



## Full wwPDB EM Validation Report ⓘ

Aug 12, 2023 – 09:42 am BST

PDB ID : 8BD3  
EMDB ID : EMD-15973  
Title : Cryo-EM structure of the Photosystem II - LHCII supercomplex from *Chlorella* ohadi  
Authors : Fadeeva, M.; Klaiman, D.; Caspy, I.; Nelson, N.  
Deposited on : 2022-10-18  
Resolution : 2.73 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

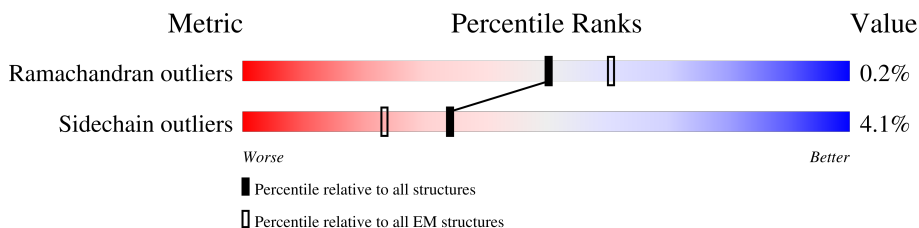
EMDB validation analysis : 0.0.1.dev50  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.73 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	214	96% .
1	7	214	98% .
2	2	222	96% .
2	4	222	95% 5%
2	9	222	97% .
2	G	222	97% .
2	g	222	96% .
2	q	222	96% .
3	3	221	95% 5%

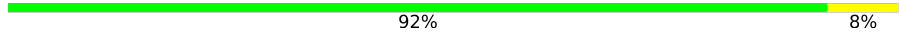

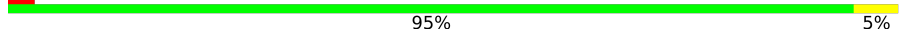
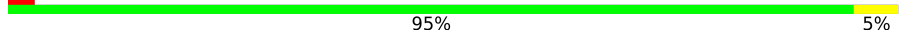
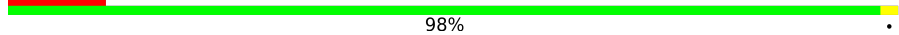
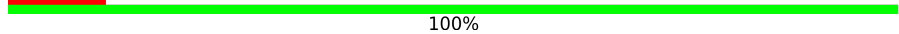
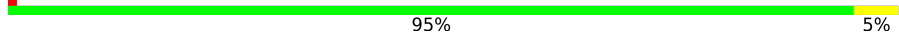
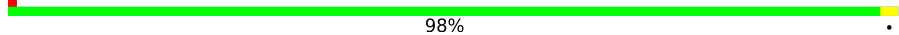
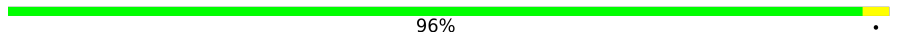
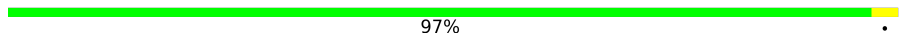
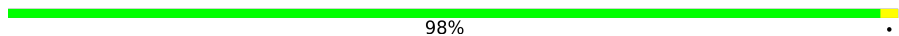
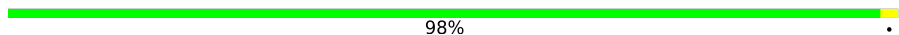
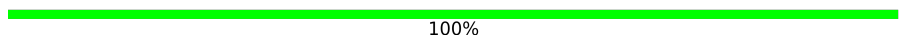
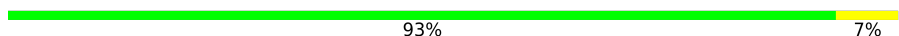
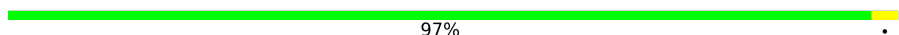
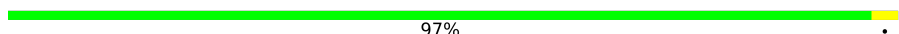
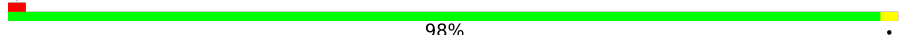
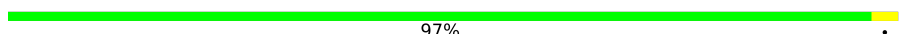
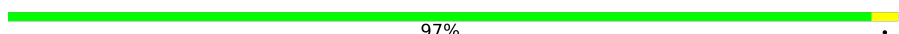
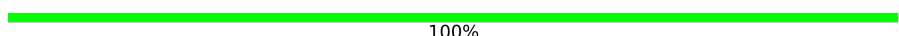
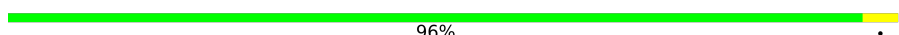
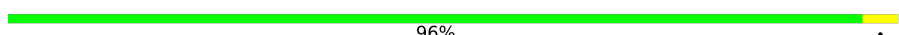
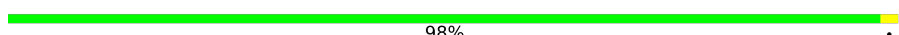
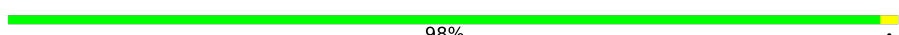
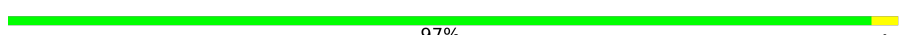
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Mol	Chain	Length	Quality of chain
3	5	221	5% 95% 5%
3	8	221	97%
3	N	221	95% 5%
3	n	221	97%
3	p	221	6% 95% 5%
4	0	217	97%
4	6	217	96%
5	A	336	97%
5	a	336	99%
6	B	504	95% 5%
6	b	504	95% 5%
7	C	448	96%
7	c	448	97%
8	D	342	97%
8	d	342	96%
9	E	81	98%
9	e	81	99%
10	F	37	100%
10	f	37	100%
11	H	67	99%
11	h	67	97%
12	I	34	97%
12	i	34	97%
13	J	38	95% 5%
13	j	38	95% 5%

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Mol	Chain	Length	Quality of chain
14	K	37	 92% 8%
14	k	37	 89% 11%
15	L	37	 95% 5%
15	l	37	 95% 5%
16	M	57	 98% 11%
16	m	57	 100%
17	O	240	 95% 5%
17	o	240	 98%
18	R	236	 96%
18	r	236	 97%
19	S	257	 98%
19	s	257	 98%
20	T	30	 100%
20	t	30	 93% 7%
21	V	32	 97%
21	v	32	 97%
22	W	60	 98%
22	w	60	 97%
23	X	37	 97%
23	x	37	 100%
24	Y	221	 96%
24	y	221	 96%
25	Z	62	 98%
25	z	62	 98%
26	U	144	 97%

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Mol	Chain	Length	Quality of chain
26	u	144	 96%
27	Q1	34	 100%
27	q1	34	 94%
28	P1	108	 98%
28	p1	108	 96%
29	F1	188	 98%
29	f1	188	 99%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	0	601	X	-	-	-
30	CHL	0	605	X	-	-	-
30	CHL	0	606	X	-	-	-
30	CHL	0	607	X	-	-	-
30	CHL	0	608	X	-	-	-
30	CHL	0	609	X	-	-	-
30	CHL	1	601	X	-	-	-
30	CHL	1	605	X	-	-	-
30	CHL	1	606	X	-	-	-
30	CHL	1	607	X	-	-	-
30	CHL	1	608	X	-	-	-
30	CHL	1	609	X	-	-	-
30	CHL	1	619	X	-	-	-
30	CHL	2	601	X	-	-	-
30	CHL	2	605	X	-	-	-
30	CHL	2	606	X	-	-	-
30	CHL	2	607	X	-	-	-
30	CHL	2	608	X	-	-	-
30	CHL	3	302	X	-	-	-
30	CHL	3	303	X	-	-	-
30	CHL	3	307	X	-	-	-
30	CHL	3	308	X	-	-	-
30	CHL	3	309	X	-	-	-
30	CHL	3	310	X	-	-	-
30	CHL	4	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	4	605	X	-	-	-
30	CHL	4	606	X	-	-	-
30	CHL	4	607	X	-	-	-
30	CHL	4	608	X	-	-	-
30	CHL	4	609	X	-	-	-
30	CHL	5	601	X	-	-	-
30	CHL	5	605	X	-	-	-
30	CHL	5	606	X	-	-	-
30	CHL	5	607	X	-	-	-
30	CHL	5	608	X	-	-	-
30	CHL	5	609	X	-	-	-
30	CHL	6	302	X	-	-	-
30	CHL	6	306	X	-	-	-
30	CHL	6	307	X	-	-	-
30	CHL	6	308	X	-	-	-
30	CHL	6	309	X	-	-	-
30	CHL	6	310	X	-	-	-
30	CHL	7	302	X	-	-	-
30	CHL	7	306	X	-	-	-
30	CHL	7	307	X	-	-	-
30	CHL	7	308	X	-	-	-
30	CHL	7	309	X	-	-	-
30	CHL	7	310	X	-	-	-
30	CHL	7	321	X	-	-	-
30	CHL	8	601	X	-	-	-
30	CHL	8	605	X	-	-	-
30	CHL	8	606	X	-	-	-
30	CHL	8	607	X	-	-	-
30	CHL	8	608	X	-	-	-
30	CHL	9	303	X	-	-	-
30	CHL	9	307	X	-	-	-
30	CHL	9	308	X	-	-	-
30	CHL	9	309	X	-	-	-
30	CHL	9	310	X	-	-	-
30	CHL	9	311	X	-	-	-
30	CHL	G	601	X	-	-	-
30	CHL	G	605	X	-	-	-
30	CHL	G	606	X	-	-	-
30	CHL	G	607	X	-	-	-
30	CHL	G	608	X	-	-	-
30	CHL	G	623	X	-	-	-
30	CHL	N	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	N	302	X	-	-	-
30	CHL	N	306	X	-	-	-
30	CHL	N	307	X	-	-	-
30	CHL	N	308	X	-	-	-
30	CHL	N	309	X	-	-	-
30	CHL	R	308	X	-	-	-
30	CHL	R	309	X	-	-	-
30	CHL	R	310	X	-	-	-
30	CHL	S	302	X	-	-	-
30	CHL	S	307	X	-	-	-
30	CHL	S	308	X	-	-	-
30	CHL	S	309	X	-	-	-
30	CHL	Y	301	X	-	-	-
30	CHL	Y	302	X	-	-	-
30	CHL	Y	306	X	-	-	-
30	CHL	Y	307	X	-	-	-
30	CHL	Y	308	X	-	-	-
30	CHL	Y	309	X	-	-	-
30	CHL	g	302	X	-	-	-
30	CHL	g	306	X	-	-	-
30	CHL	g	307	X	-	-	-
30	CHL	g	308	X	-	-	-
30	CHL	g	309	X	-	-	-
30	CHL	n	301	X	-	-	-
30	CHL	n	302	X	-	-	-
30	CHL	n	306	X	-	-	-
30	CHL	n	307	X	-	-	-
30	CHL	n	308	X	-	-	-
30	CHL	n	309	X	-	-	-
30	CHL	n	310	X	-	-	-
30	CHL	p	601	X	-	-	-
30	CHL	p	605	X	-	-	-
30	CHL	p	606	X	-	-	-
30	CHL	p	607	X	-	-	-
30	CHL	p	608	X	-	-	-
30	CHL	p	609	X	-	-	-
30	CHL	q	303	X	-	-	-
30	CHL	q	307	X	-	-	-
30	CHL	q	308	X	-	-	-
30	CHL	q	309	X	-	-	-
30	CHL	q	310	X	-	-	-
30	CHL	q	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	r	308	X	-	-	-
30	CHL	r	309	X	-	-	-
30	CHL	r	310	X	-	-	-
30	CHL	s	302	X	-	-	-
30	CHL	s	307	X	-	-	-
30	CHL	s	308	X	-	-	-
30	CHL	s	309	X	-	-	-
30	CHL	y	601	X	-	-	-
30	CHL	y	605	X	-	-	-
30	CHL	y	606	X	-	-	-
30	CHL	y	607	X	-	-	-
30	CHL	y	608	X	-	-	-
30	CHL	y	609	X	-	-	-
31	CLA	0	602	X	-	-	-
31	CLA	0	603	X	-	-	-
31	CLA	0	604	X	-	-	-
31	CLA	0	610	X	-	-	-
31	CLA	0	611	X	-	-	-
31	CLA	0	612	X	-	-	-
31	CLA	0	613	X	-	-	-
31	CLA	0	614	X	-	-	-
31	CLA	0	615	X	-	-	-
31	CLA	1	602	X	-	-	-
31	CLA	1	603	X	-	-	-
31	CLA	1	604	X	-	-	-
31	CLA	1	610	X	-	-	-
31	CLA	1	611	X	-	-	-
31	CLA	1	612	X	-	-	-
31	CLA	1	613	X	-	-	-
31	CLA	1	614	X	-	-	-
31	CLA	2	602	X	-	-	-
31	CLA	2	603	X	-	-	-
31	CLA	2	604	X	-	-	-
31	CLA	2	609	X	-	-	-
31	CLA	2	610	X	-	-	-
31	CLA	2	611	X	-	-	-
31	CLA	2	612	X	-	-	-
31	CLA	2	613	X	-	-	-
31	CLA	3	301	X	-	-	-
31	CLA	3	304	X	-	-	-
31	CLA	3	305	X	-	-	-
31	CLA	3	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	3	311	X	-	-	-
31	CLA	3	312	X	-	-	-
31	CLA	3	313	X	-	-	-
31	CLA	3	314	X	-	-	-
31	CLA	3	315	X	-	-	-
31	CLA	3	316	X	-	-	-
31	CLA	4	602	X	-	-	-
31	CLA	4	603	X	-	-	-
31	CLA	4	604	X	-	-	-
31	CLA	4	610	X	-	-	-
31	CLA	4	611	X	-	-	-
31	CLA	4	612	X	-	-	-
31	CLA	4	613	X	-	-	-
31	CLA	4	614	X	-	-	-
31	CLA	5	602	X	-	-	-
31	CLA	5	603	X	-	-	-
31	CLA	5	604	X	-	-	-
31	CLA	5	610	X	-	-	-
31	CLA	5	611	X	-	-	-
31	CLA	5	612	X	-	-	-
31	CLA	5	613	X	-	-	-
31	CLA	5	614	X	-	-	-
31	CLA	5	615	X	-	-	-
31	CLA	6	303	X	-	-	-
31	CLA	6	304	X	-	-	-
31	CLA	6	305	X	-	-	-
31	CLA	6	311	X	-	-	-
31	CLA	6	312	X	-	-	-
31	CLA	6	313	X	-	-	-
31	CLA	6	314	X	-	-	-
31	CLA	6	315	X	-	-	-
31	CLA	6	316	X	-	-	-
31	CLA	7	303	X	-	-	-
31	CLA	7	304	X	-	-	-
31	CLA	7	305	X	-	-	-
31	CLA	7	311	X	-	-	-
31	CLA	7	312	X	-	-	-
31	CLA	7	313	X	-	-	-
31	CLA	7	314	X	-	-	-
31	CLA	7	315	X	-	-	-
31	CLA	7	316	X	-	-	-
31	CLA	8	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	8	603	X	-	-	-
31	CLA	8	604	X	-	-	-
31	CLA	8	609	X	-	-	-
31	CLA	8	610	X	-	-	-
31	CLA	8	611	X	-	-	-
31	CLA	8	612	X	-	-	-
31	CLA	8	613	X	-	-	-
31	CLA	8	614	X	-	-	-
31	CLA	9	304	X	-	-	-
31	CLA	9	305	X	-	-	-
31	CLA	9	306	X	-	-	-
31	CLA	9	312	X	-	-	-
31	CLA	9	313	X	-	-	-
31	CLA	9	314	X	-	-	-
31	CLA	9	315	X	-	-	-
31	CLA	9	316	X	-	-	-
31	CLA	A	405	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	A	407	X	-	-	-
31	CLA	A	409	X	-	-	-
31	CLA	B	601	X	-	-	-
31	CLA	B	602	X	-	-	-
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31	CLA	B	605	X	-	-	-
31	CLA	B	606	X	-	-	-
31	CLA	B	607	X	-	-	-
31	CLA	B	608	X	-	-	-
31	CLA	B	609	X	-	-	-
31	CLA	B	610	X	-	-	-
31	CLA	B	611	X	-	-	-
31	CLA	B	612	X	-	-	-
31	CLA	B	613	X	-	-	-
31	CLA	B	614	X	-	-	-
31	CLA	B	615	X	-	-	-
31	CLA	B	616	X	-	-	-
31	CLA	C	601	X	-	-	-
31	CLA	C	602	X	-	-	-
31	CLA	C	603	X	-	-	-
31	CLA	C	604	X	-	-	-
31	CLA	C	605	X	-	-	-
31	CLA	C	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	C	607	X	-	-	-
31	CLA	C	608	X	-	-	-
31	CLA	C	609	X	-	-	-
31	CLA	C	610	X	-	-	-
31	CLA	C	611	X	-	-	-
31	CLA	C	612	X	-	-	-
31	CLA	C	613	X	-	-	-
31	CLA	D	403	X	-	-	-
31	CLA	D	404	X	-	-	-
31	CLA	G	602	X	-	-	-
31	CLA	G	603	X	-	-	-
31	CLA	G	604	X	-	-	-
31	CLA	G	609	X	-	-	-
31	CLA	G	610	X	-	-	-
31	CLA	G	611	X	-	-	-
31	CLA	G	612	X	-	-	-
31	CLA	G	613	X	-	-	-
31	CLA	N	303	X	-	-	-
31	CLA	N	304	X	-	-	-
31	CLA	N	305	X	-	-	-
31	CLA	N	310	X	-	-	-
31	CLA	N	311	X	-	-	-
31	CLA	N	312	X	-	-	-
31	CLA	N	313	X	-	-	-
31	CLA	N	314	X	-	-	-
31	CLA	N	315	X	-	-	-
31	CLA	N	321	X	-	-	-
31	CLA	R	303	X	-	-	-
31	CLA	R	304	X	-	-	-
31	CLA	R	305	X	-	-	-
31	CLA	R	306	X	-	-	-
31	CLA	R	307	X	-	-	-
31	CLA	R	311	X	-	-	-
31	CLA	R	312	X	-	-	-
31	CLA	R	313	X	-	-	-
31	CLA	R	314	X	-	-	-
31	CLA	R	315	X	-	-	-
31	CLA	R	316	X	-	-	-
31	CLA	S	303	X	-	-	-
31	CLA	S	304	X	-	-	-
31	CLA	S	305	X	-	-	-
31	CLA	S	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	S	310	X	-	-	-
31	CLA	S	311	X	-	-	-
31	CLA	S	312	X	-	-	-
31	CLA	S	313	X	-	-	-
31	CLA	S	314	X	-	-	-
31	CLA	S	315	X	-	-	-
31	CLA	S	316	X	-	-	-
31	CLA	Y	303	X	-	-	-
31	CLA	Y	304	X	-	-	-
31	CLA	Y	305	X	-	-	-
31	CLA	Y	310	X	-	-	-
31	CLA	Y	311	X	-	-	-
31	CLA	Y	312	X	-	-	-
31	CLA	Y	313	X	-	-	-
31	CLA	Y	314	X	-	-	-
31	CLA	a	406	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	a	409	X	-	-	-
31	CLA	b	602	X	-	-	-
31	CLA	b	603	X	-	-	-
31	CLA	b	604	X	-	-	-
31	CLA	b	605	X	-	-	-
31	CLA	b	606	X	-	-	-
31	CLA	b	607	X	-	-	-
31	CLA	b	608	X	-	-	-
31	CLA	b	609	X	-	-	-
31	CLA	b	610	X	-	-	-
31	CLA	b	611	X	-	-	-
31	CLA	b	612	X	-	-	-
31	CLA	b	613	X	-	-	-
31	CLA	b	614	X	-	-	-
31	CLA	b	615	X	-	-	-
31	CLA	b	616	X	-	-	-
31	CLA	b	617	X	-	-	-
31	CLA	c	601	X	-	-	-
31	CLA	c	602	X	-	-	-
31	CLA	c	603	X	-	-	-
31	CLA	c	604	X	-	-	-
31	CLA	c	605	X	-	-	-
31	CLA	c	606	X	-	-	-
31	CLA	c	607	X	-	-	-
31	CLA	c	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	c	609	X	-	-	-
31	CLA	c	610	X	-	-	-
31	CLA	c	611	X	-	-	-
31	CLA	c	612	X	-	-	-
31	CLA	c	613	X	-	-	-
31	CLA	d	401	X	-	-	-
31	CLA	d	404	X	-	-	-
31	CLA	d	405	X	-	-	-
31	CLA	g	303	X	-	-	-
31	CLA	g	304	X	-	-	-
31	CLA	g	305	X	-	-	-
31	CLA	g	310	X	-	-	-
31	CLA	g	311	X	-	-	-
31	CLA	g	312	X	-	-	-
31	CLA	g	313	X	-	-	-
31	CLA	g	314	X	-	-	-
31	CLA	n	303	X	-	-	-
31	CLA	n	304	X	-	-	-
31	CLA	n	305	X	-	-	-
31	CLA	n	311	X	-	-	-
31	CLA	n	312	X	-	-	-
31	CLA	n	313	X	-	-	-
31	CLA	n	314	X	-	-	-
31	CLA	n	315	X	-	-	-
31	CLA	n	316	X	-	-	-
31	CLA	p	602	X	-	-	-
31	CLA	p	603	X	-	-	-
31	CLA	p	604	X	-	-	-
31	CLA	p	610	X	-	-	-
31	CLA	p	611	X	-	-	-
31	CLA	p	612	X	-	-	-
31	CLA	p	613	X	-	-	-
31	CLA	p	614	X	-	-	-
31	CLA	p	615	X	-	-	-
31	CLA	q	304	X	-	-	-
31	CLA	q	305	X	-	-	-
31	CLA	q	306	X	-	-	-
31	CLA	q	312	X	-	-	-
31	CLA	q	313	X	-	-	-
31	CLA	q	314	X	-	-	-
31	CLA	q	315	X	-	-	-
31	CLA	q	316	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	r	303	X	-	-	-
31	CLA	r	304	X	-	-	-
31	CLA	r	305	X	-	-	-
31	CLA	r	306	X	-	-	-
31	CLA	r	307	X	-	-	-
31	CLA	r	311	X	-	-	-
31	CLA	r	312	X	-	-	-
31	CLA	r	313	X	-	-	-
31	CLA	r	314	X	-	-	-
31	CLA	r	315	X	-	-	-
31	CLA	r	316	X	-	-	-
31	CLA	s	303	X	-	-	-
31	CLA	s	304	X	-	-	-
31	CLA	s	305	X	-	-	-
31	CLA	s	306	X	-	-	-
31	CLA	s	310	X	-	-	-
31	CLA	s	311	X	-	-	-
31	CLA	s	312	X	-	-	-
31	CLA	s	313	X	-	-	-
31	CLA	s	314	X	-	-	-
31	CLA	s	315	X	-	-	-
31	CLA	s	316	X	-	-	-
31	CLA	y	602	X	-	-	-
31	CLA	y	603	X	-	-	-
31	CLA	y	604	X	-	-	-
31	CLA	y	610	X	-	-	-
31	CLA	y	611	X	-	-	-
31	CLA	y	612	X	-	-	-
31	CLA	y	613	X	-	-	-
31	CLA	y	614	X	-	-	-
31	CLA	y	615	X	-	-	-
43	BCR	c	614	-	X	-	-

## 2 Entry composition i

There are 49 unique types of molecules in this entry. The entry contains 117990 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		
1	7	214	Total	C	N	O	S	0	0
			1630	1056	265	304	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	195	LEU	PHE	conflict	UNP A0A2P6TPU9
1	225	GLU	ASP	conflict	UNP A0A2P6TPU9
1	250	ASN	THR	conflict	UNP A0A2P6TPU9
7	195	LEU	PHE	conflict	UNP A0A2P6TPU9
7	225	GLU	ASP	conflict	UNP A0A2P6TPU9
7	250	ASN	THR	conflict	UNP A0A2P6TPU9

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	4	222	Total	C	N	O	S	0	0
			1685	1088	271	321	5		
2	G	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	9	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		
2	q	222	Total	C	N	O	S	0	0
			1685	1088	271	321	5		
2	g	222	Total	C	N	O	S	0	0
			1686	1089	271	321	5		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	74	THR	SER	conflict	UNP A0A2P6TDA6
4	74	THR	SER	conflict	UNP A0A2P6TDA6
G	74	THR	SER	conflict	UNP A0A2P6TDA6
9	74	THR	SER	conflict	UNP A0A2P6TDA6
q	74	THR	SER	conflict	UNP A0A2P6TDA6
g	74	THR	SER	conflict	UNP A0A2P6TDA6

- Molecule 3 is a protein called Chlorophyll a-b binding of LHCII.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	5	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	N	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	8	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	p	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		
3	n	221	Total	C	N	O	S	0	0
			1686	1090	279	312	5		

- Molecule 4 is a protein called Chlorophyll a-b binding of LHCII.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	217	Total	C	N	O	S	0	0
			1657	1070	271	311	5		
4	0	217	Total	C	N	O	S	0	0
			1657	1070	271	311	5		

- Molecule 5 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		
5	a	336	Total	C	N	O	S	0	0
			2632	1718	431	469	14		

- Molecule 6 is a protein called Photosystem II CP47 reaction center protein.



Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	504	Total	C	N	O	S	0	0
			3954	2583	667	692	12		
6	b	504	Total	C	N	O	S	0	0
			3954	2583	667	692	12		

- Molecule 7 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	448	Total	C	N	O	S	0	0
			3482	2280	584	603	15		
7	c	448	Total	C	N	O	S	0	0
			3482	2280	584	603	15		

- Molecule 8 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	342	Total	C	N	O	S	0	0
			2730	1806	449	464	11		
8	d	342	Total	C	N	O	S	0	0
			2730	1806	449	464	11		

- Molecule 9 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	81	Total	C	N	O	0	0
			652	423	106	123		
9	e	81	Total	C	N	O	0	0
			652	423	106	123		

- Molecule 10 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	37	Total	C	N	O	S	0	0
			302	206	49	46	1		
10	f	37	Total	C	N	O	S	0	0
			302	206	49	46	1		

- Molecule 11 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	67	Total	C	N	O	S	0	0
			507	336	73	95	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	h	67	Total	C	N	O	S	0	0
			507	336	73	95	3		

- Molecule 12 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	34	Total	C	N	O	S	0	0
			274	187	41	45	1		
12	i	34	Total	C	N	O	S	0	0
			274	187	41	45	1		

- Molecule 13 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	J	38	Total	C	N	O	0	0
			270	182	42	46		
13	j	38	Total	C	N	O	0	0
			270	182	42	46		

- Molecule 14 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	K	37	Total	C	N	O	0	0
			295	204	43	48		
14	k	37	Total	C	N	O	0	0
			295	204	43	48		

- Molecule 15 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	L	37	Total	C	N	O	0	0
			303	203	48	52		
15	l	37	Total	C	N	O	0	0
			303	203	48	52		

- Molecule 16 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	57	Total	C	N	O	S	0	0
			370	242	60	67	1		
16	m	57	Total	C	N	O	S	0	0
			370	242	60	67	1		

- Molecule 17 is a protein called Chloroplast oxygen-evolving enhancer protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	240	Total	C	N	O	S	0	0
			1789	1134	287	362	6		
17	o	240	Total	C	N	O	S	0	0
			1789	1134	287	362	6		

- Molecule 18 is a protein called Chlorophyll a b binding CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	236	Total	C	N	O	S	0	0
			1818	1148	311	352	7		
18	r	236	Total	C	N	O	S	0	0
			1818	1148	311	352	7		

- Molecule 19 is a protein called Chlorophyll a b-binding CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	257	Total	C	N	O	S	0	0
			1934	1242	323	364	5		
19	s	257	Total	C	N	O	S	0	0
			1934	1242	323	364	5		

- Molecule 20 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	30	Total	C	N	O	S	0	0
			246	172	36	37	1		
20	t	30	Total	C	N	O	S	0	0
			246	172	36	37	1		

- Molecule 21 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	32	Total	C	N	O	0	0
			233	155	38	40		
21	v	32	Total	C	N	O	0	0
			233	155	38	40		

- Molecule 22 is a protein called Photosystem II reaction center W protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	W	60	Total	C	N	O	0	0
			468	301	74	93		
22	w	60	Total	C	N	O	0	0
			468	301	74	93		

- Molecule 23 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	X	37	Total	C	N	O	0	0
			247	156	43	48		
23	x	37	Total	C	N	O	0	0
			247	156	43	48		

- Molecule 24 is a protein called Multifunctional fusion protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	221	Total	C	N	O	S	0	0
			1688	1099	270	314	5		
24	y	221	Total	C	N	O	S	0	0
			1688	1099	270	314	5		

- Molecule 25 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	62	Total	C	N	O	S	0	0
			478	335	68	74	1		
25	z	62	Total	C	N	O	S	0	0
			478	335	68	74	1		

- Molecule 26 is a protein called Chloroplast oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	U	144	Total	C	N	O	0	0
			1122	701	207	214		
26	u	144	Total	C	N	O	0	0
			1122	701	207	214		

- Molecule 27 is a protein called Chloroplast PsbY.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q1	34	Total	C	N	O	S	0	0
			260	171	44	44	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	q1	34	Total	C	N	O	S	0	0
			260	171	44	44	1		

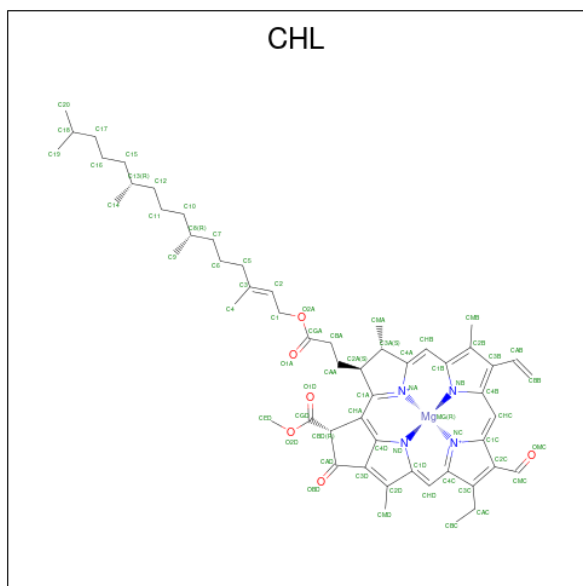
- Molecule 28 is a protein called Chloroplast photosystem II 10 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	P1	108	Total	C	N	O	S	0	0
			820	524	137	157	2		
28	p1	108	Total	C	N	O	S	0	0
			820	524	137	157	2		

- Molecule 29 is a protein called Photosystem II oxygen evolving enhancer 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F1	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		
29	f1	188	Total	C	N	O	S	0	0
			1443	918	245	279	1		

- Molecule 30 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



Mol	Chain	Residues	Atoms				AltConf	
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	1	1	66	55	1	4	6	0
30	1	1	66	55	1	4	6	0
30	1	1	50	39	1	4	6	0
30	1	1	66	55	1	4	6	0
30	1	1	61	50	1	4	6	0
30	2	1	66	55	1	4	6	0
30	2	1	46	35	1	4	6	0
30	2	1	51	40	1	4	6	0
30	2	1	50	39	1	4	6	0
30	2	1	57	46	1	4	6	0
30	3	1	57	46	1	4	6	0
30	3	1	50	39	1	4	6	0
30	3	1	46	35	1	4	6	0
30	3	1	47	36	1	4	6	0
30	3	1	50	39	1	4	6	0
30	3	1	61	50	1	4	6	0
30	4	1	66	55	1	4	6	0
30	4	1	46	35	1	4	6	0
30	4	1	51	40	1	4	6	0
30	4	1	57	46	1	4	6	0
30	4	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	4	1	57	46	1	4	6	0
30	5	1	51	40	1	4	6	0
30	5	1	46	35	1	4	6	0
30	5	1	51	40	1	4	6	0
30	5	1	51	40	1	4	6	0
30	5	1	50	39	1	4	6	0
30	5	1	56	45	1	4	6	0
30	6	1	56	45	1	4	6	0
30	6	1	46	35	1	4	6	0
30	6	1	51	40	1	4	6	0
30	6	1	66	55	1	4	6	0
30	6	1	50	39	1	4	6	0
30	6	1	61	50	1	4	6	0
30	G	1	66	55	1	4	6	0
30	G	1	48	37	1	4	6	0
30	G	1	50	39	1	4	6	0
30	G	1	51	40	1	4	6	0
30	G	1	63	52	1	4	6	0
30	G	1	66	55	1	4	6	0
30	N	1	50	39	1	4	6	0
30	N	1	56	45	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	N	1	66	55	1	4	6	0
30	N	1	58	47	1	4	6	0
30	N	1	50	39	1	4	6	0
30	N	1	66	55	1	4	6	0
30	R	1	56	45	1	4	6	0
30	R	1	56	45	1	4	6	0
30	R	1	55	44	1	4	6	0
30	S	1	46	35	1	4	6	0
30	S	1	44	35	1	4	4	0
30	S	1	43	34	1	4	4	0
30	S	1	49	38	1	4	6	0
30	Y	1	63	52	1	4	6	0
30	Y	1	66	55	1	4	6	0
30	Y	1	46	35	1	4	6	0
30	Y	1	59	48	1	4	6	0
30	Y	1	50	39	1	4	6	0
30	Y	1	66	55	1	4	6	0
30	0	1	56	45	1	4	6	0
30	0	1	52	41	1	4	6	0
30	0	1	51	40	1	4	6	0
30	0	1	66	55	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	0	1	50	39	1	4	6	0
30	0	1	61	50	1	4	6	0
30	7	1	66	55	1	4	6	0
30	7	1	66	55	1	4	6	0
30	7	1	66	55	1	4	6	0
30	7	1	66	55	1	4	6	0
30	7	1	50	39	1	4	6	0
30	7	1	66	55	1	4	6	0
30	7	1	63	52	1	4	6	0
30	8	1	56	45	1	4	6	0
30	8	1	66	55	1	4	6	0
30	8	1	58	47	1	4	6	0
30	8	1	50	39	1	4	6	0
30	8	1	66	55	1	4	6	0
30	9	1	66	55	1	4	6	0
30	9	1	46	35	1	4	6	0
30	9	1	52	41	1	4	6	0
30	9	1	53	42	1	4	6	0
30	9	1	50	39	1	4	6	0
30	9	1	61	50	1	4	6	0
30	p	1	51	40	1	4	6	0

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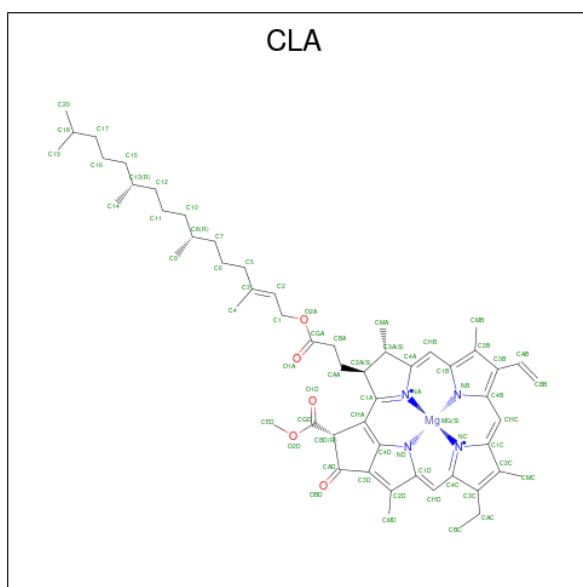
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	p	1	46	35	1	4	6	0
30	p	1	51	40	1	4	6	0
30	p	1	51	40	1	4	6	0
30	p	1	50	39	1	4	6	0
30	p	1	56	45	1	4	6	0
30	q	1	66	55	1	4	6	0
30	q	1	46	35	1	4	6	0
30	q	1	51	40	1	4	6	0
30	q	1	57	46	1	4	6	0
30	q	1	50	39	1	4	6	0
30	q	1	56	45	1	4	6	0
30	g	1	66	55	1	4	6	0
30	g	1	48	37	1	4	6	0
30	g	1	50	39	1	4	6	0
30	g	1	51	40	1	4	6	0
30	g	1	63	52	1	4	6	0
30	n	1	50	39	1	4	6	0
30	n	1	56	45	1	4	6	0
30	n	1	66	55	1	4	6	0
30	n	1	58	47	1	4	6	0
30	n	1	63	52	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	n	1	50	39	1	4	6	0
30	n	1	66	55	1	4	6	0
30	r	1	56	45	1	4	6	0
30	r	1	56	45	1	4	6	0
30	r	1	55	44	1	4	6	0
30	s	1	46	35	1	4	6	0
30	s	1	44	35	1	4	4	0
30	s	1	43	34	1	4	4	0
30	s	1	49	38	1	4	6	0
30	y	1	66	55	1	4	6	0
30	y	1	46	35	1	4	6	0
30	y	1	59	48	1	4	6	0
30	y	1	66	55	1	4	6	0
30	y	1	50	39	1	4	6	0
30	y	1	66	55	1	4	6	0

- Molecule 31 is CHLOROPHYLL A (three-letter code: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms				AltConf	
31	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	2	1	65	55	1	4	5	0
31	2	1	54	44	1	4	5	0
31	3	1	54	44	1	4	5	0
31	3	1	60	50	1	4	5	0
31	3	1	55	45	1	4	5	0
31	3	1	55	45	1	4	5	0
31	3	1	54	44	1	4	5	0
31	3	1	65	55	1	4	5	0
31	3	1	50	40	1	4	5	0
31	3	1	55	45	1	4	5	0
31	3	1	54	44	1	4	5	0
31	3	1	57	47	1	4	5	0
31	4	1	65	55	1	4	5	0
31	4	1	55	45	1	4	5	0
31	4	1	51	41	1	4	5	0
31	4	1	60	50	1	4	5	0
31	4	1	43	33	1	4	5	0
31	4	1	46	36	1	4	5	0
31	4	1	61	51	1	4	5	0
31	4	1	54	44	1	4	5	0
31	5	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	5	1	52	42	1	4	5	0
31	5	1	50	40	1	4	5	0
31	5	1	60	50	1	4	5	0
31	5	1	58	48	1	4	5	0
31	5	1	50	40	1	4	5	0
31	5	1	54	44	1	4	5	0
31	5	1	51	41	1	4	5	0
31	5	1	46	36	1	4	5	0
31	6	1	65	55	1	4	5	0
31	6	1	56	46	1	4	5	0
31	6	1	55	45	1	4	5	0
31	6	1	65	55	1	4	5	0
31	6	1	60	50	1	4	5	0
31	6	1	60	50	1	4	5	0
31	6	1	65	55	1	4	5	0
31	6	1	54	44	1	4	5	0
31	6	1	55	45	1	4	5	0
31	A	1	65	55	1	4	5	0
31	A	1	65	55	1	4	5	0
31	A	1	49	39	1	4	5	0
31	A	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	B	1	49	39	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	B	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	65	55	1	4	5	0
31	C	1	56	46	1	4	5	0
31	C	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
31	C	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	D	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	G	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	N	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	N	1	65	55	1	4	5	0
31	N	1	49	39	1	4	5	0
31	N	1	45	35	1	4	5	0
31	N	1	65	55	1	4	5	0
31	N	1	49	39	1	4	5	0
31	N	1	54	44	1	4	5	0
31	N	1	54	44	1	4	5	0
31	R	1	49	39	1	4	5	0
31	R	1	60	50	1	4	5	0
31	R	1	60	50	1	4	5	0
31	R	1	48	38	1	4	5	0
31	R	1	48	38	1	4	5	0
31	R	1	58	48	1	4	5	0
31	R	1	57	47	1	4	5	0
31	R	1	49	39	1	4	5	0
31	R	1	49	39	1	4	5	0
31	R	1	55	45	1	4	5	0
31	R	1	65	55	1	4	5	0
31	S	1	65	55	1	4	5	0
31	S	1	42	34	1	4	3	0
31	S	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	S	1	50	40	1	4	5	0
31	S	1	60	50	1	4	5	0
31	S	1	65	55	1	4	5	0
31	S	1	65	55	1	4	5	0
31	S	1	56	46	1	4	5	0
31	S	1	65	55	1	4	5	0
31	S	1	48	38	1	4	5	0
31	S	1	46	36	1	4	5	0
31	Y	1	60	50	1	4	5	0
31	Y	1	55	45	1	4	5	0
31	Y	1	55	45	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	65	55	1	4	5	0
31	Y	1	54	44	1	4	5	0
31	0	1	65	55	1	4	5	0
31	0	1	56	46	1	4	5	0
31	0	1	55	45	1	4	5	0
31	0	1	65	55	1	4	5	0
31	0	1	60	50	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	0	1	46	36	1	4	5	0
31	0	1	56	46	1	4	5	0
31	0	1	54	44	1	4	5	0
31	0	1	55	45	1	4	5	0
31	7	1	60	50	1	4	5	0
31	7	1	55	45	1	4	5	0
31	7	1	65	55	1	4	5	0
31	7	1	65	55	1	4	5	0
31	7	1	65	55	1	4	5	0
31	7	1	65	55	1	4	5	0
31	7	1	65	55	1	4	5	0
31	7	1	65	55	1	4	5	0
31	7	1	54	44	1	4	5	0
31	7	1	51	41	1	4	5	0
31	8	1	65	55	1	4	5	0
31	8	1	55	45	1	4	5	0
31	8	1	65	55	1	4	5	0
31	8	1	65	55	1	4	5	0
31	8	1	49	39	1	4	5	0
31	8	1	45	35	1	4	5	0
31	8	1	65	55	1	4	5	0
31	8	1	49	39	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	8	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	9	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	p	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	p	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	p	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	p	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	p	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	p	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	p	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	q	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	q	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	q	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	q	1	53	43	1	4	5	0
31	q	1	43	33	1	4	5	0
31	q	1	46	36	1	4	5	0
31	q	1	65	55	1	4	5	0
31	q	1	50	40	1	4	5	0
31	a	1	65	55	1	4	5	0
31	a	1	65	55	1	4	5	0
31	a	1	60	50	1	4	5	0
31	b	1	49	39	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	b	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	56	46	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	65	55	1	4	5	0
31	c	1	55	45	1	4	5	0
31	c	1	65	55	1	4	5	0
31	d	1	49	39	1	4	5	0
31	d	1	65	55	1	4	5	0
31	d	1	65	55	1	4	5	0
31	g	1	65	55	1	4	5	0
31	g	1	55	45	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	g	1	55	45	1	4	5	0
31	g	1	65	55	1	4	5	0
31	g	1	60	50	1	4	5	0
31	g	1	43	35	1	4	3	0
31	g	1	65	55	1	4	5	0
31	g	1	49	39	1	4	5	0
31	n	1	65	55	1	4	5	0
31	n	1	55	45	1	4	5	0
31	n	1	65	55	1	4	5	0
31	n	1	65	55	1	4	5	0
31	n	1	49	39	1	4	5	0
31	n	1	45	35	1	4	5	0
31	n	1	65	55	1	4	5	0
31	n	1	49	39	1	4	5	0
31	n	1	54	44	1	4	5	0
31	r	1	49	39	1	4	5	0
31	r	1	60	50	1	4	5	0
31	r	1	60	50	1	4	5	0
31	r	1	48	38	1	4	5	0
31	r	1	48	38	1	4	5	0
31	r	1	58	48	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
31	r	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

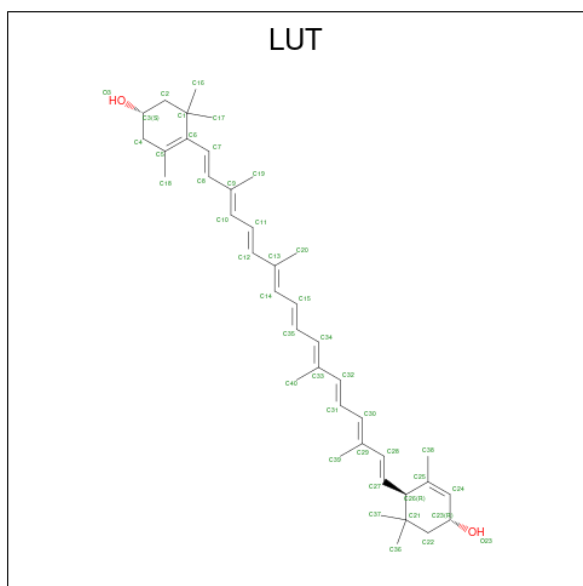
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Mol	Chain	Residues	Atoms					AltConf
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	y	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

- Molecule 32 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			42	40	2	
32	1	1	Total	C	O	0
			42	40	2	
32	2	1	Total	C	O	0
			42	40	2	
32	3	1	Total	C	O	0
			42	40	2	
32	3	1	Total	C	O	0
			42	40	2	
32	4	1	Total	C	O	0
			42	40	2	
32	5	1	Total	C	O	0
			42	40	2	

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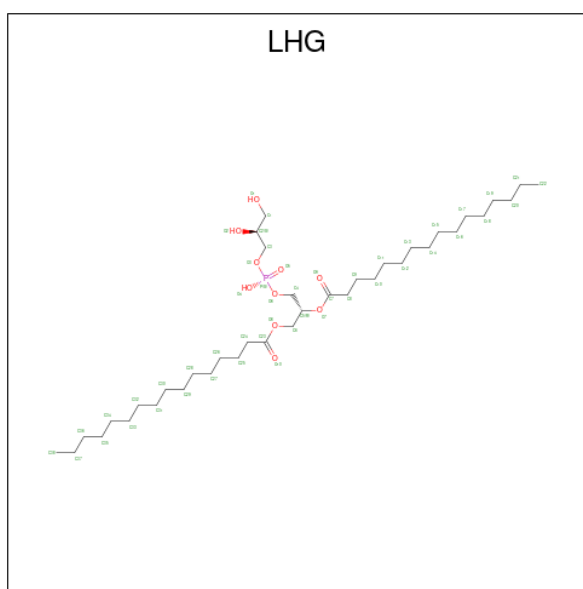
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	5	1	42	40	2	0
32	6	1	42	40	2	0
32	6	1	42	40	2	0
32	G	1	42	40	2	0
32	N	1	42	40	2	0
32	N	1	42	40	2	0
32	R	1	42	40	2	0
32	S	1	42	40	2	0
32	S	1	42	40	2	0
32	Y	1	42	40	2	0
32	Y	1	42	40	2	0
32	0	1	42	40	2	0
32	0	1	42	40	2	0
32	7	1	42	40	2	0
32	7	1	42	40	2	0
32	8	1	42	40	2	0
32	8	1	42	40	2	0
32	9	1	42	40	2	0
32	p	1	42	40	2	0
32	p	1	42	40	2	0
32	q	1	42	40	2	0

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Mol	Chain	Residues	Atoms			AltConf
32	g	1	Total	C	O	0
			42	40	2	
32	n	1	Total	C	O	0
			42	40	2	
32	n	1	Total	C	O	0
			42	40	2	
32	r	1	Total	C	O	0
			42	40	2	
32	s	1	Total	C	O	0
			42	40	2	
32	s	1	Total	C	O	0
			42	40	2	
32	y	1	Total	C	O	0
			42	40	2	
32	y	1	Total	C	O	0
			42	40	2	

- Molecule 33 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				AltConf
33	1	1	Total	C	O	P	0
			35	24	10	1	
33	2	1	Total	C	O	P	0
			49	38	10	1	
33	3	1	Total	C	O	P	0
			33	22	10	1	

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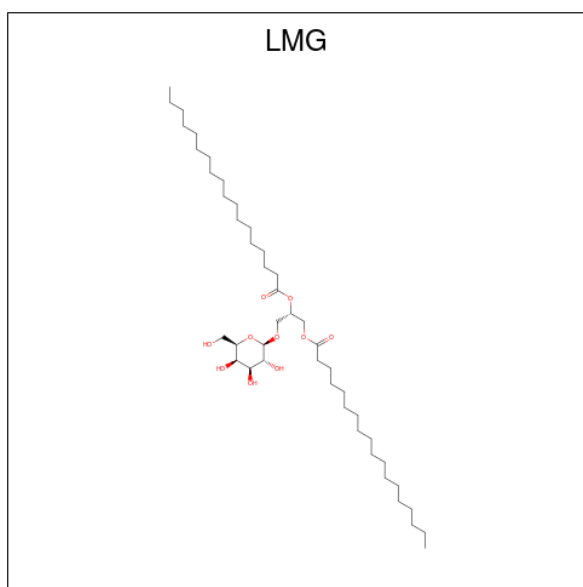
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	4	1	47	36	10	1	0
33	5	1	35	24	10	1	0
33	6	1	37	26	10	1	0
33	A	1	44	33	10	1	0
33	A	1	39	28	10	1	0
33	B	1	49	38	10	1	0
33	C	1	40	29	10	1	0
33	D	1	44	33	10	1	0
33	D	1	49	38	10	1	0
33	G	1	44	33	10	1	0
33	K	1	36	25	10	1	0
33	L	1	49	38	10	1	0
33	M	1	41	30	10	1	0
33	N	1	49	38	10	1	0
33	R	1	38	27	10	1	0
33	S	1	41	30	10	1	0
33	S	1	44	33	10	1	0
33	Y	1	42	31	10	1	0
33	0	1	36	25	10	1	0
33	7	1	35	24	10	1	0
33	8	1	49	38	10	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	g	1	33	22	10	1	0
33	p	1	35	24	10	1	0
33	q	1	46	35	10	1	0
33	a	1	39	28	10	1	0
33	b	1	44	33	10	1	0
33	b	1	49	38	10	1	0
33	c	1	47	36	10	1	0
33	d	1	49	38	10	1	0
33	e	1	44	33	10	1	0
33	g	1	44	33	10	1	0
33	j	1	49	38	10	1	0
33	l	1	49	38	10	1	0
33	n	1	49	38	10	1	0
33	r	1	38	27	10	1	0
33	s	1	41	30	10	1	0
33	s	1	44	33	10	1	0
33	t	1	41	30	10	1	0
33	y	1	46	35	10	1	0
33	z	1	36	25	10	1	0
33	F1	1	35	24	10	1	0

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	1	1	38	28	10	0
34	2	1	38	28	10	0
34	2	1	51	41	10	0
34	2	1	40	30	10	0
34	3	1	38	28	10	0
34	4	1	51	41	10	0
34	4	1	40	30	10	0
34	5	1	38	28	10	0
34	6	1	42	32	10	0
34	6	1	39	29	10	0
34	6	1	38	28	10	0
34	A	1	41	31	10	0
34	A	1	38	28	10	0
34	A	1	38	28	10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	B	1	51	41	10	0
34	B	1	38	28	10	0
34	B	1	38	28	10	0
34	C	1	51	41	10	0
34	C	1	38	28	10	0
34	C	1	32	22	10	0
34	C	1	44	34	10	0
34	D	1	46	36	10	0
34	D	1	46	36	10	0
34	D	1	51	41	10	0
34	D	1	48	38	10	0
34	G	1	38	28	10	0
34	G	1	51	41	10	0
34	G	1	40	30	10	0
34	I	1	38	28	10	0
34	J	1	51	41	10	0
34	J	1	38	28	10	0
34	N	1	38	28	10	0
34	R	1	38	28	10	0
34	S	1	41	31	10	0
34	W	1	55	45	10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	W	1	38	28	10	0
34	W	1	38	28	10	0
34	X	1	38	28	10	0
34	X	1	38	28	10	0
34	Y	1	38	28	10	0
34	0	1	42	32	10	0
34	0	1	38	28	10	0
34	7	1	39	29	10	0
34	7	1	38	28	10	0
34	7	1	38	28	10	0
34	9	1	51	41	10	0
34	9	1	40	30	10	0
34	9	1	38	28	10	0
34	p	1	38	28	10	0
34	q	1	51	41	10	0
34	q	1	40	30	10	0
34	a	1	38	28	10	0
34	a	1	38	28	10	0
34	a	1	38	28	10	0
34	b	1	45	35	10	0
34	b	1	51	41	10	0

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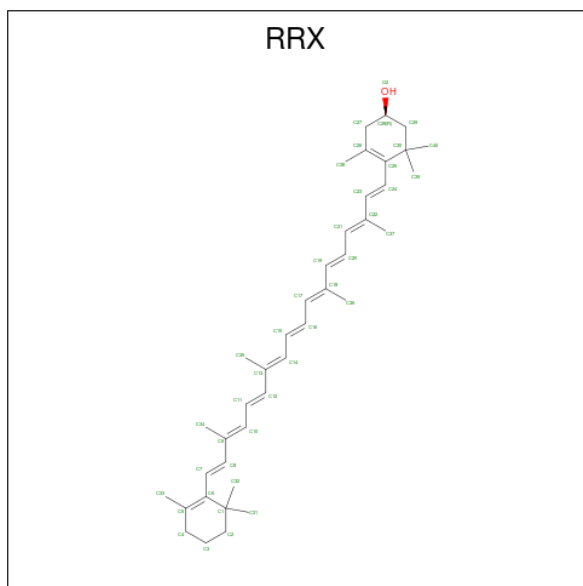
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	b	1	38	28	10	0
34	b	1	38	28	10	0
34	b	1	46	36	10	0
34	b	1	38	28	10	0
34	c	1	38	28	10	0
34	c	1	38	28	10	0
34	c	1	44	34	10	0
34	d	1	41	31	10	0
34	d	1	51	41	10	0
34	d	1	48	38	10	0
34	f	1	38	28	10	0
34	g	1	38	28	10	0
34	g	1	49	39	10	0
34	j	1	43	33	10	0
34	k	1	48	38	10	0
34	k	1	38	28	10	0
34	m	1	45	35	10	0
34	n	1	38	28	10	0
34	n	1	40	30	10	0
34	r	1	38	28	10	0
34	s	1	41	31	10	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	w	1	48	38	10	0
34	w	1	55	45	10	0
34	w	1	38	28	10	0
34	w	1	38	28	10	0
34	w	1	38	28	10	0
34	x	1	38	28	10	0
34	y	1	38	28	10	0
34	Q1	1	38	28	10	0
34	q1	1	38	28	10	0

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



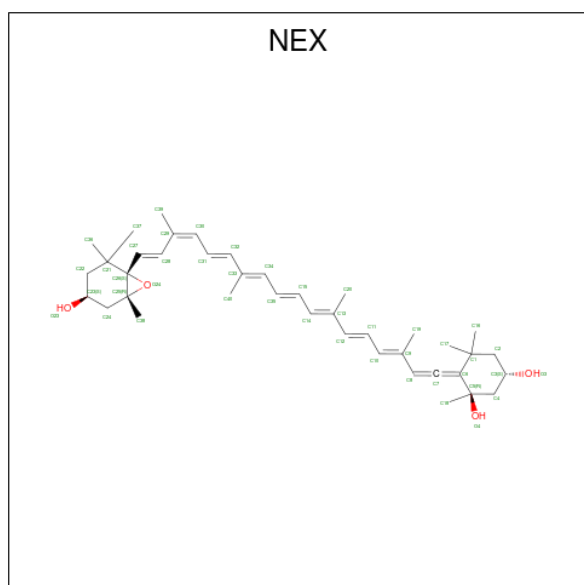
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	2	1	41	40	1	0
35	4	1	41	40	1	0

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Mol	Chain	Residues	Atoms			AltConf
35	G	1	Total	C	O	0
			41	40	1	
35	9	1	Total	C	O	0
			41	40	1	
35	q	1	Total	C	O	0
			41	40	1	
35	g	1	Total	C	O	0
			41	40	1	

- Molecule 36 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



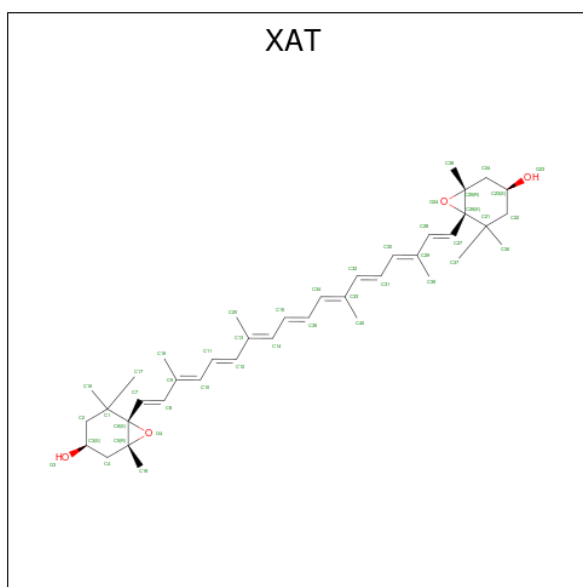
Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	O	0
			44	40	4	
36	3	1	Total	C	O	0
			44	40	4	
36	4	1	Total	C	O	0
			44	40	4	
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	G	1	Total	C	O	0
			44	40	4	

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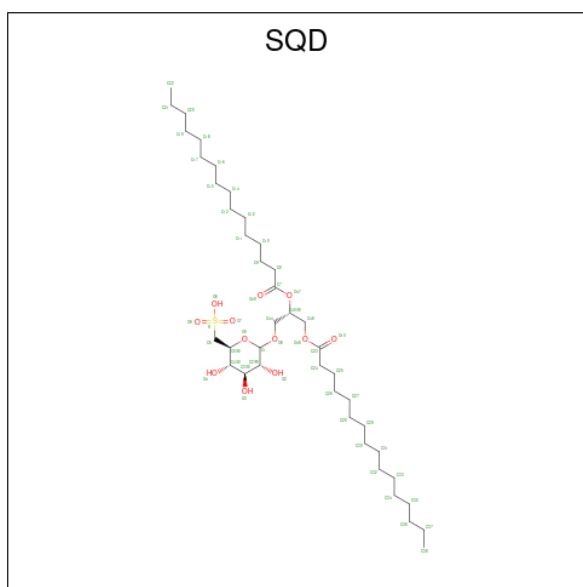
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	N	1	44	40	4	0
36	R	1	44	40	4	0
36	R	1	44	40	4	0
36	S	1	44	40	4	0
36	Y	1	44	40	4	0
36	0	1	44	40	4	0
36	8	1	44	40	4	0
36	9	1	44	40	4	0
36	p	1	44	40	4	0
36	q	1	44	40	4	0
36	g	1	44	40	4	0
36	n	1	44	40	4	0
36	r	1	44	40	4	0
36	r	1	44	40	4	0
36	s	1	44	40	4	0
36	y	1	44	40	4	0

- Molecule 37 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
37	2	1	Total	C	O	0
			44	40	4	
37	4	1	Total	C	O	0
			44	40	4	
37	G	1	Total	C	O	0
			44	40	4	
37	R	1	Total	C	O	0
			44	40	4	
37	9	1	Total	C	O	0
			44	40	4	
37	q	1	Total	C	O	0
			44	40	4	
37	g	1	Total	C	O	0
			44	40	4	
37	r	1	Total	C	O	0
			44	40	4	

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula:  $C_{41}H_{78}O_{12}S$ ).



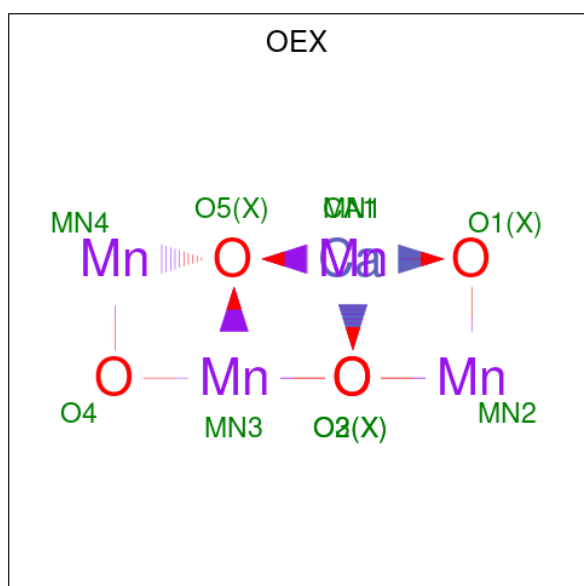
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
38	6	1	42	29	12	1	0
38	A	1	51	38	12	1	0
38	A	1	45	32	12	1	0
38	B	1	54	41	12	1	0
38	B	1	52	39	12	1	0
38	G	1	42	29	12	1	0
38	G	1	38	25	12	1	0
38	M	1	50	37	12	1	0
38	R	1	51	38	12	1	0
38	S	1	51	38	12	1	0
38	X	1	38	25	12	1	0
38	Y	1	42	29	12	1	0
38	0	1	42	29	12	1	0
38	a	1	48	35	12	1	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
38	a	1	Total 45	C 32	O 12	S 1	0
38	b	1	Total 54	C 41	O 12	S 1	0
38	b	1	Total 52	C 39	O 12	S 1	0
38	g	1	Total 38	C 25	O 12	S 1	0
38	g	1	Total 42	C 29	O 12	S 1	0
38	m	1	Total 50	C 37	O 12	S 1	0
38	r	1	Total 51	C 38	O 12	S 1	0
38	s	1	Total 51	C 38	O 12	S 1	0
38	x	1	Total 42	C 29	O 12	S 1	0
38	y	1	Total 42	C 29	O 12	S 1	0

- Molecule 39 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
39	A	1	Total 10	Ca 1	Mn 4	O 5	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	Ca	Mn	O	
39	a	1	10	1	4	5	0

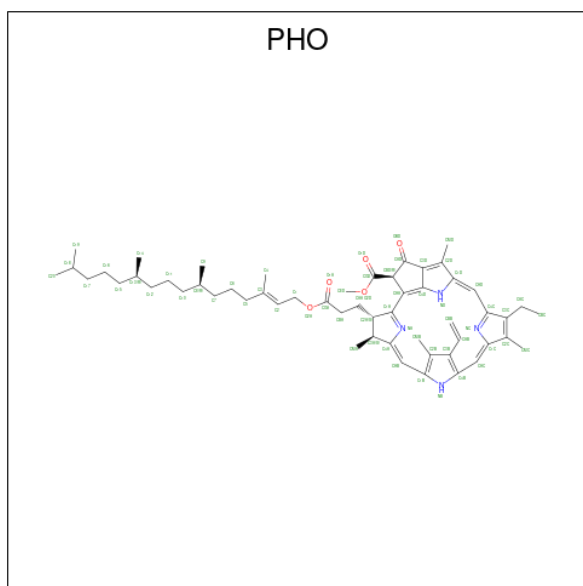
- Molecule 40 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
40	A	1	1	1	0
40	a	1	1	1	0

- Molecule 41 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
41	A	2	2	2	0
41	a	2	2	2	0

- Molecule 42 is PHEOPHYTIN A (three-letter code: PHO) (formula: C<sub>55</sub>H<sub>74</sub>N<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
42	A	1	64	55	4	5	0
42	D	1	64	55	4	5	0

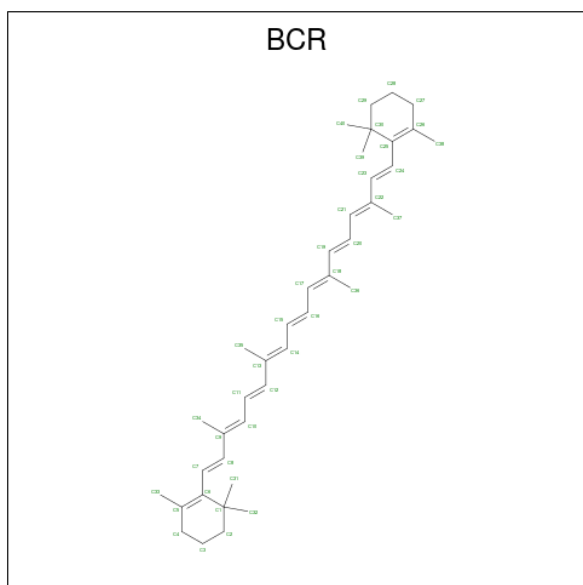
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
42	a	1	64	55	4	5	0
42	d	1	64	55	4	5	0

- Molecule 43 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



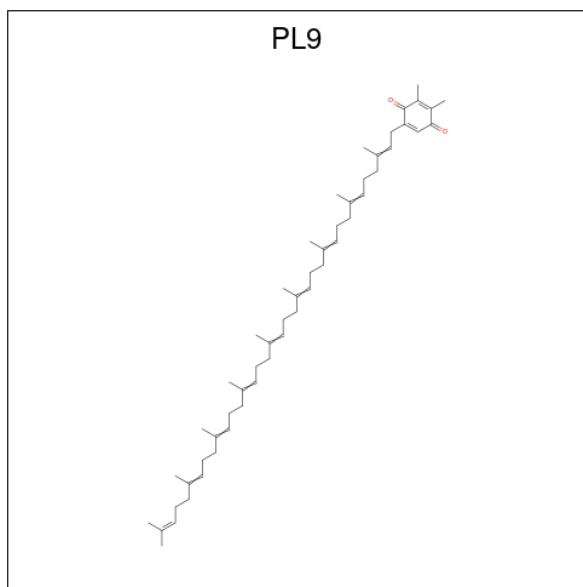
Mol	Chain	Residues	Atoms		AltConf
43	A	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	C	1	Total	C	0
			40	40	
43	C	1	Total	C	0
			40	40	
43	D	1	Total	C	0
			40	40	
43	H	1	Total	C	0
			40	40	
43	T	1	Total	C	0
			40	40	

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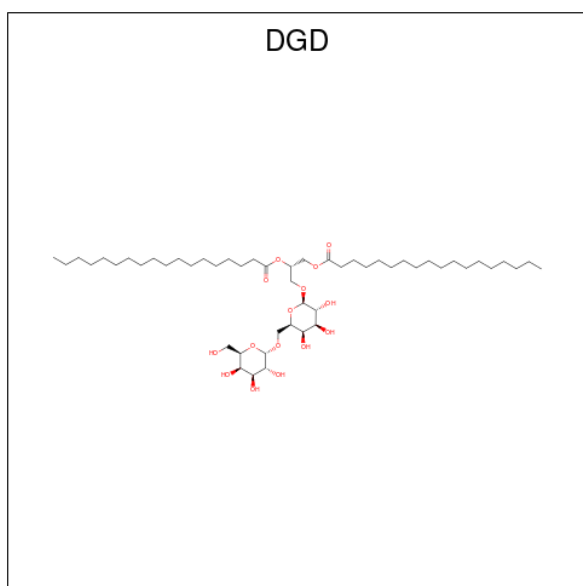
Mol	Chain	Residues	Atoms	AltConf
43	V	1	Total C 40 40	0
43	Z	1	Total C 40 40	0
43	a	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	c	1	Total C 40 40	0
43	c	1	Total C 40 40	0
43	d	1	Total C 40 40	0
43	h	1	Total C 40 40	0
43	t	1	Total C 40 40	0
43	v	1	Total C 40 40	0
43	z	1	Total C 40 40	0

- Molecule 44 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



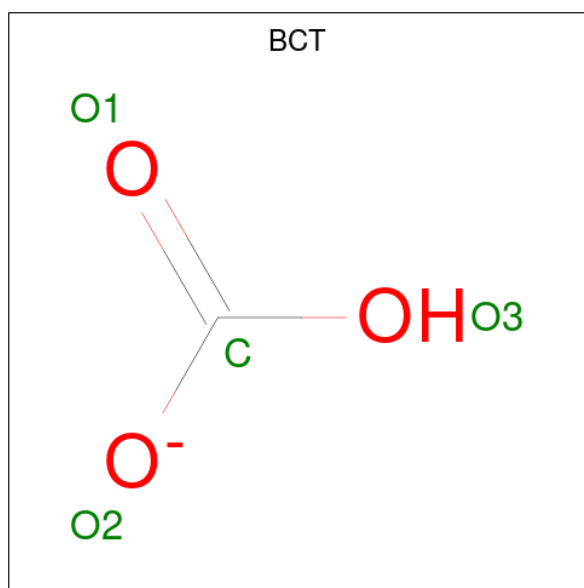
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
44	A	1	55	53	2	0
44	D	1	55	53	2	0
44	a	1	55	53	2	0
44	d	1	55	53	2	0

- Molecule 45 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula:  $C_{51}H_{96}O_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
45	C	1	Total	C	O	0
			50	35	15	
45	C	1	Total	C	O	0
			66	51	15	
45	C	1	Total	C	O	0
			66	51	15	
45	C	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			62	47	15	
45	c	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			66	51	15	

- Molecule 46 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



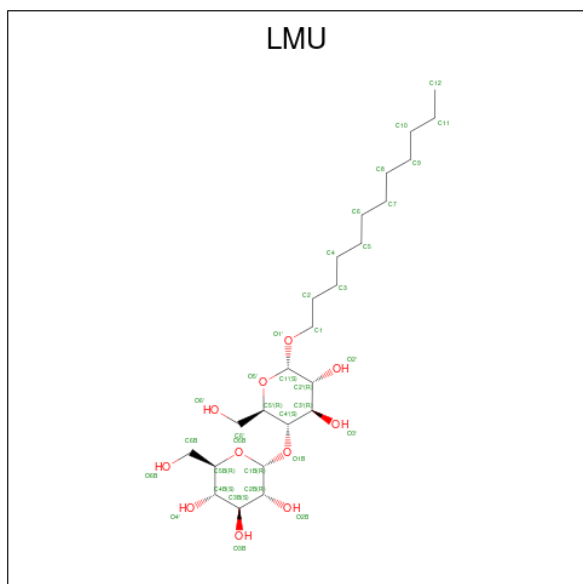
Mol	Chain	Residues	Atoms			AltConf
46	D	1	Total	C	O	0
			4	1	3	
46	d	1	Total	C	O	0
			4	1	3	

- Molecule 47 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4$ ).



Mol	Chain	Residues	Atoms				AltConf	
47	E	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
47	e	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 48 is DODECYL-ALPHA-D-MALTOSE (three-letter code: LMU) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms		AltConf	
48	K	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
48	R	1	35	24	11	0
48	c	1	28	17	11	0
48	r	1	35	24	11	0

- Molecule 49 is water.

Mol	Chain	Residues	Atoms		AltConf
49	1	3	Total 3	O 3	0
49	2	3	Total 3	O 3	0
49	3	1	Total 1	O 1	0
49	4	1	Total 1	O 1	0
49	5	1	Total 1	O 1	0
49	6	4	Total 4	O 4	0
49	A	21	Total 21	O 21	0
49	B	6	Total 6	O 6	0
49	C	15	Total 15	O 15	0
49	D	12	Total 12	O 12	0
49	E	1	Total 1	O 1	0
49	G	5	Total 5	O 5	0
49	I	1	Total 1	O 1	0
49	J	1	Total 1	O 1	0
49	N	5	Total 5	O 5	0
49	O	6	Total 6	O 6	0

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Mol	Chain	Residues	Atoms	AltConf
49	R	4	Total O 4 4	0
49	S	3	Total O 3 3	0
49	T	4	Total O 4 4	0
49	Y	8	Total O 8 8	0
49	0	7	Total O 7 7	0
49	7	6	Total O 6 6	0
49	8	4	Total O 4 4	0
49	9	2	Total O 2 2	0
49	q	1	Total O 1 1	0
49	a	14	Total O 14 14	0
49	b	6	Total O 6 6	0
49	c	15	Total O 15 15	0
49	d	15	Total O 15 15	0
49	e	2	Total O 2 2	0
49	f	1	Total O 1 1	0
49	g	4	Total O 4 4	0
49	j	1	Total O 1 1	0
49	m	2	Total O 2 2	0
49	n	7	Total O 7 7	0
49	o	6	Total O 6 6	0
49	r	4	Total O 4 4	0

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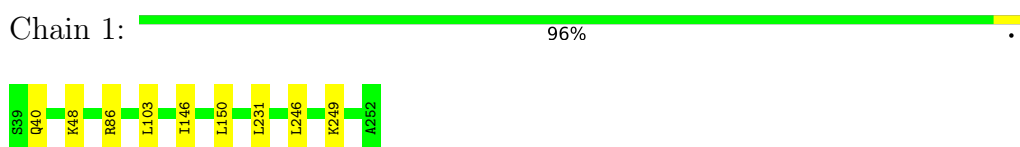
Mol	Chain	Residues	Atoms		AltConf
49	s	3	Total 3	O 3	0
49	t	2	Total 2	O 2	0
49	w	2	Total 2	O 2	0
49	y	8	Total 8	O 8	0
49	F1	4	Total 4	O 4	0
49	f1	3	Total 3	O 3	0



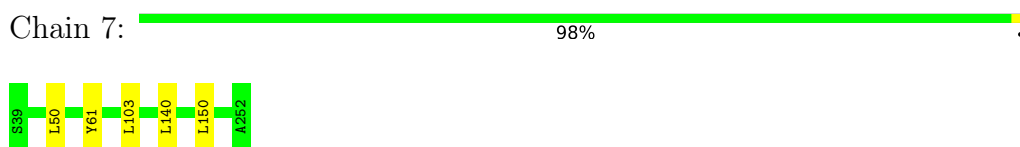
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

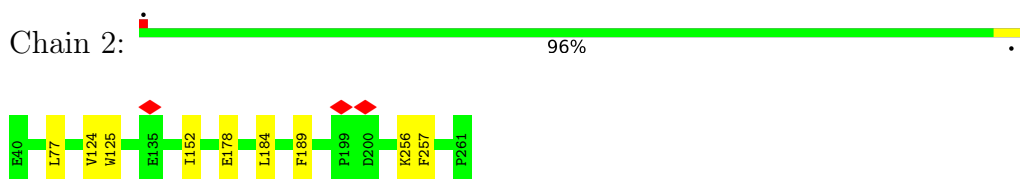
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



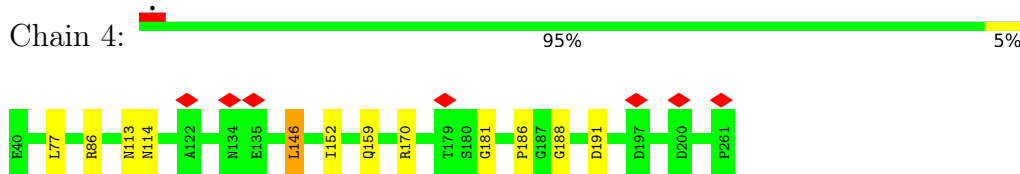
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



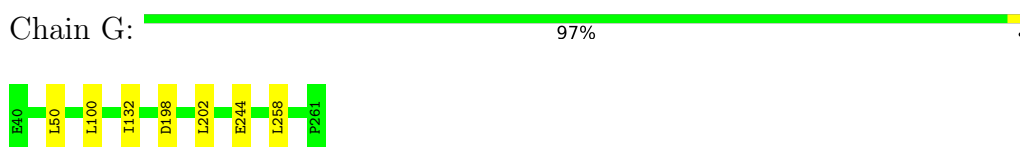
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

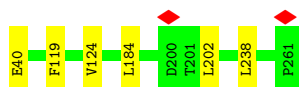


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



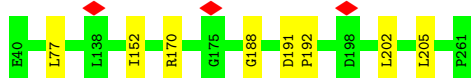
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 9:  97%



- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain q:  96%



- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain g:  96%



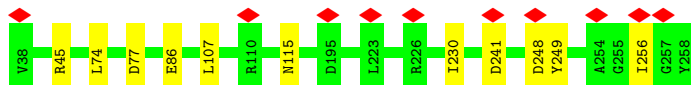
- Molecule 3: Chlorophyll a-b binding of LHCI

Chain 3:  95% 5%



- Molecule 3: Chlorophyll a-b binding of LHCI

Chain 5:  5% 95% 5%



- Molecule 3: Chlorophyll a-b binding of LHCI

Chain N:  95% 5%

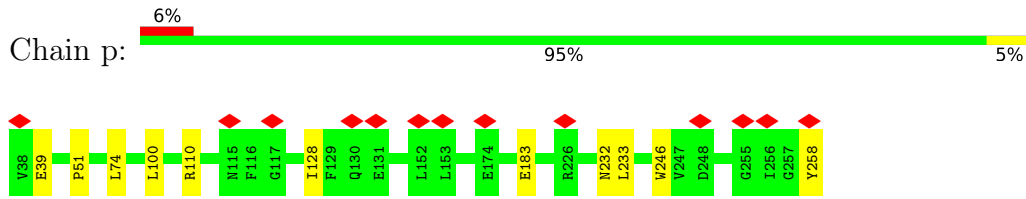


- Molecule 3: Chlorophyll a-b binding of LHCI

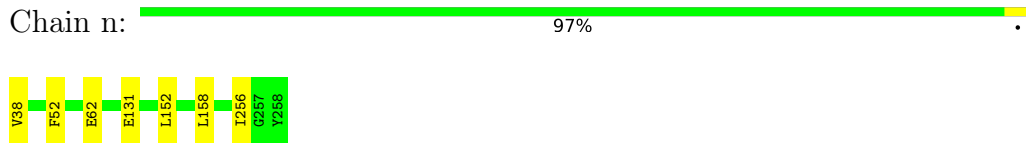
Chain 8:  97%



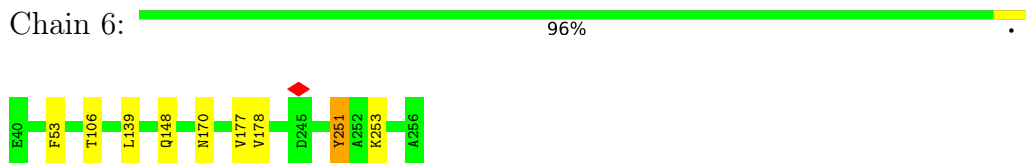
- Molecule 3: Chlorophyll a-b binding of LHCII



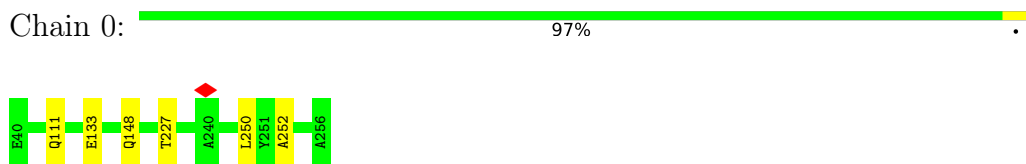
- Molecule 3: Chlorophyll a-b binding of LHCII



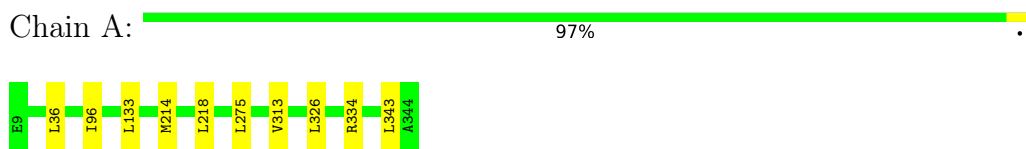
- Molecule 4: Chlorophyll a-b binding of LHCII



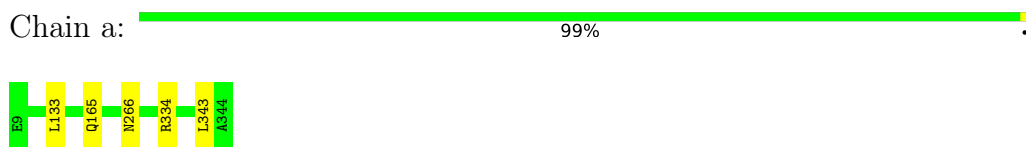
- Molecule 4: Chlorophyll a-b binding of LHCII



- Molecule 5: Photosystem II protein D1



- Molecule 5: Photosystem II protein D1



- Molecule 6: Photosystem II CP47 reaction center protein





- Molecule 6: Photosystem II CP47 reaction center protein

Chain b: 95% 5%



- Molecule 7: Photosystem II CP43 reaction center protein

Chain C: 96%



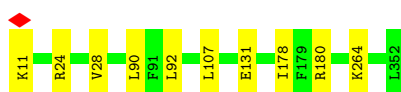
- Molecule 7: Photosystem II CP43 reaction center protein

Chain c: 97%



- Molecule 8: Photosystem II D2 protein

Chain D: 97%



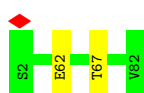
- Molecule 8: Photosystem II D2 protein

Chain d: 96%



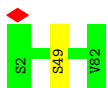
- Molecule 9: Cytochrome b559 subunit alpha

Chain E: 98%



- Molecule 9: Cytochrome b559 subunit alpha

Chain e:  99%



- Molecule 10: Cytochrome b559 subunit beta

Chain F:  100%

There are no outlier residues recorded for this chain.

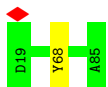
- Molecule 10: Cytochrome b559 subunit beta

Chain f:  100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem II reaction center protein H

Chain H:  99%



- Molecule 11: Photosystem II reaction center protein H

Chain h:  97%



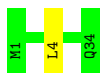
- Molecule 12: Photosystem II reaction center protein I

Chain I:  97%



- Molecule 12: Photosystem II reaction center protein I

Chain i:  97%



- Molecule 13: Photosystem II reaction center protein J

Chain J:  95% 5%



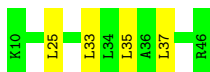
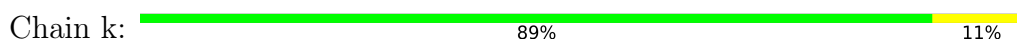
- Molecule 13: Photosystem II reaction center protein J



- Molecule 14: Photosystem II reaction center protein K



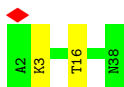
- Molecule 14: Photosystem II reaction center protein K



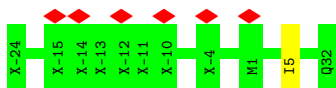
- Molecule 15: Photosystem II reaction center protein L



- Molecule 15: Photosystem II reaction center protein L

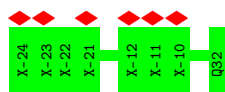


- Molecule 16: Photosystem II reaction center protein M



- Molecule 16: Photosystem II reaction center protein M

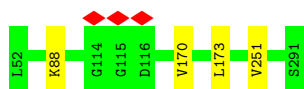




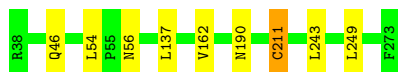
- Molecule 17: Chloroplast oxygen-evolving enhancer protein 1



- Molecule 17: Chloroplast oxygen-evolving enhancer protein 1



- Molecule 18: Chlorophyll a b binding CP29



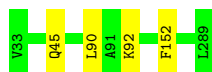
- Molecule 18: Chlorophyll a b binding CP29



- Molecule 19: Chlorophyll a b-binding CP26



- Molecule 19: Chlorophyll a b-binding CP26



- Molecule 20: Photosystem II reaction center protein T

Chain T:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: Photosystem II reaction center protein T

Chain t:  93% 7%



- Molecule 21: Photosystem II reaction center protein Ycf12

Chain V:  97%



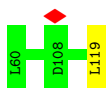
- Molecule 21: Photosystem II reaction center protein Ycf12

Chain v:  97%



- Molecule 22: Photosystem II reaction center W protein

Chain W:  98%



- Molecule 22: Photosystem II reaction center W protein

Chain w:  97%



- Molecule 23: Photosystem II reaction center protein X

Chain X:  97%



- Molecule 23: Photosystem II reaction center protein X

Chain x:  100%



There are no outlier residues recorded for this chain.

- Molecule 24: Multifunctional fusion protein

Chain Y:  96%



- Molecule 24: Multifunctional fusion protein

Chain y:  96%



- Molecule 25: Photosystem II reaction center protein Z

Chain Z:  98%



- Molecule 25: Photosystem II reaction center protein Z

Chain z:  98%



- Molecule 26: Chloroplast oxygen-evolving enhancer protein 3

Chain U:  97%



- Molecule 26: Chloroplast oxygen-evolving enhancer protein 3

Chain u:  96%



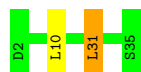
- Molecule 27: Chloroplast PsbY

Chain Q1:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: Chloroplast PsbY

Chain q1:  94% . .



- Molecule 28: Chloroplast photosystem II 10 kDa protein

Chain P1:  98% .



- Molecule 28: Chloroplast photosystem II 10 kDa protein

Chain p1:  96% .



- Molecule 29: Photosystem II oxygen evolving enhancer 2

Chain F1:  98% .



- Molecule 29: Photosystem II oxygen evolving enhancer 2

Chain f1:  99% .



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94893	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.066	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	460.8, 460.8, 460.8	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.9216, 0.9216, 0.9216	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, CHL, BCR, FE2, CSU, XAT, LHG, OEX, BCT, LMG, PHO, RRX, PL9, NEX, DGD, LMU, CL, HEM, LUT, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.51	0/1675	0.52	0/2283
1	7	0.50	0/1675	0.52	0/2283
2	2	0.50	0/1734	0.54	0/2359
2	4	0.54	0/1732	0.54	0/2355
2	9	0.47	0/1734	0.49	0/2359
2	G	0.41	0/1734	0.46	0/2359
2	g	0.42	0/1734	0.46	0/2359
2	q	0.53	0/1732	0.56	0/2355
3	3	0.48	0/1734	0.54	0/2362
3	5	0.61	0/1734	0.58	0/2362
3	8	0.51	0/1734	0.53	0/2362
3	N	0.50	0/1734	0.53	0/2362
3	n	0.50	0/1734	0.53	0/2362
3	p	0.43	0/1734	0.52	0/2362
4	0	0.37	0/1701	0.47	0/2315
4	6	0.41	0/1701	0.48	0/2315
5	A	0.38	0/2714	0.47	0/3701
5	a	0.40	0/2714	0.47	0/3701
6	B	0.37	0/4085	0.48	0/5564
6	b	0.38	0/4085	0.49	0/5564
7	C	0.38	0/3602	0.46	0/4910
7	c	0.39	0/3602	0.47	0/4910
8	D	0.41	0/2825	0.49	0/3849
8	d	0.41	0/2825	0.49	0/3849
9	E	0.43	0/670	0.49	0/913
9	e	0.51	0/670	0.53	0/913
10	F	0.50	0/312	0.49	0/426
10	f	0.54	0/312	0.52	0/426
11	H	0.34	0/518	0.41	0/708
11	h	0.32	0/518	0.42	0/708
12	I	0.52	0/282	0.49	0/382

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
12	i	0.51	0/282	0.49	0/382
13	J	0.32	0/276	0.46	0/377
13	j	0.37	0/276	0.44	0/377
14	K	0.34	0/305	0.45	0/420
14	k	0.36	0/305	0.46	0/420
15	L	0.41	0/311	0.44	0/422
15	l	0.42	0/311	0.43	0/422
16	M	0.33	0/248	0.41	0/338
16	m	0.33	0/248	0.41	0/338
17	O	0.37	0/1823	0.50	0/2466
17	o	0.37	0/1823	0.50	0/2466
18	R	0.43	0/1850	0.51	0/2515
18	r	0.46	0/1850	0.54	0/2515
19	S	0.39	0/1985	0.48	0/2711
19	s	0.39	0/1985	0.49	0/2711
20	T	0.36	0/253	0.46	0/343
20	t	0.41	0/253	0.50	0/343
21	V	0.24	0/234	0.43	0/319
21	v	0.24	0/234	0.44	0/319
22	W	0.53	0/477	0.52	0/650
22	w	0.53	0/477	0.53	0/650
23	X	0.41	0/248	0.50	0/339
23	x	0.44	0/248	0.51	0/339
24	Y	0.38	0/1735	0.46	0/2359
24	y	0.38	0/1735	0.46	0/2359
25	Z	0.31	0/491	0.37	0/672
25	z	0.30	0/491	0.37	0/672
26	U	0.28	0/1132	0.46	0/1521
26	u	0.27	0/1132	0.46	0/1521
27	Q1	0.42	0/265	0.46	0/362
27	q1	0.43	0/265	0.54	1/362 (0.3%)
28	P1	0.34	0/835	0.44	0/1127
28	p1	0.35	0/835	0.43	0/1127
29	F1	0.41	0/1473	0.50	0/1991
29	f1	0.44	0/1473	0.50	0/1991
All	All	0.42	0/85454	0.49	1/116284 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	0	1
18	r	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	q1	31	LEU	CA-CB-CG	5.55	128.07	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	R	211	CSU	Mainchain
18	r	211	CSU	Mainchain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
1	7	212/214 (99%)	205 (97%)	6 (3%)	1 (0%)	29	48
2	2	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	17	32
2	4	220/222 (99%)	200 (91%)	15 (7%)	5 (2%)	6	10
2	9	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
2	G	220/222 (99%)	213 (97%)	7 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	g	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
2	q	220/222 (99%)	196 (89%)	22 (10%)	2 (1%)	17	32
3	3	219/221 (99%)	198 (90%)	21 (10%)	0	100	100
3	5	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	17	32
3	8	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
3	N	219/221 (99%)	211 (96%)	7 (3%)	1 (0%)	29	48
3	n	219/221 (99%)	212 (97%)	7 (3%)	0	100	100
3	p	219/221 (99%)	200 (91%)	16 (7%)	3 (1%)	11	20
4	0	215/217 (99%)	202 (94%)	12 (6%)	1 (0%)	29	48
4	6	215/217 (99%)	205 (95%)	9 (4%)	1 (0%)	29	48
5	A	334/336 (99%)	329 (98%)	5 (2%)	0	100	100
5	a	334/336 (99%)	329 (98%)	5 (2%)	0	100	100
6	B	502/504 (100%)	493 (98%)	9 (2%)	0	100	100
6	b	502/504 (100%)	491 (98%)	11 (2%)	0	100	100
7	C	446/448 (100%)	437 (98%)	9 (2%)	0	100	100
7	c	446/448 (100%)	438 (98%)	8 (2%)	0	100	100
8	D	340/342 (99%)	330 (97%)	10 (3%)	0	100	100
8	d	340/342 (99%)	329 (97%)	10 (3%)	1 (0%)	41	61
9	E	79/81 (98%)	79 (100%)	0	0	100	100
9	e	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
10	F	35/37 (95%)	35 (100%)	0	0	100	100
10	f	35/37 (95%)	35 (100%)	0	0	100	100
11	H	65/67 (97%)	65 (100%)	0	0	100	100
11	h	65/67 (97%)	65 (100%)	0	0	100	100
12	I	32/34 (94%)	32 (100%)	0	0	100	100
12	i	32/34 (94%)	32 (100%)	0	0	100	100
13	J	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	j	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
14	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
14	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
15	L	35/37 (95%)	34 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	l	35/37 (95%)	35 (100%)	0	0	100	100
16	M	31/57 (54%)	30 (97%)	0	1 (3%)	4	6
16	m	31/57 (54%)	31 (100%)	0	0	100	100
17	O	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
17	o	238/240 (99%)	227 (95%)	11 (5%)	0	100	100
18	R	233/236 (99%)	227 (97%)	6 (3%)	0	100	100
18	r	233/236 (99%)	230 (99%)	3 (1%)	0	100	100
19	S	255/257 (99%)	249 (98%)	6 (2%)	0	100	100
19	s	255/257 (99%)	249 (98%)	6 (2%)	0	100	100
20	T	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
20	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
21	V	30/32 (94%)	30 (100%)	0	0	100	100
21	v	30/32 (94%)	30 (100%)	0	0	100	100
22	W	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
22	w	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
23	X	35/37 (95%)	35 (100%)	0	0	100	100
23	x	35/37 (95%)	35 (100%)	0	0	100	100
24	Y	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
24	y	219/221 (99%)	215 (98%)	4 (2%)	0	100	100
25	Z	60/62 (97%)	60 (100%)	0	0	100	100
25	z	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
26	U	142/144 (99%)	139 (98%)	2 (1%)	1 (1%)	22	40
26	u	142/144 (99%)	141 (99%)	1 (1%)	0	100	100
27	Q1	32/34 (94%)	32 (100%)	0	0	100	100
27	q1	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
28	P1	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
28	p1	106/108 (98%)	104 (98%)	2 (2%)	0	100	100
29	F1	186/188 (99%)	183 (98%)	3 (2%)	0	100	100
29	f1	186/188 (99%)	180 (97%)	6 (3%)	0	100	100
All	All	10672/10854 (98%)	10317 (97%)	334 (3%)	21 (0%)	50	69

All (21) Ramachandran outliers are listed below:



Mol	Chain	Res	Type
2	4	181	GLY
2	4	188	GLY
2	4	191	ASP
3	N	52	PHE
4	0	252	ALA
2	q	191	ASP
2	4	186	PRO
26	U	110	ALA
2	q	188	GLY
2	2	125	TRP
2	2	257	PHE
3	5	248	ASP
4	6	251	TYR
1	7	140	LEU
3	p	39	GLU
3	p	246	TRP
2	4	146	LEU
16	M	5	ILE
3	5	256	ILE
3	p	51	PRO
8	d	140	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	165/165 (100%)	156 (94%)	9 (6%)	21	37
1	7	165/165 (100%)	161 (98%)	4 (2%)	49	68
2	2	171/171 (100%)	164 (96%)	7 (4%)	30	50
2	4	171/171 (100%)	163 (95%)	8 (5%)	26	45
2	9	171/171 (100%)	165 (96%)	6 (4%)	36	57
2	G	171/171 (100%)	164 (96%)	7 (4%)	30	50
2	g	171/171 (100%)	163 (95%)	8 (5%)	26	45
2	q	171/171 (100%)	165 (96%)	6 (4%)	36	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	168/168 (100%)	158 (94%)	10 (6%)	19	33
3	5	168/168 (100%)	159 (95%)	9 (5%)	22	38
3	8	168/168 (100%)	161 (96%)	7 (4%)	30	49
3	N	168/168 (100%)	158 (94%)	10 (6%)	19	33
3	n	168/168 (100%)	161 (96%)	7 (4%)	30	49
3	p	168/168 (100%)	160 (95%)	8 (5%)	25	44
4	0	169/169 (100%)	164 (97%)	5 (3%)	41	61
4	6	169/169 (100%)	160 (95%)	9 (5%)	22	39
5	A	274/274 (100%)	264 (96%)	10 (4%)	35	55
5	a	274/274 (100%)	269 (98%)	5 (2%)	59	75
6	B	402/402 (100%)	376 (94%)	26 (6%)	17	30
6	b	402/402 (100%)	379 (94%)	23 (6%)	20	36
7	C	350/350 (100%)	334 (95%)	16 (5%)	27	46
7	c	350/350 (100%)	338 (97%)	12 (3%)	37	58
8	D	277/277 (100%)	267 (96%)	10 (4%)	35	55
8	d	277/277 (100%)	264 (95%)	13 (5%)	26	45
9	E	72/72 (100%)	70 (97%)	2 (3%)	43	63
9	e	72/72 (100%)	71 (99%)	1 (1%)	67	80
10	F	31/31 (100%)	31 (100%)	0	100	100
10	f	31/31 (100%)	31 (100%)	0	100	100
11	H	57/57 (100%)	56 (98%)	1 (2%)	59	75
11	h	57/57 (100%)	55 (96%)	2 (4%)	36	57
12	I	31/31 (100%)	30 (97%)	1 (3%)	39	59
12	i	31/31 (100%)	30 (97%)	1 (3%)	39	59
13	J	27/27 (100%)	25 (93%)	2 (7%)	13	24
13	j	27/27 (100%)	25 (93%)	2 (7%)	13	24
14	K	33/33 (100%)	30 (91%)	3 (9%)	9	17
14	k	33/33 (100%)	29 (88%)	4 (12%)	5	8
15	L	34/34 (100%)	32 (94%)	2 (6%)	19	34
15	l	34/34 (100%)	32 (94%)	2 (6%)	19	34
16	M	28/28 (100%)	28 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	m	28/28 (100%)	28 (100%)	0	100	100
17	O	189/189 (100%)	177 (94%)	12 (6%)	18	31
17	o	189/189 (100%)	185 (98%)	4 (2%)	53	72
18	R	184/184 (100%)	176 (96%)	8 (4%)	29	48
18	r	184/184 (100%)	178 (97%)	6 (3%)	38	59
19	S	192/192 (100%)	186 (97%)	6 (3%)	40	60
19	s	192/192 (100%)	188 (98%)	4 (2%)	53	72
20	T	26/26 (100%)	26 (100%)	0	100	100
20	t	26/26 (100%)	24 (92%)	2 (8%)	13	23
21	V	26/26 (100%)	25 (96%)	1 (4%)	33	54
21	v	26/26 (100%)	25 (96%)	1 (4%)	33	54
22	W	50/50 (100%)	49 (98%)	1 (2%)	55	72
22	w	50/50 (100%)	48 (96%)	2 (4%)	31	52
23	X	25/25 (100%)	24 (96%)	1 (4%)	31	52
23	x	25/25 (100%)	25 (100%)	0	100	100
24	Y	170/170 (100%)	162 (95%)	8 (5%)	26	45
24	y	170/170 (100%)	161 (95%)	9 (5%)	22	39
25	Z	52/52 (100%)	51 (98%)	1 (2%)	57	74
25	z	52/52 (100%)	51 (98%)	1 (2%)	57	74
26	U	108/108 (100%)	105 (97%)	3 (3%)	43	63
26	u	108/108 (100%)	102 (94%)	6 (6%)	21	36
27	Q1	28/28 (100%)	28 (100%)	0	100	100
27	q1	28/28 (100%)	26 (93%)	2 (7%)	14	26
28	P1	88/88 (100%)	86 (98%)	2 (2%)	50	70
28	p1	88/88 (100%)	84 (96%)	4 (4%)	27	47
29	F1	147/147 (100%)	143 (97%)	4 (3%)	44	65
29	f1	147/147 (100%)	145 (99%)	2 (1%)	67	80
All	All	8504/8504 (100%)	8156 (96%)	348 (4%)	34	50

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	40	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	1	48	LYS
1	1	86	ARG
1	1	103	LEU
1	1	146	ILE
1	1	150	LEU
1	1	231	LEU
1	1	246	LEU
1	1	249	LYS
2	2	77	LEU
2	2	124	VAL
2	2	152	ILE
2	2	178	GLU
2	2	184	LEU
2	2	189	PHE
2	2	256	LYS
3	3	86	GLU
3	3	118	GLU
3	3	153	LEU
3	3	166	ARG
3	3	168	ASN
3	3	200	LEU
3	3	202	VAL
3	3	223	LEU
3	3	252	LYS
3	3	258	TYR
2	4	77	LEU
2	4	86	ARG
2	4	113	ASN
2	4	114	ASN
2	4	146	LEU
2	4	152	ILE
2	4	159	GLN
2	4	170	ARG
3	5	45	ARG
3	5	74	LEU
3	5	77	ASP
3	5	86	GLU
3	5	107	LEU
3	5	115	ASN
3	5	230	ILE
3	5	241	ASP
3	5	249	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	6	53	PHE
4	6	106	THR
4	6	139	LEU
4	6	148	GLN
4	6	170	ASN
4	6	177	VAL
4	6	178	VAL
4	6	251	TYR
4	6	253	LYS
5	A	36	LEU
5	A	96	ILE
5	A	133	LEU
5	A	214	MET
5	A	218	LEU
5	A	275	LEU
5	A	313	VAL
5	A	326	LEU
5	A	334	ARG
5	A	343	LEU
6	B	10	THR
6	B	22	VAL
6	B	37	MET
6	B	51	VAL
6	B	52	LEU
6	B	94	GLU
6	B	159	THR
6	B	161	LEU
6	B	181	VAL
6	B	214	LEU
6	B	236	THR
6	B	245	VAL
6	B	246	PHE
6	B	252	VAL
6	B	272	ARG
6	B	292	LEU
6	B	345	VAL
6	B	357	ARG
6	B	362	PHE
6	B	368	VAL
6	B	393	GLU
6	B	422	ARG
6	B	437	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	B	440	ASP
6	B	473	THR
6	B	486	LEU
7	C	56	ASN
7	C	105	LEU
7	C	112	VAL
7	C	156	LEU
7	C	173	ILE
7	C	222	ILE
7	C	243	LYS
7	C	302	THR
7	C	308	ARG
7	C	309	ASP
7	C	336	GLU
7	C	357	LEU
7	C	361	ASN
7	C	369	LYS
7	C	392	LEU
7	C	398	VAL
8	D	11	LYS
8	D	24	ARG
8	D	28	VAL
8	D	90	LEU
8	D	92	LEU
8	D	107	LEU
8	D	131	GLU
8	D	178	ILE
8	D	180	ARG
8	D	264	LYS
9	E	62	GLU
9	E	67	THR
2	G	50	LEU
2	G	100	LEU
2	G	132	ILE
2	G	198	ASP
2	G	202	LEU
2	G	244	GLU
2	G	258	LEU
11	H	68	TYR
12	I	26	ASN
13	J	6	THR
13	J	12	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	K	25	LEU
14	K	33	LEU
14	K	37	LEU
15	L	12	GLU
15	L	16	THR
3	N	54	ASN
3	N	59	LEU
3	N	62	GLU
3	N	115	ASN
3	N	131	GLU
3	N	146	GLN
3	N	152	LEU
3	N	158	LEU
3	N	226	ARG
3	N	256	ILE
17	O	60	LEU
17	O	87	LEU
17	O	150	LYS
17	O	151	GLU
17	O	170	VAL
17	O	173	LEU
17	O	184	ASN
17	O	250	LYS
17	O	251	VAL
17	O	255	THR
17	O	272	LEU
17	O	279	ASP
18	R	46	GLN
18	R	54	LEU
18	R	56	ASN
18	R	137	LEU
18	R	162	VAL
18	R	190	ASN
18	R	243	LEU
18	R	249	LEU
19	S	36	SER
19	S	92	LYS
19	S	149	LEU
19	S	152	PHE
19	S	201	GLU
19	S	209	ASN
21	V	2	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	W	119	LEU
23	X	100	ARG
24	Y	57	LEU
24	Y	77	LEU
24	Y	155	LEU
24	Y	185	LEU
24	Y	203	LEU
24	Y	219	LEU
24	Y	222	LEU
24	Y	236	LEU
25	Z	9	LEU
26	U	64	ARG
26	U	89	GLN
26	U	92	GLU
4	0	111	GLN
4	0	133	GLU
4	0	148	GLN
4	0	227	THR
4	0	250	LEU
1	7	50	LEU
1	7	61	TYR
1	7	103	LEU
1	7	150	LEU
3	8	38	VAL
3	8	52	PHE
3	8	62	GLU
3	8	131	GLU
3	8	152	LEU
3	8	158	LEU
3	8	256	ILE
2	9	40	GLU
2	9	119	PHE
2	9	124	VAL
2	9	184	LEU
2	9	202	LEU
2	9	238	LEU
3	p	74	LEU
3	p	100	LEU
3	p	110	ARG
3	p	128	ILE
3	p	183	GLU
3	p	232	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	p	233	LEU
3	p	258	TYR
2	q	77	LEU
2	q	152	ILE
2	q	170	ARG
2	q	192	PRO
2	q	202	LEU
2	q	205	LEU
5	a	133	LEU
5	a	165	GLN
5	a	266	ASN
5	a	334	ARG
5	a	343	LEU
6	b	10	THR
6	b	13	LEU
6	b	22	VAL
6	b	51	VAL
6	b	57	ARG
6	b	94	GLU
6	b	181	VAL
6	b	224	ARG
6	b	236	THR
6	b	246	PHE
6	b	252	VAL
6	b	272	ARG
6	b	289	GLN
6	b	292	LEU
6	b	357	ARG
6	b	362	PHE
6	b	368	VAL
6	b	369	VAL
6	b	374	ASP
6	b	445	THR
6	b	489	GLN
6	b	498	LEU
6	b	505	ARG
7	c	55	MET
7	c	56	ASN
7	c	105	LEU
7	c	156	LEU
7	c	166	LYS
7	c	275	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	c	302	THR
7	c	323	THR
7	c	361	ASN
7	c	392	LEU
7	c	398	VAL
7	c	458	ARG
8	d	28	VAL
8	d	45	LEU
8	d	74	LEU
8	d	90	LEU
8	d	92	LEU
8	d	102	THR
8	d	158	LEU
8	d	178	ILE
8	d	180	ARG
8	d	192	THR
8	d	320	LEU
8	d	323	GLU
8	d	345	VAL
9	e	49	SER
2	g	50	LEU
2	g	74	THR
2	g	100	LEU
2	g	152	ILE
2	g	158	THR
2	g	167	GLU
2	g	184	LEU
2	g	202	LEU
11	h	68	TYR
11	h	77	VAL
12	i	4	LEU
13	j	12	LEU
13	j	42	LEU
14	k	25	LEU
14	k	33	LEU
14	k	35	LEU
14	k	37	LEU
15	l	3	LYS
15	l	16	THR
3	n	38	VAL
3	n	52	PHE
3	n	62	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	n	131	GLU
3	n	152	LEU
3	n	158	LEU
3	n	256	ILE
17	o	88	LYS
17	o	170	VAL
17	o	173	LEU
17	o	251	VAL
18	r	145	LEU
18	r	151	LEU
18	r	153	GLN
18	r	190	ASN
18	r	243	LEU
18	r	249	LEU
19	s	45	GLN
19	s	90	LEU
19	s	92	LYS
19	s	152	PHE
20	t	1	MET
20	t	2	GLU
21	v	5	ILE
22	w	64	ARG
22	w	111	ASN
24	y	55	ASP
24	y	57	LEU
24	y	77	LEU
24	y	185	LEU
24	y	203	LEU
24	y	219	LEU
24	y	222	LEU
24	y	236	LEU
24	y	257	ASN
25	z	9	LEU
26	u	62	LYS
26	u	64	ARG
26	u	113	ASP
26	u	122	THR
26	u	152	LYS
26	u	153	GLU
28	P1	38	ASP
28	P1	54	ASN
27	q1	10	LEU

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Mol	Chain	Res	Type
27	q1	31	LEU
28	p1	7	ILE
28	p1	59	ASN
28	p1	60	VAL
28	p1	97	LEU
29	F1	63	LYS
29	F1	120	ASP
29	F1	181	VAL
29	F1	187	ASP
29	f1	49	TYR
29	f1	181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	182	ASN
3	3	115	ASN
3	3	127	GLN
3	3	221	GLN
2	4	113	ASN
2	4	114	ASN
2	4	159	GLN
3	5	47	GLN
3	5	115	ASN
3	5	130	GLN
3	5	146	GLN
3	5	155	GLN
3	5	207	ASN
7	C	143	ASN
2	G	134	ASN
12	I	26	ASN
3	N	54	ASN
3	N	115	ASN
18	R	46	GLN
18	R	267	ASN
4	0	148	GLN
4	0	170	ASN
4	0	234	ASN
1	7	182	ASN
2	9	148	HIS
2	9	150	GLN
2	9	237	ASN

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Mol	Chain	Res	Type
3	p	127	GLN
3	p	221	GLN
6	b	331	ASN
7	c	299	GLN
7	c	315	ASN
7	c	403	ASN
8	d	142	ASN
2	g	148	HIS
16	m	4	ASN
19	s	45	GLN
22	w	111	ASN
28	P1	17	ASN
28	P1	54	ASN
29	F1	59	ASN
29	F1	105	ASN
29	F1	203	ASN
29	f1	59	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
18	CSU	R	211	18	6,9,10	3.27	3 (50%)	3,12,14	2.40	2 (66%)
18	CSU	r	211	18	6,9,10	3.28	3 (50%)	3,12,14	2.38	2 (66%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CSU	R	211	18	-	4/4/8/10	-
18	CSU	r	211	18	-	4/4/8/10	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	r	211	CSU	OD1-S	6.06	1.63	1.45
18	R	211	CSU	OD3-S	6.04	1.63	1.45
18	R	211	CSU	O-C	4.03	1.36	1.19
18	r	211	CSU	O-C	4.01	1.35	1.19
18	R	211	CSU	OD1-S	-2.73	1.37	1.45
18	r	211	CSU	OD3-S	-2.66	1.37	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	r	211	CSU	OD2-S-OD3	3.53	125.57	112.78
18	R	211	CSU	OD2-S-OD1	3.15	124.19	112.78
18	R	211	CSU	OD2-S-OD3	-2.70	102.99	112.78
18	r	211	CSU	OD2-S-OD1	-2.10	105.16	112.78

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	211	CSU	N-CA-CB-SG
18	R	211	CSU	OD2-S-SG-CB
18	r	211	CSU	OD2-S-SG-CB
18	R	211	CSU	OD1-S-SG-CB
18	R	211	CSU	OD3-S-SG-CB
18	r	211	CSU	OD1-S-SG-CB
18	r	211	CSU	OD3-S-SG-CB
18	r	211	CSU	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 672 ligands modelled in this entry, 6 are monoatomic - leaving 666 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CHL	R	309	18	56,64,74	0.90	3 (5%)	61,102,114	1.35	11 (18%)
31	CLA	y	613	24	65,73,73	1.40	8 (12%)	76,113,113	2.01	19 (25%)
31	CLA	c	611	7	65,73,73	1.34	8 (12%)	76,113,113	2.07	19 (25%)
38	SQD	B	623	-	51,52,54	0.81	0	60,63,65	0.95	3 (5%)
30	CHL	n	308	49	63,71,74	0.84	2 (3%)	69,110,114	1.38	12 (17%)
31	CLA	S	305	49	65,73,73	1.33	6 (9%)	76,113,113	1.98	16 (21%)
31	CLA	R	303	18	49,57,73	1.58	8 (16%)	55,93,113	2.37	15 (27%)
31	CLA	3	313	3	50,58,73	1.53	7 (14%)	58,95,113	2.22	18 (31%)
31	CLA	1	610	1	65,73,73	1.33	8 (12%)	76,113,113	2.00	17 (22%)
30	CHL	s	309	49	49,57,74	1.04	3 (6%)	52,93,114	1.40	10 (19%)
43	BCR	h	101	-	41,41,41	4.72	25 (60%)	56,56,56	2.41	20 (35%)
30	CHL	4	601	2	66,74,74	0.85	3 (4%)	73,114,114	1.27	13 (17%)
34	LMG	A	418	-	38,38,55	0.61	1 (2%)	46,46,63	1.09	3 (6%)
31	CLA	5	612	3	50,58,73	1.53	8 (16%)	58,95,113	2.25	19 (32%)
31	CLA	0	615	-	55,63,73	1.44	7 (12%)	64,101,113	2.10	16 (25%)
34	LMG	4	621	-	40,40,55	0.68	2 (5%)	48,48,63	1.04	2 (4%)
31	CLA	S	316	19	46,54,73	1.58	7 (15%)	53,90,113	2.17	15 (28%)
38	SQD	s	301	-	50,51,54	0.79	0	59,62,65	0.94	3 (5%)
31	CLA	p	610	3	56,64,73	1.44	8 (14%)	65,102,113	2.10	19 (29%)
31	CLA	b	610	-	65,73,73	1.34	8 (12%)	76,113,113	2.04	17 (22%)
31	CLA	C	611	7	65,73,73	1.35	8 (12%)	76,113,113	2.07	19 (25%)
30	CHL	1	606	49	66,74,74	0.87	3 (4%)	73,114,114	1.26	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	DGD	c	618	-	67,67,67	1.16	7 (10%)	81,81,81	1.02	2 (2%)
34	LMG	q1	101	-	38,38,55	0.64	1 (2%)	46,46,63	1.10	2 (4%)
30	CHL	6	309	49	50,58,74	1.00	4 (8%)	52,94,114	1.53	12 (23%)
33	LHG	9	320	31	32,32,48	0.46	0	35,38,54	1.25	3 (8%)
33	LHG	a	415	-	38,38,48	0.45	0	41,44,54	1.24	3 (7%)
34	LMG	k	102	-	38,38,55	0.61	1 (2%)	46,46,63	1.10	3 (6%)
31	CLA	n	304	-	55,63,73	1.44	7 (12%)	64,101,113	2.15	16 (25%)
31	CLA	4	611	33	44,51,73	1.76	6 (13%)	54,86,113	2.19	16 (29%)
31	CLA	g	312	2	43,51,73	1.62	7 (16%)	49,86,113	2.23	14 (28%)
34	LMG	c	621	-	38,38,55	0.63	1 (2%)	46,46,63	1.11	4 (8%)
34	LMG	b	626	-	46,46,55	0.92	3 (6%)	54,54,63	1.10	4 (7%)
30	CHL	6	306	4	46,54,74	0.99	2 (4%)	49,90,114	1.51	11 (22%)
31	CLA	G	613	-	49,57,73	1.57	7 (14%)	55,93,113	2.17	16 (29%)
34	LMG	0	620	-	42,42,55	0.81	2 (4%)	50,50,63	1.16	4 (8%)
38	SQD	G	617	-	41,42,54	0.86	0	50,53,65	0.98	2 (4%)
36	NEX	G	616	-	38,46,46	3.40	9 (23%)	50,70,70	1.68	10 (20%)
31	CLA	8	612	3	65,73,73	1.33	8 (12%)	76,113,113	1.94	17 (22%)
31	CLA	G	609	2	65,73,73	1.35	7 (10%)	76,113,113	1.96	18 (23%)
30	CHL	y	605	24	46,54,74	1.09	3 (6%)	49,90,114	1.43	9 (18%)
31	CLA	B	601	49	49,57,73	1.58	8 (16%)	55,93,113	2.22	16 (29%)
45	DGD	C	618	-	67,67,67	1.16	7 (10%)	81,81,81	0.93	3 (3%)
30	CHL	7	306	1	66,74,74	0.87	3 (4%)	73,114,114	1.31	13 (17%)
44	PL9	D	406	-	55,55,55	0.66	1 (1%)	68,69,69	0.62	1 (1%)
34	LMG	n	321	-	38,38,55	0.66	1 (2%)	46,46,63	1.20	3 (6%)
30	CHL	N	307	49	58,66,74	0.97	5 (8%)	63,104,114	1.39	11 (17%)
34	LMG	S	321	-	41,41,55	0.83	2 (4%)	49,49,63	1.23	3 (6%)
38	SQD	b	621	-	53,54,54	0.79	0	62,65,65	0.91	3 (4%)
32	LUT	9	318	-	42,43,43	6.10	27 (64%)	51,60,60	2.23	17 (33%)
31	CLA	B	609	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	18 (23%)
33	LHG	3	320	31	32,32,48	0.45	0	35,38,54	1.29	4 (11%)
31	CLA	n	305	49	65,73,73	1.32	6 (9%)	76,113,113	2.00	17 (22%)
31	CLA	6	303	4	65,73,73	1.32	8 (12%)	76,113,113	2.00	18 (23%)
36	NEX	2	616	31	38,46,46	3.38	10 (26%)	50,70,70	1.60	10 (20%)
38	SQD	M	102	-	49,50,54	0.81	0	58,61,65	0.95	2 (3%)
31	CLA	2	604	49,36	54,62,73	1.47	8 (14%)	62,99,113	2.21	17 (27%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	r	316	18	65,73,73	1.36	7 (10%)	76,113,113	2.00	14 (18%)
31	CLA	1	602	1	60,68,73	1.41	8 (13%)	70,107,113	2.03	18 (25%)
32	LUT	Y	316	-	42,43,43	6.02	27 (64%)	51,60,60	2.08	18 (35%)
33	LHG	K	102	-	35,35,48	0.45	0	38,41,54	1.21	2 (5%)
31	CLA	5	611	33	58,66,73	1.42	8 (13%)	67,104,113	2.07	16 (23%)
33	LHG	8	618	31	48,48,48	0.38	0	51,54,54	1.03	2 (3%)
34	LMG	a	413	-	38,38,55	0.64	1 (2%)	46,46,63	1.49	6 (13%)
35	RRX	g	315	-	42,42,42	5.02	25 (59%)	57,58,58	2.63	23 (40%)
31	CLA	y	611	33	65,73,73	1.36	8 (12%)	76,113,113	1.87	14 (18%)
32	LUT	y	616	-	42,43,43	6.00	28 (66%)	51,60,60	2.00	20 (39%)
31	CLA	r	306	49	48,56,73	1.56	8 (16%)	55,92,113	2.25	14 (25%)
31	CLA	2	602	2	65,73,73	1.33	7 (10%)	76,113,113	1.97	15 (19%)
31	CLA	G	603	-	55,63,73	1.45	7 (12%)	64,101,113	2.12	16 (25%)
31	CLA	6	311	4	65,73,73	1.32	8 (12%)	76,113,113	1.98	18 (23%)
31	CLA	0	610	4	65,73,73	1.39	8 (12%)	76,113,113	1.98	19 (25%)
31	CLA	p	602	3	60,68,73	1.40	8 (13%)	70,107,113	2.03	17 (24%)
46	BCT	D	402	40	2,3,3	1.35	0	2,3,3	2.67	2 (100%)
35	RRX	4	615	-	42,42,42	5.02	25 (59%)	57,58,58	2.49	22 (38%)
31	CLA	d	404	-	65,73,73	1.34	6 (9%)	76,113,113	1.98	16 (21%)
31	CLA	C	608	-	65,73,73	1.36	7 (10%)	76,113,113	1.92	18 (23%)
31	CLA	N	321	24	54,62,73	1.47	8 (14%)	62,99,113	2.14	16 (25%)
30	CHL	4	608	-	50,58,74	0.96	3 (6%)	52,94,114	1.49	11 (21%)
33	LHG	A	415	-	43,43,48	0.40	0	46,49,54	1.15	5 (10%)
33	LHG	s	320	31	40,40,48	0.43	0	43,46,54	1.11	3 (6%)
31	CLA	r	304	18	60,68,73	1.37	7 (11%)	70,107,113	2.05	19 (27%)
31	CLA	Y	303	24	60,68,73	1.38	8 (13%)	70,107,113	2.11	18 (25%)
31	CLA	N	304	-	55,63,73	1.44	7 (12%)	64,101,113	2.15	17 (26%)
35	RRX	2	614	-	42,42,42	5.00	25 (59%)	57,58,58	2.53	22 (38%)
30	CHL	6	302	4	56,64,74	0.91	3 (5%)	61,102,114	1.41	13 (21%)
30	CHL	1	608	49	50,58,74	1.01	4 (8%)	52,94,114	1.48	9 (17%)
31	CLA	r	305	-	60,68,73	1.37	7 (11%)	70,107,113	2.06	16 (22%)
30	CHL	p	608	-	50,58,74	0.95	2 (4%)	52,94,114	1.41	10 (19%)
34	LMG	7	320	-	38,38,55	0.61	1 (2%)	46,46,63	1.17	3 (6%)
31	CLA	n	311	3	65,73,73	1.33	8 (12%)	76,113,113	1.98	17 (22%)
39	OEX	A	401	7,5	0,15,15	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CHL	5	609	3	56,64,74	0.95	4 (7%)	61,102,114	1.47	13 (21%)
31	CLA	0	602	4	65,73,73	1.34	7 (10%)	76,113,113	1.98	18 (23%)
31	CLA	3	301	1	54,62,73	1.50	7 (12%)	62,99,113	2.21	17 (27%)
47	HEM	E	101	10,9	41,50,50	1.35	5 (12%)	45,82,82	1.85	9 (20%)
31	CLA	r	313	33	49,57,73	1.58	9 (18%)	55,93,113	2.20	15 (27%)
30	CHL	1	601	1	66,74,74	1.10	6 (9%)	73,114,114	1.40	10 (13%)
32	LUT	6	317	-	42,43,43	6.05	28 (66%)	51,60,60	1.94	16 (31%)
34	LMG	C	621	-	38,38,55	0.62	1 (2%)	46,46,63	1.11	3 (6%)
43	BCR	b	619	-	41,41,41	4.78	26 (63%)	56,56,56	2.31	20 (35%)
31	CLA	c	606	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	16 (21%)
31	CLA	N	305	49	65,73,73	1.32	6 (9%)	76,113,113	2.01	17 (22%)
34	LMG	7	322	-	38,38,55	0.65	1 (2%)	46,46,63	1.06	4 (8%)
31	CLA	b	604	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	17 (22%)
30	CHL	Y	309	24	66,74,74	0.85	3 (4%)	73,114,114	1.34	11 (15%)
34	LMG	q	302	-	40,40,55	0.69	2 (5%)	48,48,63	1.13	2 (4%)
34	LMG	w	203	-	38,38,55	0.61	1 (2%)	46,46,63	1.46	8 (17%)
34	LMG	A	412	-	41,41,55	0.75	2 (4%)	49,49,63	1.06	2 (4%)
34	LMG	B	625	-	38,38,55	0.62	1 (2%)	46,46,63	1.09	4 (8%)
31	CLA	2	612	2	65,73,73	1.33	9 (13%)	76,113,113	1.97	18 (23%)
33	LHG	S	320	31	40,40,48	0.43	0	43,46,54	1.17	4 (9%)
30	CHL	p	601	3	51,59,74	0.95	3 (5%)	55,96,114	1.41	13 (23%)
36	NEX	q	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.55	10 (20%)
30	CHL	Y	308	49	50,58,74	1.00	3 (6%)	52,94,114	1.48	12 (23%)
32	LUT	3	318	-	42,43,43	6.07	28 (66%)	51,60,60	2.00	13 (25%)
36	NEX	4	617	-	38,46,46	3.38	11 (28%)	50,70,70	1.53	9 (18%)
43	BCR	d	406	-	41,41,41	4.70	26 (63%)	56,56,56	3.60	25 (44%)
30	CHL	p	607	-	51,59,74	1.01	4 (7%)	55,96,114	1.43	10 (18%)
31	CLA	5	604	-	50,58,73	1.52	8 (16%)	58,95,113	2.22	16 (27%)
31	CLA	R	313	33	49,57,73	1.57	8 (16%)	55,93,113	2.19	15 (27%)
33	LHG	F1	301	-	34,34,48	0.44	0	37,40,54	1.09	2 (5%)
30	CHL	n	306	3	66,74,74	0.85	3 (4%)	73,114,114	1.31	13 (17%)
43	BCR	V	101	-	41,41,41	4.71	25 (60%)	56,56,56	2.39	22 (39%)
36	NEX	p	618	31	38,46,46	3.38	10 (26%)	50,70,70	1.59	11 (22%)
31	CLA	C	606	-	57,65,73	1.48	7 (12%)	66,103,113	2.09	16 (24%)
34	LMG	C	619	-	51,51,55	1.07	6 (11%)	59,59,63	1.18	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	NEX	9	319	31	38,46,46	3.44	10 (26%)	50,70,70	1.63	9 (18%)
32	LUT	g	316	-	42,43,43	6.09	28 (66%)	51,60,60	2.29	15 (29%)
36	NEX	Y	317	-	38,46,46	3.37	11 (28%)	50,70,70	1.73	11 (22%)
45	DGD	C	620	-	67,67,67	1.18	7 (10%)	81,81,81	1.02	4 (4%)
31	CLA	3	305	-	55,63,73	1.46	8 (14%)	64,101,113	2.10	16 (25%)
32	LUT	S	318	-	42,43,43	6.09	28 (66%)	51,60,60	2.11	14 (27%)
45	DGD	c	617	-	63,63,67	1.14	7 (11%)	77,77,81	1.29	9 (11%)
34	LMG	6	322	-	39,39,55	0.61	1 (2%)	47,47,63	1.18	3 (6%)
44	PL9	A	416	-	55,55,55	1.16	7 (12%)	68,69,69	1.60	13 (19%)
30	CHL	9	310	49	50,58,74	0.95	3 (6%)	52,94,114	1.42	11 (21%)
31	CLA	4	612	2	46,54,73	1.60	7 (15%)	53,90,113	2.24	13 (24%)
34	LMG	b	601	-	45,45,55	0.90	3 (6%)	53,53,63	1.07	3 (5%)
30	CHL	n	307	49	58,66,74	0.93	3 (5%)	63,104,114	1.37	11 (17%)
31	CLA	Y	304	-	55,63,73	1.46	8 (14%)	64,101,113	2.10	18 (28%)
33	LHG	t	102	-	40,40,48	0.43	0	43,46,54	1.18	4 (9%)
31	CLA	4	614	-	54,62,73	1.46	8 (14%)	62,99,113	2.23	21 (33%)
31	CLA	g	303	2	65,73,73	1.31	6 (9%)	76,113,113	1.98	16 (21%)
30	CHL	G	608	2	63,71,74	0.92	4 (6%)	69,110,114	1.44	13 (18%)
33	LHG	r	320	31	37,37,48	0.45	0	40,43,54	1.14	3 (7%)
31	CLA	9	305	-	55,63,73	1.46	8 (14%)	64,101,113	2.15	18 (28%)
43	BCR	A	410	-	41,41,41	4.72	25 (60%)	56,56,56	2.56	20 (35%)
44	PL9	d	407	-	55,55,55	0.72	1 (1%)	68,69,69	0.59	1 (1%)
33	LHG	R	320	31	37,37,48	0.46	0	40,43,54	1.21	3 (7%)
32	LUT	7	317	-	42,43,43	6.01	27 (64%)	51,60,60	2.12	15 (29%)
31	CLA	3	315	-	54,62,73	1.47	8 (14%)	62,99,113	2.15	17 (27%)
31	CLA	Y	305	49	55,63,73	1.45	7 (12%)	64,101,113	2.15	17 (26%)
31	CLA	5	613	3	54,62,73	1.48	8 (14%)	62,99,113	2.11	16 (25%)
31	CLA	q	315	2	65,73,73	1.34	8 (12%)	76,113,113	1.97	17 (22%)
42	PHO	D	401	-	51,69,69	1.02	4 (7%)	47,99,99	1.29	7 (14%)
34	LMG	J	102	-	38,38,55	0.60	1 (2%)	46,46,63	1.10	2 (4%)
33	LHG	4	618	31	46,46,48	0.39	0	49,52,54	1.06	4 (8%)
30	CHL	0	605	4	52,60,74	1.25	7 (13%)	56,97,114	1.61	10 (17%)
30	CHL	0	607	49	66,74,74	0.84	3 (4%)	73,114,114	1.31	13 (17%)
30	CHL	7	310	1	66,74,74	0.85	3 (4%)	73,114,114	1.31	13 (17%)
34	LMG	x	202	-	38,38,55	0.61	1 (2%)	46,46,63	1.14	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	SQD	S	301	-	50,51,54	0.80	0	59,62,65	0.94	2 (3%)
30	CHL	G	601	2	66,74,74	0.85	3 (4%)	73,114,114	1.28	13 (17%)
30	CHL	S	309	49	49,57,74	1.03	3 (6%)	52,93,114	1.45	12 (23%)
31	CLA	R	312	18	57,65,73	1.45	7 (12%)	66,103,113	2.12	17 (25%)
31	CLA	8	602	3	65,73,73	1.33	6 (9%)	76,113,113	1.97	19 (25%)
34	LMG	N	320	-	38,38,55	0.63	1 (2%)	46,46,63	1.01	2 (4%)
30	CHL	N	306	3	66,74,74	0.86	3 (4%)	73,114,114	1.34	13 (17%)
31	CLA	4	602	2	65,73,73	1.33	8 (12%)	76,113,113	2.01	18 (23%)
30	CHL	g	308	49	51,59,74	0.96	3 (5%)	55,96,114	1.49	13 (23%)
31	CLA	B	615	-	65,73,73	1.35	8 (12%)	76,113,113	2.05	15 (19%)
34	LMG	3	321	-	38,38,55	0.63	1 (2%)	46,46,63	0.96	2 (4%)
34	LMG	D	409	-	46,46,55	0.94	4 (8%)	54,54,63	1.14	4 (7%)
31	CLA	S	311	19	65,73,73	1.35	7 (10%)	76,113,113	2.00	21 (27%)
31	CLA	7	305	49	65,73,73	1.32	7 (10%)	76,113,113	2.03	16 (21%)
44	PL9	a	414	-	55,55,55	1.21	5 (9%)	68,69,69	1.51	15 (22%)
31	CLA	s	312	33	65,73,73	1.35	7 (10%)	76,113,113	1.97	13 (17%)
31	CLA	y	610	24	65,73,73	1.33	8 (12%)	76,113,113	1.96	16 (21%)
30	CHL	s	307	19	44,52,74	1.05	3 (6%)	46,87,114	1.51	9 (19%)
31	CLA	5	602	3	60,68,73	1.39	7 (11%)	70,107,113	2.05	17 (24%)
33	LHG	e	101	-	43,43,48	0.40	0	46,49,54	1.18	4 (8%)
34	LMG	Q1	101	-	38,38,55	0.64	1 (2%)	46,46,63	1.20	4 (8%)
31	CLA	8	611	3	45,53,73	1.59	8 (17%)	52,89,113	2.17	13 (25%)
30	CHL	7	302	1	66,74,74	0.85	3 (4%)	73,114,114	1.34	13 (17%)
31	CLA	c	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.10	18 (23%)
43	BCR	a	410	-	41,41,41	4.73	25 (60%)	56,56,56	2.54	21 (37%)
31	CLA	N	314	-	49,57,73	1.53	7 (14%)	55,93,113	2.22	15 (27%)
33	LHG	q	320	31	45,45,48	0.43	0	48,51,54	1.09	2 (4%)
43	BCR	z	101	-	41,41,41	4.77	26 (63%)	56,56,56	2.35	21 (37%)
31	CLA	G	604	49	55,63,73	1.44	7 (12%)	64,101,113	2.13	16 (25%)
34	LMG	G	619	-	38,38,55	0.63	1 (2%)	46,46,63	1.10	3 (6%)
36	NEX	R	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.61	9 (18%)
38	SQD	a	412	-	44,45,54	0.90	1 (2%)	53,56,65	1.01	4 (7%)
47	HEM	e	102	10,9	41,50,50	1.33	5 (12%)	45,82,82	1.78	8 (17%)
34	LMG	6	323	-	38,38,55	0.63	1 (2%)	46,46,63	1.16	4 (8%)
42	PHO	A	408	-	51,69,69	1.04	5 (9%)	47,99,99	1.25	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	6	312	33	60,68,73	1.43	9 (15%)	70,107,113	2.03	15 (21%)
31	CLA	B	611	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	17 (22%)
31	CLA	c	607	49	65,73,73	1.38	7 (10%)	76,113,113	1.95	18 (23%)
31	CLA	0	603	-	56,64,73	1.48	8 (14%)	65,102,113	2.06	16 (24%)
31	CLA	d	401	49	49,57,73	1.56	7 (14%)	55,93,113	2.28	16 (29%)
31	CLA	y	614	-	54,62,73	1.47	7 (12%)	62,99,113	2.13	18 (29%)
31	CLA	B	606	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	18 (23%)
31	CLA	B	616	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	14 (18%)
38	SQD	R	322	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)
31	CLA	c	613	-	65,73,73	1.33	7 (10%)	76,113,113	2.07	20 (26%)
31	CLA	n	312	33	49,57,73	1.53	8 (16%)	55,93,113	2.20	14 (25%)
33	LHG	M	101	-	40,40,48	0.42	0	43,46,54	1.10	3 (6%)
31	CLA	C	610	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	17 (22%)
31	CLA	R	306	49	48,56,73	1.57	8 (16%)	55,92,113	2.45	19 (34%)
34	LMG	7	301	-	39,39,55	0.62	1 (2%)	47,47,63	1.00	2 (4%)
31	CLA	S	315	-	48,56,73	1.57	7 (14%)	55,92,113	2.13	15 (27%)
31	CLA	8	613	-	49,57,73	1.53	7 (14%)	55,93,113	2.24	16 (29%)
32	LUT	Y	315	-	42,43,43	6.00	28 (66%)	51,60,60	1.95	18 (35%)
31	CLA	s	313	19	56,64,73	1.46	7 (12%)	65,102,113	2.20	17 (26%)
32	LUT	s	317	-	42,43,43	6.07	28 (66%)	51,60,60	1.89	16 (31%)
34	LMG	b	622	-	51,51,55	1.09	6 (11%)	59,59,63	1.33	7 (11%)
48	LMU	r	302	-	36,36,36	0.38	0	47,47,47	0.78	0
30	CHL	Y	307	49	59,67,74	0.94	4 (6%)	64,105,114	1.38	12 (18%)
31	CLA	6	314	4	65,73,73	1.33	6 (9%)	76,113,113	2.00	17 (22%)
45	DGD	C	616	-	51,51,67	0.82	2 (3%)	65,65,81	1.00	2 (3%)
48	LMU	c	623	-	29,29,36	0.44	0	40,40,47	1.11	2 (5%)
32	LUT	2	615	-	42,43,43	5.91	28 (66%)	51,60,60	3.00	18 (35%)
31	CLA	2	610	33	60,68,73	1.38	7 (11%)	70,107,113	2.05	15 (21%)
31	CLA	A	406	49	65,73,73	1.34	8 (12%)	76,113,113	2.09	19 (25%)
36	NEX	n	319	-	38,46,46	3.30	9 (23%)	50,70,70	1.78	14 (28%)
32	LUT	8	615	-	42,43,43	6.09	28 (66%)	51,60,60	1.83	17 (33%)
30	CHL	Y	306	24	46,54,74	1.08	4 (8%)	49,90,114	1.46	12 (24%)
33	LHG	7	319	31	34,34,48	0.44	0	37,40,54	1.11	2 (5%)
31	CLA	R	311	18	58,66,73	1.44	7 (12%)	67,104,113	2.08	17 (25%)
34	LMG	n	322	-	40,40,55	0.71	3 (7%)	48,48,63	1.39	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	y	602	24	60,68,73	1.38	8 (13%)	70,107,113	2.07	18 (25%)
33	LHG	n	320	31	48,48,48	0.38	0	51,54,54	1.03	2 (3%)
38	SQD	B	620	-	53,54,54	0.77	0	62,65,65	0.91	2 (3%)
45	DGD	C	617	-	67,67,67	1.17	7 (10%)	81,81,81	0.92	3 (3%)
31	CLA	l	614	-	54,62,73	1.44	6 (11%)	62,99,113	2.14	17 (27%)
32	LUT	N	317	-	42,43,43	6.07	28 (66%)	51,60,60	2.10	14 (27%)
34	LMG	c	620	-	38,38,55	0.62	1 (2%)	46,46,63	1.18	5 (10%)
34	LMG	d	409	-	41,41,55	0.72	2 (4%)	49,49,63	1.08	3 (6%)
31	CLA	p	614	-	51,59,73	1.51	8 (15%)	59,96,113	2.24	17 (28%)
31	CLA	b	616	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	14 (18%)
31	CLA	s	311	19	65,73,73	1.35	7 (10%)	76,113,113	2.01	22 (28%)
37	XAT	R	318	-	39,47,47	0.64	0	54,74,74	1.94	14 (25%)
31	CLA	c	601	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	16 (21%)
31	CLA	o	611	33	60,68,73	1.41	8 (13%)	70,107,113	1.97	14 (20%)
34	LMG	b	629	-	38,38,55	0.63	1 (2%)	46,46,63	1.12	2 (4%)
31	CLA	Y	314	-	54,62,73	1.46	7 (12%)	62,99,113	2.16	17 (27%)
33	LHG	p	619	31	34,34,48	0.44	0	37,40,54	1.18	3 (8%)
38	SQD	A	413	-	44,45,54	0.84	0	53,56,65	0.96	2 (3%)
38	SQD	G	624	-	37,38,54	0.94	1 (2%)	46,49,65	1.04	2 (4%)
30	CHL	Y	301	49	63,71,74	0.87	3 (4%)	69,110,114	1.36	12 (17%)
33	LHG	2	617	31	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
31	CLA	3	306	49	55,63,73	1.45	8 (14%)	64,101,113	2.14	16 (25%)
38	SQD	x	201	-	41,42,54	0.88	1 (2%)	50,53,65	0.98	4 (8%)
31	CLA	8	614	3	54,62,73	1.46	8 (14%)	62,99,113	2.13	18 (29%)
31	CLA	4	603	-	55,63,73	1.46	7 (12%)	64,101,113	2.08	17 (26%)
31	CLA	3	311	-	54,62,73	1.50	8 (14%)	62,99,113	2.19	17 (27%)
32	LUT	8	616	-	42,43,43	6.07	28 (66%)	51,60,60	1.93	14 (27%)
34	LMG	k	101	-	48,48,55	0.99	5 (10%)	56,56,63	1.14	4 (7%)
31	CLA	b	615	-	65,73,73	1.32	8 (12%)	76,113,113	2.02	17 (22%)
31	CLA	9	312	2	54,62,73	1.46	8 (14%)	62,99,113	2.27	20 (32%)
31	CLA	R	304	18	60,68,73	1.41	7 (11%)	70,107,113	2.02	17 (24%)
30	CHL	q	309	-	57,65,74	1.14	5 (8%)	62,103,114	1.35	10 (16%)
31	CLA	p	611	33	60,68,73	1.41	8 (13%)	70,107,113	2.01	15 (21%)
30	CHL	n	310	3	66,74,74	0.86	3 (4%)	73,114,114	1.42	12 (16%)
31	CLA	q	313	33	44,51,73	1.76	7 (15%)	54,86,113	2.28	17 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	LMG	9	301	-	51,51,55	1.10	6 (11%)	59,59,63	1.68	8 (13%)
31	CLA	5	615	3	46,54,73	1.57	7 (15%)	53,90,113	2.30	16 (30%)
34	LMG	r	321	-	38,38,55	0.69	2 (5%)	46,46,63	1.27	4 (8%)
34	LMG	G	622	-	40,40,55	0.69	2 (5%)	48,48,63	1.09	4 (8%)
37	XAT	r	318	-	39,47,47	0.65	0	54,74,74	1.94	12 (22%)
31	CLA	C	613	-	65,73,73	1.33	8 (12%)	76,113,113	2.14	21 (27%)
42	PHO	d	402	-	51,69,69	0.56	0	47,99,99	0.71	0
34	LMG	R	321	-	38,38,55	0.63	1 (2%)	46,46,63	1.11	2 (4%)
30	CHL	y	601	24	66,74,74	0.81	2 (3%)	73,114,114	1.31	13 (17%)
43	BCR	c	615	-	41,41,41	4.78	25 (60%)	56,56,56	2.74	24 (42%)
30	CHL	g	307	49	50,58,74	1.02	3 (6%)	52,94,114	1.49	10 (19%)
31	CLA	c	605	-	65,73,73	1.36	7 (10%)	76,113,113	1.91	15 (19%)
34	LMG	B	622	-	38,38,55	0.64	1 (2%)	46,46,63	1.22	4 (8%)
34	LMG	B	621	-	51,51,55	1.08	6 (11%)	59,59,63	1.29	4 (6%)
30	CHL	p	606	-	51,59,74	0.90	2 (3%)	55,96,114	1.47	13 (23%)
31	CLA	R	305	-	60,68,73	1.41	7 (11%)	70,107,113	2.12	15 (21%)
31	CLA	1	613	1	65,73,73	1.35	8 (12%)	76,113,113	1.95	16 (21%)
36	NEX	r	319	-	38,46,46	3.39	11 (28%)	50,70,70	1.61	10 (20%)
31	CLA	Y	310	24	65,73,73	1.33	8 (12%)	76,113,113	1.96	16 (21%)
31	CLA	8	603	-	55,63,73	1.45	7 (12%)	64,101,113	2.15	16 (25%)
32	LUT	r	317	-	42,43,43	6.02	28 (66%)	51,60,60	2.07	20 (39%)
31	CLA	g	313	2	65,73,73	1.33	7 (10%)	76,113,113	1.95	18 (23%)
31	CLA	2	613	-	54,62,73	1.46	7 (12%)	62,99,113	2.20	18 (29%)
46	BCT	d	403	40	2,3,3	1.15	0	2,3,3	4.30	2 (100%)
31	CLA	b	613	-	65,73,73	1.32	7 (10%)	76,113,113	2.04	19 (25%)
30	CHL	Y	302	24	66,74,74	0.82	2 (3%)	73,114,114	1.34	14 (19%)
31	CLA	c	609	-	65,73,73	1.37	7 (10%)	76,113,113	2.00	20 (26%)
33	LHG	D	407	-	43,43,48	0.41	0	46,49,54	1.10	3 (6%)
30	CHL	y	607	49	66,74,74	0.85	3 (4%)	73,114,114	1.30	13 (17%)
34	LMG	a	401	-	38,38,55	0.62	1 (2%)	46,46,63	1.04	3 (6%)
34	LMG	1	618	-	38,38,55	0.62	1 (2%)	46,46,63	1.04	2 (4%)
31	CLA	B	607	49	65,73,73	1.40	8 (12%)	76,113,113	2.17	20 (26%)
30	CHL	9	309	-	53,61,74	0.99	4 (7%)	57,98,114	1.52	12 (21%)
36	NEX	6	319	-	38,46,46	3.37	11 (28%)	50,70,70	1.59	11 (22%)
30	CHL	g	302	2	66,74,74	0.84	3 (4%)	73,114,114	1.29	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	NEX	5	618	-	38,46,46	3.36	10 (26%)	50,70,70	1.56	9 (18%)
32	LUT	7	318	-	42,43,43	6.07	28 (66%)	51,60,60	1.88	12 (23%)
31	CLA	B	613	-	65,73,73	1.33	8 (12%)	76,113,113	1.91	17 (22%)
31	CLA	q	314	2	46,54,73	1.59	7 (15%)	53,90,113	2.14	13 (24%)
31	CLA	g	314	-	49,57,73	1.54	7 (14%)	55,93,113	2.25	17 (30%)
34	LMG	f	101	-	38,38,55	0.58	1 (2%)	46,46,63	1.13	2 (4%)
32	LUT	4	616	-	42,43,43	6.06	28 (66%)	51,60,60	2.18	13 (25%)
45	DGD	c	616	-	67,67,67	1.16	7 (10%)	81,81,81	1.07	2 (2%)
30	CHL	q	307	2	46,54,74	0.98	2 (4%)	49,90,114	1.49	11 (22%)
31	CLA	C	609	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	16 (21%)
31	CLA	r	311	18	58,66,73	1.43	7 (12%)	67,104,113	2.13	17 (25%)
30	CHL	2	607	49	50,58,74	0.98	3 (6%)	52,94,114	1.51	11 (21%)
31	CLA	9	314	2	50,58,73	1.54	7 (14%)	58,95,113	2.18	15 (25%)
38	SQD	0	621	-	41,42,54	0.86	0	50,53,65	0.96	3 (6%)
32	LUT	1	616	-	42,43,43	6.03	27 (64%)	51,60,60	1.89	16 (31%)
30	CHL	7	308	49	66,74,74	0.81	2 (3%)	73,114,114	1.27	13 (17%)
34	LMG	X	202	-	38,38,55	0.62	1 (2%)	46,46,63	1.06	2 (4%)
31	CLA	5	610	3	60,68,73	1.38	7 (11%)	70,107,113	2.08	17 (24%)
31	CLA	c	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.06	18 (23%)
30	CHL	1	609	1	66,74,74	0.88	4 (6%)	73,114,114	1.35	13 (17%)
31	CLA	C	612	-	55,63,73	1.47	8 (14%)	64,101,113	2.25	17 (26%)
31	CLA	Y	312	24	65,73,73	1.38	7 (10%)	76,113,113	1.97	17 (22%)
31	CLA	b	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	16 (21%)
34	LMG	d	410	-	51,51,55	1.07	6 (11%)	59,59,63	1.08	3 (5%)
30	CHL	9	311	2	61,69,74	0.85	2 (3%)	67,108,114	1.38	13 (19%)
31	CLA	4	610	2	60,68,73	1.40	7 (11%)	70,107,113	2.07	21 (30%)
34	LMG	6	321	-	42,42,55	0.77	2 (4%)	50,50,63	1.24	5 (10%)
37	XAT	G	620	-	39,47,47	0.65	0	54,74,74	1.91	13 (24%)
43	BCR	Z	101	-	41,41,41	4.77	26 (63%)	56,56,56	2.36	18 (32%)
30	CHL	s	308	49	43,51,74	1.01	3 (6%)	45,86,114	1.49	10 (22%)
33	LHG	C	623	-	39,39,48	0.42	0	42,45,54	1.21	4 (9%)
36	NEX	3	319	-	38,46,46	3.45	9 (23%)	50,70,70	1.67	12 (24%)
31	CLA	7	316	1	51,59,73	1.51	8 (15%)	59,96,113	2.21	17 (28%)
34	LMG	b	624	-	38,38,55	0.66	1 (2%)	46,46,63	1.33	7 (15%)
37	XAT	2	619	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	p	612	3	46,54,73	1.59	8 (17%)	53,90,113	2.13	15 (28%)
31	CLA	C	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.08	16 (21%)
31	CLA	g	310	2	65,73,73	1.35	8 (12%)	76,113,113	1.97	20 (26%)
30	CHL	8	606	49	58,66,74	0.93	3 (5%)	63,104,114	1.37	11 (17%)
31	CLA	b	612	-	65,73,73	1.33	6 (9%)	76,113,113	1.99	18 (23%)
32	LUT	5	616	-	42,43,43	6.10	27 (64%)	51,60,60	1.89	11 (21%)
31	CLA	S	314	19	65,73,73	1.35	8 (12%)	76,113,113	1.97	18 (23%)
31	CLA	A	409	-	60,68,73	1.39	8 (13%)	70,107,113	2.18	18 (25%)
31	CLA	y	603	-	55,63,73	1.45	8 (14%)	64,101,113	2.13	18 (28%)
31	CLA	S	312	33	65,73,73	1.35	7 (10%)	76,113,113	2.00	14 (18%)
30	CHL	4	606	31	51,59,74	0.93	2 (3%)	55,96,114	1.46	11 (20%)
30	CHL	S	307	19	44,52,74	1.05	3 (6%)	46,87,114	1.50	9 (19%)
30	CHL	8	607	49	50,58,74	0.95	2 (4%)	52,94,114	1.51	12 (23%)
31	CLA	c	608	-	65,73,73	1.36	7 (10%)	76,113,113	1.90	19 (25%)
30	CHL	q	308	-	51,59,74	1.02	4 (7%)	55,96,114	1.54	9 (16%)
31	CLA	s	304	-	42,50,73	1.65	6 (14%)	48,85,113	2.26	15 (31%)
34	LMG	W	201	-	55,55,55	1.18	6 (10%)	63,63,63	1.20	4 (6%)
31	CLA	q	306	49	55,63,73	1.47	7 (12%)	64,101,113	2.09	18 (28%)
31	CLA	r	314	-	49,57,73	1.59	7 (14%)	55,93,113	2.19	16 (29%)
36	NEX	s	319	-	38,46,46	3.46	10 (26%)	50,70,70	1.56	10 (20%)
31	CLA	2	603	-	55,63,73	1.45	7 (12%)	64,101,113	2.10	17 (26%)
36	NEX	0	618	-	38,46,46	3.37	10 (26%)	50,70,70	1.59	11 (22%)
32	LUT	p	617	-	42,43,43	6.06	29 (69%)	51,60,60	2.82	20 (39%)
34	LMG	g	320	-	38,38,55	0.62	1 (2%)	46,46,63	1.12	4 (8%)
34	LMG	D	412	-	48,48,55	0.99	5 (10%)	56,56,63	1.11	2 (3%)
30	CHL	1	605	1	66,74,74	0.87	3 (4%)	73,114,114	1.29	9 (12%)
37	XAT	9	322	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
31	CLA	5	614	-	51,59,73	1.51	8 (15%)	59,96,113	2.26	17 (28%)
31	CLA	C	602	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
31	CLA	s	315	-	48,56,73	1.56	7 (14%)	55,92,113	2.13	14 (25%)
31	CLA	s	305	49	65,73,73	1.33	8 (12%)	76,113,113	2.02	16 (21%)
33	LHG	D	408	-	48,48,48	0.39	0	51,54,54	1.08	4 (7%)
43	BCR	H	101	-	41,41,41	4.74	26 (63%)	56,56,56	2.38	20 (35%)
31	CLA	n	313	3	45,53,73	1.59	7 (15%)	52,89,113	2.17	13 (25%)
30	CHL	2	606	-	51,59,74	0.91	2 (3%)	55,96,114	1.49	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	LMG	g	322	-	49,49,55	1.03	5 (10%)	57,57,63	1.22	2 (3%)
31	CLA	6	304	-	56,64,73	1.45	8 (14%)	65,102,113	2.13	19 (29%)
33	LHG	z	102	-	35,35,48	0.43	0	38,41,54	1.20	3 (7%)
36	NEX	R	301	-	38,46,46	3.42	11 (28%)	50,70,70	1.56	9 (18%)
43	BCR	B	619	-	41,41,41	4.74	25 (60%)	56,56,56	2.46	21 (37%)
33	LHG	y	619	31	45,45,48	0.43	0	48,51,54	1.05	3 (6%)
31	CLA	1	612	1	65,73,73	1.37	7 (10%)	76,113,113	1.92	16 (21%)
31	CLA	B	604	-	65,73,73	1.38	8 (12%)	76,113,113	2.13	17 (22%)
31	CLA	G	611	2	43,51,73	1.66	6 (13%)	49,86,113	2.21	15 (30%)
31	CLA	a	406	-	65,73,73	1.35	7 (10%)	76,113,113	2.03	15 (19%)
31	CLA	1	603	-	55,63,73	1.50	8 (14%)	64,101,113	2.08	15 (23%)
43	BCR	b	620	-	41,41,41	4.75	25 (60%)	56,56,56	2.33	20 (35%)
38	SQD	Y	320	-	41,42,54	0.87	0	50,53,65	0.99	2 (4%)
30	CHL	5	605	3	46,54,74	0.98	2 (4%)	49,90,114	1.43	12 (24%)
48	LMU	K	101	-	36,36,36	0.42	0	47,47,47	1.10	4 (8%)
30	CHL	6	310	4	61,69,74	0.89	3 (4%)	67,108,114	1.35	14 (20%)
30	CHL	3	302	49	57,65,74	1.08	5 (8%)	62,103,114	1.55	14 (22%)
30	CHL	0	601	4	56,64,74	0.92	3 (5%)	61,102,114	1.43	13 (21%)
31	CLA	7	315	-	54,62,73	1.45	6 (11%)	62,99,113	2.12	17 (27%)
30	CHL	3	307	3	46,54,74	1.01	3 (6%)	49,90,114	1.50	11 (22%)
38	SQD	g	318	-	41,42,54	0.88	0	50,53,65	0.96	2 (4%)
30	CHL	9	308	-	52,60,74	0.97	3 (5%)	56,97,114	1.45	12 (21%)
31	CLA	s	306	-	50,58,73	1.51	7 (14%)	58,95,113	2.30	17 (29%)
31	CLA	4	613	2	61,69,73	1.40	7 (11%)	71,108,113	2.00	18 (25%)
30	CHL	5	607	-	51,59,74	1.02	4 (7%)	55,96,114	1.40	10 (18%)
31	CLA	B	614	-	65,73,73	1.34	8 (12%)	76,113,113	1.96	17 (22%)
30	CHL	N	309	3	66,74,74	0.84	3 (4%)	73,114,114	1.38	13 (17%)
30	CHL	2	608	2	57,65,74	0.95	4 (7%)	62,103,114	1.46	13 (20%)
31	CLA	2	611	2	55,63,73	1.44	7 (12%)	64,101,113	2.08	17 (26%)
31	CLA	G	612	2	65,73,73	1.35	8 (12%)	76,113,113	2.01	17 (22%)
31	CLA	S	303	19	65,73,73	1.33	8 (12%)	76,113,113	2.02	19 (25%)
34	LMG	X	203	-	38,38,55	0.61	1 (2%)	46,46,63	1.12	2 (4%)
30	CHL	G	623	49	66,74,74	0.85	3 (4%)	73,114,114	1.31	13 (17%)
30	CHL	3	303	3	50,58,74	0.97	3 (6%)	52,94,114	1.51	12 (23%)
30	CHL	y	606	49	59,67,74	0.90	3 (5%)	64,105,114	1.36	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	SQD	6	301	-	41,42,54	0.87	0	50,53,65	1.00	2 (4%)
34	LMG	G	621	-	51,51,55	1.07	6 (11%)	59,59,63	1.07	3 (5%)
31	CLA	B	612	-	65,73,73	1.32	7 (10%)	76,113,113	1.98	17 (22%)
43	BCR	B	618	-	41,41,41	4.77	25 (60%)	56,56,56	2.19	20 (35%)
30	CHL	q	311	2	56,64,74	0.89	3 (5%)	61,102,114	1.33	11 (18%)
31	CLA	b	605	-	65,73,73	1.38	8 (12%)	76,113,113	2.04	17 (22%)
30	CHL	7	307	49	66,74,74	0.88	3 (4%)	73,114,114	1.36	13 (17%)
31	CLA	0	604	49	55,63,73	1.46	7 (12%)	64,101,113	2.18	15 (23%)
31	CLA	3	316	3	57,65,73	1.46	8 (14%)	66,103,113	2.13	19 (28%)
34	LMG	j	101	-	43,43,55	0.82	2 (4%)	51,51,63	1.03	3 (5%)
38	SQD	a	411	-	47,48,54	0.82	0	56,59,65	0.97	2 (3%)
38	SQD	y	621	-	41,42,54	0.87	0	50,53,65	1.00	2 (4%)
37	XAT	g	321	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
34	LMG	2	620	-	51,51,55	1.06	5 (9%)	59,59,63	1.06	3 (5%)
36	NEX	g	317	31	38,46,46	3.36	11 (28%)	50,70,70	1.67	10 (20%)
32	LUT	R	317	-	42,43,43	6.05	27 (64%)	51,60,60	2.98	15 (29%)
32	LUT	6	318	-	42,43,43	6.06	28 (66%)	51,60,60	1.94	12 (23%)
31	CLA	D	404	-	65,73,73	1.33	8 (12%)	76,113,113	2.12	19 (25%)
34	LMG	c	624	-	44,44,55	0.86	3 (6%)	52,52,63	1.05	3 (5%)
30	CHL	9	303	2	66,74,74	0.83	3 (4%)	73,114,114	1.29	12 (16%)
34	LMG	a	416	-	38,38,55	0.61	1 (2%)	46,46,63	1.06	3 (6%)
30	CHL	8	601	3	56,64,74	0.92	3 (5%)	61,102,114	1.44	13 (21%)
34	LMG	s	321	-	41,41,55	0.85	2 (4%)	49,49,63	1.28	5 (10%)
35	RRX	9	317	-	42,42,42	5.01	25 (59%)	57,58,58	2.49	22 (38%)
30	CHL	3	309	-	50,58,74	1.10	4 (8%)	52,94,114	1.44	9 (17%)
43	BCR	v	101	-	41,41,41	4.75	25 (60%)	56,56,56	2.24	18 (32%)
34	LMG	9	302	-	40,40,55	0.68	2 (5%)	48,48,63	1.09	3 (6%)
30	CHL	6	307	49	51,59,74	0.90	2 (3%)	55,96,114	1.45	11 (20%)
31	CLA	B	603	-	65,73,73	1.37	7 (10%)	76,113,113	1.95	16 (21%)
33	LHG	d	408	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
34	LMG	D	410	-	46,46,55	0.93	3 (6%)	54,54,63	1.07	4 (7%)
31	CLA	g	304	-	55,63,73	1.45	7 (12%)	64,101,113	2.13	16 (25%)
34	LMG	A	414	-	38,38,55	0.64	1 (2%)	46,46,63	1.14	4 (8%)
30	CHL	6	308	49	66,74,74	0.84	3 (4%)	73,114,114	1.24	12 (16%)
31	CLA	g	311	33	60,68,73	1.44	8 (13%)	70,107,113	2.02	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	r	315	18	55,63,73	1.45	8 (14%)	64,101,113	2.26	20 (31%)
31	CLA	q	312	2	54,61,73	1.60	7 (12%)	66,98,113	2.27	20 (30%)
31	CLA	N	315	3	54,62,73	1.46	7 (12%)	62,99,113	2.16	17 (27%)
31	CLA	r	303	18	49,57,73	1.58	7 (14%)	55,93,113	2.39	17 (30%)
33	LHG	b	628	-	48,48,48	0.40	0	51,54,54	1.11	3 (5%)
48	LMU	R	302	-	36,36,36	0.44	0	47,47,47	0.95	2 (4%)
31	CLA	b	609	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	16 (21%)
30	CHL	n	301	49	50,58,74	0.99	3 (6%)	52,94,114	1.45	12 (23%)
30	CHL	y	608	49	50,58,74	1.00	3 (6%)	52,94,114	1.54	12 (23%)
31	CLA	C	601	-	65,73,73	1.37	8 (12%)	76,113,113	1.96	16 (21%)
33	LHG	A	417	-	38,38,48	0.45	0	41,44,54	1.09	3 (7%)
30	CHL	7	309	49	50,58,74	0.99	3 (6%)	52,94,114	1.53	11 (21%)
30	CHL	4	607	-	57,65,74	0.98	5 (8%)	62,103,114	1.40	11 (17%)
43	BCR	t	101	-	41,41,41	4.71	25 (60%)	56,56,56	3.99	27 (48%)
31	CLA	g	305	49,36	55,63,73	1.44	8 (14%)	64,101,113	2.15	15 (23%)
37	XAT	q	321	-	39,47,47	0.65	0	54,74,74	1.91	13 (24%)
31	CLA	7	311	1	65,73,73	1.32	8 (12%)	76,113,113	1.96	17 (22%)
31	CLA	7	303	1	60,68,73	1.38	7 (11%)	70,107,113	2.02	17 (24%)
31	CLA	0	612	4	46,54,73	1.62	8 (17%)	53,90,113	2.11	15 (28%)
34	LMG	p	620	-	38,38,55	0.62	1 (2%)	46,46,63	1.10	4 (8%)
30	CHL	1	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.26	13 (17%)
31	CLA	5	603	-	52,60,73	1.48	6 (11%)	60,97,113	2.25	18 (30%)
31	CLA	7	314	1	65,73,73	1.34	8 (12%)	76,113,113	1.95	19 (25%)
31	CLA	8	604	49,36	65,73,73	1.32	7 (10%)	76,113,113	2.02	17 (22%)
31	CLA	D	403	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	16 (21%)
33	LHG	l	101	-	48,48,48	0.39	0	51,54,54	1.03	3 (5%)
43	BCR	D	405	-	41,41,41	4.84	27 (65%)	56,56,56	2.69	22 (39%)
31	CLA	8	610	33	49,57,73	1.53	8 (16%)	55,93,113	2.21	15 (27%)
31	CLA	p	615	3	46,54,73	1.59	8 (17%)	53,90,113	2.11	13 (24%)
31	CLA	r	307	49	48,56,73	1.61	7 (14%)	55,92,113	2.13	15 (27%)
31	CLA	7	313	1	65,73,73	1.36	7 (10%)	76,113,113	1.93	18 (23%)
30	CHL	0	608	49	50,58,74	1.01	3 (6%)	52,94,114	1.54	11 (21%)
30	CHL	G	605	2	48,56,74	0.98	2 (4%)	51,92,114	1.50	13 (25%)
30	CHL	p	609	3	56,64,74	0.94	4 (7%)	61,102,114	1.41	12 (19%)
31	CLA	9	313	33	47,55,73	1.60	8 (17%)	54,91,113	2.14	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	CLA	s	316	19	46,54,73	1.59	8 (17%)	53,90,113	2.16	15 (28%)
43	BCR	C	615	-	41,41,41	4.70	25 (60%)	56,56,56	4.03	31 (55%)
33	LHG	G	618	31	43,43,48	0.40	0	46,49,54	1.10	3 (6%)
30	CHL	R	310	49	55,63,74	1.05	4 (7%)	59,100,114	1.37	11 (18%)
31	CLA	B	605	-	65,73,73	1.35	6 (9%)	76,113,113	2.02	16 (21%)
43	BCR	B	617	-	41,41,41	4.69	26 (63%)	56,56,56	2.52	22 (39%)
34	LMG	J	101	-	51,51,55	1.08	6 (11%)	59,59,63	1.08	3 (5%)
31	CLA	b	602	49	49,57,73	1.56	7 (14%)	55,93,113	2.23	13 (23%)
30	CHL	S	308	49	43,51,74	1.18	4 (9%)	45,86,114	1.54	11 (24%)
31	CLA	l	604	49	65,73,73	1.35	7 (10%)	76,113,113	2.06	18 (23%)
34	LMG	b	623	-	38,38,55	0.62	1 (2%)	46,46,63	1.09	2 (4%)
30	CHL	n	309	49	50,58,74	0.95	2 (4%)	52,94,114	1.51	12 (23%)
30	CHL	G	607	49	51,59,74	0.98	2 (3%)	55,96,114	1.46	13 (23%)
34	LMG	C	624	-	44,44,55	0.88	3 (6%)	52,52,63	1.05	2 (3%)
32	LUT	y	617	-	42,43,43	6.02	28 (66%)	51,60,60	2.00	17 (33%)
31	CLA	n	315	-	49,57,73	1.53	7 (14%)	55,93,113	2.25	16 (29%)
30	CHL	R	308	18	56,64,74	0.95	3 (5%)	61,102,114	1.41	12 (19%)
34	LMG	0	622	-	38,38,55	0.65	1 (2%)	46,46,63	1.13	3 (6%)
33	LHG	N	319	31	48,48,48	0.38	0	51,54,54	1.02	2 (3%)
42	PHO	a	408	-	51,69,69	0.52	0	47,99,99	0.59	0
31	CLA	6	313	4	60,68,73	1.40	8 (13%)	70,107,113	2.01	16 (22%)
31	CLA	N	313	3	65,73,73	1.33	7 (10%)	76,113,113	1.95	16 (21%)
30	CHL	N	301	-	50,58,74	1.01	3 (6%)	52,94,114	1.42	11 (21%)
33	LHG	l	617	31	34,34,48	0.44	0	37,40,54	1.17	3 (8%)
31	CLA	c	604	49	56,64,73	1.44	7 (12%)	65,102,113	2.15	17 (26%)
31	CLA	Y	311	33	65,73,73	1.37	7 (10%)	76,113,113	1.91	14 (18%)
30	CHL	0	609	4	61,69,74	0.91	4 (6%)	67,108,114	1.41	13 (19%)
31	CLA	S	313	19	56,64,73	1.47	7 (12%)	65,102,113	2.22	20 (30%)
33	LHG	6	320	31	36,36,48	0.44	0	39,42,54	1.19	3 (7%)
31	CLA	R	316	18	65,73,73	1.35	8 (12%)	76,113,113	2.05	17 (22%)
33	LHG	s	322	-	43,43,48	0.40	0	46,49,54	1.14	3 (6%)
31	CLA	B	610	49	65,73,73	1.34	7 (10%)	76,113,113	2.01	18 (23%)
32	LUT	0	617	-	42,43,43	6.02	28 (66%)	51,60,60	1.96	14 (27%)
31	CLA	y	612	24	65,73,73	1.36	7 (10%)	76,113,113	1.98	16 (21%)
31	CLA	b	611	49	65,73,73	1.34	8 (12%)	76,113,113	1.96	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CHL	p	605	3	46,54,74	0.98	2 (4%)	49,90,114	1.50	11 (22%)
39	OEX	a	402	7,5	0,15,15	-	-	-		
31	CLA	d	405	-	65,73,73	1.33	8 (12%)	76,113,113	2.10	19 (25%)
34	LMG	d	411	-	48,48,55	0.99	5 (10%)	56,56,63	1.15	3 (5%)
32	LUT	5	617	-	42,43,43	6.08	27 (64%)	51,60,60	1.87	12 (23%)
43	BCR	c	614	-	41,41,41	4.75	26 (63%)	56,56,56	2.96	25 (44%)
31	CLA	S	306	-	50,58,73	1.52	7 (14%)	58,95,113	2.27	16 (27%)
31	CLA	s	303	19	65,73,73	1.33	8 (12%)	76,113,113	2.01	20 (26%)
35	RRX	G	614	-	42,42,42	5.01	25 (59%)	57,58,58	2.49	22 (38%)
31	CLA	c	612	-	55,63,73	1.46	8 (14%)	64,101,113	2.23	18 (28%)
30	CHL	5	608	-	50,58,74	0.93	2 (4%)	52,94,114	1.51	12 (23%)
36	NEX	y	618	-	38,46,46	3.41	11 (28%)	50,70,70	1.59	11 (22%)
31	CLA	a	407	49	65,73,73	1.35	8 (12%)	76,113,113	2.04	18 (23%)
38	SQD	g	301	-	37,38,54	0.91	0	46,49,65	1.01	2 (4%)
30	CHL	g	309	2	63,71,74	0.90	4 (6%)	69,110,114	1.44	13 (18%)
30	CHL	r	308	18	56,64,74	0.98	4 (7%)	61,102,114	1.40	13 (21%)
33	LHG	S	322	-	43,43,48	0.41	0	46,49,54	1.08	3 (6%)
31	CLA	C	604	49	56,64,73	1.45	7 (12%)	65,102,113	2.17	16 (24%)
30	CHL	8	605	3	66,74,74	0.85	3 (4%)	73,114,114	1.31	14 (19%)
31	CLA	a	409	-	60,68,73	1.38	8 (13%)	70,107,113	2.17	18 (25%)
31	CLA	R	307	49	48,56,73	1.61	8 (16%)	55,92,113	2.15	14 (25%)
30	CHL	g	306	2	48,56,74	1.00	3 (6%)	51,92,114	1.50	11 (21%)
30	CHL	3	308	-	47,55,74	1.05	3 (6%)	50,91,114	1.39	9 (18%)
31	CLA	0	614	-	54,62,73	1.45	7 (12%)	62,99,113	2.17	19 (30%)
31	CLA	7	312	33	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
34	LMG	m	102	-	45,45,55	0.91	3 (6%)	53,53,63	1.25	5 (9%)
33	LHG	0	619	31	35,35,48	0.44	0	38,41,54	1.20	4 (10%)
31	CLA	1	611	33	65,73,73	1.34	8 (12%)	76,113,113	1.93	17 (22%)
31	CLA	3	314	3	55,63,73	1.46	8 (14%)	64,101,113	2.10	18 (28%)
38	SQD	m	101	-	49,50,54	0.82	0	58,61,65	0.96	2 (3%)
30	CHL	9	307	2	46,54,74	1.02	2 (4%)	49,90,114	1.43	9 (18%)
34	LMG	5	620	-	38,38,55	0.63	1 (2%)	46,46,63	1.09	2 (4%)
32	LUT	s	318	-	42,43,43	6.04	28 (66%)	51,60,60	1.92	15 (29%)
43	BCR	C	614	-	41,41,41	4.70	25 (60%)	56,56,56	2.59	23 (41%)
31	CLA	p	613	-	54,62,73	1.45	8 (14%)	62,99,113	2.11	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LHG	5	619	31	34,34,48	0.46	0	37,40,54	1.14	3 (8%)
31	CLA	s	310	19	60,68,73	1.41	8 (13%)	70,107,113	2.09	15 (21%)
31	CLA	N	311	33	49,57,73	1.54	7 (14%)	55,93,113	2.24	15 (27%)
31	CLA	N	303	3	65,73,73	1.33	8 (12%)	76,113,113	1.98	19 (25%)
30	CHL	4	609	2	57,65,74	0.91	3 (5%)	62,103,114	1.47	14 (22%)
34	LMG	w	201	-	48,48,55	1.00	5 (10%)	56,56,63	1.08	3 (5%)
30	CHL	2	601	2	66,74,74	0.86	3 (4%)	73,114,114	1.28	13 (17%)
36	NEX	r	301	-	38,46,46	3.37	9 (23%)	50,70,70	1.69	12 (24%)
32	LUT	p	616	-	42,43,43	6.09	27 (64%)	51,60,60	2.78	18 (35%)
38	SQD	r	322	-	50,51,54	0.80	0	59,62,65	0.93	2 (3%)
30	CHL	2	605	2	46,54,74	0.99	2 (4%)	49,90,114	1.48	12 (24%)
31	CLA	y	615	24	54,62,73	1.47	8 (14%)	62,99,113	2.23	18 (29%)
38	SQD	A	411	-	50,51,54	0.80	0	59,62,65	0.97	3 (5%)
31	CLA	c	602	-	65,73,73	1.36	7 (10%)	76,113,113	2.00	16 (21%)
35	RRX	q	317	-	42,42,42	4.96	25 (59%)	57,58,58	2.57	19 (33%)
31	CLA	4	604	30	51,59,73	1.50	7 (13%)	59,96,113	2.28	16 (27%)
31	CLA	S	310	19	60,68,73	1.41	8 (13%)	70,107,113	2.05	16 (22%)
31	CLA	2	609	2	60,68,73	1.39	8 (13%)	70,107,113	2.06	19 (27%)
32	LUT	q	318	-	42,43,43	6.07	28 (66%)	51,60,60	2.12	14 (27%)
33	LHG	c	622	-	46,46,48	0.40	0	49,52,54	1.01	2 (4%)
31	CLA	A	407	49	49,57,73	1.55	7 (14%)	55,93,113	2.28	19 (34%)
31	CLA	b	614	-	65,73,73	1.32	7 (10%)	76,113,113	1.96	17 (22%)
31	CLA	b	607	-	65,73,73	1.36	7 (10%)	76,113,113	2.05	16 (21%)
30	CHL	5	606	49	51,59,74	0.95	2 (3%)	55,96,114	1.49	12 (21%)
31	CLA	3	304	3	60,68,73	1.38	7 (11%)	70,107,113	2.08	17 (24%)
31	CLA	8	609	3	65,73,73	1.33	7 (10%)	76,113,113	1.99	17 (22%)
32	LUT	N	316	-	42,43,43	6.09	28 (66%)	51,60,60	2.01	12 (23%)
31	CLA	b	617	-	65,73,73	1.39	7 (10%)	76,113,113	1.99	17 (22%)
32	LUT	0	616	-	42,43,43	6.02	27 (64%)	51,60,60	1.99	17 (33%)
31	CLA	0	613	4	56,64,73	1.46	8 (14%)	65,102,113	2.10	18 (27%)
34	LMG	2	618	-	38,38,55	0.62	1 (2%)	46,46,63	1.11	3 (6%)
31	CLA	p	603	-	55,63,73	1.48	8 (14%)	64,101,113	2.22	18 (28%)
32	LUT	1	615	-	42,43,43	6.01	27 (64%)	51,60,60	2.01	18 (35%)
31	CLA	9	306	49,36	65,73,73	1.33	7 (10%)	76,113,113	2.05	17 (22%)
30	CHL	r	310	49	55,63,74	1.01	3 (5%)	59,100,114	1.39	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LHG	Y	318	31	41,41,48	0.45	0	44,47,54	1.07	3 (6%)
31	CLA	N	312	3	45,53,73	1.60	8 (17%)	52,89,113	2.11	15 (28%)
34	LMG	W	202	-	38,38,55	0.64	1 (2%)	46,46,63	1.25	5 (10%)
36	NEX	8	617	31	38,46,46	3.38	11 (28%)	50,70,70	1.65	12 (24%)
38	SQD	b	627	-	51,52,54	0.87	0	60,63,65	1.02	2 (3%)
31	CLA	9	315	2	55,63,73	1.45	7 (12%)	64,101,113	2.07	16 (25%)
30	CHL	q	310	-	50,58,74	1.07	4 (8%)	52,94,114	1.56	12 (23%)
34	LMG	W	203	-	38,38,55	0.64	1 (2%)	46,46,63	1.12	2 (4%)
36	NEX	S	319	-	38,46,46	3.44	10 (26%)	50,70,70	1.55	11 (22%)
33	LHG	B	624	-	48,48,48	0.37	0	51,54,54	0.98	2 (3%)
34	LMG	y	620	-	38,38,55	0.60	1 (2%)	46,46,63	1.13	3 (6%)
31	CLA	9	304	2	65,73,73	1.33	7 (10%)	76,113,113	2.05	18 (23%)
34	LMG	Y	319	-	38,38,55	0.64	1 (2%)	46,46,63	1.12	3 (6%)
34	LMG	w	205	-	38,38,55	0.62	1 (2%)	46,46,63	1.13	2 (4%)
31	CLA	n	303	3	65,73,73	1.32	8 (12%)	76,113,113	1.98	19 (25%)
34	LMG	w	202	-	55,55,55	1.14	6 (10%)	63,63,63	1.13	3 (4%)
31	CLA	9	316	-	46,54,73	1.58	8 (17%)	53,90,113	2.12	14 (26%)
31	CLA	n	314	3	65,73,73	1.33	8 (12%)	76,113,113	1.95	17 (22%)
30	CHL	q	303	2	66,74,74	0.84	3 (4%)	73,114,114	1.24	12 (16%)
32	LUT	S	317	-	42,43,43	6.08	27 (64%)	51,60,60	1.94	13 (25%)
31	CLA	A	405	-	65,73,73	1.34	7 (10%)	76,113,113	2.06	20 (26%)
31	CLA	B	608	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
31	CLA	b	606	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	16 (21%)
31	CLA	r	312	18	57,65,73	1.45	7 (12%)	66,103,113	2.13	18 (27%)
32	LUT	G	615	-	42,43,43	6.12	28 (66%)	51,60,60	6.98	17 (33%)
30	CHL	s	302	19	46,54,74	0.99	2 (4%)	49,90,114	1.38	10 (20%)
31	CLA	G	610	33	60,68,73	1.41	8 (13%)	70,107,113	1.99	15 (21%)
34	LMG	I	101	-	38,38,55	0.62	1 (2%)	46,46,63	1.10	2 (4%)
36	NEX	N	318	-	38,46,46	3.36	11 (28%)	50,70,70	1.79	14 (28%)
34	LMG	9	321	-	38,38,55	0.65	1 (2%)	46,46,63	1.14	4 (8%)
30	CHL	y	609	24	66,74,74	0.85	3 (4%)	73,114,114	1.31	10 (13%)
31	CLA	3	312	33	65,73,73	1.35	8 (12%)	76,113,113	1.94	15 (19%)
31	CLA	6	305	49	55,63,73	1.44	7 (12%)	64,101,113	2.18	17 (26%)
30	CHL	7	321	49	63,71,74	0.84	2 (3%)	69,110,114	1.38	12 (17%)
30	CHL	r	309	18	56,64,74	0.89	2 (3%)	61,102,114	1.36	9 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	CHL	5	601	3	51,59,74	0.93	2 (3%)	55,96,114	1.47	12 (21%)
31	CLA	6	315	-	54,62,73	1.45	7 (12%)	62,99,113	2.21	17 (27%)
31	CLA	q	304	2	65,73,73	1.33	8 (12%)	76,113,113	2.01	18 (23%)
31	CLA	6	316	4	55,63,73	1.44	6 (10%)	64,101,113	2.16	18 (28%)
30	CHL	3	310	3	61,69,74	0.88	3 (4%)	67,108,114	1.41	12 (17%)
33	LHG	g	319	31	43,43,48	0.40	0	46,49,54	1.13	4 (8%)
31	CLA	7	304	-	55,63,73	1.46	8 (14%)	64,101,113	2.12	18 (28%)
34	LMG	w	204	-	38,38,55	0.65	1 (2%)	46,46,63	1.11	4 (8%)
30	CHL	N	308	49	50,58,74	0.98	3 (6%)	52,94,114	1.50	11 (21%)
43	BCR	T	101	-	41,41,41	4.76	27 (65%)	56,56,56	2.30	19 (33%)
34	LMG	4	620	-	51,51,55	1.06	5 (9%)	59,59,63	1.07	3 (5%)
30	CHL	4	605	2	46,54,74	0.99	2 (4%)	49,90,114	1.45	11 (22%)
37	XAT	4	619	-	39,47,47	0.64	0	54,74,74	1.91	13 (24%)
30	CHL	N	302	3	56,64,74	0.92	3 (5%)	61,102,114	1.47	13 (21%)
34	LMG	D	411	-	51,51,55	1.07	6 (11%)	59,59,63	1.08	3 (5%)
31	CLA	R	314	-	49,57,73	1.57	7 (14%)	55,93,113	2.19	16 (29%)
30	CHL	n	302	3	56,64,74	0.92	3 (5%)	61,102,114	1.44	13 (21%)
30	CHL	S	302	19	46,54,74	1.00	2 (4%)	49,90,114	1.42	10 (20%)
31	CLA	q	305	-	55,63,73	1.44	7 (12%)	64,101,113	2.13	16 (25%)
32	LUT	3	317	-	42,43,43	6.08	28 (66%)	51,60,60	1.88	12 (23%)
38	SQD	X	201	-	37,38,54	0.91	0	46,49,65	1.02	2 (4%)
31	CLA	b	608	49	65,73,73	1.34	8 (12%)	76,113,113	2.07	17 (22%)
31	CLA	n	316	3	54,62,73	1.47	8 (14%)	62,99,113	2.14	18 (29%)
31	CLA	s	314	19	65,73,73	1.36	8 (12%)	76,113,113	2.00	18 (23%)
43	BCR	b	618	-	41,41,41	4.69	25 (60%)	56,56,56	2.52	23 (41%)
33	LHG	b	625	-	43,43,48	0.41	0	46,49,54	1.07	3 (6%)
30	CHL	8	608	3	66,74,74	0.82	3 (4%)	73,114,114	1.38	12 (16%)
32	LUT	n	317	-	42,43,43	6.09	28 (66%)	51,60,60	1.83	17 (33%)
31	CLA	q	316	-	50,58,73	1.55	8 (16%)	58,95,113	2.24	16 (27%)
31	CLA	C	605	-	65,73,73	1.43	9 (13%)	76,113,113	1.96	15 (19%)
34	LMG	2	621	-	40,40,55	0.67	2 (5%)	48,48,63	1.16	4 (8%)
34	LMG	q	301	-	51,51,55	1.07	5 (9%)	59,59,63	1.16	5 (8%)
31	CLA	S	304	-	42,50,73	1.70	7 (16%)	48,85,113	2.13	16 (33%)
30	CHL	G	606	49	50,58,74	0.99	3 (6%)	52,94,114	1.44	12 (23%)
31	CLA	G	602	2	65,73,73	1.34	8 (12%)	76,113,113	1.95	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
33	LHG	j	102	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
34	LMG	C	622	-	32,32,55	0.48	0	40,40,63	1.08	2 (5%)
30	CHL	1	619	-	61,69,74	1.16	5 (8%)	67,108,114	1.53	14 (20%)
45	DGD	c	619	-	67,67,67	1.16	7 (10%)	81,81,81	1.02	3 (3%)
33	LHG	L	101	-	48,48,48	0.39	0	51,54,54	1.02	3 (5%)
30	CHL	0	606	49	51,59,74	0.95	2 (3%)	55,96,114	1.43	9 (16%)
31	CLA	R	315	18	55,63,73	1.47	7 (12%)	64,101,113	2.18	18 (28%)
32	LUT	n	318	-	42,43,43	6.07	28 (66%)	51,60,60	1.94	13 (25%)
31	CLA	y	604	49	55,63,73	1.46	7 (12%)	64,101,113	2.19	18 (28%)
31	CLA	C	607	49	65,73,73	1.38	8 (12%)	76,113,113	2.01	19 (25%)
31	CLA	p	604	36	50,58,73	1.54	10 (20%)	58,95,113	2.24	17 (29%)
31	CLA	Y	313	24	65,73,73	1.36	8 (12%)	76,113,113	1.99	18 (23%)
31	CLA	B	602	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	18 (23%)
31	CLA	N	310	3	65,73,73	1.34	8 (12%)	76,113,113	2.01	18 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	R	309	18	3/3/18/26	6/27/125/137	-
31	CLA	y	613	24	1/1/15/20	17/37/115/115	-
31	CLA	c	611	7	1/1/15/20	15/37/115/115	-
38	SQD	B	623	-	-	20/47/67/69	0/1/1/1
30	CHL	n	308	49	3/3/19/26	12/36/134/137	-
31	CLA	S	305	49	1/1/15/20	11/37/115/115	-
31	CLA	R	303	18	1/1/11/20	9/18/96/115	-
31	CLA	3	313	3	1/1/12/20	11/19/97/115	-
31	CLA	1	610	1	1/1/15/20	19/37/115/115	-
30	CHL	s	309	49	3/3/16/26	2/19/117/137	-
43	BCR	h	101	-	-	9/29/63/63	0/2/2/2
30	CHL	4	601	2	3/3/20/26	12/39/137/137	-
34	LMG	A	418	-	-	11/33/53/70	0/1/1/1
31	CLA	5	612	3	1/1/12/20	8/19/97/115	-
31	CLA	0	615	-	1/1/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	4	621	-	-	11/35/55/70	0/1/1/1
31	CLA	S	316	19	1/1/11/20	7/15/93/115	-
38	SQD	s	301	-	-	16/46/66/69	0/1/1/1
31	CLA	p	610	3	1/1/13/20	15/27/105/115	-
31	CLA	b	610	-	1/1/15/20	20/37/115/115	-
31	CLA	C	611	7	1/1/15/20	15/37/115/115	-
30	CHL	1	606	49	3/3/20/26	16/39/137/137	-
45	DGD	c	618	-	-	19/55/95/95	0/2/2/2
34	LMG	q1	101	-	-	7/33/53/70	0/1/1/1
30	CHL	6	309	49	3/3/16/26	2/20/118/137	-
33	LHG	9	320	31	-	24/37/37/53	-
33	LHG	a	415	-	-	23/43/43/53	-
34	LMG	k	102	-	-	10/33/53/70	0/1/1/1
31	CLA	n	304	-	1/1/13/20	13/25/103/115	-
31	CLA	4	611	33	1/1/11/20	5/13/89/115	-
31	CLA	g	312	2	1/1/10/20	3/11/89/115	-
34	LMG	c	621	-	-	8/33/53/70	0/1/1/1
34	LMG	b	626	-	-	14/41/61/70	0/1/1/1
30	CHL	6	306	4	3/3/16/26	7/15/113/137	-
31	CLA	G	613	-	1/1/11/20	8/18/96/115	-
34	LMG	0	620	-	-	13/37/57/70	0/1/1/1
38	SQD	G	617	-	-	11/37/57/69	0/1/1/1
36	NEX	G	616	-	-	2/27/83/83	0/3/3/3
31	CLA	8	612	3	1/1/15/20	15/37/115/115	-
31	CLA	G	609	2	1/1/15/20	7/37/115/115	-
30	CHL	y	605	24	3/3/16/26	2/15/113/137	-
31	CLA	B	601	49	1/1/11/20	8/18/96/115	-
45	DGD	C	618	-	-	16/55/95/95	0/2/2/2
30	CHL	7	306	1	3/3/20/26	17/39/137/137	-
44	PL9	D	406	-	-	9/53/73/73	0/1/1/1
34	LMG	n	321	-	-	12/33/53/70	0/1/1/1
30	CHL	N	307	49	3/3/18/26	6/30/128/137	-
34	LMG	S	321	-	-	9/36/56/70	0/1/1/1
38	SQD	b	621	-	-	13/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	LUT	9	318	-	-	5/29/67/67	0/2/2/2
31	CLA	B	609	-	1/1/15/20	20/37/115/115	-
33	LHG	3	320	31	-	25/37/37/53	-
31	CLA	n	305	49	1/1/15/20	19/37/115/115	-
31	CLA	6	303	4	1/1/15/20	15/37/115/115	-
36	NEX	2	616	31	-	14/27/83/83	0/3/3/3
38	SQD	M	102	-	-	16/45/65/69	0/1/1/1
31	CLA	2	604	49,36	1/1/12/20	11/24/102/115	-
31	CLA	r	316	18	1/1/15/20	18/37/115/115	-
31	CLA	1	602	1	1/1/14/20	14/31/109/115	-
32	LUT	Y	316	-	-	3/29/67/67	0/2/2/2
33	LHG	K	102	-	-	24/40/40/53	-
31	CLA	5	611	33	1/1/13/20	15/29/107/115	-
33	LHG	8	618	31	-	35/53/53/53	-
34	LMG	a	413	-	-	9/33/53/70	0/1/1/1
35	RRX	g	315	-	-	7/29/65/65	0/2/2/2
31	CLA	y	611	33	1/1/15/20	17/37/115/115	-
32	LUT	y	616	-	-	2/29/67/67	0/2/2/2
31	CLA	r	306	49	1/1/11/20	8/17/95/115	-
31	CLA	2	602	2	1/1/15/20	23/37/115/115	-
31	CLA	G	603	-	1/1/13/20	11/25/103/115	-
31	CLA	6	311	4	1/1/15/20	16/37/115/115	-
31	CLA	0	610	4	1/1/15/20	15/37/115/115	-
31	CLA	p	602	3	1/1/14/20	12/31/109/115	-
35	RRX	4	615	-	-	15/29/65/65	0/2/2/2
31	CLA	d	404	-	1/1/15/20	13/37/115/115	-
31	CLA	C	608	-	1/1/15/20	13/37/115/115	-
31	CLA	N	321	24	1/1/12/20	7/24/102/115	-
30	CHL	4	608	-	3/3/16/26	4/20/118/137	-
33	LHG	A	415	-	-	31/48/48/53	-
33	LHG	s	320	31	-	25/45/45/53	-
31	CLA	r	304	18	1/1/14/20	11/31/109/115	-
31	CLA	Y	303	24	1/1/14/20	10/31/109/115	-
31	CLA	N	304	-	1/1/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	RRX	2	614	-	-	15/29/65/65	0/2/2/2
30	CHL	6	302	4	3/3/18/26	5/27/125/137	-
30	CHL	1	608	49	3/3/16/26	5/20/118/137	-
31	CLA	r	305	-	1/1/14/20	14/31/109/115	-
30	CHL	p	608	-	3/3/16/26	10/20/118/137	-
34	LMG	7	320	-	-	7/33/53/70	0/1/1/1
31	CLA	n	311	3	1/1/15/20	10/37/115/115	-
30	CHL	5	609	3	3/3/18/26	5/27/125/137	-
31	CLA	0	602	4	1/1/15/20	18/37/115/115	-
31	CLA	3	301	1	1/1/12/20	13/24/102/115	-
47	HEM	E	101	10,9	-	4/12/54/54	-
31	CLA	r	313	33	1/1/11/20	6/18/96/115	-
30	CHL	1	601	1	3/3/20/26	12/39/137/137	-
32	LUT	6	317	-	-	6/29/67/67	0/2/2/2
34	LMG	C	621	-	-	9/33/53/70	0/1/1/1
43	BCR	b	619	-	-	15/29/63/63	0/2/2/2
31	CLA	c	606	-	1/1/15/20	20/37/115/115	-
31	CLA	N	305	49	1/1/15/20	18/37/115/115	-
34	LMG	7	322	-	-	13/33/53/70	0/1/1/1
31	CLA	b	604	-	1/1/15/20	16/37/115/115	-
30	CHL	Y	309	24	3/3/20/26	10/39/137/137	-
34	LMG	q	302	-	-	9/35/55/70	0/1/1/1
34	LMG	w	203	-	-	6/33/53/70	0/1/1/1
34	LMG	A	412	-	-	11/36/56/70	0/1/1/1
34	LMG	B	625	-	-	13/33/53/70	0/1/1/1
31	CLA	2	612	2	1/1/15/20	17/37/115/115	-
33	LHG	S	320	31	-	30/45/45/53	-
30	CHL	p	601	3	3/3/17/26	8/21/119/137	-
36	NEX	q	319	-	-	11/27/83/83	0/3/3/3
30	CHL	Y	308	49	3/3/16/26	7/20/118/137	-
32	LUT	3	318	-	-	8/29/67/67	0/2/2/2
36	NEX	4	617	-	-	6/27/83/83	0/3/3/3
43	BCR	d	406	-	-	11/29/63/63	0/2/2/2
30	CHL	p	607	-	3/3/17/26	7/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	5	604	-	1/1/12/20	6/19/97/115	-
31	CLA	R	313	33	1/1/11/20	6/18/96/115	-
33	LHG	F1	301	-	-	26/39/39/53	-
30	CHL	n	306	3	3/3/20/26	15/39/137/137	-
43	BCR	V	101	-	-	15/29/63/63	0/2/2/2
36	NEX	p	618	31	-	9/27/83/83	0/3/3/3
31	CLA	C	606	-	1/1/13/20	13/28/106/115	-
34	LMG	C	619	-	-	10/46/66/70	0/1/1/1
36	NEX	9	319	31	-	6/27/83/83	0/3/3/3
32	LUT	g	316	-	-	10/29/67/67	0/2/2/2
36	NEX	Y	317	-	-	2/27/83/83	0/3/3/3
45	DGD	C	620	-	-	17/55/95/95	0/2/2/2
31	CLA	3	305	-	1/1/13/20	13/25/103/115	-
32	LUT	S	318	-	-	9/29/67/67	0/2/2/2
45	DGD	c	617	-	-	23/51/91/95	0/2/2/2
34	LMG	6	322	-	-	11/34/54/70	0/1/1/1
44	PL9	A	416	-	-	13/53/73/73	0/1/1/1
30	CHL	9	310	49	3/3/16/26	7/20/118/137	-
31	CLA	4	612	2	1/1/11/20	6/15/93/115	-
34	LMG	b	601	-	-	10/40/60/70	0/1/1/1
30	CHL	n	307	49	3/3/18/26	3/30/128/137	-
31	CLA	Y	304	-	1/1/13/20	13/25/103/115	-
33	LHG	t	102	-	-	30/45/45/53	-
31	CLA	4	614	-	1/1/12/20	8/24/102/115	-
31	CLA	g	303	2	1/1/15/20	11/37/115/115	-
30	CHL	G	608	2	3/3/19/26	4/36/134/137	-
33	LHG	r	320	31	-	23/42/42/53	-
31	CLA	9	305	-	1/1/13/20	12/25/103/115	-
43	BCR	A	410	-	-	6/29/63/63	0/2/2/2
44	PL9	d	407	-	-	7/53/73/73	0/1/1/1
33	LHG	R	320	31	-	26/42/42/53	-
32	LUT	7	317	-	-	6/29/67/67	0/2/2/2
31	CLA	3	315	-	1/1/12/20	12/24/102/115	-
31	CLA	Y	305	49	1/1/13/20	13/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	5	613	3	1/1/12/20	11/24/102/115	-
31	CLA	q	315	2	1/1/15/20	15/37/115/115	-
42	PHO	D	401	-	-	12/37/103/103	0/5/6/6
34	LMG	J	102	-	-	7/33/53/70	0/1/1/1
33	LHG	4	618	31	-	28/51/51/53	-
30	CHL	0	605	4	3/3/17/26	10/23/121/137	-
30	CHL	0	607	49	3/3/20/26	19/39/137/137	-
30	CHL	7	310	1	3/3/20/26	9/39/137/137	-
34	LMG	x	202	-	-	19/33/53/70	0/1/1/1
38	SQD	S	301	-	-	14/46/66/69	0/1/1/1
30	CHL	G	601	2	3/3/20/26	10/39/137/137	-
30	CHL	S	309	49	3/3/16/26	1/19/117/137	-
31	CLA	R	312	18	1/1/13/20	12/28/106/115	-
31	CLA	8	602	3	1/1/15/20	13/37/115/115	-
34	LMG	N	320	-	-	9/33/53/70	0/1/1/1
30	CHL	N	306	3	3/3/20/26	12/39/137/137	-
31	CLA	4	602	2	1/1/15/20	15/37/115/115	-
30	CHL	g	308	49	3/3/17/26	4/21/119/137	-
31	CLA	B	615	-	1/1/15/20	9/37/115/115	-
34	LMG	3	321	-	-	10/33/53/70	0/1/1/1
34	LMG	D	409	-	-	12/41/61/70	0/1/1/1
31	CLA	S	311	19	1/1/15/20	13/37/115/115	-
31	CLA	7	305	49	1/1/15/20	14/37/115/115	-
44	PL9	a	414	-	-	16/53/73/73	0/1/1/1
31	CLA	s	312	33	1/1/15/20	23/37/115/115	-
31	CLA	y	610	24	1/1/15/20	11/37/115/115	-
30	CHL	s	307	19	3/3/15/26	0/13/111/137	-
31	CLA	5	602	3	1/1/14/20	14/31/109/115	-
33	LHG	e	101	-	-	31/48/48/53	-
34	LMG	Q1	101	-	-	10/33/53/70	0/1/1/1
31	CLA	8	611	3	1/1/11/20	4/13/91/115	-
30	CHL	7	302	1	3/3/20/26	12/39/137/137	-
31	CLA	c	610	-	1/1/15/20	14/37/115/115	-
43	BCR	a	410	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	N	314	-	1/1/11/20	9/18/96/115	-
33	LHG	q	320	31	-	31/50/50/53	-
43	BCR	z	101	-	-	4/29/63/63	0/2/2/2
31	CLA	G	604	49	1/1/13/20	14/25/103/115	-
34	LMG	G	619	-	-	11/33/53/70	0/1/1/1
36	NEX	R	319	-	-	7/27/83/83	0/3/3/3
38	SQD	a	412	-	-	18/40/60/69	0/1/1/1
47	HEM	e	102	10,9	-	4/12/54/54	-
34	LMG	6	323	-	-	14/33/53/70	0/1/1/1
42	PHO	A	408	-	-	13/37/103/103	0/5/6/6
31	CLA	6	312	33	1/1/14/20	17/31/109/115	-
31	CLA	B	611	-	1/1/15/20	12/37/115/115	-
31	CLA	c	607	49	1/1/15/20	11/37/115/115	-
31	CLA	0	603	-	1/1/13/20	15/27/105/115	-
31	CLA	d	401	49	1/1/11/20	6/18/96/115	-
31	CLA	y	614	-	1/1/12/20	10/24/102/115	-
31	CLA	B	606	-	1/1/15/20	14/37/115/115	-
31	CLA	B	616	-	1/1/15/20	15/37/115/115	-
38	SQD	R	322	-	-	16/46/66/69	0/1/1/1
31	CLA	c	613	-	1/1/15/20	10/37/115/115	-
31	CLA	n	312	33	1/1/11/20	7/18/96/115	-
33	LHG	M	101	-	-	25/45/45/53	-
31	CLA	C	610	-	1/1/15/20	14/37/115/115	-
31	CLA	R	306	49	1/1/11/20	7/17/95/115	-
34	LMG	7	301	-	-	11/34/54/70	0/1/1/1
31	CLA	S	315	-	1/1/11/20	5/17/95/115	-
31	CLA	8	613	-	1/1/11/20	8/18/96/115	-
32	LUT	Y	315	-	-	0/29/67/67	0/2/2/2
31	CLA	s	313	19	1/1/13/20	9/27/105/115	-
32	LUT	s	317	-	-	6/29/67/67	0/2/2/2
34	LMG	b	622	-	-	16/46/66/70	0/1/1/1
48	LMU	r	302	-	-	9/21/61/61	0/2/2/2
30	CHL	Y	307	49	3/3/18/26	10/31/129/137	-
31	CLA	6	314	4	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	DGD	C	616	-	-	9/39/79/95	0/2/2/2
48	LMU	c	623	-	-	5/14/54/61	0/2/2/2
32	LUT	2	615	-	-	5/29/67/67	0/2/2/2
31	CLA	2	610	33	1/1/14/20	15/31/109/115	-
31	CLA	A	406	49	1/1/15/20	12/37/115/115	-
36	NEX	n	319	-	-	10/27/83/83	0/3/3/3
32	LUT	8	615	-	-	6/29/67/67	0/2/2/2
30	CHL	Y	306	24	3/3/16/26	0/15/113/137	-
33	LHG	7	319	31	-	28/39/39/53	-
31	CLA	R	311	18	1/1/13/20	18/29/107/115	-
34	LMG	n	322	-	-	12/35/55/70	0/1/1/1
31	CLA	y	602	24	1/1/14/20	10/31/109/115	-
33	LHG	n	320	31	-	34/53/53/53	-
38	SQD	B	620	-	-	18/49/69/69	0/1/1/1
45	DGD	C	617	-	-	16/55/95/95	0/2/2/2
31	CLA	1	614	-	1/1/12/20	16/24/102/115	-
32	LUT	N	317	-	-	6/29/67/67	0/2/2/2
34	LMG	c	620	-	-	14/33/53/70	0/1/1/1
34	LMG	d	409	-	-	10/36/56/70	0/1/1/1
31	CLA	p	614	-	1/1/12/20	11/21/99/115	-
31	CLA	b	616	-	1/1/15/20	15/37/115/115	-
31	CLA	s	311	19	1/1/15/20	13/37/115/115	-
37	XAT	R	318	-	-	6/31/93/93	0/4/4/4
31	CLA	c	601	-	1/1/15/20	22/37/115/115	-
31	CLA	0	611	33	1/1/14/20	10/31/109/115	-
34	LMG	b	629	-	-	12/33/53/70	0/1/1/1
31	CLA	Y	314	-	1/1/12/20	11/24/102/115	-
33	LHG	p	619	31	-	26/39/39/53	-
38	SQD	A	413	-	-	15/40/60/69	0/1/1/1
38	SQD	G	624	-	-	12/33/53/69	0/1/1/1
30	CHL	Y	301	49	3/3/19/26	9/36/134/137	-
33	LHG	2	617	31	-	32/53/53/53	-
31	CLA	3	306	49	1/1/13/20	17/25/103/115	-
38	SQD	x	201	-	-	14/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	8	614	3	1/1/12/20	10/24/102/115	-
31	CLA	4	603	-	1/1/13/20	10/25/103/115	-
31	CLA	3	311	-	1/1/12/20	6/24/102/115	-
32	LUT	8	616	-	-	6/29/67/67	0/2/2/2
34	LMG	k	101	-	-	9/43/63/70	0/1/1/1
31	CLA	b	615	-	1/1/15/20	16/37/115/115	-
31	CLA	9	312	2	1/1/12/20	13/24/102/115	-
31	CLA	R	304	18	1/1/14/20	14/31/109/115	-
30	CHL	q	309	-	3/3/18/26	19/29/127/137	-
31	CLA	p	611	33	1/1/14/20	19/31/109/115	-
30	CHL	n	310	3	3/3/20/26	6/39/137/137	-
31	CLA	q	313	33	1/1/11/20	7/13/89/115	-
34	LMG	9	301	-	-	11/46/66/70	0/1/1/1
31	CLA	5	615	3	1/1/11/20	9/15/93/115	-
34	LMG	r	321	-	-	15/33/53/70	0/1/1/1
34	LMG	G	622	-	-	7/35/55/70	0/1/1/1
37	XAT	r	318	-	-	1/31/93/93	0/4/4/4
31	CLA	C	613	-	1/1/15/20	13/37/115/115	-
42	PHO	d	402	-	-	6/37/103/103	0/5/6/6
34	LMG	R	321	-	-	9/33/53/70	0/1/1/1
30	CHL	y	601	24	3/3/20/26	12/39/137/137	-
43	BCR	c	615	-	-	11/29/63/63	0/2/2/2
30	CHL	g	307	49	3/3/16/26	3/20/118/137	-
31	CLA	c	605	-	1/1/15/20	17/37/115/115	-
34	LMG	B	622	-	-	8/33/53/70	0/1/1/1
34	LMG	B	621	-	-	15/46/66/70	0/1/1/1
30	CHL	p	606	-	3/3/17/26	2/21/119/137	-
31	CLA	R	305	-	1/1/14/20	8/31/109/115	-
31	CLA	1	613	1	1/1/15/20	15/37/115/115	-
36	NEX	r	319	-	-	4/27/83/83	0/3/3/3
31	CLA	Y	310	24	1/1/15/20	11/37/115/115	-
31	CLA	8	603	-	1/1/13/20	13/25/103/115	-
32	LUT	r	317	-	-	5/29/67/67	0/2/2/2
31	CLA	g	313	2	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	2	613	-	1/1/12/20	13/24/102/115	-
31	CLA	b	613	-	1/1/15/20	17/37/115/115	-
30	CHL	Y	302	24	3/3/20/26	10/39/137/137	-
31	CLA	c	609	-	1/1/15/20	12/37/115/115	-
33	LHG	D	407	-	-	31/48/48/53	-
30	CHL	y	607	49	3/3/20/26	11/39/137/137	-
34	LMG	a	401	-	-	6/33/53/70	0/1/1/1
34	LMG	1	618	-	-	8/33/53/70	0/1/1/1
31	CLA	B	607	49	1/1/15/20	20/37/115/115	-
30	CHL	9	309	-	3/3/17/26	11/24/122/137	-
36	NEX	6	319	-	-	9/27/83/83	0/3/3/3
30	CHL	g	302	2	3/3/20/26	14/39/137/137	-
36	NEX	5	618	-	-	9/27/83/83	0/3/3/3
32	LUT	7	318	-	-	6/29/67/67	0/2/2/2
31	CLA	B	613	-	1/1/15/20	9/37/115/115	-
31	CLA	q	314	2	1/1/11/20	9/15/93/115	-
31	CLA	g	314	-	1/1/11/20	7/18/96/115	-
34	LMG	f	101	-	-	11/33/53/70	0/1/1/1
32	LUT	4	616	-	-	6/29/67/67	0/2/2/2
45	DGD	c	616	-	-	22/55/95/95	0/2/2/2
30	CHL	q	307	2	3/3/16/26	4/15/113/137	-
31	CLA	C	609	-	1/1/15/20	12/37/115/115	-
31	CLA	r	311	18	1/1/13/20	17/29/107/115	-
30	CHL	2	607	49	3/3/16/26	6/20/118/137	-
31	CLA	9	314	2	1/1/12/20	5/19/97/115	-
38	SQD	0	621	-	-	9/37/57/69	0/1/1/1
32	LUT	1	616	-	-	3/29/67/67	0/2/2/2
30	CHL	7	308	49	3/3/20/26	9/39/137/137	-
34	LMG	X	202	-	-	5/33/53/70	0/1/1/1
31	CLA	5	610	3	1/1/14/20	11/31/109/115	-
31	CLA	c	603	-	1/1/15/20	22/37/115/115	-
30	CHL	1	609	1	3/3/20/26	6/39/137/137	-
31	CLA	C	612	-	1/1/13/20	14/25/103/115	-
31	CLA	Y	312	24	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	603	-	1/1/15/20	17/37/115/115	-
34	LMG	d	410	-	-	15/46/66/70	0/1/1/1
30	CHL	9	311	2	3/3/19/26	14/33/131/137	-
31	CLA	4	610	2	1/1/14/20	20/31/109/115	-
34	LMG	6	321	-	-	13/37/57/70	0/1/1/1
37	XAT	G	620	-	-	9/31/93/93	0/4/4/4
43	BCR	Z	101	-	-	4/29/63/63	0/2/2/2
30	CHL	s	308	49	3/3/15/26	3/12/110/137	-
33	LHG	C	623	-	-	28/44/44/53	-
36	NEX	3	319	-	-	9/27/83/83	0/3/3/3
31	CLA	7	316	1	1/1/12/20	7/21/99/115	-
34	LMG	b	624	-	-	14/33/53/70	0/1/1/1
37	XAT	2	619	-	-	9/31/93/93	0/4/4/4
31	CLA	p	612	3	1/1/11/20	8/15/93/115	-
31	CLA	C	603	-	1/1/15/20	18/37/115/115	-
31	CLA	g	310	2	1/1/15/20	14/37/115/115	-
30	CHL	8	606	49	3/3/18/26	3/30/128/137	-
31	CLA	b	612	-	1/1/15/20	13/37/115/115	-
32	LUT	5	616	-	-	7/29/67/67	0/2/2/2
31	CLA	S	314	19	1/1/15/20	16/37/115/115	-
31	CLA	A	409	-	1/1/14/20	16/31/109/115	-
31	CLA	y	603	-	1/1/13/20	12/25/103/115	-
31	CLA	S	312	33	1/1/15/20	18/37/115/115	-
30	CHL	4	606	31	3/3/17/26	6/21/119/137	-
30	CHL	S	307	19	3/3/15/26	0/13/111/137	-
30	CHL	8	607	49	3/3/16/26	4/20/118/137	-
31	CLA	c	608	-	1/1/15/20	11/37/115/115	-
30	CHL	q	308	-	3/3/17/26	6/21/119/137	-
31	CLA	s	304	-	1/1/10/20	6/10/88/115	-
34	LMG	W	201	-	-	19/50/70/70	0/1/1/1
31	CLA	q	306	49	1/1/13/20	12/25/103/115	-
31	CLA	r	314	-	1/1/11/20	7/18/96/115	-
36	NEX	s	319	-	-	3/27/83/83	0/3/3/3
31	CLA	2	603	-	1/1/13/20	13/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	NEX	0	618	-	-	9/27/83/83	0/3/3/3
32	LUT	p	617	-	-	9/29/67/67	0/2/2/2
34	LMG	g	320	-	-	11/33/53/70	0/1/1/1
34	LMG	D	412	-	-	7/43/63/70	0/1/1/1
30	CHL	1	605	1	3/3/20/26	13/39/137/137	-
37	XAT	9	322	-	-	9/31/93/93	0/4/4/4
31	CLA	5	614	-	1/1/12/20	8/21/99/115	-
31	CLA	C	602	-	1/1/15/20	11/37/115/115	-
31	CLA	s	315	-	1/1/11/20	6/17/95/115	-
31	CLA	s	305	49	1/1/15/20	16/37/115/115	-
33	LHG	D	408	-	-	30/53/53/53	-
43	BCR	H	101	-	-	5/29/63/63	0/2/2/2
31	CLA	n	313	3	1/1/11/20	4/13/91/115	-
30	CHL	2	606	-	3/3/17/26	6/21/119/137	-
34	LMG	g	322	-	-	15/44/64/70	0/1/1/1
31	CLA	6	304	-	1/1/13/20	18/27/105/115	-
33	LHG	z	102	-	-	22/40/40/53	-
36	NEX	R	301	-	-	3/27/83/83	0/3/3/3
43	BCR	B	619	-	-	9/29/63/63	0/2/2/2
33	LHG	y	619	31	-	30/50/50/53	-
31	CLA	1	612	1	1/1/15/20	19/37/115/115	-
31	CLA	B	604	-	1/1/15/20	16/37/115/115	-
31	CLA	G	611	2	1/1/10/20	2/11/89/115	-
31	CLA	a	406	-	1/1/15/20	15/37/115/115	-
31	CLA	1	603	-	1/1/13/20	8/25/103/115	-
43	BCR	b	620	-	-	9/29/63/63	0/2/2/2
38	SQD	Y	320	-	-	8/37/57/69	0/1/1/1
30	CHL	5	605	3	3/3/16/26	3/15/113/137	-
48	LMU	K	101	-	-	7/21/61/61	0/2/2/2
30	CHL	6	310	4	3/3/19/26	12/33/131/137	-
30	CHL	3	302	49	3/3/18/26	13/29/127/137	-
30	CHL	0	601	4	3/3/18/26	8/27/125/137	-
31	CLA	7	315	-	1/1/12/20	16/24/102/115	-
30	CHL	3	307	3	3/3/16/26	7/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	SQD	g	318	-	-	3/37/57/69	0/1/1/1
30	CHL	9	308	-	3/3/17/26	6/23/121/137	-
31	CLA	s	306	-	1/1/12/20	5/19/97/115	-
31	CLA	4	613	2	1/1/14/20	15/33/111/115	-
30	CHL	5	607	-	3/3/17/26	8/21/119/137	-
31	CLA	B	614	-	1/1/15/20	19/37/115/115	-
30	CHL	N	309	3	3/3/20/26	6/39/137/137	-
30	CHL	2	608	2	3/3/18/26	7/29/127/137	-
31	CLA	2	611	2	1/1/13/20	10/25/103/115	-
31	CLA	G	612	2	1/1/15/20	19/37/115/115	-
31	CLA	S	303	19	1/1/15/20	17/37/115/115	-
34	LMG	X	203	-	-	10/33/53/70	0/1/1/1
30	CHL	G	623	49	3/3/20/26	12/39/137/137	-
30	CHL	3	303	3	3/3/16/26	6/20/118/137	-
30	CHL	y	606	49	3/3/18/26	9/31/129/137	-
38	SQD	6	301	-	-	18/37/57/69	0/1/1/1
34	LMG	G	621	-	-	13/46/66/70	0/1/1/1
31	CLA	B	612	-	1/1/15/20	11/37/115/115	-
43	BCR	B	618	-	-	10/29/63/63	0/2/2/2
30	CHL	q	311	2	3/3/18/26	3/27/125/137	-
31	CLA	b	605	-	1/1/15/20	25/37/115/115	-
30	CHL	7	307	49	3/3/20/26	9/39/137/137	-
31	CLA	0	604	49	1/1/13/20	15/25/103/115	-
31	CLA	3	316	3	1/1/13/20	13/28/106/115	-
34	LMG	j	101	-	-	12/38/58/70	0/1/1/1
38	SQD	a	411	-	-	16/43/63/69	0/1/1/1
38	SQD	y	621	-	-	9/37/57/69	0/1/1/1
37	XAT	g	321	-	-	9/31/93/93	0/4/4/4
34	LMG	2	620	-	-	18/46/66/70	0/1/1/1
36	NEX	g	317	31	-	12/27/83/83	0/3/3/3
32	LUT	R	317	-	-	8/29/67/67	0/2/2/2
32	LUT	6	318	-	-	6/29/67/67	0/2/2/2
31	CLA	D	404	-	1/1/15/20	19/37/115/115	-
34	LMG	c	624	-	-	11/39/59/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	9	303	2	3/3/20/26	10/39/137/137	-
34	LMG	a	416	-	-	11/33/53/70	0/1/1/1
30	CHL	8	601	3	3/3/18/26	8/27/125/137	-
34	LMG	s	321	-	-	11/36/56/70	0/1/1/1
35	RRX	9	317	-	-	15/29/65/65	0/2/2/2
30	CHL	3	309	-	3/3/16/26	10/20/118/137	-
43	BCR	v	101	-	-	15/29/63/63	0/2/2/2
34	LMG	9	302	-	-	13/35/55/70	0/1/1/1
30	CHL	6	307	49	3/3/17/26	5/21/119/137	-
31	CLA	B	603	-	1/1/15/20	19/37/115/115	-
33	LHG	d	408	-	-	29/53/53/53	-
34	LMG	D	410	-	-	12/41/61/70	0/1/1/1
31	CLA	g	304	-	1/1/13/20	12/25/103/115	-
34	LMG	A	414	-	-	10/33/53/70	0/1/1/1
30	CHL	6	308	49	3/3/20/26	13/39/137/137	-
31	CLA	g	311	33	1/1/14/20	13/31/109/115	-
31	CLA	r	315	18	1/1/13/20	13/25/103/115	-
31	CLA	q	312	2	1/1/13/20	11/25/101/115	-
31	CLA	N	315	3	1/1/12/20	8/24/102/115	-
31	CLA	r	303	18	1/1/11/20	9/18/96/115	-
33	LHG	b	628	-	-	31/53/53/53	-
48	LMU	R	302	-	-	12/21/61/61	0/2/2/2
31	CLA	b	609	-	1/1/15/20	14/37/115/115	-
30	CHL	n	301	49	3/3/16/26	6/20/118/137	-
30	CHL	y	608	49	3/3/16/26	3/20/118/137	-
31	CLA	C	601	-	1/1/15/20	18/37/115/115	-
33	LHG	A	417	-	-	24/43/43/53	-
30	CHL	7	309	49	3/3/16/26	7/20/118/137	-
30	CHL	4	607	-	3/3/18/26	15/29/127/137	-
43	BCR	t	101	-	-	6/29/63/63	0/2/2/2
31	CLA	g	305	49,36	1/1/13/20	13/25/103/115	-
37	XAT	q	321	-	-	9/31/93/93	0/4/4/4
31	CLA	7	311	1	1/1/15/20	17/37/115/115	-
31	CLA	7	303	1	1/1/14/20	11/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	0	612	4	1/1/11/20	8/15/93/115	-
34	LMG	p	620	-	-	7/33/53/70	0/1/1/1
30	CHL	1	607	-	3/3/20/26	13/39/137/137	-
31	CLA	5	603	-	1/1/12/20	10/22/100/115	-
31	CLA	7	314	1	1/1/15/20	17/37/115/115	-
31	CLA	8	604	49,36	1/1/15/20	21/37/115/115	-
31	CLA	D	403	-	1/1/15/20	14/37/115/115	-
33	LHG	l	101	-	-	29/53/53/53	-
43	BCR	D	405	-	-	13/29/63/63	0/2/2/2
31	CLA	8	610	33	1/1/11/20	7/18/96/115	-
31	CLA	p	615	3	1/1/11/20	7/15/93/115	-
31	CLA	r	307	49	1/1/11/20	9/17/95/115	-
31	CLA	7	313	1	1/1/15/20	15/37/115/115	-
30	CHL	0	608	49	3/3/16/26	4/20/118/137	-
30	CHL	G	605	2	3/3/16/26	5/18/116/137	-
30	CHL	p	609	3	3/3/18/26	4/27/125/137	-
31	CLA	9	313	33	1/1/11/20	8/16/94/115	-
31	CLA	s	316	19	1/1/11/20	6/15/93/115	-
43	BCR	C	615	-	-	8/29/63/63	0/2/2/2
33	LHG	G	618	31	-	29/48/48/53	-
30	CHL	R	310	49	3/3/17/26	4/26/124/137	-
31	CLA	B	605	-	1/1/15/20	19/37/115/115	-
43	BCR	B	617	-	-	14/29/63/63	0/2/2/2
34	LMG	J	101	-	-	13/46/66/70	0/1/1/1
31	CLA	b	602	49	1/1/11/20	12/18/96/115	-
30	CHL	S	308	49	3/3/15/26	1/12/110/137	-
31	CLA	l	604	49	1/1/15/20	14/37/115/115	-
34	LMG	b	623	-	-	7/33/53/70	0/1/1/1
30	CHL	n	309	49	3/3/16/26	4/20/118/137	-
30	CHL	G	607	49	3/3/17/26	5/21/119/137	-
34	LMG	C	624	-	-	13/39/59/70	0/1/1/1
32	LUT	y	617	-	-	2/29/67/67	0/2/2/2
31	CLA	n	315	-	1/1/11/20	8/18/96/115	-
30	CHL	R	308	18	3/3/18/26	5/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	0	622	-	-	15/33/53/70	0/1/1/1
33	LHG	N	319	31	-	32/53/53/53	-
42	PHO	a	408	-	-	10/37/103/103	0/5/6/6
31	CLA	6	313	4	1/1/14/20	12/31/109/115	-
31	CLA	N	313	3	1/1/15/20	13/37/115/115	-
30	CHL	N	301	-	3/3/16/26	6/20/118/137	-
33	LHG	1	617	31	-	29/39/39/53	-
31	CLA	c	604	49	1/1/13/20	9/27/105/115	-
31	CLA	Y	311	33	1/1/15/20	14/37/115/115	-
30	CHL	0	609	4	3/3/19/26	4/33/131/137	-
31	CLA	S	313	19	1/1/13/20	9/27/105/115	-
33	LHG	6	320	31	-	24/41/41/53	-
31	CLA	R	316	18	1/1/15/20	20/37/115/115	-
33	LHG	s	322	-	-	29/48/48/53	-
31	CLA	B	610	49	1/1/15/20	14/37/115/115	-
32	LUT	0	617	-	-	0/29/67/67	0/2/2/2
31	CLA	y	612	24	1/1/15/20	18/37/115/115	-
31	CLA	b	611	49	1/1/15/20	12/37/115/115	-
30	CHL	p	605	3	3/3/16/26	3/15/113/137	-
31	CLA	d	405	-	1/1/15/20	13/37/115/115	-
34	LMG	d	411	-	-	8/43/63/70	0/1/1/1
32	LUT	5	617	-	-	7/29/67/67	0/2/2/2
43	BCR	c	614	-	-	16/29/63/63	0/2/2/2
31	CLA	S	306	-	1/1/12/20	4/19/97/115	-
31	CLA	s	303	19	1/1/15/20	14/37/115/115	-
35	RRX	G	614	-	-	15/29/65/65	0/2/2/2
31	CLA	c	612	-	1/1/13/20	12/25/103/115	-
30	CHL	5	608	-	3/3/16/26	7/20/118/137	-
36	NEX	y	618	-	-	2/27/83/83	0/3/3/3
31	CLA	a	407	49	1/1/15/20	13/37/115/115	-
38	SQD	g	301	-	-	6/33/53/69	0/1/1/1
30	CHL	g	309	2	3/3/19/26	7/36/134/137	-
30	CHL	r	308	18	3/3/18/26	8/27/125/137	-
33	LHG	S	322	-	-	31/48/48/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	C	604	49	1/1/13/20	10/27/105/115	-
30	CHL	8	605	3	3/3/20/26	15/39/137/137	-
31	CLA	a	409	-	1/1/14/20	16/31/109/115	-
31	CLA	R	307	49	1/1/11/20	9/17/95/115	-
30	CHL	g	306	2	3/3/16/26	5/18/116/137	-
30	CHL	3	308	-	3/3/16/26	3/17/115/137	-
31	CLA	0	614	-	1/1/12/20	12/24/102/115	-
31	CLA	7	312	33	1/1/15/20	19/37/115/115	-
34	LMG	m	102	-	-	10/40/60/70	0/1/1/1
33	LHG	0	619	31	-	29/40/40/53	-
31	CLA	1	611	33	1/1/15/20	11/37/115/115	-
31	CLA	3	314	3	1/1/13/20	6/25/103/115	-
38	SQD	m	101	-	-	13/45/65/69	0/1/1/1
30	CHL	9	307	2	3/3/16/26	7/15/113/137	-
34	LMG	5	620	-	-	14/33/53/70	0/1/1/1
32	LUT	s	318	-	-	5/29/67/67	0/2/2/2
43	BCR	C	614	-	-	12/29/63/63	0/2/2/2
31	CLA	p	613	-	1/1/12/20	9/24/102/115	-
33	LHG	5	619	31	-	27/39/39/53	-
31	CLA	s	310	19	1/1/14/20	14/31/109/115	-
31	CLA	N	311	33	1/1/11/20	9/18/96/115	-
31	CLA	N	303	3	1/1/15/20	19/37/115/115	-
30	CHL	4	609	2	3/3/18/26	9/29/127/137	-
34	LMG	w	201	-	-	13/43/63/70	0/1/1/1
30	CHL	2	601	2	3/3/20/26	10/39/137/137	-
36	NEX	r	301	-	-	2/27/83/83	0/3/3/3
32	LUT	p	616	-	-	9/29/67/67	0/2/2/2
38	SQD	r	322	-	-	15/46/66/69	0/1/1/1
30	CHL	2	605	2	3/3/16/26	4/15/113/137	-
31	CLA	y	615	24	1/1/12/20	12/24/102/115	-
38	SQD	A	411	-	-	13/46/66/69	0/1/1/1
31	CLA	c	602	-	1/1/15/20	12/37/115/115	-
35	RRX	q	317	-	-	9/29/65/65	0/2/2/2
31	CLA	4	604	30	1/1/12/20	12/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	S	310	19	1/1/14/20	14/31/109/115	-
31	CLA	2	609	2	1/1/14/20	18/31/109/115	-
32	LUT	q	318	-	-	6/29/67/67	0/2/2/2
33	LHG	c	622	-	-	32/51/51/53	-
31	CLA	A	407	49	1/1/11/20	6/18/96/115	-
31	CLA	b	614	-	1/1/15/20	13/37/115/115	-
31	CLA	b	607	-	1/1/15/20	14/37/115/115	-
30	CHL	5	606	49	3/3/17/26	1/21/119/137	-
31	CLA	3	304	3	1/1/14/20	14/31/109/115	-
31	CLA	8	609	3	1/1/15/20	10/37/115/115	-
32	LUT	N	316	-	-	6/29/67/67	0/2/2/2
31	CLA	b	617	-	1/1/15/20	15/37/115/115	-
32	LUT	0	616	-	-	2/29/67/67	0/2/2/2
31	CLA	0	613	4	1/1/13/20	10/27/105/115	-
34	LMG	2	618	-	-	13/33/53/70	0/1/1/1
31	CLA	p	603	-	1/1/13/20	12/25/103/115	-
32	LUT	1	615	-	-	1/29/67/67	0/2/2/2
31	CLA	9	306	49,36	1/1/15/20	17/37/115/115	-
30	CHL	r	310	49	3/3/17/26	3/26/124/137	-
33	LHG	Y	318	31	-	30/46/46/53	-
31	CLA	N	312	3	1/1/11/20	6/13/91/115	-
34	LMG	W	202	-	-	11/33/53/70	0/1/1/1
36	NEX	8	617	31	-	11/27/83/83	0/3/3/3
38	SQD	b	627	-	-	14/47/67/69	0/1/1/1
31	CLA	9	315	2	1/1/13/20	8/25/103/115	-
30	CHL	q	310	-	3/3/16/26	4/20/118/137	-
34	LMG	W	203	-	-	13/33/53/70	0/1/1/1
36	NEX	S	319	-	-	2/27/83/83	0/3/3/3
33	LHG	B	624	-	-	35/53/53/53	-
34	LMG	y	620	-	-	10/33/53/70	0/1/1/1
31	CLA	9	304	2	1/1/15/20	19/37/115/115	-
34	LMG	Y	319	-	-	8/33/53/70	0/1/1/1
34	LMG	w	205	-	-	13/33/53/70	0/1/1/1
31	CLA	n	303	3	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	w	202	-	-	12/50/70/70	0/1/1/1
31	CLA	9	316	-	1/1/11/20	9/15/93/115	-
31	CLA	n	314	3	1/1/15/20	15/37/115/115	-
30	CHL	q	303	2	3/3/20/26	9/39/137/137	-
32	LUT	S	317	-	-	6/29/67/67	0/2/2/2
31	CLA	A	405	-	1/1/15/20	10/37/115/115	-
31	CLA	B	608	-	1/1/15/20	12/37/115/115	-
31	CLA	b	606	-	1/1/15/20	16/37/115/115	-
31	CLA	r	312	18	1/1/13/20	12/28/106/115	-
32	LUT	G	615	-	-	10/29/67/67	0/2/2/2
30	CHL	s	302	19	3/3/16/26	2/15/113/137	-
31	CLA	G	610	33	1/1/14/20	16/31/109/115	-
34	LMG	I	101	-	-	15/33/53/70	0/1/1/1
36	NEX	N	318	-	-	15/27/83/83	0/3/3/3
34	LMG	9	321	-	-	10/33/53/70	0/1/1/1
30	CHL	y	609	24	3/3/20/26	5/39/137/137	-
31	CLA	3	312	33	1/1/15/20	13/37/115/115	-
31	CLA	6	305	49	1/1/13/20	15/25/103/115	-
30	CHL	7	321	49	3/3/19/26	12/36/134/137	-
30	CHL	r	309	18	3/3/18/26	4/27/125/137	-
30	CHL	5	601	3	3/3/17/26	8/21/119/137	-
31	CLA	6	315	-	1/1/12/20	16/24/102/115	-
31	CLA	q	304	2	1/1/15/20	12/37/115/115	-
31	CLA	6	316	4	1/1/13/20	14/25/103/115	-
30	CHL	3	310	3	3/3/19/26	8/33/131/137	-
33	LHG	g	319	31	-	26/48/48/53	-
31	CLA	7	304	-	1/1/13/20	12/25/103/115	-
34	LMG	w	204	-	-	12/33/53/70	0/1/1/1
30	CHL	N	308	49	3/3/16/26	7/20/118/137	-
43	BCR	T	101	-	-	14/29/63/63	0/2/2/2
34	LMG	4	620	-	-	15/46/66/70	0/1/1/1
30	CHL	4	605	2	3/3/16/26	3/15/113/137	-
37	XAT	4	619	-	-	9/31/93/93	0/4/4/4
30	CHL	N	302	3	3/3/18/26	4/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	LMG	D	411	-	-	15/46/66/70	0/1/1/1
31	CLA	R	314	-	1/1/11/20	5/18/96/115	-
30	CHL	n	302	3	3/3/18/26	8/27/125/137	-
30	CHL	S	302	19	3/3/16/26	0/15/113/137	-
31	CLA	q	305	-	1/1/13/20	14/25/103/115	-
32	LUT	3	317	-	-	2/29/67/67	0/2/2/2
38	SQD	X	201	-	-	9/33/53/69	0/1/1/1
31	CLA	b	608	49	1/1/15/20	24/37/115/115	-
31	CLA	n	316	3	1/1/12/20	10/24/102/115	-
31	CLA	s	314	19	1/1/15/20	17/37/115/115	-
43	BCR	b	618	-	-	14/29/63/63	0/2/2/2
33	LHG	b	625	-	-	30/48/48/53	-
30	CHL	8	608	3	3/3/20/26	8/39/137/137	-
32	LUT	n	317	-	-	6/29/67/67	0/2/2/2
31	CLA	q	316	-	1/1/12/20	8/19/97/115	-
31	CLA	C	605	-	1/1/15/20	18/37/115/115	-
34	LMG	2	621	-	-	9/35/55/70	0/1/1/1
34	LMG	q	301	-	-	14/46/66/70	0/1/1/1
31	CLA	S	304	-	1/1/10/20	5/10/88/115	-
30	CHL	G	606	49	3/3/16/26	6/20/118/137	-
31	CLA	G	602	2	1/1/15/20	16/37/115/115	-
33	LHG	j	102	-	-	36/53/53/53	-
34	LMG	C	622	-	-	6/27/47/70	0/1/1/1
30	CHL	1	619	-	3/3/19/26	11/33/131/137	-
45	DGD	c	619	-	-	16/55/95/95	0/2/2/2
33	LHG	L	101	-	-	31/53/53/53	-
30	CHL	0	606	49	3/3/17/26	3/21/119/137	-
31	CLA	R	315	18	1/1/13/20	8/25/103/115	-
32	LUT	n	318	-	-	6/29/67/67	0/2/2/2
31	CLA	y	604	49	1/1/13/20	15/25/103/115	-
31	CLA	C	607	49	1/1/15/20	13/37/115/115	-
31	CLA	p	604	36	1/1/12/20	8/19/97/115	-
31	CLA	Y	313	24	1/1/15/20	12/37/115/115	-
31	CLA	B	602	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	N	310	3	1/1/15/20	11/37/115/115	-

All (4604) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	316	LUT	C24-C25	23.29	1.62	1.33
32	5	616	LUT	C24-C25	23.25	1.62	1.33
32	G	615	LUT	C24-C25	23.25	1.62	1.33
32	3	317	LUT	C24-C25	23.24	1.62	1.33
32	9	318	LUT	C24-C25	23.23	1.62	1.33
32	8	615	LUT	C24-C25	23.22	1.62	1.33
32	n	317	LUT	C24-C25	23.21	1.62	1.33
32	p	616	LUT	C24-C25	23.21	1.62	1.33
32	S	318	LUT	C24-C25	23.19	1.62	1.33
32	q	318	LUT	C24-C25	23.18	1.62	1.33
32	g	316	LUT	C24-C25	23.16	1.62	1.33
32	8	616	LUT	C24-C25	23.15	1.62	1.33
32	N	317	LUT	C24-C25	23.15	1.62	1.33
32	n	318	LUT	C24-C25	23.13	1.62	1.33
32	6	318	LUT	C24-C25	23.10	1.61	1.33
32	6	317	LUT	C24-C25	23.09	1.61	1.33
32	p	617	LUT	C24-C25	23.09	1.61	1.33
32	7	318	LUT	C24-C25	23.08	1.61	1.33
32	3	318	LUT	C24-C25	23.07	1.61	1.33
32	S	317	LUT	C24-C25	23.05	1.61	1.33
32	s	317	LUT	C24-C25	23.04	1.61	1.33
32	s	318	LUT	C24-C25	23.02	1.61	1.33
32	4	616	LUT	C24-C25	23.00	1.61	1.33
32	1	616	LUT	C24-C25	23.00	1.61	1.33
32	5	617	LUT	C24-C25	23.00	1.61	1.33
32	0	616	LUT	C24-C25	22.96	1.61	1.33
32	R	317	LUT	C24-C25	22.94	1.61	1.33
32	1	615	LUT	C24-C25	22.93	1.61	1.33
32	r	317	LUT	C24-C25	22.86	1.61	1.33
32	Y	315	LUT	C24-C25	22.80	1.61	1.33
32	7	317	LUT	C24-C25	22.80	1.61	1.33
32	0	617	LUT	C24-C25	22.76	1.61	1.33
32	y	617	LUT	C24-C25	22.76	1.61	1.33
32	y	616	LUT	C24-C25	22.71	1.61	1.33
32	Y	316	LUT	C24-C25	22.64	1.61	1.33
32	2	615	LUT	C24-C25	21.68	1.60	1.33
43	B	618	BCR	C26-C25	15.74	1.61	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	b	619	BCR	C26-C25	15.68	1.61	1.34
43	Z	101	BCR	C26-C25	15.46	1.61	1.34
43	z	101	BCR	C26-C25	15.43	1.61	1.34
43	D	405	BCR	C26-C25	15.38	1.61	1.34
35	9	317	RRX	C26-C25	15.35	1.61	1.34
35	4	615	RRX	C26-C25	15.35	1.61	1.34
35	G	614	RRX	C26-C25	15.32	1.61	1.34
32	8	615	LUT	C5-C6	15.32	1.61	1.34
32	n	317	LUT	C5-C6	15.32	1.61	1.34
35	2	614	RRX	C26-C25	15.32	1.61	1.34
43	b	620	BCR	C26-C25	15.29	1.60	1.34
35	g	315	RRX	C26-C25	15.27	1.60	1.34
32	G	615	LUT	C5-C6	15.25	1.60	1.34
43	t	101	BCR	C26-C25	15.25	1.60	1.34
43	c	615	BCR	C26-C25	15.25	1.60	1.34
32	s	317	LUT	C5-C6	15.25	1.60	1.34
32	5	617	LUT	C5-C6	15.25	1.60	1.34
32	S	317	LUT	C5-C6	15.23	1.60	1.34
35	q	317	RRX	C26-C25	15.23	1.60	1.34
43	H	101	BCR	C26-C25	15.23	1.60	1.34
32	6	318	LUT	C5-C6	15.23	1.60	1.34
32	7	318	LUT	C5-C6	15.23	1.60	1.34
32	5	616	LUT	C5-C6	15.21	1.60	1.34
32	9	318	LUT	C5-C6	15.21	1.60	1.34
43	T	101	BCR	C26-C25	15.21	1.60	1.34
32	8	616	LUT	C5-C6	15.20	1.60	1.34
32	n	318	LUT	C5-C6	15.19	1.60	1.34
43	c	614	BCR	C26-C25	15.19	1.60	1.34
43	v	101	BCR	C26-C25	15.18	1.60	1.34
43	a	410	BCR	C26-C25	15.18	1.60	1.34
43	C	615	BCR	C26-C25	15.16	1.60	1.34
43	B	619	BCR	C26-C25	15.15	1.60	1.34
32	p	616	LUT	C5-C6	15.15	1.60	1.34
32	4	616	LUT	C5-C6	15.14	1.60	1.34
43	h	101	BCR	C26-C25	15.13	1.60	1.34
32	3	317	LUT	C5-C6	15.12	1.60	1.34
32	0	617	LUT	C5-C6	15.10	1.60	1.34
32	N	316	LUT	C5-C6	15.08	1.60	1.34
32	g	316	LUT	C5-C6	15.08	1.60	1.34
32	r	317	LUT	C5-C6	15.07	1.60	1.34
32	S	318	LUT	C5-C6	15.07	1.60	1.34
43	d	406	BCR	C26-C25	15.07	1.60	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	y	617	LUT	C5-C6	15.03	1.60	1.34
32	Y	315	LUT	C5-C6	15.03	1.60	1.34
32	p	617	LUT	C5-C6	15.01	1.60	1.34
32	s	318	LUT	C5-C6	15.01	1.60	1.34
32	N	317	LUT	C5-C6	15.01	1.60	1.34
32	Y	316	LUT	C5-C6	15.01	1.60	1.34
43	A	410	BCR	C26-C25	15.00	1.60	1.34
32	1	616	LUT	C5-C6	14.98	1.60	1.34
32	3	318	LUT	C5-C6	14.98	1.60	1.34
32	6	317	LUT	C5-C6	14.96	1.60	1.34
32	R	317	LUT	C5-C6	14.95	1.60	1.34
32	q	318	LUT	C5-C6	14.94	1.60	1.34
32	y	616	LUT	C5-C6	14.93	1.60	1.34
43	B	617	BCR	C26-C25	14.91	1.60	1.34
32	0	616	LUT	C5-C6	14.90	1.60	1.34
32	1	615	LUT	C5-C6	14.82	1.60	1.34
32	7	317	LUT	C5-C6	14.82	1.60	1.34
32	2	615	LUT	C5-C6	14.81	1.60	1.34
43	b	618	BCR	C26-C25	14.79	1.60	1.34
43	C	614	BCR	C26-C25	14.74	1.60	1.34
43	V	101	BCR	C26-C25	14.70	1.59	1.34
35	g	315	RRX	C5-C6	14.30	1.59	1.34
35	4	615	RRX	C5-C6	14.25	1.59	1.34
43	D	405	BCR	C5-C6	14.24	1.59	1.34
35	9	317	RRX	C5-C6	14.23	1.59	1.34
35	G	614	RRX	C5-C6	14.20	1.59	1.34
35	2	614	RRX	C5-C6	14.18	1.59	1.34
43	z	101	BCR	C5-C6	14.16	1.59	1.34
43	Z	101	BCR	C5-C6	14.06	1.58	1.34
43	B	618	BCR	C5-C6	13.99	1.58	1.34
35	q	317	RRX	C5-C6	13.95	1.58	1.34
43	T	101	BCR	C5-C6	13.91	1.58	1.34
43	a	410	BCR	C5-C6	13.90	1.58	1.34
43	b	619	BCR	C5-C6	13.89	1.58	1.34
43	c	614	BCR	C5-C6	13.86	1.58	1.34
43	H	101	BCR	C5-C6	13.84	1.58	1.34
43	v	101	BCR	C5-C6	13.82	1.58	1.34
43	A	410	BCR	C5-C6	13.82	1.58	1.34
43	b	620	BCR	C5-C6	13.81	1.58	1.34
43	B	619	BCR	C5-C6	13.79	1.58	1.34
43	V	101	BCR	C5-C6	13.75	1.58	1.34
43	C	614	BCR	C5-C6	13.73	1.58	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	h	101	BCR	C5-C6	13.72	1.58	1.34
43	b	618	BCR	C5-C6	13.69	1.58	1.34
43	c	615	BCR	C5-C6	13.62	1.58	1.34
43	B	617	BCR	C5-C6	13.57	1.57	1.34
43	d	406	BCR	C5-C6	13.56	1.57	1.34
43	t	101	BCR	C5-C6	13.39	1.57	1.34
32	R	317	LUT	C22-C21	-13.33	1.38	1.54
32	y	617	LUT	C22-C21	-13.31	1.38	1.54
32	Y	315	LUT	C22-C21	-13.30	1.38	1.54
32	r	317	LUT	C22-C21	-13.29	1.38	1.54
32	y	616	LUT	C22-C21	-13.25	1.38	1.54
32	1	616	LUT	C22-C21	-13.24	1.38	1.54
32	Y	316	LUT	C22-C21	-13.18	1.38	1.54
32	1	615	LUT	C22-C21	-13.16	1.38	1.54
32	7	317	LUT	C22-C21	-13.14	1.38	1.54
32	0	616	LUT	C22-C21	-13.07	1.38	1.54
32	9	318	LUT	C22-C21	-13.06	1.38	1.54
32	S	317	LUT	C22-C21	-13.05	1.38	1.54
32	n	317	LUT	C22-C21	-13.02	1.38	1.54
32	6	317	LUT	C22-C21	-13.01	1.38	1.54
32	8	615	LUT	C22-C21	-13.00	1.38	1.54
43	C	615	BCR	C5-C6	12.98	1.56	1.34
32	N	316	LUT	C22-C21	-12.96	1.38	1.54
32	8	616	LUT	C22-C21	-12.96	1.38	1.54
32	5	616	LUT	C22-C21	-12.95	1.38	1.54
32	S	318	LUT	C22-C21	-12.95	1.38	1.54
32	G	615	LUT	C22-C21	-12.95	1.38	1.54
32	s	317	LUT	C22-C21	-12.93	1.38	1.54
32	3	317	LUT	C22-C21	-12.93	1.38	1.54
32	n	318	LUT	C22-C21	-12.89	1.38	1.54
32	q	318	LUT	C22-C21	-12.88	1.38	1.54
32	N	317	LUT	C22-C21	-12.87	1.38	1.54
32	7	318	LUT	C22-C21	-12.84	1.38	1.54
32	g	316	LUT	C22-C21	-12.84	1.38	1.54
32	3	318	LUT	C22-C21	-12.83	1.38	1.54
32	4	616	LUT	C22-C21	-12.82	1.38	1.54
32	s	318	LUT	C22-C21	-12.81	1.38	1.54
32	6	318	LUT	C22-C21	-12.78	1.38	1.54
32	0	617	LUT	C22-C21	-12.72	1.38	1.54
32	p	616	LUT	C22-C21	-12.70	1.38	1.54
32	5	617	LUT	C22-C21	-12.58	1.38	1.54
32	p	617	LUT	C22-C21	-12.49	1.39	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	2	615	LUT	C22-C21	-12.17	1.39	1.54
32	y	616	LUT	C2-C3	-11.58	1.35	1.52
32	r	317	LUT	C2-C3	-11.48	1.35	1.52
32	y	617	LUT	C2-C3	-11.45	1.35	1.52
32	Y	315	LUT	C2-C3	-11.40	1.35	1.52
32	Y	316	LUT	C2-C3	-11.40	1.35	1.52
32	8	615	LUT	C2-C3	-11.35	1.36	1.52
32	S	317	LUT	C2-C3	-11.31	1.36	1.52
32	n	317	LUT	C2-C3	-11.30	1.36	1.52
32	s	317	LUT	C2-C3	-11.29	1.36	1.52
32	1	615	LUT	C2-C3	-11.27	1.36	1.52
32	R	317	LUT	C2-C3	-11.26	1.36	1.52
32	7	317	LUT	C2-C3	-11.25	1.36	1.52
32	0	617	LUT	C2-C3	-11.24	1.36	1.52
32	1	616	LUT	C2-C3	-11.21	1.36	1.52
32	3	317	LUT	C2-C3	-11.16	1.36	1.52
32	5	616	LUT	C2-C3	-11.15	1.36	1.52
32	6	318	LUT	C2-C3	-11.13	1.36	1.52
32	N	316	LUT	C2-C3	-11.09	1.36	1.52
32	G	615	LUT	C2-C3	-11.08	1.36	1.52
32	0	616	LUT	C2-C3	-11.08	1.36	1.52
32	6	317	LUT	C2-C3	-11.08	1.36	1.52
32	4	616	LUT	C2-C3	-11.08	1.36	1.52
32	7	318	LUT	C2-C3	-11.07	1.36	1.52
32	n	318	LUT	C2-C3	-11.02	1.36	1.52
32	9	318	LUT	C2-C3	-11.01	1.36	1.52
32	S	318	LUT	C2-C3	-11.01	1.36	1.52
32	8	616	LUT	C2-C3	-10.99	1.36	1.52
32	5	617	LUT	C2-C3	-10.97	1.36	1.52
32	g	316	LUT	C2-C3	-10.96	1.36	1.52
32	N	317	LUT	C2-C3	-10.94	1.36	1.52
32	p	616	LUT	C2-C3	-10.92	1.36	1.52
32	s	318	LUT	C2-C3	-10.87	1.36	1.52
32	2	615	LUT	C2-C3	-10.86	1.36	1.52
32	3	318	LUT	C2-C3	-10.85	1.36	1.52
32	q	318	LUT	C2-C3	-10.83	1.36	1.52
32	p	617	LUT	C2-C3	-10.72	1.36	1.52
35	q	317	RRX	C29-C28	-10.36	1.37	1.52
35	G	614	RRX	C29-C28	-10.33	1.37	1.52
35	2	614	RRX	C29-C28	-10.32	1.37	1.52
35	9	317	RRX	C29-C28	-10.32	1.37	1.52
35	4	615	RRX	C29-C28	-10.29	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	g	315	RRX	C29-C28	-10.27	1.37	1.52
32	S	318	LUT	C22-C23	8.51	1.67	1.53
32	5	617	LUT	C22-C23	8.38	1.67	1.53
35	g	315	RRX	C27-C28	8.34	1.66	1.52
32	g	316	LUT	C22-C23	8.28	1.66	1.53
32	7	318	LUT	C22-C23	8.24	1.66	1.53
32	s	318	LUT	C22-C23	8.24	1.66	1.53
32	p	617	LUT	C22-C23	8.17	1.66	1.53
32	p	616	LUT	C22-C23	8.16	1.66	1.53
32	2	615	LUT	C22-C23	8.15	1.66	1.53
32	3	318	LUT	C4-C3	8.14	1.66	1.52
32	5	616	LUT	C22-C23	8.14	1.66	1.53
32	4	616	LUT	C22-C23	8.14	1.66	1.53
35	4	615	RRX	C27-C28	8.13	1.66	1.52
32	G	615	LUT	C22-C23	8.13	1.66	1.53
35	9	317	RRX	C27-C28	8.12	1.66	1.52
32	q	318	LUT	C22-C23	8.10	1.66	1.53
32	6	318	LUT	C22-C23	8.08	1.66	1.53
32	p	617	LUT	C4-C3	8.08	1.66	1.52
32	3	318	LUT	C22-C23	8.07	1.66	1.53
35	G	614	RRX	C27-C28	8.07	1.66	1.52
32	N	317	LUT	C4-C3	8.06	1.66	1.52
32	g	316	LUT	C4-C3	8.03	1.66	1.52
32	q	318	LUT	C4-C3	8.03	1.66	1.52
32	0	617	LUT	C22-C23	8.02	1.66	1.53
35	2	614	RRX	C27-C28	8.01	1.66	1.52
32	N	317	LUT	C22-C23	8.01	1.66	1.53
32	s	317	LUT	C22-C23	8.01	1.66	1.53
32	8	616	LUT	C22-C23	8.01	1.66	1.53
32	n	318	LUT	C22-C23	8.00	1.66	1.53
32	S	318	LUT	C4-C3	8.00	1.66	1.52
43	B	617	BCR	C30-C25	-7.99	1.42	1.53
32	5	617	LUT	C4-C3	7.99	1.66	1.52
32	2	615	LUT	C4-C3	7.98	1.66	1.52
32	S	317	LUT	C22-C23	7.97	1.66	1.53
32	1	615	LUT	C22-C23	7.96	1.66	1.53
32	6	317	LUT	C22-C23	7.96	1.66	1.53
32	8	616	LUT	C4-C3	7.95	1.66	1.52
32	n	318	LUT	C4-C3	7.93	1.66	1.52
36	S	319	NEX	C10-C9	-7.93	1.25	1.35
35	q	317	RRX	C27-C28	7.93	1.66	1.52
32	0	616	LUT	C22-C23	7.93	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	p	616	LUT	C4-C3	7.93	1.66	1.52
32	3	317	LUT	C22-C23	7.92	1.66	1.53
32	G	615	LUT	C32-C33	7.92	1.63	1.45
36	3	319	NEX	C14-C13	-7.91	1.25	1.35
36	3	319	NEX	C10-C9	-7.91	1.25	1.35
32	1	616	LUT	C22-C23	7.91	1.66	1.53
32	9	318	LUT	C22-C23	7.91	1.66	1.53
32	3	317	LUT	C4-C3	7.91	1.66	1.52
36	R	301	NEX	C34-C33	-7.90	1.25	1.35
36	9	319	NEX	C30-C29	-7.90	1.25	1.35
36	9	319	NEX	C34-C33	-7.89	1.25	1.35
36	R	301	NEX	C14-C13	-7.88	1.25	1.35
36	s	319	NEX	C34-C33	-7.88	1.25	1.35
32	n	317	LUT	C22-C23	7.88	1.66	1.53
32	N	316	LUT	C4-C3	7.88	1.65	1.52
32	Y	316	LUT	C22-C23	7.87	1.66	1.53
32	8	615	LUT	C22-C23	7.87	1.66	1.53
32	9	318	LUT	C4-C3	7.85	1.65	1.52
32	s	318	LUT	C4-C3	7.85	1.65	1.52
32	6	317	LUT	C4-C3	7.85	1.65	1.52
32	S	317	LUT	C4-C3	7.85	1.65	1.52
32	N	316	LUT	C22-C23	7.85	1.66	1.53
32	G	615	LUT	C4-C3	7.84	1.65	1.52
32	y	616	LUT	C22-C23	7.84	1.66	1.53
32	4	616	LUT	C4-C3	7.84	1.65	1.52
32	7	318	LUT	C4-C3	7.83	1.65	1.52
32	7	317	LUT	C22-C23	7.82	1.66	1.53
36	s	319	NEX	C30-C29	-7.81	1.25	1.35
32	0	616	LUT	C4-C3	7.80	1.65	1.52
36	s	319	NEX	C10-C9	-7.80	1.25	1.35
32	s	317	LUT	C4-C3	7.80	1.65	1.52
32	r	317	LUT	C22-C23	7.79	1.66	1.53
36	9	319	NEX	C10-C9	-7.78	1.25	1.35
32	y	617	LUT	C22-C23	7.78	1.66	1.53
32	5	616	LUT	C4-C3	7.78	1.65	1.52
36	3	319	NEX	C34-C33	-7.78	1.25	1.35
36	G	616	NEX	C34-C33	-7.78	1.25	1.35
32	0	617	LUT	C4-C3	7.77	1.65	1.52
36	G	616	NEX	C30-C29	-7.77	1.25	1.35
36	s	319	NEX	C14-C13	-7.77	1.25	1.35
32	6	318	LUT	C4-C3	7.75	1.65	1.52
36	G	616	NEX	C14-C13	-7.75	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	y	618	NEX	C34-C33	-7.75	1.25	1.35
32	Y	315	LUT	C22-C23	7.74	1.65	1.53
36	3	319	NEX	C30-C29	-7.73	1.25	1.35
32	R	317	LUT	C22-C23	7.72	1.65	1.53
32	8	615	LUT	C4-C3	7.71	1.65	1.52
36	S	319	NEX	C30-C29	-7.71	1.25	1.35
32	Y	316	LUT	C4-C3	7.71	1.65	1.52
36	N	318	NEX	C14-C13	-7.71	1.25	1.35
36	2	616	NEX	C10-C9	-7.69	1.25	1.35
32	n	317	LUT	C4-C3	7.68	1.65	1.52
36	4	617	NEX	C10-C9	-7.68	1.25	1.35
36	y	618	NEX	C10-C9	-7.68	1.25	1.35
32	p	616	LUT	C32-C33	7.68	1.62	1.45
36	R	301	NEX	C10-C9	-7.66	1.25	1.35
36	g	317	NEX	C10-C9	-7.65	1.25	1.35
32	1	615	LUT	C4-C3	7.65	1.65	1.52
36	y	618	NEX	C30-C29	-7.64	1.25	1.35
36	8	617	NEX	C34-C33	-7.64	1.25	1.35
36	S	319	NEX	C14-C13	-7.63	1.25	1.35
32	7	317	LUT	C4-C3	7.62	1.65	1.52
36	r	319	NEX	C30-C29	-7.62	1.25	1.35
36	6	319	NEX	C30-C29	-7.62	1.25	1.35
36	y	618	NEX	C14-C13	-7.62	1.25	1.35
36	R	319	NEX	C14-C13	-7.62	1.25	1.35
36	S	319	NEX	C34-C33	-7.61	1.25	1.35
32	y	617	LUT	C4-C3	7.61	1.65	1.52
36	R	319	NEX	C30-C29	-7.60	1.25	1.35
36	0	618	NEX	C30-C29	-7.60	1.25	1.35
36	R	319	NEX	C10-C9	-7.60	1.25	1.35
32	R	317	LUT	C4-C3	7.60	1.65	1.52
32	2	615	LUT	C32-C33	7.59	1.62	1.45
36	Y	317	NEX	C14-C13	-7.59	1.25	1.35
36	5	618	NEX	C14-C13	-7.59	1.25	1.35
36	r	301	NEX	C30-C29	-7.59	1.25	1.35
36	r	319	NEX	C34-C33	-7.59	1.25	1.35
43	C	615	BCR	C30-C25	-7.58	1.43	1.53
36	4	617	NEX	C14-C13	-7.58	1.25	1.35
36	p	618	NEX	C30-C29	-7.58	1.25	1.35
36	R	319	NEX	C34-C33	-7.57	1.25	1.35
36	q	319	NEX	C30-C29	-7.57	1.25	1.35
36	2	616	NEX	C34-C33	-7.57	1.25	1.35
36	9	319	NEX	C14-C13	-7.57	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	2	616	NEX	C14-C13	-7.57	1.25	1.35
36	q	319	NEX	C34-C33	-7.57	1.25	1.35
36	G	616	NEX	C10-C9	-7.56	1.25	1.35
36	Y	317	NEX	C34-C33	-7.56	1.25	1.35
32	g	316	LUT	C32-C33	7.56	1.62	1.45
43	b	618	BCR	C30-C25	-7.55	1.43	1.53
32	p	617	LUT	C32-C33	7.54	1.62	1.45
36	4	617	NEX	C30-C29	-7.54	1.25	1.35
36	8	617	NEX	C14-C13	-7.54	1.25	1.35
36	5	618	NEX	C30-C29	-7.54	1.25	1.35
36	q	319	NEX	C14-C13	-7.53	1.25	1.35
36	r	301	NEX	C10-C9	-7.53	1.25	1.35
36	p	618	NEX	C34-C33	-7.53	1.25	1.35
36	r	319	NEX	C14-C13	-7.53	1.25	1.35
32	9	318	LUT	C32-C33	7.52	1.62	1.45
32	1	616	LUT	C4-C3	7.52	1.65	1.52
36	r	301	NEX	C14-C13	-7.52	1.25	1.35
36	r	301	NEX	C34-C33	-7.52	1.25	1.35
36	Y	317	NEX	C10-C9	-7.52	1.25	1.35
32	5	617	LUT	C32-C33	7.52	1.62	1.45
36	8	617	NEX	C30-C29	-7.52	1.25	1.35
36	4	617	NEX	C34-C33	-7.52	1.25	1.35
36	5	618	NEX	C34-C33	-7.51	1.25	1.35
36	R	301	NEX	C30-C29	-7.51	1.25	1.35
36	p	618	NEX	C14-C13	-7.51	1.25	1.35
43	V	101	BCR	C30-C25	-7.50	1.43	1.53
36	g	317	NEX	C34-C33	-7.50	1.25	1.35
36	r	319	NEX	C10-C9	-7.50	1.25	1.35
32	Y	315	LUT	C4-C3	7.50	1.65	1.52
43	d	406	BCR	C30-C25	-7.50	1.43	1.53
32	3	318	LUT	C32-C33	7.50	1.62	1.45
36	2	616	NEX	C30-C29	-7.49	1.25	1.35
36	5	618	NEX	C10-C9	-7.49	1.25	1.35
36	8	617	NEX	C10-C9	-7.48	1.25	1.35
32	r	317	LUT	C4-C3	7.48	1.65	1.52
36	0	618	NEX	C34-C33	-7.48	1.25	1.35
32	5	616	LUT	C32-C33	7.48	1.62	1.45
32	q	318	LUT	C32-C33	7.47	1.62	1.45
36	6	319	NEX	C34-C33	-7.47	1.25	1.35
32	4	616	LUT	C32-C33	7.47	1.62	1.45
36	6	319	NEX	C14-C13	-7.47	1.25	1.35
36	0	618	NEX	C14-C13	-7.47	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Y	317	NEX	C30-C29	-7.46	1.25	1.35
36	g	317	NEX	C14-C13	-7.46	1.25	1.35
36	q	319	NEX	C10-C9	-7.45	1.25	1.35
32	y	616	LUT	C4-C3	7.44	1.65	1.52
32	N	317	LUT	C32-C33	7.44	1.61	1.45
36	g	317	NEX	C30-C29	-7.44	1.25	1.35
32	S	318	LUT	C32-C33	7.42	1.61	1.45
36	N	318	NEX	C30-C29	-7.41	1.26	1.35
36	N	318	NEX	C34-C33	-7.41	1.26	1.35
32	3	317	LUT	C32-C33	7.41	1.61	1.45
32	6	318	LUT	C32-C33	7.39	1.61	1.45
36	p	618	NEX	C10-C9	-7.39	1.26	1.35
36	N	318	NEX	C10-C9	-7.39	1.26	1.35
32	N	316	LUT	C32-C33	7.39	1.61	1.45
43	C	614	BCR	C30-C25	-7.38	1.43	1.53
36	n	319	NEX	C14-C13	-7.37	1.26	1.35
36	6	319	NEX	C10-C9	-7.36	1.26	1.35
32	8	616	LUT	C32-C33	7.35	1.61	1.45
32	7	318	LUT	C32-C33	7.34	1.61	1.45
36	0	618	NEX	C10-C9	-7.33	1.26	1.35
32	n	318	LUT	C32-C33	7.33	1.61	1.45
43	c	615	BCR	C30-C25	-7.31	1.43	1.53
32	n	317	LUT	C32-C33	7.28	1.61	1.45
36	n	319	NEX	C10-C9	-7.27	1.26	1.35
32	8	615	LUT	C32-C33	7.27	1.61	1.45
32	s	317	LUT	C32-C33	7.27	1.61	1.45
32	S	317	LUT	C32-C33	7.26	1.61	1.45
32	6	317	LUT	C32-C33	7.25	1.61	1.45
32	s	318	LUT	C32-C33	7.25	1.61	1.45
36	n	319	NEX	C34-C33	-7.25	1.26	1.35
43	t	101	BCR	C2-C3	-7.19	1.34	1.52
32	0	617	LUT	C32-C33	7.19	1.61	1.45
32	R	317	LUT	C32-C33	7.19	1.61	1.45
36	n	319	NEX	C30-C29	-7.17	1.26	1.35
43	A	410	BCR	C30-C25	-7.15	1.43	1.53
43	h	101	BCR	C30-C25	-7.13	1.44	1.53
43	t	101	BCR	C30-C25	-7.11	1.44	1.53
43	B	619	BCR	C30-C25	-7.09	1.44	1.53
43	Z	101	BCR	C30-C25	-7.07	1.44	1.53
32	Y	316	LUT	C32-C33	7.06	1.61	1.45
32	1	616	LUT	C32-C33	7.06	1.61	1.45
43	B	617	BCR	C1-C6	-7.06	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	H	101	BCR	C30-C25	-7.05	1.44	1.53
43	b	620	BCR	C30-C25	-7.05	1.44	1.53
43	v	101	BCR	C30-C25	-7.05	1.44	1.53
32	0	616	LUT	C32-C33	7.05	1.61	1.45
43	c	615	BCR	C1-C6	-7.02	1.44	1.53
32	7	317	LUT	C32-C33	7.02	1.61	1.45
43	c	614	BCR	C30-C25	-7.00	1.44	1.53
43	T	101	BCR	C2-C3	-7.00	1.35	1.52
43	z	101	BCR	C1-C6	-6.98	1.44	1.53
32	y	617	LUT	C32-C33	6.98	1.60	1.45
36	3	319	NEX	C35-C15	-6.96	1.17	1.36
43	d	406	BCR	C2-C3	-6.96	1.35	1.52
43	D	405	BCR	C30-C25	-6.95	1.44	1.53
43	z	101	BCR	C30-C25	-6.95	1.44	1.53
43	C	615	BCR	C2-C3	-6.94	1.35	1.52
43	Z	101	BCR	C1-C6	-6.94	1.44	1.53
32	1	615	LUT	C32-C33	6.91	1.60	1.45
36	s	319	NEX	C35-C15	-6.91	1.18	1.36
36	9	319	NEX	C35-C15	-6.90	1.18	1.36
36	R	301	NEX	C35-C15	-6.90	1.18	1.36
43	B	618	BCR	C30-C25	-6.89	1.44	1.53
36	S	319	NEX	C35-C15	-6.88	1.18	1.36
43	Z	101	BCR	C2-C3	-6.87	1.35	1.52
43	T	101	BCR	C30-C25	-6.87	1.44	1.53
36	R	319	NEX	C35-C15	-6.86	1.18	1.36
43	C	614	BCR	C1-C6	-6.85	1.44	1.53
36	r	319	NEX	C35-C15	-6.85	1.18	1.36
32	Y	315	LUT	C32-C33	6.85	1.60	1.45
36	G	616	NEX	C35-C15	-6.85	1.18	1.36
43	C	615	BCR	C1-C6	-6.84	1.44	1.53
32	1	615	LUT	C1-C6	-6.83	1.44	1.53
43	B	619	BCR	C1-C6	-6.83	1.44	1.53
36	p	618	NEX	C35-C15	-6.83	1.18	1.36
43	z	101	BCR	C2-C3	-6.83	1.35	1.52
36	y	618	NEX	C35-C15	-6.82	1.18	1.36
32	y	616	LUT	C32-C33	6.82	1.60	1.45
36	6	319	NEX	C35-C15	-6.81	1.18	1.36
43	c	614	BCR	C2-C3	-6.81	1.35	1.52
43	V	101	BCR	C1-C6	-6.81	1.44	1.53
36	0	618	NEX	C35-C15	-6.81	1.18	1.36
32	Y	316	LUT	C1-C6	-6.81	1.44	1.53
43	h	101	BCR	C2-C3	-6.80	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	r	301	NEX	C35-C15	-6.80	1.18	1.36
43	B	617	BCR	C2-C3	-6.80	1.35	1.52
43	H	101	BCR	C2-C3	-6.79	1.35	1.52
35	g	315	RRX	C30-C25	-6.79	1.44	1.53
36	q	319	NEX	C35-C15	-6.79	1.18	1.36
32	r	317	LUT	C32-C33	6.79	1.60	1.45
36	8	617	NEX	C35-C15	-6.79	1.18	1.36
43	b	619	BCR	C1-C6	-6.79	1.44	1.53
36	2	616	NEX	C35-C15	-6.79	1.18	1.36
32	R	317	LUT	C1-C6	-6.79	1.44	1.53
43	b	619	BCR	C30-C25	-6.78	1.44	1.53
36	Y	317	NEX	C35-C15	-6.77	1.18	1.36
43	b	620	BCR	C2-C3	-6.77	1.35	1.52
36	5	618	NEX	C35-C15	-6.77	1.18	1.36
32	y	617	LUT	C1-C6	-6.76	1.44	1.53
43	b	620	BCR	C1-C6	-6.76	1.44	1.53
36	4	617	NEX	C35-C15	-6.76	1.18	1.36
43	B	619	BCR	C2-C3	-6.76	1.35	1.52
43	a	410	BCR	C2-C3	-6.76	1.35	1.52
43	v	101	BCR	C2-C3	-6.74	1.35	1.52
43	v	101	BCR	C1-C6	-6.74	1.44	1.53
43	b	618	BCR	C2-C3	-6.73	1.35	1.52
43	C	615	BCR	C29-C28	-6.73	1.35	1.52
43	A	410	BCR	C2-C3	-6.73	1.35	1.52
36	g	317	NEX	C35-C15	-6.72	1.18	1.36
43	a	410	BCR	C30-C25	-6.72	1.44	1.53
36	N	318	NEX	C35-C15	-6.72	1.18	1.36
43	V	101	BCR	C2-C3	-6.71	1.36	1.52
36	n	319	NEX	C35-C15	-6.70	1.18	1.36
32	0	617	LUT	C1-C6	-6.70	1.44	1.53
43	D	405	BCR	C2-C3	-6.69	1.36	1.52
43	C	614	BCR	C2-C3	-6.69	1.36	1.52
43	h	101	BCR	C1-C6	-6.67	1.44	1.53
32	7	317	LUT	C1-C6	-6.67	1.44	1.53
32	y	616	LUT	C1-C6	-6.67	1.44	1.53
43	a	410	BCR	C1-C6	-6.67	1.44	1.53
43	c	615	BCR	C2-C3	-6.63	1.36	1.52
35	q	317	RRX	C2-C3	-6.62	1.36	1.52
43	B	618	BCR	C2-C3	-6.62	1.36	1.52
32	2	615	LUT	C1-C6	-6.60	1.44	1.53
32	3	318	LUT	C1-C6	-6.60	1.44	1.53
32	8	616	LUT	C1-C6	-6.60	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	616	LUT	C1-C6	-6.60	1.44	1.53
32	r	317	LUT	C1-C6	-6.59	1.44	1.53
32	N	317	LUT	C1-C6	-6.59	1.44	1.53
32	Y	315	LUT	C1-C6	-6.59	1.44	1.53
43	B	617	BCR	C29-C28	-6.57	1.36	1.52
43	b	619	BCR	C2-C3	-6.57	1.36	1.52
43	H	101	BCR	C1-C6	-6.56	1.44	1.53
43	a	410	BCR	C29-C28	-6.56	1.36	1.52
43	d	406	BCR	C29-C28	-6.55	1.36	1.52
32	n	318	LUT	C1-C6	-6.54	1.44	1.53
43	z	101	BCR	C29-C28	-6.52	1.36	1.52
43	Z	101	BCR	C29-C28	-6.51	1.36	1.52
43	A	410	BCR	C1-C6	-6.50	1.44	1.53
35	2	614	RRX	C2-C3	-6.50	1.36	1.52
43	c	614	BCR	C29-C28	-6.50	1.36	1.52
35	G	614	RRX	C2-C3	-6.50	1.36	1.52
31	B	604	CLA	MG-NA	6.48	2.21	2.06
43	t	101	BCR	C1-C6	-6.48	1.44	1.53
36	9	319	NEX	C11-C12	-6.47	1.17	1.34
43	B	618	BCR	C29-C28	-6.47	1.36	1.52
36	s	319	NEX	C11-C12	-6.47	1.17	1.34
35	9	317	RRX	C2-C3	-6.46	1.36	1.52
32	1	616	LUT	C1-C6	-6.46	1.44	1.53
35	4	615	RRX	C2-C3	-6.46	1.36	1.52
32	g	316	LUT	C1-C6	-6.46	1.44	1.53
31	b	605	CLA	MG-NA	6.46	2.21	2.06
31	5	615	CLA	MG-NA	6.46	2.21	2.06
35	g	315	RRX	C2-C3	-6.45	1.36	1.52
32	q	318	LUT	C1-C6	-6.45	1.44	1.53
43	b	619	BCR	C29-C28	-6.45	1.36	1.52
36	9	319	NEX	C31-C32	-6.45	1.18	1.34
43	b	618	BCR	C1-C6	-6.44	1.44	1.53
43	B	619	BCR	C29-C28	-6.43	1.36	1.52
43	B	618	BCR	C1-C6	-6.43	1.44	1.53
32	p	617	LUT	C1-C6	-6.43	1.44	1.53
43	h	101	BCR	C29-C28	-6.42	1.36	1.52
36	3	319	NEX	C11-C12	-6.42	1.18	1.34
43	T	101	BCR	C1-C6	-6.42	1.45	1.53
36	S	319	NEX	C11-C12	-6.41	1.18	1.34
36	s	319	NEX	C31-C32	-6.41	1.18	1.34
35	2	614	RRX	C30-C25	-6.40	1.45	1.53
36	G	616	NEX	C31-C32	-6.40	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	R	301	NEX	C11-C12	-6.39	1.18	1.34
36	y	618	NEX	C11-C12	-6.39	1.18	1.34
36	p	618	NEX	C11-C12	-6.39	1.18	1.34
32	6	317	LUT	C1-C6	-6.39	1.45	1.53
43	H	101	BCR	C29-C28	-6.39	1.36	1.52
43	b	620	BCR	C29-C28	-6.39	1.36	1.52
32	s	318	LUT	C1-C6	-6.39	1.45	1.53
32	N	316	LUT	C1-C6	-6.38	1.45	1.53
31	G	610	CLA	MG-NA	6.38	2.21	2.06
36	4	617	NEX	C11-C12	-6.38	1.18	1.34
36	g	317	NEX	C11-C12	-6.38	1.18	1.34
32	6	318	LUT	C1-C6	-6.37	1.45	1.53
43	T	101	BCR	C29-C28	-6.37	1.36	1.52
31	g	311	CLA	MG-NA	6.37	2.21	2.06
36	S	319	NEX	C31-C32	-6.37	1.18	1.34
31	2	604	CLA	MG-NA	6.37	2.21	2.06
43	d	406	BCR	C1-C6	-6.37	1.45	1.53
32	S	317	LUT	C1-C6	-6.37	1.45	1.53
32	4	616	LUT	C1-C6	-6.36	1.45	1.53
36	2	616	NEX	C11-C12	-6.36	1.18	1.34
36	6	319	NEX	C11-C12	-6.36	1.18	1.34
43	t	101	BCR	C29-C28	-6.36	1.36	1.52
43	v	101	BCR	C29-C28	-6.36	1.36	1.52
36	R	319	NEX	C11-C12	-6.36	1.18	1.34
36	R	319	NEX	C31-C32	-6.35	1.18	1.34
32	7	318	LUT	C1-C6	-6.35	1.45	1.53
36	y	618	NEX	C31-C32	-6.35	1.18	1.34
31	6	304	CLA	MG-NA	6.35	2.21	2.06
36	0	618	NEX	C11-C12	-6.35	1.18	1.34
36	G	616	NEX	C11-C12	-6.35	1.18	1.34
32	S	318	LUT	C1-C6	-6.34	1.45	1.53
36	0	618	NEX	C31-C32	-6.34	1.18	1.34
36	3	319	NEX	C31-C32	-6.34	1.18	1.34
36	r	319	NEX	C31-C32	-6.34	1.18	1.34
36	6	319	NEX	C31-C32	-6.33	1.18	1.34
31	G	613	CLA	MG-NA	6.33	2.21	2.06
36	5	618	NEX	C11-C12	-6.33	1.18	1.34
32	5	617	LUT	C1-C6	-6.33	1.45	1.53
35	G	614	RRX	C30-C25	-6.33	1.45	1.53
43	A	410	BCR	C29-C28	-6.32	1.37	1.52
31	q	304	CLA	MG-NA	6.32	2.21	2.06
36	Y	317	NEX	C11-C12	-6.32	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	p	618	NEX	C31-C32	-6.32	1.18	1.34
31	6	312	CLA	MG-NA	6.32	2.21	2.06
36	r	319	NEX	C11-C12	-6.32	1.18	1.34
31	q	316	CLA	MG-NA	6.31	2.21	2.06
35	4	615	RRX	C30-C25	-6.31	1.45	1.53
31	2	609	CLA	MG-NA	6.31	2.21	2.06
31	Y	313	CLA	MG-NA	6.31	2.21	2.06
31	S	314	CLA	MG-NA	6.31	2.21	2.06
36	2	616	NEX	C31-C32	-6.31	1.18	1.34
35	q	317	RRX	C30-C25	-6.30	1.45	1.53
43	c	615	BCR	C29-C28	-6.30	1.37	1.52
31	b	607	CLA	MG-NA	6.30	2.21	2.06
36	Y	317	NEX	C31-C32	-6.30	1.18	1.34
32	s	317	LUT	C1-C6	-6.30	1.45	1.53
31	4	603	CLA	MG-NA	6.30	2.21	2.06
31	7	314	CLA	MG-NA	6.30	2.21	2.06
31	p	612	CLA	MG-NA	6.30	2.21	2.06
36	8	617	NEX	C31-C32	-6.30	1.18	1.34
31	0	603	CLA	MG-NA	6.30	2.21	2.06
31	9	315	CLA	MG-NA	6.29	2.21	2.06
31	5	612	CLA	MG-NA	6.29	2.21	2.06
43	b	618	BCR	C29-C28	-6.29	1.37	1.52
31	B	606	CLA	MG-NA	6.29	2.21	2.06
32	p	616	LUT	C1-C6	-6.29	1.45	1.53
43	D	405	BCR	C1-C6	-6.29	1.45	1.53
31	n	314	CLA	MG-NA	6.29	2.21	2.06
36	5	618	NEX	C31-C32	-6.29	1.18	1.34
31	N	311	CLA	MG-NA	6.29	2.21	2.06
32	9	318	LUT	C1-C6	-6.29	1.45	1.53
31	7	304	CLA	MG-NA	6.29	2.21	2.06
31	3	305	CLA	MG-NA	6.29	2.21	2.06
36	8	617	NEX	C11-C12	-6.28	1.18	1.34
31	9	305	CLA	MG-NA	6.28	2.21	2.06
36	N	318	NEX	C31-C32	-6.28	1.18	1.34
31	7	313	CLA	MG-NA	6.28	2.21	2.06
31	N	313	CLA	MG-NA	6.28	2.21	2.06
31	8	612	CLA	MG-NA	6.27	2.21	2.06
36	r	301	NEX	C31-C32	-6.27	1.18	1.34
31	3	315	CLA	MG-NA	6.27	2.21	2.06
31	5	603	CLA	MG-NA	6.27	2.21	2.06
31	9	313	CLA	MG-NA	6.27	2.21	2.06
32	G	615	LUT	C1-C6	-6.27	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	604	CLA	MG-NA	6.27	2.21	2.06
35	9	317	RRX	C30-C25	-6.27	1.45	1.53
43	c	614	BCR	C1-C6	-6.27	1.45	1.53
36	R	301	NEX	C31-C32	-6.27	1.18	1.34
31	Y	304	CLA	MG-NA	6.27	2.21	2.06
31	q	305	CLA	MG-NA	6.27	2.21	2.06
31	4	611	CLA	MG-NA	6.27	2.21	2.06
31	5	602	CLA	MG-NA	6.27	2.21	2.06
31	G	611	CLA	MG-NA	6.27	2.21	2.06
31	0	613	CLA	MG-NA	6.26	2.21	2.06
31	b	611	CLA	MG-NA	6.26	2.21	2.06
31	R	307	CLA	MG-NA	6.26	2.21	2.06
31	n	315	CLA	MG-NA	6.26	2.21	2.06
31	s	304	CLA	MG-NA	6.26	2.21	2.06
31	0	612	CLA	MG-NA	6.26	2.21	2.06
31	p	611	CLA	MG-NA	6.26	2.21	2.06
31	3	313	CLA	MG-NA	6.26	2.21	2.06
31	8	613	CLA	MG-NA	6.26	2.21	2.06
31	s	314	CLA	MG-NA	6.26	2.21	2.06
31	g	313	CLA	MG-NA	6.25	2.21	2.06
36	4	617	NEX	C31-C32	-6.25	1.18	1.34
31	5	614	CLA	MG-NA	6.25	2.21	2.06
31	c	601	CLA	MG-NA	6.25	2.21	2.06
31	0	614	CLA	MG-NA	6.25	2.21	2.06
31	1	613	CLA	MG-NA	6.25	2.21	2.06
43	D	405	BCR	C29-C28	-6.25	1.37	1.52
31	p	602	CLA	MG-NA	6.25	2.21	2.06
31	1	612	CLA	MG-NA	6.25	2.21	2.06
31	6	314	CLA	MG-NA	6.25	2.21	2.06
31	G	602	CLA	MG-NA	6.24	2.21	2.06
31	9	316	CLA	MG-NA	6.24	2.21	2.06
31	p	610	CLA	MG-NA	6.24	2.21	2.06
31	2	602	CLA	MG-NA	6.24	2.21	2.06
43	C	614	BCR	C29-C28	-6.24	1.37	1.52
31	3	312	CLA	MG-NA	6.24	2.21	2.06
31	S	316	CLA	MG-NA	6.24	2.21	2.06
31	0	611	CLA	MG-NA	6.24	2.21	2.06
31	3	304	CLA	MG-NA	6.23	2.21	2.06
31	y	603	CLA	MG-NA	6.23	2.21	2.06
31	2	603	CLA	MG-NA	6.23	2.21	2.06
31	S	310	CLA	MG-NA	6.23	2.21	2.06
31	1	603	CLA	MG-NA	6.23	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	303	CLA	MG-NA	6.23	2.21	2.06
31	n	312	CLA	MG-NA	6.23	2.21	2.06
31	B	611	CLA	MG-NA	6.23	2.21	2.06
31	5	613	CLA	MG-NA	6.23	2.21	2.06
31	g	305	CLA	MG-NA	6.23	2.21	2.06
31	8	603	CLA	MG-NA	6.23	2.21	2.06
31	y	614	CLA	MG-NA	6.23	2.21	2.06
31	4	610	CLA	MG-NA	6.23	2.21	2.06
31	8	602	CLA	MG-NA	6.23	2.21	2.06
31	4	602	CLA	MG-NA	6.23	2.21	2.06
36	g	317	NEX	C31-C32	-6.23	1.18	1.34
36	r	301	NEX	C11-C12	-6.23	1.18	1.34
31	s	312	CLA	MG-NA	6.23	2.21	2.06
31	3	314	CLA	MG-NA	6.23	2.21	2.06
31	G	612	CLA	MG-NA	6.22	2.21	2.06
31	r	307	CLA	MG-NA	6.22	2.21	2.06
31	Y	303	CLA	MG-NA	6.22	2.21	2.06
31	n	313	CLA	MG-NA	6.22	2.21	2.06
31	C	603	CLA	MG-NA	6.22	2.21	2.06
31	b	609	CLA	MG-NA	6.22	2.21	2.06
31	S	306	CLA	MG-NA	6.22	2.21	2.06
32	8	615	LUT	C1-C6	-6.22	1.45	1.53
31	8	609	CLA	MG-NA	6.22	2.21	2.06
31	Y	310	CLA	MG-NA	6.22	2.21	2.06
31	s	306	CLA	MG-NA	6.21	2.21	2.06
31	b	612	CLA	MG-NA	6.21	2.21	2.06
31	5	611	CLA	MG-NA	6.21	2.21	2.06
36	q	319	NEX	C31-C32	-6.21	1.18	1.34
31	N	314	CLA	MG-NA	6.21	2.21	2.06
31	Y	312	CLA	MG-NA	6.21	2.21	2.06
31	c	603	CLA	MG-NA	6.21	2.21	2.06
31	g	314	CLA	MG-NA	6.21	2.21	2.06
31	n	311	CLA	MG-NA	6.21	2.21	2.06
31	7	311	CLA	MG-NA	6.21	2.21	2.06
31	8	610	CLA	MG-NA	6.21	2.21	2.06
31	7	316	CLA	MG-NA	6.21	2.21	2.06
31	p	603	CLA	MG-NA	6.21	2.21	2.06
31	7	315	CLA	MG-NA	6.21	2.21	2.06
35	q	317	RRX	C1-C6	-6.21	1.45	1.53
36	q	319	NEX	C11-C12	-6.21	1.18	1.34
31	s	316	CLA	MG-NA	6.21	2.21	2.06
31	5	604	CLA	MG-NA	6.21	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	312	CLA	MG-NA	6.21	2.21	2.06
31	7	312	CLA	MG-NA	6.21	2.21	2.06
31	4	614	CLA	MG-NA	6.20	2.21	2.06
31	N	315	CLA	MG-NA	6.20	2.21	2.06
31	b	614	CLA	MG-NA	6.20	2.21	2.06
31	6	316	CLA	MG-NA	6.20	2.21	2.06
31	B	614	CLA	MG-NA	6.20	2.21	2.06
31	S	304	CLA	MG-NA	6.20	2.21	2.06
31	8	614	CLA	MG-NA	6.20	2.21	2.06
31	2	610	CLA	MG-NA	6.20	2.21	2.06
31	1	614	CLA	MG-NA	6.20	2.21	2.06
31	1	611	CLA	MG-NA	6.20	2.21	2.06
32	n	317	LUT	C1-C6	-6.20	1.45	1.53
31	g	312	CLA	MG-NA	6.20	2.21	2.06
31	8	604	CLA	MG-NA	6.20	2.21	2.06
31	r	313	CLA	MG-NA	6.20	2.21	2.06
31	s	303	CLA	MG-NA	6.20	2.21	2.06
31	C	611	CLA	MG-NA	6.19	2.21	2.06
31	9	306	CLA	MG-NA	6.19	2.21	2.06
31	3	311	CLA	MG-NA	6.19	2.21	2.06
31	N	304	CLA	MG-NA	6.19	2.21	2.06
31	N	303	CLA	MG-NA	6.19	2.21	2.06
31	b	603	CLA	MG-NA	6.19	2.21	2.06
31	y	602	CLA	MG-NA	6.19	2.21	2.06
31	S	305	CLA	MG-NA	6.19	2.21	2.06
32	3	317	LUT	C1-C6	-6.19	1.45	1.53
31	8	611	CLA	MG-NA	6.19	2.21	2.06
31	n	303	CLA	MG-NA	6.19	2.21	2.06
31	C	601	CLA	MG-NA	6.19	2.21	2.06
31	p	614	CLA	MG-NA	6.19	2.21	2.06
36	n	319	NEX	C11-C12	-6.18	1.18	1.34
31	B	610	CLA	MG-NA	6.18	2.21	2.06
31	p	604	CLA	MG-NA	6.18	2.21	2.06
31	N	321	CLA	MG-NA	6.18	2.21	2.06
31	y	610	CLA	MG-NA	6.18	2.21	2.06
31	3	306	CLA	MG-NA	6.18	2.21	2.06
31	N	310	CLA	MG-NA	6.18	2.20	2.06
31	q	312	CLA	MG-NA	6.18	2.20	2.06
31	2	613	CLA	MG-NA	6.18	2.20	2.06
31	2	612	CLA	MG-NA	6.18	2.20	2.06
31	a	407	CLA	MG-NA	6.18	2.20	2.06
31	6	313	CLA	MG-NA	6.18	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	603	CLA	MG-NA	6.17	2.20	2.06
35	2	614	RRX	C1-C6	-6.17	1.45	1.53
31	R	303	CLA	MG-NA	6.17	2.20	2.06
31	y	604	CLA	MG-NA	6.17	2.20	2.06
31	B	613	CLA	MG-NA	6.17	2.20	2.06
31	b	613	CLA	MG-NA	6.17	2.20	2.06
31	6	311	CLA	MG-NA	6.17	2.20	2.06
31	b	604	CLA	MG-NA	6.17	2.20	2.06
31	R	306	CLA	MG-NA	6.17	2.20	2.06
31	R	313	CLA	MG-NA	6.17	2.20	2.06
31	b	615	CLA	MG-NA	6.17	2.20	2.06
31	r	314	CLA	MG-NA	6.17	2.20	2.06
31	Y	314	CLA	MG-NA	6.17	2.20	2.06
31	c	602	CLA	MG-NA	6.17	2.20	2.06
31	s	310	CLA	MG-NA	6.17	2.20	2.06
31	6	303	CLA	MG-NA	6.17	2.20	2.06
31	S	313	CLA	MG-NA	6.17	2.20	2.06
31	n	305	CLA	MG-NA	6.17	2.20	2.06
31	4	613	CLA	MG-NA	6.16	2.20	2.06
31	g	304	CLA	MG-NA	6.16	2.20	2.06
31	s	305	CLA	MG-NA	6.16	2.20	2.06
31	S	303	CLA	MG-NA	6.16	2.20	2.06
31	0	615	CLA	MG-NA	6.16	2.20	2.06
31	1	602	CLA	MG-NA	6.16	2.20	2.06
31	n	316	CLA	MG-NA	6.15	2.20	2.06
31	Y	311	CLA	MG-NA	6.15	2.20	2.06
31	B	608	CLA	MG-NA	6.15	2.20	2.06
31	Y	305	CLA	MG-NA	6.14	2.20	2.06
31	5	610	CLA	MG-NA	6.14	2.20	2.06
31	G	604	CLA	MG-NA	6.14	2.20	2.06
31	N	305	CLA	MG-NA	6.14	2.20	2.06
31	r	305	CLA	MG-NA	6.14	2.20	2.06
31	s	313	CLA	MG-NA	6.14	2.20	2.06
31	y	615	CLA	MG-NA	6.14	2.20	2.06
36	n	319	NEX	C31-C32	-6.14	1.18	1.34
31	c	611	CLA	MG-NA	6.14	2.20	2.06
31	y	612	CLA	MG-NA	6.13	2.20	2.06
31	n	304	CLA	MG-NA	6.13	2.20	2.06
31	6	315	CLA	MG-NA	6.13	2.20	2.06
31	c	607	CLA	MG-NA	6.13	2.20	2.06
31	2	611	CLA	MG-NA	6.13	2.20	2.06
31	B	612	CLA	MG-NA	6.13	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	V	101	BCR	C29-C28	-6.13	1.37	1.52
31	b	617	CLA	MG-NA	6.12	2.20	2.06
35	9	317	RRX	C19-C18	6.12	1.59	1.45
31	r	316	CLA	MG-NA	6.12	2.20	2.06
31	B	601	CLA	MG-NA	6.12	2.20	2.06
31	S	315	CLA	MG-NA	6.12	2.20	2.06
31	p	615	CLA	MG-NA	6.12	2.20	2.06
31	6	305	CLA	MG-NA	6.12	2.20	2.06
31	C	602	CLA	MG-NA	6.11	2.20	2.06
31	7	305	CLA	MG-NA	6.11	2.20	2.06
35	4	615	RRX	C19-C18	6.11	1.59	1.45
31	C	612	CLA	MG-NA	6.11	2.20	2.06
31	C	607	CLA	MG-NA	6.11	2.20	2.06
31	0	602	CLA	MG-NA	6.11	2.20	2.06
31	S	312	CLA	MG-NA	6.11	2.20	2.06
35	4	615	RRX	C1-C6	-6.11	1.45	1.53
31	9	304	CLA	MG-NA	6.11	2.20	2.06
31	B	602	CLA	MG-NA	6.10	2.20	2.06
31	c	608	CLA	MG-NA	6.10	2.20	2.06
31	b	610	CLA	MG-NA	6.10	2.20	2.06
35	9	317	RRX	C1-C6	-6.10	1.45	1.53
31	c	609	CLA	MG-NA	6.10	2.20	2.06
31	q	306	CLA	MG-NA	6.10	2.20	2.06
31	r	304	CLA	MG-NA	6.10	2.20	2.06
31	r	306	CLA	MG-NA	6.10	2.20	2.06
31	p	613	CLA	MG-NA	6.09	2.20	2.06
31	d	405	CLA	MG-NA	6.09	2.20	2.06
31	C	606	CLA	MG-NA	6.09	2.20	2.06
31	C	613	CLA	MG-NA	6.09	2.20	2.06
31	b	616	CLA	MG-NA	6.09	2.20	2.06
31	B	603	CLA	MG-NA	6.09	2.20	2.06
31	R	314	CLA	MG-NA	6.09	2.20	2.06
36	N	318	NEX	C11-C12	-6.08	1.18	1.34
35	G	614	RRX	C1-C6	-6.08	1.45	1.53
31	s	315	CLA	MG-NA	6.08	2.20	2.06
31	B	616	CLA	MG-NA	6.08	2.20	2.06
31	1	610	CLA	MG-NA	6.08	2.20	2.06
31	B	615	CLA	MG-NA	6.08	2.20	2.06
31	S	311	CLA	MG-NA	6.08	2.20	2.06
31	R	305	CLA	MG-NA	6.07	2.20	2.06
31	y	611	CLA	MG-NA	6.07	2.20	2.06
31	s	311	CLA	MG-NA	6.07	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C	610	CLA	MG-NA	6.07	2.20	2.06
31	c	613	CLA	MG-NA	6.07	2.20	2.06
31	c	612	CLA	MG-NA	6.07	2.20	2.06
35	G	614	RRX	C19-C18	6.06	1.59	1.45
31	B	609	CLA	MG-NA	6.06	2.20	2.06
31	R	304	CLA	MG-NA	6.06	2.20	2.06
31	c	605	CLA	MG-NA	6.06	2.20	2.06
31	q	314	CLA	MG-NA	6.05	2.20	2.06
31	C	609	CLA	MG-NA	6.05	2.20	2.06
31	B	605	CLA	MG-NA	6.05	2.20	2.06
31	C	604	CLA	MG-NA	6.05	2.20	2.06
31	D	403	CLA	MG-NA	6.04	2.20	2.06
31	R	312	CLA	MG-NA	6.04	2.20	2.06
31	d	401	CLA	MG-NA	6.04	2.20	2.06
31	R	316	CLA	MG-NA	6.04	2.20	2.06
31	c	606	CLA	MG-NA	6.04	2.20	2.06
35	2	614	RRX	C19-C18	6.04	1.58	1.45
31	g	310	CLA	MG-NA	6.03	2.20	2.06
32	5	616	LUT	C1-C6	-6.03	1.45	1.53
31	A	406	CLA	MG-NA	6.03	2.20	2.06
31	a	406	CLA	MG-NA	6.03	2.20	2.06
31	C	608	CLA	MG-NA	6.02	2.20	2.06
31	b	606	CLA	MG-NA	6.02	2.20	2.06
31	b	608	CLA	MG-NA	6.02	2.20	2.06
31	0	604	CLA	MG-NA	6.01	2.20	2.06
31	b	602	CLA	MG-NA	6.01	2.20	2.06
35	g	315	RRX	C19-C18	6.01	1.58	1.45
31	R	315	CLA	MG-NA	6.01	2.20	2.06
35	g	315	RRX	C1-C6	-6.00	1.45	1.53
31	c	610	CLA	MG-NA	6.00	2.20	2.06
31	D	404	CLA	MG-NA	6.00	2.20	2.06
31	d	404	CLA	MG-NA	6.00	2.20	2.06
31	R	311	CLA	MG-NA	5.99	2.20	2.06
31	G	609	CLA	MG-NA	5.99	2.20	2.06
31	0	610	CLA	MG-NA	5.99	2.20	2.06
31	A	405	CLA	MG-NA	5.98	2.20	2.06
31	A	407	CLA	MG-NA	5.96	2.20	2.06
31	r	312	CLA	MG-NA	5.96	2.20	2.06
31	l	604	CLA	MG-NA	5.96	2.20	2.06
31	y	613	CLA	MG-NA	5.95	2.20	2.06
31	c	604	CLA	MG-NA	5.95	2.20	2.06
31	r	315	CLA	MG-NA	5.93	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	301	CLA	MG-NA	5.92	2.20	2.06
31	g	303	CLA	MG-NA	5.90	2.20	2.06
31	q	312	CLA	C3B-C4B	5.89	1.46	1.39
31	A	409	CLA	MG-NA	5.88	2.20	2.06
31	9	314	CLA	MG-NA	5.88	2.20	2.06
31	3	316	CLA	MG-NA	5.88	2.20	2.06
31	r	311	CLA	MG-NA	5.88	2.20	2.06
31	q	313	CLA	MG-NA	5.88	2.20	2.06
31	4	611	CLA	C3B-C4B	5.88	1.46	1.39
31	a	409	CLA	MG-NA	5.86	2.20	2.06
31	4	612	CLA	MG-NA	5.86	2.20	2.06
31	r	303	CLA	MG-NA	5.84	2.20	2.06
43	c	614	BCR	C12-C13	5.82	1.58	1.45
43	D	405	BCR	C12-C13	5.82	1.58	1.45
31	B	607	CLA	MG-NA	5.82	2.20	2.06
31	q	315	CLA	MG-NA	5.81	2.20	2.06
31	9	312	CLA	MG-NA	5.80	2.20	2.06
43	T	101	BCR	C12-C13	5.74	1.58	1.45
31	C	605	CLA	MG-NA	5.69	2.19	2.06
35	q	317	RRX	C19-C18	5.67	1.58	1.45
43	c	615	BCR	C12-C13	5.66	1.58	1.45
31	q	313	CLA	C3B-C4B	5.65	1.46	1.39
36	p	618	NEX	C7-C8	5.56	1.41	1.32
43	v	101	BCR	C12-C13	5.56	1.57	1.45
36	y	618	NEX	C28-C29	-5.56	1.34	1.45
43	A	410	BCR	C12-C13	5.54	1.57	1.45
43	D	405	BCR	C8-C9	5.54	1.57	1.45
36	0	618	NEX	C28-C29	-5.54	1.34	1.45
36	r	319	NEX	C28-C29	-5.54	1.34	1.45
43	z	101	BCR	C12-C13	5.53	1.57	1.45
36	6	319	NEX	C28-C29	-5.53	1.34	1.45
36	N	318	NEX	C7-C8	5.53	1.41	1.32
43	B	619	BCR	C12-C13	5.53	1.57	1.45
36	R	319	NEX	C28-C29	-5.53	1.34	1.45
36	q	319	NEX	C28-C29	-5.52	1.34	1.45
36	s	319	NEX	C28-C29	-5.52	1.34	1.45
36	S	319	NEX	C28-C29	-5.52	1.34	1.45
43	C	614	BCR	C12-C13	5.52	1.57	1.45
43	H	101	BCR	C12-C13	5.50	1.57	1.45
36	9	319	NEX	C28-C29	-5.49	1.34	1.45
43	b	618	BCR	C12-C13	5.48	1.57	1.45
36	2	616	NEX	C28-C29	-5.48	1.34	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	V	101	BCR	C12-C13	5.47	1.57	1.45
36	r	301	NEX	C28-C29	-5.47	1.34	1.45
43	Z	101	BCR	C12-C13	5.47	1.57	1.45
36	4	617	NEX	C28-C29	-5.47	1.34	1.45
36	3	319	NEX	C28-C29	-5.45	1.34	1.45
36	5	618	NEX	C28-C29	-5.45	1.34	1.45
43	b	620	BCR	C12-C13	5.44	1.57	1.45
36	n	319	NEX	C7-C8	5.44	1.41	1.32
36	G	616	NEX	C28-C29	-5.44	1.34	1.45
36	8	617	NEX	C28-C29	-5.44	1.34	1.45
43	C	615	BCR	C12-C13	5.42	1.57	1.45
36	R	301	NEX	C28-C29	-5.41	1.34	1.45
36	Y	317	NEX	C28-C29	-5.41	1.34	1.45
43	h	101	BCR	C12-C13	5.40	1.57	1.45
36	q	319	NEX	C7-C8	5.40	1.41	1.32
36	p	618	NEX	C28-C29	-5.39	1.34	1.45
43	t	101	BCR	C12-C13	5.39	1.57	1.45
36	g	317	NEX	C28-C29	-5.38	1.34	1.45
36	N	318	NEX	C28-C29	-5.38	1.34	1.45
43	b	619	BCR	C12-C13	5.37	1.57	1.45
43	B	618	BCR	C12-C13	5.35	1.57	1.45
36	S	319	NEX	C7-C8	5.33	1.40	1.32
43	c	614	BCR	C8-C9	5.33	1.57	1.45
43	c	615	BCR	C8-C9	5.33	1.57	1.45
43	D	405	BCR	C23-C22	5.32	1.57	1.45
43	a	410	BCR	C12-C13	5.31	1.57	1.45
36	r	301	NEX	C7-C8	5.31	1.40	1.32
36	Y	317	NEX	C7-C8	5.31	1.40	1.32
36	s	319	NEX	C7-C8	5.30	1.40	1.32
43	t	101	BCR	C29-C30	5.30	1.66	1.54
43	v	101	BCR	C8-C9	5.29	1.57	1.45
36	3	319	NEX	C7-C8	5.28	1.40	1.32
43	T	101	BCR	C8-C9	5.28	1.57	1.45
36	n	319	NEX	C28-C29	-5.27	1.34	1.45
36	8	617	NEX	C7-C8	5.25	1.40	1.32
36	r	319	NEX	C7-C8	5.24	1.40	1.32
43	d	406	BCR	C12-C13	5.24	1.57	1.45
43	V	101	BCR	C8-C9	5.24	1.57	1.45
36	0	618	NEX	C7-C8	5.24	1.40	1.32
36	6	319	NEX	C7-C8	5.23	1.40	1.32
43	V	101	BCR	C29-C30	5.23	1.66	1.54
43	B	617	BCR	C12-C13	5.22	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	y	618	NEX	C7-C8	5.20	1.40	1.32
36	5	618	NEX	C7-C8	5.19	1.40	1.32
43	b	619	BCR	C23-C22	5.19	1.57	1.45
43	b	618	BCR	C8-C9	5.18	1.57	1.45
43	b	619	BCR	C8-C9	5.18	1.57	1.45
43	A	410	BCR	C8-C9	5.18	1.57	1.45
36	R	319	NEX	C7-C8	5.16	1.40	1.32
43	D	405	BCR	C29-C30	5.16	1.66	1.54
43	T	101	BCR	C29-C30	5.15	1.66	1.54
43	B	618	BCR	C8-C9	5.15	1.57	1.45
43	B	619	BCR	C8-C9	5.15	1.57	1.45
36	g	317	NEX	C7-C8	5.14	1.40	1.32
43	b	620	BCR	C23-C22	5.13	1.57	1.45
36	4	617	NEX	C7-C8	5.11	1.40	1.32
43	z	101	BCR	C8-C9	5.10	1.56	1.45
36	2	616	NEX	C7-C8	5.10	1.40	1.32
43	c	615	BCR	C23-C22	5.10	1.56	1.45
43	H	101	BCR	C29-C30	5.09	1.65	1.54
43	v	101	BCR	C23-C22	5.09	1.56	1.45
35	q	317	RRX	C8-C9	5.09	1.56	1.45
43	h	101	BCR	C29-C30	5.09	1.65	1.54
32	p	616	LUT	C8-C9	5.08	1.56	1.45
35	G	614	RRX	C8-C9	5.07	1.56	1.45
35	4	615	RRX	C8-C9	5.07	1.56	1.45
32	5	617	LUT	C8-C9	5.07	1.56	1.45
35	9	317	RRX	C8-C9	5.06	1.56	1.45
43	v	101	BCR	C29-C30	5.06	1.65	1.54
32	5	616	LUT	C8-C9	5.05	1.56	1.45
35	g	315	RRX	C8-C9	5.05	1.56	1.45
43	a	410	BCR	C8-C9	5.04	1.56	1.45
43	C	614	BCR	C8-C9	5.04	1.56	1.45
43	H	101	BCR	C8-C9	5.04	1.56	1.45
43	C	614	BCR	C29-C30	5.03	1.65	1.54
43	B	618	BCR	C23-C22	5.03	1.56	1.45
32	9	318	LUT	C8-C9	5.02	1.56	1.45
43	B	619	BCR	C23-C22	5.01	1.56	1.45
43	T	101	BCR	C23-C22	5.01	1.56	1.45
43	b	620	BCR	C8-C9	5.01	1.56	1.45
43	B	618	BCR	C29-C30	5.01	1.65	1.54
43	H	101	BCR	C23-C22	5.00	1.56	1.45
43	A	410	BCR	C23-C22	5.00	1.56	1.45
43	A	410	BCR	C29-C30	4.99	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	c	615	BCR	C29-C30	4.99	1.65	1.54
43	d	406	BCR	C8-C9	4.99	1.56	1.45
32	3	318	LUT	C8-C9	4.98	1.56	1.45
32	G	615	LUT	C8-C9	4.98	1.56	1.45
43	b	620	BCR	C29-C30	4.98	1.65	1.54
35	2	614	RRX	C8-C9	4.98	1.56	1.45
43	b	619	BCR	C29-C30	4.98	1.65	1.54
36	9	319	NEX	C7-C8	4.97	1.40	1.32
43	b	618	BCR	C29-C30	4.97	1.65	1.54
36	R	301	NEX	C7-C8	4.97	1.40	1.32
43	B	619	BCR	C29-C30	4.97	1.65	1.54
43	a	410	BCR	C29-C30	4.97	1.65	1.54
32	g	316	LUT	C8-C9	4.97	1.56	1.45
32	2	615	LUT	C8-C9	4.96	1.56	1.45
43	B	617	BCR	C8-C9	4.96	1.56	1.45
32	q	318	LUT	C8-C9	4.96	1.56	1.45
32	p	617	LUT	C8-C9	4.95	1.56	1.45
43	h	101	BCR	C8-C9	4.94	1.56	1.45
43	t	101	BCR	C8-C9	4.94	1.56	1.45
43	a	410	BCR	C23-C22	4.93	1.56	1.45
43	d	406	BCR	C29-C30	4.93	1.65	1.54
32	3	317	LUT	C8-C9	4.93	1.56	1.45
32	y	616	LUT	C4-C5	-4.93	1.43	1.51
36	G	616	NEX	C7-C8	4.93	1.40	1.32
35	g	315	RRX	C2-C1	4.91	1.65	1.54
43	z	101	BCR	C29-C30	4.91	1.65	1.54
32	Y	315	LUT	C4-C5	-4.91	1.43	1.51
43	h	101	BCR	C23-C22	4.91	1.56	1.45
35	4	615	RRX	C23-C22	4.90	1.56	1.45
43	Z	101	BCR	C8-C9	4.88	1.56	1.45
35	9	317	RRX	C23-C22	4.88	1.56	1.45
43	D	405	BCR	C15-C14	4.88	1.58	1.43
32	S	318	LUT	C8-C9	4.88	1.56	1.45
35	2	614	RRX	C23-C22	4.88	1.56	1.45
43	C	615	BCR	C23-C22	4.87	1.56	1.45
43	Z	101	BCR	C29-C30	4.86	1.65	1.54
32	7	317	LUT	C4-C5	-4.86	1.43	1.51
32	7	318	LUT	C8-C9	4.86	1.56	1.45
32	N	316	LUT	C8-C9	4.86	1.56	1.45
35	G	614	RRX	C23-C22	4.86	1.56	1.45
32	N	317	LUT	C8-C9	4.86	1.56	1.45
35	g	315	RRX	C23-C22	4.85	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	615	BCR	C15-C14	4.85	1.58	1.43
43	t	101	BCR	C23-C22	4.85	1.56	1.45
43	Z	101	BCR	C23-C22	4.84	1.56	1.45
32	n	318	LUT	C8-C9	4.82	1.56	1.45
43	c	615	BCR	C15-C14	4.82	1.58	1.43
32	p	616	LUT	C12-C13	4.82	1.56	1.45
32	4	616	LUT	C8-C9	4.81	1.56	1.45
32	n	317	LUT	C8-C9	4.81	1.56	1.45
43	c	614	BCR	C29-C30	4.81	1.65	1.54
32	6	317	LUT	C8-C9	4.81	1.56	1.45
32	8	616	LUT	C8-C9	4.81	1.56	1.45
43	V	101	BCR	C23-C22	4.81	1.56	1.45
35	4	615	RRX	C12-C13	4.80	1.56	1.45
43	c	614	BCR	C15-C14	4.80	1.58	1.43
32	6	318	LUT	C8-C9	4.80	1.56	1.45
35	G	614	RRX	C2-C1	4.79	1.65	1.54
32	s	318	LUT	C8-C9	4.79	1.56	1.45
32	Y	316	LUT	C4-C5	-4.79	1.43	1.51
32	s	317	LUT	C8-C9	4.79	1.56	1.45
43	c	614	BCR	C23-C22	4.79	1.56	1.45
43	C	614	BCR	C23-C22	4.78	1.56	1.45
32	8	615	LUT	C8-C9	4.78	1.56	1.45
43	a	410	BCR	C19-C18	4.78	1.56	1.45
32	r	317	LUT	C4-C5	-4.78	1.43	1.51
32	S	317	LUT	C8-C9	4.78	1.56	1.45
35	9	317	RRX	C12-C13	4.77	1.56	1.45
35	4	615	RRX	C2-C1	4.77	1.65	1.54
32	1	616	LUT	C4-C5	-4.77	1.43	1.51
35	G	614	RRX	C12-C13	4.77	1.56	1.45
35	g	315	RRX	C12-C13	4.76	1.56	1.45
43	C	615	BCR	C29-C30	4.76	1.65	1.54
43	T	101	BCR	C15-C14	4.75	1.58	1.43
35	9	317	RRX	C2-C1	4.74	1.65	1.54
43	z	101	BCR	C23-C22	4.73	1.56	1.45
35	2	614	RRX	C2-C1	4.73	1.65	1.54
43	d	406	BCR	C23-C22	4.73	1.56	1.45
43	D	405	BCR	C19-C18	4.73	1.56	1.45
32	R	317	LUT	C4-C5	-4.71	1.43	1.51
32	y	617	LUT	C4-C5	-4.71	1.43	1.51
35	2	614	RRX	C12-C13	4.70	1.56	1.45
43	b	618	BCR	C23-C22	4.70	1.56	1.45
43	C	615	BCR	C8-C9	4.69	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	A	410	BCR	C15-C14	4.69	1.58	1.43
44	d	407	PL9	C3-C4	-4.68	1.41	1.49
32	p	617	LUT	C12-C13	4.68	1.56	1.45
32	1	615	LUT	C4-C5	-4.68	1.43	1.51
35	q	317	RRX	C12-C13	4.67	1.56	1.45
43	D	405	BCR	C2-C1	4.67	1.64	1.54
43	c	615	BCR	C19-C18	4.67	1.56	1.45
43	B	617	BCR	C29-C30	4.67	1.64	1.54
32	G	615	LUT	C12-C13	4.65	1.55	1.45
32	5	616	LUT	C12-C13	4.64	1.55	1.45
32	0	616	LUT	C8-C9	4.64	1.55	1.45
35	q	317	RRX	C23-C22	4.64	1.55	1.45
32	g	316	LUT	C12-C13	4.63	1.55	1.45
32	1	616	LUT	C8-C9	4.63	1.55	1.45
32	s	318	LUT	C4-C5	-4.63	1.43	1.51
43	Z	101	BCR	C15-C14	4.63	1.57	1.43
32	0	617	LUT	C8-C9	4.62	1.55	1.45
32	5	617	LUT	C12-C13	4.61	1.55	1.45
43	v	101	BCR	C15-C14	4.61	1.57	1.43
35	4	615	RRX	C24-C25	4.60	1.61	1.45
32	9	318	LUT	C12-C13	4.59	1.55	1.45
35	g	315	RRX	C24-C25	4.58	1.61	1.45
32	7	317	LUT	C8-C9	4.58	1.55	1.45
43	V	101	BCR	C15-C14	4.58	1.57	1.43
35	9	317	RRX	C24-C25	4.58	1.61	1.45
32	4	616	LUT	C12-C13	4.57	1.55	1.45
32	q	318	LUT	C12-C13	4.57	1.55	1.45
32	N	317	LUT	C12-C13	4.57	1.55	1.45
35	G	614	RRX	C24-C25	4.57	1.61	1.45
35	2	614	RRX	C24-C25	4.56	1.61	1.45
43	d	406	BCR	C15-C14	4.56	1.57	1.43
32	Y	316	LUT	C8-C9	4.56	1.55	1.45
32	S	318	LUT	C12-C13	4.56	1.55	1.45
43	t	101	BCR	C15-C14	4.55	1.57	1.43
32	3	318	LUT	C12-C13	4.55	1.55	1.45
32	3	317	LUT	C12-C13	4.54	1.55	1.45
32	N	316	LUT	C12-C13	4.54	1.55	1.45
32	R	317	LUT	C8-C9	4.54	1.55	1.45
43	B	618	BCR	C15-C14	4.54	1.57	1.43
43	H	101	BCR	C15-C14	4.54	1.57	1.43
43	C	614	BCR	C15-C14	4.54	1.57	1.43
43	C	615	BCR	C19-C18	4.54	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	q	317	RRX	C24-C25	4.53	1.61	1.45
43	b	620	BCR	C15-C14	4.53	1.57	1.43
32	0	617	LUT	C4-C5	-4.52	1.44	1.51
32	p	616	LUT	C15-C14	4.52	1.57	1.43
43	z	101	BCR	C15-C14	4.50	1.57	1.43
43	h	101	BCR	C15-C14	4.50	1.57	1.43
32	R	317	LUT	C12-C13	4.49	1.55	1.45
32	2	615	LUT	C12-C13	4.49	1.55	1.45
43	a	410	BCR	C15-C14	4.49	1.57	1.43
32	7	318	LUT	C12-C13	4.49	1.55	1.45
35	G	614	RRX	C3-C4	4.48	1.66	1.52
32	n	317	LUT	C4-C5	-4.47	1.44	1.51
43	b	619	BCR	C15-C14	4.47	1.57	1.43
35	4	615	RRX	C3-C4	4.47	1.66	1.52
32	0	616	LUT	C4-C5	-4.46	1.44	1.51
35	2	614	RRX	C3-C4	4.46	1.66	1.52
43	b	618	BCR	C15-C14	4.45	1.57	1.43
32	8	615	LUT	C4-C5	-4.45	1.44	1.51
32	S	317	LUT	C4-C5	-4.45	1.44	1.51
32	S	318	LUT	C4-C5	-4.45	1.44	1.51
30	1	619	CHL	C3A-C2A	-4.45	1.42	1.54
32	2	615	LUT	C15-C14	4.45	1.57	1.43
35	9	317	RRX	C3-C4	4.45	1.66	1.52
32	6	318	LUT	C4-C5	-4.45	1.44	1.51
32	p	616	LUT	C31-C30	4.45	1.57	1.43
43	B	619	BCR	C15-C14	4.44	1.57	1.43
32	2	615	LUT	C35-C34	4.44	1.57	1.43
32	N	316	LUT	C4-C5	-4.44	1.44	1.51
32	r	317	LUT	C8-C9	4.44	1.55	1.45
32	7	318	LUT	C4-C5	-4.44	1.44	1.51
31	C	605	CLA	MG-ND	-4.44	1.97	2.05
32	n	317	LUT	C12-C13	4.43	1.55	1.45
32	4	616	LUT	C4-C5	-4.43	1.44	1.51
43	T	101	BCR	C19-C18	4.43	1.55	1.45
32	p	616	LUT	C35-C34	4.43	1.57	1.43
32	2	615	LUT	C31-C30	4.43	1.57	1.43
32	6	317	LUT	C4-C5	-4.42	1.44	1.51
32	p	617	LUT	C15-C14	4.42	1.57	1.43
43	b	619	BCR	C2-C1	4.41	1.64	1.54
35	q	317	RRX	C11-C10	4.41	1.57	1.43
32	q	318	LUT	C4-C5	-4.41	1.44	1.51
32	2	615	LUT	C4-C5	-4.41	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	B	619	BCR	C2-C1	4.41	1.64	1.54
43	B	618	BCR	C2-C1	4.41	1.64	1.54
32	n	318	LUT	C12-C13	4.41	1.55	1.45
32	s	318	LUT	C12-C13	4.41	1.55	1.45
32	G	615	LUT	C15-C14	4.40	1.57	1.43
32	N	317	LUT	C4-C5	-4.40	1.44	1.51
35	q	317	RRX	C2-C1	4.40	1.64	1.54
32	6	318	LUT	C12-C13	4.40	1.55	1.45
32	9	318	LUT	C4-C5	-4.40	1.44	1.51
32	p	617	LUT	C31-C30	4.40	1.57	1.43
32	8	615	LUT	C12-C13	4.39	1.55	1.45
32	6	317	LUT	C12-C13	4.39	1.55	1.45
43	c	614	BCR	C2-C1	4.39	1.64	1.54
32	8	616	LUT	C12-C13	4.39	1.55	1.45
32	1	615	LUT	C8-C9	4.39	1.55	1.45
43	c	614	BCR	C19-C18	4.39	1.55	1.45
32	3	317	LUT	C4-C5	-4.38	1.44	1.51
43	A	410	BCR	C19-C18	4.38	1.55	1.45
43	a	410	BCR	C2-C1	4.38	1.64	1.54
43	d	406	BCR	C2-C1	4.38	1.64	1.54
35	g	315	RRX	C11-C10	4.38	1.57	1.43
32	y	616	LUT	C8-C9	4.38	1.55	1.45
43	D	405	BCR	C20-C21	4.38	1.57	1.43
32	s	317	LUT	C4-C5	-4.37	1.44	1.51
43	B	617	BCR	C15-C14	4.37	1.57	1.43
43	b	618	BCR	C2-C1	4.37	1.64	1.54
43	A	410	BCR	C2-C1	4.37	1.64	1.54
43	H	101	BCR	C2-C1	4.37	1.64	1.54
32	3	318	LUT	C15-C14	4.37	1.57	1.43
43	v	101	BCR	C19-C18	4.36	1.55	1.45
32	9	318	LUT	C15-C14	4.36	1.57	1.43
32	5	617	LUT	C15-C14	4.36	1.57	1.43
32	s	317	LUT	C12-C13	4.36	1.55	1.45
43	c	615	BCR	C20-C21	4.36	1.57	1.43
43	c	615	BCR	C2-C1	4.36	1.64	1.54
43	b	619	BCR	C19-C18	4.36	1.55	1.45
32	n	318	LUT	C4-C5	-4.36	1.44	1.51
32	g	316	LUT	C31-C30	4.36	1.57	1.43
35	4	615	RRX	C11-C10	4.36	1.56	1.43
32	G	615	LUT	C4-C5	-4.36	1.44	1.51
32	q	318	LUT	C31-C30	4.35	1.56	1.43
35	9	317	RRX	C11-C10	4.35	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	615	LUT	C31-C30	4.35	1.56	1.43
32	S	317	LUT	C12-C13	4.35	1.55	1.45
32	q	318	LUT	C15-C14	4.34	1.56	1.43
35	g	315	RRX	C3-C4	4.34	1.66	1.52
32	5	617	LUT	C31-C30	4.34	1.56	1.43
32	7	317	LUT	C12-C13	4.34	1.55	1.45
32	5	616	LUT	C15-C14	4.34	1.56	1.43
32	g	316	LUT	C15-C14	4.34	1.56	1.43
35	G	614	RRX	C11-C10	4.34	1.56	1.43
43	h	101	BCR	C2-C1	4.34	1.64	1.54
43	C	614	BCR	C2-C1	4.34	1.64	1.54
32	g	316	LUT	C4-C5	-4.33	1.44	1.51
32	8	616	LUT	C4-C5	-4.33	1.44	1.51
32	p	617	LUT	C35-C34	4.33	1.56	1.43
32	0	617	LUT	C12-C13	4.33	1.55	1.45
32	5	616	LUT	C31-C30	4.33	1.56	1.43
32	9	318	LUT	C31-C30	4.33	1.56	1.43
43	b	620	BCR	C2-C1	4.33	1.64	1.54
35	q	317	RRX	C3-C4	4.33	1.66	1.52
32	p	617	LUT	C4-C5	-4.32	1.44	1.51
32	3	318	LUT	C31-C30	4.32	1.56	1.43
32	4	616	LUT	C15-C14	4.32	1.56	1.43
32	S	318	LUT	C15-C14	4.32	1.56	1.43
32	5	616	LUT	C4-C5	-4.32	1.44	1.51
32	p	616	LUT	C4-C5	-4.32	1.44	1.51
35	2	614	RRX	C11-C10	4.31	1.56	1.43
32	R	317	LUT	C15-C14	4.30	1.56	1.43
32	N	317	LUT	C31-C30	4.30	1.56	1.43
44	a	414	PL9	C7-C3	-4.30	1.46	1.51
32	N	316	LUT	C15-C14	4.30	1.56	1.43
32	g	316	LUT	C35-C34	4.29	1.56	1.43
35	2	614	RRX	C29-C30	4.29	1.68	1.54
32	S	318	LUT	C31-C30	4.29	1.56	1.43
32	G	615	LUT	C35-C34	4.29	1.56	1.43
32	4	616	LUT	C31-C30	4.29	1.56	1.43
32	5	617	LUT	C4-C5	-4.29	1.44	1.51
32	3	318	LUT	C35-C34	4.29	1.56	1.43
32	Y	315	LUT	C8-C9	4.28	1.55	1.45
35	G	614	RRX	C29-C30	4.28	1.68	1.54
43	V	101	BCR	C2-C1	4.28	1.64	1.54
32	3	317	LUT	C15-C14	4.27	1.56	1.43
32	3	317	LUT	C31-C30	4.27	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	4	615	RRX	C29-C30	4.27	1.68	1.54
32	N	317	LUT	C15-C14	4.27	1.56	1.43
35	9	317	RRX	C29-C30	4.27	1.68	1.54
35	q	317	RRX	C29-C30	4.27	1.68	1.54
43	V	101	BCR	C28-C27	4.27	1.65	1.52
32	5	616	LUT	C35-C34	4.27	1.56	1.43
43	B	617	BCR	C23-C22	4.27	1.55	1.45
32	5	617	LUT	C35-C34	4.27	1.56	1.43
32	6	318	LUT	C31-C30	4.26	1.56	1.43
43	V	101	BCR	C19-C18	4.26	1.55	1.45
32	q	318	LUT	C35-C34	4.26	1.56	1.43
32	3	318	LUT	C4-C5	-4.26	1.44	1.51
31	S	304	CLA	MG-ND	-4.26	1.97	2.05
43	b	620	BCR	C19-C18	4.26	1.55	1.45
43	Z	101	BCR	C2-C1	4.26	1.63	1.54
43	Z	101	BCR	C19-C18	4.25	1.55	1.45
43	C	615	BCR	C20-C21	4.25	1.56	1.43
32	N	316	LUT	C31-C30	4.25	1.56	1.43
31	c	607	CLA	MG-ND	-4.25	1.97	2.05
43	T	101	BCR	C2-C1	4.25	1.63	1.54
35	q	317	RRX	C27-C26	-4.25	1.44	1.51
32	1	616	LUT	C12-C13	4.25	1.55	1.45
31	b	617	CLA	MG-ND	-4.25	1.97	2.05
32	Y	316	LUT	C12-C13	4.24	1.55	1.45
43	b	619	BCR	C20-C21	4.24	1.56	1.43
43	H	101	BCR	C19-C18	4.24	1.55	1.45
43	h	101	BCR	C19-C18	4.24	1.55	1.45
32	7	318	LUT	C15-C14	4.24	1.56	1.43
43	D	405	BCR	C28-C27	4.24	1.65	1.52
32	y	617	LUT	C8-C9	4.24	1.55	1.45
43	B	617	BCR	C2-C1	4.24	1.63	1.54
44	D	406	PL9	C3-C4	-4.23	1.42	1.49
43	v	101	BCR	C2-C1	4.23	1.63	1.54
31	C	603	CLA	MG-ND	-4.23	1.97	2.05
43	B	618	BCR	C19-C18	4.22	1.55	1.45
43	z	101	BCR	C2-C1	4.22	1.63	1.54
32	7	318	LUT	C31-C30	4.22	1.56	1.43
32	6	318	LUT	C15-C14	4.22	1.56	1.43
32	R	317	LUT	C35-C34	4.22	1.56	1.43
32	N	316	LUT	C35-C34	4.22	1.56	1.43
32	s	317	LUT	C31-C30	4.22	1.56	1.43
32	n	318	LUT	C15-C14	4.21	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	317	LUT	C31-C30	4.21	1.56	1.43
43	T	101	BCR	C20-C21	4.20	1.56	1.43
31	G	611	CLA	MG-ND	-4.20	1.97	2.05
43	C	614	BCR	C19-C18	4.20	1.55	1.45
32	8	616	LUT	C15-C14	4.20	1.56	1.43
43	v	101	BCR	C28-C27	4.20	1.65	1.52
32	8	616	LUT	C31-C30	4.20	1.56	1.43
32	S	318	LUT	C35-C34	4.20	1.56	1.43
32	6	318	LUT	C35-C34	4.20	1.56	1.43
31	c	603	CLA	MG-ND	-4.20	1.97	2.05
32	n	318	LUT	C31-C30	4.20	1.56	1.43
32	4	616	LUT	C35-C34	4.19	1.56	1.43
32	s	317	LUT	C15-C14	4.19	1.56	1.43
32	s	318	LUT	C15-C14	4.19	1.56	1.43
45	C	620	DGD	O1G-C1A	4.19	1.45	1.33
32	3	317	LUT	C35-C34	4.19	1.56	1.43
43	c	615	BCR	C28-C27	4.19	1.65	1.52
32	9	318	LUT	C35-C34	4.19	1.56	1.43
32	6	317	LUT	C31-C30	4.18	1.56	1.43
32	N	317	LUT	C35-C34	4.18	1.56	1.43
32	s	318	LUT	C31-C30	4.18	1.56	1.43
32	0	617	LUT	C31-C30	4.18	1.56	1.43
32	8	615	LUT	C15-C14	4.18	1.56	1.43
32	n	317	LUT	C15-C14	4.17	1.56	1.43
31	B	603	CLA	MG-ND	-4.17	1.97	2.05
31	c	609	CLA	MG-ND	-4.17	1.97	2.05
32	0	616	LUT	C12-C13	4.17	1.54	1.45
32	6	317	LUT	C15-C14	4.17	1.56	1.43
32	S	317	LUT	C15-C14	4.16	1.56	1.43
43	C	614	BCR	C28-C27	4.16	1.65	1.52
32	7	317	LUT	C15-C14	4.16	1.56	1.43
31	B	616	CLA	MG-ND	-4.16	1.97	2.05
43	B	619	BCR	C19-C18	4.16	1.54	1.45
32	R	317	LUT	C31-C30	4.16	1.56	1.43
31	C	610	CLA	MG-ND	-4.15	1.97	2.05
32	2	615	LUT	C21-C26	4.15	1.67	1.56
43	T	101	BCR	C28-C27	4.15	1.65	1.52
31	C	607	CLA	MG-ND	-4.15	1.97	2.05
45	c	619	DGD	O1G-C1A	4.15	1.45	1.33
32	n	317	LUT	C31-C30	4.15	1.56	1.43
43	b	620	BCR	C20-C21	4.14	1.56	1.43
32	8	615	LUT	C31-C30	4.14	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	v	101	BCR	C20-C21	4.14	1.56	1.43
31	b	605	CLA	MG-ND	-4.14	1.97	2.05
32	0	617	LUT	C15-C14	4.14	1.56	1.43
43	b	618	BCR	C28-C27	4.14	1.65	1.52
45	C	618	DGD	O1G-C1A	4.14	1.45	1.33
31	c	612	CLA	MG-ND	-4.13	1.97	2.05
32	5	616	LUT	C28-C29	4.13	1.54	1.45
35	g	315	RRX	C29-C30	4.12	1.67	1.54
32	7	318	LUT	C35-C34	4.12	1.56	1.43
32	2	615	LUT	C23-C24	-4.12	1.44	1.50
32	0	617	LUT	C35-C34	4.12	1.56	1.43
43	A	410	BCR	C28-C27	4.12	1.65	1.52
32	1	615	LUT	C12-C13	4.12	1.54	1.45
32	8	616	LUT	C35-C34	4.12	1.56	1.43
43	d	406	BCR	C28-C27	4.11	1.65	1.52
31	C	612	CLA	MG-ND	-4.11	1.97	2.05
43	Z	101	BCR	C28-C27	4.11	1.65	1.52
32	n	318	LUT	C35-C34	4.11	1.56	1.43
43	a	410	BCR	C28-C27	4.11	1.65	1.52
32	p	616	LUT	C7-C6	4.11	1.59	1.45
31	C	609	CLA	MG-ND	-4.11	1.97	2.05
32	8	615	LUT	C35-C34	4.11	1.56	1.43
32	n	317	LUT	C35-C34	4.11	1.56	1.43
31	D	403	CLA	MG-ND	-4.11	1.97	2.05
31	c	606	CLA	MG-ND	-4.11	1.97	2.05
32	y	617	LUT	C12-C13	4.11	1.54	1.45
43	H	101	BCR	C28-C27	4.10	1.65	1.52
43	b	620	BCR	C28-C27	4.10	1.65	1.52
32	0	616	LUT	C15-C14	4.10	1.56	1.43
31	r	303	CLA	MG-ND	-4.10	1.97	2.05
32	Y	316	LUT	C15-C14	4.10	1.56	1.43
31	B	604	CLA	MG-ND	-4.10	1.97	2.05
43	A	410	BCR	C20-C21	4.10	1.56	1.43
31	b	604	CLA	MG-ND	-4.10	1.97	2.05
32	g	316	LUT	C28-C29	4.10	1.54	1.45
35	2	614	RRX	C27-C26	-4.10	1.44	1.51
43	z	101	BCR	C19-C18	4.09	1.54	1.45
43	b	619	BCR	C28-C27	4.09	1.65	1.52
43	t	101	BCR	C28-C27	4.09	1.65	1.52
43	t	101	BCR	C19-C18	4.09	1.54	1.45
32	S	317	LUT	C35-C34	4.09	1.56	1.43
32	5	616	LUT	C7-C6	4.09	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	Z	101	BCR	C20-C21	4.09	1.56	1.43
32	5	617	LUT	C28-C29	4.08	1.54	1.45
32	s	318	LUT	C35-C34	4.08	1.56	1.43
43	B	618	BCR	C28-C27	4.08	1.65	1.52
31	S	313	CLA	MG-ND	-4.08	1.97	2.05
43	t	101	BCR	C4-C5	-4.08	1.43	1.51
32	6	317	LUT	C35-C34	4.08	1.56	1.43
43	H	101	BCR	C20-C21	4.08	1.56	1.43
32	Y	316	LUT	C31-C30	4.08	1.56	1.43
43	t	101	BCR	C2-C1	4.07	1.63	1.54
43	B	619	BCR	C28-C27	4.07	1.65	1.52
43	B	618	BCR	C20-C21	4.07	1.56	1.43
43	c	614	BCR	C20-C21	4.07	1.56	1.43
32	s	317	LUT	C35-C34	4.07	1.56	1.43
32	p	617	LUT	C21-C26	4.07	1.67	1.56
31	r	307	CLA	MG-ND	-4.07	1.97	2.05
31	q	315	CLA	MG-ND	-4.07	1.97	2.05
32	Y	316	LUT	C35-C34	4.07	1.56	1.43
32	1	616	LUT	C31-C30	4.07	1.56	1.43
35	4	615	RRX	C15-C14	4.07	1.56	1.43
31	y	613	CLA	MG-ND	-4.07	1.97	2.05
45	C	617	DGD	O1G-C1A	4.07	1.45	1.33
31	1	604	CLA	MG-ND	-4.06	1.97	2.05
45	C	616	DGD	O1G-C1A	4.06	1.45	1.33
35	g	315	RRX	C15-C14	4.06	1.56	1.43
31	B	607	CLA	C1C-NC	-4.06	1.31	1.37
43	h	101	BCR	C28-C27	4.06	1.65	1.52
43	c	614	BCR	C28-C27	4.06	1.65	1.52
32	1	616	LUT	C15-C14	4.06	1.56	1.43
45	c	616	DGD	O1G-C1A	4.06	1.45	1.33
31	r	314	CLA	MG-ND	-4.06	1.97	2.05
43	B	619	BCR	C20-C21	4.05	1.56	1.43
43	V	101	BCR	C20-C21	4.05	1.56	1.43
35	4	615	RRX	C27-C26	-4.05	1.44	1.51
32	3	318	LUT	C28-C29	4.05	1.54	1.45
32	N	317	LUT	C28-C29	4.05	1.54	1.45
32	q	318	LUT	C28-C29	4.05	1.54	1.45
45	c	618	DGD	O1G-C1A	4.05	1.45	1.33
31	R	305	CLA	MG-ND	-4.05	1.97	2.05
31	c	602	CLA	MG-ND	-4.05	1.97	2.05
35	9	317	RRX	C15-C14	4.05	1.56	1.43
45	c	617	DGD	O1G-C1A	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	0	610	CLA	MG-ND	-4.05	1.97	2.05
32	9	318	LUT	C7-C6	4.05	1.59	1.45
43	h	101	BCR	C20-C21	4.04	1.56	1.43
35	G	614	RRX	C27-C26	-4.04	1.44	1.51
32	5	617	LUT	C7-C6	4.04	1.59	1.45
32	g	316	LUT	C7-C6	4.04	1.59	1.45
32	1	615	LUT	C31-C30	4.04	1.56	1.43
31	1	603	CLA	MG-ND	-4.04	1.97	2.05
35	G	614	RRX	C15-C14	4.04	1.56	1.43
35	9	317	RRX	C27-C26	-4.04	1.44	1.51
32	3	317	LUT	C28-C29	4.04	1.54	1.45
31	R	307	CLA	MG-ND	-4.04	1.97	2.05
32	G	615	LUT	C7-C6	4.04	1.59	1.45
32	N	316	LUT	C28-C29	4.03	1.54	1.45
31	c	613	CLA	MG-ND	-4.03	1.97	2.05
35	2	614	RRX	C15-C14	4.03	1.55	1.43
31	C	605	CLA	C1C-NC	-4.03	1.31	1.37
31	Y	312	CLA	MG-ND	-4.02	1.97	2.05
31	0	603	CLA	MG-ND	-4.02	1.97	2.05
31	p	603	CLA	MG-ND	-4.02	1.97	2.05
31	c	610	CLA	MG-ND	-4.02	1.97	2.05
43	b	618	BCR	C19-C18	4.02	1.54	1.45
31	R	306	CLA	MG-ND	-4.02	1.97	2.05
31	7	314	CLA	MG-ND	-4.02	1.97	2.05
31	0	612	CLA	MG-ND	-4.02	1.97	2.05
31	c	608	CLA	MG-ND	-4.02	1.97	2.05
32	p	617	LUT	C7-C6	4.02	1.59	1.45
32	q	318	LUT	C7-C6	4.02	1.59	1.45
31	1	613	CLA	MG-ND	-4.01	1.97	2.05
31	S	314	CLA	MG-ND	-4.01	1.97	2.05
43	C	614	BCR	C20-C21	4.01	1.55	1.43
31	g	311	CLA	MG-ND	-4.01	1.97	2.05
43	z	101	BCR	C28-C27	4.01	1.65	1.52
31	r	316	CLA	MG-ND	-4.00	1.97	2.05
32	1	616	LUT	C35-C34	4.00	1.55	1.43
31	R	313	CLA	MG-ND	-4.00	1.97	2.05
31	G	610	CLA	MG-ND	-4.00	1.97	2.05
35	q	317	RRX	C15-C14	4.00	1.55	1.43
31	b	608	CLA	MG-ND	-4.00	1.97	2.05
31	Y	311	CLA	MG-ND	-4.00	1.97	2.05
32	y	617	LUT	C15-C14	4.00	1.55	1.43
32	1	615	LUT	C15-C14	4.00	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	3	318	LUT	C7-C6	4.00	1.59	1.45
32	0	616	LUT	C31-C30	3.99	1.55	1.43
31	s	314	CLA	MG-ND	-3.99	1.97	2.05
32	7	317	LUT	C31-C30	3.99	1.55	1.43
31	Y	313	CLA	MG-ND	-3.99	1.97	2.05
32	2	615	LUT	C7-C6	3.99	1.59	1.45
43	c	614	BCR	C11-C10	3.99	1.55	1.43
31	C	602	CLA	MG-ND	-3.99	1.97	2.05
32	7	317	LUT	C35-C34	3.99	1.55	1.43
32	y	616	LUT	C12-C13	3.99	1.54	1.45
31	B	608	CLA	MG-ND	-3.99	1.97	2.05
32	7	318	LUT	C7-C6	3.98	1.59	1.45
31	R	314	CLA	MG-ND	-3.98	1.97	2.05
32	N	317	LUT	C7-C6	3.98	1.59	1.45
31	b	609	CLA	MG-ND	-3.98	1.97	2.05
32	S	318	LUT	C28-C29	3.98	1.54	1.45
32	9	318	LUT	C28-C29	3.98	1.54	1.45
32	6	318	LUT	C28-C29	3.98	1.54	1.45
31	q	315	CLA	C1C-NC	-3.98	1.31	1.37
32	4	616	LUT	C7-C6	3.98	1.59	1.45
32	6	317	LUT	C28-C29	3.98	1.54	1.45
31	d	404	CLA	MG-ND	-3.98	1.97	2.05
32	0	617	LUT	C21-C26	3.98	1.67	1.56
31	y	613	CLA	C1C-NC	-3.98	1.31	1.37
31	s	313	CLA	MG-ND	-3.98	1.97	2.05
31	l	612	CLA	MG-ND	-3.97	1.97	2.05
31	y	612	CLA	MG-ND	-3.97	1.97	2.05
32	G	615	LUT	C28-C29	3.97	1.54	1.45
43	d	406	BCR	C20-C21	3.97	1.55	1.43
32	4	616	LUT	C28-C29	3.97	1.54	1.45
43	z	101	BCR	C20-C21	3.96	1.55	1.43
32	3	317	LUT	C7-C6	3.96	1.59	1.45
32	y	616	LUT	C15-C14	3.96	1.55	1.43
31	C	604	CLA	MG-ND	-3.96	1.97	2.05
31	a	406	CLA	MG-ND	-3.96	1.97	2.05
43	t	101	BCR	C20-C21	3.96	1.55	1.43
31	c	605	CLA	MG-ND	-3.96	1.97	2.05
31	4	612	CLA	MG-ND	-3.95	1.98	2.05
31	R	303	CLA	MG-ND	-3.95	1.98	2.05
31	C	606	CLA	MG-ND	-3.95	1.98	2.05
32	0	616	LUT	C35-C34	3.95	1.55	1.43
31	C	608	CLA	MG-ND	-3.95	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	a	410	BCR	C20-C21	3.95	1.55	1.43
31	R	316	CLA	MG-ND	-3.95	1.98	2.05
31	3	301	CLA	MG-ND	-3.95	1.98	2.05
31	q	306	CLA	MG-ND	-3.95	1.98	2.05
32	s	317	LUT	C7-C6	3.95	1.59	1.45
32	n	317	LUT	C28-C29	3.94	1.54	1.45
32	6	318	LUT	C7-C6	3.94	1.59	1.45
32	N	316	LUT	C7-C6	3.94	1.59	1.45
32	S	318	LUT	C7-C6	3.94	1.59	1.45
31	3	316	CLA	MG-ND	-3.94	1.98	2.05
32	r	317	LUT	C12-C13	3.94	1.54	1.45
43	B	617	BCR	C28-C27	3.94	1.64	1.52
31	B	615	CLA	MG-ND	-3.94	1.98	2.05
31	b	606	CLA	MG-ND	-3.94	1.98	2.05
32	n	318	LUT	C7-C6	3.94	1.59	1.45
43	C	615	BCR	C2-C1	3.94	1.63	1.54
31	S	315	CLA	MG-ND	-3.94	1.98	2.05
32	1	615	LUT	C35-C34	3.94	1.55	1.43
32	8	615	LUT	C28-C29	3.94	1.54	1.45
31	B	605	CLA	MG-ND	-3.94	1.98	2.05
31	r	312	CLA	MG-ND	-3.94	1.98	2.05
32	n	317	LUT	C7-C6	3.94	1.59	1.45
32	Y	315	LUT	C12-C13	3.94	1.54	1.45
31	c	611	CLA	MG-ND	-3.94	1.98	2.05
31	r	313	CLA	MG-ND	-3.94	1.98	2.05
31	y	611	CLA	MG-ND	-3.94	1.98	2.05
31	G	612	CLA	MG-ND	-3.94	1.98	2.05
32	3	317	LUT	C21-C26	3.93	1.67	1.56
32	s	317	LUT	C28-C29	3.93	1.54	1.45
31	r	311	CLA	MG-ND	-3.93	1.98	2.05
32	8	615	LUT	C7-C6	3.93	1.59	1.45
31	R	315	CLA	MG-ND	-3.93	1.98	2.05
43	d	406	BCR	C19-C18	3.93	1.54	1.45
32	8	616	LUT	C7-C6	3.93	1.59	1.45
31	B	601	CLA	MG-ND	-3.93	1.98	2.05
31	6	312	CLA	MG-ND	-3.93	1.98	2.05
31	R	312	CLA	MG-ND	-3.93	1.98	2.05
32	y	617	LUT	C31-C30	3.93	1.55	1.43
32	p	617	LUT	C28-C29	3.93	1.54	1.45
31	C	611	CLA	MG-ND	-3.93	1.98	2.05
31	C	613	CLA	MG-ND	-3.93	1.98	2.05
32	p	616	LUT	C21-C26	3.92	1.67	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	p	602	CLA	MG-ND	-3.92	1.98	2.05
32	7	318	LUT	C28-C29	3.92	1.54	1.45
32	Y	315	LUT	C15-C14	3.92	1.55	1.43
31	b	617	CLA	C1C-NC	-3.92	1.31	1.37
32	G	615	LUT	C21-C26	3.92	1.67	1.56
31	3	311	CLA	MG-ND	-3.92	1.98	2.05
31	B	606	CLA	MG-ND	-3.91	1.98	2.05
32	S	317	LUT	C7-C6	3.91	1.59	1.45
32	n	318	LUT	C28-C29	3.91	1.54	1.45
32	y	617	LUT	C35-C34	3.91	1.55	1.43
32	8	616	LUT	C28-C29	3.91	1.54	1.45
31	0	613	CLA	MG-ND	-3.91	1.98	2.05
43	C	615	BCR	C28-C27	3.91	1.64	1.52
32	5	617	LUT	C11-C10	3.91	1.55	1.43
32	r	317	LUT	C31-C30	3.90	1.55	1.43
31	g	310	CLA	MG-ND	-3.90	1.98	2.05
32	p	616	LUT	C28-C29	3.90	1.54	1.45
32	S	317	LUT	C28-C29	3.90	1.54	1.45
31	A	405	CLA	MG-ND	-3.90	1.98	2.05
31	B	616	CLA	C1C-NC	-3.90	1.32	1.37
31	R	311	CLA	MG-ND	-3.90	1.98	2.05
32	y	616	LUT	C31-C30	3.90	1.55	1.43
43	b	619	BCR	C3-C4	3.90	1.64	1.52
32	s	318	LUT	C7-C6	3.90	1.58	1.45
31	4	610	CLA	MG-ND	-3.90	1.98	2.05
32	p	616	LUT	C11-C10	3.89	1.55	1.43
32	R	317	LUT	C7-C6	3.89	1.58	1.45
32	6	317	LUT	C7-C6	3.89	1.58	1.45
31	S	312	CLA	MG-ND	-3.89	1.98	2.05
43	B	617	BCR	C4-C5	-3.89	1.43	1.51
32	Y	315	LUT	C35-C34	3.89	1.55	1.43
31	9	314	CLA	MG-ND	-3.89	1.98	2.05
31	4	613	CLA	MG-ND	-3.89	1.98	2.05
32	R	317	LUT	C21-C26	3.89	1.67	1.56
31	0	611	CLA	MG-ND	-3.89	1.98	2.05
31	3	312	CLA	MG-ND	-3.89	1.98	2.05
43	V	101	BCR	C3-C4	3.88	1.64	1.52
32	2	615	LUT	C28-C29	3.88	1.54	1.45
32	5	617	LUT	C21-C26	3.88	1.67	1.56
31	s	312	CLA	MG-ND	-3.88	1.98	2.05
43	D	405	BCR	C16-C17	3.88	1.55	1.43
43	c	615	BCR	C3-C4	3.88	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a	407	CLA	MG-ND	-3.88	1.98	2.05
31	R	304	CLA	MG-ND	-3.87	1.98	2.05
31	0	604	CLA	MG-ND	-3.87	1.98	2.05
32	s	318	LUT	C28-C29	3.87	1.54	1.45
32	g	316	LUT	C21-C26	3.87	1.67	1.56
32	Y	316	LUT	C7-C6	3.87	1.58	1.45
31	9	313	CLA	MG-ND	-3.87	1.98	2.05
31	A	406	CLA	MG-ND	-3.87	1.98	2.05
32	Y	315	LUT	C31-C30	3.87	1.55	1.43
43	C	615	BCR	C3-C4	3.87	1.64	1.52
35	2	614	RRX	C16-C17	3.87	1.55	1.43
32	0	616	LUT	C7-C6	3.87	1.58	1.45
31	b	602	CLA	MG-ND	-3.87	1.98	2.05
43	C	615	BCR	C27-C26	-3.87	1.43	1.51
31	b	607	CLA	MG-ND	-3.87	1.98	2.05
35	G	614	RRX	C16-C17	3.87	1.55	1.43
32	9	318	LUT	C21-C26	3.87	1.67	1.56
31	1	602	CLA	MG-ND	-3.87	1.98	2.05
31	A	407	CLA	MG-ND	-3.86	1.98	2.05
31	d	401	CLA	MG-ND	-3.86	1.98	2.05
43	B	618	BCR	C3-C4	3.86	1.64	1.52
31	r	306	CLA	MG-ND	-3.86	1.98	2.05
35	9	317	RRX	C16-C17	3.86	1.55	1.43
31	S	311	CLA	MG-ND	-3.86	1.98	2.05
43	b	618	BCR	C20-C21	3.85	1.55	1.43
31	S	316	CLA	MG-ND	-3.85	1.98	2.05
32	q	318	LUT	C21-C26	3.85	1.67	1.56
31	0	602	CLA	MG-ND	-3.85	1.98	2.05
31	q	316	CLA	MG-ND	-3.85	1.98	2.05
32	S	318	LUT	C21-C26	3.85	1.67	1.56
35	4	615	RRX	C16-C17	3.85	1.55	1.43
35	g	315	RRX	C27-C26	-3.85	1.45	1.51
31	b	610	CLA	MG-ND	-3.85	1.98	2.05
31	s	310	CLA	MG-ND	-3.85	1.98	2.05
32	4	616	LUT	C21-C26	3.85	1.67	1.56
31	G	609	CLA	MG-ND	-3.85	1.98	2.05
32	y	616	LUT	C35-C34	3.85	1.55	1.43
32	s	317	LUT	C21-C26	3.85	1.67	1.56
32	N	317	LUT	C21-C26	3.85	1.67	1.56
31	C	608	CLA	C1C-NC	-3.85	1.32	1.37
32	0	617	LUT	C7-C6	3.85	1.58	1.45
31	s	311	CLA	MG-ND	-3.84	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	r	317	LUT	C15-C14	3.84	1.55	1.43
32	6	318	LUT	C21-C26	3.84	1.67	1.56
32	N	316	LUT	C21-C26	3.84	1.67	1.56
32	3	318	LUT	C11-C10	3.84	1.55	1.43
31	B	602	CLA	MG-ND	-3.84	1.98	2.05
32	S	317	LUT	C21-C26	3.84	1.67	1.56
31	G	613	CLA	MG-ND	-3.84	1.98	2.05
32	0	617	LUT	C28-C29	3.84	1.54	1.45
31	s	315	CLA	MG-ND	-3.83	1.98	2.05
35	G	614	RRX	C20-C21	3.83	1.55	1.43
31	c	604	CLA	MG-ND	-3.83	1.98	2.05
31	C	602	CLA	C1C-NC	-3.83	1.32	1.37
31	b	616	CLA	MG-ND	-3.83	1.98	2.05
43	v	101	BCR	C3-C4	3.83	1.64	1.52
35	g	315	RRX	C16-C17	3.82	1.55	1.43
32	3	318	LUT	C21-C26	3.82	1.67	1.56
32	1	616	LUT	C7-C6	3.82	1.58	1.45
32	5	616	LUT	C21-C26	3.82	1.67	1.56
32	7	317	LUT	C7-C6	3.82	1.58	1.45
32	8	615	LUT	C21-C26	3.82	1.67	1.56
31	r	303	CLA	C1C-NC	-3.82	1.32	1.37
31	r	315	CLA	MG-ND	-3.82	1.98	2.05
31	q	314	CLA	MG-ND	-3.82	1.98	2.05
31	S	310	CLA	MG-ND	-3.82	1.98	2.05
31	C	601	CLA	MG-ND	-3.81	1.98	2.05
31	B	609	CLA	MG-ND	-3.81	1.98	2.05
32	n	317	LUT	C21-C26	3.81	1.67	1.56
35	q	317	RRX	C16-C17	3.81	1.55	1.43
35	g	315	RRX	C20-C21	3.81	1.55	1.43
35	4	615	RRX	C20-C21	3.81	1.55	1.43
31	A	407	CLA	C1C-NC	-3.81	1.32	1.37
32	8	616	LUT	C21-C26	3.81	1.67	1.56
31	b	608	CLA	C1C-NC	-3.81	1.32	1.37
31	B	607	CLA	MG-ND	-3.80	1.98	2.05
31	0	615	CLA	MG-ND	-3.80	1.98	2.05
31	4	614	CLA	MG-ND	-3.80	1.98	2.05
32	7	318	LUT	C21-C26	3.80	1.67	1.56
35	9	317	RRX	C20-C21	3.80	1.55	1.43
32	6	317	LUT	C21-C26	3.79	1.67	1.56
31	b	603	CLA	MG-ND	-3.79	1.98	2.05
32	p	617	LUT	C11-C10	3.79	1.55	1.43
43	B	617	BCR	C19-C18	3.79	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	z	101	BCR	C3-C4	3.79	1.64	1.52
31	d	405	CLA	MG-ND	-3.79	1.98	2.05
32	n	318	LUT	C21-C26	3.78	1.66	1.56
32	Y	316	LUT	C28-C29	3.78	1.54	1.45
31	s	316	CLA	MG-ND	-3.78	1.98	2.05
31	a	409	CLA	MG-ND	-3.78	1.98	2.05
31	7	313	CLA	MG-ND	-3.77	1.98	2.05
32	1	615	LUT	C7-C6	3.77	1.58	1.45
43	C	614	BCR	C3-C4	3.77	1.64	1.52
32	G	615	LUT	C11-C10	3.77	1.55	1.43
32	g	316	LUT	C11-C10	3.77	1.55	1.43
32	7	317	LUT	C28-C29	3.77	1.54	1.45
35	2	614	RRX	C20-C21	3.77	1.55	1.43
32	y	616	LUT	C7-C6	3.76	1.58	1.45
31	c	601	CLA	MG-ND	-3.76	1.98	2.05
31	5	615	CLA	MG-ND	-3.76	1.98	2.05
43	B	619	BCR	C3-C4	3.76	1.64	1.52
31	A	409	CLA	MG-ND	-3.76	1.98	2.05
31	c	602	CLA	C1C-NC	-3.76	1.32	1.37
31	c	606	CLA	C1C-NC	-3.76	1.32	1.37
32	s	318	LUT	C21-C26	3.76	1.66	1.56
31	a	406	CLA	C1C-NC	-3.76	1.32	1.37
43	D	405	BCR	C11-C10	3.76	1.55	1.43
32	r	317	LUT	C35-C34	3.75	1.55	1.43
32	y	617	LUT	C7-C6	3.75	1.58	1.45
43	b	620	BCR	C3-C4	3.75	1.64	1.52
31	3	301	CLA	C1C-NC	-3.75	1.32	1.37
32	1	616	LUT	C28-C29	3.75	1.54	1.45
32	r	317	LUT	C7-C6	3.75	1.58	1.45
32	5	616	LUT	C11-C10	3.75	1.55	1.43
43	c	614	BCR	C3-C4	3.74	1.64	1.52
32	0	616	LUT	C28-C29	3.74	1.54	1.45
31	p	604	CLA	MG-ND	-3.74	1.98	2.05
31	R	311	CLA	C1C-NC	-3.74	1.32	1.37
31	r	312	CLA	C1C-NC	-3.73	1.32	1.37
31	n	315	CLA	MG-ND	-3.73	1.98	2.05
43	b	618	BCR	C3-C4	3.73	1.64	1.52
43	A	410	BCR	C3-C4	3.73	1.64	1.52
43	c	614	BCR	C16-C17	3.73	1.55	1.43
43	a	410	BCR	C3-C4	3.73	1.64	1.52
31	8	613	CLA	MG-ND	-3.72	1.98	2.05
43	D	405	BCR	C3-C4	3.72	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	609	CLA	C1C-NC	-3.72	1.32	1.37
31	d	401	CLA	C1C-NC	-3.72	1.32	1.37
32	0	616	LUT	C21-C26	3.72	1.66	1.56
31	N	314	CLA	MG-ND	-3.72	1.98	2.05
43	C	614	BCR	C27-C26	-3.72	1.43	1.51
43	Z	101	BCR	C3-C4	3.71	1.64	1.52
43	T	101	BCR	C16-C17	3.71	1.55	1.43
32	y	617	LUT	C21-C26	3.71	1.66	1.56
31	p	612	CLA	MG-ND	-3.71	1.98	2.05
31	0	610	CLA	C1C-NC	-3.71	1.32	1.37
43	h	101	BCR	C3-C4	3.71	1.64	1.52
31	r	311	CLA	C1C-NC	-3.71	1.32	1.37
32	q	318	LUT	C11-C10	3.71	1.54	1.43
32	2	615	LUT	C11-C10	3.71	1.54	1.43
43	b	618	BCR	C27-C26	-3.71	1.43	1.51
31	D	404	CLA	MG-ND	-3.70	1.98	2.05
31	A	405	CLA	C1C-NC	-3.70	1.32	1.37
31	c	608	CLA	C1C-NC	-3.70	1.32	1.37
43	B	617	BCR	C3-C4	3.70	1.64	1.52
32	Y	315	LUT	C21-C26	3.70	1.66	1.56
32	9	318	LUT	C11-C10	3.70	1.54	1.43
31	7	316	CLA	MG-ND	-3.70	1.98	2.05
32	7	317	LUT	C21-C26	3.69	1.66	1.56
31	6	316	CLA	MG-ND	-3.69	1.98	2.05
43	H	101	BCR	C3-C4	3.69	1.64	1.52
31	5	612	CLA	MG-ND	-3.69	1.98	2.05
31	2	611	CLA	MG-ND	-3.69	1.98	2.05
32	1	616	LUT	C21-C26	3.69	1.66	1.56
31	c	603	CLA	C1C-NC	-3.69	1.32	1.37
32	1	615	LUT	C21-C26	3.69	1.66	1.56
43	d	406	BCR	C4-C5	-3.69	1.43	1.51
31	5	611	CLA	MG-ND	-3.69	1.98	2.05
31	C	607	CLA	C1C-NC	-3.69	1.32	1.37
32	4	616	LUT	C11-C10	3.69	1.54	1.43
31	B	605	CLA	C1C-NC	-3.69	1.32	1.37
31	c	604	CLA	C1C-NC	-3.69	1.32	1.37
31	B	604	CLA	C1C-NC	-3.69	1.32	1.37
31	g	310	CLA	C1C-NC	-3.69	1.32	1.37
31	G	609	CLA	C1C-NC	-3.68	1.32	1.37
31	c	607	CLA	C1C-NC	-3.68	1.32	1.37
32	N	317	LUT	C11-C10	3.68	1.54	1.43
31	C	604	CLA	C1C-NC	-3.68	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	9	312	CLA	MG-ND	-3.68	1.98	2.05
32	S	318	LUT	C11-C10	3.68	1.54	1.43
32	3	317	LUT	C11-C10	3.68	1.54	1.43
31	2	612	CLA	MG-ND	-3.68	1.98	2.05
32	S	317	LUT	C38-C25	3.68	1.57	1.50
31	p	613	CLA	MG-ND	-3.67	1.98	2.05
31	3	316	CLA	C1C-NC	-3.67	1.32	1.37
32	Y	315	LUT	C7-C6	3.67	1.58	1.45
31	N	313	CLA	MG-ND	-3.67	1.98	2.05
32	N	316	LUT	C11-C10	3.67	1.54	1.43
32	s	317	LUT	C38-C25	3.67	1.57	1.50
31	b	606	CLA	C1C-NC	-3.67	1.32	1.37
30	q	309	CHL	C3A-C2A	-3.67	1.44	1.54
31	B	614	CLA	MG-ND	-3.66	1.98	2.05
32	R	317	LUT	C11-C10	3.66	1.54	1.43
31	b	605	CLA	C1C-NC	-3.66	1.32	1.37
31	R	315	CLA	C1C-NC	-3.66	1.32	1.37
31	8	610	CLA	MG-ND	-3.66	1.98	2.05
32	5	617	LUT	C19-C9	3.66	1.58	1.50
43	B	617	BCR	C27-C26	-3.66	1.43	1.51
31	3	314	CLA	MG-ND	-3.66	1.98	2.05
32	R	317	LUT	C28-C29	3.66	1.53	1.45
43	v	101	BCR	C16-C17	3.65	1.54	1.43
31	C	611	CLA	C1C-NC	-3.65	1.32	1.37
43	H	101	BCR	C4-C5	-3.65	1.43	1.51
43	d	406	BCR	C3-C4	3.65	1.63	1.52
31	s	305	CLA	MG-ND	-3.65	1.98	2.05
43	b	619	BCR	C16-C17	3.65	1.54	1.43
31	1	604	CLA	C1C-NC	-3.65	1.32	1.37
32	y	616	LUT	C21-C26	3.65	1.66	1.56
31	g	313	CLA	MG-ND	-3.65	1.98	2.05
43	t	101	BCR	C11-C10	3.65	1.54	1.43
31	N	321	CLA	MG-ND	-3.65	1.98	2.05
31	p	611	CLA	MG-ND	-3.65	1.98	2.05
31	q	313	CLA	MG-ND	-3.65	1.98	2.05
32	6	317	LUT	C38-C25	3.65	1.57	1.50
31	N	305	CLA	MG-ND	-3.65	1.98	2.05
43	T	101	BCR	C11-C10	3.65	1.54	1.43
31	A	409	CLA	C1C-NC	-3.65	1.32	1.37
32	1	615	LUT	C28-C29	3.65	1.53	1.45
31	9	312	CLA	C1C-NC	-3.65	1.32	1.37
32	7	318	LUT	C11-C10	3.64	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	604	CLA	MG-ND	-3.64	1.98	2.05
31	B	612	CLA	MG-ND	-3.64	1.98	2.05
35	q	317	RRX	C20-C21	3.64	1.54	1.43
43	c	615	BCR	C11-C10	3.64	1.54	1.43
32	4	616	LUT	C38-C25	3.64	1.57	1.50
31	g	312	CLA	MG-ND	-3.64	1.98	2.05
32	p	617	LUT	C38-C25	3.64	1.57	1.50
32	8	615	LUT	C11-C10	3.64	1.54	1.43
31	C	612	CLA	C1C-NC	-3.64	1.32	1.37
32	n	317	LUT	C11-C10	3.64	1.54	1.43
32	Y	316	LUT	C21-C26	3.64	1.66	1.56
31	D	403	CLA	C1C-NC	-3.64	1.32	1.37
31	5	614	CLA	MG-ND	-3.64	1.98	2.05
31	5	604	CLA	MG-ND	-3.64	1.98	2.05
31	B	603	CLA	C1C-NC	-3.64	1.32	1.37
31	a	409	CLA	C1C-NC	-3.63	1.32	1.37
32	g	316	LUT	C38-C25	3.63	1.57	1.50
31	2	604	CLA	MG-ND	-3.63	1.98	2.05
31	8	614	CLA	MG-ND	-3.63	1.98	2.05
31	R	304	CLA	C1C-NC	-3.63	1.32	1.37
32	Y	315	LUT	C28-C29	3.63	1.53	1.45
31	B	611	CLA	MG-ND	-3.63	1.98	2.05
31	n	312	CLA	MG-ND	-3.63	1.98	2.05
30	0	605	CHL	C3A-C2A	-3.63	1.44	1.54
31	6	313	CLA	MG-ND	-3.63	1.98	2.05
31	A	406	CLA	C1C-NC	-3.62	1.32	1.37
31	3	313	CLA	MG-ND	-3.62	1.98	2.05
43	T	101	BCR	C4-C5	-3.62	1.43	1.51
31	r	304	CLA	MG-ND	-3.62	1.98	2.05
32	8	616	LUT	C11-C10	3.62	1.54	1.43
31	p	614	CLA	MG-ND	-3.62	1.98	2.05
31	7	312	CLA	MG-ND	-3.62	1.98	2.05
31	Y	314	CLA	MG-ND	-3.62	1.98	2.05
31	C	603	CLA	C1C-NC	-3.62	1.32	1.37
31	4	611	CLA	MG-ND	-3.62	1.98	2.05
31	G	602	CLA	MG-ND	-3.62	1.98	2.05
32	n	318	LUT	C11-C10	3.62	1.54	1.43
31	2	613	CLA	MG-ND	-3.61	1.98	2.05
32	8	615	LUT	C38-C25	3.61	1.57	1.50
32	s	318	LUT	C11-C10	3.61	1.54	1.43
31	q	313	CLA	C1C-NC	-3.61	1.32	1.37
31	g	314	CLA	MG-ND	-3.61	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	B	617	BCR	C20-C21	3.61	1.54	1.43
43	t	101	BCR	C27-C26	-3.61	1.43	1.51
43	c	615	BCR	C16-C17	3.61	1.54	1.43
32	y	617	LUT	C28-C29	3.61	1.53	1.45
31	B	610	CLA	MG-ND	-3.61	1.98	2.05
43	T	101	BCR	C3-C4	3.61	1.63	1.52
31	p	610	CLA	MG-ND	-3.61	1.98	2.05
32	5	617	LUT	C38-C25	3.61	1.57	1.50
31	Y	311	CLA	C1C-NC	-3.61	1.32	1.37
32	6	317	LUT	C11-C10	3.61	1.54	1.43
32	q	318	LUT	C19-C9	3.61	1.58	1.50
31	c	613	CLA	C1C-NC	-3.61	1.32	1.37
43	C	614	BCR	C4-C5	-3.61	1.43	1.51
31	S	313	CLA	C1C-NC	-3.61	1.32	1.37
31	y	615	CLA	MG-ND	-3.61	1.98	2.05
31	S	311	CLA	C1C-NC	-3.61	1.32	1.37
43	V	101	BCR	C16-C17	3.60	1.54	1.43
31	9	316	CLA	MG-ND	-3.60	1.98	2.05
32	3	317	LUT	C38-C25	3.60	1.57	1.50
31	n	316	CLA	MG-ND	-3.60	1.98	2.05
31	G	604	CLA	MG-ND	-3.60	1.98	2.05
31	8	611	CLA	MG-ND	-3.60	1.98	2.05
31	p	615	CLA	MG-ND	-3.60	1.98	2.05
32	s	317	LUT	C11-C10	3.60	1.54	1.43
43	C	615	BCR	C11-C10	3.60	1.54	1.43
32	9	318	LUT	C19-C9	3.60	1.58	1.50
31	r	307	CLA	C1C-NC	-3.60	1.32	1.37
32	0	616	LUT	C38-C25	3.60	1.57	1.50
32	8	616	LUT	C19-C9	3.60	1.58	1.50
31	N	315	CLA	MG-ND	-3.60	1.98	2.05
32	7	318	LUT	C38-C25	3.60	1.57	1.50
32	n	317	LUT	C38-C25	3.60	1.57	1.50
31	R	312	CLA	C1C-NC	-3.60	1.32	1.37
31	3	315	CLA	MG-ND	-3.60	1.98	2.05
31	8	603	CLA	MG-ND	-3.60	1.98	2.05
31	R	314	CLA	C1C-NC	-3.60	1.32	1.37
31	N	312	CLA	MG-ND	-3.60	1.98	2.05
31	S	305	CLA	MG-ND	-3.60	1.98	2.05
31	7	315	CLA	MG-ND	-3.60	1.98	2.05
31	8	602	CLA	MG-ND	-3.60	1.98	2.05
31	7	305	CLA	MG-ND	-3.60	1.98	2.05
31	8	612	CLA	MG-ND	-3.60	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	313	CLA	C1C-NC	-3.60	1.32	1.37
31	n	314	CLA	MG-ND	-3.59	1.98	2.05
31	n	313	CLA	MG-ND	-3.59	1.98	2.05
31	6	314	CLA	MG-ND	-3.59	1.98	2.05
32	6	318	LUT	C11-C10	3.59	1.54	1.43
43	A	410	BCR	C27-C26	-3.59	1.43	1.51
32	3	318	LUT	C19-C9	3.59	1.58	1.50
31	5	613	CLA	MG-ND	-3.59	1.98	2.05
31	n	304	CLA	MG-ND	-3.59	1.98	2.05
43	h	101	BCR	C4-C5	-3.59	1.43	1.51
32	n	318	LUT	C19-C9	3.59	1.58	1.50
43	B	618	BCR	C16-C17	3.59	1.54	1.43
30	1	619	CHL	C3B-C2B	-3.59	1.35	1.40
31	B	613	CLA	MG-ND	-3.58	1.98	2.05
32	3	317	LUT	C19-C9	3.58	1.58	1.50
31	B	609	CLA	C1C-NC	-3.58	1.32	1.37
31	7	313	CLA	C1C-NC	-3.58	1.32	1.37
43	a	410	BCR	C27-C26	-3.58	1.43	1.51
35	g	315	RRX	C7-C6	3.58	1.57	1.45
32	S	317	LUT	C11-C10	3.58	1.54	1.43
31	c	605	CLA	C1C-NC	-3.58	1.32	1.37
31	a	407	CLA	C1C-NC	-3.58	1.32	1.37
31	N	304	CLA	MG-ND	-3.58	1.98	2.05
31	y	614	CLA	MG-ND	-3.58	1.98	2.05
32	6	317	LUT	C19-C9	3.58	1.58	1.50
32	N	316	LUT	C19-C9	3.58	1.58	1.50
31	g	305	CLA	MG-ND	-3.58	1.98	2.05
32	s	318	LUT	C38-C25	3.58	1.57	1.50
43	c	614	BCR	C4-C5	-3.58	1.43	1.51
32	6	318	LUT	C38-C25	3.58	1.57	1.50
31	1	614	CLA	MG-ND	-3.58	1.98	2.05
31	7	303	CLA	MG-ND	-3.58	1.98	2.05
43	C	615	BCR	C4-C5	-3.58	1.43	1.51
31	0	614	CLA	MG-ND	-3.58	1.98	2.05
32	Y	316	LUT	C23-C24	-3.58	1.45	1.50
32	S	317	LUT	C19-C9	3.58	1.58	1.50
32	s	317	LUT	C19-C9	3.58	1.58	1.50
31	6	303	CLA	MG-ND	-3.58	1.98	2.05
31	8	604	CLA	MG-ND	-3.58	1.98	2.05
43	Z	101	BCR	C16-C17	3.58	1.54	1.43
43	B	619	BCR	C4-C5	-3.57	1.43	1.51
32	9	318	LUT	C38-C25	3.57	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	611	CLA	C1C-NC	-3.57	1.32	1.37
31	y	602	CLA	MG-ND	-3.57	1.98	2.05
31	g	304	CLA	MG-ND	-3.57	1.98	2.05
31	5	602	CLA	MG-ND	-3.57	1.98	2.05
31	R	316	CLA	C1C-NC	-3.57	1.32	1.37
31	2	603	CLA	MG-ND	-3.57	1.98	2.05
31	b	611	CLA	MG-ND	-3.57	1.98	2.05
31	r	316	CLA	C1C-NC	-3.57	1.32	1.37
31	4	602	CLA	MG-ND	-3.57	1.98	2.05
31	Y	310	CLA	MG-ND	-3.57	1.98	2.05
43	A	410	BCR	C11-C10	3.57	1.54	1.43
31	n	305	CLA	MG-ND	-3.57	1.98	2.05
32	r	317	LUT	C21-C26	3.56	1.66	1.56
31	9	315	CLA	MG-ND	-3.56	1.98	2.05
32	5	616	LUT	C19-C9	3.56	1.58	1.50
32	G	615	LUT	C19-C9	3.56	1.58	1.50
32	n	317	LUT	C19-C9	3.56	1.58	1.50
31	6	304	CLA	MG-ND	-3.56	1.98	2.05
32	g	316	LUT	C19-C9	3.56	1.58	1.50
43	c	614	BCR	C27-C26	-3.56	1.44	1.51
43	B	619	BCR	C11-C10	3.56	1.54	1.43
43	b	618	BCR	C11-C10	3.56	1.54	1.43
31	B	606	CLA	C1C-NC	-3.56	1.32	1.37
31	3	306	CLA	MG-ND	-3.56	1.98	2.05
31	6	305	CLA	MG-ND	-3.56	1.98	2.05
31	Y	303	CLA	MG-ND	-3.56	1.98	2.05
31	B	602	CLA	C1C-NC	-3.56	1.32	1.37
32	7	318	LUT	C19-C9	3.56	1.58	1.50
31	N	311	CLA	MG-ND	-3.56	1.98	2.05
43	c	615	BCR	C27-C26	-3.55	1.44	1.51
31	1	603	CLA	C1C-NC	-3.55	1.32	1.37
31	9	306	CLA	MG-ND	-3.55	1.98	2.05
43	v	101	BCR	C11-C10	3.55	1.54	1.43
32	s	318	LUT	C19-C9	3.55	1.58	1.50
31	1	611	CLA	MG-ND	-3.55	1.98	2.05
32	S	318	LUT	C19-C9	3.55	1.58	1.50
43	V	101	BCR	C11-C10	3.55	1.54	1.43
31	Y	305	CLA	MG-ND	-3.55	1.98	2.05
31	B	615	CLA	C1C-NC	-3.55	1.32	1.37
31	6	311	CLA	MG-ND	-3.55	1.98	2.05
31	2	610	CLA	MG-ND	-3.55	1.98	2.05
31	C	601	CLA	C1C-NC	-3.55	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	303	CLA	MG-ND	-3.54	1.98	2.05
31	q	312	CLA	MG-ND	-3.54	1.98	2.05
32	8	615	LUT	C19-C9	3.54	1.58	1.50
43	C	614	BCR	C11-C10	3.54	1.54	1.43
31	b	613	CLA	MG-ND	-3.54	1.98	2.05
31	n	303	CLA	MG-ND	-3.54	1.98	2.05
32	G	615	LUT	C38-C25	3.54	1.57	1.50
31	N	310	CLA	MG-ND	-3.54	1.98	2.05
32	7	317	LUT	C11-C10	3.54	1.54	1.43
31	9	305	CLA	MG-ND	-3.54	1.98	2.05
32	Y	316	LUT	C11-C10	3.54	1.54	1.43
31	9	314	CLA	C1C-NC	-3.54	1.32	1.37
43	d	406	BCR	C27-C26	-3.54	1.44	1.51
43	z	101	BCR	C27-C26	-3.54	1.44	1.51
43	D	405	BCR	C24-C25	3.54	1.57	1.45
32	n	318	LUT	C38-C25	3.54	1.57	1.50
31	C	606	CLA	C1C-NC	-3.54	1.32	1.37
43	B	618	BCR	C24-C25	3.54	1.57	1.45
31	9	304	CLA	MG-ND	-3.54	1.98	2.05
43	z	101	BCR	C11-C10	3.54	1.54	1.43
32	y	617	LUT	C23-C24	-3.54	1.45	1.50
31	b	615	CLA	MG-ND	-3.54	1.98	2.05
35	9	317	RRX	C7-C6	3.54	1.57	1.45
31	s	310	CLA	C1C-NC	-3.54	1.32	1.37
31	R	306	CLA	C1C-NC	-3.53	1.32	1.37
32	p	617	LUT	C19-C9	3.53	1.58	1.50
31	G	603	CLA	MG-ND	-3.53	1.98	2.05
31	7	311	CLA	MG-ND	-3.53	1.98	2.05
31	r	306	CLA	C1C-NC	-3.53	1.32	1.37
31	R	307	CLA	C1C-NC	-3.53	1.32	1.37
35	G	614	RRX	C7-C6	3.53	1.57	1.45
32	4	616	LUT	C19-C9	3.53	1.58	1.50
32	q	318	LUT	C38-C25	3.53	1.57	1.50
43	A	410	BCR	C16-C17	3.53	1.54	1.43
32	N	317	LUT	C19-C9	3.53	1.58	1.50
31	G	612	CLA	C1C-NC	-3.53	1.32	1.37
31	1	602	CLA	C1C-NC	-3.53	1.32	1.37
32	2	615	LUT	C19-C9	3.53	1.58	1.50
32	6	318	LUT	C19-C9	3.53	1.58	1.50
31	2	602	CLA	MG-ND	-3.53	1.98	2.05
31	N	303	CLA	MG-ND	-3.53	1.98	2.05
43	h	101	BCR	C27-C26	-3.53	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	7	317	LUT	C38-C25	3.52	1.57	1.50
32	8	616	LUT	C38-C25	3.52	1.57	1.50
31	1	610	CLA	MG-ND	-3.52	1.98	2.05
31	B	601	CLA	C1C-NC	-3.52	1.32	1.37
31	d	405	CLA	C1C-NC	-3.52	1.32	1.37
43	h	101	BCR	C16-C17	3.52	1.54	1.43
31	3	304	CLA	MG-ND	-3.52	1.98	2.05
43	b	619	BCR	C24-C25	3.52	1.57	1.45
43	h	101	BCR	C11-C10	3.52	1.54	1.43
32	r	317	LUT	C28-C29	3.52	1.53	1.45
31	n	311	CLA	MG-ND	-3.52	1.98	2.05
32	0	617	LUT	C11-C10	3.52	1.54	1.43
31	2	609	CLA	MG-ND	-3.52	1.98	2.05
31	4	604	CLA	MG-ND	-3.52	1.98	2.05
32	3	318	LUT	C38-C25	3.52	1.57	1.50
43	Z	101	BCR	C11-C10	3.52	1.54	1.43
31	q	304	CLA	MG-ND	-3.52	1.98	2.05
31	b	602	CLA	C1C-NC	-3.52	1.32	1.37
31	c	612	CLA	C1C-NC	-3.52	1.32	1.37
31	C	613	CLA	C1C-NC	-3.52	1.32	1.37
32	1	616	LUT	C38-C25	3.52	1.57	1.50
31	s	303	CLA	MG-ND	-3.52	1.98	2.05
35	4	615	RRX	C7-C6	3.52	1.57	1.45
32	5	616	LUT	C38-C25	3.52	1.57	1.50
31	3	305	CLA	MG-ND	-3.51	1.98	2.05
31	s	316	CLA	C1C-NC	-3.51	1.32	1.37
31	b	612	CLA	MG-ND	-3.51	1.98	2.05
32	N	316	LUT	C38-C25	3.51	1.57	1.50
32	S	318	LUT	C38-C25	3.51	1.57	1.50
31	B	608	CLA	C1C-NC	-3.51	1.32	1.37
43	a	410	BCR	C16-C17	3.51	1.54	1.43
31	y	611	CLA	C1C-NC	-3.51	1.32	1.37
31	5	610	CLA	MG-ND	-3.51	1.98	2.05
43	B	619	BCR	C27-C26	-3.51	1.44	1.51
43	b	620	BCR	C11-C10	3.51	1.54	1.43
32	p	616	LUT	C19-C9	3.51	1.58	1.50
32	0	616	LUT	C11-C10	3.51	1.54	1.43
31	S	314	CLA	C1C-NC	-3.51	1.32	1.37
43	b	620	BCR	C16-C17	3.50	1.54	1.43
31	R	313	CLA	C1C-NC	-3.50	1.32	1.37
43	b	619	BCR	C11-C10	3.50	1.54	1.43
31	Y	312	CLA	C1C-NC	-3.50	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	311	CLA	C1C-NC	-3.50	1.32	1.37
31	4	612	CLA	C1C-NC	-3.50	1.32	1.37
31	r	315	CLA	C1C-NC	-3.50	1.32	1.37
32	y	616	LUT	C28-C29	3.50	1.53	1.45
43	b	620	BCR	C27-C26	-3.50	1.44	1.51
31	C	606	CLA	C3B-C2B	-3.50	1.35	1.40
32	1	615	LUT	C38-C25	3.50	1.57	1.50
31	g	303	CLA	C1C-NC	-3.50	1.32	1.37
32	1	616	LUT	C11-C10	3.50	1.54	1.43
31	R	303	CLA	C1C-NC	-3.49	1.32	1.37
32	N	317	LUT	C38-C25	3.49	1.57	1.50
31	r	314	CLA	C1C-NC	-3.49	1.32	1.37
31	C	609	CLA	C1C-NC	-3.49	1.32	1.37
31	b	614	CLA	MG-ND	-3.49	1.98	2.05
43	C	614	BCR	C16-C17	3.49	1.54	1.43
43	b	620	BCR	C4-C5	-3.49	1.44	1.51
31	0	602	CLA	C1C-NC	-3.49	1.32	1.37
43	v	101	BCR	C24-C25	3.49	1.57	1.45
31	s	314	CLA	C1C-NC	-3.49	1.32	1.37
32	1	616	LUT	C19-C9	3.49	1.58	1.50
31	8	609	CLA	MG-ND	-3.49	1.98	2.05
43	H	101	BCR	C16-C17	3.49	1.54	1.43
43	H	101	BCR	C11-C10	3.49	1.54	1.43
31	6	315	CLA	MG-ND	-3.49	1.98	2.05
32	r	317	LUT	C38-C25	3.49	1.57	1.50
31	b	604	CLA	C1C-NC	-3.49	1.32	1.37
32	0	616	LUT	C19-C9	3.49	1.58	1.50
35	q	317	RRX	C7-C6	3.48	1.57	1.45
32	R	317	LUT	C23-C24	-3.48	1.45	1.50
31	D	404	CLA	C1C-NC	-3.48	1.32	1.37
31	s	313	CLA	C1C-NC	-3.48	1.32	1.37
43	A	410	BCR	C4-C5	-3.48	1.44	1.51
31	y	612	CLA	C1C-NC	-3.47	1.32	1.37
31	y	610	CLA	MG-ND	-3.47	1.98	2.05
31	s	304	CLA	MG-ND	-3.47	1.98	2.05
43	z	101	BCR	C16-C17	3.47	1.54	1.43
31	0	604	CLA	C1C-NC	-3.47	1.32	1.37
31	b	610	CLA	C1C-NC	-3.47	1.32	1.37
31	Y	304	CLA	MG-ND	-3.47	1.98	2.05
31	y	603	CLA	MG-ND	-3.47	1.98	2.05
31	4	613	CLA	C1C-NC	-3.47	1.32	1.37
43	Z	101	BCR	C27-C26	-3.47	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	T	101	BCR	C24-C25	3.47	1.57	1.45
43	a	410	BCR	C4-C5	-3.47	1.44	1.51
43	b	618	BCR	C4-C5	-3.47	1.44	1.51
31	3	311	CLA	C1C-NC	-3.46	1.32	1.37
43	B	619	BCR	C16-C17	3.46	1.54	1.43
31	R	305	CLA	C1C-NC	-3.46	1.32	1.37
35	2	614	RRX	C7-C6	3.46	1.57	1.45
43	c	615	BCR	C24-C25	3.46	1.57	1.45
31	r	305	CLA	MG-ND	-3.46	1.98	2.05
31	S	315	CLA	C1C-NC	-3.46	1.32	1.37
32	0	617	LUT	C38-C25	3.46	1.57	1.50
43	B	618	BCR	C11-C10	3.46	1.54	1.43
32	Y	315	LUT	C38-C25	3.46	1.57	1.50
43	T	101	BCR	C27-C26	-3.45	1.44	1.51
31	b	607	CLA	C1C-NC	-3.45	1.32	1.37
31	5	603	CLA	MG-ND	-3.45	1.98	2.05
31	1	613	CLA	C1C-NC	-3.45	1.32	1.37
47	E	101	HEM	C1B-NB	-3.44	1.34	1.40
43	H	101	BCR	C24-C25	3.44	1.57	1.45
43	t	101	BCR	C24-C25	3.44	1.57	1.45
31	s	315	CLA	C1C-NC	-3.44	1.32	1.37
32	y	616	LUT	C38-C25	3.44	1.57	1.50
43	b	620	BCR	C24-C25	3.44	1.57	1.45
43	a	410	BCR	C11-C10	3.44	1.54	1.43
31	s	306	CLA	MG-ND	-3.44	1.99	2.05
32	p	616	LUT	C38-C25	3.44	1.57	1.50
43	a	410	BCR	C24-C25	3.43	1.57	1.45
43	b	618	BCR	C16-C17	3.43	1.54	1.43
32	0	617	LUT	C19-C9	3.43	1.58	1.50
43	D	405	BCR	C4-C5	-3.43	1.44	1.51
43	c	615	BCR	C4-C5	-3.43	1.44	1.51
43	t	101	BCR	C16-C17	3.43	1.54	1.43
31	g	303	CLA	MG-ND	-3.43	1.99	2.05
31	G	613	CLA	C1C-NC	-3.43	1.32	1.37
32	p	616	LUT	C2-C1	3.43	1.65	1.54
31	q	314	CLA	C1C-NC	-3.43	1.32	1.37
31	C	610	CLA	C1C-NC	-3.42	1.32	1.37
31	1	612	CLA	C1C-NC	-3.42	1.32	1.37
31	7	304	CLA	MG-ND	-3.42	1.99	2.05
31	b	616	CLA	C1C-NC	-3.42	1.32	1.37
32	y	617	LUT	C19-C9	3.42	1.57	1.50
47	E	101	HEM	C4D-ND	-3.42	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	406	BCR	C16-C17	3.42	1.54	1.43
32	y	616	LUT	C19-C9	3.41	1.57	1.50
31	c	610	CLA	C1C-NC	-3.41	1.32	1.37
31	S	304	CLA	CBB-CAB	3.41	1.51	1.29
43	H	101	BCR	C27-C26	-3.41	1.44	1.51
43	B	617	BCR	C11-C10	3.41	1.54	1.43
43	h	101	BCR	C24-C25	3.41	1.57	1.45
31	d	404	CLA	C1C-NC	-3.41	1.32	1.37
43	t	101	BCR	C3-C4	3.41	1.63	1.52
32	l	615	LUT	C19-C9	3.41	1.57	1.50
31	4	603	CLA	MG-ND	-3.40	1.99	2.05
32	p	617	LUT	C2-C1	3.40	1.65	1.54
31	q	306	CLA	C1C-NC	-3.40	1.32	1.37
43	B	618	BCR	C27-C26	-3.40	1.44	1.51
43	V	101	BCR	C27-C26	-3.40	1.44	1.51
31	S	312	CLA	C1C-NC	-3.40	1.32	1.37
31	9	313	CLA	C1C-NC	-3.40	1.32	1.37
43	Z	101	BCR	C4-C5	-3.40	1.44	1.51
31	6	312	CLA	C1C-NC	-3.40	1.32	1.37
31	c	601	CLA	C1C-NC	-3.40	1.32	1.37
32	q	318	LUT	C2-C1	3.40	1.65	1.54
32	7	317	LUT	C19-C9	3.39	1.57	1.50
31	0	613	CLA	C1C-NC	-3.39	1.32	1.37
43	c	614	BCR	C24-C25	3.39	1.57	1.45
32	9	318	LUT	C2-C1	3.39	1.65	1.54
32	R	317	LUT	C38-C25	3.39	1.56	1.50
31	S	310	CLA	C1C-NC	-3.39	1.32	1.37
32	r	317	LUT	C19-C9	3.39	1.57	1.50
30	S	308	CHL	C3B-C2B	-3.39	1.35	1.40
47	e	102	HEM	C1B-NB	-3.39	1.34	1.40
43	C	615	BCR	C24-C25	3.39	1.57	1.45
31	4	614	CLA	C1C-NC	-3.38	1.32	1.37
31	b	609	CLA	C1C-NC	-3.38	1.32	1.37
31	r	313	CLA	C1C-NC	-3.38	1.32	1.37
32	N	316	LUT	C2-C1	3.38	1.65	1.54
43	V	101	BCR	C24-C25	3.38	1.57	1.45
43	Z	101	BCR	C24-C25	3.38	1.57	1.45
43	A	410	BCR	C24-C25	3.38	1.57	1.45
31	p	604	CLA	CBB-CAB	3.38	1.51	1.29
31	g	311	CLA	C1C-NC	-3.38	1.32	1.37
31	0	612	CLA	C1C-NC	-3.37	1.32	1.37
31	b	603	CLA	C1C-NC	-3.37	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	z	101	BCR	C24-C25	3.37	1.57	1.45
30	p	608	CHL	CBB-CAB	3.37	1.51	1.29
32	5	616	LUT	C40-C33	3.37	1.57	1.50
43	d	406	BCR	C24-C25	3.37	1.57	1.45
32	1	615	LUT	C11-C10	3.37	1.53	1.43
31	G	611	CLA	C1C-NC	-3.37	1.32	1.37
31	7	314	CLA	C1C-NC	-3.37	1.32	1.37
43	v	101	BCR	C27-C26	-3.37	1.44	1.51
32	Y	315	LUT	C19-C9	3.37	1.57	1.50
30	9	307	CHL	CBB-CAB	3.37	1.51	1.29
31	s	316	CLA	CBB-CAB	3.36	1.51	1.29
32	8	615	LUT	C40-C33	3.36	1.57	1.50
31	4	614	CLA	CBB-CAB	3.36	1.51	1.29
30	4	609	CHL	CBB-CAB	3.36	1.51	1.29
32	5	616	LUT	C2-C1	3.36	1.65	1.54
31	3	304	CLA	CBB-CAB	3.36	1.51	1.29
32	6	317	LUT	C2-C1	3.36	1.65	1.54
30	5	605	CHL	CBB-CAB	3.36	1.51	1.29
45	c	616	DGD	CAB-C9B	-3.36	1.32	1.51
32	q	318	LUT	C40-C33	3.36	1.57	1.50
32	5	617	LUT	C2-C1	3.36	1.65	1.54
32	Y	316	LUT	C19-C9	3.36	1.57	1.50
30	3	307	CHL	CBB-CAB	3.36	1.51	1.29
47	e	102	HEM	C4D-ND	-3.36	1.34	1.40
32	s	318	LUT	C2-C1	3.36	1.65	1.54
31	0	603	CLA	C1C-NC	-3.36	1.32	1.37
31	8	602	CLA	CBB-CAB	3.36	1.51	1.29
31	s	312	CLA	C1C-NC	-3.36	1.32	1.37
31	p	602	CLA	C1C-NC	-3.35	1.32	1.37
30	p	605	CHL	CBB-CAB	3.35	1.51	1.29
43	B	619	BCR	C24-C25	3.35	1.57	1.45
31	q	305	CLA	MG-ND	-3.35	1.99	2.05
31	3	312	CLA	CBB-CAB	3.35	1.51	1.29
31	3	314	CLA	CBB-CAB	3.35	1.51	1.29
31	9	306	CLA	CBB-CAB	3.35	1.51	1.29
31	B	610	CLA	C1C-NC	-3.35	1.32	1.37
32	4	616	LUT	C40-C33	3.35	1.57	1.50
30	g	306	CHL	CBB-CAB	3.35	1.51	1.29
31	3	315	CLA	CBB-CAB	3.35	1.51	1.29
32	6	317	LUT	C40-C33	3.35	1.57	1.50
30	p	601	CHL	CBB-CAB	3.35	1.51	1.29
43	v	101	BCR	C4-C5	-3.35	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	S	317	LUT	C40-C33	3.35	1.57	1.50
31	S	306	CLA	MG-ND	-3.35	1.99	2.05
31	5	603	CLA	CBB-CAB	3.35	1.51	1.29
32	6	318	LUT	C2-C1	3.35	1.65	1.54
31	5	613	CLA	CBB-CAB	3.35	1.51	1.29
43	V	101	BCR	C4-C5	-3.35	1.44	1.51
31	3	313	CLA	CBB-CAB	3.35	1.51	1.29
43	C	615	BCR	C16-C17	3.35	1.53	1.43
30	G	605	CHL	CBB-CAB	3.35	1.51	1.29
31	5	612	CLA	CBB-CAB	3.35	1.51	1.29
31	6	315	CLA	CBB-CAB	3.35	1.51	1.29
43	d	406	BCR	C11-C10	3.35	1.53	1.43
31	5	610	CLA	CBB-CAB	3.35	1.51	1.29
31	0	611	CLA	CBB-CAB	3.35	1.51	1.29
31	p	612	CLA	CBB-CAB	3.35	1.51	1.29
32	y	617	LUT	C11-C10	3.35	1.53	1.43
31	7	303	CLA	CBB-CAB	3.35	1.51	1.29
31	b	615	CLA	CBB-CAB	3.35	1.51	1.29
31	9	304	CLA	CBB-CAB	3.35	1.51	1.29
31	q	304	CLA	CBB-CAB	3.35	1.51	1.29
31	6	313	CLA	CBB-CAB	3.35	1.51	1.29
32	6	318	LUT	C40-C33	3.35	1.57	1.50
34	B	621	LMG	C37-C36	-3.34	1.32	1.51
31	p	615	CLA	C1C-NC	-3.34	1.32	1.37
32	4	616	LUT	C2-C1	3.34	1.65	1.54
31	8	614	CLA	CBB-CAB	3.34	1.51	1.29
30	2	605	CHL	CBB-CAB	3.34	1.51	1.29
31	n	303	CLA	CBB-CAB	3.34	1.51	1.29
31	s	305	CLA	CBB-CAB	3.34	1.51	1.29
30	G	607	CHL	CBB-CAB	3.34	1.51	1.29
31	5	611	CLA	CBB-CAB	3.34	1.51	1.29
31	s	303	CLA	CBB-CAB	3.34	1.51	1.29
31	0	615	CLA	C1C-NC	-3.34	1.32	1.37
31	5	602	CLA	CBB-CAB	3.34	1.51	1.29
31	7	311	CLA	CBB-CAB	3.34	1.51	1.29
32	7	318	LUT	C2-C1	3.34	1.65	1.54
31	2	611	CLA	C1C-NC	-3.34	1.32	1.37
35	q	317	RRX	C4-C5	-3.34	1.44	1.51
31	N	312	CLA	CBB-CAB	3.34	1.51	1.29
31	7	315	CLA	CBB-CAB	3.34	1.51	1.29
32	5	617	LUT	C40-C33	3.34	1.57	1.50
31	3	306	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S	303	CLA	CBB-CAB	3.34	1.51	1.29
31	8	603	CLA	CBB-CAB	3.34	1.51	1.29
31	y	610	CLA	CBB-CAB	3.34	1.51	1.29
31	6	304	CLA	CBB-CAB	3.34	1.51	1.29
32	2	615	LUT	C2-C1	3.34	1.65	1.54
31	8	610	CLA	CBB-CAB	3.34	1.51	1.29
32	S	318	LUT	C40-C33	3.34	1.57	1.50
31	6	312	CLA	CBB-CAB	3.34	1.51	1.29
31	Y	310	CLA	CBB-CAB	3.34	1.51	1.29
31	0	612	CLA	CBB-CAB	3.34	1.51	1.29
31	9	316	CLA	CBB-CAB	3.34	1.51	1.29
32	Y	315	LUT	C11-C10	3.34	1.53	1.43
30	2	608	CHL	CBB-CAB	3.34	1.51	1.29
31	4	604	CLA	CBB-CAB	3.34	1.51	1.29
31	c	607	CLA	CBB-CAB	3.34	1.51	1.29
31	n	305	CLA	CBB-CAB	3.34	1.51	1.29
31	5	604	CLA	CBB-CAB	3.34	1.51	1.29
31	2	604	CLA	CBB-CAB	3.34	1.51	1.29
31	3	305	CLA	CBB-CAB	3.34	1.51	1.29
31	N	303	CLA	CBB-CAB	3.34	1.51	1.29
31	N	314	CLA	CBB-CAB	3.34	1.51	1.29
31	p	610	CLA	CBB-CAB	3.34	1.51	1.29
31	7	312	CLA	CBB-CAB	3.34	1.51	1.29
31	n	313	CLA	CBB-CAB	3.34	1.51	1.29
31	6	303	CLA	CBB-CAB	3.34	1.51	1.29
31	S	305	CLA	CBB-CAB	3.34	1.51	1.29
31	B	611	CLA	CBB-CAB	3.34	1.51	1.29
31	N	305	CLA	CBB-CAB	3.34	1.51	1.29
31	p	614	CLA	CBB-CAB	3.34	1.51	1.29
31	y	603	CLA	CBB-CAB	3.34	1.51	1.29
31	1	614	CLA	CBB-CAB	3.34	1.51	1.29
31	5	614	CLA	CBB-CAB	3.34	1.51	1.29
43	b	619	BCR	C27-C26	-3.34	1.44	1.51
31	3	311	CLA	CBB-CAB	3.34	1.51	1.29
31	4	603	CLA	CBB-CAB	3.34	1.51	1.29
31	r	305	CLA	CBB-CAB	3.34	1.51	1.29
31	g	314	CLA	CBB-CAB	3.34	1.51	1.29
31	2	610	CLA	CBB-CAB	3.34	1.51	1.29
31	4	602	CLA	CBB-CAB	3.34	1.51	1.29
31	N	304	CLA	CBB-CAB	3.34	1.51	1.29
31	0	614	CLA	CBB-CAB	3.34	1.51	1.29
31	G	602	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	g	322	LMG	C37-C36	-3.34	1.32	1.51
31	s	304	CLA	CBB-CAB	3.34	1.51	1.29
30	9	311	CHL	CBB-CAB	3.34	1.51	1.29
31	6	311	CLA	CBB-CAB	3.34	1.51	1.29
31	n	312	CLA	CBB-CAB	3.34	1.51	1.29
31	y	612	CLA	CBB-CAB	3.34	1.51	1.29
31	9	305	CLA	CBB-CAB	3.34	1.51	1.29
30	2	607	CHL	CBB-CAB	3.34	1.51	1.29
31	n	315	CLA	CBB-CAB	3.34	1.51	1.29
32	G	615	LUT	C2-C1	3.34	1.65	1.54
31	g	305	CLA	CBB-CAB	3.34	1.51	1.29
31	4	610	CLA	C1C-NC	-3.34	1.32	1.37
31	9	315	CLA	CBB-CAB	3.34	1.51	1.29
32	0	617	LUT	C23-C24	-3.34	1.45	1.50
31	B	614	CLA	CBB-CAB	3.34	1.51	1.29
30	p	609	CHL	CBB-CAB	3.34	1.51	1.29
31	N	313	CLA	CBB-CAB	3.33	1.51	1.29
30	Y	302	CHL	CBB-CAB	3.33	1.51	1.29
31	8	604	CLA	CBB-CAB	3.33	1.51	1.29
30	4	605	CHL	CBB-CAB	3.33	1.51	1.29
31	1	611	CLA	CBB-CAB	3.33	1.51	1.29
31	Y	303	CLA	CBB-CAB	3.33	1.51	1.29
32	3	317	LUT	C2-C1	3.33	1.65	1.54
31	8	609	CLA	CBB-CAB	3.33	1.51	1.29
31	9	312	CLA	CBB-CAB	3.33	1.51	1.29
31	6	314	CLA	CBB-CAB	3.33	1.51	1.29
30	6	306	CHL	CBB-CAB	3.33	1.51	1.29
30	q	307	CHL	CBB-CAB	3.33	1.51	1.29
31	N	310	CLA	CBB-CAB	3.33	1.51	1.29
31	s	306	CLA	CBB-CAB	3.33	1.51	1.29
31	R	313	CLA	CBB-CAB	3.33	1.51	1.29
31	Y	305	CLA	CBB-CAB	3.33	1.51	1.29
31	q	316	CLA	CBB-CAB	3.33	1.51	1.29
31	0	603	CLA	CBB-CAB	3.33	1.51	1.29
31	9	313	CLA	CBB-CAB	3.33	1.51	1.29
31	b	613	CLA	CBB-CAB	3.33	1.51	1.29
31	G	610	CLA	CBB-CAB	3.33	1.51	1.29
31	q	306	CLA	CBB-CAB	3.33	1.51	1.29
31	r	304	CLA	CBB-CAB	3.33	1.51	1.29
32	G	615	LUT	C40-C33	3.33	1.57	1.50
31	8	611	CLA	CBB-CAB	3.33	1.51	1.29
31	p	611	CLA	CBB-CAB	3.33	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	z	101	BCR	C4-C5	-3.33	1.44	1.51
34	9	301	LMG	C19-C18	-3.33	1.32	1.51
31	b	614	CLA	CBB-CAB	3.33	1.51	1.29
31	n	316	CLA	CBB-CAB	3.33	1.51	1.29
32	1	616	LUT	C2-C1	3.33	1.65	1.54
30	g	309	CHL	CBB-CAB	3.33	1.51	1.29
31	g	303	CLA	CBB-CAB	3.33	1.51	1.29
31	N	315	CLA	CBB-CAB	3.33	1.51	1.29
30	8	607	CHL	CBB-CAB	3.33	1.51	1.29
31	B	610	CLA	CBB-CAB	3.33	1.51	1.29
31	0	602	CLA	CBB-CAB	3.33	1.51	1.29
30	1	605	CHL	CBB-CAB	3.33	1.51	1.29
31	6	305	CLA	CBB-CAB	3.33	1.51	1.29
31	2	609	CLA	CBB-CAB	3.33	1.51	1.29
30	4	607	CHL	C4B-NB	3.33	1.38	1.35
32	p	616	LUT	C40-C33	3.33	1.57	1.50
30	G	608	CHL	CBB-CAB	3.33	1.51	1.29
32	n	317	LUT	C40-C33	3.33	1.57	1.50
31	8	613	CLA	CBB-CAB	3.33	1.51	1.29
31	n	314	CLA	CBB-CAB	3.33	1.51	1.29
45	c	617	DGD	CGB-CFB	-3.33	1.32	1.51
30	3	303	CHL	CBB-CAB	3.33	1.51	1.29
30	8	601	CHL	CBB-CAB	3.33	1.51	1.29
31	S	306	CLA	CBB-CAB	3.33	1.51	1.29
31	q	305	CLA	CBB-CAB	3.33	1.51	1.29
30	n	302	CHL	CBB-CAB	3.33	1.51	1.29
31	b	612	CLA	CBB-CAB	3.33	1.51	1.29
30	7	309	CHL	CBB-CAB	3.33	1.51	1.29
31	g	311	CLA	CBB-CAB	3.33	1.51	1.29
30	7	306	CHL	CBB-CAB	3.33	1.51	1.29
31	p	602	CLA	CBB-CAB	3.33	1.51	1.29
31	R	316	CLA	CBB-CAB	3.33	1.51	1.29
31	n	304	CLA	CBB-CAB	3.33	1.51	1.29
31	7	305	CLA	CBB-CAB	3.33	1.51	1.29
31	p	603	CLA	CBB-CAB	3.33	1.51	1.29
31	y	602	CLA	CBB-CAB	3.33	1.51	1.29
31	8	612	CLA	CBB-CAB	3.33	1.51	1.29
31	0	613	CLA	CBB-CAB	3.33	1.51	1.29
30	q	311	CHL	CBB-CAB	3.32	1.51	1.29
34	m	102	LMG	C37-C36	-3.32	1.32	1.51
32	8	615	LUT	C2-C1	3.32	1.65	1.54
31	y	604	CLA	CBB-CAB	3.32	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	604	CLA	CBB-CAB	3.32	1.51	1.29
31	7	316	CLA	CBB-CAB	3.32	1.51	1.29
31	s	315	CLA	CBB-CAB	3.32	1.51	1.29
31	2	613	CLA	CBB-CAB	3.32	1.51	1.29
31	r	313	CLA	CBB-CAB	3.32	1.51	1.29
30	g	308	CHL	CBB-CAB	3.32	1.51	1.29
31	1	610	CLA	CBB-CAB	3.32	1.51	1.29
31	G	613	CLA	CBB-CAB	3.32	1.51	1.29
31	7	304	CLA	CBB-CAB	3.32	1.51	1.29
30	0	609	CHL	CBB-CAB	3.32	1.51	1.29
32	n	317	LUT	C2-C1	3.32	1.65	1.54
31	y	615	CLA	CBB-CAB	3.32	1.51	1.29
31	b	611	CLA	CBB-CAB	3.32	1.51	1.29
31	g	304	CLA	CBB-CAB	3.32	1.51	1.29
32	g	316	LUT	C2-C1	3.32	1.65	1.54
31	N	311	CLA	CBB-CAB	3.32	1.51	1.29
31	s	311	CLA	CBB-CAB	3.32	1.51	1.29
32	N	316	LUT	C40-C33	3.32	1.57	1.50
30	5	609	CHL	CBB-CAB	3.32	1.51	1.29
31	N	321	CLA	CBB-CAB	3.32	1.51	1.29
30	N	302	CHL	CBB-CAB	3.32	1.51	1.29
31	G	603	CLA	CBB-CAB	3.32	1.51	1.29
31	g	313	CLA	CBB-CAB	3.32	1.51	1.29
31	2	611	CLA	CBB-CAB	3.32	1.51	1.29
31	Y	314	CLA	CBB-CAB	3.32	1.51	1.29
30	Y	309	CHL	CBB-CAB	3.32	1.51	1.29
31	0	615	CLA	CBB-CAB	3.32	1.51	1.29
30	r	309	CHL	CBB-CAB	3.32	1.51	1.29
31	g	312	CLA	CBB-CAB	3.32	1.51	1.29
30	9	310	CHL	CBB-CAB	3.32	1.51	1.29
31	B	611	CLA	C1C-NC	-3.32	1.32	1.37
32	r	317	LUT	C11-C10	3.32	1.53	1.43
31	5	615	CLA	CBB-CAB	3.32	1.51	1.29
31	G	612	CLA	CBB-CAB	3.32	1.51	1.29
32	7	318	LUT	C40-C33	3.32	1.57	1.50
30	3	310	CHL	CBB-CAB	3.32	1.51	1.29
30	n	309	CHL	CBB-CAB	3.32	1.51	1.29
45	c	618	DGD	CAA-C9A	-3.32	1.33	1.51
31	b	609	CLA	CBB-CAB	3.32	1.51	1.29
30	1	608	CHL	CBB-CAB	3.32	1.51	1.29
31	B	608	CLA	CBB-CAB	3.32	1.51	1.29
32	N	317	LUT	C40-C33	3.32	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	y	601	CHL	CBB-CAB	3.32	1.51	1.29
31	2	603	CLA	CBB-CAB	3.32	1.51	1.29
31	B	613	CLA	CBB-CAB	3.32	1.51	1.29
32	y	617	LUT	C38-C25	3.32	1.56	1.50
30	7	310	CHL	CBB-CAB	3.32	1.51	1.29
30	0	605	CHL	C3B-C2B	-3.32	1.35	1.40
31	S	316	CLA	CBB-CAB	3.31	1.51	1.29
30	g	302	CHL	CBB-CAB	3.31	1.51	1.29
31	R	314	CLA	CBB-CAB	3.31	1.51	1.29
32	s	318	LUT	C40-C33	3.31	1.57	1.50
30	y	609	CHL	CBB-CAB	3.31	1.51	1.29
31	B	612	CLA	CBB-CAB	3.31	1.51	1.29
31	C	610	CLA	CBB-CAB	3.31	1.51	1.29
31	9	314	CLA	CBB-CAB	3.31	1.51	1.29
32	y	616	LUT	C30-C29	-3.31	1.31	1.35
31	R	307	CLA	CBB-CAB	3.31	1.51	1.29
31	D	404	CLA	CBB-CAB	3.31	1.51	1.29
31	R	303	CLA	CBB-CAB	3.31	1.51	1.29
30	N	308	CHL	CBB-CAB	3.31	1.51	1.29
30	9	303	CHL	CBB-CAB	3.31	1.51	1.29
31	Y	304	CLA	CBB-CAB	3.31	1.51	1.29
32	S	318	LUT	C2-C1	3.31	1.65	1.54
31	7	314	CLA	CBB-CAB	3.31	1.51	1.29
30	n	310	CHL	CBB-CAB	3.31	1.51	1.29
30	s	308	CHL	CBB-CAB	3.31	1.51	1.29
31	n	311	CLA	CBB-CAB	3.31	1.51	1.29
34	d	410	LMG	C40-C39	-3.31	1.33	1.51
31	2	612	CLA	CBB-CAB	3.31	1.51	1.29
30	R	309	CHL	CBB-CAB	3.31	1.51	1.29
32	9	318	LUT	C40-C33	3.31	1.57	1.50
34	D	411	LMG	C40-C39	-3.31	1.33	1.51
31	7	313	CLA	CBB-CAB	3.31	1.51	1.29
31	1	612	CLA	CBB-CAB	3.31	1.51	1.29
31	p	615	CLA	CBB-CAB	3.31	1.51	1.29
31	1	613	CLA	CBB-CAB	3.31	1.51	1.29
31	4	612	CLA	CBB-CAB	3.31	1.51	1.29
30	4	606	CHL	CBB-CAB	3.31	1.51	1.29
31	3	313	CLA	C1C-NC	-3.31	1.32	1.37
31	s	310	CLA	CBB-CAB	3.31	1.51	1.29
30	5	608	CHL	CBB-CAB	3.31	1.51	1.29
31	S	310	CLA	CBB-CAB	3.31	1.51	1.29
32	0	616	LUT	C2-C1	3.31	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	602	CLA	CBB-CAB	3.31	1.51	1.29
31	s	312	CLA	CBB-CAB	3.31	1.51	1.29
31	S	312	CLA	CBB-CAB	3.31	1.51	1.29
31	S	315	CLA	CBB-CAB	3.31	1.51	1.29
30	5	601	CHL	CBB-CAB	3.31	1.51	1.29
31	4	610	CLA	CBB-CAB	3.31	1.51	1.29
31	p	613	CLA	CBB-CAB	3.30	1.51	1.29
30	8	608	CHL	CBB-CAB	3.30	1.51	1.29
30	N	309	CHL	CBB-CAB	3.30	1.51	1.29
30	9	309	CHL	CBB-CAB	3.30	1.51	1.29
32	7	317	LUT	C2-C1	3.30	1.65	1.54
31	R	311	CLA	CBB-CAB	3.30	1.51	1.29
32	s	317	LUT	C40-C33	3.30	1.57	1.50
34	b	601	LMG	C37-C36	-3.30	1.33	1.51
30	7	308	CHL	CBB-CAB	3.30	1.51	1.29
31	6	316	CLA	CBB-CAB	3.30	1.51	1.29
31	r	311	CLA	CBB-CAB	3.30	1.51	1.29
45	c	616	DGD	CGA-CFA	-3.30	1.33	1.51
31	q	316	CLA	C1C-NC	-3.30	1.32	1.37
31	s	313	CLA	CBB-CAB	3.30	1.51	1.29
30	y	608	CHL	CBB-CAB	3.30	1.51	1.29
30	S	302	CHL	CBB-CAB	3.30	1.51	1.29
32	n	318	LUT	C40-C33	3.30	1.57	1.50
43	C	614	BCR	C24-C25	3.30	1.56	1.45
31	S	313	CLA	CBB-CAB	3.30	1.51	1.29
31	B	615	CLA	CBB-CAB	3.30	1.51	1.29
32	3	318	LUT	C40-C33	3.30	1.57	1.50
30	q	303	CHL	CBB-CAB	3.30	1.51	1.29
31	2	602	CLA	CBB-CAB	3.30	1.51	1.29
31	b	606	CLA	CBB-CAB	3.30	1.51	1.29
31	c	604	CLA	CBB-CAB	3.30	1.51	1.29
31	3	301	CLA	CBB-CAB	3.30	1.51	1.29
31	r	303	CLA	CBB-CAB	3.30	1.51	1.29
31	1	603	CLA	CBB-CAB	3.30	1.51	1.29
31	Y	313	CLA	CBB-CAB	3.30	1.51	1.29
45	c	617	DGD	CAB-C9B	-3.30	1.33	1.51
31	r	314	CLA	CBB-CAB	3.30	1.51	1.29
34	D	409	LMG	C19-C18	-3.30	1.33	1.51
31	q	312	CLA	C1C-NC	-3.30	1.32	1.37
31	0	604	CLA	CBB-CAB	3.30	1.51	1.29
30	6	302	CHL	CBB-CAB	3.30	1.51	1.29
31	B	609	CLA	CBB-CAB	3.30	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	410	LMG	C37-C36	-3.30	1.33	1.51
45	c	617	DGD	CAA-C9A	-3.30	1.33	1.51
31	B	604	CLA	CBB-CAB	3.30	1.51	1.29
31	B	602	CLA	CBB-CAB	3.30	1.51	1.29
30	2	601	CHL	CBB-CAB	3.30	1.51	1.29
30	0	601	CHL	CBB-CAB	3.30	1.51	1.29
31	r	307	CLA	CBB-CAB	3.30	1.51	1.29
30	3	309	CHL	CBB-CAB	3.30	1.51	1.29
30	G	601	CHL	CBB-CAB	3.30	1.51	1.29
31	r	316	CLA	CBB-CAB	3.30	1.51	1.29
31	R	306	CLA	CBB-CAB	3.30	1.51	1.29
32	N	317	LUT	C2-C1	3.30	1.65	1.54
31	b	608	CLA	CBB-CAB	3.30	1.51	1.29
34	m	102	LMG	C40-C39	-3.30	1.33	1.51
32	3	317	LUT	C40-C33	3.30	1.57	1.50
45	C	617	DGD	CGB-CFB	-3.30	1.33	1.51
31	C	601	CLA	CBB-CAB	3.30	1.51	1.29
31	S	314	CLA	CBB-CAB	3.30	1.51	1.29
45	C	617	DGD	CAB-C9B	-3.30	1.33	1.51
30	Y	301	CHL	CBB-CAB	3.30	1.51	1.29
31	S	311	CLA	CBB-CAB	3.29	1.51	1.29
31	c	606	CLA	CBB-CAB	3.29	1.51	1.29
30	1	607	CHL	CBB-CAB	3.29	1.51	1.29
31	G	609	CLA	CBB-CAB	3.29	1.51	1.29
30	7	302	CHL	CBB-CAB	3.29	1.51	1.29
31	b	604	CLA	CBB-CAB	3.29	1.51	1.29
31	y	614	CLA	CBB-CAB	3.29	1.51	1.29
34	s	321	LMG	C19-C18	-3.29	1.33	1.51
31	G	611	CLA	CBB-CAB	3.29	1.51	1.29
34	W	201	LMG	C19-C18	-3.29	1.33	1.51
32	8	616	LUT	C40-C33	3.29	1.57	1.50
30	s	302	CHL	CBB-CAB	3.29	1.51	1.29
31	R	305	CLA	CBB-CAB	3.29	1.51	1.29
31	Y	314	CLA	C1C-NC	-3.29	1.32	1.37
31	r	315	CLA	CBB-CAB	3.29	1.51	1.29
30	n	306	CHL	CBB-CAB	3.29	1.51	1.29
31	A	406	CLA	CBB-CAB	3.29	1.51	1.29
30	4	608	CHL	CBB-CAB	3.29	1.51	1.29
31	p	614	CLA	C1C-NC	-3.29	1.32	1.37
34	b	601	LMG	C40-C39	-3.29	1.33	1.51
32	y	616	LUT	C11-C10	3.29	1.53	1.43
30	Y	308	CHL	CBB-CAB	3.29	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	315	CLA	CBB-CAB	3.29	1.51	1.29
31	q	315	CLA	CBB-CAB	3.29	1.51	1.29
31	c	610	CLA	CBB-CAB	3.29	1.51	1.29
30	4	601	CHL	CBB-CAB	3.29	1.51	1.29
31	C	608	CLA	CBB-CAB	3.29	1.51	1.29
34	w	201	LMG	C19-C18	-3.29	1.33	1.51
43	B	618	BCR	C4-C5	-3.29	1.44	1.51
30	1	609	CHL	CBB-CAB	3.29	1.51	1.29
31	q	314	CLA	CBB-CAB	3.29	1.51	1.29
31	b	605	CLA	CBB-CAB	3.29	1.51	1.29
32	0	616	LUT	C23-C24	-3.29	1.45	1.50
31	Y	312	CLA	CBB-CAB	3.29	1.51	1.29
31	c	601	CLA	CBB-CAB	3.29	1.51	1.29
30	n	301	CHL	CBB-CAB	3.29	1.51	1.29
30	5	606	CHL	CBB-CAB	3.29	1.51	1.29
30	0	608	CHL	CBB-CAB	3.29	1.51	1.29
34	b	622	LMG	C37-C36	-3.29	1.33	1.51
31	b	603	CLA	CBB-CAB	3.29	1.51	1.29
31	b	610	CLA	CBB-CAB	3.29	1.51	1.29
31	s	314	CLA	CBB-CAB	3.29	1.51	1.29
30	p	607	CHL	CBB-CAB	3.29	1.51	1.29
31	R	312	CLA	CBB-CAB	3.29	1.51	1.29
31	c	603	CLA	CBB-CAB	3.29	1.51	1.29
31	c	602	CLA	CBB-CAB	3.29	1.51	1.29
45	C	617	DGD	CDB-CCB	-3.29	1.33	1.51
31	n	316	CLA	C1C-NC	-3.29	1.32	1.37
31	r	305	CLA	C1C-NC	-3.29	1.32	1.37
31	c	605	CLA	CBB-CAB	3.29	1.51	1.29
30	Y	306	CHL	CBB-CAB	3.29	1.51	1.29
30	0	607	CHL	CBB-CAB	3.28	1.51	1.29
34	W	201	LMG	C37-C36	-3.28	1.33	1.51
45	c	618	DGD	CAB-C9B	-3.28	1.33	1.51
45	c	619	DGD	CDA-CCA	-3.28	1.33	1.51
32	n	318	LUT	C2-C1	3.28	1.65	1.54
30	S	309	CHL	CBB-CAB	3.28	1.51	1.29
30	6	310	CHL	CBB-CAB	3.28	1.51	1.29
31	b	607	CLA	CBB-CAB	3.28	1.51	1.29
31	5	615	CLA	C1C-NC	-3.28	1.32	1.37
31	g	310	CLA	CBB-CAB	3.28	1.51	1.29
31	y	611	CLA	CBB-CAB	3.28	1.51	1.29
32	g	316	LUT	C40-C33	3.28	1.57	1.50
32	7	317	LUT	C23-C24	-3.28	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	304	CLA	CBB-CAB	3.28	1.51	1.29
30	s	309	CHL	CBB-CAB	3.28	1.51	1.29
31	C	607	CLA	CBB-CAB	3.28	1.51	1.29
34	W	201	LMG	C25-C24	-3.28	1.33	1.51
32	3	318	LUT	C2-C1	3.28	1.65	1.54
31	2	613	CLA	C1C-NC	-3.28	1.32	1.37
30	p	606	CHL	CBB-CAB	3.28	1.51	1.29
30	8	605	CHL	CBB-CAB	3.28	1.51	1.29
31	C	612	CLA	CBB-CAB	3.28	1.51	1.29
30	5	607	CHL	CBB-CAB	3.28	1.51	1.29
31	C	603	CLA	CBB-CAB	3.28	1.51	1.29
45	c	616	DGD	CGB-CFB	-3.28	1.33	1.51
34	W	201	LMG	C22-C21	-3.28	1.33	1.51
31	c	611	CLA	CBB-CAB	3.28	1.51	1.29
30	N	306	CHL	CBB-CAB	3.28	1.51	1.29
35	g	315	RRX	C4-C5	-3.28	1.44	1.51
31	6	314	CLA	C1C-NC	-3.28	1.32	1.37
31	p	603	CLA	C1C-NC	-3.28	1.32	1.37
31	r	312	CLA	CBB-CAB	3.28	1.51	1.29
34	w	201	LMG	C40-C39	-3.28	1.33	1.51
45	c	619	DGD	CAB-C9B	-3.28	1.33	1.51
31	r	306	CLA	CBB-CAB	3.28	1.51	1.29
31	S	316	CLA	C1C-NC	-3.28	1.32	1.37
30	9	308	CHL	CBB-CAB	3.28	1.51	1.29
34	J	101	LMG	C37-C36	-3.28	1.33	1.51
31	C	613	CLA	CBB-CAB	3.28	1.51	1.29
31	B	606	CLA	CBB-CAB	3.28	1.51	1.29
31	Y	305	CLA	C1C-NC	-3.28	1.32	1.37
30	N	301	CHL	CBB-CAB	3.28	1.51	1.29
30	1	601	CHL	C3A-C2A	-3.28	1.45	1.54
30	n	308	CHL	CBB-CAB	3.28	1.51	1.29
30	7	321	CHL	CBB-CAB	3.28	1.51	1.29
31	6	305	CLA	C1C-NC	-3.28	1.32	1.37
30	6	308	CHL	CBB-CAB	3.28	1.51	1.29
31	b	617	CLA	CBB-CAB	3.27	1.51	1.29
34	D	411	LMG	C37-C36	-3.27	1.33	1.51
31	4	613	CLA	CBB-CAB	3.27	1.51	1.29
31	r	304	CLA	C1C-NC	-3.27	1.32	1.37
43	b	618	BCR	C24-C25	3.27	1.56	1.45
31	1	604	CLA	CBB-CAB	3.27	1.51	1.29
34	b	622	LMG	C22-C21	-3.27	1.33	1.51
34	B	621	LMG	C22-C21	-3.27	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	610	CLA	C1C-NC	-3.27	1.32	1.37
34	D	409	LMG	C22-C21	-3.27	1.33	1.51
31	a	406	CLA	CBB-CAB	3.27	1.51	1.29
45	C	617	DGD	CAA-C9A	-3.27	1.33	1.51
30	G	623	CHL	CBB-CAB	3.27	1.51	1.29
31	b	616	CLA	CBB-CAB	3.27	1.51	1.29
30	1	606	CHL	CBB-CAB	3.27	1.51	1.29
34	J	101	LMG	C19-C18	-3.27	1.33	1.51
31	N	310	CLA	C1C-NC	-3.27	1.32	1.37
31	A	405	CLA	CBB-CAB	3.27	1.51	1.29
34	2	620	LMG	C40-C39	-3.27	1.33	1.51
32	8	616	LUT	C2-C1	3.27	1.65	1.54
32	y	616	LUT	C2-C1	3.27	1.65	1.54
30	7	307	CHL	CBB-CAB	3.27	1.51	1.29
31	C	611	CLA	CBB-CAB	3.27	1.51	1.29
43	b	619	BCR	C4-C5	-3.27	1.44	1.51
34	d	410	LMG	C37-C36	-3.27	1.33	1.51
31	d	401	CLA	CBB-CAB	3.27	1.51	1.29
31	a	409	CLA	CBB-CAB	3.27	1.51	1.29
34	C	619	LMG	C40-C39	-3.27	1.33	1.51
31	A	407	CLA	CBB-CAB	3.27	1.51	1.29
31	a	407	CLA	CBB-CAB	3.27	1.51	1.29
34	J	101	LMG	C40-C39	-3.27	1.33	1.51
30	y	605	CHL	CBB-CAB	3.27	1.51	1.29
34	B	621	LMG	C19-C18	-3.27	1.33	1.51
34	D	412	LMG	C37-C36	-3.27	1.33	1.51
31	d	404	CLA	CBB-CAB	3.27	1.51	1.29
45	c	616	DGD	CDA-CCA	-3.27	1.33	1.51
31	c	608	CLA	CBB-CAB	3.27	1.51	1.29
34	9	301	LMG	C37-C36	-3.27	1.33	1.51
34	C	624	LMG	C19-C18	-3.27	1.33	1.51
31	B	603	CLA	CBB-CAB	3.27	1.50	1.29
31	B	605	CLA	CBB-CAB	3.27	1.50	1.29
31	d	405	CLA	CBB-CAB	3.26	1.50	1.29
34	b	626	LMG	C37-C36	-3.26	1.33	1.51
34	C	619	LMG	C19-C18	-3.26	1.33	1.51
31	A	409	CLA	CBB-CAB	3.26	1.50	1.29
31	B	616	CLA	CBB-CAB	3.26	1.50	1.29
34	c	624	LMG	C40-C39	-3.26	1.33	1.51
31	C	604	CLA	CBB-CAB	3.26	1.50	1.29
31	7	316	CLA	C1C-NC	-3.26	1.32	1.37
31	C	602	CLA	CBB-CAB	3.26	1.50	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	6	307	CHL	CBB-CAB	3.26	1.50	1.29
30	9	308	CHL	C4B-NB	3.26	1.38	1.35
30	Y	307	CHL	CBB-CAB	3.26	1.50	1.29
31	y	604	CLA	C1C-NC	-3.26	1.32	1.37
45	C	620	DGD	CAA-C9A	-3.26	1.33	1.51
45	c	616	DGD	CDB-CCB	-3.26	1.33	1.51
31	3	316	CLA	CBB-CAB	3.26	1.50	1.29
32	Y	315	LUT	C23-C24	-3.26	1.45	1.50
34	0	620	LMG	C19-C18	-3.26	1.33	1.51
31	s	304	CLA	C1C-NC	-3.26	1.32	1.37
34	A	412	LMG	C19-C18	-3.26	1.33	1.51
32	p	617	LUT	C40-C33	3.26	1.57	1.50
34	w	202	LMG	C37-C36	-3.26	1.33	1.51
34	j	101	LMG	C19-C18	-3.26	1.33	1.51
32	0	616	LUT	C40-C33	3.26	1.57	1.50
34	g	322	LMG	C19-C18	-3.26	1.33	1.51
31	N	312	CLA	C1C-NC	-3.26	1.32	1.37
45	c	618	DGD	CDA-CCA	-3.26	1.33	1.51
34	C	624	LMG	C22-C21	-3.26	1.33	1.51
45	C	618	DGD	CAA-C9A	-3.26	1.33	1.51
34	J	101	LMG	C22-C21	-3.26	1.33	1.51
31	c	613	CLA	CBB-CAB	3.26	1.50	1.29
34	w	202	LMG	C25-C24	-3.26	1.33	1.51
30	y	607	CHL	CBB-CAB	3.26	1.50	1.29
31	0	611	CLA	C1C-NC	-3.25	1.32	1.37
31	n	304	CLA	C1C-NC	-3.25	1.32	1.37
30	2	606	CHL	CBB-CAB	3.25	1.50	1.29
31	s	305	CLA	C1C-NC	-3.25	1.32	1.37
45	C	620	DGD	CGA-CFA	-3.25	1.33	1.51
30	6	309	CHL	CBB-CAB	3.25	1.50	1.29
45	C	620	DGD	CDB-CCB	-3.25	1.33	1.51
31	D	403	CLA	CBB-CAB	3.25	1.50	1.29
31	B	614	CLA	C1C-NC	-3.25	1.33	1.37
31	q	305	CLA	C1C-NC	-3.25	1.33	1.37
31	b	612	CLA	C1C-NC	-3.25	1.33	1.37
32	p	617	LUT	C23-C24	-3.25	1.45	1.50
34	b	622	LMG	C19-C18	-3.25	1.33	1.51
34	s	321	LMG	C22-C21	-3.25	1.33	1.51
30	N	307	CHL	C4B-NB	3.25	1.38	1.35
31	3	314	CLA	C1C-NC	-3.25	1.33	1.37
34	G	621	LMG	C22-C21	-3.25	1.33	1.51
32	R	317	LUT	C2-C1	3.25	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	y	606	CHL	CBB-CAB	3.25	1.50	1.29
45	c	617	DGD	CDB-CCB	-3.25	1.33	1.51
31	N	314	CLA	C1C-NC	-3.25	1.33	1.37
31	7	304	CLA	C1C-NC	-3.25	1.33	1.37
32	S	317	LUT	C2-C1	3.25	1.65	1.54
31	N	321	CLA	C1C-NC	-3.25	1.33	1.37
31	p	612	CLA	C1C-NC	-3.25	1.33	1.37
34	D	412	LMG	C19-C18	-3.25	1.33	1.51
34	w	202	LMG	C22-C21	-3.25	1.33	1.51
31	C	609	CLA	CBB-CAB	3.25	1.50	1.29
32	0	617	LUT	C40-C33	3.25	1.57	1.50
31	c	612	CLA	CBB-CAB	3.25	1.50	1.29
34	D	412	LMG	C40-C39	-3.25	1.33	1.51
31	8	612	CLA	C1C-NC	-3.25	1.33	1.37
34	4	620	LMG	C40-C39	-3.24	1.33	1.51
34	d	410	LMG	C22-C21	-3.24	1.33	1.51
34	d	411	LMG	C19-C18	-3.24	1.33	1.51
34	w	202	LMG	C19-C18	-3.24	1.33	1.51
30	g	307	CHL	CBB-CAB	3.24	1.50	1.29
31	2	603	CLA	C1C-NC	-3.24	1.33	1.37
45	C	617	DGD	CGA-CFA	-3.24	1.33	1.51
31	3	305	CLA	C1C-NC	-3.24	1.33	1.37
31	g	304	CLA	C1C-NC	-3.24	1.33	1.37
34	j	101	LMG	C37-C36	-3.24	1.33	1.51
34	c	624	LMG	C37-C36	-3.24	1.33	1.51
34	C	619	LMG	C22-C21	-3.24	1.33	1.51
34	W	201	LMG	C43-C42	-3.24	1.33	1.51
32	y	616	LUT	C23-C24	-3.24	1.45	1.50
32	s	317	LUT	C2-C1	3.24	1.65	1.54
30	8	606	CHL	CBB-CAB	3.24	1.50	1.29
30	s	307	CHL	CBB-CAB	3.24	1.50	1.29
43	B	617	BCR	C16-C17	3.24	1.53	1.43
45	C	617	DGD	CDA-CCA	-3.24	1.33	1.51
30	q	310	CHL	CBB-CAB	3.24	1.50	1.29
31	0	610	CLA	CBB-CAB	3.24	1.50	1.29
34	k	101	LMG	C19-C18	-3.24	1.33	1.51
31	c	609	CLA	CBB-CAB	3.24	1.50	1.29
34	D	410	LMG	C19-C18	-3.24	1.33	1.51
34	9	301	LMG	C22-C21	-3.24	1.33	1.51
30	G	606	CHL	CBB-CAB	3.24	1.50	1.29
45	C	620	DGD	CDA-CCA	-3.24	1.33	1.51
32	8	615	LUT	C23-C24	-3.24	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	D	411	LMG	C22-C21	-3.24	1.33	1.51
31	G	610	CLA	C1C-NC	-3.24	1.33	1.37
32	8	616	LUT	C23-C24	-3.24	1.45	1.50
45	c	618	DGD	CDB-CCB	-3.24	1.33	1.51
32	R	317	LUT	C19-C9	3.24	1.57	1.50
34	C	619	LMG	C37-C36	-3.24	1.33	1.51
31	N	303	CLA	C1C-NC	-3.24	1.33	1.37
34	2	620	LMG	C22-C21	-3.23	1.33	1.51
34	k	101	LMG	C40-C39	-3.23	1.33	1.51
45	C	620	DGD	CAB-C9B	-3.23	1.33	1.51
31	7	305	CLA	C1C-NC	-3.23	1.33	1.37
34	4	620	LMG	C37-C36	-3.23	1.33	1.51
34	G	621	LMG	C19-C18	-3.23	1.33	1.51
45	c	619	DGD	CGA-CFA	-3.23	1.33	1.51
34	4	620	LMG	C22-C21	-3.23	1.33	1.51
34	w	202	LMG	C40-C39	-3.23	1.33	1.51
43	D	405	BCR	C27-C26	-3.23	1.44	1.51
31	b	611	CLA	C1C-NC	-3.23	1.33	1.37
30	n	307	CHL	CBB-CAB	3.23	1.50	1.29
45	C	618	DGD	CDA-CCA	-3.23	1.33	1.51
45	c	618	DGD	CGB-CFB	-3.23	1.33	1.51
45	c	619	DGD	CAA-C9A	-3.23	1.33	1.51
34	d	411	LMG	C37-C36	-3.23	1.33	1.51
31	g	313	CLA	C1C-NC	-3.23	1.33	1.37
31	4	603	CLA	C1C-NC	-3.23	1.33	1.37
34	k	101	LMG	C37-C36	-3.23	1.33	1.51
31	g	312	CLA	C1C-NC	-3.23	1.33	1.37
31	s	306	CLA	C1C-NC	-3.23	1.33	1.37
31	B	607	CLA	CBB-CAB	3.23	1.50	1.29
31	Y	311	CLA	CBB-CAB	3.23	1.50	1.29
31	G	604	CLA	C1C-NC	-3.23	1.33	1.37
34	S	321	LMG	C22-C21	-3.23	1.33	1.51
34	q	301	LMG	C22-C21	-3.23	1.33	1.51
30	S	307	CHL	CBB-CAB	3.23	1.50	1.29
34	B	621	LMG	C40-C39	-3.23	1.33	1.51
31	B	601	CLA	CBB-CAB	3.23	1.50	1.29
31	y	603	CLA	C1C-NC	-3.23	1.33	1.37
30	q	308	CHL	CBB-CAB	3.23	1.50	1.29
34	b	622	LMG	C40-C39	-3.23	1.33	1.51
32	9	318	LUT	C23-C24	-3.23	1.45	1.50
34	d	410	LMG	C19-C18	-3.23	1.33	1.51
31	2	610	CLA	C1C-NC	-3.22	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	2	620	LMG	C37-C36	-3.22	1.33	1.51
32	r	317	LUT	C2-C1	3.22	1.64	1.54
31	6	304	CLA	C1C-NC	-3.22	1.33	1.37
45	C	618	DGD	CAB-C9B	-3.22	1.33	1.51
34	D	411	LMG	C19-C18	-3.22	1.33	1.51
45	C	618	DGD	CGB-CFB	-3.22	1.33	1.51
31	3	315	CLA	C1C-NC	-3.22	1.33	1.37
31	5	612	CLA	C1C-NC	-3.22	1.33	1.37
31	g	314	CLA	C1C-NC	-3.22	1.33	1.37
34	G	621	LMG	C37-C36	-3.22	1.33	1.51
32	n	317	LUT	C23-C24	-3.22	1.45	1.50
31	Y	304	CLA	C1C-NC	-3.22	1.33	1.37
31	9	304	CLA	C1C-NC	-3.22	1.33	1.37
34	6	321	LMG	C19-C18	-3.22	1.33	1.51
31	6	303	CLA	C1C-NC	-3.22	1.33	1.37
34	d	411	LMG	C40-C39	-3.22	1.33	1.51
31	5	613	CLA	C1C-NC	-3.21	1.33	1.37
30	R	308	CHL	CBB-CAB	3.21	1.50	1.29
32	1	615	LUT	C2-C1	3.21	1.64	1.54
31	S	305	CLA	C1C-NC	-3.21	1.33	1.37
31	y	602	CLA	C1C-NC	-3.21	1.33	1.37
34	q	301	LMG	C37-C36	-3.21	1.33	1.51
32	n	318	LUT	C23-C24	-3.21	1.45	1.50
34	S	321	LMG	C19-C18	-3.21	1.33	1.51
31	n	311	CLA	C1C-NC	-3.21	1.33	1.37
45	c	618	DGD	CGA-CFA	-3.21	1.33	1.51
31	8	610	CLA	C1C-NC	-3.21	1.33	1.37
30	N	307	CHL	CBB-CAB	3.21	1.50	1.29
31	b	602	CLA	CBB-CAB	3.21	1.50	1.29
45	C	618	DGD	CGA-CFA	-3.21	1.33	1.51
31	9	305	CLA	C1C-NC	-3.21	1.33	1.37
31	y	614	CLA	C1C-NC	-3.21	1.33	1.37
30	N	301	CHL	C4B-NB	3.21	1.38	1.35
31	5	611	CLA	C1C-NC	-3.21	1.33	1.37
31	C	606	CLA	CBB-CAB	3.21	1.50	1.29
45	c	619	DGD	CDB-CCB	-3.21	1.33	1.51
32	7	317	LUT	C40-C33	3.21	1.57	1.50
34	w	202	LMG	C43-C42	-3.21	1.33	1.51
31	G	602	CLA	C1C-NC	-3.21	1.33	1.37
31	7	312	CLA	C1C-NC	-3.21	1.33	1.37
31	n	315	CLA	C1C-NC	-3.21	1.33	1.37
34	4	620	LMG	C19-C18	-3.21	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	309	CHL	C4B-NB	3.21	1.38	1.35
31	C	605	CLA	CBB-CAB	3.20	1.50	1.29
31	N	305	CLA	C1C-NC	-3.20	1.33	1.37
31	n	305	CLA	C1C-NC	-3.20	1.33	1.37
44	A	416	PL9	C7-C3	-3.20	1.48	1.51
31	N	304	CLA	C1C-NC	-3.20	1.33	1.37
31	7	311	CLA	C1C-NC	-3.20	1.33	1.37
31	n	312	CLA	C1C-NC	-3.20	1.33	1.37
34	2	620	LMG	C19-C18	-3.20	1.33	1.51
34	q	301	LMG	C19-C18	-3.20	1.33	1.51
45	C	618	DGD	CDB-CCB	-3.20	1.33	1.51
31	p	611	CLA	C1C-NC	-3.20	1.33	1.37
31	n	314	CLA	C1C-NC	-3.20	1.33	1.37
31	5	604	CLA	C1C-NC	-3.20	1.33	1.37
31	y	610	CLA	C1C-NC	-3.20	1.33	1.37
31	Y	303	CLA	C1C-NC	-3.20	1.33	1.37
31	y	615	CLA	C1C-NC	-3.20	1.33	1.37
31	6	313	CLA	C1C-NC	-3.20	1.33	1.37
34	G	621	LMG	C40-C39	-3.20	1.33	1.51
30	0	608	CHL	C4B-NB	3.20	1.38	1.35
44	a	414	PL9	C3-C4	-3.20	1.44	1.49
31	p	604	CLA	C1C-NC	-3.19	1.33	1.37
30	4	607	CHL	CBB-CAB	3.19	1.50	1.29
30	0	606	CHL	CBB-CAB	3.19	1.50	1.29
34	g	322	LMG	C40-C39	-3.19	1.33	1.51
31	8	614	CLA	C1C-NC	-3.19	1.33	1.37
32	1	616	LUT	C40-C33	3.19	1.57	1.50
32	Y	315	LUT	C2-C1	3.19	1.64	1.54
32	Y	316	LUT	C2-C1	3.19	1.64	1.54
31	Y	310	CLA	C1C-NC	-3.19	1.33	1.37
34	W	201	LMG	C40-C39	-3.19	1.33	1.51
45	c	619	DGD	CGB-CFB	-3.19	1.33	1.51
31	1	611	CLA	C1C-NC	-3.19	1.33	1.37
31	S	306	CLA	C1C-NC	-3.19	1.33	1.37
31	s	303	CLA	C1C-NC	-3.19	1.33	1.37
30	n	307	CHL	C4B-NB	3.19	1.38	1.35
31	2	612	CLA	C1C-NC	-3.19	1.33	1.37
34	9	301	LMG	C40-C39	-3.19	1.33	1.51
30	r	310	CHL	CBB-CAB	3.19	1.50	1.29
30	r	308	CHL	CBB-CAB	3.19	1.50	1.29
31	2	609	CLA	C1C-NC	-3.19	1.33	1.37
30	1	608	CHL	C4B-NB	3.18	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	1	614	CLA	C1C-NC	-3.18	1.33	1.37
31	8	604	CLA	C1C-NC	-3.18	1.33	1.37
32	N	316	LUT	C23-C24	-3.18	1.45	1.50
31	p	613	CLA	C1C-NC	-3.18	1.33	1.37
31	3	306	CLA	C1C-NC	-3.18	1.33	1.37
30	3	302	CHL	CBB-CAB	3.18	1.50	1.29
34	w	201	LMG	C37-C36	-3.18	1.33	1.51
31	S	303	CLA	C1C-NC	-3.18	1.33	1.37
32	0	617	LUT	C2-C1	3.18	1.64	1.54
30	p	608	CHL	C4B-NB	3.18	1.38	1.35
30	r	308	CHL	C4B-NB	3.18	1.38	1.35
32	y	617	LUT	C2-C1	3.18	1.64	1.54
31	9	306	CLA	C1C-NC	-3.18	1.33	1.37
34	q	301	LMG	C40-C39	-3.18	1.33	1.51
30	6	308	CHL	C4B-NB	3.17	1.38	1.35
31	5	603	CLA	C1C-NC	-3.17	1.33	1.37
31	3	304	CLA	C1C-NC	-3.17	1.33	1.37
31	9	316	CLA	C1C-NC	-3.17	1.33	1.37
31	b	614	CLA	C1C-NC	-3.17	1.33	1.37
30	1	601	CHL	C3B-C2B	-3.17	1.36	1.40
30	7	307	CHL	C4B-NB	3.17	1.38	1.35
30	g	307	CHL	C4B-NB	3.17	1.38	1.35
34	b	626	LMG	C19-C18	-3.17	1.33	1.51
31	y	613	CLA	CBB-CAB	3.17	1.50	1.29
30	q	309	CHL	C3B-C2B	-3.17	1.36	1.40
30	0	605	CHL	CBB-CAB	3.17	1.50	1.29
31	4	602	CLA	C1C-NC	-3.17	1.33	1.37
30	3	308	CHL	CBB-CAB	3.17	1.50	1.29
31	n	303	CLA	C1C-NC	-3.17	1.33	1.37
31	n	313	CLA	C1C-NC	-3.17	1.33	1.37
31	3	312	CLA	C1C-NC	-3.16	1.33	1.37
31	9	315	CLA	C1C-NC	-3.16	1.33	1.37
31	g	305	CLA	C1C-NC	-3.16	1.33	1.37
32	1	615	LUT	C23-C24	-3.16	1.45	1.50
32	r	317	LUT	C23-C24	-3.16	1.45	1.50
30	p	609	CHL	C4B-NB	3.16	1.38	1.35
31	8	609	CLA	C1C-NC	-3.16	1.33	1.37
30	3	308	CHL	C3B-C2B	-3.16	1.36	1.40
30	9	310	CHL	C4B-NB	3.16	1.38	1.35
31	N	315	CLA	C1C-NC	-3.16	1.33	1.37
31	2	602	CLA	C1C-NC	-3.16	1.33	1.37
31	2	604	CLA	C1C-NC	-3.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	5	614	CLA	C1C-NC	-3.16	1.33	1.37
32	Y	316	LUT	C38-C25	3.16	1.56	1.50
31	8	611	CLA	C1C-NC	-3.16	1.33	1.37
32	Y	315	LUT	C40-C33	3.16	1.57	1.50
31	b	613	CLA	C1C-NC	-3.16	1.33	1.37
30	S	308	CHL	CBB-CAB	3.16	1.50	1.29
32	1	615	LUT	C40-C33	3.15	1.57	1.50
30	3	307	CHL	C4B-NB	3.15	1.38	1.35
31	B	613	CLA	C1C-NC	-3.15	1.33	1.37
31	b	615	CLA	C1C-NC	-3.15	1.33	1.37
31	7	315	CLA	C1C-NC	-3.15	1.33	1.37
30	1	601	CHL	CBB-CAB	3.15	1.50	1.29
30	2	608	CHL	C4B-NB	3.15	1.38	1.35
31	N	311	CLA	C1C-NC	-3.15	1.33	1.37
32	4	616	LUT	C23-C24	-3.15	1.45	1.50
31	5	610	CLA	C1C-NC	-3.15	1.33	1.37
31	6	315	CLA	C1C-NC	-3.15	1.33	1.37
45	C	620	DGD	CGB-CFB	-3.15	1.33	1.51
31	6	316	CLA	C1C-NC	-3.15	1.33	1.37
31	G	603	CLA	C1C-NC	-3.15	1.33	1.37
30	p	601	CHL	C4B-NB	3.15	1.38	1.35
31	8	603	CLA	C1C-NC	-3.15	1.33	1.37
30	S	307	CHL	C4B-NB	3.15	1.38	1.35
32	q	318	LUT	C23-C24	-3.15	1.45	1.50
31	5	602	CLA	C1C-NC	-3.14	1.33	1.37
34	b	626	LMG	C22-C21	-3.14	1.33	1.51
31	6	311	CLA	C1C-NC	-3.14	1.33	1.37
32	r	317	LUT	C40-C33	3.14	1.57	1.50
31	N	313	CLA	C1C-NC	-3.14	1.33	1.37
30	G	606	CHL	C4B-NB	3.14	1.38	1.35
34	D	410	LMG	C22-C21	-3.14	1.34	1.51
30	6	306	CHL	C4B-NB	3.14	1.38	1.35
32	6	317	LUT	C23-C24	-3.14	1.45	1.50
30	R	310	CHL	CBB-CAB	3.14	1.50	1.29
31	8	613	CLA	C1C-NC	-3.14	1.33	1.37
30	0	607	CHL	C4B-NB	3.13	1.38	1.35
31	7	303	CLA	C1C-NC	-3.13	1.33	1.37
32	r	317	LUT	C30-C29	-3.13	1.31	1.35
32	N	317	LUT	C23-C24	-3.13	1.45	1.50
31	0	614	CLA	C1C-NC	-3.13	1.33	1.37
31	S	304	CLA	C1C-NC	-3.13	1.33	1.37
30	8	606	CHL	C4B-NB	3.13	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	4	608	CHL	C4B-NB	3.12	1.38	1.35
31	8	602	CLA	C1C-NC	-3.12	1.33	1.37
30	G	608	CHL	C4B-NB	3.12	1.38	1.35
45	c	616	DGD	CAA-C9A	-3.12	1.34	1.51
30	n	306	CHL	C4B-NB	3.12	1.38	1.35
30	9	307	CHL	C4B-NB	3.12	1.38	1.35
31	B	612	CLA	C1C-NC	-3.12	1.33	1.37
30	R	310	CHL	C3B-C2B	-3.11	1.36	1.40
30	g	308	CHL	C4B-NB	3.11	1.38	1.35
30	1	609	CHL	C4B-NB	3.11	1.38	1.35
30	p	607	CHL	C4B-NB	3.11	1.38	1.35
32	2	615	LUT	C40-C33	3.11	1.57	1.50
32	R	317	LUT	C40-C33	3.11	1.57	1.50
31	p	610	CLA	C1C-NC	-3.11	1.33	1.37
30	y	607	CHL	C4B-NB	3.11	1.38	1.35
32	y	616	LUT	C40-C33	3.11	1.57	1.50
30	G	601	CHL	C4B-NB	3.11	1.38	1.35
30	s	308	CHL	C4B-NB	3.11	1.38	1.35
31	4	612	CLA	C3B-C2B	-3.10	1.36	1.40
32	Y	316	LUT	C40-C33	3.10	1.57	1.50
30	2	601	CHL	C4B-NB	3.10	1.38	1.35
30	2	607	CHL	C4B-NB	3.10	1.38	1.35
30	8	607	CHL	C4B-NB	3.10	1.38	1.35
32	y	617	LUT	C40-C33	3.10	1.57	1.50
30	8	605	CHL	C4B-NB	3.10	1.38	1.35
30	s	307	CHL	C4B-NB	3.10	1.38	1.35
31	4	604	CLA	C1C-NC	-3.10	1.33	1.37
32	S	317	LUT	C23-C24	-3.10	1.45	1.50
30	7	309	CHL	C4B-NB	3.09	1.38	1.35
31	4	611	CLA	C1C-NC	-3.09	1.33	1.37
30	Y	301	CHL	C4B-NB	3.09	1.38	1.35
30	Y	307	CHL	C4B-NB	3.09	1.38	1.35
43	B	617	BCR	C24-C25	3.09	1.56	1.45
30	4	605	CHL	C4B-NB	3.09	1.38	1.35
31	y	613	CLA	C4B-NB	-3.09	1.32	1.35
30	N	302	CHL	C4B-NB	3.08	1.38	1.35
30	4	601	CHL	C4B-NB	3.08	1.38	1.35
30	q	309	CHL	CBB-CAB	3.08	1.49	1.29
30	y	606	CHL	C4B-NB	3.08	1.38	1.35
30	2	605	CHL	C4B-NB	3.08	1.38	1.35
31	q	304	CLA	C1C-NC	-3.08	1.33	1.37
30	R	308	CHL	C4B-NB	3.08	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	2	614	RRX	C4-C5	-3.08	1.44	1.51
32	3	317	LUT	C23-C24	-3.07	1.45	1.50
30	5	607	CHL	C4B-NB	3.07	1.37	1.35
30	p	605	CHL	C4B-NB	3.07	1.37	1.35
30	1	605	CHL	C4B-NB	3.07	1.37	1.35
30	N	308	CHL	C4B-NB	3.07	1.37	1.35
30	q	309	CHL	C4B-NB	3.07	1.37	1.35
35	4	615	RRX	C4-C5	-3.07	1.44	1.51
30	9	303	CHL	C4B-NB	3.07	1.37	1.35
35	G	614	RRX	C4-C5	-3.07	1.45	1.51
30	y	608	CHL	C4B-NB	3.06	1.37	1.35
30	1	607	CHL	C4B-NB	3.06	1.37	1.35
32	1	616	LUT	C23-C24	-3.06	1.45	1.50
30	q	311	CHL	C4B-NB	3.06	1.37	1.35
30	G	607	CHL	C4B-NB	3.06	1.37	1.35
30	9	309	CHL	C4B-NB	3.06	1.37	1.35
30	n	302	CHL	C4B-NB	3.06	1.37	1.35
30	g	306	CHL	C4B-NB	3.05	1.37	1.35
30	n	309	CHL	C4B-NB	3.05	1.37	1.35
30	1	619	CHL	CBB-CAB	3.05	1.49	1.29
30	6	302	CHL	C4B-NB	3.05	1.37	1.35
30	N	306	CHL	C4B-NB	3.05	1.37	1.35
30	8	608	CHL	C4B-NB	3.05	1.37	1.35
30	5	609	CHL	C4B-NB	3.05	1.37	1.35
30	1	606	CHL	C4B-NB	3.04	1.37	1.35
30	Y	309	CHL	C4B-NB	3.04	1.37	1.35
30	y	605	CHL	C4B-NB	3.04	1.37	1.35
30	4	606	CHL	C4B-NB	3.04	1.37	1.35
30	n	301	CHL	C4B-NB	3.04	1.37	1.35
32	s	317	LUT	C23-C24	-3.04	1.45	1.50
35	9	317	RRX	C4-C5	-3.04	1.45	1.51
30	q	307	CHL	C4B-NB	3.03	1.37	1.35
30	G	605	CHL	C4B-NB	3.03	1.37	1.35
30	G	623	CHL	C4B-NB	3.03	1.37	1.35
32	6	318	LUT	C23-C24	-3.03	1.45	1.50
30	6	310	CHL	C4B-NB	3.03	1.37	1.35
30	7	308	CHL	C4B-NB	3.03	1.37	1.35
32	r	317	LUT	C34-C33	-3.03	1.31	1.35
32	3	318	LUT	C23-C24	-3.03	1.45	1.50
30	5	605	CHL	C4B-NB	3.03	1.37	1.35
32	y	617	LUT	C30-C29	-3.02	1.31	1.35
30	5	606	CHL	C4B-NB	3.02	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Y	308	CHL	C4B-NB	3.02	1.37	1.35
30	0	609	CHL	C4B-NB	3.02	1.37	1.35
30	8	601	CHL	C4B-NB	3.02	1.37	1.35
30	q	303	CHL	C4B-NB	3.02	1.37	1.35
30	n	310	CHL	C4B-NB	3.01	1.37	1.35
30	y	609	CHL	C4B-NB	3.01	1.37	1.35
31	R	307	CLA	C3B-C2B	-3.01	1.36	1.40
30	2	606	CHL	C4B-NB	3.01	1.37	1.35
30	3	303	CHL	C4B-NB	3.01	1.37	1.35
30	R	309	CHL	C4B-NB	3.01	1.37	1.35
30	Y	302	CHL	C4B-NB	3.00	1.37	1.35
30	5	601	CHL	C4B-NB	3.00	1.37	1.35
30	s	309	CHL	C4B-NB	3.00	1.37	1.35
30	r	309	CHL	C4B-NB	3.00	1.37	1.35
30	0	601	CHL	C4B-NB	3.00	1.37	1.35
32	1	615	LUT	C30-C29	-2.99	1.31	1.35
30	4	609	CHL	C4B-NB	2.98	1.37	1.35
30	7	310	CHL	C4B-NB	2.98	1.37	1.35
31	r	307	CLA	C3B-C2B	-2.98	1.36	1.40
31	r	314	CLA	C3B-C2B	-2.98	1.36	1.40
30	g	302	CHL	C4B-NB	2.98	1.37	1.35
30	5	608	CHL	C4B-NB	2.98	1.37	1.35
32	Y	315	LUT	C30-C29	-2.98	1.31	1.35
32	5	617	LUT	C23-C24	-2.98	1.45	1.50
31	S	304	CLA	C3B-C2B	-2.97	1.36	1.40
30	3	308	CHL	C4B-NB	2.97	1.37	1.35
30	S	309	CHL	C4B-NB	2.97	1.37	1.35
32	7	318	LUT	C23-C24	-2.97	1.46	1.50
30	7	321	CHL	C4B-NB	2.97	1.37	1.35
32	p	616	LUT	C23-C24	-2.96	1.46	1.50
30	6	309	CHL	C4B-NB	2.96	1.37	1.35
30	Y	306	CHL	C4B-NB	2.96	1.37	1.35
30	7	306	CHL	C4B-NB	2.96	1.37	1.35
30	9	311	CHL	C4B-NB	2.96	1.37	1.35
30	6	307	CHL	C4B-NB	2.95	1.37	1.35
30	n	308	CHL	C4B-NB	2.94	1.37	1.35
30	3	310	CHL	C4B-NB	2.94	1.37	1.35
31	1	603	CLA	C3B-C2B	-2.93	1.36	1.40
30	r	310	CHL	C4B-NB	2.93	1.37	1.35
32	s	318	LUT	C23-C24	-2.93	1.46	1.50
30	N	309	CHL	C4B-NB	2.92	1.37	1.35
31	9	314	CLA	C3B-C2B	-2.92	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	7	302	CHL	C4B-NB	2.92	1.37	1.35
30	r	310	CHL	C3B-C2B	-2.92	1.36	1.40
31	B	601	CLA	C3B-C2B	-2.91	1.36	1.40
31	S	312	CLA	C3B-C2B	-2.90	1.36	1.40
47	E	101	HEM	FE-NB	2.90	2.11	1.96
30	3	309	CHL	C4B-NB	2.90	1.37	1.35
32	5	616	LUT	C23-C24	-2.89	1.46	1.50
31	c	601	CLA	C3B-C2B	-2.89	1.36	1.40
30	p	606	CHL	C4B-NB	2.89	1.37	1.35
30	y	601	CHL	C4B-NB	2.89	1.37	1.35
31	C	601	CLA	C3B-C2B	-2.88	1.36	1.40
30	R	310	CHL	C4B-NB	2.88	1.37	1.35
32	G	615	LUT	C23-C24	-2.88	1.46	1.50
31	C	605	CLA	C4B-NB	-2.87	1.32	1.35
31	C	607	CLA	C3B-C2B	-2.87	1.36	1.40
31	R	314	CLA	C3B-C2B	-2.87	1.36	1.40
30	q	310	CHL	C3B-C2B	-2.87	1.36	1.40
47	e	102	HEM	FE-NB	2.86	2.11	1.96
35	q	317	RRX	C17-C18	-2.86	1.32	1.35
31	y	611	CLA	C3B-C2B	-2.85	1.36	1.40
31	R	303	CLA	C3B-C2B	-2.85	1.36	1.40
31	4	613	CLA	C3B-C2B	-2.85	1.36	1.40
30	3	302	CHL	C4B-NB	2.83	1.37	1.35
31	7	313	CLA	C3B-C2B	-2.83	1.36	1.40
31	r	303	CLA	C3B-C2B	-2.83	1.36	1.40
31	3	301	CLA	C3B-C2B	-2.82	1.36	1.40
30	3	302	CHL	C3B-C2B	-2.81	1.36	1.40
31	y	612	CLA	C3B-C2B	-2.81	1.36	1.40
32	y	617	LUT	C34-C33	-2.81	1.32	1.35
32	2	615	LUT	C38-C25	2.81	1.55	1.50
43	D	405	BCR	C34-C9	2.81	1.56	1.50
43	D	405	BCR	C7-C6	2.81	1.55	1.45
31	1	612	CLA	C3B-C2B	-2.81	1.36	1.40
32	1	616	LUT	C30-C29	-2.80	1.32	1.35
31	0	603	CLA	C3B-C2B	-2.80	1.36	1.40
31	s	306	CLA	CHC-C1C	2.80	1.42	1.35
31	b	602	CLA	C3B-C2B	-2.80	1.36	1.40
30	q	310	CHL	C3A-C2A	-2.80	1.46	1.54
31	S	306	CLA	CHC-C1C	2.80	1.42	1.35
31	B	612	CLA	CHC-C1C	2.79	1.42	1.35
32	y	617	LUT	O23-C23	-2.79	1.38	1.43
31	r	313	CLA	C3B-C2B	-2.78	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	614	CLA	CHC-C1C	2.78	1.42	1.35
42	A	408	PHO	CAC-C3C	-2.78	1.47	1.52
31	B	611	CLA	CHC-C1C	2.77	1.42	1.35
31	g	311	CLA	C3B-C2B	-2.77	1.36	1.40
31	s	312	CLA	C3B-C2B	-2.77	1.36	1.40
31	Y	312	CLA	C3B-C2B	-2.77	1.36	1.40
32	0	616	LUT	C30-C29	-2.77	1.32	1.35
31	c	604	CLA	C3B-C2B	-2.77	1.36	1.40
30	q	308	CHL	C4B-NB	2.77	1.37	1.35
31	p	611	CLA	CHC-C1C	2.77	1.42	1.35
32	y	616	LUT	C34-C33	-2.77	1.32	1.35
32	g	316	LUT	C23-C24	-2.77	1.46	1.50
42	D	401	PHO	CAC-C3C	-2.77	1.47	1.52
32	7	317	LUT	C30-C29	-2.76	1.32	1.35
43	c	614	BCR	C7-C6	2.76	1.54	1.45
35	2	614	RRX	C17-C18	-2.76	1.32	1.35
30	0	606	CHL	C4B-NB	2.76	1.37	1.35
31	y	610	CLA	CHC-C1C	2.76	1.42	1.35
31	q	315	CLA	C3B-C2B	-2.76	1.36	1.40
31	p	610	CLA	CHC-C1C	2.75	1.42	1.35
31	5	610	CLA	CHC-C1C	2.75	1.42	1.35
43	V	101	BCR	C34-C9	2.75	1.56	1.50
31	C	605	CLA	C3B-C2B	-2.75	1.36	1.40
30	Y	306	CHL	C3B-C2B	-2.75	1.36	1.40
30	3	302	CHL	C3A-C2A	-2.75	1.46	1.54
31	g	303	CLA	CHC-C1C	2.74	1.42	1.35
31	6	311	CLA	CHC-C1C	2.74	1.42	1.35
31	y	614	CLA	CHC-C1C	2.74	1.42	1.35
31	N	311	CLA	CHC-C1C	2.73	1.42	1.35
31	S	303	CLA	CHC-C1C	2.73	1.42	1.35
32	Y	315	LUT	C34-C33	-2.73	1.32	1.35
31	b	613	CLA	CHC-C1C	2.73	1.42	1.35
35	4	615	RRX	C17-C18	-2.73	1.32	1.35
31	p	615	CLA	CHC-C1C	2.73	1.42	1.35
31	2	602	CLA	CHC-C1C	2.73	1.42	1.35
31	8	611	CLA	CHC-C1C	2.73	1.42	1.35
31	8	609	CLA	CHC-C1C	2.73	1.42	1.35
31	n	303	CLA	CHC-C1C	2.73	1.42	1.35
35	G	614	RRX	C17-C18	-2.72	1.32	1.35
31	7	311	CLA	CHC-C1C	2.72	1.41	1.35
31	g	314	CLA	CHC-C1C	2.72	1.41	1.35
31	B	613	CLA	CHC-C1C	2.72	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	q	304	CLA	CHC-C1C	2.72	1.41	1.35
31	G	613	CLA	C3B-C2B	-2.72	1.36	1.40
31	c	601	CLA	CHC-C1C	2.72	1.41	1.35
31	n	316	CLA	CHC-C1C	2.72	1.41	1.35
30	q	310	CHL	C4B-NB	2.72	1.37	1.35
31	6	312	CLA	C3B-C2B	-2.72	1.36	1.40
43	v	101	BCR	C34-C9	2.72	1.56	1.50
31	1	611	CLA	CHC-C1C	2.71	1.41	1.35
31	5	602	CLA	CHC-C1C	2.71	1.41	1.35
31	N	310	CLA	CHC-C1C	2.71	1.41	1.35
31	n	313	CLA	CHC-C1C	2.71	1.41	1.35
32	r	317	LUT	O23-C23	-2.71	1.38	1.43
31	b	615	CLA	CHC-C1C	2.71	1.41	1.35
31	5	603	CLA	CHC-C1C	2.71	1.41	1.35
31	5	612	CLA	CHC-C1C	2.71	1.41	1.35
32	R	317	LUT	C30-C29	-2.71	1.32	1.35
31	5	611	CLA	CHC-C1C	2.71	1.41	1.35
31	p	604	CLA	CHC-C1C	2.71	1.41	1.35
31	N	315	CLA	CHC-C1C	2.71	1.41	1.35
31	7	312	CLA	CHC-C1C	2.71	1.41	1.35
32	R	317	LUT	O23-C23	-2.71	1.38	1.43
31	4	602	CLA	CHC-C1C	2.71	1.41	1.35
31	2	613	CLA	CHC-C1C	2.70	1.41	1.35
31	N	303	CLA	CHC-C1C	2.70	1.41	1.35
31	s	303	CLA	CHC-C1C	2.70	1.41	1.35
43	b	619	BCR	C34-C9	2.70	1.56	1.50
43	A	410	BCR	C34-C9	2.70	1.56	1.50
43	b	618	BCR	C34-C9	2.70	1.56	1.50
31	Y	310	CLA	CHC-C1C	2.70	1.41	1.35
31	2	609	CLA	CHC-C1C	2.70	1.41	1.35
31	7	304	CLA	CHC-C1C	2.70	1.41	1.35
31	b	612	CLA	CHC-C1C	2.70	1.41	1.35
30	y	605	CHL	C3B-C2B	-2.70	1.36	1.40
31	8	614	CLA	CHC-C1C	2.70	1.41	1.35
31	3	305	CLA	CHC-C1C	2.70	1.41	1.35
31	G	602	CLA	CHC-C1C	2.70	1.41	1.35
35	9	317	RRX	C17-C18	-2.70	1.32	1.35
31	p	614	CLA	CHC-C1C	2.70	1.41	1.35
30	r	308	CHL	C3B-C2B	-2.70	1.36	1.40
31	8	602	CLA	CHC-C1C	2.70	1.41	1.35
31	N	312	CLA	CHC-C1C	2.70	1.41	1.35
31	N	321	CLA	CHC-C1C	2.70	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	306	CLA	CHC-C1C	2.69	1.41	1.35
31	q	314	CLA	C3B-C2B	-2.69	1.36	1.40
31	6	313	CLA	CHC-C1C	2.69	1.41	1.35
31	C	605	CLA	C3D-C4D	-2.69	1.38	1.44
43	b	620	BCR	C34-C9	2.69	1.56	1.50
31	6	304	CLA	CHC-C1C	2.69	1.41	1.35
31	5	614	CLA	CHC-C1C	2.69	1.41	1.35
31	q	312	CLA	CHC-C1C	2.69	1.41	1.35
43	v	101	BCR	C7-C6	2.69	1.54	1.45
32	2	615	LUT	O23-C23	-2.69	1.38	1.43
43	B	617	BCR	C39-C30	-2.69	1.48	1.53
31	9	304	CLA	CHC-C1C	2.69	1.41	1.35
31	s	316	CLA	C3B-C2B	-2.68	1.36	1.40
31	6	303	CLA	CHC-C1C	2.68	1.41	1.35
34	y	620	LMG	C37-C36	-2.68	1.32	1.51
31	n	311	CLA	CHC-C1C	2.68	1.41	1.35
31	Y	304	CLA	CHC-C1C	2.68	1.41	1.35
31	1	610	CLA	CHC-C1C	2.68	1.41	1.35
31	0	610	CLA	C3B-C2B	-2.68	1.36	1.40
31	y	615	CLA	CHC-C1C	2.68	1.41	1.35
32	S	317	LUT	C18-C5	2.68	1.55	1.50
31	4	604	CLA	CHC-C1C	2.68	1.41	1.35
31	G	610	CLA	C3B-C2B	-2.68	1.36	1.40
30	S	308	CHL	C4B-NB	2.68	1.37	1.35
31	9	316	CLA	CHC-C1C	2.68	1.41	1.35
43	c	614	BCR	C34-C9	2.68	1.56	1.50
30	G	608	CHL	C3A-C2A	-2.68	1.47	1.54
32	Y	315	LUT	O23-C23	-2.68	1.38	1.43
34	0	622	LMG	C37-C36	-2.68	1.32	1.51
31	4	603	CLA	CHC-C1C	2.68	1.41	1.35
31	N	314	CLA	CHC-C1C	2.67	1.41	1.35
31	b	611	CLA	CHC-C1C	2.67	1.41	1.35
31	8	604	CLA	CHC-C1C	2.67	1.41	1.35
31	6	315	CLA	CHC-C1C	2.67	1.41	1.35
31	8	613	CLA	CHC-C1C	2.67	1.41	1.35
31	y	602	CLA	CHC-C1C	2.67	1.41	1.35
32	5	616	LUT	C18-C5	2.67	1.55	1.50
30	s	302	CHL	C4B-NB	2.67	1.37	1.35
31	1	614	CLA	CHC-C1C	2.67	1.41	1.35
31	y	603	CLA	CHC-C1C	2.67	1.41	1.35
31	2	603	CLA	CHC-C1C	2.67	1.41	1.35
32	6	318	LUT	C18-C5	2.66	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	312	CLA	CHC-C1C	2.66	1.41	1.35
31	3	304	CLA	CHC-C1C	2.66	1.41	1.35
31	3	314	CLA	CHC-C1C	2.66	1.41	1.35
31	2	610	CLA	CHC-C1C	2.66	1.41	1.35
43	B	618	BCR	C7-C6	2.66	1.54	1.45
31	9	306	CLA	CHC-C1C	2.66	1.41	1.35
32	0	616	LUT	O23-C23	-2.66	1.38	1.43
31	4	611	CLA	CHC-C1C	2.66	1.41	1.35
31	8	603	CLA	CHC-C1C	2.66	1.41	1.35
31	n	315	CLA	CHC-C1C	2.66	1.41	1.35
31	g	313	CLA	CHC-C1C	2.66	1.41	1.35
31	s	304	CLA	CHC-C1C	2.66	1.41	1.35
31	3	315	CLA	CHC-C1C	2.66	1.41	1.35
32	s	317	LUT	O23-C23	-2.66	1.38	1.43
31	Y	305	CLA	CHC-C1C	2.66	1.41	1.35
32	n	317	LUT	C18-C5	2.66	1.55	1.50
31	G	604	CLA	CHC-C1C	2.66	1.41	1.35
31	5	613	CLA	CHC-C1C	2.66	1.41	1.35
31	0	614	CLA	CHC-C1C	2.66	1.41	1.35
31	q	305	CLA	CHC-C1C	2.66	1.41	1.35
32	3	317	LUT	C18-C5	2.66	1.55	1.50
31	9	312	CLA	C3B-C2B	-2.65	1.36	1.40
30	S	302	CHL	C4B-NB	2.65	1.37	1.35
31	n	305	CLA	CHC-C1C	2.65	1.41	1.35
31	G	603	CLA	CHC-C1C	2.65	1.41	1.35
31	8	610	CLA	CHC-C1C	2.65	1.41	1.35
43	c	615	BCR	C7-C6	2.65	1.54	1.45
30	0	605	CHL	C4B-NB	2.65	1.37	1.35
31	5	604	CLA	CHC-C1C	2.65	1.41	1.35
31	R	313	CLA	C3B-C2B	-2.65	1.36	1.40
32	s	317	LUT	C18-C5	2.65	1.55	1.50
31	1	612	CLA	CHC-C1C	2.65	1.41	1.35
31	7	316	CLA	CHC-C1C	2.65	1.41	1.35
31	d	404	CLA	CHC-C1C	2.65	1.41	1.35
31	n	304	CLA	CHC-C1C	2.65	1.41	1.35
31	N	305	CLA	CHC-C1C	2.65	1.41	1.35
30	1	601	CHL	C4B-NB	2.65	1.37	1.35
31	7	303	CLA	CHC-C1C	2.64	1.41	1.35
32	6	317	LUT	C18-C5	2.64	1.55	1.50
30	5	607	CHL	C3A-C2A	-2.64	1.47	1.54
31	9	305	CLA	CHC-C1C	2.64	1.41	1.35
31	g	312	CLA	CHC-C1C	2.64	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	3	313	CLA	CHC-C1C	2.64	1.41	1.35
43	c	615	BCR	C34-C9	2.64	1.56	1.50
31	Y	304	CLA	C3B-C2B	-2.64	1.36	1.40
32	8	615	LUT	C18-C5	2.64	1.55	1.50
32	N	317	LUT	O23-C23	-2.64	1.38	1.43
32	1	615	LUT	C34-C33	-2.64	1.32	1.35
31	9	315	CLA	CHC-C1C	2.64	1.41	1.35
32	Y	316	LUT	O23-C23	-2.64	1.38	1.43
31	g	304	CLA	CHC-C1C	2.64	1.41	1.35
31	b	603	CLA	C3B-C2B	-2.64	1.36	1.40
43	B	618	BCR	C34-C9	2.64	1.56	1.50
43	a	410	BCR	C34-C9	2.63	1.56	1.50
31	6	305	CLA	CHC-C1C	2.63	1.41	1.35
31	N	313	CLA	CHC-C1C	2.63	1.41	1.35
31	Y	303	CLA	CHC-C1C	2.63	1.41	1.35
31	7	305	CLA	CHC-C1C	2.63	1.41	1.35
31	6	314	CLA	CHC-C1C	2.63	1.41	1.35
31	B	610	CLA	CHC-C1C	2.63	1.41	1.35
31	p	612	CLA	CHC-C1C	2.63	1.41	1.35
31	y	611	CLA	CHC-C1C	2.63	1.41	1.35
31	0	612	CLA	CHC-C1C	2.63	1.41	1.35
43	V	101	BCR	C7-C6	2.63	1.54	1.45
34	w	205	LMG	C37-C36	-2.63	1.33	1.51
31	G	613	CLA	CHC-C1C	2.63	1.41	1.35
32	Y	316	LUT	C30-C29	-2.63	1.32	1.35
31	2	611	CLA	CHC-C1C	2.62	1.41	1.35
31	s	311	CLA	CHC-C1C	2.62	1.41	1.35
31	3	316	CLA	C3B-C2B	-2.62	1.36	1.40
32	R	317	LUT	C34-C33	-2.62	1.32	1.35
31	s	305	CLA	CHC-C1C	2.62	1.41	1.35
34	b	624	LMG	C37-C36	-2.62	1.33	1.51
31	r	305	CLA	CHC-C1C	2.62	1.41	1.35
31	b	614	CLA	CHC-C1C	2.62	1.41	1.35
32	S	317	LUT	O23-C23	-2.62	1.38	1.43
31	S	305	CLA	CHC-C1C	2.62	1.41	1.35
34	r	321	LMG	C37-C36	-2.62	1.33	1.51
31	Y	314	CLA	CHC-C1C	2.62	1.41	1.35
31	9	313	CLA	C3B-C2B	-2.62	1.36	1.40
32	N	316	LUT	C18-C5	2.61	1.55	1.50
30	n	310	CHL	C3A-C2A	-2.61	1.47	1.54
32	8	615	LUT	C30-C29	-2.61	1.32	1.35
43	b	619	BCR	C7-C6	2.61	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	607	CLA	C3D-C4D	-2.61	1.38	1.44
32	8	616	LUT	O23-C23	-2.61	1.38	1.43
32	0	617	LUT	O23-C23	-2.61	1.38	1.43
31	y	604	CLA	CHC-C1C	2.61	1.41	1.35
31	7	315	CLA	CHC-C1C	2.61	1.41	1.35
34	n	321	LMG	C37-C36	-2.61	1.33	1.51
31	p	602	CLA	CHC-C1C	2.61	1.41	1.35
34	R	321	LMG	C37-C36	-2.61	1.33	1.51
32	y	616	LUT	O23-C23	-2.60	1.38	1.43
32	7	317	LUT	C34-C33	-2.60	1.32	1.35
31	c	607	CLA	C3B-C2B	-2.60	1.36	1.40
31	9	314	CLA	CHC-C1C	2.60	1.41	1.35
34	6	321	LMG	C37-C36	-2.60	1.33	1.51
32	7	318	LUT	C18-C5	2.60	1.55	1.50
31	g	305	CLA	CHC-C1C	2.60	1.41	1.35
45	c	617	DGD	CDA-CCA	-2.60	1.33	1.51
43	T	101	BCR	C34-C9	2.60	1.56	1.50
31	9	313	CLA	CHC-C1C	2.60	1.41	1.35
31	b	602	CLA	CHC-C1C	2.60	1.41	1.35
34	C	621	LMG	C37-C36	-2.60	1.33	1.51
31	3	311	CLA	C3B-C2B	-2.60	1.36	1.40
31	2	604	CLA	CHC-C1C	2.60	1.41	1.35
31	7	313	CLA	CHC-C1C	2.60	1.41	1.35
43	C	615	BCR	C39-C30	-2.60	1.48	1.53
45	C	616	DGD	CAB-C9B	-2.60	1.33	1.51
43	T	101	BCR	C7-C6	2.60	1.54	1.45
32	5	617	LUT	C18-C5	2.60	1.55	1.50
34	Q1	101	LMG	C37-C36	-2.60	1.33	1.51
34	b	623	LMG	C37-C36	-2.60	1.33	1.51
32	p	616	LUT	C18-C5	2.60	1.55	1.50
31	C	601	CLA	CHC-C1C	2.60	1.41	1.35
31	3	312	CLA	CHC-C1C	2.59	1.41	1.35
31	N	304	CLA	CHC-C1C	2.59	1.41	1.35
31	q	316	CLA	CHC-C1C	2.59	1.41	1.35
31	Y	311	CLA	C3B-C2B	-2.59	1.36	1.40
32	6	318	LUT	O23-C23	-2.59	1.38	1.43
31	B	601	CLA	CHC-C1C	2.59	1.41	1.35
31	g	311	CLA	CHC-C1C	2.59	1.41	1.35
31	r	304	CLA	CHC-C1C	2.59	1.41	1.35
34	w	203	LMG	C37-C36	-2.59	1.33	1.51
32	n	317	LUT	O23-C23	-2.59	1.38	1.43
32	n	318	LUT	O23-C23	-2.59	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	A	418	LMG	C37-C36	-2.59	1.33	1.51
34	B	625	LMG	C37-C36	-2.59	1.33	1.51
31	r	315	CLA	CHC-C1C	2.59	1.41	1.35
31	6	316	CLA	CHC-C1C	2.59	1.41	1.35
30	3	309	CHL	C3B-C2B	-2.59	1.36	1.40
34	A	414	LMG	C37-C36	-2.59	1.33	1.51
34	Y	319	LMG	C37-C36	-2.59	1.33	1.51
34	d	409	LMG	C19-C18	-2.58	1.33	1.51
31	n	314	CLA	CHC-C1C	2.58	1.41	1.35
34	4	621	LMG	C19-C18	-2.58	1.33	1.51
34	G	619	LMG	C37-C36	-2.58	1.33	1.51
31	2	612	CLA	CHC-C1C	2.58	1.41	1.35
34	7	322	LMG	C37-C36	-2.58	1.33	1.51
34	f	101	LMG	C37-C36	-2.58	1.33	1.51
31	3	301	CLA	CHC-C1C	2.58	1.41	1.35
31	r	313	CLA	CHC-C1C	2.58	1.41	1.35
34	m	102	LMG	C19-C18	-2.58	1.33	1.51
32	6	317	LUT	C30-C29	-2.58	1.32	1.35
32	g	316	LUT	C18-C5	2.58	1.55	1.50
34	3	321	LMG	C37-C36	-2.58	1.33	1.51
32	S	318	LUT	C18-C5	2.58	1.55	1.50
34	6	322	LMG	C19-C18	-2.58	1.33	1.51
32	9	318	LUT	O23-C23	-2.58	1.38	1.43
34	X	203	LMG	C37-C36	-2.58	1.33	1.51
43	z	101	BCR	C34-C9	2.58	1.56	1.50
34	d	409	LMG	C37-C36	-2.58	1.33	1.51
32	1	616	LUT	O23-C23	-2.57	1.38	1.43
31	G	603	CLA	C3B-C2B	-2.57	1.36	1.40
31	r	316	CLA	C3B-C2B	-2.57	1.36	1.40
43	h	101	BCR	C34-C9	2.57	1.56	1.50
34	N	320	LMG	C37-C36	-2.57	1.33	1.51
34	9	321	LMG	C37-C36	-2.57	1.33	1.51
31	R	312	CLA	CHC-C1C	2.57	1.41	1.35
31	S	311	CLA	CHC-C1C	2.57	1.41	1.35
31	8	612	CLA	CHC-C1C	2.57	1.41	1.35
34	7	320	LMG	C37-C36	-2.57	1.33	1.51
32	1	615	LUT	O23-C23	-2.57	1.38	1.43
32	g	316	LUT	C26-C27	2.57	1.54	1.50
32	6	317	LUT	O23-C23	-2.57	1.38	1.43
31	0	611	CLA	CHC-C1C	2.57	1.41	1.35
31	G	612	CLA	CHC-C1C	2.57	1.41	1.35
34	2	618	LMG	C37-C36	-2.57	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	613	CLA	CHC-C1C	2.57	1.41	1.35
34	5	620	LMG	C37-C36	-2.57	1.33	1.51
34	9	302	LMG	C19-C18	-2.57	1.33	1.51
31	4	612	CLA	CHC-C1C	2.57	1.41	1.35
32	N	317	LUT	C18-C5	2.57	1.55	1.50
31	0	612	CLA	C3B-C2B	-2.57	1.36	1.40
34	g	320	LMG	C37-C36	-2.57	1.33	1.51
34	p	620	LMG	C37-C36	-2.57	1.33	1.51
32	8	615	LUT	O23-C23	-2.57	1.39	1.43
34	X	202	LMG	C37-C36	-2.57	1.33	1.51
34	1	618	LMG	C37-C36	-2.57	1.33	1.51
34	b	629	LMG	C37-C36	-2.57	1.33	1.51
32	n	317	LUT	C30-C29	-2.57	1.32	1.35
34	q1	101	LMG	C37-C36	-2.57	1.33	1.51
34	k	102	LMG	C37-C36	-2.57	1.33	1.51
30	7	306	CHL	C3A-C2A	-2.57	1.47	1.54
34	2	621	LMG	C19-C18	-2.57	1.33	1.51
32	3	317	LUT	O23-C23	-2.57	1.39	1.43
34	W	203	LMG	C37-C36	-2.57	1.33	1.51
31	B	602	CLA	C3B-C2B	-2.57	1.36	1.40
34	c	621	LMG	C37-C36	-2.57	1.33	1.51
31	r	314	CLA	CHC-C1C	2.56	1.41	1.35
34	B	622	LMG	C37-C36	-2.56	1.33	1.51
43	B	619	BCR	C7-C6	2.56	1.54	1.45
34	I	101	LMG	C37-C36	-2.56	1.33	1.51
35	g	315	RRX	C17-C18	-2.56	1.32	1.35
34	q	302	LMG	C19-C18	-2.56	1.33	1.51
31	R	313	CLA	CHC-C1C	2.56	1.41	1.35
31	S	310	CLA	C3B-C2B	-2.56	1.36	1.40
34	6	323	LMG	C37-C36	-2.56	1.33	1.51
32	7	317	LUT	C18-C5	2.56	1.55	1.50
34	b	601	LMG	C19-C18	-2.56	1.33	1.51
31	D	404	CLA	CHC-C1C	2.56	1.41	1.35
34	g	322	LMG	C22-C21	-2.56	1.33	1.51
34	0	620	LMG	C37-C36	-2.56	1.33	1.51
32	0	617	LUT	C18-C5	2.56	1.55	1.50
34	7	301	LMG	C19-C18	-2.56	1.33	1.51
31	6	312	CLA	CHC-C1C	2.56	1.41	1.35
31	R	314	CLA	CHC-C1C	2.56	1.41	1.35
34	n	322	LMG	C19-C18	-2.56	1.33	1.51
32	9	318	LUT	C18-C5	2.56	1.55	1.50
34	a	401	LMG	C37-C36	-2.56	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	G	615	LUT	C18-C5	2.55	1.55	1.50
34	J	102	LMG	C37-C36	-2.55	1.33	1.51
34	c	620	LMG	C37-C36	-2.55	1.33	1.51
31	y	614	CLA	C3B-C2B	-2.55	1.36	1.40
34	D	409	LMG	C37-C36	-2.55	1.33	1.51
34	W	202	LMG	C37-C36	-2.55	1.33	1.51
34	a	416	LMG	C37-C36	-2.55	1.33	1.51
31	4	614	CLA	CHC-C1C	2.55	1.41	1.35
32	Y	315	LUT	C18-C5	2.55	1.55	1.50
31	B	615	CLA	C3B-C2B	-2.55	1.36	1.40
31	p	613	CLA	CHC-C1C	2.55	1.41	1.35
31	7	304	CLA	C3B-C2B	-2.55	1.36	1.40
31	1	602	CLA	CHC-C1C	2.55	1.41	1.35
43	B	619	BCR	C34-C9	2.55	1.56	1.50
31	g	310	CLA	CHC-C1C	2.55	1.41	1.35
34	G	622	LMG	C19-C18	-2.55	1.33	1.51
31	D	403	CLA	CHC-C1C	2.55	1.41	1.35
31	0	615	CLA	CHC-C1C	2.55	1.41	1.35
43	C	614	BCR	C34-C9	2.55	1.56	1.50
31	0	602	CLA	CHC-C1C	2.55	1.41	1.35
34	w	204	LMG	C37-C36	-2.55	1.33	1.51
31	0	613	CLA	CHC-C1C	2.55	1.41	1.35
31	R	305	CLA	C3B-C2B	-2.55	1.36	1.40
32	0	616	LUT	C18-C5	2.54	1.55	1.50
43	A	410	BCR	C7-C6	2.54	1.54	1.45
31	b	616	CLA	C3B-C2B	-2.54	1.36	1.40
31	b	617	CLA	C3B-C2B	-2.54	1.36	1.40
32	q	318	LUT	O23-C23	-2.54	1.39	1.43
31	s	313	CLA	CHC-C1C	2.54	1.41	1.35
31	R	303	CLA	CHC-C1C	2.54	1.41	1.35
31	y	612	CLA	CHC-C1C	2.54	1.41	1.35
31	0	604	CLA	CHC-C1C	2.54	1.41	1.35
31	R	304	CLA	CHC-C1C	2.54	1.41	1.35
31	q	313	CLA	CHC-C1C	2.54	1.41	1.35
34	a	413	LMG	C37-C36	-2.54	1.33	1.51
32	p	617	LUT	C18-C5	2.54	1.55	1.50
31	N	321	CLA	C3B-C2B	-2.54	1.36	1.40
32	G	615	LUT	O23-C23	-2.54	1.39	1.43
31	B	602	CLA	CHC-C1C	2.54	1.41	1.35
31	d	401	CLA	C3B-C2B	-2.53	1.36	1.40
31	S	316	CLA	CHC-C1C	2.53	1.41	1.35
32	7	317	LUT	O23-C23	-2.53	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	608	CLA	CHC-C1C	2.53	1.41	1.35
32	r	317	LUT	C18-C5	2.53	1.55	1.50
34	x	202	LMG	C37-C36	-2.53	1.33	1.51
32	S	317	LUT	C30-C29	-2.53	1.32	1.35
32	5	617	LUT	O23-C23	-2.53	1.39	1.43
32	S	318	LUT	C23-C24	-2.53	1.46	1.50
43	H	101	BCR	C34-C9	2.53	1.56	1.50
31	s	304	CLA	C3B-C2B	-2.53	1.36	1.40
31	3	316	CLA	CHC-C1C	2.53	1.41	1.35
43	C	614	BCR	C7-C6	2.53	1.54	1.45
43	b	618	BCR	C7-C6	2.53	1.54	1.45
32	N	316	LUT	O23-C23	-2.53	1.39	1.43
31	G	609	CLA	CHC-C1C	2.53	1.41	1.35
31	b	603	CLA	CHC-C1C	2.53	1.41	1.35
32	s	318	LUT	C18-C5	2.52	1.55	1.50
31	y	615	CLA	C3B-C2B	-2.52	1.36	1.40
31	p	615	CLA	C3B-C2B	-2.52	1.36	1.40
31	R	311	CLA	CHC-C1C	2.52	1.41	1.35
31	b	607	CLA	CHC-C1C	2.52	1.41	1.35
31	4	610	CLA	CHC-C1C	2.52	1.41	1.35
32	3	318	LUT	O23-C23	-2.52	1.39	1.43
31	A	405	CLA	CHC-C1C	2.52	1.41	1.35
32	q	318	LUT	C18-C5	2.52	1.55	1.50
32	4	616	LUT	O23-C23	-2.52	1.39	1.43
31	0	611	CLA	C3B-C2B	-2.52	1.36	1.40
31	S	313	CLA	CHC-C1C	2.52	1.41	1.35
32	8	616	LUT	C18-C5	2.52	1.55	1.50
31	1	604	CLA	CHC-C1C	2.52	1.41	1.35
31	p	613	CLA	C3B-C2B	-2.52	1.36	1.40
32	4	616	LUT	C18-C5	2.52	1.55	1.50
31	c	604	CLA	CHC-C1C	2.52	1.41	1.35
31	5	613	CLA	C3B-C2B	-2.52	1.36	1.40
31	0	615	CLA	C3B-C2B	-2.52	1.36	1.40
31	s	315	CLA	C3B-C2B	-2.52	1.36	1.40
31	0	603	CLA	CHC-C1C	2.52	1.41	1.35
32	0	617	LUT	C30-C29	-2.51	1.32	1.35
31	c	603	CLA	C3B-C2B	-2.51	1.36	1.40
31	S	312	CLA	CHC-C1C	2.51	1.41	1.35
31	y	613	CLA	C3D-C4D	-2.51	1.38	1.44
31	q	305	CLA	C3B-C2B	-2.51	1.36	1.40
32	n	318	LUT	C18-C5	2.51	1.55	1.50
31	r	311	CLA	CHC-C1C	2.51	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	g	307	CHL	C3B-C2B	-2.51	1.36	1.40
31	B	606	CLA	C3B-C2B	-2.51	1.36	1.40
31	7	312	CLA	C3B-C2B	-2.51	1.36	1.40
31	C	610	CLA	CHC-C1C	2.51	1.41	1.35
31	r	312	CLA	CHC-C1C	2.51	1.41	1.35
30	1	619	CHL	C4B-NB	2.51	1.37	1.35
31	3	312	CLA	C3B-C2B	-2.51	1.36	1.40
31	s	315	CLA	CHC-C1C	2.50	1.41	1.35
31	G	611	CLA	CHC-C1C	2.50	1.41	1.35
32	1	616	LUT	C34-C33	-2.50	1.32	1.35
31	c	610	CLA	CHC-C1C	2.50	1.41	1.35
32	3	318	LUT	C18-C5	2.50	1.55	1.50
31	S	315	CLA	CHC-C1C	2.50	1.41	1.35
31	Y	312	CLA	CHC-C1C	2.50	1.41	1.35
31	b	604	CLA	CHC-C1C	2.50	1.41	1.35
31	b	609	CLA	CHC-C1C	2.50	1.41	1.35
31	c	611	CLA	CHC-C1C	2.50	1.41	1.35
31	3	311	CLA	CHC-C1C	2.50	1.41	1.35
31	C	613	CLA	CHC-C1C	2.50	1.41	1.35
31	g	304	CLA	C3B-C2B	-2.50	1.36	1.40
32	s	317	LUT	C30-C29	-2.49	1.32	1.35
44	a	414	PL9	C6-C1	-2.49	1.44	1.48
31	2	603	CLA	C3B-C2B	-2.49	1.36	1.40
31	a	406	CLA	CHC-C1C	2.49	1.41	1.35
31	6	304	CLA	C3B-C2B	-2.49	1.36	1.40
31	s	316	CLA	CHC-C1C	2.49	1.41	1.35
31	B	605	CLA	CHC-C1C	2.49	1.41	1.35
31	g	314	CLA	C3B-C2B	-2.49	1.36	1.40
43	Z	101	BCR	C34-C9	2.49	1.56	1.50
30	N	307	CHL	C3B-C2B	-2.49	1.36	1.40
30	R	308	CHL	C3B-C2B	-2.49	1.36	1.40
43	d	406	BCR	C34-C9	2.49	1.56	1.50
31	1	611	CLA	C3B-C2B	-2.49	1.36	1.40
31	5	614	CLA	C3B-C2B	-2.49	1.36	1.40
31	c	607	CLA	CHC-C1C	2.49	1.41	1.35
31	G	610	CLA	CHC-C1C	2.48	1.41	1.35
32	y	616	LUT	C18-C5	2.48	1.55	1.50
31	q	314	CLA	CHC-C1C	2.48	1.41	1.35
31	S	310	CLA	CHC-C1C	2.48	1.41	1.35
31	p	603	CLA	C3B-C2B	-2.48	1.36	1.40
31	p	612	CLA	C3B-C2B	-2.48	1.36	1.40
31	d	401	CLA	CHC-C1C	2.48	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	g	316	LUT	O23-C23	-2.48	1.39	1.43
31	C	606	CLA	CHC-C1C	2.48	1.41	1.35
31	q	306	CLA	CHC-C1C	2.48	1.41	1.35
32	1	616	LUT	C18-C5	2.48	1.55	1.50
31	a	409	CLA	CHC-C1C	2.48	1.41	1.35
31	3	313	CLA	C3B-C2B	-2.48	1.36	1.40
32	0	616	LUT	C34-C33	-2.47	1.32	1.35
31	c	608	CLA	CHC-C1C	2.47	1.41	1.35
31	r	306	CLA	CHC-C1C	2.47	1.41	1.35
31	c	608	CLA	C3B-C2B	-2.47	1.36	1.40
31	A	409	CLA	CHC-C1C	2.47	1.41	1.35
43	B	617	BCR	C34-C9	2.47	1.56	1.50
31	B	607	CLA	C3B-C2B	-2.47	1.36	1.40
31	0	610	CLA	C3D-C4D	-2.47	1.38	1.44
32	1	615	LUT	C18-C5	2.47	1.55	1.50
31	c	605	CLA	CHC-C1C	2.47	1.41	1.35
32	7	318	LUT	O23-C23	-2.47	1.39	1.43
31	B	609	CLA	CHC-C1C	2.47	1.41	1.35
31	b	610	CLA	CHC-C1C	2.47	1.41	1.35
31	B	616	CLA	C3B-C2B	-2.47	1.36	1.40
31	s	314	CLA	CHC-C1C	2.47	1.41	1.35
31	p	603	CLA	CHC-C1C	2.47	1.41	1.35
43	b	620	BCR	C7-C6	2.46	1.53	1.45
31	Y	311	CLA	CHC-C1C	2.46	1.41	1.35
31	C	603	CLA	CHC-C1C	2.46	1.41	1.35
31	d	405	CLA	CHC-C1C	2.46	1.41	1.35
31	s	312	CLA	CHC-C1C	2.46	1.41	1.35
43	d	406	BCR	C7-C6	2.46	1.53	1.45
31	9	305	CLA	C3B-C2B	-2.46	1.37	1.40
43	a	410	BCR	C7-C6	2.46	1.53	1.45
32	G	615	LUT	C26-C27	2.46	1.53	1.50
31	B	607	CLA	C4B-NB	-2.46	1.33	1.35
31	7	314	CLA	CHC-C1C	2.46	1.41	1.35
31	N	312	CLA	C3B-C2B	-2.45	1.37	1.40
31	R	316	CLA	C3B-C2B	-2.45	1.37	1.40
31	4	610	CLA	C3B-C2B	-2.45	1.37	1.40
31	S	314	CLA	CHC-C1C	2.45	1.41	1.35
36	q	319	NEX	O24-C25	-2.45	1.42	1.46
31	y	613	CLA	C3B-C2B	-2.45	1.37	1.40
31	r	303	CLA	C3D-C4D	-2.45	1.38	1.44
31	0	604	CLA	C3B-C2B	-2.45	1.37	1.40
31	9	312	CLA	CHC-C1C	2.45	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	z	101	BCR	C7-C6	2.45	1.53	1.45
43	C	615	BCR	C7-C6	2.45	1.53	1.45
32	s	318	LUT	C30-C29	-2.45	1.32	1.35
31	a	407	CLA	CHC-C1C	2.44	1.41	1.35
31	B	606	CLA	CHC-C1C	2.44	1.41	1.35
31	s	310	CLA	CHC-C1C	2.44	1.41	1.35
31	G	609	CLA	C3B-C2B	-2.44	1.37	1.40
32	5	616	LUT	O23-C23	-2.44	1.39	1.43
31	3	314	CLA	C3B-C2B	-2.44	1.37	1.40
31	Y	313	CLA	CHC-C1C	2.44	1.41	1.35
31	4	603	CLA	C3B-C2B	-2.44	1.37	1.40
43	b	618	BCR	C39-C30	-2.44	1.49	1.53
32	Y	316	LUT	C18-C5	2.44	1.54	1.50
32	s	318	LUT	O23-C23	-2.44	1.39	1.43
31	r	303	CLA	CHC-C1C	2.44	1.41	1.35
31	c	605	CLA	C3B-C2B	-2.44	1.37	1.40
31	r	312	CLA	C3B-C2B	-2.44	1.37	1.40
31	C	602	CLA	CHC-C1C	2.44	1.41	1.35
32	2	615	LUT	C18-C5	2.44	1.54	1.50
31	r	307	CLA	CHC-C1C	2.44	1.41	1.35
31	s	310	CLA	C3B-C2B	-2.44	1.37	1.40
35	9	317	RRX	C34-C9	2.44	1.55	1.50
31	r	311	CLA	C3B-C2B	-2.44	1.37	1.40
32	7	318	LUT	C30-C29	-2.43	1.32	1.35
31	0	610	CLA	CHC-C1C	2.43	1.41	1.35
31	C	611	CLA	CHC-C1C	2.43	1.41	1.35
44	a	414	PL9	C53-C6	-2.43	1.45	1.50
31	C	608	CLA	C3B-C2B	-2.43	1.37	1.40
31	q	316	CLA	C3B-C2B	-2.43	1.37	1.40
31	2	610	CLA	C3B-C2B	-2.43	1.37	1.40
31	6	313	CLA	C3B-C2B	-2.43	1.37	1.40
31	R	315	CLA	CHC-C1C	2.43	1.41	1.35
30	6	309	CHL	C3B-C2B	-2.43	1.37	1.40
30	0	608	CHL	C3B-C2B	-2.43	1.37	1.40
43	H	101	BCR	C7-C6	2.43	1.53	1.45
31	R	316	CLA	CHC-C1C	2.43	1.41	1.35
32	p	617	LUT	O23-C23	-2.43	1.39	1.43
31	1	613	CLA	CHC-C1C	2.43	1.41	1.35
31	8	610	CLA	C3B-C2B	-2.42	1.37	1.40
31	C	608	CLA	CHC-C1C	2.42	1.41	1.35
31	A	407	CLA	CHC-C1C	2.42	1.41	1.35
35	4	615	RRX	C34-C9	2.42	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	607	CLA	C3B-C2B	-2.42	1.37	1.40
31	c	602	CLA	CHC-C1C	2.42	1.41	1.35
31	C	609	CLA	CHC-C1C	2.42	1.41	1.35
30	5	609	CHL	C3A-C2A	-2.42	1.47	1.54
31	c	609	CLA	CHC-C1C	2.42	1.41	1.35
31	c	606	CLA	C3B-C2B	-2.42	1.37	1.40
31	p	614	CLA	C3B-C2B	-2.41	1.37	1.40
31	C	604	CLA	CHC-C1C	2.41	1.41	1.35
31	b	611	CLA	C3B-C2B	-2.41	1.37	1.40
31	n	312	CLA	C3B-C2B	-2.41	1.37	1.40
31	S	304	CLA	CHC-C1C	2.41	1.41	1.35
31	b	605	CLA	CHC-C1C	2.41	1.41	1.35
30	S	307	CHL	C3B-C2B	-2.41	1.37	1.40
31	S	315	CLA	C3B-C2B	-2.41	1.37	1.40
31	A	406	CLA	CHC-C1C	2.41	1.41	1.35
30	8	606	CHL	C3B-C2B	-2.41	1.37	1.40
31	c	603	CLA	CHC-C1C	2.40	1.41	1.35
31	r	306	CLA	C3B-C2B	-2.40	1.37	1.40
32	y	617	LUT	C18-C5	2.40	1.54	1.50
31	3	315	CLA	C3B-C2B	-2.40	1.37	1.40
43	T	101	BCR	C36-C18	2.40	1.55	1.50
31	5	611	CLA	C3B-C2B	-2.40	1.37	1.40
31	C	612	CLA	CHC-C1C	2.40	1.41	1.35
31	3	301	CLA	C3D-C4D	-2.40	1.38	1.44
31	R	306	CLA	CHC-C1C	2.40	1.41	1.35
31	S	311	CLA	C3B-C2B	-2.40	1.37	1.40
32	8	616	LUT	C30-C29	-2.40	1.32	1.35
32	p	616	LUT	O23-C23	-2.40	1.39	1.43
35	G	614	RRX	C34-C9	2.40	1.55	1.50
31	B	603	CLA	CHC-C1C	2.40	1.41	1.35
32	S	318	LUT	O23-C23	-2.40	1.39	1.43
31	A	409	CLA	C3D-C4D	-2.40	1.38	1.44
30	2	608	CHL	C3A-C2A	-2.39	1.47	1.54
30	9	309	CHL	C3A-C2A	-2.39	1.47	1.54
30	n	307	CHL	C3B-C2B	-2.39	1.37	1.40
43	C	615	BCR	C34-C9	2.39	1.55	1.50
31	B	604	CLA	CHC-C1C	2.39	1.41	1.35
32	n	318	LUT	C30-C29	-2.39	1.32	1.35
31	R	307	CLA	CHC-C1C	2.39	1.41	1.35
44	A	416	PL9	C3-C4	-2.39	1.45	1.49
43	t	101	BCR	C34-C9	2.39	1.55	1.50
31	c	608	CLA	C3D-C4D	-2.38	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	q	306	CLA	C3B-C2B	-2.38	1.37	1.40
43	H	101	BCR	C39-C30	-2.38	1.49	1.53
31	l	613	CLA	C3B-C2B	-2.38	1.37	1.40
31	b	606	CLA	CHC-C1C	2.38	1.41	1.35
30	p	607	CHL	C3A-C2A	-2.38	1.47	1.54
31	5	615	CLA	C3B-C2B	-2.38	1.37	1.40
31	a	409	CLA	C3D-C4D	-2.38	1.38	1.44
31	p	611	CLA	C3B-C2B	-2.38	1.37	1.40
31	l	603	CLA	CHC-C1C	2.37	1.41	1.35
31	r	316	CLA	CHC-C1C	2.37	1.41	1.35
43	h	101	BCR	C7-C6	2.37	1.53	1.45
31	N	311	CLA	C3B-C2B	-2.37	1.37	1.40
43	c	615	BCR	C39-C30	-2.37	1.49	1.53
31	R	312	CLA	C3B-C2B	-2.37	1.37	1.40
30	2	601	CHL	C3B-C2B	-2.37	1.37	1.40
35	g	315	RRX	C34-C9	2.37	1.55	1.50
31	5	615	CLA	CHC-C1C	2.36	1.41	1.35
30	y	607	CHL	C3B-C2B	-2.36	1.37	1.40
31	C	605	CLA	C1D-ND	-2.36	1.34	1.37
43	Z	101	BCR	C7-C6	2.36	1.53	1.45
43	a	410	BCR	C36-C18	2.36	1.55	1.50
43	h	101	BCR	C39-C30	-2.36	1.49	1.53
30	Y	308	CHL	C3B-C2B	-2.36	1.37	1.40
31	B	607	CLA	CHC-C1C	2.36	1.41	1.35
30	S	309	CHL	C3B-C2B	-2.36	1.37	1.40
43	d	406	BCR	C39-C30	-2.36	1.49	1.53
32	S	318	LUT	C26-C27	2.35	1.53	1.50
31	4	610	CLA	C3D-C4D	-2.35	1.38	1.44
30	R	310	CHL	C3A-C2A	-2.35	1.47	1.54
31	c	605	CLA	C3D-C4D	-2.35	1.38	1.44
31	C	607	CLA	CHC-C1C	2.35	1.41	1.35
32	0	617	LUT	C34-C33	-2.35	1.32	1.35
31	c	613	CLA	CHC-C1C	2.35	1.41	1.35
43	b	620	BCR	C39-C30	-2.35	1.49	1.53
31	B	603	CLA	C3D-C4D	-2.35	1.38	1.44
36	S	319	NEX	C1-C6	-2.35	1.50	1.54
43	C	614	BCR	C39-C30	-2.35	1.49	1.53
31	b	604	CLA	C3D-C4D	-2.35	1.38	1.44
36	R	301	NEX	C1-C6	-2.35	1.50	1.54
43	A	410	BCR	C39-C30	-2.35	1.49	1.53
43	c	614	BCR	C39-C30	-2.35	1.49	1.53
30	Y	307	CHL	C3B-C2B	-2.35	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	616	CLA	CHC-C1C	2.35	1.41	1.35
45	c	617	DGD	O5D-C1E	2.35	1.44	1.40
43	V	101	BCR	C39-C30	-2.35	1.49	1.53
31	R	311	CLA	C3B-C2B	-2.34	1.37	1.40
32	R	317	LUT	C18-C5	2.34	1.54	1.50
32	N	316	LUT	C30-C29	-2.34	1.32	1.35
30	s	309	CHL	C3B-C2B	-2.34	1.37	1.40
31	Y	312	CLA	C3D-C4D	-2.34	1.38	1.44
30	G	623	CHL	C3B-C2B	-2.33	1.37	1.40
31	b	607	CLA	C3D-C4D	-2.33	1.38	1.44
30	s	307	CHL	C3B-C2B	-2.33	1.37	1.40
30	G	606	CHL	C3B-C2B	-2.33	1.37	1.40
31	C	608	CLA	C3D-C4D	-2.33	1.38	1.44
31	b	609	CLA	C3D-C4D	-2.33	1.38	1.44
31	B	610	CLA	C3B-C2B	-2.33	1.37	1.40
31	R	305	CLA	C3D-C4D	-2.33	1.38	1.44
31	b	608	CLA	CHC-C1C	2.33	1.40	1.35
35	2	614	RRX	C34-C9	2.33	1.55	1.50
32	S	317	LUT	C34-C33	-2.32	1.32	1.35
43	a	410	BCR	C39-C30	-2.32	1.49	1.53
31	c	606	CLA	CHC-C1C	2.32	1.40	1.35
30	1	601	CHL	C1D-ND	-2.32	1.34	1.37
43	z	101	BCR	C39-C30	-2.32	1.49	1.53
31	S	316	CLA	C3B-C2B	-2.32	1.37	1.40
43	Z	101	BCR	C39-C30	-2.31	1.49	1.53
30	N	308	CHL	C3A-C2A	-2.31	1.48	1.54
31	c	612	CLA	CHC-C1C	2.31	1.40	1.35
30	g	309	CHL	C3A-C2A	-2.31	1.48	1.54
30	1	609	CHL	C3A-C2A	-2.31	1.48	1.54
30	3	310	CHL	C3A-C2A	-2.31	1.48	1.54
31	s	311	CLA	C3B-C2B	-2.31	1.37	1.40
31	C	609	CLA	C3B-C2B	-2.31	1.37	1.40
31	B	605	CLA	C3D-C4D	-2.31	1.39	1.44
43	t	101	BCR	C7-C6	2.31	1.53	1.45
30	q	309	CHL	CHC-C1C	2.31	1.40	1.35
30	7	310	CHL	C3B-C2B	-2.30	1.37	1.40
31	1	604	CLA	C3B-C2B	-2.30	1.37	1.40
31	9	315	CLA	C3B-C2B	-2.30	1.37	1.40
30	0	609	CHL	C3A-C2A	-2.30	1.48	1.54
43	D	405	BCR	C36-C18	2.30	1.55	1.50
30	y	608	CHL	C3B-C2B	-2.30	1.37	1.40
31	B	615	CLA	C3D-C4D	-2.30	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	s	318	LUT	C34-C33	-2.30	1.32	1.35
30	q	303	CHL	C3B-C2B	-2.30	1.37	1.40
43	b	619	BCR	C39-C30	-2.29	1.49	1.53
30	s	308	CHL	C3B-C2B	-2.29	1.37	1.40
31	4	612	CLA	C3D-C4D	-2.29	1.39	1.44
31	y	612	CLA	C3D-C4D	-2.29	1.39	1.44
30	G	608	CHL	C3B-C2B	-2.29	1.37	1.40
32	6	317	LUT	C34-C33	-2.29	1.32	1.35
43	B	619	BCR	C39-C30	-2.29	1.49	1.53
31	S	305	CLA	C3B-C2B	-2.29	1.37	1.40
31	9	312	CLA	C3D-C4D	-2.29	1.39	1.44
31	b	617	CLA	CHC-C1C	2.29	1.40	1.35
32	5	617	LUT	C26-C27	2.29	1.53	1.50
31	a	406	CLA	C3B-C2B	-2.29	1.37	1.40
31	D	403	CLA	C3D-C4D	-2.29	1.39	1.44
31	A	407	CLA	C3D-C4D	-2.29	1.39	1.44
31	d	404	CLA	C3D-C4D	-2.29	1.39	1.44
32	9	318	LUT	C26-C27	2.28	1.53	1.50
31	B	608	CLA	C3D-C4D	-2.28	1.39	1.44
42	A	408	PHO	CMB-C2B	-2.28	1.46	1.51
44	A	416	PL9	C6-C1	-2.28	1.44	1.48
43	v	101	BCR	C39-C30	-2.28	1.49	1.53
31	a	406	CLA	C3D-C4D	-2.28	1.39	1.44
31	C	606	CLA	C3D-C4D	-2.28	1.39	1.44
31	q	315	CLA	C3D-C4D	-2.28	1.39	1.44
43	b	620	BCR	C36-C18	2.27	1.55	1.50
31	9	314	CLA	C3D-C4D	-2.27	1.39	1.44
31	s	313	CLA	C3D-C4D	-2.27	1.39	1.44
31	R	304	CLA	C3D-C4D	-2.27	1.39	1.44
30	6	310	CHL	C3B-C2B	-2.27	1.37	1.40
31	g	310	CLA	C3B-C2B	-2.27	1.37	1.40
31	B	604	CLA	C3D-C4D	-2.27	1.39	1.44
31	2	612	CLA	C3B-C2B	-2.27	1.37	1.40
31	y	613	CLA	CHC-C1C	2.27	1.40	1.35
31	G	611	CLA	C3D-C4D	-2.27	1.39	1.44
31	B	606	CLA	C3D-C4D	-2.27	1.39	1.44
31	b	616	CLA	C3D-C4D	-2.27	1.39	1.44
30	N	306	CHL	C3B-C2B	-2.27	1.37	1.40
31	B	615	CLA	CHC-C1C	2.27	1.40	1.35
43	B	618	BCR	C39-C30	-2.27	1.49	1.53
30	N	309	CHL	C3A-C2A	-2.27	1.48	1.54
42	D	401	PHO	CMC-C2C	-2.27	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	t	101	BCR	C39-C30	-2.27	1.49	1.53
30	7	307	CHL	C3B-C2B	-2.27	1.37	1.40
31	s	313	CLA	C3B-C2B	-2.27	1.37	1.40
31	B	616	CLA	CHC-C1C	2.26	1.40	1.35
30	y	609	CHL	C3B-C2B	-2.26	1.37	1.40
31	D	404	CLA	C3D-C4D	-2.26	1.39	1.44
31	b	606	CLA	C3D-C4D	-2.26	1.39	1.44
31	n	311	CLA	C3B-C2B	-2.26	1.37	1.40
31	q	313	CLA	C4B-CHC	-2.26	1.39	1.43
31	R	305	CLA	CHC-C1C	2.26	1.40	1.35
43	c	614	BCR	C36-C18	2.26	1.55	1.50
43	B	617	BCR	C7-C6	2.26	1.53	1.45
31	C	603	CLA	C3D-C4D	-2.26	1.39	1.44
31	d	401	CLA	C3D-C4D	-2.26	1.39	1.44
31	R	312	CLA	C3D-C4D	-2.26	1.39	1.44
42	D	401	PHO	CMD-C2D	-2.26	1.46	1.51
31	c	607	CLA	C3D-C4D	-2.26	1.39	1.44
31	B	609	CLA	C3D-C4D	-2.26	1.39	1.44
31	R	306	CLA	C3B-C2B	-2.25	1.37	1.40
31	c	602	CLA	C3D-C4D	-2.25	1.39	1.44
30	1	619	CHL	C1D-ND	-2.25	1.35	1.37
42	A	408	PHO	CMC-C2C	-2.25	1.46	1.51
43	H	101	BCR	C36-C18	2.25	1.55	1.50
30	1	606	CHL	C3B-C2B	-2.25	1.37	1.40
31	C	610	CLA	C3B-C2B	-2.25	1.37	1.40
31	p	604	CLA	C3B-C2B	-2.25	1.37	1.40
36	2	616	NEX	C1-C6	-2.25	1.50	1.54
42	A	408	PHO	CMD-C2D	-2.25	1.46	1.51
31	A	405	CLA	C3D-C4D	-2.25	1.39	1.44
30	6	308	CHL	C3B-C2B	-2.25	1.37	1.40
31	A	406	CLA	C3D-C4D	-2.25	1.39	1.44
30	4	607	CHL	CHC-C1C	2.25	1.40	1.35
43	v	101	BCR	C36-C18	2.25	1.55	1.50
31	1	602	CLA	C3B-C2B	-2.25	1.37	1.40
31	b	610	CLA	C3B-C2B	-2.24	1.37	1.40
32	3	317	LUT	C30-C29	-2.24	1.32	1.35
36	r	319	NEX	O24-C25	-2.24	1.43	1.46
31	0	602	CLA	C3B-C2B	-2.24	1.37	1.40
30	1	609	CHL	C3B-C2B	-2.24	1.37	1.40
32	6	318	LUT	C30-C29	-2.24	1.32	1.35
31	b	606	CLA	C3B-C2B	-2.24	1.37	1.40
30	n	301	CHL	C3B-C2B	-2.24	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	n	318	LUT	C34-C33	-2.24	1.32	1.35
32	3	317	LUT	C26-C27	2.24	1.53	1.50
32	r	317	LUT	C14-C13	-2.24	1.32	1.35
31	s	315	CLA	C3D-C4D	-2.24	1.39	1.44
31	c	606	CLA	C3D-C4D	-2.24	1.39	1.44
31	a	407	CLA	C3D-C4D	-2.24	1.39	1.44
31	R	314	CLA	C3D-C4D	-2.24	1.39	1.44
32	5	616	LUT	C30-C29	-2.24	1.32	1.35
31	R	311	CLA	C3D-C4D	-2.24	1.39	1.44
31	b	617	CLA	C3D-C4D	-2.24	1.39	1.44
32	5	616	LUT	C26-C27	2.24	1.53	1.50
32	N	316	LUT	C26-C27	2.24	1.53	1.50
32	N	317	LUT	C26-C27	2.24	1.53	1.50
32	8	616	LUT	C34-C33	-2.23	1.32	1.35
31	2	604	CLA	C3B-C2B	-2.23	1.37	1.40
31	C	604	CLA	C3D-C4D	-2.23	1.39	1.44
31	B	612	CLA	C1C-C2C	2.23	1.48	1.44
31	q	314	CLA	C3D-C4D	-2.23	1.39	1.44
31	C	602	CLA	C3D-C4D	-2.23	1.39	1.44
36	9	319	NEX	C1-C6	-2.23	1.50	1.54
30	y	606	CHL	C3B-C2B	-2.23	1.37	1.40
31	c	609	CLA	C3D-C4D	-2.23	1.39	1.44
31	N	310	CLA	C3B-C2B	-2.23	1.37	1.40
32	8	615	LUT	C34-C33	-2.23	1.32	1.35
35	q	317	RRX	C34-C9	2.23	1.55	1.50
30	N	301	CHL	C3B-C2B	-2.23	1.37	1.40
31	0	610	CLA	C4B-NB	-2.23	1.33	1.35
31	r	311	CLA	C3D-C4D	-2.23	1.39	1.44
31	A	407	CLA	C3B-C2B	-2.23	1.37	1.40
30	Y	309	CHL	C3B-C2B	-2.23	1.37	1.40
31	n	315	CLA	C3B-C2B	-2.23	1.37	1.40
43	V	101	BCR	C36-C18	2.23	1.55	1.50
30	Y	301	CHL	C3A-C2A	-2.23	1.48	1.54
36	N	318	NEX	C1-C6	-2.22	1.50	1.54
31	S	304	CLA	C3D-C4D	-2.22	1.39	1.44
31	0	615	CLA	C3D-C4D	-2.22	1.39	1.44
31	C	602	CLA	C3B-C2B	-2.22	1.37	1.40
31	N	314	CLA	C3B-C2B	-2.22	1.37	1.40
31	b	605	CLA	C3D-C4D	-2.22	1.39	1.44
32	S	318	LUT	C30-C29	-2.22	1.32	1.35
30	7	302	CHL	C3B-C2B	-2.22	1.37	1.40
32	7	318	LUT	C34-C33	-2.22	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	N	317	LUT	C30-C29	-2.22	1.32	1.35
32	Y	316	LUT	C34-C33	-2.22	1.32	1.35
31	c	611	CLA	C3B-C2B	-2.22	1.37	1.40
31	0	612	CLA	C3D-C4D	-2.22	1.39	1.44
31	R	307	CLA	C3D-C4D	-2.22	1.39	1.44
30	4	607	CHL	C3B-C2B	-2.22	1.37	1.40
30	g	309	CHL	C3B-C2B	-2.22	1.37	1.40
42	A	408	PHO	C3B-C2B	-2.22	1.37	1.40
31	n	304	CLA	C3B-C2B	-2.22	1.37	1.40
31	b	613	CLA	C1C-C2C	2.22	1.48	1.44
36	r	319	NEX	C1-C6	-2.22	1.50	1.54
30	p	601	CHL	C3B-C2B	-2.22	1.37	1.40
31	C	610	CLA	C3D-C4D	-2.22	1.39	1.44
31	7	316	CLA	C3B-C2B	-2.21	1.37	1.40
30	9	308	CHL	C3B-C2B	-2.21	1.37	1.40
30	n	306	CHL	C3B-C2B	-2.21	1.37	1.40
31	2	602	CLA	C1C-C2C	2.21	1.48	1.44
43	B	619	BCR	C36-C18	2.21	1.55	1.50
30	0	609	CHL	C3B-C2B	-2.21	1.37	1.40
30	8	605	CHL	C3B-C2B	-2.21	1.37	1.40
35	4	615	RRX	C33-C5	2.21	1.54	1.50
43	Z	101	BCR	C36-C18	2.21	1.55	1.50
31	R	315	CLA	C3D-C4D	-2.21	1.39	1.44
35	G	614	RRX	C33-C5	2.21	1.54	1.50
31	s	305	CLA	C3B-C2B	-2.21	1.37	1.40
44	A	416	PL9	C36-C34	-2.21	1.46	1.51
31	0	613	CLA	C3B-C2B	-2.21	1.37	1.40
32	n	317	LUT	C34-C33	-2.21	1.32	1.35
31	8	603	CLA	C3B-C2B	-2.21	1.37	1.40
31	C	609	CLA	C3D-C4D	-2.21	1.39	1.44
32	s	317	LUT	C34-C33	-2.21	1.32	1.35
31	B	602	CLA	C3D-C4D	-2.21	1.39	1.44
31	1	612	CLA	C3D-C4D	-2.21	1.39	1.44
43	h	101	BCR	C36-C18	2.20	1.55	1.50
31	b	610	CLA	C3D-C4D	-2.20	1.39	1.44
38	a	412	SQD	O47-C45	-2.20	1.41	1.46
32	4	616	LUT	C30-C29	-2.20	1.32	1.35
31	p	610	CLA	C1C-C2C	2.20	1.48	1.44
31	c	610	CLA	C3D-C4D	-2.20	1.39	1.44
31	4	604	CLA	C3B-C2B	-2.20	1.37	1.40
31	q	315	CLA	CHC-C1C	2.20	1.40	1.35
36	8	617	NEX	O24-C25	-2.20	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r	312	CLA	C3D-C4D	-2.20	1.39	1.44
31	b	602	CLA	C3D-C4D	-2.20	1.39	1.44
36	4	617	NEX	O24-C25	-2.20	1.43	1.46
44	A	416	PL9	C31-C29	-2.20	1.46	1.51
31	d	405	CLA	C3B-C2B	-2.20	1.37	1.40
32	q	318	LUT	C26-C27	2.20	1.53	1.50
31	B	609	CLA	C3B-C2B	-2.20	1.37	1.40
31	g	303	CLA	C3D-C4D	-2.19	1.39	1.44
32	2	615	LUT	C26-C27	2.19	1.53	1.50
35	9	317	RRX	C33-C5	2.19	1.54	1.50
31	1	610	CLA	C3B-C2B	-2.19	1.37	1.40
31	r	305	CLA	C3B-C2B	-2.19	1.37	1.40
31	1	603	CLA	C3D-C4D	-2.19	1.39	1.44
30	3	309	CHL	C1D-ND	-2.19	1.35	1.37
36	g	317	NEX	O24-C25	-2.19	1.43	1.46
31	b	608	CLA	C3D-C4D	-2.19	1.39	1.44
30	Y	307	CHL	C3A-C2A	-2.19	1.48	1.54
30	0	607	CHL	C3B-C2B	-2.19	1.37	1.40
31	A	405	CLA	C3B-C2B	-2.19	1.37	1.40
31	3	316	CLA	C3D-C4D	-2.19	1.39	1.44
31	c	603	CLA	C3D-C4D	-2.19	1.39	1.44
43	T	101	BCR	C39-C30	-2.19	1.49	1.53
31	r	315	CLA	C3D-C4D	-2.19	1.39	1.44
31	B	603	CLA	C3B-C2B	-2.19	1.37	1.40
44	a	414	PL9	C52-C5	-2.19	1.46	1.50
31	Y	311	CLA	C3D-C4D	-2.19	1.39	1.44
31	7	315	CLA	C3B-C2B	-2.19	1.37	1.40
30	6	309	CHL	C3A-C2A	-2.18	1.48	1.54
43	c	615	BCR	C36-C18	2.18	1.55	1.50
31	q	306	CLA	C3D-C4D	-2.18	1.39	1.44
31	0	603	CLA	C3D-C4D	-2.18	1.39	1.44
31	s	314	CLA	C3B-C2B	-2.18	1.37	1.40
31	S	313	CLA	C3D-C4D	-2.18	1.39	1.44
31	G	613	CLA	C3D-C4D	-2.18	1.39	1.44
43	C	614	BCR	C36-C18	2.18	1.55	1.50
31	B	616	CLA	C3D-C4D	-2.18	1.39	1.44
31	y	611	CLA	C3D-C4D	-2.18	1.39	1.44
31	q	304	CLA	C1C-C2C	2.18	1.48	1.44
30	5	609	CHL	C3B-C2B	-2.18	1.37	1.40
31	b	605	CLA	C3B-C2B	-2.18	1.37	1.40
31	S	315	CLA	C3D-C4D	-2.18	1.39	1.44
31	5	604	CLA	C3B-C2B	-2.18	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	q	313	CLA	C3D-C4D	-2.18	1.39	1.44
32	3	318	LUT	C26-C27	2.17	1.53	1.50
31	r	314	CLA	C3D-C4D	-2.17	1.39	1.44
31	B	601	CLA	C3D-C4D	-2.17	1.39	1.44
30	9	309	CHL	C3B-C2B	-2.17	1.37	1.40
31	C	607	CLA	C3D-C4D	-2.17	1.39	1.44
31	1	602	CLA	C3D-C4D	-2.17	1.39	1.44
31	8	609	CLA	C3B-C2B	-2.17	1.37	1.40
31	7	313	CLA	C3D-C4D	-2.17	1.39	1.44
31	b	603	CLA	C3D-C4D	-2.17	1.39	1.44
31	1	614	CLA	C3B-C2B	-2.17	1.37	1.40
30	9	303	CHL	C3B-C2B	-2.17	1.37	1.40
31	9	304	CLA	C3B-C2B	-2.17	1.37	1.40
32	p	616	LUT	C28-C27	2.17	1.37	1.32
31	r	316	CLA	C3D-C4D	-2.17	1.39	1.44
32	6	318	LUT	C34-C33	-2.17	1.32	1.35
31	3	306	CLA	C3B-C2B	-2.17	1.37	1.40
31	c	611	CLA	C3D-C4D	-2.17	1.39	1.44
30	1	608	CHL	C3B-C2B	-2.17	1.37	1.40
31	R	304	CLA	C3B-C2B	-2.17	1.37	1.40
30	5	607	CHL	C3B-C2B	-2.17	1.37	1.40
36	8	617	NEX	C1-C6	-2.17	1.50	1.54
44	A	416	PL9	C53-C6	-2.16	1.46	1.50
36	0	618	NEX	O24-C25	-2.16	1.43	1.46
31	8	613	CLA	C3B-C2B	-2.16	1.37	1.40
31	s	314	CLA	C3D-C4D	-2.16	1.39	1.44
31	r	306	CLA	C3D-C4D	-2.16	1.39	1.44
31	A	406	CLA	C3B-C2B	-2.16	1.37	1.40
32	q	318	LUT	C30-C29	-2.16	1.32	1.35
32	6	318	LUT	C26-C27	2.16	1.53	1.50
32	N	317	LUT	C34-C33	-2.16	1.32	1.35
31	2	609	CLA	C3B-C2B	-2.16	1.37	1.40
31	a	409	CLA	C3B-C2B	-2.16	1.37	1.40
31	C	612	CLA	C3D-C4D	-2.16	1.39	1.44
31	C	613	CLA	C3D-C4D	-2.16	1.39	1.44
31	c	612	CLA	C3D-C4D	-2.16	1.39	1.44
31	S	303	CLA	C1C-C2C	2.16	1.48	1.44
31	c	602	CLA	C3B-C2B	-2.16	1.37	1.40
31	Y	313	CLA	C3D-C4D	-2.15	1.39	1.44
31	r	315	CLA	C3B-C2B	-2.15	1.37	1.40
32	2	615	LUT	C34-C33	-2.15	1.32	1.35
32	4	616	LUT	C34-C33	-2.15	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	b	619	BCR	C36-C18	2.15	1.55	1.50
31	p	611	CLA	C1C-C2C	2.15	1.48	1.44
43	b	618	BCR	C36-C18	2.15	1.55	1.50
31	6	304	CLA	C3D-C4D	-2.15	1.39	1.44
32	2	615	LUT	C28-C27	2.15	1.37	1.32
31	9	304	CLA	C1C-C2C	2.15	1.48	1.44
32	G	615	LUT	C34-C33	-2.15	1.32	1.35
31	5	612	CLA	C1C-C2C	2.15	1.48	1.44
35	2	614	RRX	C33-C5	2.15	1.54	1.50
31	d	405	CLA	C3D-C4D	-2.15	1.39	1.44
31	c	610	CLA	C3B-C2B	-2.15	1.37	1.40
31	R	306	CLA	C3D-C4D	-2.15	1.39	1.44
31	N	314	CLA	C1C-C2C	2.15	1.48	1.44
43	z	101	BCR	C36-C18	2.15	1.55	1.50
30	6	302	CHL	C3B-C2B	-2.15	1.37	1.40
31	5	610	CLA	C3B-C2B	-2.15	1.37	1.40
31	b	609	CLA	C3B-C2B	-2.15	1.37	1.40
31	8	613	CLA	C1C-C2C	2.15	1.48	1.44
31	y	610	CLA	C3B-C2B	-2.15	1.37	1.40
36	g	317	NEX	C1-C6	-2.15	1.51	1.54
31	C	601	CLA	C3D-C4D	-2.15	1.39	1.44
31	S	312	CLA	C3D-C4D	-2.15	1.39	1.44
31	a	407	CLA	C3B-C2B	-2.15	1.37	1.40
36	R	319	NEX	O24-C25	-2.14	1.43	1.46
31	R	315	CLA	C3B-C2B	-2.14	1.37	1.40
31	R	316	CLA	C3D-C4D	-2.14	1.39	1.44
31	8	602	CLA	C1C-C2C	2.14	1.48	1.44
43	D	405	BCR	C39-C30	-2.14	1.49	1.53
30	1	608	CHL	C3A-C2A	-2.14	1.48	1.54
31	n	315	CLA	C1C-C2C	2.14	1.48	1.44
30	1	601	CHL	C1A-CHA	-2.14	1.34	1.43
31	R	306	CLA	C1A-CHA	2.14	1.52	1.43
47	e	102	HEM	C1D-ND	-2.14	1.34	1.38
31	2	609	CLA	C1C-C2C	2.14	1.48	1.44
31	N	313	CLA	C3B-C2B	-2.14	1.37	1.40
31	q	312	CLA	C1C-C2C	2.14	1.48	1.44
43	A	410	BCR	C36-C18	2.14	1.55	1.50
31	p	615	CLA	C1C-C2C	2.14	1.48	1.44
32	y	617	LUT	C14-C13	-2.14	1.32	1.35
36	4	617	NEX	C1-C6	-2.14	1.51	1.54
31	s	306	CLA	C1C-C2C	2.14	1.48	1.44
31	0	604	CLA	C3D-C4D	-2.14	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	3	318	LUT	C30-C29	-2.14	1.32	1.35
31	2	613	CLA	C3B-C2B	-2.14	1.37	1.40
31	C	611	CLA	C3B-C2B	-2.14	1.37	1.40
31	6	314	CLA	C3B-C2B	-2.14	1.37	1.40
31	s	312	CLA	C3D-C4D	-2.14	1.39	1.44
30	8	601	CHL	C3B-C2B	-2.14	1.37	1.40
31	Y	310	CLA	C3B-C2B	-2.14	1.37	1.40
31	n	314	CLA	C3B-C2B	-2.14	1.37	1.40
31	C	611	CLA	C3D-C4D	-2.14	1.39	1.44
31	c	604	CLA	C3D-C4D	-2.14	1.39	1.44
31	3	305	CLA	C3B-C2B	-2.14	1.37	1.40
31	N	305	CLA	C3B-C2B	-2.14	1.37	1.40
31	8	603	CLA	C3D-C4D	-2.13	1.39	1.44
31	4	602	CLA	C1C-C2C	2.13	1.48	1.44
31	3	305	CLA	C3D-C4D	-2.13	1.39	1.44
31	0	611	CLA	C3D-C4D	-2.13	1.39	1.44
32	9	318	LUT	C34-C33	-2.13	1.33	1.35
31	Y	314	CLA	C3B-C2B	-2.13	1.37	1.40
31	1	604	CLA	C3D-C4D	-2.13	1.39	1.44
31	r	307	CLA	C3D-C4D	-2.13	1.39	1.44
32	N	316	LUT	C34-C33	-2.13	1.33	1.35
31	r	313	CLA	C3D-C4D	-2.13	1.39	1.44
31	Y	305	CLA	C3B-C2B	-2.13	1.37	1.40
31	7	304	CLA	C3D-C4D	-2.13	1.39	1.44
31	G	612	CLA	C3D-C4D	-2.13	1.39	1.44
31	y	603	CLA	C3B-C2B	-2.13	1.37	1.40
36	q	319	NEX	C1-C6	-2.13	1.51	1.54
35	g	315	RRX	C33-C5	2.13	1.54	1.50
31	N	315	CLA	C3B-C2B	-2.13	1.37	1.40
31	c	601	CLA	C3D-C4D	-2.13	1.39	1.44
31	6	316	CLA	C3B-C2B	-2.13	1.37	1.40
31	p	603	CLA	C3D-C4D	-2.13	1.39	1.44
36	6	319	NEX	O24-C25	-2.12	1.43	1.46
36	p	618	NEX	C1-C6	-2.12	1.51	1.54
31	p	615	CLA	C3D-C4D	-2.12	1.39	1.44
31	g	310	CLA	C3D-C4D	-2.12	1.39	1.44
30	0	605	CHL	C3D-C4D	-2.12	1.39	1.44
31	6	315	CLA	C3B-C2B	-2.12	1.37	1.40
32	4	616	LUT	C26-C27	2.12	1.53	1.50
31	G	610	CLA	C1A-CHA	2.12	1.51	1.43
31	A	409	CLA	C3B-C2B	-2.12	1.37	1.40
36	5	618	NEX	C1-C6	-2.12	1.51	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	314	CLA	C3D-C4D	-2.12	1.39	1.44
31	q	316	CLA	C3D-C4D	-2.12	1.39	1.44
31	N	311	CLA	C1C-C2C	2.12	1.48	1.44
31	0	613	CLA	C3D-C4D	-2.12	1.39	1.44
31	b	605	CLA	C1A-CHA	2.12	1.51	1.43
31	0	602	CLA	C3D-C4D	-2.12	1.39	1.44
31	N	304	CLA	C3B-C2B	-2.12	1.37	1.40
31	y	604	CLA	C3B-C2B	-2.12	1.37	1.40
31	p	604	CLA	C1C-C2C	2.12	1.48	1.44
31	3	304	CLA	C3B-C2B	-2.12	1.37	1.40
31	y	603	CLA	C3D-C4D	-2.12	1.39	1.44
31	g	314	CLA	C1C-C2C	2.12	1.48	1.44
31	3	315	CLA	C1C-C2C	2.11	1.48	1.44
31	c	613	CLA	C3D-C4D	-2.11	1.39	1.44
31	8	612	CLA	C3B-C2B	-2.11	1.37	1.40
31	b	604	CLA	C3B-C2B	-2.11	1.37	1.40
32	8	615	LUT	C26-C27	2.11	1.53	1.50
31	7	303	CLA	C3B-C2B	-2.11	1.37	1.40
31	s	311	CLA	C3D-C4D	-2.11	1.39	1.44
30	0	601	CHL	C3B-C2B	-2.11	1.37	1.40
30	0	605	CHL	C1D-ND	-2.11	1.35	1.37
31	p	604	CLA	C1B-NB	2.11	1.37	1.35
31	S	306	CLA	C1C-C2C	2.11	1.48	1.44
31	G	609	CLA	C3D-C4D	-2.11	1.39	1.44
32	S	318	LUT	C34-C33	-2.11	1.33	1.35
31	8	609	CLA	C1C-C2C	2.11	1.48	1.44
31	S	310	CLA	C3D-C4D	-2.11	1.39	1.44
31	3	312	CLA	C1C-C2C	2.11	1.48	1.44
31	p	613	CLA	C3D-C4D	-2.11	1.39	1.44
31	1	603	CLA	C1A-CHA	2.11	1.51	1.43
31	4	604	CLA	C1C-C2C	2.10	1.48	1.44
31	r	305	CLA	C3D-C4D	-2.10	1.39	1.44
42	D	401	PHO	CMB-C2B	-2.10	1.46	1.51
31	y	602	CLA	C1C-C2C	2.10	1.48	1.44
31	2	602	CLA	C3B-C2B	-2.10	1.37	1.40
31	s	303	CLA	C1C-C2C	2.10	1.48	1.44
31	N	310	CLA	C1C-C2C	2.10	1.48	1.44
31	N	321	CLA	C1C-C2C	2.10	1.48	1.44
31	n	316	CLA	C3B-C2B	-2.10	1.37	1.40
31	7	311	CLA	C3B-C2B	-2.10	1.37	1.40
31	7	311	CLA	C1C-C2C	2.10	1.48	1.44
32	7	318	LUT	C26-C27	2.10	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	7	303	CLA	C1C-C2C	2.10	1.48	1.44
31	n	311	CLA	C1C-C2C	2.10	1.48	1.44
36	Y	317	NEX	C1-C6	-2.10	1.51	1.54
43	t	101	BCR	C36-C18	2.10	1.55	1.50
31	G	602	CLA	C3B-C2B	-2.10	1.37	1.40
31	y	615	CLA	C1C-C2C	2.10	1.48	1.44
31	c	609	CLA	C3B-C2B	-2.10	1.37	1.40
31	5	602	CLA	C1C-C2C	2.10	1.48	1.44
31	B	612	CLA	C3D-C4D	-2.10	1.39	1.44
30	g	308	CHL	C3B-C2B	-2.09	1.37	1.40
31	n	312	CLA	C1C-C2C	2.09	1.48	1.44
30	2	608	CHL	C3B-C2B	-2.09	1.37	1.40
30	n	302	CHL	C3B-C2B	-2.09	1.37	1.40
31	C	613	CLA	C3B-C2B	-2.09	1.37	1.40
32	8	616	LUT	C26-C27	2.09	1.53	1.50
32	s	318	LUT	C26-C27	2.09	1.53	1.50
30	3	303	CHL	C3B-C2B	-2.09	1.37	1.40
31	p	602	CLA	C3B-C2B	-2.09	1.37	1.40
38	G	624	SQD	O47-C45	-2.09	1.41	1.46
31	N	312	CLA	C1C-C2C	2.09	1.48	1.44
31	C	605	CLA	CHC-C1C	2.09	1.40	1.35
43	d	406	BCR	C14-C13	-2.09	1.33	1.35
30	3	302	CHL	C1D-ND	-2.09	1.35	1.37
31	4	603	CLA	C3D-C4D	-2.09	1.39	1.44
31	S	303	CLA	C3B-C2B	-2.09	1.37	1.40
31	S	314	CLA	C3D-C4D	-2.09	1.39	1.44
31	q	312	CLA	C3D-C4D	-2.09	1.39	1.44
31	4	614	CLA	C3D-C4D	-2.09	1.39	1.44
31	9	313	CLA	C3D-C4D	-2.09	1.39	1.44
31	9	316	CLA	C3B-C2B	-2.09	1.37	1.40
31	y	602	CLA	C3D-C4D	-2.09	1.39	1.44
31	b	612	CLA	C1C-C2C	2.09	1.48	1.44
47	E	101	HEM	C1D-ND	-2.09	1.34	1.38
32	n	317	LUT	C26-C27	2.09	1.53	1.50
31	g	305	CLA	C3B-C2B	-2.09	1.37	1.40
30	4	609	CHL	C3B-C2B	-2.09	1.37	1.40
31	g	311	CLA	C1A-CHA	2.09	1.51	1.43
31	N	312	CLA	C3D-C4D	-2.09	1.39	1.44
31	b	615	CLA	C1C-C2C	2.09	1.48	1.44
31	S	316	CLA	C3D-C4D	-2.09	1.39	1.44
30	7	309	CHL	C3B-C2B	-2.09	1.37	1.40
31	6	311	CLA	C3B-C2B	-2.09	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	406	CLA	C1A-CHA	2.09	1.51	1.43
32	g	316	LUT	C30-C29	-2.09	1.33	1.35
31	Y	313	CLA	C3B-C2B	-2.09	1.37	1.40
31	r	304	CLA	C3B-C2B	-2.09	1.37	1.40
43	z	101	BCR	C38-C26	2.09	1.54	1.50
31	d	405	CLA	C1A-CHA	2.09	1.51	1.43
30	r	308	CHL	C3A-C2A	-2.08	1.48	1.54
30	4	601	CHL	C3B-C2B	-2.08	1.37	1.40
31	B	604	CLA	C1A-CHA	2.08	1.51	1.43
31	D	404	CLA	C3B-C2B	-2.08	1.37	1.40
36	Y	317	NEX	O24-C25	-2.08	1.43	1.46
31	1	611	CLA	C1C-C2C	2.08	1.48	1.44
31	6	313	CLA	C1C-C2C	2.08	1.48	1.44
31	6	303	CLA	C3B-C2B	-2.08	1.37	1.40
31	g	312	CLA	C3D-C4D	-2.08	1.39	1.44
43	D	405	BCR	C38-C26	2.08	1.54	1.50
31	B	613	CLA	C3D-C4D	-2.08	1.39	1.44
31	5	612	CLA	C3B-C2B	-2.08	1.37	1.40
31	b	608	CLA	C3B-C2B	-2.08	1.37	1.40
31	1	613	CLA	C3D-C4D	-2.08	1.39	1.44
31	S	306	CLA	C3B-C2B	-2.08	1.37	1.40
43	Z	101	BCR	C38-C26	2.08	1.54	1.50
31	6	313	CLA	C3D-C4D	-2.08	1.39	1.44
31	S	311	CLA	C3D-C4D	-2.08	1.39	1.44
31	G	602	CLA	C1C-C2C	2.08	1.48	1.44
31	C	613	CLA	C1A-CHA	2.08	1.51	1.43
30	g	306	CHL	C3B-C2B	-2.08	1.37	1.40
31	N	303	CLA	C3B-C2B	-2.08	1.37	1.40
30	S	308	CHL	C1D-ND	-2.08	1.35	1.37
31	6	312	CLA	C3D-C4D	-2.08	1.39	1.44
31	D	404	CLA	C1A-CHA	2.08	1.51	1.43
31	a	407	CLA	C1A-CHA	2.08	1.51	1.43
31	3	304	CLA	C1C-C2C	2.08	1.48	1.44
31	B	614	CLA	C1C-C2C	2.08	1.48	1.44
31	C	610	CLA	C1A-CHA	2.08	1.51	1.43
32	0	617	LUT	C26-C27	2.08	1.53	1.50
31	7	314	CLA	C3B-C2B	-2.08	1.37	1.40
31	6	312	CLA	C1A-CHA	2.08	1.51	1.43
31	6	305	CLA	C3B-C2B	-2.08	1.37	1.40
31	G	604	CLA	C3D-C4D	-2.07	1.39	1.44
31	c	613	CLA	C1A-CHA	2.07	1.51	1.43
31	6	304	CLA	C1C-C2C	2.07	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	303	CLA	C1C-C2C	2.07	1.48	1.44
31	B	604	CLA	C3B-C2B	-2.07	1.37	1.40
43	B	617	BCR	C10-C9	-2.07	1.33	1.35
31	5	610	CLA	C1C-C2C	2.07	1.48	1.44
31	g	304	CLA	C3D-C4D	-2.07	1.39	1.44
31	C	603	CLA	C3B-C2B	-2.07	1.37	1.40
31	s	303	CLA	C3B-C2B	-2.07	1.37	1.40
31	B	602	CLA	C1A-CHA	2.07	1.51	1.43
31	B	613	CLA	C1C-C2C	2.07	1.48	1.44
31	p	614	CLA	C1C-C2C	2.07	1.48	1.44
31	s	310	CLA	C3D-C4D	-2.07	1.39	1.44
31	4	611	CLA	C1C-C2C	2.07	1.48	1.44
31	y	610	CLA	C1C-C2C	2.07	1.48	1.44
43	D	405	BCR	C37-C22	2.07	1.55	1.50
32	p	616	LUT	C26-C27	2.07	1.53	1.50
31	Y	310	CLA	C1C-C2C	2.07	1.48	1.44
30	N	307	CHL	C3A-C2A	-2.07	1.48	1.54
31	G	602	CLA	C3D-C4D	-2.07	1.39	1.44
31	g	311	CLA	C3D-C4D	-2.07	1.39	1.44
31	8	611	CLA	C1C-C2C	2.07	1.48	1.44
30	N	302	CHL	C3B-C2B	-2.07	1.37	1.40
31	2	613	CLA	C3D-C4D	-2.07	1.39	1.44
31	p	602	CLA	C1A-CHA	2.07	1.51	1.43
31	G	603	CLA	C3D-C4D	-2.07	1.39	1.44
31	7	304	CLA	C1C-C2C	2.07	1.48	1.44
31	9	305	CLA	C3D-C4D	-2.07	1.39	1.44
31	s	316	CLA	C3D-C4D	-2.07	1.39	1.44
31	p	610	CLA	C3B-C2B	-2.07	1.37	1.40
31	B	615	CLA	C1A-CHA	2.07	1.51	1.43
30	2	607	CHL	C3B-C2B	-2.07	1.37	1.40
31	S	314	CLA	C3B-C2B	-2.07	1.37	1.40
31	5	611	CLA	C3D-C4D	-2.07	1.39	1.44
31	8	610	CLA	C1C-C2C	2.07	1.48	1.44
31	3	306	CLA	C3D-C4D	-2.07	1.39	1.44
31	8	614	CLA	C3B-C2B	-2.07	1.37	1.40
31	9	306	CLA	C3B-C2B	-2.07	1.37	1.40
31	n	304	CLA	C3D-C4D	-2.07	1.39	1.44
31	1	610	CLA	C3D-C4D	-2.06	1.39	1.44
31	3	312	CLA	C3D-C4D	-2.06	1.39	1.44
31	p	614	CLA	C3D-C4D	-2.06	1.39	1.44
31	2	611	CLA	C3D-C4D	-2.06	1.39	1.44
31	q	305	CLA	C3D-C4D	-2.06	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R	303	CLA	C1A-CHA	2.06	1.51	1.43
31	7	314	CLA	C1A-CHA	2.06	1.51	1.43
31	8	614	CLA	C1C-C2C	2.06	1.48	1.44
31	8	612	CLA	C1C-C2C	2.06	1.48	1.44
31	8	612	CLA	C3D-C4D	-2.06	1.39	1.44
31	N	304	CLA	C3D-C4D	-2.06	1.39	1.44
32	3	317	LUT	C34-C33	-2.06	1.33	1.35
31	b	613	CLA	C3D-C4D	-2.06	1.39	1.44
31	b	614	CLA	C3D-C4D	-2.06	1.39	1.44
30	0	605	CHL	C1B-NB	-2.06	1.33	1.35
31	n	316	CLA	C3D-C4D	-2.06	1.39	1.44
31	7	316	CLA	C1C-C2C	2.06	1.48	1.44
30	p	609	CHL	C3B-C2B	-2.06	1.37	1.40
31	c	612	CLA	C3B-C2B	-2.06	1.37	1.40
32	n	318	LUT	C26-C27	2.06	1.53	1.50
31	B	614	CLA	C3D-C4D	-2.06	1.39	1.44
30	8	608	CHL	C3A-C2A	-2.06	1.48	1.54
30	4	608	CHL	C3B-C2B	-2.06	1.37	1.40
30	g	302	CHL	C3B-C2B	-2.06	1.37	1.40
47	e	102	HEM	C4B-NB	-2.06	1.34	1.38
31	N	321	CLA	C3D-C4D	-2.06	1.39	1.44
31	p	610	CLA	C3D-C4D	-2.06	1.39	1.44
31	B	611	CLA	C1C-C2C	2.06	1.48	1.44
31	7	305	CLA	C3B-C2B	-2.06	1.37	1.40
32	p	617	LUT	C28-C27	2.06	1.37	1.32
31	n	316	CLA	C1C-C2C	2.06	1.48	1.44
31	5	602	CLA	C3B-C2B	-2.06	1.37	1.40
36	y	618	NEX	O24-C25	-2.06	1.43	1.46
43	C	615	BCR	C36-C18	2.06	1.55	1.50
31	b	614	CLA	C3B-C2B	-2.05	1.37	1.40
31	n	305	CLA	C3B-C2B	-2.05	1.37	1.40
30	p	609	CHL	C3A-C2A	-2.05	1.48	1.54
30	q	308	CHL	C3A-C2A	-2.05	1.48	1.54
31	b	608	CLA	C1A-CHA	2.05	1.51	1.43
31	Y	304	CLA	C3D-C4D	-2.05	1.39	1.44
31	2	610	CLA	C1C-C2C	2.05	1.48	1.44
31	C	601	CLA	C1C-C2C	2.05	1.48	1.44
31	g	313	CLA	C1C-C2C	2.05	1.48	1.44
31	5	614	CLA	C1C-C2C	2.05	1.48	1.44
31	p	612	CLA	C1C-C2C	2.05	1.48	1.44
31	Y	303	CLA	C3B-C2B	-2.05	1.37	1.40
31	S	310	CLA	C1A-CHA	2.05	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	313	CLA	C1C-C2C	2.05	1.48	1.44
31	n	314	CLA	C1C-C2C	2.05	1.48	1.44
31	N	303	CLA	C3D-C4D	-2.05	1.39	1.44
30	3	307	CHL	C3B-C2B	-2.05	1.37	1.40
31	2	604	CLA	C1C-C2C	2.05	1.48	1.44
31	9	306	CLA	C1C-C2C	2.05	1.48	1.44
31	Y	313	CLA	C1A-CHA	2.05	1.51	1.43
32	p	617	LUT	C30-C29	-2.05	1.33	1.35
31	4	614	CLA	C1C-C2C	2.05	1.48	1.44
31	R	313	CLA	C3D-C4D	-2.05	1.39	1.44
36	R	319	NEX	C1-C6	-2.05	1.51	1.54
30	q	311	CHL	C3B-C2B	-2.05	1.37	1.40
31	B	608	CLA	C3B-C2B	-2.05	1.37	1.40
31	8	611	CLA	C3B-C2B	-2.05	1.37	1.40
31	6	312	CLA	C1C-C2C	2.05	1.48	1.44
31	3	314	CLA	C3D-C4D	-2.05	1.39	1.44
31	2	611	CLA	C3B-C2B	-2.05	1.37	1.40
31	C	612	CLA	C3B-C2B	-2.05	1.37	1.40
34	g	322	LMG	C43-C42	-2.05	1.33	1.49
31	7	316	CLA	C3D-C4D	-2.05	1.39	1.44
43	T	101	BCR	C38-C26	2.05	1.54	1.50
31	N	303	CLA	C1C-C2C	2.05	1.48	1.44
32	p	617	LUT	C34-C33	-2.05	1.33	1.35
32	y	616	LUT	C14-C13	-2.05	1.33	1.35
31	2	604	CLA	C3D-C4D	-2.05	1.39	1.44
31	y	615	CLA	C3D-C4D	-2.05	1.39	1.44
30	p	607	CHL	C3B-C2B	-2.05	1.37	1.40
31	0	614	CLA	C3B-C2B	-2.05	1.37	1.40
31	0	612	CLA	C1C-C2C	2.05	1.48	1.44
31	p	604	CLA	C3D-C4D	-2.05	1.39	1.44
31	R	313	CLA	C1A-CHA	2.05	1.51	1.43
31	n	303	CLA	C3B-C2B	-2.05	1.37	1.40
31	2	612	CLA	C1C-C2C	2.05	1.48	1.44
31	9	316	CLA	C1C-C2C	2.05	1.48	1.44
31	b	603	CLA	C1A-CHA	2.05	1.51	1.43
30	N	307	CHL	CHC-C1C	2.04	1.40	1.35
31	5	604	CLA	C1C-C2C	2.04	1.48	1.44
31	Y	303	CLA	C1C-C2C	2.04	1.48	1.44
31	8	604	CLA	C1C-C2C	2.04	1.48	1.44
31	r	306	CLA	C1A-CHA	2.04	1.51	1.43
31	1	613	CLA	C1A-CHA	2.04	1.51	1.43
31	c	603	CLA	C1A-CHA	2.04	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	613	CLA	C3D-C4D	-2.04	1.39	1.44
31	6	305	CLA	C3D-C4D	-2.04	1.39	1.44
31	4	602	CLA	C3B-C2B	-2.04	1.37	1.40
31	S	313	CLA	C3B-C2B	-2.04	1.37	1.40
34	C	624	LMG	C25-C24	-2.04	1.33	1.49
31	3	311	CLA	C1A-CHA	2.04	1.51	1.43
31	N	310	CLA	C3D-C4D	-2.04	1.39	1.44
31	R	303	CLA	C3D-C4D	-2.04	1.39	1.44
31	b	616	CLA	C1A-CHA	2.04	1.51	1.43
31	9	312	CLA	C4B-NB	-2.04	1.33	1.35
31	Y	310	CLA	C3D-C4D	-2.04	1.39	1.44
43	T	101	BCR	C37-C22	2.04	1.55	1.50
31	b	611	CLA	C1C-C2C	2.04	1.48	1.44
31	N	313	CLA	C3D-C4D	-2.04	1.39	1.44
31	7	311	CLA	C3D-C4D	-2.04	1.39	1.44
31	9	316	CLA	C3D-C4D	-2.04	1.39	1.44
34	n	322	LMG	C37-C36	-2.04	1.33	1.49
30	4	607	CHL	C3A-C2A	-2.04	1.48	1.54
30	R	309	CHL	C3B-C2B	-2.04	1.37	1.40
36	6	319	NEX	C1-C6	-2.04	1.51	1.54
31	6	311	CLA	C1C-C2C	2.04	1.48	1.44
31	S	314	CLA	C1A-CHA	2.04	1.51	1.43
31	B	611	CLA	C3B-C2B	-2.04	1.37	1.40
31	C	604	CLA	C3B-C2B	-2.04	1.37	1.40
31	D	403	CLA	C3B-C2B	-2.04	1.37	1.40
31	Y	303	CLA	C3D-C4D	-2.04	1.39	1.44
31	n	314	CLA	C3D-C4D	-2.04	1.39	1.44
31	6	303	CLA	C1C-C2C	2.04	1.48	1.44
31	6	315	CLA	C1C-C2C	2.04	1.48	1.44
31	0	603	CLA	C1A-CHA	2.04	1.51	1.43
31	n	312	CLA	C3D-C4D	-2.04	1.39	1.44
36	N	318	NEX	O24-C25	-2.03	1.43	1.46
31	y	610	CLA	C3D-C4D	-2.03	1.39	1.44
31	5	611	CLA	C1C-C2C	2.03	1.48	1.44
31	3	311	CLA	C3D-C4D	-2.03	1.39	1.44
36	R	301	NEX	O24-C25	-2.03	1.43	1.46
31	3	314	CLA	C1C-C2C	2.03	1.48	1.44
31	p	612	CLA	C3D-C4D	-2.03	1.39	1.44
31	q	304	CLA	C3B-C2B	-2.03	1.37	1.40
32	5	617	LUT	C30-C29	-2.03	1.33	1.35
43	B	617	BCR	C17-C18	-2.03	1.33	1.35
31	2	612	CLA	C3D-C4D	-2.03	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	n	322	LMG	O1-C1	2.03	1.43	1.40
31	s	306	CLA	C3B-C2B	-2.03	1.37	1.40
43	b	619	BCR	C38-C26	2.03	1.54	1.50
34	d	410	LMG	C25-C24	-2.03	1.33	1.49
35	q	317	RRX	C14-C13	-2.03	1.33	1.35
31	5	613	CLA	C1C-C2C	2.03	1.48	1.44
31	G	612	CLA	C1A-CHA	2.03	1.51	1.43
31	s	314	CLA	C1A-CHA	2.03	1.51	1.43
31	p	603	CLA	C1A-CHA	2.03	1.51	1.43
32	g	316	LUT	C34-C33	-2.03	1.33	1.35
34	w	201	LMG	C22-C21	-2.03	1.33	1.49
31	y	603	CLA	C1C-C2C	2.03	1.48	1.44
34	J	101	LMG	C25-C24	-2.03	1.33	1.49
31	y	614	CLA	C1C-C2C	2.03	1.48	1.44
31	8	610	CLA	C3D-C4D	-2.03	1.39	1.44
31	5	603	CLA	C3B-C2B	-2.03	1.37	1.40
34	d	411	LMG	C22-C21	-2.03	1.33	1.49
31	C	612	CLA	C1A-CHA	2.03	1.51	1.43
43	B	618	BCR	C36-C18	2.03	1.55	1.50
43	H	101	BCR	C38-C26	2.03	1.54	1.50
31	9	315	CLA	C3D-C4D	-2.03	1.39	1.44
34	k	101	LMG	C43-C42	-2.03	1.33	1.49
31	y	611	CLA	C1C-C2C	2.03	1.48	1.44
31	A	409	CLA	C1A-CHA	2.03	1.51	1.43
31	5	613	CLA	C3D-C4D	-2.03	1.39	1.44
31	5	614	CLA	C1A-CHA	2.03	1.51	1.43
34	r	321	LMG	O7-C8	-2.03	1.41	1.46
31	s	305	CLA	C1C-C2C	2.03	1.48	1.44
34	D	411	LMG	C43-C42	-2.03	1.33	1.49
32	3	318	LUT	C34-C33	-2.03	1.33	1.35
31	p	602	CLA	C3D-C4D	-2.03	1.39	1.44
43	d	406	BCR	C36-C18	2.03	1.55	1.50
31	B	614	CLA	C3B-C2B	-2.03	1.37	1.40
31	7	312	CLA	C1C-C2C	2.03	1.48	1.44
34	D	411	LMG	C25-C24	-2.03	1.33	1.49
31	0	611	CLA	C1C-C2C	2.03	1.48	1.44
31	8	604	CLA	C3B-C2B	-2.03	1.37	1.40
31	3	306	CLA	C1C-C2C	2.03	1.48	1.44
34	d	410	LMG	C43-C42	-2.03	1.33	1.49
32	Y	315	LUT	C14-C13	-2.03	1.33	1.35
34	B	621	LMG	C25-C24	-2.03	1.33	1.49
34	A	412	LMG	C22-C21	-2.03	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	305	CLA	C3D-C4D	-2.03	1.39	1.44
38	x	201	SQD	O47-C45	-2.03	1.41	1.46
31	a	409	CLA	C1A-CHA	2.03	1.51	1.43
31	G	604	CLA	C3B-C2B	-2.03	1.37	1.40
31	n	313	CLA	C3B-C2B	-2.02	1.37	1.40
34	w	201	LMG	C43-C42	-2.02	1.33	1.49
30	Y	306	CHL	C3A-C2A	-2.02	1.48	1.54
31	b	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	6	303	CLA	C3D-C4D	-2.02	1.39	1.44
34	D	412	LMG	C22-C21	-2.02	1.33	1.49
32	G	615	LUT	C30-C29	-2.02	1.33	1.35
31	G	612	CLA	C3B-C2B	-2.02	1.37	1.40
31	3	316	CLA	C1C-C2C	2.02	1.48	1.44
31	C	609	CLA	C1A-CHA	2.02	1.51	1.43
31	n	311	CLA	C3D-C4D	-2.02	1.39	1.44
34	C	619	LMG	C43-C42	-2.02	1.33	1.49
34	c	624	LMG	C43-C42	-2.02	1.33	1.49
47	E	101	HEM	C4B-NB	-2.02	1.34	1.38
31	1	610	CLA	C1C-C2C	2.02	1.48	1.44
31	b	615	CLA	C3D-C4D	-2.02	1.39	1.44
31	9	313	CLA	C1A-CHA	2.02	1.51	1.43
31	N	315	CLA	C1C-C2C	2.02	1.48	1.44
31	p	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	2	612	CLA	C1A-CHA	2.02	1.51	1.43
34	D	409	LMG	C25-C24	-2.02	1.33	1.49
31	B	610	CLA	C3D-C4D	-2.02	1.39	1.44
34	9	301	LMG	C43-C42	-2.02	1.33	1.49
36	s	319	NEX	O24-C25	-2.02	1.43	1.46
31	R	316	CLA	C1A-CHA	2.02	1.51	1.43
34	D	412	LMG	C43-C42	-2.02	1.33	1.49
30	1	605	CHL	C3B-C2B	-2.02	1.37	1.40
31	6	311	CLA	C3D-C4D	-2.02	1.39	1.44
36	y	618	NEX	C1-C6	-2.02	1.51	1.54
31	g	310	CLA	C1A-CHA	2.02	1.51	1.43
30	G	601	CHL	C3B-C2B	-2.02	1.37	1.40
31	G	610	CLA	C3D-C4D	-2.02	1.39	1.44
31	g	305	CLA	C1C-C2C	2.02	1.48	1.44
31	B	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	Y	314	CLA	C3D-C4D	-2.02	1.39	1.44
31	y	602	CLA	C3B-C2B	-2.02	1.37	1.40
34	q	302	LMG	C37-C36	-2.01	1.33	1.49
34	b	622	LMG	C25-C24	-2.01	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	612	CLA	C1A-CHA	2.01	1.51	1.43
31	s	310	CLA	C1A-CHA	2.01	1.51	1.43
34	9	302	LMG	C37-C36	-2.01	1.33	1.49
31	4	602	CLA	C3D-C4D	-2.01	1.39	1.44
32	p	617	LUT	C26-C27	2.01	1.53	1.50
31	5	604	CLA	C3D-C4D	-2.01	1.39	1.44
31	7	305	CLA	C3D-C4D	-2.01	1.39	1.44
34	9	301	LMG	C25-C24	-2.01	1.33	1.49
31	c	601	CLA	C1C-C2C	2.01	1.48	1.44
34	2	621	LMG	C37-C36	-2.01	1.33	1.49
44	A	416	PL9	C52-C5	-2.01	1.46	1.50
34	J	101	LMG	C43-C42	-2.01	1.33	1.49
31	0	613	CLA	C1A-CHA	2.01	1.51	1.43
34	b	622	LMG	C43-C42	-2.01	1.33	1.49
32	6	317	LUT	C26-C27	2.01	1.53	1.50
43	c	614	BCR	C37-C22	2.01	1.55	1.50
31	S	303	CLA	C3D-C4D	-2.01	1.39	1.44
31	g	313	CLA	C3D-C4D	-2.01	1.39	1.44
31	q	304	CLA	C1A-CHA	2.01	1.51	1.43
30	9	310	CHL	C3B-C2B	-2.01	1.37	1.40
31	r	313	CLA	C1A-CHA	2.01	1.51	1.43
34	4	620	LMG	C43-C42	-2.01	1.33	1.49
31	n	303	CLA	C3D-C4D	-2.01	1.39	1.44
31	3	305	CLA	C1C-C2C	2.01	1.48	1.44
31	C	607	CLA	C1A-CHA	2.01	1.51	1.43
31	C	603	CLA	C1A-CHA	2.01	1.51	1.43
34	4	621	LMG	C37-C36	-2.01	1.33	1.49
31	s	316	CLA	C1A-CHA	2.01	1.51	1.43
31	1	611	CLA	C3D-C4D	-2.01	1.39	1.44
31	g	312	CLA	C1C-C2C	2.01	1.48	1.44
32	s	317	LUT	C26-C27	2.01	1.53	1.50
31	2	609	CLA	C3D-C4D	-2.01	1.39	1.44
31	y	604	CLA	C3D-C4D	-2.01	1.39	1.44
31	g	305	CLA	C3D-C4D	-2.01	1.39	1.44
34	d	411	LMG	C43-C42	-2.01	1.33	1.49
34	C	619	LMG	C25-C24	-2.01	1.33	1.49
31	5	612	CLA	C3D-C4D	-2.01	1.39	1.44
31	R	307	CLA	C1A-CHA	2.01	1.51	1.43
32	q	318	LUT	C34-C33	-2.01	1.33	1.35
31	1	602	CLA	C1C-C2C	2.01	1.48	1.44
31	2	603	CLA	C1C-C2C	2.01	1.48	1.44
31	b	610	CLA	C1A-CHA	2.01	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	0	614	CLA	C3D-C4D	-2.00	1.39	1.44
31	p	604	CLA	C1A-CHA	2.00	1.51	1.43
31	p	613	CLA	C1C-C2C	2.00	1.48	1.44
34	2	620	LMG	C25-C24	-2.00	1.33	1.49
31	c	611	CLA	C1A-CHA	2.00	1.51	1.43
34	k	101	LMG	C22-C21	-2.00	1.33	1.49
31	9	305	CLA	C1C-C2C	2.00	1.48	1.44
31	3	315	CLA	C3D-C4D	-2.00	1.39	1.44
31	5	615	CLA	C3D-C4D	-2.00	1.39	1.44
34	B	621	LMG	C43-C42	-2.00	1.33	1.49
31	Y	304	CLA	C1C-C2C	2.00	1.48	1.44
31	q	316	CLA	C1C-C2C	2.00	1.48	1.44
34	q	301	LMG	C43-C42	-2.00	1.33	1.49
31	B	613	CLA	C3B-C2B	-2.00	1.37	1.40
31	b	615	CLA	C3B-C2B	-2.00	1.37	1.40
31	r	313	CLA	C1C-C2C	2.00	1.48	1.44
34	G	621	LMG	C43-C42	-2.00	1.33	1.49
31	3	313	CLA	C1C-C2C	2.00	1.48	1.44
31	B	601	CLA	C1C-C2C	2.00	1.48	1.44
34	G	621	LMG	C25-C24	-2.00	1.33	1.49
31	8	614	CLA	C3D-C4D	-2.00	1.39	1.44
31	s	303	CLA	C3D-C4D	-2.00	1.39	1.44
31	4	614	CLA	C1A-CHA	2.00	1.51	1.43
31	8	611	CLA	C3D-C4D	-2.00	1.39	1.44
31	q	315	CLA	C4B-NB	-2.00	1.33	1.35
34	G	622	LMG	C37-C36	-2.00	1.33	1.49
31	r	315	CLA	C1A-CHA	2.00	1.51	1.43
31	C	611	CLA	C1A-CHA	2.00	1.51	1.43
31	r	304	CLA	C3D-C4D	-2.00	1.39	1.44
31	s	305	CLA	C3D-C4D	-2.00	1.39	1.44
30	q	308	CHL	C1D-ND	-2.00	1.35	1.37

All (8064) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	G	615	LUT	C40-C33-C34	-33.47	76.04	122.92
32	G	615	LUT	C32-C33-C34	25.38	157.89	118.94
32	G	615	LUT	C40-C33-C32	-22.99	81.85	118.08
43	C	615	BCR	C15-C14-C13	-12.84	108.99	127.31
43	t	101	BCR	C11-C10-C9	-11.88	110.35	127.31
43	d	406	BCR	C15-C14-C13	-11.80	110.48	127.31
43	d	406	BCR	C7-C8-C9	-11.71	108.55	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	t	101	BCR	C15-C14-C13	-11.67	110.65	127.31
43	C	615	BCR	C7-C8-C9	-11.50	108.85	126.23
32	R	317	LUT	C35-C34-C33	-10.67	112.09	127.31
32	p	617	LUT	C35-C34-C33	-10.40	112.47	127.31
43	t	101	BCR	C7-C8-C9	-10.37	110.56	126.23
32	p	616	LUT	C35-C34-C33	-10.37	112.52	127.31
31	B	607	CLA	C4A-NA-C1A	10.23	111.31	106.71
43	c	614	BCR	C20-C21-C22	-10.11	112.88	127.31
31	b	608	CLA	C4A-NA-C1A	9.96	111.19	106.71
31	d	405	CLA	C4A-NA-C1A	9.94	111.18	106.71
31	B	615	CLA	C4A-NA-C1A	9.82	111.12	106.71
31	c	613	CLA	C4A-NA-C1A	9.78	111.11	106.71
31	R	306	CLA	C4A-NA-C1A	9.67	111.06	106.71
31	a	409	CLA	C4A-NA-C1A	9.64	111.04	106.71
31	A	409	CLA	C4A-NA-C1A	9.62	111.03	106.71
31	b	610	CLA	C4A-NA-C1A	9.60	111.02	106.71
31	g	305	CLA	C4A-NA-C1A	9.60	111.02	106.71
32	2	615	LUT	C35-C34-C33	-9.57	113.64	127.31
31	b	616	CLA	C4A-NA-C1A	9.57	111.01	106.71
31	D	404	CLA	C4A-NA-C1A	9.57	111.01	106.71
31	q	315	CLA	C4A-NA-C1A	9.55	111.00	106.71
31	C	612	CLA	C4A-NA-C1A	9.50	110.98	106.71
31	C	607	CLA	C4A-NA-C1A	9.48	110.97	106.71
31	c	606	CLA	C4A-NA-C1A	9.48	110.97	106.71
31	c	612	CLA	C4A-NA-C1A	9.45	110.95	106.71
31	R	316	CLA	C4A-NA-C1A	9.43	110.95	106.71
31	A	406	CLA	C4A-NA-C1A	9.42	110.94	106.71
31	b	609	CLA	C4A-NA-C1A	9.42	110.94	106.71
31	r	315	CLA	C4A-NA-C1A	9.40	110.93	106.71
31	A	405	CLA	C4A-NA-C1A	9.40	110.93	106.71
31	q	313	CLA	C4A-NA-C1A	9.40	110.93	106.71
31	C	609	CLA	C4A-NA-C1A	9.39	110.93	106.71
31	2	604	CLA	C4A-NA-C1A	9.38	110.92	106.71
31	9	312	CLA	C4A-NA-C1A	9.38	110.92	106.71
31	r	312	CLA	C4A-NA-C1A	9.37	110.92	106.71
31	4	612	CLA	C4A-NA-C1A	9.35	110.91	106.71
31	b	613	CLA	C4A-NA-C1A	9.34	110.90	106.71
31	s	310	CLA	C4A-NA-C1A	9.33	110.90	106.71
31	C	613	CLA	C4A-NA-C1A	9.33	110.90	106.71
31	B	609	CLA	C4A-NA-C1A	9.32	110.89	106.71
31	y	604	CLA	C4A-NA-C1A	9.29	110.88	106.71
31	c	610	CLA	C4A-NA-C1A	9.28	110.88	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	p	613	CLA	C4A-NA-C1A	9.28	110.88	106.71
31	7	305	CLA	C4A-NA-C1A	9.25	110.86	106.71
31	c	611	CLA	C4A-NA-C1A	9.20	110.84	106.71
31	y	613	CLA	C4A-NA-C1A	9.19	110.84	106.71
31	6	305	CLA	C4A-NA-C1A	9.17	110.83	106.71
31	a	406	CLA	C4A-NA-C1A	9.16	110.82	106.71
31	2	602	CLA	C4A-NA-C1A	9.15	110.82	106.71
31	4	604	CLA	C4A-NA-C1A	9.13	110.81	106.71
31	c	609	CLA	C4A-NA-C1A	9.13	110.81	106.71
31	G	604	CLA	C4A-NA-C1A	9.12	110.81	106.71
31	a	407	CLA	C4A-NA-C1A	9.12	110.80	106.71
31	0	604	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	n	315	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	R	312	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	r	306	CLA	C4A-NA-C1A	9.11	110.80	106.71
31	4	610	CLA	C4A-NA-C1A	9.10	110.80	106.71
31	B	616	CLA	C4A-NA-C1A	9.09	110.79	106.71
31	S	306	CLA	C4A-NA-C1A	9.07	110.78	106.71
31	8	613	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	9	306	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	C	611	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	1	613	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	0	615	CLA	C4A-NA-C1A	9.04	110.77	106.71
31	0	610	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	D	403	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	N	314	CLA	C4A-NA-C1A	9.03	110.77	106.71
31	R	315	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	S	310	CLA	C4A-NA-C1A	9.02	110.76	106.71
31	S	314	CLA	C4A-NA-C1A	9.01	110.76	106.71
31	s	312	CLA	C4A-NA-C1A	9.01	110.76	106.71
31	2	610	CLA	C4A-NA-C1A	9.00	110.75	106.71
31	q	304	CLA	C4A-NA-C1A	9.00	110.75	106.71
31	Y	305	CLA	C4A-NA-C1A	8.99	110.75	106.71
31	B	604	CLA	C4A-NA-C1A	8.98	110.75	106.71
31	y	615	CLA	C4A-NA-C1A	8.98	110.74	106.71
31	r	311	CLA	C4A-NA-C1A	8.98	110.74	106.71
31	q	312	CLA	C4A-NA-C1A	8.97	110.74	106.71
31	b	606	CLA	C4A-NA-C1A	8.96	110.74	106.71
31	R	303	CLA	C4A-NA-C1A	8.95	110.73	106.71
31	S	313	CLA	C4A-NA-C1A	8.95	110.73	106.71
31	Y	311	CLA	C4A-NA-C1A	8.95	110.73	106.71
31	N	304	CLA	C4A-NA-C1A	8.94	110.73	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	612	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	9	314	CLA	C4A-NA-C1A	8.93	110.72	106.71
31	N	305	CLA	C4A-NA-C1A	8.92	110.72	106.71
31	N	311	CLA	C4A-NA-C1A	8.91	110.71	106.71
43	D	405	BCR	C7-C8-C9	-8.90	112.78	126.23
31	G	610	CLA	C4A-NA-C1A	8.90	110.71	106.71
31	c	605	CLA	C4A-NA-C1A	8.90	110.71	106.71
31	g	310	CLA	C4A-NA-C1A	8.90	110.71	106.71
31	l	603	CLA	C4A-NA-C1A	8.89	110.70	106.71
31	n	304	CLA	C4A-NA-C1A	8.89	110.70	106.71
31	b	614	CLA	C4A-NA-C1A	8.89	110.70	106.71
31	G	612	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	b	605	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	s	313	CLA	C4A-NA-C1A	8.88	110.70	106.71
31	2	611	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	5	615	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	6	314	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	B	608	CLA	C4A-NA-C1A	8.86	110.69	106.71
31	5	603	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	1	604	CLA	C4A-NA-C1A	8.85	110.69	106.71
31	1	614	CLA	C4A-NA-C1A	8.85	110.68	106.71
31	S	305	CLA	C4A-NA-C1A	8.85	110.68	106.71
31	0	602	CLA	C4A-NA-C1A	8.84	110.68	106.71
31	r	316	CLA	C4A-NA-C1A	8.84	110.68	106.71
31	8	604	CLA	C4A-NA-C1A	8.83	110.68	106.71
31	g	303	CLA	C4A-NA-C1A	8.83	110.68	106.71
31	s	305	CLA	C4A-NA-C1A	8.83	110.68	106.71
31	s	304	CLA	C4A-NA-C1A	8.83	110.67	106.71
31	G	611	CLA	C4A-NA-C1A	8.82	110.67	106.71
31	B	612	CLA	C4A-NA-C1A	8.82	110.67	106.71
31	n	305	CLA	C4A-NA-C1A	8.81	110.67	106.71
31	r	303	CLA	C4A-NA-C1A	8.81	110.67	106.71
31	3	306	CLA	C4A-NA-C1A	8.80	110.66	106.71
31	3	311	CLA	C4A-NA-C1A	8.80	110.66	106.71
31	b	602	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	C	610	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	Y	313	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	c	604	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	s	303	CLA	C4A-NA-C1A	8.78	110.66	106.71
31	S	303	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	y	612	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	R	305	CLA	C4A-NA-C1A	8.77	110.65	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	p	602	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	c	607	CLA	C4A-NA-C1A	8.77	110.65	106.71
31	6	311	CLA	C4A-NA-C1A	8.76	110.64	106.71
31	0	614	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	2	613	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	3	313	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	7	314	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	5	604	CLA	C4A-NA-C1A	8.75	110.64	106.71
31	0	613	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	s	316	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	A	407	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	d	401	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	G	609	CLA	C4A-NA-C1A	8.74	110.64	106.71
31	R	313	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	9	304	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	n	314	CLA	C4A-NA-C1A	8.73	110.63	106.71
31	C	602	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	5	602	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	C	608	CLA	C4A-NA-C1A	8.72	110.63	106.71
31	2	609	CLA	C4A-NA-C1A	8.72	110.62	106.71
31	y	611	CLA	C4A-NA-C1A	8.72	110.62	106.71
31	g	312	CLA	C4A-NA-C1A	8.71	110.62	106.71
31	g	313	CLA	C4A-NA-C1A	8.71	110.62	106.71
31	r	313	CLA	C4A-NA-C1A	8.71	110.62	106.71
31	5	611	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	8	603	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	9	305	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	n	312	CLA	C4A-NA-C1A	8.69	110.61	106.71
31	r	305	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	q	316	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	n	303	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	s	306	CLA	C4A-NA-C1A	8.68	110.61	106.71
31	c	603	CLA	C4A-NA-C1A	8.67	110.61	106.71
31	q	314	CLA	C4A-NA-C1A	8.67	110.61	106.71
31	s	314	CLA	C4A-NA-C1A	8.67	110.61	106.71
31	6	313	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	5	614	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	3	312	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	5	610	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	B	610	CLA	C4A-NA-C1A	8.67	110.60	106.71
31	B	603	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	6	315	CLA	C4A-NA-C1A	8.66	110.60	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	615	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	4	614	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	S	311	CLA	C4A-NA-C1A	8.66	110.60	106.71
31	Y	303	CLA	C4A-NA-C1A	8.65	110.60	106.71
31	8	612	CLA	C4A-NA-C1A	8.65	110.60	106.71
31	1	602	CLA	C4A-NA-C1A	8.65	110.59	106.71
31	7	315	CLA	C4A-NA-C1A	8.65	110.59	106.71
31	8	610	CLA	C4A-NA-C1A	8.64	110.59	106.71
31	c	602	CLA	C4A-NA-C1A	8.64	110.59	106.71
31	G	603	CLA	C4A-NA-C1A	8.63	110.58	106.71
31	N	313	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	S	312	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	8	609	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	3	316	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	B	605	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	g	304	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	N	303	CLA	C4A-NA-C1A	8.62	110.58	106.71
31	b	612	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	r	304	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	7	303	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	9	315	CLA	C4A-NA-C1A	8.61	110.58	106.71
31	n	311	CLA	C4A-NA-C1A	8.60	110.57	106.71
31	b	607	CLA	C4A-NA-C1A	8.60	110.57	106.71
31	R	307	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	6	316	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	y	603	CLA	C4A-NA-C1A	8.59	110.57	106.71
31	b	617	CLA	C4A-NA-C1A	8.58	110.56	106.71
31	N	315	CLA	C4A-NA-C1A	8.58	110.56	106.71
31	Y	312	CLA	C4A-NA-C1A	8.57	110.56	106.71
31	7	312	CLA	C4A-NA-C1A	8.57	110.56	106.71
31	n	313	CLA	C4A-NA-C1A	8.57	110.56	106.71
31	S	316	CLA	C4A-NA-C1A	8.56	110.55	106.71
31	N	310	CLA	C4A-NA-C1A	8.55	110.55	106.71
31	p	611	CLA	C4A-NA-C1A	8.55	110.55	106.71
31	8	611	CLA	C4A-NA-C1A	8.54	110.54	106.71
31	Y	314	CLA	C4A-NA-C1A	8.53	110.54	106.71
31	d	404	CLA	C4A-NA-C1A	8.53	110.54	106.71
31	5	612	CLA	C4A-NA-C1A	8.52	110.54	106.71
31	3	314	CLA	C4A-NA-C1A	8.51	110.53	106.71
31	B	606	CLA	C4A-NA-C1A	8.51	110.53	106.71
31	C	601	CLA	C4A-NA-C1A	8.51	110.53	106.71
31	4	602	CLA	C4A-NA-C1A	8.50	110.53	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	6	303	CLA	C4A-NA-C1A	8.49	110.53	106.71
31	C	604	CLA	C4A-NA-C1A	8.49	110.52	106.71
31	p	603	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	y	602	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	4	611	CLA	C4A-NA-C1A	8.48	110.52	106.71
31	g	314	CLA	C4A-NA-C1A	8.47	110.52	106.71
31	Y	304	CLA	C4A-NA-C1A	8.47	110.52	106.71
31	1	612	CLA	C4A-NA-C1A	8.47	110.51	106.71
31	8	602	CLA	C4A-NA-C1A	8.47	110.51	106.71
31	3	301	CLA	C4A-NA-C1A	8.46	110.51	106.71
31	p	612	CLA	C4A-NA-C1A	8.45	110.51	106.71
31	7	304	CLA	C4A-NA-C1A	8.45	110.50	106.71
31	y	610	CLA	C4A-NA-C1A	8.44	110.50	106.71
31	3	305	CLA	C4A-NA-C1A	8.44	110.50	106.71
31	7	316	CLA	C4A-NA-C1A	8.44	110.50	106.71
31	q	305	CLA	C4A-NA-C1A	8.43	110.50	106.71
31	R	304	CLA	C4A-NA-C1A	8.43	110.50	106.71
31	6	304	CLA	C4A-NA-C1A	8.42	110.49	106.71
31	2	603	CLA	C4A-NA-C1A	8.42	110.49	106.71
31	3	304	CLA	C4A-NA-C1A	8.41	110.49	106.71
31	B	601	CLA	C4A-NA-C1A	8.41	110.49	106.71
31	7	311	CLA	C4A-NA-C1A	8.41	110.49	106.71
31	g	311	CLA	C4A-NA-C1A	8.40	110.48	106.71
31	6	312	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	B	602	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	4	613	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	R	314	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	3	315	CLA	C4A-NA-C1A	8.36	110.46	106.71
31	5	613	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	R	311	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	r	314	CLA	C4A-NA-C1A	8.35	110.46	106.71
31	B	611	CLA	C4A-NA-C1A	8.34	110.46	106.71
31	G	602	CLA	C4A-NA-C1A	8.34	110.46	106.71
31	n	316	CLA	C4A-NA-C1A	8.34	110.46	106.71
31	p	604	CLA	C4A-NA-C1A	8.33	110.45	106.71
31	C	605	CLA	C4A-NA-C1A	8.32	110.45	106.71
31	s	311	CLA	C4A-NA-C1A	8.32	110.45	106.71
31	N	321	CLA	C4A-NA-C1A	8.32	110.45	106.71
31	b	604	CLA	C4A-NA-C1A	8.31	110.44	106.71
31	Y	310	CLA	C4A-NA-C1A	8.31	110.44	106.71
31	C	606	CLA	C4A-NA-C1A	8.29	110.43	106.71
31	b	611	CLA	C4A-NA-C1A	8.29	110.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	313	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	p	610	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	9	316	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	0	611	CLA	C4A-NA-C1A	8.26	110.42	106.71
31	4	603	CLA	C4A-NA-C1A	8.26	110.42	106.71
31	0	612	CLA	C4A-NA-C1A	8.25	110.42	106.71
31	r	307	CLA	C4A-NA-C1A	8.25	110.41	106.71
31	q	306	CLA	C4A-NA-C1A	8.24	110.41	106.71
31	1	611	CLA	C4A-NA-C1A	8.23	110.41	106.71
31	p	614	CLA	C4A-NA-C1A	8.23	110.41	106.71
31	c	608	CLA	C4A-NA-C1A	8.22	110.40	106.71
31	B	614	CLA	C4A-NA-C1A	8.22	110.40	106.71
31	c	601	CLA	C4A-NA-C1A	8.20	110.39	106.71
31	s	315	CLA	C4A-NA-C1A	8.20	110.39	106.71
31	0	603	CLA	C4A-NA-C1A	8.19	110.39	106.71
31	N	312	CLA	C4A-NA-C1A	8.17	110.38	106.71
31	b	603	CLA	C4A-NA-C1A	8.17	110.38	106.71
31	y	614	CLA	C4A-NA-C1A	8.17	110.38	106.71
31	1	610	CLA	C4A-NA-C1A	8.16	110.38	106.71
31	C	603	CLA	C4A-NA-C1A	8.13	110.36	106.71
31	8	614	CLA	C4A-NA-C1A	8.07	110.34	106.71
31	B	613	CLA	C4A-NA-C1A	8.07	110.33	106.71
43	D	405	BCR	C15-C14-C13	-8.03	115.85	127.31
31	S	315	CLA	C4A-NA-C1A	8.02	110.31	106.71
43	C	615	BCR	C20-C21-C22	-7.95	115.96	127.31
31	p	615	CLA	C4A-NA-C1A	7.95	110.28	106.71
31	7	313	CLA	C4A-NA-C1A	7.81	110.22	106.71
31	G	613	CLA	C4A-NA-C1A	7.67	110.16	106.71
31	r	303	CLA	O2D-CGD-CBD	7.59	124.75	111.27
43	c	614	BCR	C24-C23-C22	-7.58	114.78	126.23
43	c	615	BCR	C20-C21-C22	-7.40	116.76	127.31
43	C	615	BCR	C8-C9-C10	7.35	130.21	118.94
43	A	410	BCR	C15-C14-C13	-7.24	116.97	127.31
43	t	101	BCR	C33-C5-C6	-7.23	116.40	124.53
43	t	101	BCR	C15-C16-C17	-7.22	108.68	123.47
31	R	303	CLA	O2D-CGD-CBD	7.17	124.01	111.27
32	G	615	LUT	C31-C30-C29	-7.16	117.09	127.31
43	z	101	BCR	C11-C10-C9	-7.16	117.10	127.31
43	C	615	BCR	C12-C13-C14	6.99	129.66	118.94
31	R	306	CLA	O2D-CGD-CBD	6.88	123.49	111.27
43	c	615	BCR	C15-C14-C13	-6.71	117.73	127.31
43	d	406	BCR	C8-C9-C10	6.60	129.07	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	g	315	RRX	C11-C10-C9	-6.58	117.92	127.31
32	g	316	LUT	C31-C30-C29	-6.56	117.94	127.31
43	H	101	BCR	C11-C10-C9	-6.56	117.95	127.31
43	c	614	BCR	C16-C17-C18	-6.55	117.97	127.31
31	S	312	CLA	O2A-C1-C2	6.54	125.81	108.64
43	B	619	BCR	C11-C10-C9	-6.52	118.00	127.31
35	g	315	RRX	C15-C14-C13	-6.51	118.02	127.31
32	Y	316	LUT	C11-C10-C9	-6.51	118.03	127.31
43	a	410	BCR	C24-C23-C22	-6.44	116.50	126.23
43	C	615	BCR	C10-C11-C12	-6.43	103.16	123.22
43	d	406	BCR	C10-C11-C12	-6.43	103.16	123.22
43	a	410	BCR	C20-C21-C22	-6.42	118.15	127.31
43	Z	101	BCR	C7-C8-C9	-6.34	116.65	126.23
31	3	316	CLA	CMD-C2D-C1D	6.34	135.88	124.71
43	c	615	BCR	C1-C6-C5	-6.33	113.70	122.61
31	p	614	CLA	CMD-C2D-C1D	6.27	135.77	124.71
32	4	616	LUT	C11-C10-C9	-6.26	118.38	127.31
43	t	101	BCR	C20-C21-C22	-6.25	118.39	127.31
35	q	317	RRX	C15-C14-C13	-6.24	118.40	127.31
31	r	315	CLA	O2A-C1-C2	6.23	125.00	108.64
31	5	615	CLA	CMD-C2D-C1D	6.23	135.68	124.71
32	3	318	LUT	C15-C14-C13	-6.22	118.43	127.31
43	Z	101	BCR	C11-C10-C9	-6.22	118.44	127.31
43	C	615	BCR	C11-C10-C9	6.21	136.17	127.31
43	T	101	BCR	C33-C5-C6	-6.21	117.56	124.53
31	B	604	CLA	O2D-CGD-CBD	6.18	122.26	111.27
43	B	618	BCR	C15-C14-C13	-6.13	118.56	127.31
35	4	615	RRX	C20-C21-C22	-6.12	118.58	127.31
32	R	317	LUT	C30-C31-C32	-6.11	104.15	123.22
43	B	619	BCR	C15-C14-C13	-6.10	118.60	127.31
31	s	306	CLA	O2D-CGD-CBD	6.10	122.11	111.27
43	V	101	BCR	C16-C17-C18	-6.10	118.61	127.31
32	2	615	LUT	C38-C25-C24	-6.09	110.53	123.56
43	C	615	BCR	C1-C6-C5	-6.09	114.04	122.61
35	9	317	RRX	C20-C21-C22	-6.08	118.64	127.31
35	G	614	RRX	C20-C21-C22	-6.08	118.64	127.31
35	q	317	RRX	C1-C6-C5	-6.06	114.07	122.61
43	b	620	BCR	C7-C8-C9	-6.05	117.09	126.23
31	C	605	CLA	O2D-CGD-CBD	6.04	122.00	111.27
37	r	318	XAT	C31-C30-C29	-6.02	118.71	127.31
43	b	618	BCR	C38-C26-C25	-6.01	117.78	124.53
31	R	312	CLA	CMD-C2D-C1D	6.00	135.29	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	2	614	RRX	C20-C21-C22	-6.00	118.74	127.31
32	2	615	LUT	C28-C29-C30	5.99	128.13	118.94
43	C	614	BCR	C38-C26-C25	-5.98	117.81	124.53
31	5	614	CLA	O2D-CGD-CBD	5.97	121.87	111.27
31	B	606	CLA	O2D-CGD-CBD	5.97	121.87	111.27
31	1	604	CLA	O2D-CGD-CBD	5.96	121.86	111.27
31	S	313	CLA	O2D-CGD-CBD	5.95	121.84	111.27
32	2	615	LUT	C30-C31-C32	-5.94	104.67	123.22
31	c	612	CLA	O2D-CGD-CBD	5.94	121.83	111.27
31	S	304	CLA	C4A-NA-C1A	5.94	109.38	106.71
43	A	410	BCR	C38-C26-C25	-5.93	117.87	124.53
31	q	312	CLA	CMD-C2D-C1D	5.92	135.15	124.71
43	t	101	BCR	C27-C26-C25	-5.92	114.14	122.73
31	9	312	CLA	O2A-C1-C2	5.91	124.18	108.64
31	D	404	CLA	O2A-C1-C2	5.91	124.17	108.64
31	8	603	CLA	CMD-C2D-C1D	5.89	135.09	124.71
31	1	610	CLA	CMD-C2D-C1D	5.88	135.07	124.71
43	C	614	BCR	C11-C10-C9	-5.86	118.94	127.31
31	7	305	CLA	CMD-C2D-C1D	5.86	135.04	124.71
43	v	101	BCR	C16-C17-C18	-5.84	118.98	127.31
44	A	416	PL9	C7-C3-C4	5.83	121.62	116.88
43	b	618	BCR	C33-C5-C6	-5.82	117.99	124.53
31	r	311	CLA	O2A-C1-C2	5.82	123.94	108.64
31	C	613	CLA	O2A-C1-C2	5.82	123.94	108.64
35	q	317	RRX	C20-C21-C22	-5.82	119.01	127.31
43	d	406	BCR	C38-C26-C25	-5.82	118.00	124.53
32	S	318	LUT	C35-C34-C33	-5.81	119.02	127.31
31	R	306	CLA	CMD-C2D-C1D	5.80	134.94	124.71
43	h	101	BCR	C11-C10-C9	-5.80	119.04	127.31
31	S	315	CLA	CMD-C2D-C1D	5.79	134.92	124.71
43	T	101	BCR	C7-C8-C9	-5.78	117.51	126.23
31	d	401	CLA	CMD-C2D-C1D	5.77	134.88	124.71
31	2	613	CLA	CMD-C2D-C1D	5.77	134.88	124.71
31	r	313	CLA	O2A-C1-C2	5.77	122.45	108.97
32	9	318	LUT	C31-C30-C29	-5.77	119.08	127.31
43	C	615	BCR	C33-C5-C6	-5.76	118.06	124.53
31	7	313	CLA	O2D-CGD-CBD	5.76	121.50	111.27
31	D	404	CLA	O2D-CGD-CBD	5.76	121.50	111.27
31	C	603	CLA	CMD-C2D-C1D	5.76	134.86	124.71
32	g	316	LUT	C11-C10-C9	-5.76	119.09	127.31
31	7	304	CLA	CMD-C2D-C1D	5.75	134.85	124.71
31	b	607	CLA	CMD-C2D-C1D	5.75	134.85	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	614	CLA	CMD-C2D-C1D	5.75	134.84	124.71
31	r	316	CLA	CMD-C2D-C1D	5.75	134.84	124.71
43	t	101	BCR	C11-C12-C13	-5.74	110.28	126.42
31	7	313	CLA	CMD-C2D-C1D	5.73	134.82	124.71
31	0	612	CLA	CMD-C2D-C1D	5.73	134.81	124.71
31	y	610	CLA	CMD-C2D-C1D	5.72	134.80	124.71
31	9	304	CLA	O2A-C1-C2	5.72	123.67	108.64
31	p	604	CLA	CMD-C2D-C1D	5.72	134.79	124.71
31	N	310	CLA	CMD-C2D-C1D	5.71	134.78	124.71
31	c	607	CLA	O2D-CGD-CBD	5.71	121.41	111.27
31	R	314	CLA	CMD-C2D-C1D	5.70	134.76	124.71
31	q	316	CLA	CMD-C2D-C1D	5.70	134.76	124.71
31	d	404	CLA	O2A-C1-C2	5.70	123.61	108.64
32	p	617	LUT	C21-C26-C27	-5.69	105.50	112.70
43	d	406	BCR	C24-C23-C22	-5.69	117.64	126.23
31	s	315	CLA	CMD-C2D-C1D	5.69	134.74	124.71
43	b	619	BCR	C20-C21-C22	-5.69	119.19	127.31
31	B	605	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	5	610	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	p	610	CLA	CMD-C2D-C1D	5.67	134.71	124.71
31	g	304	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	g	303	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	s	303	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	G	602	CLA	CMD-C2D-C1D	5.67	134.70	124.71
31	b	603	CLA	CAA-C2A-C3A	-5.66	97.27	112.78
43	B	617	BCR	C4-C5-C6	-5.66	114.51	122.73
43	b	620	BCR	C11-C10-C9	-5.66	119.23	127.31
31	C	607	CLA	O2D-CGD-CBD	5.66	121.32	111.27
31	G	603	CLA	CMD-C2D-C1D	5.66	134.68	124.71
31	p	603	CLA	O2A-C1-C2	5.65	123.48	108.64
31	G	613	CLA	CMD-C2D-C1D	5.65	134.66	124.71
43	v	101	BCR	C38-C26-C25	-5.65	118.19	124.53
37	R	318	XAT	C31-C30-C29	-5.64	119.25	127.31
31	9	316	CLA	CMD-C2D-C1D	5.64	134.66	124.71
31	B	616	CLA	O2D-CGD-CBD	5.64	121.29	111.27
31	N	315	CLA	CMD-C2D-C1D	5.64	134.65	124.71
31	R	304	CLA	CMD-C2D-C1D	5.64	134.65	124.71
31	6	312	CLA	O2A-C1-C2	5.64	123.45	108.64
31	7	311	CLA	CMD-C2D-C1D	5.64	134.65	124.71
31	y	612	CLA	O2D-CGD-CBD	5.63	121.28	111.27
32	7	317	LUT	C7-C8-C9	-5.63	117.73	126.23
31	0	604	CLA	O2D-CGD-CBD	5.63	121.27	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	316	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	6	304	CLA	CMD-C2D-C1D	5.63	134.63	124.71
31	q	304	CLA	CMD-C2D-C1D	5.62	134.62	124.71
32	9	318	LUT	C15-C14-C13	-5.62	119.29	127.31
31	B	605	CLA	O2D-CGD-CBD	5.62	121.25	111.27
31	r	304	CLA	CMD-C2D-C1D	5.62	134.61	124.71
31	s	306	CLA	CMD-C2D-C1D	5.62	134.61	124.71
31	9	312	CLA	CMD-C2D-C1D	5.62	134.61	124.71
31	B	604	CLA	CMD-C2D-C1D	5.62	134.61	124.71
31	7	305	CLA	O2D-CGD-CBD	5.61	121.24	111.27
31	9	305	CLA	CMD-C2D-C1D	5.61	134.60	124.71
31	2	603	CLA	CMD-C2D-C1D	5.61	134.60	124.71
31	6	303	CLA	CMD-C2D-C1D	5.61	134.59	124.71
31	B	601	CLA	O2D-CGD-CBD	5.60	121.22	111.27
31	4	610	CLA	CMD-C2D-C1D	5.60	134.59	124.71
31	C	612	CLA	O2D-CGD-CBD	5.60	121.22	111.27
31	b	603	CLA	O2A-C1-C2	5.60	123.35	108.64
31	2	609	CLA	CMD-C2D-C1D	5.60	134.58	124.71
31	6	311	CLA	CMD-C2D-C1D	5.60	134.58	124.71
31	y	615	CLA	CMD-C2D-C1D	5.60	134.58	124.71
43	V	101	BCR	C33-C5-C6	-5.59	118.25	124.53
31	g	312	CLA	CMD-C2D-C1D	5.59	134.56	124.71
31	B	606	CLA	CMD-C2D-C1D	5.58	134.56	124.71
31	1	602	CLA	O2D-CGD-CBD	5.58	121.19	111.27
35	4	615	RRX	C24-C23-C22	-5.58	117.80	126.23
31	B	615	CLA	O2D-CGD-CBD	5.58	121.19	111.27
31	3	304	CLA	CMD-C2D-C1D	5.58	134.55	124.71
31	c	601	CLA	CMD-C2D-C1D	5.58	134.55	124.71
31	6	315	CLA	CMD-C2D-C1D	5.58	134.54	124.71
31	b	605	CLA	O2D-CGD-CBD	5.58	121.18	111.27
31	R	303	CLA	O2A-C1-C2	5.58	122.01	108.97
31	r	312	CLA	CMD-C2D-C1D	5.57	134.54	124.71
35	9	317	RRX	C24-C23-C22	-5.57	117.81	126.23
31	p	603	CLA	CMD-C2D-C1D	5.57	134.53	124.71
31	n	316	CLA	CMD-C2D-C1D	5.57	134.53	124.71
31	4	602	CLA	CMD-C2D-C1D	5.57	134.52	124.71
31	q	314	CLA	CMD-C2D-C1D	5.56	134.52	124.71
31	b	607	CLA	O2D-CGD-CBD	5.56	121.15	111.27
31	1	614	CLA	CMD-C2D-C1D	5.56	134.52	124.71
31	p	615	CLA	CMD-C2D-C1D	5.56	134.52	124.71
35	G	614	RRX	C24-C23-C22	-5.56	117.84	126.23
31	2	602	CLA	CMD-C2D-C1D	5.56	134.51	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	602	CLA	CMD-C2D-C1D	5.56	134.51	124.71
31	R	315	CLA	CMD-C2D-C1D	5.56	134.51	124.71
31	6	305	CLA	CMD-C2D-C1D	5.56	134.50	124.71
31	N	303	CLA	CMD-C2D-C1D	5.55	134.50	124.71
31	q	312	CLA	O2D-CGD-CBD	5.55	121.13	111.27
32	g	316	LUT	C35-C34-C33	-5.55	119.39	127.31
43	c	615	BCR	C11-C10-C9	-5.55	119.39	127.31
31	C	610	CLA	O2D-CGD-CBD	5.55	121.13	111.27
31	G	604	CLA	CMD-C2D-C1D	5.55	134.49	124.71
31	g	314	CLA	CMD-C2D-C1D	5.54	134.49	124.71
31	8	614	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	A	406	CLA	CMD-C2D-C1D	5.54	134.48	124.71
43	h	101	BCR	C15-C14-C13	-5.54	119.40	127.31
43	b	619	BCR	C16-C17-C18	-5.54	119.40	127.31
31	3	313	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	S	303	CLA	CMD-C2D-C1D	5.54	134.48	124.71
31	C	611	CLA	O2D-CGD-CBD	5.54	121.11	111.27
43	b	618	BCR	C27-C26-C25	-5.54	114.69	122.73
31	R	305	CLA	O2D-CGD-CBD	5.54	121.11	111.27
31	S	306	CLA	CMD-C2D-C1D	5.54	134.47	124.71
31	b	608	CLA	CMD-C2D-C1D	5.54	134.47	124.71
31	p	612	CLA	CMD-C2D-C1D	5.54	134.47	124.71
31	y	615	CLA	O2D-CGD-CBD	5.53	121.10	111.27
31	6	314	CLA	CMD-C2D-C1D	5.53	134.47	124.71
31	5	603	CLA	CMD-C2D-C1D	5.53	134.47	124.71
31	B	602	CLA	O2D-CGD-CBD	5.53	121.10	111.27
31	q	305	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	n	303	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	b	615	CLA	CMD-C2D-C1D	5.53	134.46	124.71
31	c	603	CLA	CMD-C2D-C1D	5.53	134.46	124.71
43	d	406	BCR	C34-C9-C10	-5.53	115.18	122.92
31	Y	310	CLA	CMD-C2D-C1D	5.53	134.46	124.71
35	2	614	RRX	C24-C23-C22	-5.53	117.88	126.23
31	N	321	CLA	CMD-C2D-C1D	5.53	134.45	124.71
31	C	604	CLA	CMD-C2D-C1D	5.52	134.45	124.71
31	A	409	CLA	O2D-CGD-CBD	5.52	121.08	111.27
35	g	315	RRX	C20-C21-C22	-5.52	119.43	127.31
31	3	306	CLA	CMD-C2D-C1D	5.52	134.45	124.71
31	6	313	CLA	CMD-C2D-C1D	5.52	134.44	124.71
31	R	313	CLA	O2A-C1-C2	5.52	121.88	108.97
31	2	604	CLA	CMD-C2D-C1D	5.52	134.44	124.71
31	Y	304	CLA	CMD-C2D-C1D	5.52	134.44	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	306	CLA	CMD-C2D-C1D	5.52	134.44	124.71
31	8	609	CLA	CMD-C2D-C1D	5.51	134.43	124.71
31	a	406	CLA	C1-C2-C3	-5.51	116.51	126.04
31	Y	305	CLA	CMD-C2D-C1D	5.51	134.43	124.71
31	4	604	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	0	614	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	Y	303	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	y	614	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	7	303	CLA	CMD-C2D-C1D	5.51	134.42	124.71
31	S	316	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	y	603	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	C	602	CLA	O2D-CGD-CBD	5.50	121.04	111.27
31	r	314	CLA	O2A-C1-C2	5.50	121.83	108.97
31	5	602	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	8	602	CLA	CMD-C2D-C1D	5.50	134.41	124.71
31	s	304	CLA	CMD-C2D-C1D	5.50	134.40	124.71
31	s	313	CLA	O2D-CGD-CBD	5.50	121.04	111.27
31	N	313	CLA	CMD-C2D-C1D	5.50	134.40	124.71
31	1	604	CLA	CMD-C2D-C1D	5.49	134.40	124.71
31	a	409	CLA	O2D-CGD-CBD	5.49	121.03	111.27
31	1	612	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	c	604	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	n	304	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	R	311	CLA	O2A-C1-C2	5.49	123.07	108.64
31	r	315	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	N	304	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	Y	312	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	b	612	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	n	313	CLA	CMD-C2D-C1D	5.49	134.39	124.71
31	7	316	CLA	CMD-C2D-C1D	5.49	134.38	124.71
31	d	405	CLA	O2D-CGD-CBD	5.49	121.02	111.27
31	s	313	CLA	CMD-C2D-C1D	5.49	134.38	124.71
31	9	304	CLA	CMD-C2D-C1D	5.48	134.38	124.71
31	5	614	CLA	CMD-C2D-C1D	5.48	134.38	124.71
31	B	615	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	G	612	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	7	315	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	C	607	CLA	CMD-C2D-C1D	5.48	134.37	124.71
31	c	602	CLA	O2A-C1-C2	5.48	123.03	108.64
31	8	611	CLA	CMD-C2D-C1D	5.47	134.36	124.71
31	n	311	CLA	CMD-C2D-C1D	5.47	134.36	124.71
31	N	312	CLA	CMD-C2D-C1D	5.47	134.36	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	317	LUT	C11-C10-C9	-5.47	119.50	127.31
31	r	306	CLA	O2D-CGD-CBD	5.47	120.99	111.27
32	S	318	LUT	C31-C30-C29	-5.47	119.50	127.31
31	c	609	CLA	CMD-C2D-C1D	5.47	134.35	124.71
37	R	318	XAT	C38-C25-C24	5.47	120.43	114.28
37	r	318	XAT	C38-C25-C24	5.47	120.43	114.28
43	v	101	BCR	C33-C5-C6	-5.47	118.39	124.53
31	5	612	CLA	CMD-C2D-C1D	5.46	134.34	124.71
31	5	604	CLA	CMD-C2D-C1D	5.46	134.34	124.71
31	0	602	CLA	CMD-C2D-C1D	5.46	134.34	124.71
31	3	315	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	3	311	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	r	305	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	y	602	CLA	CMD-C2D-C1D	5.46	134.33	124.71
31	c	610	CLA	CMD-C2D-C1D	5.45	134.32	124.71
32	7	317	LUT	C11-C10-C9	-5.45	119.53	127.31
31	9	315	CLA	CMD-C2D-C1D	5.45	134.32	124.71
31	b	606	CLA	CMD-C2D-C1D	5.45	134.31	124.71
31	0	603	CLA	CMD-C2D-C1D	5.45	134.31	124.71
31	0	615	CLA	CMD-C2D-C1D	5.45	134.31	124.71
32	N	317	LUT	C11-C10-C9	-5.45	119.54	127.31
31	B	614	CLA	CMD-C2D-C1D	5.44	134.30	124.71
31	0	613	CLA	CMD-C2D-C1D	5.44	134.30	124.71
31	A	405	CLA	CMD-C2D-C1D	5.44	134.30	124.71
47	e	102	HEM	CHC-C4B-NB	5.44	130.34	124.43
31	b	603	CLA	O2D-CGD-CBD	5.44	120.93	111.27
31	g	313	CLA	CMD-C2D-C1D	5.44	134.29	124.71
31	4	603	CLA	CMD-C2D-C1D	5.43	134.29	124.71
31	r	314	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	p	603	CLA	O2D-CGD-CBD	5.43	120.92	111.27
43	H	101	BCR	C7-C8-C9	-5.43	118.03	126.23
31	b	604	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	b	602	CLA	O2D-CGD-CBD	5.43	120.92	111.27
31	S	304	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	c	609	CLA	O2D-CGD-CBD	5.43	120.91	111.27
31	g	305	CLA	CMD-C2D-C1D	5.43	134.28	124.71
31	C	603	CLA	C1-C2-C3	-5.43	116.66	126.04
31	4	613	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	b	614	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	c	607	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	Y	314	CLA	CMD-C2D-C1D	5.42	134.27	124.71
31	s	310	CLA	CMD-C2D-C1D	5.42	134.27	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	p	613	CLA	O2D-CGD-CBD	5.42	120.90	111.27
31	S	305	CLA	CMD-C2D-C1D	5.42	134.26	124.71
31	S	310	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	B	602	CLA	CAA-C2A-C3A	-5.41	97.96	112.78
31	R	316	CLA	O2D-CGD-CBD	5.41	120.89	111.27
31	N	305	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	0	610	CLA	CMD-C2D-C1D	5.41	134.25	124.71
31	r	315	CLA	O2D-CGD-CBD	5.41	120.88	111.27
32	R	317	LUT	C28-C29-C30	5.40	127.23	118.94
31	a	406	CLA	O2A-C1-C2	5.40	122.84	108.64
31	B	601	CLA	CMD-C2D-C1D	5.40	134.24	124.71
31	b	611	CLA	CMD-C2D-C1D	5.40	134.24	124.71
31	y	604	CLA	CMD-C2D-C1D	5.40	134.23	124.71
43	C	614	BCR	C7-C8-C9	-5.40	118.08	126.23
31	B	612	CLA	O2D-CGD-CBD	5.40	120.86	111.27
31	8	604	CLA	CMD-C2D-C1D	5.40	134.23	124.71
31	3	314	CLA	CMD-C2D-C1D	5.40	134.23	124.71
31	G	611	CLA	O2D-CGD-CBD	5.40	120.86	111.27
31	n	305	CLA	CMD-C2D-C1D	5.40	134.23	124.71
31	S	313	CLA	CMD-C2D-C1D	5.40	134.22	124.71
31	s	316	CLA	CMD-C2D-C1D	5.40	134.22	124.71
31	r	316	CLA	O2D-CGD-CBD	5.39	120.85	111.27
31	A	409	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	a	409	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	B	610	CLA	O2D-CGD-CBD	5.39	120.85	111.27
32	N	316	LUT	C7-C8-C9	-5.39	118.09	126.23
31	C	610	CLA	CMD-C2D-C1D	5.39	134.22	124.71
31	B	613	CLA	CMD-C2D-C1D	5.39	134.21	124.71
32	5	616	LUT	C18-C5-C6	-5.39	118.48	124.53
31	b	607	CLA	O2A-C1-C2	5.39	122.79	108.64
31	A	407	CLA	CMD-C2D-C1D	5.39	134.21	124.71
31	A	407	CLA	O2A-C1-C2	5.39	121.56	108.97
31	a	406	CLA	CMD-C2D-C1D	5.39	134.21	124.71
31	7	316	CLA	O2D-CGD-CBD	5.38	120.84	111.27
31	s	311	CLA	CMD-C2D-C1D	5.38	134.20	124.71
31	R	307	CLA	O2D-CGD-CBD	5.38	120.84	111.27
31	b	617	CLA	O2D-CGD-CBD	5.38	120.83	111.27
35	q	317	RRX	C33-C5-C6	-5.38	118.49	124.53
31	3	301	CLA	O2A-C1-C2	5.38	122.77	108.64
31	B	604	CLA	O2A-C1-C2	5.38	122.76	108.64
31	C	606	CLA	O2D-CGD-CBD	5.38	120.82	111.27
31	B	610	CLA	CMD-C2D-C1D	5.37	134.19	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	2	614	RRX	C11-C10-C9	-5.37	119.64	127.31
43	d	406	BCR	C33-C5-C6	-5.37	118.50	124.53
31	S	310	CLA	O2A-C1-C2	5.37	122.75	108.64
31	5	615	CLA	O2D-CGD-CBD	5.37	120.81	111.27
31	y	613	CLA	O2D-CGD-CBD	5.37	120.81	111.27
31	C	604	CLA	O2D-CGD-CBD	5.37	120.81	111.27
31	6	316	CLA	CMD-C2D-C1D	5.37	134.17	124.71
32	2	615	LUT	C39-C29-C30	-5.36	115.41	122.92
31	B	611	CLA	CMD-C2D-C1D	5.36	134.17	124.71
31	C	611	CLA	CMD-C2D-C1D	5.36	134.17	124.71
31	3	305	CLA	CMD-C2D-C1D	5.36	134.16	124.71
31	B	602	CLA	O2A-C1-C2	5.36	122.71	108.64
31	6	315	CLA	O2A-C1-C2	5.36	122.71	108.64
31	S	311	CLA	CMD-C2D-C1D	5.35	134.15	124.71
31	1	611	CLA	CMD-C2D-C1D	5.35	134.15	124.71
31	s	305	CLA	CMD-C2D-C1D	5.35	134.15	124.71
31	b	616	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	0	604	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	8	612	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	n	314	CLA	CMD-C2D-C1D	5.35	134.14	124.71
31	1	604	CLA	O2A-C1-C2	5.35	122.69	108.64
31	c	604	CLA	O2D-CGD-CBD	5.35	120.77	111.27
31	c	605	CLA	O2D-CGD-CBD	5.35	120.77	111.27
31	b	605	CLA	O2A-C1-C2	5.35	122.69	108.64
43	z	101	BCR	C24-C23-C22	-5.34	118.16	126.23
31	9	313	CLA	O2D-CGD-CBD	5.34	120.76	111.27
31	2	611	CLA	CMD-C2D-C1D	5.34	134.13	124.71
31	B	609	CLA	CMD-C2D-C1D	5.34	134.12	124.71
31	G	613	CLA	O2D-CGD-CBD	5.34	120.76	111.27
31	R	315	CLA	O2D-CGD-CBD	5.34	120.76	111.27
31	8	610	CLA	O2A-C1-C2	5.34	121.45	108.97
31	n	312	CLA	O2A-C1-C2	5.34	121.45	108.97
32	p	616	LUT	C32-C33-C34	5.33	127.13	118.94
31	p	604	CLA	O2D-CGD-CBD	5.33	120.75	111.27
31	c	610	CLA	O2A-C1-C2	5.33	122.65	108.64
36	2	616	NEX	C38-C25-C24	5.33	120.28	114.28
31	3	312	CLA	O2A-C1-C2	5.33	122.64	108.64
47	E	101	HEM	CHC-C4B-NB	5.32	130.22	124.43
31	s	314	CLA	CMD-C2D-C1D	5.32	134.09	124.71
31	b	606	CLA	O2D-CGD-CBD	5.32	120.72	111.27
31	c	611	CLA	CMD-C2D-C1D	5.32	134.09	124.71
31	s	310	CLA	O2A-C1-C2	5.32	122.62	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	601	CLA	CMD-C2D-C1D	5.32	134.09	124.71
31	C	602	CLA	CMD-C2D-C1D	5.32	134.09	124.71
31	9	313	CLA	CMD-C2D-C1D	5.32	134.09	124.71
32	R	317	LUT	C21-C26-C27	-5.32	105.98	112.70
32	R	317	LUT	C32-C33-C34	5.32	127.10	118.94
31	d	405	CLA	CMD-C2D-C1D	5.32	134.08	124.71
31	b	616	CLA	O2D-CGD-CBD	5.31	120.71	111.27
31	4	612	CLA	CMD-C2D-C1D	5.31	134.08	124.71
31	D	404	CLA	CMD-C2D-C1D	5.31	134.08	124.71
31	B	607	CLA	O2A-C1-C2	5.31	122.60	108.64
31	4	611	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	G	609	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	g	310	CLA	CMD-C2D-C1D	5.31	134.07	124.71
43	D	405	BCR	C8-C9-C10	5.31	127.09	118.94
31	d	404	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	C	606	CLA	CMD-C2D-C1D	5.31	134.07	124.71
31	r	305	CLA	O2D-CGD-CBD	5.30	120.69	111.27
31	4	612	CLA	O2D-CGD-CBD	5.30	120.69	111.27
43	B	617	BCR	C38-C26-C25	-5.30	118.58	124.53
31	c	603	CLA	O2D-CGD-CBD	5.30	120.68	111.27
31	r	306	CLA	CMD-C2D-C1D	5.30	134.05	124.71
31	4	614	CLA	O2A-C1-C2	5.30	122.56	108.64
31	c	602	CLA	O2D-CGD-CBD	5.30	120.68	111.27
35	q	317	RRX	C38-C26-C25	-5.29	118.58	124.53
31	n	315	CLA	CMD-C2D-C1D	5.29	134.04	124.71
43	A	410	BCR	C16-C17-C18	-5.29	119.76	127.31
31	2	610	CLA	CMD-C2D-C1D	5.29	134.04	124.71
31	Y	312	CLA	O2A-C1-C2	5.29	122.53	108.64
31	8	613	CLA	CMD-C2D-C1D	5.29	134.03	124.71
31	g	314	CLA	O2A-C1-C2	5.29	121.34	108.97
31	B	614	CLA	O2A-C1-C2	5.29	122.53	108.64
31	C	612	CLA	O2A-C1-C2	5.29	122.53	108.64
31	N	311	CLA	O2A-C1-C2	5.29	121.33	108.97
31	b	603	CLA	CMD-C2D-C1D	5.28	134.03	124.71
31	s	313	CLA	O2A-C1-C2	5.28	122.52	108.64
31	2	612	CLA	CMD-C2D-C1D	5.28	134.02	124.71
31	5	613	CLA	CMD-C2D-C1D	5.28	134.02	124.71
31	g	314	CLA	O2D-CGD-CBD	5.28	120.65	111.27
31	Y	312	CLA	O2D-CGD-CBD	5.28	120.64	111.27
31	G	611	CLA	CMD-C2D-C1D	5.27	134.01	124.71
31	c	604	CLA	O2A-C1-C2	5.27	122.50	108.64
31	S	314	CLA	CMD-C2D-C1D	5.27	134.01	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	7	314	CLA	CMD-C2D-C1D	5.27	134.00	124.71
31	s	311	CLA	O2D-CGD-CBD	5.27	120.63	111.27
31	p	615	CLA	O2D-CGD-CBD	5.27	120.63	111.27
31	d	401	CLA	O2A-C1-C2	5.27	121.28	108.97
31	q	306	CLA	CMD-C2D-C1D	5.26	133.99	124.71
31	3	311	CLA	O2D-CGD-CBD	5.26	120.62	111.27
43	B	619	BCR	C16-C17-C18	-5.26	119.80	127.31
31	7	312	CLA	CMD-C2D-C1D	5.26	133.99	124.71
31	B	602	CLA	CMD-C2D-C1D	5.26	133.99	124.71
35	G	614	RRX	C15-C14-C13	-5.26	119.80	127.31
43	Z	101	BCR	C24-C23-C22	-5.26	118.29	126.23
31	c	605	CLA	CMD-C2D-C1D	5.26	133.98	124.71
43	c	614	BCR	C15-C14-C13	-5.26	119.81	127.31
32	2	615	LUT	C31-C30-C29	5.25	134.81	127.31
31	R	305	CLA	O2A-C1-C2	5.25	122.44	108.64
35	4	615	RRX	C15-C14-C13	-5.25	119.81	127.31
43	C	615	BCR	C34-C9-C10	-5.25	115.56	122.92
31	g	311	CLA	O2A-C1-C2	5.25	122.44	108.64
31	r	311	CLA	CMD-C2D-C1D	5.25	133.97	124.71
31	g	311	CLA	O2D-CGD-CBD	5.24	120.59	111.27
31	R	303	CLA	CMD-C2D-C1D	5.24	133.95	124.71
31	s	312	CLA	O2D-CGD-CBD	5.24	120.58	111.27
43	C	615	BCR	C4-C5-C6	-5.24	115.12	122.73
31	d	401	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	S	315	CLA	O2D-CGD-CBD	5.24	120.58	111.27
36	5	618	NEX	C38-C25-C24	5.24	120.18	114.28
31	q	313	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	b	610	CLA	O2D-CGD-CBD	5.24	120.58	111.27
31	R	311	CLA	CMD-C2D-C1D	5.24	133.95	124.71
31	B	603	CLA	CMD-C2D-C1D	5.24	133.94	124.71
31	b	617	CLA	CMD-C2D-C1D	5.24	133.94	124.71
31	B	616	CLA	O2A-C1-C2	5.23	122.38	108.64
31	q	315	CLA	O2D-CGD-CBD	5.23	120.56	111.27
32	5	617	LUT	C15-C14-C13	-5.23	119.85	127.31
31	D	403	CLA	CMD-C2D-C1D	5.23	133.93	124.71
35	9	317	RRX	C15-C14-C13	-5.23	119.85	127.31
31	N	311	CLA	CMD-C2D-C1D	5.23	133.92	124.71
31	0	603	CLA	O2D-CGD-CBD	5.23	120.55	111.27
31	N	311	CLA	O2D-CGD-CBD	5.22	120.55	111.27
31	6	305	CLA	O2D-CGD-CBD	5.22	120.55	111.27
31	2	609	CLA	O2D-CGD-CBD	5.22	120.55	111.27
31	9	314	CLA	CMD-C2D-C1D	5.22	133.91	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	d	406	BCR	C12-C13-C14	5.22	126.95	118.94
31	A	407	CLA	O2D-CGD-CBD	5.22	120.54	111.27
31	C	601	CLA	O2D-CGD-CBD	5.22	120.53	111.27
31	N	305	CLA	O2D-CGD-CBD	5.21	120.53	111.27
31	S	304	CLA	O2D-CGD-CBD	5.21	120.53	111.27
35	g	315	RRX	C30-C25-C26	-5.21	115.27	122.61
43	z	101	BCR	C7-C8-C9	-5.21	118.36	126.23
36	q	319	NEX	C27-C28-C29	-5.21	117.44	125.53
31	3	314	CLA	O2D-CGD-CBD	5.21	120.53	111.27
31	p	612	CLA	O2D-CGD-CBD	5.21	120.53	111.27
31	C	603	CLA	O2D-CGD-CBD	5.21	120.52	111.27
31	6	304	CLA	O2D-CGD-CBD	5.21	120.52	111.27
46	d	403	BCT	O2-C-O1	5.20	133.04	119.55
32	4	616	LUT	C15-C14-C13	-5.20	119.89	127.31
43	b	619	BCR	C15-C14-C13	-5.20	119.89	127.31
31	B	611	CLA	O2A-C1-C2	5.20	122.29	108.64
43	C	614	BCR	C27-C26-C25	-5.20	115.19	122.73
31	8	611	CLA	O2D-CGD-CBD	5.20	120.50	111.27
31	r	307	CLA	O2D-CGD-CBD	5.20	120.50	111.27
31	Y	313	CLA	CMD-C2D-C1D	5.20	133.87	124.71
32	G	615	LUT	C35-C15-C14	-5.20	112.83	123.47
31	8	604	CLA	O2D-CGD-CBD	5.20	120.50	111.27
31	1	602	CLA	CMD-C2D-C1D	5.19	133.87	124.71
31	b	613	CLA	O2D-CGD-CBD	5.19	120.48	111.27
31	b	613	CLA	CMD-C2D-C1D	5.18	133.85	124.71
31	2	613	CLA	O2D-CGD-CBD	5.18	120.48	111.27
31	r	307	CLA	CMD-C2D-C1D	5.18	133.85	124.71
43	C	614	BCR	C15-C14-C13	-5.18	119.92	127.31
31	d	405	CLA	O2A-C1-C2	5.18	122.25	108.64
31	c	613	CLA	O2D-CGD-CBD	5.18	120.47	111.27
32	N	317	LUT	C7-C8-C9	-5.18	118.41	126.23
31	B	607	CLA	O2D-CGD-CBD	5.18	120.47	111.27
31	c	603	CLA	C1-C2-C3	-5.18	117.09	126.04
31	0	613	CLA	O2D-CGD-CBD	5.18	120.47	111.27
31	0	612	CLA	O2D-CGD-CBD	5.18	120.46	111.27
31	C	602	CLA	O2A-C1-C2	5.17	122.23	108.64
31	6	312	CLA	O2D-CGD-CBD	5.17	120.46	111.27
31	b	615	CLA	O2A-C1-C2	5.17	122.23	108.64
32	s	317	LUT	C35-C34-C33	-5.17	119.93	127.31
31	s	315	CLA	O2D-CGD-CBD	5.17	120.46	111.27
31	5	611	CLA	CMD-C2D-C1D	5.17	133.82	124.71
31	B	609	CLA	O2D-CGD-CBD	5.17	120.45	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	313	CLA	O2D-CGD-CBD	5.17	120.45	111.27
31	B	601	CLA	O2A-C1-C2	5.17	121.06	108.97
37	2	619	XAT	C15-C14-C13	-5.17	119.94	127.31
31	Y	303	CLA	O2D-CGD-CBD	5.17	120.45	111.27
31	5	610	CLA	O2D-CGD-CBD	5.16	120.44	111.27
35	2	614	RRX	C15-C14-C13	-5.16	119.94	127.31
31	5	612	CLA	O2D-CGD-CBD	5.16	120.44	111.27
31	q	316	CLA	O2A-C1-C2	5.16	122.20	108.64
31	b	602	CLA	O2A-C1-C2	5.16	121.04	108.97
31	3	301	CLA	CMD-C2D-C1D	5.16	133.81	124.71
31	r	303	CLA	CMD-C2D-C1D	5.16	133.81	124.71
31	y	612	CLA	CMD-C2D-C1D	5.16	133.81	124.71
31	c	606	CLA	O2D-CGD-CBD	5.16	120.43	111.27
31	s	312	CLA	O2A-C1-C2	5.16	122.19	108.64
31	9	306	CLA	O2D-CGD-CBD	5.16	120.43	111.27
31	b	617	CLA	O2A-C1-C2	5.16	122.18	108.64
31	3	312	CLA	O2D-CGD-CBD	5.15	120.43	111.27
37	4	619	XAT	C15-C14-C13	-5.15	119.95	127.31
36	R	319	NEX	C38-C25-C24	5.15	120.08	114.28
31	b	605	CLA	CMD-C2D-C1D	5.15	133.79	124.71
31	q	305	CLA	O2D-CGD-CBD	5.15	120.42	111.27
31	S	316	CLA	O2D-CGD-CBD	5.15	120.42	111.27
37	G	620	XAT	C15-C14-C13	-5.15	119.96	127.31
31	b	611	CLA	O2D-CGD-CBD	5.15	120.42	111.27
31	p	602	CLA	CMD-C2D-C1D	5.15	133.78	124.71
31	s	311	CLA	O2A-C1-C2	5.15	122.16	108.64
31	C	604	CLA	O2A-C1-C2	5.15	122.16	108.64
31	B	608	CLA	O2D-CGD-CBD	5.14	120.41	111.27
32	6	317	LUT	C35-C34-C33	-5.14	119.97	127.31
37	g	321	XAT	C15-C14-C13	-5.14	119.97	127.31
31	C	609	CLA	O2D-CGD-CBD	5.14	120.41	111.27
31	C	611	CLA	O2A-C1-C2	5.14	122.15	108.64
31	a	407	CLA	CMD-C2D-C1D	5.14	133.78	124.71
37	q	321	XAT	C15-C14-C13	-5.14	119.97	127.31
31	Y	311	CLA	O2D-CGD-CBD	5.14	120.40	111.27
31	q	313	CLA	CMD-C2D-C1D	5.14	133.77	124.71
35	G	614	RRX	C11-C10-C9	-5.13	119.98	127.31
43	t	101	BCR	C38-C26-C25	-5.13	118.76	124.53
31	3	306	CLA	O2D-CGD-CBD	5.13	120.39	111.27
31	r	303	CLA	O2A-C1-C2	5.13	120.97	108.97
31	3	315	CLA	O2D-CGD-CBD	5.13	120.39	111.27
31	S	313	CLA	O2A-C1-C2	5.13	122.11	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	610	CLA	O2A-C1-C2	5.13	122.11	108.64
31	c	603	CLA	O2A-C1-C2	5.13	122.11	108.64
31	c	608	CLA	CMD-C2D-C1D	5.13	133.75	124.71
31	c	613	CLA	CMD-C2D-C1D	5.13	133.75	124.71
31	n	305	CLA	O2D-CGD-CBD	5.13	120.38	111.27
31	0	604	CLA	O2A-C1-C2	5.12	122.10	108.64
31	n	312	CLA	O2D-CGD-CBD	5.12	120.37	111.27
31	c	611	CLA	O2A-C1-C2	5.12	122.10	108.64
31	1	612	CLA	O2D-CGD-CBD	5.12	120.37	111.27
35	9	317	RRX	C11-C10-C9	-5.12	120.00	127.31
37	9	322	XAT	C15-C14-C13	-5.12	120.00	127.31
32	2	615	LUT	C32-C33-C34	5.12	126.80	118.94
31	c	610	CLA	O2D-CGD-CBD	5.12	120.36	111.27
31	1	603	CLA	CMD-C2D-C1D	5.12	133.73	124.71
31	8	610	CLA	O2D-CGD-CBD	5.11	120.36	111.27
44	a	414	PL9	C7-C3-C4	5.11	121.03	116.88
31	C	609	CLA	CMD-C2D-C1D	5.11	133.72	124.71
31	y	603	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	G	613	CLA	O2A-C1-C2	5.11	120.92	108.97
43	C	615	BCR	C16-C17-C18	-5.11	120.02	127.31
31	Y	304	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	c	601	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	y	614	CLA	O2D-CGD-CBD	5.11	120.35	111.27
31	Y	313	CLA	O2D-CGD-CBD	5.11	120.35	111.27
32	p	616	LUT	C11-C10-C9	-5.11	120.02	127.31
31	y	604	CLA	O2D-CGD-CBD	5.11	120.34	111.27
32	9	318	LUT	C35-C34-C33	-5.11	120.02	127.31
32	p	616	LUT	C28-C29-C30	5.11	126.78	118.94
31	G	609	CLA	O2D-CGD-CBD	5.11	120.34	111.27
36	8	617	NEX	C38-C25-C24	5.11	120.02	114.28
31	8	610	CLA	CMD-C2D-C1D	5.10	133.71	124.71
31	B	603	CLA	O2D-CGD-CBD	5.10	120.33	111.27
31	0	611	CLA	O2D-CGD-CBD	5.10	120.33	111.27
43	c	614	BCR	C33-C5-C6	-5.10	118.80	124.53
31	B	612	CLA	CMD-C2D-C1D	5.10	133.70	124.71
31	b	612	CLA	O2D-CGD-CBD	5.10	120.33	111.27
31	5	611	CLA	O2D-CGD-CBD	5.10	120.33	111.27
31	C	603	CLA	O2A-C1-C2	5.10	122.03	108.64
31	S	312	CLA	O2D-CGD-CBD	5.10	120.33	111.27
35	4	615	RRX	C11-C10-C9	-5.10	120.04	127.31
31	p	611	CLA	CMD-C2D-C1D	5.09	133.69	124.71
31	C	613	CLA	CMD-C2D-C1D	5.09	133.69	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	312	CLA	CMD-C2D-C1D	5.09	133.69	124.71
31	N	312	CLA	O2D-CGD-CBD	5.09	120.31	111.27
31	n	312	CLA	CMD-C2D-C1D	5.09	133.68	124.71
31	6	311	CLA	O2D-CGD-CBD	5.08	120.30	111.27
31	Y	305	CLA	O2D-CGD-CBD	5.08	120.30	111.27
36	r	301	NEX	C38-C25-C24	5.08	120.00	114.28
31	Y	303	CLA	O2A-C1-C2	5.08	121.98	108.64
31	y	612	CLA	O2A-C1-C2	5.08	121.98	108.64
32	q	318	LUT	C11-C10-C9	-5.08	120.07	127.31
31	b	610	CLA	CMD-C2D-C1D	5.08	133.66	124.71
43	z	101	BCR	C33-C5-C6	-5.08	118.83	124.53
43	h	101	BCR	C7-C8-C9	-5.07	118.57	126.23
31	7	314	CLA	O2D-CGD-CBD	5.07	120.28	111.27
31	A	405	CLA	O2A-C1-C2	5.07	121.96	108.64
31	4	604	CLA	O2D-CGD-CBD	5.07	120.28	111.27
31	s	303	CLA	O2D-CGD-CBD	5.07	120.27	111.27
36	r	319	NEX	C38-C25-C24	5.07	119.98	114.28
31	n	315	CLA	O2A-C1-C2	5.07	120.82	108.97
31	4	614	CLA	O2D-CGD-CBD	5.06	120.27	111.27
31	N	314	CLA	CMD-C2D-C1D	5.06	133.64	124.71
31	C	608	CLA	CMD-C2D-C1D	5.06	133.64	124.71
32	R	317	LUT	C39-C29-C30	-5.06	115.83	122.92
31	1	603	CLA	O2D-CGD-CBD	5.06	120.27	111.27
31	G	602	CLA	O2D-CGD-CBD	5.06	120.27	111.27
31	0	602	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	4	603	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	y	611	CLA	O2D-CGD-CBD	5.06	120.26	111.27
31	R	305	CLA	CMD-C2D-C1D	5.06	133.63	124.71
31	S	311	CLA	O2A-C1-C2	5.06	121.93	108.64
31	c	602	CLA	CMD-C2D-C1D	5.06	133.63	124.71
31	y	602	CLA	O2D-CGD-CBD	5.06	120.25	111.27
31	b	604	CLA	O2D-CGD-CBD	5.06	120.25	111.27
31	2	604	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	6	315	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	3	304	CLA	O2A-C1-C2	5.05	121.92	108.64
31	1	611	CLA	O2D-CGD-CBD	5.05	120.25	111.27
31	B	611	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	N	313	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	9	306	CLA	O2A-C1-C2	5.05	121.90	108.64
32	q	318	LUT	C7-C8-C9	-5.05	118.61	126.23
31	5	604	CLA	O2D-CGD-CBD	5.05	120.24	111.27
31	5	614	CLA	O2A-C1-C2	5.05	121.90	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	B	617	BCR	C33-C5-C6	-5.04	118.86	124.53
31	8	613	CLA	O2A-C1-C2	5.04	120.76	108.97
31	s	312	CLA	CMD-C2D-C1D	5.04	133.60	124.71
32	0	617	LUT	C7-C8-C9	-5.04	118.62	126.23
31	q	306	CLA	O2D-CGD-CBD	5.04	120.22	111.27
31	7	303	CLA	O2D-CGD-CBD	5.04	120.22	111.27
31	N	314	CLA	O2A-C1-C2	5.04	120.75	108.97
31	0	611	CLA	CMD-C2D-C1D	5.04	133.59	124.71
31	N	303	CLA	O2D-CGD-CBD	5.03	120.21	111.27
31	y	611	CLA	CMD-C2D-C1D	5.03	133.58	124.71
32	6	318	LUT	C7-C8-C9	-5.03	118.63	126.23
31	1	613	CLA	O2D-CGD-CBD	5.03	120.21	111.27
31	S	305	CLA	O2D-CGD-CBD	5.03	120.20	111.27
43	A	410	BCR	C20-C21-C22	-5.03	120.13	127.31
31	r	304	CLA	O2D-CGD-CBD	5.03	120.20	111.27
31	p	602	CLA	O2D-CGD-CBD	5.03	120.20	111.27
31	N	315	CLA	O2D-CGD-CBD	5.03	120.20	111.27
31	5	613	CLA	O2D-CGD-CBD	5.03	120.20	111.27
31	p	613	CLA	CMD-C2D-C1D	5.02	133.57	124.71
31	R	304	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	S	311	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	c	611	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	y	602	CLA	O2A-C1-C2	5.02	121.83	108.64
31	n	303	CLA	O2D-CGD-CBD	5.02	120.19	111.27
43	c	615	BCR	C33-C5-C6	-5.02	118.89	124.53
31	3	301	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	8	612	CLA	O2D-CGD-CBD	5.02	120.19	111.27
31	B	607	CLA	CMD-C2D-C1D	5.02	133.56	124.71
31	R	314	CLA	O2A-C1-C2	5.02	120.70	108.97
31	B	614	CLA	O2D-CGD-CBD	5.01	120.18	111.27
31	s	316	CLA	O2D-CGD-CBD	5.01	120.17	111.27
31	n	314	CLA	O2D-CGD-CBD	5.01	120.17	111.27
43	t	101	BCR	C20-C19-C18	-5.00	112.36	126.42
31	b	608	CLA	O2D-CGD-CBD	5.00	120.16	111.27
37	9	322	XAT	C38-C25-C24	5.00	119.91	114.28
37	g	321	XAT	C38-C25-C24	5.00	119.90	114.28
43	C	614	BCR	C33-C5-C6	-5.00	118.92	124.53
31	b	609	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	7	304	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	R	311	CLA	O2D-CGD-CBD	4.99	120.14	111.27
31	3	315	CLA	O2A-C1-C2	4.99	121.75	108.64
31	b	608	CLA	O2A-C1-C2	4.99	121.75	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	6	303	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	4	610	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	s	305	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	1	610	CLA	O2D-CGD-CBD	4.99	120.13	111.27
31	p	611	CLA	O2D-CGD-CBD	4.99	120.13	111.27
37	2	619	XAT	C38-C25-C24	4.99	119.89	114.28
37	G	620	XAT	C38-C25-C24	4.99	119.89	114.28
31	G	609	CLA	O2A-C1-C2	4.98	121.74	108.64
43	b	618	BCR	C16-C17-C18	-4.98	120.20	127.31
31	9	316	CLA	O2D-CGD-CBD	4.98	120.12	111.27
31	g	304	CLA	O2D-CGD-CBD	4.98	120.12	111.27
31	6	312	CLA	CMD-C2D-C1D	4.98	133.49	124.71
43	h	101	BCR	C24-C23-C22	-4.98	118.71	126.23
31	S	303	CLA	O2D-CGD-CBD	4.98	120.12	111.27
43	Z	101	BCR	C33-C5-C6	-4.98	118.94	124.53
31	p	614	CLA	O2D-CGD-CBD	4.98	120.11	111.27
32	S	317	LUT	C35-C34-C33	-4.98	120.21	127.31
31	s	304	CLA	O2D-CGD-CBD	4.98	120.11	111.27
31	b	612	CLA	O2A-C1-C2	4.98	121.71	108.64
31	D	403	CLA	O2D-CGD-CBD	4.98	120.11	111.27
37	4	619	XAT	C38-C25-C24	4.97	119.88	114.28
31	N	310	CLA	O2A-C1-C2	4.97	121.70	108.64
31	7	312	CLA	O2D-CGD-CBD	4.97	120.10	111.27
31	Y	314	CLA	O2A-C1-C2	4.97	121.70	108.64
43	c	615	BCR	C38-C26-C25	-4.96	118.95	124.53
31	0	610	CLA	O2D-CGD-CBD	4.96	120.09	111.27
31	C	601	CLA	O2A-C1-C2	4.96	121.68	108.64
31	6	316	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	S	306	CLA	O2A-C1-C2	4.96	121.67	108.64
35	g	315	RRX	C38-C26-C25	-4.96	118.96	124.53
31	8	604	CLA	O2A-C1-C2	4.96	121.67	108.64
37	q	321	XAT	C38-C25-C24	4.96	119.86	114.28
31	g	310	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	n	316	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	9	305	CLA	O2D-CGD-CBD	4.96	120.08	111.27
31	1	612	CLA	O2A-C1-C2	4.96	121.66	108.64
31	5	613	CLA	O2A-C1-C2	4.96	121.66	108.64
32	q	318	LUT	C15-C14-C13	-4.95	120.24	127.31
35	q	317	RRX	C16-C17-C18	-4.95	120.24	127.31
31	r	313	CLA	CMD-C2D-C1D	4.95	133.44	124.71
36	g	317	NEX	C38-C25-C24	4.95	119.85	114.28
32	5	616	LUT	C35-C34-C33	-4.95	120.24	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	613	CLA	CMD-C2D-C1D	4.95	133.43	124.71
31	8	602	CLA	O2D-CGD-CBD	4.95	120.06	111.27
31	p	610	CLA	O2D-CGD-CBD	4.94	120.05	111.27
31	c	612	CLA	O2A-C1-C2	4.94	121.62	108.64
32	g	316	LUT	C15-C14-C13	-4.94	120.26	127.31
31	0	611	CLA	O2A-C1-C2	4.94	121.61	108.64
31	4	611	CLA	O2D-CGD-CBD	4.94	120.04	111.27
32	0	616	LUT	C35-C34-C33	-4.94	120.26	127.31
31	G	604	CLA	O2D-CGD-CBD	4.94	120.04	111.27
31	4	604	CLA	C1-C2-C3	-4.94	117.51	126.04
31	G	610	CLA	O2D-CGD-CBD	4.94	120.04	111.27
32	4	616	LUT	C7-C8-C9	-4.94	118.78	126.23
31	C	608	CLA	O2D-CGD-CBD	4.93	120.04	111.27
32	y	616	LUT	C21-C26-C27	-4.93	106.46	112.70
31	p	614	CLA	O2A-C1-C2	4.93	121.60	108.64
31	n	304	CLA	O2D-CGD-CBD	4.93	120.03	111.27
31	G	612	CLA	O2D-CGD-CBD	4.93	120.02	111.27
31	R	313	CLA	CMD-C2D-C1D	4.93	133.40	124.71
36	r	319	NEX	C27-C28-C29	-4.93	117.89	125.53
31	N	304	CLA	O2D-CGD-CBD	4.93	120.02	111.27
31	n	305	CLA	O2A-C1-C2	4.93	121.58	108.64
31	N	315	CLA	O2A-C1-C2	4.92	121.57	108.64
31	A	405	CLA	C1-C2-C3	-4.92	117.53	126.04
31	B	616	CLA	CMD-C2D-C1D	4.92	133.38	124.71
31	N	305	CLA	O2A-C1-C2	4.92	121.56	108.64
43	a	410	BCR	C38-C26-C25	-4.92	119.01	124.53
32	3	317	LUT	C35-C34-C33	-4.91	120.30	127.31
31	9	304	CLA	O2D-CGD-CBD	4.91	120.00	111.27
36	6	319	NEX	C38-C25-C24	4.91	119.81	114.28
31	9	305	CLA	O2A-C1-C2	4.91	121.54	108.64
31	G	610	CLA	CMD-C2D-C1D	4.91	133.37	124.71
31	g	311	CLA	CMD-C2D-C1D	4.91	133.37	124.71
36	4	617	NEX	C38-C25-C24	4.91	119.80	114.28
31	A	406	CLA	O2A-C1-C2	4.91	121.53	108.64
31	5	603	CLA	O2D-CGD-CBD	4.91	119.99	111.27
31	S	306	CLA	O2D-CGD-CBD	4.91	119.99	111.27
31	b	616	CLA	O2A-C1-C2	4.91	121.53	108.64
43	V	101	BCR	C38-C26-C25	-4.90	119.02	124.53
31	D	403	CLA	O2A-C1-C2	4.90	121.52	108.64
31	N	310	CLA	O2D-CGD-CBD	4.90	119.98	111.27
31	r	312	CLA	O2D-CGD-CBD	4.90	119.98	111.27
31	C	613	CLA	O2D-CGD-CBD	4.90	119.98	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	307	CLA	CMD-C2D-C1D	4.90	133.34	124.71
31	2	610	CLA	O2D-CGD-CBD	4.90	119.97	111.27
31	8	609	CLA	O2D-CGD-CBD	4.89	119.97	111.27
31	g	305	CLA	O2D-CGD-CBD	4.89	119.97	111.27
32	s	318	LUT	C35-C34-C33	-4.89	120.33	127.31
31	g	313	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	3	313	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	d	404	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	0	603	CLA	O2A-C1-C2	4.89	121.49	108.64
31	g	312	CLA	O2D-CGD-CBD	4.89	119.96	111.27
31	3	312	CLA	CMD-C2D-C1D	4.89	133.33	124.71
31	9	315	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	0	615	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	3	304	CLA	O2D-CGD-CBD	4.89	119.95	111.27
31	b	606	CLA	O2A-C1-C2	4.89	121.47	108.64
31	b	610	CLA	O2A-C1-C2	4.88	121.47	108.64
31	2	613	CLA	O2A-C1-C2	4.88	121.47	108.64
31	4	613	CLA	O2D-CGD-CBD	4.88	119.94	111.27
43	B	619	BCR	C38-C26-C25	-4.88	119.05	124.53
31	5	612	CLA	O2A-C1-C2	4.88	121.46	108.64
31	q	316	CLA	O2D-CGD-CBD	4.88	119.94	111.27
36	0	618	NEX	C38-C25-C24	4.88	119.77	114.28
31	4	613	CLA	O2A-C1-C2	4.88	121.45	108.64
31	b	615	CLA	O2D-CGD-CBD	4.88	119.93	111.27
31	N	321	CLA	O2A-C1-C2	4.88	121.45	108.64
31	s	305	CLA	O2A-C1-C2	4.88	121.45	108.64
31	p	604	CLA	O2A-C1-C2	4.88	121.45	108.64
31	s	310	CLA	O2D-CGD-CBD	4.88	119.93	111.27
31	7	312	CLA	O2A-C1-C2	4.87	121.44	108.64
31	b	609	CLA	CMD-C2D-C1D	4.87	133.30	124.71
31	R	315	CLA	O2A-C1-C2	4.87	121.44	108.64
43	b	620	BCR	C15-C14-C13	-4.87	120.36	127.31
31	a	407	CLA	O2D-CGD-CBD	4.87	119.92	111.27
31	B	610	CLA	O2A-C1-C2	4.87	121.42	108.64
31	c	601	CLA	O2A-C1-C2	4.86	121.42	108.64
31	y	615	CLA	O2A-C1-C2	4.86	121.41	108.64
31	s	313	CLA	C1-C2-C3	-4.86	117.64	126.04
31	s	314	CLA	O2A-C1-C2	4.86	121.40	108.64
43	A	410	BCR	C33-C5-C6	-4.86	119.07	124.53
31	R	312	CLA	O2D-CGD-CBD	4.86	119.90	111.27
31	3	301	CLA	C1-C2-C3	-4.85	117.65	126.04
31	8	614	CLA	O2D-CGD-CBD	4.85	119.89	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	0	614	CLA	O2D-CGD-CBD	4.85	119.89	111.27
31	y	613	CLA	CMD-C2D-C1D	4.85	133.26	124.71
31	R	314	CLA	O2D-CGD-CBD	4.85	119.88	111.27
31	6	314	CLA	O2D-CGD-CBD	4.84	119.87	111.27
31	n	311	CLA	O2A-C1-C2	4.84	121.36	108.64
31	y	604	CLA	O2A-C1-C2	4.84	121.36	108.64
31	r	313	CLA	O2D-CGD-CBD	4.84	119.87	111.27
31	3	305	CLA	O2D-CGD-CBD	4.84	119.87	111.27
43	a	410	BCR	C15-C14-C13	-4.84	120.40	127.31
32	4	616	LUT	C35-C34-C33	-4.84	120.40	127.31
31	7	315	CLA	O2D-CGD-CBD	4.84	119.86	111.27
32	6	318	LUT	C35-C34-C33	-4.83	120.41	127.31
32	N	317	LUT	C15-C14-C13	-4.83	120.41	127.31
31	C	606	CLA	O2A-C1-C2	4.83	121.33	108.64
31	4	602	CLA	O2D-CGD-CBD	4.83	119.85	111.27
37	g	321	XAT	C31-C30-C29	-4.83	120.42	127.31
31	S	310	CLA	O2D-CGD-CBD	4.83	119.85	111.27
36	8	617	NEX	C27-C28-C29	-4.83	118.04	125.53
31	B	605	CLA	O2A-C1-C2	4.83	121.32	108.64
31	n	311	CLA	O2D-CGD-CBD	4.82	119.84	111.27
31	1	614	CLA	O2D-CGD-CBD	4.82	119.84	111.27
31	c	608	CLA	O2D-CGD-CBD	4.82	119.84	111.27
37	G	620	XAT	C31-C30-C29	-4.82	120.43	127.31
32	9	318	LUT	C11-C10-C9	-4.82	120.44	127.31
34	m	102	LMG	O7-C10-C11	4.82	121.88	111.50
31	8	603	CLA	O2D-CGD-CBD	4.81	119.82	111.27
31	Y	311	CLA	CMD-C2D-C1D	4.81	133.20	124.71
31	g	310	CLA	O2A-C1-C2	4.81	121.28	108.64
37	q	321	XAT	C31-C30-C29	-4.81	120.44	127.31
37	2	619	XAT	C31-C30-C29	-4.81	120.45	127.31
37	4	619	XAT	C31-C30-C29	-4.80	120.45	127.31
43	V	101	BCR	C27-C26-C25	-4.80	115.76	122.73
31	q	304	CLA	O2D-CGD-CBD	4.80	119.80	111.27
31	B	608	CLA	O2A-C1-C2	4.80	121.25	108.64
31	B	608	CLA	CMD-C2D-C1D	4.80	133.17	124.71
31	1	603	CLA	O2A-C1-C2	4.80	121.24	108.64
31	A	406	CLA	O2D-CGD-CBD	4.79	119.79	111.27
31	9	314	CLA	O2D-CGD-CBD	4.79	119.78	111.27
31	6	303	CLA	O2A-C1-C2	4.79	121.22	108.64
37	9	322	XAT	C31-C30-C29	-4.79	120.48	127.31
31	s	306	CLA	O2A-C1-C2	4.79	121.21	108.64
43	c	615	BCR	C4-C5-C6	-4.79	115.78	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	604	CLA	C1-C2-C3	-4.79	117.77	126.04
31	q	314	CLA	O2D-CGD-CBD	4.78	119.77	111.27
31	Y	305	CLA	O2A-C1-C2	4.78	121.20	108.64
31	q	315	CLA	CMD-C2D-C1D	4.78	133.14	124.71
31	y	610	CLA	O2A-C1-C2	4.78	121.20	108.64
34	9	301	LMG	C1-O6-C5	-4.78	104.30	113.69
31	C	610	CLA	O2A-C1-C2	4.78	121.20	108.64
43	C	614	BCR	C20-C21-C22	-4.78	120.49	127.31
31	Y	314	CLA	O2D-CGD-CBD	4.78	119.76	111.27
31	p	602	CLA	O2A-C1-C2	4.78	121.20	108.64
31	5	602	CLA	O2D-CGD-CBD	4.78	119.76	111.27
43	h	101	BCR	C33-C5-C6	-4.77	119.17	124.53
31	N	321	CLA	O2D-CGD-CBD	4.77	119.75	111.27
31	C	605	CLA	CMD-C2D-C1D	4.77	133.12	124.71
31	b	609	CLA	O2A-C1-C2	4.77	121.17	108.64
31	6	316	CLA	O2A-C1-C2	4.76	121.15	108.64
36	9	319	NEX	C27-C28-C29	-4.76	118.15	125.53
30	4	607	CHL	CHD-C1D-ND	-4.76	120.08	124.45
31	6	313	CLA	O2D-CGD-CBD	4.76	119.72	111.27
36	9	319	NEX	C38-C25-C24	4.76	119.63	114.28
36	g	317	NEX	C27-C28-C29	-4.76	118.15	125.53
31	n	316	CLA	O2A-C1-C2	4.76	121.14	108.64
31	a	407	CLA	O2A-C1-C2	4.75	121.13	108.64
31	q	305	CLA	O2A-C1-C2	4.75	121.12	108.64
36	R	319	NEX	C27-C28-C29	-4.75	118.16	125.53
34	w	203	LMG	O7-C10-C11	4.75	121.74	111.50
31	Y	310	CLA	O2D-CGD-CBD	4.75	119.70	111.27
31	2	603	CLA	O2D-CGD-CBD	4.75	119.70	111.27
31	s	314	CLA	O2D-CGD-CBD	4.74	119.70	111.27
43	H	101	BCR	C16-C17-C18	-4.74	120.54	127.31
43	B	617	BCR	C15-C14-C13	-4.74	120.55	127.31
31	Y	310	CLA	O2A-C1-C2	4.74	121.09	108.64
30	1	601	CHL	CHD-C1D-ND	-4.74	120.10	124.45
31	0	610	CLA	O2A-C1-C2	4.74	121.08	108.64
43	T	101	BCR	C38-C26-C25	-4.74	119.21	124.53
31	5	611	CLA	O2A-C1-C2	4.73	121.07	108.64
31	S	305	CLA	O2A-C1-C2	4.73	121.07	108.64
43	c	614	BCR	C38-C26-C25	-4.73	119.22	124.53
43	H	101	BCR	C24-C23-C22	-4.73	119.09	126.23
31	a	409	CLA	O2A-C1-C2	4.73	121.06	108.64
31	A	409	CLA	O2A-C1-C2	4.73	121.06	108.64
31	q	312	CLA	O2A-C1-C2	4.73	121.06	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	4	616	LUT	C18-C5-C6	-4.73	119.22	124.53
43	a	410	BCR	C11-C10-C9	-4.72	120.57	127.31
31	6	304	CLA	O2A-C1-C2	4.72	121.05	108.64
31	7	316	CLA	O2A-C1-C2	4.72	121.04	108.64
32	1	615	LUT	C18-C5-C6	-4.72	119.23	124.53
31	5	602	CLA	O2A-C1-C2	4.72	121.03	108.64
31	G	603	CLA	O2A-C1-C2	4.71	121.02	108.64
31	n	314	CLA	O2A-C1-C2	4.71	121.02	108.64
31	A	405	CLA	O2D-CGD-CBD	4.71	119.64	111.27
43	a	410	BCR	C33-C5-C6	-4.71	119.24	124.53
32	N	316	LUT	C18-C5-C6	-4.70	119.25	124.53
43	c	615	BCR	C27-C26-C25	-4.70	115.90	122.73
31	5	603	CLA	O2A-C1-C2	4.70	120.99	108.64
31	8	612	CLA	O2A-C1-C2	4.70	120.99	108.64
31	C	612	CLA	CMD-C2D-C1D	4.70	133.00	124.71
34	n	322	LMG	O7-C10-C11	4.70	121.63	111.50
31	c	612	CLA	CMD-C2D-C1D	4.70	133.00	124.71
31	b	604	CLA	O2A-C1-C2	4.70	120.99	108.64
31	R	313	CLA	O2D-CGD-CBD	4.70	119.61	111.27
31	b	614	CLA	O2D-CGD-CBD	4.69	119.61	111.27
31	7	311	CLA	O2D-CGD-CBD	4.69	119.61	111.27
31	n	315	CLA	O2D-CGD-CBD	4.69	119.61	111.27
35	g	315	RRX	C24-C23-C22	-4.69	119.15	126.23
31	r	314	CLA	O2D-CGD-CBD	4.69	119.60	111.27
34	b	622	LMG	O7-C10-C11	4.69	121.60	111.50
31	0	614	CLA	O2A-C1-C2	4.68	120.94	108.64
31	8	614	CLA	O2A-C1-C2	4.68	120.94	108.64
30	Y	309	CHL	CHD-C1D-ND	-4.68	120.15	124.45
31	8	609	CLA	O2A-C1-C2	4.68	120.93	108.64
31	C	606	CLA	C1-C2-C3	-4.68	117.95	126.04
31	2	612	CLA	O2D-CGD-CBD	4.67	119.57	111.27
31	3	305	CLA	O2A-C1-C2	4.67	120.91	108.64
36	g	317	NEX	C5-C4-C3	-4.67	106.22	111.75
31	4	602	CLA	O2A-C1-C2	4.67	120.91	108.64
31	r	305	CLA	O2A-C1-C2	4.67	120.91	108.64
31	2	602	CLA	O2D-CGD-CBD	4.67	119.56	111.27
32	n	317	LUT	C35-C34-C33	-4.67	120.65	127.31
31	S	303	CLA	O2A-C1-C2	4.67	120.90	108.64
31	y	614	CLA	O2A-C1-C2	4.67	120.90	108.64
31	p	611	CLA	O2A-C1-C2	4.66	120.89	108.64
34	w	205	LMG	O7-C10-C11	4.66	121.55	111.50
36	n	319	NEX	C27-C28-C29	-4.66	118.30	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	D	405	BCR	C33-C5-C6	-4.66	119.30	124.53
37	r	318	XAT	C15-C14-C13	-4.66	120.66	127.31
35	4	615	RRX	C1-C6-C5	-4.66	116.05	122.61
35	9	317	RRX	C1-C6-C5	-4.66	116.06	122.61
31	G	603	CLA	O2D-CGD-CBD	4.66	119.54	111.27
43	A	410	BCR	C11-C10-C9	-4.66	120.67	127.31
31	3	311	CLA	O2A-C1-C2	4.65	120.87	108.64
32	p	616	LUT	C30-C31-C32	-4.65	108.69	123.22
32	8	615	LUT	C35-C34-C33	-4.65	120.67	127.31
35	G	614	RRX	C1-C6-C5	-4.65	116.06	122.61
32	p	617	LUT	C35-C15-C14	-4.65	113.96	123.47
31	g	304	CLA	O2A-C1-C2	4.65	120.85	108.64
31	C	613	CLA	CAA-C2A-C3A	-4.64	100.06	112.78
37	R	318	XAT	C15-C14-C13	-4.64	120.68	127.31
31	G	610	CLA	O2A-C1-C2	4.64	120.84	108.64
36	r	301	NEX	C27-C28-C29	-4.64	118.33	125.53
31	B	613	CLA	O2A-C1-C2	4.64	120.83	108.64
31	q	304	CLA	O2A-C1-C2	4.64	120.83	108.64
43	B	618	BCR	C11-C10-C9	-4.64	120.69	127.31
31	9	312	CLA	O2D-CGD-CBD	4.64	119.51	111.27
31	7	311	CLA	O2A-C1-C2	4.63	120.81	108.64
31	8	602	CLA	O2A-C1-C2	4.63	120.81	108.64
43	b	619	BCR	C33-C5-C6	-4.63	119.33	124.53
30	6	306	CHL	CHD-C1D-ND	-4.63	120.20	124.45
30	n	310	CHL	CHD-C1D-ND	-4.63	120.20	124.45
32	8	616	LUT	C35-C34-C33	-4.63	120.70	127.31
31	3	313	CLA	O2A-C1-C2	4.63	120.80	108.64
33	z	102	LHG	O7-C7-C8	4.63	121.47	111.50
31	B	609	CLA	O2A-C1-C2	4.62	120.79	108.64
36	2	616	NEX	C27-C28-C29	-4.62	118.35	125.53
43	T	101	BCR	C20-C21-C22	-4.62	120.72	127.31
30	q	308	CHL	CHD-C1D-ND	-4.62	120.21	124.45
34	W	201	LMG	O7-C10-C11	4.62	121.46	111.50
31	B	613	CLA	O2D-CGD-CBD	4.62	119.47	111.27
32	N	316	LUT	C15-C14-C13	-4.61	120.72	127.31
35	2	614	RRX	C16-C17-C18	-4.61	120.73	127.31
31	a	406	CLA	O2D-CGD-CBD	4.61	119.46	111.27
32	n	318	LUT	C35-C34-C33	-4.61	120.73	127.31
43	C	615	BCR	C35-C13-C14	-4.61	116.47	122.92
31	4	604	CLA	O2A-C1-C2	4.61	120.75	108.64
35	q	317	RRX	C24-C23-C22	-4.61	119.27	126.23
32	6	317	LUT	C18-C5-C6	-4.61	119.36	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	B	618	BCR	C33-C5-C6	-4.60	119.36	124.53
35	g	315	RRX	C16-C17-C18	-4.60	120.74	127.31
43	D	405	BCR	C34-C9-C10	-4.60	116.48	122.92
36	y	618	NEX	C38-C25-C24	4.60	119.45	114.28
31	2	611	CLA	O2D-CGD-CBD	4.60	119.44	111.27
31	0	602	CLA	O2A-C1-C2	4.60	120.71	108.64
31	3	316	CLA	O2D-CGD-CBD	4.60	119.43	111.27
37	r	318	XAT	C18-C5-C4	4.59	119.45	114.28
34	c	620	LMG	O7-C10-C11	4.59	121.40	111.50
31	B	607	CLA	C1-C2-C3	-4.59	118.10	126.04
31	8	613	CLA	O2D-CGD-CBD	4.59	119.42	111.27
36	G	616	NEX	C38-C25-C24	4.59	119.44	114.28
31	2	610	CLA	O2A-C1-C2	4.59	120.70	108.64
31	b	611	CLA	O2A-C1-C2	4.59	120.69	108.64
31	y	610	CLA	O2D-CGD-CBD	4.59	119.42	111.27
32	2	615	LUT	C1-C6-C5	-4.59	116.15	122.61
30	0	608	CHL	CHD-C1D-ND	-4.58	120.24	124.45
32	Y	316	LUT	C7-C8-C9	-4.58	119.31	126.23
32	R	317	LUT	C18-C5-C6	-4.58	119.39	124.53
36	Y	317	NEX	C2-C1-C6	4.58	113.66	109.21
32	p	617	LUT	C32-C33-C34	4.58	125.96	118.94
31	N	313	CLA	O2A-C1-C2	4.58	120.66	108.64
31	1	611	CLA	O2A-C1-C2	4.58	120.66	108.64
35	2	614	RRX	C1-C6-C5	-4.57	116.17	122.61
32	0	617	LUT	C35-C34-C33	-4.57	120.79	127.31
31	2	604	CLA	O2A-C1-C2	4.57	120.64	108.64
33	C	623	LHG	O7-C7-C8	4.56	121.34	111.50
30	y	608	CHL	CHD-C1D-ND	-4.56	120.27	124.45
36	R	301	NEX	C27-C28-C29	-4.56	118.46	125.53
36	s	319	NEX	C38-C25-C24	4.56	119.41	114.28
30	3	302	CHL	C1-C2-C3	-4.56	118.16	126.04
34	B	621	LMG	O7-C10-C11	4.56	121.32	111.50
31	r	311	CLA	O2D-CGD-CBD	4.55	119.36	111.27
31	2	612	CLA	O2A-C1-C2	4.55	120.60	108.64
32	3	318	LUT	C1-C6-C5	-4.55	116.20	122.61
43	V	101	BCR	C24-C23-C22	-4.55	119.36	126.23
33	K	102	LHG	O7-C7-C8	4.55	121.30	111.50
30	1	605	CHL	CHD-C1D-ND	-4.54	120.28	124.45
37	g	321	XAT	C18-C5-C4	4.54	119.39	114.28
32	p	617	LUT	C28-C29-C30	4.54	125.91	118.94
30	g	307	CHL	CHD-C1D-ND	-4.54	120.28	124.45
32	7	318	LUT	C7-C8-C9	-4.54	119.37	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	t	101	BCR	C4-C5-C6	-4.54	116.14	122.73
31	8	603	CLA	O2A-C1-C2	4.54	120.56	108.64
31	n	304	CLA	O2A-C1-C2	4.54	120.56	108.64
32	7	317	LUT	C15-C14-C13	-4.53	120.84	127.31
35	G	614	RRX	C16-C17-C18	-4.53	120.84	127.31
43	D	405	BCR	C24-C23-C22	-4.53	119.39	126.23
33	a	415	LHG	O7-C7-C8	4.53	121.26	111.50
32	p	616	LUT	C18-C5-C6	-4.52	119.45	124.53
31	b	614	CLA	O2A-C1-C2	4.52	120.53	108.64
31	5	610	CLA	O2A-C1-C2	4.52	120.53	108.64
32	p	617	LUT	C11-C10-C9	-4.52	120.86	127.31
30	0	605	CHL	C1-O2A-CGA	4.52	128.30	116.44
31	6	316	CLA	C1-C2-C3	-4.52	118.22	126.04
37	G	620	XAT	C18-C5-C4	4.52	119.36	114.28
37	R	318	XAT	C18-C5-C4	4.52	119.36	114.28
37	4	619	XAT	C18-C5-C4	4.52	119.36	114.28
31	S	314	CLA	O2D-CGD-CBD	4.52	119.30	111.27
43	b	618	BCR	C7-C8-C9	-4.52	119.41	126.23
31	1	614	CLA	O2A-C1-C2	4.52	120.51	108.64
43	d	406	BCR	C11-C10-C9	4.52	133.76	127.31
43	C	614	BCR	C4-C5-C6	-4.52	116.17	122.73
35	4	615	RRX	C16-C17-C18	-4.51	120.87	127.31
31	c	606	CLA	CMD-C2D-C1D	4.51	132.66	124.71
43	t	101	BCR	C8-C9-C10	4.51	125.86	118.94
43	z	101	BCR	C20-C21-C22	-4.51	120.88	127.31
36	y	618	NEX	C27-C28-C29	-4.50	118.54	125.53
31	N	314	CLA	O2D-CGD-CBD	4.50	119.27	111.27
31	1	602	CLA	O2A-C1-C2	4.50	120.47	108.64
31	G	604	CLA	O2A-C1-C2	4.50	120.47	108.64
43	d	406	BCR	C35-C13-C14	-4.50	116.62	122.92
31	B	615	CLA	O2A-C1-C2	4.50	120.47	108.64
37	q	321	XAT	C18-C5-C4	4.50	119.34	114.28
35	g	315	RRX	C29-C28-C27	4.50	116.47	110.30
43	B	617	BCR	C7-C8-C9	-4.50	119.44	126.23
43	c	614	BCR	C7-C8-C9	-4.50	119.44	126.23
43	b	618	BCR	C15-C14-C13	-4.50	120.89	127.31
32	3	317	LUT	C18-C5-C6	-4.49	119.48	124.53
31	n	303	CLA	O2A-C1-C2	4.49	120.44	108.64
36	3	319	NEX	C38-C25-C24	4.49	119.33	114.28
37	9	322	XAT	C18-C5-C4	4.49	119.33	114.28
31	y	603	CLA	O2A-C1-C2	4.49	120.44	108.64
45	c	618	DGD	O2G-C1B-C2B	4.49	121.17	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	6	314	CLA	O2A-C1-C2	4.49	120.43	108.64
35	9	317	RRX	C16-C17-C18	-4.49	120.91	127.31
32	N	316	LUT	C11-C10-C9	-4.48	120.91	127.31
31	2	603	CLA	O2A-C1-C2	4.48	120.41	108.64
31	N	303	CLA	O2A-C1-C2	4.48	120.41	108.64
32	S	317	LUT	C18-C5-C6	-4.48	119.50	124.53
34	6	321	LMG	O7-C10-C11	4.48	121.15	111.50
31	4	603	CLA	O2A-C1-C2	4.48	120.40	108.64
36	p	618	NEX	C38-C25-C24	4.47	119.31	114.28
32	q	318	LUT	C35-C34-C33	-4.47	120.93	127.31
43	C	614	BCR	C16-C17-C18	-4.47	120.93	127.31
37	2	619	XAT	C18-C5-C4	4.47	119.31	114.28
31	7	304	CLA	O2A-C1-C2	4.47	120.37	108.64
34	g	320	LMG	O7-C10-C11	4.47	121.12	111.50
30	1	608	CHL	CHD-C1D-ND	-4.46	120.35	124.45
36	Y	317	NEX	C27-C28-C29	-4.46	118.60	125.53
31	N	304	CLA	O2A-C1-C2	4.46	120.37	108.64
31	R	316	CLA	O2A-C1-C2	4.46	120.35	108.64
31	p	610	CLA	O2A-C1-C2	4.46	120.35	108.64
32	p	617	LUT	C1-C6-C5	-4.46	116.34	122.61
35	g	315	RRX	C1-C6-C5	-4.46	116.34	122.61
31	b	613	CLA	O2A-C1-C2	4.45	120.34	108.64
31	6	311	CLA	O2A-C1-C2	4.45	120.33	108.64
31	9	314	CLA	O2A-C1-C2	4.45	120.32	108.64
32	9	318	LUT	C18-C5-C6	-4.45	119.53	124.53
30	7	309	CHL	CHD-C1D-ND	-4.45	120.37	124.45
32	4	616	LUT	C31-C30-C29	-4.43	120.98	127.31
47	E	101	HEM	CHD-C1D-ND	4.43	129.25	124.43
34	d	411	LMG	O7-C10-C11	4.43	121.06	111.50
33	t	102	LHG	O7-C7-C8	4.43	121.05	111.50
43	a	410	BCR	C36-C18-C19	4.43	125.06	118.08
34	B	622	LMG	O7-C10-C11	4.43	121.05	111.50
31	3	306	CLA	O2A-C1-C2	4.43	120.28	108.64
31	7	313	CLA	O2A-C1-C2	4.43	120.27	108.64
43	B	617	BCR	C11-C10-C9	-4.42	121.00	127.31
43	z	101	BCR	C15-C14-C13	-4.42	121.00	127.31
36	S	319	NEX	C27-C28-C29	-4.42	118.67	125.53
31	s	305	CLA	C1-C2-C3	-4.42	118.40	126.04
30	7	307	CHL	CHD-C1D-ND	-4.42	120.39	124.45
36	R	301	NEX	C38-C25-C24	4.42	119.25	114.28
31	2	602	CLA	O2A-C1-C2	4.41	120.24	108.64
31	q	306	CLA	O2A-C1-C2	4.41	120.24	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	304	CLA	O2A-C1-C2	4.41	120.23	108.64
32	7	318	LUT	C35-C34-C33	-4.41	121.01	127.31
34	C	621	LMG	O7-C10-C11	4.41	121.01	111.50
30	7	302	CHL	CHD-C1D-ND	-4.41	120.40	124.45
36	n	319	NEX	C38-C25-C24	4.41	119.24	114.28
32	1	616	LUT	C35-C34-C33	-4.41	121.02	127.31
31	0	613	CLA	O2A-C1-C2	4.41	120.21	108.64
31	G	612	CLA	O2A-C1-C2	4.40	120.21	108.64
36	Y	317	NEX	C38-C25-C24	4.40	119.23	114.28
30	Y	307	CHL	CHD-C1D-ND	-4.40	120.41	124.45
31	Y	304	CLA	O2A-C1-C2	4.40	120.20	108.64
34	G	622	LMG	O7-C10-C11	4.40	120.98	111.50
32	S	318	LUT	C22-C23-C24	4.40	116.75	111.74
32	y	617	LUT	C18-C5-C6	-4.40	119.59	124.53
30	9	309	CHL	CHD-C1D-ND	-4.40	120.42	124.45
30	0	601	CHL	CHD-C1D-ND	-4.39	120.42	124.45
31	7	315	CLA	O2A-C1-C2	4.39	120.18	108.64
31	c	608	CLA	O2A-C1-C2	4.39	120.17	108.64
32	p	616	LUT	C40-C33-C34	-4.38	116.78	122.92
31	c	606	CLA	O2A-C1-C2	4.38	120.15	108.64
43	h	101	BCR	C20-C21-C22	-4.38	121.06	127.31
32	9	318	LUT	C7-C8-C9	-4.38	119.62	126.23
34	9	301	LMG	C8-O7-C10	-4.38	107.01	117.79
36	N	318	NEX	C38-C25-C24	4.38	119.20	114.28
30	s	307	CHL	CHD-C1D-ND	-4.38	120.43	124.45
35	2	614	RRX	C38-C26-C25	-4.38	119.61	124.53
30	g	309	CHL	CHD-C1D-ND	-4.37	120.44	124.45
31	s	303	CLA	O2A-C1-C2	4.37	120.13	108.64
33	3	320	LHG	O7-C7-C8	4.37	120.92	111.50
43	B	619	BCR	C24-C23-C22	-4.37	119.63	126.23
31	g	303	CLA	O2D-CGD-CBD	4.37	119.03	111.27
30	3	303	CHL	CHD-C1D-ND	-4.37	120.44	124.45
31	6	305	CLA	O2A-C1-C2	4.37	120.11	108.64
32	2	615	LUT	C40-C33-C34	-4.36	116.81	122.92
30	N	309	CHL	CHD-C1D-ND	-4.36	120.44	124.45
47	e	102	HEM	CHD-C1D-ND	4.36	129.17	124.43
32	s	317	LUT	C18-C5-C6	-4.36	119.64	124.53
43	V	101	BCR	C20-C21-C22	-4.36	121.09	127.31
43	h	101	BCR	C16-C17-C18	-4.35	121.09	127.31
35	g	315	RRX	C4-C5-C6	-4.35	116.41	122.73
31	5	604	CLA	O2A-C1-C2	4.35	120.08	108.64
31	B	612	CLA	O2A-C1-C2	4.35	120.07	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	311	CLA	O2A-C1-C2	4.35	120.07	108.64
30	2	607	CHL	CHD-C1D-ND	-4.35	120.46	124.45
30	9	308	CHL	CHD-C1D-ND	-4.35	120.46	124.45
30	8	608	CHL	CHD-C1D-ND	-4.35	120.46	124.45
35	G	614	RRX	C38-C26-C25	-4.34	119.65	124.53
31	R	305	CLA	C1-C2-C3	-4.34	118.54	126.04
32	p	617	LUT	C30-C31-C32	-4.34	109.67	123.22
30	p	609	CHL	CHD-C1D-ND	-4.34	120.47	124.45
35	9	317	RRX	C38-C26-C25	-4.34	119.66	124.53
30	y	609	CHL	CHD-C1D-ND	-4.34	120.47	124.45
31	S	313	CLA	C1-C2-C3	-4.34	118.55	126.04
35	4	615	RRX	C38-C26-C25	-4.33	119.67	124.53
34	b	624	LMG	O7-C10-C11	4.33	120.83	111.50
30	0	605	CHL	CHD-C1D-ND	-4.33	120.47	124.45
43	b	620	BCR	C16-C17-C18	-4.33	121.13	127.31
30	p	607	CHL	CHD-C1D-ND	-4.32	120.48	124.45
32	n	318	LUT	C7-C8-C9	-4.32	119.70	126.23
30	r	308	CHL	CHD-C1D-ND	-4.32	120.48	124.45
31	7	303	CLA	O2A-C1-C2	4.32	119.98	108.64
31	g	303	CLA	O2A-C1-C2	4.32	119.98	108.64
36	N	318	NEX	C27-C28-C29	-4.32	118.83	125.53
31	3	316	CLA	O2A-C1-C2	4.31	119.97	108.64
32	q	318	LUT	C1-C6-C5	-4.31	116.54	122.61
31	g	305	CLA	O2A-C1-C2	4.31	119.96	108.64
31	1	613	CLA	O2A-C1-C2	4.31	119.95	108.64
32	5	617	LUT	C18-C5-C6	-4.30	119.69	124.53
34	9	301	LMG	O1-C7-C8	-4.30	100.51	110.90
36	s	319	NEX	C17-C1-C6	-4.30	106.62	110.47
34	a	413	LMG	O7-C10-C11	4.30	120.77	111.50
34	W	203	LMG	O7-C10-C11	4.30	120.77	111.50
43	b	620	BCR	C33-C5-C6	-4.30	119.70	124.53
30	S	307	CHL	CHD-C1D-ND	-4.30	120.50	124.45
35	2	614	RRX	C33-C5-C6	-4.30	119.70	124.53
32	y	617	LUT	C35-C34-C33	-4.30	121.17	127.31
30	5	606	CHL	CHD-C1D-ND	-4.30	120.50	124.45
30	4	608	CHL	CHD-C1D-ND	-4.30	120.50	124.45
30	1	609	CHL	CHD-C1D-ND	-4.29	120.51	124.45
43	A	410	BCR	C27-C26-C25	-4.29	116.50	122.73
36	G	616	NEX	C27-C28-C29	-4.29	118.87	125.53
30	N	307	CHL	CHD-C1D-ND	-4.29	120.51	124.45
31	S	314	CLA	O2A-C1-C2	4.29	119.91	108.64
32	Y	316	LUT	C15-C14-C13	-4.29	121.19	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	2	614	RRX	C4-C5-C6	-4.29	116.50	122.73
30	n	309	CHL	CHD-C1D-ND	-4.29	120.52	124.45
32	8	616	LUT	C7-C8-C9	-4.29	119.76	126.23
34	q	302	LMG	O7-C10-C11	4.28	120.73	111.50
43	Z	101	BCR	C20-C21-C22	-4.28	121.20	127.31
32	3	318	LUT	C18-C5-C6	-4.28	119.72	124.53
31	2	611	CLA	O2A-C1-C2	4.28	119.88	108.64
30	Y	308	CHL	CHD-C1D-ND	-4.28	120.52	124.45
30	5	609	CHL	CHD-C1D-ND	-4.28	120.52	124.45
32	G	615	LUT	C18-C5-C6	-4.28	119.73	124.53
45	c	619	DGD	O2G-C1B-C2B	4.27	120.71	111.50
30	7	310	CHL	CHD-C1D-ND	-4.27	120.53	124.45
30	n	307	CHL	CHD-C1D-ND	-4.27	120.53	124.45
31	6	313	CLA	O2A-C1-C2	4.27	119.85	108.64
33	9	320	LHG	O7-C7-C8	4.27	120.70	111.50
30	0	609	CHL	CHD-C1D-ND	-4.27	120.53	124.45
30	8	607	CHL	CHD-C1D-ND	-4.26	120.54	124.45
30	R	308	CHL	CHD-C1D-ND	-4.26	120.54	124.45
30	N	302	CHL	CHD-C1D-ND	-4.26	120.54	124.45
43	C	615	BCR	C16-C15-C14	4.26	132.20	123.47
34	S	321	LMG	O7-C10-C11	4.26	120.68	111.50
32	3	318	LUT	C7-C8-C9	-4.26	119.80	126.23
33	R	320	LHG	O7-C7-C8	4.26	120.67	111.50
34	w	202	LMG	O7-C10-C11	4.25	120.67	111.50
36	S	319	NEX	C38-C25-C24	4.25	119.06	114.28
31	Y	313	CLA	O2A-C1-C2	4.25	119.80	108.64
33	s	322	LHG	O7-C7-C8	4.25	120.66	111.50
34	b	601	LMG	O7-C10-C11	4.25	120.65	111.50
34	2	618	LMG	O7-C10-C11	4.24	120.65	111.50
31	Y	303	CLA	C1-C2-C3	-4.24	118.70	126.04
30	5	601	CHL	CHD-C1D-ND	-4.24	120.56	124.45
35	q	317	RRX	C4-C5-C6	-4.24	116.57	122.73
43	c	615	BCR	C16-C17-C18	-4.24	121.26	127.31
30	1	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
32	7	317	LUT	C35-C34-C33	-4.24	121.26	127.31
30	2	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
30	G	608	CHL	CHD-C1D-ND	-4.24	120.56	124.45
43	B	617	BCR	C23-C24-C25	-4.24	115.30	127.20
30	p	606	CHL	CHD-C1D-ND	-4.24	120.56	124.45
30	6	308	CHL	CHD-C1D-ND	-4.24	120.56	124.45
31	r	304	CLA	O2A-C1-C2	4.23	119.76	108.64
30	8	606	CHL	CHD-C1D-ND	-4.23	120.56	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	613	CLA	O2A-C1-C2	4.23	119.76	108.64
31	3	314	CLA	O2A-C1-C2	4.23	119.75	108.64
32	p	617	LUT	C40-C33-C34	-4.22	117.00	122.92
32	p	616	LUT	C35-C15-C14	-4.22	114.82	123.47
34	f	101	LMG	O7-C10-C11	4.22	120.60	111.50
36	s	319	NEX	C27-C28-C29	-4.22	118.99	125.53
31	0	615	CLA	O2A-C1-C2	4.22	119.72	108.64
30	4	609	CHL	CHD-C1D-ND	-4.21	120.58	124.45
30	5	608	CHL	CHD-C1D-ND	-4.21	120.58	124.45
30	6	309	CHL	CHD-C1D-ND	-4.21	120.58	124.45
34	I	101	LMG	O7-C10-C11	4.21	120.57	111.50
31	2	609	CLA	O2A-C1-C2	4.21	119.69	108.64
43	V	101	BCR	C30-C25-C26	-4.21	116.69	122.61
32	p	616	LUT	C39-C29-C30	-4.21	117.03	122.92
30	8	605	CHL	CHD-C1D-ND	-4.20	120.59	124.45
32	1	616	LUT	C7-C8-C9	-4.20	119.89	126.23
31	7	312	CLA	C1-C2-C3	-4.20	118.78	126.04
30	2	608	CHL	CHD-C1D-ND	-4.20	120.60	124.45
30	G	606	CHL	CHD-C1D-ND	-4.19	120.60	124.45
30	g	308	CHL	CHD-C1D-ND	-4.19	120.60	124.45
30	6	310	CHL	CHD-C1D-ND	-4.19	120.60	124.45
36	3	319	NEX	C2-C1-C6	4.19	113.28	109.21
43	H	101	BCR	C15-C14-C13	-4.19	121.33	127.31
32	8	615	LUT	C18-C5-C6	-4.19	119.83	124.53
32	g	316	LUT	C7-C8-C9	-4.18	119.91	126.23
34	Y	319	LMG	O7-C10-C11	4.18	120.51	111.50
32	n	317	LUT	C18-C5-C6	-4.18	119.83	124.53
38	b	627	SQD	O7-S-C6	-4.18	101.97	106.94
43	t	101	BCR	C34-C9-C10	-4.18	117.07	122.92
30	n	306	CHL	CHD-C1D-ND	-4.18	120.61	124.45
43	C	615	BCR	C20-C19-C18	-4.18	114.67	126.42
32	S	317	LUT	C7-C8-C9	-4.18	119.92	126.23
31	7	314	CLA	O2A-C1-C2	4.17	119.61	108.64
31	b	605	CLA	C1-C2-C3	-4.17	118.83	126.04
31	C	607	CLA	O2A-C1-C2	4.17	119.60	108.64
32	N	316	LUT	C35-C34-C33	-4.17	121.36	127.31
43	B	619	BCR	C20-C21-C22	-4.17	121.36	127.31
31	B	611	CLA	C1-C2-C3	-4.17	118.83	126.04
45	C	620	DGD	O2G-C1B-C2B	4.17	120.49	111.50
34	7	320	LMG	O7-C10-C11	4.16	120.48	111.50
31	8	604	CLA	C1-C2-C3	-4.16	118.84	126.04
30	3	307	CHL	CHD-C1D-ND	-4.16	120.63	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Y	315	LUT	C18-C5-C6	-4.16	119.86	124.53
30	q	307	CHL	CHD-C1D-ND	-4.16	120.63	124.45
31	y	615	CLA	C1-C2-C3	-4.16	118.85	126.04
30	N	308	CHL	CHD-C1D-ND	-4.16	120.63	124.45
33	p	619	LHG	O7-C7-C8	4.16	120.46	111.50
34	J	102	LMG	O7-C10-C11	4.16	120.46	111.50
32	r	317	LUT	C18-C5-C6	-4.16	119.86	124.53
30	0	607	CHL	CHD-C1D-ND	-4.16	120.63	124.45
34	6	322	LMG	O7-C10-C11	4.16	120.46	111.50
34	2	621	LMG	O7-C10-C11	4.16	120.46	111.50
30	6	307	CHL	CHD-C1D-ND	-4.15	120.64	124.45
33	A	415	LHG	O7-C7-C8	4.15	120.45	111.50
34	Q1	101	LMG	O7-C10-C11	4.15	120.44	111.50
30	3	309	CHL	CHD-C1D-ND	-4.15	120.64	124.45
31	b	615	CLA	C1-C2-C3	-4.15	118.87	126.04
31	g	313	CLA	O2A-C1-C2	4.15	119.53	108.64
33	D	407	LHG	O7-C7-C8	4.15	120.44	111.50
36	q	319	NEX	C38-C25-C24	4.15	118.94	114.28
34	G	619	LMG	O7-C10-C11	4.15	120.44	111.50
31	B	603	CLA	O2A-C1-C2	4.15	119.53	108.64
36	4	617	NEX	C27-C28-C29	-4.15	119.10	125.53
32	R	317	LUT	C35-C15-C14	-4.15	114.98	123.47
32	r	317	LUT	C35-C34-C33	-4.14	121.40	127.31
43	A	410	BCR	C24-C23-C22	-4.14	119.98	126.23
32	N	317	LUT	C35-C34-C33	-4.14	121.40	127.31
43	a	410	BCR	C15-C16-C17	-4.14	115.00	123.47
43	c	614	BCR	C11-C12-C13	-4.13	114.80	126.42
30	y	605	CHL	CHD-C1D-ND	-4.13	120.66	124.45
30	N	306	CHL	CHD-C1D-ND	-4.12	120.66	124.45
32	6	318	LUT	C15-C14-C13	-4.12	121.43	127.31
34	b	629	LMG	O7-C10-C11	4.12	120.38	111.50
30	n	301	CHL	CHD-C1D-ND	-4.12	120.67	124.45
31	C	604	CLA	C1-C2-C3	-4.12	118.92	126.04
31	S	306	CLA	C1-C2-C3	-4.12	120.09	126.75
32	0	616	LUT	C18-C5-C6	-4.11	119.91	124.53
34	7	322	LMG	O7-C10-C11	4.11	120.37	111.50
31	9	315	CLA	O2A-C1-C2	4.11	119.44	108.64
31	9	306	CLA	C1-C2-C3	-4.11	118.93	126.04
43	t	101	BCR	C30-C25-C26	-4.11	116.82	122.61
30	r	309	CHL	CHD-C1D-ND	-4.11	120.67	124.45
43	Z	101	BCR	C15-C14-C13	-4.11	121.44	127.31
34	b	623	LMG	O7-C10-C11	4.11	120.36	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	605	CLA	O2A-C1-C2	4.11	119.44	108.64
34	A	412	LMG	O7-C10-C11	4.11	120.36	111.50
43	t	101	BCR	C36-C18-C17	-4.11	117.17	122.92
34	D	412	LMG	O7-C10-C11	4.11	120.35	111.50
32	0	616	LUT	C21-C26-C27	-4.10	107.51	112.70
30	y	606	CHL	CHD-C1D-ND	-4.10	120.68	124.45
33	S	320	LHG	O7-C7-C8	4.10	120.34	111.50
30	n	308	CHL	CHD-C1D-ND	-4.10	120.68	124.45
31	B	606	CLA	O2A-C1-C2	4.10	119.42	108.64
43	d	406	BCR	C2-C1-C6	4.10	116.80	110.48
30	2	605	CHL	CHD-C1D-ND	-4.10	120.69	124.45
30	7	321	CHL	CHD-C1D-ND	-4.10	120.69	124.45
30	p	608	CHL	CHD-C1D-ND	-4.10	120.69	124.45
31	q	316	CLA	C1-C2-C3	-4.09	120.13	126.75
30	9	303	CHL	CHD-C1D-ND	-4.09	120.69	124.45
36	5	618	NEX	C27-C28-C29	-4.09	119.18	125.53
32	n	318	LUT	C15-C14-C13	-4.09	121.47	127.31
30	G	601	CHL	CHD-C1D-ND	-4.09	120.70	124.45
32	8	616	LUT	C15-C14-C13	-4.09	121.48	127.31
34	w	204	LMG	O7-C10-C11	4.09	120.31	111.50
43	d	406	BCR	C27-C26-C25	-4.08	116.81	122.73
43	b	619	BCR	C11-C10-C9	-4.08	121.49	127.31
43	B	617	BCR	C16-C17-C18	-4.08	121.49	127.31
34	X	203	LMG	O7-C10-C11	4.08	120.29	111.50
30	n	302	CHL	CHD-C1D-ND	-4.08	120.71	124.45
43	B	618	BCR	C20-C21-C22	-4.08	121.49	127.31
31	5	615	CLA	C2C-C1C-NC	4.08	113.79	109.97
30	3	310	CHL	CHD-C1D-ND	-4.08	120.71	124.45
30	7	308	CHL	CHD-C1D-ND	-4.07	120.71	124.45
34	J	101	LMG	O7-C10-C11	4.07	120.27	111.50
45	c	617	DGD	O2G-C1B-C2B	4.07	120.27	111.50
30	p	605	CHL	CHD-C1D-ND	-4.07	120.72	124.45
30	R	309	CHL	CHD-C1D-ND	-4.07	120.72	124.45
30	Y	302	CHL	CHD-C1D-ND	-4.07	120.72	124.45
31	c	609	CLA	O2A-C1-C2	4.06	119.32	108.64
34	k	102	LMG	O7-C10-C11	4.06	120.26	111.50
30	q	308	CHL	C4D-CHA-C1A	4.06	126.19	121.25
43	b	619	BCR	C4-C5-C6	-4.06	116.83	122.73
34	y	620	LMG	O7-C10-C11	4.06	120.25	111.50
30	8	601	CHL	CHD-C1D-ND	-4.06	120.72	124.45
32	y	617	LUT	C15-C14-C13	-4.06	121.52	127.31
33	b	625	LHG	O7-C7-C8	4.06	120.25	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	602	CLA	C1-C2-C3	-4.06	119.03	126.04
43	b	620	BCR	C24-C23-C22	-4.05	120.11	126.23
31	6	305	CLA	C1-C2-C3	-4.05	119.03	126.04
34	a	413	LMG	C1-O6-C5	-4.05	105.73	113.69
30	G	623	CHL	CHD-C1D-ND	-4.05	120.73	124.45
30	4	605	CHL	CHD-C1D-ND	-4.05	120.73	124.45
30	g	306	CHL	CHD-C1D-ND	-4.05	120.74	124.45
30	9	310	CHL	CHD-C1D-ND	-4.04	120.74	124.45
36	3	319	NEX	C27-C28-C29	-4.04	119.25	125.53
31	y	604	CLA	C1-C2-C3	-4.04	119.05	126.04
30	G	605	CHL	CHD-C1D-ND	-4.04	120.74	124.45
34	s	321	LMG	O7-C10-C11	4.04	120.21	111.50
30	r	310	CHL	CHD-C1D-ND	-4.04	120.74	124.45
30	y	607	CHL	CHD-C1D-ND	-4.04	120.74	124.45
43	H	101	BCR	C33-C5-C6	-4.04	119.99	124.53
32	2	615	LUT	C31-C32-C33	4.04	137.75	126.42
31	C	610	CLA	CAA-C2A-C3A	-4.03	101.73	112.78
32	p	617	LUT	C39-C29-C30	-4.03	117.27	122.92
31	N	321	CLA	C1-C2-C3	-4.03	119.07	126.04
33	c	622	LHG	O7-C7-C8	4.03	120.18	111.50
31	S	314	CLA	C1-C2-C3	-4.03	119.08	126.04
33	j	102	LHG	O7-C7-C8	4.02	120.17	111.50
31	C	612	CLA	C1-C2-C3	-4.02	119.09	126.04
31	c	605	CLA	O2A-C1-C2	4.02	119.19	108.64
33	0	619	LHG	O7-C7-C8	4.02	120.16	111.50
34	c	621	LMG	O7-C10-C11	4.02	120.16	111.50
32	2	615	LUT	C18-C5-C6	-4.01	120.02	124.53
31	C	608	CLA	O2A-C1-C2	4.01	119.18	108.64
32	R	317	LUT	C31-C30-C29	4.01	133.04	127.31
34	W	202	LMG	O7-C10-C11	4.01	120.15	111.50
48	c	623	LMU	C1B-O1B-C4'	-4.01	108.05	117.96
31	5	612	CLA	C1-C2-C3	-4.01	120.27	126.75
33	L	101	LHG	O7-C7-C8	4.00	120.12	111.50
43	t	101	BCR	C19-C18-C17	4.00	125.08	118.94
43	c	614	BCR	C15-C16-C17	-4.00	115.28	123.47
34	b	626	LMG	O7-C10-C11	4.00	120.12	111.50
32	N	317	LUT	C1-C6-C5	-4.00	116.98	122.61
32	g	316	LUT	C1-C6-C5	-4.00	116.98	122.61
43	t	101	BCR	C35-C13-C14	-4.00	117.32	122.92
35	9	317	RRX	C4-C5-C6	-4.00	116.93	122.73
33	1	617	LHG	O7-C7-C8	3.99	120.11	111.50
43	B	619	BCR	C4-C5-C6	-3.99	116.93	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	6	320	LHG	O7-C7-C8	3.99	120.11	111.50
30	G	607	CHL	CHD-C1D-ND	-3.99	120.78	124.45
32	Y	315	LUT	C35-C34-C33	-3.99	121.61	127.31
30	3	308	CHL	CHD-C1D-ND	-3.99	120.79	124.45
43	Z	101	BCR	C38-C26-C25	-3.99	120.05	124.53
35	4	615	RRX	C33-C5-C6	-3.99	120.05	124.53
32	Y	316	LUT	C35-C34-C33	-3.99	121.62	127.31
33	D	408	LHG	O7-C7-C8	3.99	120.09	111.50
43	b	618	BCR	C4-C5-C6	-3.99	116.94	122.73
33	d	408	LHG	O7-C7-C8	3.99	120.09	111.50
31	9	314	CLA	C1-C2-C3	-3.98	120.31	126.75
34	R	321	LMG	O7-C10-C11	3.98	120.08	111.50
34	B	625	LMG	O7-C10-C11	3.98	120.08	111.50
36	r	301	NEX	C5-C4-C3	3.98	116.46	111.75
43	A	410	BCR	C7-C8-C9	-3.98	120.22	126.23
32	Y	315	LUT	C21-C26-C27	-3.98	107.67	112.70
34	j	101	LMG	O7-C10-C11	3.98	120.07	111.50
30	N	301	CHL	CHD-C1D-ND	-3.98	120.80	124.45
30	4	601	CHL	CHD-C1D-ND	-3.97	120.80	124.45
30	y	601	CHL	CHD-C1D-ND	-3.97	120.80	124.45
34	d	409	LMG	O7-C10-C11	3.97	120.06	111.50
30	0	606	CHL	CHD-C1D-ND	-3.97	120.80	124.45
31	y	602	CLA	C1-C2-C3	-3.97	119.17	126.04
30	0	605	CHL	C3C-C4C-NC	-3.97	106.12	110.57
34	A	414	LMG	O7-C10-C11	3.97	120.06	111.50
35	G	614	RRX	C4-C5-C6	-3.97	116.97	122.73
34	9	302	LMG	O7-C10-C11	3.97	120.05	111.50
31	r	306	CLA	O2A-C1-C2	3.97	122.91	109.49
30	1	619	CHL	CMA-C3A-C4A	3.97	122.44	111.77
31	3	304	CLA	C1-C2-C3	-3.97	119.18	126.04
30	4	606	CHL	CHD-C1D-ND	-3.97	120.81	124.45
31	5	604	CLA	C1-C2-C3	-3.96	120.34	126.75
32	1	616	LUT	C15-C14-C13	-3.96	121.65	127.31
34	q	301	LMG	O7-C10-C11	3.96	120.04	111.50
35	4	615	RRX	C4-C5-C6	-3.96	116.98	122.73
32	7	317	LUT	C21-C26-C27	-3.96	107.69	112.70
35	G	614	RRX	C33-C5-C6	-3.96	120.08	124.53
30	Y	301	CHL	CHD-C1D-ND	-3.96	120.82	124.45
30	q	311	CHL	CHD-C1D-ND	-3.96	120.82	124.45
35	2	614	RRX	C7-C8-C9	-3.95	120.26	126.23
43	b	619	BCR	C1-C6-C5	-3.95	117.05	122.61
32	5	617	LUT	C35-C34-C33	-3.95	121.67	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	607	CHL	CHD-C1D-ND	-3.95	120.83	124.45
31	C	605	CLA	C1-C2-C3	-3.95	119.22	126.04
35	9	317	RRX	C33-C5-C6	-3.94	120.10	124.53
31	N	305	CLA	C1-C2-C3	-3.94	119.22	126.04
34	C	619	LMG	O7-C10-C11	3.94	119.99	111.50
32	r	317	LUT	C21-C26-C27	-3.94	107.72	112.70
43	d	406	BCR	C15-C16-C17	-3.94	115.41	123.47
31	R	306	CLA	O2A-C1-C2	3.93	122.79	109.49
30	5	607	CHL	CHD-C1D-ND	-3.93	120.84	124.45
32	r	317	LUT	C15-C14-C13	-3.93	121.70	127.31
30	9	311	CHL	CHD-C1D-ND	-3.93	120.84	124.45
43	Z	101	BCR	C16-C17-C18	-3.93	121.70	127.31
33	M	101	LHG	O7-C7-C8	3.93	119.97	111.50
33	e	101	LHG	O7-C7-C8	3.92	119.96	111.50
33	5	619	LHG	O7-C7-C8	3.92	119.95	111.50
34	r	321	LMG	O7-C10-C11	3.92	119.94	111.50
43	b	620	BCR	C4-C5-C6	-3.92	117.05	122.73
31	C	603	CLA	CHD-C1D-ND	-3.92	120.86	124.45
31	c	612	CLA	C1-C2-C3	-3.91	119.28	126.04
30	S	309	CHL	CHD-C1D-ND	-3.91	120.86	124.45
30	5	605	CHL	CHD-C1D-ND	-3.91	120.86	124.45
34	n	321	LMG	O7-C10-C11	3.91	119.92	111.50
30	q	303	CHL	CHD-C1D-ND	-3.90	120.87	124.45
43	b	618	BCR	C11-C10-C9	-3.90	121.74	127.31
32	0	617	LUT	C15-C14-C13	-3.90	121.74	127.31
43	B	618	BCR	C1-C6-C5	-3.90	117.12	122.61
34	D	411	LMG	O7-C10-C11	3.90	119.91	111.50
31	n	305	CLA	C1-C2-C3	-3.90	119.30	126.04
43	H	101	BCR	C27-C26-C25	-3.90	117.07	122.73
43	H	101	BCR	C4-C5-C6	-3.90	117.07	122.73
47	E	101	HEM	CBA-CAA-C2A	-3.90	105.97	112.62
43	B	618	BCR	C4-C5-C6	-3.90	117.07	122.73
30	g	302	CHL	CHD-C1D-ND	-3.90	120.87	124.45
34	d	410	LMG	O7-C10-C11	3.89	119.89	111.50
32	6	318	LUT	C11-C10-C9	-3.89	121.75	127.31
30	Y	306	CHL	CHD-C1D-ND	-3.89	120.88	124.45
33	G	618	LHG	O7-C7-C8	3.89	119.89	111.50
31	C	609	CLA	O2A-C1-C2	3.89	118.86	108.64
43	H	101	BCR	C38-C26-C25	-3.89	120.16	124.53
31	g	303	CLA	C1D-ND-C4D	-3.89	103.57	106.33
30	2	601	CHL	CHD-C1D-ND	-3.89	120.88	124.45
30	6	302	CHL	CHD-C1D-ND	-3.89	120.88	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	615	LUT	C21-C26-C27	-3.88	107.79	112.70
31	3	313	CLA	C1-C2-C3	-3.88	120.47	126.75
31	Y	305	CLA	C1-C2-C3	-3.88	119.33	126.04
33	r	320	LHG	O7-C7-C8	3.88	119.87	111.50
31	B	615	CLA	C2C-C1C-NC	3.88	113.61	109.97
31	B	608	CLA	C1-C2-C3	-3.88	119.33	126.04
32	y	616	LUT	C18-C5-C6	-3.88	120.17	124.53
31	R	312	CLA	O2A-C1-C2	3.88	118.83	108.64
32	y	616	LUT	C35-C34-C33	-3.88	121.77	127.31
32	1	615	LUT	C21-C26-C27	-3.88	107.80	112.70
30	s	308	CHL	CHD-C1D-ND	-3.88	120.89	124.45
43	B	617	BCR	C1-C6-C5	-3.88	117.15	122.61
33	2	617	LHG	O7-C7-C8	3.87	119.85	111.50
31	r	312	CLA	O2A-C1-C2	3.87	118.81	108.64
34	X	202	LMG	O7-C10-C11	3.87	119.84	111.50
30	1	619	CHL	C1-C2-C3	-3.87	119.35	126.04
43	c	614	BCR	C4-C5-C6	-3.87	117.11	122.73
48	K	101	LMU	C1B-O1B-C4'	-3.87	108.40	117.96
34	C	622	LMG	O7-C10-C11	3.86	119.82	111.50
32	s	318	LUT	C15-C14-C13	-3.86	121.81	127.31
30	s	309	CHL	CHD-C1D-ND	-3.85	120.91	124.45
34	6	323	LMG	O7-C10-C11	3.85	119.80	111.50
43	t	101	BCR	C24-C23-C22	-3.85	120.42	126.23
31	Y	313	CLA	C1-C2-C3	-3.85	119.38	126.04
45	C	616	DGD	O2G-C1B-C2B	3.85	119.79	111.50
33	S	322	LHG	O7-C7-C8	3.84	119.78	111.50
33	s	320	LHG	O7-C7-C8	3.84	119.78	111.50
30	q	309	CHL	C1-O2A-CGA	3.84	126.53	116.44
34	5	620	LMG	O7-C10-C11	3.84	119.78	111.50
34	0	620	LMG	O7-C10-C11	3.84	119.78	111.50
43	v	101	BCR	C27-C26-C25	-3.84	117.16	122.73
31	r	316	CLA	CHD-C1D-ND	-3.84	120.93	124.45
43	t	101	BCR	C12-C13-C14	3.83	124.83	118.94
30	1	601	CHL	CMA-C3A-C4A	3.83	122.08	111.77
34	k	101	LMG	O7-C10-C11	3.83	119.76	111.50
30	3	302	CHL	C1-O2A-CGA	3.83	126.50	116.44
34	7	301	LMG	O7-C10-C11	3.83	119.76	111.50
31	y	612	CLA	C1-C2-C3	-3.83	119.42	126.04
33	g	319	LHG	O7-C7-C8	3.83	119.75	111.50
33	A	417	LHG	O7-C7-C8	3.83	119.75	111.50
34	4	621	LMG	O7-C10-C11	3.83	119.75	111.50
34	p	620	LMG	O7-C10-C11	3.82	119.74	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	314	CLA	C1-C2-C3	-3.82	119.43	126.04
43	h	101	BCR	C27-C26-C25	-3.82	117.18	122.73
31	0	614	CLA	C1-C2-C3	-3.82	119.43	126.04
32	S	318	LUT	C1-C6-C5	-3.82	117.23	122.61
43	V	101	BCR	C38-C26-C27	3.82	120.95	113.62
30	n	310	CHL	CMA-C3A-C4A	3.82	122.04	111.77
31	c	613	CLA	CAA-C2A-C3A	-3.82	102.32	112.78
31	s	306	CLA	C1-C2-C3	-3.82	120.58	126.75
32	n	317	LUT	C15-C14-C13	-3.82	121.86	127.31
34	G	621	LMG	O7-C10-C11	3.82	119.72	111.50
43	c	614	BCR	C30-C25-C26	-3.81	117.24	122.61
30	p	601	CHL	CHD-C1D-ND	-3.81	120.95	124.45
31	c	606	CLA	C1-C2-C3	-3.81	119.45	126.04
34	D	409	LMG	O7-C10-C11	3.81	119.71	111.50
34	g	322	LMG	O7-C10-C11	3.81	119.71	111.50
31	0	604	CLA	C1-C2-C3	-3.81	119.46	126.04
32	y	617	LUT	C21-C26-C27	-3.81	107.89	112.70
32	q	318	LUT	C18-C5-C6	-3.81	120.25	124.53
33	N	319	LHG	O7-C7-C8	3.81	119.70	111.50
31	G	612	CLA	C1-C2-C3	-3.81	119.46	126.04
30	7	306	CHL	CHD-C1D-ND	-3.81	120.96	124.45
30	9	303	CHL	C1-C2-C3	-3.80	119.46	126.04
34	x	202	LMG	O7-C10-C11	3.80	119.69	111.50
34	9	321	LMG	O7-C10-C11	3.80	119.69	111.50
32	7	318	LUT	C18-C5-C6	-3.80	120.26	124.53
31	B	605	CLA	C1-C2-C3	-3.80	119.47	126.04
32	y	617	LUT	C7-C8-C9	-3.80	120.50	126.23
32	p	616	LUT	C1-C6-C5	-3.80	117.27	122.61
31	0	602	CLA	C1-C2-C3	-3.80	119.48	126.04
31	R	312	CLA	CHD-C1D-ND	-3.80	120.97	124.45
35	q	317	RRX	C20-C19-C18	-3.79	115.76	126.42
31	R	316	CLA	CHD-C1D-ND	-3.79	120.97	124.45
30	3	309	CHL	C3C-C4C-NC	-3.79	106.32	110.57
32	7	318	LUT	C15-C14-C13	-3.79	121.90	127.31
31	c	604	CLA	C1-C2-C3	-3.79	119.48	126.04
43	v	101	BCR	C20-C21-C22	-3.79	121.90	127.31
34	0	622	LMG	O7-C10-C11	3.79	119.67	111.50
31	a	407	CLA	C1-C2-C3	-3.79	119.49	126.04
43	v	101	BCR	C1-C6-C5	-3.79	117.28	122.61
32	8	615	LUT	C15-C14-C13	-3.79	121.91	127.31
30	9	307	CHL	CHD-C1D-ND	-3.79	120.97	124.45
31	0	613	CLA	C1-C2-C3	-3.79	119.49	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	q	317	RRX	C27-C26-C25	-3.79	112.41	120.85
45	c	616	DGD	O2G-C1B-C2B	3.78	119.66	111.50
36	p	618	NEX	C27-C28-C29	-3.78	119.66	125.53
31	G	602	CLA	O2A-C1-C2	3.78	118.56	108.64
33	F1	301	LHG	O7-C7-C8	3.77	119.63	111.50
31	1	610	CLA	C1-C2-C3	-3.77	119.52	126.04
30	R	310	CHL	CHD-C1D-ND	-3.77	120.99	124.45
30	1	619	CHL	CHD-C1D-ND	-3.77	120.99	124.45
31	4	614	CLA	C1-C2-C3	-3.77	119.53	126.04
34	w	201	LMG	O7-C10-C11	3.77	119.62	111.50
36	N	318	NEX	C20-C13-C14	-3.76	117.65	122.92
30	q	310	CHL	CHD-C1D-ND	-3.76	121.00	124.45
31	y	611	CLA	O2A-C1-C2	3.76	118.53	108.64
31	y	614	CLA	C1-C2-C3	-3.76	119.53	126.04
31	Y	314	CLA	C1-C2-C3	-3.76	119.54	126.04
31	s	312	CLA	C1-C2-C3	-3.76	119.54	126.04
32	p	617	LUT	C7-C8-C9	-3.76	120.56	126.23
31	4	610	CLA	O2A-C1-C2	3.76	118.51	108.64
47	e	102	HEM	C1B-NB-C4B	3.76	108.95	105.07
31	b	609	CLA	C1-C2-C3	-3.76	119.55	126.04
31	S	305	CLA	C1-C2-C3	-3.75	119.55	126.04
33	l	101	LHG	O7-C7-C8	3.75	119.59	111.50
43	T	101	BCR	C27-C26-C25	-3.75	117.28	122.73
31	b	612	CLA	C1-C2-C3	-3.75	119.55	126.04
31	g	303	CLA	C2D-C1D-ND	3.75	112.87	110.10
34	2	620	LMG	O7-C10-C11	3.75	119.58	111.50
33	n	320	LHG	O7-C7-C8	3.75	119.58	111.50
33	8	618	LHG	O7-C7-C8	3.74	119.57	111.50
34	n	322	LMG	C8-O7-C10	-3.74	108.58	117.79
32	5	617	LUT	C7-C8-C9	-3.74	120.58	126.23
31	R	314	CLA	CHD-C1D-ND	-3.74	121.02	124.45
43	B	619	BCR	C27-C26-C25	-3.74	117.30	122.73
31	7	305	CLA	O2A-C1-C2	3.74	118.46	108.64
43	T	101	BCR	C16-C15-C14	-3.74	115.82	123.47
31	1	613	CLA	C1-C2-C3	-3.74	119.58	126.04
30	G	608	CHL	CMA-C3A-C4A	3.74	121.81	111.77
31	2	604	CLA	C1-C2-C3	-3.73	119.58	126.04
43	t	101	BCR	C7-C6-C5	-3.73	112.42	121.46
31	R	307	CLA	O2A-C1-C2	3.73	122.11	109.49
31	b	617	CLA	CHD-C1D-ND	-3.73	121.03	124.45
36	n	319	NEX	C2-C1-C6	3.73	112.84	109.21
38	G	624	SQD	O7-S-C6	-3.73	102.51	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	h	101	BCR	C4-C5-C6	-3.73	117.32	122.73
31	2	612	CLA	C1-C2-C3	-3.72	119.60	126.04
31	b	606	CLA	C1-C2-C3	-3.72	119.60	126.04
31	C	613	CLA	C1-O2A-CGA	3.72	126.21	116.44
44	A	416	PL9	C7-C3-C2	-3.72	118.41	123.30
43	z	101	BCR	C16-C17-C18	-3.72	122.00	127.31
31	r	311	CLA	C1-C2-C3	-3.72	119.61	126.04
33	q	320	LHG	O7-C7-C8	3.72	119.52	111.50
32	5	616	LUT	C15-C14-C13	-3.72	122.00	127.31
32	2	615	LUT	C35-C15-C14	-3.72	115.86	123.47
31	N	315	CLA	C1-C2-C3	-3.72	119.61	126.04
34	c	624	LMG	O7-C10-C11	3.72	119.51	111.50
32	s	318	LUT	C1-C6-C5	-3.72	117.38	122.61
32	p	617	LUT	C18-C5-C6	-3.72	120.36	124.53
35	g	315	RRX	C33-C5-C6	-3.71	120.36	124.53
34	a	401	LMG	O7-C10-C11	3.71	119.50	111.50
33	7	319	LHG	O7-C7-C8	3.71	119.50	111.50
43	d	406	BCR	C4-C5-C6	-3.71	117.35	122.73
43	V	101	BCR	C1-C6-C5	-3.70	117.39	122.61
31	c	610	CLA	C1-C2-C3	-3.70	119.64	126.04
43	b	620	BCR	C20-C21-C22	-3.70	122.02	127.31
33	y	619	LHG	O7-C7-C8	3.70	119.48	111.50
34	q1	101	LMG	O7-C10-C11	3.70	119.48	111.50
31	C	613	CLA	C1-C2-C3	-3.70	119.64	126.04
36	N	318	NEX	C12-C13-C14	3.70	124.61	118.94
30	r	309	CHL	C1-C2-C3	-3.70	119.65	126.04
31	r	316	CLA	O2A-C1-C2	3.70	118.35	108.64
30	S	302	CHL	CHD-C1D-ND	-3.69	121.06	124.45
43	C	614	BCR	C30-C25-C26	-3.69	117.41	122.61
30	S	308	CHL	CHD-C1D-ND	-3.69	121.06	124.45
31	7	314	CLA	C1-C2-C3	-3.69	119.67	126.04
32	S	317	LUT	C31-C30-C29	-3.69	122.05	127.31
31	c	607	CLA	O2A-C1-C2	3.68	118.32	108.64
33	b	628	LHG	O7-C7-C8	3.68	119.44	111.50
43	b	619	BCR	C38-C26-C25	-3.68	120.39	124.53
31	B	616	CLA	C1-C2-C3	-3.68	119.67	126.04
32	5	617	LUT	C31-C30-C29	-3.68	122.05	127.31
31	y	613	CLA	O2A-C1-C2	3.68	118.31	108.64
31	r	307	CLA	O2A-C1-C2	3.68	121.92	109.49
31	c	606	CLA	C2C-C1C-NC	3.68	113.42	109.97
32	3	318	LUT	C35-C34-C33	-3.67	122.07	127.31
32	Y	315	LUT	C15-C14-C13	-3.67	122.07	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	609	CLA	C1-C2-C3	-3.67	119.69	126.04
32	q	318	LUT	C31-C30-C29	-3.67	122.07	127.31
31	C	601	CLA	C1-C2-C3	-3.67	119.70	126.04
31	9	304	CLA	C1-C2-C3	-3.67	119.70	126.04
31	b	603	CLA	C1-C2-C3	-3.66	119.71	126.04
32	0	617	LUT	C18-C5-C6	-3.66	120.42	124.53
31	9	313	CLA	O2A-C1-C2	3.66	121.87	108.42
31	p	604	CLA	CHD-C1D-ND	-3.66	121.09	124.45
38	X	201	SQD	O7-S-C6	-3.66	102.59	106.94
34	a	413	LMG	O1-C7-C8	-3.66	102.08	110.90
30	1	601	CHL	C4D-CHA-C1A	3.65	125.70	121.25
43	b	618	BCR	C30-C25-C26	-3.65	117.47	122.61
31	A	406	CLA	C1-C2-C3	-3.65	119.72	126.04
32	7	318	LUT	C31-C30-C29	-3.65	122.10	127.31
42	D	401	PHO	CMB-C2B-C3B	3.65	131.51	124.68
32	r	317	LUT	C8-C7-C6	-3.65	116.95	127.20
32	0	617	LUT	C11-C10-C9	-3.65	122.10	127.31
31	5	602	CLA	C1-C2-C3	-3.65	119.73	126.04
44	D	406	PL9	C7-C3-C4	3.65	119.84	116.88
43	Z	101	BCR	C27-C26-C25	-3.65	117.44	122.73
31	b	616	CLA	C2C-C1C-NC	3.64	113.39	109.97
31	B	613	CLA	C1-C2-C3	-3.64	119.75	126.04
43	a	410	BCR	C4-C5-C6	-3.64	117.45	122.73
34	4	620	LMG	O7-C10-C11	3.64	119.34	111.50
31	r	314	CLA	CHD-C1D-ND	-3.63	121.11	124.45
33	Y	318	LHG	O7-C7-C8	3.63	119.33	111.50
43	C	615	BCR	C11-C12-C13	3.63	136.62	126.42
31	g	305	CLA	C1-C2-C3	-3.63	119.76	126.04
30	3	310	CHL	C1-O2A-CGA	3.63	125.97	116.44
34	D	410	LMG	O7-C10-C11	3.63	119.32	111.50
30	S	308	CHL	C3C-C4C-NC	-3.63	106.50	110.57
43	d	406	BCR	C16-C17-C18	-3.63	122.14	127.31
31	d	405	CLA	C1-C2-C3	-3.62	119.77	126.04
30	1	601	CHL	C3C-C4C-NC	-3.62	106.51	110.57
30	7	302	CHL	C4D-CHA-C1A	3.62	125.66	121.25
31	1	610	CLA	CHD-C1D-ND	-3.62	121.12	124.45
43	B	617	BCR	C20-C21-C22	-3.62	122.14	127.31
32	1	615	LUT	C35-C34-C33	-3.62	122.14	127.31
31	c	601	CLA	C1-C2-C3	-3.62	119.78	126.04
32	R	317	LUT	C40-C33-C34	-3.62	117.85	122.92
38	6	301	SQD	O7-S-C6	-3.62	102.64	106.94
31	n	316	CLA	C1-C2-C3	-3.62	119.79	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	1	605	CHL	C4D-CHA-C1A	3.62	125.65	121.25
31	C	609	CLA	C2C-C1C-NC	3.62	113.36	109.97
31	D	404	CLA	C1-C2-C3	-3.61	119.80	126.04
30	9	309	CHL	C1-O2A-CGA	3.61	125.92	116.44
32	3	317	LUT	C15-C14-C13	-3.61	122.16	127.31
31	g	303	CLA	CHD-C1D-ND	-3.61	121.14	124.45
34	9	301	LMG	C3-C4-C5	3.61	116.68	110.24
38	a	411	SQD	O7-S-C6	-3.61	102.65	106.94
43	C	614	BCR	C23-C24-C25	-3.61	117.08	127.20
31	R	305	CLA	CHD-C1D-ND	-3.61	121.14	124.45
30	3	302	CHL	C3C-C4C-NC	-3.60	106.53	110.57
38	s	301	SQD	O7-S-C6	-3.60	102.66	106.94
31	8	603	CLA	C1-C2-C3	-3.60	119.82	126.04
31	s	311	CLA	CHD-C1D-ND	-3.60	121.15	124.45
32	S	317	LUT	C15-C14-C13	-3.60	122.18	127.31
33	4	618	LHG	O7-C7-C8	3.60	119.25	111.50
31	q	306	CLA	C1-C2-C3	-3.60	119.83	126.04
30	8	608	CHL	C1-O2A-CGA	3.59	125.88	116.44
34	w	203	LMG	O8-C28-C29	3.59	123.18	111.91
43	C	615	BCR	C33-C5-C4	3.59	120.52	113.62
34	a	416	LMG	O7-C10-C11	3.59	119.24	111.50
31	N	310	CLA	C1-C2-C3	-3.59	119.84	126.04
30	1	619	CHL	C3C-C4C-NC	-3.58	106.55	110.57
31	c	603	CLA	CHD-C1D-ND	-3.58	121.16	124.45
38	R	322	SQD	O7-S-C6	-3.58	102.69	106.94
38	r	322	SQD	O7-S-C6	-3.58	102.69	106.94
30	3	302	CHL	CHD-C1D-ND	-3.58	121.17	124.45
31	3	311	CLA	C1-C2-C3	-3.58	119.86	126.04
47	e	102	HEM	CHA-C4D-ND	3.57	128.80	124.38
32	1	616	LUT	C18-C5-C6	-3.57	120.52	124.53
30	Y	309	CHL	CMA-C3A-C4A	3.57	121.37	111.77
36	6	319	NEX	C27-C28-C29	-3.57	119.99	125.53
31	p	604	CLA	C1-C2-C3	-3.57	120.98	126.75
43	a	410	BCR	C30-C25-C26	-3.57	117.59	122.61
43	B	617	BCR	C27-C26-C25	-3.57	117.55	122.73
38	G	617	SQD	O7-S-C6	-3.57	102.70	106.94
31	B	614	CLA	C1-C2-C3	-3.57	119.87	126.04
35	q	317	RRX	C30-C25-C26	-3.57	117.59	122.61
34	1	618	LMG	O7-C10-C11	3.57	119.19	111.50
43	b	618	BCR	C24-C23-C22	-3.57	120.85	126.23
36	0	618	NEX	C27-C28-C29	-3.57	120.00	125.53
31	p	603	CLA	CHD-C1D-ND	-3.57	121.18	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	9	318	LUT	C1-C6-C5	-3.56	117.59	122.61
38	A	411	SQD	O7-S-C6	-3.56	102.70	106.94
47	E	101	HEM	C1B-NB-C4B	3.56	108.75	105.07
31	q	315	CLA	O2A-C1-C2	3.56	117.99	108.64
31	S	304	CLA	CAA-C2A-C3A	-3.56	105.37	114.26
43	B	617	BCR	C24-C23-C22	-3.56	120.86	126.23
31	5	615	CLA	C1C-C2C-C3C	-3.55	103.22	106.96
31	4	612	CLA	C2D-C1D-ND	3.55	112.72	110.10
34	A	418	LMG	O7-C10-C11	3.55	119.16	111.50
31	p	602	CLA	C1-C2-C3	-3.55	119.90	126.04
30	Y	302	CHL	C3C-C4C-NC	-3.55	106.59	110.57
32	1	615	LUT	C8-C7-C6	-3.55	117.24	127.20
30	s	307	CHL	C4D-CHA-C1A	3.55	125.57	121.25
38	g	301	SQD	O7-S-C6	-3.55	102.72	106.94
31	6	314	CLA	C1-C2-C3	-3.54	119.91	126.04
30	n	302	CHL	C3C-C4C-NC	-3.54	106.60	110.57
31	0	603	CLA	CHD-C1D-ND	-3.54	121.20	124.45
35	G	614	RRX	C7-C8-C9	-3.54	120.89	126.23
38	m	101	SQD	O7-S-C6	-3.54	102.73	106.94
31	p	615	CLA	CHD-C1D-ND	-3.54	121.20	124.45
38	M	102	SQD	O7-S-C6	-3.54	102.74	106.94
30	8	601	CHL	C3C-C4C-NC	-3.53	106.61	110.57
30	G	608	CHL	C3C-C4C-NC	-3.53	106.61	110.57
30	9	309	CHL	C4D-CHA-C1A	3.53	125.55	121.25
30	2	608	CHL	CMA-C3A-C4A	3.53	121.26	111.77
30	y	609	CHL	CMA-C3A-C4A	3.53	121.26	111.77
30	8	608	CHL	CMA-C3A-C4A	3.53	121.26	111.77
30	S	307	CHL	C4D-CHA-C1A	3.53	125.54	121.25
43	A	410	BCR	C30-C25-C26	-3.53	117.65	122.61
31	r	306	CLA	CHD-C1D-ND	-3.52	121.22	124.45
31	R	304	CLA	CHD-C1D-ND	-3.52	121.22	124.45
30	g	309	CHL	C3C-C4C-NC	-3.52	106.62	110.57
31	S	311	CLA	CHD-C1D-ND	-3.52	121.22	124.45
43	b	620	BCR	C27-C26-C25	-3.52	117.62	122.73
32	Y	315	LUT	C7-C8-C9	-3.52	120.92	126.23
32	Y	316	LUT	C21-C26-C27	-3.52	108.25	112.70
38	B	620	SQD	O7-S-C6	-3.52	102.76	106.94
31	s	315	CLA	O2A-C1-C2	3.52	121.38	109.49
30	4	601	CHL	C1-C2-C3	-3.51	119.97	126.04
31	R	305	CLA	CBC-CAC-C3C	-3.51	102.74	112.43
38	y	621	SQD	O7-S-C6	-3.51	102.76	106.94
30	7	307	CHL	C1-C2-C3	-3.51	119.97	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	R	310	CHL	C3C-C4C-NC	-3.51	106.63	110.57
30	g	309	CHL	CMA-C3A-C4A	3.51	121.21	111.77
43	B	619	BCR	C7-C8-C9	-3.51	120.93	126.23
31	b	617	CLA	C1-C2-C3	-3.51	119.97	126.04
32	N	317	LUT	C18-C5-C4	3.51	120.86	114.36
31	B	601	CLA	CHD-C1D-ND	-3.51	121.23	124.45
35	4	615	RRX	C7-C8-C9	-3.51	120.93	126.23
30	N	309	CHL	C3C-C4C-NC	-3.51	106.64	110.57
35	9	317	RRX	C7-C8-C9	-3.51	120.93	126.23
31	3	306	CLA	C1-C2-C3	-3.51	119.97	126.04
37	R	318	XAT	C7-C8-C9	-3.51	120.09	125.53
31	r	307	CLA	C2C-C1C-NC	3.51	113.26	109.97
32	6	318	LUT	C18-C5-C6	-3.51	120.59	124.53
30	3	310	CHL	CMA-C3A-C4A	3.51	121.20	111.77
36	3	319	NEX	C16-C1-C6	-3.51	107.33	110.47
31	d	401	CLA	CHD-C1D-ND	-3.51	121.23	124.45
43	b	618	BCR	C23-C24-C25	-3.51	117.36	127.20
31	B	610	CLA	C1-C2-C3	-3.50	119.98	126.04
31	Y	312	CLA	C1-C2-C3	-3.50	119.98	126.04
31	b	607	CLA	CHD-C1D-ND	-3.50	121.23	124.45
31	S	303	CLA	C1-C2-C3	-3.50	119.98	126.04
31	7	316	CLA	C1-C2-C3	-3.50	119.98	126.04
31	c	611	CLA	C1-C2-C3	-3.50	119.99	126.04
34	C	624	LMG	O7-C10-C11	3.50	119.03	111.50
35	2	614	RRX	C30-C25-C26	-3.49	117.69	122.61
30	5	609	CHL	CMA-C3A-C4A	3.49	121.16	111.77
31	c	610	CLA	CHD-C1D-ND	-3.49	121.24	124.45
30	n	310	CHL	C3C-C4C-NC	-3.49	106.66	110.57
43	b	620	BCR	C38-C26-C25	-3.49	120.61	124.53
43	T	101	BCR	C4-C5-C6	-3.49	117.66	122.73
38	b	621	SQD	O7-S-C6	-3.49	102.79	106.94
31	c	604	CLA	CHD-C1D-ND	-3.49	121.25	124.45
31	R	307	CLA	C2C-C1C-NC	3.49	113.24	109.97
43	D	405	BCR	C38-C26-C27	3.49	120.31	113.62
32	y	616	LUT	C8-C7-C6	-3.48	117.42	127.20
30	N	309	CHL	CMA-C3A-C4A	3.48	121.14	111.77
31	b	610	CLA	C1-C2-C3	-3.48	120.02	126.04
31	p	613	CLA	C1-O2A-CGA	3.48	125.58	116.44
30	7	309	CHL	C3C-C4C-NC	-3.48	106.67	110.57
32	n	318	LUT	C18-C5-C6	-3.48	120.62	124.53
38	B	623	SQD	O7-S-C6	-3.48	102.80	106.94
31	A	409	CLA	C1-C2-C3	-3.48	120.02	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	p	614	CLA	CHD-C1D-ND	-3.48	121.26	124.45
30	y	605	CHL	C3C-C4C-NC	-3.48	106.67	110.57
43	z	101	BCR	C27-C26-C25	-3.48	117.68	122.73
32	g	316	LUT	C18-C5-C6	-3.48	120.62	124.53
43	t	101	BCR	C2-C1-C6	3.48	115.83	110.48
32	S	318	LUT	C18-C5-C4	3.48	120.80	114.36
38	S	301	SQD	O7-S-C6	-3.47	102.81	106.94
31	N	310	CLA	CHD-C1D-ND	-3.47	121.26	124.45
30	0	609	CHL	CMA-C3A-C4A	3.47	121.10	111.77
30	5	601	CHL	C1-C2-C3	-3.47	121.14	126.75
32	y	616	LUT	C30-C31-C32	-3.47	112.39	123.22
32	6	317	LUT	C21-C26-C27	-3.47	108.32	112.70
32	3	317	LUT	C11-C10-C9	-3.47	122.36	127.31
31	q	305	CLA	C1-C2-C3	-3.47	120.05	126.04
38	g	318	SQD	O7-S-C6	-3.47	102.82	106.94
43	T	101	BCR	C20-C19-C18	-3.47	116.68	126.42
38	Y	320	SQD	O7-S-C6	-3.46	102.82	106.94
31	a	409	CLA	C1-C2-C3	-3.46	120.05	126.04
31	S	315	CLA	O2A-C1-C2	3.46	121.20	109.49
30	4	607	CHL	C3C-C4C-NC	-3.46	106.69	110.57
32	Y	315	LUT	C8-C7-C6	-3.46	117.48	127.20
31	C	610	CLA	CHD-C1D-ND	-3.46	121.27	124.45
31	2	613	CLA	C1-C2-C3	-3.46	120.06	126.04
45	c	617	DGD	C1E-O6E-C5E	3.46	120.48	113.69
32	8	616	LUT	C18-C5-C6	-3.46	120.64	124.53
30	6	309	CHL	C3C-C4C-NC	-3.46	106.69	110.57
30	s	302	CHL	CHD-C1D-ND	-3.46	121.28	124.45
44	a	414	PL9	C7-C3-C2	-3.46	118.75	123.30
43	B	618	BCR	C8-C7-C6	-3.46	117.49	127.20
47	e	102	HEM	CHB-C1B-NB	3.46	128.65	124.38
31	9	312	CLA	C1-C2-C3	-3.46	120.06	126.04
31	B	604	CLA	C2C-C1C-NC	3.46	113.21	109.97
31	q	312	CLA	C2D-C1D-ND	3.46	112.65	110.10
32	1	615	LUT	C7-C8-C9	-3.45	121.02	126.23
31	8	614	CLA	C1-C2-C3	-3.45	120.07	126.04
31	b	613	CLA	C2D-C1D-ND	3.45	112.65	110.10
31	s	306	CLA	C2D-C1D-ND	3.45	112.65	110.10
34	N	320	LMG	O7-C10-C11	3.45	118.94	111.50
32	N	317	LUT	C31-C30-C29	-3.45	122.38	127.31
32	1	615	LUT	C11-C10-C9	-3.45	122.39	127.31
31	S	315	CLA	CHD-C1D-ND	-3.45	121.28	124.45
43	a	410	BCR	C27-C26-C25	-3.45	117.72	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	7	306	CHL	CMA-C3A-C4A	3.45	121.04	111.77
30	Y	309	CHL	C4D-CHA-C1A	3.45	125.44	121.25
43	v	101	BCR	C24-C23-C22	-3.45	121.03	126.23
36	G	616	NEX	C2-C1-C6	3.44	112.56	109.21
31	0	615	CLA	C1-C2-C3	-3.44	120.09	126.04
31	6	303	CLA	C1-C2-C3	-3.44	120.09	126.04
30	7	321	CHL	C1-C2-C3	-3.44	120.09	126.04
31	y	613	CLA	C1-C2-C3	-3.44	120.10	126.04
32	8	616	LUT	C1-C6-C5	-3.44	117.77	122.61
30	r	310	CHL	C3C-C4C-NC	-3.44	106.72	110.57
32	S	318	LUT	C15-C14-C13	-3.44	122.41	127.31
32	5	617	LUT	C1-C6-C5	-3.44	117.78	122.61
32	s	317	LUT	C15-C14-C13	-3.43	122.41	127.31
31	C	612	CLA	C2C-C1C-NC	3.43	113.19	109.97
32	3	317	LUT	C7-C8-C9	-3.43	121.05	126.23
32	n	318	LUT	C1-C6-C5	-3.43	117.78	122.61
31	3	314	CLA	C1-C2-C3	-3.43	120.11	126.04
47	E	101	HEM	CHA-C4D-ND	3.43	128.62	124.38
31	s	313	CLA	C2C-C1C-NC	3.43	113.18	109.97
30	R	308	CHL	C4D-CHA-C1A	3.42	125.42	121.25
36	y	618	NEX	C17-C1-C6	-3.42	107.41	110.47
31	6	315	CLA	CHD-C1D-ND	-3.42	121.31	124.45
30	1	609	CHL	CMA-C3A-C4A	3.42	120.97	111.77
31	r	303	CLA	O2D-CGD-O1D	-3.42	117.14	123.84
31	C	604	CLA	CHD-C1D-ND	-3.42	121.31	124.45
34	3	321	LMG	O7-C10-C11	3.42	118.87	111.50
31	q	312	CLA	C1B-NB-C4B	3.42	109.45	106.32
30	n	308	CHL	C1-C2-C3	-3.42	120.13	126.04
31	r	312	CLA	CHD-C1D-ND	-3.42	121.31	124.45
30	R	308	CHL	C1-C2-C3	-3.42	120.13	126.04
31	c	612	CLA	C2C-C1C-NC	3.42	113.17	109.97
30	7	309	CHL	C2C-C3C-C4C	3.42	108.92	106.49
32	R	317	LUT	C7-C8-C9	-3.41	121.08	126.23
30	Y	301	CHL	C3C-C4C-NC	-3.41	106.74	110.57
31	s	313	CLA	CHD-C1D-ND	-3.41	121.32	124.45
38	A	413	SQD	O7-S-C6	-3.41	102.89	106.94
31	n	311	CLA	C1-C2-C3	-3.41	120.15	126.04
32	0	617	LUT	C21-C26-C27	-3.41	108.39	112.70
43	D	405	BCR	C38-C26-C25	-3.41	120.70	124.53
31	2	603	CLA	C1-C2-C3	-3.40	120.15	126.04
30	3	303	CHL	C4D-CHA-C1A	3.40	125.39	121.25
30	4	608	CHL	C3C-C4C-NC	-3.40	106.75	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	7	304	CLA	C1-C2-C3	-3.40	120.17	126.04
30	3	302	CHL	CMA-C3A-C4A	3.40	120.91	111.77
30	y	609	CHL	C4D-CHA-C1A	3.40	125.38	121.25
30	G	607	CHL	C1-C2-C3	-3.40	121.26	126.75
43	c	614	BCR	C21-C20-C19	3.40	133.81	123.22
31	A	406	CLA	CHD-C1D-ND	-3.39	121.34	124.45
31	A	407	CLA	CHD-C1D-ND	-3.39	121.34	124.45
30	1	601	CHL	C1B-CHB-C4A	-3.39	123.40	130.12
31	B	609	CLA	C1-C2-C3	-3.39	120.18	126.04
31	R	316	CLA	C1-C2-C3	-3.39	120.18	126.04
31	B	616	CLA	CHD-C1D-ND	-3.39	121.34	124.45
30	9	309	CHL	CMA-C3A-C4A	3.39	120.88	111.77
30	0	608	CHL	C3C-C4C-NC	-3.39	106.77	110.57
31	s	310	CLA	C1-C2-C3	-3.39	120.19	126.04
32	s	317	LUT	C7-C8-C9	-3.38	121.12	126.23
31	r	315	CLA	CHD-C1D-ND	-3.38	121.34	124.45
32	Y	315	LUT	C10-C11-C12	-3.38	112.66	123.22
31	A	406	CLA	C2C-C1C-NC	3.38	113.14	109.97
31	4	613	CLA	C1-C2-C3	-3.38	120.19	126.04
30	Y	306	CHL	C3C-C4C-NC	-3.38	106.78	110.57
31	G	609	CLA	CHD-C1D-ND	-3.38	121.35	124.45
31	B	616	CLA	C2C-C1C-NC	3.38	113.14	109.97
37	9	322	XAT	C6-C7-C8	-3.38	118.85	125.99
37	q	321	XAT	C6-C7-C8	-3.38	118.85	125.99
43	V	101	BCR	C4-C5-C6	-3.38	117.83	122.73
31	Y	310	CLA	C1-C2-C3	-3.38	120.20	126.04
31	q	315	CLA	C2C-C1C-NC	3.38	113.14	109.97
43	H	101	BCR	C2-C1-C6	3.37	115.68	110.48
31	R	311	CLA	CHD-C1D-ND	-3.37	121.35	124.45
37	4	619	XAT	C6-C7-C8	-3.37	118.86	125.99
31	y	610	CLA	CHD-C1D-ND	-3.37	121.36	124.45
31	S	313	CLA	C2C-C1C-NC	3.37	113.13	109.97
33	B	624	LHG	O7-C7-C8	3.37	118.77	111.50
43	D	405	BCR	C30-C25-C26	-3.37	117.87	122.61
31	b	605	CLA	C2C-C1C-NC	3.37	113.13	109.97
43	c	615	BCR	C20-C19-C18	-3.37	116.95	126.42
31	5	610	CLA	C1-C2-C3	-3.37	120.22	126.04
38	x	201	SQD	O7-S-C6	-3.37	102.94	106.94
32	6	318	LUT	C31-C30-C29	-3.37	122.50	127.31
31	S	306	CLA	C2D-C1D-ND	3.37	112.59	110.10
31	b	602	CLA	CHD-C1D-ND	-3.37	121.36	124.45
37	2	619	XAT	C6-C7-C8	-3.37	118.87	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	310	CLA	C2C-C1C-NC	3.37	113.13	109.97
37	g	321	XAT	C6-C7-C8	-3.37	118.88	125.99
38	a	412	SQD	O7-S-C6	-3.37	102.94	106.94
43	A	410	BCR	C20-C19-C18	-3.36	116.96	126.42
37	G	620	XAT	C6-C7-C8	-3.36	118.88	125.99
31	b	611	CLA	C1-C2-C3	-3.36	120.22	126.04
31	c	602	CLA	C2C-C1C-NC	3.36	113.12	109.97
31	n	304	CLA	C1-C2-C3	-3.36	120.23	126.04
44	d	407	PL9	C7-C3-C4	3.36	119.61	116.88
35	9	317	RRX	C30-C25-C26	-3.36	117.88	122.61
31	9	304	CLA	C2D-C1D-ND	3.36	112.58	110.10
31	C	609	CLA	CHD-C1D-ND	-3.36	121.37	124.45
30	q	308	CHL	C1-C2-C3	-3.36	121.32	126.75
34	9	301	LMG	O8-C28-C29	3.36	122.45	111.91
32	n	318	LUT	C11-C10-C9	-3.36	122.52	127.31
43	D	405	BCR	C27-C26-C25	-3.36	117.86	122.73
33	e	101	LHG	O8-C23-C24	3.36	122.44	111.91
31	S	312	CLA	C1-O2A-CGA	3.36	125.25	116.44
32	5	616	LUT	C11-C10-C9	-3.36	122.52	127.31
30	G	623	CHL	C3C-C4C-NC	-3.36	106.81	110.57
35	G	614	RRX	C30-C25-C26	-3.35	117.89	122.61
31	8	609	CLA	CHD-C1D-ND	-3.35	121.37	124.45
31	r	316	CLA	C2C-C1C-NC	3.35	113.11	109.97
30	S	309	CHL	C3C-C4C-NC	-3.35	106.81	110.57
31	R	306	CLA	C2C-C1C-NC	3.35	113.11	109.97
43	v	101	BCR	C15-C14-C13	-3.35	122.53	127.31
31	5	603	CLA	CHD-C1D-ND	-3.35	121.38	124.45
30	N	308	CHL	CMA-C3A-C4A	3.35	120.78	111.77
43	D	405	BCR	C10-C11-C12	-3.35	112.77	123.22
30	3	309	CHL	C2C-C3C-C4C	3.35	108.88	106.49
30	0	607	CHL	C4D-CHA-C1A	3.35	125.32	121.25
30	2	601	CHL	C3C-C4C-NC	-3.35	106.82	110.57
32	G	615	LUT	C7-C8-C9	-3.35	121.18	126.23
30	7	307	CHL	C4D-CHA-C1A	3.35	125.32	121.25
47	E	101	HEM	CHB-C1B-NB	3.35	128.51	124.38
31	D	404	CLA	C2D-C1D-ND	3.34	112.57	110.10
31	3	311	CLA	C2C-C1C-NC	3.34	113.11	109.97
31	9	304	CLA	CHD-C1D-ND	-3.34	121.38	124.45
32	s	317	LUT	C31-C30-C29	-3.34	122.54	127.31
31	g	304	CLA	C1-C2-C3	-3.34	120.26	126.04
31	3	316	CLA	CHD-C1D-ND	-3.34	121.38	124.45
31	s	303	CLA	CHD-C1D-ND	-3.34	121.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N	304	CLA	C1-C2-C3	-3.34	120.27	126.04
35	4	615	RRX	C30-C25-C26	-3.34	117.91	122.61
36	p	618	NEX	C38-C25-C26	-3.34	116.67	122.26
30	5	607	CHL	C1-C2-C3	-3.34	121.35	126.75
30	8	608	CHL	C3C-C4C-NC	-3.34	106.83	110.57
32	8	616	LUT	C11-C10-C9	-3.33	122.55	127.31
31	6	311	CLA	CHD-C1D-ND	-3.33	121.39	124.45
32	s	318	LUT	C8-C7-C6	-3.33	117.84	127.20
30	N	302	CHL	C4D-CHA-C1A	3.33	125.31	121.25
31	n	311	CLA	CHD-C1D-ND	-3.33	121.39	124.45
31	s	315	CLA	CHD-C1D-ND	-3.33	121.39	124.45
32	3	317	LUT	C31-C30-C29	-3.33	122.56	127.31
30	n	301	CHL	C4D-CHA-C1A	3.33	125.30	121.25
31	7	311	CLA	CHD-C1D-ND	-3.33	121.39	124.45
31	r	303	CLA	C2D-C1D-ND	3.33	112.56	110.10
36	G	616	NEX	C17-C1-C6	-3.33	107.49	110.47
30	p	607	CHL	C1-C2-C3	-3.33	121.37	126.75
30	q	309	CHL	CMA-C3A-C4A	3.33	120.71	111.77
30	7	308	CHL	C3C-C4C-NC	-3.32	106.84	110.57
32	0	616	LUT	C8-C7-C6	-3.32	117.87	127.20
31	R	315	CLA	C1-C2-C3	-3.32	120.30	126.04
32	S	318	LUT	C11-C10-C9	-3.32	122.57	127.31
32	y	617	LUT	C31-C30-C29	-3.32	122.57	127.31
43	h	101	BCR	C38-C26-C25	-3.32	120.80	124.53
30	n	310	CHL	C1-O2A-CGA	3.32	125.16	116.44
30	1	619	CHL	C2C-C3C-C4C	3.32	108.86	106.49
31	2	604	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	q	306	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	c	609	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	1	603	CLA	C2C-C1C-NC	3.32	113.08	109.97
31	q	312	CLA	C1-C2-C3	-3.32	120.30	126.04
30	7	321	CHL	C3C-C4C-NC	-3.32	106.85	110.57
31	3	306	CLA	CHD-C1D-ND	-3.32	121.41	124.45
30	p	609	CHL	CMA-C3A-C4A	3.32	120.69	111.77
30	N	307	CHL	C3C-C4C-NC	-3.32	106.85	110.57
31	6	303	CLA	CHD-C1D-ND	-3.32	121.41	124.45
30	R	309	CHL	C1-C2-C3	-3.31	120.31	126.04
43	B	619	BCR	C33-C5-C4	3.31	119.98	113.62
31	R	316	CLA	C2C-C1C-NC	3.31	113.08	109.97
31	b	614	CLA	C1-C2-C3	-3.31	120.31	126.04
31	6	316	CLA	C2C-C1C-NC	3.31	113.07	109.97
30	N	308	CHL	C3C-C4C-NC	-3.31	106.86	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	0	604	CLA	CHD-C1D-ND	-3.31	121.41	124.45
31	1	604	CLA	C1-C2-C3	-3.31	120.32	126.04
30	q	308	CHL	CMA-C3A-C4A	3.31	120.66	111.77
30	7	310	CHL	C4D-CHA-C1A	3.31	125.27	121.25
30	5	607	CHL	C3C-C4C-NC	-3.30	106.86	110.57
31	1	604	CLA	CHD-C1D-ND	-3.30	121.42	124.45
30	N	302	CHL	C3C-C4C-NC	-3.30	106.87	110.57
30	g	302	CHL	C3C-C4C-NC	-3.30	106.87	110.57
31	b	608	CLA	C1-C2-C3	-3.30	120.33	126.04
30	y	608	CHL	C3C-C4C-NC	-3.30	106.87	110.57
30	q	310	CHL	C3C-C4C-NC	-3.30	106.87	110.57
31	B	615	CLA	CHD-C1D-ND	-3.30	121.42	124.45
30	n	308	CHL	C3C-C4C-NC	-3.30	106.87	110.57
31	B	604	CLA	CMA-C3A-C4A	3.30	120.64	111.77
31	1	603	CLA	CHD-C1D-ND	-3.30	121.42	124.45
43	b	618	BCR	C20-C21-C22	-3.30	122.61	127.31
31	3	313	CLA	C2C-C1C-NC	3.30	113.06	109.97
30	2	607	CHL	C3C-C4C-NC	-3.29	106.88	110.57
30	1	608	CHL	CMA-C3A-C4A	3.29	120.62	111.77
30	N	306	CHL	C1-O2A-CGA	3.29	125.08	116.44
31	n	315	CLA	C2D-C1D-ND	3.29	112.53	110.10
31	Y	310	CLA	CHD-C1D-ND	-3.29	121.43	124.45
43	D	405	BCR	C12-C13-C14	3.29	123.99	118.94
30	Y	307	CHL	CMA-C3A-C4A	3.29	120.62	111.77
31	s	306	CLA	C1D-ND-C4D	-3.29	104.00	106.33
36	r	319	NEX	C17-C1-C6	-3.29	107.53	110.47
31	S	316	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	y	610	CLA	C1-C2-C3	-3.29	120.35	126.04
31	9	315	CLA	C2C-C1C-NC	3.29	113.05	109.97
32	s	318	LUT	C18-C5-C4	3.29	120.45	114.36
30	q	307	CHL	C4D-CHA-C1A	3.29	125.25	121.25
31	p	611	CLA	C1-C2-C3	-3.29	120.36	126.04
31	3	305	CLA	C1-C2-C3	-3.29	120.36	126.04
31	c	601	CLA	CHD-C1D-ND	-3.29	121.43	124.45
32	Y	316	LUT	C1-C6-C5	-3.29	117.98	122.61
31	5	602	CLA	CHD-C1D-ND	-3.29	121.43	124.45
43	Z	101	BCR	C4-C5-C6	-3.29	117.96	122.73
43	B	618	BCR	C30-C25-C26	-3.29	117.98	122.61
37	R	318	XAT	C38-C25-C26	-3.29	116.75	122.26
30	N	306	CHL	C1-C2-C3	-3.28	120.36	126.04
31	B	607	CLA	C2C-C1C-NC	3.28	113.05	109.97
31	4	614	CLA	CHD-C1D-ND	-3.28	121.44	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	T	101	BCR	C23-C24-C25	-3.28	117.99	127.20
30	7	321	CHL	C4D-CHA-C1A	3.28	125.24	121.25
30	1	605	CHL	CMA-C3A-C4A	3.28	120.59	111.77
30	1	607	CHL	C3C-C4C-NC	-3.28	106.89	110.57
30	0	606	CHL	C1-C2-C3	-3.28	121.45	126.75
30	9	308	CHL	C4D-CHA-C1A	3.28	125.24	121.25
31	N	314	CLA	C2D-C1D-ND	3.28	112.52	110.10
31	5	603	CLA	C6-C5-C3	-3.28	109.26	114.62
30	y	608	CHL	C4D-CHA-C1A	3.28	125.24	121.25
31	2	602	CLA	C2D-C1D-ND	3.28	112.52	110.10
31	R	305	CLA	C2C-C1C-NC	3.27	113.04	109.97
31	q	304	CLA	C1-C2-C3	-3.27	120.38	126.04
32	r	317	LUT	C31-C30-C29	-3.27	122.64	127.31
30	0	601	CHL	C4D-CHA-C1A	3.27	125.23	121.25
30	7	306	CHL	C1-C2-C3	-3.27	120.39	126.04
31	c	609	CLA	CHD-C1D-ND	-3.27	121.45	124.45
30	8	605	CHL	C3C-C4C-NC	-3.27	106.91	110.57
30	5	601	CHL	C4D-CHA-C1A	3.27	125.23	121.25
31	G	603	CLA	C1-C2-C3	-3.27	120.39	126.04
30	y	601	CHL	C3C-C4C-NC	-3.27	106.91	110.57
43	c	615	BCR	C8-C7-C6	-3.27	118.03	127.20
31	S	303	CLA	CHD-C1D-ND	-3.27	121.45	124.45
31	b	616	CLA	CHD-C1D-ND	-3.27	121.45	124.45
31	C	605	CLA	C2C-C1C-NC	3.27	113.03	109.97
32	3	317	LUT	C21-C26-C27	-3.27	108.57	112.70
31	2	602	CLA	C1-C2-C3	-3.27	120.39	126.04
30	q	309	CHL	CHD-C1D-ND	-3.27	121.45	124.45
30	n	306	CHL	C3C-C4C-NC	-3.27	106.91	110.57
31	N	303	CLA	CHD-C1D-ND	-3.26	121.45	124.45
30	6	310	CHL	C3C-C4C-NC	-3.26	106.91	110.57
30	p	607	CHL	C3C-C4C-NC	-3.26	106.91	110.57
31	5	615	CLA	CHD-C1D-ND	-3.26	121.46	124.45
31	Y	313	CLA	C2C-C1C-NC	3.26	113.03	109.97
31	G	602	CLA	CHD-C1D-ND	-3.26	121.46	124.45
31	5	610	CLA	CHD-C1D-ND	-3.26	121.46	124.45
30	7	308	CHL	C2C-C3C-C4C	3.26	108.81	106.49
30	g	306	CHL	C4D-CHA-C1A	3.26	125.21	121.25
31	S	310	CLA	CHD-C1D-ND	-3.26	121.46	124.45
30	8	607	CHL	C3C-C4C-NC	-3.26	106.92	110.57
32	6	317	LUT	C7-C8-C9	-3.26	121.31	126.23
31	q	312	CLA	C1D-ND-C4D	-3.26	104.02	106.33
30	6	306	CHL	C4D-CHA-C1A	3.26	125.21	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	S	302	CHL	C3C-C4C-NC	-3.26	106.92	110.57
30	n	310	CHL	C4D-CHA-C1A	3.25	125.21	121.25
31	C	607	CLA	CHD-C1D-ND	-3.25	121.46	124.45
31	7	305	CLA	C1-C2-C3	-3.25	120.41	126.04
31	b	605	CLA	O2D-CGD-O1D	-3.25	117.47	123.84
43	h	101	BCR	C38-C26-C27	3.25	119.86	113.62
31	R	305	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
30	5	606	CHL	C4D-CHA-C1A	3.25	125.21	121.25
30	6	309	CHL	CMA-C3A-C4A	3.25	120.51	111.77
31	R	306	CLA	CHD-C1D-ND	-3.25	121.47	124.45
30	n	308	CHL	C4D-CHA-C1A	3.25	125.20	121.25
43	D	405	BCR	C2-C1-C6	3.25	115.48	110.48
30	8	608	CHL	C4D-CHA-C1A	3.25	125.20	121.25
31	G	603	CLA	CHD-C1D-ND	-3.25	121.47	124.45
30	q	308	CHL	C1B-CHB-C4A	-3.25	123.69	130.12
30	g	307	CHL	C3C-C4C-NC	-3.25	106.93	110.57
43	b	618	BCR	C16-C15-C14	-3.25	116.82	123.47
31	1	613	CLA	C2C-C1C-NC	3.25	113.01	109.97
31	p	613	CLA	C2C-C1C-NC	3.25	113.01	109.97
30	1	609	CHL	C1-C2-C3	-3.25	120.43	126.04
30	1	608	CHL	C3C-C4C-NC	-3.25	106.93	110.57
35	q	317	RRX	C8-C7-C6	-3.25	118.09	127.20
31	r	311	CLA	CHD-C1D-ND	-3.24	121.47	124.45
31	p	610	CLA	CHD-C1D-ND	-3.24	121.47	124.45
32	2	615	LUT	C7-C8-C9	-3.24	121.33	126.23
34	9	301	LMG	O7-C10-C11	3.24	118.49	111.50
43	B	617	BCR	C16-C15-C14	-3.24	116.83	123.47
31	S	310	CLA	C2C-C1C-NC	3.24	113.01	109.97
43	C	615	BCR	C19-C18-C17	3.24	123.92	118.94
32	7	317	LUT	C18-C5-C6	-3.24	120.89	124.53
31	B	602	CLA	C1-C2-C3	-3.24	120.44	126.04
31	g	305	CLA	C2C-C1C-NC	3.24	113.01	109.97
31	y	613	CLA	C2C-C1C-NC	3.24	113.01	109.97
31	C	606	CLA	CHD-C1D-ND	-3.24	121.47	124.45
31	9	305	CLA	C1-C2-C3	-3.24	120.44	126.04
30	3	310	CHL	C3C-C4C-NC	-3.24	106.94	110.57
30	4	609	CHL	C3C-C4C-NC	-3.24	106.94	110.57
30	Y	307	CHL	C4D-CHA-C1A	3.24	125.19	121.25
30	0	609	CHL	C3C-C4C-NC	-3.24	106.94	110.57
35	9	317	RRX	C33-C5-C4	3.24	119.84	113.62
30	Y	301	CHL	CMA-C3A-C4A	3.24	120.47	111.77
31	R	303	CLA	O2D-CGD-O1D	-3.24	117.51	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	610	CLA	C1-C2-C3	-3.24	120.45	126.04
43	z	101	BCR	C38-C26-C25	-3.24	120.89	124.53
35	4	615	RRX	C33-C5-C4	3.24	119.83	113.62
31	q	313	CLA	C2D-C1D-ND	3.23	112.49	110.10
30	y	607	CHL	C3C-C4C-NC	-3.23	106.94	110.57
31	G	610	CLA	C2C-C1C-NC	3.23	113.00	109.97
31	s	314	CLA	C2C-C1C-NC	3.23	113.00	109.97
31	p	612	CLA	C2D-C1D-ND	3.23	112.49	110.10
31	r	304	CLA	C2D-C1D-ND	3.23	112.49	110.10
30	0	605	CHL	C1-C2-C3	-3.23	120.45	126.04
36	n	319	NEX	C31-C30-C29	3.23	131.92	127.31
31	g	304	CLA	CHD-C1D-ND	-3.23	121.48	124.45
36	S	319	NEX	C17-C1-C6	-3.23	107.58	110.47
43	D	405	BCR	C35-C13-C14	-3.23	118.40	122.92
30	9	309	CHL	C1B-CHB-C4A	-3.23	123.73	130.12
30	s	308	CHL	C3C-C4C-NC	-3.23	106.95	110.57
30	y	601	CHL	C1-C2-C3	-3.23	120.47	126.04
31	y	603	CLA	C1-C2-C3	-3.23	120.47	126.04
30	0	608	CHL	C4D-CHA-C1A	3.23	125.17	121.25
31	b	607	CLA	C1-C2-C3	-3.22	120.47	126.04
31	s	303	CLA	C1-C2-C3	-3.22	120.47	126.04
31	r	305	CLA	CHD-C1D-ND	-3.22	121.49	124.45
31	2	610	CLA	C1-C2-C3	-3.22	120.47	126.04
31	6	315	CLA	C1-C2-C3	-3.22	120.47	126.04
43	A	410	BCR	C4-C5-C6	-3.22	118.05	122.73
31	r	304	CLA	CHD-C1D-ND	-3.22	121.49	124.45
31	p	603	CLA	C2C-C1C-NC	3.22	112.99	109.97
31	7	304	CLA	CHD-C1D-ND	-3.22	121.50	124.45
43	H	101	BCR	C20-C21-C22	-3.22	122.72	127.31
32	0	616	LUT	C35-C15-C14	-3.22	116.88	123.47
31	B	602	CLA	CHD-C1D-ND	-3.22	121.50	124.45
35	2	614	RRX	C29-C28-C27	3.22	114.71	110.30
31	p	603	CLA	C1-C2-C3	-3.22	120.48	126.04
31	a	407	CLA	CHD-C1D-ND	-3.22	121.50	124.45
31	b	603	CLA	CHD-C1D-ND	-3.22	121.50	124.45
31	R	304	CLA	C1-C2-C3	-3.22	120.48	126.04
31	n	304	CLA	CHD-C1D-ND	-3.22	121.50	124.45
30	y	601	CHL	C1-O2A-CGA	3.22	124.88	116.44
31	8	602	CLA	C1-C2-C3	-3.21	120.48	126.04
31	4	610	CLA	C2D-C1D-ND	3.21	112.47	110.10
31	8	613	CLA	C2D-C1D-ND	3.21	112.47	110.10
31	0	602	CLA	CHD-C1D-ND	-3.21	121.50	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	310	CLA	CHD-C1D-ND	-3.21	121.50	124.45
35	G	614	RRX	C33-C5-C4	3.21	119.79	113.62
30	4	607	CHL	C1B-CHB-C4A	-3.21	123.75	130.12
31	4	602	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	C	608	CLA	CHD-C1D-ND	-3.21	121.50	124.45
30	G	623	CHL	C2C-C3C-C4C	3.21	108.78	106.49
31	S	304	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	3	311	CLA	CHD-C1D-ND	-3.21	121.50	124.45
32	1	616	LUT	C21-C26-C27	-3.21	108.64	112.70
31	8	603	CLA	CHD-C1D-ND	-3.21	121.50	124.45
31	8	614	CLA	CHD-C1D-ND	-3.21	121.50	124.45
43	C	615	BCR	C36-C18-C17	-3.21	118.43	122.92
30	6	308	CHL	C4D-CHA-C1A	3.21	125.15	121.25
31	4	604	CLA	C2C-C1C-NC	3.21	112.98	109.97
30	3	308	CHL	CMA-C3A-C4A	3.21	120.39	111.77
32	p	616	LUT	C21-C26-C27	-3.21	108.65	112.70
31	2	613	CLA	CHD-C1D-ND	-3.21	121.51	124.45
31	n	314	CLA	C2C-C1C-NC	3.21	112.98	109.97
30	5	608	CHL	C4D-CHA-C1A	3.21	125.15	121.25
31	9	316	CLA	CHD-C1D-ND	-3.21	121.51	124.45
43	B	617	BCR	C38-C26-C27	3.21	119.77	113.62
30	2	605	CHL	C4D-CHA-C1A	3.20	125.15	121.25
32	0	617	LUT	C31-C30-C29	-3.20	122.74	127.31
31	y	603	CLA	CHD-C1D-ND	-3.20	121.51	124.45
31	G	611	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	a	407	CLA	C2C-C1C-NC	3.20	112.97	109.97
30	Y	302	CHL	C1-O2A-CGA	3.20	124.84	116.44
30	5	608	CHL	C3C-C4C-NC	-3.20	106.98	110.57
35	g	315	RRX	C20-C19-C18	-3.20	117.42	126.42
31	C	607	CLA	C2C-C1C-NC	3.20	112.97	109.97
30	g	306	CHL	CMA-C3A-C4A	3.20	120.38	111.77
30	6	302	CHL	C3C-C4C-NC	-3.20	106.98	110.57
31	6	315	CLA	C2D-C1D-ND	3.20	112.46	110.10
30	9	308	CHL	C1-C2-C3	-3.20	120.51	126.04
31	G	604	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	7	314	CLA	C2C-C1C-NC	3.20	112.97	109.97
32	N	316	LUT	C1-C6-C5	-3.20	118.11	122.61
31	A	407	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	6	311	CLA	C2D-C1D-ND	3.20	112.46	110.10
31	8	612	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	g	313	CLA	C2C-C1C-NC	3.20	112.97	109.97
31	N	303	CLA	C1-C2-C3	-3.20	120.51	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	y	605	CHL	C2C-C3C-C4C	3.20	108.77	106.49
31	q	313	CLA	C1B-NB-C4B	3.20	109.25	106.32
31	7	315	CLA	CHD-C1D-ND	-3.20	121.52	124.45
31	C	604	CLA	CMB-C2B-C3B	3.20	130.66	124.68
43	b	620	BCR	C30-C25-C26	-3.19	118.11	122.61
31	s	312	CLA	C2C-C1C-NC	3.19	112.96	109.97
36	R	319	NEX	C38-C25-C26	-3.19	116.91	122.26
43	d	406	BCR	C30-C25-C26	-3.19	118.11	122.61
43	t	101	BCR	C23-C24-C25	-3.19	118.23	127.20
30	N	307	CHL	C2C-C3C-C4C	3.19	108.77	106.49
30	Y	302	CHL	C2C-C3C-C4C	3.19	108.77	106.49
31	3	312	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	Y	314	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	n	305	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	3	304	CLA	CHD-C1D-ND	-3.19	121.52	124.45
31	G	613	CLA	CHD-C1D-ND	-3.19	121.52	124.45
31	4	611	CLA	C1B-NB-C4B	3.19	109.25	106.32
31	y	604	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	1	612	CLA	CHD-C1D-ND	-3.19	121.52	124.45
30	9	311	CHL	C3C-C4C-NC	-3.19	106.99	110.57
32	R	317	LUT	C8-C7-C6	-3.19	118.24	127.20
43	c	614	BCR	C1-C6-C5	-3.19	118.12	122.61
31	0	613	CLA	C2C-C1C-NC	3.19	112.96	109.97
30	5	609	CHL	C3C-C4C-NC	-3.19	106.99	110.57
31	3	301	CLA	C2D-C1D-ND	3.19	112.45	110.10
31	N	313	CLA	C1-C2-C3	-3.19	120.53	126.04
31	5	614	CLA	C1-C2-C3	-3.19	120.53	126.04
31	s	316	CLA	C2C-C1C-NC	3.19	112.96	109.97
31	N	311	CLA	C2D-C1D-ND	3.19	112.45	110.10
36	R	301	NEX	C40-C33-C34	-3.19	118.46	122.92
30	5	606	CHL	CMA-C3A-C4A	3.18	120.33	111.77
31	6	305	CLA	CHD-C1D-ND	-3.18	121.53	124.45
30	p	606	CHL	C1-C2-C3	-3.18	121.60	126.75
31	n	303	CLA	C2D-C1D-ND	3.18	112.45	110.10
31	2	603	CLA	CHD-C1D-ND	-3.18	121.53	124.45
32	6	317	LUT	C8-C7-C6	-3.18	118.27	127.20
30	4	607	CHL	C2C-C3C-C4C	3.18	108.76	106.49
30	q	308	CHL	C1-O2A-CGA	3.18	124.79	116.44
31	Y	311	CLA	C2C-C1C-NC	3.18	112.95	109.97
43	C	615	BCR	C38-C26-C25	-3.18	120.96	124.53
30	7	307	CHL	C1-O2A-CGA	3.18	124.79	116.44
30	n	309	CHL	C3C-C4C-NC	-3.18	107.00	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	311	CLA	C2C-C1C-NC	3.18	112.95	109.97
31	n	316	CLA	CHD-C1D-ND	-3.18	121.53	124.45
30	p	605	CHL	C4D-CHA-C1A	3.18	125.11	121.25
31	5	612	CLA	C2D-C1D-ND	3.18	112.44	110.10
30	Y	301	CHL	C2C-C3C-C4C	3.17	108.75	106.49
31	6	312	CLA	CMA-C3A-C4A	3.17	120.31	111.77
31	G	604	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	y	615	CLA	C2D-C1D-ND	3.17	112.44	110.10
30	3	307	CHL	C3C-C4C-NC	-3.17	107.01	110.57
32	y	616	LUT	C10-C11-C12	-3.17	113.31	123.22
32	S	317	LUT	C11-C10-C9	-3.17	122.78	127.31
30	4	605	CHL	C4D-CHA-C1A	3.17	125.11	121.25
43	a	410	BCR	C8-C7-C6	-3.17	118.29	127.20
31	b	610	CLA	C2C-C1C-NC	3.17	112.94	109.97
32	S	318	LUT	C7-C8-C9	-3.17	121.44	126.23
30	2	606	CHL	C4D-CHA-C1A	3.17	125.11	121.25
30	s	309	CHL	C3C-C4C-NC	-3.17	107.02	110.57
30	q	310	CHL	C4D-CHA-C1A	3.17	125.11	121.25
31	N	304	CLA	C2C-C1C-NC	3.17	112.94	109.97
31	N	312	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	d	404	CLA	CHD-C1D-ND	-3.17	121.54	124.45
31	p	614	CLA	C1D-ND-C4D	-3.17	104.08	106.33
30	g	309	CHL	C4D-CHA-C1A	3.17	125.11	121.25
31	g	311	CLA	C2C-C1C-NC	3.17	112.94	109.97
32	n	317	LUT	C7-C8-C9	-3.17	121.45	126.23
30	q	310	CHL	C1-O2A-CGA	3.17	124.75	116.44
30	N	307	CHL	CMA-C3A-C4A	3.17	120.29	111.77
43	T	101	BCR	C15-C14-C13	-3.17	122.79	127.31
31	N	304	CLA	CHD-C1D-ND	-3.17	121.54	124.45
30	2	601	CHL	C1-O2A-CGA	3.17	124.75	116.44
30	r	308	CHL	C4D-CHA-C1A	3.17	125.10	121.25
30	6	308	CHL	C3C-C4C-NC	-3.17	107.02	110.57
31	B	606	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	Y	303	CLA	C2C-C1C-NC	3.16	112.94	109.97
31	2	611	CLA	C1-C2-C3	-3.16	120.57	126.04
30	1	619	CHL	CAA-C2A-C3A	-3.16	104.12	112.78
31	0	611	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	y	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	p	612	CLA	C2C-C1C-NC	3.16	112.93	109.97
31	2	609	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	y	602	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	Y	313	CLA	CMA-C3A-C4A	3.16	120.27	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	3	318	LUT	C15-C35-C34	-3.16	117.00	123.47
31	7	313	CLA	CHD-C1D-ND	-3.16	121.55	124.45
34	W	201	LMG	O8-C28-C29	3.16	121.82	111.91
31	C	602	CLA	C2C-C1C-NC	3.16	112.93	109.97
43	v	101	BCR	C4-C5-C6	-3.16	118.15	122.73
31	1	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	g	310	CLA	CHD-C1D-ND	-3.16	121.55	124.45
31	2	609	CLA	C2D-C1D-ND	3.16	112.43	110.10
30	1	606	CHL	C3C-C4C-NC	-3.16	107.03	110.57
32	S	318	LUT	C18-C5-C6	-3.16	120.98	124.53
31	0	614	CLA	CHD-C1D-ND	-3.16	121.55	124.45
30	p	606	CHL	C4D-CHA-C1A	3.16	125.09	121.25
43	d	406	BCR	C1-C6-C5	-3.16	118.17	122.61
31	3	314	CLA	C2C-C1C-NC	3.16	112.93	109.97
35	2	614	RRX	C33-C5-C4	3.16	119.68	113.62
42	A	408	PHO	CMB-C2B-C3B	3.15	130.58	124.68
31	B	612	CLA	C2D-C1D-ND	3.15	112.43	110.10
31	8	604	CLA	C2C-C1C-NC	3.15	112.93	109.97
32	8	615	LUT	C7-C8-C9	-3.15	121.47	126.23
30	5	609	CHL	C4D-CHA-C1A	3.15	125.08	121.25
31	b	613	CLA	C1D-ND-C4D	-3.15	104.10	106.33
30	G	601	CHL	C3C-C4C-NC	-3.15	107.04	110.57
31	2	612	CLA	CMA-C3A-C4A	3.15	120.24	111.77
31	c	605	CLA	C2C-C1C-NC	3.15	112.92	109.97
30	2	608	CHL	C3C-C4C-NC	-3.15	107.04	110.57
31	B	609	CLA	C2C-C1C-NC	3.15	112.92	109.97
34	g	322	LMG	O8-C28-C29	3.15	121.79	111.91
31	S	312	CLA	C1-C2-C3	-3.15	120.60	126.04
43	B	617	BCR	C8-C7-C6	-3.15	118.36	127.20
31	n	303	CLA	CHD-C1D-ND	-3.15	121.56	124.45
30	g	302	CHL	C1-C2-C3	-3.15	120.60	126.04
32	3	318	LUT	C18-C5-C4	3.15	120.18	114.36
43	v	101	BCR	C30-C25-C26	-3.14	118.18	122.61
31	6	314	CLA	C2C-C1C-NC	3.14	112.92	109.97
30	q	310	CHL	CMA-C3A-C4A	3.14	120.22	111.77
31	5	602	CLA	C2D-C1D-ND	3.14	112.42	110.10
30	4	606	CHL	C1-C2-C3	-3.14	121.67	126.75
31	G	604	CLA	C1-C2-C3	-3.14	120.61	126.04
30	4	609	CHL	C4D-CHA-C1A	3.14	125.07	121.25
31	N	321	CLA	CHD-C1D-ND	-3.14	121.57	124.45
37	9	322	XAT	C7-C8-C9	-3.14	120.65	125.53
30	0	608	CHL	C2C-C3C-C4C	3.14	108.73	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	R	317	LUT	C1-C6-C5	-3.14	118.19	122.61
31	7	316	CLA	C2C-C1C-NC	3.14	112.92	109.97
31	n	304	CLA	C2C-C1C-NC	3.14	112.92	109.97
42	A	408	PHO	O2D-CGD-O1D	-3.14	117.70	123.84
31	R	306	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
37	q	321	XAT	C7-C8-C9	-3.14	120.66	125.53
31	q	304	CLA	CHD-C1D-ND	-3.14	121.57	124.45
31	d	401	CLA	C2C-C1C-NC	3.14	112.91	109.97
30	5	606	CHL	C1-C2-C3	-3.14	121.67	126.75
30	y	609	CHL	C3C-C4C-NC	-3.14	107.05	110.57
31	A	409	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	8	611	CLA	CHD-C1D-ND	-3.14	121.57	124.45
43	v	101	BCR	C8-C7-C6	-3.14	118.39	127.20
31	R	303	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	q	312	CLA	CHD-C1D-ND	-3.14	121.57	124.45
46	d	403	BCT	O3-C-O1	-3.14	111.41	119.55
31	b	608	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	n	313	CLA	CHD-C1D-ND	-3.14	121.57	124.45
30	n	309	CHL	CMA-C3A-C4A	3.14	120.20	111.77
31	b	617	CLA	C2C-C1C-NC	3.14	112.91	109.97
31	Y	304	CLA	C1-C2-C3	-3.13	120.62	126.04
43	B	617	BCR	C21-C20-C19	-3.13	113.43	123.22
30	9	307	CHL	C4D-CHA-C1A	3.13	125.06	121.25
32	S	318	LUT	C8-C7-C6	-3.13	118.40	127.20
34	n	322	LMG	O1-C1-C2	3.13	113.20	108.30
31	5	604	CLA	C2C-C1C-NC	3.13	112.91	109.97
30	y	607	CHL	C2C-C3C-C4C	3.13	108.72	106.49
31	b	606	CLA	CHD-C1D-ND	-3.13	121.57	124.45
32	n	318	LUT	C31-C30-C29	-3.13	122.84	127.31
30	3	303	CHL	C3C-C4C-NC	-3.13	107.06	110.57
30	p	605	CHL	C3C-C4C-NC	-3.13	107.06	110.57
30	0	606	CHL	C4D-CHA-C1A	3.13	125.06	121.25
31	b	606	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	b	614	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	g	304	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	c	611	CLA	CHD-C1D-ND	-3.13	121.58	124.45
30	N	301	CHL	C4D-CHA-C1A	3.13	125.06	121.25
31	7	311	CLA	C1-C2-C3	-3.13	120.63	126.04
31	a	409	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	s	305	CLA	C2C-C1C-NC	3.13	112.91	109.97
31	0	610	CLA	C2D-C1D-ND	3.13	112.41	110.10
38	0	621	SQD	O7-S-C6	-3.13	103.22	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	311	CLA	C1-C2-C3	-3.13	120.63	126.04
30	2	608	CHL	C4D-CHA-C1A	3.13	125.06	121.25
31	8	609	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	n	311	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	S	314	CLA	C2C-C1C-NC	3.13	112.90	109.97
31	0	610	CLA	CHD-C1D-ND	-3.13	121.58	124.45
30	R	309	CHL	C3C-C4C-NC	-3.13	107.06	110.57
30	g	307	CHL	CMA-C3A-C4A	3.13	120.18	111.77
31	b	614	CLA	CHD-C1D-ND	-3.13	121.58	124.45
31	r	303	CLA	O1D-CGD-CBD	-3.13	118.08	124.48
31	p	613	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	b	612	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	3	316	CLA	C2C-C1C-NC	3.13	112.90	109.97
31	6	312	CLA	C2C-C1C-NC	3.13	112.90	109.97
31	Y	304	CLA	CHD-C1D-ND	-3.13	121.58	124.45
32	8	616	LUT	C31-C30-C29	-3.13	122.85	127.31
31	2	602	CLA	C1D-ND-C4D	-3.13	104.11	106.33
30	0	607	CHL	C3C-C4C-NC	-3.13	107.06	110.57
37	2	619	XAT	C7-C8-C9	-3.12	120.68	125.53
37	G	620	XAT	C7-C8-C9	-3.12	120.68	125.53
37	g	321	XAT	C7-C8-C9	-3.12	120.68	125.53
30	p	608	CHL	C3C-C4C-NC	-3.12	107.07	110.57
36	5	618	NEX	C17-C1-C6	-3.12	107.68	110.47
30	6	306	CHL	C3C-C4C-NC	-3.12	107.07	110.57
30	G	605	CHL	C3C-C4C-NC	-3.12	107.07	110.57
30	1	609	CHL	C4D-CHA-C1A	3.12	125.05	121.25
30	G	605	CHL	C4D-CHA-C1A	3.12	125.05	121.25
31	r	304	CLA	C2C-C1C-NC	3.12	112.90	109.97
37	4	619	XAT	C7-C8-C9	-3.12	120.69	125.53
31	g	311	CLA	C1-C2-C3	-3.12	120.65	126.04
31	Y	303	CLA	CHD-C1D-ND	-3.12	121.59	124.45
31	s	316	CLA	CHD-C1D-ND	-3.12	121.59	124.45
30	s	307	CHL	C1B-CHB-C4A	-3.12	123.94	130.12
31	8	603	CLA	C2C-C1C-NC	3.12	112.89	109.97
32	y	617	LUT	C8-C7-C6	-3.12	118.44	127.20
31	4	603	CLA	C1-C2-C3	-3.12	120.65	126.04
30	6	302	CHL	C1-C2-C3	-3.12	120.65	126.04
30	1	605	CHL	C1B-CHB-C4A	-3.12	123.94	130.12
43	a	410	BCR	C7-C8-C9	-3.12	121.53	126.23
31	C	603	CLA	CMB-C2B-C3B	3.11	130.51	124.68
31	9	305	CLA	C2C-C1C-NC	3.11	112.89	109.97
31	B	613	CLA	CHD-C1D-ND	-3.11	121.59	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	305	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	4	602	CLA	C2D-C1D-ND	3.11	112.40	110.10
32	r	317	LUT	C30-C31-C32	-3.11	113.50	123.22
31	6	313	CLA	C2D-C1D-ND	3.11	112.40	110.10
43	b	619	BCR	C24-C23-C22	-3.11	121.53	126.23
30	Y	309	CHL	C3C-C4C-NC	-3.11	107.08	110.57
30	2	606	CHL	C3C-C4C-NC	-3.11	107.08	110.57
43	b	619	BCR	C8-C7-C6	-3.11	118.47	127.20
31	2	611	CLA	C2C-C1C-NC	3.11	112.89	109.97
30	Y	309	CHL	C1B-CHB-C4A	-3.11	123.96	130.12
33	t	102	LHG	C5-O7-C7	-3.11	110.14	117.79
31	B	610	CLA	C2C-C1C-NC	3.11	112.88	109.97
31	8	602	CLA	CHD-C1D-ND	-3.11	121.60	124.45
31	r	306	CLA	C2C-C1C-NC	3.11	112.88	109.97
31	r	311	CLA	C2C-C1C-NC	3.11	112.88	109.97
31	6	304	CLA	C2D-C1D-ND	3.11	112.39	110.10
30	0	609	CHL	C4D-CHA-C1A	3.11	125.03	121.25
30	p	609	CHL	C4D-CHA-C1A	3.11	125.03	121.25
30	3	307	CHL	C4D-CHA-C1A	3.11	125.03	121.25
30	7	309	CHL	C4D-CHA-C1A	3.11	125.03	121.25
31	b	608	CLA	CHD-C1D-ND	-3.10	121.60	124.45
30	4	608	CHL	C2C-C3C-C4C	3.10	108.70	106.49
33	b	628	LHG	O8-C23-C24	3.10	121.64	111.91
31	Y	314	CLA	CHD-C1D-ND	-3.10	121.60	124.45
31	0	615	CLA	C2D-C1D-ND	3.10	112.39	110.10
30	2	606	CHL	C1-C2-C3	-3.10	121.73	126.75
30	1	606	CHL	CMA-C3A-C4A	3.10	120.11	111.77
34	9	321	LMG	O8-C28-C29	3.10	121.64	111.91
30	n	307	CHL	C3C-C4C-NC	-3.10	107.09	110.57
31	S	305	CLA	C2C-C1C-NC	3.10	112.88	109.97
43	T	101	BCR	C30-C25-C26	-3.10	118.25	122.61
30	8	606	CHL	C3C-C4C-NC	-3.10	107.09	110.57
30	y	606	CHL	C3C-C4C-NC	-3.10	107.09	110.57
31	7	305	CLA	C2C-C1C-NC	3.10	112.88	109.97
31	s	315	CLA	C2C-C1C-NC	3.10	112.88	109.97
31	9	304	CLA	C1D-ND-C4D	-3.10	104.13	106.33
31	B	611	CLA	C2D-C1D-ND	3.10	112.39	110.10
30	y	606	CHL	C1-O2A-CGA	3.10	124.58	116.44
31	r	307	CLA	CHD-C1D-ND	-3.10	121.61	124.45
31	2	610	CLA	C2D-C1D-ND	3.10	112.39	110.10
31	p	611	CLA	C2D-C1D-ND	3.10	112.39	110.10
43	B	618	BCR	C24-C23-C22	-3.10	121.55	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	312	CLA	C2C-C1C-NC	3.10	112.87	109.97
30	q	307	CHL	C3C-C4C-NC	-3.10	107.10	110.57
31	Y	305	CLA	C2C-C1C-NC	3.10	112.87	109.97
31	S	310	CLA	C1-C2-C3	-3.10	120.69	126.04
32	N	316	LUT	C21-C26-C27	-3.10	108.79	112.70
30	1	609	CHL	C3C-C4C-NC	-3.10	107.10	110.57
31	g	305	CLA	CHD-C1D-ND	-3.10	121.61	124.45
31	N	313	CLA	C2C-C1C-NC	3.10	112.87	109.97
31	7	315	CLA	C2C-C1C-NC	3.10	112.87	109.97
32	g	316	LUT	C18-C5-C4	3.10	120.09	114.36
31	2	610	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	B	606	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	9	313	CLA	C2C-C1C-NC	3.09	112.87	109.97
31	1	602	CLA	C1-C2-C3	-3.09	120.69	126.04
30	9	310	CHL	C3C-C4C-NC	-3.09	107.10	110.57
31	0	604	CLA	C2C-C1C-NC	3.09	112.87	109.97
32	p	617	LUT	C18-C5-C4	3.09	120.08	114.36
30	N	306	CHL	C3C-C4C-NC	-3.09	107.11	110.57
31	n	313	CLA	C2D-C1D-ND	3.09	112.38	110.10
30	7	306	CHL	C3C-C4C-NC	-3.09	107.11	110.57
31	q	316	CLA	CHD-C1D-ND	-3.09	121.61	124.45
31	n	315	CLA	C2C-C1C-NC	3.09	112.87	109.97
30	S	307	CHL	C1B-CHB-C4A	-3.09	124.00	130.12
30	1	608	CHL	C2C-C3C-C4C	3.09	108.69	106.49
30	0	606	CHL	CMA-C3A-C4A	3.09	120.07	111.77
31	3	313	CLA	C2D-C1D-ND	3.09	112.38	110.10
31	S	306	CLA	C1D-ND-C4D	-3.09	104.14	106.33
31	s	306	CLA	CHD-C1D-ND	-3.09	121.62	124.45
31	c	613	CLA	C2C-C1C-NC	3.09	112.86	109.97
30	S	308	CHL	C2C-C3C-C4C	3.09	108.69	106.49
32	s	318	LUT	C18-C5-C6	-3.09	121.06	124.53
32	q	318	LUT	C18-C5-C4	3.09	120.07	114.36
30	g	309	CHL	C2C-C3C-C4C	3.09	108.69	106.49
34	B	621	LMG	O8-C28-C29	3.09	121.59	111.91
31	4	604	CLA	CHD-C1D-ND	-3.09	121.62	124.45
31	A	409	CLA	CHD-C1D-ND	-3.09	121.62	124.45
31	S	303	CLA	C2D-C1D-ND	3.09	112.38	110.10
43	C	615	BCR	C23-C22-C21	3.09	123.68	118.94
30	p	609	CHL	C3C-C4C-NC	-3.09	107.11	110.57
36	g	317	NEX	C38-C25-C26	-3.09	117.09	122.26
31	7	313	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	r	303	CLA	C2C-C1C-NC	3.08	112.86	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	9	317	RRX	C29-C28-C27	3.08	114.53	110.30
31	R	315	CLA	C2C-C1C-NC	3.08	112.86	109.97
30	g	309	CHL	C1B-CHB-C4A	-3.08	124.01	130.12
31	g	310	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	N	315	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	S	312	CLA	CHD-C1D-ND	-3.08	121.62	124.45
30	4	601	CHL	C3C-C4C-NC	-3.08	107.11	110.57
31	b	609	CLA	C2C-C1C-NC	3.08	112.86	109.97
30	q	303	CHL	C3C-C4C-NC	-3.08	107.11	110.57
31	5	613	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	3	315	CLA	C2D-C1D-ND	3.08	112.37	110.10
30	Y	307	CHL	C3C-C4C-NC	-3.08	107.12	110.57
31	3	315	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	C	611	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	b	615	CLA	CHD-C1D-ND	-3.08	121.62	124.45
31	4	611	CLA	C2D-C1D-ND	3.08	112.37	110.10
33	g	319	LHG	O8-C23-C24	3.08	121.57	111.91
31	q	305	CLA	CMA-C3A-C4A	3.08	120.05	111.77
31	8	611	CLA	C2D-C1D-ND	3.08	112.37	110.10
31	c	607	CLA	C2C-C1C-NC	3.08	112.86	109.97
31	7	316	CLA	CHD-C1D-ND	-3.08	121.63	124.45
30	s	302	CHL	C3C-C4C-NC	-3.08	107.12	110.57
35	4	615	RRX	C29-C28-C27	3.08	114.52	110.30
46	D	402	BCT	O2-C-O1	-3.08	111.56	119.55
32	6	317	LUT	C15-C14-C13	-3.08	122.92	127.31
31	S	316	CLA	C2C-C1C-NC	3.08	112.85	109.97
31	s	304	CLA	C2C-C1C-NC	3.08	112.85	109.97
31	y	612	CLA	CHD-C1D-ND	-3.08	121.63	124.45
32	s	318	LUT	C11-C10-C9	-3.08	122.92	127.31
30	8	607	CHL	CMA-C3A-C4A	3.08	120.04	111.77
31	1	614	CLA	C2D-C1D-ND	3.07	112.37	110.10
31	S	304	CLA	C2D-C1D-ND	3.07	112.37	110.10
30	Y	307	CHL	C1B-CHB-C4A	-3.07	124.03	130.12
31	8	613	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	d	405	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	C	612	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
32	6	318	LUT	C21-C26-C27	-3.07	108.82	112.70
31	9	306	CLA	C2C-C1C-NC	3.07	112.85	109.97
30	p	607	CHL	C1B-CHB-C4A	-3.07	124.03	130.12
31	g	312	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	q	316	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	c	601	CLA	O2D-CGD-O1D	-3.07	117.83	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	315	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	c	612	CLA	CHD-C1D-ND	-3.07	121.63	124.45
30	2	607	CHL	C1-O2A-CGA	3.07	124.50	116.44
31	c	606	CLA	C1C-C2C-C3C	-3.07	103.73	106.96
34	k	101	LMG	O8-C28-C29	3.07	121.55	111.91
31	N	305	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	g	314	CLA	C2D-C1D-ND	3.07	112.37	110.10
31	Y	305	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	p	602	CLA	C2C-C1C-NC	3.07	112.85	109.97
31	7	305	CLA	CHD-C1D-ND	-3.07	121.63	124.45
31	0	612	CLA	CHD-C1D-ND	-3.07	121.63	124.45
30	7	321	CHL	CMA-C3A-C4A	3.07	120.02	111.77
30	g	308	CHL	C3C-C4C-NC	-3.07	107.13	110.57
35	G	614	RRX	C29-C28-C27	3.07	114.50	110.30
31	p	614	CLA	C2D-C1D-ND	3.07	112.36	110.10
30	5	608	CHL	CMA-C3A-C4A	3.07	120.02	111.77
31	3	304	CLA	CMA-C3A-C4A	3.07	120.02	111.77
31	0	613	CLA	CHD-C1D-ND	-3.07	121.64	124.45
32	5	616	LUT	C31-C30-C29	-3.07	122.93	127.31
31	Y	314	CLA	C2D-C1D-ND	3.07	112.36	110.10
37	r	318	XAT	C6-C7-C8	-3.07	119.51	125.99
31	5	611	CLA	C1-C2-C3	-3.07	120.74	126.04
43	B	619	BCR	C1-C6-C5	-3.06	118.30	122.61
30	6	307	CHL	C3C-C4C-NC	-3.06	107.14	110.57
31	8	602	CLA	C2D-C1D-ND	3.06	112.36	110.10
30	y	607	CHL	C1-O2A-CGA	3.06	124.48	116.44
31	7	313	CLA	C1-C2-C3	-3.06	120.75	126.04
31	C	611	CLA	C2C-C1C-NC	3.06	112.84	109.97
31	b	615	CLA	C2D-C1D-ND	3.06	112.36	110.10
31	b	611	CLA	CHD-C1D-ND	-3.06	121.64	124.45
30	n	308	CHL	CMA-C3A-C4A	3.06	120.00	111.77
31	2	602	CLA	C2C-C1C-NC	3.06	112.84	109.97
30	N	309	CHL	C2C-C3C-C4C	3.06	108.67	106.49
30	8	601	CHL	C2C-C3C-C4C	3.06	108.67	106.49
36	2	616	NEX	C38-C25-C26	-3.06	117.13	122.26
31	s	304	CLA	C2D-C1D-ND	3.06	112.36	110.10
30	6	309	CHL	C2C-C3C-C4C	3.06	108.67	106.49
31	0	611	CLA	C2C-C1C-NC	3.06	112.84	109.97
30	y	609	CHL	C1-O2A-CGA	3.06	124.47	116.44
31	5	602	CLA	C2C-C1C-NC	3.06	112.84	109.97
30	g	307	CHL	C4D-CHA-C1A	3.06	124.97	121.25
43	B	619	BCR	C8-C7-C6	-3.06	118.62	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	611	CLA	C2C-C1C-NC	3.06	112.83	109.97
31	s	304	CLA	CHD-C1D-ND	-3.06	121.65	124.45
30	8	605	CHL	C2C-C3C-C4C	3.06	108.67	106.49
43	c	615	BCR	C30-C25-C26	-3.06	118.31	122.61
31	R	304	CLA	C2C-C1C-NC	3.06	112.83	109.97
31	2	603	CLA	C2D-C1D-ND	3.05	112.36	110.10
31	d	405	CLA	C2D-C1D-ND	3.05	112.36	110.10
31	9	313	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	3	306	CLA	C2C-C1C-NC	3.05	112.83	109.97
31	7	312	CLA	C2C-C1C-NC	3.05	112.83	109.97
30	p	601	CHL	C1-C2-C3	-3.05	121.81	126.75
31	C	601	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	G	612	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	7	303	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	9	306	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	2	607	CHL	C2C-C3C-C4C	3.05	108.67	106.49
36	q	319	NEX	O24-C25-C38	-3.05	111.40	115.06
31	5	611	CLA	C2C-C1C-NC	3.05	112.83	109.97
43	Z	101	BCR	C30-C25-C26	-3.05	118.31	122.61
32	p	616	LUT	C31-C30-C29	3.05	131.66	127.31
32	Y	315	LUT	C30-C31-C32	-3.05	113.70	123.22
31	0	613	CLA	CMA-C3A-C4A	3.05	119.97	111.77
30	R	310	CHL	C2C-C3C-C4C	3.05	108.66	106.49
31	c	608	CLA	CHD-C1D-ND	-3.05	121.65	124.45
30	n	302	CHL	C2C-C3C-C4C	3.05	108.66	106.49
30	n	306	CHL	C2C-C3C-C4C	3.05	108.66	106.49
31	y	611	CLA	CHD-C1D-ND	-3.05	121.65	124.45
31	B	610	CLA	C2D-C1D-ND	3.05	112.35	110.10
30	6	306	CHL	CMA-C3A-C4A	3.05	119.96	111.77
31	p	603	CLA	C1-O2A-CGA	3.05	124.44	116.44
31	S	305	CLA	CHD-C1D-ND	-3.05	121.66	124.45
31	n	304	CLA	CMA-C3A-C4A	3.05	119.96	111.77
30	q	311	CHL	C4D-CHA-C1A	3.05	124.95	121.25
30	7	302	CHL	C3C-C4C-NC	-3.05	107.16	110.57
31	6	303	CLA	C2C-C1C-NC	3.04	112.82	109.97
32	0	616	LUT	C1-C6-C5	-3.04	118.33	122.61
30	s	309	CHL	CMA-C3A-C4A	3.04	119.95	111.77
31	3	304	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	8	610	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	c	603	CLA	CMA-C3A-C4A	3.04	119.95	111.77
31	6	314	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	B	605	CLA	CHD-C1D-ND	-3.04	121.66	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	n	310	CHL	C1B-CHB-C4A	-3.04	124.09	130.12
31	q	304	CLA	CMA-C3A-C4A	3.04	119.95	111.77
31	4	604	CLA	C2D-C1D-ND	3.04	112.34	110.10
31	Y	310	CLA	C2D-C1D-ND	3.04	112.34	110.10
31	9	315	CLA	CMA-C3A-C4A	3.04	119.95	111.77
30	p	601	CHL	CMA-C3A-C4A	3.04	119.94	111.77
32	6	317	LUT	C11-C10-C9	-3.04	122.97	127.31
30	y	609	CHL	C1B-CHB-C4A	-3.04	124.10	130.12
31	2	613	CLA	C2C-C1C-NC	3.04	112.82	109.97
30	7	309	CHL	CMA-C3A-C4A	3.04	119.94	111.77
31	7	303	CLA	C2D-C1D-ND	3.04	112.34	110.10
31	6	313	CLA	C2C-C1C-NC	3.04	112.82	109.97
31	N	314	CLA	C2C-C1C-NC	3.04	112.82	109.97
43	A	410	BCR	C23-C24-C25	-3.04	118.67	127.20
31	C	612	CLA	CHD-C1D-ND	-3.04	121.66	124.45
30	g	306	CHL	C3C-C4C-NC	-3.04	107.17	110.57
30	G	623	CHL	C4D-CHA-C1A	3.04	124.94	121.25
31	s	303	CLA	C2D-C1D-ND	3.04	112.34	110.10
30	r	309	CHL	C3C-C4C-NC	-3.04	107.17	110.57
31	G	609	CLA	C1-C2-C3	-3.04	120.79	126.04
31	a	409	CLA	CHD-C1D-ND	-3.04	121.66	124.45
31	4	603	CLA	C2C-C1C-NC	3.04	112.82	109.97
30	G	608	CHL	C4D-CHA-C1A	3.04	124.94	121.25
34	0	620	LMG	O1-C1-C2	3.04	113.04	108.30
31	4	603	CLA	CMA-C3A-C4A	3.04	119.93	111.77
32	1	615	LUT	C35-C15-C14	-3.03	117.26	123.47
31	B	602	CLA	C2C-C1C-NC	3.03	112.81	109.97
30	Y	301	CHL	C4D-CHA-C1A	3.03	124.94	121.25
31	2	611	CLA	C2D-C1D-ND	3.03	112.34	110.10
36	8	617	NEX	C38-C25-C26	-3.03	117.18	122.26
31	4	613	CLA	CHD-C1D-ND	-3.03	121.67	124.45
36	4	617	NEX	O24-C25-C38	-3.03	111.42	115.06
31	1	614	CLA	C2C-C1C-NC	3.03	112.81	109.97
30	8	607	CHL	C4D-CHA-C1A	3.03	124.94	121.25
31	B	605	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	A	406	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
31	r	305	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	b	604	CLA	C1-C2-C3	-3.03	120.80	126.04
31	S	313	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
30	q	310	CHL	C2C-C3C-C4C	3.03	108.65	106.49
43	b	619	BCR	C38-C26-C27	3.03	119.44	113.62
32	1	615	LUT	C30-C31-C32	-3.03	113.76	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	R	308	CHL	C1B-CHB-C4A	-3.03	124.12	130.12
31	5	614	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	b	604	CLA	CMB-C2B-C3B	3.03	130.34	124.68
31	q	313	CLA	C2C-C1C-NC	3.03	112.81	109.97
31	c	611	CLA	CMA-C3A-C4A	3.03	119.91	111.77
36	0	618	NEX	C17-C1-C6	-3.03	107.76	110.47
30	7	306	CHL	C1-O2A-CGA	3.03	124.39	116.44
30	5	606	CHL	C1B-CHB-C4A	-3.03	124.12	130.12
33	A	415	LHG	C5-O7-C7	-3.03	110.34	117.79
31	C	610	CLA	C2C-C1C-NC	3.03	112.81	109.97
30	7	307	CHL	C3C-C4C-NC	-3.03	107.18	110.57
32	r	317	LUT	C35-C15-C14	-3.03	117.27	123.47
30	g	308	CHL	C1-O2A-CGA	3.03	124.39	116.44
30	g	308	CHL	C4D-CHA-C1A	3.03	124.93	121.25
31	6	303	CLA	C2D-C1D-ND	3.03	112.33	110.10
31	N	321	CLA	C2D-C1D-ND	3.03	112.33	110.10
31	6	313	CLA	CMA-C3A-C4A	3.03	119.91	111.77
30	6	307	CHL	C1-C2-C3	-3.03	121.86	126.75
31	6	311	CLA	CMA-C3A-C4A	3.03	119.91	111.77
30	7	310	CHL	C3C-C4C-NC	-3.03	107.18	110.57
31	y	615	CLA	CHD-C1D-ND	-3.03	121.67	124.45
31	8	603	CLA	CMA-C3A-C4A	3.02	119.90	111.77
32	s	318	LUT	C31-C30-C29	-3.02	122.99	127.31
31	S	311	CLA	C2C-C1C-NC	3.02	112.81	109.97
31	q	314	CLA	C2C-C1C-NC	3.02	112.81	109.97
30	0	609	CHL	C1B-CHB-C4A	-3.02	124.13	130.12
30	9	303	CHL	C4D-CHA-C1A	3.02	124.93	121.25
30	7	302	CHL	C1-O2A-CGA	3.02	124.38	116.44
34	C	619	LMG	O8-C28-C29	3.02	121.40	111.91
31	2	604	CLA	C2D-C1D-ND	3.02	112.33	110.10
32	s	318	LUT	C7-C8-C9	-3.02	121.67	126.23
31	y	612	CLA	C2C-C1C-NC	3.02	112.80	109.97
33	A	415	LHG	O8-C23-C24	3.02	121.39	111.91
30	n	301	CHL	C3C-C4C-NC	-3.02	107.18	110.57
31	B	610	CLA	CMA-C3A-C4A	3.02	119.90	111.77
31	d	404	CLA	C1-C2-C3	-3.02	120.82	126.04
31	5	604	CLA	C2D-C1D-ND	3.02	112.33	110.10
43	v	101	BCR	C23-C24-C25	-3.02	118.72	127.20
31	B	603	CLA	CMB-C2B-C3B	3.02	130.33	124.68
43	T	101	BCR	C2-C1-C6	3.02	115.13	110.48
31	3	301	CLA	CMA-C3A-C4A	3.02	119.89	111.77
31	s	314	CLA	CHD-C1D-ND	-3.02	121.68	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	302	CHL	C1B-CHB-C4A	-3.02	124.14	130.12
32	r	317	LUT	C10-C11-C12	-3.02	113.79	123.22
31	5	612	CLA	CMA-C3A-C4A	3.02	119.89	111.77
33	K	102	LHG	O8-C23-C24	3.02	121.39	111.91
31	G	603	CLA	C2C-C1C-NC	3.02	112.80	109.97
31	q	305	CLA	CHD-C1D-ND	-3.02	121.68	124.45
36	Y	317	NEX	C17-C1-C6	-3.02	107.77	110.47
30	s	308	CHL	C2C-C3C-C4C	3.02	108.64	106.49
31	2	603	CLA	C2C-C1C-NC	3.02	112.80	109.97
31	3	315	CLA	CHD-C1D-ND	-3.02	121.68	124.45
30	7	310	CHL	C1-C2-C3	-3.02	120.82	126.04
30	6	302	CHL	C4D-CHA-C1A	3.02	124.92	121.25
30	n	309	CHL	C4D-CHA-C1A	3.02	124.92	121.25
37	g	321	XAT	C38-C25-C26	-3.02	117.20	122.26
30	7	302	CHL	C1B-CHB-C4A	-3.02	124.14	130.12
31	C	605	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
31	b	611	CLA	C2C-C1C-NC	3.02	112.80	109.97
30	5	605	CHL	C3C-C4C-NC	-3.02	107.19	110.57
30	6	307	CHL	C4D-CHA-C1A	3.02	124.92	121.25
30	Y	308	CHL	CMA-C3A-C4A	3.02	119.88	111.77
31	3	304	CLA	C2D-C1D-ND	3.02	112.33	110.10
31	7	312	CLA	C2D-C1D-ND	3.02	112.33	110.10
31	8	610	CLA	C2D-C1D-ND	3.02	112.33	110.10
30	9	307	CHL	CMA-C3A-C4A	3.01	119.88	111.77
30	6	309	CHL	C4D-CHA-C1A	3.01	124.92	121.25
30	0	601	CHL	C3C-C4C-NC	-3.01	107.19	110.57
30	6	308	CHL	C2C-C3C-C4C	3.01	108.64	106.49
31	9	304	CLA	C2C-C1C-NC	3.01	112.80	109.97
43	B	619	BCR	C15-C16-C17	-3.01	117.30	123.47
37	r	318	XAT	C7-C8-C9	-3.01	120.85	125.53
31	4	602	CLA	C2C-C1C-NC	3.01	112.80	109.97
31	0	614	CLA	C2C-C1C-NC	3.01	112.80	109.97
31	8	614	CLA	C2C-C1C-NC	3.01	112.80	109.97
31	r	316	CLA	CMA-C3A-C4A	3.01	119.87	111.77
30	Y	309	CHL	C1-C2-C3	-3.01	120.83	126.04
30	6	310	CHL	CMA-C3A-C4A	3.01	119.87	111.77
30	7	307	CHL	CMA-C3A-C4A	3.01	119.87	111.77
31	3	312	CLA	CMA-C3A-C4A	3.01	119.87	111.77
35	g	315	RRX	C11-C12-C13	-3.01	117.95	126.42
31	6	315	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	9	312	CLA	C2D-C1D-ND	3.01	112.32	110.10
31	S	313	CLA	CHD-C1D-ND	-3.01	121.69	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	616	LUT	C15-C14-C13	-3.01	123.01	127.31
31	3	305	CLA	CMA-C3A-C4A	3.01	119.86	111.77
31	0	603	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	0	603	CLA	C1-C2-C3	-3.01	120.84	126.04
31	B	603	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	R	313	CLA	C2C-C1C-NC	3.01	112.79	109.97
34	0	620	LMG	C8-O7-C10	-3.01	110.39	117.79
31	6	305	CLA	C2C-C1C-NC	3.01	112.79	109.97
30	1	609	CHL	C1B-CHB-C4A	-3.01	124.16	130.12
43	B	618	BCR	C16-C17-C18	-3.01	123.02	127.31
31	n	312	CLA	C2C-C1C-NC	3.01	112.79	109.97
31	g	310	CLA	C1-C2-C3	-3.01	120.84	126.04
30	q	303	CHL	C4D-CHA-C1A	3.01	124.91	121.25
43	c	614	BCR	C27-C26-C25	-3.01	118.37	122.73
30	3	302	CHL	C2C-C3C-C4C	3.01	108.63	106.49
31	8	604	CLA	CHD-C1D-ND	-3.01	121.69	124.45
30	Y	308	CHL	C3C-C4C-NC	-3.00	107.20	110.57
30	1	607	CHL	C2C-C3C-C4C	3.00	108.63	106.49
31	g	313	CLA	CHD-C1D-ND	-3.00	121.69	124.45
31	D	404	CLA	O2D-CGD-O1D	-3.00	117.96	123.84
31	5	610	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	5	614	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	8	612	CLA	C2D-C1D-ND	3.00	112.32	110.10
31	c	605	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
31	S	306	CLA	CHD-C1D-ND	-3.00	121.69	124.45
31	b	612	CLA	CHD-C1D-ND	-3.00	121.69	124.45
31	2	603	CLA	CMA-C3A-C4A	3.00	119.84	111.77
31	6	314	CLA	C2D-C1D-ND	3.00	112.32	110.10
30	4	606	CHL	CMA-C3A-C4A	3.00	119.84	111.77
31	S	315	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	5	613	CLA	CHD-C1D-ND	-3.00	121.69	124.45
31	C	603	CLA	CMA-C3A-C4A	3.00	119.84	111.77
30	0	605	CHL	C1B-CHB-C4A	-3.00	124.17	130.12
31	b	611	CLA	C2D-C1D-ND	3.00	112.32	110.10
30	r	308	CHL	C3C-C4C-NC	-3.00	107.20	110.57
31	p	610	CLA	C1-C2-C3	-3.00	120.86	126.04
31	6	313	CLA	CHD-C1D-ND	-3.00	121.70	124.45
31	N	312	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	p	611	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	c	603	CLA	C2C-C1C-NC	3.00	112.78	109.97
37	q	321	XAT	C38-C25-C26	-3.00	117.24	122.26
31	5	604	CLA	CHD-C1D-ND	-3.00	121.70	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	609	CLA	CHD-C1D-ND	-3.00	121.70	124.45
30	5	608	CHL	C1B-CHB-C4A	-3.00	124.18	130.12
31	y	610	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	y	614	CLA	C2D-C1D-ND	3.00	112.31	110.10
31	2	609	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	4	614	CLA	C2C-C1C-NC	3.00	112.78	109.97
31	B	612	CLA	C1-C2-C3	-3.00	120.86	126.04
31	9	306	CLA	C2D-C1D-ND	3.00	112.31	110.10
36	N	318	NEX	C39-C29-C30	-3.00	118.73	122.92
43	a	410	BCR	C16-C17-C18	-3.00	123.03	127.31
31	C	611	CLA	CMA-C3A-C4A	3.00	119.83	111.77
31	N	311	CLA	C2C-C1C-NC	3.00	112.78	109.97
34	0	622	LMG	O8-C28-C29	3.00	121.31	111.91
31	0	612	CLA	C2C-C1C-NC	2.99	112.78	109.97
31	7	311	CLA	C1D-ND-C4D	-2.99	104.21	106.33
31	6	314	CLA	CMA-C3A-C4A	2.99	119.82	111.77
31	r	304	CLA	C1-C2-C3	-2.99	120.87	126.04
43	T	101	BCR	C24-C23-C22	-2.99	121.71	126.23
37	2	619	XAT	C38-C25-C26	-2.99	117.24	122.26
31	6	311	CLA	C2C-C1C-NC	2.99	112.78	109.97
30	0	607	CHL	C1-C2-C3	-2.99	120.87	126.04
31	6	315	CLA	C1D-ND-C4D	-2.99	104.21	106.33
32	r	317	LUT	C15-C35-C34	-2.99	117.34	123.47
31	B	609	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	D	403	CLA	C2C-C1C-NC	2.99	112.78	109.97
43	h	101	BCR	C2-C1-C6	2.99	115.09	110.48
30	0	609	CHL	C1-O2A-CGA	2.99	124.29	116.44
31	C	609	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
31	1	610	CLA	C1D-ND-C4D	-2.99	104.21	106.33
31	5	610	CLA	C1D-ND-C4D	-2.99	104.21	106.33
31	N	310	CLA	CMA-C3A-C4A	2.99	119.81	111.77
31	N	303	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	c	611	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	5	611	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	N	310	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	n	314	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	B	610	CLA	CHD-C1D-ND	-2.99	121.71	124.45
31	9	315	CLA	CHD-C1D-ND	-2.99	121.71	124.45
31	1	611	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	2	612	CLA	CHD-C1D-ND	-2.99	121.71	124.45
31	N	315	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	s	303	CLA	C2C-C1C-NC	2.99	112.77	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1	615	LUT	C10-C11-C12	-2.99	113.89	123.22
30	Y	301	CHL	C1-C2-C3	-2.99	120.88	126.04
31	n	305	CLA	CHD-C1D-ND	-2.99	121.71	124.45
31	3	305	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	6	304	CLA	C2C-C1C-NC	2.99	112.77	109.97
31	4	614	CLA	CMA-C3A-C4A	2.99	119.80	111.77
30	9	303	CHL	C3C-C4C-NC	-2.99	107.22	110.57
45	C	618	DGD	O2G-C1B-C2B	2.99	117.94	111.50
31	N	305	CLA	C2D-C1D-ND	2.99	112.31	110.10
34	n	322	LMG	O8-C28-C29	2.99	121.28	111.91
31	4	610	CLA	C1-C2-C3	-2.99	120.88	126.04
31	r	313	CLA	C2C-C1C-NC	2.99	112.77	109.97
43	c	614	BCR	C38-C26-C27	2.98	119.35	113.62
30	7	308	CHL	C4D-CHA-C1A	2.98	124.88	121.25
30	r	308	CHL	CMA-C3A-C4A	2.98	119.79	111.77
31	N	304	CLA	C2D-C1D-ND	2.98	112.30	110.10
31	7	315	CLA	C2D-C1D-ND	2.98	112.30	110.10
31	n	316	CLA	C2D-C1D-ND	2.98	112.30	110.10
31	g	314	CLA	CHD-C1D-ND	-2.98	121.71	124.45
31	B	613	CLA	C2C-C1C-NC	2.98	112.77	109.97
30	1	619	CHL	C4D-CHA-C1A	2.98	124.88	121.25
31	c	607	CLA	CHD-C1D-ND	-2.98	121.71	124.45
30	G	606	CHL	C3C-C4C-NC	-2.98	107.23	110.57
31	N	303	CLA	C2D-C1D-ND	2.98	112.30	110.10
31	7	303	CLA	C2C-C1C-NC	2.98	112.77	109.97
37	4	619	XAT	C38-C25-C26	-2.98	117.26	122.26
31	Y	310	CLA	C1D-ND-C4D	-2.98	104.22	106.33
31	q	305	CLA	C2C-C1C-NC	2.98	112.76	109.97
34	b	622	LMG	O8-C28-C29	2.98	121.26	111.91
30	6	302	CHL	C1-O2A-CGA	2.98	124.26	116.44
31	y	604	CLA	CHD-C1D-ND	-2.98	121.72	124.45
31	g	314	CLA	C2C-C1C-NC	2.98	112.76	109.97
31	r	315	CLA	C1-O2A-CGA	2.98	124.26	116.44
36	6	319	NEX	C17-C1-C6	-2.98	107.81	110.47
31	8	604	CLA	C2D-C1D-ND	2.98	112.30	110.10
30	p	606	CHL	C3C-C4C-NC	-2.98	107.23	110.57
31	y	602	CLA	C2C-C1C-NC	2.98	112.76	109.97
30	r	309	CHL	C4D-CHA-C1A	2.98	124.87	121.25
31	7	315	CLA	C1-C2-C3	-2.98	120.89	126.04
31	S	304	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
31	a	407	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
31	g	312	CLA	C2D-C1D-ND	2.98	112.30	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	621	LMG	O8-C28-C29	2.98	121.25	111.91
33	5	619	LHG	C5-O7-C7	-2.98	110.46	117.79
31	4	602	CLA	CMA-C3A-C4A	2.98	119.77	111.77
36	n	319	NEX	C39-C29-C30	-2.98	118.75	122.92
33	e	101	LHG	C5-O7-C7	-2.98	110.46	117.79
42	D	401	PHO	O2D-CGD-O1D	-2.98	118.02	123.84
45	C	617	DGD	O2G-C1B-C2B	2.98	117.92	111.50
30	8	608	CHL	C1B-CHB-C4A	-2.98	124.22	130.12
30	p	605	CHL	C2C-C3C-C4C	2.98	108.61	106.49
31	8	609	CLA	CMA-C3A-C4A	2.98	119.77	111.77
31	G	612	CLA	C2C-C1C-NC	2.97	112.76	109.97
35	2	614	RRX	C20-C19-C18	-2.97	118.06	126.42
31	n	303	CLA	CMA-C3A-C4A	2.97	119.77	111.77
30	7	321	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
30	N	302	CHL	C1-O2A-CGA	2.97	124.25	116.44
31	9	304	CLA	CMA-C3A-C4A	2.97	119.77	111.77
31	b	607	CLA	O2A-CGA-CBA	2.97	121.24	111.91
30	n	308	CHL	C1B-CHB-C4A	-2.97	124.23	130.12
31	s	312	CLA	CHD-C1D-ND	-2.97	121.72	124.45
31	C	608	CLA	C2C-C1C-NC	2.97	112.76	109.97
30	N	301	CHL	C3C-C4C-NC	-2.97	107.24	110.57
32	7	317	LUT	C1-C6-C5	-2.97	118.42	122.61
37	9	322	XAT	C38-C25-C26	-2.97	117.28	122.26
43	V	101	BCR	C8-C7-C6	-2.97	118.85	127.20
30	G	623	CHL	C1-O2A-CGA	2.97	124.24	116.44
30	N	309	CHL	C4D-CHA-C1A	2.97	124.87	121.25
31	q	314	CLA	CHD-C1D-ND	-2.97	121.72	124.45
31	0	615	CLA	C2C-C1C-NC	2.97	112.76	109.97
31	r	311	CLA	O2A-CGA-CBA	2.97	121.24	111.91
31	C	602	CLA	C1-C2-C3	-2.97	120.90	126.04
31	5	603	CLA	C2D-C1D-ND	2.97	112.29	110.10
31	p	615	CLA	C2D-C1D-ND	2.97	112.29	110.10
31	r	304	CLA	CMA-C3A-C4A	2.97	119.76	111.77
32	8	615	LUT	C21-C26-C27	-2.97	108.94	112.70
31	1	611	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	3	313	CLA	CHD-C1D-ND	-2.97	121.72	124.45
30	0	608	CHL	CMA-C3A-C4A	2.97	119.75	111.77
31	R	307	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
30	G	601	CHL	C4D-CHA-C1A	2.97	124.86	121.25
31	1	604	CLA	C2C-C1C-NC	2.97	112.75	109.97
43	c	615	BCR	C33-C5-C4	2.97	119.32	113.62
31	2	613	CLA	C2D-C1D-ND	2.97	112.29	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	304	CLA	C2D-C1D-ND	2.97	112.29	110.10
31	8	602	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	0	610	CLA	C1D-ND-C4D	-2.97	104.23	106.33
31	B	608	CLA	C2C-C1C-NC	2.97	112.75	109.97
31	2	609	CLA	C1-C2-C3	-2.97	120.91	126.04
43	v	101	BCR	C10-C11-C12	-2.97	113.96	123.22
30	2	607	CHL	CMA-C3A-C4A	2.97	119.74	111.77
30	8	608	CHL	C2C-C3C-C4C	2.97	108.60	106.49
30	n	310	CHL	C2C-C3C-C4C	2.97	108.60	106.49
30	6	309	CHL	C1B-CHB-C4A	-2.97	124.24	130.12
43	B	618	BCR	C15-C16-C17	-2.97	117.40	123.47
31	b	602	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
30	y	608	CHL	CMA-C3A-C4A	2.96	119.74	111.77
31	r	305	CLA	CMA-C3A-C4A	2.96	119.74	111.77
31	5	612	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	y	610	CLA	C1D-ND-C4D	-2.96	104.23	106.33
36	6	319	NEX	C26-C27-C28	-2.96	119.73	125.99
30	9	309	CHL	C3C-C4C-NC	-2.96	107.25	110.57
30	7	307	CHL	C1B-CHB-C4A	-2.96	124.25	130.12
31	y	602	CLA	C2D-C1D-ND	2.96	112.29	110.10
31	C	604	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	2	609	CLA	C1D-ND-C4D	-2.96	104.23	106.33
30	G	607	CHL	CMA-C3A-C4A	2.96	119.73	111.77
31	8	602	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	g	303	CLA	C1-O2A-CGA	2.96	124.21	116.44
36	N	318	NEX	C17-C1-C6	-2.96	107.82	110.47
31	B	616	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
37	G	620	XAT	C38-C25-C26	-2.96	117.30	122.26
31	p	602	CLA	CHD-C1D-ND	-2.96	121.73	124.45
30	R	309	CHL	C4D-CHA-C1A	2.96	124.85	121.25
31	r	313	CLA	CHD-C1D-ND	-2.96	121.73	124.45
33	A	417	LHG	O8-C23-C24	2.96	121.19	111.91
31	R	313	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	N	321	CLA	C2C-C1C-NC	2.96	112.74	109.97
31	b	604	CLA	C2C-C1C-NC	2.96	112.74	109.97
30	2	605	CHL	C3C-C4C-NC	-2.96	107.25	110.57
30	4	606	CHL	C3C-C4C-NC	-2.96	107.25	110.57
32	0	616	LUT	C30-C31-C32	-2.96	113.99	123.22
31	B	607	CLA	C1C-C2C-C3C	-2.96	103.85	106.96
31	D	403	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	G	604	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	N	315	CLA	C2D-C1D-ND	2.96	112.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	p	610	CLA	C2D-C1D-ND	2.96	112.28	110.10
31	N	312	CLA	C2C-C1C-NC	2.96	112.74	109.97
31	n	313	CLA	C2C-C1C-NC	2.96	112.74	109.97
31	B	615	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
36	0	618	NEX	C26-C27-C28	-2.96	119.74	125.99
30	q	310	CHL	C1B-CHB-C4A	-2.96	124.26	130.12
30	y	608	CHL	C1B-CHB-C4A	-2.96	124.26	130.12
31	1	614	CLA	C1-C2-C3	-2.96	120.93	126.04
30	N	309	CHL	C1B-CHB-C4A	-2.96	124.26	130.12
35	9	317	RRX	C38-C26-C27	2.96	119.83	114.36
31	B	615	CLA	C1-C2-C3	-2.96	120.93	126.04
31	C	601	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
31	n	311	CLA	C1D-ND-C4D	-2.95	104.24	106.33
31	n	303	CLA	C2C-C1C-NC	2.95	112.74	109.97
32	n	317	LUT	C21-C26-C27	-2.95	108.97	112.70
31	b	613	CLA	C1-C2-C3	-2.95	120.93	126.04
30	7	321	CHL	C2C-C3C-C4C	2.95	108.59	106.49
31	b	603	CLA	C2C-C1C-NC	2.95	112.74	109.97
31	N	305	CLA	CHD-C1D-ND	-2.95	121.74	124.45
30	q	311	CHL	C3C-C4C-NC	-2.95	107.26	110.57
43	C	614	BCR	C1-C6-C5	-2.95	118.45	122.61
31	n	303	CLA	C1-C2-C3	-2.95	120.94	126.04
30	0	605	CHL	CHC-C1C-NC	2.95	128.68	124.20
31	R	306	CLA	C1C-C2C-C3C	-2.95	103.85	106.96
31	s	305	CLA	C2D-C1D-ND	2.95	112.28	110.10
36	6	319	NEX	C38-C25-C26	-2.95	117.31	122.26
30	2	608	CHL	C1B-CHB-C4A	-2.95	124.27	130.12
31	5	602	CLA	C1D-ND-C4D	-2.95	104.24	106.33
36	r	319	NEX	C38-C25-C26	-2.95	117.32	122.26
30	g	307	CHL	C2C-C3C-C4C	2.95	108.59	106.49
31	7	311	CLA	C2D-C1D-ND	2.95	112.28	110.10
36	6	319	NEX	C2-C1-C6	2.95	112.08	109.21
32	s	317	LUT	C21-C26-C27	-2.95	108.97	112.70
33	9	320	LHG	C5-O7-C7	-2.95	110.53	117.79
31	3	315	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	C	613	CLA	C2C-C1C-NC	2.95	112.73	109.97
30	p	607	CHL	C4D-CHA-C1A	2.95	124.84	121.25
30	s	308	CHL	CMA-C3A-C4A	2.95	119.70	111.77
31	9	312	CLA	CHD-C1D-ND	-2.95	121.74	124.45
30	3	302	CHL	C1B-CHB-C4A	-2.95	124.28	130.12
31	9	305	CLA	C2D-C1D-ND	2.95	112.28	110.10
31	4	604	CLA	CMA-C3A-C4A	2.95	119.70	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	303	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	G	602	CLA	C2C-C1C-NC	2.95	112.73	109.97
30	r	308	CHL	C1-C2-C3	-2.95	120.94	126.04
31	1	612	CLA	C1-C2-C3	-2.95	120.94	126.04
31	p	613	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
31	4	602	CLA	C1D-ND-C4D	-2.95	104.24	106.33
31	6	311	CLA	C1D-ND-C4D	-2.95	104.24	106.33
35	4	615	RRX	C38-C26-C27	2.95	119.82	114.36
43	B	619	BCR	C33-C5-C6	-2.95	121.22	124.53
31	y	602	CLA	CMA-C3A-C4A	2.95	119.69	111.77
33	s	322	LHG	O8-C23-C24	2.95	121.16	111.91
31	2	610	CLA	CHD-C1D-ND	-2.95	121.75	124.45
30	N	308	CHL	C4D-CHA-C1A	2.95	124.83	121.25
35	G	614	RRX	C38-C26-C27	2.95	119.81	114.36
30	3	307	CHL	C2C-C3C-C4C	2.95	108.59	106.49
30	n	308	CHL	C2C-C3C-C4C	2.95	108.59	106.49
31	y	611	CLA	C2D-C1D-ND	2.95	112.28	110.10
34	9	302	LMG	O8-C28-C29	2.95	121.15	111.91
31	B	615	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
31	b	607	CLA	C2C-C1C-NC	2.95	112.73	109.97
31	N	310	CLA	C1D-ND-C4D	-2.94	104.24	106.33
31	p	611	CLA	C1D-ND-C4D	-2.94	104.24	106.33
31	n	312	CLA	C2D-C1D-ND	2.94	112.27	110.10
31	6	303	CLA	CMA-C3A-C4A	2.94	119.69	111.77
30	0	601	CHL	C1-C2-C3	-2.94	120.95	126.04
31	C	610	CLA	CMB-C2B-C3B	2.94	130.19	124.68
36	0	618	NEX	C2-C1-C6	2.94	112.07	109.21
30	9	311	CHL	CMA-C3A-C4A	2.94	119.68	111.77
31	0	614	CLA	C2D-C1D-ND	2.94	112.27	110.10
30	9	308	CHL	C1B-CHB-C4A	-2.94	124.29	130.12
43	a	410	BCR	C1-C6-C5	-2.94	118.47	122.61
31	N	310	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	S	312	CLA	C2C-C1C-NC	2.94	112.73	109.97
30	G	608	CHL	C1B-CHB-C4A	-2.94	124.29	130.12
31	c	612	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
31	1	611	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	p	612	CLA	CMA-C3A-C4A	2.94	119.68	111.77
31	8	611	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	A	406	CLA	CMB-C2B-C3B	2.94	130.18	124.68
31	1	611	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	A	409	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
31	q	306	CLA	CMA-C3A-C4A	2.94	119.68	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	305	CLA	CHD-C1D-ND	-2.94	121.75	124.45
30	s	308	CHL	C4D-CHA-C1A	2.94	124.83	121.25
30	5	609	CHL	C1-O2A-CGA	2.94	124.16	116.44
31	4	613	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	C	603	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	8	609	CLA	C2C-C1C-NC	2.94	112.73	109.97
31	R	303	CLA	O1D-CGD-CBD	-2.94	118.47	124.48
31	2	604	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	p	614	CLA	C2C-C1C-NC	2.94	112.72	109.97
31	q	304	CLA	C2C-C1C-NC	2.94	112.72	109.97
30	7	310	CHL	C1B-CHB-C4A	-2.94	124.30	130.12
30	S	309	CHL	CMA-C3A-C4A	2.94	119.67	111.77
31	N	313	CLA	CMA-C3A-C4A	2.94	119.67	111.77
32	0	616	LUT	C7-C8-C9	-2.94	121.80	126.23
34	C	619	LMG	C8-O7-C10	-2.94	110.56	117.79
31	R	314	CLA	C2C-C1C-NC	2.94	112.72	109.97
30	G	605	CHL	CMA-C3A-C4A	2.94	119.67	111.77
31	4	603	CLA	CHD-C1D-ND	-2.94	121.75	124.45
31	B	611	CLA	CHD-C1D-ND	-2.94	121.75	124.45
30	9	311	CHL	C1B-CHB-C4A	-2.94	124.30	130.12
36	0	618	NEX	C38-C25-C26	-2.94	117.34	122.26
30	y	607	CHL	C4D-CHA-C1A	2.94	124.82	121.25
31	C	602	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
31	0	604	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
30	g	308	CHL	C1-C2-C3	-2.94	122.00	126.75
31	s	316	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
31	S	303	CLA	C1D-ND-C4D	-2.94	104.25	106.33
31	D	404	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	Y	312	CLA	C2C-C1C-NC	2.93	112.72	109.97
31	0	602	CLA	C2C-C1C-NC	2.93	112.72	109.97
31	S	305	CLA	C2D-C1D-ND	2.93	112.27	110.10
31	q	304	CLA	C2D-C1D-ND	2.93	112.27	110.10
31	s	304	CLA	CMA-C3A-C4A	2.93	119.66	111.77
30	9	310	CHL	C2C-C3C-C4C	2.93	108.58	106.49
31	n	311	CLA	C2C-C1C-NC	2.93	112.72	109.97
30	g	306	CHL	C1B-CHB-C4A	-2.93	124.31	130.12
30	Y	308	CHL	C1-O2A-CGA	2.93	124.14	116.44
31	5	614	CLA	CMA-C3A-C4A	2.93	119.66	111.77
31	4	611	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	1	610	CLA	C2D-C1D-ND	2.93	112.27	110.10
31	b	614	CLA	C2D-C1D-ND	2.93	112.27	110.10
31	s	303	CLA	C1D-ND-C4D	-2.93	104.25	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	611	CLA	CHD-C1D-ND	-2.93	121.76	124.45
30	3	303	CHL	CMA-C3A-C4A	2.93	119.65	111.77
42	A	408	PHO	O1D-CGD-CBD	2.93	129.62	124.74
30	G	607	CHL	C4D-CHA-C1A	2.93	124.82	121.25
34	b	626	LMG	O8-C28-C29	2.93	121.11	111.91
43	b	619	BCR	C33-C5-C4	2.93	119.25	113.62
36	9	319	NEX	C38-C25-C26	-2.93	117.35	122.26
30	6	306	CHL	C1B-CHB-C4A	-2.93	124.31	130.12
43	C	615	BCR	C27-C26-C25	-2.93	118.48	122.73
31	3	316	CLA	C2D-C1D-ND	2.93	112.26	110.10
32	1	616	LUT	C31-C30-C29	-2.93	123.13	127.31
31	5	602	CLA	CMA-C3A-C4A	2.93	119.64	111.77
30	0	608	CHL	C1B-CHB-C4A	-2.93	124.32	130.12
36	G	616	NEX	C5-C6-C1	2.93	122.60	119.70
31	3	314	CLA	C2D-C1D-ND	2.93	112.26	110.10
31	n	305	CLA	C2D-C1D-ND	2.93	112.26	110.10
31	N	314	CLA	CMA-C3A-C4A	2.93	119.64	111.77
31	9	316	CLA	C2C-C1C-NC	2.93	112.72	109.97
30	4	609	CHL	C1-C2-C3	-2.93	120.98	126.04
31	c	612	CLA	CMB-C2B-C3B	2.93	130.16	124.68
31	7	303	CLA	CMA-C3A-C4A	2.93	119.64	111.77
37	9	322	XAT	C27-C28-C29	2.93	130.07	125.53
31	b	605	CLA	CMA-C3A-C4A	2.93	119.64	111.77
31	1	603	CLA	C1C-C2C-C3C	-2.93	103.88	106.96
32	5	616	LUT	C21-C26-C27	-2.93	109.00	112.70
30	7	302	CHL	C1-C2-C3	-2.93	120.98	126.04
31	y	614	CLA	C2C-C1C-NC	2.92	112.71	109.97
30	S	309	CHL	C1-O2A-CGA	2.92	124.12	116.44
31	b	610	CLA	C2D-C1D-ND	2.92	112.26	110.10
31	3	301	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	y	603	CLA	C2C-C1C-NC	2.92	112.71	109.97
31	p	614	CLA	C1-C2-C3	-2.92	120.99	126.04
31	b	606	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
31	N	311	CLA	CMA-C3A-C4A	2.92	119.63	111.77
33	d	408	LHG	C5-O7-C7	-2.92	110.60	117.79
31	C	612	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
30	G	601	CHL	C1-C2-C3	-2.92	120.99	126.04
34	2	620	LMG	O8-C28-C29	2.92	121.08	111.91
31	7	314	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	6	312	CLA	C1-C2-C3	-2.92	120.99	126.04
31	9	316	CLA	C2D-C1D-ND	2.92	112.26	110.10
31	s	312	CLA	CMA-C3A-C4A	2.92	119.62	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	612	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
43	V	101	BCR	C23-C24-C25	-2.92	119.00	127.20
30	p	606	CHL	C1B-CHB-C4A	-2.92	124.33	130.12
31	B	608	CLA	CMB-C2B-C3B	2.92	130.14	124.68
31	N	313	CLA	C2D-C1D-ND	2.92	112.26	110.10
37	q	321	XAT	C27-C28-C29	2.92	130.06	125.53
34	c	620	LMG	C8-O7-C10	-2.92	110.60	117.79
31	2	602	CLA	CMA-C3A-C4A	2.92	119.62	111.77
30	8	601	CHL	C4D-CHA-C1A	2.92	124.80	121.25
31	N	313	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	3	306	CLA	C1D-ND-C4D	-2.92	104.26	106.33
31	n	315	CLA	CMA-C3A-C4A	2.92	119.62	111.77
33	D	408	LHG	O8-C23-C24	2.92	121.06	111.91
31	C	610	CLA	C1C-C2C-C3C	-2.92	103.89	106.96
31	a	409	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
31	4	612	CLA	C1D-ND-C4D	-2.92	104.26	106.33
44	A	416	PL9	C36-C34-C33	-2.92	115.22	121.12
30	G	606	CHL	CMA-C3A-C4A	2.92	119.61	111.77
31	c	602	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
31	B	605	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
31	1	602	CLA	CHD-C1D-ND	-2.92	121.78	124.45
31	r	314	CLA	C2D-C1D-ND	2.91	112.25	110.10
31	8	613	CLA	CMA-C3A-C4A	2.91	119.61	111.77
30	3	310	CHL	C4D-CHA-C1A	2.91	124.80	121.25
32	y	617	LUT	C30-C31-C32	-2.91	114.12	123.22
30	r	308	CHL	C1B-CHB-C4A	-2.91	124.35	130.12
31	Y	303	CLA	C2D-C1D-ND	2.91	112.25	110.10
31	2	612	CLA	C2C-C1C-NC	2.91	112.70	109.97
31	7	304	CLA	CMA-C3A-C4A	2.91	119.60	111.77
31	C	613	CLA	C2D-C1D-ND	2.91	112.25	110.10
34	6	322	LMG	O8-C28-C29	2.91	121.05	111.91
30	y	606	CHL	C4D-CHA-C1A	2.91	124.79	121.25
31	r	304	CLA	C1D-ND-C4D	-2.91	104.27	106.33
36	2	616	NEX	C17-C1-C6	-2.91	107.87	110.47
31	g	304	CLA	CMA-C3A-C4A	2.91	119.60	111.77
31	s	315	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
32	6	317	LUT	C1-C6-C5	-2.91	118.52	122.61
31	R	315	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	7	312	CLA	CHD-C1D-ND	-2.91	121.78	124.45
31	Y	314	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	R	307	CLA	CHD-C1D-ND	-2.91	121.78	124.45
43	T	101	BCR	C11-C10-C9	-2.91	123.16	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	303	CHL	C1B-CHB-C4A	-2.91	124.36	130.12
30	s	307	CHL	CMA-C3A-C4A	2.91	119.59	111.77
30	9	311	CHL	C4D-CHA-C1A	2.91	124.79	121.25
31	N	304	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	G	603	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	c	610	CLA	O2A-CGA-CBA	2.91	121.03	111.91
30	N	302	CHL	CMA-C3A-C4A	2.91	119.58	111.77
31	4	611	CLA	CMA-C3A-C4A	2.91	119.58	111.77
34	b	624	LMG	O8-C28-C29	2.91	121.03	111.91
34	d	411	LMG	O8-C28-C29	2.91	121.03	111.91
31	8	612	CLA	CHD-C1D-ND	-2.91	121.78	124.45
30	n	302	CHL	C4D-CHA-C1A	2.91	124.79	121.25
31	C	607	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
30	9	307	CHL	C3C-C4C-NC	-2.91	107.31	110.57
32	s	317	LUT	C11-C10-C9	-2.91	123.16	127.31
31	c	610	CLA	CMB-C2B-C3B	2.90	130.11	124.68
36	9	319	NEX	C2-C1-C6	2.90	112.03	109.21
31	5	603	CLA	C2C-C1C-NC	2.90	112.69	109.97
43	d	406	BCR	C20-C21-C22	-2.90	123.17	127.31
31	8	614	CLA	CMA-C3A-C4A	2.90	119.58	111.77
30	p	601	CHL	C3C-C4C-NC	-2.90	107.31	110.57
31	6	304	CLA	CHD-C1D-ND	-2.90	121.79	124.45
37	g	321	XAT	C27-C28-C29	2.90	130.03	125.53
31	B	614	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	G	602	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	8	612	CLA	CMA-C3A-C4A	2.90	119.57	111.77
31	c	602	CLA	C1-C2-C3	-2.90	121.02	126.04
43	B	618	BCR	C27-C26-C25	-2.90	118.52	122.73
32	3	318	LUT	C31-C30-C29	-2.90	123.17	127.31
34	7	320	LMG	C7-O1-C1	-2.90	108.07	113.74
31	N	311	CLA	C1D-ND-C4D	-2.90	104.27	106.33
31	9	314	CLA	C2D-C1D-ND	2.90	112.24	110.10
31	N	303	CLA	CMA-C3A-C4A	2.90	119.57	111.77
31	B	607	CLA	CHD-C1D-ND	-2.90	121.79	124.45
31	2	609	CLA	CMA-C3A-C4A	2.90	119.57	111.77
31	n	311	CLA	CMA-C3A-C4A	2.90	119.57	111.77
34	Q1	101	LMG	O8-C28-C29	2.90	121.01	111.91
31	5	610	CLA	C2C-C1C-NC	2.90	112.69	109.97
31	n	314	CLA	CMA-C3A-C4A	2.90	119.56	111.77
31	B	614	CLA	CHD-C1D-ND	-2.90	121.79	124.45
33	2	617	LHG	C5-O7-C7	-2.90	110.66	117.79
31	d	404	CLA	C2D-C1D-ND	2.90	112.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	n	302	CHL	CMA-C3A-C4A	2.90	119.56	111.77
43	C	615	BCR	C23-C24-C25	-2.90	119.06	127.20
31	y	615	CLA	C2C-C1C-NC	2.90	112.69	109.97
30	5	609	CHL	C1B-CHB-C4A	-2.90	124.38	130.12
43	T	101	BCR	C38-C26-C27	2.90	119.18	113.62
32	2	615	LUT	C11-C10-C9	-2.90	123.17	127.31
37	4	619	XAT	C27-C28-C29	2.90	130.03	125.53
34	b	629	LMG	O8-C28-C29	2.90	121.00	111.91
31	q	312	CLA	CMA-C3A-C4A	2.90	119.56	111.77
31	y	603	CLA	CMA-C3A-C4A	2.90	119.56	111.77
31	5	603	CLA	C1-C2-C3	-2.90	121.03	126.04
31	b	613	CLA	CHD-C1D-ND	-2.90	121.79	124.45
37	g	321	XAT	C18-C5-C6	-2.90	117.41	122.26
30	4	609	CHL	C1B-CHB-C4A	-2.90	124.38	130.12
43	C	614	BCR	C11-C12-C13	-2.90	118.28	126.42
32	N	317	LUT	C18-C5-C6	-2.90	121.28	124.53
30	0	601	CHL	C1B-CHB-C4A	-2.89	124.38	130.12
31	b	616	CLA	C1C-C2C-C3C	-2.89	103.91	106.96
31	p	612	CLA	CHD-C1D-ND	-2.89	121.79	124.45
31	b	604	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
31	n	316	CLA	C2C-C1C-NC	2.89	112.68	109.97
30	Y	308	CHL	C4D-CHA-C1A	2.89	124.77	121.25
30	0	601	CHL	CMA-C3A-C4A	2.89	119.55	111.77
31	a	406	CLA	C2D-C1D-ND	2.89	112.24	110.10
34	y	620	LMG	O8-C28-C29	2.89	120.99	111.91
31	5	611	CLA	C1D-ND-C4D	-2.89	104.28	106.33
31	8	609	CLA	C1D-ND-C4D	-2.89	104.28	106.33
37	G	620	XAT	C18-C5-C6	-2.89	117.41	122.26
35	G	614	RRX	C20-C19-C18	-2.89	118.29	126.42
30	9	308	CHL	C3C-C4C-NC	-2.89	107.33	110.57
32	Y	316	LUT	C30-C31-C32	-2.89	114.19	123.22
30	n	307	CHL	C4D-CHA-C1A	2.89	124.77	121.25
31	C	606	CLA	C2C-C1C-NC	2.89	112.68	109.97
31	p	610	CLA	C2C-C1C-NC	2.89	112.68	109.97
31	g	313	CLA	C2D-C1D-ND	2.89	112.23	110.10
30	r	310	CHL	C4D-CHA-C1A	2.89	124.77	121.25
34	B	625	LMG	O8-C28-C29	2.89	120.98	111.91
31	G	609	CLA	C2C-C1C-NC	2.89	112.68	109.97
35	9	317	RRX	C20-C19-C18	-2.89	118.30	126.42
32	G	615	LUT	C1-C6-C5	-2.89	118.54	122.61
31	S	313	CLA	C2D-C1D-ND	2.89	112.23	110.10
30	8	601	CHL	CMA-C3A-C4A	2.89	119.53	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	5	620	LMG	O8-C28-C29	2.89	120.97	111.91
31	Y	305	CLA	C2D-C1D-ND	2.89	112.23	110.10
35	4	615	RRX	C20-C19-C18	-2.89	118.31	126.42
37	2	619	XAT	C27-C28-C29	2.89	130.01	125.53
31	8	610	CLA	CMA-C3A-C4A	2.89	119.53	111.77
37	q	321	XAT	C18-C5-C6	-2.89	117.42	122.26
31	Y	312	CLA	CHD-C1D-ND	-2.89	121.80	124.45
31	p	613	CLA	CHD-C1D-ND	-2.89	121.80	124.45
31	B	601	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
45	c	618	DGD	O1G-C1A-C2A	2.89	120.97	111.91
30	5	606	CHL	C3C-C4C-NC	-2.89	107.33	110.57
32	5	616	LUT	C1-C6-C5	-2.89	118.55	122.61
43	D	405	BCR	C33-C5-C4	2.89	119.16	113.62
37	4	619	XAT	C18-C5-C6	-2.89	117.42	122.26
31	C	613	CLA	CMB-C2B-C3B	2.89	130.08	124.68
30	4	605	CHL	C3C-C4C-NC	-2.89	107.33	110.57
31	R	316	CLA	C2D-C1D-ND	2.88	112.23	110.10
31	g	313	CLA	CMA-C3A-C4A	2.88	119.53	111.77
30	0	607	CHL	C2C-C3C-C4C	2.88	108.55	106.49
30	N	306	CHL	CMA-C3A-C4A	2.88	119.53	111.77
31	D	404	CLA	C2C-C1C-NC	2.88	112.67	109.97
32	S	317	LUT	C21-C26-C27	-2.88	109.06	112.70
31	b	610	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
30	q	309	CHL	C3C-C4C-NC	-2.88	107.34	110.57
31	g	305	CLA	C2D-C1D-ND	2.88	112.23	110.10
30	8	606	CHL	C4D-CHA-C1A	2.88	124.76	121.25
45	c	617	DGD	O1G-C1A-C2A	2.88	120.95	111.91
30	8	607	CHL	C2C-C3C-C4C	2.88	108.54	106.49
35	2	614	RRX	C38-C26-C27	2.88	119.69	114.36
34	a	401	LMG	C8-O7-C10	-2.88	110.70	117.79
31	q	312	CLA	C2C-C1C-NC	2.88	112.67	109.97
31	C	612	CLA	CMB-C2B-C3B	2.88	130.07	124.68
33	j	102	LHG	C5-O7-C7	-2.88	110.70	117.79
31	9	315	CLA	C1-C2-C3	-2.88	121.06	126.04
31	1	612	CLA	O2A-CGA-CBA	2.88	120.95	111.91
31	3	305	CLA	CHD-C1D-ND	-2.88	121.81	124.45
42	D	401	PHO	O1D-CGD-CBD	2.88	129.54	124.74
31	N	312	CLA	C1D-ND-C4D	-2.88	104.29	106.33
30	1	607	CHL	C4D-CHA-C1A	2.88	124.75	121.25
31	Y	310	CLA	CMA-C3A-C4A	2.88	119.51	111.77
31	b	615	CLA	C2C-C1C-NC	2.88	112.67	109.97
30	8	605	CHL	C1-C2-C3	-2.88	121.06	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	316	CLA	CMA-C3A-C4A	2.88	119.51	111.77
34	I	101	LMG	O8-C28-C29	2.88	120.94	111.91
30	y	601	CHL	C4D-CHA-C1A	2.88	124.75	121.25
30	4	609	CHL	CMA-C3A-C4A	2.88	119.51	111.77
31	C	611	CLA	C1-C2-C3	-2.88	121.06	126.04
31	b	603	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
31	p	604	CLA	C2C-C1C-NC	2.88	112.67	109.97
31	b	609	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
31	s	314	CLA	CMA-C3A-C4A	2.88	119.51	111.77
31	S	314	CLA	C2D-C1D-ND	2.88	112.22	110.10
34	s	321	LMG	C7-O1-C1	-2.88	108.12	113.74
31	R	316	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
30	8	606	CHL	C1-C2-C3	-2.88	121.07	126.04
30	n	306	CHL	C1-C2-C3	-2.88	121.07	126.04
31	2	610	CLA	CMA-C3A-C4A	2.88	119.50	111.77
31	5	611	CLA	CMA-C3A-C4A	2.88	119.50	111.77
31	5	612	CLA	CHD-C1D-ND	-2.88	121.81	124.45
31	5	613	CLA	C1-C2-C3	-2.88	121.07	126.04
30	N	308	CHL	C2C-C3C-C4C	2.88	108.54	106.49
31	s	306	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
31	7	316	CLA	C2D-C1D-ND	2.88	112.22	110.10
31	R	311	CLA	O2A-CGA-CBA	2.88	120.93	111.91
31	b	610	CLA	CHD-C1D-ND	-2.87	121.81	124.45
31	n	314	CLA	CHD-C1D-ND	-2.87	121.81	124.45
31	4	612	CLA	C1C-C2C-C3C	-2.87	103.93	106.96
31	Y	304	CLA	C2C-C1C-NC	2.87	112.67	109.97
32	Y	315	LUT	C35-C15-C14	-2.87	117.59	123.47
31	B	614	CLA	CMA-C3A-C4A	2.87	119.50	111.77
31	p	610	CLA	CMA-C3A-C4A	2.87	119.50	111.77
31	Y	304	CLA	C2D-C1D-ND	2.87	112.22	110.10
43	Z	101	BCR	C11-C12-C13	-2.87	118.34	126.42
34	W	202	LMG	O8-C28-C29	2.87	120.92	111.91
43	B	619	BCR	C38-C26-C27	2.87	119.14	113.62
31	a	406	CLA	CHD-C1D-ND	-2.87	121.81	124.45
31	Y	310	CLA	C2C-C1C-NC	2.87	112.66	109.97
37	G	620	XAT	C27-C28-C29	2.87	129.99	125.53
32	p	616	LUT	C7-C8-C9	-2.87	121.90	126.23
31	S	303	CLA	C2C-C1C-NC	2.87	112.66	109.97
30	2	605	CHL	C2C-C3C-C4C	2.87	108.53	106.49
31	N	315	CLA	CMA-C3A-C4A	2.87	119.49	111.77
31	6	305	CLA	C2D-C1D-ND	2.87	112.22	110.10
32	s	317	LUT	C8-C7-C6	-2.87	119.14	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	613	CLA	CMB-C2B-C3B	2.87	130.05	124.68
36	4	617	NEX	C17-C1-C6	-2.87	107.90	110.47
31	3	301	CLA	C2C-C1C-NC	2.87	112.66	109.97
37	9	322	XAT	C18-C5-C6	-2.87	117.45	122.26
36	g	317	NEX	C39-C29-C30	-2.87	118.90	122.92
31	S	306	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	4	608	CHL	C4D-CHA-C1A	2.87	124.74	121.25
31	1	614	CLA	CMA-C3A-C4A	2.87	119.48	111.77
30	g	307	CHL	C1B-CHB-C4A	-2.87	124.44	130.12
30	G	608	CHL	C2C-C3C-C4C	2.87	108.53	106.49
31	b	607	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
30	N	307	CHL	C4D-CHA-C1A	2.87	124.74	121.25
30	R	308	CHL	CMA-C3A-C4A	2.87	119.48	111.77
31	n	312	CLA	CMA-C3A-C4A	2.87	119.48	111.77
30	5	601	CHL	C3C-C4C-NC	-2.87	107.36	110.57
30	R	308	CHL	C3C-C4C-NC	-2.87	107.36	110.57
31	B	602	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
31	3	314	CLA	CHD-C1D-ND	-2.87	121.82	124.45
31	Y	313	CLA	CHD-C1D-ND	-2.87	121.82	124.45
33	8	618	LHG	O8-C23-C24	2.87	120.90	111.91
31	4	612	CLA	C2C-C1C-NC	2.87	112.66	109.97
34	R	321	LMG	O8-C28-C29	2.86	120.90	111.91
32	y	616	LUT	C35-C15-C14	-2.86	117.61	123.47
31	4	610	CLA	C1C-C2C-C3C	-2.86	103.94	106.96
30	p	609	CHL	C1B-CHB-C4A	-2.86	124.44	130.12
31	p	603	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
31	R	307	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
31	q	305	CLA	C2D-C1D-ND	2.86	112.21	110.10
30	8	606	CHL	C1-O2A-CGA	2.86	123.96	116.44
31	5	615	CLA	CMA-C3A-C4A	2.86	119.47	111.77
32	y	616	LUT	C15-C14-C13	-2.86	123.22	127.31
30	G	623	CHL	C1-C2-C3	-2.86	121.09	126.04
37	2	619	XAT	C18-C5-C6	-2.86	117.46	122.26
31	7	313	CLA	C2D-C1D-ND	2.86	112.21	110.10
31	3	301	CLA	C1D-ND-C4D	-2.86	104.30	106.33
31	B	606	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
31	s	311	CLA	C1-C2-C3	-2.86	121.09	126.04
31	1	612	CLA	C2C-C1C-NC	2.86	112.65	109.97
31	3	314	CLA	CMA-C3A-C4A	2.86	119.46	111.77
33	n	320	LHG	O8-C23-C24	2.86	120.88	111.91
32	y	617	LUT	C15-C35-C34	-2.86	117.62	123.47
31	B	612	CLA	CHD-C1D-ND	-2.86	121.83	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	613	CLA	C2C-C1C-NC	2.86	112.65	109.97
31	7	311	CLA	C2C-C1C-NC	2.86	112.65	109.97
31	p	611	CLA	CMA-C3A-C4A	2.86	119.46	111.77
43	C	614	BCR	C24-C23-C22	-2.86	121.92	126.23
31	g	312	CLA	CMA-C3A-C4A	2.86	119.46	111.77
31	5	603	CLA	CMA-C3A-C4A	2.86	119.46	111.77
31	r	315	CLA	CMB-C2B-C3B	2.86	130.03	124.68
30	3	307	CHL	CMA-C3A-C4A	2.86	119.45	111.77
31	c	613	CLA	C2D-C1D-ND	2.86	112.21	110.10
31	y	613	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
31	c	608	CLA	C2C-C1C-NC	2.86	112.65	109.97
30	6	307	CHL	CMA-C3A-C4A	2.86	119.45	111.77
30	8	607	CHL	C1-O2A-CGA	2.86	123.94	116.44
31	S	306	CLA	CMA-C3A-C4A	2.86	119.45	111.77
31	N	304	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
31	r	315	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
31	R	306	CLA	CAA-C2A-C3A	-2.86	104.96	112.78
31	S	316	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
43	V	101	BCR	C10-C11-C12	-2.85	114.31	123.22
31	S	313	CLA	CMB-C2B-C3B	2.85	130.02	124.68
31	B	612	CLA	C1D-ND-C4D	-2.85	104.31	106.33
45	C	616	DGD	O1G-C1A-C2A	2.85	120.86	111.91
31	9	306	CLA	CMA-C3A-C4A	2.85	119.44	111.77
31	R	303	CLA	C2D-C1D-ND	2.85	112.21	110.10
31	G	611	CLA	CHD-C1D-ND	-2.85	121.83	124.45
31	y	615	CLA	C1D-ND-C4D	-2.85	104.31	106.33
30	p	605	CHL	CMA-C3A-C4A	2.85	119.44	111.77
32	5	616	LUT	C7-C8-C9	-2.85	121.93	126.23
31	y	604	CLA	C2D-C1D-ND	2.85	112.20	110.10
31	S	314	CLA	CHD-C1D-ND	-2.85	121.83	124.45
30	n	302	CHL	C1-O2A-CGA	2.85	123.92	116.44
31	R	315	CLA	CMB-C2B-C3B	2.85	130.01	124.68
31	7	312	CLA	CMA-C3A-C4A	2.85	119.43	111.77
30	S	308	CHL	C4D-CHA-C1A	2.85	124.72	121.25
30	y	606	CHL	CMA-C3A-C4A	2.85	119.43	111.77
45	c	616	DGD	O1G-C1A-C2A	2.85	120.85	111.91
30	Y	306	CHL	C2C-C3C-C4C	2.85	108.52	106.49
31	G	604	CLA	C1D-ND-C4D	-2.85	104.31	106.33
31	q	304	CLA	C1D-ND-C4D	-2.85	104.31	106.33
31	A	405	CLA	CHD-C1D-ND	-2.85	121.84	124.45
31	b	611	CLA	CMA-C3A-C4A	2.85	119.43	111.77
31	b	606	CLA	C2D-C1D-ND	2.85	112.20	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	p	608	CHL	C4D-CHA-C1A	2.85	124.72	121.25
43	c	614	BCR	C35-C13-C14	-2.85	118.93	122.92
31	a	407	CLA	CMA-C3A-C4A	2.85	119.43	111.77
43	c	614	BCR	C23-C22-C21	2.85	123.31	118.94
31	8	614	CLA	C2D-C1D-ND	2.85	112.20	110.10
31	r	305	CLA	C2D-C1D-ND	2.85	112.20	110.10
31	2	610	CLA	C1D-ND-C4D	-2.85	104.31	106.33
31	C	610	CLA	O2A-CGA-CBA	2.85	120.84	111.91
31	1	603	CLA	C1-C2-C3	-2.85	121.12	126.04
31	A	406	CLA	CAA-C2A-C3A	-2.85	104.99	112.78
30	n	307	CHL	C1-O2A-CGA	2.85	123.91	116.44
31	3	316	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
31	7	314	CLA	CMA-C3A-C4A	2.85	119.42	111.77
31	A	409	CLA	CMB-C2B-C3B	2.85	130.00	124.68
31	b	602	CLA	C2C-C1C-NC	2.84	112.64	109.97
31	3	312	CLA	C1-C2-C3	-2.84	121.12	126.04
30	8	607	CHL	C1B-CHB-C4A	-2.84	124.48	130.12
31	B	613	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
30	8	601	CHL	C1-O2A-CGA	2.84	123.91	116.44
31	0	614	CLA	CMA-C3A-C4A	2.84	119.42	111.77
31	d	401	CLA	CMA-C3A-C4A	2.84	119.42	111.77
30	q	307	CHL	C1B-CHB-C4A	-2.84	124.49	130.12
31	p	602	CLA	C2D-C1D-ND	2.84	112.20	110.10
31	c	602	CLA	CHD-C1D-ND	-2.84	121.84	124.45
31	C	606	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
31	p	610	CLA	C1D-ND-C4D	-2.84	104.32	106.33
31	r	305	CLA	C1-C2-C3	-2.84	121.13	126.04
31	p	611	CLA	CHD-C1D-ND	-2.84	121.84	124.45
30	G	601	CHL	CMA-C3A-C4A	2.84	119.41	111.77
31	6	315	CLA	CMA-C3A-C4A	2.84	119.41	111.77
31	1	610	CLA	C2C-C1C-NC	2.84	112.63	109.97
36	4	617	NEX	C26-C27-C28	-2.84	119.99	125.99
31	R	313	CLA	CHD-C1D-ND	-2.84	121.84	124.45
31	S	315	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
30	g	302	CHL	C2C-C3C-C4C	2.84	108.51	106.49
30	2	606	CHL	C1B-CHB-C4A	-2.84	124.49	130.12
43	A	410	BCR	C33-C5-C4	2.84	119.07	113.62
30	n	307	CHL	C1-C2-C3	-2.84	121.13	126.04
31	a	409	CLA	CMB-C2B-C3B	2.84	129.99	124.68
31	6	303	CLA	C1D-ND-C4D	-2.84	104.32	106.33
31	n	304	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
43	T	101	BCR	C11-C12-C13	-2.84	118.44	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	306	CLA	C2C-C1C-NC	2.84	112.63	109.97
31	3	306	CLA	C2D-C1D-ND	2.84	112.19	110.10
31	5	613	CLA	C2D-C1D-ND	2.84	112.19	110.10
31	G	602	CLA	CMA-C3A-C4A	2.84	119.39	111.77
31	C	613	CLA	CHD-C1D-ND	-2.84	121.85	124.45
31	p	614	CLA	CMA-C3A-C4A	2.84	119.39	111.77
31	g	314	CLA	CMA-C3A-C4A	2.84	119.39	111.77
30	1	606	CHL	C1B-CHB-C4A	-2.84	124.50	130.12
31	r	306	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
31	c	612	CLA	C2D-C1D-ND	2.83	112.19	110.10
31	S	303	CLA	CMA-C3A-C4A	2.83	119.39	111.77
32	7	318	LUT	C11-C10-C9	-2.83	123.27	127.31
31	r	312	CLA	C2C-C1C-NC	2.83	112.63	109.97
30	G	606	CHL	C4D-CHA-C1A	2.83	124.70	121.25
30	6	306	CHL	C2C-C3C-C4C	2.83	108.51	106.49
31	n	303	CLA	C1D-ND-C4D	-2.83	104.32	106.33
30	N	306	CHL	C1B-CHB-C4A	-2.83	124.51	130.12
30	q	303	CHL	C1-O2A-CGA	2.83	123.88	116.44
31	c	609	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
30	9	308	CHL	CMA-C3A-C4A	2.83	119.39	111.77
30	n	301	CHL	C1B-CHB-C4A	-2.83	124.51	130.12
30	3	310	CHL	C1B-CHB-C4A	-2.83	124.51	130.12
31	p	614	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
31	D	403	CLA	CHD-C1D-ND	-2.83	121.85	124.45
31	C	605	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
30	Y	302	CHL	C4D-CHA-C1A	2.83	124.69	121.25
31	9	305	CLA	CMA-C3A-C4A	2.83	119.38	111.77
31	b	612	CLA	C1D-ND-C4D	-2.83	104.33	106.33
31	b	615	CLA	C1D-ND-C4D	-2.83	104.33	106.33
34	D	410	LMG	O8-C28-C29	2.83	120.79	111.91
30	1	605	CHL	C3C-C4C-NC	-2.83	107.40	110.57
31	C	609	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
31	c	610	CLA	C2C-C1C-NC	2.83	112.62	109.97
31	n	316	CLA	CMA-C3A-C4A	2.83	119.38	111.77
31	n	313	CLA	C1D-ND-C4D	-2.83	104.33	106.33
31	1	602	CLA	C2C-C1C-NC	2.83	112.62	109.97
37	r	318	XAT	C38-C25-C26	-2.83	117.52	122.26
31	1	613	CLA	CMA-C3A-C4A	2.83	119.37	111.77
31	y	613	CLA	O2A-CGA-CBA	2.83	120.78	111.91
31	r	304	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
31	r	305	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
31	6	316	CLA	CHD-C1D-ND	-2.83	121.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	308	CHL	C1B-CHB-C4A	-2.83	124.52	130.12
31	B	601	CLA	C2C-C1C-NC	2.83	112.62	109.97
31	C	605	CLA	CHA-C4D-ND	2.83	138.41	132.50
31	8	610	CLA	CHD-C1D-ND	-2.83	121.86	124.45
31	5	614	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
31	S	304	CLA	C2C-C1C-NC	2.83	112.62	109.97
31	s	306	CLA	C2C-C1C-NC	2.83	112.62	109.97
31	2	613	CLA	CMA-C3A-C4A	2.83	119.37	111.77
30	g	309	CHL	C1-C2-C3	-2.83	121.16	126.04
31	Y	311	CLA	CHD-C1D-ND	-2.82	121.86	124.45
31	s	303	CLA	CMA-C3A-C4A	2.82	119.36	111.77
32	n	317	LUT	C8-C7-C6	-2.82	119.27	127.20
31	q	305	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
31	q	314	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
30	3	307	CHL	C1B-CHB-C4A	-2.82	124.53	130.12
34	X	202	LMG	O8-C28-C29	2.82	120.76	111.91
31	b	609	CLA	C2D-C1D-ND	2.82	112.18	110.10
31	c	611	CLA	O2A-CGA-CBA	2.82	120.76	111.91
30	R	310	CHL	C1-C2-C3	-2.82	121.17	126.04
30	8	606	CHL	C2C-C3C-C4C	2.82	108.50	106.49
31	6	313	CLA	C1D-ND-C4D	-2.82	104.33	106.33
43	C	614	BCR	C21-C20-C19	-2.82	114.42	123.22
31	B	608	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
34	2	621	LMG	O8-C28-C29	2.82	120.75	111.91
30	n	309	CHL	C1B-CHB-C4A	-2.82	124.54	130.12
32	R	317	LUT	C31-C32-C33	2.82	134.33	126.42
31	3	312	CLA	CHD-C1D-ND	-2.82	121.86	124.45
32	8	616	LUT	C21-C26-C27	-2.82	109.14	112.70
30	n	307	CHL	C2C-C3C-C4C	2.82	108.50	106.49
31	s	312	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
33	q	320	LHG	O8-C23-C24	2.82	120.75	111.91
31	c	607	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
31	d	405	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
31	B	614	CLA	C2C-C1C-NC	2.82	112.61	109.97
31	3	311	CLA	C1C-C2C-C3C	-2.82	104.00	106.96
43	c	615	BCR	C36-C18-C17	-2.82	118.98	122.92
31	b	617	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
36	Y	317	NEX	C39-C29-C30	-2.81	118.98	122.92
31	N	321	CLA	C1D-ND-C4D	-2.81	104.34	106.33
43	B	617	BCR	C10-C11-C12	-2.81	114.44	123.22
43	T	101	BCR	C16-C17-C18	-2.81	123.30	127.31
31	8	611	CLA	C1D-ND-C4D	-2.81	104.34	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	n	318	LUT	C21-C26-C27	-2.81	109.15	112.70
31	C	604	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
30	g	302	CHL	C4D-CHA-C1A	2.81	124.67	121.25
43	c	615	BCR	C24-C23-C22	-2.81	121.99	126.23
31	r	312	CLA	C1-C2-C3	-2.81	121.18	126.04
31	g	305	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
31	7	304	CLA	C2C-C1C-NC	2.81	112.61	109.97
30	G	607	CHL	C3C-C4C-NC	-2.81	107.42	110.57
31	q	315	CLA	C1-C2-C3	-2.81	121.18	126.04
31	9	315	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
31	r	314	CLA	C2C-C1C-NC	2.81	112.60	109.97
31	5	613	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	B	611	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	s	305	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
31	y	614	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	c	601	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	C	607	CLA	C2D-C1D-ND	2.81	112.17	110.10
30	7	309	CHL	C1B-CHB-C4A	-2.81	124.56	130.12
31	b	614	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
31	b	608	CLA	CMB-C2B-C3B	2.81	129.93	124.68
31	C	601	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	7	311	CLA	CMA-C3A-C4A	2.81	119.32	111.77
31	C	602	CLA	CHD-C1D-ND	-2.81	121.88	124.45
31	3	312	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
31	r	316	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
31	2	612	CLA	C2D-C1D-ND	2.81	112.17	110.10
34	q	302	LMG	O8-C28-C29	2.81	120.71	111.91
31	7	316	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
31	n	305	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
31	3	306	CLA	CMA-C3A-C4A	2.80	119.31	111.77
31	B	606	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	2	603	CLA	C1D-ND-C4D	-2.80	104.34	106.33
31	N	314	CLA	C1D-ND-C4D	-2.80	104.34	106.33
32	8	615	LUT	C8-C7-C6	-2.80	119.33	127.20
31	9	315	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	R	303	CLA	CHD-C1D-ND	-2.80	121.88	124.45
31	C	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
30	p	606	CHL	CMA-C3A-C4A	2.80	119.31	111.77
36	G	616	NEX	C19-C9-C10	-2.80	119.00	122.92
30	N	302	CHL	C1-C2-C3	-2.80	121.20	126.04
31	d	401	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	g	313	CLA	C1C-C2C-C3C	-2.80	104.01	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	601	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	q	314	CLA	CMA-C3A-C4A	2.80	119.30	111.77
31	9	314	CLA	CHD-C1D-ND	-2.80	121.88	124.45
31	8	612	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	1	612	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	g	310	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	s	316	CLA	C2D-C1D-ND	2.80	112.17	110.10
31	4	610	CLA	C2C-C1C-NC	2.80	112.59	109.97
31	1	614	CLA	C1D-ND-C4D	-2.80	104.35	106.33
30	4	601	CHL	CMA-C3A-C4A	2.80	119.29	111.77
31	4	613	CLA	CMA-C3A-C4A	2.80	119.29	111.77
43	c	615	BCR	C23-C24-C25	-2.80	119.35	127.20
31	C	601	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
31	c	611	CLA	C2D-C1D-ND	2.80	112.17	110.10
32	r	317	LUT	C7-C8-C9	-2.80	122.01	126.23
43	c	614	BCR	C20-C19-C18	2.80	134.27	126.42
31	7	313	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
31	9	304	CLA	C1C-C2C-C3C	-2.80	104.02	106.96
31	B	603	CLA	CMB-C2B-C1B	-2.80	124.17	128.46
31	B	604	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
30	g	308	CHL	CMA-C3A-C4A	2.80	119.29	111.77
31	0	615	CLA	CMA-C3A-C4A	2.80	119.29	111.77
31	q	316	CLA	CMA-C3A-C4A	2.80	119.29	111.77
31	n	314	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
30	5	605	CHL	CMA-C3A-C4A	2.79	119.28	111.77
31	c	611	CLA	CAA-CBA-CGA	-2.79	105.09	113.25
31	N	314	CLA	O2A-CGA-CBA	2.79	120.67	111.91
31	8	610	CLA	C1D-ND-C4D	-2.79	104.35	106.33
31	c	601	CLA	C2D-C1D-ND	2.79	112.16	110.10
31	3	316	CLA	CMD-C2D-C3D	-2.79	121.19	127.61
31	s	310	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
34	b	622	LMG	O1-C1-C2	2.79	112.66	108.30
30	G	605	CHL	C2C-C3C-C4C	2.79	108.48	106.49
31	B	611	CLA	C2C-C1C-NC	2.79	112.59	109.97
30	n	302	CHL	C1B-CHB-C4A	-2.79	124.59	130.12
31	3	313	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
31	S	311	CLA	C1-C2-C3	-2.79	121.22	126.04
43	C	615	BCR	C30-C25-C26	-2.79	118.68	122.61
31	3	316	CLA	CMA-C3A-C4A	2.79	119.27	111.77
31	6	316	CLA	CMA-C3A-C4A	2.79	119.27	111.77
31	G	602	CLA	C1D-ND-C4D	-2.79	104.35	106.33
31	7	303	CLA	C1-C2-C3	-2.79	121.22	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	303	CLA	CMA-C3A-C4A	2.79	119.26	111.77
31	a	407	CLA	CMB-C2B-C3B	2.79	129.89	124.68
31	B	609	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
30	G	605	CHL	C1B-CHB-C4A	-2.79	124.60	130.12
31	s	306	CLA	CMA-C3A-C4A	2.79	119.26	111.77
31	C	611	CLA	O2A-CGA-CBA	2.79	120.65	111.91
36	n	319	NEX	C20-C13-C14	-2.79	119.02	122.92
32	3	317	LUT	C1-C6-C5	-2.79	118.69	122.61
43	b	620	BCR	C38-C26-C27	2.79	118.97	113.62
31	C	610	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
30	Y	308	CHL	C1B-CHB-C4A	-2.79	124.60	130.12
31	b	604	CLA	O2A-CGA-CBA	2.78	120.65	111.91
30	4	601	CHL	C4D-CHA-C1A	2.78	124.64	121.25
30	n	309	CHL	C2C-C3C-C4C	2.78	108.47	106.49
31	G	610	CLA	CHD-C1D-ND	-2.78	121.89	124.45
30	8	605	CHL	CMA-C3A-C4A	2.78	119.26	111.77
31	C	608	CLA	C2D-C1D-ND	2.78	112.16	110.10
31	G	603	CLA	C2D-C1D-ND	2.78	112.16	110.10
31	7	305	CLA	C2D-C1D-ND	2.78	112.16	110.10
31	2	611	CLA	C1D-ND-C4D	-2.78	104.36	106.33
32	r	317	LUT	C20-C13-C12	2.78	122.46	118.08
35	q	317	RRX	C35-C13-C14	-2.78	119.02	122.92
34	d	410	LMG	O8-C28-C29	2.78	120.64	111.91
31	n	312	CLA	CHD-C1D-ND	-2.78	121.90	124.45
31	p	602	CLA	CMA-C3A-C4A	2.78	119.25	111.77
30	p	608	CHL	C2C-C3C-C4C	2.78	108.47	106.49
31	D	404	CLA	C1D-ND-C4D	-2.78	104.36	106.33
30	8	601	CHL	C1B-CHB-C4A	-2.78	124.61	130.12
30	S	307	CHL	CMA-C3A-C4A	2.78	119.25	111.77
31	6	304	CLA	C1-C2-C3	-2.78	121.23	126.04
31	9	305	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
34	D	411	LMG	O8-C28-C29	2.78	120.64	111.91
34	S	321	LMG	O8-C28-C29	2.78	120.64	111.91
36	8	617	NEX	C17-C1-C6	-2.78	107.98	110.47
31	1	604	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
31	1	613	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
31	R	305	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	b	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
31	2	602	CLA	CHD-C1D-ND	-2.78	121.90	124.45
34	q1	101	LMG	O8-C28-C29	2.78	120.63	111.91
31	c	604	CLA	C2D-C1D-ND	2.78	112.15	110.10
31	8	613	CLA	C1D-ND-C4D	-2.78	104.36	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	405	CLA	C2D-C1D-ND	2.78	112.15	110.10
31	N	312	CLA	CMA-C3A-C4A	2.78	119.24	111.77
36	5	618	NEX	C26-C27-C28	-2.78	120.12	125.99
35	g	315	RRX	C8-C7-C6	-2.78	119.41	127.20
31	N	303	CLA	C1D-ND-C4D	-2.78	104.36	106.33
31	a	409	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
30	G	608	CHL	C1-O2A-CGA	2.78	123.73	116.44
43	B	619	BCR	C23-C24-C25	-2.78	119.41	127.20
43	H	101	BCR	C38-C26-C27	2.78	118.95	113.62
31	7	304	CLA	C2D-C1D-ND	2.77	112.15	110.10
30	4	606	CHL	C2C-C3C-C4C	2.77	108.47	106.49
30	N	302	CHL	C2C-C3C-C4C	2.77	108.47	106.49
31	b	613	CLA	C2C-C1C-NC	2.77	112.57	109.97
30	4	606	CHL	C4D-CHA-C1A	2.77	124.62	121.25
31	4	604	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
30	n	306	CHL	CMA-C3A-C4A	2.77	119.23	111.77
31	N	311	CLA	CHD-C1D-ND	-2.77	121.91	124.45
31	R	306	CLA	O1D-CGD-CBD	-2.77	118.81	124.48
31	B	607	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	g	308	CHL	C1B-CHB-C4A	-2.77	124.63	130.12
30	1	619	CHL	CHB-C4A-NA	2.77	128.34	124.51
30	N	301	CHL	CMA-C3A-C4A	2.77	119.22	111.77
31	G	612	CLA	CMA-C3A-C4A	2.77	119.22	111.77
31	4	613	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	C	611	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	0	602	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	s	311	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	3	315	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	0	615	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	n	315	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	C	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
31	B	608	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
31	R	304	CLA	O2A-CGA-CBA	2.77	120.60	111.91
34	s	321	LMG	O8-C28-C29	2.77	120.60	111.91
31	2	611	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
31	S	310	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
30	s	302	CHL	CHB-C4A-NA	2.77	128.34	124.51
31	y	602	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	b	616	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
30	2	607	CHL	C4D-CHA-C1A	2.77	124.62	121.25
31	C	605	CLA	C1-O2A-CGA	2.77	123.71	116.44
30	s	307	CHL	C3C-C4C-NC	-2.77	107.47	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	608	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
31	R	304	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
43	A	410	BCR	C1-C6-C5	-2.77	118.72	122.61
30	3	308	CHL	C3C-C4C-NC	-2.77	107.47	110.57
30	2	601	CHL	C4D-CHA-C1A	2.77	124.62	121.25
30	N	301	CHL	C1B-CHB-C4A	-2.77	124.64	130.12
31	0	610	CLA	CMA-C3A-C4A	2.77	119.21	111.77
33	R	320	LHG	C5-O7-C7	-2.77	110.98	117.79
31	3	314	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	9	306	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	p	612	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	n	316	CLA	C1D-ND-C4D	-2.77	104.37	106.33
31	q	314	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
30	0	606	CHL	C3C-C4C-NC	-2.77	107.47	110.57
30	y	606	CHL	C1B-CHB-C4A	-2.77	124.64	130.12
31	p	603	CLA	O2A-CGA-CBA	2.77	120.59	111.91
31	b	615	CLA	CMA-C3A-C4A	2.77	119.21	111.77
31	8	603	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
31	B	602	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
34	g	320	LMG	C8-O7-C10	-2.76	110.98	117.79
31	4	614	CLA	C2D-C1D-ND	2.76	112.14	110.10
30	7	310	CHL	CMA-C3A-C4A	2.76	119.20	111.77
31	A	407	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
31	c	609	CLA	CMB-C2B-C3B	2.76	129.85	124.68
31	r	315	CLA	C2D-C1D-ND	2.76	112.14	110.10
31	1	604	CLA	CMB-C2B-C3B	2.76	129.85	124.68
32	3	317	LUT	C8-C7-C6	-2.76	119.44	127.20
31	B	611	CLA	C1D-ND-C4D	-2.76	104.37	106.33
31	G	612	CLA	CMB-C2B-C3B	2.76	129.84	124.68
32	4	616	LUT	C21-C26-C27	-2.76	109.21	112.70
31	g	310	CLA	O2A-CGA-CBA	2.76	120.57	111.91
31	y	613	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
33	C	623	LHG	O8-C23-C24	2.76	120.57	111.91
32	3	318	LUT	C21-C26-C27	-2.76	109.21	112.70
31	6	314	CLA	C1D-ND-C4D	-2.76	104.37	106.33
31	C	607	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
31	S	316	CLA	CMA-C3A-C4A	2.76	119.19	111.77
35	g	315	RRX	C38-C26-C27	2.76	119.47	114.36
31	N	321	CLA	CMA-C3A-C4A	2.76	119.19	111.77
43	b	620	BCR	C33-C5-C4	2.76	118.92	113.62
31	N	314	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
30	q	307	CHL	C2C-C3C-C4C	2.76	108.46	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	413	LMG	O8-C28-C29	2.76	120.56	111.91
31	n	313	CLA	CMA-C3A-C4A	2.76	119.19	111.77
31	g	311	CLA	CHD-C1D-ND	-2.76	121.92	124.45
35	g	315	RRX	C34-C9-C10	-2.76	119.06	122.92
31	G	613	CLA	CMA-C3A-C4A	2.76	119.19	111.77
31	y	603	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
31	8	602	CLA	C1D-ND-C4D	-2.76	104.38	106.33
31	3	316	CLA	C1-C2-C3	-2.76	121.27	126.04
32	1	615	LUT	C31-C30-C29	-2.76	123.38	127.31
30	S	307	CHL	C3C-C4C-NC	-2.76	107.48	110.57
31	A	407	CLA	CMA-C3A-C4A	2.76	119.18	111.77
30	N	307	CHL	C1B-CHB-C4A	-2.76	124.66	130.12
30	N	306	CHL	C4D-CHA-C1A	2.76	124.60	121.25
31	c	603	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
33	t	102	LHG	O8-C23-C24	2.76	120.56	111.91
31	D	403	CLA	C1-C2-C3	-2.76	121.28	126.04
31	6	305	CLA	C1D-ND-C4D	-2.76	104.38	106.33
31	5	604	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
43	B	618	BCR	C20-C19-C18	-2.76	118.68	126.42
31	9	316	CLA	C1D-ND-C4D	-2.75	104.38	106.33
33	z	102	LHG	O8-C23-C24	2.75	120.55	111.91
31	4	612	CLA	CMA-C3A-C4A	2.75	119.17	111.77
31	b	612	CLA	C2C-C1C-NC	2.75	112.55	109.97
31	7	304	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
30	r	310	CHL	C2C-C3C-C4C	2.75	108.45	106.49
32	2	615	LUT	C18-C5-C4	2.75	119.46	114.36
31	r	312	CLA	C2D-C1D-ND	2.75	112.13	110.10
31	6	312	CLA	CHD-C1D-ND	-2.75	121.92	124.45
31	3	314	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	c	610	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
30	0	607	CHL	C1B-CHB-C4A	-2.75	124.67	130.12
31	7	315	CLA	CMA-C3A-C4A	2.75	119.17	111.77
31	R	311	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	7	314	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	s	304	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
30	s	309	CHL	C1-O2A-CGA	2.75	123.66	116.44
31	c	602	CLA	C6-C5-C3	-2.75	106.24	113.45
32	0	617	LUT	C1-C6-C5	-2.75	118.74	122.61
31	5	603	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	5	613	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
31	c	611	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
31	y	603	CLA	C2D-C1D-ND	2.75	112.13	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	304	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
30	9	307	CHL	C2C-C3C-C4C	2.75	108.45	106.49
31	8	611	CLA	CMA-C3A-C4A	2.75	119.16	111.77
31	b	610	CLA	O2A-CGA-CBA	2.75	120.54	111.91
31	b	603	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	2	604	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	g	312	CLA	C1D-ND-C4D	-2.75	104.38	106.33
32	6	317	LUT	C30-C31-C32	-2.75	114.64	123.22
32	0	617	LUT	C18-C5-C4	2.75	119.44	114.36
31	r	306	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
31	r	312	CLA	O2A-CGA-CBA	2.75	120.53	111.91
31	5	614	CLA	CHD-C1D-ND	-2.75	121.93	124.45
31	R	314	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	g	312	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
31	q	315	CLA	CMA-C3A-C4A	2.75	119.15	111.77
31	Y	304	CLA	CMA-C3A-C4A	2.75	119.15	111.77
30	y	608	CHL	C1-O2A-CGA	2.75	123.65	116.44
31	Y	314	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
43	h	101	BCR	C29-C30-C25	2.75	114.71	110.48
31	g	304	CLA	C2D-C1D-ND	2.75	112.13	110.10
31	y	610	CLA	CMA-C3A-C4A	2.75	119.15	111.77
31	p	613	CLA	C1D-ND-C4D	-2.74	104.39	106.33
31	1	610	CLA	CMA-C3A-C4A	2.74	119.15	111.77
36	3	319	NEX	C19-C9-C10	-2.74	119.08	122.92
32	6	317	LUT	C35-C15-C14	-2.74	117.85	123.47
31	6	314	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
31	b	607	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
31	y	615	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
30	N	309	CHL	C1-O2A-CGA	2.74	123.64	116.44
31	8	604	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
43	C	615	BCR	C35-C13-C12	-2.74	113.76	118.08
31	9	312	CLA	C2C-C1C-NC	2.74	112.54	109.97
31	y	610	CLA	C2C-C1C-NC	2.74	112.54	109.97
31	C	605	CLA	CHD-C1D-ND	-2.74	121.94	124.45
31	g	313	CLA	C1-C2-C3	-2.74	121.31	126.04
31	n	312	CLA	C1D-ND-C4D	-2.74	104.39	106.33
43	c	615	BCR	C19-C18-C17	2.74	123.14	118.94
31	B	603	CLA	O2A-CGA-CBA	2.74	120.50	111.91
34	W	203	LMG	O8-C28-C29	2.74	120.50	111.91
32	g	316	LUT	C11-C12-C13	-2.74	118.72	126.42
31	6	304	CLA	CMA-C3A-C4A	2.74	119.13	111.77
31	q	306	CLA	CHD-C1D-ND	-2.74	121.94	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	315	CLA	CHD-C1D-ND	-2.74	121.94	124.45
30	0	606	CHL	C1-O2A-CGA	2.74	123.62	116.44
31	q	306	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
31	b	604	CLA	CHD-C1D-ND	-2.74	121.94	124.45
30	4	609	CHL	C1-O2A-CGA	2.74	123.62	116.44
32	n	318	LUT	C18-C5-C4	2.74	119.42	114.36
31	G	603	CLA	C1D-ND-C4D	-2.74	104.39	106.33
31	p	613	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
31	b	616	CLA	C1-C2-C3	-2.74	121.31	126.04
31	1	614	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
31	3	304	CLA	C1D-ND-C4D	-2.74	104.39	106.33
31	A	409	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	B	605	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	Y	311	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
31	g	310	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
30	Y	301	CHL	C1B-CHB-C4A	-2.73	124.70	130.12
31	b	602	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
32	5	616	LUT	C8-C7-C6	-2.73	119.52	127.20
34	7	320	LMG	O8-C28-C29	2.73	120.49	111.91
32	5	617	LUT	C15-C35-C34	-2.73	117.88	123.47
31	A	409	CLA	C2D-C1D-ND	2.73	112.12	110.10
30	n	307	CHL	CMA-C3A-C4A	2.73	119.12	111.77
31	C	602	CLA	C6-C5-C3	-2.73	106.29	113.45
34	A	418	LMG	C8-O7-C10	-2.73	111.06	117.79
31	N	314	CLA	CHD-C1D-ND	-2.73	121.94	124.45
31	c	613	CLA	CHD-C1D-ND	-2.73	121.94	124.45
31	5	603	CLA	C1D-ND-C4D	-2.73	104.39	106.33
31	N	315	CLA	C1D-ND-C4D	-2.73	104.39	106.33
31	n	304	CLA	C1D-ND-C4D	-2.73	104.39	106.33
43	A	410	BCR	C11-C12-C13	-2.73	118.75	126.42
36	3	319	NEX	C38-C25-C26	-2.73	117.69	122.26
31	c	609	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
34	6	321	LMG	O8-C28-C29	2.73	120.47	111.91
31	b	604	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
31	g	311	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
31	D	403	CLA	CMB-C2B-C3B	2.73	129.78	124.68
30	6	308	CHL	C1B-CHB-C4A	-2.73	124.71	130.12
30	7	302	CHL	CMA-C3A-C4A	2.73	119.11	111.77
37	R	318	XAT	C6-C7-C8	-2.73	120.22	125.99
30	8	606	CHL	CMA-C3A-C4A	2.73	119.11	111.77
31	c	608	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
32	1	615	LUT	C15-C14-C13	-2.73	123.42	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	G	603	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
31	n	315	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
32	0	616	LUT	C11-C10-C9	-2.73	123.42	127.31
31	B	613	CLA	C2D-C1D-ND	2.73	112.11	110.10
30	n	301	CHL	C1-O2A-CGA	2.73	123.60	116.44
31	Y	303	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
31	0	604	CLA	C1C-C2C-C3C	-2.73	104.09	106.96
31	c	608	CLA	CMB-C2B-C3B	2.73	129.78	124.68
31	A	407	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
31	2	613	CLA	C1D-ND-C4D	-2.73	104.40	106.33
31	3	313	CLA	C1D-ND-C4D	-2.73	104.40	106.33
31	r	315	CLA	C2C-C1C-NC	2.73	112.53	109.97
31	c	610	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	d	405	CLA	CHD-C1D-ND	-2.72	121.95	124.45
32	7	317	LUT	C30-C31-C32	-2.72	114.71	123.22
30	0	605	CHL	CHD-C4C-C3C	2.72	128.84	124.84
33	B	624	LHG	O8-C23-C24	2.72	120.45	111.91
31	r	307	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
31	q	315	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	c	607	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	2	610	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
31	G	604	CLA	C1C-C2C-C3C	-2.72	104.09	106.96
32	8	616	LUT	C18-C5-C4	2.72	119.40	114.36
31	p	615	CLA	C2C-C1C-NC	2.72	112.52	109.97
31	r	313	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
34	W	202	LMG	O1-C1-C2	2.72	112.55	108.30
48	R	302	LMU	C1B-O1B-C4'	-2.72	111.23	117.96
31	6	313	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
30	9	310	CHL	C1-O2A-CGA	2.72	123.58	116.44
31	c	606	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
31	p	615	CLA	C1D-ND-C4D	-2.72	104.40	106.33
31	y	613	CLA	CMA-C3A-C4A	2.72	119.08	111.77
31	6	316	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
31	c	611	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
30	q	311	CHL	C1B-CHB-C4A	-2.72	124.73	130.12
31	7	303	CLA	C1D-ND-C4D	-2.72	104.40	106.33
30	2	605	CHL	C1B-CHB-C4A	-2.72	124.73	130.12
31	d	404	CLA	CMB-C2B-C3B	2.72	129.76	124.68
31	s	313	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
31	A	405	CLA	C2C-C1C-NC	2.72	112.52	109.97
32	y	616	LUT	C7-C8-C9	-2.72	122.13	126.23
31	9	306	CLA	C1C-C2C-C3C	-2.71	104.10	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	g	316	LUT	C39-C29-C30	-2.71	119.12	122.92
30	5	607	CHL	C1B-CHB-C4A	-2.71	124.74	130.12
31	8	612	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	g	305	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	6	315	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
31	7	315	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
31	c	613	CLA	C1C-C2C-C3C	-2.71	104.10	106.96
31	R	306	CLA	C2D-C1D-ND	2.71	112.10	110.10
31	s	311	CLA	C2C-C1C-NC	2.71	112.51	109.97
31	4	614	CLA	O2A-CGA-CBA	2.71	120.42	111.91
32	q	318	LUT	C11-C12-C13	-2.71	118.80	126.42
31	7	312	CLA	C1D-ND-C4D	-2.71	104.41	106.33
43	C	615	BCR	C24-C23-C22	-2.71	122.14	126.23
32	9	318	LUT	C21-C26-C27	-2.71	109.28	112.70
31	7	311	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	6	304	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	B	603	CLA	CHD-C1D-ND	-2.71	121.96	124.45
31	1	602	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
30	2	601	CHL	CMA-C3A-C4A	2.71	119.05	111.77
31	4	604	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	g	304	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	R	303	CLA	CMA-C3A-C4A	2.71	119.05	111.77
36	r	301	NEX	C5-C6-C1	2.71	122.38	119.70
31	p	603	CLA	CMA-C3A-C4A	2.71	119.05	111.77
30	y	601	CHL	C2C-C3C-C4C	2.71	108.42	106.49
34	r	321	LMG	O1-C1-C2	2.71	112.53	108.30
31	p	612	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	r	311	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	1	613	CLA	C2D-C1D-ND	2.71	112.10	110.10
32	8	615	LUT	C11-C10-C9	-2.71	123.45	127.31
31	c	607	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
31	Y	311	CLA	O2D-CGD-O1D	-2.71	118.55	123.84
33	S	322	LHG	O8-C23-C24	2.71	120.40	111.91
30	g	306	CHL	C2C-C3C-C4C	2.71	108.42	106.49
34	6	321	LMG	C8-O7-C10	-2.71	111.13	117.79
31	c	604	CLA	C2C-C1C-NC	2.71	112.51	109.97
43	t	101	BCR	C16-C15-C14	2.71	129.02	123.47
31	d	404	CLA	O2A-CGA-CBA	2.71	120.40	111.91
31	1	611	CLA	C1D-ND-C4D	-2.71	104.41	106.33
31	5	610	CLA	CMA-C3A-C4A	2.71	119.04	111.77
31	B	612	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
31	8	614	CLA	C1C-C2C-C3C	-2.70	104.11	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	9	307	CHL	C1B-CHB-C4A	-2.70	124.76	130.12
32	0	617	LUT	C10-C11-C12	-2.70	114.78	123.22
30	4	607	CHL	C4D-CHA-C1A	2.70	124.54	121.25
30	Y	307	CHL	C1-C2-C3	-2.70	121.37	126.04
31	1	613	CLA	CHD-C1D-ND	-2.70	121.97	124.45
30	n	306	CHL	C1B-CHB-C4A	-2.70	124.76	130.12
31	C	604	CLA	CMB-C2B-C1B	-2.70	124.31	128.46
31	3	305	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
30	r	310	CHL	C1-C2-C3	-2.70	121.37	126.04
30	4	605	CHL	C1B-CHB-C4A	-2.70	124.77	130.12
31	3	315	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	s	314	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
30	Y	306	CHL	CMA-C3A-C4A	2.70	119.03	111.77
31	R	311	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
31	6	313	CLA	C1-C2-C3	-2.70	121.37	126.04
30	q	307	CHL	CMA-C3A-C4A	2.70	119.03	111.77
31	p	615	CLA	O1D-CGD-CBD	-2.70	118.96	124.48
31	g	314	CLA	C1D-ND-C4D	-2.70	104.42	106.33
30	2	601	CHL	C1-C2-C3	-2.70	121.37	126.04
31	C	601	CLA	C2C-C1C-NC	2.70	112.50	109.97
30	G	601	CHL	C1B-CHB-C4A	-2.70	124.77	130.12
31	9	314	CLA	O2A-CGA-CBA	2.70	120.38	111.91
34	w	204	LMG	O8-C28-C29	2.70	120.38	111.91
33	N	319	LHG	O8-C23-C24	2.70	120.38	111.91
31	C	603	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	8	613	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	g	311	CLA	CAA-C2A-C3A	-2.70	105.39	112.78
31	b	611	CLA	C1D-ND-C4D	-2.70	104.42	106.33
31	d	404	CLA	C2C-C1C-NC	2.70	112.50	109.97
43	b	620	BCR	C11-C12-C13	-2.70	118.84	126.42
32	0	616	LUT	C18-C5-C4	2.70	119.35	114.36
34	w	203	LMG	C9-C8-C7	-2.70	105.41	111.79
31	S	304	CLA	CHA-C4D-ND	2.70	138.14	132.50
31	N	305	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	r	313	CLA	C2D-C1D-ND	2.70	112.09	110.10
30	6	307	CHL	C1B-CHB-C4A	-2.70	124.78	130.12
31	N	310	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
30	y	609	CHL	CHC-C1C-NC	2.70	128.29	124.20
31	q	312	CLA	O1D-CGD-CBD	-2.70	118.97	124.48
30	8	605	CHL	C1B-CHB-C4A	-2.70	124.78	130.12
37	R	318	XAT	C18-C5-C6	-2.70	117.74	122.26
31	c	608	CLA	CAA-C2A-C3A	-2.70	105.40	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	k	101	LMG	C8-O7-C10	-2.70	111.16	117.79
31	N	321	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	B	601	CLA	C2D-C1D-ND	2.69	112.09	110.10
32	n	317	LUT	C11-C10-C9	-2.69	123.46	127.31
34	d	409	LMG	O8-C28-C29	2.69	120.36	111.91
30	S	302	CHL	CMA-C3A-C4A	2.69	119.01	111.77
31	y	614	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	4	610	CLA	CMA-C3A-C4A	2.69	119.01	111.77
31	2	612	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	S	305	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
31	b	604	CLA	C1C-C2C-C3C	-2.69	104.12	106.96
30	G	606	CHL	C1B-CHB-C4A	-2.69	124.78	130.12
30	4	605	CHL	CMA-C3A-C4A	2.69	119.01	111.77
31	S	314	CLA	CMA-C3A-C4A	2.69	119.01	111.77
30	1	601	CHL	CMA-C3A-C2A	2.69	124.69	113.83
31	s	311	CLA	CMB-C2B-C3B	2.69	129.72	124.68
31	q	313	CLA	CHD-C1D-ND	-2.69	121.98	124.45
31	Y	310	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
30	9	310	CHL	C4D-CHA-C1A	2.69	124.53	121.25
31	7	316	CLA	CMA-C3A-C4A	2.69	119.01	111.77
34	q	301	LMG	O8-C28-C29	2.69	120.36	111.91
37	r	318	XAT	C26-C27-C28	-2.69	120.30	125.99
31	4	610	CLA	C1D-ND-C4D	-2.69	104.42	106.33
43	b	619	BCR	C23-C24-C25	-2.69	119.64	127.20
31	b	612	CLA	CMA-C3A-C4A	2.69	119.01	111.77
31	y	604	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	Y	311	CLA	C1-C2-C3	-2.69	121.39	126.04
31	5	615	CLA	CHA-C1A-NA	-2.69	120.24	126.40
34	k	102	LMG	O8-C28-C29	2.69	120.35	111.91
31	6	303	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	S	311	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
30	5	601	CHL	C1B-CHB-C4A	-2.69	124.79	130.12
31	S	305	CLA	C1D-ND-C4D	-2.69	104.42	106.33
31	7	304	CLA	C1D-ND-C4D	-2.69	104.42	106.33
31	8	603	CLA	C1D-ND-C4D	-2.69	104.42	106.33
31	r	305	CLA	C1D-ND-C4D	-2.69	104.42	106.33
32	7	317	LUT	C18-C5-C4	2.69	119.34	114.36
43	b	619	BCR	C7-C8-C9	-2.69	122.17	126.23
31	1	610	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	R	312	CLA	C2C-C1C-NC	2.69	112.49	109.97
30	6	310	CHL	C1-C2-C3	-2.69	121.39	126.04
31	b	604	CLA	CHA-C4D-ND	2.69	138.12	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	4	614	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	5	614	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	8	613	CLA	CHD-C1D-ND	-2.69	121.98	124.45
31	5	610	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
30	s	309	CHL	C4D-CHA-C1A	2.69	124.52	121.25
31	6	316	CLA	C2D-C1D-ND	2.69	112.08	110.10
31	B	602	CLA	C2D-C1D-ND	2.69	112.08	110.10
31	G	609	CLA	C2D-C1D-ND	2.69	112.08	110.10
31	C	611	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
31	c	604	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
31	N	303	CLA	C1C-C2C-C3C	-2.68	104.13	106.96
31	a	409	CLA	C2D-C1D-ND	2.68	112.08	110.10
30	n	301	CHL	CMA-C3A-C4A	2.68	118.99	111.77
31	s	305	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	q	314	CLA	C2D-C1D-ND	2.68	112.08	110.10
31	r	307	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
31	d	404	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	B	612	CLA	C2C-C1C-NC	2.68	112.48	109.97
34	s	321	LMG	O1-C1-C2	2.68	112.49	108.30
31	6	311	CLA	C1-C2-C3	-2.68	121.41	126.04
34	C	624	LMG	O8-C28-C29	2.68	120.32	111.91
31	5	604	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	q	305	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	d	404	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
30	g	309	CHL	C1-O2A-CGA	2.68	123.47	116.44
31	5	613	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	4	604	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
31	s	314	CLA	O2A-CGA-CBA	2.68	120.31	111.91
30	4	608	CHL	C1B-CHB-C4A	-2.68	124.81	130.12
31	5	615	CLA	CHA-C4D-ND	2.68	138.10	132.50
31	2	613	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	p	615	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	y	614	CLA	C1D-ND-C4D	-2.68	104.43	106.33
31	C	612	CLA	C2D-C1D-ND	2.68	112.08	110.10
31	q	306	CLA	C2D-C1D-ND	2.68	112.08	110.10
30	p	601	CHL	C4D-CHA-C1A	2.68	124.51	121.25
31	3	306	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	s	313	CLA	C2D-C1D-ND	2.68	112.08	110.10
30	Y	302	CHL	C1-C2-C3	-2.67	121.42	126.04
31	C	603	CLA	CMB-C2B-C1B	-2.67	124.35	128.46
31	C	605	CLA	C2D-C1D-ND	2.67	112.08	110.10
34	G	621	LMG	O8-C28-C29	2.67	120.30	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	303	CLA	C1D-ND-C4D	-2.67	104.44	106.33
31	S	312	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
30	4	609	CHL	C2C-C3C-C4C	2.67	108.39	106.49
31	3	301	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	5	602	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
34	N	320	LMG	O8-C28-C29	2.67	120.29	111.91
31	n	314	CLA	C1D-ND-C4D	-2.67	104.44	106.33
31	4	613	CLA	O2A-CGA-CBA	2.67	120.29	111.91
31	G	609	CLA	O2A-CGA-CBA	2.67	120.29	111.91
31	2	603	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
30	4	608	CHL	CMA-C3A-C4A	2.67	118.95	111.77
31	S	311	CLA	C2D-C1D-ND	2.67	112.07	110.10
31	s	304	CLA	C1D-ND-C4D	-2.67	104.44	106.33
36	N	318	NEX	C2-C1-C6	2.67	111.81	109.21
36	9	319	NEX	C39-C29-C30	-2.67	119.18	122.92
30	1	606	CHL	C4D-CHA-C1A	2.67	124.50	121.25
30	n	306	CHL	C4D-CHA-C1A	2.67	124.50	121.25
31	5	615	CLA	CMD-C2D-C3D	-2.67	121.47	127.61
31	R	314	CLA	C2D-C1D-ND	2.67	112.07	110.10
31	8	604	CLA	C1D-ND-C4D	-2.67	104.44	106.33
31	3	315	CLA	C1-C2-C3	-2.67	121.43	126.04
31	q	312	CLA	C4B-C3B-C2B	2.67	108.47	106.36
31	8	612	CLA	O2A-CGA-CBA	2.67	120.28	111.91
31	0	614	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	1	602	CLA	CMA-C3A-C4A	2.67	118.94	111.77
30	8	605	CHL	C4D-CHA-C1A	2.67	124.50	121.25
30	y	607	CHL	C1B-CHB-C4A	-2.67	124.83	130.12
34	x	202	LMG	O8-C28-C29	2.67	120.28	111.91
32	N	317	LUT	C21-C26-C27	-2.67	109.33	112.70
31	Y	313	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	0	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
33	1	617	LHG	C5-O7-C7	-2.67	111.23	117.79
31	B	615	CLA	C2D-C1D-ND	2.67	112.07	110.10
31	2	602	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	C	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	s	303	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
33	3	320	LHG	C6-C5-C4	-2.67	105.48	111.79
31	0	611	CLA	C1-C2-C3	-2.67	121.43	126.04
31	4	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
31	c	613	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
31	B	610	CLA	C1D-ND-C4D	-2.66	104.44	106.33
31	N	313	CLA	C1C-C2C-C3C	-2.66	104.16	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	7	305	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	n	314	CLA	O2A-CGA-CBA	2.66	120.27	111.91
33	j	102	LHG	O8-C23-C24	2.66	120.26	111.91
31	b	602	CLA	C2D-C1D-ND	2.66	112.07	110.10
31	b	614	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
33	b	625	LHG	O8-C23-C24	2.66	120.26	111.91
31	7	312	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	4	612	CLA	CHD-C1D-ND	-2.66	122.01	124.45
34	b	622	LMG	C8-O7-C10	-2.66	111.24	117.79
31	r	316	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
31	0	611	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	s	312	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
34	n	322	LMG	O7-C10-O9	-2.66	117.27	123.70
30	s	302	CHL	CMA-C3A-C4A	2.66	118.92	111.77
31	b	606	CLA	O2A-CGA-CBA	2.66	120.26	111.91
34	b	601	LMG	O8-C28-C29	2.66	120.26	111.91
30	2	605	CHL	CMA-C3A-C4A	2.66	118.92	111.77
30	1	608	CHL	C4D-CHA-C1A	2.66	124.49	121.25
31	C	606	CLA	C2D-C1D-ND	2.66	112.06	110.10
31	Y	311	CLA	C1-O2A-CGA	2.66	123.42	116.44
31	y	615	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	4	611	CLA	C1D-ND-C4D	-2.66	104.45	106.33
30	6	310	CHL	C4D-CHA-C1A	2.66	124.48	121.25
31	C	608	CLA	CMB-C2B-C3B	2.66	129.65	124.68
34	D	412	LMG	O8-C28-C29	2.66	120.25	111.91
31	0	610	CLA	C2C-C1C-NC	2.66	112.46	109.97
31	G	611	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	b	615	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
30	S	302	CHL	CHB-C4A-NA	2.66	128.19	124.51
31	q	316	CLA	C2D-C1D-ND	2.66	112.06	110.10
31	n	303	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
31	9	314	CLA	C2C-C1C-NC	2.66	112.46	109.97
31	y	611	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
32	2	615	LUT	C8-C7-C6	-2.66	119.74	127.20
31	S	304	CLA	CHA-C1A-NA	-2.66	120.32	126.40
34	w	204	LMG	C8-O7-C10	-2.66	111.25	117.79
30	n	302	CHL	C1-C2-C3	-2.65	121.45	126.04
30	0	607	CHL	C1-O2A-CGA	2.65	123.41	116.44
30	2	606	CHL	CMA-C3A-C4A	2.65	118.91	111.77
34	A	414	LMG	O8-C28-C29	2.65	120.23	111.91
34	w	202	LMG	O8-C28-C29	2.65	120.23	111.91
30	5	608	CHL	C2C-C3C-C4C	2.65	108.38	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	610	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
30	8	601	CHL	C1-C2-C3	-2.65	121.46	126.04
36	y	618	NEX	C38-C25-C26	-2.65	117.82	122.26
30	n	309	CHL	C1-O2A-CGA	2.65	123.40	116.44
31	Y	305	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	r	314	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	G	602	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
30	r	310	CHL	CMA-C3A-C4A	2.65	118.89	111.77
48	K	101	LMU	O5'-C1'-C2'	2.65	115.96	110.35
31	Y	305	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
31	p	610	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
34	D	409	LMG	O8-C28-C29	2.65	120.22	111.91
31	Y	314	CLA	C1D-ND-C4D	-2.65	104.45	106.33
33	M	101	LHG	C5-O7-C7	-2.65	111.27	117.79
31	0	612	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
31	Y	312	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
31	B	608	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
32	9	318	LUT	C31-C32-C33	-2.65	118.98	126.42
30	2	608	CHL	C1-O2A-CGA	2.65	123.39	116.44
31	9	313	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
30	r	310	CHL	C1B-CHB-C4A	-2.65	124.88	130.12
36	g	317	NEX	C17-C1-C6	-2.65	108.10	110.47
30	G	601	CHL	C2C-C3C-C4C	2.65	108.38	106.49
31	7	315	CLA	C1D-ND-C4D	-2.65	104.46	106.33
31	c	608	CLA	C2D-C1D-ND	2.64	112.05	110.10
31	4	603	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	B	604	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	8	609	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	R	312	CLA	CMD-C2D-C3D	-2.64	121.53	127.61
47	E	101	HEM	CHD-C1D-C2D	-2.64	120.85	124.98
30	G	623	CHL	CMA-C3A-C4A	2.64	118.88	111.77
32	6	317	LUT	C18-C5-C4	2.64	119.25	114.36
30	p	605	CHL	C1B-CHB-C4A	-2.64	124.88	130.12
43	Z	101	BCR	C2-C1-C6	2.64	114.55	110.48
31	0	615	CLA	CHD-C1D-ND	-2.64	122.03	124.45
31	c	605	CLA	CHD-C1D-ND	-2.64	122.03	124.45
31	n	311	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	8	603	CLA	CMD-C2D-C3D	-2.64	121.54	127.61
34	n	321	LMG	O1-C1-C2	2.64	112.43	108.30
33	9	320	LHG	O8-C23-C24	2.64	120.20	111.91
32	Y	316	LUT	C18-C5-C4	2.64	119.25	114.36
31	r	303	CLA	C1D-ND-C4D	-2.64	104.46	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	609	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	c	610	CLA	O2D-CGD-O1D	-2.64	118.68	123.84
31	B	603	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	0	603	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	q	304	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
30	6	302	CHL	C1B-CHB-C4A	-2.64	124.89	130.12
45	C	617	DGD	O1G-C1A-C2A	2.64	120.19	111.91
30	6	302	CHL	CMA-C3A-C4A	2.64	118.87	111.77
31	7	316	CLA	C1D-ND-C4D	-2.64	104.46	106.33
31	G	613	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	C	606	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
31	9	316	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
30	Y	306	CHL	C4D-CHA-C1A	2.64	124.46	121.25
30	9	303	CHL	C1-O2A-CGA	2.64	123.36	116.44
30	N	306	CHL	C2C-C3C-C4C	2.64	108.37	106.49
31	s	316	CLA	CMA-C3A-C4A	2.64	118.86	111.77
30	1	601	CHL	CHC-C1C-NC	2.64	128.20	124.20
30	6	310	CHL	C1B-CHB-C4A	-2.64	124.90	130.12
33	c	622	LHG	O8-C23-C24	2.64	120.18	111.91
31	4	602	CLA	C1C-C2C-C3C	-2.64	104.19	106.96
31	5	612	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	G	611	CLA	CHA-C4D-ND	2.63	138.01	132.50
32	1	616	LUT	C11-C10-C9	-2.63	123.55	127.31
43	B	618	BCR	C23-C24-C25	-2.63	119.81	127.20
33	6	320	LHG	O8-C23-C24	2.63	120.17	111.91
31	N	305	CLA	C1D-ND-C4D	-2.63	104.47	106.33
31	A	409	CLA	CMA-C3A-C4A	2.63	118.85	111.77
31	N	315	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	p	614	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	c	602	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	n	313	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	7	314	CLA	C2D-C1D-ND	2.63	112.04	110.10
30	G	608	CHL	C1-C2-C3	-2.63	121.49	126.04
30	9	310	CHL	CMA-C3A-C4A	2.63	118.84	111.77
33	M	101	LHG	O8-C23-C24	2.63	120.16	111.91
31	a	406	CLA	C2C-C1C-NC	2.63	112.44	109.97
31	0	602	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	a	409	CLA	CMA-C3A-C4A	2.63	118.84	111.77
31	8	613	CLA	O2A-CGA-CBA	2.63	120.16	111.91
45	C	618	DGD	O1G-C1A-C2A	2.63	120.16	111.91
30	9	303	CHL	C1B-CHB-C4A	-2.63	124.91	130.12
35	g	315	RRX	C35-C13-C14	-2.63	119.24	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	3	304	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
31	p	615	CLA	CMA-C3A-C4A	2.63	118.84	111.77
34	w	203	LMG	C7-O1-C1	-2.63	108.61	113.74
31	5	611	CLA	CHD-C1D-ND	-2.63	122.04	124.45
34	G	619	LMG	C8-O7-C10	-2.63	111.32	117.79
31	g	311	CLA	CMA-C3A-C4A	2.63	118.83	111.77
31	4	614	CLA	CMB-C2B-C3B	2.63	129.59	124.68
31	3	312	CLA	C2D-C1D-ND	2.63	112.04	110.10
32	9	318	LUT	C11-C12-C13	-2.63	119.04	126.42
31	D	403	CLA	O2A-CGA-CBA	2.63	120.15	111.91
30	1	607	CHL	C1B-CHB-C4A	-2.63	124.92	130.12
43	h	101	BCR	C8-C7-C6	-2.63	119.83	127.20
36	R	319	NEX	C17-C1-C6	-2.63	108.12	110.47
34	2	618	LMG	O8-C28-C29	2.63	120.15	111.91
30	1	607	CHL	CMA-C3A-C4A	2.63	118.83	111.77
31	y	602	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
33	G	618	LHG	O8-C23-C24	2.63	120.15	111.91
31	2	609	CLA	O1D-CGD-CBD	-2.62	119.11	124.48
32	g	316	LUT	C31-C32-C33	-2.62	119.04	126.42
31	D	404	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	R	313	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	c	609	CLA	C1-C2-C3	-2.62	121.50	126.04
32	1	616	LUT	C30-C31-C32	-2.62	115.03	123.22
31	S	315	CLA	CMD-C2D-C3D	-2.62	121.58	127.61
31	b	608	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	y	612	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
30	Y	309	CHL	CHC-C1C-NC	2.62	128.18	124.20
33	L	101	LHG	O8-C23-C24	2.62	120.14	111.91
31	1	604	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
31	7	303	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	p	611	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	b	613	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	C	609	CLA	C2D-C1D-ND	2.62	112.04	110.10
31	0	612	CLA	C2D-C1D-ND	2.62	112.04	110.10
43	c	615	BCR	C37-C22-C21	-2.62	119.25	122.92
30	y	601	CHL	C1B-CHB-C4A	-2.62	124.93	130.12
34	f	101	LMG	O8-C28-C29	2.62	120.13	111.91
31	Y	312	CLA	C2D-C1D-ND	2.62	112.03	110.10
31	6	311	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	9	312	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
31	3	311	CLA	CMA-C3A-C4A	2.62	118.81	111.77
31	0	613	CLA	C2D-C1D-ND	2.62	112.03	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	607	CLA	C2D-C1D-ND	2.62	112.03	110.10
31	c	607	CLA	O2A-CGA-CBA	2.62	120.12	111.91
30	7	306	CHL	C1B-CHB-C4A	-2.62	124.93	130.12
31	A	407	CLA	CMB-C2B-C3B	2.62	129.58	124.68
31	0	612	CLA	CHA-C4D-ND	2.62	137.97	132.50
31	R	311	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
30	3	308	CHL	C4D-CHA-C1A	2.62	124.43	121.25
36	R	301	NEX	C39-C29-C30	-2.62	119.26	122.92
36	Y	317	NEX	C40-C33-C34	-2.62	119.26	122.92
32	y	617	LUT	C10-C11-C12	-2.62	115.05	123.22
31	8	610	CLA	C1C-C2C-C3C	-2.62	104.21	106.96
43	D	405	BCR	C4-C5-C6	-2.62	118.93	122.73
30	2	607	CHL	C1B-CHB-C4A	-2.62	124.94	130.12
31	S	310	CLA	CMA-C3A-C4A	2.62	118.80	111.77
33	7	319	LHG	O8-C23-C24	2.61	120.11	111.91
31	S	312	CLA	C2D-C1D-ND	2.61	112.03	110.10
33	s	320	LHG	C6-C5-C4	-2.61	105.60	111.79
33	6	320	LHG	C5-O7-C7	-2.61	111.35	117.79
31	g	303	CLA	C2C-C1C-NC	2.61	112.42	109.97
43	H	101	BCR	C16-C15-C14	-2.61	118.12	123.47
31	0	602	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	q	316	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	B	604	CLA	CHA-C4D-ND	2.61	137.97	132.50
31	p	604	CLA	C2D-C1D-ND	2.61	112.03	110.10
31	1	611	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	Y	304	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	n	316	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
43	A	410	BCR	C8-C7-C6	-2.61	119.86	127.20
30	y	607	CHL	CMA-C3A-C4A	2.61	118.80	111.77
31	B	603	CLA	CMA-C3A-C4A	2.61	118.80	111.77
31	6	312	CLA	O2A-CGA-CBA	2.61	120.11	111.91
30	2	608	CHL	C1-C2-C3	-2.61	121.53	126.04
31	r	306	CLA	CAA-C2A-C3A	-2.61	105.63	112.78
31	q	313	CLA	C1D-ND-C4D	-2.61	104.48	106.33
36	G	616	NEX	C38-C25-C26	-2.61	117.89	122.26
30	5	605	CHL	C2C-C3C-C4C	2.61	108.35	106.49
31	A	406	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
31	G	610	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	8	611	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
31	2	611	CLA	O2A-CGA-CBA	2.61	120.10	111.91
31	4	611	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
34	C	622	LMG	O8-C28-C29	2.61	120.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	318	LUT	C1-C6-C5	-2.61	118.94	122.61
31	B	606	CLA	C1-C2-C3	-2.61	121.53	126.04
31	R	312	CLA	C2D-C1D-ND	2.61	112.03	110.10
33	1	617	LHG	O8-C23-C24	2.61	120.09	111.91
31	p	602	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
30	1	608	CHL	C1B-CHB-C4A	-2.61	124.95	130.12
33	D	407	LHG	O8-C23-C24	2.61	120.09	111.91
34	6	323	LMG	O8-C28-C29	2.61	120.09	111.91
31	N	313	CLA	C1D-ND-C4D	-2.61	104.48	106.33
31	s	315	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
30	Y	302	CHL	C1B-CHB-C4A	-2.61	124.95	130.12
31	4	610	CLA	CHA-C4D-ND	2.61	137.95	132.50
31	5	612	CLA	C1D-ND-C4D	-2.61	104.48	106.33
31	5	614	CLA	C1D-ND-C4D	-2.61	104.48	106.33
31	8	602	CLA	C1C-C2C-C3C	-2.61	104.22	106.96
31	n	315	CLA	O2A-CGA-CBA	2.61	120.08	111.91
31	B	604	CLA	CHD-C1D-ND	-2.61	122.06	124.45
32	S	317	LUT	C8-C7-C6	-2.60	119.89	127.20
31	S	314	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	b	609	CLA	CMB-C2B-C3B	2.60	129.55	124.68
30	8	606	CHL	C1B-CHB-C4A	-2.60	124.96	130.12
30	4	607	CHL	C1-C2-C3	-2.60	121.54	126.04
31	B	606	CLA	O2A-CGA-CBA	2.60	120.08	111.91
31	b	617	CLA	O2A-CGA-CBA	2.60	120.08	111.91
31	Y	313	CLA	CMB-C2B-C3B	2.60	129.55	124.68
33	C	623	LHG	C5-O7-C7	-2.60	111.38	117.79
45	C	620	DGD	C2G-O2G-C1B	-2.60	111.38	117.79
30	n	307	CHL	C1B-CHB-C4A	-2.60	124.96	130.12
31	G	612	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	N	312	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
31	S	310	CLA	C2D-C1D-ND	2.60	112.02	110.10
30	7	308	CHL	C1B-CHB-C4A	-2.60	124.96	130.12
32	3	317	LUT	C18-C5-C4	2.60	119.18	114.36
47	e	102	HEM	CHD-C1D-C2D	-2.60	120.91	124.98
31	R	316	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	6	312	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	s	310	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	G	604	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	d	405	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
34	J	101	LMG	O8-C28-C29	2.60	120.07	111.91
31	D	403	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
31	3	305	CLA	C2D-C1D-ND	2.60	112.02	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	314	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
32	1	616	LUT	C15-C35-C34	-2.60	118.15	123.47
43	z	101	BCR	C4-C5-C6	-2.60	118.96	122.73
31	R	313	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	3	313	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	r	303	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
34	B	622	LMG	C8-O7-C10	-2.60	111.39	117.79
31	s	312	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	9	312	CLA	C1D-ND-C4D	-2.60	104.49	106.33
31	b	609	CLA	CMA-C3A-C4A	2.60	118.76	111.77
30	6	306	CHL	C4A-NA-C1A	2.60	107.87	106.71
31	c	602	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
34	j	101	LMG	O8-C28-C29	2.60	120.06	111.91
31	1	602	CLA	C2D-C1D-ND	2.60	112.02	110.10
31	n	305	CLA	C1D-ND-C4D	-2.60	104.49	106.33
32	1	616	LUT	C8-C7-C6	-2.60	119.91	127.20
30	5	609	CHL	C2C-C3C-C4C	2.60	108.34	106.49
30	S	309	CHL	C4D-CHA-C1A	2.60	124.41	121.25
30	4	607	CHL	C1-O2A-CGA	2.60	123.26	116.44
31	b	611	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
31	g	314	CLA	C1C-C2C-C3C	-2.60	104.23	106.96
31	B	605	CLA	CMB-C2B-C3B	2.60	129.53	124.68
32	G	615	LUT	C39-C29-C30	-2.60	119.29	122.92
34	b	624	LMG	O1-C1-C2	2.59	112.35	108.30
31	R	304	CLA	C2D-C1D-ND	2.59	112.02	110.10
31	8	603	CLA	C2D-C1D-ND	2.59	112.02	110.10
30	7	302	CHL	CHC-C1C-NC	2.59	128.14	124.20
31	y	613	CLA	C2D-C1D-ND	2.59	112.02	110.10
31	5	611	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	n	312	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	B	609	CLA	O2A-CGA-CBA	2.59	120.05	111.91
36	0	618	NEX	C19-C9-C10	-2.59	119.29	122.92
31	C	604	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
30	1	619	CHL	C1B-CHB-C4A	-2.59	124.98	130.12
31	G	613	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
31	b	605	CLA	CHA-C4D-ND	2.59	137.92	132.50
30	y	601	CHL	CMA-C3A-C4A	2.59	118.74	111.77
30	G	607	CHL	C1B-CHB-C4A	-2.59	124.99	130.12
31	0	611	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
31	3	316	CLA	CHA-C4D-ND	2.59	137.91	132.50
31	2	604	CLA	C1D-ND-C4D	-2.59	104.50	106.33
43	B	617	BCR	C2-C1-C6	2.59	114.47	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	p	604	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
31	b	615	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
31	2	604	CLA	CMA-C3A-C4A	2.59	118.73	111.77
31	c	602	CLA	C1-O2A-CGA	2.59	123.23	116.44
43	H	101	BCR	C33-C5-C4	2.59	118.59	113.62
31	0	602	CLA	O2A-CGA-CBA	2.59	120.03	111.91
31	y	612	CLA	C2D-C1D-ND	2.59	112.01	110.10
32	1	615	LUT	C1-C6-C5	-2.59	118.97	122.61
31	G	610	CLA	CMA-C3A-C4A	2.59	118.73	111.77
31	3	312	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
31	s	313	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
31	9	313	CLA	CMA-C3A-C4A	2.59	118.72	111.77
30	4	609	CHL	CHB-C4A-NA	2.59	128.09	124.51
34	1	618	LMG	O8-C28-C29	2.59	120.02	111.91
30	Y	302	CHL	CMA-C3A-C4A	2.59	118.72	111.77
30	0	601	CHL	C1-O2A-CGA	2.59	123.23	116.44
31	G	611	CLA	CMB-C2B-C3B	2.59	129.51	124.68
31	A	407	CLA	C2D-C1D-ND	2.59	112.01	110.10
31	B	608	CLA	C2D-C1D-ND	2.59	112.01	110.10
31	4	603	CLA	C2D-C1D-ND	2.58	112.01	110.10
31	y	610	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	B	614	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
31	B	604	CLA	CMD-C2D-C3D	-2.58	121.67	127.61
31	6	312	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
36	q	319	NEX	C40-C33-C34	-2.58	119.31	122.92
32	6	318	LUT	C18-C5-C4	2.58	119.14	114.36
31	D	403	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	r	312	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
32	y	616	LUT	C39-C29-C28	2.58	122.14	118.08
37	R	318	XAT	C26-C27-C28	-2.58	120.53	125.99
31	q	313	CLA	CMA-C3A-C4A	2.58	118.71	111.77
31	r	313	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	r	315	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
30	1	601	CHL	CHB-C4A-NA	2.58	128.08	124.51
30	G	623	CHL	C1B-CHB-C4A	-2.58	125.00	130.12
30	S	308	CHL	CMA-C3A-C4A	2.58	118.71	111.77
30	2	606	CHL	C2C-C3C-C4C	2.58	108.33	106.49
31	7	305	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
31	6	305	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	B	614	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	b	605	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
31	9	305	CLA	C1D-ND-C4D	-2.58	104.50	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	3	311	CLA	O2A-CGA-CBA	2.58	120.00	111.91
34	0	620	LMG	O8-C28-C29	2.58	120.00	111.91
31	a	407	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
30	R	310	CHL	CHB-C4A-NA	2.58	128.08	124.51
31	7	313	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
43	c	615	BCR	C23-C22-C21	2.58	122.90	118.94
31	R	312	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	S	303	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	G	611	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
30	p	608	CHL	CMA-C3A-C4A	2.58	118.70	111.77
34	C	621	LMG	O8-C28-C29	2.58	120.00	111.91
31	G	610	CLA	C2D-C1D-ND	2.58	112.00	110.10
30	G	608	CHL	CMA-C3A-C2A	2.58	124.22	113.83
31	9	314	CLA	CHA-C4D-ND	2.58	137.89	132.50
31	9	304	CLA	O2A-CGA-CBA	2.58	119.99	111.91
31	9	313	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
31	c	601	CLA	CHA-C4D-ND	2.58	137.89	132.50
31	S	316	CLA	C2D-C1D-ND	2.58	112.00	110.10
31	C	609	CLA	C1-C2-C3	-2.58	121.59	126.04
36	p	618	NEX	C26-C27-C28	-2.58	120.55	125.99
31	4	610	CLA	CHD-C1D-ND	-2.57	122.09	124.45
36	p	618	NEX	C17-C1-C6	-2.57	108.17	110.47
31	a	407	CLA	C2D-C1D-ND	2.57	112.00	110.10
31	B	610	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
30	2	601	CHL	C2C-C3C-C4C	2.57	108.32	106.49
31	B	608	CLA	CMA-C3A-C4A	2.57	118.69	111.77
30	9	311	CHL	CHC-C1C-NC	2.57	128.11	124.20
31	d	405	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
31	y	611	CLA	C1-O2A-CGA	2.57	123.19	116.44
43	h	101	BCR	C15-C16-C17	-2.57	118.21	123.47
30	s	308	CHL	C1B-CHB-C4A	-2.57	125.03	130.12
30	4	608	CHL	C1-O2A-CGA	2.57	123.19	116.44
31	6	305	CLA	CMA-C3A-C4A	2.57	118.68	111.77
31	c	603	CLA	O2A-CGA-CBA	2.57	119.97	111.91
32	y	617	LUT	C11-C10-C9	-2.57	123.64	127.31
34	c	620	LMG	O8-C28-C29	2.57	119.97	111.91
31	6	304	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
31	a	409	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
31	C	602	CLA	CMA-C3A-C4A	2.57	118.67	111.77
34	Y	319	LMG	O8-C28-C29	2.57	119.97	111.91
31	B	608	CLA	CHD-C1D-ND	-2.57	122.09	124.45
31	7	305	CLA	CHA-C4D-ND	2.57	137.87	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	d	406	BCR	C11-C12-C13	2.57	133.63	126.42
31	6	312	CLA	C1-O2A-CGA	2.56	123.17	116.44
31	B	605	CLA	C2D-C1D-ND	2.56	111.99	110.10
31	B	601	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
37	2	619	XAT	C26-C27-C28	-2.56	120.57	125.99
31	6	304	CLA	OBD-CAD-C3D	-2.56	122.35	128.52
31	g	311	CLA	CHA-C4D-ND	2.56	137.86	132.50
31	B	603	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
31	R	315	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
31	R	313	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
31	y	611	CLA	C2C-C1C-NC	2.56	112.37	109.97
31	g	311	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
30	R	310	CHL	CMA-C3A-C4A	2.56	118.66	111.77
31	b	616	CLA	C2D-C1D-ND	2.56	111.99	110.10
31	c	605	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
32	p	617	LUT	C15-C14-C13	-2.56	123.65	127.31
31	N	311	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
43	B	618	BCR	C33-C5-C4	2.56	118.53	113.62
33	5	619	LHG	O8-C23-C24	2.56	119.94	111.91
31	6	312	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
31	C	609	CLA	CMB-C2B-C3B	2.56	129.47	124.68
44	A	416	PL9	C7-C8-C9	-2.56	122.53	126.79
36	R	301	NEX	C20-C13-C14	-2.56	119.34	122.92
31	s	314	CLA	C2D-C1D-ND	2.56	111.99	110.10
31	5	604	CLA	CMA-C3A-C4A	2.56	118.65	111.77
31	S	306	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
31	C	613	CLA	CBA-CAA-C2A	2.56	121.42	113.86
31	a	407	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
31	q	312	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
30	s	308	CHL	C4A-NA-C1A	2.56	107.86	106.71
31	G	613	CLA	C2D-C1D-ND	2.56	111.99	110.10
36	6	319	NEX	C19-C9-C10	-2.56	119.34	122.92
32	0	616	LUT	C39-C29-C28	2.56	122.11	118.08
31	N	304	CLA	C1D-ND-C4D	-2.56	104.52	106.33
32	7	318	LUT	C1-C6-C5	-2.56	119.01	122.61
31	c	610	CLA	C1-O2A-CGA	2.56	123.15	116.44
31	Y	312	CLA	CHA-C4D-ND	2.56	137.85	132.50
37	G	620	XAT	C26-C27-C28	-2.56	120.59	125.99
30	4	606	CHL	C1B-CHB-C4A	-2.56	125.05	130.12
34	X	203	LMG	O8-C28-C29	2.56	119.93	111.91
30	2	601	CHL	C1B-CHB-C4A	-2.56	125.06	130.12
31	A	409	CLA	CAA-C2A-C3A	-2.55	105.78	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	v	101	BCR	C38-C26-C27	2.55	118.52	113.62
31	Y	305	CLA	C1D-ND-C4D	-2.55	104.52	106.33
31	9	314	CLA	C1D-ND-C4D	-2.55	104.52	106.33
30	y	607	CHL	C1-C2-C3	-2.55	121.63	126.04
31	1	604	CLA	O2A-CGA-CBA	2.55	119.92	111.91
31	r	316	CLA	O2A-CGA-CBA	2.55	119.92	111.91
30	6	309	CHL	CHD-C4C-C3C	2.55	128.59	124.84
31	s	306	CLA	C1C-C2C-C3C	-2.55	104.27	106.96
31	R	306	CLA	CHA-C4D-ND	2.55	137.84	132.50
36	q	319	NEX	C17-C1-C6	-2.55	108.19	110.47
30	S	309	CHL	C2C-C3C-C4C	2.55	108.31	106.49
31	d	401	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
31	D	404	CLA	CMB-C2B-C3B	2.55	129.45	124.68
43	t	101	BCR	C29-C30-C25	2.55	114.41	110.48
30	R	309	CHL	C1B-CHB-C4A	-2.55	125.07	130.12
32	p	616	LUT	C19-C9-C10	-2.55	119.35	122.92
31	7	304	CLA	CHA-C4D-ND	2.55	137.83	132.50
31	3	316	CLA	CBA-CAA-C2A	-2.55	106.34	113.86
30	y	608	CHL	C2C-C3C-C4C	2.55	108.31	106.49
31	Y	313	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
32	4	616	LUT	C1-C6-C5	-2.55	119.02	122.61
43	b	620	BCR	C23-C24-C25	-2.55	120.05	127.20
43	h	101	BCR	C23-C24-C25	-2.55	120.05	127.20
31	9	315	CLA	C1D-ND-C4D	-2.55	104.53	106.33
31	1	610	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
30	4	601	CHL	C1B-CHB-C4A	-2.55	125.07	130.12
31	b	609	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
30	3	309	CHL	CMA-C3A-C4A	2.55	118.62	111.77
30	2	605	CHL	C4A-NA-C1A	2.55	107.85	106.71
34	G	622	LMG	O8-C28-C29	2.55	119.90	111.91
31	0	614	CLA	C1D-ND-C4D	-2.55	104.53	106.33
30	9	311	CHL	C1-O2A-CGA	2.55	123.12	116.44
30	7	306	CHL	C4D-CHA-C1A	2.55	124.35	121.25
31	q	316	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
31	b	613	CLA	CMA-C3A-C4A	2.55	118.61	111.77
35	2	614	RRX	C8-C7-C6	-2.55	120.05	127.20
31	7	313	CLA	CHA-C4D-ND	2.55	137.82	132.50
33	d	408	LHG	O8-C23-C24	2.54	119.89	111.91
31	y	613	CLA	CHA-C4D-ND	2.54	137.82	132.50
30	0	608	CHL	C1-O2A-CGA	2.54	123.12	116.44
31	B	606	CLA	CHA-C4D-ND	2.54	137.82	132.50
30	5	605	CHL	C4D-CHA-C1A	2.54	124.34	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	7	305	CLA	CMD-C2D-C3D	-2.54	121.76	127.61
33	0	619	LHG	C6-C5-C4	-2.54	105.77	111.79
43	b	619	BCR	C30-C25-C26	-2.54	119.03	122.61
31	B	607	CLA	CHA-C4D-ND	2.54	137.82	132.50
33	4	618	LHG	O8-C23-C24	2.54	119.89	111.91
37	q	321	XAT	C26-C27-C28	-2.54	120.62	125.99
31	a	409	CLA	O2A-CGA-CBA	2.54	119.89	111.91
31	s	305	CLA	CMA-C3A-C4A	2.54	118.61	111.77
31	y	604	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
31	p	614	CLA	CHA-C4D-ND	2.54	137.81	132.50
37	4	619	XAT	C26-C27-C28	-2.54	120.62	125.99
31	8	611	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
31	A	409	CLA	O2A-CGA-CBA	2.54	119.88	111.91
31	r	316	CLA	C2D-C1D-ND	2.54	111.98	110.10
30	n	310	CHL	CMA-C3A-C2A	2.54	124.08	113.83
32	q	318	LUT	C21-C26-C27	-2.54	109.49	112.70
31	N	305	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
31	l	612	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
31	y	612	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
34	w	201	LMG	O8-C28-C29	2.54	119.88	111.91
31	b	608	CLA	CMA-C3A-C4A	2.54	118.60	111.77
43	B	618	BCR	C38-C26-C25	-2.54	121.68	124.53
31	b	606	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
31	Y	313	CLA	C2D-C1D-ND	2.54	111.97	110.10
30	y	605	CHL	C4D-CHA-C1A	2.54	124.34	121.25
31	R	314	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
31	R	304	CLA	CMB-C2B-C3B	2.54	129.43	124.68
31	B	614	CLA	C1D-ND-C4D	-2.54	104.53	106.33
31	l	604	CLA	C2D-C1D-ND	2.54	111.97	110.10
31	0	611	CLA	C2D-C1D-ND	2.54	111.97	110.10
31	S	313	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
31	q	306	CLA	CHA-C4D-ND	2.54	137.80	132.50
30	g	302	CHL	CMA-C3A-C4A	2.54	118.59	111.77
43	C	614	BCR	C15-C16-C17	-2.54	118.28	123.47
31	r	307	CLA	CAA-C2A-C3A	-2.54	105.84	112.78
34	w	205	LMG	O8-C28-C29	2.54	119.86	111.91
31	C	612	CLA	O2A-CGA-CBA	2.53	119.86	111.91
31	A	406	CLA	CMA-C3A-C4A	2.53	118.58	111.77
31	7	314	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
31	Y	312	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
31	p	604	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
35	q	317	RRX	C29-C28-C27	2.53	113.77	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	607	CLA	O2A-CGA-CBA	2.53	119.86	111.91
32	1	616	LUT	C10-C11-C12	-2.53	115.31	123.22
31	2	604	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	G	612	CLA	C2D-C1D-ND	2.53	111.97	110.10
34	n	321	LMG	O8-C28-C29	2.53	119.86	111.91
31	B	607	CLA	CMA-C3A-C4A	2.53	118.58	111.77
31	R	312	CLA	O2A-CGA-CBA	2.53	119.86	111.91
31	S	313	CLA	CHA-C4D-ND	2.53	137.80	132.50
31	c	605	CLA	CHA-C4D-ND	2.53	137.79	132.50
33	3	320	LHG	O8-C23-C24	2.53	119.85	111.91
30	S	302	CHL	CHC-C1C-NC	2.53	128.04	124.20
31	B	609	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
30	6	302	CHL	C2C-C3C-C4C	2.53	108.29	106.49
31	b	612	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
31	4	610	CLA	O2A-CGA-CBA	2.53	119.85	111.91
31	n	313	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
34	q	301	LMG	C8-O7-C10	-2.53	111.56	117.79
36	n	319	NEX	C38-C25-C26	-2.53	118.02	122.26
37	9	322	XAT	C26-C27-C28	-2.53	120.64	125.99
33	L	101	LHG	C5-O7-C7	-2.53	111.56	117.79
32	y	616	LUT	C15-C35-C34	-2.53	118.29	123.47
30	0	607	CHL	CMA-C3A-C4A	2.53	118.57	111.77
31	C	608	CLA	CAA-C2A-C3A	-2.53	105.85	112.78
30	q	310	CHL	CHD-C4C-C3C	2.53	128.56	124.84
43	b	618	BCR	C1-C6-C5	-2.53	119.05	122.61
31	q	313	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
31	8	614	CLA	C1D-ND-C4D	-2.53	104.54	106.33
31	S	305	CLA	CMA-C3A-C4A	2.53	118.57	111.77
33	r	320	LHG	C5-O7-C7	-2.53	111.57	117.79
37	g	321	XAT	C26-C27-C28	-2.53	120.65	125.99
31	B	611	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
34	p	620	LMG	O8-C28-C29	2.53	119.84	111.91
35	q	317	RRX	C23-C24-C25	-2.53	120.11	127.20
31	b	607	CLA	CHA-C4D-ND	2.53	137.78	132.50
31	b	611	CLA	C1C-C2C-C3C	-2.53	104.30	106.96
31	d	404	CLA	C1D-ND-C4D	-2.53	104.54	106.33
34	a	416	LMG	C8-O7-C10	-2.53	111.57	117.79
31	3	313	CLA	O2A-CGA-CBA	2.53	119.83	111.91
31	S	312	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
31	B	612	CLA	CMA-C3A-C4A	2.52	118.56	111.77
31	d	405	CLA	CMA-C3A-C4A	2.52	118.56	111.77
34	r	321	LMG	O8-C28-C29	2.52	119.83	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	b	618	BCR	C38-C26-C27	2.52	118.46	113.62
31	b	613	CLA	C6-C5-C3	-2.52	106.84	113.45
32	y	616	LUT	C31-C30-C29	-2.52	123.71	127.31
31	0	610	CLA	C1-C2-C3	-2.52	121.68	126.04
30	p	608	CHL	C1B-CHB-C4A	-2.52	125.12	130.12
31	B	616	CLA	O2A-CGA-CBA	2.52	119.82	111.91
31	3	305	CLA	C1D-ND-C4D	-2.52	104.54	106.33
31	4	611	CLA	C4B-C3B-C2B	2.52	108.36	106.36
30	4	609	CHL	CHC-C1C-NC	2.52	128.03	124.20
33	D	408	LHG	C5-O7-C7	-2.52	111.59	117.79
31	s	311	CLA	C6-C5-C3	-2.52	106.85	113.45
30	5	607	CHL	CHC-C1C-NC	2.52	128.03	124.20
31	4	603	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	B	614	CLA	CHA-C4D-ND	2.52	137.77	132.50
31	1	602	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
36	y	618	NEX	C39-C29-C30	-2.52	119.40	122.92
31	y	612	CLA	CHA-C4D-ND	2.52	137.77	132.50
43	T	101	BCR	C29-C30-C25	2.52	114.36	110.48
31	p	603	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
31	Y	313	CLA	O2A-CGA-CBA	2.52	119.81	111.91
36	G	616	NEX	C20-C13-C14	-2.52	119.40	122.92
31	p	604	CLA	O2A-CGA-CBA	2.52	119.81	111.91
32	Y	316	LUT	C18-C5-C6	-2.52	121.70	124.53
31	q	305	CLA	CHA-C4D-ND	2.52	137.76	132.50
32	p	617	LUT	C8-C7-C6	-2.52	120.14	127.20
36	4	617	NEX	C39-C29-C30	-2.51	119.40	122.92
31	9	313	CLA	CHA-C4D-ND	2.51	137.76	132.50
31	B	604	CLA	CMB-C2B-C3B	2.51	129.38	124.68
31	0	612	CLA	CMA-C3A-C4A	2.51	118.53	111.77
31	y	604	CLA	C1D-ND-C4D	-2.51	104.55	106.33
30	2	608	CHL	CHC-C1C-NC	2.51	128.02	124.20
33	0	619	LHG	O8-C23-C24	2.51	119.80	111.91
31	G	612	CLA	O2A-CGA-CBA	2.51	119.80	111.91
31	0	615	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
31	r	311	CLA	CMB-C2B-C3B	2.51	129.38	124.68
33	D	407	LHG	C5-O7-C7	-2.51	111.60	117.79
34	B	622	LMG	O8-C28-C29	2.51	119.79	111.91
31	B	603	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	G	610	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	q	314	CLA	CHA-C4D-ND	2.51	137.75	132.50
31	C	601	CLA	O2A-CGA-CBA	2.51	119.79	111.91
31	q	314	CLA	C1D-ND-C4D	-2.51	104.55	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	605	CLA	CHA-C4D-ND	2.51	137.75	132.50
36	R	301	NEX	C31-C30-C29	2.51	130.89	127.31
31	R	303	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
30	3	303	CHL	C1-O2A-CGA	2.51	123.03	116.44
30	7	310	CHL	CHC-C1C-NC	2.51	128.01	124.20
31	C	611	CLA	CMB-C2B-C3B	2.51	129.37	124.68
31	R	306	CLA	CMB-C2B-C3B	2.51	129.37	124.68
31	1	612	CLA	CHA-C4D-ND	2.51	137.75	132.50
30	7	306	CHL	CHB-C4A-NA	2.51	127.98	124.51
32	9	318	LUT	C40-C33-C34	-2.51	119.41	122.92
31	R	315	CLA	CHA-C4D-ND	2.51	137.75	132.50
30	9	311	CHL	CHD-C4C-C3C	2.51	128.53	124.84
31	q	316	CLA	CHA-C4D-ND	2.51	137.74	132.50
34	3	321	LMG	O8-C28-C29	2.51	119.78	111.91
43	a	410	BCR	C19-C18-C17	-2.51	115.09	118.94
31	N	313	CLA	O2A-CGA-CBA	2.51	119.77	111.91
31	r	315	CLA	O2A-CGA-CBA	2.51	119.77	111.91
31	c	606	CLA	C2D-C1D-ND	2.51	111.95	110.10
30	1	619	CHL	CMA-C3A-C2A	2.51	123.94	113.83
34	2	618	LMG	C8-O7-C10	-2.51	111.62	117.79
37	r	318	XAT	C18-C5-C6	-2.51	118.06	122.26
31	2	613	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
43	C	615	BCR	C37-C22-C21	-2.50	119.41	122.92
31	c	609	CLA	C2D-C1D-ND	2.50	111.95	110.10
31	6	316	CLA	CHA-C4D-ND	2.50	137.74	132.50
30	8	608	CHL	CMA-C3A-C2A	2.50	123.93	113.83
30	r	309	CHL	C1B-CHB-C4A	-2.50	125.16	130.12
31	Y	304	CLA	C1D-ND-C4D	-2.50	104.56	106.33
31	G	603	CLA	O2A-CGA-CBA	2.50	119.77	111.91
30	g	309	CHL	CMA-C3A-C2A	2.50	123.93	113.83
32	p	617	LUT	C21-C26-C25	2.50	115.90	111.42
31	G	611	CLA	C2D-C1D-ND	2.50	111.95	110.10
31	c	611	CLA	CMB-C2B-C3B	2.50	129.36	124.68
34	G	619	LMG	O8-C28-C29	2.50	119.76	111.91
31	b	614	CLA	C1D-ND-C4D	-2.50	104.56	106.33
31	A	406	CLA	C2D-C1D-ND	2.50	111.95	110.10
36	R	319	NEX	C26-C27-C28	-2.50	120.70	125.99
32	y	616	LUT	C19-C9-C8	2.50	122.02	118.08
30	G	608	CHL	CHB-C4A-NA	2.50	127.97	124.51
35	G	614	RRX	C8-C7-C6	-2.50	120.18	127.20
30	8	608	CHL	CHD-C4C-C3C	2.50	128.52	124.84
31	3	315	CLA	O2D-CGD-O1D	-2.50	118.95	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	s	310	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
33	r	320	LHG	O8-C23-C24	2.50	119.75	111.91
31	6	305	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
32	s	318	LUT	C30-C31-C32	-2.50	115.42	123.22
30	1	609	CHL	CHC-C1C-NC	2.50	128.00	124.20
31	B	604	CLA	O1D-CGD-CBD	-2.50	119.37	124.48
31	2	602	CLA	CHA-C4D-ND	2.50	137.73	132.50
31	b	609	CLA	CHD-C1D-ND	-2.50	122.16	124.45
35	4	615	RRX	C8-C7-C6	-2.50	120.19	127.20
45	c	617	DGD	O6E-C1E-O5D	2.50	115.89	109.97
31	8	603	CLA	CHA-C4D-ND	2.50	137.72	132.50
31	S	311	CLA	CAA-C2A-C3A	-2.50	105.94	112.78
34	J	102	LMG	O8-C28-C29	2.50	119.75	111.91
30	p	607	CHL	C1-O2A-CGA	2.50	123.00	116.44
33	p	619	LHG	O8-C23-C24	2.50	119.74	111.91
30	1	605	CHL	CHC-C1C-NC	2.50	127.99	124.20
43	a	410	BCR	C33-C5-C4	2.50	118.41	113.62
34	m	102	LMG	C4-C3-C2	-2.50	106.47	110.82
31	g	312	CLA	CHA-C4D-ND	2.50	137.72	132.50
32	Y	315	LUT	C39-C29-C28	2.50	122.01	118.08
31	r	303	CLA	CHA-C4D-ND	2.50	137.72	132.50
30	q	303	CHL	CMA-C3A-C4A	2.50	118.48	111.77
30	3	303	CHL	CHC-C1C-NC	2.50	127.99	124.20
31	3	311	CLA	C2D-C1D-ND	2.50	111.94	110.10
30	Y	309	CHL	C1-O2A-CGA	2.50	122.99	116.44
31	5	614	CLA	CHA-C4D-ND	2.50	137.72	132.50
31	2	611	CLA	CMA-C3A-C4A	2.49	118.48	111.77
31	g	313	CLA	C1D-ND-C4D	-2.49	104.56	106.33
36	s	319	NEX	C4-C3-C2	2.49	115.59	110.77
34	g	320	LMG	O8-C28-C29	2.49	119.73	111.91
31	c	607	CLA	CHA-C4D-ND	2.49	137.71	132.50
30	S	302	CHL	C4D-CHA-C1A	2.49	124.28	121.25
31	7	304	CLA	CMD-C2D-C3D	-2.49	121.88	127.61
36	s	319	NEX	C38-C25-C26	-2.49	118.08	122.26
31	y	615	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
43	D	405	BCR	C20-C21-C22	-2.49	123.75	127.31
43	V	101	BCR	C15-C14-C13	-2.49	123.75	127.31
31	G	603	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	G	602	CLA	C1-C2-C3	-2.49	121.73	126.04
35	9	317	RRX	C8-C7-C6	-2.49	120.20	127.20
31	C	611	CLA	CHA-C4D-ND	2.49	137.71	132.50
36	N	318	NEX	C31-C30-C29	2.49	130.86	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	612	CLA	O2A-CGA-CBA	2.49	119.72	111.91
30	9	311	CHL	CMA-C3A-C2A	2.49	123.87	113.83
31	c	606	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
32	r	317	LUT	C19-C9-C8	2.49	122.00	118.08
43	D	405	BCR	C1-C6-C7	2.49	122.82	115.78
31	9	305	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	S	311	CLA	CMB-C2B-C3B	2.49	129.34	124.68
30	6	307	CHL	C2C-C3C-C4C	2.49	108.26	106.49
31	3	305	CLA	CHA-C4D-ND	2.49	137.71	132.50
31	c	613	CLA	CHA-C4D-ND	2.49	137.70	132.50
43	b	618	BCR	C21-C20-C19	-2.49	115.45	123.22
36	p	618	NEX	C20-C13-C14	-2.49	119.44	122.92
31	R	307	CLA	C2D-C1D-ND	2.49	111.94	110.10
30	6	310	CHL	C2C-C3C-C4C	2.49	108.26	106.49
31	y	615	CLA	CHA-C4D-ND	2.49	137.70	132.50
43	d	406	BCR	C33-C5-C4	2.49	118.39	113.62
31	2	609	CLA	O2A-CGA-CBA	2.49	119.71	111.91
32	G	615	LUT	C8-C7-C6	-2.49	120.22	127.20
30	q	309	CHL	C2C-C3C-C4C	2.49	108.26	106.49
31	6	304	CLA	CHA-C4D-ND	2.49	137.70	132.50
31	c	611	CLA	CHA-C4D-ND	2.49	137.70	132.50
30	y	605	CHL	CMA-C3A-C4A	2.49	118.45	111.77
31	S	315	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
30	5	605	CHL	CHB-C4A-NA	2.48	127.95	124.51
31	d	401	CLA	C2D-C1D-ND	2.48	111.94	110.10
31	b	602	CLA	CHA-C4D-ND	2.48	137.70	132.50
31	s	315	CLA	CHA-C4D-ND	2.48	137.70	132.50
31	s	315	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
31	5	604	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	0	610	CLA	C1C-C2C-C3C	-2.48	104.34	106.96
31	g	304	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	B	605	CLA	O2A-CGA-CBA	2.48	119.70	111.91
31	B	613	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	C	610	CLA	CHA-C4D-ND	2.48	137.69	132.50
36	n	319	NEX	C19-C9-C10	-2.48	119.44	122.92
31	6	313	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	b	612	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
36	r	319	NEX	C39-C29-C30	-2.48	119.45	122.92
31	C	608	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
31	7	305	CLA	C1D-ND-C4D	-2.48	104.57	106.33
31	S	316	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
33	S	320	LHG	C5-O7-C7	-2.48	111.68	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	612	CLA	CMA-C3A-C4A	2.48	118.44	111.77
31	p	614	CLA	O2A-CGA-CBA	2.48	119.69	111.91
30	3	302	CHL	CHD-C4C-C3C	2.48	128.49	124.84
31	A	405	CLA	CMB-C2B-C3B	2.48	129.32	124.68
42	A	408	PHO	C1-C2-C3	-2.48	121.75	126.04
45	c	617	DGD	C2G-O2G-C1B	-2.48	111.68	117.79
31	1	602	CLA	O2A-CGA-CBA	2.48	119.69	111.91
30	3	309	CHL	CHB-C4A-NA	2.48	127.94	124.51
43	b	618	BCR	C37-C22-C23	2.48	121.98	118.08
31	D	403	CLA	C1D-ND-C4D	-2.48	104.57	106.33
30	y	608	CHL	CHC-C1C-NC	2.48	127.97	124.20
30	q	308	CHL	C3C-C4C-NC	-2.48	107.79	110.57
32	1	615	LUT	C20-C13-C12	2.48	121.98	118.08
31	C	601	CLA	CHA-C4D-ND	2.48	137.69	132.50
31	r	311	CLA	C2D-C1D-ND	2.48	111.93	110.10
31	R	316	CLA	O2A-CGA-CBA	2.48	119.69	111.91
31	S	315	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	p	612	CLA	CHA-C4D-ND	2.48	137.68	132.50
36	q	319	NEX	C20-C13-C14	-2.48	119.45	122.92
30	p	607	CHL	CHC-C1C-NC	2.48	127.96	124.20
31	4	612	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	s	304	CLA	CHA-C4D-ND	2.48	137.68	132.50
30	5	601	CHL	C4A-NA-C1A	2.48	107.82	106.71
36	r	301	NEX	C38-C25-C26	-2.48	118.11	122.26
31	1	610	CLA	O2A-CGA-CBA	2.48	119.68	111.91
31	N	305	CLA	CHA-C4D-ND	2.48	137.68	132.50
32	G	615	LUT	C10-C11-C12	-2.48	115.48	123.22
30	2	601	CHL	CHB-C4A-NA	2.48	127.94	124.51
30	9	311	CHL	CHB-C4A-NA	2.48	127.94	124.51
43	a	410	BCR	C38-C26-C27	2.48	118.38	113.62
31	b	608	CLA	CHA-C4D-ND	2.48	137.68	132.50
30	n	306	CHL	C1-O2A-CGA	2.48	122.94	116.44
31	0	604	CLA	C2D-C1D-ND	2.48	111.93	110.10
32	N	316	LUT	C31-C30-C29	-2.48	123.78	127.31
31	5	612	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	Y	304	CLA	CHA-C4D-ND	2.48	137.68	132.50
31	C	603	CLA	CMD-C2D-C3D	-2.48	121.92	127.61
31	7	315	CLA	O2A-CGA-CBA	2.48	119.68	111.91
31	G	609	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
31	Y	311	CLA	C2D-C1D-ND	2.48	111.93	110.10
34	A	412	LMG	O8-C28-C29	2.47	119.67	111.91
31	2	613	CLA	CHA-C4D-ND	2.47	137.68	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	p	613	CLA	CHA-C4D-ND	2.47	137.68	132.50
33	a	415	LHG	C5-O7-C7	-2.47	111.70	117.79
30	N	309	CHL	CMA-C3A-C2A	2.47	123.81	113.83
31	G	610	CLA	CHA-C1A-NA	-2.47	120.73	126.40
30	p	609	CHL	C1-O2A-CGA	2.47	122.93	116.44
32	S	318	LUT	C35-C15-C14	-2.47	118.41	123.47
31	B	607	CLA	O2A-CGA-CBA	2.47	119.67	111.91
31	Y	305	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	r	307	CLA	CHA-C4D-ND	2.47	137.67	132.50
31	b	614	CLA	CMA-C3A-C4A	2.47	118.42	111.77
32	0	617	LUT	C30-C31-C32	-2.47	115.50	123.22
30	2	608	CHL	CMA-C3A-C2A	2.47	123.80	113.83
30	Y	302	CHL	CHB-C4A-NA	2.47	127.93	124.51
43	c	614	BCR	C1-C6-C7	2.47	122.77	115.78
31	B	606	CLA	C2D-C1D-ND	2.47	111.92	110.10
31	c	603	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
31	7	314	CLA	CMB-C2B-C3B	2.47	129.30	124.68
31	y	603	CLA	C1D-ND-C4D	-2.47	104.58	106.33
30	s	309	CHL	C2C-C3C-C4C	2.47	108.25	106.49
36	S	319	NEX	C26-C27-C28	-2.47	120.77	125.99
33	S	320	LHG	O8-C23-C24	2.47	119.66	111.91
34	B	621	LMG	C8-O7-C10	-2.47	111.71	117.79
31	N	304	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	2	610	CLA	O2A-CGA-CBA	2.47	119.66	111.91
30	g	302	CHL	CHB-C4A-NA	2.47	127.93	124.51
32	Y	315	LUT	C15-C35-C34	-2.47	118.42	123.47
31	q	315	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	b	615	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	1	604	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
31	C	602	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
30	q	303	CHL	C1B-CHB-C4A	-2.47	125.23	130.12
31	N	311	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
43	b	619	BCR	C15-C16-C17	-2.47	118.42	123.47
31	R	303	CLA	CHA-C4D-ND	2.47	137.66	132.50
30	G	606	CHL	C1-O2A-CGA	2.47	122.92	116.44
31	r	307	CLA	CMA-C3A-C4A	2.47	118.41	111.77
31	c	610	CLA	CMB-C2B-C1B	-2.47	124.67	128.46
32	1	615	LUT	C15-C35-C34	-2.47	118.42	123.47
31	1	604	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	4	604	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	C	602	CLA	C2D-C1D-ND	2.47	111.92	110.10
33	S	322	LHG	C5-O7-C7	-2.47	111.72	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	7	318	LUT	C18-C5-C4	2.47	118.92	114.36
31	b	605	CLA	CMB-C2B-C3B	2.47	129.29	124.68
31	B	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
30	6	310	CHL	CHB-C4A-NA	2.47	127.92	124.51
31	S	306	CLA	CHA-C4D-ND	2.47	137.66	132.50
31	9	305	CLA	O2A-CGA-CBA	2.47	119.64	111.91
31	b	613	CLA	O2A-CGA-CBA	2.47	119.64	111.91
43	V	101	BCR	C30-C25-C24	2.47	122.75	115.78
31	2	610	CLA	CHA-C4D-ND	2.46	137.66	132.50
30	0	606	CHL	C1B-CHB-C4A	-2.46	125.24	130.12
33	s	320	LHG	O8-C23-C24	2.46	119.64	111.91
34	c	624	LMG	O8-C28-C29	2.46	119.64	111.91
31	s	310	CLA	CMA-C3A-C4A	2.46	118.40	111.77
30	3	310	CHL	CHC-C1C-NC	2.46	127.94	124.20
30	4	601	CHL	CHB-C4A-NA	2.46	127.92	124.51
43	H	101	BCR	C23-C24-C25	-2.46	120.28	127.20
44	a	414	PL9	C40-C39-C41	2.46	119.41	115.27
30	n	310	CHL	CHD-C4C-C3C	2.46	128.46	124.84
43	C	615	BCR	C34-C9-C8	-2.46	114.20	118.08
36	N	318	NEX	C38-C25-C26	-2.46	118.13	122.26
31	8	604	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
32	Y	316	LUT	C8-C7-C6	-2.46	120.29	127.20
31	7	316	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
36	2	616	NEX	C16-C1-C6	-2.46	108.27	110.47
31	p	604	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
31	B	612	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
33	0	619	LHG	C5-O7-C7	-2.46	111.73	117.79
31	r	313	CLA	CMA-C3A-C4A	2.46	118.38	111.77
34	x	202	LMG	O1-C7-C8	-2.46	104.96	110.90
30	p	608	CHL	C1-O2A-CGA	2.46	122.90	116.44
31	G	613	CLA	CHA-C4D-ND	2.46	137.64	132.50
30	8	605	CHL	C1-O2A-CGA	2.46	122.90	116.44
31	1	611	CLA	C1-C2-C3	-2.46	121.79	126.04
31	g	311	CLA	C2D-C1D-ND	2.46	111.92	110.10
36	Y	317	NEX	C38-C25-C26	-2.46	118.14	122.26
31	G	609	CLA	CAA-C2A-C3A	-2.46	106.05	112.78
30	s	302	CHL	C4A-NA-C1A	2.46	107.81	106.71
31	b	609	CLA	C1D-ND-C4D	-2.46	104.59	106.33
30	p	606	CHL	C2C-C3C-C4C	2.46	108.24	106.49
31	b	603	CLA	CMA-C3A-C4A	2.46	118.38	111.77
31	B	607	CLA	C2D-C1D-ND	2.46	111.92	110.10
30	3	310	CHL	CMA-C3A-C2A	2.46	123.74	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	609	CHL	CMA-C3A-C2A	2.46	123.74	113.83
31	1	614	CLA	O2A-CGA-CBA	2.46	119.62	111.91
31	g	304	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
36	3	319	NEX	C17-C1-C6	-2.46	108.27	110.47
31	b	609	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
32	N	317	LUT	C11-C12-C13	-2.45	119.52	126.42
31	B	612	CLA	O2A-CGA-CBA	2.45	119.61	111.91
31	G	604	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	g	305	CLA	CHA-C4D-ND	2.45	137.63	132.50
30	g	302	CHL	C1-O2A-CGA	2.45	122.88	116.44
31	G	612	CLA	CHA-C4D-ND	2.45	137.63	132.50
33	G	618	LHG	C5-O7-C7	-2.45	111.75	117.79
31	1	613	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
30	q	309	CHL	C4D-CHA-C1A	2.45	124.23	121.25
31	s	311	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
31	3	315	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	B	601	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	9	306	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	y	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	8	604	CLA	CMA-C3A-C4A	2.45	118.37	111.77
32	g	316	LUT	C19-C9-C10	-2.45	119.49	122.92
30	Y	301	CHL	CHD-C4C-C3C	2.45	128.44	124.84
31	2	603	CLA	CHA-C4D-ND	2.45	137.63	132.50
43	C	615	BCR	C38-C26-C27	2.45	118.33	113.62
43	b	618	BCR	C33-C5-C4	2.45	118.33	113.62
31	C	608	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
31	C	612	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
45	c	619	DGD	O1G-C1A-C2A	2.45	119.60	111.91
31	N	313	CLA	CHA-C4D-ND	2.45	137.63	132.50
31	8	614	CLA	CMB-C2B-C3B	2.45	129.26	124.68
31	g	314	CLA	CHA-C4D-ND	2.45	137.63	132.50
30	0	609	CHL	C2C-C3C-C4C	2.45	108.24	106.49
30	q	303	CHL	C2C-C3C-C4C	2.45	108.24	106.49
31	B	611	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
31	p	613	CLA	O2A-C1-C2	2.45	115.07	108.64
32	Y	316	LUT	C31-C30-C29	-2.45	123.81	127.31
31	5	611	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	0	615	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	7	303	CLA	CHA-C4D-ND	2.45	137.62	132.50
33	y	619	LHG	O8-C23-C24	2.45	119.59	111.91
31	B	605	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
32	p	616	LUT	C8-C7-C6	-2.45	120.32	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	w	201	LMG	C8-O7-C10	-2.45	111.76	117.79
31	r	314	CLA	CMA-C3A-C4A	2.45	118.35	111.77
36	p	618	NEX	C16-C1-C6	-2.45	108.28	110.47
31	C	603	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	R	304	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
30	q	311	CHL	CMA-C3A-C4A	2.45	118.35	111.77
31	G	603	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
31	3	314	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	n	312	CLA	CHA-C4D-ND	2.45	137.62	132.50
43	H	101	BCR	C30-C25-C26	-2.45	119.17	122.61
31	r	306	CLA	C2D-C1D-ND	2.45	111.91	110.10
34	7	301	LMG	O8-C28-C29	2.45	119.58	111.91
31	g	313	CLA	CHA-C4D-ND	2.45	137.62	132.50
31	n	305	CLA	CHA-C4D-ND	2.45	137.62	132.50
30	5	609	CHL	CHC-C1C-NC	2.45	127.91	124.20
31	q	312	CLA	CHA-C4D-ND	2.45	137.61	132.50
31	n	312	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
31	r	316	CLA	CMD-C2D-C3D	-2.44	121.99	127.61
31	c	601	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
31	G	609	CLA	CMB-C2B-C3B	2.44	129.25	124.68
42	D	401	PHO	C4A-C3A-C2A	-2.44	100.51	102.84
31	7	312	CLA	CHA-C4D-ND	2.44	137.61	132.50
32	3	318	LUT	C8-C7-C6	-2.44	120.34	127.20
31	q	315	CLA	C1D-ND-C4D	-2.44	104.60	106.33
31	c	610	CLA	CAA-CBA-CGA	-2.44	106.11	113.25
31	b	612	CLA	O2A-CGA-CBA	2.44	119.58	111.91
31	g	303	CLA	O2A-CGA-CBA	2.44	119.58	111.91
31	R	316	CLA	CMA-C3A-C4A	2.44	118.34	111.77
30	0	609	CHL	CHB-C4A-NA	2.44	127.89	124.51
31	9	312	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	d	404	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	B	613	CLA	CMA-C3A-C4A	2.44	118.34	111.77
36	8	617	NEX	C39-C29-C30	-2.44	119.50	122.92
31	q	315	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
31	g	303	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
43	z	101	BCR	C34-C9-C10	-2.44	119.50	122.92
31	y	604	CLA	CHA-C4D-ND	2.44	137.61	132.50
31	r	315	CLA	CMA-C3A-C4A	2.44	118.33	111.77
31	3	313	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	Y	313	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	8	610	CLA	CHA-C4D-ND	2.44	137.60	132.50
30	g	302	CHL	C1B-CHB-C4A	-2.44	125.28	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	604	CLA	CHA-C4D-ND	2.44	137.60	132.50
30	Y	306	CHL	C1B-CHB-C4A	-2.44	125.29	130.12
31	7	314	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	G	613	CLA	O2A-CGA-CBA	2.44	119.56	111.91
31	c	606	CLA	CHD-C1D-ND	-2.44	122.21	124.45
45	c	617	DGD	C3G-O3G-C1D	-2.44	108.97	113.74
43	z	101	BCR	C29-C30-C25	2.44	114.23	110.48
31	8	613	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	p	611	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	g	311	CLA	CHA-C1A-NA	-2.44	120.81	126.40
31	r	306	CLA	CMB-C2B-C3B	2.44	129.24	124.68
30	q	311	CHL	CHC-C1C-NC	2.44	127.90	124.20
31	C	610	CLA	CMB-C2B-C1B	-2.44	124.72	128.46
31	d	405	CLA	CMB-C2B-C3B	2.44	129.24	124.68
31	r	311	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
31	G	602	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	d	401	CLA	CMD-C2D-C3D	-2.44	122.01	127.61
36	p	618	NEX	C40-C33-C34	-2.44	119.51	122.92
31	b	603	CLA	CHA-C4D-ND	2.44	137.60	132.50
31	3	304	CLA	O2A-CGA-CBA	2.44	119.56	111.91
31	4	611	CLA	CHA-C4D-ND	2.44	137.60	132.50
43	A	410	BCR	C35-C13-C14	-2.44	119.51	122.92
33	2	617	LHG	O8-C23-C24	2.44	119.55	111.91
32	r	317	LUT	C22-C23-C24	2.44	114.51	111.74
30	1	609	CHL	CMA-C3A-C2A	2.44	123.65	113.83
45	c	619	DGD	C3G-O3G-C1D	-2.43	108.98	113.74
34	w	203	LMG	O8-C28-O10	-2.43	117.45	123.59
31	C	604	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	8	602	CLA	CHA-C4D-ND	2.43	137.59	132.50
34	6	321	LMG	O1-C1-C2	2.43	112.10	108.30
30	3	309	CHL	C1-O2A-CGA	2.43	122.83	116.44
31	g	304	CLA	O2A-CGA-CBA	2.43	119.55	111.91
31	s	305	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	5	615	CLA	CMB-C2B-C3B	2.43	129.23	124.68
31	N	315	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	n	315	CLA	CHA-C4D-ND	2.43	137.59	132.50
30	Y	308	CHL	CHB-C4A-NA	2.43	127.88	124.51
30	y	601	CHL	CHB-C4A-NA	2.43	127.88	124.51
30	R	309	CHL	CMA-C3A-C4A	2.43	118.31	111.77
31	7	316	CLA	CHA-C4D-ND	2.43	137.59	132.50
31	s	311	CLA	O2A-CGA-CBA	2.43	119.54	111.91
36	s	319	NEX	O24-C25-C38	-2.43	112.14	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	b	618	BCR	C8-C7-C6	-2.43	120.38	127.20
31	2	613	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
31	b	607	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
30	G	605	CHL	C1-O2A-CGA	2.43	123.79	116.73
31	c	608	CLA	C1-C2-C3	-2.43	121.84	126.04
31	s	312	CLA	CHA-C4D-ND	2.43	137.58	132.50
34	b	623	LMG	O8-C28-C29	2.43	119.53	111.91
30	6	310	CHL	CHC-C1C-NC	2.43	127.89	124.20
36	5	618	NEX	C38-C25-C26	-2.43	118.19	122.26
31	C	613	CLA	CHA-C4D-ND	2.43	137.58	132.50
31	R	312	CLA	CHA-C4D-ND	2.43	137.58	132.50
30	1	607	CHL	C1-C2-C3	-2.43	121.84	126.04
31	p	610	CLA	CHA-C4D-ND	2.43	137.58	132.50
31	0	611	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
36	q	319	NEX	C19-C9-C10	-2.43	119.52	122.92
31	p	603	CLA	CHA-C4D-ND	2.43	137.58	132.50
43	Z	101	BCR	C21-C20-C19	-2.43	115.64	123.22
31	8	610	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
32	N	317	LUT	C15-C35-C34	-2.43	118.50	123.47
43	V	101	BCR	C7-C8-C9	-2.43	122.57	126.23
30	5	607	CHL	CHD-C4C-C3C	2.43	128.41	124.84
30	N	309	CHL	CHD-C4C-C3C	2.43	128.41	124.84
34	a	401	LMG	O8-C28-C29	2.43	119.52	111.91
31	y	610	CLA	CMD-C2D-C3D	-2.43	122.03	127.61
31	N	303	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	s	313	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	S	312	CLA	CMA-C3A-C4A	2.43	118.29	111.77
31	4	614	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	B	602	CLA	CHA-C4D-ND	2.43	137.57	132.50
31	b	613	CLA	C16-C15-C13	-2.42	108.08	115.92
31	6	312	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	n	303	CLA	CHA-C4D-ND	2.42	137.57	132.50
43	z	101	BCR	C11-C12-C13	-2.42	119.61	126.42
30	9	311	CHL	C1-C2-C3	-2.42	121.85	126.04
31	d	401	CLA	CAA-C2A-C3A	-2.42	106.14	112.78
31	R	312	CLA	CMA-C3A-C4A	2.42	118.29	111.77
43	h	101	BCR	C33-C5-C4	2.42	118.27	113.62
31	3	304	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	p	604	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	B	609	CLA	C1D-ND-C4D	-2.42	104.61	106.33
31	s	316	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
32	1	615	LUT	C39-C29-C28	2.42	121.90	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	611	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	3	312	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	b	614	CLA	CHA-C4D-ND	2.42	137.57	132.50
31	2	609	CLA	CHA-C4D-ND	2.42	137.57	132.50
30	9	303	CHL	CMA-C3A-C4A	2.42	118.28	111.77
31	C	609	CLA	O2A-CGA-CBA	2.42	119.51	111.91
31	N	321	CLA	CHA-C4D-ND	2.42	137.57	132.50
30	p	607	CHL	CHD-C4C-C3C	2.42	128.40	124.84
34	4	621	LMG	O8-C28-C29	2.42	119.51	111.91
32	5	617	LUT	C22-C23-C24	2.42	114.50	111.74
31	c	610	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	r	303	CLA	CHD-C1D-ND	-2.42	122.23	124.45
30	5	608	CHL	CHC-C1C-NC	2.42	127.88	124.20
31	y	611	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
32	S	317	LUT	C35-C15-C14	-2.42	118.52	123.47
31	9	315	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	c	603	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	s	313	CLA	CMB-C2B-C3B	2.42	129.21	124.68
30	Y	306	CHL	CHD-C4C-C3C	2.42	128.40	124.84
33	p	619	LHG	C5-O7-C7	-2.42	111.83	117.79
36	Y	317	NEX	C16-C1-C6	-2.42	108.31	110.47
31	G	613	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
30	G	606	CHL	C2C-C3C-C4C	2.42	108.21	106.49
31	p	611	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
30	0	601	CHL	CHC-C1C-NC	2.42	127.87	124.20
30	4	606	CHL	C1-O2A-CGA	2.42	122.79	116.44
31	b	604	CLA	CMA-C3A-C4A	2.42	118.28	111.77
44	A	416	PL9	C32-C33-C34	-2.42	121.83	127.66
31	q	312	CLA	CMD-C2D-C3D	-2.42	122.05	127.61
36	r	301	NEX	C20-C13-C14	-2.42	119.53	122.92
31	0	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	b	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
30	S	302	CHL	C4A-NA-C1A	2.42	107.79	106.71
31	6	304	CLA	O2A-CGA-CBA	2.42	119.50	111.91
34	4	620	LMG	O8-C28-C29	2.42	119.50	111.91
31	C	613	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
34	c	621	LMG	C8-O7-C10	-2.42	111.84	117.79
31	b	612	CLA	CHA-C4D-ND	2.42	137.56	132.50
31	8	603	CLA	O2A-CGA-CBA	2.42	119.49	111.91
32	7	317	LUT	C15-C35-C34	-2.42	118.52	123.47
31	1	603	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
31	y	610	CLA	O2A-CGA-CBA	2.42	119.49	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D	404	CLA	CMA-C3A-C4A	2.42	118.27	111.77
31	4	613	CLA	C1-O2A-CGA	2.42	122.78	116.44
31	n	305	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
31	A	409	CLA	C1D-ND-C4D	-2.42	104.62	106.33
31	s	314	CLA	CHA-C4D-ND	2.42	137.55	132.50
36	r	301	NEX	C40-C33-C34	-2.42	119.54	122.92
36	9	319	NEX	C17-C1-C6	-2.41	108.31	110.47
43	c	615	BCR	C29-C30-C25	2.41	114.20	110.48
32	9	318	LUT	C38-C25-C24	-2.41	118.39	123.56
31	5	610	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
31	r	313	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
31	N	311	CLA	CHA-C4D-ND	2.41	137.55	132.50
48	K	101	LMU	C1'-C2'-C3'	2.41	115.02	110.00
36	G	616	NEX	C39-C29-C30	-2.41	119.54	122.92
30	p	601	CHL	CHB-C4A-NA	2.41	127.85	124.51
31	B	610	CLA	CHA-C4D-ND	2.41	137.55	132.50
34	Y	319	LMG	C8-O7-C10	-2.41	111.85	117.79
32	Y	315	LUT	C20-C13-C12	2.41	121.88	118.08
31	7	313	CLA	C1D-ND-C4D	-2.41	104.62	106.33
32	n	317	LUT	C31-C30-C29	-2.41	123.87	127.31
31	q	315	CLA	CHD-C1D-ND	-2.41	122.24	124.45
30	3	310	CHL	CHB-C4A-NA	2.41	127.85	124.51
30	S	309	CHL	CHB-C4A-NA	2.41	127.85	124.51
30	5	601	CHL	CHC-C1C-NC	2.41	127.86	124.20
33	a	415	LHG	O8-C23-C24	2.41	119.48	111.91
34	a	413	LMG	C3-C4-C5	2.41	114.54	110.24
30	N	309	CHL	C1-C2-C3	-2.41	121.87	126.04
33	3	320	LHG	C5-O7-C7	-2.41	111.85	117.79
31	B	616	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
31	b	608	CLA	C2D-C1D-ND	2.41	111.88	110.10
30	5	609	CHL	CMA-C3A-C2A	2.41	123.56	113.83
31	c	609	CLA	CHA-C4D-ND	2.41	137.54	132.50
30	N	301	CHL	C1-O2A-CGA	2.41	122.77	116.44
31	0	614	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
31	b	604	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
31	n	304	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	c	613	CLA	C1-O2A-CGA	2.41	122.77	116.44
31	n	314	CLA	CHA-C4D-ND	2.41	137.54	132.50
30	7	321	CHL	CHD-C4C-C3C	2.41	128.38	124.84
31	g	314	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
31	6	311	CLA	CHA-C4D-ND	2.41	137.54	132.50
31	C	602	CLA	CHA-C4D-ND	2.41	137.54	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	R	304	CLA	C1D-ND-C4D	-2.41	104.62	106.33
31	1	611	CLA	CHA-C4D-ND	2.41	137.54	132.50
30	S	308	CHL	C1B-CHB-C4A	-2.41	125.35	130.12
32	8	615	LUT	C31-C30-C29	-2.41	123.87	127.31
31	y	602	CLA	O2A-CGA-CBA	2.41	119.47	111.91
34	A	418	LMG	O8-C28-C29	2.41	119.47	111.91
31	R	307	CLA	CHA-C4D-ND	2.41	137.53	132.50
30	0	609	CHL	CHC-C1C-NC	2.41	127.86	124.20
30	g	308	CHL	CHC-C1C-NC	2.41	127.86	124.20
31	q	304	CLA	CHA-C4D-ND	2.41	137.53	132.50
31	q	312	CLA	C3B-C4B-NB	-2.41	107.49	110.36
30	6	307	CHL	C4A-NA-C1A	2.41	107.79	106.71
30	S	308	CHL	C4A-NA-C1A	2.41	107.79	106.71
31	0	614	CLA	CHA-C4D-ND	2.41	137.53	132.50
42	A	408	PHO	CMC-C2C-C3C	2.41	129.48	124.94
32	7	318	LUT	C21-C26-C27	-2.41	109.66	112.70
30	3	310	CHL	CHD-C4C-C3C	2.41	128.38	124.84
31	5	603	CLA	O2A-CGA-CBA	2.41	119.46	111.91
31	5	603	CLA	CHA-C4D-ND	2.41	137.53	132.50
31	5	610	CLA	CHA-C4D-ND	2.41	137.53	132.50
31	S	303	CLA	O2A-CGA-CBA	2.41	119.46	111.91
30	g	309	CHL	CHD-C4C-C3C	2.41	128.38	124.84
43	b	619	BCR	C29-C30-C25	2.41	114.18	110.48
31	C	602	CLA	C1-O2A-CGA	2.41	122.75	116.44
31	p	610	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
43	t	101	BCR	C1-C6-C5	-2.41	119.23	122.61
32	s	317	LUT	C30-C31-C32	-2.40	115.71	123.22
36	Y	317	NEX	C31-C30-C29	2.40	130.74	127.31
34	r	321	LMG	O6-C1-C2	-2.40	105.26	110.35
30	9	309	CHL	CHC-C1C-NC	2.40	127.85	124.20
30	p	601	CHL	CHC-C1C-NC	2.40	127.85	124.20
31	7	311	CLA	O2A-CGA-CBA	2.40	119.45	111.91
30	n	302	CHL	CHD-C4C-C3C	2.40	128.37	124.84
31	0	613	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	9	316	CLA	CHA-C4D-ND	2.40	137.53	132.50
31	6	314	CLA	O2A-CGA-CBA	2.40	119.45	111.91
31	Y	310	CLA	O2A-CGA-CBA	2.40	119.45	111.91
36	r	301	NEX	C39-C29-C30	-2.40	119.56	122.92
31	q	313	CLA	CHA-C4D-ND	2.40	137.53	132.50
30	N	302	CHL	CHC-C1C-NC	2.40	127.85	124.20
31	A	407	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
32	7	317	LUT	C11-C12-C13	-2.40	119.67	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	R	302	LMU	O5'-C5'-C4'	-2.40	104.69	109.75
31	Y	303	CLA	CHA-C4D-ND	2.40	137.53	132.50
33	b	625	LHG	C5-O7-C7	-2.40	111.88	117.79
31	8	611	CLA	CHA-C4D-ND	2.40	137.52	132.50
35	g	315	RRX	C33-C5-C4	2.40	118.23	113.62
30	4	605	CHL	C2C-C3C-C4C	2.40	108.20	106.49
32	8	616	LUT	C30-C31-C32	-2.40	115.72	123.22
31	R	311	CLA	CMB-C2B-C3B	2.40	129.17	124.68
44	A	416	PL9	C27-C28-C29	-2.40	121.88	127.66
31	s	303	CLA	CMD-C2D-C3D	-2.40	122.09	127.61
43	c	614	BCR	C19-C18-C17	2.40	122.62	118.94
31	3	306	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	b	606	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	a	406	CLA	CMB-C2B-C3B	2.40	129.17	124.68
31	c	606	CLA	CMB-C2B-C3B	2.40	129.17	124.68
31	y	614	CLA	CHA-C4D-ND	2.40	137.52	132.50
36	R	301	NEX	C38-C25-C26	-2.40	118.24	122.26
30	S	308	CHL	CHB-C4A-NA	2.40	127.83	124.51
31	S	314	CLA	CHA-C4D-ND	2.40	137.52	132.50
32	n	318	LUT	C30-C31-C32	-2.40	115.73	123.22
30	S	309	CHL	CHC-C1C-NC	2.40	127.84	124.20
30	n	308	CHL	CHD-C4C-C3C	2.40	128.37	124.84
31	4	603	CLA	C1D-ND-C4D	-2.40	104.63	106.33
34	m	102	LMG	O8-C28-C29	2.40	119.44	111.91
32	r	317	LUT	C40-C33-C32	2.40	121.86	118.08
31	r	303	CLA	CMA-C3A-C4A	2.40	118.22	111.77
31	8	614	CLA	CHA-C4D-ND	2.40	137.52	132.50
31	Y	303	CLA	O2A-CGA-CBA	2.40	119.43	111.91
30	8	601	CHL	CHD-C4C-C3C	2.40	128.37	124.84
33	l	101	LHG	O8-C23-C24	2.40	119.43	111.91
30	2	608	CHL	C2C-C3C-C4C	2.40	108.20	106.49
31	r	312	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	S	305	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
31	N	310	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
32	0	616	LUT	C20-C13-C12	2.40	121.85	118.08
31	7	315	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	r	316	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	c	604	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
30	3	303	CHL	C2C-C3C-C4C	2.40	108.20	106.49
30	6	302	CHL	CHC-C1C-NC	2.40	127.84	124.20
31	s	316	CLA	CHA-C4D-ND	2.40	137.51	132.50
31	n	304	CLA	O2A-CGA-CBA	2.40	119.43	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	q	305	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
31	4	614	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
31	n	303	CLA	O2A-CGA-CBA	2.39	119.42	111.91
31	5	615	CLA	O1D-CGD-CBD	-2.39	119.58	124.48
30	7	306	CHL	C2C-C3C-C4C	2.39	108.20	106.49
30	G	608	CHL	CHC-C1C-NC	2.39	127.83	124.20
31	b	603	CLA	C2D-C1D-ND	2.39	111.87	110.10
30	S	309	CHL	C1B-CHB-C4A	-2.39	125.38	130.12
31	G	602	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
31	6	314	CLA	CHA-C4D-ND	2.39	137.50	132.50
32	7	318	LUT	C15-C35-C34	-2.39	118.57	123.47
36	y	618	NEX	C40-C33-C34	-2.39	119.57	122.92
31	G	611	CLA	CMA-C3A-C4A	2.39	118.20	111.77
31	R	307	CLA	CMA-C3A-C4A	2.39	118.20	111.77
31	5	615	CLA	C2D-C1D-ND	2.39	111.87	110.10
31	6	303	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	c	606	CLA	CHA-C4D-ND	2.39	137.50	132.50
30	3	308	CHL	C1B-CHB-C4A	-2.39	125.38	130.12
31	q	312	CLA	O2A-CGA-CBA	2.39	119.41	111.91
31	6	303	CLA	O2A-CGA-CBA	2.39	119.41	111.91
31	R	304	CLA	CMD-C2D-C3D	-2.39	122.11	127.61
31	n	313	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	c	601	CLA	C2C-C1C-NC	2.39	112.21	109.97
31	b	605	CLA	CHA-C1A-NA	-2.39	120.92	126.40
31	b	608	CLA	O2A-CGA-CBA	2.39	119.41	111.91
31	5	613	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	b	613	CLA	CHA-C4D-ND	2.39	137.50	132.50
33	S	320	LHG	C6-C5-C4	-2.39	106.14	111.79
31	B	607	CLA	CMB-C2B-C3B	2.39	129.15	124.68
32	g	316	LUT	C40-C33-C34	-2.39	119.58	122.92
30	3	307	CHL	CHD-C4C-C3C	2.39	128.35	124.84
31	8	612	CLA	CHA-C4D-ND	2.39	137.50	132.50
43	t	101	BCR	C28-C27-C26	-2.39	109.81	114.08
31	1	610	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	s	303	CLA	CHA-C4D-ND	2.39	137.50	132.50
31	S	305	CLA	CHA-C4D-ND	2.39	137.50	132.50
32	0	617	LUT	C8-C7-C6	-2.39	120.50	127.20
31	G	610	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
30	R	310	CHL	C4D-CHA-C1A	2.39	124.16	121.25
31	4	602	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	C	606	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	r	306	CLA	CHA-C4D-ND	2.39	137.49	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	3	314	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
31	n	305	CLA	CMA-C3A-C4A	2.39	118.19	111.77
30	Y	307	CHL	CMA-C3A-C2A	2.39	123.46	113.83
31	6	305	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	R	316	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	S	310	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	d	401	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	r	304	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	r	313	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	s	306	CLA	CHA-C4D-ND	2.39	137.49	132.50
38	a	412	SQD	O5-C1-O6	-2.39	104.32	109.97
30	6	310	CHL	CMA-C3A-C2A	2.39	123.46	113.83
31	B	611	CLA	O2A-CGA-CBA	2.39	119.40	111.91
30	9	308	CHL	CHC-C1C-NC	2.39	127.82	124.20
30	0	608	CHL	CHD-C4C-C3C	2.39	128.35	124.84
32	n	317	LUT	C35-C15-C14	-2.39	118.59	123.47
31	c	602	CLA	CHA-C4D-ND	2.39	137.49	132.50
31	r	311	CLA	CAA-C2A-C3A	-2.39	106.25	112.78
31	7	313	CLA	CMD-C2D-C3D	-2.39	122.13	127.61
31	r	305	CLA	O2D-CGD-O1D	-2.38	119.17	123.84
31	D	403	CLA	CHA-C4D-ND	2.38	137.49	132.50
30	g	309	CHL	CHC-C1C-NC	2.38	127.82	124.20
34	D	409	LMG	O1-C7-C8	-2.38	105.15	110.90
35	G	614	RRX	C37-C22-C21	-2.38	119.58	122.92
43	B	618	BCR	C10-C11-C12	-2.38	115.78	123.22
30	n	301	CHL	CHC-C1C-NC	2.38	127.82	124.20
32	5	617	LUT	C8-C7-C6	-2.38	120.51	127.20
31	S	313	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
30	N	307	CHL	C1-O2A-CGA	2.38	122.69	116.44
31	y	602	CLA	CHA-C4D-ND	2.38	137.48	132.50
36	r	319	NEX	C26-C27-C28	-2.38	120.96	125.99
31	0	611	CLA	O2A-CGA-CBA	2.38	119.38	111.91
31	R	313	CLA	CHA-C4D-ND	2.38	137.48	132.50
30	q	303	CHL	CHC-C1C-NC	2.38	127.82	124.20
43	c	614	BCR	C33-C5-C4	2.38	118.19	113.62
30	G	605	CHL	CHB-C4A-NA	2.38	127.80	124.51
30	y	608	CHL	CHD-C4C-C3C	2.38	128.34	124.84
31	0	612	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
31	c	613	CLA	CHA-C1A-NA	-2.38	120.95	126.40
31	p	602	CLA	O2A-CGA-CBA	2.38	119.38	111.91
31	0	603	CLA	O2A-CGA-CBA	2.38	119.37	111.91
31	B	616	CLA	CHA-C4D-ND	2.38	137.47	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	316	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	r	315	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	A	405	CLA	CAA-C2A-C1A	-2.38	104.18	111.97
31	S	314	CLA	C1-O2A-CGA	2.38	122.68	116.44
31	r	305	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	y	610	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	9	313	CLA	C2D-C1D-ND	2.38	111.86	110.10
43	D	405	BCR	C23-C24-C25	-2.38	120.53	127.20
31	5	611	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
31	R	314	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	0	602	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	g	311	CLA	O2A-CGA-CBA	2.38	119.37	111.91
31	q	313	CLA	C4B-C3B-C2B	2.38	108.24	106.36
35	9	317	RRX	C37-C22-C21	-2.38	119.59	122.92
44	A	416	PL9	C40-C39-C41	2.38	119.27	115.27
36	S	319	NEX	O24-C25-C38	-2.38	112.21	115.06
31	1	613	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	A	405	CLA	CHA-C4D-ND	2.38	137.47	132.50
31	N	310	CLA	CHA-C4D-ND	2.38	137.47	132.50
36	3	319	NEX	C40-C33-C34	-2.38	119.59	122.92
31	7	311	CLA	CMD-C2D-C3D	-2.38	122.15	127.61
31	c	605	CLA	C1-O2A-CGA	2.38	122.68	116.44
31	4	602	CLA	O2A-CGA-CBA	2.38	119.36	111.91
31	c	604	CLA	CHA-C4D-ND	2.37	137.47	132.50
47	E	101	HEM	C4D-ND-C1D	2.37	107.53	105.07
31	q	315	CLA	O1D-CGD-CBD	-2.37	119.62	124.48
43	B	619	BCR	C35-C13-C14	-2.37	119.60	122.92
31	5	612	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
31	N	312	CLA	CHA-C4D-ND	2.37	137.47	132.50
44	a	414	PL9	C22-C23-C24	-2.37	121.94	127.66
33	Y	318	LHG	O8-C23-C24	2.37	119.36	111.91
42	D	401	PHO	CMC-C2C-C3C	2.37	129.42	124.94
30	5	605	CHL	C1B-CHB-C4A	-2.37	125.42	130.12
30	1	605	CHL	C1-O2A-CGA	2.37	122.67	116.44
30	7	308	CHL	CHD-C4C-C3C	2.37	128.33	124.84
31	R	306	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
43	B	617	BCR	C3-C4-C5	-2.37	109.84	114.08
31	q	314	CLA	CMD-C2D-C3D	-2.37	122.16	127.61
31	s	310	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	p	610	CLA	O2A-CGA-CBA	2.37	119.35	111.91
31	c	612	CLA	CMB-C2B-C1B	-2.37	124.82	128.46
31	7	303	CLA	O2A-CGA-CBA	2.37	119.35	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	p	605	CHL	C4A-NA-C1A	2.37	107.77	106.71
31	0	604	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	3	316	CLA	O2A-CGA-CBA	2.37	119.35	111.91
34	7	322	LMG	C8-O7-C10	-2.37	111.95	117.79
31	1	611	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
31	1	602	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	b	617	CLA	CHA-C4D-ND	2.37	137.46	132.50
30	s	302	CHL	CHC-C1C-NC	2.37	127.80	124.20
35	G	614	RRX	C36-C18-C17	-2.37	119.60	122.92
32	p	616	LUT	C31-C32-C33	2.37	133.07	126.42
31	1	614	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	R	311	CLA	CHA-C4D-ND	2.37	137.46	132.50
31	4	613	CLA	CHA-C4D-ND	2.37	137.45	132.50
31	c	608	CLA	CHA-C4D-ND	2.37	137.45	132.50
34	6	323	LMG	O6-C5-C6	2.37	112.33	106.44
31	3	316	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
31	B	612	CLA	C6-C5-C3	-2.37	107.24	113.45
31	p	603	CLA	CMD-C2D-C3D	-2.37	122.17	127.61
30	p	609	CHL	CHC-C1C-NC	2.37	127.80	124.20
30	1	606	CHL	C2C-C3C-C4C	2.37	108.18	106.49
43	c	615	BCR	C7-C8-C9	-2.37	122.66	126.23
31	R	303	CLA	CAA-CBA-CGA	-2.37	106.33	113.25
31	0	610	CLA	C1-O2A-CGA	2.37	122.66	116.44
32	8	615	LUT	C35-C15-C14	-2.37	118.62	123.47
32	y	616	LUT	C18-C5-C4	2.37	118.74	114.36
31	2	612	CLA	CHA-C4D-ND	2.37	137.45	132.50
32	8	615	LUT	C30-C31-C32	-2.37	115.83	123.22
32	n	317	LUT	C30-C31-C32	-2.37	115.83	123.22
35	q	317	RRX	C11-C10-C9	-2.37	123.93	127.31
31	B	613	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
32	n	318	LUT	C8-C7-C6	-2.37	120.56	127.20
31	r	313	CLA	O2A-CGA-CBA	2.37	119.33	111.91
31	c	601	CLA	O2A-CGA-CBA	2.37	119.33	111.91
31	y	613	CLA	C6-C5-C3	-2.36	107.25	113.45
31	s	305	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	s	314	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
31	9	314	CLA	CMA-C3A-C4A	2.36	118.13	111.77
34	w	202	LMG	C8-O7-C10	-2.36	111.97	117.79
31	B	606	CLA	CMD-C2D-C3D	-2.36	122.17	127.61
34	7	322	LMG	O8-C28-C29	2.36	119.33	111.91
31	N	315	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
30	R	309	CHL	C2C-C3C-C4C	2.36	108.17	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	407	CLA	CMB-C2B-C1B	-2.36	124.83	128.46
31	S	303	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	S	316	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	A	406	CLA	O2D-CGD-O1D	-2.36	119.22	123.84
30	N	306	CHL	CHB-C4A-NA	2.36	127.78	124.51
31	c	602	CLA	C2D-C1D-ND	2.36	111.84	110.10
31	7	311	CLA	CHA-C4D-ND	2.36	137.44	132.50
30	9	310	CHL	C1B-CHB-C4A	-2.36	125.44	130.12
34	c	624	LMG	C8-O7-C10	-2.36	111.98	117.79
31	3	316	CLA	C1D-ND-C4D	-2.36	104.66	106.33
43	C	614	BCR	C2-C1-C6	2.36	114.11	110.48
31	0	610	CLA	CHA-C4D-ND	2.36	137.44	132.50
32	7	317	LUT	C8-C7-C6	-2.36	120.57	127.20
31	c	608	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
31	N	314	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	Y	314	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	3	311	CLA	O1D-CGD-CBD	-2.36	119.66	124.48
36	3	319	NEX	C26-C27-C28	-2.36	121.00	125.99
31	5	610	CLA	O2A-CGA-CBA	2.36	119.31	111.91
30	n	302	CHL	CHC-C1C-NC	2.36	127.78	124.20
31	8	609	CLA	CHA-C4D-ND	2.36	137.44	132.50
31	r	312	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
31	a	406	CLA	CHA-C4D-ND	2.36	137.43	132.50
44	A	416	PL9	C22-C23-C24	-2.36	121.98	127.66
30	y	609	CHL	CHD-C4C-C3C	2.36	128.31	124.84
32	6	317	LUT	C39-C29-C28	2.36	121.79	118.08
31	3	306	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
36	2	616	NEX	C26-C27-C28	-2.36	121.01	125.99
31	Y	312	CLA	O2A-CGA-CBA	2.36	119.31	111.91
36	y	618	NEX	C2-C1-C6	2.36	111.50	109.21
30	8	601	CHL	CHC-C1C-NC	2.36	127.78	124.20
31	Y	305	CLA	O2A-CGA-CBA	2.36	119.30	111.91
31	N	321	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
31	g	305	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
30	3	310	CHL	C2C-C3C-C4C	2.36	108.17	106.49
30	y	605	CHL	C1B-CHB-C4A	-2.36	125.45	130.12
43	H	101	BCR	C8-C7-C6	-2.36	120.58	127.20
30	G	608	CHL	CHD-C4C-C3C	2.36	128.30	124.84
31	R	304	CLA	CHA-C4D-ND	2.36	137.43	132.50
31	0	603	CLA	O2D-CGD-O1D	-2.36	119.23	123.84
43	v	101	BCR	C33-C5-C4	2.36	118.14	113.62
31	c	605	CLA	CMD-C2D-C3D	-2.36	122.20	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	311	CLA	CHA-C4D-ND	2.35	137.43	132.50
31	q	313	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
31	3	316	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
31	5	612	CLA	O2A-CGA-CBA	2.35	119.30	111.91
31	s	306	CLA	O1D-CGD-CBD	-2.35	119.67	124.48
30	g	308	CHL	C2C-C3C-C4C	2.35	108.17	106.49
31	B	611	CLA	CHA-C4D-ND	2.35	137.42	132.50
32	3	318	LUT	C20-C13-C14	-2.35	119.63	122.92
31	5	602	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	Y	310	CLA	CHA-C4D-ND	2.35	137.42	132.50
31	N	310	CLA	O2A-CGA-CBA	2.35	119.29	111.91
31	6	316	CLA	C1D-ND-C4D	-2.35	104.66	106.33
31	c	612	CLA	CHA-C4D-ND	2.35	137.42	132.50
30	1	601	CHL	CHD-C4C-C3C	2.35	128.30	124.84
32	9	318	LUT	C18-C5-C4	2.35	118.71	114.36
35	4	615	RRX	C37-C22-C21	-2.35	119.63	122.92
30	1	607	CHL	C1-O2A-CGA	2.35	122.61	116.44
30	4	609	CHL	CHD-C4C-C3C	2.35	128.30	124.84
30	9	303	CHL	C2C-C3C-C4C	2.35	108.17	106.49
31	9	313	CLA	O2A-CGA-CBA	2.35	119.29	111.91
36	s	319	NEX	C39-C29-C30	-2.35	119.63	122.92
32	8	616	LUT	C8-C7-C6	-2.35	120.60	127.20
31	5	610	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
31	a	409	CLA	C1D-ND-C4D	-2.35	104.67	106.33
31	y	611	CLA	CHA-C4D-ND	2.35	137.41	132.50
31	c	609	CLA	CMB-C2B-C1B	-2.35	124.85	128.46
32	0	617	LUT	C15-C35-C34	-2.35	118.66	123.47
30	Y	306	CHL	CHB-C4A-NA	2.35	127.76	124.51
31	N	303	CLA	O2A-CGA-CBA	2.35	119.28	111.91
31	S	312	CLA	CHA-C4D-ND	2.35	137.41	132.50
34	d	409	LMG	C8-O7-C10	-2.35	112.01	117.79
30	1	607	CHL	CHD-C4C-C3C	2.35	128.29	124.84
30	p	609	CHL	CMA-C3A-C2A	2.35	123.30	113.83
31	C	607	CLA	CHA-C4D-ND	2.35	137.41	132.50
31	4	611	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
31	c	609	CLA	C6-C5-C3	-2.35	107.30	113.45
43	b	620	BCR	C8-C7-C6	-2.35	120.61	127.20
31	q	316	CLA	CMD-C2D-C3D	-2.35	122.22	127.61
30	S	302	CHL	C1B-CHB-C4A	-2.35	125.47	130.12
31	R	315	CLA	C2D-C1D-ND	2.34	111.83	110.10
30	q	307	CHL	CHC-C1C-NC	2.34	127.76	124.20
34	a	416	LMG	O8-C28-C29	2.34	119.27	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	1	603	CLA	CMA-C3A-C4A	2.34	118.07	111.77
31	G	612	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
31	2	610	CLA	O2D-CGD-O1D	-2.34	119.25	123.84
31	9	304	CLA	CHA-C4D-ND	2.34	137.40	132.50
31	q	306	CLA	C6-C5-C3	-2.34	107.31	113.45
35	2	614	RRX	C27-C26-C25	-2.34	115.63	120.85
31	g	310	CLA	CHA-C4D-ND	2.34	137.40	132.50
31	B	601	CLA	O2A-CGA-CBA	2.34	119.26	111.91
43	c	615	BCR	C35-C13-C14	-2.34	119.64	122.92
31	S	304	CLA	CMA-C3A-C4A	2.34	118.06	111.77
44	a	414	PL9	C27-C28-C29	-2.34	122.02	127.66
31	q	305	CLA	O2A-CGA-CBA	2.34	119.25	111.91
31	q	304	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
32	S	318	LUT	C31-C32-C33	-2.34	119.84	126.42
30	1	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
32	p	616	LUT	C18-C5-C4	2.34	118.69	114.36
34	x	202	LMG	C8-O7-C10	-2.34	112.03	117.79
31	y	611	CLA	C1D-ND-C4D	-2.34	104.67	106.33
35	9	317	RRX	C35-C13-C14	-2.34	119.65	122.92
43	d	406	BCR	C38-C26-C27	2.34	118.11	113.62
43	C	614	BCR	C8-C7-C6	-2.34	120.63	127.20
30	Y	302	CHL	CHD-C4C-C3C	2.34	128.28	124.84
31	8	602	CLA	O2A-CGA-CBA	2.34	119.25	111.91
31	A	406	CLA	CHA-C4D-ND	2.34	137.39	132.50
31	7	313	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
31	7	313	CLA	O2A-CGA-CBA	2.34	119.24	111.91
31	C	613	CLA	CMA-C3A-C4A	2.34	118.06	111.77
31	B	609	CLA	CHA-C4D-ND	2.34	137.39	132.50
43	V	101	BCR	C11-C10-C9	-2.34	123.97	127.31
31	6	304	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
31	g	305	CLA	CMA-C3A-C4A	2.34	118.05	111.77
35	2	614	RRX	C36-C18-C17	-2.34	119.65	122.92
31	C	603	CLA	O2A-CGA-CBA	2.34	119.24	111.91
32	N	317	LUT	C19-C9-C10	-2.34	119.65	122.92
31	p	602	CLA	CHA-C4D-ND	2.34	137.38	132.50
36	r	301	NEX	C26-C27-C28	-2.34	121.06	125.99
31	C	610	CLA	C2D-C1D-ND	2.34	111.83	110.10
31	y	611	CLA	C1-C2-C3	-2.34	122.00	126.04
35	4	615	RRX	C36-C18-C17	-2.34	119.65	122.92
31	4	603	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
31	9	316	CLA	CMD-C2D-C3D	-2.33	122.24	127.61
30	6	309	CHL	CHC-C1C-NC	2.33	127.75	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	2	604	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
31	Y	303	CLA	O2D-CGD-O1D	-2.33	119.27	123.84
30	N	309	CHL	CHB-C4A-NA	2.33	127.74	124.51
31	d	405	CLA	C1D-ND-C4D	-2.33	104.68	106.33
31	G	609	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	9	306	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	b	610	CLA	CHA-C4D-ND	2.33	137.38	132.50
30	8	605	CHL	CHD-C4C-C3C	2.33	128.27	124.84
34	p	620	LMG	C8-O7-C10	-2.33	112.05	117.79
31	b	602	CLA	O2A-CGA-CBA	2.33	119.23	111.91
30	q	311	CHL	CHB-C4A-NA	2.33	127.74	124.51
36	G	616	NEX	C26-C27-C28	-2.33	121.06	125.99
31	y	613	CLA	C16-C15-C13	-2.33	108.38	115.92
38	B	620	SQD	O3-C3-C2	-2.33	104.96	110.35
31	8	612	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	b	613	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	s	306	CLA	O2A-CGA-CBA	2.33	119.22	111.91
30	n	310	CHL	CHC-C1C-NC	2.33	127.74	124.20
31	7	312	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
45	C	620	DGD	O1G-C1A-C2A	2.33	119.22	111.91
31	R	315	CLA	CMA-C3A-C4A	2.33	118.04	111.77
30	N	307	CHL	C1-C2-C3	-2.33	122.01	126.04
43	b	620	BCR	C21-C20-C19	-2.33	115.94	123.22
30	5	601	CHL	CMA-C3A-C4A	2.33	118.04	111.77
32	s	317	LUT	C35-C15-C14	-2.33	118.70	123.47
31	6	305	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
31	C	604	CLA	CMD-C2D-C3D	-2.33	122.25	127.61
31	3	301	CLA	CHA-C4D-ND	2.33	137.37	132.50
31	C	612	CLA	CHA-C4D-ND	2.33	137.37	132.50
30	0	601	CHL	CMA-C3A-C2A	2.33	123.22	113.83
31	Y	304	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	p	604	CLA	CMA-C3A-C4A	2.33	118.03	111.77
31	n	314	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
31	y	603	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
30	2	608	CHL	CHB-C4A-NA	2.33	127.73	124.51
31	S	310	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
36	0	618	NEX	C40-C33-C34	-2.33	119.66	122.92
31	1	603	CLA	O2A-CGA-CBA	2.33	119.21	111.91
34	a	413	LMG	O1-C1-C2	2.33	111.94	108.30
31	G	609	CLA	CHA-C4D-ND	2.33	137.37	132.50
47	e	102	HEM	C4D-ND-C1D	2.33	107.48	105.07
31	1	604	CLA	CMB-C2B-C1B	-2.33	124.89	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	Y	308	CHL	CHC-C1C-NC	2.33	127.73	124.20
31	R	312	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
38	Y	320	SQD	O3-C3-C2	-2.33	104.97	110.35
31	r	315	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
31	B	615	CLA	CHA-C4D-ND	2.33	137.36	132.50
31	n	304	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
31	g	314	CLA	O2A-CGA-CBA	2.33	119.20	111.91
31	A	406	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
31	S	311	CLA	O2A-CGA-CBA	2.32	119.20	111.91
30	S	309	CHL	CHD-C4C-C3C	2.32	128.26	124.84
35	2	614	RRX	C37-C22-C21	-2.32	119.67	122.92
30	n	306	CHL	CHD-C4C-C3C	2.32	128.26	124.84
31	S	311	CLA	CHA-C4D-ND	2.32	137.36	132.50
31	g	313	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	R	315	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
31	R	315	CLA	O2A-CGA-CBA	2.32	119.20	111.91
30	4	607	CHL	CHD-C4C-C3C	2.32	128.25	124.84
31	C	608	CLA	CHA-C4D-ND	2.32	137.36	132.50
31	a	407	CLA	CHA-C4D-ND	2.32	137.36	132.50
44	a	414	PL9	C36-C34-C33	-2.32	116.42	121.12
31	n	311	CLA	CHA-C4D-ND	2.32	137.36	132.50
31	g	310	CLA	CMB-C2B-C3B	2.32	129.02	124.68
31	6	316	CLA	CMB-C2B-C3B	2.32	129.02	124.68
32	S	318	LUT	C40-C33-C34	-2.32	119.67	122.92
31	p	604	CLA	C1D-ND-C4D	-2.32	104.69	106.33
31	r	304	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	b	602	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
31	G	602	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	9	306	CLA	O2A-CGA-CBA	2.32	119.19	111.91
31	s	314	CLA	CMB-C2B-C3B	2.32	129.02	124.68
31	c	613	CLA	C2A-C1A-CHA	2.32	127.92	123.86
31	N	312	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	y	614	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
31	0	612	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
30	Y	307	CHL	CHC-C1C-NC	2.32	127.72	124.20
34	9	302	LMG	C8-O7-C10	-2.32	112.08	117.79
33	R	320	LHG	O8-C23-C24	2.32	119.19	111.91
38	s	301	SQD	O3-C3-C2	-2.32	104.99	110.35
31	0	603	CLA	CHA-C4D-ND	2.32	137.35	132.50
32	G	615	LUT	C20-C13-C12	2.32	121.73	118.08
30	6	306	CHL	CHC-C1C-NC	2.32	127.72	124.20
31	N	313	CLA	O2D-CGD-O1D	-2.32	119.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	304	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
31	6	303	CLA	CMD-C2D-C3D	-2.32	122.28	127.61
31	B	611	CLA	CMB-C2B-C3B	2.32	129.01	124.68
31	y	613	CLA	CHD-C1D-ND	-2.32	122.33	124.45
35	9	317	RRX	C27-C26-C25	-2.32	115.69	120.85
31	3	301	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
31	c	605	CLA	C1-C2-C3	-2.32	122.04	126.04
31	R	314	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
43	c	614	BCR	C37-C22-C21	-2.32	119.68	122.92
31	G	612	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
31	c	608	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
30	7	307	CHL	CHC-C1C-NC	2.31	127.72	124.20
31	6	315	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
31	p	615	CLA	CHA-C4D-ND	2.31	137.34	132.50
30	5	608	CHL	CHD-C4C-C3C	2.31	128.24	124.84
31	b	610	CLA	CAA-CBA-CGA	-2.31	106.49	113.25
35	G	614	RRX	C35-C13-C14	-2.31	119.68	122.92
31	R	315	CLA	CMB-C2B-C1B	-2.31	124.91	128.46
38	B	623	SQD	O3-C3-C2	-2.31	105.00	110.35
31	1	603	CLA	C2D-C1D-ND	2.31	111.81	110.10
35	9	317	RRX	C36-C18-C17	-2.31	119.68	122.92
31	r	312	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
44	A	416	PL9	C37-C38-C39	-2.31	122.09	127.66
31	c	603	CLA	C2D-C1D-ND	2.31	111.81	110.10
31	s	311	CLA	CHA-C4D-ND	2.31	137.33	132.50
36	S	319	NEX	C38-C25-C26	-2.31	118.39	122.26
30	g	306	CHL	CHB-C4A-NA	2.31	127.71	124.51
30	7	309	CHL	CHD-C4C-C3C	2.31	128.24	124.84
31	R	307	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
31	C	608	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
31	r	314	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
30	5	607	CHL	C4D-CHA-C1A	2.31	124.06	121.25
30	1	606	CHL	CHC-C1C-NC	2.31	127.71	124.20
30	R	308	CHL	CHC-C1C-NC	2.31	127.71	124.20
32	S	317	LUT	C1-C6-C5	-2.31	119.36	122.61
30	9	309	CHL	C2C-C3C-C4C	2.31	108.14	106.49
30	p	605	CHL	CHD-C4C-C3C	2.31	128.23	124.84
38	b	621	SQD	O3-C3-C2	-2.31	105.01	110.35
36	n	319	NEX	C12-C13-C14	2.31	122.48	118.94
31	7	315	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
31	2	603	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
31	R	316	CLA	CMD-C2D-C3D	-2.31	122.30	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	602	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
31	B	602	CLA	CHA-C1A-NA	-2.31	121.11	126.40
30	N	307	CHL	CMA-C3A-C2A	2.31	123.14	113.83
31	0	604	CLA	O2A-CGA-CBA	2.31	119.15	111.91
30	5	606	CHL	C2C-C3C-C4C	2.31	108.13	106.49
30	9	311	CHL	C2C-C3C-C4C	2.31	108.13	106.49
30	1	609	CHL	C1-O2A-CGA	2.31	122.50	116.44
34	9	301	LMG	O8-C9-C8	2.31	115.15	108.43
31	3	315	CLA	O2A-CGA-CBA	2.31	119.15	111.91
31	3	311	CLA	CHA-C4D-ND	2.31	137.32	132.50
31	S	315	CLA	O2A-CGA-CBA	2.31	119.15	111.91
31	Y	313	CLA	C1-O2A-CGA	2.31	122.50	116.44
30	7	308	CHL	C1-C2-C3	-2.31	122.05	126.04
30	2	606	CHL	CHD-C4C-C3C	2.31	128.23	124.84
31	9	316	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
37	r	318	XAT	O4-C5-C18	-2.31	112.29	115.06
31	r	312	CLA	C1D-ND-C4D	-2.31	104.70	106.33
31	7	303	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
30	s	309	CHL	C1B-CHB-C4A	-2.31	125.55	130.12
30	R	309	CHL	CHC-C1C-NC	2.30	127.70	124.20
35	4	615	RRX	C27-C26-C25	-2.30	115.71	120.85
36	6	319	NEX	C40-C33-C34	-2.30	119.69	122.92
30	p	609	CHL	CHB-C4A-NA	2.30	127.70	124.51
35	G	614	RRX	C27-C26-C25	-2.30	115.71	120.85
31	0	610	CLA	O2A-CGA-CBA	2.30	119.14	111.91
31	b	614	CLA	O2A-CGA-CBA	2.30	119.14	111.91
32	4	616	LUT	C19-C9-C10	-2.30	119.70	122.92
31	9	314	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
31	B	607	CLA	CAA-C2A-C1A	-2.30	104.43	111.97
30	7	310	CHL	CHD-C4C-C3C	2.30	128.23	124.84
31	9	312	CLA	CMA-C3A-C4A	2.30	117.96	111.77
31	s	311	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
31	G	604	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
32	7	318	LUT	C30-C31-C32	-2.30	116.03	123.22
30	0	605	CHL	C4D-CHA-C1A	2.30	124.05	121.25
31	4	611	CLA	C3B-C4B-NB	-2.30	107.61	110.36
31	8	612	CLA	C1-C2-C3	-2.30	122.06	126.04
31	N	321	CLA	O2A-CGA-CBA	2.30	119.13	111.91
31	n	311	CLA	O2A-CGA-CBA	2.30	119.13	111.91
31	s	303	CLA	C6-C7-C8	-2.30	108.48	115.92
31	p	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
31	S	311	CLA	CMA-C3A-C4A	2.30	117.96	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	R	322	SQD	O3-C3-C2	-2.30	105.03	110.35
38	S	301	SQD	O3-C3-C2	-2.30	105.03	110.35
31	5	613	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
31	N	304	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
30	4	605	CHL	CHC-C1C-NC	2.30	127.69	124.20
31	9	305	CLA	CMD-C2D-C3D	-2.30	122.32	127.61
31	1	612	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
35	g	315	RRX	C36-C18-C17	-2.30	119.70	122.92
36	4	617	NEX	C40-C33-C34	-2.30	119.70	122.92
31	C	606	CLA	O2A-CGA-CBA	2.30	119.12	111.91
31	y	603	CLA	O2A-CGA-CBA	2.30	119.12	111.91
30	n	306	CHL	CHB-C4A-NA	2.30	127.69	124.51
31	A	407	CLA	CHA-C4D-ND	2.30	137.31	132.50
33	F1	301	LHG	O8-C23-C24	2.30	119.12	111.91
32	Y	316	LUT	C11-C12-C13	-2.30	119.96	126.42
34	b	626	LMG	C8-O7-C10	-2.30	112.13	117.79
38	6	301	SQD	O3-C3-C2	-2.30	105.04	110.35
38	m	101	SQD	O3-C3-C2	-2.30	105.04	110.35
31	d	405	CLA	CHA-C4D-ND	2.30	137.31	132.50
31	A	405	CLA	O2A-CGA-CBA	2.30	119.12	111.91
31	Y	311	CLA	CMA-C3A-C4A	2.30	117.95	111.77
30	5	609	CHL	CHB-C4A-NA	2.30	127.69	124.51
30	4	608	CHL	CHD-C4C-C3C	2.30	128.22	124.84
31	d	404	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
30	5	606	CHL	CMA-C3A-C2A	2.30	123.09	113.83
43	b	620	BCR	C15-C16-C17	-2.30	118.77	123.47
43	B	618	BCR	C37-C22-C23	2.30	121.69	118.08
36	r	301	NEX	C16-C1-C6	-2.30	108.42	110.47
31	C	612	CLA	C6-C5-C3	-2.30	107.43	113.45
31	N	303	CLA	C6-C5-C3	-2.30	107.43	113.45
31	0	613	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
31	B	603	CLA	C2D-C1D-ND	2.30	111.80	110.10
31	S	314	CLA	O2A-CGA-CBA	2.30	119.11	111.91
43	h	101	BCR	C30-C25-C26	-2.30	119.38	122.61
31	g	312	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
31	b	616	CLA	CHA-C4D-ND	2.30	137.30	132.50
31	Y	304	CLA	O2A-CGA-CBA	2.29	119.11	111.91
31	5	614	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
31	C	607	CLA	C1-C2-C3	-2.29	122.08	126.04
30	8	605	CHL	CHB-C4A-NA	2.29	127.68	124.51
30	6	302	CHL	CHD-C4C-C3C	2.29	128.21	124.84
31	r	307	CLA	CHA-C1A-NA	-2.29	121.15	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	315	CLA	C2D-C1D-ND	2.29	111.79	110.10
31	B	613	CLA	C1D-ND-C4D	-2.29	104.71	106.33
31	1	602	CLA	CMB-C2B-C3B	2.29	128.97	124.68
31	B	604	CLA	CHA-C1A-NA	-2.29	121.15	126.40
31	1	611	CLA	O2A-CGA-CBA	2.29	119.10	111.91
30	7	307	CHL	C2C-C3C-C4C	2.29	108.12	106.49
35	4	615	RRX	C35-C13-C14	-2.29	119.71	122.92
31	s	311	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
31	s	311	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
30	Y	309	CHL	CHD-C4C-C3C	2.29	128.21	124.84
30	q	311	CHL	CHD-C4C-C3C	2.29	128.21	124.84
38	X	201	SQD	O3-C3-C2	-2.29	105.05	110.35
31	y	615	CLA	C6-C5-C3	-2.29	107.45	113.45
31	1	603	CLA	CHA-C4D-ND	2.29	137.29	132.50
36	0	618	NEX	C31-C30-C29	2.29	130.58	127.31
31	B	608	CLA	CHA-C4D-ND	2.29	137.29	132.50
31	r	311	CLA	CHA-C4D-ND	2.29	137.29	132.50
30	q	303	CHL	CHB-C4A-NA	2.29	127.68	124.51
37	R	318	XAT	C39-C29-C30	-2.29	119.72	122.92
36	8	617	NEX	C26-C27-C28	-2.29	121.15	125.99
31	5	604	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
31	8	614	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
30	N	301	CHL	CHC-C1C-NC	2.29	127.68	124.20
31	R	312	CLA	C1D-ND-C4D	-2.29	104.71	106.33
30	4	606	CHL	CMA-C3A-C2A	2.29	123.06	113.83
31	3	306	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
30	1	609	CHL	CHB-C4A-NA	2.29	127.68	124.51
43	b	619	BCR	C37-C22-C21	-2.29	119.72	122.92
34	W	202	LMG	O6-C1-O1	-2.29	104.55	109.97
32	s	318	LUT	C35-C15-C14	-2.29	118.79	123.47
31	p	615	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
31	0	614	CLA	C6-C5-C3	-2.29	107.45	113.45
32	1	616	LUT	C18-C5-C4	2.29	118.59	114.36
30	3	302	CHL	CHC-C1C-NC	2.29	127.67	124.20
36	6	319	NEX	C31-C30-C29	2.29	130.57	127.31
31	5	613	CLA	O2A-CGA-CBA	2.29	119.09	111.91
31	g	304	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
31	4	603	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
30	2	601	CHL	CHC-C1C-NC	2.29	127.67	124.20
30	4	608	CHL	CHC-C1C-NC	2.29	127.67	124.20
30	Y	302	CHL	CHC-C1C-NC	2.29	127.67	124.20
30	G	601	CHL	CHC-C1C-NC	2.29	127.67	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	309	CHL	CHC-C1C-NC	2.29	127.67	124.20
36	2	616	NEX	C39-C29-C30	-2.29	119.72	122.92
31	3	311	CLA	CMD-C2D-C3D	-2.29	122.36	127.61
31	4	610	CLA	CHA-C1A-NA	-2.29	121.16	126.40
31	n	316	CLA	O2D-CGD-O1D	-2.29	119.37	123.84
43	B	619	BCR	C34-C9-C10	-2.29	119.72	122.92
43	A	410	BCR	C38-C26-C27	2.28	118.00	113.62
36	n	319	NEX	C40-C33-C34	-2.28	119.72	122.92
31	q	305	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
30	4	609	CHL	CMA-C3A-C2A	2.28	123.04	113.83
33	z	102	LHG	O7-C7-O9	-2.28	118.18	123.70
31	3	314	CLA	O2A-CGA-CBA	2.28	119.07	111.91
31	b	611	CLA	O2A-CGA-CBA	2.28	119.07	111.91
43	C	615	BCR	C7-C6-C5	-2.28	115.93	121.46
36	r	301	NEX	C19-C9-C10	-2.28	119.73	122.92
31	2	609	CLA	CMD-C2D-C3D	-2.28	122.36	127.61
32	y	617	LUT	C40-C33-C32	2.28	121.67	118.08
30	7	306	CHL	CHC-C1C-NC	2.28	127.66	124.20
30	r	309	CHL	CHC-C1C-NC	2.28	127.66	124.20
43	b	618	BCR	C10-C11-C12	-2.28	116.10	123.22
31	G	610	CLA	O2A-CGA-CBA	2.28	119.06	111.91
31	R	314	CLA	CMA-C3A-C4A	2.28	117.90	111.77
31	y	603	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
31	3	304	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
31	8	614	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
43	C	614	BCR	C29-C30-C25	2.28	113.99	110.48
43	H	101	BCR	C29-C30-C25	2.28	113.99	110.48
30	y	606	CHL	CHC-C1C-NC	2.28	127.66	124.20
32	2	615	LUT	C2-C3-C4	2.28	113.42	110.30
31	b	606	CLA	C1D-ND-C4D	-2.28	104.72	106.33
31	4	614	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
31	8	609	CLA	O2A-CGA-CBA	2.28	119.06	111.91
31	2	602	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
38	A	413	SQD	O3-C3-C2	-2.28	105.08	110.35
34	4	620	LMG	C8-O7-C10	-2.28	112.19	117.79
31	y	615	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
31	r	315	CLA	C1-C2-C3	-2.28	122.11	126.04
31	R	312	CLA	CMB-C2B-C3B	2.28	128.94	124.68
31	1	604	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
30	p	601	CHL	C1B-CHB-C4A	-2.28	125.61	130.12
31	b	603	CLA	CHA-C1A-NA	-2.28	121.19	126.40
31	G	602	CLA	O2D-CGD-O1D	-2.28	119.39	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	r	317	LUT	C39-C29-C28	2.28	121.66	118.08
31	n	314	CLA	C1-C2-C3	-2.28	122.11	126.04
30	p	606	CHL	CHD-C4C-C3C	2.28	128.19	124.84
31	Y	312	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
31	S	310	CLA	C1-O2A-CGA	2.28	122.41	116.44
30	G	607	CHL	CHC-C1C-NC	2.28	127.66	124.20
31	Y	310	CLA	CMD-C2D-C3D	-2.28	122.38	127.61
30	y	607	CHL	CHB-C4A-NA	2.28	127.66	124.51
32	r	317	LUT	C8-C9-C10	-2.27	115.45	118.94
31	9	312	CLA	CHA-C1A-NA	-2.27	121.19	126.40
30	g	306	CHL	CMA-C3A-C2A	2.27	123.00	113.83
31	3	305	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
32	y	616	LUT	C11-C10-C9	-2.27	124.06	127.31
30	N	308	CHL	CMA-C3A-C2A	2.27	123.00	113.83
31	q	315	CLA	CHA-C1A-NA	-2.27	121.19	126.40
31	s	315	CLA	O2A-CGA-CBA	2.27	119.04	111.91
31	6	315	CLA	CHA-C4D-ND	2.27	137.25	132.50
31	S	303	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
31	0	603	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
30	8	607	CHL	CHC-C1C-NC	2.27	127.65	124.20
31	B	610	CLA	O2A-CGA-CBA	2.27	119.04	111.91
30	N	308	CHL	CHB-C4A-NA	2.27	127.66	124.51
36	n	319	NEX	C11-C10-C9	2.27	130.55	127.31
36	S	319	NEX	C40-C33-C34	-2.27	119.74	122.92
43	C	614	BCR	C38-C26-C27	2.27	117.98	113.62
31	R	316	CLA	C1D-ND-C4D	-2.27	104.72	106.33
32	8	616	LUT	C15-C35-C34	-2.27	118.82	123.47
31	D	404	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
30	g	307	CHL	CMA-C3A-C2A	2.27	122.99	113.83
31	n	316	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
33	e	101	LHG	O8-C23-O10	-2.27	117.86	123.59
30	G	607	CHL	CHB-C4A-NA	2.27	127.65	124.51
31	a	406	CLA	C1D-ND-C4D	-2.27	104.72	106.33
32	N	316	LUT	C11-C12-C13	-2.27	120.04	126.42
31	Y	314	CLA	O2A-CGA-CBA	2.27	119.03	111.91
31	S	316	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
30	0	608	CHL	CHC-C1C-NC	2.27	127.65	124.20
31	b	608	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
34	b	624	LMG	C8-O7-C10	-2.27	112.20	117.79
30	3	302	CHL	CHB-C4A-NA	2.27	127.65	124.51
43	A	410	BCR	C29-C30-C25	2.27	113.97	110.48
31	b	605	CLA	O2A-CGA-CBA	2.27	119.02	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	304	CLA	C6-C5-C3	-2.27	107.51	113.45
30	r	308	CHL	CHC-C1C-NC	2.27	127.64	124.20
30	5	607	CHL	C2C-C3C-C4C	2.27	108.11	106.49
30	5	605	CHL	C4A-NA-C1A	2.27	107.72	106.71
31	Y	304	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
31	4	614	CLA	C1D-ND-C4D	-2.27	104.72	106.33
30	9	303	CHL	CHC-C1C-NC	2.27	127.64	124.20
31	B	602	CLA	CMB-C2B-C3B	2.27	128.92	124.68
31	C	604	CLA	CMA-C3A-C4A	2.27	117.86	111.77
31	R	306	CLA	CHA-C1A-NA	-2.27	121.21	126.40
31	p	613	CLA	CMA-C3A-C4A	2.27	117.86	111.77
31	b	609	CLA	CHA-C4D-ND	2.26	137.24	132.50
31	c	601	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
30	r	308	CHL	CMA-C3A-C2A	2.26	122.96	113.83
31	r	315	CLA	C1D-ND-C4D	-2.26	104.73	106.33
31	N	303	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
31	Y	305	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
31	9	306	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
30	1	606	CHL	CHB-C4A-NA	2.26	127.64	124.51
37	g	321	XAT	C25-C24-C23	-2.26	108.27	112.75
31	7	304	CLA	O2A-CGA-CBA	2.26	119.01	111.91
31	N	303	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
36	2	616	NEX	C19-C9-C10	-2.26	119.75	122.92
30	r	308	CHL	C2C-C3C-C4C	2.26	108.10	106.49
31	r	314	CLA	CHA-C4D-ND	2.26	137.23	132.50
30	6	302	CHL	CHB-C4A-NA	2.26	127.64	124.51
30	r	308	CHL	CHB-C4A-NA	2.26	127.64	124.51
31	N	304	CLA	O2A-CGA-CBA	2.26	119.00	111.91
31	S	314	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
31	9	315	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
31	5	603	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	6	311	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	4	612	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
38	A	411	SQD	O3-C3-C2	-2.26	105.13	110.35
30	7	310	CHL	CMA-C3A-C2A	2.26	122.94	113.83
31	N	321	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
30	4	601	CHL	CHC-C1C-NC	2.26	127.63	124.20
30	q	307	CHL	CHD-C4C-C3C	2.26	128.16	124.84
31	7	316	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	b	615	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
43	z	101	BCR	C21-C20-C19	-2.26	116.17	123.22
36	n	319	NEX	C28-C29-C30	2.26	122.41	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	6	314	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	9	312	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
31	g	314	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
43	a	410	BCR	C29-C30-C25	2.26	113.95	110.48
31	y	613	CLA	CMB-C2B-C3B	2.26	128.90	124.68
30	N	302	CHL	CMA-C3A-C2A	2.26	122.93	113.83
31	6	316	CLA	CHA-C1A-NA	-2.26	121.23	126.40
31	q	313	CLA	C3B-C4B-NB	-2.26	107.67	110.36
31	b	610	CLA	CHA-C1A-NA	-2.25	121.23	126.40
31	4	602	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
32	5	617	LUT	C18-C5-C4	2.25	118.53	114.36
31	4	610	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
35	4	615	RRX	C34-C9-C10	-2.25	119.77	122.92
30	s	302	CHL	CMB-C2B-C1B	-2.25	125.00	128.46
31	C	613	CLA	CMB-C2B-C1B	-2.25	125.00	128.46
30	p	609	CHL	C2C-C3C-C4C	2.25	108.10	106.49
37	4	619	XAT	C25-C24-C23	-2.25	108.29	112.75
43	z	101	BCR	C23-C24-C25	-2.25	120.87	127.20
36	q	319	NEX	C26-C27-C28	-2.25	121.23	125.99
37	q	321	XAT	C25-C24-C23	-2.25	108.29	112.75
31	q	304	CLA	O2A-CGA-CBA	2.25	118.98	111.91
30	s	309	CHL	CHB-C4A-NA	2.25	127.63	124.51
30	6	307	CHL	CHD-C4C-C3C	2.25	128.15	124.84
31	6	311	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
31	R	313	CLA	O2A-CGA-CBA	2.25	118.98	111.91
31	b	615	CLA	O2A-CGA-CBA	2.25	118.98	111.91
30	2	606	CHL	CHC-C1C-NC	2.25	127.62	124.20
31	r	304	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
30	g	306	CHL	CHD-C4C-C3C	2.25	128.15	124.84
31	C	609	CLA	CHA-C4D-ND	2.25	137.21	132.50
38	a	412	SQD	O3-C3-C2	-2.25	105.14	110.35
36	p	618	NEX	C5-C4-C3	2.25	114.41	111.75
38	g	301	SQD	O3-C3-C2	-2.25	105.14	110.35
43	z	101	BCR	C1-C6-C5	-2.25	119.44	122.61
30	p	607	CHL	C2C-C3C-C4C	2.25	108.09	106.49
30	q	311	CHL	C2C-C3C-C4C	2.25	108.09	106.49
31	B	606	CLA	O1D-CGD-CBD	-2.25	119.88	124.48
43	b	620	BCR	C1-C6-C5	-2.25	119.44	122.61
30	p	601	CHL	C4A-NA-C1A	2.25	107.72	106.71
43	B	619	BCR	C21-C20-C19	-2.25	116.19	123.22
30	7	309	CHL	C1-O2A-CGA	2.25	122.35	116.44
31	q	304	CLA	O2D-CGD-O1D	-2.25	119.44	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	N	318	NEX	C11-C10-C9	2.25	130.52	127.31
30	7	308	CHL	CHB-C4A-NA	2.25	127.62	124.51
43	v	101	BCR	C16-C15-C14	-2.25	118.87	123.47
31	6	303	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
31	B	607	CLA	CBC-CAC-C3C	-2.25	106.23	112.43
30	7	308	CHL	CMA-C3A-C4A	2.25	117.82	111.77
31	C	608	CLA	CMA-C3A-C4A	2.25	117.82	111.77
47	e	102	HEM	CHA-C4D-C3D	-2.25	121.11	125.33
36	s	319	NEX	C26-C27-C28	-2.25	121.24	125.99
31	s	306	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
30	6	309	CHL	CMA-C3A-C2A	2.25	122.90	113.83
30	5	601	CHL	C1-O2A-CGA	2.25	122.34	116.44
31	p	615	CLA	CHA-C1A-NA	-2.25	121.25	126.40
31	Y	313	CLA	CMB-C2B-C1B	-2.25	125.01	128.46
37	2	619	XAT	C25-C24-C23	-2.25	108.30	112.75
32	S	317	LUT	C30-C31-C32	-2.25	116.20	123.22
31	0	615	CLA	CHA-C1A-NA	-2.25	121.25	126.40
31	1	614	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
30	r	309	CHL	C2C-C3C-C4C	2.25	108.09	106.49
35	2	614	RRX	C35-C13-C14	-2.25	119.78	122.92
30	8	608	CHL	CHC-C1C-NC	2.25	127.61	124.20
31	5	611	CLA	O2A-CGA-CBA	2.25	118.96	111.91
31	a	406	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
31	s	303	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
44	A	416	PL9	C31-C32-C33	-2.25	104.50	111.88
31	G	613	CLA	C1D-ND-C4D	-2.25	104.74	106.33
30	0	606	CHL	CMB-C2B-C1B	-2.25	125.01	128.46
31	b	608	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
30	G	607	CHL	C1-O2A-CGA	2.25	122.34	116.44
31	B	609	CLA	CMB-C2B-C3B	2.25	128.88	124.68
37	G	620	XAT	C25-C24-C23	-2.25	108.31	112.75
38	G	617	SQD	O3-C3-C2	-2.25	105.16	110.35
32	n	318	LUT	C15-C35-C34	-2.25	118.87	123.47
43	V	101	BCR	C16-C15-C14	-2.25	118.87	123.47
31	4	612	CLA	O2D-CGD-O1D	-2.25	119.45	123.84
30	S	302	CHL	CHD-C4C-C3C	2.25	128.14	124.84
31	R	305	CLA	CHA-C4D-ND	2.25	137.20	132.50
31	Y	303	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
43	z	101	BCR	C15-C16-C17	-2.24	118.88	123.47
30	7	309	CHL	CMA-C3A-C2A	2.24	122.88	113.83
36	y	618	NEX	C19-C9-C10	-2.24	119.78	122.92
31	y	612	CLA	O2A-CGA-CBA	2.24	118.95	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	607	CLA	CHA-C1A-NA	-2.24	121.26	126.40
31	c	603	CLA	CMD-C2D-C3D	-2.24	122.45	127.61
31	6	305	CLA	C6-C5-C3	-2.24	107.57	113.45
31	G	604	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
30	1	606	CHL	CHD-C4C-C3C	2.24	128.14	124.84
30	2	601	CHL	CHD-C4C-C3C	2.24	128.14	124.84
30	7	321	CHL	CHC-C1C-NC	2.24	127.61	124.20
35	9	317	RRX	C34-C9-C10	-2.24	119.78	122.92
43	Z	101	BCR	C23-C24-C25	-2.24	120.90	127.20
31	A	405	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
31	g	305	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
30	G	605	CHL	CMA-C3A-C2A	2.24	122.87	113.83
34	A	414	LMG	C8-O7-C10	-2.24	112.27	117.79
30	1	608	CHL	CMA-C3A-C2A	2.24	122.87	113.83
30	2	607	CHL	CHB-C4A-NA	2.24	127.61	124.51
43	c	614	BCR	C36-C18-C17	-2.24	119.78	122.92
31	D	404	CLA	CHA-C4D-ND	2.24	137.19	132.50
31	R	303	CLA	O2A-CGA-CBA	2.24	118.94	111.91
43	C	615	BCR	C29-C30-C25	2.24	113.93	110.48
30	5	608	CHL	C1-O2A-CGA	2.24	122.32	116.44
30	N	301	CHL	CHB-C4A-NA	2.24	127.61	124.51
31	s	304	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
31	r	305	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
31	b	607	CLA	CMB-C2B-C3B	2.24	128.87	124.68
31	3	305	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
38	G	624	SQD	O3-C3-C2	-2.24	105.17	110.35
37	9	322	XAT	C25-C24-C23	-2.24	108.32	112.75
30	3	302	CHL	C4D-CHA-C1A	2.24	123.97	121.25
30	G	606	CHL	CHC-C1C-NC	2.24	127.60	124.20
38	a	411	SQD	O3-C3-C2	-2.24	105.17	110.35
31	g	312	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
34	W	201	LMG	O8-C28-O10	-2.24	117.94	123.59
31	b	603	CLA	CMB-C2B-C3B	2.24	128.87	124.68
36	Y	317	NEX	O24-C25-C38	-2.24	112.37	115.06
32	9	318	LUT	C20-C13-C14	-2.24	119.79	122.92
37	r	318	XAT	C40-C33-C34	-2.24	119.79	122.92
31	6	315	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
31	S	305	CLA	O2A-CGA-CBA	2.24	118.93	111.91
43	c	615	BCR	C11-C12-C13	-2.24	120.13	126.42
30	y	605	CHL	CHB-C4A-NA	2.24	127.61	124.51
30	r	309	CHL	CMA-C3A-C4A	2.24	117.79	111.77
30	r	310	CHL	CHD-C4C-C3C	2.24	128.13	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	S	319	NEX	C2-C1-C6	2.24	111.39	109.21
31	c	604	CLA	CMA-C3A-C4A	2.24	117.78	111.77
35	G	614	RRX	C34-C9-C10	-2.24	119.79	122.92
30	S	307	CHL	CMA-C3A-C2A	2.24	122.85	113.83
31	0	603	CLA	CMA-C3A-C4A	2.24	117.78	111.77
31	b	605	CLA	CHD-C1D-ND	-2.24	122.40	124.45
31	4	613	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
31	A	406	CLA	O2A-CGA-CBA	2.24	118.92	111.91
31	g	303	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
31	C	613	CLA	CHA-C1A-NA	-2.24	121.28	126.40
31	r	304	CLA	C6-C5-C3	-2.24	107.59	113.45
31	r	312	CLA	C1-O2A-CGA	2.24	122.31	116.44
31	A	409	CLA	CHA-C4D-ND	2.24	137.18	132.50
31	c	609	CLA	O2A-CGA-CBA	2.24	118.92	111.91
31	D	403	CLA	CMB-C2B-C1B	-2.23	125.03	128.46
30	G	623	CHL	CMA-C3A-C2A	2.23	122.84	113.83
36	s	319	NEX	C40-C33-C34	-2.23	119.79	122.92
31	r	315	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
34	b	622	LMG	C7-O1-C1	2.23	118.10	113.74
31	s	314	CLA	C1-O2A-CGA	2.23	122.31	116.44
31	y	614	CLA	O2A-CGA-CBA	2.23	118.92	111.91
30	9	309	CHL	CHD-C4C-C3C	2.23	128.12	124.84
31	5	614	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
31	B	608	CLA	O2A-CGA-CBA	2.23	118.92	111.91
31	N	313	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	a	409	CLA	CHA-C4D-ND	2.23	137.17	132.50
36	p	618	NEX	C2-C1-C6	2.23	111.38	109.21
31	c	608	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	c	612	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	4	603	CLA	OBD-CAD-C3D	-2.23	123.15	128.52
36	q	319	NEX	C38-C25-C26	-2.23	118.52	122.26
37	R	318	XAT	C40-C33-C34	-2.23	119.80	122.92
30	8	607	CHL	CHD-C4C-C3C	2.23	128.12	124.84
31	1	612	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	B	601	CLA	CMA-C3A-C4A	2.23	117.77	111.77
31	S	304	CLA	C1D-ND-C4D	-2.23	104.75	106.33
33	4	618	LHG	C6-C5-C4	-2.23	106.51	111.79
31	C	604	CLA	C2D-C1D-ND	2.23	111.75	110.10
30	s	302	CHL	CHD-C4C-C3C	2.23	128.12	124.84
30	Y	308	CHL	CMA-C3A-C2A	2.23	122.83	113.83
30	6	307	CHL	CHC-C1C-NC	2.23	127.59	124.20
31	c	602	CLA	CMB-C2B-C3B	2.23	128.85	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	409	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
32	y	616	LUT	C20-C13-C12	2.23	121.59	118.08
30	4	606	CHL	CHB-C4A-NA	2.23	127.60	124.51
30	N	308	CHL	CHD-C4C-C3C	2.23	128.12	124.84
31	n	304	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
31	4	610	CLA	CMB-C2B-C3B	2.23	128.85	124.68
31	s	316	CLA	C1D-ND-C4D	-2.23	104.75	106.33
30	q	309	CHL	CHB-C4A-NA	2.23	127.59	124.51
31	4	602	CLA	C6-C5-C3	-2.23	107.61	113.45
30	q	308	CHL	CHC-C1C-NC	2.23	127.58	124.20
33	A	417	LHG	O8-C23-O10	-2.23	117.97	123.59
31	9	315	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
36	g	317	NEX	C26-C27-C28	-2.23	121.28	125.99
30	s	308	CHL	CHD-C4C-C3C	2.23	128.12	124.84
31	7	304	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
31	8	603	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
36	q	319	NEX	C39-C29-C30	-2.23	119.80	122.92
44	a	414	PL9	O2-C1-C6	2.23	124.45	120.59
31	B	613	CLA	O2A-CGA-CBA	2.23	118.90	111.91
32	4	616	LUT	C8-C7-C6	-2.23	120.95	127.20
32	1	616	LUT	C1-C6-C5	-2.23	119.48	122.61
38	0	621	SQD	O3-C3-C2	-2.23	105.20	110.35
30	N	302	CHL	CHD-C4C-C3C	2.23	128.11	124.84
31	R	306	CLA	C2A-C1A-CHA	2.23	127.75	123.86
30	N	301	CHL	C2C-C3C-C4C	2.23	108.08	106.49
31	6	304	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
31	n	313	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
32	1	616	LUT	C38-C25-C24	-2.23	118.80	123.56
36	p	618	NEX	C39-C29-C30	-2.23	119.81	122.92
36	8	617	NEX	C16-C1-C6	-2.23	108.48	110.47
34	2	620	LMG	O8-C28-O10	-2.23	117.97	123.59
31	D	404	CLA	C1-O2A-CGA	2.23	122.28	116.44
43	B	619	BCR	C30-C25-C26	-2.23	119.48	122.61
31	r	303	CLA	O2A-CGA-CBA	2.23	118.89	111.91
30	q	310	CHL	CHC-C1C-NC	2.23	127.58	124.20
31	y	615	CLA	O1D-CGD-CBD	-2.23	119.93	124.48
31	A	409	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
31	b	617	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
31	4	604	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
30	7	310	CHL	CHB-C4A-NA	2.22	127.59	124.51
31	1	614	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
32	0	616	LUT	C10-C11-C12	-2.22	116.28	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Y	316	LUT	C35-C15-C14	-2.22	118.92	123.47
31	G	612	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
31	S	303	CLA	O2D-CGD-O1D	-2.22	119.49	123.84
30	9	303	CHL	CHB-C4A-NA	2.22	127.58	124.51
43	z	101	BCR	C8-C7-C6	-2.22	120.96	127.20
31	B	614	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
36	R	319	NEX	C39-C29-C30	-2.22	119.81	122.92
31	2	612	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
31	9	305	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
31	N	315	CLA	O2A-CGA-CBA	2.22	118.88	111.91
31	r	305	CLA	O2A-CGA-CBA	2.22	118.88	111.91
30	6	309	CHL	CHB-C4A-NA	2.22	127.58	124.51
30	S	302	CHL	CMB-C2B-C1B	-2.22	125.05	128.46
31	q	306	CLA	C1D-ND-C4D	-2.22	104.76	106.33
34	b	622	LMG	O6-C1-O1	-2.22	104.72	109.97
30	5	606	CHL	CHC-C1C-NC	2.22	127.57	124.20
31	y	613	CLA	CHA-C1A-NA	-2.22	121.32	126.40
31	q	312	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
30	r	310	CHL	CHB-C4A-NA	2.22	127.58	124.51
32	9	318	LUT	C8-C7-C6	-2.22	120.97	127.20
38	r	322	SQD	O3-C3-C2	-2.22	105.22	110.35
31	s	311	CLA	C1D-ND-C4D	-2.22	104.76	106.33
30	R	310	CHL	C1B-CHB-C4A	-2.22	125.72	130.12
31	s	310	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
35	2	614	RRX	C34-C9-C10	-2.22	119.82	122.92
30	n	308	CHL	CHC-C1C-NC	2.22	127.57	124.20
31	7	303	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
32	0	616	LUT	C19-C9-C8	2.22	121.57	118.08
32	y	617	LUT	C39-C29-C28	2.22	121.57	118.08
31	8	609	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
31	R	311	CLA	C2D-C1D-ND	2.22	111.74	110.10
30	5	608	CHL	CMA-C3A-C2A	2.22	122.77	113.83
32	0	616	LUT	C38-C25-C24	-2.22	118.82	123.56
30	n	309	CHL	CMA-C3A-C2A	2.22	122.77	113.83
30	4	601	CHL	C1-O2A-CGA	2.22	122.26	116.44
34	b	624	LMG	O7-C10-O9	-2.22	118.35	123.70
42	D	401	PHO	C1-C2-C3	-2.22	122.21	126.04
30	5	606	CHL	CMB-C2B-C1B	-2.22	125.06	128.46
30	r	310	CHL	CHC-C1C-NC	2.22	127.56	124.20
35	q	317	RRX	C32-C1-C6	2.22	113.89	110.30
31	6	316	CLA	O2A-CGA-CBA	2.22	118.86	111.91
30	G	606	CHL	CMA-C3A-C2A	2.22	122.77	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	303	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
31	n	315	CLA	CHA-C1A-NA	-2.22	121.32	126.40
31	q	315	CLA	O2A-CGA-CBA	2.22	118.86	111.91
30	3	308	CHL	C4A-NA-C1A	2.22	107.70	106.71
30	y	601	CHL	CHC-C1C-NC	2.22	127.56	124.20
31	8	613	CLA	CHA-C1A-NA	-2.22	121.33	126.40
43	B	618	BCR	C29-C30-C25	2.22	113.89	110.48
31	B	607	CLA	C16-C15-C13	-2.21	108.76	115.92
30	s	307	CHL	CMA-C3A-C2A	2.21	122.76	113.83
31	s	304	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
30	G	623	CHL	CHB-C4A-NA	2.21	127.57	124.51
31	8	602	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
32	s	317	LUT	C1-C6-C5	-2.21	119.50	122.61
31	3	314	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
31	6	316	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
32	7	318	LUT	C8-C7-C6	-2.21	120.99	127.20
30	p	606	CHL	CMA-C3A-C2A	2.21	122.76	113.83
31	b	617	CLA	C2D-C1D-ND	2.21	111.73	110.10
31	3	313	CLA	CMD-C2D-C3D	-2.21	122.52	127.61
32	g	316	LUT	C20-C13-C14	-2.21	119.82	122.92
30	5	607	CHL	C1-O2A-CGA	2.21	122.25	116.44
30	g	309	CHL	CHB-C4A-NA	2.21	127.57	124.51
30	s	302	CHL	C4D-CHA-C1A	2.21	123.94	121.25
31	B	609	CLA	CHA-C1A-NA	-2.21	121.33	126.40
30	1	609	CHL	CHD-C4C-C3C	2.21	128.09	124.84
32	Y	316	LUT	C38-C25-C24	-2.21	118.83	123.56
31	g	303	CLA	CHA-C4D-ND	2.21	137.13	132.50
30	2	606	CHL	C1-O2A-CGA	2.21	122.25	116.44
31	S	305	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
34	9	301	LMG	C4-C3-C2	2.21	114.68	110.82
31	1	612	CLA	C1D-ND-C4D	-2.21	104.76	106.33
32	6	317	LUT	C10-C11-C12	-2.21	116.32	123.22
31	7	316	CLA	O2A-CGA-CBA	2.21	118.85	111.91
31	6	316	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	0	614	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	4	613	CLA	C1D-ND-C4D	-2.21	104.77	106.33
31	b	610	CLA	C1D-ND-C4D	-2.21	104.77	106.33
31	s	313	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	R	312	CLA	C1-C2-C3	-2.21	122.22	126.04
30	2	605	CHL	CHD-C4C-C3C	2.21	128.09	124.84
30	5	609	CHL	CHD-C4C-C3C	2.21	128.09	124.84
30	G	605	CHL	CHD-C4C-C3C	2.21	128.09	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	S	313	CLA	C6-C5-C3	-2.21	107.66	113.45
30	y	608	CHL	CMA-C3A-C2A	2.21	122.74	113.83
30	N	306	CHL	CMA-C3A-C2A	2.21	122.74	113.83
34	b	622	LMG	O7-C10-O9	-2.21	118.36	123.70
31	C	610	CLA	CHA-C1A-NA	-2.21	121.34	126.40
30	7	306	CHL	CMA-C3A-C2A	2.21	122.74	113.83
31	b	610	CLA	CMB-C2B-C3B	2.21	128.81	124.68
48	K	101	LMU	C1-O1'-C1'	-2.21	110.18	113.84
30	S	307	CHL	CHC-C1C-NC	2.21	127.55	124.20
31	7	305	CLA	O1D-CGD-CBD	-2.21	119.97	124.48
31	8	611	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
31	y	614	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
30	n	301	CHL	C2C-C3C-C4C	2.21	108.06	106.49
31	0	602	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
31	b	616	CLA	C1-O2A-CGA	2.21	122.24	116.44
36	R	301	NEX	C17-C1-C6	-2.21	108.50	110.47
30	7	306	CHL	CHD-C4C-C3C	2.21	128.09	124.84
30	4	608	CHL	CHB-C4A-NA	2.21	127.56	124.51
31	6	314	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
31	c	604	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
43	V	101	BCR	C33-C5-C4	2.21	117.86	113.62
36	8	617	NEX	C40-C33-C34	-2.21	119.83	122.92
32	5	616	LUT	C18-C5-C4	2.21	118.44	114.36
31	2	604	CLA	O2A-CGA-CBA	2.21	118.83	111.91
31	c	613	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
31	C	607	CLA	C6-C5-C3	-2.21	107.67	113.45
31	0	604	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
31	8	602	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
31	C	602	CLA	CMB-C2B-C3B	2.21	128.80	124.68
31	c	607	CLA	OBD-CAD-C3D	-2.21	123.21	128.52
43	z	101	BCR	C16-C15-C14	-2.21	118.96	123.47
37	r	318	XAT	C39-C29-C30	-2.20	119.83	122.92
31	N	312	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
31	S	306	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
30	y	608	CHL	CHB-C4A-NA	2.20	127.56	124.51
31	b	607	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
32	s	317	LUT	C15-C35-C34	-2.20	118.96	123.47
31	6	315	CLA	O2A-CGA-CBA	2.20	118.82	111.91
31	4	613	CLA	CMD-C2D-C3D	-2.20	122.54	127.61
31	R	307	CLA	CHA-C1A-NA	-2.20	121.35	126.40
30	Y	301	CHL	CMA-C3A-C2A	2.20	122.72	113.83
30	p	605	CHL	CHC-C1C-NC	2.20	127.55	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N	314	CLA	CHA-C1A-NA	-2.20	121.35	126.40
32	g	316	LUT	C8-C7-C6	-2.20	121.01	127.20
30	Y	309	CHL	C3A-C2A-C1A	2.20	104.64	101.34
31	n	311	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
31	R	313	CLA	CAA-C2A-C3A	-2.20	106.75	112.78
31	2	609	CLA	CHA-C1A-NA	-2.20	121.35	126.40
31	N	315	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
34	w	203	LMG	C8-O7-C10	-2.20	112.37	117.79
30	5	601	CHL	CHB-C4A-NA	2.20	127.56	124.51
30	G	601	CHL	CHB-C4A-NA	2.20	127.56	124.51
43	B	618	BCR	C38-C26-C27	2.20	117.85	113.62
30	2	608	CHL	CHD-C4C-C3C	2.20	128.08	124.84
30	1	619	CHL	CHA-C1A-NA	-2.20	121.36	126.40
31	7	315	CLA	CHA-C1A-NA	-2.20	121.36	126.40
31	5	604	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
43	a	410	BCR	C36-C18-C17	-2.20	119.84	122.92
31	6	313	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
46	D	402	BCT	O3-C-O1	-2.20	113.84	119.55
31	N	311	CLA	O2A-CGA-CBA	2.20	118.81	111.91
30	y	606	CHL	CMA-C3A-C2A	2.20	122.70	113.83
31	3	314	CLA	C6-C5-C3	-2.20	107.69	113.45
31	b	606	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
31	G	610	CLA	C2A-C1A-CHA	2.20	127.70	123.86
31	8	609	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
31	2	612	CLA	O2A-CGA-CBA	2.20	118.81	111.91
32	7	317	LUT	C39-C29-C28	2.20	121.54	118.08
30	s	307	CHL	CHC-C1C-NC	2.20	127.54	124.20
34	6	321	LMG	O7-C10-O9	-2.20	118.39	123.70
31	5	602	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
31	R	304	CLA	CMA-C3A-C4A	2.20	117.68	111.77
31	B	613	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
31	c	603	CLA	CMB-C2B-C3B	2.20	128.79	124.68
31	b	605	CLA	C2D-C1D-ND	2.20	111.72	110.10
32	s	317	LUT	C18-C5-C4	2.20	118.42	114.36
31	b	617	CLA	CMB-C2B-C3B	2.20	128.79	124.68
34	W	201	LMG	C8-O7-C10	-2.20	112.38	117.79
30	1	607	CHL	CMB-C2B-C1B	-2.20	125.09	128.46
43	b	620	BCR	C16-C15-C14	-2.20	118.97	123.47
31	5	602	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
31	N	305	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
30	p	601	CHL	C1-O2A-CGA	2.20	122.20	116.44
31	2	603	CLA	O2D-CGD-O1D	-2.20	119.55	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	614	CLA	O2A-CGA-CBA	2.20	118.80	111.91
30	2	607	CHL	CHC-C1C-NC	2.20	127.53	124.20
43	d	406	BCR	C23-C24-C25	-2.20	121.04	127.20
31	4	610	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
31	G	604	CLA	O2A-CGA-CBA	2.20	118.80	111.91
31	n	305	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
30	p	606	CHL	CHC-C1C-NC	2.19	127.53	124.20
31	d	404	CLA	CMD-C2D-C3D	-2.19	122.56	127.61
30	0	601	CHL	CHB-C4A-NA	2.19	127.55	124.51
30	0	609	CHL	C1-C2-C3	-2.19	122.25	126.04
30	s	308	CHL	CHC-C1C-NC	2.19	127.53	124.20
31	n	303	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
31	7	314	CLA	O2A-CGA-CBA	2.19	118.79	111.91
31	c	604	CLA	C1D-ND-C4D	-2.19	104.78	106.33
30	1	606	CHL	CMA-C3A-C2A	2.19	122.67	113.83
31	7	315	CLA	CMD-C2D-C3D	-2.19	122.57	127.61
34	k	102	LMG	C8-O7-C10	-2.19	112.39	117.79
31	p	602	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
32	7	317	LUT	C35-C15-C14	-2.19	118.98	123.47
30	y	606	CHL	CHB-C4A-NA	2.19	127.54	124.51
31	s	313	CLA	C1D-ND-C4D	-2.19	104.78	106.33
31	5	615	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
30	3	310	CHL	CMB-C2B-C1B	-2.19	125.10	128.46
38	M	102	SQD	O3-C3-C2	-2.19	105.28	110.35
30	y	606	CHL	C2C-C3C-C4C	2.19	108.05	106.49
31	n	303	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
31	r	306	CLA	CHA-C1A-NA	-2.19	121.38	126.40
31	p	612	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
33	l	101	LHG	C5-O7-C7	-2.19	112.40	117.79
30	G	623	CHL	CHD-C4C-C3C	2.19	128.06	124.84
31	5	603	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	y	602	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	4	612	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	s	304	CLA	CHA-C1A-NA	-2.19	121.38	126.40
31	C	608	CLA	C6-C5-C3	-2.19	107.71	113.45
31	s	311	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	0	615	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
30	3	303	CHL	CHB-C4A-NA	2.19	127.54	124.51
30	n	302	CHL	CMA-C3A-C2A	2.19	122.66	113.83
36	5	618	NEX	C39-C29-C30	-2.19	119.86	122.92
31	4	610	CLA	CMC-C2C-C1C	2.19	128.37	125.04
31	4	610	CLA	CMD-C2D-C3D	-2.19	122.58	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	304	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
31	y	612	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
32	p	617	LUT	C15-C35-C34	2.19	127.96	123.47
31	4	604	CLA	O2A-CGA-CBA	2.19	118.78	111.91
30	g	302	CHL	CHC-C1C-NC	2.19	127.52	124.20
31	b	612	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	N	310	CLA	C11-C10-C8	-2.19	108.85	115.92
30	8	601	CHL	CMA-C3A-C2A	2.19	122.66	113.83
30	7	308	CHL	C1-O2A-CGA	2.19	122.19	116.44
31	R	315	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
30	q	303	CHL	C1-C2-C3	-2.19	122.26	126.04
31	8	604	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	B	612	CLA	CMB-C2B-C3B	2.19	128.77	124.68
31	q	304	CLA	C6-C5-C3	-2.19	107.72	113.45
30	1	619	CHL	CMB-C2B-C1B	-2.19	125.10	128.46
30	6	307	CHL	CMB-C2B-C1B	-2.19	125.10	128.46
31	y	604	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
31	a	406	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
31	b	609	CLA	O2A-CGA-CBA	2.19	118.77	111.91
31	r	311	CLA	C1-O2A-CGA	2.19	122.18	116.44
31	2	604	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
32	r	317	LUT	C12-C13-C14	-2.19	115.59	118.94
30	1	606	CHL	C1-C2-C3	-2.19	122.26	126.04
31	c	606	CLA	O2A-CGA-CBA	2.19	118.77	111.91
30	2	605	CHL	CHC-C1C-NC	2.19	127.52	124.20
30	q	309	CHL	C1B-CHB-C4A	-2.19	125.79	130.12
30	Y	301	CHL	CMB-C2B-C1B	-2.19	125.11	128.46
30	7	308	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
30	9	311	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
43	D	405	BCR	C11-C10-C9	2.18	130.43	127.31
31	R	305	CLA	CMB-C2B-C3B	2.18	128.76	124.68
30	3	307	CHL	CHC-C1C-NC	2.18	127.52	124.20
31	q	306	CLA	O2A-CGA-CBA	2.18	118.76	111.91
30	n	309	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
34	C	621	LMG	O7-C10-O9	-2.18	118.43	123.70
31	R	311	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
35	g	315	RRX	C8-C9-C10	2.18	122.29	118.94
32	s	318	LUT	C22-C23-C24	2.18	114.22	111.74
31	Y	304	CLA	CHA-C1A-NA	-2.18	121.40	126.40
30	7	308	CHL	C4A-NA-C1A	2.18	107.69	106.71
30	N	308	CHL	CHC-C1C-NC	2.18	127.51	124.20
31	B	607	CLA	CBA-CAA-C2A	-2.18	107.42	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	304	CLA	O2A-CGA-CBA	2.18	118.75	111.91
32	S	317	LUT	C15-C35-C34	-2.18	119.00	123.47
32	q	318	LUT	C38-C25-C24	-2.18	118.89	123.56
30	Y	302	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
32	1	615	LUT	C19-C9-C8	2.18	121.51	118.08
30	6	308	CHL	CMA-C3A-C4A	2.18	117.63	111.77
32	p	617	LUT	C2-C3-C4	2.18	113.29	110.30
31	9	313	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
34	9	321	LMG	C8-O7-C10	-2.18	112.42	117.79
30	5	608	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
36	6	319	NEX	C20-C13-C14	-2.18	119.87	122.92
31	s	312	CLA	O2A-CGA-CBA	2.18	118.75	111.91
32	1	615	LUT	C12-C13-C14	-2.18	115.60	118.94
34	q	301	LMG	O7-C10-O9	-2.18	118.43	123.70
31	N	305	CLA	CMA-C3A-C4A	2.18	117.63	111.77
35	2	614	RRX	C1-C6-C7	2.18	121.94	115.78
31	S	315	CLA	C1D-ND-C4D	-2.18	104.79	106.33
30	p	606	CHL	C1-O2A-CGA	2.18	122.16	116.44
43	H	101	BCR	C11-C12-C13	-2.18	120.30	126.42
30	4	601	CHL	C2C-C3C-C4C	2.18	108.04	106.49
30	7	302	CHL	CHD-C4C-C3C	2.18	128.04	124.84
31	B	606	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
31	C	607	CLA	CMA-C3A-C4A	2.18	117.63	111.77
32	S	318	LUT	C39-C29-C30	-2.18	119.87	122.92
31	7	305	CLA	CMB-C2B-C3B	2.18	128.75	124.68
31	C	606	CLA	CMA-C3A-C4A	2.18	117.62	111.77
31	c	613	CLA	CBA-CAA-C2A	2.18	120.29	113.86
32	G	615	LUT	C38-C25-C24	-2.18	118.90	123.56
30	2	606	CHL	CMB-C2B-C1B	-2.18	125.12	128.46
36	R	319	NEX	C19-C9-C10	-2.18	119.87	122.92
31	N	304	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
31	g	313	CLA	CMD-C2D-C3D	-2.18	122.61	127.61
31	R	311	CLA	C1-O2A-CGA	2.18	122.15	116.44
34	s	321	LMG	C8-O7-C10	-2.18	112.43	117.79
30	7	307	CHL	CMA-C3A-C2A	2.18	122.60	113.83
31	n	313	CLA	CMB-C2B-C3B	2.18	128.75	124.68
34	B	625	LMG	C9-C8-C7	-2.18	106.64	111.79
31	0	613	CLA	O2A-CGA-CBA	2.18	118.73	111.91
31	0	603	CLA	C2D-C1D-ND	2.18	111.71	110.10
30	3	303	CHL	CHD-C4C-C3C	2.17	128.04	124.84
31	B	614	CLA	O2A-CGA-CBA	2.17	118.73	111.91
31	g	313	CLA	O2A-CGA-CBA	2.17	118.73	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	c	615	BCR	C34-C9-C10	-2.17	119.88	122.92
30	n	308	CHL	CMB-C2B-C1B	-2.17	125.12	128.46
31	8	614	CLA	CMB-C2B-C1B	-2.17	125.12	128.46
31	B	609	CLA	C6-C5-C3	-2.17	107.75	113.45
30	G	606	CHL	CHB-C4A-NA	2.17	127.52	124.51
43	z	101	BCR	C2-C1-C6	2.17	113.83	110.48
31	S	310	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
31	S	313	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
31	S	306	CLA	O2A-CGA-CBA	2.17	118.73	111.91
30	y	607	CHL	CMA-C3A-C2A	2.17	122.59	113.83
30	N	308	CHL	CMB-C2B-C1B	-2.17	125.12	128.46
36	4	617	NEX	C38-C25-C26	-2.17	118.62	122.26
32	Y	315	LUT	C11-C10-C9	-2.17	124.21	127.31
30	2	606	CHL	CMA-C3A-C2A	2.17	122.59	113.83
31	A	407	CLA	O2A-CGA-CBA	2.17	118.73	111.91
31	1	610	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
30	4	605	CHL	CHB-C4A-NA	2.17	127.52	124.51
31	6	304	CLA	CHA-C1A-NA	-2.17	121.42	126.40
43	D	405	BCR	C20-C19-C18	-2.17	120.31	126.42
31	5	612	CLA	CMB-C2B-C3B	2.17	128.74	124.68
30	Y	302	CHL	CMA-C3A-C2A	2.17	122.59	113.83
31	0	602	CLA	C1D-ND-C4D	-2.17	104.79	106.33
30	7	302	CHL	CHB-C4A-NA	2.17	127.52	124.51
31	C	605	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
31	s	316	CLA	CHA-C1A-NA	-2.17	121.43	126.40
31	B	603	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
31	6	313	CLA	O2A-CGA-CBA	2.17	118.72	111.91
31	2	613	CLA	CMB-C2B-C3B	2.17	128.74	124.68
34	w	203	LMG	C30-C29-C28	-2.17	105.73	113.62
31	n	303	CLA	C6-C5-C3	-2.17	107.76	113.45
30	0	607	CHL	CHC-C1C-NC	2.17	127.50	124.20
30	8	607	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
30	g	308	CHL	CHD-C4C-C3C	2.17	128.03	124.84
31	q	306	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
31	B	614	CLA	CMB-C2B-C3B	2.17	128.74	124.68
31	0	612	CLA	CHA-C1A-NA	-2.17	121.43	126.40
32	q	318	LUT	C15-C35-C34	-2.17	119.03	123.47
31	c	608	CLA	CHA-C1A-NA	-2.17	121.43	126.40
32	9	318	LUT	C39-C29-C30	-2.17	119.89	122.92
31	y	614	CLA	CHA-C1A-NA	-2.17	121.43	126.40
31	5	613	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
31	0	613	CLA	CMD-C2D-C3D	-2.17	122.63	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	9	317	RRX	C1-C6-C7	2.17	121.91	115.78
31	b	617	CLA	CHA-C1A-NA	-2.17	121.43	126.40
32	N	316	LUT	C30-C31-C32	-2.17	116.45	123.22
31	r	312	CLA	CMB-C2B-C3B	2.17	128.73	124.68
34	B	621	LMG	O7-C10-O9	-2.17	118.47	123.70
30	r	309	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
35	4	615	RRX	C1-C6-C7	2.17	121.91	115.78
31	S	314	CLA	CMB-C2B-C3B	2.17	128.73	124.68
31	5	602	CLA	O2A-CGA-CBA	2.17	118.70	111.91
30	4	606	CHL	CMB-C2B-C1B	-2.17	125.14	128.46
31	b	611	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
31	6	304	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
31	c	607	CLA	CMB-C2B-C3B	2.17	128.73	124.68
31	2	612	CLA	C1D-ND-C4D	-2.17	104.80	106.33
31	4	611	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	A	405	CLA	CMD-C2D-C3D	-2.16	122.63	127.61
31	c	609	CLA	CMA-C3A-C4A	2.16	117.59	111.77
30	Y	307	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
31	5	615	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
36	5	618	NEX	C40-C33-C34	-2.16	119.89	122.92
36	8	617	NEX	C19-C9-C10	-2.16	119.89	122.92
43	b	618	BCR	C2-C1-C6	2.16	113.81	110.48
31	B	615	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
30	q	311	CHL	CMA-C3A-C2A	2.16	122.56	113.83
36	0	618	NEX	C20-C13-C14	-2.16	119.89	122.92
31	3	315	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	c	610	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	S	311	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
31	a	407	CLA	O2A-CGA-CBA	2.16	118.70	111.91
30	s	309	CHL	CHC-C1C-NC	2.16	127.48	124.20
31	g	310	CLA	CMA-C3A-C4A	2.16	117.59	111.77
31	3	312	CLA	C1-O2A-CGA	2.16	122.12	116.44
31	p	603	CLA	C2D-C1D-ND	2.16	111.70	110.10
30	3	303	CHL	CMA-C3A-C2A	2.16	122.55	113.83
30	s	302	CHL	C1B-CHB-C4A	-2.16	125.83	130.12
34	6	323	LMG	C1-O6-C5	2.16	117.93	113.69
31	5	612	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
32	n	317	LUT	C38-C25-C24	-2.16	118.93	123.56
30	n	310	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
30	y	605	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
38	b	627	SQD	O3-C3-C2	-2.16	105.35	110.35
30	0	607	CHL	CHD-C4C-C3C	2.16	128.02	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	318	LUT	C15-C35-C34	-2.16	119.05	123.47
31	d	405	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	Y	314	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
36	N	318	NEX	O24-C25-C38	-2.16	112.47	115.06
31	B	602	CLA	CMA-C3A-C4A	2.16	117.58	111.77
31	a	409	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	b	614	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
31	s	315	CLA	C2D-C1D-ND	2.16	111.70	110.10
30	N	306	CHL	CHD-C4C-C3C	2.16	128.01	124.84
36	n	319	NEX	C16-C1-C6	-2.16	108.54	110.47
31	N	305	CLA	CHA-C1A-NA	-2.16	121.45	126.40
43	V	101	BCR	C15-C16-C17	-2.16	119.05	123.47
31	S	304	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
31	3	304	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
30	p	601	CHL	CHD-C4C-C3C	2.16	128.01	124.84
31	C	605	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	9	305	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	C	611	CLA	CHA-C1A-NA	-2.16	121.45	126.40
31	2	612	CLA	CMB-C2B-C3B	2.16	128.72	124.68
31	S	303	CLA	C11-C10-C8	-2.16	108.94	115.92
36	S	319	NEX	C39-C29-C30	-2.16	119.90	122.92
34	y	620	LMG	C9-C8-C7	-2.16	106.68	111.79
31	b	602	CLA	C1D-ND-C4D	-2.16	104.80	106.33
31	C	610	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
31	s	305	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
35	q	317	RRX	C19-C18-C17	2.16	122.25	118.94
31	b	617	CLA	C1-O2A-CGA	2.16	122.11	116.44
31	B	613	CLA	CHA-C1A-NA	-2.16	121.46	126.40
31	8	611	CLA	CMB-C2B-C3B	2.16	128.71	124.68
32	N	316	LUT	C18-C5-C4	2.16	118.35	114.36
30	8	608	CHL	CMB-C2B-C1B	-2.16	125.15	128.46
31	G	602	CLA	CHA-C1A-NA	-2.16	121.46	126.40
31	r	303	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
32	p	616	LUT	C15-C35-C34	2.16	127.89	123.47
31	g	305	CLA	O2A-CGA-CBA	2.16	118.67	111.91
30	6	309	CHL	C1-O2A-CGA	2.16	122.10	116.44
32	1	616	LUT	C39-C29-C28	2.16	121.47	118.08
35	g	315	RRX	C23-C24-C25	-2.16	121.15	127.20
31	D	404	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
31	s	314	CLA	CHA-C1A-NA	-2.16	121.46	126.40
30	n	309	CHL	CHB-C4A-NA	2.16	127.49	124.51
34	Q1	101	LMG	C8-O7-C10	-2.16	112.48	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	q	304	CLA	CMB-C2B-C3B	2.16	128.71	124.68
30	G	601	CHL	CMB-C2B-C1B	-2.16	125.15	128.46
31	4	614	CLA	CMB-C2B-C1B	-2.16	125.15	128.46
31	7	316	CLA	CHA-C1A-NA	-2.16	121.46	126.40
31	c	602	CLA	CHA-C1A-NA	-2.16	121.46	126.40
32	n	317	LUT	C18-C5-C4	2.16	118.35	114.36
31	0	614	CLA	O2A-CGA-CBA	2.16	118.67	111.91
31	p	602	CLA	C1D-ND-C4D	-2.16	104.80	106.33
32	8	615	LUT	C38-C25-C24	-2.15	118.95	123.56
31	S	313	CLA	CMA-C3A-C4A	2.15	117.56	111.77
32	3	318	LUT	C11-C10-C9	-2.15	124.23	127.31
31	A	409	CLA	CMD-C2D-C3D	-2.15	122.66	127.61
43	b	618	BCR	C36-C18-C19	2.15	121.47	118.08
31	3	315	CLA	CHA-C1A-NA	-2.15	121.47	126.40
30	0	607	CHL	CMA-C3A-C2A	2.15	122.52	113.83
42	D	401	PHO	O2A-CGA-O1A	-2.15	118.16	123.59
31	2	604	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	r	307	CLA	C2D-C1D-ND	2.15	111.69	110.10
30	6	308	CHL	CHC-C1C-NC	2.15	127.47	124.20
43	t	101	BCR	C3-C4-C5	-2.15	110.23	114.08
31	9	312	CLA	C1-O2A-CGA	2.15	122.09	116.44
31	2	603	CLA	O2A-CGA-CBA	2.15	118.66	111.91
31	R	314	CLA	O2A-CGA-CBA	2.15	118.66	111.91
30	n	309	CHL	CHC-C1C-NC	2.15	127.47	124.20
30	n	306	CHL	CMA-C3A-C2A	2.15	122.51	113.83
31	B	608	CLA	C1D-ND-C4D	-2.15	104.81	106.33
31	8	612	CLA	C6-C5-C3	-2.15	107.81	113.45
31	n	314	CLA	C6-C5-C3	-2.15	107.81	113.45
31	9	312	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
30	7	321	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
32	1	615	LUT	C18-C5-C4	2.15	118.34	114.36
30	Y	308	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
31	y	612	CLA	CHA-C1A-NA	-2.15	121.47	126.40
32	n	317	LUT	C39-C29-C28	2.15	121.47	118.08
43	b	618	BCR	C35-C13-C12	2.15	121.47	118.08
31	R	305	CLA	C1-O2A-CGA	2.15	122.09	116.44
30	n	301	CHL	CHB-C4A-NA	2.15	127.49	124.51
30	y	607	CHL	CHD-C4C-C3C	2.15	128.00	124.84
36	N	318	NEX	C4-C3-C2	2.15	114.93	110.77
30	8	606	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
30	9	309	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
30	y	601	CHL	CMB-C2B-C1B	-2.15	125.16	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	g	318	SQD	O3-C3-C2	-2.15	105.38	110.35
31	p	611	CLA	O2A-CGA-CBA	2.15	118.66	111.91
30	g	306	CHL	CHC-C1C-NC	2.15	127.47	124.20
31	q	316	CLA	CHA-C1A-NA	-2.15	121.47	126.40
31	C	607	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
30	p	606	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
35	G	614	RRX	C1-C6-C7	2.15	121.86	115.78
31	0	602	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
31	c	609	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
36	r	319	NEX	C20-C13-C14	-2.15	119.91	122.92
31	4	602	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
31	c	612	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
34	Q1	101	LMG	O1-C1-C2	2.15	111.66	108.30
30	1	607	CHL	CHC-C1C-NC	2.15	127.46	124.20
31	B	616	CLA	C2D-C1D-ND	2.15	111.69	110.10
30	2	606	CHL	CHB-C4A-NA	2.15	127.48	124.51
30	0	605	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
32	Y	315	LUT	C31-C30-C29	-2.15	124.25	127.31
32	N	316	LUT	C15-C35-C34	-2.15	119.08	123.47
30	G	601	CHL	C1-O2A-CGA	2.15	122.08	116.44
30	5	605	CHL	CMA-C3A-C2A	2.15	122.49	113.83
30	5	605	CHL	CHC-C1C-NC	2.15	127.46	124.20
32	8	615	LUT	C18-C5-C4	2.15	118.33	114.36
36	r	319	NEX	O24-C25-C38	-2.15	112.48	115.06
30	4	605	CHL	C4A-NA-C1A	2.15	107.67	106.71
30	g	308	CHL	CMB-C2B-C1B	-2.15	125.17	128.46
31	R	306	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	r	314	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
30	2	601	CHL	CMA-C3A-C2A	2.15	122.48	113.83
31	8	612	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
31	q	316	CLA	O2A-CGA-CBA	2.15	118.64	111.91
31	9	312	CLA	O2A-CGA-CBA	2.15	118.64	111.91
34	w	203	LMG	O7-C10-O9	-2.15	118.52	123.70
31	s	310	CLA	O2A-CGA-CBA	2.15	118.64	111.91
31	1	614	CLA	CHA-C1A-NA	-2.14	121.49	126.40
30	3	309	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
30	n	301	CHL	CHD-C4C-C3C	2.14	127.99	124.84
30	R	309	CHL	CHB-C4A-NA	2.14	127.48	124.51
32	0	616	LUT	C31-C30-C29	-2.14	124.25	127.31
30	7	302	CHL	CMA-C3A-C2A	2.14	122.48	113.83
30	g	302	CHL	CMA-C3A-C2A	2.14	122.48	113.83
31	c	605	CLA	CMB-C2B-C3B	2.14	128.69	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	5	609	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
30	q	309	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
31	c	613	CLA	CMA-C3A-C4A	2.14	117.53	111.77
35	g	315	RRX	C37-C22-C21	-2.14	119.92	122.92
31	p	610	CLA	CMB-C2B-C3B	2.14	128.69	124.68
44	A	416	PL9	C41-C39-C38	-2.14	116.78	121.12
32	s	317	LUT	C20-C13-C12	2.14	121.45	118.08
31	1	612	CLA	CHA-C1A-NA	-2.14	121.49	126.40
30	5	605	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
31	2	609	CLA	C6-C7-C8	-2.14	108.99	115.92
30	3	302	CHL	CMA-C3A-C2A	2.14	122.47	113.83
31	b	616	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
31	p	604	CLA	CMB-C2B-C3B	2.14	128.69	124.68
31	B	612	CLA	O1D-CGD-CBD	-2.14	120.10	124.48
31	3	313	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
30	g	302	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
31	Y	314	CLA	CHA-C1A-NA	-2.14	121.49	126.40
30	6	308	CHL	CHD-C4C-C3C	2.14	127.99	124.84
31	S	316	CLA	CHA-C1A-NA	-2.14	121.49	126.40
30	q	308	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
31	b	615	CLA	CMB-C2B-C3B	2.14	128.68	124.68
32	G	615	LUT	C15-C35-C34	2.14	127.86	123.47
31	s	303	CLA	C6-C5-C3	-2.14	107.84	113.45
31	p	612	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
31	d	405	CLA	C1-O2A-CGA	2.14	122.06	116.44
30	1	605	CHL	CMA-C3A-C2A	2.14	122.46	113.83
30	s	309	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
31	Y	305	CLA	CMA-C3A-C4A	2.14	117.53	111.77
36	Y	317	NEX	C20-C13-C14	-2.14	119.92	122.92
31	5	612	CLA	CHA-C1A-NA	-2.14	121.50	126.40
31	8	614	CLA	O2A-CGA-CBA	2.14	118.62	111.91
31	3	301	CLA	C6-C5-C3	-2.14	107.84	113.45
31	q	313	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	C	608	CLA	C1D-ND-C4D	-2.14	104.81	106.33
31	q	306	CLA	CHA-C1A-NA	-2.14	121.50	126.40
43	h	101	BCR	C31-C1-C6	-2.14	106.83	110.30
31	0	610	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
43	Z	101	BCR	C16-C15-C14	-2.14	119.09	123.47
30	4	601	CHL	CMA-C3A-C2A	2.14	122.46	113.83
30	8	605	CHL	CMA-C3A-C2A	2.14	122.46	113.83
31	G	603	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
30	9	307	CHL	CHD-C4C-C3C	2.14	127.98	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	605	CHL	CHC-C1C-NC	2.14	127.45	124.20
32	s	318	LUT	C15-C35-C34	-2.14	119.09	123.47
30	R	309	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
30	p	608	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
31	C	606	CLA	C1D-ND-C4D	-2.14	104.82	106.33
36	3	319	NEX	C39-C29-C30	-2.14	119.93	122.92
30	N	307	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
31	7	304	CLA	CHA-C1A-NA	-2.14	121.50	126.40
30	Y	301	CHL	CHB-C4A-NA	2.14	127.47	124.51
32	p	617	LUT	C38-C25-C24	-2.14	118.98	123.56
31	s	311	CLA	CMA-C3A-C4A	2.14	117.52	111.77
31	9	304	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	s	316	CLA	CMD-C2D-C3D	-2.14	122.70	127.61
31	2	611	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
31	9	313	CLA	CHA-C1A-NA	-2.14	121.50	126.40
31	3	305	CLA	CHA-C1A-NA	-2.14	121.50	126.40
31	c	612	CLA	CHA-C1A-NA	-2.14	121.50	126.40
30	0	609	CHL	CHD-C4C-C3C	2.14	127.98	124.84
31	3	311	CLA	C1D-ND-C4D	-2.14	104.82	106.33
31	n	305	CLA	CHA-C1A-NA	-2.14	121.50	126.40
30	R	309	CHL	CHD-C4C-C3C	2.14	127.98	124.84
30	r	310	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
43	C	614	BCR	C34-C9-C10	-2.14	119.93	122.92
31	c	605	CLA	C2D-C1D-ND	2.14	111.68	110.10
30	R	310	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
31	A	405	CLA	CAA-CBA-CGA	-2.14	107.01	113.25
36	9	319	NEX	C26-C27-C28	-2.13	121.48	125.99
31	B	615	CLA	C6-C5-C3	-2.13	107.86	113.45
34	c	620	LMG	O7-C10-O9	-2.13	118.54	123.70
31	C	611	CLA	CAA-CBA-CGA	-2.13	107.02	113.25
43	h	101	BCR	C20-C19-C18	-2.13	120.42	126.42
34	m	102	LMG	O7-C10-O9	-2.13	118.54	123.70
31	5	602	CLA	CHA-C1A-NA	-2.13	121.51	126.40
30	5	601	CHL	C2C-C3C-C4C	2.13	108.01	106.49
30	0	601	CHL	C2C-C3C-C4C	2.13	108.01	106.49
31	1	611	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
30	N	302	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
34	A	414	LMG	C1-O6-C5	-2.13	109.50	113.69
31	0	604	CLA	CMB-C2B-C3B	2.13	128.67	124.68
36	3	319	NEX	C20-C13-C14	-2.13	119.94	122.92
31	8	614	CLA	CHA-C1A-NA	-2.13	121.51	126.40
30	6	309	CHL	CMB-C2B-C1B	-2.13	125.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	n	301	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
31	0	610	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	9	304	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
33	y	619	LHG	C6-C5-C4	-2.13	106.75	111.79
31	N	313	CLA	CHA-C1A-NA	-2.13	121.52	126.40
30	5	606	CHL	CHD-C4C-C3C	2.13	127.97	124.84
31	Y	305	CLA	CMB-C2B-C3B	2.13	128.67	124.68
31	B	601	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	N	304	CLA	CHA-C1A-NA	-2.13	121.52	126.40
30	6	308	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
30	G	605	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
30	9	310	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
31	0	615	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
43	D	405	BCR	C1-C6-C5	-2.13	119.61	122.61
31	d	405	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	N	310	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
31	p	614	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
30	n	302	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
30	7	309	CHL	CHC-C1C-NC	2.13	127.44	124.20
30	7	310	CHL	C1-O2A-CGA	2.13	122.03	116.44
31	3	316	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
30	G	608	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
31	2	610	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	n	314	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	2	602	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
30	1	605	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
30	N	309	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
34	S	321	LMG	C8-O7-C10	-2.13	112.55	117.79
30	1	619	CHL	CHC-C1C-NC	2.13	127.43	124.20
30	2	605	CHL	CHB-C4A-NA	2.13	127.46	124.51
30	0	601	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
30	p	609	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
31	s	311	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
33	g	319	LHG	C5-O7-C7	-2.13	112.55	117.79
31	Y	314	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
31	3	316	CLA	CHA-C1A-NA	-2.13	121.52	126.40
31	8	602	CLA	CHA-C1A-NA	-2.13	121.52	126.40
30	6	306	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
33	Y	318	LHG	C6-C5-C4	-2.13	106.75	111.79
31	q	313	CLA	CHA-C1A-NA	-2.13	121.53	126.40
30	7	307	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
30	y	606	CHL	CMB-C2B-C1B	-2.13	125.19	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	611	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
31	A	405	CLA	C1D-ND-C4D	-2.13	104.82	106.33
32	y	617	LUT	C35-C15-C14	-2.13	119.12	123.47
31	r	305	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
30	S	307	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
31	2	613	CLA	O2A-CGA-CBA	2.13	118.58	111.91
30	0	601	CHL	CHD-C4C-C3C	2.13	127.97	124.84
31	S	314	CLA	CHA-C1A-NA	-2.13	121.53	126.40
30	q	310	CHL	CMB-C2B-C1B	-2.13	125.20	128.46
31	B	610	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
30	6	308	CHL	CHB-C4A-NA	2.13	127.45	124.51
30	0	605	CHL	CHB-C4A-NA	2.13	127.45	124.51
31	Y	303	CLA	C6-C5-C3	-2.13	107.88	113.45
33	t	102	LHG	O7-C7-O9	-2.13	118.56	123.70
31	p	612	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
30	N	306	CHL	CHC-C1C-NC	2.13	127.43	124.20
30	1	609	CHL	CMB-C2B-C1B	-2.13	125.20	128.46
30	7	309	CHL	CMB-C2B-C1B	-2.13	125.20	128.46
31	C	601	CLA	CMD-C2D-C3D	-2.13	122.72	127.61
31	n	314	CLA	CHA-C1A-NA	-2.13	121.53	126.40
31	B	602	CLA	C6-C7-C8	-2.13	109.05	115.92
31	B	616	CLA	CMB-C2B-C3B	2.13	128.65	124.68
30	9	307	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
44	a	414	PL9	C12-C13-C14	-2.12	122.54	127.66
31	7	316	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
31	a	406	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
31	G	611	CLA	CHA-C1A-NA	-2.12	121.53	126.40
30	6	310	CHL	C4A-NA-C1A	2.12	107.66	106.71
31	r	303	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
31	5	603	CLA	CMB-C2B-C3B	2.12	128.65	124.68
31	n	316	CLA	O2A-CGA-CBA	2.12	118.57	111.91
31	s	305	CLA	O2A-CGA-CBA	2.12	118.57	111.91
32	G	615	LUT	C18-C5-C4	2.12	118.29	114.36
37	G	620	XAT	C40-C33-C34	-2.12	119.95	122.92
30	7	307	CHL	CHD-C4C-C3C	2.12	127.96	124.84
32	n	317	LUT	C10-C11-C12	-2.12	116.59	123.22
34	C	619	LMG	O8-C28-O10	-2.12	118.23	123.59
30	n	307	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
31	r	311	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
31	b	616	CLA	C6-C5-C3	-2.12	107.89	113.45
30	G	601	CHL	CMA-C3A-C2A	2.12	122.39	113.83
30	y	605	CHL	C4A-NA-C1A	2.12	107.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	9	312	CLA	CAA-C2A-C3A	-2.12	106.97	112.78
31	6	314	CLA	C6-C5-C3	-2.12	107.89	113.45
30	3	308	CHL	CHC-C1C-NC	2.12	127.42	124.20
30	n	310	CHL	CHB-C4A-NA	2.12	127.45	124.51
31	3	311	CLA	CHA-C1A-NA	-2.12	121.54	126.40
30	g	307	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
33	4	618	LHG	C5-O7-C7	-2.12	112.57	117.79
31	r	306	CLA	CMD-C2D-C3D	-2.12	122.73	127.61
31	B	606	CLA	C6-C5-C3	-2.12	107.89	113.45
31	D	404	CLA	O2A-CGA-CBA	2.12	118.56	111.91
30	8	601	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
31	5	615	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
31	n	315	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
32	G	615	LUT	C31-C32-C33	-2.12	120.46	126.42
31	C	607	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
32	8	615	LUT	C39-C29-C28	2.12	121.42	118.08
31	G	613	CLA	CHA-C1A-NA	-2.12	121.54	126.40
30	1	606	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
30	q	309	CHL	CMA-C3A-C2A	2.12	122.38	113.83
30	4	608	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
30	4	609	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	D	403	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
30	G	607	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	8	604	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	C	605	CLA	C7-C6-C5	-2.12	107.60	113.36
31	4	603	CLA	O2A-CGA-CBA	2.12	118.56	111.91
31	A	407	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
30	1	608	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
30	2	605	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
30	N	306	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	S	310	CLA	O2A-CGA-CBA	2.12	118.56	111.91
31	4	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	g	310	CLA	CAA-C2A-C3A	-2.12	106.98	112.78
36	5	618	NEX	C19-C9-C10	-2.12	119.96	122.92
31	9	304	CLA	C1-O2A-CGA	2.12	122.00	116.44
30	Y	301	CHL	CHC-C1C-NC	2.12	127.42	124.20
30	9	310	CHL	CMA-C3A-C2A	2.12	122.37	113.83
36	y	618	NEX	C26-C27-C28	-2.12	121.52	125.99
45	C	618	DGD	C1D-O6D-C5D	-2.12	109.53	113.69
34	0	622	LMG	C8-O7-C10	-2.12	112.58	117.79
31	g	312	CLA	CMB-C2B-C3B	2.12	128.64	124.68
32	r	317	LUT	C38-C25-C24	-2.12	119.03	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	r	310	CHL	C1-O2A-CGA	2.12	122.00	116.44
38	y	621	SQD	O3-C3-C2	-2.12	105.46	110.35
31	5	604	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	C	601	CLA	C1D-ND-C4D	-2.12	104.83	106.33
31	3	312	CLA	O2A-CGA-CBA	2.12	118.55	111.91
32	y	617	LUT	C38-C25-C24	-2.12	119.03	123.56
43	C	614	BCR	C29-C28-C27	2.12	116.10	111.38
30	G	606	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
30	n	306	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	n	311	CLA	CHA-C1A-NA	-2.12	121.55	126.40
31	2	611	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
43	V	101	BCR	C21-C20-C19	-2.11	116.62	123.22
30	3	302	CHL	CMB-C2B-C1B	-2.11	125.21	128.46
30	q	307	CHL	CMB-C2B-C1B	-2.11	125.21	128.46
30	g	309	CHL	CMB-C2B-C1B	-2.11	125.21	128.46
30	8	605	CHL	CHC-C1C-NC	2.11	127.41	124.20
31	S	316	CLA	CMB-C2B-C3B	2.11	128.63	124.68
31	g	313	CLA	CMB-C2B-C3B	2.11	128.63	124.68
31	b	603	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
31	c	607	CLA	CMD-C2D-C3D	-2.11	122.75	127.61
30	7	302	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
30	9	308	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
30	y	601	CHL	CHD-C4C-C3C	2.11	127.95	124.84
30	R	308	CHL	CMA-C3A-C2A	2.11	122.35	113.83
31	3	311	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
31	S	303	CLA	CMB-C2B-C3B	2.11	128.63	124.68
31	s	306	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
32	7	317	LUT	C31-C30-C29	-2.11	124.29	127.31
31	S	304	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
31	6	311	CLA	O2A-CGA-CBA	2.11	118.54	111.91
31	R	313	CLA	CHA-C1A-NA	-2.11	121.56	126.40
31	q	305	CLA	CHA-C1A-NA	-2.11	121.56	126.40
31	A	407	CLA	C1D-ND-C4D	-2.11	104.83	106.33
30	8	607	CHL	CMA-C3A-C2A	2.11	122.35	113.83
31	r	312	CLA	C6-C5-C3	-2.11	107.92	113.45
30	y	607	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	p	603	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
30	3	307	CHL	CHB-C4A-NA	2.11	127.43	124.51
30	1	609	CHL	C2C-C3C-C4C	2.11	107.99	106.49
30	R	308	CHL	C2C-C3C-C4C	2.11	107.99	106.49
30	S	309	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	8	612	CLA	CHA-C1A-NA	-2.11	121.56	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	p	602	CLA	CMB-C2B-C3B	2.11	128.63	124.68
30	2	607	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
30	Y	309	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
32	8	615	LUT	C10-C11-C12	-2.11	116.63	123.22
30	R	308	CHL	CHD-C4C-C3C	2.11	127.94	124.84
32	S	317	LUT	C20-C13-C12	2.11	121.40	118.08
31	G	609	CLA	CMD-C2D-C3D	-2.11	122.76	127.61
30	Y	306	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	2	603	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	R	314	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	A	405	CLA	CMA-C3A-C4A	2.11	117.44	111.77
31	0	611	CLA	CHA-C1A-NA	-2.11	121.57	126.40
30	7	310	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	b	617	CLA	CMA-C3A-C4A	2.11	117.44	111.77
30	0	608	CHL	CMA-C3A-C2A	2.11	122.34	113.83
32	4	616	LUT	C11-C12-C13	-2.11	120.49	126.42
31	r	314	CLA	O2A-CGA-CBA	2.11	118.53	111.91
31	p	610	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
31	9	315	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	7	313	CLA	C6-C5-C3	-2.11	107.93	113.45
31	y	604	CLA	CMB-C2B-C3B	2.11	128.62	124.68
36	R	319	NEX	C16-C1-C6	-2.11	108.58	110.47
31	S	311	CLA	CHA-C1A-NA	-2.11	121.57	126.40
36	2	616	NEX	C40-C33-C34	-2.11	119.97	122.92
30	8	601	CHL	CHB-C4A-NA	2.11	127.43	124.51
31	B	606	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
31	S	316	CLA	CBC-CAC-C3C	-2.11	106.62	112.43
32	y	617	LUT	C19-C9-C8	2.11	121.40	118.08
31	g	310	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
30	9	303	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	6	313	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
43	B	617	BCR	C33-C5-C4	2.11	117.66	113.62
31	r	304	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
30	p	605	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
30	g	306	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
34	m	102	LMG	C8-O7-C10	-2.11	112.61	117.79
30	Y	306	CHL	C4A-NA-C1A	2.11	107.65	106.71
30	q	310	CHL	CMA-C3A-C2A	2.11	122.33	113.83
31	1	611	CLA	CHA-C1A-NA	-2.11	121.57	126.40
31	3	304	CLA	CHA-C1A-NA	-2.11	121.57	126.40
30	S	308	CHL	CHD-C4C-C3C	2.11	127.94	124.84
30	3	303	CHL	CMB-C2B-C1B	-2.11	125.23	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	4	616	LUT	C15-C35-C34	-2.11	119.16	123.47
31	p	603	CLA	CHA-C1A-NA	-2.11	121.58	126.40
37	g	321	XAT	C40-C33-C34	-2.11	119.97	122.92
30	n	309	CHL	CHD-C4C-C3C	2.11	127.94	124.84
31	3	313	CLA	CHA-C1A-NA	-2.11	121.58	126.40
31	1	604	CLA	C1-O2A-CGA	2.11	121.97	116.44
31	B	602	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
43	T	101	BCR	C8-C7-C6	-2.10	121.29	127.20
31	Y	312	CLA	C1D-ND-C4D	-2.10	104.84	106.33
30	Y	308	CHL	C2C-C3C-C4C	2.10	107.99	106.49
31	6	312	CLA	CHA-C1A-NA	-2.10	121.58	126.40
30	R	308	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
30	p	607	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
36	8	617	NEX	C20-C13-C14	-2.10	119.98	122.92
30	8	605	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
30	s	308	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
31	5	612	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
30	p	601	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
36	y	618	NEX	C31-C30-C29	2.10	130.31	127.31
30	3	302	CHL	C3A-C2A-C1A	2.10	104.49	101.34
30	9	307	CHL	CHB-C4A-NA	2.10	127.42	124.51
30	4	605	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
30	6	302	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
43	a	410	BCR	C10-C11-C12	-2.10	116.66	123.22
31	S	311	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
37	9	322	XAT	C40-C33-C34	-2.10	119.98	122.92
43	Z	101	BCR	C15-C16-C17	-2.10	119.17	123.47
31	C	606	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	0	614	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	7	314	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	S	311	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
31	7	312	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	r	307	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	5	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	p	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	g	313	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	d	401	CLA	C1D-ND-C4D	-2.10	104.84	106.33
30	0	609	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
30	q	311	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
30	s	307	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
31	0	613	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
34	W	202	LMG	C8-O7-C10	-2.10	112.62	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	g	314	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	4	611	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
31	q	306	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
30	7	306	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
30	y	609	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
31	7	305	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	9	312	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
30	3	308	CHL	CHB-C4A-NA	2.10	127.42	124.51
31	2	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	4	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	s	311	CLA	CHA-C1A-NA	-2.10	121.59	126.40
30	n	306	CHL	CHC-C1C-NC	2.10	127.39	124.20
32	G	615	LUT	C11-C10-C9	-2.10	124.31	127.31
31	0	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	y	610	CLA	CHA-C1A-NA	-2.10	121.59	126.40
30	5	607	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
31	1	602	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
31	p	604	CLA	C1-O2A-CGA	2.10	121.95	116.44
30	5	605	CHL	CHD-C4C-C3C	2.10	127.92	124.84
31	5	613	CLA	CHA-C1A-NA	-2.10	121.59	126.40
31	y	603	CLA	CHA-C1A-NA	-2.10	121.59	126.40
37	q	321	XAT	C40-C33-C34	-2.10	119.98	122.92
31	c	606	CLA	C6-C7-C8	-2.10	109.14	115.92
30	3	308	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
30	q	303	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
31	7	314	CLA	C1-O2A-CGA	2.10	121.95	116.44
31	S	316	CLA	C1D-ND-C4D	-2.10	104.84	106.33
30	4	607	CHL	CHD-C1D-C2D	2.10	129.88	125.48
30	p	601	CHL	C2C-C3C-C4C	2.10	107.98	106.49
31	G	613	CLA	CAA-C2A-C3A	-2.10	107.03	112.78
30	4	607	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
31	G	611	CLA	CMB-C2B-C1B	-2.10	125.24	128.46
32	q	318	LUT	C19-C9-C10	-2.10	119.99	122.92
31	s	303	CLA	C11-C10-C8	-2.10	109.14	115.92
32	5	617	LUT	C21-C26-C27	-2.10	110.05	112.70
30	r	308	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
31	7	304	CLA	OBD-CAD-C3D	-2.10	123.48	128.52
30	Y	307	CHL	C2C-C3C-C4C	2.10	107.98	106.49
30	7	308	CHL	CHC-C1C-NC	2.10	127.38	124.20
32	r	317	LUT	C11-C10-C9	-2.10	124.32	127.31
31	n	303	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
30	2	601	CHL	CMB-C2B-C1B	-2.09	125.24	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	3	307	CHL	CMB-C2B-C1B	-2.09	125.24	128.46
30	N	307	CHL	CHB-C4A-NA	2.09	127.41	124.51
30	n	302	CHL	CHB-C4A-NA	2.09	127.41	124.51
31	a	407	CLA	C6-C5-C3	-2.09	107.96	113.45
34	G	621	LMG	C8-O7-C10	-2.09	112.63	117.79
36	g	317	NEX	C40-C33-C34	-2.09	119.99	122.92
30	N	301	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
30	y	608	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
31	g	310	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
36	3	319	NEX	O24-C25-C38	-2.09	112.55	115.06
37	4	619	XAT	C40-C33-C34	-2.09	119.99	122.92
31	C	602	CLA	CHA-C1A-NA	-2.09	121.60	126.40
30	y	609	CHL	C3A-C2A-C1A	2.09	104.47	101.34
30	1	601	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
30	y	606	CHL	C1-C2-C3	-2.09	122.42	126.04
31	s	313	CLA	CMA-C3A-C4A	2.09	117.40	111.77
32	6	317	LUT	C38-C25-C24	-2.09	119.08	123.56
30	1	607	CHL	CHB-C4A-NA	2.09	127.41	124.51
35	g	315	RRX	C19-C18-C17	2.09	122.15	118.94
31	3	314	CLA	CHA-C1A-NA	-2.09	121.61	126.40
30	G	623	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
31	n	311	CLA	O1D-CGD-CBD	-2.09	120.20	124.48
31	9	314	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
30	7	321	CHL	C1-O2A-CGA	2.09	121.93	116.44
31	C	607	CLA	CHA-C1A-NA	-2.09	121.61	126.40
30	0	607	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
36	5	618	NEX	O24-C25-C38	-2.09	112.55	115.06
30	Y	307	CHL	CHB-C4A-NA	2.09	127.40	124.51
31	0	615	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	c	607	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
33	A	415	LHG	O8-C23-O10	-2.09	118.31	123.59
32	p	617	LUT	C19-C9-C10	-2.09	119.99	122.92
30	Y	302	CHL	C4A-NA-C1A	2.09	107.65	106.71
31	7	303	CLA	CHA-C1A-NA	-2.09	121.61	126.40
36	N	318	NEX	C15-C14-C13	-2.09	124.33	127.31
30	4	607	CHL	CHC-C1C-NC	2.09	127.37	124.20
31	2	604	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	c	609	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
36	r	319	NEX	C19-C9-C10	-2.09	120.00	122.92
31	c	607	CLA	CMA-C3A-C4A	2.09	117.39	111.77
30	9	310	CHL	CHC-C1C-NC	2.09	127.37	124.20
30	G	607	CHL	CMA-C3A-C2A	2.09	122.26	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	3	301	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
34	p	620	LMG	C7-O1-C1	-2.09	109.66	113.74
30	g	308	CHL	CMA-C3A-C2A	2.09	122.25	113.83
36	8	617	NEX	C2-C1-C6	2.09	111.24	109.21
43	c	614	BCR	C8-C7-C6	-2.09	121.34	127.20
47	E	101	HEM	CHA-C4D-C3D	-2.09	121.41	125.33
30	r	308	CHL	CHD-C4C-C3C	2.09	127.91	124.84
31	6	304	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
31	q	313	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
43	v	101	BCR	C35-C13-C12	2.09	121.37	118.08
32	6	318	LUT	C30-C31-C32	-2.09	116.70	123.22
30	p	609	CHL	CHD-C4C-C3C	2.09	127.91	124.84
31	b	605	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
34	q	301	LMG	O6-C5-C6	2.09	111.63	106.44
31	p	614	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
31	A	407	CLA	CMB-C2B-C1B	-2.09	125.26	128.46
31	Y	310	CLA	CHA-C1A-NA	-2.09	121.62	126.40
31	r	314	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
34	D	410	LMG	C8-O7-C10	-2.09	112.65	117.79
31	S	306	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	0	603	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
31	0	613	CLA	CHA-C1A-NA	-2.09	121.62	126.40
45	C	620	DGD	O2G-C1B-O1B	-2.09	118.66	123.70
31	C	602	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
30	n	308	CHL	CMA-C3A-C2A	2.09	122.24	113.83
31	g	314	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
31	C	611	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
31	A	405	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
30	0	607	CHL	CHB-C4A-NA	2.08	127.39	124.51
36	s	319	NEX	C2-C1-C6	2.08	111.24	109.21
31	6	311	CLA	CMB-C2B-C3B	2.08	128.58	124.68
31	0	602	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
30	4	609	CHL	C4A-NA-C1A	2.08	107.64	106.71
31	1	611	CLA	CAA-C2A-C3A	-2.08	107.07	112.78
31	C	607	CLA	C6-C7-C8	-2.08	109.18	115.92
30	2	608	CHL	CMB-C2B-C1B	-2.08	125.26	128.46
31	N	305	CLA	O2A-CGA-CBA	2.08	118.45	111.91
31	8	602	CLA	C6-C5-C3	-2.08	107.99	113.45
31	6	315	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	y	604	CLA	O2A-CGA-CBA	2.08	118.44	111.91
30	6	306	CHL	CHD-C4C-C3C	2.08	127.90	124.84
43	V	101	BCR	C35-C13-C12	2.08	121.36	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	n	305	CLA	O2A-CGA-CBA	2.08	118.44	111.91
31	9	306	CLA	CMB-C2B-C3B	2.08	128.57	124.68
31	1	604	CLA	CHA-C1A-NA	-2.08	121.63	126.40
30	7	307	CHL	CHB-C4A-NA	2.08	127.39	124.51
31	2	612	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
31	C	608	CLA	O2A-CGA-CBA	2.08	118.44	111.91
30	7	321	CHL	CMA-C3A-C2A	2.08	122.23	113.83
31	B	613	CLA	CMB-C2B-C3B	2.08	128.57	124.68
32	6	318	LUT	C8-C7-C6	-2.08	121.36	127.20
30	6	310	CHL	C1-O2A-CGA	2.08	121.91	116.44
30	4	601	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
30	4	605	CHL	CHD-C4C-C3C	2.08	127.90	124.84
30	G	601	CHL	CHD-C4C-C3C	2.08	127.90	124.84
30	N	301	CHL	CHD-C4C-C3C	2.08	127.90	124.84
30	6	306	CHL	C3A-C2A-C1A	2.08	104.46	101.34
36	S	319	NEX	C19-C9-C10	-2.08	120.01	122.92
45	c	617	DGD	C6D-O5D-C1E	2.08	117.80	113.74
31	6	305	CLA	CMB-C2B-C3B	2.08	128.57	124.68
30	0	608	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
31	0	602	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	0	612	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
31	G	611	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
31	B	615	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	C	609	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	S	314	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	7	311	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	d	401	CLA	C1-O2A-CGA	2.08	121.90	116.44
31	8	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40
34	j	101	LMG	C8-O7-C10	-2.08	112.67	117.79
36	R	301	NEX	O24-C25-C38	-2.08	112.57	115.06
31	B	603	CLA	C1-C2-C3	-2.08	122.45	126.04
30	y	601	CHL	CMA-C3A-C2A	2.08	122.21	113.83
31	p	610	CLA	O2D-CGD-O1D	-2.08	119.78	123.84
31	r	313	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	3	306	CLA	OBD-CAD-C3D	-2.08	123.52	128.52
31	p	610	CLA	C6-C5-C3	-2.08	108.01	113.45
30	n	308	CHL	C1-O2A-CGA	2.08	121.89	116.44
31	6	305	CLA	O2A-CGA-CBA	2.08	118.43	111.91
31	9	316	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	d	401	CLA	O2A-CGA-CBA	2.08	118.42	111.91
31	b	613	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
31	p	610	CLA	CHA-C1A-NA	-2.08	121.64	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	N	317	LUT	C2-C3-C4	2.08	113.15	110.30
30	6	310	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
31	3	313	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
31	y	615	CLA	O2A-CGA-CBA	2.08	118.42	111.91
31	9	304	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	C	607	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
32	Y	315	LUT	C19-C9-C8	2.08	121.35	118.08
31	n	316	CLA	CMB-C2B-C3B	2.08	128.56	124.68
31	N	315	CLA	CHA-C1A-NA	-2.08	121.64	126.40
31	S	310	CLA	CHA-C1A-NA	-2.08	121.64	126.40
30	p	608	CHL	CHC-C1C-NC	2.07	127.35	124.20
31	S	313	CLA	O2A-CGA-CBA	2.07	118.42	111.91
44	A	416	PL9	O2-C1-C6	2.07	124.18	120.59
30	8	607	CHL	CHB-C4A-NA	2.07	127.38	124.51
31	N	304	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	b	607	CLA	C1D-ND-C4D	-2.07	104.86	106.33
31	8	613	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
34	g	320	LMG	O7-C10-O9	-2.07	118.69	123.70
38	A	411	SQD	O8-S-C6	-2.07	102.44	105.74
31	b	606	CLA	CMB-C2B-C3B	2.07	128.56	124.68
31	g	311	CLA	C2A-C1A-CHA	2.07	127.48	123.86
30	6	308	CHL	C4A-NA-C1A	2.07	107.64	106.71
31	5	614	CLA	CHA-C1A-NA	-2.07	121.65	126.40
31	B	604	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
31	B	602	CLA	O2A-CGA-CBA	2.07	118.41	111.91
37	R	318	XAT	C19-C9-C10	-2.07	120.02	122.92
30	g	302	CHL	CHD-C4C-C3C	2.07	127.88	124.84
31	6	311	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	6	313	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	S	313	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
31	p	602	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
33	b	628	LHG	C5-O7-C7	-2.07	112.69	117.79
30	9	308	CHL	C2C-C3C-C4C	2.07	107.97	106.49
31	s	303	CLA	CMB-C2B-C3B	2.07	128.55	124.68
31	b	611	CLA	CHA-C1A-NA	-2.07	121.66	126.40
30	S	308	CHL	CMA-C3A-C2A	2.07	122.18	113.83
30	9	309	CHL	C1-C2-C3	-2.07	122.46	126.04
31	S	315	CLA	CHA-C1A-NA	-2.07	121.66	126.40
31	9	305	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
31	G	609	CLA	C1D-ND-C4D	-2.07	104.86	106.33
31	3	306	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
30	5	609	CHL	C1-C2-C3	-2.07	122.47	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	611	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
31	q	306	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
31	R	303	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
30	q	307	CHL	CHB-C4A-NA	2.07	127.37	124.51
30	3	307	CHL	CMA-C3A-C2A	2.07	122.17	113.83
43	z	101	BCR	C38-C26-C27	2.07	117.59	113.62
34	c	621	LMG	O8-C28-O10	-2.07	118.37	123.59
31	S	311	CLA	C1D-ND-C4D	-2.07	104.87	106.33
31	y	613	CLA	C1D-ND-C4D	-2.07	104.87	106.33
31	c	607	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
31	n	303	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
31	A	407	CLA	C1-O2A-CGA	2.07	121.87	116.44
31	r	313	CLA	C1-O2A-CGA	2.07	121.87	116.44
30	Y	308	CHL	CHD-C4C-C3C	2.07	127.88	124.84
30	g	307	CHL	CHB-C4A-NA	2.07	127.37	124.51
34	d	411	LMG	O7-C10-O9	-2.07	118.71	123.70
31	y	604	CLA	CMA-C3A-C4A	2.07	117.33	111.77
31	g	304	CLA	CHA-C1A-NA	-2.07	121.67	126.40
36	0	618	NEX	C4-C3-C2	2.07	114.76	110.77
32	3	318	LUT	C30-C31-C32	-2.07	116.77	123.22
32	y	616	LUT	C40-C33-C32	2.07	121.33	118.08
31	B	609	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	Y	314	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	B	609	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
30	q	307	CHL	CMA-C3A-C2A	2.07	122.16	113.83
38	B	623	SQD	O8-S-C6	-2.07	102.45	105.74
31	b	612	CLA	CMB-C2B-C3B	2.07	128.54	124.68
31	5	604	CLA	O2A-CGA-CBA	2.07	118.39	111.91
31	7	312	CLA	O2A-CGA-CBA	2.07	118.39	111.91
31	s	314	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
37	2	619	XAT	C40-C33-C34	-2.07	120.03	122.92
43	H	101	BCR	C34-C9-C10	-2.07	120.03	122.92
43	Z	101	BCR	C8-C7-C6	-2.07	121.40	127.20
30	S	307	CHL	CHB-C4A-NA	2.06	127.37	124.51
34	6	322	LMG	C8-O7-C10	-2.06	112.71	117.79
37	2	619	XAT	C19-C9-C10	-2.06	120.03	122.92
30	9	309	CHL	CMA-C3A-C2A	2.06	122.15	113.83
31	1	602	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	g	310	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	c	611	CLA	CHA-C1A-NA	-2.06	121.67	126.40
31	1	602	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
31	C	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	0	610	CLA	O2D-CGD-O1D	-2.06	119.80	123.84
31	b	606	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
44	a	414	PL9	C20-C19-C21	2.06	118.74	115.27
31	0	610	CLA	CHA-C1A-NA	-2.06	121.67	126.40
30	5	601	CHL	CMB-C2B-C1B	-2.06	125.29	128.46
36	6	319	NEX	C4-C3-C2	2.06	114.76	110.77
30	p	606	CHL	CHB-C4A-NA	2.06	127.36	124.51
31	A	406	CLA	C1D-ND-C4D	-2.06	104.87	106.33
30	G	607	CHL	C4A-NA-C1A	2.06	107.63	106.71
31	A	406	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	C	608	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	r	315	CLA	CAA-C2A-C1A	-2.06	105.22	111.97
31	y	612	CLA	C1-O2A-CGA	2.06	121.85	116.44
31	s	303	CLA	O2A-CGA-CBA	2.06	118.38	111.91
30	G	623	CHL	CHC-C1C-NC	2.06	127.33	124.20
44	a	414	PL9	O2-C1-C2	-2.06	117.06	121.78
31	6	314	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	c	601	CLA	C1D-ND-C4D	-2.06	104.87	106.33
31	q	315	CLA	O2D-CGD-O1D	-2.06	119.81	123.84
30	S	308	CHL	CMB-C2B-C1B	-2.06	125.30	128.46
31	B	605	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
31	N	315	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
30	p	605	CHL	CHB-C4A-NA	2.06	127.36	124.51
31	7	313	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	g	312	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	l	602	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
31	s	315	CLA	CMB-C2B-C3B	2.06	128.53	124.68
31	q	316	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
30	p	608	CHL	CHB-C4A-NA	2.06	127.36	124.51
31	b	604	CLA	CHA-C1A-NA	-2.06	121.68	126.40
31	R	306	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
31	4	614	CLA	C1-O2A-CGA	2.06	121.85	116.44
36	R	319	NEX	C2-C1-C6	2.06	111.21	109.21
36	9	319	NEX	C4-C3-C2	2.06	114.75	110.77
31	s	315	CLA	CHA-C1A-NA	-2.06	121.68	126.40
32	Y	316	LUT	C2-C3-C4	2.06	113.12	110.30
31	D	404	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
32	3	317	LUT	C30-C31-C32	-2.06	116.79	123.22
31	r	303	CLA	CHA-C1A-NA	-2.06	121.69	126.40
31	8	613	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
31	c	611	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
32	q	318	LUT	C2-C3-C4	2.06	113.12	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Y	303	CLA	CHA-C1A-NA	-2.06	121.69	126.40
31	C	604	CLA	C6-C7-C8	-2.06	109.27	115.92
34	D	409	LMG	C8-O7-C10	-2.06	112.73	117.79
31	g	310	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
31	l	610	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
31	Y	303	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
32	5	617	LUT	C20-C13-C14	-2.06	120.04	122.92
32	Y	316	LUT	C19-C9-C10	-2.06	120.04	122.92
30	n	307	CHL	CHB-C4A-NA	2.06	127.36	124.51
38	b	621	SQD	O8-S-C6	-2.06	102.46	105.74
33	C	623	LHG	O7-C7-O9	-2.06	118.73	123.70
30	9	303	CHL	CMA-C3A-C2A	2.06	122.12	113.83
32	y	616	LUT	C8-C9-C10	-2.06	115.79	118.94
31	3	301	CLA	CHA-C1A-NA	-2.06	121.69	126.40
31	c	611	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	6	311	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
31	B	615	CLA	CMA-C3A-C4A	2.05	117.29	111.77
31	g	303	CLA	CMB-C2B-C3B	2.05	128.52	124.68
31	g	310	CLA	CHA-C1A-NA	-2.05	121.69	126.40
30	y	607	CHL	CHC-C1C-NC	2.05	127.32	124.20
31	s	316	CLA	CBC-CAC-C3C	-2.05	106.77	112.43
31	s	303	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
31	B	614	CLA	CHA-C1A-NA	-2.05	121.69	126.40
31	3	301	CLA	O2A-CGA-CBA	2.05	118.35	111.91
31	7	312	CLA	CHA-C1A-NA	-2.05	121.70	126.40
30	r	308	CHL	C1-O2A-CGA	2.05	121.83	116.44
31	n	303	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	n	312	CLA	O2A-CGA-CBA	2.05	118.35	111.91
30	9	308	CHL	CHD-C4C-C3C	2.05	127.86	124.84
44	a	414	PL9	C32-C33-C34	-2.05	122.72	127.66
38	x	201	SQD	O3-C3-C2	-2.05	105.60	110.35
31	c	609	CLA	C16-C15-C13	-2.05	109.28	115.92
32	n	317	LUT	C15-C35-C34	-2.05	119.27	123.47
31	N	303	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	8	603	CLA	CHA-C1A-NA	-2.05	121.70	126.40
43	B	617	BCR	C30-C25-C26	-2.05	119.72	122.61
31	R	305	CLA	CMD-C2D-C3D	-2.05	122.89	127.61
31	2	611	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	b	617	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	8	610	CLA	O2A-CGA-CBA	2.05	118.35	111.91
31	s	305	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	1	612	CLA	O1D-CGD-CBD	-2.05	120.29	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	3	315	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	0	613	CLA	C1D-ND-C4D	-2.05	104.88	106.33
31	p	612	CLA	CHA-C1A-NA	-2.05	121.70	126.40
32	Y	315	LUT	C28-C29-C30	-2.05	115.79	118.94
30	6	310	CHL	CHD-C4C-C3C	2.05	127.85	124.84
30	Y	306	CHL	C3A-C2A-C1A	2.05	104.41	101.34
31	b	612	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
30	9	308	CHL	CHB-C4A-NA	2.05	127.35	124.51
32	1	616	LUT	C20-C13-C12	2.05	121.31	118.08
35	q	317	RRX	C38-C26-C27	2.05	118.15	114.36
30	Y	306	CHL	CHC-C1C-NC	2.05	127.31	124.20
31	n	315	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
31	r	314	CLA	CHA-C1A-NA	-2.05	121.70	126.40
31	3	312	CLA	C1D-ND-C4D	-2.05	104.88	106.33
30	G	607	CHL	C2C-C3C-C4C	2.05	107.95	106.49
31	N	311	CLA	CMD-C2D-C3D	-2.05	122.90	127.61
31	5	610	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	S	315	CLA	CMB-C2B-C3B	2.05	128.51	124.68
31	Y	312	CLA	C6-C5-C3	-2.05	108.08	113.45
30	8	605	CHL	C4A-NA-C1A	2.05	107.63	106.71
43	c	614	BCR	C24-C25-C26	-2.05	116.50	121.46
31	5	602	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	b	615	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	y	602	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	y	610	CLA	CMB-C2B-C3B	2.05	128.51	124.68
32	6	317	LUT	C20-C13-C12	2.05	121.30	118.08
31	S	305	CLA	CHA-C1A-NA	-2.05	121.71	126.40
31	N	314	CLA	O2D-CGD-O1D	-2.05	119.83	123.84
32	3	317	LUT	C35-C15-C14	-2.05	119.28	123.47
31	R	311	CLA	CHA-C1A-NA	-2.05	121.71	126.40
30	7	310	CHL	C2C-C3C-C4C	2.05	107.95	106.49
31	y	603	CLA	CMB-C2B-C3B	2.05	128.51	124.68
30	6	302	CHL	CMA-C3A-C2A	2.05	122.08	113.83
31	9	306	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
31	G	603	CLA	CHA-C1A-NA	-2.05	121.71	126.40
30	0	606	CHL	CHC-C1C-NC	2.05	127.31	124.20
31	1	614	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	c	610	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
30	R	308	CHL	CHB-C4A-NA	2.05	127.34	124.51
31	c	603	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
44	A	416	PL9	O2-C1-C2	-2.05	117.09	121.78
31	B	611	CLA	CHA-C1A-NA	-2.05	121.71	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	N	321	CLA	CHA-C1A-NA	-2.04	121.72	126.40
31	a	407	CLA	CHA-C1A-NA	-2.04	121.72	126.40
44	a	414	PL9	C7-C8-C9	-2.04	123.39	126.79
34	G	622	LMG	C8-O7-C10	-2.04	112.76	117.79
31	S	313	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
31	c	613	CLA	C1-C2-C3	-2.04	122.51	126.04
31	n	305	CLA	CMB-C2B-C3B	2.04	128.50	124.68
31	0	610	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
30	2	605	CHL	CMA-C3A-C2A	2.04	122.07	113.83
34	2	621	LMG	C9-C8-C7	-2.04	106.95	111.79
31	3	314	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
31	6	315	CLA	CMB-C2B-C3B	2.04	128.50	124.68
30	1	619	CHL	C3A-C2A-C1A	2.04	104.40	101.34
31	Y	312	CLA	CMA-C3A-C4A	2.04	117.26	111.77
31	B	605	CLA	C1D-ND-C4D	-2.04	104.88	106.33
31	r	311	CLA	C1D-ND-C4D	-2.04	104.88	106.33
32	s	318	LUT	C39-C29-C28	2.04	121.30	118.08
31	s	314	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
31	1	610	CLA	CHA-C1A-NA	-2.04	121.72	126.40
31	C	612	CLA	CHA-C1A-NA	-2.04	121.72	126.40
30	n	307	CHL	CMA-C3A-C2A	2.04	122.06	113.83
31	g	310	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	Y	313	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
31	7	314	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
32	8	615	LUT	C15-C35-C34	-2.04	119.29	123.47
32	9	318	LUT	C19-C9-C10	-2.04	120.06	122.92
36	r	319	NEX	C40-C33-C34	-2.04	120.06	122.92
30	Y	307	CHL	CHD-C4C-C3C	2.04	127.84	124.84
31	S	313	CLA	CHA-C1A-NA	-2.04	121.72	126.40
31	R	313	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	c	601	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
30	8	608	CHL	CHB-C4A-NA	2.04	127.33	124.51
32	s	318	LUT	C20-C13-C12	2.04	121.29	118.08
31	n	316	CLA	CHA-C1A-NA	-2.04	121.72	126.40
32	y	617	LUT	C1-C6-C5	-2.04	119.74	122.61
31	y	615	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	1	613	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	Y	312	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	r	307	CLA	O2A-CGA-CBA	2.04	118.31	111.91
32	8	616	LUT	C38-C25-C24	-2.04	119.19	123.56
31	c	611	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
31	2	611	CLA	CMB-C2B-C3B	2.04	128.49	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	4	617	NEX	C19-C9-C10	-2.04	120.07	122.92
31	4	613	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
32	5	616	LUT	C35-C15-C14	-2.04	119.30	123.47
32	n	318	LUT	C38-C25-C24	-2.04	119.20	123.56
43	B	617	BCR	C37-C22-C23	2.04	121.29	118.08
31	9	315	CLA	O2A-CGA-CBA	2.04	118.31	111.91
31	y	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B	616	CLA	CHA-C1A-NA	-2.04	121.73	126.40
37	R	318	XAT	C20-C13-C14	-2.04	120.07	122.92
31	r	315	CLA	CAA-C2A-C3A	-2.04	107.20	112.78
31	b	610	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	G	609	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	1	613	CLA	CMB-C2B-C3B	2.04	128.49	124.68
31	p	603	CLA	CMB-C2B-C3B	2.04	128.49	124.68
31	b	612	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	4	602	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	0	612	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	0	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B	601	CLA	C1D-ND-C4D	-2.04	104.89	106.33
37	G	620	XAT	C19-C9-C10	-2.04	120.07	122.92
31	6	303	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	R	314	CLA	C1-O2A-CGA	2.04	121.79	116.44
30	5	606	CHL	CHB-C4A-NA	2.04	127.33	124.51
31	4	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	A	407	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	0	614	CLA	CMB-C2B-C3B	2.04	128.49	124.68
31	N	310	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	6	303	CLA	C6-C5-C3	-2.04	108.12	113.45
31	3	305	CLA	O2A-CGA-CBA	2.04	118.30	111.91
31	2	609	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B	601	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	7	313	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B	601	CLA	CHA-C1A-NA	-2.04	121.74	126.40
30	8	606	CHL	CMA-C3A-C2A	2.04	122.04	113.83
31	p	614	CLA	CHA-C1A-NA	-2.04	121.74	126.40
31	8	604	CLA	O2A-CGA-CBA	2.04	118.29	111.91
31	7	311	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
36	y	618	NEX	C4-C3-C2	2.04	114.70	110.77
31	4	610	CLA	C6-C5-C3	-2.03	108.12	113.45
44	a	414	PL9	C37-C38-C39	-2.03	122.76	127.66
36	g	317	NEX	C19-C9-C10	-2.03	120.07	122.92
31	0	602	CLA	CMB-C2B-C3B	2.03	128.48	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	8	609	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
32	s	317	LUT	C19-C9-C8	2.03	121.28	118.08
31	y	602	CLA	CMB-C2B-C3B	2.03	128.48	124.68
31	C	606	CLA	CHA-C1A-NA	-2.03	121.74	126.40
31	8	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
34	9	321	LMG	O8-C28-O10	-2.03	118.46	123.59
30	n	301	CHL	CMA-C3A-C2A	2.03	122.03	113.83
31	b	605	CLA	C2A-C1A-CHA	2.03	127.41	123.86
31	c	603	CLA	CHA-C1A-NA	-2.03	121.74	126.40
31	r	312	CLA	CMA-C3A-C4A	2.03	117.24	111.77
30	8	606	CHL	CHB-C4A-NA	2.03	127.32	124.51
31	0	612	CLA	C1D-ND-C4D	-2.03	104.89	106.33
31	c	608	CLA	C1D-ND-C4D	-2.03	104.89	106.33
31	p	611	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
45	C	617	DGD	O1G-C1A-O1A	-2.03	118.46	123.59
37	R	318	XAT	C24-C23-C22	-2.03	106.85	110.77
31	8	604	CLA	CMB-C2B-C3B	2.03	128.48	124.68
31	C	613	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	R	306	CLA	O2A-CGA-CBA	2.03	118.28	111.91
32	Y	316	LUT	C15-C35-C34	-2.03	119.31	123.47
31	N	311	CLA	CHA-C1A-NA	-2.03	121.75	126.40
33	g	319	LHG	O8-C23-O10	-2.03	118.47	123.59
37	4	619	XAT	C19-C9-C10	-2.03	120.08	122.92
32	Y	316	LUT	C39-C29-C28	2.03	121.28	118.08
31	b	614	CLA	CHA-C1A-NA	-2.03	121.75	126.40
31	n	304	CLA	CHA-C1A-NA	-2.03	121.75	126.40
31	C	609	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
31	Y	310	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
30	g	307	CHL	CHC-C1C-NC	2.03	127.28	124.20
38	a	412	SQD	O8-S-C6	-2.03	102.50	105.74
31	s	304	CLA	CAA-C2A-C3A	-2.03	109.19	114.26
31	c	605	CLA	C6-C5-C3	-2.03	108.13	113.45
30	q	310	CHL	CHB-C4A-NA	2.03	127.32	124.51
31	c	612	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	n	315	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
36	N	318	NEX	C19-C9-C10	-2.03	120.08	122.92
43	b	619	BCR	C10-C11-C12	-2.03	116.88	123.22
32	y	616	LUT	C12-C13-C14	-2.03	115.83	118.94
34	k	101	LMG	O8-C28-O10	-2.03	118.47	123.59
31	N	314	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	R	307	CLA	O2A-CGA-CBA	2.03	118.28	111.91
36	8	617	NEX	O24-C25-C38	-2.03	112.62	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	g	321	XAT	C19-C9-C10	-2.03	120.08	122.92
31	y	613	CLA	C6-C7-C8	-2.03	109.36	115.92
30	y	606	CHL	CHD-C4C-C3C	2.03	127.82	124.84
31	N	312	CLA	CHA-C1A-NA	-2.03	121.75	126.40
48	c	623	LMU	O5B-C1B-C2B	2.03	114.64	110.35
31	7	315	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
36	9	319	NEX	C19-C9-C10	-2.03	120.08	122.92
31	c	608	CLA	C1-O2A-CGA	2.03	121.76	116.44
31	b	604	CLA	C2D-C1D-ND	2.03	111.60	110.10
31	G	611	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
31	r	304	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	R	316	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
32	0	617	LUT	C38-C25-C24	-2.03	119.22	123.56
31	R	304	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
32	n	317	LUT	C20-C13-C12	2.03	121.27	118.08
34	c	620	LMG	O8-C28-O10	-2.03	118.48	123.59
30	1	607	CHL	CMA-C3A-C2A	2.03	122.00	113.83
31	6	316	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
31	B	607	CLA	C1D-ND-C4D	-2.03	104.90	106.33
31	B	610	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	a	406	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
32	N	317	LUT	C30-C31-C32	-2.03	116.90	123.22
34	d	410	LMG	O8-C28-O10	-2.03	118.48	123.59
31	C	613	CLA	C2A-C1A-CHA	2.03	127.40	123.86
34	2	621	LMG	O7-C10-O9	-2.03	118.81	123.70
34	w	204	LMG	O7-C10-O9	-2.03	118.81	123.70
36	r	301	NEX	C31-C30-C29	2.02	130.20	127.31
31	q	312	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
31	B	610	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
31	A	405	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	5	610	CLA	O2D-CGD-O1D	-2.02	119.88	123.84
30	7	302	CHL	C2C-C3C-C4C	2.02	107.93	106.49
31	b	613	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	5	611	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	y	604	CLA	CHA-C1A-NA	-2.02	121.76	126.40
37	9	322	XAT	C19-C9-C10	-2.02	120.09	122.92
36	g	317	NEX	C31-C30-C29	2.02	130.20	127.31
31	4	614	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	S	312	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	G	602	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
31	c	604	CLA	O2A-CGA-CBA	2.02	118.26	111.91
34	J	101	LMG	C8-O7-C10	-2.02	112.81	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	604	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	B	606	CLA	CMB-C2B-C3B	2.02	128.46	124.68
31	b	613	CLA	CMB-C2B-C3B	2.02	128.46	124.68
31	c	609	CLA	C11-C10-C8	-2.02	109.38	115.92
31	s	313	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	S	311	CLA	C6-C5-C3	-2.02	108.15	113.45
34	b	624	LMG	O6-C5-C4	2.02	113.37	109.69
31	S	311	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
36	S	319	NEX	C20-C13-C14	-2.02	120.09	122.92
34	B	625	LMG	O8-C28-O10	-2.02	118.49	123.59
31	2	612	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	7	311	CLA	CMB-C2B-C3B	2.02	128.46	124.68
31	4	614	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
31	y	614	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
31	7	303	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
43	B	619	BCR	C29-C30-C25	2.02	113.59	110.48
44	a	414	PL9	O1-C4-C3	-2.02	118.49	120.72
30	2	607	CHL	CHD-C4C-C3C	2.02	127.81	124.84
31	S	304	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	1	603	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
31	R	305	CLA	C2D-C1D-ND	2.02	111.59	110.10
31	0	613	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
32	8	615	LUT	C20-C13-C12	2.02	121.26	118.08
30	s	307	CHL	C2C-C3C-C4C	2.02	107.93	106.49
31	Y	305	CLA	CHA-C1A-NA	-2.02	121.77	126.40
31	R	312	CLA	CAA-CBA-CGA	-2.02	107.35	113.25
31	c	604	CLA	C1-O2A-CGA	2.02	121.74	116.44
38	x	201	SQD	O5-C1-O6	-2.02	105.19	109.97
31	2	612	CLA	C1-O2A-CGA	2.02	121.74	116.44
30	4	601	CHL	CHD-C4C-C3C	2.02	127.81	124.84
30	R	310	CHL	C3A-C2A-C1A	2.02	104.36	101.34
30	R	310	CHL	CHC-C1C-NC	2.02	127.27	124.20
32	4	616	LUT	C20-C13-C14	-2.02	120.09	122.92
31	c	613	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	N	310	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
31	q	315	CLA	C11-C10-C8	-2.02	109.39	115.92
30	6	308	CHL	CMA-C3A-C2A	2.02	121.97	113.83
36	n	319	NEX	C11-C12-C13	2.02	132.09	126.42
30	N	302	CHL	CHB-C4A-NA	2.02	127.30	124.51
43	C	614	BCR	C33-C5-C4	2.02	117.49	113.62
31	9	305	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	1	603	CLA	CHA-C1A-NA	-2.02	121.78	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	G	605	CHL	C4A-NA-C1A	2.02	107.61	106.71
31	R	315	CLA	C6-C5-C3	-2.02	108.17	113.45
31	3	304	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	r	316	CLA	C1D-ND-C4D	-2.02	104.90	106.33
31	y	604	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
31	4	604	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	304	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
43	d	406	BCR	C21-C20-C19	-2.02	116.92	123.22
31	G	612	CLA	CHA-C1A-NA	-2.02	121.78	126.40
45	c	617	DGD	O5D-C6D-C5D	2.02	112.78	109.05
31	b	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	311	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	s	316	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	q	304	CLA	C6-C7-C8	-2.02	109.40	115.92
31	y	603	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
34	b	601	LMG	C9-C8-C7	-2.02	107.02	111.79
30	9	310	CHL	CHB-C4A-NA	2.02	127.30	124.51
31	5	612	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
31	r	304	CLA	C6-C7-C8	-2.01	109.41	115.92
32	Y	315	LUT	C18-C5-C4	2.01	118.09	114.36
32	y	616	LUT	C38-C25-C24	-2.01	119.25	123.56
31	Y	304	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
31	n	316	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
30	g	308	CHL	CHB-C4A-NA	2.01	127.30	124.51
34	7	322	LMG	O7-C10-O9	-2.01	118.83	123.70
31	C	603	CLA	CHA-C1A-NA	-2.01	121.79	126.40
31	R	314	CLA	CHA-C1A-NA	-2.01	121.79	126.40
30	G	606	CHL	CHD-C4C-C3C	2.01	127.80	124.84
31	R	316	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
30	3	309	CHL	CMA-C3A-C2A	2.01	121.95	113.83
31	1	613	CLA	O2A-CGA-CBA	2.01	118.23	111.91
30	5	608	CHL	CHB-C4A-NA	2.01	127.30	124.51
32	Y	315	LUT	C38-C25-C24	-2.01	119.25	123.56
43	v	101	BCR	C30-C25-C24	2.01	121.47	115.78
31	7	314	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
44	a	414	PL9	C31-C32-C33	-2.01	105.27	111.88
31	4	610	CLA	C6-C7-C8	-2.01	109.41	115.92
31	B	604	CLA	O2A-CGA-CBA	2.01	118.22	111.91
45	c	617	DGD	O2G-C1B-O1B	-2.01	118.84	123.70
31	2	609	CLA	C11-C10-C8	-2.01	109.41	115.92
43	d	406	BCR	C29-C30-C25	2.01	113.58	110.48
31	b	614	CLA	C3D-C2D-C1D	-2.01	103.08	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	9	308	CHL	CMA-C3A-C2A	2.01	121.94	113.83
32	8	615	LUT	C19-C9-C8	2.01	121.25	118.08
31	B	607	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
31	7	314	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
31	G	609	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
32	8	616	LUT	C35-C15-C14	-2.01	119.35	123.47
31	N	305	CLA	CMB-C2B-C3B	2.01	128.44	124.68
37	q	321	XAT	C19-C9-C10	-2.01	120.11	122.92
31	8	613	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	s	313	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	y	612	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
31	Y	311	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	N	303	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
31	S	303	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	8	610	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	q	314	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
31	9	312	CLA	CMB-C2B-C3B	2.01	128.44	124.68
31	0	604	CLA	C1D-ND-C4D	-2.01	104.91	106.33
31	7	304	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
30	S	309	CHL	C4A-NA-C1A	2.01	107.61	106.71
31	c	603	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
33	A	415	LHG	O7-C7-O9	-2.01	118.85	123.70
34	G	622	LMG	O7-C10-O9	-2.01	118.85	123.70
31	d	405	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
31	c	608	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	g	314	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
34	D	411	LMG	O8-C28-O10	-2.01	118.53	123.59
31	2	613	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	B	610	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	C	602	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	N	303	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
32	n	317	LUT	C19-C9-C8	2.01	121.24	118.08
31	8	610	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
31	s	310	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	C	611	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
31	S	314	CLA	CMD-C2D-C3D	-2.01	123.00	127.61
31	n	311	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
32	6	317	LUT	C19-C9-C8	2.01	121.24	118.08
38	x	201	SQD	O8-S-C6	-2.01	102.54	105.74
34	b	624	LMG	O6-C1-C2	-2.01	106.10	110.35
31	G	604	CLA	CMB-C2B-C3B	2.00	128.43	124.68
31	4	613	CLA	CHA-C1A-NA	-2.00	121.81	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	r	314	CLA	C1D-ND-C4D	-2.00	104.91	106.33
30	q	303	CHL	CMA-C3A-C2A	2.00	121.91	113.83
31	G	602	CLA	C1-O2A-CGA	2.00	121.70	116.44
31	n	312	CLA	CMD-C2D-C3D	-2.00	123.00	127.61
34	B	622	LMG	O7-C10-O9	-2.00	118.86	123.70
31	2	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	N	312	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
33	s	322	LHG	O7-C7-O9	-2.00	118.86	123.70
43	b	619	BCR	C35-C13-C14	-2.00	120.12	122.92
31	N	312	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
31	A	405	CLA	CMB-C2B-C1B	-2.00	125.39	128.46
36	2	616	NEX	C20-C13-C14	-2.00	120.12	122.92
31	3	313	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
31	y	602	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
38	s	301	SQD	O8-S-C6	-2.00	102.55	105.74
31	S	303	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
30	3	309	CHL	C1B-CHB-C4A	-2.00	126.15	130.12
31	8	602	CLA	CMB-C2B-C3B	2.00	128.42	124.68
31	c	606	CLA	CHA-C1A-NA	-2.00	121.81	126.40
31	y	611	CLA	CHA-C1A-NA	-2.00	121.81	126.40
31	C	613	CLA	C1D-ND-C4D	-2.00	104.91	106.33
33	D	408	LHG	O8-C23-O10	-2.00	118.54	123.59
31	1	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	2	603	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	9	316	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	C	601	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
31	C	609	CLA	CMA-C3A-C4A	2.00	117.15	111.77
31	Y	313	CLA	CHA-C1A-NA	-2.00	121.82	126.40
31	6	303	CLA	CMB-C2B-C3B	2.00	128.42	124.68
34	b	626	LMG	O8-C28-O10	-2.00	118.54	123.59
38	0	621	SQD	O8-S-C6	-2.00	102.55	105.74
32	s	317	LUT	C39-C29-C28	2.00	121.23	118.08
31	g	313	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
31	G	610	CLA	CAA-C2A-C3A	-2.00	107.30	112.78
34	D	410	LMG	O8-C28-O10	-2.00	118.54	123.59

All (636) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	1	601	CHL	NA
30	1	601	CHL	NC
30	1	601	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	1	605	CHL	NA
30	1	605	CHL	NC
30	1	605	CHL	ND
30	1	606	CHL	NA
30	1	606	CHL	NC
30	1	606	CHL	ND
30	1	607	CHL	NA
30	1	607	CHL	NC
30	1	607	CHL	ND
30	1	608	CHL	NA
30	1	608	CHL	NC
30	1	608	CHL	ND
30	1	609	CHL	NA
30	1	609	CHL	NC
30	1	609	CHL	ND
30	1	619	CHL	NA
30	1	619	CHL	NC
30	1	619	CHL	ND
30	2	601	CHL	NA
30	2	601	CHL	NC
30	2	601	CHL	ND
30	2	605	CHL	NA
30	2	605	CHL	NC
30	2	605	CHL	ND
30	2	606	CHL	NA
30	2	606	CHL	NC
30	2	606	CHL	ND
30	2	607	CHL	NA
30	2	607	CHL	NC
30	2	607	CHL	ND
30	2	608	CHL	NA
30	2	608	CHL	NC
30	2	608	CHL	ND
30	3	302	CHL	NA
30	3	302	CHL	NC
30	3	302	CHL	ND
30	3	303	CHL	NA
30	3	303	CHL	NC
30	3	303	CHL	ND
30	3	307	CHL	NA
30	3	307	CHL	NC
30	3	307	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	3	308	CHL	NA
30	3	308	CHL	NC
30	3	308	CHL	ND
30	3	309	CHL	NA
30	3	309	CHL	NC
30	3	309	CHL	ND
30	3	310	CHL	NA
30	3	310	CHL	NC
30	3	310	CHL	ND
30	4	601	CHL	NA
30	4	601	CHL	NC
30	4	601	CHL	ND
30	4	605	CHL	NA
30	4	605	CHL	NC
30	4	605	CHL	ND
30	4	606	CHL	NA
30	4	606	CHL	NC
30	4	606	CHL	ND
30	4	607	CHL	NA
30	4	607	CHL	NC
30	4	607	CHL	ND
30	4	608	CHL	NA
30	4	608	CHL	NC
30	4	608	CHL	ND
30	4	609	CHL	NA
30	4	609	CHL	NC
30	4	609	CHL	ND
30	5	601	CHL	NA
30	5	601	CHL	NC
30	5	601	CHL	ND
30	5	605	CHL	NA
30	5	605	CHL	NC
30	5	605	CHL	ND
30	5	606	CHL	NA
30	5	606	CHL	NC
30	5	606	CHL	ND
30	5	607	CHL	NA
30	5	607	CHL	NC
30	5	607	CHL	ND
30	5	608	CHL	NA
30	5	608	CHL	NC
30	5	608	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	5	609	CHL	NA
30	5	609	CHL	NC
30	5	609	CHL	ND
30	6	302	CHL	NA
30	6	302	CHL	NC
30	6	302	CHL	ND
30	6	306	CHL	NA
30	6	306	CHL	NC
30	6	306	CHL	ND
30	6	307	CHL	NA
30	6	307	CHL	NC
30	6	307	CHL	ND
30	6	308	CHL	NA
30	6	308	CHL	NC
30	6	308	CHL	ND
30	6	309	CHL	NA
30	6	309	CHL	NC
30	6	309	CHL	ND
30	6	310	CHL	NA
30	6	310	CHL	NC
30	6	310	CHL	ND
30	G	601	CHL	NA
30	G	601	CHL	NC
30	G	601	CHL	ND
30	G	605	CHL	NA
30	G	605	CHL	NC
30	G	605	CHL	ND
30	G	606	CHL	NA
30	G	606	CHL	NC
30	G	606	CHL	ND
30	G	607	CHL	NA
30	G	607	CHL	NC
30	G	607	CHL	ND
30	G	608	CHL	NA
30	G	608	CHL	NC
30	G	608	CHL	ND
30	G	623	CHL	NA
30	G	623	CHL	NC
30	G	623	CHL	ND
30	N	301	CHL	NA
30	N	301	CHL	NC
30	N	301	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	N	302	CHL	NA
30	N	302	CHL	NC
30	N	302	CHL	ND
30	N	306	CHL	NA
30	N	306	CHL	NC
30	N	306	CHL	ND
30	N	307	CHL	NA
30	N	307	CHL	NC
30	N	307	CHL	ND
30	N	308	CHL	NA
30	N	308	CHL	NC
30	N	308	CHL	ND
30	N	309	CHL	NA
30	N	309	CHL	NC
30	N	309	CHL	ND
30	R	308	CHL	NA
30	R	308	CHL	NC
30	R	308	CHL	ND
30	R	309	CHL	NA
30	R	309	CHL	NC
30	R	309	CHL	ND
30	R	310	CHL	NA
30	R	310	CHL	NC
30	R	310	CHL	ND
30	S	302	CHL	NA
30	S	302	CHL	NC
30	S	302	CHL	ND
30	S	307	CHL	NA
30	S	307	CHL	NC
30	S	307	CHL	ND
30	S	308	CHL	NA
30	S	308	CHL	NC
30	S	308	CHL	ND
30	S	309	CHL	NA
30	S	309	CHL	NC
30	S	309	CHL	ND
30	Y	301	CHL	NA
30	Y	301	CHL	NC
30	Y	301	CHL	ND
30	Y	302	CHL	NA
30	Y	302	CHL	NC
30	Y	302	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	Y	306	CHL	NA
30	Y	306	CHL	NC
30	Y	306	CHL	ND
30	Y	307	CHL	NA
30	Y	307	CHL	NC
30	Y	307	CHL	ND
30	Y	308	CHL	NA
30	Y	308	CHL	NC
30	Y	308	CHL	ND
30	Y	309	CHL	NA
30	Y	309	CHL	NC
30	Y	309	CHL	ND
30	0	601	CHL	NA
30	0	601	CHL	NC
30	0	601	CHL	ND
30	0	605	CHL	NA
30	0	605	CHL	NC
30	0	605	CHL	ND
30	0	606	CHL	NA
30	0	606	CHL	NC
30	0	606	CHL	ND
30	0	607	CHL	NA
30	0	607	CHL	NC
30	0	607	CHL	ND
30	0	608	CHL	NA
30	0	608	CHL	NC
30	0	608	CHL	ND
30	0	609	CHL	NA
30	0	609	CHL	NC
30	0	609	CHL	ND
30	7	302	CHL	NA
30	7	302	CHL	NC
30	7	302	CHL	ND
30	7	306	CHL	NA
30	7	306	CHL	NC
30	7	306	CHL	ND
30	7	307	CHL	NA
30	7	307	CHL	NC
30	7	307	CHL	ND
30	7	308	CHL	NA
30	7	308	CHL	NC
30	7	308	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	7	309	CHL	NA
30	7	309	CHL	NC
30	7	309	CHL	ND
30	7	310	CHL	NA
30	7	310	CHL	NC
30	7	310	CHL	ND
30	7	321	CHL	NA
30	7	321	CHL	NC
30	7	321	CHL	ND
30	8	601	CHL	NA
30	8	601	CHL	NC
30	8	601	CHL	ND
30	8	605	CHL	NA
30	8	605	CHL	NC
30	8	605	CHL	ND
30	8	606	CHL	NA
30	8	606	CHL	NC
30	8	606	CHL	ND
30	8	607	CHL	NA
30	8	607	CHL	NC
30	8	607	CHL	ND
30	8	608	CHL	NA
30	8	608	CHL	NC
30	8	608	CHL	ND
30	9	303	CHL	NA
30	9	303	CHL	NC
30	9	303	CHL	ND
30	9	307	CHL	NA
30	9	307	CHL	NC
30	9	307	CHL	ND
30	9	308	CHL	NA
30	9	308	CHL	NC
30	9	308	CHL	ND
30	9	309	CHL	NA
30	9	309	CHL	NC
30	9	309	CHL	ND
30	9	310	CHL	NA
30	9	310	CHL	NC
30	9	310	CHL	ND
30	9	311	CHL	NA
30	9	311	CHL	NC
30	9	311	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	p	601	CHL	NA
30	p	601	CHL	NC
30	p	601	CHL	ND
30	p	605	CHL	NA
30	p	605	CHL	NC
30	p	605	CHL	ND
30	p	606	CHL	NA
30	p	606	CHL	NC
30	p	606	CHL	ND
30	p	607	CHL	NA
30	p	607	CHL	NC
30	p	607	CHL	ND
30	p	608	CHL	NA
30	p	608	CHL	NC
30	p	608	CHL	ND
30	p	609	CHL	NA
30	p	609	CHL	NC
30	p	609	CHL	ND
30	q	303	CHL	NA
30	q	303	CHL	NC
30	q	303	CHL	ND
30	q	307	CHL	NA
30	q	307	CHL	NC
30	q	307	CHL	ND
30	q	308	CHL	NA
30	q	308	CHL	NC
30	q	308	CHL	ND
30	q	309	CHL	NA
30	q	309	CHL	NC
30	q	309	CHL	ND
30	q	310	CHL	NA
30	q	310	CHL	NC
30	q	310	CHL	ND
30	q	311	CHL	NA
30	q	311	CHL	NC
30	q	311	CHL	ND
30	g	302	CHL	NA
30	g	302	CHL	NC
30	g	302	CHL	ND
30	g	306	CHL	NA
30	g	306	CHL	NC
30	g	306	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	g	307	CHL	NA
30	g	307	CHL	NC
30	g	307	CHL	ND
30	g	308	CHL	NA
30	g	308	CHL	NC
30	g	308	CHL	ND
30	g	309	CHL	NA
30	g	309	CHL	NC
30	g	309	CHL	ND
30	n	301	CHL	NA
30	n	301	CHL	NC
30	n	301	CHL	ND
30	n	302	CHL	NA
30	n	302	CHL	NC
30	n	302	CHL	ND
30	n	306	CHL	NA
30	n	306	CHL	NC
30	n	306	CHL	ND
30	n	307	CHL	NA
30	n	307	CHL	NC
30	n	307	CHL	ND
30	n	308	CHL	NA
30	n	308	CHL	NC
30	n	308	CHL	ND
30	n	309	CHL	NA
30	n	309	CHL	NC
30	n	309	CHL	ND
30	n	310	CHL	NA
30	n	310	CHL	NC
30	n	310	CHL	ND
30	r	308	CHL	NA
30	r	308	CHL	NC
30	r	308	CHL	ND
30	r	309	CHL	NA
30	r	309	CHL	NC
30	r	309	CHL	ND
30	r	310	CHL	NA
30	r	310	CHL	NC
30	r	310	CHL	ND
30	s	302	CHL	NA
30	s	302	CHL	NC
30	s	302	CHL	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
30	s	307	CHL	NA
30	s	307	CHL	NC
30	s	307	CHL	ND
30	s	308	CHL	NA
30	s	308	CHL	NC
30	s	308	CHL	ND
30	s	309	CHL	NA
30	s	309	CHL	NC
30	s	309	CHL	ND
30	y	601	CHL	NA
30	y	601	CHL	NC
30	y	601	CHL	ND
30	y	605	CHL	NA
30	y	605	CHL	NC
30	y	605	CHL	ND
30	y	606	CHL	NA
30	y	606	CHL	NC
30	y	606	CHL	ND
30	y	607	CHL	NA
30	y	607	CHL	NC
30	y	607	CHL	ND
30	y	608	CHL	NA
30	y	608	CHL	NC
30	y	608	CHL	ND
30	y	609	CHL	NA
30	y	609	CHL	NC
30	y	609	CHL	ND
31	1	602	CLA	ND
31	1	603	CLA	ND
31	1	604	CLA	ND
31	1	610	CLA	ND
31	1	611	CLA	ND
31	1	612	CLA	ND
31	1	613	CLA	ND
31	1	614	CLA	ND
31	2	602	CLA	ND
31	2	603	CLA	ND
31	2	604	CLA	ND
31	2	609	CLA	ND
31	2	610	CLA	ND
31	2	611	CLA	ND
31	2	612	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	2	613	CLA	ND
31	3	301	CLA	ND
31	3	304	CLA	ND
31	3	305	CLA	ND
31	3	306	CLA	ND
31	3	311	CLA	ND
31	3	312	CLA	ND
31	3	313	CLA	ND
31	3	314	CLA	ND
31	3	315	CLA	ND
31	3	316	CLA	ND
31	4	602	CLA	ND
31	4	603	CLA	ND
31	4	604	CLA	ND
31	4	610	CLA	ND
31	4	611	CLA	ND
31	4	612	CLA	ND
31	4	613	CLA	ND
31	4	614	CLA	ND
31	5	602	CLA	ND
31	5	603	CLA	ND
31	5	604	CLA	ND
31	5	610	CLA	ND
31	5	611	CLA	ND
31	5	612	CLA	ND
31	5	613	CLA	ND
31	5	614	CLA	ND
31	5	615	CLA	ND
31	6	303	CLA	ND
31	6	304	CLA	ND
31	6	305	CLA	ND
31	6	311	CLA	ND
31	6	312	CLA	ND
31	6	313	CLA	ND
31	6	314	CLA	ND
31	6	315	CLA	ND
31	6	316	CLA	ND
31	A	405	CLA	ND
31	A	406	CLA	ND
31	A	407	CLA	ND
31	A	409	CLA	ND
31	B	601	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	B	602	CLA	ND
31	B	603	CLA	ND
31	B	604	CLA	ND
31	B	605	CLA	ND
31	B	606	CLA	ND
31	B	607	CLA	ND
31	B	608	CLA	ND
31	B	609	CLA	ND
31	B	610	CLA	ND
31	B	611	CLA	ND
31	B	612	CLA	ND
31	B	613	CLA	ND
31	B	614	CLA	ND
31	B	615	CLA	ND
31	B	616	CLA	ND
31	C	601	CLA	ND
31	C	602	CLA	ND
31	C	603	CLA	ND
31	C	604	CLA	ND
31	C	605	CLA	ND
31	C	606	CLA	ND
31	C	607	CLA	ND
31	C	608	CLA	ND
31	C	609	CLA	ND
31	C	610	CLA	ND
31	C	611	CLA	ND
31	C	612	CLA	ND
31	C	613	CLA	ND
31	D	403	CLA	ND
31	D	404	CLA	ND
31	G	602	CLA	ND
31	G	603	CLA	ND
31	G	604	CLA	ND
31	G	609	CLA	ND
31	G	610	CLA	ND
31	G	611	CLA	ND
31	G	612	CLA	ND
31	G	613	CLA	ND
31	N	303	CLA	ND
31	N	304	CLA	ND
31	N	305	CLA	ND
31	N	310	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	N	311	CLA	ND
31	N	312	CLA	ND
31	N	313	CLA	ND
31	N	314	CLA	ND
31	N	315	CLA	ND
31	N	321	CLA	ND
31	R	303	CLA	ND
31	R	304	CLA	ND
31	R	305	CLA	ND
31	R	306	CLA	ND
31	R	307	CLA	ND
31	R	311	CLA	ND
31	R	312	CLA	ND
31	R	313	CLA	ND
31	R	314	CLA	ND
31	R	315	CLA	ND
31	R	316	CLA	ND
31	S	303	CLA	ND
31	S	304	CLA	ND
31	S	305	CLA	ND
31	S	306	CLA	ND
31	S	310	CLA	ND
31	S	311	CLA	ND
31	S	312	CLA	ND
31	S	313	CLA	ND
31	S	314	CLA	ND
31	S	315	CLA	ND
31	S	316	CLA	ND
31	Y	303	CLA	ND
31	Y	304	CLA	ND
31	Y	305	CLA	ND
31	Y	310	CLA	ND
31	Y	311	CLA	ND
31	Y	312	CLA	ND
31	Y	313	CLA	ND
31	Y	314	CLA	ND
31	0	602	CLA	ND
31	0	603	CLA	ND
31	0	604	CLA	ND
31	0	610	CLA	ND
31	0	611	CLA	ND
31	0	612	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	0	613	CLA	ND
31	0	614	CLA	ND
31	0	615	CLA	ND
31	7	303	CLA	ND
31	7	304	CLA	ND
31	7	305	CLA	ND
31	7	311	CLA	ND
31	7	312	CLA	ND
31	7	313	CLA	ND
31	7	314	CLA	ND
31	7	315	CLA	ND
31	7	316	CLA	ND
31	8	602	CLA	ND
31	8	603	CLA	ND
31	8	604	CLA	ND
31	8	609	CLA	ND
31	8	610	CLA	ND
31	8	611	CLA	ND
31	8	612	CLA	ND
31	8	613	CLA	ND
31	8	614	CLA	ND
31	9	304	CLA	ND
31	9	305	CLA	ND
31	9	306	CLA	ND
31	9	312	CLA	ND
31	9	313	CLA	ND
31	9	314	CLA	ND
31	9	315	CLA	ND
31	9	316	CLA	ND
31	p	602	CLA	ND
31	p	603	CLA	ND
31	p	604	CLA	ND
31	p	610	CLA	ND
31	p	611	CLA	ND
31	p	612	CLA	ND
31	p	613	CLA	ND
31	p	614	CLA	ND
31	p	615	CLA	ND
31	q	304	CLA	ND
31	q	305	CLA	ND
31	q	306	CLA	ND
31	q	312	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	q	313	CLA	ND
31	q	314	CLA	ND
31	q	315	CLA	ND
31	q	316	CLA	ND
31	a	406	CLA	ND
31	a	407	CLA	ND
31	a	409	CLA	ND
31	b	602	CLA	ND
31	b	603	CLA	ND
31	b	604	CLA	ND
31	b	605	CLA	ND
31	b	606	CLA	ND
31	b	607	CLA	ND
31	b	608	CLA	ND
31	b	609	CLA	ND
31	b	610	CLA	ND
31	b	611	CLA	ND
31	b	612	CLA	ND
31	b	613	CLA	ND
31	b	614	CLA	ND
31	b	615	CLA	ND
31	b	616	CLA	ND
31	b	617	CLA	ND
31	c	601	CLA	ND
31	c	602	CLA	ND
31	c	603	CLA	ND
31	c	604	CLA	ND
31	c	605	CLA	ND
31	c	606	CLA	ND
31	c	607	CLA	ND
31	c	608	CLA	ND
31	c	609	CLA	ND
31	c	610	CLA	ND
31	c	611	CLA	ND
31	c	612	CLA	ND
31	c	613	CLA	ND
31	d	401	CLA	ND
31	d	404	CLA	ND
31	d	405	CLA	ND
31	g	303	CLA	ND
31	g	304	CLA	ND
31	g	305	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
31	g	310	CLA	ND
31	g	311	CLA	ND
31	g	312	CLA	ND
31	g	313	CLA	ND
31	g	314	CLA	ND
31	n	303	CLA	ND
31	n	304	CLA	ND
31	n	305	CLA	ND
31	n	311	CLA	ND
31	n	312	CLA	ND
31	n	313	CLA	ND
31	n	314	CLA	ND
31	n	315	CLA	ND
31	n	316	CLA	ND
31	r	303	CLA	ND
31	r	304	CLA	ND
31	r	305	CLA	ND
31	r	306	CLA	ND
31	r	307	CLA	ND
31	r	311	CLA	ND
31	r	312	CLA	ND
31	r	313	CLA	ND
31	r	314	CLA	ND
31	r	315	CLA	ND
31	r	316	CLA	ND
31	s	303	CLA	ND
31	s	304	CLA	ND
31	s	305	CLA	ND
31	s	306	CLA	ND
31	s	310	CLA	ND
31	s	311	CLA	ND
31	s	312	CLA	ND
31	s	313	CLA	ND
31	s	314	CLA	ND
31	s	315	CLA	ND
31	s	316	CLA	ND
31	y	602	CLA	ND
31	y	603	CLA	ND
31	y	604	CLA	ND
31	y	610	CLA	ND
31	y	611	CLA	ND
31	y	612	CLA	ND

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Mol	Chain	Res	Type	Atom
31	y	613	CLA	ND
31	y	614	CLA	ND
31	y	615	CLA	ND

All (7812) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	1	601	CHL	CHA-CBD-CGD-O1D
30	1	601	CHL	CHA-CBD-CGD-O2D
30	1	606	CHL	CAD-CBD-CGD-O1D
30	1	606	CHL	CAD-CBD-CGD-O2D
30	1	607	CHL	C1A-C2A-CAA-CBA
30	1	607	CHL	C3A-C2A-CAA-CBA
30	1	609	CHL	C11-C12-C13-C14
30	2	601	CHL	C1A-C2A-CAA-CBA
30	2	601	CHL	C3A-C2A-CAA-CBA
30	2	605	CHL	CHA-CBD-CGD-O1D
30	2	605	CHL	CHA-CBD-CGD-O2D
30	3	302	CHL	C2-C1-O2A-CGA
30	3	302	CHL	CHA-CBD-CGD-O1D
30	3	302	CHL	CAD-CBD-CGD-O1D
30	3	302	CHL	CAD-CBD-CGD-O2D
30	3	307	CHL	CAD-CBD-CGD-O1D
30	3	307	CHL	CAD-CBD-CGD-O2D
30	3	308	CHL	CHA-CBD-CGD-O1D
30	3	308	CHL	CHA-CBD-CGD-O2D
30	3	309	CHL	CHA-CBD-CGD-O1D
30	3	309	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	C1A-C2A-CAA-CBA
30	4	601	CHL	C3A-C2A-CAA-CBA
30	4	605	CHL	CHA-CBD-CGD-O1D
30	4	605	CHL	CHA-CBD-CGD-O2D
30	4	607	CHL	C1A-C2A-CAA-CBA
30	4	607	CHL	C2-C1-O2A-CGA
30	5	607	CHL	CAD-CBD-CGD-O2D
30	5	609	CHL	CHA-CBD-CGD-O1D
30	5	609	CHL	CHA-CBD-CGD-O2D
30	6	302	CHL	C1A-C2A-CAA-CBA
30	6	302	CHL	C3A-C2A-CAA-CBA
30	6	306	CHL	CHA-CBD-CGD-O1D
30	6	306	CHL	CHA-CBD-CGD-O2D
30	6	307	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	G	601	CHL	C1A-C2A-CAA-CBA
30	G	601	CHL	CHA-CBD-CGD-O1D
30	G	601	CHL	CHA-CBD-CGD-O2D
30	G	601	CHL	C11-C12-C13-C14
30	G	605	CHL	C1A-C2A-CAA-CBA
30	G	606	CHL	CHA-CBD-CGD-O1D
30	G	606	CHL	CHA-CBD-CGD-O2D
30	G	608	CHL	C11-C12-C13-C14
30	N	306	CHL	CHA-CBD-CGD-O1D
30	N	306	CHL	CHA-CBD-CGD-O2D
30	R	310	CHL	C2A-CAA-CBA-CGA
30	Y	302	CHL	C3A-C2A-CAA-CBA
30	0	605	CHL	C2-C1-O2A-CGA
30	0	605	CHL	CAD-CBD-CGD-O2D
30	0	605	CHL	C4-C3-C5-C6
30	0	606	CHL	C1A-C2A-CAA-CBA
30	7	302	CHL	C3A-C2A-CAA-CBA
30	7	306	CHL	CAD-CBD-CGD-O1D
30	7	306	CHL	CAD-CBD-CGD-O2D
30	7	307	CHL	CBD-CGD-O2D-CED
30	7	308	CHL	C1A-C2A-CAA-CBA
30	8	608	CHL	C1A-C2A-CAA-CBA
30	8	608	CHL	C3A-C2A-CAA-CBA
30	9	307	CHL	CHA-CBD-CGD-O1D
30	9	307	CHL	CHA-CBD-CGD-O2D
30	9	308	CHL	C2-C3-C5-C6
30	9	308	CHL	C4-C3-C5-C6
30	9	309	CHL	CBD-CGD-O2D-CED
30	9	310	CHL	C1A-C2A-CAA-CBA
30	9	310	CHL	C3A-C2A-CAA-CBA
30	9	311	CHL	CHA-CBD-CGD-O1D
30	9	311	CHL	CHA-CBD-CGD-O2D
30	p	601	CHL	C1A-C2A-CAA-CBA
30	p	601	CHL	C3A-C2A-CAA-CBA
30	p	605	CHL	CHA-CBD-CGD-O1D
30	p	605	CHL	CHA-CBD-CGD-O2D
30	p	607	CHL	CAD-CBD-CGD-O1D
30	p	607	CHL	CAD-CBD-CGD-O2D
30	q	303	CHL	C1A-C2A-CAA-CBA
30	q	303	CHL	C3A-C2A-CAA-CBA
30	q	307	CHL	CHA-CBD-CGD-O1D
30	q	307	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
30	q	309	CHL	C1A-C2A-CAA-CBA
30	q	309	CHL	C2-C1-O2A-CGA
30	q	309	CHL	CAD-CBD-CGD-O1D
30	q	309	CHL	CAD-CBD-CGD-O2D
30	q	311	CHL	C1A-C2A-CAA-CBA
30	g	302	CHL	C1A-C2A-CAA-CBA
30	g	302	CHL	CHA-CBD-CGD-O1D
30	g	302	CHL	CHA-CBD-CGD-O2D
30	g	302	CHL	C11-C12-C13-C14
30	g	306	CHL	C1A-C2A-CAA-CBA
30	g	307	CHL	CHA-CBD-CGD-O1D
30	g	307	CHL	CHA-CBD-CGD-O2D
30	g	309	CHL	C11-C12-C13-C14
30	n	310	CHL	C1A-C2A-CAA-CBA
30	y	601	CHL	C3A-C2A-CAA-CBA
31	1	603	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	CHA-CBD-CGD-O1D
31	1	604	CLA	CHA-CBD-CGD-O2D
31	1	610	CLA	CBD-CGD-O2D-CED
31	1	610	CLA	C11-C10-C8-C9
31	1	611	CLA	C2-C1-O2A-CGA
31	1	612	CLA	C2-C1-O2A-CGA
31	1	613	CLA	CBD-CGD-O2D-CED
31	1	614	CLA	C1A-C2A-CAA-CBA
31	1	614	CLA	C2-C1-O2A-CGA
31	1	614	CLA	CBD-CGD-O2D-CED
31	2	602	CLA	CBD-CGD-O2D-CED
31	2	609	CLA	C2-C1-O2A-CGA
31	2	609	CLA	CHA-CBD-CGD-O1D
31	2	609	CLA	CHA-CBD-CGD-O2D
31	2	609	CLA	CBD-CGD-O2D-CED
31	2	610	CLA	C1A-C2A-CAA-CBA
31	2	611	CLA	C2-C1-O2A-CGA
31	2	612	CLA	CHA-CBD-CGD-O1D
31	2	612	CLA	CHA-CBD-CGD-O2D
31	2	613	CLA	C1A-C2A-CAA-CBA
31	2	613	CLA	C3A-C2A-CAA-CBA
31	2	613	CLA	C2-C1-O2A-CGA
31	2	613	CLA	CBD-CGD-O2D-CED
31	3	305	CLA	C1A-C2A-CAA-CBA
31	3	305	CLA	CBD-CGD-O2D-CED
31	3	306	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	3	312	CLA	C1A-C2A-CAA-CBA
31	3	312	CLA	C3A-C2A-CAA-CBA
31	3	312	CLA	C2-C1-O2A-CGA
31	3	312	CLA	CHA-CBD-CGD-O1D
31	3	312	CLA	CHA-CBD-CGD-O2D
31	3	312	CLA	CBD-CGD-O2D-CED
31	3	313	CLA	C2-C1-O2A-CGA
31	3	316	CLA	C2-C1-O2A-CGA
31	3	316	CLA	CBD-CGD-O2D-CED
31	4	604	CLA	C3A-C2A-CAA-CBA
31	4	604	CLA	CAD-CBD-CGD-O1D
31	4	604	CLA	CAD-CBD-CGD-O2D
31	4	604	CLA	C2-C3-C5-C6
31	4	610	CLA	C2-C1-O2A-CGA
31	4	610	CLA	CHA-CBD-CGD-O1D
31	4	610	CLA	CHA-CBD-CGD-O2D
31	4	610	CLA	C2-C3-C5-C6
31	4	610	CLA	C4-C3-C5-C6
31	4	612	CLA	CHA-CBD-CGD-O2D
31	4	614	CLA	CBA-CGA-O2A-C1
31	4	614	CLA	O1A-CGA-O2A-C1
31	5	602	CLA	CBD-CGD-O2D-CED
31	5	603	CLA	CBA-CGA-O2A-C1
31	5	603	CLA	O1A-CGA-O2A-C1
31	5	611	CLA	C3A-C2A-CAA-CBA
31	5	611	CLA	CHA-CBD-CGD-O1D
31	5	611	CLA	CHA-CBD-CGD-O2D
31	5	612	CLA	CBA-CGA-O2A-C1
31	5	612	CLA	O1A-CGA-O2A-C1
31	5	612	CLA	CHA-CBD-CGD-O1D
31	5	612	CLA	CHA-CBD-CGD-O2D
31	5	613	CLA	C2-C1-O2A-CGA
31	5	614	CLA	C1A-C2A-CAA-CBA
31	5	614	CLA	CBD-CGD-O2D-CED
31	5	615	CLA	C1A-C2A-CAA-CBA
31	5	615	CLA	CBD-CGD-O2D-CED
31	6	304	CLA	C1A-C2A-CAA-CBA
31	6	304	CLA	C2-C1-O2A-CGA
31	6	305	CLA	C1A-C2A-CAA-CBA
31	6	305	CLA	C3A-C2A-CAA-CBA
31	6	305	CLA	CHA-CBD-CGD-O1D
31	6	311	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	6	311	CLA	C3A-C2A-CAA-CBA
31	6	312	CLA	C2-C1-O2A-CGA
31	6	312	CLA	CHA-CBD-CGD-O1D
31	6	312	CLA	CHA-CBD-CGD-O2D
31	6	316	CLA	C1A-C2A-CAA-CBA
31	6	316	CLA	C3A-C2A-CAA-CBA
31	6	316	CLA	C2-C1-O2A-CGA
31	6	316	CLA	CBD-CGD-O2D-CED
31	A	406	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C3A-C2A-CAA-CBA
31	A	406	CLA	CHA-CBD-CGD-O1D
31	A	406	CLA	CHA-CBD-CGD-O2D
31	A	407	CLA	CHA-CBD-CGD-O1D
31	A	407	CLA	CHA-CBD-CGD-O2D
31	A	409	CLA	C2-C3-C5-C6
31	A	409	CLA	C4-C3-C5-C6
31	B	601	CLA	CHA-CBD-CGD-O1D
31	B	601	CLA	CHA-CBD-CGD-O2D
31	B	602	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	CBA-CGA-O2A-C1
31	B	602	CLA	CHA-CBD-CGD-O1D
31	B	602	CLA	CHA-CBD-CGD-O2D
31	B	602	CLA	C2-C3-C5-C6
31	B	602	CLA	C4-C3-C5-C6
31	B	603	CLA	CBD-CGD-O2D-CED
31	B	603	CLA	C2-C3-C5-C6
31	B	603	CLA	C4-C3-C5-C6
31	B	604	CLA	C1A-C2A-CAA-CBA
31	B	604	CLA	C2-C3-C5-C6
31	B	604	CLA	C4-C3-C5-C6
31	B	605	CLA	CBD-CGD-O2D-CED
31	B	606	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	C1A-C2A-CAA-CBA
31	B	607	CLA	C3A-C2A-CAA-CBA
31	B	607	CLA	CHA-CBD-CGD-O1D
31	B	607	CLA	CHA-CBD-CGD-O2D
31	B	607	CLA	CAD-CBD-CGD-O1D
31	B	607	CLA	CAD-CBD-CGD-O2D
31	B	609	CLA	C1A-C2A-CAA-CBA
31	B	609	CLA	C3A-C2A-CAA-CBA
31	B	609	CLA	CBD-CGD-O2D-CED
31	B	609	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	B	610	CLA	C2-C1-O2A-CGA
31	B	610	CLA	C11-C12-C13-C14
31	B	612	CLA	C1A-C2A-CAA-CBA
31	B	612	CLA	C3A-C2A-CAA-CBA
31	B	612	CLA	C2-C1-O2A-CGA
31	B	613	CLA	CBD-CGD-O2D-CED
31	B	613	CLA	C4-C3-C5-C6
31	B	614	CLA	C2A-CAA-CBA-CGA
31	B	614	CLA	CBD-CGD-O2D-CED
31	B	614	CLA	C6-C7-C8-C9
31	C	601	CLA	CHA-CBD-CGD-O1D
31	C	601	CLA	CHA-CBD-CGD-O2D
31	C	601	CLA	CAD-CBD-CGD-O1D
31	C	601	CLA	CAD-CBD-CGD-O2D
31	C	602	CLA	CHA-CBD-CGD-O1D
31	C	602	CLA	CHA-CBD-CGD-O2D
31	C	602	CLA	CAD-CBD-CGD-O1D
31	C	604	CLA	CHA-CBD-CGD-O1D
31	C	604	CLA	CHA-CBD-CGD-O2D
31	C	605	CLA	CHA-CBD-CGD-O1D
31	C	605	CLA	CHA-CBD-CGD-O2D
31	C	606	CLA	C1A-C2A-CAA-CBA
31	C	606	CLA	C3A-C2A-CAA-CBA
31	C	606	CLA	CHA-CBD-CGD-O1D
31	C	606	CLA	CHA-CBD-CGD-O2D
31	C	606	CLA	CAD-CBD-CGD-O1D
31	C	607	CLA	CHA-CBD-CGD-O1D
31	C	607	CLA	CHA-CBD-CGD-O2D
31	C	608	CLA	CHA-CBD-CGD-O1D
31	C	608	CLA	CHA-CBD-CGD-O2D
31	C	609	CLA	C2-C1-O2A-CGA
31	C	610	CLA	C1A-C2A-CAA-CBA
31	C	612	CLA	CBA-CGA-O2A-C1
31	C	612	CLA	O1A-CGA-O2A-C1
31	C	613	CLA	C1A-C2A-CAA-CBA
31	D	403	CLA	C6-C7-C8-C9
31	D	404	CLA	C1A-C2A-CAA-CBA
31	D	404	CLA	C4-C3-C5-C6
31	G	603	CLA	C1A-C2A-CAA-CBA
31	G	603	CLA	CBA-CGA-O2A-C1
31	G	604	CLA	C1A-C2A-CAA-CBA
31	G	604	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	G	610	CLA	C1A-C2A-CAA-CBA
31	G	610	CLA	C3A-C2A-CAA-CBA
31	G	610	CLA	C2-C3-C5-C6
31	G	610	CLA	C4-C3-C5-C6
31	G	612	CLA	CBD-CGD-O2D-CED
31	G	613	CLA	C2-C1-O2A-CGA
31	N	305	CLA	C1A-C2A-CAA-CBA
31	N	305	CLA	CHA-CBD-CGD-O1D
31	N	305	CLA	CAD-CBD-CGD-O1D
31	N	305	CLA	C11-C10-C8-C9
31	N	310	CLA	C1A-C2A-CAA-CBA
31	N	310	CLA	C3A-C2A-CAA-CBA
31	N	311	CLA	C1A-C2A-CAA-CBA
31	N	311	CLA	C3A-C2A-CAA-CBA
31	N	313	CLA	C6-C7-C8-C9
31	N	314	CLA	C1A-C2A-CAA-CBA
31	N	314	CLA	C3A-C2A-CAA-CBA
31	N	321	CLA	C2-C1-O2A-CGA
31	N	321	CLA	CBD-CGD-O2D-CED
31	R	303	CLA	C3A-C2A-CAA-CBA
31	R	304	CLA	CHA-CBD-CGD-O1D
31	R	304	CLA	CHA-CBD-CGD-O2D
31	R	306	CLA	C1A-C2A-CAA-CBA
31	R	306	CLA	C3A-C2A-CAA-CBA
31	R	306	CLA	CHA-CBD-CGD-O2D
31	R	312	CLA	C1A-C2A-CAA-CBA
31	R	312	CLA	C3A-C2A-CAA-CBA
31	R	313	CLA	CBD-CGD-O2D-CED
31	R	314	CLA	C2-C1-O2A-CGA
31	R	314	CLA	CBD-CGD-O2D-CED
31	R	315	CLA	C2-C1-O2A-CGA
31	R	316	CLA	C1A-C2A-CAA-CBA
31	R	316	CLA	C3A-C2A-CAA-CBA
31	R	316	CLA	CHA-CBD-CGD-O1D
31	S	303	CLA	C1A-C2A-CAA-CBA
31	S	303	CLA	C3A-C2A-CAA-CBA
31	S	304	CLA	C1A-C2A-CAA-CBA
31	S	304	CLA	C3A-C2A-CAA-CBA
31	S	306	CLA	C2-C1-O2A-CGA
31	S	310	CLA	C1A-C2A-CAA-CBA
31	S	310	CLA	C3A-C2A-CAA-CBA
31	S	310	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	S	310	CLA	C2-C3-C5-C6
31	S	310	CLA	C4-C3-C5-C6
31	S	312	CLA	C1A-C2A-CAA-CBA
31	S	312	CLA	C3A-C2A-CAA-CBA
31	S	312	CLA	C2A-CAA-CBA-CGA
31	S	312	CLA	C2-C1-O2A-CGA
31	S	312	CLA	CHA-CBD-CGD-O1D
31	S	312	CLA	CHA-CBD-CGD-O2D
31	S	313	CLA	CHA-CBD-CGD-O1D
31	S	314	CLA	CHA-CBD-CGD-O1D
31	S	314	CLA	CHA-CBD-CGD-O2D
31	S	314	CLA	CBD-CGD-O2D-CED
31	S	314	CLA	C11-C10-C8-C9
31	S	315	CLA	C3A-C2A-CAA-CBA
31	S	316	CLA	CBA-CGA-O2A-C1
31	S	316	CLA	CBD-CGD-O2D-CED
31	Y	305	CLA	CHA-CBD-CGD-O1D
31	Y	305	CLA	CHA-CBD-CGD-O2D
31	Y	305	CLA	CAD-CBD-CGD-O1D
31	Y	305	CLA	CAD-CBD-CGD-O2D
31	Y	311	CLA	C1A-C2A-CAA-CBA
31	Y	311	CLA	C3A-C2A-CAA-CBA
31	Y	313	CLA	CBD-CGD-O2D-CED
31	0	602	CLA	C2-C3-C5-C6
31	0	602	CLA	C4-C3-C5-C6
31	0	603	CLA	C1A-C2A-CAA-CBA
31	0	603	CLA	C3A-C2A-CAA-CBA
31	0	603	CLA	C2-C1-O2A-CGA
31	0	603	CLA	CHA-CBD-CGD-O2D
31	0	604	CLA	C1A-C2A-CAA-CBA
31	0	604	CLA	C3A-C2A-CAA-CBA
31	0	604	CLA	CHA-CBD-CGD-O1D
31	0	604	CLA	CHA-CBD-CGD-O2D
31	0	604	CLA	CAD-CBD-CGD-O1D
31	0	610	CLA	C1A-C2A-CAA-CBA
31	0	610	CLA	C3A-C2A-CAA-CBA
31	0	610	CLA	C2-C3-C5-C6
31	0	610	CLA	C4-C3-C5-C6
31	0	610	CLA	C11-C10-C8-C9
31	0	611	CLA	C2-C1-O2A-CGA
31	0	611	CLA	CHA-CBD-CGD-O1D
31	0	611	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	0	612	CLA	CBA-CGA-O2A-C1
31	0	612	CLA	O1A-CGA-O2A-C1
31	0	613	CLA	CBD-CGD-O2D-CED
31	0	614	CLA	C1A-C2A-CAA-CBA
31	0	614	CLA	C3A-C2A-CAA-CBA
31	0	614	CLA	CBD-CGD-O2D-CED
31	0	614	CLA	O1D-CGD-O2D-CED
31	0	615	CLA	C1A-C2A-CAA-CBA
31	0	615	CLA	C3A-C2A-CAA-CBA
31	7	305	CLA	CHA-CBD-CGD-O1D
31	7	305	CLA	CHA-CBD-CGD-O2D
31	7	312	CLA	C1A-C2A-CAA-CBA
31	7	312	CLA	C3A-C2A-CAA-CBA
31	7	314	CLA	CBD-CGD-O2D-CED
31	7	315	CLA	C1A-C2A-CAA-CBA
31	7	315	CLA	C2-C1-O2A-CGA
31	7	315	CLA	CHA-CBD-CGD-O1D
31	7	315	CLA	CHA-CBD-CGD-O2D
31	7	315	CLA	CBD-CGD-O2D-CED
31	7	316	CLA	C1A-C2A-CAA-CBA
31	7	316	CLA	C2-C1-O2A-CGA
31	8	603	CLA	CBA-CGA-O2A-C1
31	8	603	CLA	O1A-CGA-O2A-C1
31	8	604	CLA	C1A-C2A-CAA-CBA
31	8	609	CLA	C1A-C2A-CAA-CBA
31	8	609	CLA	C3A-C2A-CAA-CBA
31	8	609	CLA	C6-C7-C8-C9
31	8	610	CLA	C1A-C2A-CAA-CBA
31	8	610	CLA	C3A-C2A-CAA-CBA
31	8	612	CLA	C2-C1-O2A-CGA
31	8	612	CLA	CBD-CGD-O2D-CED
31	8	612	CLA	C6-C7-C8-C9
31	8	613	CLA	C1A-C2A-CAA-CBA
31	8	613	CLA	C3A-C2A-CAA-CBA
31	8	613	CLA	C2-C1-O2A-CGA
31	8	614	CLA	CBD-CGD-O2D-CED
31	9	304	CLA	C1A-C2A-CAA-CBA
31	9	304	CLA	C2-C1-O2A-CGA
31	9	306	CLA	C1A-C2A-CAA-CBA
31	9	306	CLA	C3A-C2A-CAA-CBA
31	9	306	CLA	CHA-CBD-CGD-O1D
31	9	306	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	9	312	CLA	C1A-C2A-CAA-CBA
31	9	312	CLA	CHA-CBD-CGD-O1D
31	9	312	CLA	CHA-CBD-CGD-O2D
31	9	313	CLA	CHA-CBD-CGD-O1D
31	9	313	CLA	CHA-CBD-CGD-O2D
31	9	314	CLA	C2-C1-O2A-CGA
31	9	314	CLA	CBD-CGD-O2D-CED
31	9	315	CLA	CBD-CGD-O2D-CED
31	p	610	CLA	C2A-CAA-CBA-CGA
31	p	610	CLA	CHA-CBD-CGD-O1D
31	p	610	CLA	CHA-CBD-CGD-O2D
31	p	610	CLA	CBD-CGD-O2D-CED
31	p	611	CLA	C1A-C2A-CAA-CBA
31	p	611	CLA	C3A-C2A-CAA-CBA
31	p	611	CLA	CHA-CBD-CGD-O1D
31	p	611	CLA	CHA-CBD-CGD-O2D
31	p	611	CLA	C11-C10-C8-C7
31	p	612	CLA	CHA-CBD-CGD-O2D
31	p	613	CLA	CBD-CGD-O2D-CED
31	p	614	CLA	CBD-CGD-O2D-CED
31	p	614	CLA	O1D-CGD-O2D-CED
31	q	305	CLA	CHA-CBD-CGD-O1D
31	q	305	CLA	CHA-CBD-CGD-O2D
31	q	312	CLA	C2A-CAA-CBA-CGA
31	q	312	CLA	O1A-CGA-O2A-C1
31	q	312	CLA	CBD-CGD-O2D-CED
31	q	313	CLA	CHA-CBD-CGD-O1D
31	q	313	CLA	CHA-CBD-CGD-O2D
31	q	314	CLA	CAD-CBD-CGD-O1D
31	q	314	CLA	CAD-CBD-CGD-O2D
31	q	316	CLA	C1A-C2A-CAA-CBA
31	q	316	CLA	C3A-C2A-CAA-CBA
31	q	316	CLA	CBD-CGD-O2D-CED
31	a	407	CLA	C1A-C2A-CAA-CBA
31	a	407	CLA	CHA-CBD-CGD-O1D
31	a	407	CLA	CHA-CBD-CGD-O2D
31	a	409	CLA	C2-C3-C5-C6
31	a	409	CLA	C4-C3-C5-C6
31	b	602	CLA	C1A-C2A-CAA-CBA
31	b	602	CLA	C3A-C2A-CAA-CBA
31	b	603	CLA	C1A-C2A-CAA-CBA
31	b	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	b	603	CLA	O1A-CGA-O2A-C1
31	b	603	CLA	C4-C3-C5-C6
31	b	604	CLA	CBD-CGD-O2D-CED
31	b	605	CLA	C1A-C2A-CAA-CBA
31	b	605	CLA	CHA-CBD-CGD-O1D
31	b	605	CLA	CHA-CBD-CGD-O2D
31	b	605	CLA	CAD-CBD-CGD-O1D
31	b	605	CLA	CAD-CBD-CGD-O2D
31	b	606	CLA	CBD-CGD-O2D-CED
31	b	606	CLA	C4-C3-C5-C6
31	b	607	CLA	CHA-CBD-CGD-O1D
31	b	607	CLA	CHA-CBD-CGD-O2D
31	b	607	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	C1A-C2A-CAA-CBA
31	b	608	CLA	C3A-C2A-CAA-CBA
31	b	608	CLA	CHA-CBD-CGD-O1D
31	b	608	CLA	CHA-CBD-CGD-O2D
31	b	608	CLA	CAD-CBD-CGD-O1D
31	b	608	CLA	CAD-CBD-CGD-O2D
31	b	609	CLA	C1A-C2A-CAA-CBA
31	b	609	CLA	C2-C3-C5-C6
31	b	609	CLA	C4-C3-C5-C6
31	b	610	CLA	C1A-C2A-CAA-CBA
31	b	610	CLA	C3A-C2A-CAA-CBA
31	b	610	CLA	CHA-CBD-CGD-O1D
31	b	610	CLA	CHA-CBD-CGD-O2D
31	b	610	CLA	CAD-CBD-CGD-O1D
31	b	610	CLA	CBD-CGD-O2D-CED
31	b	610	CLA	C11-C10-C8-C9
31	b	613	CLA	C1A-C2A-CAA-CBA
31	b	613	CLA	C3A-C2A-CAA-CBA
31	b	614	CLA	CBD-CGD-O2D-CED
31	b	614	CLA	C2-C3-C5-C6
31	b	614	CLA	C4-C3-C5-C6
31	b	615	CLA	C6-C7-C8-C9
31	b	616	CLA	CHA-CBD-CGD-O1D
31	b	616	CLA	CHA-CBD-CGD-O2D
31	b	617	CLA	CBA-CGA-O2A-C1
31	b	617	CLA	O1A-CGA-O2A-C1
31	c	601	CLA	CAD-CBD-CGD-O1D
31	c	601	CLA	CAD-CBD-CGD-O2D
31	c	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	c	602	CLA	CHA-CBD-CGD-O2D
31	c	602	CLA	CAD-CBD-CGD-O1D
31	c	602	CLA	CAD-CBD-CGD-O2D
31	c	603	CLA	CBD-CGD-O2D-CED
31	c	604	CLA	CHA-CBD-CGD-O1D
31	c	604	CLA	CHA-CBD-CGD-O2D
31	c	605	CLA	CHA-CBD-CGD-O1D
31	c	605	CLA	CHA-CBD-CGD-O2D
31	c	605	CLA	CAD-CBD-CGD-O1D
31	c	605	CLA	CAD-CBD-CGD-O2D
31	c	606	CLA	C1A-C2A-CAA-CBA
31	c	606	CLA	C3A-C2A-CAA-CBA
31	c	606	CLA	CHA-CBD-CGD-O1D
31	c	606	CLA	CHA-CBD-CGD-O2D
31	c	606	CLA	CAD-CBD-CGD-O1D
31	c	608	CLA	CHA-CBD-CGD-O1D
31	c	608	CLA	CHA-CBD-CGD-O2D
31	c	609	CLA	C2-C1-O2A-CGA
31	c	609	CLA	C6-C7-C8-C9
31	c	610	CLA	CBA-CGA-O2A-C1
31	c	610	CLA	O1A-CGA-O2A-C1
31	c	612	CLA	CBA-CGA-O2A-C1
31	c	612	CLA	O1A-CGA-O2A-C1
31	c	613	CLA	C1A-C2A-CAA-CBA
31	d	401	CLA	CHA-CBD-CGD-O1D
31	d	401	CLA	CHA-CBD-CGD-O2D
31	d	404	CLA	C2-C3-C5-C6
31	d	404	CLA	C4-C3-C5-C6
31	d	405	CLA	C1A-C2A-CAA-CBA
31	d	405	CLA	C3A-C2A-CAA-CBA
31	d	405	CLA	CBD-CGD-O2D-CED
31	g	303	CLA	C2-C1-O2A-CGA
31	g	304	CLA	C1A-C2A-CAA-CBA
31	g	304	CLA	C3A-C2A-CAA-CBA
31	g	305	CLA	C1A-C2A-CAA-CBA
31	g	305	CLA	C3A-C2A-CAA-CBA
31	g	311	CLA	C1A-C2A-CAA-CBA
31	g	311	CLA	C3A-C2A-CAA-CBA
31	g	311	CLA	C6-C7-C8-C10
31	g	313	CLA	CHA-CBD-CGD-O1D
31	g	313	CLA	CHA-CBD-CGD-O2D
31	g	314	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	n	304	CLA	CBA-CGA-O2A-C1
31	n	304	CLA	O1A-CGA-O2A-C1
31	n	305	CLA	C1A-C2A-CAA-CBA
31	n	311	CLA	C1A-C2A-CAA-CBA
31	n	311	CLA	C3A-C2A-CAA-CBA
31	n	312	CLA	C1A-C2A-CAA-CBA
31	n	312	CLA	C3A-C2A-CAA-CBA
31	n	314	CLA	C2-C1-O2A-CGA
31	n	314	CLA	CBD-CGD-O2D-CED
31	n	314	CLA	C6-C7-C8-C9
31	n	315	CLA	C1A-C2A-CAA-CBA
31	n	315	CLA	C3A-C2A-CAA-CBA
31	n	315	CLA	C2-C1-O2A-CGA
31	r	303	CLA	C1A-C2A-CAA-CBA
31	r	303	CLA	C3A-C2A-CAA-CBA
31	r	303	CLA	CHA-CBD-CGD-O1D
31	r	303	CLA	CHA-CBD-CGD-O2D
31	r	306	CLA	C1A-C2A-CAA-CBA
31	r	306	CLA	C3A-C2A-CAA-CBA
31	r	311	CLA	CBD-CGD-O2D-CED
31	r	312	CLA	C1A-C2A-CAA-CBA
31	r	312	CLA	C3A-C2A-CAA-CBA
31	r	313	CLA	CBD-CGD-O2D-CED
31	r	314	CLA	C2-C1-O2A-CGA
31	r	314	CLA	CHA-CBD-CGD-O1D
31	r	315	CLA	C1A-C2A-CAA-CBA
31	r	315	CLA	C3A-C2A-CAA-CBA
31	r	315	CLA	C2-C1-O2A-CGA
31	r	316	CLA	C1A-C2A-CAA-CBA
31	r	316	CLA	C3A-C2A-CAA-CBA
31	r	316	CLA	CHA-CBD-CGD-O1D
31	r	316	CLA	CHA-CBD-CGD-O2D
31	s	303	CLA	C3A-C2A-CAA-CBA
31	s	303	CLA	CBA-CGA-O2A-C1
31	s	303	CLA	O1A-CGA-O2A-C1
31	s	304	CLA	C1A-C2A-CAA-CBA
31	s	306	CLA	CHA-CBD-CGD-O2D
31	s	310	CLA	C1A-C2A-CAA-CBA
31	s	310	CLA	C3A-C2A-CAA-CBA
31	s	312	CLA	C1A-C2A-CAA-CBA
31	s	312	CLA	C3A-C2A-CAA-CBA
31	s	312	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	s	312	CLA	CHA-CBD-CGD-O2D
31	s	313	CLA	CHA-CBD-CGD-O1D
31	s	313	CLA	CHA-CBD-CGD-O2D
31	s	314	CLA	CBD-CGD-O2D-CED
31	s	315	CLA	C3A-C2A-CAA-CBA
31	s	316	CLA	C1A-C2A-CAA-CBA
31	s	316	CLA	CBA-CGA-O2A-C1
31	s	316	CLA	CBD-CGD-O2D-CED
31	y	604	CLA	CHA-CBD-CGD-O1D
31	y	604	CLA	CHA-CBD-CGD-O2D
31	y	604	CLA	CAD-CBD-CGD-O1D
31	y	612	CLA	C6-C7-C8-C9
31	y	614	CLA	CBA-CGA-O2A-C1
31	y	614	CLA	O1A-CGA-O2A-C1
31	y	615	CLA	C1A-C2A-CAA-CBA
31	y	615	CLA	C3A-C2A-CAA-CBA
31	y	615	CLA	CHA-CBD-CGD-O1D
31	y	615	CLA	CHA-CBD-CGD-O2D
32	1	616	LUT	C7-C8-C9-C10
32	1	616	LUT	C7-C8-C9-C19
32	3	317	LUT	C11-C12-C13-C14
32	3	317	LUT	C11-C12-C13-C20
32	3	318	LUT	C11-C12-C13-C14
32	3	318	LUT	C11-C12-C13-C20
32	4	616	LUT	C7-C8-C9-C10
32	4	616	LUT	C7-C8-C9-C19
32	4	616	LUT	C31-C32-C33-C34
32	4	616	LUT	C31-C32-C33-C40
32	5	616	LUT	C11-C12-C13-C14
32	5	616	LUT	C11-C12-C13-C20
32	5	616	LUT	C31-C32-C33-C34
32	5	616	LUT	C31-C32-C33-C40
32	5	617	LUT	C7-C8-C9-C10
32	5	617	LUT	C7-C8-C9-C19
32	5	617	LUT	C31-C32-C33-C34
32	5	617	LUT	C31-C32-C33-C40
32	6	317	LUT	C11-C12-C13-C14
32	6	317	LUT	C11-C12-C13-C20
32	6	317	LUT	C31-C32-C33-C34
32	6	317	LUT	C31-C32-C33-C40
32	6	318	LUT	C7-C8-C9-C10
32	6	318	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
32	6	318	LUT	C31-C32-C33-C34
32	6	318	LUT	C31-C32-C33-C40
32	G	615	LUT	C21-C26-C27-C28
32	G	615	LUT	C25-C26-C27-C28
32	G	615	LUT	C31-C32-C33-C40
32	G	615	LUT	C33-C34-C35-C15
32	N	316	LUT	C11-C12-C13-C14
32	N	316	LUT	C11-C12-C13-C20
32	N	317	LUT	C31-C32-C33-C34
32	N	317	LUT	C31-C32-C33-C40
32	R	317	LUT	C11-C12-C13-C14
32	R	317	LUT	C11-C12-C13-C20
32	S	317	LUT	C7-C8-C9-C10
32	S	317	LUT	C7-C8-C9-C19
32	S	317	LUT	C11-C12-C13-C14
32	S	317	LUT	C11-C12-C13-C20
32	S	317	LUT	C31-C32-C33-C34
32	S	317	LUT	C31-C32-C33-C40
32	S	318	LUT	C11-C12-C13-C14
32	S	318	LUT	C11-C12-C13-C20
32	S	318	LUT	C21-C26-C27-C28
32	S	318	LUT	C27-C28-C29-C30
32	S	318	LUT	C27-C28-C29-C39
32	S	318	LUT	C31-C32-C33-C34
32	S	318	LUT	C31-C32-C33-C40
32	0	616	LUT	C11-C12-C13-C14
32	0	616	LUT	C11-C12-C13-C20
32	7	317	LUT	C11-C12-C13-C14
32	7	317	LUT	C11-C12-C13-C20
32	7	318	LUT	C7-C8-C9-C10
32	7	318	LUT	C7-C8-C9-C19
32	8	615	LUT	C7-C8-C9-C10
32	8	615	LUT	C7-C8-C9-C19
32	8	615	LUT	C11-C12-C13-C14
32	8	615	LUT	C11-C12-C13-C20
32	8	615	LUT	C31-C32-C33-C34
32	8	615	LUT	C31-C32-C33-C40
32	8	616	LUT	C31-C32-C33-C34
32	8	616	LUT	C31-C32-C33-C40
32	p	617	LUT	C7-C8-C9-C10
32	q	318	LUT	C11-C12-C13-C14
32	q	318	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
32	q	318	LUT	C31-C32-C33-C34
32	q	318	LUT	C31-C32-C33-C40
32	g	316	LUT	C11-C12-C13-C20
32	g	316	LUT	C21-C26-C27-C28
32	g	316	LUT	C25-C26-C27-C28
32	g	316	LUT	C31-C32-C33-C34
32	g	316	LUT	C31-C32-C33-C40
32	n	317	LUT	C7-C8-C9-C10
32	n	317	LUT	C7-C8-C9-C19
32	n	317	LUT	C11-C12-C13-C14
32	n	317	LUT	C11-C12-C13-C20
32	n	317	LUT	C31-C32-C33-C34
32	n	317	LUT	C31-C32-C33-C40
32	n	318	LUT	C31-C32-C33-C34
32	n	318	LUT	C31-C32-C33-C40
32	r	317	LUT	C11-C12-C13-C14
32	r	317	LUT	C11-C12-C13-C20
32	s	317	LUT	C7-C8-C9-C10
32	s	317	LUT	C7-C8-C9-C19
32	s	317	LUT	C11-C12-C13-C14
32	s	317	LUT	C11-C12-C13-C20
32	s	317	LUT	C31-C32-C33-C34
32	s	317	LUT	C31-C32-C33-C40
32	s	318	LUT	C11-C12-C13-C14
32	s	318	LUT	C11-C12-C13-C20
32	y	617	LUT	C7-C8-C9-C10
32	y	617	LUT	C7-C8-C9-C19
33	1	617	LHG	O1-C1-C2-C3
33	1	617	LHG	C1-C2-C3-O3
33	1	617	LHG	C3-O3-P-O4
33	1	617	LHG	C4-O6-P-O4
33	2	617	LHG	C3-O3-P-O4
33	2	617	LHG	C4-O6-P-O3
33	2	617	LHG	C4-O6-P-O4
33	2	617	LHG	C4-O6-P-O5
33	3	320	LHG	C4-O6-P-O3
33	3	320	LHG	C4-O6-P-O4
33	3	320	LHG	C4-O6-P-O5
33	3	320	LHG	O7-C5-C6-O8
33	4	618	LHG	C1-C2-C3-O3
33	4	618	LHG	C4-O6-P-O3
33	4	618	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	4	618	LHG	C4-O6-P-O5
33	4	618	LHG	O9-C7-O7-C5
33	4	618	LHG	C8-C7-O7-C5
33	5	619	LHG	O1-C1-C2-O2
33	5	619	LHG	C3-O3-P-O5
33	5	619	LHG	C3-O3-P-O6
33	5	619	LHG	C4-O6-P-O5
33	5	619	LHG	O9-C7-O7-C5
33	6	320	LHG	C4-O6-P-O3
33	6	320	LHG	C4-O6-P-O4
33	6	320	LHG	C4-O6-P-O5
33	A	415	LHG	O1-C1-C2-C3
33	A	415	LHG	C4-O6-P-O4
33	A	415	LHG	O7-C5-C6-O8
33	A	417	LHG	C3-O3-P-O5
33	A	417	LHG	C4-O6-P-O3
33	A	417	LHG	O6-C4-C5-O7
33	C	623	LHG	O1-C1-C2-C3
33	C	623	LHG	C1-C2-C3-O3
33	C	623	LHG	C4-O6-P-O5
33	C	623	LHG	C8-C7-O7-C5
33	D	407	LHG	O1-C1-C2-C3
33	D	407	LHG	C1-C2-C3-O3
33	D	407	LHG	C3-O3-P-O5
33	D	407	LHG	C3-O3-P-O6
33	D	407	LHG	C4-O6-P-O5
33	D	408	LHG	O1-C1-C2-C3
33	D	408	LHG	C1-C2-C3-O3
33	D	408	LHG	C4-O6-P-O3
33	D	408	LHG	C4-O6-P-O5
33	G	618	LHG	C4-O6-P-O4
33	G	618	LHG	C4-O6-P-O5
33	K	102	LHG	O1-C1-C2-O2
33	K	102	LHG	O1-C1-C2-C3
33	K	102	LHG	C1-C2-C3-O3
33	K	102	LHG	C3-O3-P-O4
33	K	102	LHG	C3-O3-P-O5
33	K	102	LHG	C3-O3-P-O6
33	K	102	LHG	C4-O6-P-O5
33	K	102	LHG	O9-C7-O7-C5
33	K	102	LHG	C8-C7-O7-C5
33	L	101	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
33	M	101	LHG	C3-O3-P-O5
33	M	101	LHG	O7-C5-C6-O8
33	M	101	LHG	C8-C7-O7-C5
33	N	319	LHG	O1-C1-C2-O2
33	N	319	LHG	O1-C1-C2-C3
33	N	319	LHG	C3-O3-P-O5
33	N	319	LHG	C4-O6-P-O4
33	R	320	LHG	O1-C1-C2-C3
33	R	320	LHG	C4-O6-P-O4
33	S	320	LHG	O1-C1-C2-O2
33	S	320	LHG	O1-C1-C2-C3
33	S	320	LHG	C1-C2-C3-O3
33	S	320	LHG	C3-O3-P-O5
33	S	320	LHG	C4-O6-P-O3
33	S	320	LHG	C4-O6-P-O4
33	S	320	LHG	C4-O6-P-O5
33	S	322	LHG	C1-C2-C3-O3
33	S	322	LHG	O2-C2-C3-O3
33	Y	318	LHG	C1-C2-C3-O3
33	Y	318	LHG	C3-O3-P-O4
33	0	619	LHG	O1-C1-C2-C3
33	0	619	LHG	C4-O6-P-O5
33	0	619	LHG	O7-C5-C6-O8
33	0	619	LHG	C8-C7-O7-C5
33	7	319	LHG	C1-C2-C3-O3
33	7	319	LHG	C4-O6-P-O4
33	8	618	LHG	O1-C1-C2-O2
33	8	618	LHG	C1-C2-C3-O3
33	8	618	LHG	O2-C2-C3-O3
33	8	618	LHG	C4-O6-P-O4
33	8	618	LHG	C4-C5-O7-C7
33	9	320	LHG	O1-C1-C2-C3
33	9	320	LHG	C1-C2-C3-O3
33	9	320	LHG	C4-O6-P-O5
33	p	619	LHG	O1-C1-C2-O2
33	p	619	LHG	C1-C2-C3-O3
33	p	619	LHG	C4-O6-P-O4
33	p	619	LHG	C8-C7-O7-C5
33	q	320	LHG	O1-C1-C2-C3
33	q	320	LHG	C1-C2-C3-O3
33	q	320	LHG	C3-O3-P-O4
33	q	320	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
33	a	415	LHG	C1-C2-C3-O3
33	a	415	LHG	C3-O3-P-O6
33	a	415	LHG	C4-O6-P-O3
33	a	415	LHG	O6-C4-C5-O7
33	b	625	LHG	C4-O6-P-O5
33	b	628	LHG	C3-O3-P-O5
33	b	628	LHG	C4-O6-P-O4
33	c	622	LHG	O1-C1-C2-C3
33	c	622	LHG	C3-O3-P-O5
33	c	622	LHG	C4-O6-P-O4
33	d	408	LHG	O1-C1-C2-C3
33	d	408	LHG	C1-C2-C3-O3
33	d	408	LHG	C4-O6-P-O5
33	e	101	LHG	C4-O6-P-O4
33	g	319	LHG	O1-C1-C2-C3
33	g	319	LHG	C3-O3-P-O5
33	j	102	LHG	C3-O3-P-O4
33	j	102	LHG	C3-O3-P-O5
33	j	102	LHG	C3-O3-P-O6
33	j	102	LHG	O7-C5-C6-O8
33	l	101	LHG	C4-O6-P-O4
33	l	101	LHG	C4-O6-P-O5
33	n	320	LHG	O1-C1-C2-O2
33	n	320	LHG	C1-C2-C3-O3
33	n	320	LHG	O2-C2-C3-O3
33	n	320	LHG	C4-O6-P-O4
33	r	320	LHG	O1-C1-C2-C3
33	r	320	LHG	C4-O6-P-O4
33	s	320	LHG	C1-C2-C3-O3
33	s	320	LHG	C4-O6-P-O3
33	s	320	LHG	C4-O6-P-O4
33	s	320	LHG	C4-O6-P-O5
33	s	320	LHG	O7-C5-C6-O8
33	s	322	LHG	C4-O6-P-O3
33	s	322	LHG	C8-C7-O7-C5
33	t	102	LHG	O1-C1-C2-C3
33	t	102	LHG	C1-C2-C3-O3
33	t	102	LHG	C4-O6-P-O3
33	y	619	LHG	C1-C2-C3-O3
33	y	619	LHG	C3-O3-P-O4
33	y	619	LHG	C3-O3-P-O5
33	y	619	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
33	z	102	LHG	O1-C1-C2-C3
33	z	102	LHG	C1-C2-C3-O3
33	z	102	LHG	C4-O6-P-O3
33	z	102	LHG	C4-O6-P-O5
33	z	102	LHG	O6-C4-C5-O7
33	z	102	LHG	O9-C7-O7-C5
33	z	102	LHG	C8-C7-O7-C5
33	F1	301	LHG	O2-C2-C3-O3
33	F1	301	LHG	C3-O3-P-O5
33	F1	301	LHG	O7-C5-C6-O8
34	4	620	LMG	O6-C1-O1-C7
34	4	620	LMG	C11-C10-O7-C8
34	4	621	LMG	O6-C1-O1-C7
34	4	621	LMG	C11-C10-O7-C8
34	5	620	LMG	C11-C10-O7-C8
34	6	321	LMG	O6-C1-O1-C7
34	6	322	LMG	C2-C1-O1-C7
34	6	322	LMG	O6-C1-O1-C7
34	6	322	LMG	O9-C10-O7-C8
34	6	322	LMG	C11-C10-O7-C8
34	6	323	LMG	O10-C28-O8-C9
34	A	412	LMG	O6-C1-O1-C7
34	A	412	LMG	C9-C8-O7-C10
34	A	414	LMG	O9-C10-O7-C8
34	A	414	LMG	C11-C10-O7-C8
34	A	418	LMG	C11-C10-O7-C8
34	B	622	LMG	C11-C10-O7-C8
34	B	625	LMG	O10-C28-O8-C9
34	C	621	LMG	O9-C10-O7-C8
34	C	621	LMG	C11-C10-O7-C8
34	C	622	LMG	C11-C10-O7-C8
34	G	622	LMG	C2-C1-O1-C7
34	G	622	LMG	O6-C1-O1-C7
34	G	622	LMG	C11-C10-O7-C8
34	I	101	LMG	C11-C10-O7-C8
34	J	102	LMG	C11-C10-O7-C8
34	N	320	LMG	C8-C7-O1-C1
34	N	320	LMG	C11-C10-O7-C8
34	W	202	LMG	O6-C1-O1-C7
34	W	203	LMG	O1-C7-C8-O7
34	W	203	LMG	C11-C10-O7-C8
34	X	202	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	X	203	LMG	O7-C8-C9-O8
34	Y	319	LMG	O6-C1-O1-C7
34	0	620	LMG	C2-C1-O1-C7
34	0	620	LMG	O6-C1-O1-C7
34	0	620	LMG	C11-C10-O7-C8
34	0	622	LMG	C2-C1-O1-C7
34	0	622	LMG	O6-C1-O1-C7
34	7	301	LMG	C2-C1-O1-C7
34	7	301	LMG	O6-C1-O1-C7
34	7	301	LMG	C8-C7-O1-C1
34	7	301	LMG	C11-C10-O7-C8
34	7	322	LMG	C8-C7-O1-C1
34	7	322	LMG	C11-C10-O7-C8
34	9	301	LMG	O9-C10-O7-C8
34	9	301	LMG	C11-C10-O7-C8
34	9	302	LMG	O6-C1-O1-C7
34	9	321	LMG	O6-C1-O1-C7
34	9	321	LMG	C11-C10-O7-C8
34	p	620	LMG	C11-C10-O7-C8
34	q	301	LMG	C2-C1-O1-C7
34	q	301	LMG	C8-C7-O1-C1
34	q	302	LMG	O9-C10-O7-C8
34	a	401	LMG	O9-C10-O7-C8
34	a	401	LMG	C11-C10-O7-C8
34	a	413	LMG	C11-C10-O7-C8
34	b	601	LMG	O6-C1-O1-C7
34	b	601	LMG	C11-C10-O7-C8
34	b	622	LMG	O6-C1-O1-C7
34	b	623	LMG	C11-C10-O7-C8
34	b	624	LMG	O6-C1-O1-C7
34	b	624	LMG	C8-C9-O8-C28
34	b	624	LMG	C11-C10-O7-C8
34	b	624	LMG	O10-C28-O8-C9
34	b	629	LMG	C11-C10-O7-C8
34	c	620	LMG	O6-C1-O1-C7
34	c	621	LMG	C11-C10-O7-C8
34	c	624	LMG	C11-C10-O7-C8
34	f	101	LMG	C11-C10-O7-C8
34	g	322	LMG	O6-C1-O1-C7
34	j	101	LMG	O10-C28-O8-C9
34	k	101	LMG	C11-C10-O7-C8
34	k	102	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	k	102	LMG	O6-C1-O1-C7
34	k	102	LMG	C11-C10-O7-C8
34	m	102	LMG	O6-C1-O1-C7
34	m	102	LMG	C11-C10-O7-C8
34	n	321	LMG	O6-C1-O1-C7
34	n	322	LMG	O6-C1-O1-C7
34	w	201	LMG	O6-C1-O1-C7
34	w	201	LMG	O1-C7-C8-O7
34	w	203	LMG	C11-C10-O7-C8
34	w	204	LMG	C2-C1-O1-C7
34	w	204	LMG	O6-C1-O1-C7
34	w	204	LMG	O9-C10-O7-C8
34	w	204	LMG	C11-C10-O7-C8
34	w	205	LMG	C2-C1-O1-C7
34	w	205	LMG	O6-C1-O1-C7
34	w	205	LMG	O9-C10-O7-C8
34	x	202	LMG	O9-C10-O7-C8
34	x	202	LMG	C11-C10-O7-C8
34	y	620	LMG	C11-C10-O7-C8
34	Q1	101	LMG	O6-C1-O1-C7
34	Q1	101	LMG	O9-C10-O7-C8
34	Q1	101	LMG	C11-C10-O7-C8
34	q1	101	LMG	C8-C7-O1-C1
34	q1	101	LMG	C11-C10-O7-C8
35	2	614	RRX	C23-C24-C25-C30
35	2	614	RRX	C23-C24-C25-C26
35	2	614	RRX	C37-C22-C23-C24
35	2	614	RRX	C21-C22-C23-C24
35	2	614	RRX	C36-C18-C19-C20
35	2	614	RRX	C17-C18-C19-C20
35	2	614	RRX	C11-C12-C13-C14
35	2	614	RRX	C11-C12-C13-C35
35	2	614	RRX	C7-C8-C9-C10
35	2	614	RRX	C7-C8-C9-C34
35	4	615	RRX	C23-C24-C25-C30
35	4	615	RRX	C23-C24-C25-C26
35	4	615	RRX	C37-C22-C23-C24
35	4	615	RRX	C21-C22-C23-C24
35	4	615	RRX	C36-C18-C19-C20
35	4	615	RRX	C17-C18-C19-C20
35	4	615	RRX	C11-C12-C13-C14
35	4	615	RRX	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
35	4	615	RRX	C9-C10-C11-C12
35	4	615	RRX	C7-C8-C9-C10
35	4	615	RRX	C7-C8-C9-C34
35	4	615	RRX	C1-C6-C7-C8
35	G	614	RRX	C23-C24-C25-C30
35	G	614	RRX	C23-C24-C25-C26
35	G	614	RRX	C37-C22-C23-C24
35	G	614	RRX	C21-C22-C23-C24
35	G	614	RRX	C36-C18-C19-C20
35	G	614	RRX	C17-C18-C19-C20
35	G	614	RRX	C11-C12-C13-C14
35	G	614	RRX	C11-C12-C13-C35
35	G	614	RRX	C9-C10-C11-C12
35	G	614	RRX	C7-C8-C9-C10
35	G	614	RRX	C7-C8-C9-C34
35	G	614	RRX	C1-C6-C7-C8
35	9	317	RRX	C23-C24-C25-C30
35	9	317	RRX	C23-C24-C25-C26
35	9	317	RRX	C37-C22-C23-C24
35	9	317	RRX	C21-C22-C23-C24
35	9	317	RRX	C36-C18-C19-C20
35	9	317	RRX	C17-C18-C19-C20
35	9	317	RRX	C11-C12-C13-C14
35	9	317	RRX	C11-C12-C13-C35
35	9	317	RRX	C9-C10-C11-C12
35	9	317	RRX	C7-C8-C9-C10
35	9	317	RRX	C7-C8-C9-C34
35	9	317	RRX	C1-C6-C7-C8
35	q	317	RRX	C23-C24-C25-C30
35	q	317	RRX	C37-C22-C23-C24
35	q	317	RRX	C21-C22-C23-C24
35	q	317	RRX	C7-C8-C9-C10
35	q	317	RRX	C7-C8-C9-C34
35	g	315	RRX	C37-C22-C23-C24
35	g	315	RRX	C7-C8-C9-C10
36	2	616	NEX	C10-C11-C12-C13
36	2	616	NEX	C12-C13-C14-C15
36	2	616	NEX	C20-C13-C14-C15
36	2	616	NEX	C28-C29-C30-C31
36	2	616	NEX	C39-C29-C30-C31
36	2	616	NEX	C31-C32-C33-C34
36	2	616	NEX	C31-C32-C33-C40

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Mol	Chain	Res	Type	Atoms
36	3	319	NEX	C32-C33-C34-C35
36	3	319	NEX	C40-C33-C34-C35
36	4	617	NEX	C10-C11-C12-C13
36	4	617	NEX	C26-C27-C28-C29
36	4	617	NEX	C39-C29-C30-C31
36	5	618	NEX	C10-C11-C12-C13
36	5	618	NEX	C11-C12-C13-C14
36	5	618	NEX	C11-C12-C13-C20
36	5	618	NEX	C14-C15-C35-C34
36	5	618	NEX	C30-C31-C32-C33
36	6	319	NEX	C28-C29-C30-C31
36	6	319	NEX	C39-C29-C30-C31
36	6	319	NEX	C29-C30-C31-C32
36	6	319	NEX	C30-C31-C32-C33
36	N	318	NEX	C10-C11-C12-C13
36	N	318	NEX	C11-C12-C13-C14
36	N	318	NEX	C11-C12-C13-C20
36	N	318	NEX	C32-C33-C34-C35
36	N	318	NEX	C40-C33-C34-C35
36	0	618	NEX	C28-C29-C30-C31
36	0	618	NEX	C39-C29-C30-C31
36	0	618	NEX	C29-C30-C31-C32
36	0	618	NEX	C30-C31-C32-C33
36	8	617	NEX	C11-C12-C13-C14
36	8	617	NEX	C11-C12-C13-C20
36	9	319	NEX	C9-C10-C11-C12
36	9	319	NEX	C10-C11-C12-C13
36	9	319	NEX	C14-C15-C35-C34
36	p	618	NEX	C11-C10-C9-C8
36	p	618	NEX	C11-C10-C9-C19
36	q	319	NEX	C10-C11-C12-C13
36	q	319	NEX	C11-C12-C13-C14
36	q	319	NEX	C11-C12-C13-C20
36	q	319	NEX	C14-C15-C35-C34
36	q	319	NEX	C32-C33-C34-C35
36	q	319	NEX	C40-C33-C34-C35
36	g	317	NEX	C10-C11-C12-C13
36	g	317	NEX	C11-C12-C13-C14
36	g	317	NEX	C11-C12-C13-C20
36	g	317	NEX	C12-C13-C14-C15
36	g	317	NEX	C20-C13-C14-C15
36	g	317	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
36	g	317	NEX	C39-C29-C30-C31
36	n	319	NEX	C11-C10-C9-C8
36	n	319	NEX	C11-C10-C9-C19
36	n	319	NEX	C10-C11-C12-C13
36	n	319	NEX	C11-C12-C13-C14
36	n	319	NEX	C11-C12-C13-C20
36	r	319	NEX	C7-C8-C9-C10
36	r	319	NEX	C28-C29-C30-C31
37	2	619	XAT	C21-C26-C27-C28
37	2	619	XAT	C25-C26-C27-C28
37	2	619	XAT	O24-C26-C27-C28
37	2	619	XAT	C26-C27-C28-C29
37	4	619	XAT	C21-C26-C27-C28
37	4	619	XAT	C25-C26-C27-C28
37	4	619	XAT	O24-C26-C27-C28
37	4	619	XAT	C26-C27-C28-C29
37	G	620	XAT	C21-C26-C27-C28
37	G	620	XAT	C25-C26-C27-C28
37	G	620	XAT	O24-C26-C27-C28
37	G	620	XAT	C26-C27-C28-C29
37	9	322	XAT	C21-C26-C27-C28
37	9	322	XAT	C25-C26-C27-C28
37	9	322	XAT	O24-C26-C27-C28
37	9	322	XAT	C26-C27-C28-C29
37	q	321	XAT	C21-C26-C27-C28
37	q	321	XAT	C25-C26-C27-C28
37	q	321	XAT	O24-C26-C27-C28
37	q	321	XAT	C26-C27-C28-C29
37	g	321	XAT	C21-C26-C27-C28
37	g	321	XAT	C25-C26-C27-C28
37	g	321	XAT	O24-C26-C27-C28
37	g	321	XAT	C26-C27-C28-C29
38	6	301	SQD	O5-C5-C6-S
38	A	411	SQD	O47-C45-C46-O48
38	A	413	SQD	C2-C1-O6-C44
38	A	413	SQD	O5-C1-O6-C44
38	A	413	SQD	O5-C5-C6-S
38	B	620	SQD	O5-C1-O6-C44
38	B	620	SQD	O49-C7-O47-C45
38	B	620	SQD	C8-C7-O47-C45
38	B	623	SQD	C2-C1-O6-C44
38	B	623	SQD	O5-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
38	B	623	SQD	O5-C5-C6-S
38	G	617	SQD	C2-C1-O6-C44
38	G	617	SQD	C8-C7-O47-C45
38	G	617	SQD	O5-C5-C6-S
38	R	322	SQD	O5-C5-C6-S
38	S	301	SQD	O6-C44-C45-O47
38	Y	320	SQD	O5-C1-O6-C44
38	Y	320	SQD	C8-C7-O47-C45
38	0	621	SQD	C2-C1-O6-C44
38	0	621	SQD	O5-C1-O6-C44
38	0	621	SQD	C8-C7-O47-C45
38	0	621	SQD	O5-C5-C6-S
38	a	412	SQD	C2-C1-O6-C44
38	a	412	SQD	O5-C1-O6-C44
38	a	412	SQD	O5-C5-C6-S
38	b	621	SQD	C8-C7-O47-C45
38	b	621	SQD	O5-C5-C6-S
38	b	627	SQD	O5-C5-C6-S
38	g	301	SQD	O5-C1-O6-C44
38	g	301	SQD	O5-C5-C6-S
38	g	318	SQD	C2-C1-O6-C44
38	g	318	SQD	O5-C1-O6-C44
38	r	322	SQD	C2-C1-O6-C44
38	r	322	SQD	O5-C1-O6-C44
38	r	322	SQD	O49-C7-O47-C45
38	r	322	SQD	C8-C7-O47-C45
38	r	322	SQD	O5-C5-C6-S
38	s	301	SQD	C2-C1-O6-C44
38	s	301	SQD	O5-C1-O6-C44
38	s	301	SQD	O5-C5-C6-S
38	x	201	SQD	O5-C5-C6-S
38	y	621	SQD	O6-C44-C45-O47
38	y	621	SQD	C8-C7-O47-C45
42	A	408	PHO	C11-C10-C8-C9
43	B	617	BCR	C7-C8-C9-C10
43	B	617	BCR	C7-C8-C9-C34
43	B	617	BCR	C11-C12-C13-C14
43	B	617	BCR	C11-C12-C13-C35
43	B	617	BCR	C37-C22-C23-C24
43	B	618	BCR	C7-C8-C9-C10
43	B	618	BCR	C7-C8-C9-C34
43	B	618	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
43	B	618	BCR	C11-C12-C13-C35
43	B	618	BCR	C17-C18-C19-C20
43	B	618	BCR	C36-C18-C19-C20
43	B	619	BCR	C1-C6-C7-C8
43	B	619	BCR	C7-C8-C9-C34
43	B	619	BCR	C11-C12-C13-C14
43	B	619	BCR	C11-C12-C13-C35
43	C	614	BCR	C11-C12-C13-C14
43	C	614	BCR	C11-C12-C13-C35
43	C	614	BCR	C17-C18-C19-C20
43	C	614	BCR	C36-C18-C19-C20
43	C	614	BCR	C21-C22-C23-C24
43	C	614	BCR	C37-C22-C23-C24
43	C	615	BCR	C11-C12-C13-C14
43	C	615	BCR	C11-C12-C13-C35
43	D	405	BCR	C11-C12-C13-C14
43	D	405	BCR	C11-C12-C13-C35
43	D	405	BCR	C17-C18-C19-C20
43	D	405	BCR	C36-C18-C19-C20
43	D	405	BCR	C19-C20-C21-C22
43	D	405	BCR	C23-C24-C25-C30
43	H	101	BCR	C7-C8-C9-C10
43	H	101	BCR	C7-C8-C9-C34
43	T	101	BCR	C9-C10-C11-C12
43	T	101	BCR	C21-C22-C23-C24
43	T	101	BCR	C37-C22-C23-C24
43	V	101	BCR	C11-C12-C13-C14
43	V	101	BCR	C11-C12-C13-C35
43	V	101	BCR	C37-C22-C23-C24
43	Z	101	BCR	C11-C12-C13-C14
43	Z	101	BCR	C11-C12-C13-C35
43	a	410	BCR	C1-C6-C7-C8
43	b	618	BCR	C5-C6-C7-C8
43	b	618	BCR	C11-C12-C13-C14
43	b	618	BCR	C11-C12-C13-C35
43	b	618	BCR	C13-C14-C15-C16
43	b	618	BCR	C37-C22-C23-C24
43	b	619	BCR	C7-C8-C9-C10
43	b	619	BCR	C7-C8-C9-C34
43	b	619	BCR	C9-C10-C11-C12
43	b	619	BCR	C17-C18-C19-C20
43	b	619	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
43	b	620	BCR	C11-C12-C13-C14
43	b	620	BCR	C11-C12-C13-C35
43	b	620	BCR	C17-C18-C19-C20
43	b	620	BCR	C36-C18-C19-C20
43	c	614	BCR	C5-C6-C7-C8
43	c	614	BCR	C17-C18-C19-C20
43	c	614	BCR	C36-C18-C19-C20
43	c	614	BCR	C21-C22-C23-C24
43	c	614	BCR	C37-C22-C23-C24
43	c	614	BCR	C23-C24-C25-C26
43	c	615	BCR	C7-C8-C9-C10
43	c	615	BCR	C7-C8-C9-C34
43	c	615	BCR	C11-C12-C13-C14
43	c	615	BCR	C11-C12-C13-C35
43	d	406	BCR	C17-C18-C19-C20
43	d	406	BCR	C36-C18-C19-C20
43	d	406	BCR	C23-C24-C25-C26
43	h	101	BCR	C7-C8-C9-C10
43	h	101	BCR	C7-C8-C9-C34
43	t	101	BCR	C5-C6-C7-C8
43	t	101	BCR	C11-C12-C13-C14
43	t	101	BCR	C11-C12-C13-C35
43	v	101	BCR	C7-C8-C9-C34
43	v	101	BCR	C11-C12-C13-C14
43	v	101	BCR	C11-C12-C13-C35
43	z	101	BCR	C7-C8-C9-C10
43	z	101	BCR	C7-C8-C9-C34
44	A	416	PL9	C7-C8-C9-C11
44	A	416	PL9	C12-C13-C14-C16
44	A	416	PL9	C17-C18-C19-C21
44	A	416	PL9	C32-C33-C34-C36
44	A	416	PL9	C45-C44-C46-C47
44	a	414	PL9	C7-C8-C9-C10
44	a	414	PL9	C7-C8-C9-C11
44	a	414	PL9	C9-C11-C12-C13
44	a	414	PL9	C27-C28-C29-C31
44	a	414	PL9	C32-C33-C34-C35
44	a	414	PL9	C32-C33-C34-C36
44	a	414	PL9	C37-C38-C39-C40
44	a	414	PL9	C37-C38-C39-C41
45	C	616	DGD	C2A-C1A-O1G-C1G
45	C	616	DGD	O1A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
45	C	618	DGD	C2D-C1D-O3G-C3G
45	C	618	DGD	O6D-C1D-O3G-C3G
45	C	620	DGD	C2A-C1A-O1G-C1G
45	C	620	DGD	O1A-C1A-O1G-C1G
45	C	620	DGD	C2B-C1B-O2G-C2G
45	c	616	DGD	O1B-C1B-O2G-C2G
45	c	617	DGD	O1B-C1B-O2G-C2G
45	c	617	DGD	O6E-C1E-O5D-C6D
45	c	618	DGD	C2B-C1B-O2G-C2G
45	c	619	DGD	C2B-C1B-O2G-C2G
48	R	302	LMU	O5'-C1'-O1'-C1
31	1	614	CLA	O1D-CGD-O2D-CED
31	3	316	CLA	O1D-CGD-O2D-CED
31	5	615	CLA	O1D-CGD-O2D-CED
31	6	316	CLA	O1D-CGD-O2D-CED
31	N	315	CLA	O1D-CGD-O2D-CED
31	8	614	CLA	O1D-CGD-O2D-CED
31	9	315	CLA	O1D-CGD-O2D-CED
31	p	613	CLA	O1D-CGD-O2D-CED
31	p	615	CLA	O1D-CGD-O2D-CED
31	g	305	CLA	O1D-CGD-O2D-CED
31	n	316	CLA	O1D-CGD-O2D-CED
31	r	314	CLA	O1D-CGD-O2D-CED
31	s	314	CLA	O1D-CGD-O2D-CED
31	9	306	CLA	C5-C6-C7-C8
31	2	609	CLA	O1D-CGD-O2D-CED
31	6	314	CLA	O1D-CGD-O2D-CED
31	A	405	CLA	O1D-CGD-O2D-CED
31	N	321	CLA	O1D-CGD-O2D-CED
31	7	315	CLA	O1D-CGD-O2D-CED
31	8	611	CLA	O1D-CGD-O2D-CED
31	n	313	CLA	O1D-CGD-O2D-CED
30	2	607	CHL	CBD-CGD-O2D-CED
30	4	606	CHL	CBD-CGD-O2D-CED
30	0	605	CHL	CBD-CGD-O2D-CED
30	p	608	CHL	CBD-CGD-O2D-CED
31	1	611	CLA	CBD-CGD-O2D-CED
31	2	603	CLA	CBD-CGD-O2D-CED
31	2	604	CLA	CBD-CGD-O2D-CED
31	2	610	CLA	CBD-CGD-O2D-CED
31	2	611	CLA	CBD-CGD-O2D-CED
31	2	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	3	304	CLA	CBD-CGD-O2D-CED
31	3	314	CLA	CBD-CGD-O2D-CED
31	3	315	CLA	CBD-CGD-O2D-CED
31	4	602	CLA	CBD-CGD-O2D-CED
31	4	603	CLA	CBD-CGD-O2D-CED
31	4	610	CLA	CBD-CGD-O2D-CED
31	4	611	CLA	CBD-CGD-O2D-CED
31	4	613	CLA	CBD-CGD-O2D-CED
31	4	614	CLA	CBD-CGD-O2D-CED
31	5	603	CLA	CBD-CGD-O2D-CED
31	5	610	CLA	CBD-CGD-O2D-CED
31	5	613	CLA	CBD-CGD-O2D-CED
31	6	303	CLA	CBD-CGD-O2D-CED
31	6	304	CLA	CBD-CGD-O2D-CED
31	6	311	CLA	CBD-CGD-O2D-CED
31	6	312	CLA	CBD-CGD-O2D-CED
31	6	314	CLA	CBD-CGD-O2D-CED
31	A	405	CLA	CBD-CGD-O2D-CED
31	A	409	CLA	CBD-CGD-O2D-CED
31	B	601	CLA	CBD-CGD-O2D-CED
31	B	602	CLA	CBD-CGD-O2D-CED
31	B	608	CLA	CBD-CGD-O2D-CED
31	B	616	CLA	CBD-CGD-O2D-CED
31	C	602	CLA	CBD-CGD-O2D-CED
31	C	603	CLA	CBD-CGD-O2D-CED
31	C	604	CLA	CBD-CGD-O2D-CED
31	C	606	CLA	CBD-CGD-O2D-CED
31	C	611	CLA	CBD-CGD-O2D-CED
31	C	612	CLA	CBD-CGD-O2D-CED
31	D	404	CLA	CBD-CGD-O2D-CED
31	G	609	CLA	CBD-CGD-O2D-CED
31	G	611	CLA	CBD-CGD-O2D-CED
31	G	613	CLA	CBD-CGD-O2D-CED
31	N	312	CLA	CBD-CGD-O2D-CED
31	N	313	CLA	CBD-CGD-O2D-CED
31	N	315	CLA	CBD-CGD-O2D-CED
31	R	303	CLA	CBD-CGD-O2D-CED
31	R	305	CLA	CBD-CGD-O2D-CED
31	R	311	CLA	CBD-CGD-O2D-CED
31	R	312	CLA	CBD-CGD-O2D-CED
31	S	304	CLA	CBD-CGD-O2D-CED
31	S	305	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	S	315	CLA	CBD-CGD-O2D-CED
31	Y	305	CLA	CBD-CGD-O2D-CED
31	Y	310	CLA	CBD-CGD-O2D-CED
31	0	603	CLA	CBD-CGD-O2D-CED
31	0	604	CLA	CBD-CGD-O2D-CED
31	0	611	CLA	CBD-CGD-O2D-CED
31	7	304	CLA	CBD-CGD-O2D-CED
31	7	305	CLA	CBD-CGD-O2D-CED
31	7	311	CLA	CBD-CGD-O2D-CED
31	8	609	CLA	CBD-CGD-O2D-CED
31	8	611	CLA	CBD-CGD-O2D-CED
31	8	613	CLA	CBD-CGD-O2D-CED
31	9	306	CLA	CBD-CGD-O2D-CED
31	9	313	CLA	CBD-CGD-O2D-CED
31	p	602	CLA	CBD-CGD-O2D-CED
31	p	603	CLA	CBD-CGD-O2D-CED
31	p	604	CLA	CBD-CGD-O2D-CED
31	p	615	CLA	CBD-CGD-O2D-CED
31	q	304	CLA	CBD-CGD-O2D-CED
31	q	305	CLA	CBD-CGD-O2D-CED
31	q	306	CLA	CBD-CGD-O2D-CED
31	q	314	CLA	CBD-CGD-O2D-CED
31	q	315	CLA	CBD-CGD-O2D-CED
31	a	406	CLA	CBD-CGD-O2D-CED
31	a	409	CLA	CBD-CGD-O2D-CED
31	b	602	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	CBD-CGD-O2D-CED
31	b	609	CLA	CBD-CGD-O2D-CED
31	b	615	CLA	CBD-CGD-O2D-CED
31	b	617	CLA	CBD-CGD-O2D-CED
31	c	602	CLA	CBD-CGD-O2D-CED
31	c	606	CLA	CBD-CGD-O2D-CED
31	c	610	CLA	CBD-CGD-O2D-CED
31	c	611	CLA	CBD-CGD-O2D-CED
31	c	613	CLA	CBD-CGD-O2D-CED
31	g	305	CLA	CBD-CGD-O2D-CED
31	g	311	CLA	CBD-CGD-O2D-CED
31	g	312	CLA	CBD-CGD-O2D-CED
31	g	313	CLA	CBD-CGD-O2D-CED
31	n	313	CLA	CBD-CGD-O2D-CED
31	n	315	CLA	CBD-CGD-O2D-CED
31	n	316	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	r	305	CLA	CBD-CGD-O2D-CED
31	r	306	CLA	CBD-CGD-O2D-CED
31	r	312	CLA	CBD-CGD-O2D-CED
31	r	314	CLA	CBD-CGD-O2D-CED
31	r	315	CLA	CBD-CGD-O2D-CED
31	r	316	CLA	CBD-CGD-O2D-CED
31	s	304	CLA	CBD-CGD-O2D-CED
31	s	311	CLA	CBD-CGD-O2D-CED
31	y	603	CLA	CBD-CGD-O2D-CED
31	y	604	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	O1A-CGA-O2A-C1
31	1	611	CLA	O1A-CGA-O2A-C1
31	2	610	CLA	O1A-CGA-O2A-C1
31	5	604	CLA	O1A-CGA-O2A-C1
31	5	610	CLA	O1A-CGA-O2A-C1
31	5	614	CLA	O1A-CGA-O2A-C1
31	6	313	CLA	O1A-CGA-O2A-C1
31	6	315	CLA	O1A-CGA-O2A-C1
31	B	601	CLA	O1A-CGA-O2A-C1
31	B	602	CLA	O1A-CGA-O2A-C1
31	B	614	CLA	O1A-CGA-O2A-C1
31	B	616	CLA	O1A-CGA-O2A-C1
31	G	603	CLA	O1A-CGA-O2A-C1
31	N	304	CLA	O1A-CGA-O2A-C1
31	R	316	CLA	O1A-CGA-O2A-C1
31	S	306	CLA	O1A-CGA-O2A-C1
31	p	610	CLA	O1A-CGA-O2A-C1
31	b	615	CLA	O1A-CGA-O2A-C1
31	g	304	CLA	O1A-CGA-O2A-C1
31	r	312	CLA	O1A-CGA-O2A-C1
31	r	313	CLA	O1A-CGA-O2A-C1
33	K	102	LHG	O10-C'23-O8-C6
34	4	620	LMG	O10-C'28-O8-C9
34	A	418	LMG	O10-C'28-O8-C9
34	B	621	LMG	O10-C'28-O8-C9
34	C	624	LMG	O10-C'28-O8-C9
34	D	410	LMG	O10-C'28-O8-C9
34	G	621	LMG	O10-C'28-O8-C9
34	0	620	LMG	O10-C'28-O8-C9
34	a	416	LMG	O10-C'28-O8-C9
34	b	629	LMG	O10-C'28-O8-C9
34	f	101	LMG	O10-C'28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	w	203	LMG	O10-C28-O8-C9
38	0	621	SQD	O10-C23-O48-C46
38	g	301	SQD	O10-C23-O48-C46
31	4	612	CLA	O1A-CGA-O2A-C1
31	5	615	CLA	O1A-CGA-O2A-C1
31	S	316	CLA	O1A-CGA-O2A-C1
31	q	314	CLA	O1A-CGA-O2A-C1
48	c	623	LMU	C4B-C5B-C6B-O6B
30	7	307	CHL	O1D-CGD-O2D-CED
30	9	309	CHL	O1D-CGD-O2D-CED
31	2	602	CLA	O1D-CGD-O2D-CED
31	2	612	CLA	O1D-CGD-O2D-CED
31	4	613	CLA	O1D-CGD-O2D-CED
31	5	614	CLA	O1D-CGD-O2D-CED
31	6	311	CLA	O1D-CGD-O2D-CED
31	S	314	CLA	O1D-CGD-O2D-CED
31	0	613	CLA	O1D-CGD-O2D-CED
31	q	314	CLA	O1D-CGD-O2D-CED
31	q	315	CLA	O1D-CGD-O2D-CED
31	a	406	CLA	O1D-CGD-O2D-CED
31	g	313	CLA	O1D-CGD-O2D-CED
31	n	314	CLA	O1D-CGD-O2D-CED
31	4	612	CLA	CBA-CGA-O2A-C1
31	5	615	CLA	CBA-CGA-O2A-C1
31	9	316	CLA	CBA-CGA-O2A-C1
31	q	314	CLA	CBA-CGA-O2A-C1
48	r	302	LMU	O5B-C1B-O1B-C4'
30	4	606	CHL	O1D-CGD-O2D-CED
31	2	613	CLA	O1D-CGD-O2D-CED
31	3	305	CLA	O1D-CGD-O2D-CED
31	3	312	CLA	O1D-CGD-O2D-CED
31	B	605	CLA	O1D-CGD-O2D-CED
31	C	603	CLA	O1D-CGD-O2D-CED
31	R	314	CLA	O1D-CGD-O2D-CED
31	S	310	CLA	O1D-CGD-O2D-CED
31	S	316	CLA	O1D-CGD-O2D-CED
31	Y	313	CLA	O1D-CGD-O2D-CED
31	7	314	CLA	O1D-CGD-O2D-CED
31	8	612	CLA	O1D-CGD-O2D-CED
31	9	314	CLA	O1D-CGD-O2D-CED
31	p	610	CLA	O1D-CGD-O2D-CED
31	q	312	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	b	607	CLA	O1D-CGD-O2D-CED
31	c	603	CLA	O1D-CGD-O2D-CED
31	r	313	CLA	O1D-CGD-O2D-CED
31	s	316	CLA	O1D-CGD-O2D-CED
31	1	604	CLA	CBA-CGA-O2A-C1
31	1	611	CLA	CBA-CGA-O2A-C1
31	2	610	CLA	CBA-CGA-O2A-C1
31	5	604	CLA	CBA-CGA-O2A-C1
31	5	610	CLA	CBA-CGA-O2A-C1
31	5	614	CLA	CBA-CGA-O2A-C1
31	6	313	CLA	CBA-CGA-O2A-C1
31	6	315	CLA	CBA-CGA-O2A-C1
31	B	616	CLA	CBA-CGA-O2A-C1
31	S	306	CLA	CBA-CGA-O2A-C1
31	0	611	CLA	CBA-CGA-O2A-C1
31	p	610	CLA	CBA-CGA-O2A-C1
31	q	312	CLA	CBA-CGA-O2A-C1
31	b	615	CLA	CBA-CGA-O2A-C1
31	g	304	CLA	CBA-CGA-O2A-C1
31	r	312	CLA	CBA-CGA-O2A-C1
31	r	313	CLA	CBA-CGA-O2A-C1
33	K	102	LHG	C24-C23-O8-C6
34	A	418	LMG	C29-C28-O8-C9
34	B	621	LMG	C29-C28-O8-C9
34	D	410	LMG	C29-C28-O8-C9
34	G	621	LMG	C29-C28-O8-C9
34	a	416	LMG	C29-C28-O8-C9
34	f	101	LMG	C29-C28-O8-C9
34	w	203	LMG	C29-C28-O8-C9
34	x	202	LMG	C29-C28-O8-C9
38	B	620	SQD	C24-C23-O48-C46
38	g	301	SQD	C24-C23-O48-C46
30	1	607	CHL	CBD-CGD-O2D-CED
30	q	307	CHL	CBD-CGD-O2D-CED
30	q	309	CHL	CBD-CGD-O2D-CED
30	q	310	CHL	CBD-CGD-O2D-CED
30	g	308	CHL	CBD-CGD-O2D-CED
30	n	301	CHL	CBD-CGD-O2D-CED
31	1	602	CLA	CBD-CGD-O2D-CED
31	1	604	CLA	CBD-CGD-O2D-CED
31	3	311	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	C	610	CLA	CBD-CGD-O2D-CED
31	C	613	CLA	CBD-CGD-O2D-CED
31	G	603	CLA	CBD-CGD-O2D-CED
31	G	604	CLA	CBD-CGD-O2D-CED
31	G	610	CLA	CBD-CGD-O2D-CED
31	N	303	CLA	CBD-CGD-O2D-CED
31	N	310	CLA	CBD-CGD-O2D-CED
31	R	307	CLA	CBD-CGD-O2D-CED
31	R	315	CLA	CBD-CGD-O2D-CED
31	R	316	CLA	CBD-CGD-O2D-CED
31	S	312	CLA	CBD-CGD-O2D-CED
31	Y	304	CLA	CBD-CGD-O2D-CED
31	Y	311	CLA	CBD-CGD-O2D-CED
31	Y	312	CLA	CBD-CGD-O2D-CED
31	0	602	CLA	CBD-CGD-O2D-CED
31	0	610	CLA	CBD-CGD-O2D-CED
31	0	612	CLA	CBD-CGD-O2D-CED
31	7	303	CLA	CBD-CGD-O2D-CED
31	8	602	CLA	CBD-CGD-O2D-CED
31	8	603	CLA	CBD-CGD-O2D-CED
31	8	604	CLA	CBD-CGD-O2D-CED
31	9	304	CLA	CBD-CGD-O2D-CED
31	9	312	CLA	CBD-CGD-O2D-CED
31	9	316	CLA	CBD-CGD-O2D-CED
31	b	603	CLA	CBD-CGD-O2D-CED
31	b	612	CLA	CBD-CGD-O2D-CED
31	b	616	CLA	CBD-CGD-O2D-CED
31	c	604	CLA	CBD-CGD-O2D-CED
31	c	612	CLA	CBD-CGD-O2D-CED
31	d	404	CLA	CBD-CGD-O2D-CED
31	g	303	CLA	CBD-CGD-O2D-CED
31	g	304	CLA	CBD-CGD-O2D-CED
31	g	310	CLA	CBD-CGD-O2D-CED
31	n	303	CLA	CBD-CGD-O2D-CED
31	n	304	CLA	CBD-CGD-O2D-CED
31	n	305	CLA	CBD-CGD-O2D-CED
31	n	311	CLA	CBD-CGD-O2D-CED
31	r	303	CLA	CBD-CGD-O2D-CED
31	r	307	CLA	CBD-CGD-O2D-CED
31	s	310	CLA	CBD-CGD-O2D-CED
31	s	312	CLA	CBD-CGD-O2D-CED
31	s	315	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	y	615	CLA	CBD-CGD-O2D-CED
31	3	315	CLA	O1A-CGA-O2A-C1
31	5	611	CLA	O1A-CGA-O2A-C1
31	5	613	CLA	O1A-CGA-O2A-C1
31	6	312	CLA	O1A-CGA-O2A-C1
31	6	314	CLA	O1A-CGA-O2A-C1
31	B	610	CLA	O1A-CGA-O2A-C1
31	R	303	CLA	O1A-CGA-O2A-C1
31	R	311	CLA	O1A-CGA-O2A-C1
31	R	312	CLA	O1A-CGA-O2A-C1
31	R	313	CLA	O1A-CGA-O2A-C1
31	R	315	CLA	O1A-CGA-O2A-C1
31	S	303	CLA	O1A-CGA-O2A-C1
31	Y	304	CLA	O1A-CGA-O2A-C1
31	Y	305	CLA	O1A-CGA-O2A-C1
31	0	611	CLA	O1A-CGA-O2A-C1
31	0	615	CLA	O1A-CGA-O2A-C1
31	7	304	CLA	O1A-CGA-O2A-C1
31	7	305	CLA	O1A-CGA-O2A-C1
31	7	316	CLA	O1A-CGA-O2A-C1
31	9	305	CLA	O1A-CGA-O2A-C1
31	9	313	CLA	O1A-CGA-O2A-C1
31	9	314	CLA	O1A-CGA-O2A-C1
31	p	603	CLA	O1A-CGA-O2A-C1
31	p	604	CLA	O1A-CGA-O2A-C1
31	p	614	CLA	O1A-CGA-O2A-C1
31	q	306	CLA	O1A-CGA-O2A-C1
31	g	314	CLA	O1A-CGA-O2A-C1
31	r	303	CLA	O1A-CGA-O2A-C1
31	r	311	CLA	O1A-CGA-O2A-C1
31	y	603	CLA	O1A-CGA-O2A-C1
33	p	619	LHG	O10-C'23-O8-C6
33	q	320	LHG	O10-C'23-O8-C6
33	z	102	LHG	O10-C'23-O8-C6
34	1	618	LMG	O10-C'28-O8-C9
34	2	618	LMG	O10-C'28-O8-C9
34	6	321	LMG	O10-C'28-O8-C9
34	6	322	LMG	O10-C'28-O8-C9
34	D	409	LMG	O10-C'28-O8-C9
34	G	619	LMG	O10-C'28-O8-C9
34	G	622	LMG	O10-C'28-O8-C9
34	I	101	LMG	O10-C'28-O8-C9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
34	J	101	LMG	O10-C28-O8-C9
34	N	320	LMG	O10-C28-O8-C9
34	R	321	LMG	O10-C28-O8-C9
34	W	201	LMG	O10-C28-O8-C9
34	W	202	LMG	O10-C28-O8-C9
34	X	202	LMG	O10-C28-O8-C9
34	7	320	LMG	O10-C28-O8-C9
34	7	322	LMG	O10-C28-O8-C9
34	9	302	LMG	O10-C28-O8-C9
34	9	321	LMG	O10-C28-O8-C9
34	p	620	LMG	O10-C28-O8-C9
34	q	301	LMG	O10-C28-O8-C9
34	q	302	LMG	O10-C28-O8-C9
34	a	401	LMG	O10-C28-O8-C9
34	b	601	LMG	O10-C28-O8-C9
34	b	626	LMG	O10-C28-O8-C9
34	c	620	LMG	O10-C28-O8-C9
34	c	624	LMG	O10-C28-O8-C9
34	g	320	LMG	O10-C28-O8-C9
34	g	322	LMG	O10-C28-O8-C9
34	m	102	LMG	O10-C28-O8-C9
34	n	322	LMG	O10-C28-O8-C9
34	x	202	LMG	O10-C28-O8-C9
34	Q1	101	LMG	O10-C28-O8-C9
34	q1	101	LMG	O10-C28-O8-C9
38	B	620	SQD	O10-C23-O48-C46
38	G	624	SQD	O10-C23-O48-C46
38	R	322	SQD	O10-C23-O48-C46
38	X	201	SQD	O10-C23-O48-C46
31	9	316	CLA	O1A-CGA-O2A-C1
31	s	316	CLA	O1A-CGA-O2A-C1
31	1	610	CLA	O1D-CGD-O2D-CED
31	1	613	CLA	O1D-CGD-O2D-CED
31	q	316	CLA	O1D-CGD-O2D-CED
31	b	606	CLA	O1D-CGD-O2D-CED
31	b	614	CLA	O1D-CGD-O2D-CED
31	1	603	CLA	O1D-CGD-O2D-CED
31	5	602	CLA	O1D-CGD-O2D-CED
31	B	613	CLA	O1D-CGD-O2D-CED
31	B	614	CLA	O1D-CGD-O2D-CED
31	G	612	CLA	O1D-CGD-O2D-CED
31	R	313	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	b	610	CLA	O1D-CGD-O2D-CED
31	d	405	CLA	O1D-CGD-O2D-CED
31	g	314	CLA	O1D-CGD-O2D-CED
31	r	311	CLA	O1D-CGD-O2D-CED
30	4	609	CHL	CBD-CGD-O2D-CED
30	N	301	CHL	CBD-CGD-O2D-CED
30	Y	308	CHL	CBD-CGD-O2D-CED
31	5	612	CLA	CBD-CGD-O2D-CED
31	6	305	CLA	CBD-CGD-O2D-CED
31	C	601	CLA	CBD-CGD-O2D-CED
31	N	305	CLA	CBD-CGD-O2D-CED
31	7	313	CLA	CBD-CGD-O2D-CED
31	c	601	CLA	CBD-CGD-O2D-CED
31	c	607	CLA	CBD-CGD-O2D-CED
31	B	603	CLA	O1D-CGD-O2D-CED
31	B	606	CLA	O1D-CGD-O2D-CED
31	B	609	CLA	O1D-CGD-O2D-CED
31	N	313	CLA	O1D-CGD-O2D-CED
31	R	311	CLA	O1D-CGD-O2D-CED
31	S	315	CLA	O1D-CGD-O2D-CED
31	b	604	CLA	O1D-CGD-O2D-CED
31	s	311	CLA	O1D-CGD-O2D-CED
33	1	617	LHG	O9-C7-O7-C5
33	C	623	LHG	O9-C7-O7-C5
33	0	619	LHG	O9-C7-O7-C5
33	7	319	LHG	O9-C7-O7-C5
33	p	619	LHG	O9-C7-O7-C5
33	s	322	LHG	O9-C7-O7-C5
34	2	621	LMG	O9-C10-O7-C8
34	4	620	LMG	O9-C10-O7-C8
34	4	621	LMG	O9-C10-O7-C8
34	A	412	LMG	O9-C10-O7-C8
34	B	622	LMG	O9-C10-O7-C8
34	C	622	LMG	O9-C10-O7-C8
34	G	622	LMG	O9-C10-O7-C8
34	I	101	LMG	O9-C10-O7-C8
34	J	102	LMG	O9-C10-O7-C8
34	N	320	LMG	O9-C10-O7-C8
34	W	203	LMG	O9-C10-O7-C8
34	0	620	LMG	O9-C10-O7-C8
34	7	301	LMG	O9-C10-O7-C8
34	9	321	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
34	p	620	LMG	O9-C10-O7-C8
34	a	413	LMG	O9-C10-O7-C8
34	a	416	LMG	O9-C10-O7-C8
34	b	601	LMG	O9-C10-O7-C8
34	b	623	LMG	O9-C10-O7-C8
34	b	624	LMG	O9-C10-O7-C8
34	b	629	LMG	O9-C10-O7-C8
34	c	620	LMG	O9-C10-O7-C8
34	c	621	LMG	O9-C10-O7-C8
34	c	624	LMG	O9-C10-O7-C8
34	f	101	LMG	O9-C10-O7-C8
34	g	320	LMG	O9-C10-O7-C8
34	k	101	LMG	O9-C10-O7-C8
34	k	102	LMG	O9-C10-O7-C8
34	m	102	LMG	O9-C10-O7-C8
34	w	203	LMG	O9-C10-O7-C8
34	y	620	LMG	O9-C10-O7-C8
34	q1	101	LMG	O9-C10-O7-C8
38	G	617	SQD	O49-C7-O47-C45
38	0	621	SQD	O49-C7-O47-C45
38	b	621	SQD	O49-C7-O47-C45
38	y	621	SQD	O49-C7-O47-C45
45	C	620	DGD	O1B-C1B-O2G-C2G
45	c	619	DGD	O1B-C1B-O2G-C2G
48	K	101	LMU	C4B-C5B-C6B-O6B
31	p	612	CLA	O1A-CGA-O2A-C1
31	p	615	CLA	O1A-CGA-O2A-C1
31	1	613	CLA	C3-C5-C6-C7
31	2	603	CLA	C3-C5-C6-C7
31	2	611	CLA	C3-C5-C6-C7
31	2	612	CLA	C3-C5-C6-C7
31	2	613	CLA	C3-C5-C6-C7
31	3	301	CLA	C3-C5-C6-C7
31	4	602	CLA	C3-C5-C6-C7
31	6	304	CLA	C3-C5-C6-C7
31	6	305	CLA	C3-C5-C6-C7
31	6	311	CLA	C3-C5-C6-C7
31	6	313	CLA	C3-C5-C6-C7
31	6	314	CLA	C3-C5-C6-C7
31	A	409	CLA	C3-C5-C6-C7
31	B	602	CLA	C3-C5-C6-C7
31	B	604	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	C	604	CLA	C3-C5-C6-C7
31	C	609	CLA	C3-C5-C6-C7
31	D	403	CLA	C3-C5-C6-C7
31	G	603	CLA	C3-C5-C6-C7
31	G	612	CLA	C3-C5-C6-C7
31	N	304	CLA	C3-C5-C6-C7
31	R	312	CLA	C3-C5-C6-C7
31	S	311	CLA	C3-C5-C6-C7
31	S	313	CLA	C3-C5-C6-C7
31	Y	305	CLA	C3-C5-C6-C7
31	0	604	CLA	C3-C5-C6-C7
31	0	610	CLA	C3-C5-C6-C7
31	0	613	CLA	C3-C5-C6-C7
31	8	612	CLA	C3-C5-C6-C7
31	p	603	CLA	C3-C5-C6-C7
31	q	315	CLA	C3-C5-C6-C7
31	a	409	CLA	C3-C5-C6-C7
31	b	605	CLA	C3-C5-C6-C7
31	b	608	CLA	C3-C5-C6-C7
31	b	615	CLA	C3-C5-C6-C7
31	b	617	CLA	C3-C5-C6-C7
31	c	606	CLA	C3-C5-C6-C7
31	c	608	CLA	C3-C5-C6-C7
31	c	613	CLA	C3-C5-C6-C7
31	d	405	CLA	C3-C5-C6-C7
31	n	314	CLA	C3-C5-C6-C7
31	r	315	CLA	C3-C5-C6-C7
31	s	311	CLA	C3-C5-C6-C7
31	s	313	CLA	C3-C5-C6-C7
31	y	612	CLA	C3-C5-C6-C7
31	y	614	CLA	C3-C5-C6-C7
42	D	401	PHO	C3-C5-C6-C7
42	d	402	PHO	C3-C5-C6-C7
30	5	607	CHL	CBA-CGA-O2A-C1
31	3	315	CLA	CBA-CGA-O2A-C1
31	4	613	CLA	CBA-CGA-O2A-C1
31	5	613	CLA	CBA-CGA-O2A-C1
31	6	304	CLA	CBA-CGA-O2A-C1
31	6	312	CLA	CBA-CGA-O2A-C1
31	6	314	CLA	CBA-CGA-O2A-C1
31	A	409	CLA	CBA-CGA-O2A-C1
31	B	601	CLA	CBA-CGA-O2A-C1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
31	B	610	CLA	CBA-CGA-O2A-C1
31	B	614	CLA	CBA-CGA-O2A-C1
31	N	304	CLA	CBA-CGA-O2A-C1
31	R	303	CLA	CBA-CGA-O2A-C1
31	R	311	CLA	CBA-CGA-O2A-C1
31	R	313	CLA	CBA-CGA-O2A-C1
31	R	316	CLA	CBA-CGA-O2A-C1
31	S	303	CLA	CBA-CGA-O2A-C1
31	Y	304	CLA	CBA-CGA-O2A-C1
31	0	615	CLA	CBA-CGA-O2A-C1
31	7	305	CLA	CBA-CGA-O2A-C1
31	9	305	CLA	CBA-CGA-O2A-C1
31	9	313	CLA	CBA-CGA-O2A-C1
31	p	614	CLA	CBA-CGA-O2A-C1
31	q	306	CLA	CBA-CGA-O2A-C1
31	a	409	CLA	CBA-CGA-O2A-C1
31	c	609	CLA	CBA-CGA-O2A-C1
31	y	603	CLA	CBA-CGA-O2A-C1
33	q	320	LHG	C24-C23-O8-C6
33	z	102	LHG	C24-C23-O8-C6
34	1	618	LMG	C29-C28-O8-C9
34	2	618	LMG	C29-C28-O8-C9
34	4	620	LMG	C29-C28-O8-C9
34	6	323	LMG	C29-C28-O8-C9
34	B	625	LMG	C29-C28-O8-C9
34	C	624	LMG	C29-C28-O8-C9
34	D	409	LMG	C29-C28-O8-C9
34	G	619	LMG	C29-C28-O8-C9
34	I	101	LMG	C29-C28-O8-C9
34	J	101	LMG	C29-C28-O8-C9
34	N	320	LMG	C29-C28-O8-C9
34	R	321	LMG	C29-C28-O8-C9
34	0	620	LMG	C29-C28-O8-C9
34	7	320	LMG	C29-C28-O8-C9
34	7	322	LMG	C29-C28-O8-C9
34	9	321	LMG	C29-C28-O8-C9
34	q	301	LMG	C29-C28-O8-C9
34	b	601	LMG	C29-C28-O8-C9
34	b	624	LMG	C29-C28-O8-C9
34	b	626	LMG	C29-C28-O8-C9
34	b	629	LMG	C29-C28-O8-C9
34	c	620	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
34	j	101	LMG	C29-C28-O8-C9
34	m	102	LMG	C29-C28-O8-C9
34	n	322	LMG	C29-C28-O8-C9
34	Q1	101	LMG	C29-C28-O8-C9
34	q1	101	LMG	C29-C28-O8-C9
38	G	624	SQD	C24-C23-O48-C46
38	X	201	SQD	C24-C23-O48-C46
38	0	621	SQD	C24-C23-O48-C46
31	9	313	CLA	C2-C1-O2A-CGA
31	1	610	CLA	C5-C6-C7-C8
33	1	617	LHG	C8-C7-O7-C5
33	5	619	LHG	C8-C7-O7-C5
33	7	319	LHG	C8-C7-O7-C5
34	2	621	LMG	C11-C10-O7-C8
34	6	321	LMG	C11-C10-O7-C8
34	q	302	LMG	C11-C10-O7-C8
34	a	416	LMG	C11-C10-O7-C8
34	c	620	LMG	C11-C10-O7-C8
34	g	320	LMG	C11-C10-O7-C8
34	w	205	LMG	C11-C10-O7-C8
45	c	616	DGD	C2B-C1B-O2G-C2G
45	c	617	DGD	C2B-C1B-O2G-C2G
31	3	314	CLA	O1D-CGD-O2D-CED
31	3	315	CLA	O1D-CGD-O2D-CED
31	4	602	CLA	O1D-CGD-O2D-CED
31	C	606	CLA	O1D-CGD-O2D-CED
31	S	304	CLA	O1D-CGD-O2D-CED
31	9	313	CLA	O1D-CGD-O2D-CED
31	n	315	CLA	O1D-CGD-O2D-CED
30	7	310	CHL	CBD-CGD-O2D-CED
31	3	313	CLA	CBD-CGD-O2D-CED
31	C	609	CLA	CBD-CGD-O2D-CED
31	y	602	CLA	CBD-CGD-O2D-CED
31	y	610	CLA	CBD-CGD-O2D-CED
31	N	310	CLA	O1A-CGA-O2A-C1
48	c	623	LMU	O5B-C5B-C6B-O6B
31	p	612	CLA	CBA-CGA-O2A-C1
31	p	615	CLA	CBA-CGA-O2A-C1
31	D	403	CLA	C4-C3-C5-C6
31	p	602	CLA	C4-C3-C5-C6
31	b	605	CLA	C4-C3-C5-C6
31	s	310	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	D	404	CLA	C2-C3-C5-C6
30	R	309	CHL	CBD-CGD-O2D-CED
30	0	607	CHL	CBD-CGD-O2D-CED
31	1	612	CLA	CBD-CGD-O2D-CED
31	B	611	CLA	CBD-CGD-O2D-CED
31	p	611	CLA	CBD-CGD-O2D-CED
31	p	612	CLA	CBD-CGD-O2D-CED
31	b	611	CLA	CBD-CGD-O2D-CED
31	c	609	CLA	CBD-CGD-O2D-CED
30	y	605	CHL	C2A-CAA-CBA-CGA
31	2	609	CLA	C2A-CAA-CBA-CGA
31	3	312	CLA	C2A-CAA-CBA-CGA
31	6	314	CLA	C2A-CAA-CBA-CGA
31	B	606	CLA	C2A-CAA-CBA-CGA
31	D	404	CLA	C2A-CAA-CBA-CGA
31	R	316	CLA	C2A-CAA-CBA-CGA
31	S	303	CLA	C2A-CAA-CBA-CGA
31	7	312	CLA	C2A-CAA-CBA-CGA
31	9	316	CLA	C2A-CAA-CBA-CGA
31	a	406	CLA	C2A-CAA-CBA-CGA
31	r	312	CLA	C2A-CAA-CBA-CGA
31	s	312	CLA	C2A-CAA-CBA-CGA
31	s	314	CLA	C2A-CAA-CBA-CGA
31	A	409	CLA	O1A-CGA-O2A-C1
31	a	409	CLA	O1A-CGA-O2A-C1
30	0	605	CHL	O1D-CGD-O2D-CED
31	2	611	CLA	O1D-CGD-O2D-CED
31	5	603	CLA	O1D-CGD-O2D-CED
31	b	615	CLA	O1D-CGD-O2D-CED
33	G	618	LHG	C13-C14-C15-C16
34	2	620	LMG	C17-C18-C19-C20
34	2	620	LMG	C35-C36-C37-C38
34	2	620	LMG	C38-C39-C40-C41
34	4	620	LMG	C17-C18-C19-C20
34	4	620	LMG	C35-C36-C37-C38
34	4	620	LMG	C38-C39-C40-C41
34	B	621	LMG	C17-C18-C19-C20
34	B	621	LMG	C20-C21-C22-C23
34	C	619	LMG	C20-C21-C22-C23
34	C	619	LMG	C35-C36-C37-C38
34	C	624	LMG	C17-C18-C19-C20
34	D	410	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
34	D	410	LMG	C20-C21-C22-C23
34	D	411	LMG	C17-C18-C19-C20
34	D	411	LMG	C20-C21-C22-C23
34	D	411	LMG	C35-C36-C37-C38
34	D	412	LMG	C35-C36-C37-C38
34	D	412	LMG	C38-C39-C40-C41
34	G	621	LMG	C20-C21-C22-C23
34	G	621	LMG	C35-C36-C37-C38
34	G	621	LMG	C38-C39-C40-C41
34	J	101	LMG	C20-C21-C22-C23
34	J	101	LMG	C35-C36-C37-C38
34	S	321	LMG	C17-C18-C19-C20
34	W	201	LMG	C38-C39-C40-C41
34	9	301	LMG	C20-C21-C22-C23
34	9	301	LMG	C35-C36-C37-C38
34	9	301	LMG	C38-C39-C40-C41
34	q	301	LMG	C17-C18-C19-C20
34	q	301	LMG	C35-C36-C37-C38
34	q	301	LMG	C38-C39-C40-C41
34	b	622	LMG	C17-C18-C19-C20
34	b	622	LMG	C20-C21-C22-C23
34	b	626	LMG	C17-C18-C19-C20
34	b	626	LMG	C20-C21-C22-C23
34	c	624	LMG	C35-C36-C37-C38
34	c	624	LMG	C38-C39-C40-C41
34	d	410	LMG	C17-C18-C19-C20
34	d	410	LMG	C20-C21-C22-C23
34	d	410	LMG	C35-C36-C37-C38
34	d	411	LMG	C35-C36-C37-C38
34	d	411	LMG	C38-C39-C40-C41
34	g	322	LMG	C35-C36-C37-C38
34	g	322	LMG	C38-C39-C40-C41
34	k	101	LMG	C17-C18-C19-C20
34	k	101	LMG	C35-C36-C37-C38
34	s	321	LMG	C17-C18-C19-C20
34	w	201	LMG	C35-C36-C37-C38
45	C	617	DGD	CBB-CCB-CDB-CEB
45	C	618	DGD	CEA-CFA-CGA-CHA
45	C	618	DGD	C8B-C9B-CAB-CBB
45	C	618	DGD	CBB-CCB-CDB-CEB
45	C	620	DGD	CBA-CCA-CDA-CEA
45	C	620	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
45	C	620	DGD	CEB-CFB-CGB-CHB
45	c	616	DGD	C8A-C9A-CAA-CBA
45	c	616	DGD	CBB-CCB-CDB-CEB
45	c	616	DGD	CEB-CFB-CGB-CHB
45	c	617	DGD	C8B-C9B-CAB-CBB
45	c	617	DGD	CBB-CCB-CDB-CEB
45	c	618	DGD	C8A-C9A-CAA-CBA
45	c	618	DGD	CBB-CCB-CDB-CEB
45	c	619	DGD	CEA-CFA-CGA-CHA
45	c	619	DGD	CBB-CCB-CDB-CEB
45	c	619	DGD	CEB-CFB-CGB-CHB
30	4	607	CHL	C3-C5-C6-C7
30	7	302	CHL	C3-C5-C6-C7
31	1	602	CLA	C3-C5-C6-C7
31	1	604	CLA	C3-C5-C6-C7
31	1	610	CLA	C3-C5-C6-C7
31	3	304	CLA	C3-C5-C6-C7
31	3	316	CLA	C3-C5-C6-C7
31	B	614	CLA	C3-C5-C6-C7
31	C	612	CLA	C3-C5-C6-C7
31	R	315	CLA	C3-C5-C6-C7
31	R	316	CLA	C3-C5-C6-C7
31	Y	303	CLA	C3-C5-C6-C7
31	0	614	CLA	C3-C5-C6-C7
31	9	312	CLA	C3-C5-C6-C7
31	q	306	CLA	C3-C5-C6-C7
31	a	406	CLA	C3-C5-C6-C7
31	b	603	CLA	C3-C5-C6-C7
31	c	603	CLA	C3-C5-C6-C7
31	c	604	CLA	C3-C5-C6-C7
31	g	304	CLA	C3-C5-C6-C7
31	s	312	CLA	C3-C5-C6-C7
31	y	602	CLA	C3-C5-C6-C7
31	y	613	CLA	C3-C5-C6-C7
31	1	612	CLA	CBA-CGA-O2A-C1
31	2	603	CLA	CBA-CGA-O2A-C1
31	2	609	CLA	CBA-CGA-O2A-C1
31	2	611	CLA	CBA-CGA-O2A-C1
31	2	613	CLA	CBA-CGA-O2A-C1
31	5	611	CLA	CBA-CGA-O2A-C1
31	C	609	CLA	CBA-CGA-O2A-C1
31	N	314	CLA	CBA-CGA-O2A-C1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
31	R	312	CLA	CBA-CGA-O2A-C1
31	R	315	CLA	CBA-CGA-O2A-C1
31	Y	305	CLA	CBA-CGA-O2A-C1
31	0	610	CLA	CBA-CGA-O2A-C1
31	7	304	CLA	CBA-CGA-O2A-C1
31	7	316	CLA	CBA-CGA-O2A-C1
31	8	613	CLA	CBA-CGA-O2A-C1
31	9	314	CLA	CBA-CGA-O2A-C1
31	p	603	CLA	CBA-CGA-O2A-C1
31	p	604	CLA	CBA-CGA-O2A-C1
31	b	613	CLA	CBA-CGA-O2A-C1
31	c	611	CLA	CBA-CGA-O2A-C1
31	g	314	CLA	CBA-CGA-O2A-C1
31	n	311	CLA	CBA-CGA-O2A-C1
31	n	315	CLA	CBA-CGA-O2A-C1
31	r	303	CLA	CBA-CGA-O2A-C1
31	r	311	CLA	CBA-CGA-O2A-C1
31	r	316	CLA	CBA-CGA-O2A-C1
33	p	619	LHG	C24-C23-O8-C6
34	4	621	LMG	C29-C28-O8-C9
34	6	321	LMG	C29-C28-O8-C9
34	6	322	LMG	C29-C28-O8-C9
34	D	411	LMG	C29-C28-O8-C9
34	G	622	LMG	C29-C28-O8-C9
34	W	201	LMG	C29-C28-O8-C9
34	W	202	LMG	C29-C28-O8-C9
34	X	202	LMG	C29-C28-O8-C9
34	9	302	LMG	C29-C28-O8-C9
34	p	620	LMG	C29-C28-O8-C9
34	q	302	LMG	C29-C28-O8-C9
34	a	401	LMG	C29-C28-O8-C9
34	c	624	LMG	C29-C28-O8-C9
34	d	410	LMG	C29-C28-O8-C9
34	g	320	LMG	C29-C28-O8-C9
34	g	322	LMG	C29-C28-O8-C9
38	R	322	SQD	C24-C23-O48-C46
42	A	408	PHO	CBA-CGA-O2A-C1
34	W	201	LMG	C41-C42-C43-C44
34	w	202	LMG	C38-C39-C40-C41
34	w	202	LMG	C41-C42-C43-C44
31	D	404	CLA	O1D-CGD-O2D-CED
31	R	305	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	S	305	CLA	O1D-CGD-O2D-CED
31	Y	305	CLA	O1D-CGD-O2D-CED
31	0	611	CLA	O1D-CGD-O2D-CED
31	7	304	CLA	O1D-CGD-O2D-CED
31	p	604	CLA	O1D-CGD-O2D-CED
31	g	311	CLA	O1D-CGD-O2D-CED
44	A	416	PL9	C32-C33-C34-C35
30	N	306	CHL	CBD-CGD-O2D-CED
31	A	407	CLA	CBD-CGD-O2D-CED
31	B	610	CLA	CBD-CGD-O2D-CED
31	G	602	CLA	CBD-CGD-O2D-CED
31	d	401	CLA	CBD-CGD-O2D-CED
31	s	306	CLA	CBD-CGD-O2D-CED
31	y	612	CLA	CBD-CGD-O2D-CED
30	2	607	CHL	O1D-CGD-O2D-CED
31	2	604	CLA	O1D-CGD-O2D-CED
31	4	610	CLA	O1D-CGD-O2D-CED
31	4	614	CLA	O1D-CGD-O2D-CED
31	5	613	CLA	O1D-CGD-O2D-CED
31	6	304	CLA	O1D-CGD-O2D-CED
31	B	602	CLA	O1D-CGD-O2D-CED
31	G	613	CLA	O1D-CGD-O2D-CED
31	R	312	CLA	O1D-CGD-O2D-CED
31	Y	310	CLA	O1D-CGD-O2D-CED
31	9	306	CLA	O1D-CGD-O2D-CED
31	p	603	CLA	O1D-CGD-O2D-CED
31	q	305	CLA	O1D-CGD-O2D-CED
31	b	608	CLA	O1D-CGD-O2D-CED
31	c	610	CLA	O1D-CGD-O2D-CED
31	c	611	CLA	O1D-CGD-O2D-CED
31	g	312	CLA	O1D-CGD-O2D-CED
31	r	306	CLA	O1D-CGD-O2D-CED
31	r	312	CLA	O1D-CGD-O2D-CED
31	s	304	CLA	O1D-CGD-O2D-CED
31	y	603	CLA	O1D-CGD-O2D-CED
33	M	101	LHG	O9-C7-O7-C5
34	5	620	LMG	O9-C10-O7-C8
34	6	321	LMG	O9-C10-O7-C8
34	6	323	LMG	O9-C10-O7-C8
34	A	418	LMG	O9-C10-O7-C8
34	X	202	LMG	O9-C10-O7-C8
34	7	322	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
38	Y	320	SQD	O49-C7-O47-C45
45	c	618	DGD	O1B-C1B-O2G-C2G
30	5	607	CHL	O1A-CGA-O2A-C1
31	1	603	CLA	O1A-CGA-O2A-C1
31	2	603	CLA	O1A-CGA-O2A-C1
31	2	604	CLA	O1A-CGA-O2A-C1
31	2	609	CLA	O1A-CGA-O2A-C1
31	4	613	CLA	O1A-CGA-O2A-C1
31	6	304	CLA	O1A-CGA-O2A-C1
31	6	316	CLA	O1A-CGA-O2A-C1
31	C	609	CLA	O1A-CGA-O2A-C1
31	N	314	CLA	O1A-CGA-O2A-C1
31	8	609	CLA	O1A-CGA-O2A-C1
31	n	311	CLA	O1A-CGA-O2A-C1
31	r	316	CLA	O1A-CGA-O2A-C1
34	2	621	LMG	O10-C28-O8-C9
34	4	621	LMG	O10-C28-O8-C9
38	a	411	SQD	O10-C23-O48-C46
33	l	101	LHG	C11-C12-C13-C14
31	C	602	CLA	O1D-CGD-O2D-CED
31	C	611	CLA	O1D-CGD-O2D-CED
31	8	609	CLA	O1D-CGD-O2D-CED
31	b	617	CLA	O1D-CGD-O2D-CED
35	2	614	RRX	C19-C20-C21-C22
35	4	615	RRX	C19-C20-C21-C22
35	G	614	RRX	C19-C20-C21-C22
35	9	317	RRX	C19-C20-C21-C22
43	C	614	BCR	C19-C20-C21-C22
43	D	405	BCR	C13-C14-C15-C16
43	T	101	BCR	C15-C16-C17-C18
43	V	101	BCR	C13-C14-C15-C16
31	7	311	CLA	C5-C6-C7-C8
48	R	302	LMU	C3'-C4'-O1B-C1B
30	1	606	CHL	CBD-CGD-O2D-CED
30	5	601	CHL	CBD-CGD-O2D-CED
30	G	607	CHL	CBD-CGD-O2D-CED
30	Y	307	CHL	CBD-CGD-O2D-CED
30	8	607	CHL	CBD-CGD-O2D-CED
30	q	308	CHL	CBD-CGD-O2D-CED
30	n	309	CHL	CBD-CGD-O2D-CED
31	4	612	CLA	CBD-CGD-O2D-CED
31	B	615	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	C	607	CLA	CBD-CGD-O2D-CED
31	D	403	CLA	CBD-CGD-O2D-CED
31	N	311	CLA	CBD-CGD-O2D-CED
31	S	311	CLA	CBD-CGD-O2D-CED
31	Y	303	CLA	CBD-CGD-O2D-CED
31	3	304	CLA	O1D-CGD-O2D-CED
31	6	303	CLA	O1D-CGD-O2D-CED
31	B	616	CLA	O1D-CGD-O2D-CED
31	C	604	CLA	O1D-CGD-O2D-CED
31	b	602	CLA	O1D-CGD-O2D-CED
31	b	609	CLA	O1D-CGD-O2D-CED
31	c	602	CLA	O1D-CGD-O2D-CED
31	c	606	CLA	O1D-CGD-O2D-CED
33	1	617	LHG	O2-C2-C3-O3
33	3	320	LHG	O2-C2-C3-O3
33	5	619	LHG	O2-C2-C3-O3
33	A	417	LHG	O2-C2-C3-O3
33	B	624	LHG	O2-C2-C3-O3
33	C	623	LHG	O2-C2-C3-O3
33	K	102	LHG	O2-C2-C3-O3
33	N	319	LHG	O2-C2-C3-O3
33	R	320	LHG	O2-C2-C3-O3
33	Y	318	LHG	O2-C2-C3-O3
33	9	320	LHG	O2-C2-C3-O3
33	p	619	LHG	O2-C2-C3-O3
33	b	628	LHG	O2-C2-C3-O3
33	j	102	LHG	O2-C2-C3-O3
33	s	322	LHG	O2-C2-C3-O3
33	z	102	LHG	O2-C2-C3-O3
31	2	604	CLA	C3-C5-C6-C7
31	B	609	CLA	C3-C5-C6-C7
31	Y	312	CLA	C3-C5-C6-C7
31	Y	314	CLA	C3-C5-C6-C7
31	0	602	CLA	C3-C5-C6-C7
31	0	615	CLA	C3-C5-C6-C7
31	7	312	CLA	C3-C5-C6-C7
31	7	314	CLA	C3-C5-C6-C7
31	8	602	CLA	C3-C5-C6-C7
31	8	604	CLA	C3-C5-C6-C7
31	b	610	CLA	C3-C5-C6-C7
31	b	612	CLA	C3-C5-C6-C7
31	n	303	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	n	305	CLA	C3-C5-C6-C7
31	r	304	CLA	C3-C5-C6-C7
31	1	614	CLA	CBA-CGA-O2A-C1
31	2	604	CLA	CBA-CGA-O2A-C1
31	3	313	CLA	CBA-CGA-O2A-C1
31	4	610	CLA	CBA-CGA-O2A-C1
31	6	311	CLA	CBA-CGA-O2A-C1
31	G	613	CLA	CBA-CGA-O2A-C1
31	N	310	CLA	CBA-CGA-O2A-C1
31	N	315	CLA	CBA-CGA-O2A-C1
31	S	310	CLA	CBA-CGA-O2A-C1
31	7	315	CLA	CBA-CGA-O2A-C1
31	8	609	CLA	CBA-CGA-O2A-C1
31	g	305	CLA	CBA-CGA-O2A-C1
31	r	307	CLA	CBA-CGA-O2A-C1
31	s	314	CLA	CBA-CGA-O2A-C1
33	5	619	LHG	C24-C23-O8-C6
38	a	411	SQD	C24-C23-O48-C46
31	0	610	CLA	O1A-CGA-O2A-C1
31	b	613	CLA	O1A-CGA-O2A-C1
31	c	609	CLA	O1A-CGA-O2A-C1
31	s	314	CLA	O1A-CGA-O2A-C1
42	A	408	PHO	O1A-CGA-O2A-C1
30	p	608	CHL	O1D-CGD-O2D-CED
31	1	611	CLA	O1D-CGD-O2D-CED
31	2	603	CLA	O1D-CGD-O2D-CED
31	B	608	CLA	O1D-CGD-O2D-CED
31	C	612	CLA	O1D-CGD-O2D-CED
31	G	609	CLA	O1D-CGD-O2D-CED
31	G	611	CLA	O1D-CGD-O2D-CED
31	0	604	CLA	O1D-CGD-O2D-CED
31	7	305	CLA	O1D-CGD-O2D-CED
31	7	311	CLA	O1D-CGD-O2D-CED
31	8	613	CLA	O1D-CGD-O2D-CED
31	p	602	CLA	O1D-CGD-O2D-CED
31	q	304	CLA	O1D-CGD-O2D-CED
31	r	305	CLA	O1D-CGD-O2D-CED
31	r	315	CLA	O1D-CGD-O2D-CED
31	r	316	CLA	O1D-CGD-O2D-CED
33	N	319	LHG	C8-C7-O7-C5
33	8	618	LHG	C8-C7-O7-C5
33	n	320	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
34	1	618	LMG	C11-C10-O7-C8
34	2	618	LMG	C11-C10-O7-C8
34	6	323	LMG	C11-C10-O7-C8
34	A	412	LMG	C11-C10-O7-C8
34	B	621	LMG	C11-C10-O7-C8
34	J	101	LMG	C11-C10-O7-C8
34	7	320	LMG	C11-C10-O7-C8
34	s	321	LMG	C11-C10-O7-C8
33	2	617	LHG	C13-C14-C15-C16
30	3	303	CHL	CBD-CGD-O2D-CED
30	4	607	CHL	CBD-CGD-O2D-CED
30	9	311	CHL	CBD-CGD-O2D-CED
31	q	313	CLA	CBD-CGD-O2D-CED
31	s	305	CLA	CBD-CGD-O2D-CED
48	K	101	LMU	O5B-C5B-C6B-O6B
33	2	617	LHG	C11-C12-C13-C14
33	2	617	LHG	C28-C29-C30-C31
33	S	320	LHG	C28-C29-C30-C31
33	l	101	LHG	C9-C10-C11-C12
33	r	320	LHG	C11-C12-C13-C14
33	s	320	LHG	C28-C29-C30-C31
31	0	610	CLA	C5-C6-C7-C8
34	x	202	LMG	C8-C9-O8-C28
38	M	102	SQD	C45-C46-O48-C23
45	c	616	DGD	C2G-C1G-O1G-C1A
31	0	603	CLA	O1D-CGD-O2D-CED
31	1	614	CLA	O1A-CGA-O2A-C1
31	2	611	CLA	O1A-CGA-O2A-C1
31	G	613	CLA	O1A-CGA-O2A-C1
34	D	411	LMG	O10-C28-O8-C9
34	d	410	LMG	O10-C28-O8-C9
33	q	320	LHG	C26-C27-C28-C29
33	b	625	LHG	C31-C32-C33-C34
33	s	322	LHG	C28-C29-C30-C31
36	N	318	NEX	C14-C15-C35-C34
31	4	611	CLA	O1D-CGD-O2D-CED
31	5	610	CLA	O1D-CGD-O2D-CED
31	6	312	CLA	O1D-CGD-O2D-CED
33	5	619	LHG	C7-C8-C9-C10
33	G	618	LHG	C11-C10-C9-C8
33	b	625	LHG	C25-C26-C27-C28
33	g	319	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	6	308	CHL	CBD-CGD-O2D-CED
31	N	304	CLA	C5-C6-C7-C8
31	1	614	CLA	C3-C5-C6-C7
31	3	314	CLA	C3-C5-C6-C7
31	5	611	CLA	C3-C5-C6-C7
31	N	305	CLA	C3-C5-C6-C7
31	7	311	CLA	C3-C5-C6-C7
31	1	603	CLA	CBA-CGA-O2A-C1
31	6	316	CLA	CBA-CGA-O2A-C1
33	t	102	LHG	C24-C23-O8-C6
34	2	621	LMG	C29-C28-O8-C9
31	A	409	CLA	O1D-CGD-O2D-CED
31	a	409	CLA	O1D-CGD-O2D-CED
48	R	302	LMU	O5B-C5B-C6B-O6B
33	8	618	LHG	O9-C7-O7-C5
33	n	320	LHG	O9-C7-O7-C5
48	r	302	LMU	C4B-C5B-C6B-O6B
33	c	622	LHG	C33-C34-C35-C36
33	K	102	LHG	C2-C3-O3-P
31	4	610	CLA	O1A-CGA-O2A-C1
31	7	315	CLA	O1A-CGA-O2A-C1
31	8	613	CLA	O1A-CGA-O2A-C1
31	c	611	CLA	O1A-CGA-O2A-C1
31	g	305	CLA	O1A-CGA-O2A-C1
30	9	309	CHL	C3-C5-C6-C7
31	4	602	CLA	C8-C10-C11-C12
31	6	311	CLA	C5-C6-C7-C8
31	G	603	CLA	C5-C6-C7-C8
30	1	619	CHL	C4-C3-C5-C6
30	2	608	CHL	C4-C3-C5-C6
30	5	609	CHL	C4-C3-C5-C6
30	6	308	CHL	C4-C3-C5-C6
30	Y	302	CHL	C4-C3-C5-C6
30	0	609	CHL	C4-C3-C5-C6
30	y	606	CHL	C4-C3-C5-C6
31	B	605	CLA	C4-C3-C5-C6
30	1	619	CHL	C2-C3-C5-C6
30	2	608	CHL	C2-C3-C5-C6
30	5	609	CHL	C2-C3-C5-C6
30	6	308	CHL	C2-C3-C5-C6
30	Y	302	CHL	C2-C3-C5-C6
30	0	609	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	y	606	CHL	C2-C3-C5-C6
31	B	605	CLA	C2-C3-C5-C6
31	B	613	CLA	C2-C3-C5-C6
31	b	603	CLA	C2-C3-C5-C6
31	b	606	CLA	C2-C3-C5-C6
30	1	608	CHL	CBD-CGD-O2D-CED
31	9	305	CLA	CBD-CGD-O2D-CED
33	e	101	LHG	C7-C8-C9-C10
31	2	613	CLA	C2A-CAA-CBA-CGA
31	B	610	CLA	C2A-CAA-CBA-CGA
31	9	312	CLA	C2A-CAA-CBA-CGA
31	p	614	CLA	C2A-CAA-CBA-CGA
31	N	312	CLA	O1D-CGD-O2D-CED
31	R	303	CLA	O1D-CGD-O2D-CED
31	8	603	CLA	O1D-CGD-O2D-CED
31	g	304	CLA	O1D-CGD-O2D-CED
31	1	612	CLA	O1A-CGA-O2A-C1
31	2	613	CLA	O1A-CGA-O2A-C1
31	3	312	CLA	O1A-CGA-O2A-C1
31	3	313	CLA	O1A-CGA-O2A-C1
31	6	311	CLA	O1A-CGA-O2A-C1
31	N	315	CLA	O1A-CGA-O2A-C1
31	S	310	CLA	O1A-CGA-O2A-C1
31	n	315	CLA	O1A-CGA-O2A-C1
31	r	307	CLA	O1A-CGA-O2A-C1
31	s	310	CLA	O1A-CGA-O2A-C1
34	q	301	LMG	O6-C1-O1-C7
38	G	617	SQD	O5-C1-O6-C44
38	M	102	SQD	O5-C1-O6-C44
38	S	301	SQD	O5-C1-O6-C44
38	b	621	SQD	O5-C1-O6-C44
38	b	627	SQD	O5-C1-O6-C44
31	2	610	CLA	O1D-CGD-O2D-CED
31	q	306	CLA	O1D-CGD-O2D-CED
44	A	416	PL9	C19-C21-C22-C23
31	3	312	CLA	CBA-CGA-O2A-C1
31	B	605	CLA	CBA-CGA-O2A-C1
31	B	612	CLA	CBA-CGA-O2A-C1
31	C	611	CLA	CBA-CGA-O2A-C1
31	R	307	CLA	CBA-CGA-O2A-C1
31	Y	313	CLA	CBA-CGA-O2A-C1
31	c	607	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	s	310	CLA	CBA-CGA-O2A-C1
31	y	604	CLA	CBA-CGA-O2A-C1
45	C	618	DGD	C2A-C1A-O1G-C1G
45	c	619	DGD	C2A-C1A-O1G-C1G
31	N	315	CLA	C5-C6-C7-C8
33	q	320	LHG	C34-C35-C36-C37
33	g	319	LHG	C11-C10-C9-C8
30	9	307	CHL	CBD-CGD-O2D-CED
31	4	603	CLA	O1D-CGD-O2D-CED
48	r	302	LMU	O5B-C5B-C6B-O6B
33	d	408	LHG	C31-C32-C33-C34
48	r	302	LMU	C5-C6-C7-C8
31	B	601	CLA	O1D-CGD-O2D-CED
31	B	607	CLA	O1D-CGD-O2D-CED
31	C	613	CLA	O1D-CGD-O2D-CED
31	N	303	CLA	O1D-CGD-O2D-CED
31	Y	304	CLA	O1D-CGD-O2D-CED
31	9	304	CLA	O1D-CGD-O2D-CED
31	9	312	CLA	O1D-CGD-O2D-CED
31	c	612	CLA	O1D-CGD-O2D-CED
31	c	613	CLA	O1D-CGD-O2D-CED
31	d	404	CLA	O1D-CGD-O2D-CED
31	n	311	CLA	O1D-CGD-O2D-CED
31	s	310	CLA	O1D-CGD-O2D-CED
31	y	604	CLA	O1D-CGD-O2D-CED
33	t	102	LHG	O10-C23-O8-C6
33	R	320	LHG	C8-C7-O7-C5
34	2	620	LMG	C11-C10-O7-C8
34	0	622	LMG	C11-C10-O7-C8
34	w	202	LMG	C11-C10-O7-C8
31	5	613	CLA	C5-C6-C7-C8
33	j	102	LHG	C24-C25-C26-C27
44	A	416	PL9	C12-C13-C14-C15
30	n	301	CHL	O1D-CGD-O2D-CED
31	1	604	CLA	O1D-CGD-O2D-CED
31	3	311	CLA	O1D-CGD-O2D-CED
31	C	610	CLA	O1D-CGD-O2D-CED
31	G	610	CLA	O1D-CGD-O2D-CED
31	R	316	CLA	O1D-CGD-O2D-CED
31	7	303	CLA	O1D-CGD-O2D-CED
31	b	616	CLA	O1D-CGD-O2D-CED
31	c	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	g	303	CLA	O1D-CGD-O2D-CED
31	s	312	CLA	O1D-CGD-O2D-CED
31	7	312	CLA	CBD-CGD-O2D-CED
31	y	611	CLA	CBD-CGD-O2D-CED
31	g	304	CLA	C5-C6-C7-C8
31	s	303	CLA	C8-C10-C11-C12
31	9	304	CLA	C2C-C3C-CAC-CBC
31	s	315	CLA	O1D-CGD-O2D-CED
33	2	617	LHG	C1-C2-C3-O3
33	5	619	LHG	C1-C2-C3-O3
33	6	320	LHG	C1-C2-C3-O3
33	A	417	LHG	C1-C2-C3-O3
33	G	618	LHG	C1-C2-C3-O3
33	L	101	LHG	C1-C2-C3-O3
33	N	319	LHG	C1-C2-C3-O3
33	b	625	LHG	C1-C2-C3-O3
33	c	622	LHG	C1-C2-C3-O3
33	g	319	LHG	C1-C2-C3-O3
33	j	102	LHG	C1-C2-C3-O3
33	l	101	LHG	C1-C2-C3-O3
33	F1	301	LHG	C1-C2-C3-O3
33	N	319	LHG	O9-C7-O7-C5
34	1	618	LMG	O9-C10-O7-C8
34	2	618	LMG	O9-C10-O7-C8
34	J	101	LMG	O9-C10-O7-C8
34	s	321	LMG	O9-C10-O7-C8
31	3	311	CLA	O1A-CGA-O2A-C1
31	A	406	CLA	O1A-CGA-O2A-C1
31	B	612	CLA	O1A-CGA-O2A-C1
31	C	611	CLA	O1A-CGA-O2A-C1
31	R	307	CLA	O1A-CGA-O2A-C1
31	p	611	CLA	O1A-CGA-O2A-C1
33	5	619	LHG	O10-C23-O8-C6
45	C	618	DGD	O1A-C1A-O1G-C1G
31	B	607	CLA	C3-C5-C6-C7
31	c	611	CLA	C3-C5-C6-C7
31	N	310	CLA	O1D-CGD-O2D-CED
31	Y	312	CLA	O1D-CGD-O2D-CED
31	0	602	CLA	O1D-CGD-O2D-CED
31	8	602	CLA	O1D-CGD-O2D-CED
31	b	612	CLA	O1D-CGD-O2D-CED
31	n	304	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	r	303	CLA	O1D-CGD-O2D-CED
31	1	602	CLA	CBA-CGA-O2A-C1
31	3	311	CLA	CBA-CGA-O2A-C1
31	3	316	CLA	CBA-CGA-O2A-C1
31	A	406	CLA	CBA-CGA-O2A-C1
31	C	607	CLA	CBA-CGA-O2A-C1
31	C	610	CLA	CBA-CGA-O2A-C1
31	G	604	CLA	CBA-CGA-O2A-C1
31	G	610	CLA	CBA-CGA-O2A-C1
31	N	305	CLA	CBA-CGA-O2A-C1
31	N	321	CLA	CBA-CGA-O2A-C1
31	R	314	CLA	CBA-CGA-O2A-C1
31	0	603	CLA	CBA-CGA-O2A-C1
31	8	604	CLA	CBA-CGA-O2A-C1
31	8	614	CLA	CBA-CGA-O2A-C1
31	9	304	CLA	CBA-CGA-O2A-C1
31	9	312	CLA	CBA-CGA-O2A-C1
31	p	611	CLA	CBA-CGA-O2A-C1
31	q	316	CLA	CBA-CGA-O2A-C1
31	a	407	CLA	CBA-CGA-O2A-C1
31	b	606	CLA	CBA-CGA-O2A-C1
31	b	612	CLA	CBA-CGA-O2A-C1
31	d	405	CLA	CBA-CGA-O2A-C1
31	g	311	CLA	CBA-CGA-O2A-C1
31	n	305	CLA	CBA-CGA-O2A-C1
31	n	316	CLA	CBA-CGA-O2A-C1
33	G	618	LHG	C24-C23-O8-C6
38	M	102	SQD	C24-C23-O48-C46
38	m	101	SQD	C24-C23-O48-C46
42	a	408	PHO	CBA-CGA-O2A-C1
45	c	618	DGD	C2A-C1A-O1G-C1G
30	N	309	CHL	CBD-CGD-O2D-CED
31	4	604	CLA	CBD-CGD-O2D-CED
33	M	101	LHG	C34-C35-C36-C37
35	2	614	RRX	C9-C10-C11-C12
36	5	618	NEX	C29-C30-C31-C32
36	N	318	NEX	C13-C14-C15-C35
43	B	618	BCR	C19-C20-C21-C22
43	B	619	BCR	C9-C10-C11-C12
43	T	101	BCR	C19-C20-C21-C22
43	c	615	BCR	C9-C10-C11-C12
33	d	408	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
33	p	619	LHG	C24-C25-C26-C27
31	c	612	CLA	C5-C6-C7-C8
33	6	320	LHG	C11-C10-C9-C8
31	r	307	CLA	O1D-CGD-O2D-CED
31	2	613	CLA	C5-C6-C7-C8
33	M	101	LHG	C26-C27-C28-C29
33	b	628	LHG	C29-C30-C31-C32
33	y	619	LHG	C29-C30-C31-C32
48	R	302	LMU	C4B-C5B-C6B-O6B
31	A	409	CLA	C8-C10-C11-C12
31	B	606	CLA	C13-C15-C16-C17
31	a	409	CLA	C8-C10-C11-C12
33	4	618	LHG	O2-C2-C3-O3
33	6	320	LHG	O2-C2-C3-O3
33	A	415	LHG	O2-C2-C3-O3
33	D	407	LHG	O2-C2-C3-O3
33	L	101	LHG	O2-C2-C3-O3
33	S	320	LHG	O2-C2-C3-O3
33	7	319	LHG	O2-C2-C3-O3
33	a	415	LHG	O2-C2-C3-O3
33	d	408	LHG	O2-C2-C3-O3
33	l	101	LHG	O2-C2-C3-O3
33	t	102	LHG	O2-C2-C3-O3
33	y	619	LHG	O2-C2-C3-O3
33	3	320	LHG	C7-C8-C9-C10
33	S	322	LHG	C23-C24-C25-C26
33	p	619	LHG	C7-C8-C9-C10
33	b	625	LHG	C23-C24-C25-C26
33	F1	301	LHG	C23-C24-C25-C26
31	5	603	CLA	C3-C5-C6-C7
34	4	621	LMG	C2-C1-O1-C7
34	W	202	LMG	C2-C1-O1-C7
34	9	301	LMG	C2-C1-O1-C7
34	a	413	LMG	C2-C1-O1-C7
34	b	624	LMG	C2-C1-O1-C7
34	m	102	LMG	C2-C1-O1-C7
34	n	321	LMG	C2-C1-O1-C7
34	n	322	LMG	C2-C1-O1-C7
34	r	321	LMG	C2-C1-O1-C7
34	Q1	101	LMG	C2-C1-O1-C7
38	B	620	SQD	C2-C1-O6-C44
38	M	102	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
38	b	627	SQD	C2-C1-O6-C44
33	4	618	LHG	O7-C5-C6-O8
33	R	320	LHG	O7-C5-C6-O8
33	8	618	LHG	O7-C5-C6-O8
33	9	320	LHG	O7-C5-C6-O8
33	e	101	LHG	O7-C5-C6-O8
33	n	320	LHG	O7-C5-C6-O8
45	c	617	DGD	C2A-C1A-O1G-C1G
33	C	623	LHG	C26-C27-C28-C29
34	q	302	LMG	C31-C32-C33-C34
31	1	602	CLA	O1A-CGA-O2A-C1
31	G	610	CLA	O1A-CGA-O2A-C1
31	N	305	CLA	O1A-CGA-O2A-C1
31	8	604	CLA	O1A-CGA-O2A-C1
31	8	614	CLA	O1A-CGA-O2A-C1
31	a	407	CLA	O1A-CGA-O2A-C1
31	d	405	CLA	O1A-CGA-O2A-C1
31	n	305	CLA	O1A-CGA-O2A-C1
31	3	301	CLA	C4-C3-C5-C6
30	G	601	CHL	C2-C3-C5-C6
30	7	310	CHL	C2-C3-C5-C6
31	D	403	CLA	C2-C3-C5-C6
31	p	602	CLA	C2-C3-C5-C6
31	b	605	CLA	C2-C3-C5-C6
31	s	310	CLA	C2-C3-C5-C6
44	A	416	PL9	C43-C44-C46-C47
30	1	605	CHL	C6-C7-C8-C9
30	1	605	CHL	C11-C10-C8-C9
30	1	607	CHL	C14-C13-C15-C16
30	3	310	CHL	C11-C10-C8-C9
30	6	308	CHL	C11-C10-C8-C9
30	6	308	CHL	C14-C13-C15-C16
30	6	310	CHL	C11-C10-C8-C9
30	G	623	CHL	C11-C10-C8-C9
30	G	623	CHL	C14-C13-C15-C16
30	N	306	CHL	C11-C10-C8-C9
30	N	309	CHL	C11-C10-C8-C9
30	Y	309	CHL	C11-C10-C8-C9
30	0	607	CHL	C11-C10-C8-C9
30	0	607	CHL	C14-C13-C15-C16
30	7	306	CHL	C11-C10-C8-C9
30	7	307	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
30	7	308	CHL	C14-C13-C15-C16
30	8	605	CHL	C11-C10-C8-C9
30	9	303	CHL	C14-C13-C15-C16
30	9	311	CHL	C6-C7-C8-C9
30	9	311	CHL	C11-C10-C8-C9
30	g	302	CHL	C11-C10-C8-C9
30	n	306	CHL	C11-C10-C8-C9
30	y	601	CHL	C11-C10-C8-C9
30	y	607	CHL	C14-C13-C15-C16
31	1	604	CLA	C6-C7-C8-C9
31	2	602	CLA	C11-C10-C8-C9
31	2	610	CLA	C6-C7-C8-C9
31	3	316	CLA	C6-C7-C8-C9
31	5	602	CLA	C6-C7-C8-C9
31	5	610	CLA	C6-C7-C8-C9
31	5	611	CLA	C6-C7-C8-C9
31	6	303	CLA	C6-C7-C8-C9
31	6	303	CLA	C11-C10-C8-C9
31	6	312	CLA	C11-C10-C8-C9
31	A	406	CLA	C14-C13-C15-C16
31	A	409	CLA	C6-C7-C8-C9
31	B	605	CLA	C11-C10-C8-C9
31	B	607	CLA	C11-C12-C13-C14
31	C	601	CLA	C11-C12-C13-C14
31	C	607	CLA	C14-C13-C15-C16
31	C	608	CLA	C11-C10-C8-C9
31	C	613	CLA	C11-C12-C13-C14
31	D	404	CLA	C6-C7-C8-C9
31	N	303	CLA	C11-C10-C8-C9
31	N	303	CLA	C11-C12-C13-C14
31	N	310	CLA	C6-C7-C8-C9
31	R	304	CLA	C6-C7-C8-C9
31	R	311	CLA	C11-C10-C8-C9
31	R	316	CLA	C14-C13-C15-C16
31	S	305	CLA	C6-C7-C8-C9
31	Y	311	CLA	C11-C12-C13-C14
31	Y	312	CLA	C11-C12-C13-C14
31	7	311	CLA	C11-C10-C8-C9
31	7	313	CLA	C11-C10-C8-C9
31	9	304	CLA	C11-C10-C8-C9
31	p	602	CLA	C6-C7-C8-C9
31	p	610	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	a	409	CLA	C6-C7-C8-C9
31	b	605	CLA	C6-C7-C8-C9
31	b	606	CLA	C14-C13-C15-C16
31	b	609	CLA	C14-C13-C15-C16
31	b	611	CLA	C6-C7-C8-C9
31	b	611	CLA	C11-C12-C13-C14
31	b	612	CLA	C6-C7-C8-C9
31	b	612	CLA	C11-C12-C13-C14
31	b	614	CLA	C6-C7-C8-C9
31	b	616	CLA	C11-C10-C8-C9
31	c	608	CLA	C6-C7-C8-C9
31	c	613	CLA	C14-C13-C15-C16
31	d	404	CLA	C6-C7-C8-C9
31	g	313	CLA	C6-C7-C8-C9
31	n	311	CLA	C6-C7-C8-C9
31	r	304	CLA	C6-C7-C8-C9
31	r	311	CLA	C11-C10-C8-C9
31	s	310	CLA	C6-C7-C8-C9
31	s	312	CLA	C6-C7-C8-C9
31	y	613	CLA	C11-C10-C8-C9
30	q	310	CHL	O1D-CGD-O2D-CED
31	1	602	CLA	O1D-CGD-O2D-CED
31	S	312	CLA	O1D-CGD-O2D-CED
31	Y	311	CLA	O1D-CGD-O2D-CED
31	g	310	CLA	O1D-CGD-O2D-CED
31	y	615	CLA	O1D-CGD-O2D-CED
31	2	602	CLA	C2C-C3C-CAC-CBC
31	C	603	CLA	C8-C10-C11-C12
31	C	610	CLA	C13-C15-C16-C17
31	c	610	CLA	C15-C16-C17-C18
42	A	408	PHO	C8-C10-C11-C12
30	4	608	CHL	C2A-CAA-CBA-CGA
30	N	306	CHL	C2A-CAA-CBA-CGA
30	Y	307	CHL	C2A-CAA-CBA-CGA
30	q	310	CHL	C2A-CAA-CBA-CGA
31	1	614	CLA	C2A-CAA-CBA-CGA
31	3	306	CLA	C2A-CAA-CBA-CGA
31	4	610	CLA	C2A-CAA-CBA-CGA
31	4	613	CLA	C2A-CAA-CBA-CGA
31	B	604	CLA	C2A-CAA-CBA-CGA
31	7	315	CLA	C2A-CAA-CBA-CGA
32	3	318	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
32	5	617	LUT	C11-C12-C13-C20
32	6	318	LUT	C11-C12-C13-C20
32	G	615	LUT	C7-C8-C9-C19
32	G	615	LUT	C27-C28-C29-C39
32	N	316	LUT	C7-C8-C9-C19
32	N	316	LUT	C31-C32-C33-C40
32	N	317	LUT	C11-C12-C13-C20
32	R	317	LUT	C7-C8-C9-C19
32	R	317	LUT	C31-C32-C33-C40
32	8	616	LUT	C7-C8-C9-C19
32	p	616	LUT	C7-C8-C9-C19
32	p	616	LUT	C11-C12-C13-C20
32	g	316	LUT	C27-C28-C29-C39
32	n	318	LUT	C7-C8-C9-C19
36	6	319	NEX	C31-C32-C33-C40
36	R	319	NEX	C31-C32-C33-C40
36	0	618	NEX	C31-C32-C33-C40
36	p	618	NEX	C11-C12-C13-C20
37	2	619	XAT	C27-C28-C29-C39
37	4	619	XAT	C27-C28-C29-C39
37	G	620	XAT	C27-C28-C29-C39
37	9	322	XAT	C27-C28-C29-C39
37	q	321	XAT	C27-C28-C29-C39
37	g	321	XAT	C27-C28-C29-C39
43	B	617	BCR	C36-C18-C19-C20
43	C	614	BCR	C7-C8-C9-C34
43	V	101	BCR	C36-C18-C19-C20
43	Z	101	BCR	C7-C8-C9-C34
43	a	410	BCR	C36-C18-C19-C20
43	b	618	BCR	C36-C18-C19-C20
43	b	619	BCR	C11-C12-C13-C35
43	b	619	BCR	C37-C22-C23-C24
43	c	614	BCR	C7-C8-C9-C34
43	c	614	BCR	C11-C12-C13-C35
43	d	406	BCR	C11-C12-C13-C35
43	d	406	BCR	C37-C22-C23-C24
43	h	101	BCR	C11-C12-C13-C35
43	v	101	BCR	C36-C18-C19-C20
43	v	101	BCR	C37-C22-C23-C24
32	3	318	LUT	C7-C8-C9-C10
32	5	617	LUT	C11-C12-C13-C14
32	G	615	LUT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
32	G	615	LUT	C27-C28-C29-C30
32	N	316	LUT	C7-C8-C9-C10
32	R	317	LUT	C7-C8-C9-C10
32	R	317	LUT	C31-C32-C33-C34
32	Y	316	LUT	C7-C8-C9-C10
32	7	317	LUT	C7-C8-C9-C10
32	8	616	LUT	C7-C8-C9-C10
32	p	616	LUT	C7-C8-C9-C10
32	p	616	LUT	C31-C32-C33-C34
32	g	316	LUT	C27-C28-C29-C30
32	n	318	LUT	C7-C8-C9-C10
35	g	315	RRX	C21-C22-C23-C24
36	6	319	NEX	C31-C32-C33-C34
36	0	618	NEX	C31-C32-C33-C34
37	2	619	XAT	C27-C28-C29-C30
37	4	619	XAT	C27-C28-C29-C30
37	G	620	XAT	C27-C28-C29-C30
37	9	322	XAT	C27-C28-C29-C30
37	q	321	XAT	C27-C28-C29-C30
37	g	321	XAT	C27-C28-C29-C30
43	B	617	BCR	C17-C18-C19-C20
43	C	614	BCR	C7-C8-C9-C10
43	V	101	BCR	C17-C18-C19-C20
43	b	618	BCR	C21-C22-C23-C24
43	b	619	BCR	C11-C12-C13-C14
43	c	614	BCR	C7-C8-C9-C10
43	c	614	BCR	C11-C12-C13-C14
43	d	406	BCR	C11-C12-C13-C14
43	d	406	BCR	C21-C22-C23-C24
43	h	101	BCR	C11-C12-C13-C14
43	v	101	BCR	C17-C18-C19-C20
34	3	321	LMG	C11-C10-O7-C8
34	B	625	LMG	C11-C10-O7-C8
34	W	201	LMG	C11-C10-O7-C8
34	X	203	LMG	C11-C10-O7-C8
34	n	321	LMG	C11-C10-O7-C8
33	A	417	LHG	C31-C32-C33-C34
34	r	321	LMG	C11-C12-C13-C14
33	M	101	LHG	C23-C24-C25-C26
33	F1	301	LHG	C7-C8-C9-C10
31	3	316	CLA	O1A-CGA-O2A-C1
31	N	321	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	9	304	CLA	O1A-CGA-O2A-C1
31	q	316	CLA	O1A-CGA-O2A-C1
31	b	606	CLA	O1A-CGA-O2A-C1
31	n	316	CLA	O1A-CGA-O2A-C1
42	a	408	PHO	O1A-CGA-O2A-C1
31	6	312	CLA	C5-C6-C7-C8
31	B	603	CLA	C15-C16-C17-C18
31	B	616	CLA	C5-C6-C7-C8
31	b	612	CLA	C8-C10-C11-C12
31	c	601	CLA	C8-C10-C11-C12
30	1	607	CHL	O1D-CGD-O2D-CED
30	g	308	CHL	O1D-CGD-O2D-CED
31	n	303	CLA	O1D-CGD-O2D-CED
33	C	623	LHG	C33-C34-C35-C36
30	7	306	CHL	CBD-CGD-O2D-CED
31	G	603	CLA	O1D-CGD-O2D-CED
31	G	604	CLA	O1D-CGD-O2D-CED
31	G	610	CLA	C3-C5-C6-C7
31	g	303	CLA	C3-C5-C6-C7
31	c	608	CLA	CBA-CGA-O2A-C1
33	g	319	LHG	C24-C23-O8-C6
34	A	412	LMG	C29-C28-O8-C9
31	1	613	CLA	C15-C16-C17-C18
31	R	311	CLA	C5-C6-C7-C8
31	S	303	CLA	C5-C6-C7-C8
31	S	312	CLA	C10-C11-C12-C13
31	0	602	CLA	C5-C6-C7-C8
31	q	306	CLA	C5-C6-C7-C8
31	a	407	CLA	C13-C15-C16-C17
31	b	607	CLA	C13-C15-C16-C17
31	c	606	CLA	C8-C10-C11-C12
31	s	310	CLA	C5-C6-C7-C8
31	y	613	CLA	C8-C10-C11-C12
34	w	202	LMG	C29-C30-C31-C32
33	2	617	LHG	C7-C8-C9-C10
33	4	618	LHG	C23-C24-C25-C26
33	A	415	LHG	C7-C8-C9-C10
33	D	407	LHG	C23-C24-C25-C26
33	0	619	LHG	C7-C8-C9-C10
33	9	320	LHG	C7-C8-C9-C10
34	n	322	LMG	C28-C29-C30-C31
38	b	627	SQD	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	R	315	CLA	O1D-CGD-O2D-CED
31	N	304	CLA	CBD-CGD-O2D-CED
36	g	317	NEX	C14-C15-C35-C34
30	y	607	CHL	C8-C10-C11-C12
31	l	612	CLA	C8-C10-C11-C12
31	A	409	CLA	C5-C6-C7-C8
31	B	606	CLA	C8-C10-C11-C12
31	B	609	CLA	C8-C10-C11-C12
31	C	613	CLA	C5-C6-C7-C8
31	G	604	CLA	C5-C6-C7-C8
31	S	303	CLA	C8-C10-C11-C12
31	S	314	CLA	C13-C15-C16-C17
31	8	612	CLA	C5-C6-C7-C8
31	p	602	CLA	C5-C6-C7-C8
31	a	409	CLA	C5-C6-C7-C8
31	b	606	CLA	C13-C15-C16-C17
31	n	314	CLA	C5-C6-C7-C8
31	s	311	CLA	C8-C10-C11-C12
31	s	311	CLA	C10-C11-C12-C13
31	s	312	CLA	C13-C15-C16-C17
31	y	611	CLA	C13-C15-C16-C17
44	D	406	PL9	C47-C48-C49-C51
31	R	307	CLA	O1D-CGD-O2D-CED
31	9	316	CLA	O1D-CGD-O2D-CED
31	n	305	CLA	O1D-CGD-O2D-CED
33	C	623	LHG	O1-C1-C2-O2
33	D	407	LHG	O1-C1-C2-O2
33	S	322	LHG	O1-C1-C2-O2
33	7	319	LHG	O1-C1-C2-O2
33	9	320	LHG	O1-C1-C2-O2
33	b	628	LHG	O1-C1-C2-O2
33	l	101	LHG	O1-C1-C2-O2
33	z	102	LHG	O1-C1-C2-O2
33	3	320	LHG	C23-C24-C25-C26
33	6	320	LHG	C23-C24-C25-C26
33	B	624	LHG	C7-C8-C9-C10
33	B	624	LHG	C23-C24-C25-C26
33	C	623	LHG	C7-C8-C9-C10
33	C	623	LHG	C23-C24-C25-C26
33	G	618	LHG	C23-C24-C25-C26
33	K	102	LHG	C7-C8-C9-C10
33	M	101	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	N	319	LHG	C23-C24-C25-C26
33	7	319	LHG	C7-C8-C9-C10
33	b	628	LHG	C7-C8-C9-C10
33	b	628	LHG	C23-C24-C25-C26
33	g	319	LHG	C23-C24-C25-C26
33	s	320	LHG	C7-C8-C9-C10
33	s	320	LHG	C23-C24-C25-C26
33	t	102	LHG	C7-C8-C9-C10
33	z	102	LHG	C23-C24-C25-C26
34	J	101	LMG	C10-C11-C12-C13
34	n	321	LMG	C28-C29-C30-C31
45	C	616	DGD	O6E-C5E-C6E-O5E
38	s	301	SQD	C30-C31-C32-C33
31	6	315	CLA	CBD-CGD-O2D-CED
42	d	402	PHO	CBD-CGD-O2D-CED
30	1	601	CHL	C10-C11-C12-C13
30	y	607	CHL	C5-C6-C7-C8
31	R	305	CLA	C8-C10-C11-C12
31	7	313	CLA	C13-C15-C16-C17
31	a	406	CLA	C15-C16-C17-C18
31	y	610	CLA	C8-C10-C11-C12
31	N	313	CLA	C3-C5-C6-C7
31	3	306	CLA	CBA-CGA-O2A-C1
31	B	603	CLA	CBA-CGA-O2A-C1
31	R	304	CLA	CBA-CGA-O2A-C1
31	S	305	CLA	CBA-CGA-O2A-C1
31	b	614	CLA	CBA-CGA-O2A-C1
31	0	610	CLA	O1D-CGD-O2D-CED
31	0	612	CLA	O1D-CGD-O2D-CED
31	8	604	CLA	O1D-CGD-O2D-CED
31	b	603	CLA	O1D-CGD-O2D-CED
34	x	202	LMG	O6-C5-C6-O5
34	2	620	LMG	O9-C10-O7-C8
34	B	621	LMG	O9-C10-O7-C8
34	W	201	LMG	O9-C10-O7-C8
34	0	622	LMG	O9-C10-O7-C8
34	7	320	LMG	O9-C10-O7-C8
31	1	603	CLA	C2-C1-O2A-CGA
31	1	604	CLA	C2-C1-O2A-CGA
31	3	315	CLA	C2-C1-O2A-CGA
31	6	315	CLA	C2-C1-O2A-CGA
31	A	407	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	B	601	CLA	C2-C1-O2A-CGA
31	C	602	CLA	C2-C1-O2A-CGA
31	0	614	CLA	C2-C1-O2A-CGA
31	7	305	CLA	C2-C1-O2A-CGA
31	9	312	CLA	C2-C1-O2A-CGA
31	p	604	CLA	C2-C1-O2A-CGA
31	p	614	CLA	C2-C1-O2A-CGA
31	q	306	CLA	C2-C1-O2A-CGA
31	a	407	CLA	C2-C1-O2A-CGA
31	b	605	CLA	C2-C1-O2A-CGA
31	b	613	CLA	C2-C1-O2A-CGA
31	b	614	CLA	C2-C1-O2A-CGA
31	b	616	CLA	C2-C1-O2A-CGA
31	c	602	CLA	C2-C1-O2A-CGA
31	d	401	CLA	C2-C1-O2A-CGA
31	d	405	CLA	C2-C1-O2A-CGA
33	9	320	LHG	C24-C25-C26-C27
31	2	602	CLA	C13-C15-C16-C17
31	6	312	CLA	C10-C11-C12-C13
31	B	602	CLA	C15-C16-C17-C18
31	B	614	CLA	C8-C10-C11-C12
31	G	610	CLA	C5-C6-C7-C8
33	4	618	LHG	C7-C8-C9-C10
33	S	320	LHG	C23-C24-C25-C26
33	0	619	LHG	C23-C24-C25-C26
33	7	319	LHG	C23-C24-C25-C26
33	q	320	LHG	C7-C8-C9-C10
45	c	618	DGD	C1B-C2B-C3B-C4B
30	G	606	CHL	CBD-CGD-O2D-CED
30	r	309	CHL	CBD-CGD-O2D-CED
31	7	316	CLA	CBD-CGD-O2D-CED
34	5	620	LMG	C12-C13-C14-C15
34	G	619	LMG	C11-C10-O7-C8
34	Y	319	LMG	C11-C10-O7-C8
31	B	608	CLA	C15-C16-C17-C18
31	S	312	CLA	C5-C6-C7-C8
31	b	607	CLA	C10-C11-C12-C13
30	G	601	CHL	C4-C3-C5-C6
30	Y	309	CHL	C11-C12-C13-C15
30	q	309	CHL	C6-C7-C8-C10
31	1	611	CLA	C11-C10-C8-C7
31	1	612	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	3	316	CLA	C11-C10-C8-C7
31	4	613	CLA	C11-C10-C8-C7
31	6	314	CLA	C11-C10-C8-C7
31	B	605	CLA	C11-C12-C13-C15
31	C	603	CLA	C6-C7-C8-C10
31	0	610	CLA	C6-C7-C8-C10
31	7	312	CLA	C11-C10-C8-C7
31	a	406	CLA	C11-C10-C8-C7
31	b	608	CLA	C11-C10-C8-C7
31	b	613	CLA	C6-C7-C8-C10
31	b	614	CLA	C11-C12-C13-C15
31	c	603	CLA	C6-C7-C8-C10
48	r	302	LMU	C1-C2-C3-C4
31	Y	304	CLA	C3-C5-C6-C7
31	C	607	CLA	O1A-CGA-O2A-C1
31	C	610	CLA	O1A-CGA-O2A-C1
31	G	604	CLA	O1A-CGA-O2A-C1
31	Y	313	CLA	O1A-CGA-O2A-C1
31	0	603	CLA	O1A-CGA-O2A-C1
31	b	612	CLA	O1A-CGA-O2A-C1
38	m	101	SQD	O10-C23-O48-C46
32	3	318	LUT	C9-C10-C11-C12
32	4	616	LUT	C9-C10-C11-C12
36	g	317	NEX	C13-C14-C15-C35
36	n	319	NEX	C9-C10-C11-C12
43	B	618	BCR	C9-C10-C11-C12
43	D	405	BCR	C15-C16-C17-C18
43	V	101	BCR	C15-C16-C17-C18
43	b	620	BCR	C9-C10-C11-C12
43	c	614	BCR	C15-C16-C17-C18
31	C	608	CLA	CBA-CGA-O2A-C1
33	b	625	LHG	C24-C23-O8-C6
30	5	608	CHL	C2A-CAA-CBA-CGA
30	G	623	CHL	C2A-CAA-CBA-CGA
30	Y	301	CHL	C2A-CAA-CBA-CGA
30	Y	302	CHL	C2A-CAA-CBA-CGA
30	0	601	CHL	C2A-CAA-CBA-CGA
30	0	607	CHL	C2A-CAA-CBA-CGA
30	8	601	CHL	C2A-CAA-CBA-CGA
30	9	308	CHL	C2A-CAA-CBA-CGA
30	n	302	CHL	C2A-CAA-CBA-CGA
30	y	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	2	604	CLA	C2A-CAA-CBA-CGA
31	5	603	CLA	C2A-CAA-CBA-CGA
31	5	610	CLA	C2A-CAA-CBA-CGA
31	R	312	CLA	C2A-CAA-CBA-CGA
31	p	603	CLA	C2A-CAA-CBA-CGA
30	4	609	CHL	O1D-CGD-O2D-CED
30	N	301	CHL	O1D-CGD-O2D-CED
30	q	307	CHL	O1D-CGD-O2D-CED
30	q	309	CHL	O1D-CGD-O2D-CED
31	5	612	CLA	O1D-CGD-O2D-CED
31	6	305	CLA	O1D-CGD-O2D-CED
31	C	601	CLA	O1D-CGD-O2D-CED
31	7	313	CLA	O1D-CGD-O2D-CED
31	c	601	CLA	O1D-CGD-O2D-CED
31	c	607	CLA	O1D-CGD-O2D-CED
31	y	610	CLA	O1D-CGD-O2D-CED
31	4	613	CLA	C8-C10-C11-C12
31	D	403	CLA	C15-C16-C17-C18
31	7	313	CLA	C8-C10-C11-C12
31	8	612	CLA	C8-C10-C11-C12
31	b	607	CLA	C8-C10-C11-C12
31	b	613	CLA	C8-C10-C11-C12
31	b	617	CLA	C5-C6-C7-C8
31	c	611	CLA	C5-C6-C7-C8
31	n	314	CLA	C8-C10-C11-C12
31	s	310	CLA	C8-C10-C11-C12
31	y	611	CLA	C15-C16-C17-C18
31	y	612	CLA	C15-C16-C17-C18
31	B	605	CLA	O1A-CGA-O2A-C1
31	R	314	CLA	O1A-CGA-O2A-C1
31	c	607	CLA	O1A-CGA-O2A-C1
33	G	618	LHG	O10-C23-O8-C6
38	M	102	SQD	O10-C23-O48-C46
30	N	308	CHL	CBD-CGD-O2D-CED
30	y	607	CHL	CBD-CGD-O2D-CED
34	B	621	LMG	O6-C1-O1-C7
34	j	101	LMG	O6-C1-O1-C7
38	X	201	SQD	O5-C1-O6-C44
31	2	602	CLA	C15-C16-C17-C18
31	C	603	CLA	C10-C11-C12-C13
31	S	313	CLA	C5-C6-C7-C8
31	g	310	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	y	602	CLA	O1D-CGD-O2D-CED
44	A	416	PL9	C44-C46-C47-C48
44	D	406	PL9	C44-C46-C47-C48
33	7	319	LHG	C10-C11-C12-C13
33	8	618	LHG	C23-C24-C25-C26
33	c	622	LHG	C7-C8-C9-C10
33	n	320	LHG	C23-C24-C25-C26
36	8	617	NEX	C10-C11-C12-C13
36	p	618	NEX	C30-C31-C32-C33
36	q	319	NEX	C30-C31-C32-C33
37	R	318	XAT	C10-C11-C12-C13
37	r	318	XAT	C10-C11-C12-C13
33	4	618	LHG	C16-C17-C18-C19
34	2	618	LMG	C35-C36-C37-C38
34	6	321	LMG	C35-C36-C37-C38
34	A	418	LMG	C35-C36-C37-C38
34	C	621	LMG	C35-C36-C37-C38
34	G	619	LMG	C35-C36-C37-C38
34	W	203	LMG	C35-C36-C37-C38
34	X	203	LMG	C35-C36-C37-C38
34	Y	319	LMG	C35-C36-C37-C38
34	0	620	LMG	C35-C36-C37-C38
34	0	622	LMG	C35-C36-C37-C38
34	7	301	LMG	C17-C18-C19-C20
34	a	416	LMG	C35-C36-C37-C38
34	f	101	LMG	C35-C36-C37-C38
34	g	320	LMG	C35-C36-C37-C38
34	w	204	LMG	C35-C36-C37-C38
45	C	616	DGD	C8B-C9B-CAB-CBB
48	R	302	LMU	O1'-C1-C2-C3
31	C	609	CLA	O1D-CGD-O2D-CED
34	W	203	LMG	O6-C5-C6-O5
33	2	617	LHG	O2-C2-C3-O3
33	D	408	LHG	O2-C2-C3-O3
33	G	618	LHG	O2-C2-C3-O3
33	0	619	LHG	O2-C2-C3-O3
33	q	320	LHG	O2-C2-C3-O3
33	b	625	LHG	O2-C2-C3-O3
33	c	622	LHG	O2-C2-C3-O3
33	e	101	LHG	O2-C2-C3-O3
33	g	319	LHG	O2-C2-C3-O3
33	s	320	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
33	R	320	LHG	O9-C7-O7-C5
34	3	321	LMG	O9-C10-O7-C8
34	B	625	LMG	O9-C10-O7-C8
34	X	203	LMG	O9-C10-O7-C8
31	2	602	CLA	C3-C5-C6-C7
31	3	311	CLA	C3-C5-C6-C7
31	N	321	CLA	C3-C5-C6-C7
31	7	315	CLA	C3-C5-C6-C7
31	1	604	CLA	C8-C10-C11-C12
31	1	610	CLA	C8-C10-C11-C12
31	C	605	CLA	C5-C6-C7-C8
31	C	611	CLA	C13-C15-C16-C17
31	D	403	CLA	C13-C15-C16-C17
31	G	612	CLA	C5-C6-C7-C8
31	Y	312	CLA	C10-C11-C12-C13
31	Y	313	CLA	C10-C11-C12-C13
31	Y	313	CLA	C13-C15-C16-C17
31	0	602	CLA	C13-C15-C16-C17
31	b	604	CLA	C5-C6-C7-C8
31	r	305	CLA	C8-C10-C11-C12
31	s	305	CLA	C8-C10-C11-C12
31	4	604	CLA	CBA-CGA-O2A-C1
31	G	612	CLA	CBA-CGA-O2A-C1
34	6	323	LMG	C35-C36-C37-C38
34	w	203	LMG	C35-C36-C37-C38
34	Q1	101	LMG	C35-C36-C37-C38
38	B	623	SQD	C14-C15-C16-C17
30	Y	308	CHL	O1D-CGD-O2D-CED
31	9	312	CLA	O1A-CGA-O2A-C1
31	g	311	CLA	O1A-CGA-O2A-C1
31	y	604	CLA	O1A-CGA-O2A-C1
45	c	617	DGD	O1A-C1A-O1G-C1G
45	c	618	DGD	O1A-C1A-O1G-C1G
45	c	619	DGD	O1A-C1A-O1G-C1G
33	D	407	LHG	C7-C8-C9-C10
33	L	101	LHG	C23-C24-C25-C26
33	b	625	LHG	C7-C8-C9-C10
33	l	101	LHG	C7-C8-C9-C10
38	a	412	SQD	C7-C8-C9-C10
33	G	618	LHG	C24-C25-C26-C27
33	K	102	LHG	C25-C26-C27-C28
34	6	322	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
34	W	202	LMG	C35-C36-C37-C38
34	c	620	LMG	C35-C36-C37-C38
34	x	202	LMG	C35-C36-C37-C38
34	y	620	LMG	C35-C36-C37-C38
31	3	313	CLA	O1D-CGD-O2D-CED
30	1	607	CHL	C5-C6-C7-C8
30	G	623	CHL	C8-C10-C11-C12
31	5	602	CLA	C5-C6-C7-C8
31	A	406	CLA	C13-C15-C16-C17
31	B	604	CLA	C8-C10-C11-C12
31	Y	310	CLA	C5-C6-C7-C8
31	9	304	CLA	C5-C6-C7-C8
31	b	611	CLA	C5-C6-C7-C8
31	b	612	CLA	C13-C15-C16-C17
31	b	614	CLA	C5-C6-C7-C8
31	b	614	CLA	C8-C10-C11-C12
31	c	608	CLA	C10-C11-C12-C13
31	r	305	CLA	C5-C6-C7-C8
31	r	316	CLA	C5-C6-C7-C8
31	s	311	CLA	C15-C16-C17-C18
31	y	610	CLA	C5-C6-C7-C8
33	L	101	LHG	C30-C31-C32-C33
33	0	619	LHG	C9-C10-C11-C12
30	8	601	CHL	CBD-CGD-O2D-CED
30	n	302	CHL	CBD-CGD-O2D-CED
31	B	603	CLA	O1A-CGA-O2A-C1
31	b	614	CLA	O1A-CGA-O2A-C1
33	r	320	LHG	C8-C7-O7-C5
34	9	302	LMG	C11-C10-O7-C8
34	g	322	LMG	C20-C21-C22-C23
30	4	607	CHL	C5-C6-C7-C8
30	y	609	CHL	C5-C6-C7-C8
31	2	610	CLA	C8-C10-C11-C12
31	B	611	CLA	C8-C10-C11-C12
31	B	613	CLA	C5-C6-C7-C8
31	C	605	CLA	C13-C15-C16-C17
31	C	610	CLA	C8-C10-C11-C12
31	C	610	CLA	C15-C16-C17-C18
31	S	311	CLA	C8-C10-C11-C12
31	p	610	CLA	C5-C6-C7-C8
31	b	615	CLA	C8-C10-C11-C12
31	b	617	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	s	314	CLA	C13-C15-C16-C17
33	1	617	LHG	C3-O3-P-O6
33	1	617	LHG	C4-O6-P-O3
33	2	617	LHG	C3-O3-P-O6
33	5	619	LHG	C4-O6-P-O3
33	A	415	LHG	C3-O3-P-O6
33	A	415	LHG	C4-O6-P-O3
33	D	407	LHG	C4-O6-P-O3
33	D	408	LHG	C3-O3-P-O6
33	G	618	LHG	C4-O6-P-O3
33	L	101	LHG	C4-O6-P-O3
33	M	101	LHG	C3-O3-P-O6
33	N	319	LHG	C3-O3-P-O6
33	N	319	LHG	C4-O6-P-O3
33	R	320	LHG	C4-O6-P-O3
33	S	322	LHG	C3-O3-P-O6
33	S	322	LHG	C4-O6-P-O3
33	Y	318	LHG	C4-O6-P-O3
33	7	319	LHG	C4-O6-P-O3
33	8	618	LHG	C4-O6-P-O3
33	p	619	LHG	C4-O6-P-O3
33	q	320	LHG	C3-O3-P-O6
33	q	320	LHG	C4-O6-P-O3
33	b	628	LHG	C4-O6-P-O3
33	c	622	LHG	C3-O3-P-O6
33	c	622	LHG	C4-O6-P-O3
33	d	408	LHG	C4-O6-P-O3
33	e	101	LHG	C3-O3-P-O6
33	g	319	LHG	C4-O6-P-O3
33	j	102	LHG	C4-O6-P-O3
33	l	101	LHG	C4-O6-P-O3
33	n	320	LHG	C4-O6-P-O3
33	r	320	LHG	C4-O6-P-O3
33	t	102	LHG	C3-O3-P-O6
33	y	619	LHG	C4-O6-P-O3
33	F1	301	LHG	C3-O3-P-O6
33	a	415	LHG	C7-C8-C9-C10
34	A	414	LMG	C28-C29-C30-C31
44	d	407	PL9	C47-C48-C49-C51
31	C	601	CLA	C3-C5-C6-C7
31	8	614	CLA	C3-C5-C6-C7
31	n	316	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	Y	314	CLA	CBA-CGA-O2A-C1
31	0	602	CLA	CBA-CGA-O2A-C1
31	a	406	CLA	CBA-CGA-O2A-C1
31	c	605	CLA	CBA-CGA-O2A-C1
31	c	613	CLA	CBA-CGA-O2A-C1
31	r	314	CLA	CBA-CGA-O2A-C1
34	0	622	LMG	C29-C28-O8-C9
31	B	611	CLA	O1D-CGD-O2D-CED
31	N	305	CLA	O1D-CGD-O2D-CED
31	C	602	CLA	C13-C15-C16-C17
31	G	602	CLA	O1D-CGD-O2D-CED
31	p	611	CLA	O1D-CGD-O2D-CED
33	B	624	LHG	C29-C30-C31-C32
31	r	312	CLA	C8-C10-C11-C12
33	K	102	LHG	C23-C24-C25-C26
33	N	319	LHG	C7-C8-C9-C10
33	r	320	LHG	C23-C24-C25-C26
34	7	301	LMG	C28-C29-C30-C31
34	b	623	LMG	C28-C29-C30-C31
38	6	301	SQD	C23-C24-C25-C26
38	B	620	SQD	C7-C8-C9-C10
31	p	612	CLA	O1D-CGD-O2D-CED
31	y	612	CLA	O1D-CGD-O2D-CED
33	3	320	LHG	C1-C2-C3-O3
33	A	415	LHG	C1-C2-C3-O3
33	B	624	LHG	C1-C2-C3-O3
33	R	320	LHG	C1-C2-C3-O3
33	0	619	LHG	C1-C2-C3-O3
33	b	628	LHG	C1-C2-C3-O3
33	e	101	LHG	C1-C2-C3-O3
33	s	322	LHG	C1-C2-C3-O3
33	r	320	LHG	O9-C7-O7-C5
34	G	619	LMG	O9-C10-O7-C8
34	Y	319	LMG	O9-C10-O7-C8
34	9	302	LMG	O9-C10-O7-C8
34	n	321	LMG	O9-C10-O7-C8
34	n	322	LMG	O9-C10-O7-C8
34	w	202	LMG	O9-C10-O7-C8
30	3	310	CHL	C4-C3-C5-C6
30	7	310	CHL	C4-C3-C5-C6
30	y	601	CHL	C4-C3-C5-C6
31	7	311	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
33	8	618	LHG	C24-C25-C26-C27
33	n	320	LHG	C24-C25-C26-C27
31	Y	310	CLA	C8-C10-C11-C12
31	g	310	CLA	C5-C6-C7-C8
33	A	417	LHG	C29-C30-C31-C32
30	1	619	CHL	C2A-CAA-CBA-CGA
30	3	307	CHL	C2A-CAA-CBA-CGA
30	3	309	CHL	C2A-CAA-CBA-CGA
30	4	605	CHL	C2A-CAA-CBA-CGA
30	5	601	CHL	C2A-CAA-CBA-CGA
30	5	605	CHL	C2A-CAA-CBA-CGA
30	6	308	CHL	C2A-CAA-CBA-CGA
30	G	606	CHL	C2A-CAA-CBA-CGA
30	N	302	CHL	C2A-CAA-CBA-CGA
30	R	308	CHL	C2A-CAA-CBA-CGA
30	7	302	CHL	C2A-CAA-CBA-CGA
30	7	309	CHL	C2A-CAA-CBA-CGA
30	8	605	CHL	C2A-CAA-CBA-CGA
30	9	307	CHL	C2A-CAA-CBA-CGA
30	9	310	CHL	C2A-CAA-CBA-CGA
30	p	605	CHL	C2A-CAA-CBA-CGA
30	p	606	CHL	C2A-CAA-CBA-CGA
30	p	607	CHL	C2A-CAA-CBA-CGA
30	p	608	CHL	C2A-CAA-CBA-CGA
30	n	306	CHL	C2A-CAA-CBA-CGA
30	r	308	CHL	C2A-CAA-CBA-CGA
30	y	601	CHL	C2A-CAA-CBA-CGA
31	3	311	CLA	C2A-CAA-CBA-CGA
31	G	612	CLA	C2A-CAA-CBA-CGA
31	b	615	CLA	C2A-CAA-CBA-CGA
31	r	316	CLA	C2A-CAA-CBA-CGA
31	3	314	CLA	C6-C7-C8-C9
31	4	603	CLA	C6-C7-C8-C9
31	p	603	CLA	C6-C7-C8-C10
30	7	321	CHL	C3-C5-C6-C7
30	n	308	CHL	C3-C5-C6-C7
31	p	613	CLA	C3-C5-C6-C7
31	s	310	CLA	C3-C5-C6-C7
30	7	310	CHL	O1D-CGD-O2D-CED
31	N	303	CLA	CBA-CGA-O2A-C1
31	S	314	CLA	CBA-CGA-O2A-C1
31	7	303	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	D	404	CLA	C8-C10-C11-C12
33	L	101	LHG	C7-C8-C9-C10
31	b	605	CLA	C8-C10-C11-C12
43	h	101	BCR	C9-C10-C11-C12
43	v	101	BCR	C13-C14-C15-C16
33	A	417	LHG	C7-C8-C9-C10
33	7	319	LHG	C11-C12-C13-C14
33	g	319	LHG	C11-C12-C13-C14
33	g	319	LHG	C28-C29-C30-C31
34	D	409	LMG	C32-C33-C34-C35
34	q	301	LMG	C16-C17-C18-C19
30	0	607	CHL	O1D-CGD-O2D-CED
31	1	612	CLA	O1D-CGD-O2D-CED
31	c	609	CLA	O1D-CGD-O2D-CED
33	6	320	LHG	C8-C7-O7-C5
33	D	407	LHG	C8-C7-O7-C5
33	9	320	LHG	C8-C7-O7-C5
33	j	102	LHG	C8-C7-O7-C5
34	C	619	LMG	C11-C10-O7-C8
34	W	202	LMG	C11-C10-O7-C8
34	n	322	LMG	C11-C10-O7-C8
34	w	201	LMG	C11-C10-O7-C8
31	C	609	CLA	C13-C15-C16-C17
31	p	611	CLA	C8-C10-C11-C12
36	2	616	NEX	C40-C33-C34-C35
36	3	319	NEX	C11-C10-C9-C19
36	4	617	NEX	C20-C13-C14-C15
36	N	318	NEX	C20-C13-C14-C15
36	N	318	NEX	C39-C29-C30-C31
36	R	319	NEX	C39-C29-C30-C31
36	R	319	NEX	C40-C33-C34-C35
36	8	617	NEX	C11-C10-C9-C19
36	8	617	NEX	C40-C33-C34-C35
36	p	618	NEX	C39-C29-C30-C31
36	n	319	NEX	C40-C33-C34-C35
36	r	301	NEX	C39-C29-C30-C31
36	r	319	NEX	C39-C29-C30-C31
37	R	318	XAT	C20-C13-C14-C15
31	6	315	CLA	C3-C5-C6-C7
31	c	601	CLA	C3-C5-C6-C7
33	1	617	LHG	C11-C12-C13-C14
33	5	619	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	S	320	LHG	C29-C30-C31-C32
33	S	322	LHG	C13-C14-C15-C16
33	c	622	LHG	C11-C12-C13-C14
33	c	622	LHG	C13-C14-C15-C16
33	l	101	LHG	C13-C14-C15-C16
33	s	322	LHG	C13-C14-C15-C16
34	W	203	LMG	C30-C31-C32-C33
38	y	621	SQD	C25-C26-C27-C28
31	3	306	CLA	O1A-CGA-O2A-C1
31	A	407	CLA	O1D-CGD-O2D-CED
31	B	610	CLA	O1D-CGD-O2D-CED
31	S	311	CLA	O1D-CGD-O2D-CED
31	b	611	CLA	O1D-CGD-O2D-CED
31	d	401	CLA	O1D-CGD-O2D-CED
31	2	611	CLA	C6-C7-C8-C9
31	6	305	CLA	C6-C7-C8-C10
31	0	604	CLA	C6-C7-C8-C9
31	c	612	CLA	C6-C7-C8-C9
31	g	305	CLA	C6-C7-C8-C9
31	r	315	CLA	C6-C7-C8-C9
31	r	316	CLA	C16-C17-C18-C20
31	b	610	CLA	CBA-CGA-O2A-C1
31	c	604	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C11-C12-C13-C14
33	L	101	LHG	C11-C10-C9-C8
33	R	320	LHG	C13-C14-C15-C16
33	S	320	LHG	C9-C10-C11-C12
33	b	625	LHG	C13-C14-C15-C16
33	b	628	LHG	C11-C12-C13-C14
33	s	320	LHG	C29-C30-C31-C32
33	z	102	LHG	C9-C10-C11-C12
33	n	320	LHG	C4-C5-O7-C7
34	q1	101	LMG	C7-C8-O7-C10
33	6	320	LHG	O9-C7-O7-C5
33	D	407	LHG	O9-C7-O7-C5
33	9	320	LHG	O9-C7-O7-C5
33	j	102	LHG	O9-C7-O7-C5
34	C	619	LMG	O9-C10-O7-C8
34	G	621	LMG	O9-C10-O7-C8
34	W	202	LMG	O9-C10-O7-C8
34	w	201	LMG	O9-C10-O7-C8
31	b	616	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	g	313	CLA	C8-C10-C11-C12
31	r	312	CLA	C5-C6-C7-C8
33	q	320	LHG	C23-C24-C25-C26
34	D	410	LMG	C10-C11-C12-C13
31	a	407	CLA	CBD-CGD-O2D-CED
33	Y	318	LHG	C28-C29-C30-C31
33	g	319	LHG	C34-C35-C36-C37
33	r	320	LHG	C26-C27-C28-C29
33	z	102	LHG	C11-C12-C13-C14
38	B	620	SQD	C31-C32-C33-C34
38	a	411	SQD	C10-C11-C12-C13
31	G	612	CLA	O1A-CGA-O2A-C1
31	c	613	CLA	O1A-CGA-O2A-C1
33	4	618	LHG	C11-C10-C9-C8
33	4	618	LHG	C28-C29-C30-C31
33	D	408	LHG	C13-C14-C15-C16
33	M	101	LHG	C30-C31-C32-C33
33	S	322	LHG	C11-C12-C13-C14
33	8	618	LHG	C31-C32-C33-C34
33	n	320	LHG	C31-C32-C33-C34
33	y	619	LHG	C28-C29-C30-C31
38	r	322	SQD	C27-C28-C29-C30
38	s	301	SQD	C11-C10-C9-C8
31	B	615	CLA	O1D-CGD-O2D-CED
31	C	611	CLA	C15-C16-C17-C18
33	D	407	LHG	C13-C14-C15-C16
33	K	102	LHG	C13-C14-C15-C16
33	N	319	LHG	C13-C14-C15-C16
33	8	618	LHG	C15-C16-C17-C18
33	c	622	LHG	C29-C30-C31-C32
33	n	320	LHG	C15-C16-C17-C18
34	4	620	LMG	C16-C17-C18-C19
48	c	623	LMU	O1'-C1-C2-C3
31	y	603	CLA	C3-C5-C6-C7
33	d	408	LHG	C7-C8-C9-C10
30	N	306	CHL	O1D-CGD-O2D-CED
30	R	309	CHL	O1D-CGD-O2D-CED
34	R	321	LMG	C2-C1-O1-C7
34	q	302	LMG	C2-C1-O1-C7
34	j	101	LMG	C2-C1-O1-C7
36	2	616	NEX	C32-C33-C34-C35
36	3	319	NEX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
36	4	617	NEX	C12-C13-C14-C15
36	4	617	NEX	C28-C29-C30-C31
36	N	318	NEX	C12-C13-C14-C15
36	N	318	NEX	C28-C29-C30-C31
36	R	319	NEX	C28-C29-C30-C31
36	R	319	NEX	C32-C33-C34-C35
36	8	617	NEX	C11-C10-C9-C8
36	8	617	NEX	C32-C33-C34-C35
36	p	618	NEX	C28-C29-C30-C31
36	q	319	NEX	C28-C29-C30-C31
36	n	319	NEX	C32-C33-C34-C35
36	r	301	NEX	C28-C29-C30-C31
37	R	318	XAT	C12-C13-C14-C15
38	6	301	SQD	C2-C1-O6-C44
38	R	322	SQD	C2-C1-O6-C44
38	X	201	SQD	C2-C1-O6-C44
45	C	617	DGD	C2E-C1E-O5D-C6D
45	c	617	DGD	C2E-C1E-O5D-C6D
31	r	315	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C15-C16-C17-C18
33	C	623	LHG	C11-C10-C9-C8
33	Y	318	LHG	C11-C10-C9-C8
33	8	618	LHG	C28-C29-C30-C31
33	9	320	LHG	C25-C26-C27-C28
33	p	619	LHG	C11-C12-C13-C14
33	p	619	LHG	C26-C27-C28-C29
33	b	625	LHG	C26-C27-C28-C29
33	c	622	LHG	C9-C10-C11-C12
33	n	320	LHG	C26-C27-C28-C29
33	n	320	LHG	C28-C29-C30-C31
34	D	411	LMG	C32-C33-C34-C35
34	b	601	LMG	C30-C31-C32-C33
38	A	411	SQD	C12-C13-C14-C15
30	9	303	CHL	C8-C10-C11-C12
31	2	602	CLA	C5-C6-C7-C8
31	c	603	CLA	C8-C10-C11-C12
31	N	303	CLA	O1A-CGA-O2A-C1
31	S	305	CLA	O1A-CGA-O2A-C1
34	0	622	LMG	O10-C28-O8-C9
31	1	602	CLA	C11-C12-C13-C15
31	2	603	CLA	C6-C7-C8-C10
31	0	615	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	q	306	CLA	C6-C7-C8-C10
31	s	311	CLA	C16-C17-C18-C19
30	G	607	CHL	O1D-CGD-O2D-CED
30	Y	307	CHL	O1D-CGD-O2D-CED
30	8	607	CHL	O1D-CGD-O2D-CED
31	Y	303	CLA	O1D-CGD-O2D-CED
31	s	306	CLA	O1D-CGD-O2D-CED
34	d	409	LMG	O6-C5-C6-O5
30	1	607	CHL	C4-C3-C5-C6
31	2	612	CLA	C4-C3-C5-C6
31	A	405	CLA	C4-C3-C5-C6
31	B	609	CLA	C4-C3-C5-C6
31	S	303	CLA	C4-C3-C5-C6
31	a	406	CLA	C4-C3-C5-C6
31	b	610	CLA	C4-C3-C5-C6
31	s	314	CLA	C4-C3-C5-C6
33	N	319	LHG	C31-C32-C33-C34
33	R	320	LHG	C11-C12-C13-C14
33	Y	318	LHG	C11-C12-C13-C14
33	8	618	LHG	C26-C27-C28-C29
33	e	101	LHG	C26-C27-C28-C29
33	e	101	LHG	C28-C29-C30-C31
34	d	410	LMG	C32-C33-C34-C35
30	3	310	CHL	C2-C3-C5-C6
30	q	309	CHL	C2-C3-C5-C6
30	1	607	CHL	C11-C12-C13-C14
30	0	607	CHL	C6-C7-C8-C9
31	1	610	CLA	C6-C7-C8-C9
31	1	613	CLA	C14-C13-C15-C16
31	4	610	CLA	C6-C7-C8-C9
31	C	605	CLA	C14-C13-C15-C16
31	S	312	CLA	C6-C7-C8-C9
31	Y	312	CLA	C11-C10-C8-C9
31	9	304	CLA	C6-C7-C8-C9
31	b	614	CLA	C11-C12-C13-C14
31	b	617	CLA	C6-C7-C8-C9
31	c	601	CLA	C11-C10-C8-C9
31	c	603	CLA	C6-C7-C8-C9
31	g	311	CLA	C6-C7-C8-C9
30	q	308	CHL	O1D-CGD-O2D-CED
33	1	617	LHG	C23-C24-C25-C26
33	p	619	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
33	s	322	LHG	C23-C24-C25-C26
33	5	619	LHG	C11-C12-C13-C14
33	6	320	LHG	C11-C12-C13-C14
33	D	407	LHG	C9-C10-C11-C12
33	D	407	LHG	C11-C12-C13-C14
33	G	618	LHG	C11-C12-C13-C14
33	q	320	LHG	C11-C12-C13-C14
33	q	320	LHG	C28-C29-C30-C31
33	b	625	LHG	C11-C12-C13-C14
33	e	101	LHG	C13-C14-C15-C16
33	g	319	LHG	C13-C14-C15-C16
38	0	621	SQD	C11-C12-C13-C14
31	6	313	CLA	C5-C6-C7-C8
31	C	602	CLA	C15-C16-C17-C18
31	q	315	CLA	C8-C10-C11-C12
30	5	607	CHL	C2A-CAA-CBA-CGA
30	6	307	CHL	C2A-CAA-CBA-CGA
30	7	321	CHL	C2A-CAA-CBA-CGA
30	n	308	CHL	C2A-CAA-CBA-CGA
31	9	304	CLA	C2A-CAA-CBA-CGA
31	c	610	CLA	C2A-CAA-CBA-CGA
31	r	315	CLA	C2A-CAA-CBA-CGA
31	y	615	CLA	C2A-CAA-CBA-CGA
31	C	608	CLA	O1A-CGA-O2A-C1
31	R	304	CLA	O1A-CGA-O2A-C1
31	S	314	CLA	O1A-CGA-O2A-C1
31	0	602	CLA	O1A-CGA-O2A-C1
31	c	608	CLA	O1A-CGA-O2A-C1
31	r	314	CLA	O1A-CGA-O2A-C1
33	b	625	LHG	O10-C23-O8-C6
33	g	319	LHG	O10-C23-O8-C6
34	A	412	LMG	O10-C28-O8-C9
32	Y	316	LUT	C7-C8-C9-C19
32	7	317	LUT	C7-C8-C9-C19
32	9	318	LUT	C7-C8-C9-C19
32	p	616	LUT	C31-C32-C33-C40
32	p	617	LUT	C7-C8-C9-C19
32	q	318	LUT	C7-C8-C9-C19
35	g	315	RRX	C7-C8-C9-C34
43	A	410	BCR	C7-C8-C9-C34
43	T	101	BCR	C11-C12-C13-C35
43	c	615	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
33	3	320	LHG	C26-C27-C28-C29
33	L	101	LHG	C11-C12-C13-C14
33	R	320	LHG	C26-C27-C28-C29
33	s	320	LHG	C26-C27-C28-C29
33	z	102	LHG	C13-C14-C15-C16
34	b	624	LMG	C13-C14-C15-C16
38	X	201	SQD	C25-C26-C27-C28
33	2	617	LHG	O1-C1-C2-C3
33	3	320	LHG	O1-C1-C2-C3
33	5	619	LHG	O1-C1-C2-C3
33	6	320	LHG	O1-C1-C2-C3
33	A	417	LHG	O1-C1-C2-C3
33	B	624	LHG	O1-C1-C2-C3
33	G	618	LHG	O1-C1-C2-C3
33	L	101	LHG	O1-C1-C2-C3
33	S	322	LHG	O1-C1-C2-C3
33	Y	318	LHG	O1-C1-C2-C3
33	7	319	LHG	O1-C1-C2-C3
33	8	618	LHG	O1-C1-C2-C3
33	p	619	LHG	O1-C1-C2-C3
33	b	625	LHG	O1-C1-C2-C3
33	b	628	LHG	O1-C1-C2-C3
33	e	101	LHG	O1-C1-C2-C3
33	j	102	LHG	O1-C1-C2-C3
33	l	101	LHG	O1-C1-C2-C3
33	n	320	LHG	O1-C1-C2-C3
33	s	320	LHG	O1-C1-C2-C3
33	s	322	LHG	O1-C1-C2-C3
33	y	619	LHG	O1-C1-C2-C3
33	F1	301	LHG	O1-C1-C2-C3
32	N	317	LUT	C7-C8-C9-C10
32	9	318	LUT	C7-C8-C9-C10
32	q	318	LUT	C7-C8-C9-C10
32	g	316	LUT	C11-C12-C13-C14
43	B	617	BCR	C21-C22-C23-C24
43	B	619	BCR	C7-C8-C9-C10
43	T	101	BCR	C11-C12-C13-C14
43	V	101	BCR	C21-C22-C23-C24
43	Z	101	BCR	C7-C8-C9-C10
43	b	618	BCR	C17-C18-C19-C20
43	b	619	BCR	C21-C22-C23-C24
43	c	615	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
43	v	101	BCR	C7-C8-C9-C10
43	v	101	BCR	C21-C22-C23-C24
31	3	315	CLA	C3-C5-C6-C7
31	5	602	CLA	C3-C5-C6-C7
31	R	304	CLA	C3-C5-C6-C7
31	S	305	CLA	C3-C5-C6-C7
31	7	304	CLA	C3-C5-C6-C7
34	b	626	LMG	O9-C10-O7-C8
30	Y	302	CHL	C10-C11-C12-C13
31	R	316	CLA	C13-C15-C16-C17
31	c	610	CLA	C13-C15-C16-C17
34	G	621	LMG	C11-C10-O7-C8
34	b	626	LMG	C11-C10-O7-C8
33	4	618	LHG	C11-C12-C13-C14
33	A	415	LHG	C29-C30-C31-C32
33	S	320	LHG	C25-C26-C27-C28
33	S	322	LHG	C33-C34-C35-C36
33	b	625	LHG	C28-C29-C30-C31
33	e	101	LHG	C25-C26-C27-C28
33	l	101	LHG	C34-C35-C36-C37
34	6	321	LMG	C29-C30-C31-C32
34	0	620	LMG	C13-C14-C15-C16
33	2	617	LHG	C23-C24-C25-C26
33	5	619	LHG	C23-C24-C25-C26
33	A	415	LHG	C23-C24-C25-C26
33	D	408	LHG	C7-C8-C9-C10
33	R	320	LHG	C23-C24-C25-C26
33	8	618	LHG	C7-C8-C9-C10
33	9	320	LHG	C23-C24-C25-C26
33	j	102	LHG	C23-C24-C25-C26
33	n	320	LHG	C7-C8-C9-C10
34	9	302	LMG	C10-C11-C12-C13
38	G	624	SQD	C23-C24-C25-C26
31	D	403	CLA	O1D-CGD-O2D-CED
33	D	408	LHG	C9-C10-C11-C12
33	D	408	LHG	C26-C27-C28-C29
33	L	101	LHG	C33-C34-C35-C36
33	N	319	LHG	C11-C10-C9-C8
33	S	320	LHG	C13-C14-C15-C16
33	q	320	LHG	C13-C14-C15-C16
33	a	415	LHG	C28-C29-C30-C31
33	b	625	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
33	b	625	LHG	C10-C11-C12-C13
33	b	628	LHG	C28-C29-C30-C31
33	d	408	LHG	C13-C14-C15-C16
33	z	102	LHG	C25-C26-C27-C28
33	F1	301	LHG	C11-C10-C9-C8
34	m	102	LMG	C30-C31-C32-C33
45	c	617	DGD	C3B-C4B-C5B-C6B
48	r	302	LMU	C6-C7-C8-C9
30	1	619	CHL	C11-C12-C13-C15
31	2	611	CLA	C6-C7-C8-C10
31	3	305	CLA	C6-C7-C8-C10
31	4	603	CLA	C6-C7-C8-C10
31	N	304	CLA	C6-C7-C8-C9
31	Y	304	CLA	C6-C7-C8-C9
31	g	305	CLA	C6-C7-C8-C10
31	r	315	CLA	C6-C7-C8-C10
31	r	316	CLA	C16-C17-C18-C19
31	y	603	CLA	C6-C7-C8-C9
34	b	626	LMG	C8-C9-O8-C28
34	q	302	LMG	O6-C1-O1-C7
38	6	301	SQD	O5-C1-O6-C44
38	R	322	SQD	O5-C1-O6-C44
45	C	617	DGD	O6E-C1E-O5D-C6D
31	S	311	CLA	C10-C11-C12-C13
31	d	404	CLA	C15-C16-C17-C18
42	a	408	PHO	C5-C6-C7-C8
30	1	606	CHL	O1D-CGD-O2D-CED
33	5	619	LHG	C9-C10-C11-C12
33	B	624	LHG	C13-C14-C15-C16
33	D	407	LHG	C34-C35-C36-C37
33	D	408	LHG	C11-C12-C13-C14
33	K	102	LHG	C11-C12-C13-C14
33	S	320	LHG	C11-C10-C9-C8
33	s	320	LHG	C13-C14-C15-C16
45	c	616	DGD	CAA-CBA-CCA-CDA
30	p	609	CHL	CBD-CGD-O2D-CED
31	C	608	CLA	CBD-CGD-O2D-CED
31	8	610	CLA	CBD-CGD-O2D-CED
31	n	312	CLA	CBD-CGD-O2D-CED
31	4	612	CLA	O1D-CGD-O2D-CED
33	4	618	LHG	C13-C14-C15-C16
33	M	101	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
33	M	101	LHG	C33-C34-C35-C36
33	8	618	LHG	C33-C34-C35-C36
33	n	320	LHG	C33-C34-C35-C36
33	s	320	LHG	C25-C26-C27-C28
33	y	619	LHG	C11-C10-C9-C8
34	a	416	LMG	C11-C12-C13-C14
34	a	416	LMG	C30-C31-C32-C33
33	l	101	LHG	C23-C24-C25-C26
45	C	616	DGD	C1A-C2A-C3A-C4A
30	G	601	CHL	C8-C10-C11-C12
31	0	603	CLA	C5-C6-C7-C8
31	c	605	CLA	O1A-CGA-O2A-C1
33	t	102	LHG	C28-C29-C30-C31
33	F1	301	LHG	C11-C12-C13-C14
34	6	321	LMG	C32-C33-C34-C35
38	B	620	SQD	C25-C26-C27-C28
31	G	602	CLA	C3-C5-C6-C7
31	8	603	CLA	C3-C5-C6-C7
31	s	305	CLA	C3-C5-C6-C7
31	C	606	CLA	CBA-CGA-O2A-C1
31	c	603	CLA	CBA-CGA-O2A-C1
45	C	617	DGD	C2A-C1A-O1G-C1G
33	d	408	LHG	C11-C12-C13-C14
33	y	619	LHG	C11-C12-C13-C14
34	D	412	LMG	C16-C17-C18-C19
34	n	321	LMG	C11-C12-C13-C14
48	R	302	LMU	C6-C7-C8-C9
30	4	607	CHL	O1D-CGD-O2D-CED
30	n	309	CHL	O1D-CGD-O2D-CED
30	3	303	CHL	C3A-C2A-CAA-CBA
30	4	608	CHL	C3A-C2A-CAA-CBA
30	6	307	CHL	C3A-C2A-CAA-CBA
30	G	601	CHL	C3A-C2A-CAA-CBA
30	0	606	CHL	C3A-C2A-CAA-CBA
30	7	306	CHL	C3A-C2A-CAA-CBA
30	7	308	CHL	C3A-C2A-CAA-CBA
30	g	302	CHL	C3A-C2A-CAA-CBA
30	n	310	CHL	C3A-C2A-CAA-CBA
31	1	603	CLA	C3A-C2A-CAA-CBA
31	1	614	CLA	C3A-C2A-CAA-CBA
31	2	603	CLA	C3A-C2A-CAA-CBA
31	3	305	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	4	603	CLA	C3A-C2A-CAA-CBA
31	5	603	CLA	C3A-C2A-CAA-CBA
31	5	615	CLA	C3A-C2A-CAA-CBA
31	6	304	CLA	C3A-C2A-CAA-CBA
31	6	313	CLA	C3A-C2A-CAA-CBA
31	B	604	CLA	C3A-C2A-CAA-CBA
31	B	610	CLA	C3A-C2A-CAA-CBA
31	C	612	CLA	C3A-C2A-CAA-CBA
31	C	613	CLA	C3A-C2A-CAA-CBA
31	G	603	CLA	C3A-C2A-CAA-CBA
31	N	304	CLA	C3A-C2A-CAA-CBA
31	R	307	CLA	C3A-C2A-CAA-CBA
31	Y	304	CLA	C3A-C2A-CAA-CBA
31	0	612	CLA	C3A-C2A-CAA-CBA
31	7	304	CLA	C3A-C2A-CAA-CBA
31	7	315	CLA	C3A-C2A-CAA-CBA
31	8	603	CLA	C3A-C2A-CAA-CBA
31	9	305	CLA	C3A-C2A-CAA-CBA
31	p	603	CLA	C3A-C2A-CAA-CBA
31	q	305	CLA	C3A-C2A-CAA-CBA
31	a	407	CLA	C3A-C2A-CAA-CBA
31	b	605	CLA	C3A-C2A-CAA-CBA
31	c	610	CLA	C3A-C2A-CAA-CBA
31	c	612	CLA	C3A-C2A-CAA-CBA
31	c	613	CLA	C3A-C2A-CAA-CBA
31	n	304	CLA	C3A-C2A-CAA-CBA
31	r	307	CLA	C3A-C2A-CAA-CBA
31	y	603	CLA	C3A-C2A-CAA-CBA
31	1	612	CLA	C15-C16-C17-C18
31	B	611	CLA	C13-C15-C16-C17
31	Y	312	CLA	C15-C16-C17-C18
31	q	305	CLA	C5-C6-C7-C8
31	c	610	CLA	C8-C10-C11-C12
34	X	202	LMG	C8-C9-O8-C28
31	9	304	CLA	C4C-C3C-CAC-CBC
33	M	101	LHG	C31-C32-C33-C34
33	8	618	LHG	C13-C14-C15-C16
33	n	320	LHG	C13-C14-C15-C16
34	B	625	LMG	C33-C34-C35-C36
34	D	409	LMG	C18-C19-C20-C21
31	C	607	CLA	O1D-CGD-O2D-CED
30	1	619	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	6	305	CLA	C6-C7-C8-C9
31	Y	305	CLA	C6-C7-C8-C9
31	0	604	CLA	C6-C7-C8-C10
33	2	617	LHG	C9-C10-C11-C12
33	4	618	LHG	C26-C27-C28-C29
33	B	624	LHG	C28-C29-C30-C31
33	D	408	LHG	C27-C28-C29-C30
33	M	101	LHG	C9-C10-C11-C12
33	q	320	LHG	C24-C25-C26-C27
33	a	415	LHG	C33-C34-C35-C36
33	b	628	LHG	C31-C32-C33-C34
33	t	102	LHG	C9-C10-C11-C12
34	b	624	LMG	C33-C34-C35-C36
34	x	202	LMG	C33-C34-C35-C36
34	y	620	LMG	C30-C31-C32-C33
33	S	320	LHG	C4-C5-C6-O8
34	D	409	LMG	O1-C7-C8-C9
38	B	620	SQD	O6-C44-C45-C46
38	M	102	SQD	C44-C45-C46-O48
31	N	321	CLA	C5-C6-C7-C8
31	7	315	CLA	C5-C6-C7-C8
33	1	617	LHG	C25-C26-C27-C28
33	5	619	LHG	C25-C26-C27-C28
33	A	415	LHG	C28-C29-C30-C31
33	D	408	LHG	C28-C29-C30-C31
33	L	101	LHG	C31-C32-C33-C34
33	j	102	LHG	C28-C29-C30-C31
33	t	102	LHG	C30-C31-C32-C33
34	C	619	LMG	C19-C20-C21-C22
34	c	621	LMG	C32-C33-C34-C35
36	2	616	NEX	C14-C15-C35-C34
37	R	318	XAT	C14-C15-C35-C34
31	B	616	CLA	C3-C5-C6-C7
31	a	407	CLA	C3-C5-C6-C7
38	s	301	SQD	C7-C8-C9-C10
33	S	320	LHG	C11-C12-C13-C14
33	d	408	LHG	C28-C29-C30-C31
31	4	604	CLA	O1A-CGA-O2A-C1
31	c	609	CLA	C10-C11-C12-C13
31	r	316	CLA	C8-C10-C11-C12
30	6	302	CHL	C4-C3-C5-C6
30	G	623	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	Y	311	CLA	C4-C3-C5-C6
31	0	603	CLA	C4-C3-C5-C6
31	7	314	CLA	C4-C3-C5-C6
31	y	611	CLA	C4-C3-C5-C6
31	9	306	CLA	CBA-CGA-O2A-C1
31	r	306	CLA	CBA-CGA-O2A-C1
31	A	405	CLA	C2-C3-C5-C6
31	Y	311	CLA	C2-C3-C5-C6
31	0	603	CLA	C2-C3-C5-C6
31	7	314	CLA	C2-C3-C5-C6
31	a	406	CLA	C2-C3-C5-C6
31	b	610	CLA	C2-C3-C5-C6
31	s	314	CLA	C2-C3-C5-C6
31	y	611	CLA	C2-C3-C5-C6
44	a	414	PL9	C12-C11-C9-C8
33	A	415	LHG	C8-C7-O7-C5
34	C	624	LMG	C11-C10-O7-C8
34	D	411	LMG	C11-C10-O7-C8
34	q	301	LMG	C11-C10-O7-C8
34	b	622	LMG	C11-C10-O7-C8
34	d	410	LMG	C11-C10-O7-C8
34	B	621	LMG	C8-C9-O8-C28
33	p	619	LHG	C10-C11-C12-C13
33	t	102	LHG	C26-C27-C28-C29
34	W	203	LMG	C4-C5-C6-O5
31	Y	311	CLA	C2A-CAA-CBA-CGA
31	Y	313	CLA	C2A-CAA-CBA-CGA
31	b	605	CLA	C2A-CAA-CBA-CGA
33	1	617	LHG	O1-C1-C2-O2
33	2	617	LHG	O1-C1-C2-O2
33	6	320	LHG	O1-C1-C2-O2
33	A	415	LHG	O1-C1-C2-O2
33	D	408	LHG	O1-C1-C2-O2
33	G	618	LHG	O1-C1-C2-O2
33	0	619	LHG	O1-C1-C2-O2
33	q	320	LHG	O1-C1-C2-O2
33	b	625	LHG	O1-C1-C2-O2
33	c	622	LHG	O1-C1-C2-O2
33	d	408	LHG	O1-C1-C2-O2
33	j	102	LHG	O1-C1-C2-O2
33	r	320	LHG	O1-C1-C2-O2
33	s	322	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
33	t	102	LHG	O1-C1-C2-O2
33	F1	301	LHG	O1-C1-C2-O2
33	4	618	LHG	C30-C31-C32-C33
33	D	407	LHG	C10-C11-C12-C13
33	M	101	LHG	C11-C10-C9-C8
33	0	619	LHG	C11-C12-C13-C14
33	j	102	LHG	C13-C14-C15-C16
34	B	622	LMG	C32-C33-C34-C35
34	B	622	LMG	C33-C34-C35-C36
45	C	617	DGD	C2A-C3A-C4A-C5A
31	3	316	CLA	C8-C10-C11-C12
31	q	313	CLA	O1D-CGD-O2D-CED
31	Y	314	CLA	O1A-CGA-O2A-C1
31	b	610	CLA	O1A-CGA-O2A-C1
31	1	602	CLA	C11-C12-C13-C14
31	9	315	CLA	C6-C7-C8-C9
30	g	302	CHL	C5-C6-C7-C8
31	7	311	CLA	C8-C10-C11-C12
45	c	619	DGD	CCA-CDA-CEA-CFA
30	7	308	CHL	C3-C5-C6-C7
31	9	315	CLA	C3-C5-C6-C7
31	g	313	CLA	C3-C5-C6-C7
48	c	623	LMU	C1-C2-C3-C4
31	s	305	CLA	CBA-CGA-O2A-C1
33	p	619	LHG	C5-C6-O8-C23
33	A	417	LHG	C26-C27-C28-C29
31	7	303	CLA	O1A-CGA-O2A-C1
31	a	406	CLA	O1A-CGA-O2A-C1
33	j	102	LHG	C7-C8-C9-C10
31	Y	304	CLA	C5-C6-C7-C8
34	D	409	LMG	O6-C5-C6-O5
31	2	602	CLA	C4C-C3C-CAC-CBC
33	e	101	LHG	C33-C34-C35-C36
34	C	624	LMG	O9-C10-O7-C8
34	D	411	LMG	O9-C10-O7-C8
34	q	301	LMG	O9-C10-O7-C8
34	b	622	LMG	O9-C10-O7-C8
34	d	410	LMG	O9-C10-O7-C8
31	2	604	CLA	C2-C1-O2A-CGA
31	3	314	CLA	C2-C1-O2A-CGA
31	5	604	CLA	C2-C1-O2A-CGA
31	A	406	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	B	604	CLA	C2-C1-O2A-CGA
31	B	613	CLA	C2-C1-O2A-CGA
31	B	616	CLA	C2-C1-O2A-CGA
31	C	613	CLA	C2-C1-O2A-CGA
31	D	404	CLA	C2-C1-O2A-CGA
31	G	610	CLA	C2-C1-O2A-CGA
31	N	313	CLA	C2-C1-O2A-CGA
31	R	303	CLA	C2-C1-O2A-CGA
31	S	315	CLA	C2-C1-O2A-CGA
31	Y	304	CLA	C2-C1-O2A-CGA
31	Y	314	CLA	C2-C1-O2A-CGA
31	8	604	CLA	C2-C1-O2A-CGA
31	q	316	CLA	C2-C1-O2A-CGA
31	b	602	CLA	C2-C1-O2A-CGA
31	g	305	CLA	C2-C1-O2A-CGA
31	r	305	CLA	C2-C1-O2A-CGA
31	r	307	CLA	C2-C1-O2A-CGA
31	s	306	CLA	C2-C1-O2A-CGA
31	s	310	CLA	C2-C1-O2A-CGA
31	s	315	CLA	C2-C1-O2A-CGA
31	0	614	CLA	C5-C6-C7-C8
33	A	415	LHG	C31-C32-C33-C34
33	s	322	LHG	C26-C27-C28-C29
31	C	608	CLA	C5-C6-C7-C8
31	c	604	CLA	O1A-CGA-O2A-C1
31	r	315	CLA	O1A-CGA-O2A-C1
45	C	617	DGD	O1A-C1A-O1G-C1G
31	3	301	CLA	C6-C7-C8-C9
33	y	619	LHG	C27-C28-C29-C30
31	Y	304	CLA	C6-C7-C8-C10
31	8	603	CLA	C6-C7-C8-C9
31	c	612	CLA	C6-C7-C8-C10
33	s	322	LHG	C7-C8-C9-C10
34	b	622	LMG	C10-C11-C12-C13
31	1	612	CLA	C3-C5-C6-C7
31	p	602	CLA	C3-C5-C6-C7
32	5	616	LUT	C5-C6-C7-C8
32	p	617	LUT	C1-C6-C7-C8
35	2	614	RRX	C1-C6-C7-C8
35	q	317	RRX	C23-C24-C25-C26
43	A	410	BCR	C1-C6-C7-C8
43	A	410	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
43	B	617	BCR	C1-C6-C7-C8
43	B	618	BCR	C1-C6-C7-C8
43	C	614	BCR	C23-C24-C25-C26
43	D	405	BCR	C23-C24-C25-C26
43	T	101	BCR	C23-C24-C25-C26
43	V	101	BCR	C1-C6-C7-C8
43	V	101	BCR	C5-C6-C7-C8
43	V	101	BCR	C23-C24-C25-C26
43	V	101	BCR	C23-C24-C25-C30
43	a	410	BCR	C23-C24-C25-C26
43	b	618	BCR	C1-C6-C7-C8
43	b	618	BCR	C23-C24-C25-C26
43	b	619	BCR	C1-C6-C7-C8
43	b	619	BCR	C23-C24-C25-C26
43	c	614	BCR	C1-C6-C7-C8
43	c	615	BCR	C5-C6-C7-C8
43	d	406	BCR	C23-C24-C25-C30
43	t	101	BCR	C1-C6-C7-C8
43	v	101	BCR	C1-C6-C7-C8
43	v	101	BCR	C5-C6-C7-C8
43	v	101	BCR	C23-C24-C25-C30
33	A	417	LHG	C25-C26-C27-C28
33	D	407	LHG	C30-C31-C32-C33
33	D	407	LHG	C31-C32-C33-C34
33	N	319	LHG	C28-C29-C30-C31
33	Y	318	LHG	C33-C34-C35-C36
33	y	619	LHG	C13-C14-C15-C16
38	a	411	SQD	C9-C10-C11-C12
30	1	619	CHL	CBA-CGA-O2A-C1
30	G	605	CHL	CBA-CGA-O2A-C1
31	G	602	CLA	CBA-CGA-O2A-C1
31	R	306	CLA	CBA-CGA-O2A-C1
31	y	612	CLA	CBA-CGA-O2A-C1
31	y	613	CLA	CBA-CGA-O2A-C1
31	4	602	CLA	C5-C6-C7-C8
31	0	610	CLA	C8-C10-C11-C12
31	7	314	CLA	C13-C15-C16-C17
34	d	409	LMG	C11-C10-O7-C8
33	A	415	LHG	C11-C12-C13-C14
33	q	320	LHG	C11-C10-C9-C8
34	b	601	LMG	C15-C16-C17-C18
34	f	101	LMG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
34	y	620	LMG	C29-C30-C31-C32
30	5	601	CHL	O1D-CGD-O2D-CED
31	N	311	CLA	O1D-CGD-O2D-CED
31	c	603	CLA	O1A-CGA-O2A-C1
30	9	310	CHL	CBD-CGD-O2D-CED
33	s	322	LHG	C11-C12-C13-C14
33	s	322	LHG	C34-C35-C36-C37
34	y	620	LMG	C12-C13-C14-C15
44	D	406	PL9	C47-C48-C49-C50
31	4	602	CLA	C13-C15-C16-C17
31	b	608	CLA	C15-C16-C17-C18
31	y	612	CLA	C8-C10-C11-C12
31	s	305	CLA	O1D-CGD-O2D-CED
33	t	102	LHG	C35-C36-C37-C38
30	1	605	CHL	C4-C3-C5-C6
30	1	609	CHL	C4-C3-C5-C6
30	4	601	CHL	C4-C3-C5-C6
30	N	302	CHL	C4-C3-C5-C6
30	Y	307	CHL	C4-C3-C5-C6
30	0	601	CHL	C4-C3-C5-C6
30	8	601	CHL	C4-C3-C5-C6
30	9	303	CHL	C4-C3-C5-C6
30	q	303	CHL	C4-C3-C5-C6
30	q	309	CHL	C4-C3-C5-C6
30	g	302	CHL	C4-C3-C5-C6
30	n	302	CHL	C4-C3-C5-C6
30	r	308	CHL	C4-C3-C5-C6
31	C	610	CLA	C4-C3-C5-C6
31	b	608	CLA	C4-C3-C5-C6
31	s	305	CLA	C4-C3-C5-C6
30	3	303	CHL	O1D-CGD-O2D-CED
30	1	601	CHL	C11-C12-C13-C15
30	1	605	CHL	C2-C3-C5-C6
30	1	605	CHL	C6-C7-C8-C10
30	1	607	CHL	C2-C3-C5-C6
30	1	609	CHL	C2-C3-C5-C6
30	G	623	CHL	C2-C3-C5-C6
30	N	302	CHL	C2-C3-C5-C6
30	Y	307	CHL	C2-C3-C5-C6
30	0	607	CHL	C2-C3-C5-C6
30	0	607	CHL	C6-C7-C8-C10
30	8	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	9	303	CHL	C2-C3-C5-C6
30	9	311	CHL	C6-C7-C8-C10
30	g	302	CHL	C2-C3-C5-C6
30	n	302	CHL	C2-C3-C5-C6
30	r	308	CHL	C2-C3-C5-C6
30	y	601	CHL	C2-C3-C5-C6
30	y	601	CHL	C11-C12-C13-C15
31	1	610	CLA	C6-C7-C8-C10
31	2	602	CLA	C12-C13-C15-C16
31	2	610	CLA	C11-C10-C8-C7
31	5	611	CLA	C11-C10-C8-C7
31	6	303	CLA	C11-C10-C8-C7
31	6	312	CLA	C11-C10-C8-C7
31	B	602	CLA	C11-C10-C8-C7
31	B	609	CLA	C2-C3-C5-C6
31	C	605	CLA	C12-C13-C15-C16
31	C	607	CLA	C11-C12-C13-C15
31	C	613	CLA	C11-C12-C13-C15
31	G	610	CLA	C6-C7-C8-C10
31	N	303	CLA	C6-C7-C8-C10
31	N	303	CLA	C11-C12-C13-C15
31	N	305	CLA	C6-C7-C8-C10
31	N	305	CLA	C11-C10-C8-C7
31	R	316	CLA	C12-C13-C15-C16
31	S	314	CLA	C6-C7-C8-C10
31	Y	312	CLA	C11-C10-C8-C7
31	Y	312	CLA	C11-C12-C13-C15
31	7	311	CLA	C6-C7-C8-C10
31	7	311	CLA	C11-C10-C8-C7
31	7	313	CLA	C6-C7-C8-C10
31	8	602	CLA	C6-C7-C8-C10
31	8	604	CLA	C6-C7-C8-C10
31	9	304	CLA	C6-C7-C8-C10
31	q	304	CLA	C6-C7-C8-C10
31	b	604	CLA	C6-C7-C8-C10
31	b	605	CLA	C6-C7-C8-C10
31	b	608	CLA	C2-C3-C5-C6
31	b	611	CLA	C11-C12-C13-C15
31	b	616	CLA	C11-C10-C8-C7
31	b	617	CLA	C6-C7-C8-C10
31	c	601	CLA	C11-C10-C8-C7
31	c	605	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	c	606	CLA	C6-C7-C8-C10
31	n	303	CLA	C6-C7-C8-C10
31	n	305	CLA	C6-C7-C8-C10
31	y	604	CLA	C2-C3-C5-C6
31	y	611	CLA	C11-C10-C8-C7
31	y	613	CLA	C11-C10-C8-C7
42	A	408	PHO	C11-C10-C8-C7
42	a	408	PHO	C11-C12-C13-C15
31	6	312	CLA	C3-C5-C6-C7
31	g	305	CLA	C3-C5-C6-C7
30	1	619	CHL	O1A-CGA-O2A-C1
31	G	602	CLA	O1A-CGA-O2A-C1
31	9	306	CLA	O1A-CGA-O2A-C1
31	y	612	CLA	O1A-CGA-O2A-C1
31	y	613	CLA	O1A-CGA-O2A-C1
33	b	628	LHG	C13-C14-C15-C16
33	j	102	LHG	C26-C27-C28-C29
30	7	307	CHL	C5-C6-C7-C8
31	3	312	CLA	C13-C15-C16-C17
31	C	605	CLA	C8-C10-C11-C12
31	D	404	CLA	C13-C15-C16-C17
35	g	315	RRX	C19-C20-C21-C22
36	8	617	NEX	C9-C10-C11-C12
43	b	618	BCR	C15-C16-C17-C18
31	n	304	CLA	C6-C7-C8-C9
33	S	320	LHG	O9-C7-O7-C5
34	D	410	LMG	O9-C10-O7-C8
34	g	322	LMG	O9-C10-O7-C8
38	a	412	SQD	O49-C7-O47-C45
38	a	412	SQD	C23-C24-C25-C26
30	2	606	CHL	CBA-CGA-O2A-C1
31	B	609	CLA	CBA-CGA-O2A-C1
31	B	613	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C16-C17-C18-C19
33	l	101	LHG	C25-C26-C27-C28
30	9	309	CHL	C2A-CAA-CBA-CGA
30	q	309	CHL	C2A-CAA-CBA-CGA
31	3	315	CLA	C2A-CAA-CBA-CGA
31	A	405	CLA	C2A-CAA-CBA-CGA
31	C	601	CLA	C2A-CAA-CBA-CGA
31	N	305	CLA	C2A-CAA-CBA-CGA
31	N	311	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	0	602	CLA	C2A-CAA-CBA-CGA
31	q	316	CLA	C2A-CAA-CBA-CGA
31	n	305	CLA	C2A-CAA-CBA-CGA
31	r	307	CLA	C2A-CAA-CBA-CGA
31	R	311	CLA	C8-C10-C11-C12
31	c	601	CLA	C15-C16-C17-C18
33	Y	318	LHG	C9-C10-C11-C12
31	9	305	CLA	O1D-CGD-O2D-CED
33	N	319	LHG	C33-C34-C35-C36
33	Y	318	LHG	C30-C31-C32-C33
34	m	102	LMG	C29-C30-C31-C32
38	a	412	SQD	C11-C10-C9-C8
45	c	616	DGD	C6A-C7A-C8A-C9A
33	1	617	LHG	C7-C8-C9-C10
34	m	102	LMG	C10-C11-C12-C13
38	x	201	SQD	C23-C24-C25-C26
31	y	611	CLA	O1D-CGD-O2D-CED
31	B	610	CLA	C5-C6-C7-C8
33	1	617	LHG	C26-C27-C28-C29
33	4	618	LHG	C14-C15-C16-C17
33	L	101	LHG	C13-C14-C15-C16
34	2	620	LMG	C18-C19-C20-C21
38	m	101	SQD	C26-C27-C28-C29
45	C	620	DGD	C4B-C5B-C6B-C7B
45	c	616	DGD	CCB-CDB-CEB-CFB
48	r	302	LMU	C2-C3-C4-C5
33	z	102	LHG	C5-C6-O8-C23
33	G	618	LHG	C33-C34-C35-C36
33	d	408	LHG	C26-C27-C28-C29
34	Q1	101	LMG	C31-C32-C33-C34
45	c	618	DGD	CCA-CDA-CEA-CFA
31	C	606	CLA	O1A-CGA-O2A-C1
31	r	306	CLA	O1A-CGA-O2A-C1
31	s	305	CLA	O1A-CGA-O2A-C1
30	n	310	CHL	CBD-CGD-O2D-CED
30	y	606	CHL	CBD-CGD-O2D-CED
31	7	304	CLA	C6-C7-C8-C9
31	q	312	CLA	C6-C7-C8-C9
34	R	321	LMG	O6-C1-O1-C7
31	B	605	CLA	C5-C6-C7-C8
31	B	608	CLA	C13-C15-C16-C17
30	6	308	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	3	301	CLA	C5-C6-C7-C8
33	D	408	LHG	C16-C17-C18-C19
33	8	618	LHG	C11-C10-C9-C8
33	n	320	LHG	C11-C10-C9-C8
34	d	411	LMG	C13-C14-C15-C16
38	a	412	SQD	C9-C10-C11-C12
34	x	202	LMG	C28-C29-C30-C31
38	S	301	SQD	C7-C8-C9-C10
33	3	320	LHG	C8-C7-O7-C5
33	S	320	LHG	C8-C7-O7-C5
33	b	628	LHG	C8-C7-O7-C5
33	s	320	LHG	C8-C7-O7-C5
33	t	102	LHG	C8-C7-O7-C5
34	D	409	LMG	C11-C10-O7-C8
34	D	410	LMG	C11-C10-O7-C8
34	S	321	LMG	C11-C10-O7-C8
34	g	322	LMG	C11-C10-O7-C8
34	r	321	LMG	C11-C10-O7-C8
38	a	412	SQD	C8-C7-O47-C45
45	C	616	DGD	C2B-C1B-O2G-C2G
31	1	614	CLA	C5-C6-C7-C8
33	c	622	LHG	C34-C35-C36-C37
34	S	321	LMG	C14-C15-C16-C17
34	q	302	LMG	C11-C12-C13-C14
38	R	322	SQD	C11-C12-C13-C14
48	r	302	LMU	O1'-C1-C2-C3
31	G	612	CLA	C13-C15-C16-C17
31	c	605	CLA	C5-C6-C7-C8
33	4	618	LHG	C24-C25-C26-C27
33	j	102	LHG	C31-C32-C33-C34
33	A	415	LHG	O9-C7-O7-C5
33	b	628	LHG	O9-C7-O7-C5
34	D	409	LMG	O9-C10-O7-C8
34	S	321	LMG	O9-C10-O7-C8
34	d	409	LMG	O9-C10-O7-C8
34	r	321	LMG	O9-C10-O7-C8
45	C	616	DGD	O1B-C1B-O2G-C2G
31	S	310	CLA	C3-C5-C6-C7
31	n	304	CLA	C3-C5-C6-C7
34	g	322	LMG	C12-C13-C14-C15
34	n	321	LMG	C12-C13-C14-C15
34	4	620	LMG	C2-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
34	B	625	LMG	C2-C1-O1-C7
34	C	621	LMG	C2-C1-O1-C7
34	C	624	LMG	C2-C1-O1-C7
34	9	302	LMG	C2-C1-O1-C7
34	9	321	LMG	C2-C1-O1-C7
34	b	601	LMG	C2-C1-O1-C7
34	b	626	LMG	C2-C1-O1-C7
34	b	629	LMG	C2-C1-O1-C7
45	C	617	DGD	C2D-C1D-O3G-C3G
45	c	619	DGD	C2D-C1D-O3G-C3G
31	b	608	CLA	C13-C15-C16-C17
33	1	617	LHG	O7-C5-C6-O8
33	S	320	LHG	O7-C5-C6-O8
33	7	319	LHG	O7-C5-C6-O8
33	b	625	LHG	O7-C5-C6-O8
33	r	320	LHG	O7-C5-C6-O8
33	s	322	LHG	O7-C5-C6-O8
34	A	418	LMG	O1-C7-C8-O7
34	D	412	LMG	O7-C8-C9-O8
34	R	321	LMG	O7-C8-C9-O8
34	a	416	LMG	O1-C7-C8-O7
34	n	321	LMG	O7-C8-C9-O8
38	6	301	SQD	O47-C45-C46-O48
38	G	624	SQD	O47-C45-C46-O48
34	7	322	LMG	O6-C5-C6-O5
38	s	301	SQD	C24-C23-O48-C46
33	2	617	LHG	C27-C28-C29-C30
33	r	320	LHG	C13-C14-C15-C16
31	3	314	CLA	C6-C7-C8-C10
31	9	305	CLA	C6-C7-C8-C9
33	2	617	LHG	C26-C27-C28-C29
33	e	101	LHG	C24-C25-C26-C27
33	n	320	LHG	C34-C35-C36-C37
33	s	322	LHG	C33-C34-C35-C36
45	c	616	DGD	C9B-CAB-CBB-CCB
34	g	320	LMG	O6-C5-C6-O5
34	w	202	LMG	O6-C5-C6-O5
34	Q1	101	LMG	O6-C5-C6-O5
31	C	601	CLA	C8-C10-C11-C12
31	s	312	CLA	C8-C10-C11-C12
30	R	309	CHL	C4-C3-C5-C6
30	0	607	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	7	302	CHL	C4-C3-C5-C6
30	9	311	CHL	C4-C3-C5-C6
30	r	309	CHL	C4-C3-C5-C6
31	7	315	CLA	C4-C3-C5-C6
31	y	604	CLA	C4-C3-C5-C6
34	0	620	LMG	C28-C29-C30-C31
30	3	302	CHL	C2-C3-C5-C6
30	N	306	CHL	C2-C3-C5-C6
30	q	303	CHL	C2-C3-C5-C6
31	2	612	CLA	C2-C3-C5-C6
31	3	301	CLA	C2-C3-C5-C6
31	C	610	CLA	C2-C3-C5-C6
31	S	303	CLA	C2-C3-C5-C6
31	s	305	CLA	C2-C3-C5-C6
44	D	406	PL9	C4-C3-C7-C8
44	a	414	PL9	C4-C3-C7-C8
44	d	407	PL9	C4-C3-C7-C8
33	B	624	LHG	C31-C32-C33-C34
33	8	618	LHG	C34-C35-C36-C37
30	1	606	CHL	C11-C10-C8-C9
30	2	608	CHL	C6-C7-C8-C9
30	Y	307	CHL	C11-C10-C8-C9
30	8	606	CHL	C11-C10-C8-C9
30	n	307	CHL	C11-C10-C8-C9
31	B	605	CLA	C11-C12-C13-C14
31	B	609	CLA	C6-C7-C8-C9
31	C	603	CLA	C6-C7-C8-C9
31	C	607	CLA	C11-C12-C13-C14
31	C	610	CLA	C14-C13-C15-C16
31	G	602	CLA	C6-C7-C8-C9
31	G	610	CLA	C6-C7-C8-C9
31	N	303	CLA	C6-C7-C8-C9
31	N	305	CLA	C6-C7-C8-C9
31	R	316	CLA	C6-C7-C8-C9
31	0	602	CLA	C11-C10-C8-C9
31	0	610	CLA	C6-C7-C8-C9
31	7	311	CLA	C6-C7-C8-C9
31	7	312	CLA	C11-C10-C8-C9
31	7	313	CLA	C6-C7-C8-C9
31	8	602	CLA	C6-C7-C8-C9
31	8	604	CLA	C6-C7-C8-C9
31	9	306	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	p	611	CLA	C6-C7-C8-C9
31	p	611	CLA	C11-C10-C8-C9
31	q	304	CLA	C6-C7-C8-C9
31	b	608	CLA	C11-C10-C8-C9
31	c	606	CLA	C6-C7-C8-C9
31	g	303	CLA	C14-C13-C15-C16
31	n	303	CLA	C6-C7-C8-C9
31	n	305	CLA	C6-C7-C8-C9
34	B	625	LMG	C8-C9-O8-C28
33	B	624	LHG	C10-C11-C12-C13
33	G	618	LHG	C30-C31-C32-C33
33	j	102	LHG	C34-C35-C36-C37
31	G	604	CLA	C3-C5-C6-C7
30	9	311	CHL	O1D-CGD-O2D-CED
30	q	308	CHL	C2A-CAA-CBA-CGA
31	R	306	CLA	C2A-CAA-CBA-CGA
31	8	604	CLA	C2A-CAA-CBA-CGA
31	b	613	CLA	C2A-CAA-CBA-CGA
31	d	405	CLA	C2A-CAA-CBA-CGA
33	C	623	LHG	C9-C10-C11-C12
33	S	322	LHG	C26-C27-C28-C29
33	7	319	LHG	C24-C25-C26-C27
34	B	622	LMG	O6-C5-C6-O5
34	R	321	LMG	O6-C5-C6-O5
34	w	201	LMG	O6-C5-C6-O5
45	C	620	DGD	O6E-C5E-C6E-O5E
32	2	615	LUT	C31-C32-C33-C40
32	3	318	LUT	C31-C32-C33-C40
32	N	317	LUT	C7-C8-C9-C19
32	s	318	LUT	C31-C32-C33-C40
43	T	101	BCR	C7-C8-C9-C34
43	V	101	BCR	C7-C8-C9-C34
43	a	410	BCR	C7-C8-C9-C34
43	z	101	BCR	C36-C18-C19-C20
31	7	312	CLA	O1D-CGD-O2D-CED
33	s	322	LHG	C31-C32-C33-C34
34	b	622	LMG	C19-C20-C21-C22
32	N	317	LUT	C11-C12-C13-C14
43	T	101	BCR	C7-C8-C9-C10
31	B	609	CLA	O1A-CGA-O2A-C1
31	R	306	CLA	O1A-CGA-O2A-C1
30	1	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
30	3	303	CHL	C1A-C2A-CAA-CBA
30	4	608	CHL	C1A-C2A-CAA-CBA
30	4	609	CHL	C1A-C2A-CAA-CBA
30	Y	302	CHL	C1A-C2A-CAA-CBA
30	Y	308	CHL	C1A-C2A-CAA-CBA
30	7	302	CHL	C1A-C2A-CAA-CBA
30	7	306	CHL	C1A-C2A-CAA-CBA
30	s	309	CHL	C1A-C2A-CAA-CBA
30	y	601	CHL	C1A-C2A-CAA-CBA
30	y	608	CHL	C1A-C2A-CAA-CBA
31	1	602	CLA	C1A-C2A-CAA-CBA
31	1	603	CLA	C1A-C2A-CAA-CBA
31	1	610	CLA	C1A-C2A-CAA-CBA
31	2	602	CLA	C1A-C2A-CAA-CBA
31	2	603	CLA	C1A-C2A-CAA-CBA
31	2	604	CLA	C1A-C2A-CAA-CBA
31	2	609	CLA	C1A-C2A-CAA-CBA
31	3	304	CLA	C1A-C2A-CAA-CBA
31	3	306	CLA	C1A-C2A-CAA-CBA
31	3	315	CLA	C1A-C2A-CAA-CBA
31	3	316	CLA	C1A-C2A-CAA-CBA
31	4	602	CLA	C1A-C2A-CAA-CBA
31	4	603	CLA	C1A-C2A-CAA-CBA
31	4	604	CLA	C1A-C2A-CAA-CBA
31	4	610	CLA	C1A-C2A-CAA-CBA
31	4	611	CLA	C1A-C2A-CAA-CBA
31	5	602	CLA	C1A-C2A-CAA-CBA
31	5	603	CLA	C1A-C2A-CAA-CBA
31	5	604	CLA	C1A-C2A-CAA-CBA
31	5	611	CLA	C1A-C2A-CAA-CBA
31	6	303	CLA	C1A-C2A-CAA-CBA
31	6	313	CLA	C1A-C2A-CAA-CBA
31	6	314	CLA	C1A-C2A-CAA-CBA
31	6	315	CLA	C1A-C2A-CAA-CBA
31	A	407	CLA	C1A-C2A-CAA-CBA
31	B	610	CLA	C1A-C2A-CAA-CBA
31	C	601	CLA	C1A-C2A-CAA-CBA
31	C	603	CLA	C1A-C2A-CAA-CBA
31	C	608	CLA	C1A-C2A-CAA-CBA
31	C	611	CLA	C1A-C2A-CAA-CBA
31	C	612	CLA	C1A-C2A-CAA-CBA
31	G	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	G	609	CLA	C1A-C2A-CAA-CBA
31	N	304	CLA	C1A-C2A-CAA-CBA
31	R	303	CLA	C1A-C2A-CAA-CBA
31	R	307	CLA	C1A-C2A-CAA-CBA
31	S	311	CLA	C1A-C2A-CAA-CBA
31	S	315	CLA	C1A-C2A-CAA-CBA
31	S	316	CLA	C1A-C2A-CAA-CBA
31	Y	303	CLA	C1A-C2A-CAA-CBA
31	Y	304	CLA	C1A-C2A-CAA-CBA
31	Y	310	CLA	C1A-C2A-CAA-CBA
31	Y	314	CLA	C1A-C2A-CAA-CBA
31	0	612	CLA	C1A-C2A-CAA-CBA
31	7	303	CLA	C1A-C2A-CAA-CBA
31	7	304	CLA	C1A-C2A-CAA-CBA
31	7	305	CLA	C1A-C2A-CAA-CBA
31	7	311	CLA	C1A-C2A-CAA-CBA
31	8	602	CLA	C1A-C2A-CAA-CBA
31	8	603	CLA	C1A-C2A-CAA-CBA
31	9	305	CLA	C1A-C2A-CAA-CBA
31	9	313	CLA	C1A-C2A-CAA-CBA
31	p	602	CLA	C1A-C2A-CAA-CBA
31	p	603	CLA	C1A-C2A-CAA-CBA
31	p	604	CLA	C1A-C2A-CAA-CBA
31	p	610	CLA	C1A-C2A-CAA-CBA
31	p	613	CLA	C1A-C2A-CAA-CBA
31	p	614	CLA	C1A-C2A-CAA-CBA
31	q	304	CLA	C1A-C2A-CAA-CBA
31	q	305	CLA	C1A-C2A-CAA-CBA
31	q	312	CLA	C1A-C2A-CAA-CBA
31	b	604	CLA	C1A-C2A-CAA-CBA
31	b	607	CLA	C1A-C2A-CAA-CBA
31	b	615	CLA	C1A-C2A-CAA-CBA
31	c	601	CLA	C1A-C2A-CAA-CBA
31	c	603	CLA	C1A-C2A-CAA-CBA
31	c	608	CLA	C1A-C2A-CAA-CBA
31	c	610	CLA	C1A-C2A-CAA-CBA
31	c	611	CLA	C1A-C2A-CAA-CBA
31	d	401	CLA	C1A-C2A-CAA-CBA
31	g	303	CLA	C1A-C2A-CAA-CBA
31	g	310	CLA	C1A-C2A-CAA-CBA
31	n	303	CLA	C1A-C2A-CAA-CBA
31	n	304	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	r	304	CLA	C1A-C2A-CAA-CBA
31	r	307	CLA	C1A-C2A-CAA-CBA
31	r	313	CLA	C1A-C2A-CAA-CBA
31	s	303	CLA	C1A-C2A-CAA-CBA
31	s	311	CLA	C1A-C2A-CAA-CBA
31	s	315	CLA	C1A-C2A-CAA-CBA
31	y	602	CLA	C1A-C2A-CAA-CBA
31	y	603	CLA	C1A-C2A-CAA-CBA
31	y	604	CLA	C1A-C2A-CAA-CBA
31	y	610	CLA	C1A-C2A-CAA-CBA
31	y	614	CLA	C1A-C2A-CAA-CBA
31	C	603	CLA	C16-C17-C18-C20
31	C	612	CLA	C6-C7-C8-C9
31	N	304	CLA	C6-C7-C8-C10
31	7	304	CLA	C6-C7-C8-C10
31	8	603	CLA	C6-C7-C8-C10
31	9	315	CLA	C6-C7-C8-C10
31	p	611	CLA	C11-C12-C13-C15
31	q	312	CLA	C6-C7-C8-C10
31	n	304	CLA	C6-C7-C8-C10
31	y	603	CLA	C6-C7-C8-C10
33	3	320	LHG	O9-C7-O7-C5
33	b	625	LHG	C8-C7-O7-C5
33	9	320	LHG	C26-C27-C28-C29
33	g	319	LHG	C30-C31-C32-C33
34	k	101	LMG	C18-C19-C20-C21
38	x	201	SQD	C27-C28-C29-C30
43	C	614	BCR	C9-C10-C11-C12
43	c	614	BCR	C13-C14-C15-C16
43	v	101	BCR	C9-C10-C11-C12
31	N	304	CLA	O1D-CGD-O2D-CED
31	B	603	CLA	C10-C11-C12-C13
31	b	609	CLA	C5-C6-C7-C8
31	c	602	CLA	C8-C10-C11-C12
31	c	603	CLA	C15-C16-C17-C18
33	B	624	LHG	C3-O3-P-O6
33	Y	318	LHG	C3-O3-P-O6
33	b	625	LHG	C4-O6-P-O3
33	e	101	LHG	C4-O6-P-O3
33	L	101	LHG	C29-C30-C31-C32
34	6	323	LMG	C29-C30-C31-C32
38	B	623	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
34	b	623	LMG	C10-C11-C12-C13
34	C	621	LMG	O6-C5-C6-O5
44	d	407	PL9	C47-C48-C49-C50
31	q	305	CLA	C3-C5-C6-C7
31	y	604	CLA	C3-C5-C6-C7
31	4	604	CLA	O1D-CGD-O2D-CED
33	N	319	LHG	C11-C12-C13-C14
38	s	301	SQD	C9-C10-C11-C12
30	G	605	CHL	O1A-CGA-O2A-C1
31	4	610	CLA	C10-C11-C12-C13
31	C	605	CLA	CBA-CGA-O2A-C1
31	g	310	CLA	CBA-CGA-O2A-C1
33	B	624	LHG	C24-C23-O8-C6
34	G	619	LMG	O6-C5-C6-O5
33	1	617	LHG	O6-C4-C5-C6
33	2	617	LHG	O6-C4-C5-C6
33	6	320	LHG	O6-C4-C5-C6
33	A	417	LHG	O6-C4-C5-C6
33	G	618	LHG	O6-C4-C5-C6
33	N	319	LHG	O6-C4-C5-C6
33	R	320	LHG	O6-C4-C5-C6
33	8	618	LHG	O6-C4-C5-C6
33	9	320	LHG	O6-C4-C5-C6
33	a	415	LHG	O6-C4-C5-C6
33	n	320	LHG	O6-C4-C5-C6
33	z	102	LHG	O6-C4-C5-C6
33	F1	301	LHG	O6-C4-C5-C6
34	B	621	LMG	C29-C30-C31-C32
34	k	101	LMG	C30-C31-C32-C33
48	R	302	LMU	C5'-C4'-O1B-C1B
33	1	617	LHG	C11-C10-C9-C8
33	a	415	LHG	C31-C32-C33-C34
33	l	101	LHG	C31-C32-C33-C34
34	W	201	LMG	O6-C5-C6-O5
34	c	620	LMG	O6-C5-C6-O5
31	N	310	CLA	C5-C6-C7-C8
34	w	205	LMG	C8-C9-O8-C28
33	2	617	LHG	C10-C11-C12-C13
33	b	628	LHG	C11-C10-C9-C8
34	D	412	LMG	C36-C37-C38-C39
45	c	618	DGD	C3A-C4A-C5A-C6A
30	1	606	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
33	b	628	LHG	C30-C31-C32-C33
33	s	320	LHG	C11-C12-C13-C14
30	N	307	CHL	CBA-CGA-O2A-C1
45	c	616	DGD	C2A-C1A-O1G-C1G
34	k	102	LMG	O6-C5-C6-O5
30	3	302	CHL	C4-C3-C5-C6
31	c	605	CLA	C4-C3-C5-C6
31	s	313	CLA	C4-C3-C5-C6
31	y	613	CLA	C4-C3-C5-C6
31	c	610	CLA	C2-C3-C5-C6
31	s	304	CLA	C3A-C2A-CAA-CBA
33	B	624	LHG	C12-C13-C14-C15
38	b	621	SQD	C26-C27-C28-C29
31	B	611	CLA	C15-C16-C17-C18
31	c	611	CLA	C8-C10-C11-C12
33	6	320	LHG	C9-C10-C11-C12
33	A	417	LHG	C33-C34-C35-C36
33	D	408	LHG	C17-C18-C19-C20
33	b	628	LHG	C15-C16-C17-C18
34	D	409	LMG	C11-C12-C13-C14
33	r	320	LHG	C7-C8-C9-C10
30	2	606	CHL	O1A-CGA-O2A-C1
31	B	613	CLA	O1A-CGA-O2A-C1
31	C	605	CLA	O1A-CGA-O2A-C1
33	e	101	LHG	C11-C12-C13-C14
34	b	626	LMG	C31-C32-C33-C34
34	c	624	LMG	C29-C30-C31-C32
30	y	606	CHL	C2A-CAA-CBA-CGA
31	b	602	CLA	C2A-CAA-CBA-CGA
31	c	601	CLA	C2A-CAA-CBA-CGA
31	q	305	CLA	C6-C7-C8-C9
31	g	304	CLA	C6-C7-C8-C9
34	b	626	LMG	O6-C5-C6-O5
30	9	307	CHL	O1D-CGD-O2D-CED
33	1	617	LHG	C4-C5-C6-O8
33	5	619	LHG	C4-C5-C6-O8
33	D	408	LHG	C4-C5-C6-O8
33	L	101	LHG	C4-C5-C6-O8
33	R	320	LHG	C4-C5-C6-O8
33	S	322	LHG	C9-C10-C11-C12
33	0	619	LHG	C4-C5-C6-O8
33	e	101	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
33	j	102	LHG	C4-C5-C6-O8
33	r	320	LHG	C4-C5-C6-O8
34	2	618	LMG	O1-C7-C8-C9
34	A	414	LMG	O1-C7-C8-C9
34	A	418	LMG	O1-C7-C8-C9
34	B	621	LMG	C7-C8-C9-O8
34	B	625	LMG	C7-C8-C9-O8
34	C	621	LMG	C7-C8-C9-O8
34	G	619	LMG	O1-C7-C8-C9
34	N	320	LMG	O1-C7-C8-C9
34	W	203	LMG	O1-C7-C8-C9
34	X	203	LMG	C7-C8-C9-O8
34	7	322	LMG	O1-C7-C8-C9
34	9	301	LMG	O1-C7-C8-C9
34	b	629	LMG	C7-C8-C9-O8
34	g	320	LMG	O1-C7-C8-C9
34	n	322	LMG	C33-C34-C35-C36
34	r	321	LMG	O1-C7-C8-C9
34	s	321	LMG	C7-C8-C9-O8
38	6	301	SQD	O6-C44-C45-C46
38	A	411	SQD	C44-C45-C46-O48
38	A	413	SQD	C44-C45-C46-O48
38	B	623	SQD	O6-C44-C45-C46
38	G	617	SQD	C44-C45-C46-O48
38	R	322	SQD	O6-C44-C45-C46
38	S	301	SQD	C44-C45-C46-O48
38	b	627	SQD	C44-C45-C46-O48
38	r	322	SQD	O6-C44-C45-C46
38	y	621	SQD	C44-C45-C46-O48
33	j	102	LHG	C24-C23-O8-C6
34	C	624	LMG	O6-C5-C6-O5
31	1	604	CLA	C13-C15-C16-C17
31	0	604	CLA	C5-C6-C7-C8
31	r	316	CLA	C13-C15-C16-C17
33	b	628	LHG	C9-C10-C11-C12
33	t	102	LHG	C11-C12-C13-C14
45	c	616	DGD	CDB-CEB-CFB-CGB
34	2	618	LMG	C8-C7-O1-C1
34	2	620	LMG	C8-C7-O1-C1
34	2	621	LMG	C8-C7-O1-C1
34	6	323	LMG	C8-C7-O1-C1
34	G	619	LMG	C8-C7-O1-C1

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Mol	Chain	Res	Type	Atoms
34	G	621	LMG	C8-C7-O1-C1
34	I	101	LMG	C8-C7-O1-C1
34	J	102	LMG	C8-C7-O1-C1
34	R	321	LMG	C8-C7-O1-C1
34	W	202	LMG	C8-C7-O1-C1
34	Y	319	LMG	C8-C7-O1-C1
34	0	622	LMG	C8-C7-O1-C1
34	9	321	LMG	C8-C7-O1-C1
34	b	622	LMG	C8-C7-O1-C1
34	c	621	LMG	C8-C7-O1-C1
34	f	101	LMG	C8-C7-O1-C1
34	g	320	LMG	C8-C7-O1-C1
34	y	620	LMG	C8-C7-O1-C1
34	Q1	101	LMG	C8-C7-O1-C1
38	6	301	SQD	C45-C44-O6-C1
38	R	322	SQD	C45-C44-O6-C1
38	X	201	SQD	C45-C44-O6-C1
38	b	621	SQD	C45-C44-O6-C1
45	C	617	DGD	C5D-C6D-O5D-C1E
45	c	619	DGD	C5D-C6D-O5D-C1E
30	N	309	CHL	O1D-CGD-O2D-CED
33	C	623	LHG	C35-C36-C37-C38
33	9	320	LHG	C28-C29-C30-C31
34	D	409	LMG	C12-C13-C14-C15
31	B	607	CLA	C10-C11-C12-C13
31	9	305	CLA	C5-C6-C7-C8
31	b	610	CLA	C13-C15-C16-C17
33	A	417	LHG	C28-C29-C30-C31
33	p	619	LHG	C25-C26-C27-C28
33	F1	301	LHG	C9-C10-C11-C12
34	2	621	LMG	C31-C32-C33-C34
34	d	411	LMG	C12-C13-C14-C15
45	c	617	DGD	C7A-C8A-C9A-CAA
34	2	618	LMG	O7-C10-C11-C12
34	6	323	LMG	O7-C10-C11-C12
34	I	101	LMG	O6-C5-C6-O5
34	p	620	LMG	O6-C5-C6-O5
34	d	411	LMG	O6-C5-C6-O5
33	A	417	LHG	C23-C24-C25-C26
38	B	620	SQD	C23-C24-C25-C26
33	s	320	LHG	C10-C11-C12-C13
38	B	623	SQD	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
48	R	302	LMU	C1-C2-C3-C4
34	a	413	LMG	O6-C1-O1-C7
44	a	414	PL9	C39-C41-C42-C43
33	D	408	LHG	C33-C34-C35-C36
33	p	619	LHG	C28-C29-C30-C31
30	g	306	CHL	CBA-CGA-O2A-C1
34	2	618	LMG	O6-C5-C6-O5
34	s	321	LMG	O6-C5-C6-O5
45	C	618	DGD	O6E-C5E-C6E-O5E
33	3	320	LHG	O1-C1-C2-O2
33	L	101	LHG	O1-C1-C2-O2
33	R	320	LHG	O1-C1-C2-O2
33	Y	318	LHG	O1-C1-C2-O2
33	g	319	LHG	O1-C1-C2-O2
34	3	321	LMG	C8-C9-O8-C28
34	b	629	LMG	C8-C9-O8-C28
33	A	415	LHG	C33-C34-C35-C36
33	S	322	LHG	C35-C36-C37-C38
33	b	625	LHG	C29-C30-C31-C32
33	l	101	LHG	C16-C17-C18-C19
33	r	320	LHG	C25-C26-C27-C28
33	F1	301	LHG	C13-C14-C15-C16
38	r	322	SQD	C10-C11-C12-C13
38	s	301	SQD	C25-C26-C27-C28
33	s	322	LHG	C29-C30-C31-C32
30	g	302	CHL	CAA-CBA-CGA-O2A
48	K	101	LMU	C1-C2-C3-C4
33	B	624	LHG	C35-C36-C37-C38
33	S	320	LHG	C26-C27-C28-C29
33	b	628	LHG	C33-C34-C35-C36
33	l	101	LHG	C30-C31-C32-C33
34	w	205	LMG	C31-C32-C33-C34
38	s	301	SQD	C28-C29-C30-C31
31	5	610	CLA	C5-C6-C7-C8
31	7	313	CLA	C5-C6-C7-C8
31	8	609	CLA	C5-C6-C7-C8
42	A	408	PHO	C5-C6-C7-C8
34	S	321	LMG	O6-C5-C6-O5
36	2	616	NEX	C11-C10-C9-C19
36	3	319	NEX	C39-C29-C30-C31
36	N	318	NEX	C11-C10-C9-C19
36	R	301	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
36	q	319	NEX	C39-C29-C30-C31
36	g	317	NEX	C40-C33-C34-C35
37	2	619	XAT	C20-C13-C14-C15
37	4	619	XAT	C20-C13-C14-C15
37	G	620	XAT	C20-C13-C14-C15
37	9	322	XAT	C20-C13-C14-C15
37	q	321	XAT	C20-C13-C14-C15
37	g	321	XAT	C20-C13-C14-C15
45	c	618	DGD	O6E-C5E-C6E-O5E
30	N	306	CHL	C4-C3-C5-C6
31	c	603	CLA	C4-C3-C5-C6
31	c	610	CLA	C4-C3-C5-C6
31	n	316	CLA	C5-C6-C7-C8
48	K	101	LMU	C6-C7-C8-C9
31	c	603	CLA	C2-C3-C5-C6
31	r	316	CLA	C2-C3-C5-C6
34	6	322	LMG	C10-C11-C12-C13
31	0	615	CLA	C6-C7-C8-C9
31	b	603	CLA	C16-C17-C18-C20
31	7	313	CLA	CBA-CGA-O2A-C1
31	q	304	CLA	CBA-CGA-O2A-C1
33	M	101	LHG	C24-C23-O8-C6
33	F1	301	LHG	C24-C23-O8-C6
34	r	321	LMG	C29-C28-O8-C9
34	5	620	LMG	C8-C9-O8-C28
33	c	622	LHG	C30-C31-C32-C33
34	D	411	LMG	C37-C38-C39-C40
34	d	410	LMG	C37-C38-C39-C40
38	b	627	SQD	C16-C17-C18-C19
31	3	306	CLA	CBD-CGD-O2D-CED
31	R	315	CLA	C5-C6-C7-C8
31	S	312	CLA	C13-C15-C16-C17
31	b	603	CLA	C15-C16-C17-C18
31	c	609	CLA	C13-C15-C16-C17
31	7	315	CLA	C6-C7-C8-C9
33	6	320	LHG	C13-C14-C15-C16
33	0	619	LHG	C12-C13-C14-C15
38	b	621	SQD	C17-C18-C19-C20
33	N	319	LHG	C4-C5-O7-C7
34	3	321	LMG	C9-C8-O7-C10
34	7	320	LMG	C9-C8-O7-C10
45	c	619	DGD	C1G-C2G-O2G-C1B

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Mol	Chain	Res	Type	Atoms
31	a	407	CLA	O1D-CGD-O2D-CED
34	4	620	LMG	O6-C5-C6-O5
30	4	609	CHL	C2A-CAA-CBA-CGA
30	r	310	CHL	C2A-CAA-CBA-CGA
31	3	305	CLA	C2A-CAA-CBA-CGA
31	6	315	CLA	C2A-CAA-CBA-CGA
31	R	304	CLA	C2A-CAA-CBA-CGA
31	9	306	CLA	C8-C10-C11-C12
31	c	603	CLA	C10-C11-C12-C13
31	C	604	CLA	C2-C1-O2A-CGA
31	C	605	CLA	C2-C1-O2A-CGA
31	N	311	CLA	C2-C1-O2A-CGA
31	N	315	CLA	C2-C1-O2A-CGA
31	R	307	CLA	C2-C1-O2A-CGA
31	Y	311	CLA	C2-C1-O2A-CGA
31	Y	313	CLA	C2-C1-O2A-CGA
31	g	314	CLA	C2-C1-O2A-CGA
33	n	320	LHG	C11-C12-C13-C14
33	s	320	LHG	C31-C32-C33-C34
33	y	619	LHG	C9-C10-C11-C12
33	y	619	LHG	C35-C36-C37-C38
33	a	415	LHG	C23-C24-C25-C26
30	G	606	CHL	O1D-CGD-O2D-CED
30	7	306	CHL	O1D-CGD-O2D-CED
30	8	608	CHL	CBD-CGD-O2D-CED
48	K	101	LMU	O5'-C5'-C6'-O6'
31	b	604	CLA	C3-C5-C6-C7
33	8	618	LHG	C11-C12-C13-C14
33	q	320	LHG	C30-C31-C32-C33
33	q	320	LHG	C33-C34-C35-C36
33	s	322	LHG	C27-C28-C29-C30
31	B	608	CLA	C8-C10-C11-C12
31	C	601	CLA	C10-C11-C12-C13
31	b	604	CLA	C13-C15-C16-C17
42	A	408	PHO	C10-C11-C12-C13
33	j	102	LHG	C11-C12-C13-C14
30	4	607	CHL	CBA-CGA-O2A-C1
31	2	612	CLA	CBA-CGA-O2A-C1
31	B	611	CLA	CBA-CGA-O2A-C1
31	8	602	CLA	CBA-CGA-O2A-C1
31	y	611	CLA	CBA-CGA-O2A-C1
33	5	619	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
33	g	319	LHG	O6-C4-C5-O7
33	r	320	LHG	O6-C4-C5-O7
33	y	619	LHG	O6-C4-C5-O7
34	G	619	LMG	O7-C10-C11-C12
34	c	620	LMG	O7-C10-C11-C12
31	6	315	CLA	O1D-CGD-O2D-CED
31	C	612	CLA	C6-C7-C8-C10
31	c	603	CLA	C16-C17-C18-C20
31	g	304	CLA	C6-C7-C8-C10
31	r	304	CLA	C11-C12-C13-C15
33	e	101	LHG	C23-C24-C25-C26
34	C	622	LMG	C28-C29-C30-C31
33	R	320	LHG	C28-C29-C30-C31
34	x	202	LMG	C34-C35-C36-C37
48	R	302	LMU	O5B-C1B-O1B-C4'
31	7	316	CLA	O1D-CGD-O2D-CED
30	1	619	CHL	C5-C6-C7-C8
30	g	309	CHL	C5-C6-C7-C8
30	y	609	CHL	C8-C10-C11-C12
31	2	602	CLA	C10-C11-C12-C13
31	B	614	CLA	C10-C11-C12-C13
34	b	629	LMG	C33-C34-C35-C36
31	C	608	CLA	O1D-CGD-O2D-CED
31	7	313	CLA	O1A-CGA-O2A-C1
45	c	616	DGD	O1A-C1A-O1G-C1G
33	j	102	LHG	C11-C10-C9-C8
45	c	619	DGD	C4D-C5D-C6D-O5D
33	S	322	LHG	C7-C8-C9-C10
38	m	101	SQD	C23-C24-C25-C26
31	N	305	CLA	C5-C6-C7-C8
31	y	604	CLA	C5-C6-C7-C8
34	6	321	LMG	C2-C1-O1-C7
34	A	414	LMG	C2-C1-O1-C7
34	D	410	LMG	C2-C1-O1-C7
34	W	201	LMG	C2-C1-O1-C7
34	b	622	LMG	C2-C1-O1-C7
34	c	620	LMG	C2-C1-O1-C7
34	w	202	LMG	C2-C1-O1-C7
36	6	319	NEX	C32-C33-C34-C35
36	0	618	NEX	C32-C33-C34-C35
37	2	619	XAT	C12-C13-C14-C15
45	C	620	DGD	C2D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
33	S	320	LHG	C30-C31-C32-C33
34	q1	101	LMG	C8-C9-O8-C28
30	5	601	CHL	CAA-CBA-CGA-O2A
34	g	320	LMG	O7-C10-C11-C12
33	6	320	LHG	O7-C5-C6-O8
34	2	620	LMG	O1-C7-C8-O7
34	2	620	LMG	O7-C8-C9-O8
34	5	620	LMG	O1-C7-C8-O7
34	D	409	LMG	O1-C7-C8-O7
34	G	621	LMG	O1-C7-C8-O7
34	I	101	LMG	O1-C7-C8-O7
34	0	620	LMG	O1-C7-C8-O7
34	7	322	LMG	O7-C8-C9-O8
34	w	205	LMG	O1-C7-C8-O7
34	x	202	LMG	O1-C7-C8-O7
45	C	617	DGD	O2G-C2G-C3G-O3G
45	C	620	DGD	O2G-C2G-C3G-O3G
31	2	604	CLA	C6-C7-C8-C9
33	2	617	LHG	C34-C35-C36-C37
33	9	320	LHG	C11-C10-C9-C8
34	q	301	LMG	C11-C12-C13-C14
33	t	102	LHG	O9-C7-O7-C5
30	1	606	CHL	C5-C6-C7-C8
31	6	316	CLA	C5-C6-C7-C8
31	d	405	CLA	C10-C11-C12-C13
31	n	311	CLA	C5-C6-C7-C8
31	g	310	CLA	O1A-CGA-O2A-C1
31	p	611	CLA	C11-C12-C13-C14
42	d	402	PHO	CHA-CBD-CGD-O1D
42	d	402	PHO	CHA-CBD-CGD-O2D
33	t	102	LHG	C11-C10-C9-C8
31	2	602	CLA	C4-C3-C5-C6
31	0	613	CLA	C4-C3-C5-C6
31	r	316	CLA	C4-C3-C5-C6
34	2	620	LMG	C34-C35-C36-C37
30	1	605	CHL	C11-C10-C8-C7
30	1	605	CHL	C12-C13-C15-C16
30	1	606	CHL	C11-C10-C8-C7
30	1	606	CHL	C11-C12-C13-C15
30	1	607	CHL	C12-C13-C15-C16
30	2	601	CHL	C11-C10-C8-C7
30	2	608	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
30	6	310	CHL	C11-C10-C8-C7
30	G	623	CHL	C12-C13-C15-C16
30	N	306	CHL	C11-C10-C8-C7
30	Y	301	CHL	C12-C13-C15-C16
30	Y	307	CHL	C11-C10-C8-C7
30	Y	309	CHL	C12-C13-C15-C16
30	7	302	CHL	C11-C12-C13-C15
30	7	302	CHL	C12-C13-C15-C16
30	7	306	CHL	C6-C7-C8-C10
30	7	306	CHL	C11-C12-C13-C15
30	7	306	CHL	C12-C13-C15-C16
30	7	307	CHL	C12-C13-C15-C16
30	7	308	CHL	C12-C13-C15-C16
30	8	605	CHL	C11-C10-C8-C7
30	8	605	CHL	C11-C12-C13-C15
30	8	605	CHL	C12-C13-C15-C16
30	8	606	CHL	C11-C10-C8-C7
30	9	311	CHL	C11-C10-C8-C7
30	g	302	CHL	C11-C10-C8-C7
30	n	306	CHL	C11-C10-C8-C7
30	n	306	CHL	C11-C12-C13-C15
30	n	306	CHL	C12-C13-C15-C16
30	n	307	CHL	C11-C10-C8-C7
30	y	607	CHL	C11-C12-C13-C15
31	1	613	CLA	C6-C7-C8-C10
31	2	602	CLA	C2-C3-C5-C6
31	4	602	CLA	C6-C7-C8-C10
31	6	311	CLA	C6-C7-C8-C10
31	6	314	CLA	C6-C7-C8-C10
31	B	607	CLA	C11-C10-C8-C7
31	B	607	CLA	C11-C12-C13-C15
31	B	609	CLA	C6-C7-C8-C10
31	B	615	CLA	C6-C7-C8-C10
31	C	601	CLA	C11-C12-C13-C15
31	C	602	CLA	C6-C7-C8-C10
31	C	603	CLA	C11-C12-C13-C15
31	C	605	CLA	C11-C10-C8-C7
31	C	608	CLA	C11-C10-C8-C7
31	C	610	CLA	C12-C13-C15-C16
31	D	403	CLA	C11-C12-C13-C15
31	D	404	CLA	C6-C7-C8-C10
31	G	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	N	303	CLA	C11-C10-C8-C7
31	N	313	CLA	C6-C7-C8-C10
31	N	313	CLA	C11-C12-C13-C15
31	R	304	CLA	C6-C7-C8-C10
31	R	304	CLA	C11-C10-C8-C7
31	R	311	CLA	C11-C10-C8-C7
31	R	316	CLA	C6-C7-C8-C10
31	Y	311	CLA	C11-C10-C8-C7
31	Y	311	CLA	C11-C12-C13-C15
31	0	602	CLA	C6-C7-C8-C10
31	0	603	CLA	C6-C7-C8-C10
31	0	610	CLA	C11-C10-C8-C7
31	7	312	CLA	C6-C7-C8-C10
31	8	612	CLA	C6-C7-C8-C10
31	9	304	CLA	C11-C10-C8-C7
31	9	306	CLA	C6-C7-C8-C10
31	9	306	CLA	C11-C10-C8-C7
31	p	611	CLA	C6-C7-C8-C10
31	b	606	CLA	C12-C13-C15-C16
31	b	608	CLA	C11-C12-C13-C15
31	b	612	CLA	C11-C12-C13-C15
31	c	603	CLA	C11-C12-C13-C15
31	c	608	CLA	C6-C7-C8-C10
31	c	611	CLA	C11-C10-C8-C7
31	c	613	CLA	C12-C13-C15-C16
31	d	405	CLA	C6-C7-C8-C10
31	g	310	CLA	C11-C12-C13-C15
31	n	314	CLA	C6-C7-C8-C10
31	r	305	CLA	C6-C7-C8-C10
31	r	311	CLA	C6-C7-C8-C10
31	s	314	CLA	C11-C10-C8-C7
31	s	314	CLA	C12-C13-C15-C16
31	y	602	CLA	C6-C7-C8-C10
31	y	610	CLA	C11-C12-C13-C15
42	D	401	PHO	C11-C10-C8-C7
31	3	313	CLA	CAA-CBA-CGA-O2A
31	4	603	CLA	C3-C5-C6-C7
31	S	303	CLA	C3-C5-C6-C7
30	N	307	CHL	O1A-CGA-O2A-C1
38	s	301	SQD	O10-C23-O48-C46
31	Y	314	CLA	C6-C7-C8-C9
33	c	622	LHG	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
34	B	622	LMG	C12-C13-C14-C15
30	Y	301	CHL	C14-C13-C15-C16
30	Y	309	CHL	C14-C13-C15-C16
30	7	307	CHL	C14-C13-C15-C16
30	7	310	CHL	C11-C12-C13-C14
30	8	605	CHL	C14-C13-C15-C16
30	n	306	CHL	C14-C13-C15-C16
31	1	612	CLA	C6-C7-C8-C9
31	1	613	CLA	C6-C7-C8-C9
31	2	602	CLA	C6-C7-C8-C9
31	2	609	CLA	C6-C7-C8-C9
31	3	304	CLA	C6-C7-C8-C9
31	4	602	CLA	C6-C7-C8-C9
31	6	304	CLA	C6-C7-C8-C9
31	6	311	CLA	C6-C7-C8-C9
31	6	314	CLA	C6-C7-C8-C9
31	B	602	CLA	C11-C12-C13-C14
31	B	603	CLA	C11-C12-C13-C14
31	B	604	CLA	C14-C13-C15-C16
31	B	605	CLA	C14-C13-C15-C16
31	B	615	CLA	C6-C7-C8-C9
31	B	616	CLA	C6-C7-C8-C9
31	C	601	CLA	C6-C7-C8-C9
31	C	603	CLA	C11-C12-C13-C14
31	C	605	CLA	C11-C10-C8-C9
31	C	608	CLA	C6-C7-C8-C9
31	D	403	CLA	C11-C12-C13-C14
31	R	311	CLA	C6-C7-C8-C9
31	Y	303	CLA	C6-C7-C8-C9
31	Y	303	CLA	C11-C10-C8-C9
31	0	602	CLA	C6-C7-C8-C9
31	0	603	CLA	C6-C7-C8-C9
31	0	613	CLA	C6-C7-C8-C9
31	7	312	CLA	C6-C7-C8-C9
31	7	314	CLA	C11-C12-C13-C14
31	8	604	CLA	C11-C10-C8-C9
31	8	612	CLA	C11-C12-C13-C14
31	b	604	CLA	C6-C7-C8-C9
31	b	605	CLA	C14-C13-C15-C16
31	b	616	CLA	C11-C12-C13-C14
31	c	607	CLA	C11-C12-C13-C14
31	d	405	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	g	303	CLA	C6-C7-C8-C9
31	n	305	CLA	C11-C10-C8-C9
31	n	314	CLA	C11-C12-C13-C14
31	y	602	CLA	C6-C7-C8-C9
42	D	401	PHO	C11-C12-C13-C14
31	c	605	CLA	CBD-CGD-O2D-CED
34	W	201	LMG	C39-C40-C41-C42
34	q	301	LMG	C18-C19-C20-C21
31	C	601	CLA	CBA-CGA-O2A-C1
31	Y	311	CLA	CBA-CGA-O2A-C1
30	1	609	CHL	C10-C11-C12-C13
31	B	603	CLA	C8-C10-C11-C12
31	C	613	CLA	C8-C10-C11-C12
31	C	613	CLA	C13-C15-C16-C17
31	b	610	CLA	C8-C10-C11-C12
30	1	608	CHL	C2A-CAA-CBA-CGA
31	B	603	CLA	C2A-CAA-CBA-CGA
31	p	615	CLA	C2A-CAA-CBA-CGA
33	2	617	LHG	C16-C17-C18-C19
38	R	322	SQD	C12-C13-C14-C15
32	6	317	LUT	C27-C28-C29-C39
43	C	615	BCR	C37-C22-C23-C24
43	D	405	BCR	C37-C22-C23-C24
43	T	101	BCR	C36-C18-C19-C20
31	6	316	CLA	C6-C7-C8-C9
31	r	305	CLA	C11-C12-C13-C15
33	1	617	LHG	C28-C29-C30-C31
33	M	101	LHG	C11-C12-C13-C14
32	2	615	LUT	C31-C32-C33-C34
32	G	615	LUT	C31-C32-C33-C34
36	R	319	NEX	C31-C32-C33-C34
33	B	624	LHG	C17-C18-C19-C20
33	K	102	LHG	C26-C27-C28-C29
34	X	203	LMG	C11-C12-C13-C14
30	N	307	CHL	C3-C5-C6-C7
31	C	611	CLA	C3-C5-C6-C7
31	9	305	CLA	C3-C5-C6-C7
30	N	308	CHL	O1D-CGD-O2D-CED
30	n	302	CHL	O1D-CGD-O2D-CED
31	s	313	CLA	C5-C6-C7-C8
33	D	407	LHG	C26-C27-C28-C29
33	L	101	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
44	A	416	PL9	C37-C38-C39-C41
30	9	309	CHL	CBA-CGA-O2A-C1
31	C	603	CLA	CBA-CGA-O2A-C1
31	7	314	CLA	CBA-CGA-O2A-C1
31	c	606	CLA	CBA-CGA-O2A-C1
33	3	320	LHG	C24-C23-O8-C6
33	C	623	LHG	C24-C23-O8-C6
34	3	321	LMG	C29-C28-O8-C9
31	9	312	CLA	C6-C7-C8-C9
34	d	409	LMG	C10-C11-C12-C13
31	A	405	CLA	C5-C6-C7-C8
31	7	305	CLA	C5-C6-C7-C8
31	r	315	CLA	C5-C6-C7-C8
30	8	601	CHL	O1D-CGD-O2D-CED
33	D	407	LHG	C35-C36-C37-C38
33	G	618	LHG	C28-C29-C30-C31
34	C	624	LMG	C15-C16-C17-C18
38	R	322	SQD	C26-C27-C28-C29
45	c	619	DGD	O6D-C5D-C6D-O5D
30	2	601	CHL	C8-C10-C11-C12
33	A	415	LHG	O6-C4-C5-C6
33	D	408	LHG	O6-C4-C5-C6
33	K	102	LHG	O6-C4-C5-C6
33	S	320	LHG	O6-C4-C5-C6
33	j	102	LHG	O6-C4-C5-C6
33	r	320	LHG	O6-C4-C5-C6
33	s	320	LHG	O6-C4-C5-C6
33	y	619	LHG	O6-C4-C5-C6
33	q	320	LHG	C25-C26-C27-C28
33	b	628	LHG	C34-C35-C36-C37
33	R	320	LHG	C7-C8-C9-C10
45	c	616	DGD	C1B-C2B-C3B-C4B
33	0	619	LHG	C13-C14-C15-C16
34	w	204	LMG	C11-C12-C13-C14
31	1	612	CLA	C5-C6-C7-C8
31	B	606	CLA	C10-C11-C12-C13
31	R	304	CLA	C10-C11-C12-C13
31	0	611	CLA	C5-C6-C7-C8
31	8	612	CLA	C15-C16-C17-C18
31	n	314	CLA	C15-C16-C17-C18
31	2	613	CLA	CAA-CBA-CGA-O2A
30	y	607	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	B	624	LHG	C25-C26-C27-C28
38	b	621	SQD	C35-C36-C37-C38
30	R	308	CHL	C4-C3-C5-C6
30	9	309	CHL	C4-C3-C5-C6
31	1	610	CLA	C4-C3-C5-C6
31	c	606	CLA	C4-C3-C5-C6
30	6	302	CHL	C2-C3-C5-C6
31	0	613	CLA	C2-C3-C5-C6
33	G	618	LHG	C7-C8-C9-C10
34	n	322	LMG	C10-C11-C12-C13
38	M	102	SQD	C23-C24-C25-C26
33	j	102	LHG	C30-C31-C32-C33
38	b	621	SQD	C30-C31-C32-C33
42	a	408	PHO	C8-C10-C11-C12
30	2	608	CHL	C11-C10-C8-C9
30	q	309	CHL	C11-C10-C8-C9
30	g	306	CHL	O1A-CGA-O2A-C1
34	r	321	LMG	O10-C28-O8-C9
33	y	619	LHG	C34-C35-C36-C37
34	9	301	LMG	C11-C12-C13-C14
38	a	411	SQD	C32-C33-C34-C35
31	n	312	CLA	O1D-CGD-O2D-CED
30	3	310	CHL	C11-C12-C13-C14
31	G	603	CLA	C6-C7-C8-C9
31	Y	312	CLA	C16-C17-C18-C19
31	c	601	CLA	C16-C17-C18-C20
34	w	204	LMG	O6-C5-C6-O5
33	b	628	LHG	C25-C26-C27-C28
30	0	607	CHL	C8-C10-C11-C12
30	8	605	CHL	C8-C10-C11-C12
30	n	306	CHL	C8-C10-C11-C12
30	3	302	CHL	CBA-CGA-O2A-C1
30	3	309	CHL	CBA-CGA-O2A-C1
31	6	303	CLA	CBA-CGA-O2A-C1
31	6	305	CLA	CBA-CGA-O2A-C1
31	7	312	CLA	CBA-CGA-O2A-C1
33	R	320	LHG	O8-C23-C24-C25
34	5	620	LMG	O7-C10-C11-C12
34	B	622	LMG	C28-C29-C30-C31
33	Y	318	LHG	C35-C36-C37-C38
34	4	620	LMG	C32-C33-C34-C35
34	0	620	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
33	N	319	LHG	C2-C3-O3-P
33	8	618	LHG	C5-C4-O6-P
33	n	320	LHG	C5-C4-O6-P
30	1	601	CHL	C3A-C2A-CAA-CBA
30	4	607	CHL	C3A-C2A-CAA-CBA
30	6	310	CHL	C3A-C2A-CAA-CBA
30	0	608	CHL	C3A-C2A-CAA-CBA
30	q	309	CHL	C3A-C2A-CAA-CBA
30	q	311	CHL	C3A-C2A-CAA-CBA
31	2	610	CLA	C3A-C2A-CAA-CBA
31	3	301	CLA	C3A-C2A-CAA-CBA
31	3	313	CLA	C3A-C2A-CAA-CBA
31	B	608	CLA	C3A-C2A-CAA-CBA
31	7	316	CLA	C3A-C2A-CAA-CBA
31	p	613	CLA	C3A-C2A-CAA-CBA
31	b	609	CLA	C3A-C2A-CAA-CBA
31	y	611	CLA	C3A-C2A-CAA-CBA
31	7	305	CLA	C8-C10-C11-C12
31	s	305	CLA	C5-C6-C7-C8
31	3	315	CLA	C6-C7-C8-C9
31	8	614	CLA	C5-C6-C7-C8
33	S	322	LHG	C24-C25-C26-C27
33	0	619	LHG	C26-C27-C28-C29
45	C	616	DGD	C5B-C6B-C7B-C8B
31	8	610	CLA	O1D-CGD-O2D-CED
36	R	319	NEX	C13-C14-C15-C35
36	q	319	NEX	C29-C30-C31-C32
43	b	618	BCR	C19-C20-C21-C22
43	d	406	BCR	C19-C20-C21-C22
43	h	101	BCR	C19-C20-C21-C22
33	G	618	LHG	C9-C10-C11-C12
33	L	101	LHG	C34-C35-C36-C37
34	C	624	LMG	C11-C12-C13-C14
34	C	624	LMG	C18-C19-C20-C21
38	A	413	SQD	C10-C11-C12-C13
31	5	613	CLA	C3-C5-C6-C7
31	8	614	CLA	C6-C7-C8-C9
31	n	316	CLA	C6-C7-C8-C9
33	D	408	LHG	C34-C35-C36-C37
31	q	305	CLA	C6-C7-C8-C10
31	r	304	CLA	C11-C12-C13-C14
30	7	321	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
30	n	308	CHL	CBA-CGA-O2A-C1
31	C	604	CLA	CBA-CGA-O2A-C1
31	b	608	CLA	CBA-CGA-O2A-C1
31	n	303	CLA	CBA-CGA-O2A-C1
34	k	102	LMG	C29-C28-O8-C9
33	D	407	LHG	C25-C26-C27-C28
34	B	621	LMG	C37-C38-C39-C40
34	9	302	LMG	C31-C32-C33-C34
38	S	301	SQD	C27-C28-C29-C30
31	4	610	CLA	C8-C10-C11-C12
31	b	616	CLA	C10-C11-C12-C13
33	2	617	LHG	C4-C5-C6-O8
33	4	618	LHG	C4-C5-C6-O8
33	6	320	LHG	C4-C5-C6-O8
33	A	415	LHG	C4-C5-C6-O8
33	C	623	LHG	C4-C5-C6-O8
33	M	101	LHG	C4-C5-C6-O8
33	7	319	LHG	C4-C5-C6-O8
33	8	618	LHG	C4-C5-C6-O8
33	9	320	LHG	C4-C5-C6-O8
33	b	625	LHG	C4-C5-C6-O8
33	c	622	LHG	C4-C5-C6-O8
33	n	320	LHG	C4-C5-C6-O8
33	y	619	LHG	C4-C5-C6-O8
34	2	620	LMG	O1-C7-C8-C9
34	A	412	LMG	C7-C8-C9-O8
34	D	412	LMG	C7-C8-C9-O8
34	G	621	LMG	O1-C7-C8-C9
34	I	101	LMG	O1-C7-C8-C9
34	J	101	LMG	O1-C7-C8-C9
34	R	321	LMG	C7-C8-C9-O8
34	0	622	LMG	O1-C7-C8-C9
34	7	322	LMG	C7-C8-C9-O8
34	a	416	LMG	O1-C7-C8-C9
34	b	624	LMG	C7-C8-C9-O8
34	n	321	LMG	C7-C8-C9-O8
34	n	322	LMG	O1-C7-C8-C9
34	w	201	LMG	O1-C7-C8-C9
34	w	205	LMG	O1-C7-C8-C9
34	w	205	LMG	C7-C8-C9-O8
38	A	411	SQD	O6-C44-C45-C46
38	G	624	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
38	Y	320	SQD	O6-C44-C45-C46
38	Y	320	SQD	C44-C45-C46-O48
38	a	412	SQD	C44-C45-C46-O48
38	b	621	SQD	C44-C45-C46-O48
38	x	201	SQD	O6-C44-C45-C46
33	b	625	LHG	O9-C7-O7-C5
33	s	320	LHG	O9-C7-O7-C5
33	3	320	LHG	C9-C10-C11-C12
33	6	320	LHG	C28-C29-C30-C31
33	y	619	LHG	C26-C27-C28-C29
34	4	620	LMG	C34-C35-C36-C37
34	G	621	LMG	C34-C35-C36-C37
33	g	319	LHG	C7-C8-C9-C10
31	2	612	CLA	O1A-CGA-O2A-C1
34	x	202	LMG	C11-C12-C13-C14
45	C	616	DGD	C4A-C5A-C6A-C7A
30	7	302	CHL	C8-C10-C11-C12
31	B	606	CLA	C3-C5-C6-C7
31	5	615	CLA	C2C-C3C-CAC-CBC
33	Y	318	LHG	C31-C32-C33-C34
31	y	612	CLA	C5-C6-C7-C8
30	2	601	CHL	C4-C3-C5-C6
30	4	609	CHL	C4-C3-C5-C6
30	r	310	CHL	C4-C3-C5-C6
31	9	304	CLA	C4-C3-C5-C6
42	D	401	PHO	C4-C3-C5-C6
31	2	603	CLA	C6-C7-C8-C9
31	9	305	CLA	C6-C7-C8-C10
31	s	311	CLA	C16-C17-C18-C20
31	7	311	CLA	C2-C3-C5-C6
31	c	606	CLA	C2-C3-C5-C6
33	g	319	LHG	C33-C34-C35-C36
33	q	320	LHG	C29-C30-C31-C32
30	p	609	CHL	O1D-CGD-O2D-CED
31	N	313	CLA	C15-C16-C17-C18
33	A	417	LHG	C3-O3-P-O6
33	0	619	LHG	C4-O6-P-O3
33	B	624	LHG	O10-C23-O8-C6
33	j	102	LHG	O10-C23-O8-C6
33	e	101	LHG	C31-C32-C33-C34
30	5	609	CHL	C3-C5-C6-C7
30	4	607	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
30	8	607	CHL	C2A-CAA-CBA-CGA
30	n	309	CHL	C2A-CAA-CBA-CGA
31	b	608	CLA	C2A-CAA-CBA-CGA
31	s	303	CLA	C2A-CAA-CBA-CGA
33	e	101	LHG	O1-C1-C2-O2
31	1	611	CLA	C5-C6-C7-C8
31	s	303	CLA	C10-C11-C12-C13
33	K	102	LHG	C11-C10-C9-C8
33	7	319	LHG	C28-C29-C30-C31
33	e	101	LHG	C11-C10-C9-C8
33	s	322	LHG	C35-C36-C37-C38
34	A	418	LMG	C12-C13-C14-C15
45	C	620	DGD	C5A-C6A-C7A-C8A
33	1	617	LHG	O6-C4-C5-O7
33	C	623	LHG	O6-C4-C5-O7
33	D	408	LHG	O6-C4-C5-O7
33	M	101	LHG	O6-C4-C5-O7
33	R	320	LHG	O6-C4-C5-O7
33	8	618	LHG	O6-C4-C5-O7
33	q	320	LHG	O6-C4-C5-O7
33	n	320	LHG	O6-C4-C5-O7
33	s	320	LHG	O6-C4-C5-O7
31	b	602	CLA	CBA-CGA-O2A-C1
45	C	618	DGD	CAB-CBB-CCB-CDB
30	4	607	CHL	O1A-CGA-O2A-C1
31	C	601	CLA	O1A-CGA-O2A-C1
31	7	314	CLA	O1A-CGA-O2A-C1
31	8	602	CLA	O1A-CGA-O2A-C1
33	F1	301	LHG	O10-C23-O8-C6
34	3	321	LMG	O10-C28-O8-C9
38	B	623	SQD	C23-C24-C25-C26
31	C	603	CLA	C16-C17-C18-C19
31	Y	312	CLA	C16-C17-C18-C20
31	c	603	CLA	C16-C17-C18-C19
31	6	304	CLA	CAA-CBA-CGA-O2A
34	W	202	LMG	O7-C10-C11-C12
45	c	619	DGD	O1G-C1A-C2A-C3A
33	N	319	LHG	C29-C30-C31-C32
33	R	320	LHG	C25-C26-C27-C28
33	1	101	LHG	C35-C36-C37-C38
34	4	620	LMG	C18-C19-C20-C21
31	2	609	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	B	611	CLA	O1A-CGA-O2A-C1
31	q	304	CLA	O1A-CGA-O2A-C1
31	y	611	CLA	O1A-CGA-O2A-C1
33	M	101	LHG	O10-C23-O8-C6
33	2	617	LHG	C35-C36-C37-C38
38	y	621	SQD	C13-C14-C15-C16
34	y	620	LMG	C10-C11-C12-C13
31	2	613	CLA	C6-C7-C8-C9
33	g	319	LHG	C35-C36-C37-C38
45	c	618	DGD	C6B-C7B-C8B-C9B
33	2	617	LHG	O7-C5-C6-O8
33	5	619	LHG	O7-C5-C6-O8
33	C	623	LHG	O7-C5-C6-O8
33	N	319	LHG	O7-C5-C6-O8
33	q	320	LHG	O7-C5-C6-O8
33	c	622	LHG	O7-C5-C6-O8
33	y	619	LHG	O7-C5-C6-O8
34	A	412	LMG	O7-C8-C9-O8
34	A	414	LMG	O1-C7-C8-O7
34	B	625	LMG	O7-C8-C9-O8
34	C	621	LMG	O7-C8-C9-O8
34	X	203	LMG	O1-C7-C8-O7
34	0	622	LMG	O1-C7-C8-O7
34	7	322	LMG	O1-C7-C8-O7
34	b	624	LMG	O7-C8-C9-O8
38	B	620	SQD	O6-C44-C45-O47
38	R	322	SQD	O6-C44-C45-O47
38	y	621	SQD	O47-C45-C46-O48
38	x	201	SQD	C24-C23-O48-C46
33	N	319	LHG	C34-C35-C36-C37
33	a	415	LHG	C9-C10-C11-C12
32	5	617	LUT	C9-C10-C11-C12
30	n	310	CHL	O1D-CGD-O2D-CED
30	6	310	CHL	C11-C12-C13-C14
31	G	603	CLA	C6-C7-C8-C10
31	G	604	CLA	C6-C7-C8-C9
31	Y	305	CLA	C6-C7-C8-C10
31	b	603	CLA	C16-C17-C18-C19
31	r	305	CLA	C11-C12-C13-C14
33	G	618	LHG	C34-C35-C36-C37
33	Y	318	LHG	C29-C30-C31-C32
45	c	617	DGD	CFB-CGB-CHB-CIB

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Mol	Chain	Res	Type	Atoms
45	c	618	DGD	O6D-C1D-O3G-C3G
31	3	312	CLA	C15-C16-C17-C18
31	b	605	CLA	CBD-CGD-O2D-CED
44	A	416	PL9	C9-C11-C12-C13
31	1	614	CLA	C6-C7-C8-C9
33	a	415	LHG	C24-C25-C26-C27
38	B	623	SQD	C26-C27-C28-C29
31	p	610	CLA	C3-C5-C6-C7
30	R	310	CHL	C2-C1-O2A-CGA
31	4	602	CLA	C2-C1-O2A-CGA
31	R	304	CLA	C2-C1-O2A-CGA
31	R	311	CLA	C2-C1-O2A-CGA
31	b	604	CLA	C2-C1-O2A-CGA
31	c	613	CLA	C2-C1-O2A-CGA
31	7	315	CLA	C2-C3-C5-C6
31	Y	311	CLA	O1A-CGA-O2A-C1
30	1	601	CHL	C11-C12-C13-C14
30	1	606	CHL	C11-C12-C13-C14
30	Y	301	CHL	C11-C12-C13-C14
30	7	302	CHL	C11-C12-C13-C14
30	7	308	CHL	C11-C12-C13-C14
30	y	601	CHL	C11-C12-C13-C14
31	6	313	CLA	C6-C7-C8-C9
31	B	603	CLA	C6-C7-C8-C9
31	B	614	CLA	C11-C10-C8-C9
31	N	310	CLA	C11-C12-C13-C14
31	R	304	CLA	C11-C10-C8-C9
31	R	312	CLA	C11-C10-C8-C9
31	S	303	CLA	C6-C7-C8-C9
31	7	305	CLA	C6-C7-C8-C9
31	q	315	CLA	C11-C10-C8-C9
31	b	604	CLA	C11-C12-C13-C14
31	b	605	CLA	C11-C12-C13-C14
31	b	606	CLA	C6-C7-C8-C9
31	b	613	CLA	C6-C7-C8-C9
31	c	601	CLA	C6-C7-C8-C9
31	c	601	CLA	C11-C12-C13-C14
31	c	603	CLA	C11-C12-C13-C14
31	c	603	CLA	C14-C13-C15-C16
31	n	305	CLA	C14-C13-C15-C16
31	r	311	CLA	C6-C7-C8-C9
31	s	305	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	s	313	CLA	C6-C7-C8-C9
31	y	610	CLA	C6-C7-C8-C9
31	y	612	CLA	C14-C13-C15-C16
42	D	401	PHO	C6-C7-C8-C9
42	a	408	PHO	C11-C10-C8-C9
38	R	322	SQD	C9-C10-C11-C12
33	B	624	LHG	C9-C10-C11-C12
33	b	625	LHG	C11-C10-C9-C8
30	7	307	CHL	C8-C10-C11-C12
31	c	601	CLA	C5-C6-C7-C8
31	4	604	CLA	C4-C3-C5-C6
33	3	320	LHG	C2-C3-O3-P
33	A	417	LHG	C2-C3-O3-P
33	7	319	LHG	C5-C4-O6-P
33	9	320	LHG	C5-C4-O6-P
33	p	619	LHG	C5-C4-O6-P
33	b	628	LHG	C2-C3-O3-P
33	y	619	LHG	C2-C3-O3-P
33	z	102	LHG	C2-C3-O3-P
33	F1	301	LHG	C2-C3-O3-P
33	G	618	LHG	C26-C27-C28-C29
33	G	618	LHG	C29-C30-C31-C32
33	8	618	LHG	C27-C28-C29-C30
33	n	320	LHG	C27-C28-C29-C30
34	J	102	LMG	C33-C34-C35-C36
30	2	606	CHL	C2A-CAA-CBA-CGA
31	1	602	CLA	C2A-CAA-CBA-CGA
31	G	602	CLA	C2A-CAA-CBA-CGA
30	9	311	CHL	C11-C12-C13-C15
31	6	316	CLA	C6-C7-C8-C10
31	p	603	CLA	C6-C7-C8-C9
31	B	615	CLA	C3-C5-C6-C7
31	r	311	CLA	C3-C5-C6-C7
32	2	615	LUT	C5-C6-C7-C8
32	5	616	LUT	C1-C6-C7-C8
32	S	318	LUT	C5-C6-C7-C8
32	p	617	LUT	C5-C6-C7-C8
32	s	318	LUT	C5-C6-C7-C8
35	q	317	RRX	C1-C6-C7-C8
43	B	617	BCR	C23-C24-C25-C26
43	B	619	BCR	C5-C6-C7-C8
43	B	619	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
43	C	614	BCR	C1-C6-C7-C8
43	b	618	BCR	C23-C24-C25-C30
43	b	619	BCR	C5-C6-C7-C8
43	b	620	BCR	C1-C6-C7-C8
43	v	101	BCR	C23-C24-C25-C26
42	A	408	PHO	C15-C16-C17-C18
33	3	320	LHG	C28-C29-C30-C31
33	C	623	LHG	C28-C29-C30-C31
33	z	102	LHG	C26-C27-C28-C29
34	a	416	LMG	C12-C13-C14-C15
33	b	628	LHG	C19-C20-C21-C22
38	B	623	SQD	C16-C17-C18-C19
32	6	318	LUT	C11-C12-C13-C14
32	N	316	LUT	C31-C32-C33-C34
32	p	616	LUT	C11-C12-C13-C14
36	p	618	NEX	C11-C12-C13-C14
43	A	410	BCR	C7-C8-C9-C10
43	C	615	BCR	C21-C22-C23-C24
43	D	405	BCR	C21-C22-C23-C24
43	z	101	BCR	C17-C18-C19-C20
31	7	304	CLA	C5-C6-C7-C8
31	b	605	CLA	C15-C16-C17-C18
31	r	304	CLA	C8-C10-C11-C12
30	r	309	CHL	O1D-CGD-O2D-CED
31	y	614	CLA	C6-C7-C8-C9
34	w	201	LMG	C33-C34-C35-C36
38	R	322	SQD	C31-C32-C33-C34
33	a	415	LHG	C26-C27-C28-C29
38	B	620	SQD	C18-C19-C20-C21
45	C	617	DGD	C6B-C7B-C8B-C9B
31	3	305	CLA	C6-C7-C8-C9
31	6	312	CLA	C11-C12-C13-C15
31	G	604	CLA	C6-C7-C8-C10
31	q	306	CLA	C6-C7-C8-C9
31	c	601	CLA	C16-C17-C18-C19
30	3	302	CHL	C11-C10-C8-C9
31	6	304	CLA	C11-C10-C8-C9
38	B	623	SQD	C19-C20-C21-C22
31	3	306	CLA	C5-C6-C7-C8
30	9	310	CHL	O1D-CGD-O2D-CED
34	a	413	LMG	C11-C12-C13-C14
30	y	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	c	605	CLA	O1D-CGD-O2D-CED
33	l	101	LHG	C26-C27-C28-C29
34	c	624	LMG	C32-C33-C34-C35
33	S	322	LHG	O6-C4-C5-C6
33	q	320	LHG	O6-C4-C5-C6
33	c	622	LHG	O6-C4-C5-C6
33	D	407	LHG	C33-C34-C35-C36
33	y	619	LHG	C16-C17-C18-C19
30	1	607	CHL	C11-C10-C8-C7
30	G	601	CHL	C11-C12-C13-C15
30	G	608	CHL	C11-C12-C13-C15
30	G	623	CHL	C11-C12-C13-C15
30	Y	301	CHL	C11-C12-C13-C15
30	0	607	CHL	C12-C13-C15-C16
30	8	608	CHL	C12-C13-C15-C16
30	g	302	CHL	C11-C12-C13-C15
30	g	309	CHL	C11-C10-C8-C7
30	g	309	CHL	C11-C12-C13-C15
30	r	310	CHL	C2-C3-C5-C6
30	y	606	CHL	C11-C10-C8-C7
31	1	610	CLA	C11-C10-C8-C7
31	2	602	CLA	C6-C7-C8-C10
31	3	304	CLA	C6-C7-C8-C10
31	4	602	CLA	C11-C10-C8-C7
31	4	610	CLA	C11-C10-C8-C7
31	5	610	CLA	C6-C7-C8-C10
31	6	303	CLA	C6-C7-C8-C10
31	6	304	CLA	C6-C7-C8-C10
31	6	312	CLA	C6-C7-C8-C10
31	6	313	CLA	C6-C7-C8-C10
31	A	409	CLA	C6-C7-C8-C10
31	B	602	CLA	C11-C12-C13-C15
31	B	603	CLA	C6-C7-C8-C10
31	B	603	CLA	C11-C12-C13-C15
31	B	604	CLA	C12-C13-C15-C16
31	B	605	CLA	C11-C10-C8-C7
31	B	609	CLA	C11-C10-C8-C7
31	B	610	CLA	C11-C12-C13-C15
31	B	611	CLA	C6-C7-C8-C10
31	B	613	CLA	C11-C12-C13-C15
31	B	614	CLA	C6-C7-C8-C10
31	B	616	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	B	616	CLA	C11-C10-C8-C7
31	C	608	CLA	C6-C7-C8-C10
31	C	611	CLA	C11-C12-C13-C15
31	D	403	CLA	C6-C7-C8-C10
31	D	403	CLA	C11-C10-C8-C7
31	G	612	CLA	C11-C12-C13-C15
31	R	311	CLA	C6-C7-C8-C10
31	R	312	CLA	C11-C10-C8-C7
31	S	305	CLA	C6-C7-C8-C10
31	S	311	CLA	C11-C10-C8-C7
31	S	313	CLA	C6-C7-C8-C10
31	S	314	CLA	C11-C10-C8-C7
31	Y	303	CLA	C6-C7-C8-C10
31	0	613	CLA	C6-C7-C8-C10
31	7	305	CLA	C11-C10-C8-C7
31	8	602	CLA	C11-C10-C8-C7
31	8	604	CLA	C12-C13-C15-C16
31	8	612	CLA	C11-C12-C13-C15
31	q	315	CLA	C11-C10-C8-C7
31	a	409	CLA	C6-C7-C8-C10
31	b	604	CLA	C11-C12-C13-C15
31	b	605	CLA	C11-C12-C13-C15
31	b	605	CLA	C12-C13-C15-C16
31	b	610	CLA	C6-C7-C8-C10
31	b	610	CLA	C11-C10-C8-C7
31	b	612	CLA	C6-C7-C8-C10
31	b	613	CLA	C11-C12-C13-C15
31	b	615	CLA	C6-C7-C8-C10
31	b	616	CLA	C11-C12-C13-C15
31	c	607	CLA	C11-C12-C13-C15
31	c	609	CLA	C6-C7-C8-C10
31	g	303	CLA	C6-C7-C8-C10
31	g	313	CLA	C6-C7-C8-C10
31	n	303	CLA	C11-C10-C8-C7
31	n	305	CLA	C12-C13-C15-C16
31	n	314	CLA	C11-C12-C13-C15
31	r	304	CLA	C6-C7-C8-C10
31	s	305	CLA	C11-C12-C13-C15
31	s	311	CLA	C11-C10-C8-C7
31	s	312	CLA	C12-C13-C15-C16
31	y	612	CLA	C6-C7-C8-C10
31	y	612	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
30	1	609	CHL	C8-C10-C11-C12
31	6	304	CLA	C5-C6-C7-C8
31	s	312	CLA	C5-C6-C7-C8
43	H	101	BCR	C19-C20-C21-C22
43	T	101	BCR	C13-C14-C15-C16
43	a	410	BCR	C15-C16-C17-C18
43	b	619	BCR	C15-C16-C17-C18
43	b	619	BCR	C19-C20-C21-C22
43	b	620	BCR	C19-C20-C21-C22
43	c	614	BCR	C9-C10-C11-C12
43	c	614	BCR	C19-C20-C21-C22
43	h	101	BCR	C13-C14-C15-C16
30	3	310	CHL	C11-C12-C13-C15
30	9	311	CHL	C11-C12-C13-C14
31	3	306	CLA	C6-C7-C8-C9
33	5	619	LHG	C26-C27-C28-C29
34	j	101	LMG	O9-C10-O7-C8
33	6	320	LHG	C26-C27-C28-C29
34	B	625	LMG	C31-C32-C33-C34
30	Y	301	CHL	C5-C6-C7-C8
31	3	304	CLA	C8-C10-C11-C12
31	G	609	CLA	C5-C6-C7-C8
33	B	624	LHG	O7-C7-C8-C9
33	3	320	LHG	O10-C23-O8-C6
30	1	606	CHL	C2A-CAA-CBA-CGA
30	4	606	CHL	C2A-CAA-CBA-CGA
30	6	306	CHL	C2A-CAA-CBA-CGA
30	6	309	CHL	C2A-CAA-CBA-CGA
30	G	607	CHL	C2A-CAA-CBA-CGA
30	N	308	CHL	C2A-CAA-CBA-CGA
30	0	605	CHL	C2A-CAA-CBA-CGA
30	0	608	CHL	C2A-CAA-CBA-CGA
30	g	308	CHL	C2A-CAA-CBA-CGA
31	C	612	CLA	C2A-CAA-CBA-CGA
31	R	307	CLA	C2A-CAA-CBA-CGA
31	S	314	CLA	C2A-CAA-CBA-CGA
33	C	623	LHG	C31-C32-C33-C34
33	s	322	LHG	C9-C10-C11-C12
34	w	202	LMG	C39-C40-C41-C42
34	j	101	LMG	C11-C10-O7-C8
36	6	319	NEX	C40-C33-C34-C35
36	0	618	NEX	C40-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
38	a	411	SQD	C31-C32-C33-C34
31	g	311	CLA	C3-C5-C6-C7
45	c	616	DGD	CAB-CBB-CCB-CDB
30	9	309	CHL	O1A-CGA-O2A-C1
31	S	310	CLA	C11-C12-C13-C15
30	4	601	CHL	CBA-CGA-O2A-C1
31	B	604	CLA	CBA-CGA-O2A-C1
31	Y	312	CLA	CBA-CGA-O2A-C1
31	b	605	CLA	CBA-CGA-O2A-C1
31	r	305	CLA	CBA-CGA-O2A-C1
33	A	415	LHG	C24-C23-O8-C6
38	B	623	SQD	C24-C23-O48-C46
33	0	619	LHG	C27-C28-C29-C30
30	2	608	CHL	C11-C10-C8-C7
30	3	302	CHL	C11-C10-C8-C7
30	q	309	CHL	C11-C10-C8-C7
33	2	617	LHG	C30-C31-C32-C33
33	g	319	LHG	C9-C10-C11-C12
30	0	609	CHL	C8-C10-C11-C12
31	C	612	CLA	C5-C6-C7-C8
31	s	303	CLA	C13-C15-C16-C17
33	b	625	LHG	C30-C31-C32-C33
33	d	408	LHG	C9-C10-C11-C12
30	0	606	CHL	CAD-CBD-CGD-O2D
31	2	602	CLA	CAD-CBD-CGD-O2D
31	2	611	CLA	CAD-CBD-CGD-O2D
31	B	612	CLA	CAD-CBD-CGD-O2D
31	G	603	CLA	CAD-CBD-CGD-O2D
31	G	604	CLA	CAD-CBD-CGD-O2D
31	S	304	CLA	CAD-CBD-CGD-O2D
31	Y	312	CLA	CAD-CBD-CGD-O2D
31	b	610	CLA	CAD-CBD-CGD-O2D
31	c	603	CLA	CAD-CBD-CGD-O2D
31	c	606	CLA	CAD-CBD-CGD-O2D
31	r	307	CLA	CAD-CBD-CGD-O2D
31	y	604	CLA	CAD-CBD-CGD-O2D
31	y	612	CLA	CAD-CBD-CGD-O2D
33	7	319	LHG	C4-C5-O7-C7
34	1	618	LMG	C9-C8-O7-C10
34	I	101	LMG	C7-C8-O7-C10
34	f	101	LMG	C9-C8-O7-C10
36	r	319	NEX	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
36	s	319	NEX	C7-C8-C9-C19
42	A	408	PHO	CAD-CBD-CGD-O2D
45	c	616	DGD	C1G-C2G-O2G-C1B
47	E	101	HEM	C2B-C3B-CAB-CBB
47	e	102	HEM	C2B-C3B-CAB-CBB
34	b	622	LMG	C34-C35-C36-C37
34	b	623	LMG	C31-C32-C33-C34
31	B	607	CLA	C8-C10-C11-C12
34	W	203	LMG	C10-C11-C12-C13
38	b	627	SQD	C12-C13-C14-C15
48	R	302	LMU	C5-C6-C7-C8
31	b	616	CLA	CBA-CGA-O2A-C1
34	r	321	LMG	O6-C1-O1-C7
30	8	605	CHL	C13-C15-C16-C17
30	n	306	CHL	C13-C15-C16-C17
30	7	302	CHL	C2-C3-C5-C6
31	3	306	CLA	C2C-C3C-CAC-CBC
45	C	618	DGD	C1B-C2B-C3B-C4B
33	3	320	LHG	C4-C5-C6-O8
33	C	623	LHG	C2-C3-O3-P
33	N	319	LHG	C5-C4-O6-P
33	S	322	LHG	C4-C5-C6-O8
33	Y	318	LHG	C2-C3-O3-P
33	s	320	LHG	C4-C5-C6-O8
33	s	322	LHG	C4-C5-C6-O8
33	F1	301	LHG	C5-C4-O6-P
33	F1	301	LHG	C4-C5-C6-O8
34	X	203	LMG	O1-C7-C8-C9
34	Y	319	LMG	O1-C7-C8-C9
34	0	620	LMG	O1-C7-C8-C9
34	c	621	LMG	O1-C7-C8-C9
34	f	101	LMG	C7-C8-C9-O8
38	6	301	SQD	C44-C45-C46-O48
38	S	301	SQD	O6-C44-C45-C46
38	a	412	SQD	O6-C44-C45-C46
38	r	322	SQD	C44-C45-C46-O48
38	y	621	SQD	O6-C44-C45-C46
45	C	618	DGD	O1G-C1G-C2G-C3G
45	c	619	DGD	O1G-C1G-C2G-C3G
31	C	603	CLA	O1A-CGA-O2A-C1
31	n	303	CLA	O1A-CGA-O2A-C1
31	r	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
33	S	322	LHG	C30-C31-C32-C33
34	I	101	LMG	C31-C32-C33-C34
33	6	320	LHG	O6-C4-C5-O7
33	D	407	LHG	O6-C4-C5-O7
33	L	101	LHG	O6-C4-C5-O7
33	S	320	LHG	O6-C4-C5-O7
33	b	628	LHG	O6-C4-C5-O7
33	c	622	LHG	O6-C4-C5-O7
33	j	102	LHG	O6-C4-C5-O7
33	l	101	LHG	O6-C4-C5-O7
30	7	308	CHL	C5-C6-C7-C8
30	q	303	CHL	C5-C6-C7-C8
31	1	602	CLA	C5-C6-C7-C8
31	1	613	CLA	C13-C15-C16-C17
31	4	603	CLA	C5-C6-C7-C8
31	5	602	CLA	C8-C10-C11-C12
31	B	609	CLA	C15-C16-C17-C18
31	S	305	CLA	C5-C6-C7-C8
31	b	611	CLA	C8-C10-C11-C12
30	p	601	CHL	CAA-CBA-CGA-O2A
31	N	314	CLA	CAA-CBA-CGA-O2A
45	c	617	DGD	O1G-C1A-C2A-C3A
31	9	312	CLA	C5-C6-C7-C8
45	C	617	DGD	C2B-C3B-C4B-C5B
30	1	605	CHL	C2A-CAA-CBA-CGA
30	2	607	CHL	C2A-CAA-CBA-CGA
31	p	611	CLA	C2A-CAA-CBA-CGA
36	3	319	NEX	C14-C15-C35-C34
31	y	613	CLA	C5-C6-C7-C8
30	3	302	CHL	O1A-CGA-O2A-C1
31	B	611	CLA	C16-C17-C18-C19
30	3	302	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	CHA-CBD-CGD-O1D
30	5	601	CHL	CHA-CBD-CGD-O1D
30	0	601	CHL	CHA-CBD-CGD-O1D
30	8	601	CHL	CHA-CBD-CGD-O1D
30	9	303	CHL	CHA-CBD-CGD-O1D
30	p	601	CHL	CHA-CBD-CGD-O1D
30	p	601	CHL	CHA-CBD-CGD-O2D
30	q	303	CHL	CHA-CBD-CGD-O1D
30	n	302	CHL	CHA-CBD-CGD-O1D
30	s	308	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
30	s	308	CHL	CHA-CBD-CGD-O2D
30	y	601	CHL	CHA-CBD-CGD-O1D
31	1	602	CLA	CHA-CBD-CGD-O1D
31	1	602	CLA	CHA-CBD-CGD-O2D
31	2	604	CLA	CHA-CBD-CGD-O1D
31	2	604	CLA	CHA-CBD-CGD-O2D
31	3	313	CLA	CHA-CBD-CGD-O1D
31	3	313	CLA	CHA-CBD-CGD-O2D
31	4	603	CLA	CHA-CBD-CGD-O1D
31	4	603	CLA	CHA-CBD-CGD-O2D
31	4	612	CLA	CHA-CBD-CGD-O1D
31	5	603	CLA	CHA-CBD-CGD-O1D
31	5	603	CLA	CHA-CBD-CGD-O2D
31	5	604	CLA	CHA-CBD-CGD-O1D
31	5	604	CLA	CHA-CBD-CGD-O2D
31	5	614	CLA	CHA-CBD-CGD-O1D
31	5	614	CLA	CHA-CBD-CGD-O2D
31	6	304	CLA	CHA-CBD-CGD-O1D
31	6	304	CLA	CHA-CBD-CGD-O2D
31	6	305	CLA	CHA-CBD-CGD-O2D
31	6	313	CLA	CHA-CBD-CGD-O1D
31	6	313	CLA	CHA-CBD-CGD-O2D
31	B	605	CLA	CHA-CBD-CGD-O1D
31	B	605	CLA	CHA-CBD-CGD-O2D
31	B	606	CLA	CHA-CBD-CGD-O1D
31	B	606	CLA	CHA-CBD-CGD-O2D
31	B	609	CLA	CHA-CBD-CGD-O1D
31	B	609	CLA	CHA-CBD-CGD-O2D
31	C	609	CLA	CHA-CBD-CGD-O1D
31	C	612	CLA	CHA-CBD-CGD-O1D
31	C	612	CLA	CHA-CBD-CGD-O2D
31	G	602	CLA	CHA-CBD-CGD-O1D
31	G	602	CLA	CHA-CBD-CGD-O2D
31	N	303	CLA	CHA-CBD-CGD-O1D
31	N	303	CLA	CHA-CBD-CGD-O2D
31	N	304	CLA	CHA-CBD-CGD-O1D
31	N	305	CLA	CHA-CBD-CGD-O2D
31	R	303	CLA	CHA-CBD-CGD-O1D
31	R	303	CLA	CHA-CBD-CGD-O2D
31	R	306	CLA	CHA-CBD-CGD-O1D
31	R	316	CLA	CHA-CBD-CGD-O2D
31	S	313	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	Y	303	CLA	CHA-CBD-CGD-O1D
31	Y	303	CLA	CHA-CBD-CGD-O2D
31	Y	304	CLA	CHA-CBD-CGD-O1D
31	Y	304	CLA	CHA-CBD-CGD-O2D
31	0	603	CLA	CHA-CBD-CGD-O1D
31	7	303	CLA	CHA-CBD-CGD-O1D
31	7	303	CLA	CHA-CBD-CGD-O2D
31	7	304	CLA	CHA-CBD-CGD-O1D
31	7	304	CLA	CHA-CBD-CGD-O2D
31	7	313	CLA	CHA-CBD-CGD-O1D
31	7	313	CLA	CHA-CBD-CGD-O2D
31	8	602	CLA	CHA-CBD-CGD-O1D
31	8	602	CLA	CHA-CBD-CGD-O2D
31	8	604	CLA	CHA-CBD-CGD-O1D
31	8	604	CLA	CHA-CBD-CGD-O2D
31	9	304	CLA	CHA-CBD-CGD-O1D
31	9	304	CLA	CHA-CBD-CGD-O2D
31	9	305	CLA	CHA-CBD-CGD-O1D
31	9	305	CLA	CHA-CBD-CGD-O2D
31	p	612	CLA	CHA-CBD-CGD-O1D
31	p	613	CLA	CHA-CBD-CGD-O1D
31	p	613	CLA	CHA-CBD-CGD-O2D
31	q	304	CLA	CHA-CBD-CGD-O1D
31	q	304	CLA	CHA-CBD-CGD-O2D
31	q	312	CLA	CHA-CBD-CGD-O1D
31	q	312	CLA	CHA-CBD-CGD-O2D
31	b	602	CLA	CHA-CBD-CGD-O1D
31	b	602	CLA	CHA-CBD-CGD-O2D
31	b	611	CLA	CHA-CBD-CGD-O1D
31	b	611	CLA	CHA-CBD-CGD-O2D
31	c	607	CLA	CHA-CBD-CGD-O1D
31	c	607	CLA	CHA-CBD-CGD-O2D
31	c	609	CLA	CHA-CBD-CGD-O1D
31	g	303	CLA	CHA-CBD-CGD-O1D
31	n	303	CLA	CHA-CBD-CGD-O1D
31	n	303	CLA	CHA-CBD-CGD-O2D
31	n	305	CLA	CHA-CBD-CGD-O1D
31	n	305	CLA	CHA-CBD-CGD-O2D
31	r	305	CLA	CHA-CBD-CGD-O1D
31	r	305	CLA	CHA-CBD-CGD-O2D
31	r	314	CLA	CHA-CBD-CGD-O2D
31	s	304	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	s	304	CLA	CHA-CBD-CGD-O2D
31	s	305	CLA	CHA-CBD-CGD-O1D
31	s	305	CLA	CHA-CBD-CGD-O2D
31	s	306	CLA	CHA-CBD-CGD-O1D
31	y	603	CLA	CHA-CBD-CGD-O1D
31	y	603	CLA	CHA-CBD-CGD-O2D
31	3	305	CLA	C3-C5-C6-C7
30	3	309	CHL	O1A-CGA-O2A-C1
31	6	303	CLA	O1A-CGA-O2A-C1
31	C	604	CLA	O1A-CGA-O2A-C1
31	Y	312	CLA	O1A-CGA-O2A-C1
31	7	312	CLA	O1A-CGA-O2A-C1
31	b	608	CLA	O1A-CGA-O2A-C1
31	c	606	CLA	O1A-CGA-O2A-C1
33	C	623	LHG	O10-C23-O8-C6
34	k	102	LMG	O10-C28-O8-C9
33	q	320	LHG	C31-C32-C33-C34
36	2	616	NEX	C11-C10-C9-C8
36	3	319	NEX	C28-C29-C30-C31
36	N	318	NEX	C11-C10-C9-C8
36	g	317	NEX	C32-C33-C34-C35
37	4	619	XAT	C12-C13-C14-C15
37	G	620	XAT	C12-C13-C14-C15
37	9	322	XAT	C12-C13-C14-C15
37	q	321	XAT	C12-C13-C14-C15
37	g	321	XAT	C12-C13-C14-C15
34	j	101	LMG	C11-C12-C13-C14
33	D	408	LHG	O7-C5-C6-O8
33	Y	318	LHG	O7-C5-C6-O8
34	4	621	LMG	O1-C7-C8-O7
34	c	621	LMG	O1-C7-C8-O7
34	r	321	LMG	O1-C7-C8-O7
34	s	321	LMG	O7-C8-C9-O8
34	w	205	LMG	O7-C8-C9-O8
38	6	301	SQD	O6-C44-C45-O47
38	A	413	SQD	O6-C44-C45-O47
38	G	624	SQD	O6-C44-C45-O47
38	M	102	SQD	O47-C45-C46-O48
38	Y	320	SQD	O47-C45-C46-O48
38	g	318	SQD	O6-C44-C45-O47
38	s	301	SQD	O6-C44-C45-O47
38	x	201	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
45	C	620	DGD	O1G-C1G-C2G-O2G
45	c	618	DGD	O2G-C2G-C3G-O3G
30	N	309	CHL	CBA-CGA-O2A-C1
34	b	622	LMG	C16-C17-C18-C19
38	M	102	SQD	C25-C26-C27-C28
30	6	307	CHL	CBD-CGD-O2D-CED
31	0	611	CLA	C10-C11-C12-C13
31	c	606	CLA	C5-C6-C7-C8
31	6	305	CLA	O1A-CGA-O2A-C1
33	5	619	LHG	C28-C29-C30-C31
33	A	415	LHG	C27-C28-C29-C30
34	b	622	LMG	C18-C19-C20-C21
48	K	101	LMU	C2-C3-C4-C5
33	A	417	LHG	C11-C10-C9-C8
34	1	618	LMG	C11-C12-C13-C14
31	p	611	CLA	C5-C6-C7-C8
31	6	315	CLA	C4-C3-C5-C6
31	G	612	CLA	C4-C3-C5-C6
33	3	320	LHG	C11-C10-C9-C8
33	M	101	LHG	C29-C30-C31-C32
33	j	102	LHG	C9-C10-C11-C12
31	b	616	CLA	O1A-CGA-O2A-C1
34	b	629	LMG	C10-C11-C12-C13
31	y	613	CLA	C2-C3-C5-C6
31	3	306	CLA	O1D-CGD-O2D-CED
34	a	401	LMG	C11-C12-C13-C14
30	G	623	CHL	C11-C12-C13-C14
30	Y	309	CHL	C11-C12-C13-C14
30	0	607	CHL	C11-C12-C13-C14
30	7	306	CHL	C11-C12-C13-C14
30	8	605	CHL	C11-C12-C13-C14
30	n	306	CHL	C11-C12-C13-C14
30	y	607	CHL	C11-C12-C13-C14
31	3	316	CLA	C11-C10-C8-C9
31	4	610	CLA	C11-C10-C8-C9
31	4	613	CLA	C11-C10-C8-C9
31	b	613	CLA	C11-C12-C13-C14
31	c	605	CLA	C6-C7-C8-C9
31	g	313	CLA	C11-C10-C8-C9
42	d	402	PHO	O1D-CGD-O2D-CED
34	2	618	LMG	C8-C9-O8-C28
31	y	614	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	A	415	LHG	C34-C35-C36-C37
38	R	322	SQD	C32-C33-C34-C35
34	W	202	LMG	O6-C5-C6-O5
30	4	601	CHL	O1A-CGA-O2A-C1
38	x	201	SQD	O10-C23-O48-C46
33	S	322	LHG	C11-C10-C9-C8
33	7	319	LHG	C26-C27-C28-C29
31	N	310	CLA	C15-C16-C17-C18
31	b	610	CLA	C15-C16-C17-C18
38	6	301	SQD	C4-C5-C6-S
38	A	411	SQD	C5-C6-S-O8
38	A	413	SQD	C4-C5-C6-S
38	B	623	SQD	C4-C5-C6-S
38	G	617	SQD	C4-C5-C6-S
38	R	322	SQD	C4-C5-C6-S
38	0	621	SQD	C4-C5-C6-S
38	b	627	SQD	C4-C5-C6-S
38	r	322	SQD	C4-C5-C6-S
38	s	301	SQD	C5-C6-S-O8
33	c	622	LHG	C35-C36-C37-C38
33	t	102	LHG	C34-C35-C36-C37
30	y	608	CHL	C2A-CAA-CBA-CGA
31	c	606	CLA	C2A-CAA-CBA-CGA
31	y	611	CLA	C2A-CAA-CBA-CGA
33	r	320	LHG	O8-C23-C24-C25
34	X	203	LMG	O7-C10-C11-C12
34	g	322	LMG	O7-C10-C11-C12
34	2	620	LMG	C37-C38-C39-C40
31	b	602	CLA	O1A-CGA-O2A-C1
31	D	404	CLA	CBA-CGA-O2A-C1
32	7	318	LUT	C11-C12-C13-C20
32	p	617	LUT	C31-C32-C33-C40
32	g	316	LUT	C7-C8-C9-C19
43	b	620	BCR	C7-C8-C9-C34
33	6	320	LHG	C29-C30-C31-C32
34	W	201	LMG	C12-C13-C14-C15
48	c	623	LMU	C2-C3-C4-C5
31	C	605	CLA	C10-C11-C12-C13
33	b	628	LHG	C12-C13-C14-C15
33	s	322	LHG	C10-C11-C12-C13
38	B	620	SQD	C10-C11-C12-C13
38	x	201	SQD	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	7	318	LUT	C11-C12-C13-C14
32	p	617	LUT	C31-C32-C33-C34
32	g	316	LUT	C7-C8-C9-C10
32	s	318	LUT	C31-C32-C33-C34
43	T	101	BCR	C17-C18-C19-C20
43	a	410	BCR	C7-C8-C9-C10
43	b	620	BCR	C7-C8-C9-C10
38	a	412	SQD	C11-C12-C13-C14
30	1	601	CHL	C1A-C2A-CAA-CBA
30	6	310	CHL	C1A-C2A-CAA-CBA
30	0	608	CHL	C1A-C2A-CAA-CBA
31	1	611	CLA	C1A-C2A-CAA-CBA
31	3	313	CLA	C1A-C2A-CAA-CBA
31	5	610	CLA	C1A-C2A-CAA-CBA
31	B	608	CLA	C1A-C2A-CAA-CBA
31	N	303	CLA	C1A-C2A-CAA-CBA
31	Y	305	CLA	C1A-C2A-CAA-CBA
31	0	602	CLA	C1A-C2A-CAA-CBA
31	q	306	CLA	C1A-C2A-CAA-CBA
31	c	612	CLA	C1A-C2A-CAA-CBA
31	2	612	CLA	C16-C17-C18-C19
31	7	303	CLA	C11-C12-C13-C15
33	y	619	LHG	C14-C15-C16-C17
30	S	309	CHL	C2-C1-O2A-CGA
31	G	612	CLA	C2-C1-O2A-CGA
31	N	314	CLA	C2-C1-O2A-CGA
31	8	614	CLA	C2-C1-O2A-CGA
31	p	611	CLA	C2-C1-O2A-CGA
31	c	604	CLA	C2-C1-O2A-CGA
31	n	316	CLA	C2-C1-O2A-CGA
31	3	301	CLA	CBA-CGA-O2A-C1
31	y	615	CLA	CBA-CGA-O2A-C1
33	0	619	LHG	C24-C23-O8-C6
38	S	301	SQD	C24-C23-O48-C46
33	A	417	LHG	C24-C25-C26-C27
38	B	623	SQD	O10-C23-O48-C46
33	G	618	LHG	C3-O3-P-O6
33	M	101	LHG	C4-O6-P-O3
33	R	320	LHG	C3-O3-P-O6
33	b	628	LHG	C3-O3-P-O6
33	s	322	LHG	C3-O3-P-O6
30	8	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	b	605	CLA	O1D-CGD-O2D-CED
33	D	407	LHG	C11-C10-C9-C8
31	B	614	CLA	C4-C3-C5-C6
34	D	412	LMG	O7-C10-C11-C12
31	s	314	CLA	C3-C5-C6-C7
33	S	322	LHG	C2-C3-O3-P
33	S	322	LHG	C5-C4-O6-P
33	9	320	LHG	C2-C3-O3-P
33	c	622	LHG	C2-C3-O3-P
33	j	102	LHG	C2-C3-O3-P
30	0	601	CHL	C2-C3-C5-C6
30	9	311	CHL	C2-C3-C5-C6
30	r	309	CHL	C2-C3-C5-C6
42	D	401	PHO	C2-C3-C5-C6
44	a	414	PL9	C13-C14-C16-C17
34	d	409	LMG	C32-C33-C34-C35
30	7	321	CHL	O1A-CGA-O2A-C1
30	n	308	CHL	O1A-CGA-O2A-C1
31	B	604	CLA	O1A-CGA-O2A-C1
33	5	619	LHG	C4-O6-P-O4
33	A	415	LHG	C3-O3-P-O5
33	A	415	LHG	C4-O6-P-O5
33	A	417	LHG	C4-O6-P-O4
33	B	624	LHG	C3-O3-P-O4
33	D	407	LHG	C4-O6-P-O4
33	D	408	LHG	C3-O3-P-O5
33	L	101	LHG	C4-O6-P-O4
33	M	101	LHG	C3-O3-P-O4
33	N	319	LHG	C3-O3-P-O4
33	S	322	LHG	C3-O3-P-O5
33	S	322	LHG	C4-O6-P-O5
33	Y	318	LHG	C3-O3-P-O5
33	Y	318	LHG	C4-O6-P-O5
33	0	619	LHG	C4-O6-P-O4
33	p	619	LHG	C4-O6-P-O5
33	a	415	LHG	C3-O3-P-O5
33	a	415	LHG	C4-O6-P-O4
33	b	625	LHG	C4-O6-P-O4
33	c	622	LHG	C3-O3-P-O4
33	d	408	LHG	C4-O6-P-O4
33	e	101	LHG	C3-O3-P-O5
33	e	101	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
33	g	319	LHG	C4-O6-P-O5
33	j	102	LHG	C4-O6-P-O5
33	r	320	LHG	C4-O6-P-O5
33	s	322	LHG	C4-O6-P-O4
33	t	102	LHG	C3-O3-P-O5
33	t	102	LHG	C4-O6-P-O4
33	y	619	LHG	C4-O6-P-O5
33	F1	301	LHG	C3-O3-P-O4
31	2	602	CLA	C16-C17-C18-C19
31	A	409	CLA	C11-C12-C13-C15
31	S	311	CLA	C16-C17-C18-C20
31	a	409	CLA	C11-C12-C13-C15
33	j	102	LHG	C18-C19-C20-C21
34	5	620	LMG	C31-C32-C33-C34
45	c	616	DGD	C4B-C5B-C6B-C7B
34	x	202	LMG	C4-C5-C6-O5
31	B	609	CLA	C13-C15-C16-C17
30	Y	309	CHL	CBA-CGA-O2A-C1
33	4	618	LHG	O6-C4-C5-C6
33	5	619	LHG	O6-C4-C5-C6
33	C	623	LHG	O6-C4-C5-C6
33	D	407	LHG	O6-C4-C5-C6
33	L	101	LHG	O6-C4-C5-C6
33	M	101	LHG	O6-C4-C5-C6
33	b	628	LHG	O6-C4-C5-C6
33	e	101	LHG	O6-C4-C5-C6
33	g	319	LHG	O6-C4-C5-C6
33	l	101	LHG	O6-C4-C5-C6
33	t	102	LHG	O6-C4-C5-C6
34	6	322	LMG	C11-C12-C13-C14
38	A	411	SQD	C9-C10-C11-C12
38	b	621	SQD	C9-C10-C11-C12
31	b	605	CLA	O1A-CGA-O2A-C1
31	y	615	CLA	O1A-CGA-O2A-C1
30	y	609	CHL	C10-C11-C12-C13
31	g	313	CLA	C15-C16-C17-C18
30	Y	308	CHL	C2A-CAA-CBA-CGA
30	s	309	CHL	C2A-CAA-CBA-CGA
31	b	617	CLA	C2A-CAA-CBA-CGA
31	r	306	CLA	C2A-CAA-CBA-CGA
31	A	406	CLA	C3-C5-C6-C7
30	2	608	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
33	s	322	LHG	C30-C31-C32-C33
33	2	617	LHG	C12-C13-C14-C15
33	3	320	LHG	C10-C11-C12-C13
34	C	619	LMG	C12-C13-C14-C15
34	D	410	LMG	C16-C17-C18-C19
38	A	411	SQD	C27-C28-C29-C30
38	m	101	SQD	C32-C33-C34-C35
45	C	618	DGD	C6A-C7A-C8A-C9A
30	4	601	CHL	CAD-CBD-CGD-O1D
30	4	607	CHL	CAD-CBD-CGD-O1D
30	5	601	CHL	CAD-CBD-CGD-O1D
30	0	601	CHL	CAD-CBD-CGD-O1D
30	0	605	CHL	C2-C3-C5-C6
30	8	601	CHL	CAD-CBD-CGD-O1D
30	9	303	CHL	CAD-CBD-CGD-O1D
30	p	601	CHL	CAD-CBD-CGD-O1D
30	q	303	CHL	CAD-CBD-CGD-O1D
30	n	302	CHL	CAD-CBD-CGD-O1D
30	s	308	CHL	CAD-CBD-CGD-O1D
30	y	601	CHL	CAD-CBD-CGD-O1D
31	6	305	CLA	CAD-CBD-CGD-O1D
31	B	605	CLA	CAD-CBD-CGD-O1D
31	B	609	CLA	CAD-CBD-CGD-O1D
31	C	603	CLA	CAD-CBD-CGD-O1D
31	C	604	CLA	CAD-CBD-CGD-O1D
31	C	605	CLA	CAD-CBD-CGD-O1D
31	C	612	CLA	CAD-CBD-CGD-O1D
31	S	306	CLA	CAD-CBD-CGD-O1D
31	0	615	CLA	CAD-CBD-CGD-O1D
31	8	604	CLA	CAD-CBD-CGD-O1D
31	b	606	CLA	CAD-CBD-CGD-O1D
31	c	604	CLA	CAD-CBD-CGD-O1D
31	n	305	CLA	CAD-CBD-CGD-O1D
38	A	411	SQD	C5-C6-S-O7
38	B	620	SQD	O5-C5-C6-S
38	a	411	SQD	O5-C5-C6-S
47	e	102	HEM	C4D-C3D-CAD-CBD
31	1	614	CLA	CAA-CBA-CGA-O2A
34	b	629	LMG	O7-C10-C11-C12
31	2	603	CLA	C5-C6-C7-C8
31	N	311	CLA	O1A-CGA-O2A-C1
33	p	619	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	N	311	CLA	CBA-CGA-O2A-C1
31	5	611	CLA	O1D-CGD-O2D-CED
31	y	604	CLA	C6-C7-C8-C10
42	a	408	PHO	C16-C17-C18-C19
30	6	306	CHL	CBD-CGD-O2D-CED
31	4	614	CLA	C4-C3-C5-C6
31	C	613	CLA	C4-C3-C5-C6
30	1	601	CHL	C6-C7-C8-C10
30	1	601	CHL	C12-C13-C15-C16
30	1	609	CHL	C11-C12-C13-C15
30	1	619	CHL	C11-C10-C8-C7
30	3	310	CHL	C11-C10-C8-C7
30	4	601	CHL	C6-C7-C8-C10
30	6	308	CHL	C11-C10-C8-C7
30	6	308	CHL	C12-C13-C15-C16
30	G	601	CHL	C12-C13-C15-C16
30	G	608	CHL	C12-C13-C15-C16
30	G	623	CHL	C11-C10-C8-C7
30	N	307	CHL	C11-C10-C8-C7
30	N	309	CHL	C11-C10-C8-C7
30	Y	309	CHL	C11-C10-C8-C7
30	0	607	CHL	C11-C10-C8-C7
30	7	307	CHL	C11-C10-C8-C7
30	7	310	CHL	C12-C13-C15-C16
30	7	321	CHL	C12-C13-C15-C16
30	9	303	CHL	C11-C10-C8-C7
30	9	303	CHL	C12-C13-C15-C16
30	g	302	CHL	C12-C13-C15-C16
30	g	309	CHL	C12-C13-C15-C16
30	n	308	CHL	C12-C13-C15-C16
30	n	310	CHL	C12-C13-C15-C16
30	y	601	CHL	C11-C10-C8-C7
30	y	607	CHL	C12-C13-C15-C16
31	1	604	CLA	C6-C7-C8-C10
31	2	609	CLA	C11-C10-C8-C7
31	2	610	CLA	C6-C7-C8-C10
31	5	602	CLA	C6-C7-C8-C10
31	5	602	CLA	C11-C10-C8-C7
31	5	610	CLA	C11-C10-C8-C7
31	6	311	CLA	C11-C12-C13-C15
31	6	313	CLA	C11-C10-C8-C7
31	A	409	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	B	602	CLA	C3A-C2A-CAA-CBA
31	B	606	CLA	C6-C7-C8-C10
31	B	614	CLA	C11-C10-C8-C7
31	B	614	CLA	C11-C12-C13-C15
31	B	615	CLA	C11-C12-C13-C15
31	C	602	CLA	C11-C12-C13-C15
31	C	606	CLA	C6-C7-C8-C10
31	G	602	CLA	C11-C12-C13-C15
31	G	609	CLA	C11-C12-C13-C15
31	N	313	CLA	C11-C10-C8-C7
31	S	303	CLA	C11-C10-C8-C7
31	S	312	CLA	C11-C10-C8-C7
31	Y	310	CLA	C11-C12-C13-C15
31	Y	312	CLA	C12-C13-C15-C16
31	7	313	CLA	C11-C10-C8-C7
31	p	610	CLA	C6-C7-C8-C10
31	p	615	CLA	C3A-C2A-CAA-CBA
31	q	304	CLA	C11-C10-C8-C7
31	a	409	CLA	C11-C10-C8-C7
31	b	615	CLA	C11-C12-C13-C15
31	b	616	CLA	C6-C7-C8-C10
31	c	605	CLA	C6-C7-C8-C10
31	c	607	CLA	C11-C10-C8-C7
31	c	611	CLA	C12-C13-C15-C16
31	d	404	CLA	C6-C7-C8-C10
31	d	404	CLA	C11-C10-C8-C7
31	g	313	CLA	C11-C10-C8-C7
31	r	311	CLA	C11-C10-C8-C7
31	s	303	CLA	C11-C10-C8-C7
31	s	312	CLA	C6-C7-C8-C10
31	s	313	CLA	C6-C7-C8-C10
31	y	613	CLA	C12-C13-C15-C16
32	S	318	LUT	C25-C26-C27-C28
33	2	617	LHG	O6-C4-C5-O7
33	4	618	LHG	O6-C4-C5-O7
33	A	415	LHG	O6-C4-C5-O7
33	B	624	LHG	O6-C4-C5-O7
33	G	618	LHG	O6-C4-C5-O7
33	K	102	LHG	O6-C4-C5-O7
33	N	319	LHG	O6-C4-C5-O7
33	S	322	LHG	O6-C4-C5-O7
33	7	319	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
33	9	320	LHG	O6-C4-C5-O7
33	e	101	LHG	O6-C4-C5-O7
33	t	102	LHG	O6-C4-C5-O7
34	n	321	LMG	C10-C11-C12-C13
42	A	408	PHO	C6-C7-C8-C10
33	4	618	LHG	C29-C30-C31-C32
33	A	415	LHG	O10-C23-O8-C6
33	4	618	LHG	C33-C34-C35-C36
33	S	322	LHG	C31-C32-C33-C34
31	6	311	CLA	C8-C10-C11-C12
31	n	304	CLA	C5-C6-C7-C8
33	a	415	LHG	C29-C30-C31-C32
38	b	621	SQD	C14-C15-C16-C17
30	N	309	CHL	O1A-CGA-O2A-C1
33	0	619	LHG	O10-C23-O8-C6
30	6	310	CHL	C2A-CAA-CBA-CGA
30	p	601	CHL	C2A-CAA-CBA-CGA
31	8	610	CLA	C2A-CAA-CBA-CGA
31	p	602	CLA	C2A-CAA-CBA-CGA
31	g	305	CLA	C2A-CAA-CBA-CGA
31	n	312	CLA	C2A-CAA-CBA-CGA
31	y	613	CLA	C2A-CAA-CBA-CGA
31	2	609	CLA	C11-C12-C13-C14
33	L	101	LHG	C26-C27-C28-C29
33	F1	301	LHG	C26-C27-C28-C29
34	2	620	LMG	C16-C17-C18-C19
31	9	304	CLA	CAA-CBA-CGA-O2A
34	C	619	LMG	O7-C10-C11-C12
34	S	321	LMG	O7-C10-C11-C12
31	b	604	CLA	C8-C10-C11-C12
33	B	624	LHG	C14-C15-C16-C17
34	2	620	LMG	C7-C8-C9-O8
34	4	621	LMG	O1-C7-C8-C9
34	5	620	LMG	O1-C7-C8-C9
34	w	202	LMG	O1-C7-C8-C9
34	x	202	LMG	O1-C7-C8-C9
38	A	413	SQD	O6-C44-C45-C46
38	B	623	SQD	C44-C45-C46-O48
38	X	201	SQD	C44-C45-C46-O48
38	a	411	SQD	C44-C45-C46-O48
38	m	101	SQD	O6-C44-C45-C46
45	C	620	DGD	O1G-C1G-C2G-C3G

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Mol	Chain	Res	Type	Atoms
33	L	101	LHG	O7-C5-C6-O8
34	A	412	LMG	O1-C7-C8-O7
34	B	621	LMG	O7-C8-C9-O8
34	N	320	LMG	O1-C7-C8-O7
34	Y	319	LMG	O1-C7-C8-O7
34	9	301	LMG	O1-C7-C8-O7
34	b	629	LMG	O7-C8-C9-O8
34	f	101	LMG	O7-C8-C9-O8
34	g	320	LMG	O1-C7-C8-O7
34	w	202	LMG	O1-C7-C8-O7
34	w	204	LMG	O1-C7-C8-O7
38	A	411	SQD	O6-C44-C45-O47
38	A	413	SQD	O47-C45-C46-O48
38	B	623	SQD	O6-C44-C45-O47
38	B	623	SQD	O47-C45-C46-O48
38	G	617	SQD	O47-C45-C46-O48
38	a	411	SQD	O47-C45-C46-O48
38	a	412	SQD	O6-C44-C45-O47
38	a	412	SQD	O47-C45-C46-O48
38	b	627	SQD	O47-C45-C46-O48
38	m	101	SQD	O6-C44-C45-O47
38	r	322	SQD	O6-C44-C45-O47
38	r	322	SQD	O47-C45-C46-O48
33	1	617	LHG	C9-C10-C11-C12
34	5	620	LMG	C8-C7-O1-C1
34	C	624	LMG	C8-C7-O1-C1
34	D	411	LMG	C8-C7-O1-C1
34	G	622	LMG	C8-C7-O1-C1
34	W	203	LMG	C8-C7-O1-C1
34	X	203	LMG	C8-C7-O1-C1
34	q	302	LMG	C8-C7-O1-C1
34	d	410	LMG	C8-C7-O1-C1
34	g	322	LMG	C8-C7-O1-C1
34	j	101	LMG	C8-C7-O1-C1
34	w	205	LMG	C8-C7-O1-C1
38	A	411	SQD	C45-C44-O6-C1
38	G	617	SQD	C45-C44-O6-C1
38	x	201	SQD	C45-C44-O6-C1
45	C	617	DGD	C2G-C3G-O3G-C1D
45	c	617	DGD	C5D-C6D-O5D-C1E
31	3	306	CLA	C6-C7-C8-C10
31	6	312	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	G	609	CLA	C8-C10-C11-C12
31	N	313	CLA	C8-C10-C11-C12
31	c	606	CLA	C15-C16-C17-C18
34	r	321	LMG	C13-C14-C15-C16
38	A	413	SQD	C28-C29-C30-C31
48	r	302	LMU	C7-C8-C9-C10
33	l	617	LHG	C5-C4-O6-P
33	d	408	LHG	C11-C10-C9-C8
33	g	319	LHG	C25-C26-C27-C28
33	r	320	LHG	C28-C29-C30-C31
34	5	620	LMG	C29-C30-C31-C32
31	3	301	CLA	O1A-CGA-O2A-C1
38	S	301	SQD	O10-C23-O48-C46
31	2	609	CLA	C10-C11-C12-C13
44	D	406	PL9	C15-C14-C16-C17
30	4	609	CHL	C11-C10-C8-C9
38	A	411	SQD	C29-C30-C31-C32
33	L	101	LHG	C25-C26-C27-C28
30	7	321	CHL	C11-C12-C13-C14
30	q	303	CHL	C11-C12-C13-C14
30	n	308	CHL	C11-C12-C13-C14
31	3	304	CLA	C11-C10-C8-C9
31	3	312	CLA	C6-C7-C8-C9
31	4	602	CLA	C11-C10-C8-C9
31	6	312	CLA	C6-C7-C8-C9
31	B	607	CLA	C11-C10-C8-C9
31	B	611	CLA	C6-C7-C8-C9
31	B	616	CLA	C11-C10-C8-C9
31	C	602	CLA	C11-C12-C13-C14
31	C	611	CLA	C11-C12-C13-C14
31	D	403	CLA	C11-C10-C8-C9
31	D	404	CLA	C14-C13-C15-C16
31	G	612	CLA	C11-C10-C8-C9
31	G	612	CLA	C11-C12-C13-C14
31	N	313	CLA	C11-C12-C13-C14
31	S	313	CLA	C6-C7-C8-C9
31	7	305	CLA	C11-C10-C8-C9
31	8	602	CLA	C11-C10-C8-C9
31	8	604	CLA	C14-C13-C15-C16
31	b	610	CLA	C6-C7-C8-C9
31	b	616	CLA	C6-C7-C8-C9
31	c	607	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	n	303	CLA	C11-C10-C8-C9
31	r	316	CLA	C14-C13-C15-C16
31	s	305	CLA	C11-C12-C13-C14
31	s	311	CLA	C11-C10-C8-C9
31	s	312	CLA	C14-C13-C15-C16
31	s	314	CLA	C11-C10-C8-C9
31	B	603	CLA	C3-C5-C6-C7
31	S	310	CLA	C11-C12-C13-C14
31	S	311	CLA	C16-C17-C18-C19
33	S	320	LHG	C24-C25-C26-C27
33	d	408	LHG	C34-C35-C36-C37
38	G	624	SQD	O5-C1-O6-C44
30	Y	309	CHL	O1A-CGA-O2A-C1
31	D	404	CLA	O1A-CGA-O2A-C1
31	8	613	CLA	CAA-CBA-CGA-O2A
33	y	619	LHG	O1-C1-C2-O2
31	r	316	CLA	C15-C16-C17-C18
31	6	315	CLA	C6-C7-C8-C9
33	A	415	LHG	C13-C14-C15-C16
43	a	410	BCR	C18-C19-C20-C21
43	c	614	BCR	C18-C19-C20-C21
43	v	101	BCR	C15-C16-C17-C18
34	b	622	LMG	C29-C30-C31-C32
30	Y	302	CHL	O1A-CGA-O2A-C1
31	4	602	CLA	C16-C17-C18-C20
33	D	408	LHG	C31-C32-C33-C34
32	3	318	LUT	C31-C32-C33-C34
32	6	317	LUT	C27-C28-C29-C30
30	Y	301	CHL	CBA-CGA-O2A-C1
33	L	101	LHG	C10-C11-C12-C13
30	3	309	CHL	CBD-CGD-O2D-CED
33	c	622	LHG	C17-C18-C19-C20
34	W	201	LMG	C16-C17-C18-C19
31	1	604	CLA	C10-C11-C12-C13
31	N	303	CLA	C13-C15-C16-C17
33	7	319	LHG	C12-C13-C14-C15
31	1	613	CLA	C4-C3-C5-C6
31	7	315	CLA	CAA-CBA-CGA-O2A
34	d	411	LMG	O7-C10-C11-C12
31	B	605	CLA	C13-C15-C16-C17
31	C	613	CLA	C15-C16-C17-C18
31	q	315	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
38	m	101	SQD	C24-C25-C26-C27
31	B	612	CLA	C13-C15-C16-C17
30	1	608	CHL	C1-C2-C3-C4
30	2	607	CHL	C1-C2-C3-C4
30	3	303	CHL	C1-C2-C3-C4
30	3	309	CHL	C1-C2-C3-C4
30	5	608	CHL	C1-C2-C3-C4
30	6	309	CHL	C1-C2-C3-C4
30	G	606	CHL	C1-C2-C3-C4
30	N	301	CHL	C1-C2-C3-C4
30	N	308	CHL	C1-C2-C3-C4
30	Y	308	CHL	C1-C2-C3-C4
30	0	608	CHL	C1-C2-C3-C4
30	7	309	CHL	C1-C2-C3-C4
30	8	607	CHL	C1-C2-C3-C4
30	9	310	CHL	C1-C2-C3-C4
30	p	608	CHL	C1-C2-C3-C4
30	q	310	CHL	C1-C2-C3-C4
30	g	307	CHL	C1-C2-C3-C4
30	n	301	CHL	C1-C2-C3-C4
30	n	309	CHL	C1-C2-C3-C4
30	y	608	CHL	C1-C2-C3-C4
31	B	601	CLA	C1-C2-C3-C4
31	G	613	CLA	C1-C2-C3-C4
31	R	313	CLA	C1-C2-C3-C4
31	b	602	CLA	C1-C2-C3-C4
31	g	314	CLA	C1-C2-C3-C4
31	r	313	CLA	C1-C2-C3-C4
33	7	319	LHG	C9-C10-C11-C12
31	N	315	CLA	C3-C5-C6-C7
31	q	312	CLA	C3-C5-C6-C7
31	g	314	CLA	CAA-CBA-CGA-O2A
31	n	315	CLA	CAA-CBA-CGA-O2A
34	B	625	LMG	O7-C10-C11-C12
33	B	624	LHG	C30-C31-C32-C33
34	6	323	LMG	C9-C8-O7-C10
34	D	411	LMG	C9-C8-O7-C10
34	a	413	LMG	C7-C8-O7-C10
34	b	624	LMG	C7-C8-O7-C10
34	d	410	LMG	C9-C8-O7-C10
34	w	203	LMG	C9-C8-O7-C10
38	r	322	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
33	B	624	LHG	O6-C4-C5-C6
33	7	319	LHG	O6-C4-C5-C6
30	7	306	CHL	C2A-CAA-CBA-CGA
31	2	612	CLA	C2A-CAA-CBA-CGA
31	c	605	CLA	C2A-CAA-CBA-CGA
34	W	201	LMG	C11-C12-C13-C14
31	2	603	CLA	C2-C1-O2A-CGA
31	2	610	CLA	C2-C1-O2A-CGA
31	3	301	CLA	C2-C1-O2A-CGA
31	3	306	CLA	C2-C1-O2A-CGA
31	A	409	CLA	C2-C1-O2A-CGA
31	S	310	CLA	C2-C1-O2A-CGA
31	S	313	CLA	C2-C1-O2A-CGA
31	0	615	CLA	C2-C1-O2A-CGA
31	a	409	CLA	C2-C1-O2A-CGA
31	b	615	CLA	C2-C1-O2A-CGA
31	n	305	CLA	C2-C1-O2A-CGA
31	r	311	CLA	C2-C1-O2A-CGA
31	s	305	CLA	C2-C1-O2A-CGA
31	y	603	CLA	C2-C1-O2A-CGA
34	A	414	LMG	C29-C30-C31-C32
34	c	624	LMG	C31-C32-C33-C34
31	B	608	CLA	C16-C17-C18-C20
33	4	618	LHG	C9-C10-C11-C12
38	B	620	SQD	C14-C15-C16-C17
34	s	321	LMG	O7-C10-C11-C12
31	c	601	CLA	O1A-CGA-O2A-C1
30	6	307	CHL	O1D-CGD-O2D-CED
31	Y	310	CLA	C3-C5-C6-C7
31	b	613	CLA	C3-C5-C6-C7
33	a	415	LHG	C2-C3-O3-P
33	L	101	LHG	C14-C15-C16-C17
30	Y	302	CHL	CBA-CGA-O2A-C1
36	p	618	NEX	C13-C14-C15-C35
33	F1	301	LHG	O6-C4-C5-O7
31	B	605	CLA	C15-C16-C17-C18
31	8	603	CLA	C5-C6-C7-C8
31	R	311	CLA	C4-C3-C5-C6
31	b	604	CLA	C4-C3-C5-C6
34	9	301	LMG	C30-C31-C32-C33
34	b	623	LMG	C33-C34-C35-C36
31	d	404	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
32	1	615	LUT	C5-C6-C7-C8
43	T	101	BCR	C5-C6-C7-C8
31	G	612	CLA	C2-C3-C5-C6
33	D	408	LHG	C30-C31-C32-C33
34	b	626	LMG	C29-C30-C31-C32
33	7	319	LHG	C25-C26-C27-C28
45	C	617	DGD	C1A-C2A-C3A-C4A
31	B	607	CLA	CBA-CGA-O2A-C1
33	e	101	LHG	C10-C11-C12-C13
38	b	627	SQD	C13-C14-C15-C16
31	B	616	CLA	C13-C15-C16-C17
31	b	603	CLA	C13-C15-C16-C17
30	6	306	CHL	O1D-CGD-O2D-CED
31	3	304	CLA	C11-C12-C13-C15
31	N	303	CLA	C16-C17-C18-C20
31	6	305	CLA	C2A-CAA-CBA-CGA
31	B	607	CLA	C2A-CAA-CBA-CGA
31	7	314	CLA	C2A-CAA-CBA-CGA
36	R	301	NEX	C28-C29-C30-C31
36	n	319	NEX	C28-C29-C30-C31
36	y	618	NEX	C28-C29-C30-C31
45	c	618	DGD	C2D-C1D-O3G-C3G
33	S	322	LHG	O7-C5-C6-O8
34	2	618	LMG	O1-C7-C8-O7
34	J	101	LMG	O1-C7-C8-O7
34	W	201	LMG	O1-C7-C8-O7
34	n	322	LMG	O1-C7-C8-O7
38	S	301	SQD	O47-C45-C46-O48
38	Y	320	SQD	O6-C44-C45-O47
31	s	311	CLA	C5-C6-C7-C8
33	b	628	LHG	C24-C25-C26-C27
33	d	408	LHG	C29-C30-C31-C32
34	6	322	LMG	C31-C32-C33-C34
34	f	101	LMG	C31-C32-C33-C34
33	4	618	LHG	C3-O3-P-O6
33	6	320	LHG	C3-O3-P-O6
33	B	624	LHG	C4-O6-P-O3
33	C	623	LHG	C4-O6-P-O3
33	K	102	LHG	C4-O6-P-O3
33	S	320	LHG	C3-O3-P-O6
33	0	619	LHG	C3-O3-P-O6
33	7	319	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
33	8	618	LHG	C3-O3-P-O6
33	9	320	LHG	C4-O6-P-O3
33	d	408	LHG	C3-O3-P-O6
33	g	319	LHG	C3-O3-P-O6
33	n	320	LHG	C3-O3-P-O6
33	r	320	LHG	C3-O3-P-O6
33	s	320	LHG	C3-O3-P-O6
33	B	624	LHG	C26-C27-C28-C29
34	2	621	LMG	C30-C31-C32-C33
34	0	620	LMG	C32-C33-C34-C35
42	D	401	PHO	CHA-CBD-CGD-O1D
42	D	401	PHO	CHA-CBD-CGD-O2D
31	7	305	CLA	C15-C16-C17-C18
34	w	201	LMG	C29-C28-O8-C9
33	Y	318	LHG	C4-C5-C6-O8
33	q	320	LHG	C4-C5-C6-O8
34	W	201	LMG	O1-C7-C8-C9
34	7	301	LMG	C7-C8-C9-O8
34	y	620	LMG	O1-C7-C8-C9
38	G	624	SQD	C44-C45-C46-O48
45	C	620	DGD	C1G-C2G-C3G-O3G
31	7	313	CLA	C4-C3-C5-C6
44	a	414	PL9	C30-C29-C31-C32
33	t	102	LHG	C29-C30-C31-C32
34	6	321	LMG	C4-C5-C6-O5
30	3	302	CHL	C6-C7-C8-C10
30	4	601	CHL	C2-C3-C5-C6
30	7	306	CHL	C11-C10-C8-C7
30	7	321	CHL	C11-C12-C13-C15
30	n	308	CHL	C11-C12-C13-C15
31	6	303	CLA	C11-C12-C13-C15
31	A	406	CLA	C12-C13-C15-C16
31	R	311	CLA	C2-C3-C5-C6
31	S	311	CLA	C12-C13-C15-C16
31	0	602	CLA	C11-C10-C8-C7
31	7	314	CLA	C11-C12-C13-C15
31	b	611	CLA	C11-C10-C8-C7
31	s	313	CLA	C2-C3-C5-C6
31	y	612	CLA	C11-C10-C8-C7
42	a	408	PHO	C11-C10-C8-C7
31	4	610	CLA	CAA-CBA-CGA-O2A
38	r	322	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
30	1	601	CHL	C6-C7-C8-C9
30	4	601	CHL	C6-C7-C8-C9
30	q	309	CHL	C6-C7-C8-C9
31	1	611	CLA	C11-C10-C8-C9
31	2	609	CLA	C11-C10-C8-C9
31	6	311	CLA	C11-C12-C13-C14
31	B	614	CLA	C11-C12-C13-C14
31	B	615	CLA	C11-C12-C13-C14
31	G	609	CLA	C11-C12-C13-C14
31	N	313	CLA	C11-C10-C8-C9
31	S	303	CLA	C11-C10-C8-C9
31	S	312	CLA	C11-C10-C8-C9
31	Y	310	CLA	C11-C12-C13-C14
31	q	304	CLA	C11-C10-C8-C9
31	b	608	CLA	C11-C12-C13-C14
31	b	615	CLA	C11-C12-C13-C14
31	c	611	CLA	C11-C10-C8-C9
31	g	310	CLA	C11-C12-C13-C14
31	s	312	CLA	C11-C12-C13-C14
31	s	314	CLA	C14-C13-C15-C16
31	y	610	CLA	C11-C12-C13-C14
30	9	303	CHL	C10-C11-C12-C13
31	c	603	CLA	C5-C6-C7-C8
36	3	319	NEX	C13-C14-C15-C35
36	g	317	NEX	C9-C10-C11-C12
43	B	617	BCR	C9-C10-C11-C12
43	B	617	BCR	C13-C14-C15-C16
43	B	617	BCR	C19-C20-C21-C22
43	V	101	BCR	C9-C10-C11-C12
31	2	612	CLA	C16-C17-C18-C20
31	4	610	CLA	C11-C12-C13-C14
33	g	319	LHG	C31-C32-C33-C34
33	S	322	LHG	C25-C26-C27-C28
31	s	312	CLA	CBA-CGA-O2A-C1
33	D	408	LHG	C25-C26-C27-C28
31	5	611	CLA	CBD-CGD-O2D-CED
31	p	612	CLA	CAA-CBA-CGA-O2A
31	b	615	CLA	C15-C16-C17-C18
33	8	618	LHG	C17-C18-C19-C20
33	n	320	LHG	C17-C18-C19-C20
32	7	317	LUT	C27-C28-C29-C39
32	y	616	LUT	C7-C8-C9-C19

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Mol	Chain	Res	Type	Atoms
31	a	409	CLA	C11-C12-C13-C14
31	y	613	CLA	C16-C17-C18-C19
31	3	315	CLA	C5-C6-C7-C8
33	A	415	LHG	C11-C10-C9-C8
34	7	320	LMG	C33-C34-C35-C36
33	c	622	LHG	C24-C23-O8-C6
33	5	619	LHG	C2-C3-O3-P
33	5	619	LHG	C5-C4-O6-P
33	D	407	LHG	C2-C3-O3-P
33	s	322	LHG	C2-C3-O3-P
45	c	618	DGD	C1A-C2A-C3A-C4A
43	V	101	BCR	C7-C8-C9-C10
33	G	618	LHG	C31-C32-C33-C34
34	C	619	LMG	C32-C33-C34-C35
45	C	617	DGD	C3B-C4B-C5B-C6B
30	4	607	CHL	C11-C10-C8-C7
30	4	609	CHL	C11-C10-C8-C7
31	6	304	CLA	C11-C10-C8-C7
33	d	408	LHG	O9-C7-O7-C5
31	1	614	CLA	C4-C3-C5-C6
44	d	407	PL9	C16-C17-C18-C19
33	A	417	LHG	O1-C1-C2-O2
33	B	624	LHG	O1-C1-C2-O2
30	6	310	CHL	CBD-CGD-O2D-CED
31	6	315	CLA	C2-C3-C5-C6
31	Y	314	CLA	C5-C6-C7-C8
33	1	617	LHG	C27-C28-C29-C30
33	t	102	LHG	C24-C25-C26-C27
31	y	602	CLA	C11-C12-C13-C15
30	r	308	CHL	CBA-CGA-O2A-C1
31	c	601	CLA	CBA-CGA-O2A-C1
38	6	301	SQD	C24-C23-O48-C46
31	3	301	CLA	C2C-C3C-CAC-CBC
34	6	322	LMG	C8-C9-O8-C28
44	D	406	PL9	C2-C3-C7-C8
34	w	201	LMG	O10-C28-O8-C9
34	B	622	LMG	C29-C30-C31-C32
38	S	301	SQD	C30-C31-C32-C33
34	2	618	LMG	O9-C10-C11-C12
34	6	323	LMG	O9-C10-C11-C12
31	d	404	CLA	CAA-CBA-CGA-O2A
30	Y	301	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	S	313	CLA	O1A-CGA-O2A-C1
38	6	301	SQD	O10-C23-O48-C46
33	d	408	LHG	C10-C11-C12-C13
31	6	304	CLA	C2A-CAA-CBA-CGA
31	B	616	CLA	C2A-CAA-CBA-CGA
31	g	310	CLA	C2A-CAA-CBA-CGA
31	A	409	CLA	C11-C12-C13-C14
30	g	302	CHL	CAA-CBA-CGA-O1A
34	A	418	LMG	O6-C1-O1-C7
32	Y	316	LUT	C29-C30-C31-C32
36	R	301	NEX	C13-C14-C15-C35
36	8	617	NEX	C13-C14-C15-C35
43	H	101	BCR	C9-C10-C11-C12
43	b	618	BCR	C9-C10-C11-C12
43	c	615	BCR	C19-C20-C21-C22
34	S	321	LMG	C18-C19-C20-C21
45	c	617	DGD	C7B-C8B-C9B-CAB
31	s	312	CLA	O1A-CGA-O2A-C1
31	R	316	CLA	C8-C10-C11-C12
31	7	312	CLA	C10-C11-C12-C13
31	c	610	CLA	C5-C6-C7-C8
34	d	409	LMG	C11-C12-C13-C14
34	d	410	LMG	C21-C22-C23-C24
33	C	623	LHG	C34-C35-C36-C37
33	e	101	LHG	C12-C13-C14-C15
30	5	607	CHL	CBD-CGD-O2D-CED
33	l	101	LHG	C29-C30-C31-C32
33	y	619	LHG	C25-C26-C27-C28
33	z	102	LHG	C11-C10-C9-C8
34	C	619	LMG	C39-C40-C41-C42
34	D	411	LMG	C21-C22-C23-C24
47	E	101	HEM	C4B-C3B-CAB-CBB
47	e	102	HEM	C4B-C3B-CAB-CBB
31	4	613	CLA	C3-C5-C6-C7
31	y	615	CLA	C3-C5-C6-C7
31	R	311	CLA	C2C-C3C-CAC-CBC
34	w	201	LMG	C12-C13-C14-C15
38	m	101	SQD	C25-C26-C27-C28
31	N	315	CLA	C4-C3-C5-C6
31	6	314	CLA	C8-C10-C11-C12
31	C	611	CLA	C8-C10-C11-C12
30	R	308	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	1	614	CLA	C2-C3-C5-C6
33	1	617	LHG	C24-C25-C26-C27
33	L	101	LHG	C16-C17-C18-C19
34	7	322	LMG	C30-C31-C32-C33
34	k	102	LMG	C11-C12-C13-C14
45	c	617	DGD	CAB-CBB-CCB-CDB
31	S	314	CLA	C2-C1-O2A-CGA
31	p	603	CLA	C2-C1-O2A-CGA
31	b	608	CLA	C2-C1-O2A-CGA
31	b	617	CLA	C2-C1-O2A-CGA
31	c	605	CLA	C2-C1-O2A-CGA
31	c	606	CLA	C2-C1-O2A-CGA
31	s	303	CLA	C2-C1-O2A-CGA
31	y	611	CLA	C2-C1-O2A-CGA
31	2	602	CLA	C16-C17-C18-C20
34	5	620	LMG	C33-C34-C35-C36
31	q	313	CLA	C2C-C3C-CAC-CBC
31	7	314	CLA	C8-C10-C11-C12
30	3	308	CHL	C2A-CAA-CBA-CGA
30	7	310	CHL	C2A-CAA-CBA-CGA
31	A	406	CLA	C2A-CAA-CBA-CGA
31	G	604	CLA	C2A-CAA-CBA-CGA
31	N	303	CLA	C2A-CAA-CBA-CGA
31	7	303	CLA	C2A-CAA-CBA-CGA
31	b	607	CLA	C2A-CAA-CBA-CGA
34	c	620	LMG	O1-C7-C8-O7
38	b	621	SQD	O47-C45-C46-O48
47	E	101	HEM	C4D-C3D-CAD-CBD
31	3	306	CLA	C4C-C3C-CAC-CBC
34	C	624	LMG	C16-C17-C18-C19
33	B	624	LHG	C2-C3-O3-P
30	3	309	CHL	C3A-C2A-CAA-CBA
30	5	607	CHL	C3A-C2A-CAA-CBA
30	7	309	CHL	C3A-C2A-CAA-CBA
30	9	309	CHL	C3A-C2A-CAA-CBA
30	p	608	CHL	C3A-C2A-CAA-CBA
31	1	612	CLA	C3A-C2A-CAA-CBA
31	C	610	CLA	C3A-C2A-CAA-CBA
31	b	603	CLA	C3A-C2A-CAA-CBA
31	s	312	CLA	C16-C17-C18-C19
33	8	618	LHG	C35-C36-C37-C38
33	n	320	LHG	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
31	2	609	CLA	CAA-CBA-CGA-O2A
31	D	403	CLA	CAA-CBA-CGA-O2A
31	0	614	CLA	CAA-CBA-CGA-O2A
34	R	321	LMG	O7-C10-C11-C12
31	5	615	CLA	C4C-C3C-CAC-CBC
33	A	415	LHG	C35-C36-C37-C38
33	M	101	LHG	C32-C33-C34-C35
34	s	321	LMG	C11-C12-C13-C14
43	a	410	BCR	C13-C14-C15-C16
34	W	201	LMG	C42-C43-C44-C45
31	q	315	CLA	C4-C3-C5-C6
44	A	416	PL9	C40-C39-C41-C42
33	D	407	LHG	C28-C29-C30-C31
33	G	618	LHG	C25-C26-C27-C28
33	e	101	LHG	C34-C35-C36-C37
34	C	621	LMG	C12-C13-C14-C15
34	7	320	LMG	C29-C30-C31-C32
30	1	605	CHL	C14-C13-C15-C16
30	6	308	CHL	C11-C12-C13-C14
30	7	302	CHL	C14-C13-C15-C16
31	1	613	CLA	C11-C12-C13-C14
31	6	314	CLA	C11-C10-C8-C9
31	6	314	CLA	C14-C13-C15-C16
31	B	606	CLA	C11-C12-C13-C14
31	B	611	CLA	C11-C12-C13-C14
31	C	603	CLA	C14-C13-C15-C16
31	R	305	CLA	C6-C7-C8-C9
31	8	609	CLA	C11-C12-C13-C14
31	b	608	CLA	C6-C7-C8-C9
31	r	312	CLA	C6-C7-C8-C9
34	k	102	LMG	C30-C31-C32-C33
30	2	605	CHL	CAA-CBA-CGA-O2A
30	3	307	CHL	CAA-CBA-CGA-O2A
30	5	605	CHL	CAA-CBA-CGA-O2A
30	9	307	CHL	CAA-CBA-CGA-O2A
33	2	617	LHG	C31-C32-C33-C34
38	A	411	SQD	C26-C27-C28-C29
32	2	615	LUT	C39-C29-C30-C31
32	G	615	LUT	C40-C33-C34-C35
32	R	317	LUT	C39-C29-C30-C31
32	9	318	LUT	C40-C33-C34-C35
32	p	616	LUT	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
32	p	617	LUT	C39-C29-C30-C31
33	N	319	LHG	C4-C5-C6-O8
34	A	412	LMG	O1-C7-C8-C9
34	W	203	LMG	C7-C8-C9-O8
34	b	623	LMG	C7-C8-C9-O8
34	r	321	LMG	C7-C8-C9-O8
35	2	614	RRX	C16-C17-C18-C36
35	4	615	RRX	C16-C17-C18-C36
35	G	614	RRX	C16-C17-C18-C36
35	9	317	RRX	C16-C17-C18-C36
35	q	317	RRX	C16-C17-C18-C36
35	g	315	RRX	C16-C17-C18-C36
36	5	618	NEX	C39-C29-C30-C31
36	n	319	NEX	C39-C29-C30-C31
36	s	319	NEX	C39-C29-C30-C31
36	y	618	NEX	C39-C29-C30-C31
37	4	619	XAT	C40-C33-C34-C35
37	g	321	XAT	C40-C33-C34-C35
43	A	410	BCR	C16-C17-C18-C36
43	C	615	BCR	C11-C10-C9-C34
43	C	615	BCR	C16-C17-C18-C36
43	D	405	BCR	C11-C10-C9-C34
43	a	410	BCR	C20-C21-C22-C37
43	c	615	BCR	C16-C17-C18-C36
43	d	406	BCR	C11-C10-C9-C34
43	t	101	BCR	C16-C17-C18-C36
45	C	617	DGD	C1G-C2G-C3G-O3G
45	c	617	DGD	O1G-C1G-C2G-C3G
38	6	301	SQD	O49-C7-O47-C45
33	d	408	LHG	C25-C26-C27-C28
31	0	604	CLA	C2A-CAA-CBA-CGA
33	Y	318	LHG	C26-C27-C28-C29
34	c	620	LMG	O9-C10-C11-C12
34	g	320	LMG	O9-C10-C11-C12
33	0	619	LHG	C28-C29-C30-C31
34	9	301	LMG	C15-C16-C17-C18
31	2	609	CLA	C11-C12-C13-C15
31	3	304	CLA	C11-C12-C13-C14
31	B	607	CLA	C16-C17-C18-C20
31	S	312	CLA	C16-C17-C18-C19
31	y	604	CLA	C6-C7-C8-C9
42	d	402	PHO	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	r	304	CLA	CBA-CGA-O2A-C1
33	p	619	LHG	C9-C10-C11-C12
30	3	307	CHL	CAA-CBA-CGA-O1A
30	5	605	CHL	CAA-CBA-CGA-O1A
32	8	616	LUT	C11-C12-C13-C20
32	n	318	LUT	C11-C12-C13-C20
32	r	317	LUT	C7-C8-C9-C19
44	d	407	PL9	C2-C3-C7-C8
30	r	308	CHL	O1A-CGA-O2A-C1
34	d	411	LMG	C33-C34-C35-C36
38	B	620	SQD	C9-C10-C11-C12
45	c	616	DGD	C7A-C8A-C9A-CAA
47	e	102	HEM	C2D-C3D-CAD-CBD
30	3	310	CHL	C10-C11-C12-C13
31	y	614	CLA	CBD-CGD-O2D-CED
34	w	202	LMG	C14-C15-C16-C17
34	S	321	LMG	C10-C11-C12-C13
33	C	623	LHG	C29-C30-C31-C32
33	y	619	LHG	C31-C32-C33-C34
34	c	624	LMG	C15-C16-C17-C18
34	2	620	LMG	C7-C8-O7-C10
34	2	620	LMG	C9-C8-O7-C10
34	J	101	LMG	C9-C8-O7-C10
34	W	201	LMG	C9-C8-O7-C10
34	W	203	LMG	C7-C8-O7-C10
34	W	203	LMG	C9-C8-O7-C10
34	0	622	LMG	C7-C8-O7-C10
34	0	622	LMG	C9-C8-O7-C10
34	9	302	LMG	C9-C8-O7-C10
34	p	620	LMG	C7-C8-O7-C10
34	w	205	LMG	C7-C8-O7-C10
34	w	205	LMG	C9-C8-O7-C10
38	r	322	SQD	C44-C45-O47-C7
45	C	617	DGD	C3G-C2G-O2G-C1B
45	C	618	DGD	C1G-C2G-O2G-C1B
45	c	617	DGD	C1G-C2G-O2G-C1B
31	g	311	CLA	C5-C6-C7-C8
45	C	618	DGD	O6D-C5D-C6D-O5D
45	c	616	DGD	O6D-C5D-C6D-O5D
30	2	607	CHL	C1A-C2A-CAA-CBA
30	3	309	CHL	C1A-C2A-CAA-CBA
30	0	601	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	0	607	CHL	C1A-C2A-CAA-CBA
30	p	608	CHL	C1A-C2A-CAA-CBA
31	3	301	CLA	C1A-C2A-CAA-CBA
31	G	613	CLA	C1A-C2A-CAA-CBA
31	R	304	CLA	C1A-C2A-CAA-CBA
31	R	313	CLA	C1A-C2A-CAA-CBA
31	a	406	CLA	C1A-C2A-CAA-CBA
33	D	408	LHG	C35-C36-C37-C38
33	j	102	LHG	C10-C11-C12-C13
31	2	611	CLA	CAA-CBA-CGA-O2A
30	3	310	CHL	C6-C7-C8-C10
30	R	309	CHL	C2-C3-C5-C6
31	1	610	CLA	C12-C13-C15-C16
31	3	316	CLA	C6-C7-C8-C10
31	B	603	CLA	C11-C10-C8-C7
31	B	610	CLA	C11-C10-C8-C7
31	B	611	CLA	C11-C10-C8-C7
31	B	612	CLA	C11-C10-C8-C7
31	C	607	CLA	C11-C10-C8-C7
31	C	607	CLA	C12-C13-C15-C16
31	G	602	CLA	C11-C10-C8-C7
31	R	316	CLA	C11-C10-C8-C7
31	7	314	CLA	C11-C10-C8-C7
31	q	315	CLA	C11-C12-C13-C15
31	b	609	CLA	C12-C13-C15-C16
31	b	614	CLA	C6-C7-C8-C10
31	b	617	CLA	C11-C12-C13-C15
31	g	303	CLA	C12-C13-C15-C16
31	r	311	CLA	C2-C3-C5-C6
31	s	310	CLA	C6-C7-C8-C10
30	n	306	CHL	O1D-CGD-O2D-CED
31	N	305	CLA	C13-C15-C16-C17
31	D	404	CLA	C3-C5-C6-C7
31	7	303	CLA	C3-C5-C6-C7
30	q	309	CHL	O1A-CGA-O2A-C1
31	r	304	CLA	O1A-CGA-O2A-C1
30	9	307	CHL	CAA-CBA-CGA-O1A
33	0	619	LHG	C10-C11-C12-C13
33	d	408	LHG	C33-C34-C35-C36
38	6	301	SQD	O47-C7-C8-C9
38	a	411	SQD	C7-C8-C9-C10
31	R	305	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	R	311	CLA	C4C-C3C-CAC-CBC
45	C	620	DGD	C9B-CAB-CBB-CCB
30	7	321	CHL	C10-C11-C12-C13
34	G	619	LMG	O9-C10-C11-C12
31	y	610	CLA	C3-C5-C6-C7
30	6	310	CHL	O1D-CGD-O2D-CED
30	9	311	CHL	C2A-CAA-CBA-CGA
31	1	613	CLA	C2A-CAA-CBA-CGA
31	4	602	CLA	C2A-CAA-CBA-CGA
31	C	606	CLA	C2A-CAA-CBA-CGA
31	8	602	CLA	C2A-CAA-CBA-CGA
30	4	609	CHL	C5-C6-C7-C8
30	n	308	CHL	C10-C11-C12-C13
31	S	312	CLA	C8-C10-C11-C12
38	m	101	SQD	C7-C8-C9-C10
38	x	201	SQD	O47-C7-C8-C9
44	a	414	PL9	C3-C7-C8-C9
30	2	605	CHL	CAA-CBA-CGA-O1A
33	c	622	LHG	C31-C32-C33-C34
30	4	608	CHL	O2A-C1-C2-C3
30	7	310	CHL	C8-C10-C11-C12
31	S	313	CLA	CBA-CGA-O2A-C1
33	a	415	LHG	C11-C10-C9-C8
30	5	607	CHL	O1D-CGD-O2D-CED
38	S	301	SQD	C31-C32-C33-C34
45	c	618	DGD	O6D-C5D-C6D-O5D
38	6	301	SQD	C8-C7-O47-C45
30	4	607	CHL	C11-C10-C8-C9
34	s	321	LMG	C13-C14-C15-C16
30	R	310	CHL	C4-C3-C5-C6
31	q	305	CLA	C4-C3-C5-C6
33	j	102	LHG	C29-C30-C31-C32
34	q	301	LMG	C37-C38-C39-C40
34	a	413	LMG	C29-C30-C31-C32
45	c	618	DGD	C6A-C7A-C8A-C9A
31	a	407	CLA	C8-C10-C11-C12
31	7	313	CLA	C2-C3-C5-C6
31	9	306	CLA	C2-C3-C5-C6
31	q	315	CLA	C2-C3-C5-C6
33	2	617	LHG	C25-C26-C27-C28
31	D	404	CLA	C10-C11-C12-C13
30	8	605	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	l	101	LHG	C28-C29-C30-C31
34	5	620	LMG	C11-C12-C13-C14
38	Y	320	SQD	C13-C14-C15-C16
32	2	615	LUT	C28-C29-C30-C31
32	R	317	LUT	C28-C29-C30-C31
32	9	318	LUT	C32-C33-C34-C35
32	p	616	LUT	C28-C29-C30-C31
32	p	617	LUT	C28-C29-C30-C31
35	2	614	RRX	C16-C17-C18-C19
35	4	615	RRX	C16-C17-C18-C19
35	G	614	RRX	C16-C17-C18-C19
35	9	317	RRX	C16-C17-C18-C19
35	q	317	RRX	C16-C17-C18-C19
35	g	315	RRX	C16-C17-C18-C19
36	5	618	NEX	C28-C29-C30-C31
36	8	617	NEX	C28-C29-C30-C31
36	s	319	NEX	C28-C29-C30-C31
43	A	410	BCR	C16-C17-C18-C19
43	C	615	BCR	C11-C10-C9-C8
43	C	615	BCR	C16-C17-C18-C19
43	D	405	BCR	C11-C10-C9-C8
43	a	410	BCR	C20-C21-C22-C23
43	c	615	BCR	C16-C17-C18-C19
43	d	406	BCR	C11-C10-C9-C8
43	t	101	BCR	C16-C17-C18-C19
31	3	305	CLA	C5-C6-C7-C8
33	r	320	LHG	C24-C25-C26-C27
34	w	201	LMG	C16-C17-C18-C19
33	G	618	LHG	O7-C5-C6-O8
34	G	619	LMG	O1-C7-C8-O7
34	d	411	LMG	O7-C8-C9-O8
34	r	321	LMG	O7-C8-C9-O8
38	x	201	SQD	O47-C45-C46-O48
45	c	616	DGD	O2G-C2G-C3G-O3G
45	c	617	DGD	O1G-C1G-C2G-O2G
34	B	625	LMG	C10-C11-C12-C13
30	q	311	CHL	C2A-CAA-CBA-CGA
34	a	413	LMG	C34-C35-C36-C37
38	m	101	SQD	C13-C14-C15-C16
36	N	318	NEX	C33-C34-C35-C15
37	R	318	XAT	C13-C14-C15-C35
33	Y	318	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
33	q	320	LHG	C35-C36-C37-C38
38	A	413	SQD	C27-C28-C29-C30
31	B	608	CLA	C16-C17-C18-C19
31	0	614	CLA	C6-C7-C8-C9
33	K	102	LHG	C9-C10-C11-C12
33	b	625	LHG	C34-C35-C36-C37
33	d	408	LHG	C35-C36-C37-C38
34	5	620	LMG	C30-C31-C32-C33
34	b	629	LMG	C29-C30-C31-C32
31	p	602	CLA	C8-C10-C11-C12
34	J	101	LMG	C18-C19-C20-C21
31	6	303	CLA	C3-C5-C6-C7
30	G	608	CHL	C4-C3-C5-C6
30	8	605	CHL	C4-C3-C5-C6
31	Y	305	CLA	C2-C1-O2A-CGA
31	Y	312	CLA	C2-C1-O2A-CGA
31	p	610	CLA	C2-C1-O2A-CGA
31	B	607	CLA	O1A-CGA-O2A-C1
30	1	606	CHL	C8-C10-C11-C12
31	2	612	CLA	C8-C10-C11-C12
31	c	605	CLA	C10-C11-C12-C13
31	A	405	CLA	C14-C13-C15-C16
31	b	606	CLA	C11-C12-C13-C14
31	c	608	CLA	C11-C10-C8-C9
31	y	611	CLA	C11-C12-C13-C14
31	y	613	CLA	C6-C7-C8-C9
33	j	102	LHG	C35-C36-C37-C38
33	n	320	LHG	C16-C17-C18-C19
33	8	618	LHG	C16-C17-C18-C19
34	W	201	LMG	C40-C41-C42-C43
31	B	605	CLA	C8-C10-C11-C12
30	5	601	CHL	CAA-CBA-CGA-O1A
31	C	610	CLA	CAA-CBA-CGA-O2A
30	9	308	CHL	O1D-CGD-O2D-CED
33	C	623	LHG	C25-C26-C27-C28
33	G	618	LHG	C35-C36-C37-C38
31	b	605	CLA	C13-C15-C16-C17
31	c	602	CLA	C13-C15-C16-C17
47	E	101	HEM	C2D-C3D-CAD-CBD
31	C	605	CLA	C2A-CAA-CBA-CGA
31	0	613	CLA	C2A-CAA-CBA-CGA
31	q	304	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	b	604	CLA	C2A-CAA-CBA-CGA
31	5	602	CLA	C11-C12-C13-C15
31	N	303	CLA	C16-C17-C18-C19
31	y	612	CLA	C16-C17-C18-C20
32	p	616	LUT	C1-C6-C7-C8
43	B	618	BCR	C23-C24-C25-C30
43	B	619	BCR	C23-C24-C25-C26
43	h	101	BCR	C23-C24-C25-C30
34	d	410	LMG	C33-C34-C35-C36
31	1	612	CLA	CAA-CBA-CGA-O2A
33	F1	301	LHG	O7-C7-C8-C9
33	D	408	LHG	C14-C15-C16-C17
33	q	320	LHG	C9-C10-C11-C12
34	3	321	LMG	C7-C8-C9-O8
34	6	323	LMG	O1-C7-C8-C9
34	C	622	LMG	O1-C7-C8-C9
34	D	411	LMG	C33-C34-C35-C36
34	c	620	LMG	O1-C7-C8-C9
34	w	204	LMG	O1-C7-C8-C9
31	q	313	CLA	CAA-CBA-CGA-O2A
33	D	407	LHG	C27-C28-C29-C30
33	N	319	LHG	C35-C36-C37-C38
32	1	616	LUT	C29-C30-C31-C32
36	6	319	NEX	C13-C14-C15-C35
36	0	618	NEX	C13-C14-C15-C35
36	p	618	NEX	C29-C30-C31-C32
43	B	617	BCR	C15-C16-C17-C18
34	G	621	LMG	C11-C12-C13-C14
30	n	306	CHL	C4-C3-C5-C6
31	2	609	CLA	C4-C3-C5-C6
31	9	306	CLA	C4-C3-C5-C6
31	c	602	CLA	C4-C3-C5-C6
31	s	312	CLA	C4-C3-C5-C6
43	a	410	BCR	C17-C18-C19-C20
31	R	305	CLA	C5-C6-C7-C8
31	d	404	CLA	C13-C15-C16-C17
48	R	302	LMU	C2B-C1B-O1B-C4'
33	N	319	LHG	C10-C11-C12-C13
33	l	101	LHG	C33-C34-C35-C36
31	1	610	CLA	C2-C3-C5-C6
31	1	613	CLA	C2-C3-C5-C6
44	D	406	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
31	N	312	CLA	CAA-CBA-CGA-O2A
38	M	102	SQD	C45-C44-O6-C1
33	8	618	LHG	C14-C15-C16-C17
34	a	416	LMG	C8-C9-O8-C28
33	n	320	LHG	C14-C15-C16-C17
34	9	321	LMG	C13-C14-C15-C16
30	4	601	CHL	C10-C11-C12-C13
33	c	622	LHG	O10-C23-O8-C6
33	R	320	LHG	O10-C23-C24-C25
33	R	320	LHG	C10-C11-C12-C13
38	S	301	SQD	C12-C13-C14-C15
30	6	310	CHL	C11-C12-C13-C15
30	Y	302	CHL	C16-C17-C18-C20
45	c	618	DGD	C9A-CAA-CBA-CCA
31	4	613	CLA	C5-C6-C7-C8
31	B	603	CLA	C5-C6-C7-C8
31	B	610	CLA	C15-C16-C17-C18
31	p	610	CLA	C11-C10-C8-C9
34	D	409	LMG	C10-C11-C12-C13
33	s	322	LHG	C32-C33-C34-C35
34	0	622	LMG	C32-C33-C34-C35
31	c	612	CLA	C2A-CAA-CBA-CGA
34	1	618	LMG	C13-C14-C15-C16
30	9	308	CHL	CBD-CGD-O2D-CED
33	a	415	LHG	C24-C23-O8-C6
33	c	622	LHG	C16-C17-C18-C19
34	B	621	LMG	C10-C11-C12-C13
33	e	101	LHG	O9-C7-O7-C5
38	B	623	SQD	C13-C14-C15-C16
38	a	412	SQD	C24-C25-C26-C27
33	R	320	LHG	C12-C13-C14-C15
30	0	607	CHL	C13-C15-C16-C17
31	9	312	CLA	CAA-CBA-CGA-O2A
34	n	321	LMG	O7-C10-C11-C12
30	6	310	CHL	C4-C3-C5-C6
30	Y	309	CHL	C4-C3-C5-C6
30	p	609	CHL	C4-C3-C5-C6
34	c	620	LMG	C34-C35-C36-C37
34	k	102	LMG	C12-C13-C14-C15
34	s	321	LMG	C21-C22-C23-C24
30	1	606	CHL	C2-C3-C5-C6
30	2	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	2	612	CLA	C11-C12-C13-C15
31	A	405	CLA	C12-C13-C15-C16
31	Y	303	CLA	C11-C10-C8-C7
31	8	604	CLA	C11-C10-C8-C7
31	b	604	CLA	C2-C3-C5-C6
31	b	612	CLA	C11-C10-C8-C7
31	b	613	CLA	C11-C10-C8-C7
31	b	613	CLA	C12-C13-C15-C16
31	c	602	CLA	C6-C7-C8-C10
31	n	305	CLA	C11-C10-C8-C7
31	y	613	CLA	C6-C7-C8-C10
42	D	401	PHO	C6-C7-C8-C10
30	7	321	CHL	C5-C6-C7-C8
30	n	308	CHL	C5-C6-C7-C8
31	b	608	CLA	C5-C6-C7-C8
33	e	101	LHG	C30-C31-C32-C33
33	s	320	LHG	O1-C1-C2-O2
33	7	319	LHG	C11-C10-C9-C8
34	w	201	LMG	C36-C37-C38-C39
38	s	301	SQD	C14-C15-C16-C17
48	K	101	LMU	C9-C10-C11-C12
31	b	609	CLA	C8-C10-C11-C12
31	c	605	CLA	C13-C15-C16-C17
31	6	304	CLA	CAA-CBA-CGA-O1A
34	5	620	LMG	O9-C10-C11-C12
34	6	323	LMG	C2-C1-O1-C7
33	l	101	LHG	C5-C4-O6-P
38	X	201	SQD	O47-C45-C46-O48
38	g	301	SQD	O47-C45-C46-O48
31	2	613	CLA	CAA-CBA-CGA-O1A
31	3	313	CLA	CAA-CBA-CGA-O1A
30	7	308	CHL	CBD-CGD-O2D-CED
31	4	610	CLA	C5-C6-C7-C8
31	r	312	CLA	C3-C5-C6-C7
34	7	322	LMG	O7-C10-C11-C12
30	7	308	CHL	O1D-CGD-O2D-CED
31	1	612	CLA	C10-C11-C12-C13
31	a	407	CLA	C5-C6-C7-C8
31	g	310	CLA	C15-C16-C17-C18
33	b	625	LHG	C35-C36-C37-C38
31	R	305	CLA	CBA-CGA-O2A-C1
36	G	616	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
36	S	319	NEX	C39-C29-C30-C31
36	Y	317	NEX	C39-C29-C30-C31
36	8	617	NEX	C39-C29-C30-C31
36	9	319	NEX	C20-C13-C14-C15
36	9	319	NEX	C39-C29-C30-C31
37	2	619	XAT	C40-C33-C34-C35
37	G	620	XAT	C40-C33-C34-C35
37	9	322	XAT	C40-C33-C34-C35
37	q	321	XAT	C40-C33-C34-C35
45	c	616	DGD	C4A-C5A-C6A-C7A
34	D	410	LMG	C8-C9-O8-C28
30	1	606	CHL	C4-C3-C5-C6
30	y	607	CHL	C4-C3-C5-C6
30	y	609	CHL	C4-C3-C5-C6
31	S	312	CLA	C4-C3-C5-C6
31	c	612	CLA	C4-C3-C5-C6
31	y	612	CLA	C4-C3-C5-C6
30	Y	301	CHL	C8-C10-C11-C12
31	1	602	CLA	C10-C11-C12-C13
31	6	312	CLA	C8-C10-C11-C12
31	N	303	CLA	C8-C10-C11-C12
31	6	316	CLA	C2C-C3C-CAC-CBC
34	A	414	LMG	C11-C12-C13-C14
34	J	101	LMG	C30-C31-C32-C33
34	d	409	LMG	C16-C17-C18-C19
34	j	101	LMG	C29-C30-C31-C32
48	R	302	LMU	C4-C5-C6-C7
30	R	310	CHL	C2-C3-C5-C6
31	4	614	CLA	C2-C3-C5-C6
31	C	613	CLA	C2-C3-C5-C6
31	9	304	CLA	C2-C3-C5-C6
31	s	312	CLA	C2-C3-C5-C6
34	b	626	LMG	C30-C31-C32-C33
31	0	603	CLA	C11-C10-C8-C7
31	p	610	CLA	C11-C10-C8-C7
30	N	307	CHL	C11-C10-C8-C9
30	7	306	CHL	C14-C13-C15-C16
30	g	309	CHL	C11-C10-C8-C9
31	4	613	CLA	C6-C7-C8-C9
31	5	602	CLA	C11-C10-C8-C9
31	5	610	CLA	C11-C10-C8-C9
31	5	611	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	6	313	CLA	C11-C10-C8-C9
31	A	409	CLA	C11-C10-C8-C9
31	B	606	CLA	C6-C7-C8-C9
31	B	612	CLA	C11-C10-C8-C9
31	C	601	CLA	C11-C10-C8-C9
31	C	605	CLA	C6-C7-C8-C9
31	C	606	CLA	C6-C7-C8-C9
31	C	607	CLA	C11-C10-C8-C9
31	G	602	CLA	C11-C10-C8-C9
31	G	602	CLA	C11-C12-C13-C14
31	G	602	CLA	C14-C13-C15-C16
31	S	311	CLA	C11-C10-C8-C9
31	a	409	CLA	C11-C10-C8-C9
31	c	607	CLA	C11-C10-C8-C9
31	c	611	CLA	C14-C13-C15-C16
31	d	404	CLA	C11-C10-C8-C9
31	n	311	CLA	C11-C12-C13-C14
31	s	303	CLA	C11-C10-C8-C9
31	y	602	CLA	C11-C10-C8-C9
42	A	408	PHO	C6-C7-C8-C9
42	A	408	PHO	C14-C13-C15-C16
42	a	408	PHO	C14-C13-C15-C16
34	g	322	LMG	C34-C35-C36-C37
38	B	620	SQD	C27-C28-C29-C30
33	0	619	LHG	C25-C26-C27-C28
30	0	601	CHL	C3A-C2A-CAA-CBA
31	4	614	CLA	C3A-C2A-CAA-CBA
31	5	612	CLA	C3A-C2A-CAA-CBA
31	N	305	CLA	C3A-C2A-CAA-CBA
31	8	612	CLA	C3A-C2A-CAA-CBA
31	a	406	CLA	C3A-C2A-CAA-CBA
31	n	305	CLA	C3A-C2A-CAA-CBA
31	n	314	CLA	C3A-C2A-CAA-CBA
38	M	102	SQD	C17-C18-C19-C20
33	d	408	LHG	O7-C7-C8-C9
34	N	320	LMG	O7-C10-C11-C12
34	9	321	LMG	O8-C28-C29-C30
34	x	202	LMG	O8-C28-C29-C30
38	M	102	SQD	O47-C7-C8-C9
38	x	201	SQD	O48-C23-C24-C25
34	j	101	LMG	C18-C19-C20-C21
38	M	102	SQD	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
30	1	605	CHL	CAD-CBD-CGD-O2D
30	1	607	CHL	CAD-CBD-CGD-O2D
30	2	601	CHL	CAD-CBD-CGD-O2D
30	2	607	CHL	CAD-CBD-CGD-O2D
30	3	303	CHL	CAD-CBD-CGD-O2D
30	5	608	CHL	CAD-CBD-CGD-O2D
30	6	302	CHL	CAD-CBD-CGD-O2D
30	6	308	CHL	CAD-CBD-CGD-O2D
30	6	310	CHL	CAD-CBD-CGD-O2D
30	G	605	CHL	CAD-CBD-CGD-O2D
30	G	607	CHL	CAD-CBD-CGD-O2D
30	G	623	CHL	CAD-CBD-CGD-O2D
30	N	301	CHL	CAD-CBD-CGD-O2D
30	N	302	CHL	CAD-CBD-CGD-O2D
30	N	307	CHL	CAD-CBD-CGD-O2D
30	S	308	CHL	CAD-CBD-CGD-O2D
30	Y	302	CHL	CAD-CBD-CGD-O2D
30	Y	307	CHL	CAD-CBD-CGD-O2D
30	0	607	CHL	CAD-CBD-CGD-O2D
30	0	609	CHL	CAD-CBD-CGD-O2D
30	7	307	CHL	CAD-CBD-CGD-O2D
30	8	606	CHL	CAD-CBD-CGD-O2D
30	9	308	CHL	CAD-CBD-CGD-O2D
30	9	309	CHL	CAD-CBD-CGD-O2D
30	p	608	CHL	CAD-CBD-CGD-O2D
30	g	306	CHL	CAD-CBD-CGD-O2D
30	n	301	CHL	CAD-CBD-CGD-O2D
30	n	307	CHL	CAD-CBD-CGD-O2D
30	r	308	CHL	CAD-CBD-CGD-O2D
30	y	606	CHL	CAD-CBD-CGD-O2D
31	1	603	CLA	CAD-CBD-CGD-O2D
31	4	614	CLA	CAD-CBD-CGD-O2D
31	B	604	CLA	CAD-CBD-CGD-O2D
31	B	614	CLA	CAD-CBD-CGD-O2D
31	C	606	CLA	CAD-CBD-CGD-O2D
31	R	305	CLA	CAD-CBD-CGD-O2D
31	R	307	CLA	CAD-CBD-CGD-O2D
31	0	604	CLA	CAD-CBD-CGD-O2D
31	b	615	CLA	CAD-CBD-CGD-O2D
31	b	617	CLA	CAD-CBD-CGD-O2D
31	s	315	CLA	CAD-CBD-CGD-O2D
34	g	322	LMG	C9-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
42	a	408	PHO	CAD-CBD-CGD-O2D
34	b	622	LMG	C39-C40-C41-C42
31	S	314	CLA	C15-C16-C17-C18
31	b	608	CLA	C8-C10-C11-C12
34	w	202	LMG	C21-C22-C23-C24
31	1	613	CLA	C2-C1-O2A-CGA
31	G	604	CLA	C2-C1-O2A-CGA
33	c	622	LHG	C25-C26-C27-C28
34	6	321	LMG	C10-C11-C12-C13
33	S	320	LHG	O7-C7-C8-C9
34	D	410	LMG	O8-C28-C29-C30
38	6	301	SQD	O48-C23-C24-C25
38	B	623	SQD	C31-C32-C33-C34
38	X	201	SQD	C10-C11-C12-C13
33	B	624	LHG	C11-C10-C9-C8
33	b	628	LHG	C14-C15-C16-C17
34	6	321	LMG	C14-C15-C16-C17
34	C	621	LMG	C32-C33-C34-C35
30	4	607	CHL	C4-C3-C5-C6
30	7	321	CHL	C4-C3-C5-C6
30	n	308	CHL	C4-C3-C5-C6
31	B	606	CLA	C4-C3-C5-C6
31	C	609	CLA	C4-C3-C5-C6
31	C	611	CLA	C4-C3-C5-C6
31	r	311	CLA	C4-C3-C5-C6
31	8	611	CLA	CAA-CBA-CGA-O2A
31	n	313	CLA	CAA-CBA-CGA-O2A
31	s	313	CLA	C4C-C3C-CAC-CBC
42	D	401	PHO	C8-C10-C11-C12
30	4	607	CHL	C2-C3-C5-C6
31	C	611	CLA	C2-C3-C5-C6
31	q	305	CLA	C2-C3-C5-C6
31	C	603	CLA	CAA-CBA-CGA-O2A
31	G	612	CLA	CAA-CBA-CGA-O2A
31	7	314	CLA	CAA-CBA-CGA-O2A
33	2	617	LHG	O8-C23-C24-C25
33	4	618	LHG	O8-C23-C24-C25
33	p	619	LHG	O8-C23-C24-C25
34	7	301	LMG	O7-C10-C11-C12
34	r	321	LMG	O7-C10-C11-C12
33	a	415	LHG	O10-C23-O8-C6
32	7	317	LUT	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
32	8	616	LUT	C11-C12-C13-C14
32	n	318	LUT	C11-C12-C13-C14
32	r	317	LUT	C7-C8-C9-C10
32	y	616	LUT	C7-C8-C9-C10
36	2	616	NEX	C11-C12-C13-C14
43	H	101	BCR	C17-C18-C19-C20
43	h	101	BCR	C17-C18-C19-C20
34	W	201	LMG	C7-C8-C9-O8
36	5	618	NEX	O24-C26-C27-C28
36	q	319	NEX	O24-C26-C27-C28
38	G	617	SQD	O6-C44-C45-C46
45	c	618	DGD	C1G-C2G-C3G-O3G
45	c	619	DGD	O1A-C1A-C2A-C3A
31	7	311	CLA	CBA-CGA-O2A-C1
33	Y	318	LHG	O9-C7-O7-C5
30	2	601	CHL	O1A-CGA-O2A-C1
30	2	601	CHL	C5-C6-C7-C8
31	C	605	CLA	CAA-CBA-CGA-O2A
31	S	314	CLA	CAA-CBA-CGA-O2A
31	Y	313	CLA	CAA-CBA-CGA-O2A
31	0	613	CLA	CAA-CBA-CGA-O2A
31	a	406	CLA	CAA-CBA-CGA-O2A
33	3	320	LHG	O8-C23-C24-C25
33	8	618	LHG	C19-C20-C21-C22
33	n	320	LHG	C19-C20-C21-C22
34	6	323	LMG	C34-C35-C36-C37
31	N	312	CLA	CAA-CBA-CGA-O1A
31	q	313	CLA	CAA-CBA-CGA-O1A
30	1	601	CHL	O2A-C1-C2-C3
30	2	606	CHL	O2A-C1-C2-C3
30	4	606	CHL	O2A-C1-C2-C3
30	5	606	CHL	O2A-C1-C2-C3
30	G	607	CHL	O2A-C1-C2-C3
30	G	623	CHL	O2A-C1-C2-C3
30	N	306	CHL	O2A-C1-C2-C3
30	8	605	CHL	O2A-C1-C2-C3
30	p	606	CHL	O2A-C1-C2-C3
30	q	308	CHL	O2A-C1-C2-C3
30	g	308	CHL	O2A-C1-C2-C3
30	n	306	CHL	O2A-C1-C2-C3
30	y	607	CHL	O2A-C1-C2-C3
31	2	610	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	8	603	CLA	O2A-C1-C2-C3
31	n	304	CLA	O2A-C1-C2-C3
42	D	401	PHO	O2A-C1-C2-C3
33	b	625	LHG	C33-C34-C35-C36
34	4	621	LMG	C13-C14-C15-C16
31	n	303	CLA	C2A-CAA-CBA-CGA
31	s	305	CLA	C2A-CAA-CBA-CGA
30	1	605	CHL	C5-C6-C7-C8
31	b	603	CLA	C10-C11-C12-C13
45	C	618	DGD	C2B-C3B-C4B-C5B
31	6	316	CLA	CAA-CBA-CGA-O2A
31	7	312	CLA	CAA-CBA-CGA-O2A
33	S	320	LHG	O8-C23-C24-C25
33	0	619	LHG	O8-C23-C24-C25
33	1	101	LHG	O8-C23-C24-C25
34	C	622	LMG	O7-C10-C11-C12
34	W	202	LMG	O9-C10-C11-C12
33	S	322	LHG	O9-C7-O7-C5
38	A	411	SQD	C33-C34-C35-C36
31	7	311	CLA	O1A-CGA-O2A-C1
30	1	606	CHL	CHA-CBD-CGD-O1D
30	1	606	CHL	CHA-CBD-CGD-O2D
30	3	307	CHL	CHA-CBD-CGD-O1D
30	3	307	CHL	CHA-CBD-CGD-O2D
30	4	601	CHL	CHA-CBD-CGD-O2D
30	5	601	CHL	CHA-CBD-CGD-O2D
30	0	601	CHL	CHA-CBD-CGD-O2D
30	7	306	CHL	CHA-CBD-CGD-O1D
30	7	306	CHL	CHA-CBD-CGD-O2D
30	8	601	CHL	CHA-CBD-CGD-O2D
30	9	303	CHL	CHA-CBD-CGD-O2D
30	p	607	CHL	CHA-CBD-CGD-O1D
30	p	607	CHL	CHA-CBD-CGD-O2D
30	q	303	CHL	CHA-CBD-CGD-O2D
30	q	309	CHL	CHA-CBD-CGD-O1D
30	q	309	CHL	CHA-CBD-CGD-O2D
30	n	302	CHL	CHA-CBD-CGD-O2D
30	y	601	CHL	CHA-CBD-CGD-O2D
31	1	610	CLA	CHA-CBD-CGD-O2D
31	1	612	CLA	CHA-CBD-CGD-O1D
31	1	612	CLA	CHA-CBD-CGD-O2D
31	1	614	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	1	614	CLA	CHA-CBD-CGD-O2D
31	2	603	CLA	CHA-CBD-CGD-O1D
31	2	603	CLA	CHA-CBD-CGD-O2D
31	2	610	CLA	CHA-CBD-CGD-O1D
31	2	610	CLA	CHA-CBD-CGD-O2D
31	3	304	CLA	CHA-CBD-CGD-O1D
31	3	304	CLA	CHA-CBD-CGD-O2D
31	3	305	CLA	CHA-CBD-CGD-O1D
31	3	305	CLA	CHA-CBD-CGD-O2D
31	3	306	CLA	CHA-CBD-CGD-O1D
31	3	306	CLA	CHA-CBD-CGD-O2D
31	4	602	CLA	CHA-CBD-CGD-O1D
31	4	604	CLA	CHA-CBD-CGD-O1D
31	4	604	CLA	CHA-CBD-CGD-O2D
31	4	613	CLA	CHA-CBD-CGD-O1D
31	4	613	CLA	CHA-CBD-CGD-O2D
31	5	602	CLA	CHA-CBD-CGD-O1D
31	5	602	CLA	CHA-CBD-CGD-O2D
31	5	613	CLA	CHA-CBD-CGD-O1D
31	5	613	CLA	CHA-CBD-CGD-O2D
31	6	303	CLA	CHA-CBD-CGD-O1D
31	6	303	CLA	CHA-CBD-CGD-O2D
31	6	311	CLA	CHA-CBD-CGD-O1D
31	6	311	CLA	CHA-CBD-CGD-O2D
31	6	315	CLA	CHA-CBD-CGD-O1D
31	6	315	CLA	CHA-CBD-CGD-O2D
31	B	608	CLA	CHA-CBD-CGD-O1D
31	B	608	CLA	CHA-CBD-CGD-O2D
31	B	610	CLA	CHA-CBD-CGD-O1D
31	C	603	CLA	CHA-CBD-CGD-O1D
31	C	611	CLA	CHA-CBD-CGD-O1D
31	C	611	CLA	CHA-CBD-CGD-O2D
31	G	610	CLA	CHA-CBD-CGD-O2D
31	G	612	CLA	CHA-CBD-CGD-O1D
31	G	612	CLA	CHA-CBD-CGD-O2D
31	N	304	CLA	CHA-CBD-CGD-O2D
31	N	312	CLA	CHA-CBD-CGD-O1D
31	N	312	CLA	CHA-CBD-CGD-O2D
31	N	313	CLA	CHA-CBD-CGD-O2D
31	N	314	CLA	CHA-CBD-CGD-O1D
31	N	314	CLA	CHA-CBD-CGD-O2D
31	R	311	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	R	311	CLA	CHA-CBD-CGD-O2D
31	S	303	CLA	CHA-CBD-CGD-O1D
31	S	303	CLA	CHA-CBD-CGD-O2D
31	S	305	CLA	CHA-CBD-CGD-O2D
31	Y	310	CLA	CHA-CBD-CGD-O1D
31	Y	310	CLA	CHA-CBD-CGD-O2D
31	Y	313	CLA	CHA-CBD-CGD-O1D
31	Y	313	CLA	CHA-CBD-CGD-O2D
31	Y	314	CLA	CHA-CBD-CGD-O1D
31	Y	314	CLA	CHA-CBD-CGD-O2D
31	0	602	CLA	CHA-CBD-CGD-O1D
31	0	602	CLA	CHA-CBD-CGD-O2D
31	0	612	CLA	CHA-CBD-CGD-O1D
31	0	612	CLA	CHA-CBD-CGD-O2D
31	0	614	CLA	CHA-CBD-CGD-O1D
31	0	614	CLA	CHA-CBD-CGD-O2D
31	0	615	CLA	CHA-CBD-CGD-O1D
31	7	311	CLA	CHA-CBD-CGD-O1D
31	7	311	CLA	CHA-CBD-CGD-O2D
31	7	312	CLA	CHA-CBD-CGD-O1D
31	7	312	CLA	CHA-CBD-CGD-O2D
31	7	314	CLA	CHA-CBD-CGD-O1D
31	7	314	CLA	CHA-CBD-CGD-O2D
31	8	603	CLA	CHA-CBD-CGD-O1D
31	8	603	CLA	CHA-CBD-CGD-O2D
31	8	610	CLA	CHA-CBD-CGD-O2D
31	8	612	CLA	CHA-CBD-CGD-O2D
31	9	315	CLA	CHA-CBD-CGD-O1D
31	9	315	CLA	CHA-CBD-CGD-O2D
31	9	316	CLA	CHA-CBD-CGD-O1D
31	9	316	CLA	CHA-CBD-CGD-O2D
31	p	602	CLA	CHA-CBD-CGD-O1D
31	p	603	CLA	CHA-CBD-CGD-O1D
31	p	604	CLA	CHA-CBD-CGD-O1D
31	p	604	CLA	CHA-CBD-CGD-O2D
31	p	614	CLA	CHA-CBD-CGD-O1D
31	p	614	CLA	CHA-CBD-CGD-O2D
31	q	306	CLA	CHA-CBD-CGD-O1D
31	q	306	CLA	CHA-CBD-CGD-O2D
31	q	314	CLA	CHA-CBD-CGD-O1D
31	q	314	CLA	CHA-CBD-CGD-O2D
31	q	315	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	q	315	CLA	CHA-CBD-CGD-O2D
31	b	603	CLA	CHA-CBD-CGD-O1D
31	b	603	CLA	CHA-CBD-CGD-O2D
31	b	606	CLA	CHA-CBD-CGD-O1D
31	b	609	CLA	CHA-CBD-CGD-O1D
31	b	609	CLA	CHA-CBD-CGD-O2D
31	b	613	CLA	CHA-CBD-CGD-O1D
31	b	613	CLA	CHA-CBD-CGD-O2D
31	c	601	CLA	CHA-CBD-CGD-O1D
31	c	601	CLA	CHA-CBD-CGD-O2D
31	c	611	CLA	CHA-CBD-CGD-O1D
31	c	611	CLA	CHA-CBD-CGD-O2D
31	c	612	CLA	CHA-CBD-CGD-O1D
31	g	303	CLA	CHA-CBD-CGD-O2D
31	g	304	CLA	CHA-CBD-CGD-O1D
31	g	304	CLA	CHA-CBD-CGD-O2D
31	g	305	CLA	CHA-CBD-CGD-O1D
31	g	305	CLA	CHA-CBD-CGD-O2D
31	g	310	CLA	CHA-CBD-CGD-O1D
31	g	310	CLA	CHA-CBD-CGD-O2D
31	g	311	CLA	CHA-CBD-CGD-O1D
31	g	311	CLA	CHA-CBD-CGD-O2D
31	n	304	CLA	CHA-CBD-CGD-O1D
31	n	304	CLA	CHA-CBD-CGD-O2D
31	n	312	CLA	CHA-CBD-CGD-O2D
31	n	314	CLA	CHA-CBD-CGD-O2D
31	n	316	CLA	CHA-CBD-CGD-O2D
31	r	304	CLA	CHA-CBD-CGD-O1D
31	r	304	CLA	CHA-CBD-CGD-O2D
31	r	311	CLA	CHA-CBD-CGD-O1D
31	r	311	CLA	CHA-CBD-CGD-O2D
31	s	303	CLA	CHA-CBD-CGD-O2D
31	s	314	CLA	CHA-CBD-CGD-O1D
31	s	314	CLA	CHA-CBD-CGD-O2D
31	y	602	CLA	CHA-CBD-CGD-O1D
31	y	602	CLA	CHA-CBD-CGD-O2D
31	y	610	CLA	CHA-CBD-CGD-O2D
31	y	614	CLA	CHA-CBD-CGD-O1D
31	y	614	CLA	CHA-CBD-CGD-O2D
36	3	319	NEX	C9-C10-C11-C12
31	3	315	CLA	CAA-CBA-CGA-O2A
31	S	316	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	p	614	CLA	CAA-CBA-CGA-O2A
31	y	613	CLA	CAA-CBA-CGA-O2A
34	0	622	LMG	O7-C10-C11-C12
44	a	414	PL9	C17-C18-C19-C21
31	B	606	CLA	C2-C3-C5-C6
31	S	312	CLA	C2-C3-C5-C6
44	a	414	PL9	C38-C39-C41-C42
33	d	408	LHG	C8-C7-O7-C5
33	e	101	LHG	C8-C7-O7-C5
33	Y	318	LHG	O6-C4-C5-C6
36	G	616	NEX	C28-C29-C30-C31
36	S	319	NEX	C28-C29-C30-C31
36	Y	317	NEX	C28-C29-C30-C31
36	9	319	NEX	C28-C29-C30-C31
38	R	322	SQD	C29-C30-C31-C32
31	B	612	CLA	C10-C11-C12-C13
31	S	311	CLA	C5-C6-C7-C8
30	p	607	CHL	CAA-CBA-CGA-O2A
31	4	613	CLA	CAA-CBA-CGA-O2A
31	5	613	CLA	CAA-CBA-CGA-O2A
31	S	303	CLA	CAA-CBA-CGA-O2A
31	0	615	CLA	CAA-CBA-CGA-O2A
33	L	101	LHG	O7-C7-C8-C9
33	a	415	LHG	O8-C23-C24-C25
33	F1	301	LHG	O8-C23-C24-C25
34	b	601	LMG	O7-C10-C11-C12
34	k	101	LMG	O7-C10-C11-C12
38	S	301	SQD	O47-C7-C8-C9
34	g	322	LMG	C30-C31-C32-C33
34	2	618	LMG	O7-C8-C9-O8
34	2	621	LMG	O7-C8-C9-O8
34	3	321	LMG	O7-C8-C9-O8
45	C	618	DGD	O2G-C2G-C3G-O3G
30	2	601	CHL	CBA-CGA-O2A-C1
30	9	311	CHL	C8-C10-C11-C12
31	C	608	CLA	C13-C15-C16-C17
31	7	311	CLA	C13-C15-C16-C17
30	6	306	CHL	CAA-CBA-CGA-O1A
33	j	102	LHG	C33-C34-C35-C36
30	N	306	CHL	CAA-CBA-CGA-O2A
30	8	605	CHL	CAA-CBA-CGA-O2A
30	n	306	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	1	613	CLA	CAA-CBA-CGA-O2A
31	b	609	CLA	CAA-CBA-CGA-O2A
33	3	320	LHG	O7-C7-C8-C9
33	6	320	LHG	O7-C7-C8-C9
33	y	619	LHG	O8-C23-C24-C25
34	I	101	LMG	O7-C10-C11-C12
34	I	101	LMG	O8-C28-C29-C30
34	9	302	LMG	O7-C10-C11-C12
34	j	101	LMG	O7-C10-C11-C12
38	G	624	SQD	O47-C7-C8-C9
38	m	101	SQD	O47-C7-C8-C9
34	Y	319	LMG	C30-C31-C32-C33
31	S	311	CLA	C2A-CAA-CBA-CGA
31	4	610	CLA	C11-C12-C13-C15
34	6	321	LMG	O6-C5-C6-O5
31	8	612	CLA	C10-C11-C12-C13
31	b	615	CLA	C10-C11-C12-C13
31	n	314	CLA	C10-C11-C12-C13
30	Y	308	CHL	CBA-CGA-O2A-C1
30	q	309	CHL	CBA-CGA-O2A-C1
33	B	624	LHG	O9-C7-C8-C9
33	Y	318	LHG	C8-C7-O7-C5
30	p	608	CHL	CAA-CBA-CGA-O2A
30	q	308	CHL	CAA-CBA-CGA-O2A
30	n	301	CHL	CAA-CBA-CGA-O2A
31	9	306	CLA	CAA-CBA-CGA-O2A
33	A	415	LHG	O7-C7-C8-C9
33	R	320	LHG	O7-C7-C8-C9
34	7	301	LMG	C13-C14-C15-C16
34	d	410	LMG	C31-C32-C33-C34
33	N	319	LHG	C27-C28-C29-C30
34	A	418	LMG	C29-C30-C31-C32
34	D	411	LMG	C31-C32-C33-C34
30	7	302	CHL	C10-C11-C12-C13
30	1	607	CHL	C11-C12-C13-C15
30	6	310	CHL	C2-C3-C5-C6
30	Y	309	CHL	C2-C3-C5-C6
30	p	609	CHL	C2-C3-C5-C6
30	y	609	CHL	C2-C3-C5-C6
31	1	611	CLA	C11-C12-C13-C15
31	C	601	CLA	C11-C10-C8-C7
31	8	609	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	p	602	CLA	C6-C7-C8-C10
31	b	607	CLA	C6-C7-C8-C10
31	b	611	CLA	C6-C7-C8-C10
31	c	601	CLA	C11-C12-C13-C15
31	c	603	CLA	C12-C13-C15-C16
31	c	609	CLA	C11-C10-C8-C7
31	s	312	CLA	C11-C10-C8-C7
33	B	624	LHG	C18-C19-C20-C21
33	c	622	LHG	C26-C27-C28-C29
34	c	621	LMG	O6-C1-O1-C7
30	r	308	CHL	CAA-CBA-CGA-O2A
31	2	612	CLA	CAA-CBA-CGA-O2A
31	6	315	CLA	CAA-CBA-CGA-O2A
31	B	604	CLA	CAA-CBA-CGA-O2A
31	B	614	CLA	CAA-CBA-CGA-O2A
31	B	616	CLA	CAA-CBA-CGA-O2A
33	1	617	LHG	O7-C7-C8-C9
33	t	102	LHG	O8-C23-C24-C25
34	x	202	LMG	O7-C10-C11-C12
30	1	619	CHL	C11-C10-C8-C9
31	1	610	CLA	C11-C12-C13-C14
31	1	610	CLA	C14-C13-C15-C16
31	2	602	CLA	C14-C13-C15-C16
31	6	303	CLA	C11-C12-C13-C14
31	B	603	CLA	C11-C10-C8-C9
31	R	316	CLA	C11-C10-C8-C9
31	S	314	CLA	C6-C7-C8-C9
31	7	312	CLA	C11-C12-C13-C14
31	a	406	CLA	C11-C10-C8-C9
31	b	607	CLA	C6-C7-C8-C9
32	p	617	LUT	C13-C14-C15-C35
37	R	318	XAT	C29-C30-C31-C32
43	b	619	BCR	C13-C14-C15-C16
31	6	311	CLA	C15-C16-C17-C18
30	5	608	CHL	O2A-C1-C2-C3
30	7	309	CHL	O2A-C1-C2-C3
30	9	310	CHL	O2A-C1-C2-C3
31	b	602	CLA	O2A-C1-C2-C3
30	6	308	CHL	CAA-CBA-CGA-O2A
30	Y	307	CHL	CAA-CBA-CGA-O2A
31	R	316	CLA	CAA-CBA-CGA-O2A
31	b	607	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	r	320	LHG	O7-C7-C8-C9
38	a	411	SQD	C5-C6-S-O8
38	a	412	SQD	C4-C5-C6-S
38	g	301	SQD	C4-C5-C6-S
38	s	301	SQD	C4-C5-C6-S
38	x	201	SQD	C4-C5-C6-S
31	g	310	CLA	C16-C17-C18-C20
38	b	627	SQD	C28-C29-C30-C31
34	9	302	LMG	C13-C14-C15-C16
44	D	406	PL9	C21-C22-C23-C24
44	d	407	PL9	C11-C12-C13-C14
31	C	603	CLA	CAA-CBA-CGA-O1A
33	S	320	LHG	O9-C7-C8-C9
30	N	301	CHL	CAA-CBA-CGA-O2A
34	b	626	LMG	O8-C28-C29-C30
30	s	302	CHL	CAA-CBA-CGA-O2A
31	4	611	CLA	CAA-CBA-CGA-O2A
36	2	616	NEX	C11-C12-C13-C20
34	7	322	LMG	O9-C10-C11-C12
38	6	301	SQD	O10-C23-C24-C25
31	B	615	CLA	C16-C17-C18-C19
31	c	610	CLA	C16-C17-C18-C20
31	y	612	CLA	C16-C17-C18-C19
42	A	408	PHO	C16-C17-C18-C19
33	L	101	LHG	C27-C28-C29-C30
34	w	204	LMG	C33-C34-C35-C36
38	b	627	SQD	C27-C28-C29-C30
30	Y	308	CHL	O1A-CGA-O2A-C1
30	4	609	CHL	C2-C3-C5-C6
30	9	309	CHL	C2-C3-C5-C6
31	G	612	CLA	CAA-CBA-CGA-O1A
33	4	618	LHG	O10-C23-C24-C25
33	d	408	LHG	O9-C7-C8-C9
32	7	318	LUT	C31-C32-C33-C34
38	y	621	SQD	C24-C23-O48-C46
31	B	604	CLA	C13-C15-C16-C17
34	G	621	LMG	C32-C33-C34-C35
31	y	614	CLA	O1D-CGD-O2D-CED
30	3	302	CHL	C1A-C2A-CAA-CBA
30	5	608	CHL	C1A-C2A-CAA-CBA
30	0	605	CHL	C1A-C2A-CAA-CBA
30	7	309	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
30	7	310	CHL	C1A-C2A-CAA-CBA
30	9	309	CHL	C1A-C2A-CAA-CBA
31	1	612	CLA	C1A-C2A-CAA-CBA
31	5	612	CLA	C1A-C2A-CAA-CBA
31	A	405	CLA	C1A-C2A-CAA-CBA
31	C	607	CLA	C1A-C2A-CAA-CBA
31	R	311	CLA	C1A-C2A-CAA-CBA
31	8	612	CLA	C1A-C2A-CAA-CBA
31	9	316	CLA	C1A-C2A-CAA-CBA
31	p	612	CLA	C1A-C2A-CAA-CBA
31	p	615	CLA	C1A-C2A-CAA-CBA
31	g	312	CLA	C1A-C2A-CAA-CBA
31	n	314	CLA	C1A-C2A-CAA-CBA
31	y	611	CLA	C1A-C2A-CAA-CBA
34	A	414	LMG	C34-C35-C36-C37
34	s	321	LMG	C15-C16-C17-C18
31	0	615	CLA	CAA-CBA-CGA-O1A
31	a	406	CLA	CAA-CBA-CGA-O1A
30	5	608	CHL	CAA-CBA-CGA-O2A
31	8	611	CLA	CAA-CBA-CGA-O1A
34	n	322	LMG	C11-C12-C13-C14
31	B	603	CLA	C2-C1-O2A-CGA
31	0	602	CLA	C2-C1-O2A-CGA
31	b	607	CLA	C5-C6-C7-C8
30	N	308	CHL	CBA-CGA-O2A-C1
31	S	314	CLA	CAA-CBA-CGA-O1A
31	S	316	CLA	CAA-CBA-CGA-O1A
33	p	619	LHG	O10-C23-C24-C25
33	r	320	LHG	O9-C7-C8-C9
34	r	321	LMG	O9-C10-C11-C12
38	M	102	SQD	O49-C7-C8-C9
31	n	313	CLA	CAA-CBA-CGA-O1A
33	p	619	LHG	C4-C5-C6-O8
38	s	301	SQD	O6-C44-C45-C46
30	8	608	CHL	CAA-CBA-CGA-O2A
31	s	314	CLA	CAA-CBA-CGA-O2A
33	2	617	LHG	C19-C20-C21-C22
33	c	622	LHG	C28-C29-C30-C31
34	W	201	LMG	C18-C19-C20-C21
31	R	304	CLA	C8-C10-C11-C12
31	8	604	CLA	C8-C10-C11-C12
31	2	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	5	615	CLA	C2A-CAA-CBA-CGA
31	s	311	CLA	C2A-CAA-CBA-CGA
31	5	602	CLA	C11-C12-C13-C14
31	g	311	CLA	C11-C12-C13-C14
31	C	605	CLA	CAA-CBA-CGA-O1A
34	9	321	LMG	O10-C28-C29-C30
31	C	609	CLA	C8-C10-C11-C12
31	r	311	CLA	C4C-C3C-CAC-CBC
33	L	101	LHG	C17-C18-C19-C20
45	c	617	DGD	C4B-C5B-C6B-C7B
30	N	308	CHL	O1A-CGA-O2A-C1
33	0	619	LHG	C24-C25-C26-C27
33	l	101	LHG	C10-C11-C12-C13
30	y	606	CHL	CAA-CBA-CGA-O2A
31	R	312	CLA	CAA-CBA-CGA-O2A
31	b	605	CLA	CAA-CBA-CGA-O2A
34	9	302	LMG	O8-C28-C29-C30
33	F1	301	LHG	C25-C26-C27-C28
34	k	101	LMG	C37-C38-C39-C40
31	3	315	CLA	CAA-CBA-CGA-O1A
31	B	604	CLA	CAA-CBA-CGA-O1A
31	7	314	CLA	CAA-CBA-CGA-O1A
33	S	320	LHG	O10-C23-C24-C25
34	N	320	LMG	O9-C10-C11-C12
34	0	622	LMG	O9-C10-C11-C12
34	k	101	LMG	O9-C10-C11-C12
34	x	202	LMG	O10-C28-C29-C30
31	B	614	CLA	C2-C3-C5-C6
38	a	411	SQD	C29-C30-C31-C32
38	G	624	SQD	C2-C1-O6-C44
31	6	305	CLA	C5-C6-C7-C8
31	B	607	CLA	C5-C6-C7-C8
31	B	615	CLA	C13-C15-C16-C17
34	m	102	LMG	C31-C32-C33-C34
33	B	624	LHG	C4-O6-P-O5
33	Y	318	LHG	C4-O6-P-O4
33	0	619	LHG	C3-O3-P-O5
33	d	408	LHG	C3-O3-P-O5
34	r	321	LMG	O6-C5-C6-O5
31	B	612	CLA	C16-C17-C18-C19
31	y	613	CLA	C16-C17-C18-C20
34	a	413	LMG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
31	1	613	CLA	CAA-CBA-CGA-O1A
31	4	613	CLA	CAA-CBA-CGA-O1A
31	S	303	CLA	CAA-CBA-CGA-O1A
31	0	613	CLA	CAA-CBA-CGA-O1A
31	y	613	CLA	CAA-CBA-CGA-O1A
33	2	617	LHG	O10-C23-C24-C25
33	0	619	LHG	O10-C23-C24-C25
33	F1	301	LHG	O10-C23-C24-C25
34	j	101	LMG	O9-C10-C11-C12
38	m	101	SQD	O49-C7-C8-C9
30	1	608	CHL	O2A-C1-C2-C3
30	N	308	CHL	O2A-C1-C2-C3
31	3	306	CLA	CAA-CBA-CGA-O2A
34	b	624	LMG	O7-C10-C11-C12
38	a	411	SQD	O47-C7-C8-C9
34	D	411	LMG	O6-C1-O1-C7
34	d	410	LMG	O6-C1-O1-C7
31	0	614	CLA	O1A-CGA-O2A-C1
34	c	620	LMG	C29-C30-C31-C32
32	3	318	LUT	C5-C6-C7-C8
33	t	102	LHG	C33-C34-C35-C36
34	I	101	LMG	C11-C12-C13-C14
31	r	311	CLA	C5-C6-C7-C8
31	2	612	CLA	CAA-CBA-CGA-O1A
31	6	316	CLA	CAA-CBA-CGA-O1A
31	B	616	CLA	CAA-CBA-CGA-O1A
31	7	312	CLA	CAA-CBA-CGA-O1A
33	3	320	LHG	O9-C7-C8-C9
34	D	410	LMG	O10-C28-C29-C30
34	9	302	LMG	O9-C10-C11-C12
34	b	626	LMG	O10-C28-C29-C30
38	x	201	SQD	O10-C23-C24-C25
34	n	321	LMG	C34-C35-C36-C37
38	G	617	SQD	C24-C25-C26-C27
38	a	411	SQD	C25-C26-C27-C28
31	2	610	CLA	CAA-CBA-CGA-O2A
31	C	604	CLA	CAA-CBA-CGA-O2A
31	g	313	CLA	CAA-CBA-CGA-O2A
38	M	102	SQD	C13-C14-C15-C16
30	N	306	CHL	CAA-CBA-CGA-O1A
31	Y	313	CLA	CAA-CBA-CGA-O1A
33	1	617	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
33	a	415	LHG	O10-C23-C24-C25
34	C	622	LMG	O9-C10-C11-C12
34	7	301	LMG	O9-C10-C11-C12
31	6	315	CLA	C5-C6-C7-C8
33	t	102	LHG	C10-C11-C12-C13
30	n	310	CHL	CAA-CBA-CGA-O2A
31	N	305	CLA	CAA-CBA-CGA-O2A
33	D	407	LHG	O8-C23-C24-C25
33	8	618	LHG	O8-C23-C24-C25
34	C	624	LMG	O7-C10-C11-C12
31	6	303	CLA	C10-C11-C12-C13
31	b	611	CLA	C15-C16-C17-C18
33	l	101	LHG	C17-C18-C19-C20
31	p	614	CLA	CAA-CBA-CGA-O1A
33	y	619	LHG	O10-C23-C24-C25
38	G	624	SQD	O49-C7-C8-C9
31	1	602	CLA	C4-C3-C5-C6
32	4	616	LUT	C13-C14-C15-C35
32	7	318	LUT	C13-C14-C15-C35
34	4	621	LMG	C14-C15-C16-C17
34	J	102	LMG	C31-C32-C33-C34
34	x	202	LMG	C29-C30-C31-C32
30	3	309	CHL	O1D-CGD-O2D-CED
44	D	406	PL9	C11-C12-C13-C14
44	d	407	PL9	C31-C32-C33-C34
34	2	620	LMG	C40-C41-C42-C43
31	4	611	CLA	CAA-CBA-CGA-O1A
30	5	607	CHL	CAD-CBD-CGD-O1D
30	0	605	CHL	CAD-CBD-CGD-O1D
30	y	605	CHL	CAD-CBD-CGD-O1D
31	1	610	CLA	CAD-CBD-CGD-O1D
31	3	301	CLA	CAD-CBD-CGD-O1D
31	N	311	CLA	CAD-CBD-CGD-O1D
31	R	315	CLA	CAD-CBD-CGD-O1D
31	8	610	CLA	CAD-CBD-CGD-O1D
31	8	614	CLA	CAD-CBD-CGD-O1D
31	n	312	CLA	CAD-CBD-CGD-O1D
31	n	316	CLA	CAD-CBD-CGD-O1D
31	r	315	CLA	CAD-CBD-CGD-O1D
31	y	610	CLA	CAD-CBD-CGD-O1D
31	y	611	CLA	CAD-CBD-CGD-O1D
34	2	621	LMG	C7-C8-O7-C10

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Mol	Chain	Res	Type	Atoms
34	A	414	LMG	C7-C8-O7-C10
34	p	620	LMG	C9-C8-O7-C10
34	g	322	LMG	C7-C8-O7-C10
38	G	624	SQD	O5-C5-C6-S
38	a	411	SQD	C5-C6-S-O7
45	c	617	DGD	C3G-C2G-O2G-C1B
30	p	607	CHL	CAA-CBA-CGA-O1A
30	p	608	CHL	CAA-CBA-CGA-O1A
30	q	308	CHL	CAA-CBA-CGA-O1A
31	b	609	CLA	CAA-CBA-CGA-O1A
33	3	320	LHG	O10-C23-C24-C25
33	l	101	LHG	O10-C23-C24-C25
34	I	101	LMG	O10-C28-C29-C30
30	1	605	CHL	CAA-CBA-CGA-O2A
30	2	606	CHL	CAA-CBA-CGA-O2A
30	4	606	CHL	CAA-CBA-CGA-O2A
30	R	308	CHL	CAA-CBA-CGA-O2A
30	7	309	CHL	CAA-CBA-CGA-O2A
31	q	315	CLA	CAA-CBA-CGA-O2A
33	n	320	LHG	O8-C23-C24-C25
31	0	611	CLA	C8-C10-C11-C12
31	y	612	CLA	C10-C11-C12-C13
30	1	601	CHL	C14-C13-C15-C16
30	7	306	CHL	C6-C7-C8-C9
30	g	309	CHL	C14-C13-C15-C16
31	1	611	CLA	C11-C12-C13-C14
31	1	612	CLA	C11-C10-C8-C9
31	2	612	CLA	C6-C7-C8-C9
31	C	609	CLA	C11-C12-C13-C14
31	S	305	CLA	C14-C13-C15-C16
31	Y	310	CLA	C6-C7-C8-C9
31	7	303	CLA	C11-C10-C8-C9
31	q	315	CLA	C14-C13-C15-C16
31	b	603	CLA	C11-C12-C13-C14
31	b	604	CLA	C14-C13-C15-C16
31	b	612	CLA	C14-C13-C15-C16
31	b	613	CLA	C11-C10-C8-C9
31	r	305	CLA	C6-C7-C8-C9
31	s	312	CLA	C11-C10-C8-C9
38	6	301	SQD	C26-C27-C28-C29
30	8	605	CHL	CBD-CGD-O2D-CED
30	6	306	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
30	s	302	CHL	CAA-CBA-CGA-O1A
30	q	309	CHL	C5-C6-C7-C8
31	l	610	CLA	C13-C15-C16-C17
31	Y	312	CLA	C8-C10-C11-C12
31	c	601	CLA	C10-C11-C12-C13
33	t	102	LHG	O10-C23-C24-C25
33	A	417	LHG	C10-C11-C12-C13
38	B	623	SQD	C24-C25-C26-C27
30	R	309	CHL	CAA-CBA-CGA-O2A
31	Y	311	CLA	CAA-CBA-CGA-O2A
31	Y	314	CLA	CAA-CBA-CGA-O2A
31	0	604	CLA	CAA-CBA-CGA-O2A
31	8	604	CLA	CAA-CBA-CGA-O2A
31	9	316	CLA	CAA-CBA-CGA-O2A
31	b	617	CLA	CAA-CBA-CGA-O2A
31	s	303	CLA	CAA-CBA-CGA-O2A
33	Y	318	LHG	O8-C23-C24-C25
33	7	319	LHG	O8-C23-C24-C25
33	9	320	LHG	O7-C7-C8-C9
33	9	320	LHG	O8-C23-C24-C25
34	1	618	LMG	O7-C10-C11-C12
34	3	321	LMG	O7-C10-C11-C12
34	B	621	LMG	O7-C10-C11-C12
34	b	622	LMG	O7-C10-C11-C12
34	w	204	LMG	O7-C10-C11-C12
38	A	413	SQD	O47-C7-C8-C9
31	6	316	CLA	C4C-C3C-CAC-CBC
38	a	411	SQD	C11-C10-C9-C8
31	3	316	CLA	C5-C6-C7-C8
31	5	611	CLA	C8-C10-C11-C12
31	s	314	CLA	C10-C11-C12-C13
30	n	306	CHL	CBD-CGD-O2D-CED
33	D	408	LHG	C19-C20-C21-C22
38	b	627	SQD	C17-C18-C19-C20
45	c	617	DGD	C4A-C5A-C6A-C7A
45	c	617	DGD	C2B-C3B-C4B-C5B
31	5	613	CLA	CAA-CBA-CGA-O1A
33	L	101	LHG	O9-C7-C8-C9
34	4	621	LMG	C12-C13-C14-C15
34	S	321	LMG	C19-C20-C21-C22
31	B	605	CLA	C10-C11-C12-C13
33	A	417	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
33	C	623	LHG	C30-C31-C32-C33
30	7	321	CHL	CAA-CBA-CGA-O2A
30	n	308	CHL	CAA-CBA-CGA-O2A
31	2	602	CLA	CAA-CBA-CGA-O2A
31	3	305	CLA	CAA-CBA-CGA-O2A
31	B	608	CLA	CAA-CBA-CGA-O2A
31	D	404	CLA	CAA-CBA-CGA-O2A
31	p	611	CLA	CAA-CBA-CGA-O2A
31	p	613	CLA	CAA-CBA-CGA-O2A
31	q	305	CLA	CAA-CBA-CGA-O2A
31	y	615	CLA	CAA-CBA-CGA-O2A
33	S	322	LHG	O7-C7-C8-C9
33	s	322	LHG	O7-C7-C8-C9
34	J	101	LMG	O7-C10-C11-C12
34	c	621	LMG	O7-C10-C11-C12
34	d	409	LMG	O7-C10-C11-C12
38	a	412	SQD	O47-C7-C8-C9
30	0	607	CHL	C5-C6-C7-C8
31	N	303	CLA	C15-C16-C17-C18
31	b	606	CLA	C10-C11-C12-C13
38	A	413	SQD	C13-C14-C15-C16
30	5	608	CHL	CAA-CBA-CGA-O1A
30	N	301	CHL	CAA-CBA-CGA-O1A
31	6	315	CLA	CAA-CBA-CGA-O1A
31	b	617	CLA	CAA-CBA-CGA-O1A
31	s	303	CLA	CAA-CBA-CGA-O1A
31	b	606	CLA	C16-C17-C18-C20
31	r	311	CLA	C2C-C3C-CAC-CBC
34	2	620	LMG	C11-C12-C13-C14
34	C	619	LMG	C22-C23-C24-C25
31	r	306	CLA	O2A-C1-C2-C3
30	G	605	CHL	C3A-C2A-CAA-CBA
30	0	607	CHL	C3A-C2A-CAA-CBA
30	g	306	CHL	C3A-C2A-CAA-CBA
31	1	604	CLA	C11-C10-C8-C7
31	1	610	CLA	C11-C12-C13-C15
31	3	304	CLA	C11-C10-C8-C7
31	5	611	CLA	C6-C7-C8-C10
31	5	614	CLA	C3A-C2A-CAA-CBA
31	B	609	CLA	C12-C13-C15-C16
31	C	609	CLA	C11-C12-C13-C15
31	D	404	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	G	612	CLA	C11-C10-C8-C7
31	N	310	CLA	C11-C12-C13-C15
31	S	305	CLA	C12-C13-C15-C16
31	7	312	CLA	C11-C12-C13-C15
31	8	604	CLA	C3A-C2A-CAA-CBA
31	q	315	CLA	C12-C13-C15-C16
31	b	606	CLA	C11-C12-C13-C15
31	c	608	CLA	C11-C10-C8-C7
31	d	404	CLA	C11-C12-C13-C15
31	n	311	CLA	C6-C7-C8-C10
31	r	305	CLA	C11-C10-C8-C7
31	s	316	CLA	C3A-C2A-CAA-CBA
42	D	401	PHO	C3A-C2A-CAA-CBA
30	R	309	CHL	CAA-CBA-CGA-O1A
30	Y	307	CHL	CAA-CBA-CGA-O1A
30	7	309	CHL	CAA-CBA-CGA-O1A
30	8	605	CHL	CAA-CBA-CGA-O1A
30	p	601	CHL	CAA-CBA-CGA-O1A
30	n	301	CHL	CAA-CBA-CGA-O1A
30	r	308	CHL	CAA-CBA-CGA-O1A
31	B	614	CLA	CAA-CBA-CGA-O1A
31	N	314	CLA	CAA-CBA-CGA-O1A
31	p	613	CLA	CAA-CBA-CGA-O1A
33	1	617	LHG	O10-C23-C24-C25
33	9	320	LHG	O10-C23-C24-C25
34	I	101	LMG	O9-C10-C11-C12
38	a	412	SQD	O49-C7-C8-C9
34	A	412	LMG	C11-C12-C13-C14
30	0	605	CHL	CAA-CBA-CGA-O2A
31	A	405	CLA	CAA-CBA-CGA-O2A
31	G	610	CLA	CAA-CBA-CGA-O2A
31	9	315	CLA	CAA-CBA-CGA-O2A
31	c	603	CLA	CAA-CBA-CGA-O2A
31	r	303	CLA	CAA-CBA-CGA-O2A
31	y	611	CLA	CAA-CBA-CGA-O2A
33	1	617	LHG	O8-C23-C24-C25
33	D	408	LHG	O8-C23-C24-C25
33	S	322	LHG	O8-C23-C24-C25
33	b	625	LHG	O8-C23-C24-C25
33	d	408	LHG	O8-C23-C24-C25
34	4	620	LMG	O7-C10-C11-C12
34	J	102	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	c	624	LMG	O7-C10-C11-C12
38	b	627	SQD	O48-C23-C24-C25
34	3	321	LMG	C11-C12-C13-C14
30	p	608	CHL	O2A-C1-C2-C3
32	5	616	LUT	C27-C28-C29-C30
32	9	318	LUT	C31-C32-C33-C34
32	r	317	LUT	C27-C28-C29-C30
30	1	605	CHL	CAA-CBA-CGA-O1A
30	2	606	CHL	CAA-CBA-CGA-O1A
30	6	308	CHL	CAA-CBA-CGA-O1A
30	7	321	CHL	CAA-CBA-CGA-O1A
30	8	608	CHL	CAA-CBA-CGA-O1A
30	n	306	CHL	CAA-CBA-CGA-O1A
30	n	308	CHL	CAA-CBA-CGA-O1A
31	3	306	CLA	CAA-CBA-CGA-O1A
31	R	312	CLA	CAA-CBA-CGA-O1A
31	Y	314	CLA	CAA-CBA-CGA-O1A
31	9	306	CLA	CAA-CBA-CGA-O1A
31	y	615	CLA	CAA-CBA-CGA-O1A
34	B	621	LMG	O9-C10-C11-C12
34	b	601	LMG	O9-C10-C11-C12
34	b	622	LMG	O9-C10-C11-C12
38	A	413	SQD	O49-C7-C8-C9
36	N	318	NEX	C9-C10-C11-C12
33	q	320	LHG	C12-C13-C14-C15
31	5	611	CLA	CAA-CBA-CGA-O2A
31	6	305	CLA	CAA-CBA-CGA-O2A
31	G	613	CLA	CAA-CBA-CGA-O2A
31	q	314	CLA	CAA-CBA-CGA-O2A
31	n	305	CLA	CAA-CBA-CGA-O2A
31	r	312	CLA	CAA-CBA-CGA-O2A
33	e	101	LHG	O7-C7-C8-C9
33	j	102	LHG	O7-C7-C8-C9
33	s	320	LHG	O8-C23-C24-C25
38	M	102	SQD	O48-C23-C24-C25
33	t	102	LHG	C31-C32-C33-C34
45	C	620	DGD	C6B-C7B-C8B-C9B
34	6	323	LMG	O6-C1-O1-C7
30	0	607	CHL	C10-C11-C12-C13
31	S	310	CLA	C8-C10-C11-C12
33	Y	318	LHG	C25-C26-C27-C28
30	4	606	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
30	R	308	CHL	CAA-CBA-CGA-O1A
30	y	606	CHL	CAA-CBA-CGA-O1A
31	2	602	CLA	CAA-CBA-CGA-O1A
31	D	404	CLA	CAA-CBA-CGA-O1A
31	b	607	CLA	CAA-CBA-CGA-O1A
33	6	320	LHG	O9-C7-C8-C9
33	A	415	LHG	O9-C7-C8-C9
33	R	320	LHG	O9-C7-C8-C9
33	Y	318	LHG	O10-C23-C24-C25
34	d	409	LMG	O9-C10-C11-C12
34	w	204	LMG	O9-C10-C11-C12
34	x	202	LMG	O9-C10-C11-C12
38	S	301	SQD	O49-C7-C8-C9
34	a	401	LMG	C14-C15-C16-C17
34	y	620	LMG	C31-C32-C33-C34
45	c	616	DGD	C4D-C5D-C6D-O5D
30	1	619	CHL	CAA-CBA-CGA-O2A
31	3	304	CLA	CAA-CBA-CGA-O2A
31	8	614	CLA	CAA-CBA-CGA-O2A
33	A	417	LHG	O8-C23-C24-C25
34	d	409	LMG	C15-C16-C17-C18
30	8	608	CHL	C10-C11-C12-C13
31	G	610	CLA	CAA-CBA-CGA-O1A
31	R	316	CLA	CAA-CBA-CGA-O1A
31	8	604	CLA	CAA-CBA-CGA-O1A
31	g	313	CLA	CAA-CBA-CGA-O1A
33	S	322	LHG	O9-C7-C8-C9
34	b	624	LMG	O9-C10-C11-C12
31	3	301	CLA	C2A-CAA-CBA-CGA
31	S	310	CLA	C2A-CAA-CBA-CGA
31	c	602	CLA	C2A-CAA-CBA-CGA
31	1	612	CLA	C16-C17-C18-C20
31	c	609	CLA	C8-C10-C11-C12
33	z	102	LHG	C12-C13-C14-C15
38	A	413	SQD	C7-C8-C9-C10
31	3	305	CLA	CAA-CBA-CGA-O1A
31	0	604	CLA	CAA-CBA-CGA-O1A
31	q	305	CLA	CAA-CBA-CGA-O1A
31	y	611	CLA	CAA-CBA-CGA-O1A
33	7	319	LHG	O10-C23-C24-C25
33	8	618	LHG	O10-C23-C24-C25
34	J	102	LMG	O9-C10-C11-C12

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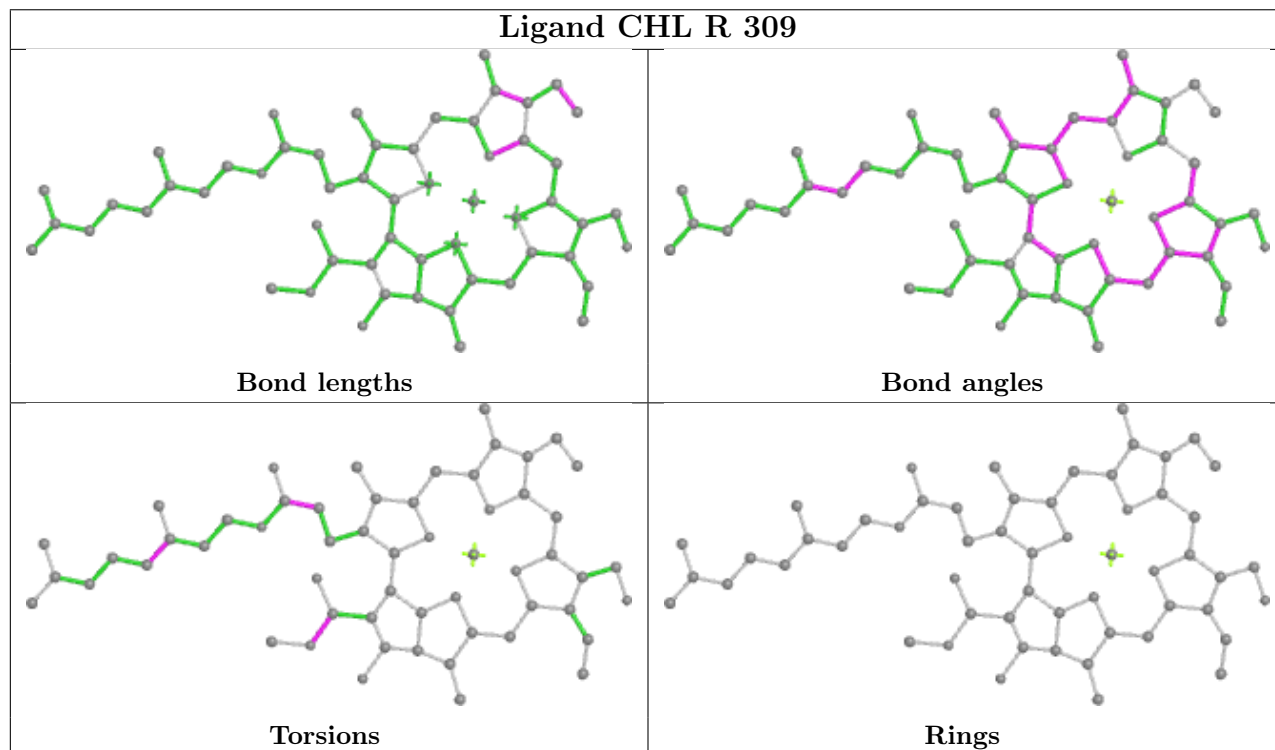
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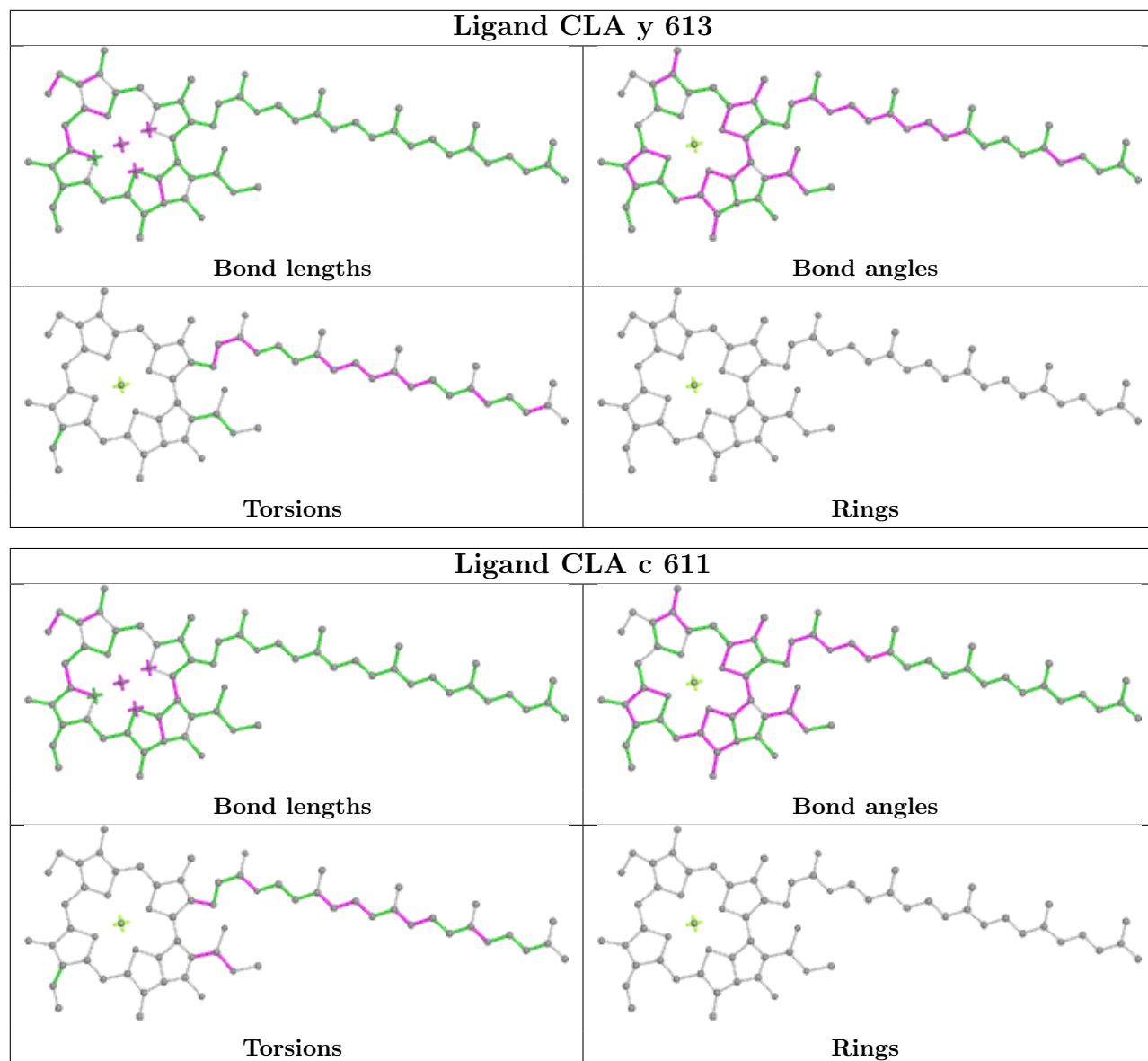
Mol	Chain	Res	Type	Atoms
45	c	617	DGD	O1A-C1A-C2A-C3A
31	G	604	CLA	C4-C3-C5-C6
31	c	611	CLA	C4-C3-C5-C6
31	d	405	CLA	C4-C3-C5-C6
33	N	319	LHG	C17-C18-C19-C20
34	B	625	LMG	C32-C33-C34-C35
34	A	418	LMG	O7-C10-C11-C12

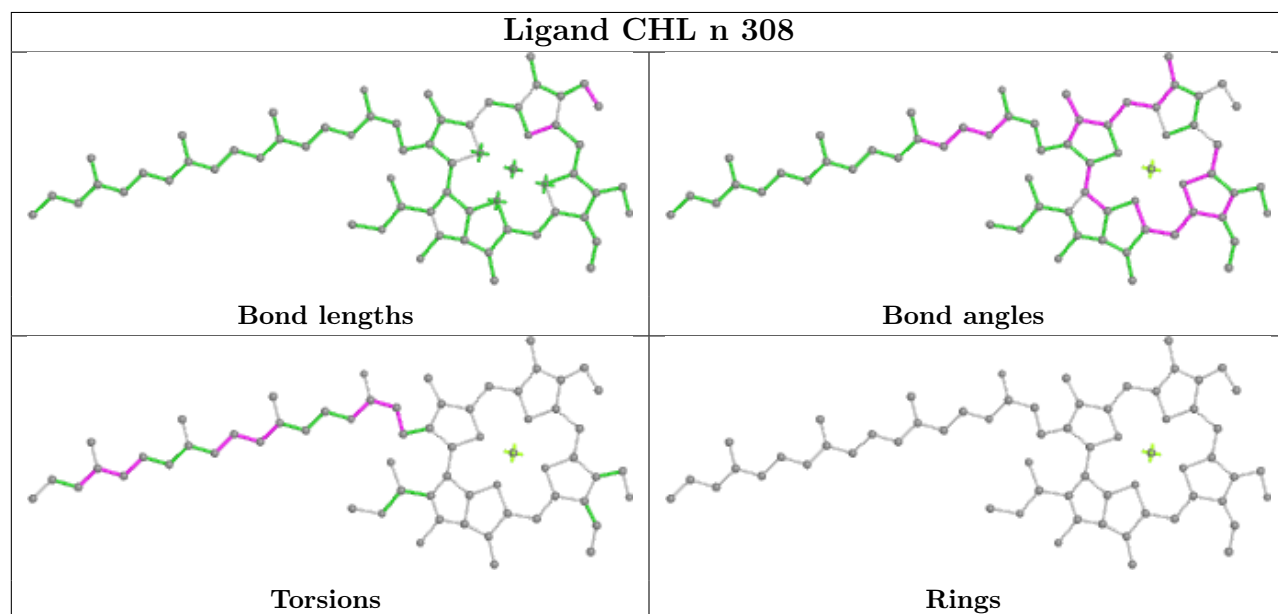
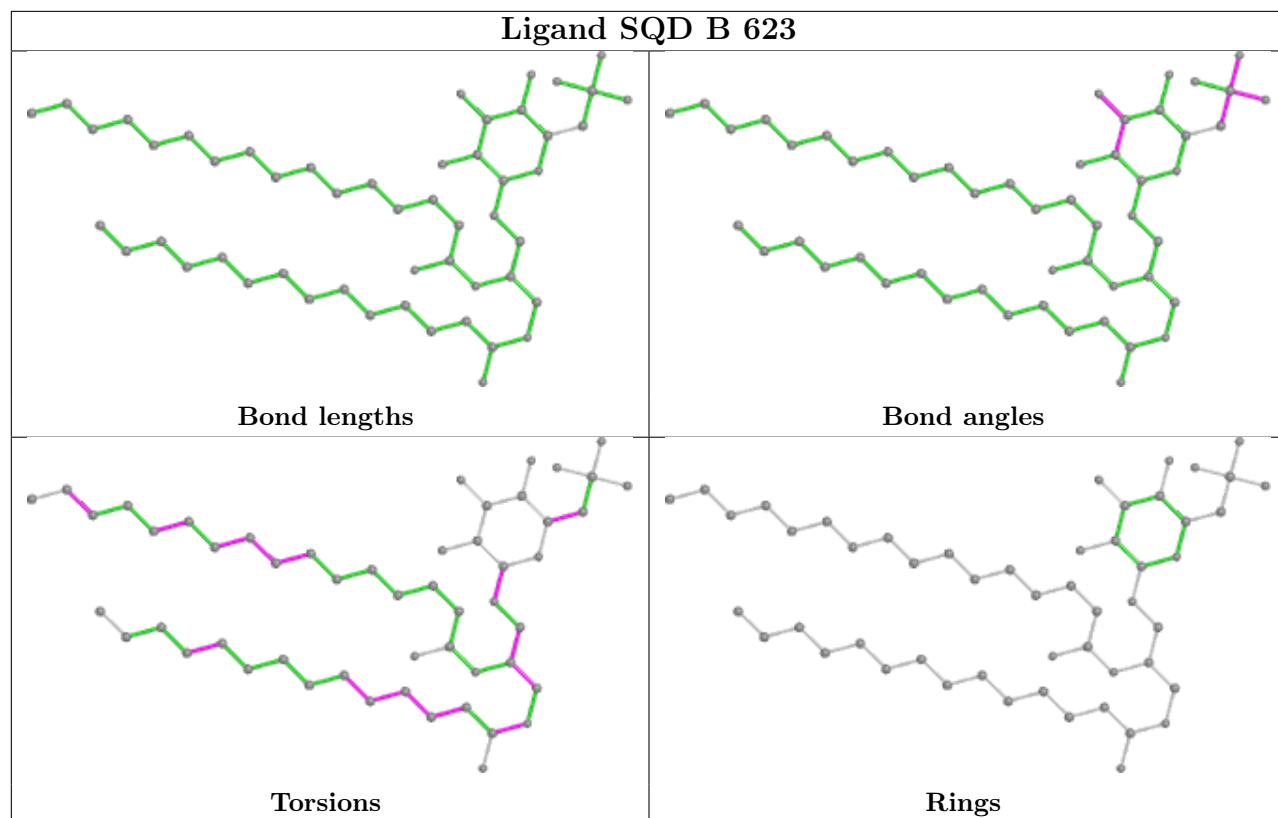
There are no ring outliers.

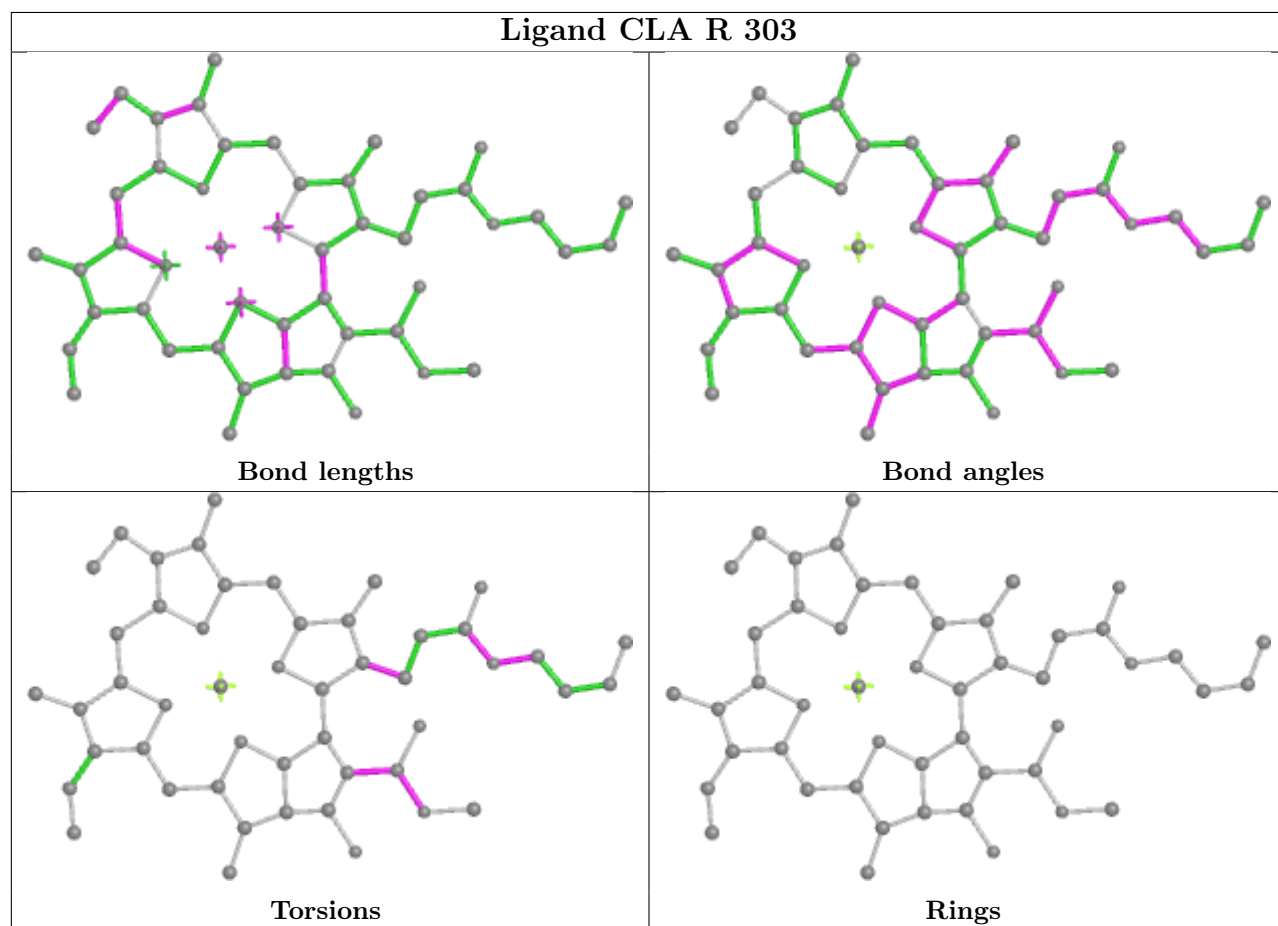
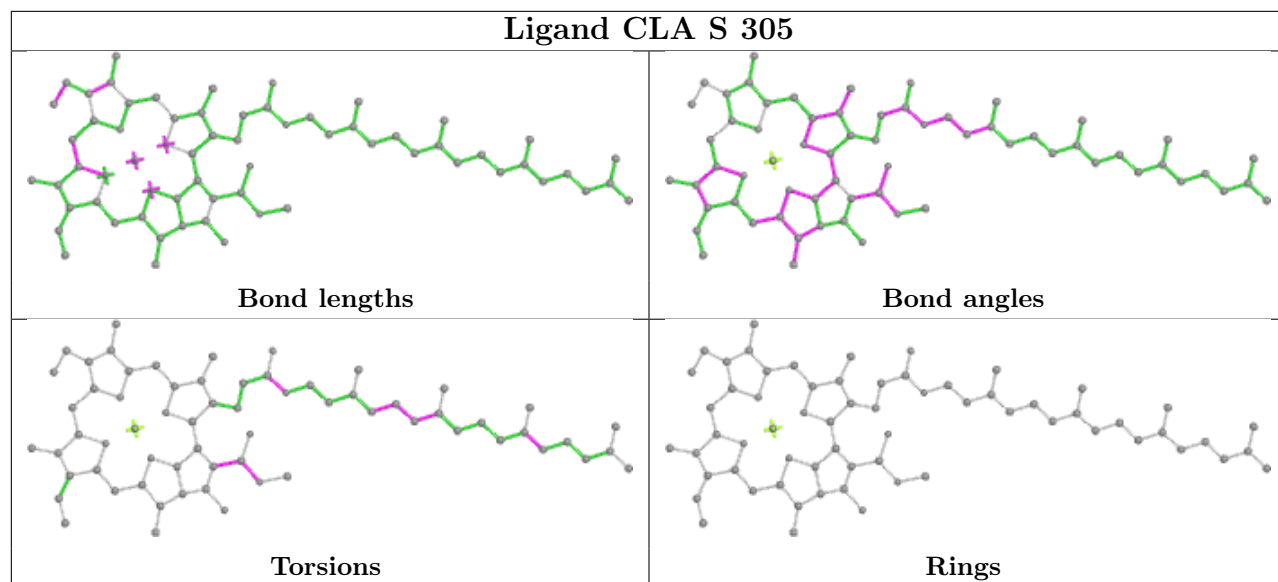
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

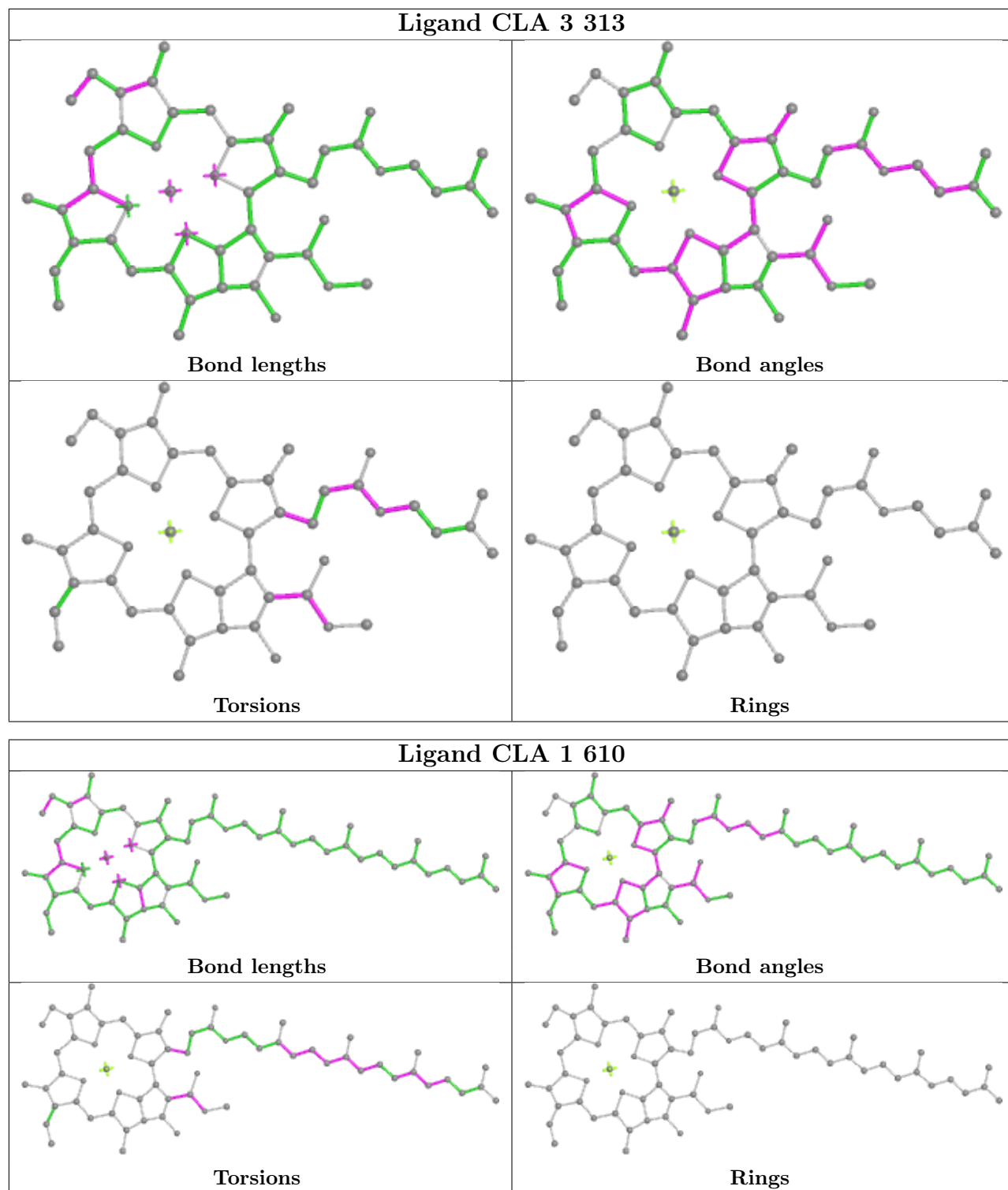


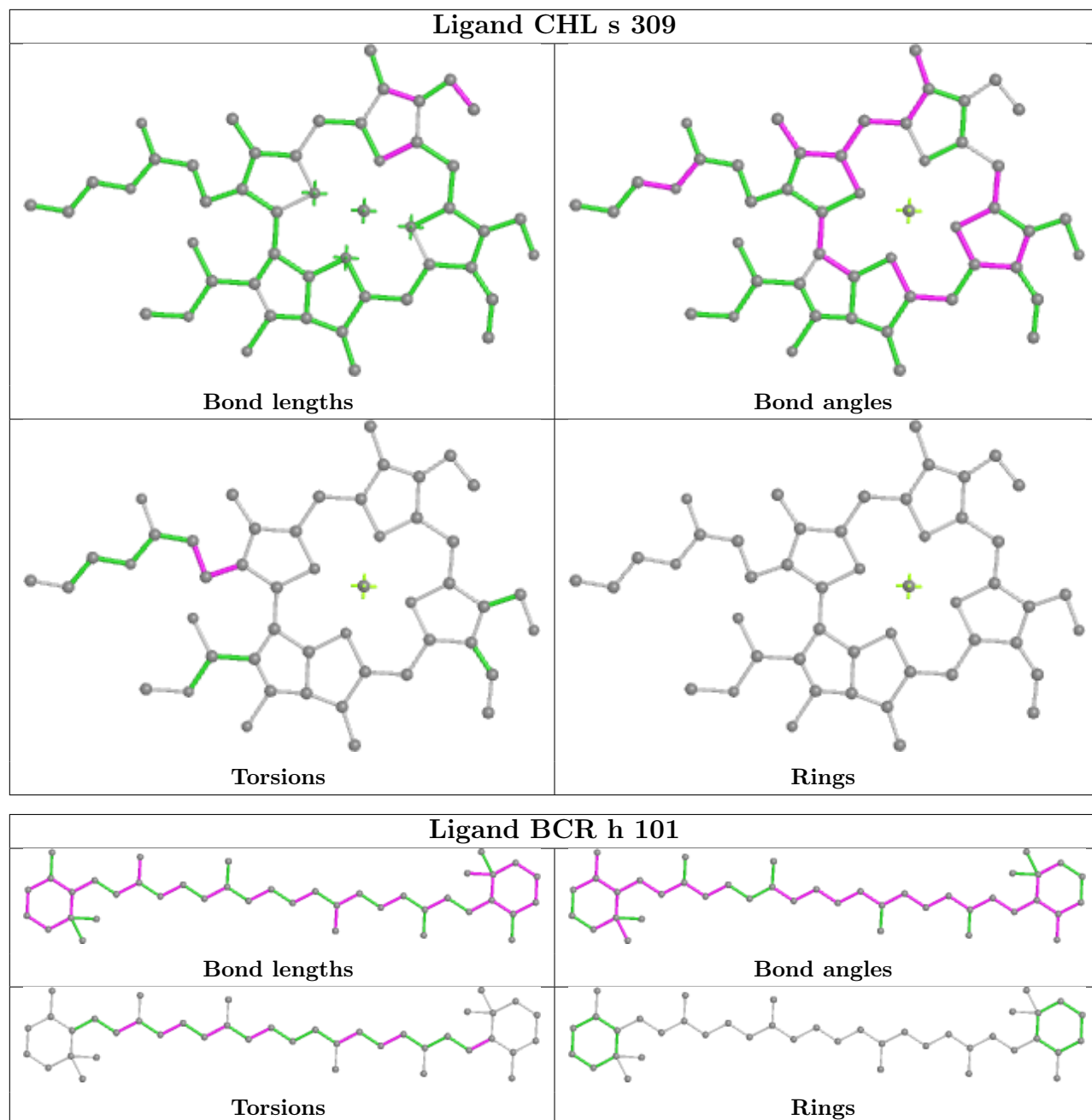


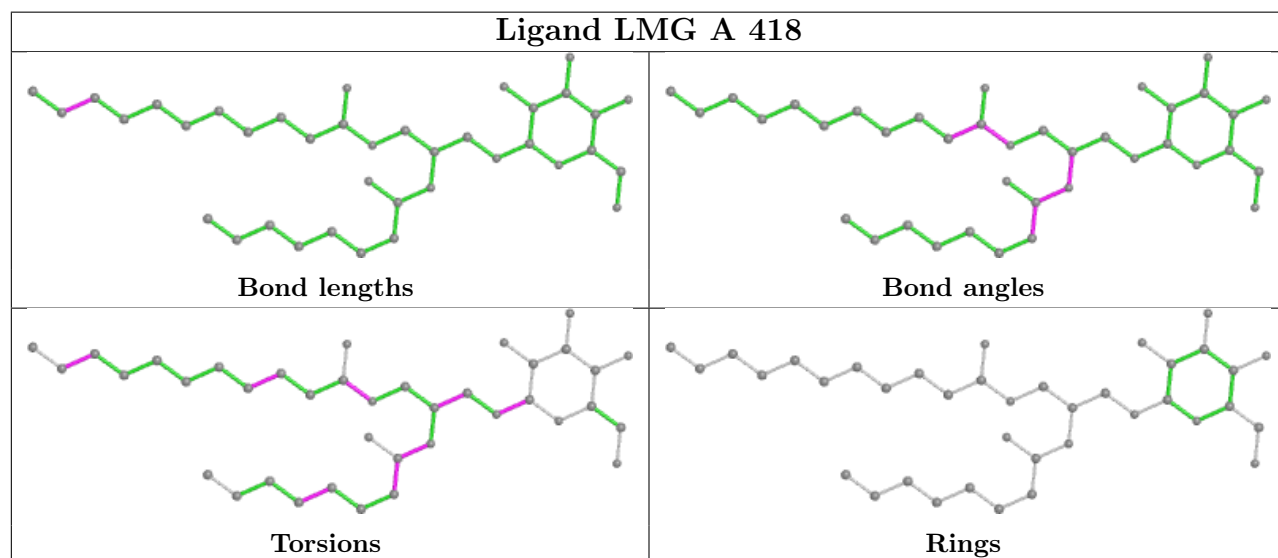
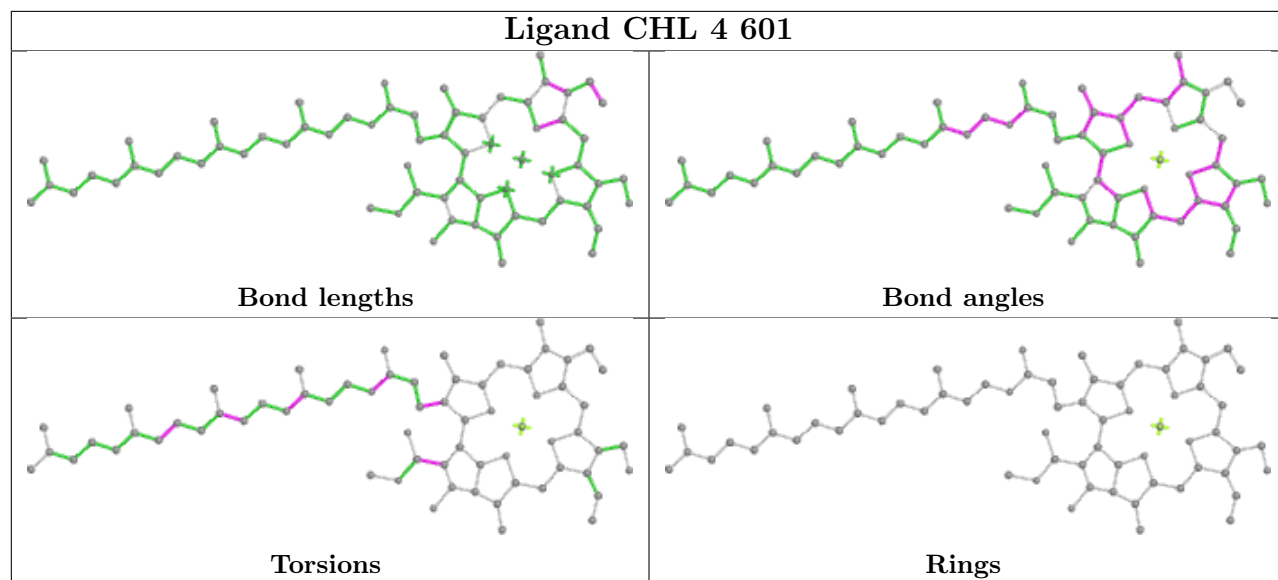


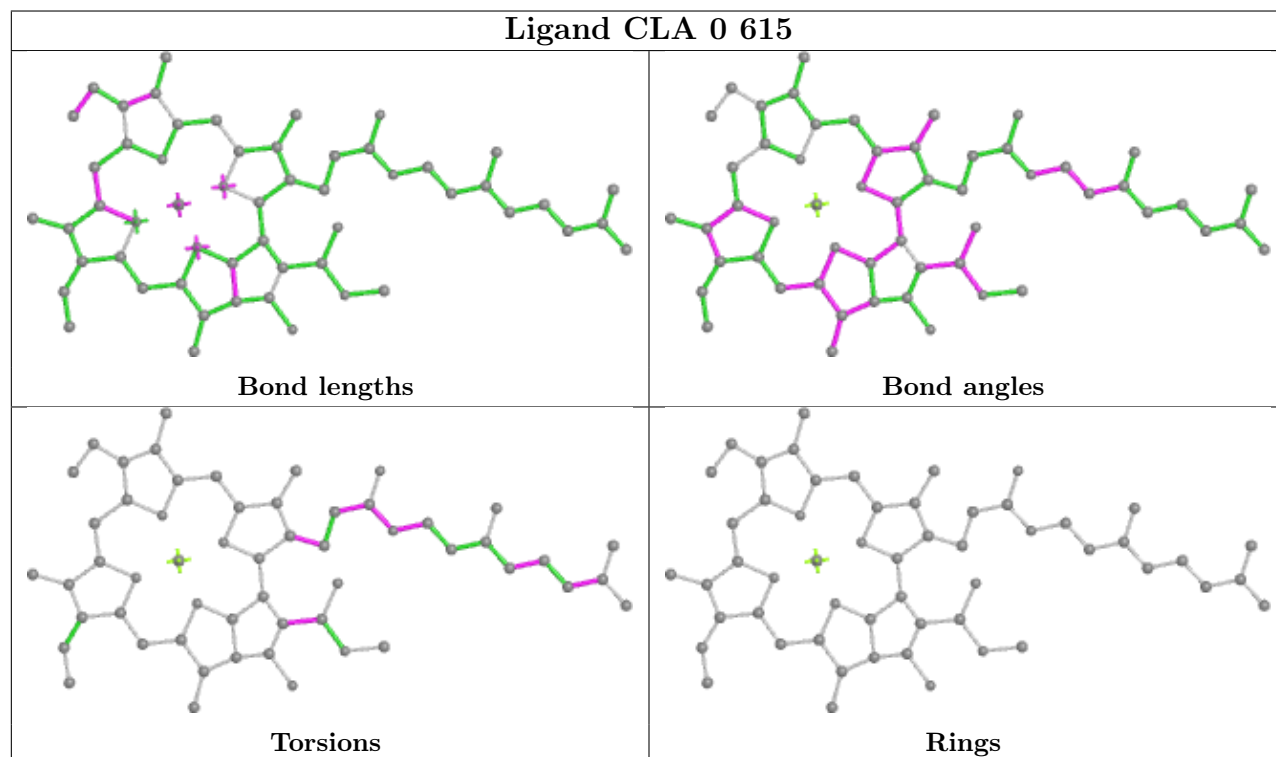
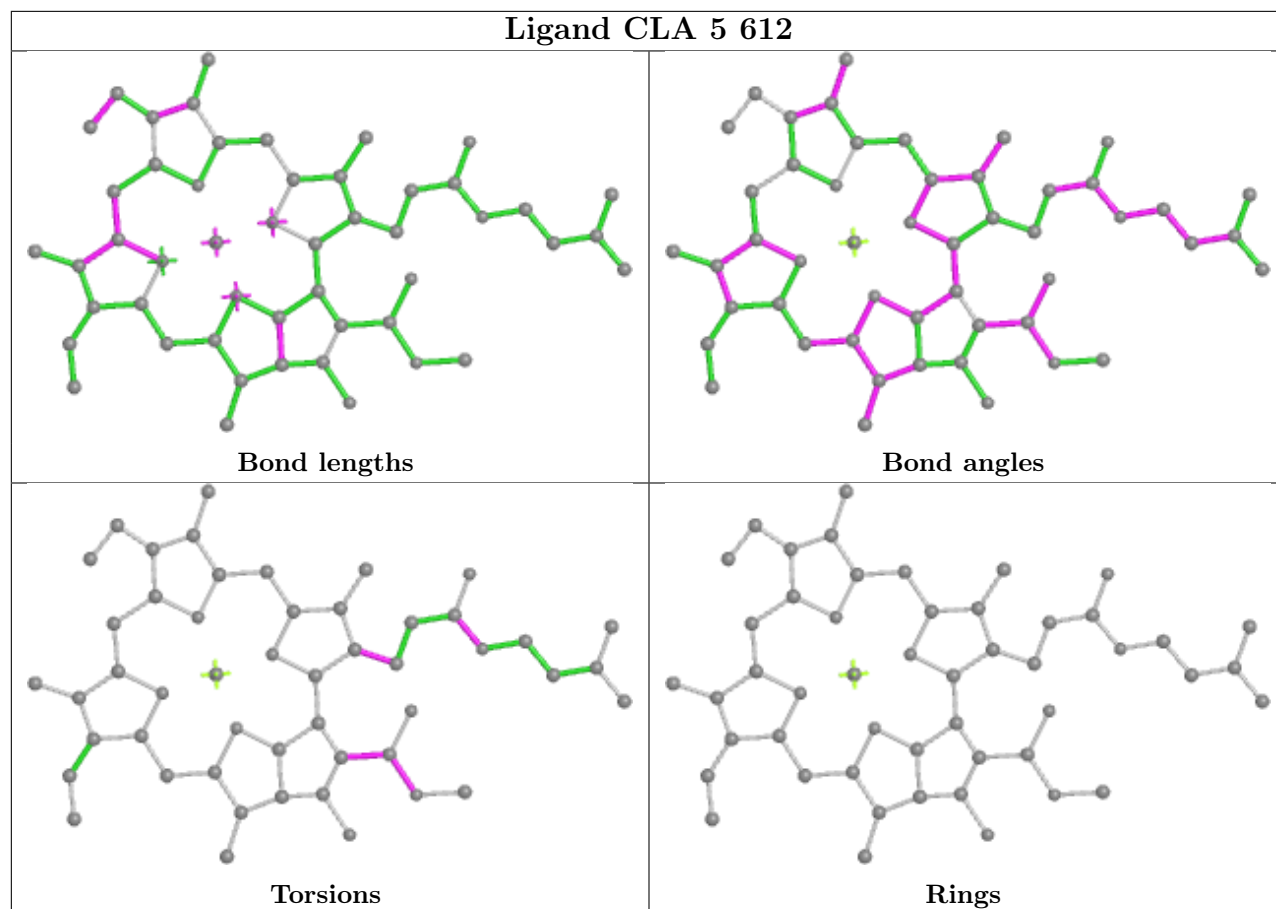


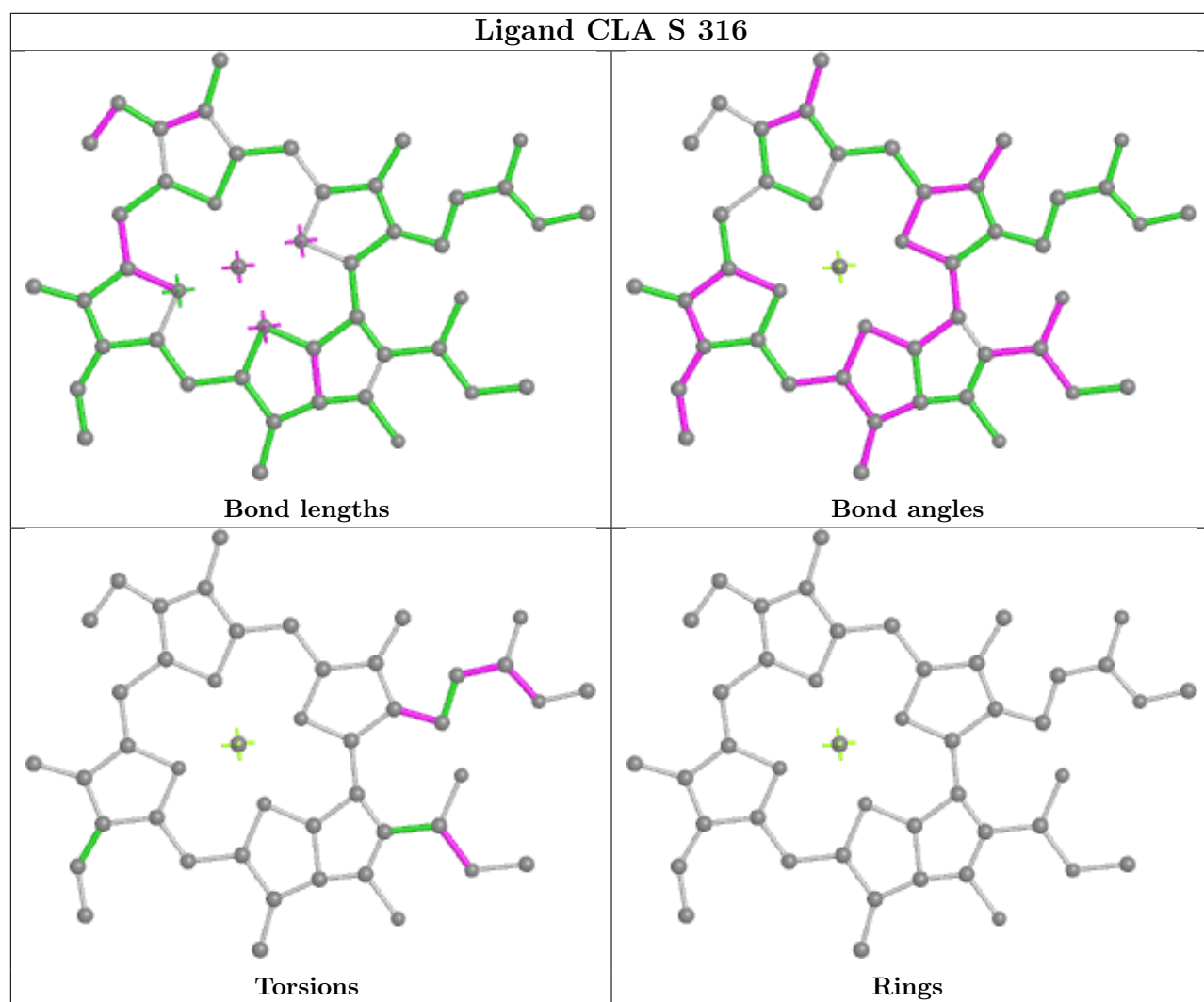
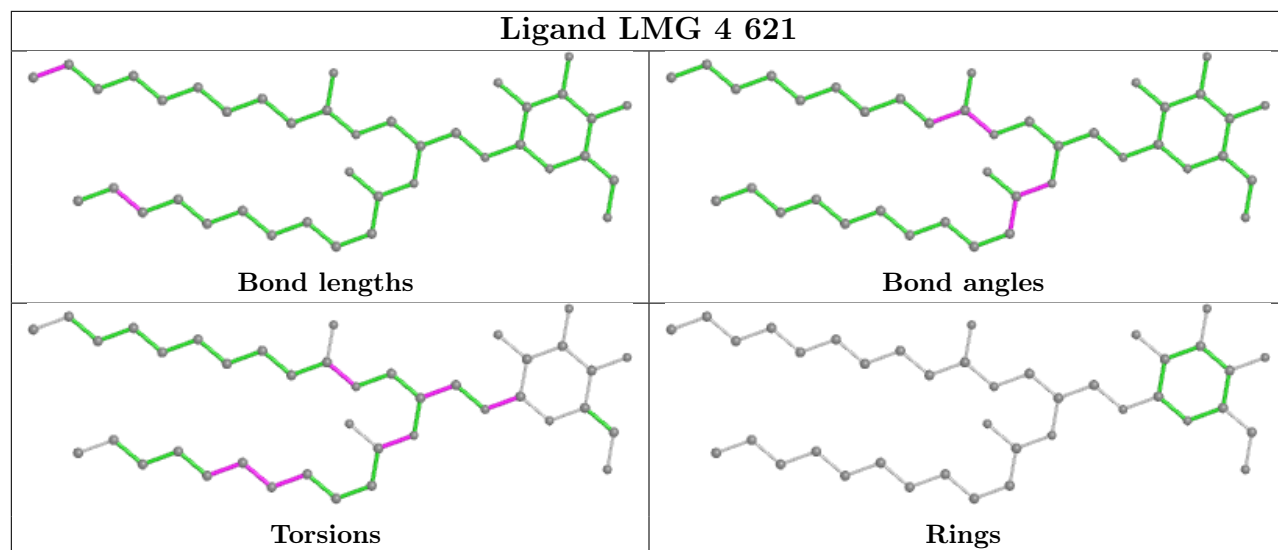


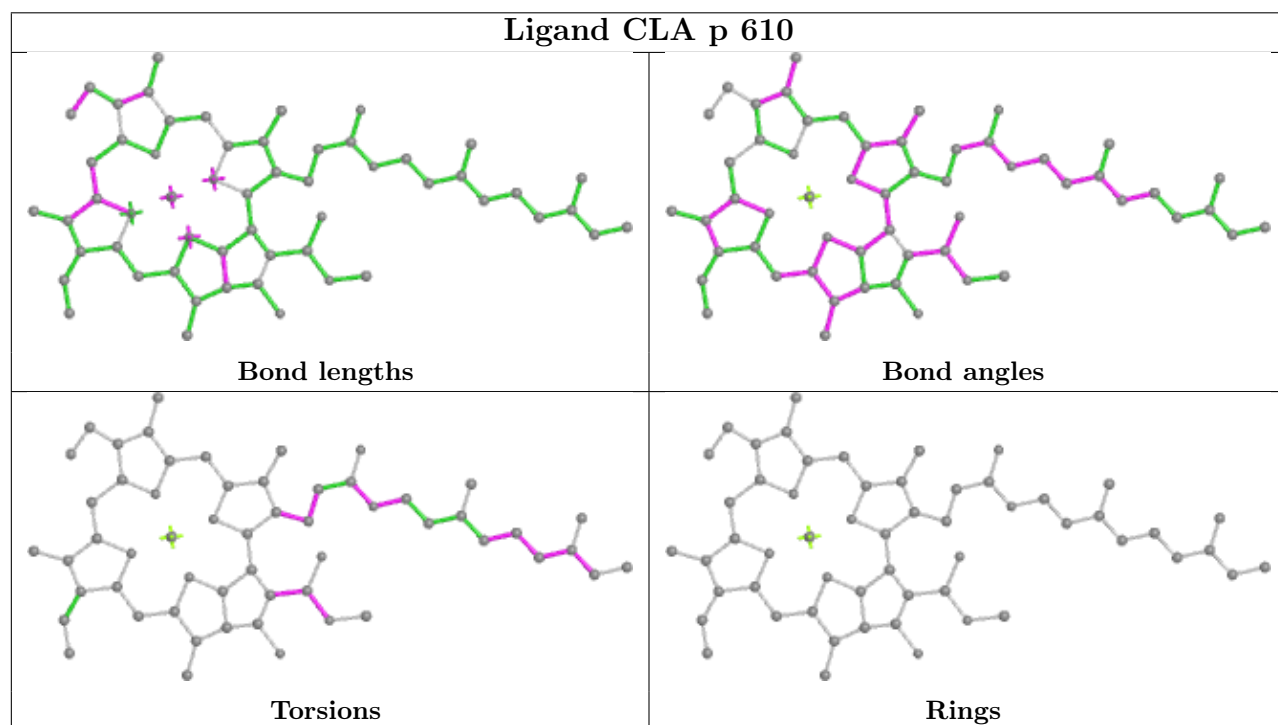
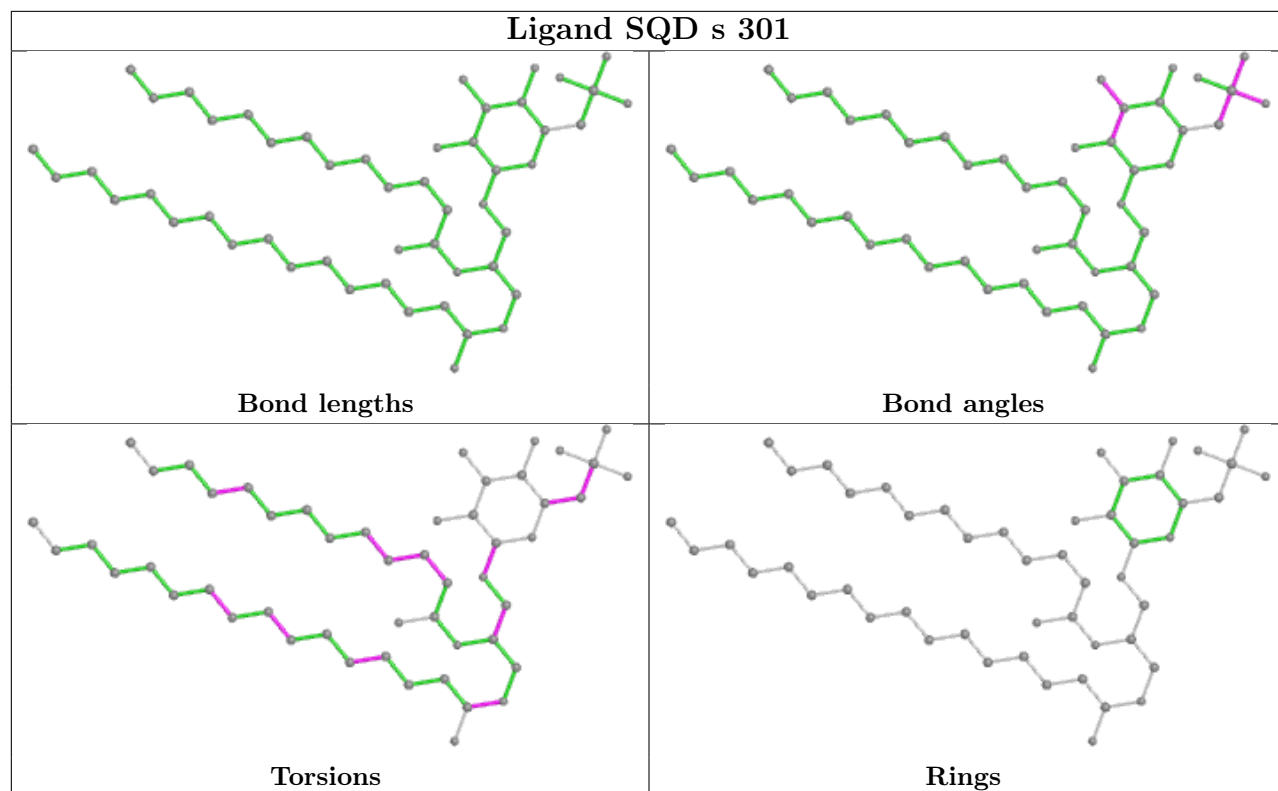


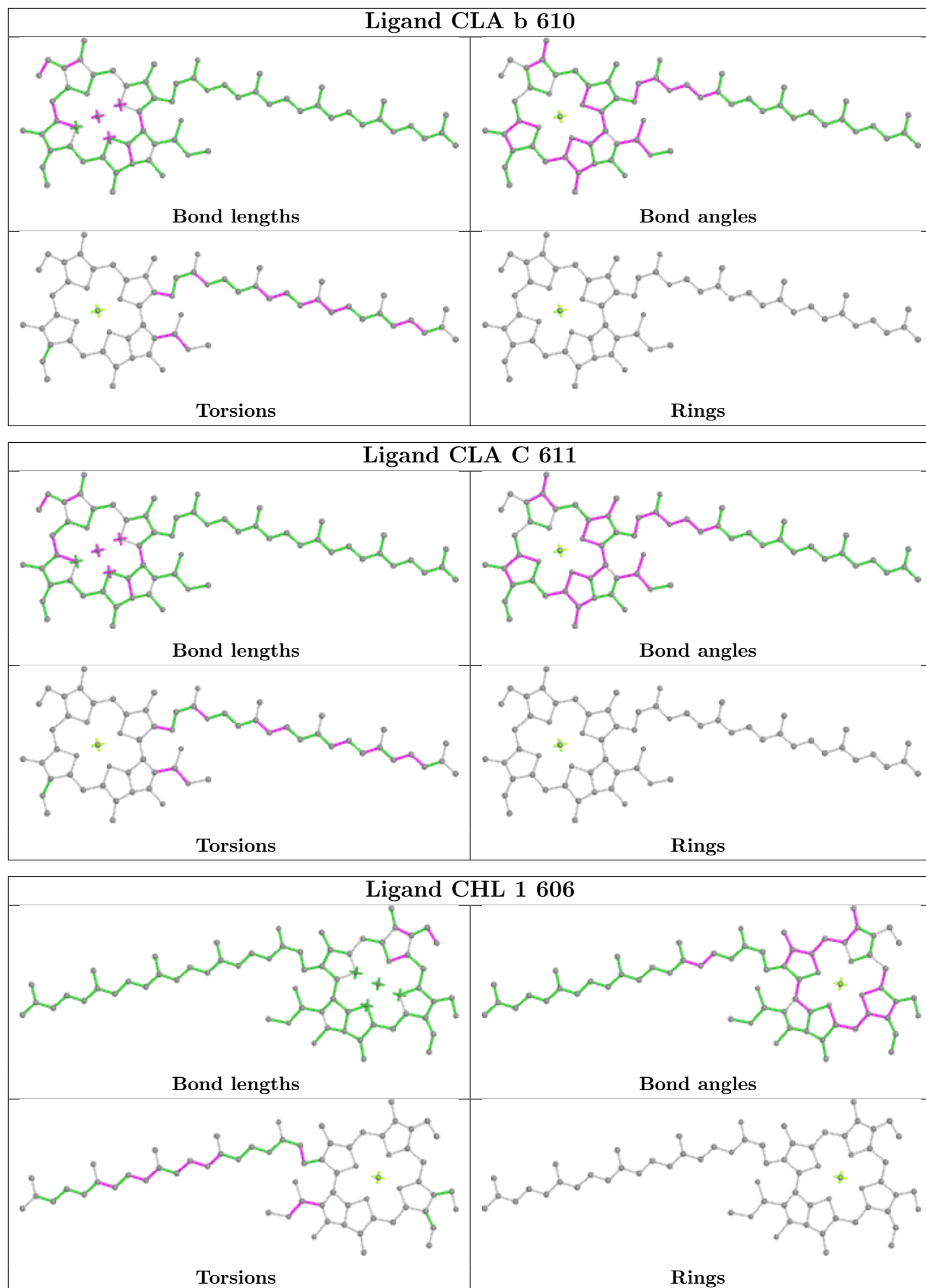


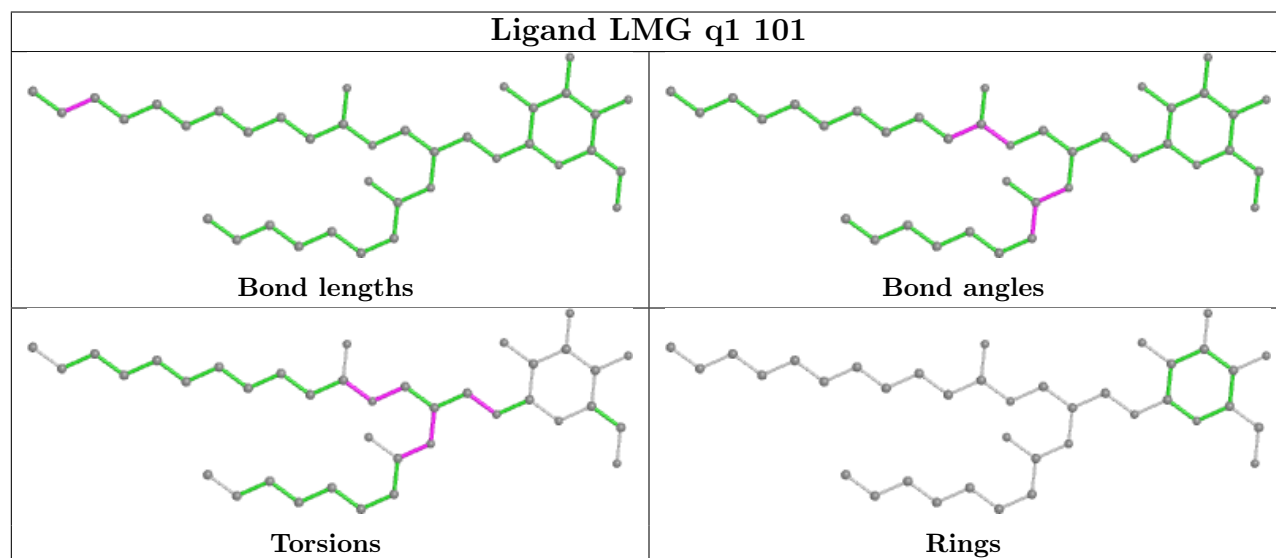
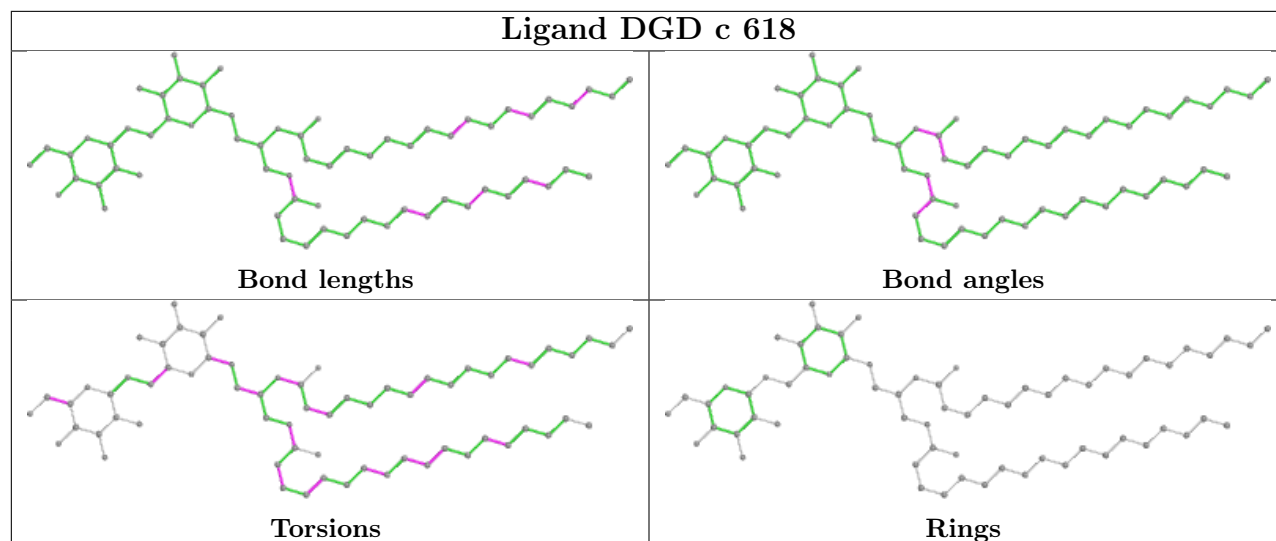




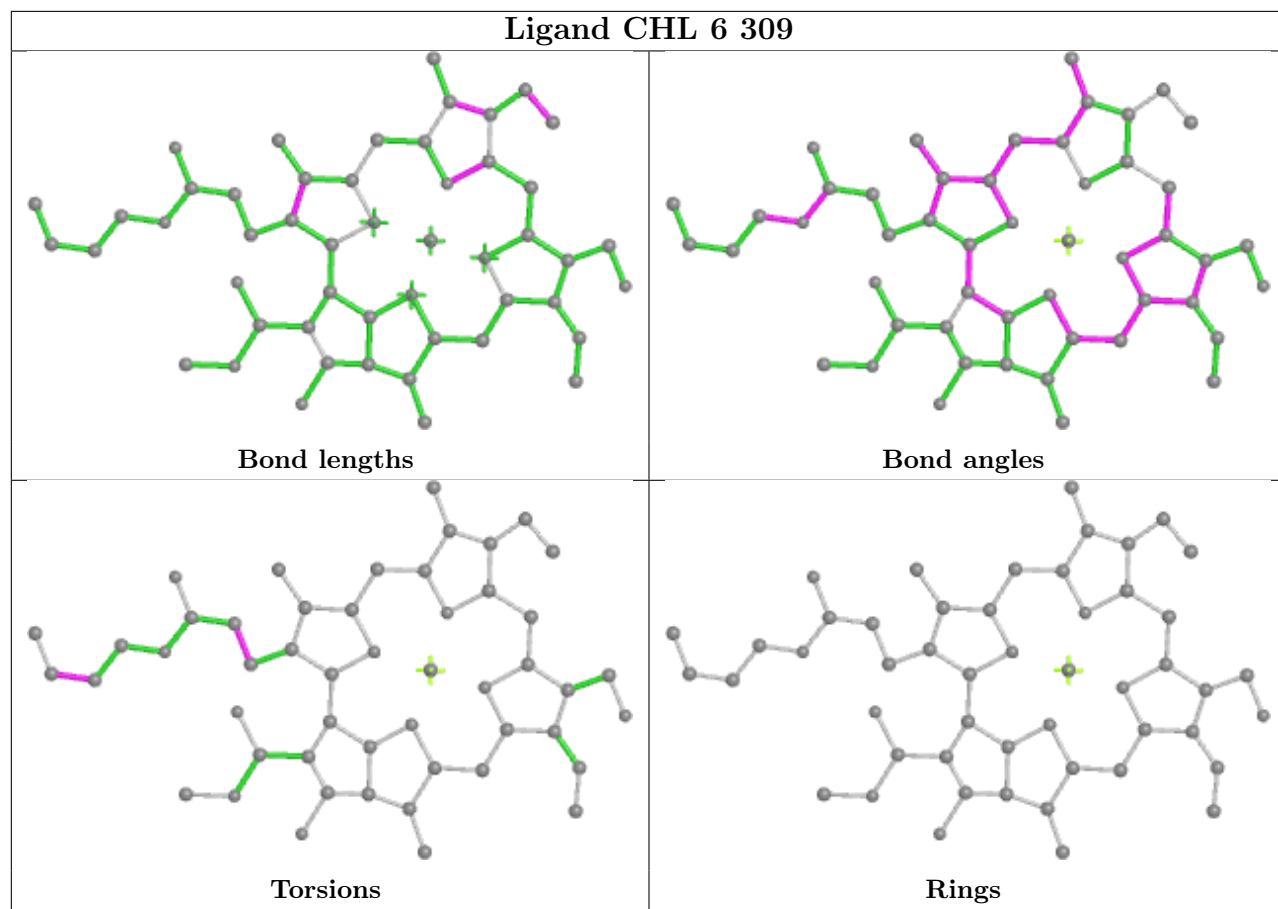


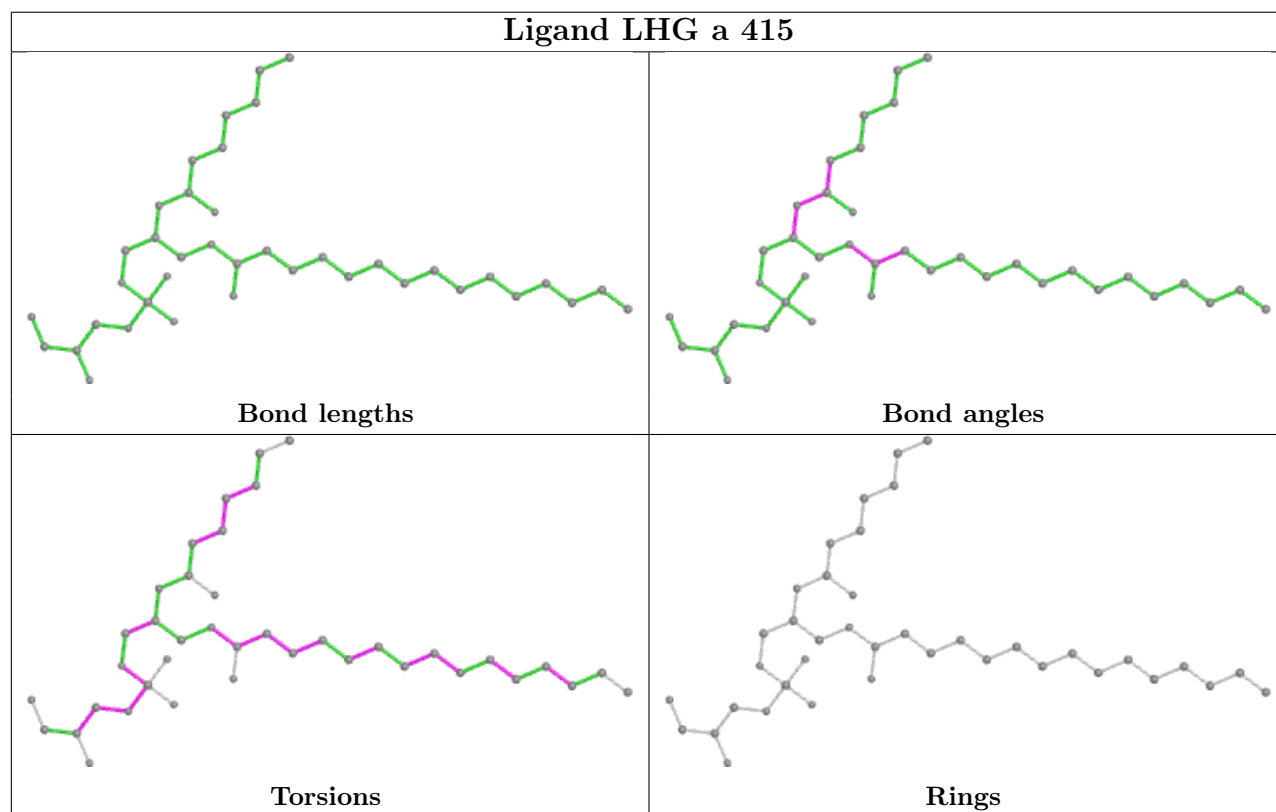
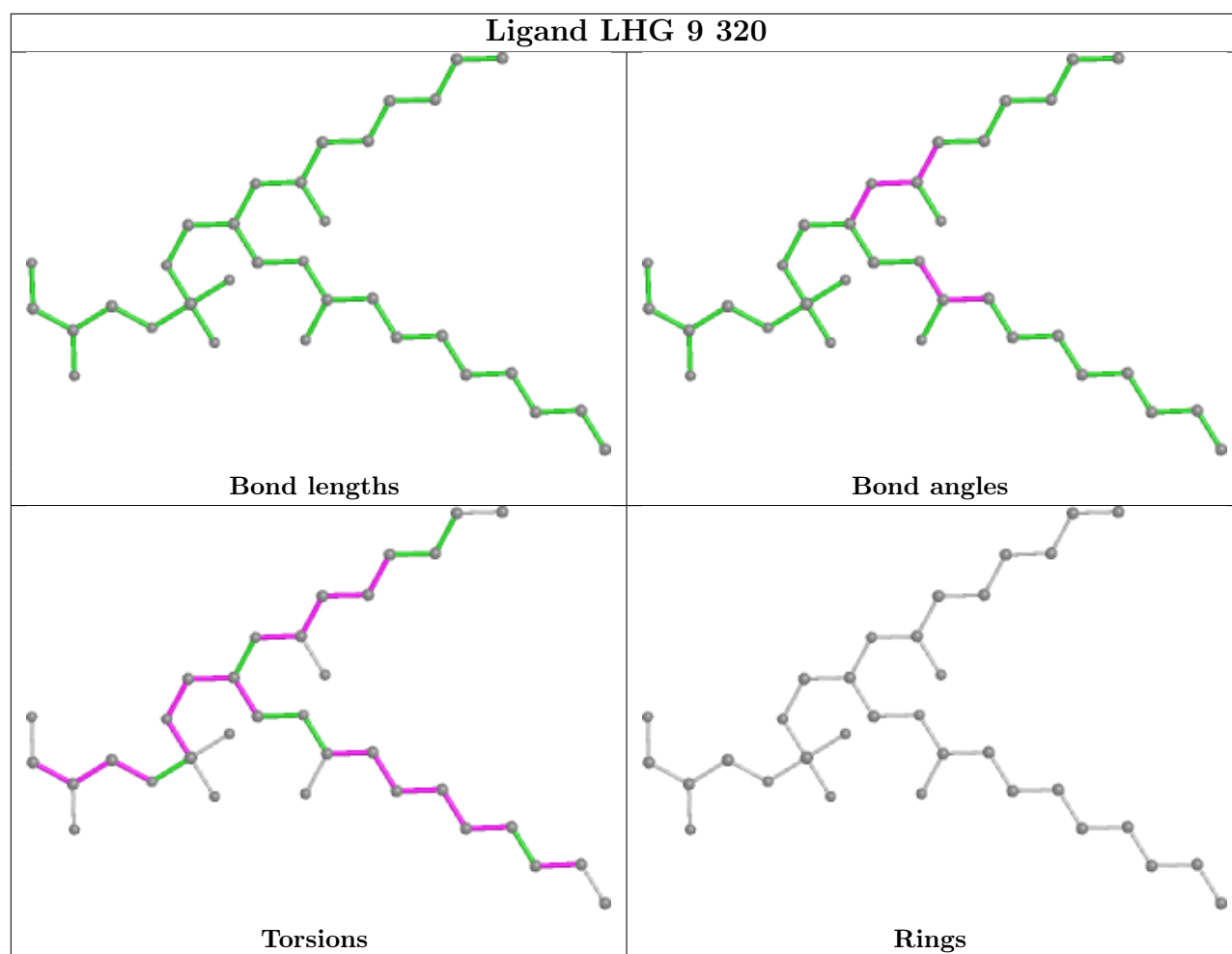


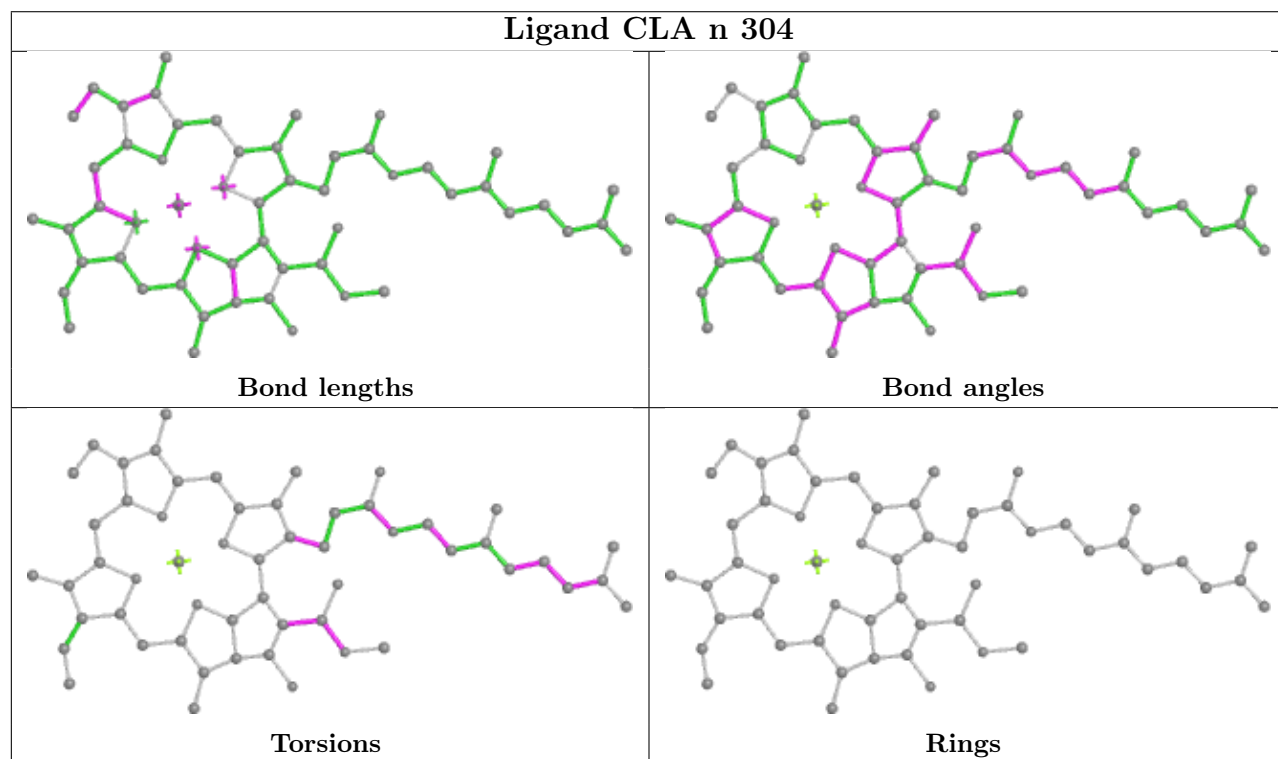
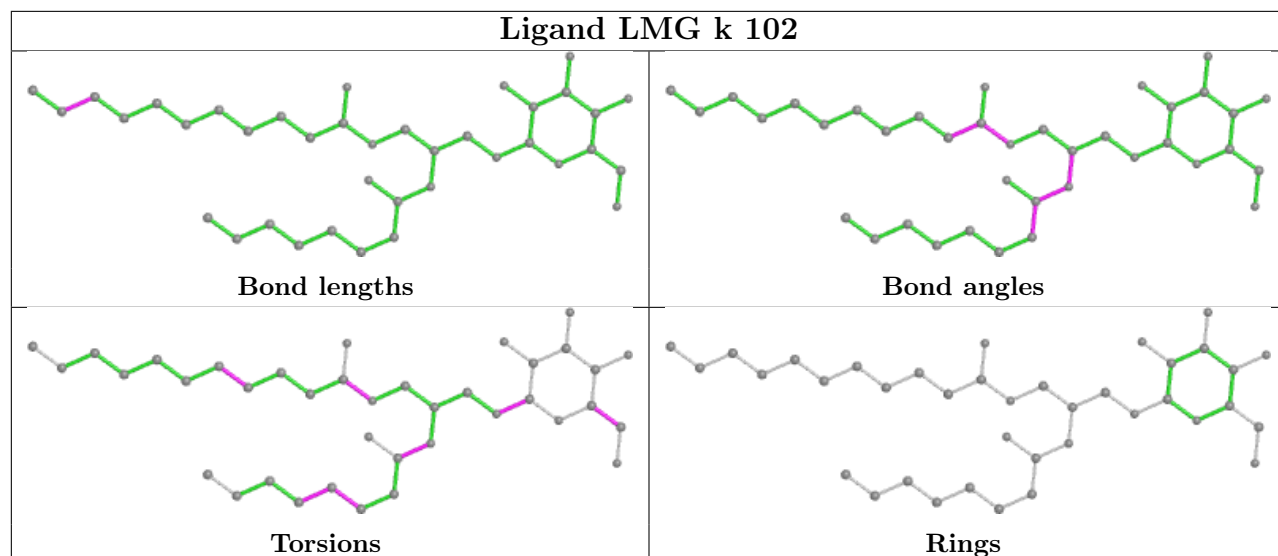


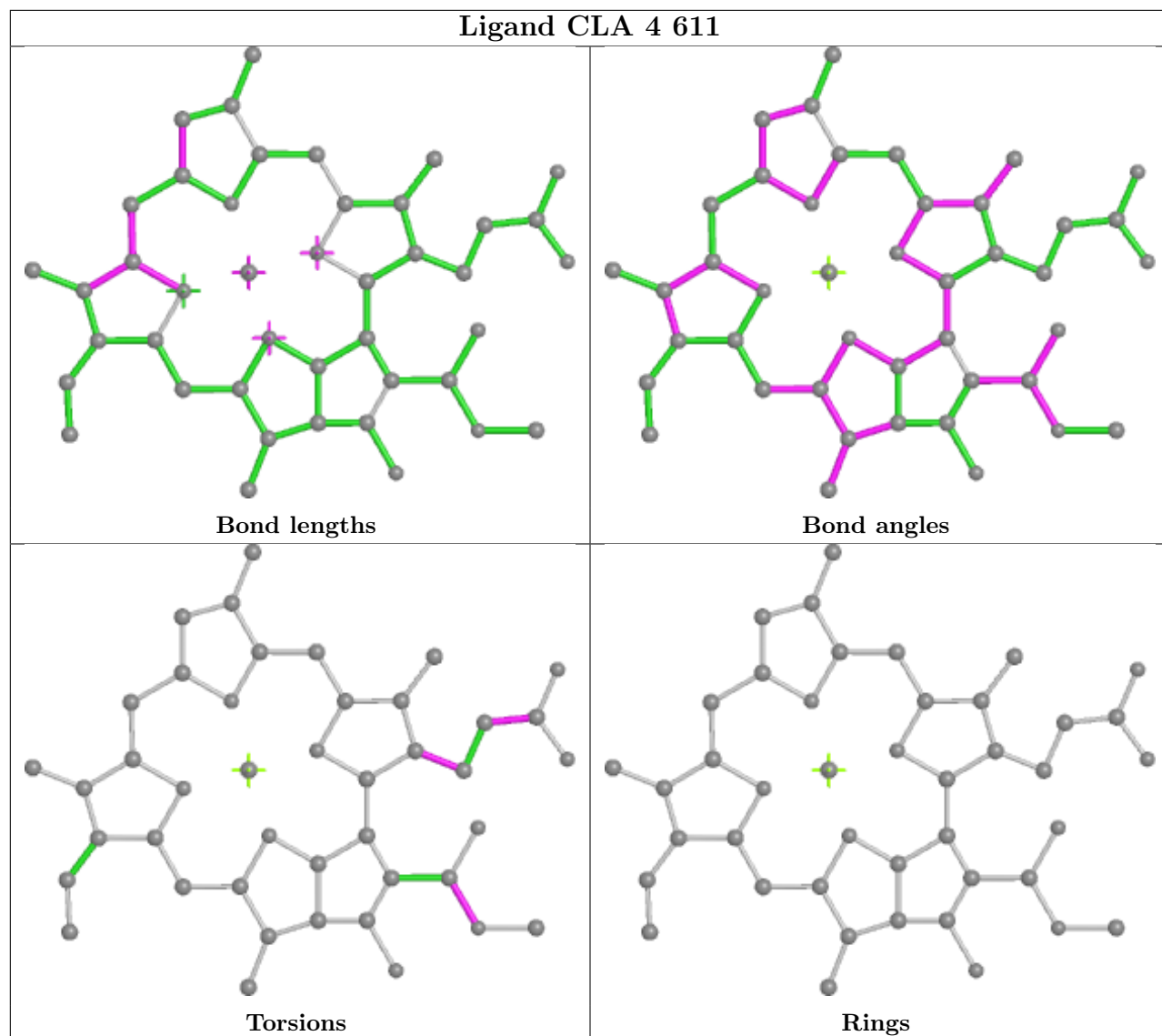


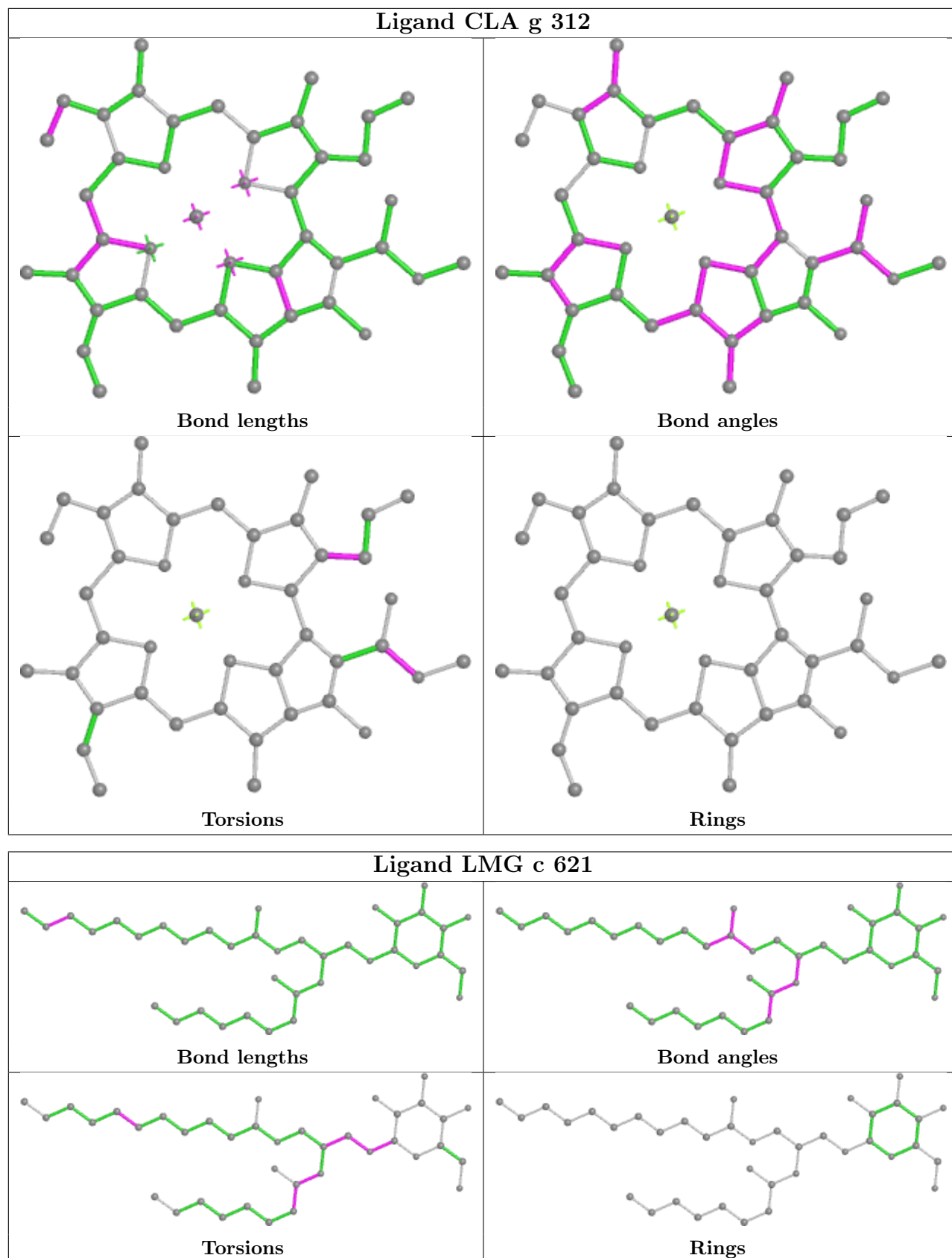


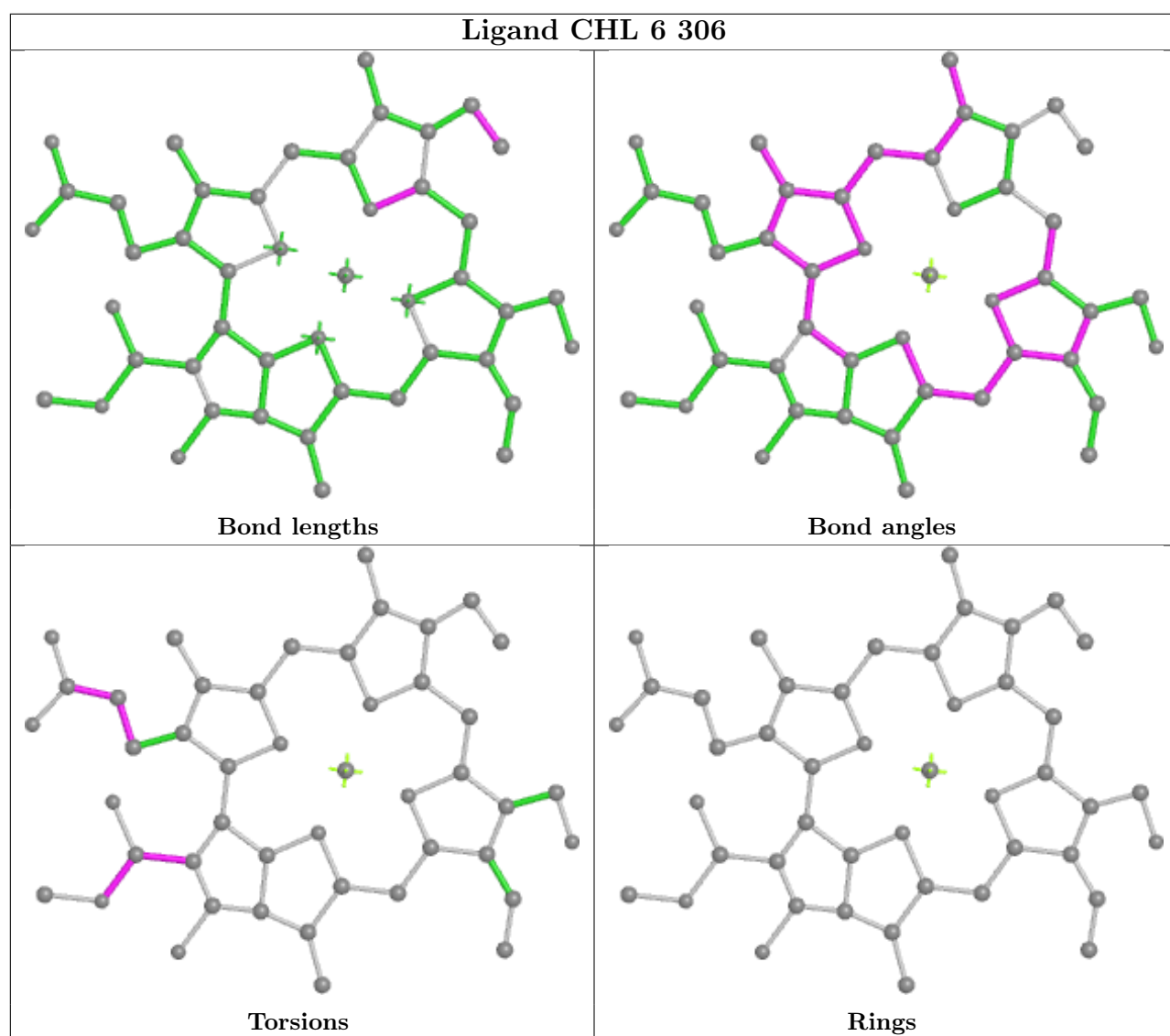
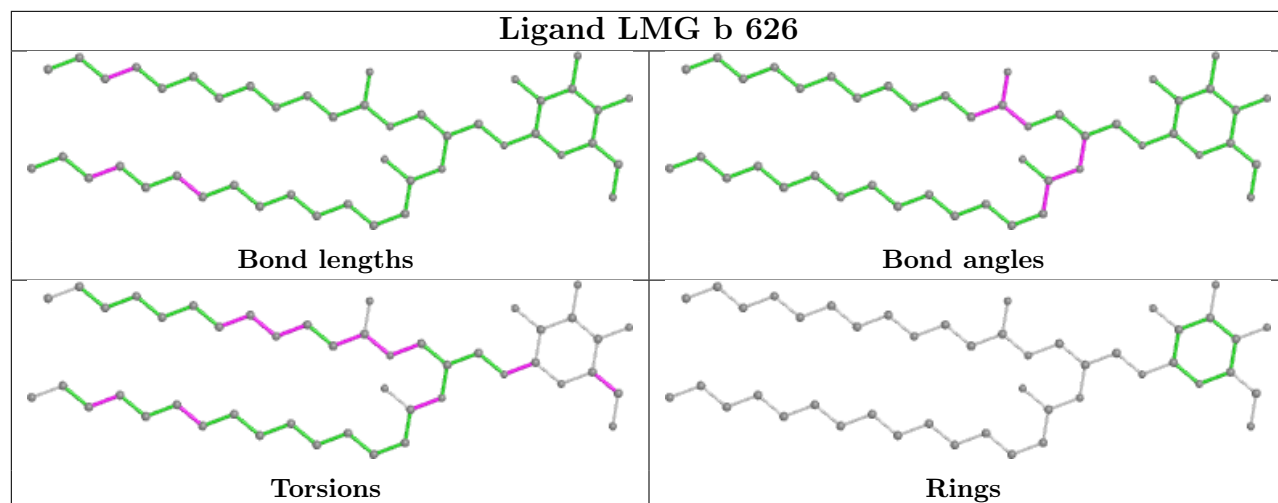


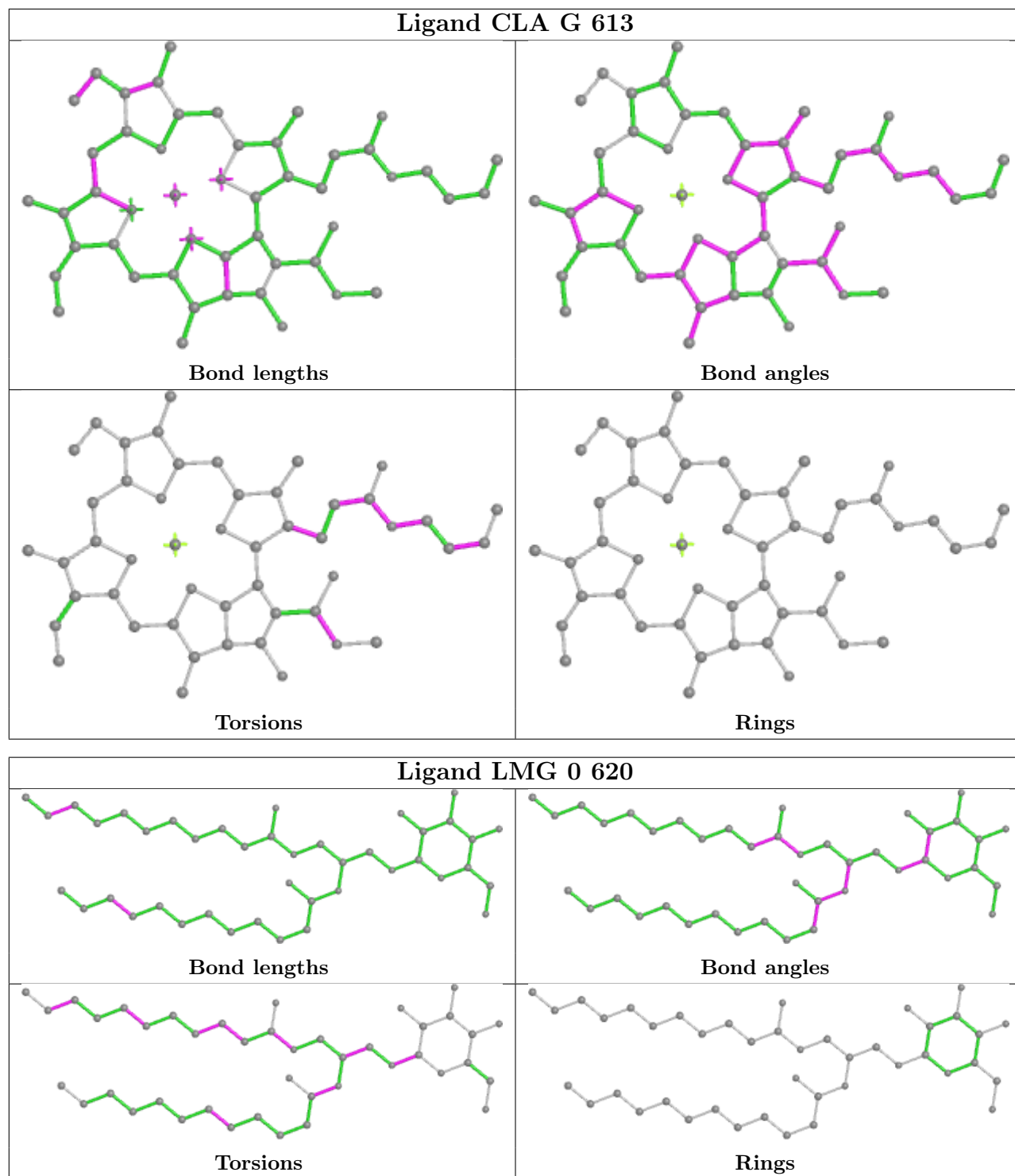


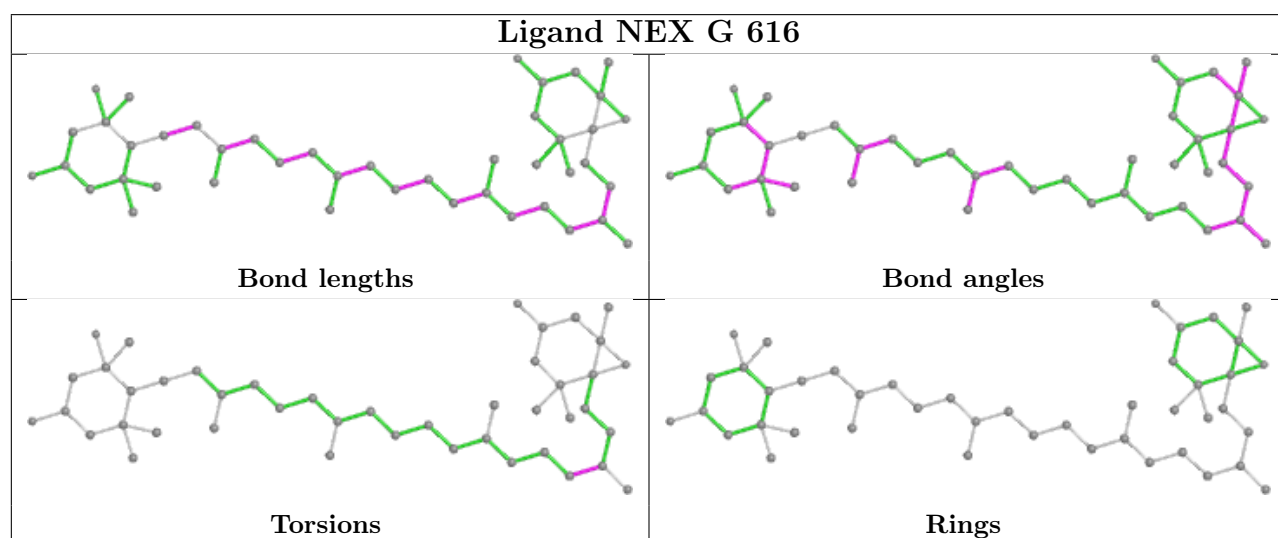
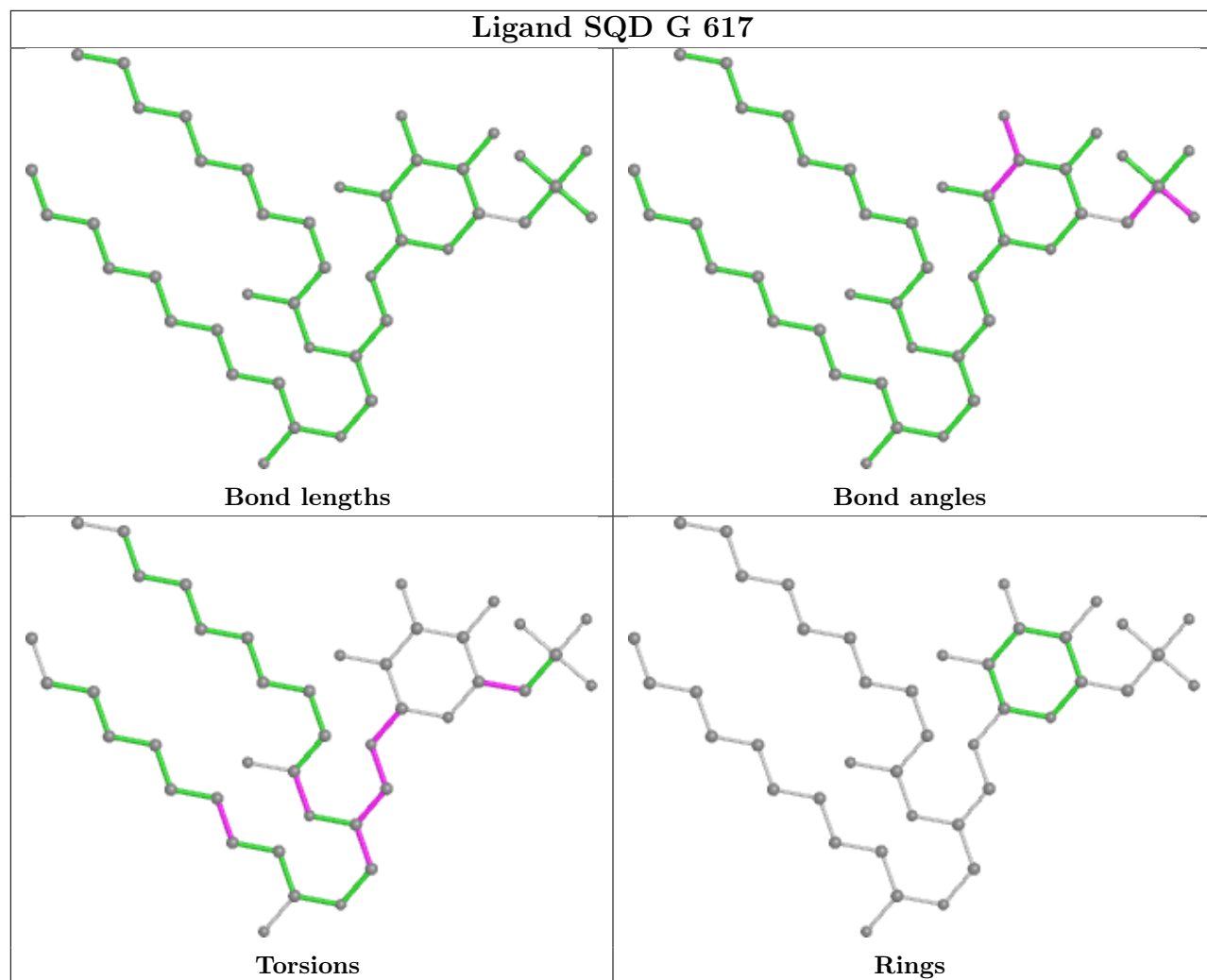




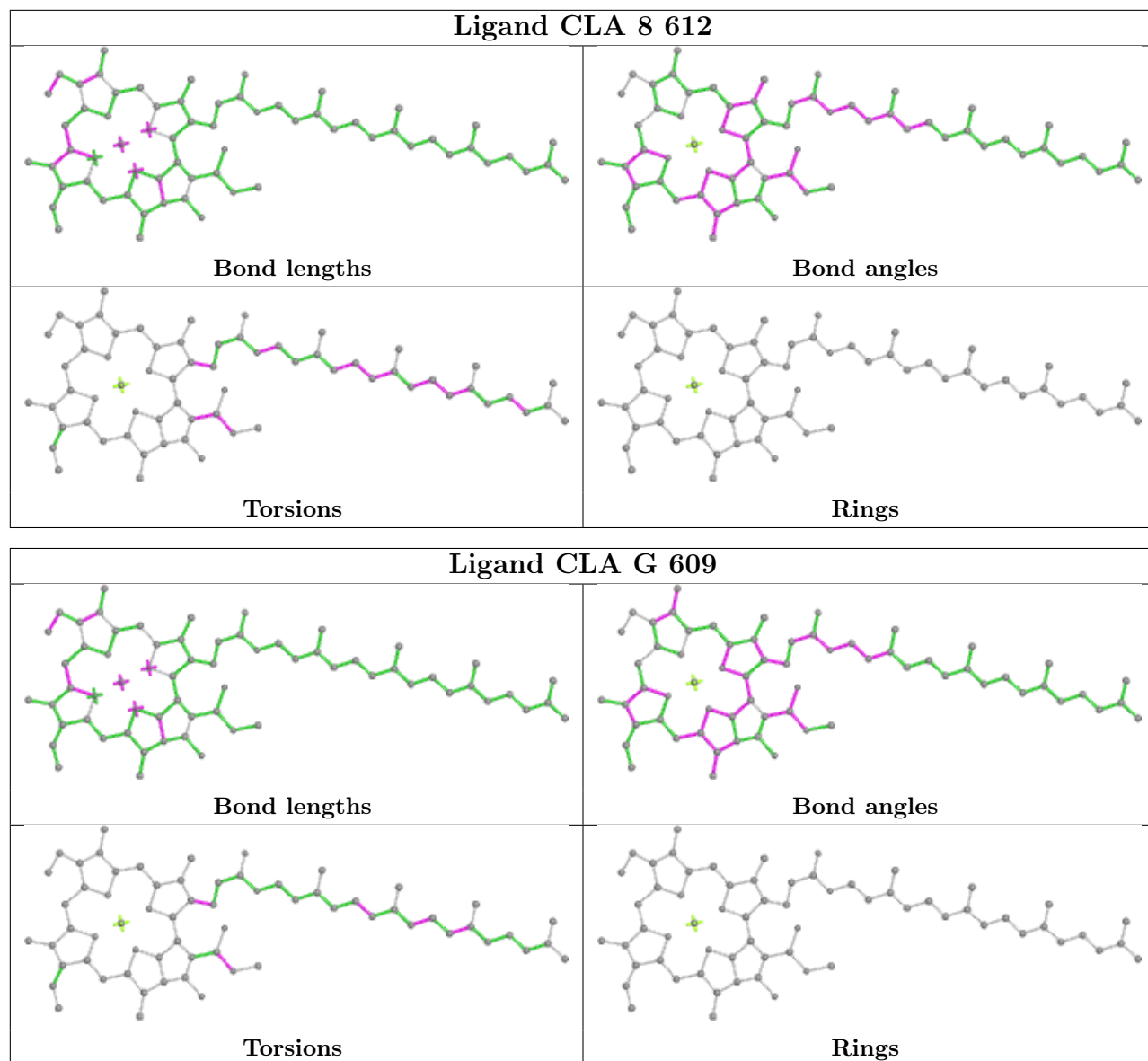


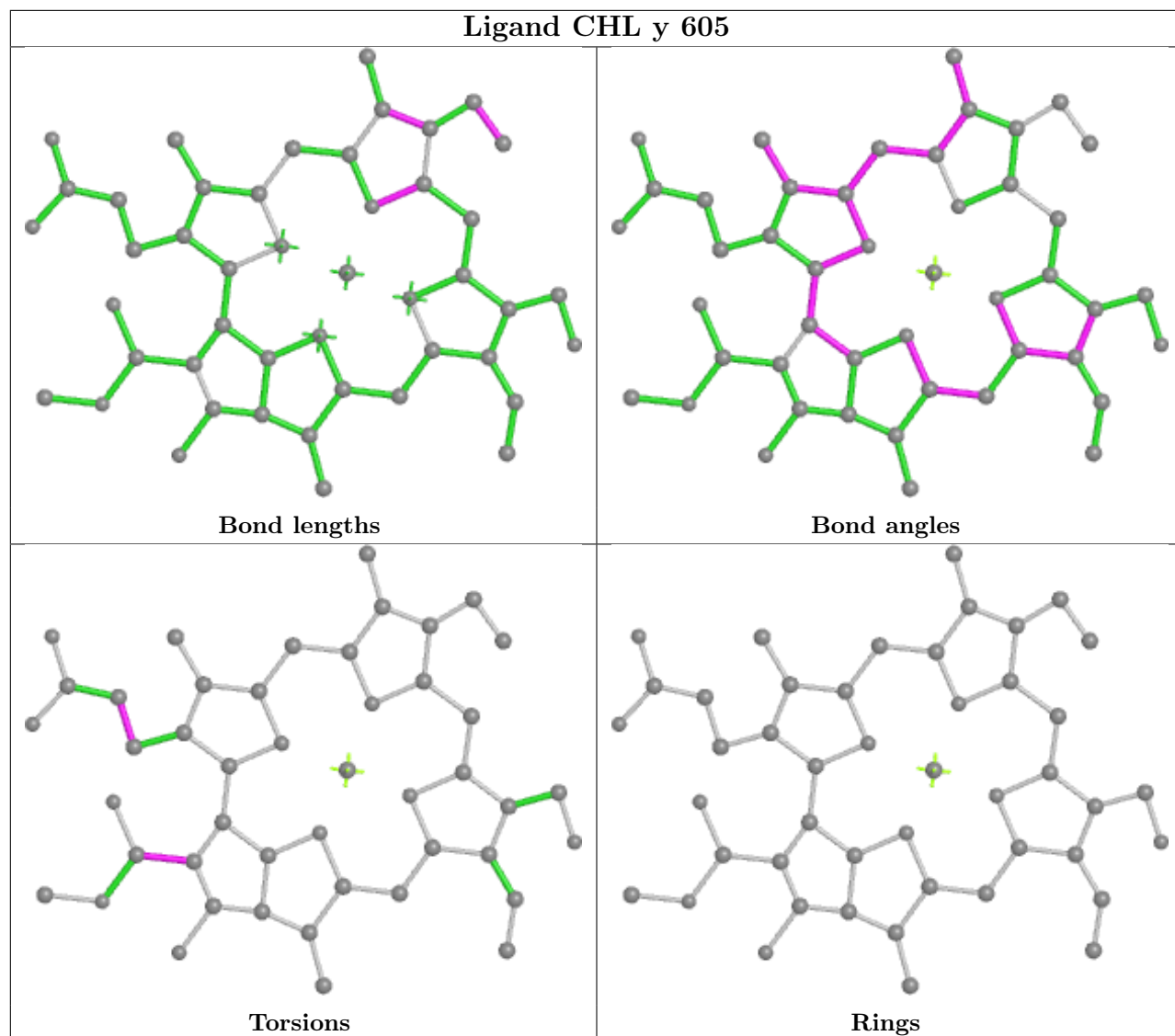


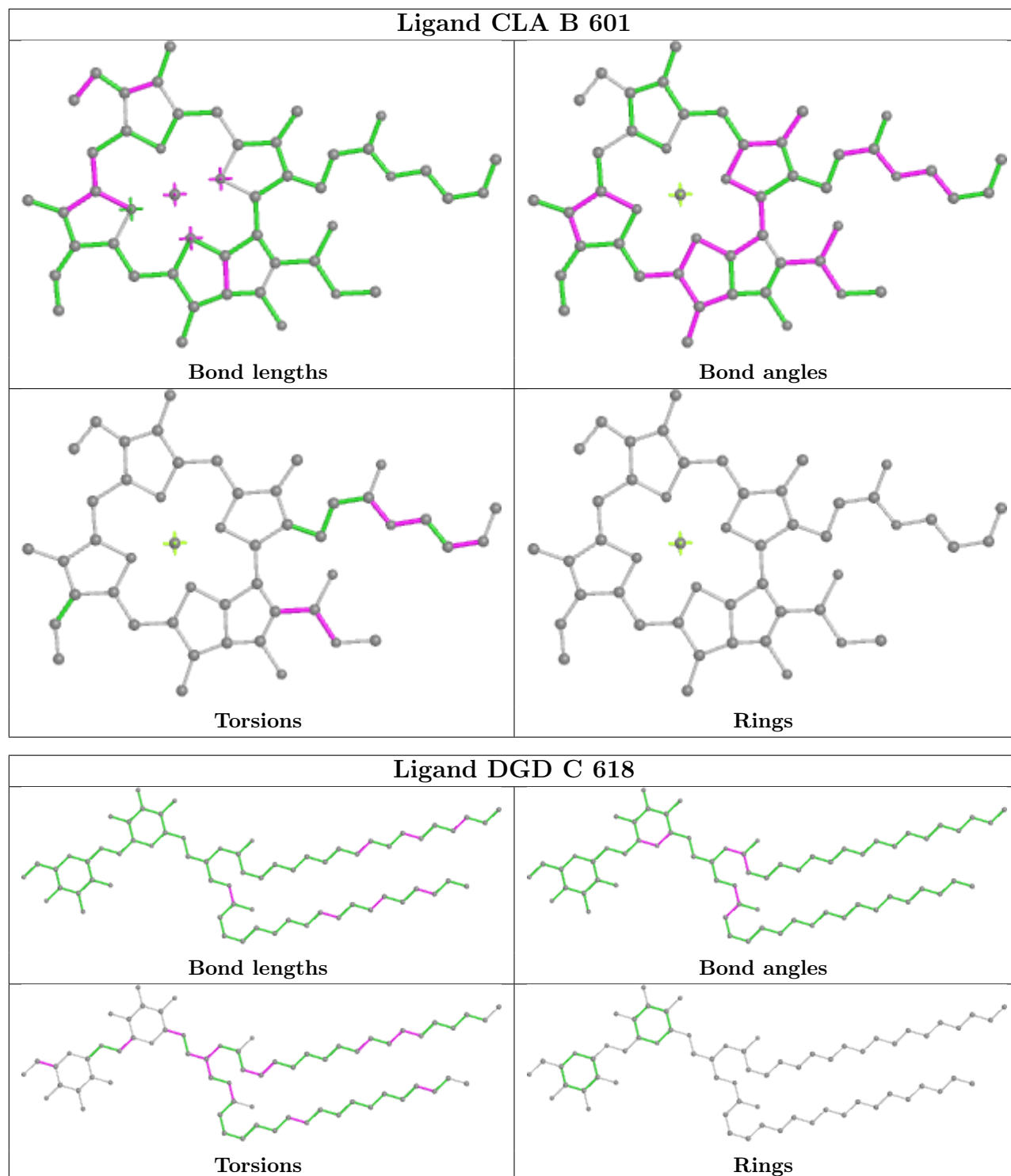


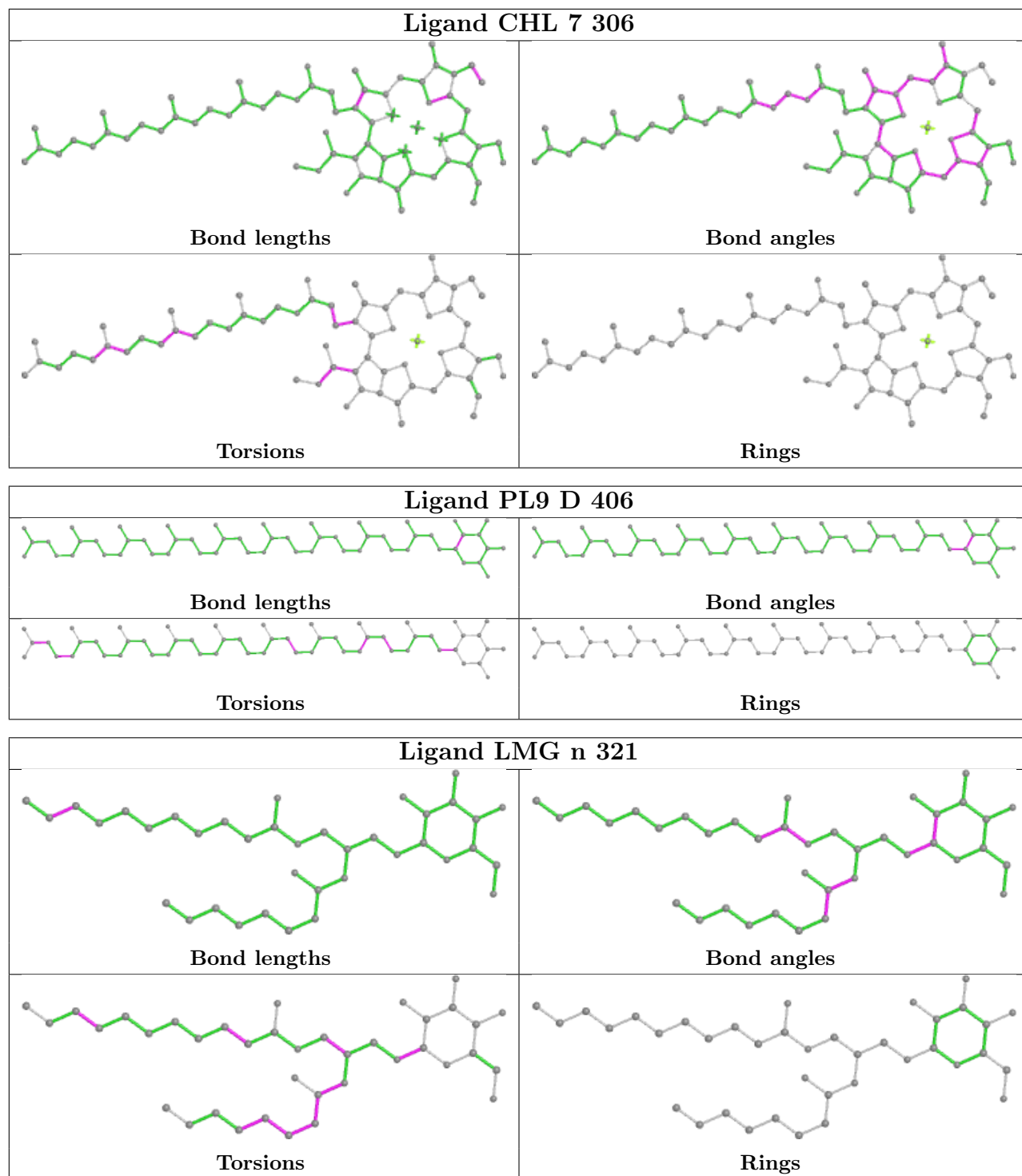


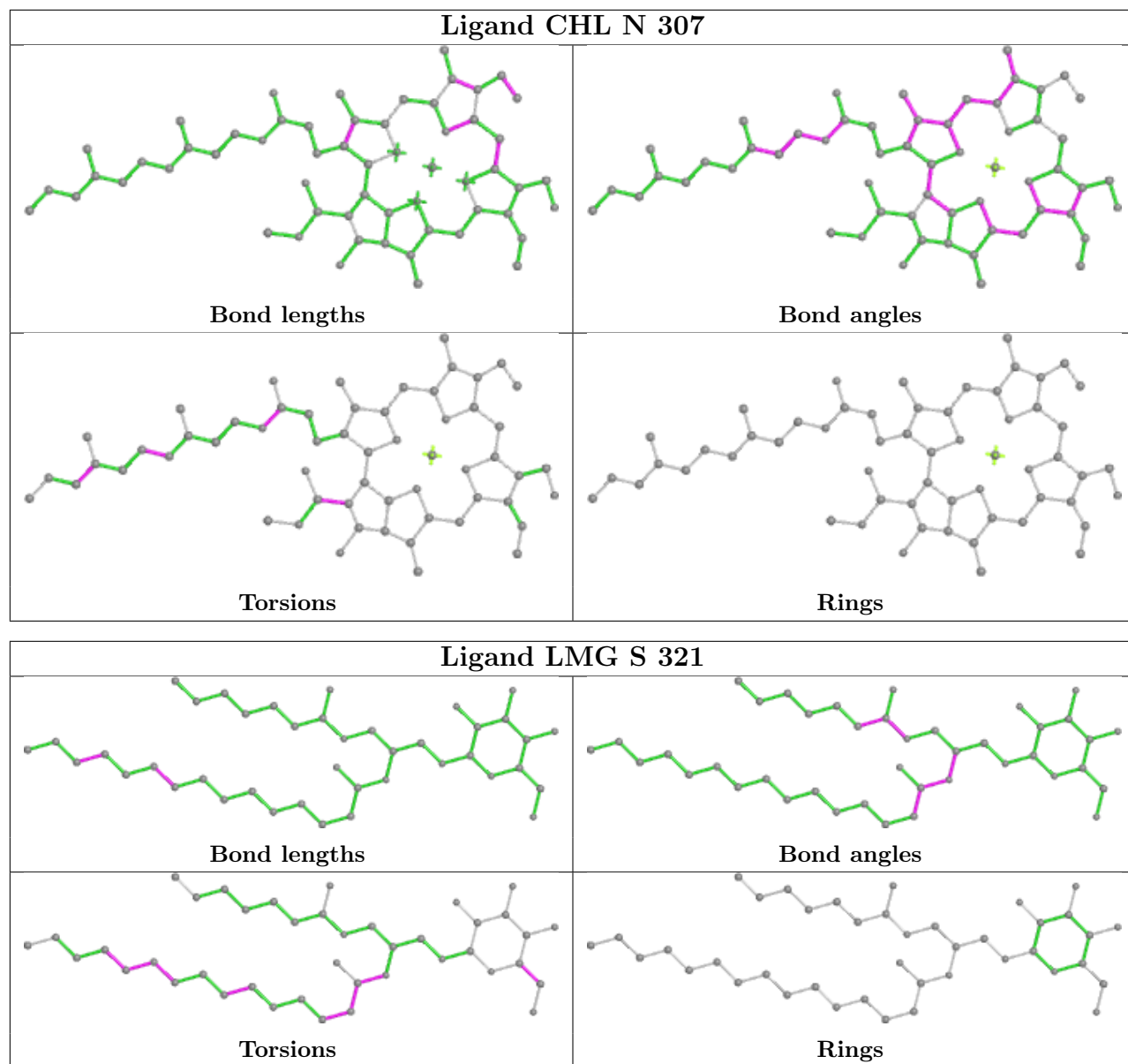


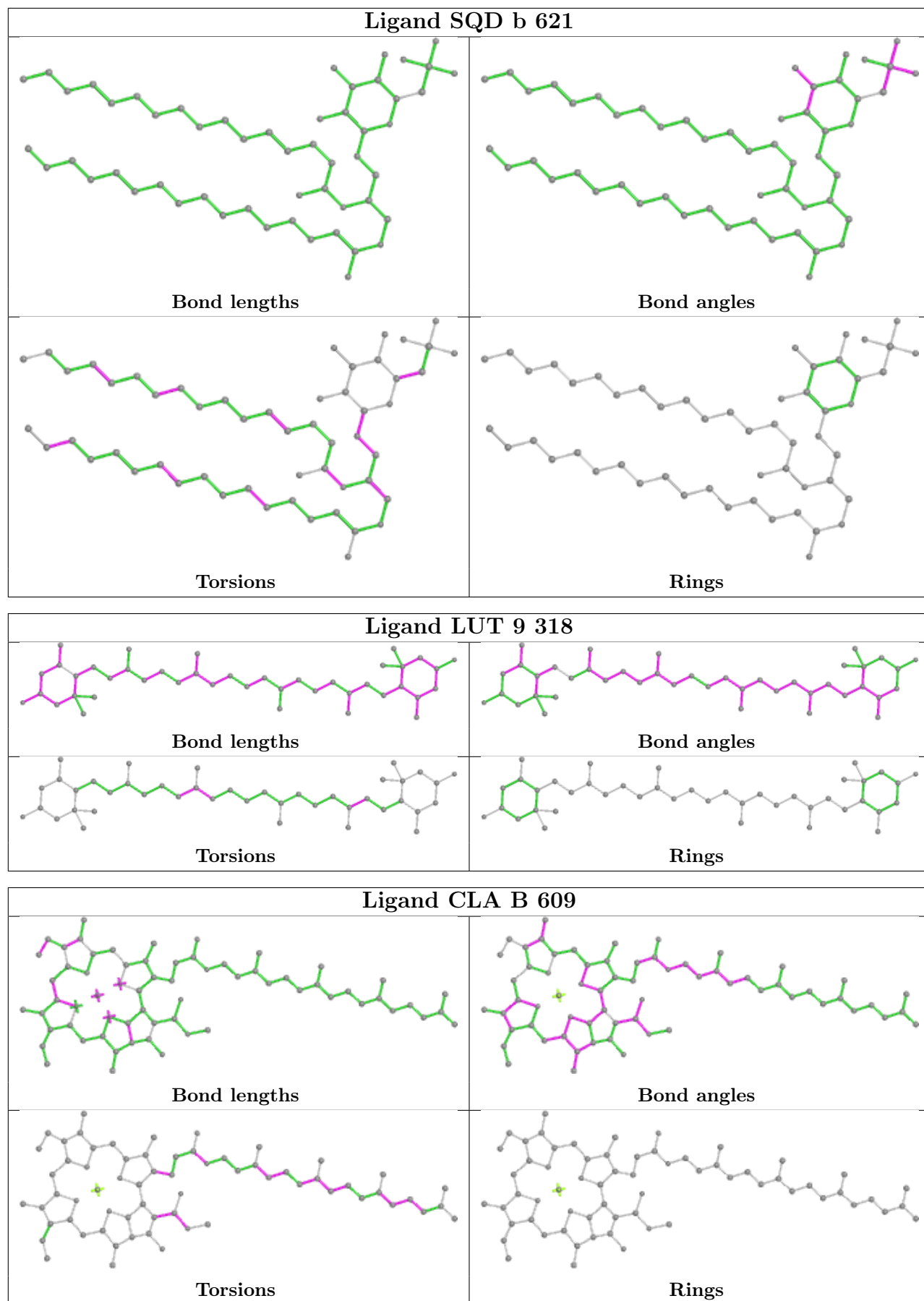


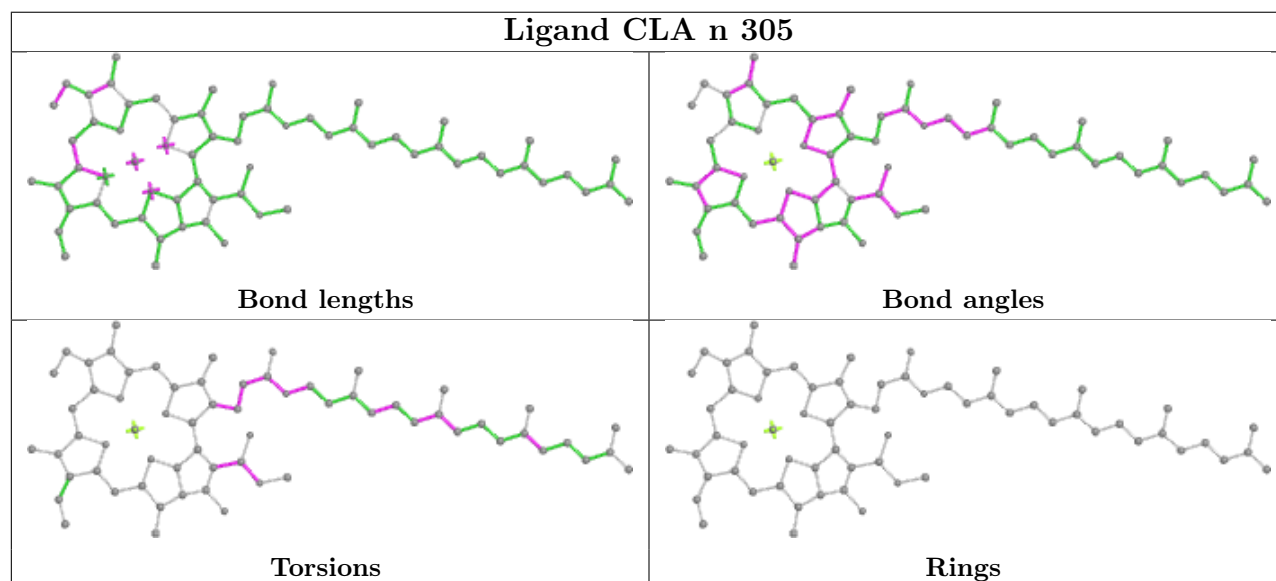
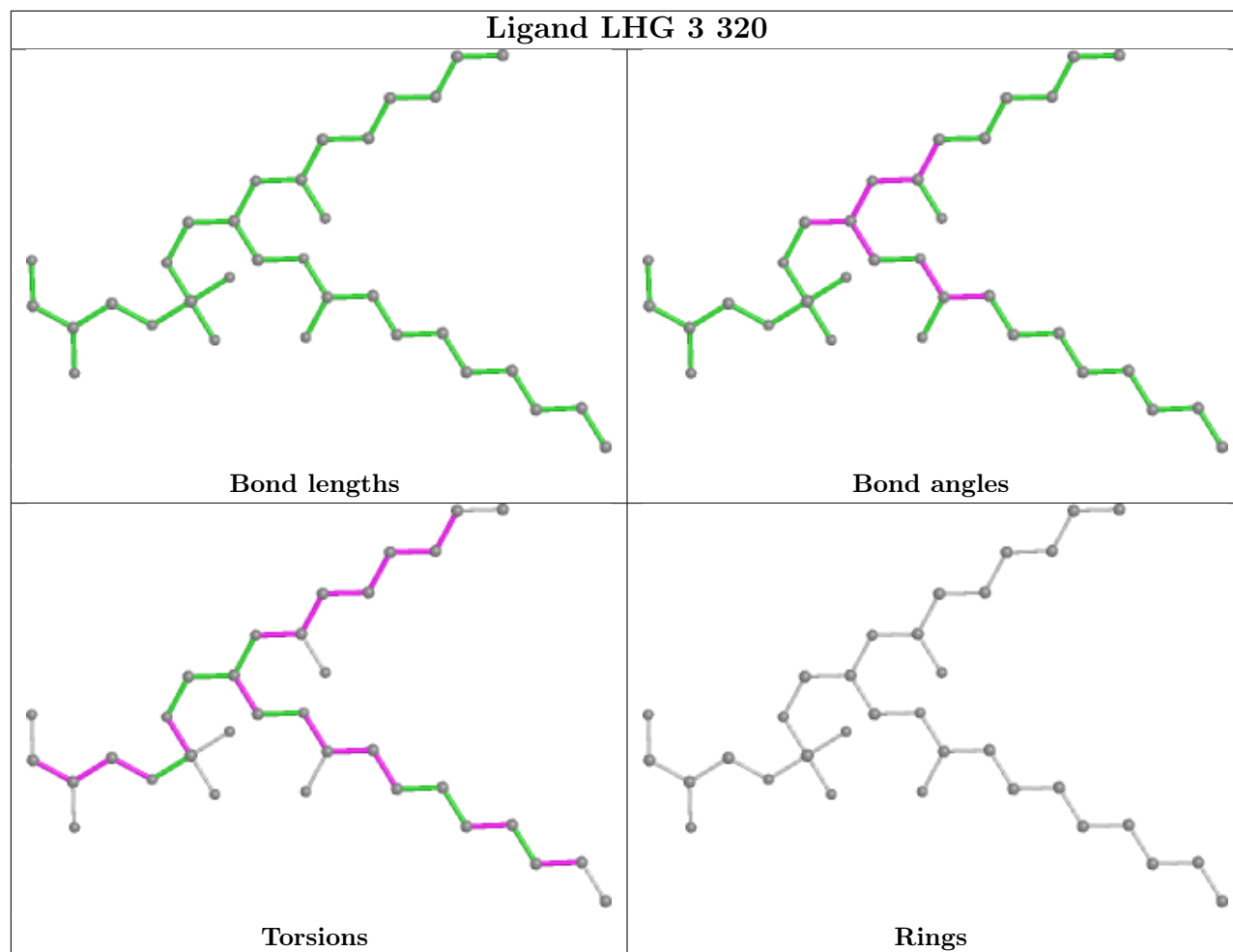


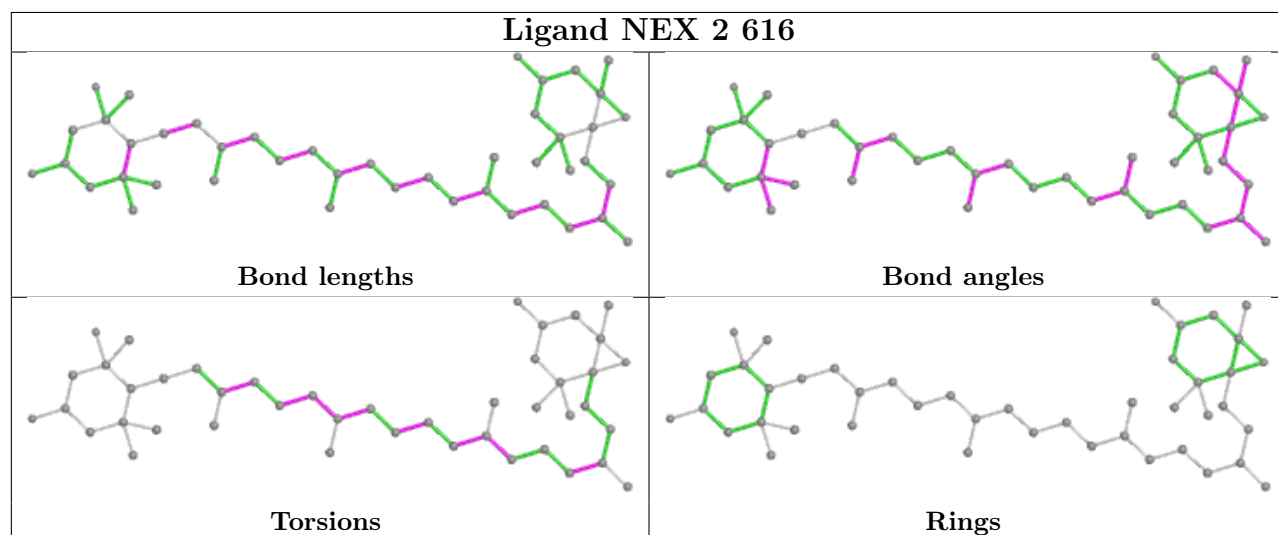
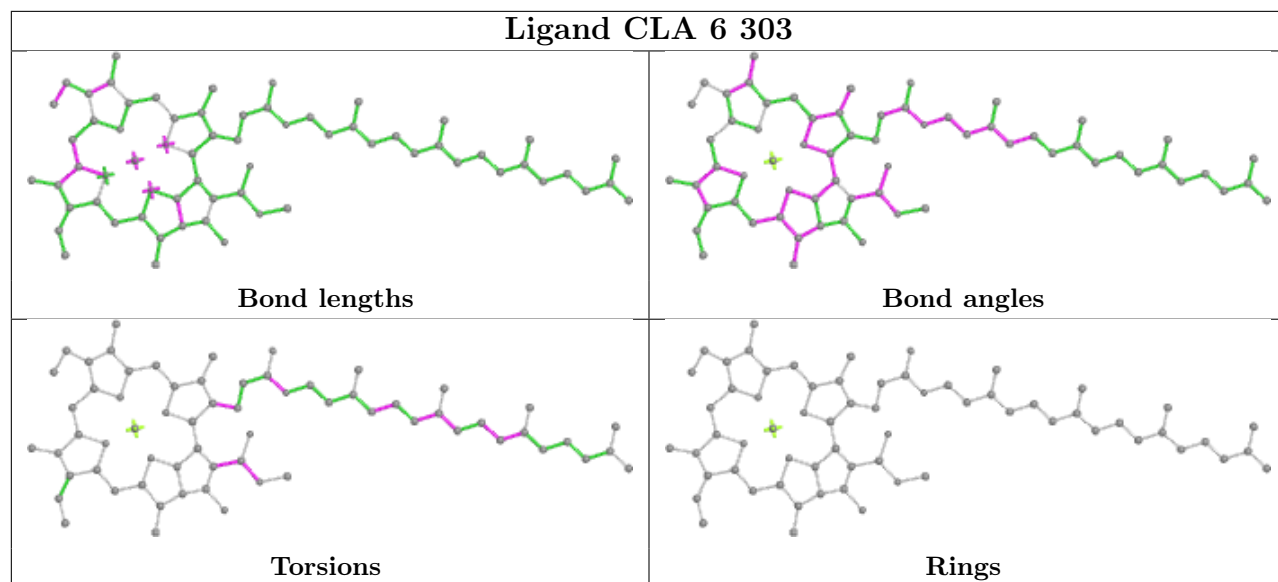




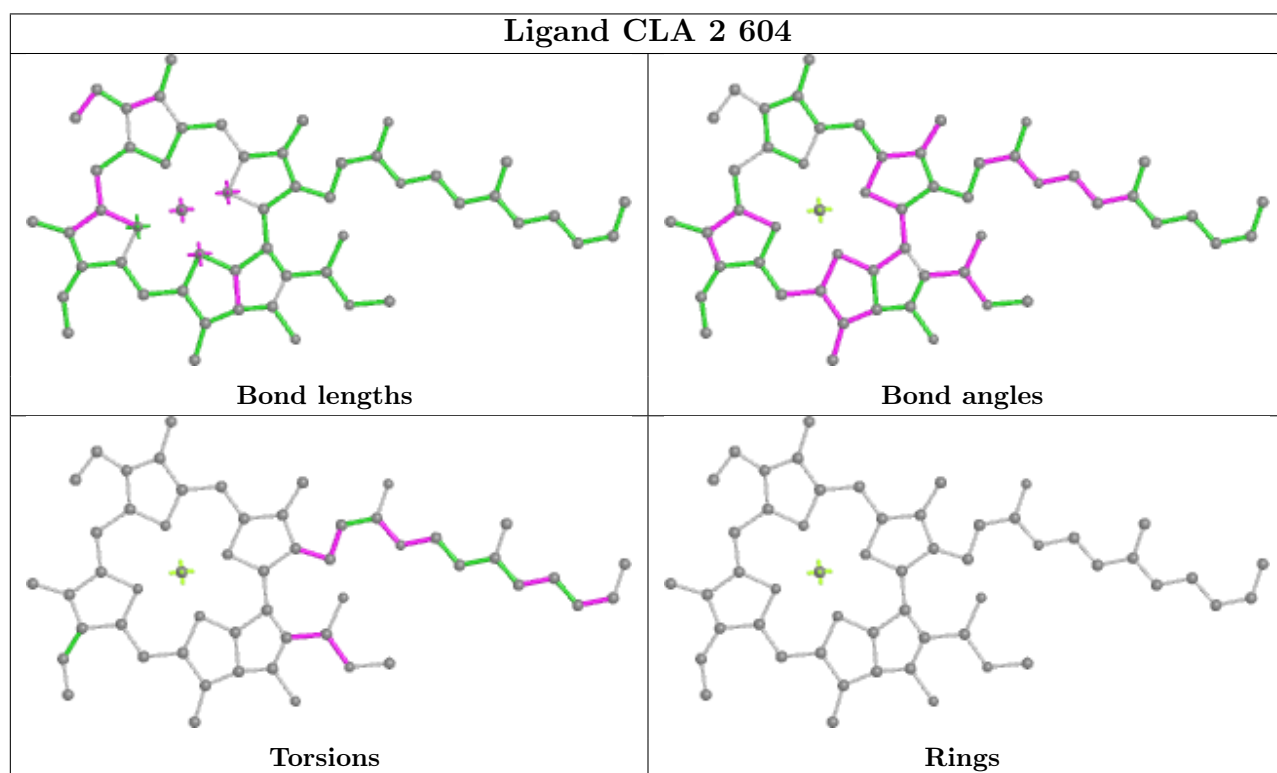
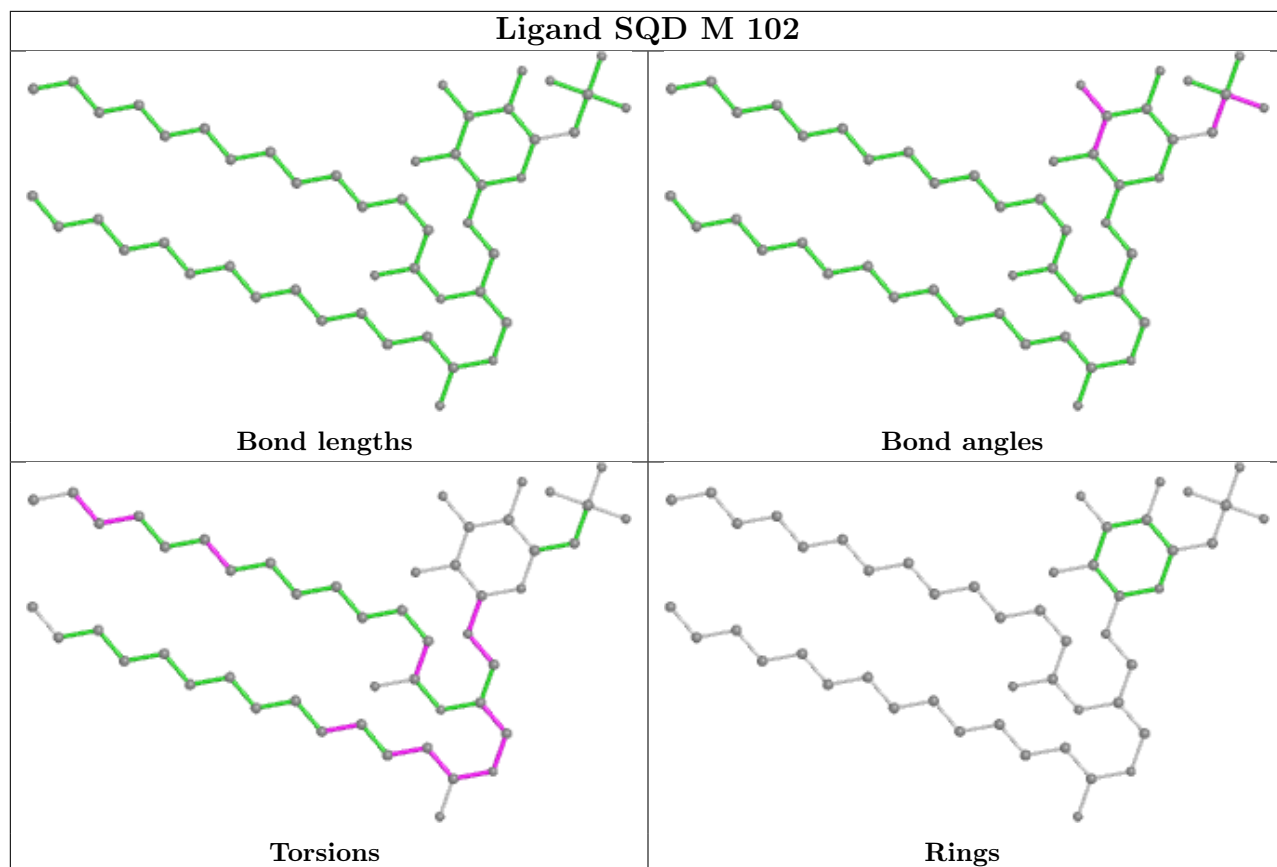


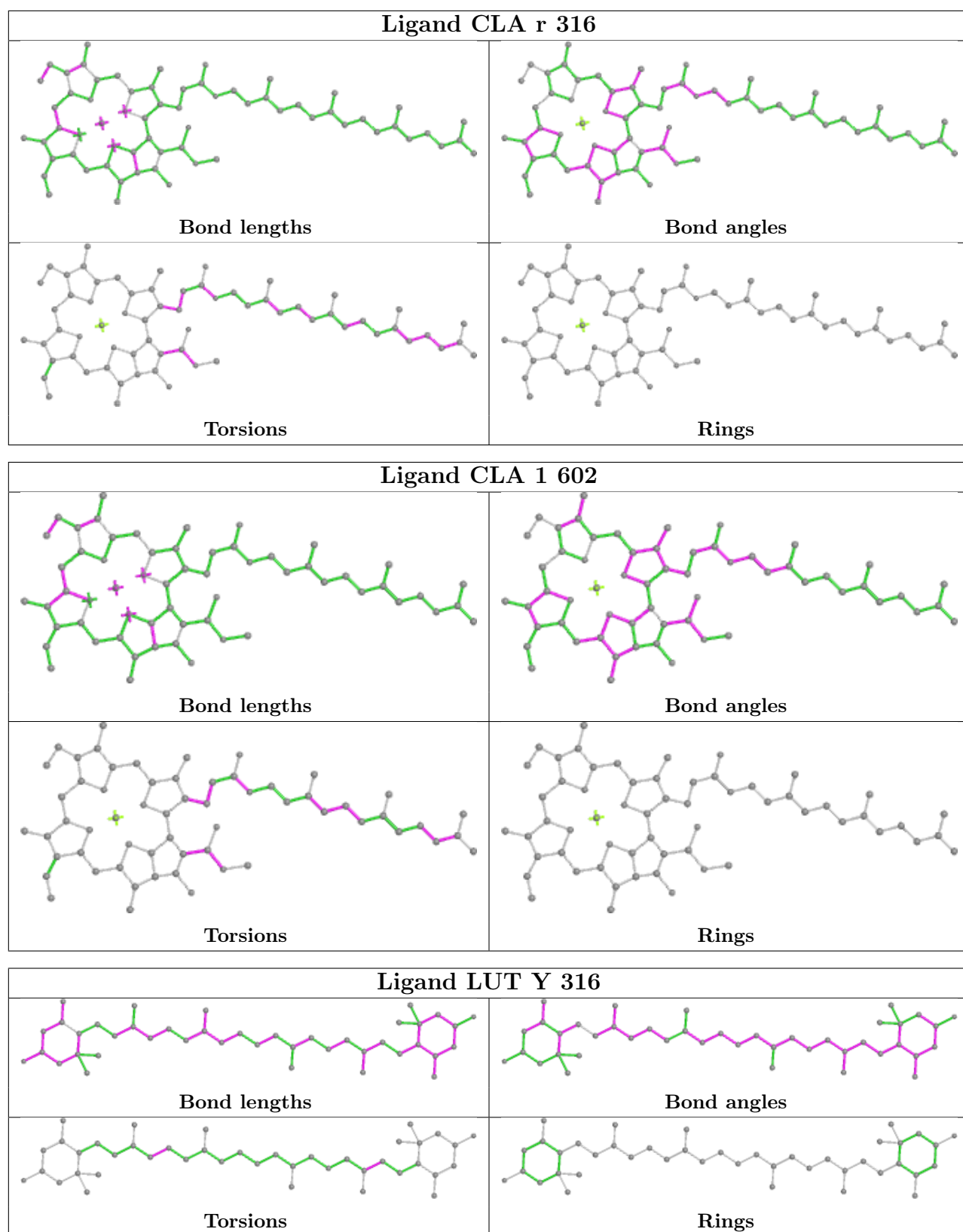


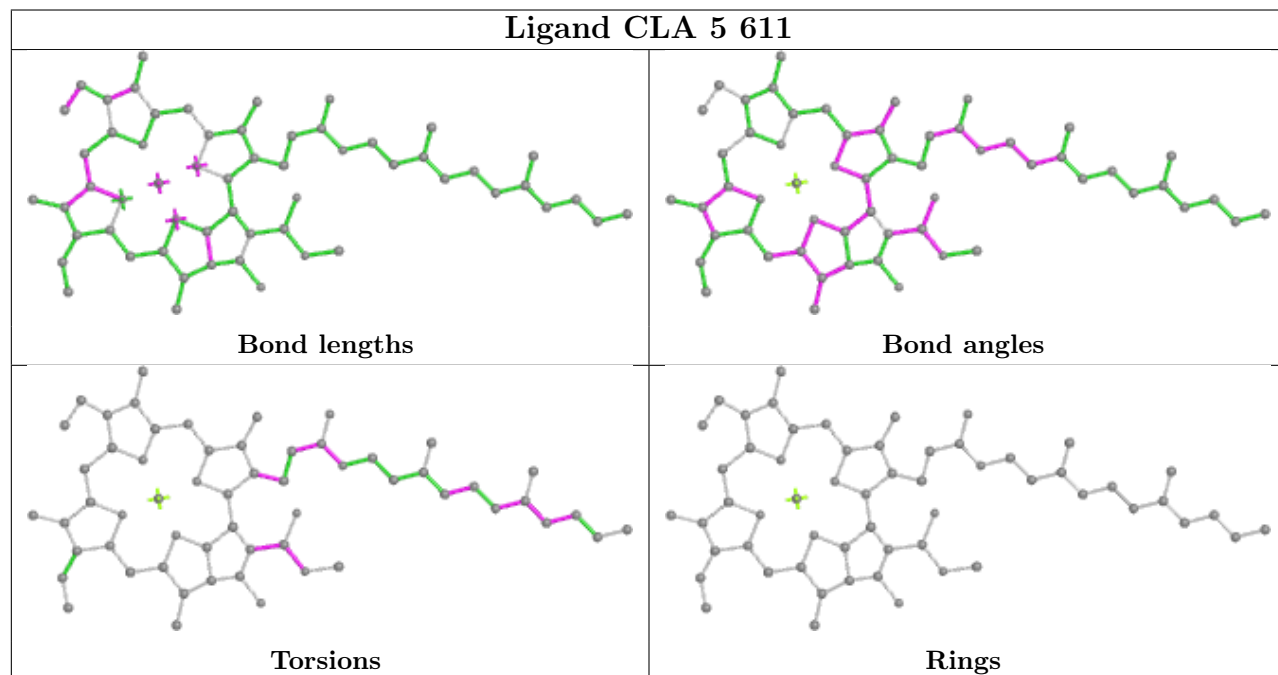
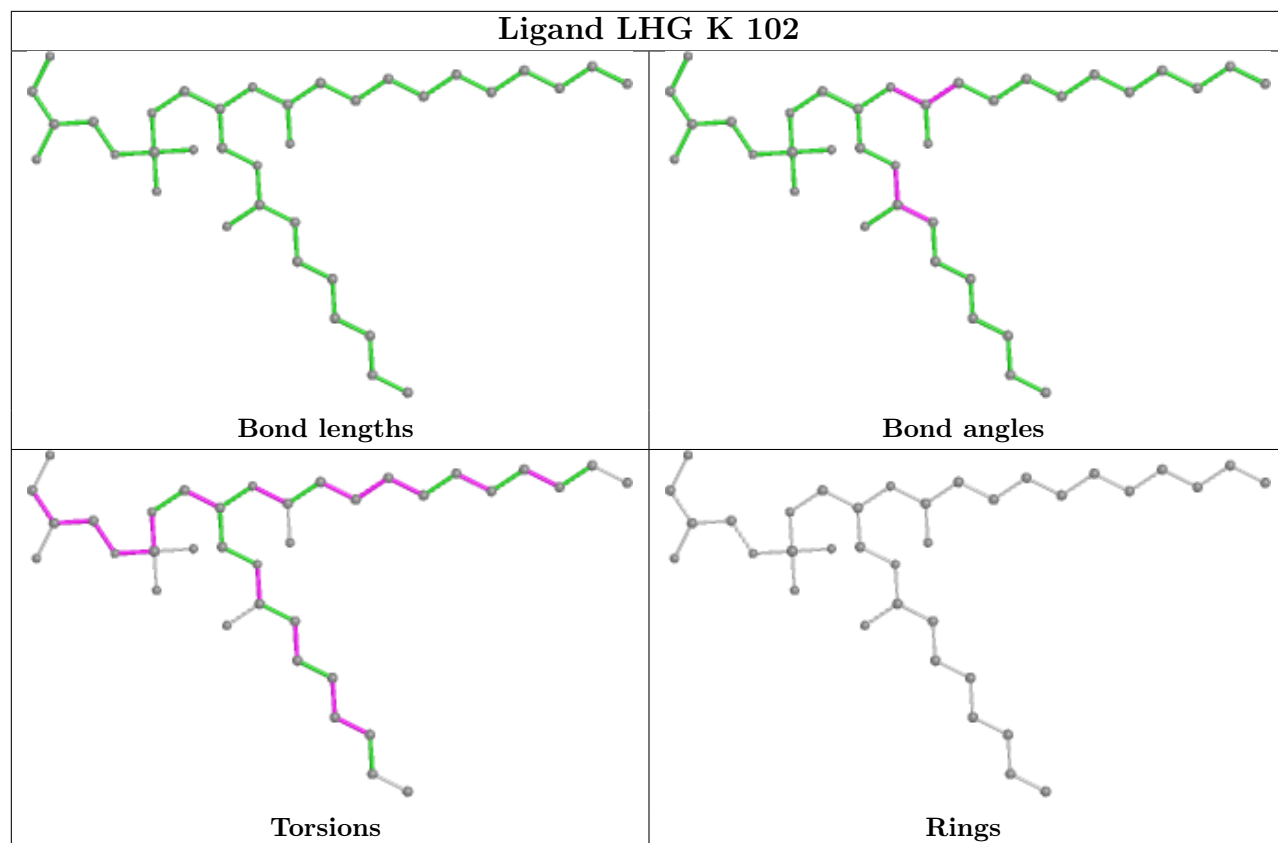


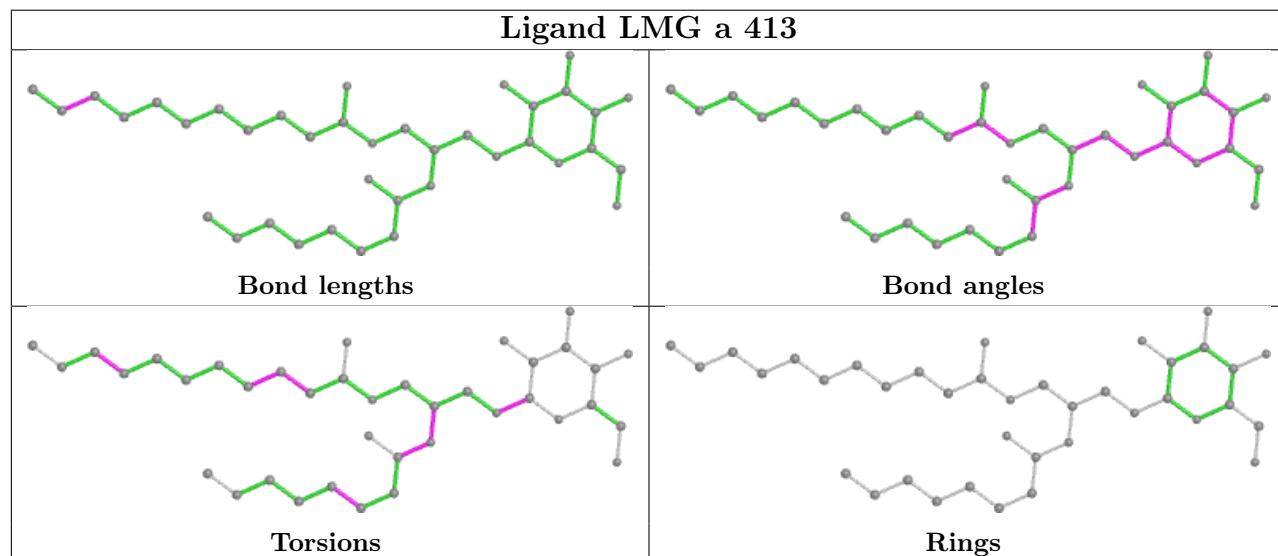
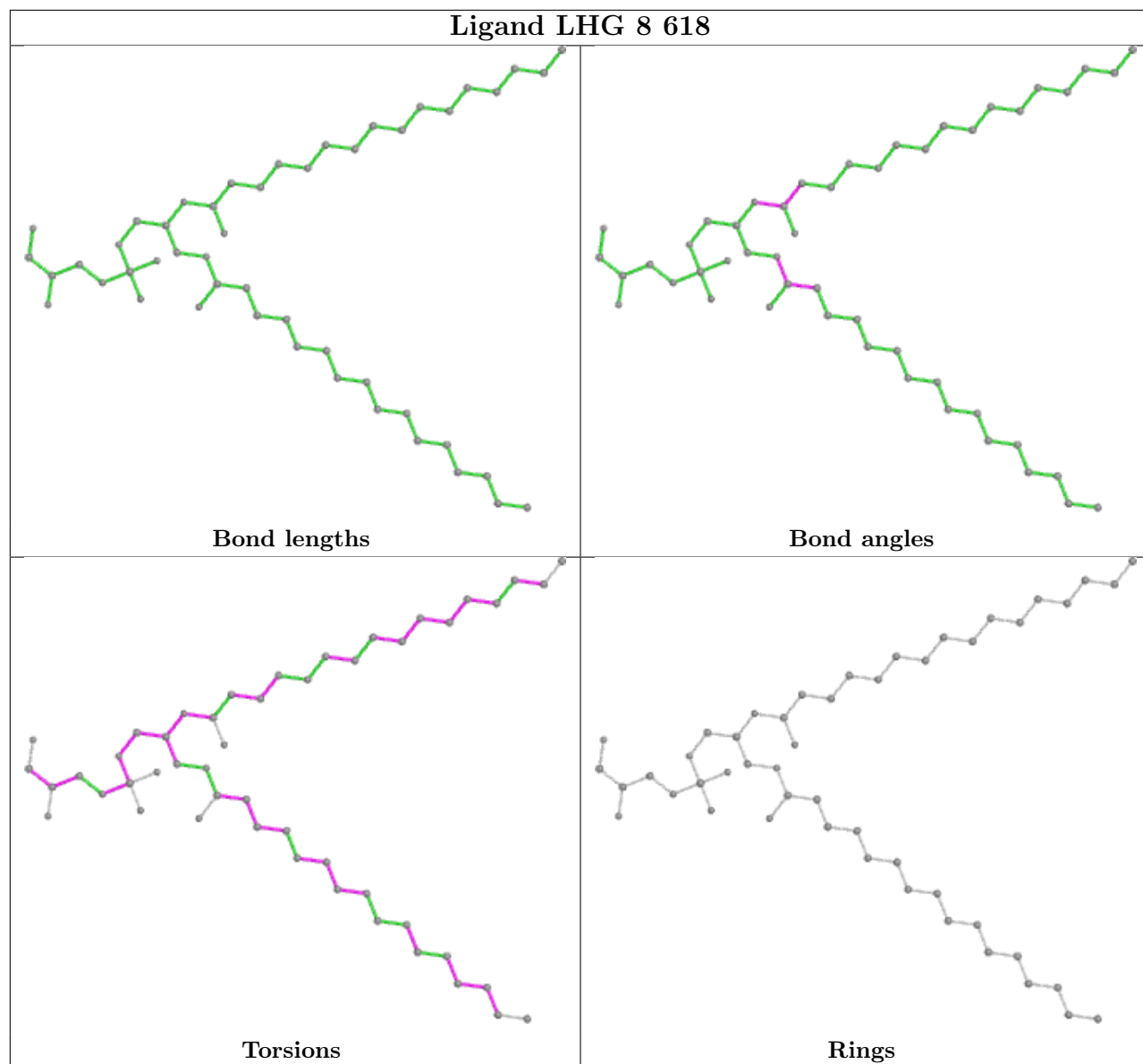


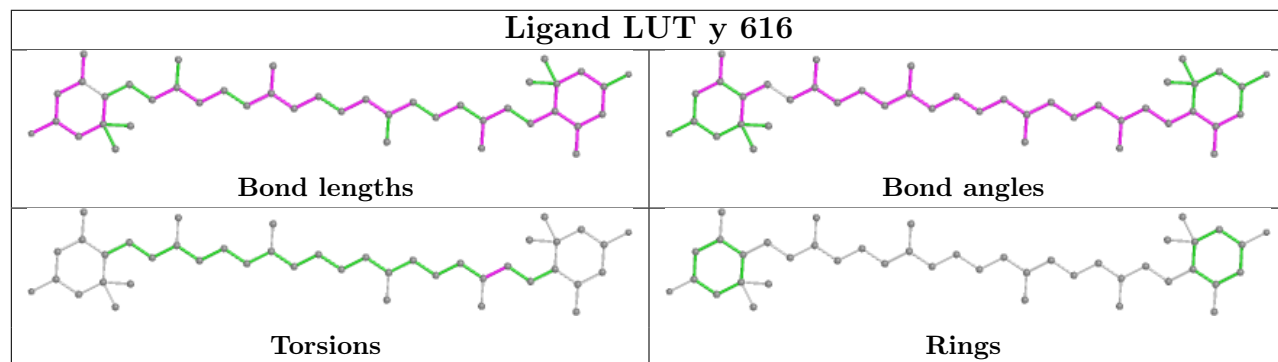
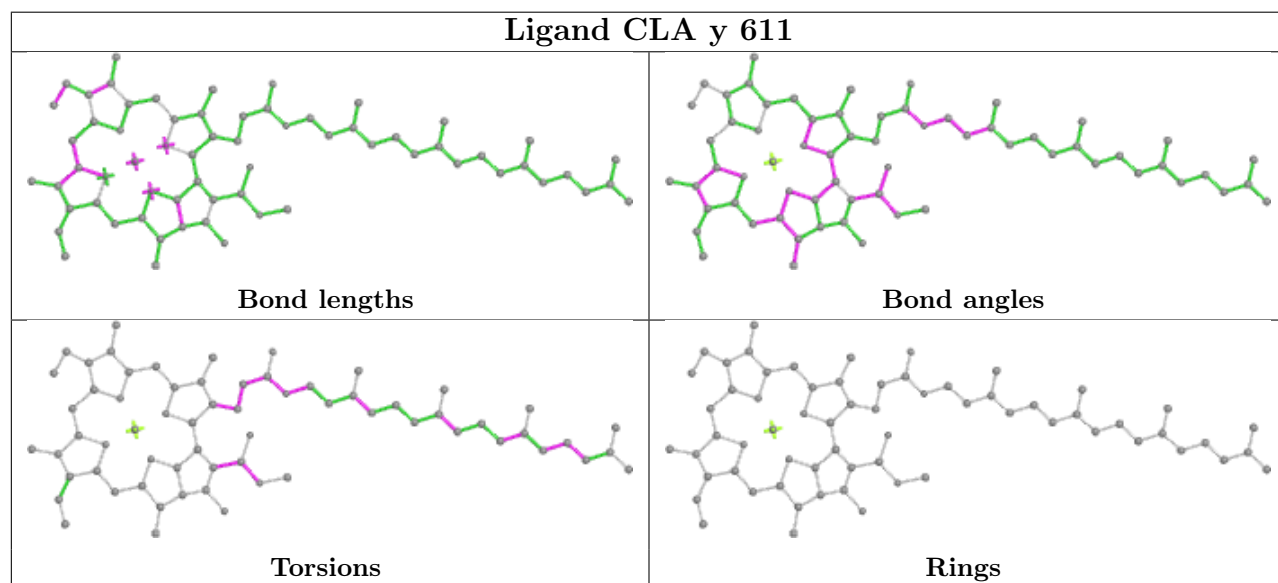
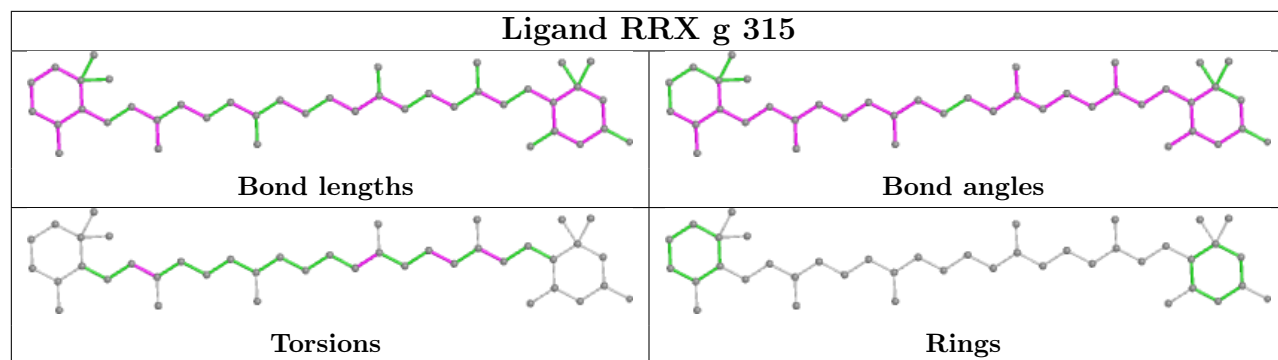


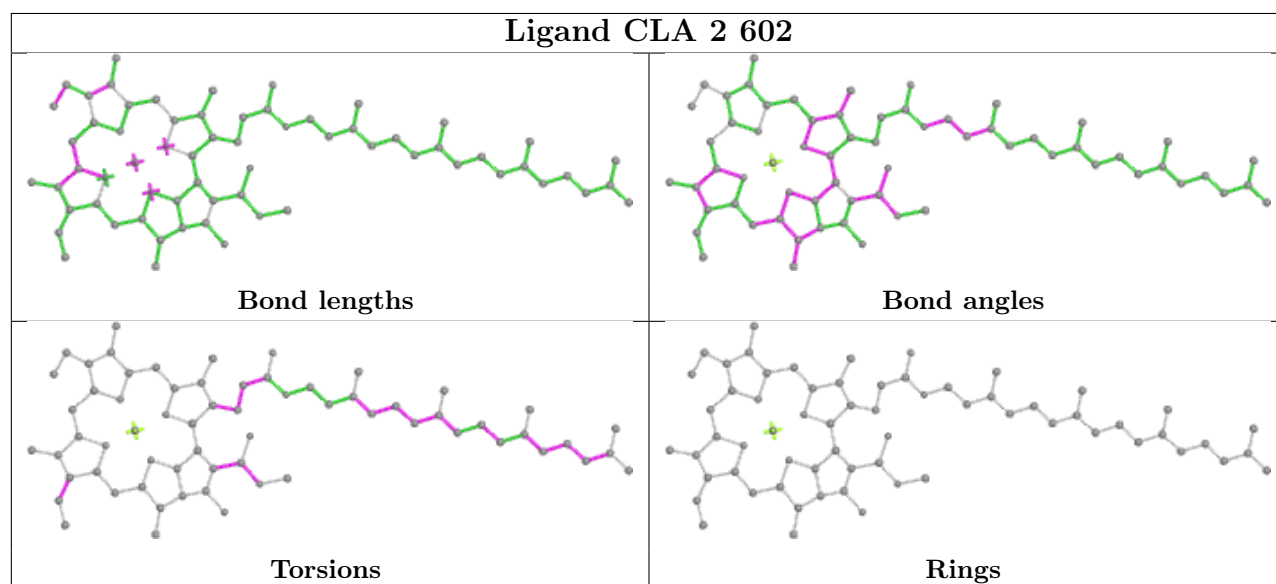
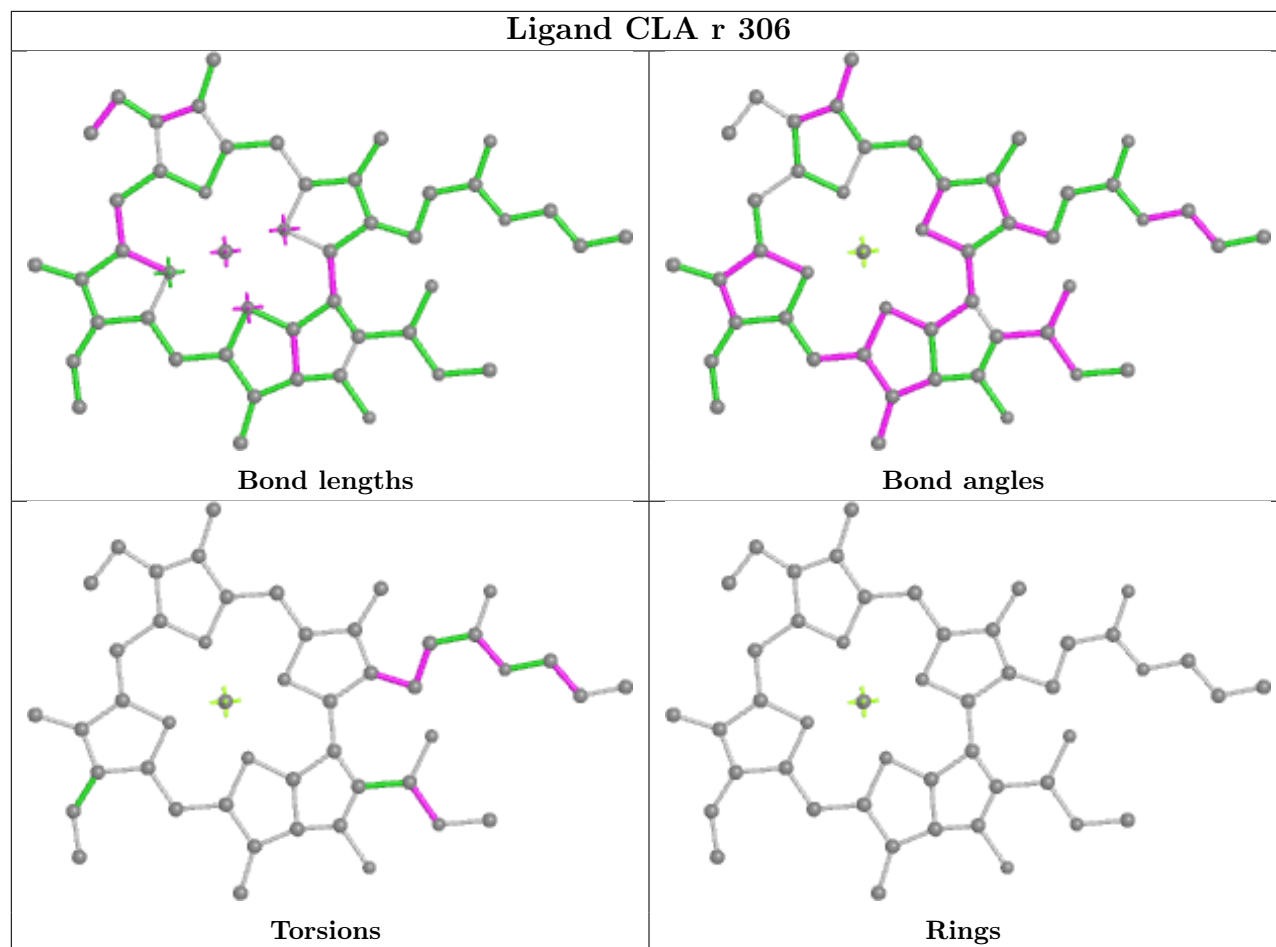


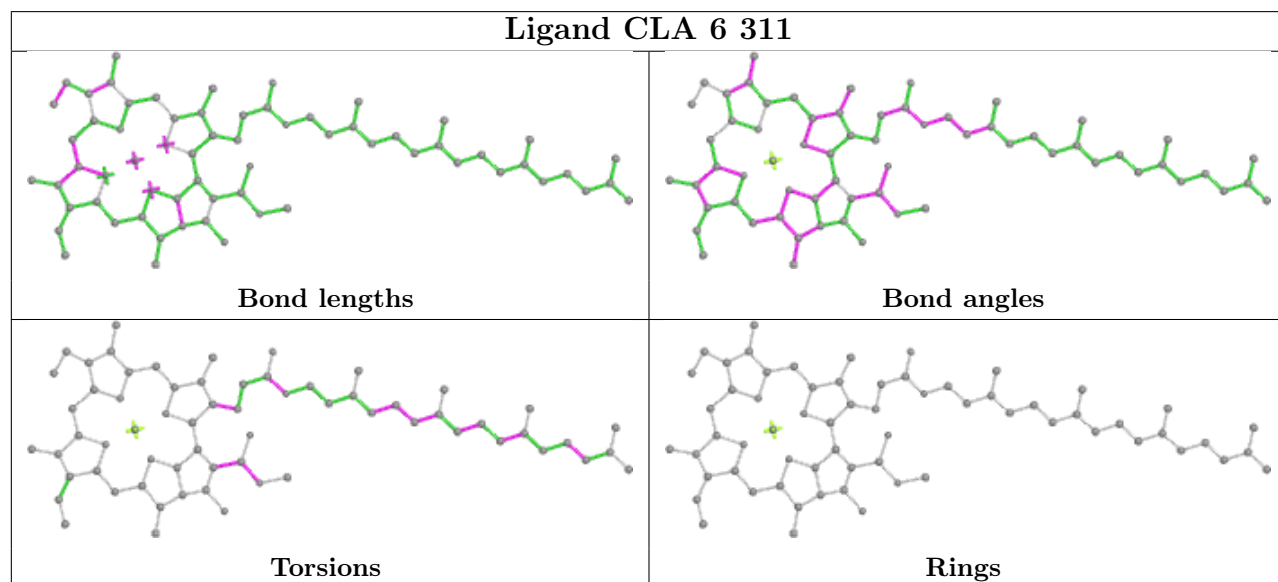
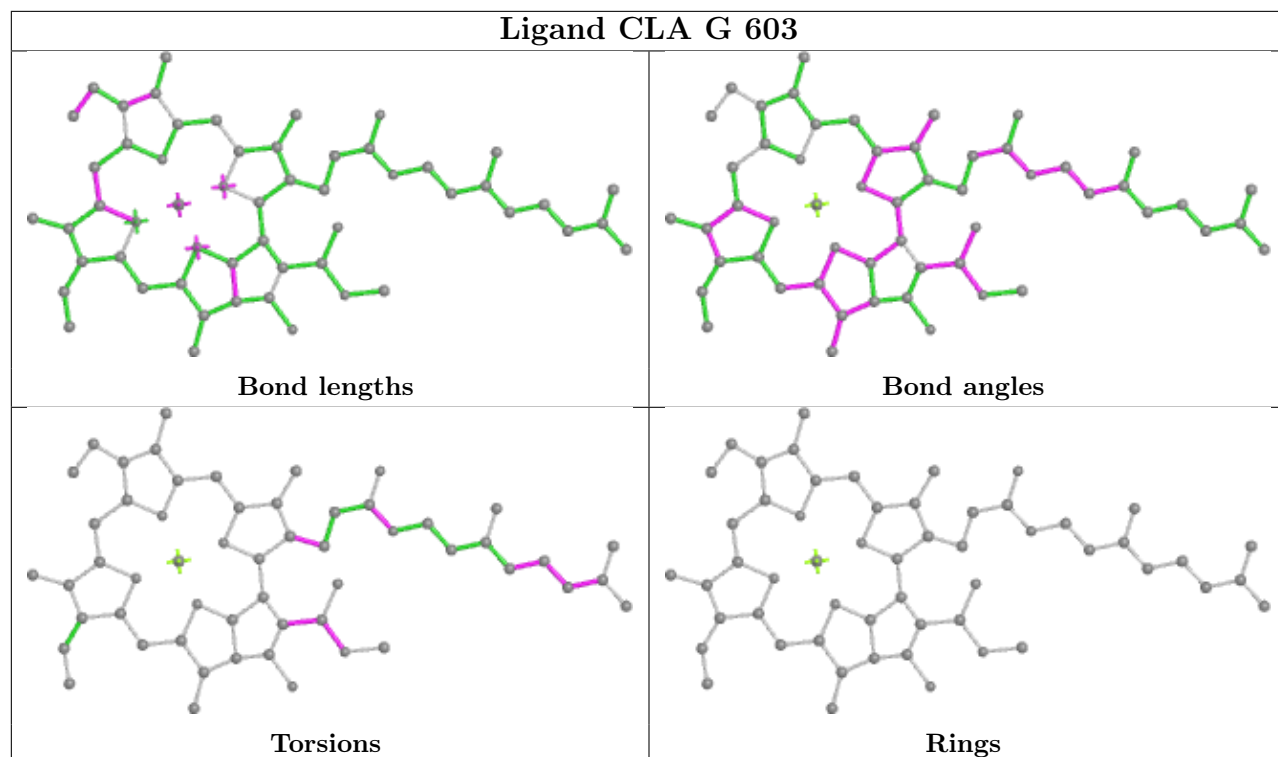


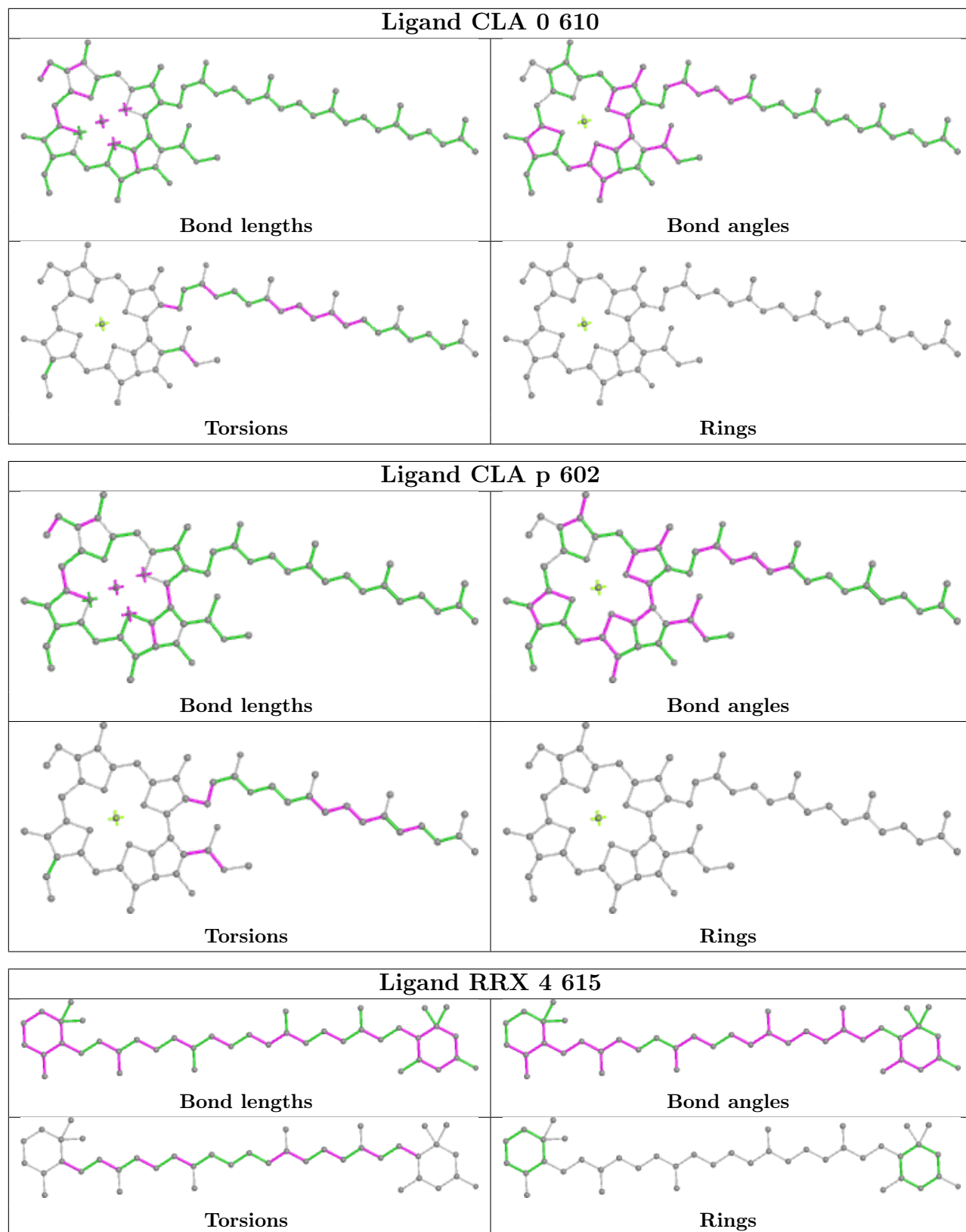




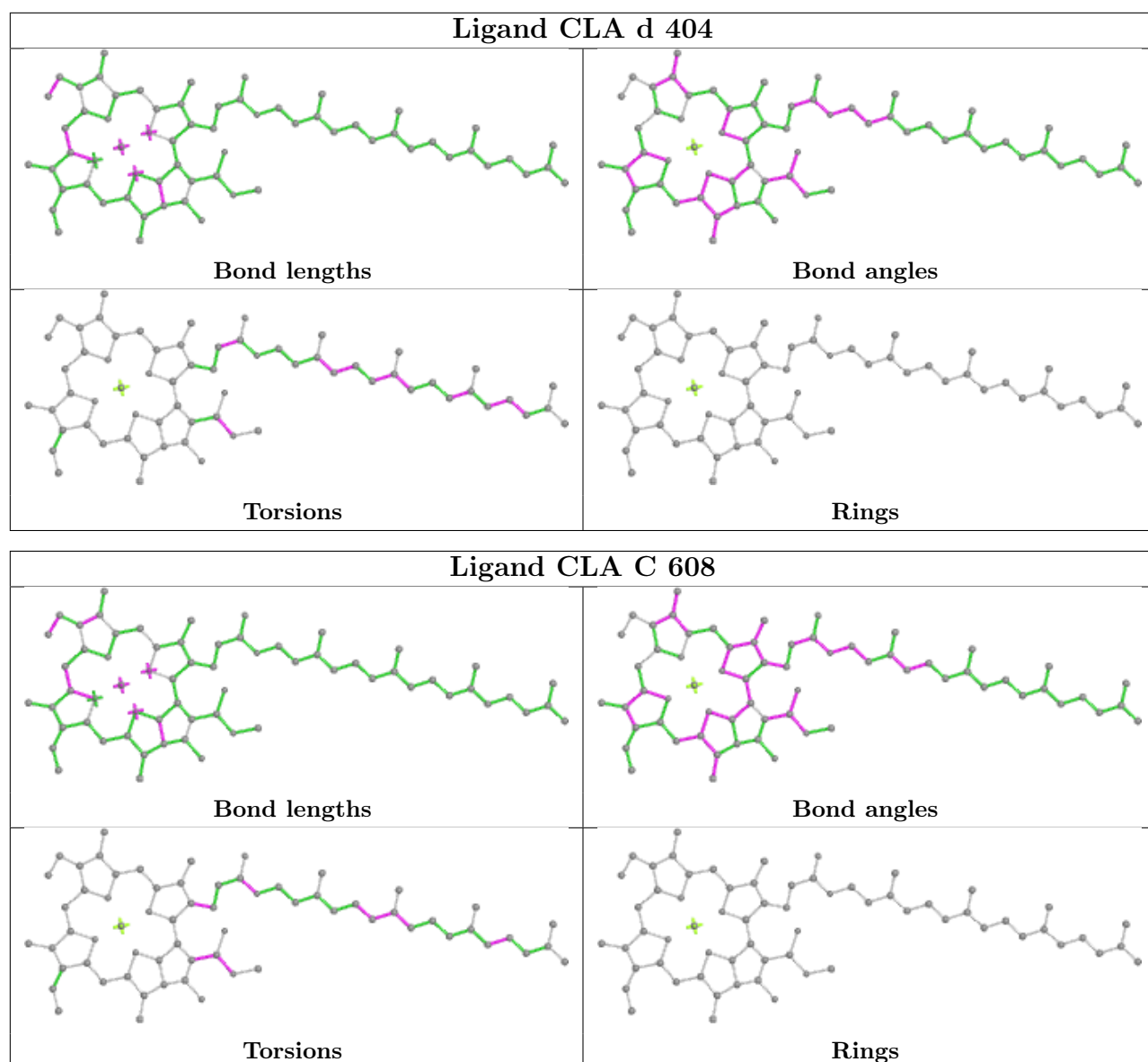


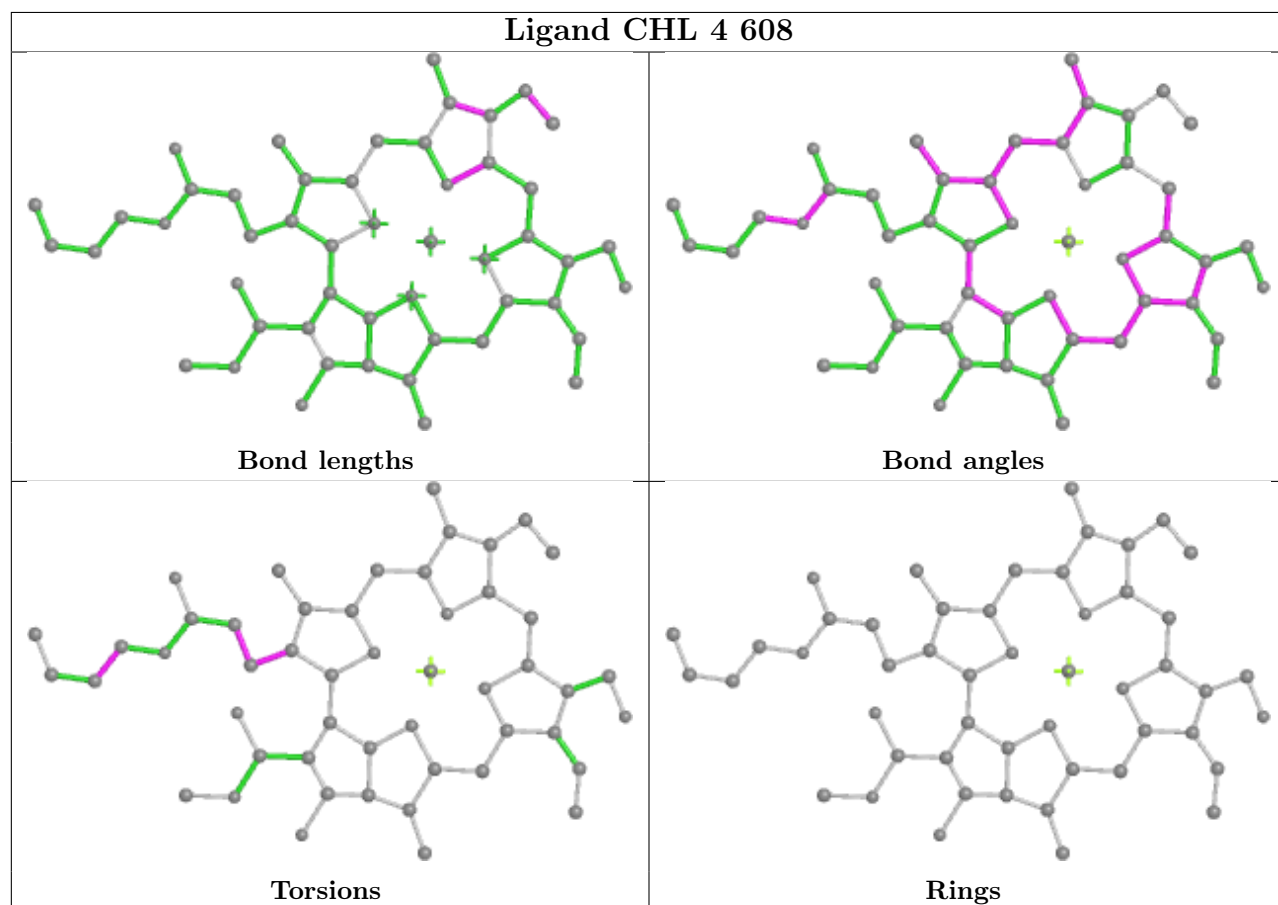
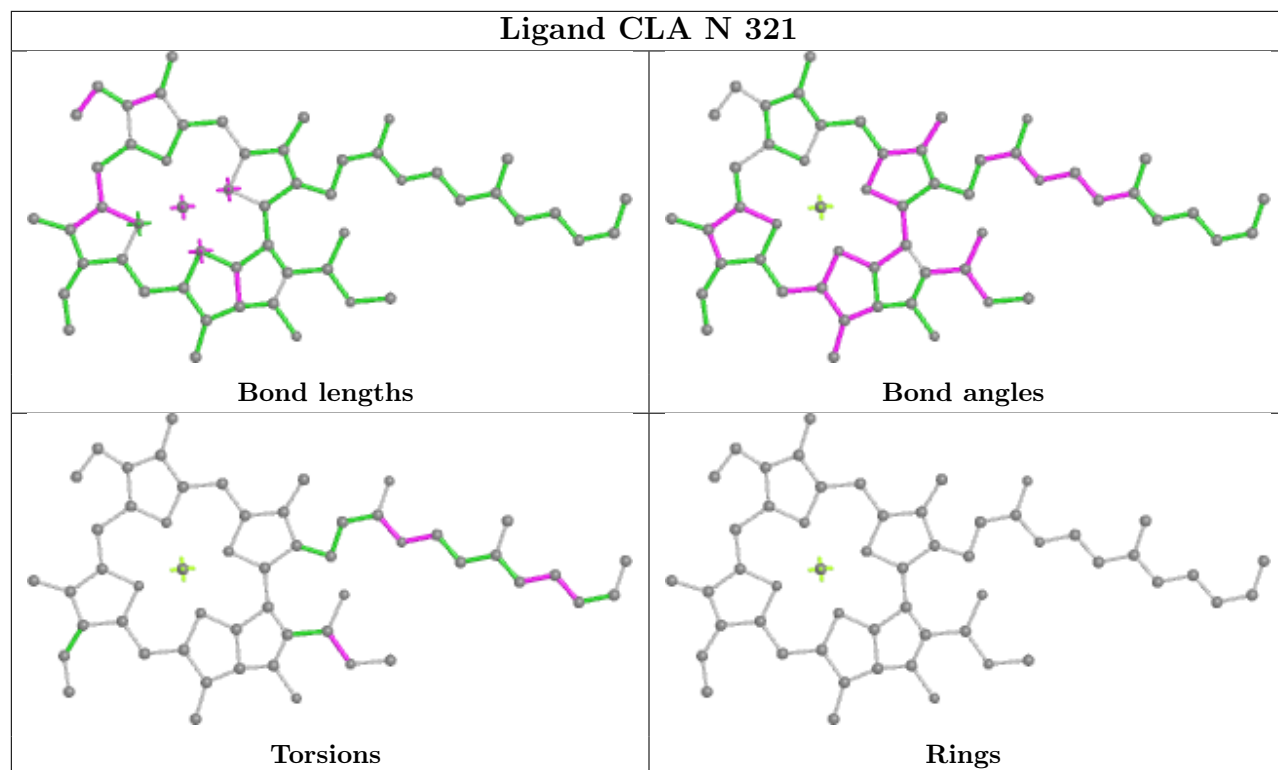


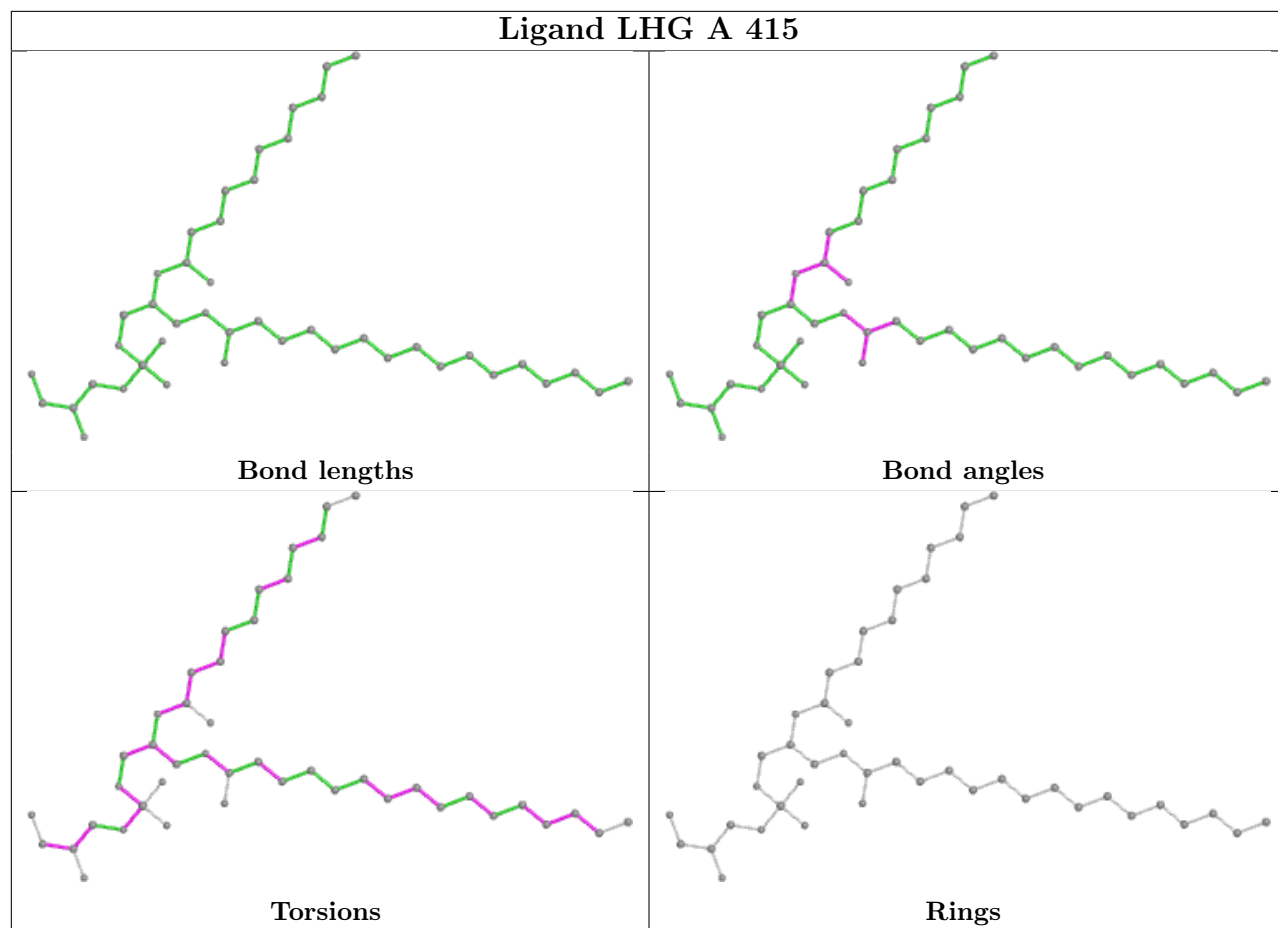


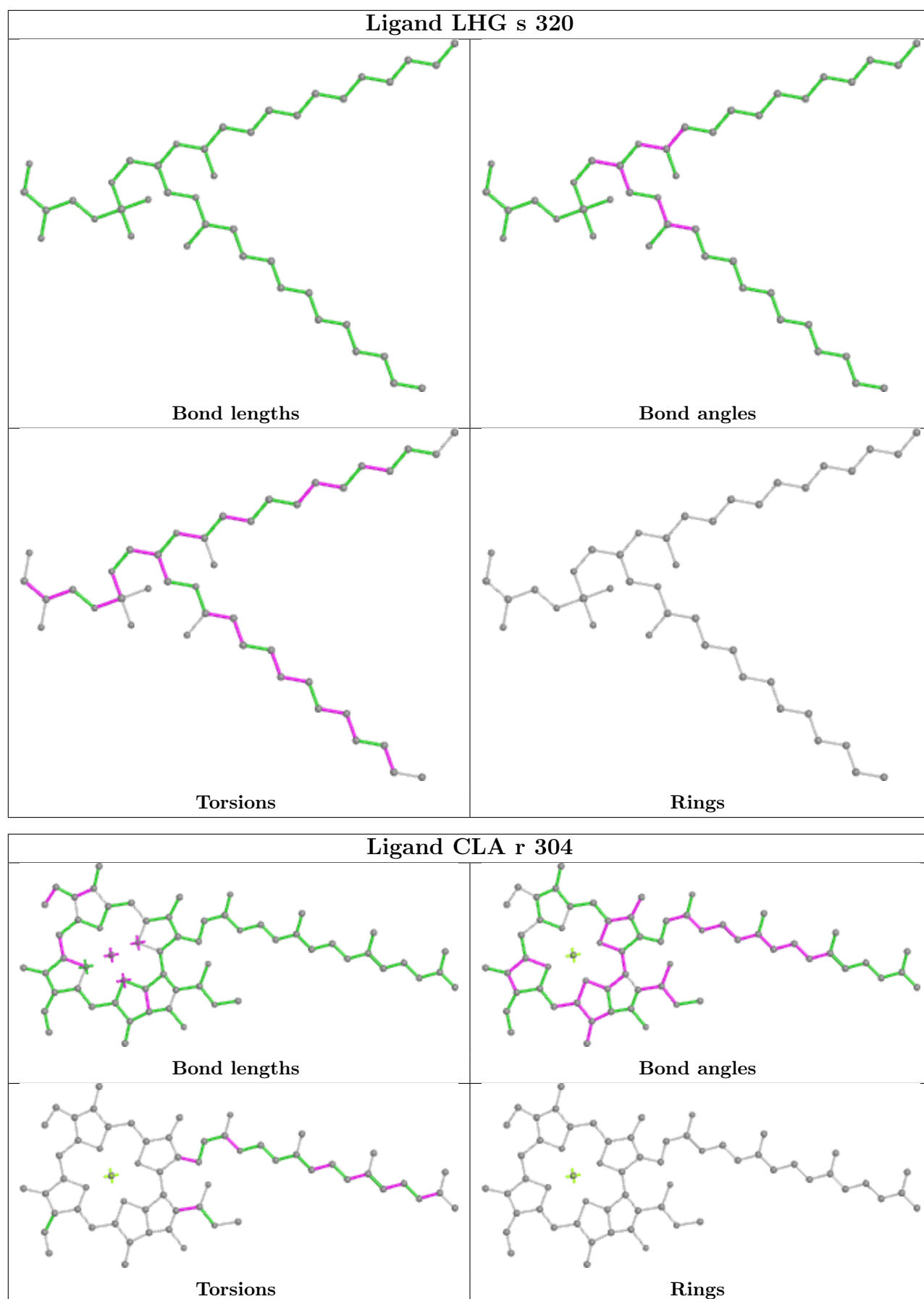


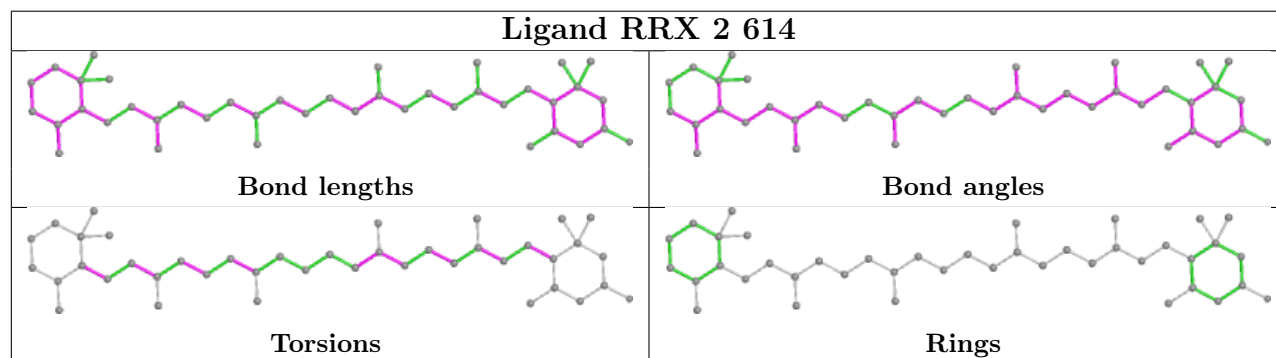
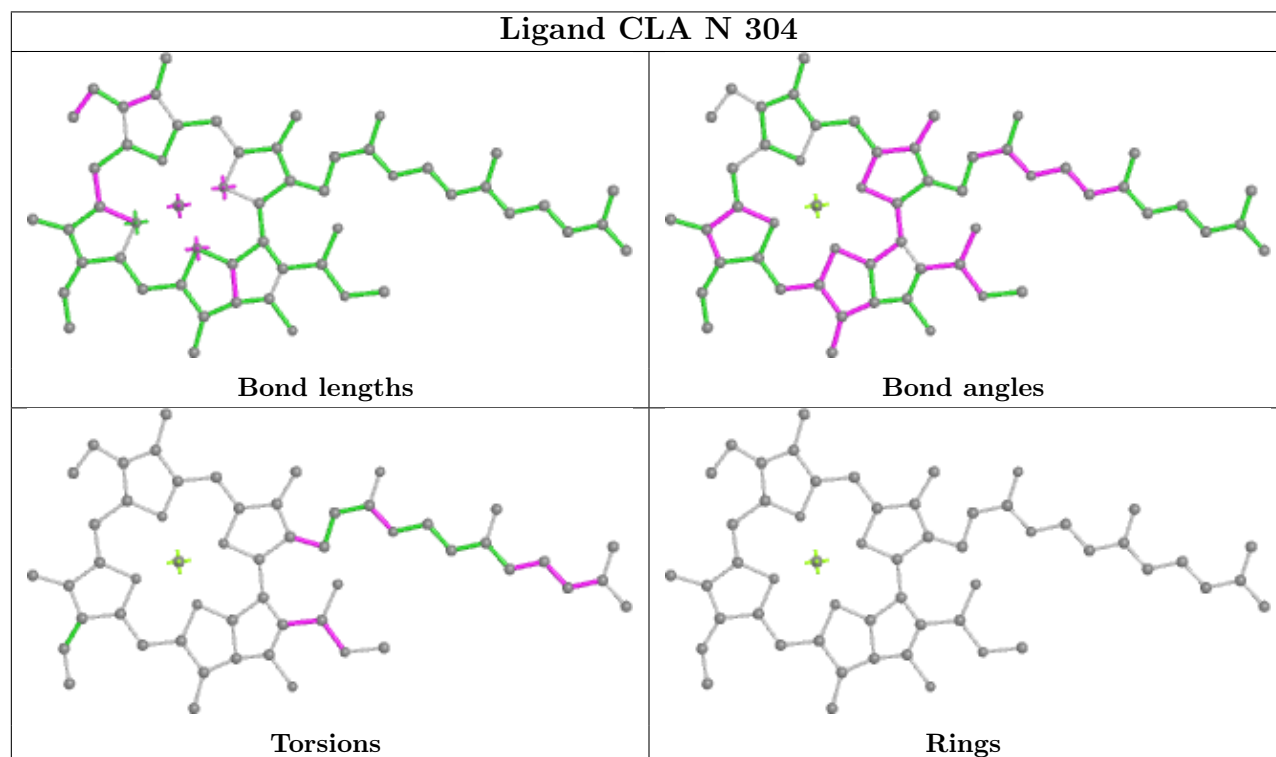
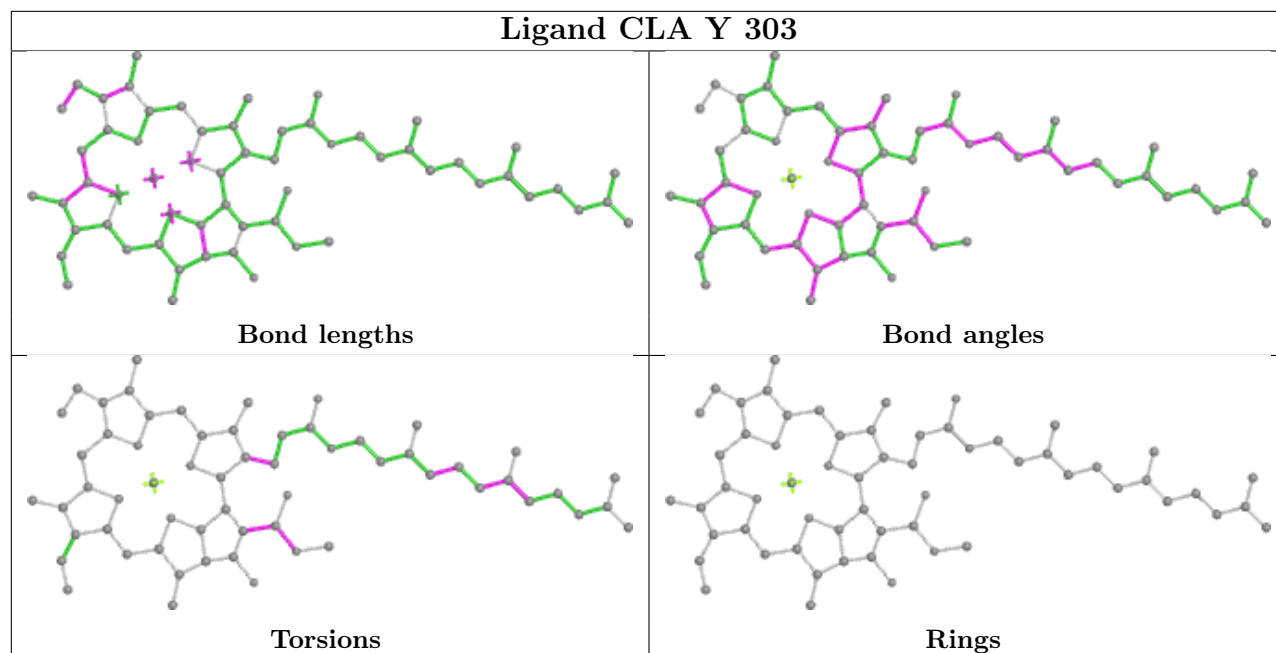


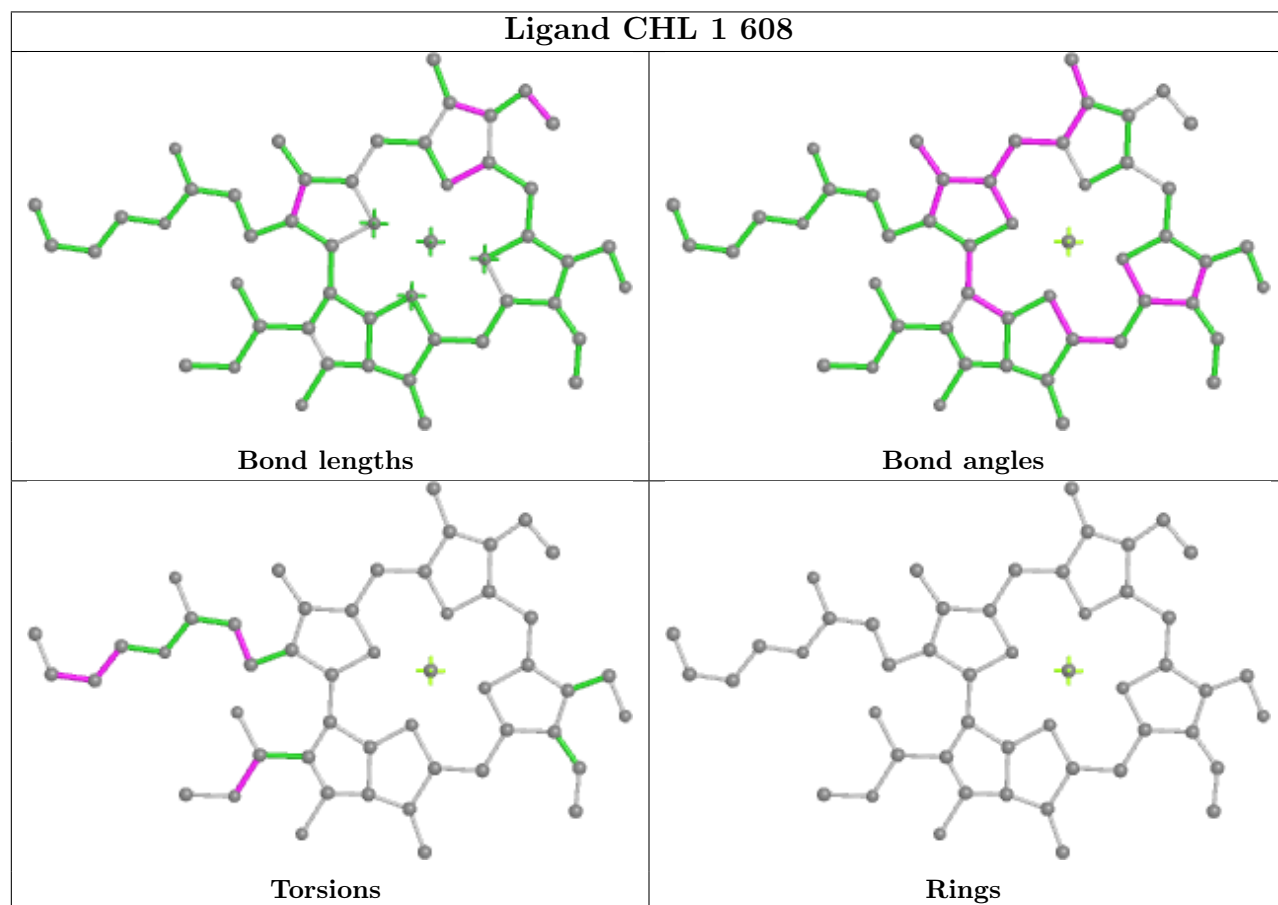
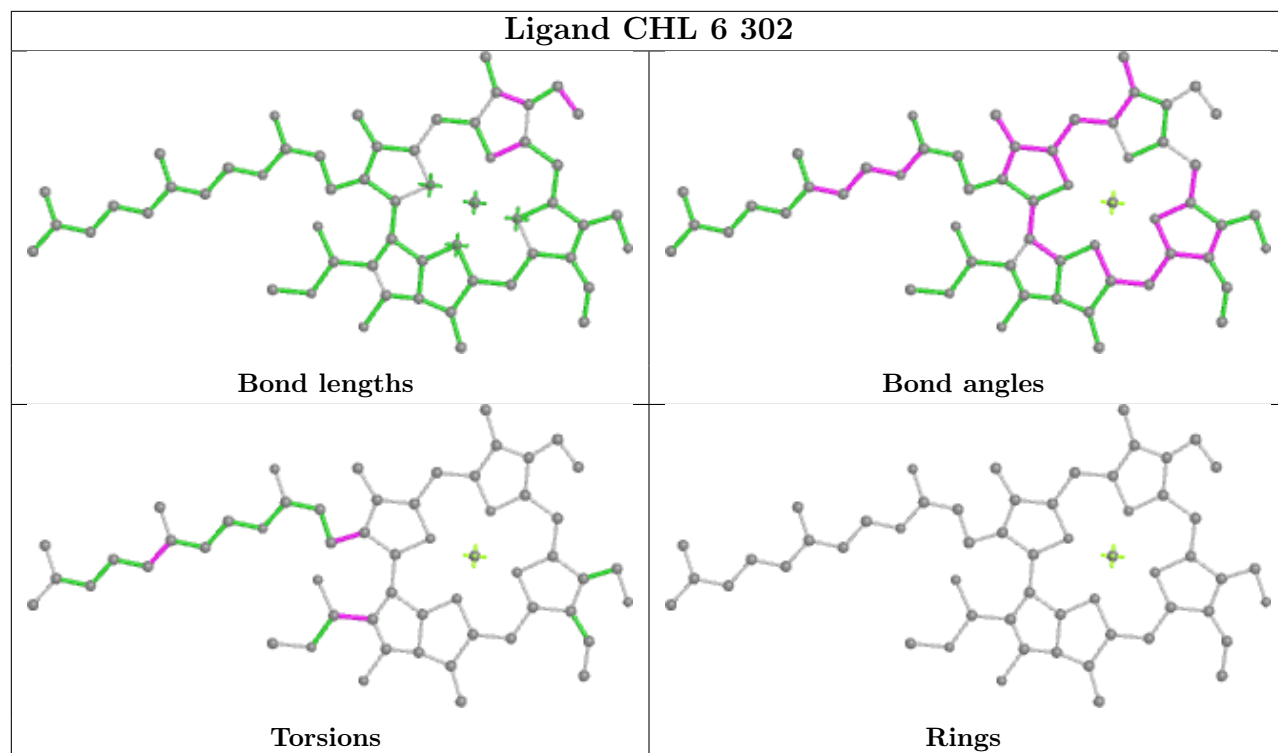


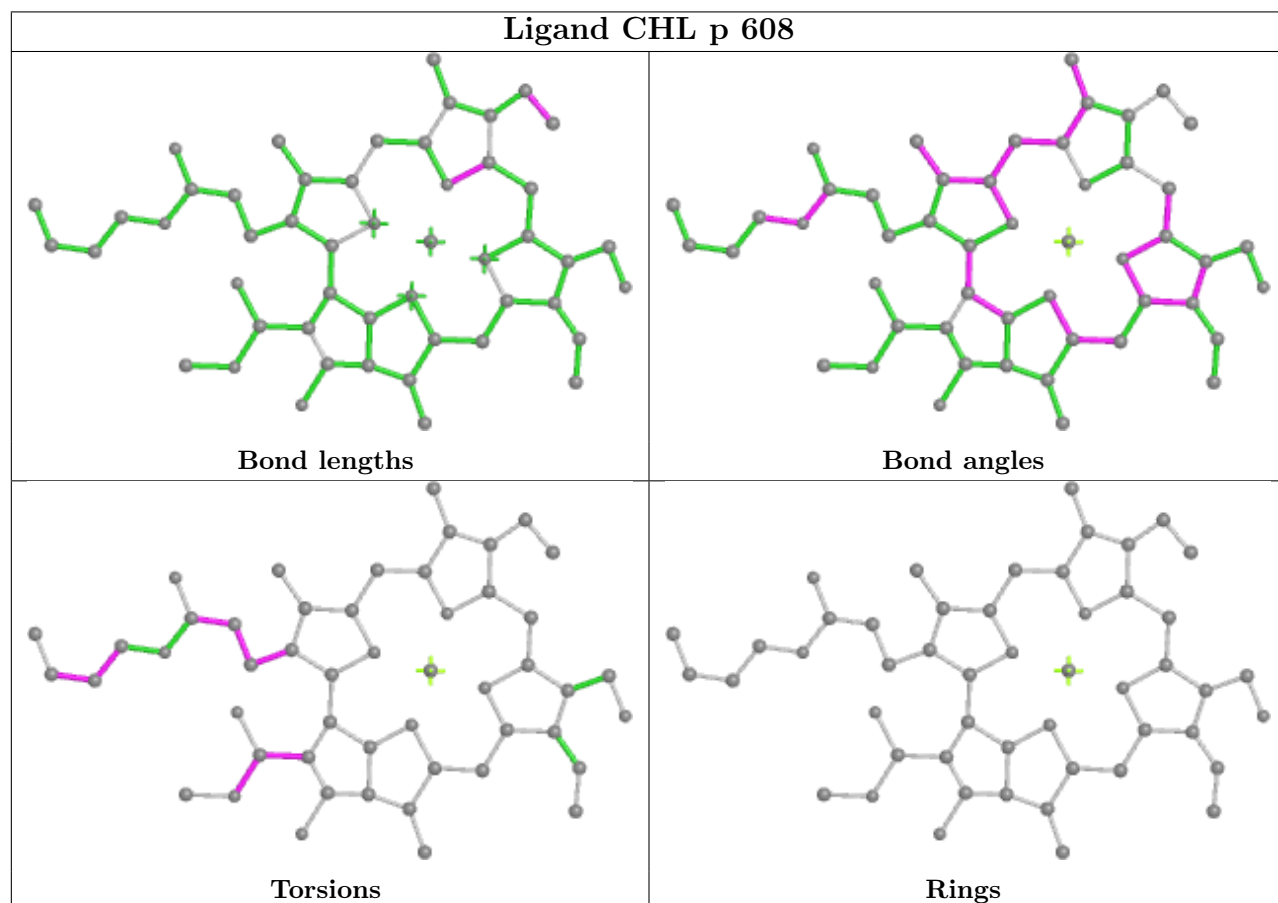
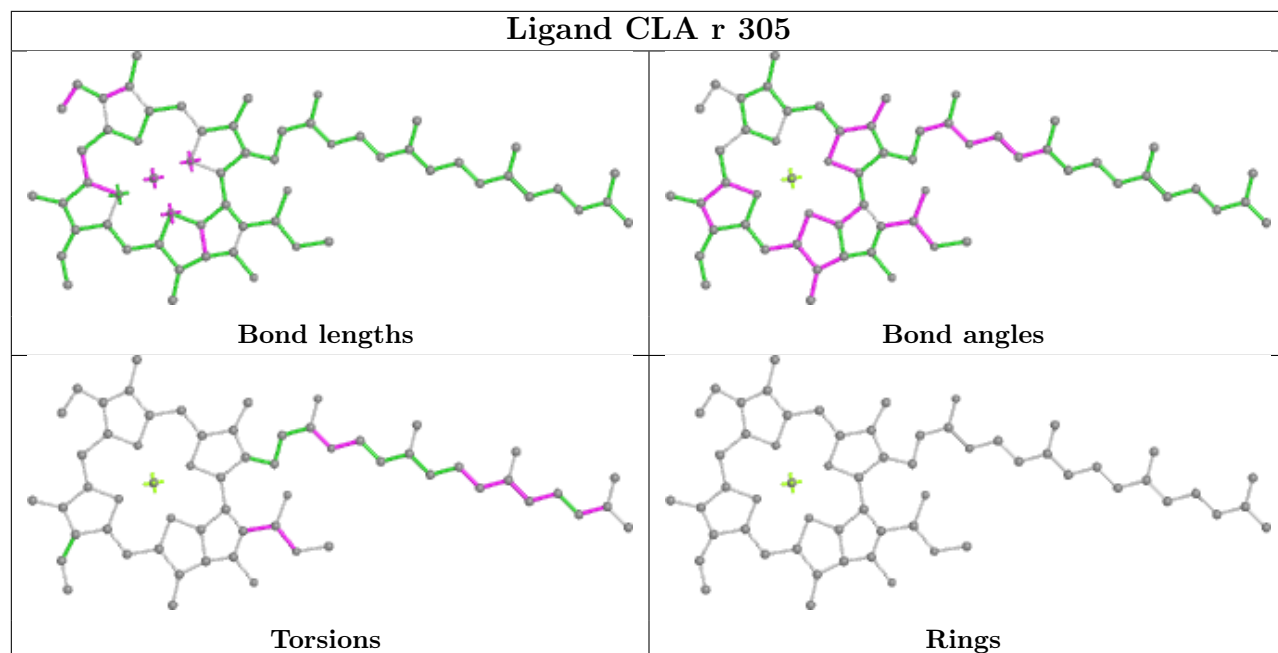


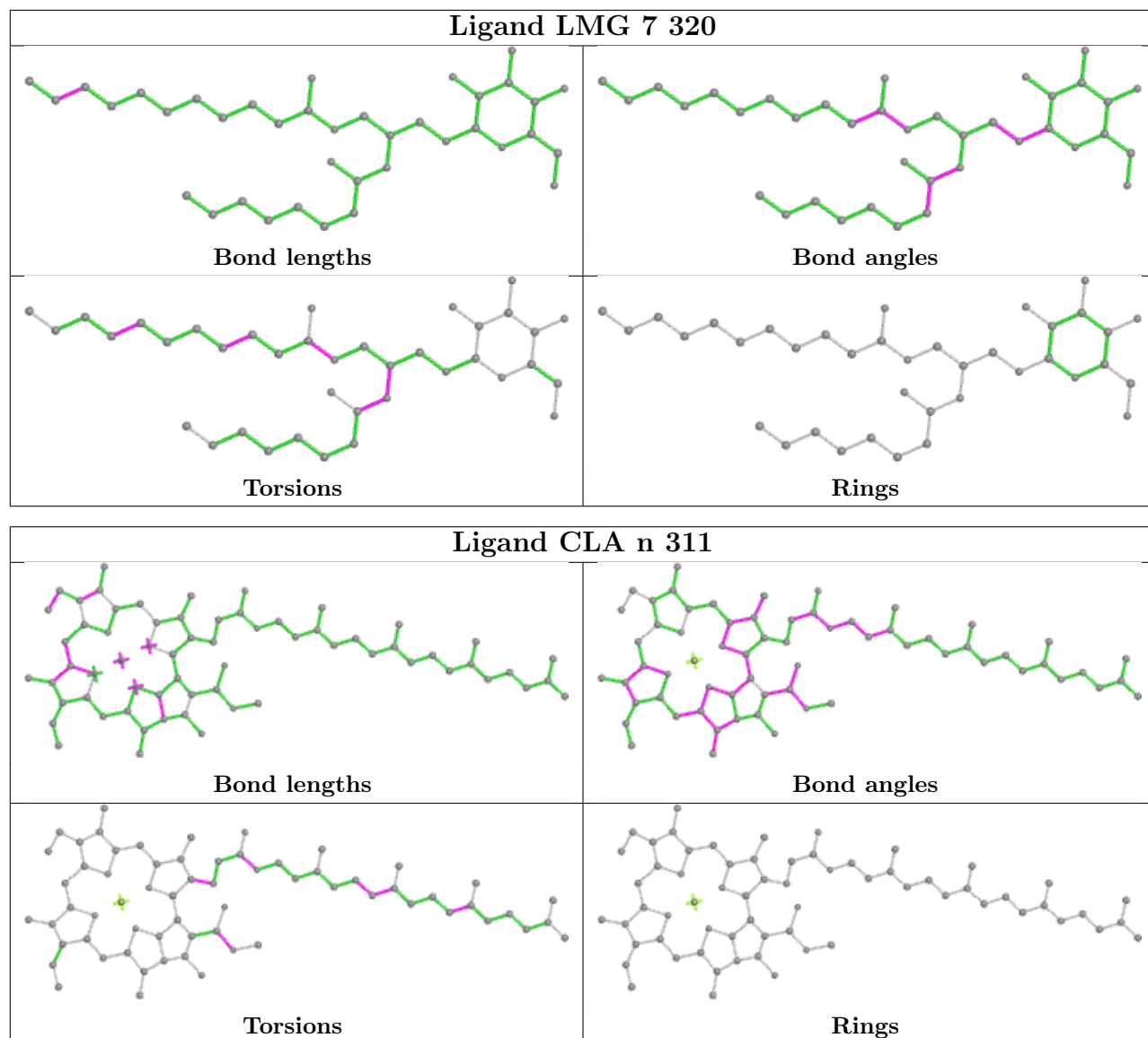




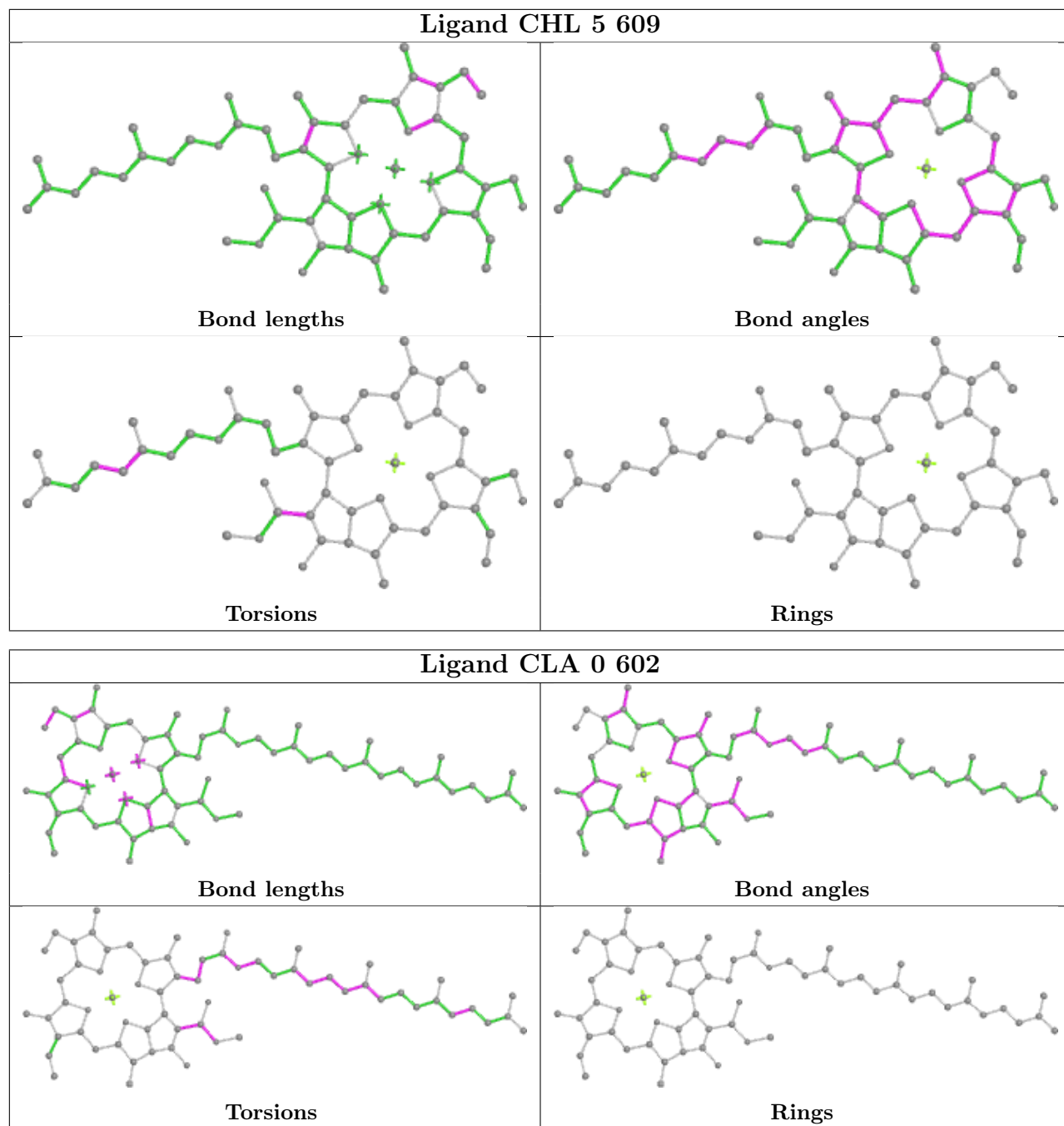


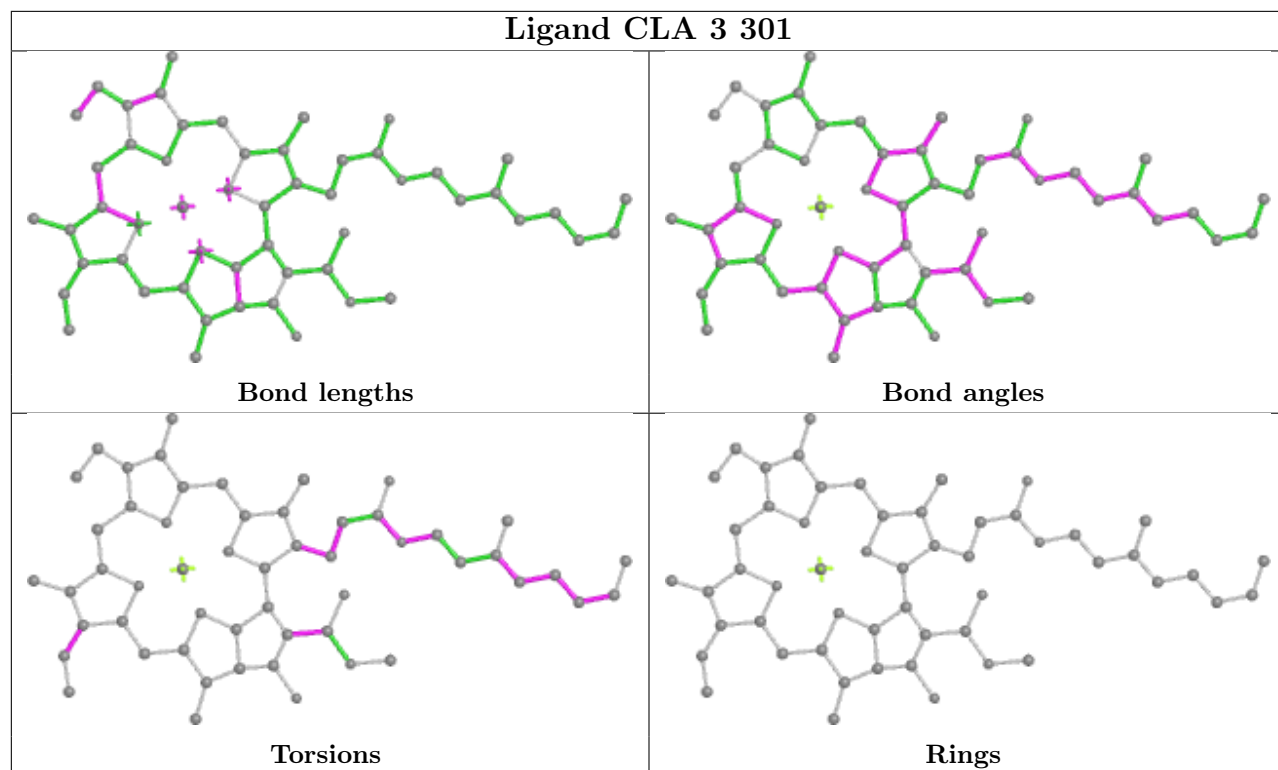


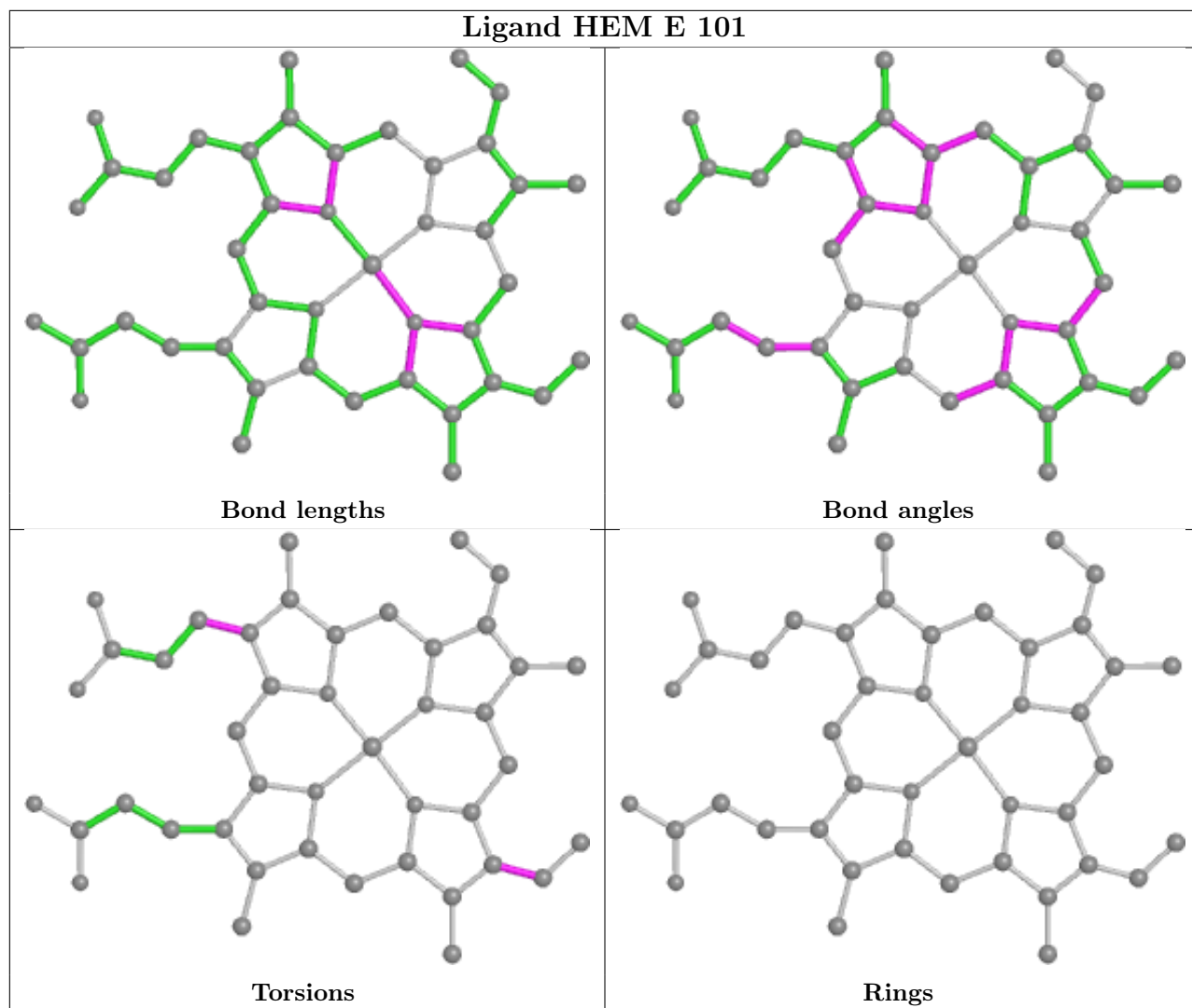


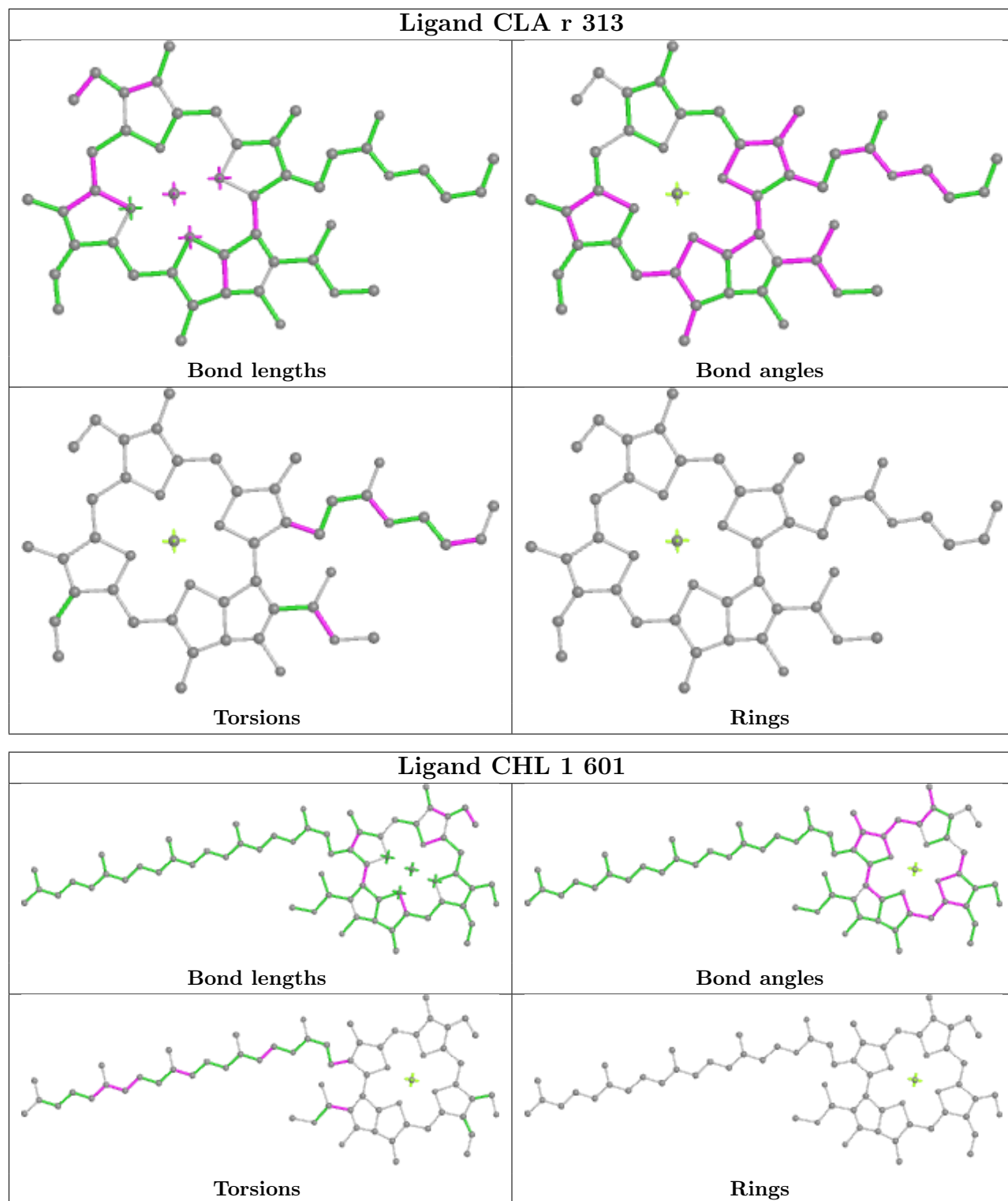


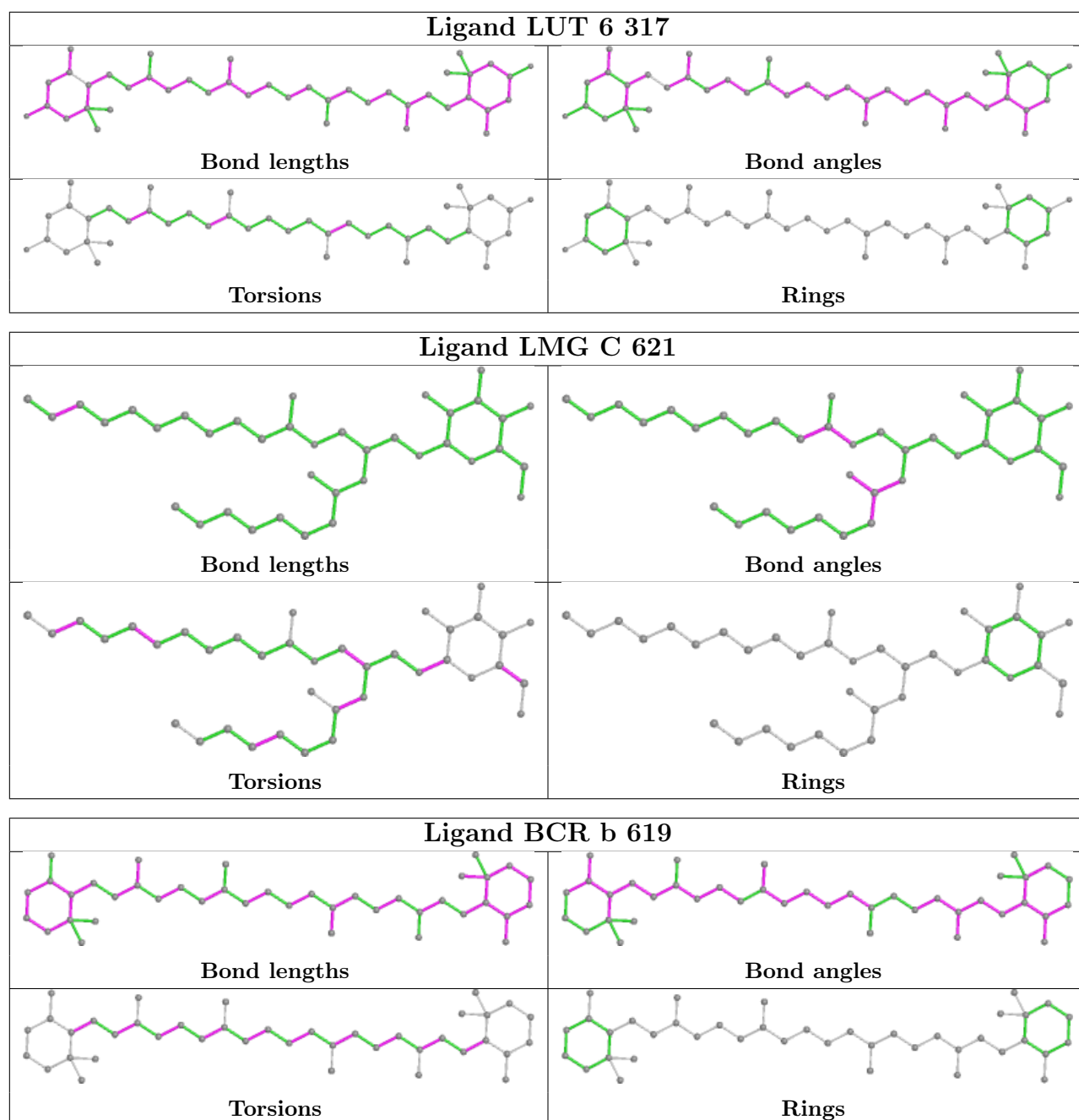


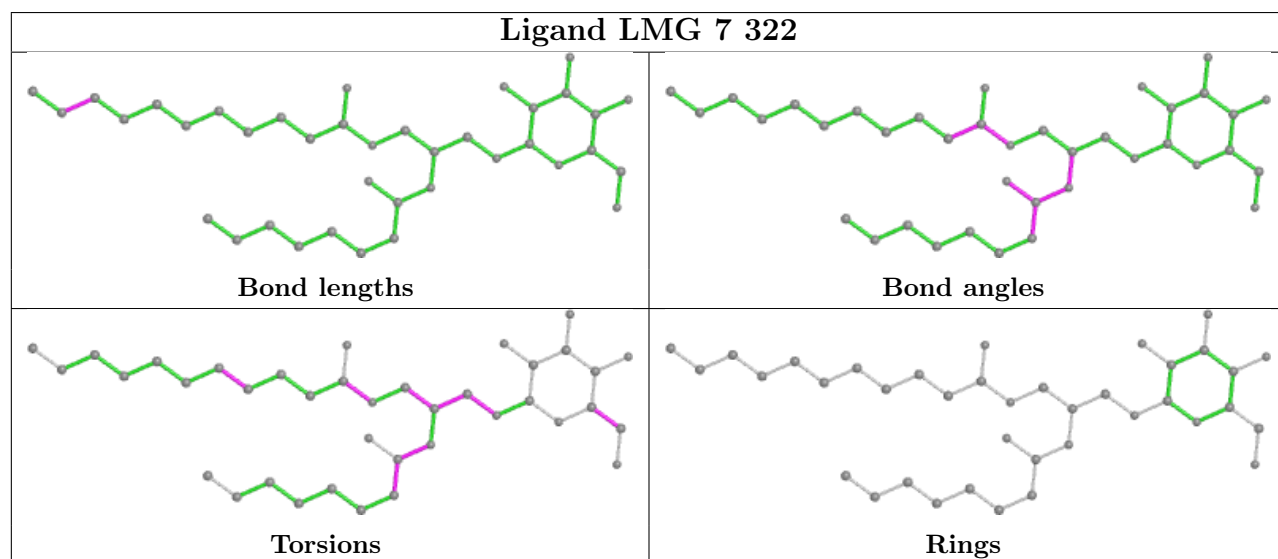
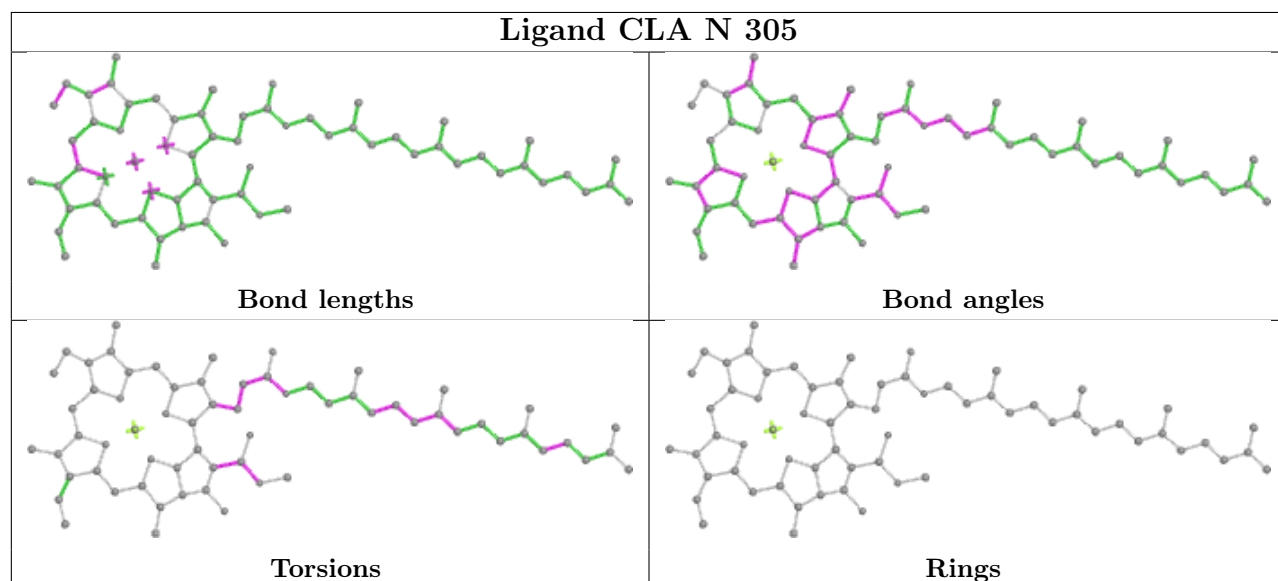
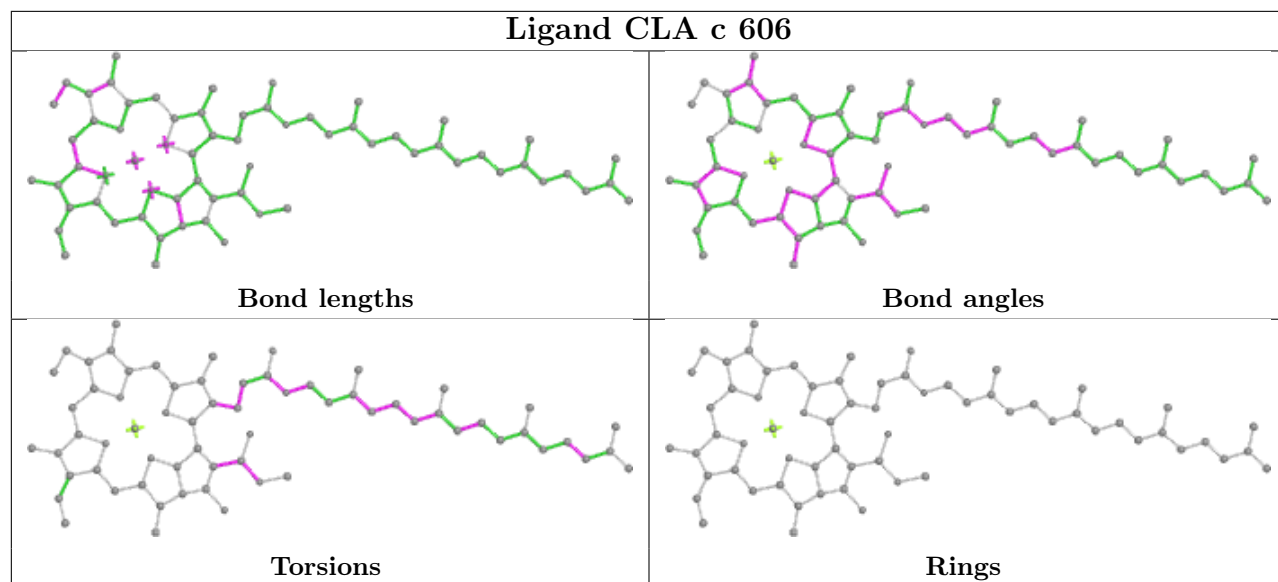


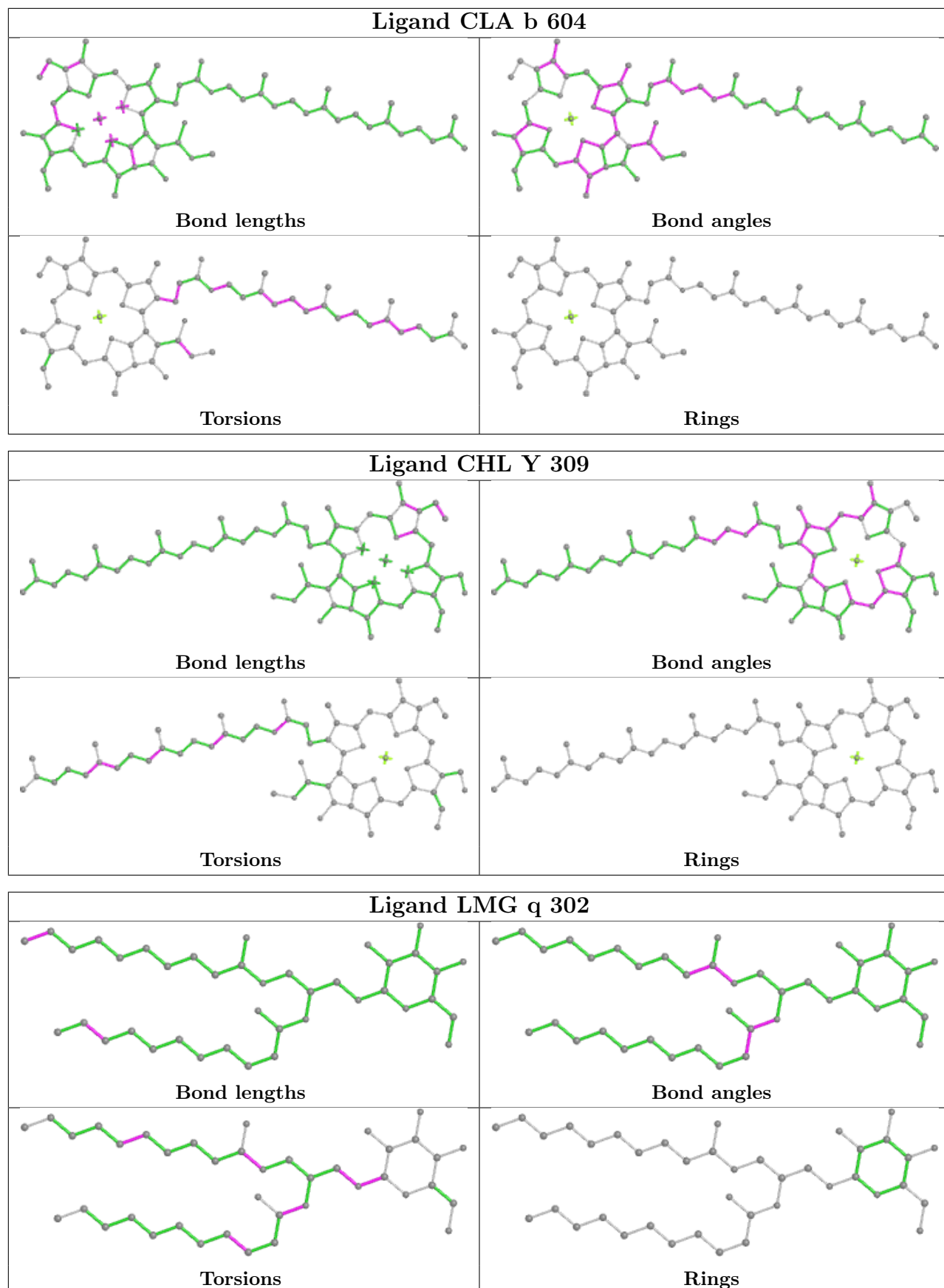


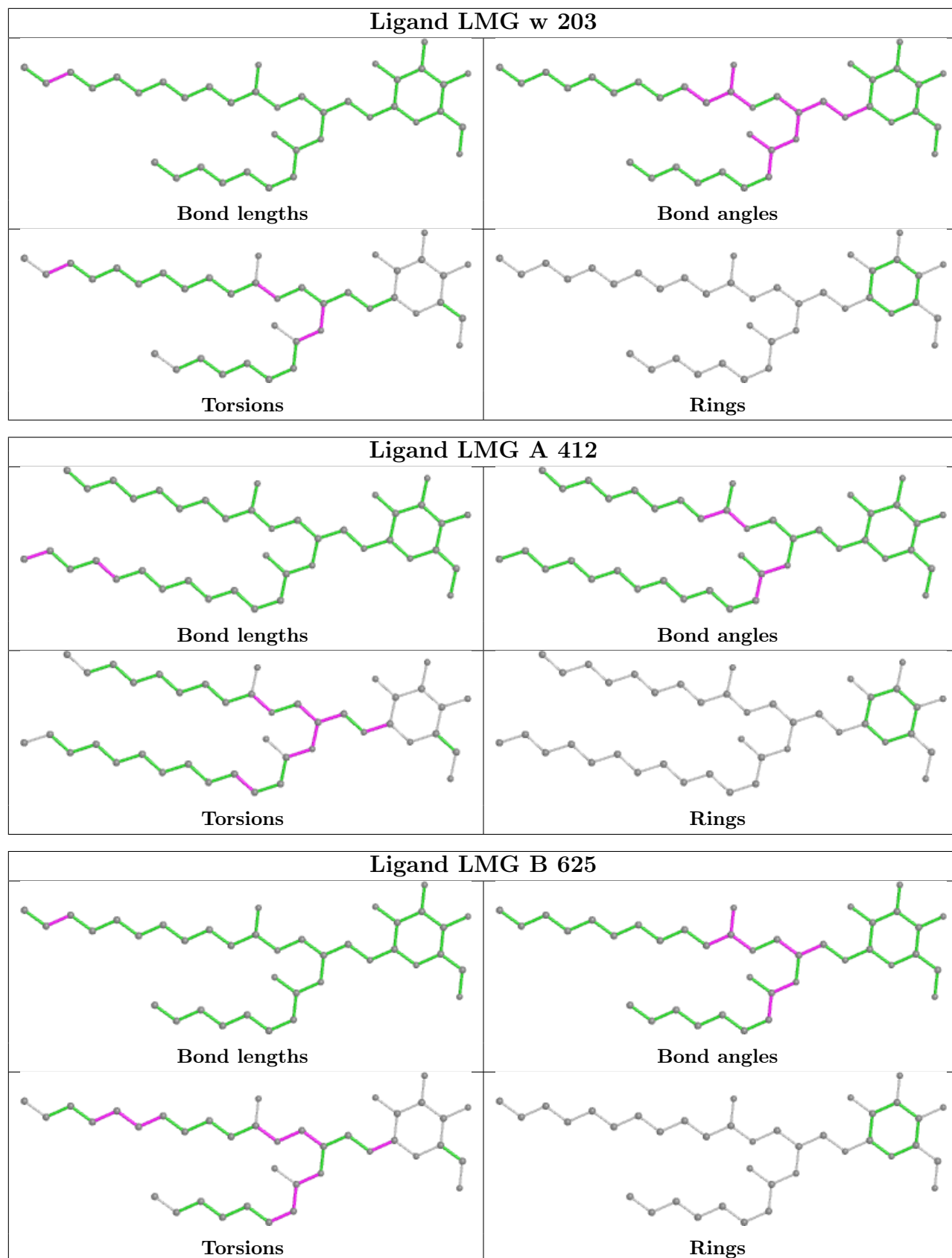




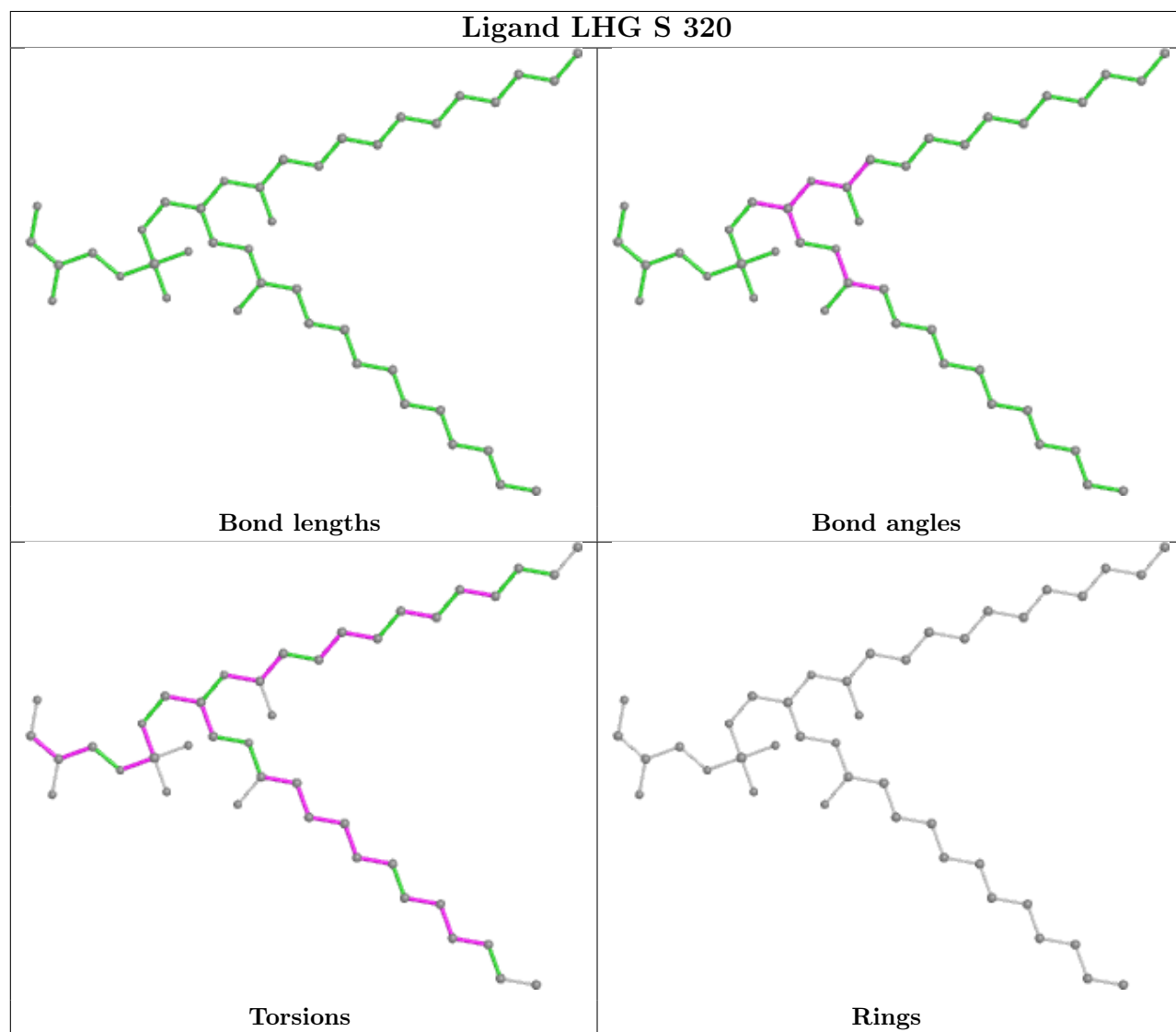
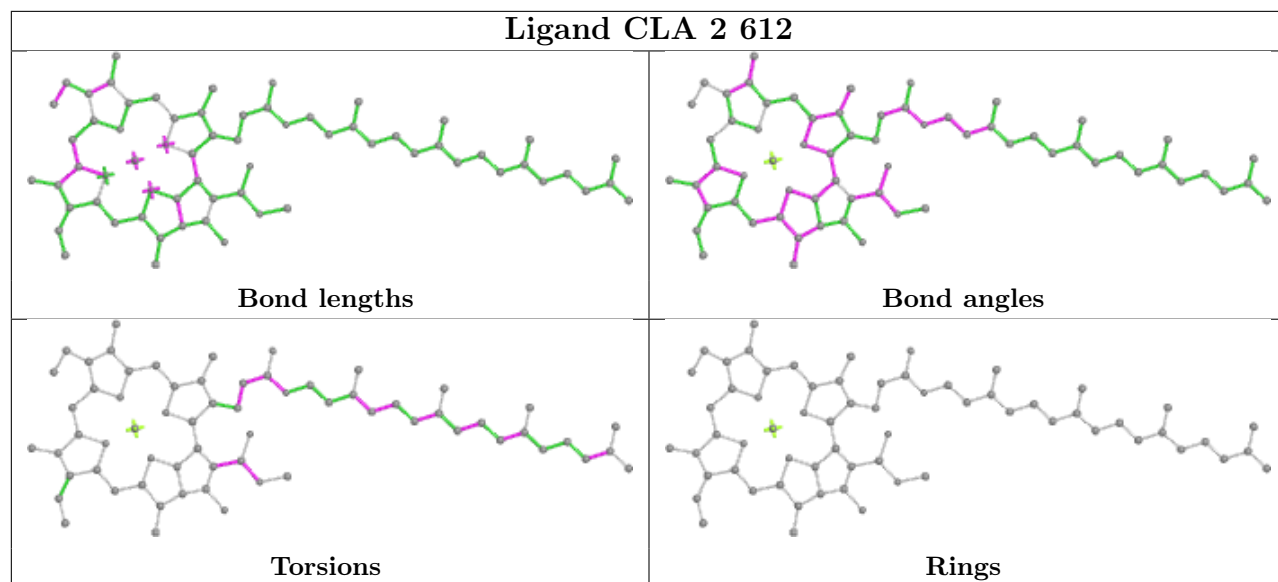


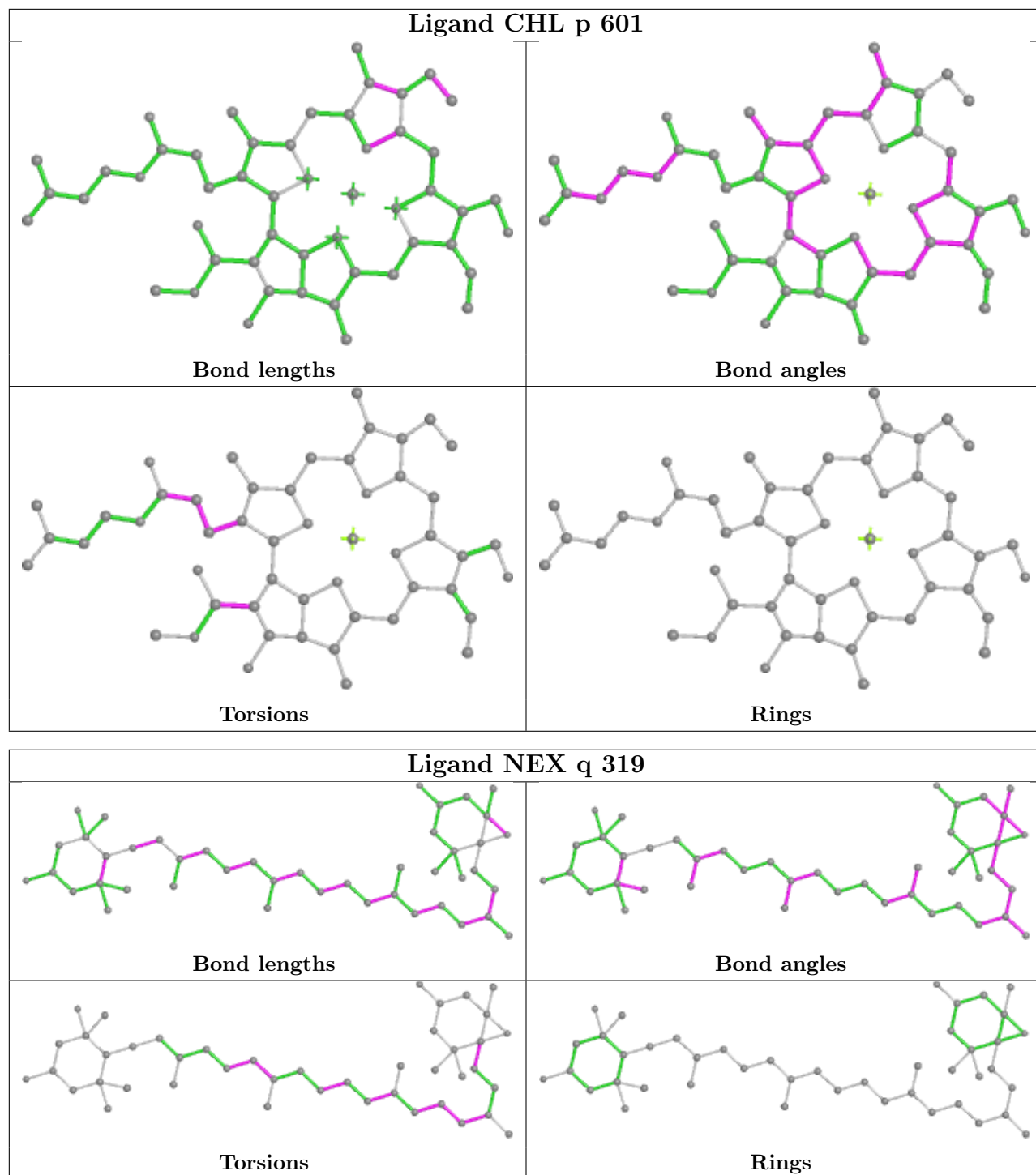


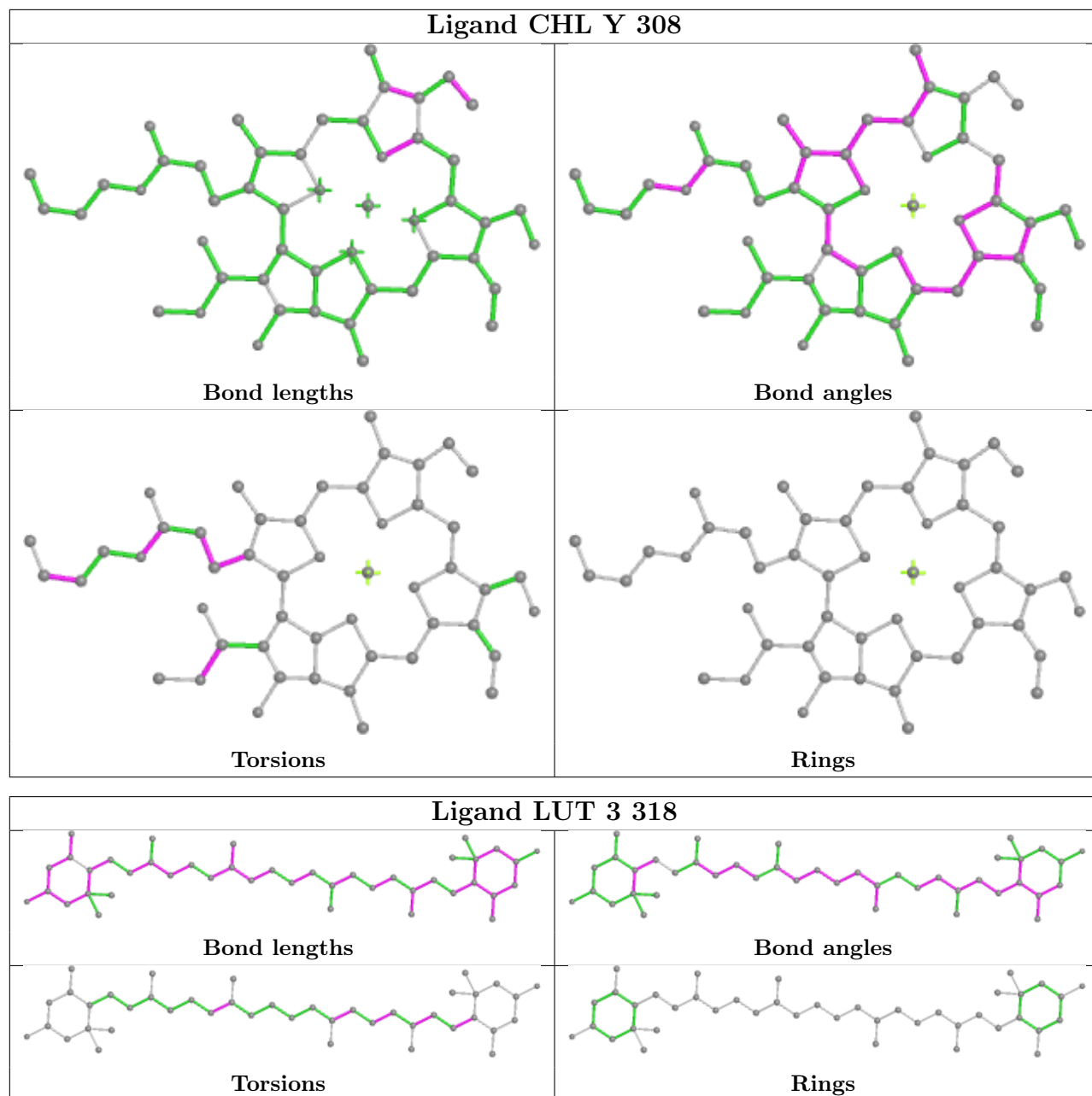


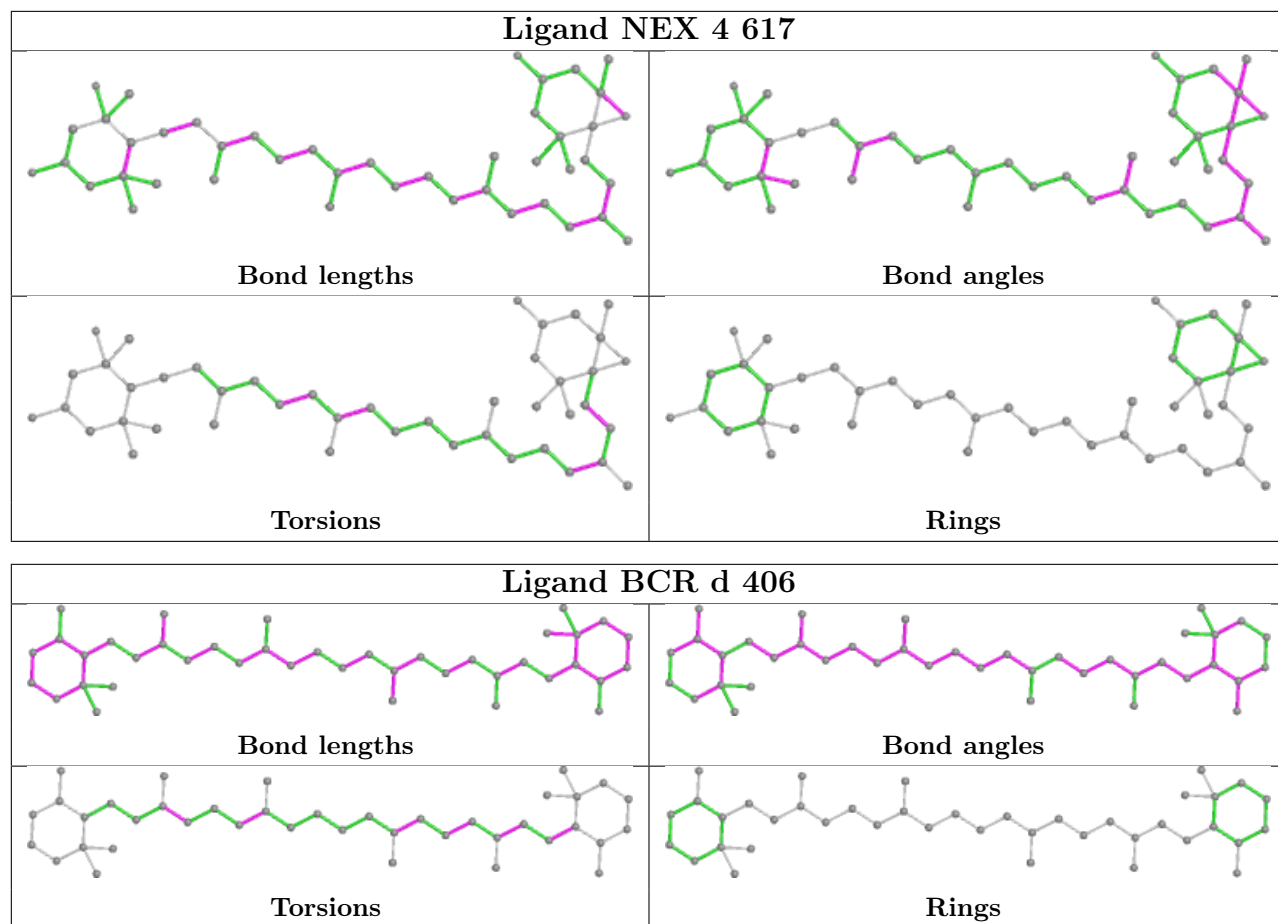


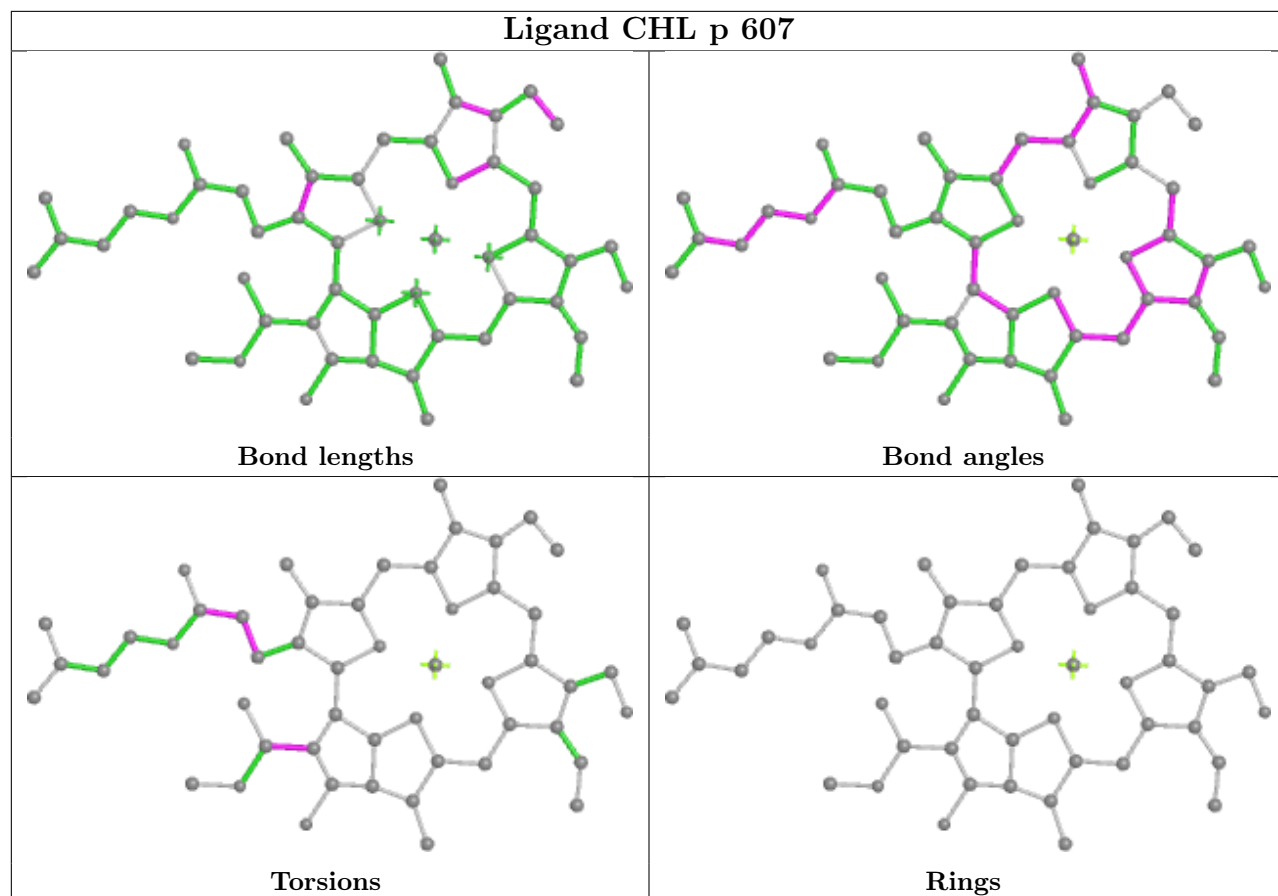


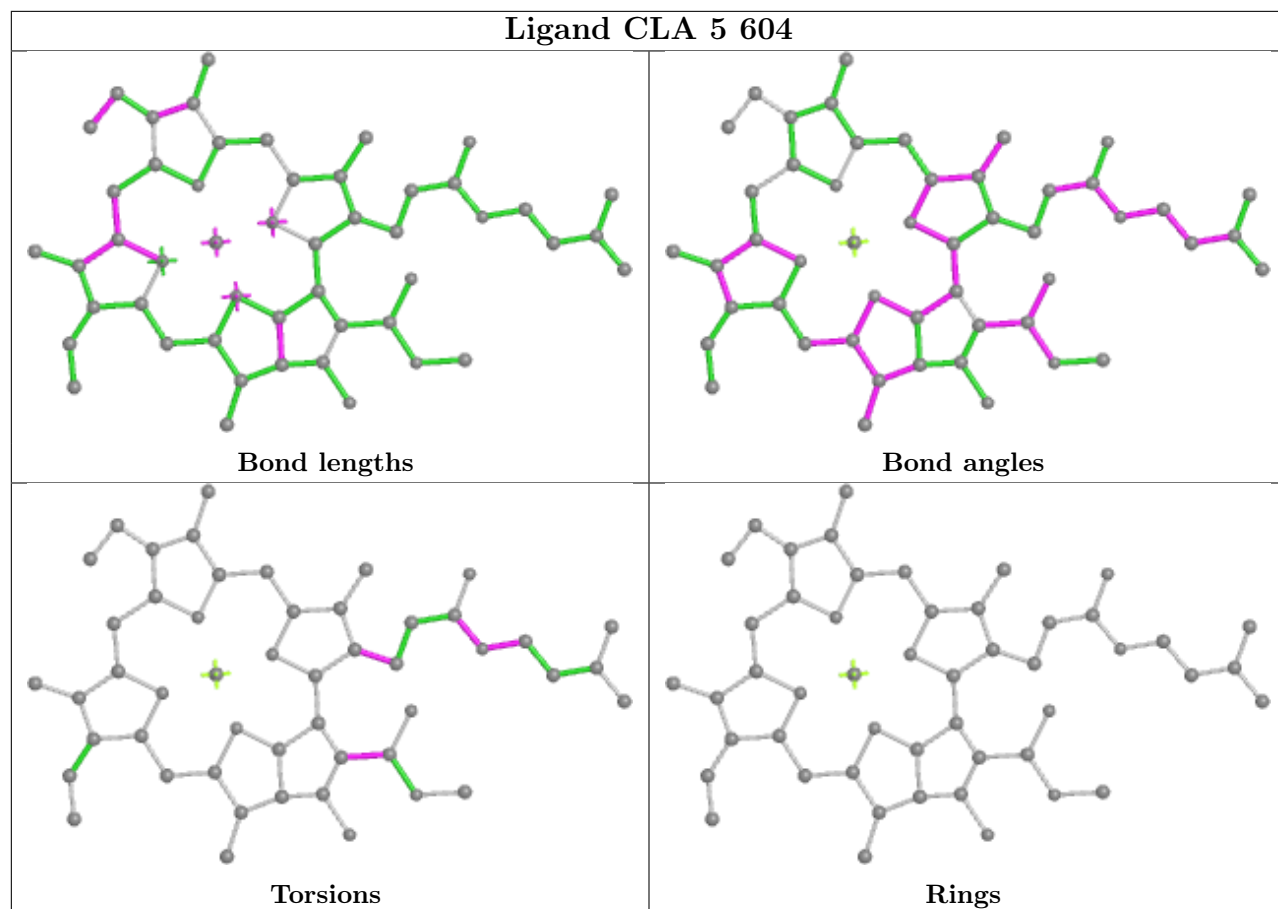


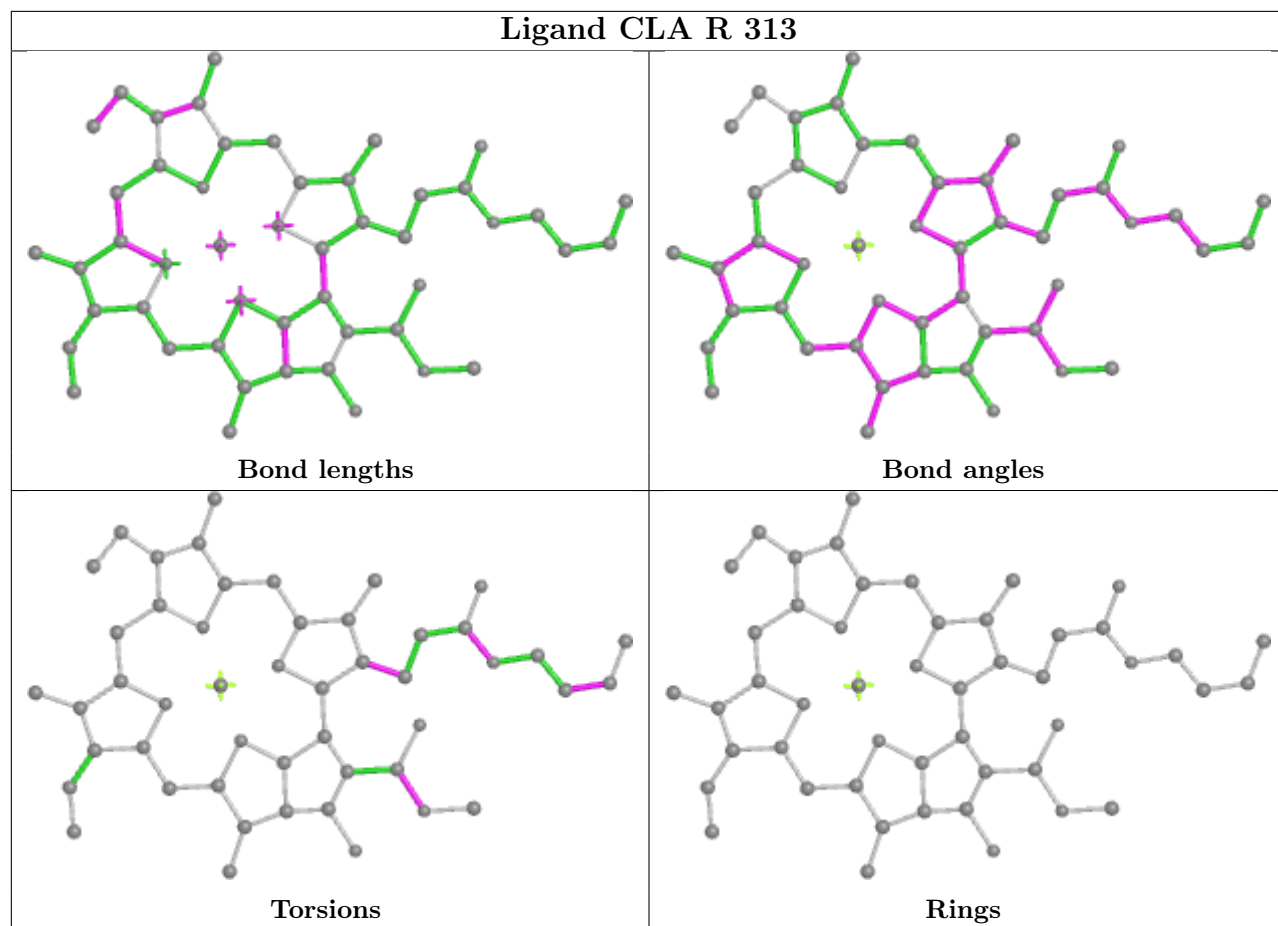


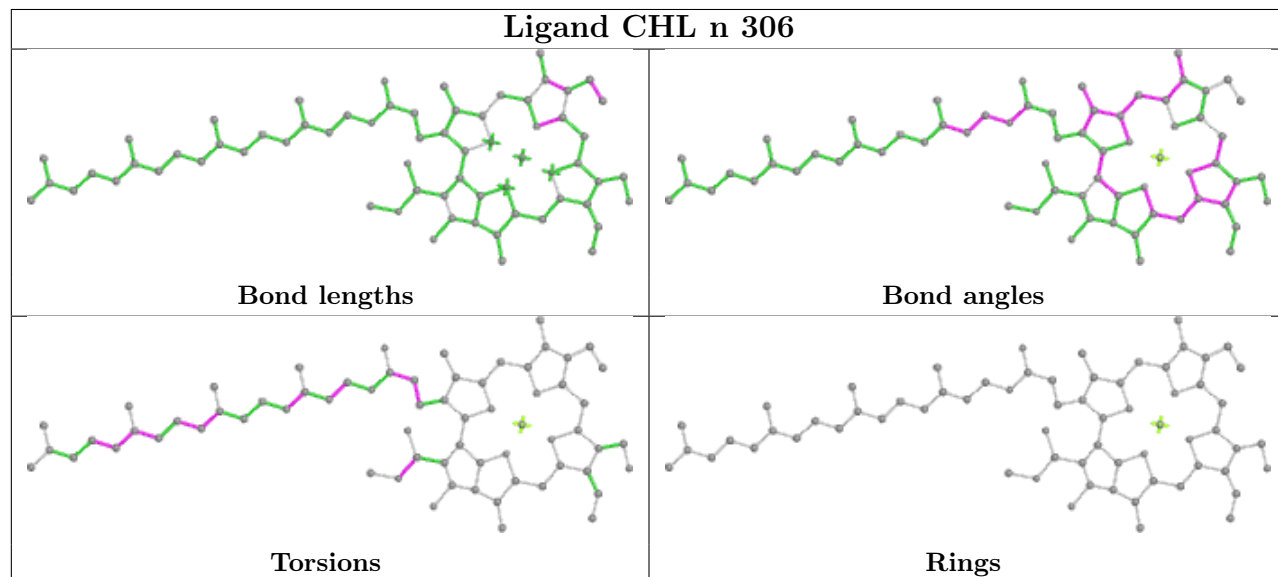
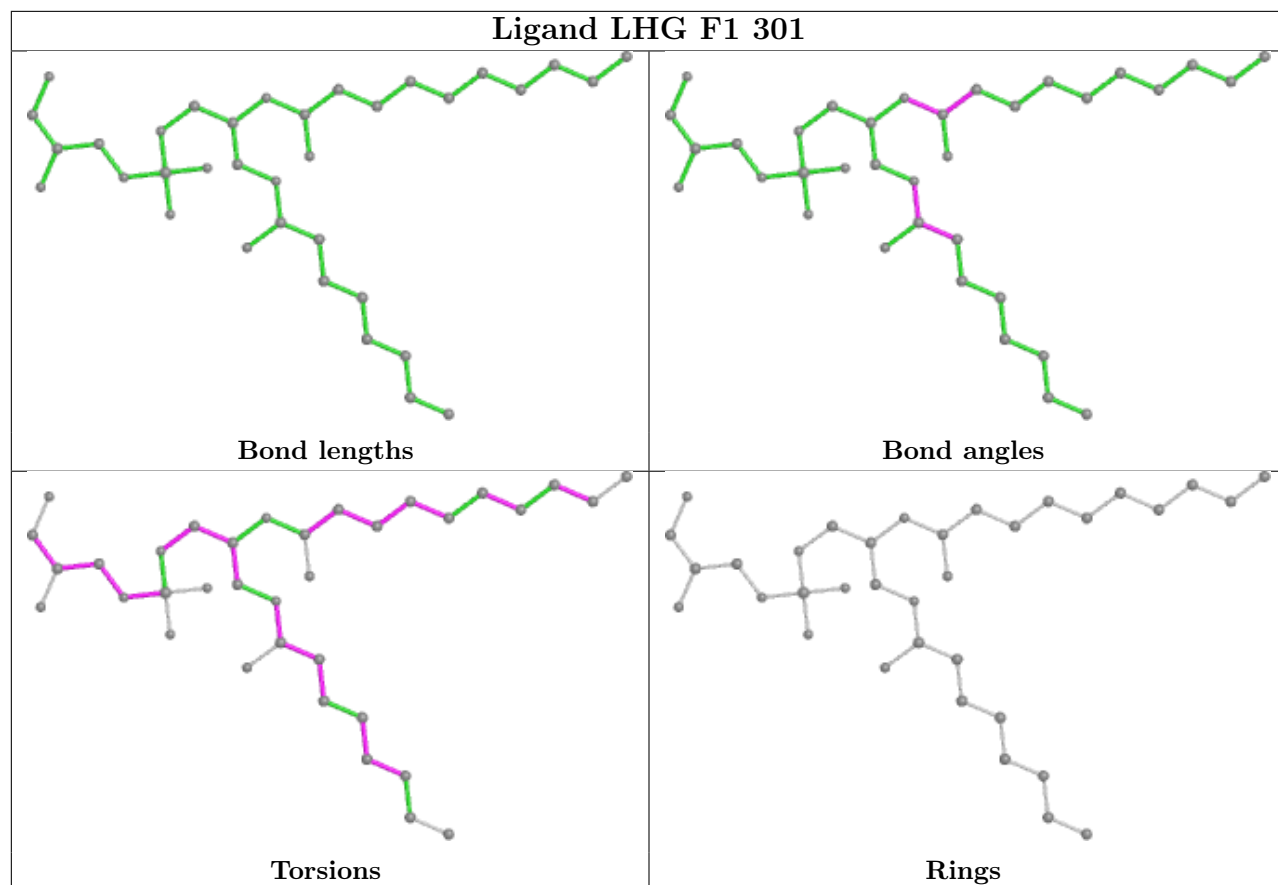




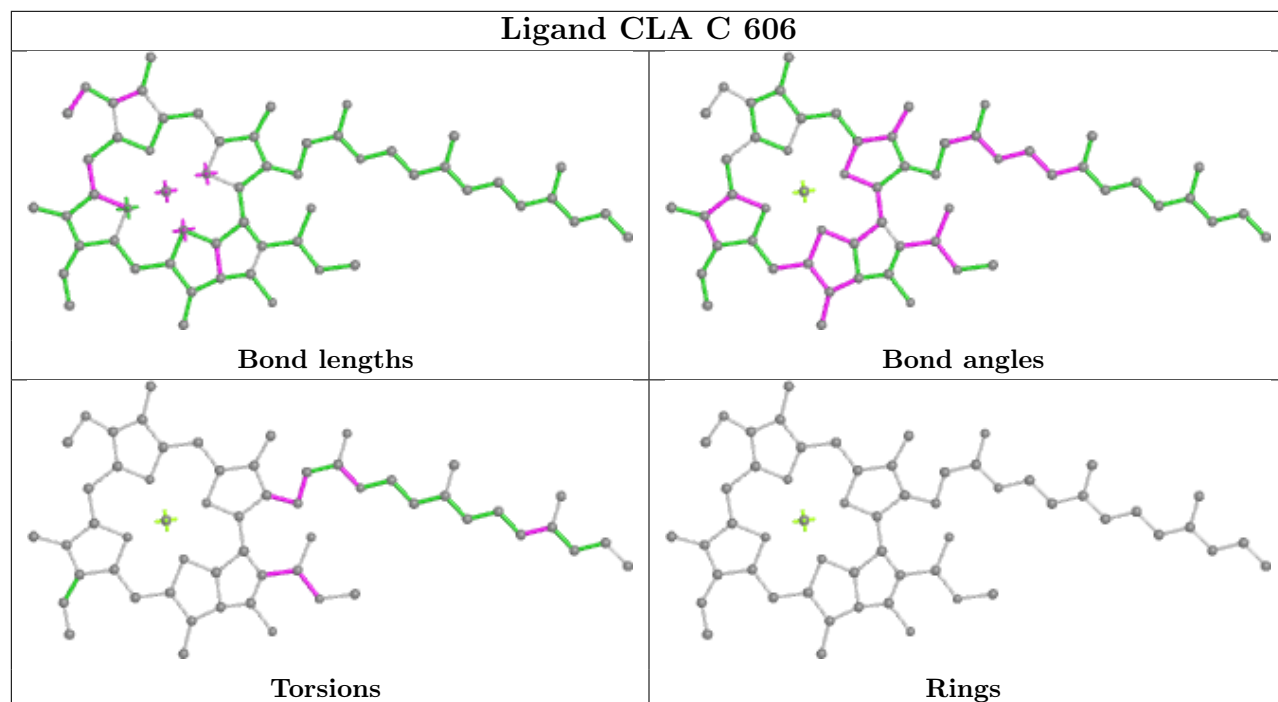
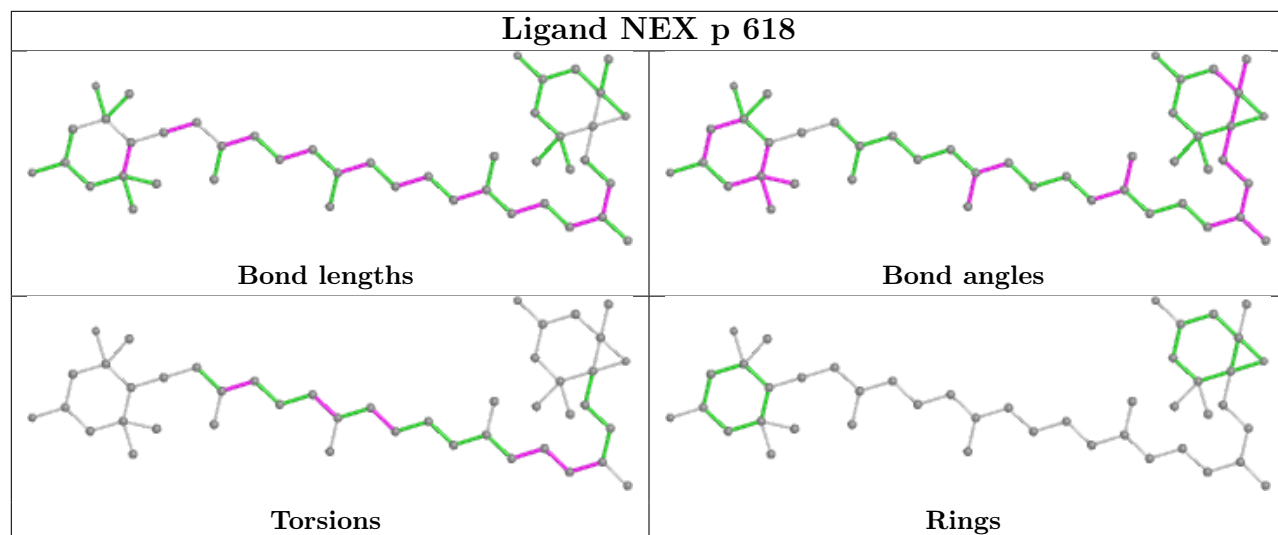
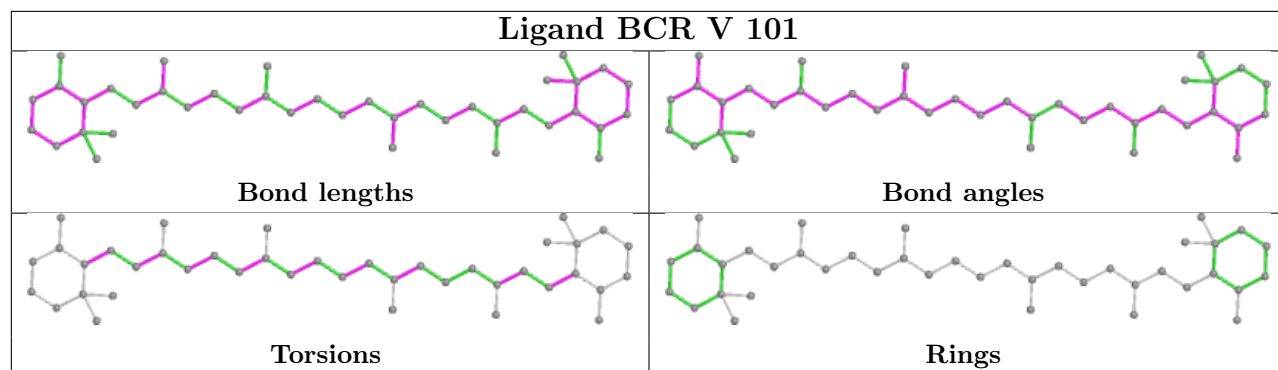


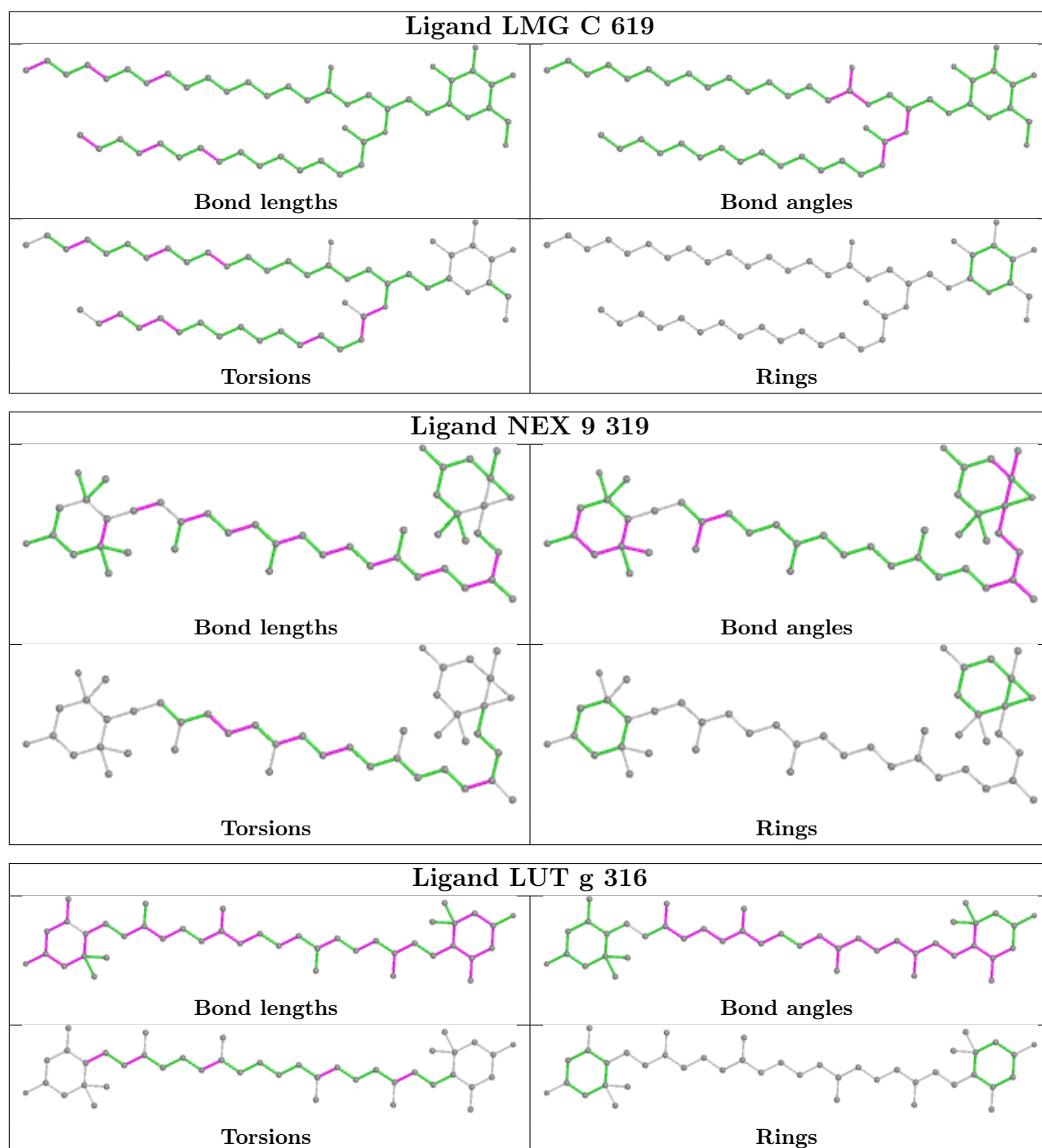


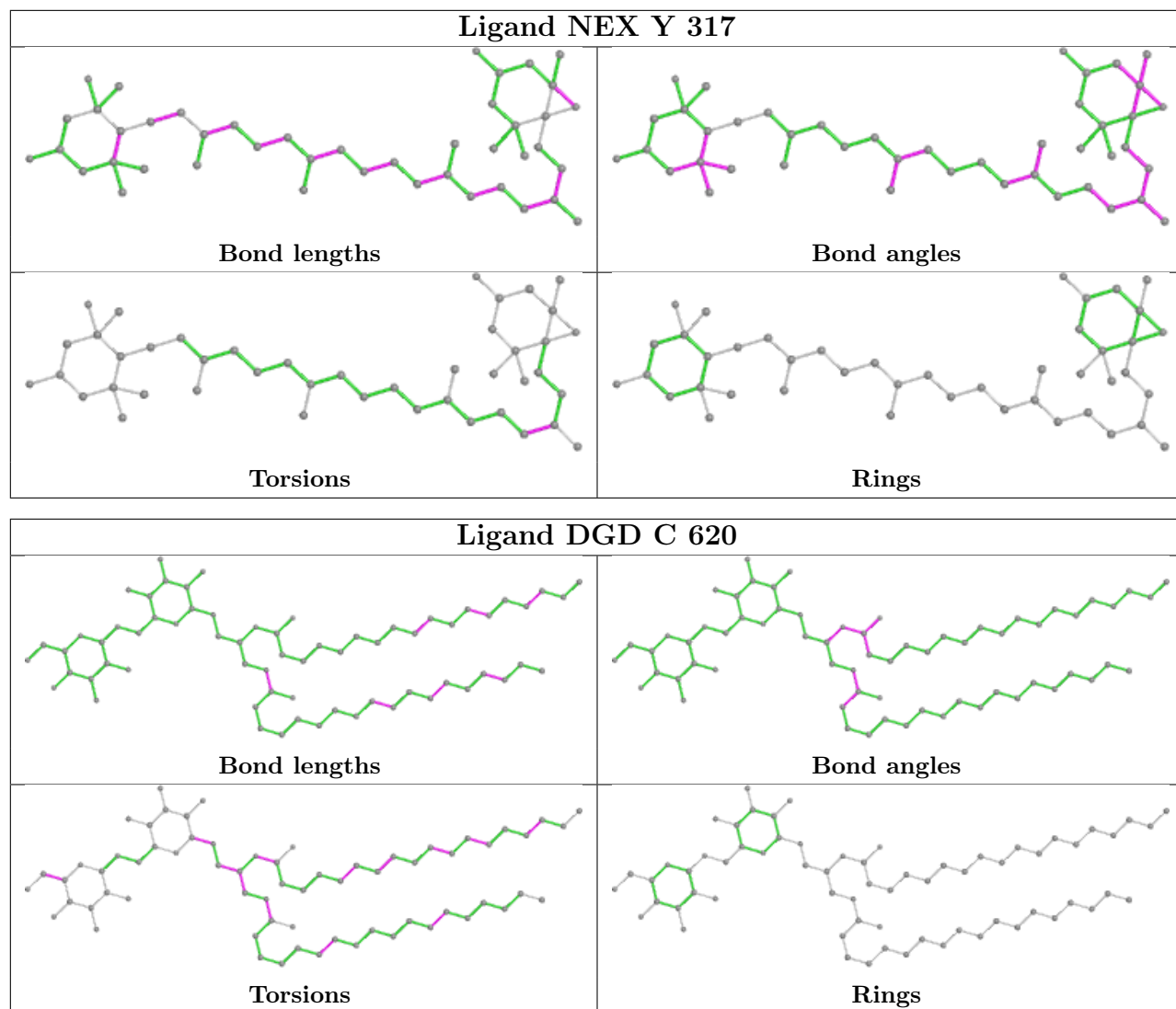


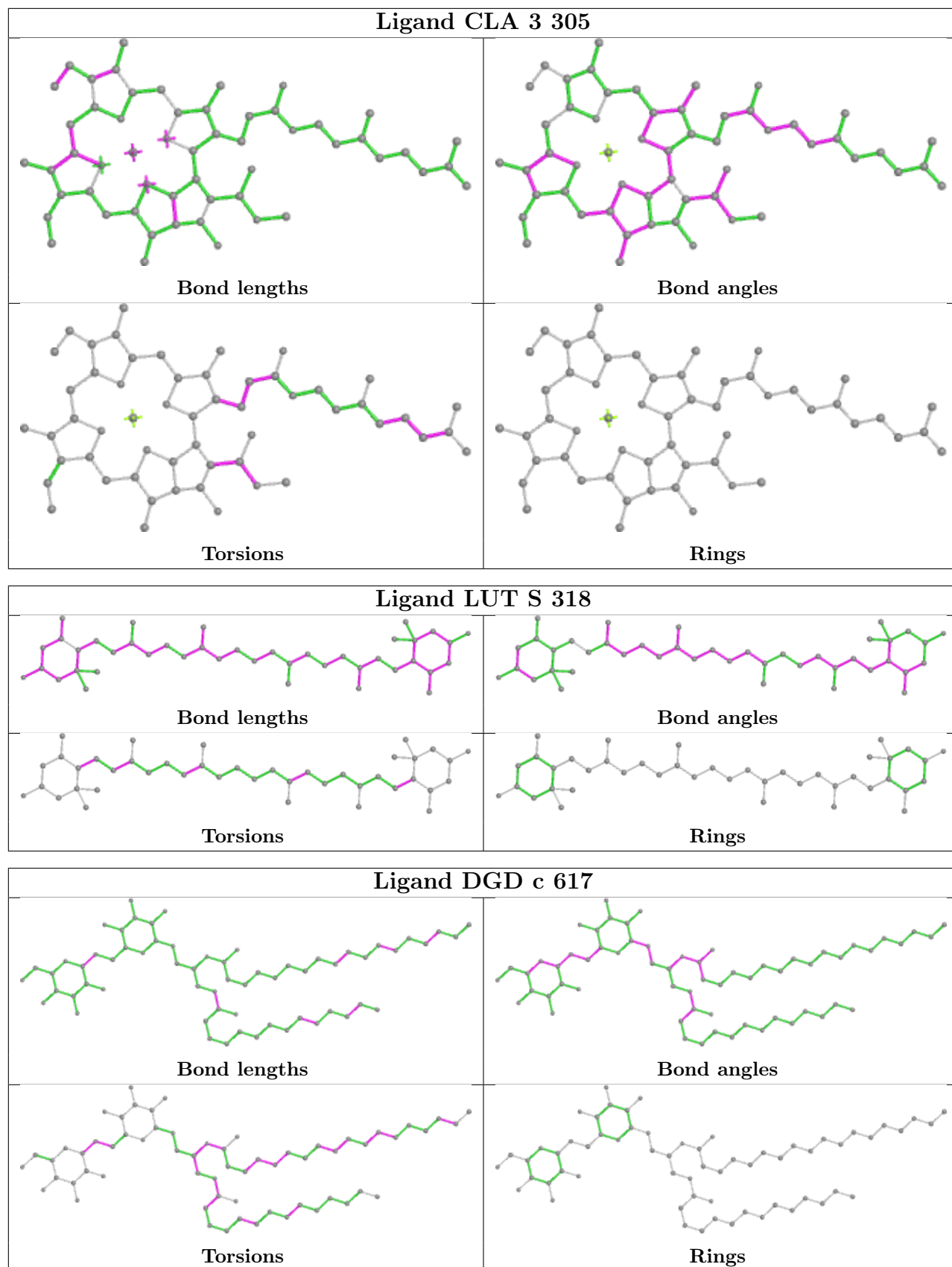


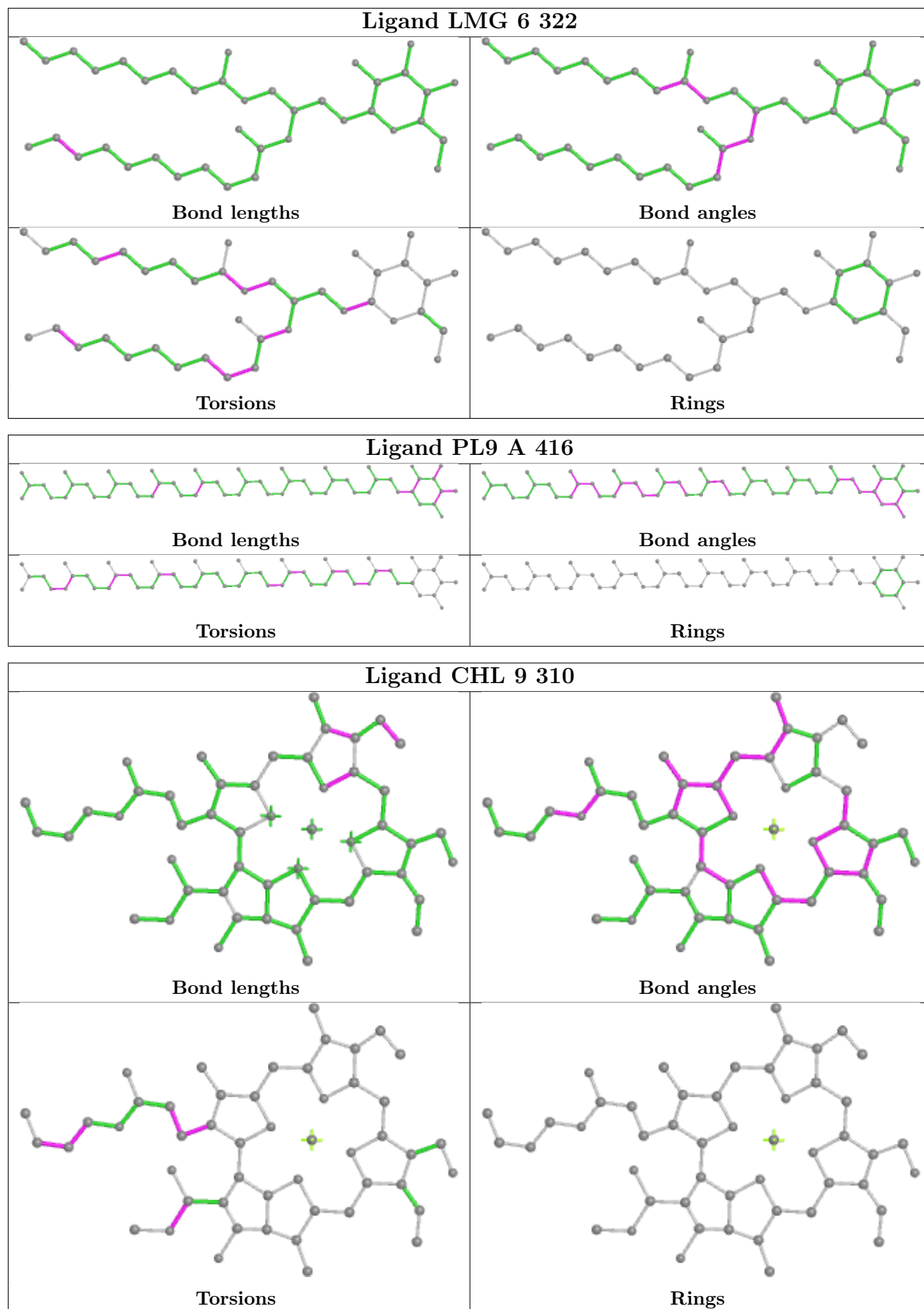


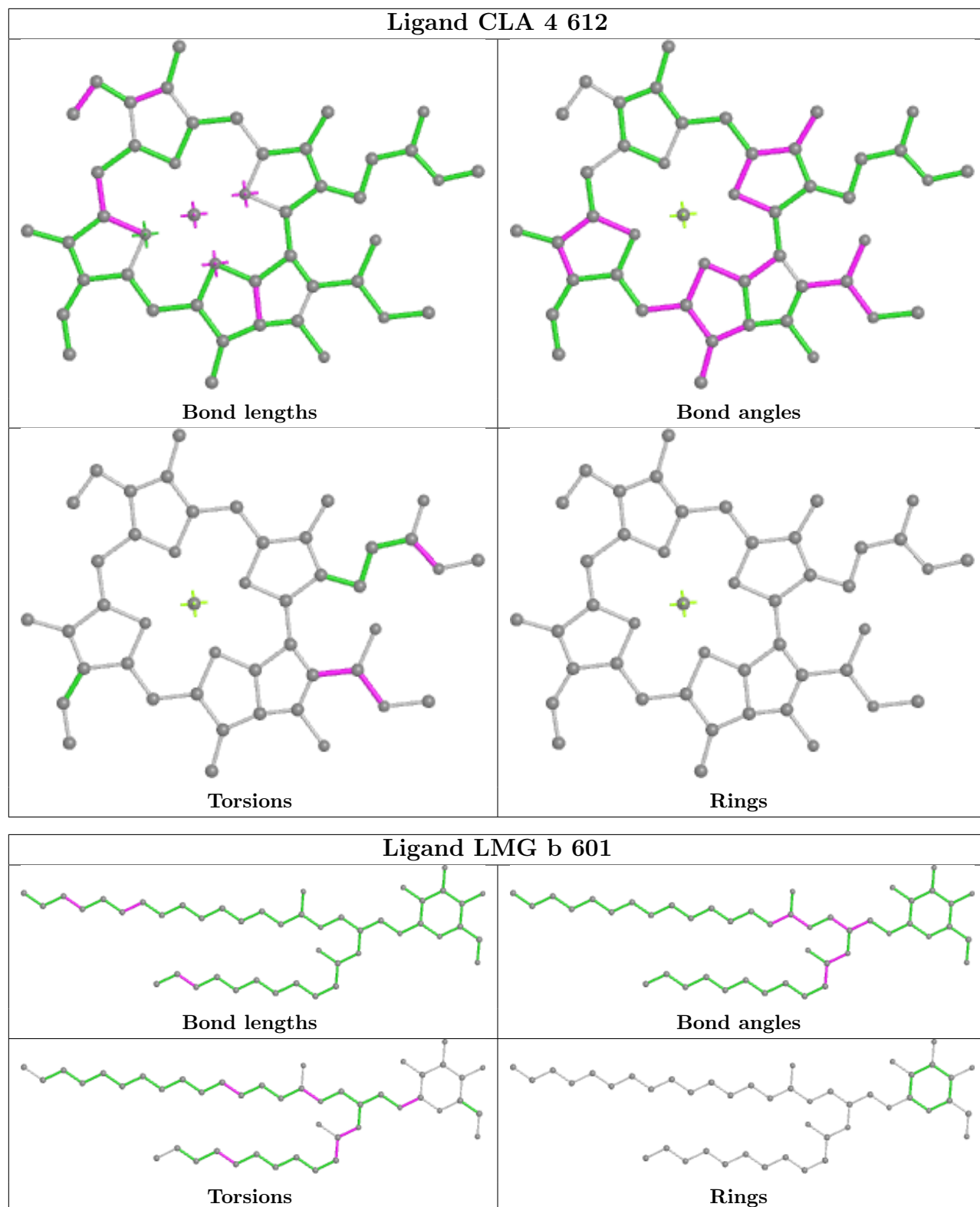


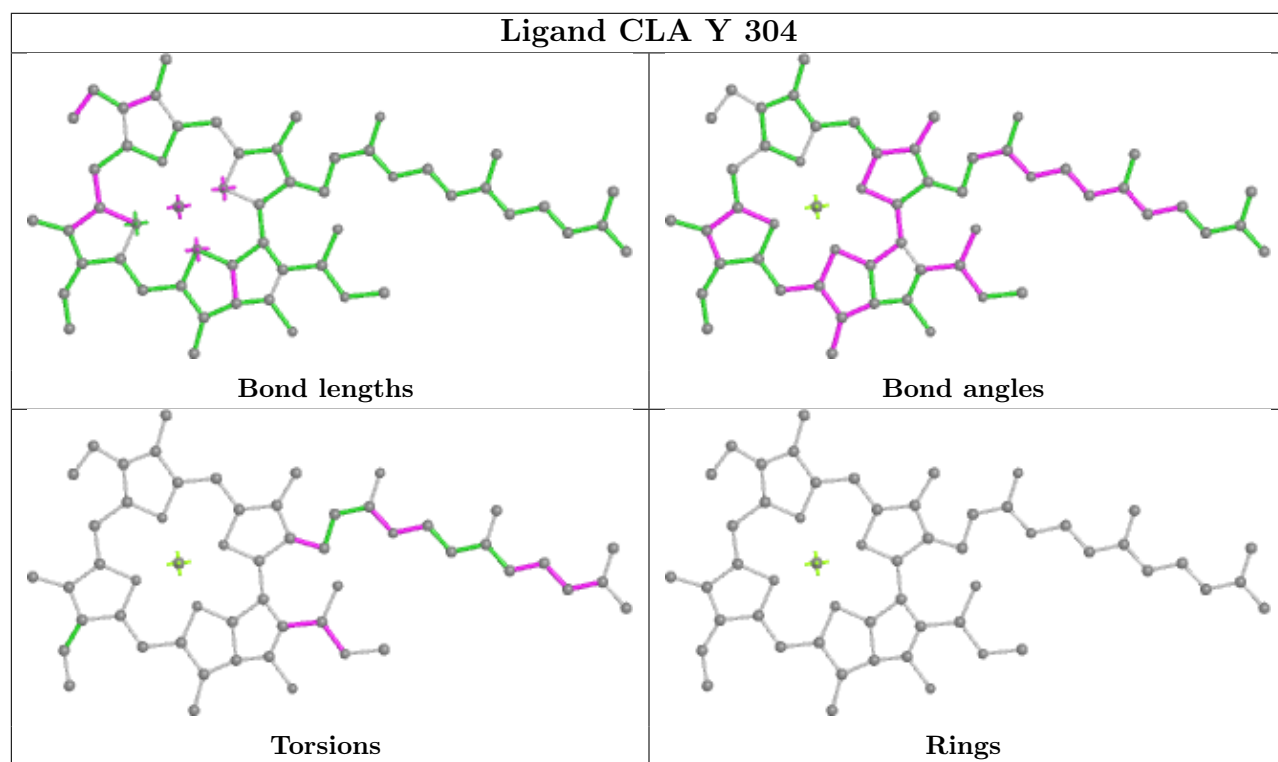
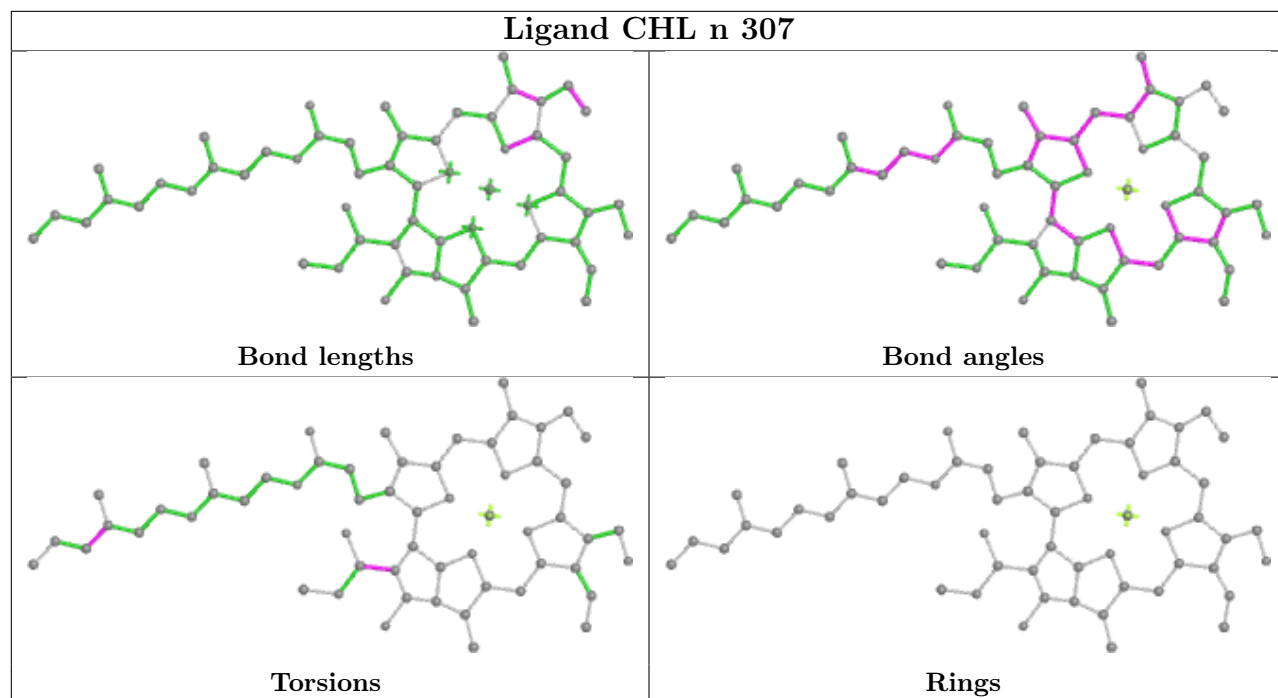


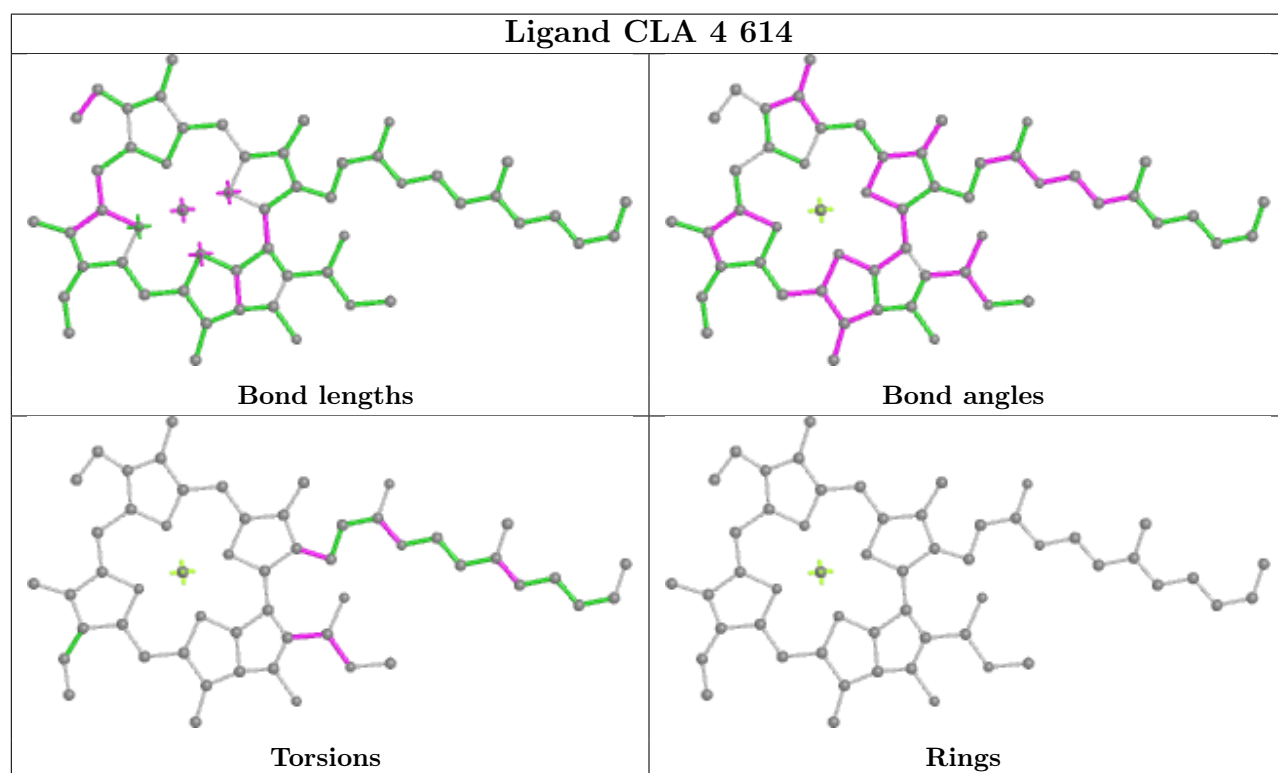
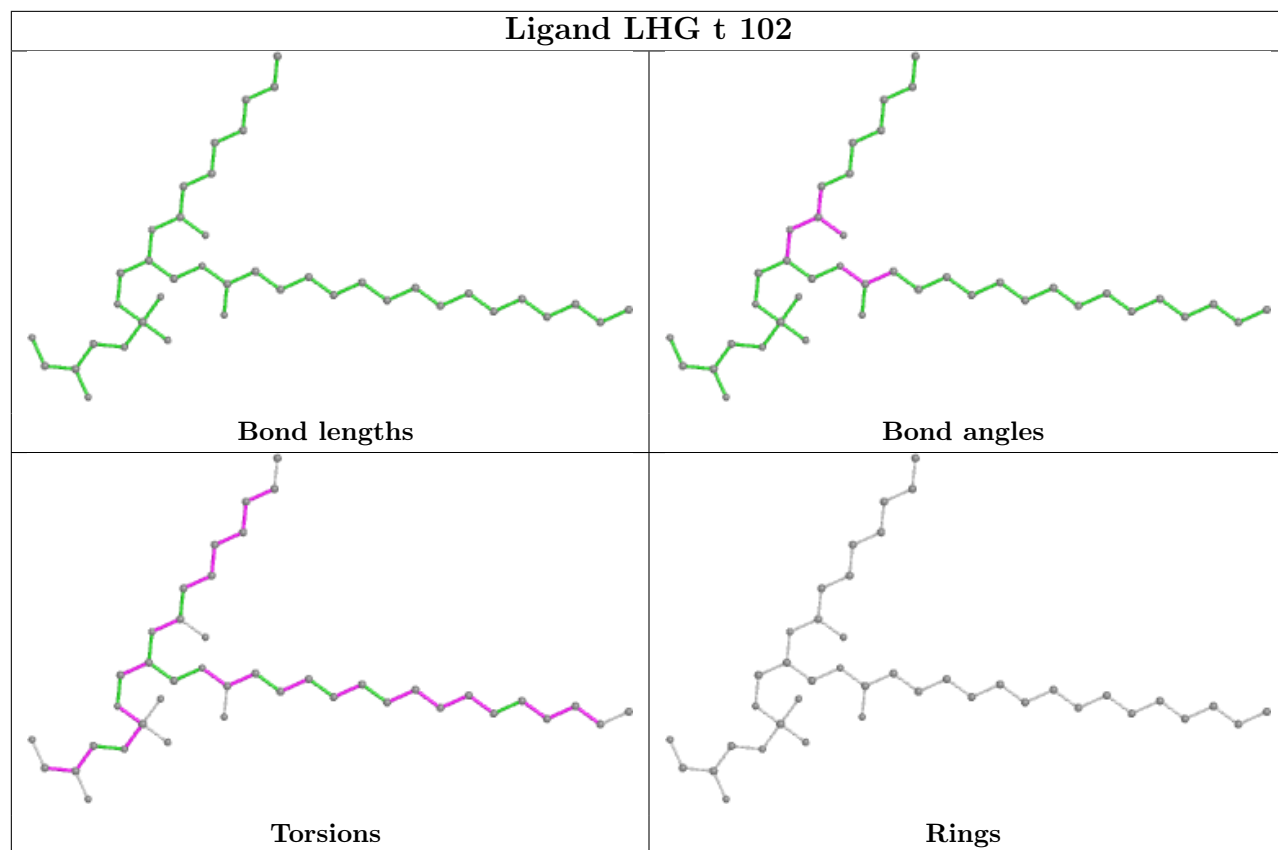




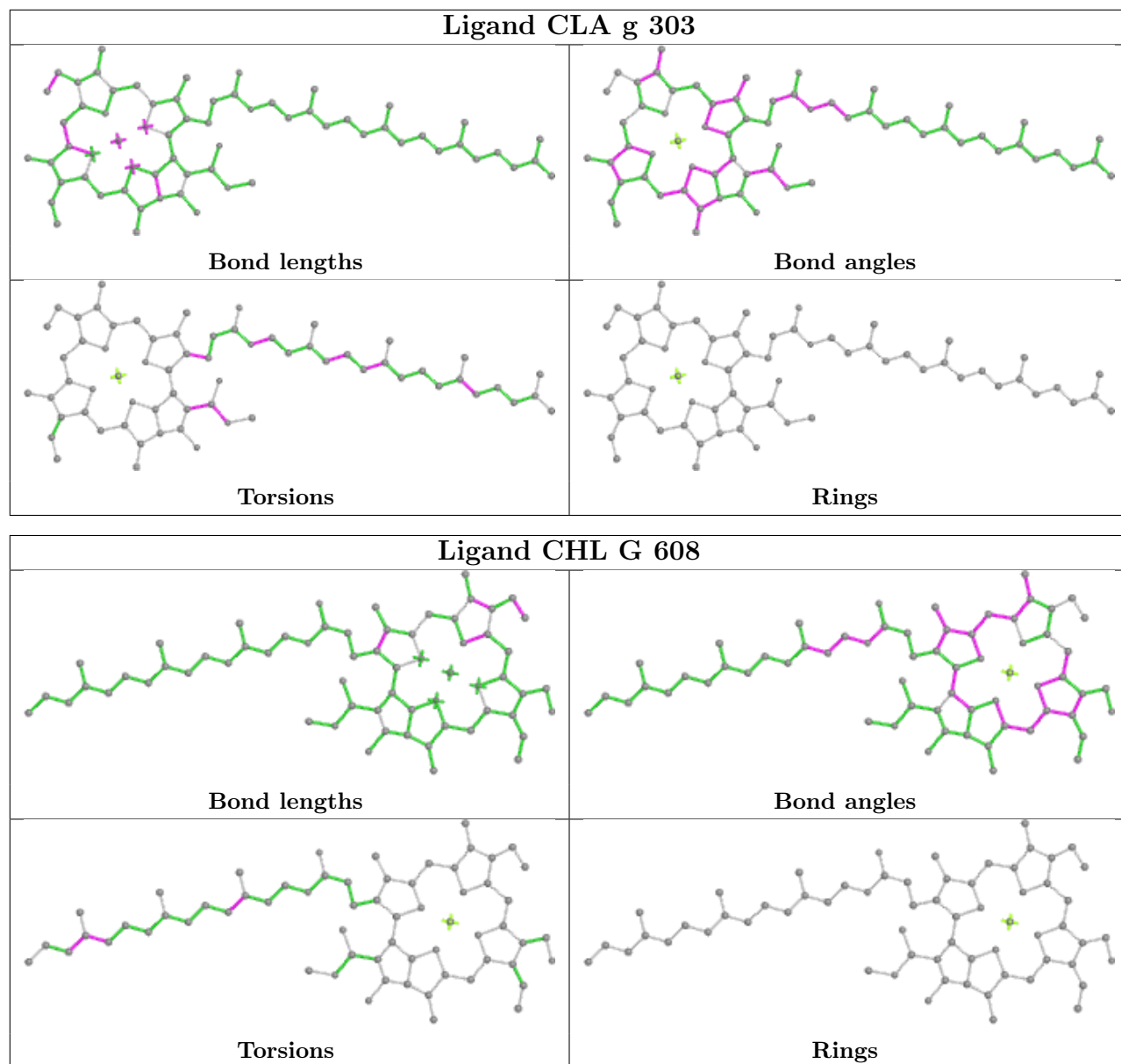


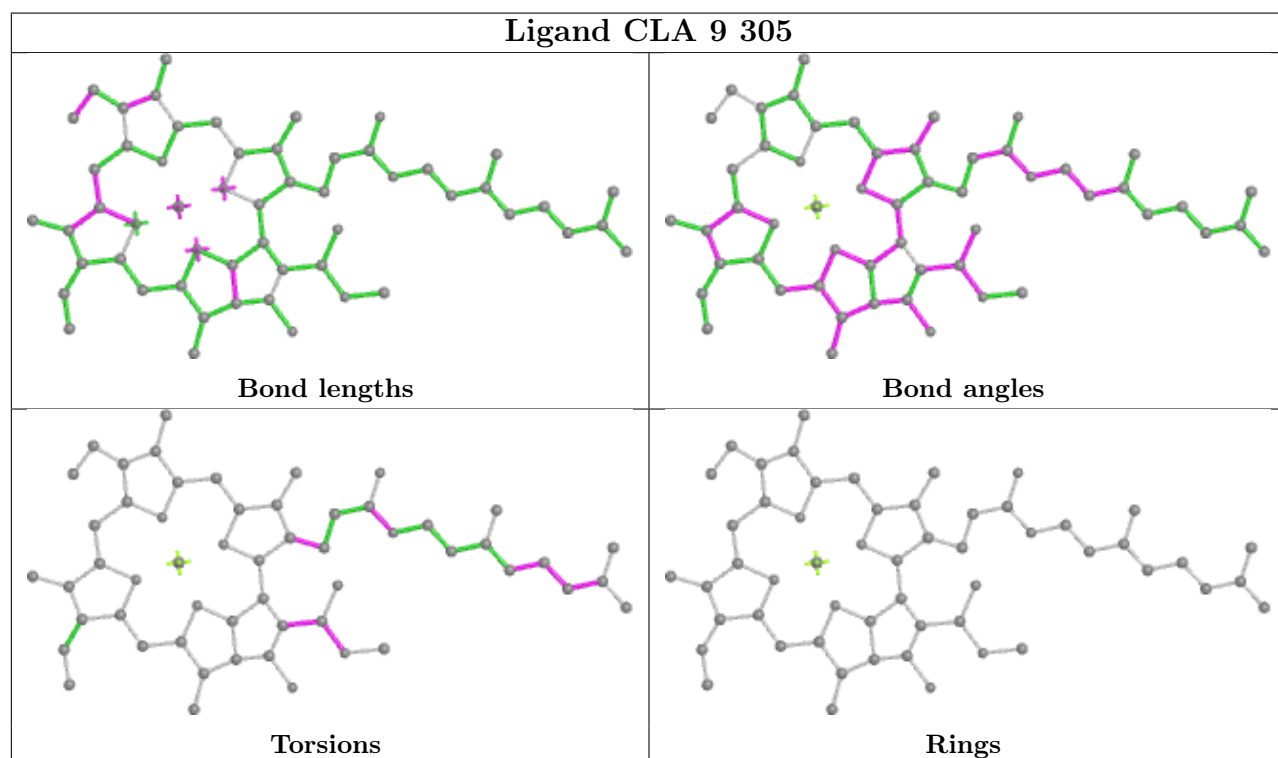
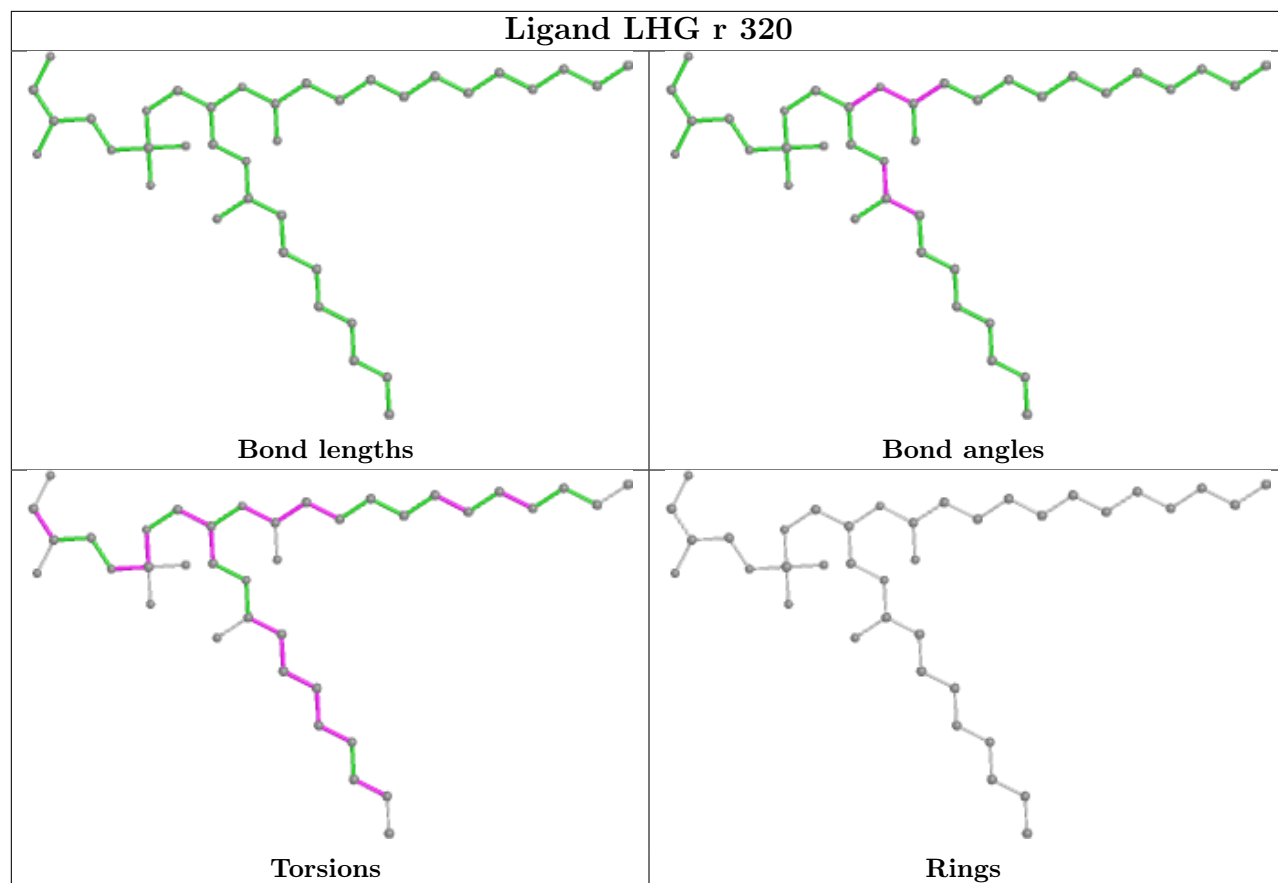


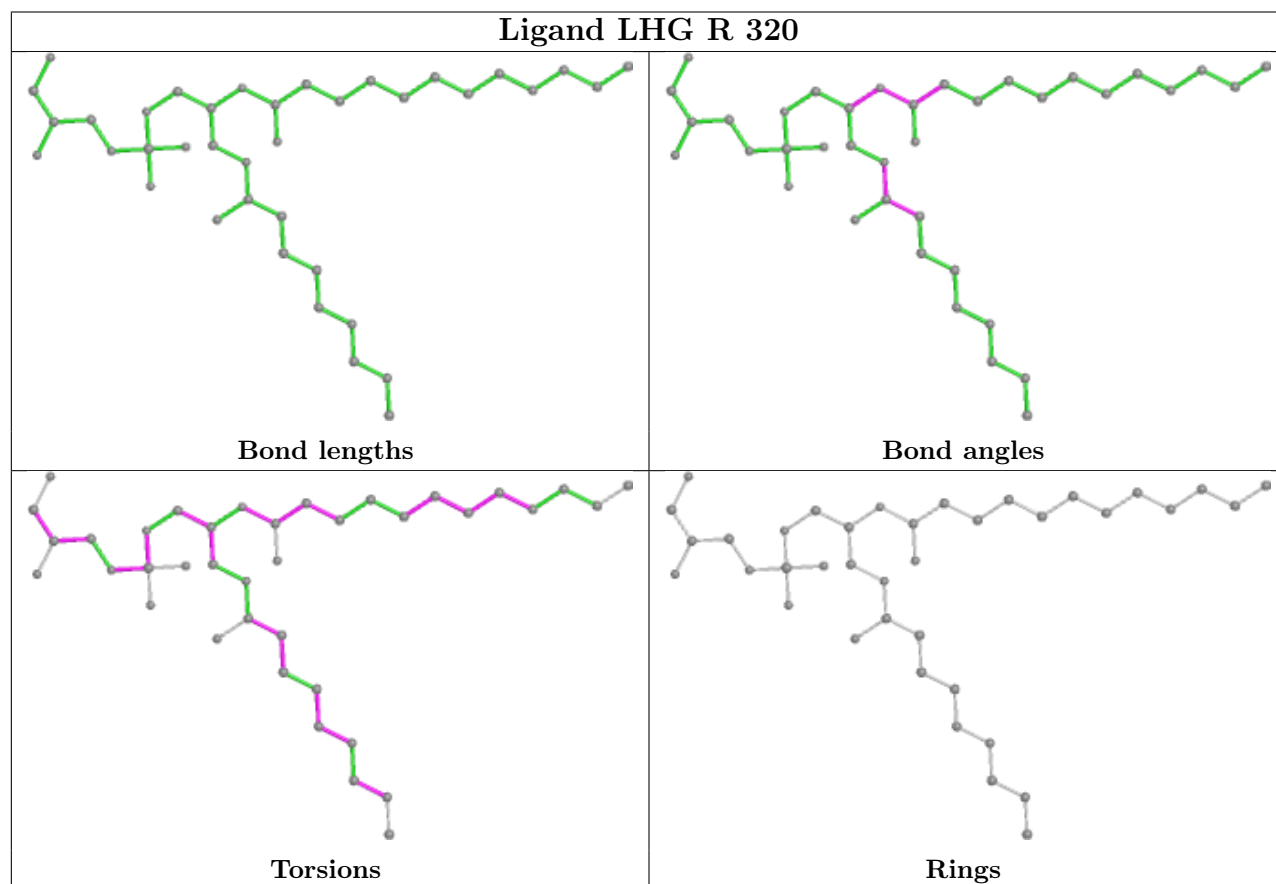
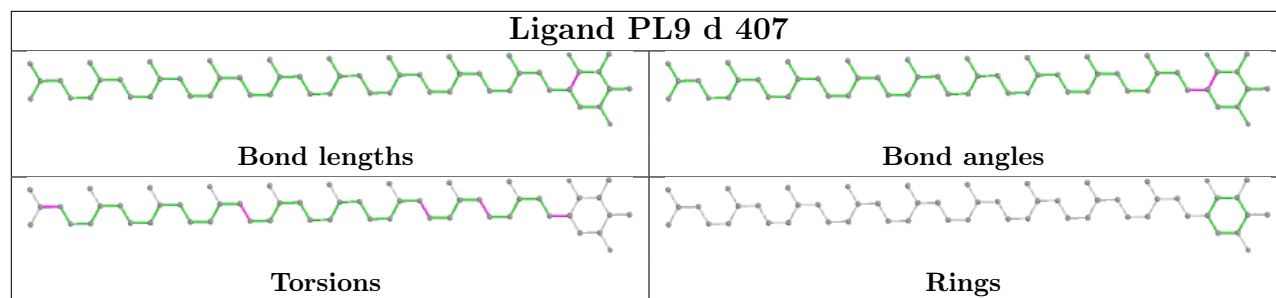
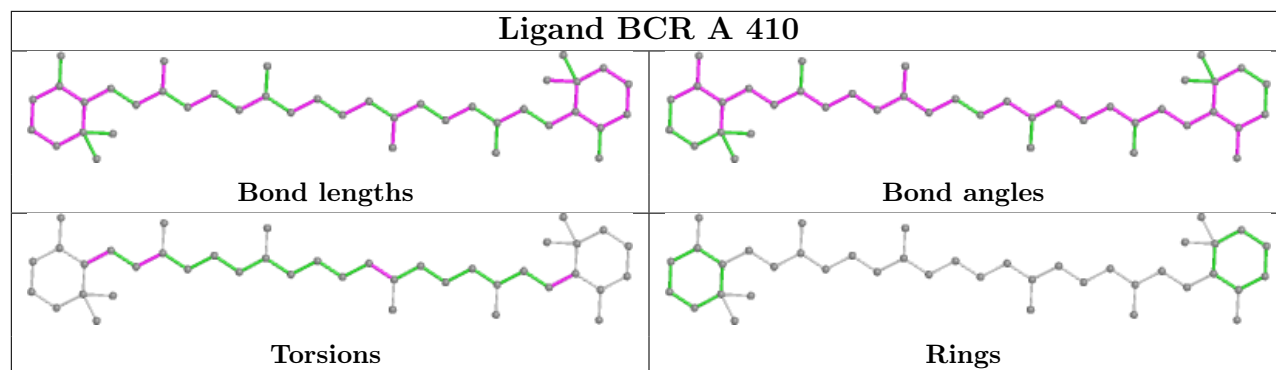


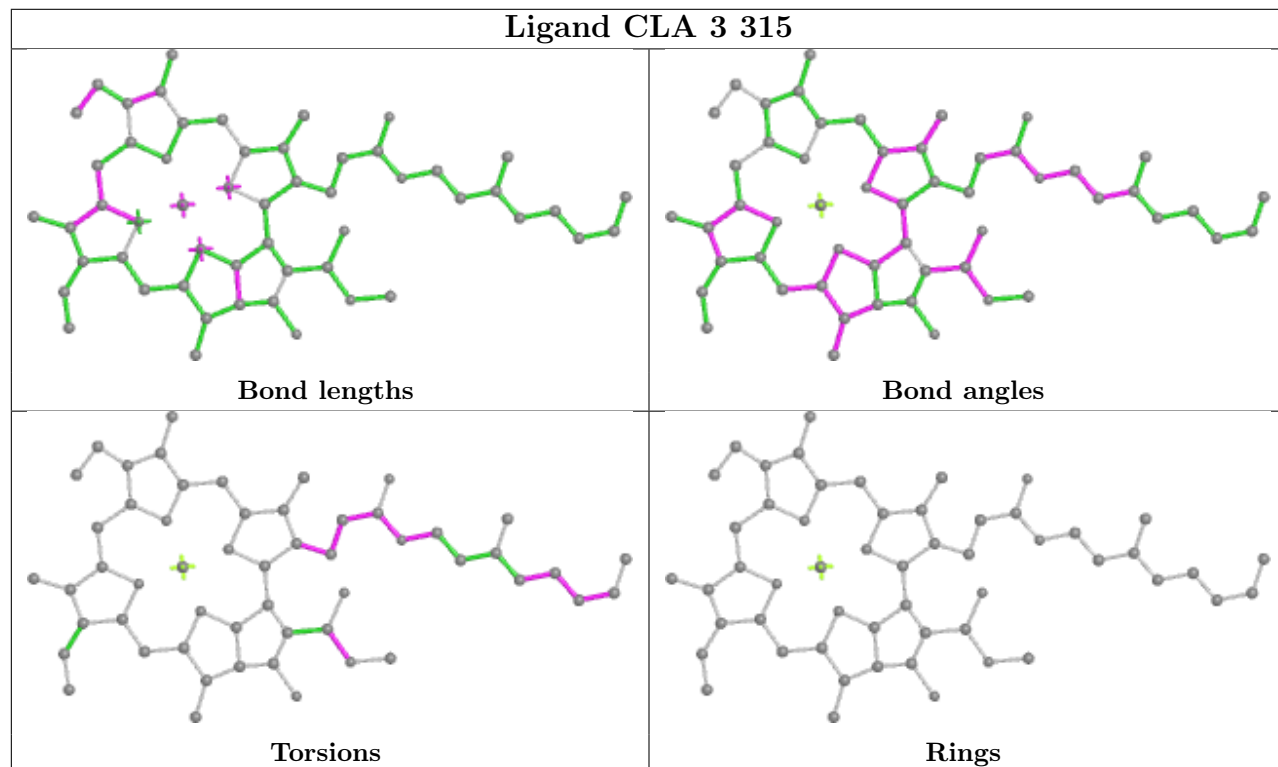
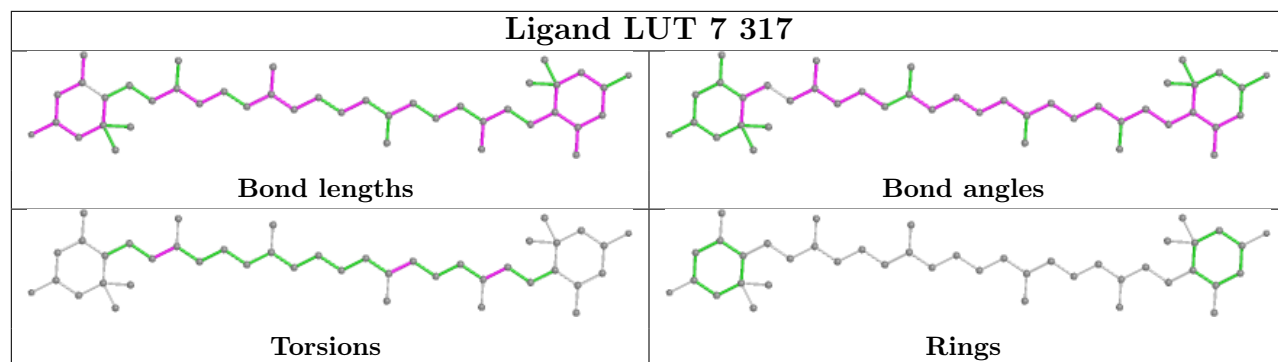


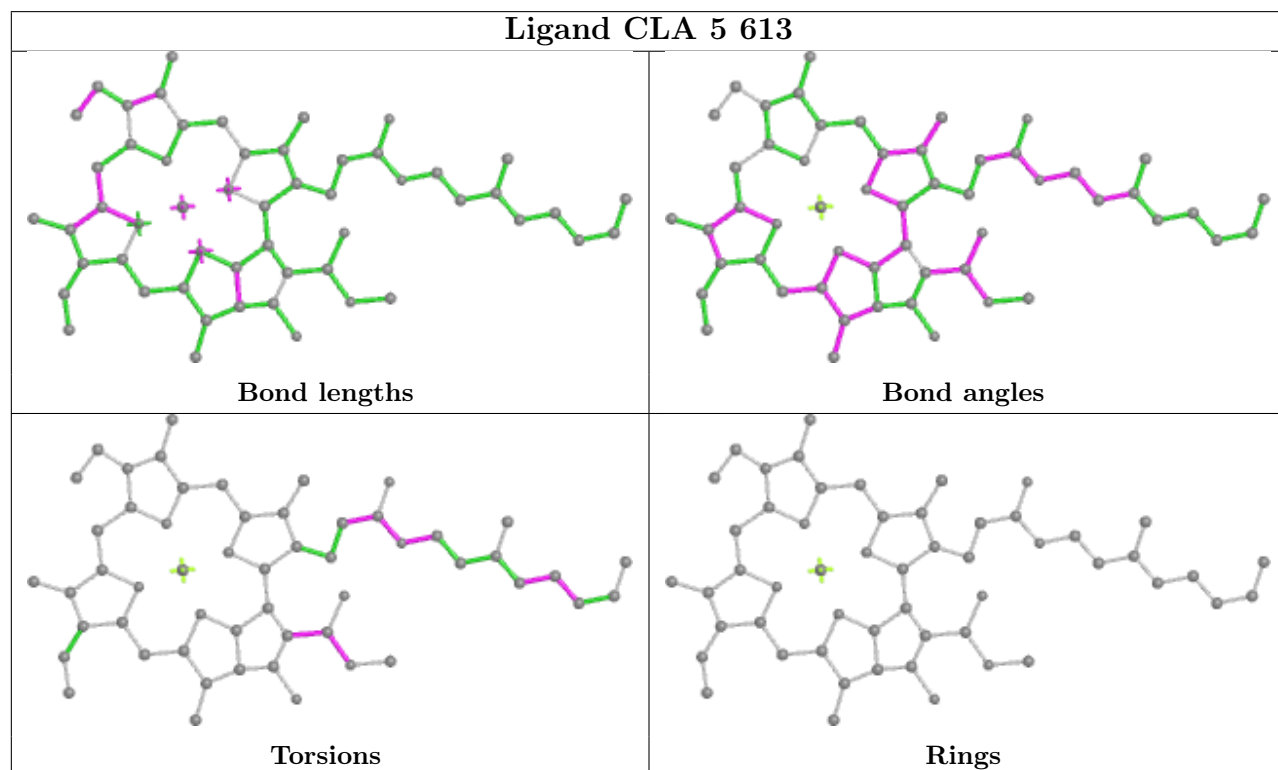
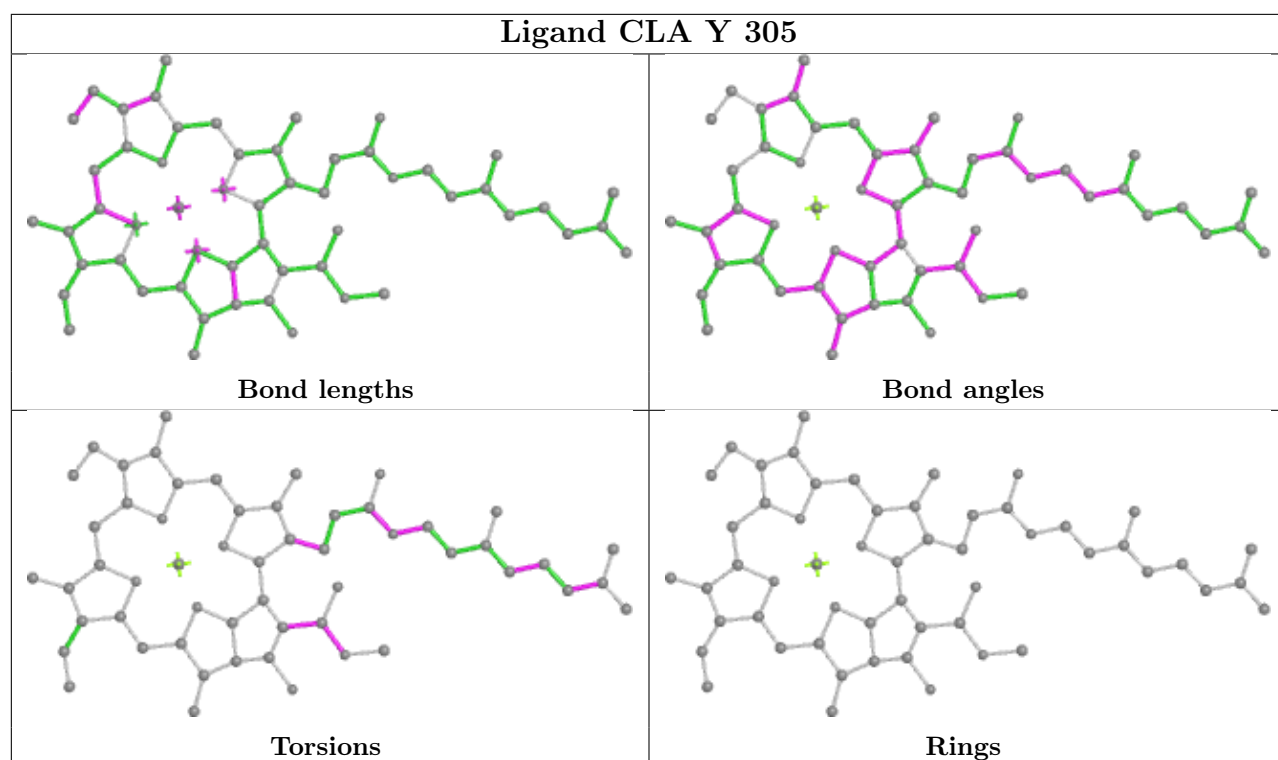


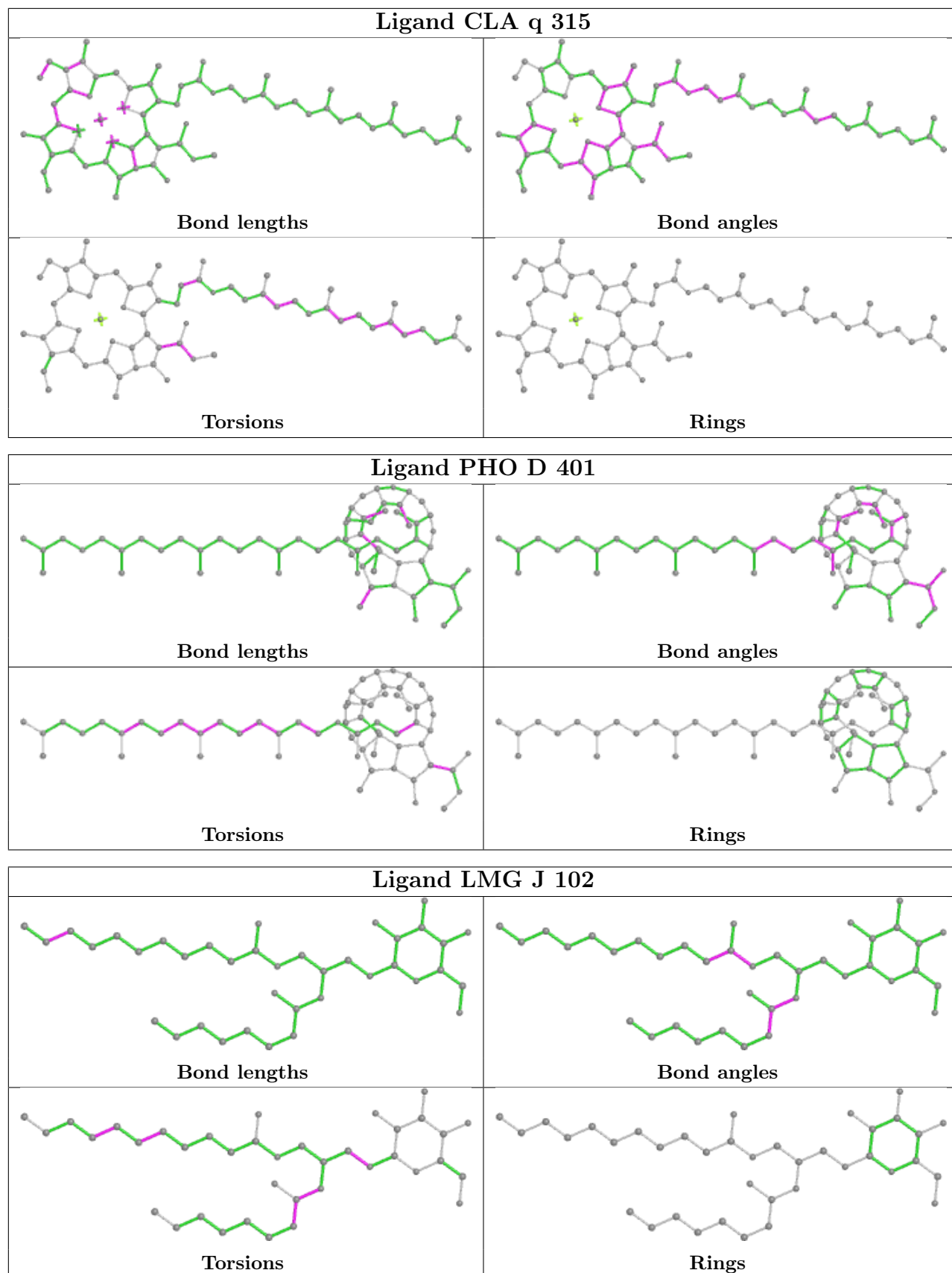


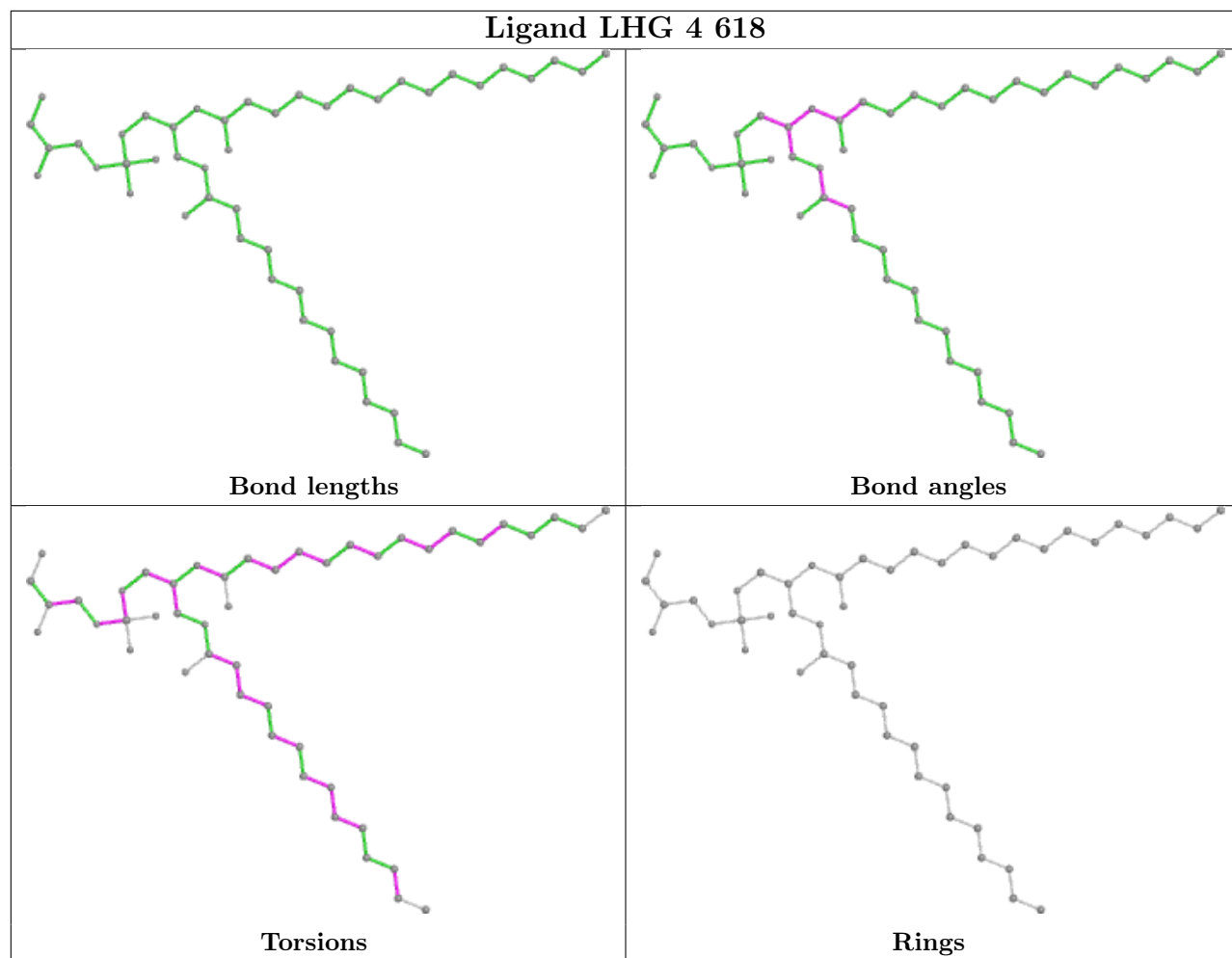


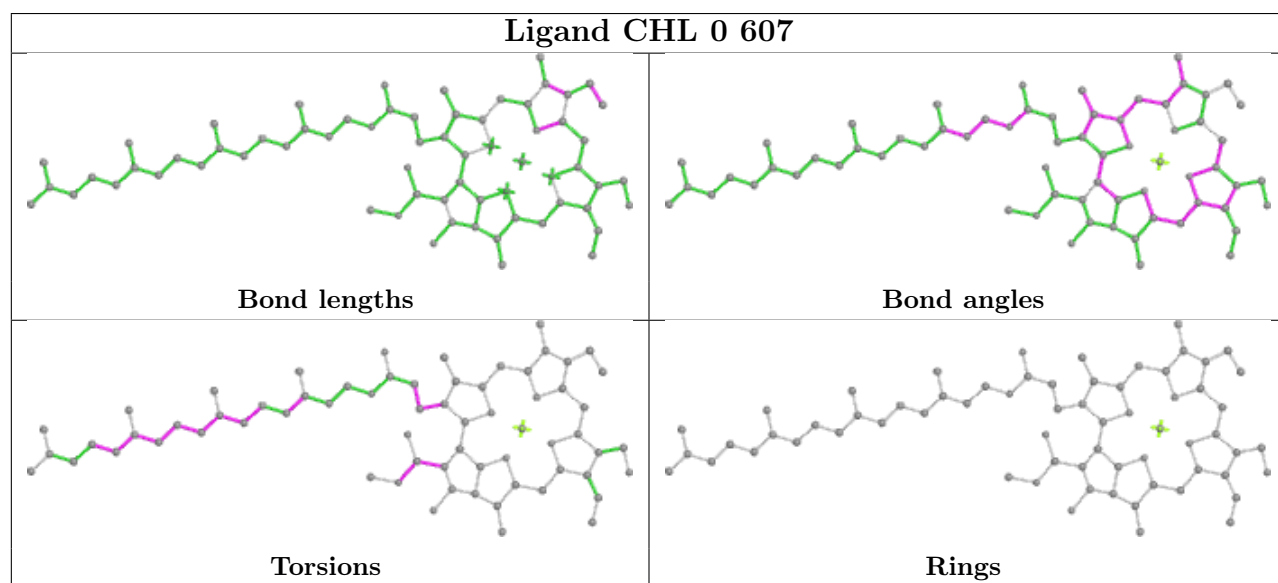
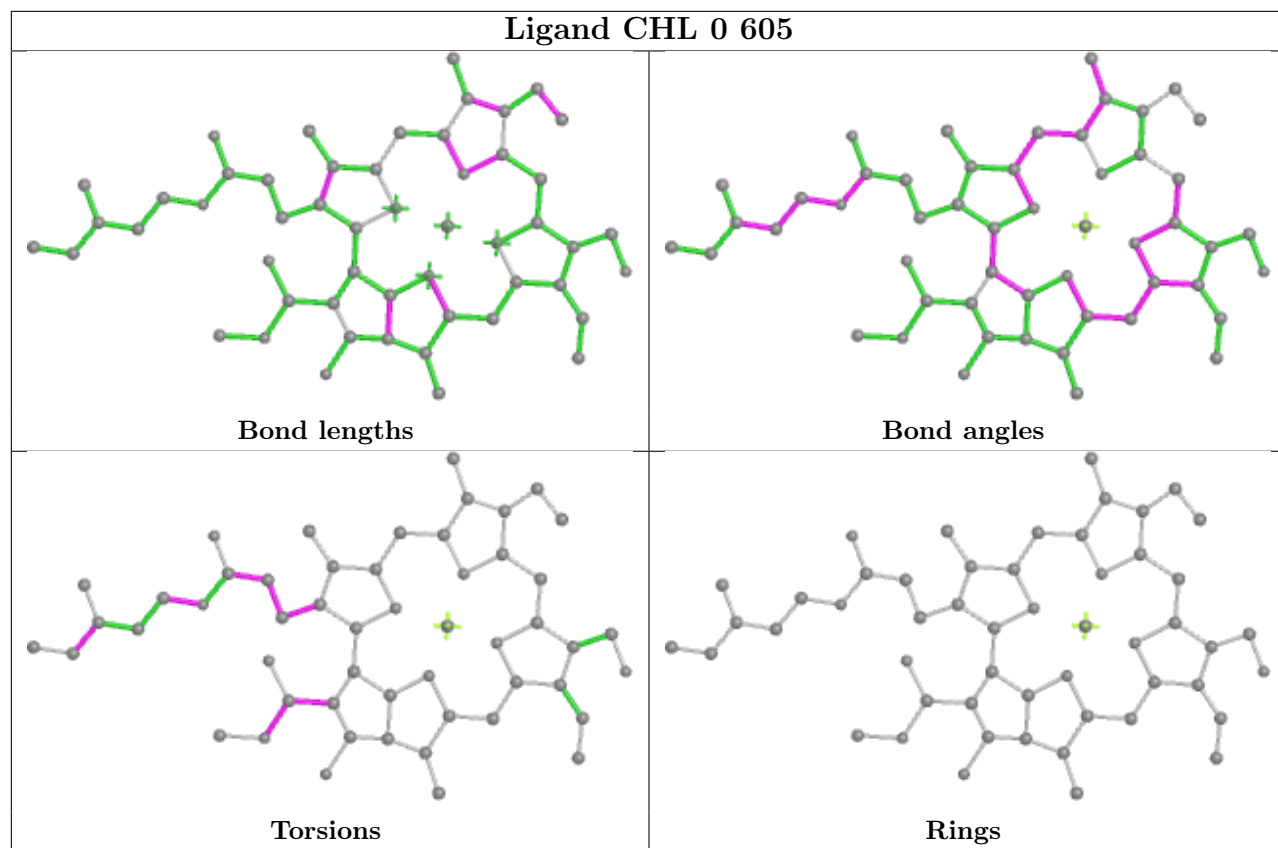




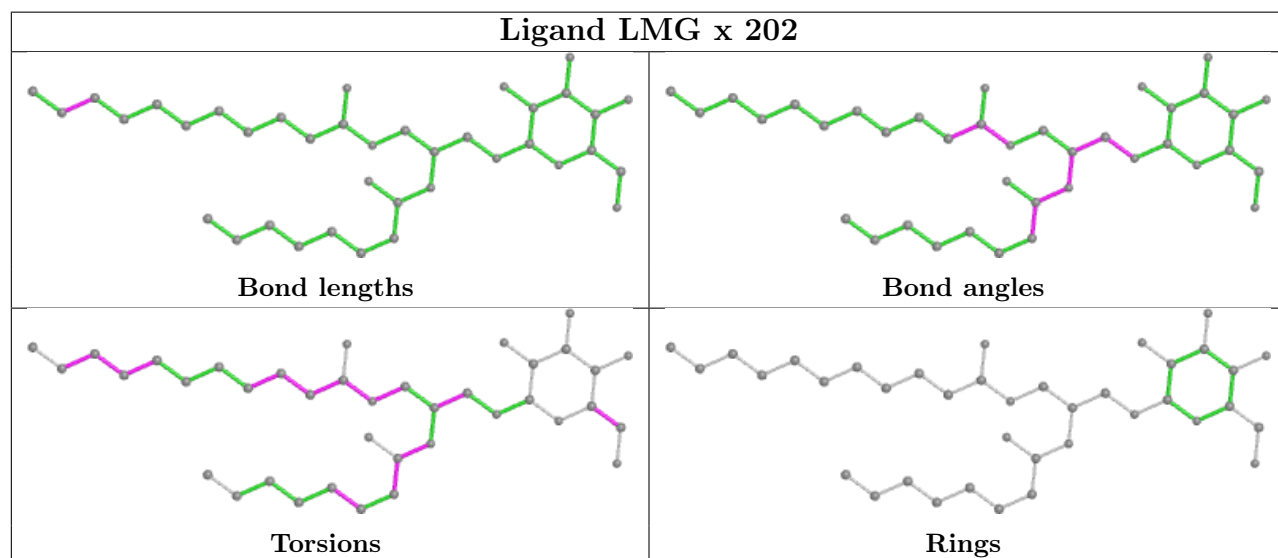
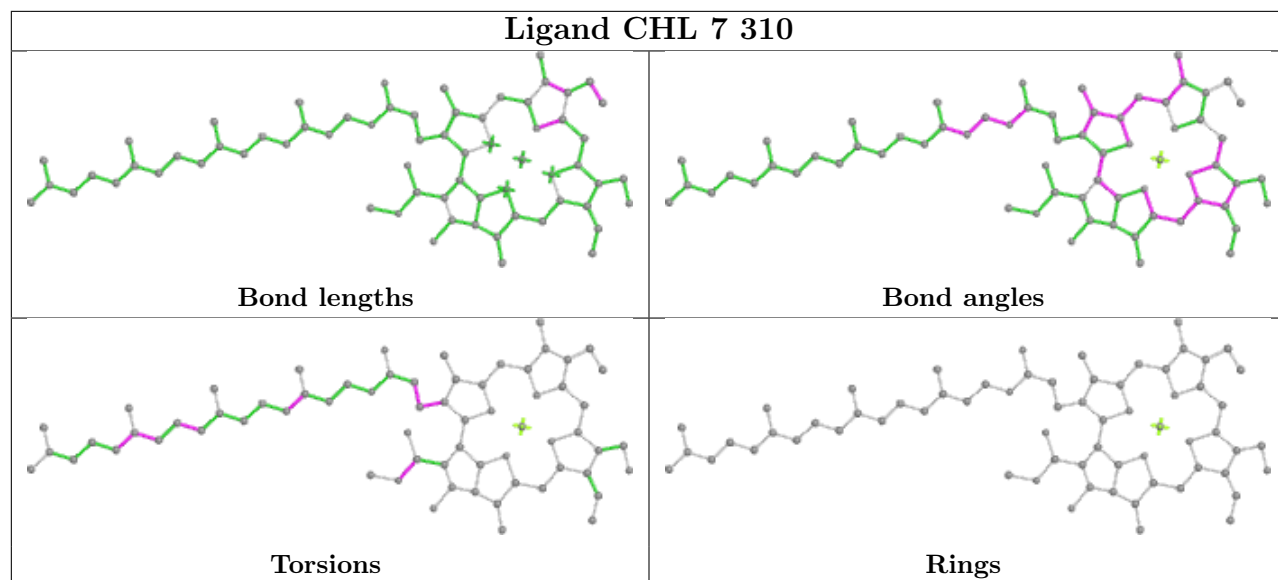


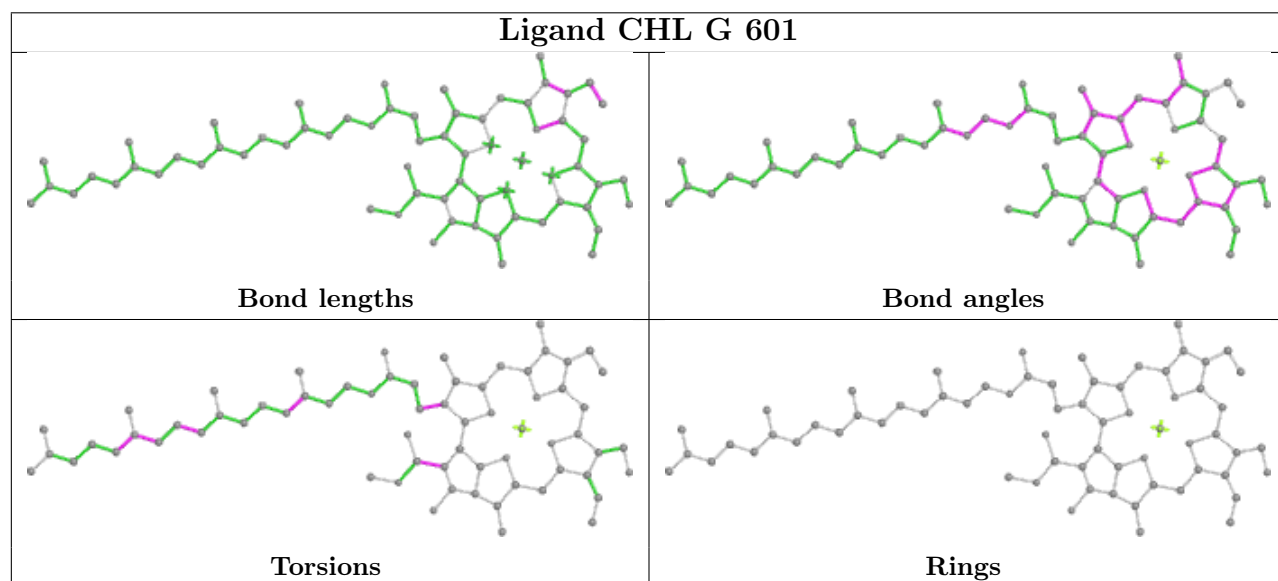
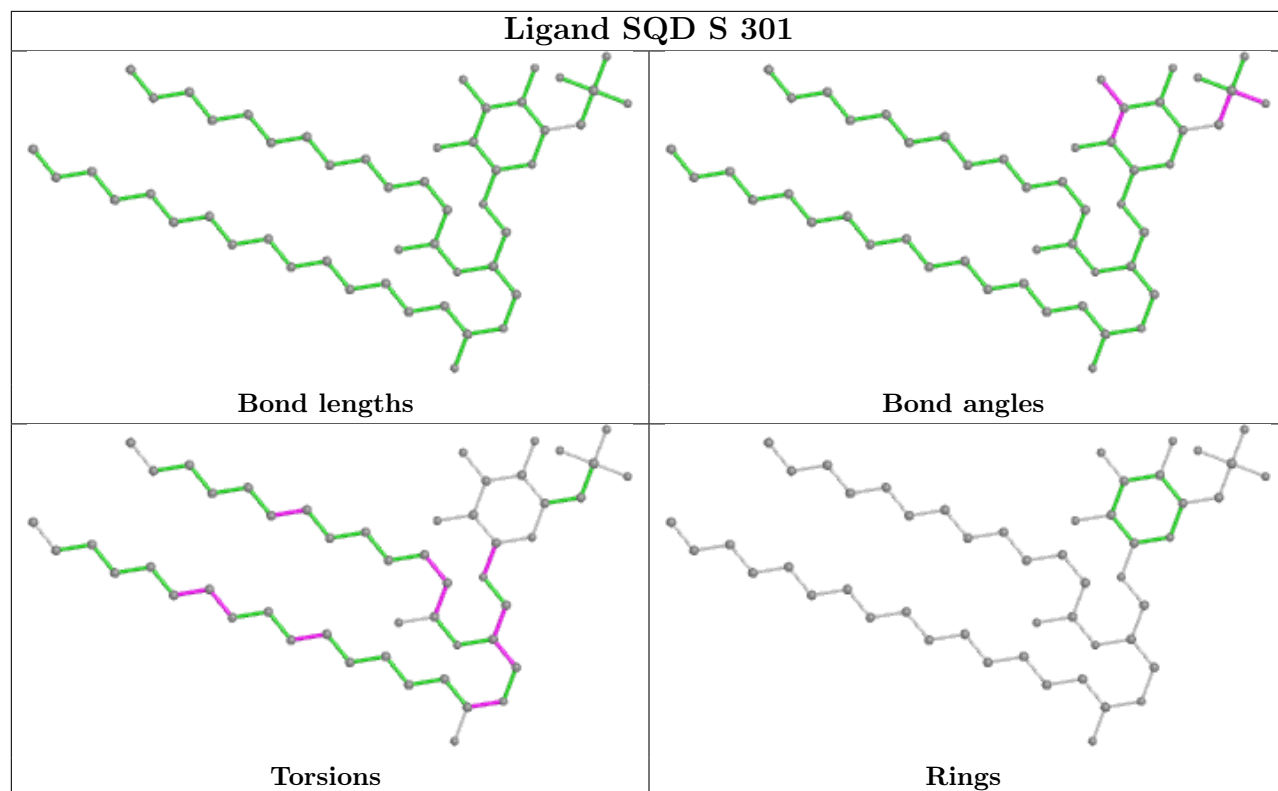


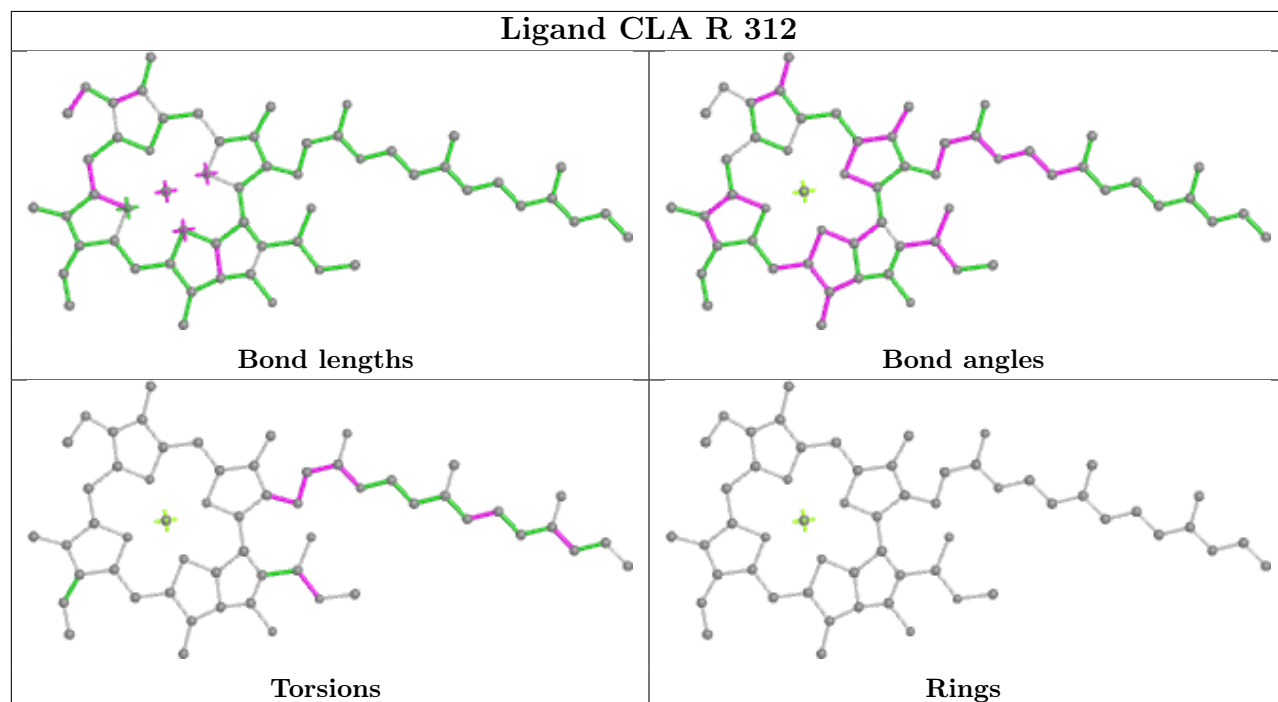
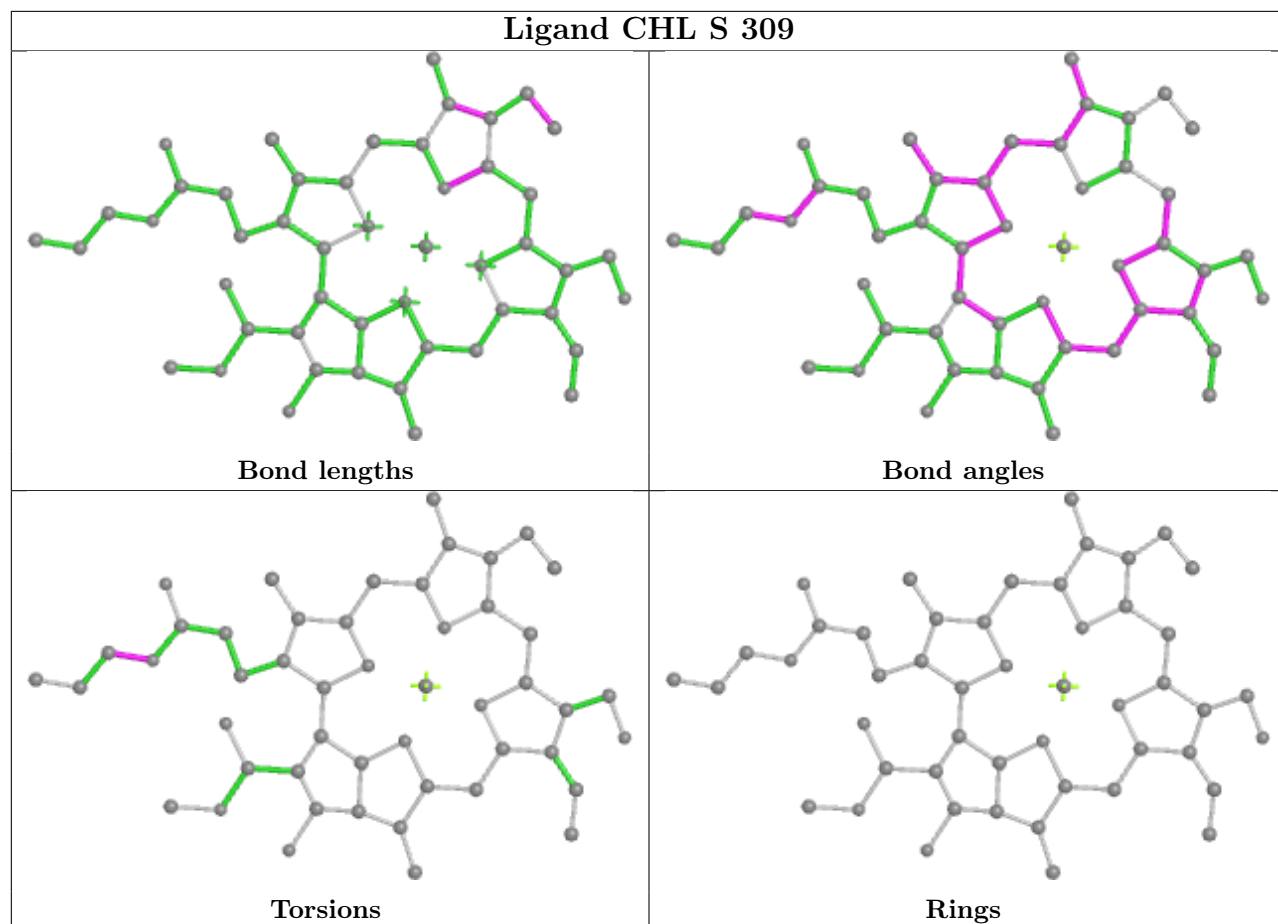


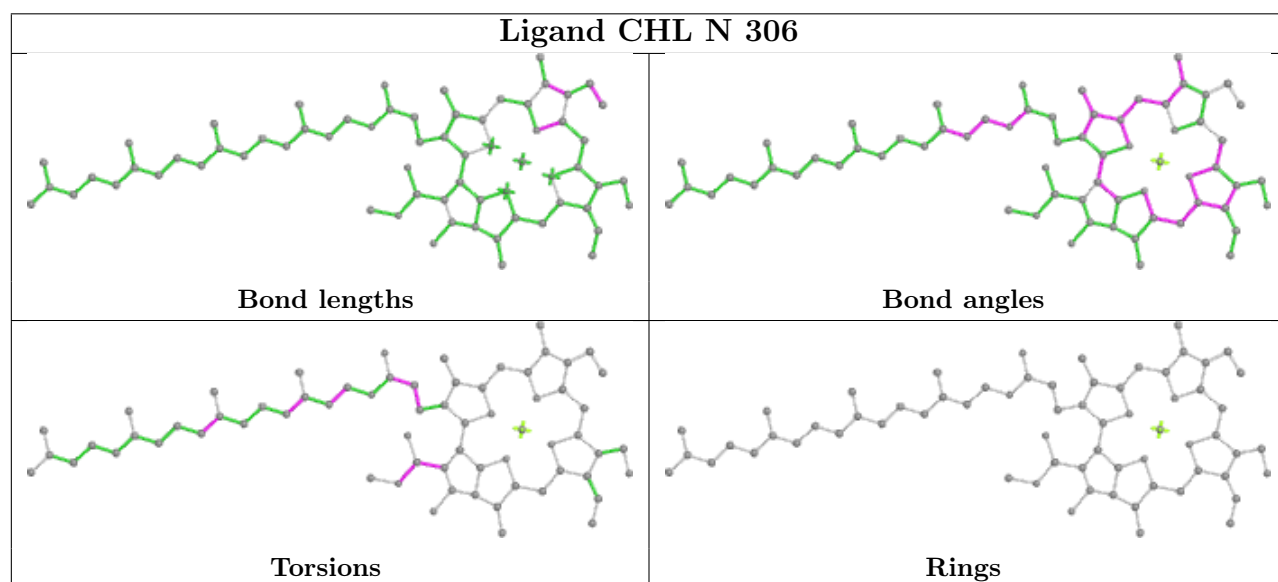
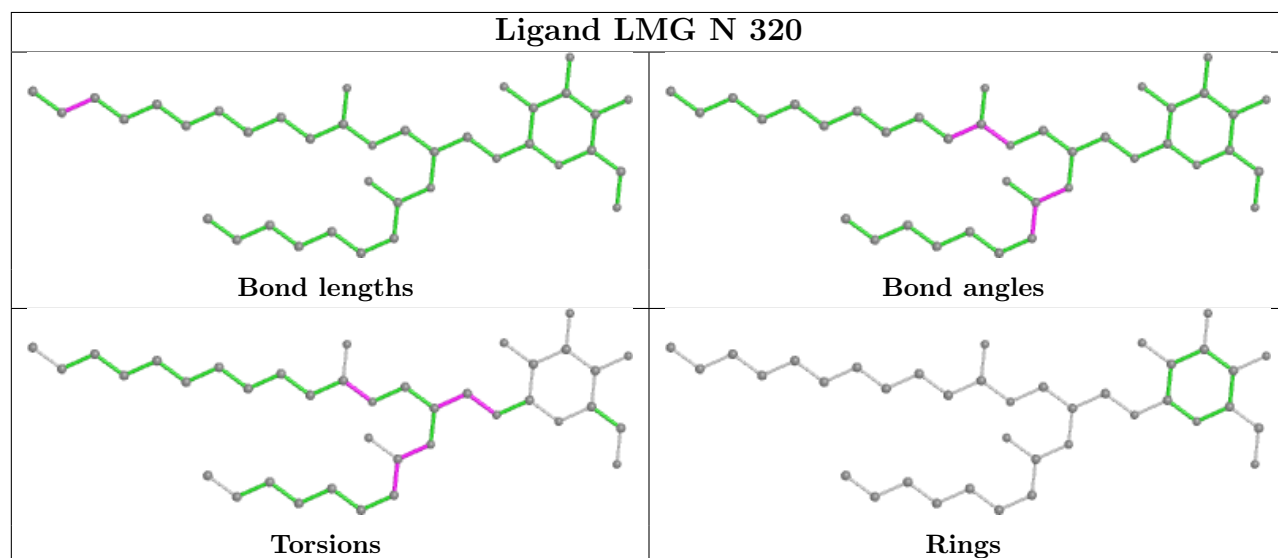
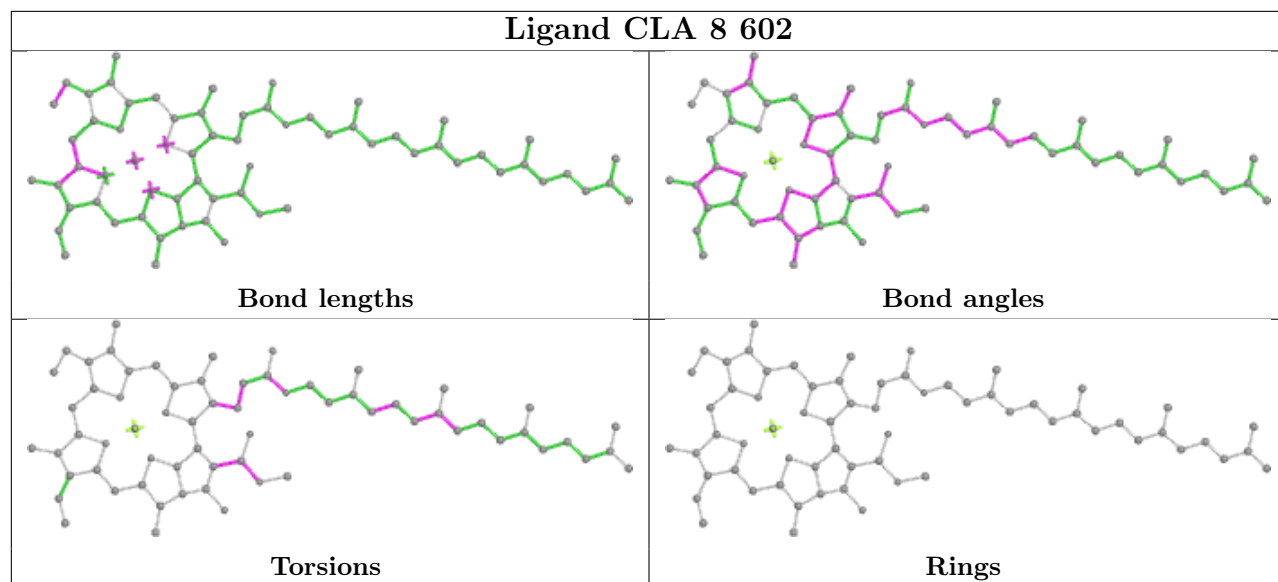


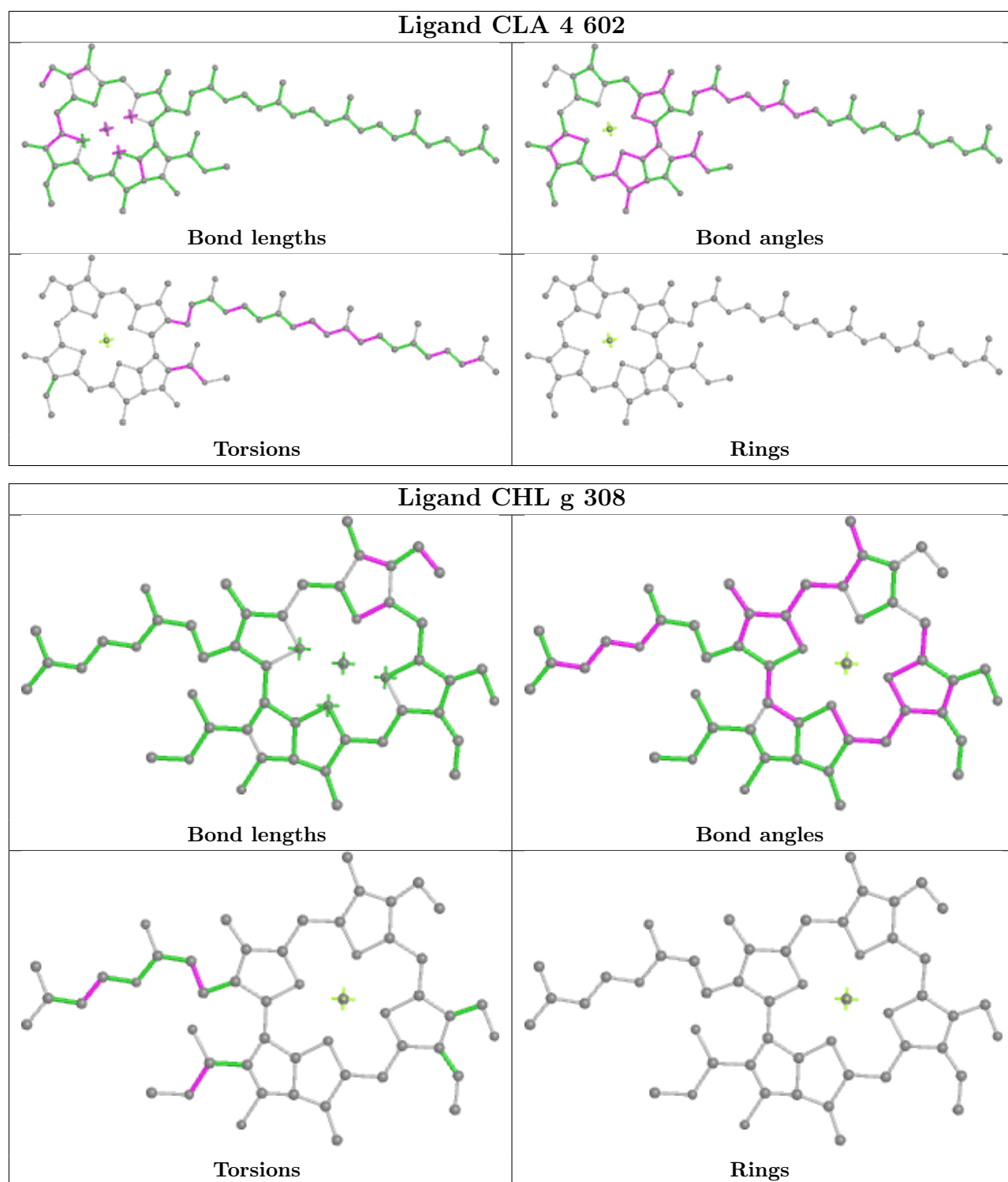


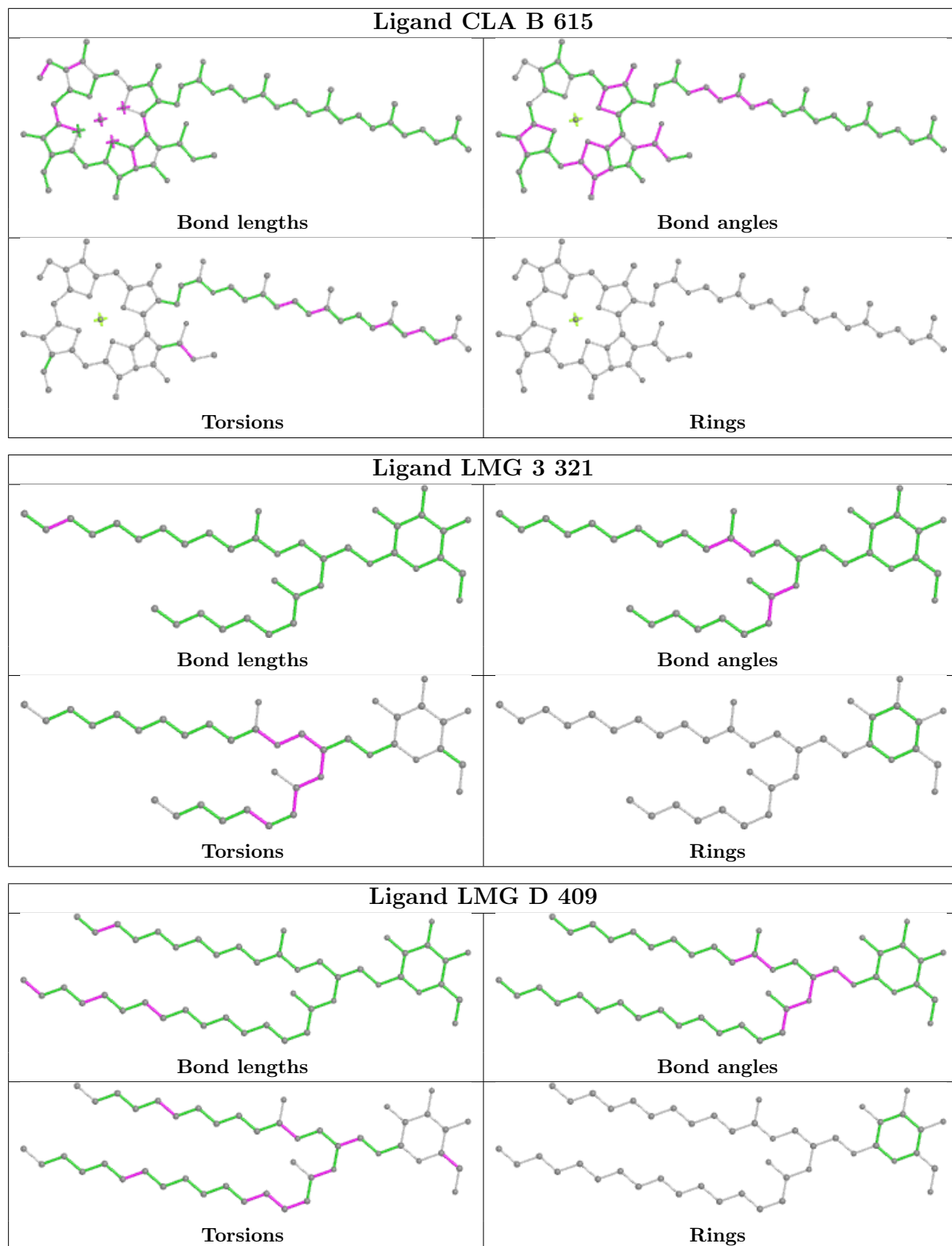


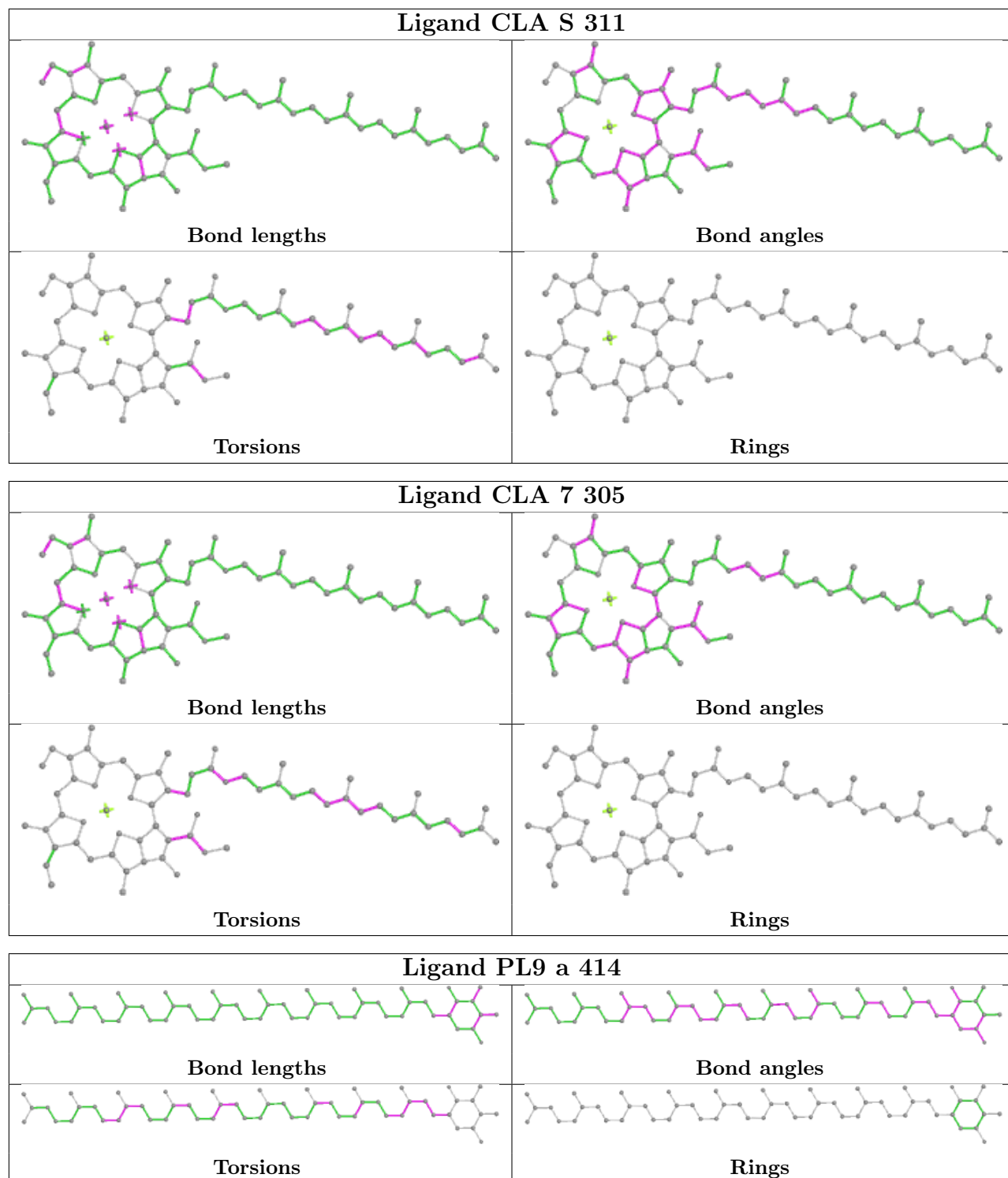


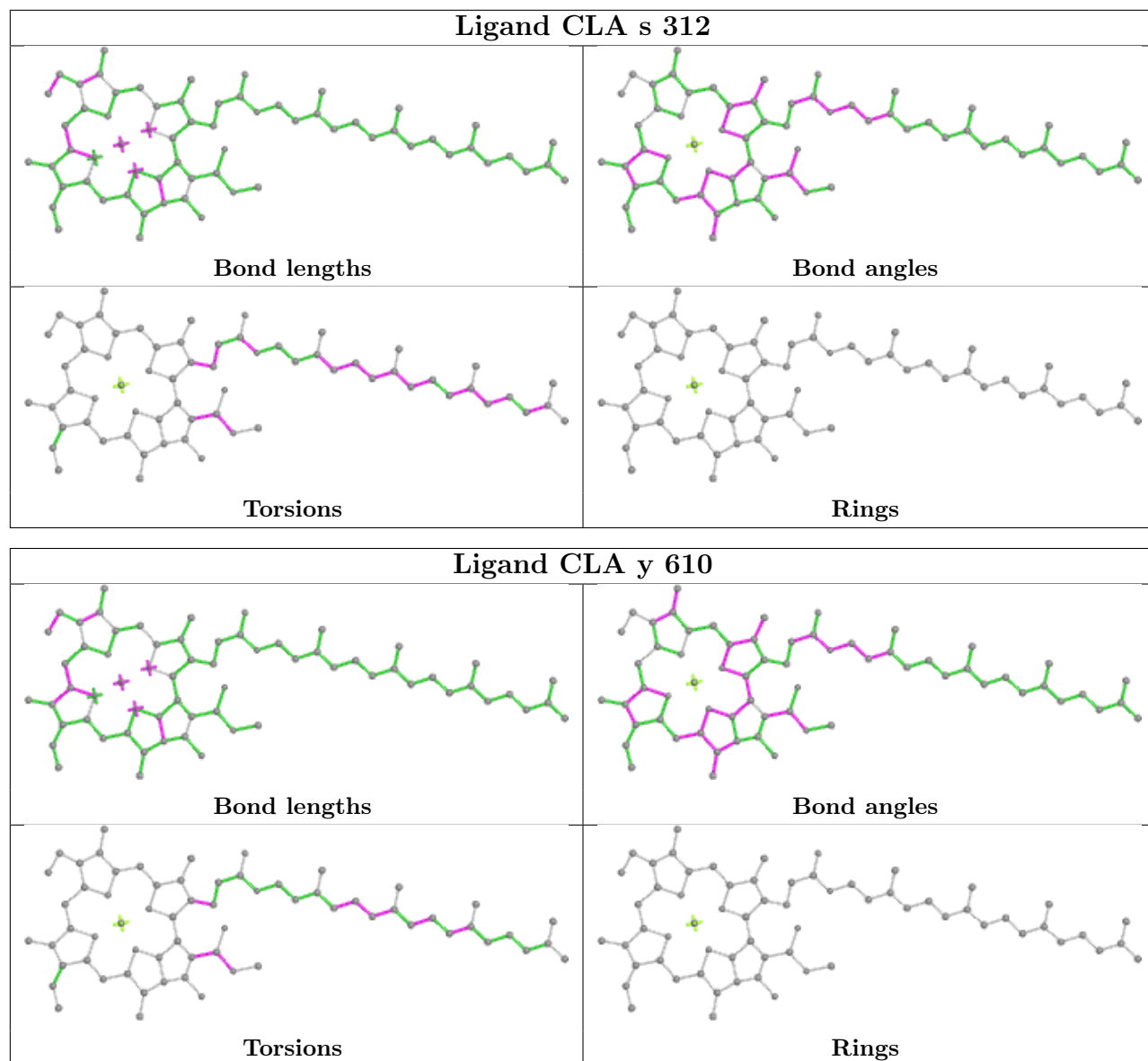




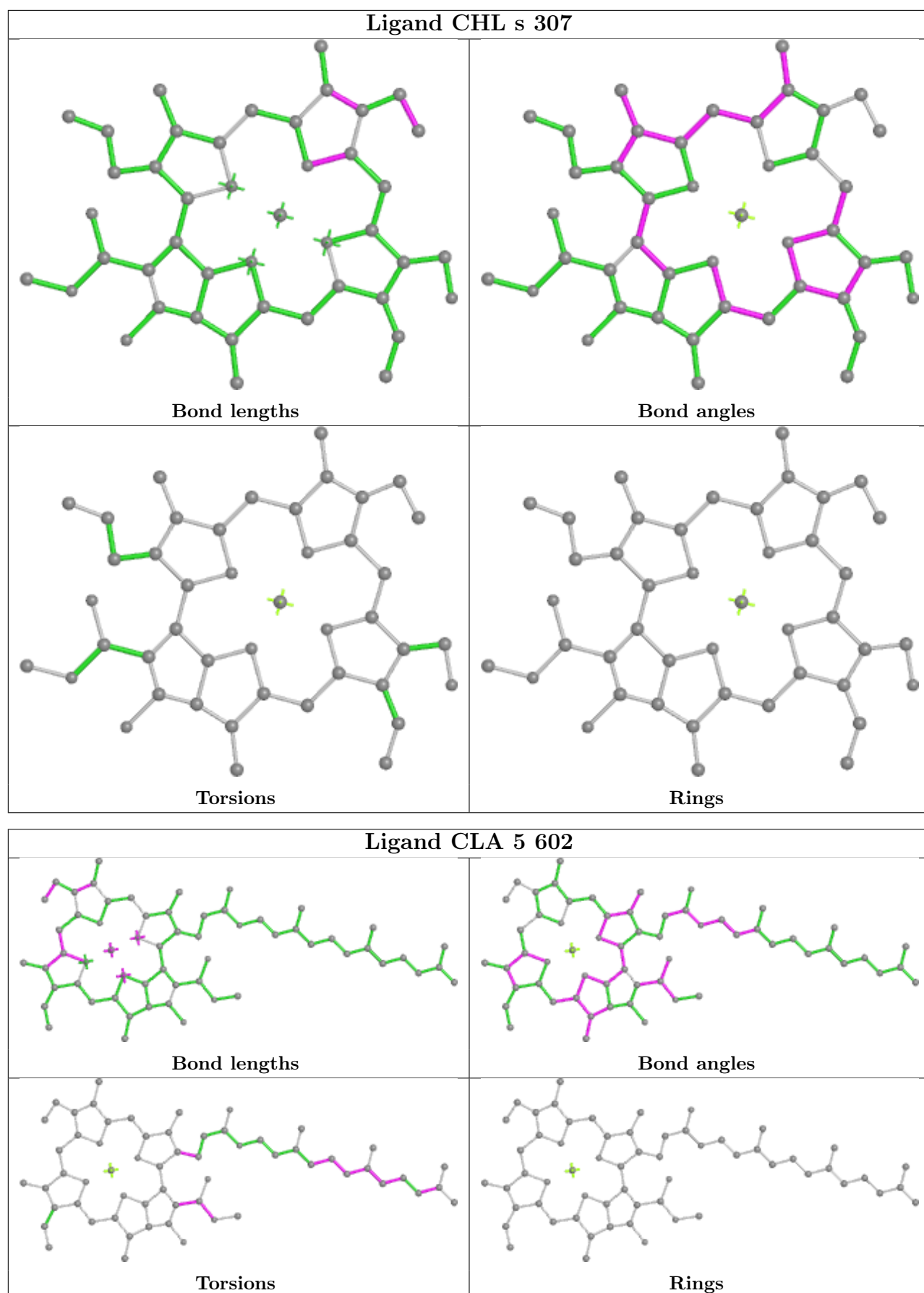


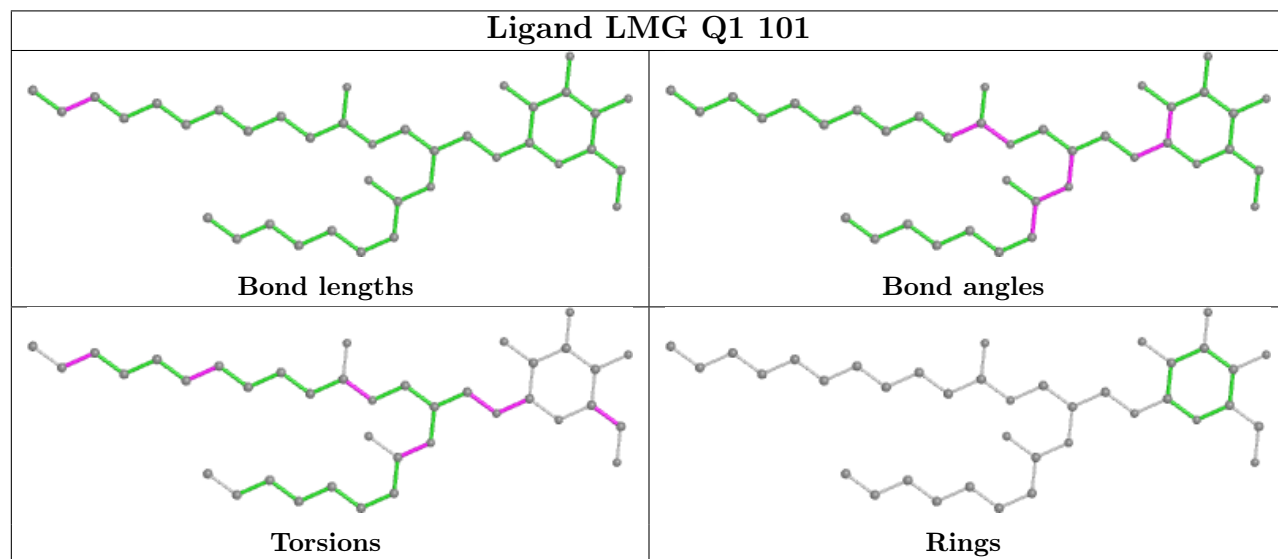
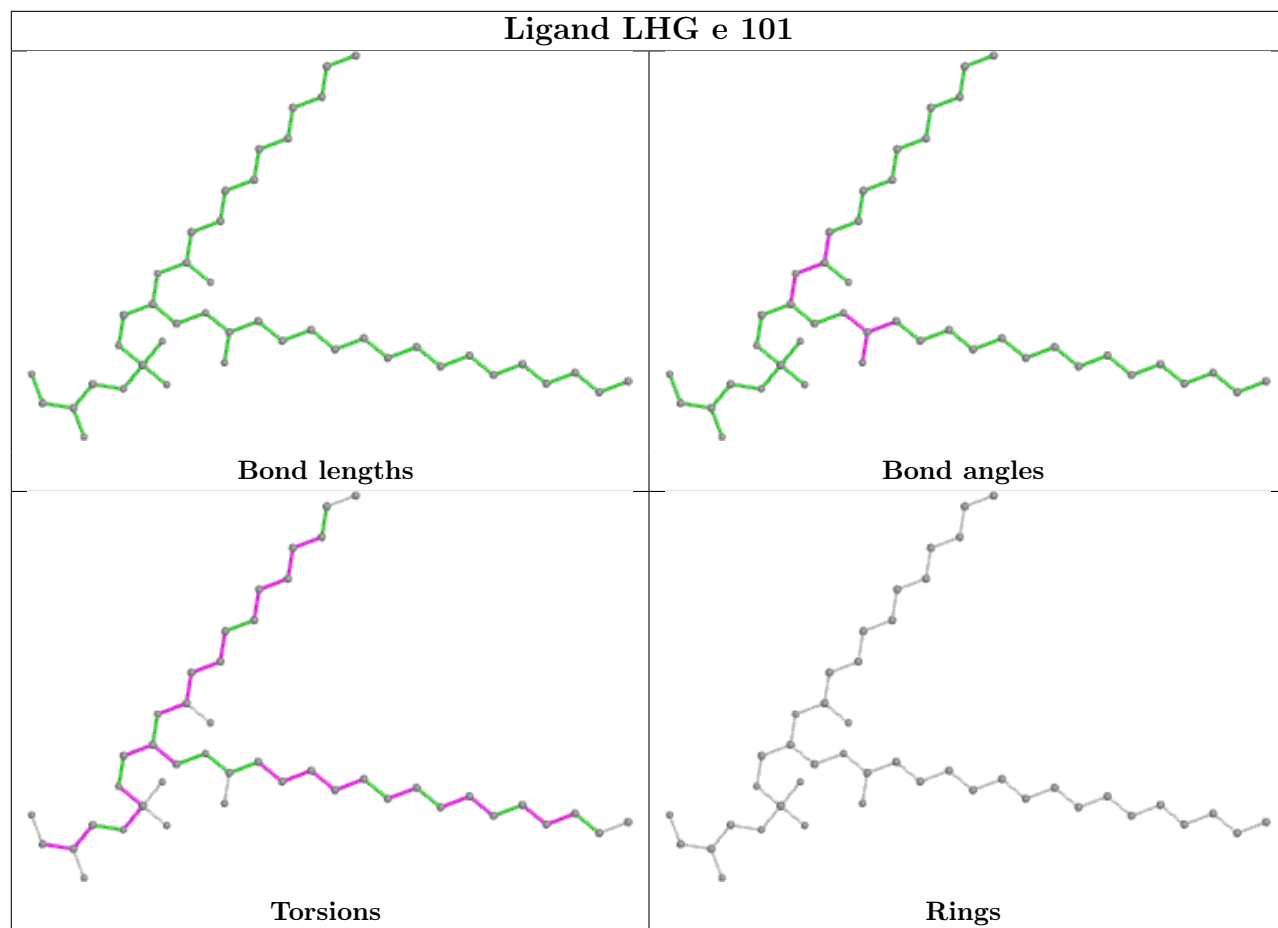


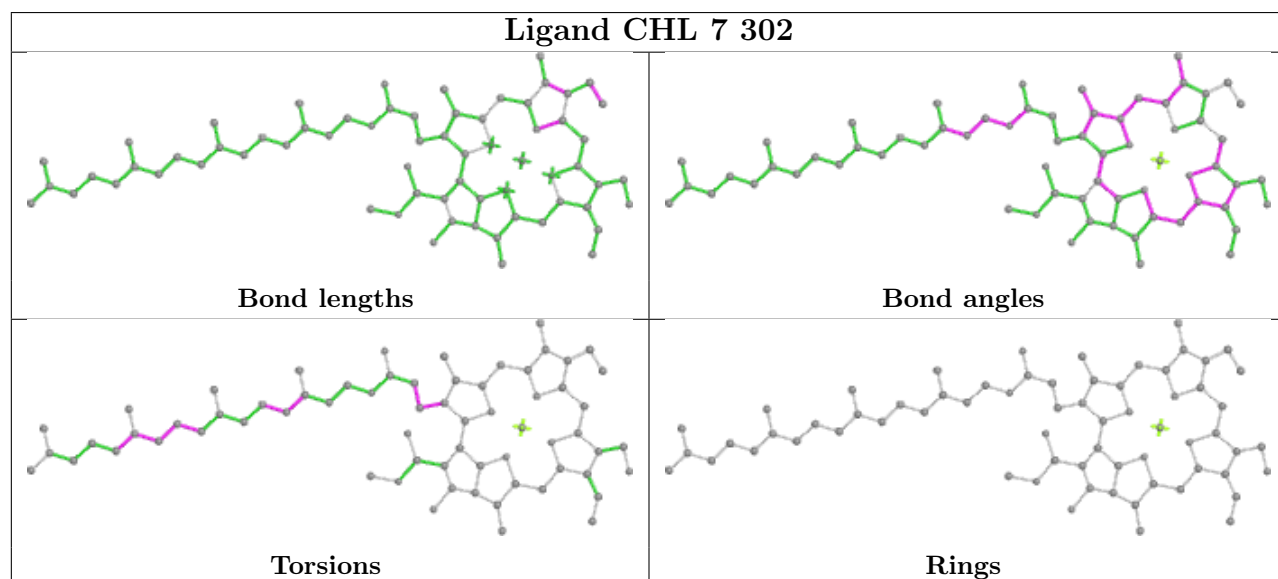
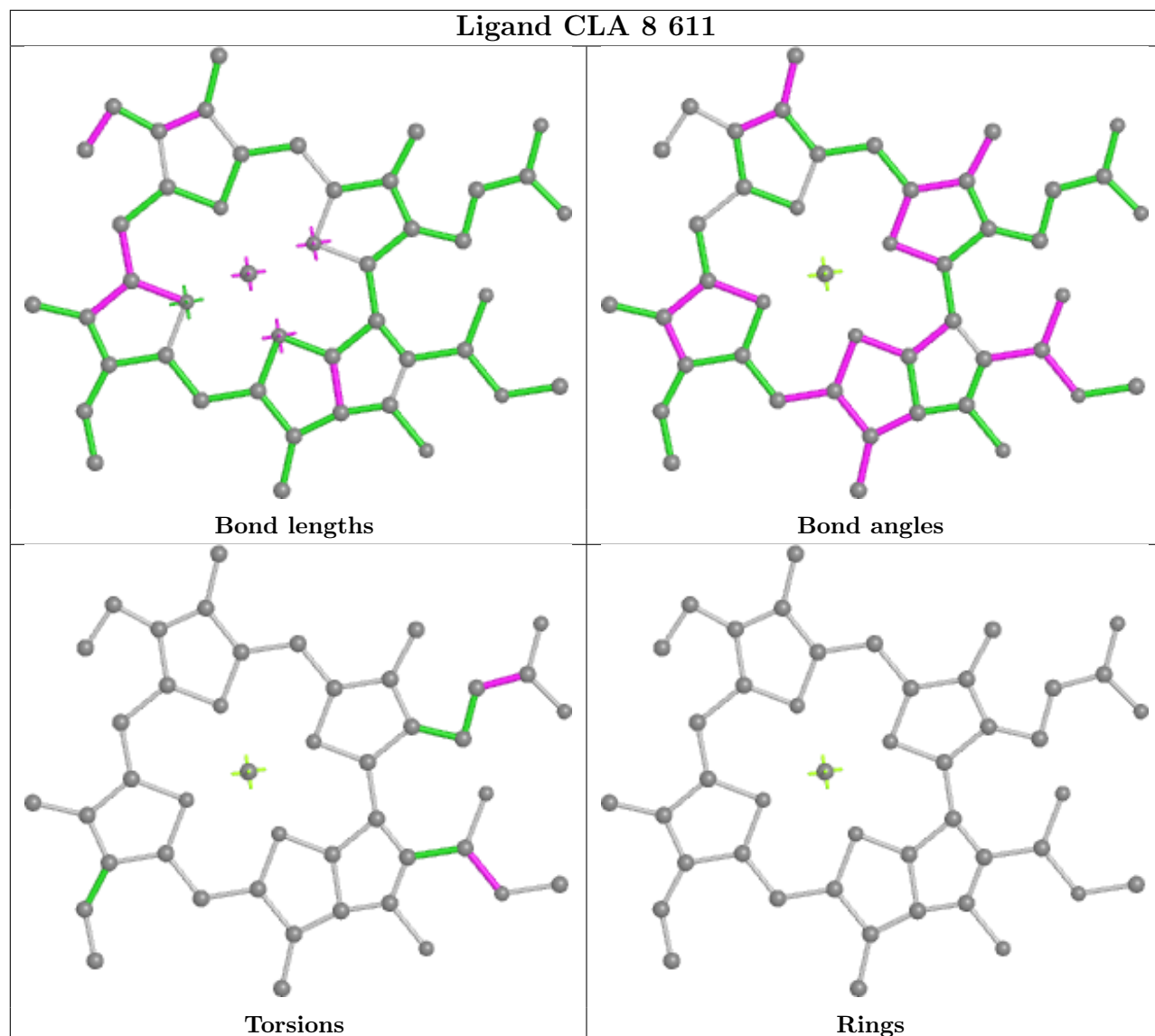


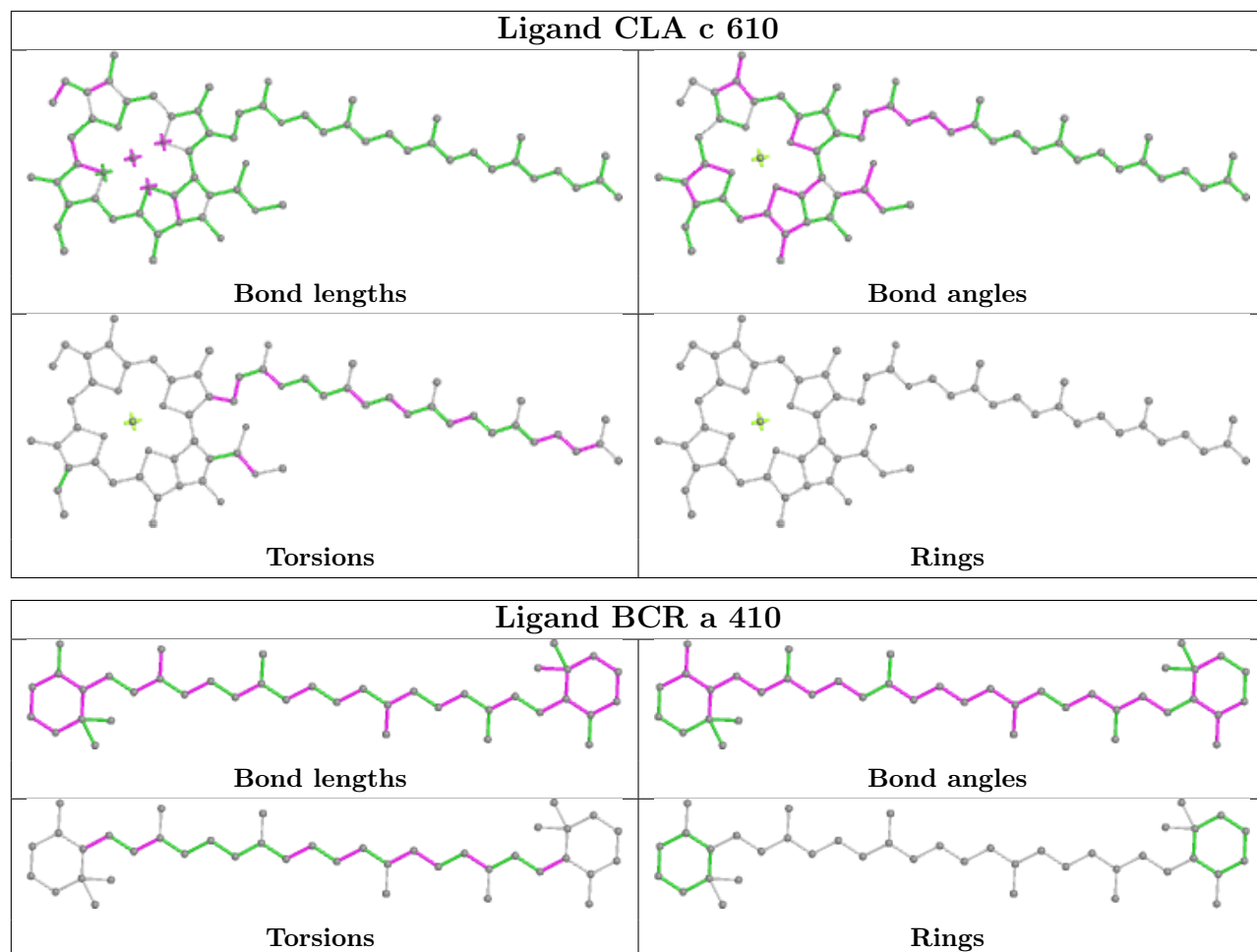


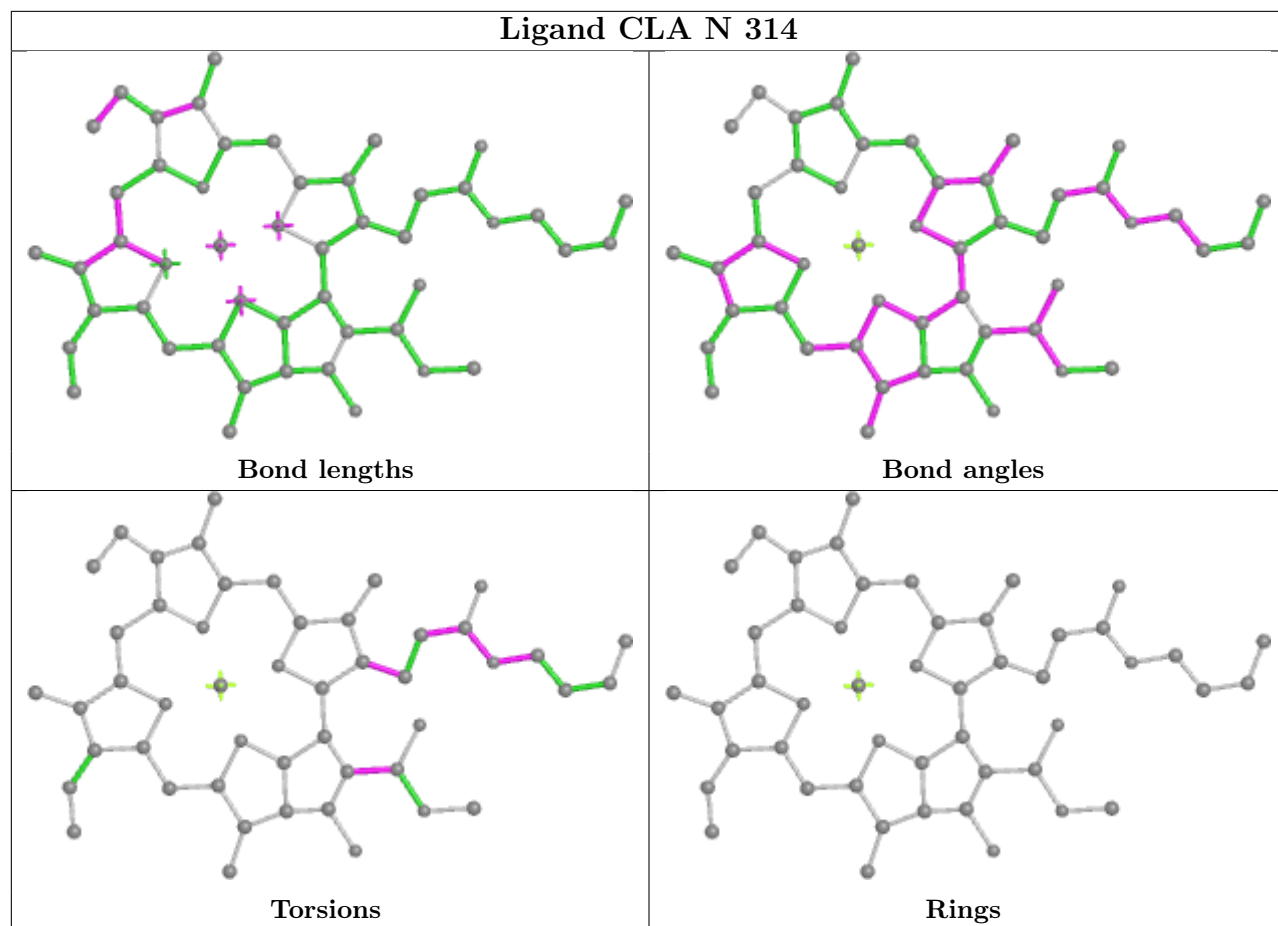


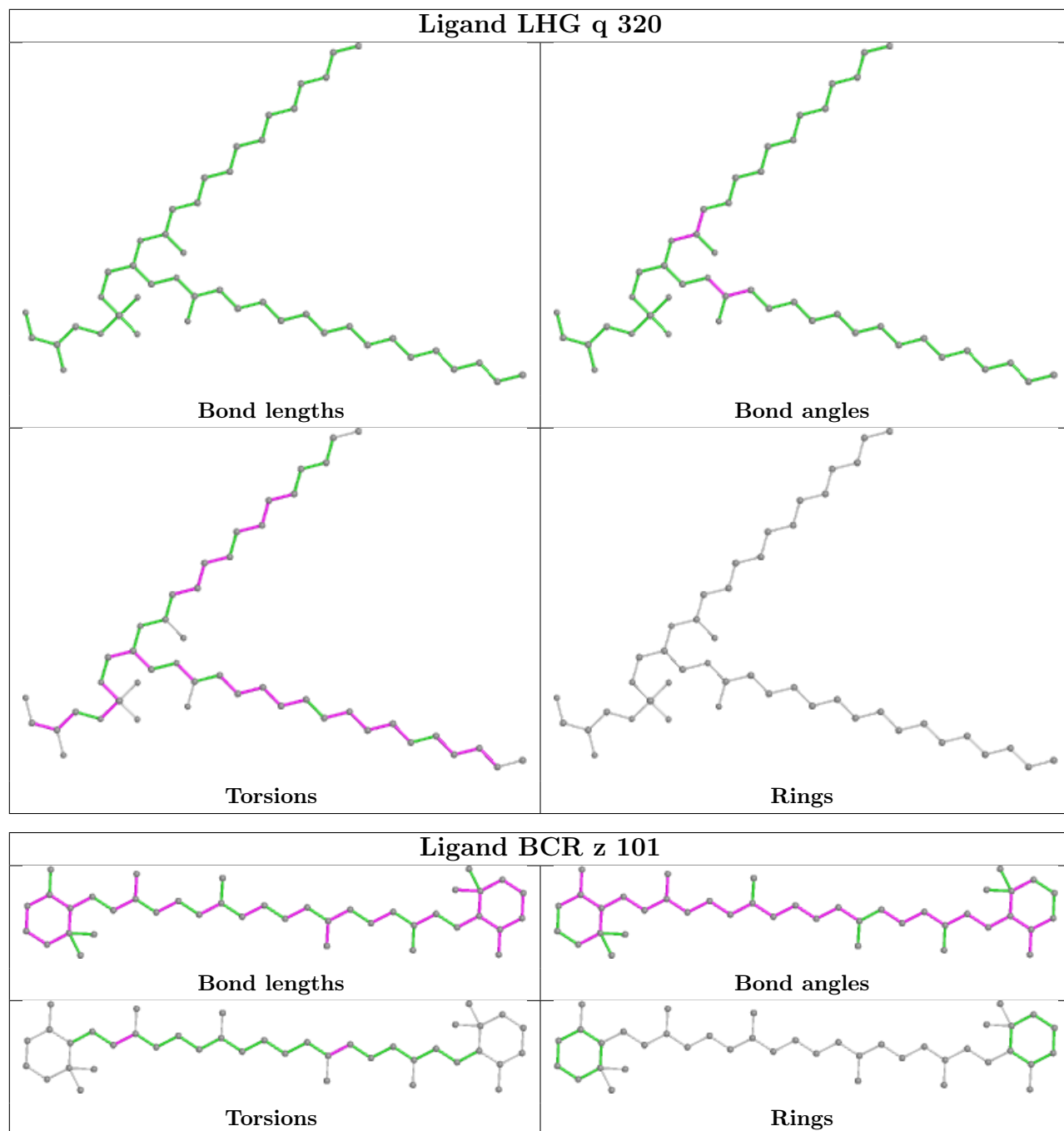


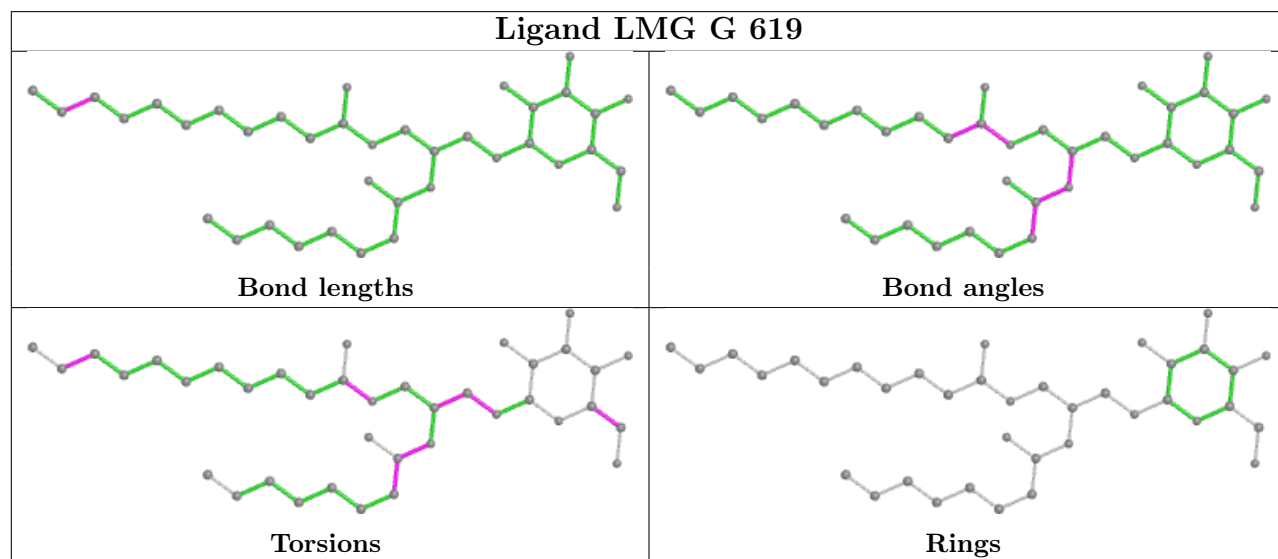
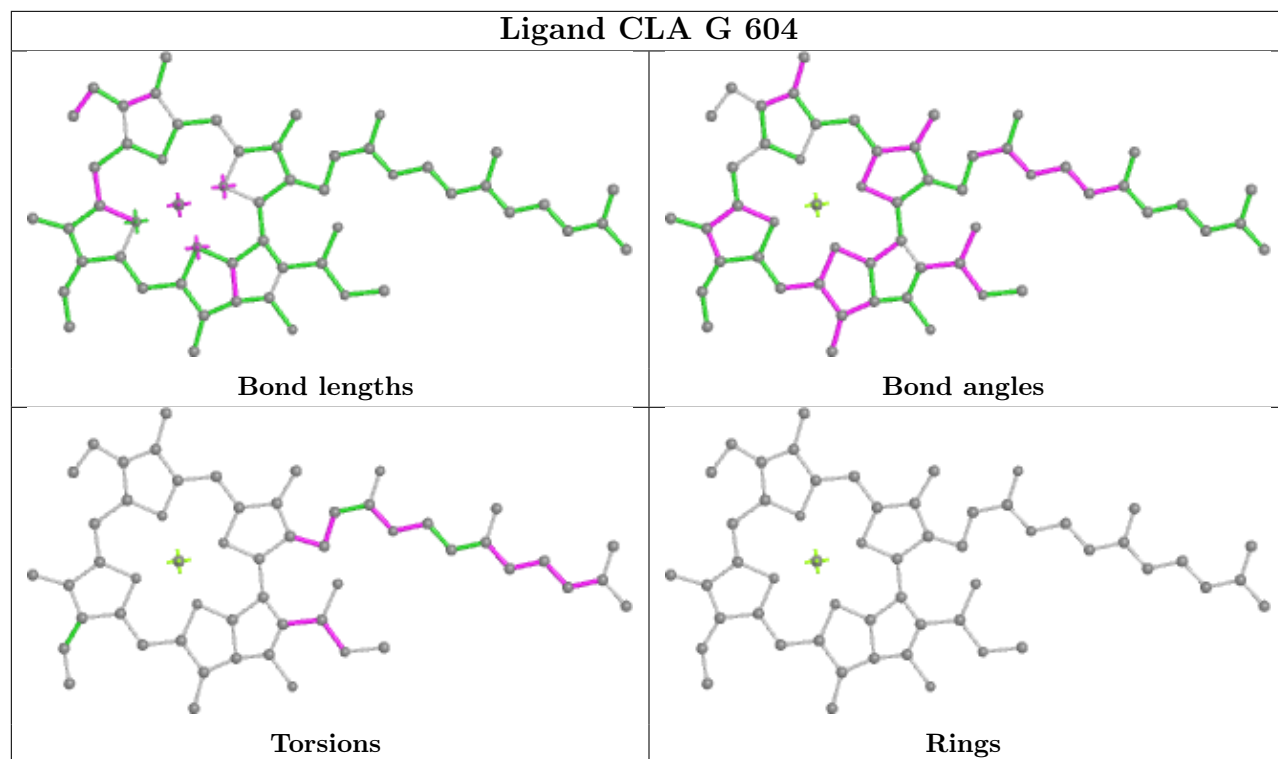


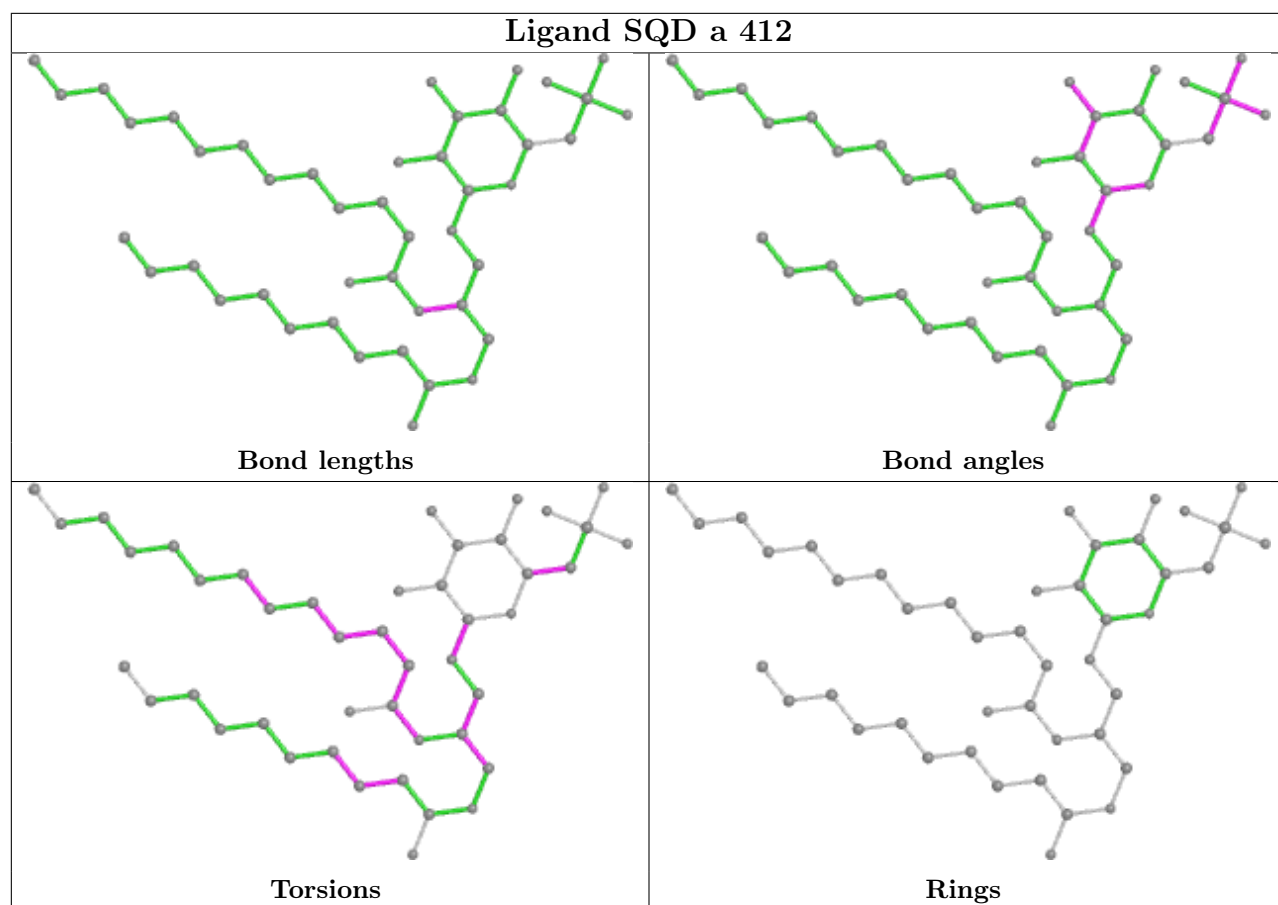
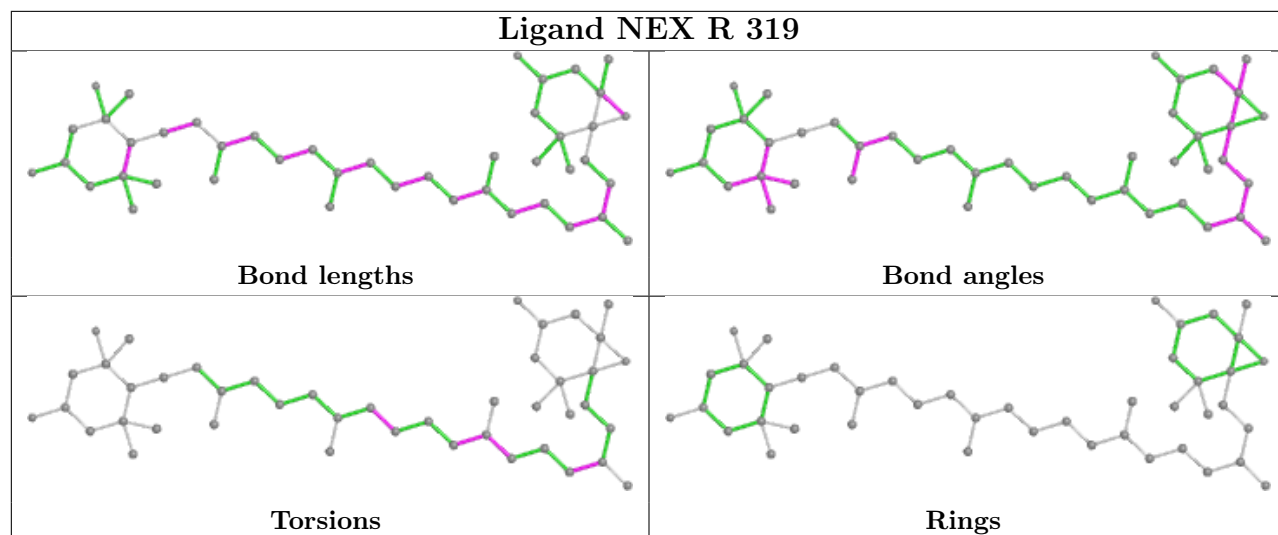




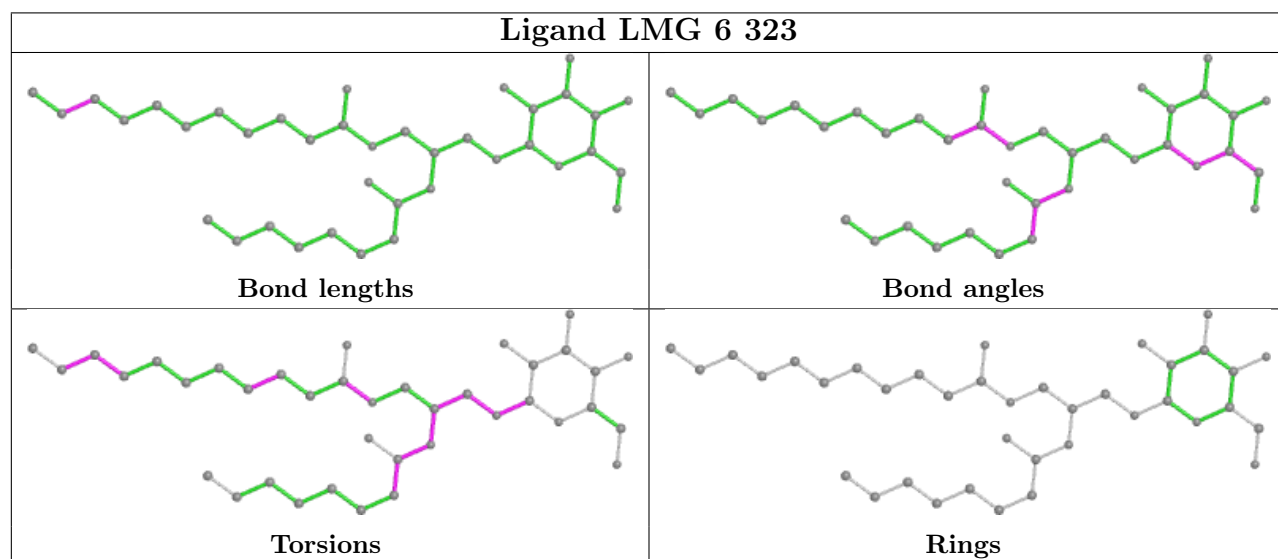
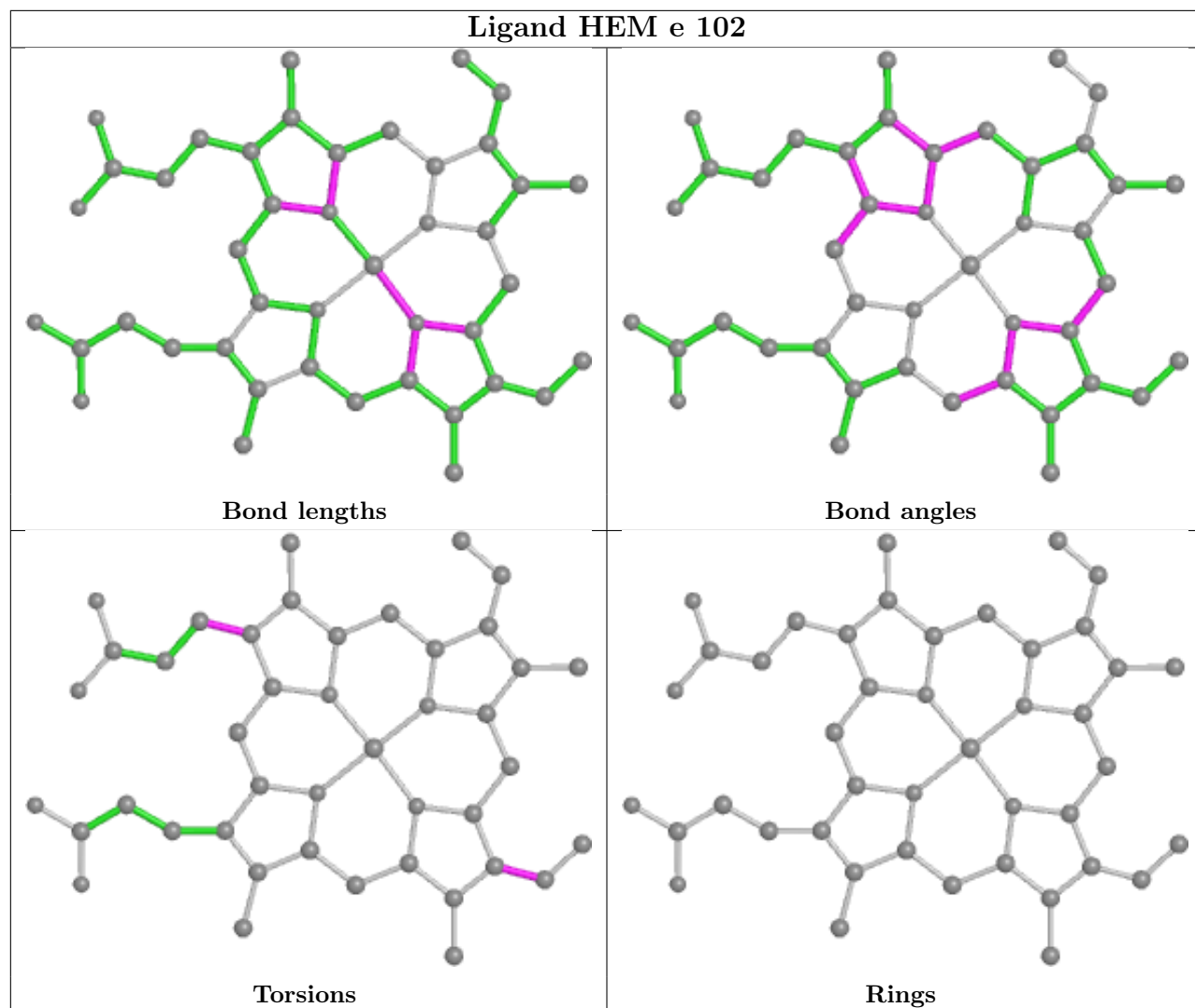


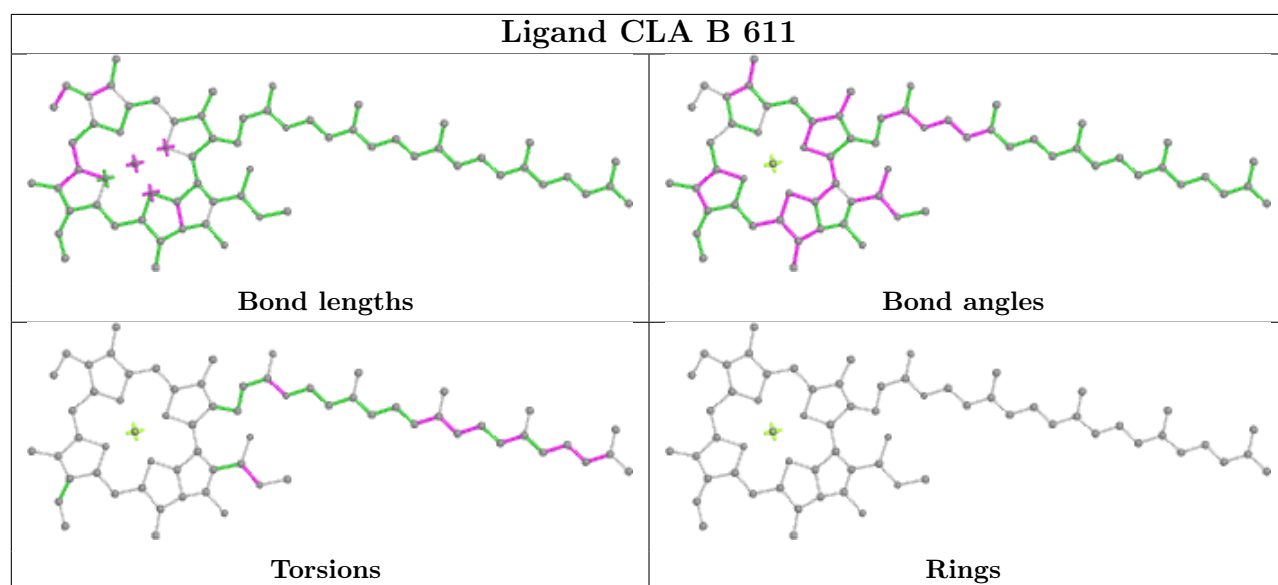
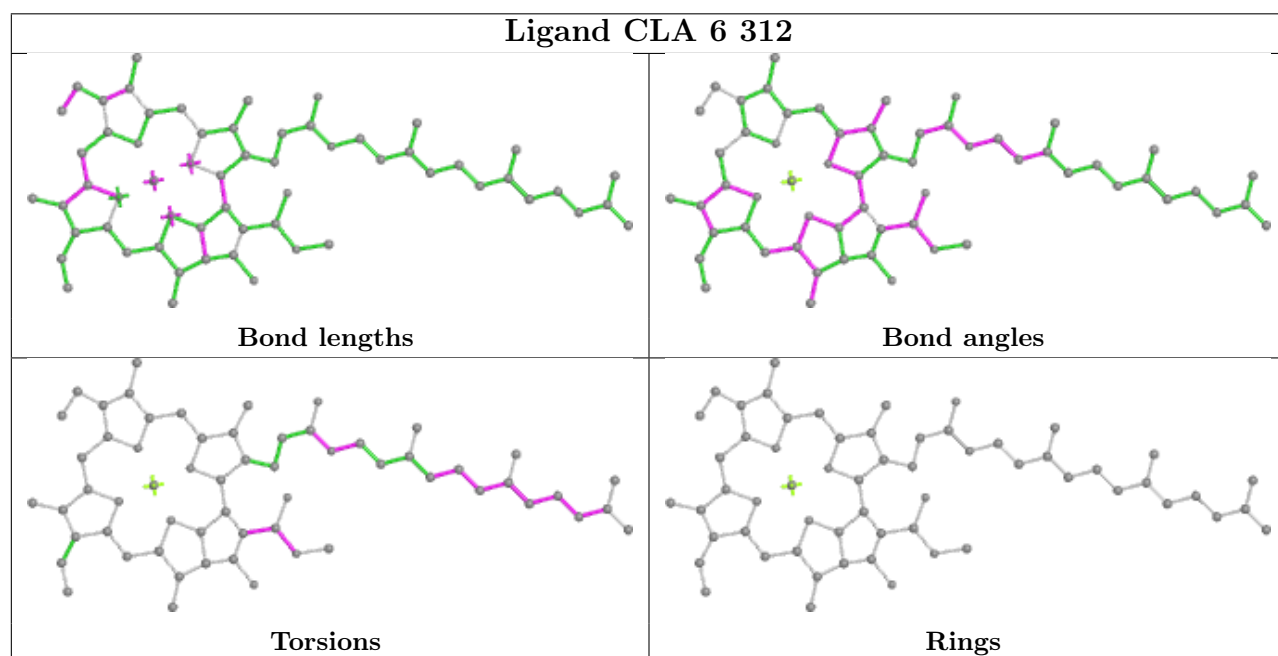
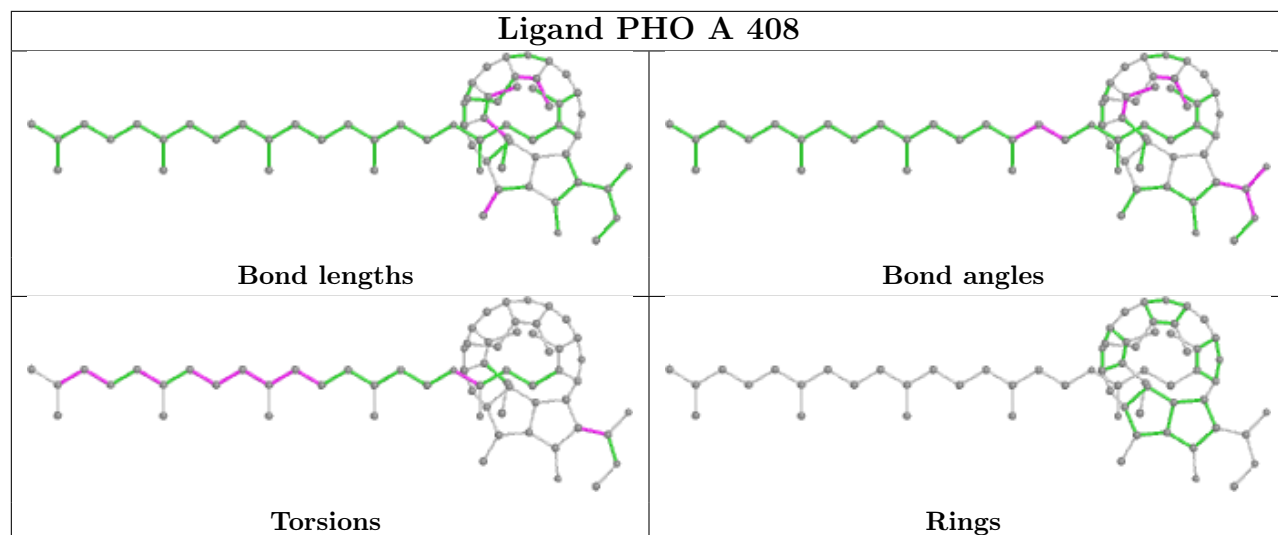


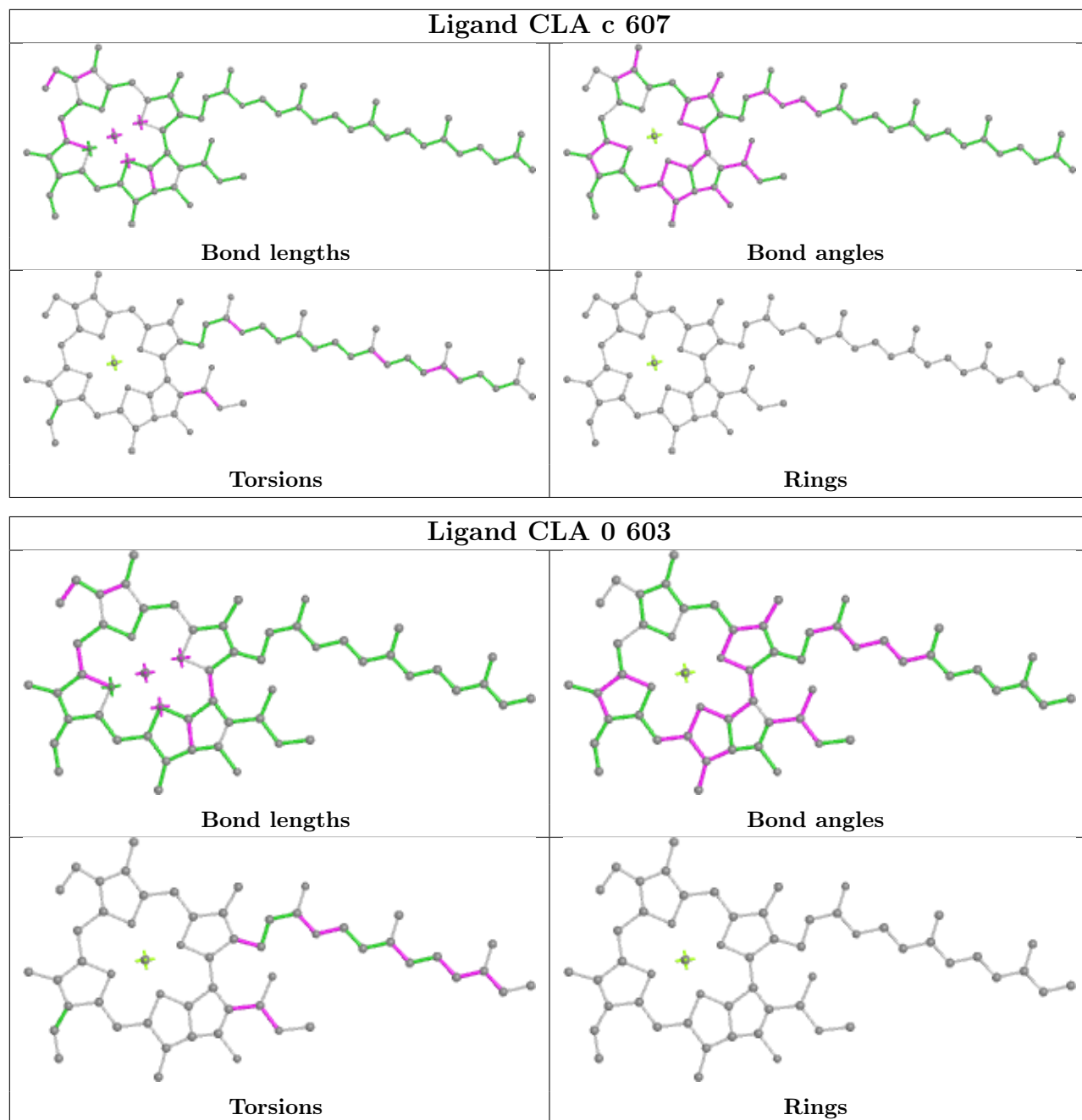


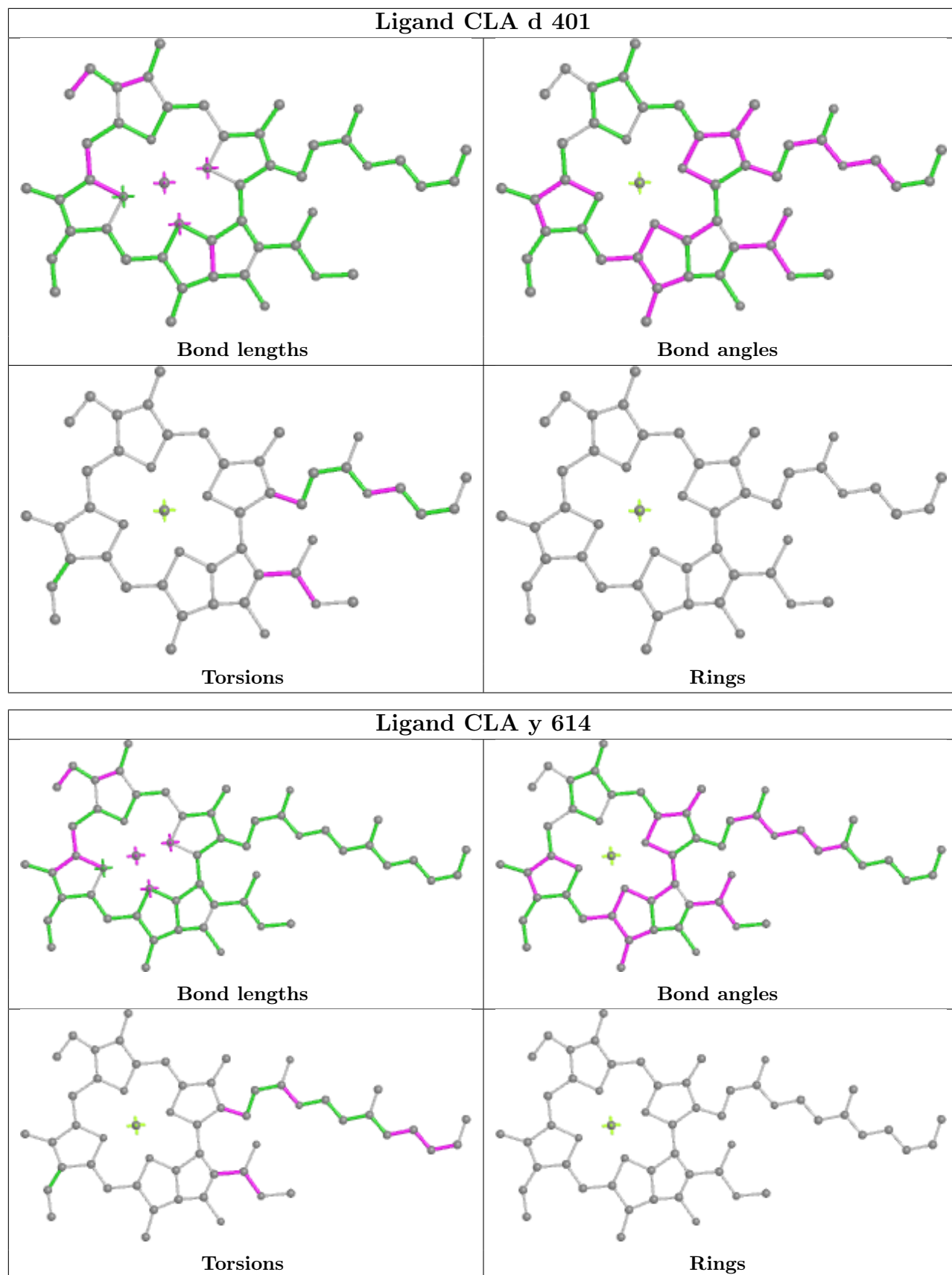


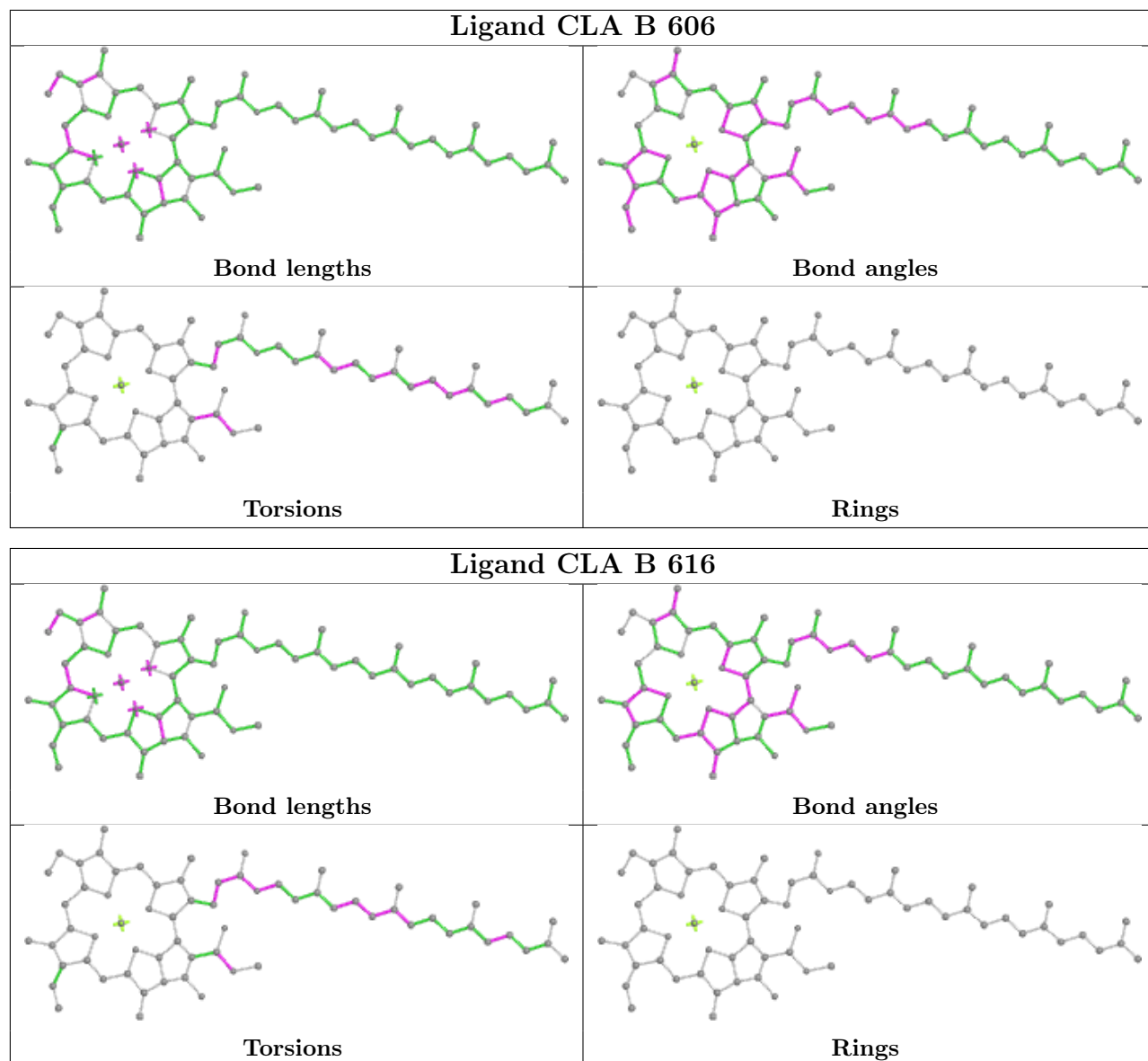


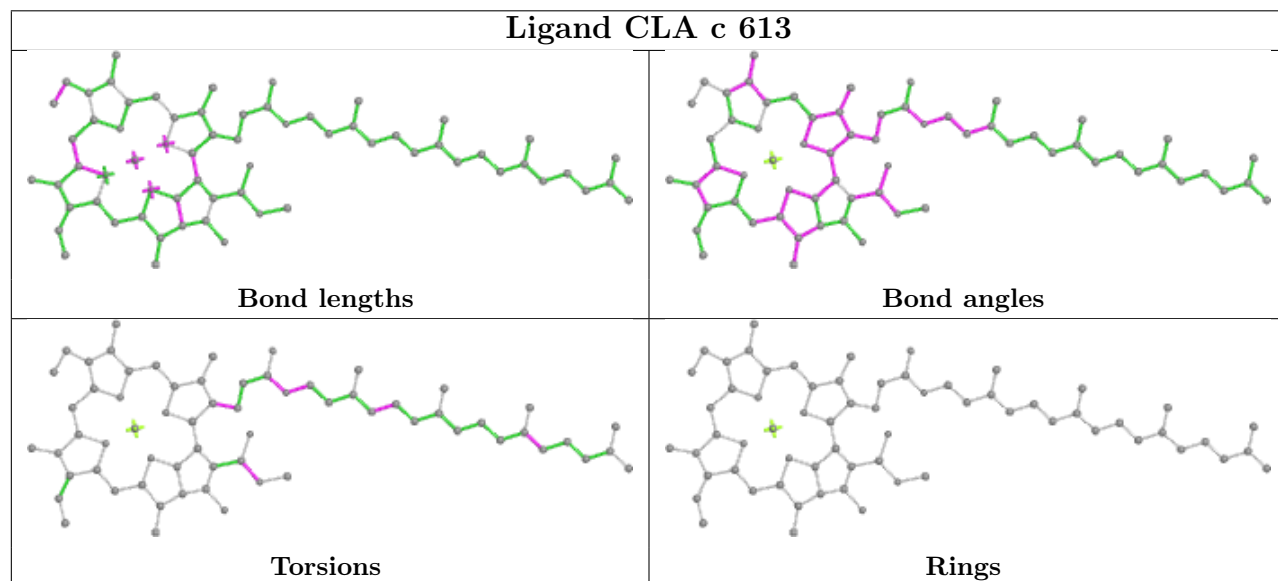
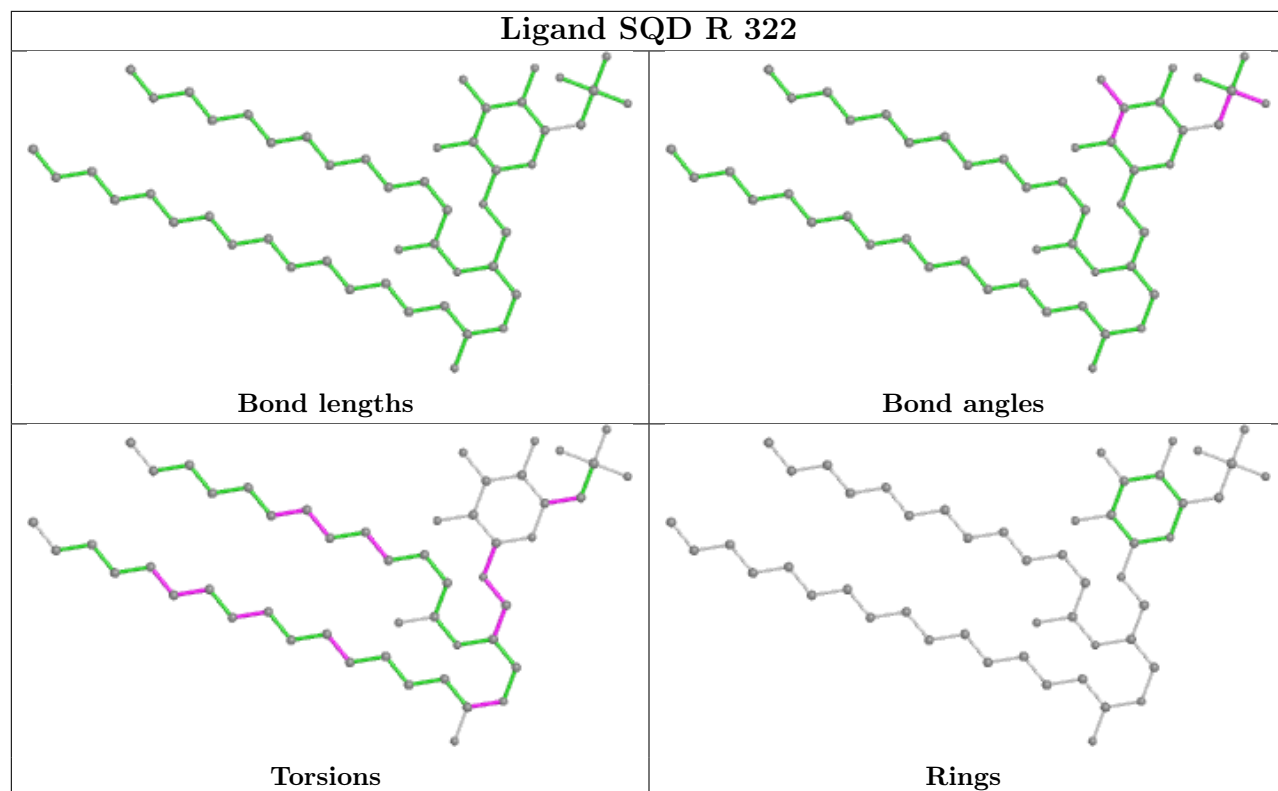


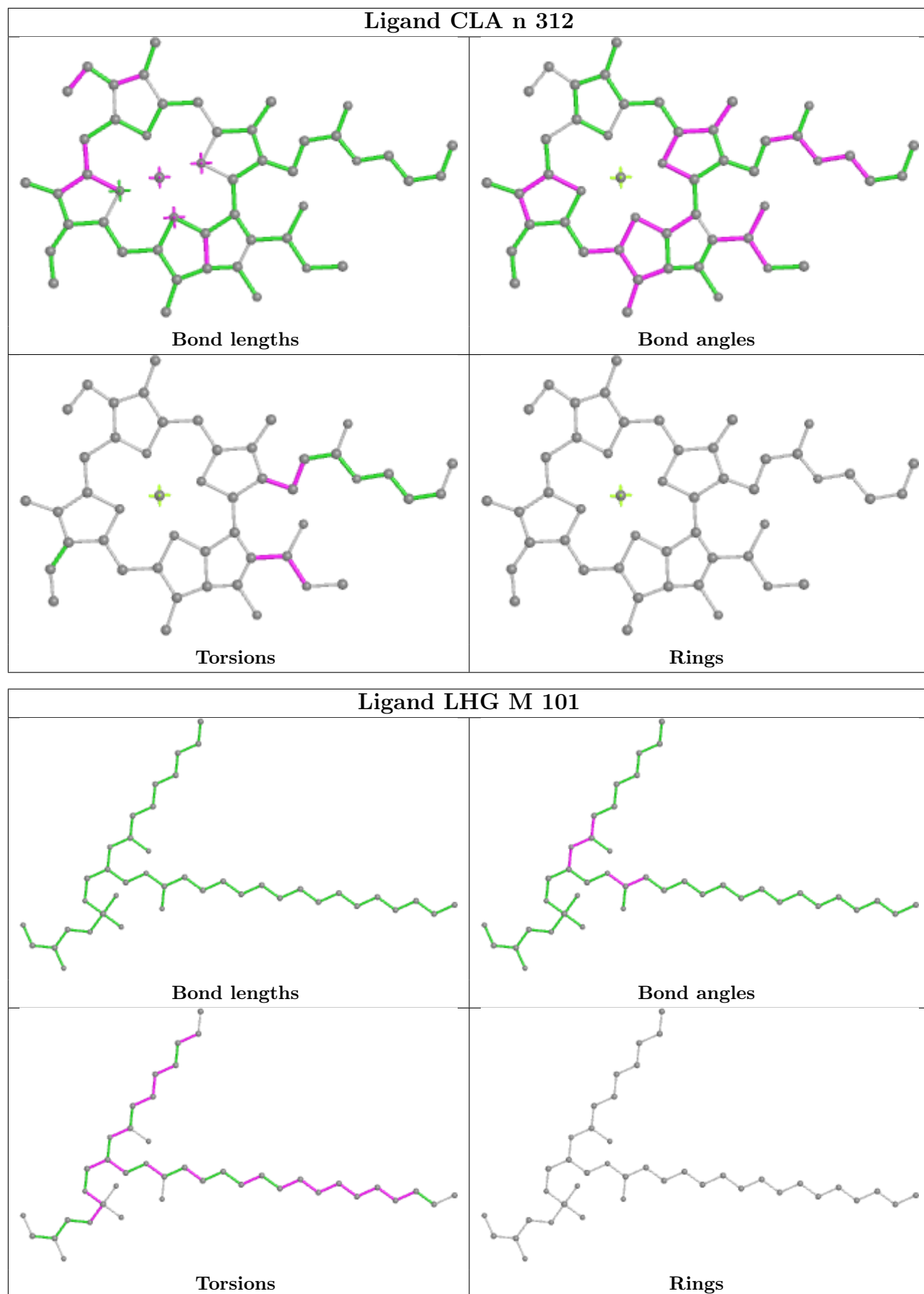


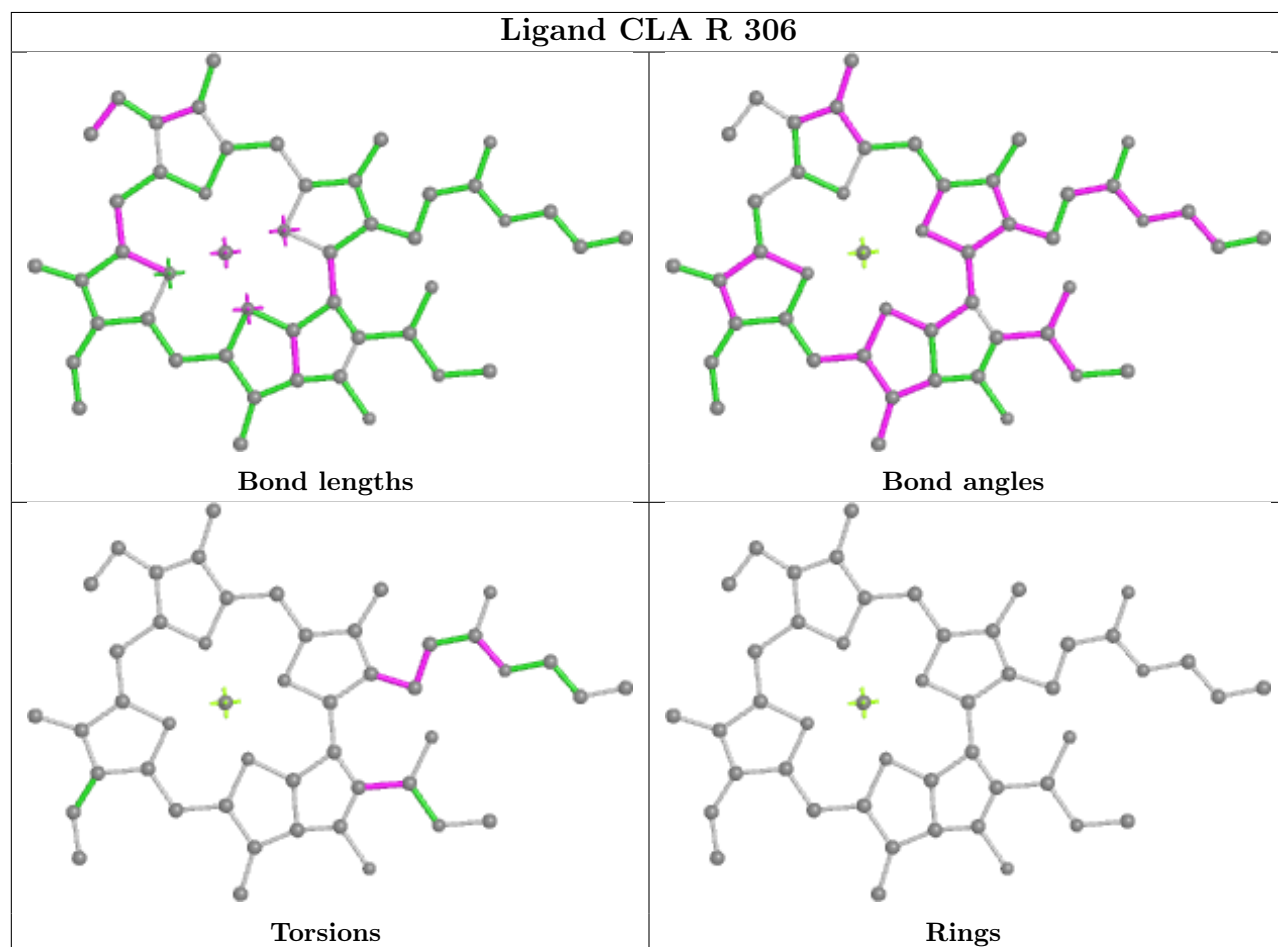
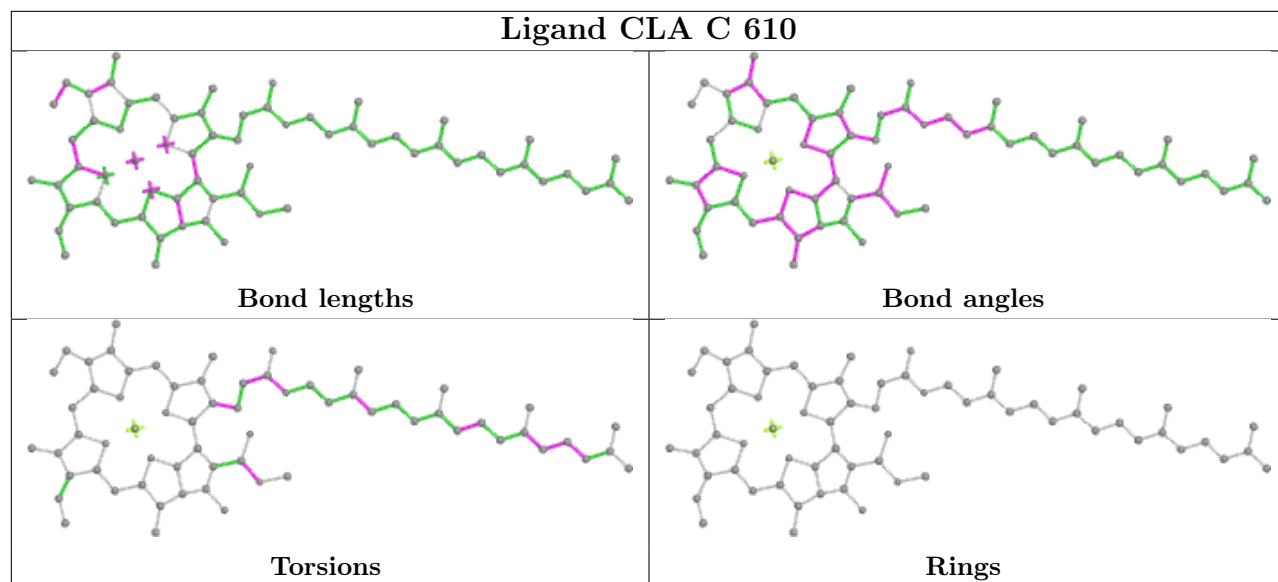




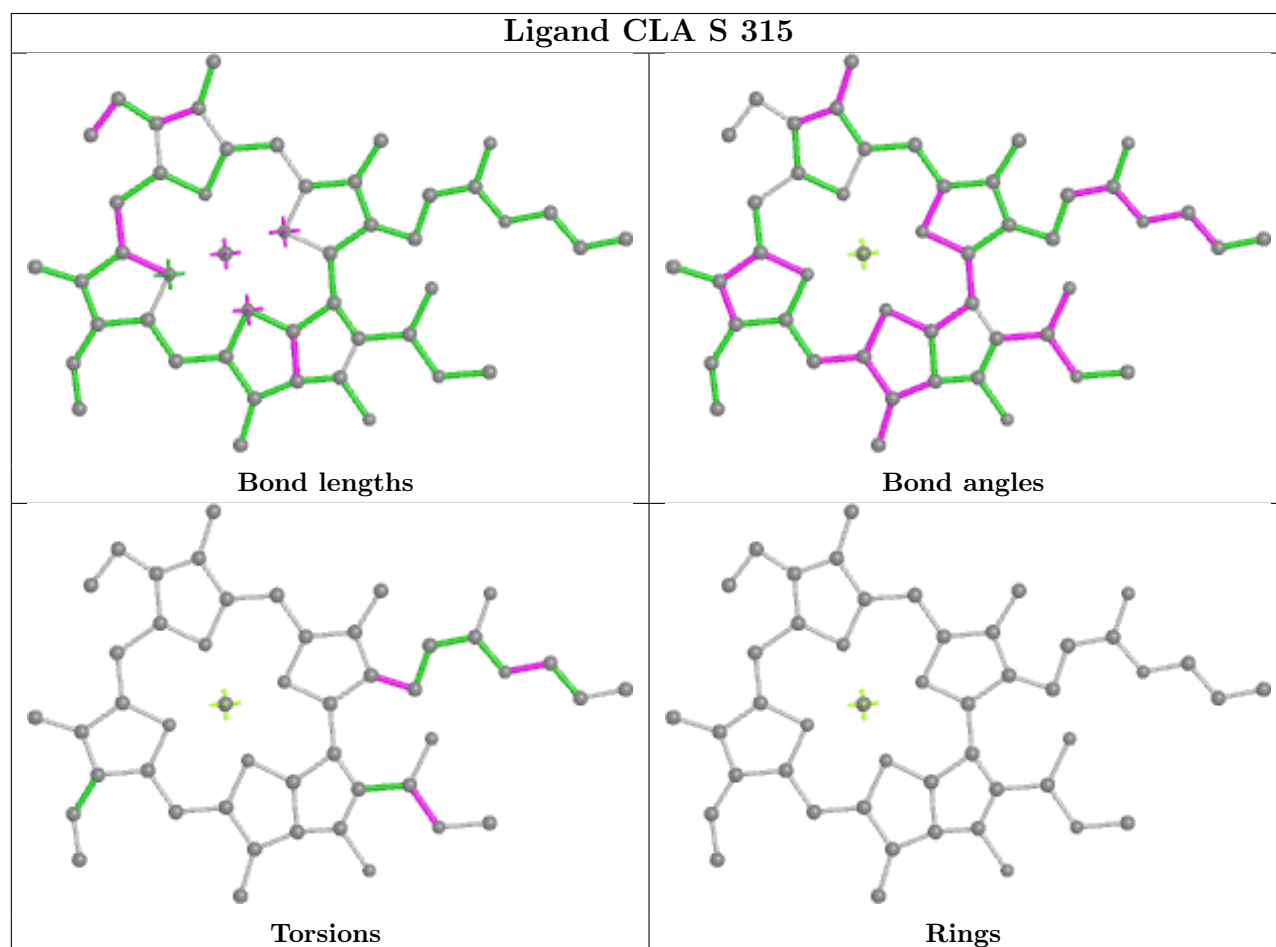
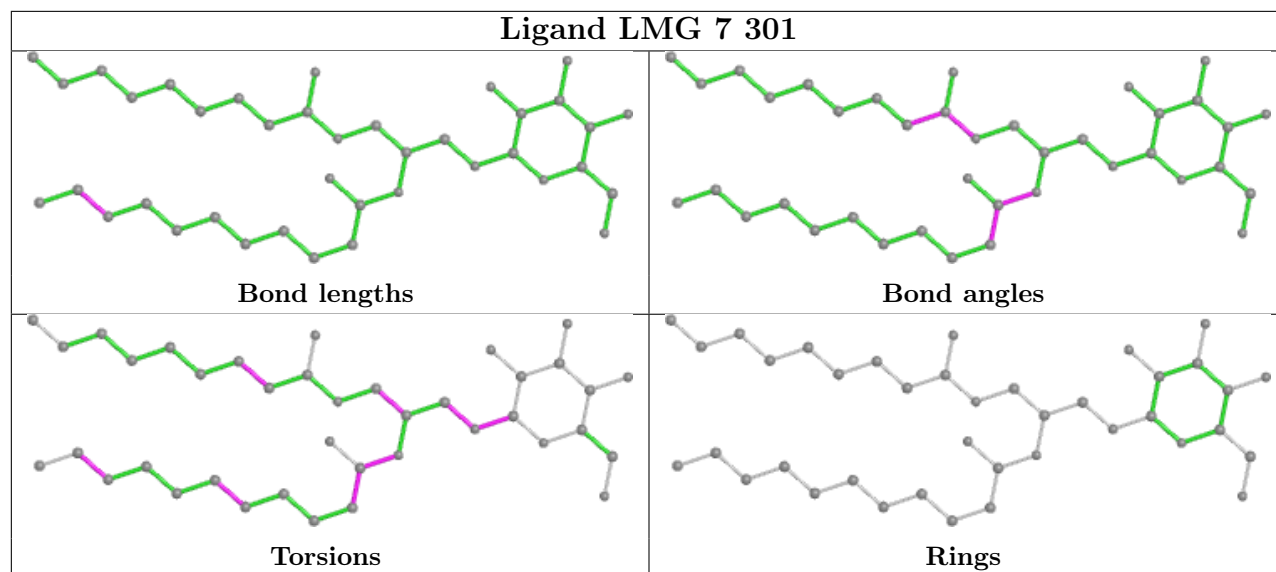


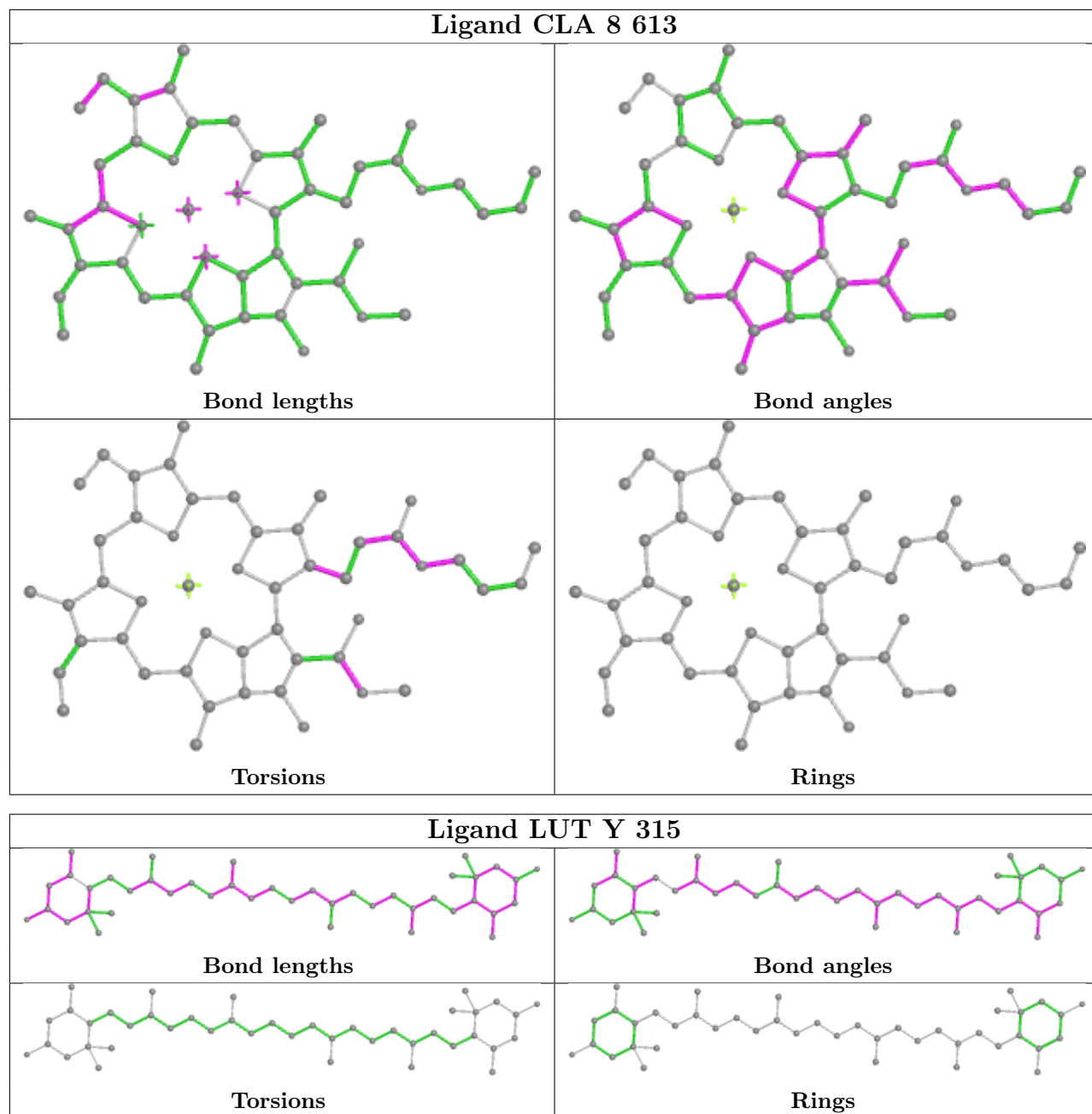


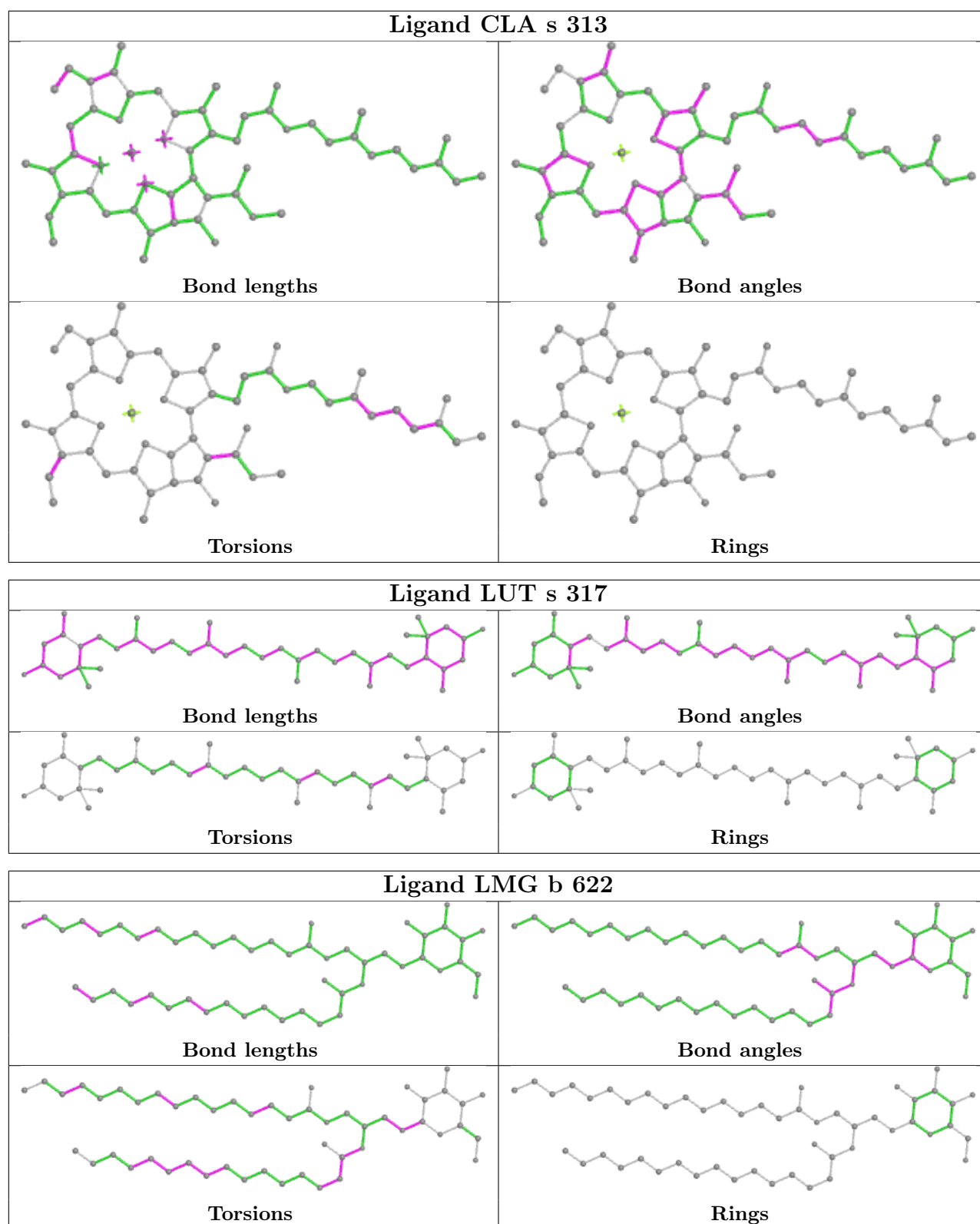


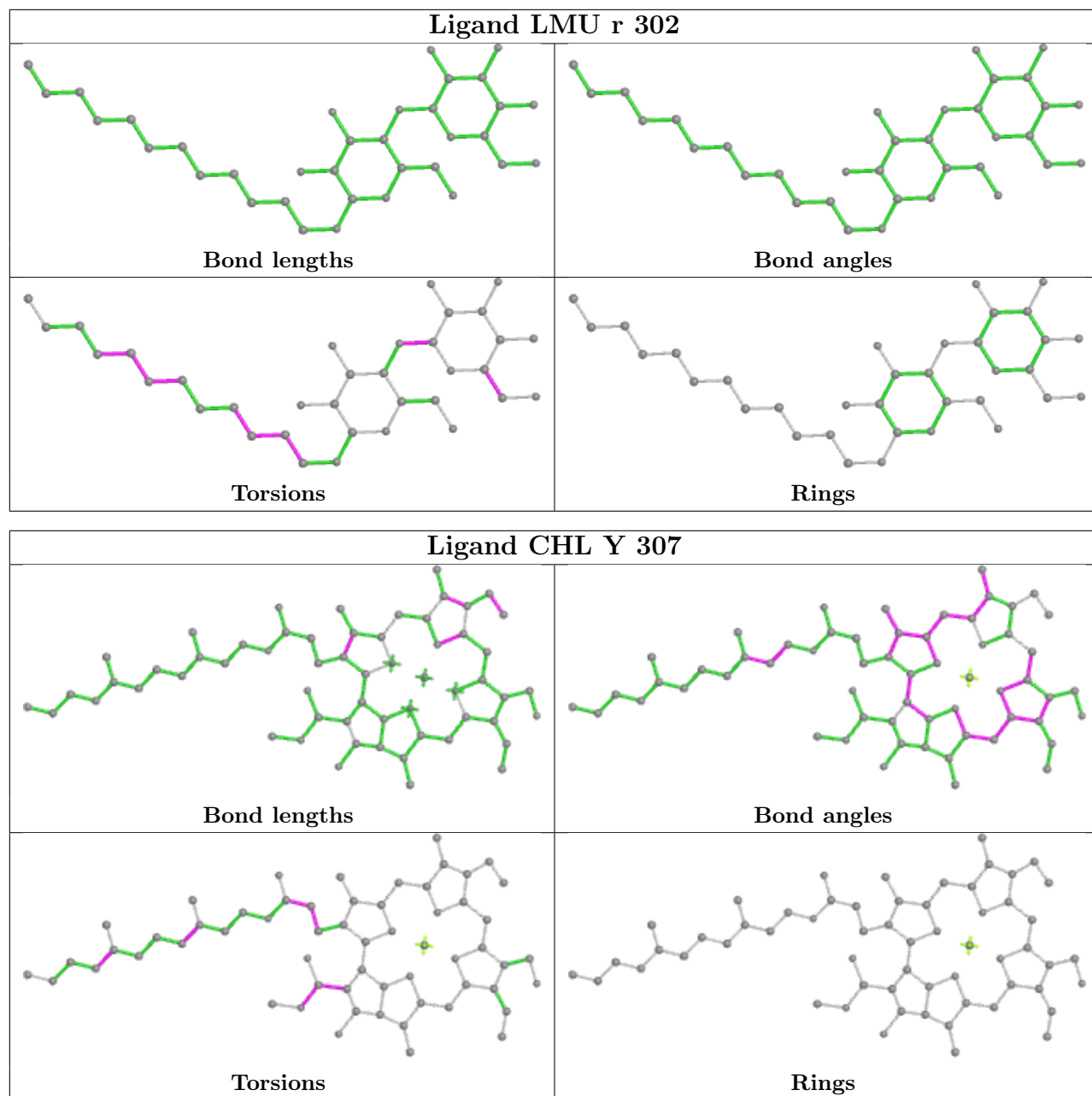


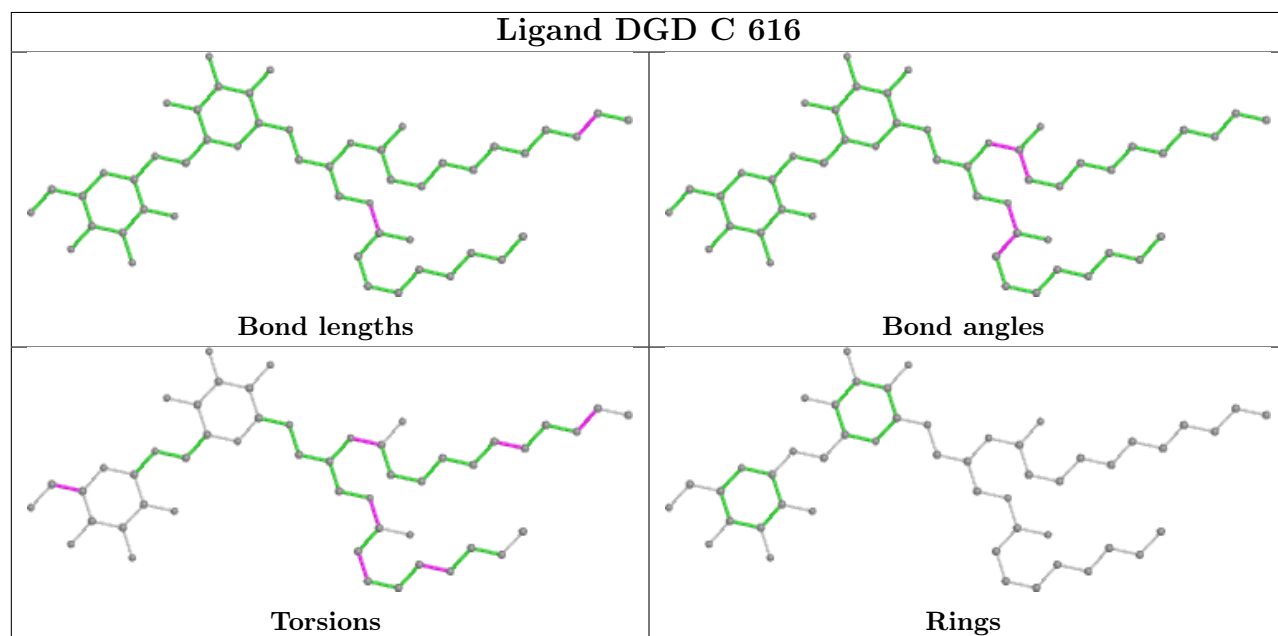
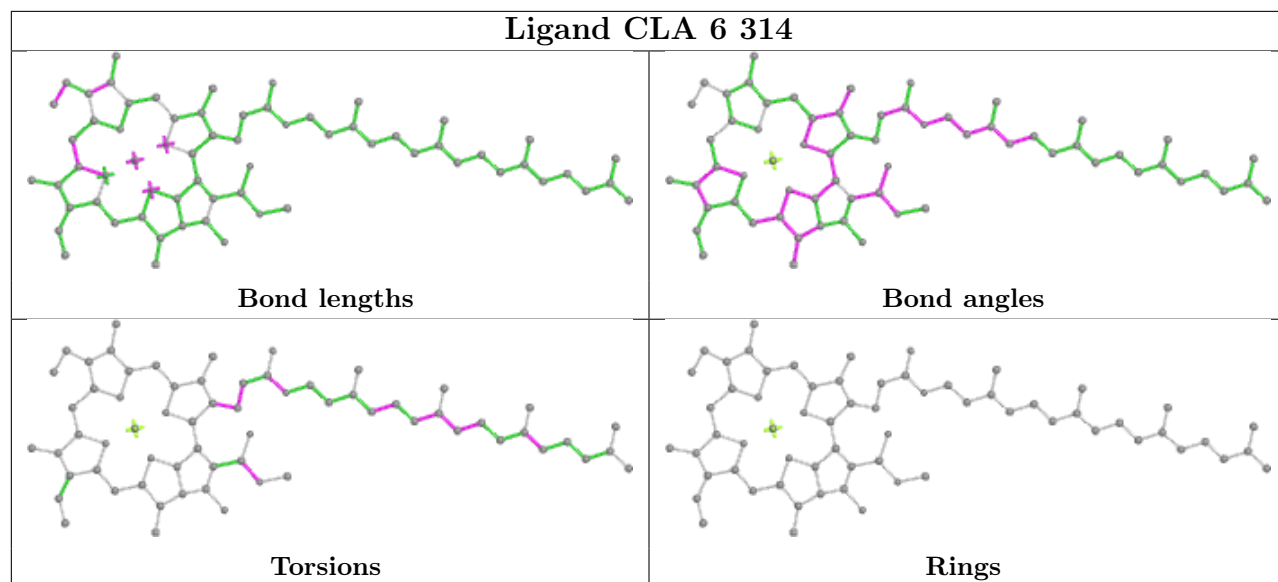


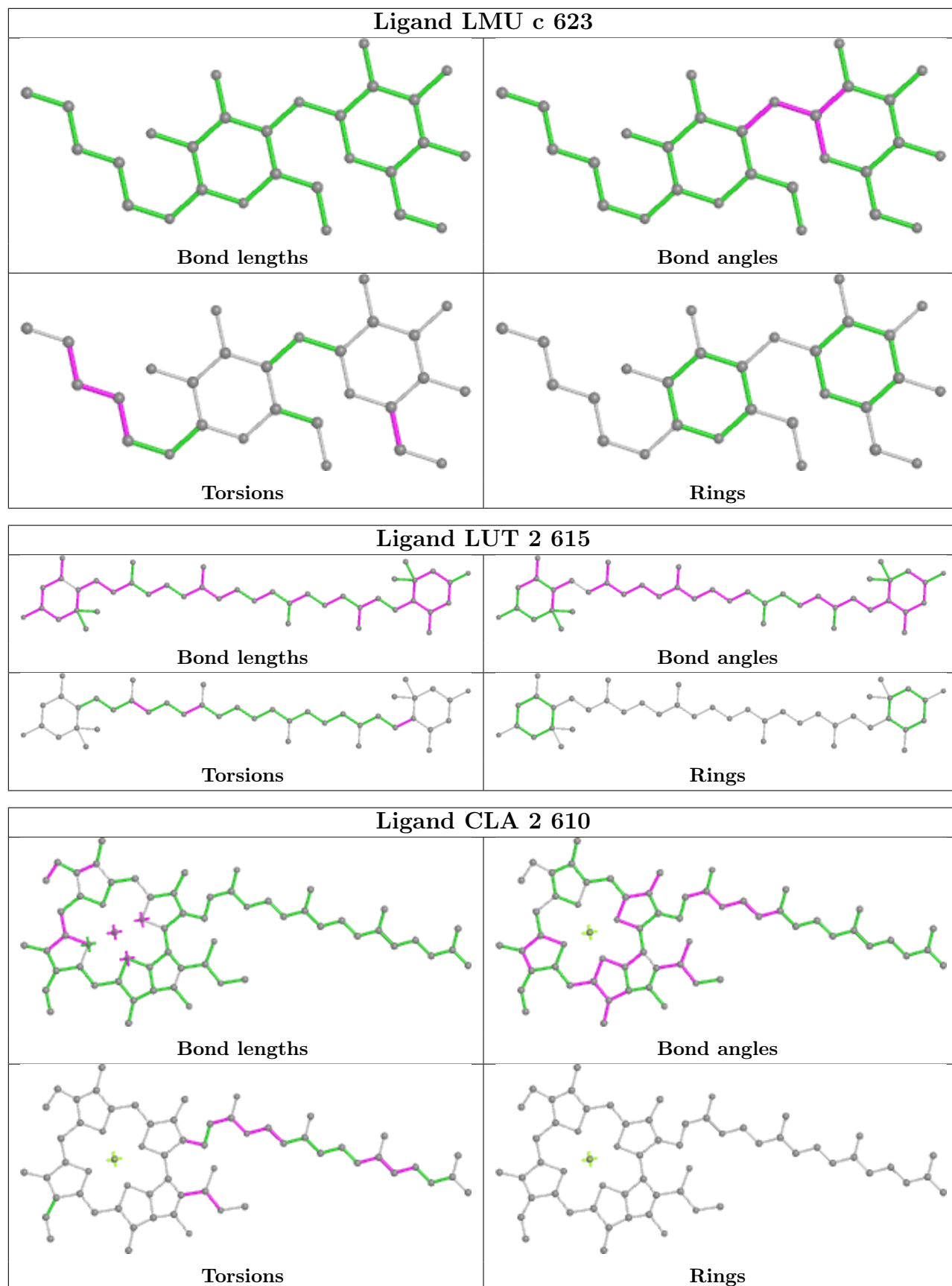


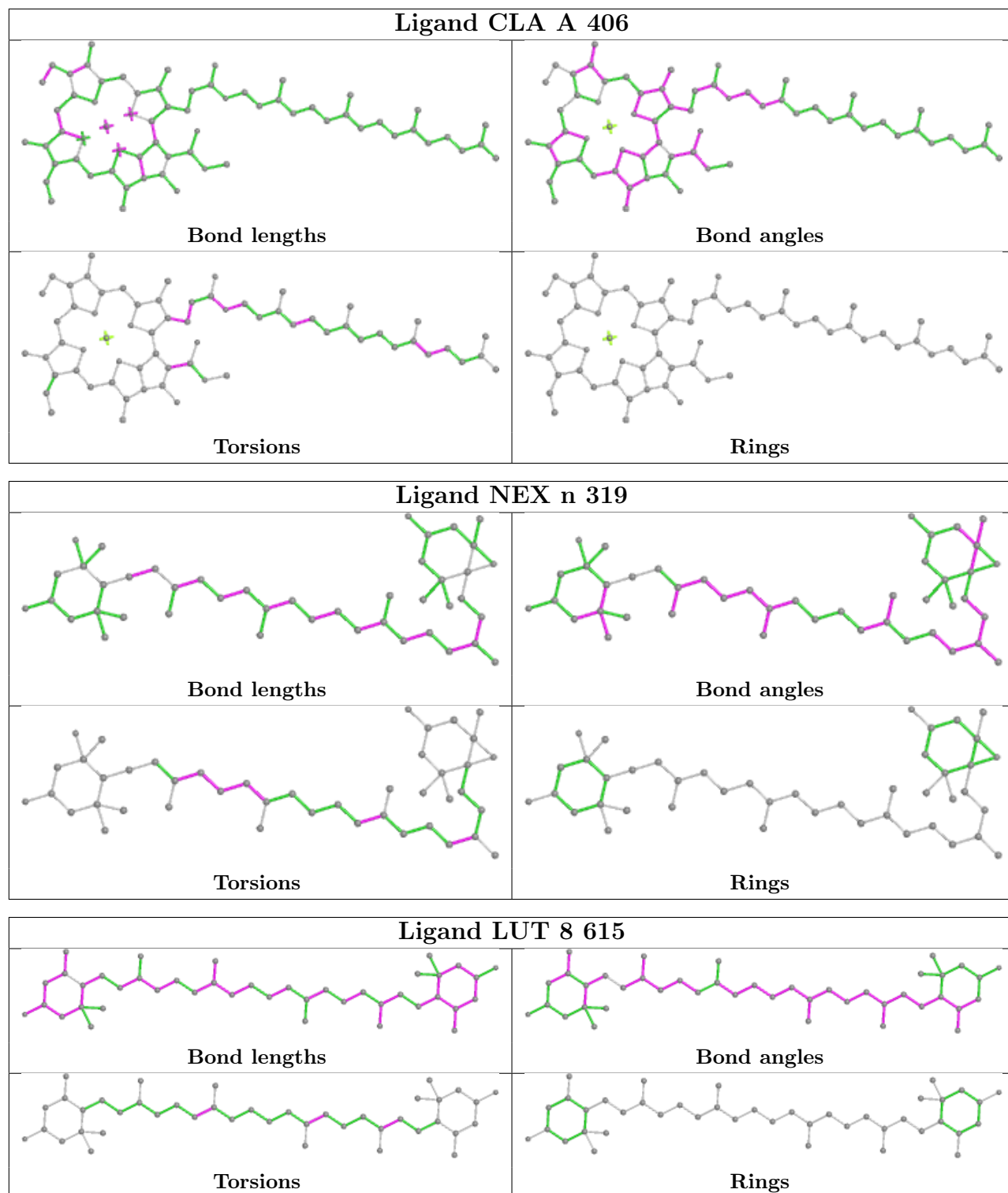


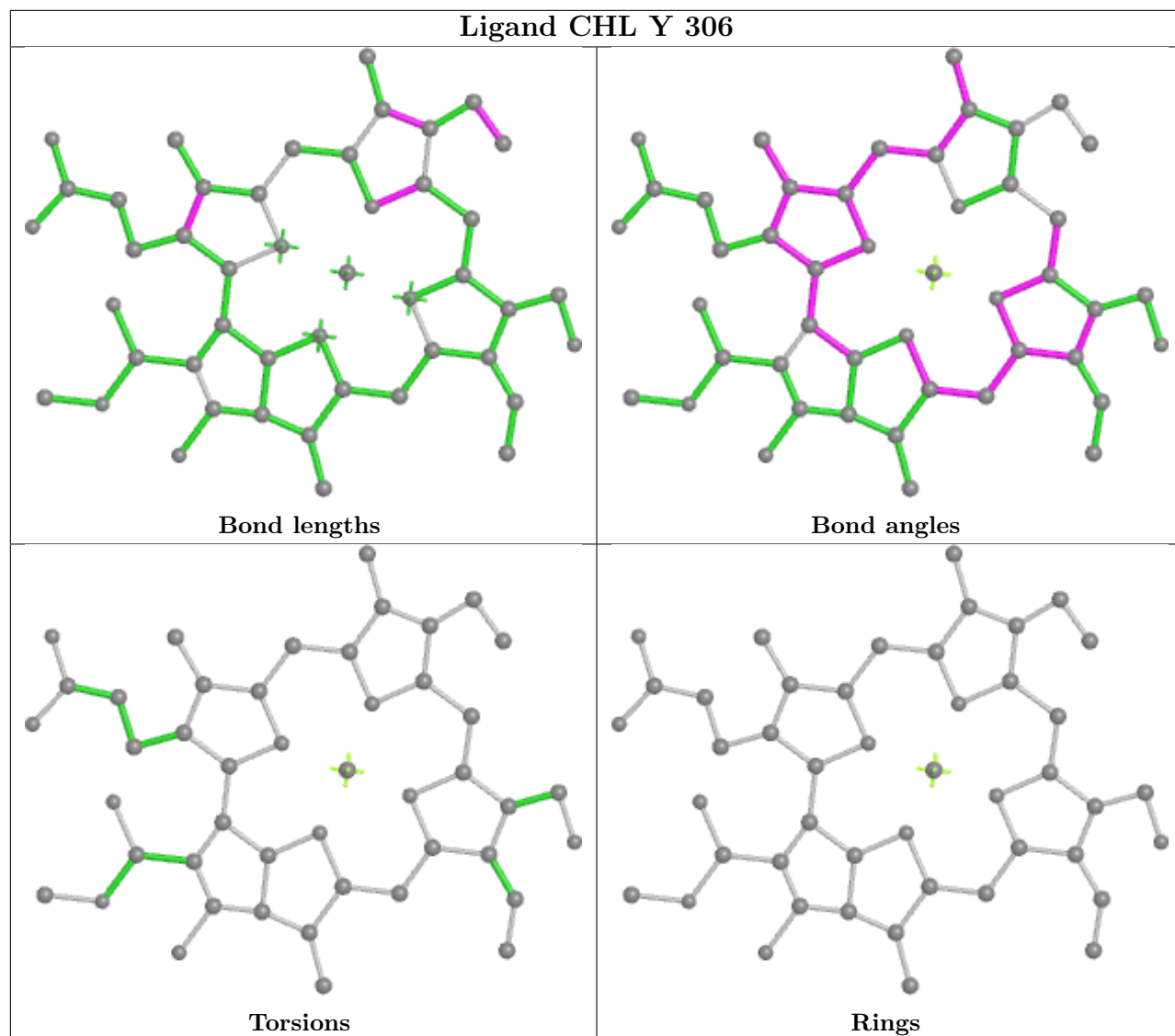




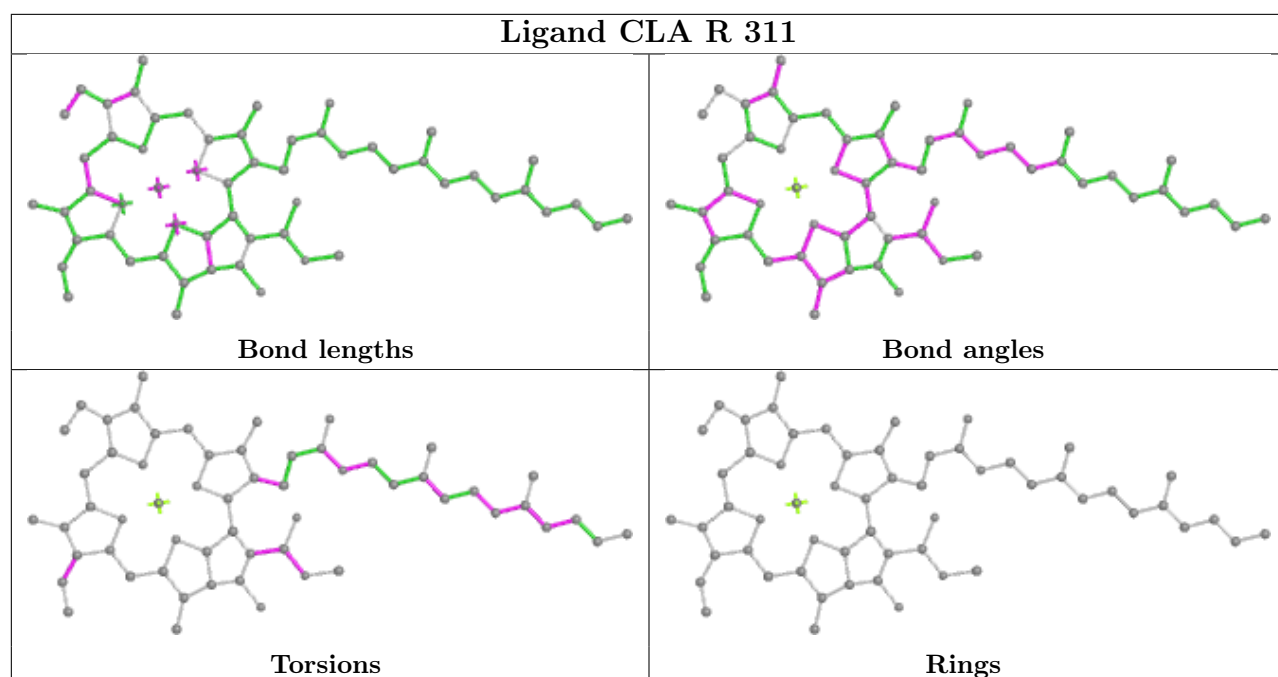
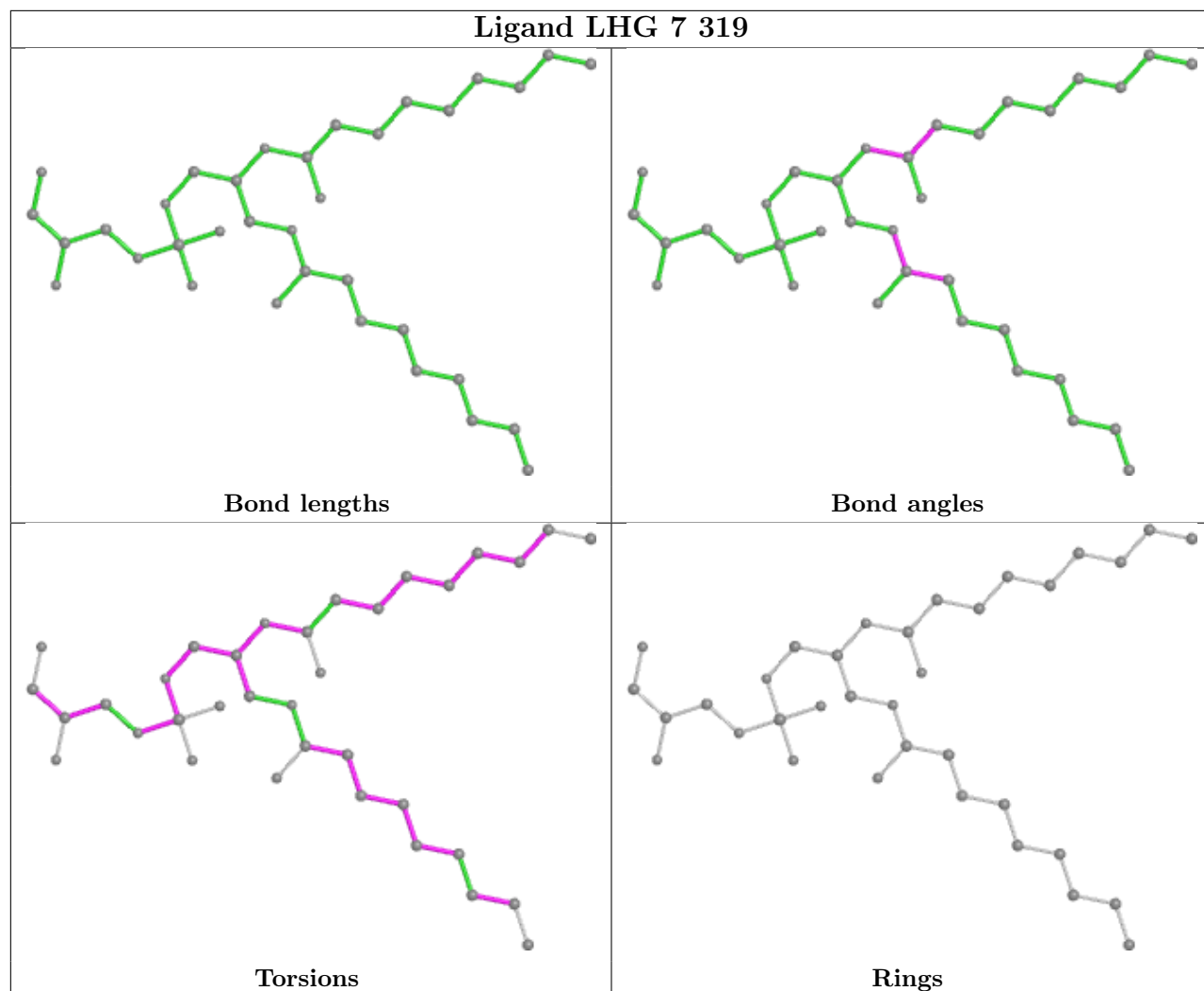


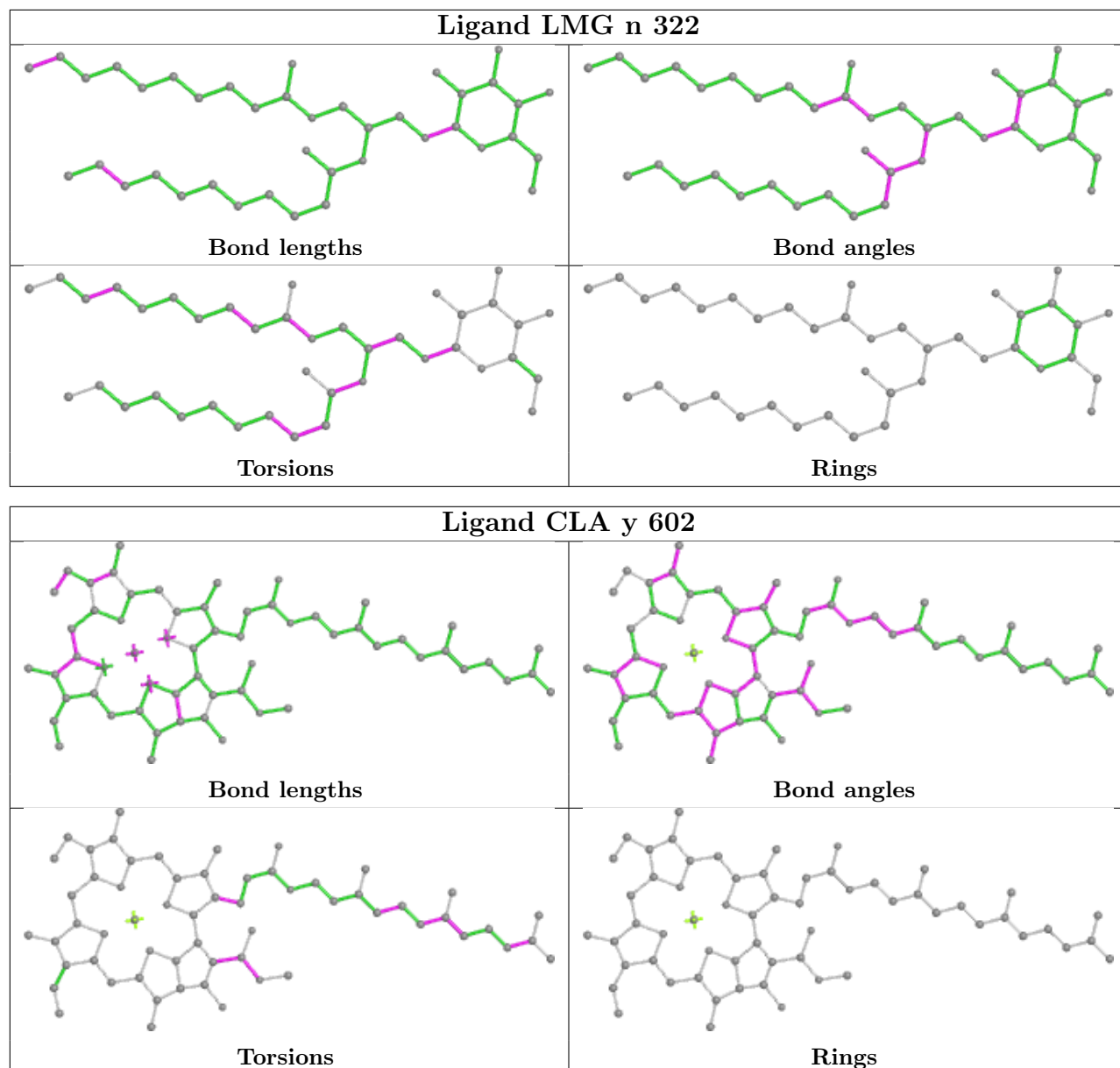


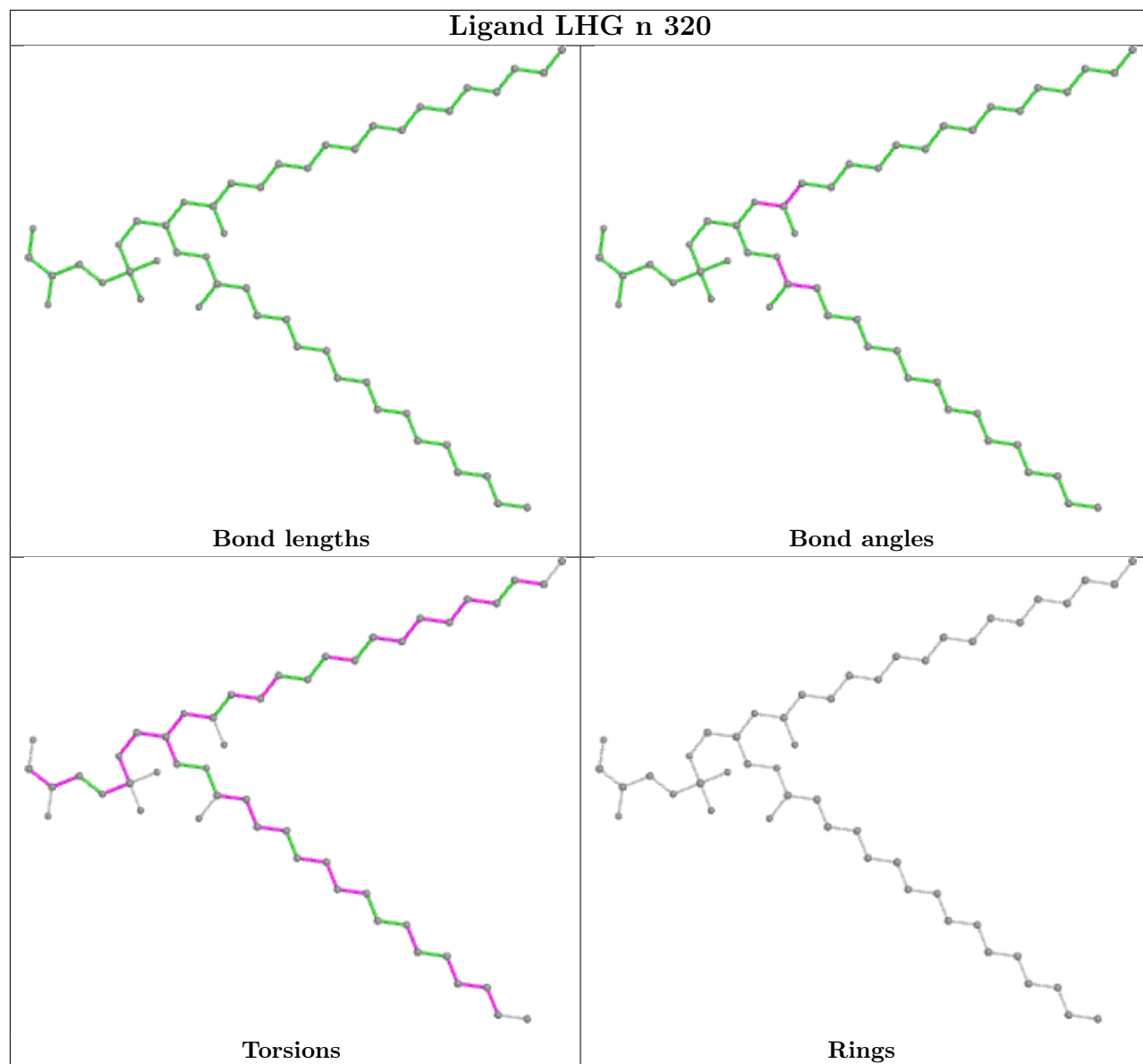


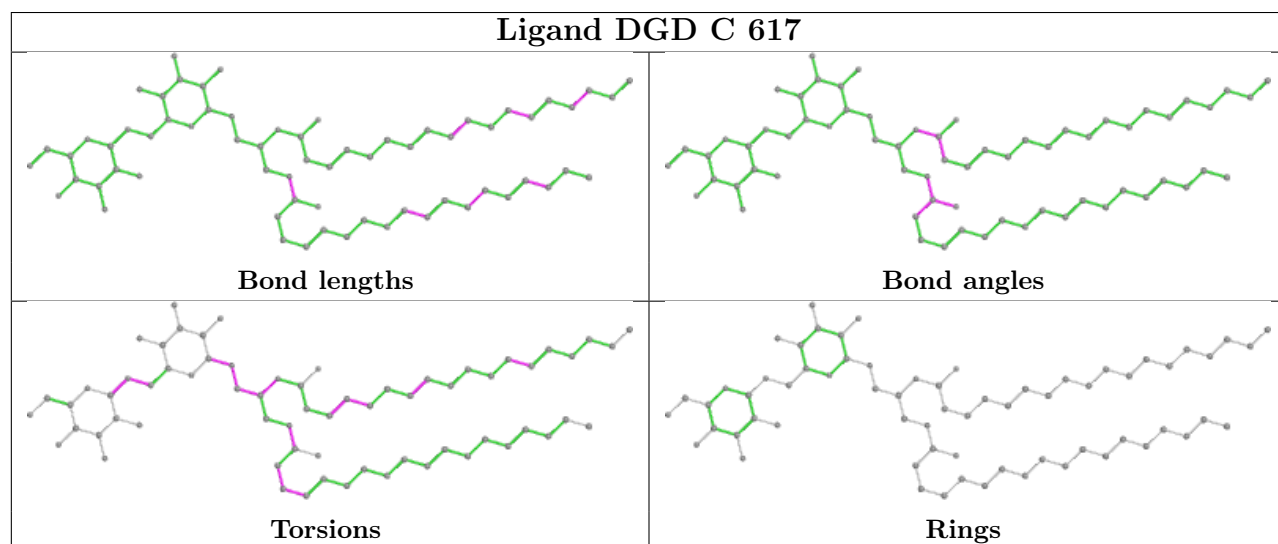
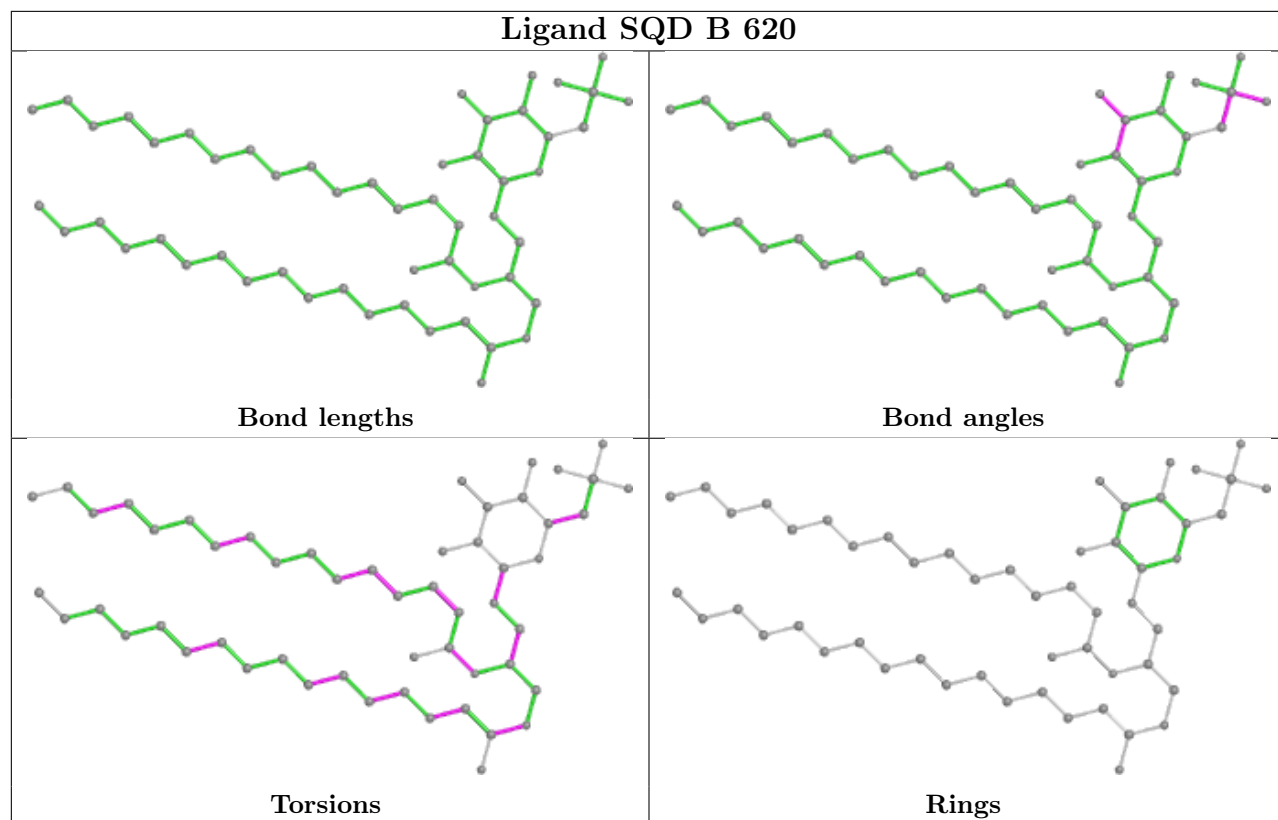


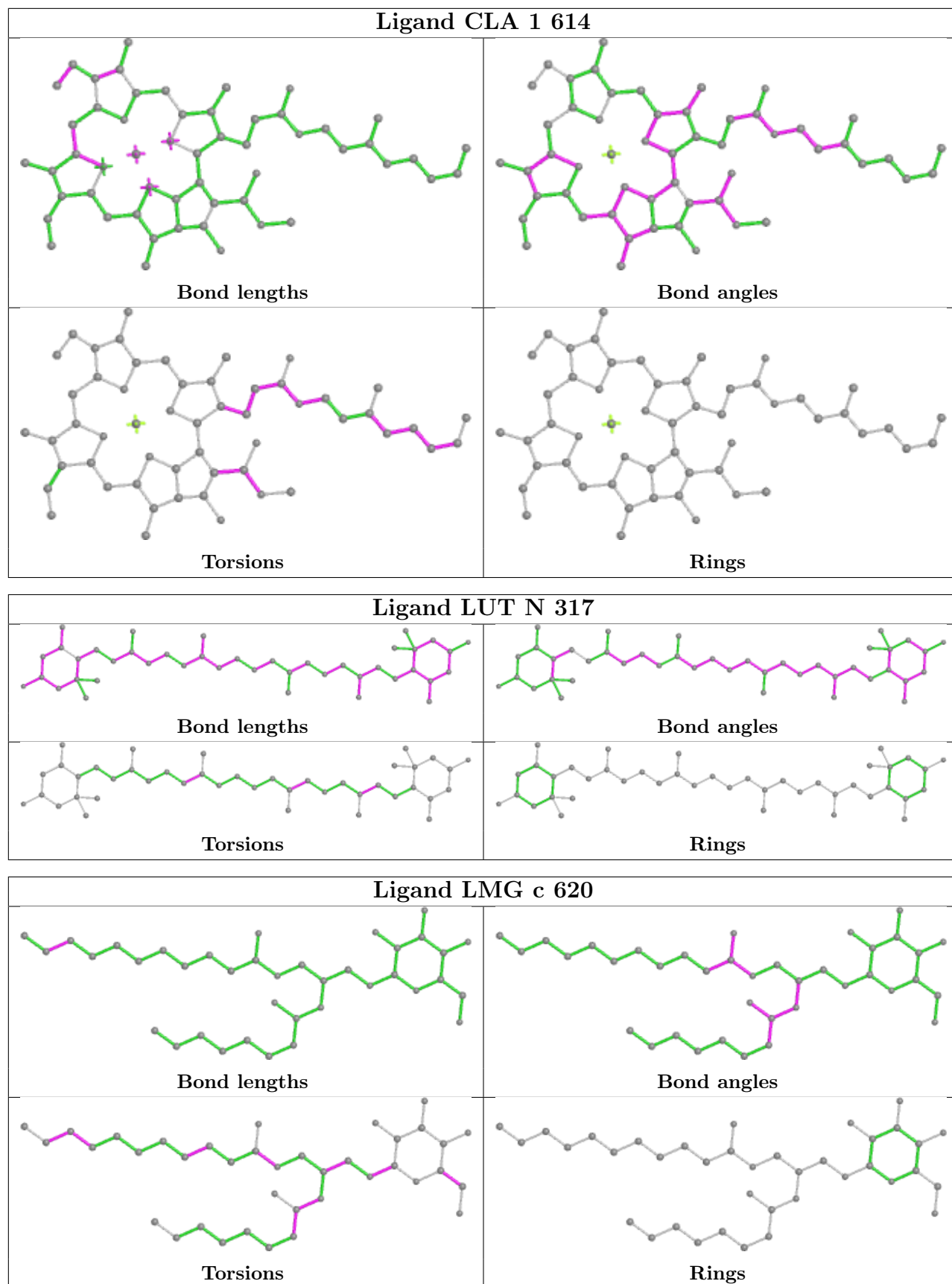


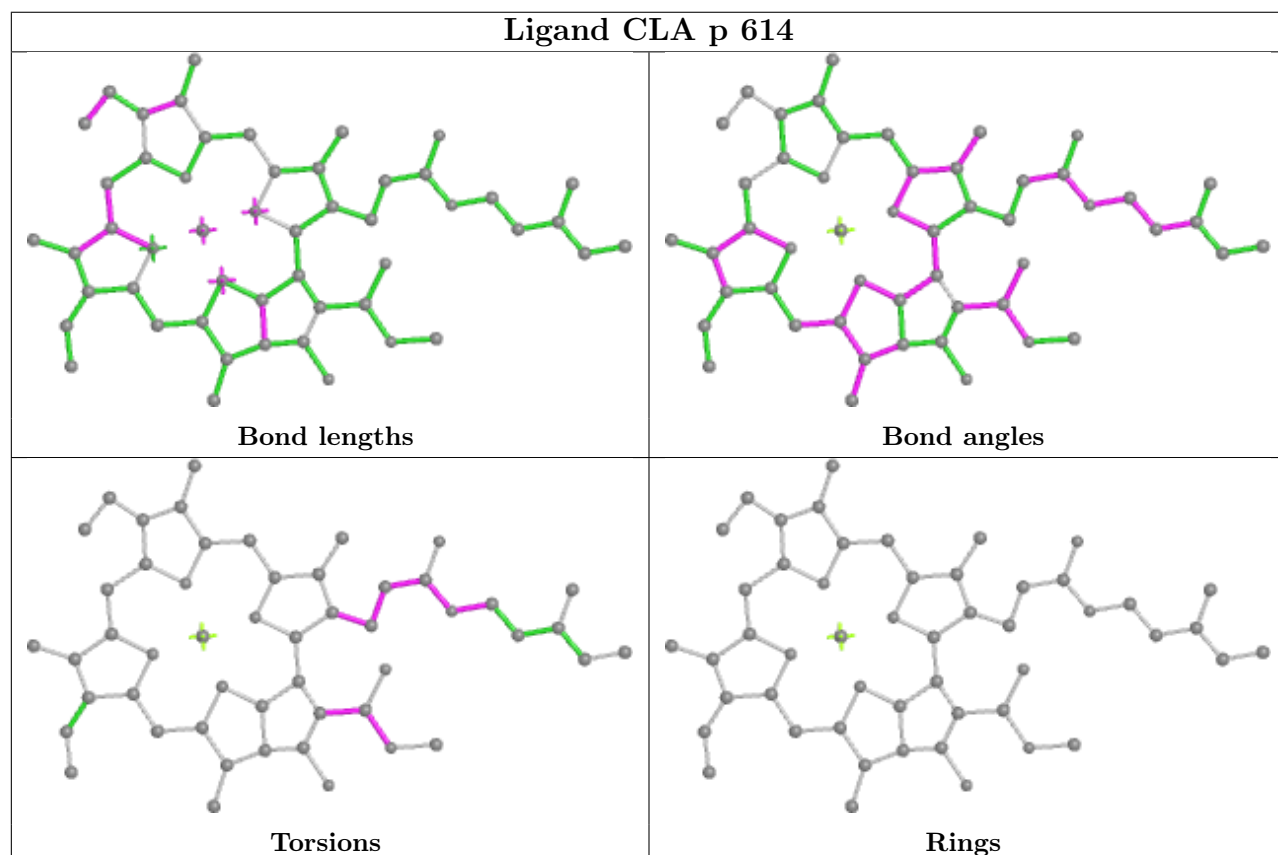
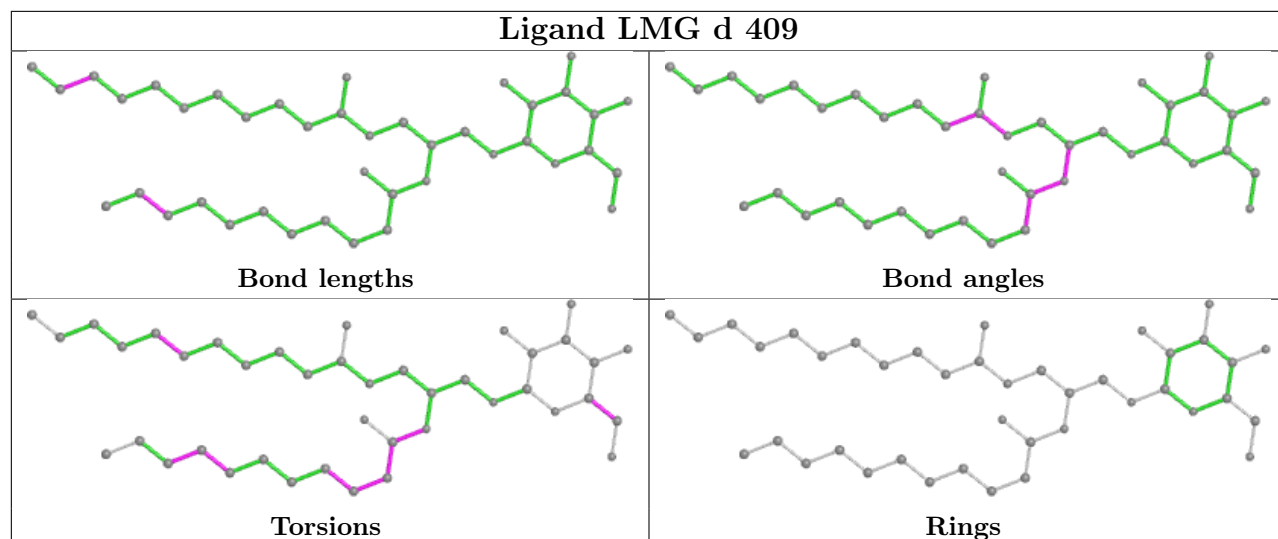


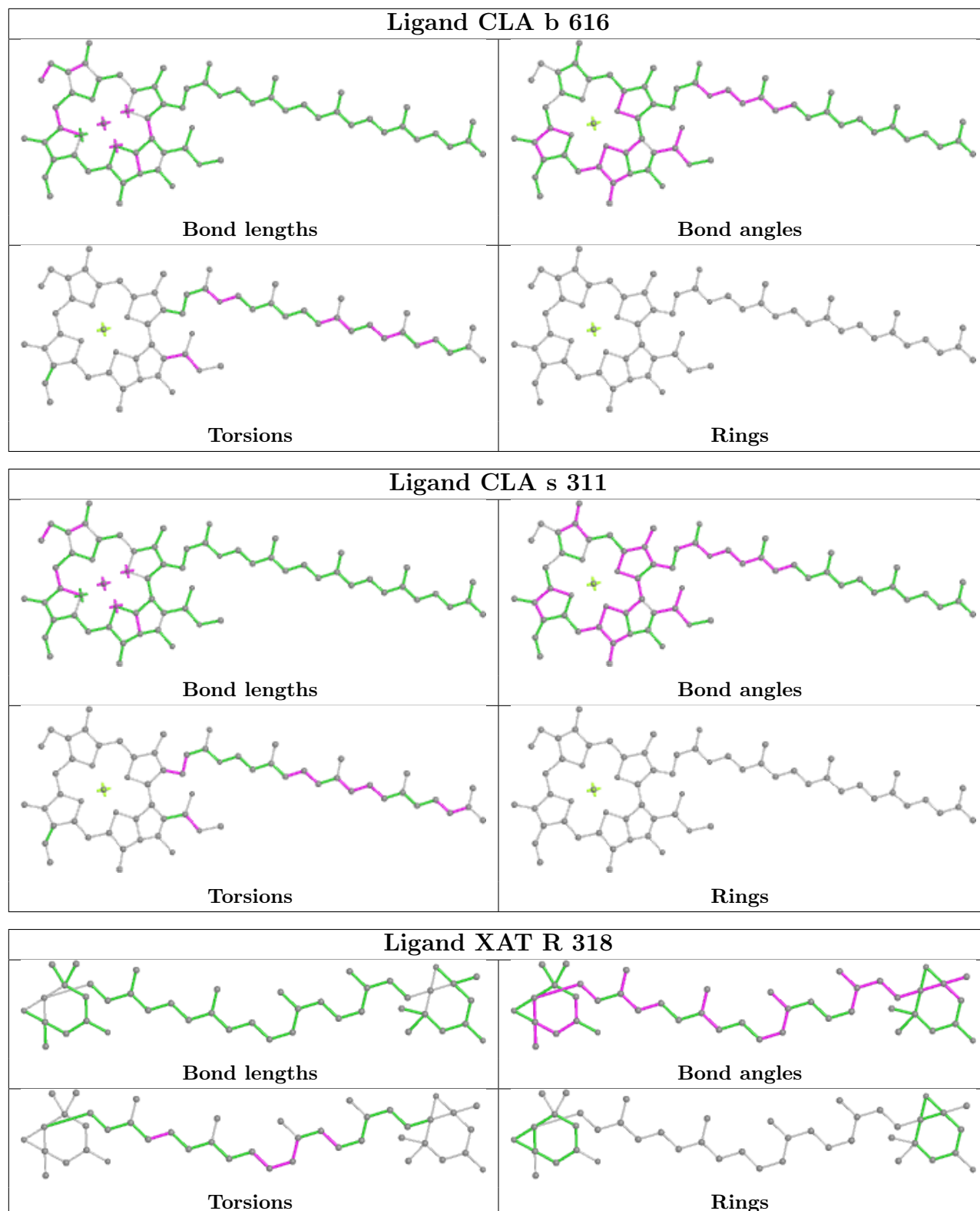


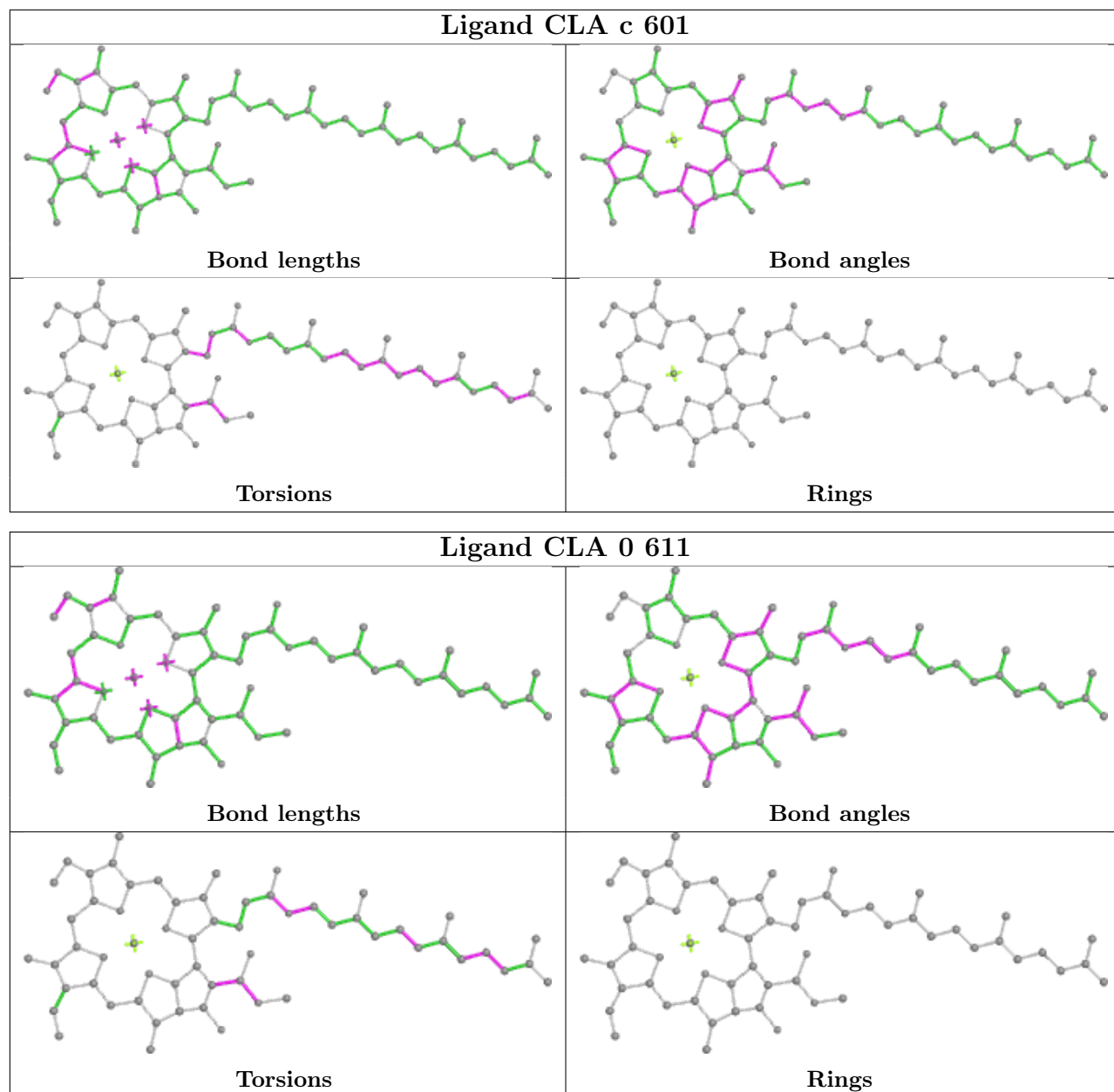




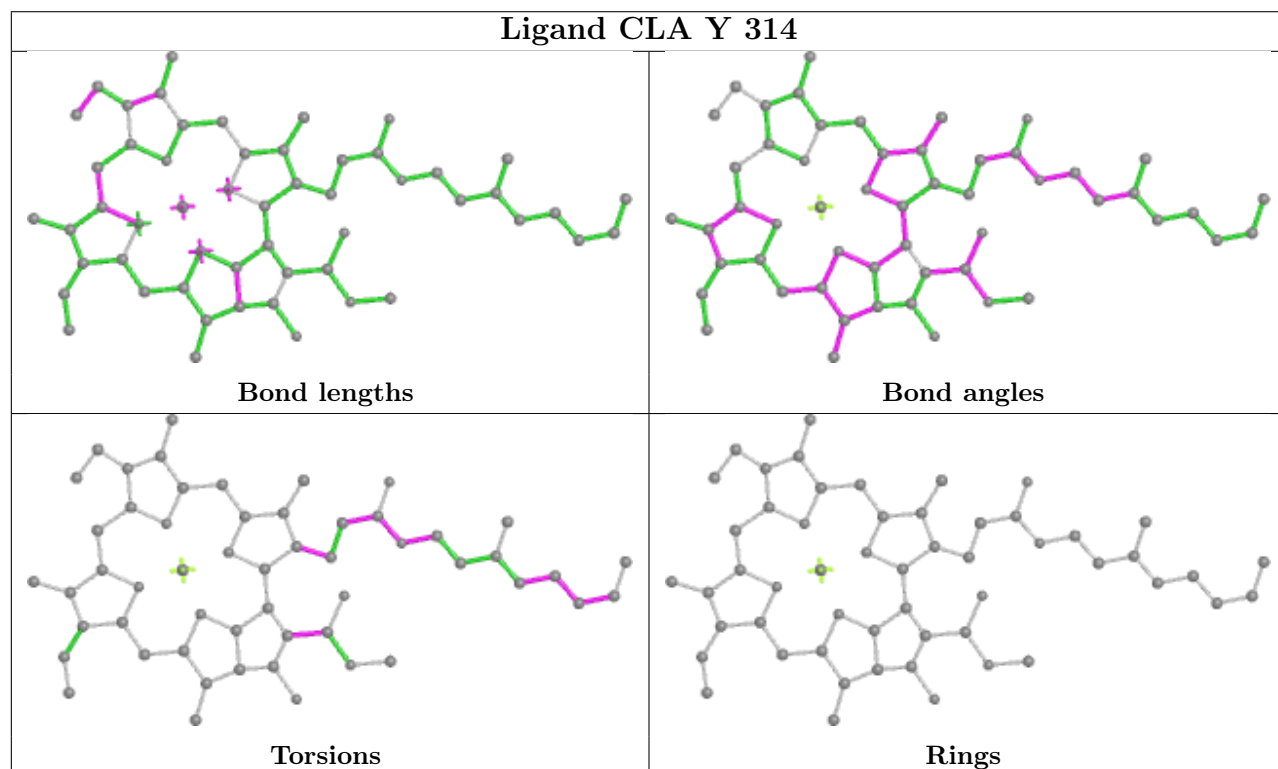
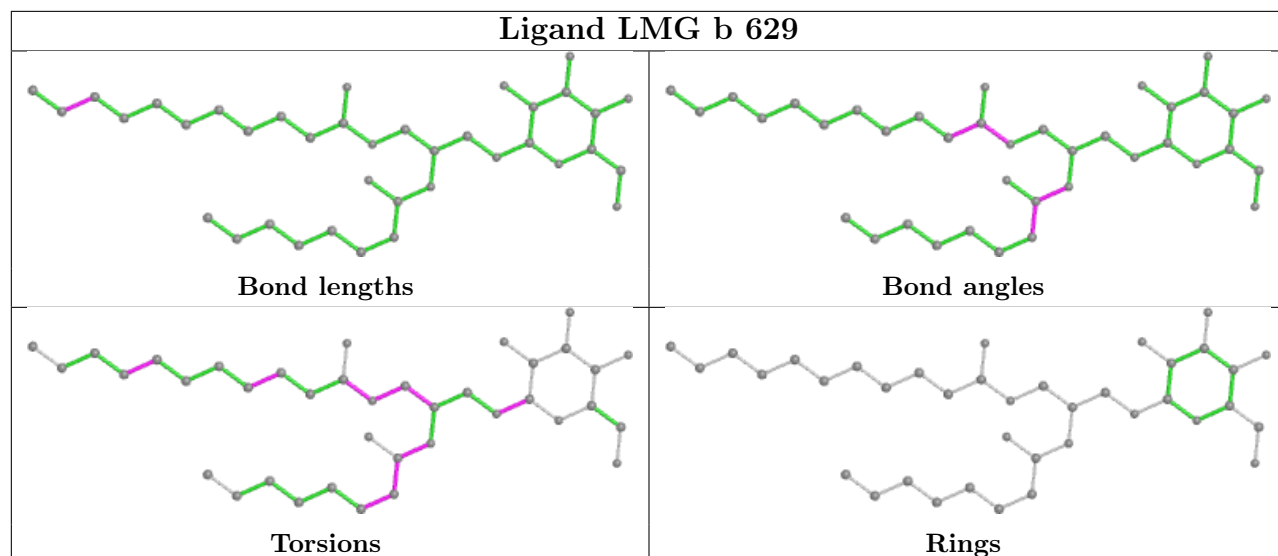


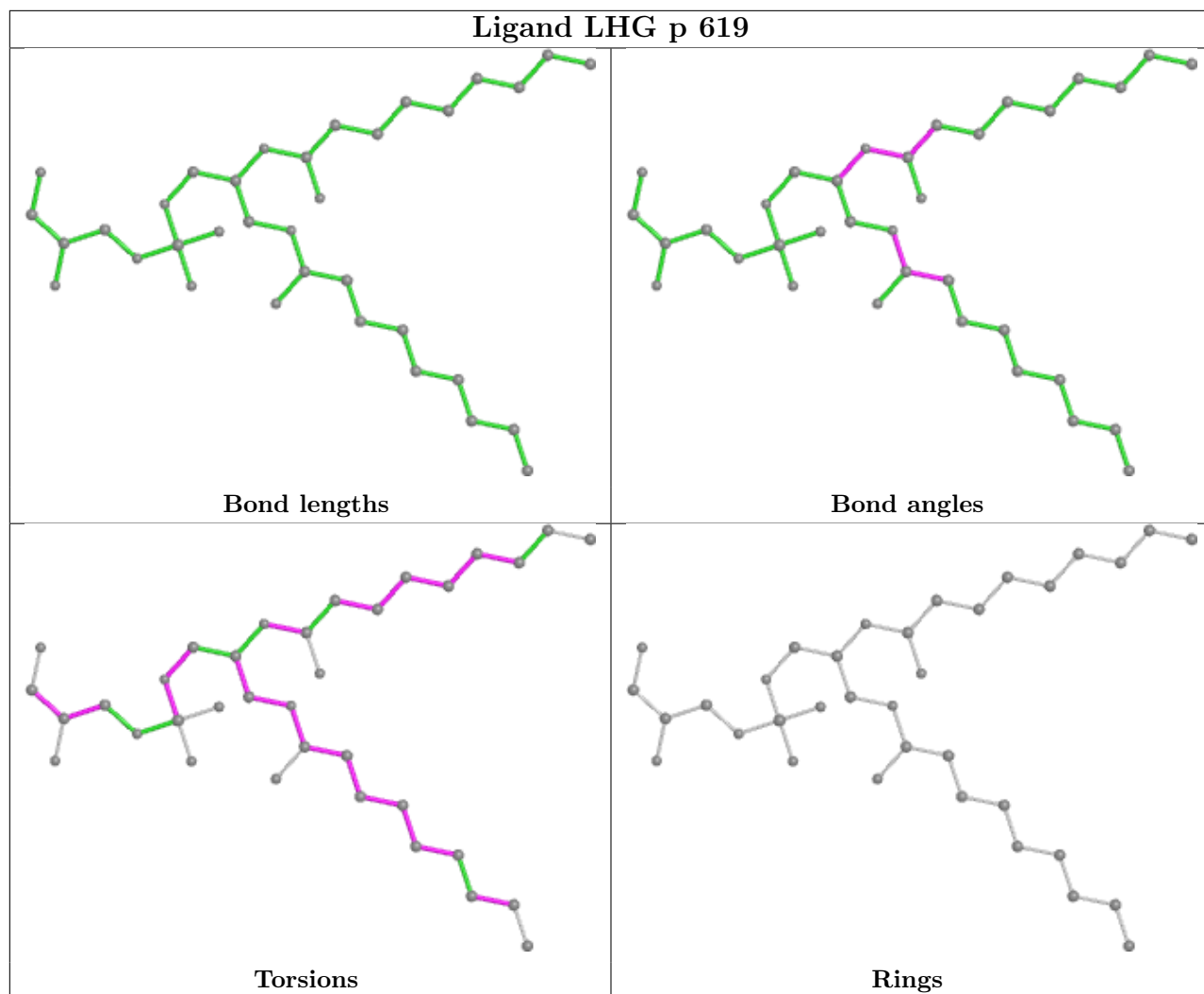


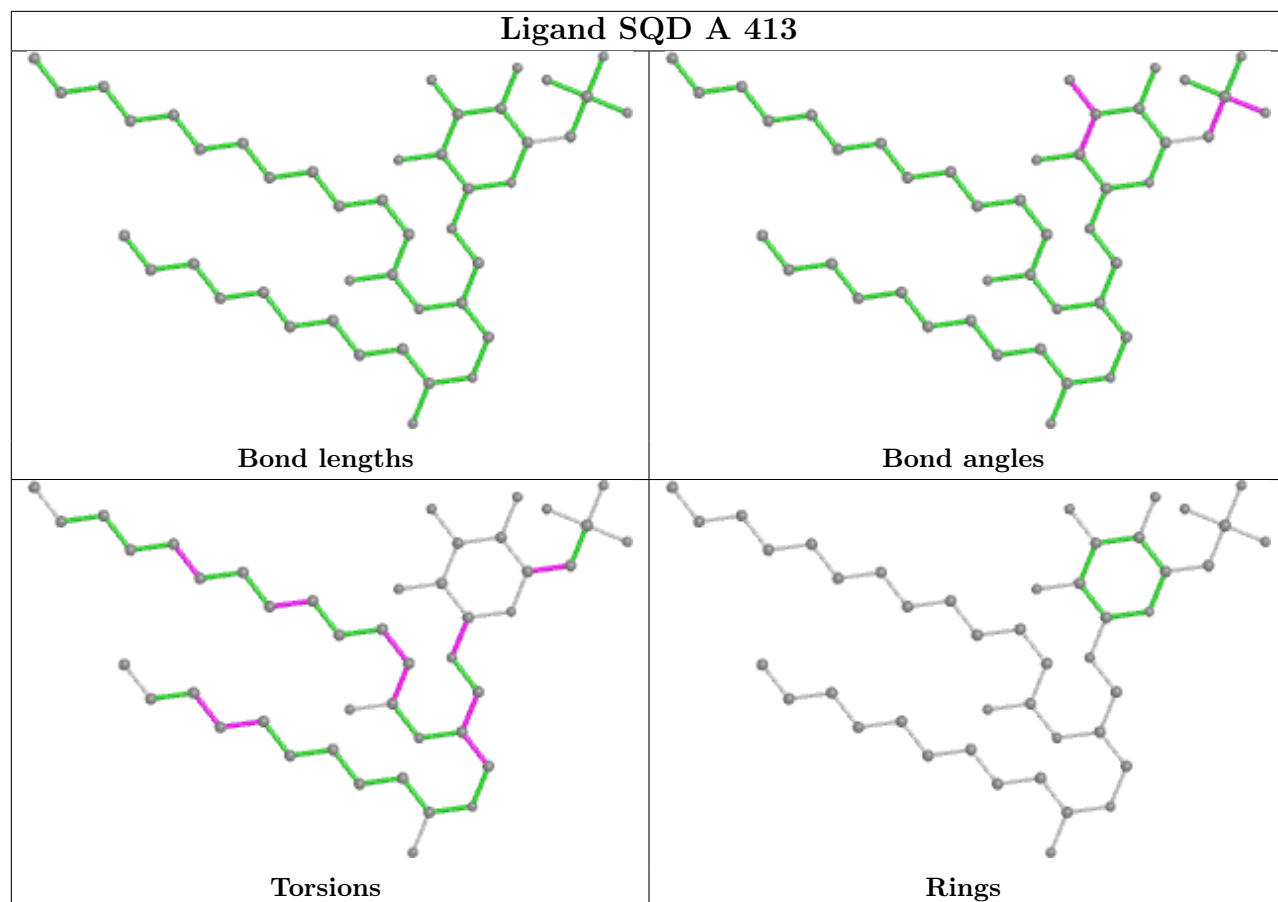


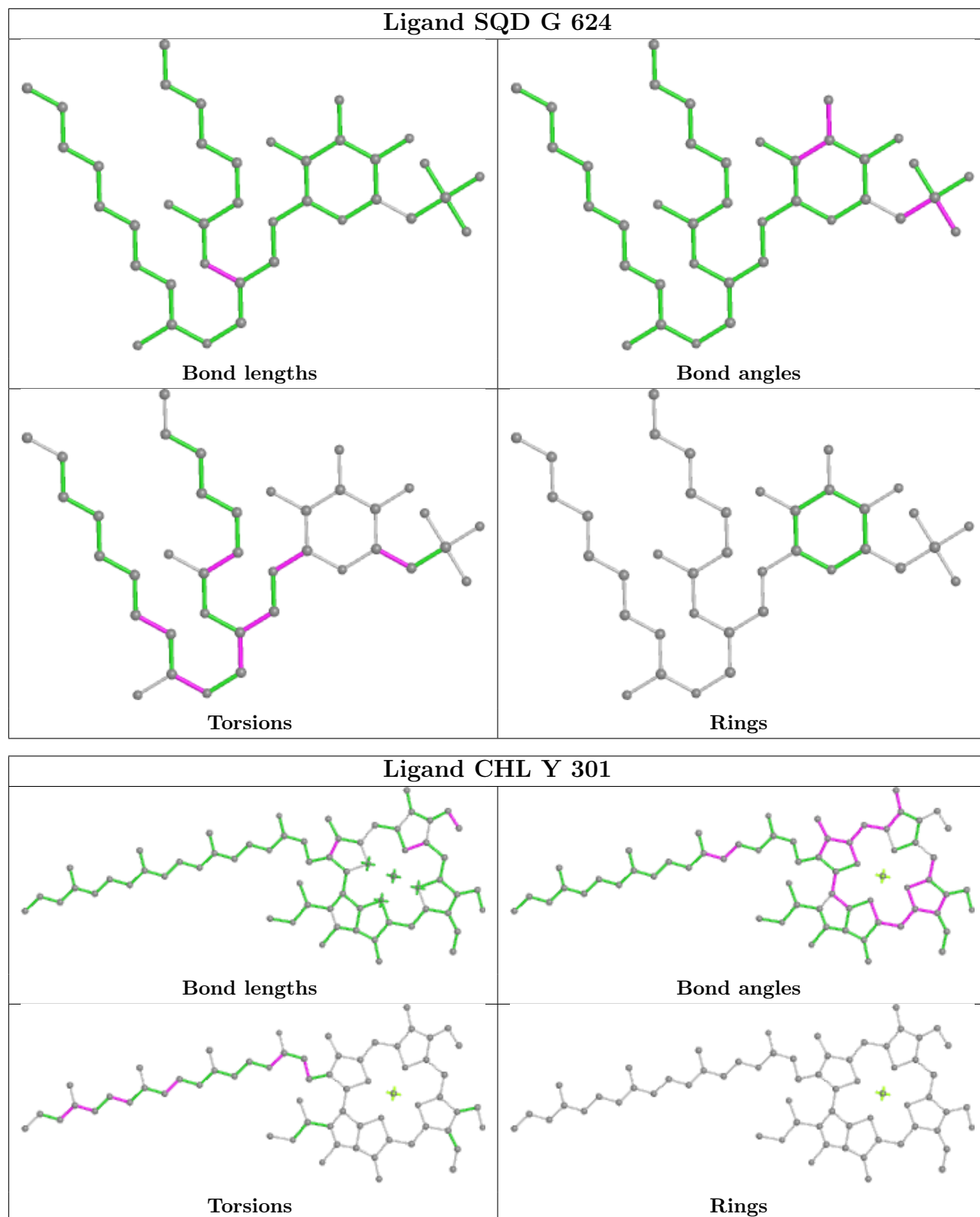


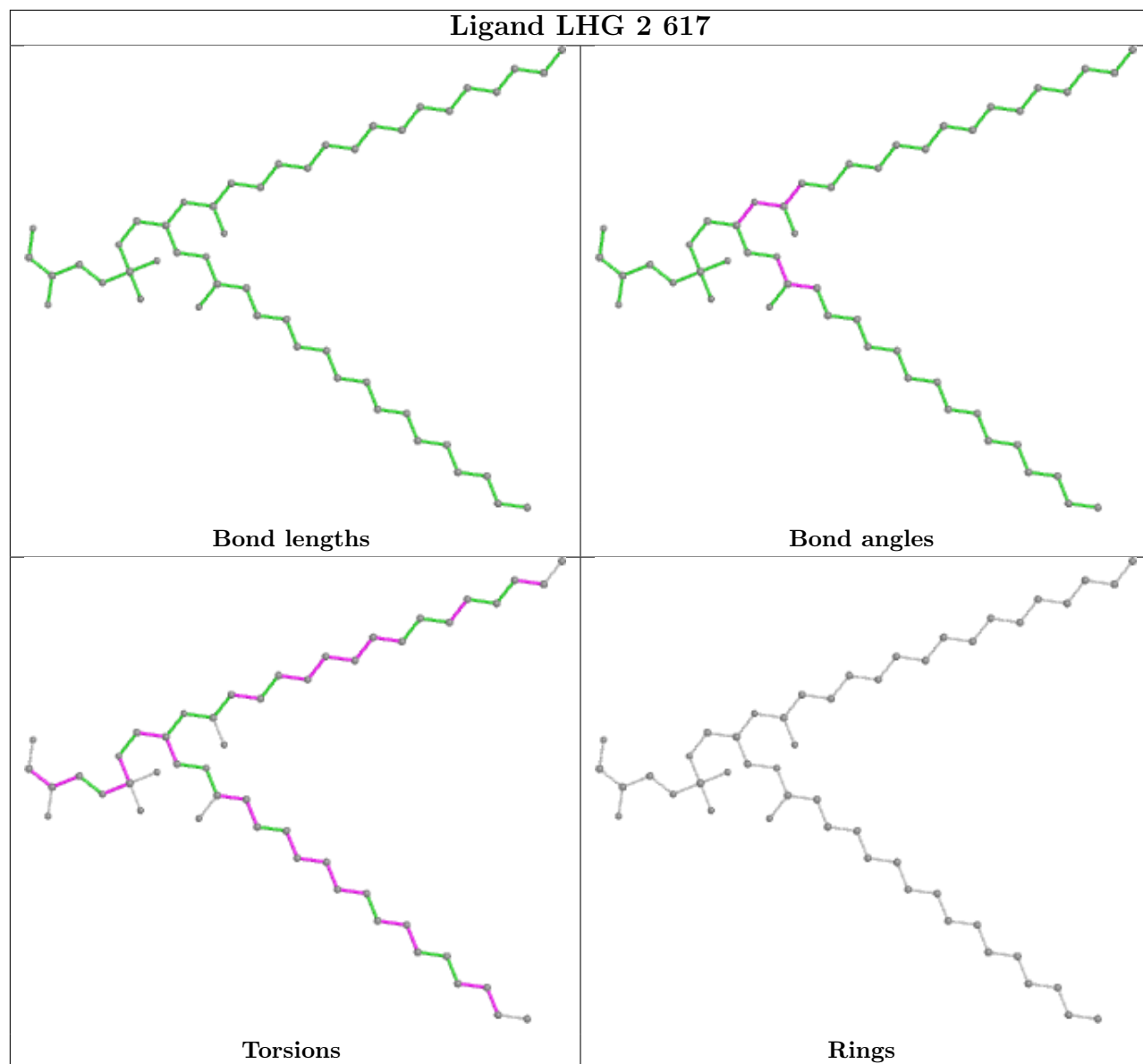


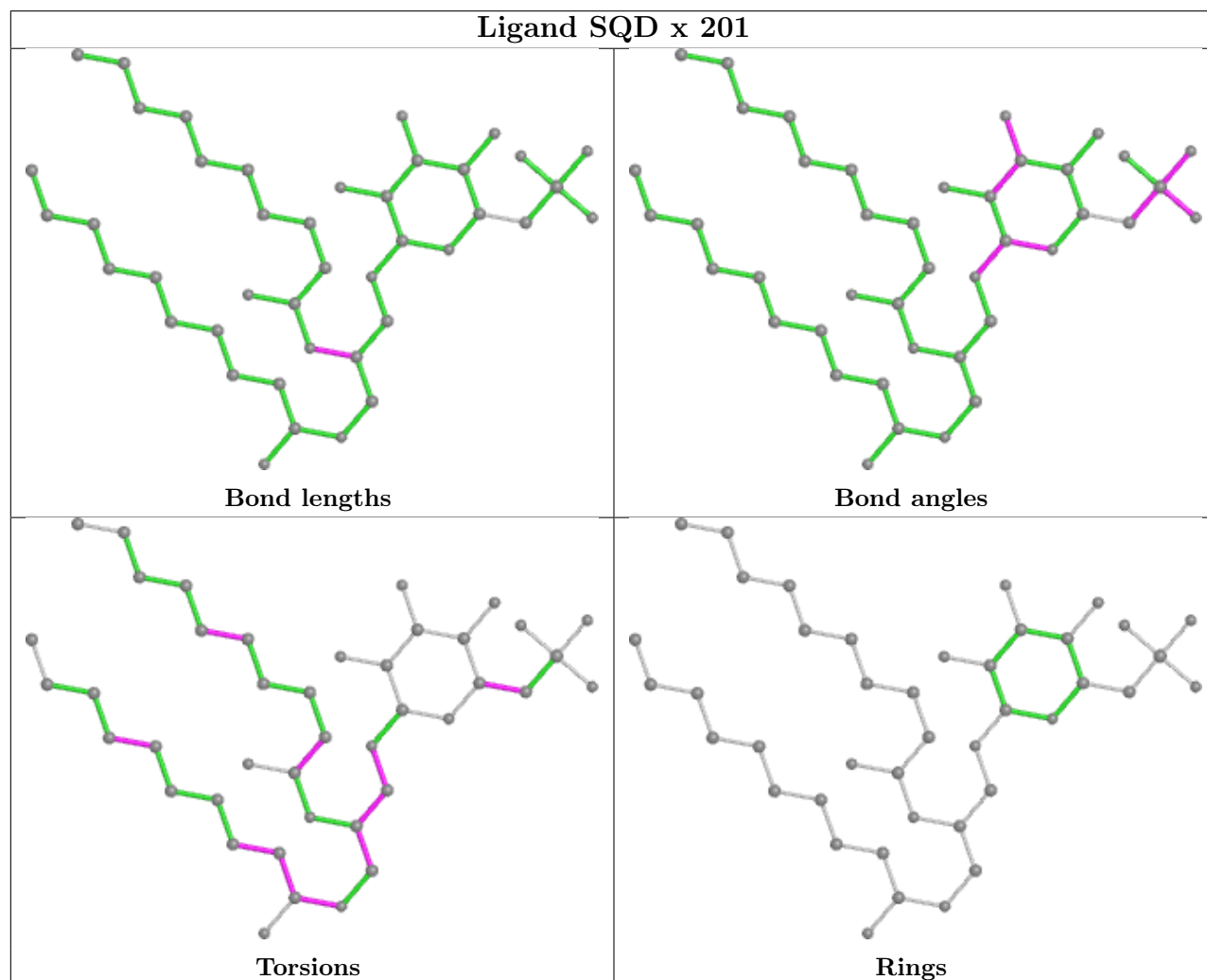
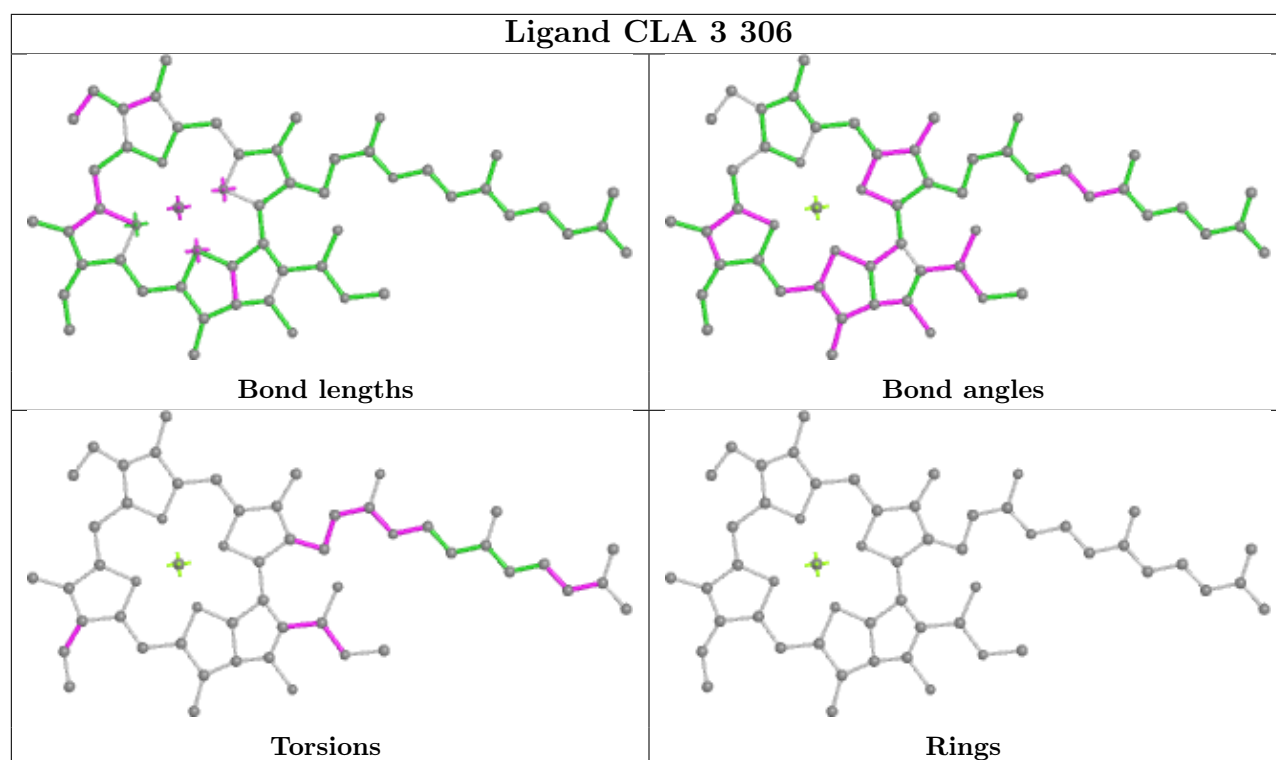


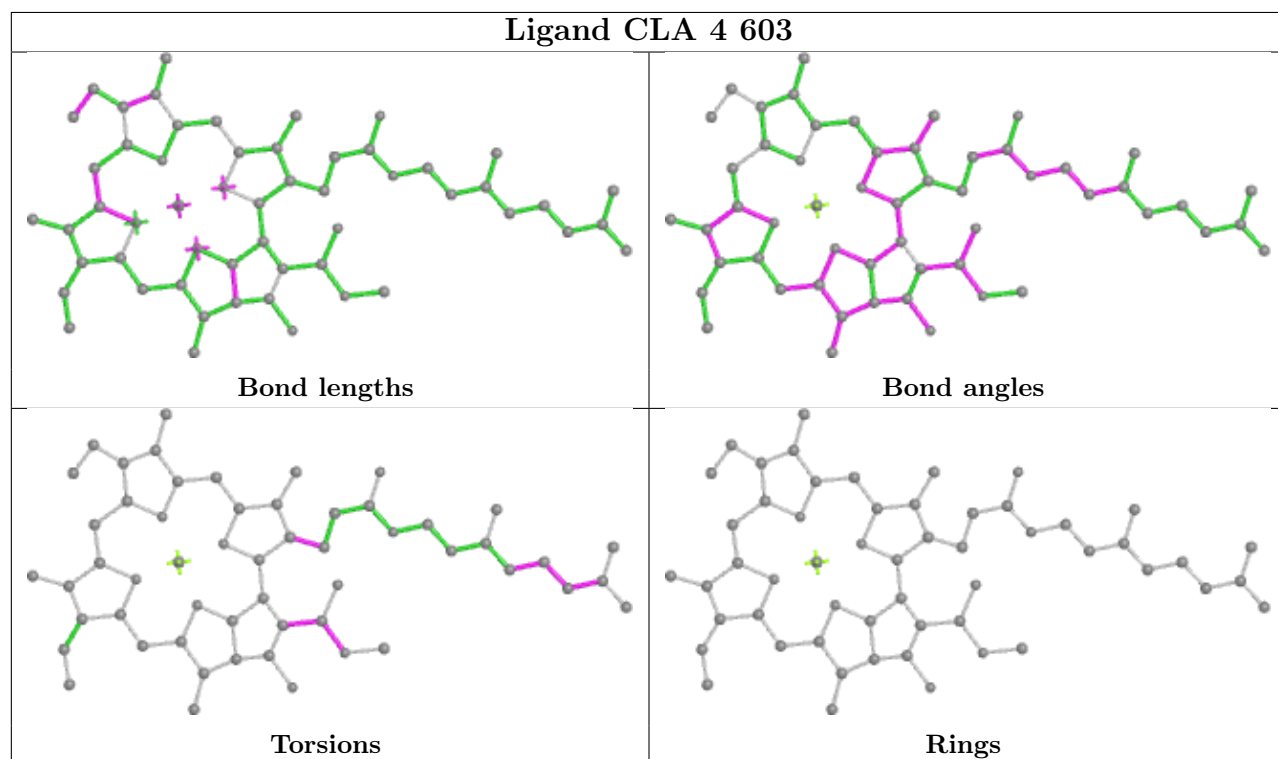
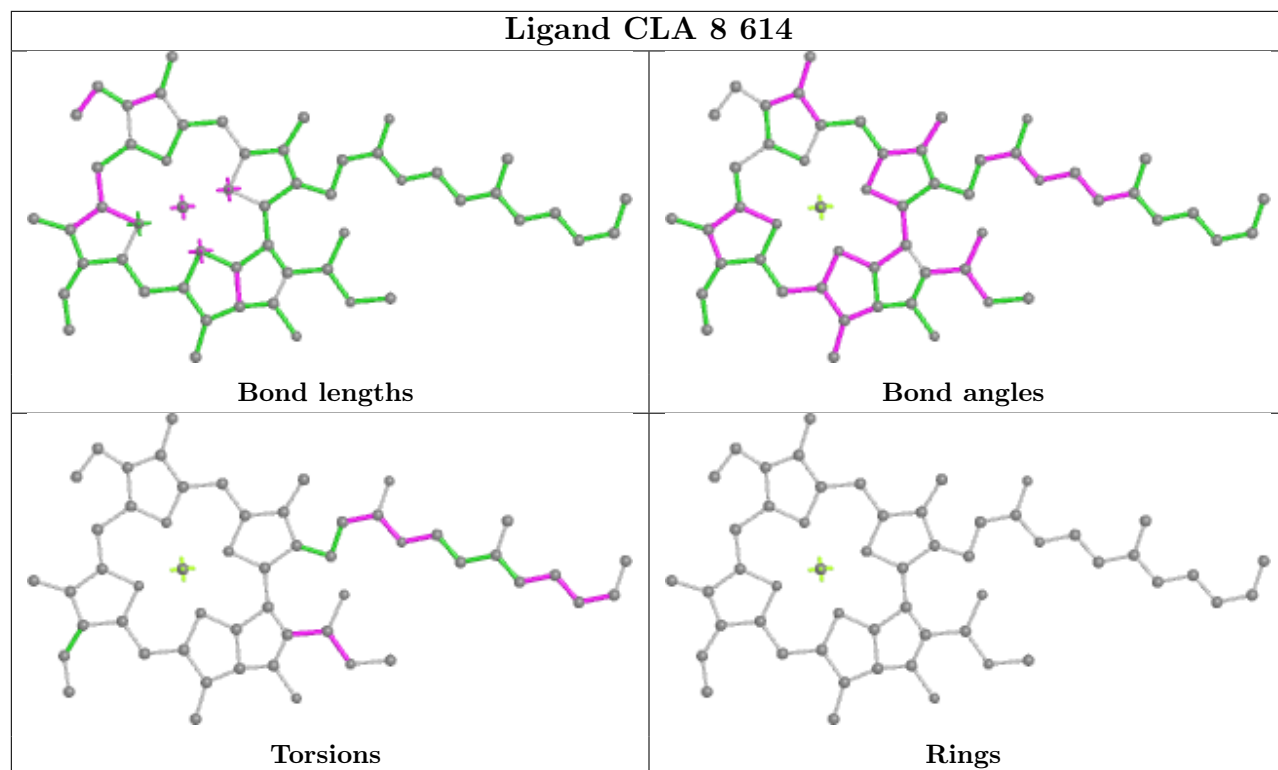


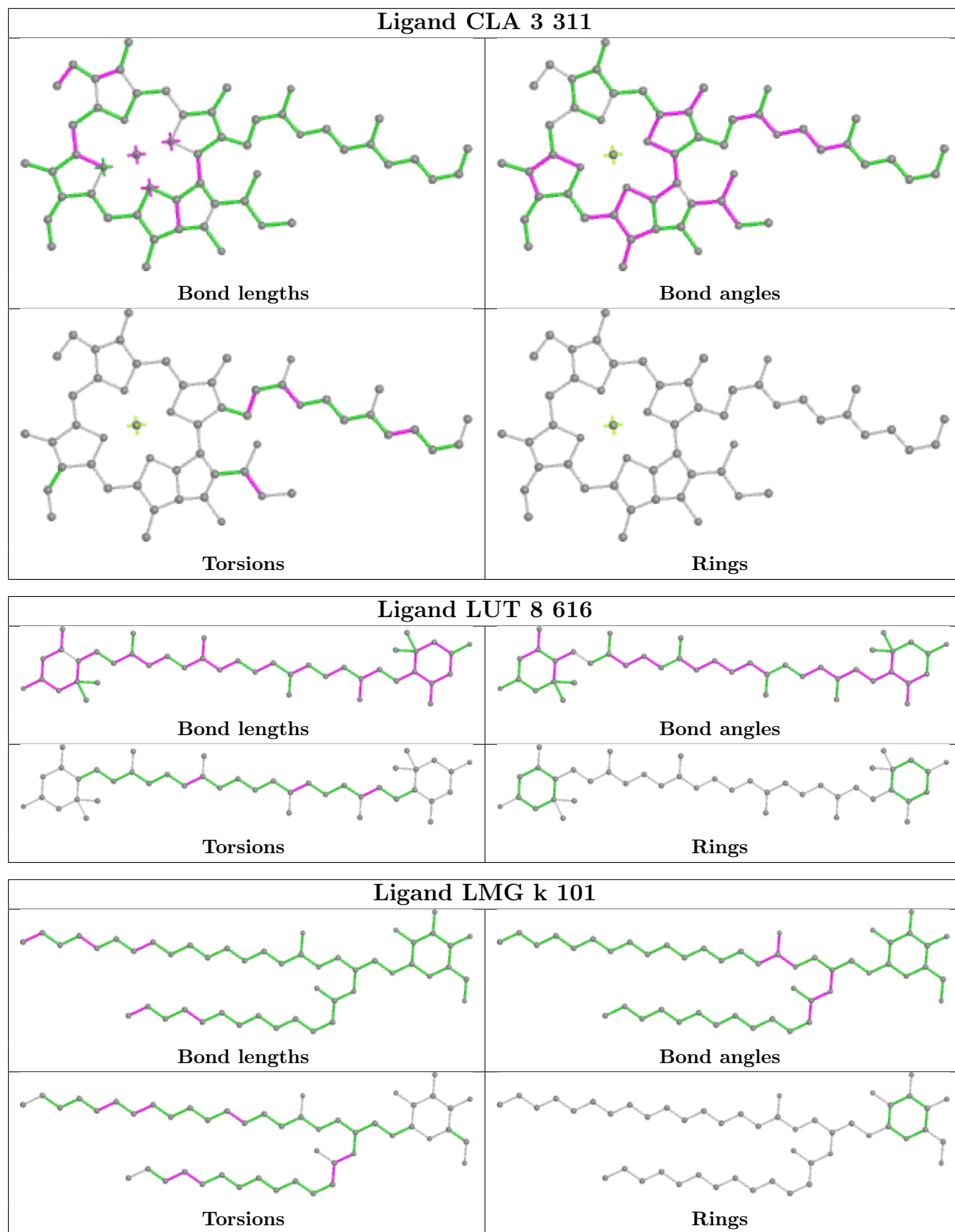




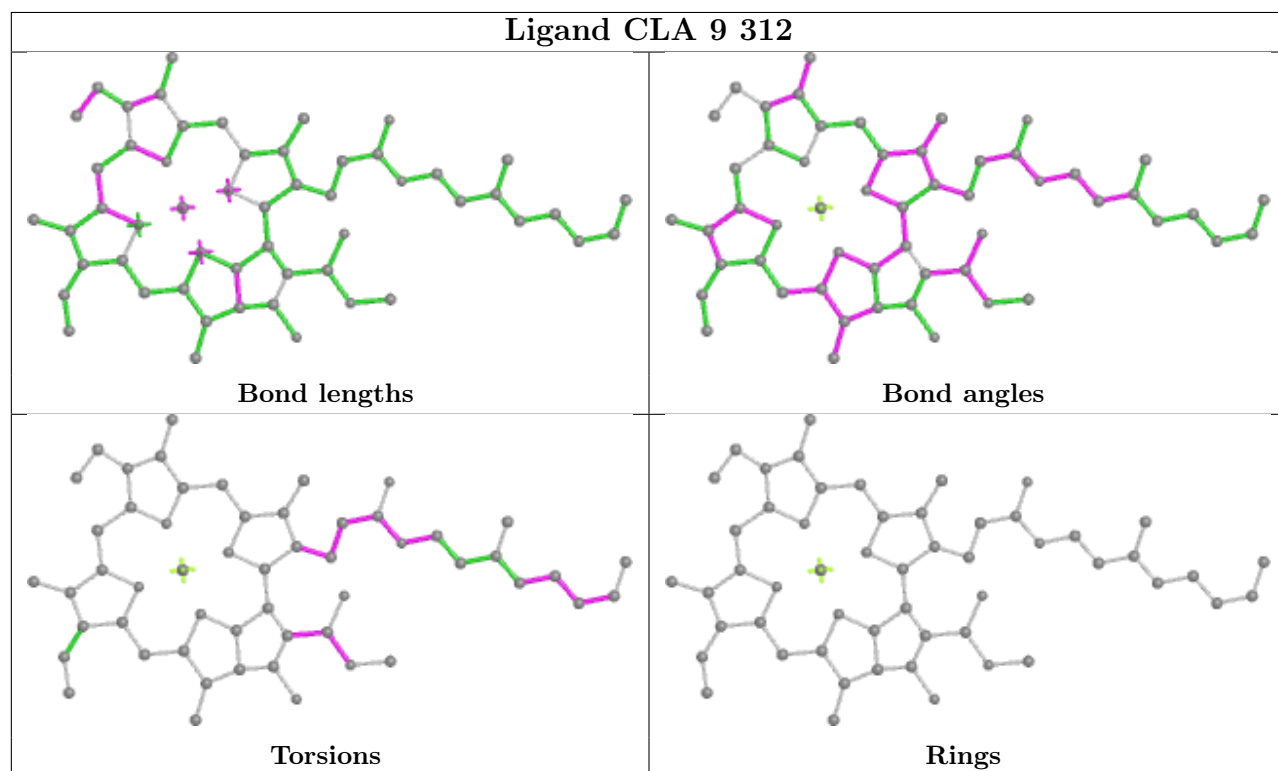
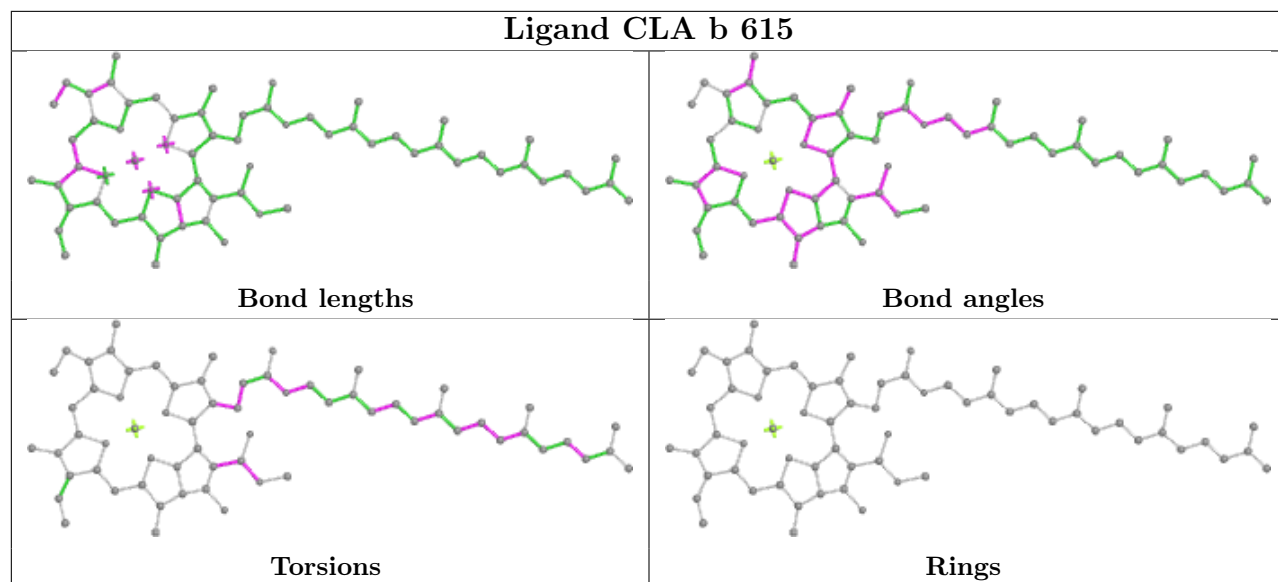


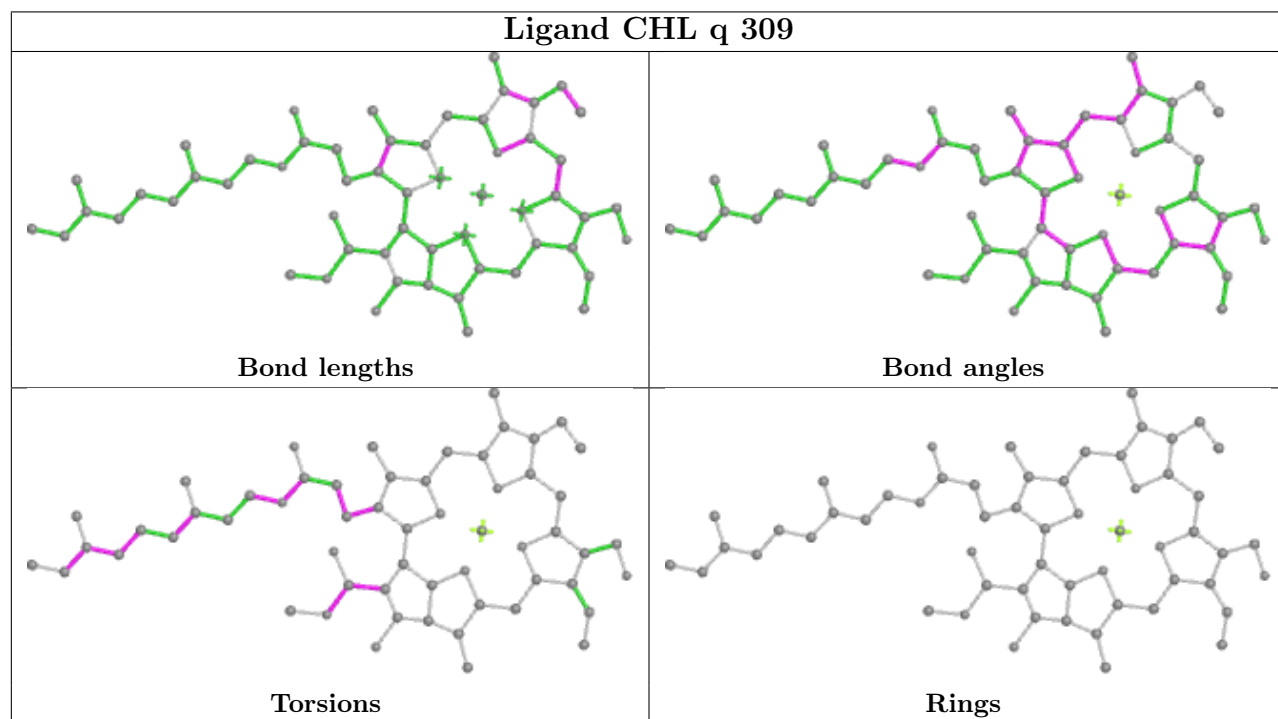
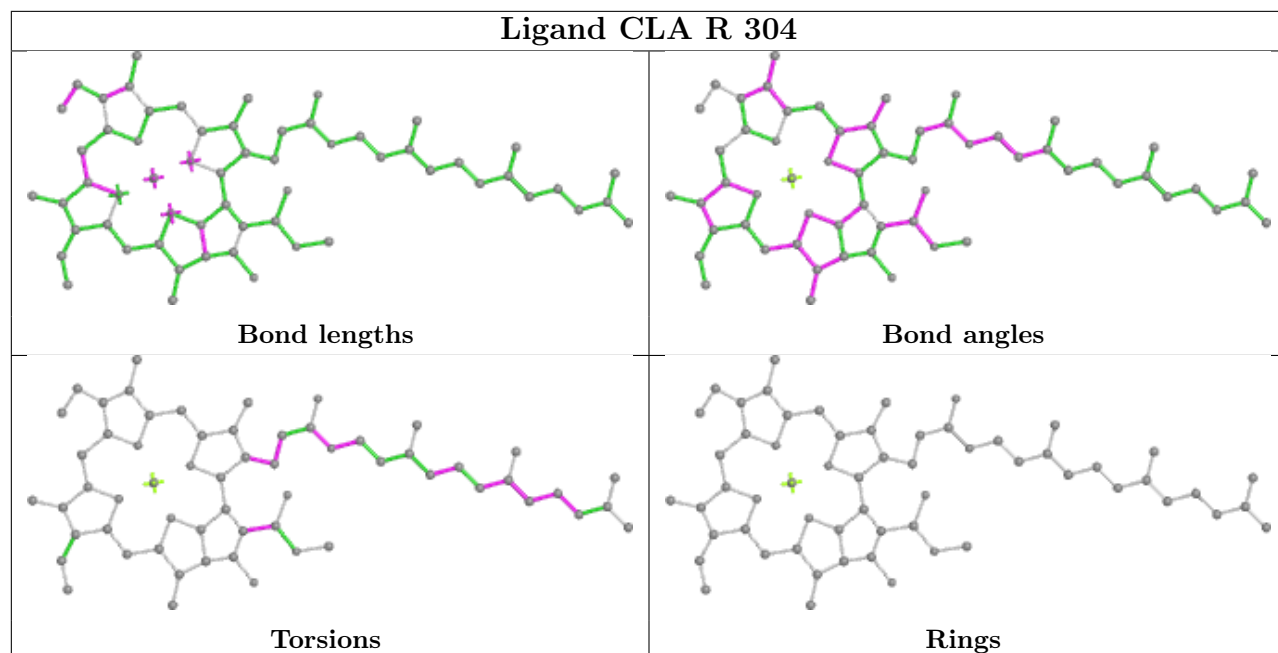


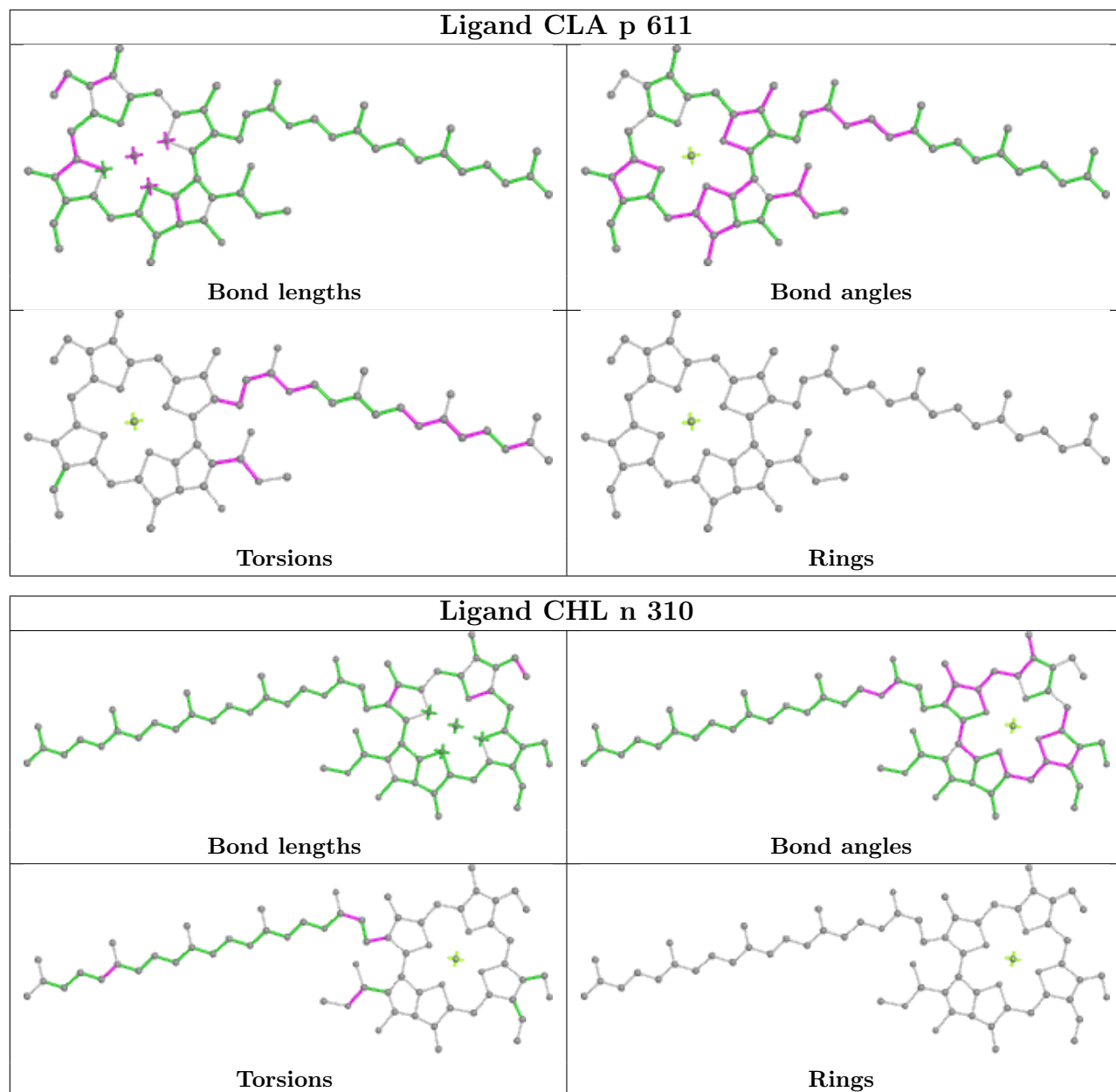


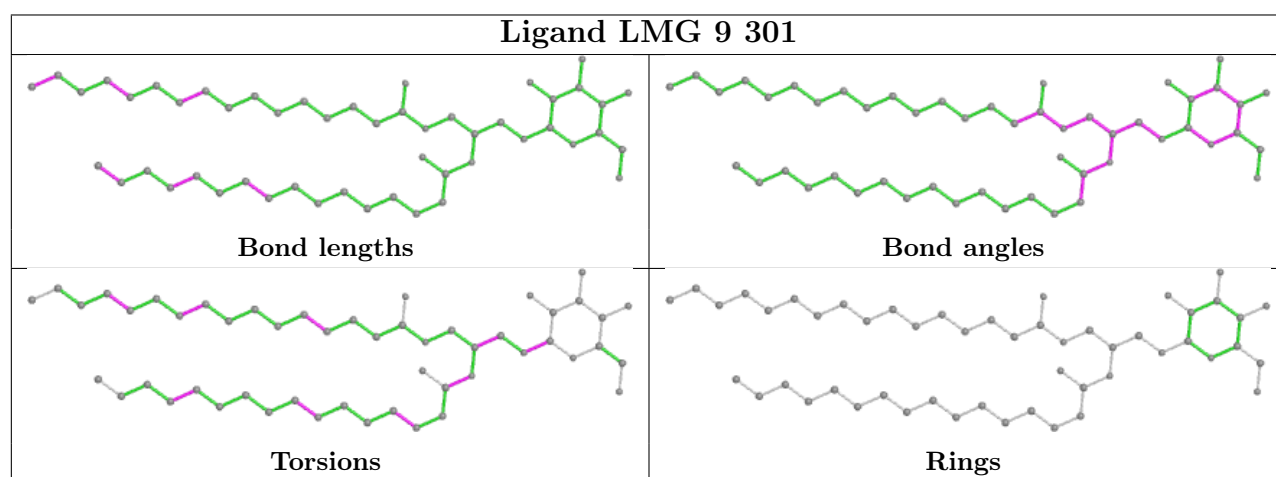
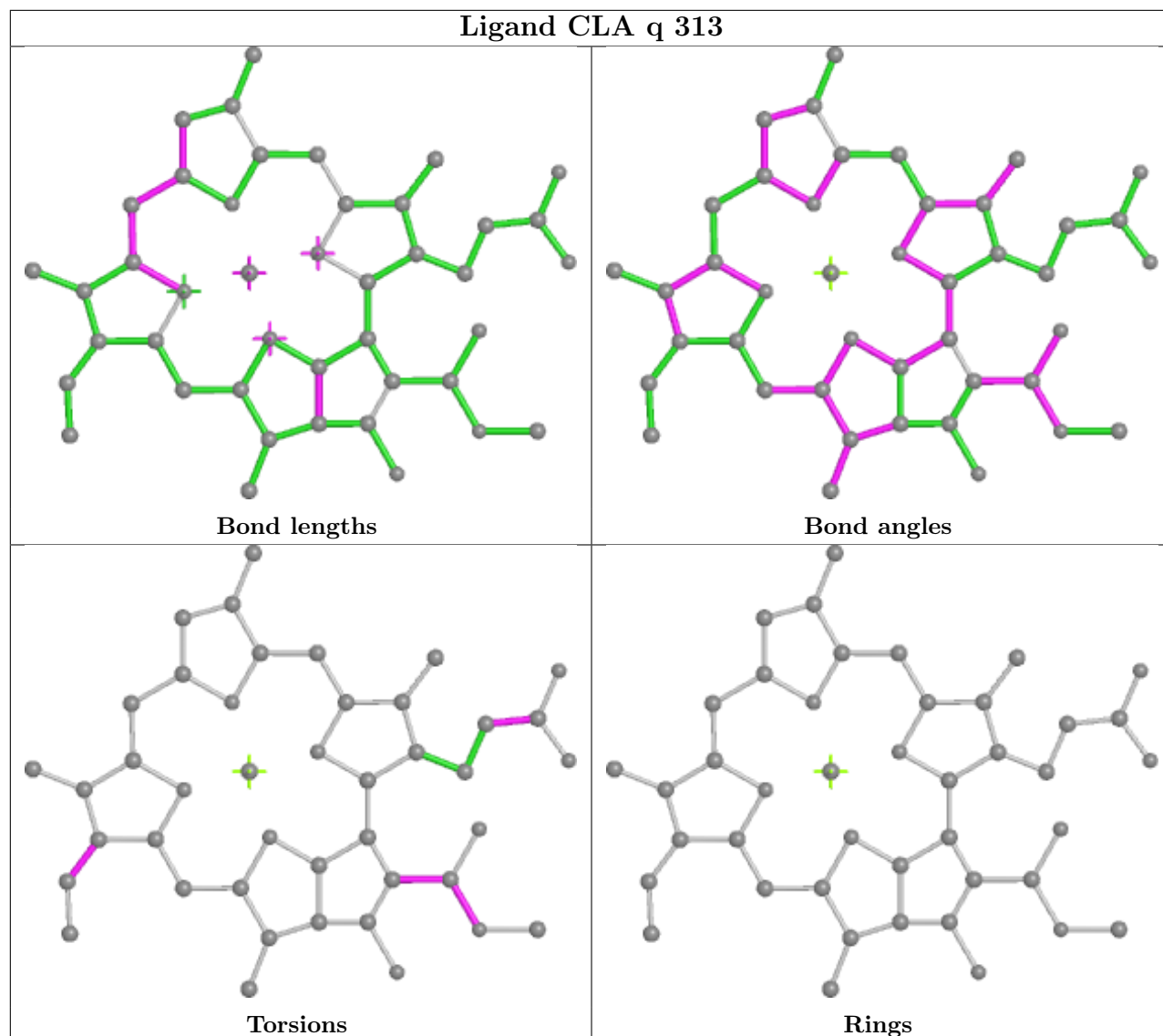


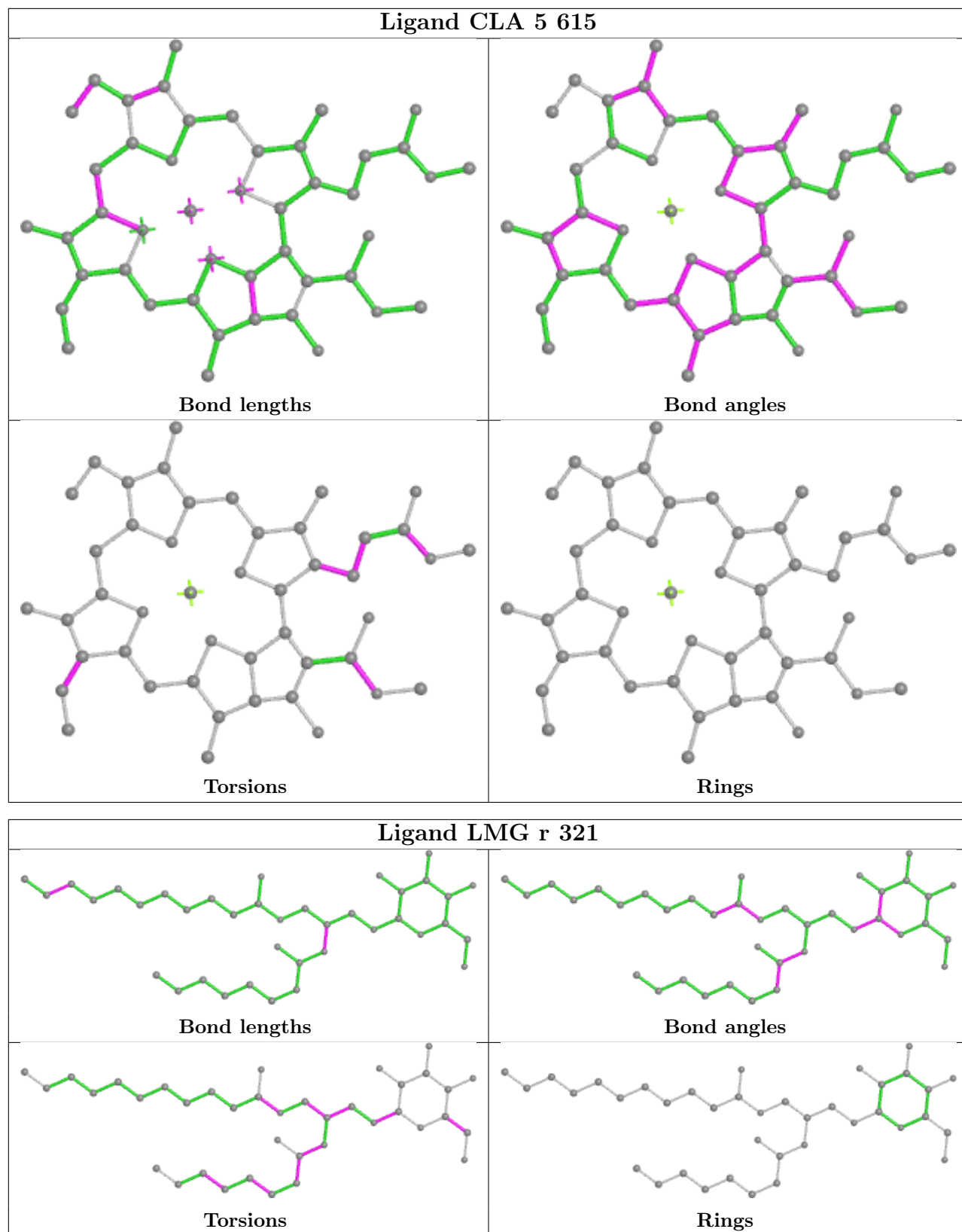


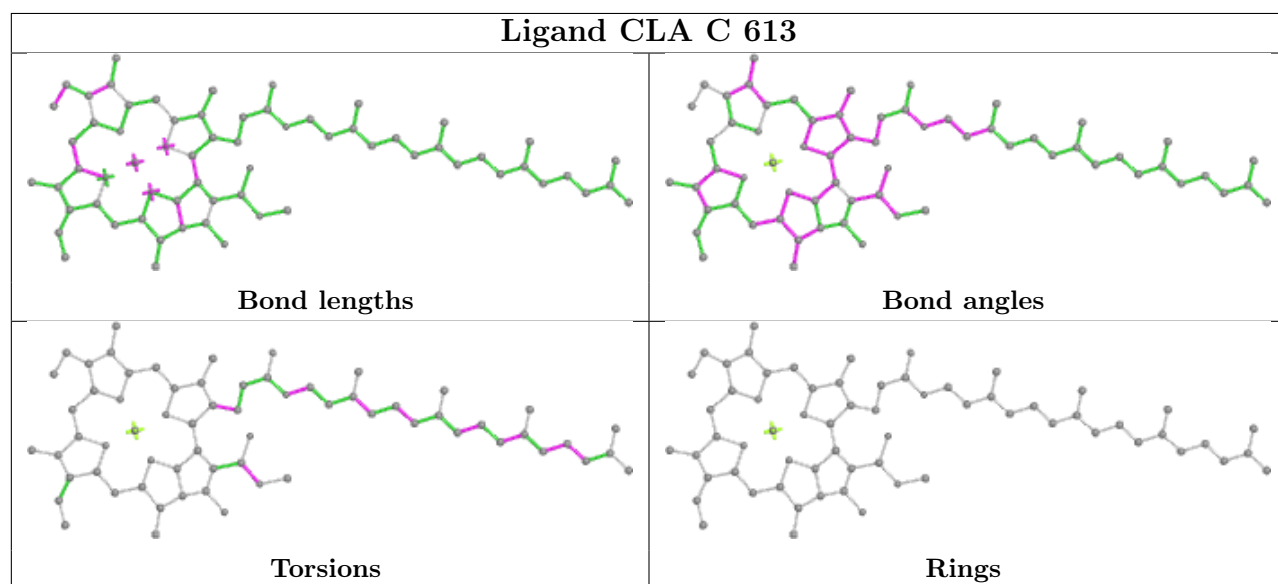
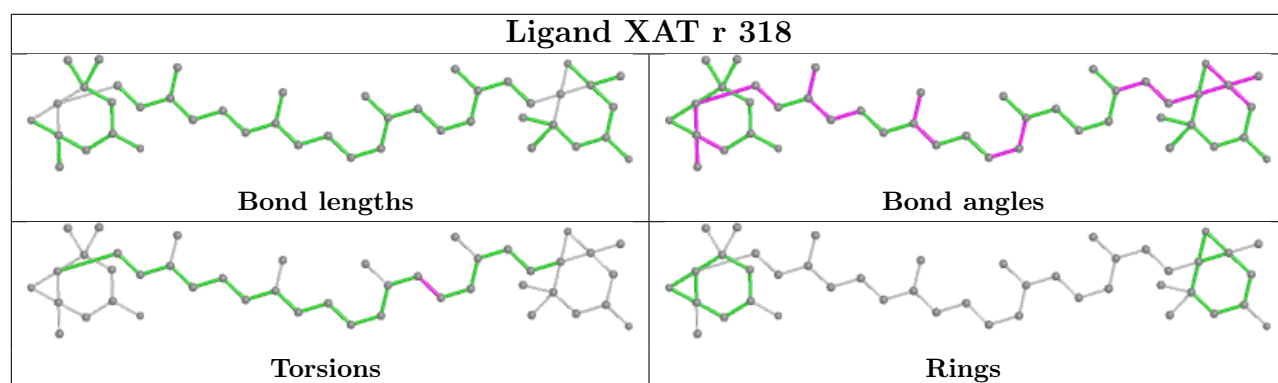
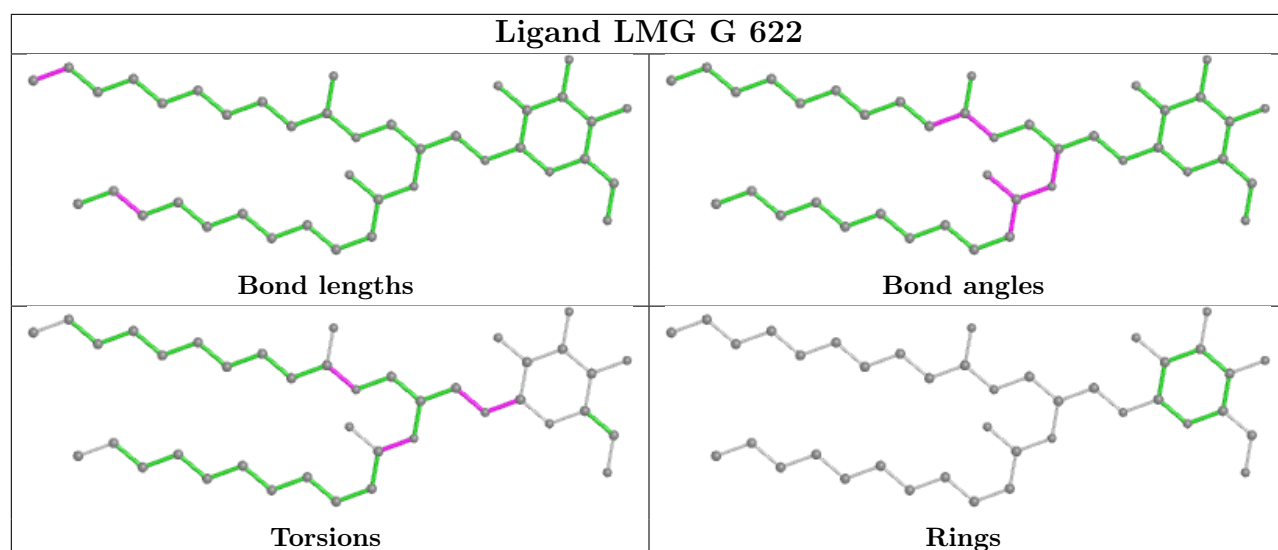


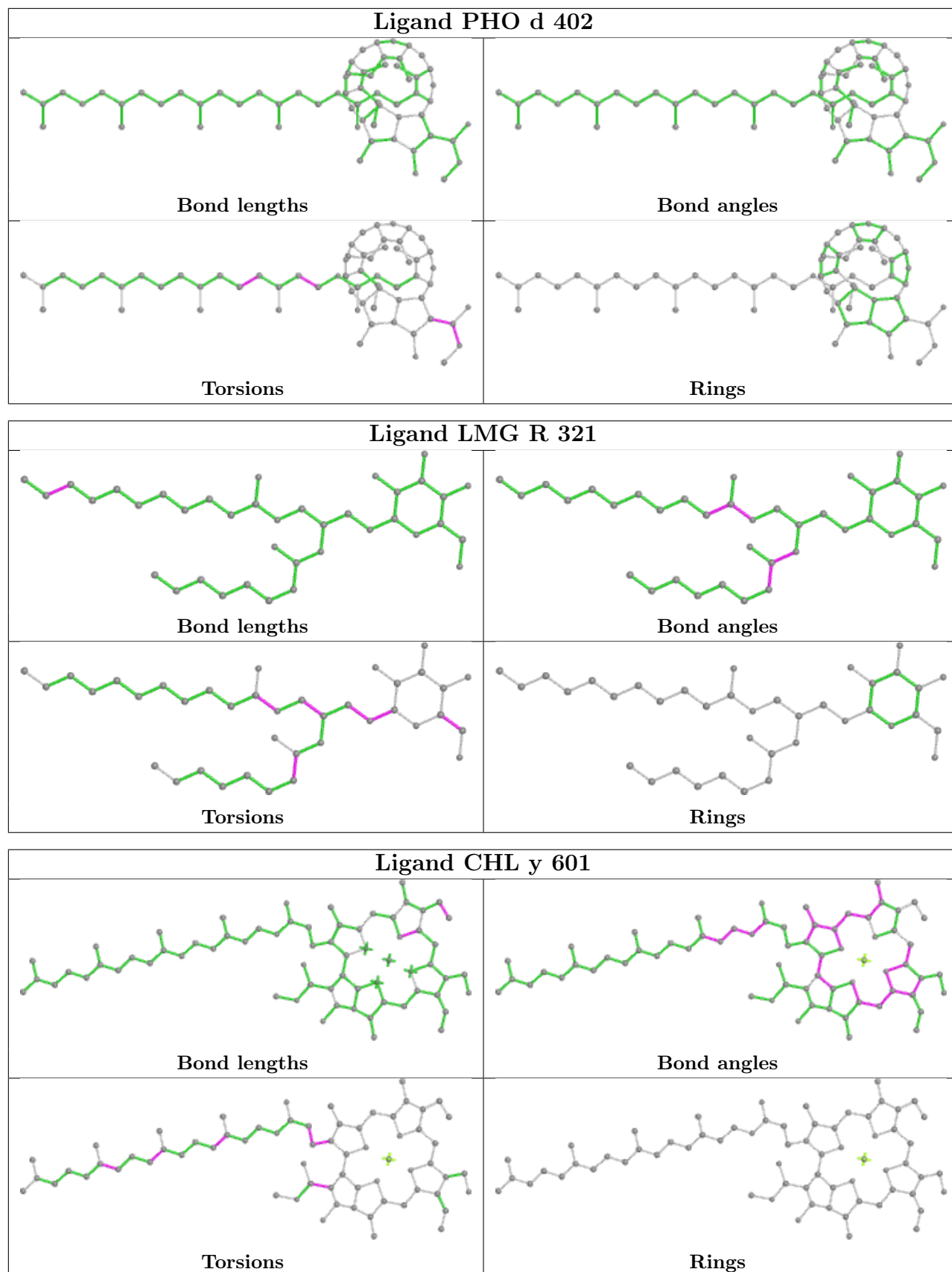


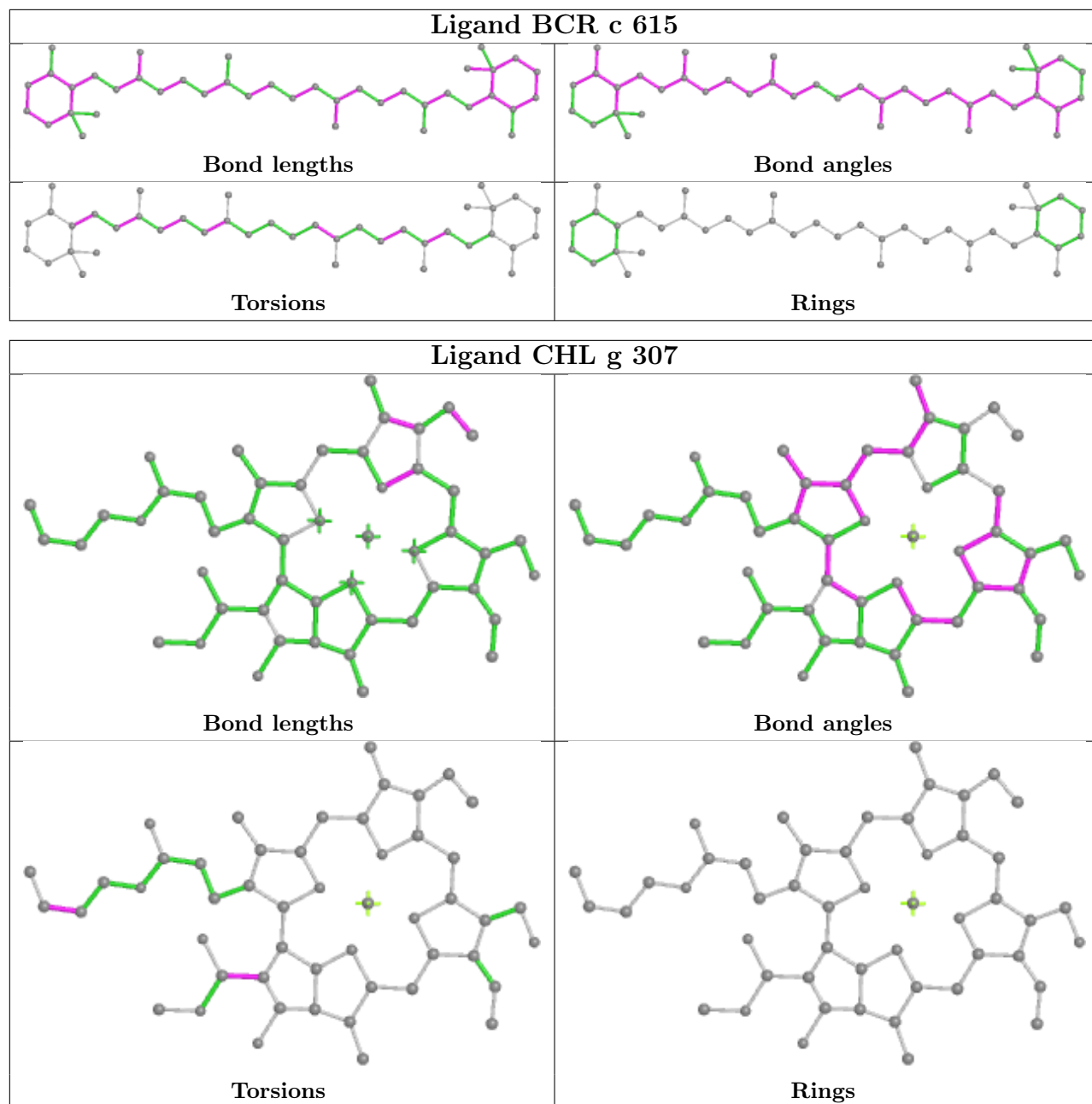




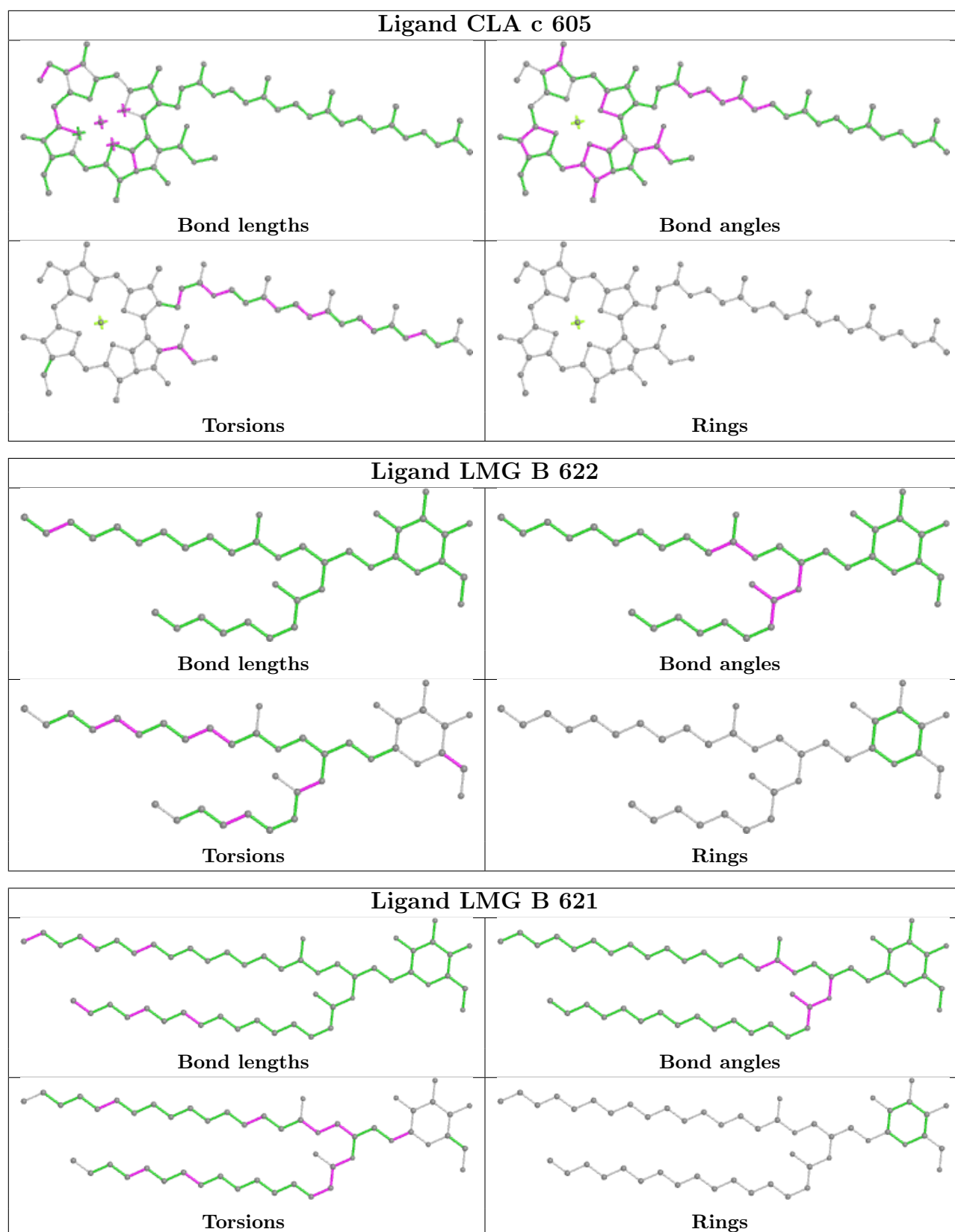


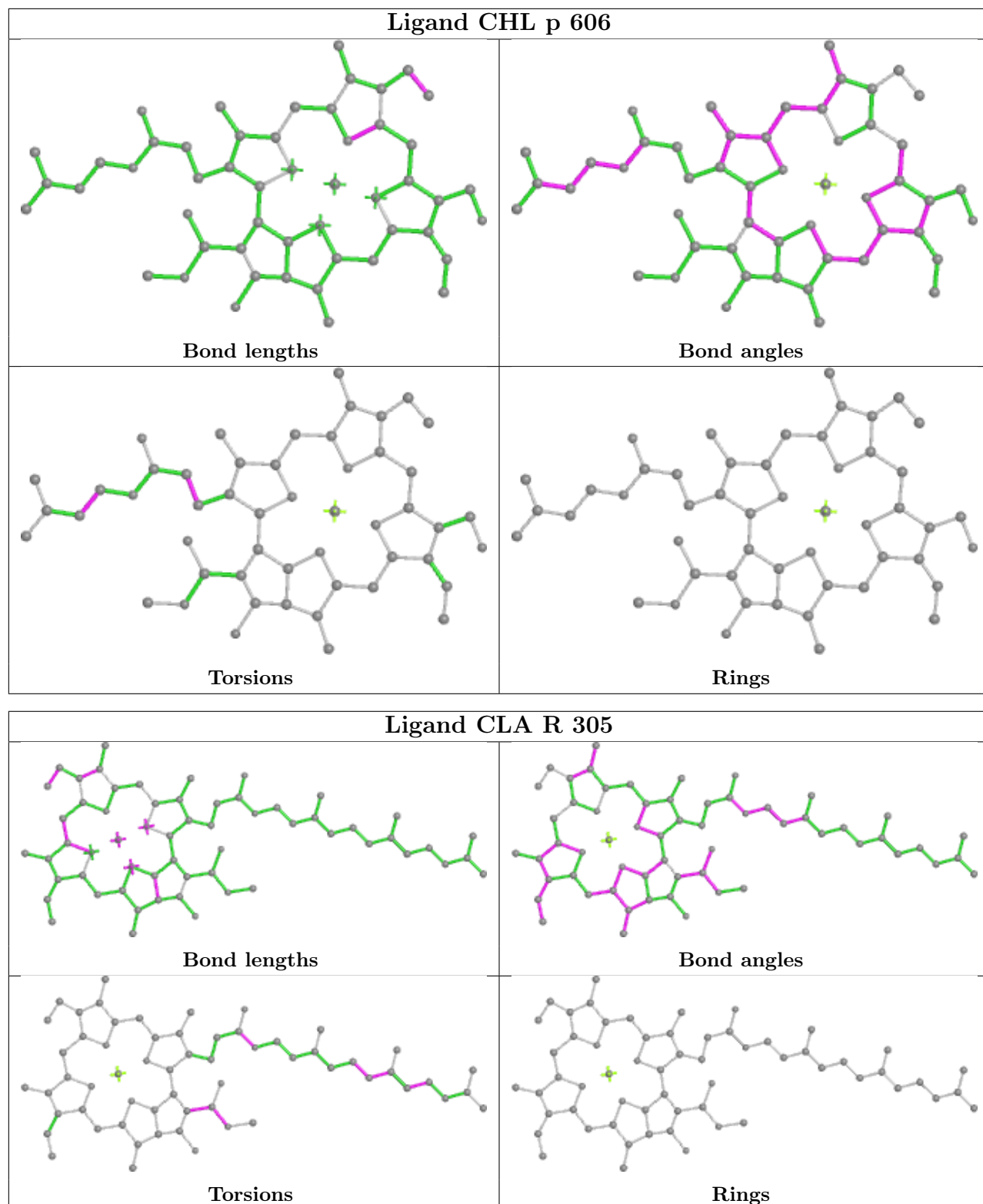


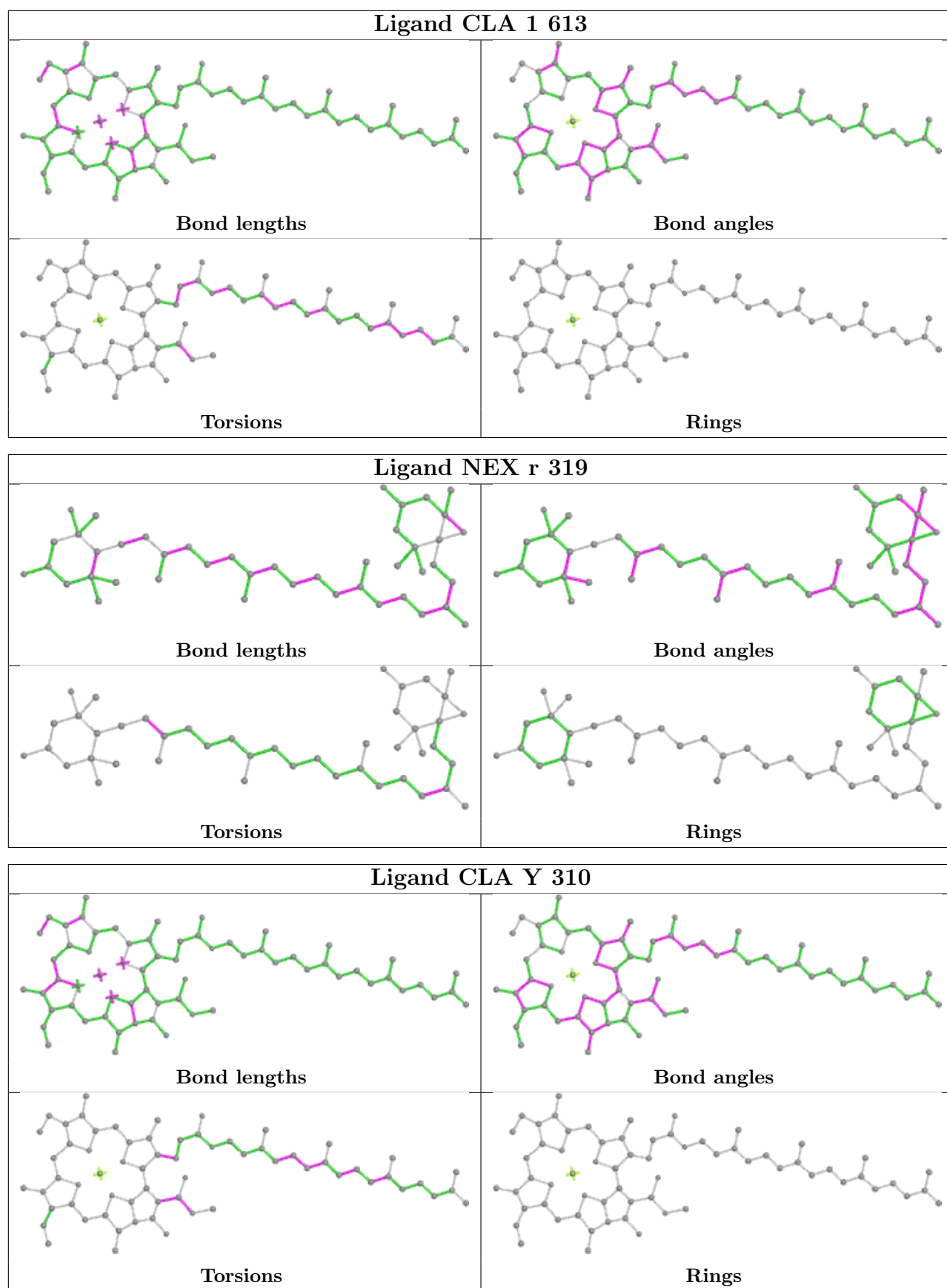


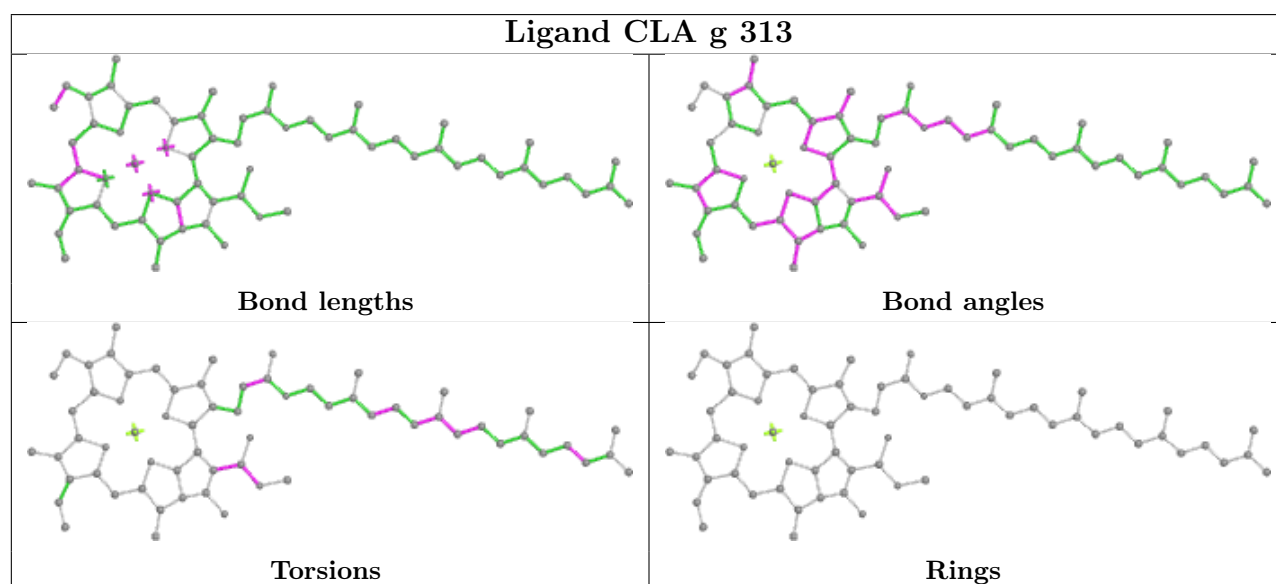
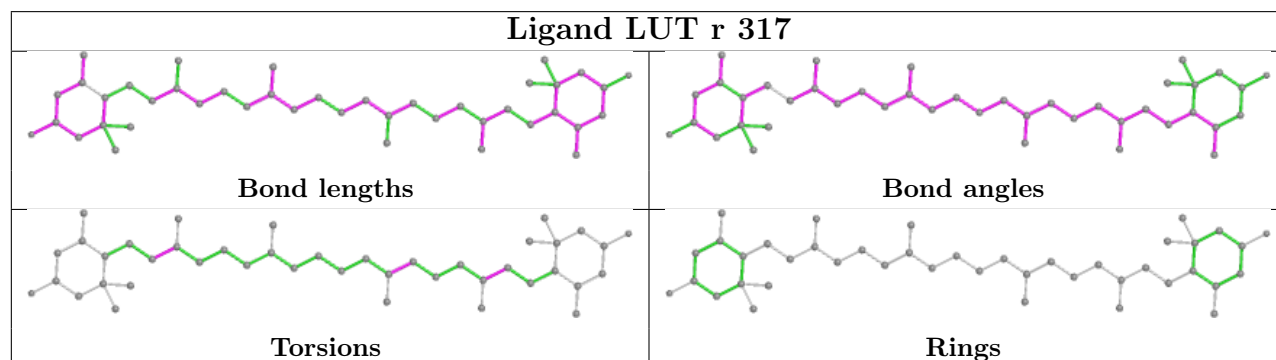
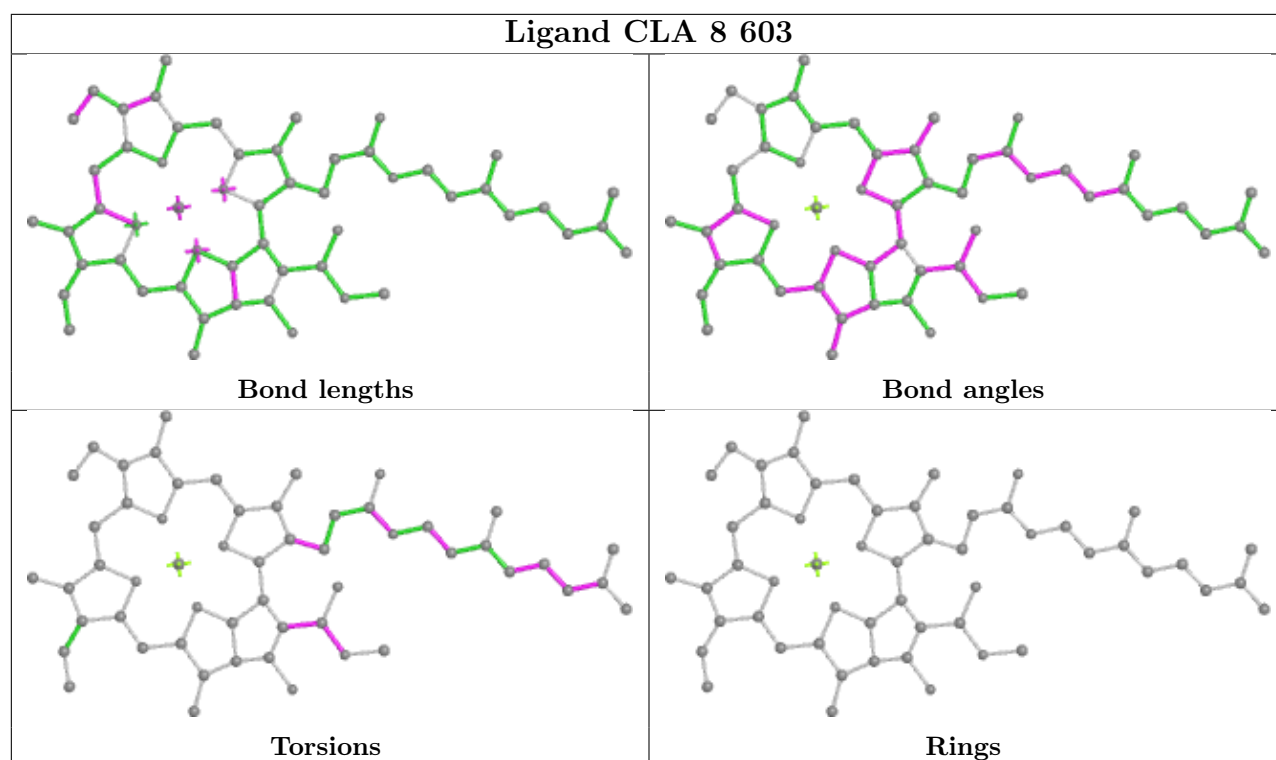


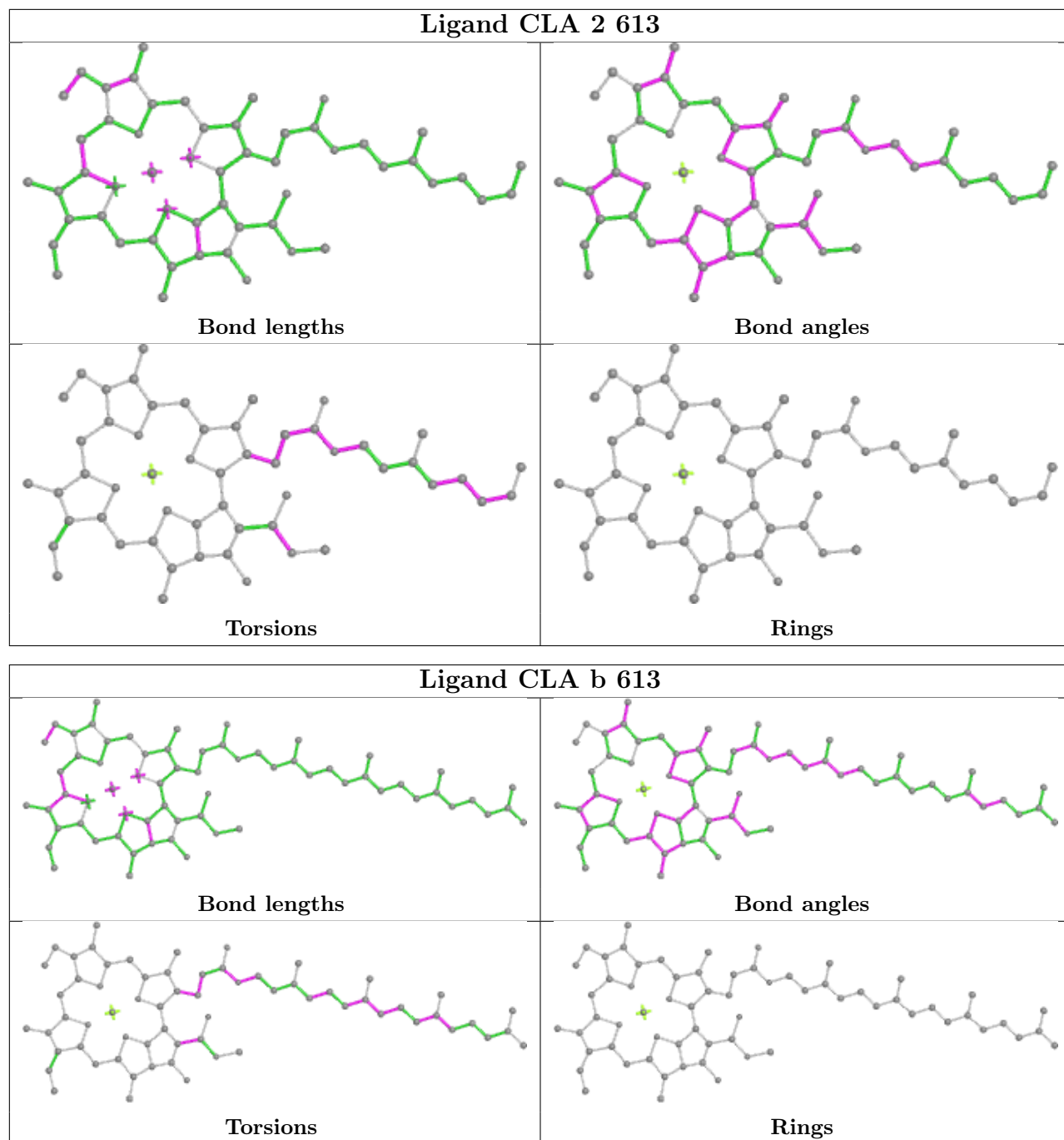


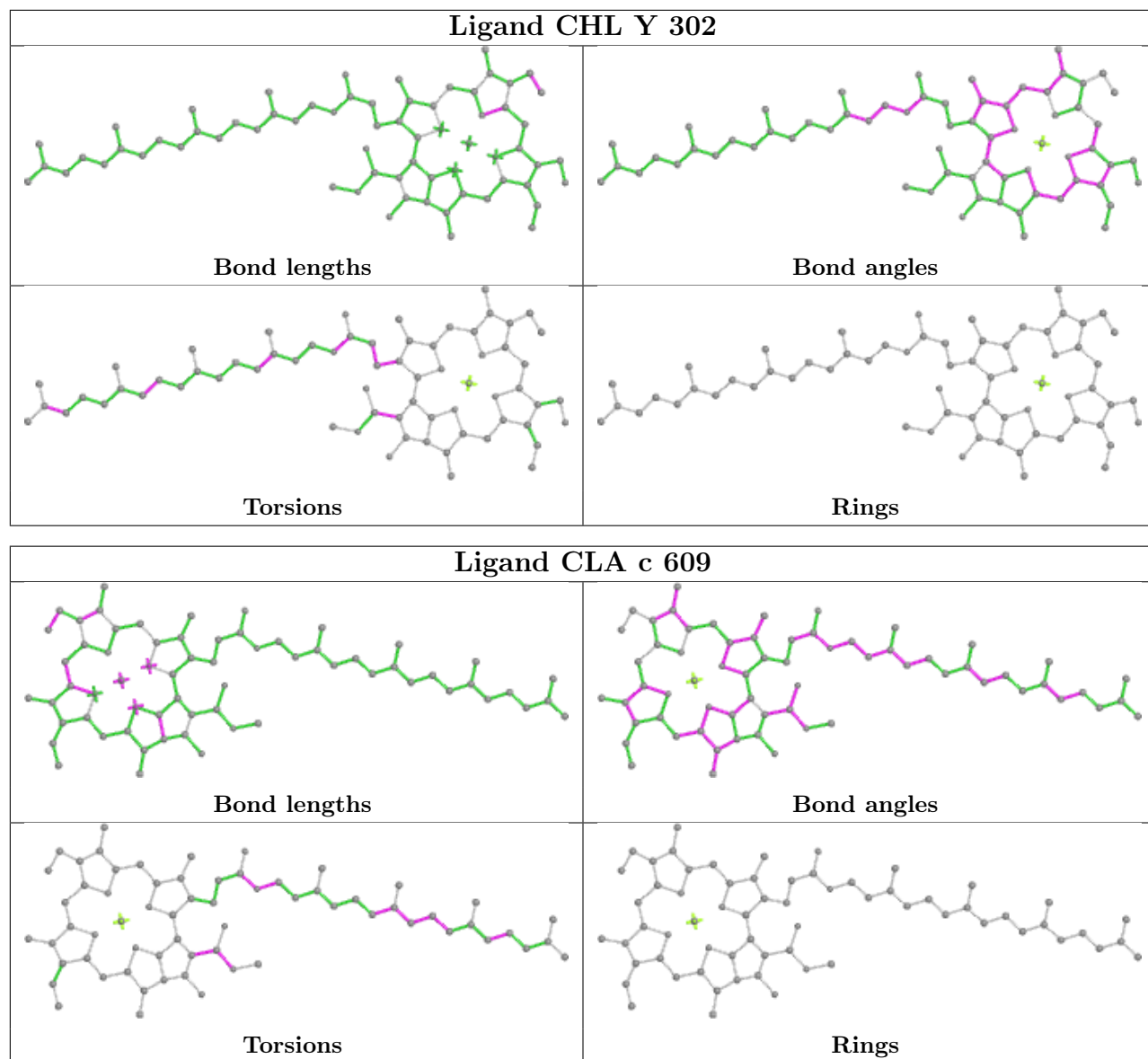


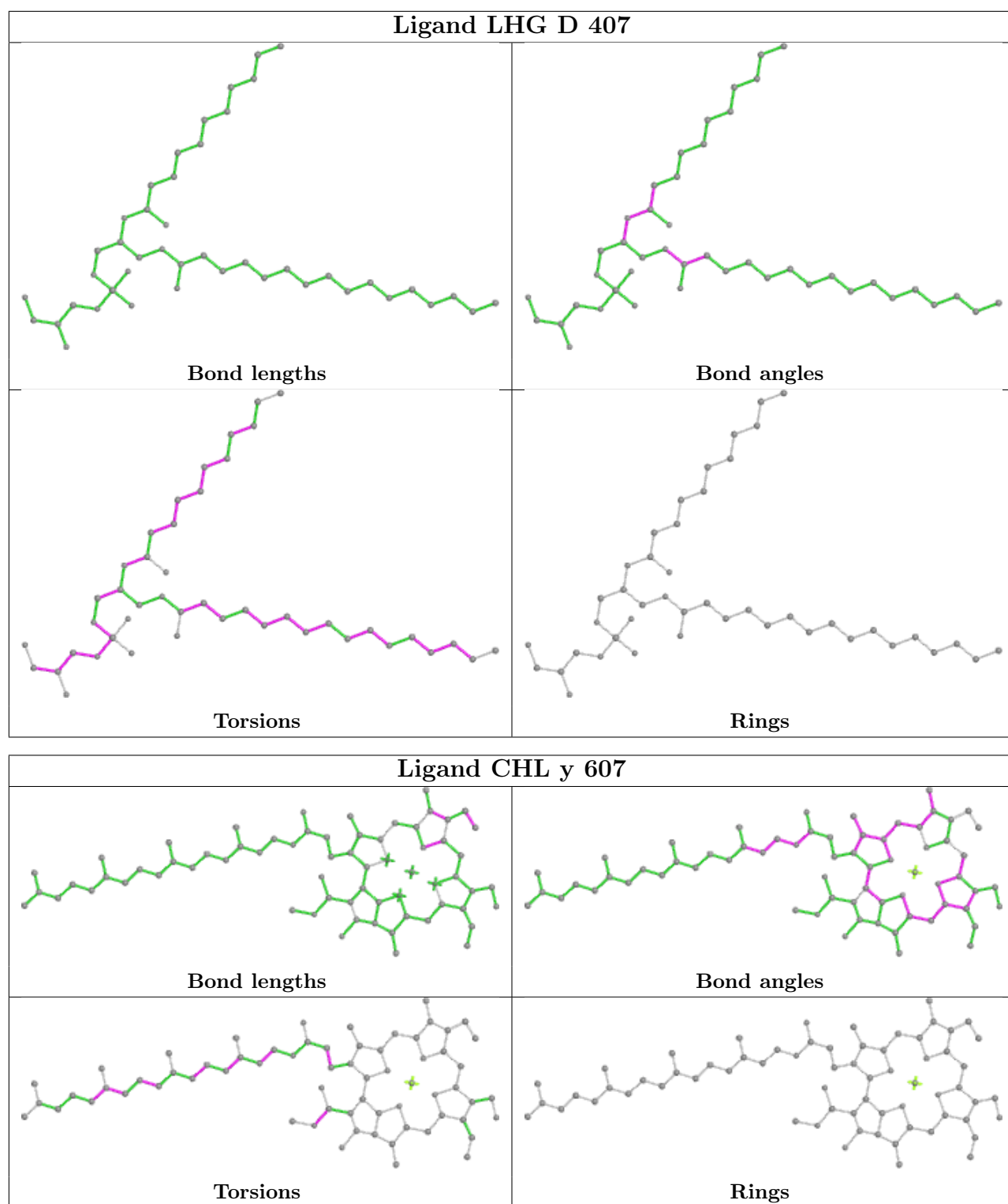


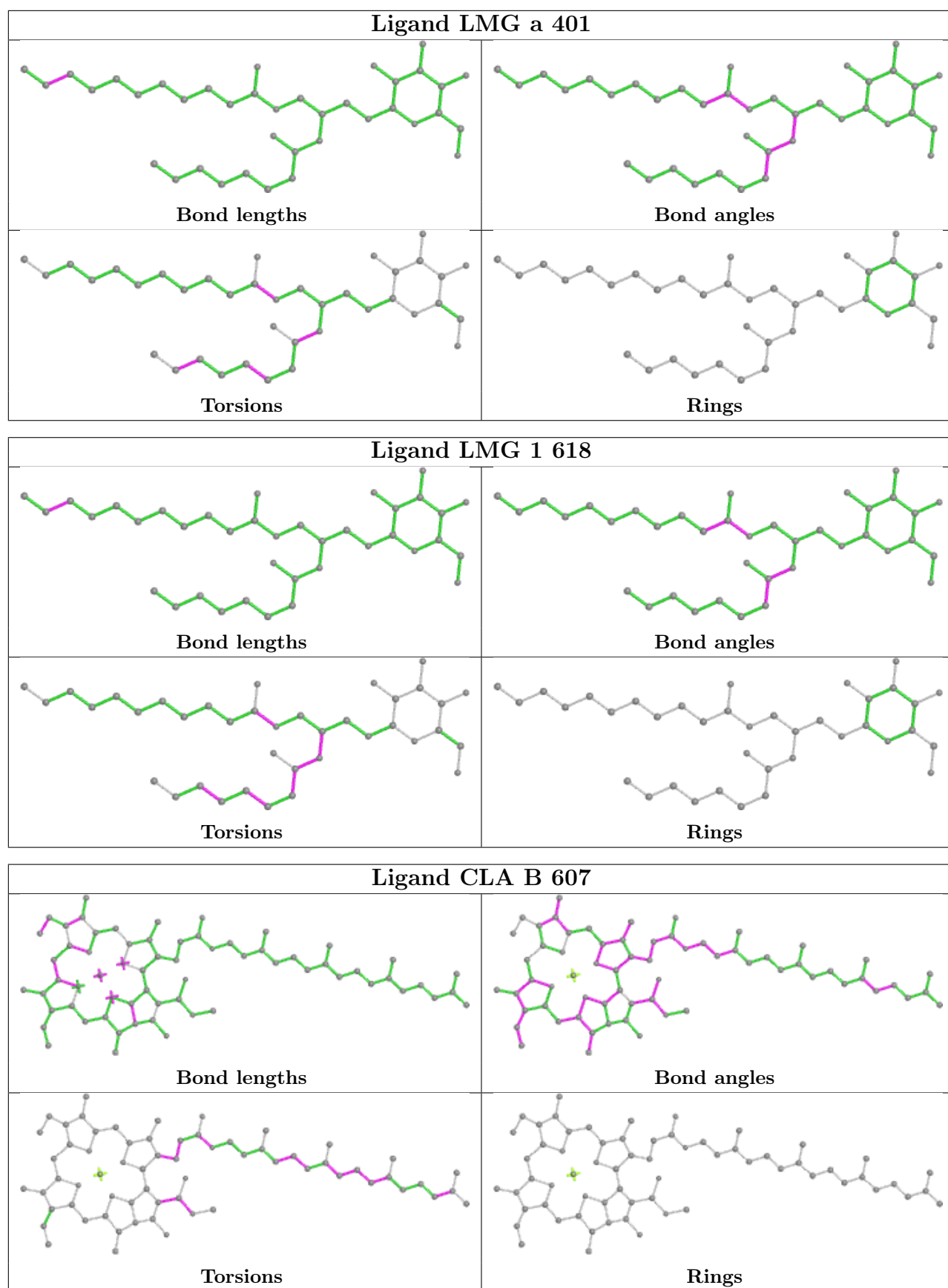




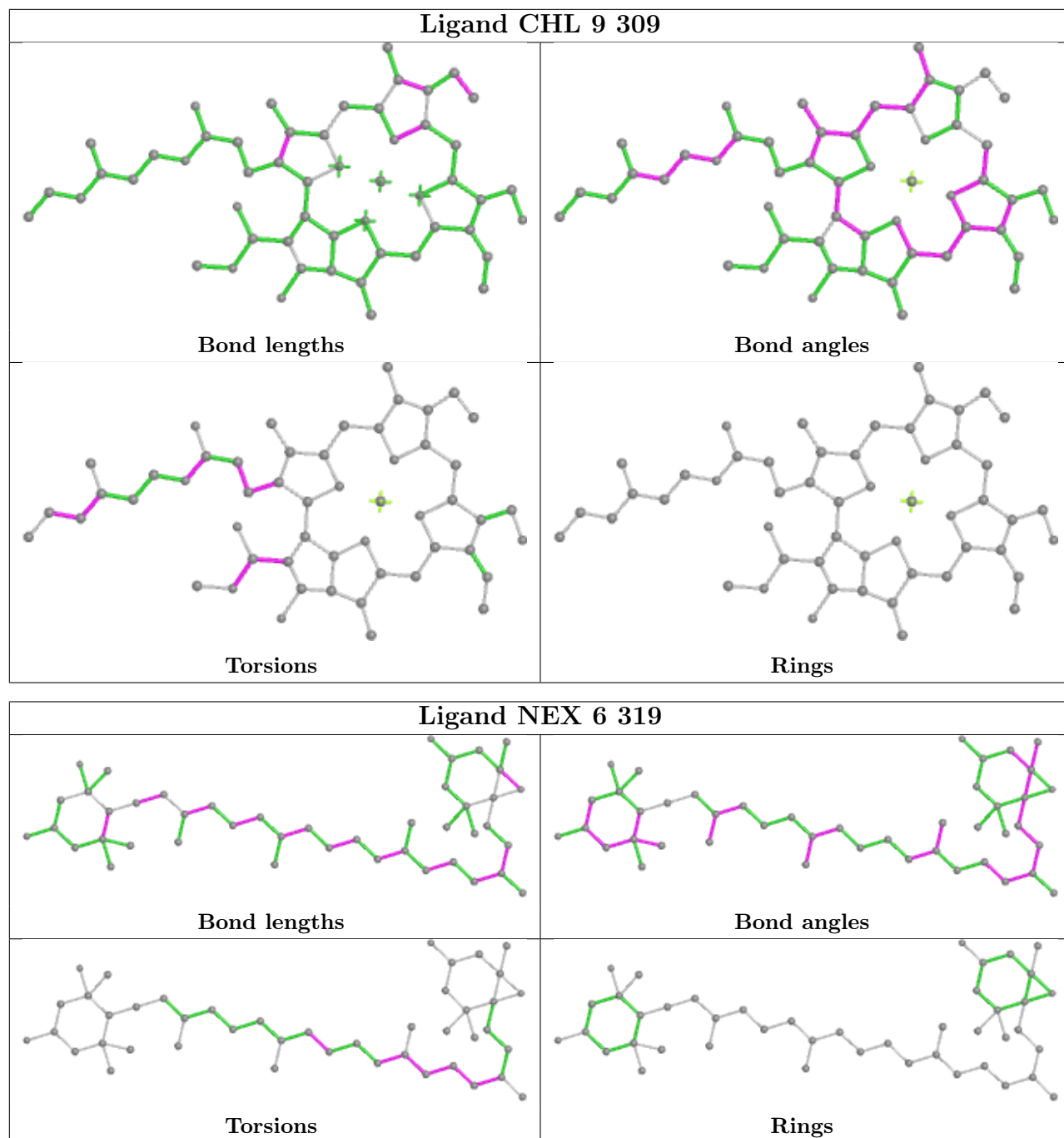


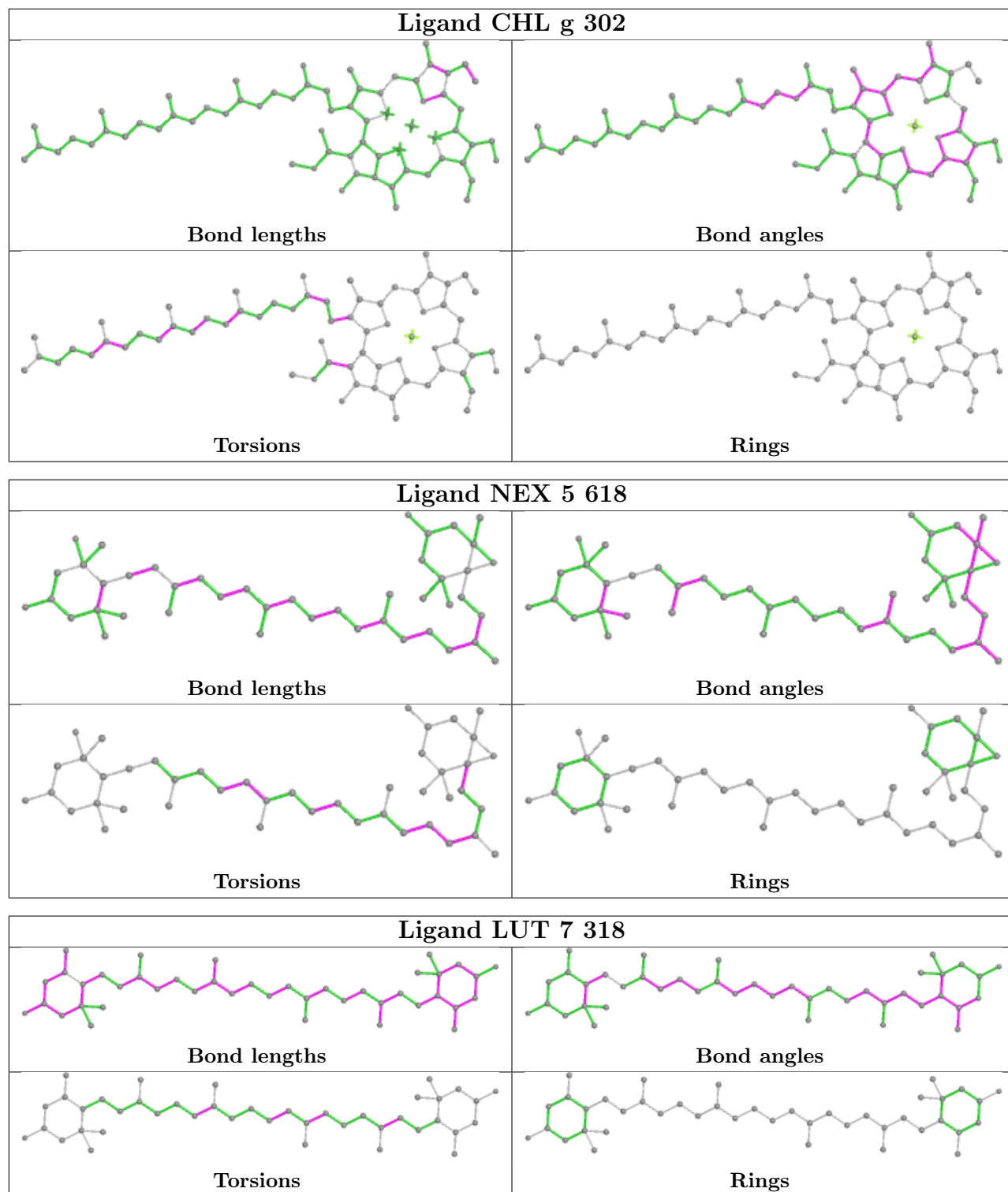


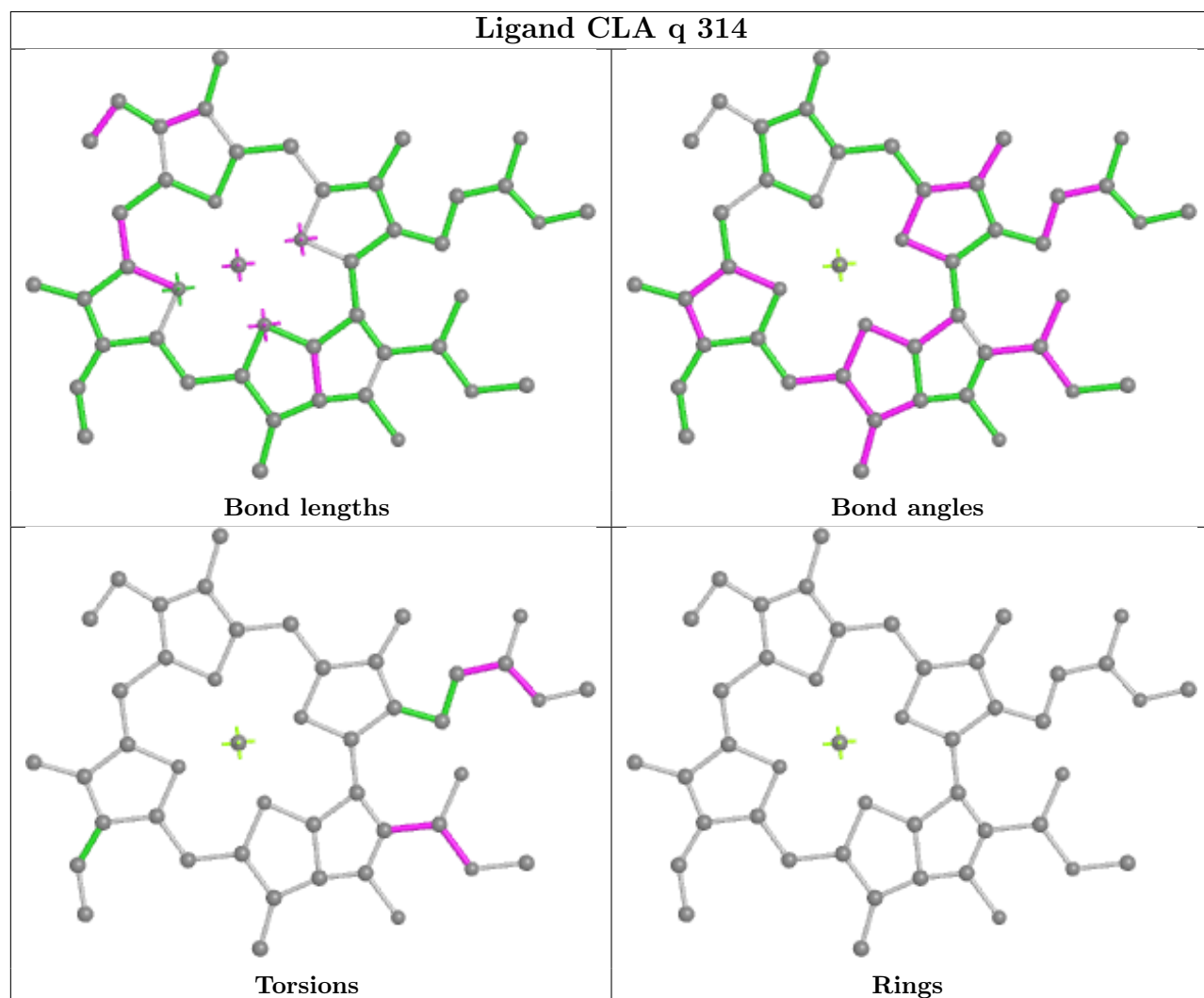
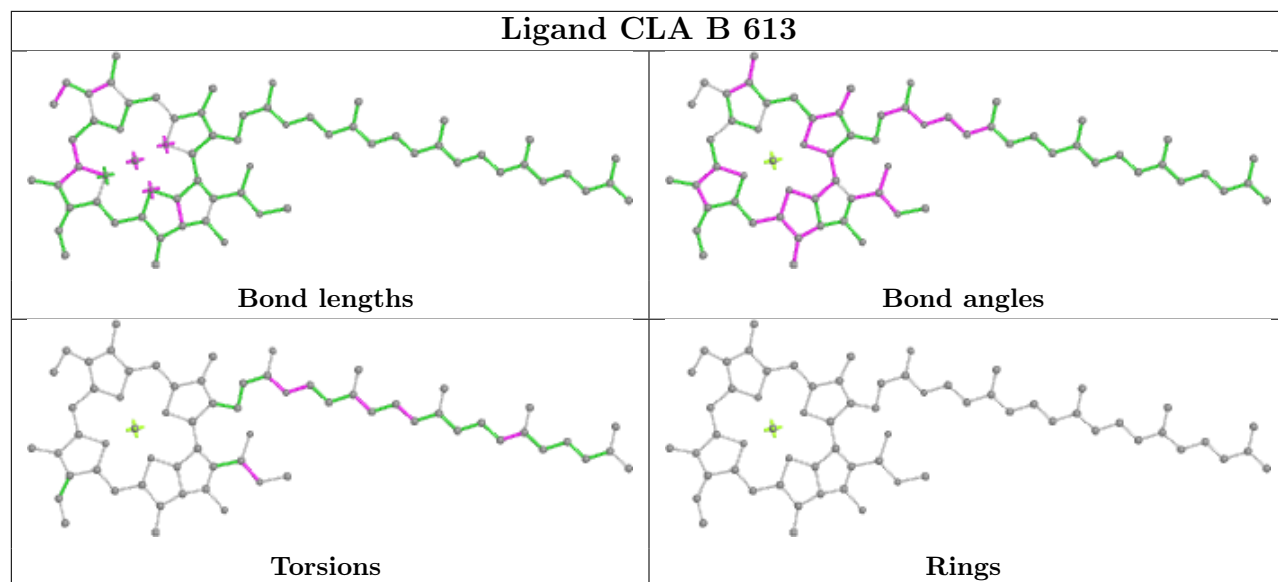


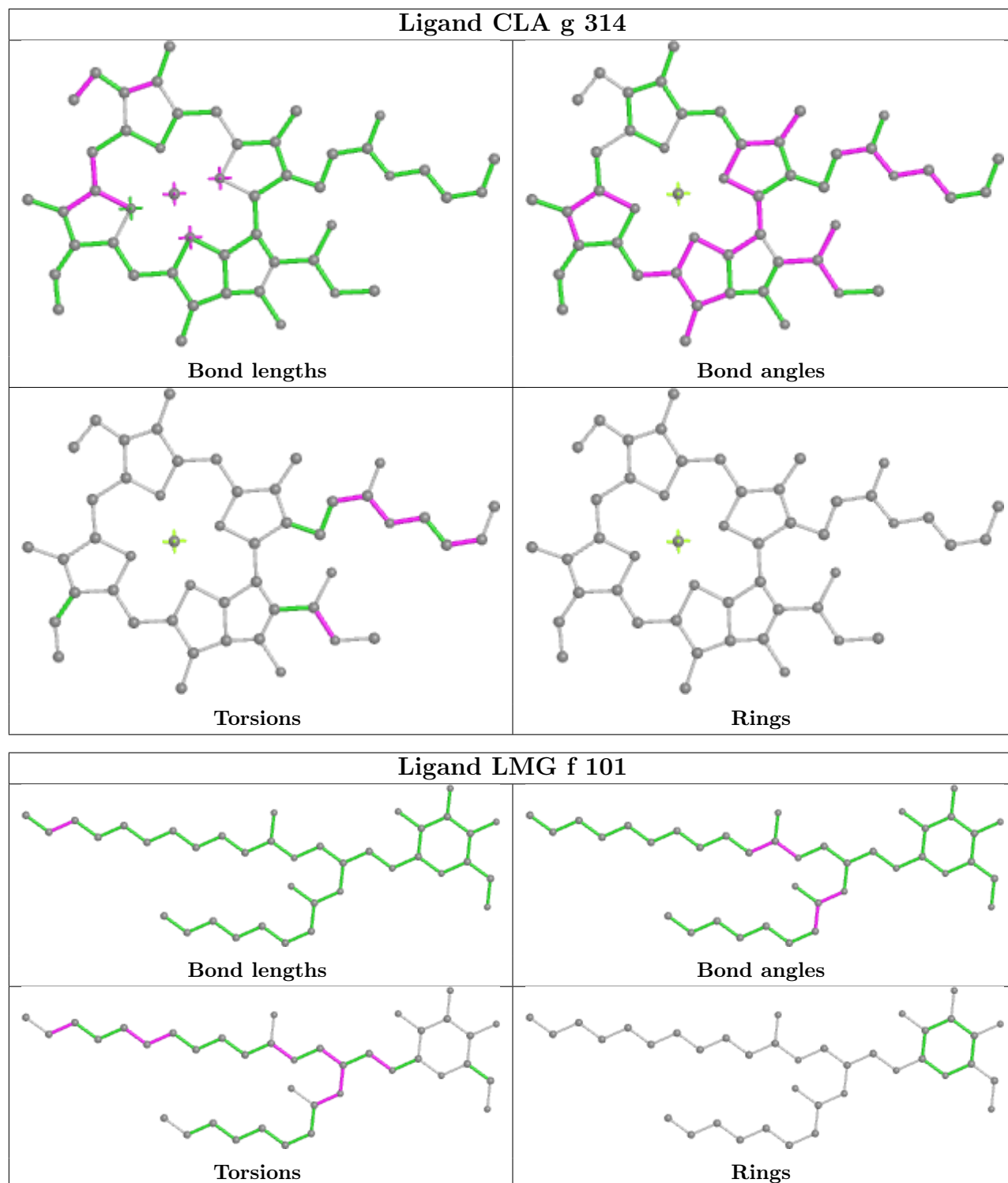


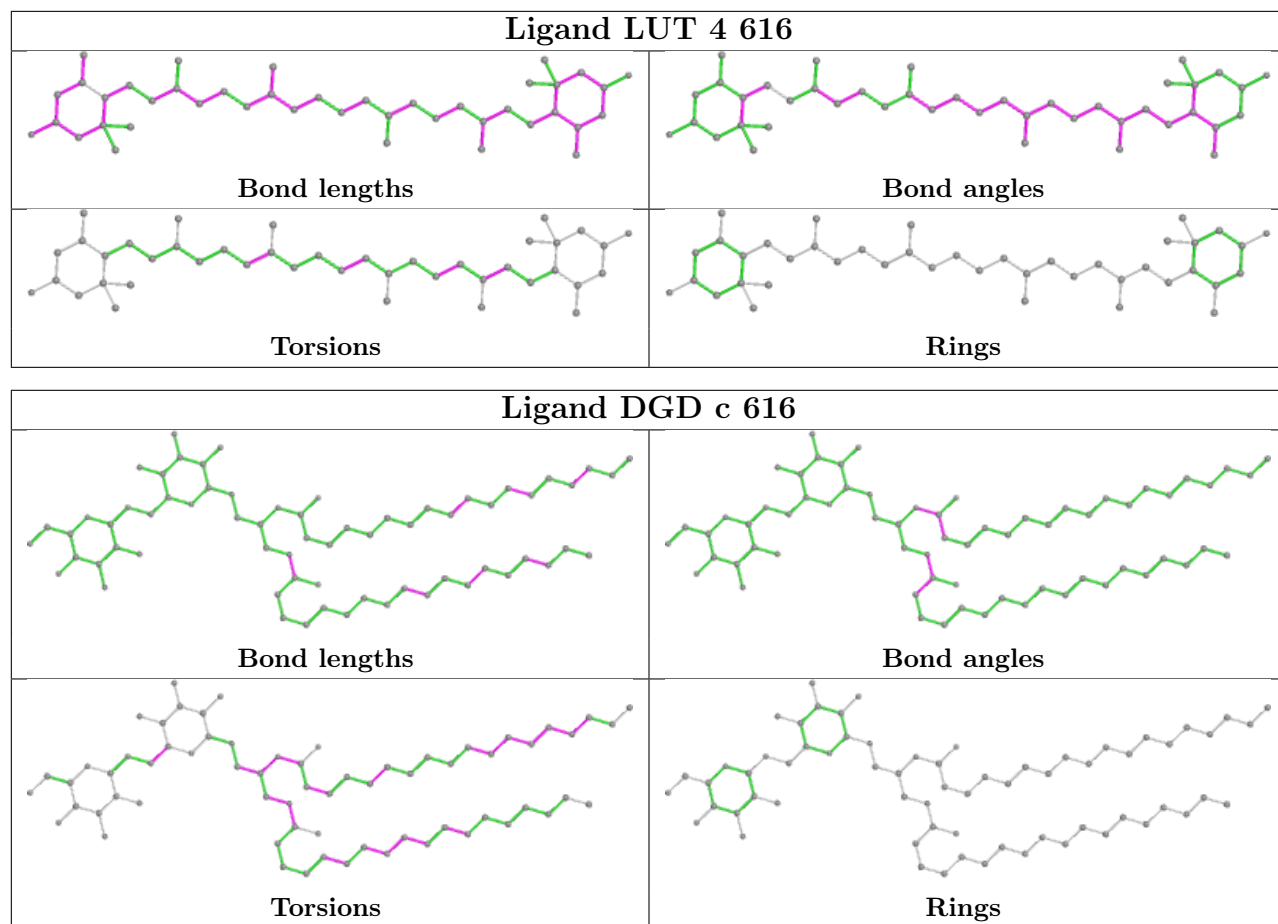


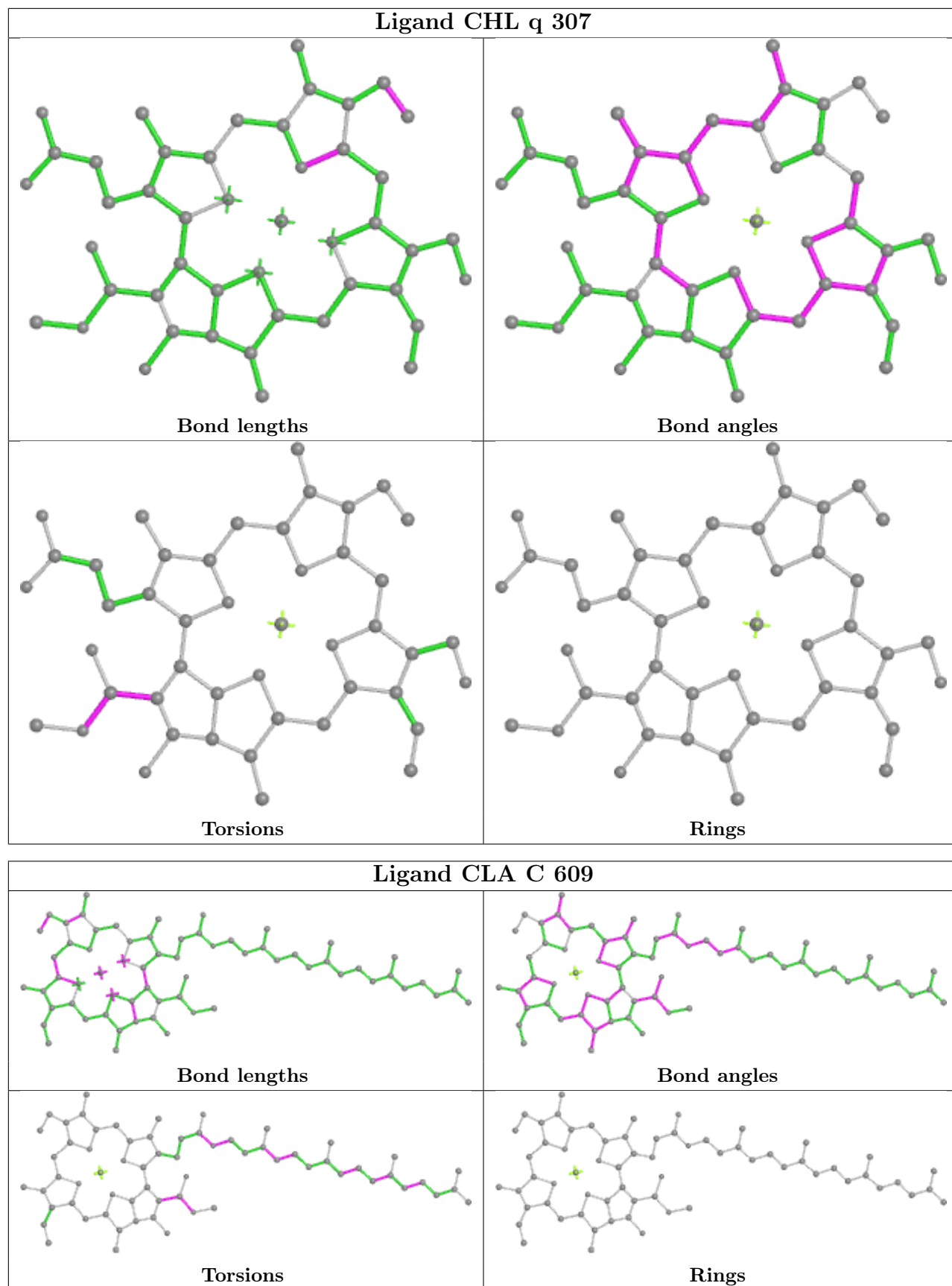


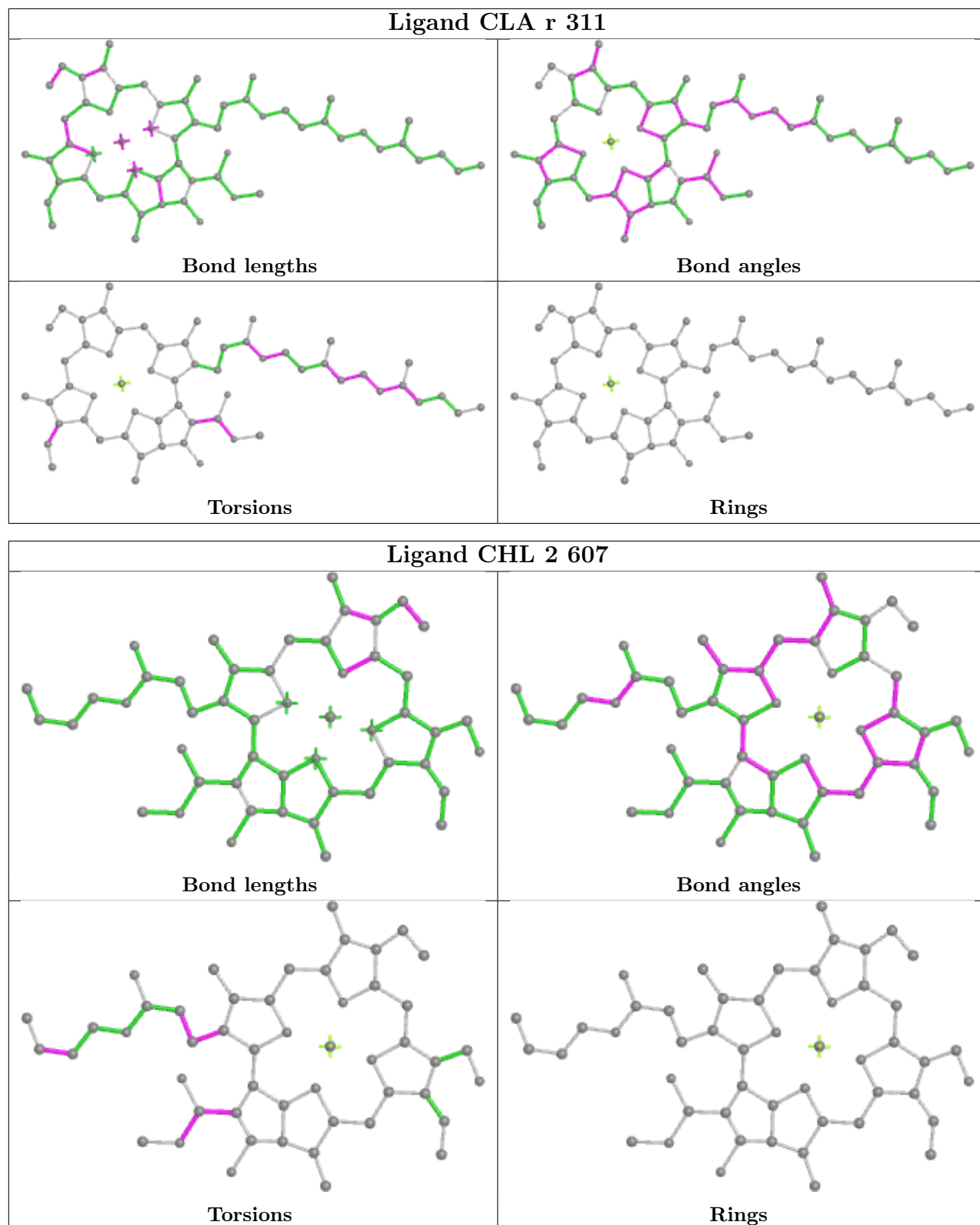


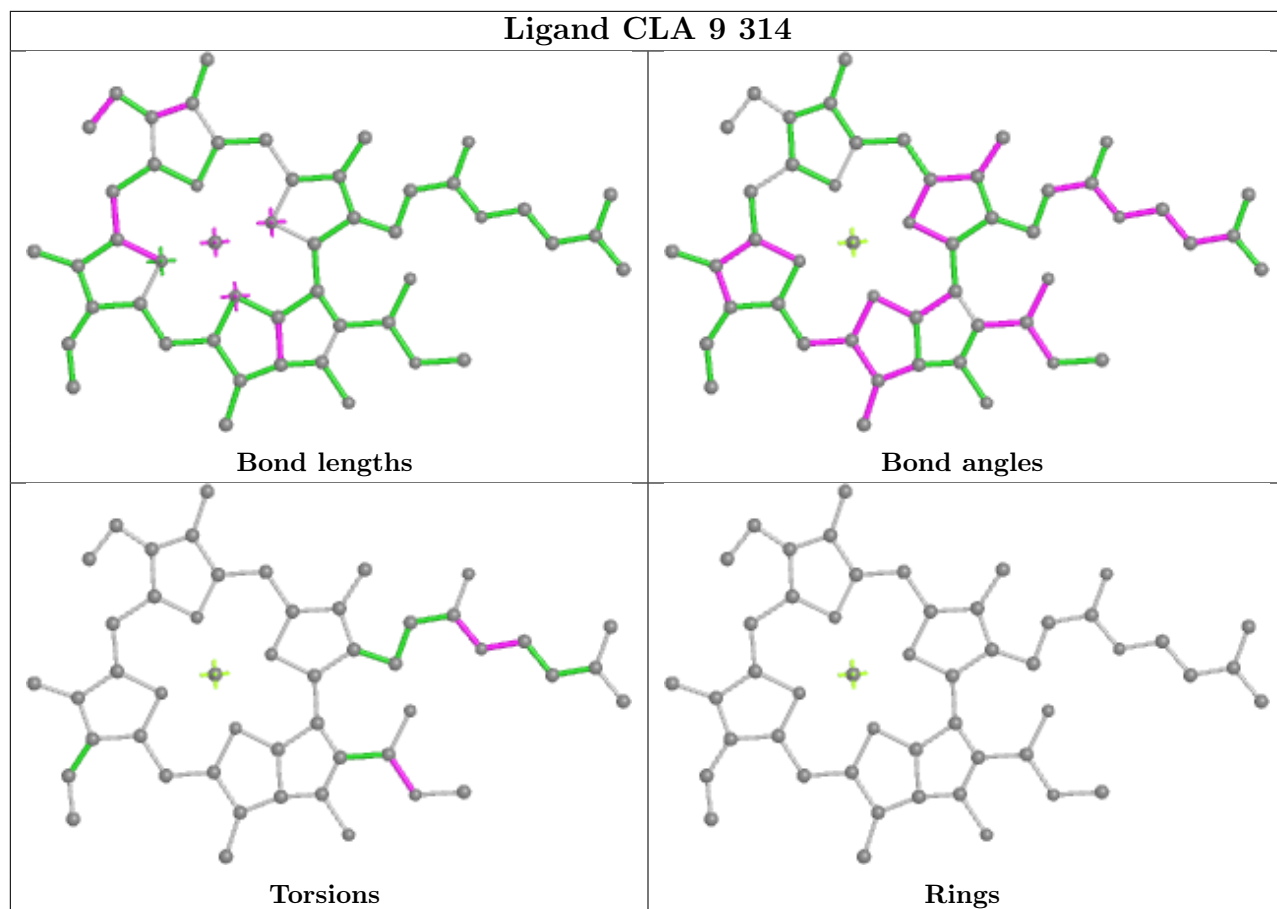




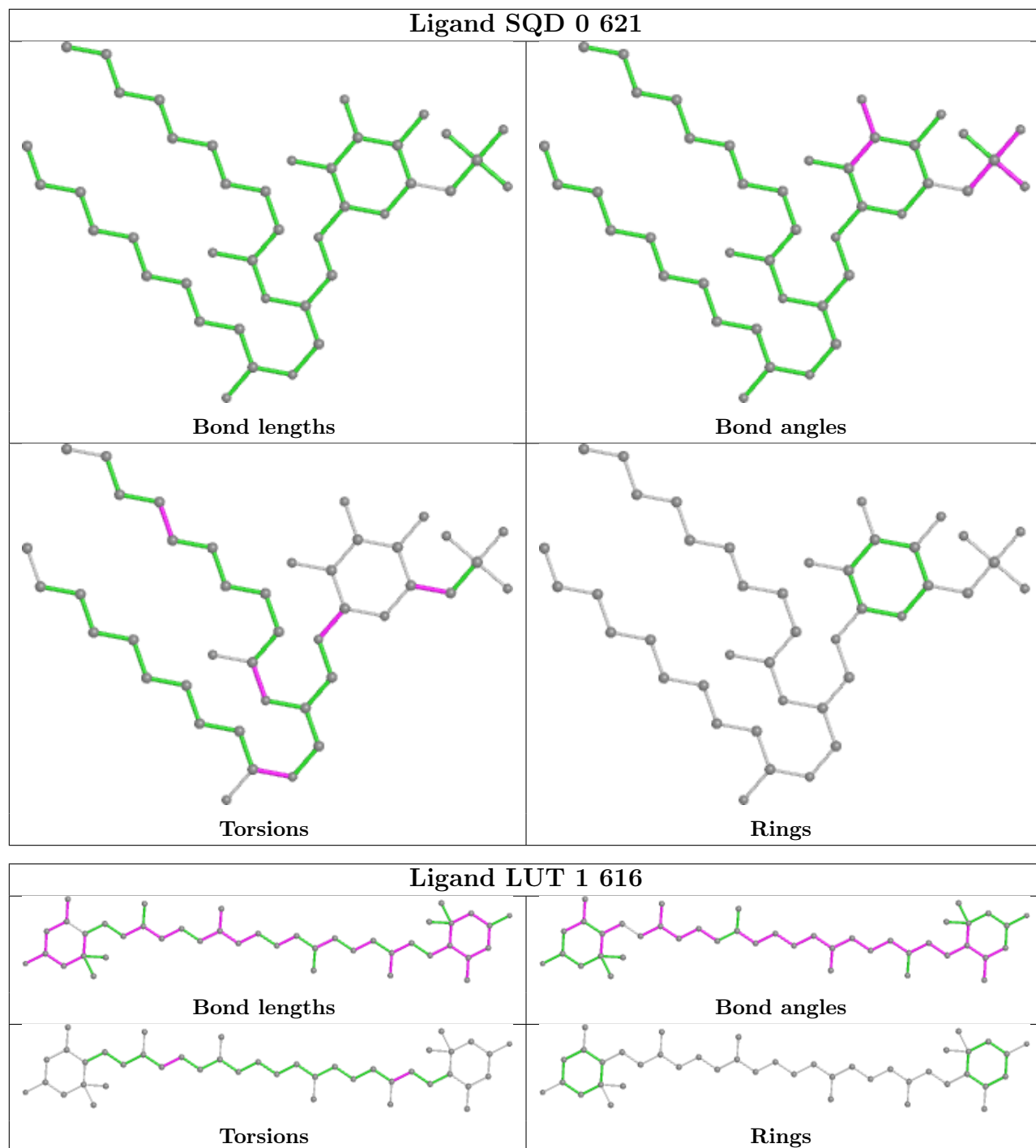


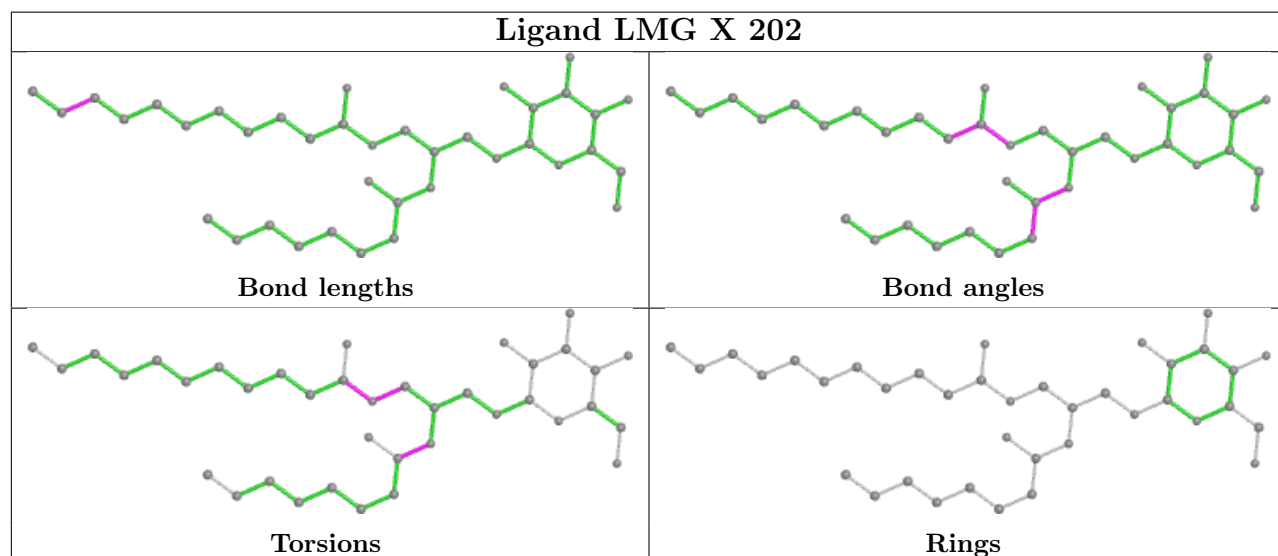
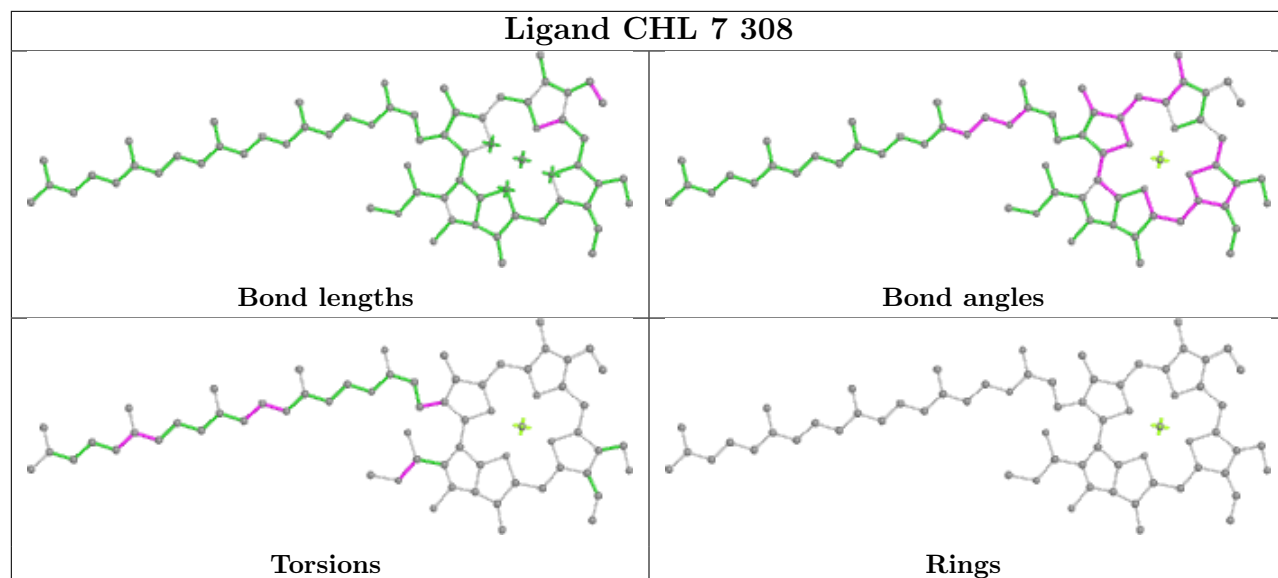


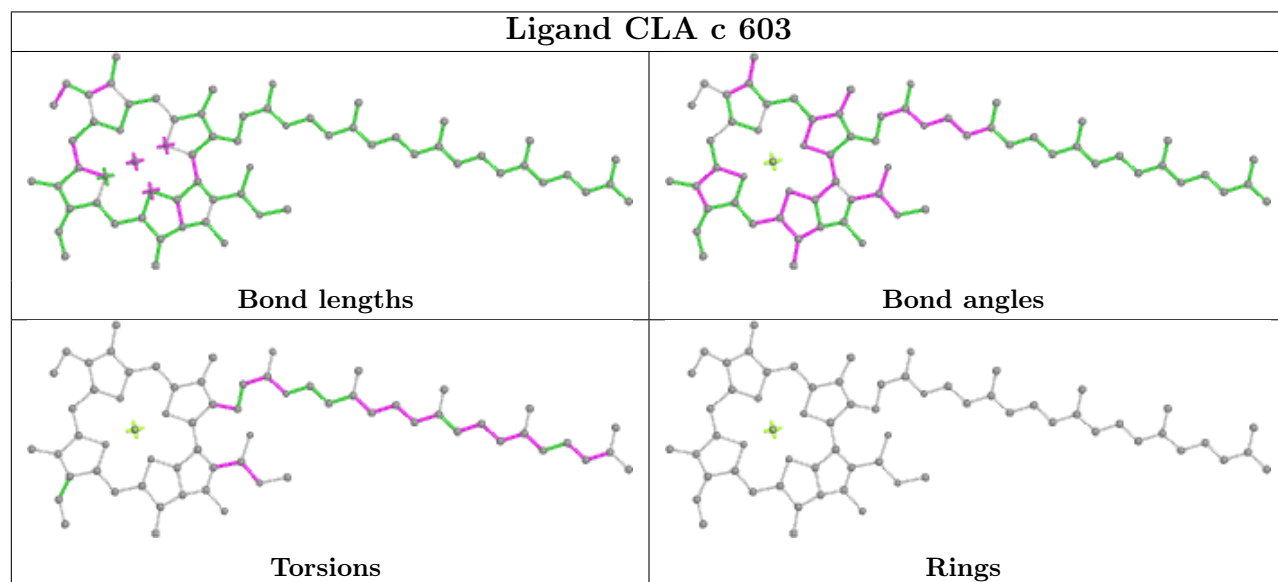
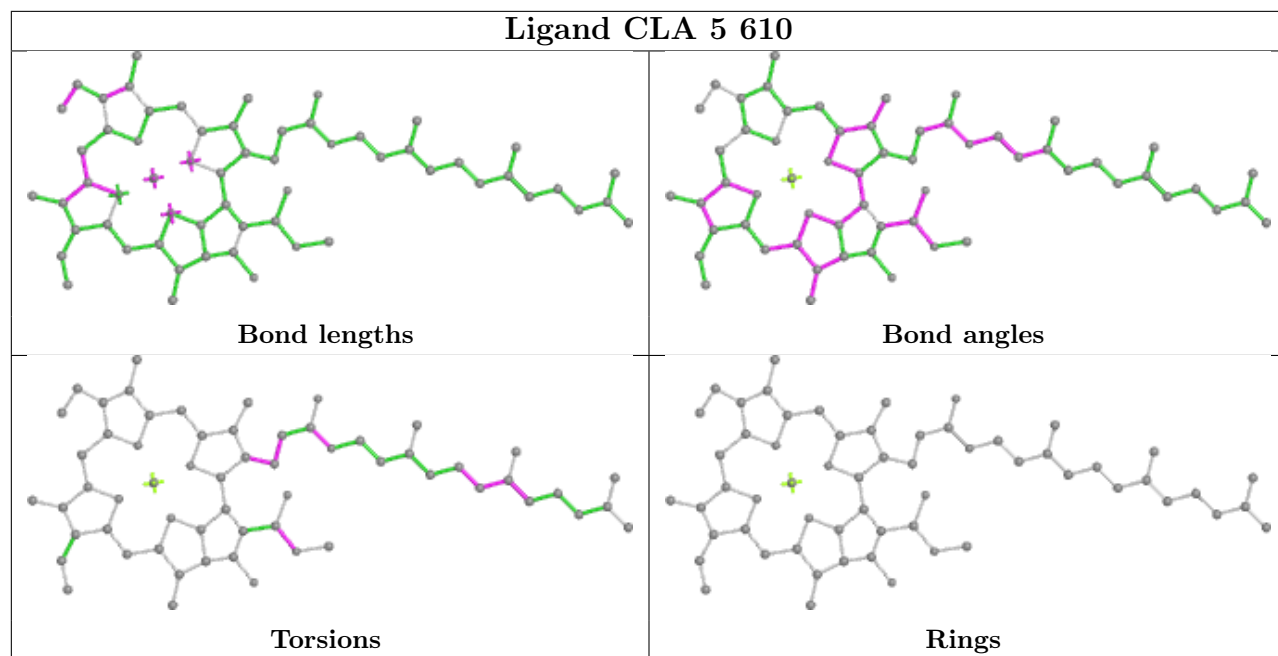


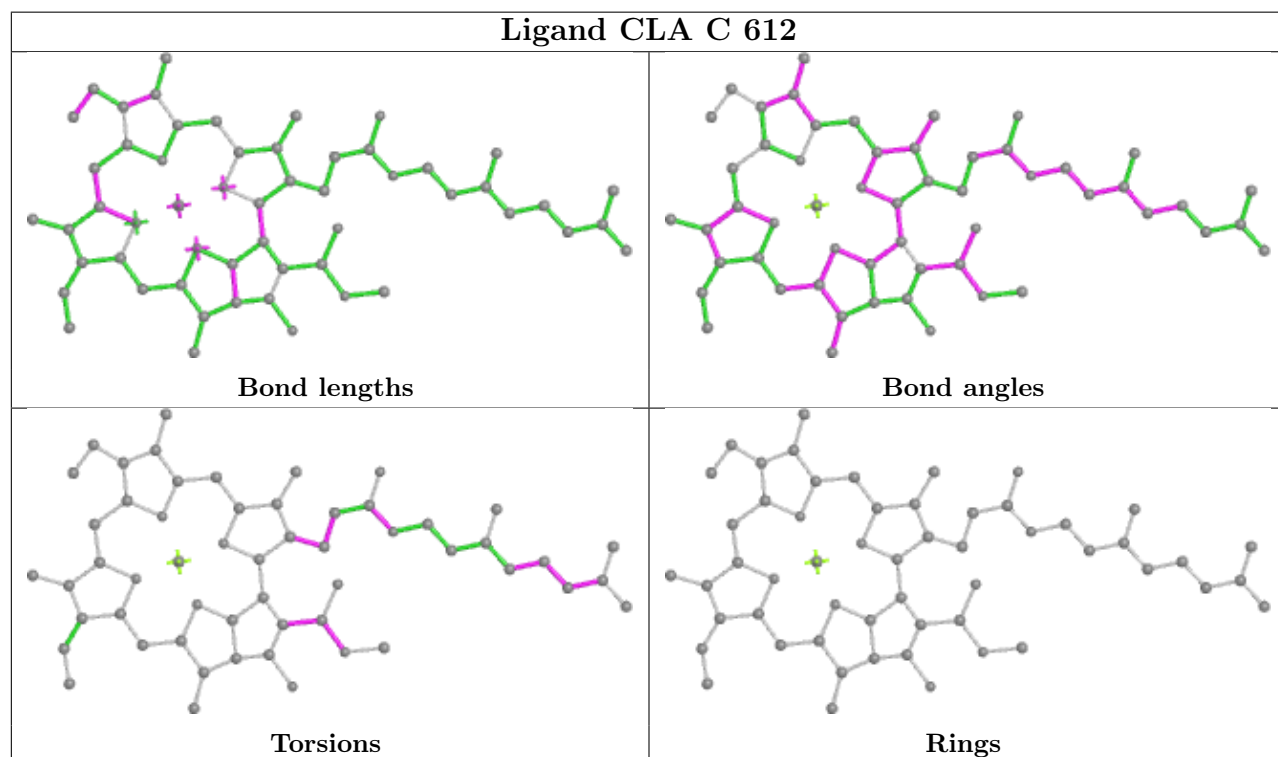
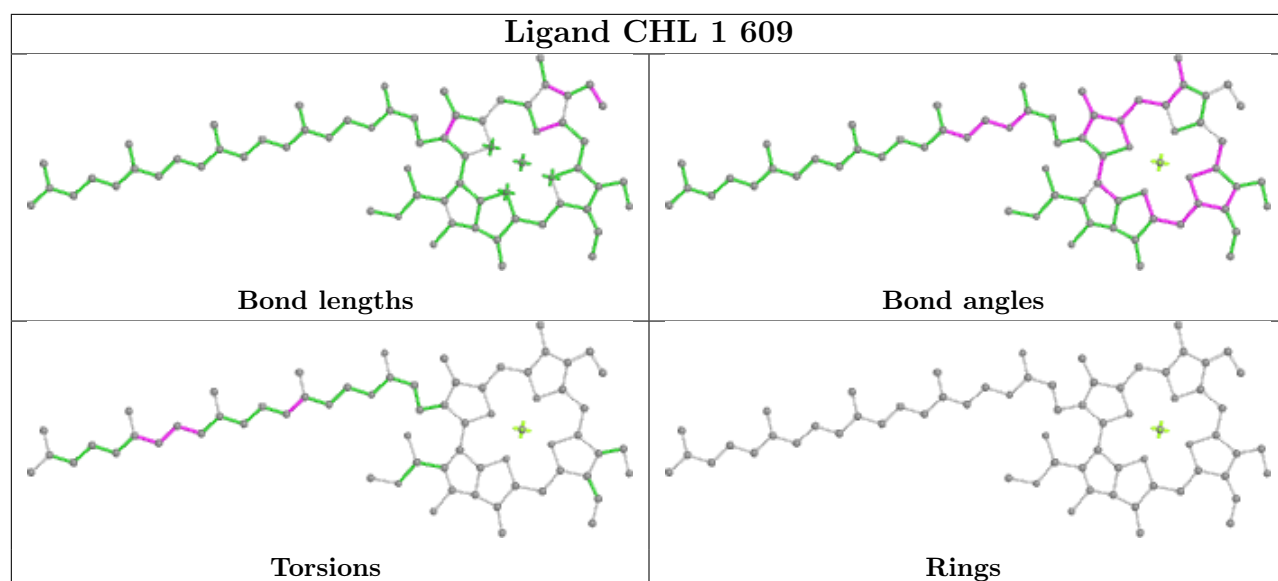


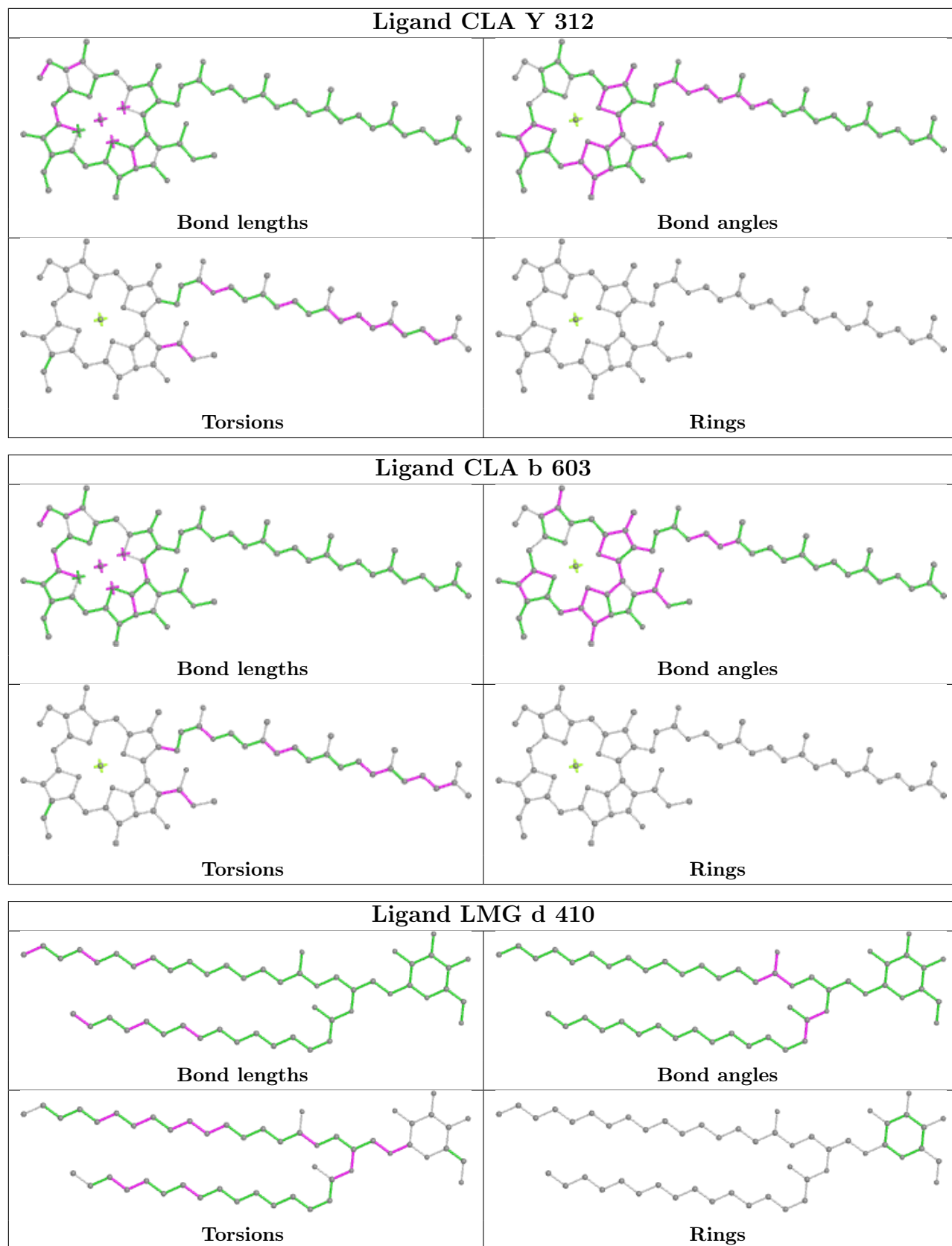


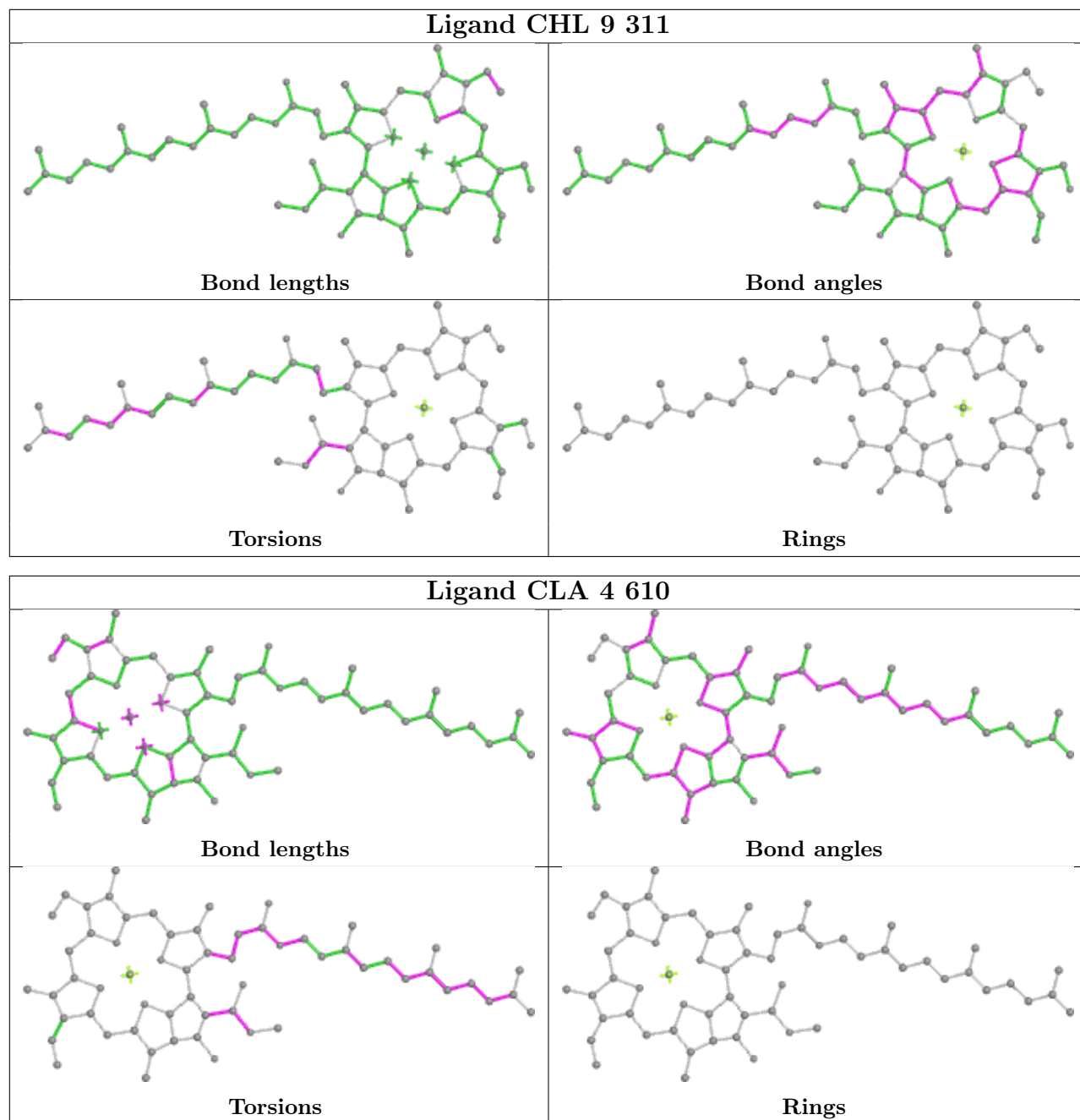


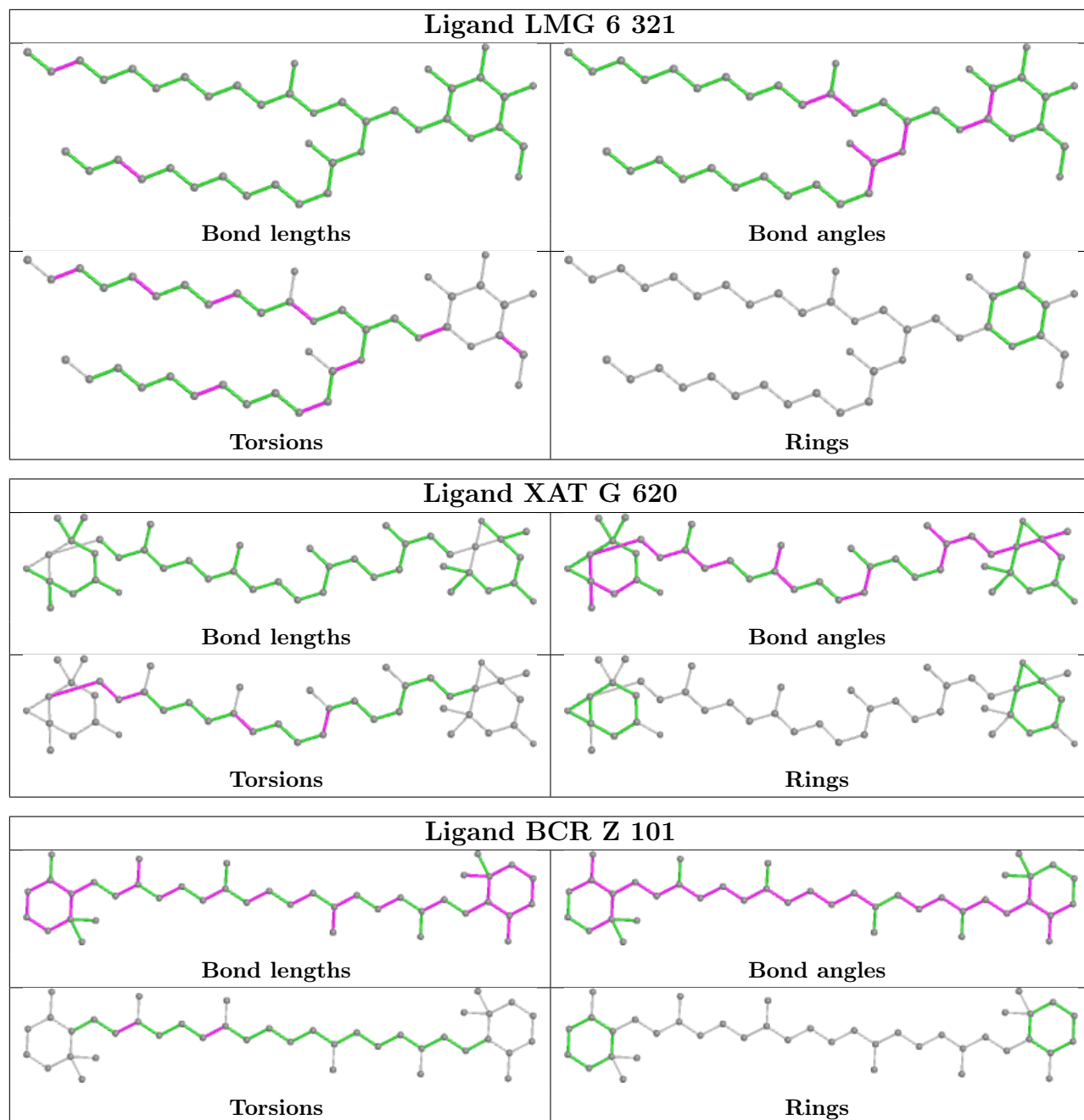


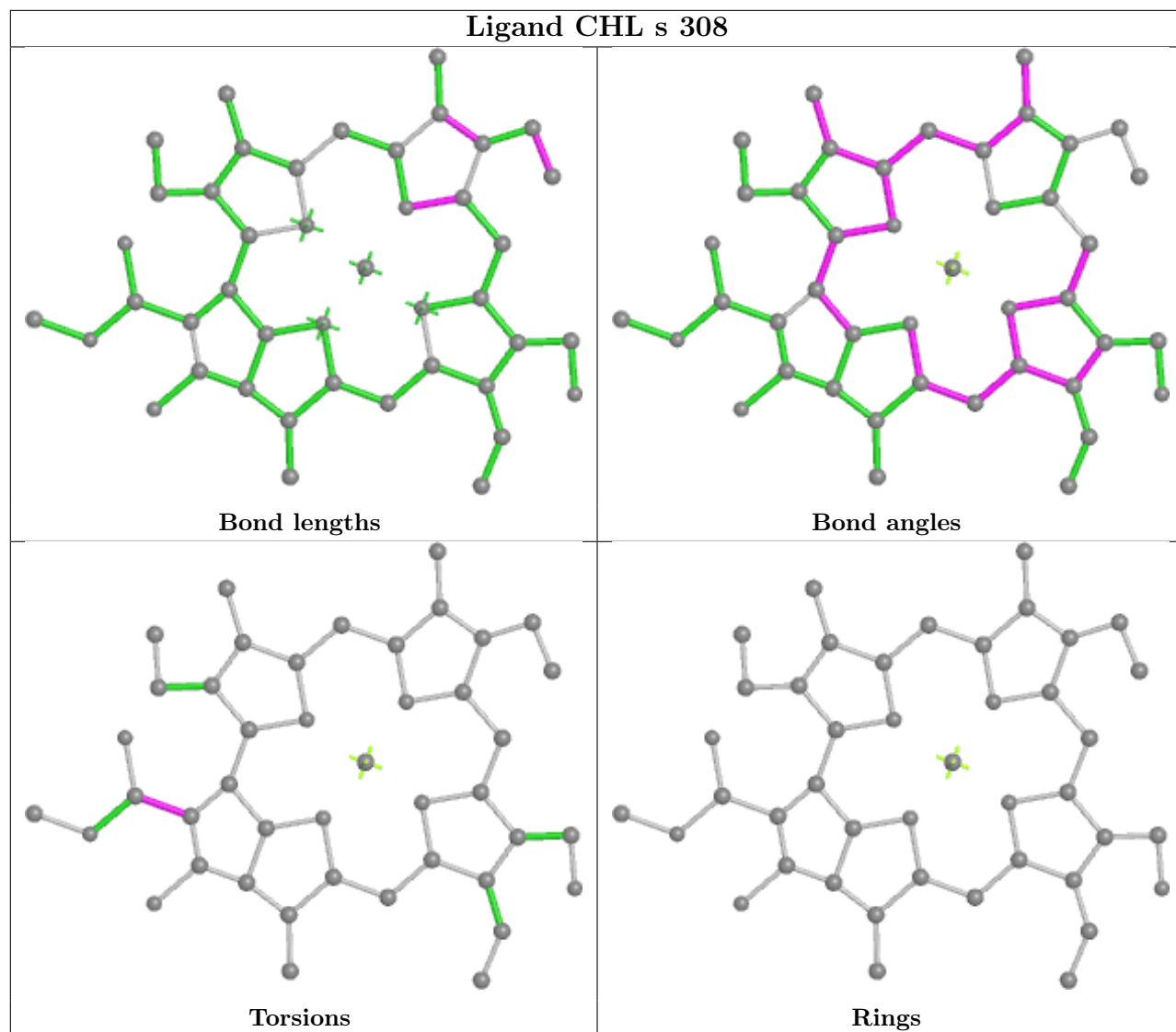




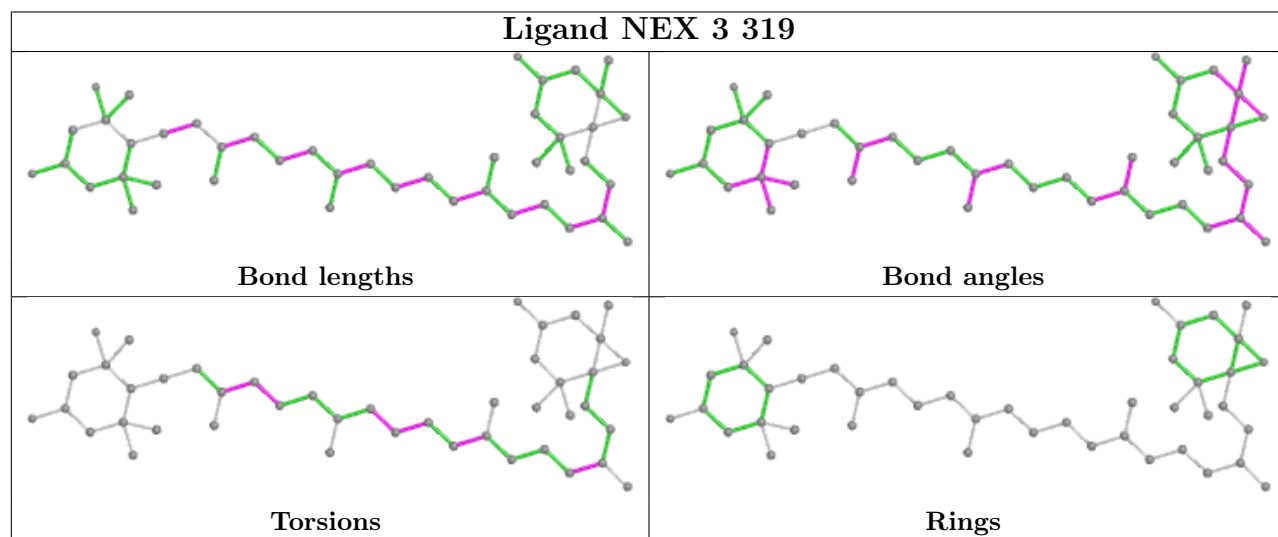
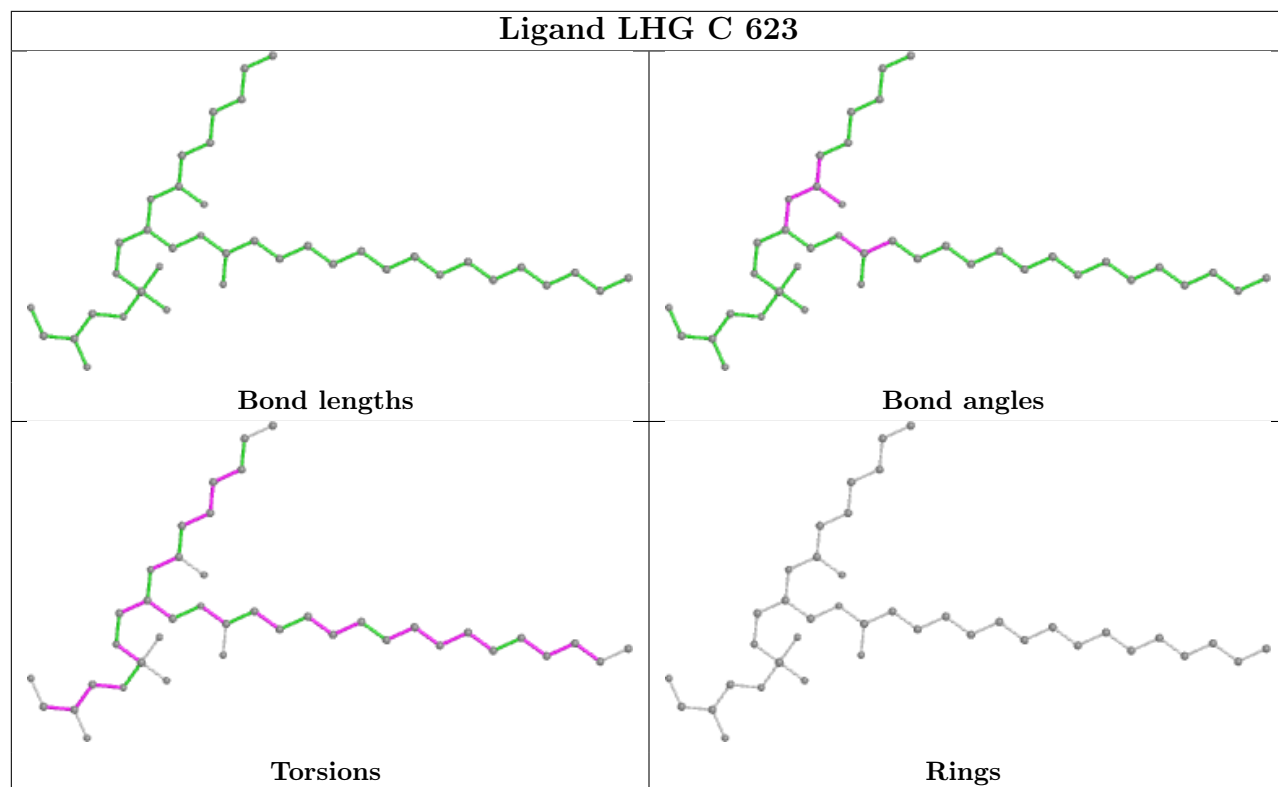


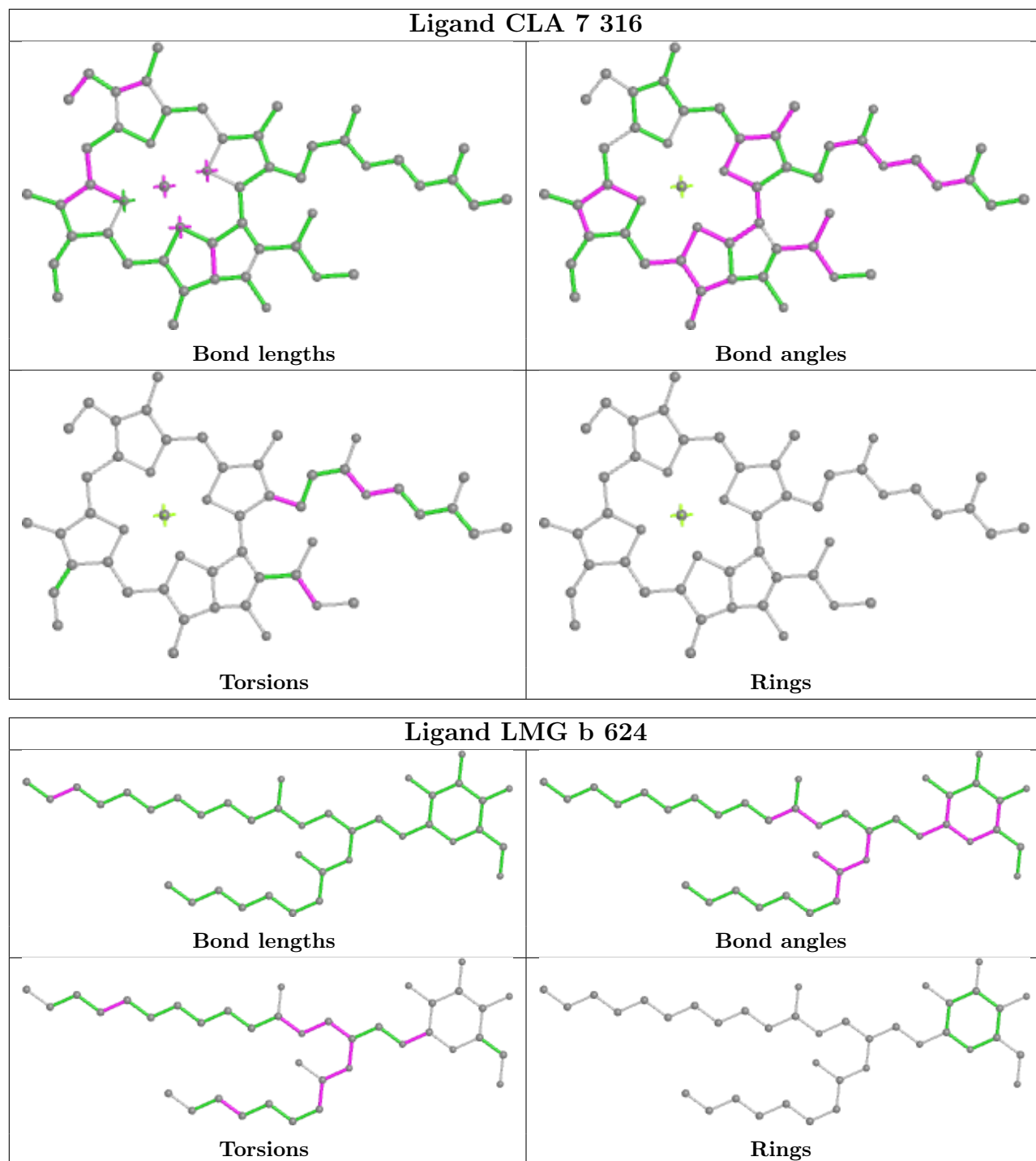


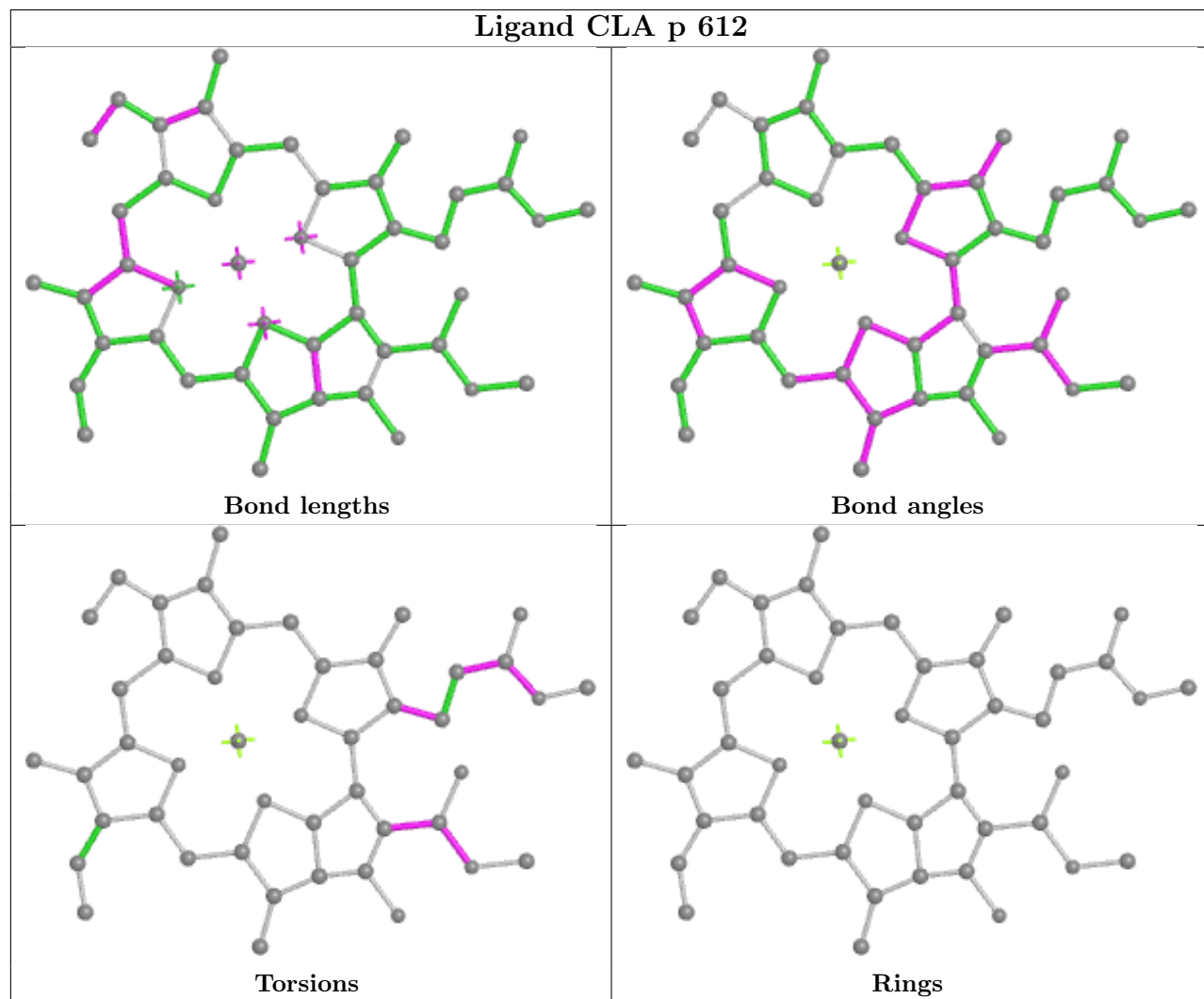
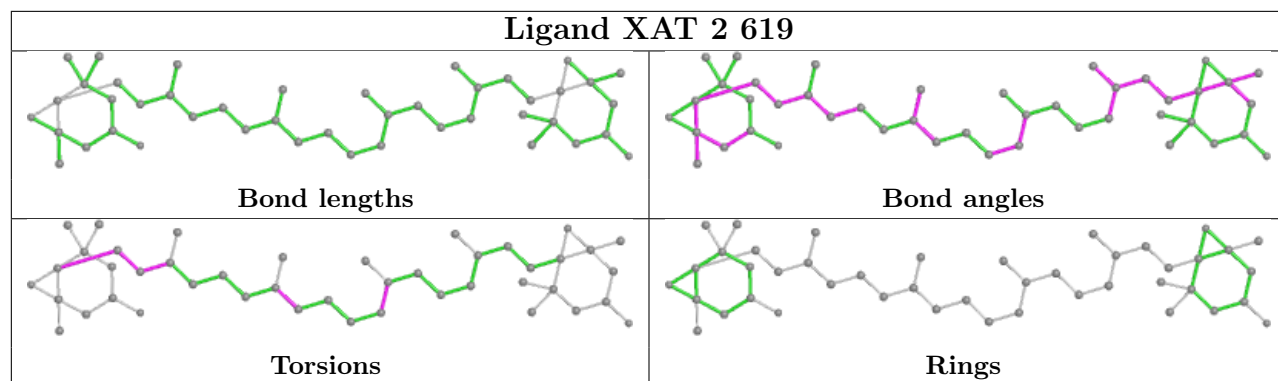


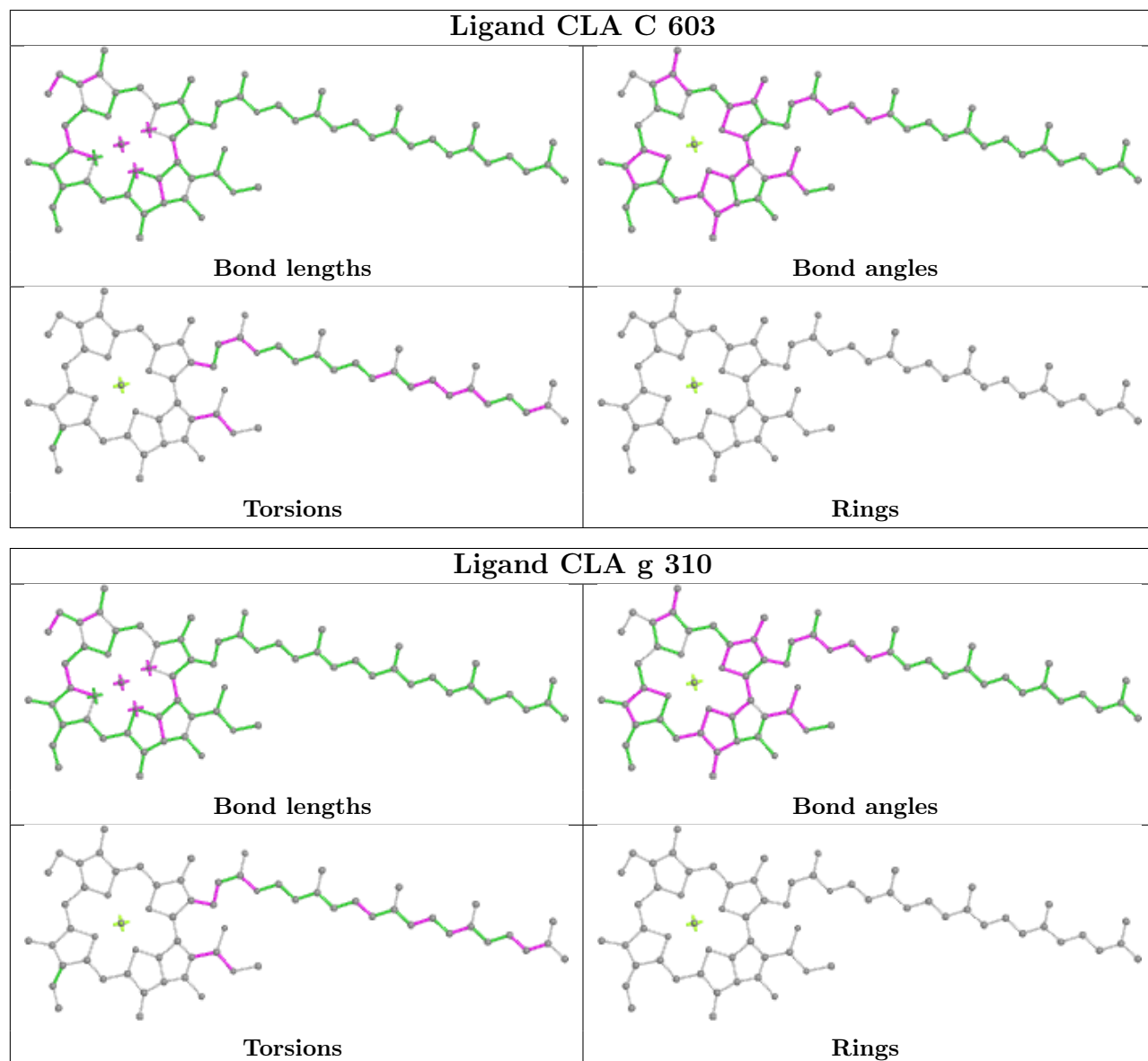


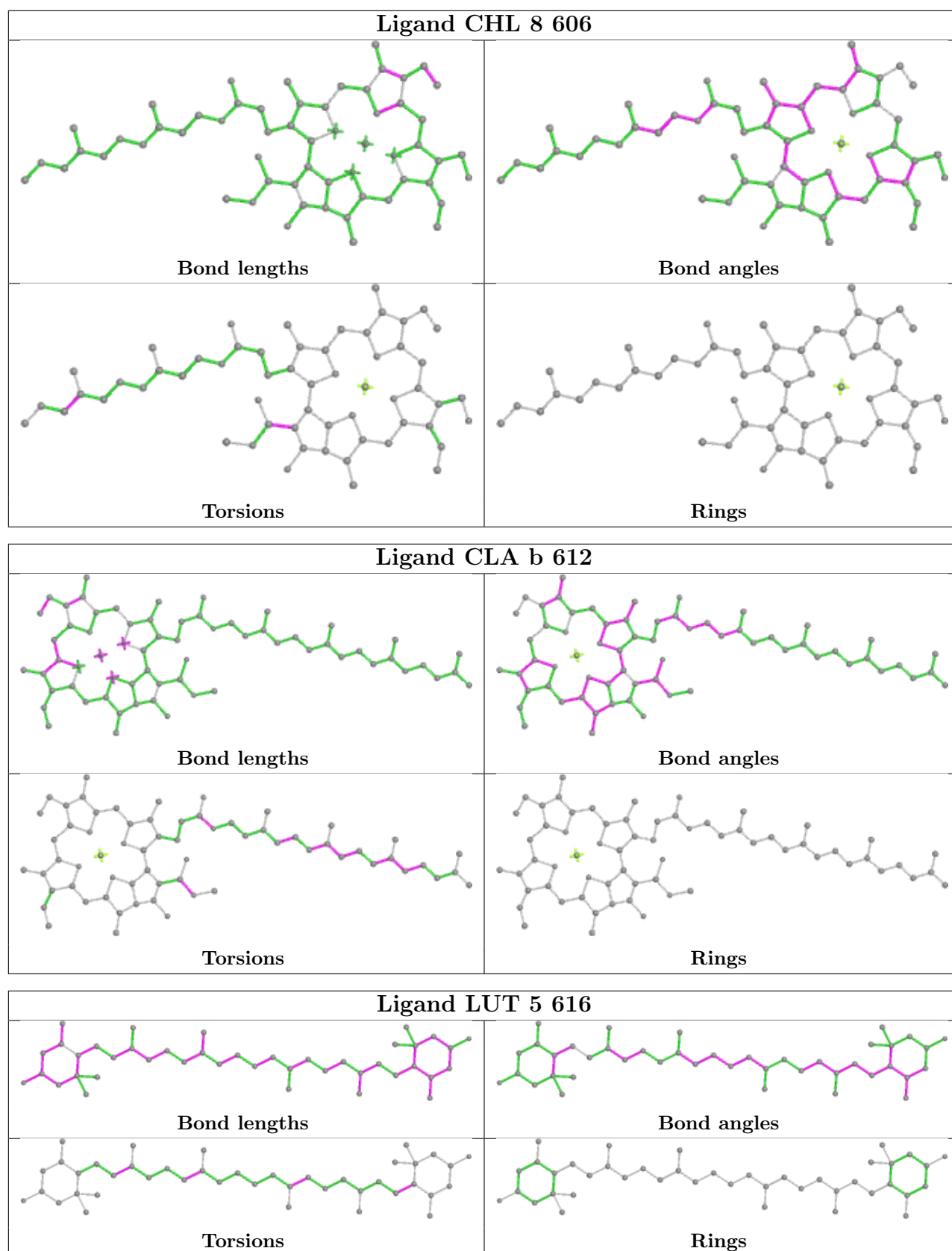


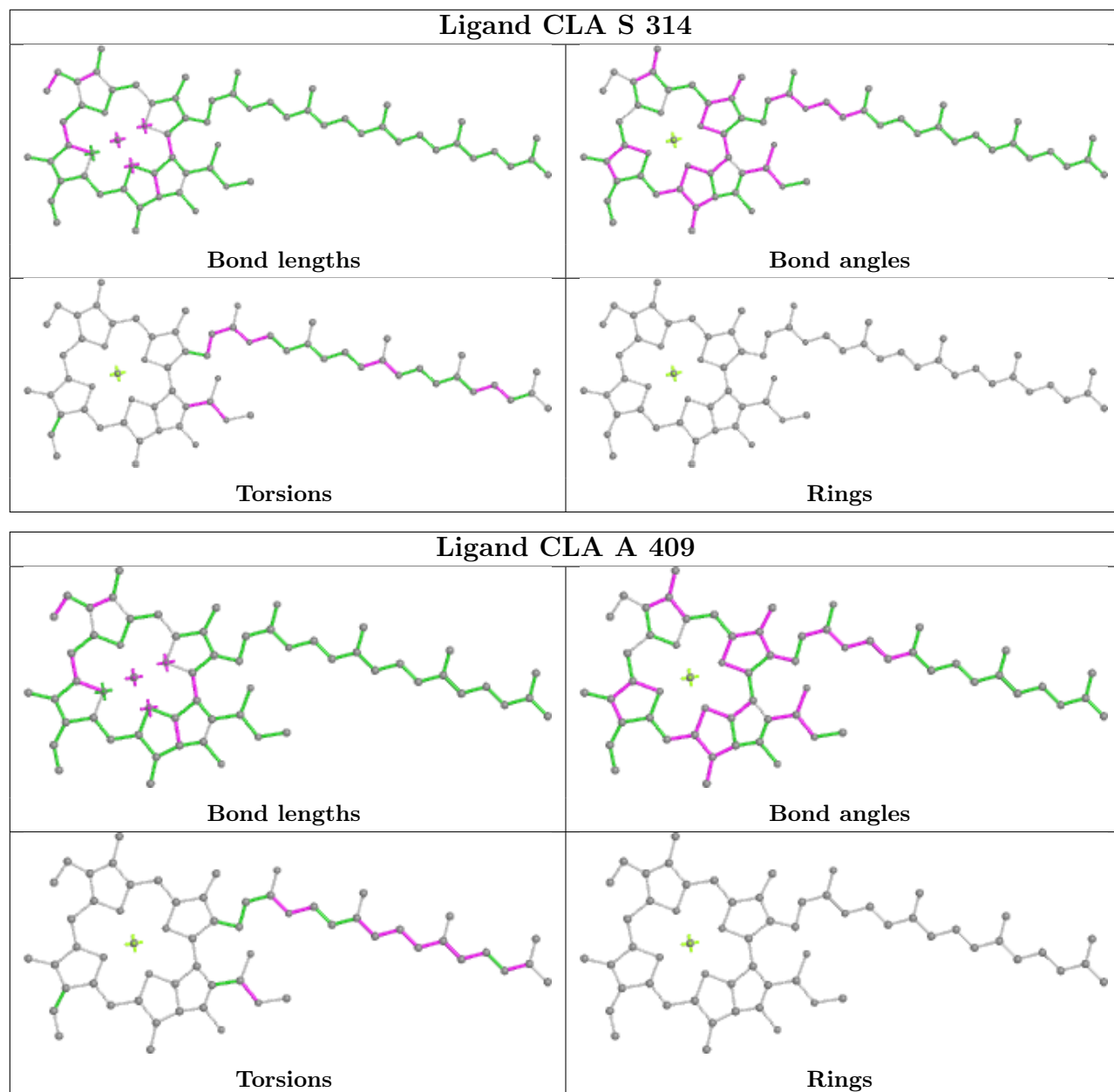


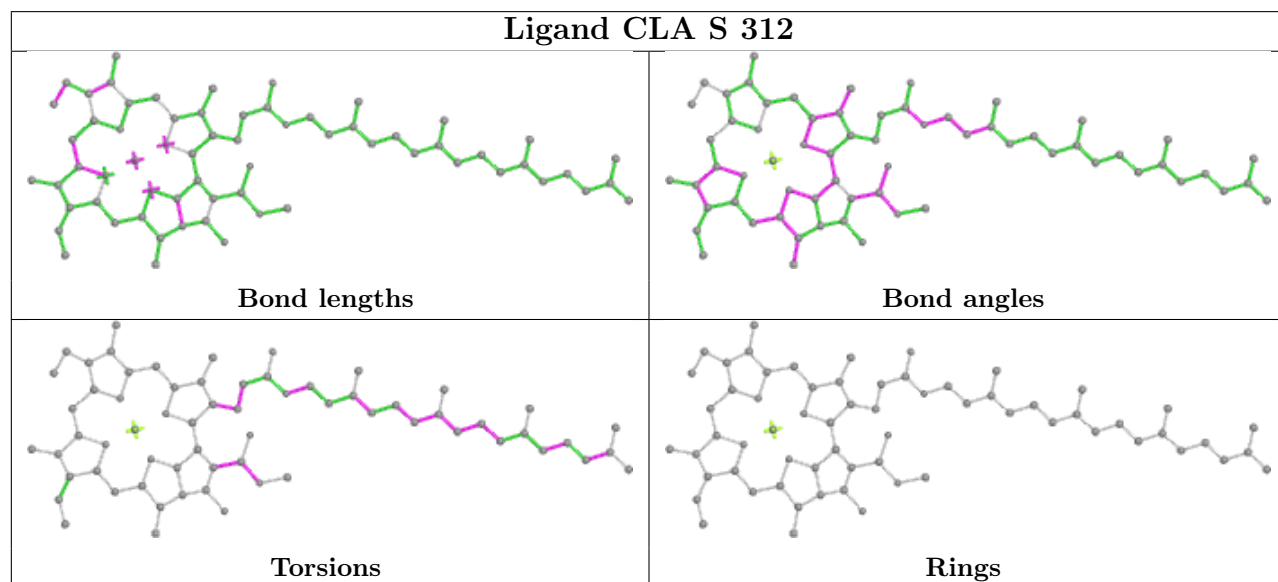
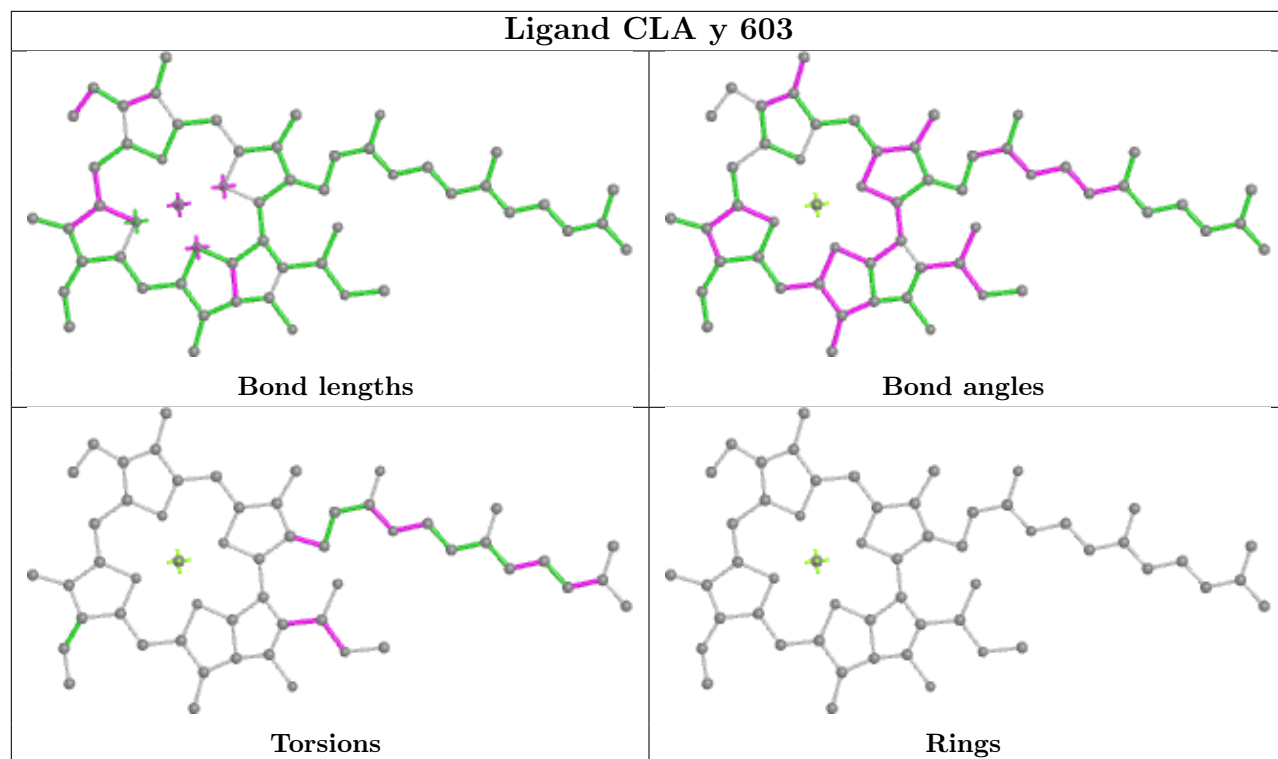


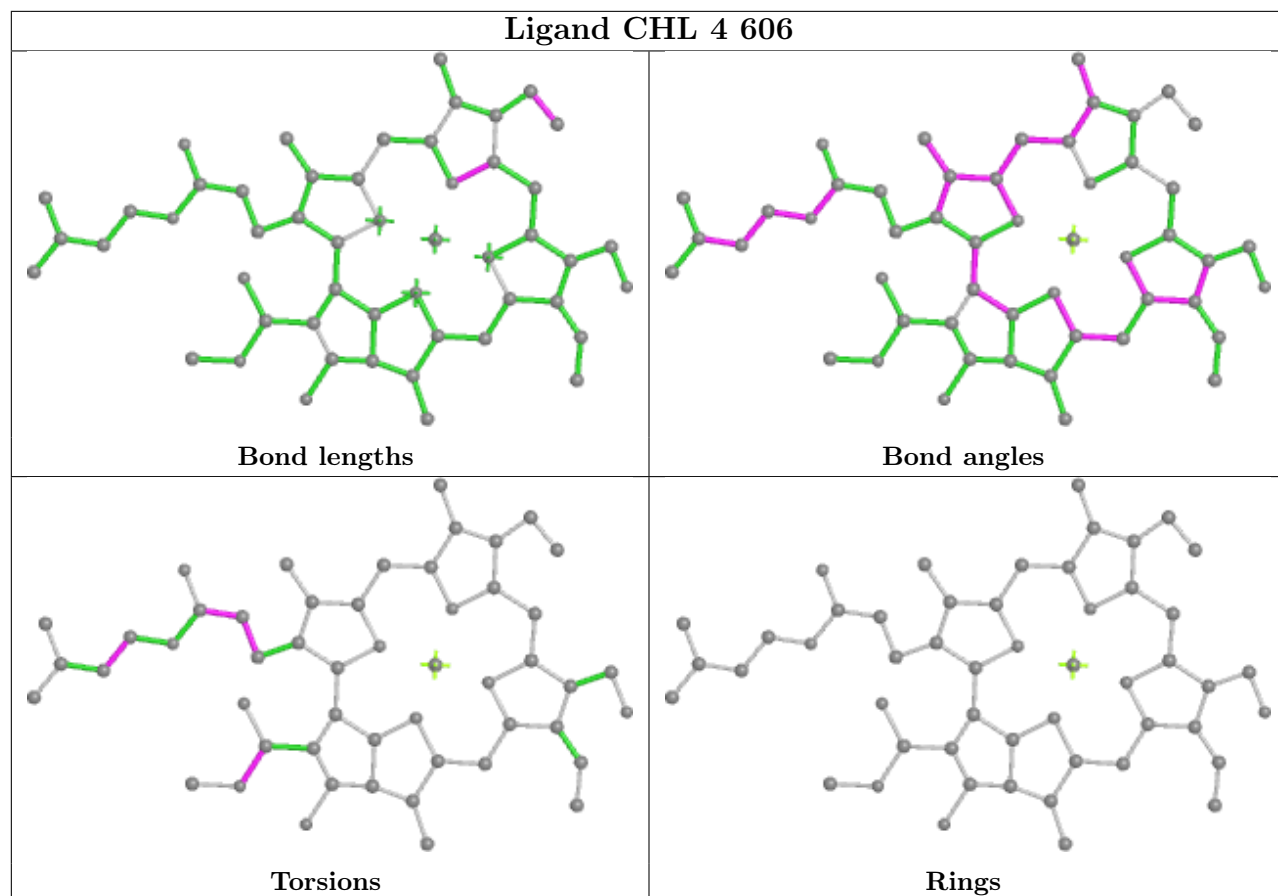




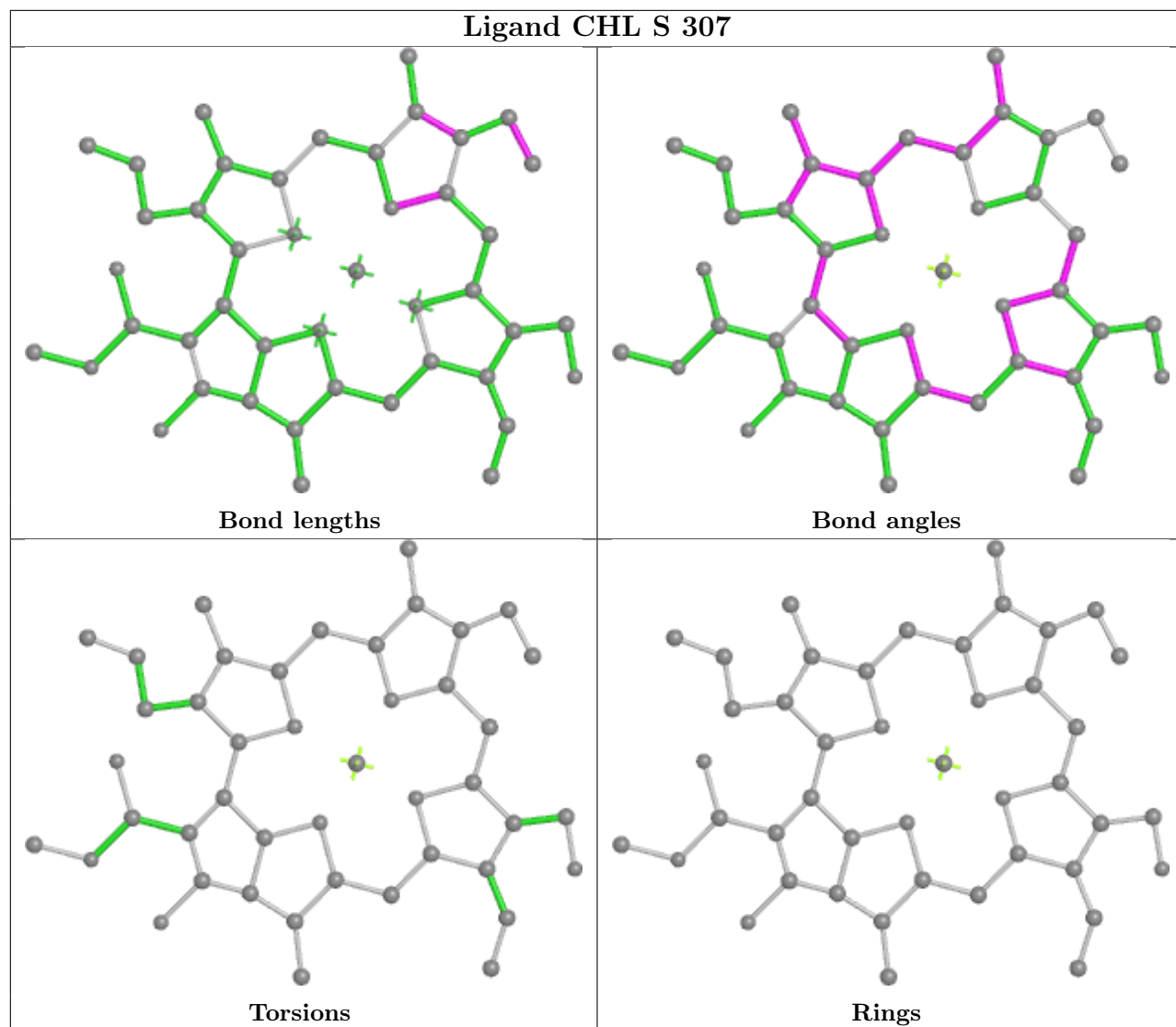


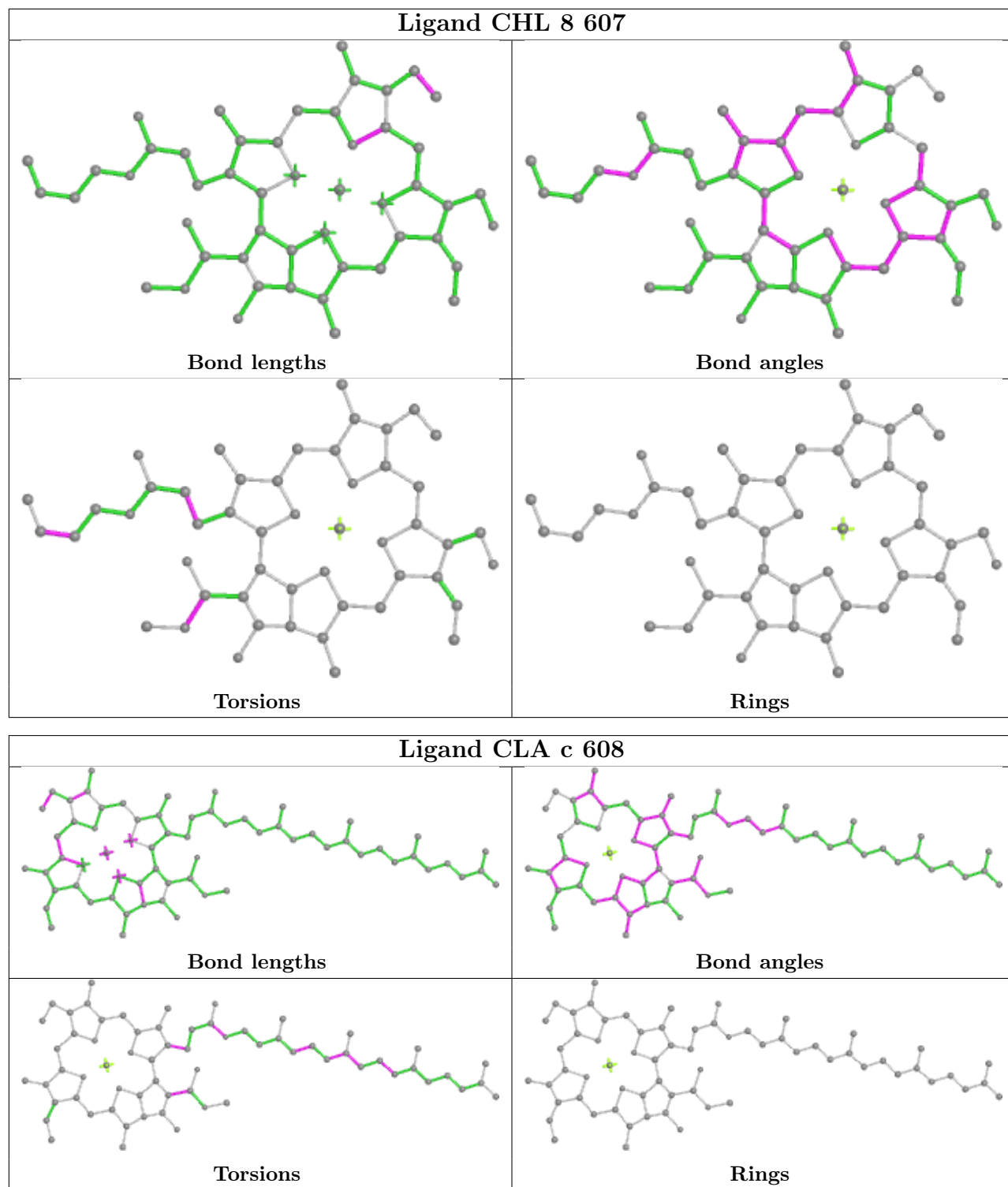


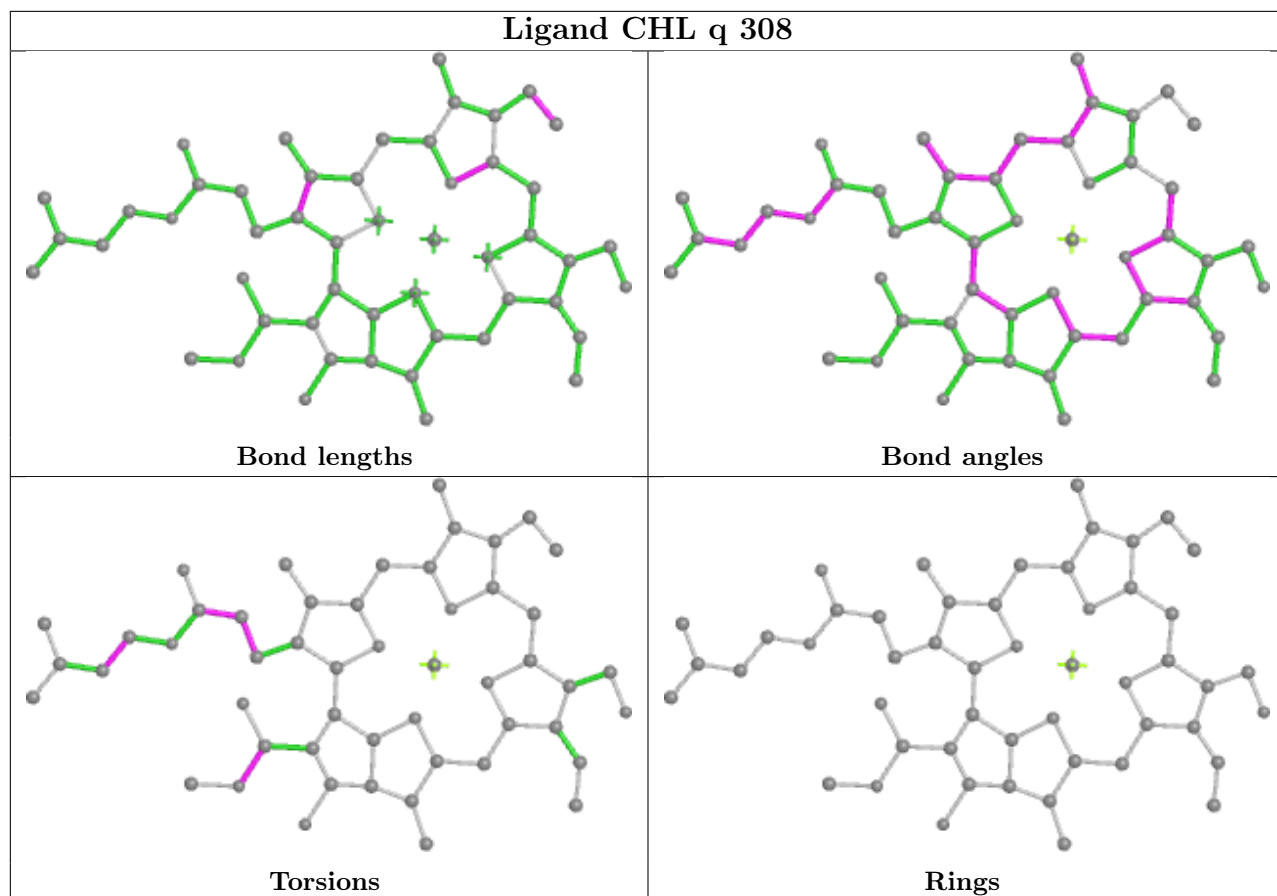


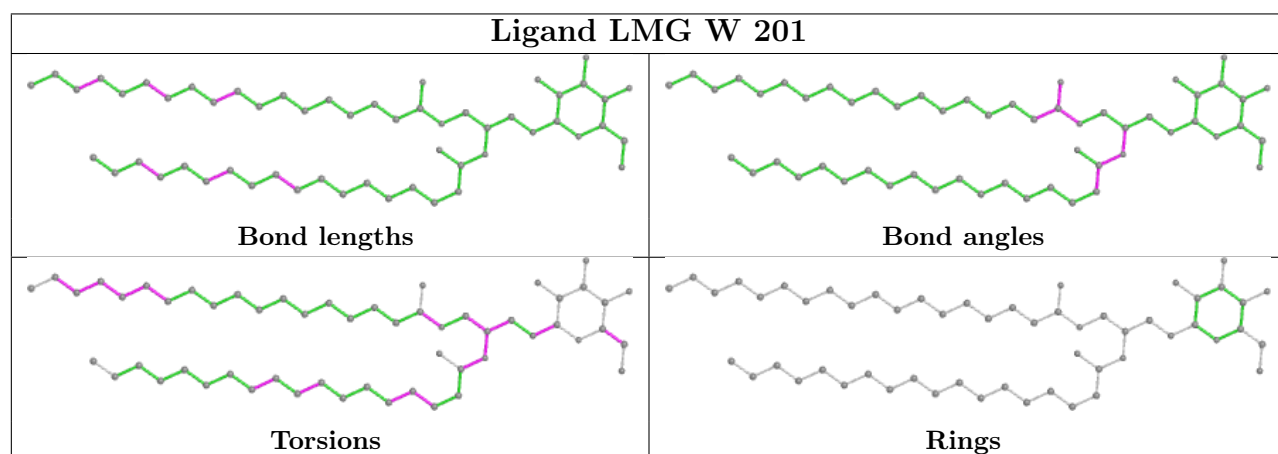
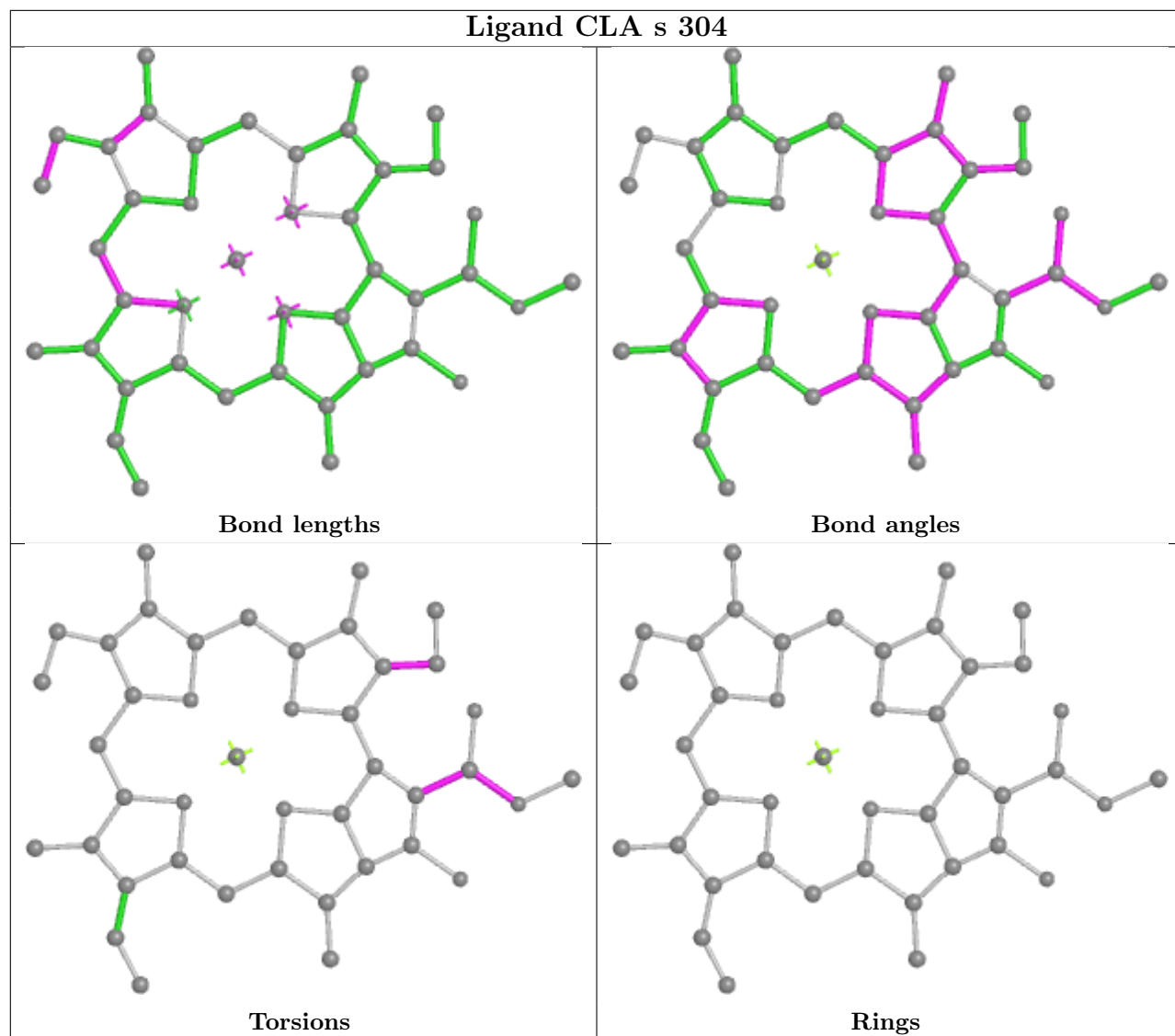


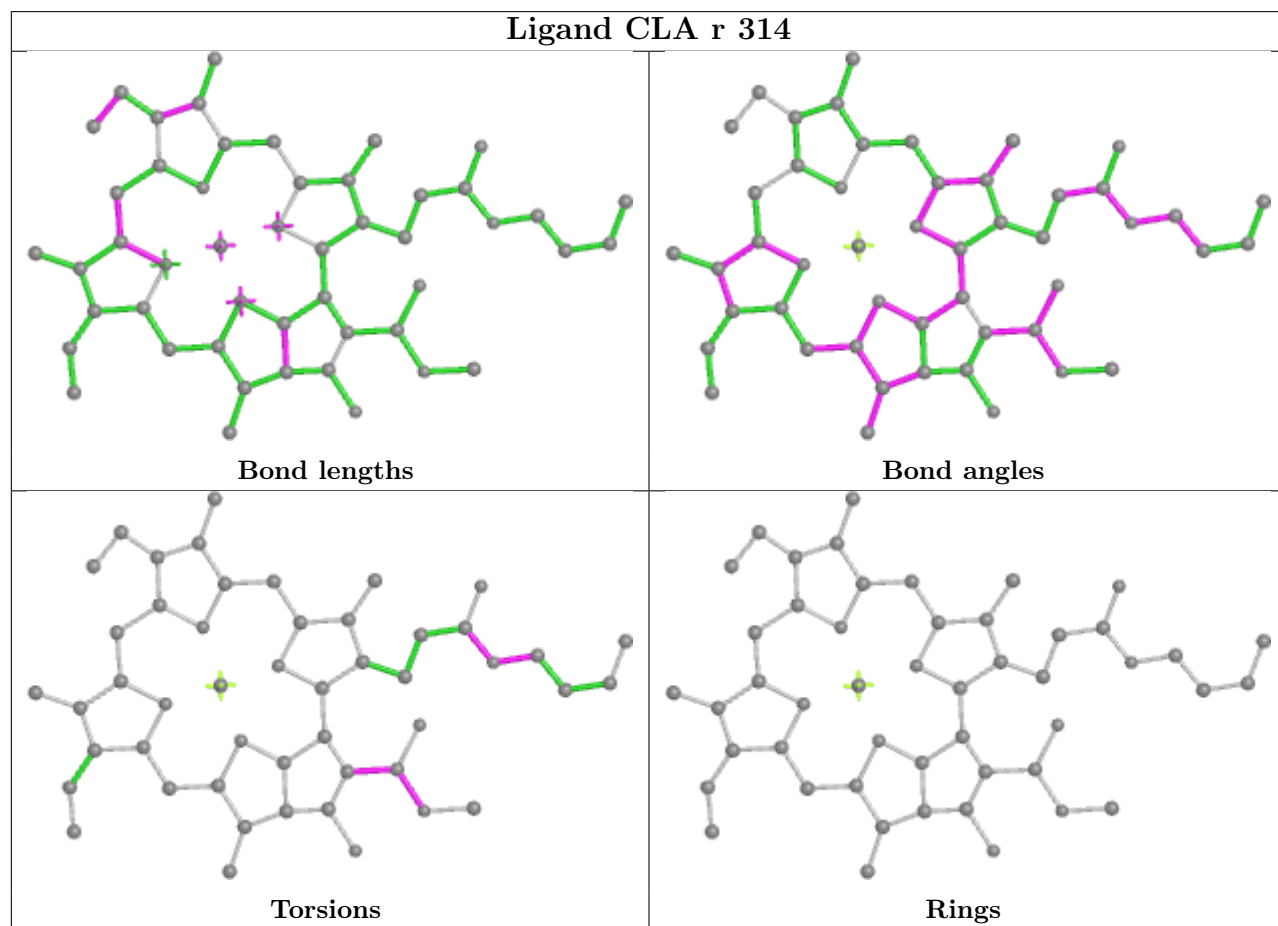
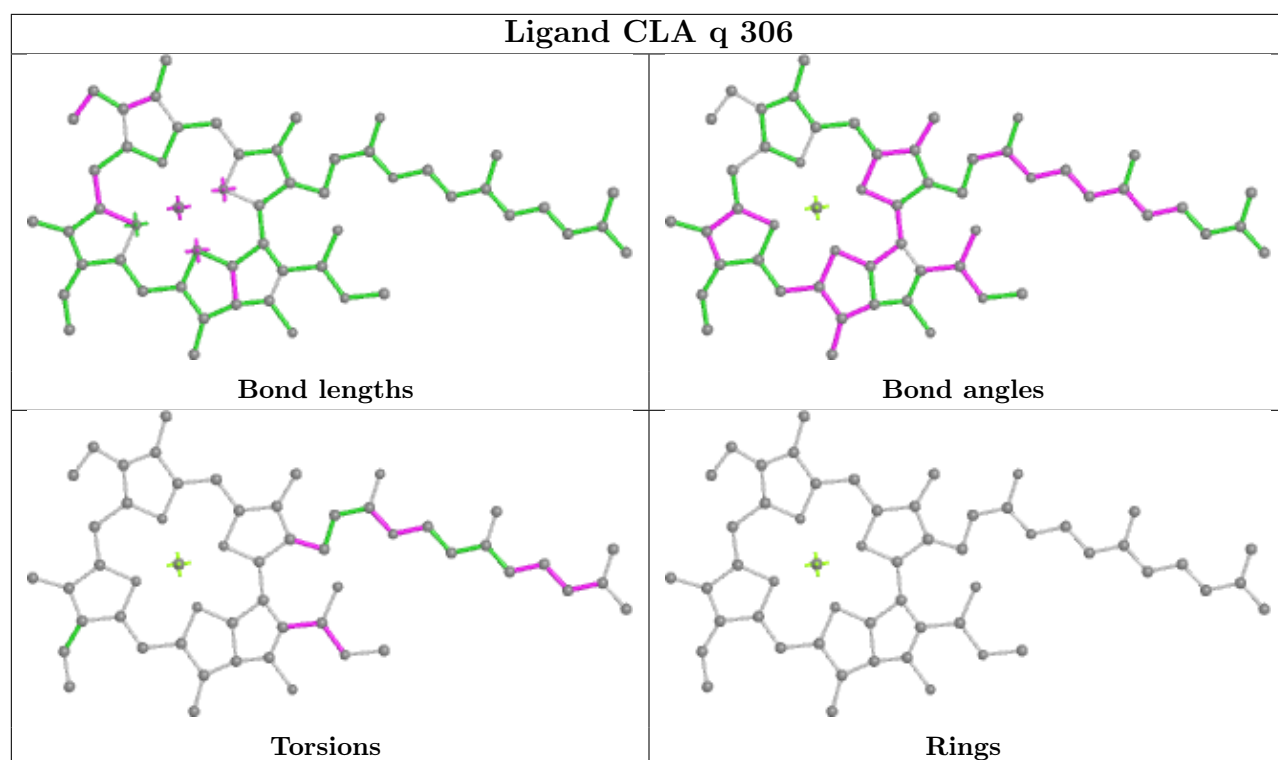


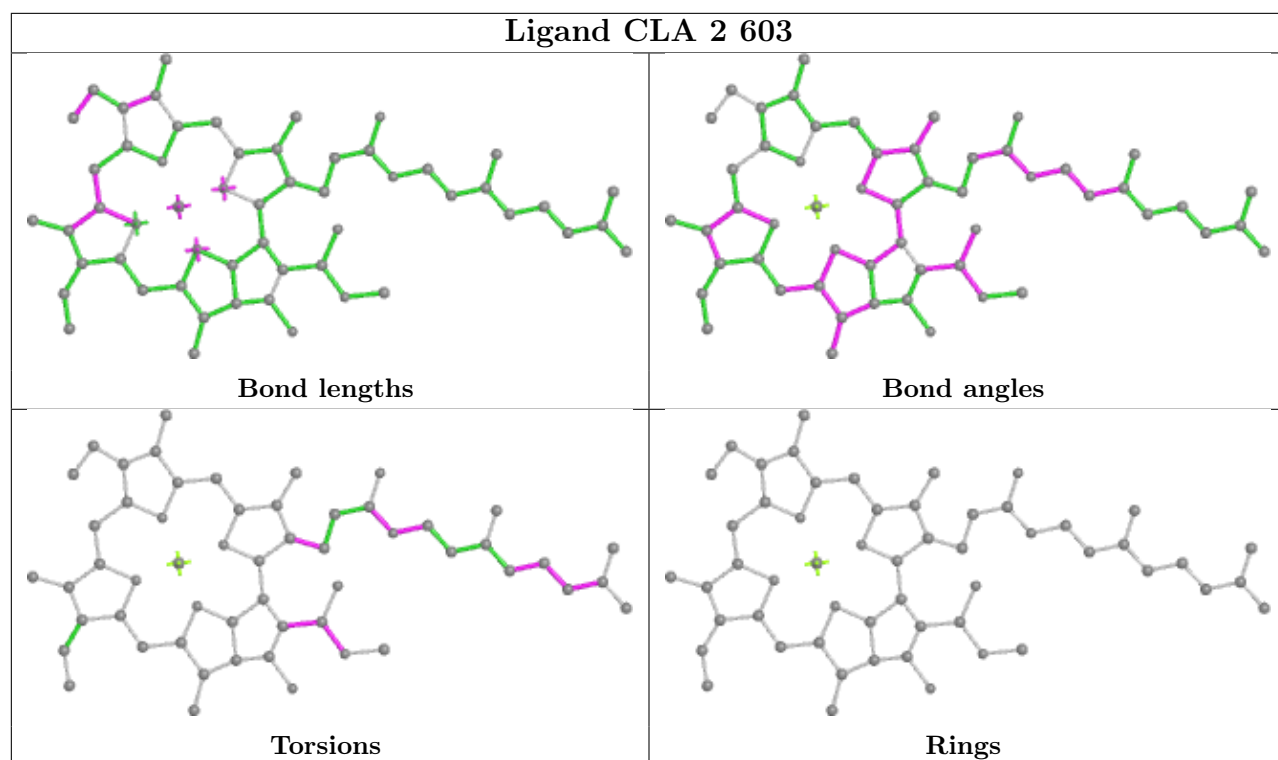
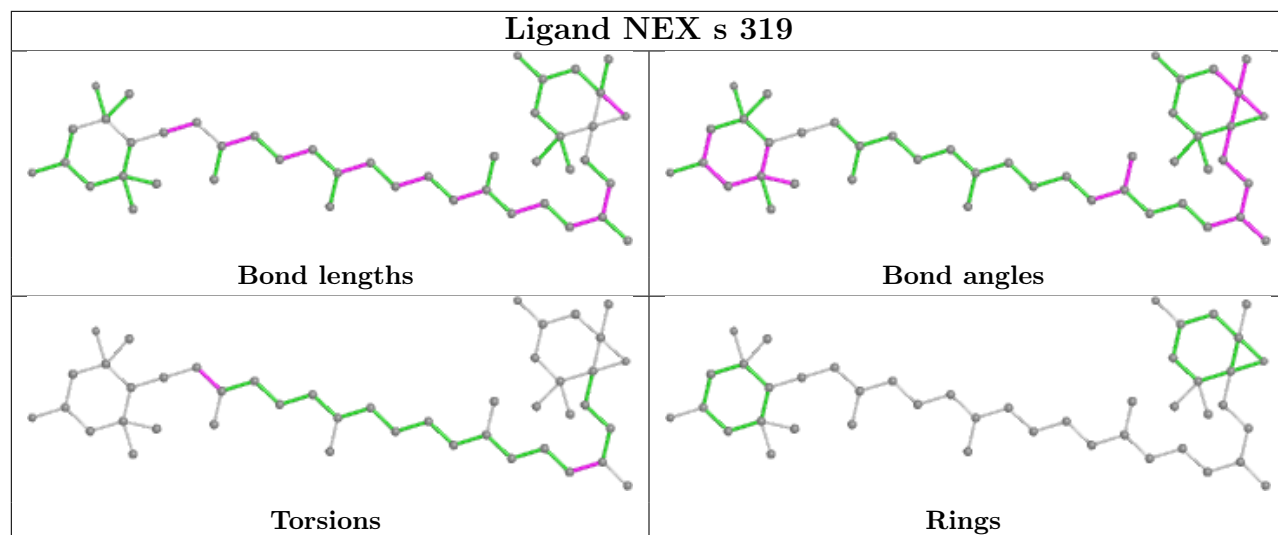


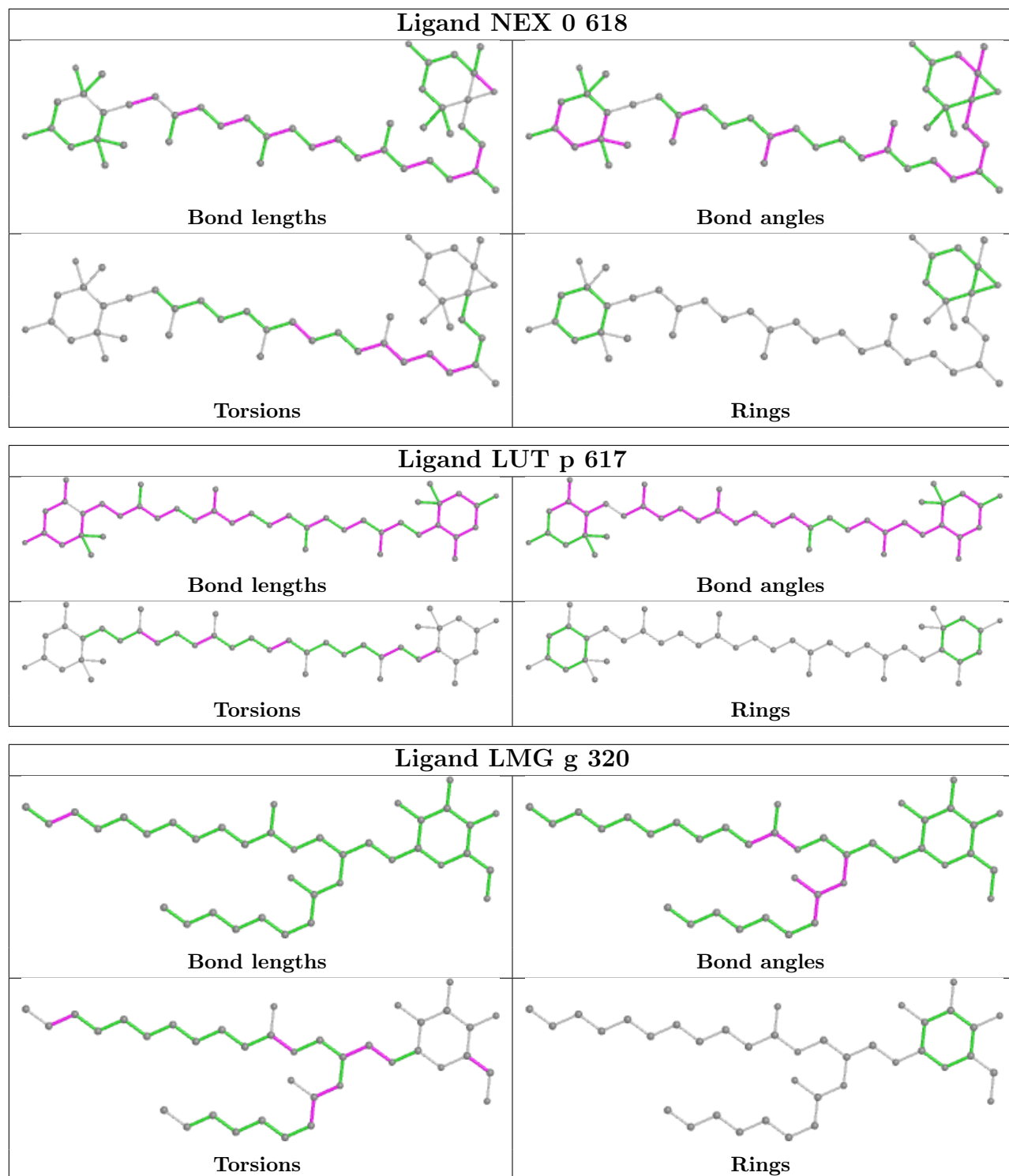


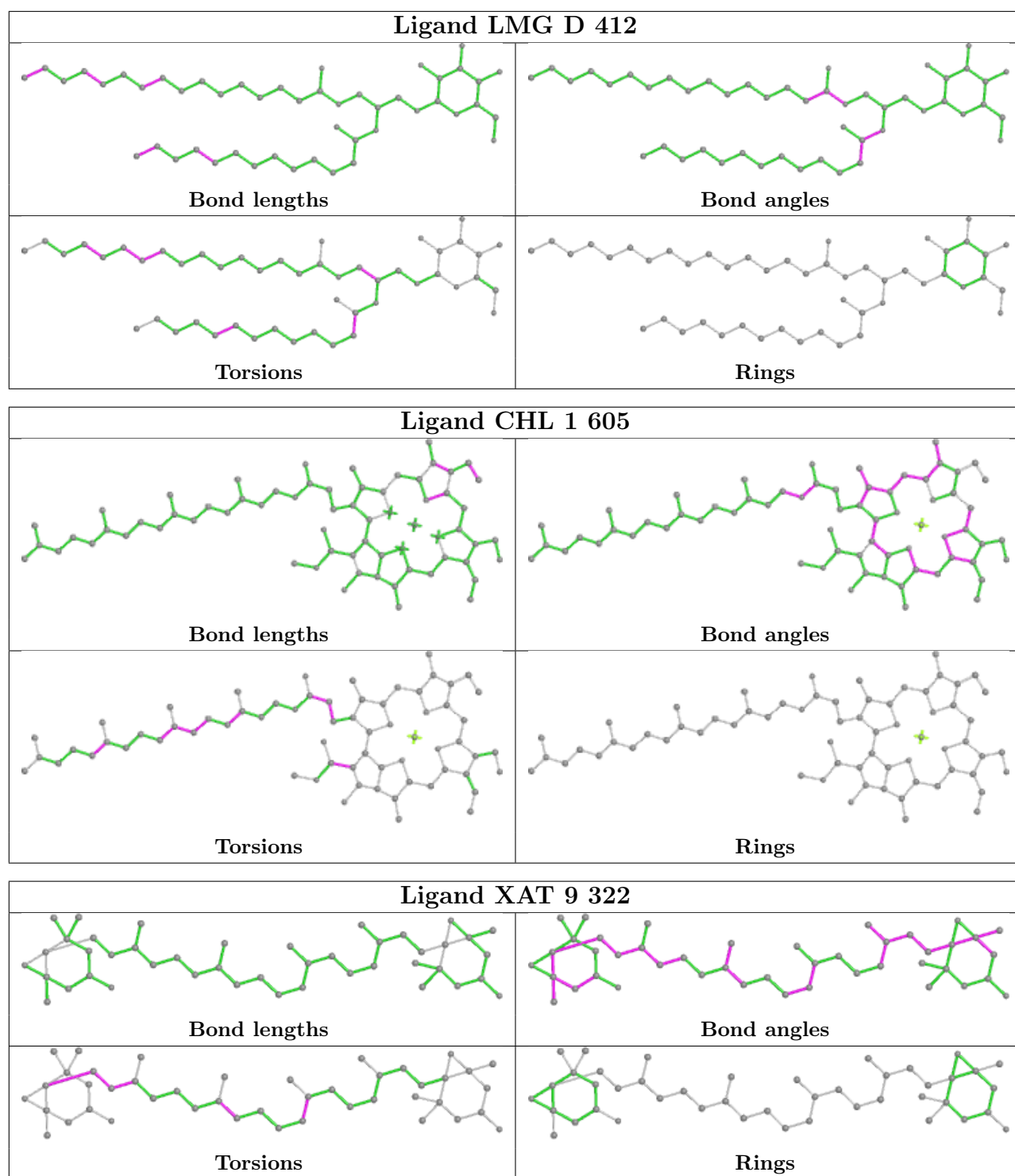




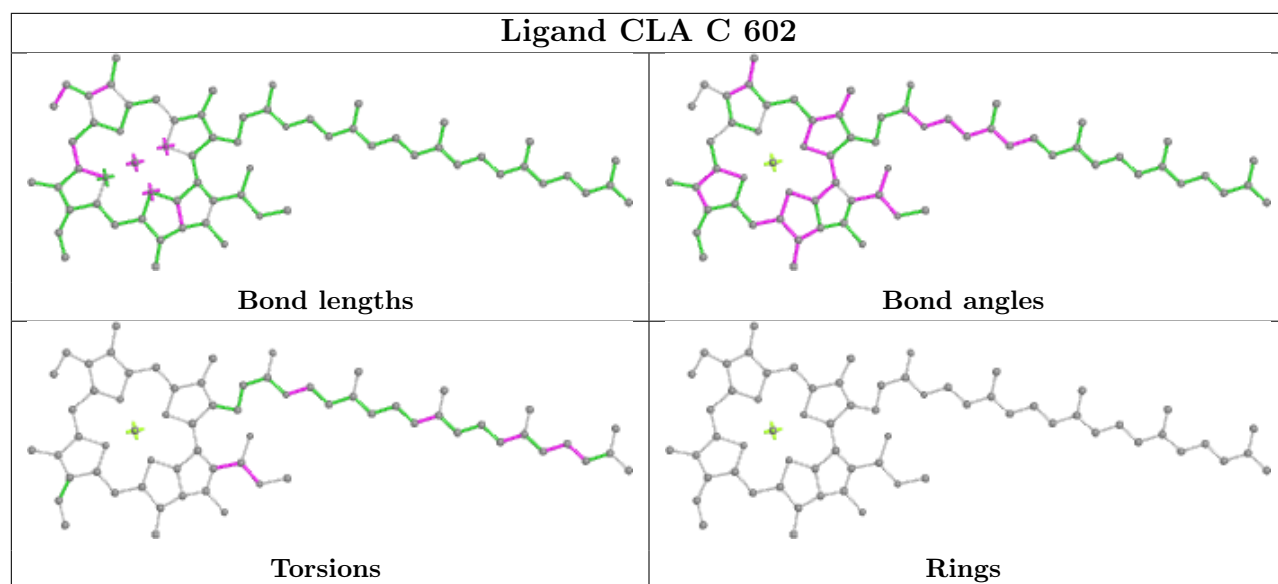
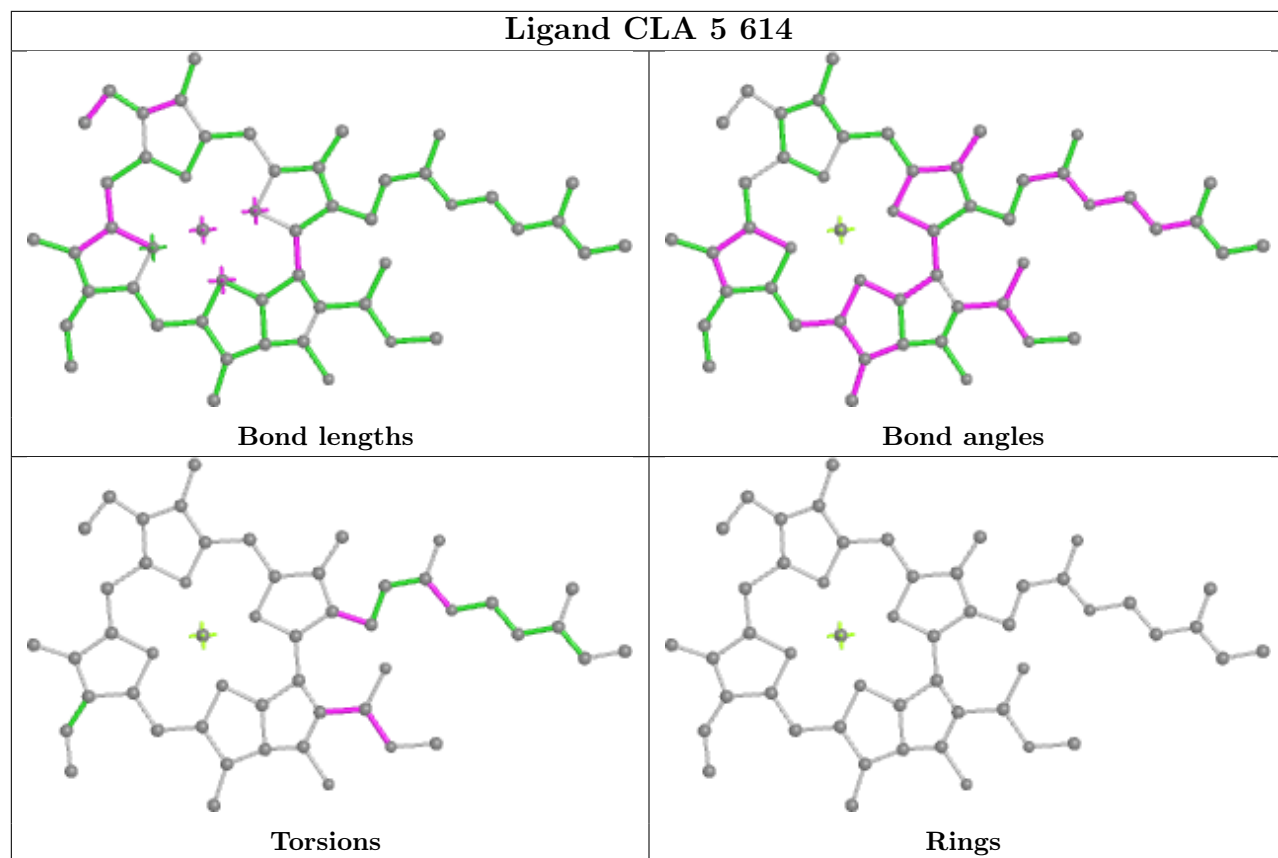


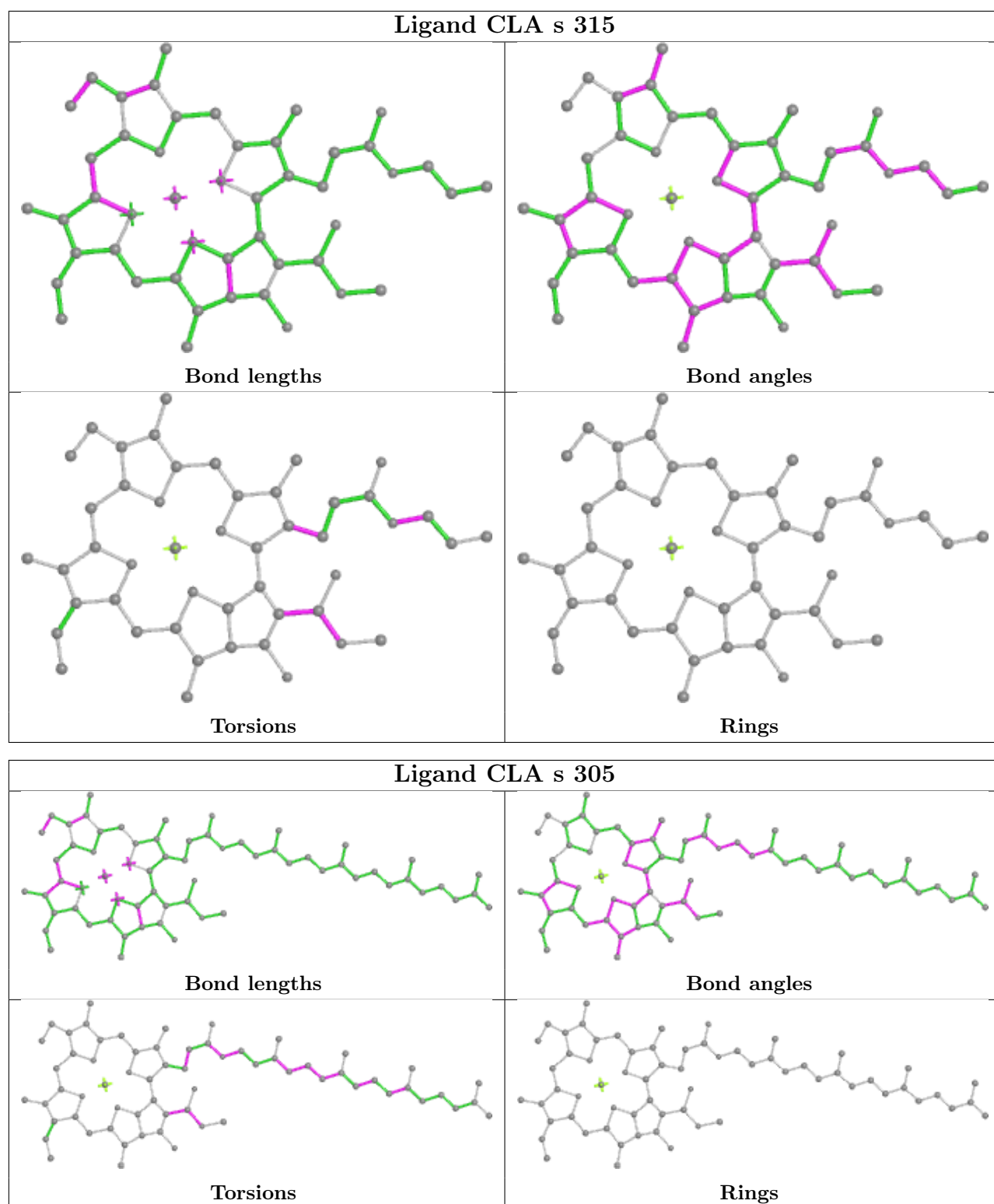


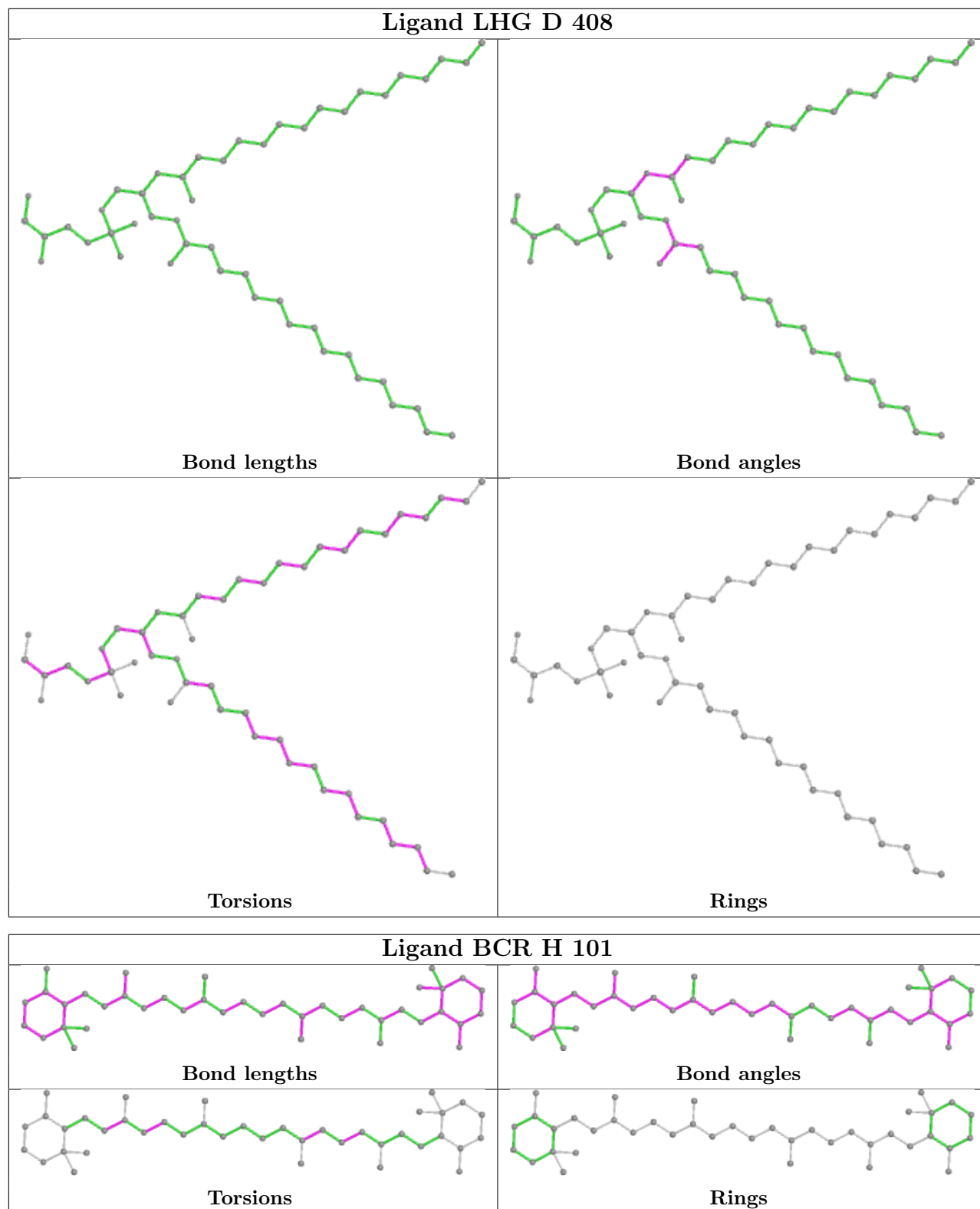


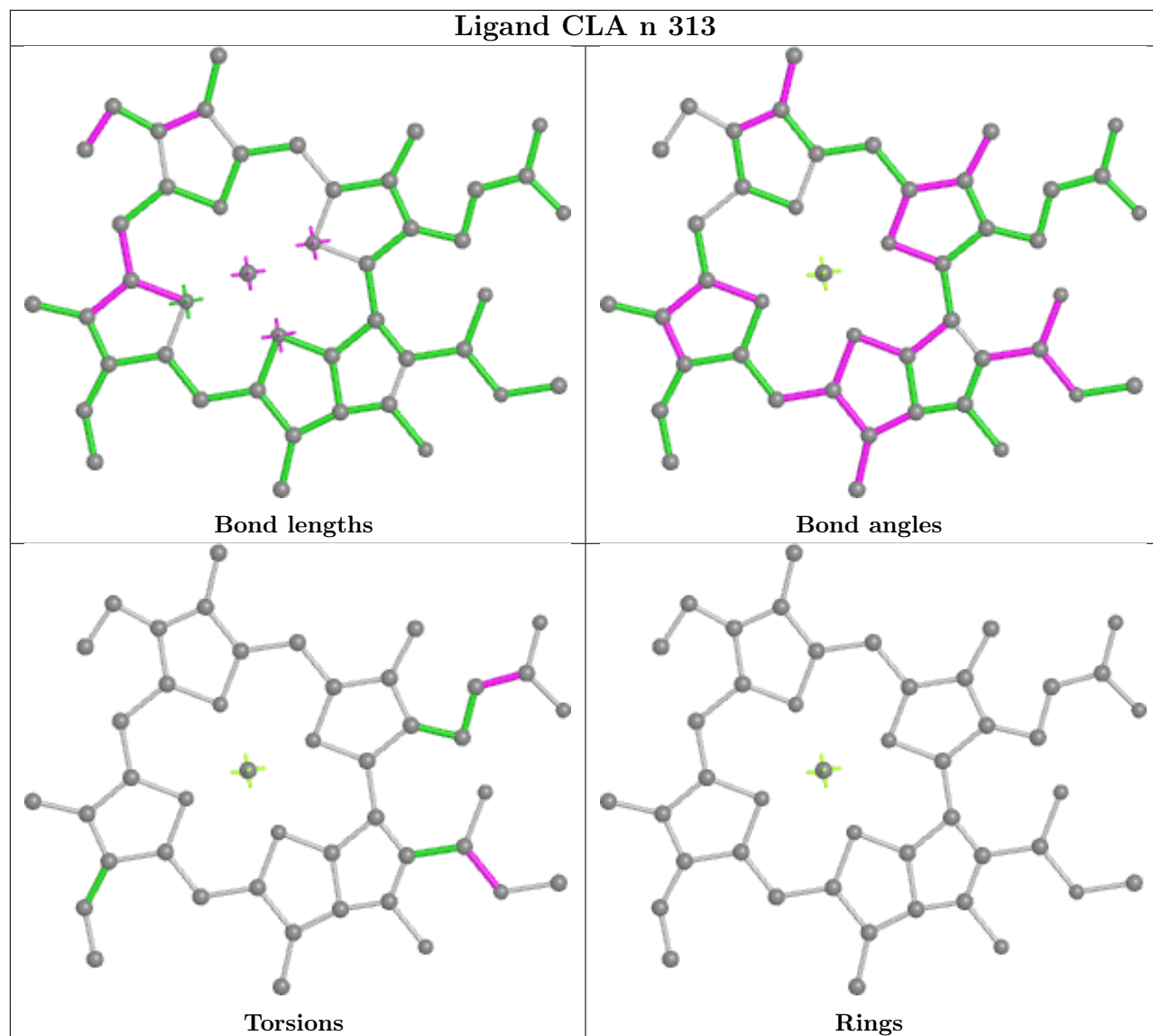


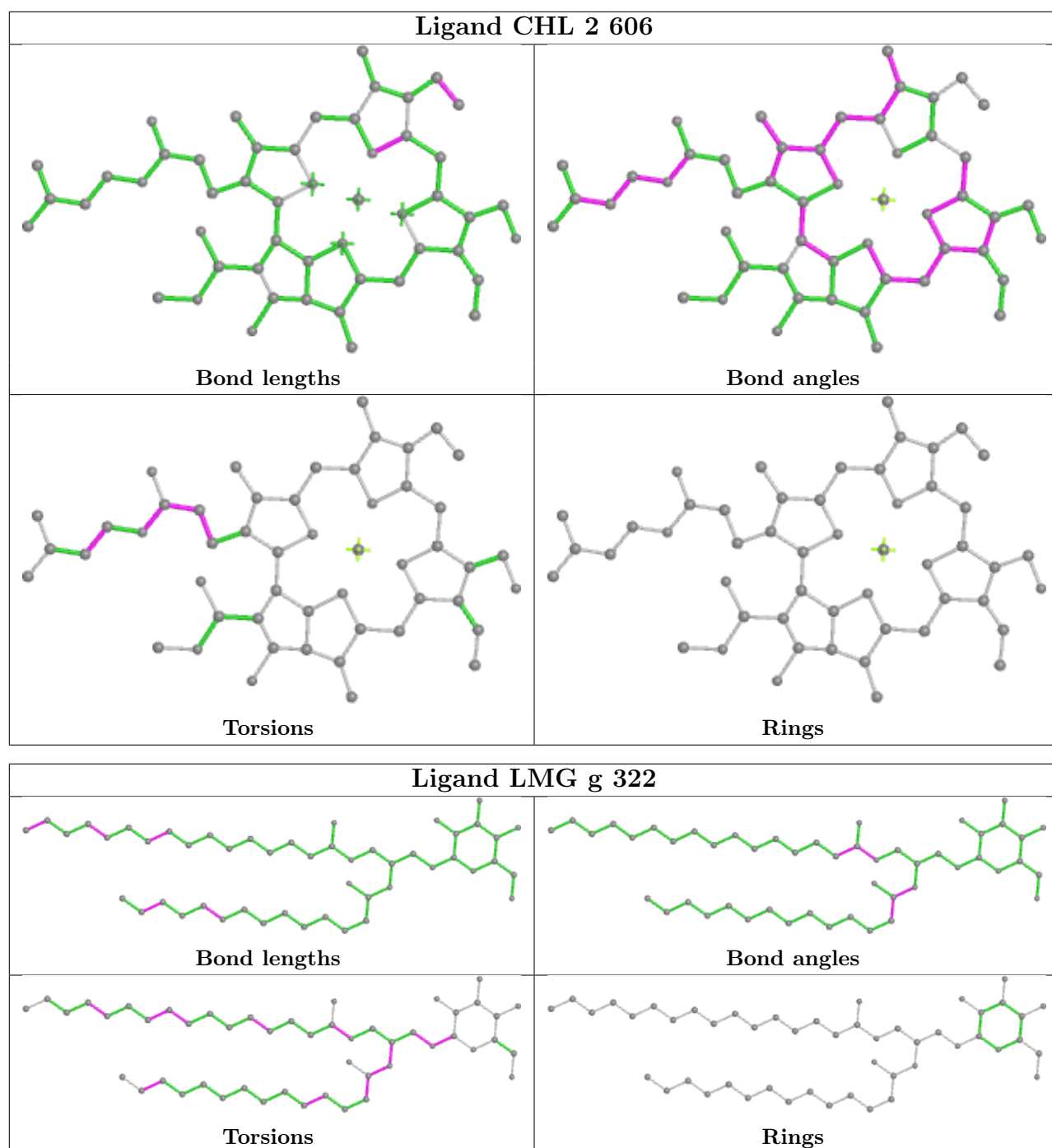


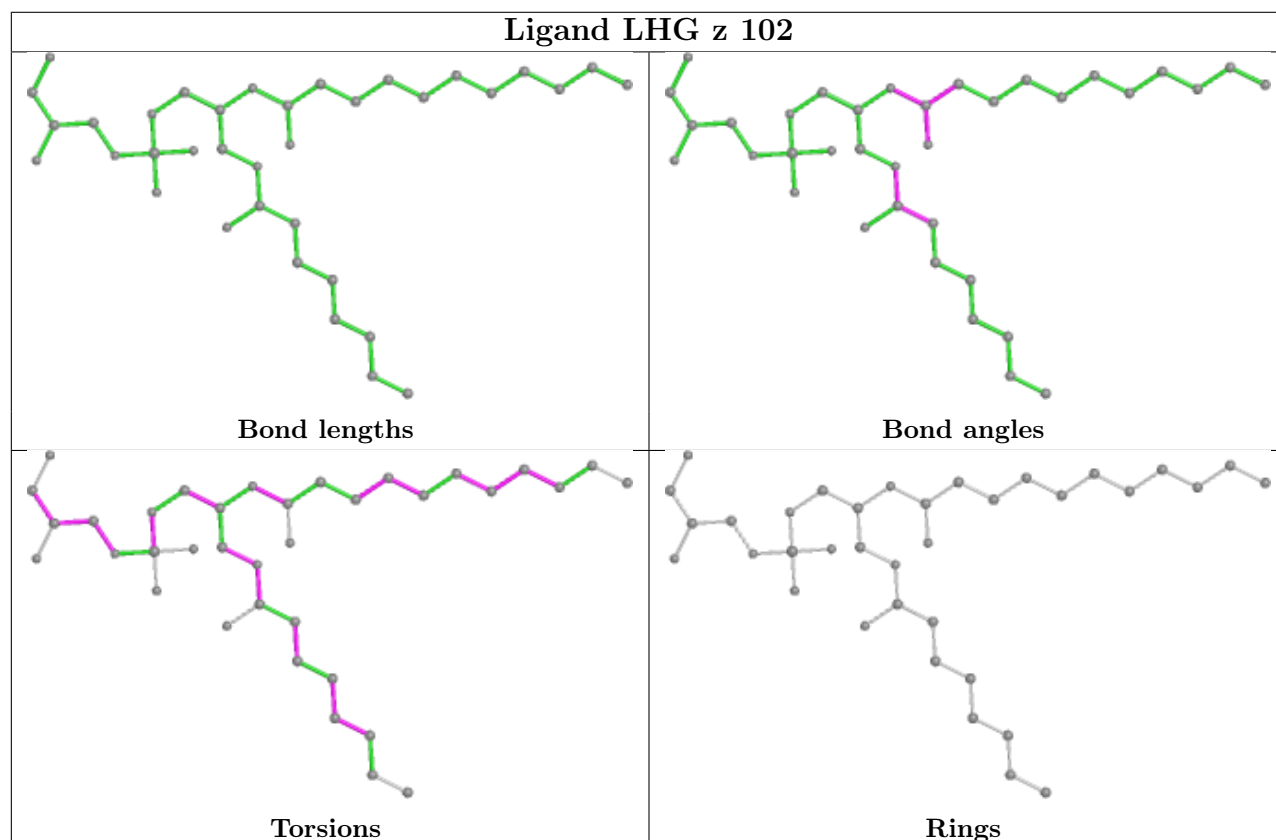
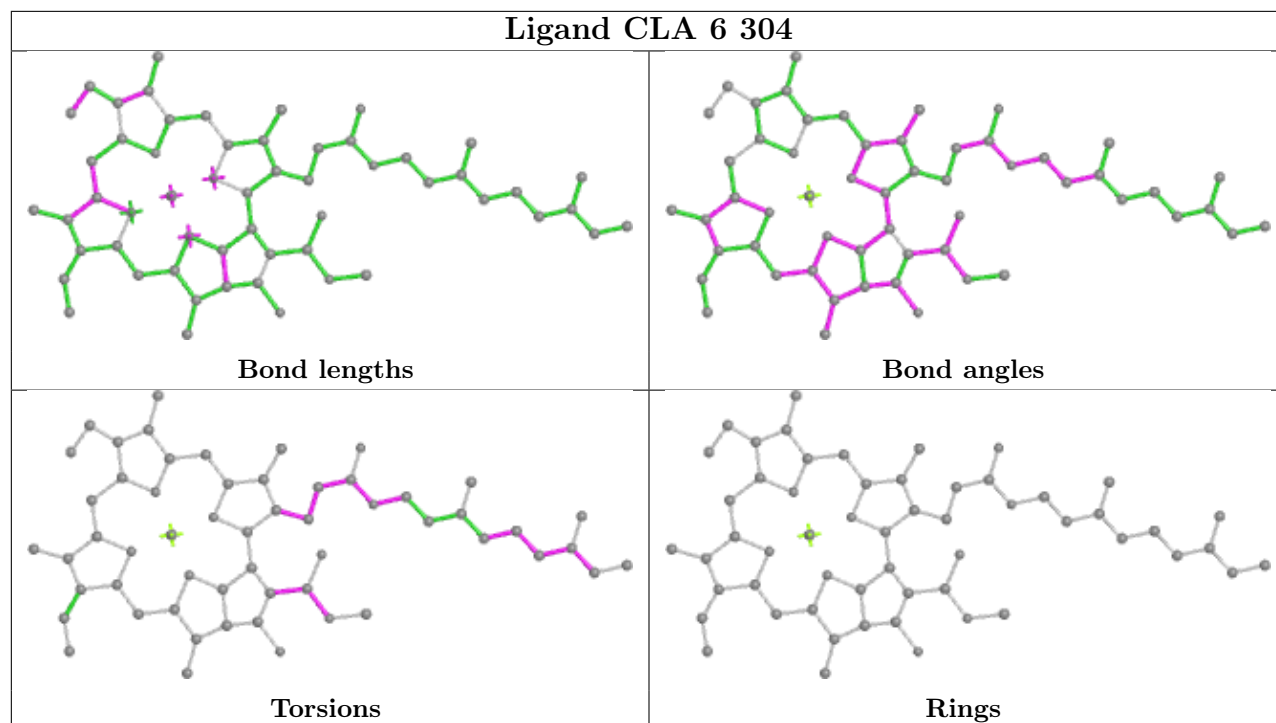


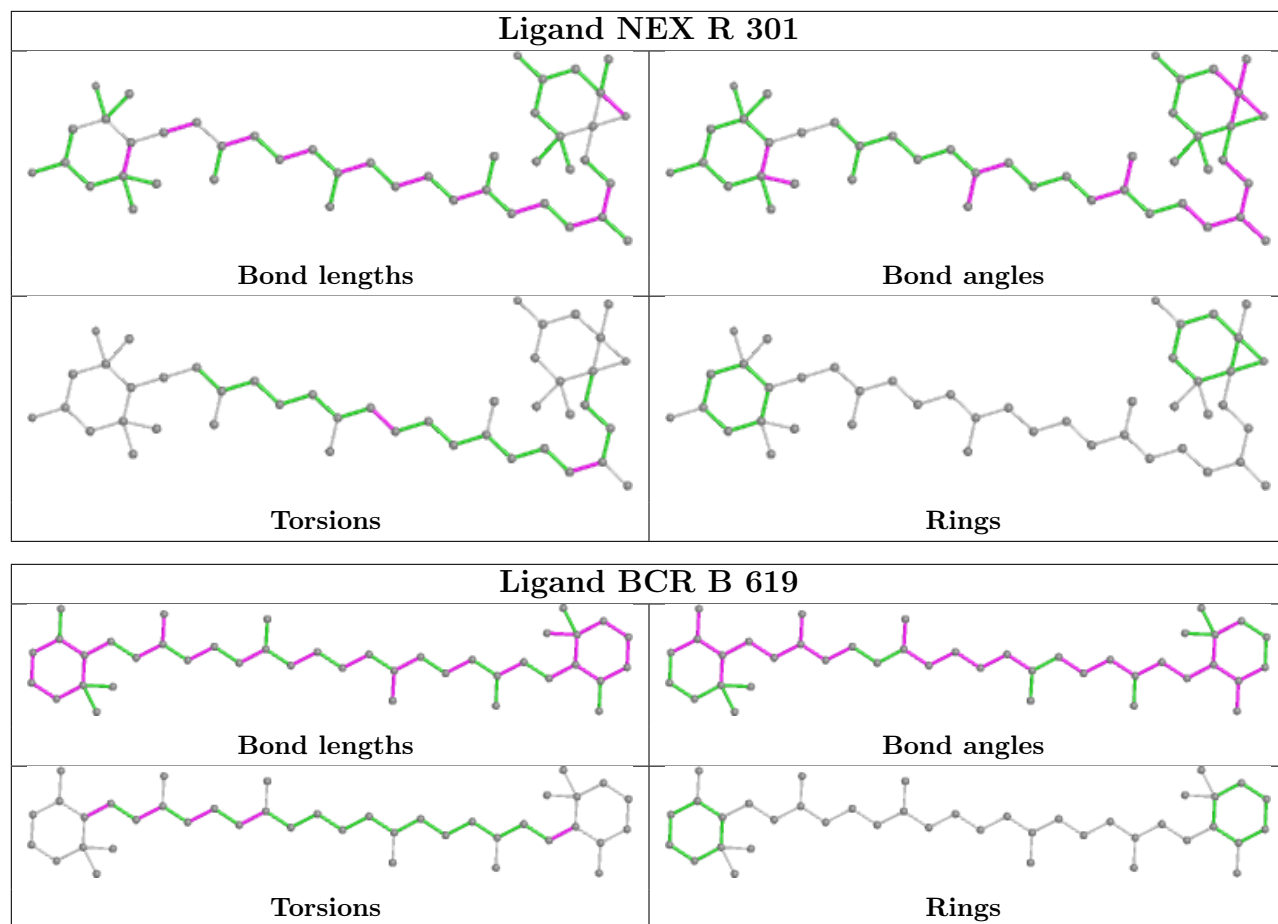


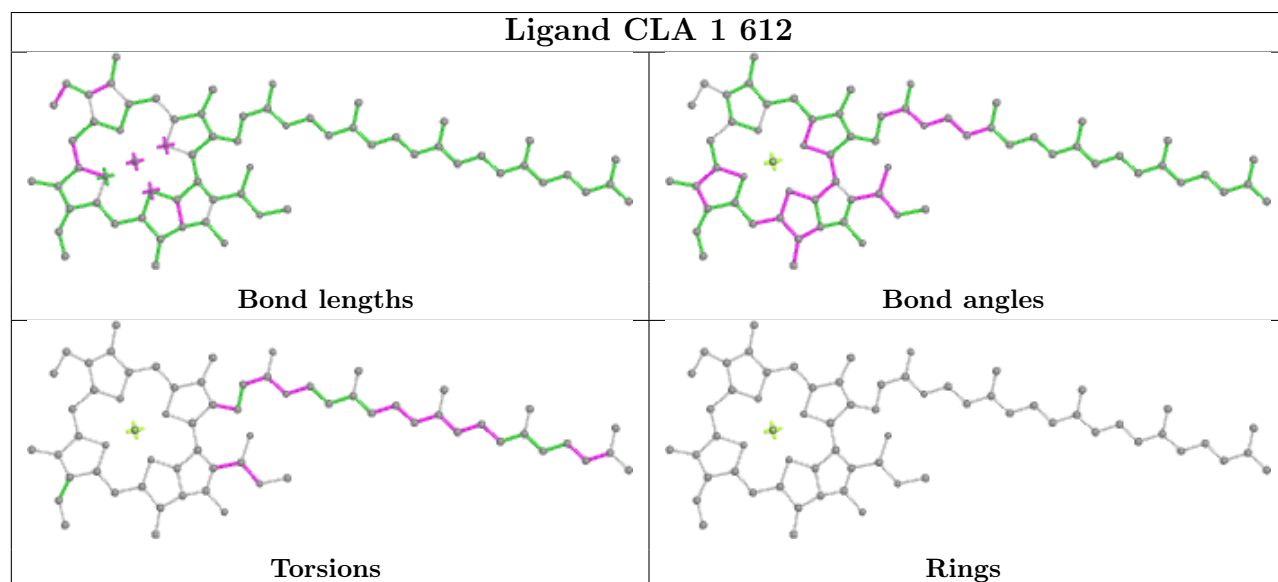
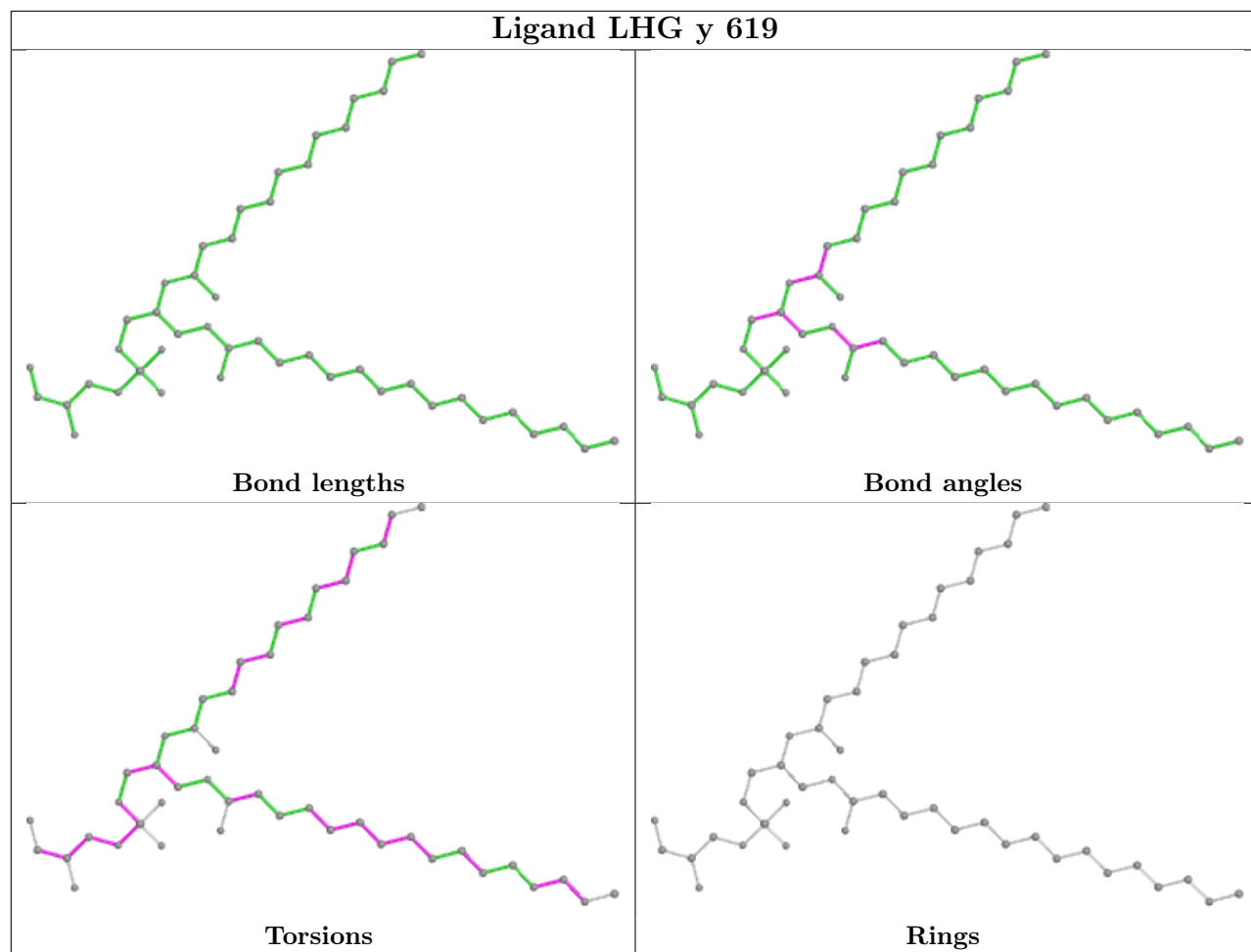




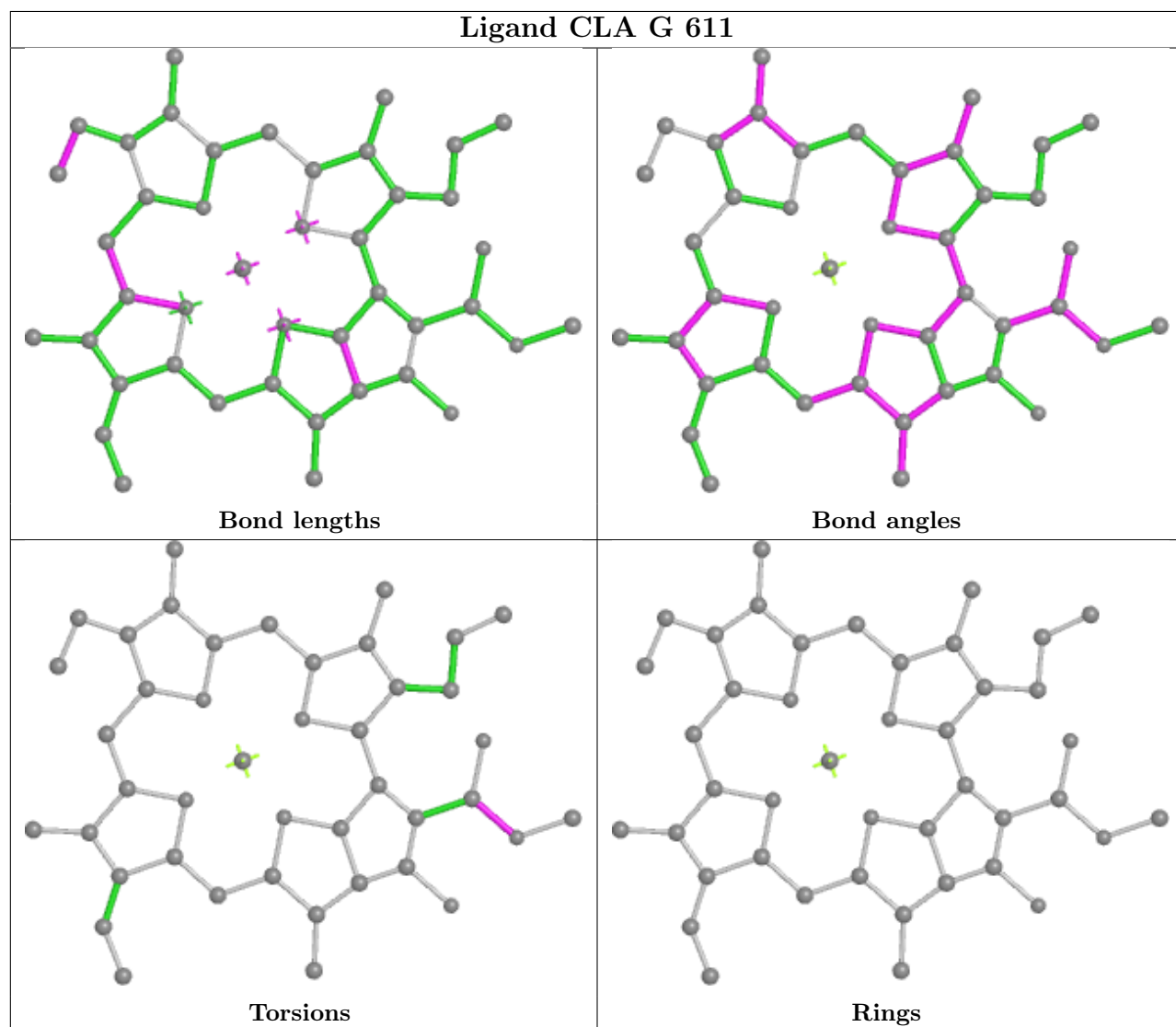
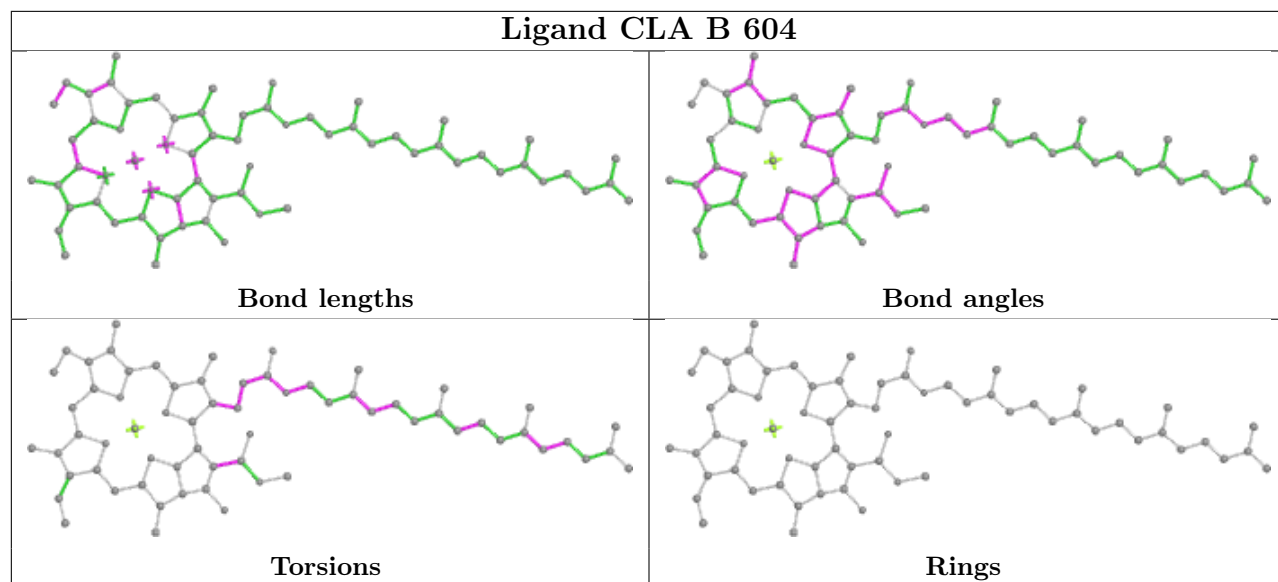


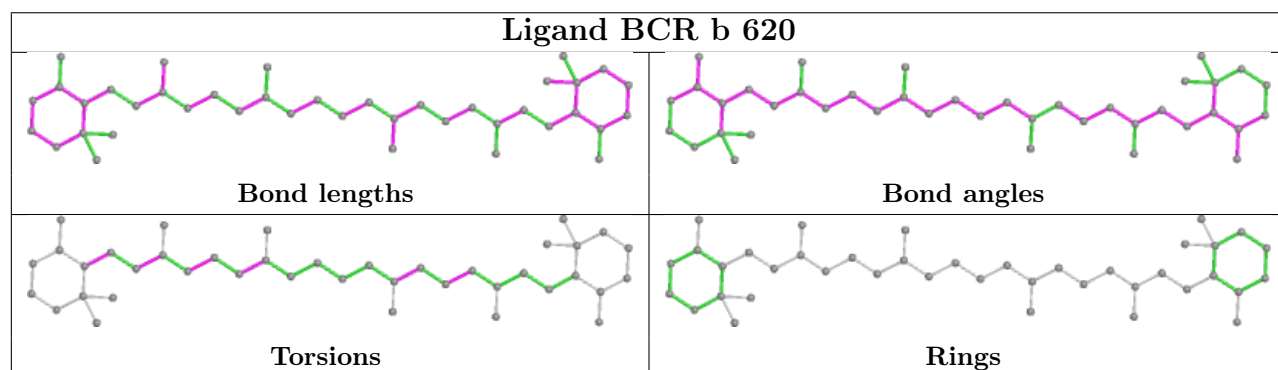
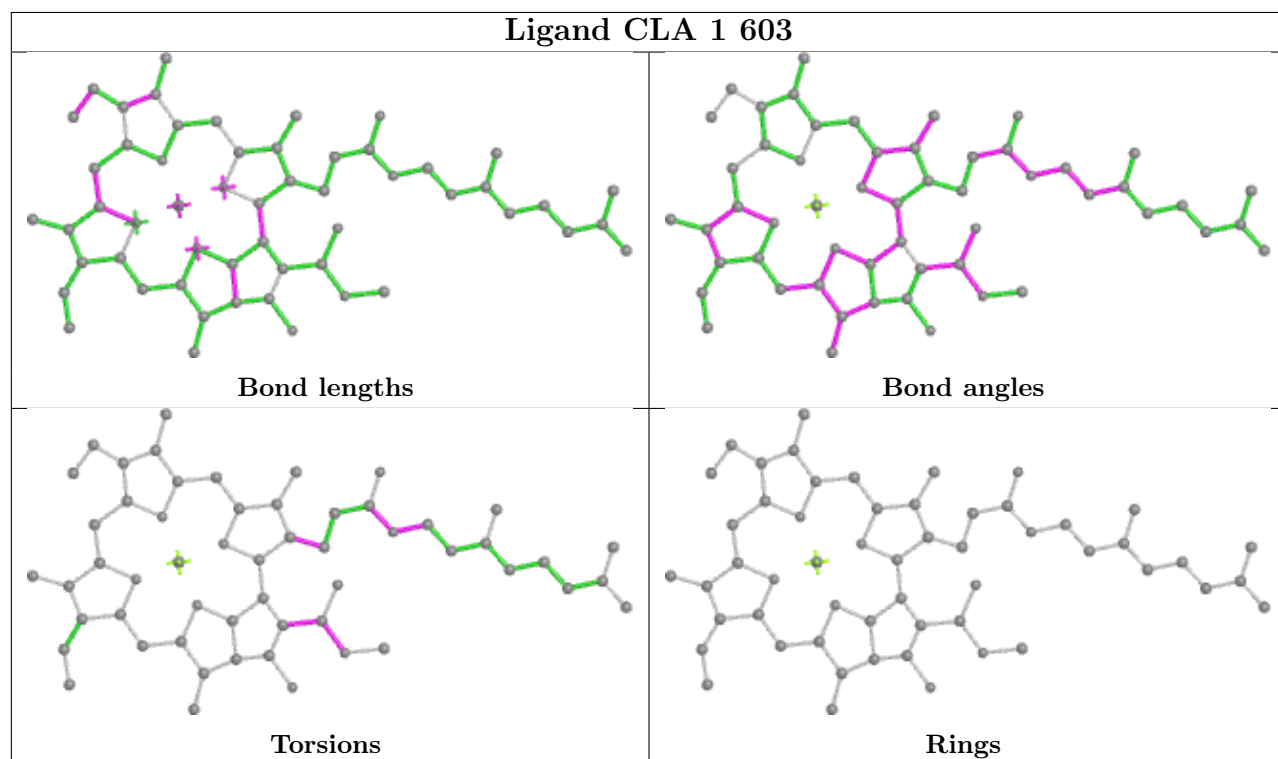
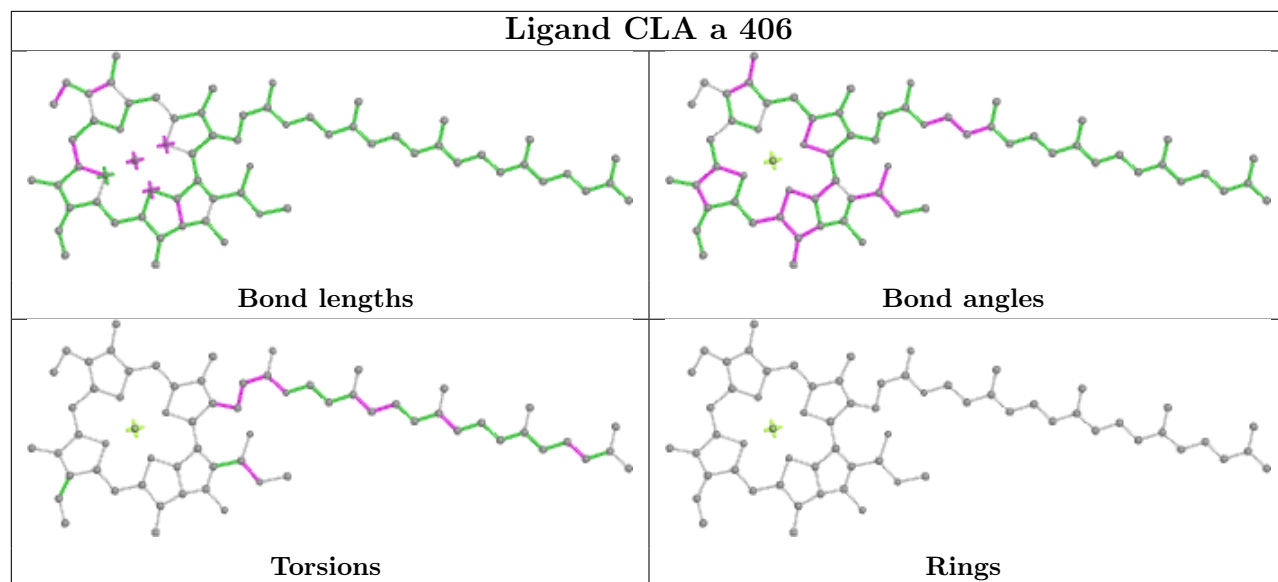


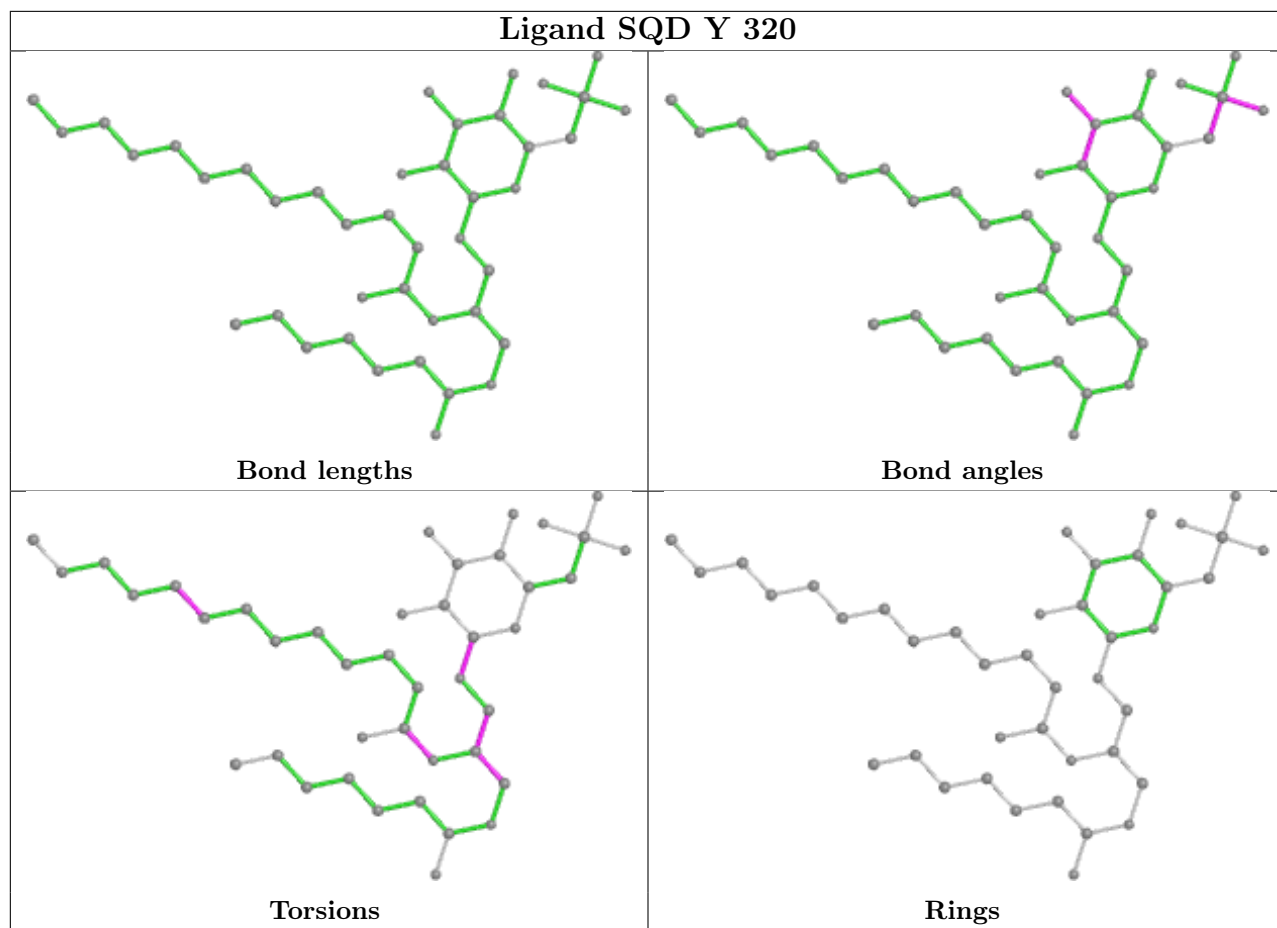


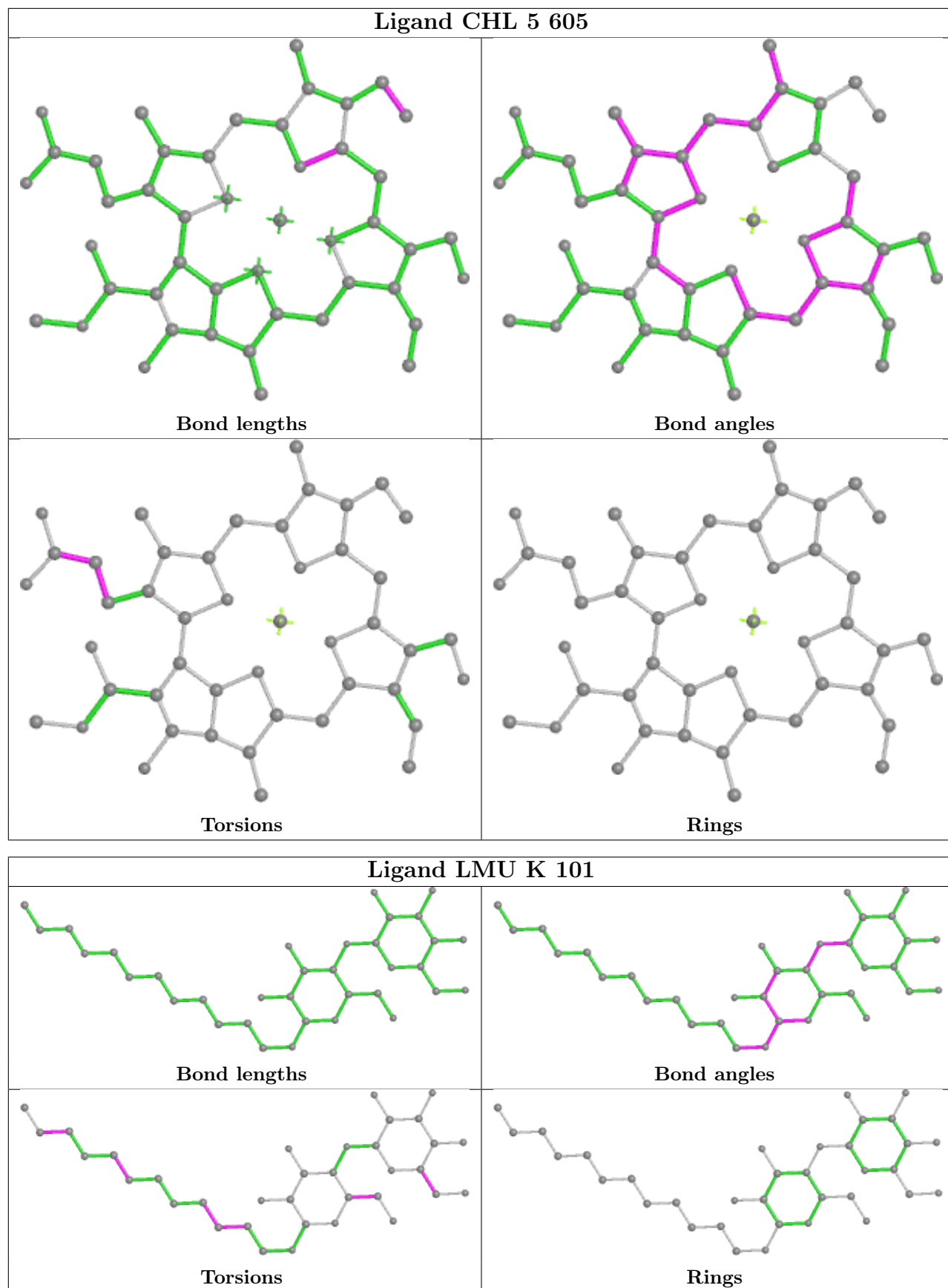


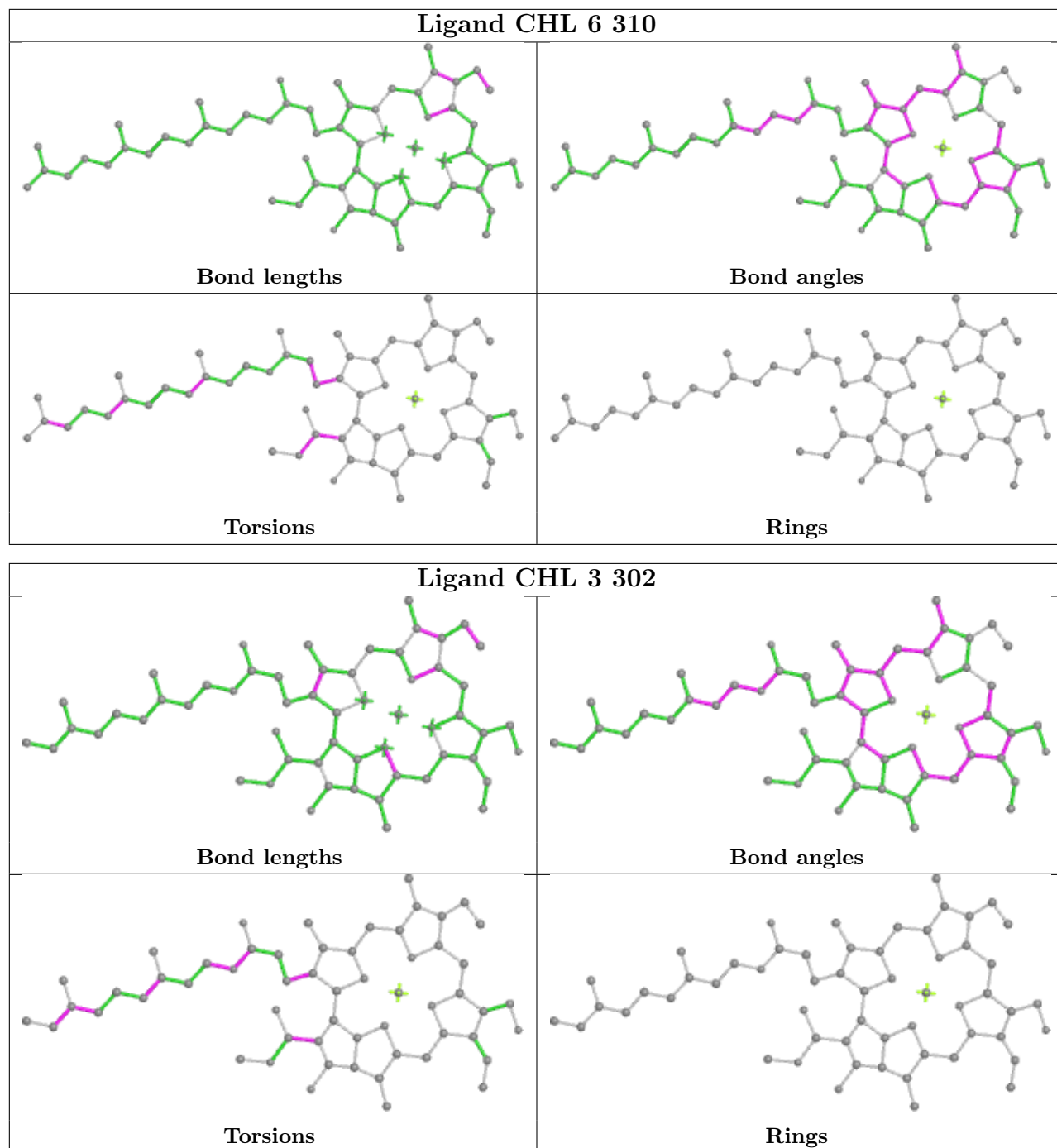


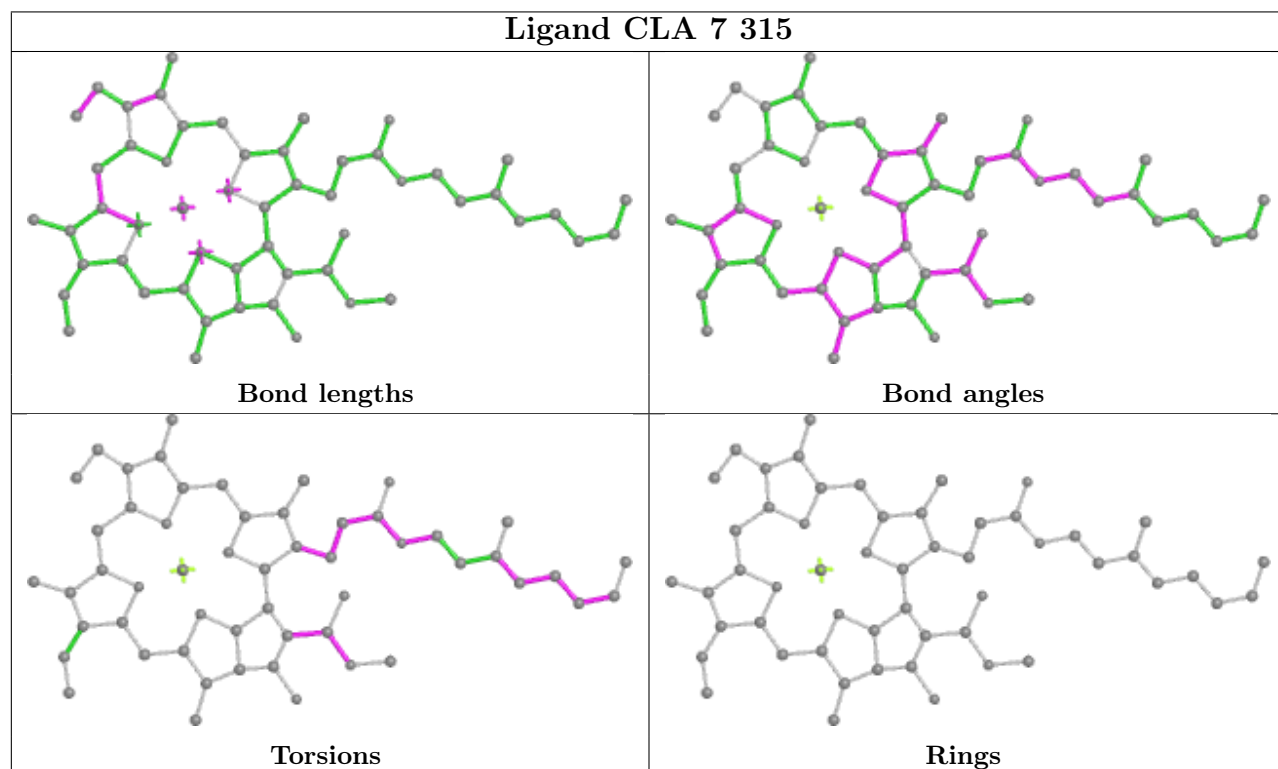
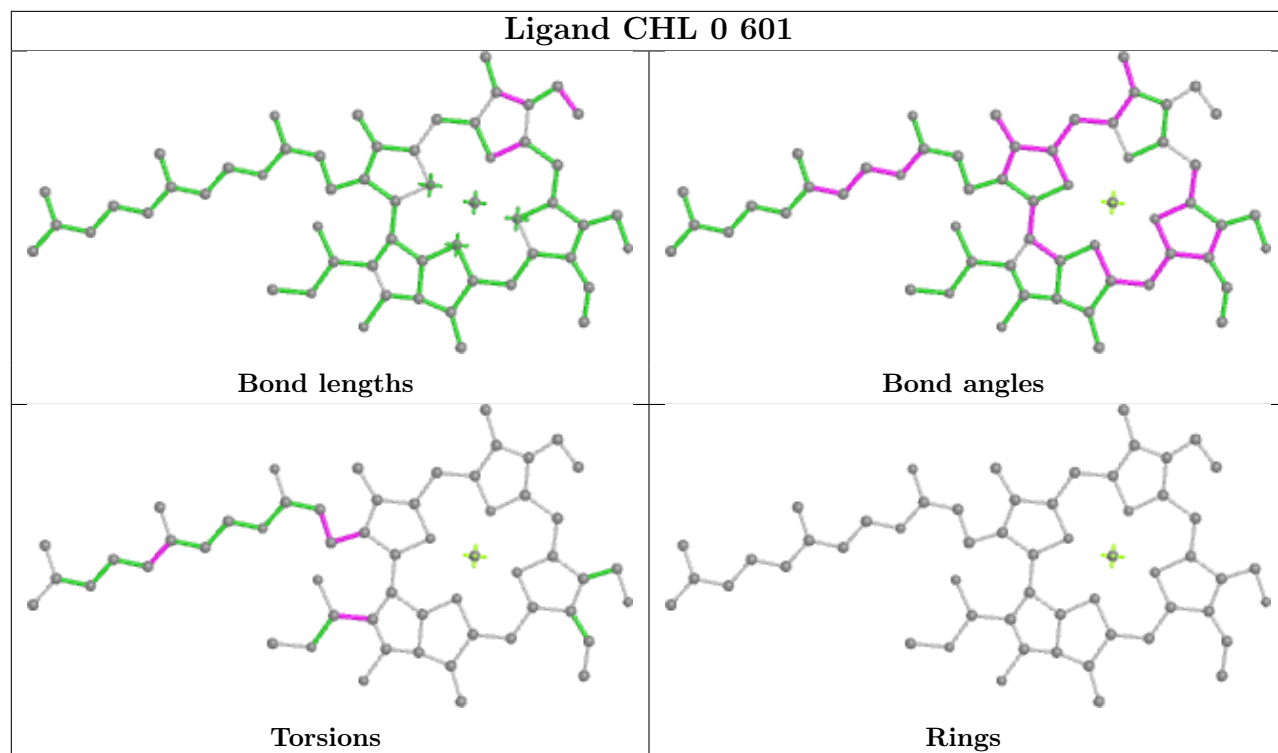


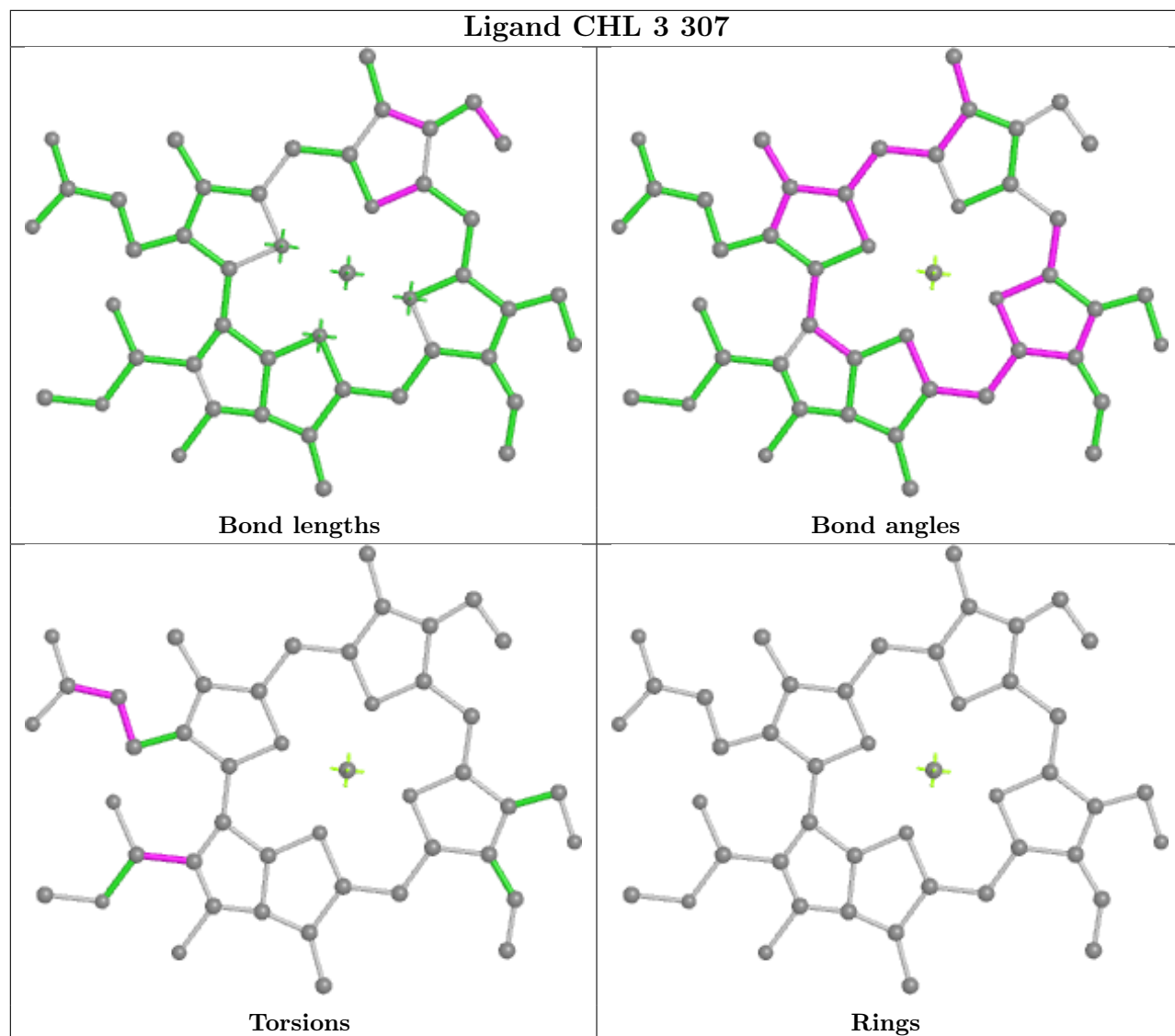


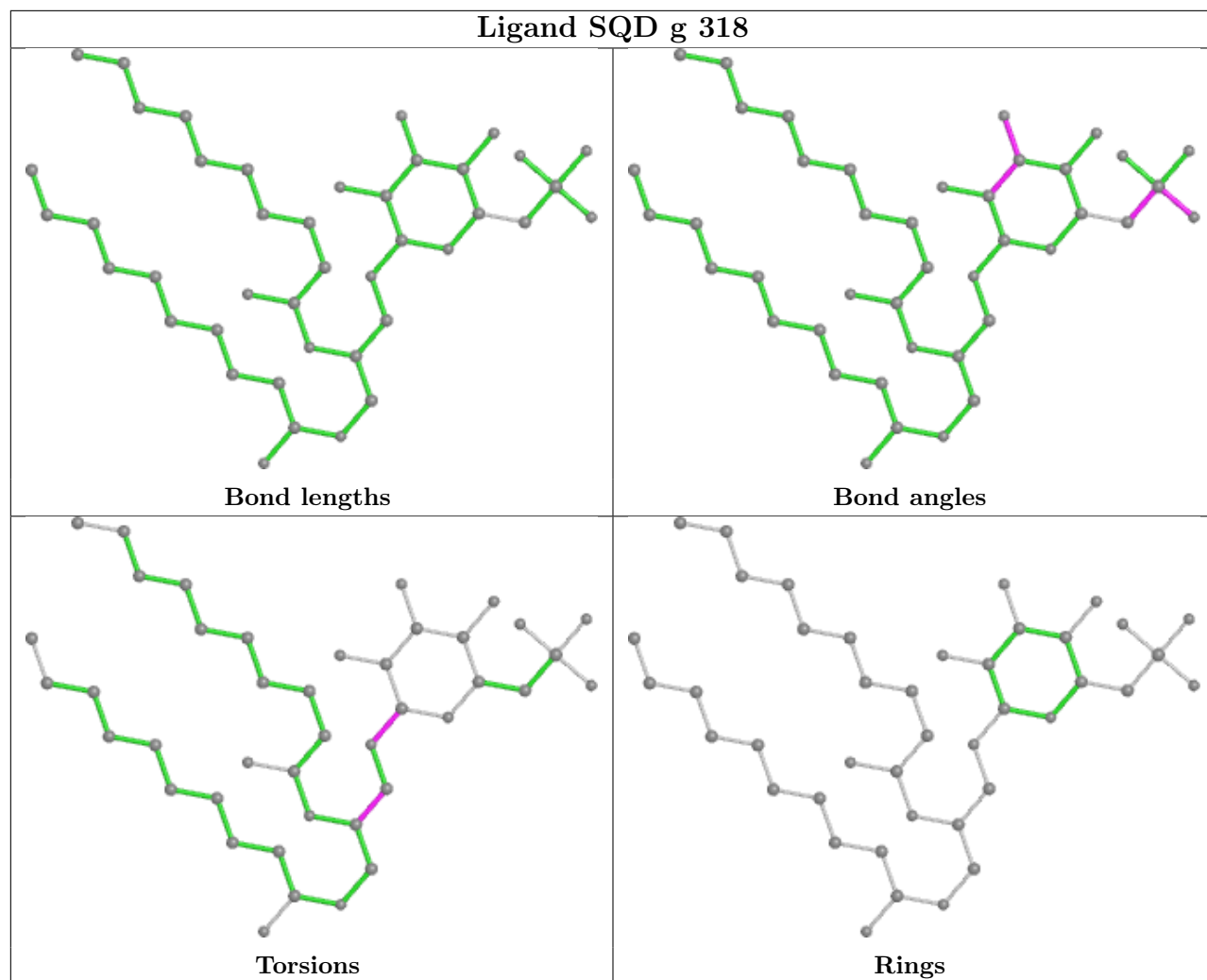




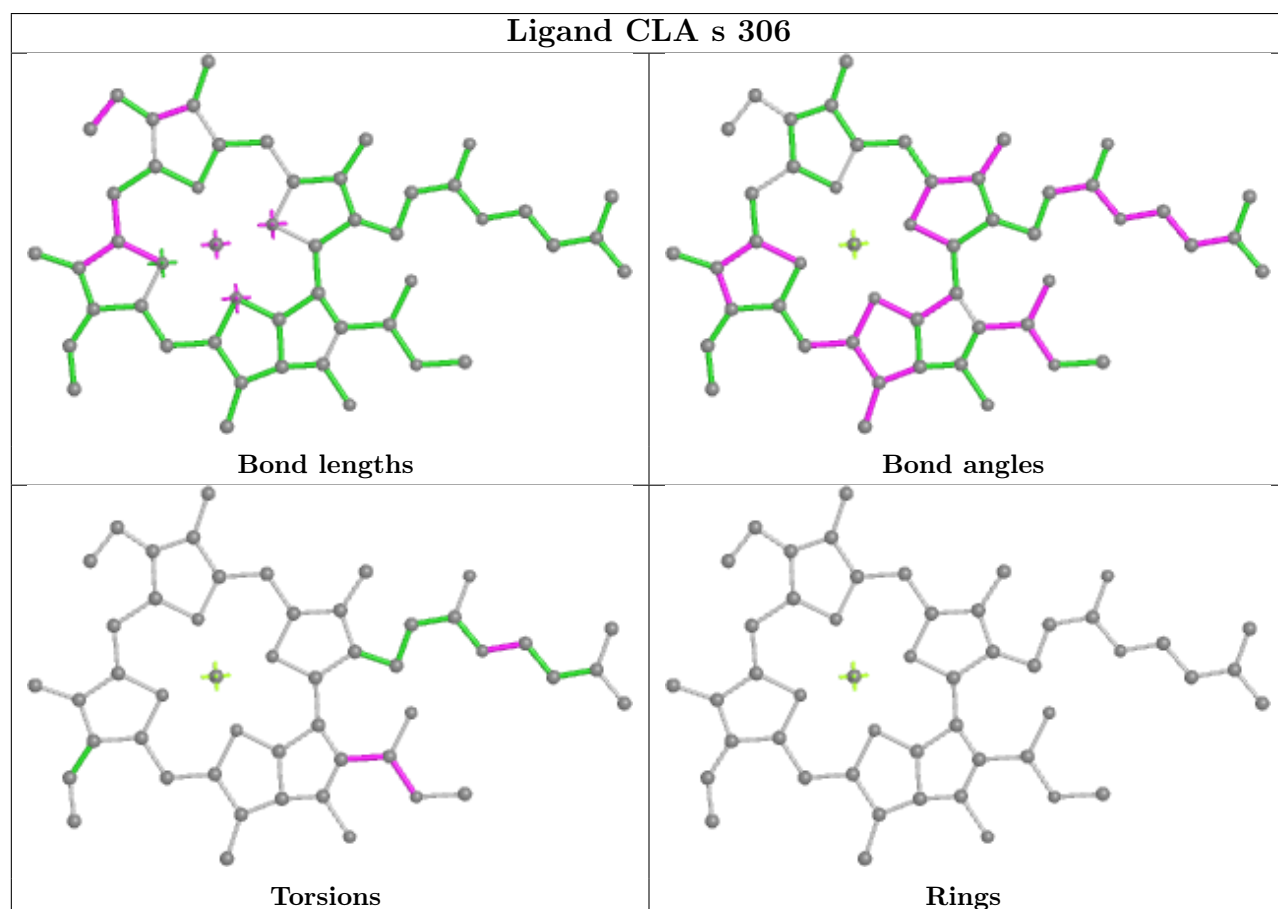
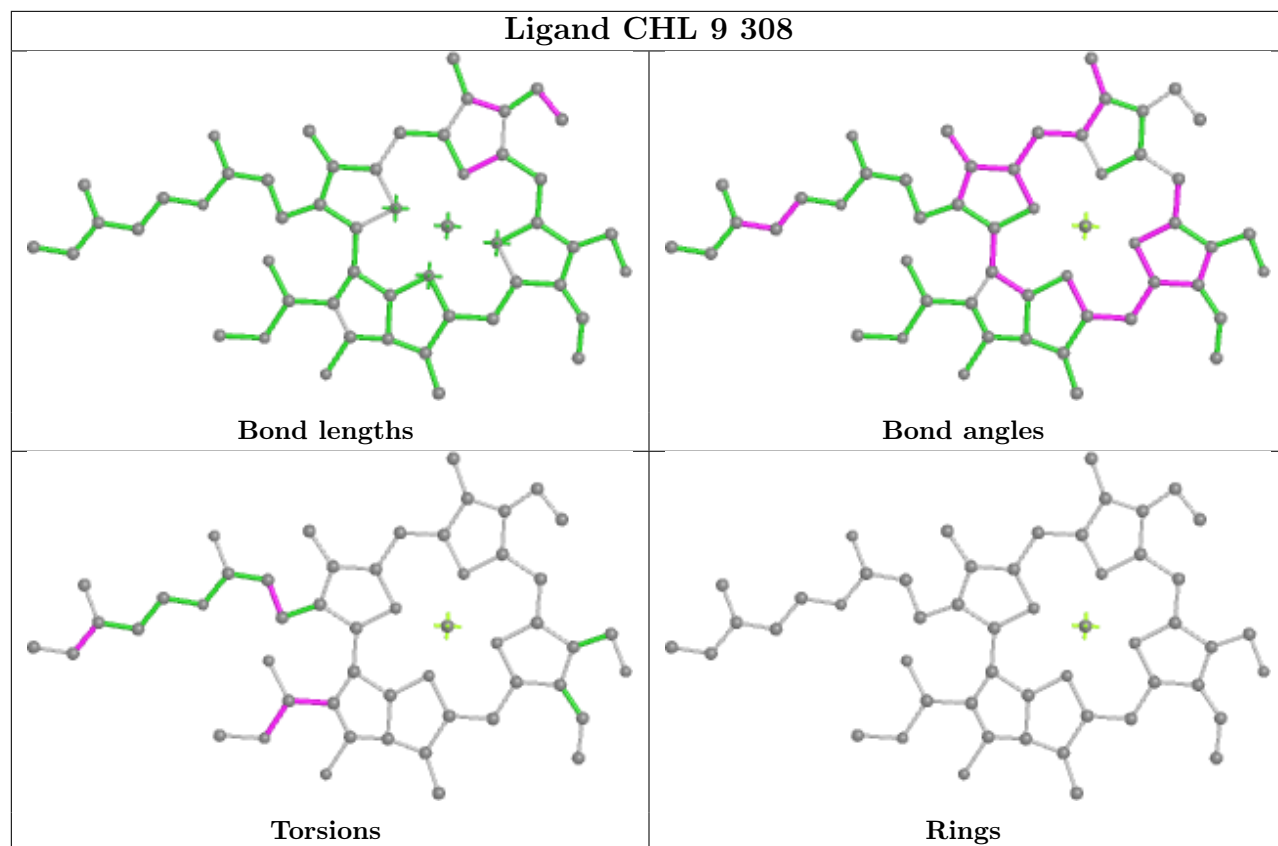


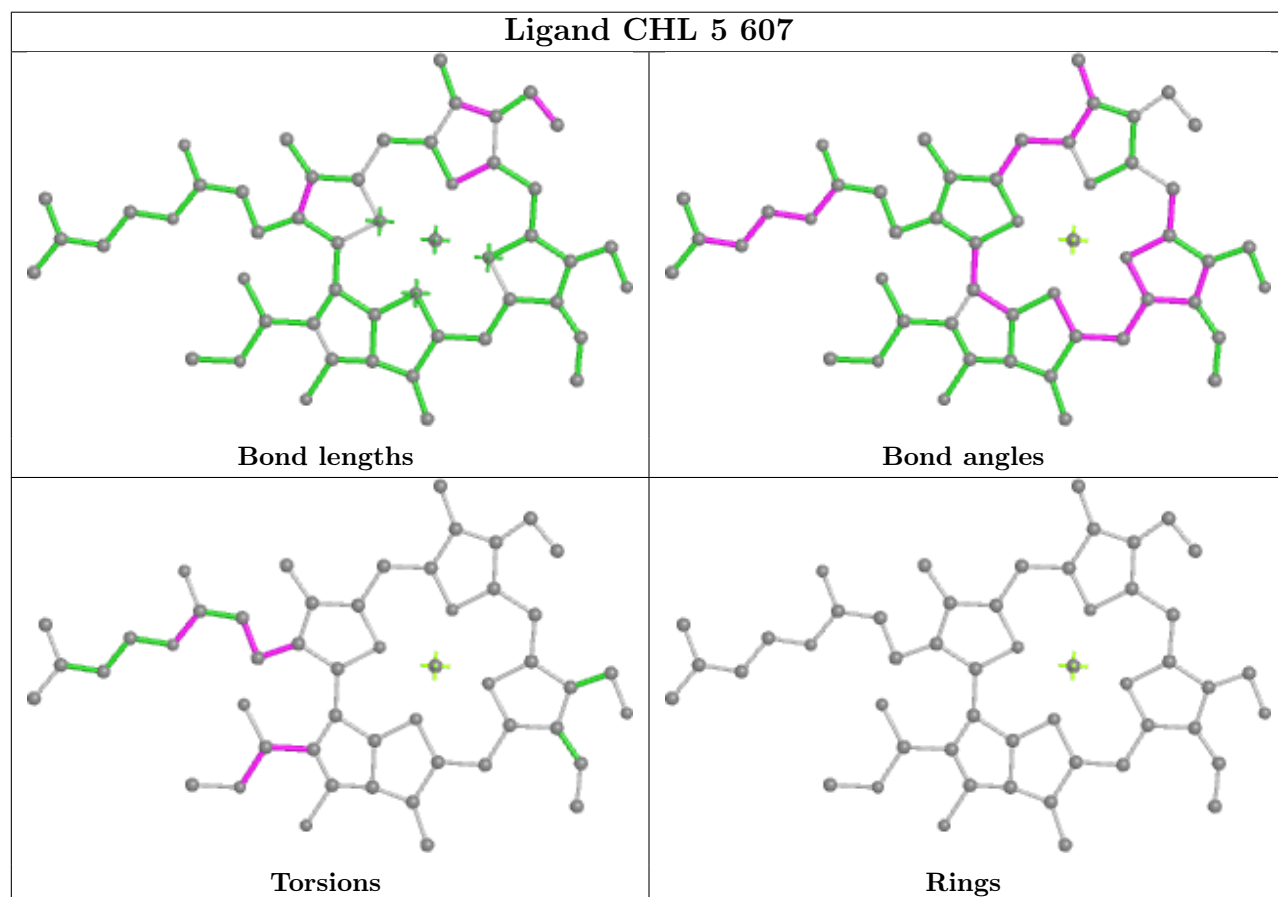
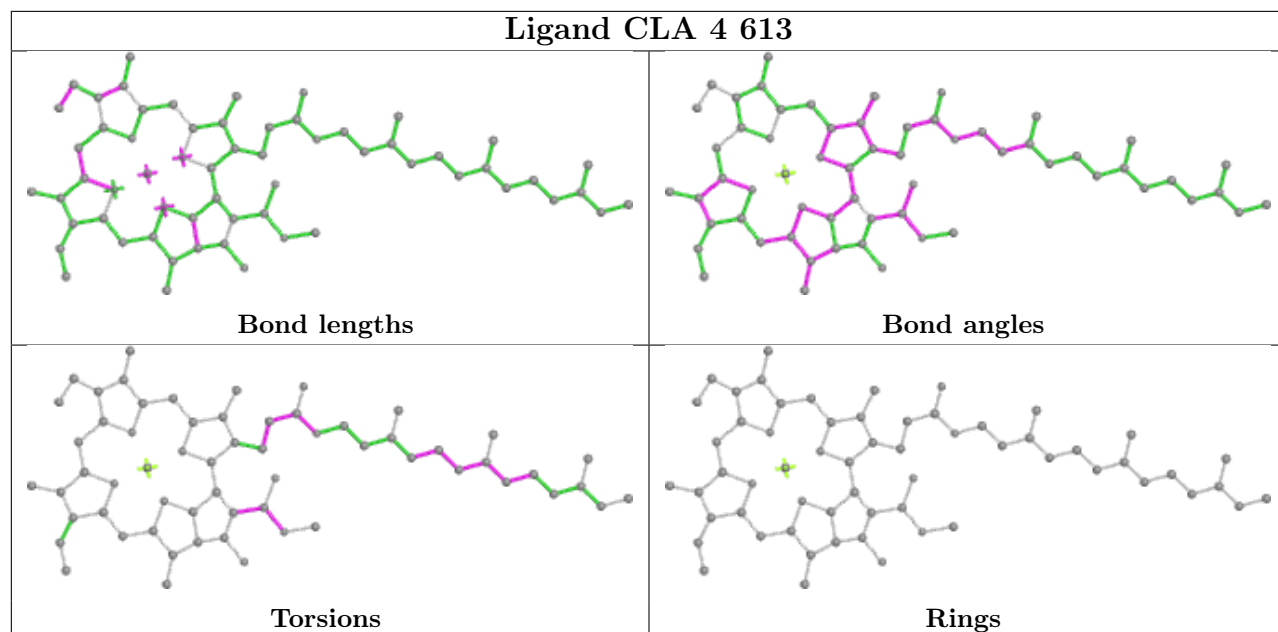


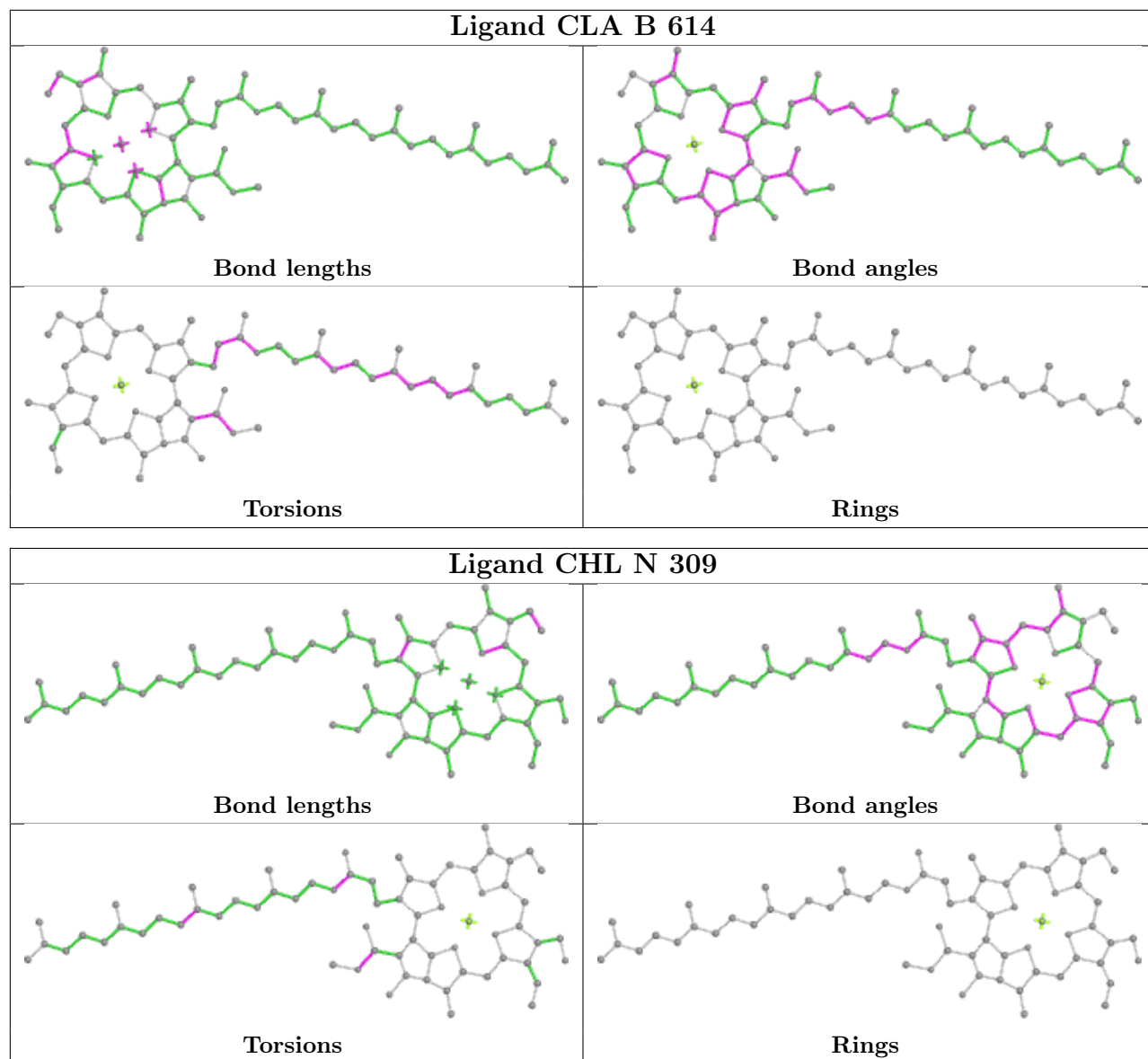


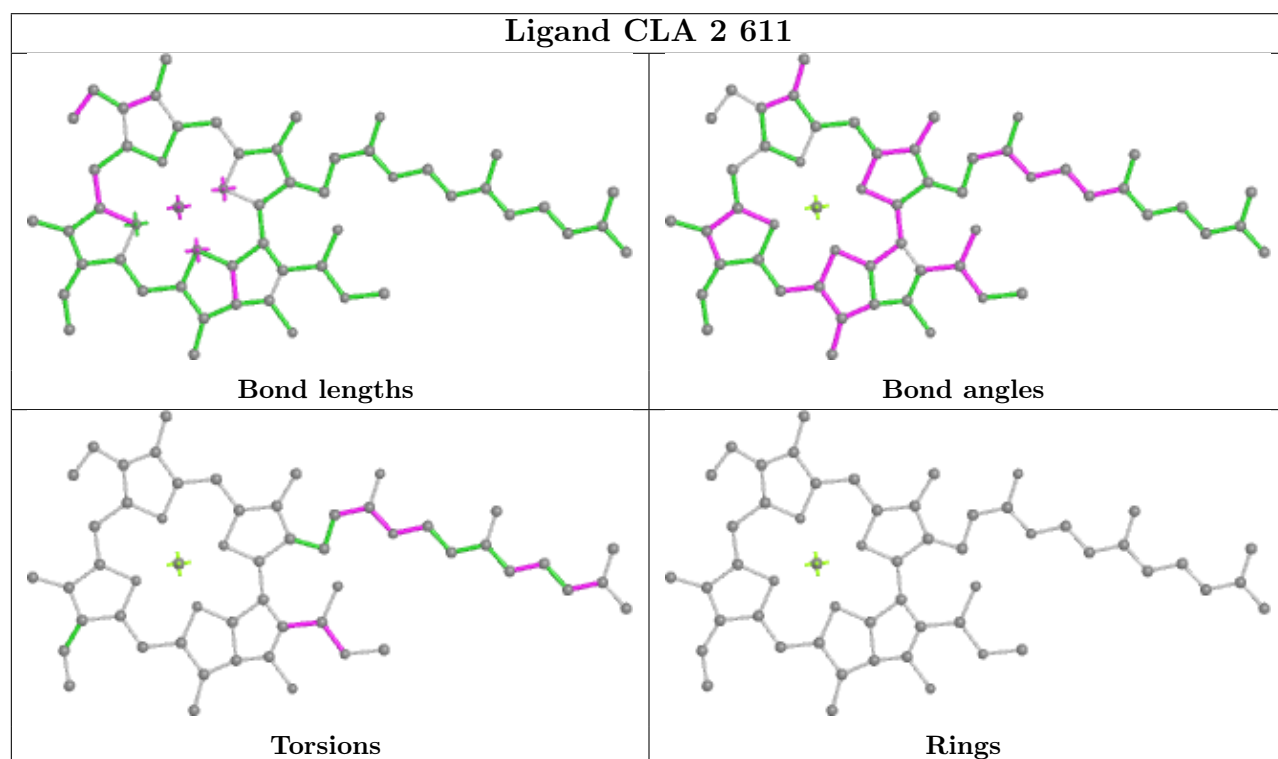
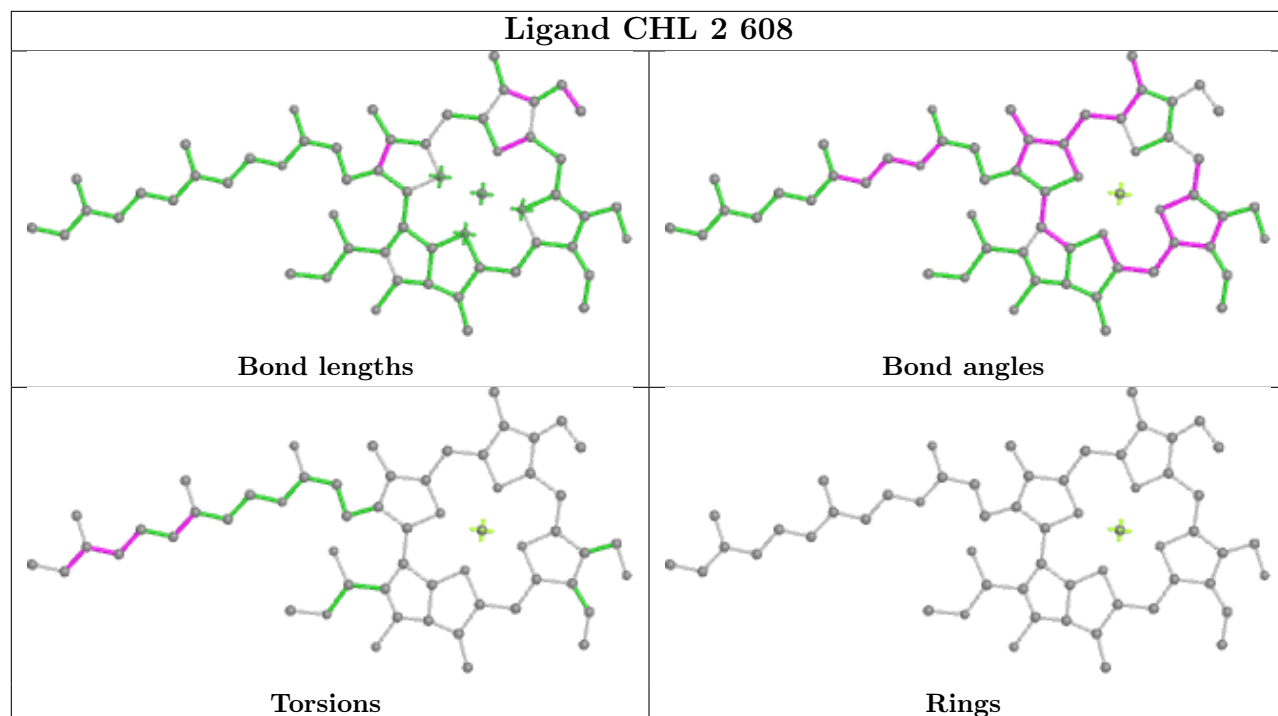


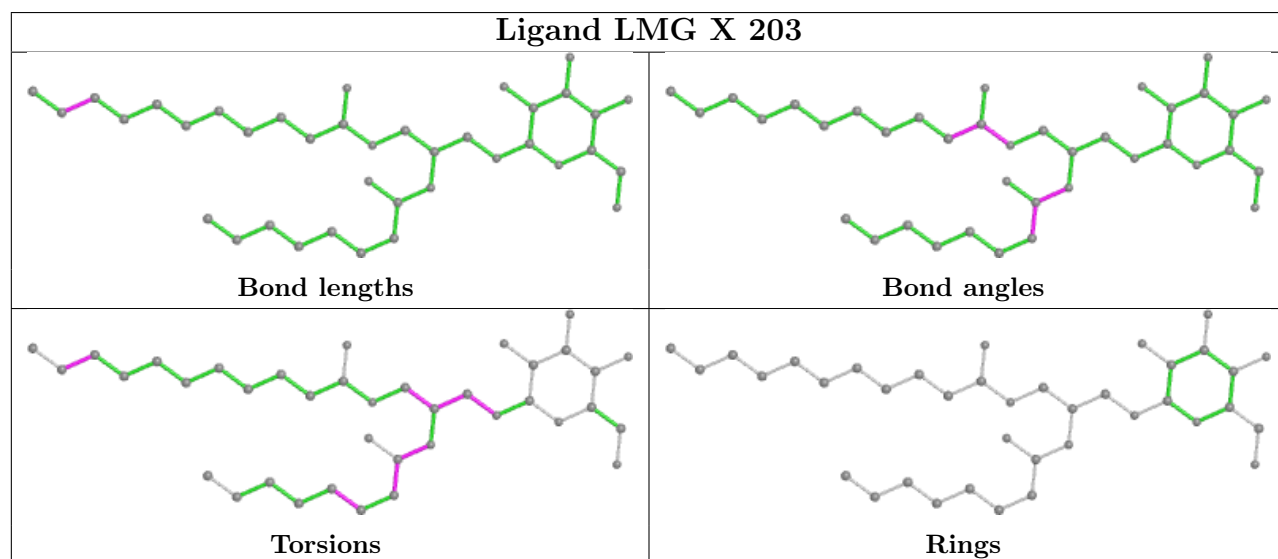
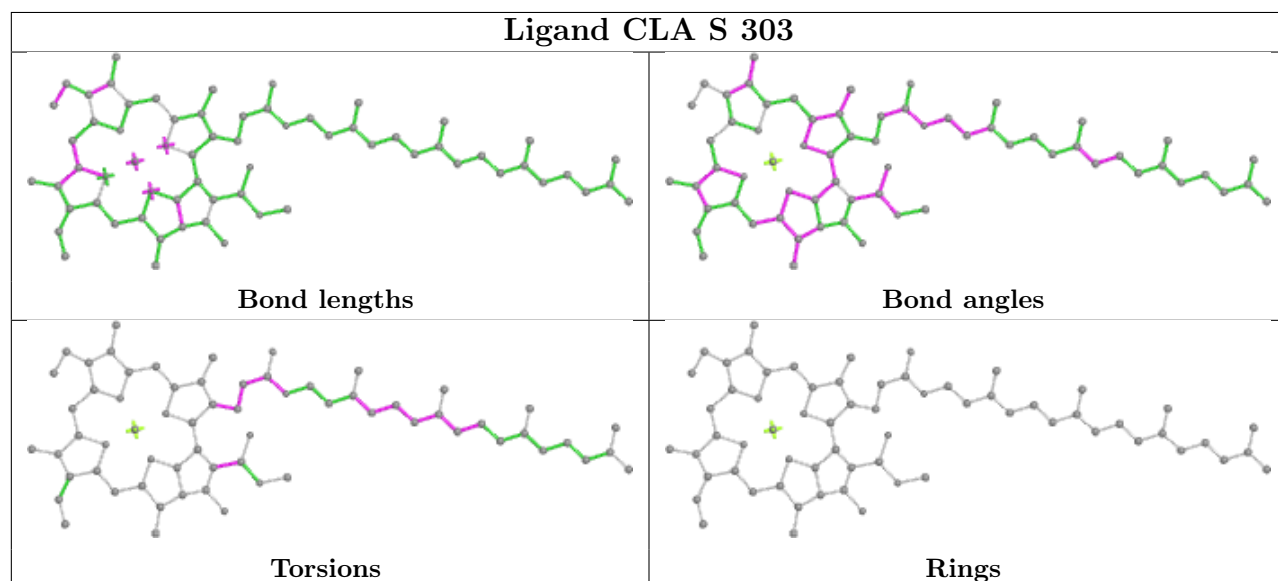
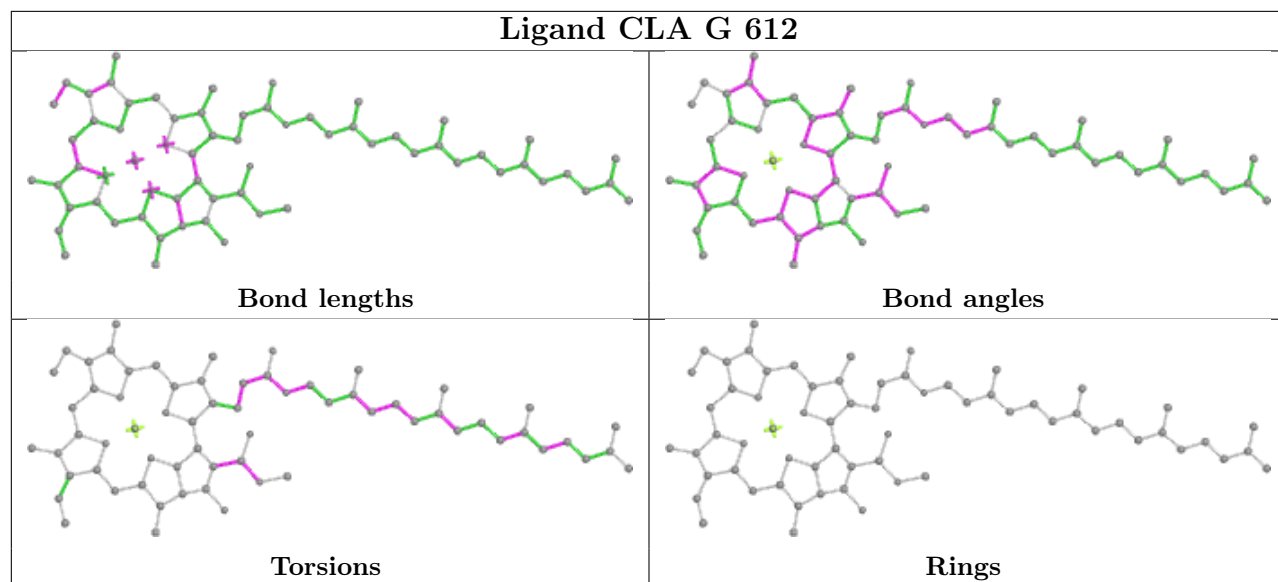


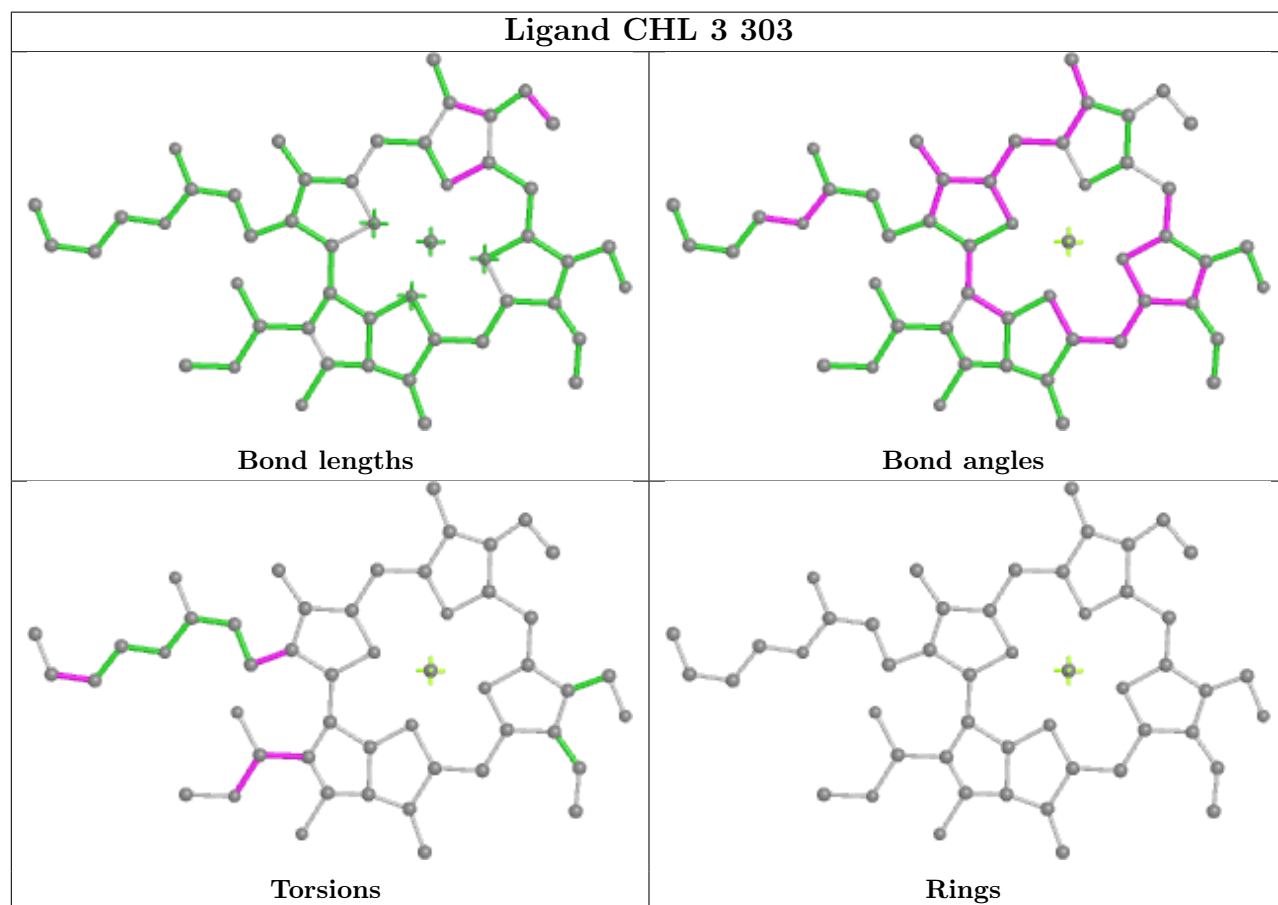
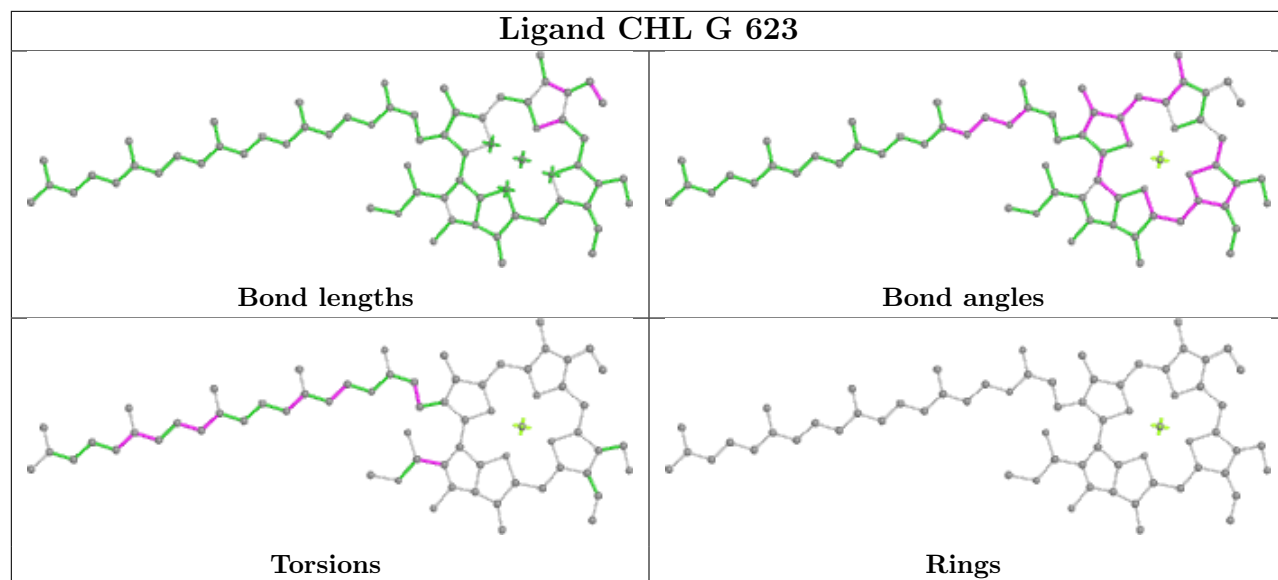


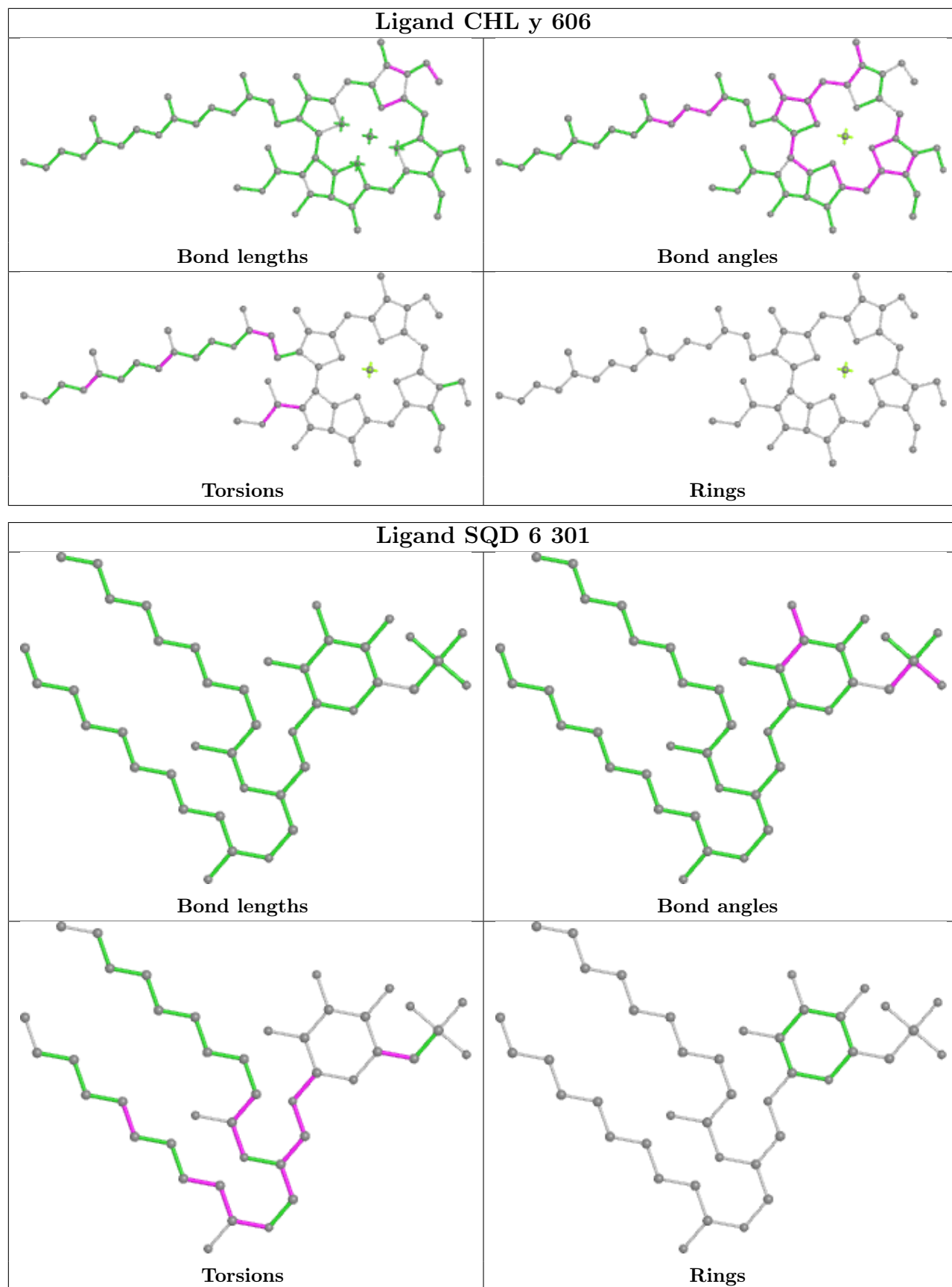


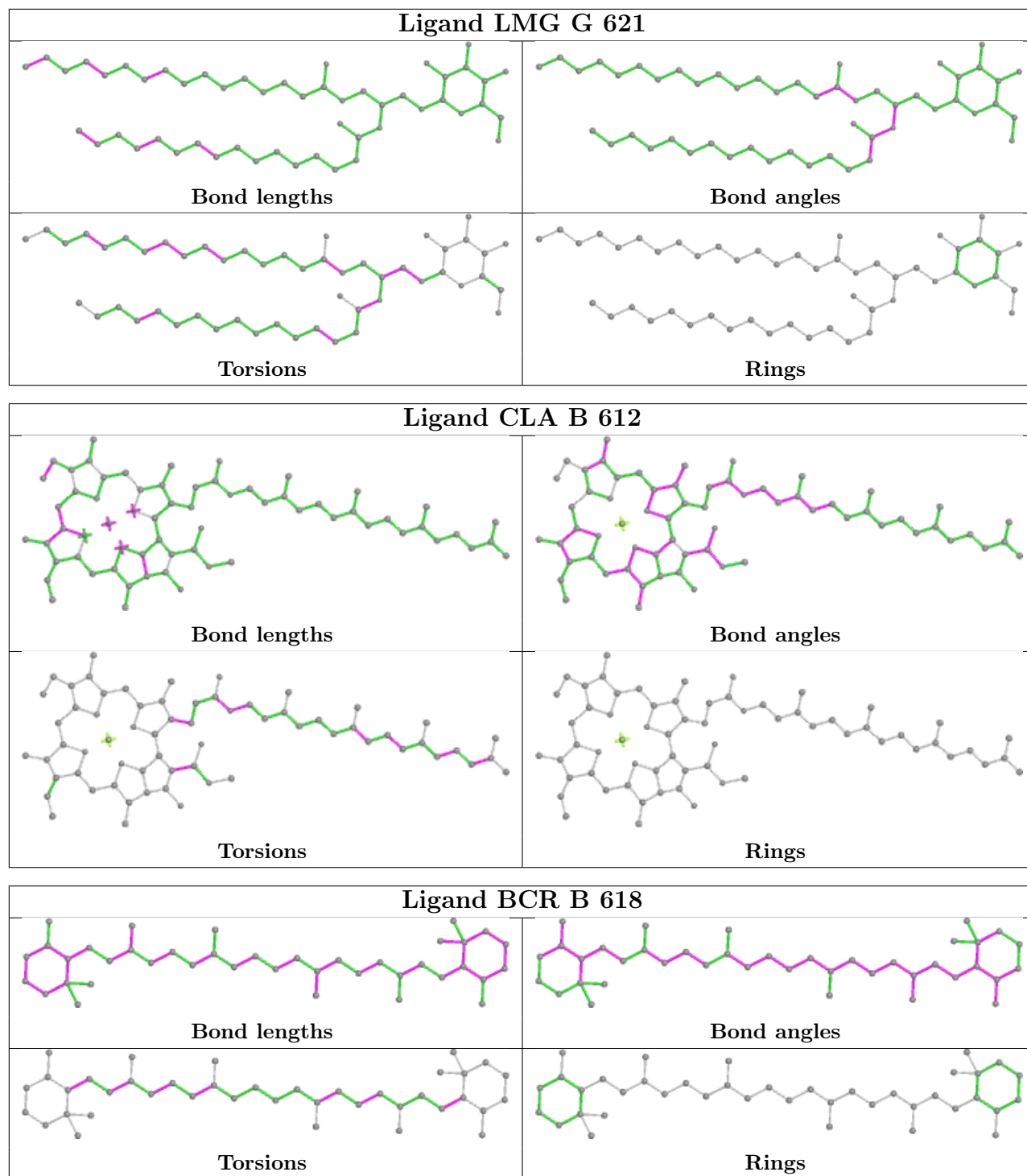




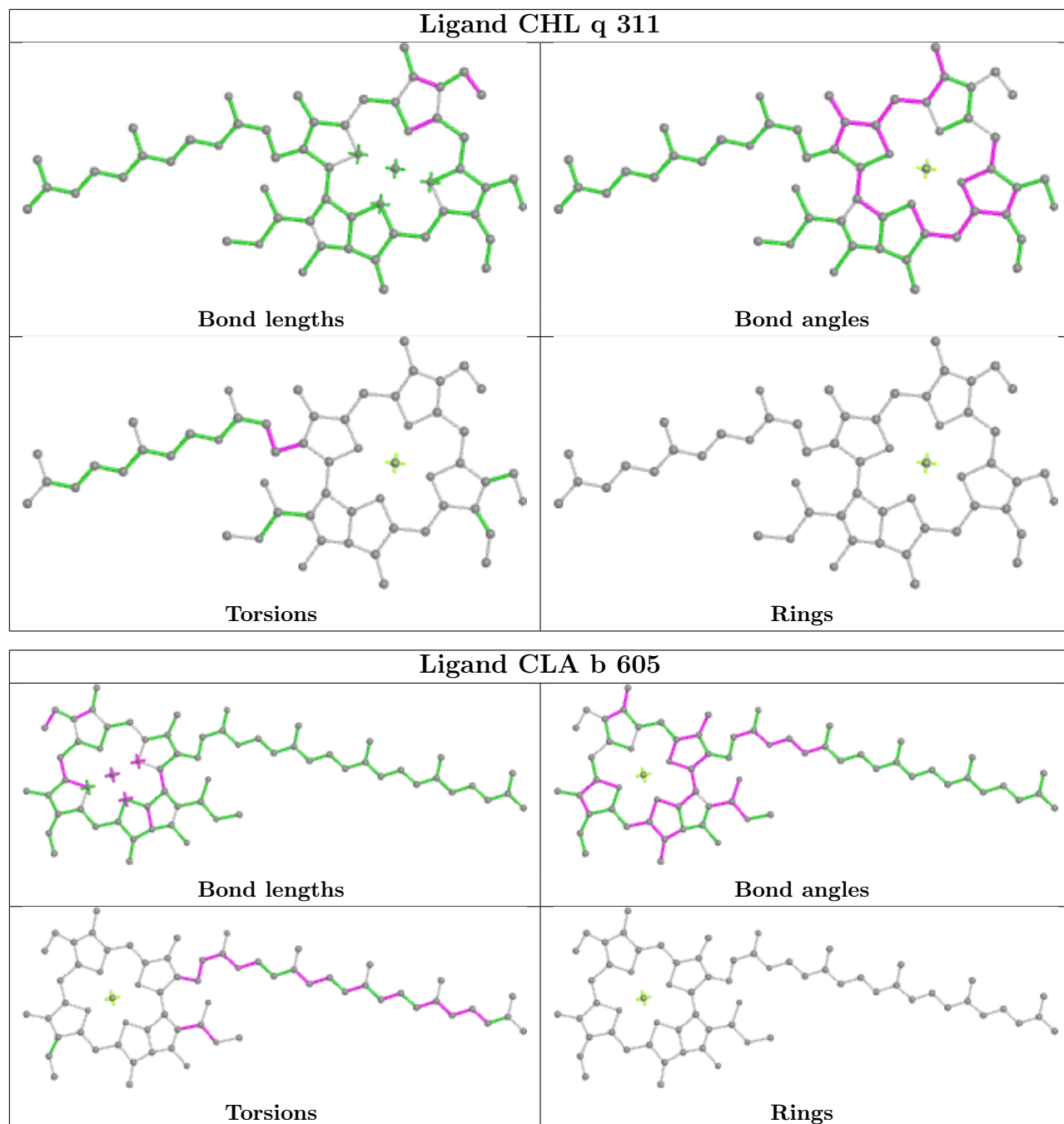


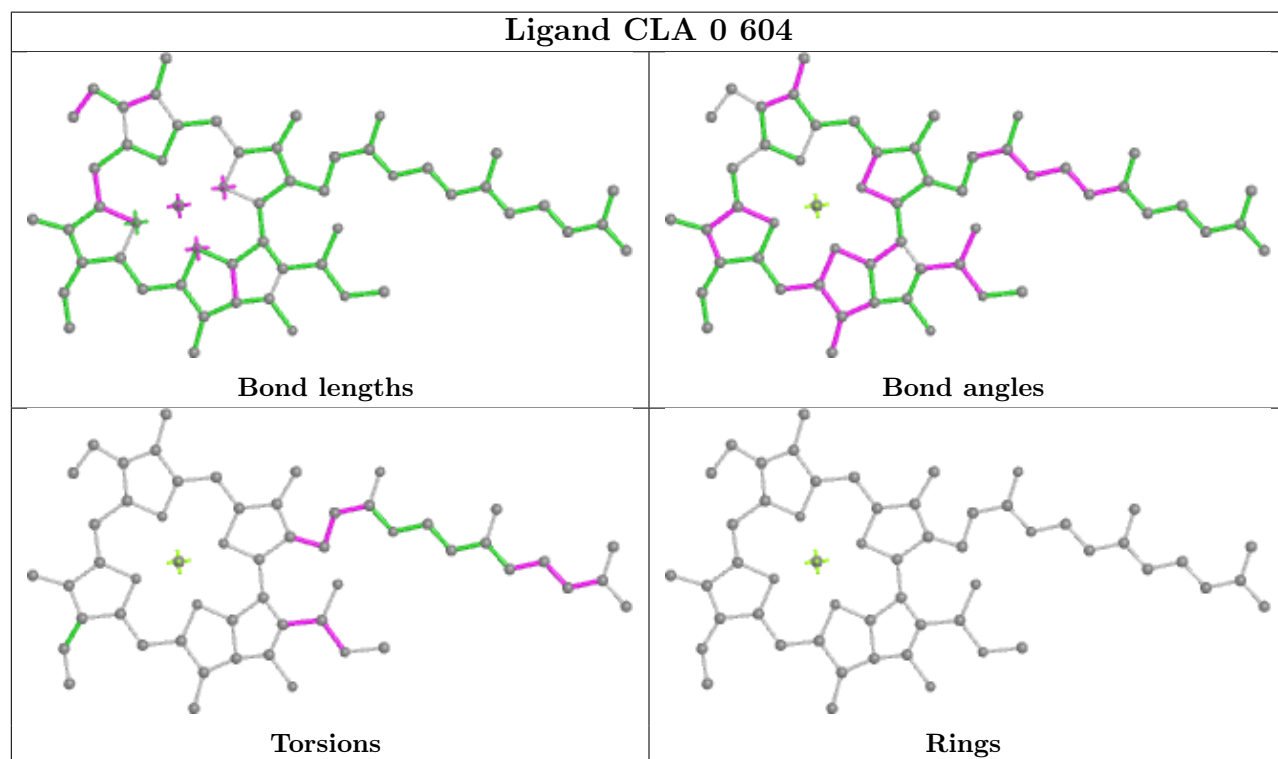
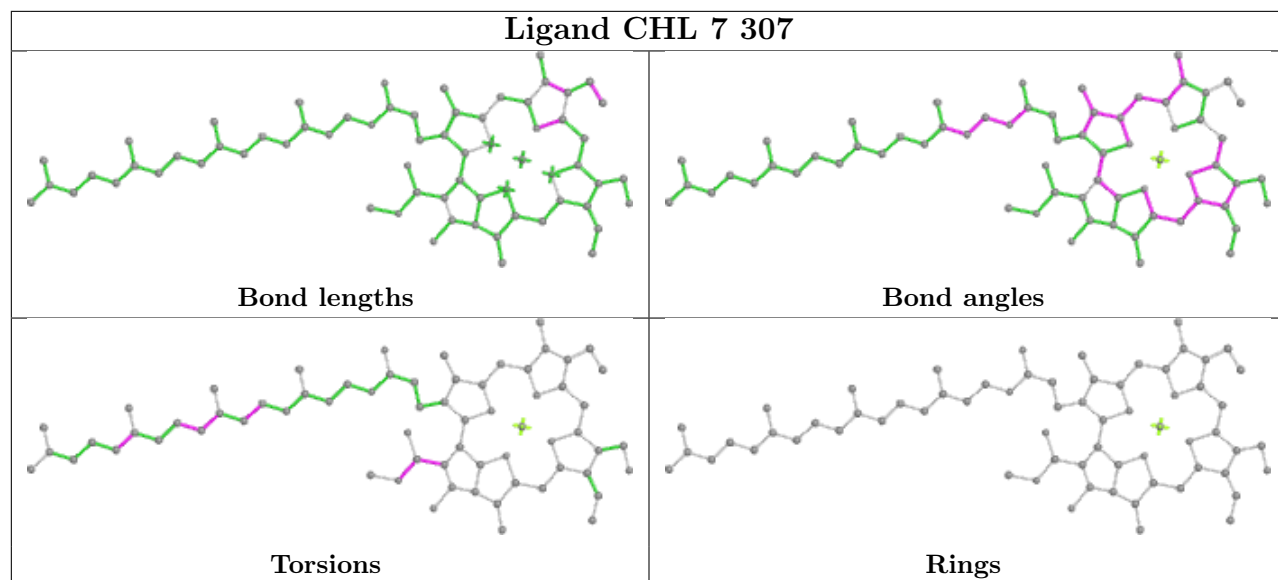


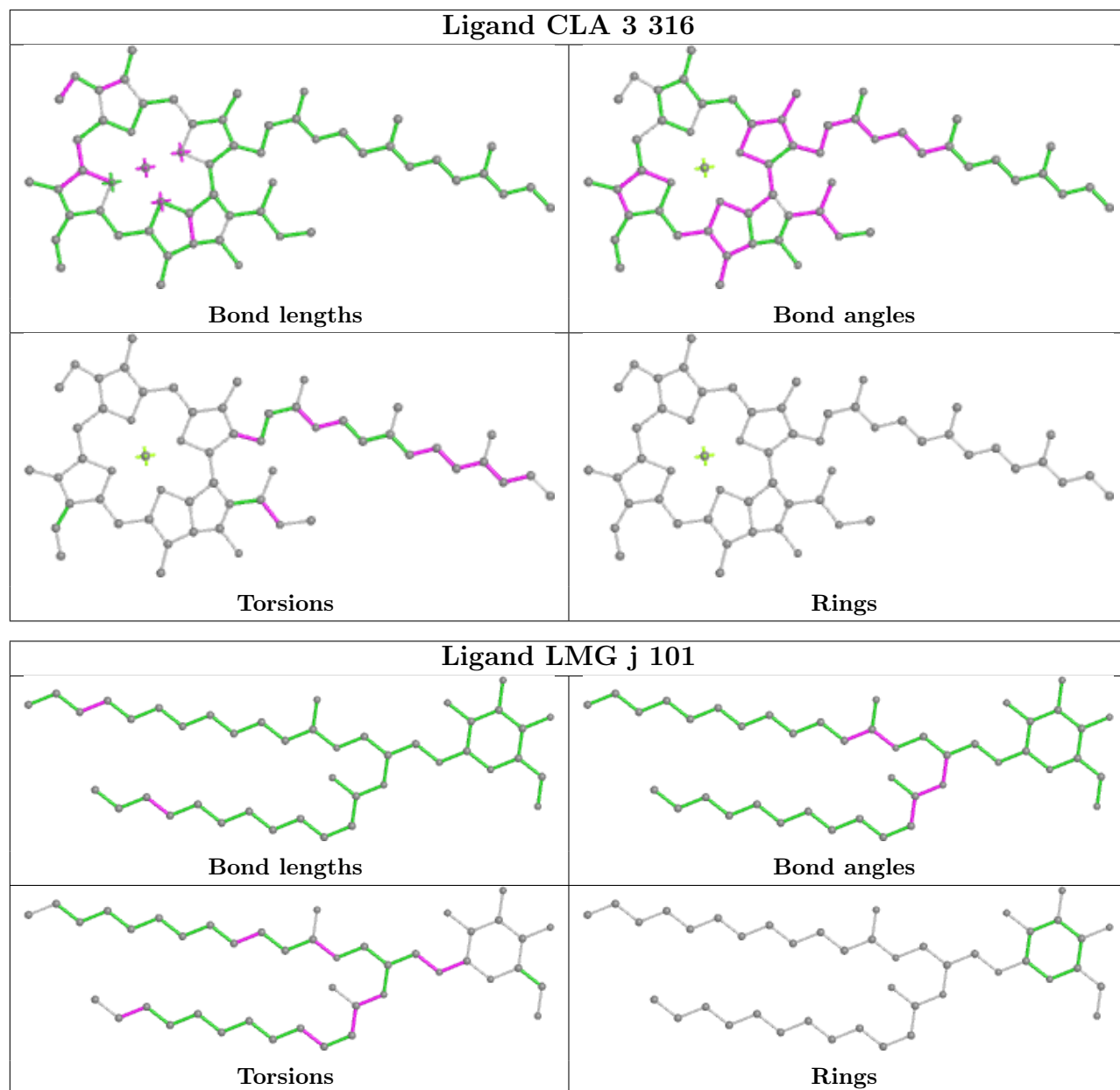


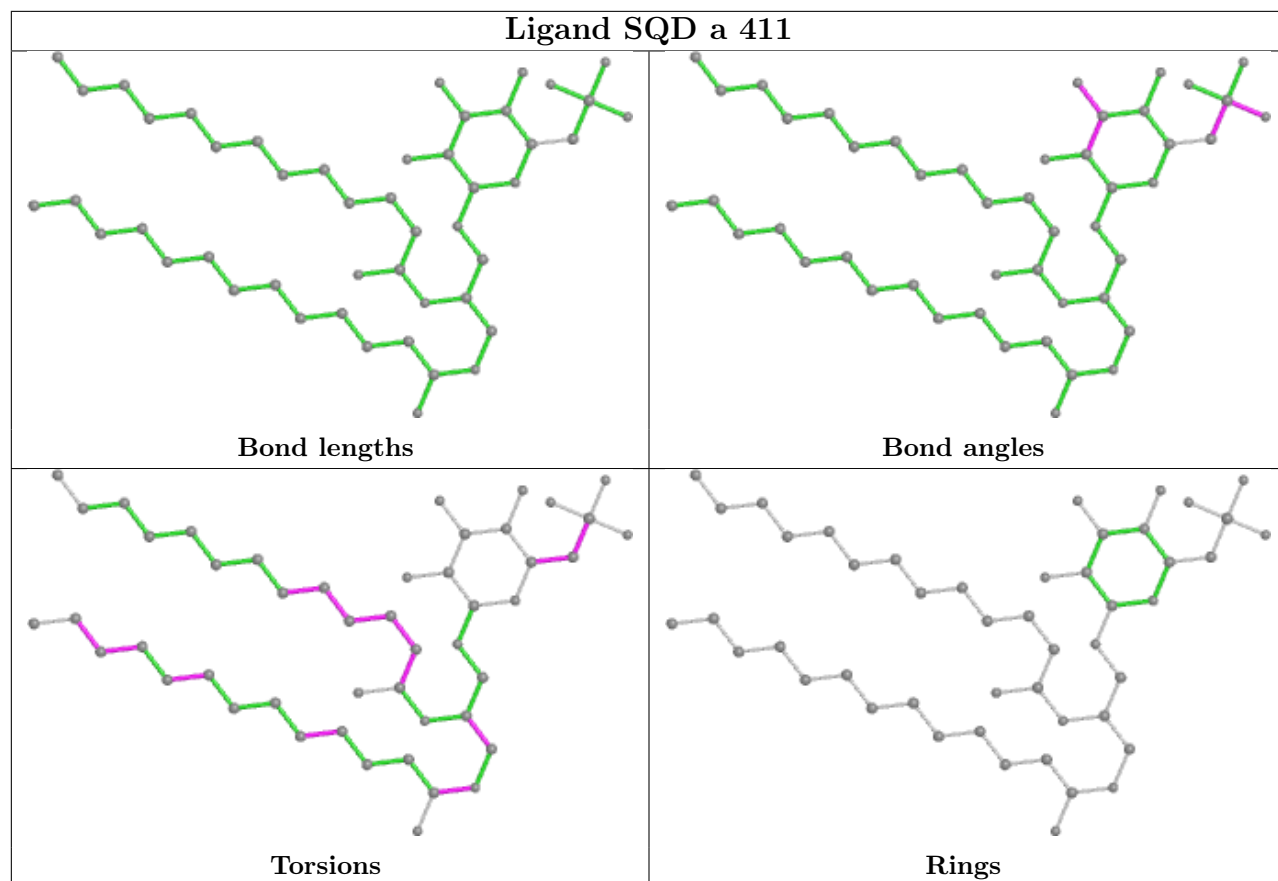


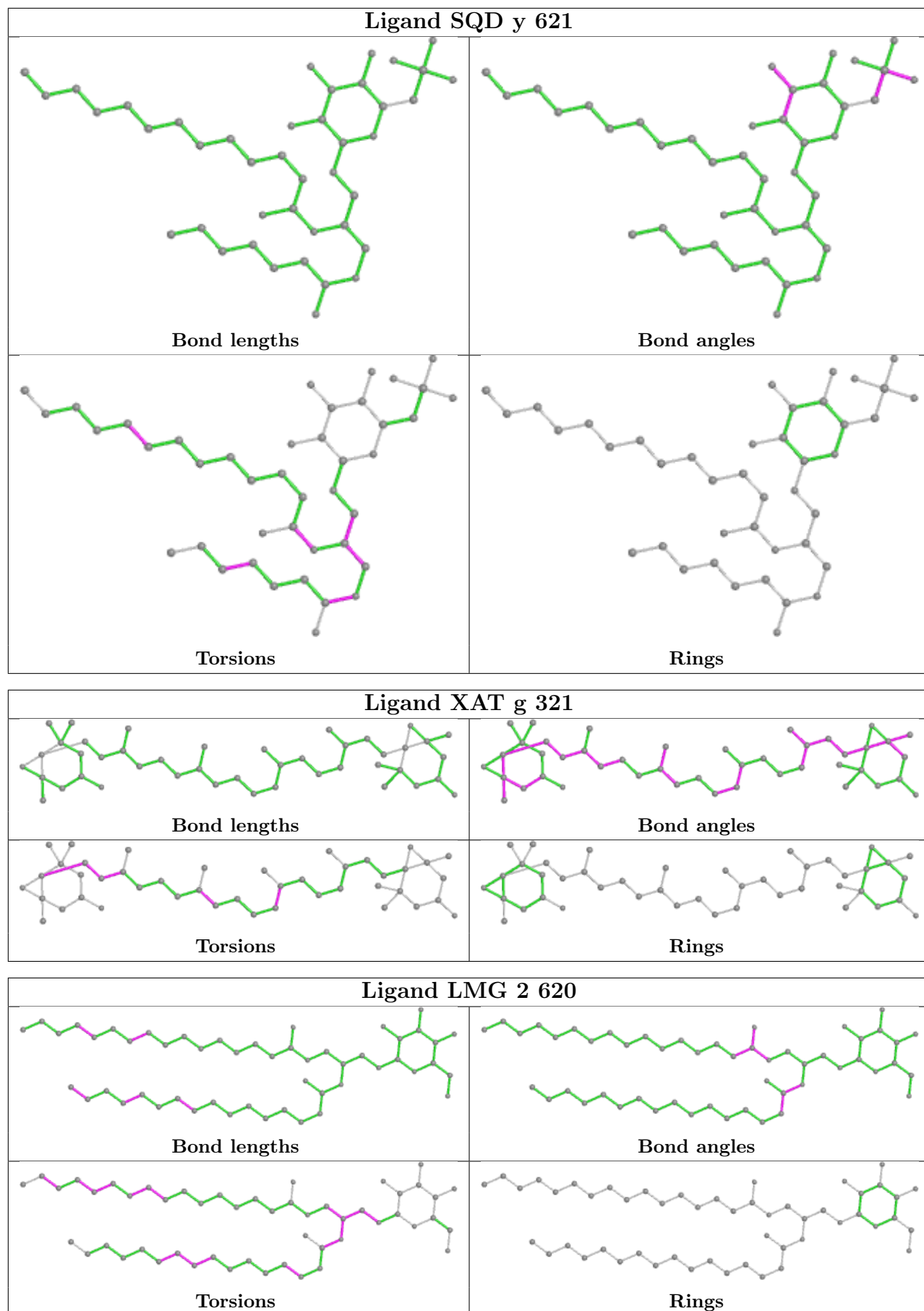


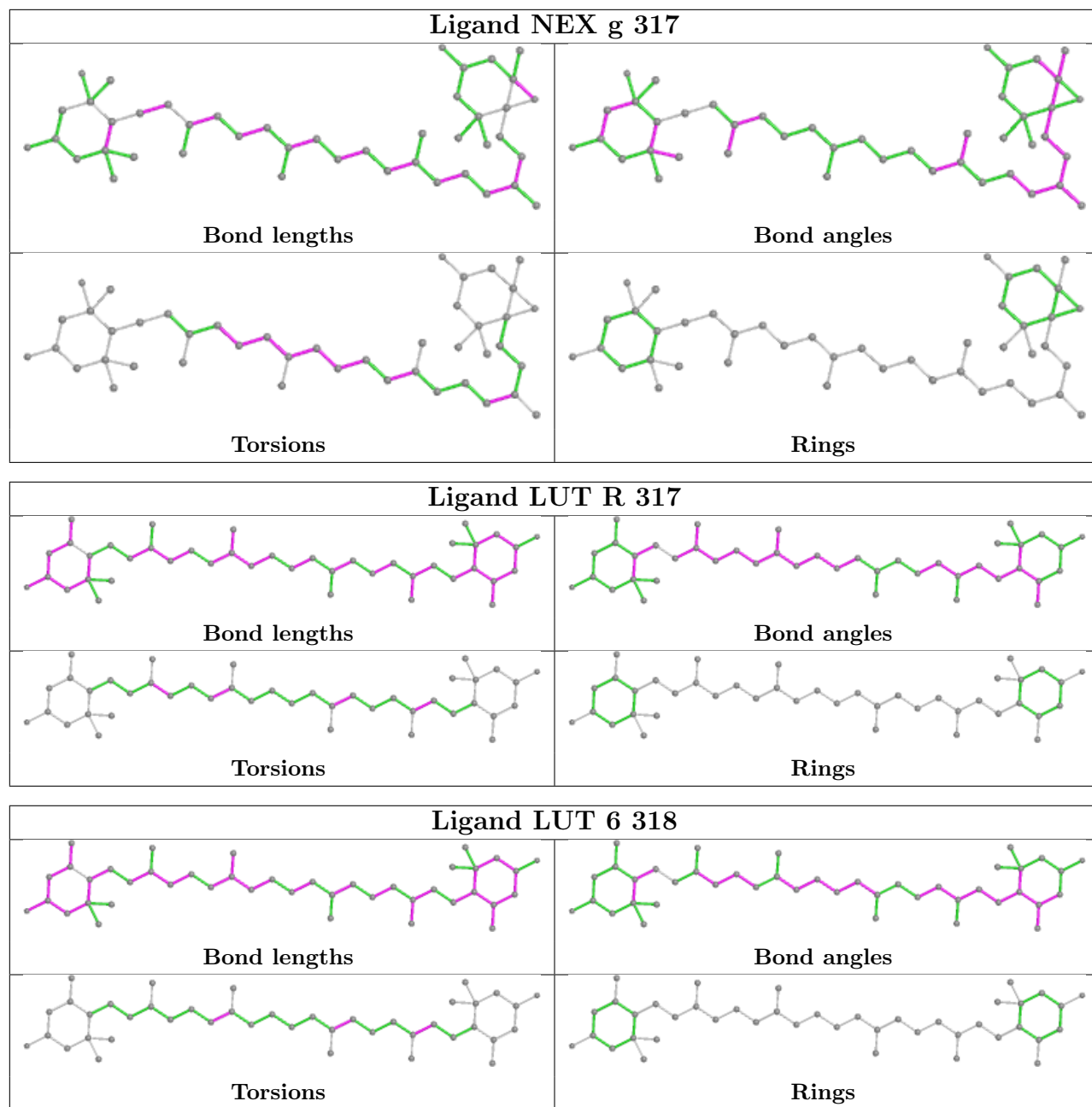


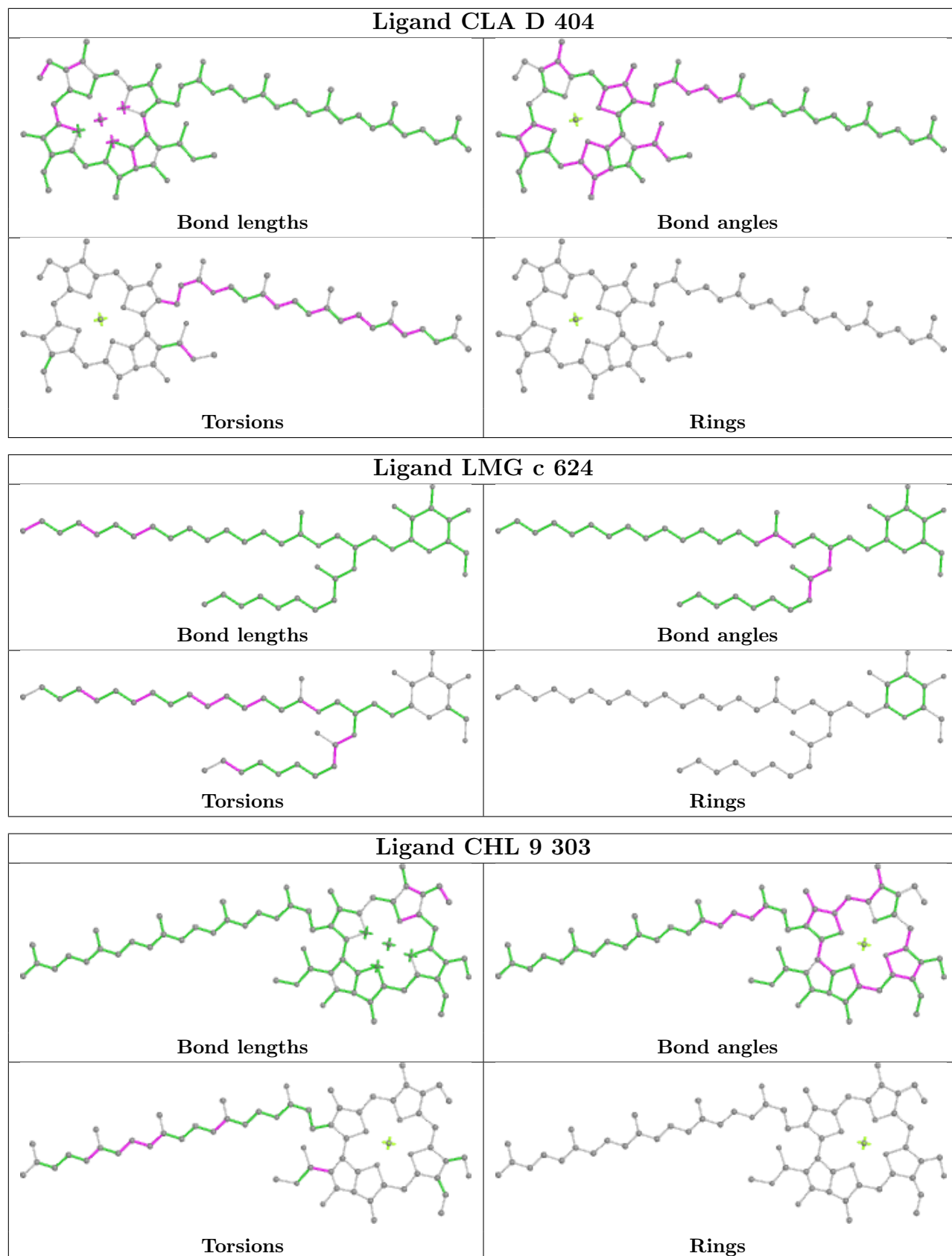


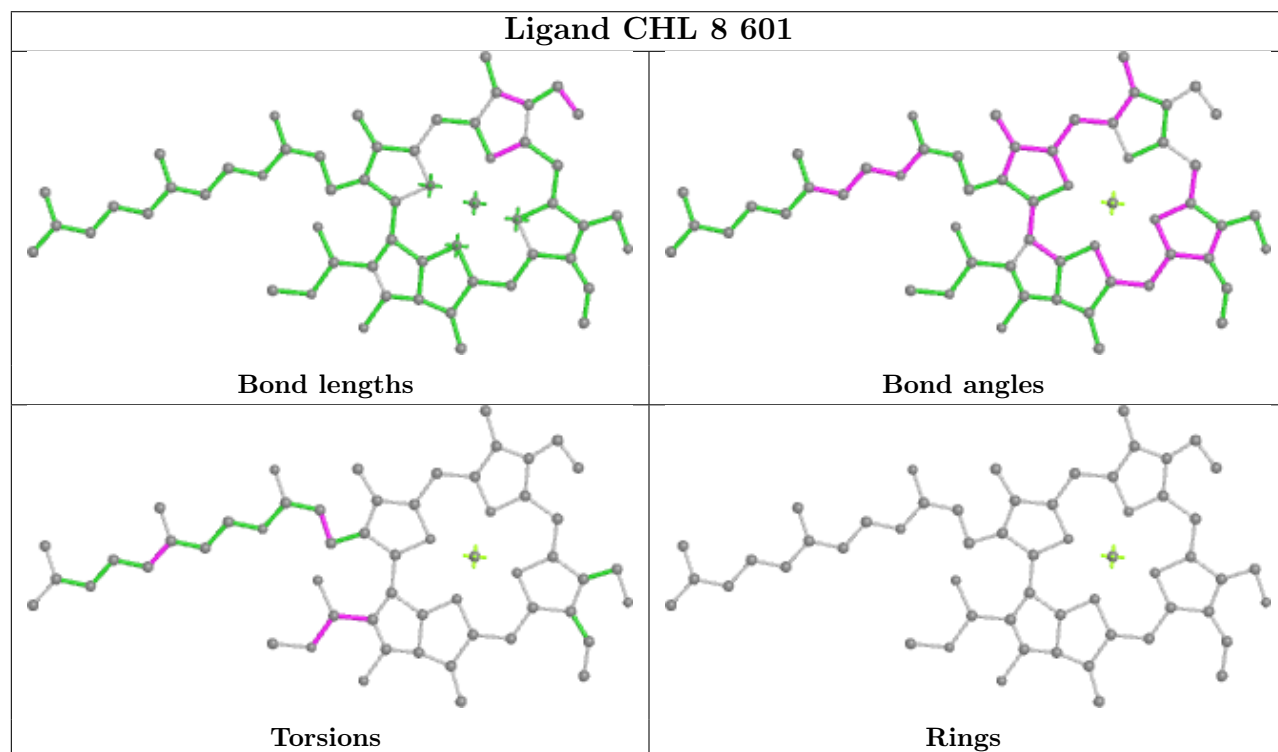
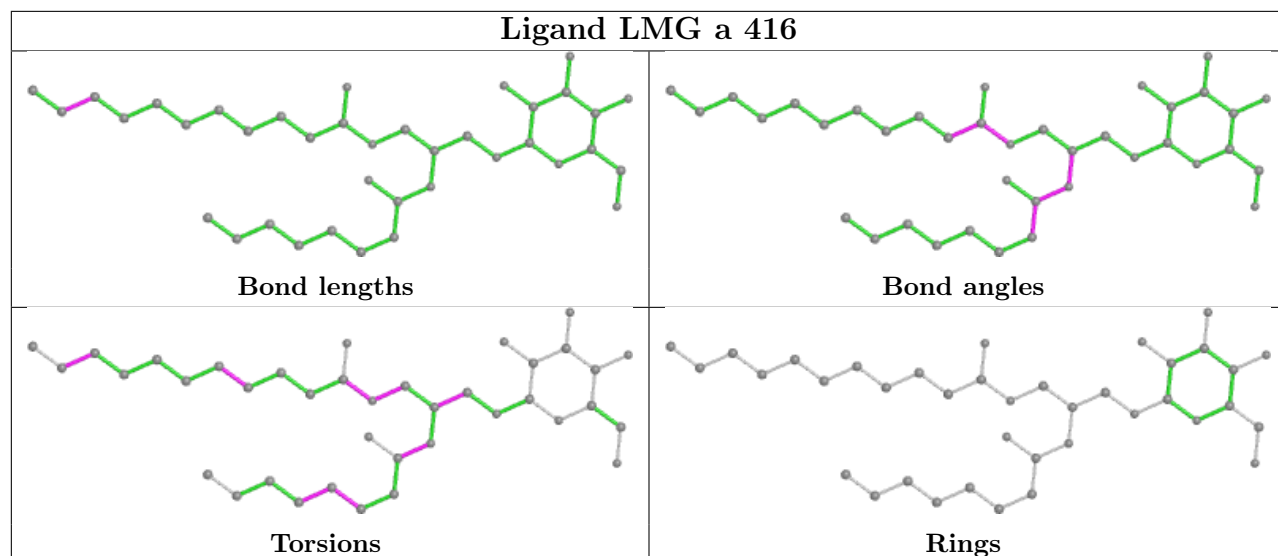




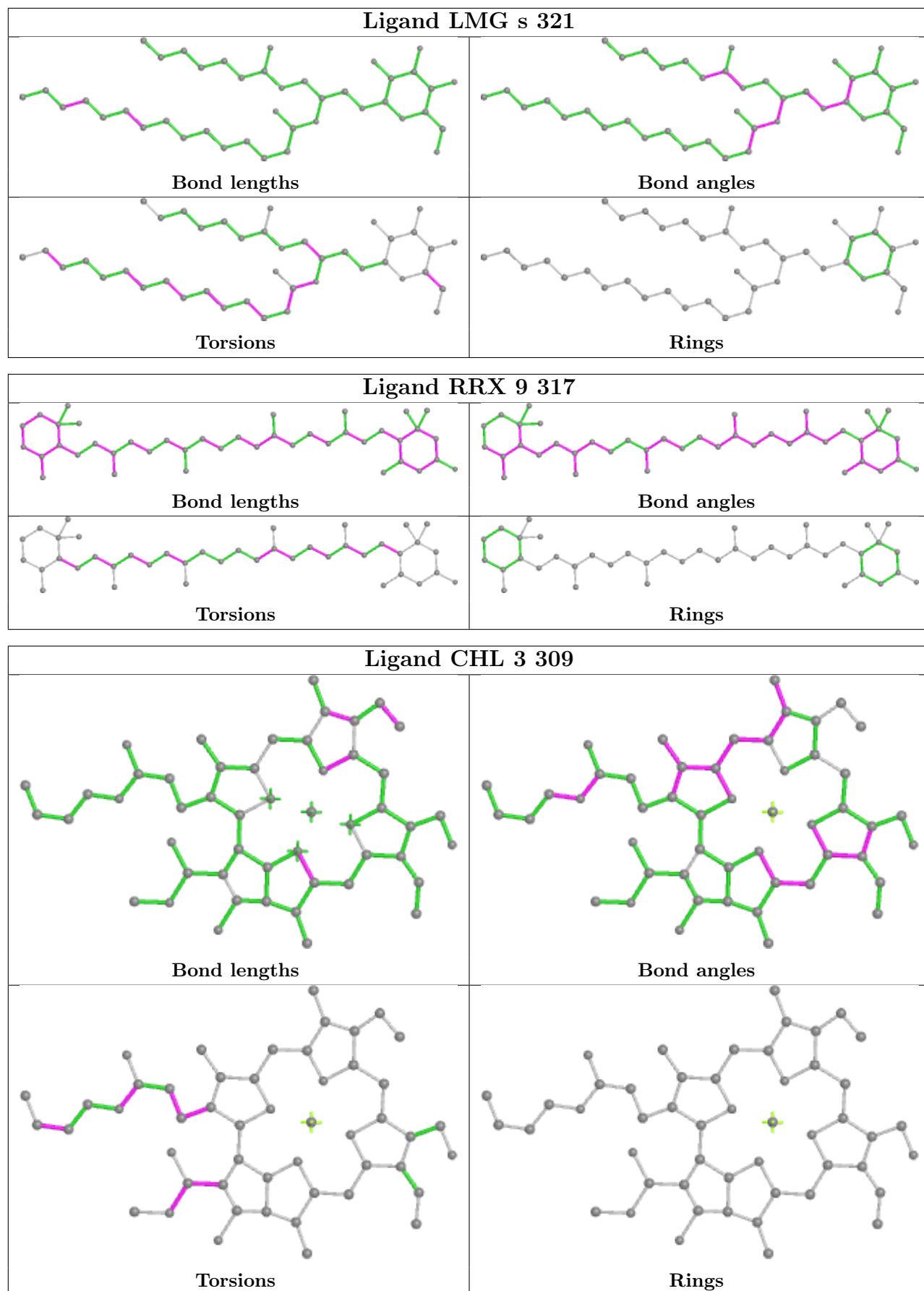


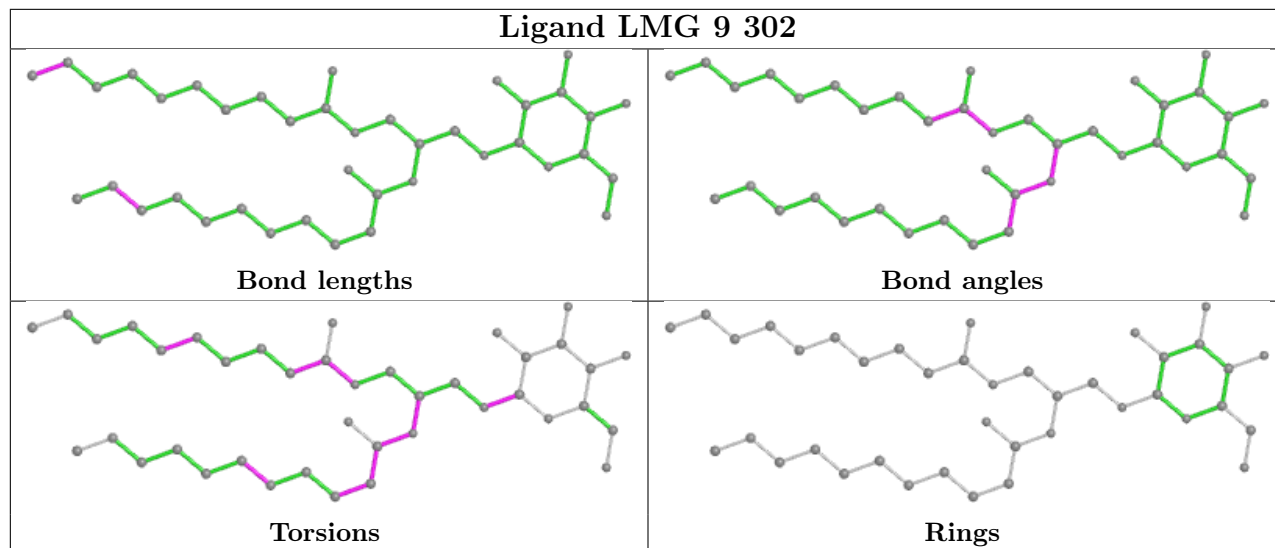
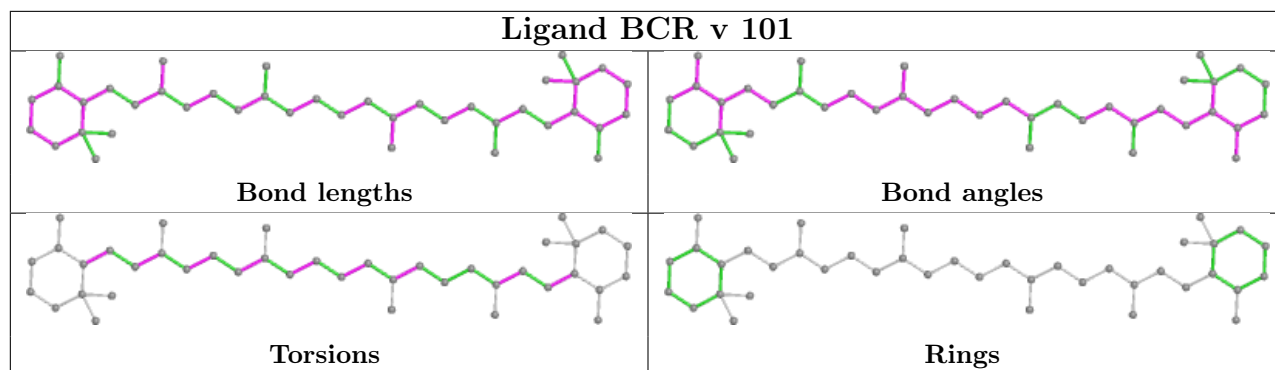


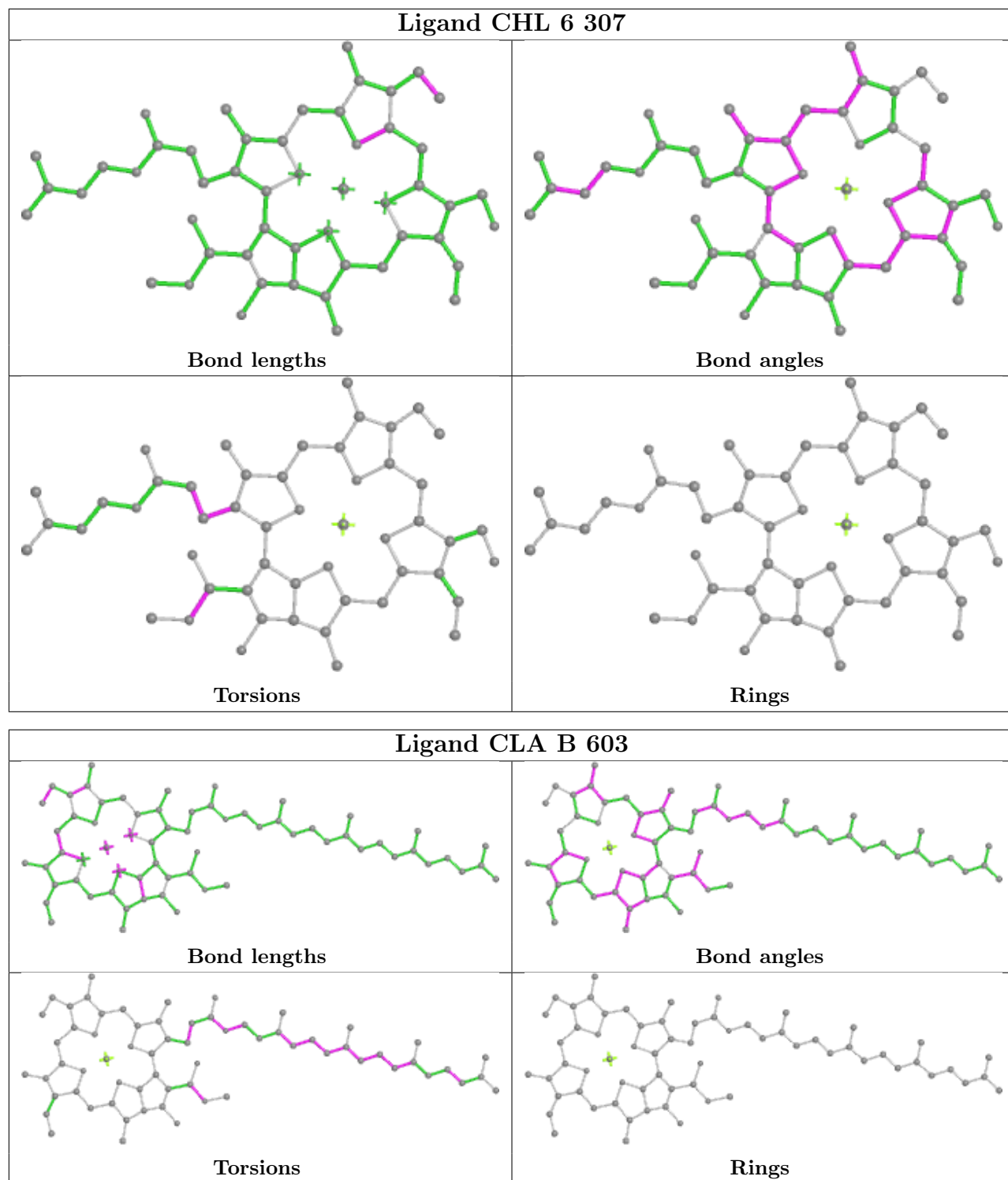


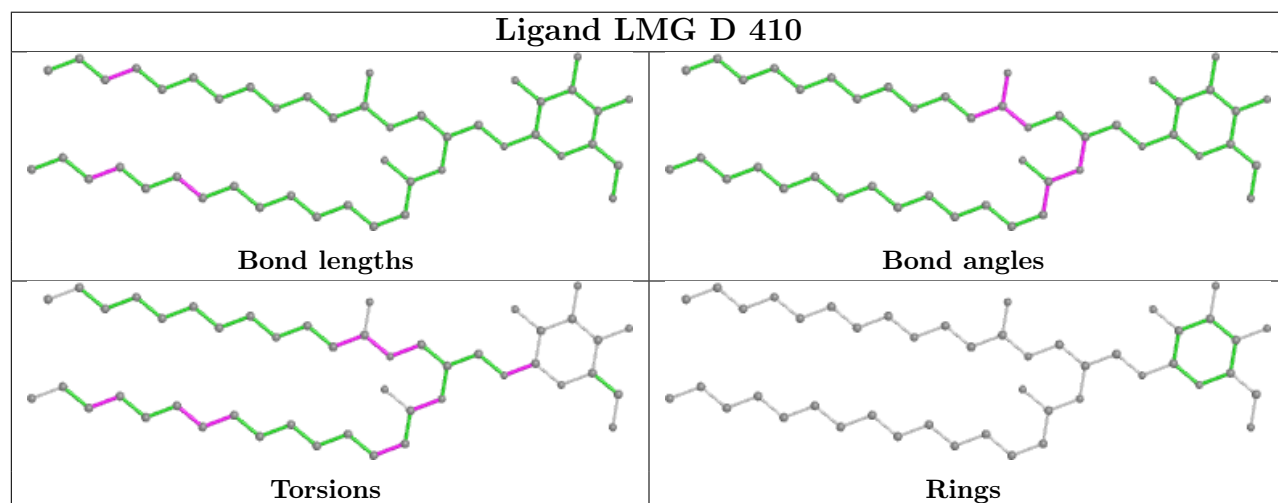
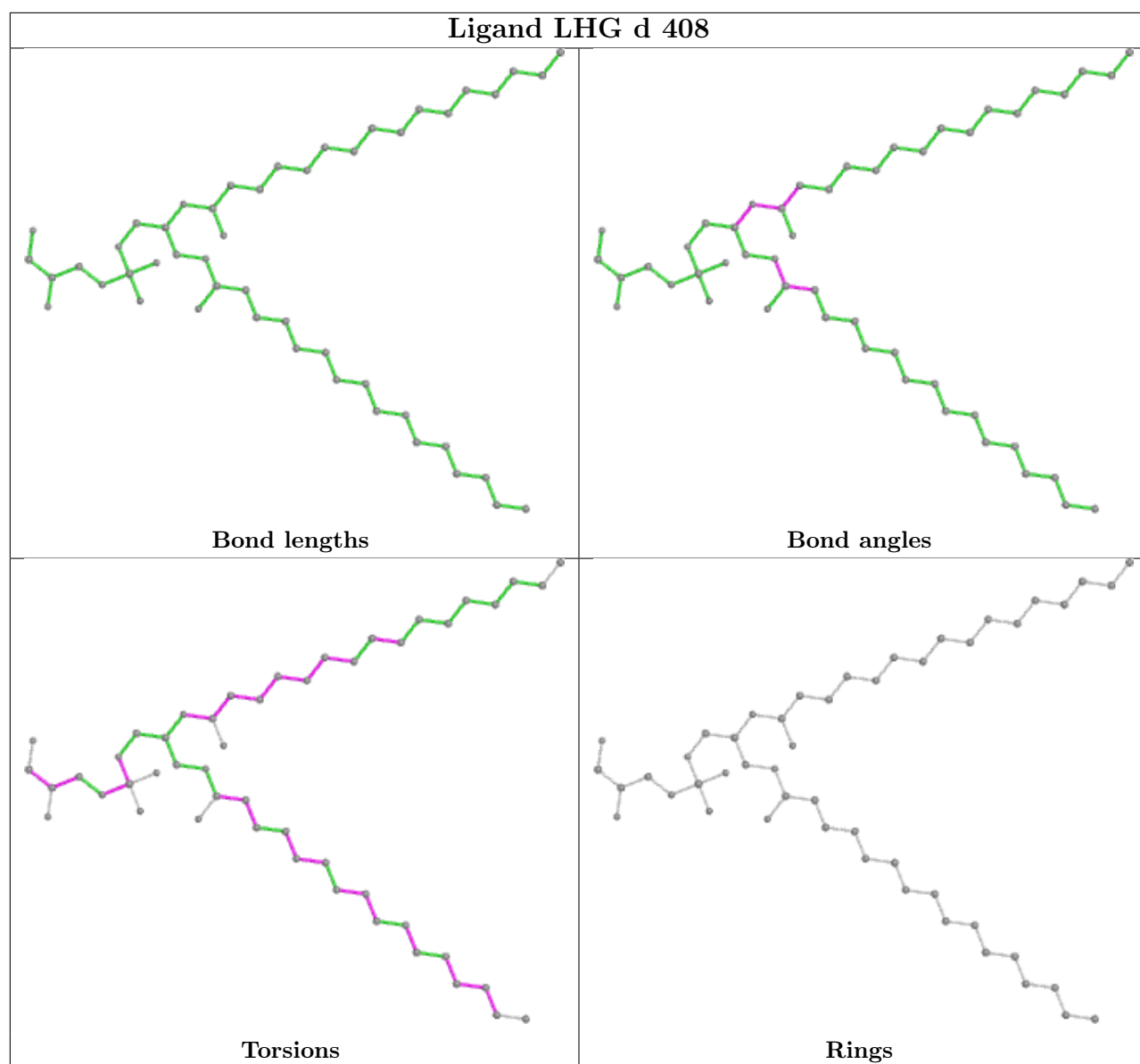


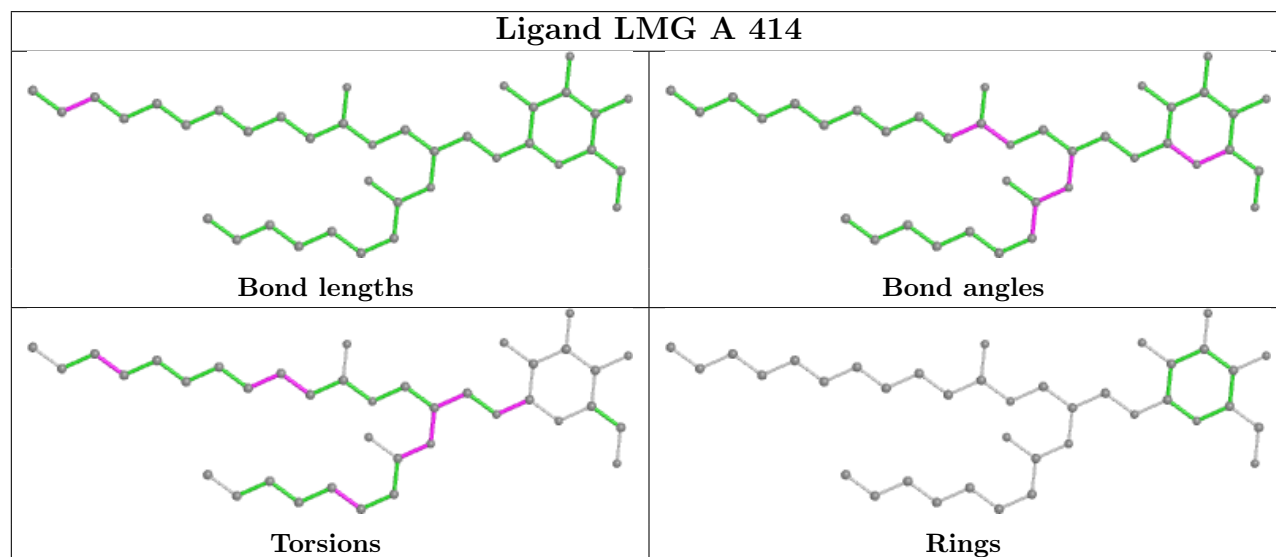
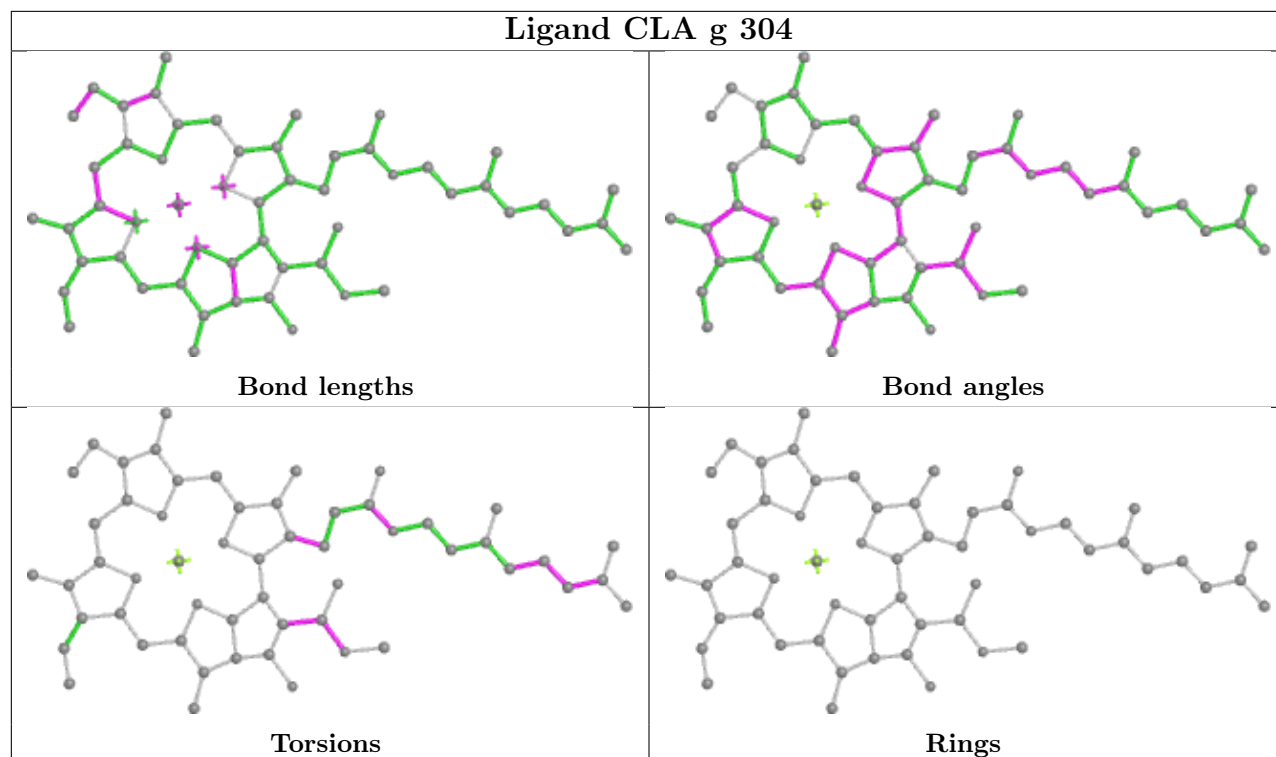


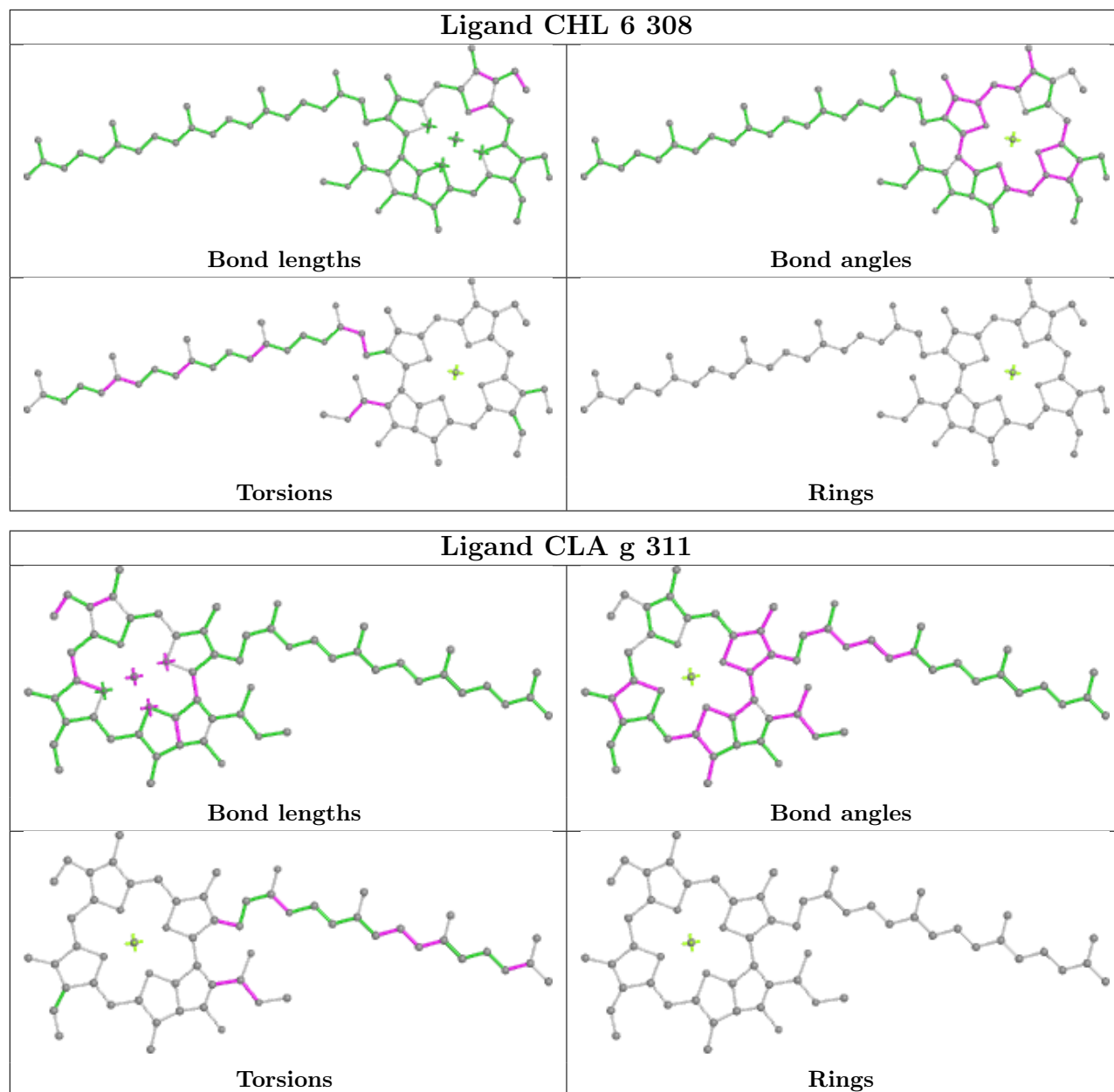


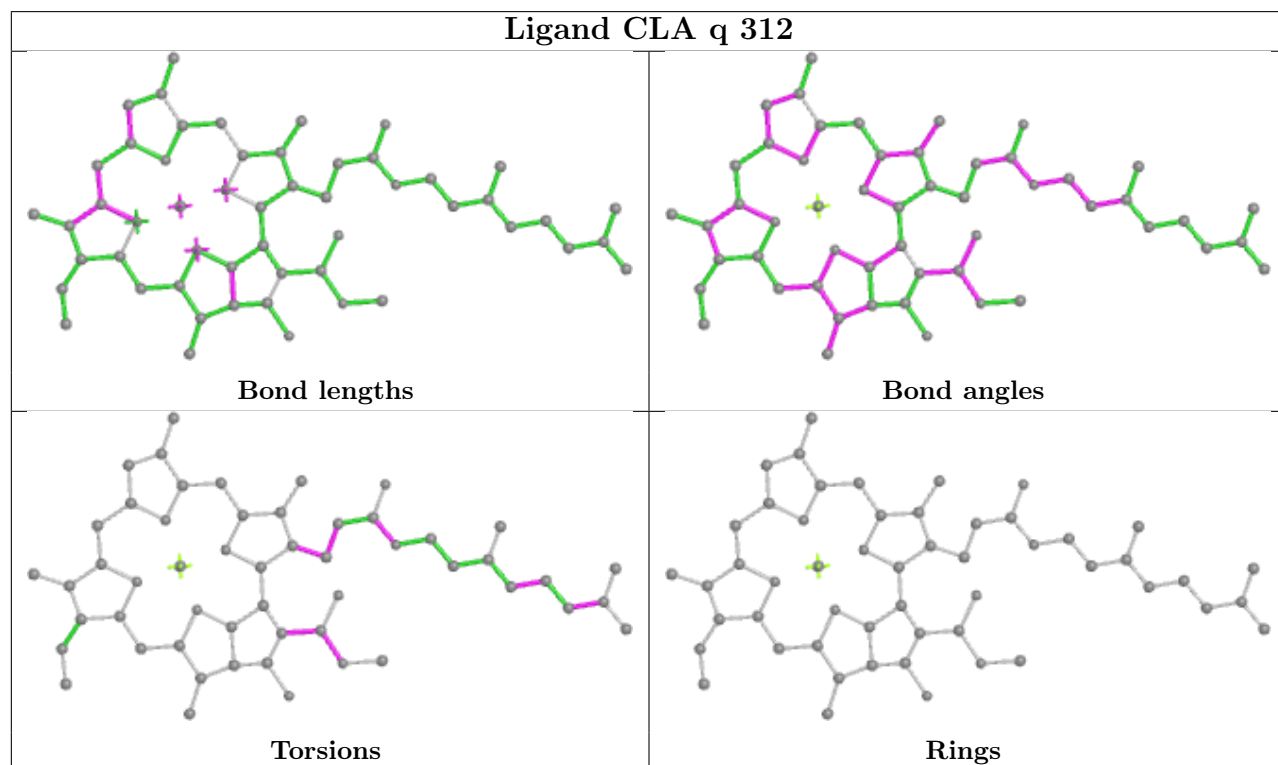
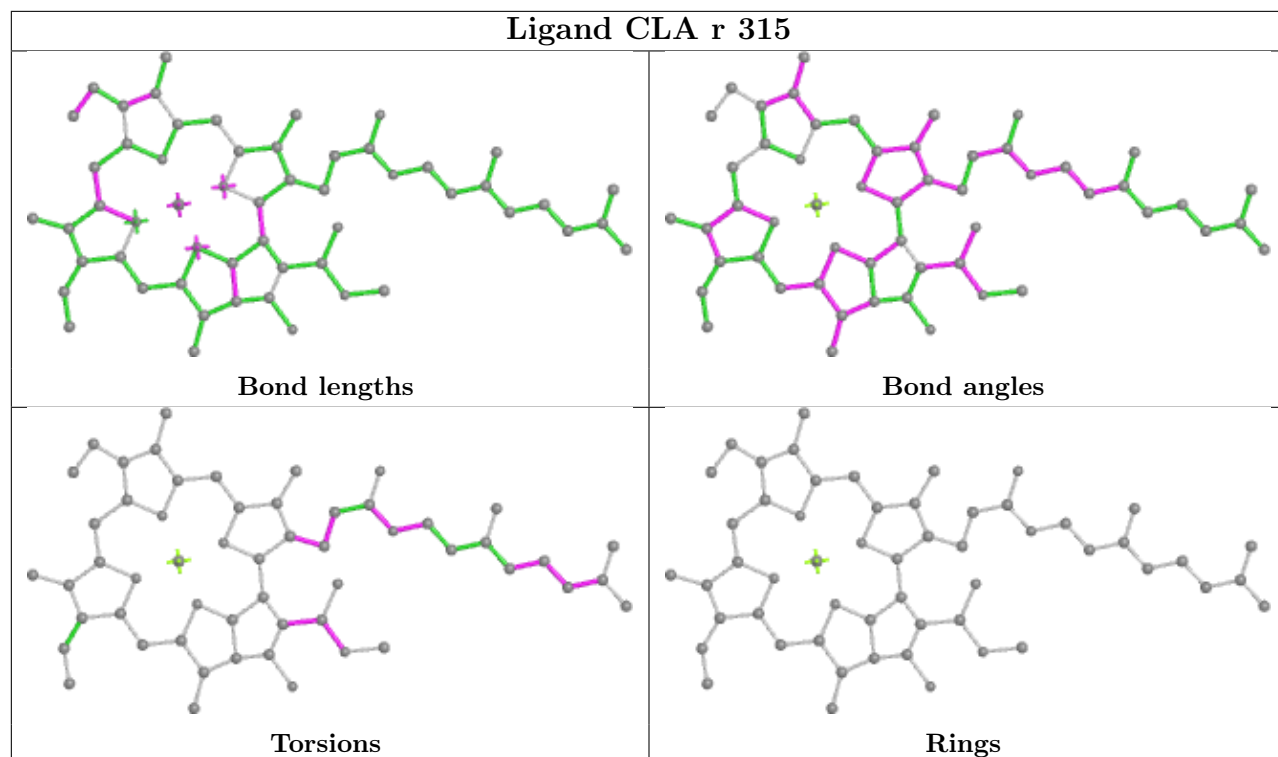


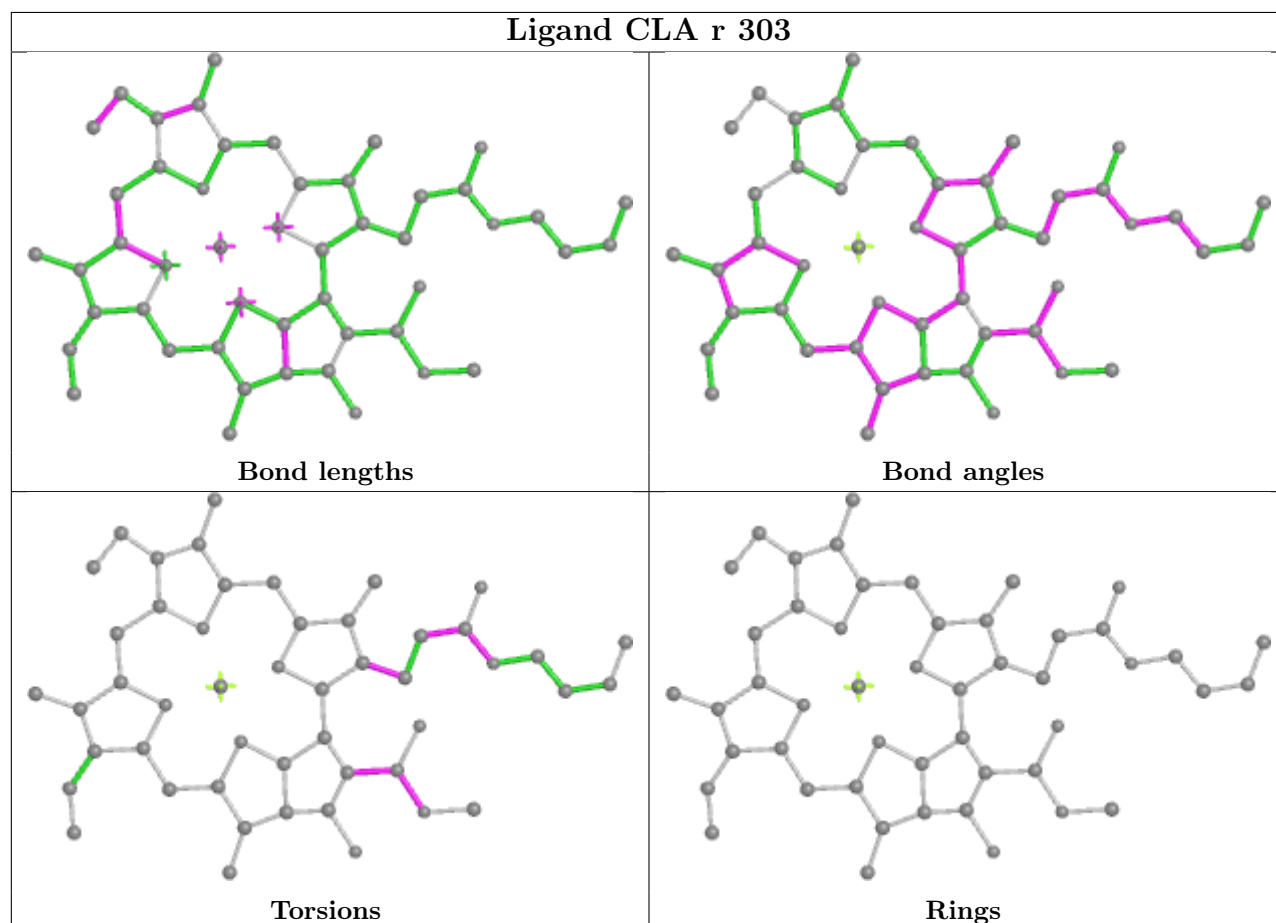
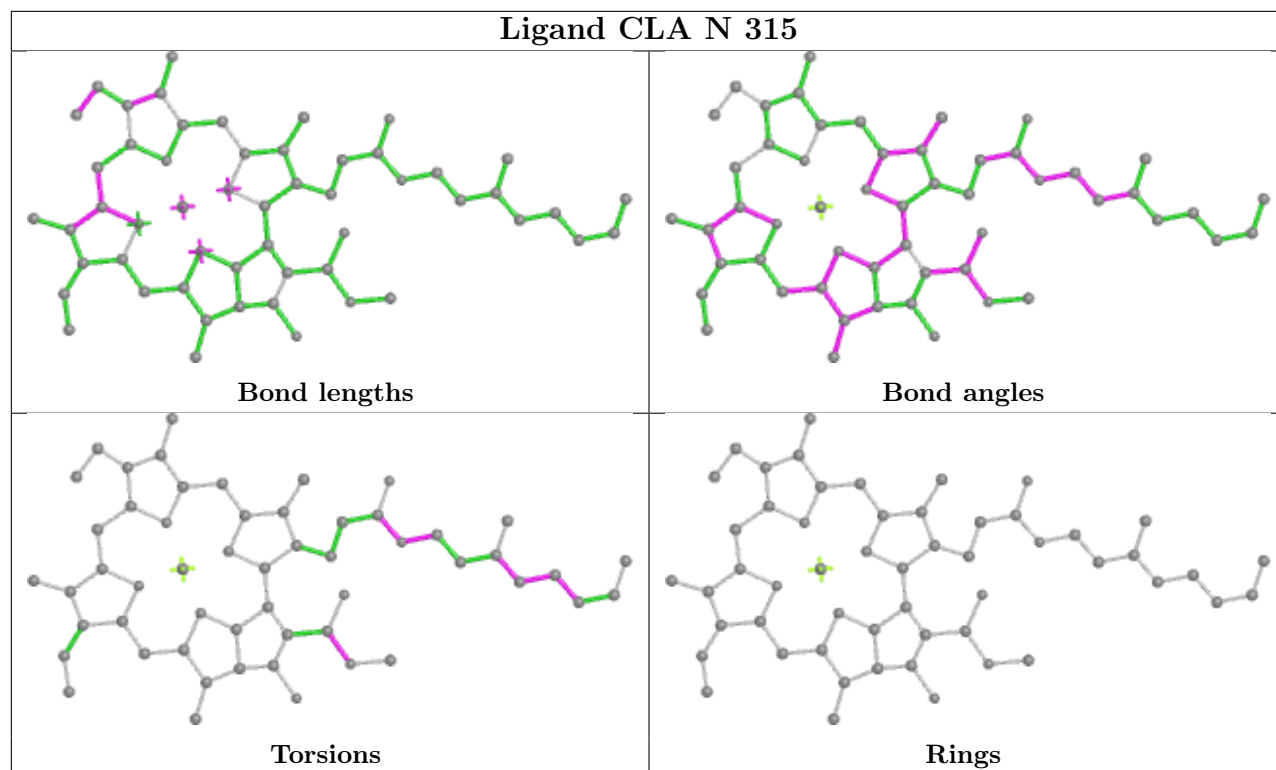




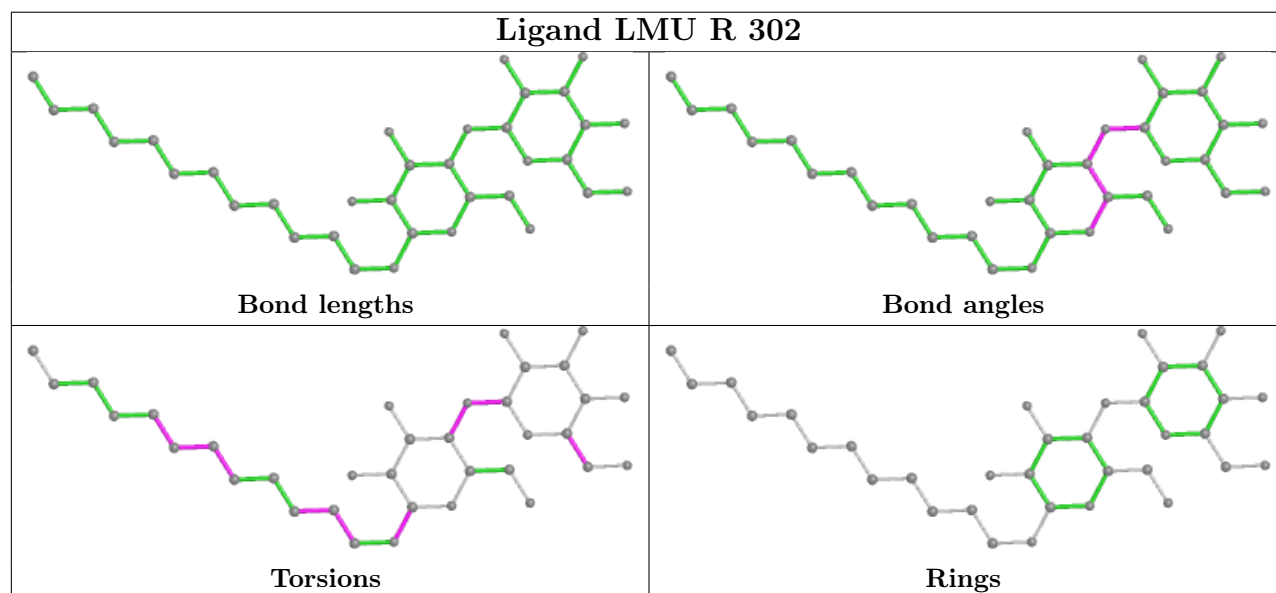
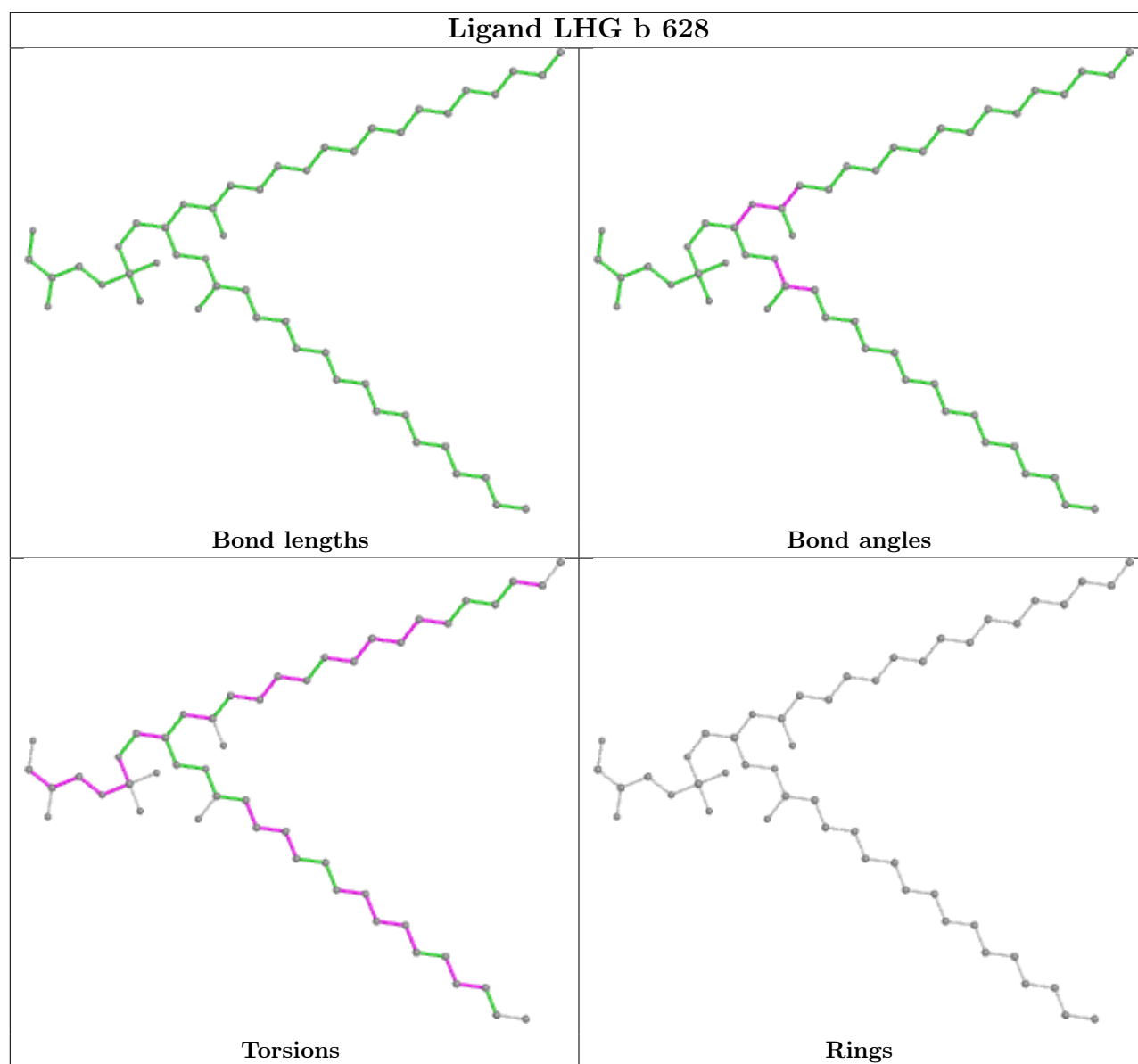


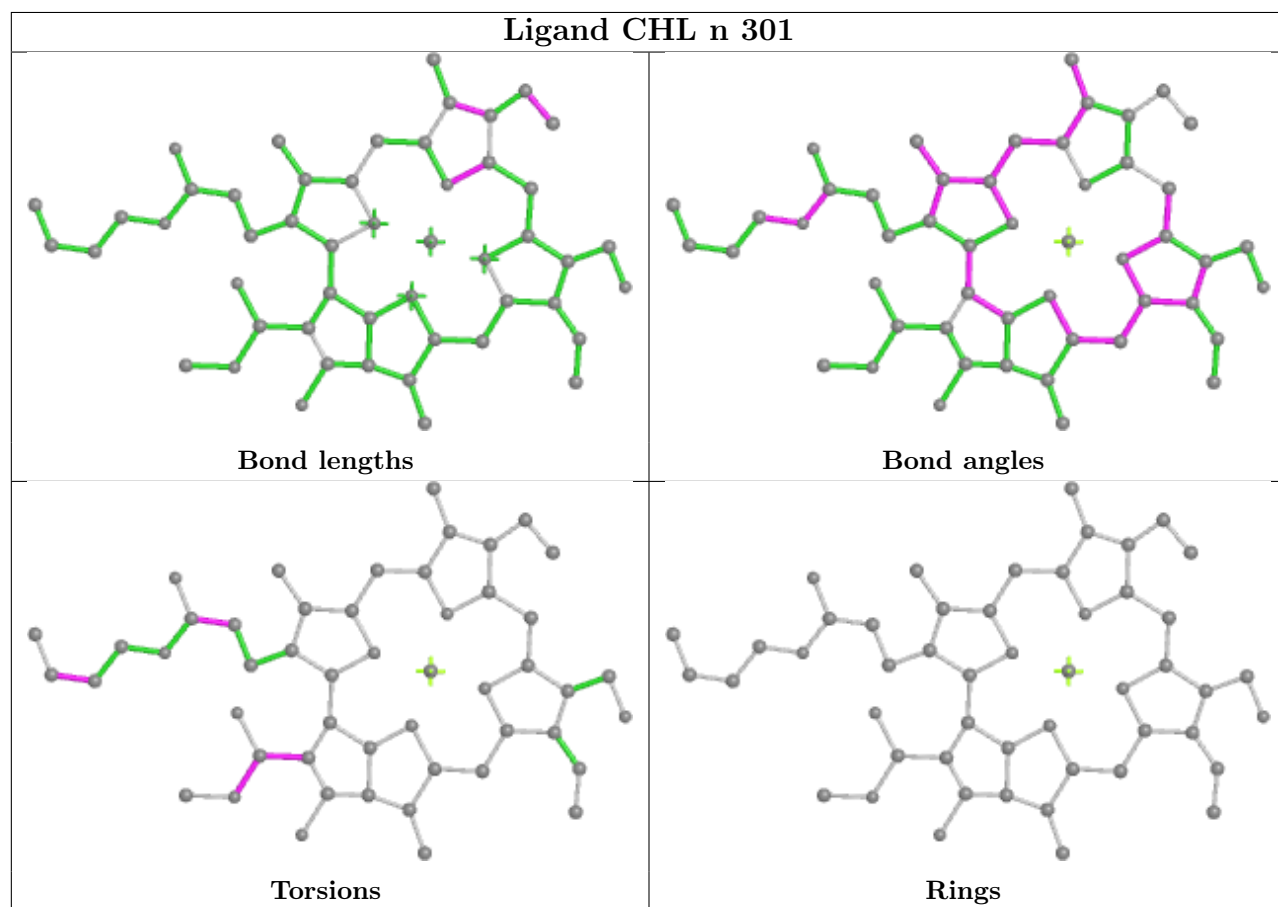
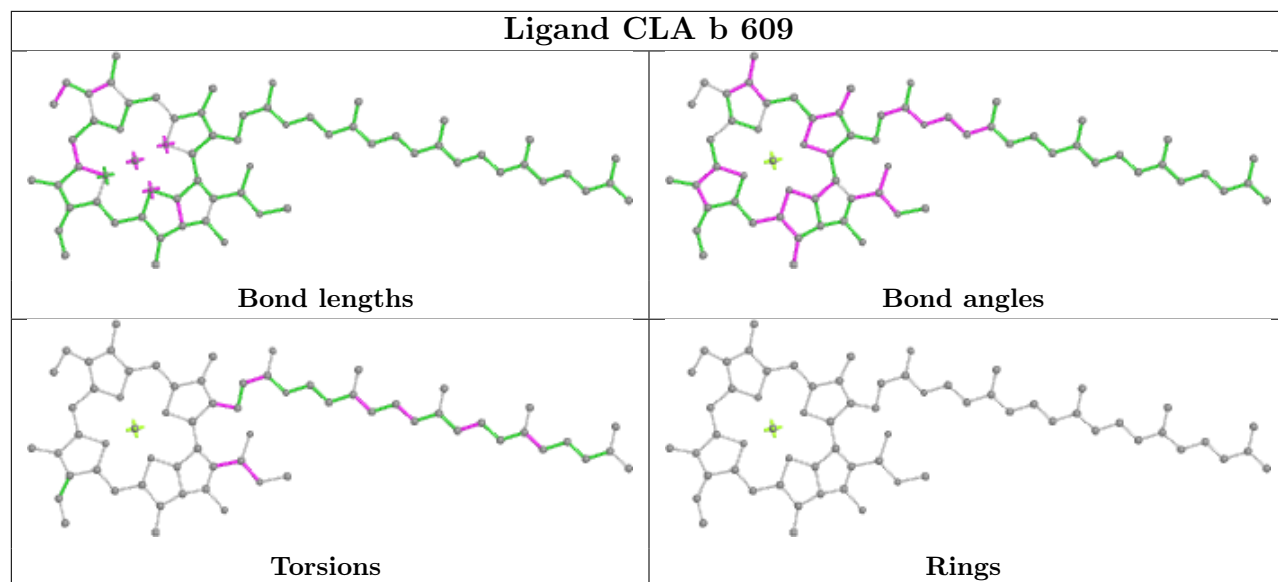


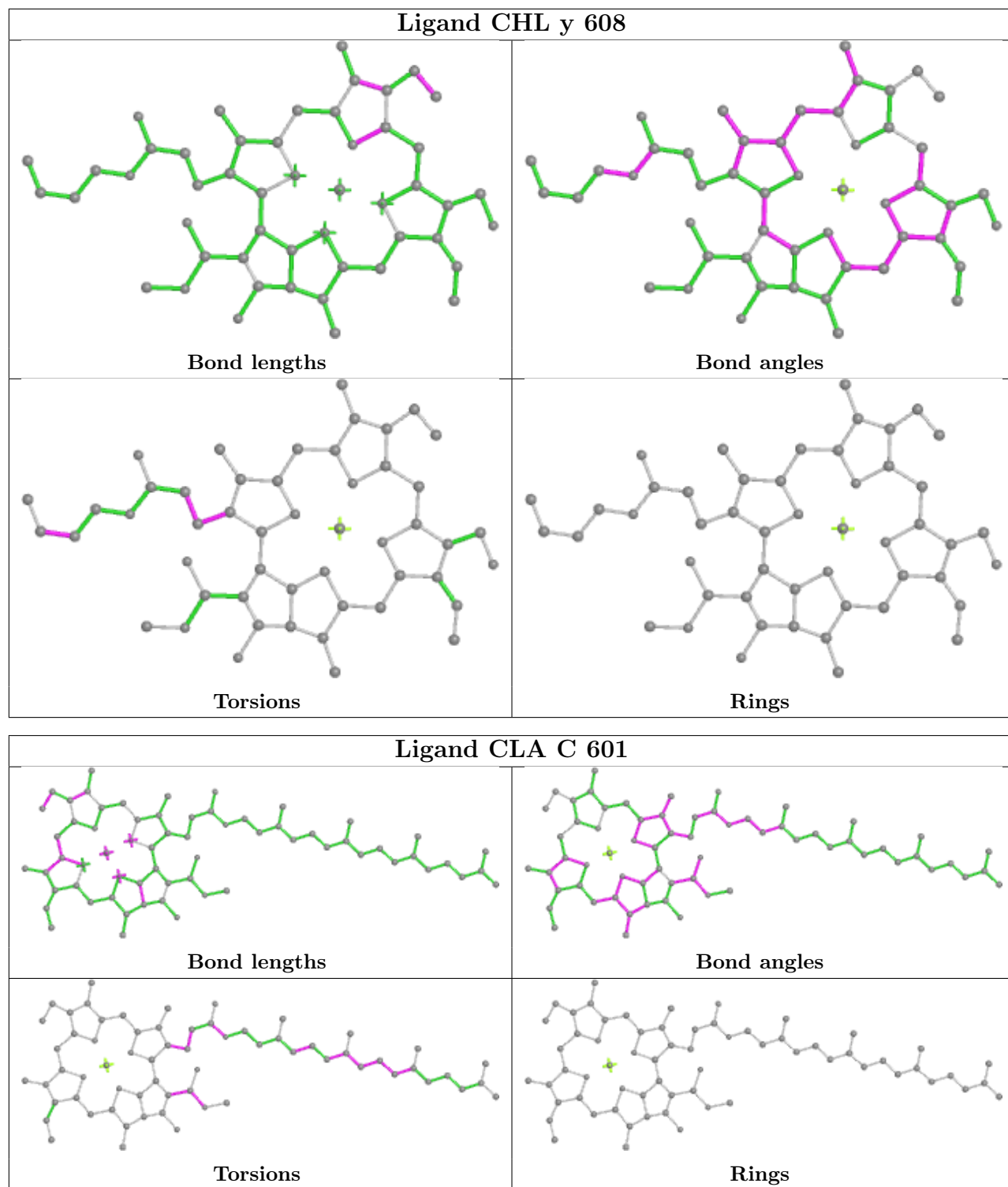


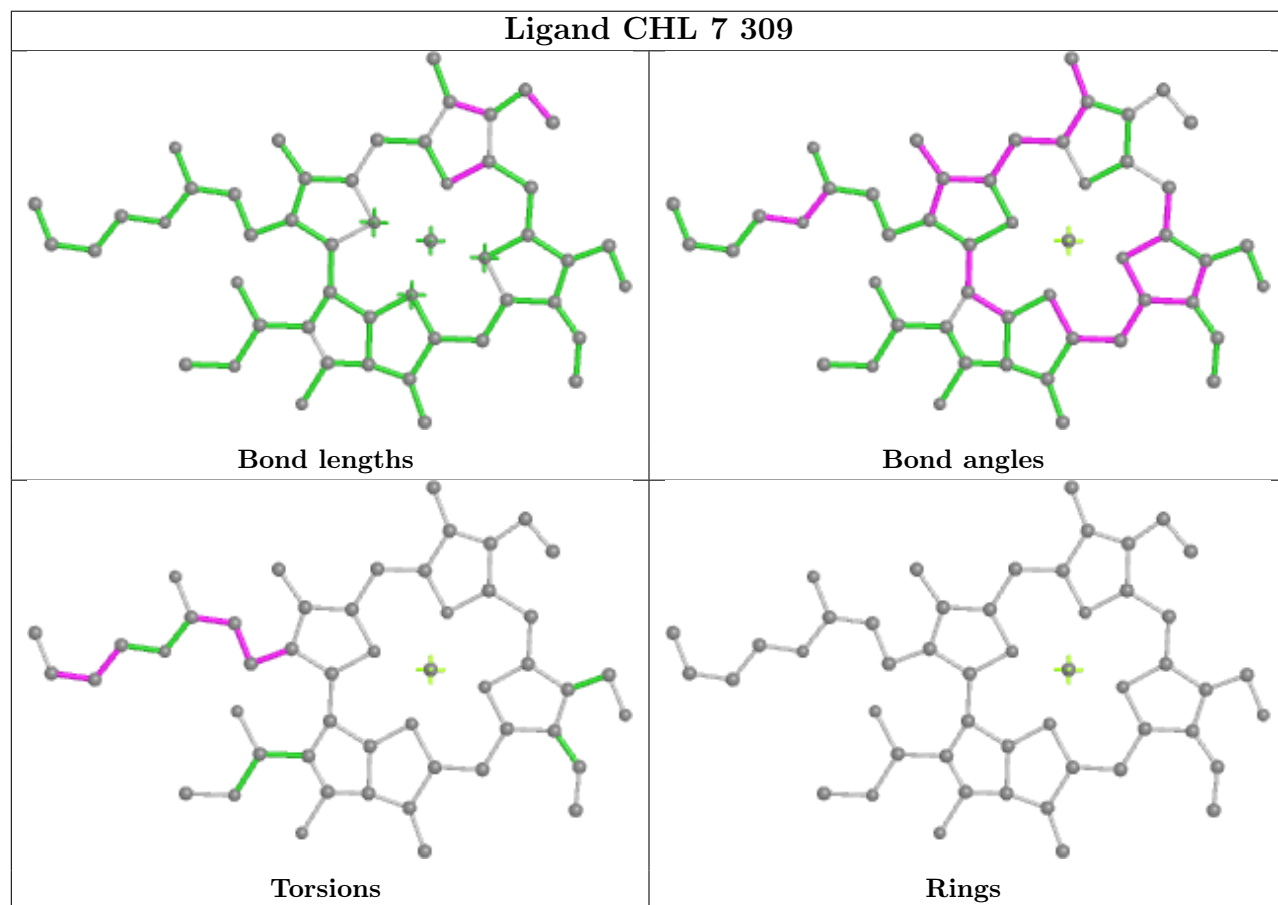
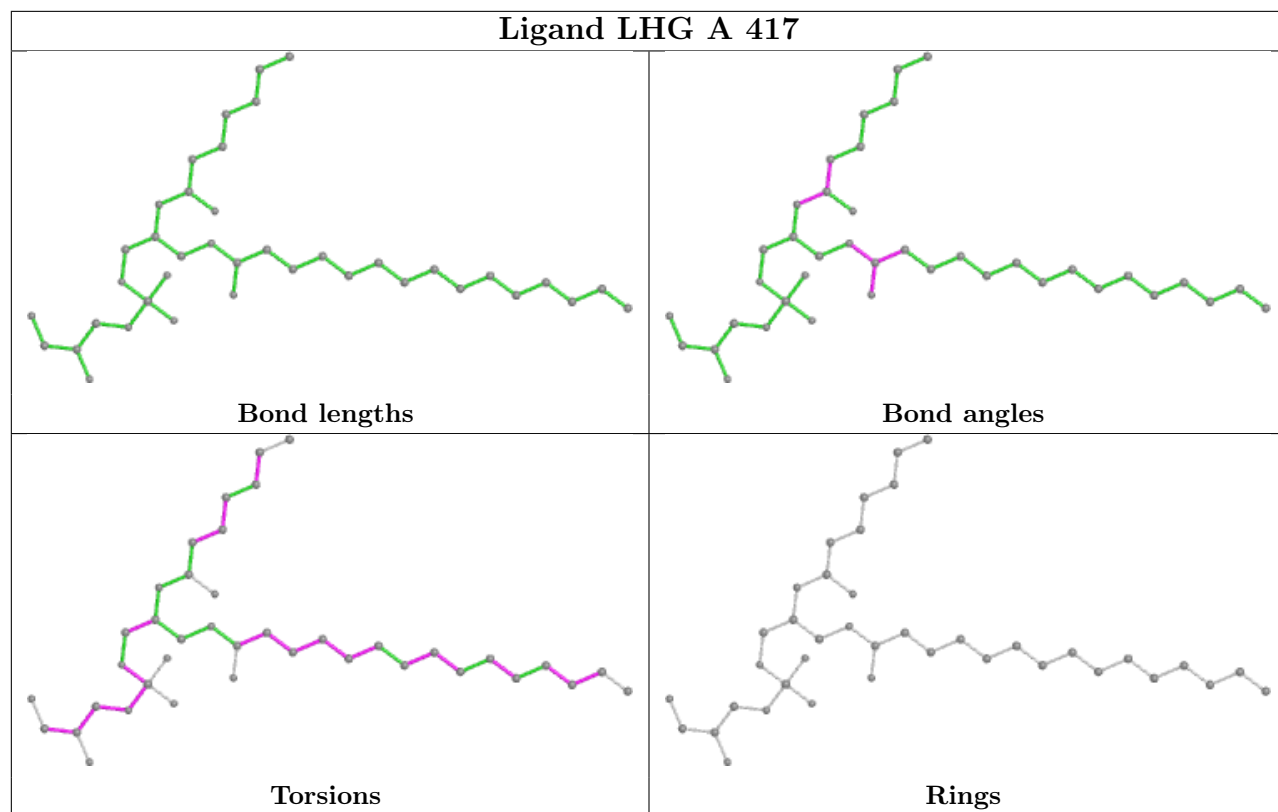


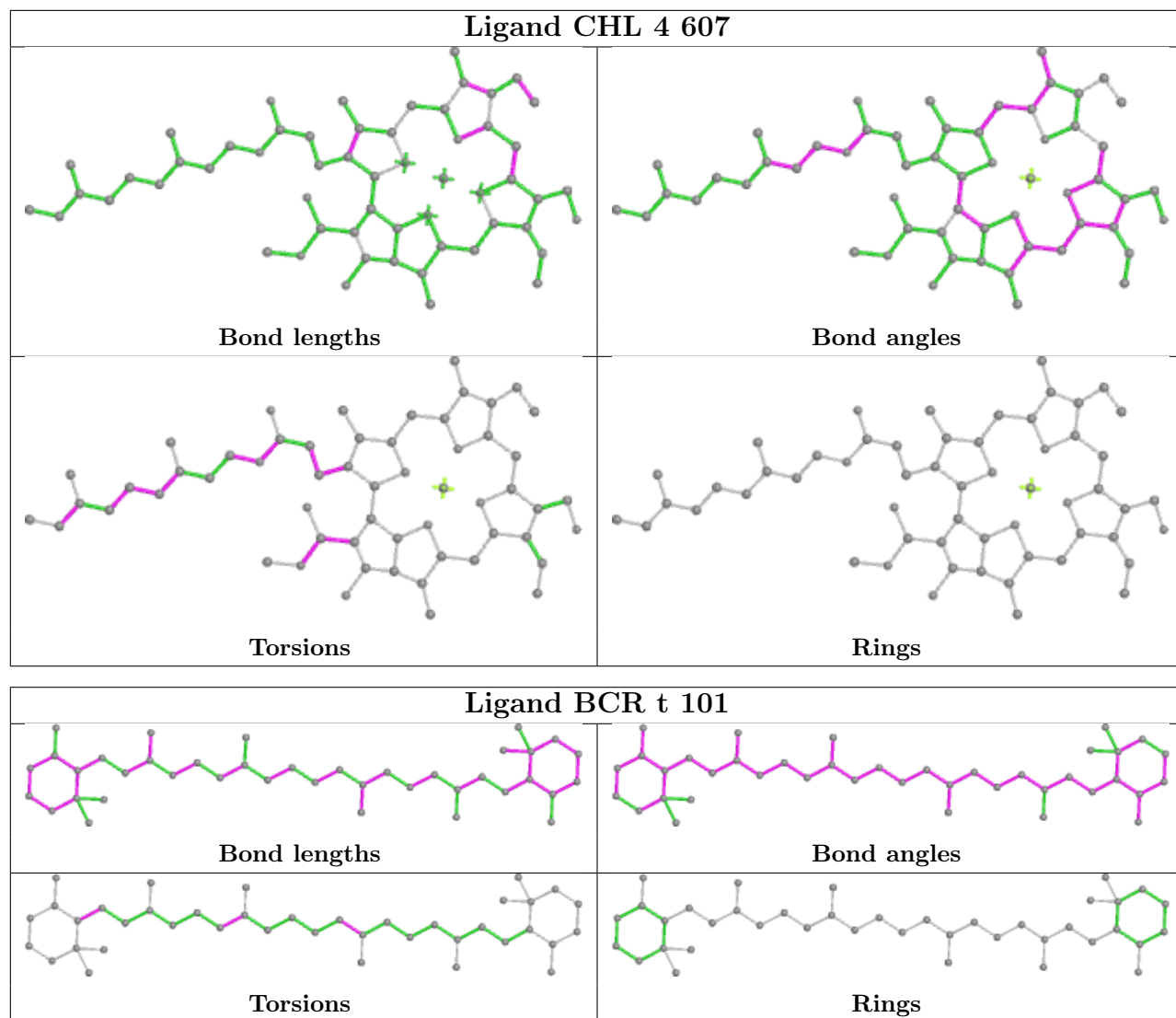


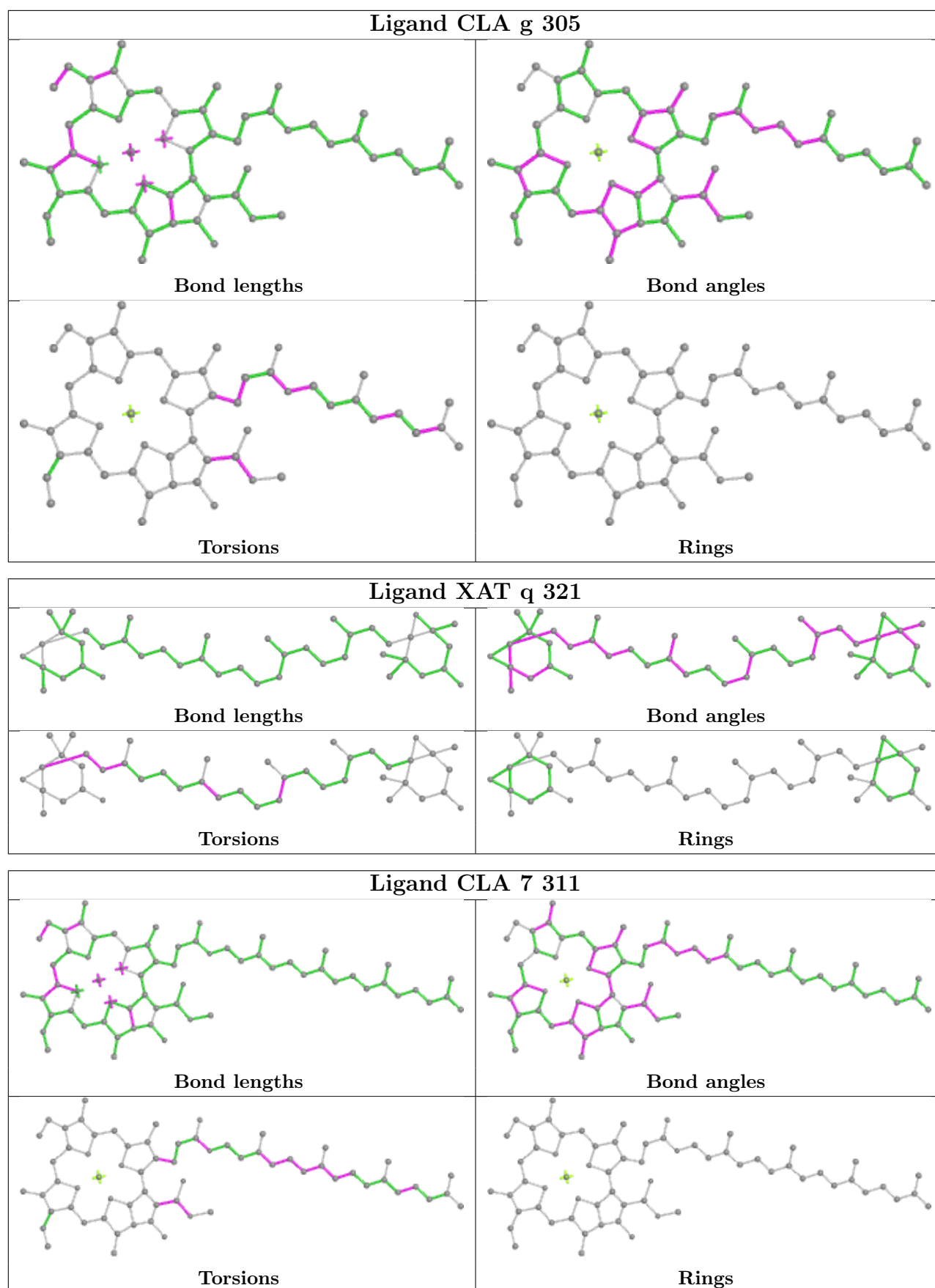


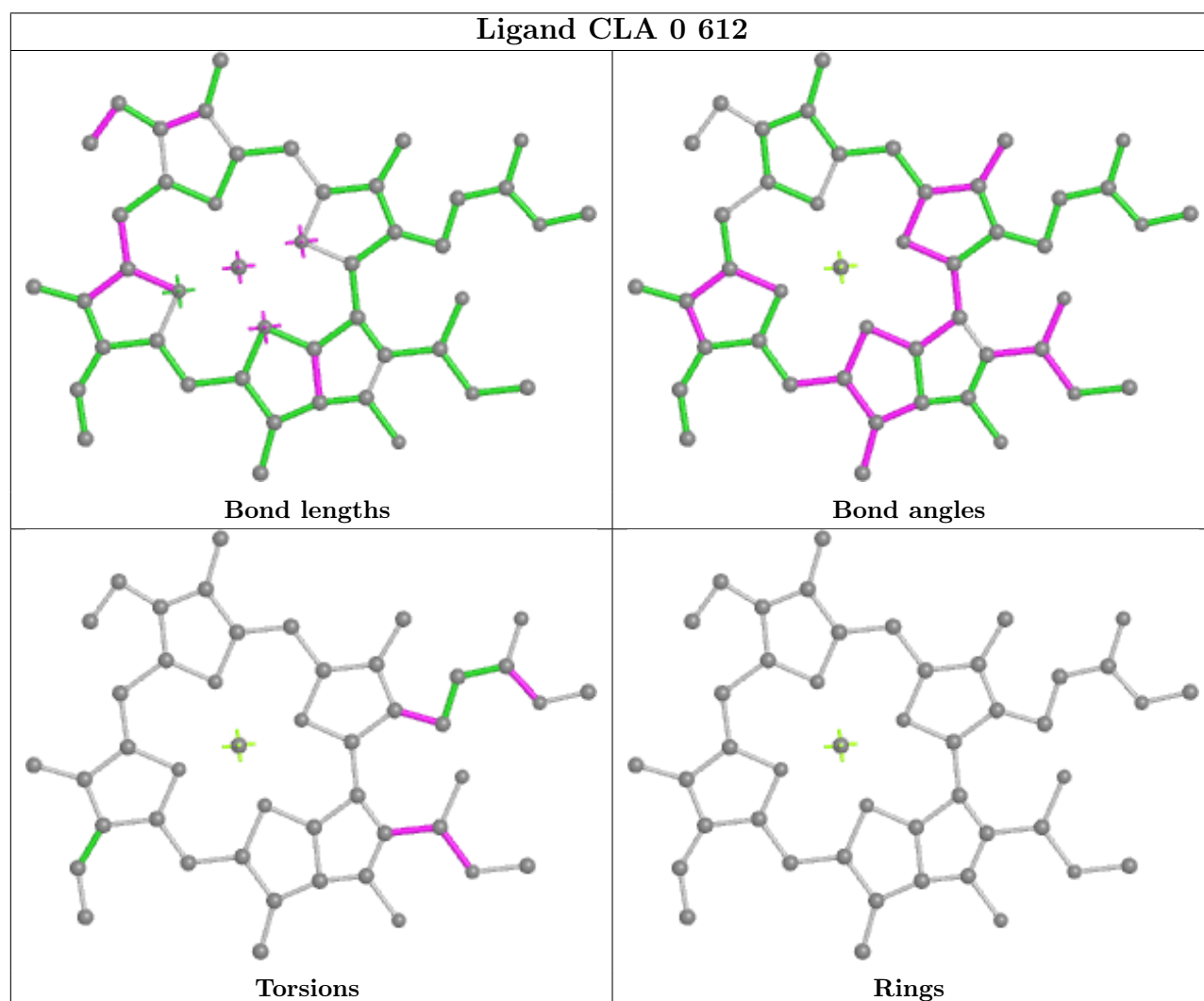
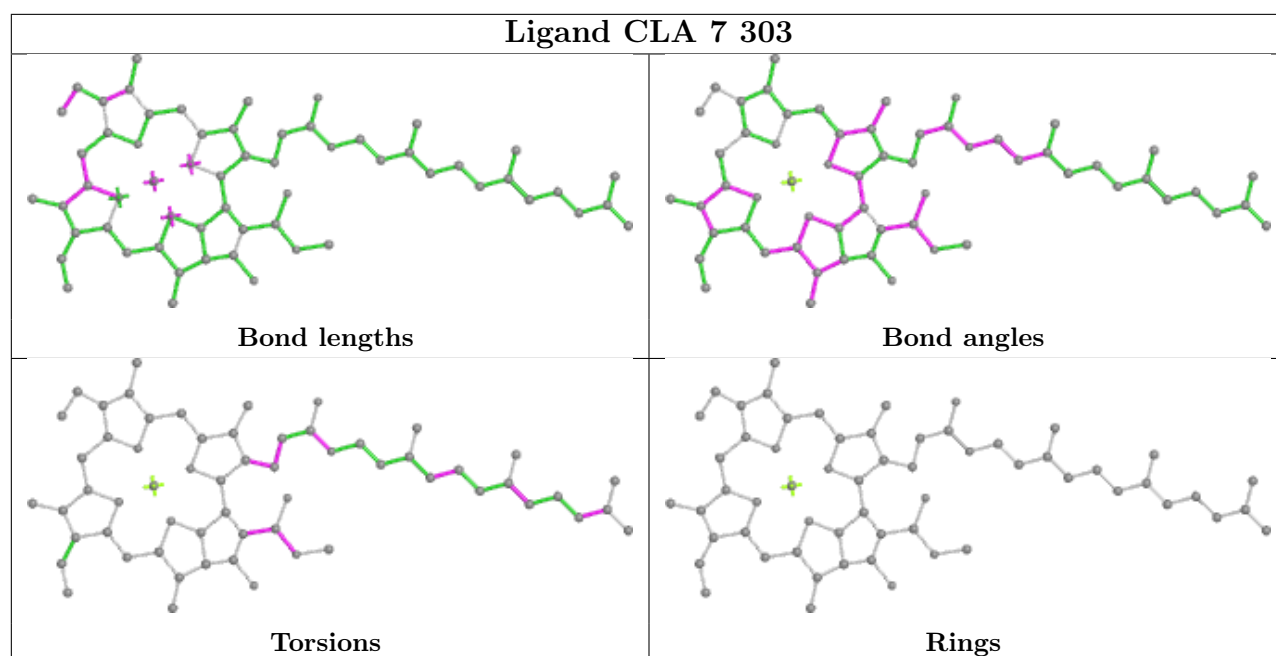


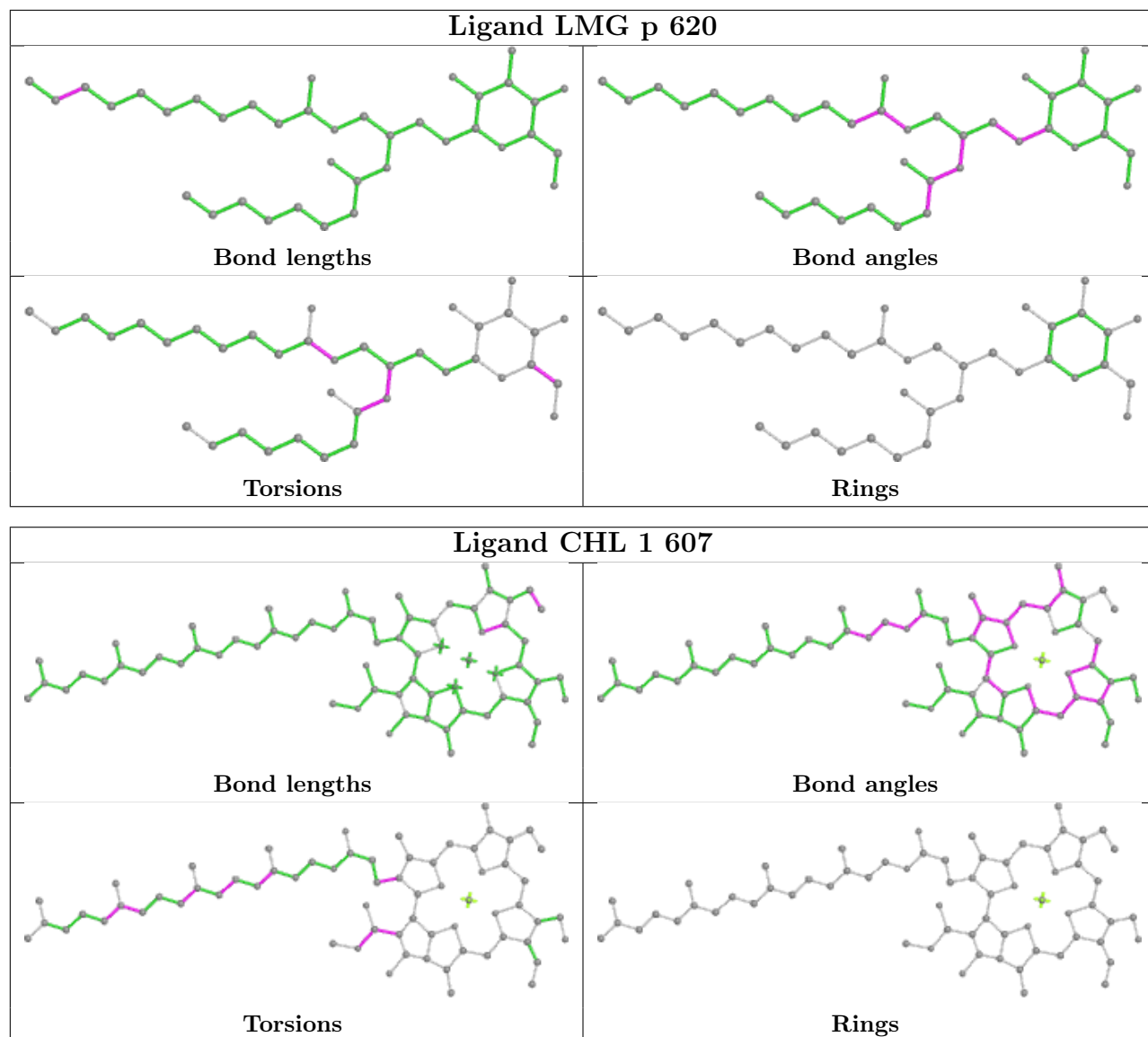




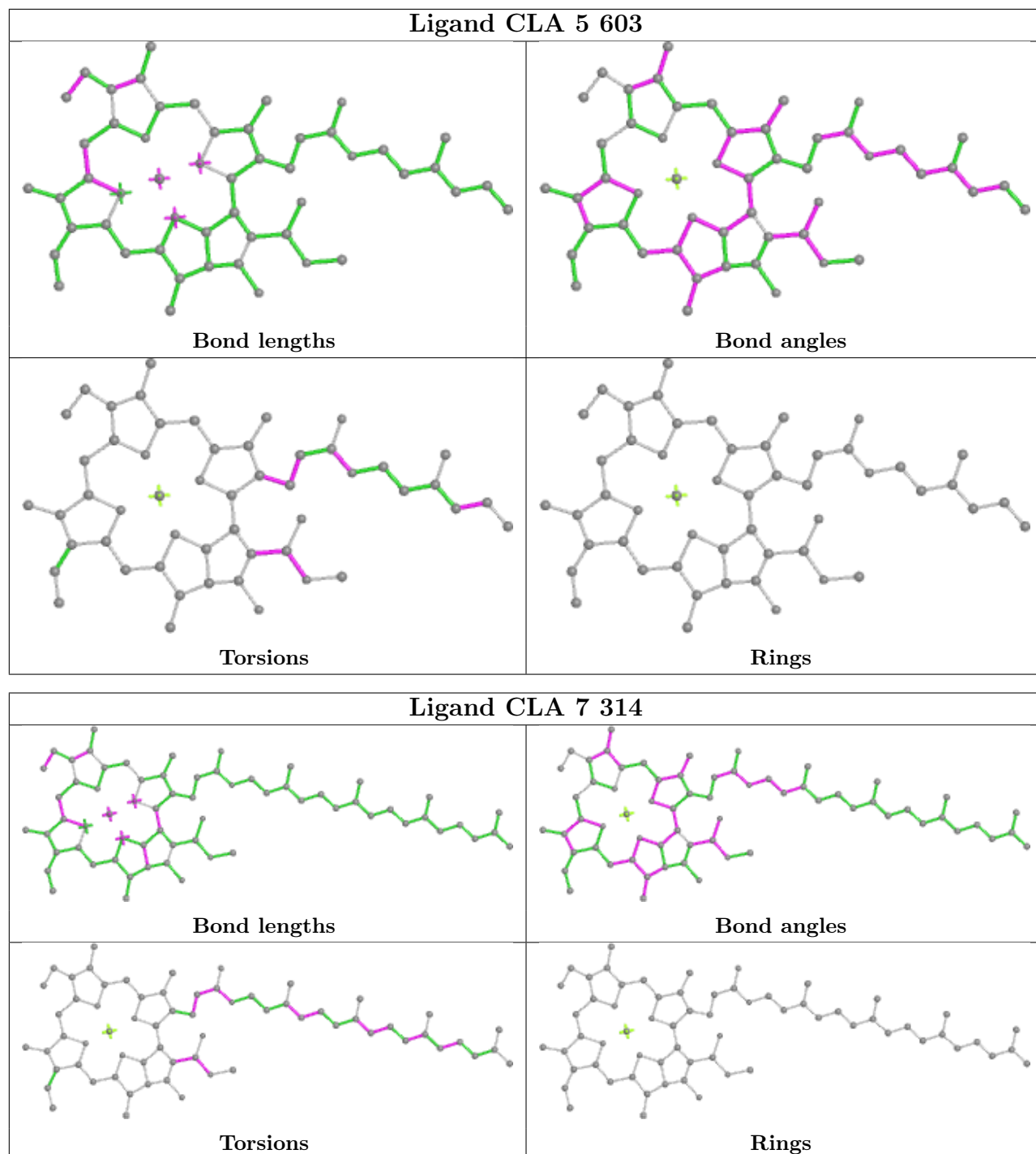


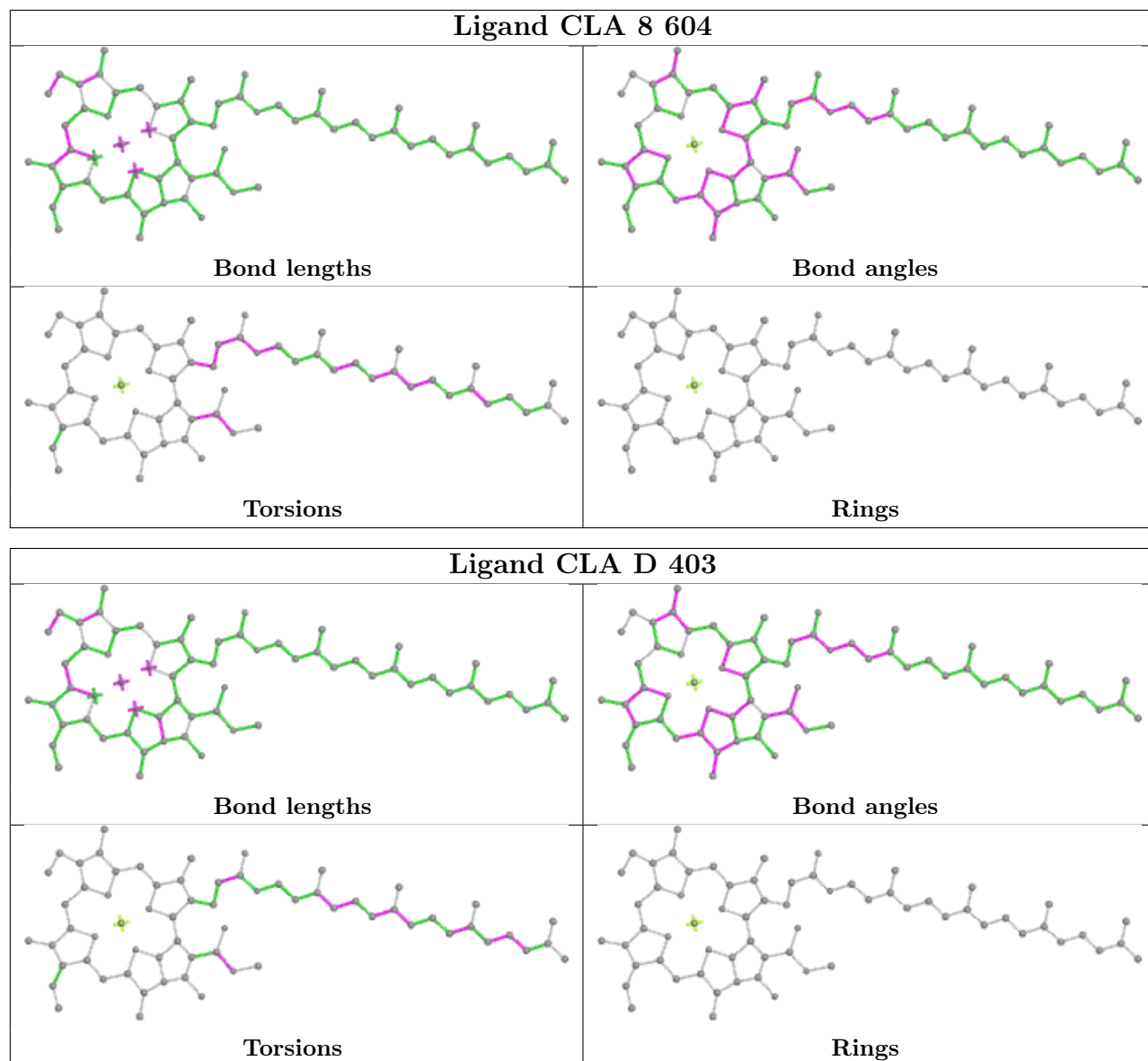


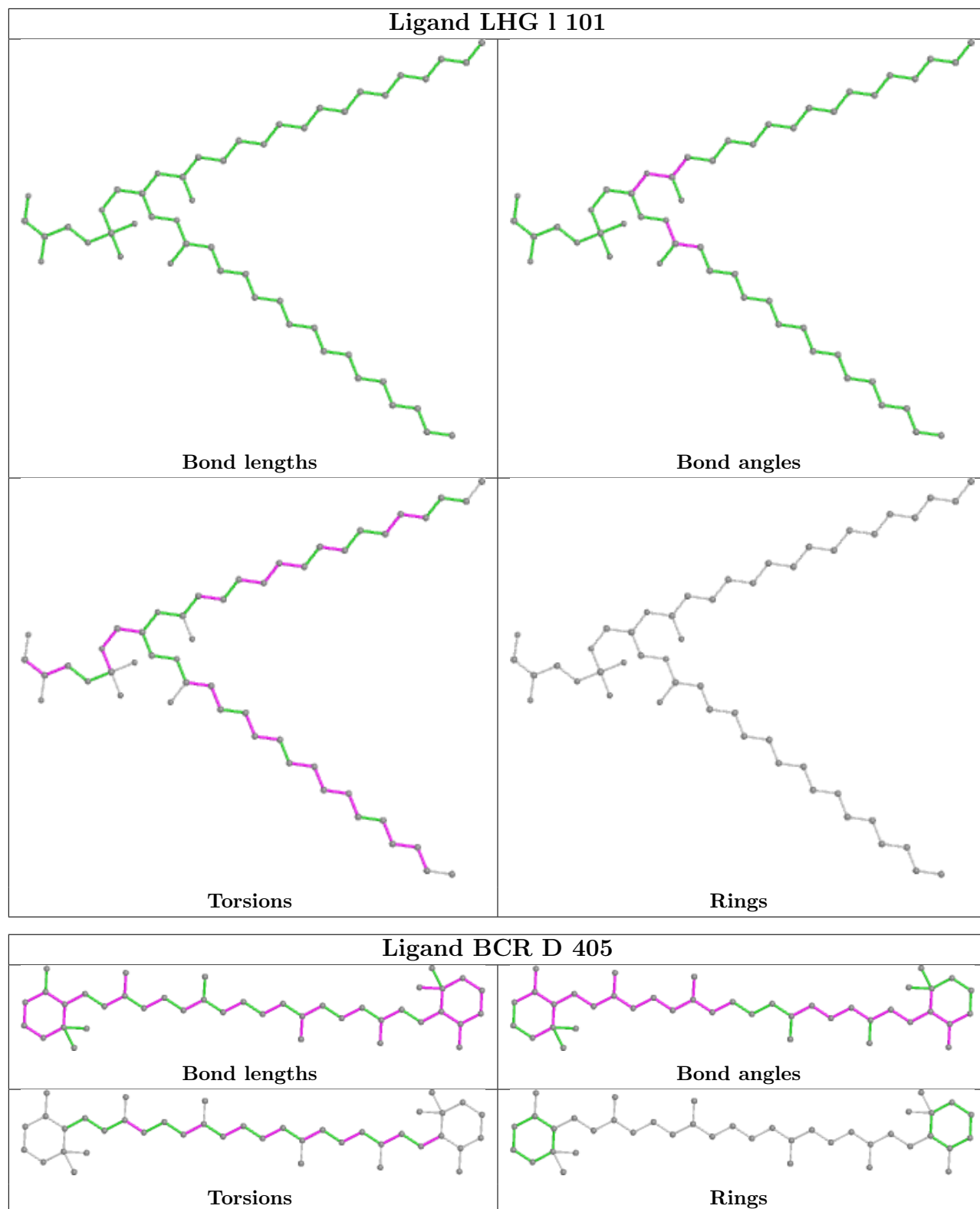


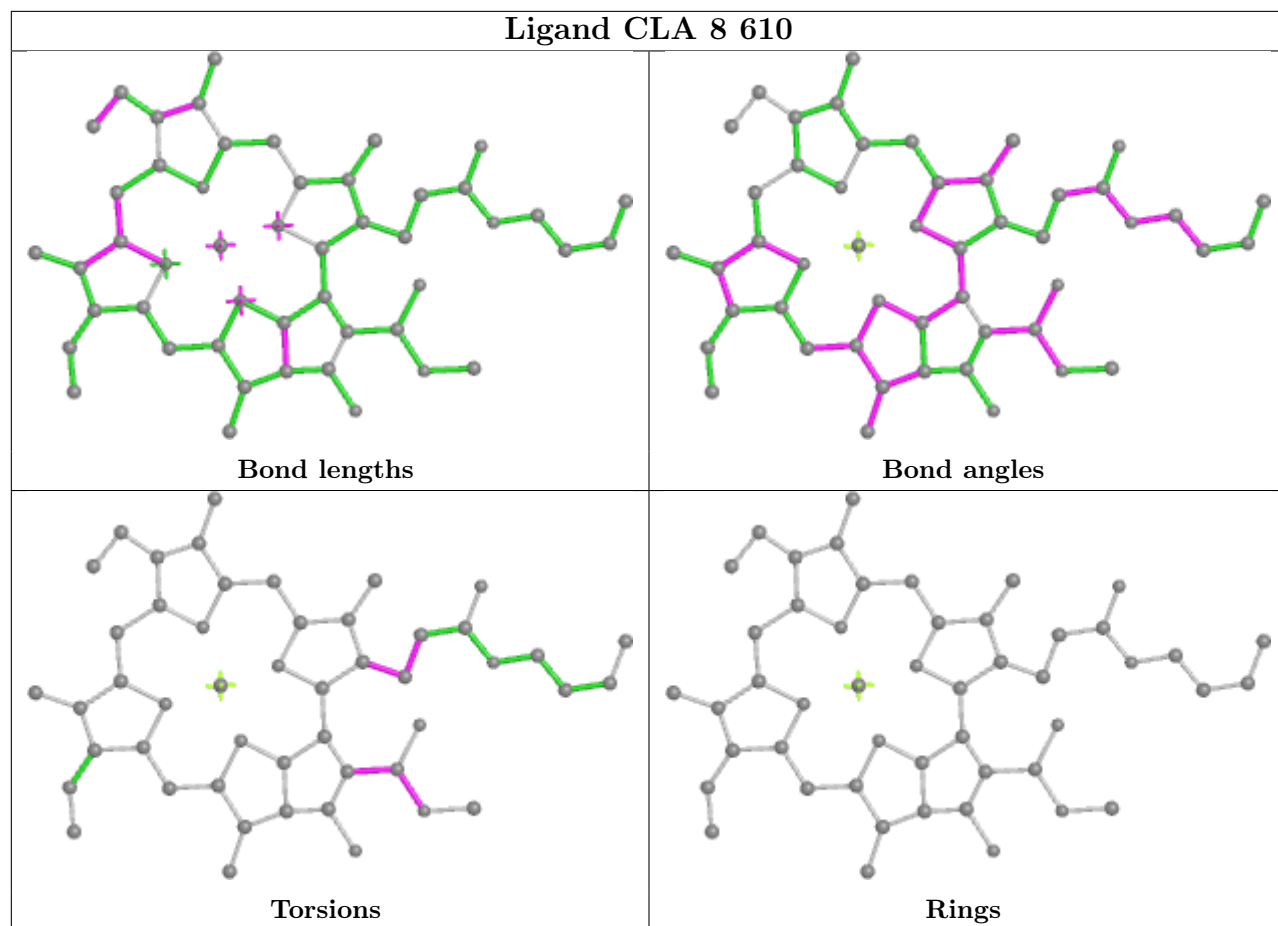


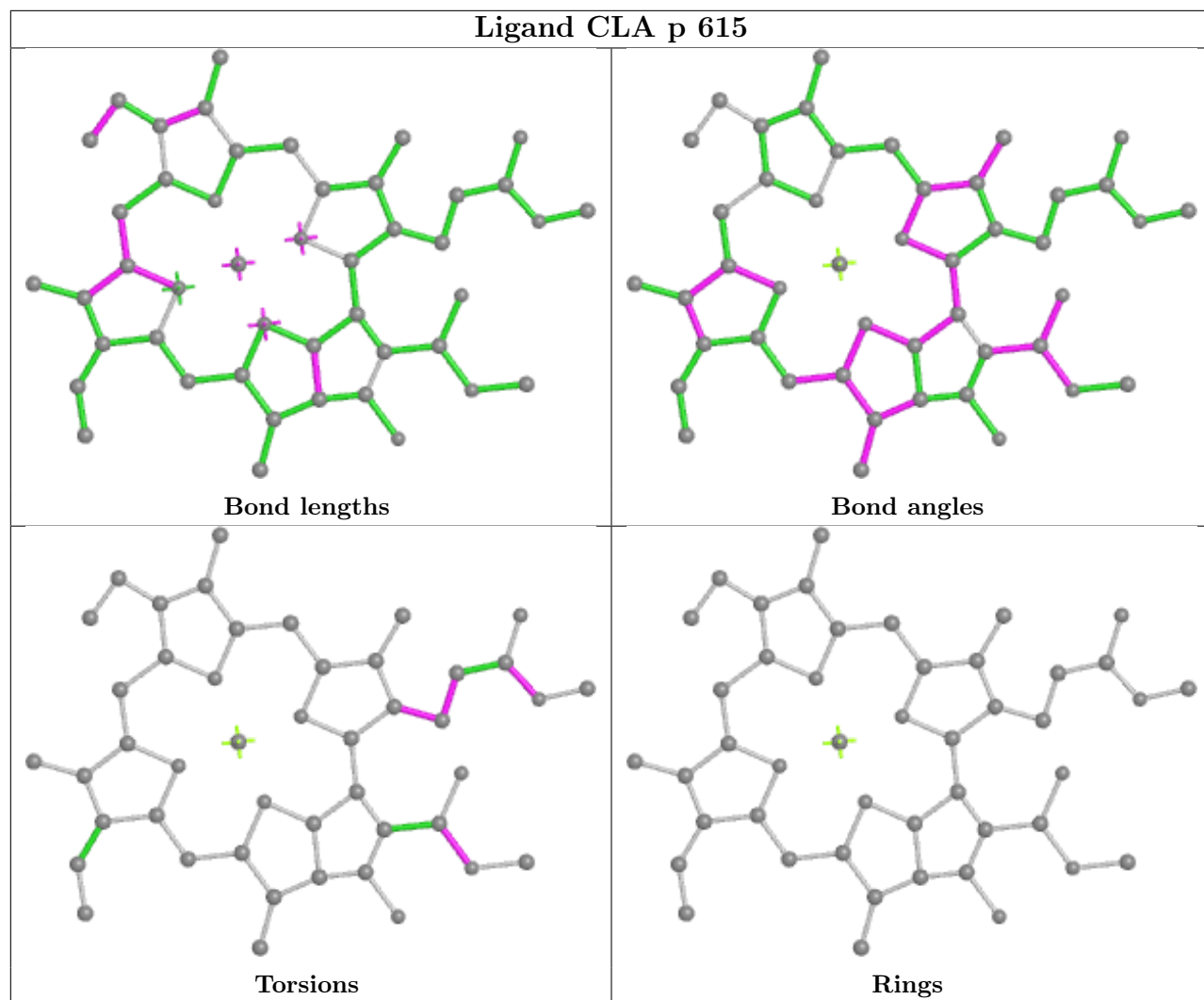


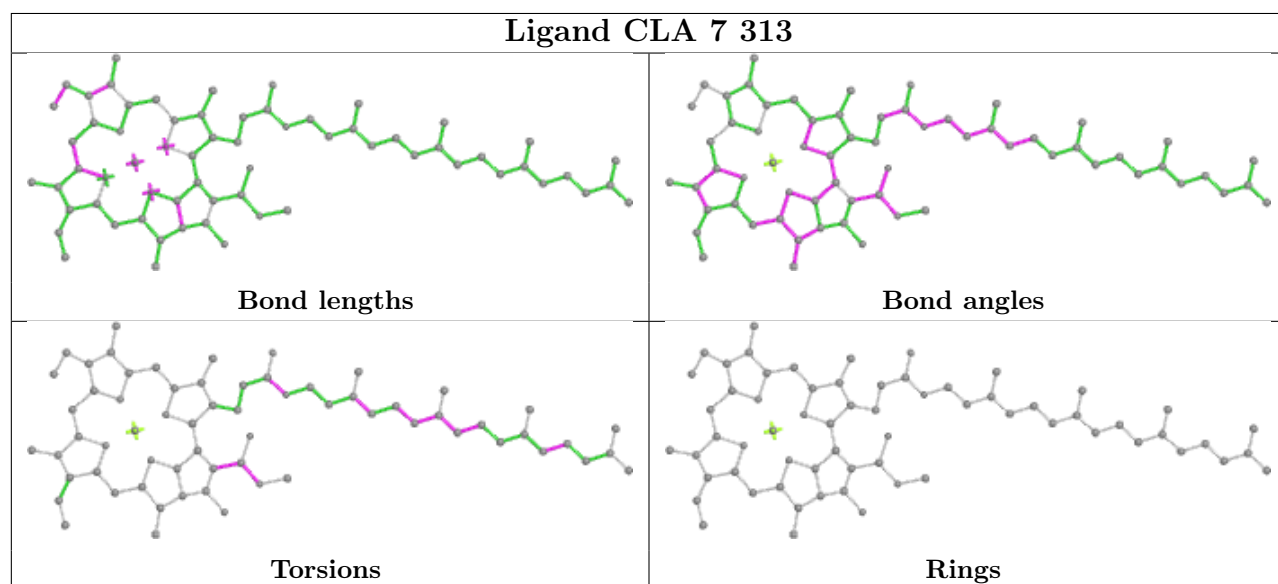
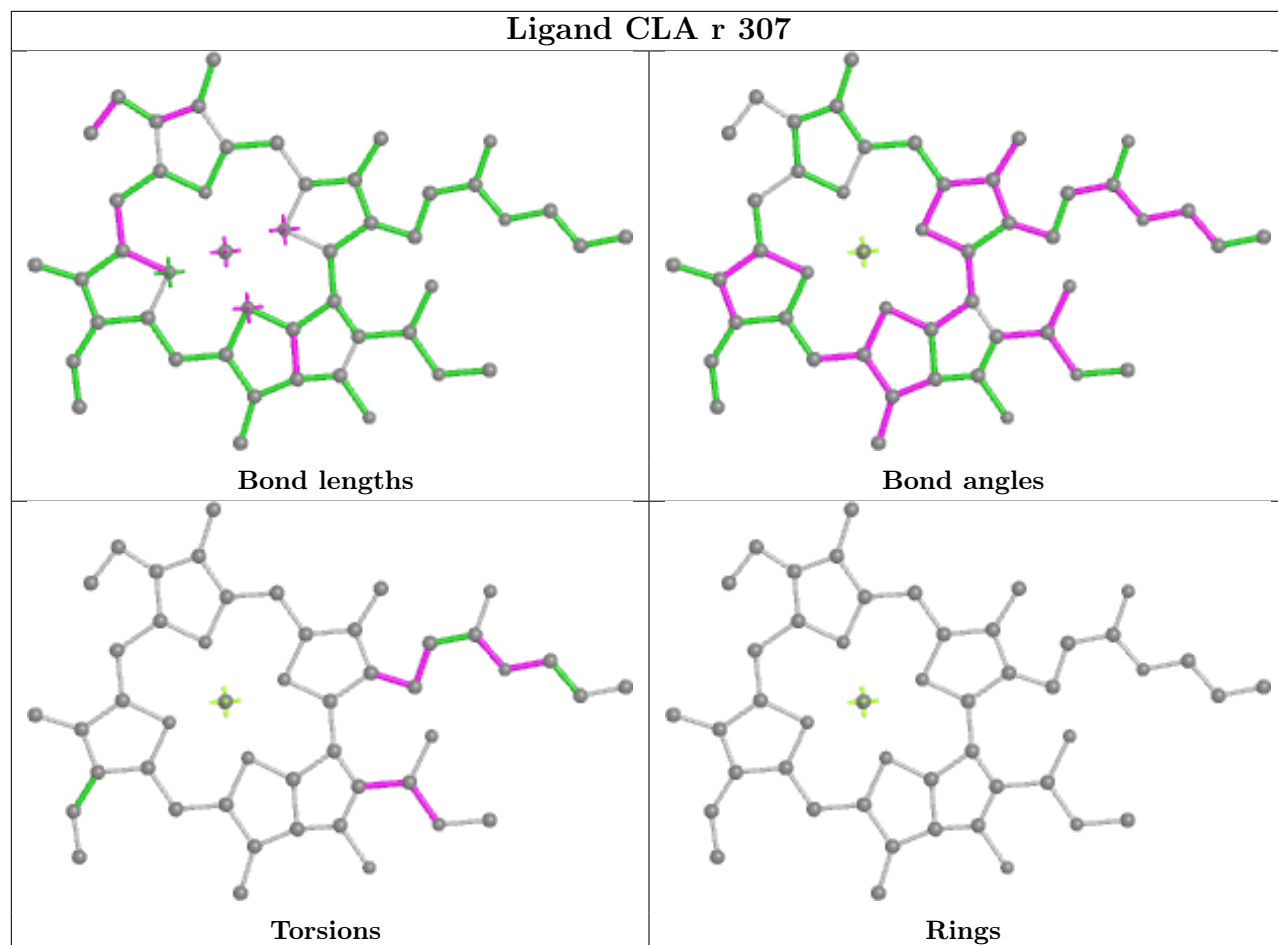


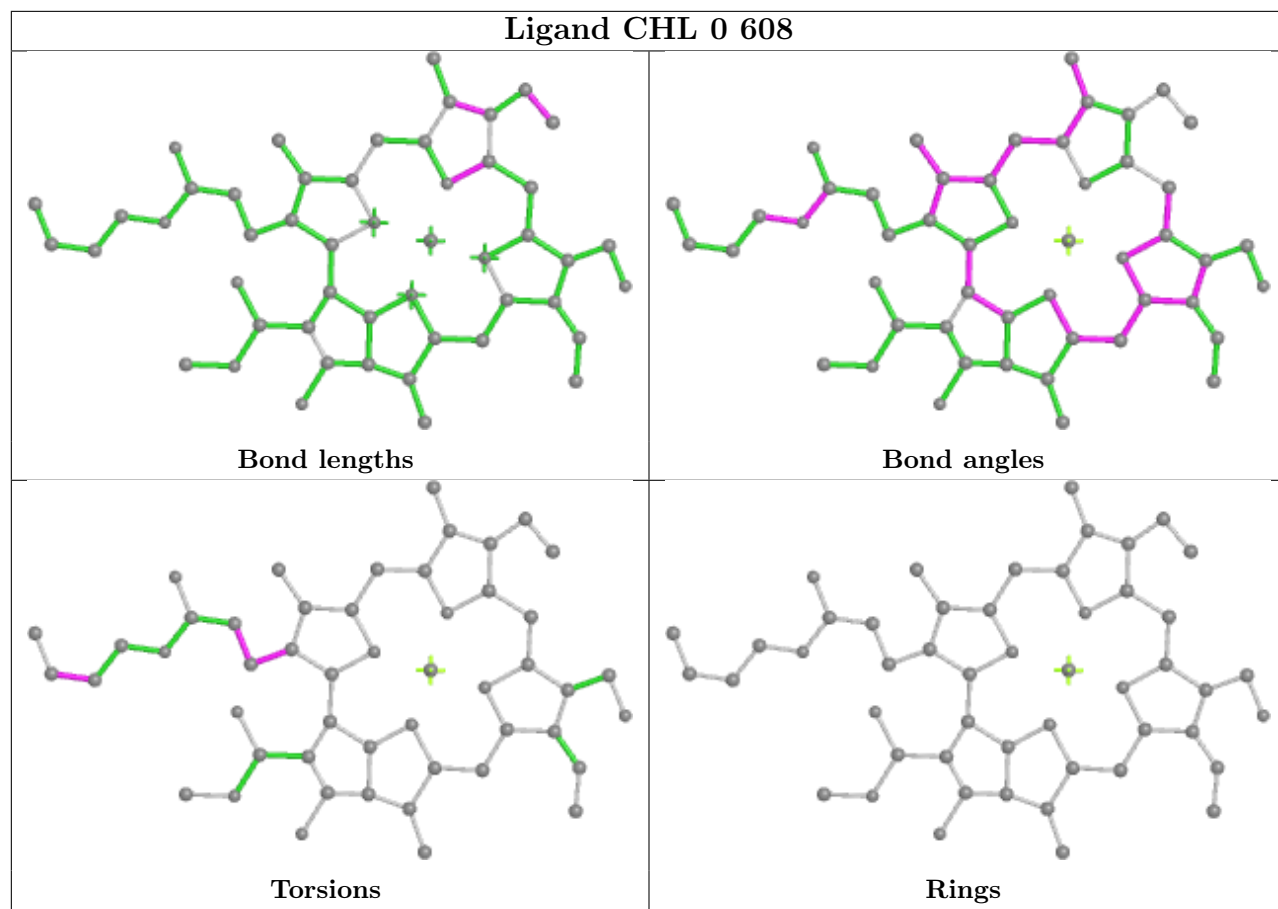


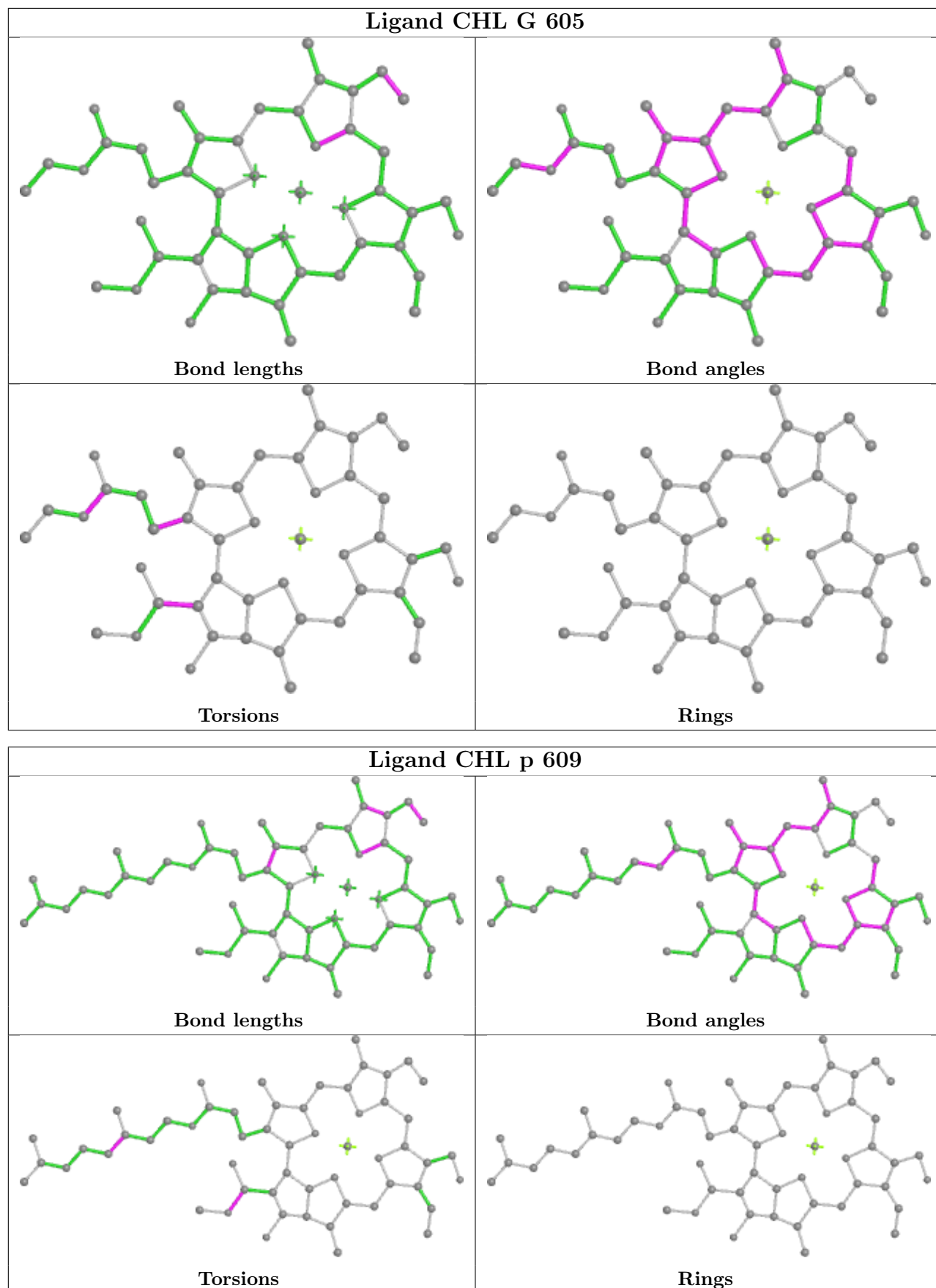




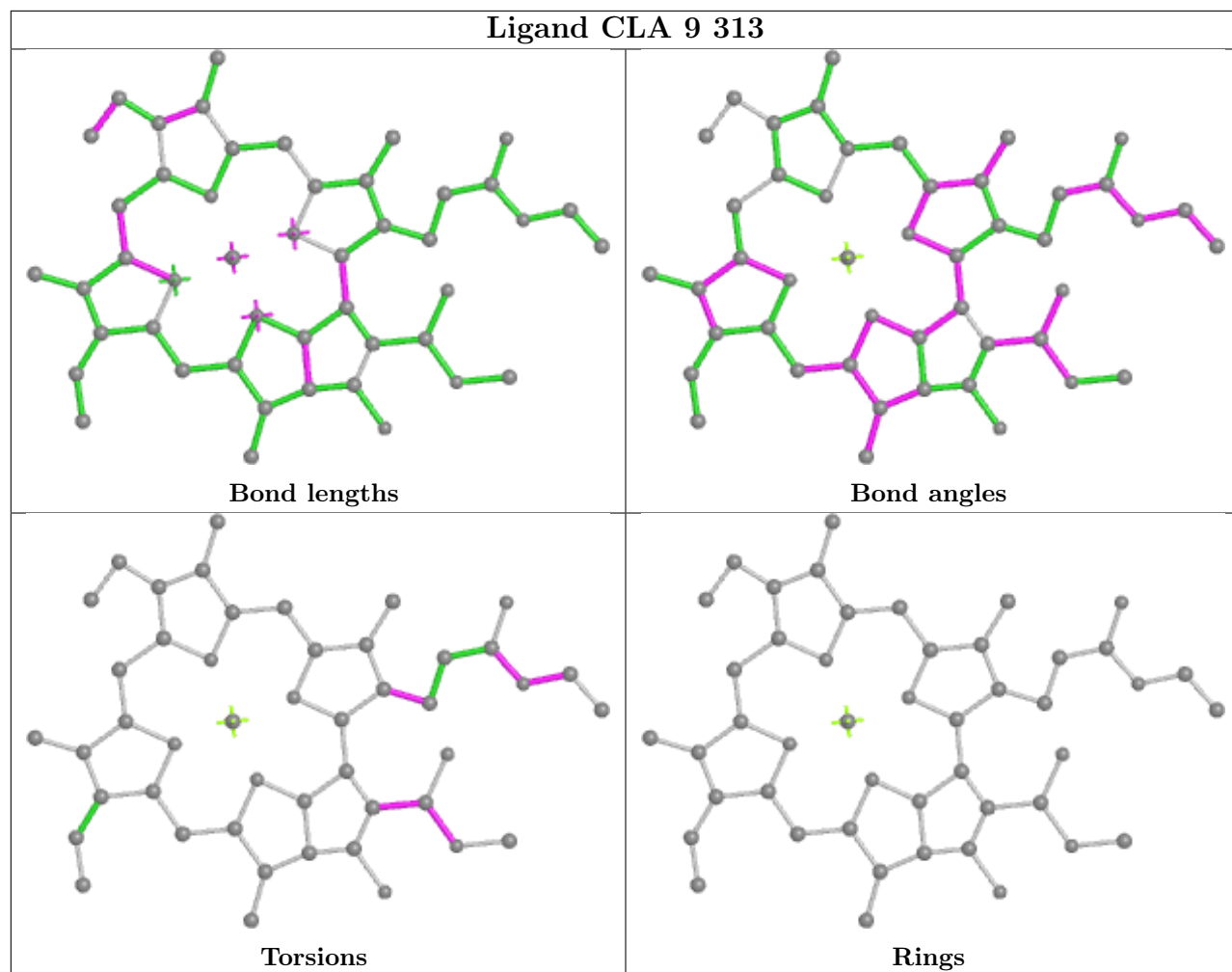


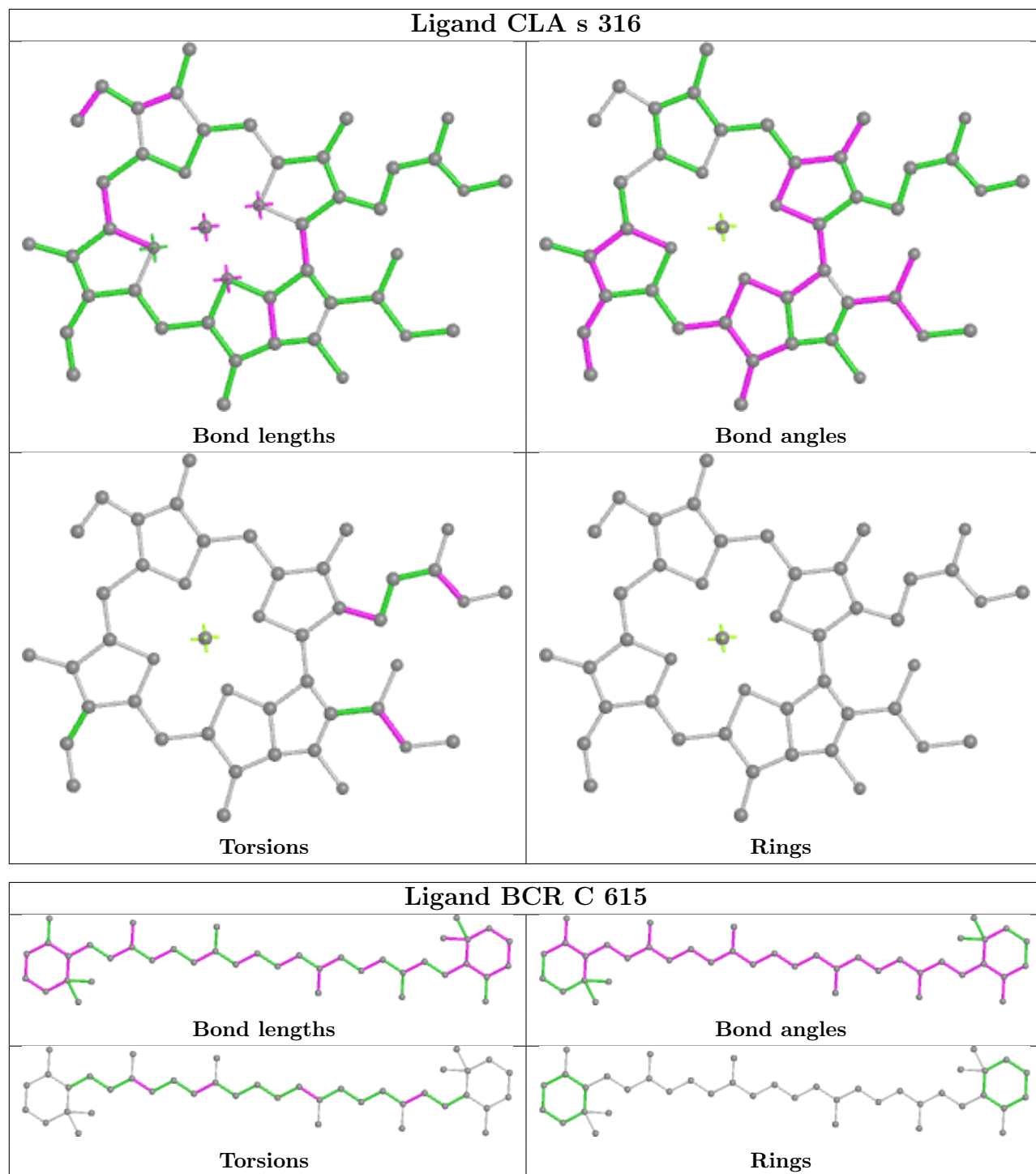


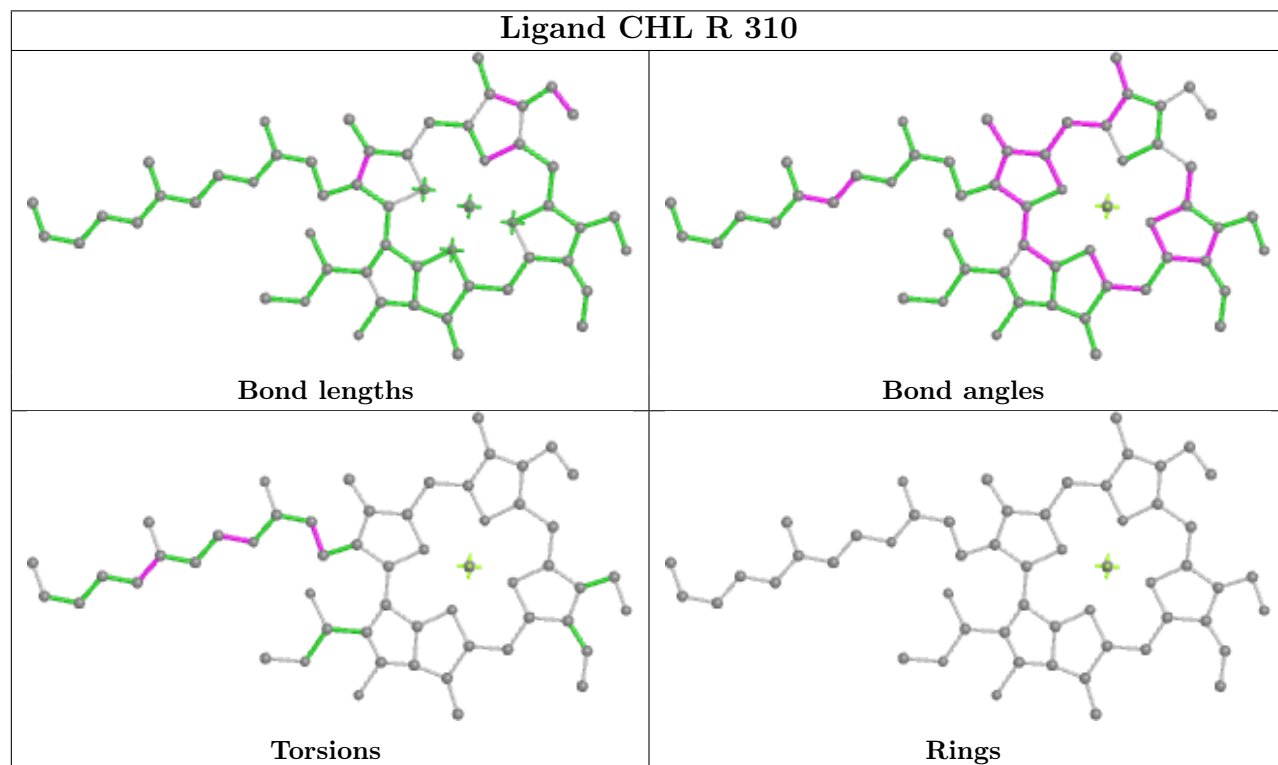
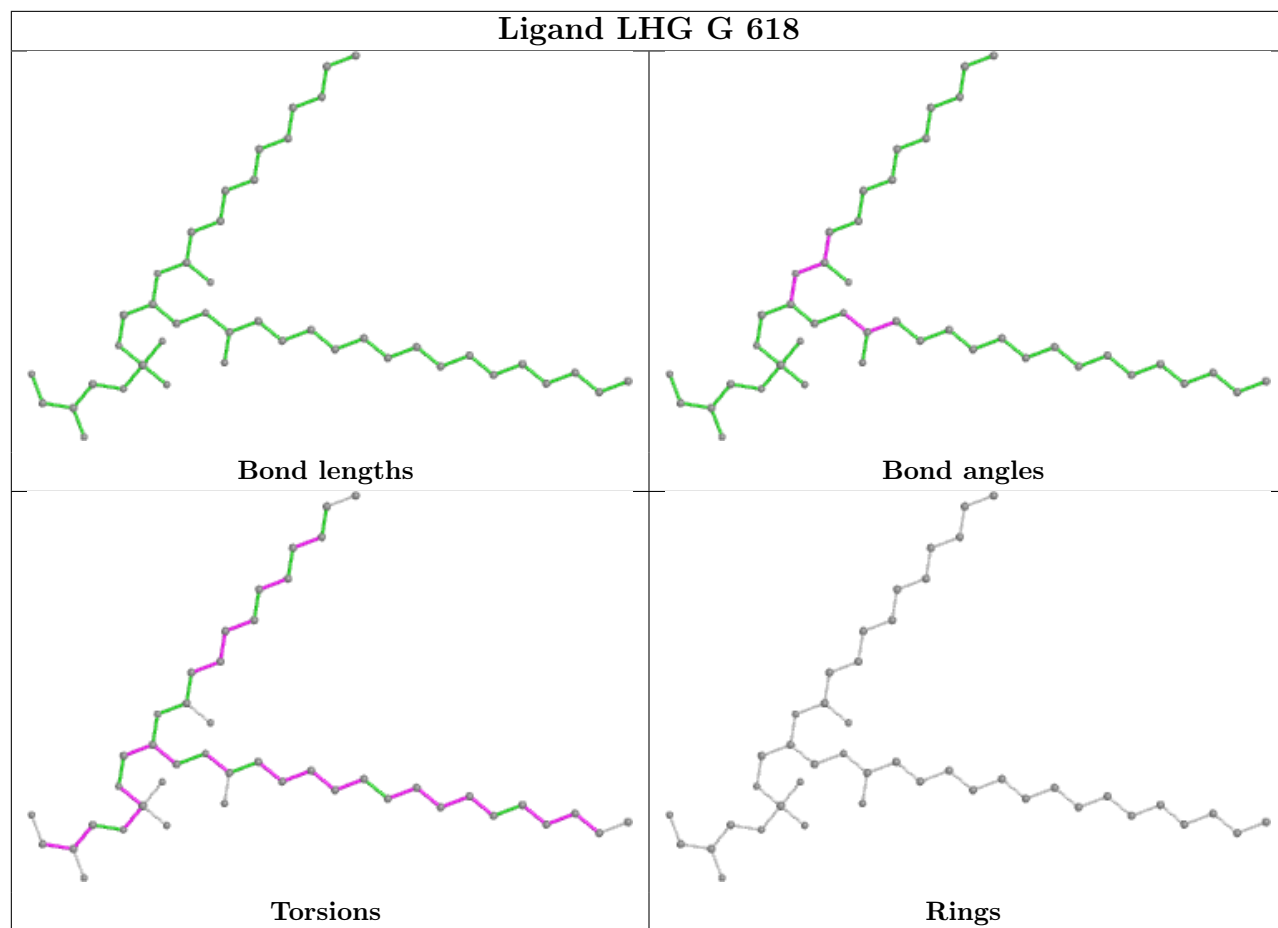


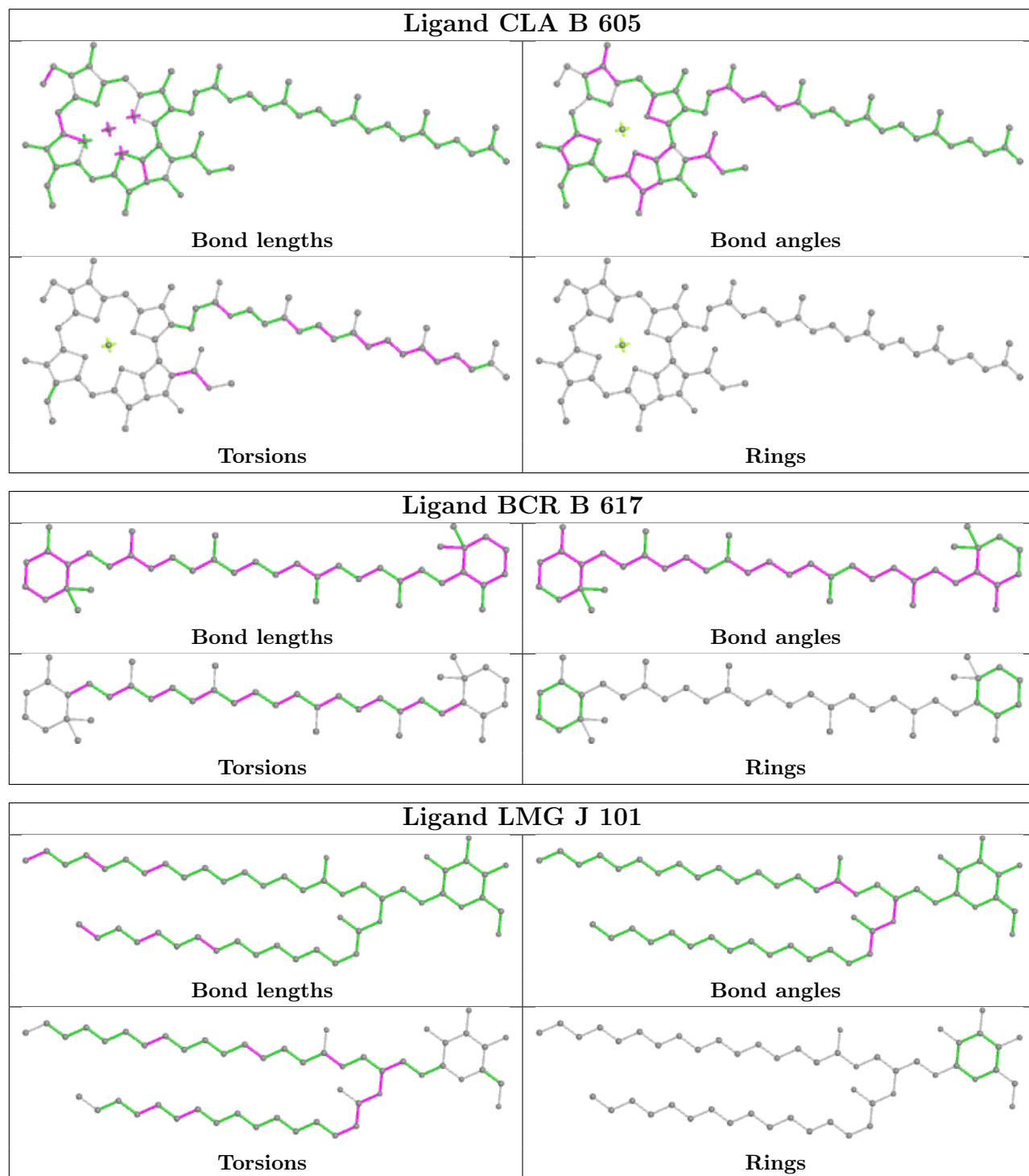


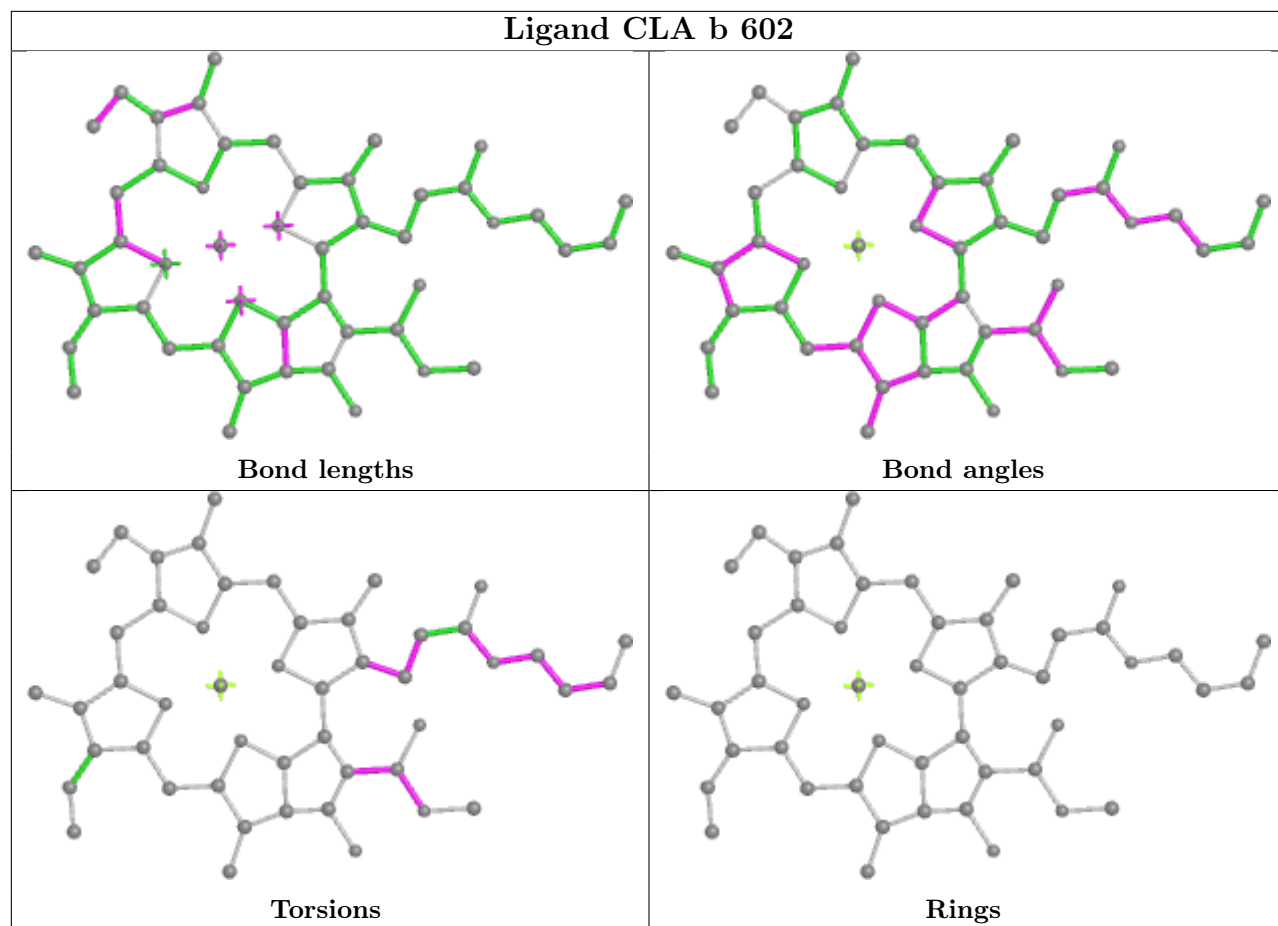


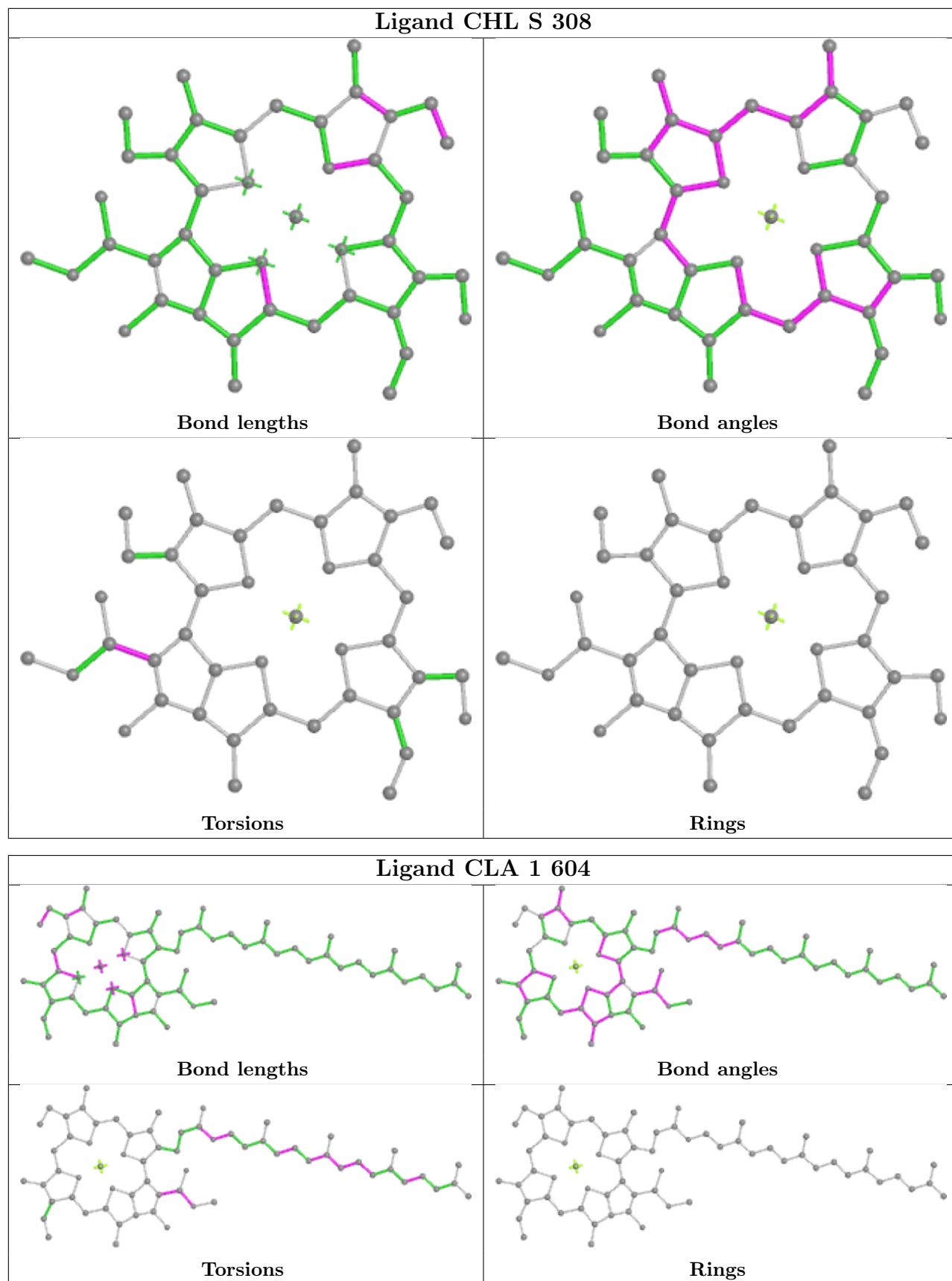


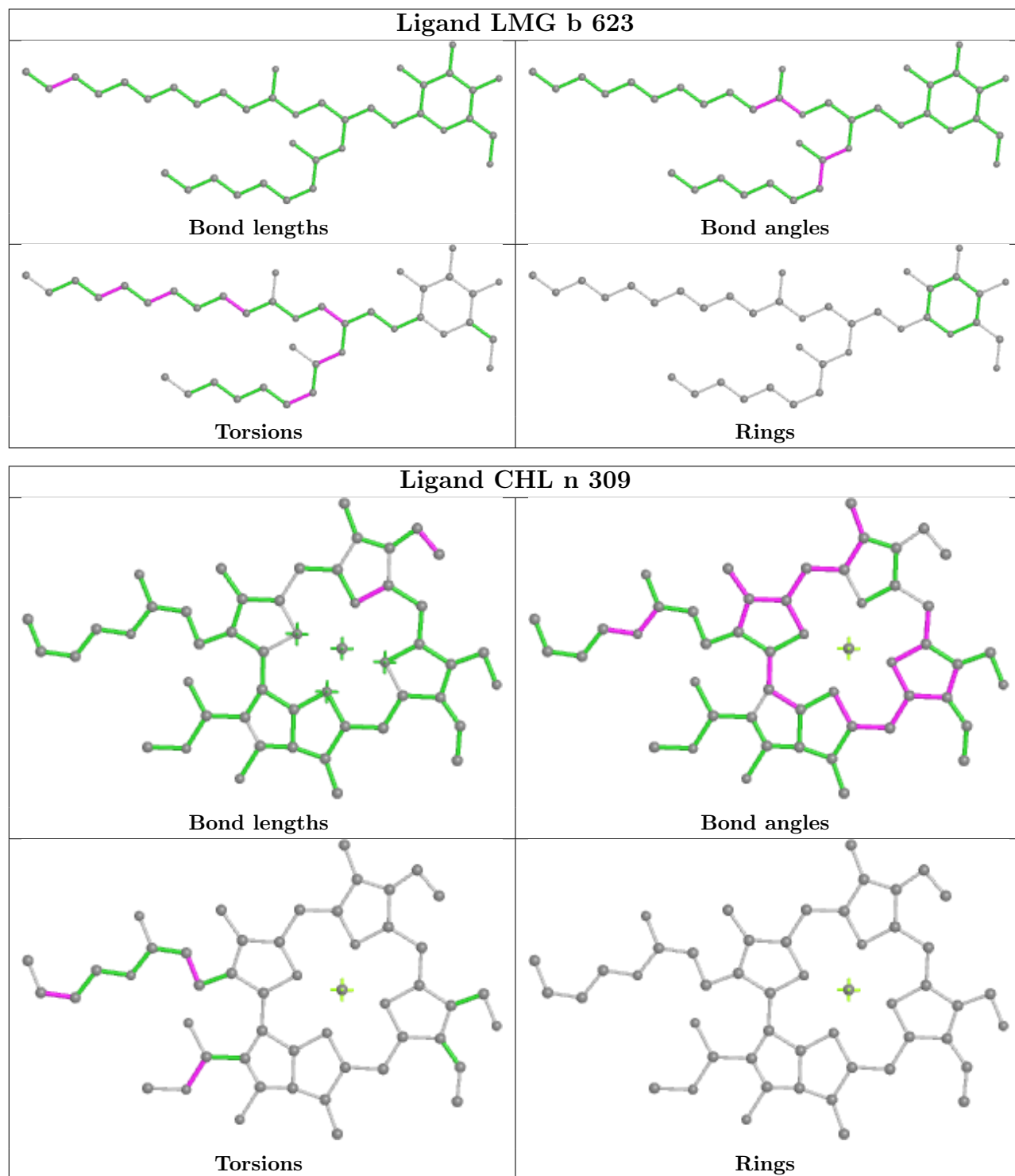


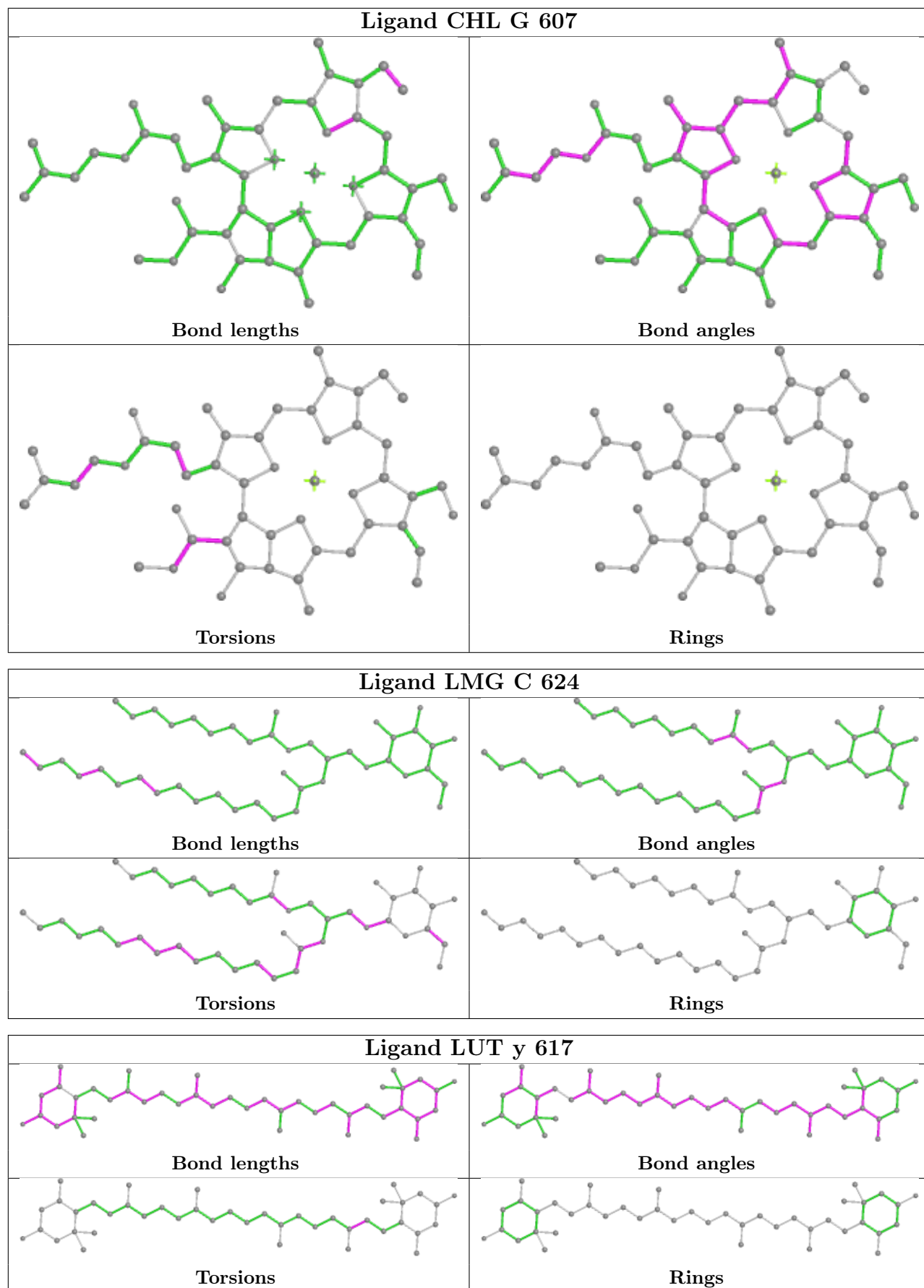




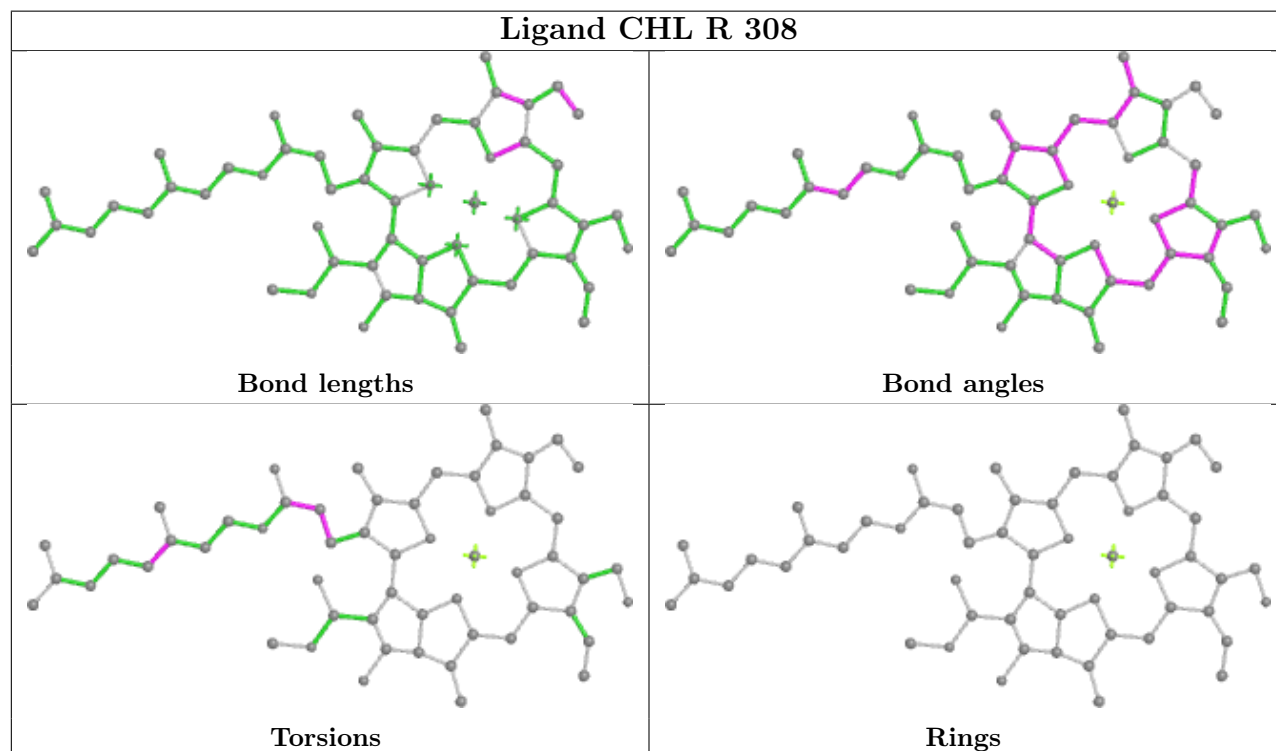
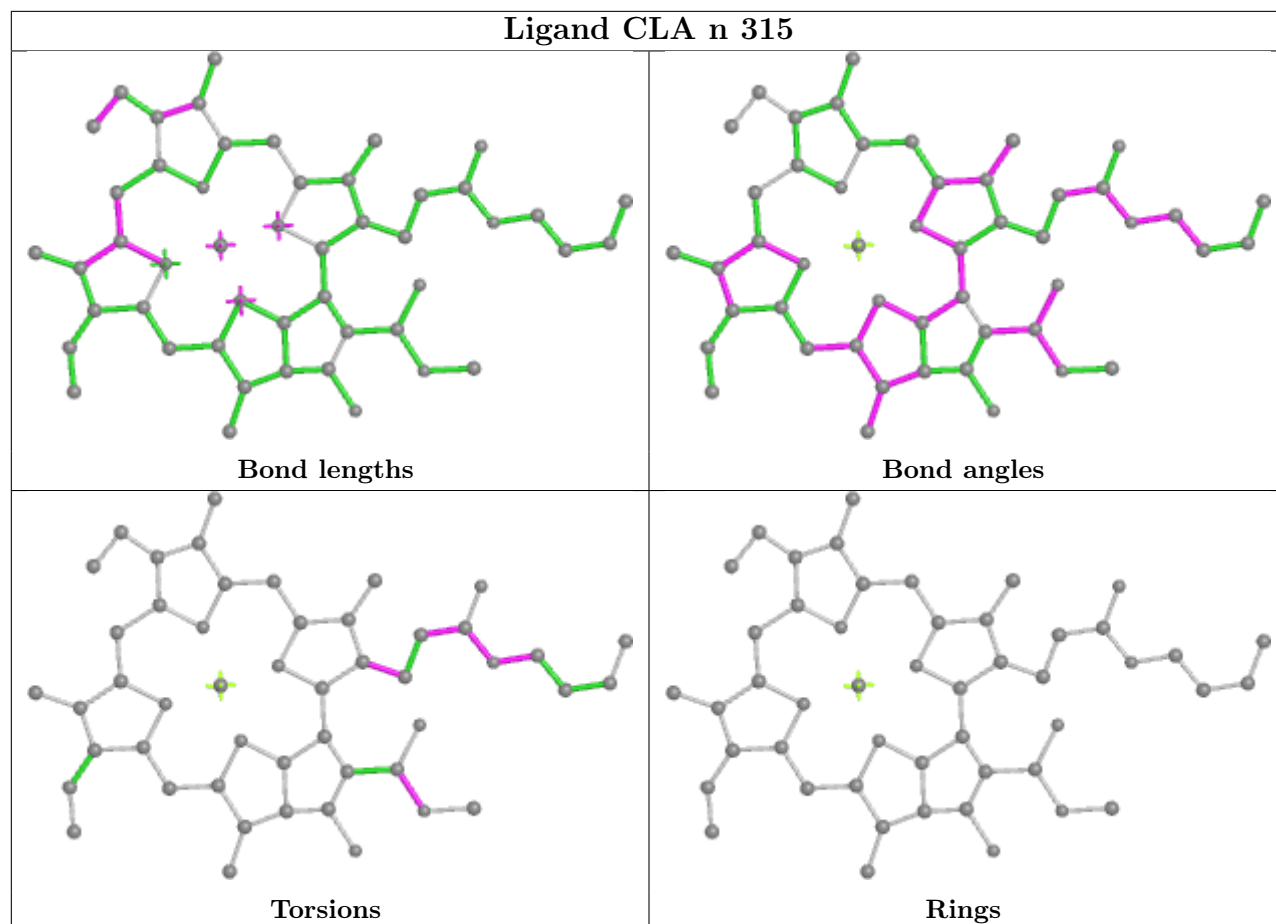


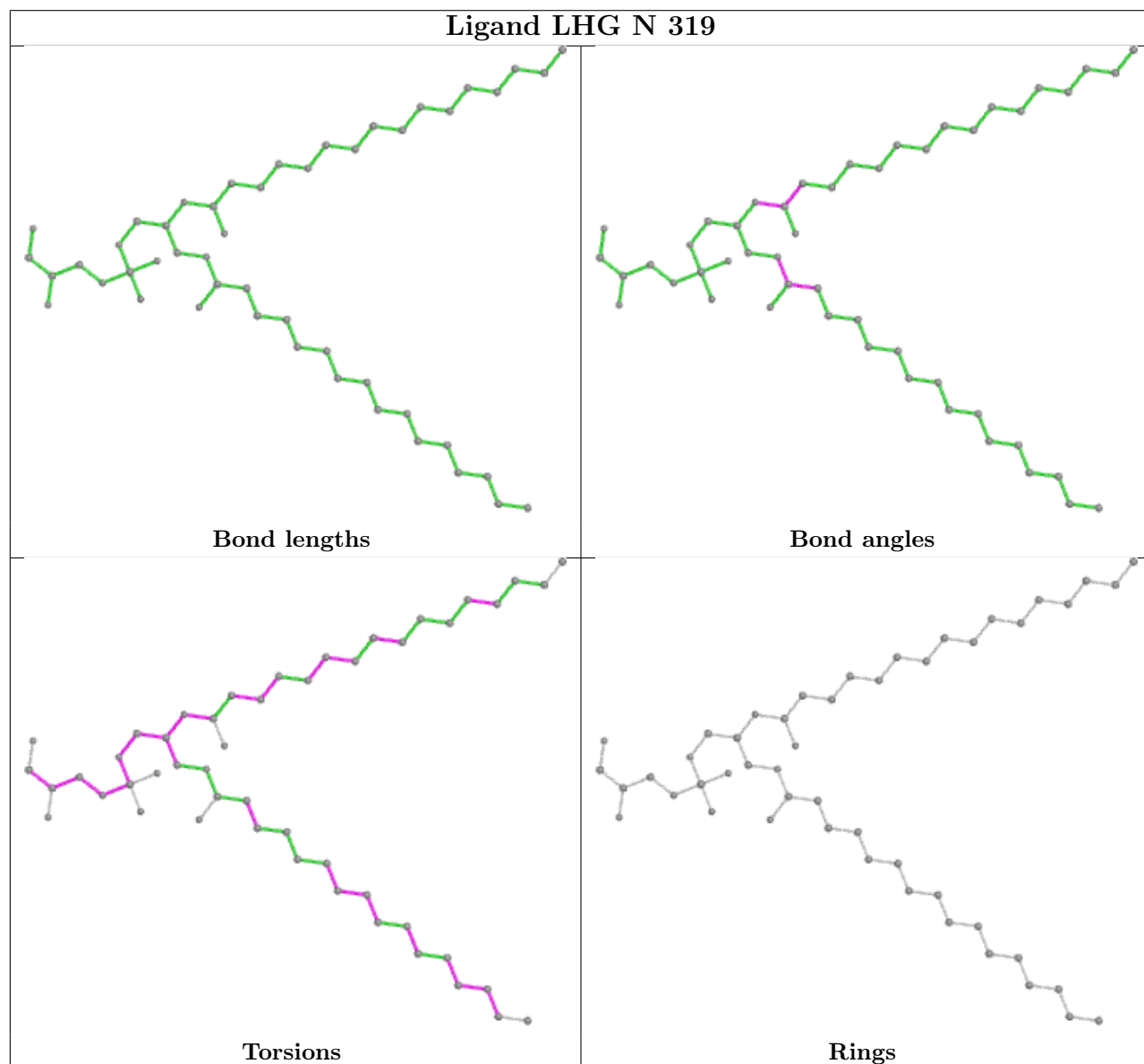
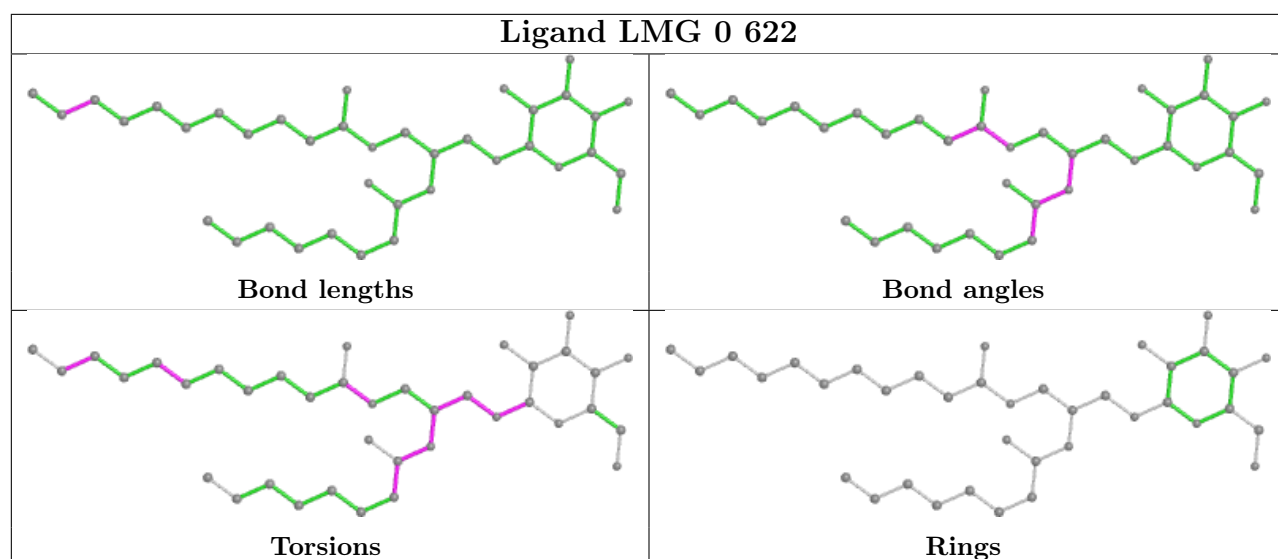


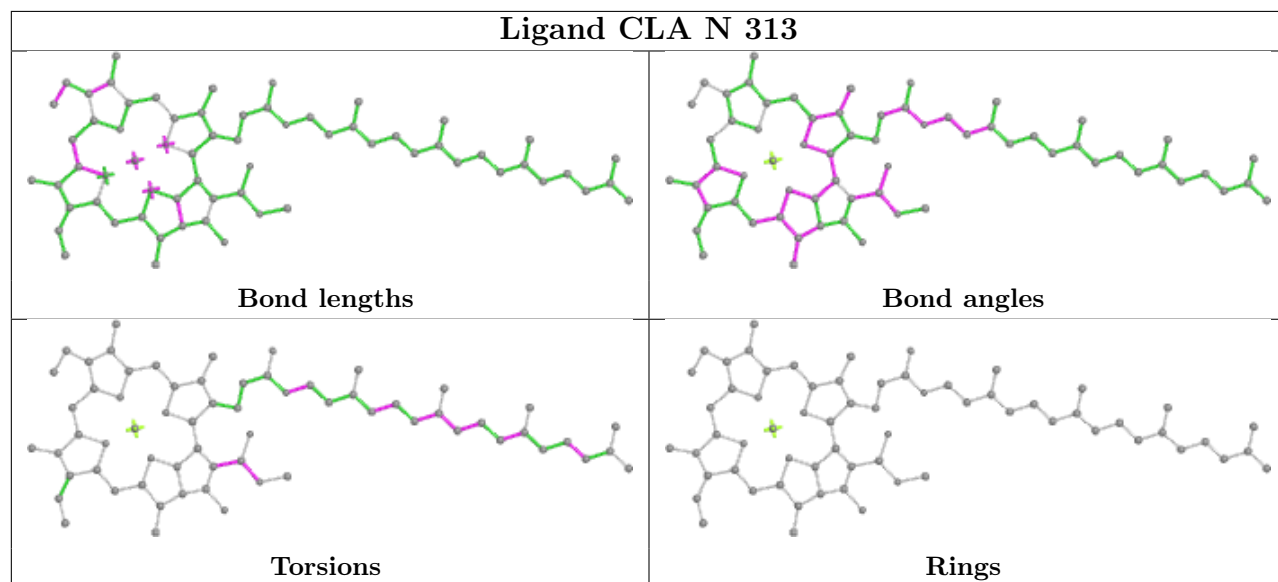
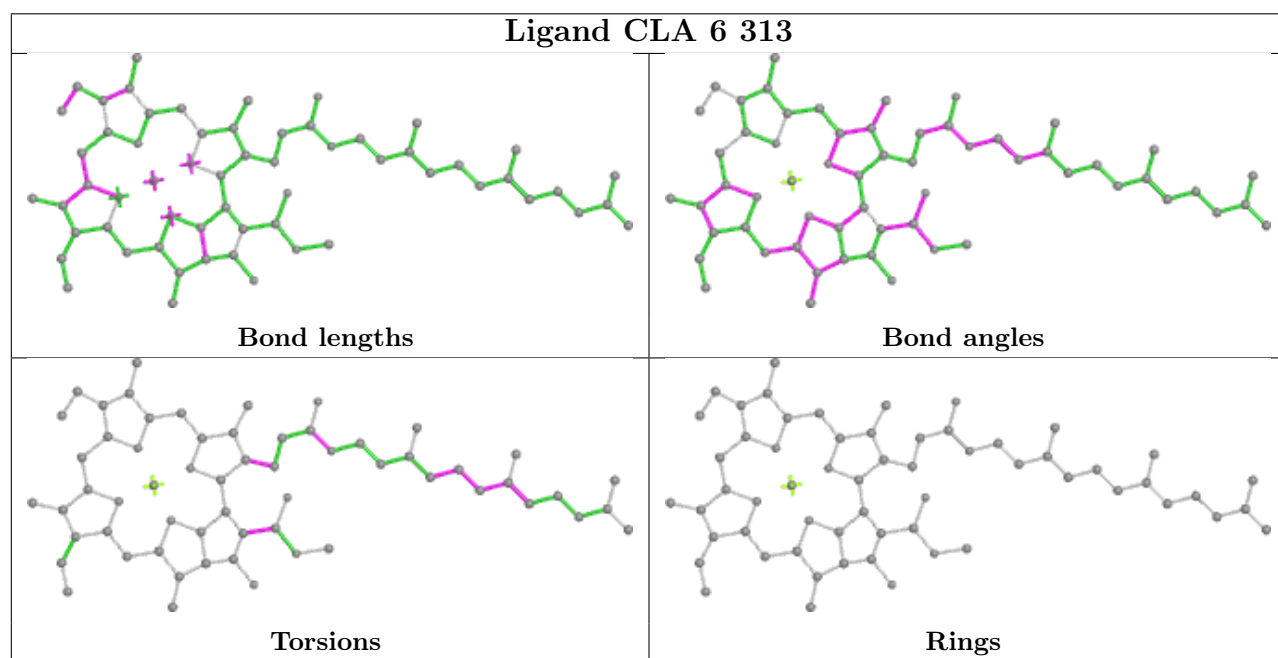
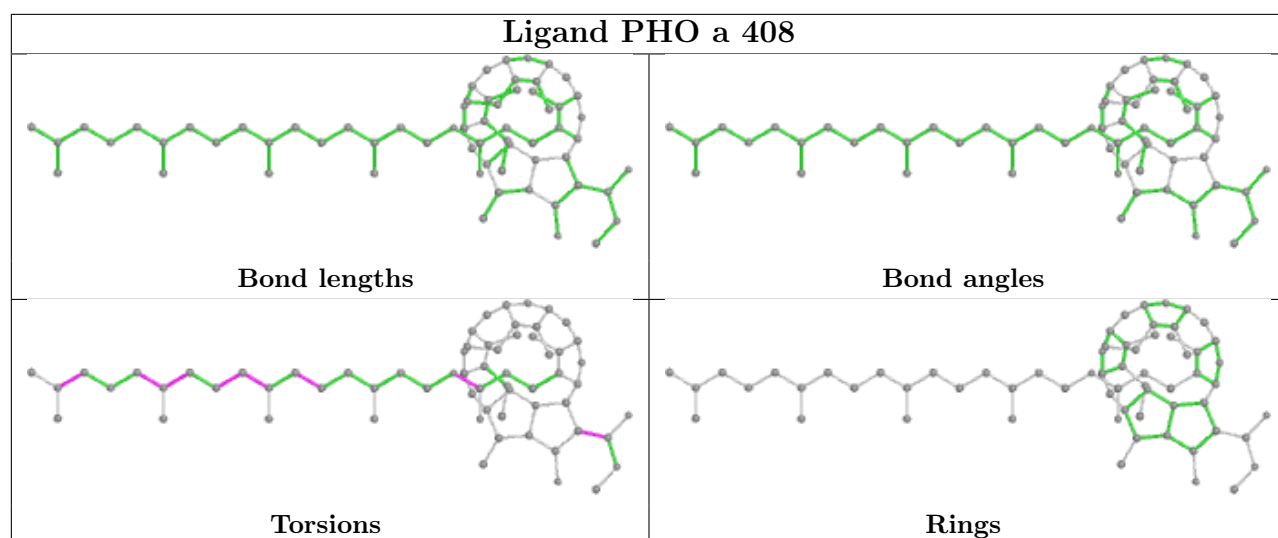


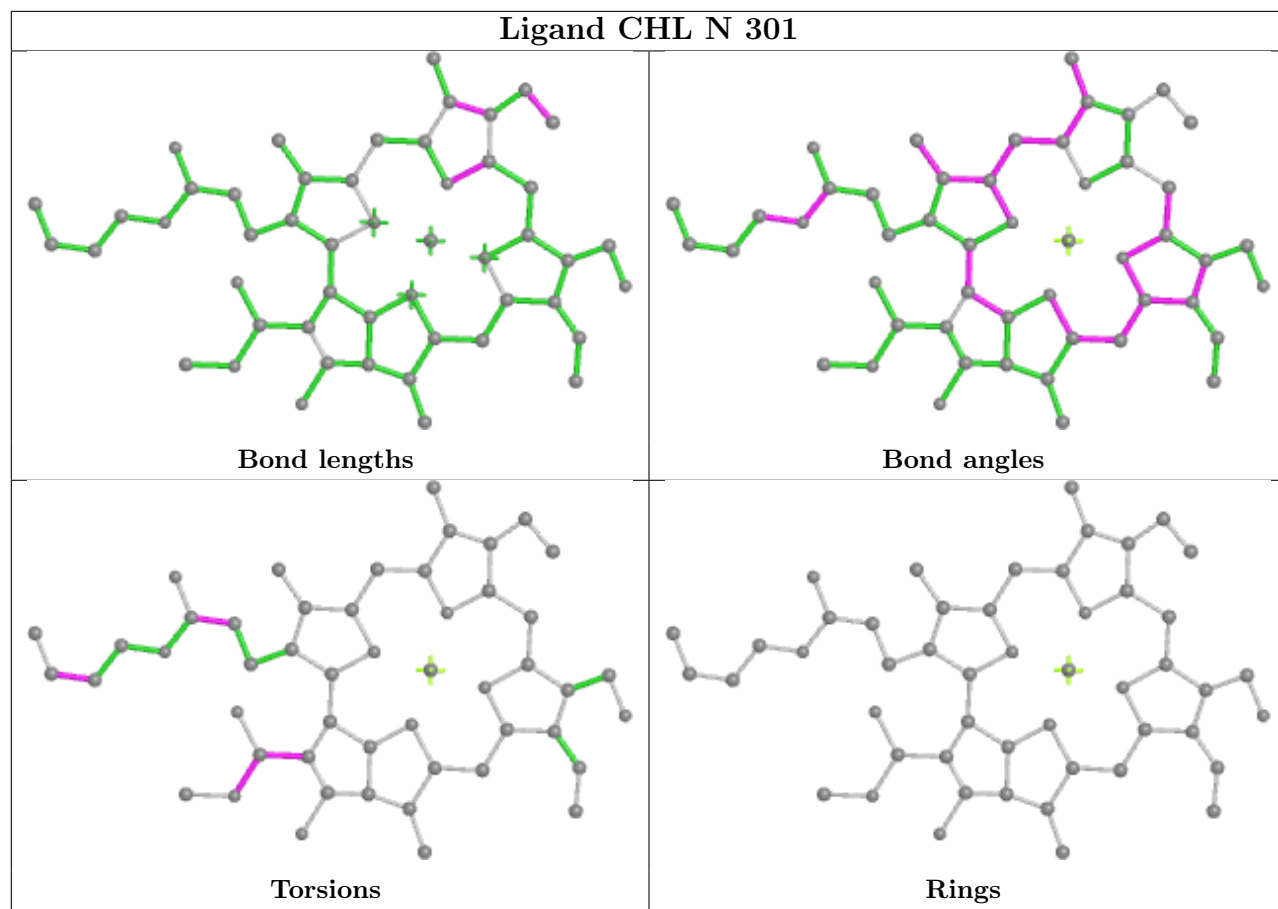


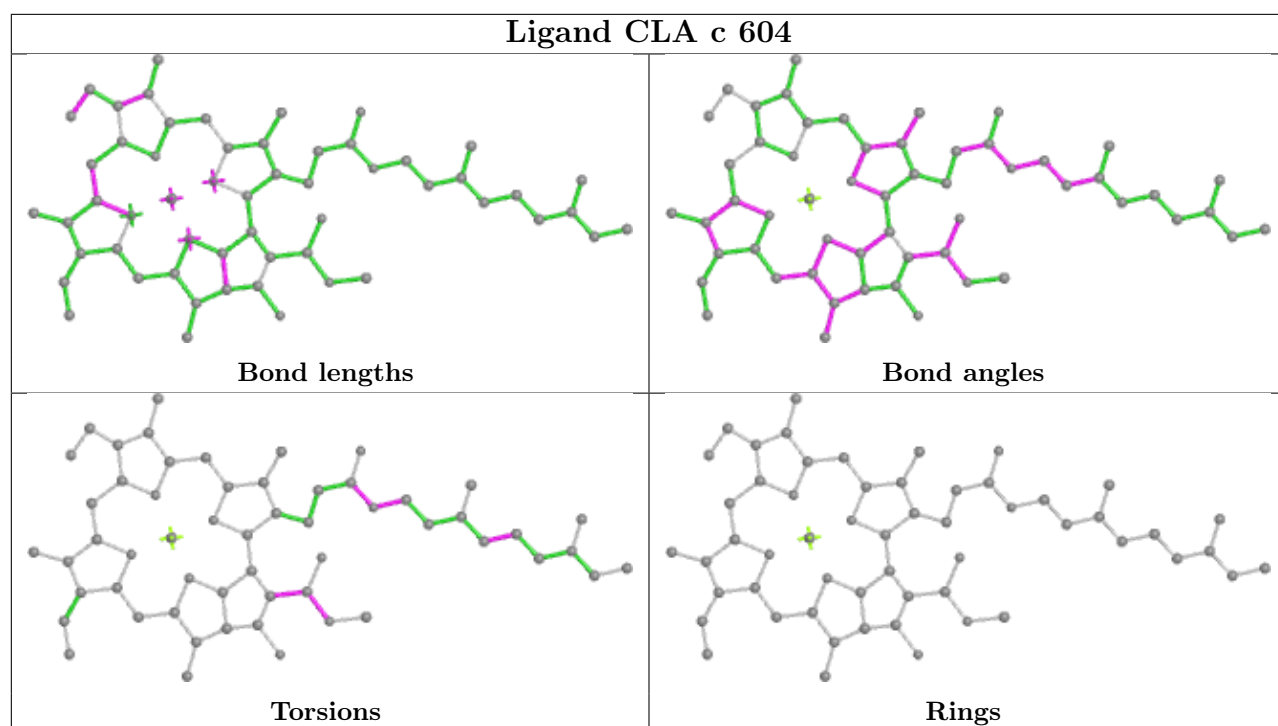
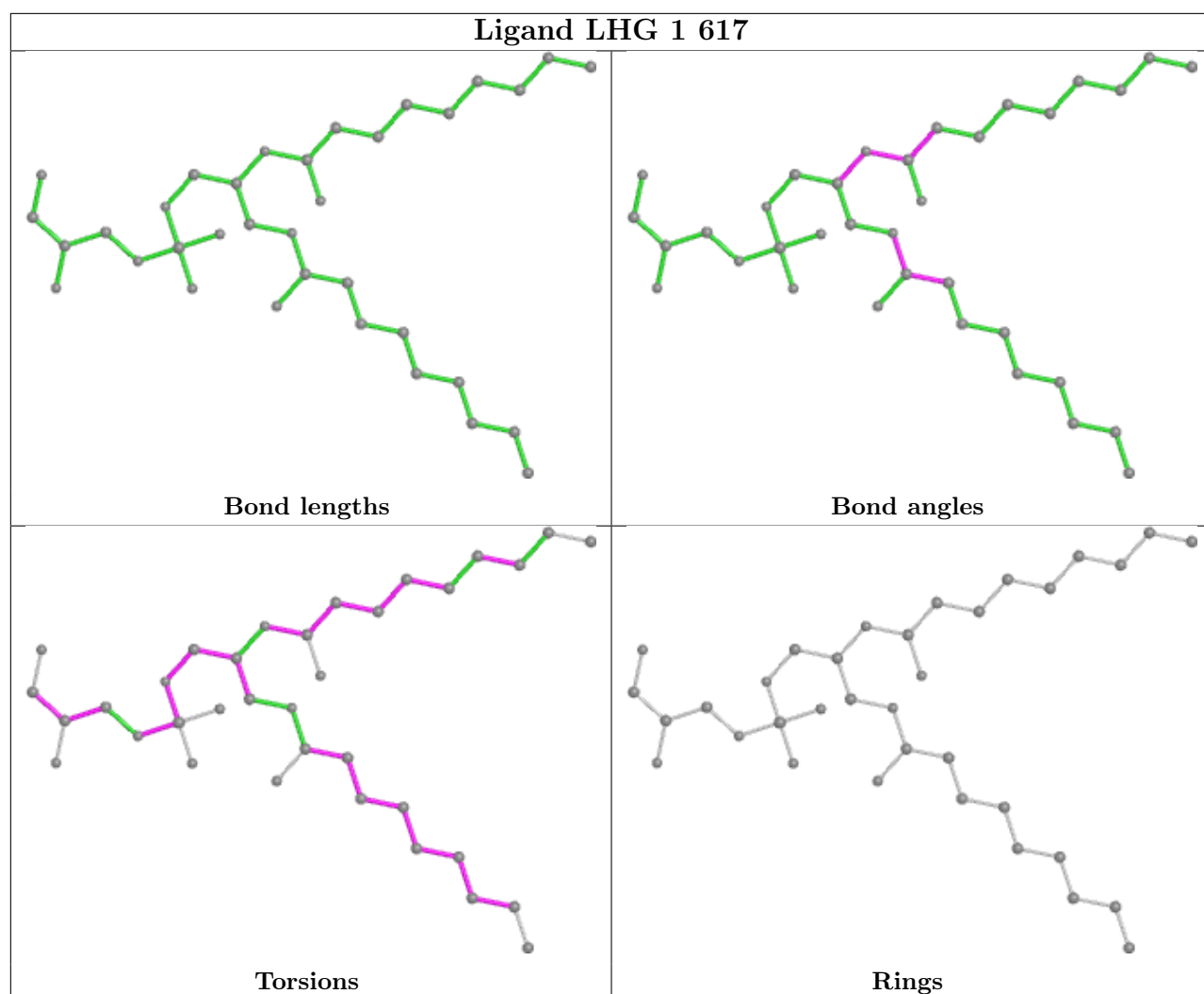


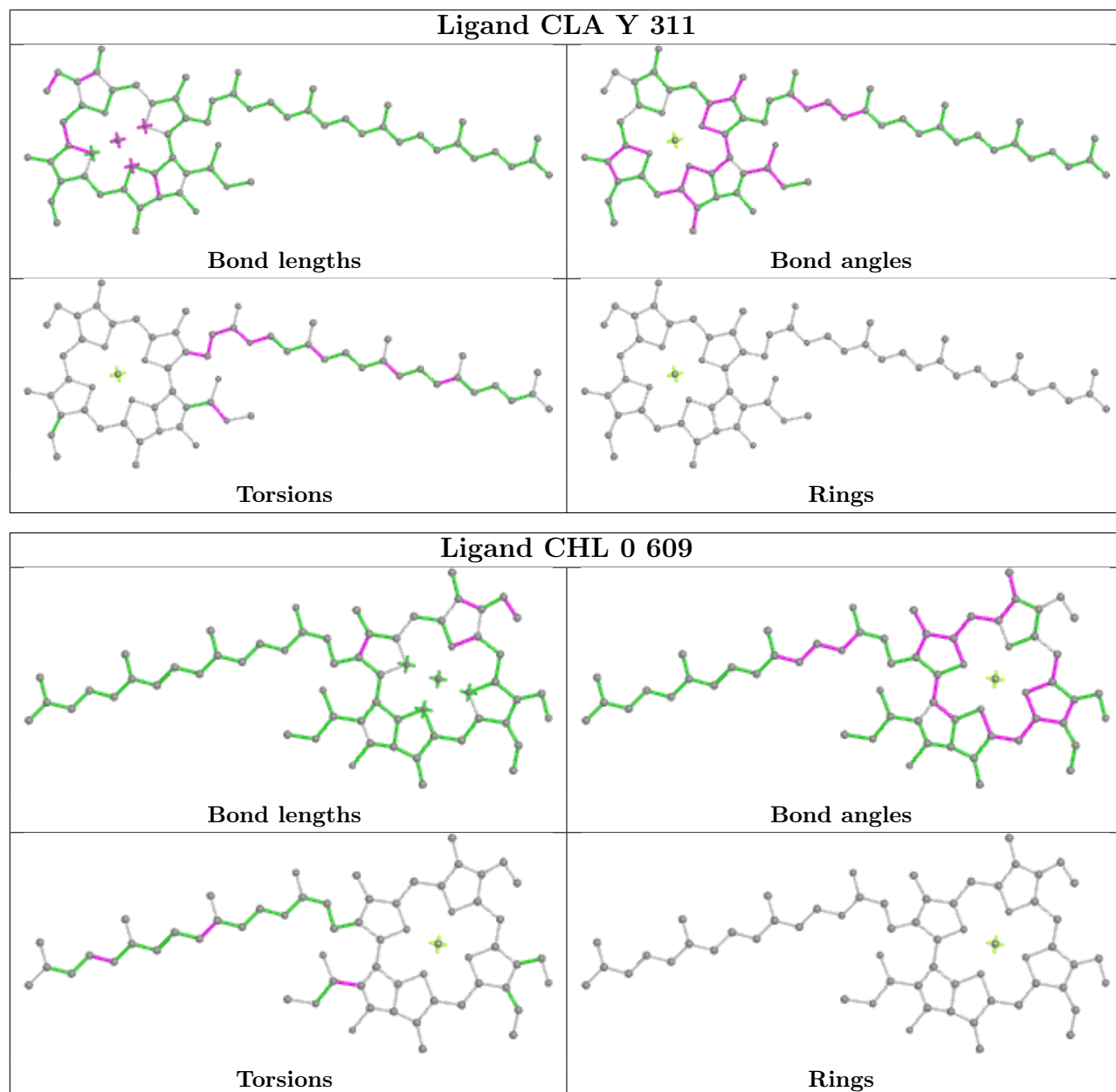


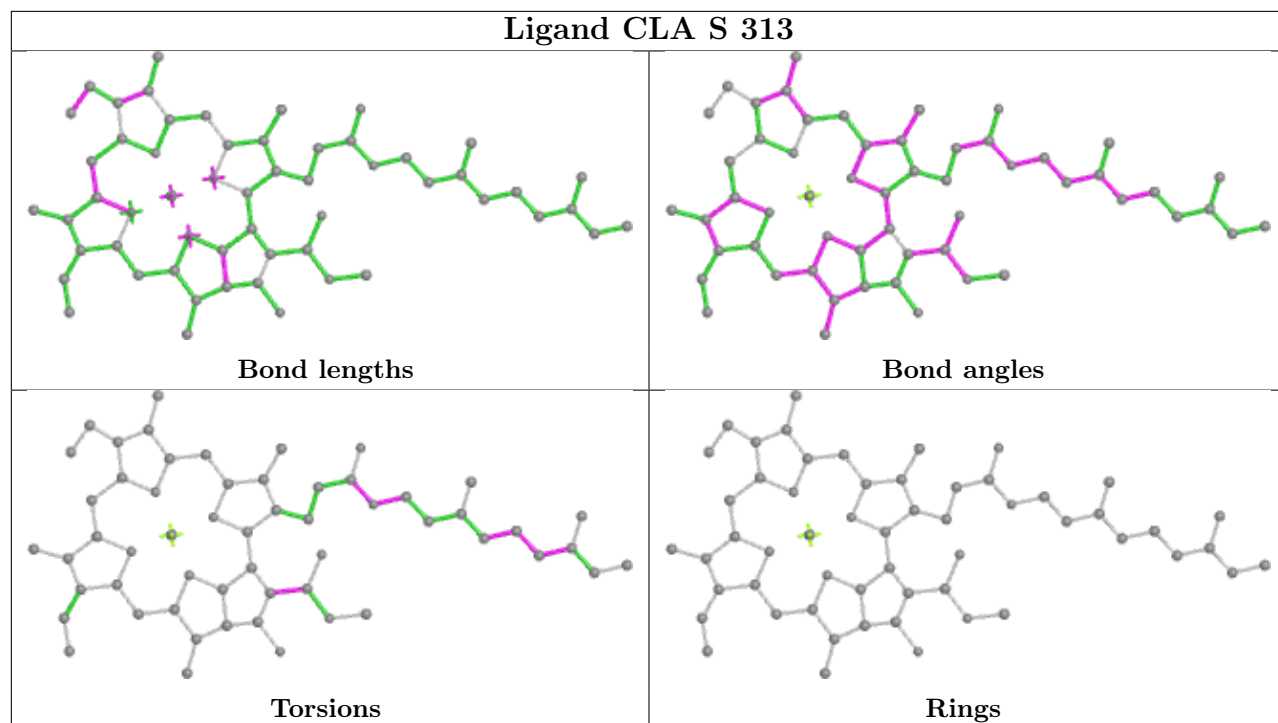


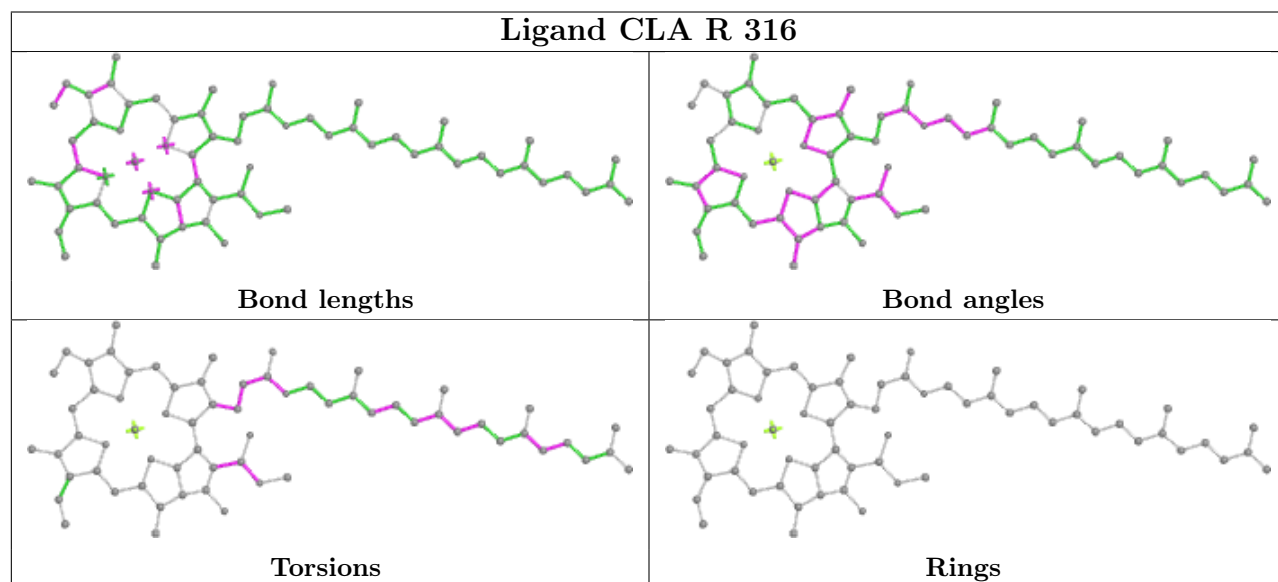
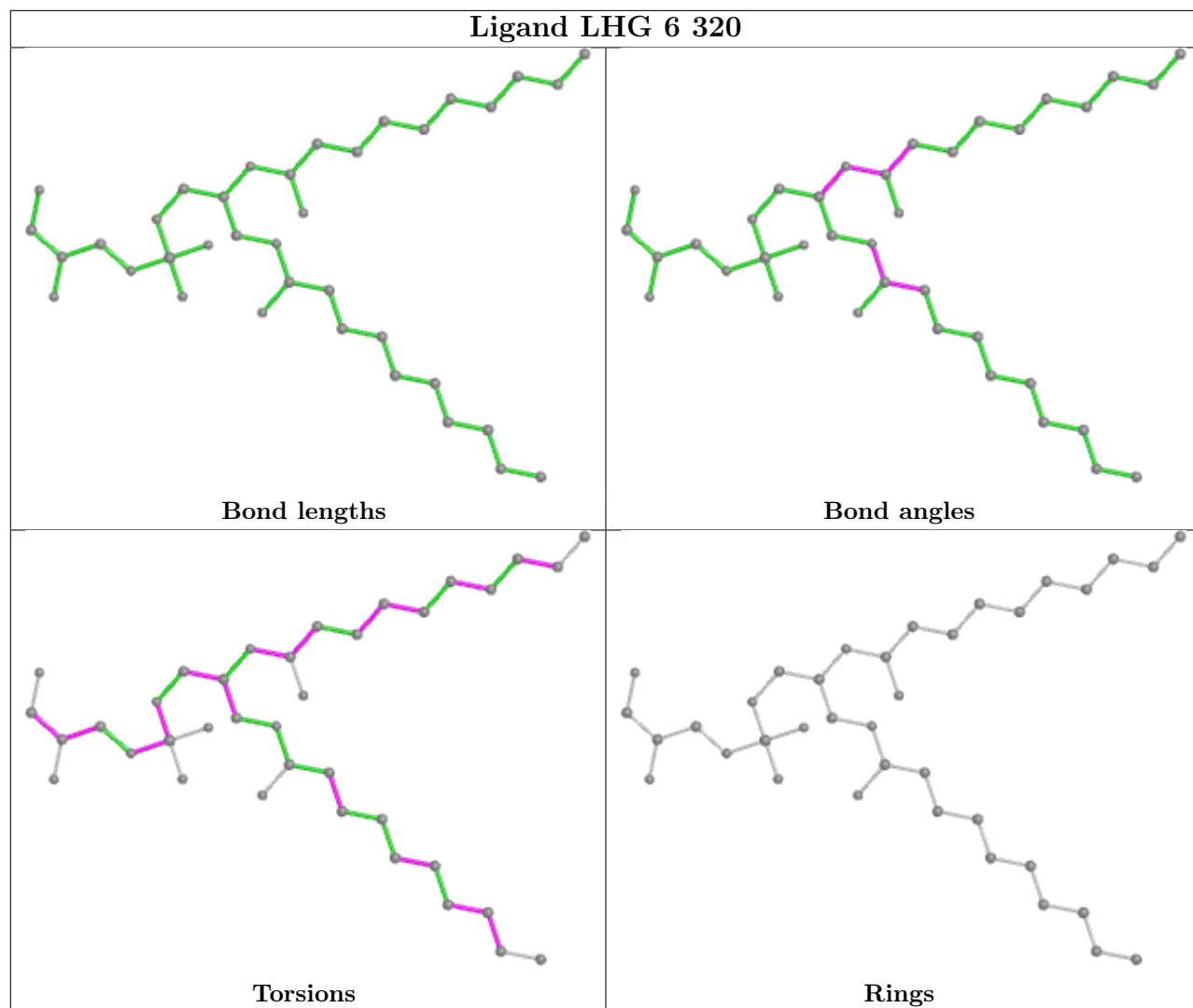




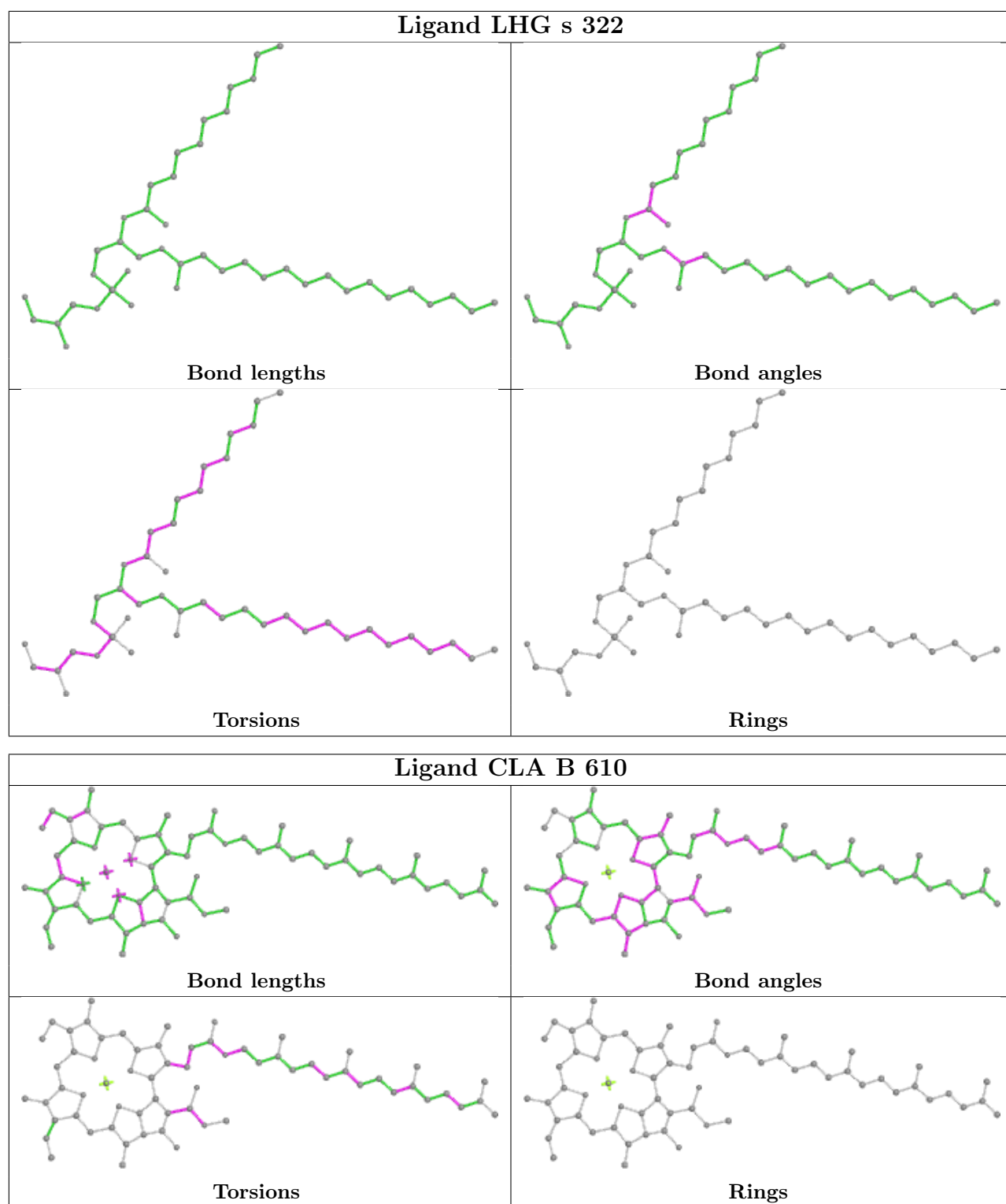


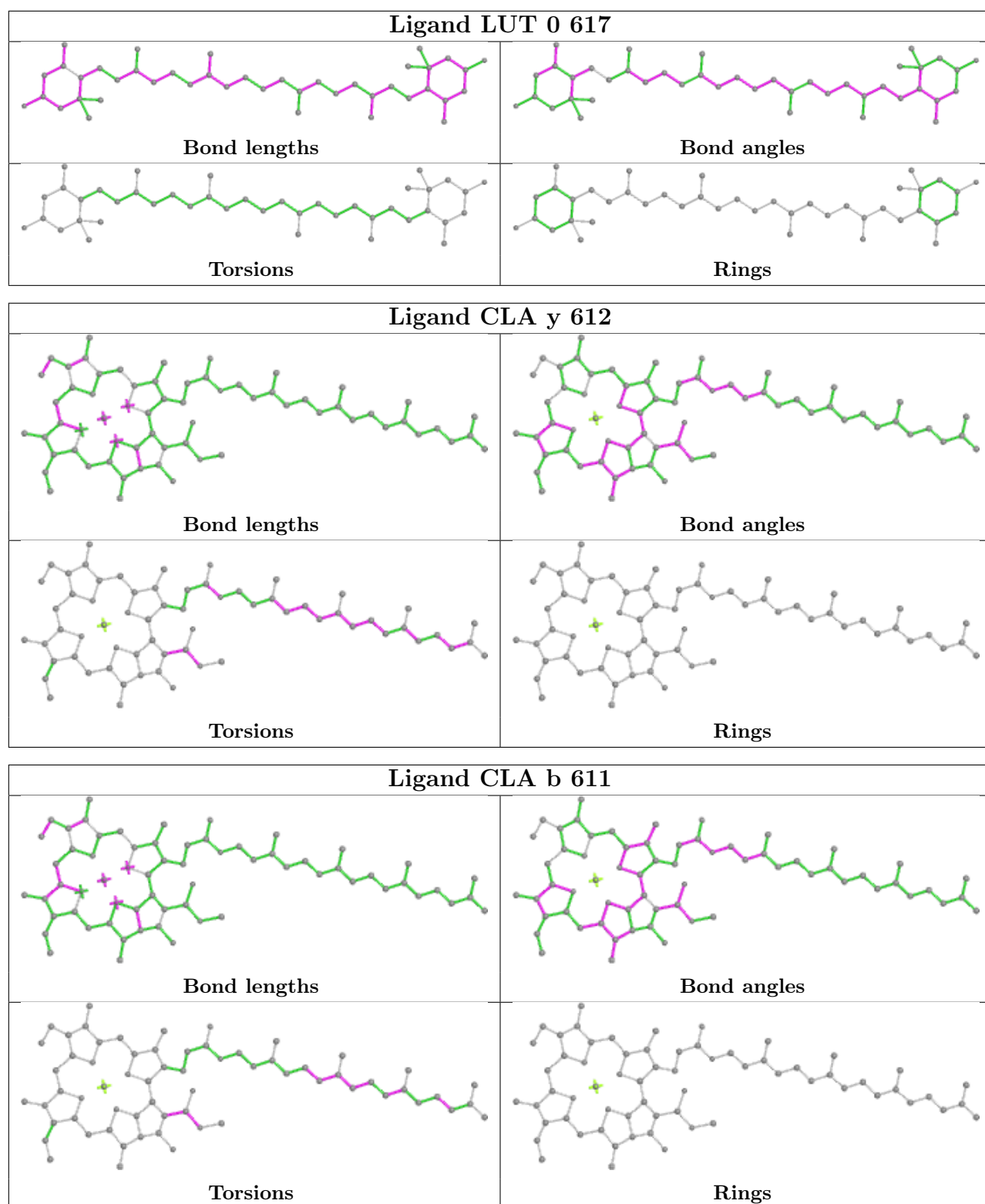


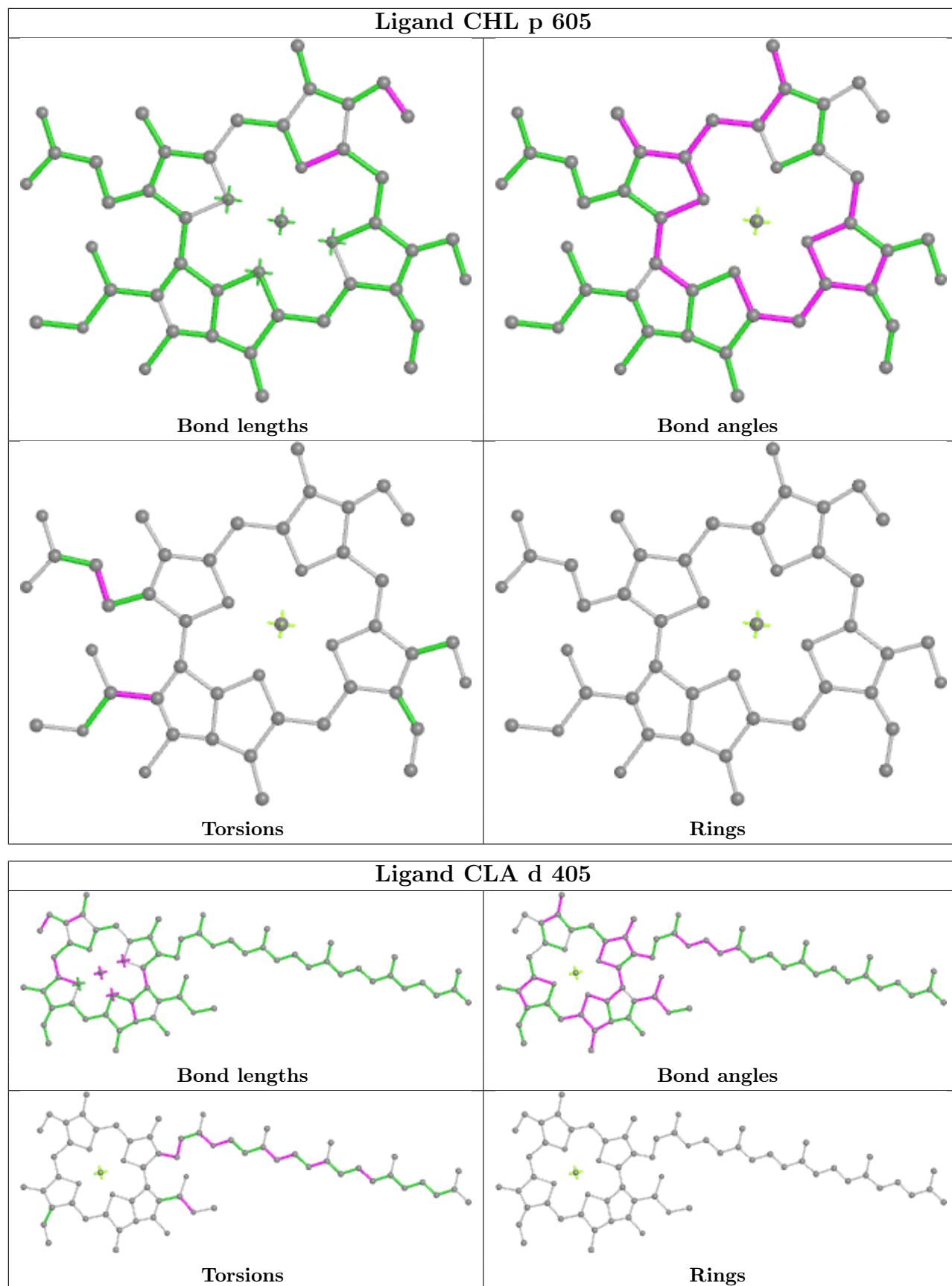


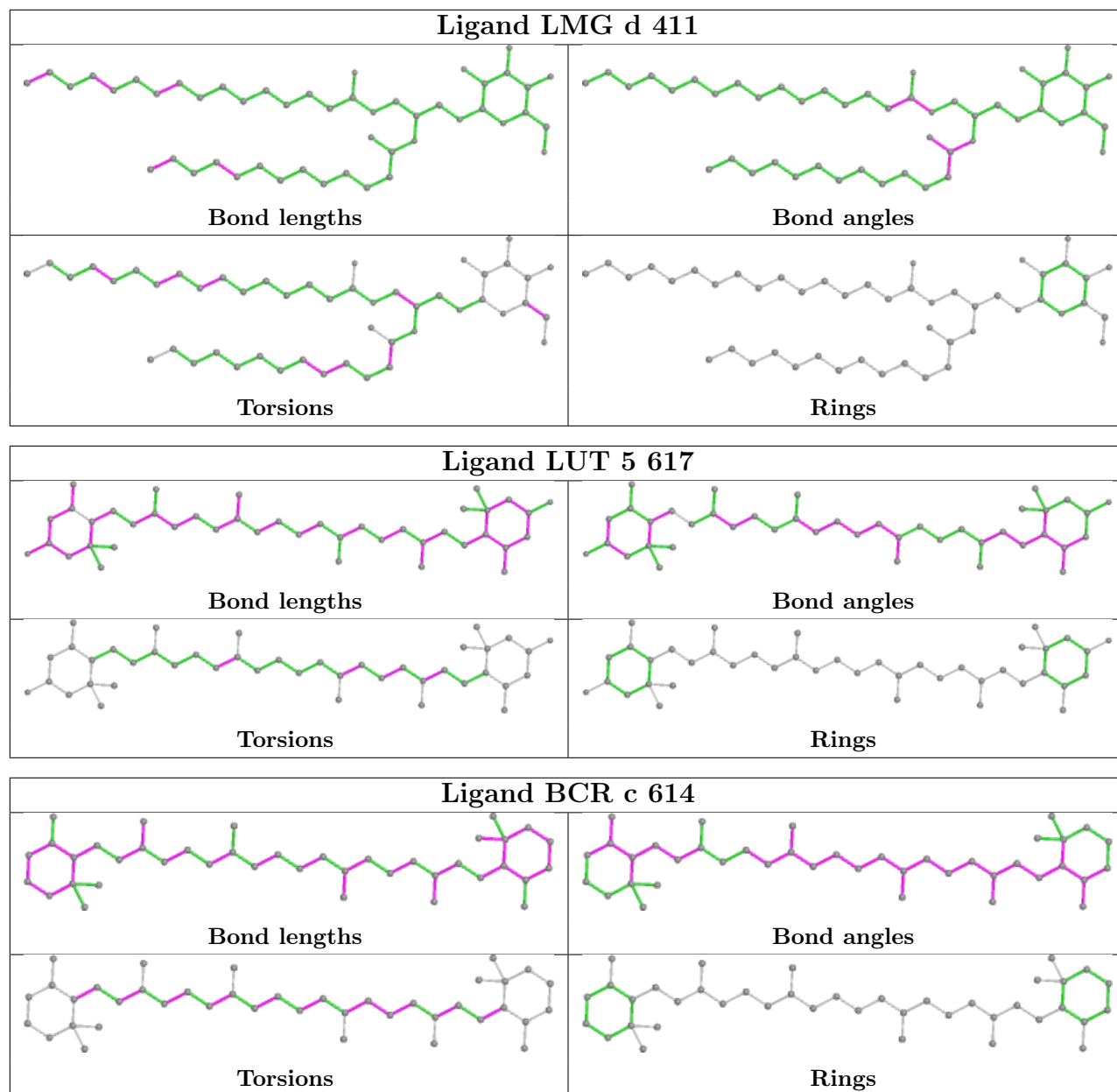


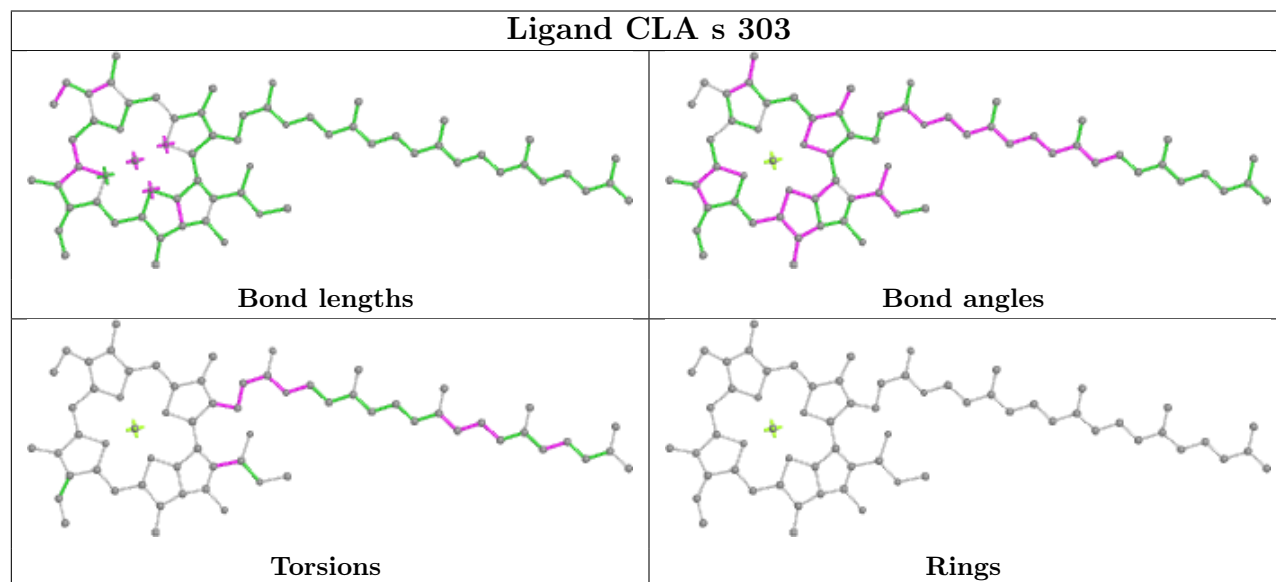
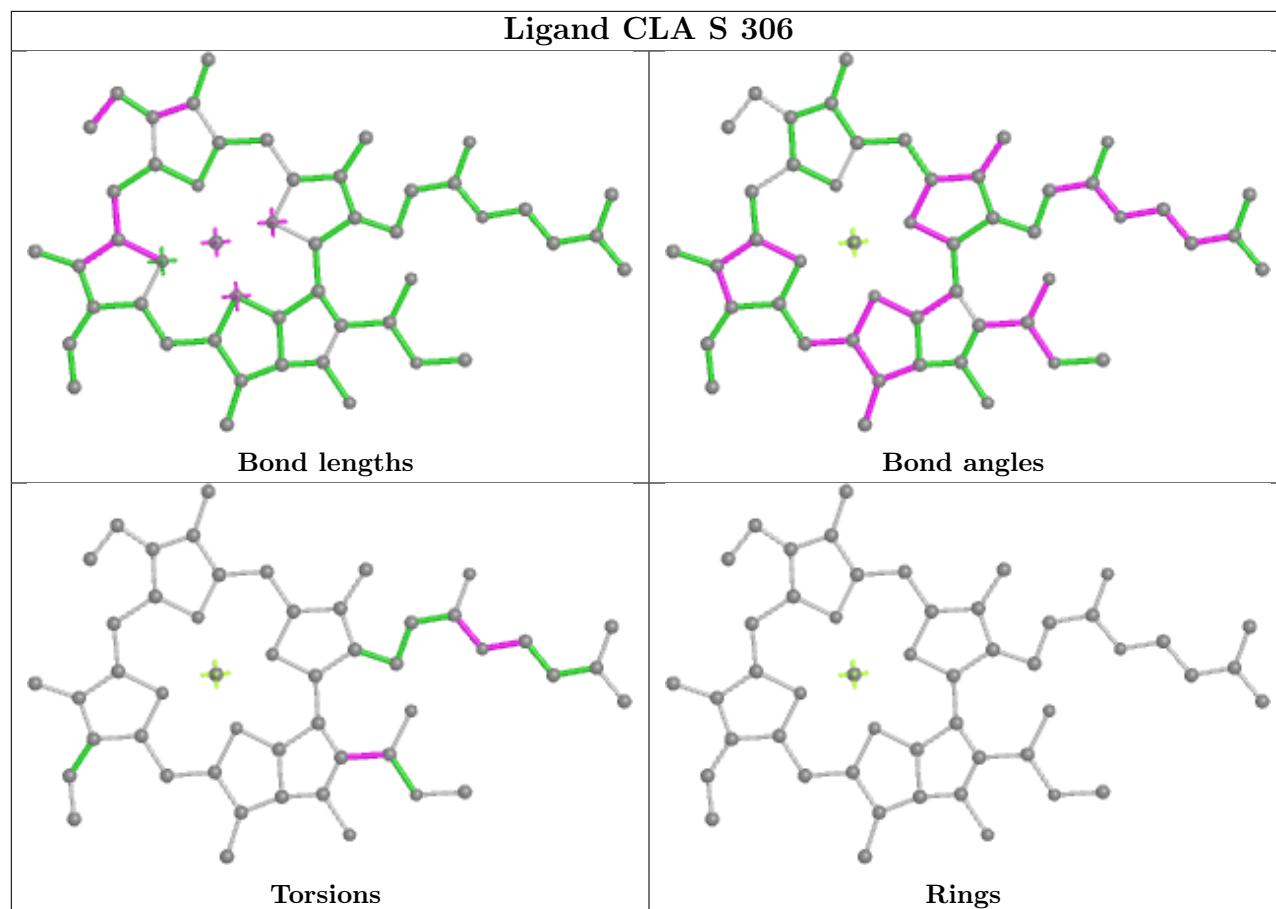


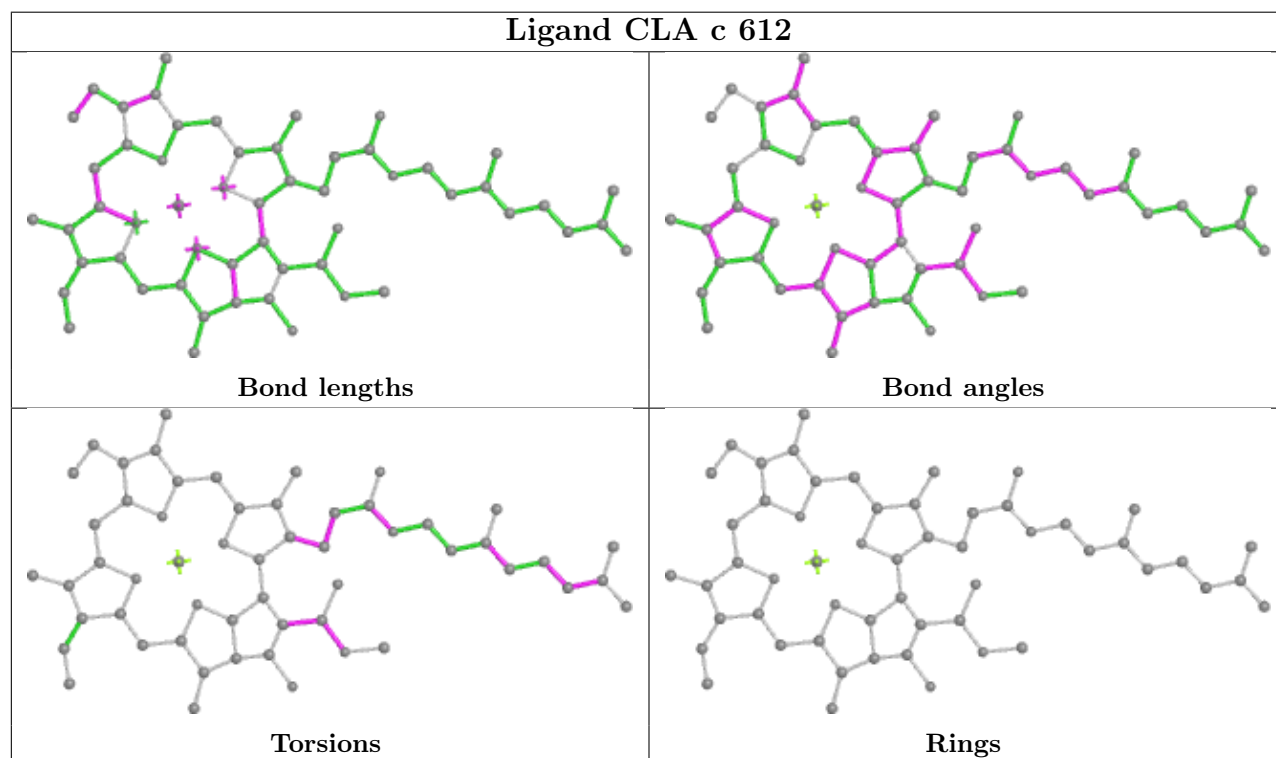
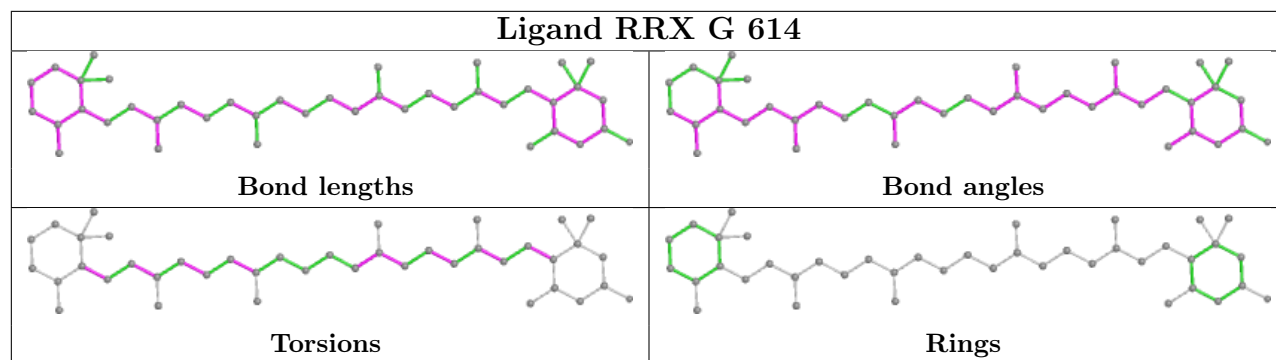


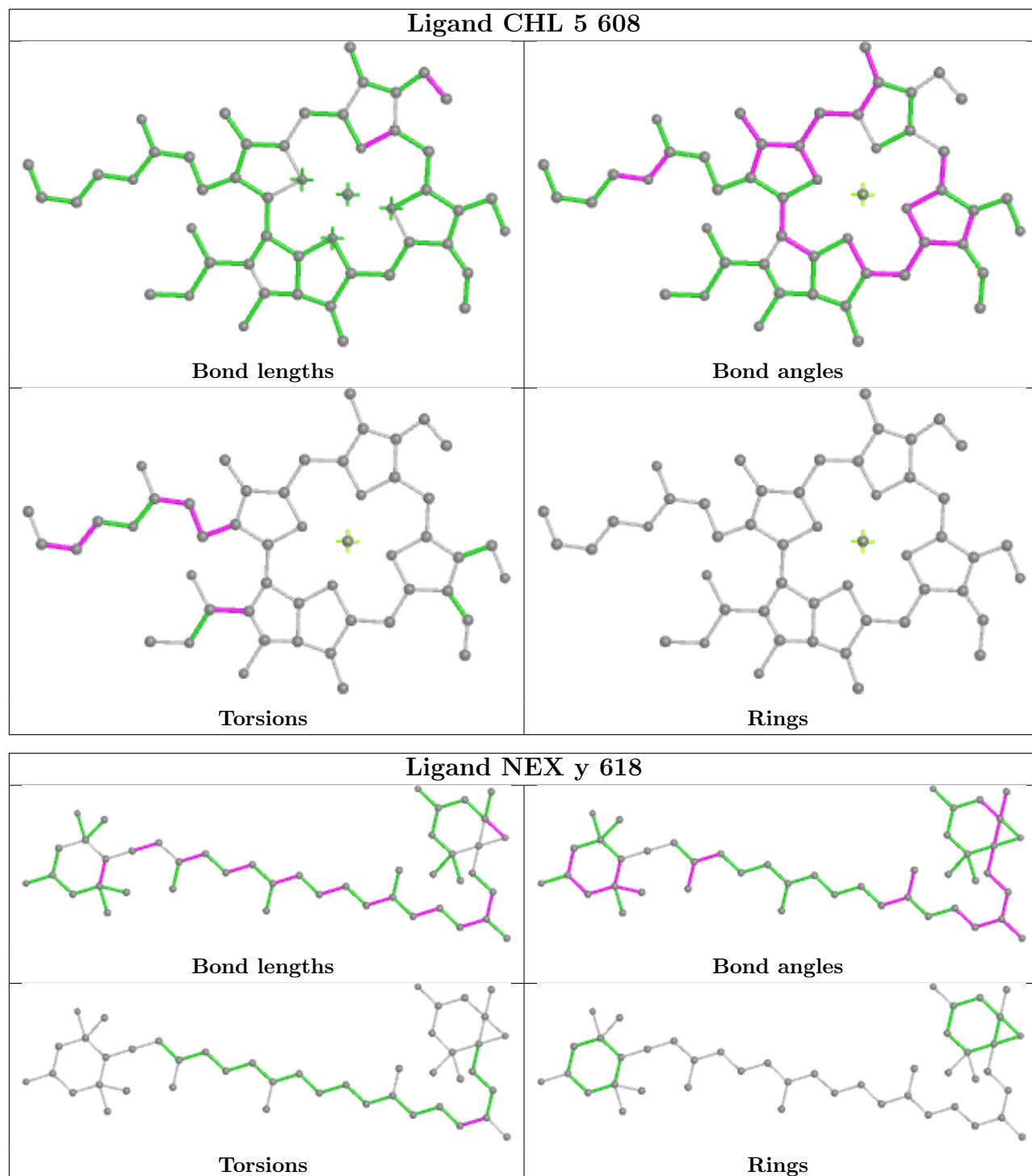


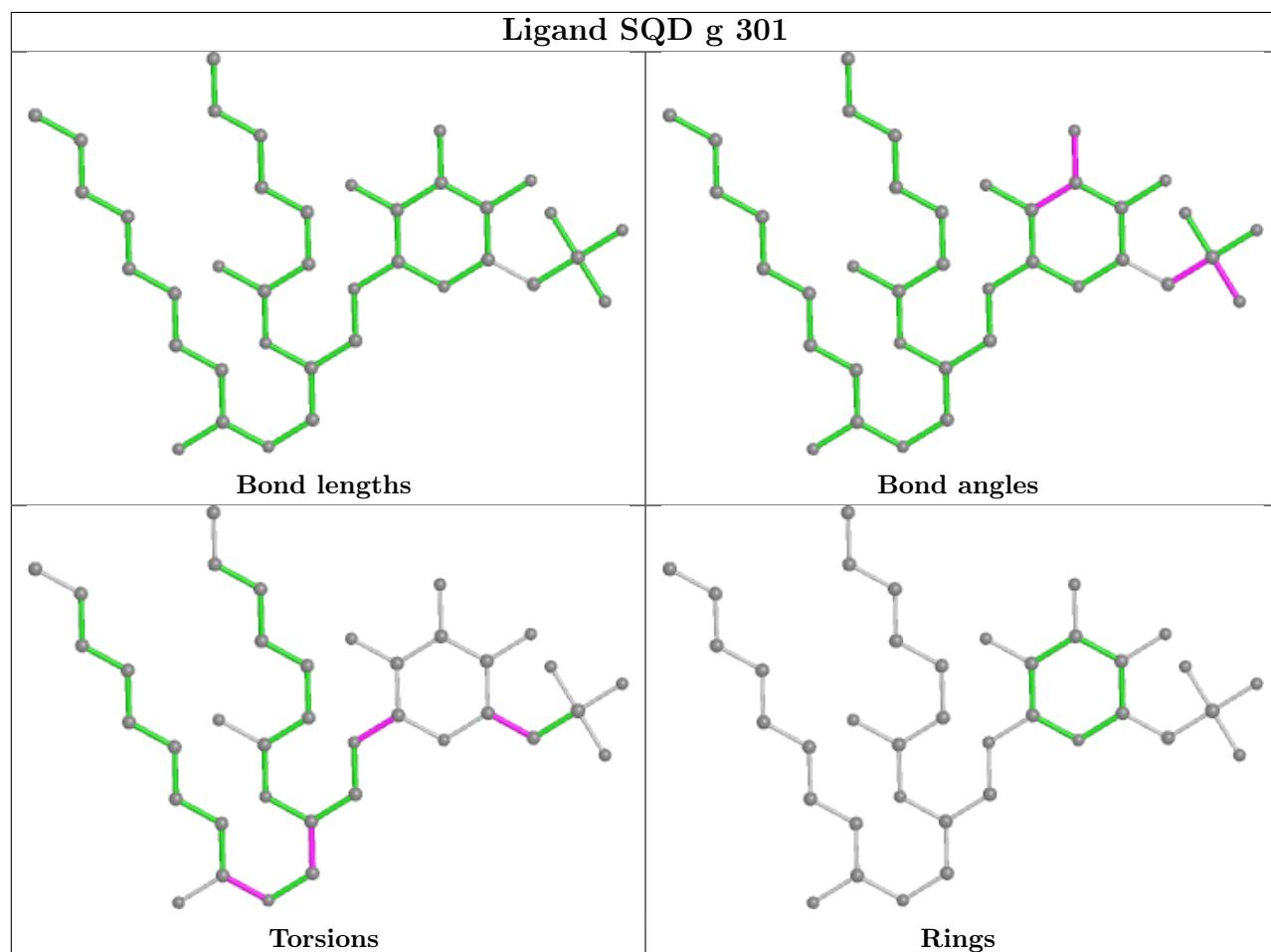
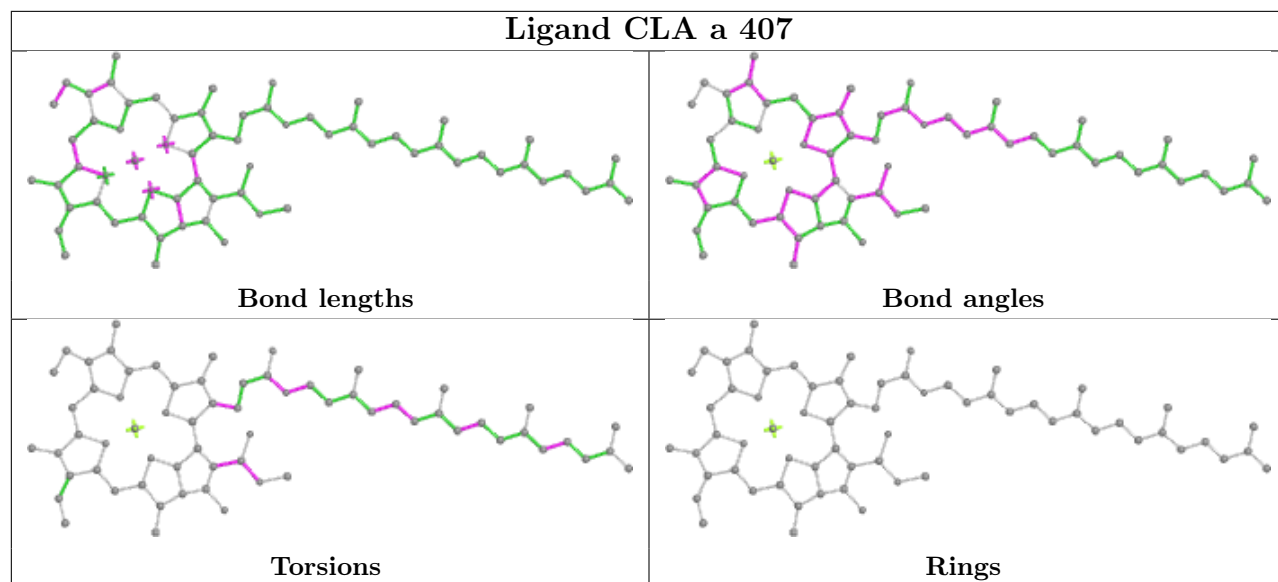




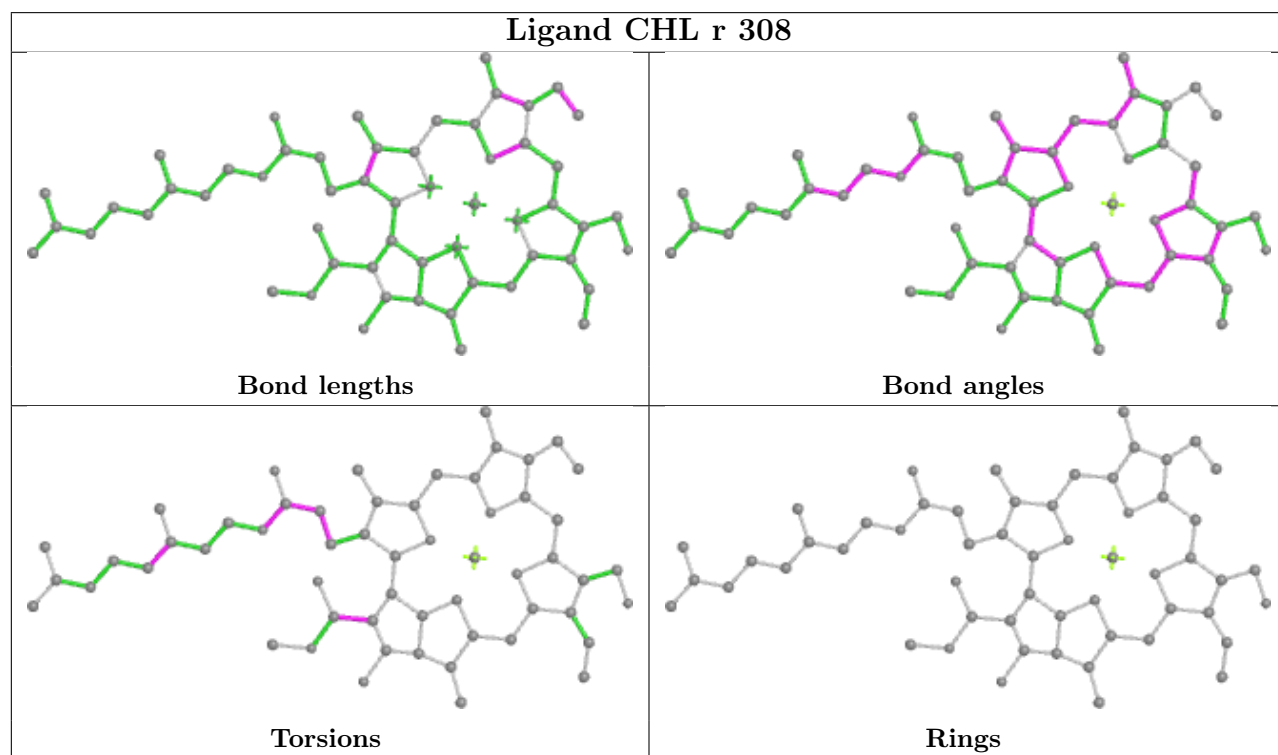
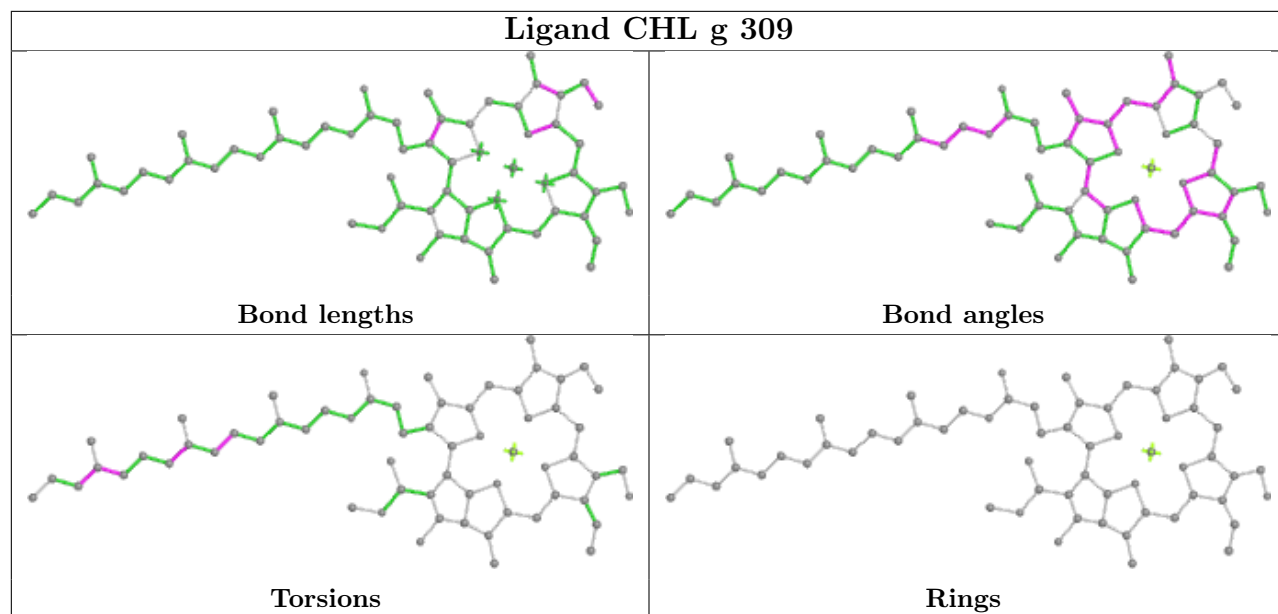


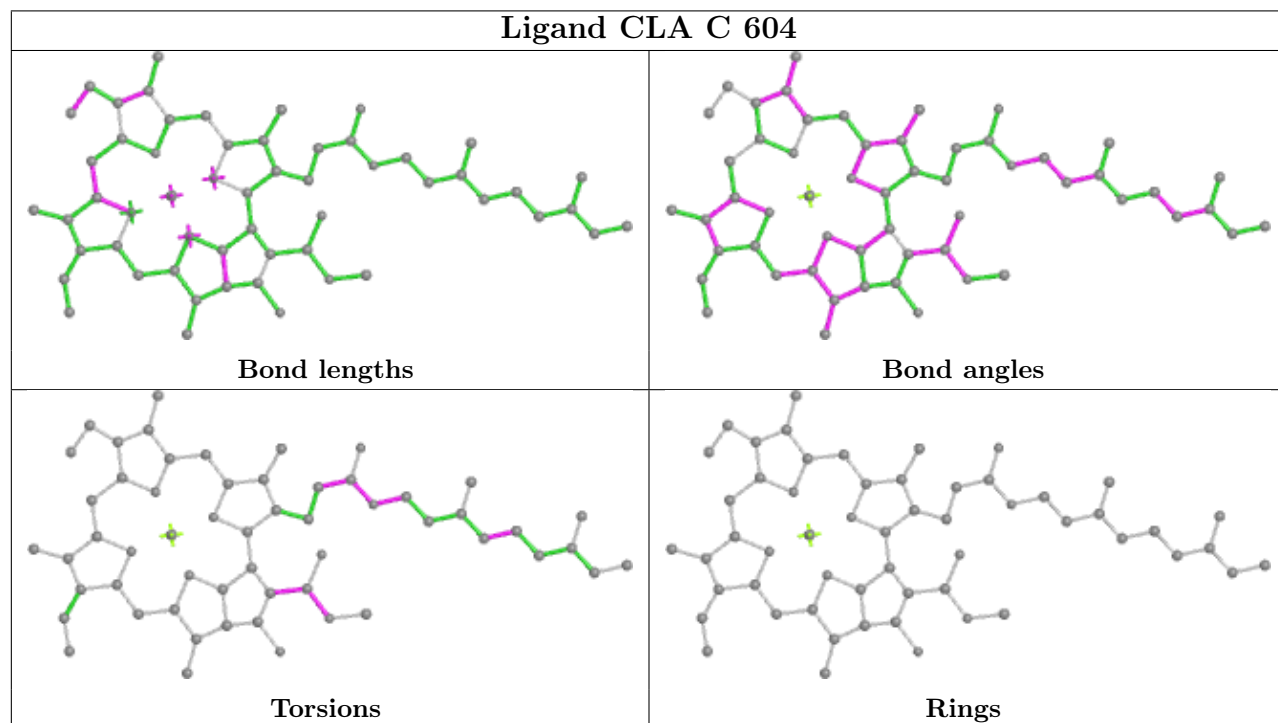
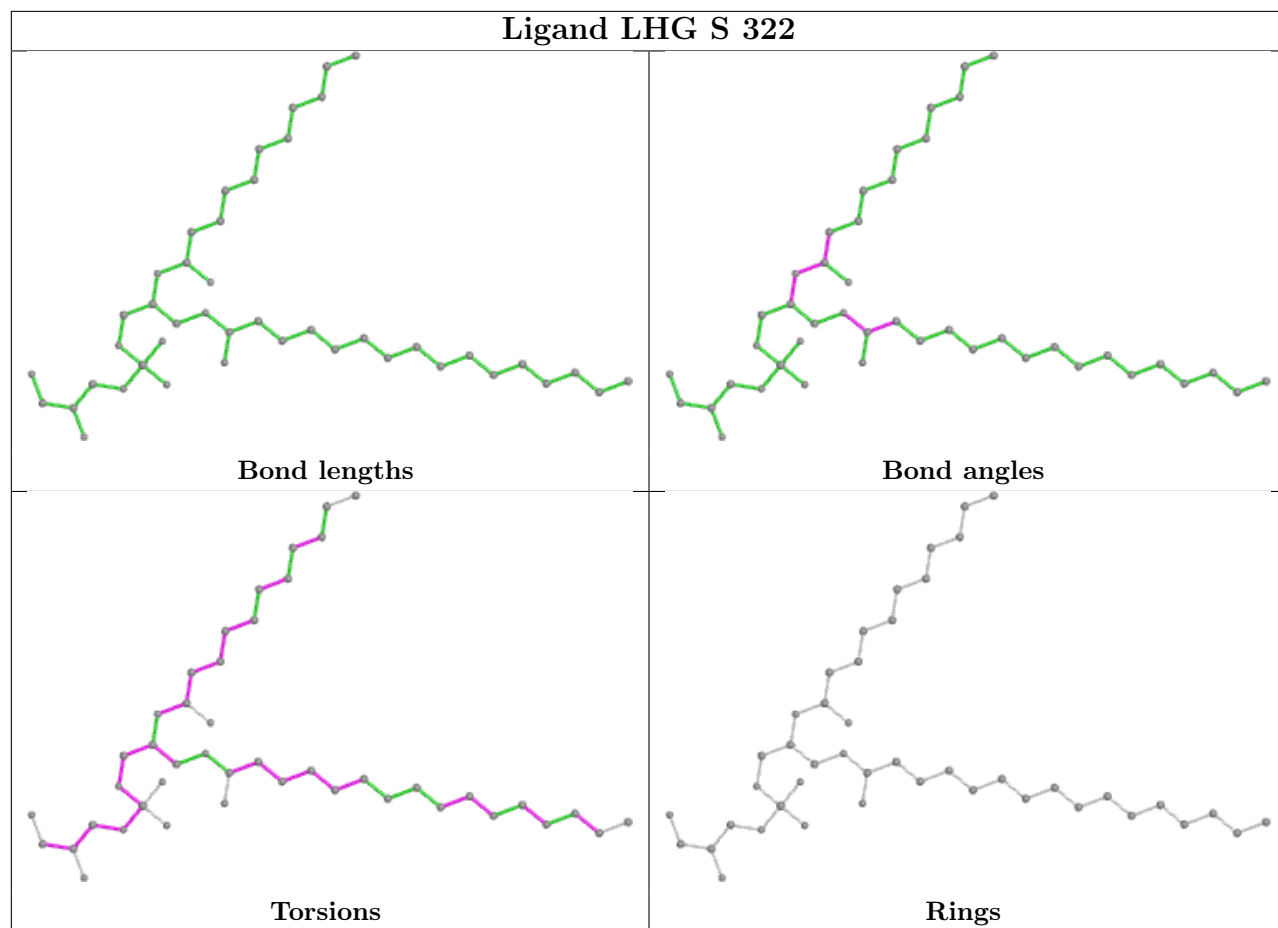


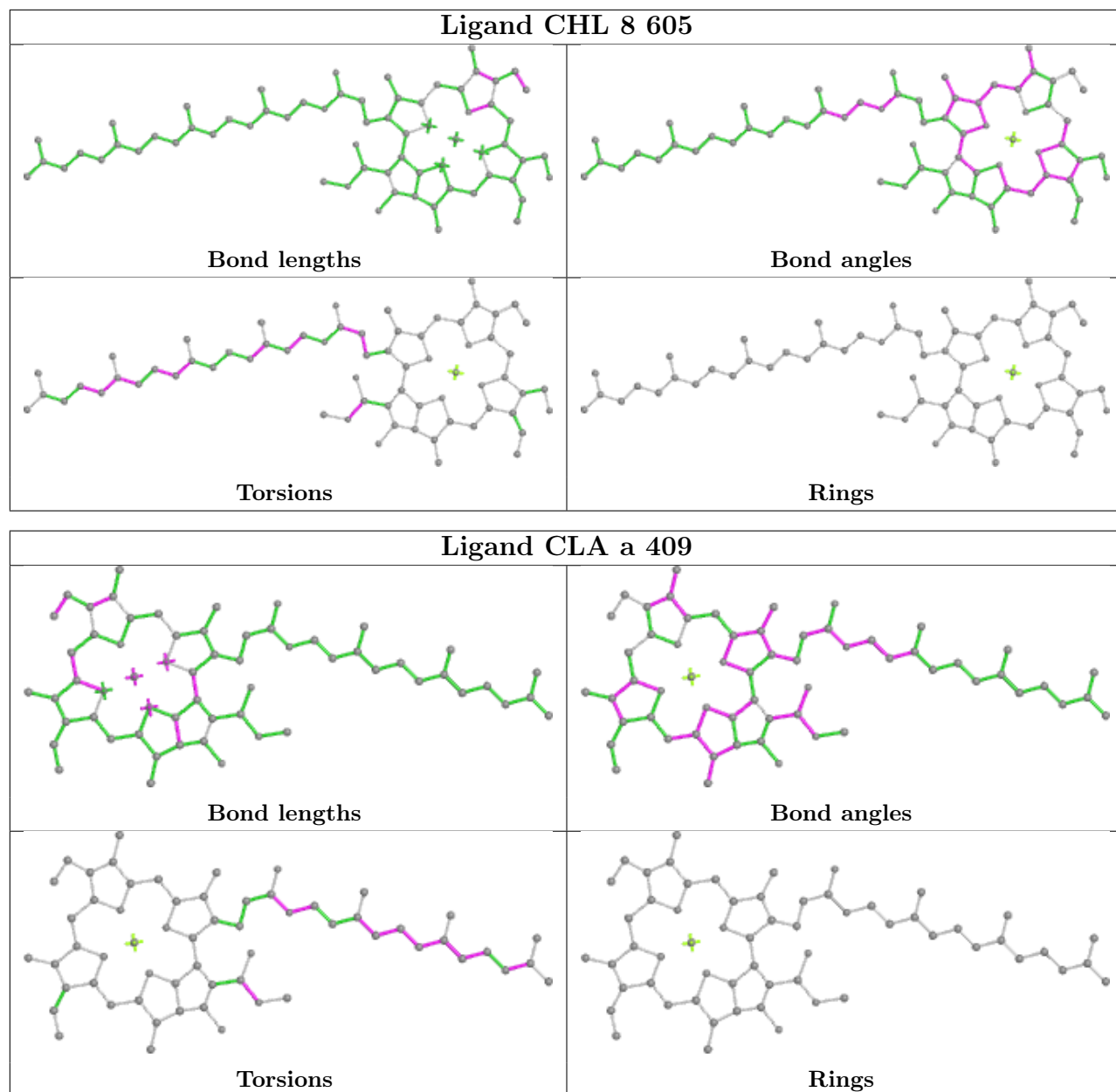


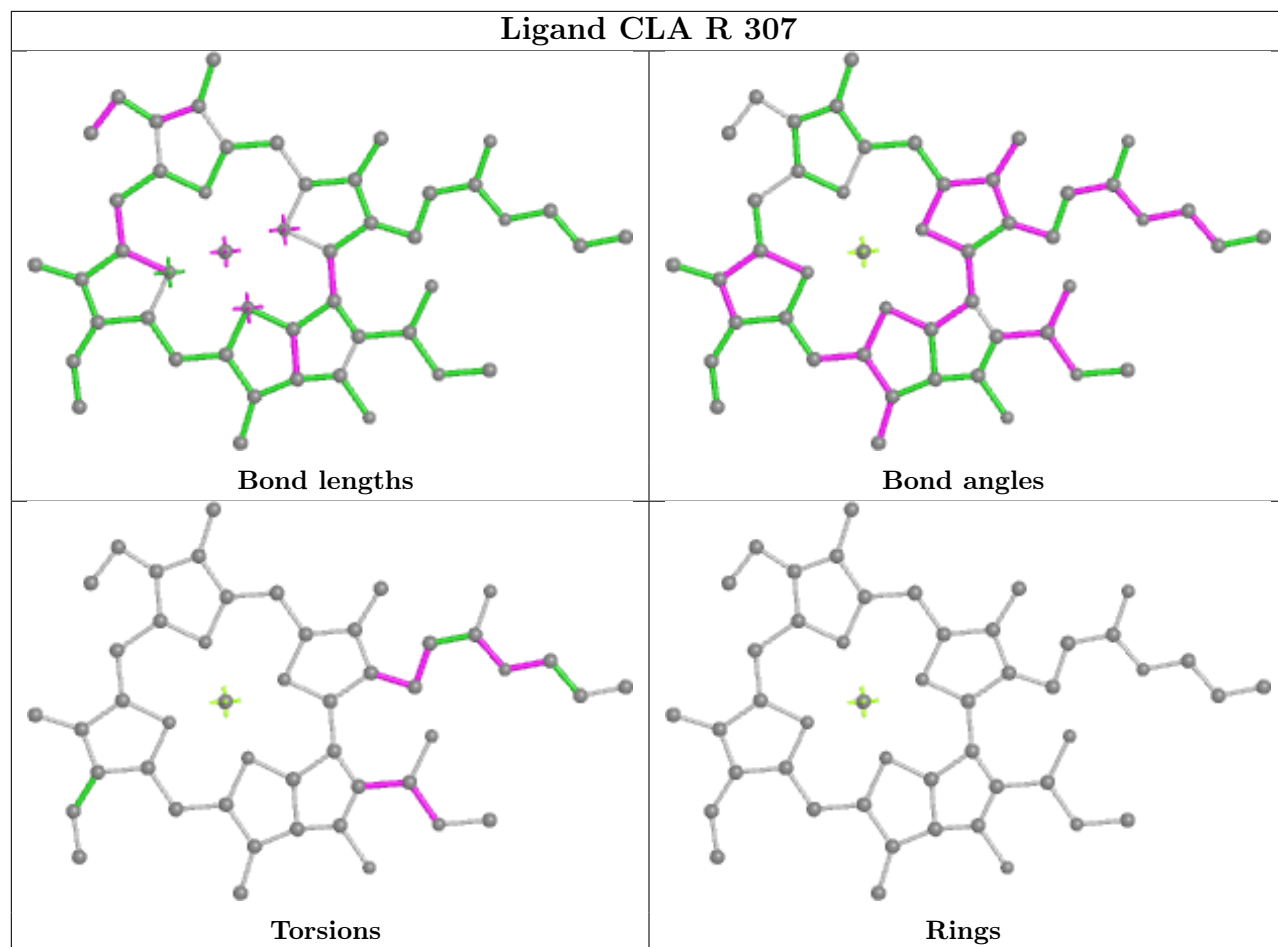


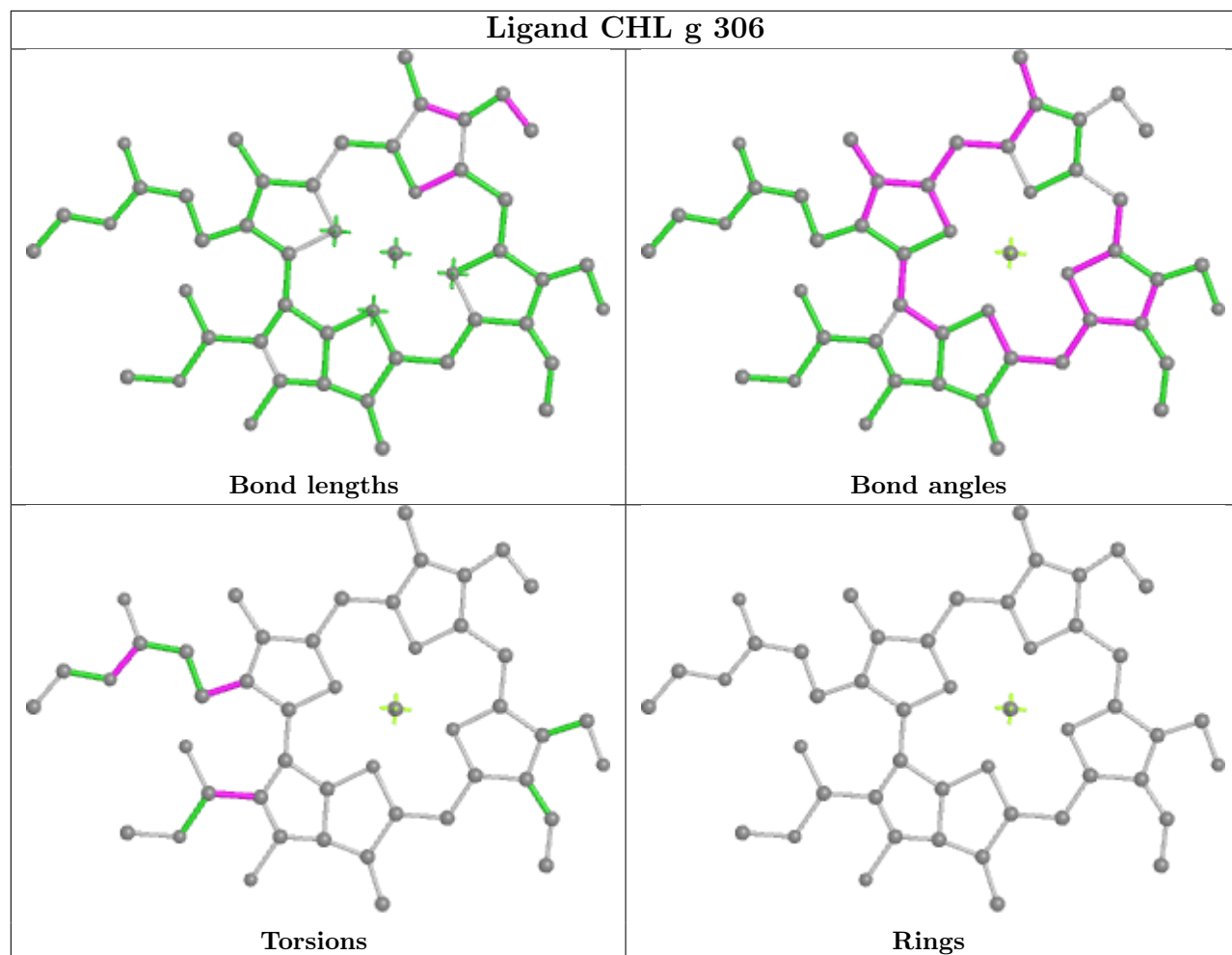


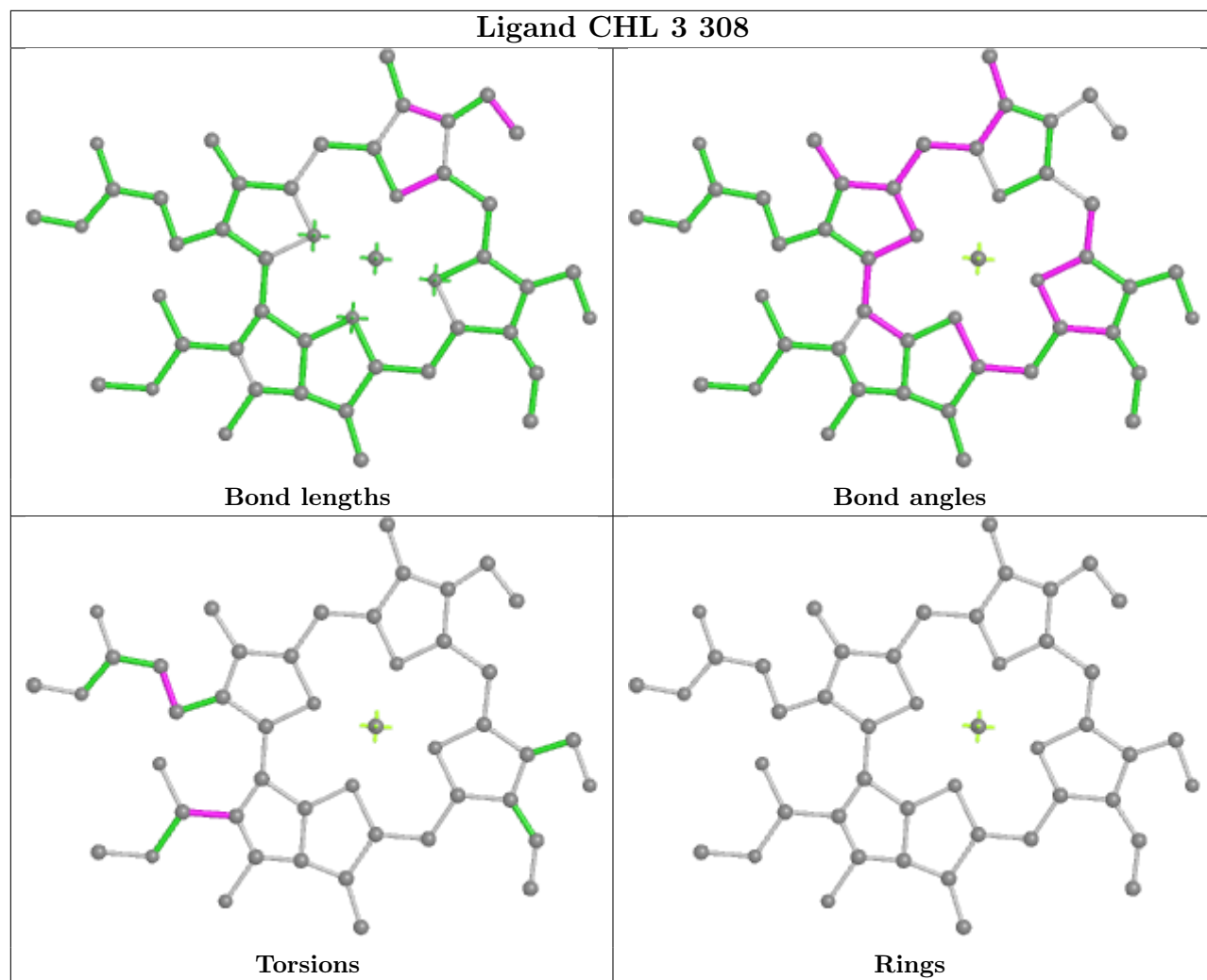


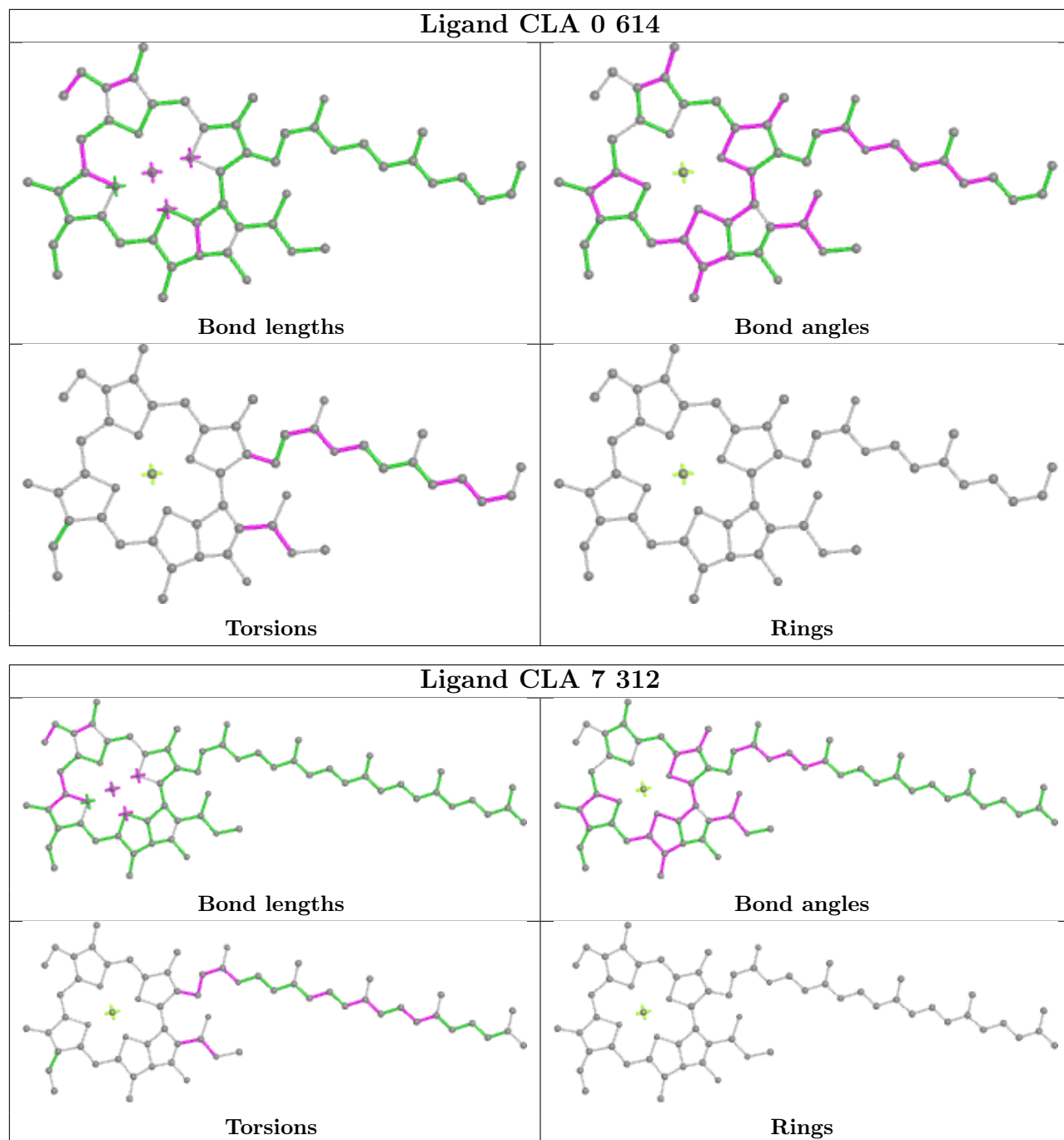


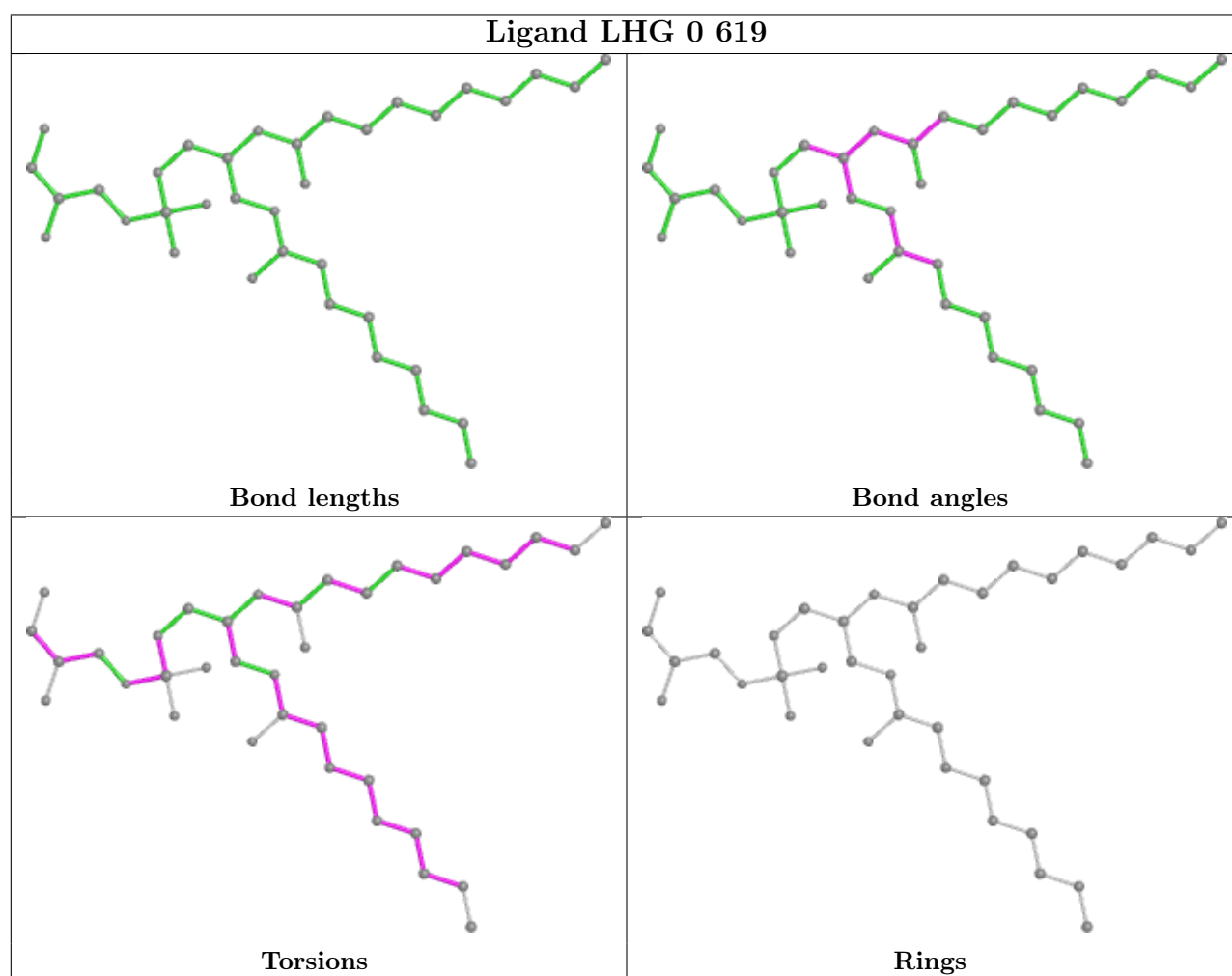
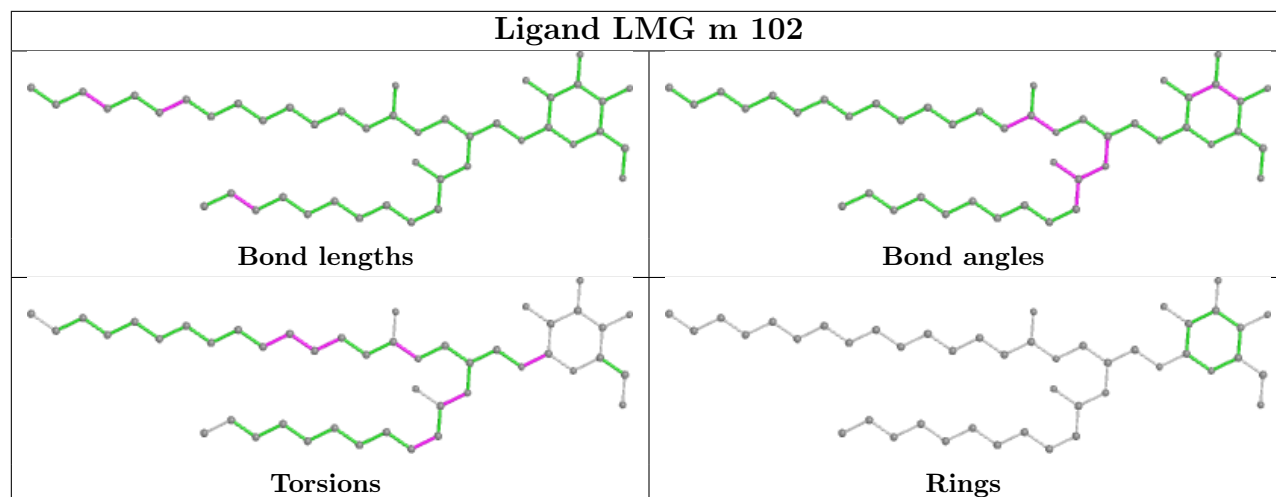




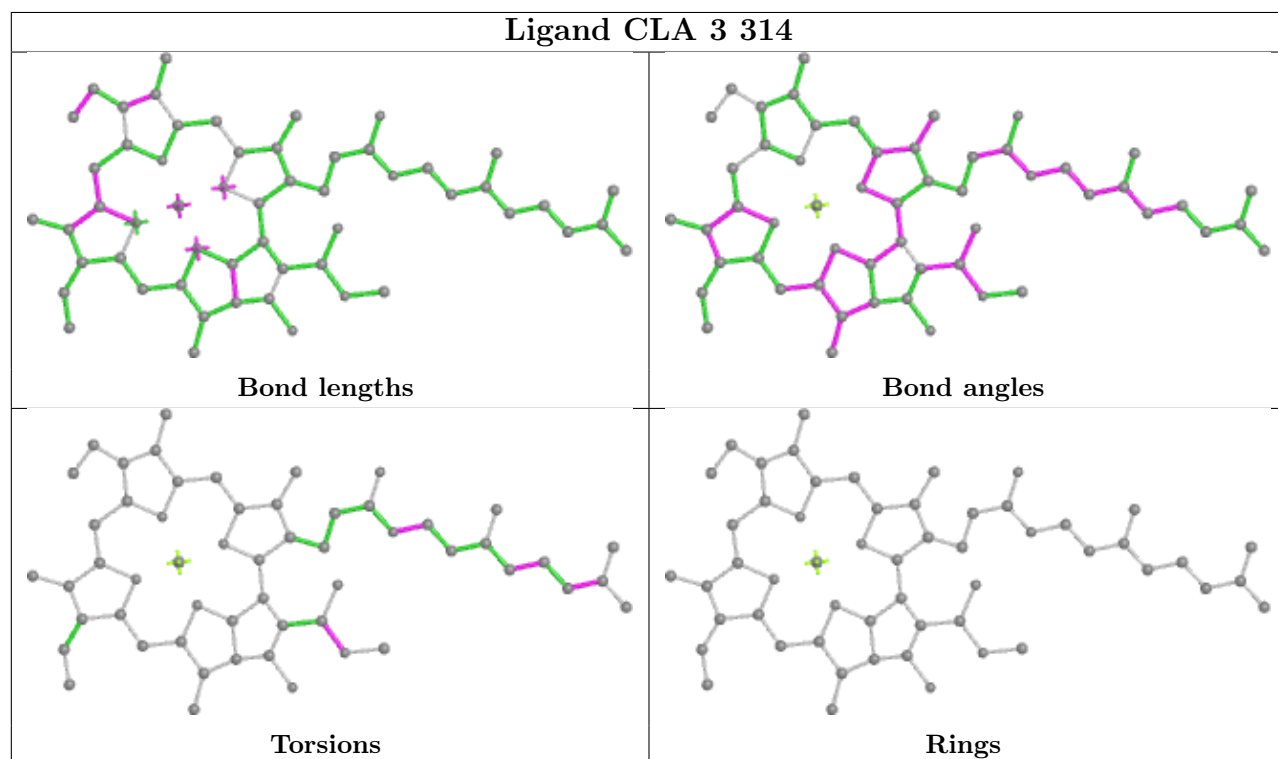
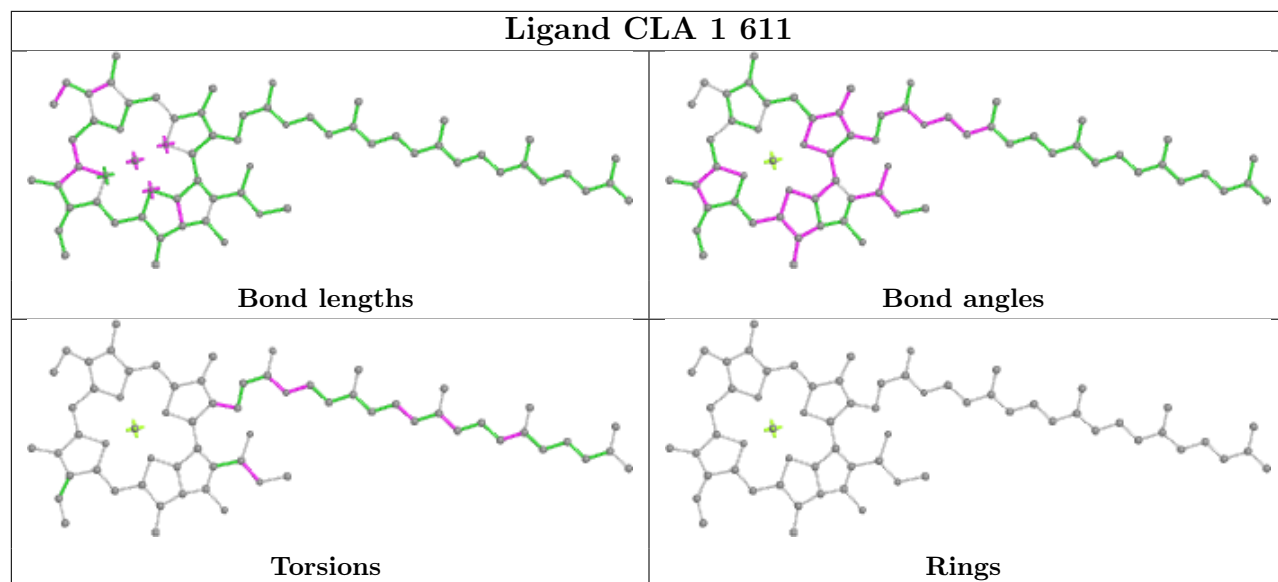


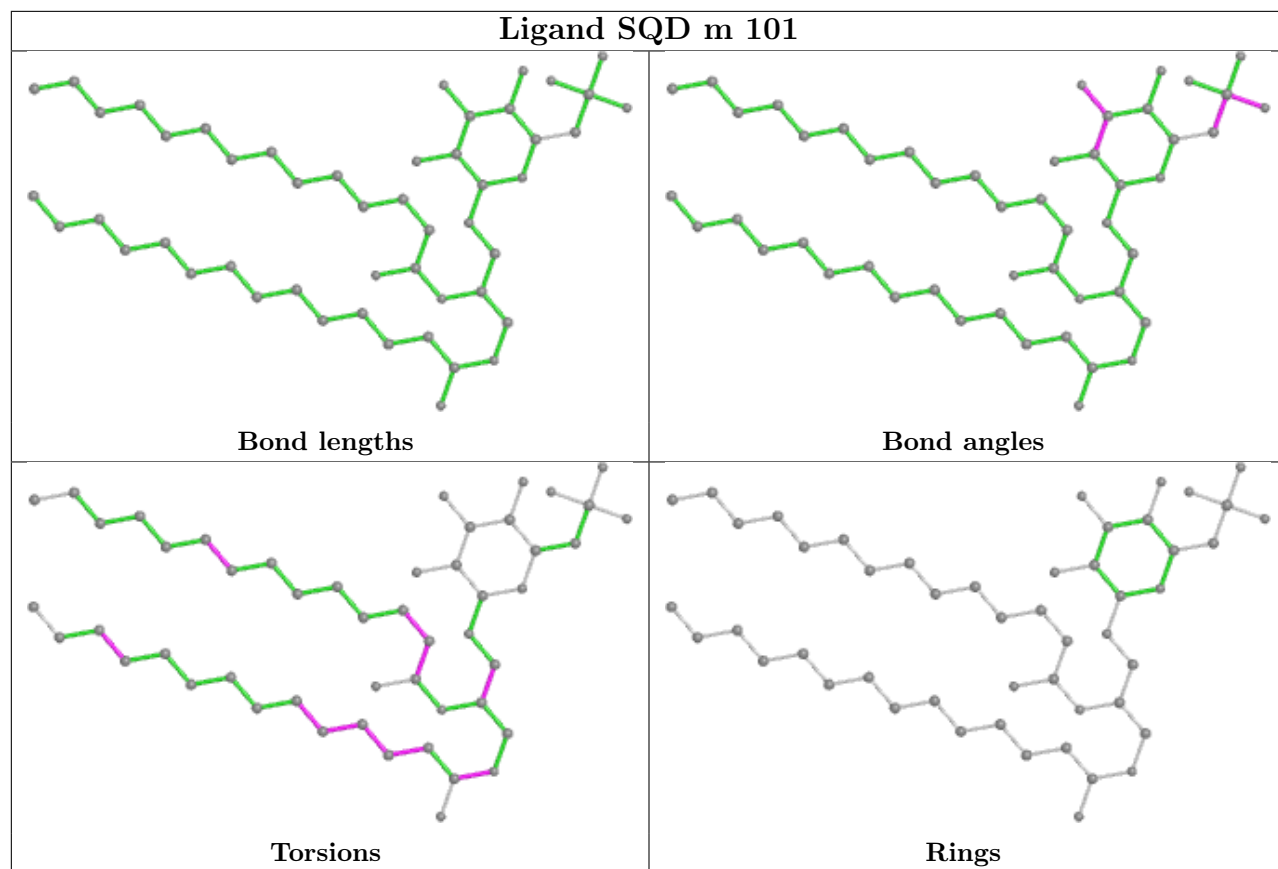


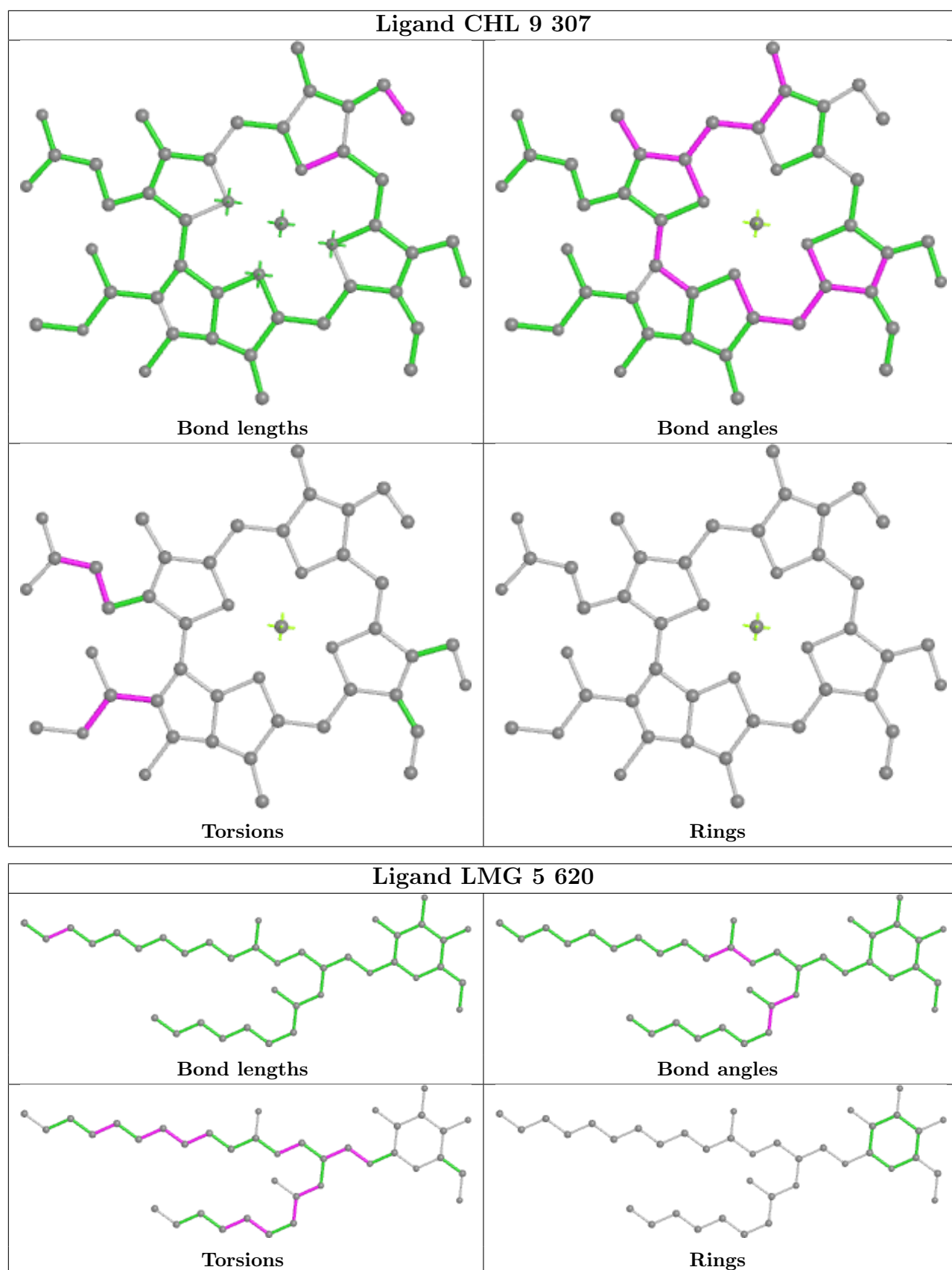


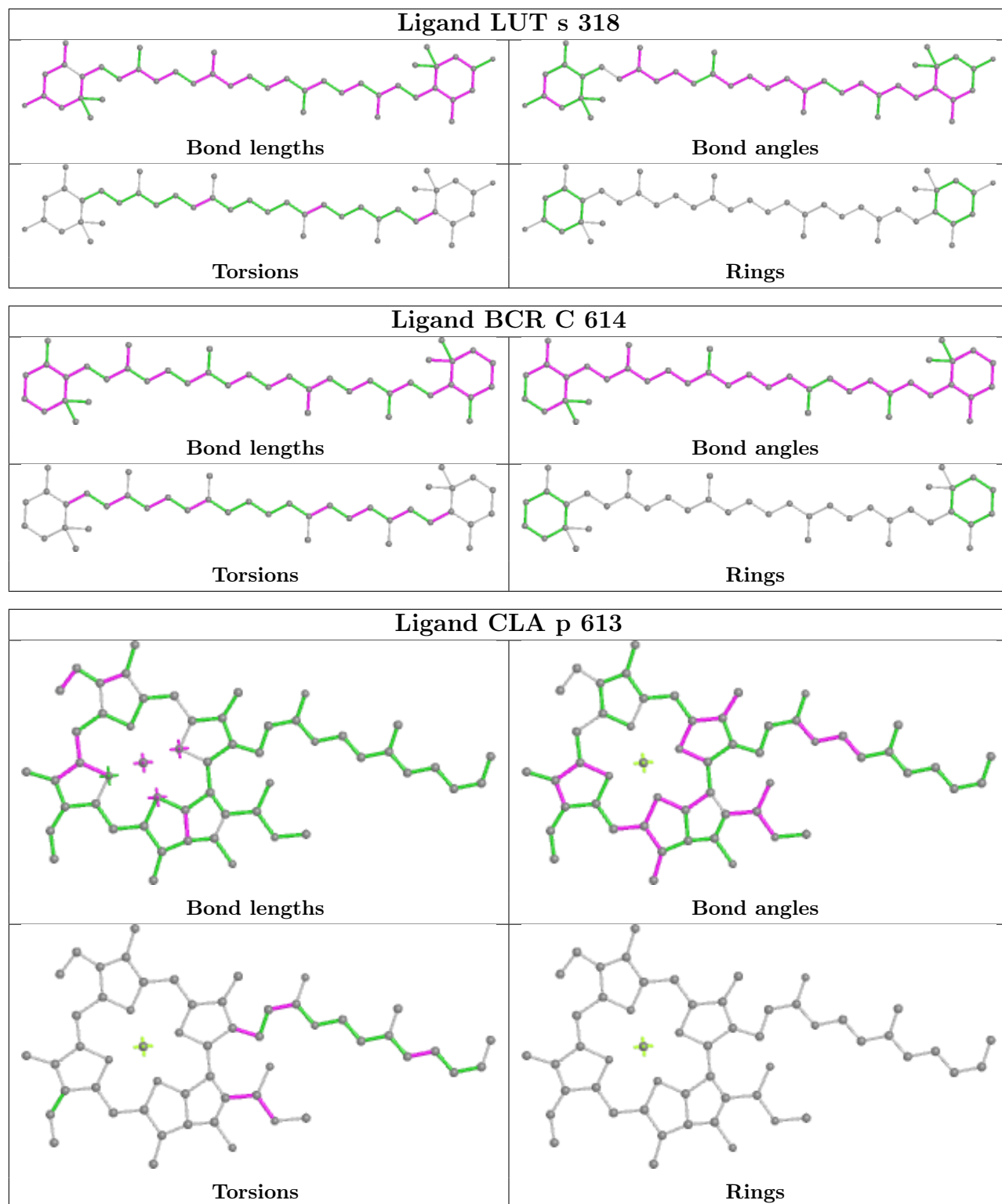


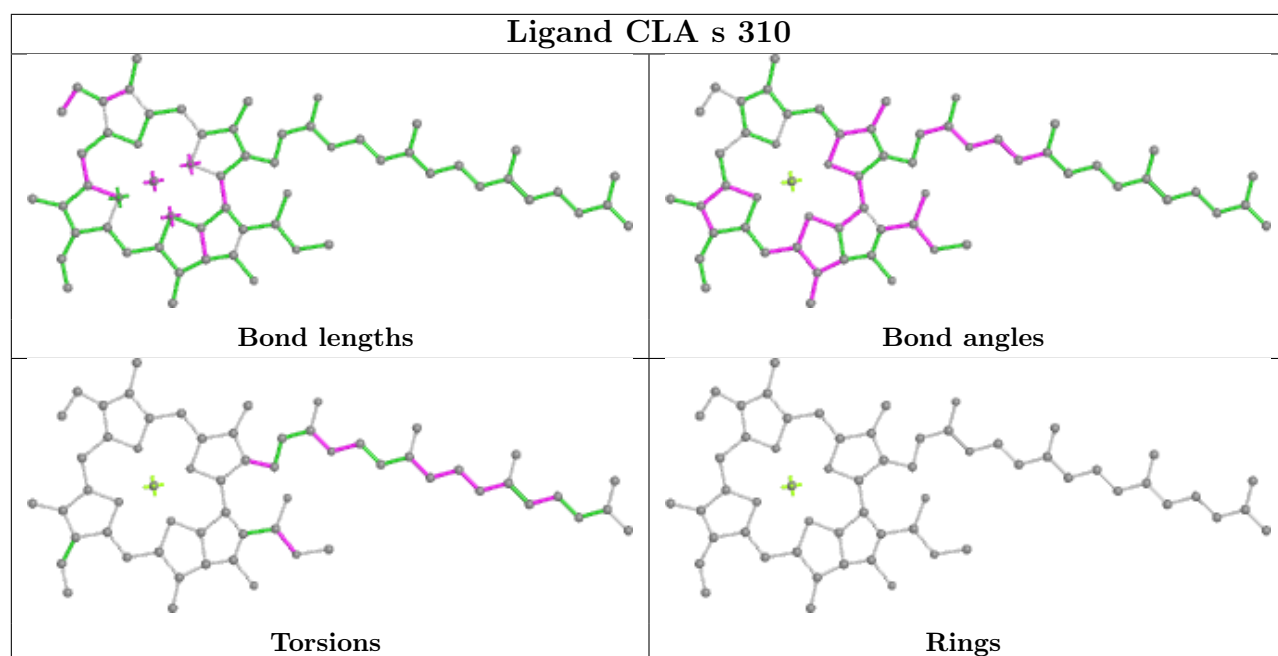
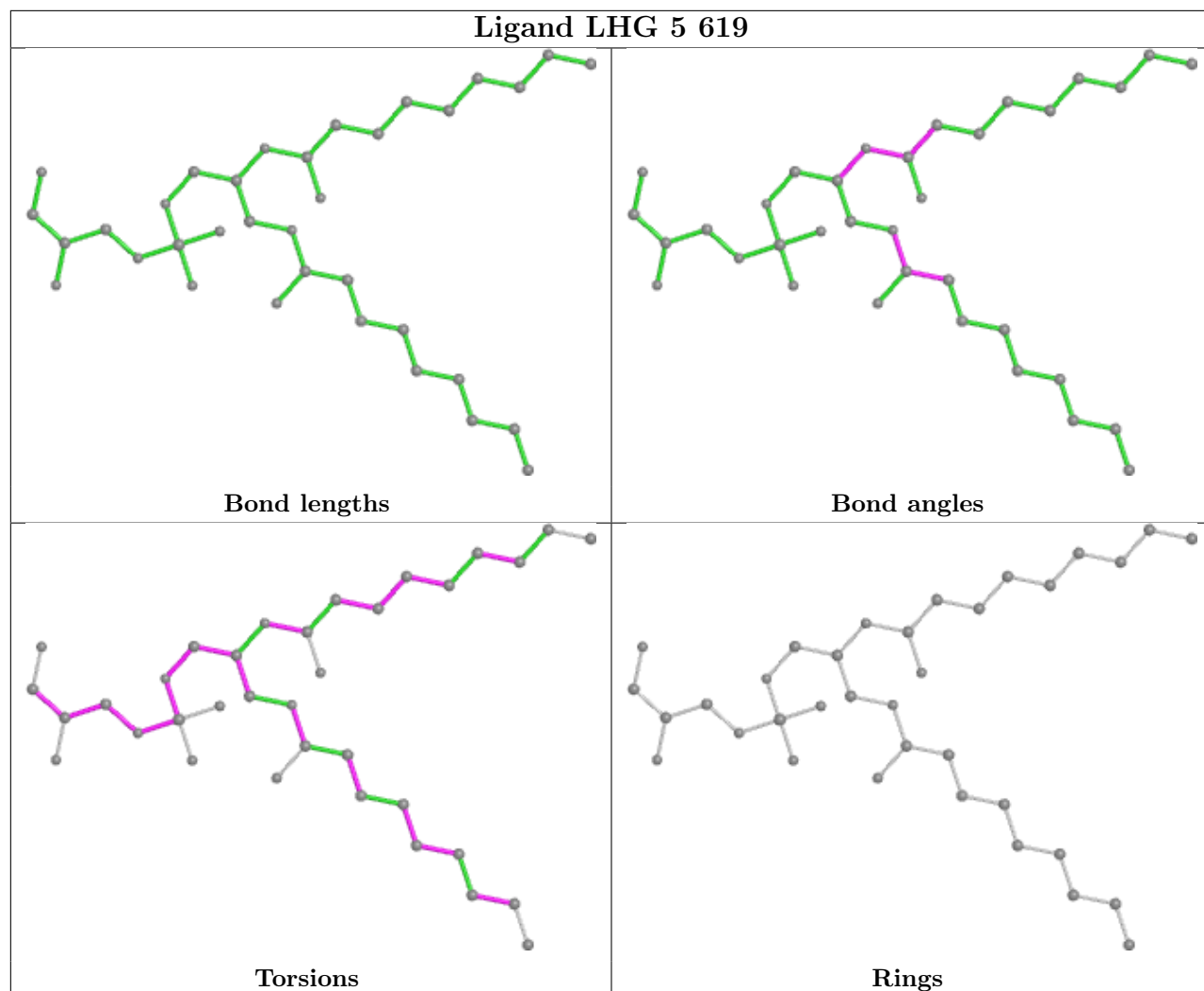


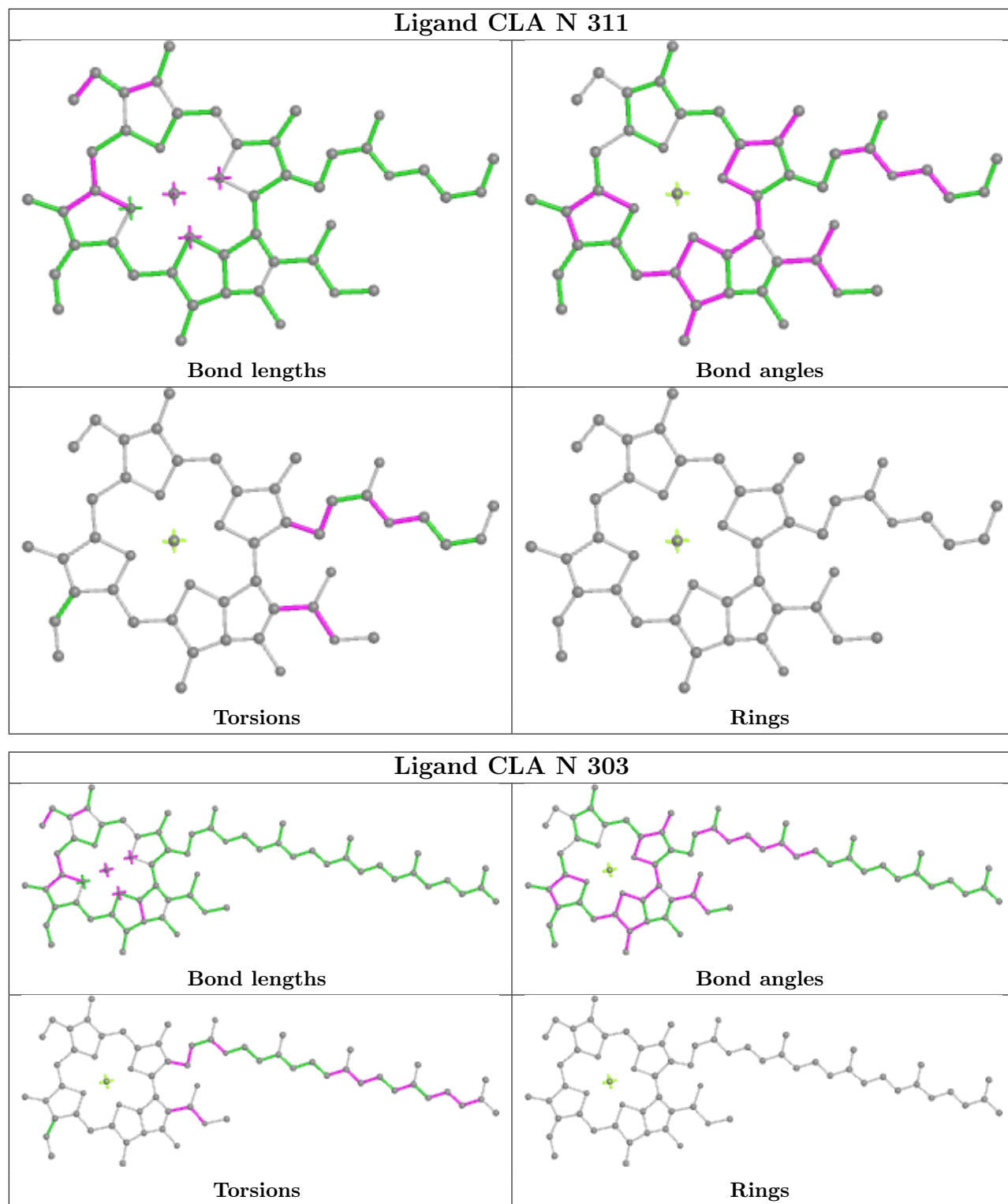


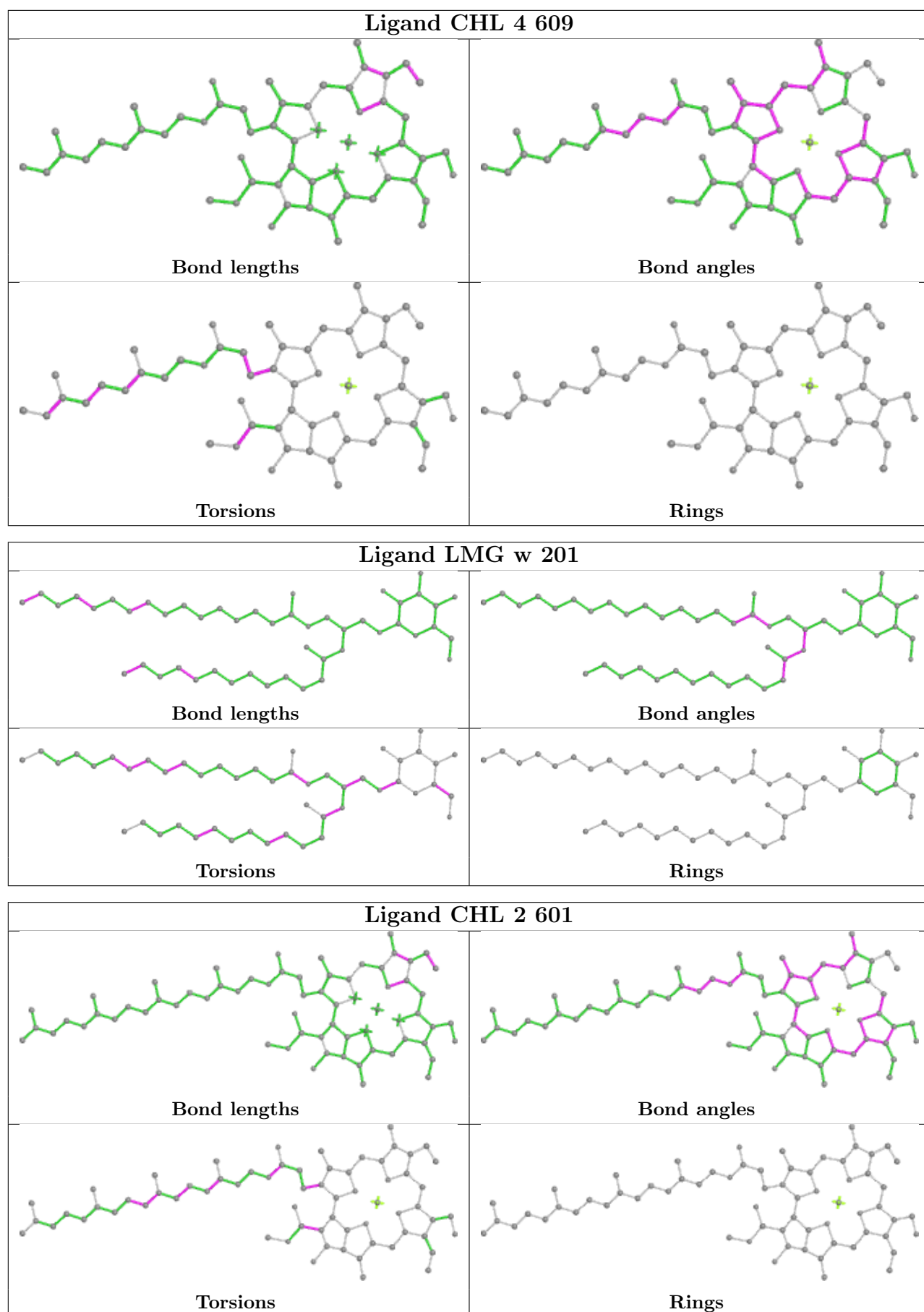


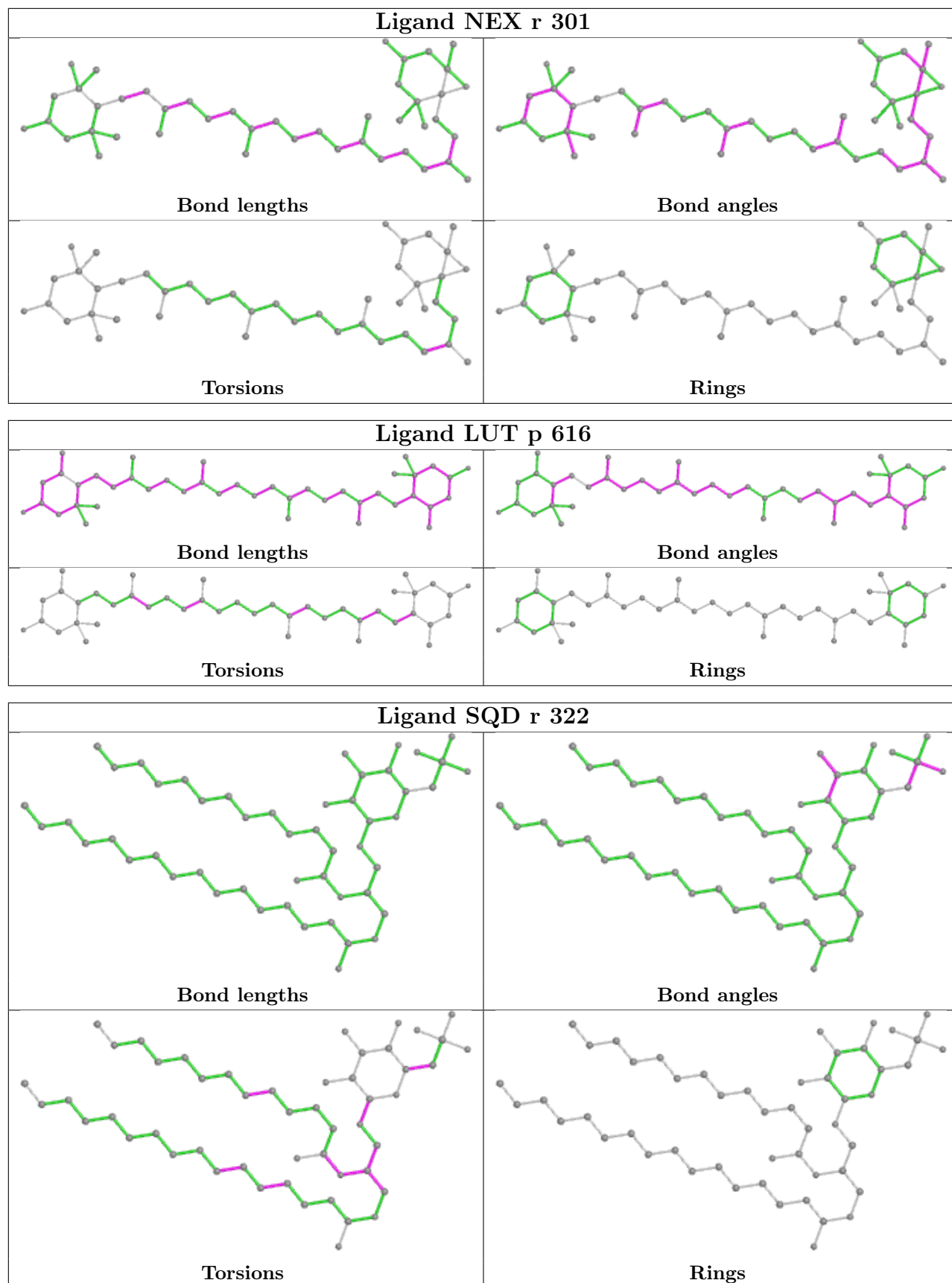




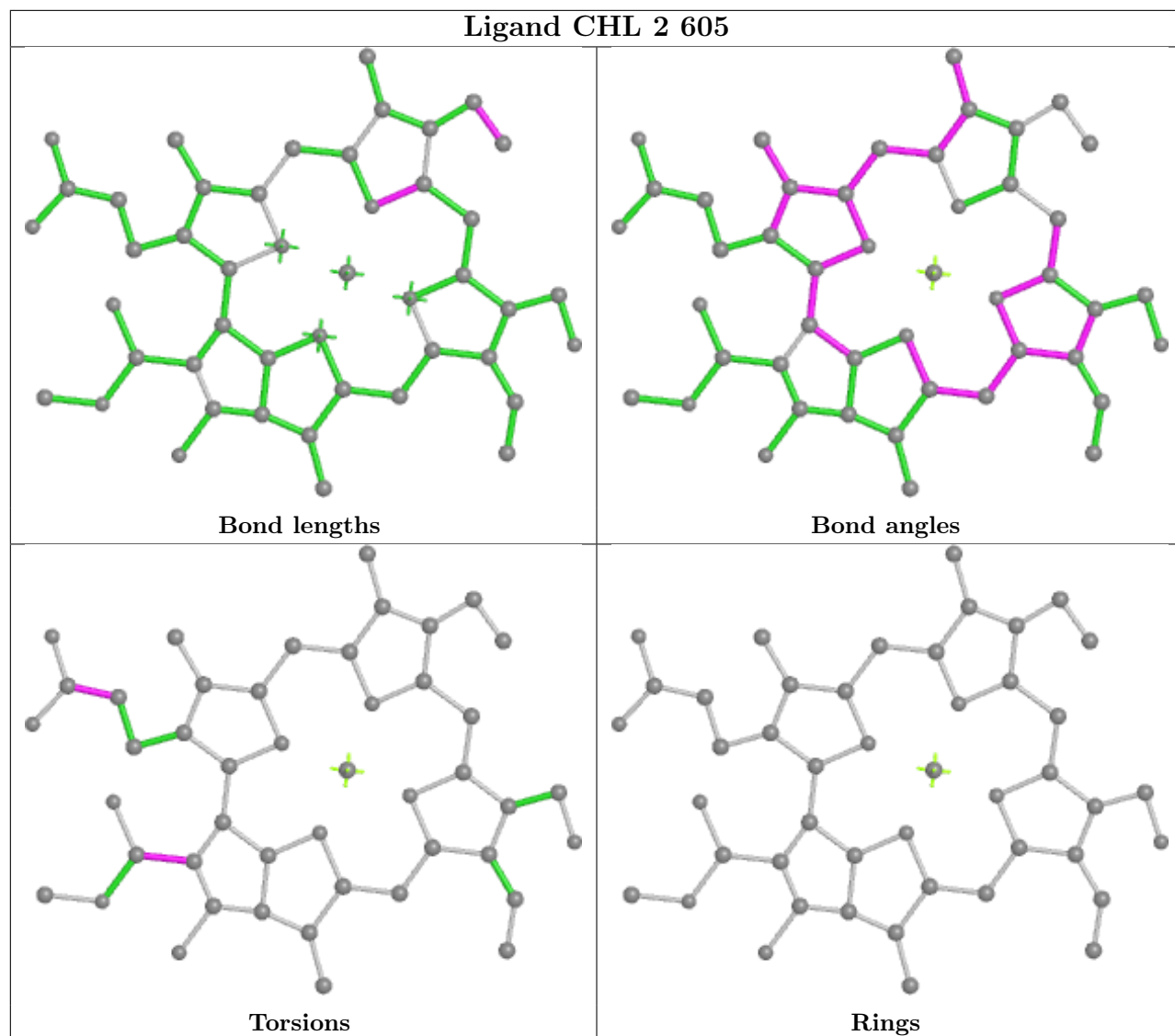


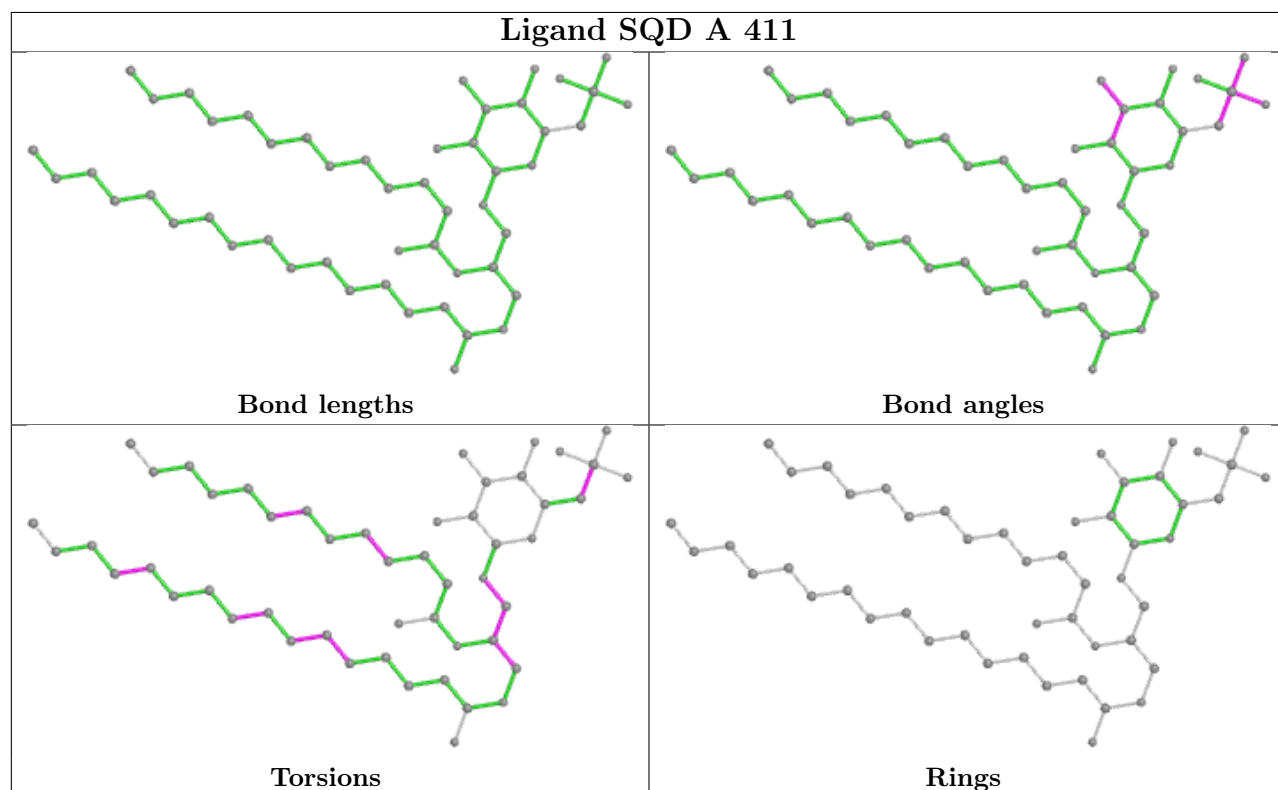
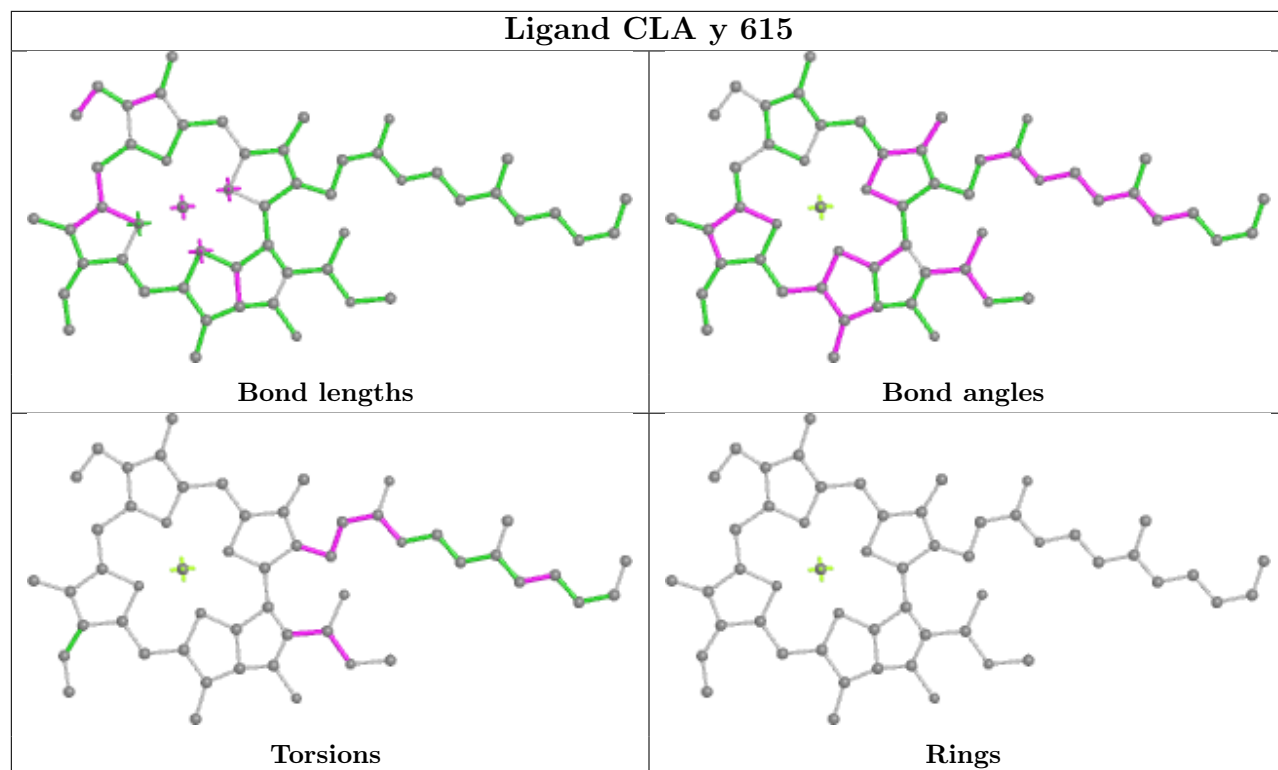


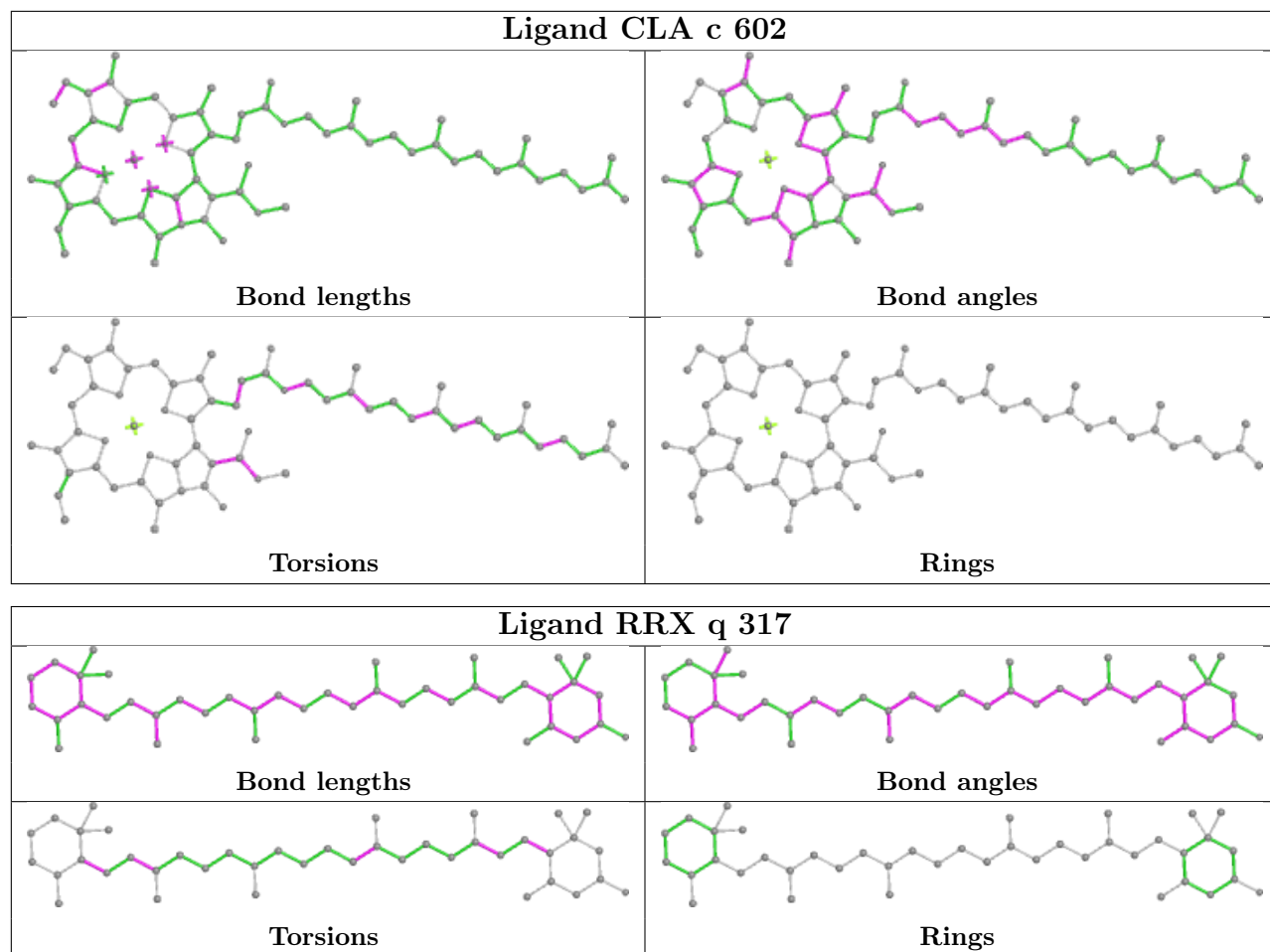


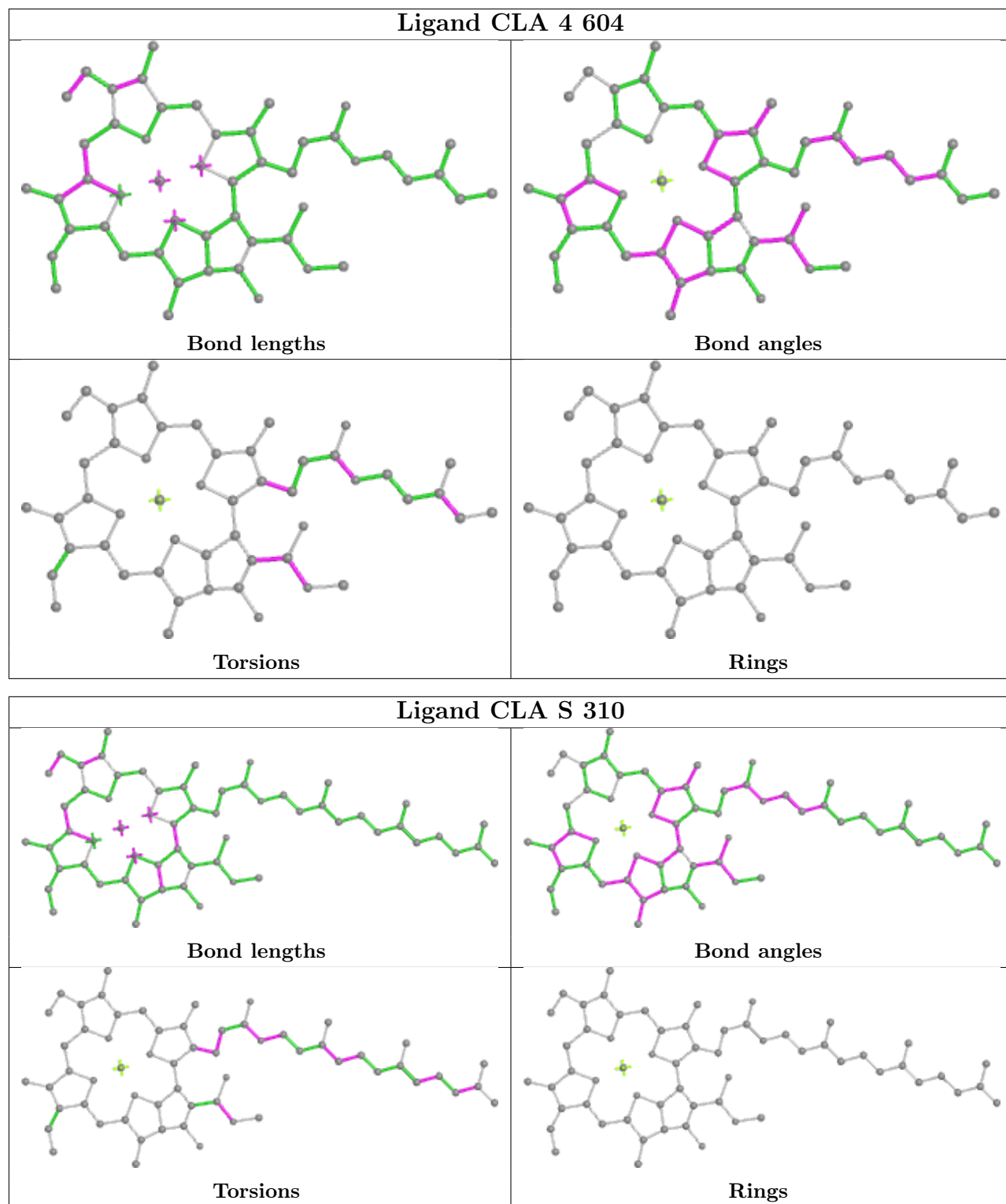


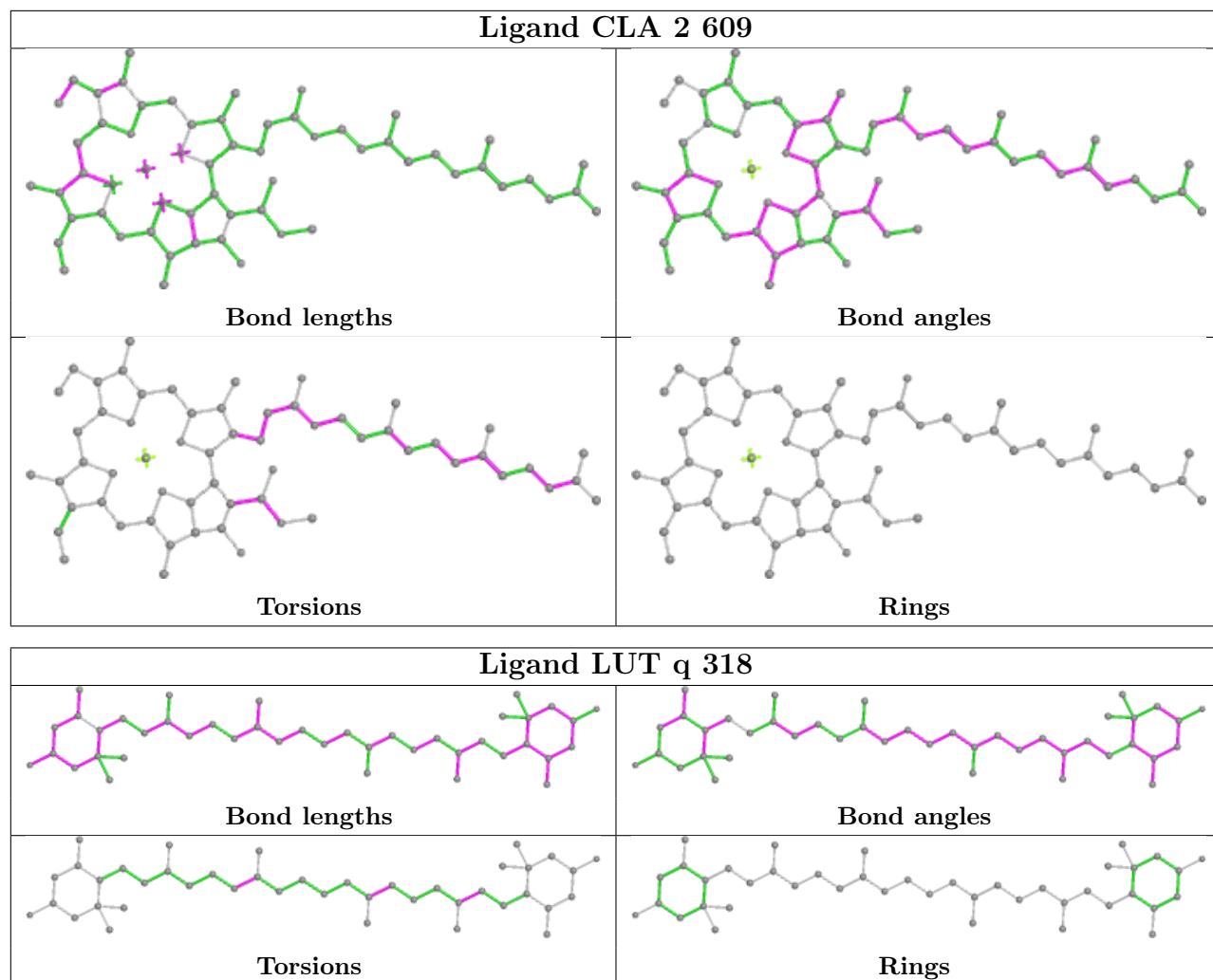


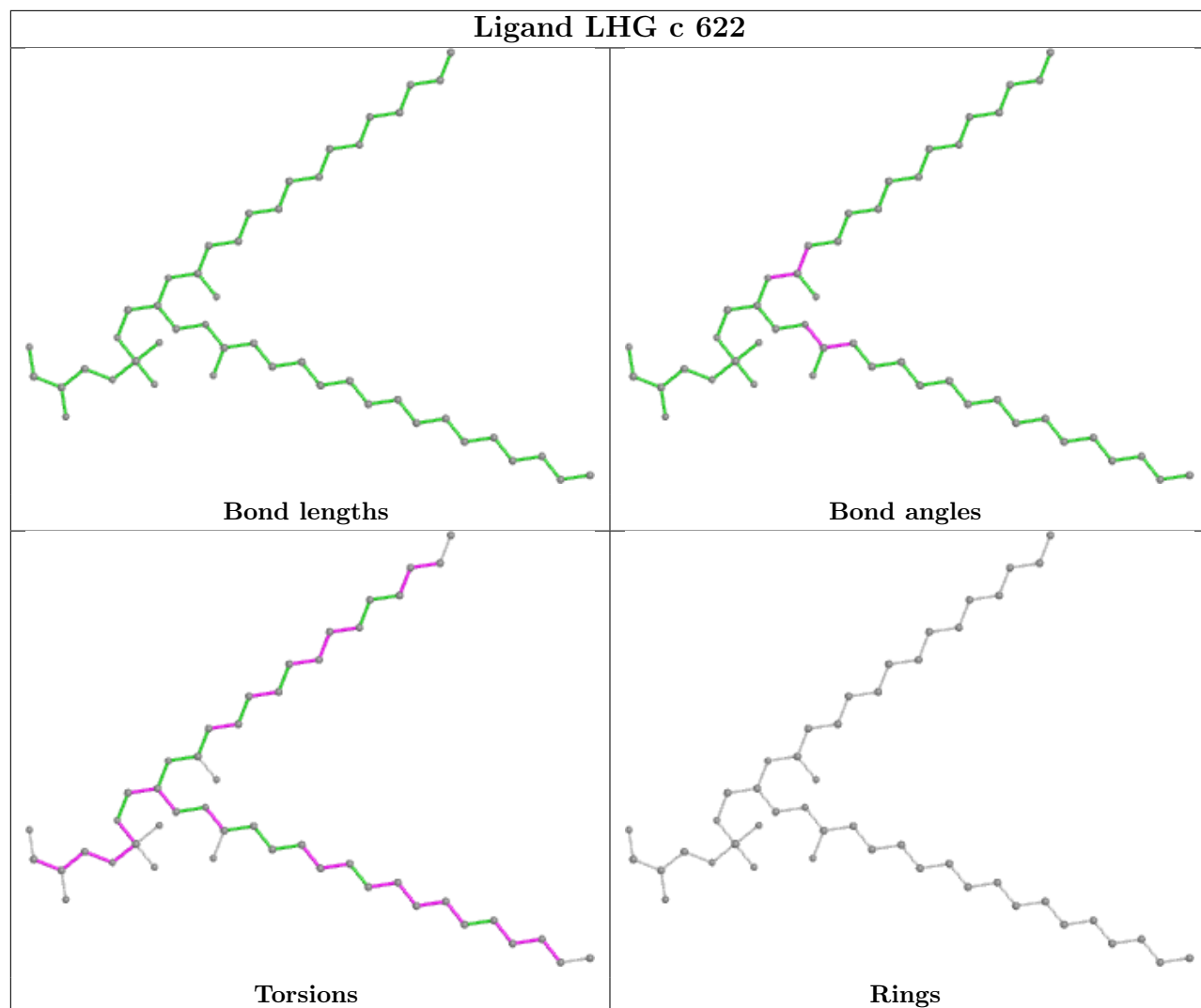


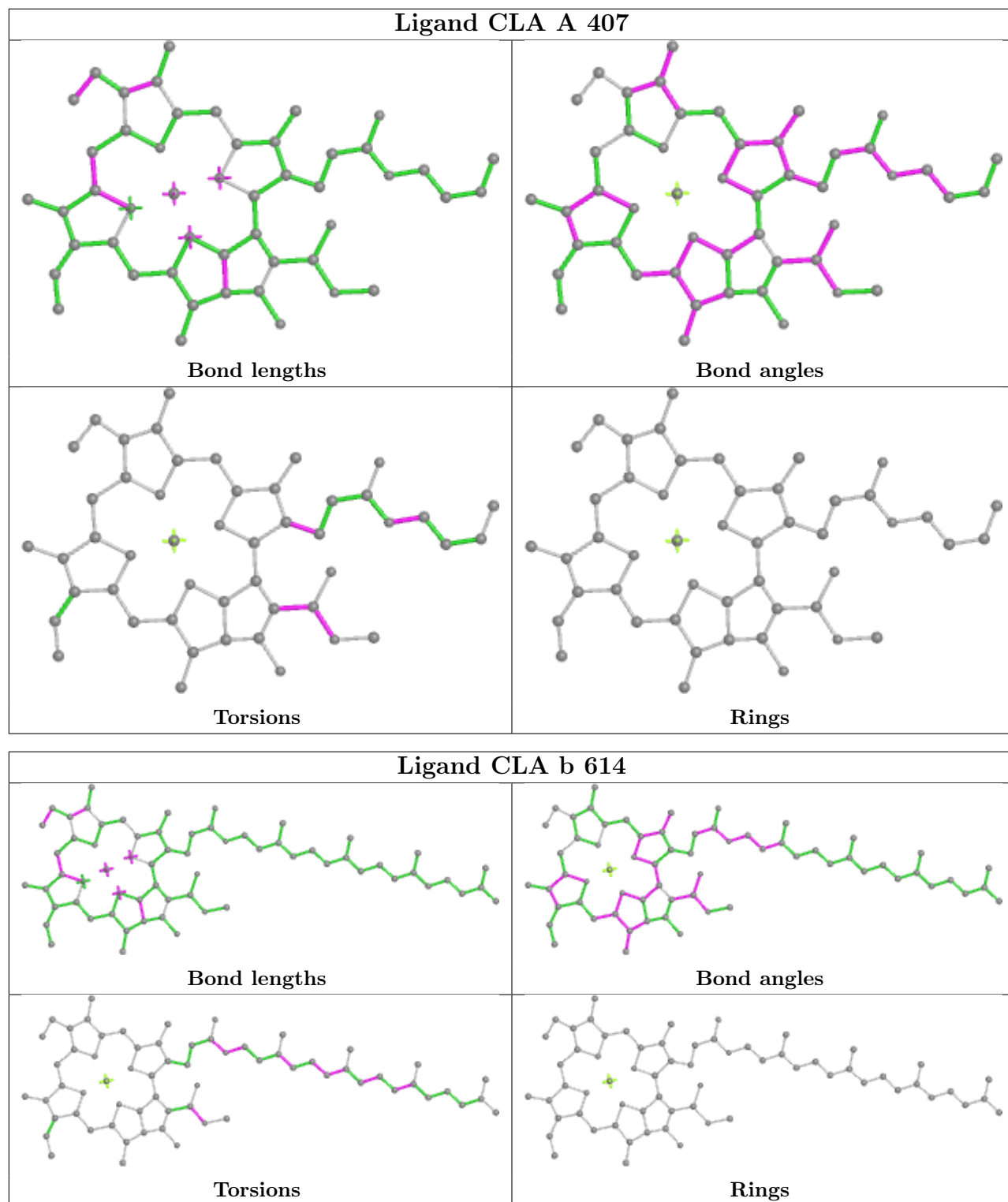


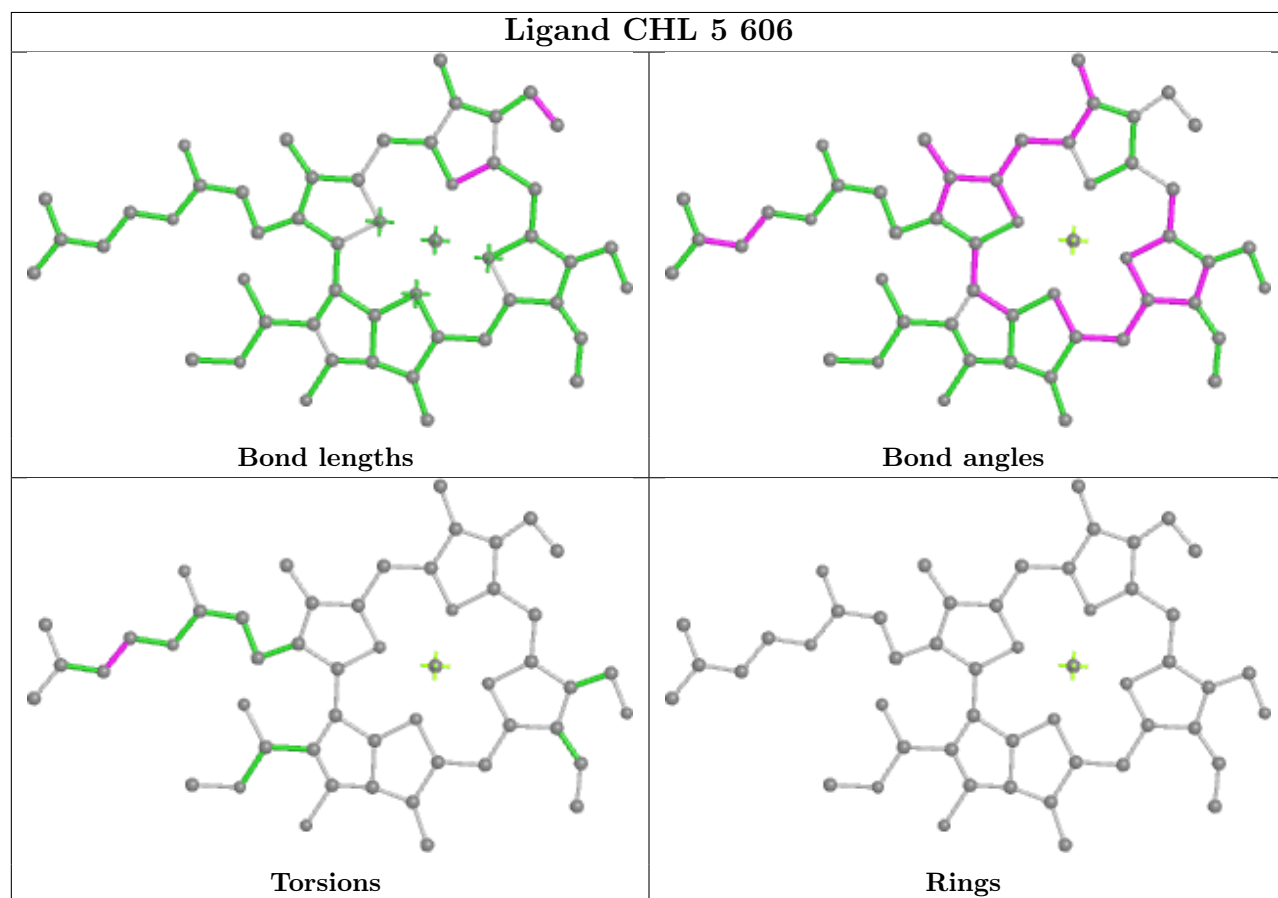
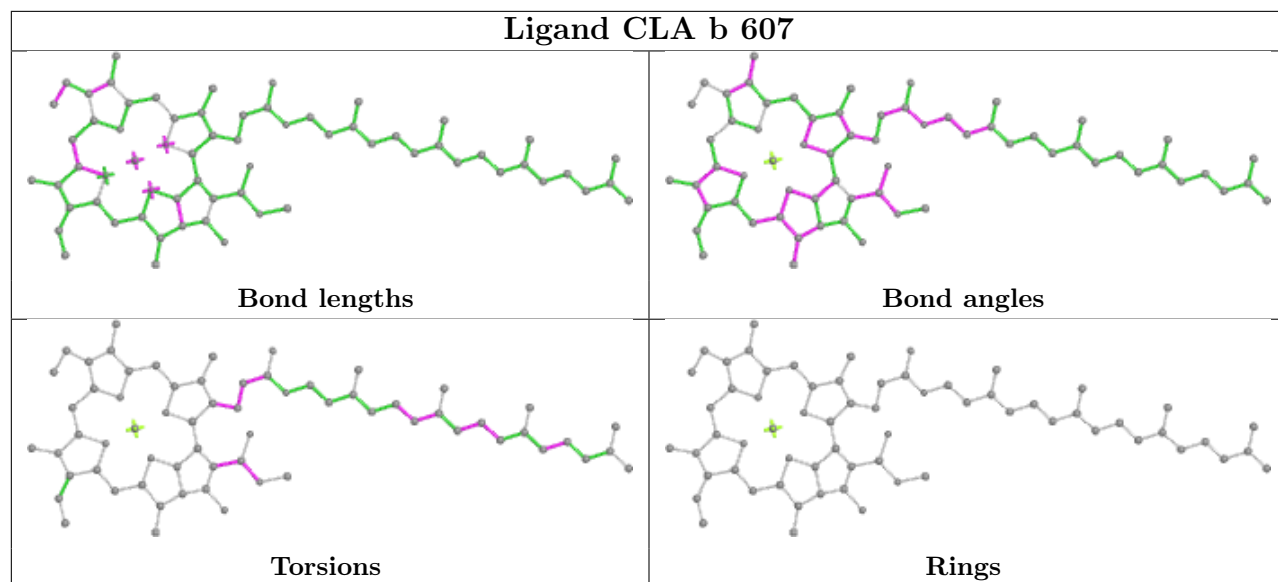




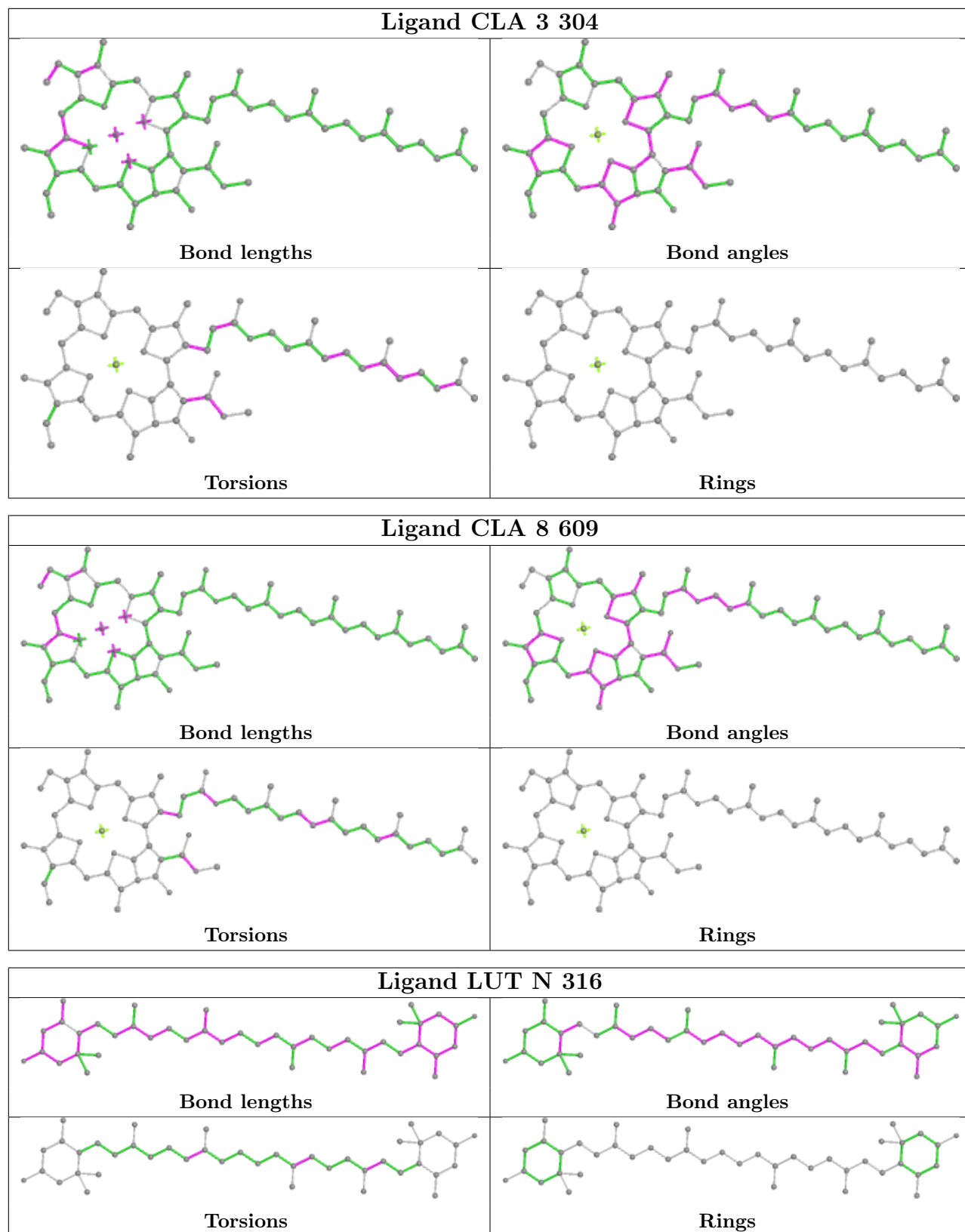


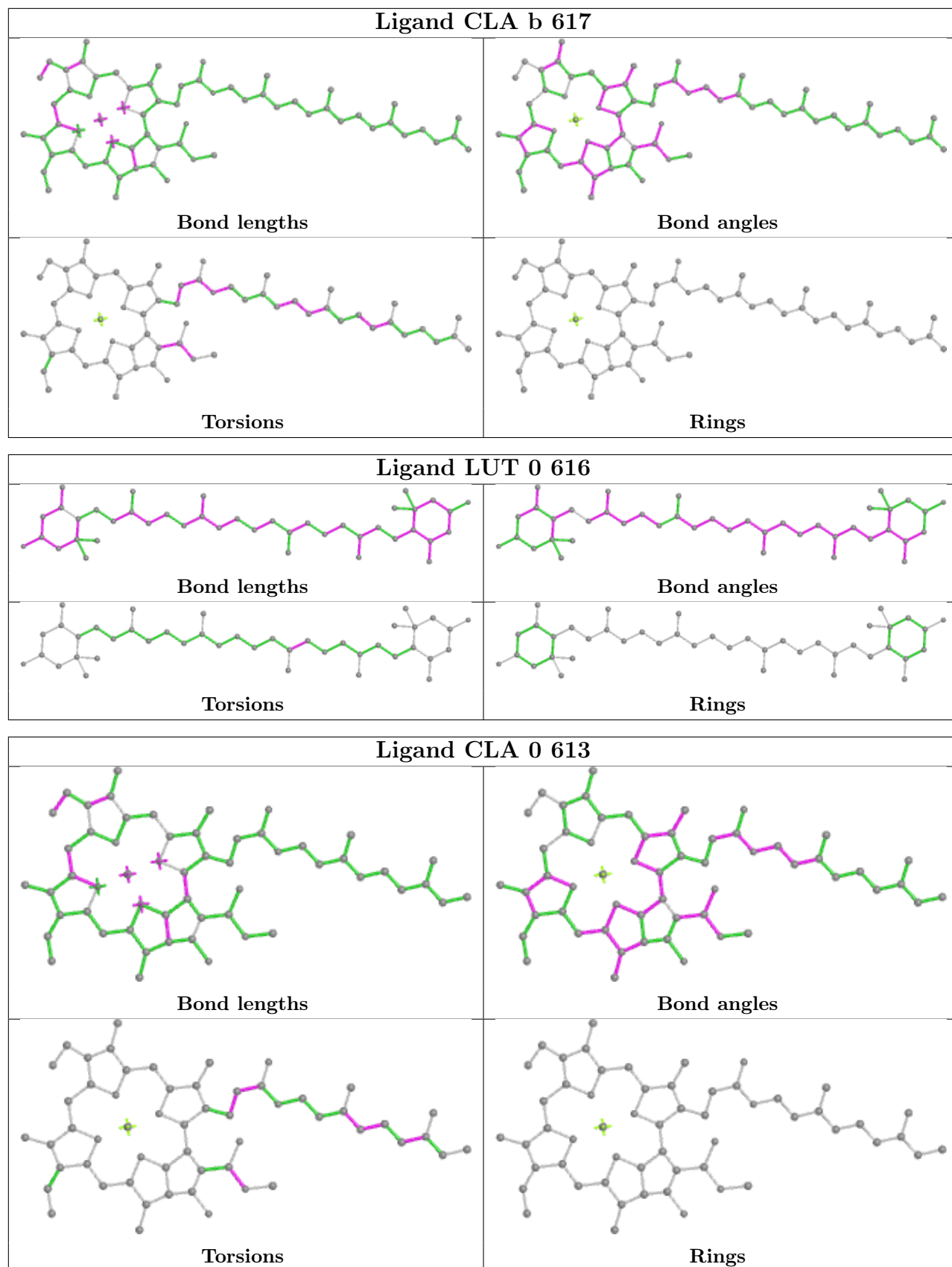


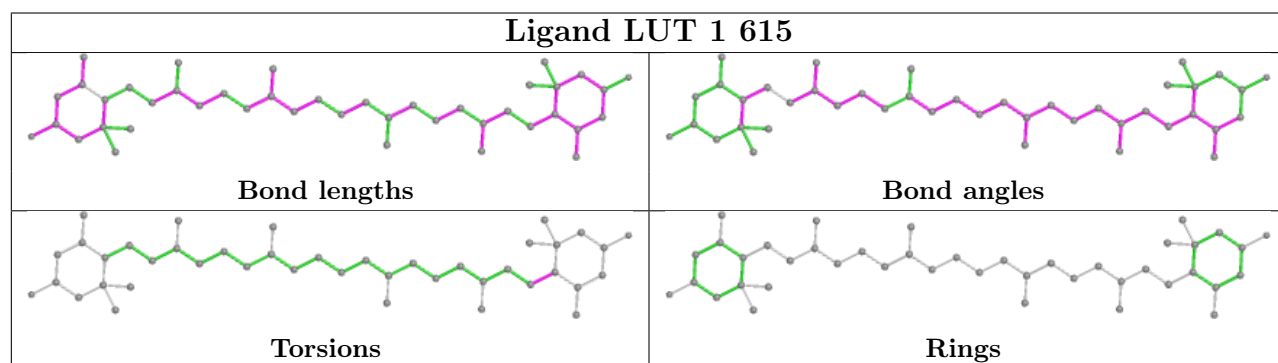
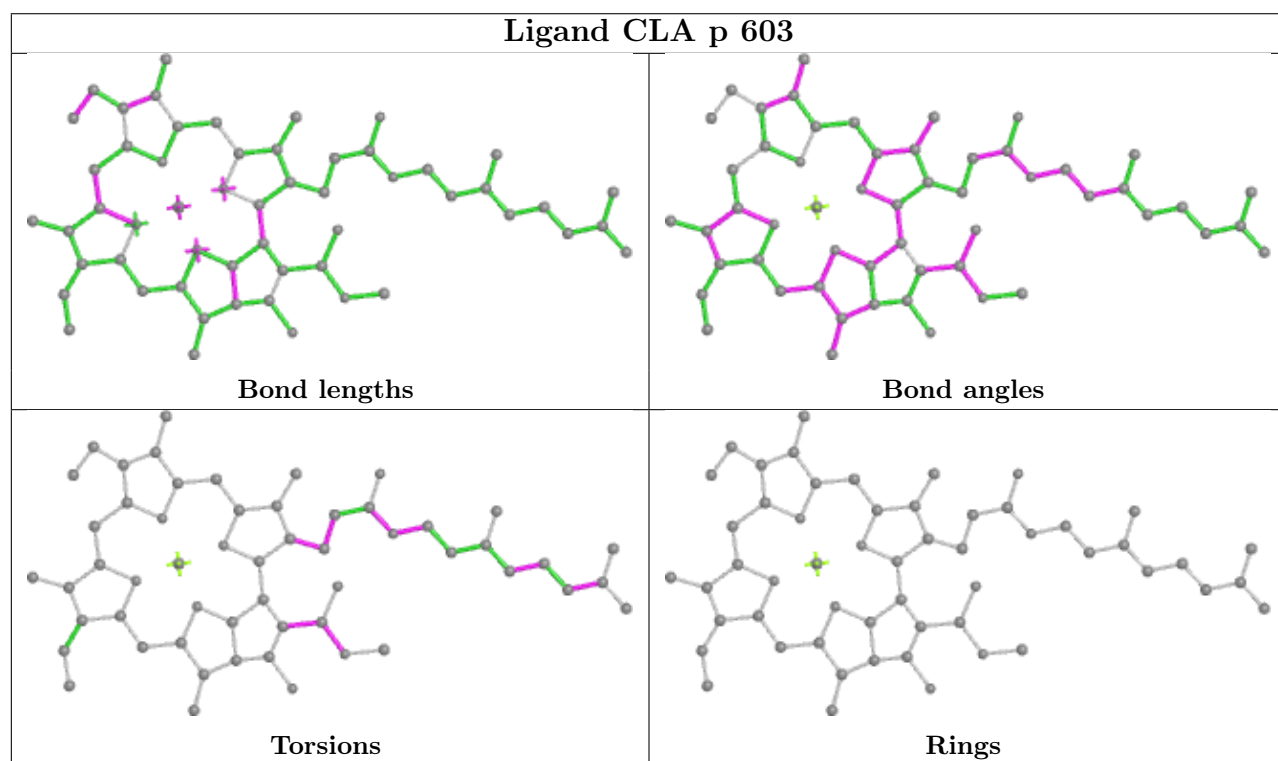
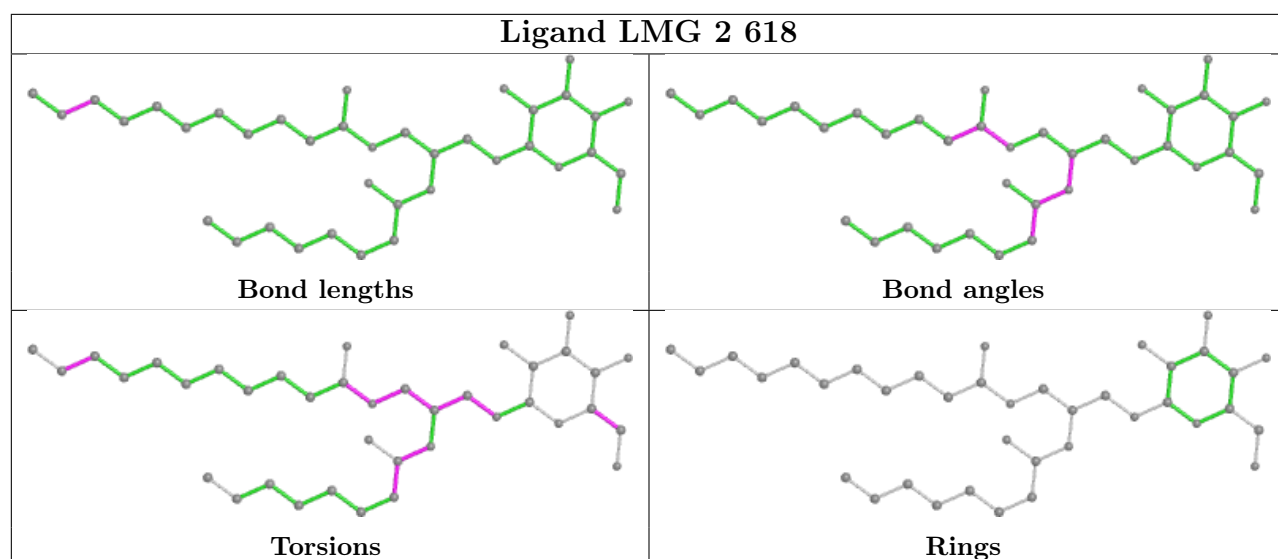


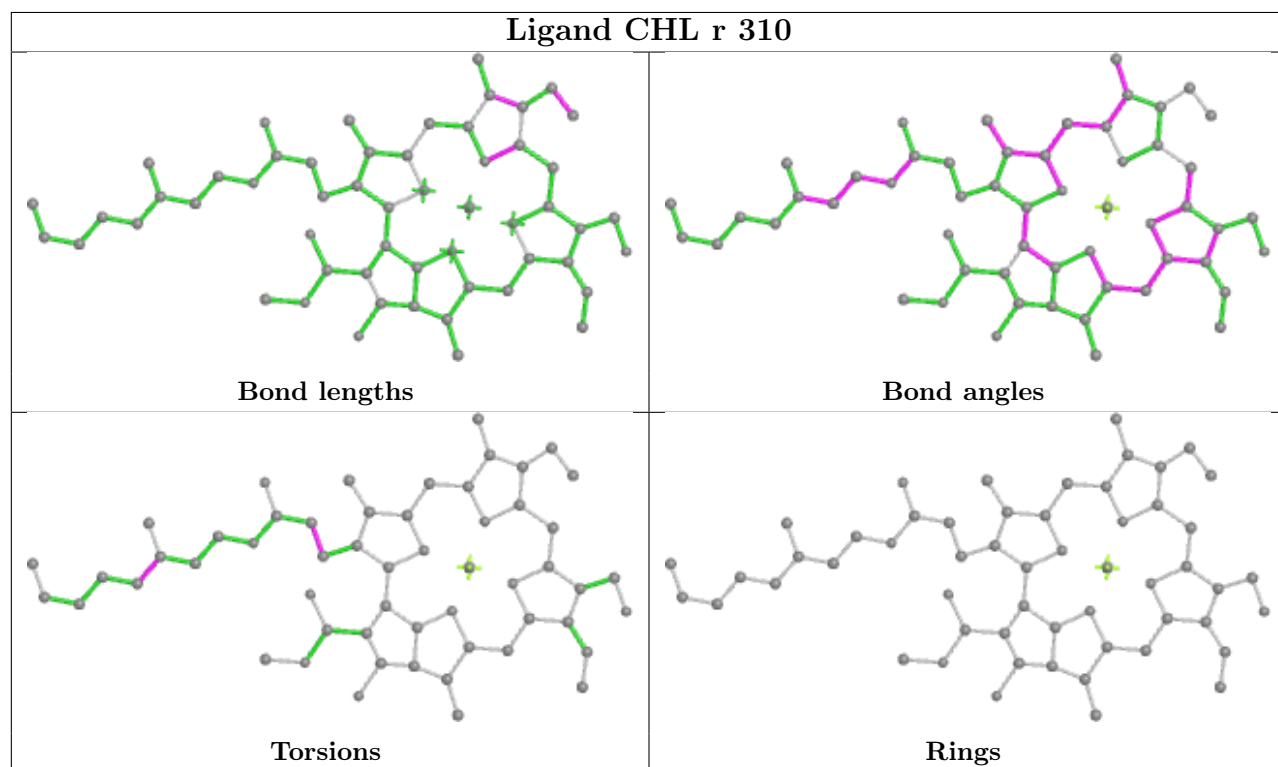
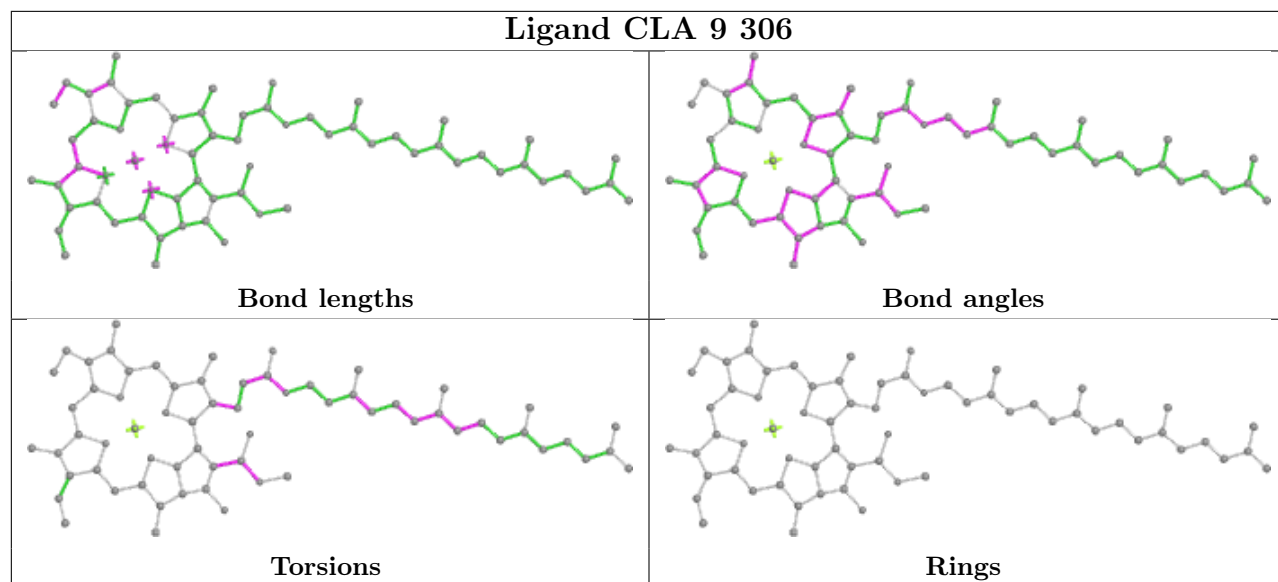


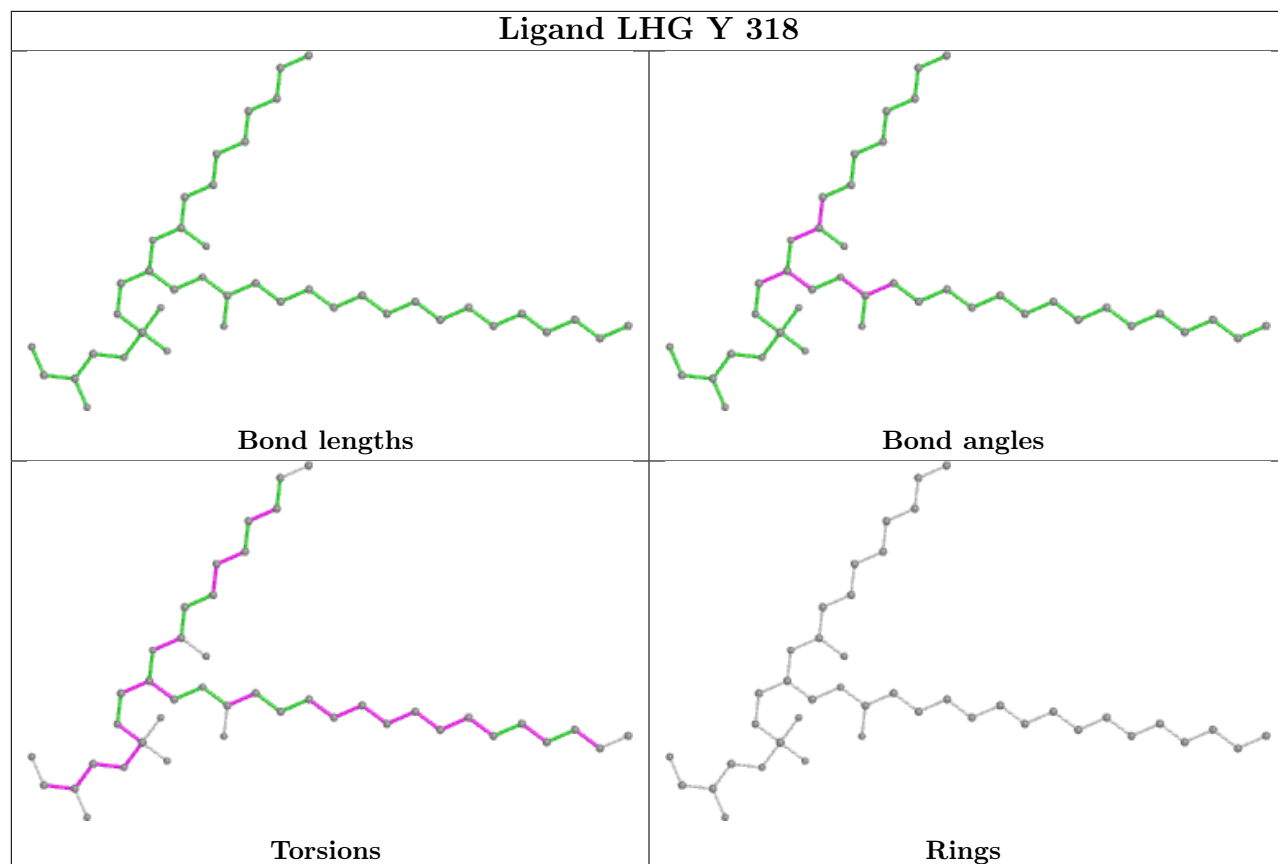


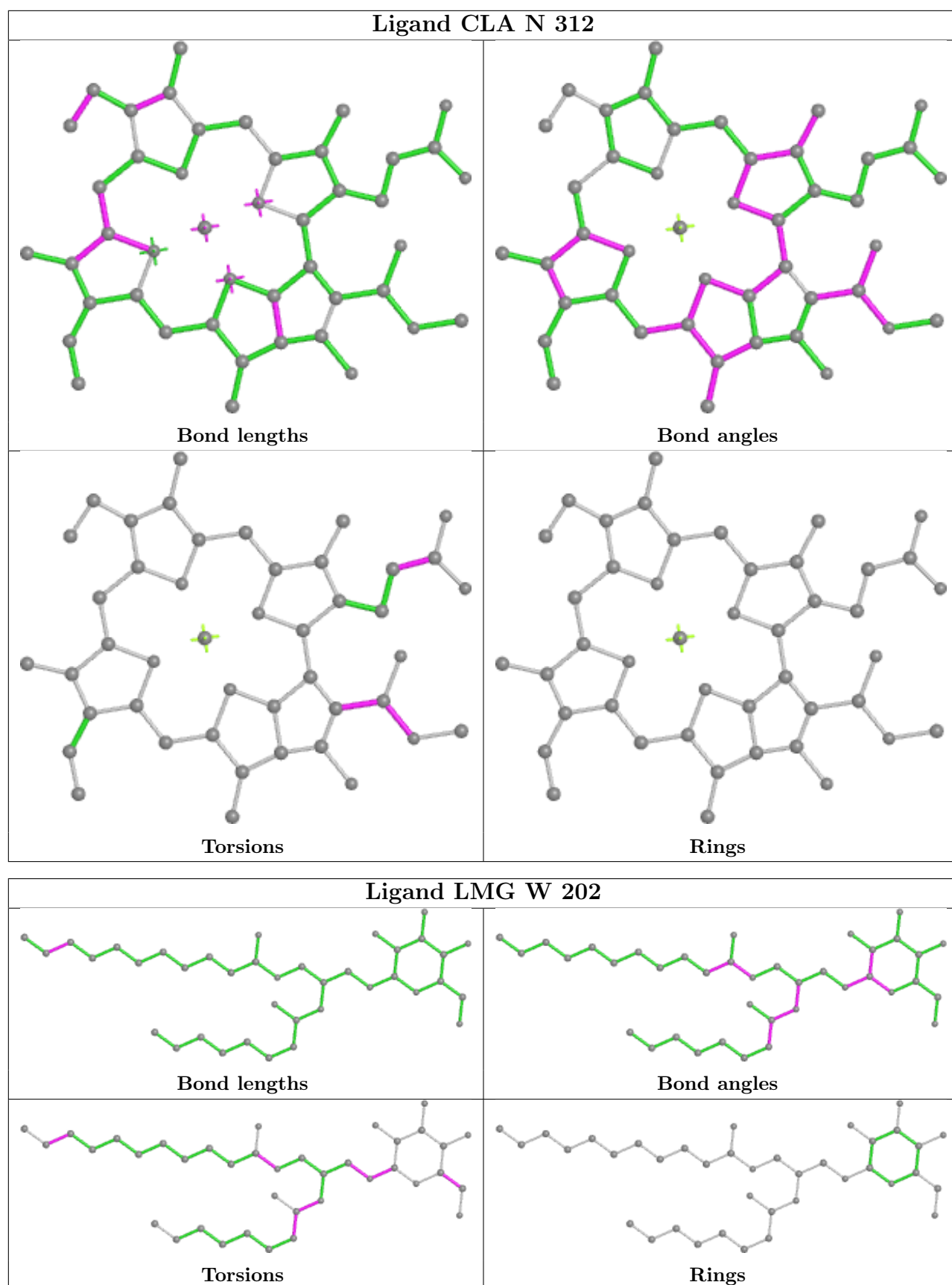


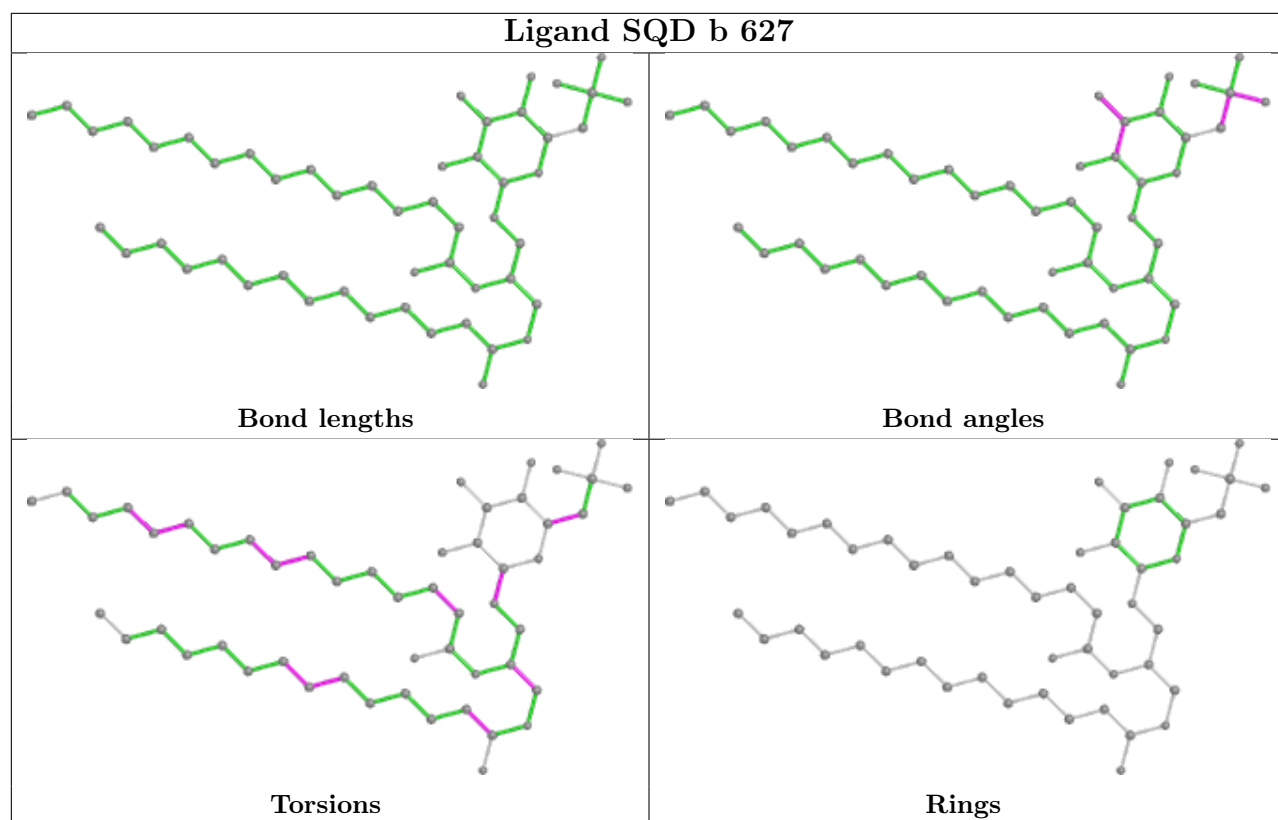
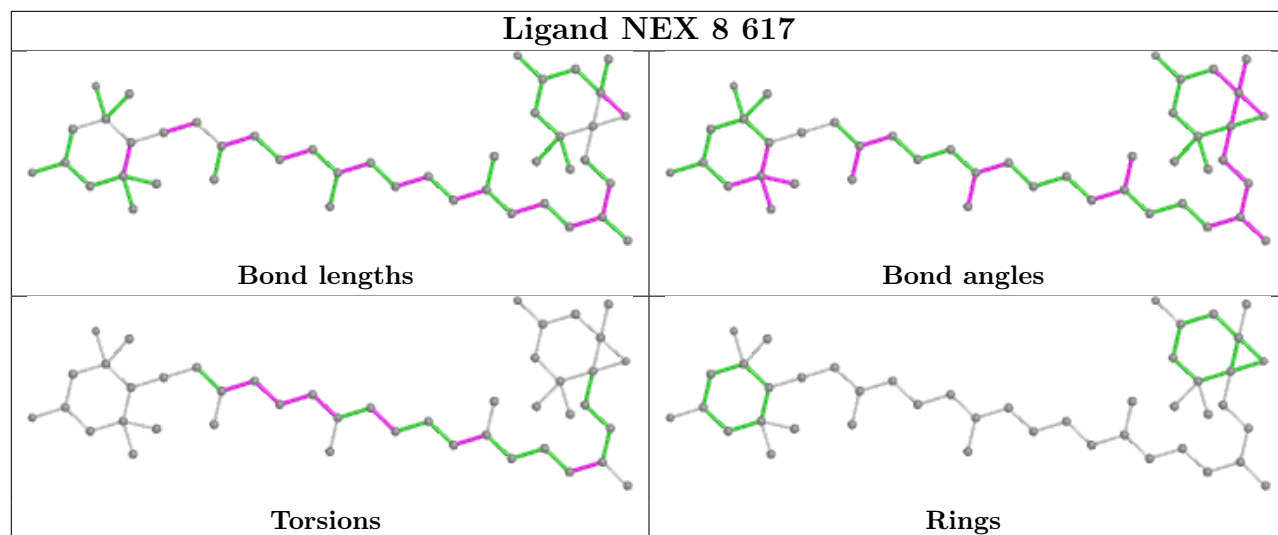


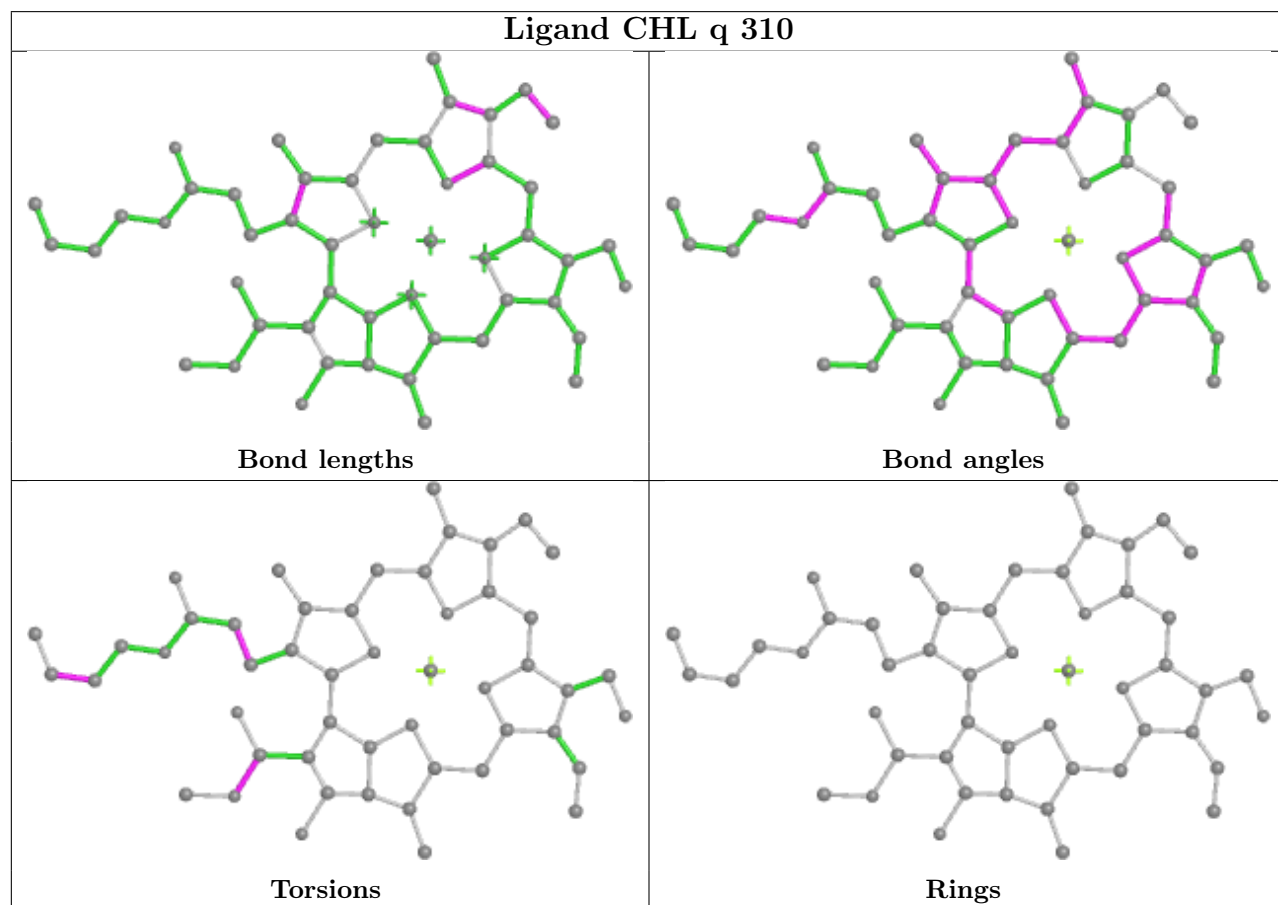
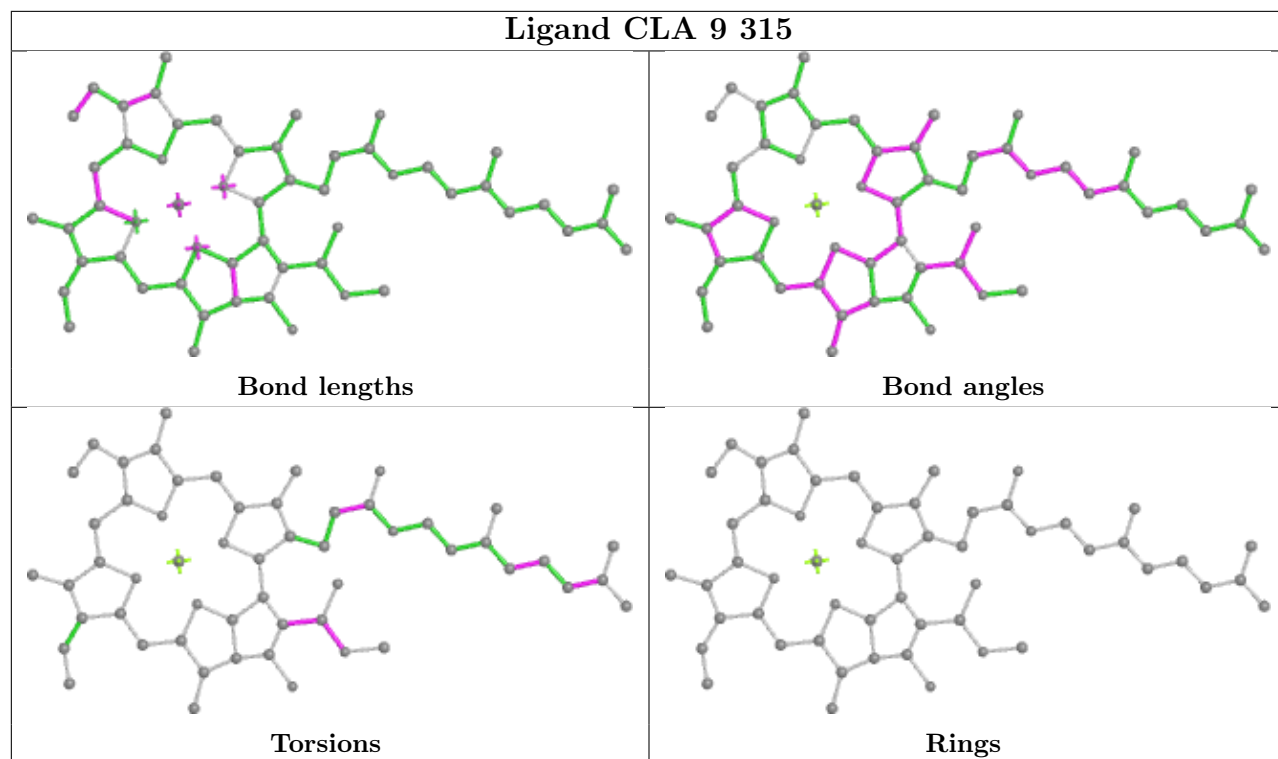




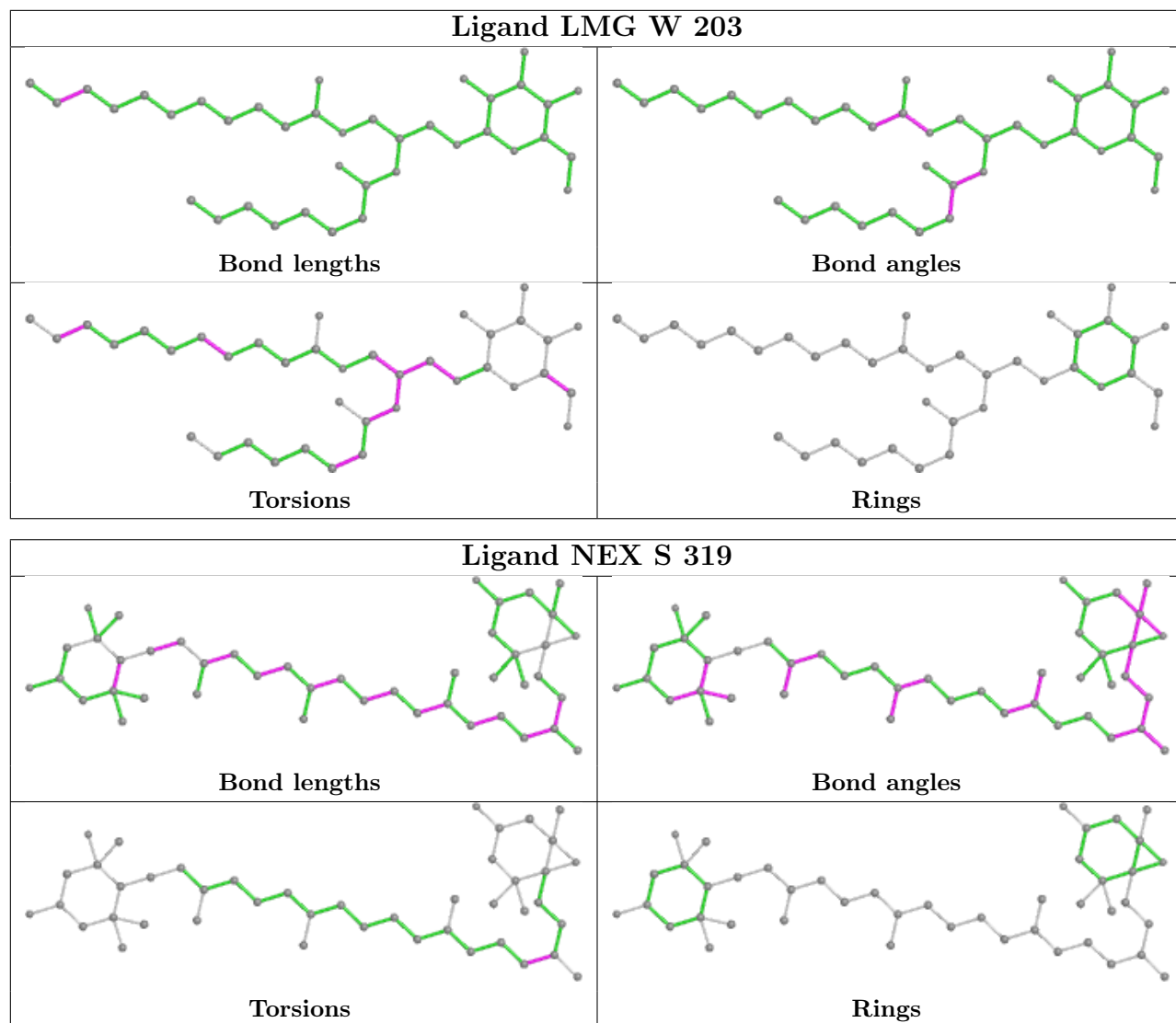


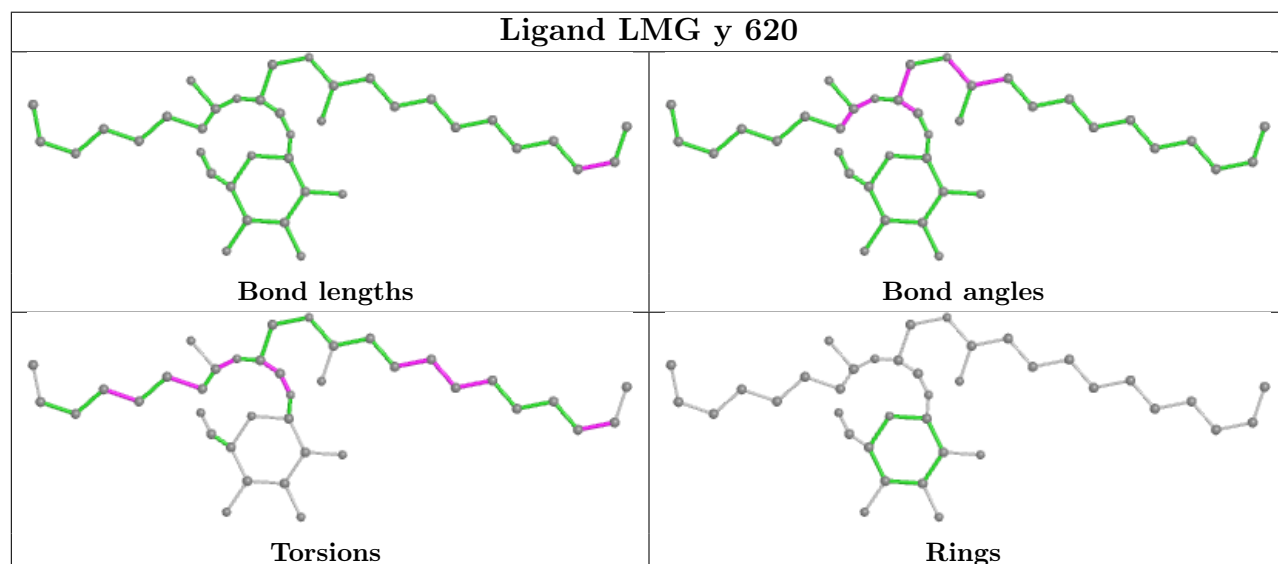
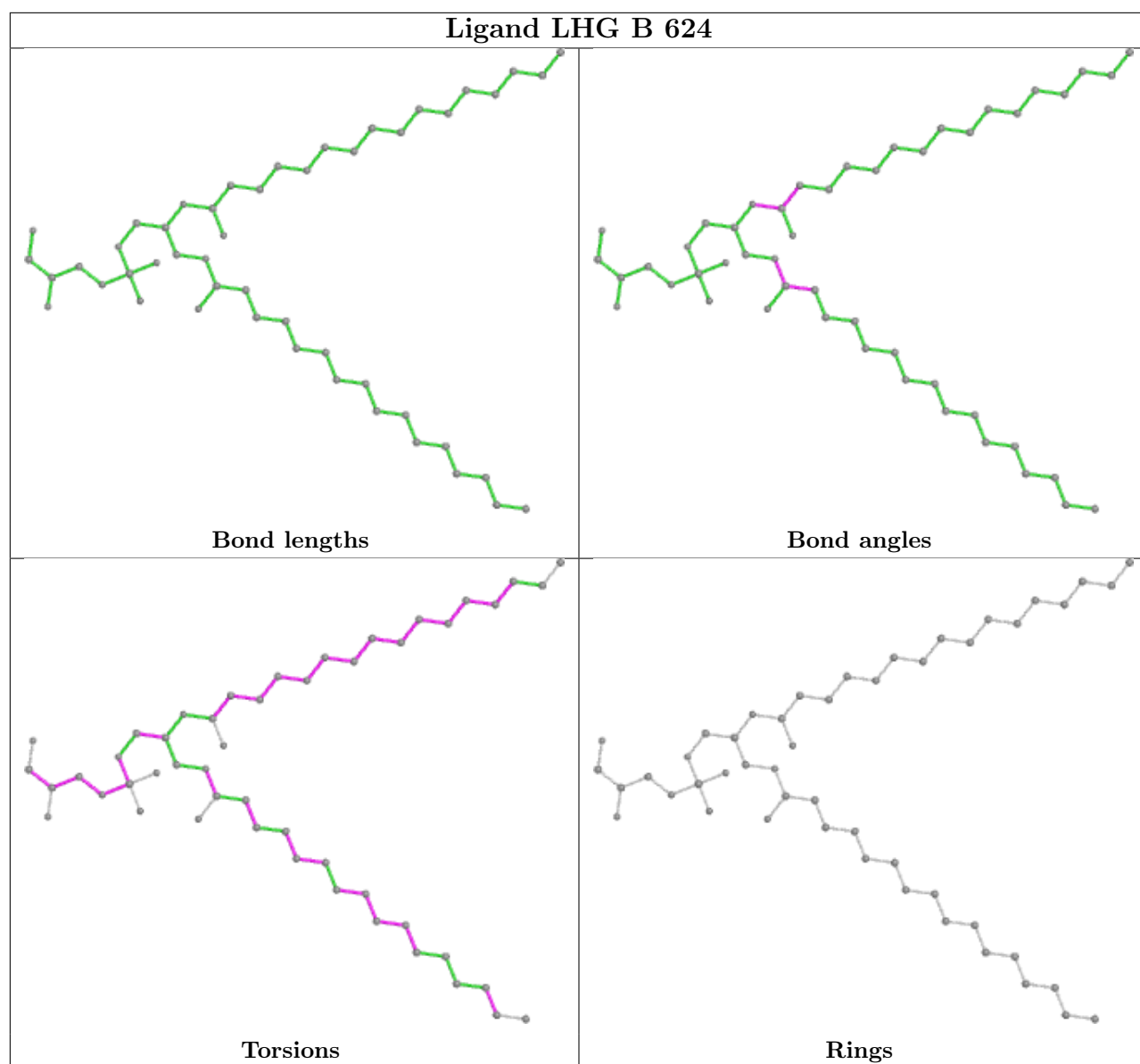


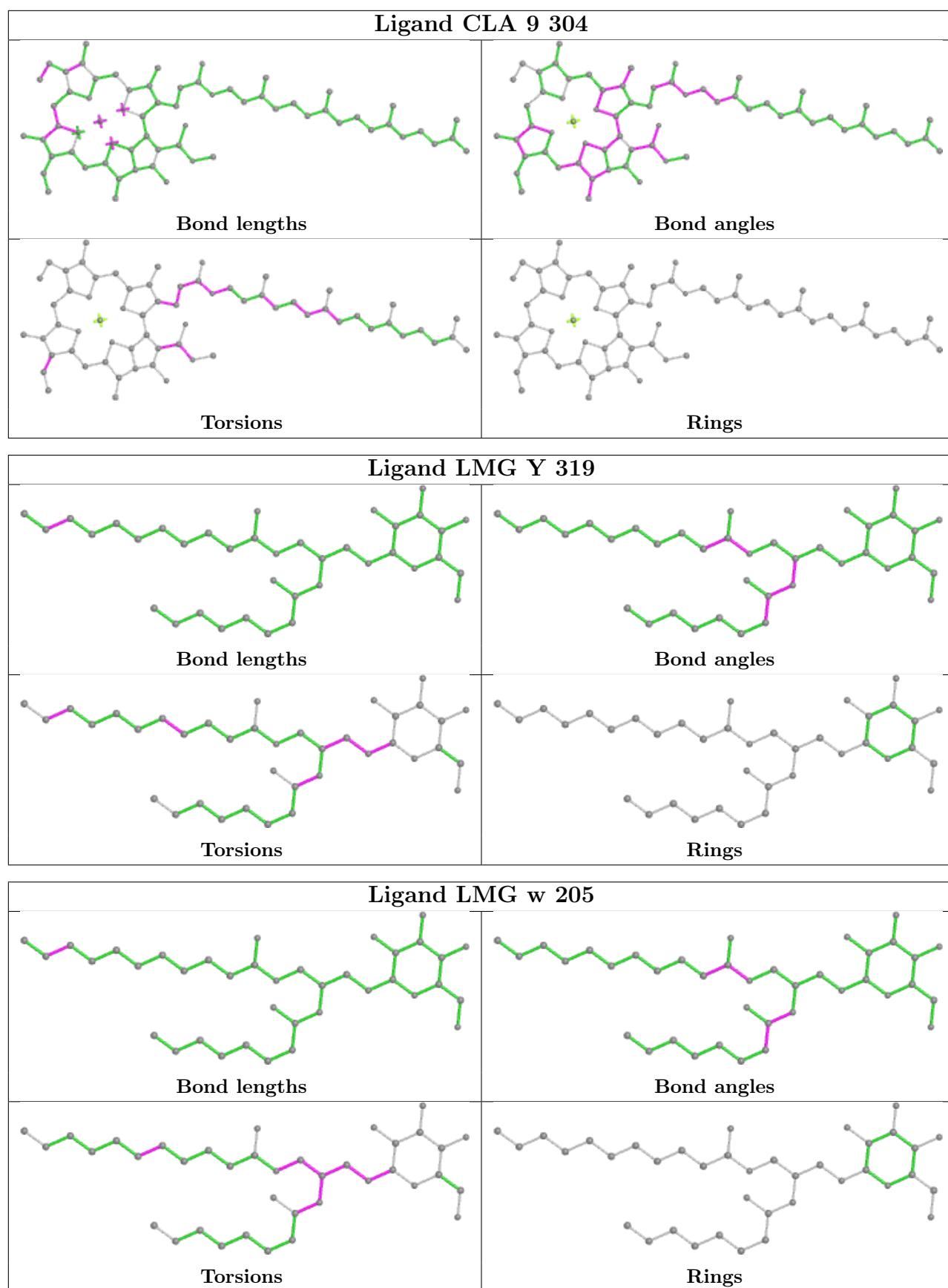


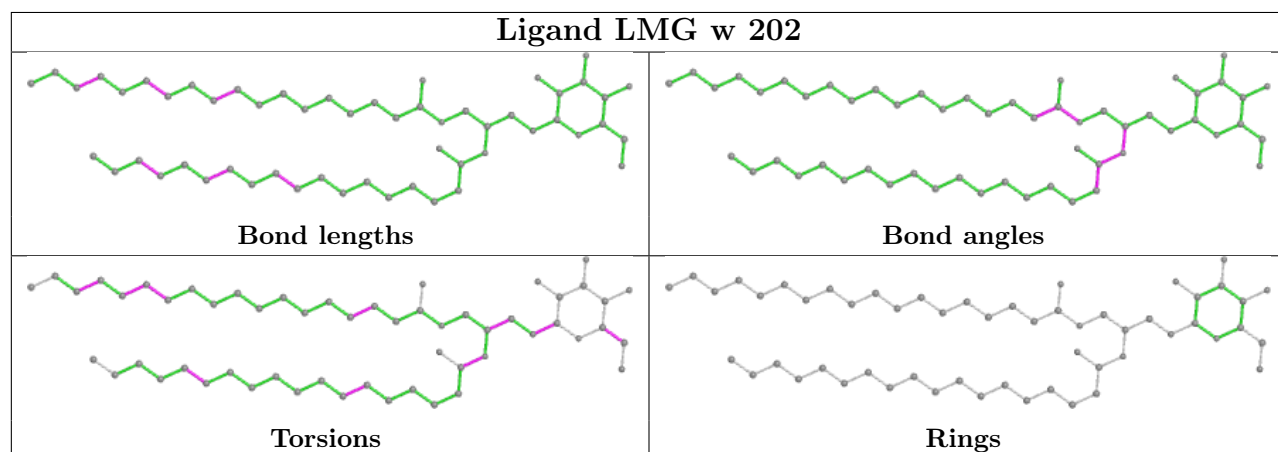
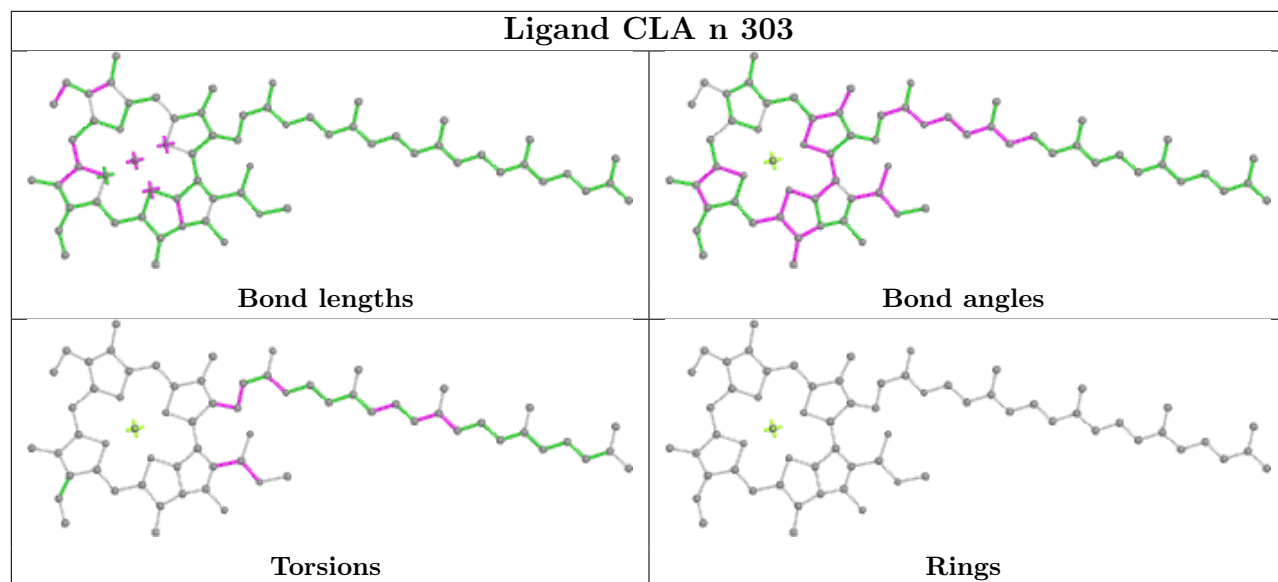


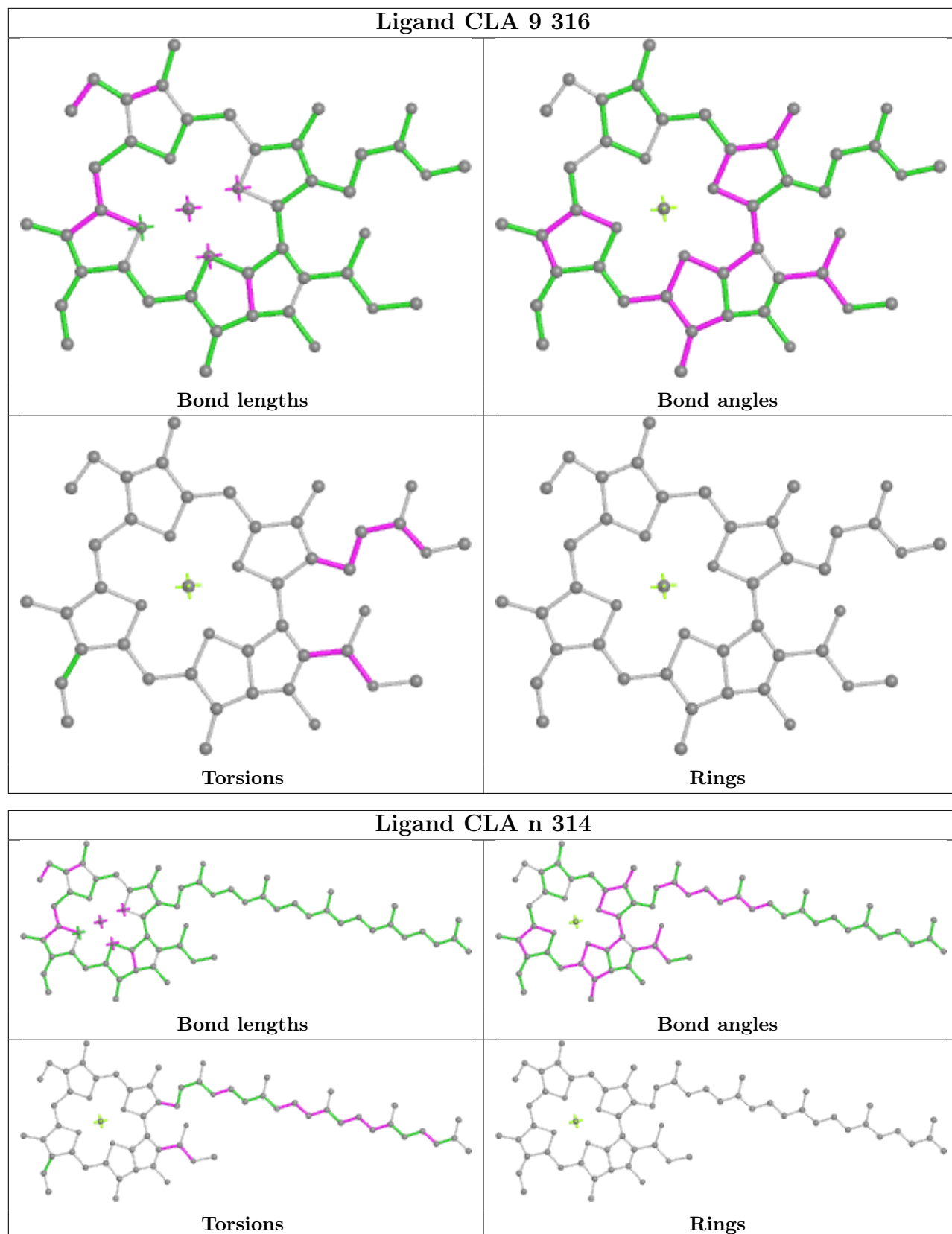


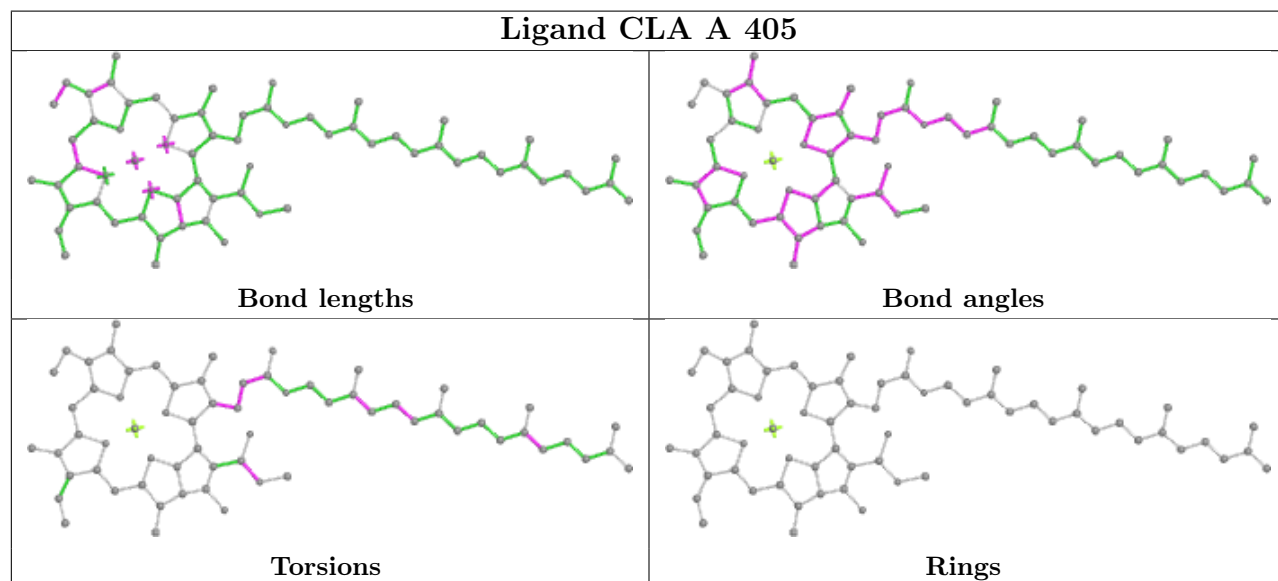
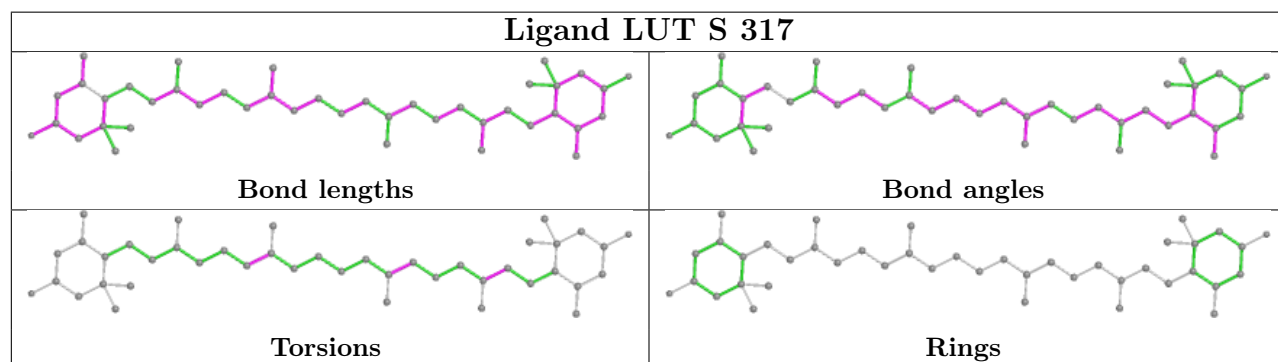
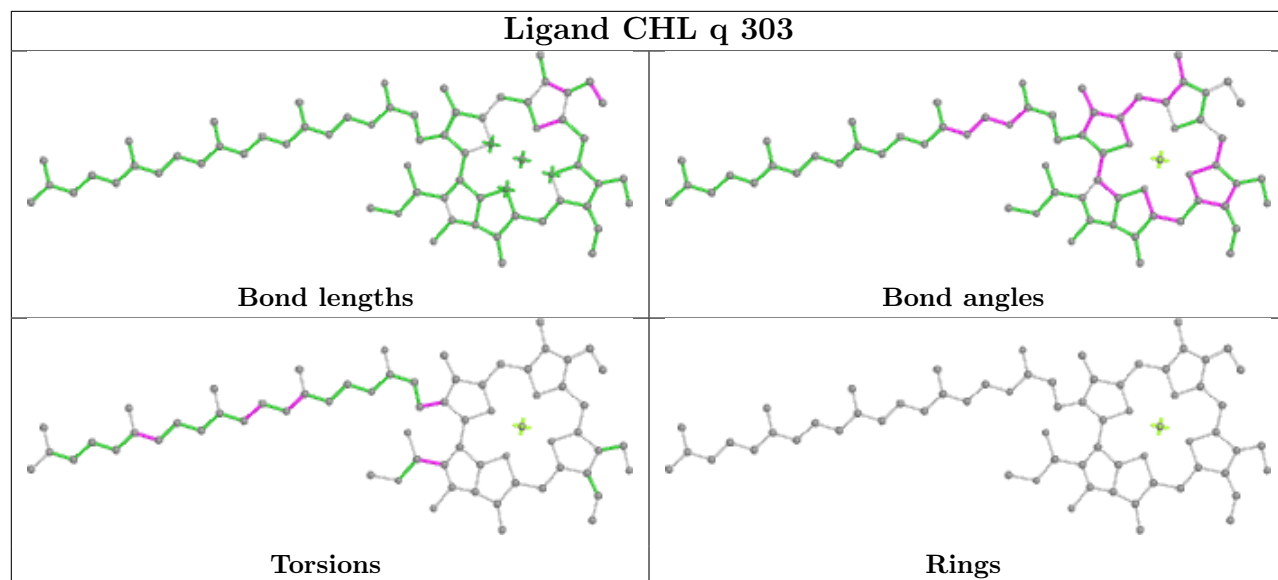


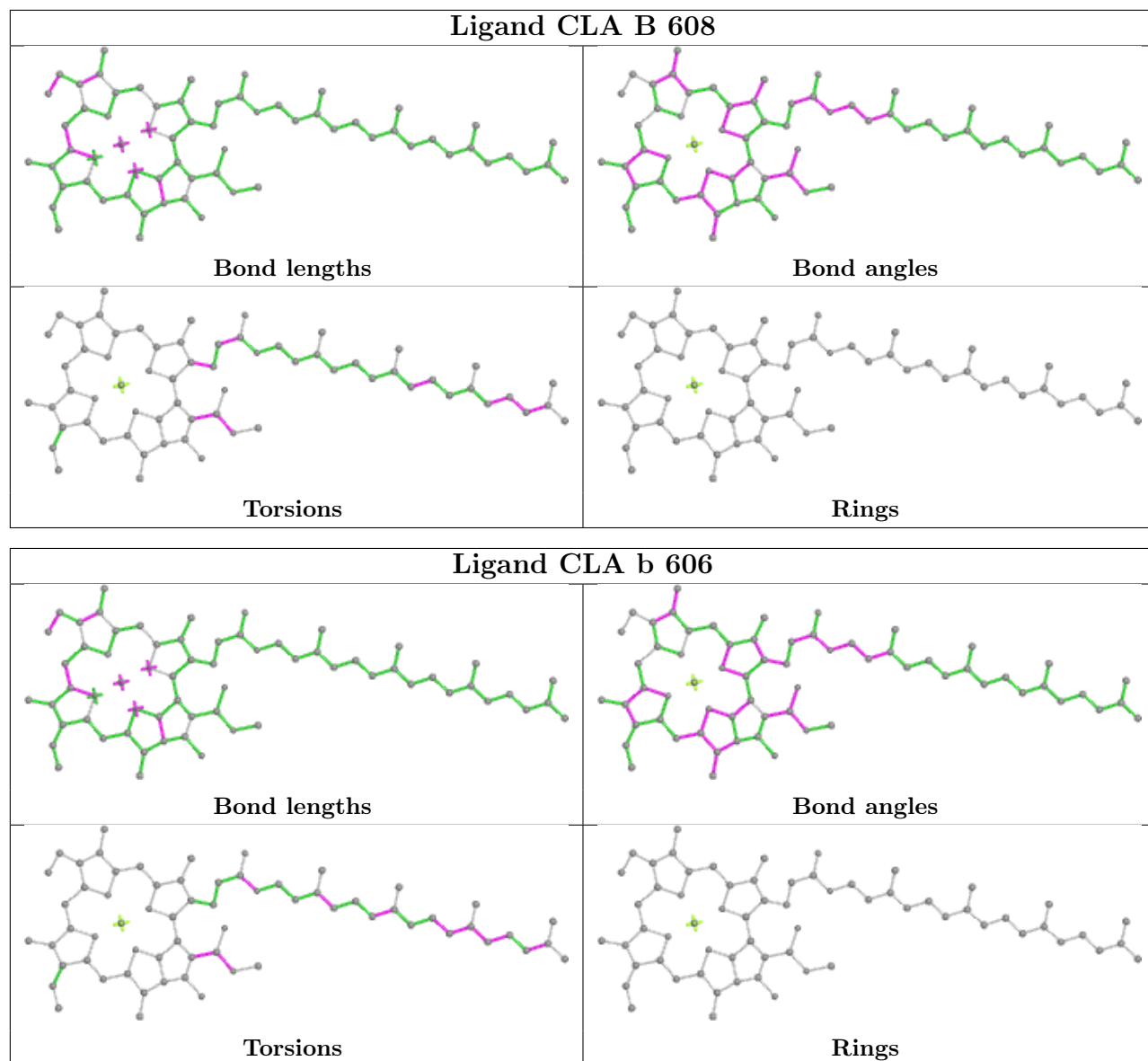


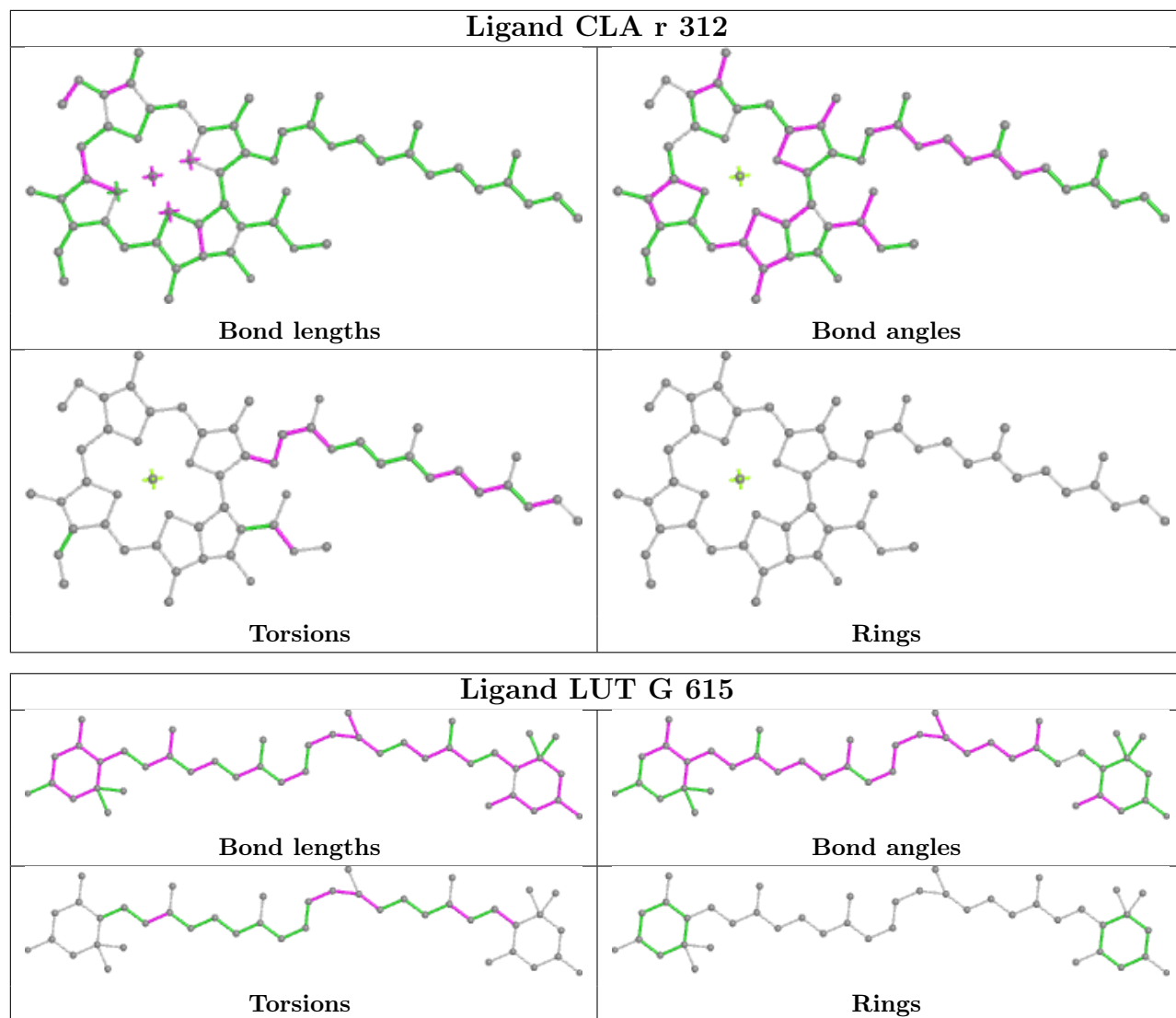




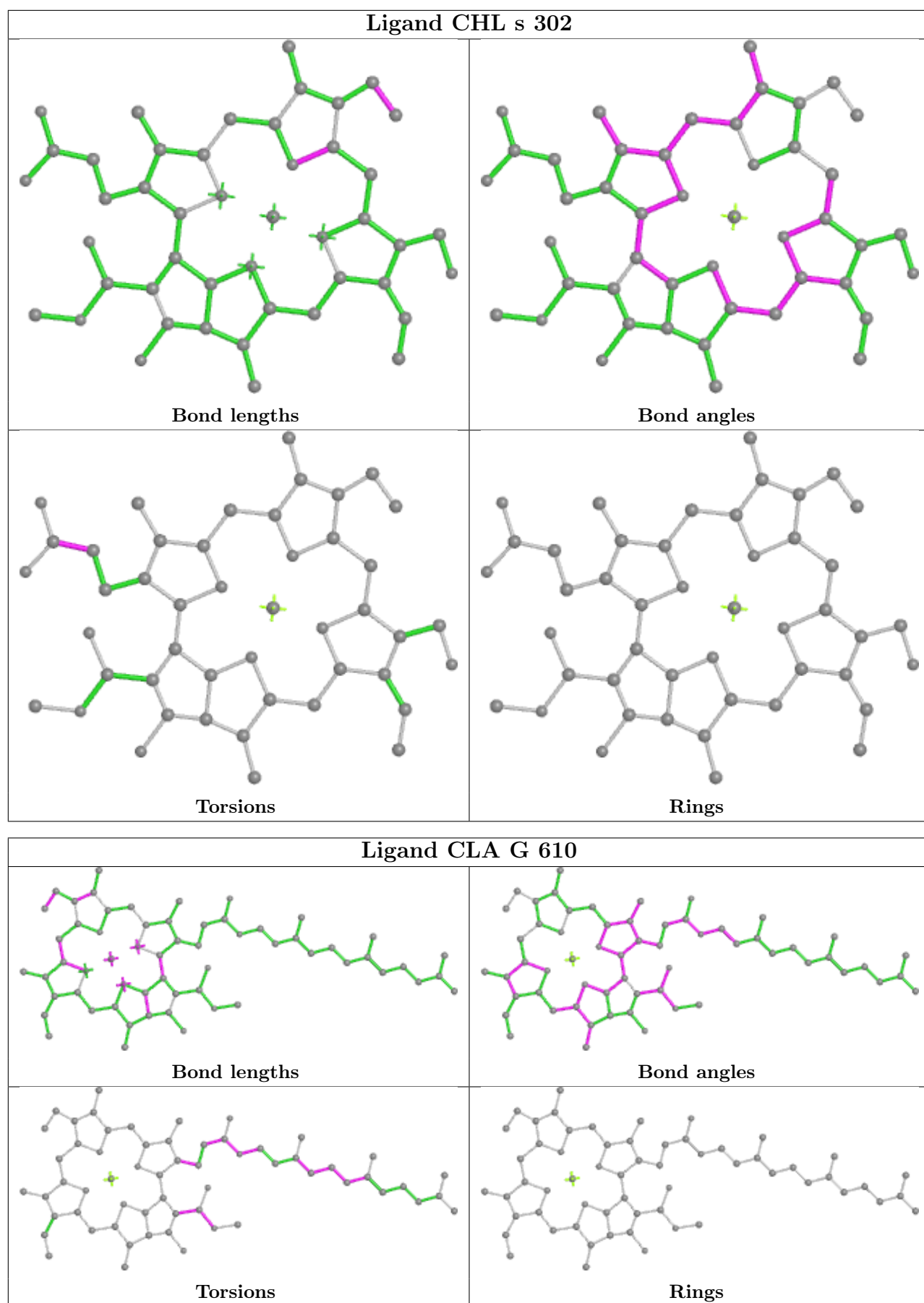


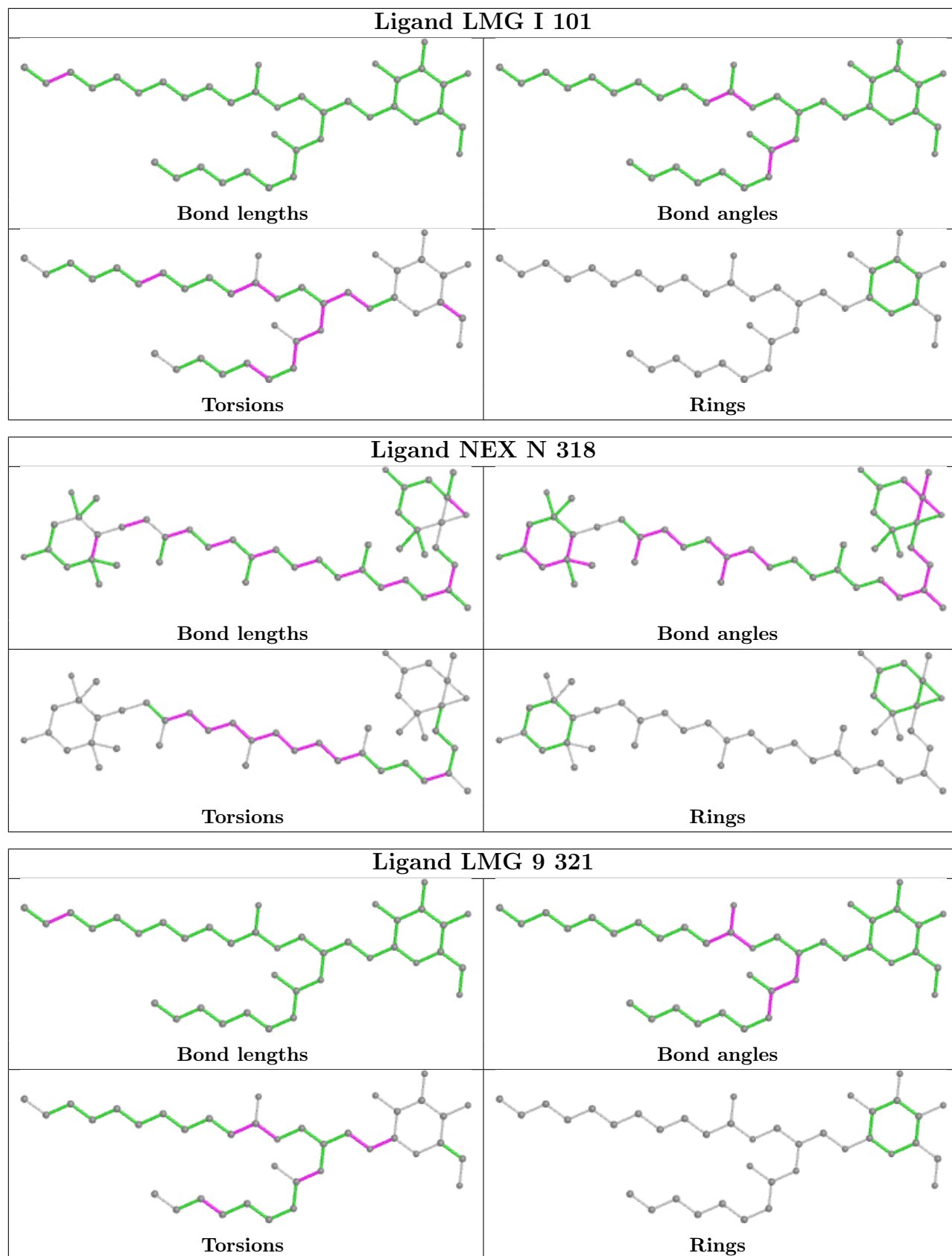


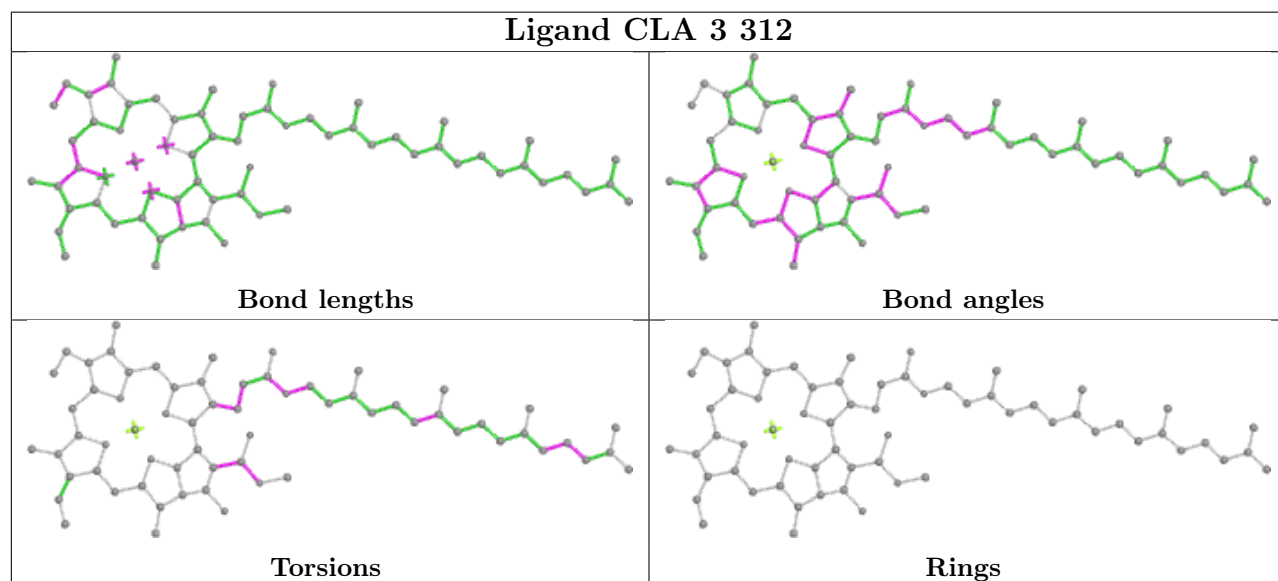
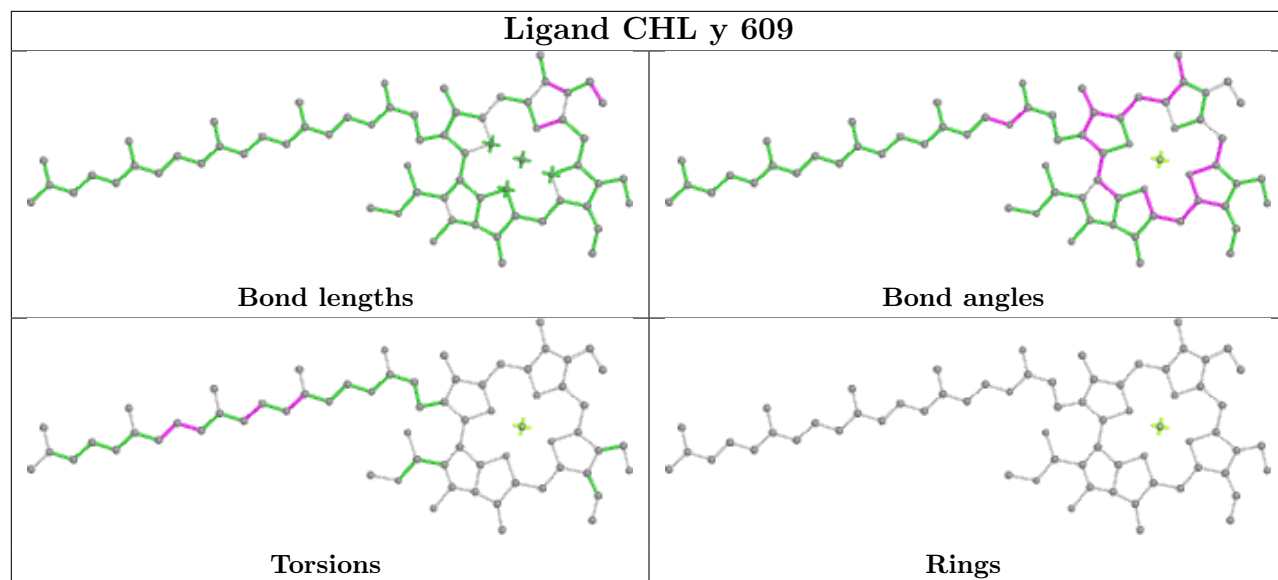


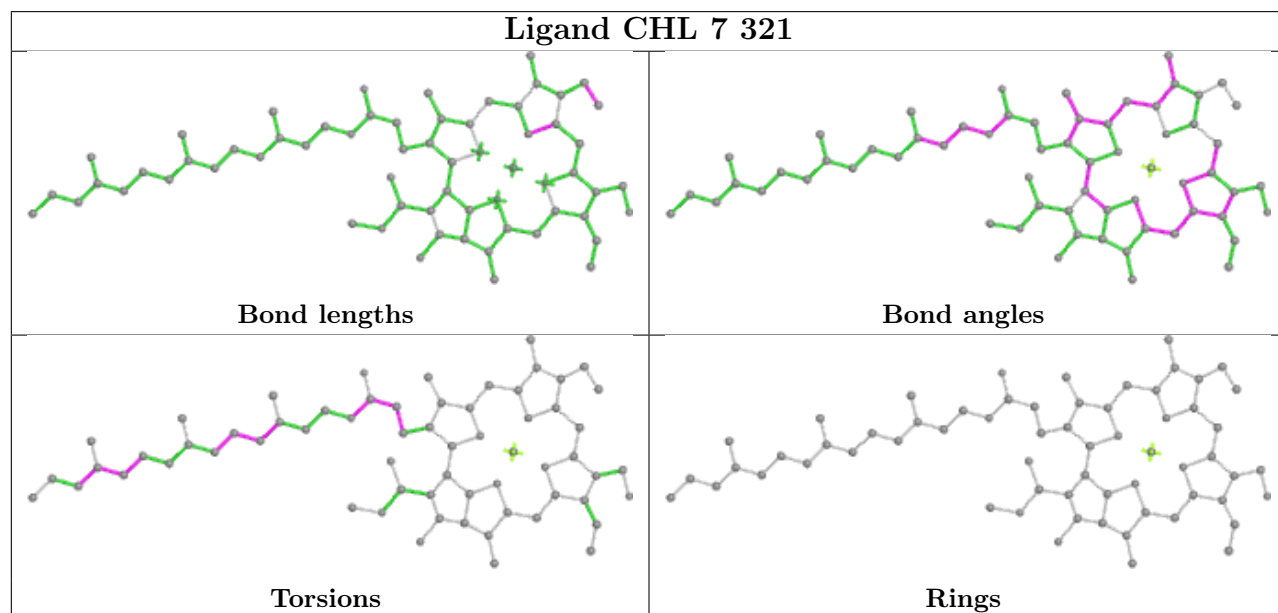
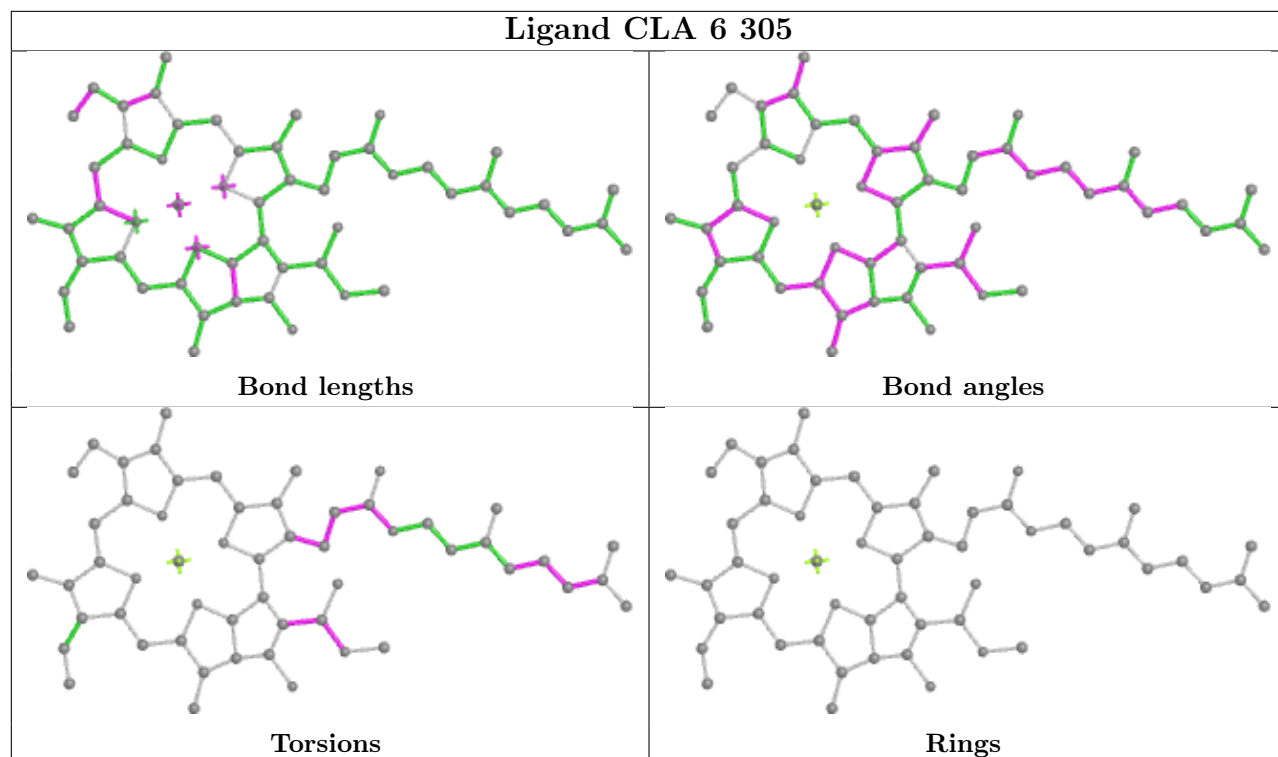


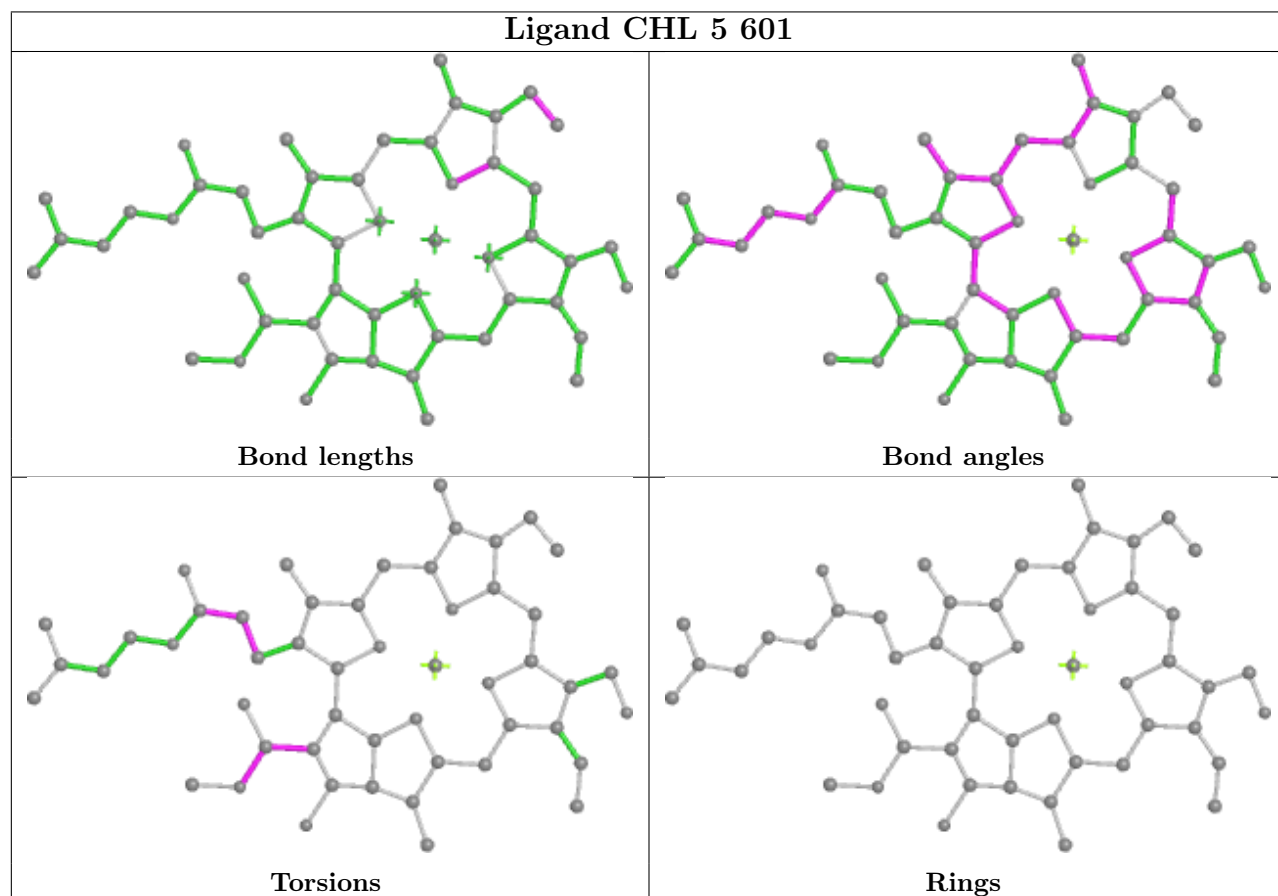
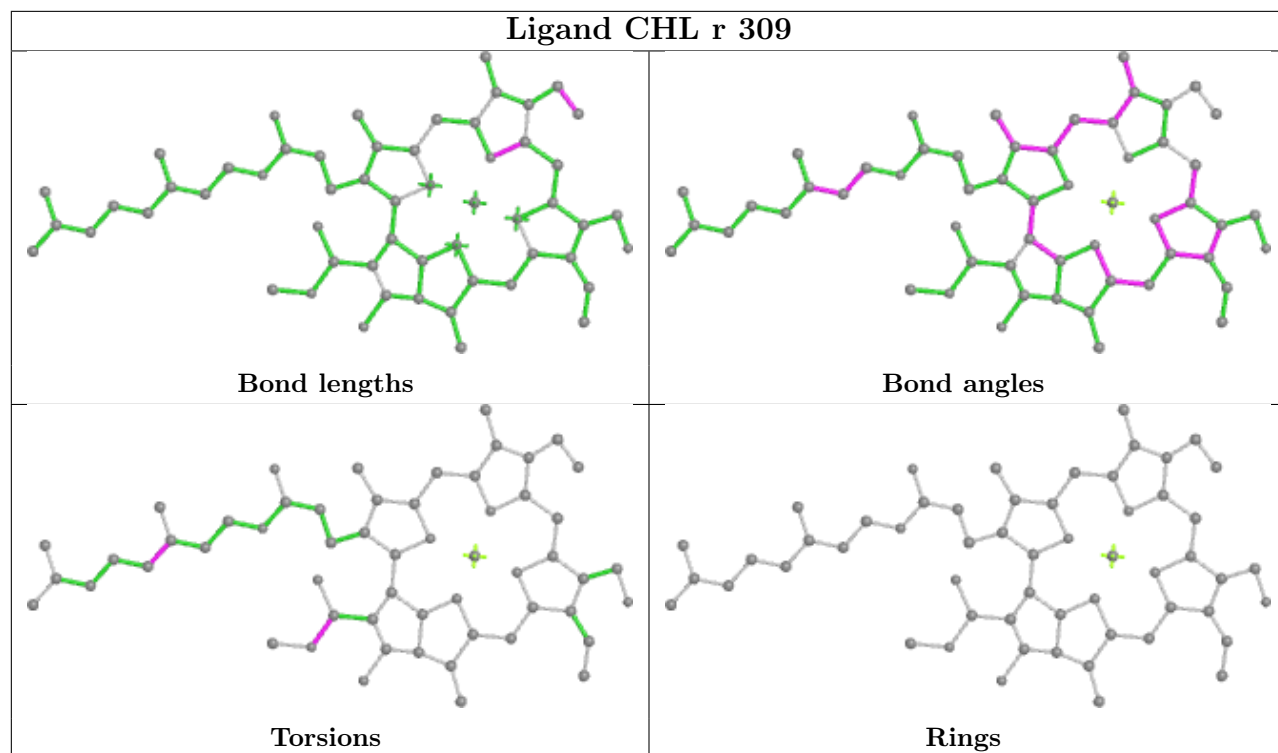


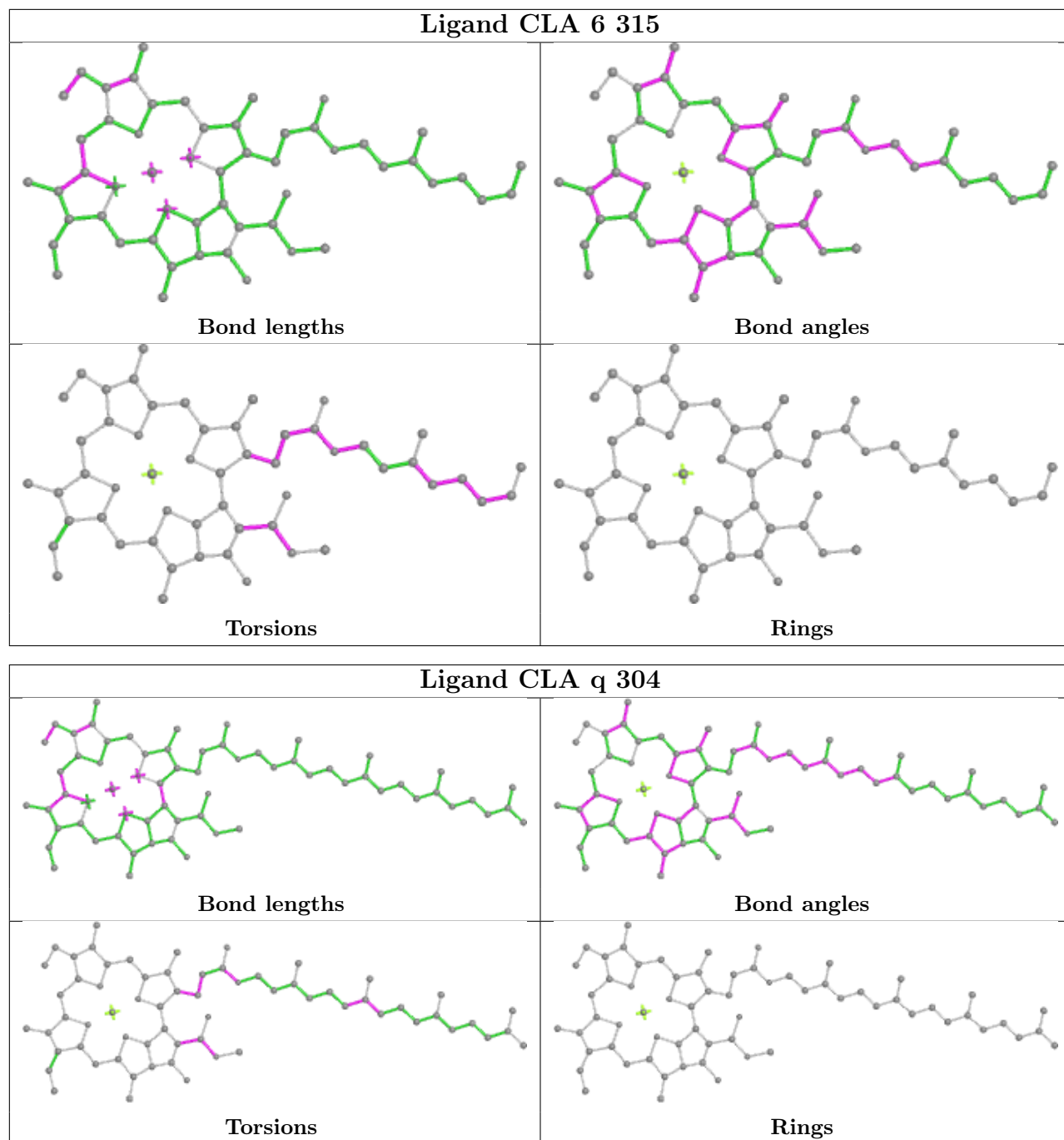


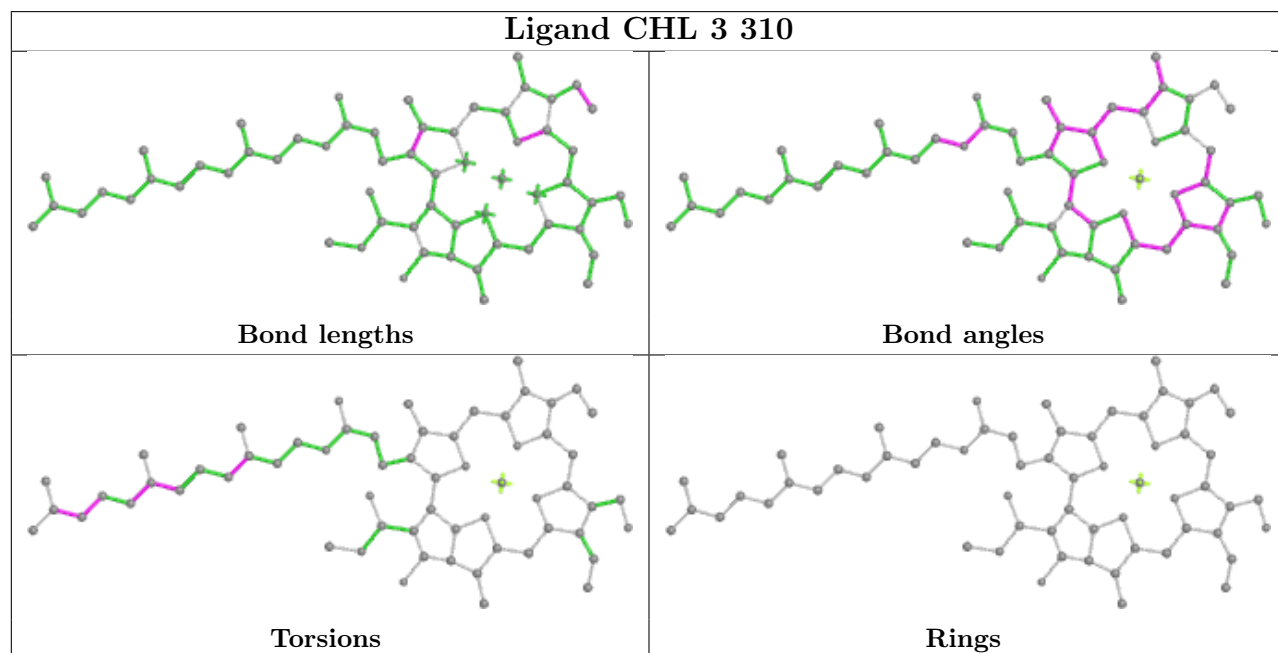
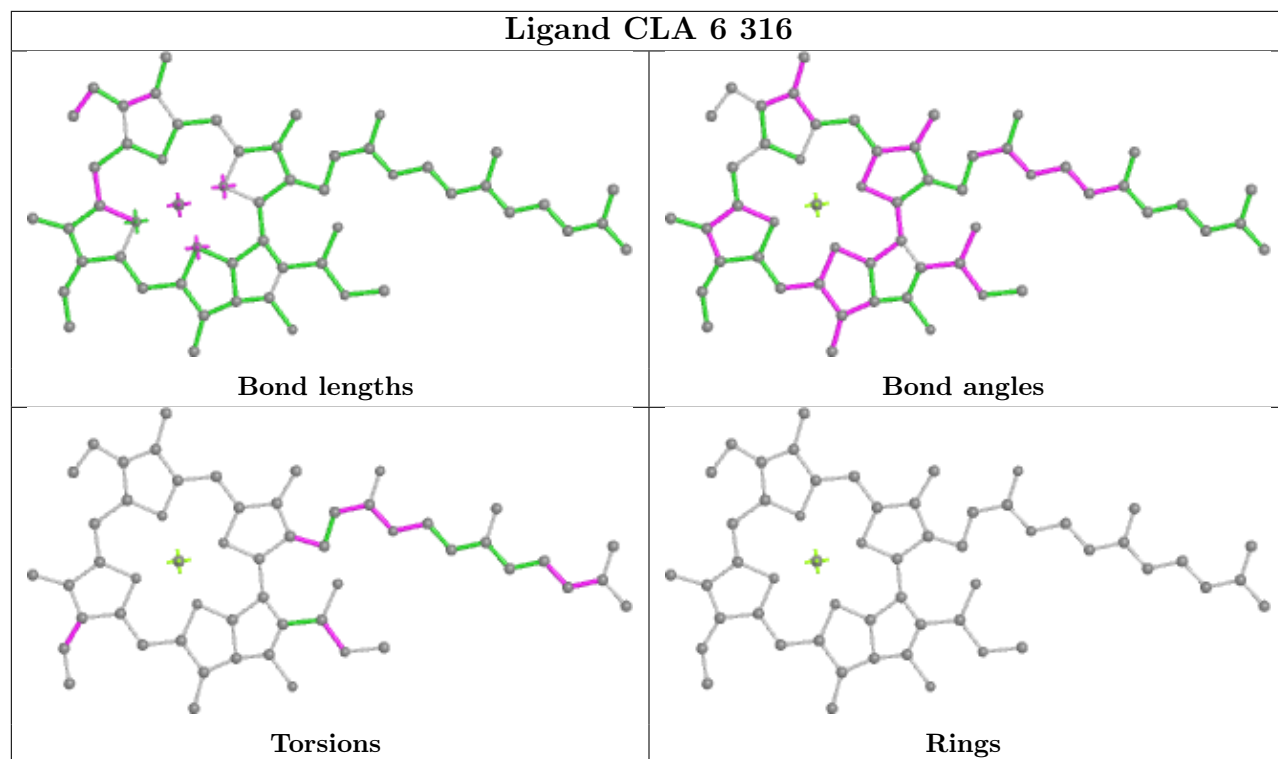




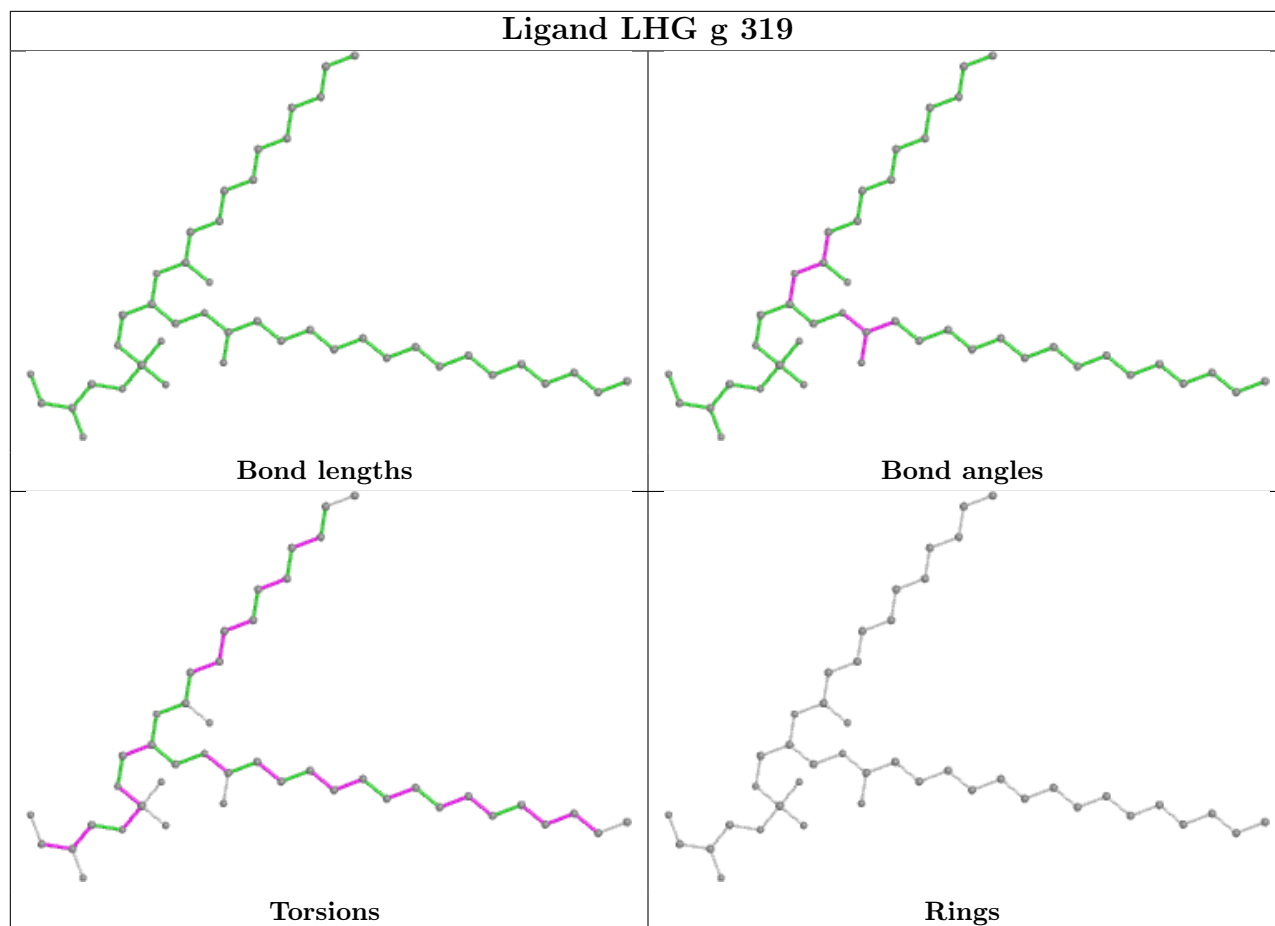




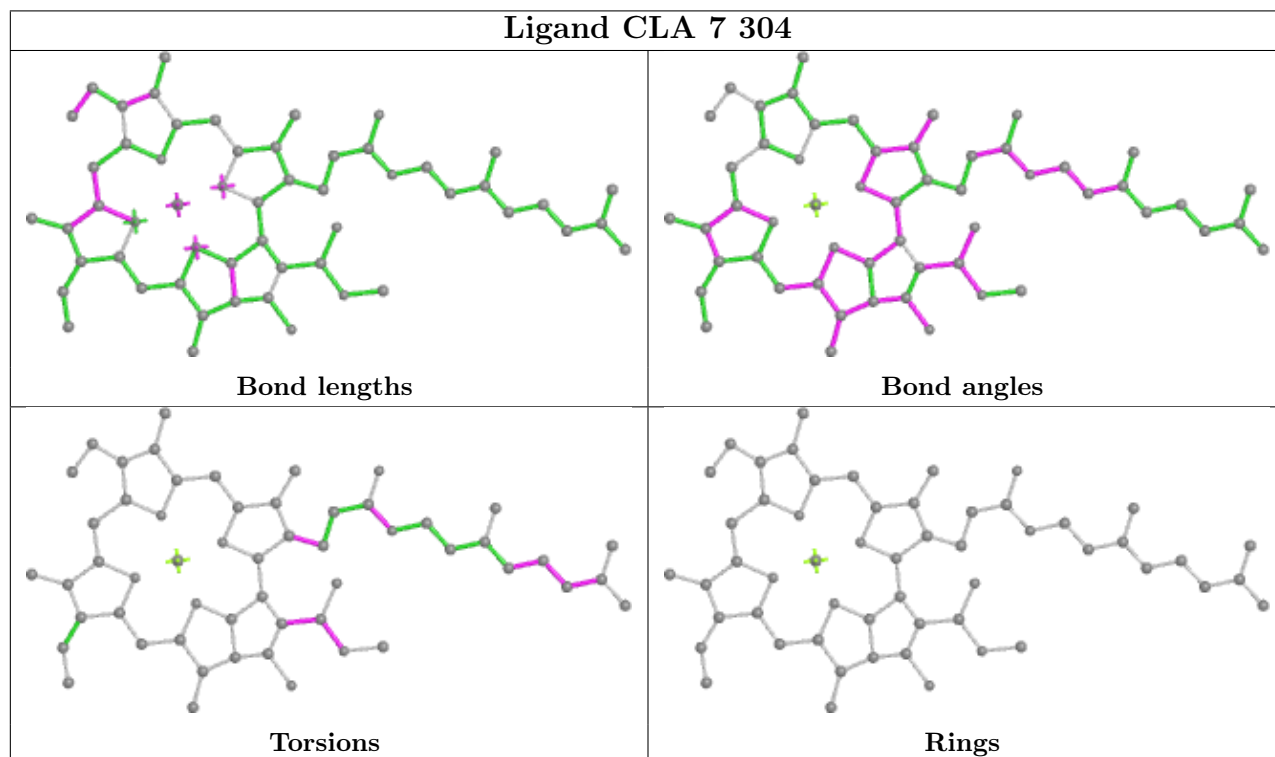




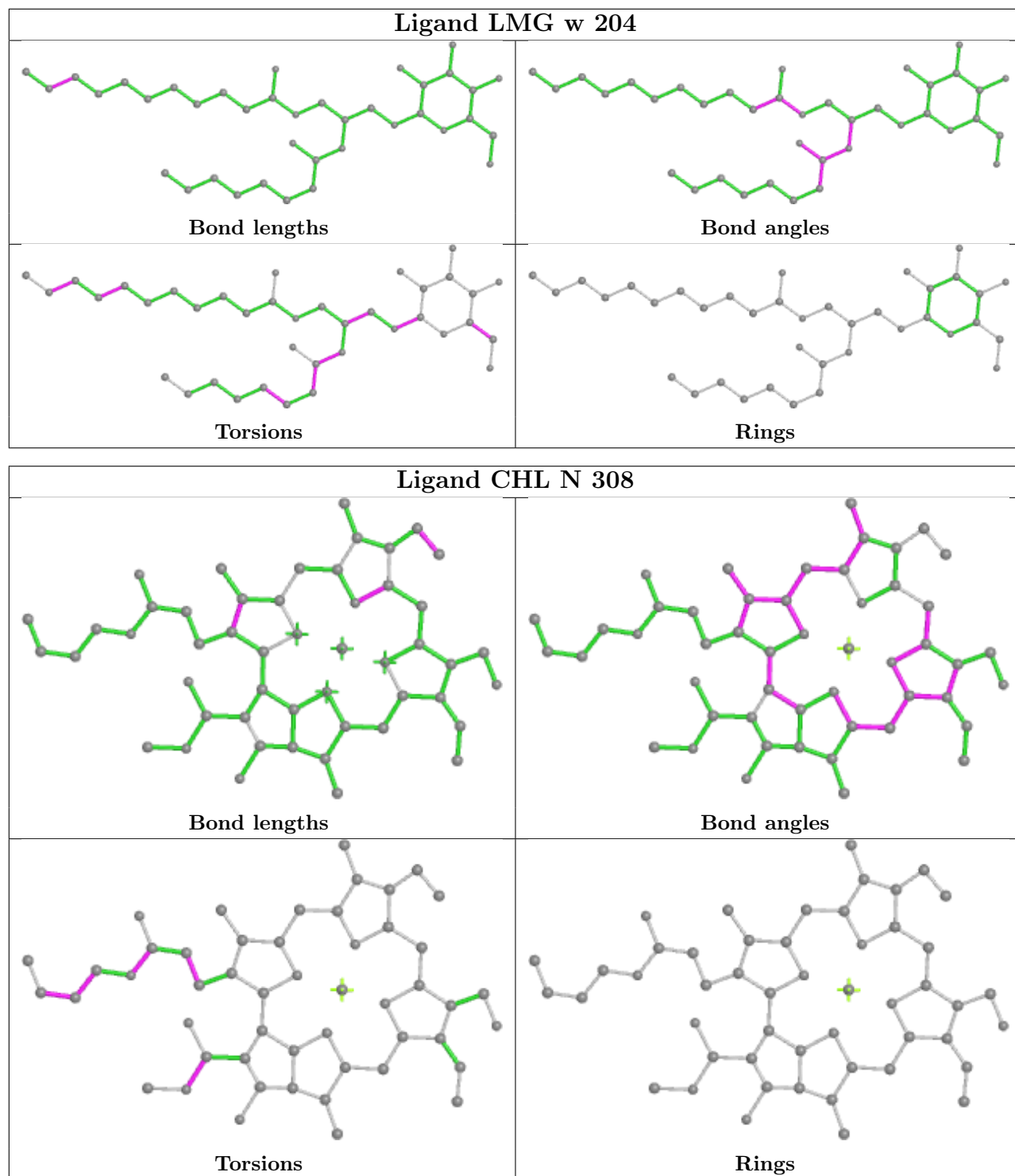
## Ligand LHG g 319

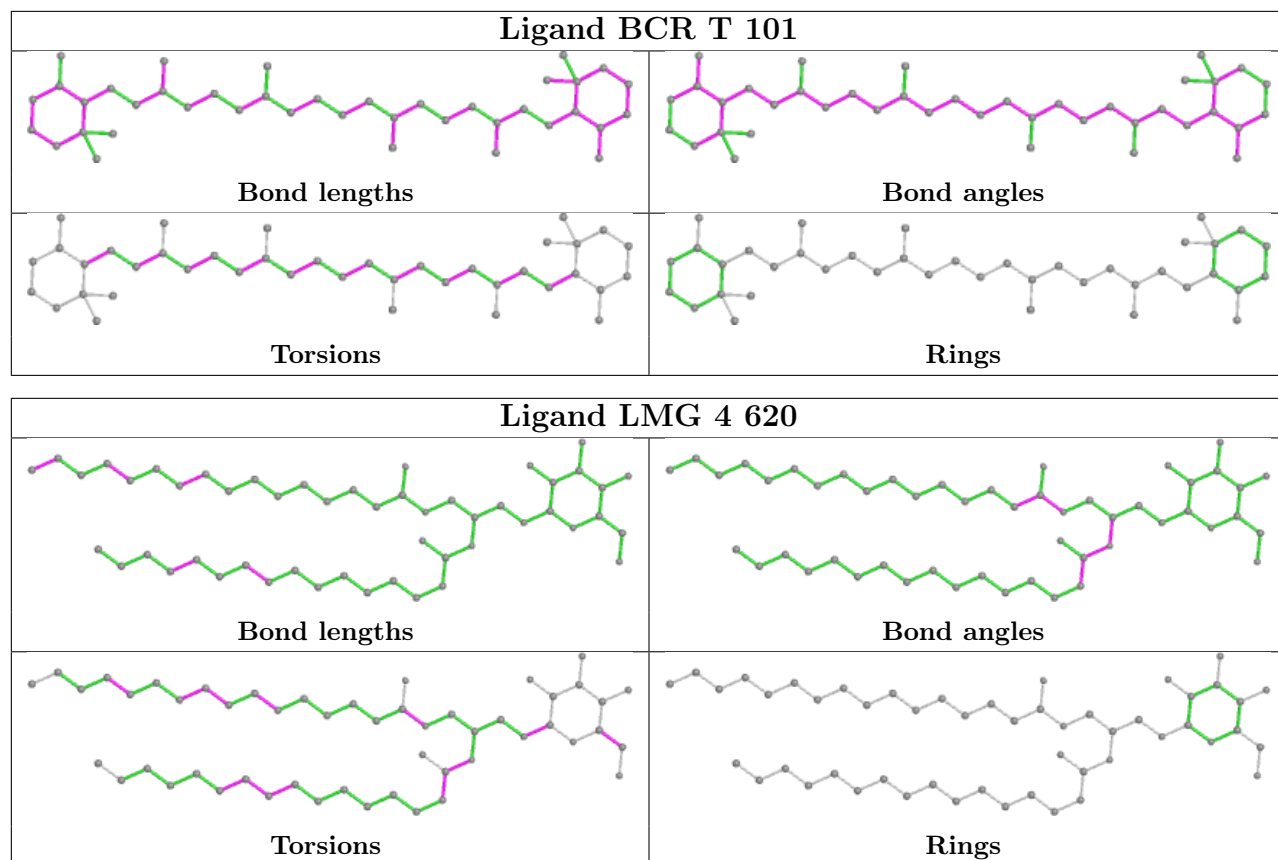


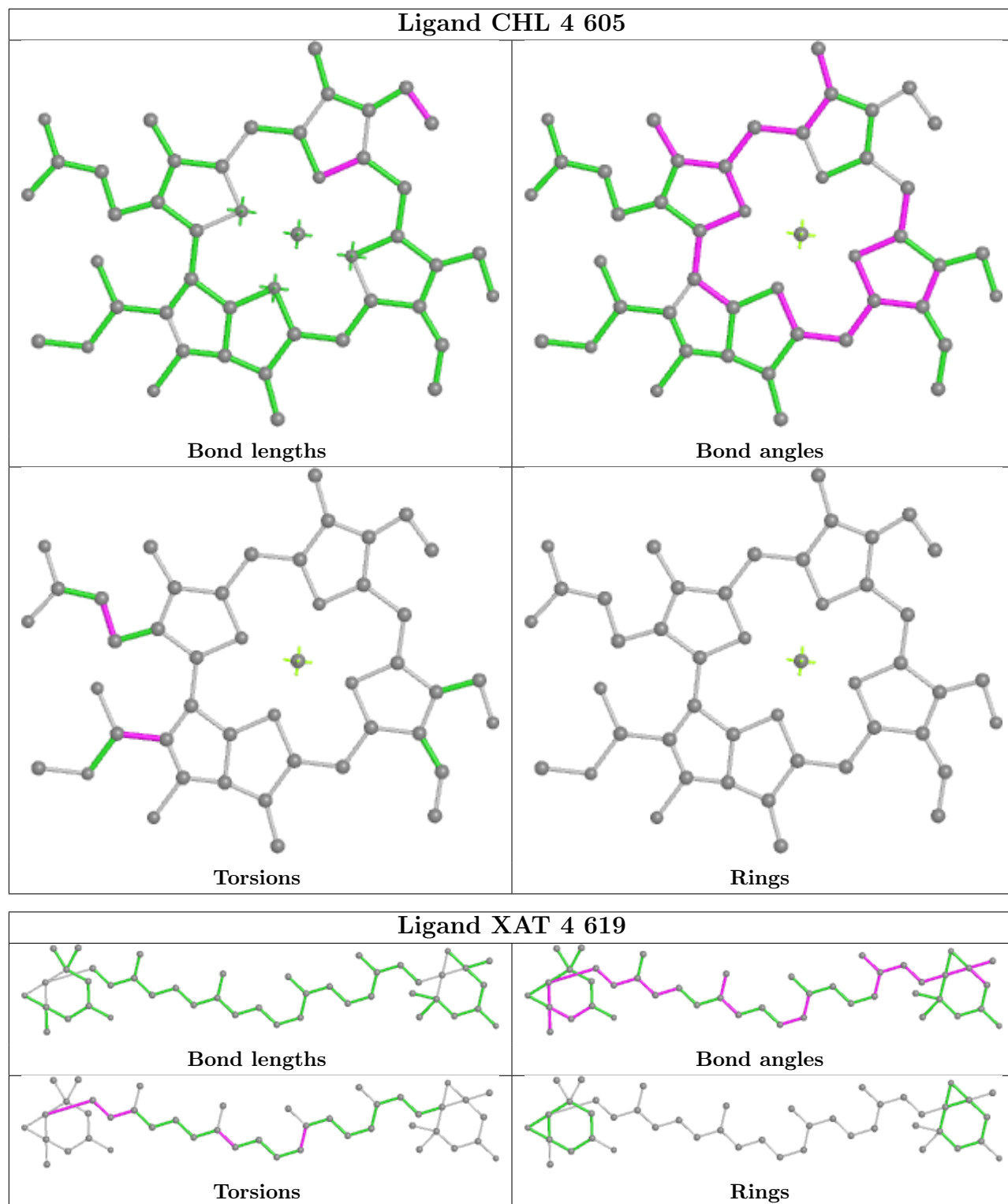
## Ligand CLA 7 304

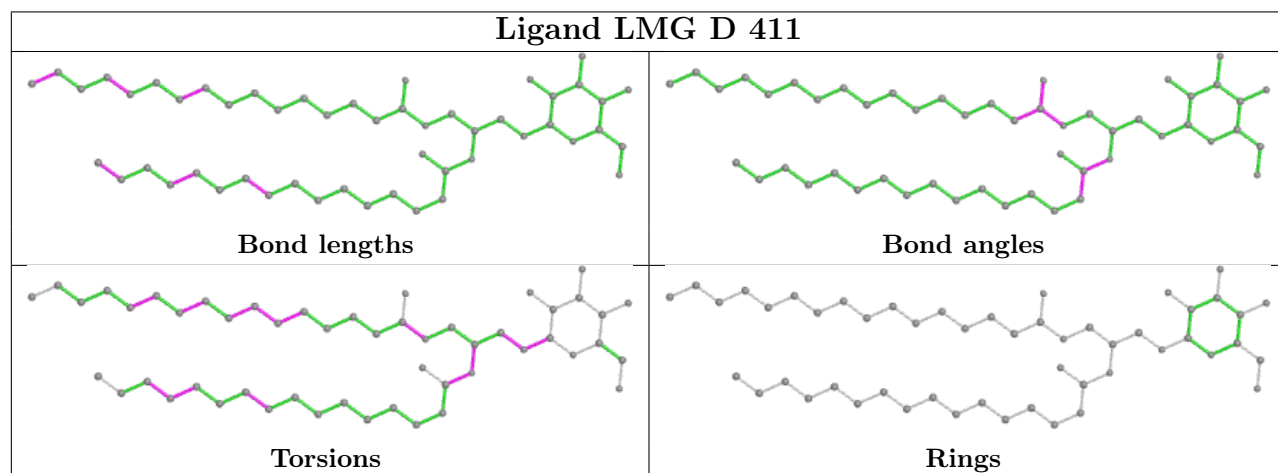
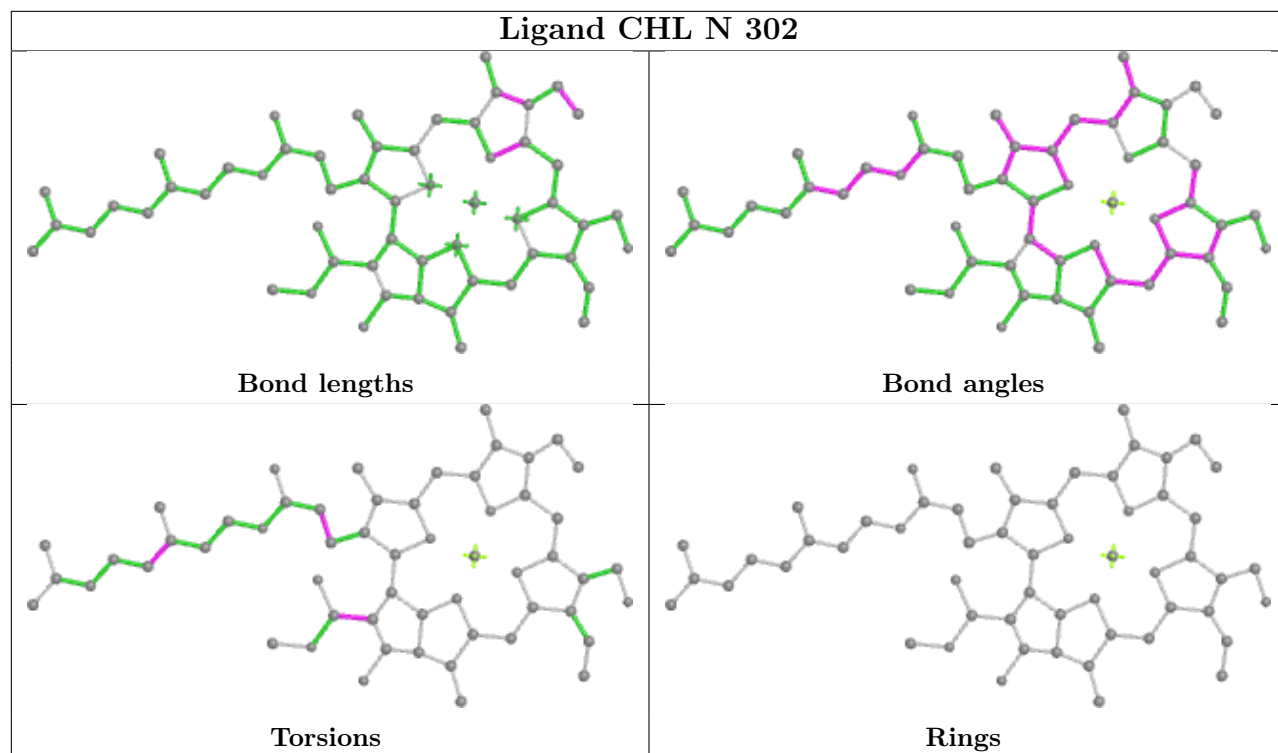


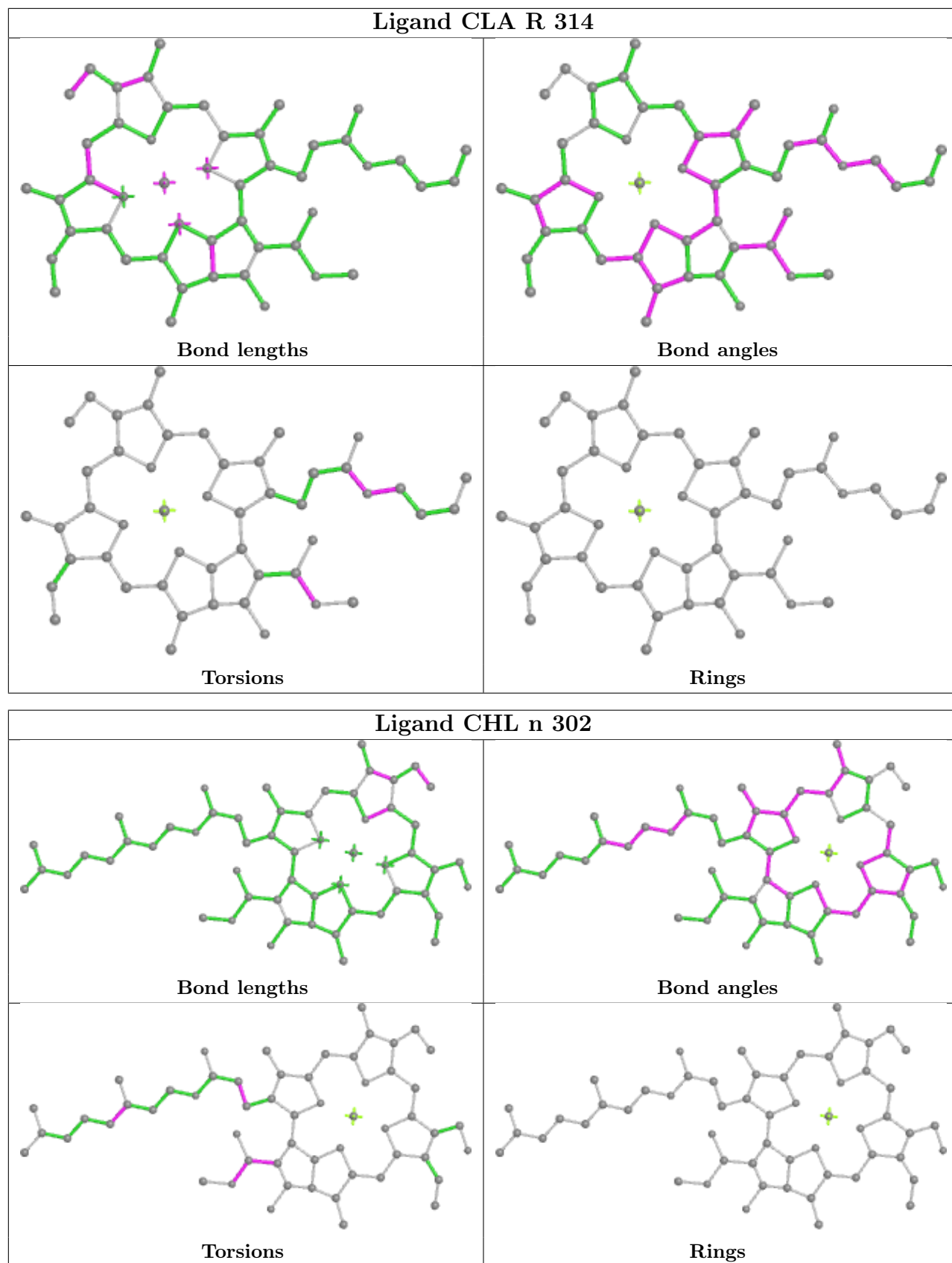


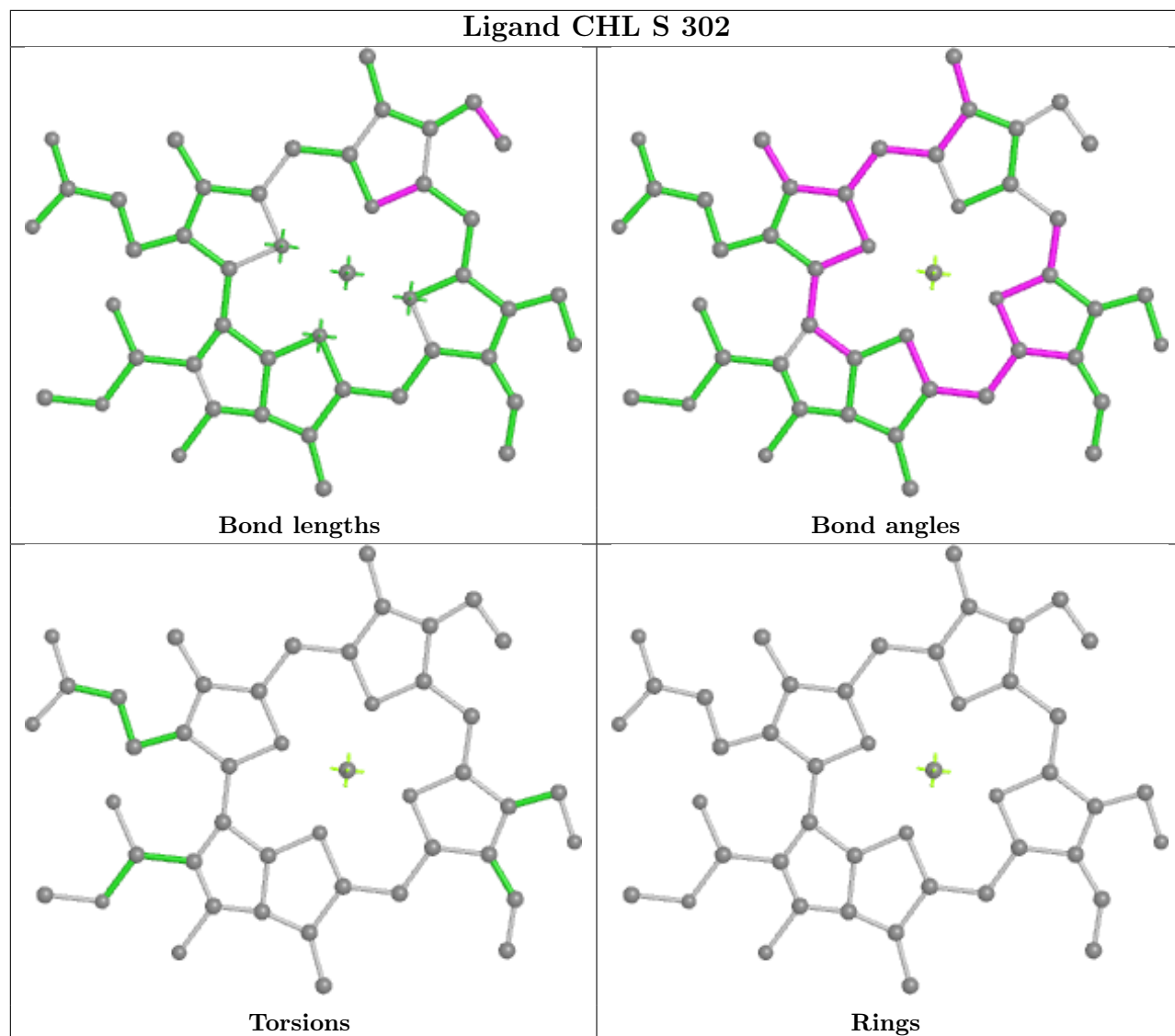


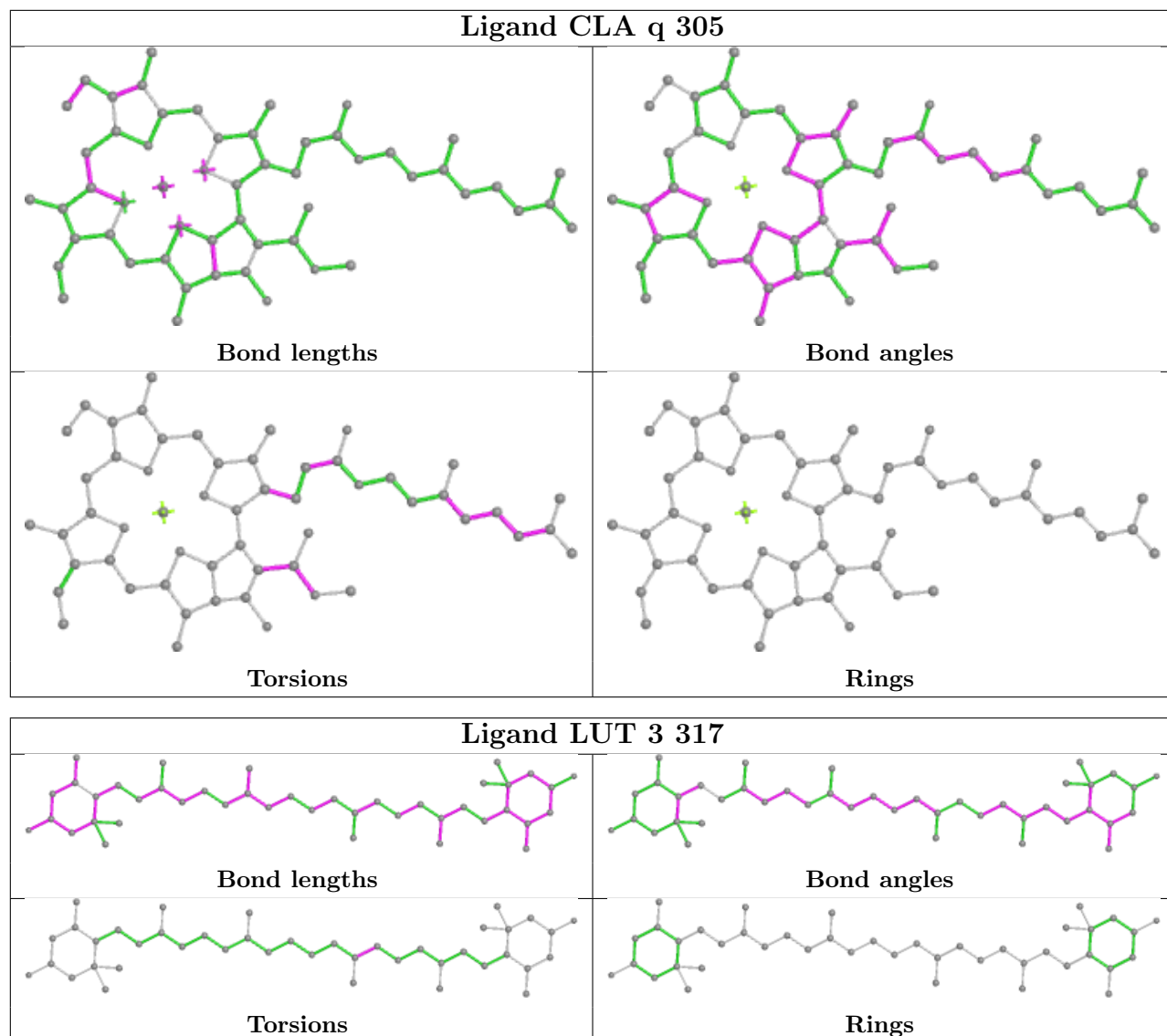


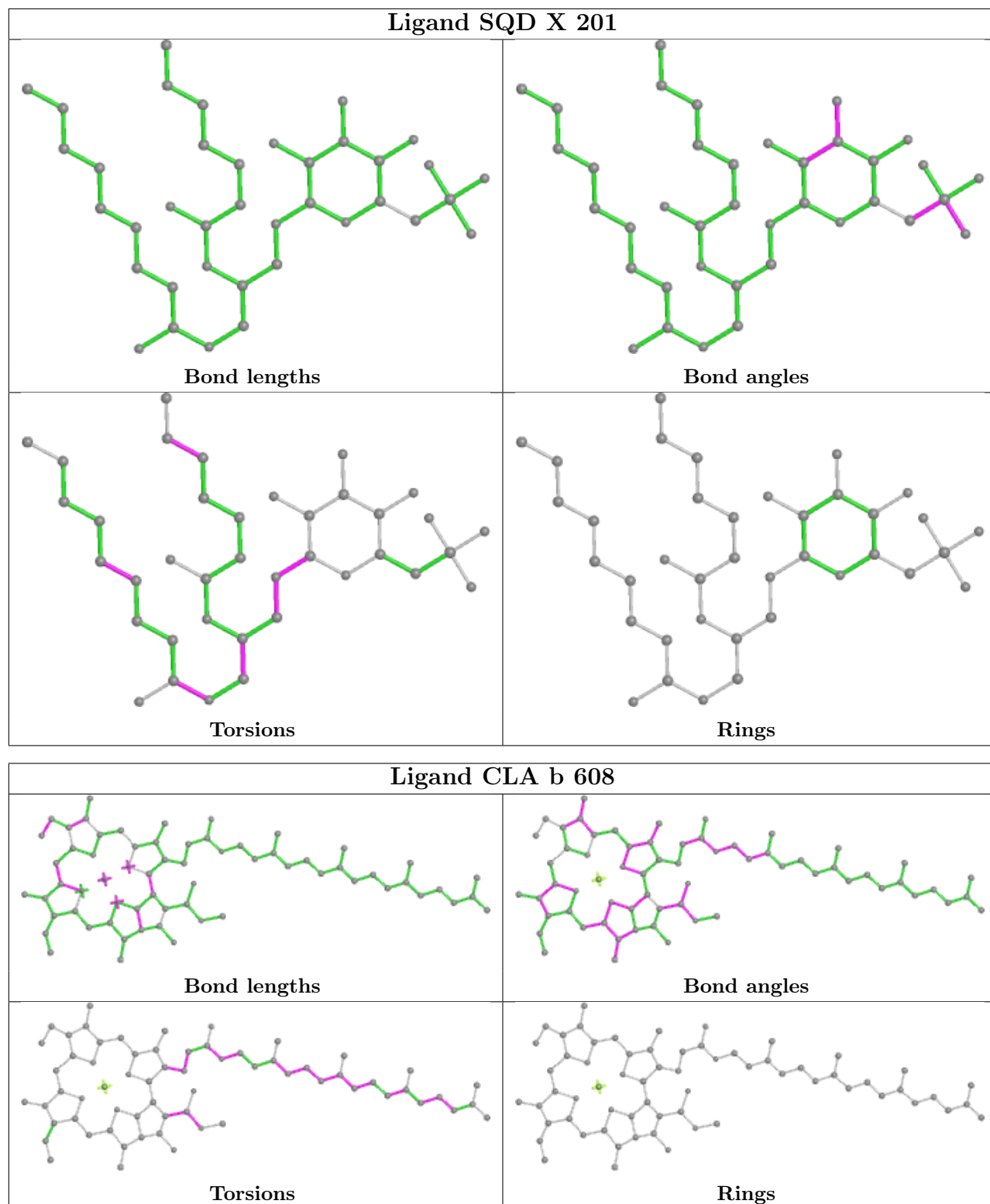




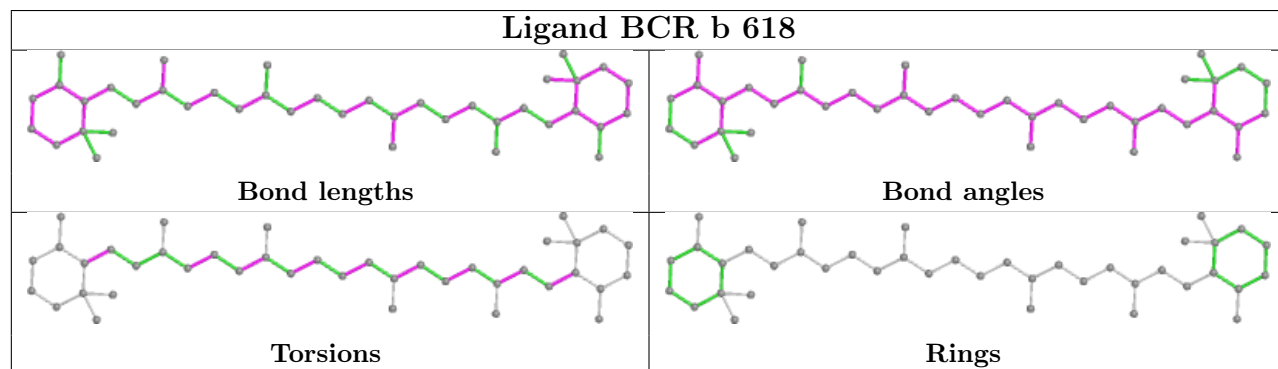
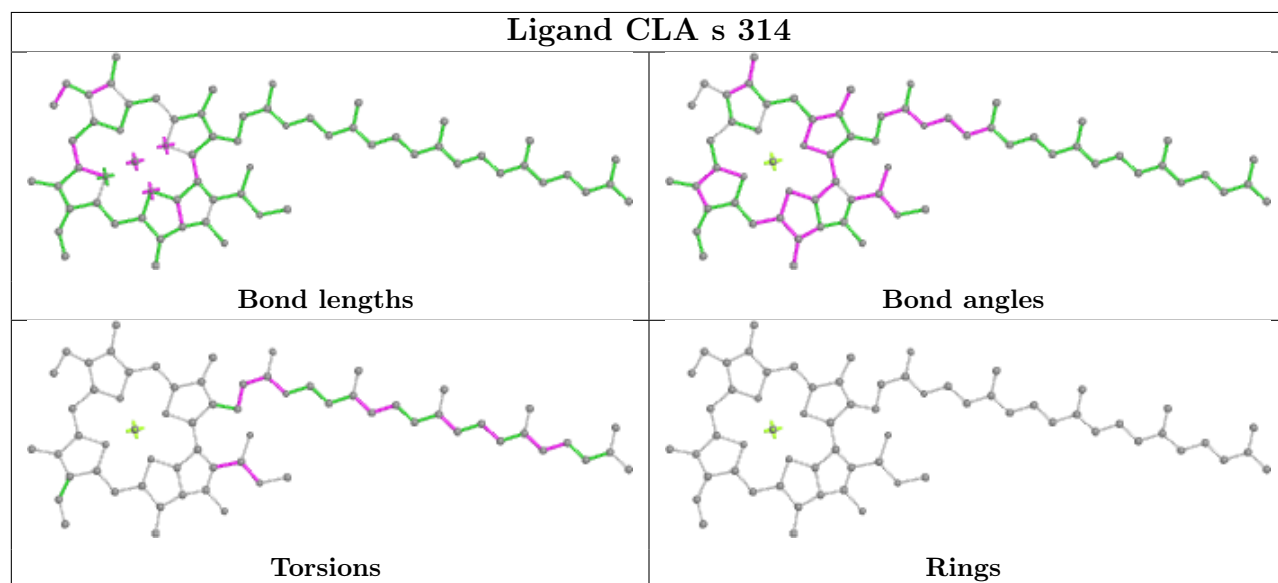
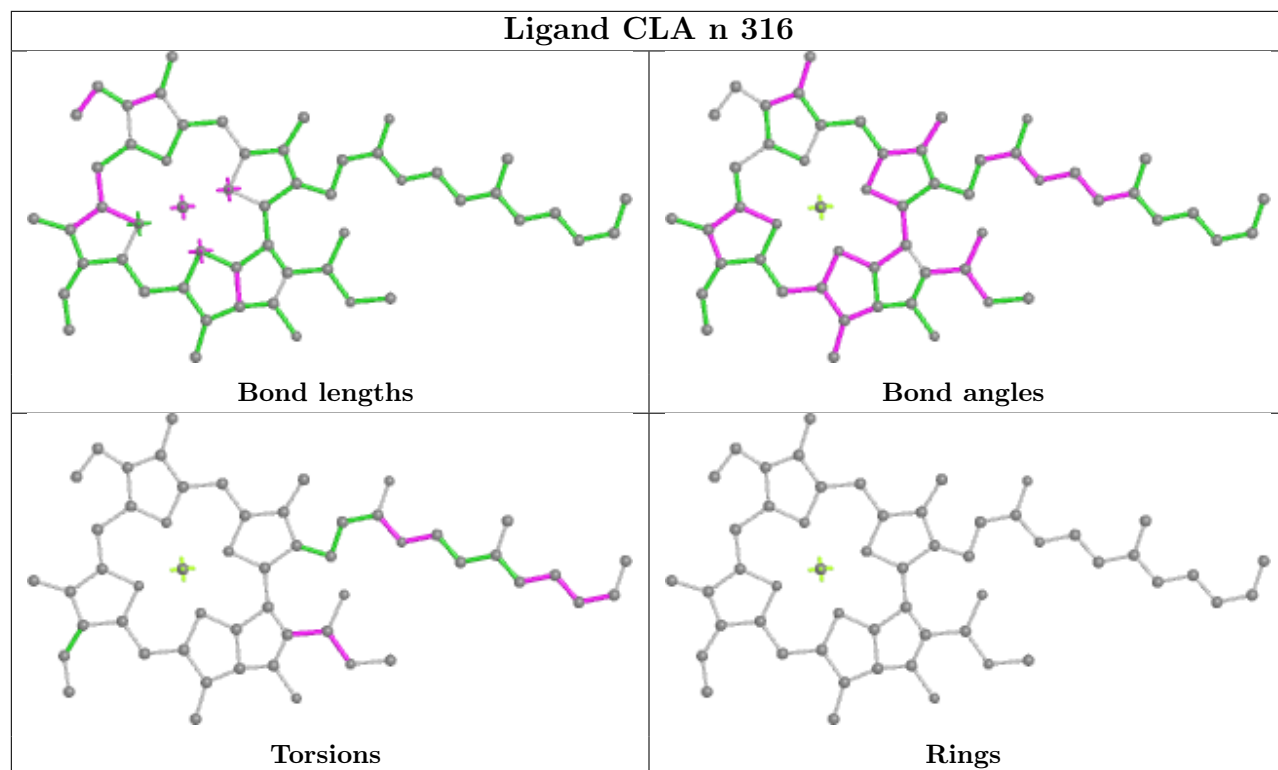


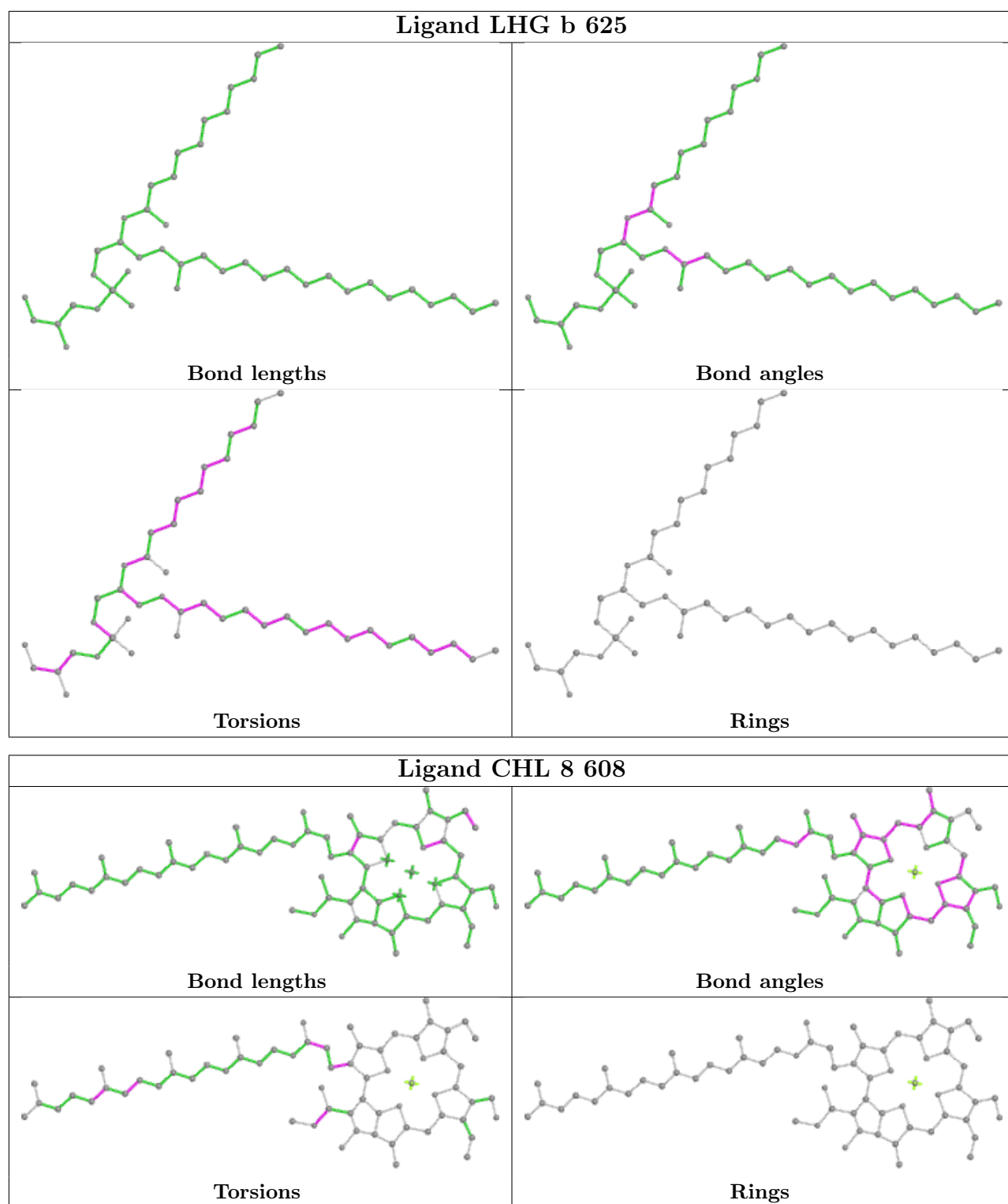


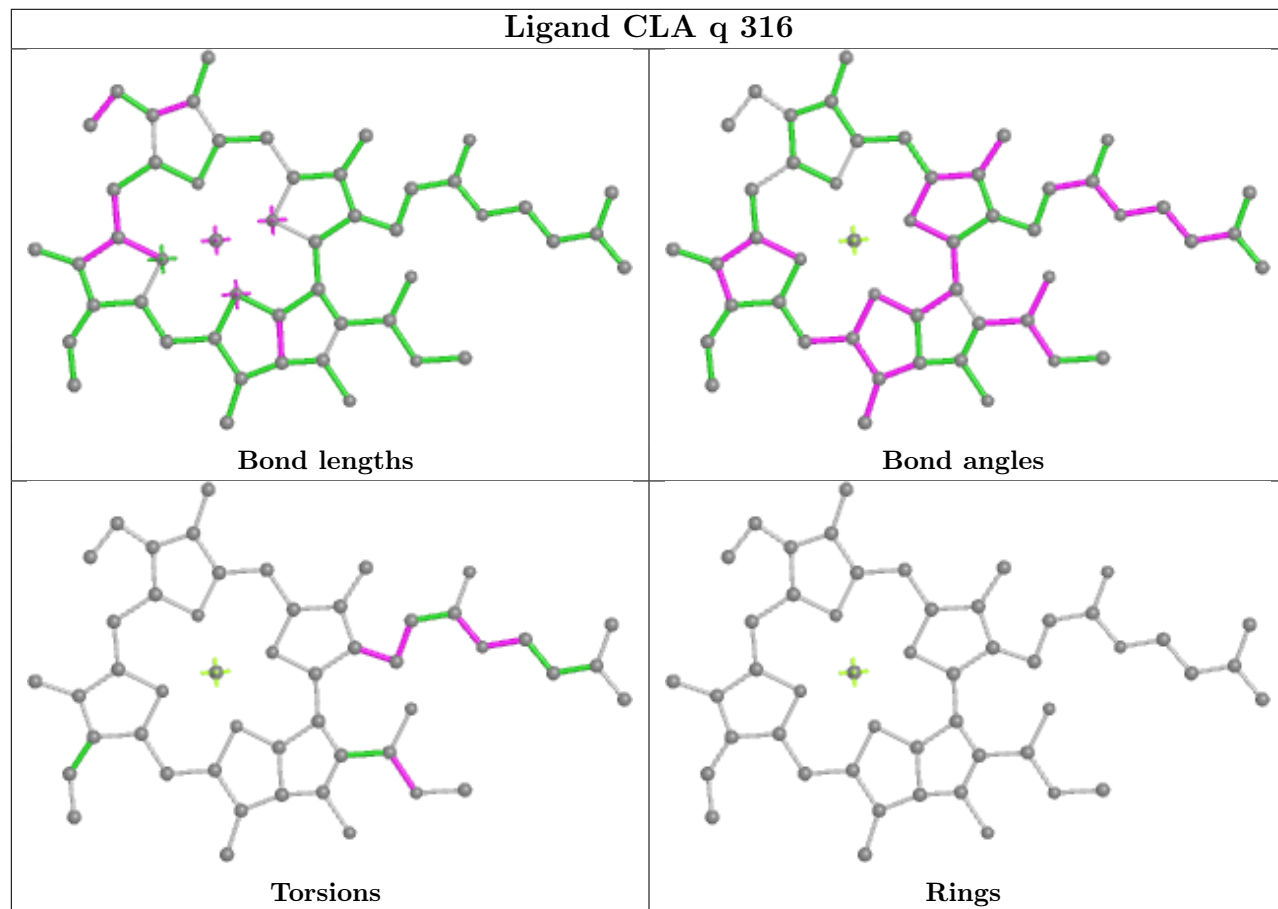
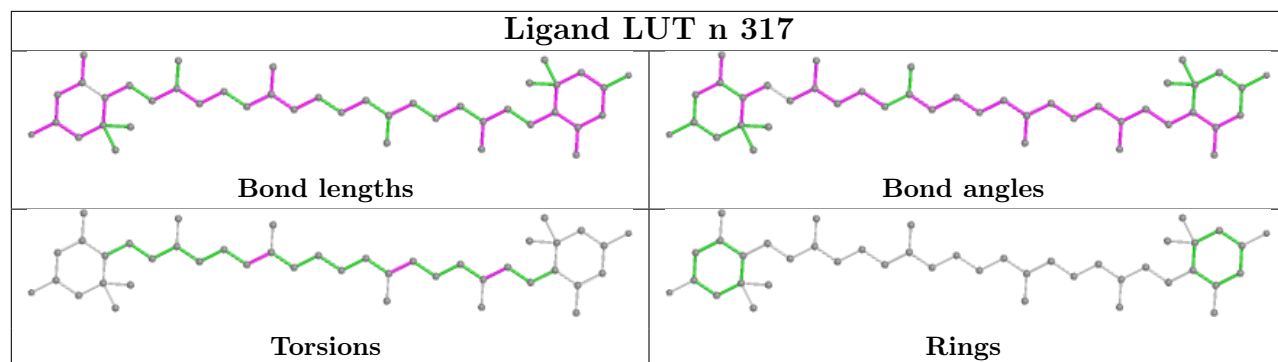


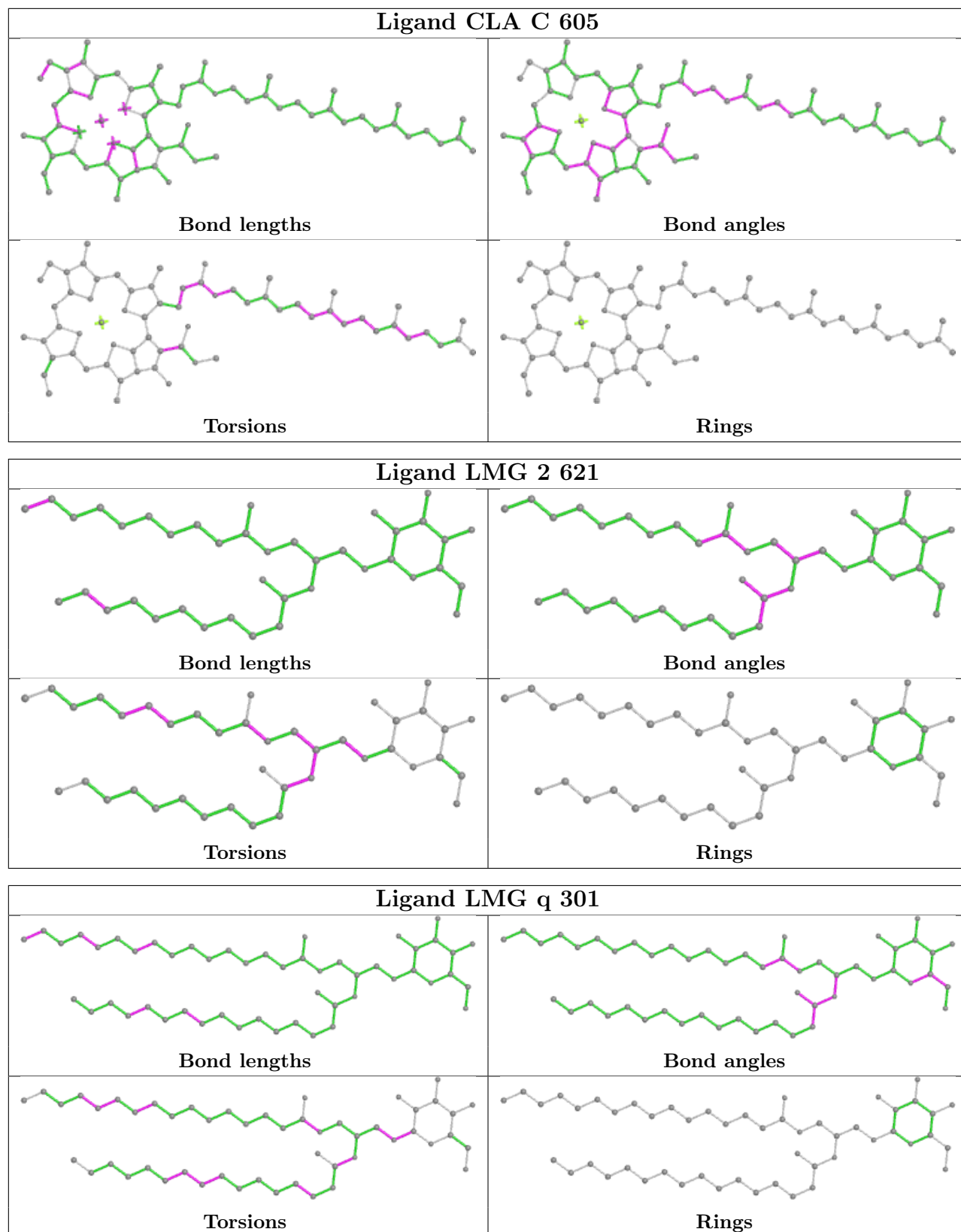


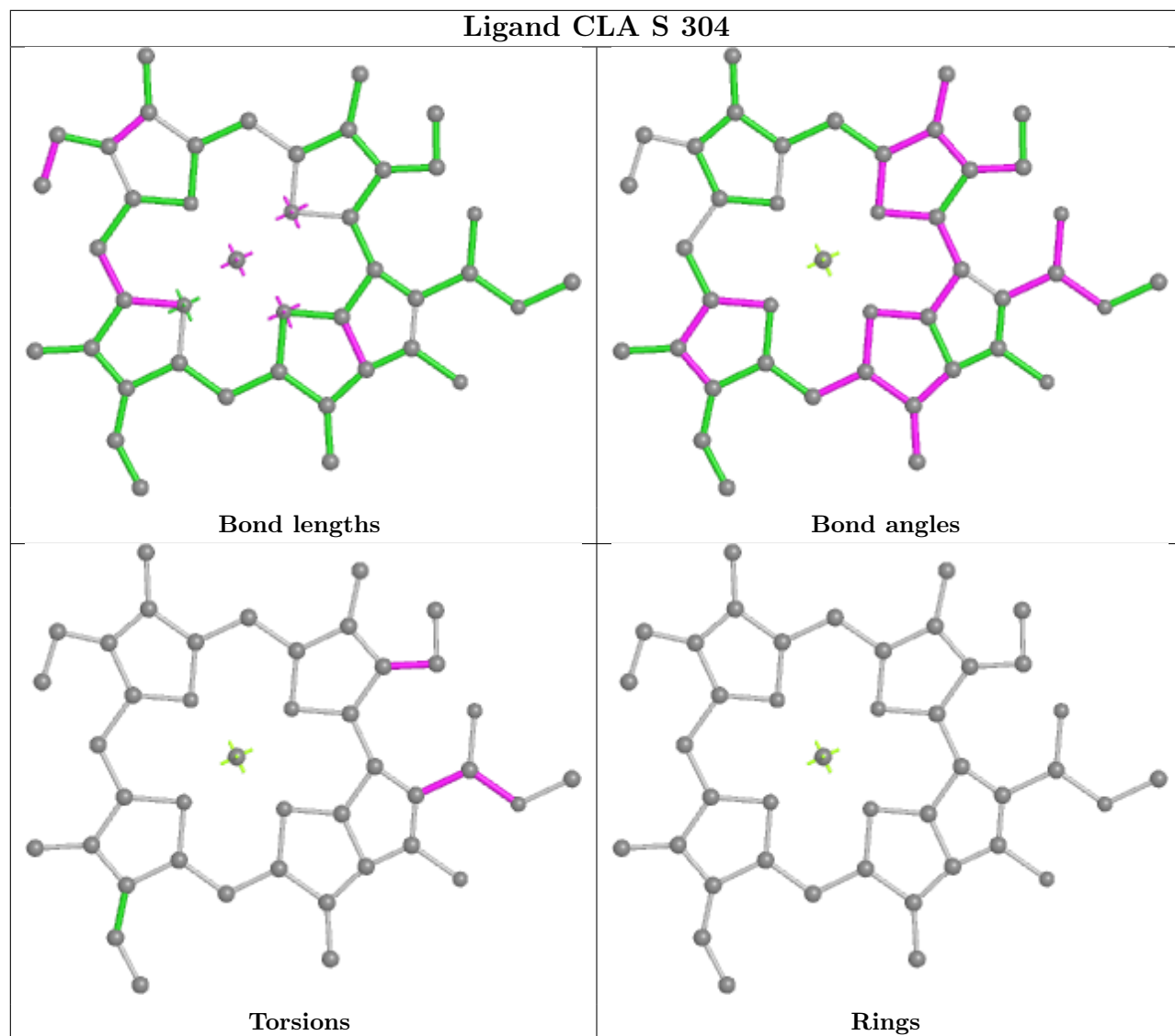


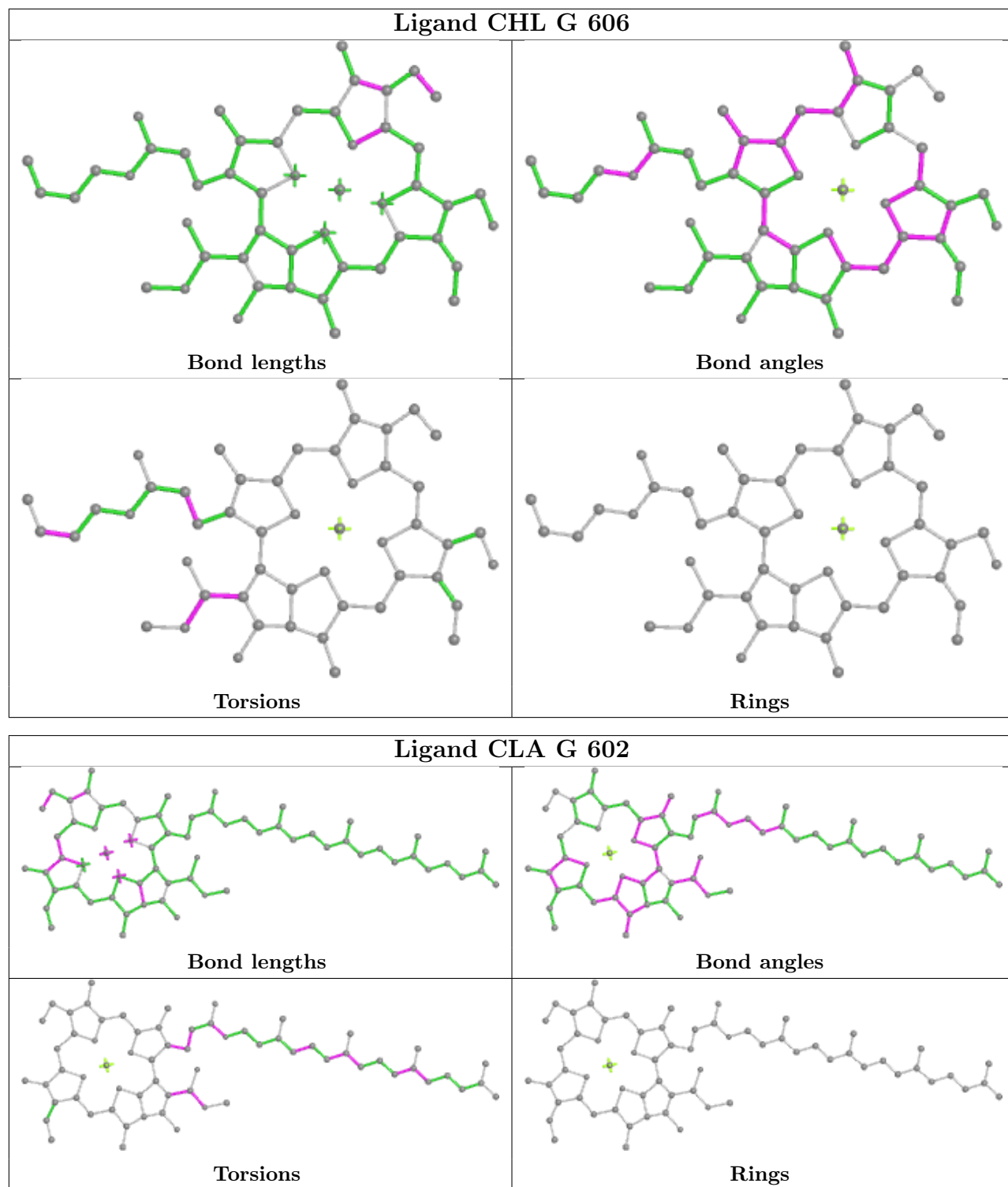


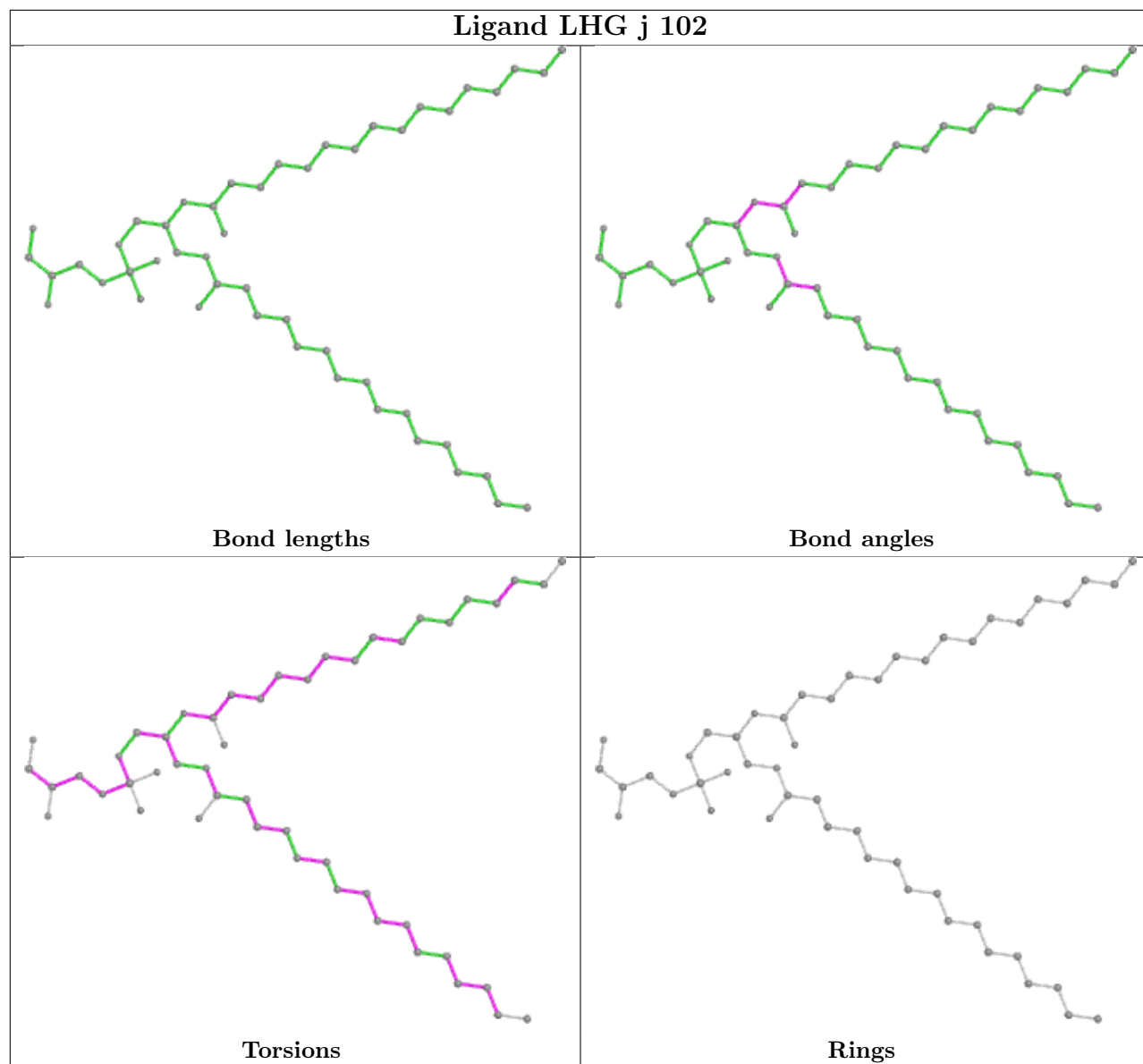


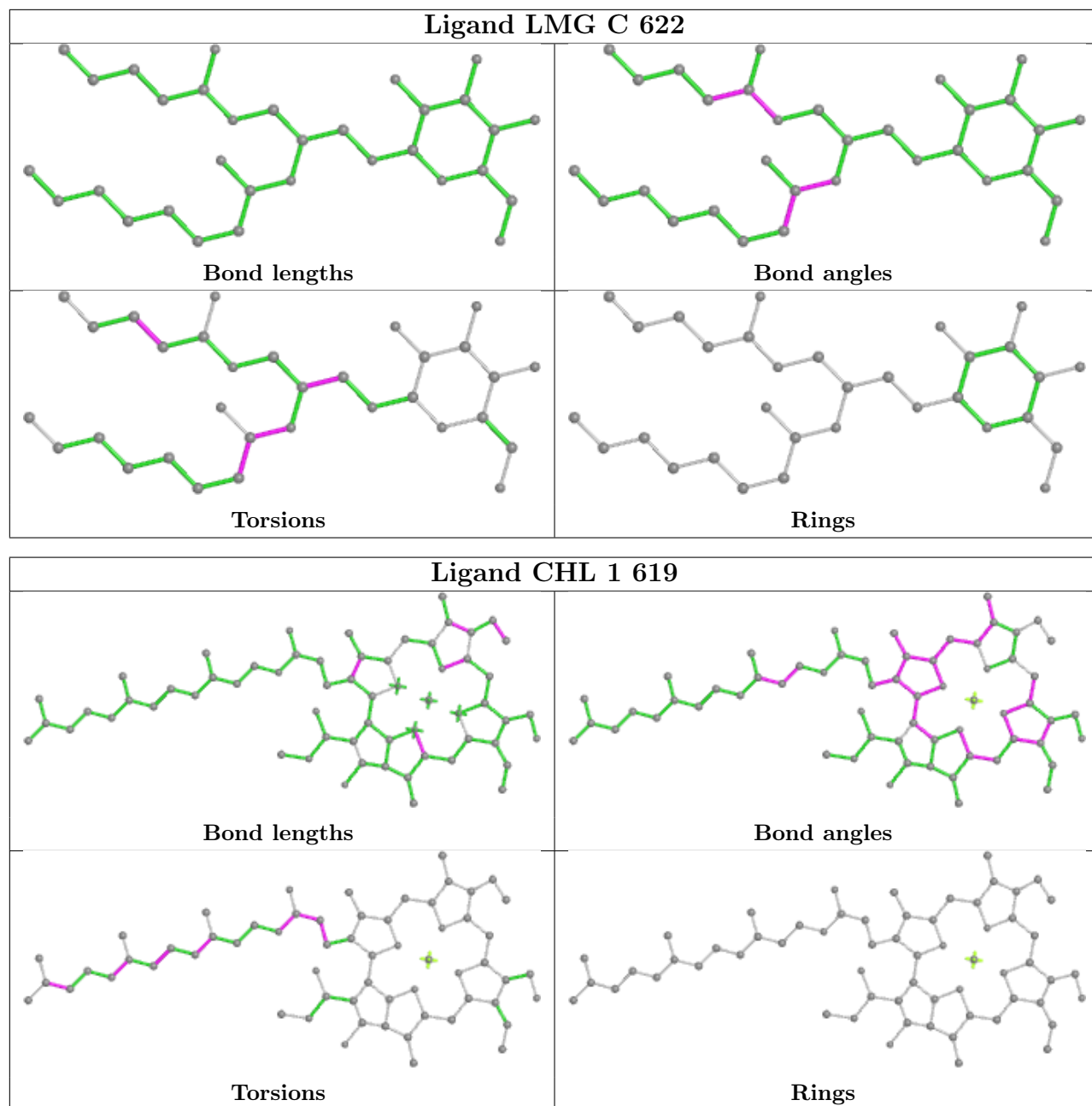




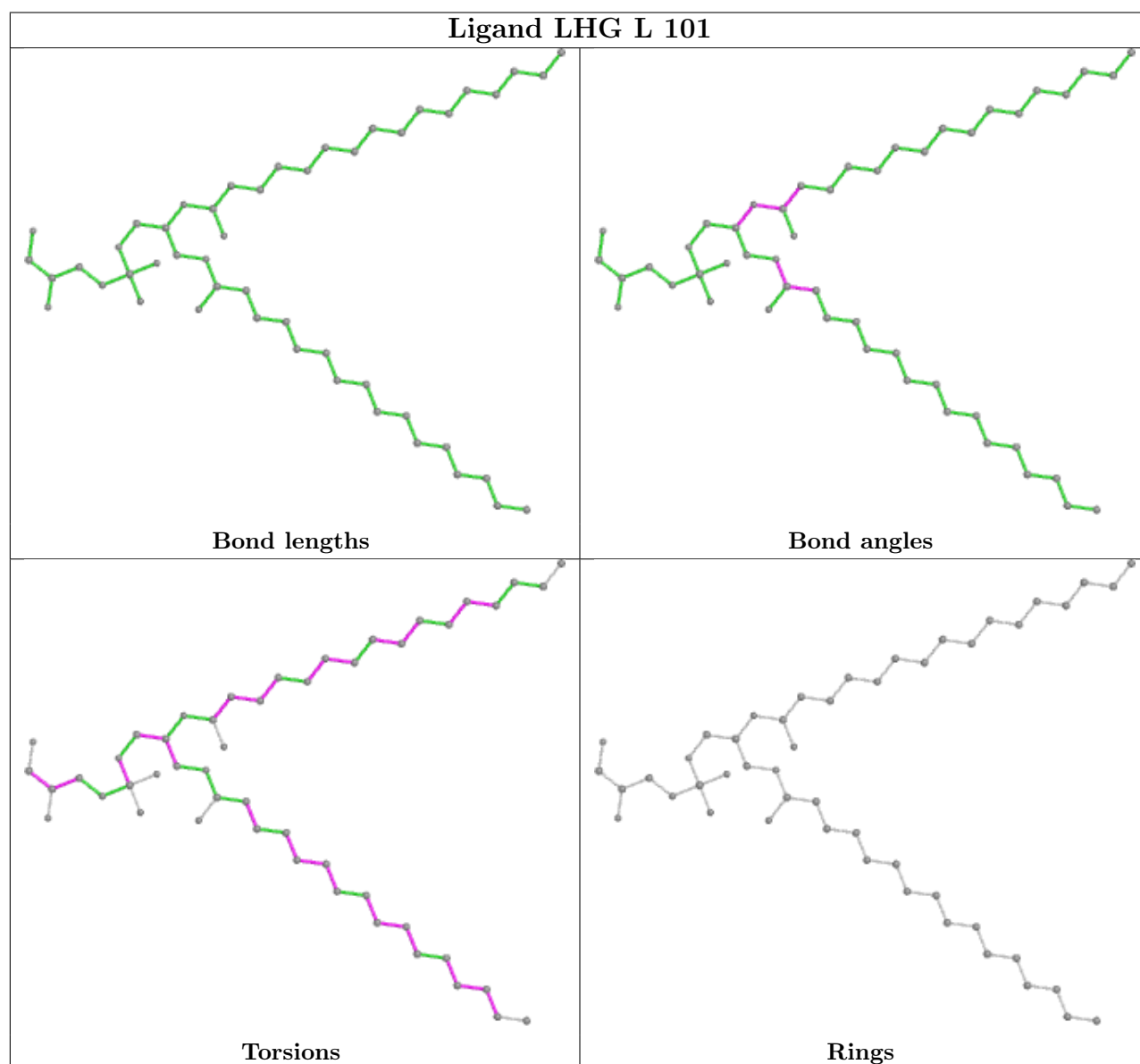
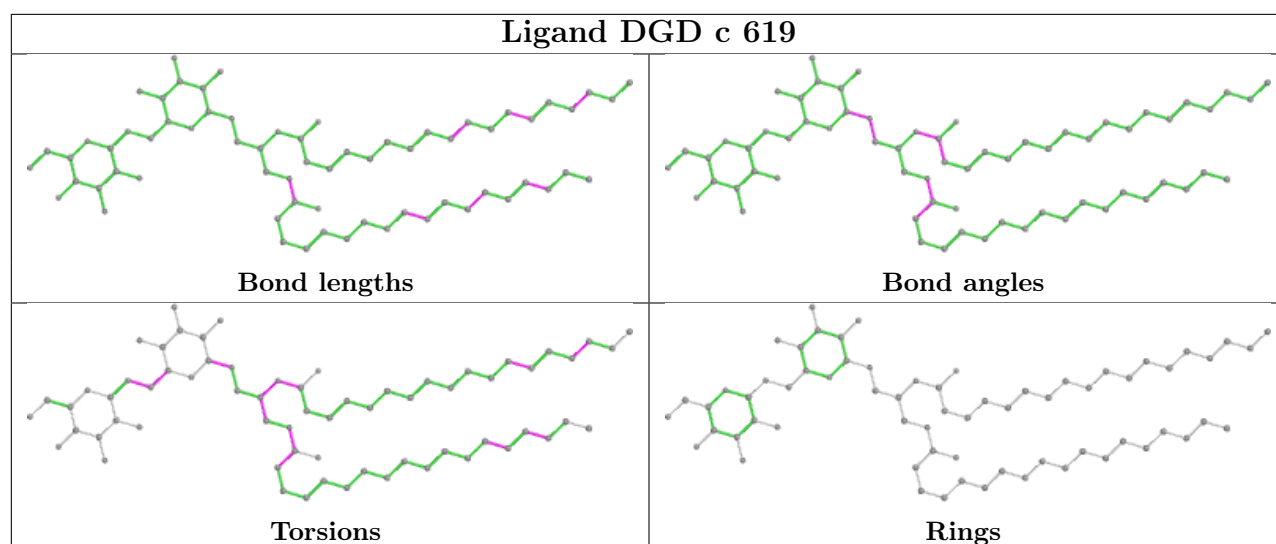


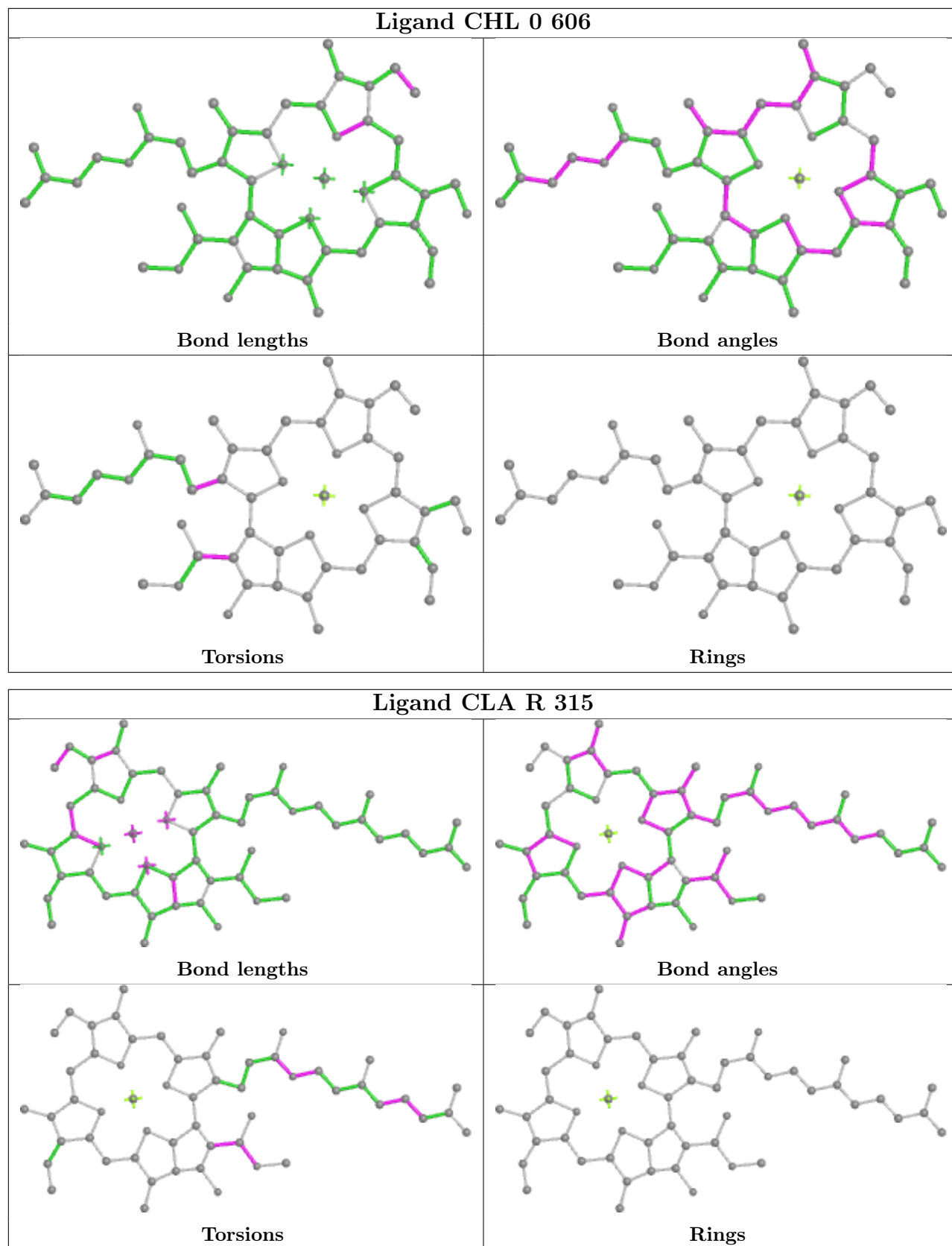


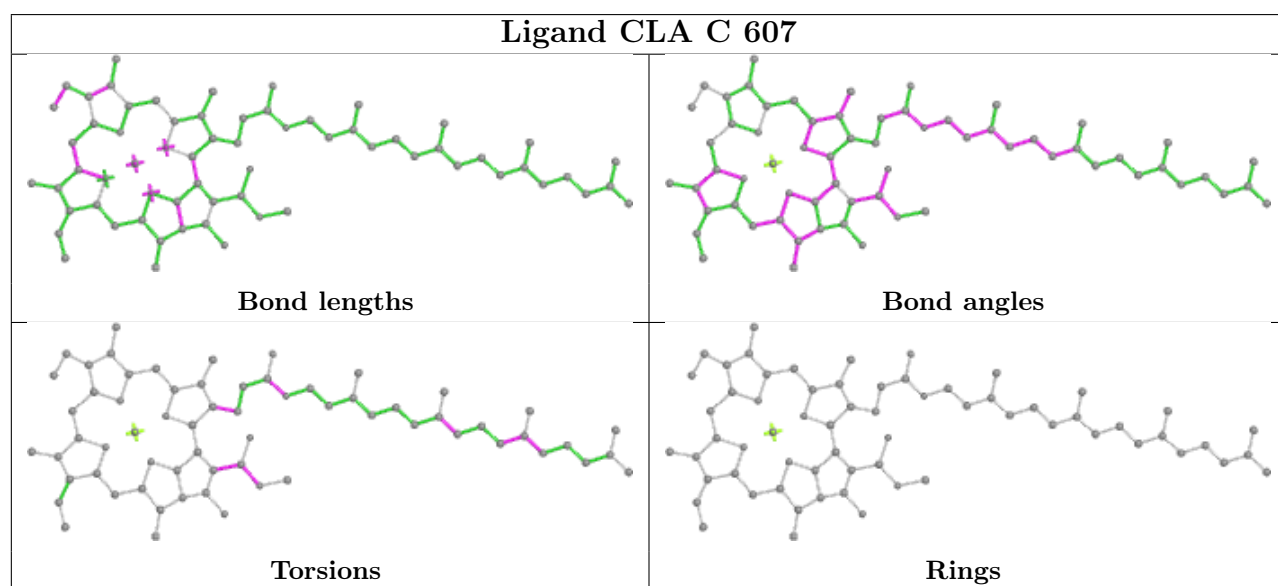
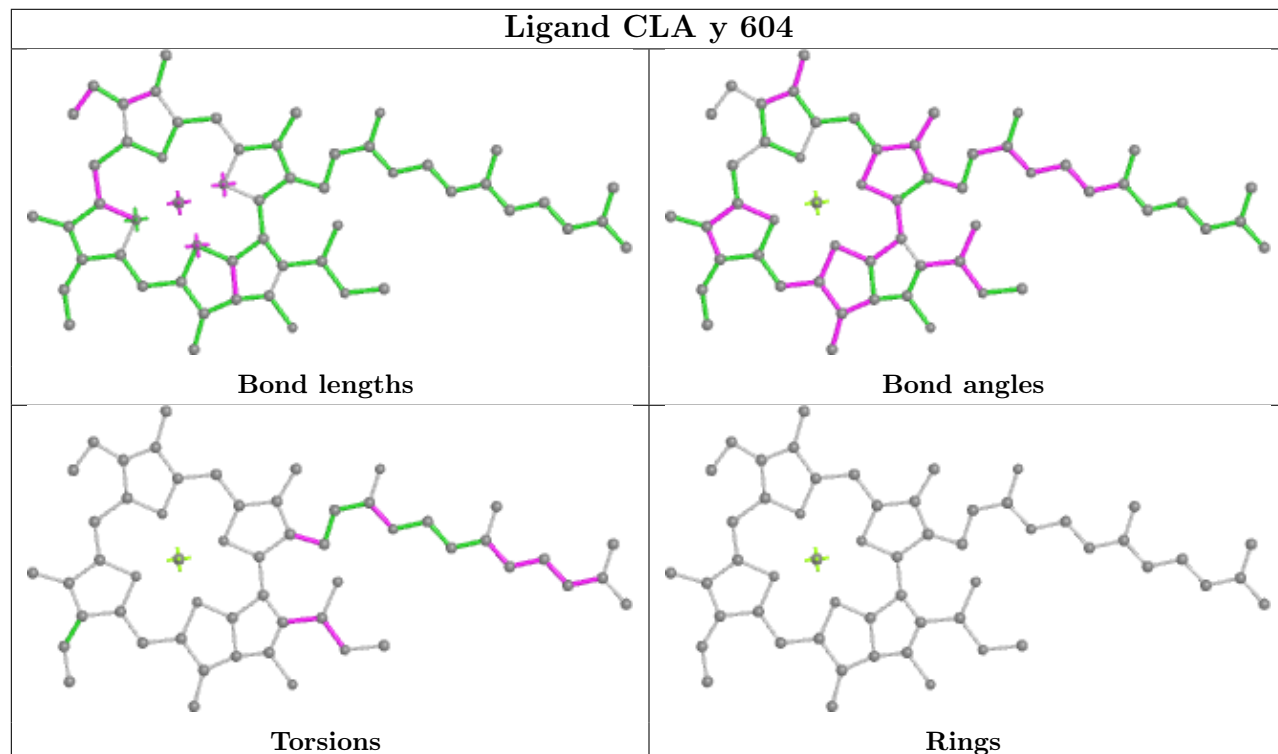
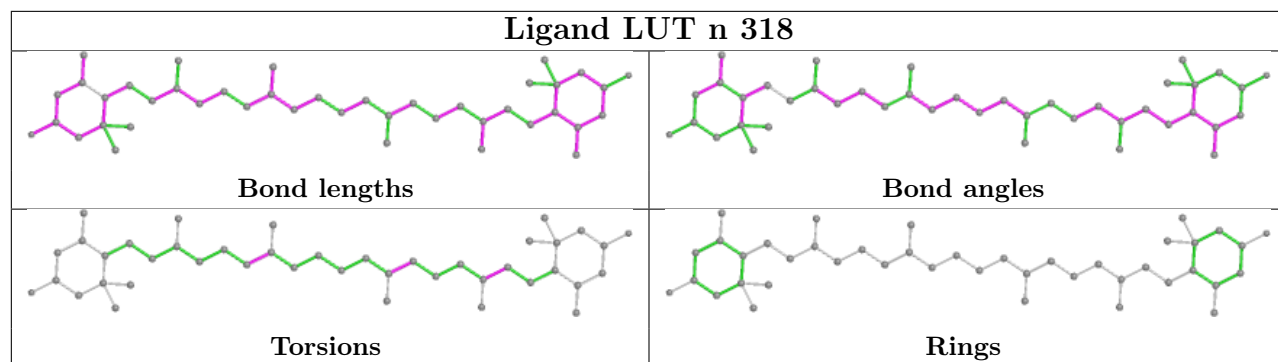


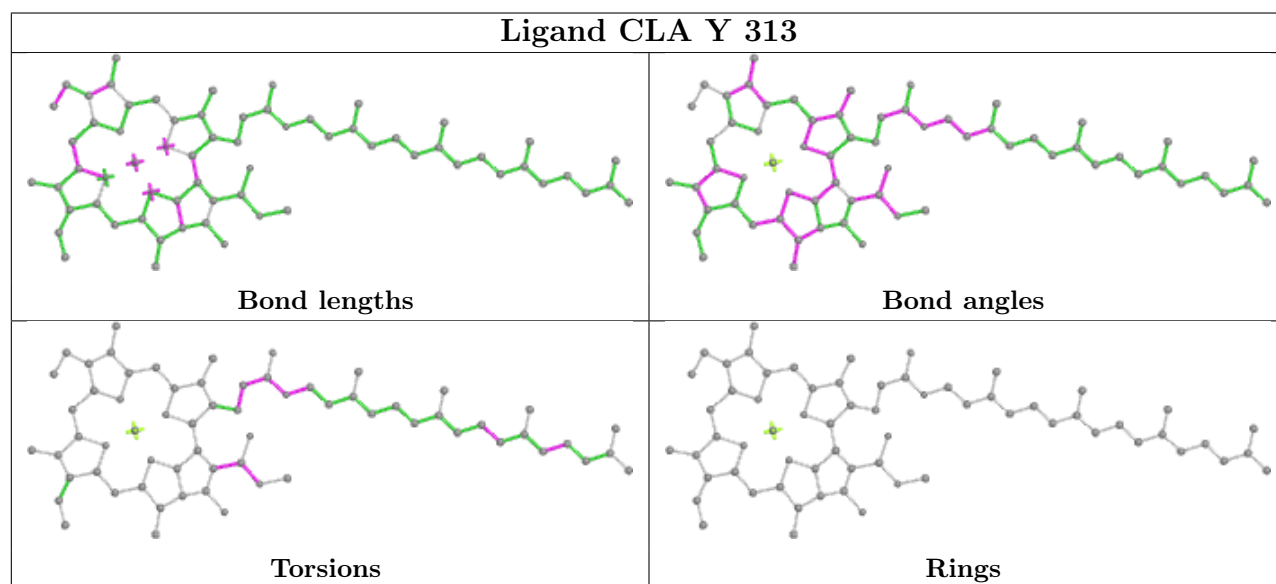
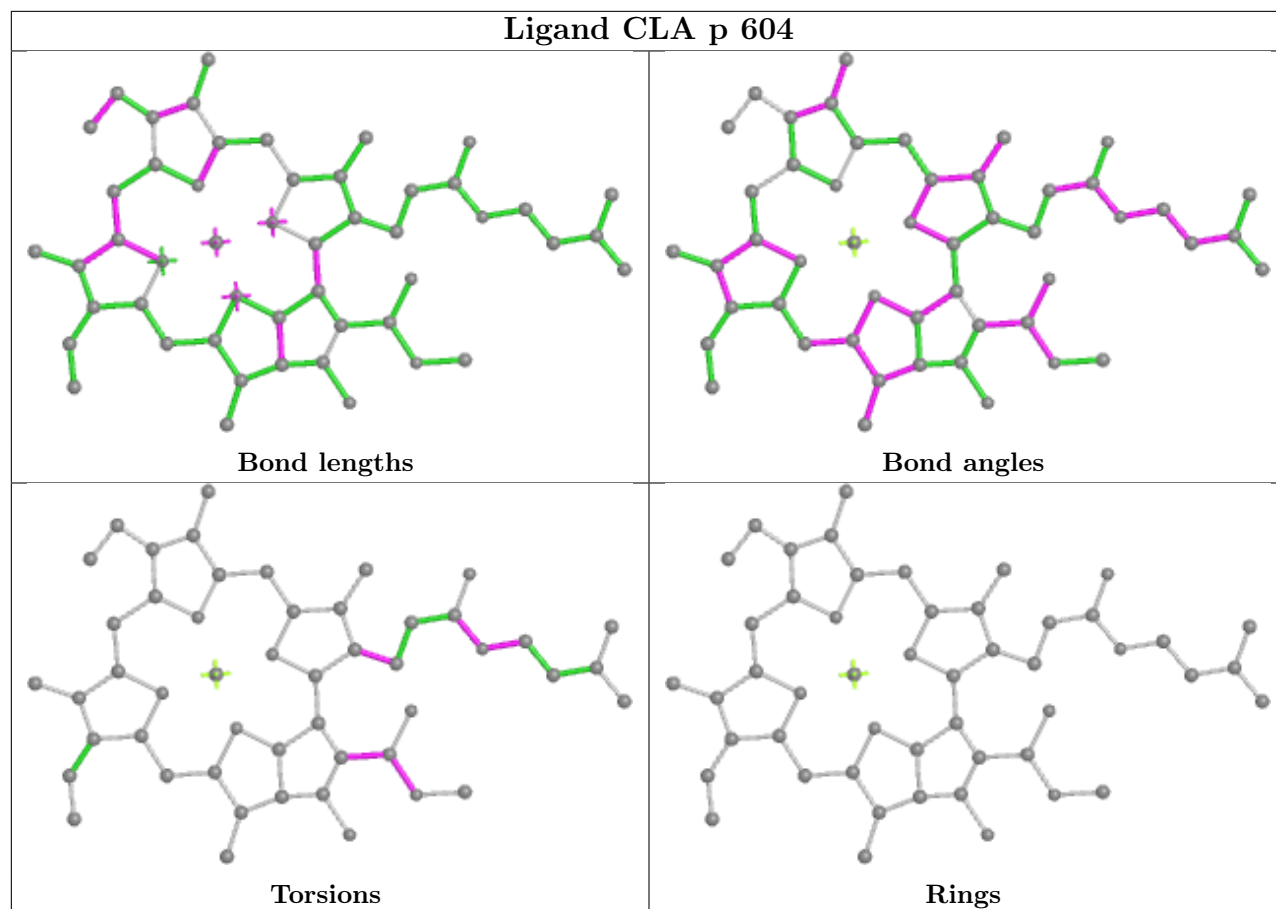


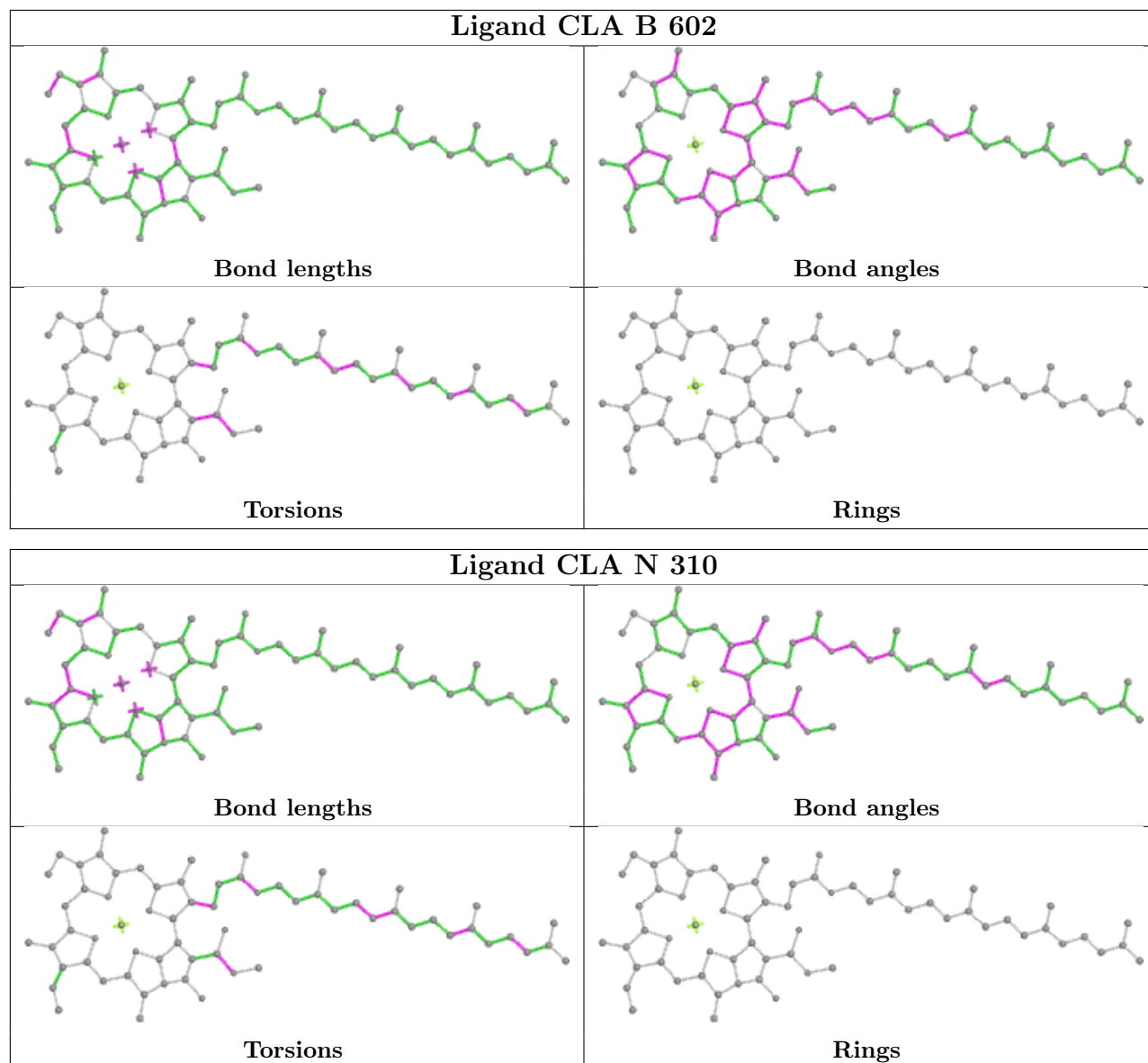












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

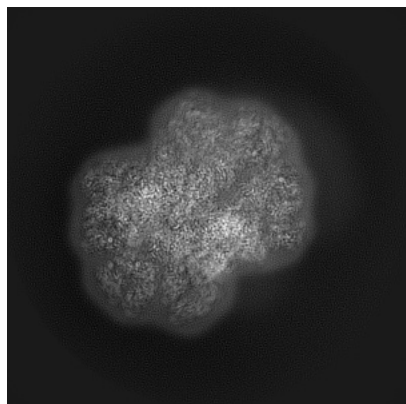
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15973. These allow visual inspection of the internal detail of the map and identification of artifacts.

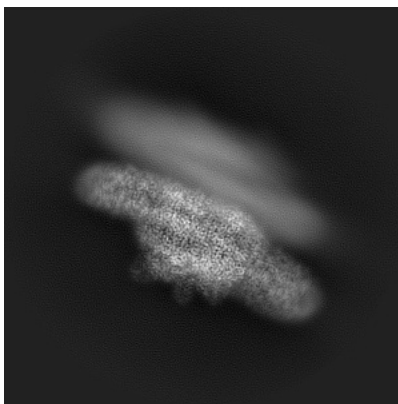
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

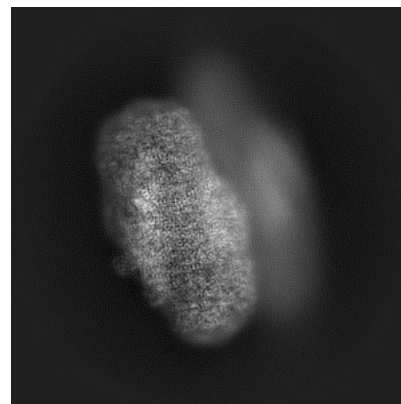
#### 6.1.1 Primary map



X

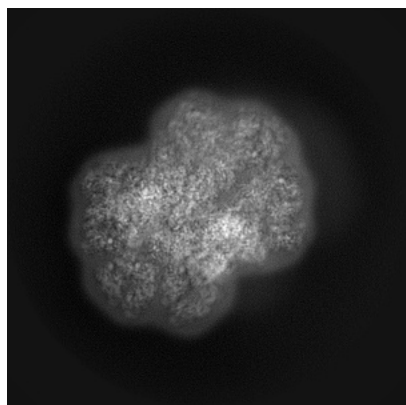


Y

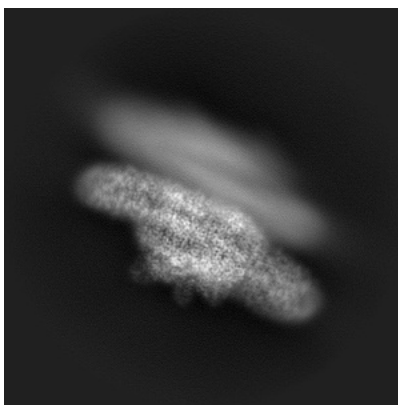


Z

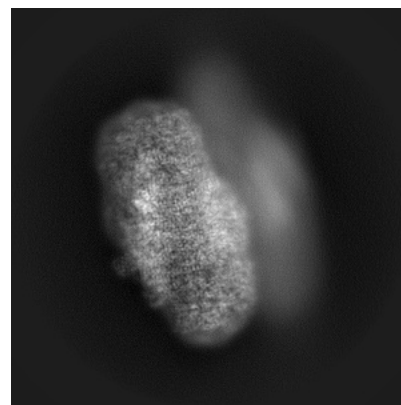
#### 6.1.2 Raw map



X



Y

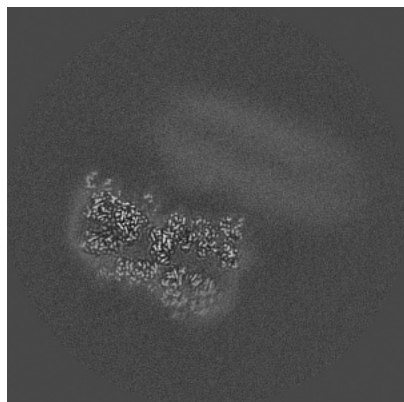


Z

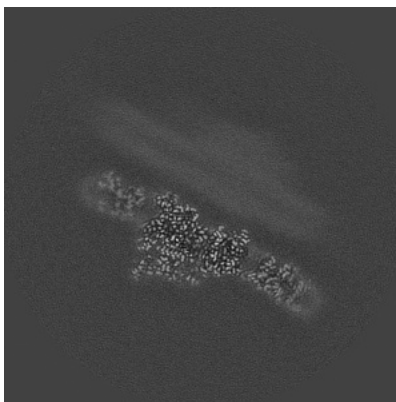
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

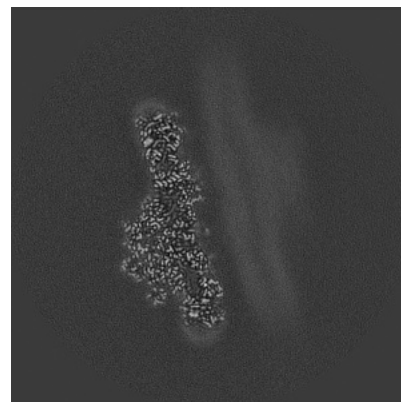
### 6.2.1 Primary map



X Index: 250

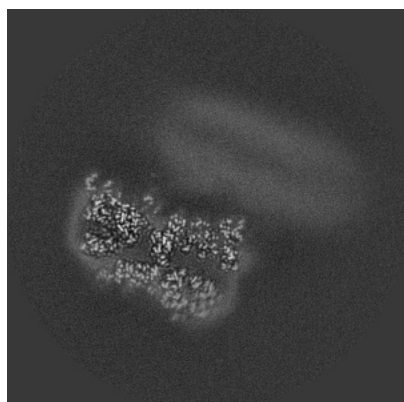


Y Index: 250

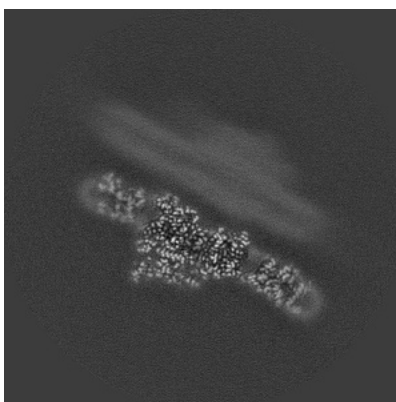


Z Index: 250

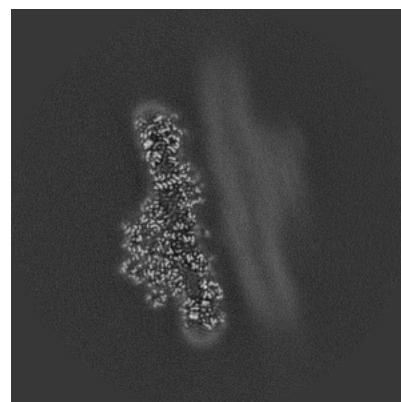
### 6.2.2 Raw map



X Index: 250



Y Index: 250

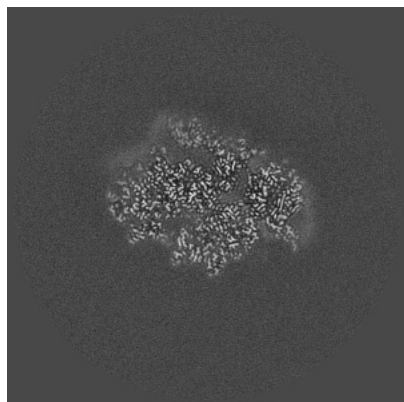


Z Index: 250

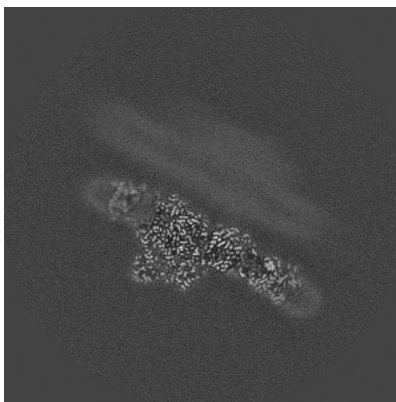
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

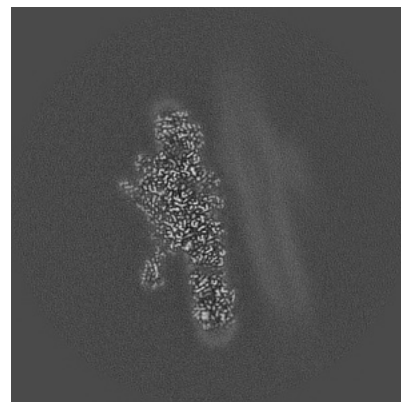
### 6.3.1 Primary map



X Index: 183

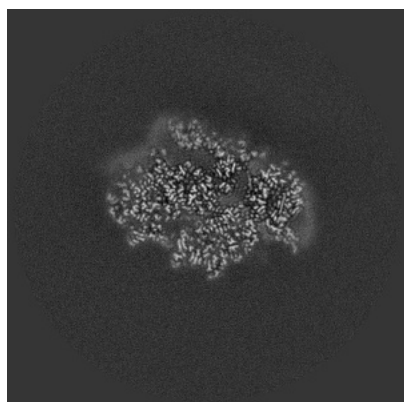


Y Index: 257

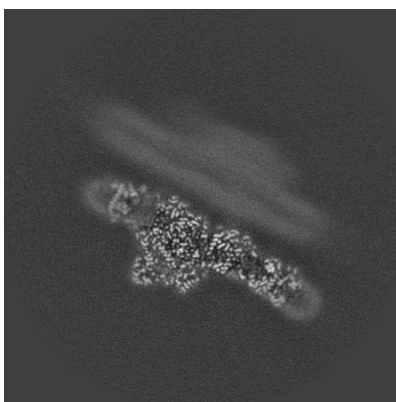


Z Index: 213

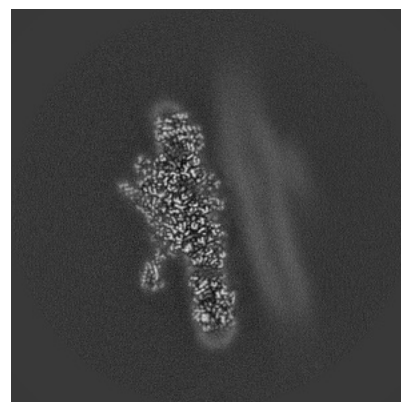
### 6.3.2 Raw map



X Index: 183



Y Index: 257



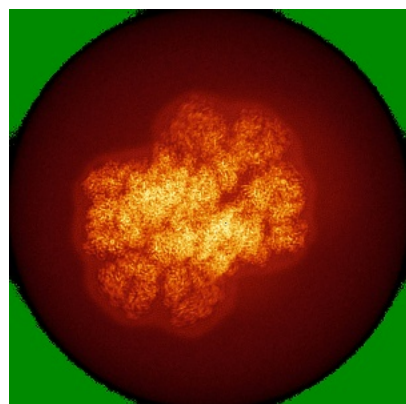
Z Index: 213

The images above show the largest variance slices of the map in three orthogonal directions.

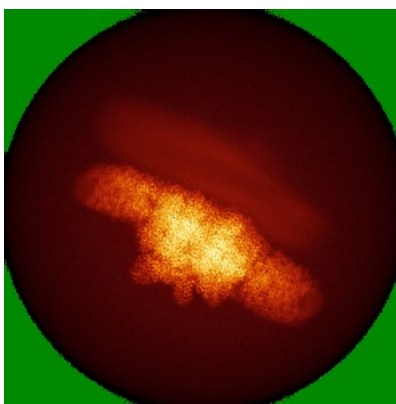


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

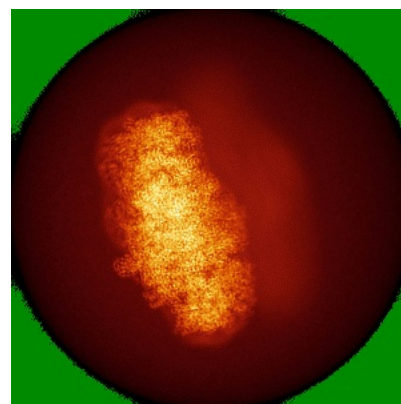
### 6.4.1 Primary map



X

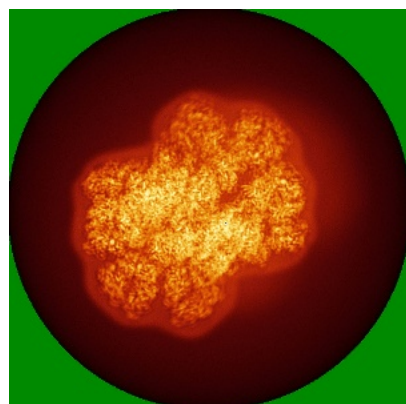


Y

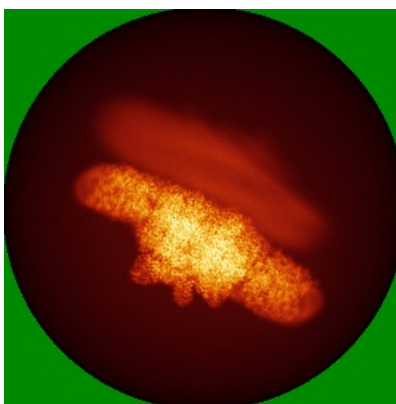


Z

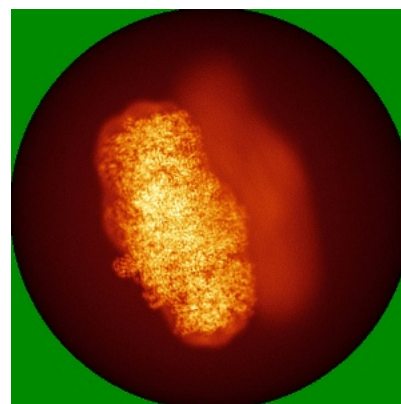
### 6.4.2 Raw map



X



Y

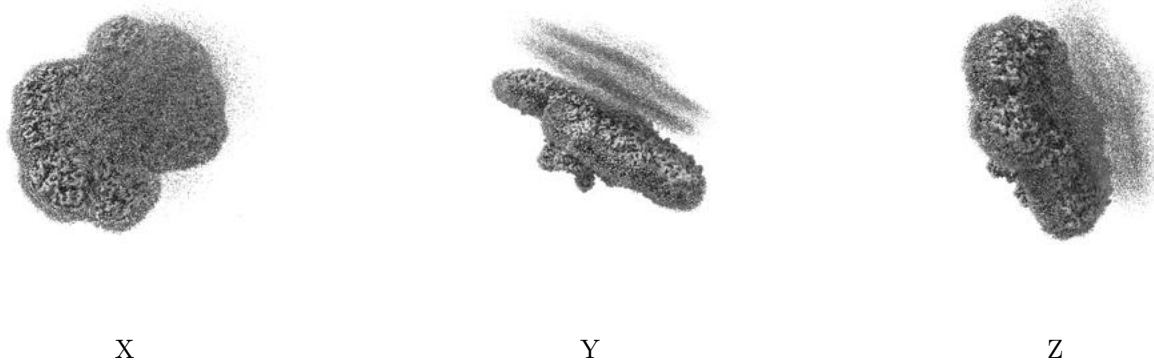


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

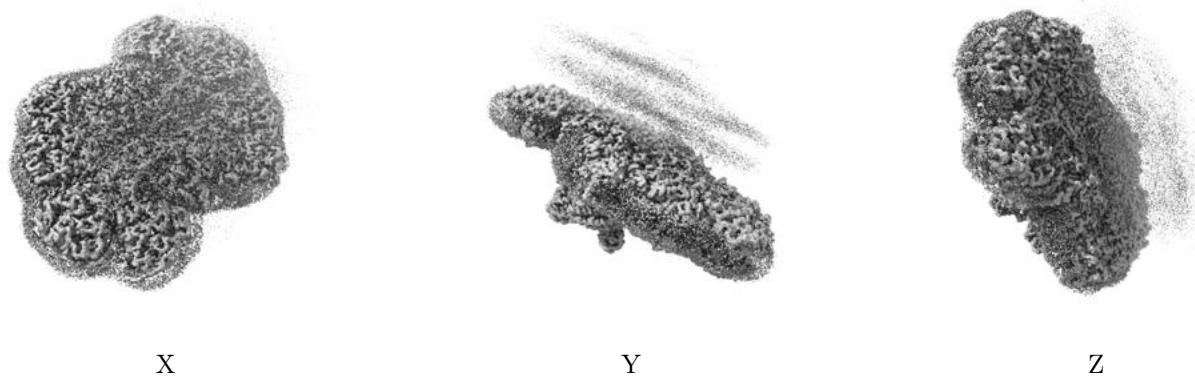
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

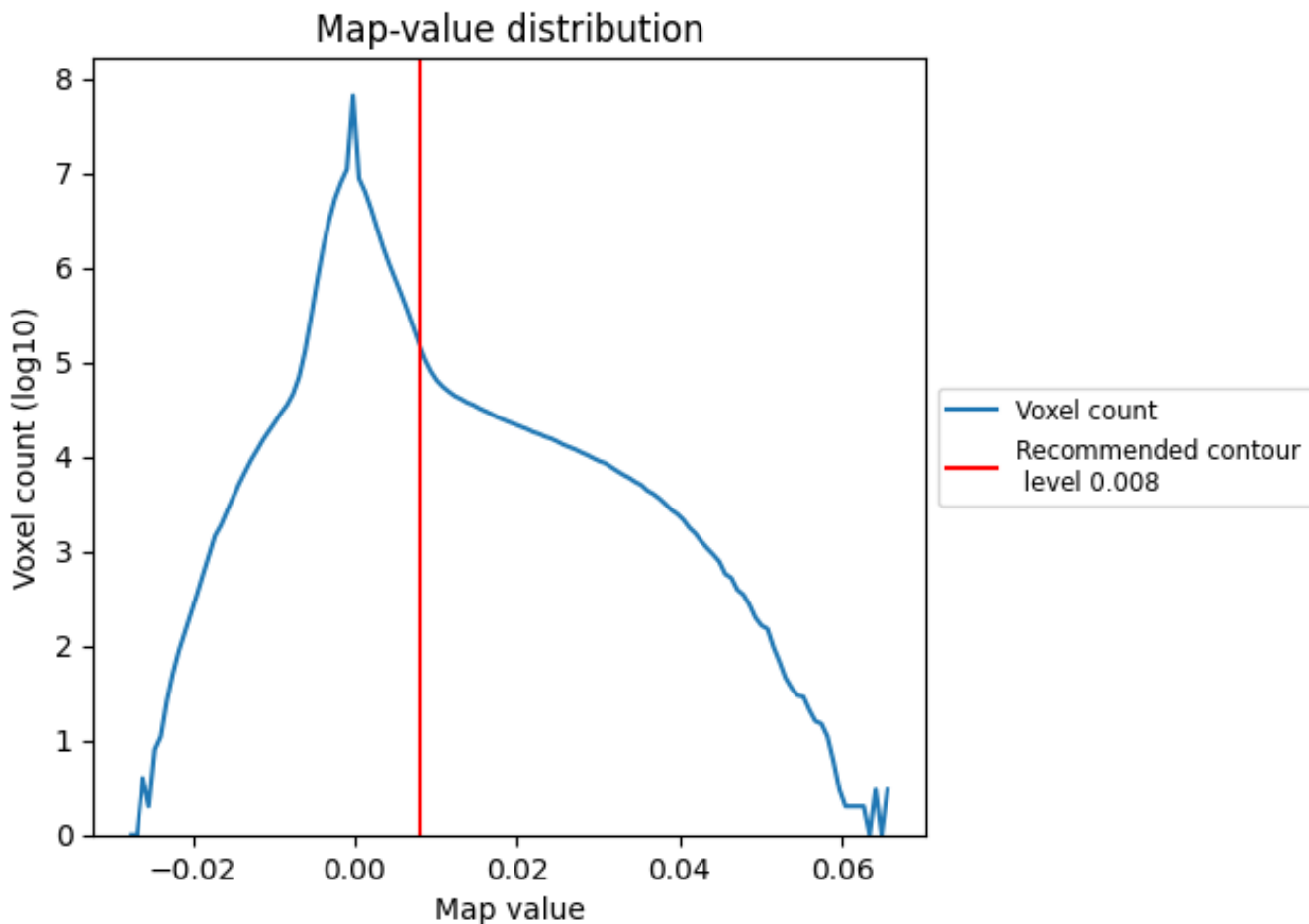
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

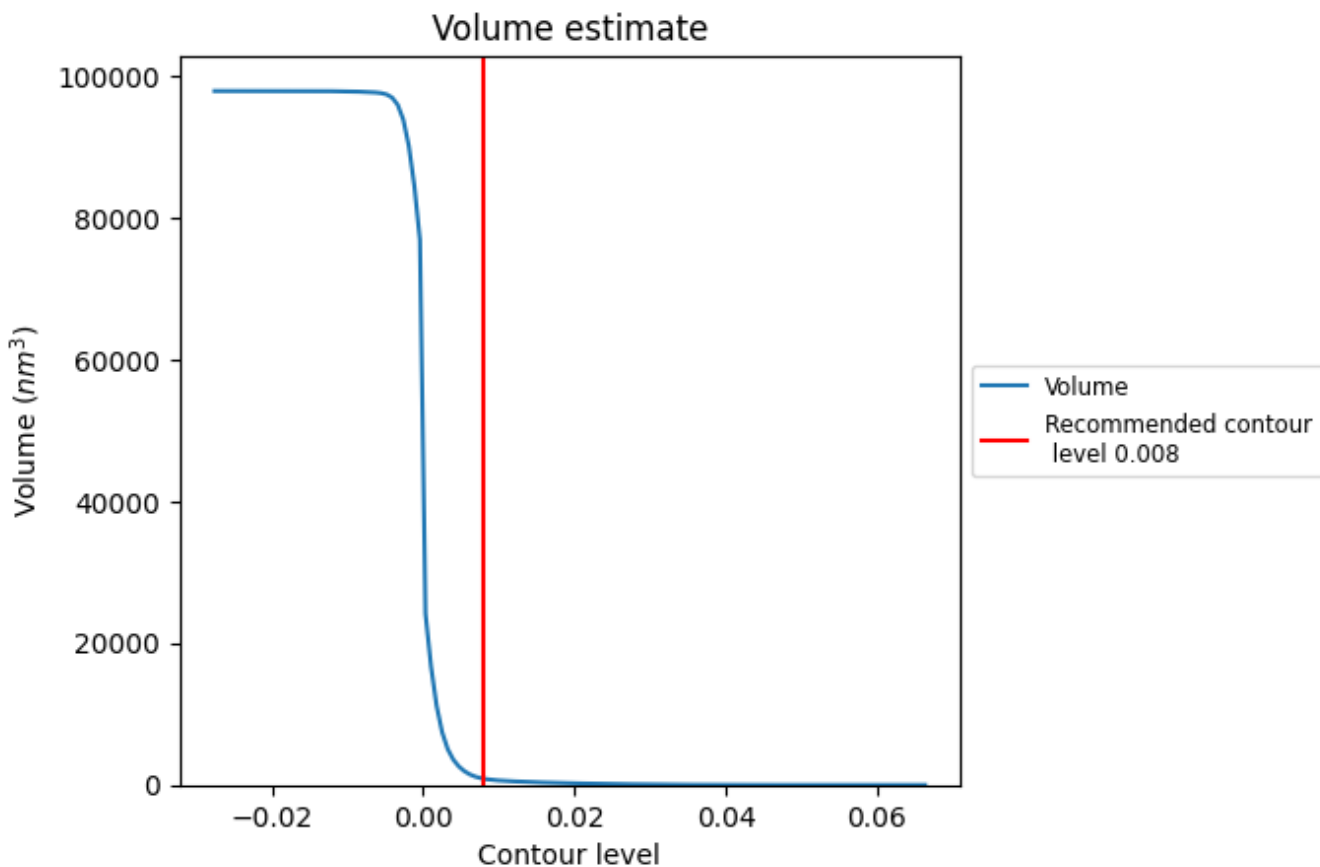
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

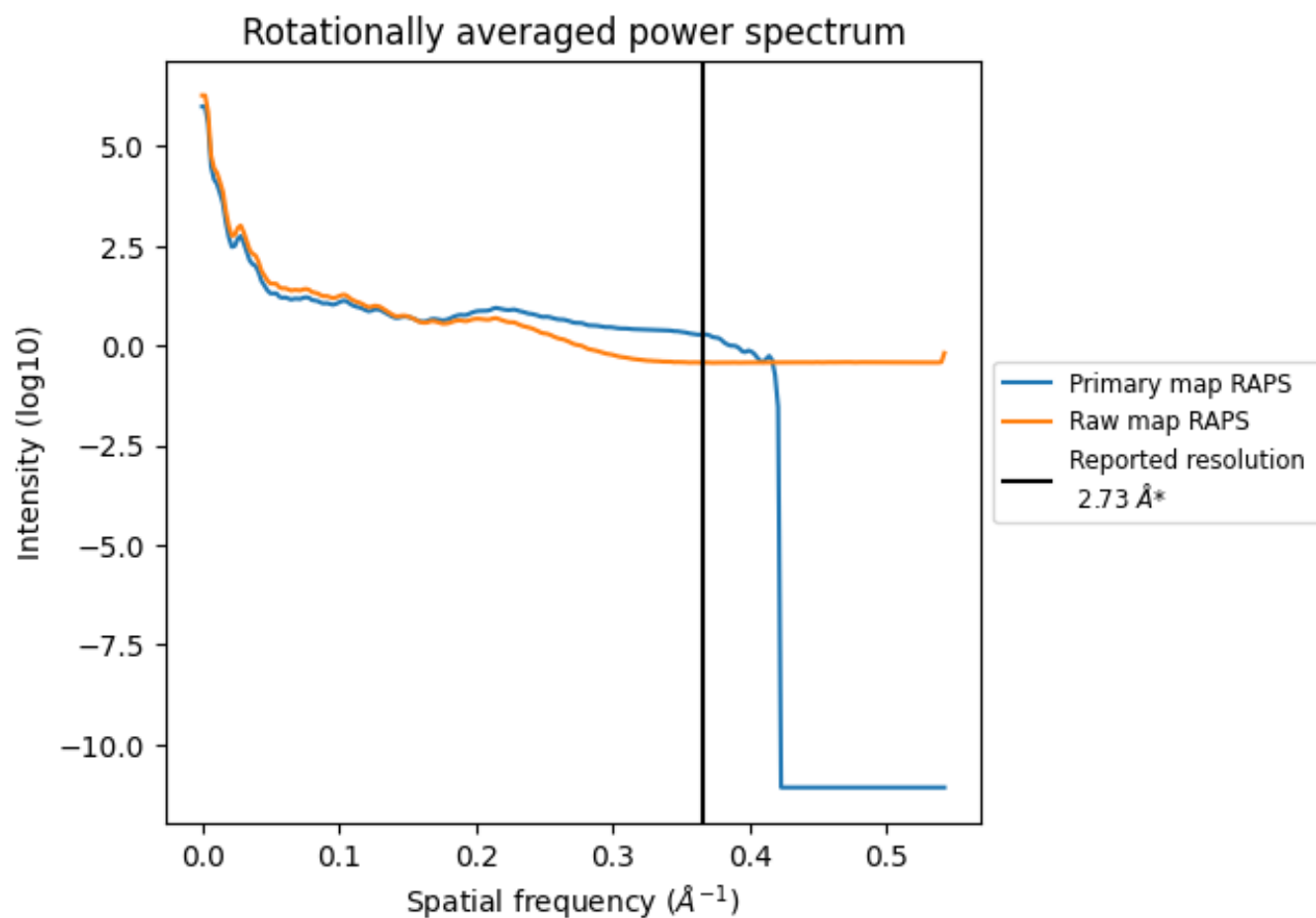
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 885  $\text{nm}^3$ ; this corresponds to an approximate mass of 799 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

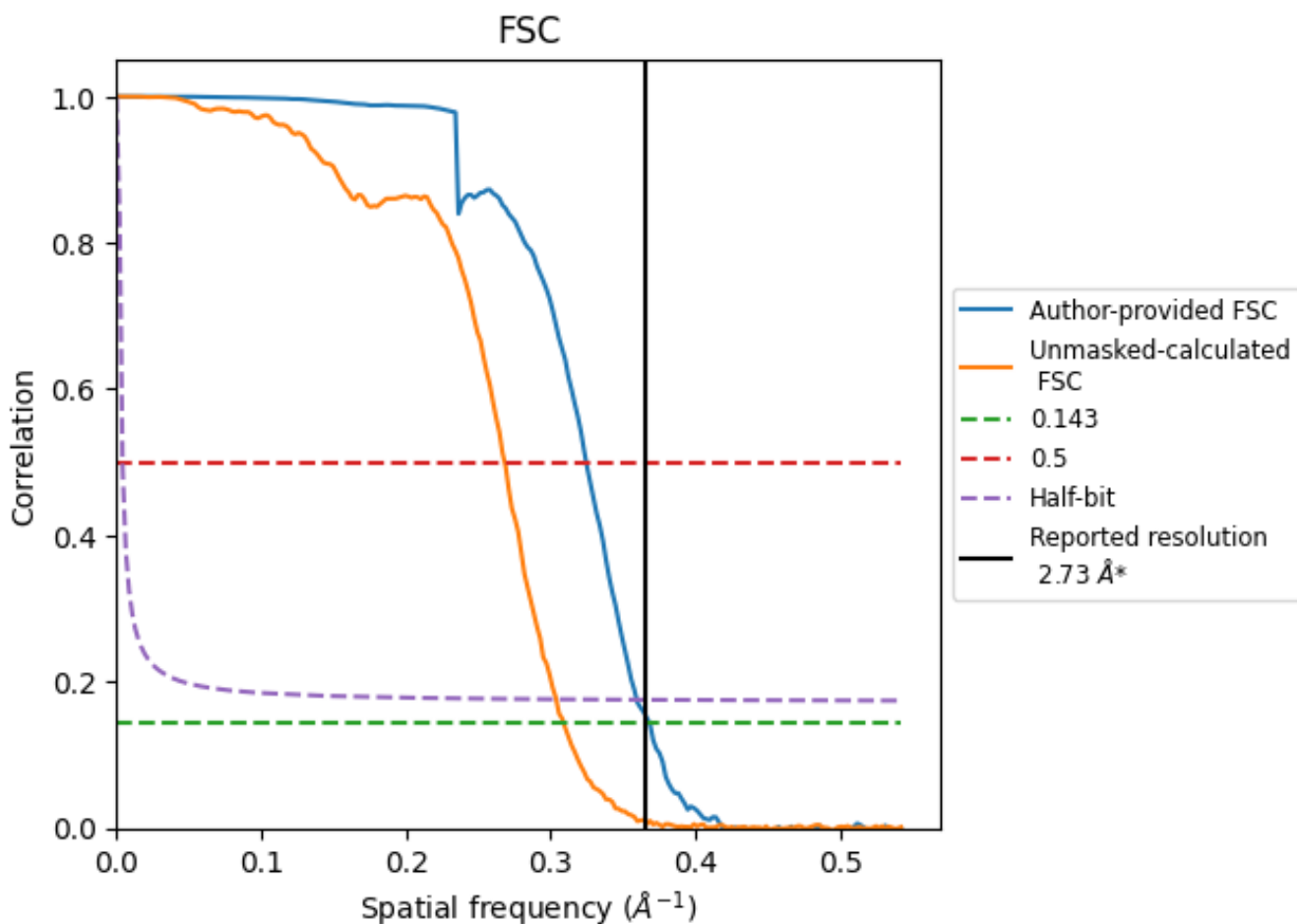


\*Reported resolution corresponds to spatial frequency of  $0.366 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.366 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

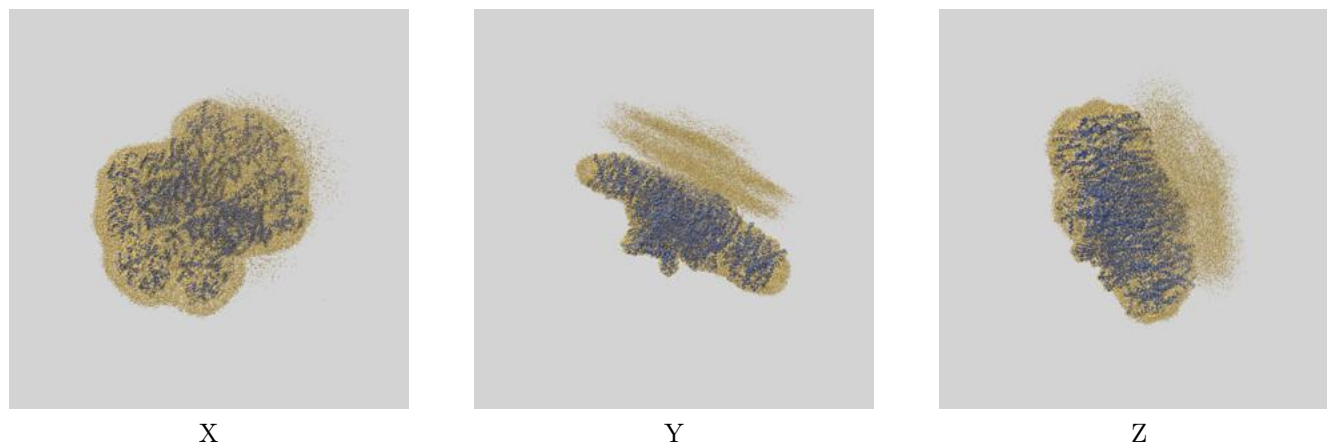
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.73	-	-
Author-provided FSC curve	2.71	3.08	2.78
Unmasked-calculated*	3.23	3.73	3.29

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.73 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15973 and PDB model 8BD3. Per-residue inclusion information can be found in section 3 on page 65.

### 9.1 Map-model overlay [i](#)



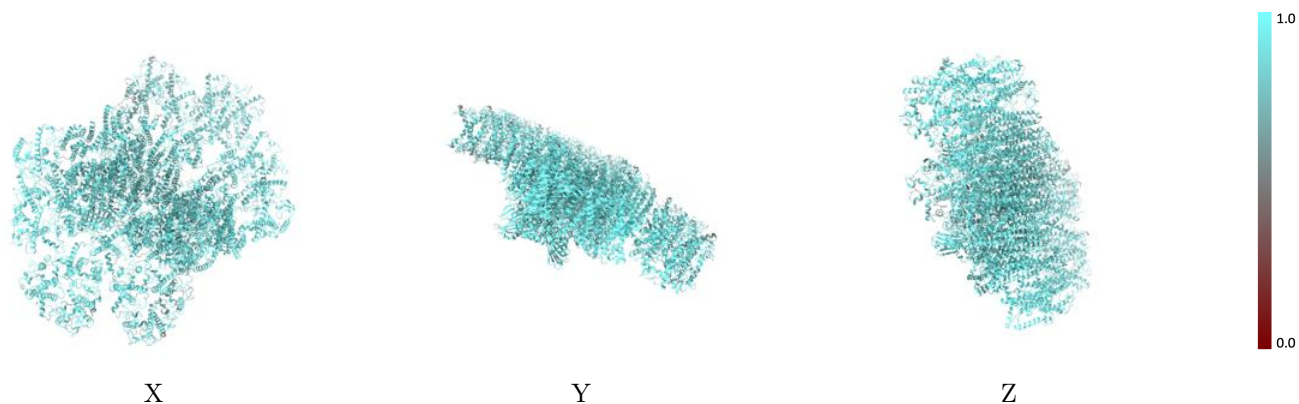
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



## 9.2 Q-score mapped to coordinate model [i](#)

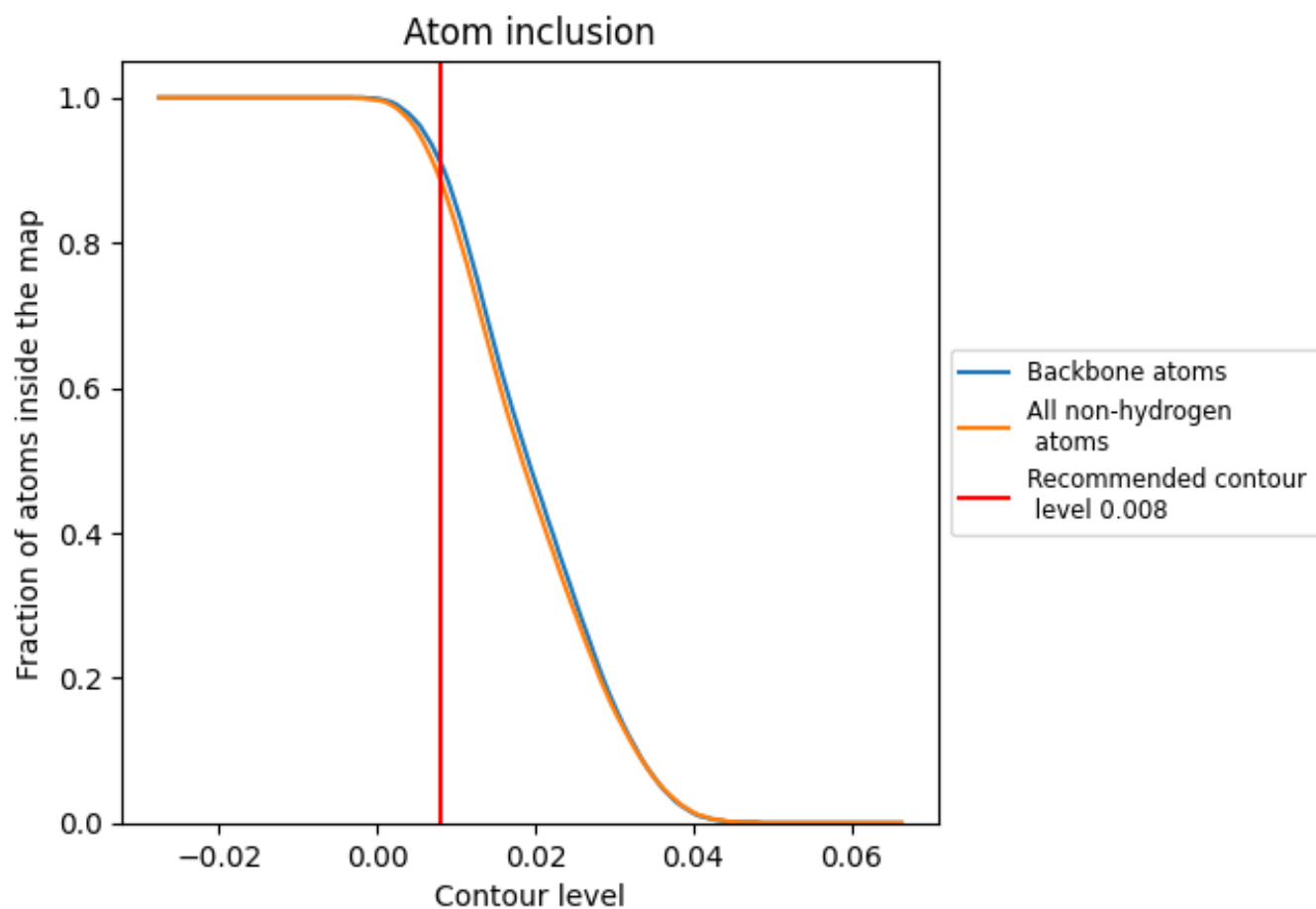
This section was not generated.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).




































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

































The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion
All	 0.8870
0	 0.8560
1	 0.8750
2	 0.8000
3	 0.8160
4	 0.7510
5	 0.7340
6	 0.8510
7	 0.8590
8	 0.7870
9	 0.7940
A	 0.9550
B	 0.9450
C	 0.9450
D	 0.9590
E	 0.9350
F	 0.9590
F1	 0.9210
G	 0.8990
H	 0.9560
I	 0.9350
J	 0.8950
K	 0.8510
L	 0.9280
M	 0.7890
N	 0.9150
O	 0.8970
P1	 0.8790
Q1	 0.7590
R	 0.9020
S	 0.8980
T	 0.9070
U	 0.8870
V	 0.8380
W	 0.8310



*Continued on next page...*

Continued from previous page...

Chain	Atom inclusion
X	 0.8580
Y	 0.9280
Z	 0.9200
a	 0.9540
b	 0.9410
c	 0.9370
d	 0.9640
e	 0.9260
f	 0.9310
fl	 0.9180
g	 0.8950
h	 0.9580
i	 0.9740
j	 0.8940
k	 0.9420
l	 0.9340
m	 0.8210
n	 0.9170
o	 0.8930
p	 0.7040
p1	 0.8800
q	 0.7420
q1	 0.7490
r	 0.9090
s	 0.9000
t	 0.8760
u	 0.8940
v	 0.8520
w	 0.8480
x	 0.8280
y	 0.9350
z	 0.8880