



wwPDB EM Validation Summary 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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at 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>.

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

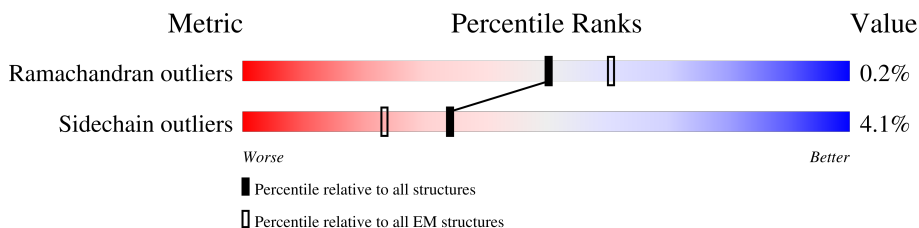
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA)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



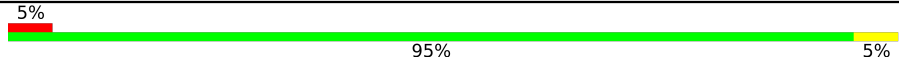
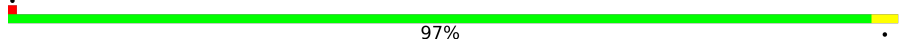
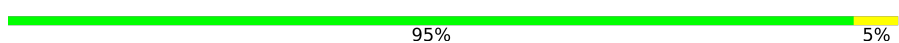
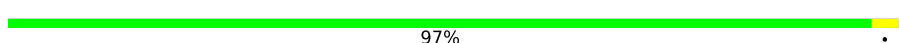
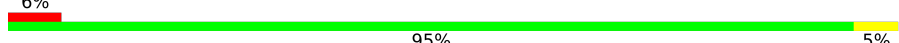
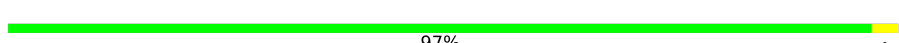
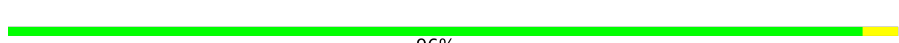

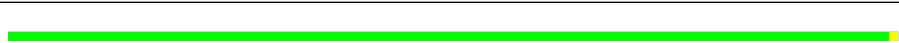

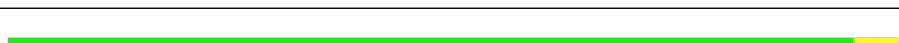

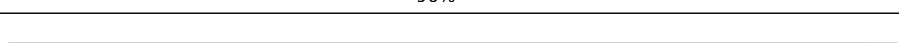
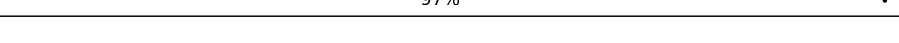
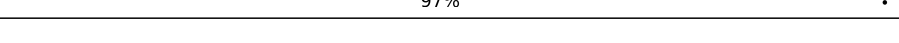
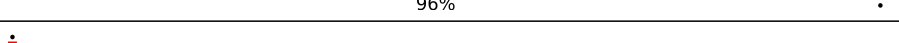
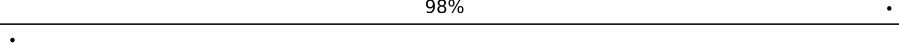
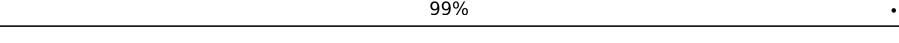
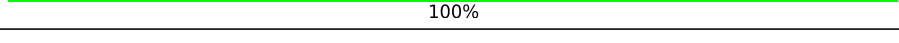
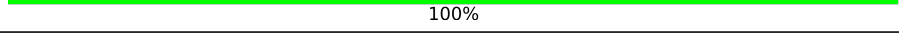
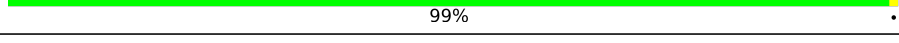
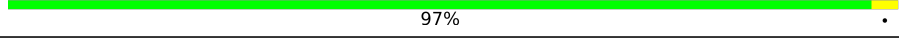
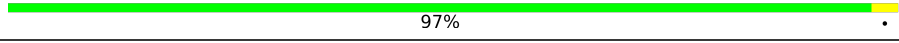
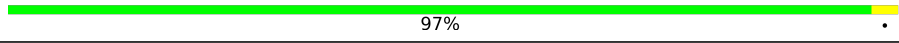
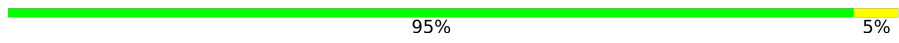
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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 ≥ 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	 95% 5%
3	8	221	 97%
3	N	221	 95% 5%
3	n	221	 97%
3	p	221	 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% 11%
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	-	-	-
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	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
			Total	C	N	O	S		
6	B	504	3954	2583	667	692	12	0	0
6	b	504	3954	2583	667	692	12	0	0

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

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

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

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

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

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

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

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

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

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

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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
			Total	C	N	O	S		
27	q1	34	Total 260	C 171	N 44	O 44	S 1	0	0

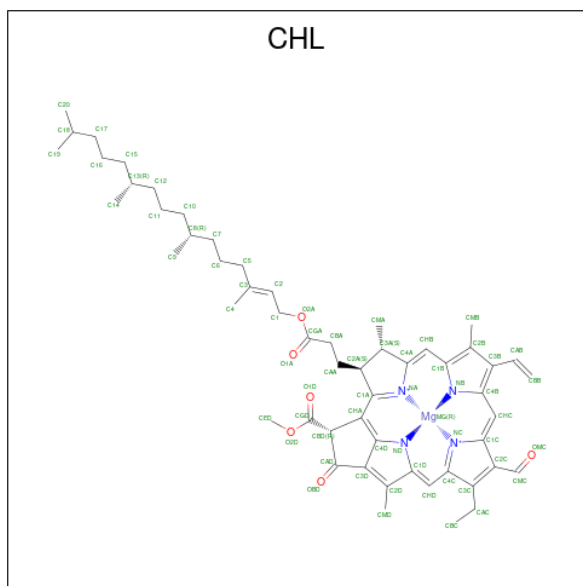
- Molecule 28 is a protein called Chloroplast photosystem II 10 kDa protein.

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

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

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

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



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

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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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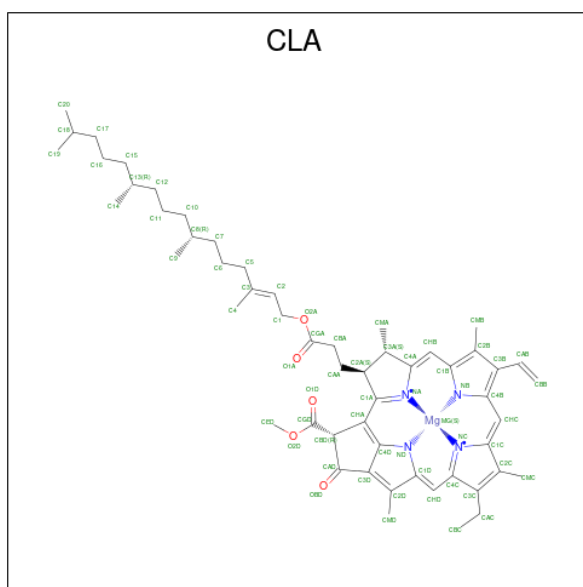
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	p	1	46	35	1	4	6	0
30	p	1	51	40	1	4	6	0
30	p	1	51	40	1	4	6	0
30	p	1	50	39	1	4	6	0
30	p	1	56	45	1	4	6	0
30	q	1	66	55	1	4	6	0
30	q	1	46	35	1	4	6	0
30	q	1	51	40	1	4	6	0
30	q	1	57	46	1	4	6	0
30	q	1	50	39	1	4	6	0
30	q	1	56	45	1	4	6	0
30	g	1	66	55	1	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
30	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
30	r	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
30	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
30	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
30	s	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			59	48	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
30	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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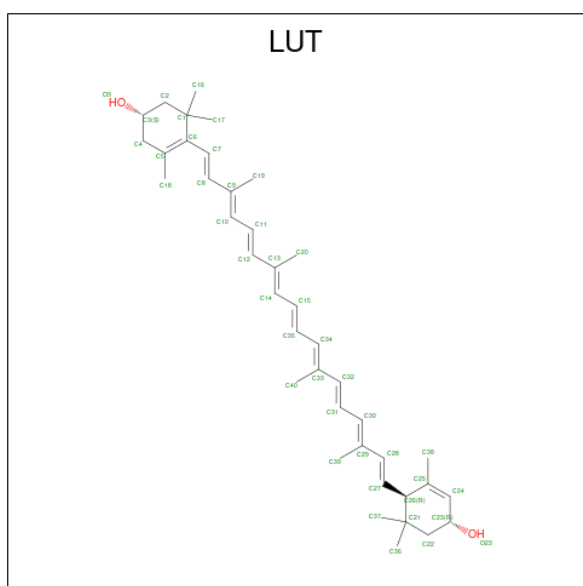
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
31	r	1	57	47	1	4	5	0
31	r	1	49	39	1	4	5	0
31	r	1	49	39	1	4	5	0
31	r	1	55	45	1	4	5	0
31	r	1	65	55	1	4	5	0
31	s	1	65	55	1	4	5	0
31	s	1	42	34	1	4	3	0
31	s	1	65	55	1	4	5	0
31	s	1	50	40	1	4	5	0
31	s	1	60	50	1	4	5	0
31	s	1	65	55	1	4	5	0
31	s	1	65	55	1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

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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: C₄₀H₅₆O₂).



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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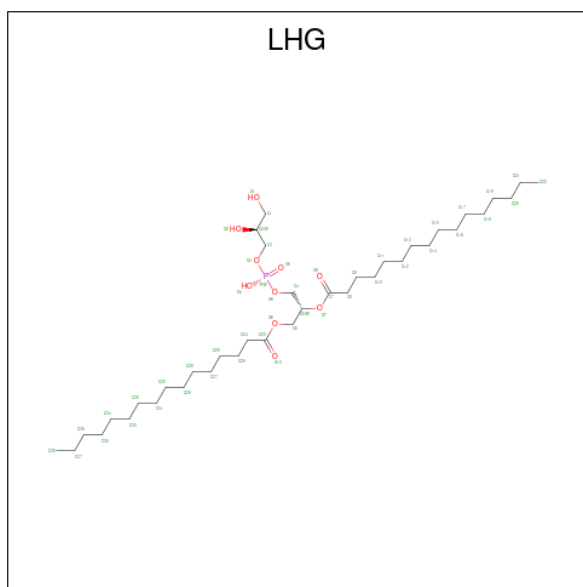
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	5	1	42	40	2	0
32	6	1	42	40	2	0
32	6	1	42	40	2	0
32	G	1	42	40	2	0
32	N	1	42	40	2	0
32	N	1	42	40	2	0
32	R	1	42	40	2	0
32	S	1	42	40	2	0
32	S	1	42	40	2	0
32	Y	1	42	40	2	0
32	Y	1	42	40	2	0
32	0	1	42	40	2	0
32	0	1	42	40	2	0
32	7	1	42	40	2	0
32	7	1	42	40	2	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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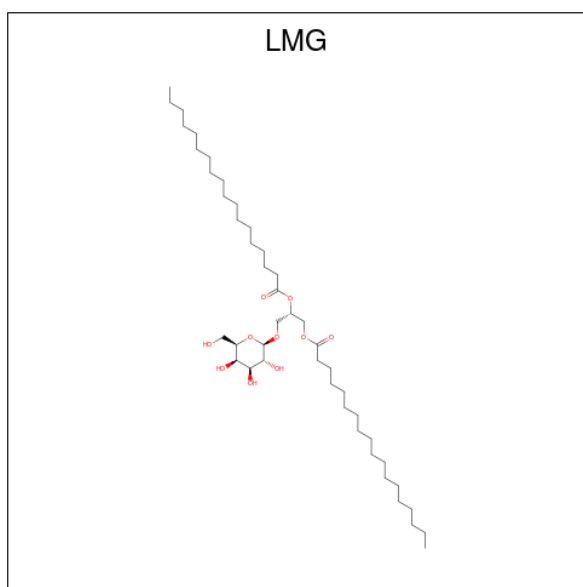
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
33	4	1	47	36	10	1	0
33	5	1	35	24	10	1	0
33	6	1	37	26	10	1	0
33	A	1	44	33	10	1	0
33	A	1	39	28	10	1	0
33	B	1	49	38	10	1	0
33	C	1	40	29	10	1	0
33	D	1	44	33	10	1	0
33	D	1	49	38	10	1	0
33	G	1	44	33	10	1	0
33	K	1	36	25	10	1	0
33	L	1	49	38	10	1	0
33	M	1	41	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	9	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: C₄₅H₈₆O₁₀).



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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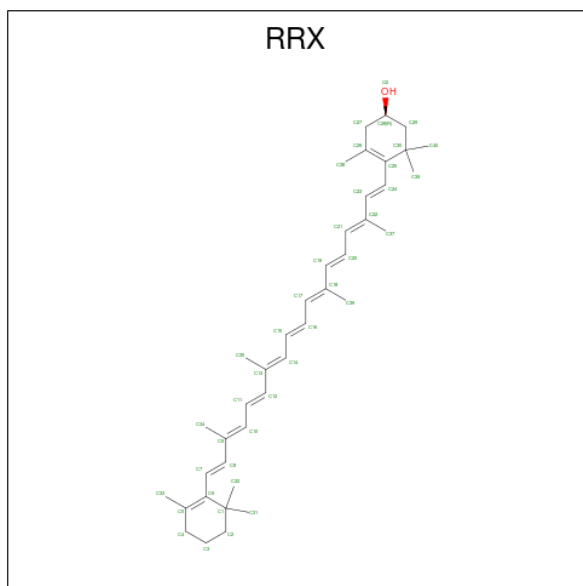
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	b	1	38	28	10	0
34	b	1	38	28	10	0
34	b	1	46	36	10	0
34	b	1	38	28	10	0
34	c	1	38	28	10	0
34	c	1	38	28	10	0
34	c	1	44	34	10	0
34	d	1	41	31	10	0
34	d	1	51	41	10	0
34	d	1	48	38	10	0
34	f	1	38	28	10	0
34	g	1	38	28	10	0
34	g	1	49	39	10	0
34	j	1	43	33	10	0
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: C₄₀H₅₆O).



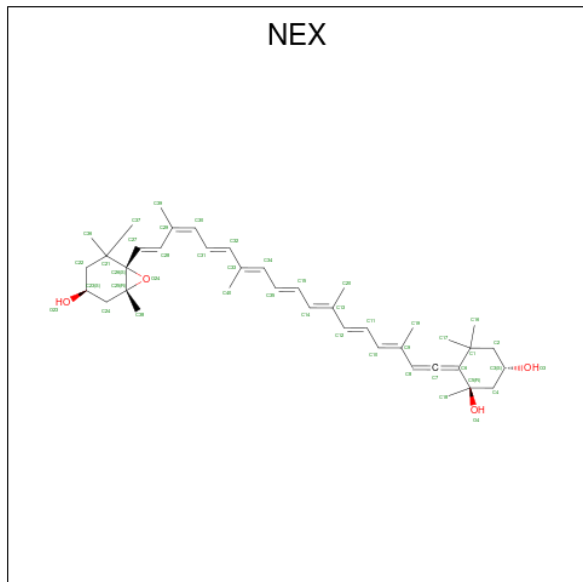
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
35	2	1	41	40	1	0
35	4	1	41	40	1	0

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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: C₄₀H₅₆O₄).



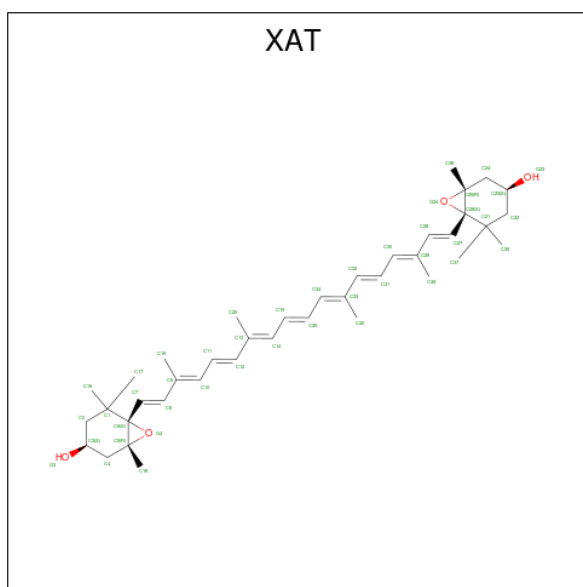
Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	O	0
			44	40	4	
36	3	1	Total	C	O	0
			44	40	4	
36	4	1	Total	C	O	0
			44	40	4	
36	5	1	Total	C	O	0
			44	40	4	
36	6	1	Total	C	O	0
			44	40	4	
36	G	1	Total	C	O	0
			44	40	4	

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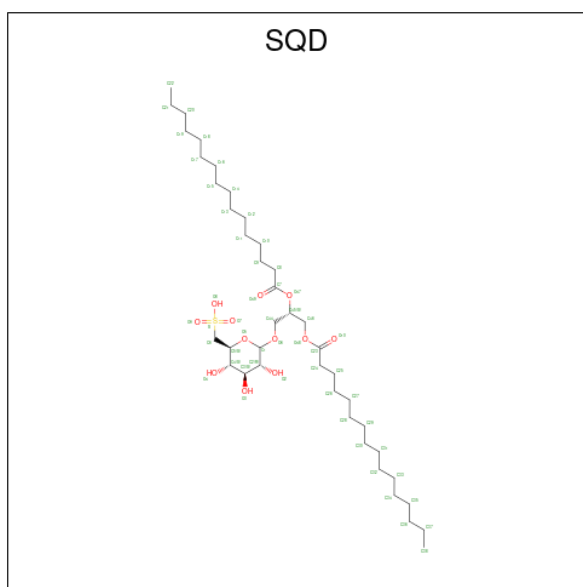
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
36	N	1	44	40	4	0
36	R	1	44	40	4	0
36	R	1	44	40	4	0
36	S	1	44	40	4	0
36	Y	1	44	40	4	0
36	0	1	44	40	4	0
36	8	1	44	40	4	0
36	9	1	44	40	4	0
36	p	1	44	40	4	0
36	q	1	44	40	4	0
36	g	1	44	40	4	0
36	n	1	44	40	4	0
36	r	1	44	40	4	0
36	r	1	44	40	4	0
36	s	1	44	40	4	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: C₄₀H₅₆O₄).



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

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



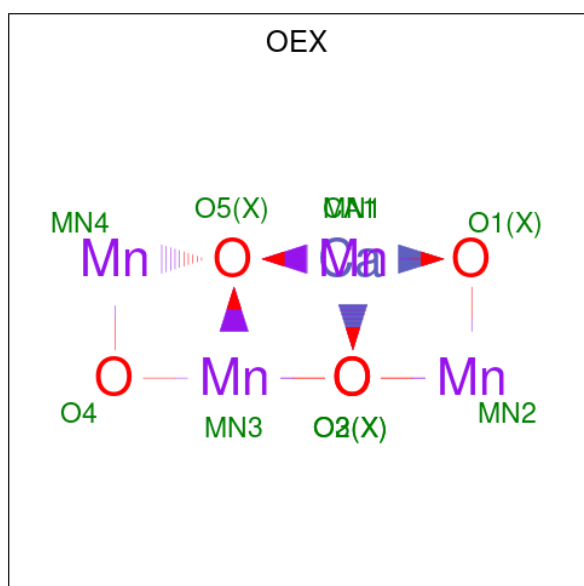
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
38	6	1	42	29	12	1	0
38	A	1	51	38	12	1	0
38	A	1	45	32	12	1	0
38	B	1	54	41	12	1	0
38	B	1	52	39	12	1	0
38	G	1	42	29	12	1	0
38	G	1	38	25	12	1	0
38	M	1	50	37	12	1	0
38	R	1	51	38	12	1	0
38	S	1	51	38	12	1	0
38	X	1	38	25	12	1	0
38	Y	1	42	29	12	1	0
38	0	1	42	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: CaMn_4O_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

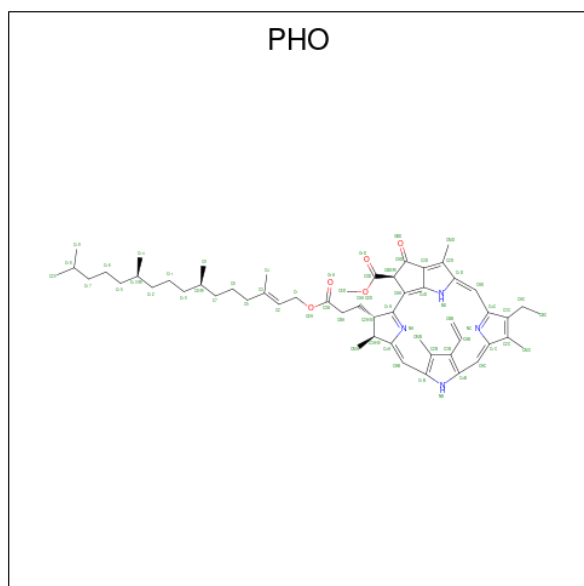
- Molecule 40 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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: C₅₅H₇₄N₄O₅).



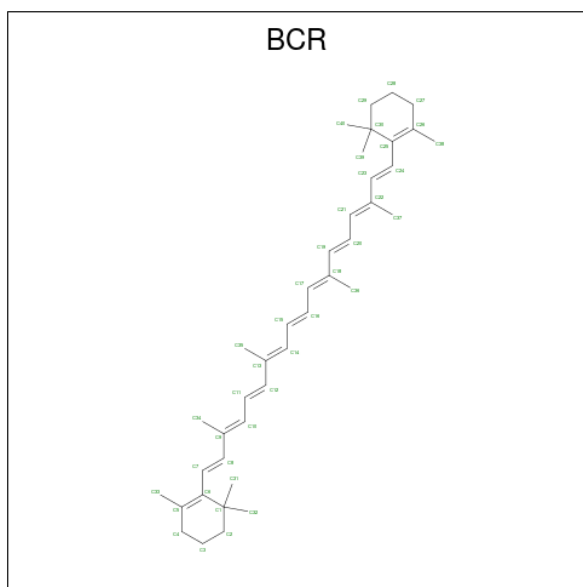
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
42	A	1	64	55	4	5	0
42	D	1	64	55	4	5	0

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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: C₄₀H₅₆).



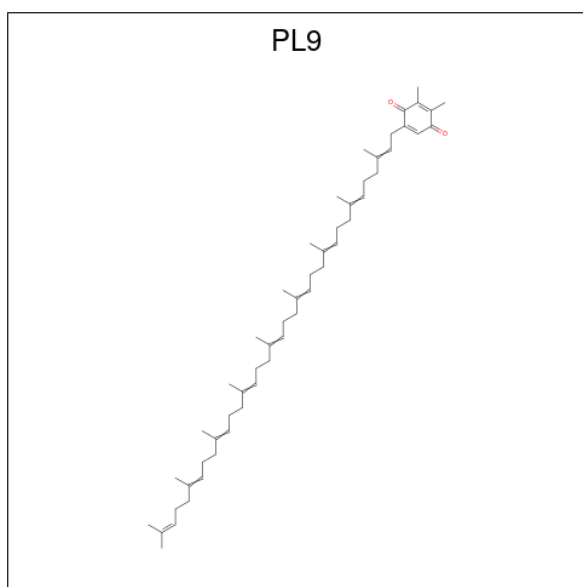
Mol	Chain	Residues	Atoms		AltConf
43	A	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	B	1	Total	C	0
			40	40	
43	C	1	Total	C	0
			40	40	
43	C	1	Total	C	0
			40	40	
43	D	1	Total	C	0
			40	40	
43	H	1	Total	C	0
			40	40	
43	T	1	Total	C	0
			40	40	

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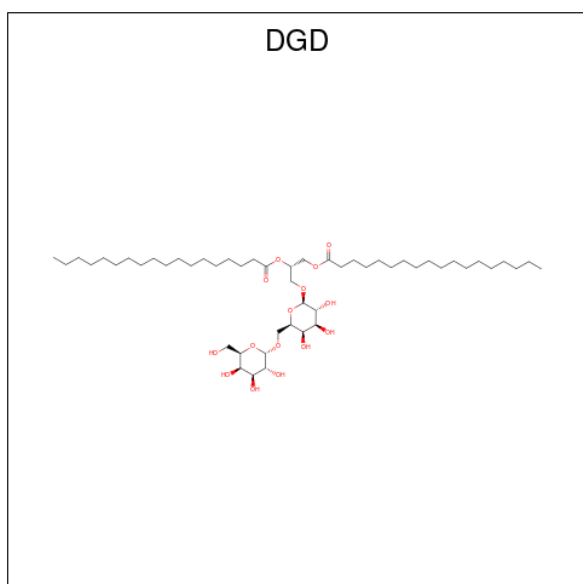
Mol	Chain	Residues	Atoms	AltConf
43	V	1	Total C 40 40	0
43	Z	1	Total C 40 40	0
43	a	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	b	1	Total C 40 40	0
43	c	1	Total C 40 40	0
43	c	1	Total C 40 40	0
43	d	1	Total C 40 40	0
43	h	1	Total C 40 40	0
43	t	1	Total C 40 40	0
43	v	1	Total C 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: C₅₃H₈₀O₂).



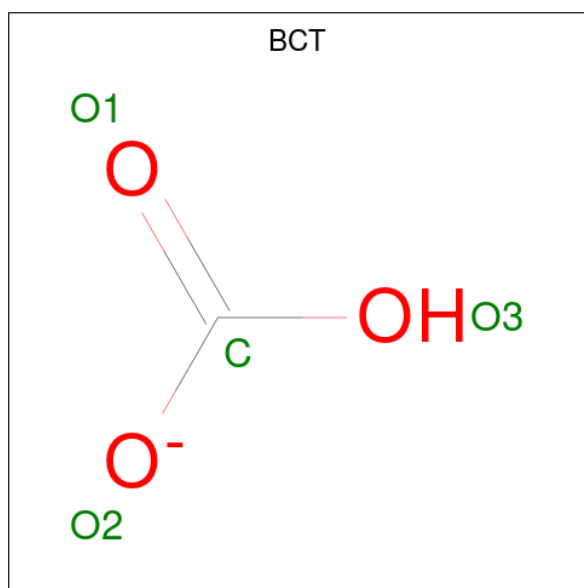
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
44	A	1	55	53	2	0
44	D	1	55	53	2	0
44	a	1	55	53	2	0
44	d	1	55	53	2	0

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



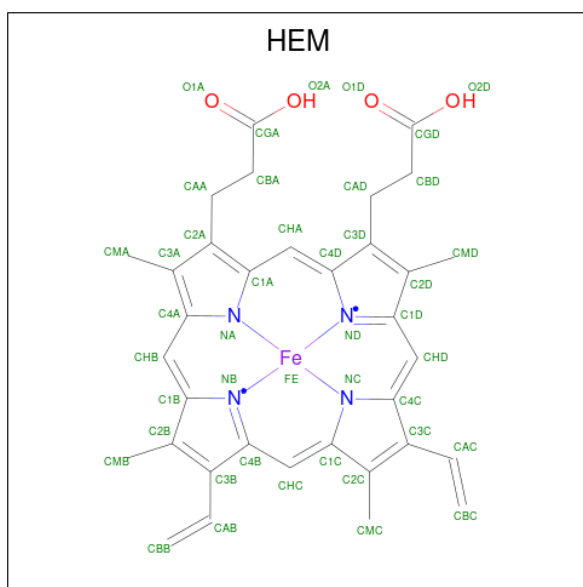
Mol	Chain	Residues	Atoms			AltConf
45	C	1	Total	C	O	0
			50	35	15	
45	C	1	Total	C	O	0
			66	51	15	
45	C	1	Total	C	O	0
			66	51	15	
45	C	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			62	47	15	
45	c	1	Total	C	O	0
			66	51	15	
45	c	1	Total	C	O	0
			66	51	15	

- Molecule 46 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



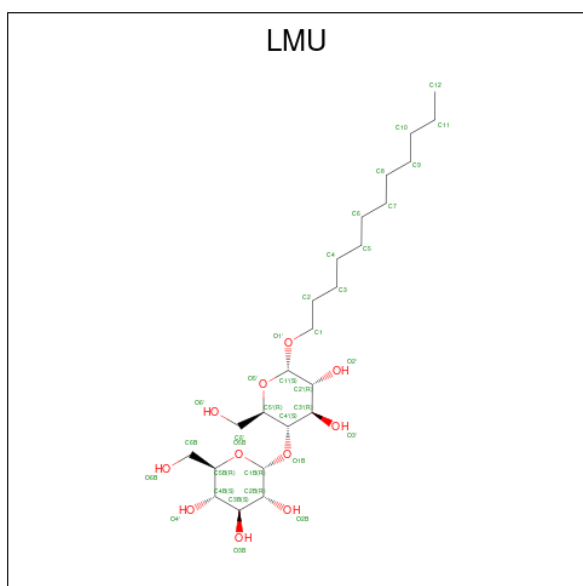
Mol	Chain	Residues	Atoms			AltConf
46	D	1	Total	C	O	0
			4	1	3	
46	d	1	Total	C	O	0
			4	1	3	

- 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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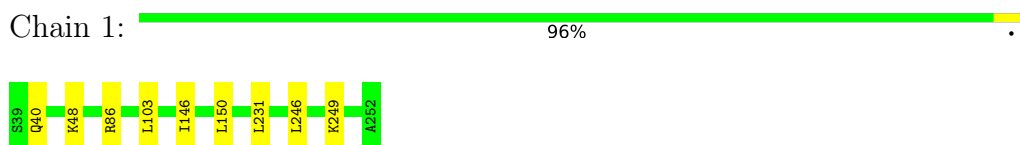
Continued from previous page...

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

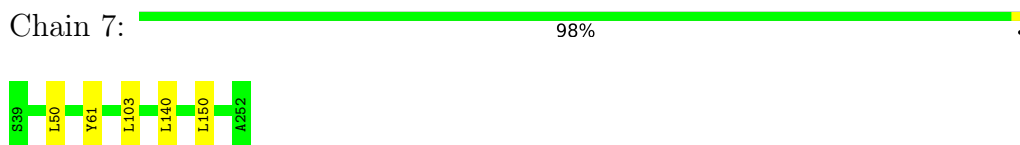
3 Residue-property plots [i](#)

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.

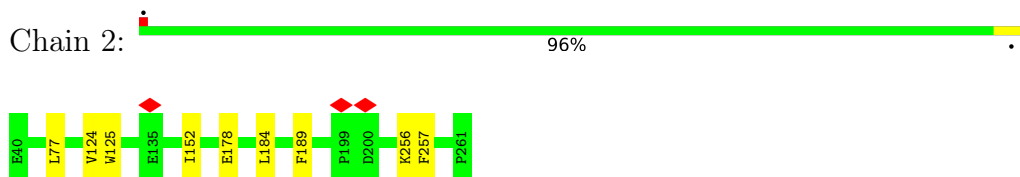
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



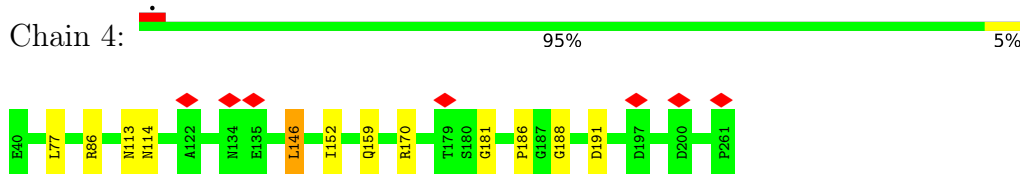
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



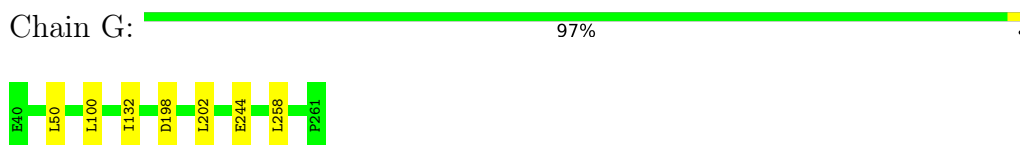
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



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

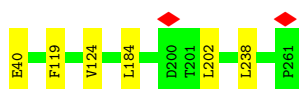


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



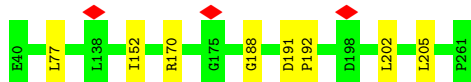
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

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%



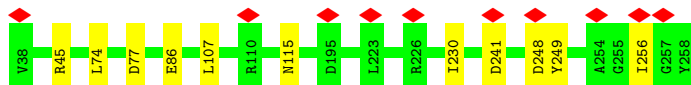
- Molecule 3: Chlorophyll a-b binding of LHCI

Chain 3:  95% 5%



- Molecule 3: Chlorophyll a-b binding of LHCI

Chain 5:  5% 95% 5%



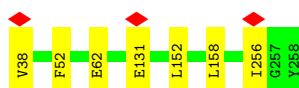
- Molecule 3: Chlorophyll a-b binding of LHCI

Chain N:  95% 5%

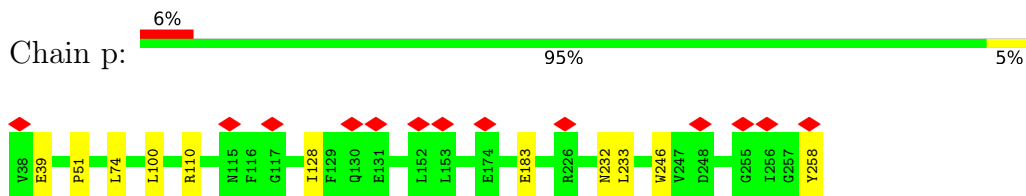


- Molecule 3: Chlorophyll a-b binding of LHCI

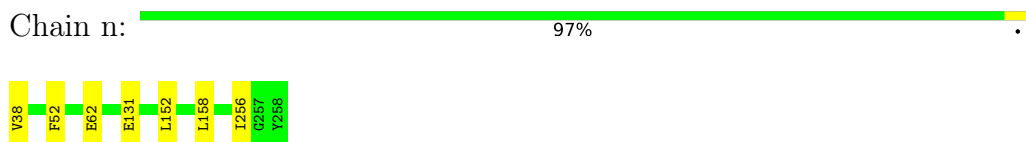
Chain 8:  97%



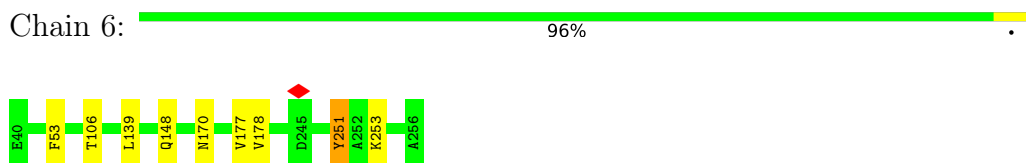
- Molecule 3: Chlorophyll a-b binding of LHCII



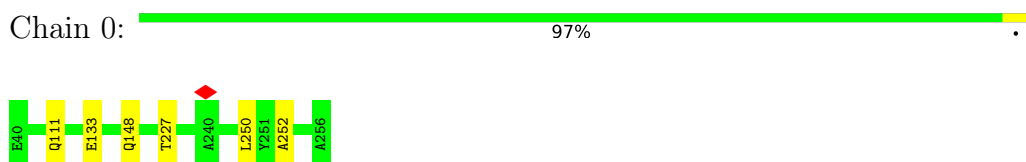
- Molecule 3: Chlorophyll a-b binding of LHCII



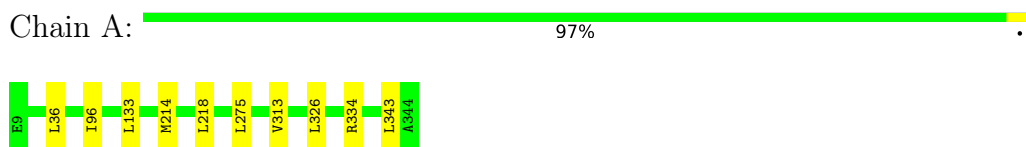
- Molecule 4: Chlorophyll a-b binding of LHCII



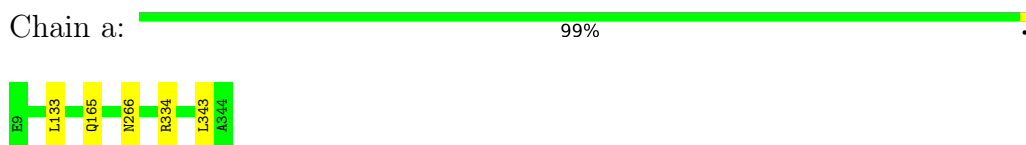
- Molecule 4: Chlorophyll a-b binding of LHCII



- 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%



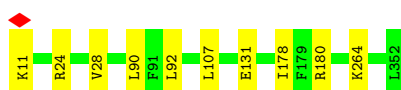
- Molecule 7: Photosystem II CP43 reaction center protein

Chain c: 97%



- Molecule 8: Photosystem II D2 protein

Chain D: 97%



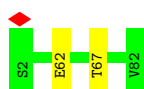
- Molecule 8: Photosystem II D2 protein

Chain d: 96%



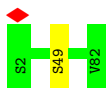
- Molecule 9: Cytochrome b559 subunit alpha

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.

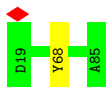
- Molecule 10: Cytochrome b559 subunit beta

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%



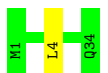
- Molecule 12: Photosystem II reaction center protein I

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%



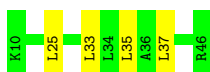
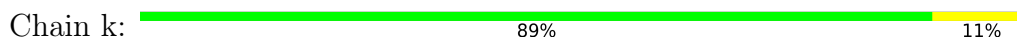
- Molecule 13: Photosystem II reaction center protein J



- Molecule 14: Photosystem II reaction center protein K



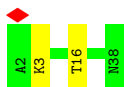
- Molecule 14: Photosystem II reaction center protein K



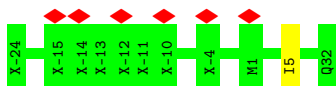
- Molecule 15: Photosystem II reaction center protein L



- Molecule 15: Photosystem II reaction center protein L

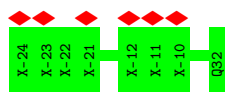


- Molecule 16: Photosystem II reaction center protein M



- Molecule 16: Photosystem II reaction center protein M

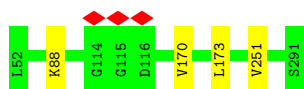




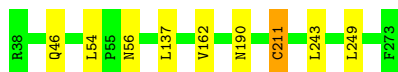
- Molecule 17: Chloroplast oxygen-evolving enhancer protein 1



- Molecule 17: Chloroplast oxygen-evolving enhancer protein 1



- Molecule 18: Chlorophyll a b binding CP29



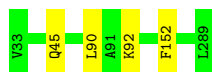
- Molecule 18: Chlorophyll a b binding CP29



- 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%



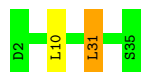
- Molecule 27: Chloroplast PsbY

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

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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

5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 348 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	b	224	ARG
14	k	25	LEU
6	b	357	ARG
8	d	45	LEU
17	o	170	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
3	p	221	GLN
16	m	4	ASN
6	b	331	ASN
7	c	403	ASN
22	w	111	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	-

The worst 5 of 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

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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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.

5 of 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

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	-	-	-	-	-
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	0	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	l	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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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	1	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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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%)
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	l	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	-
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	l	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	1	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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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

The worst 5 of 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

The worst 5 of 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

5 of 636 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	1	601	CHL	NA

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Mol	Chain	Res	Type	Atom
30	1	601	CHL	NC
30	1	601	CHL	ND
30	1	605	CHL	NA
30	1	605	CHL	NC

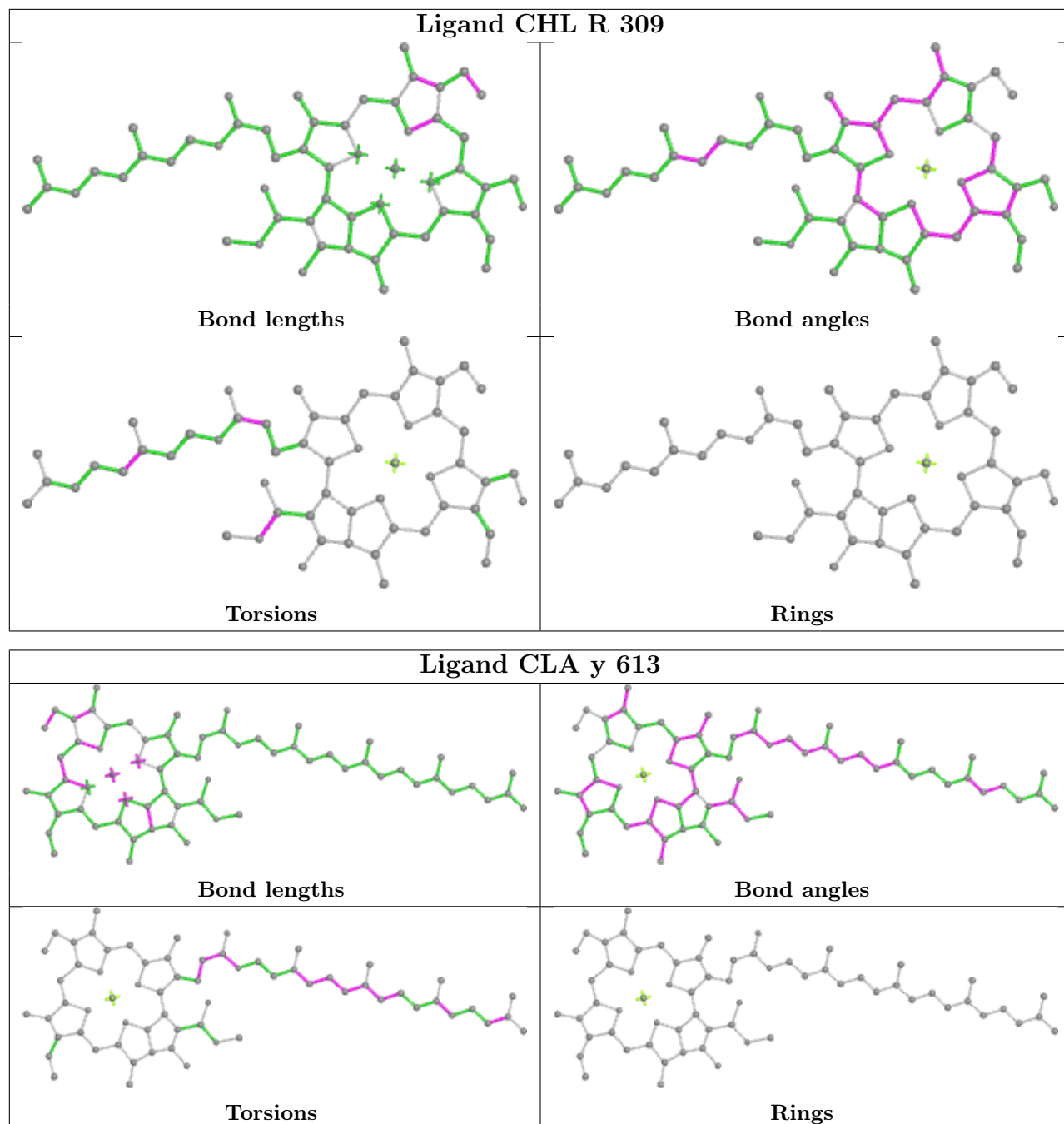
5 of 7812 torsion outliers are listed below:

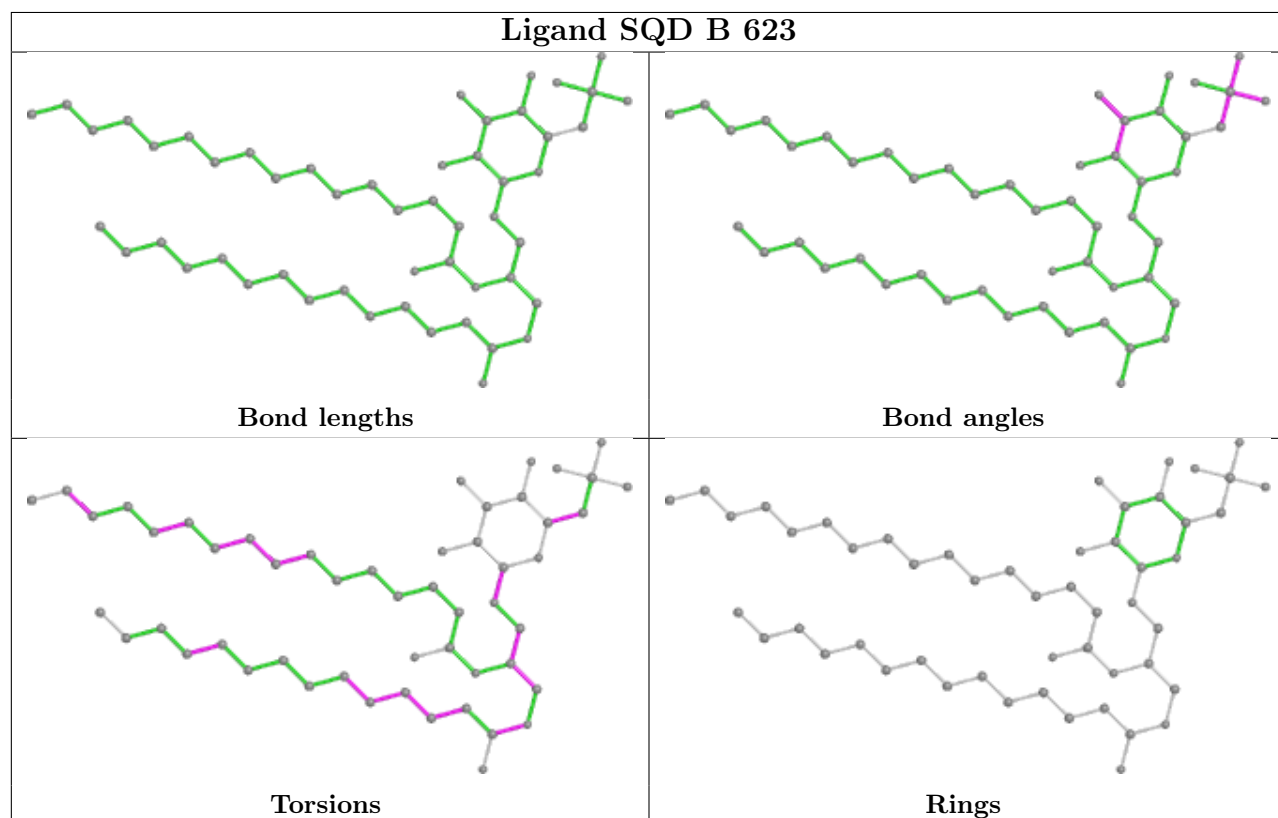
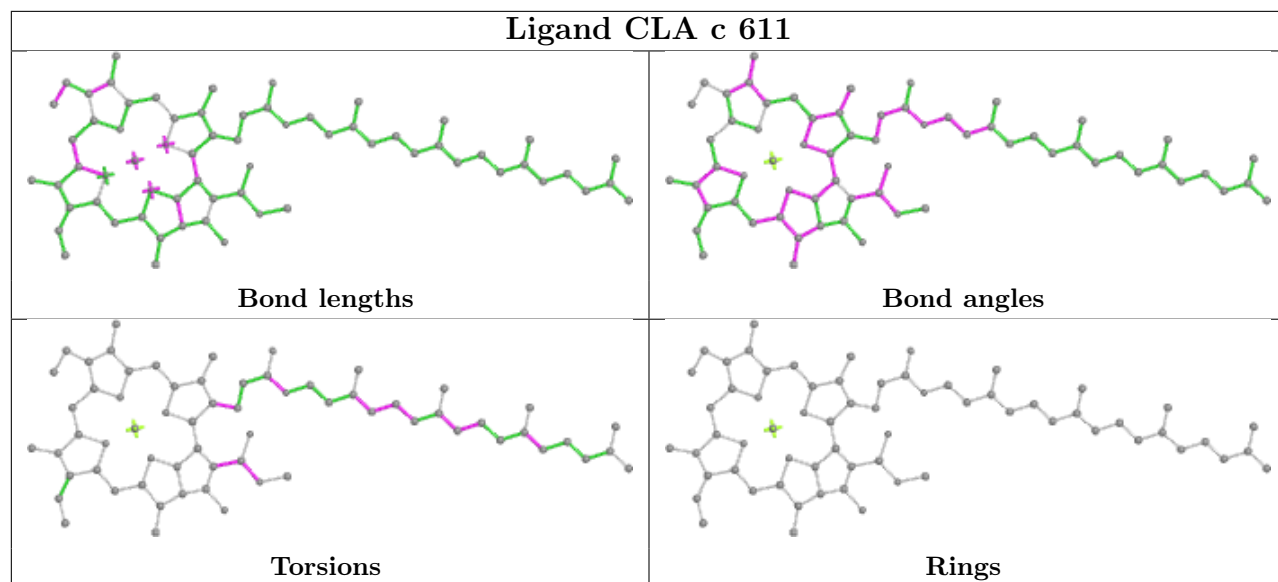
Mol	Chain	Res	Type	Atoms
30	1	601	CHL	CHA-CBD-CGD-O1D
30	1	601	CHL	CHA-CBD-CGD-O2D
30	1	606	CHL	CAD-CBD-CGD-O1D
30	1	606	CHL	CAD-CBD-CGD-O2D
30	1	607	CHL	C1A-C2A-CAA-CBA

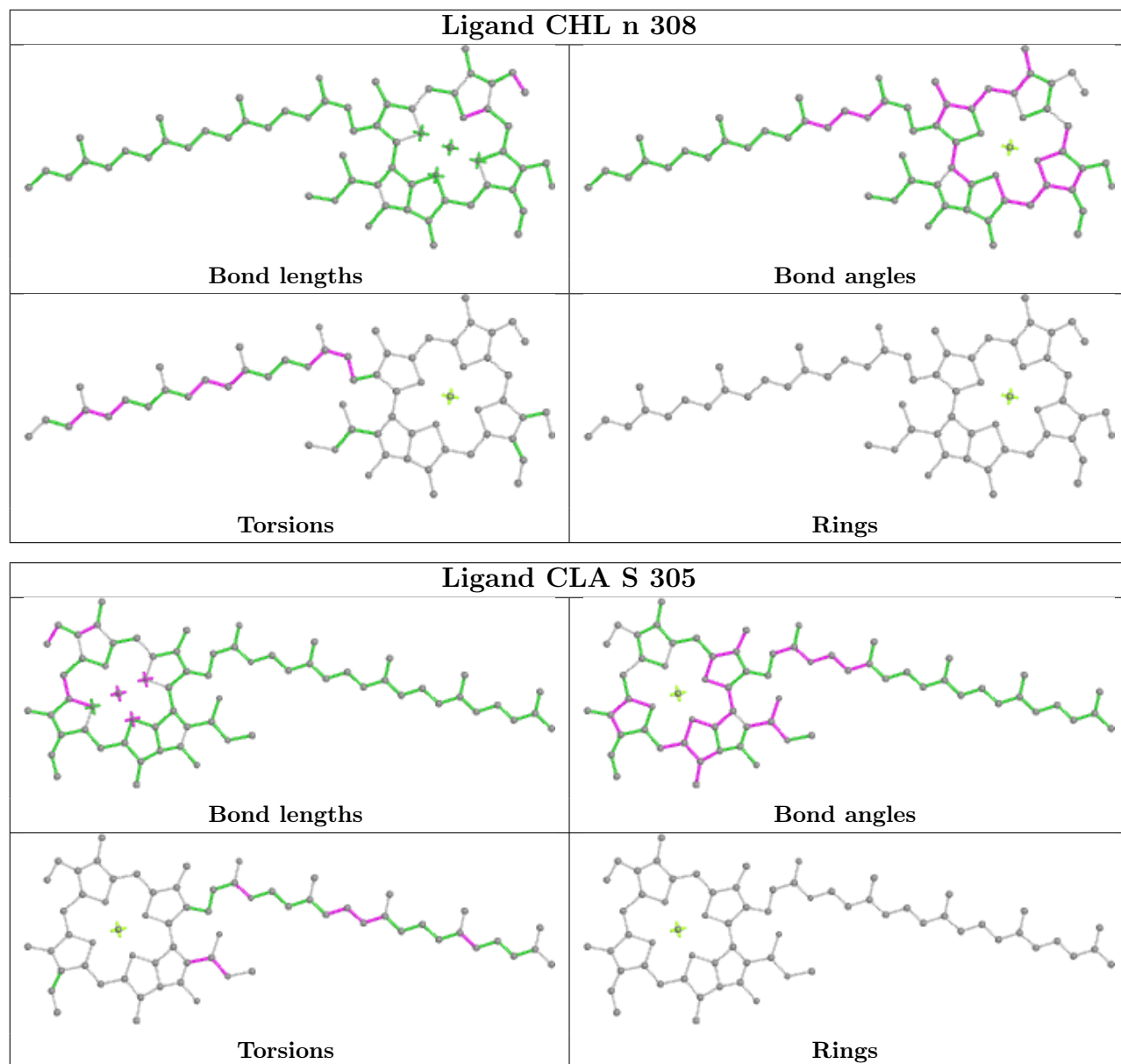
There are no ring outliers.

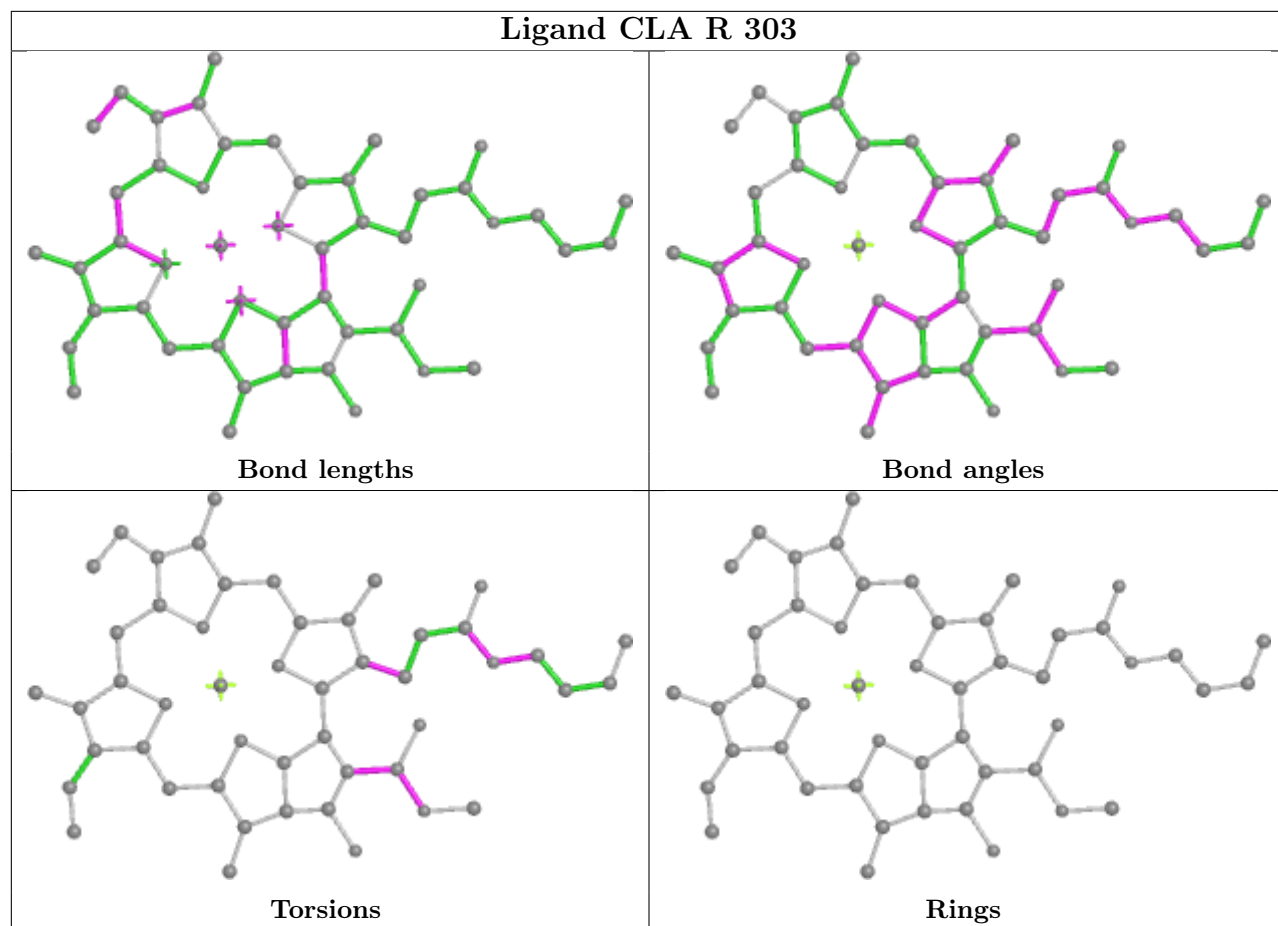
No monomer is involved in short contacts.

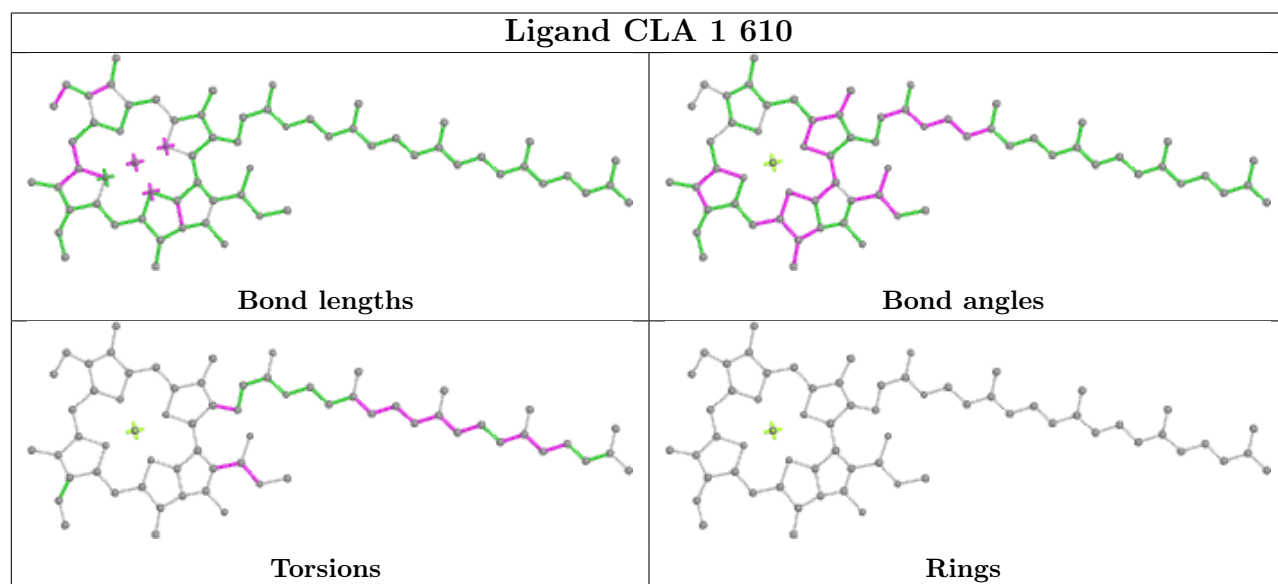
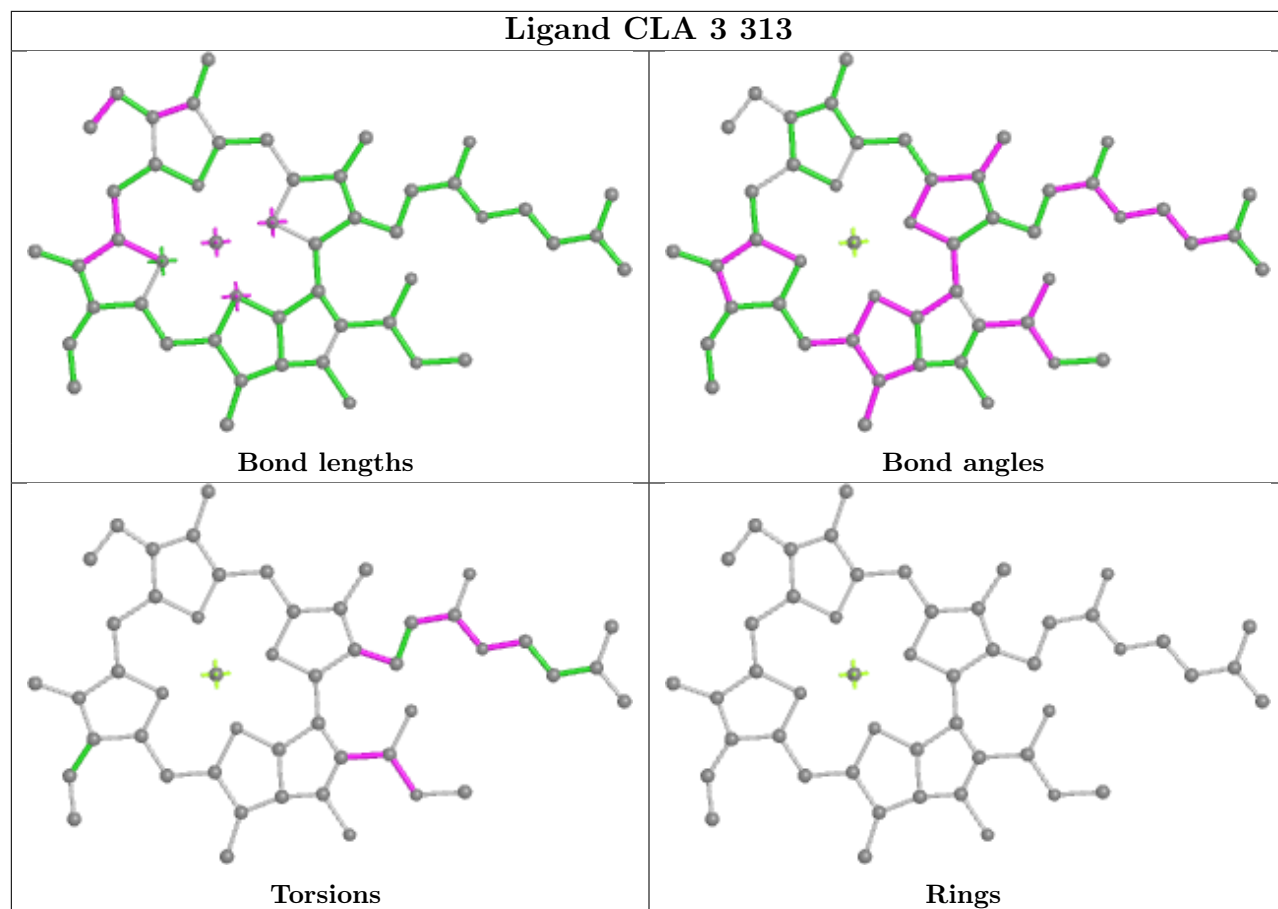
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

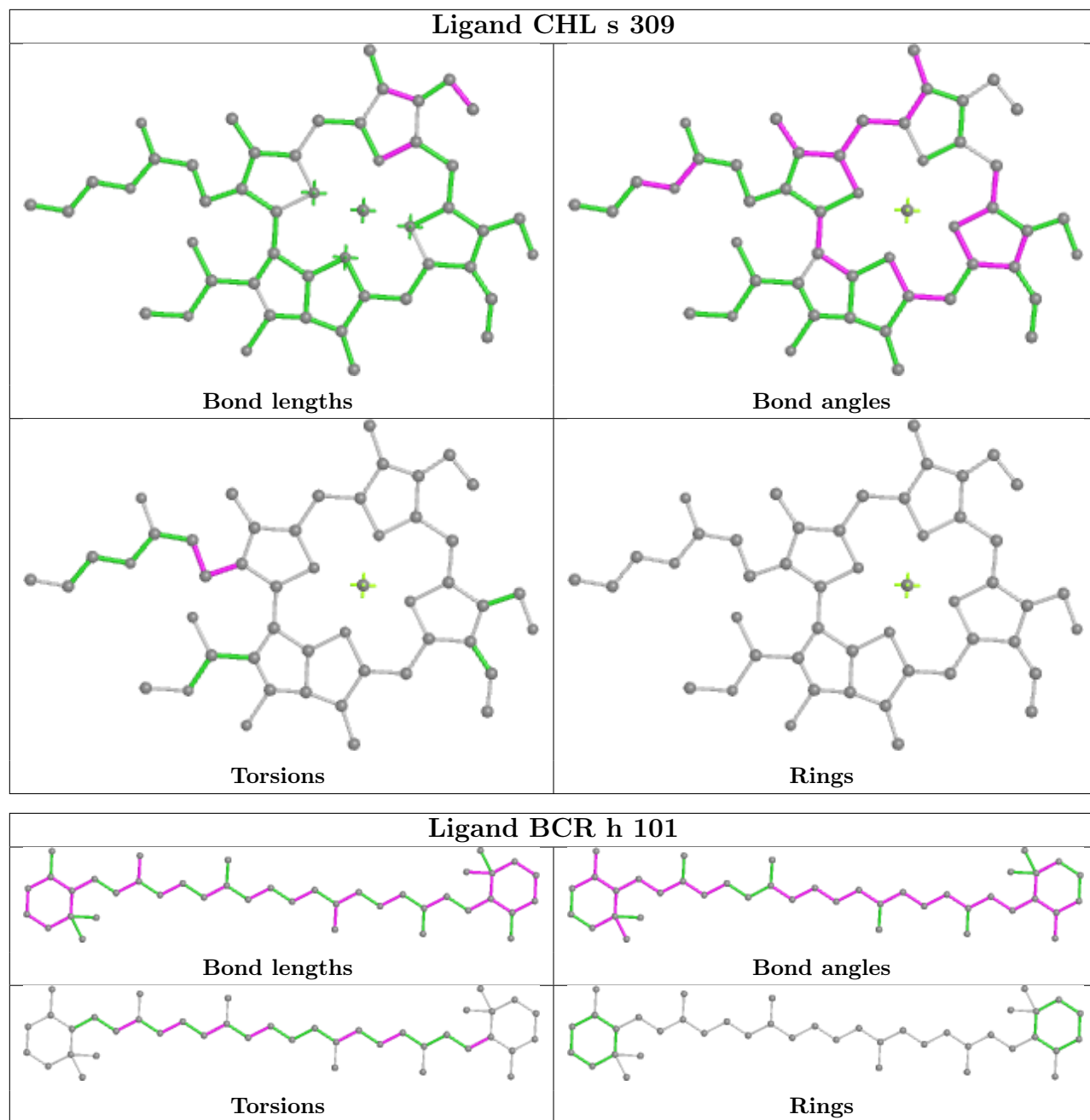


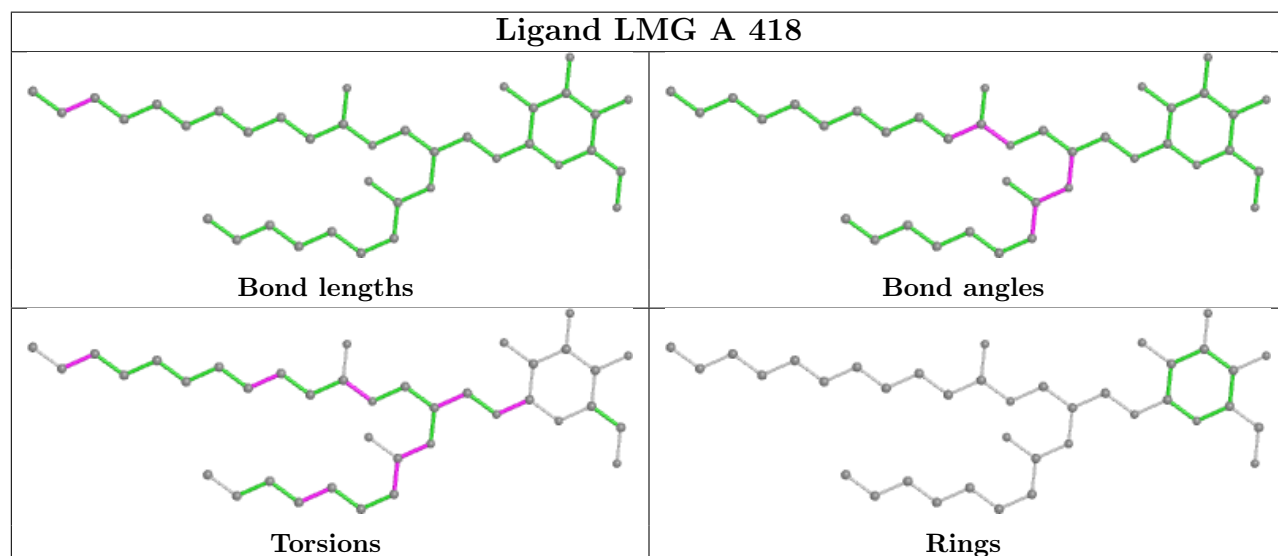
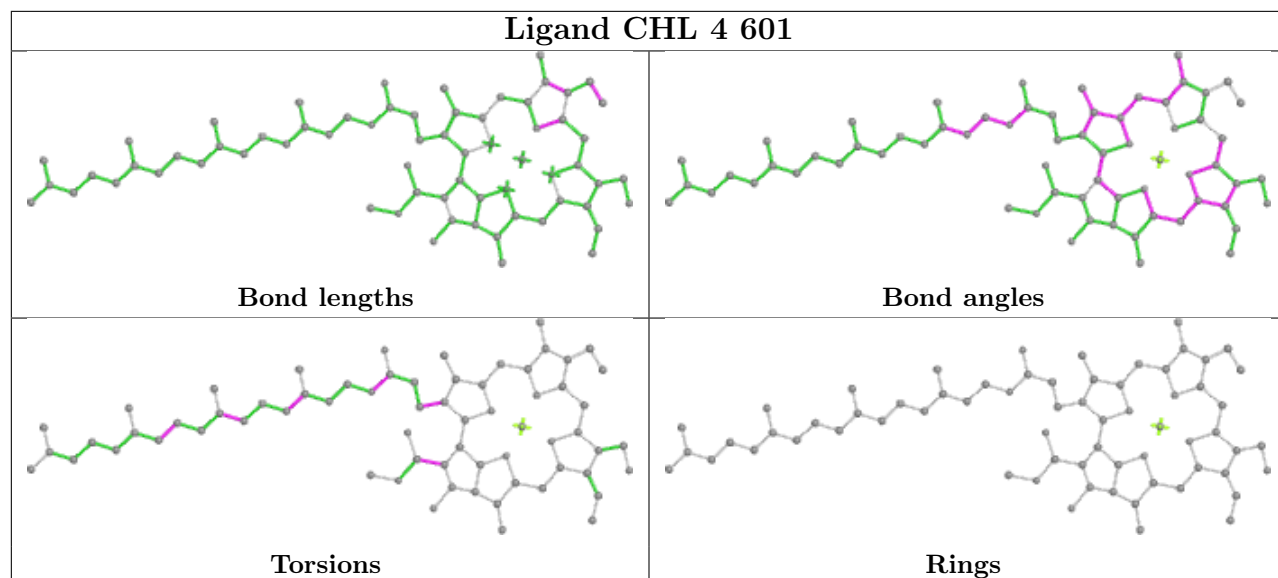


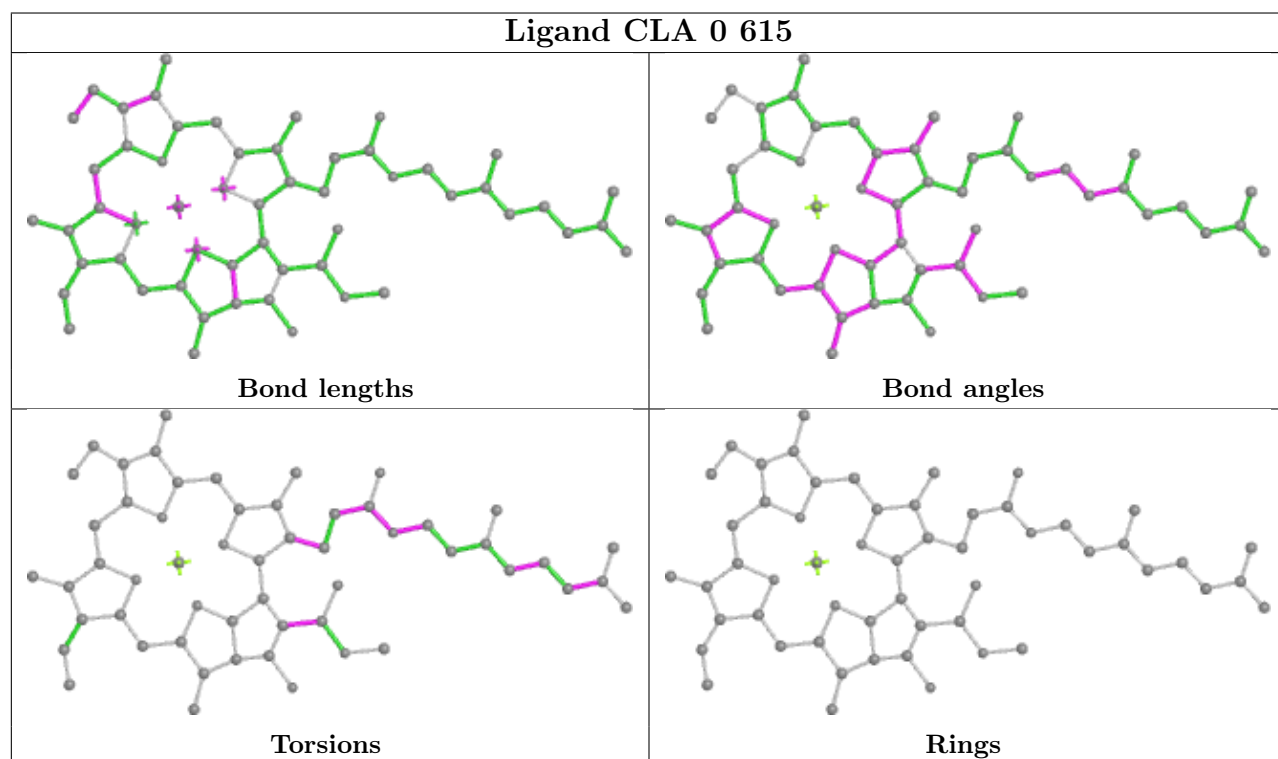
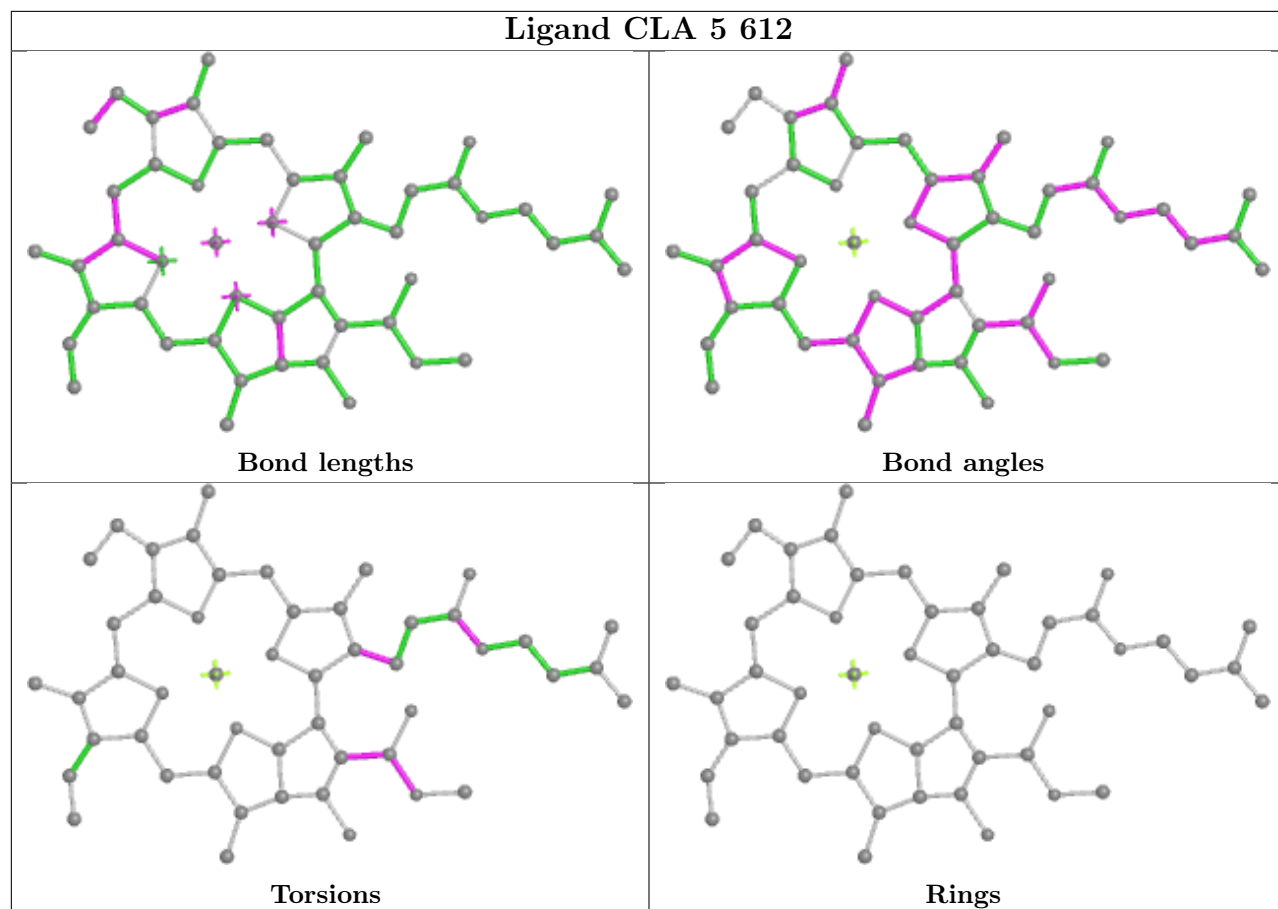


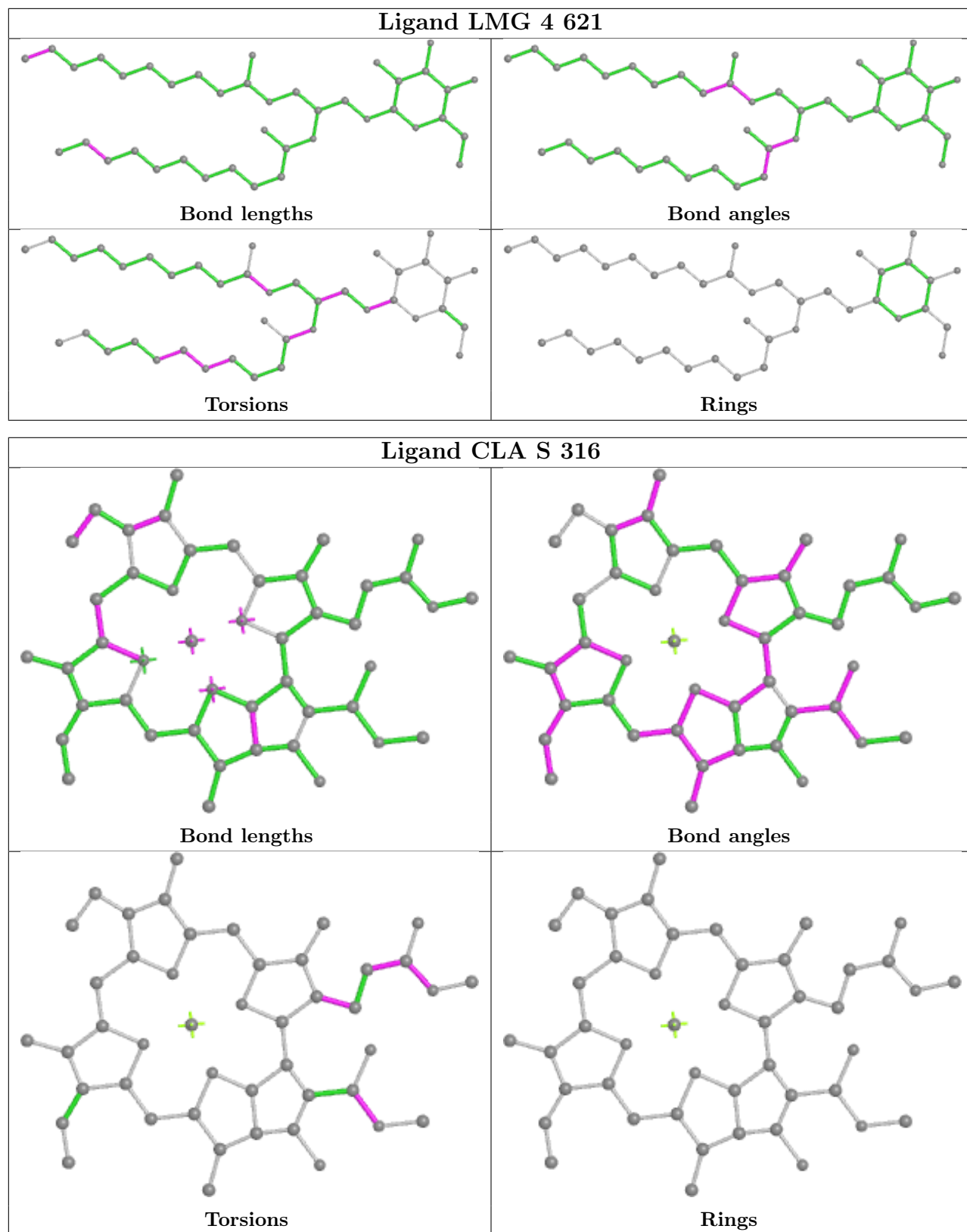


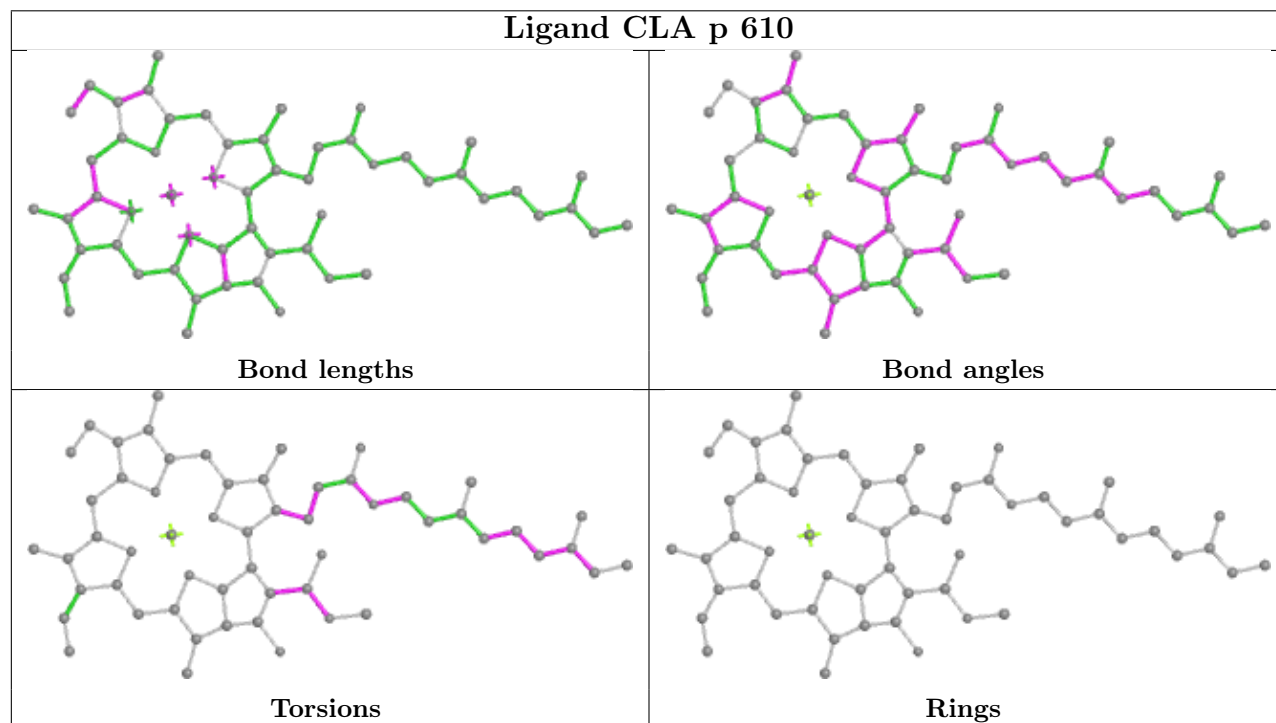
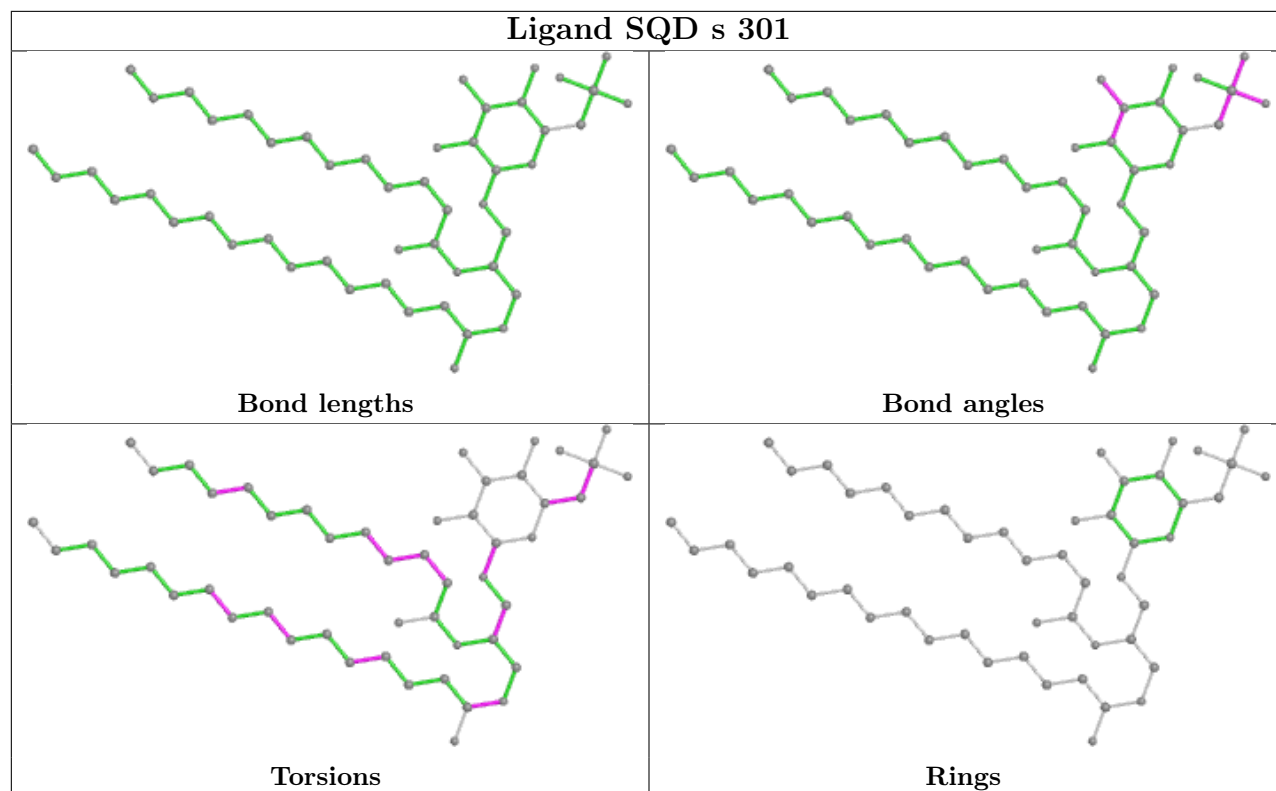


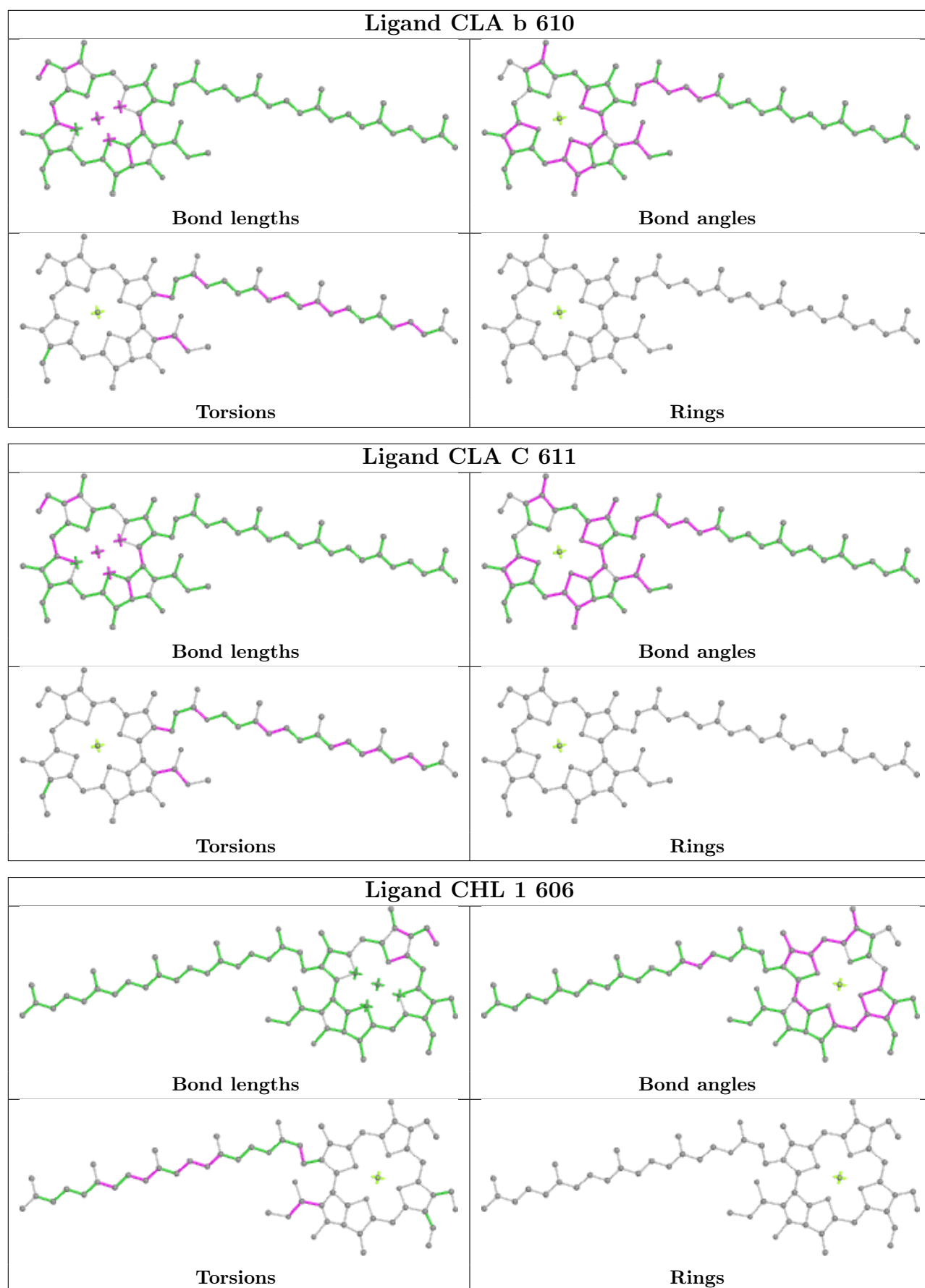


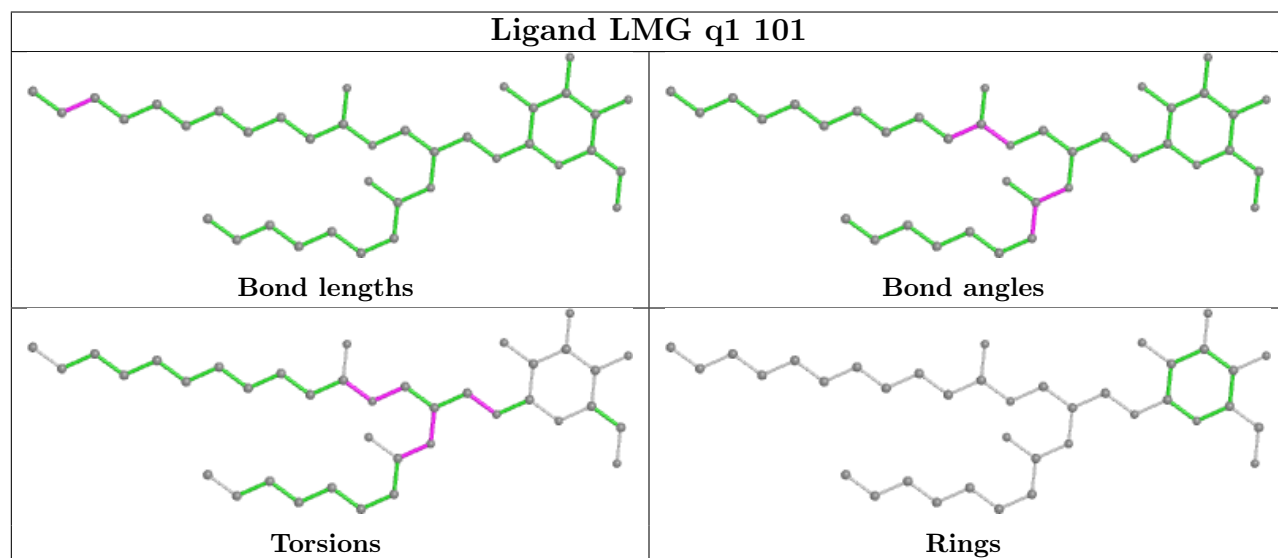
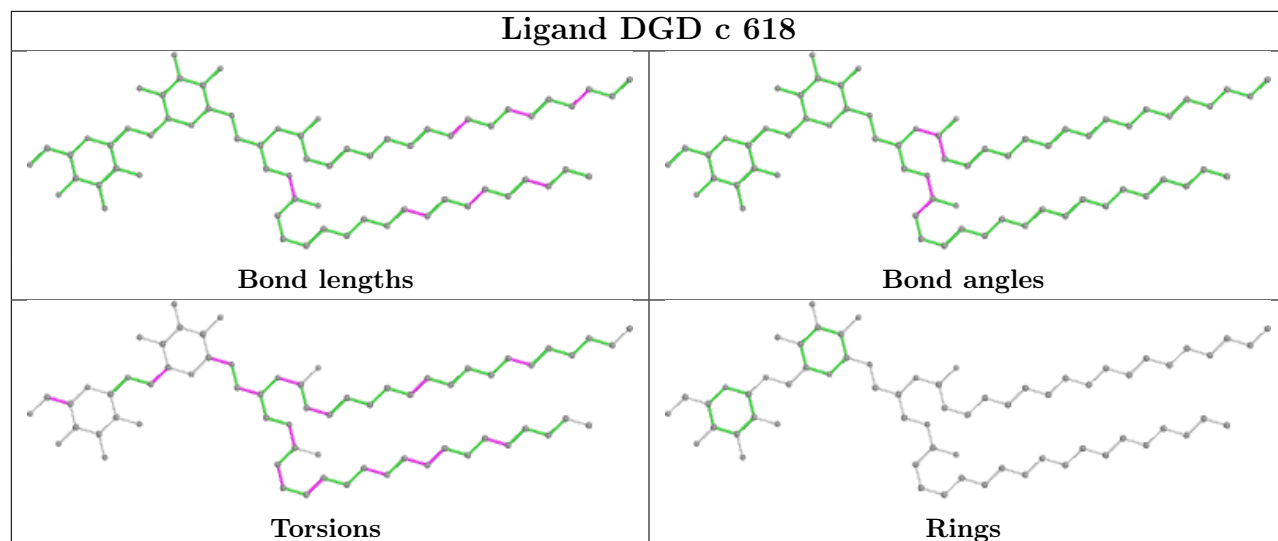


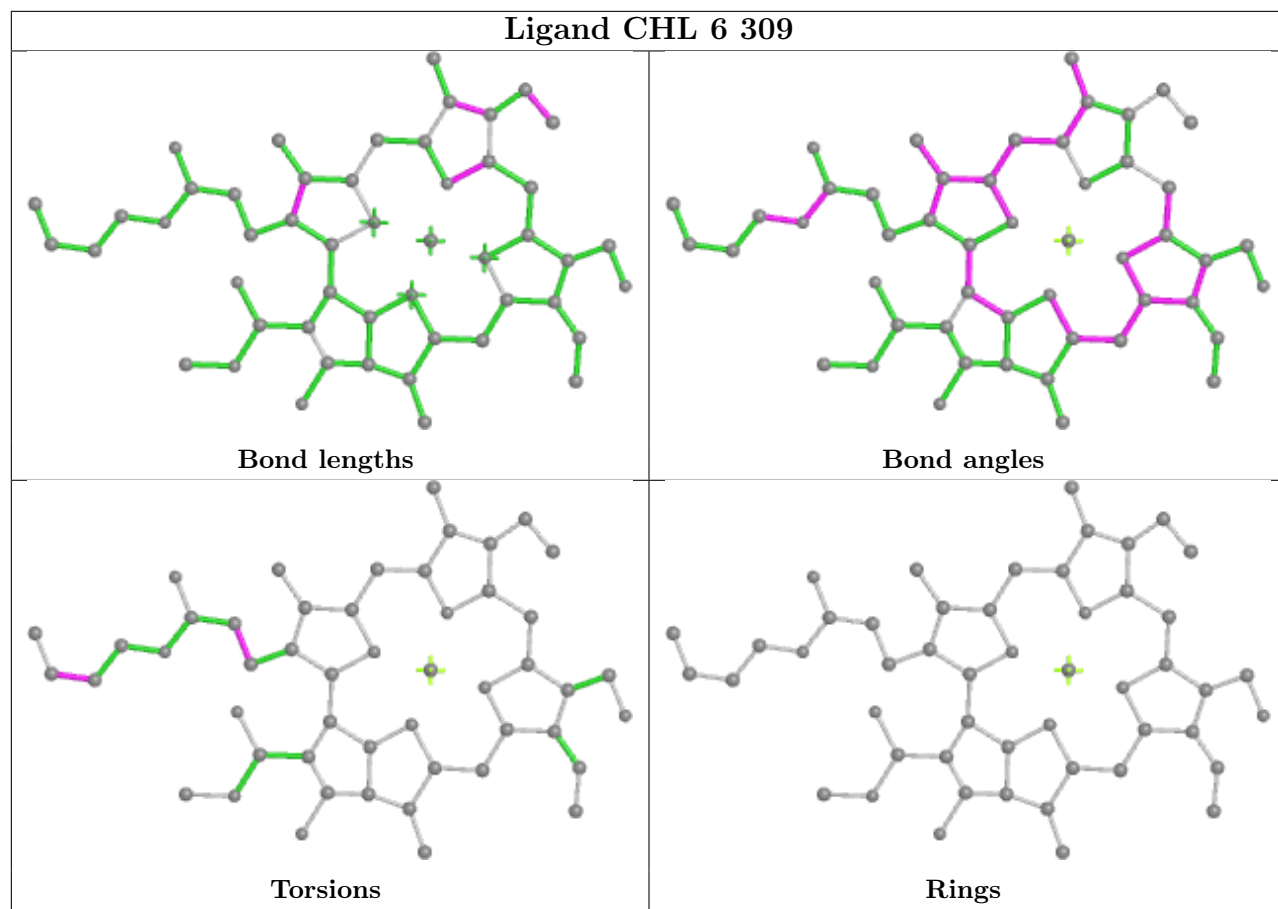


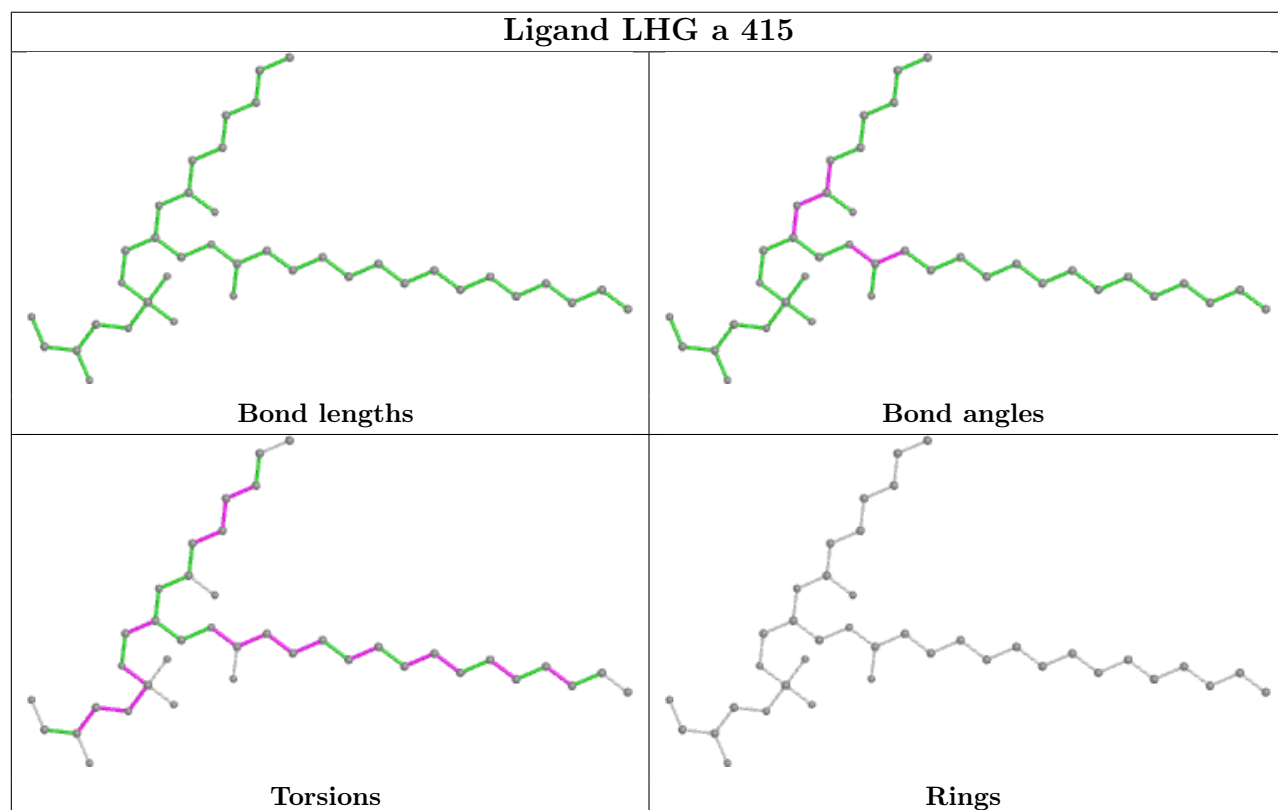
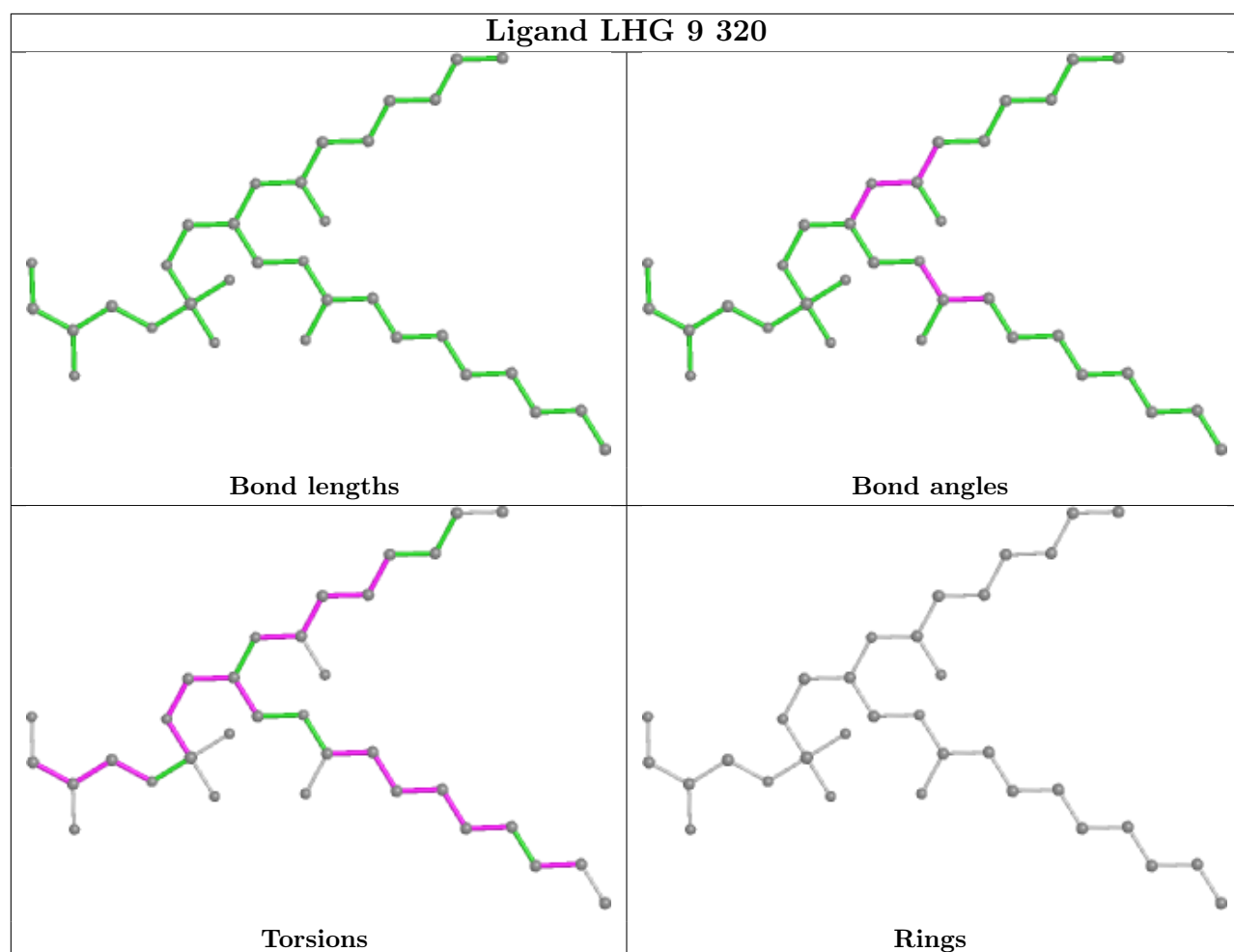


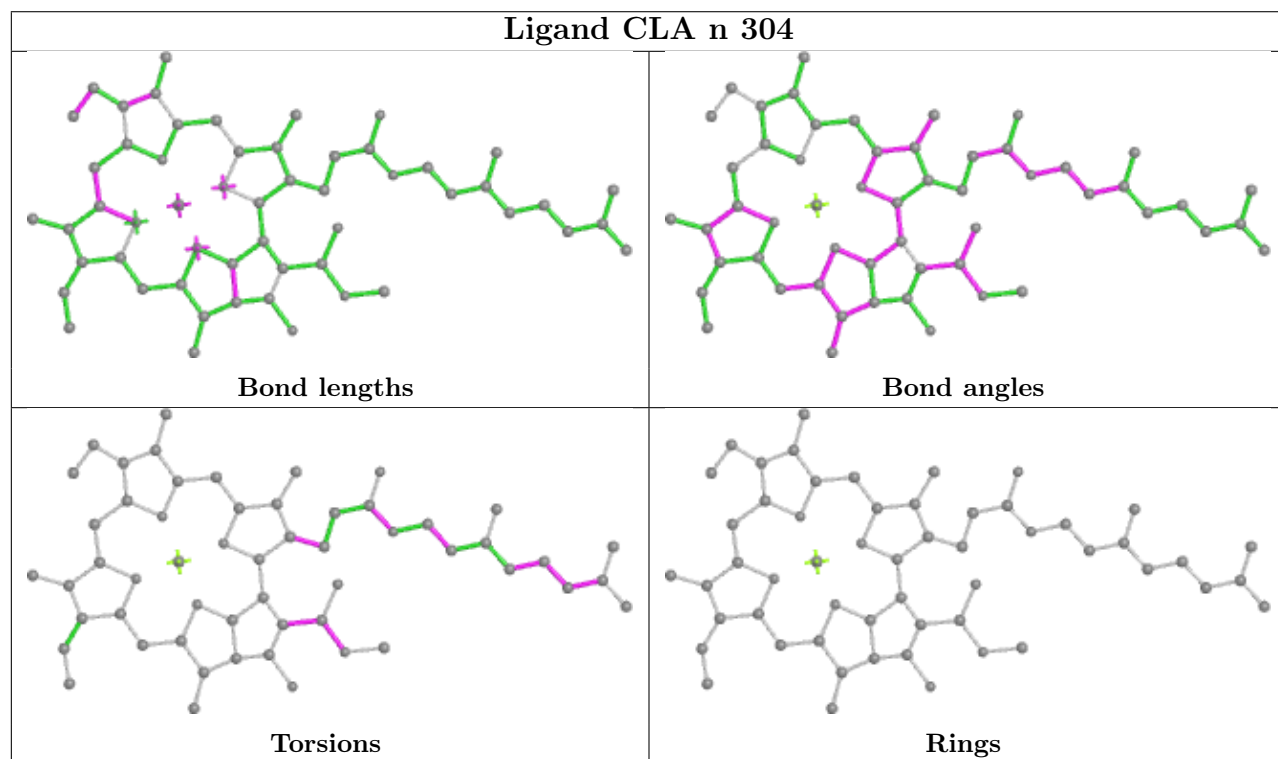
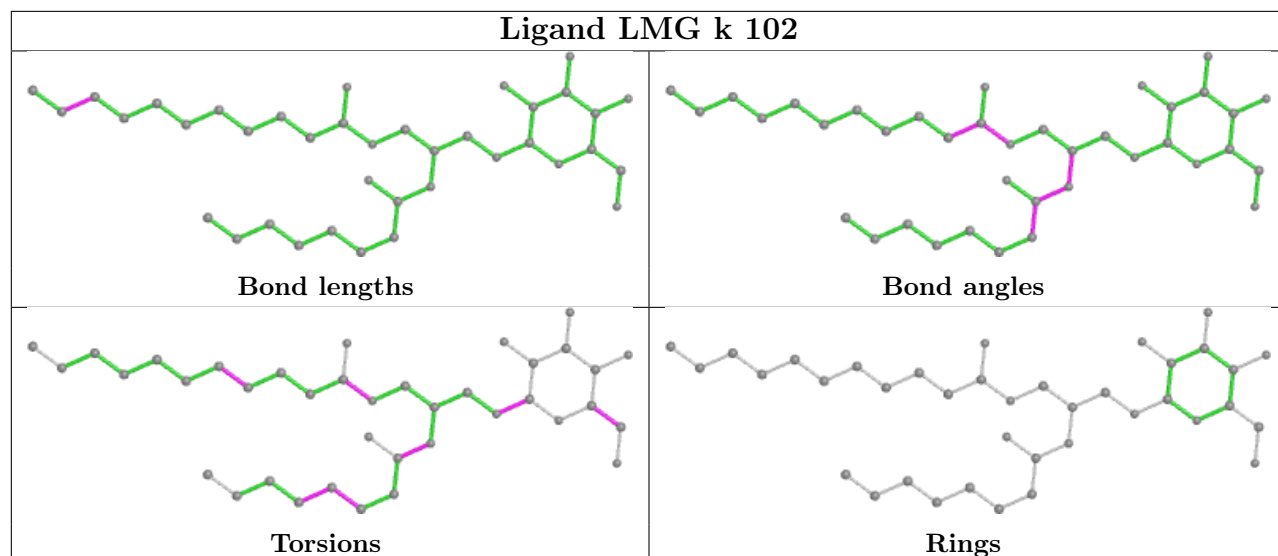


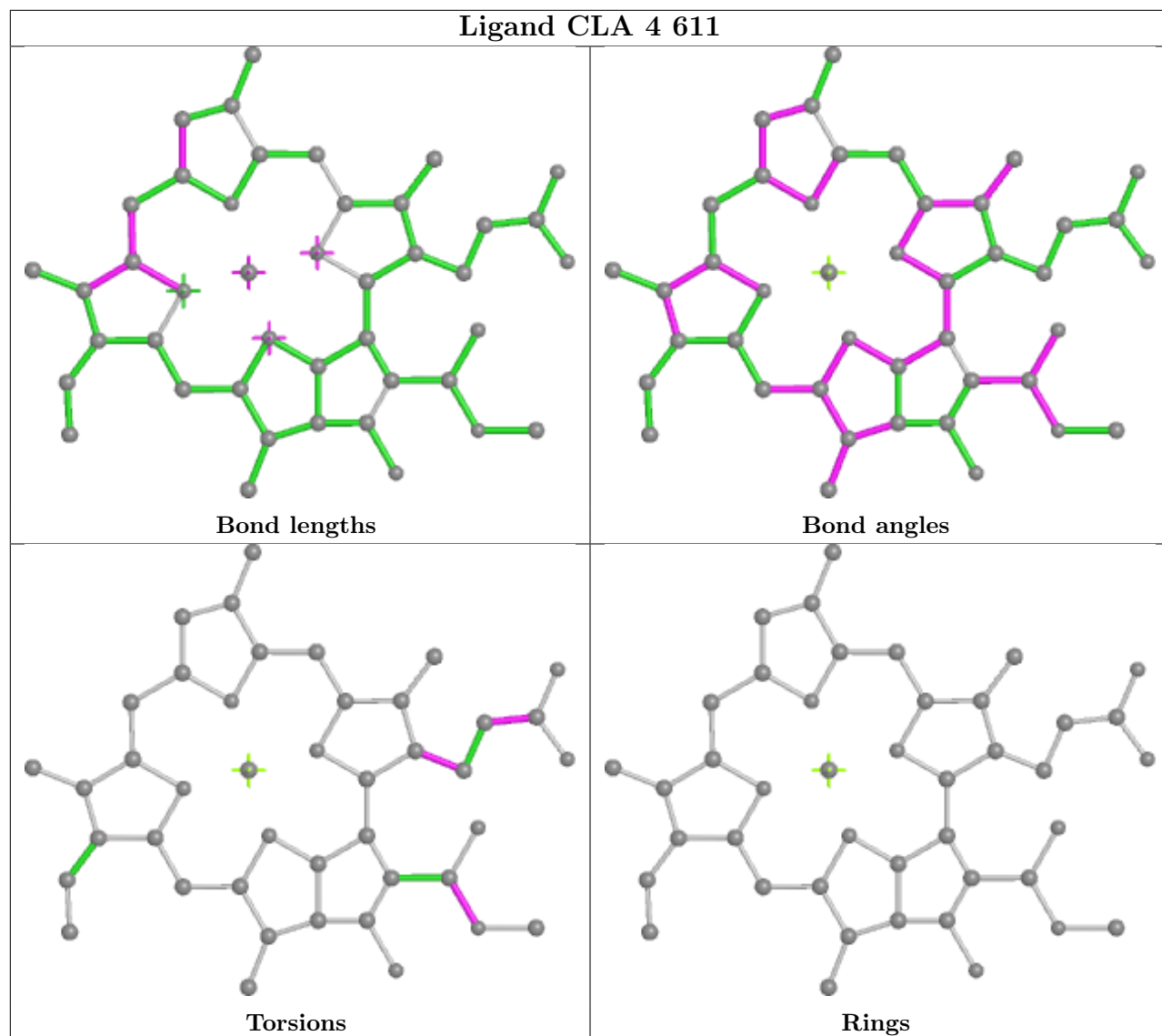


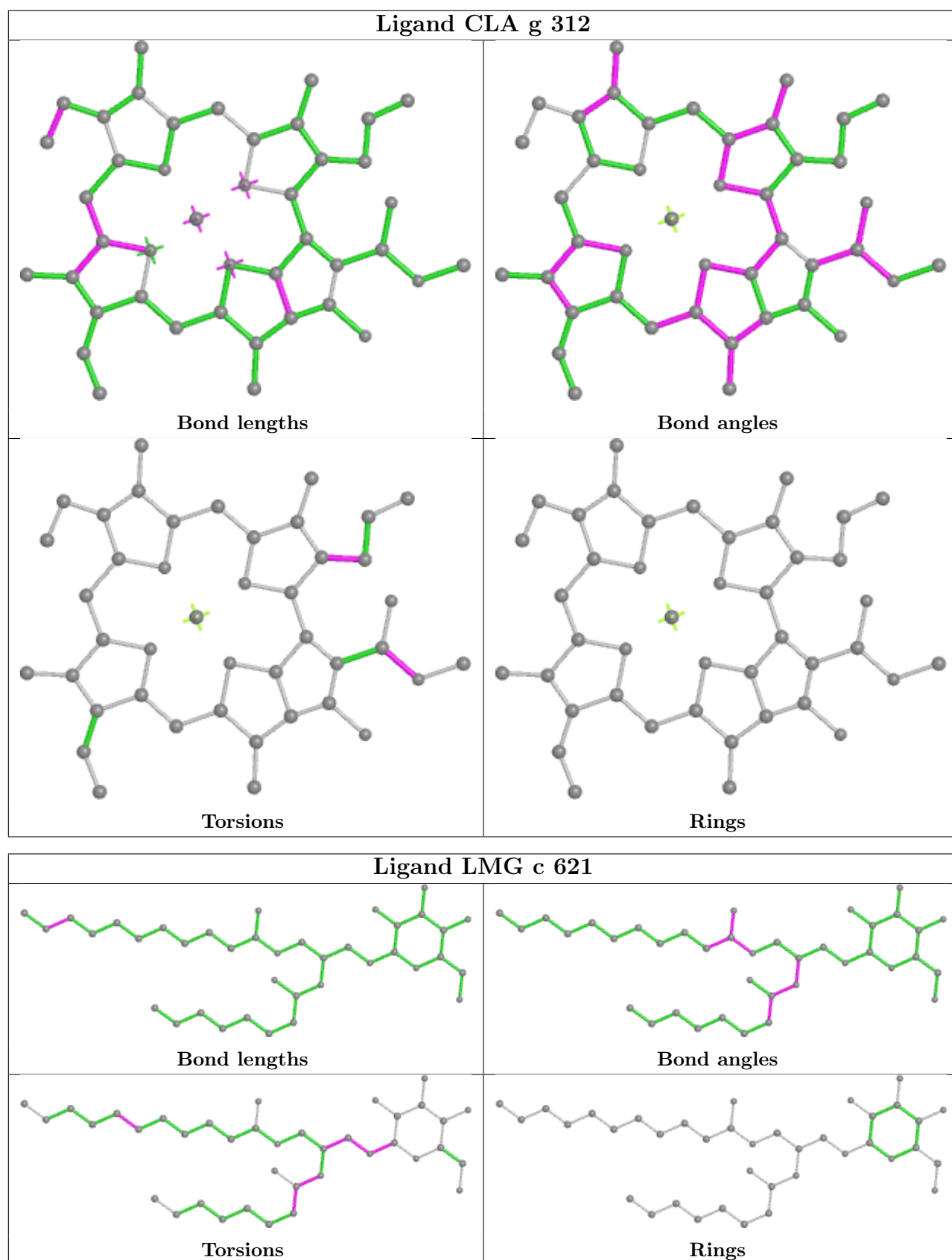


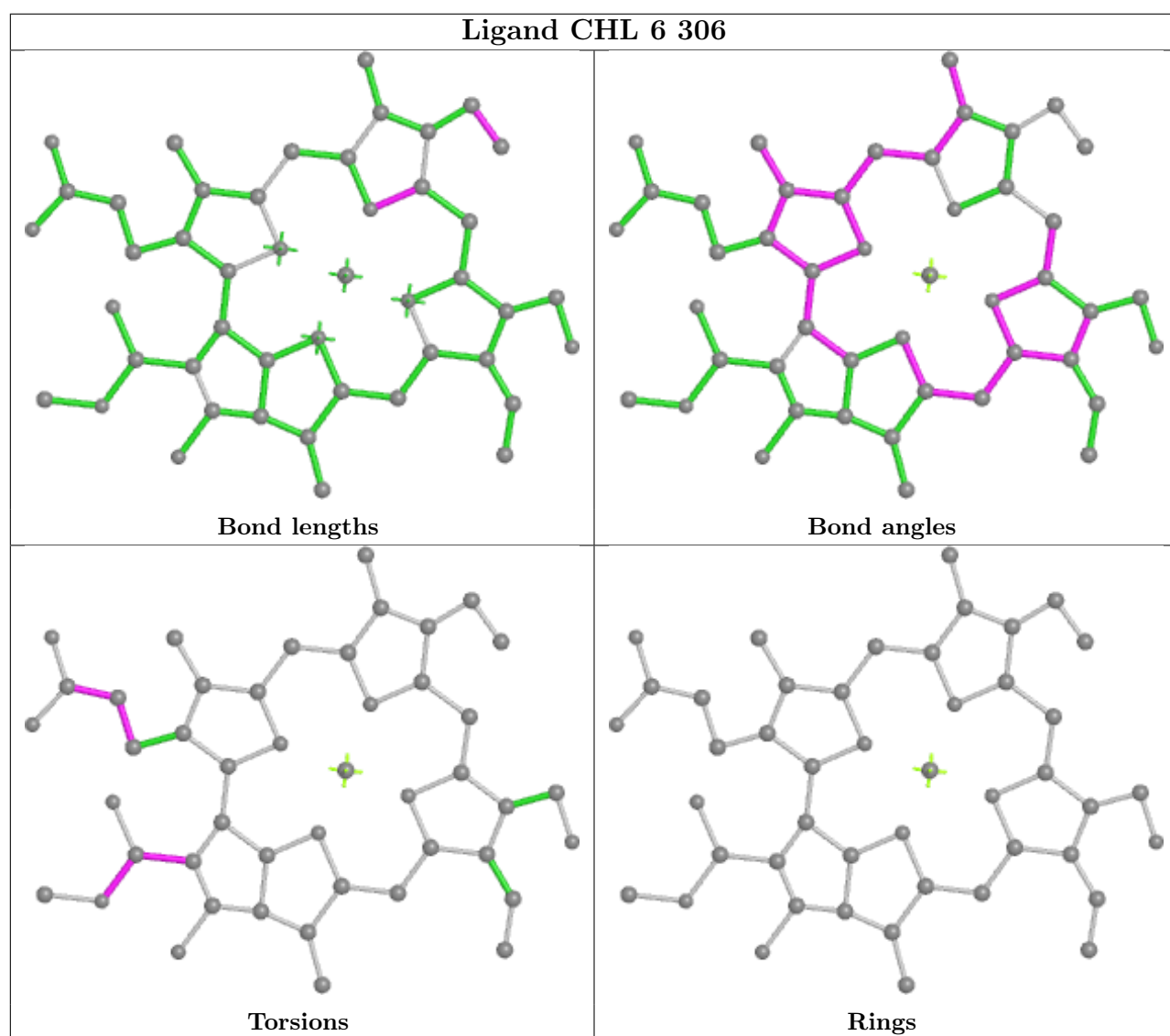
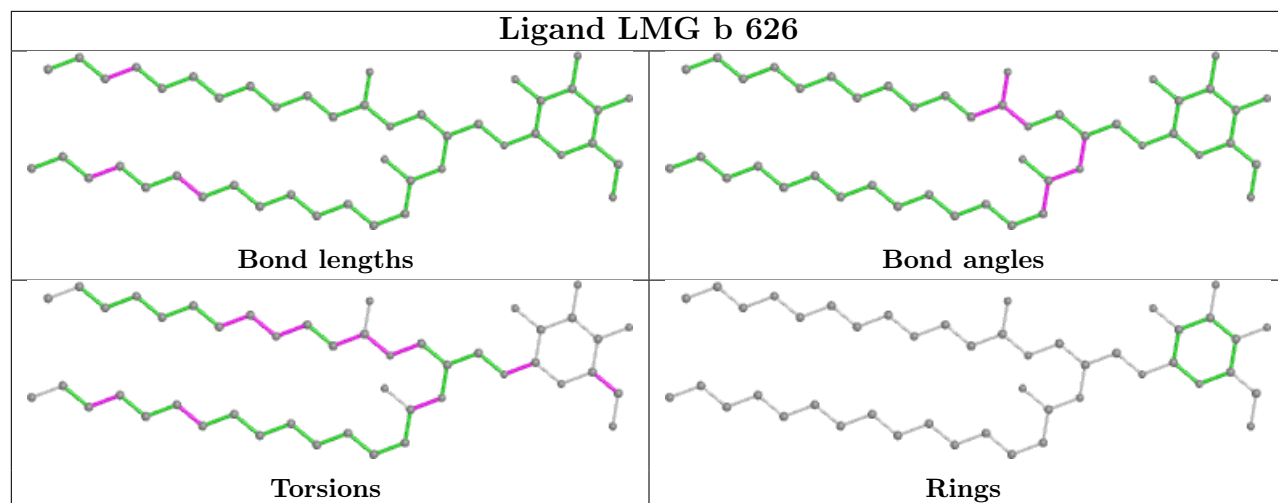


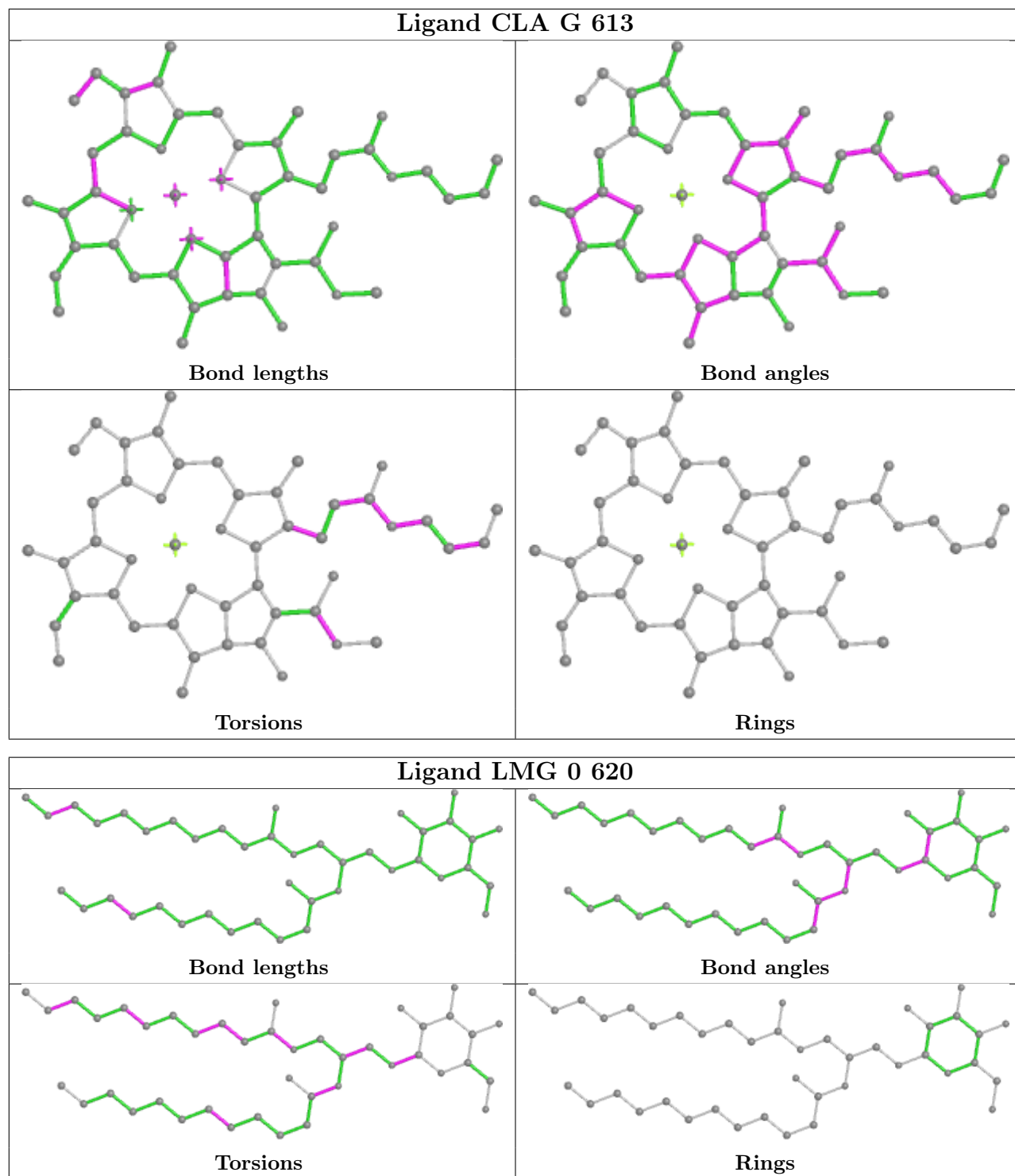


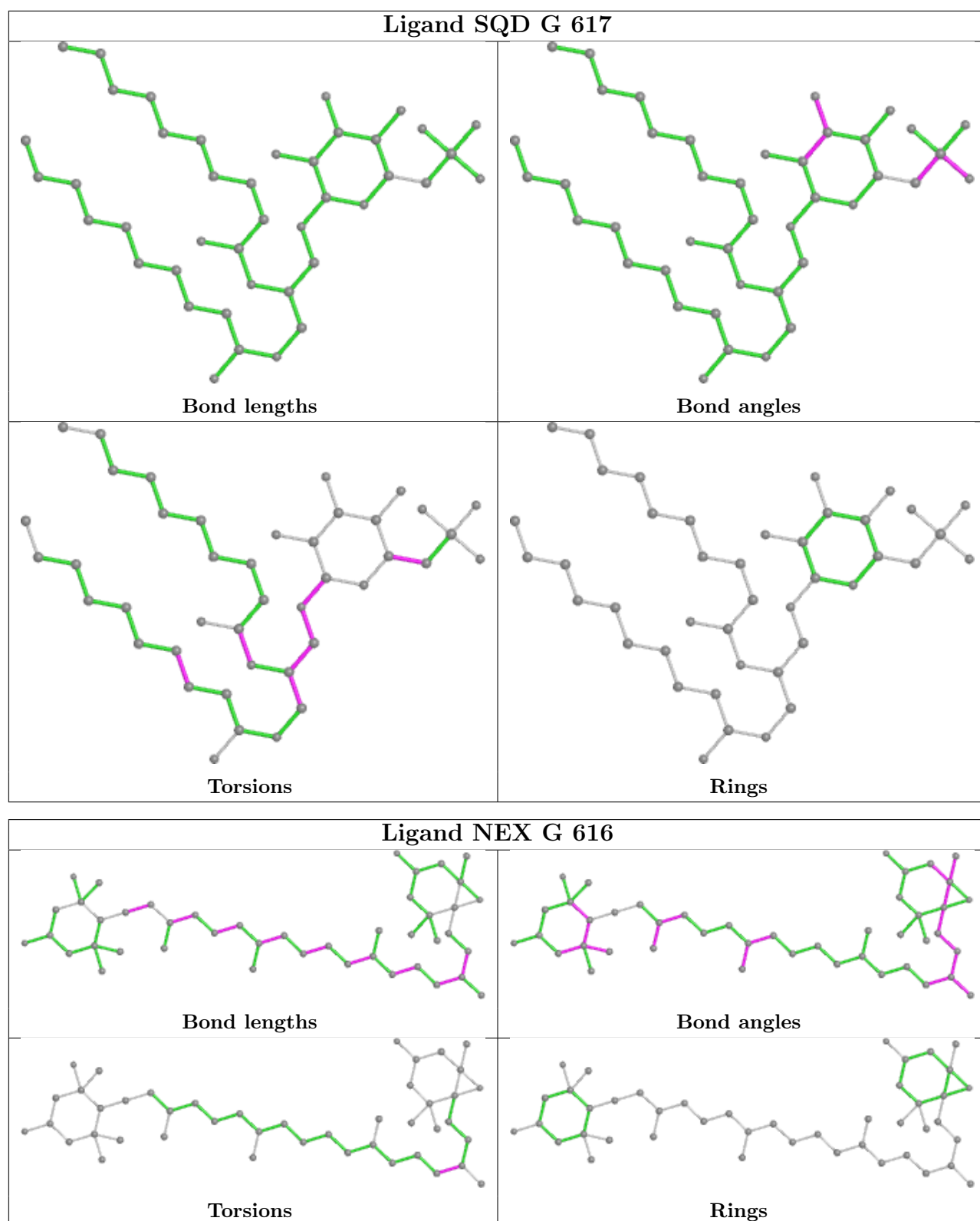


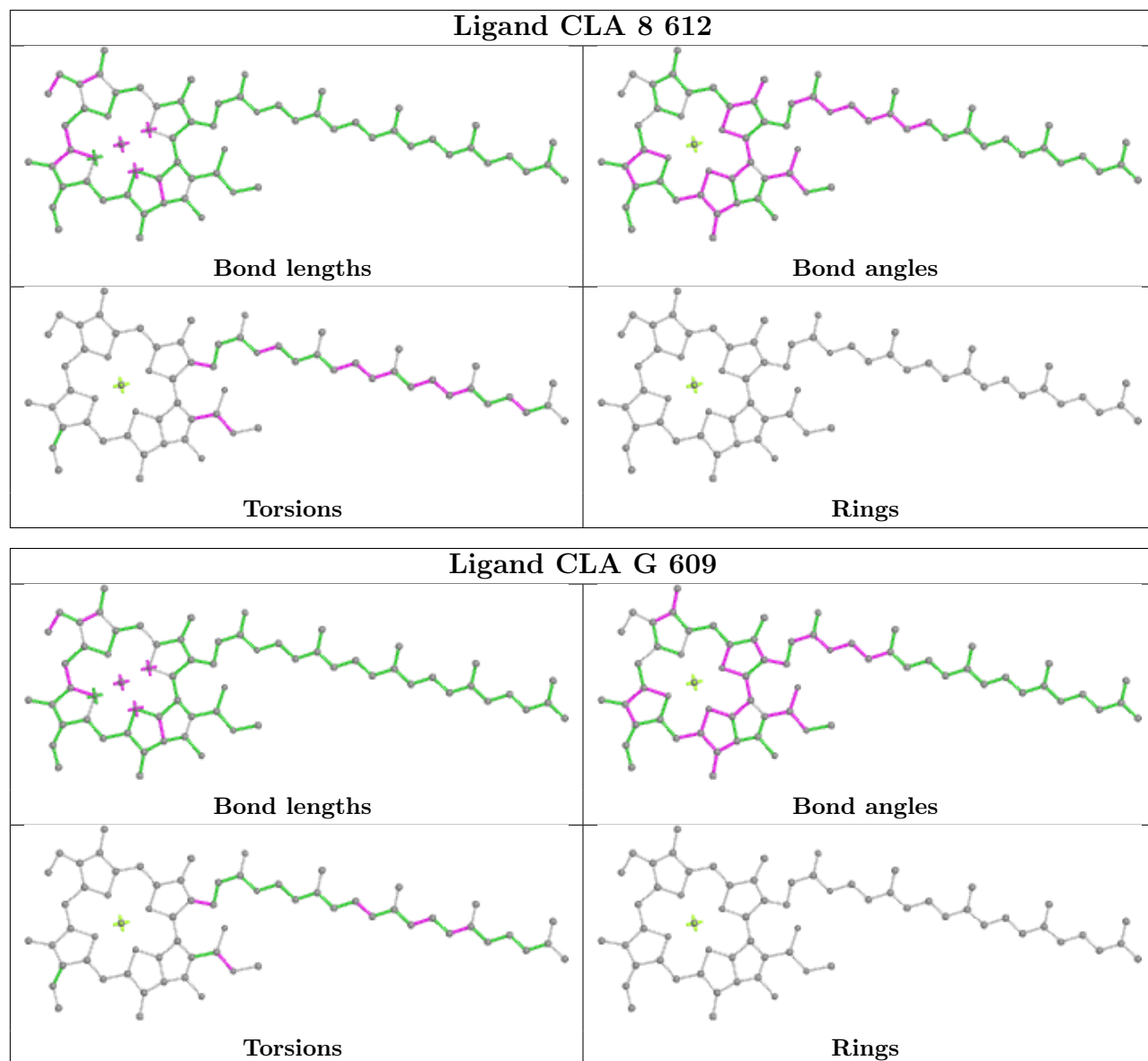


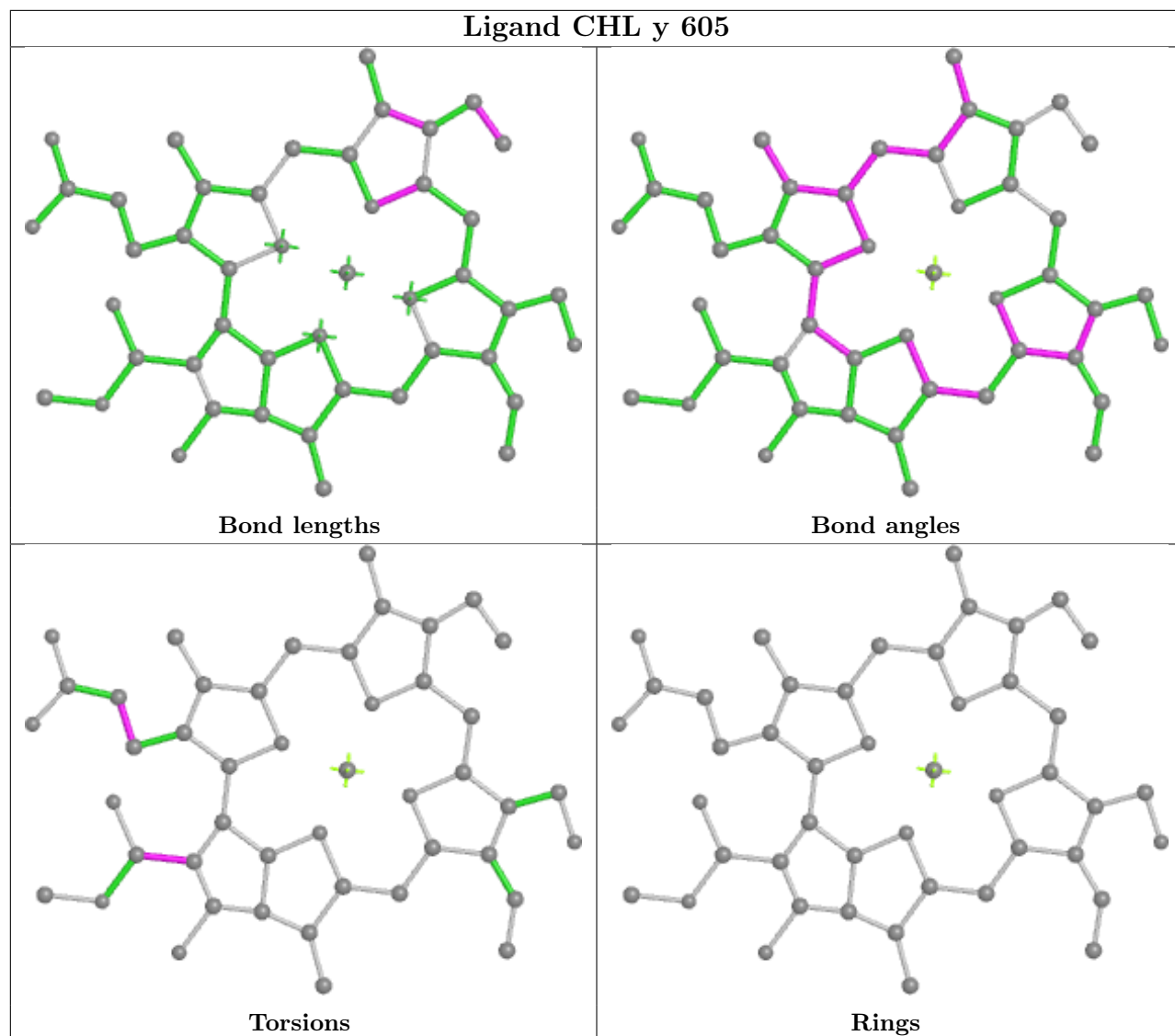


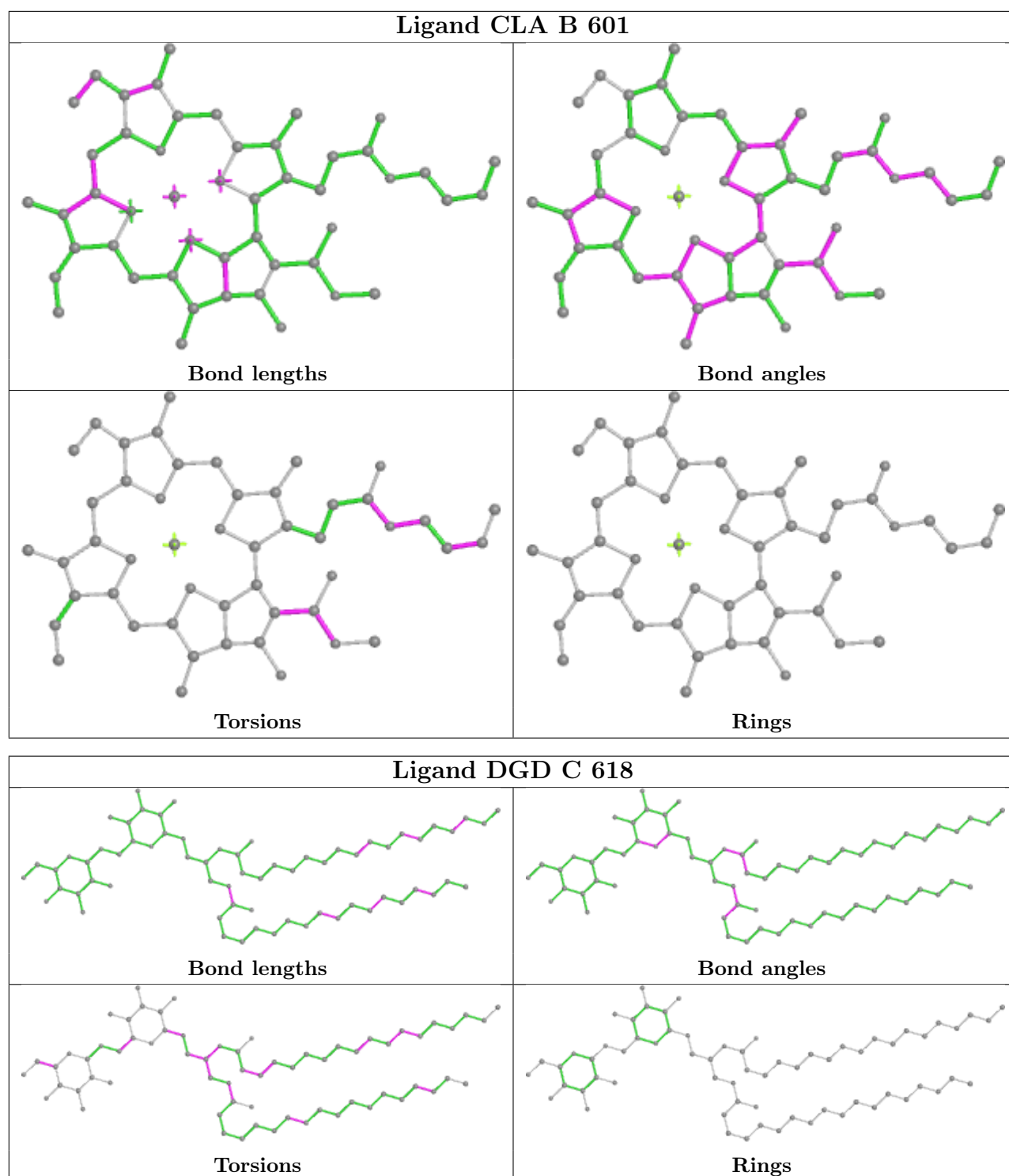


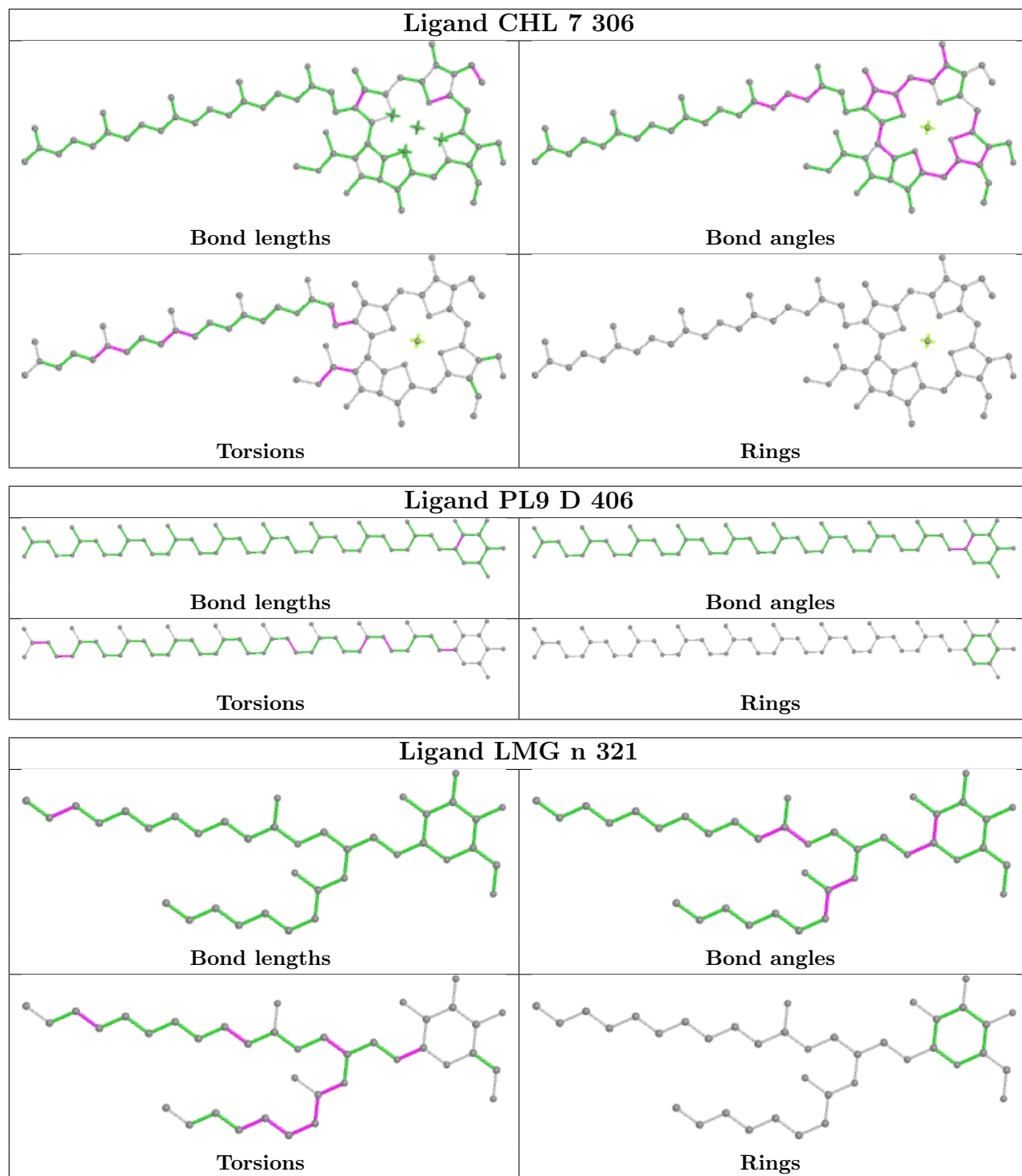


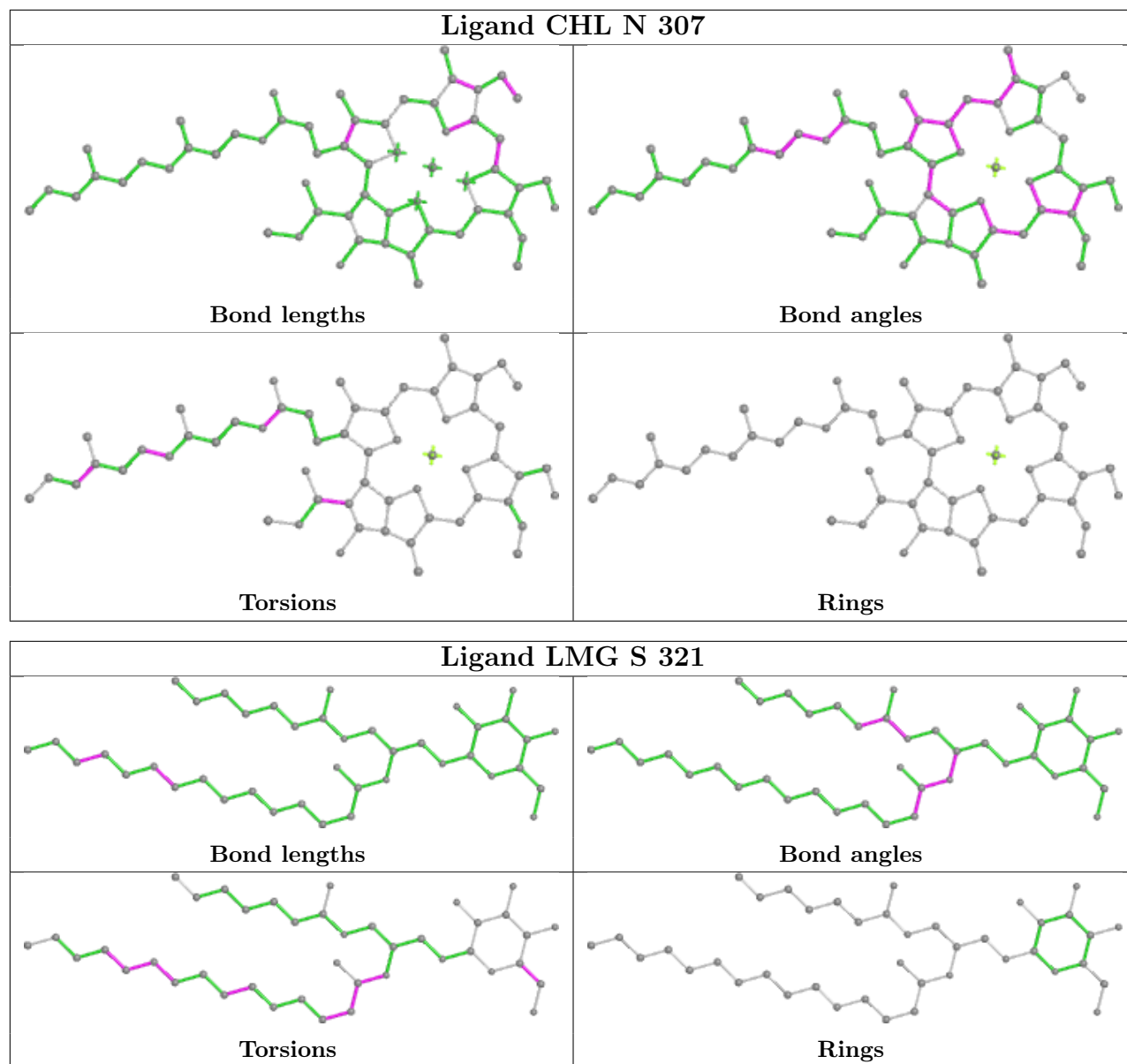


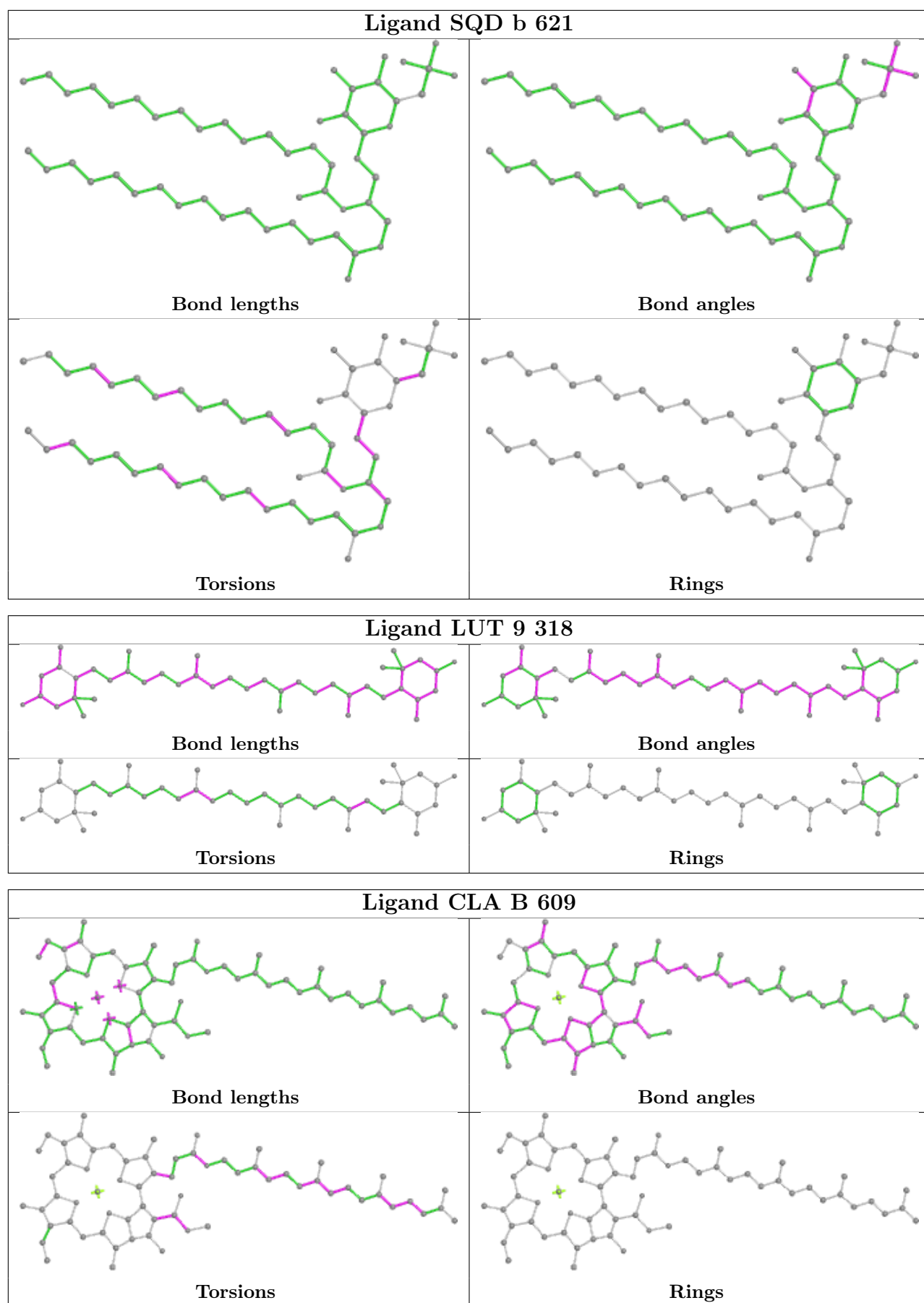


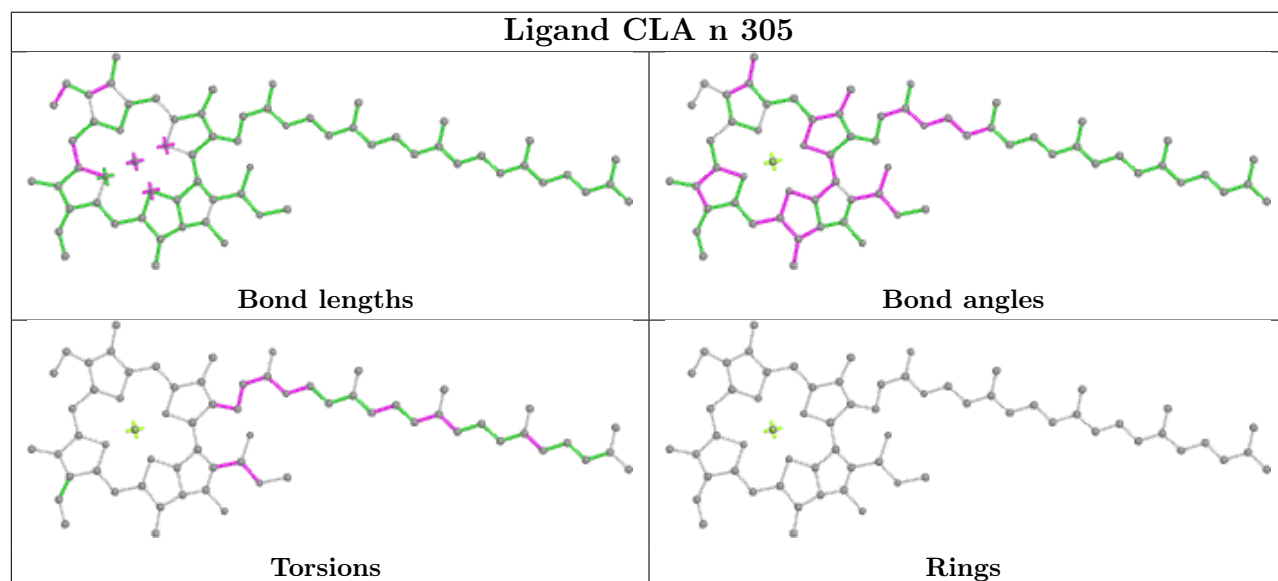
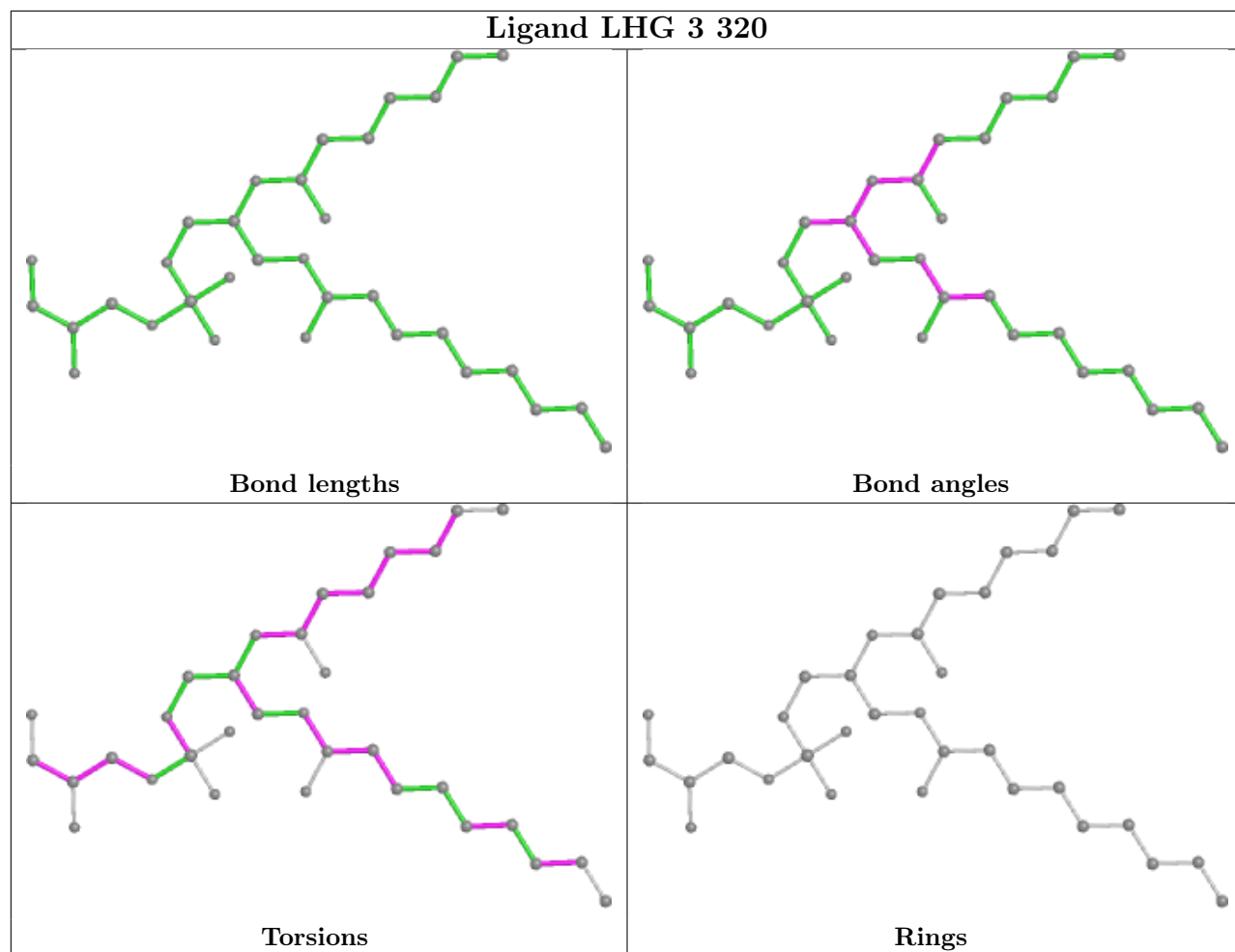


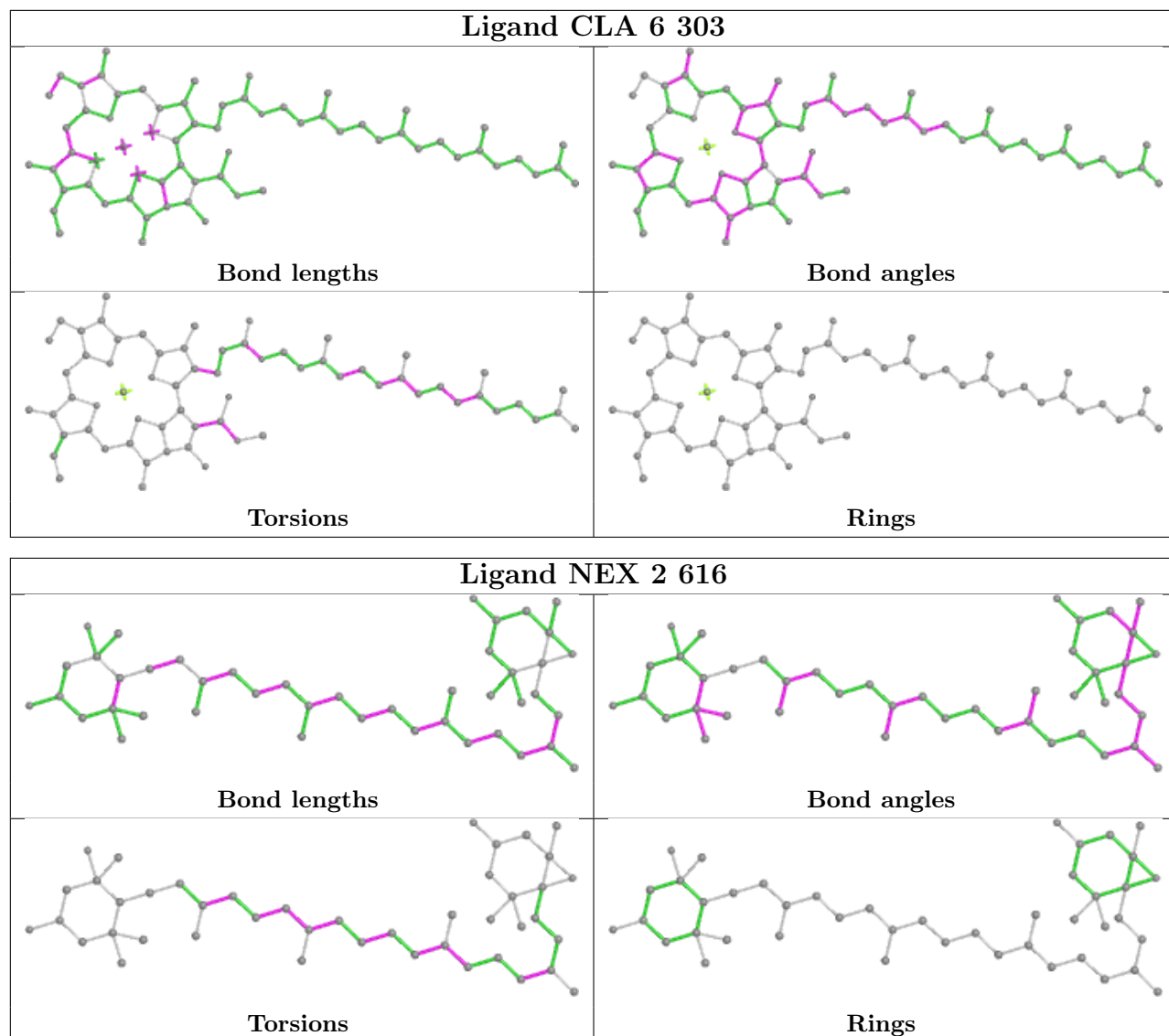


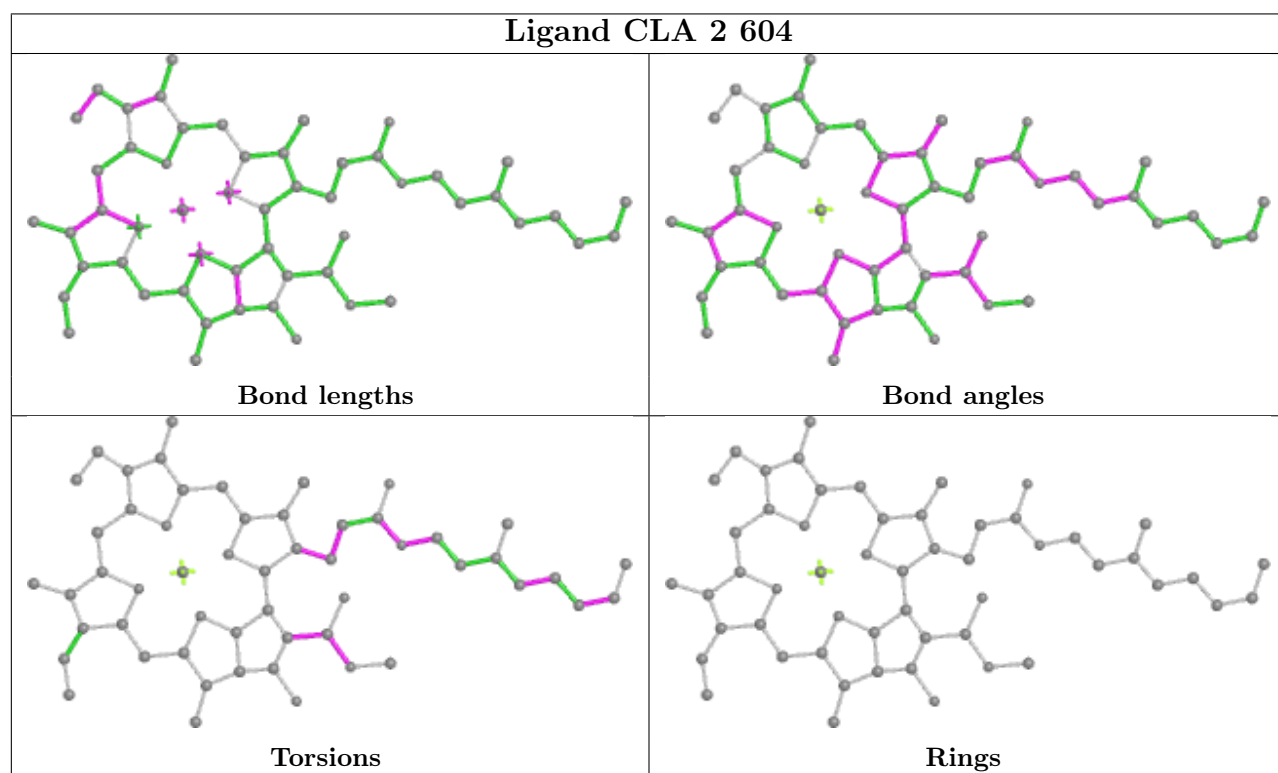
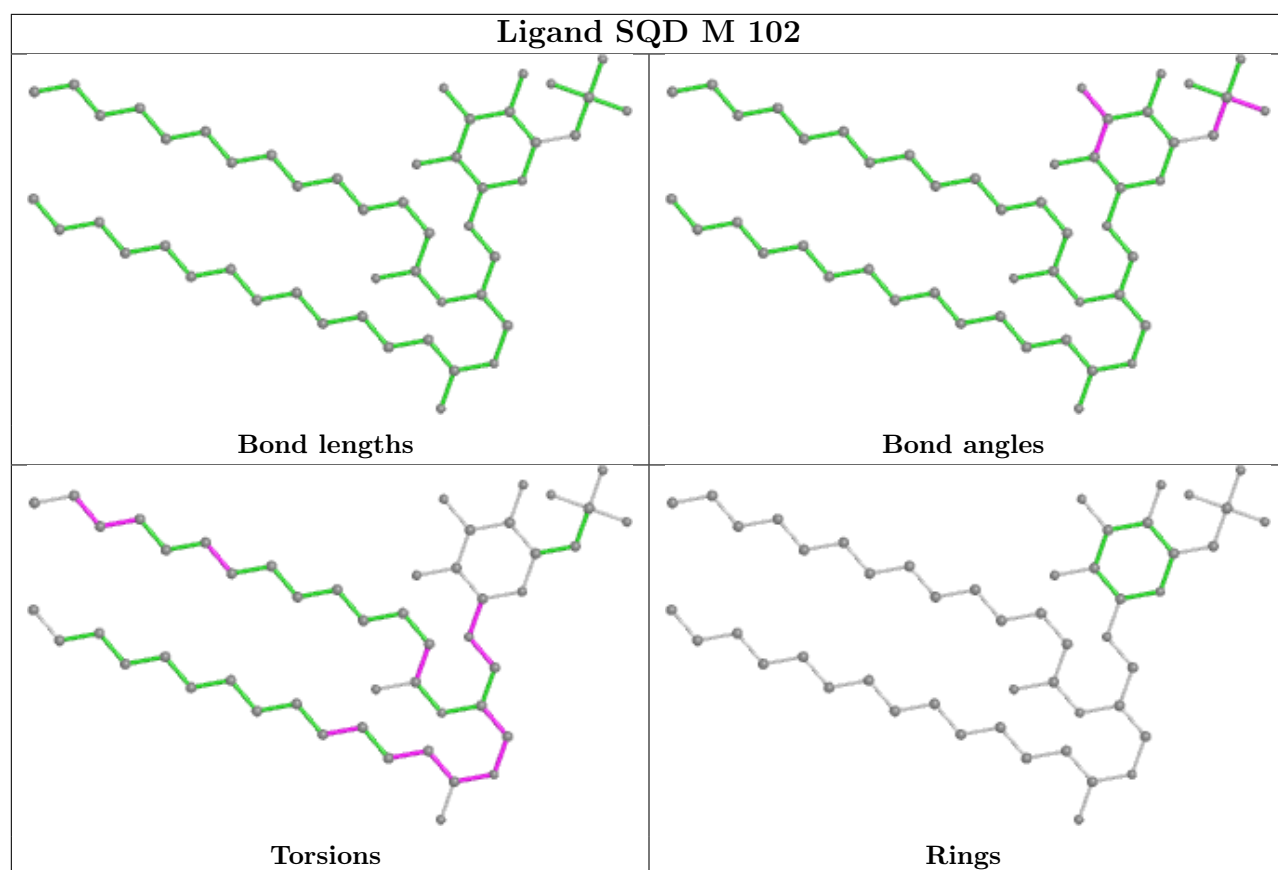


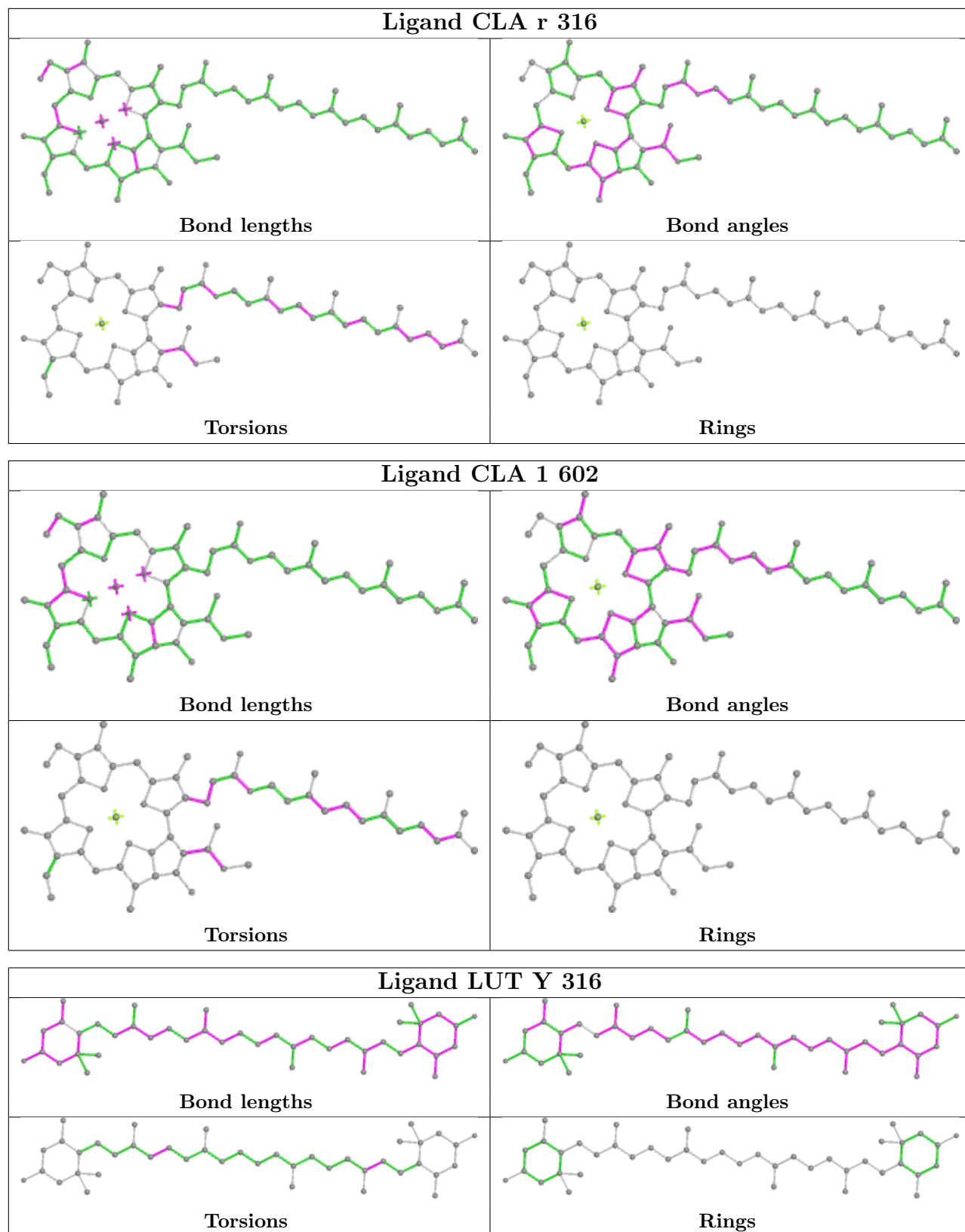


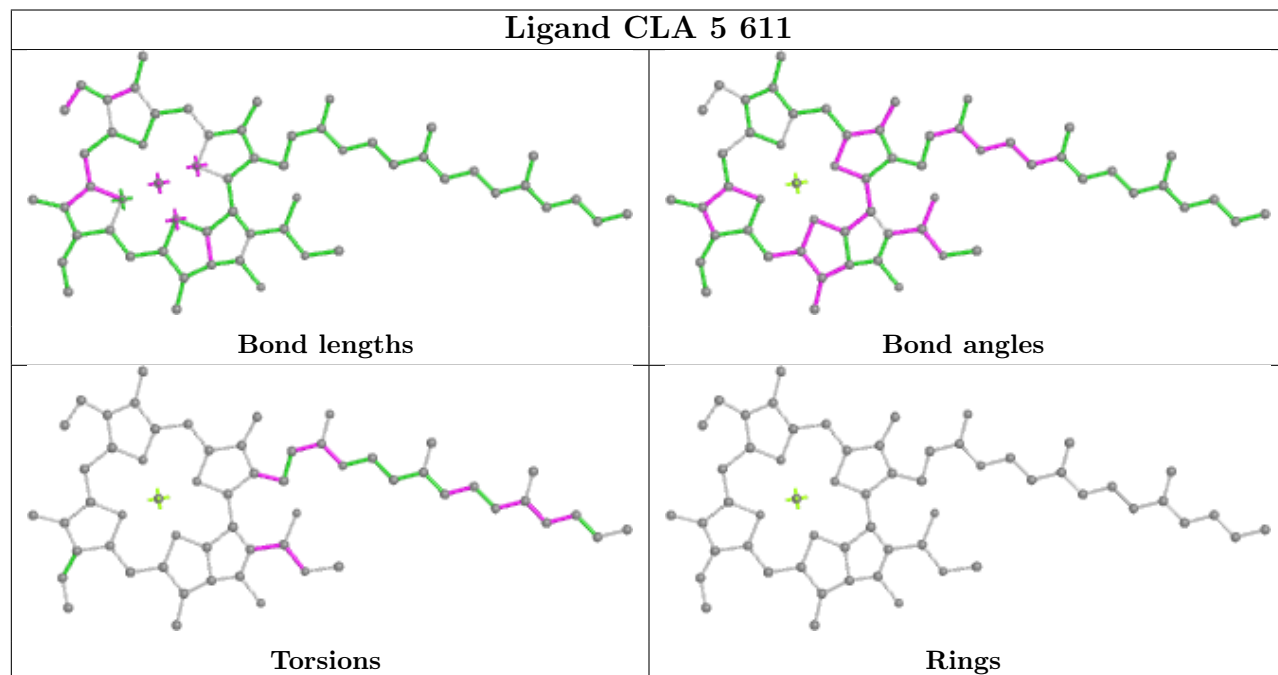
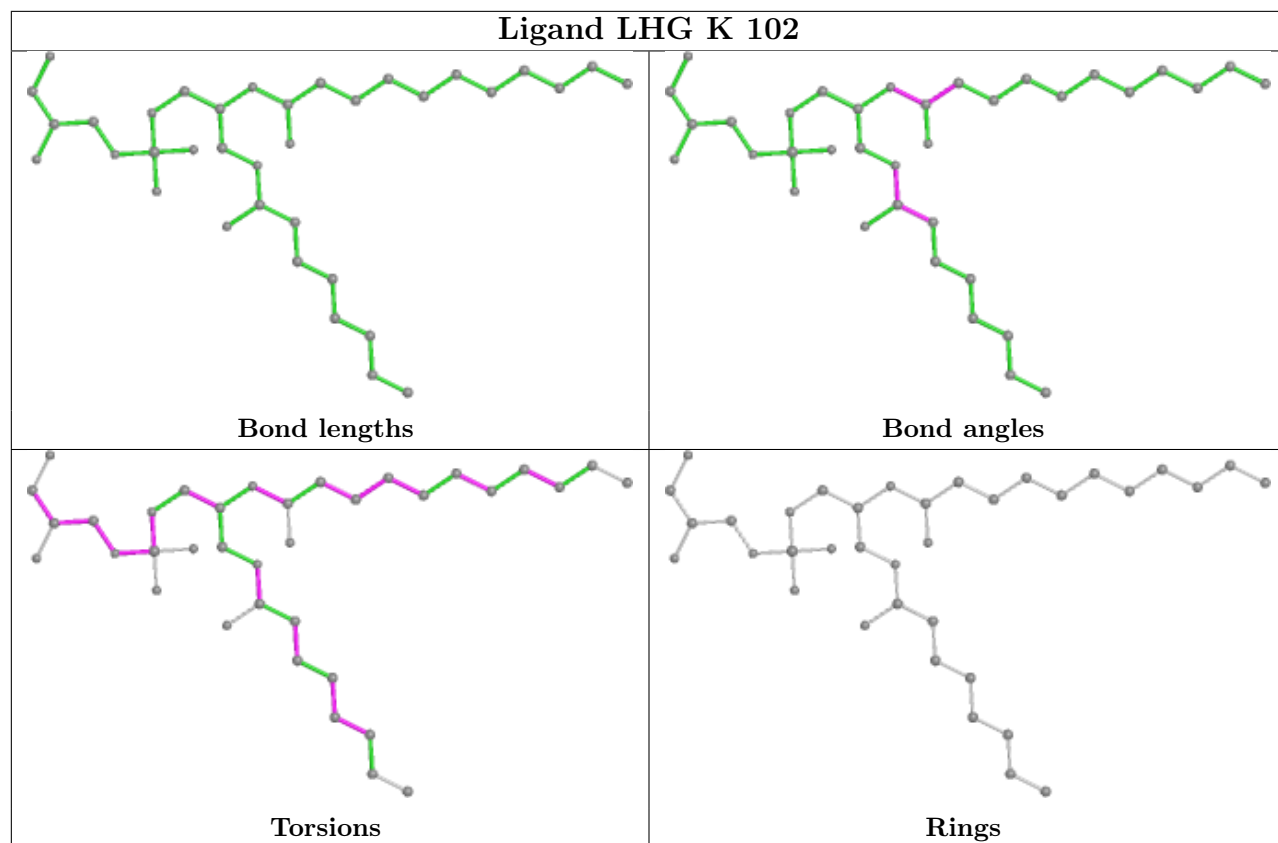


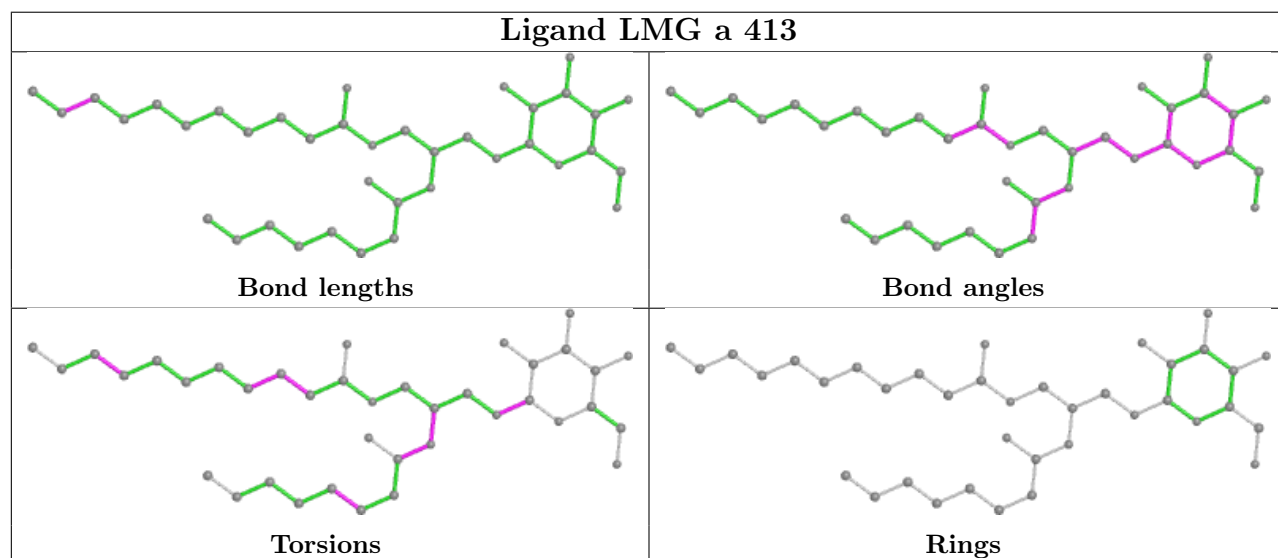
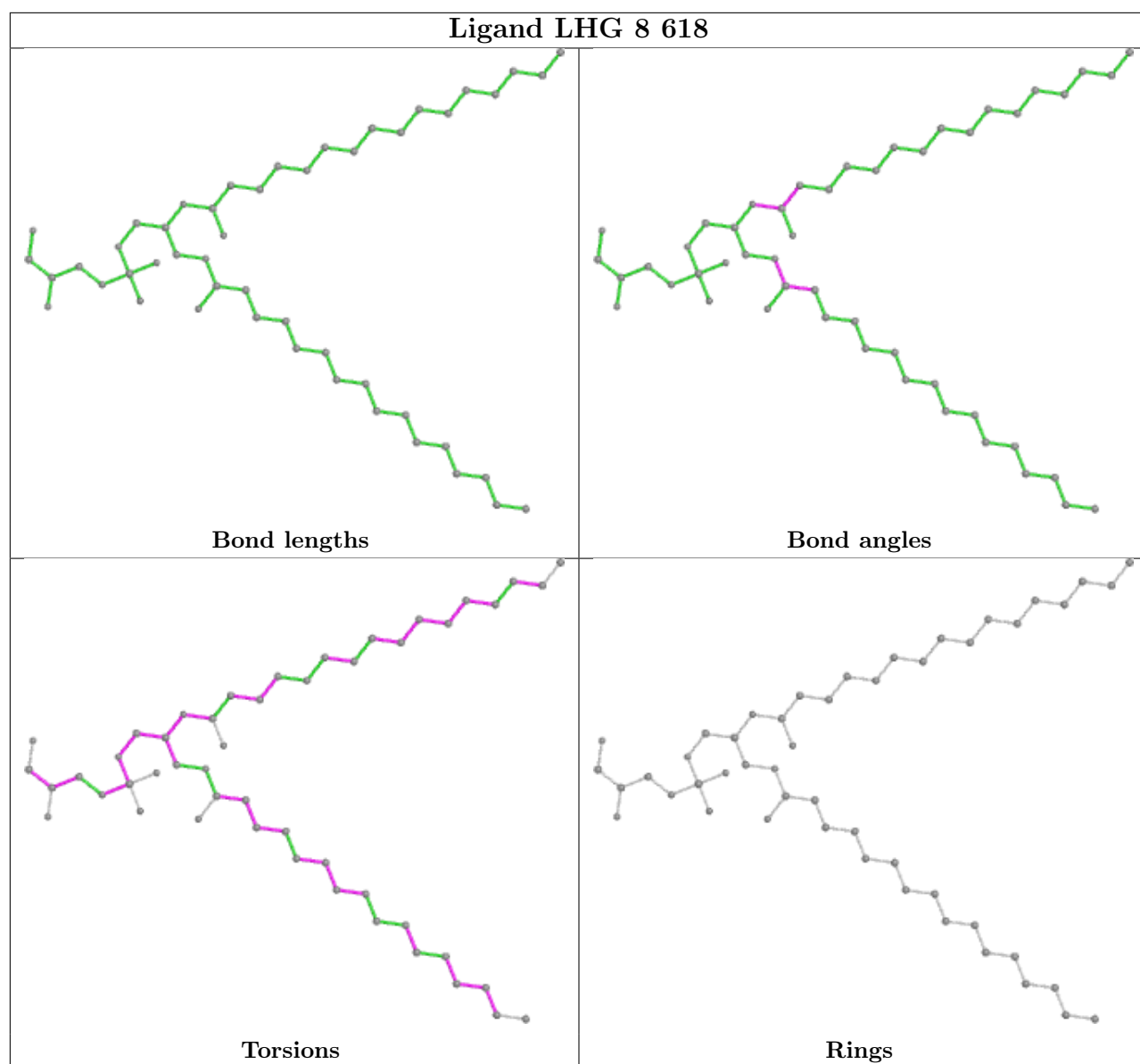


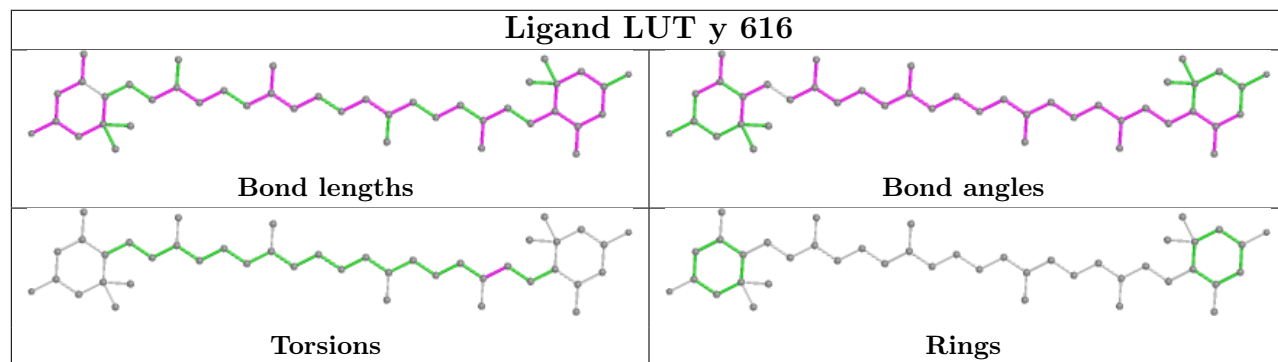
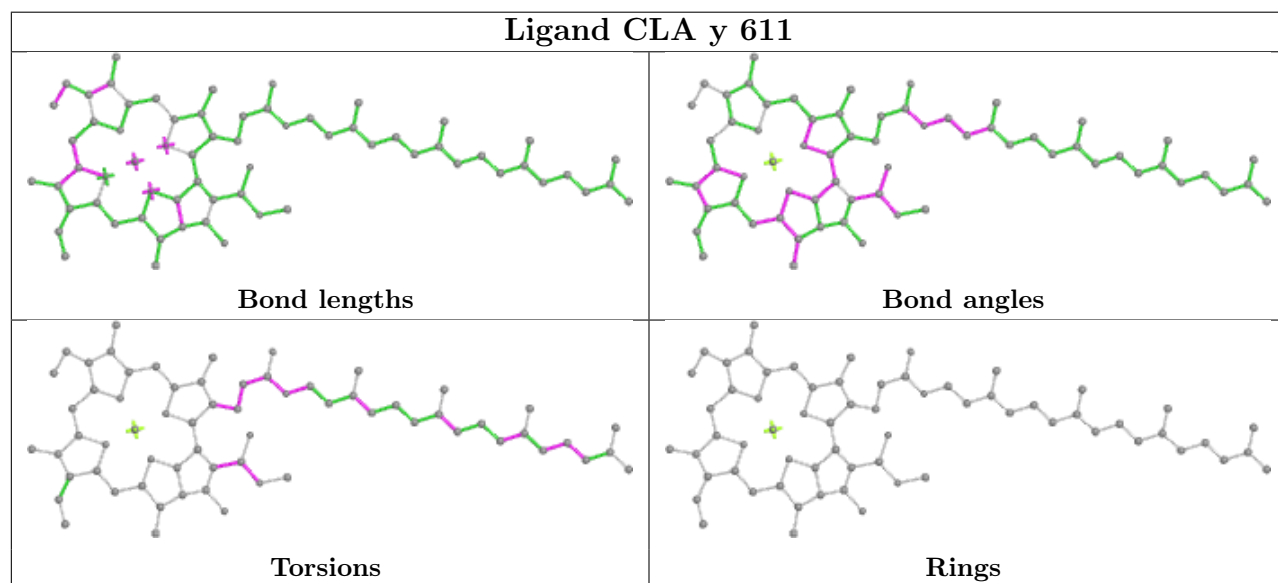
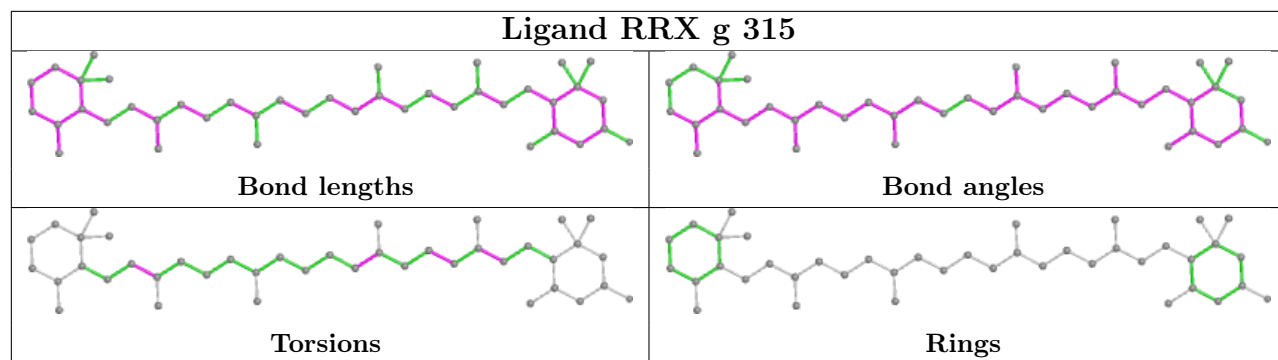


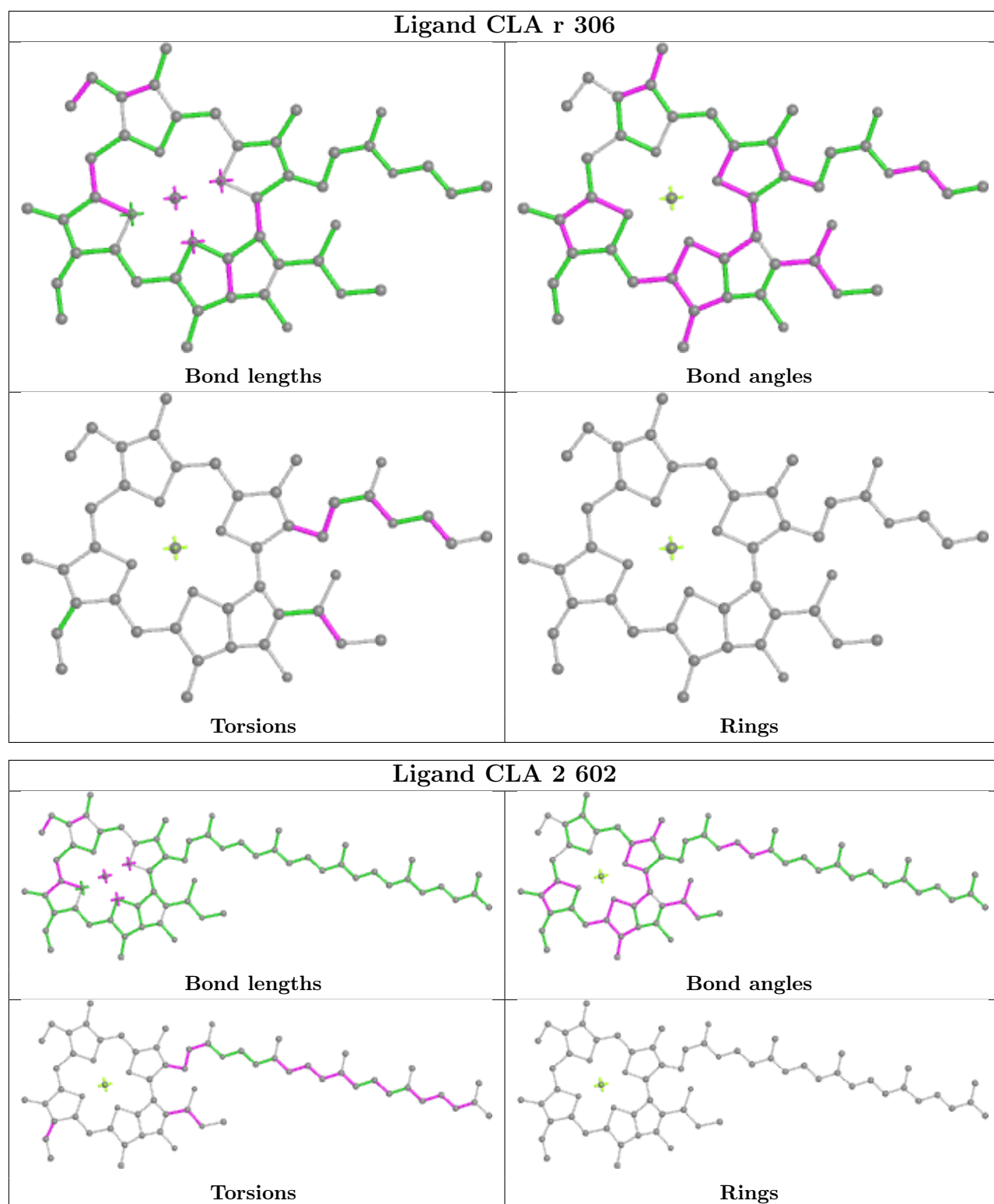


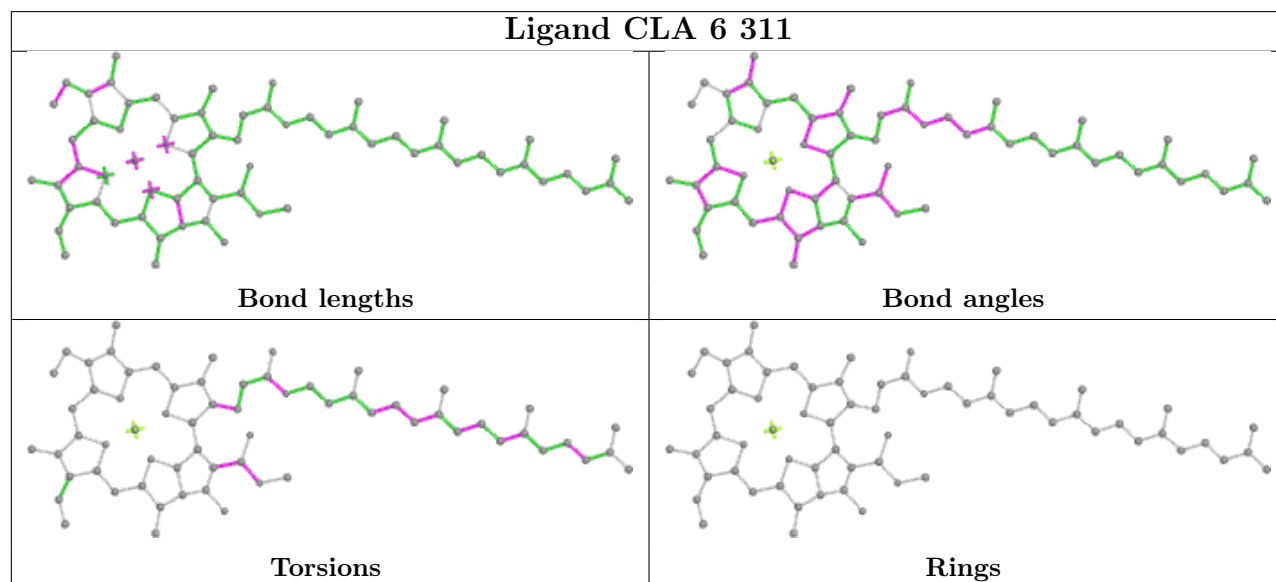
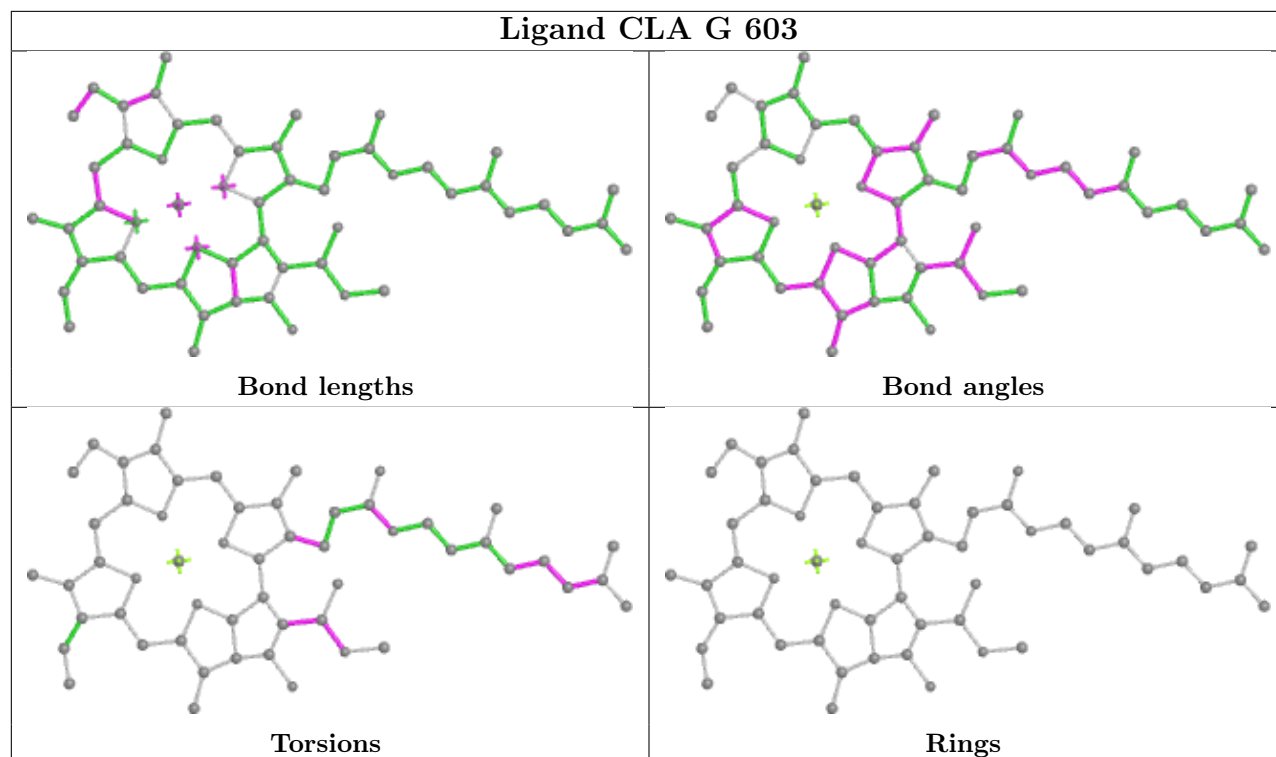


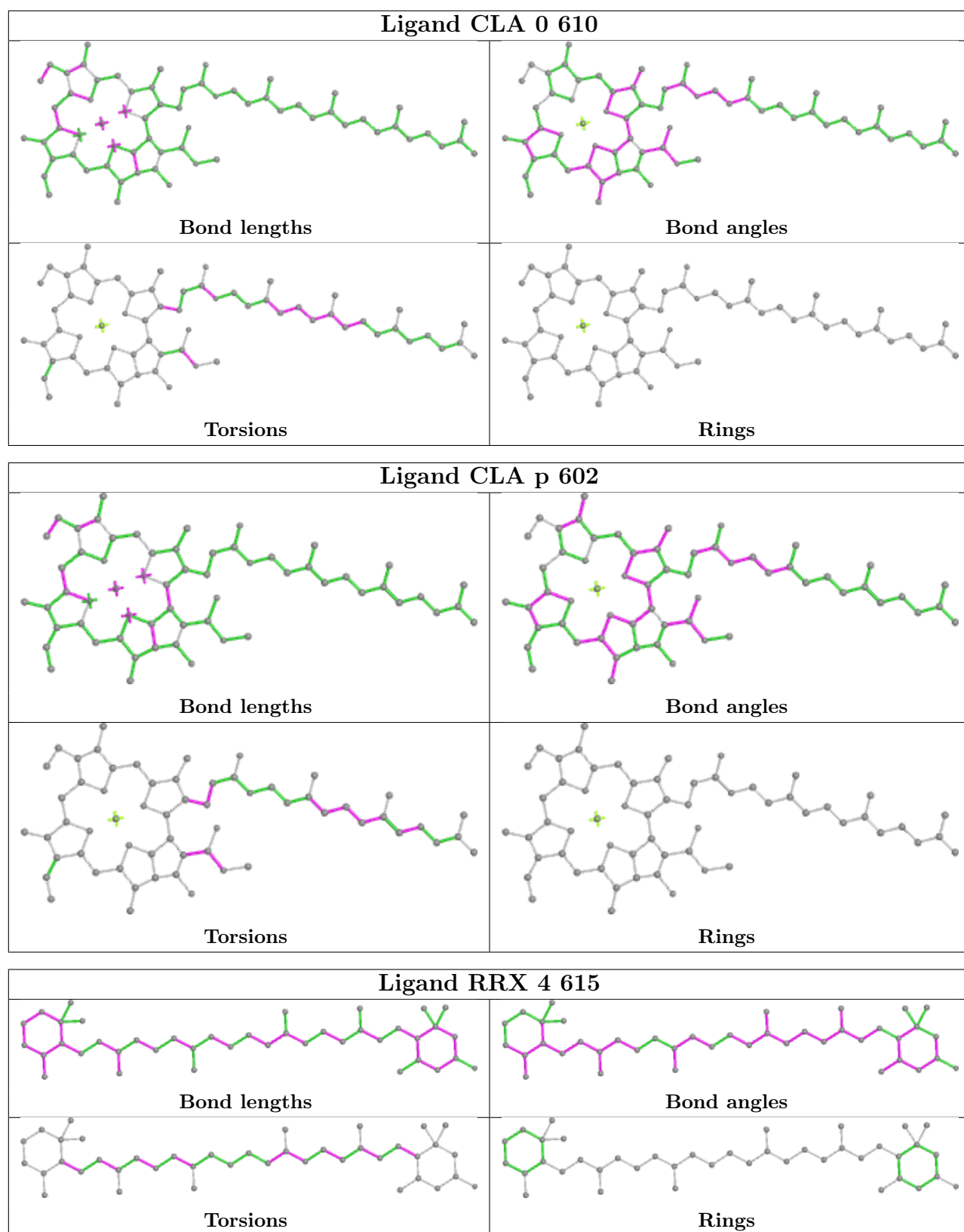


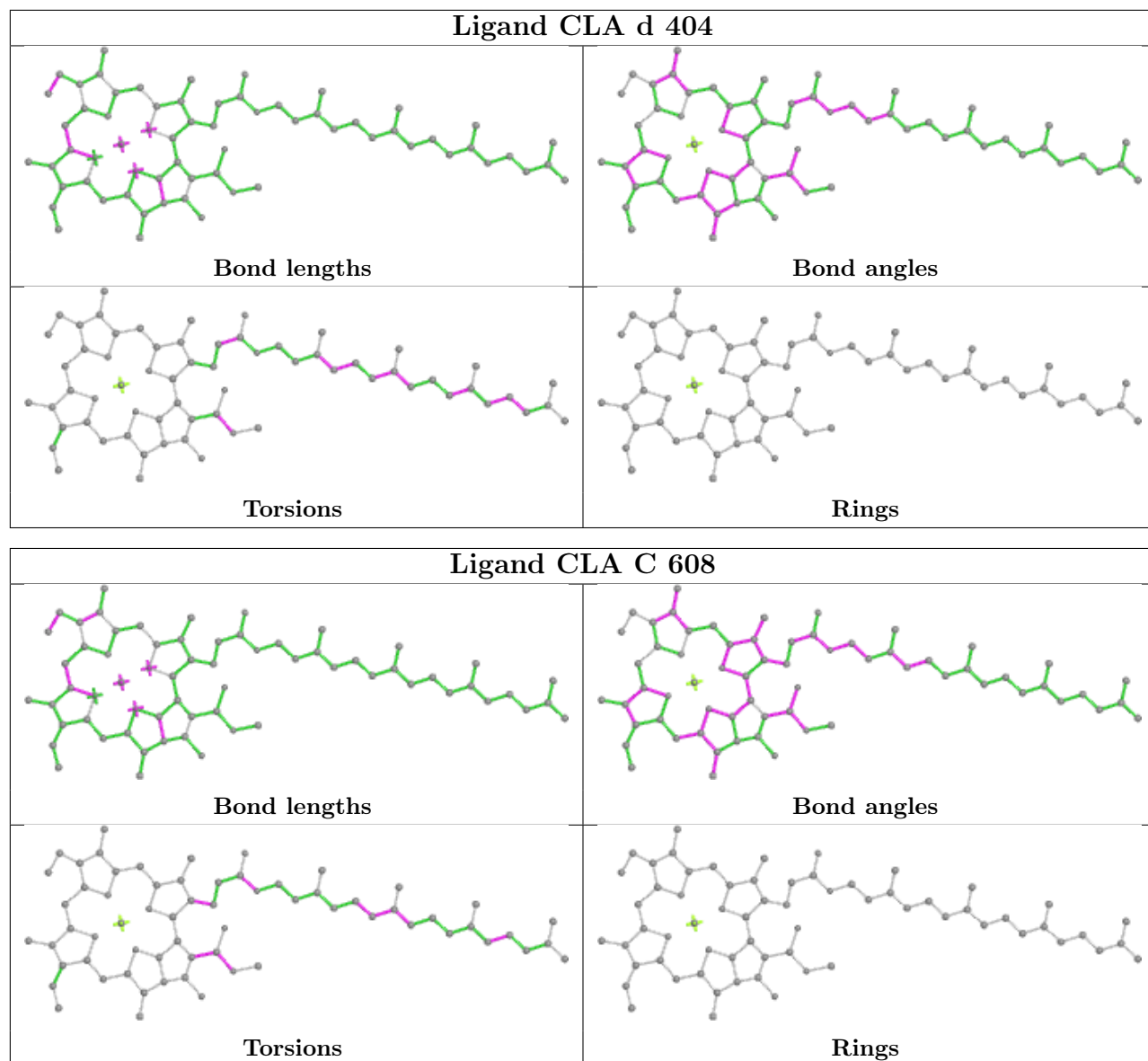


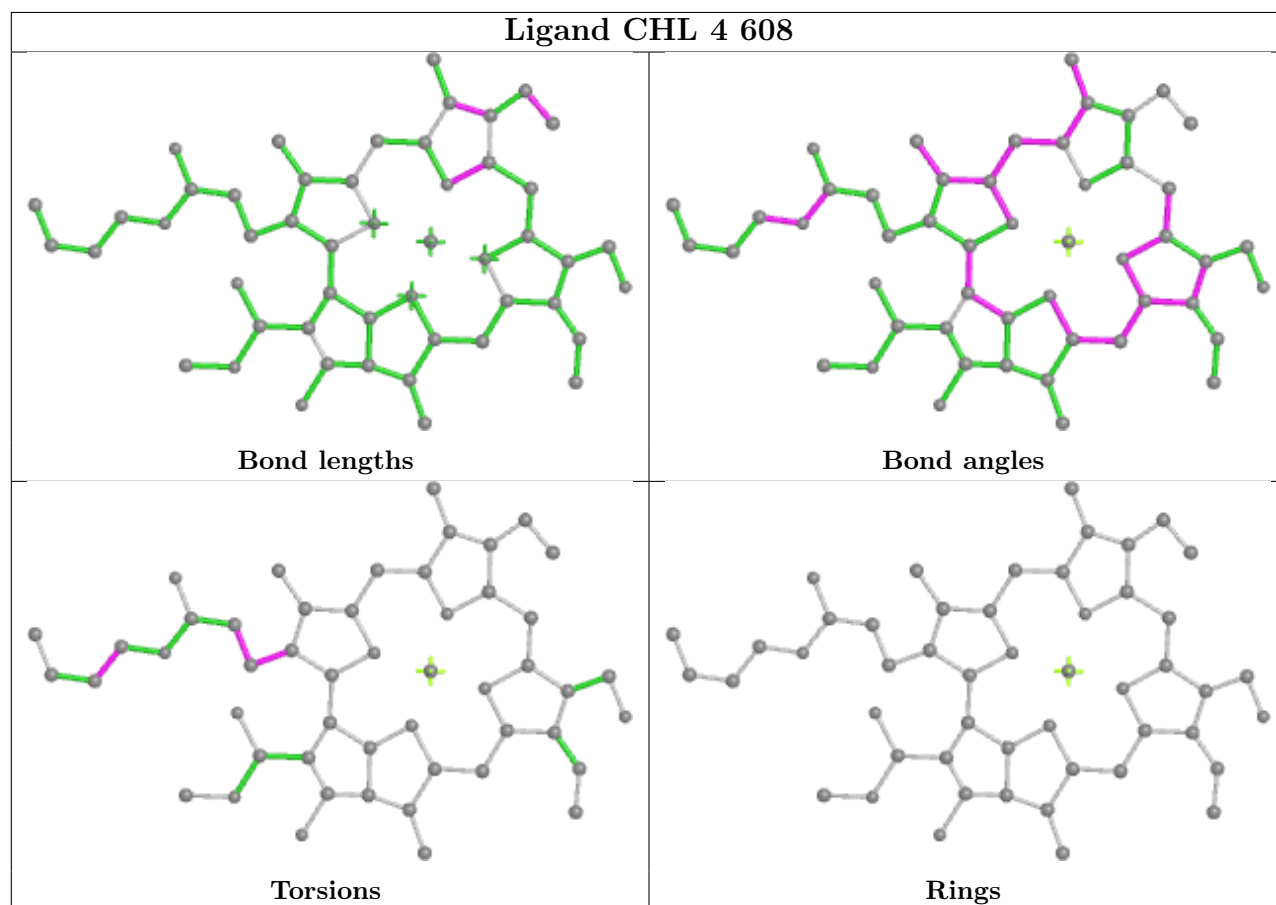
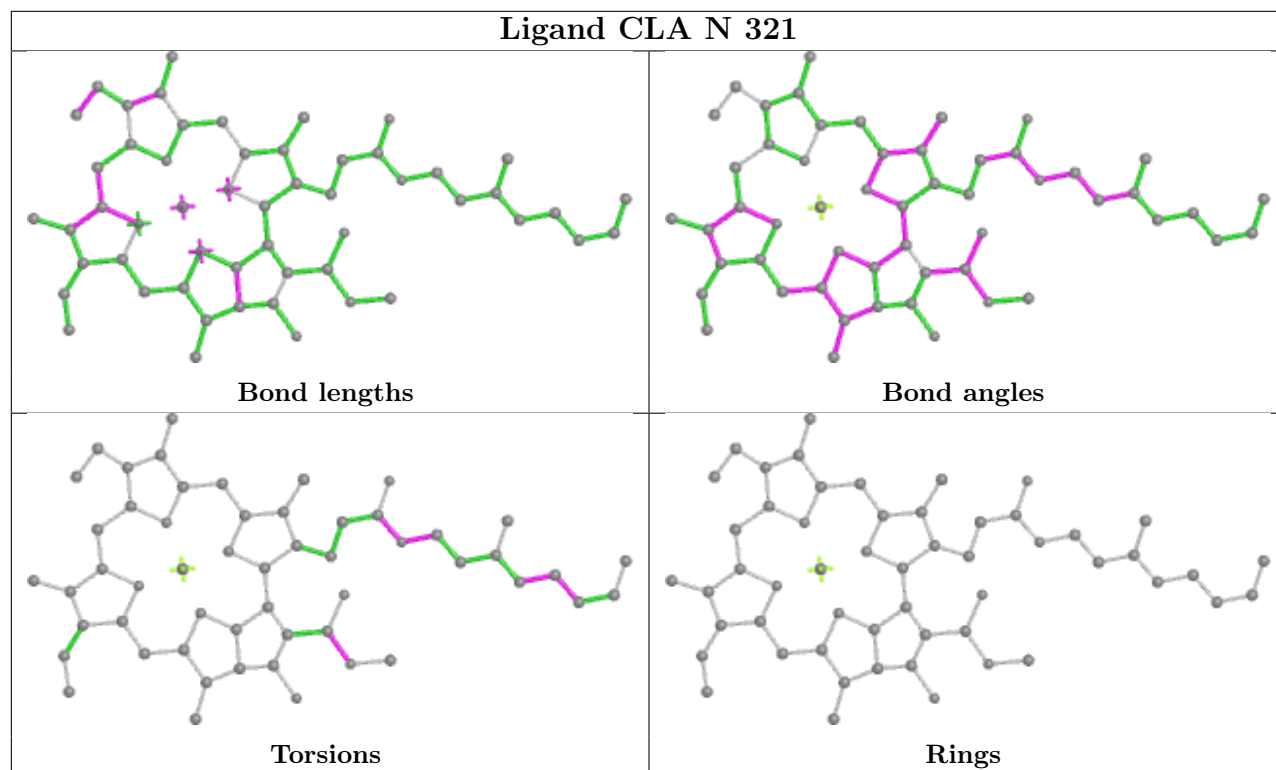


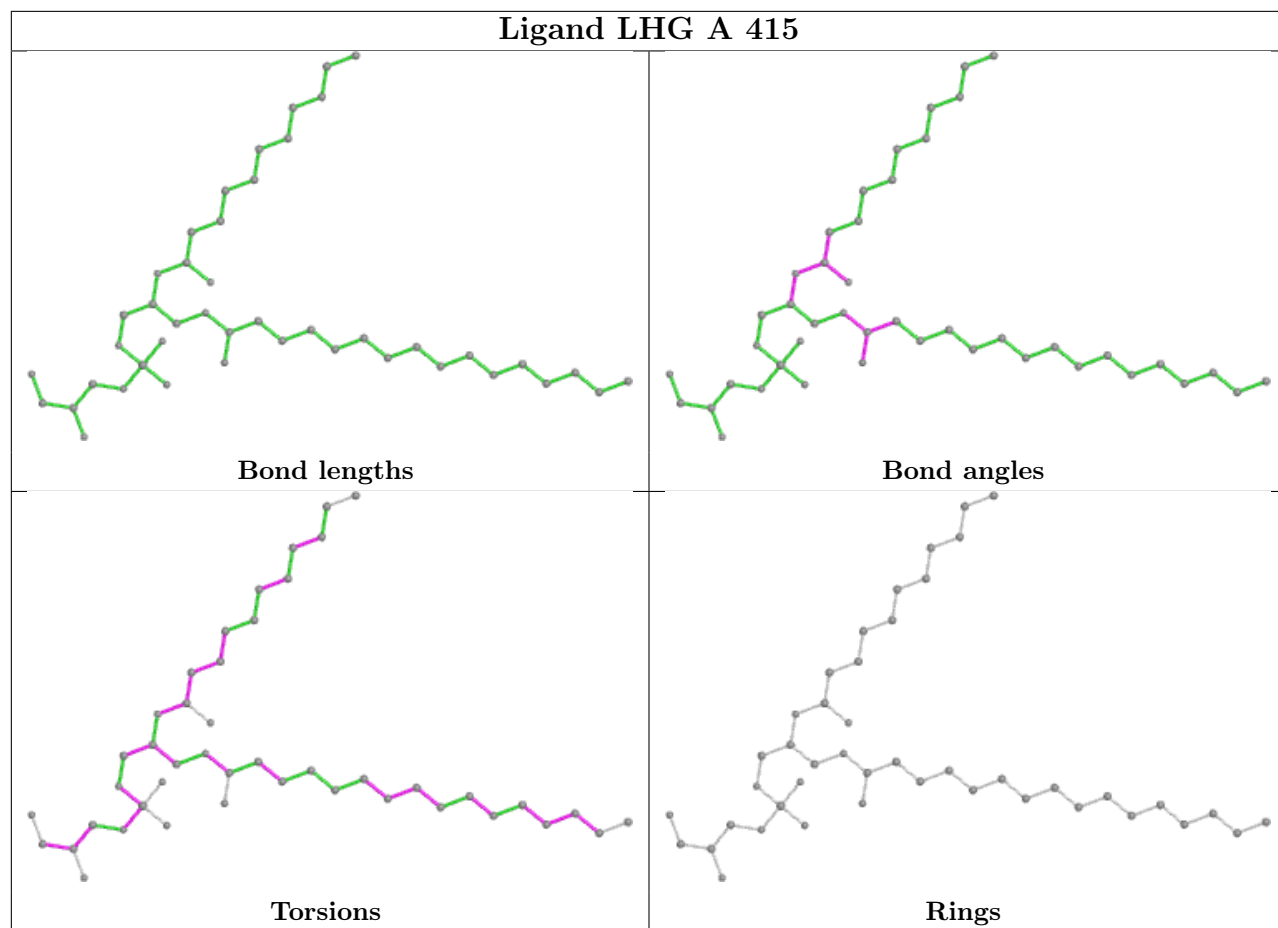


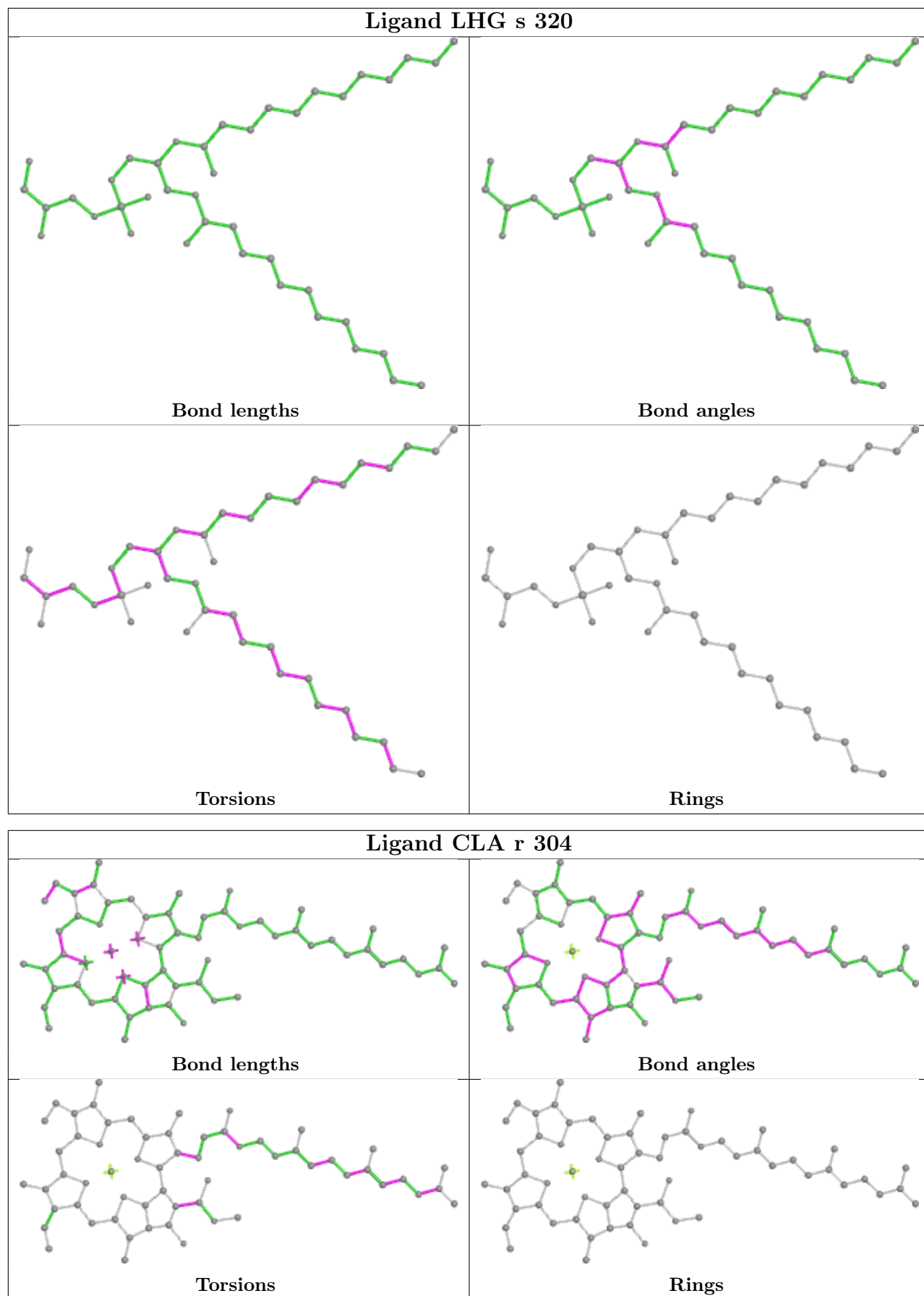


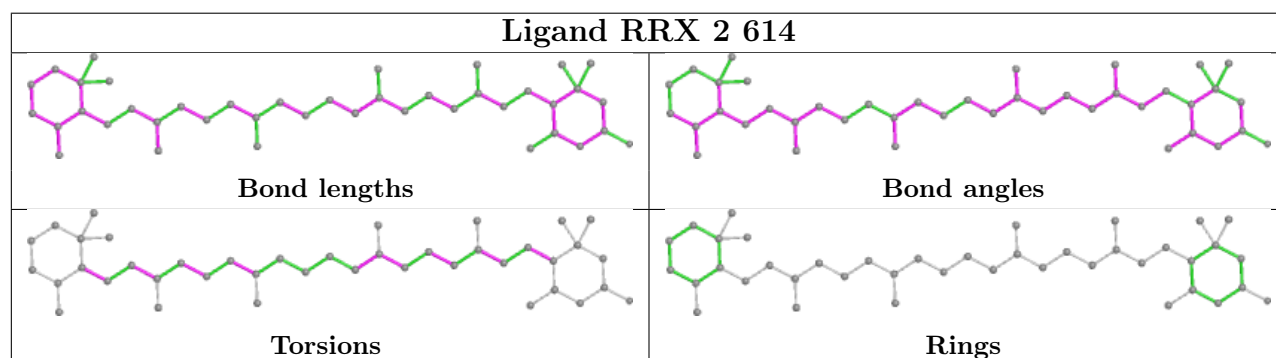
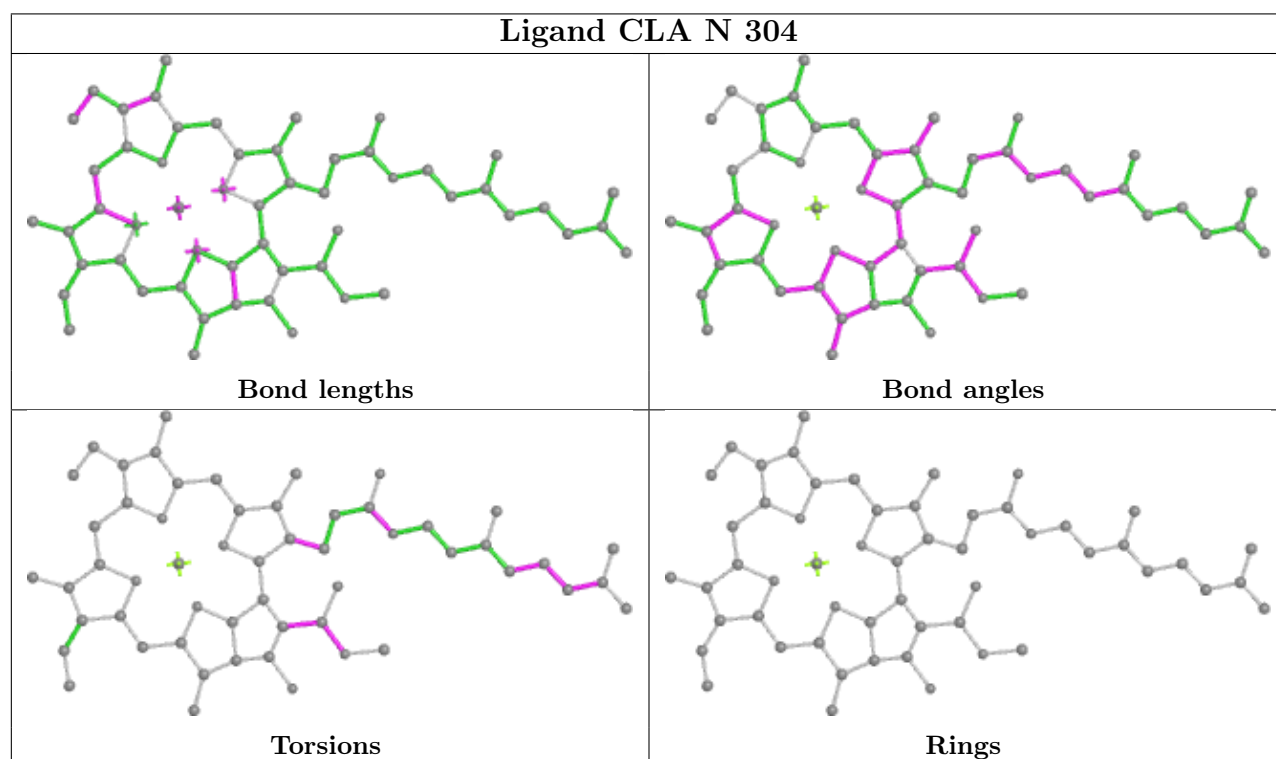
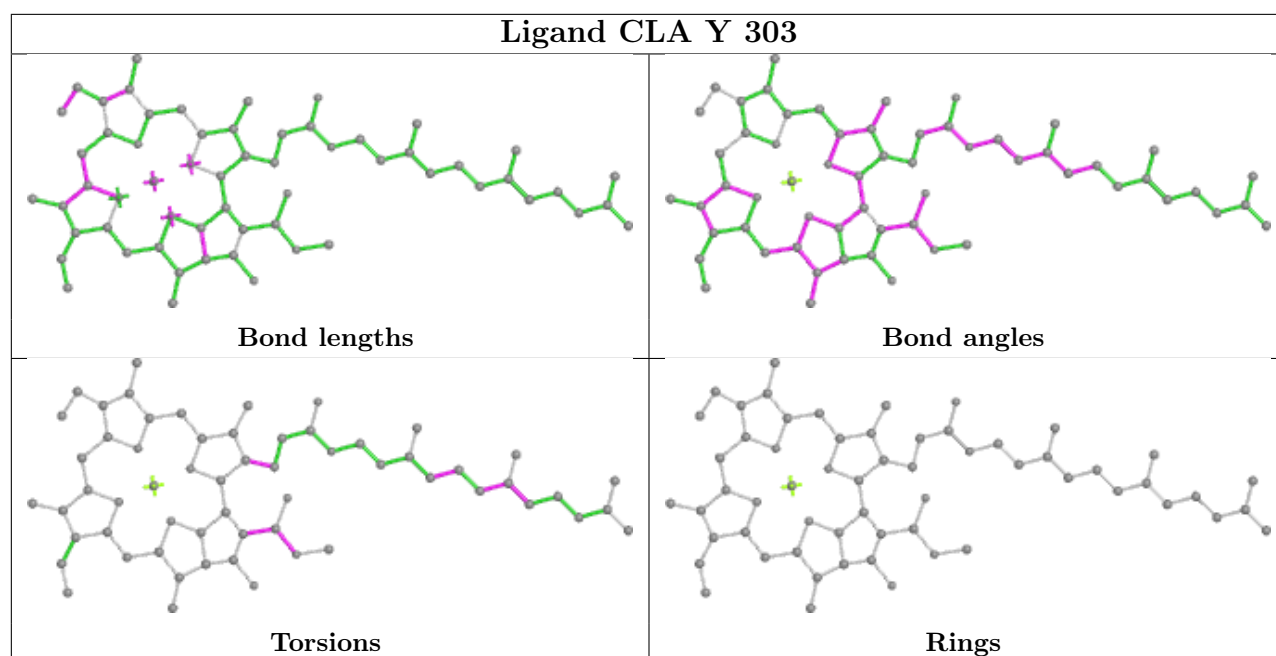


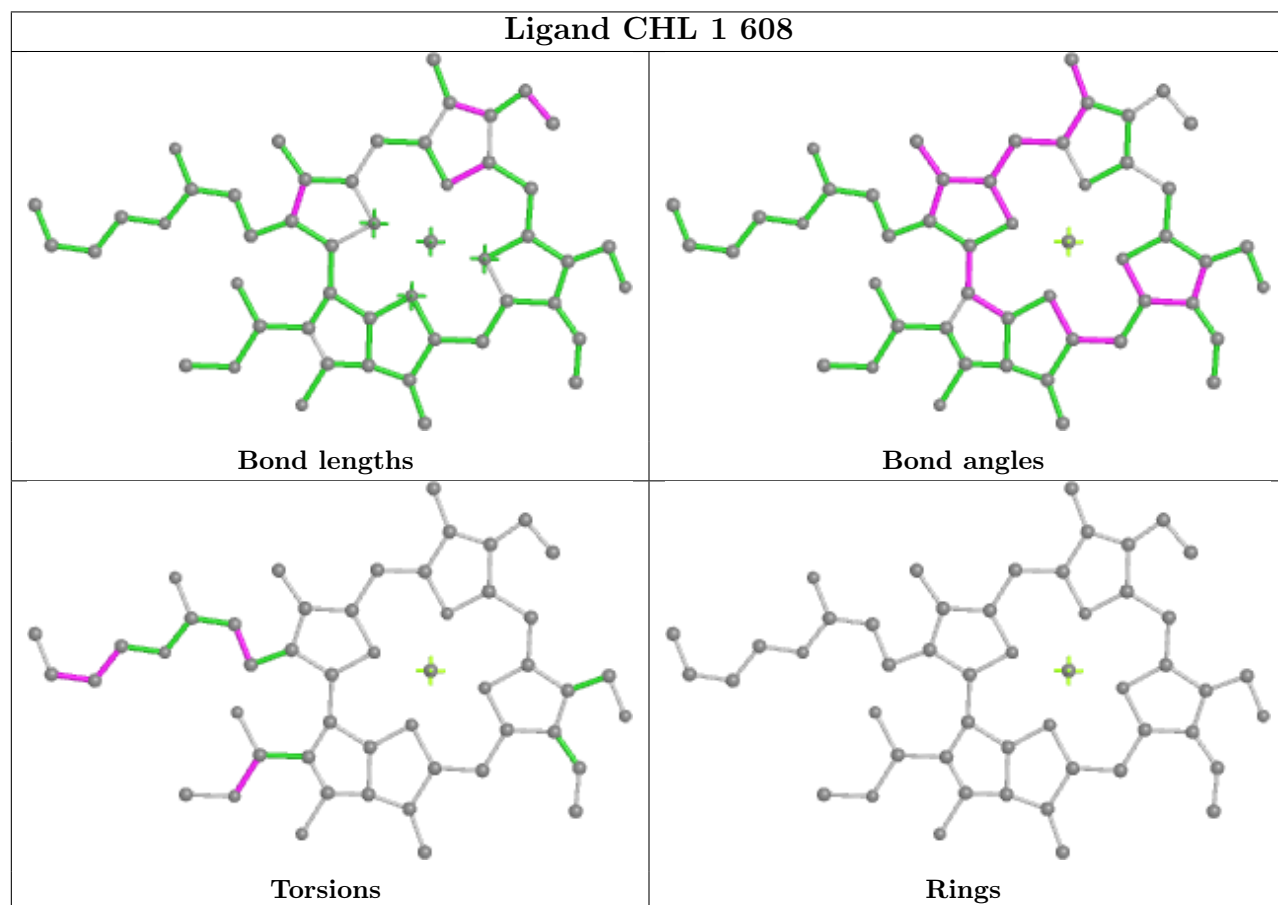
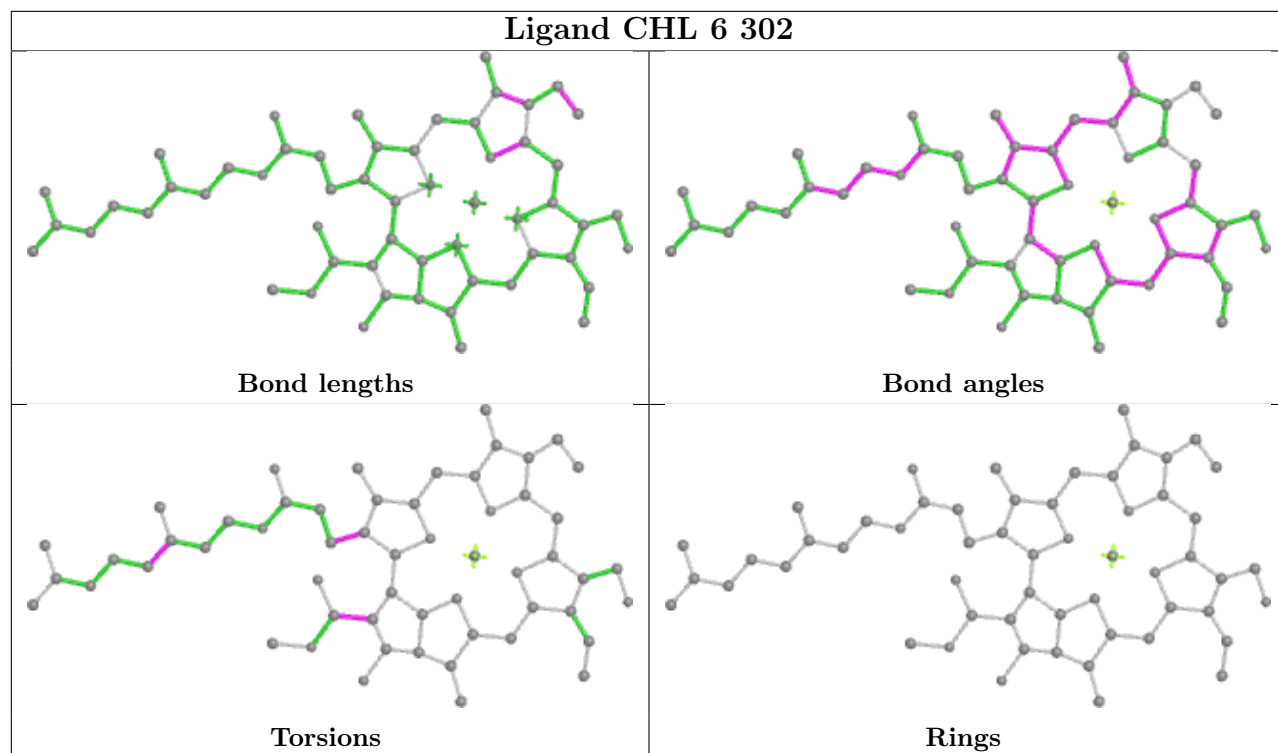


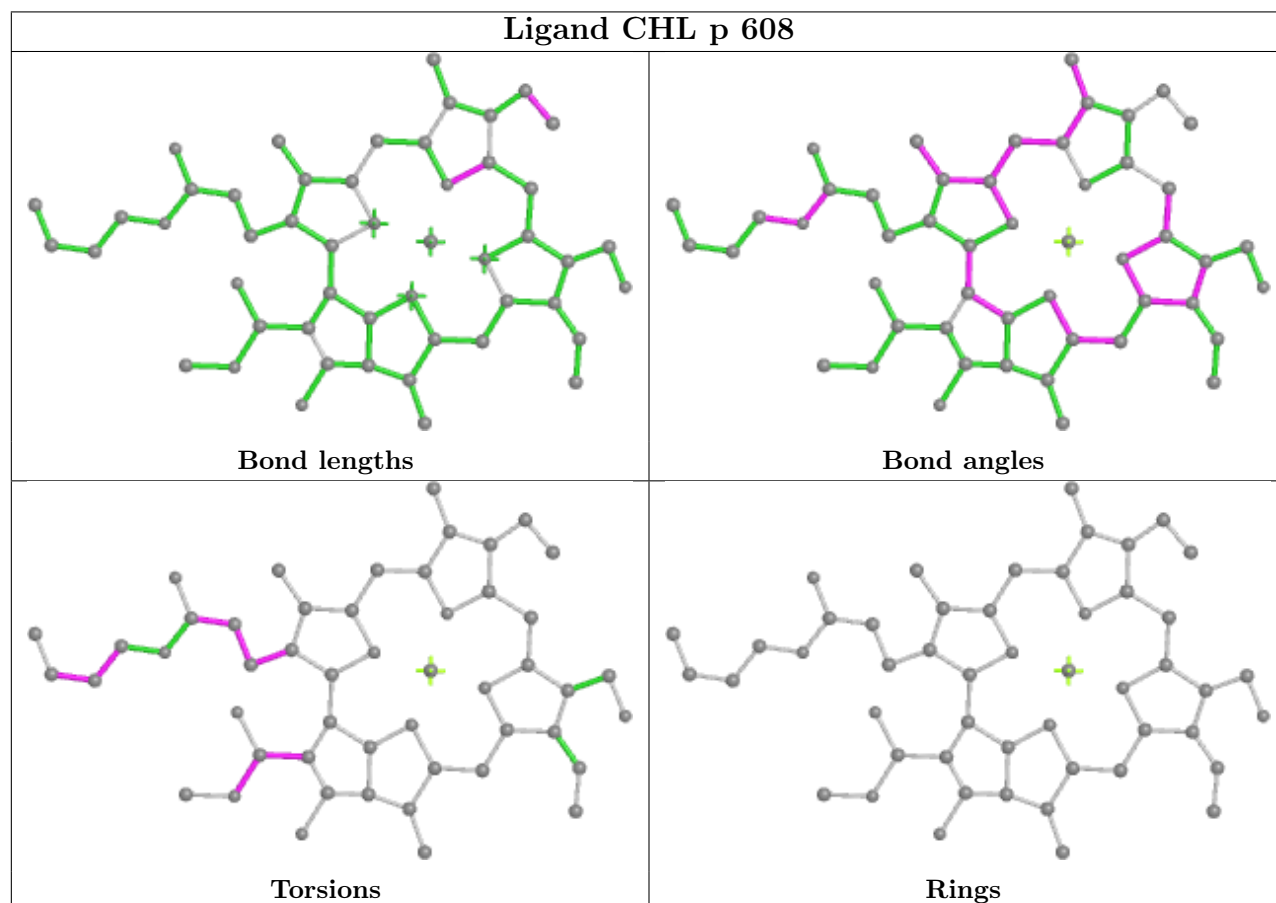
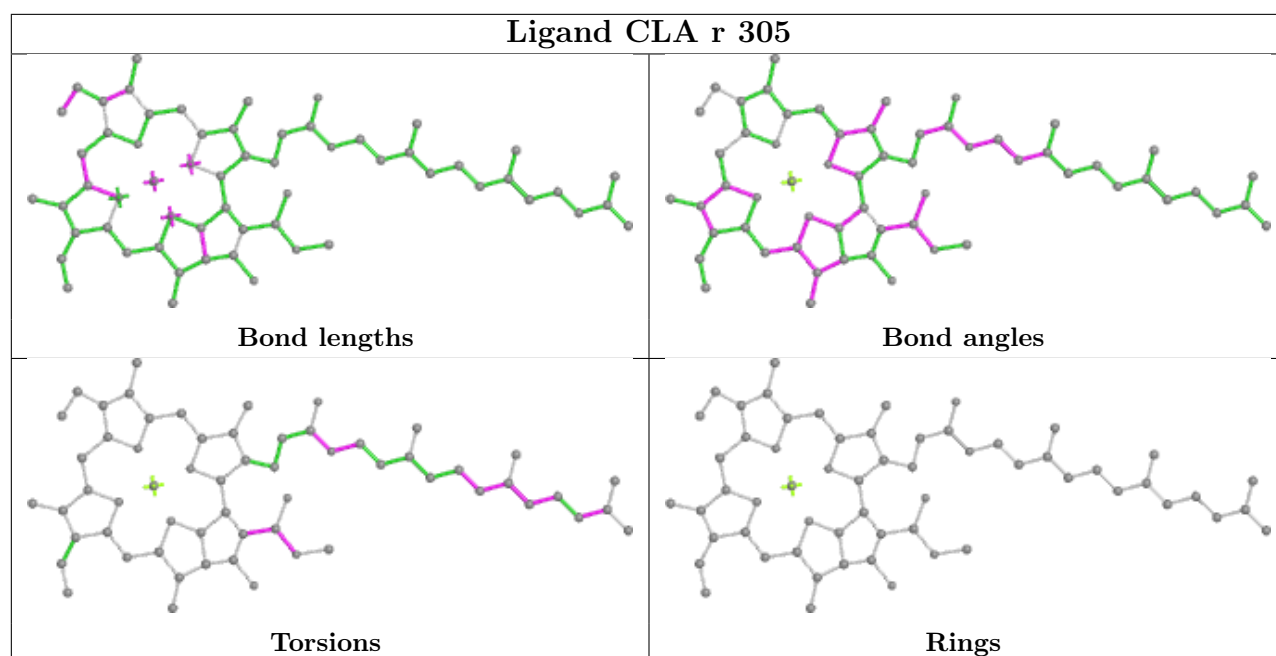


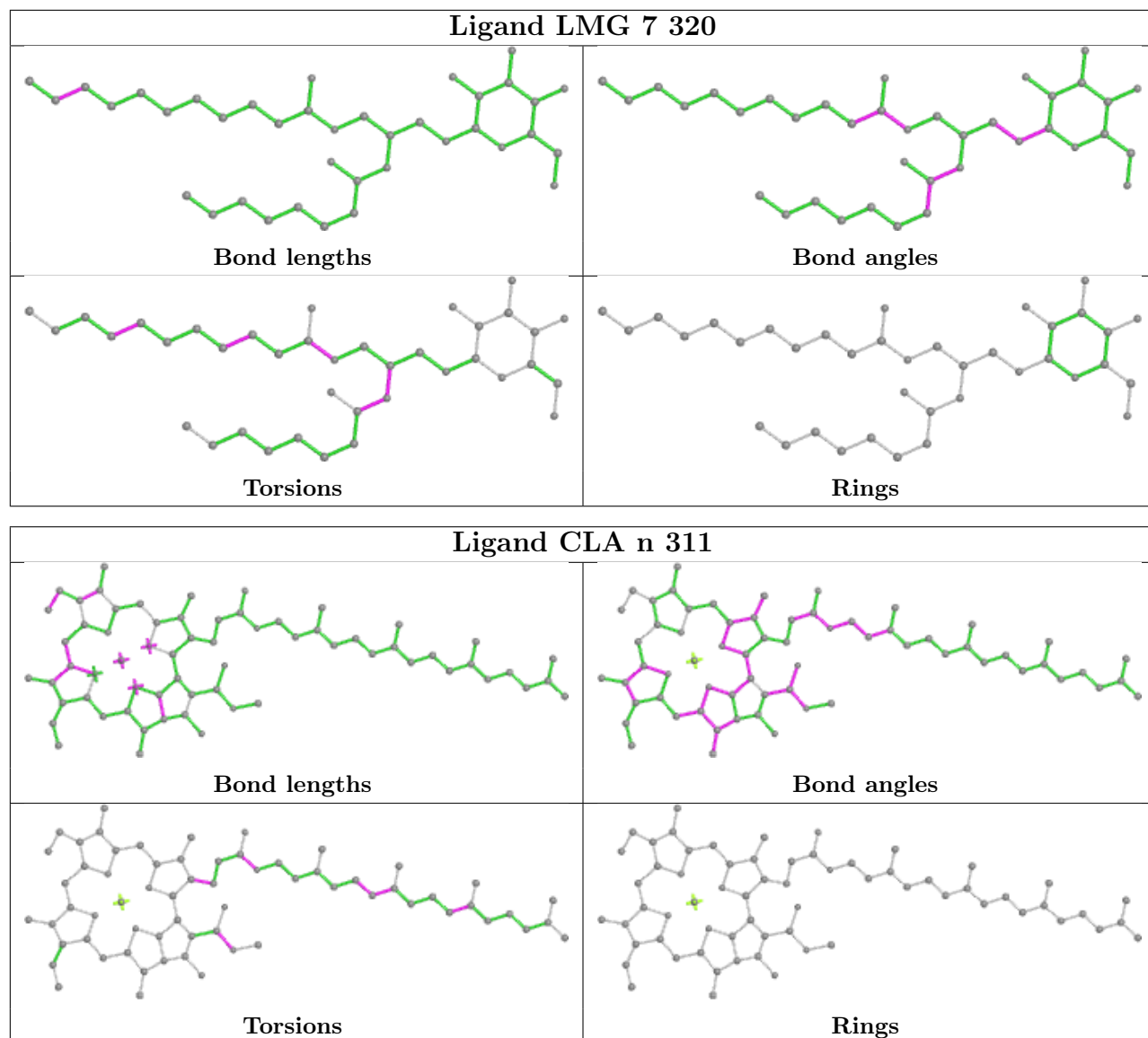


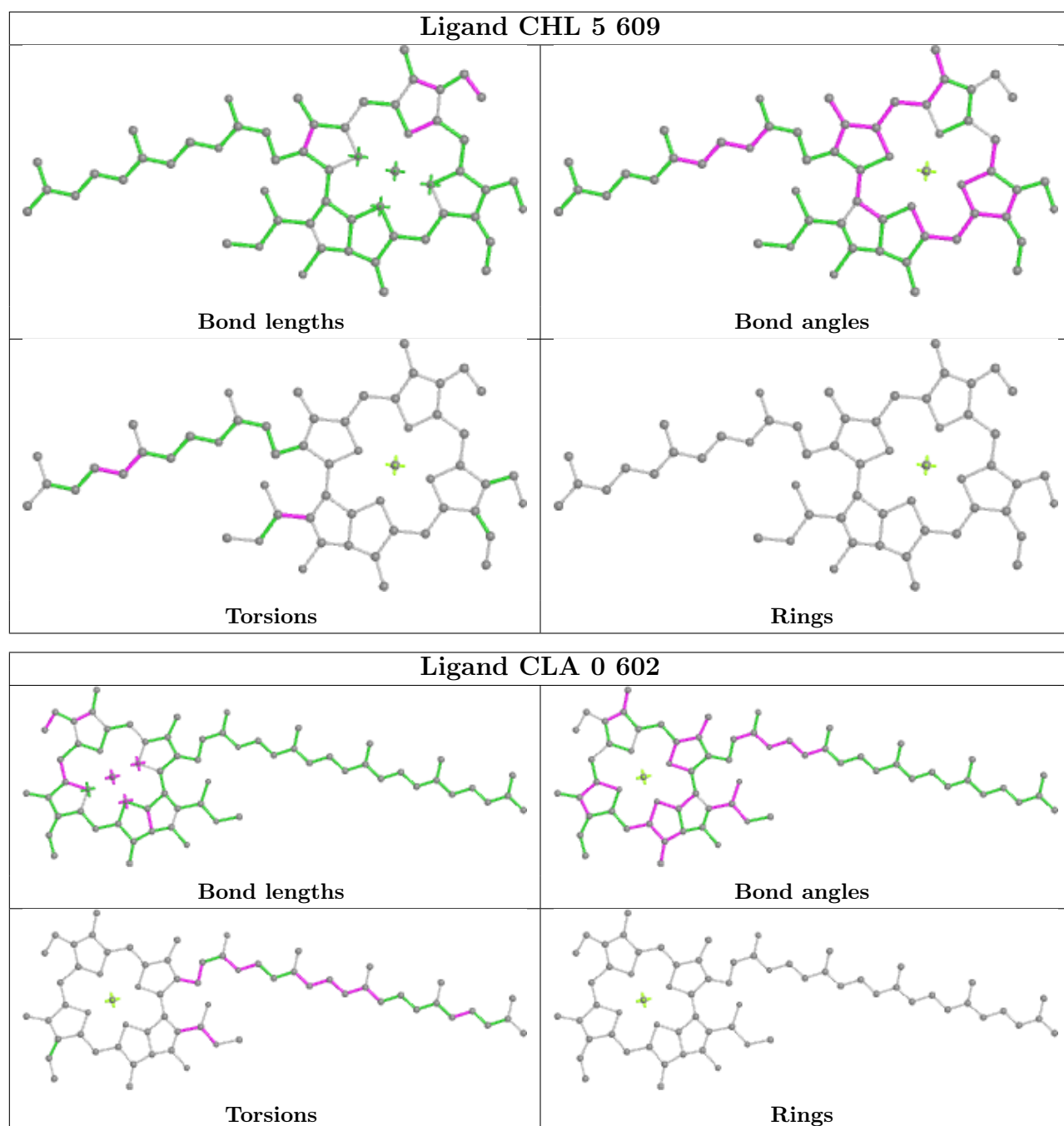


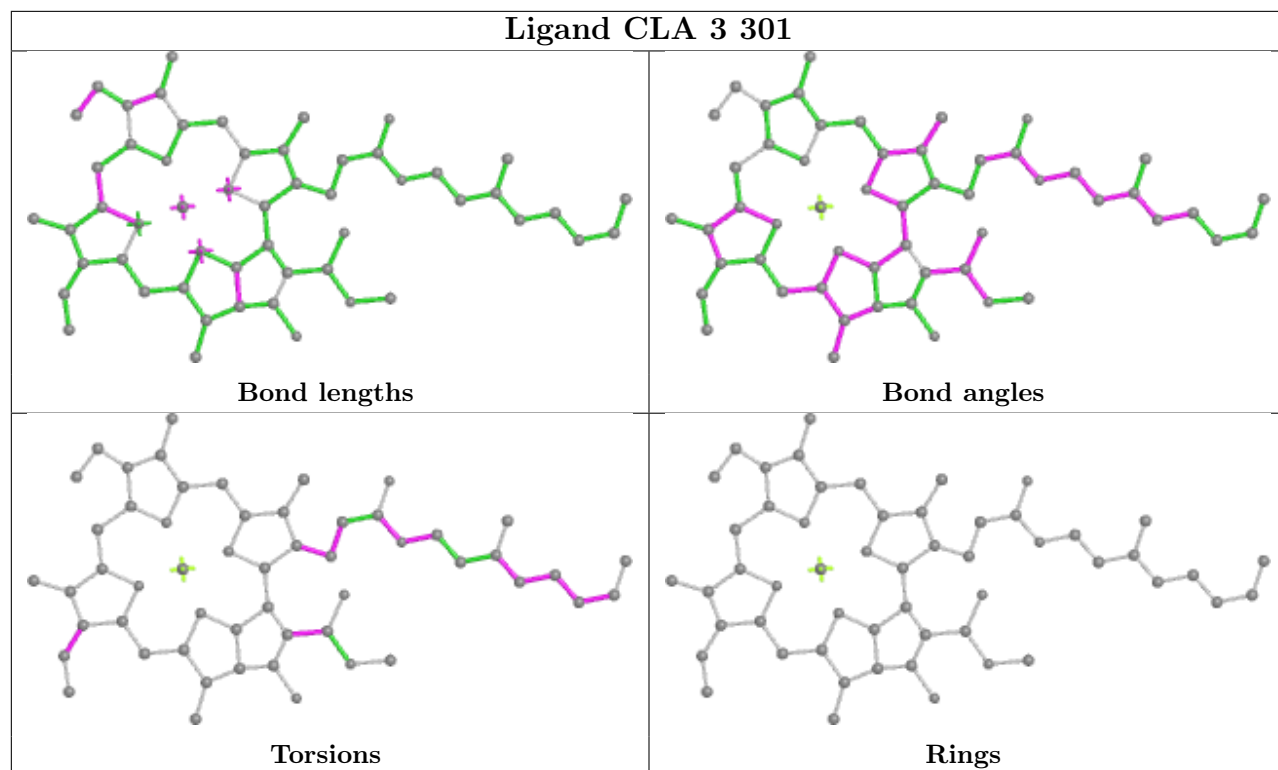


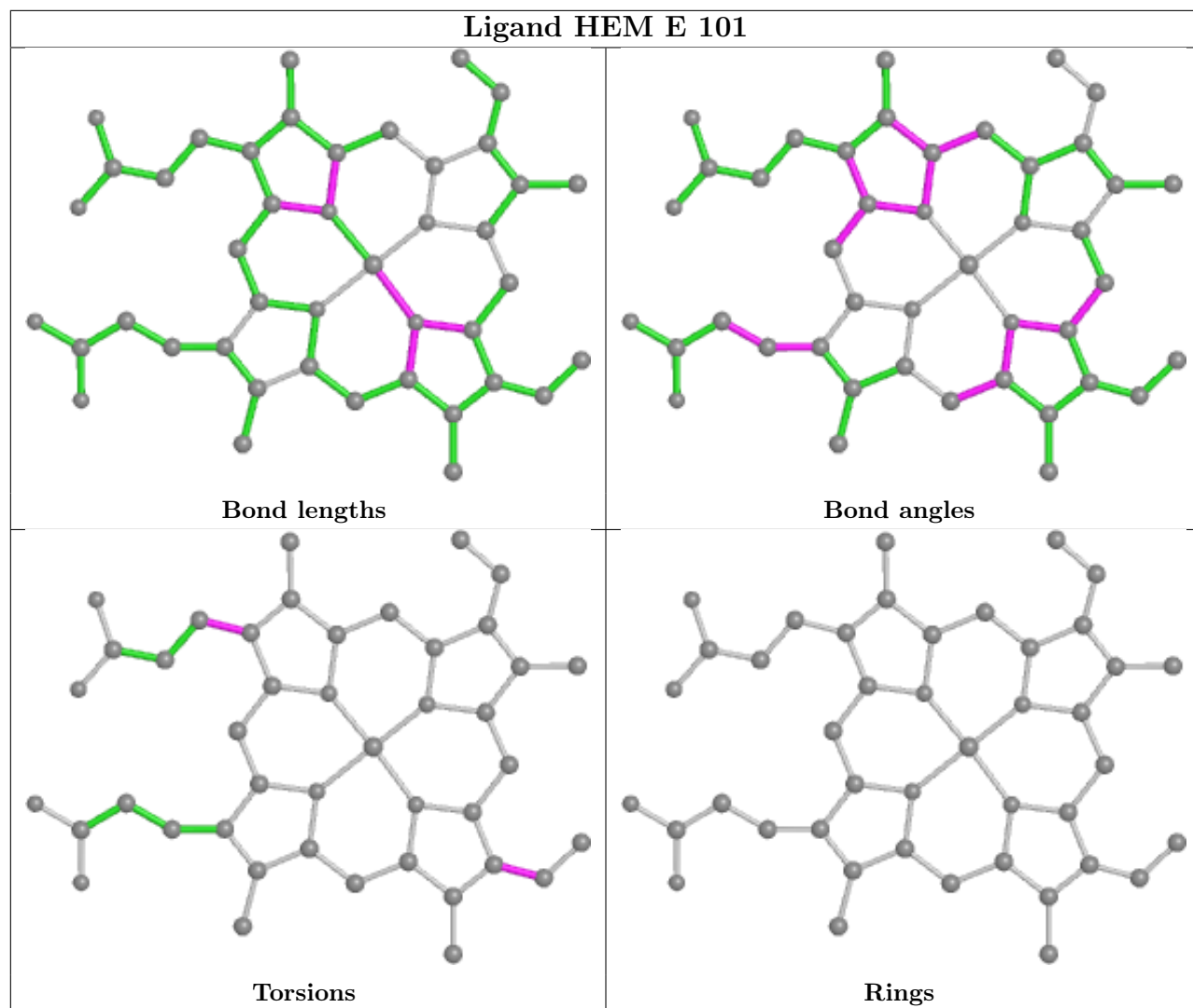


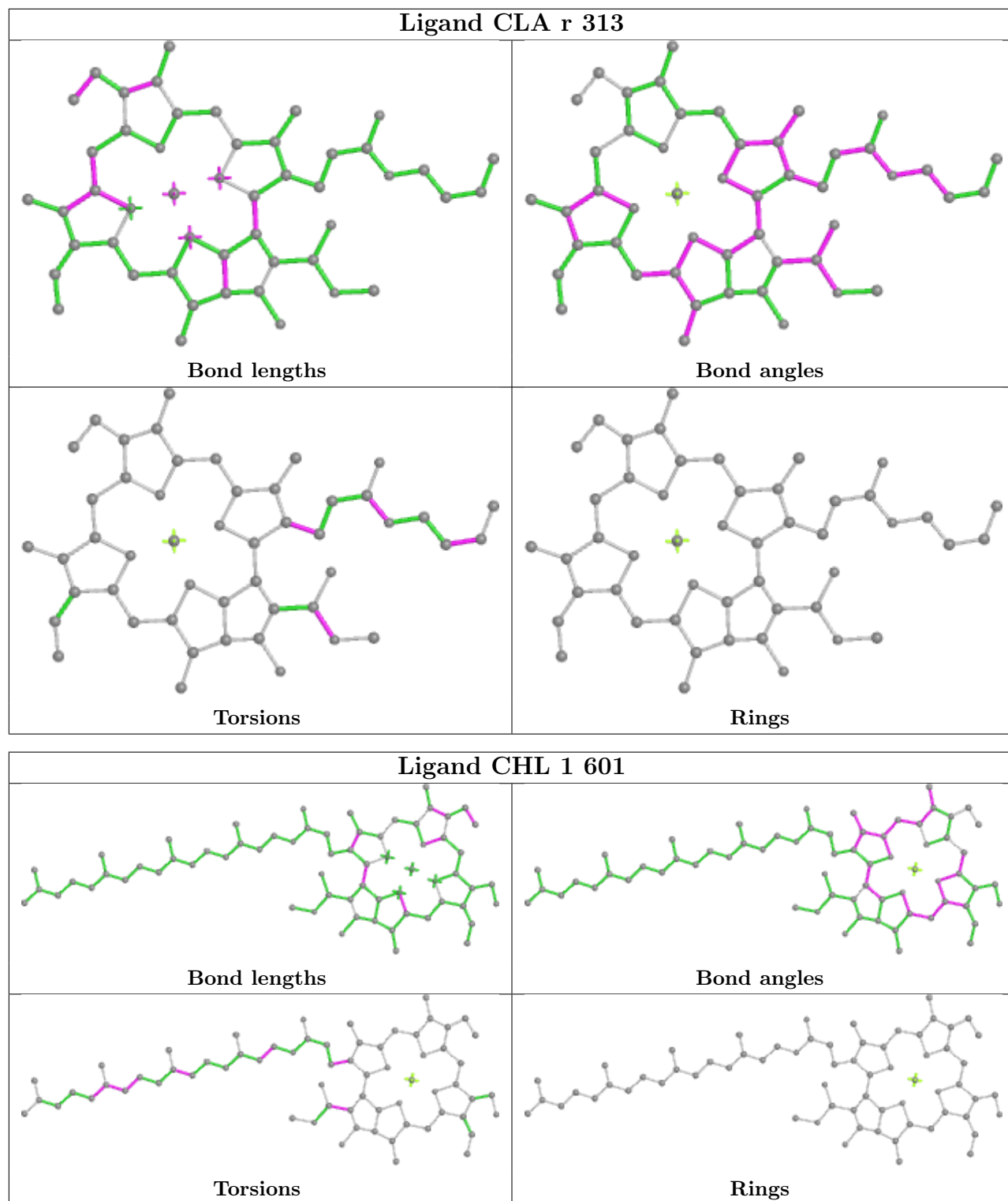


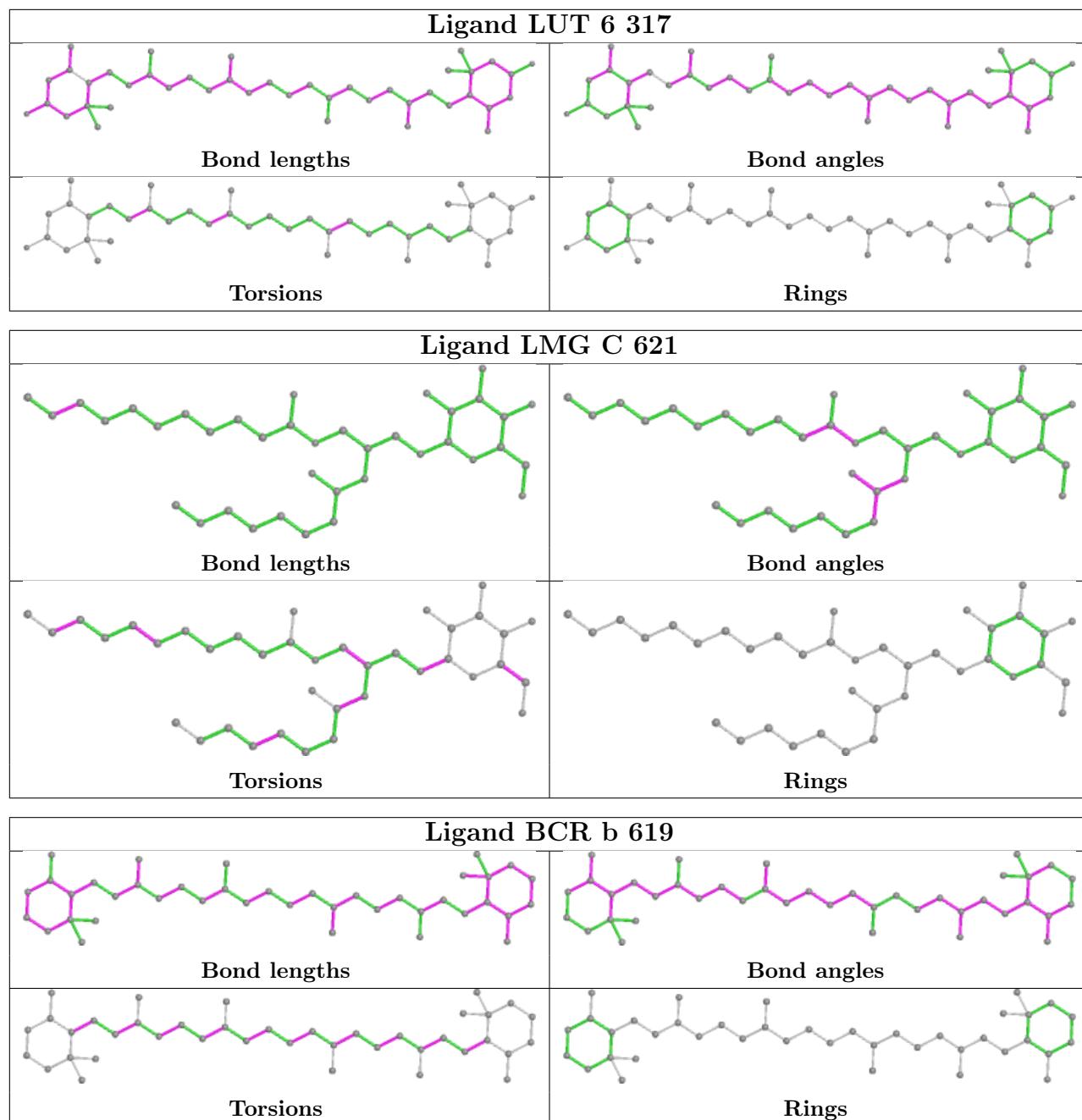


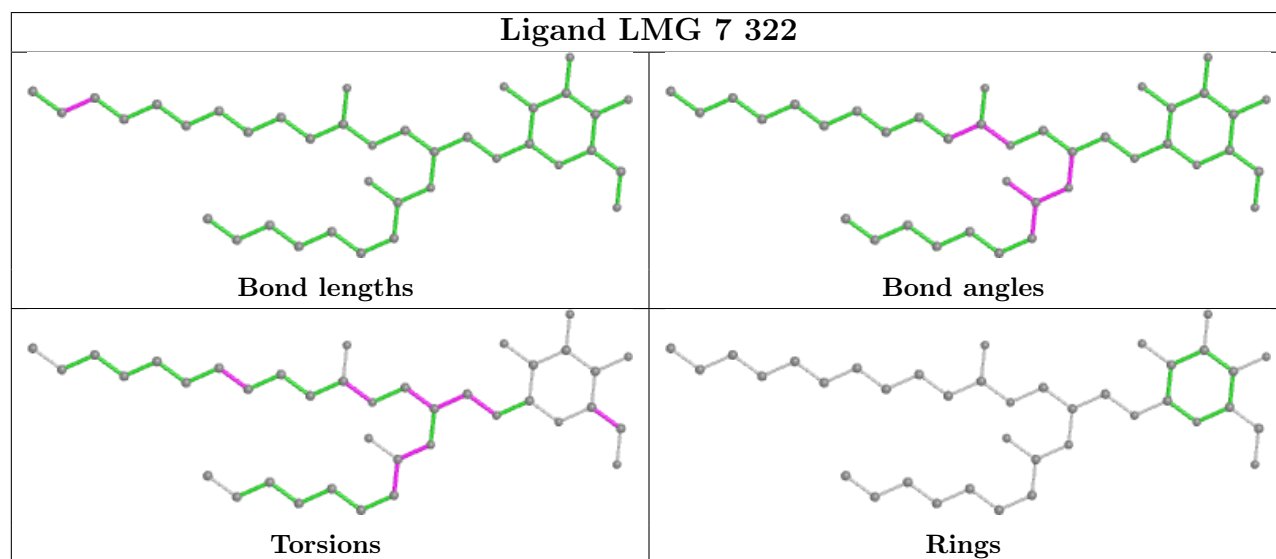
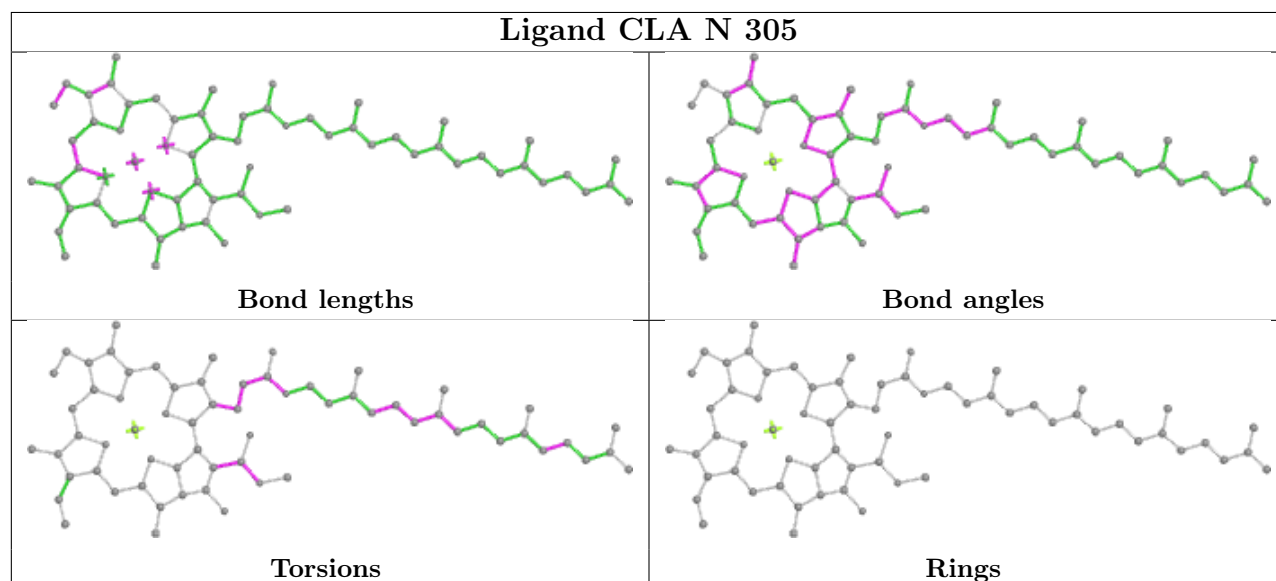
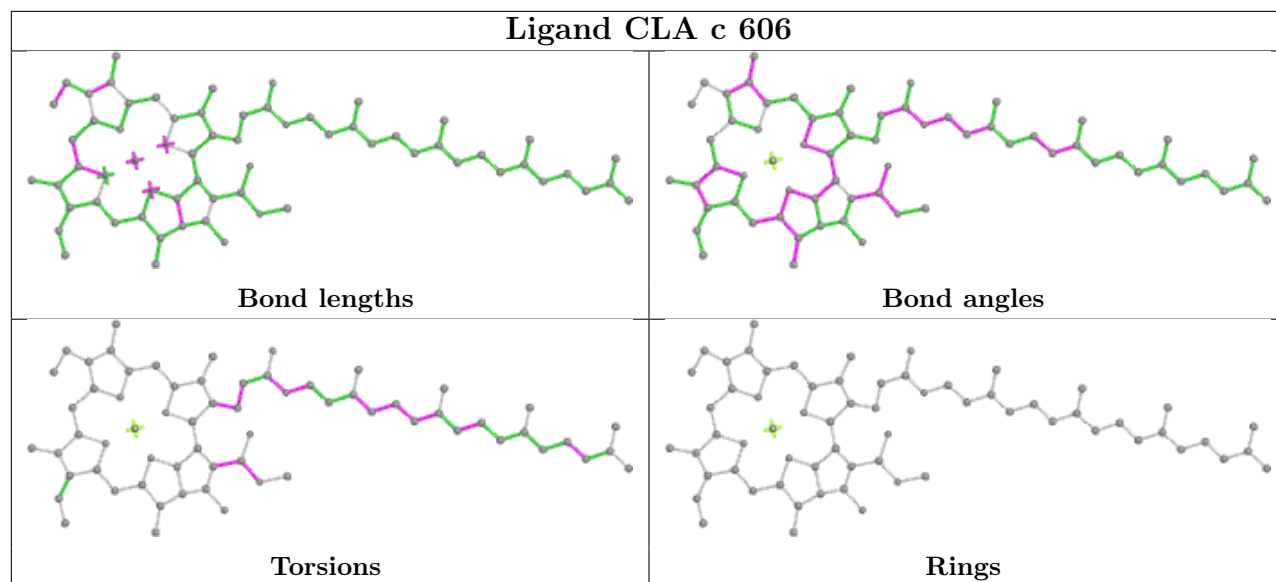


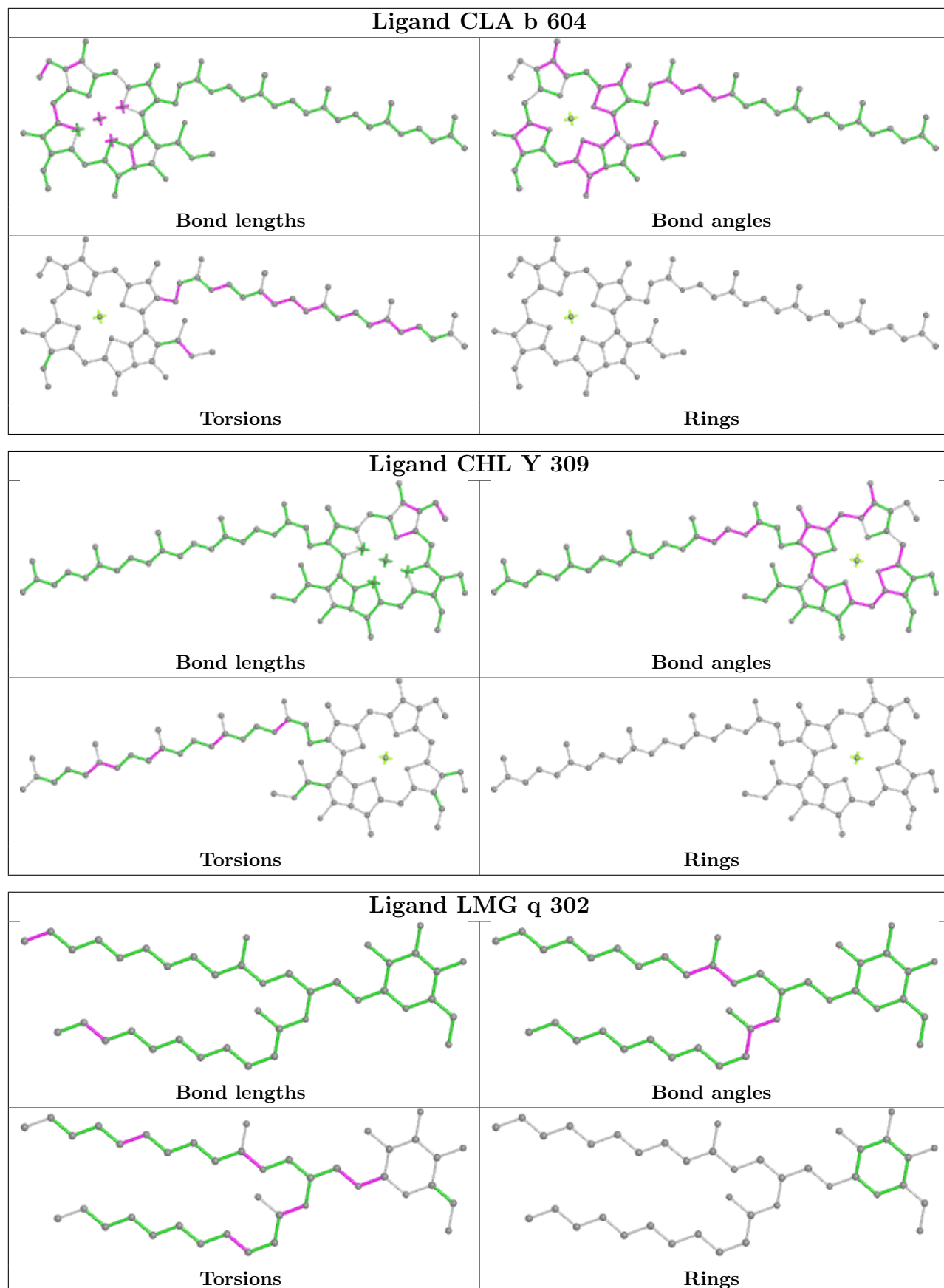


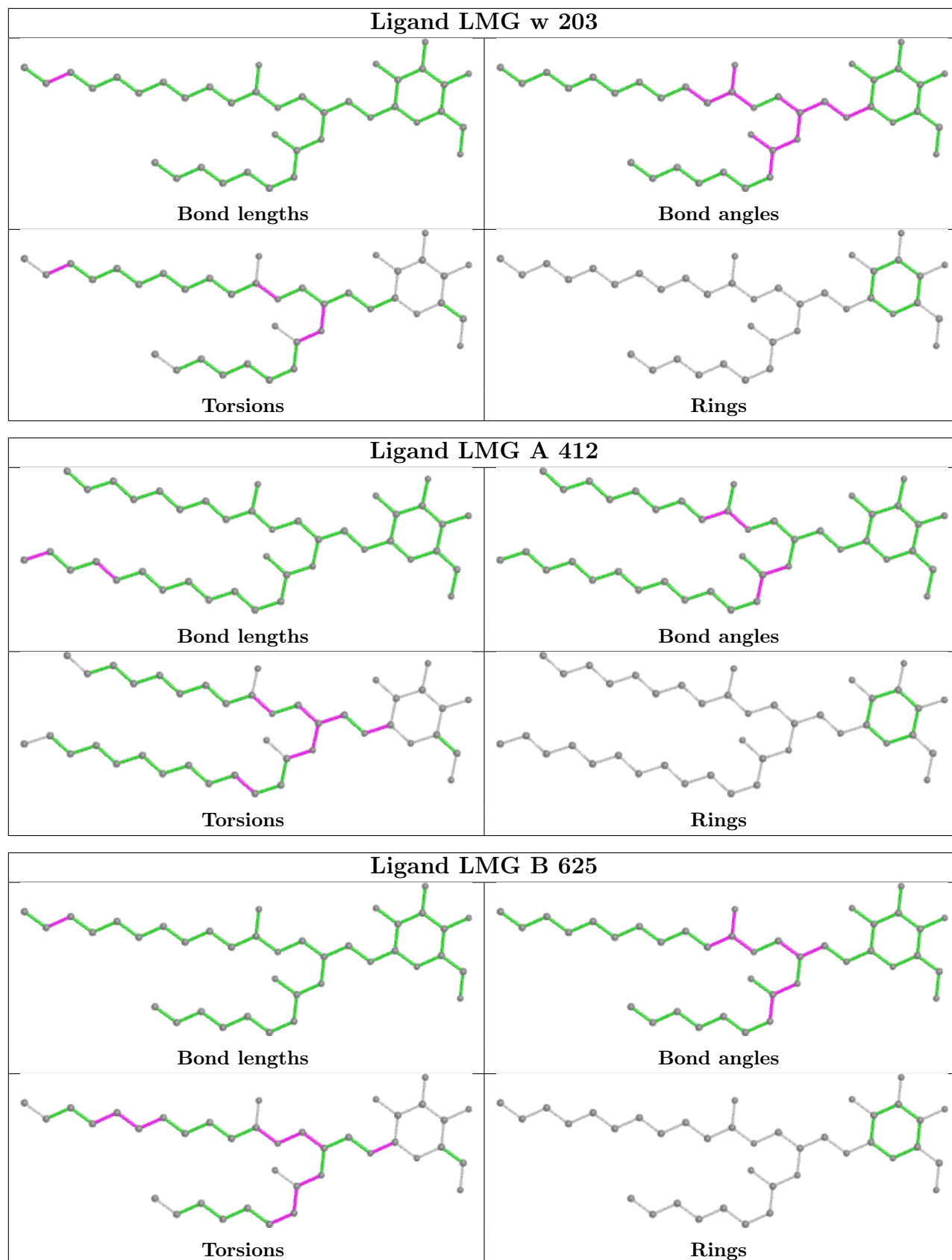


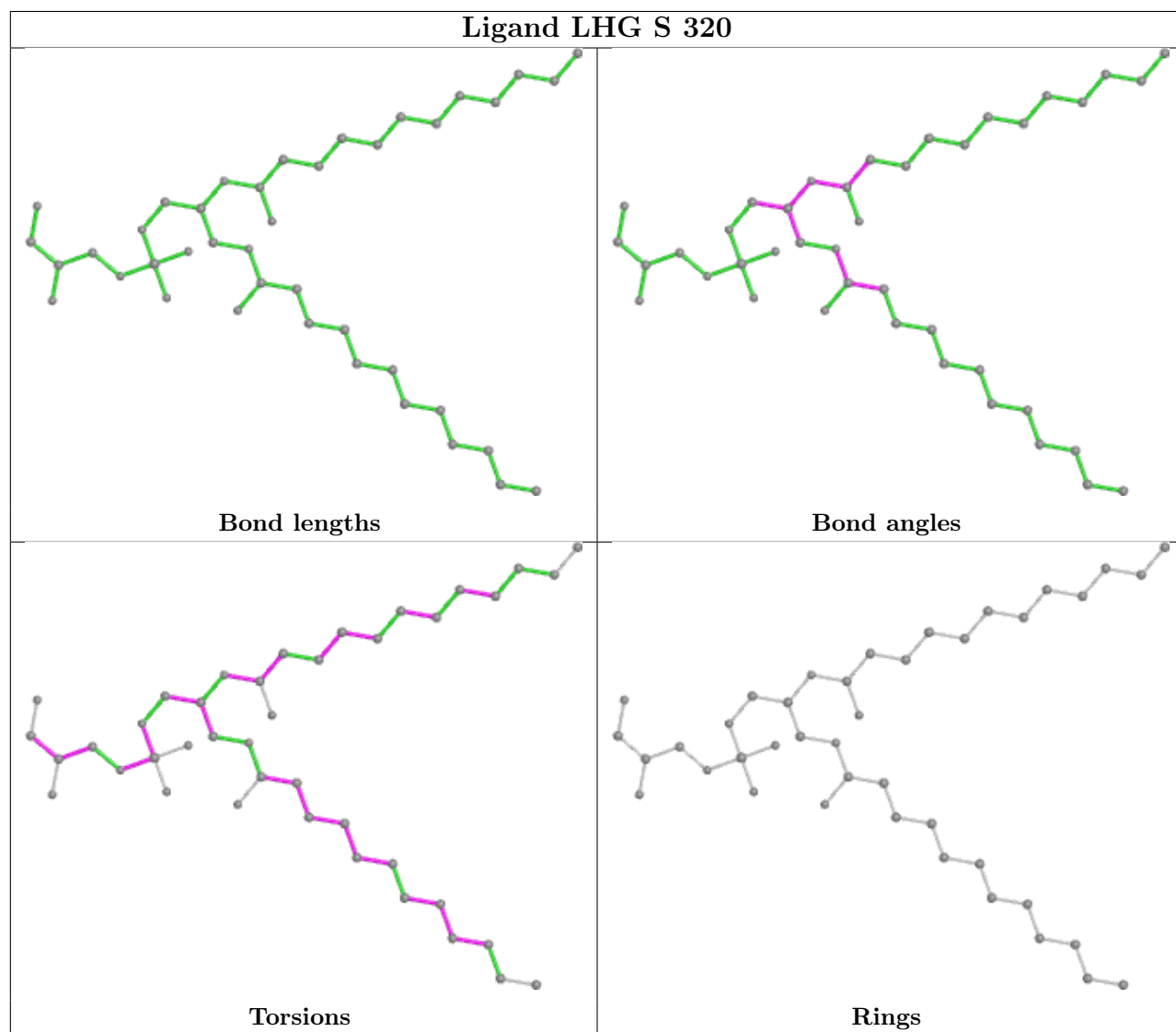
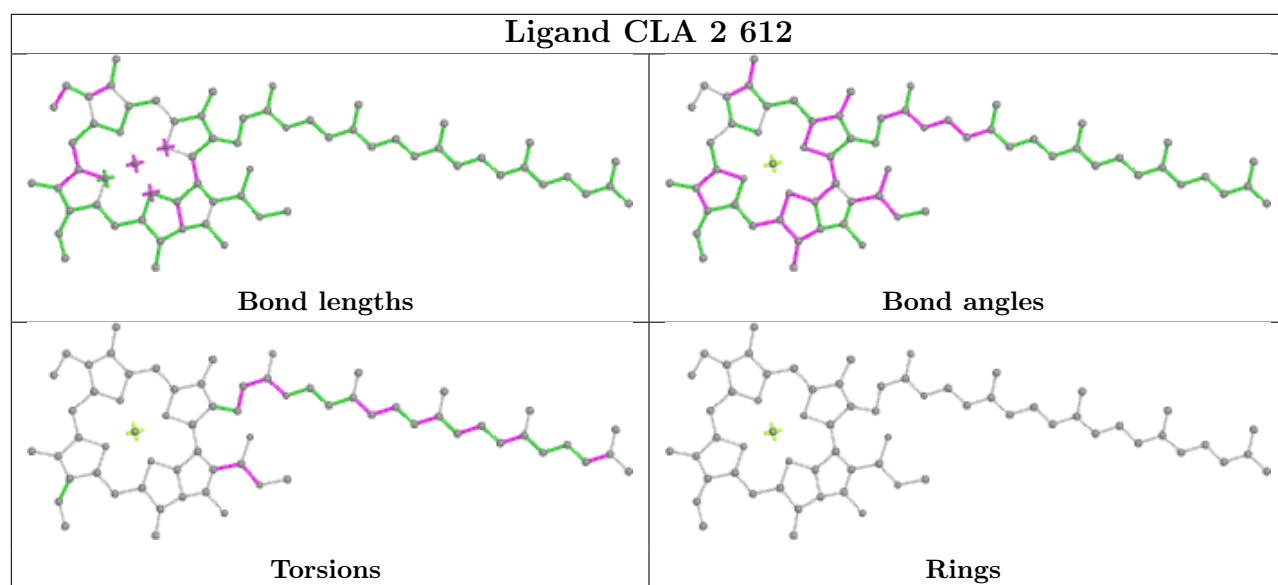


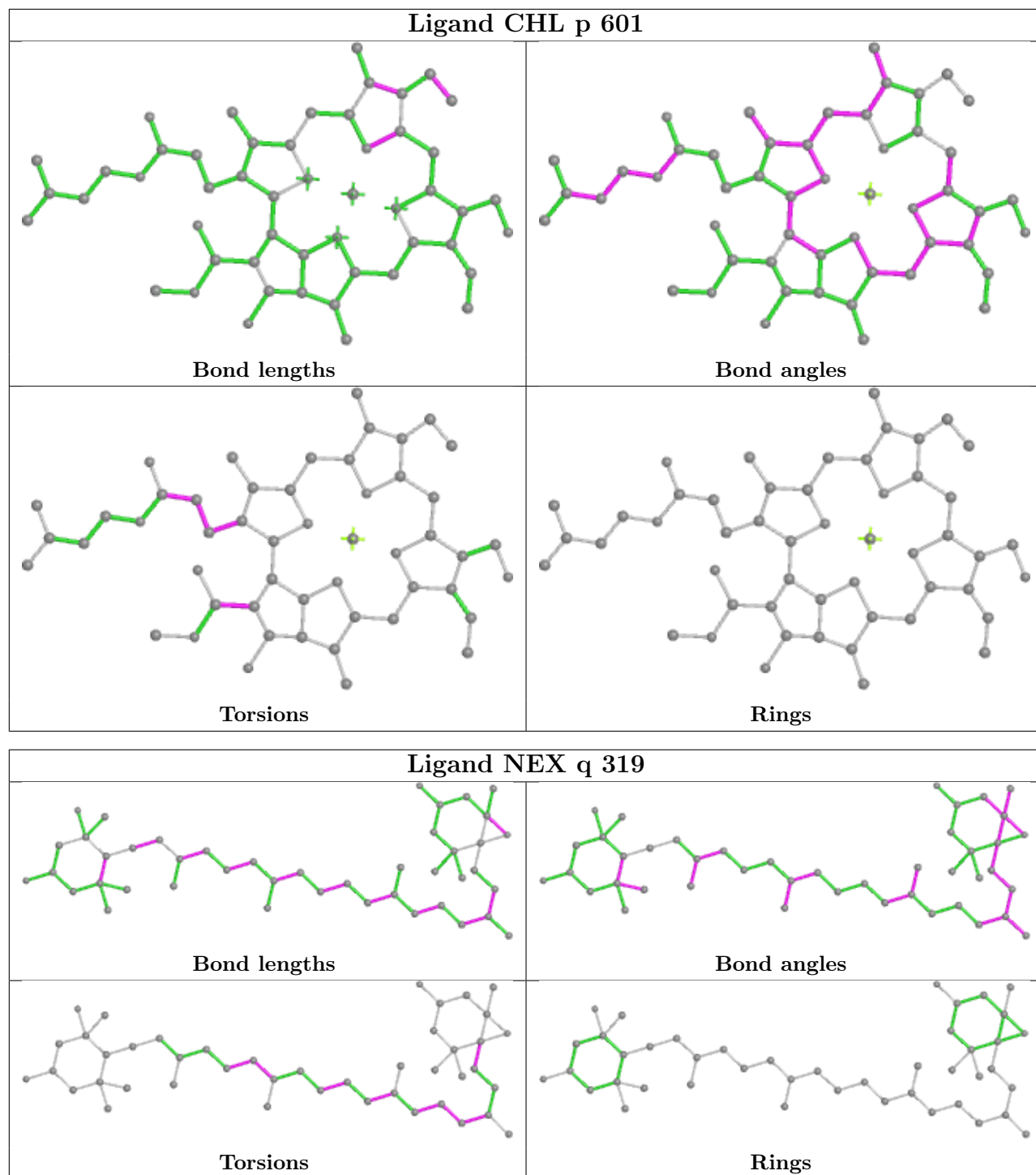


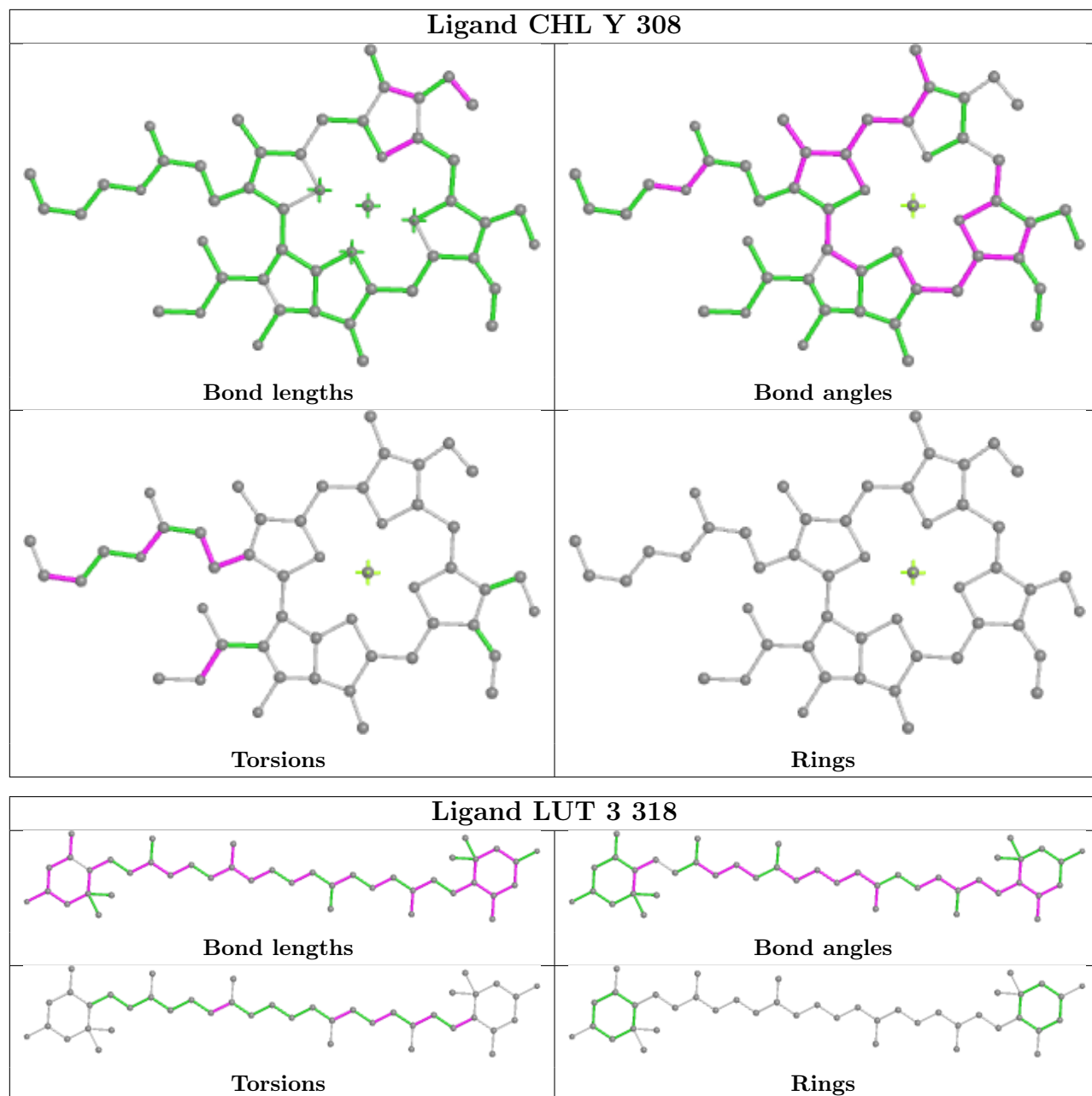


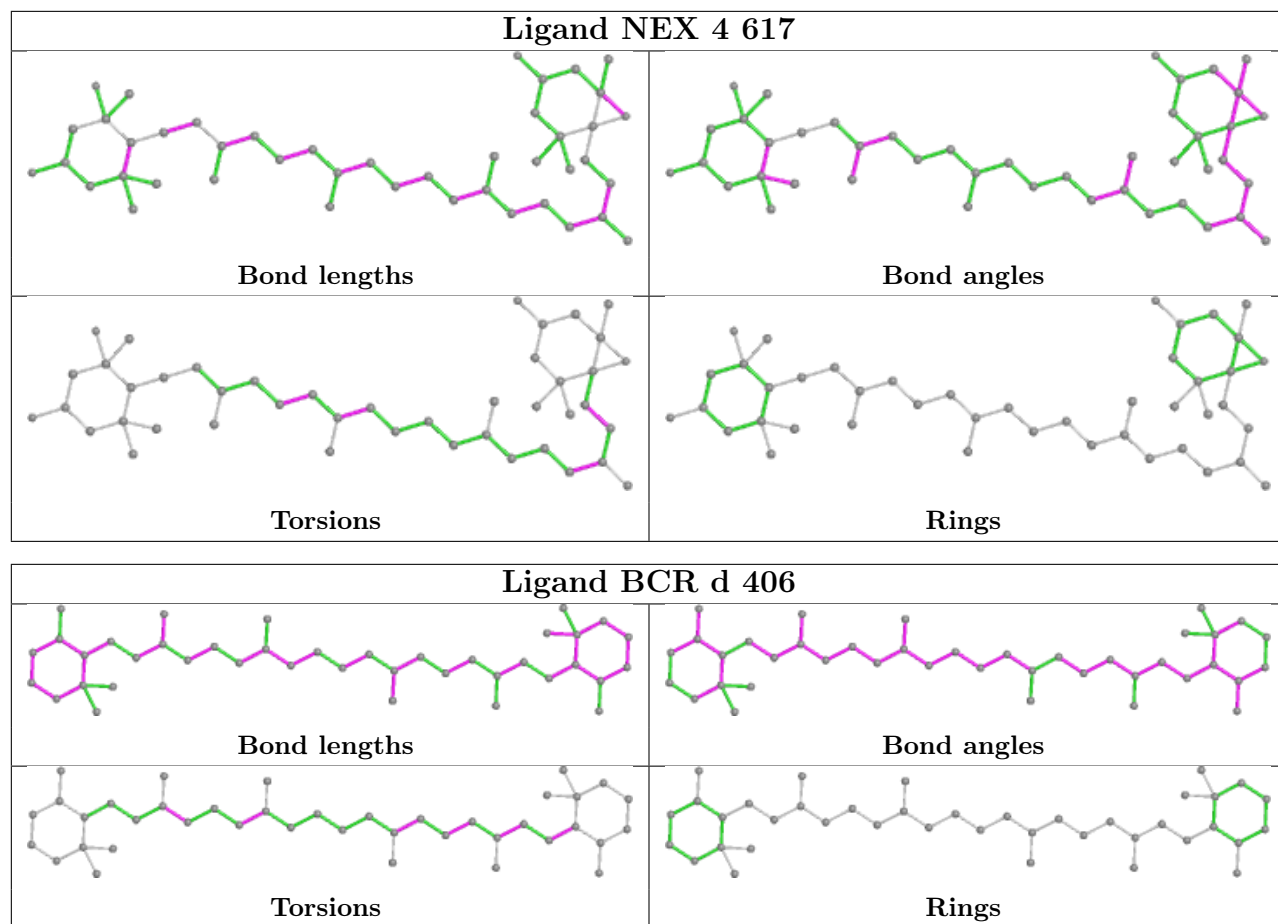


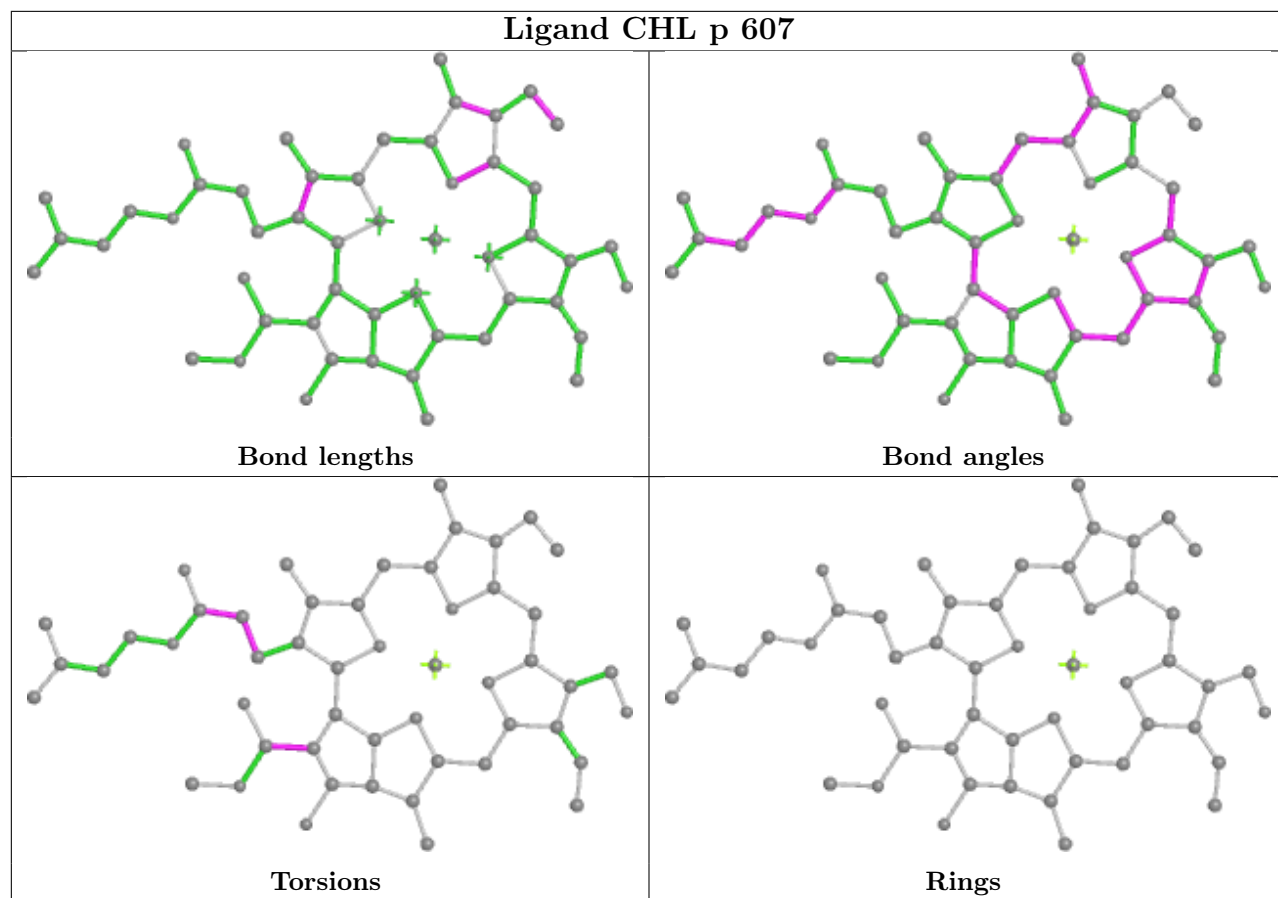


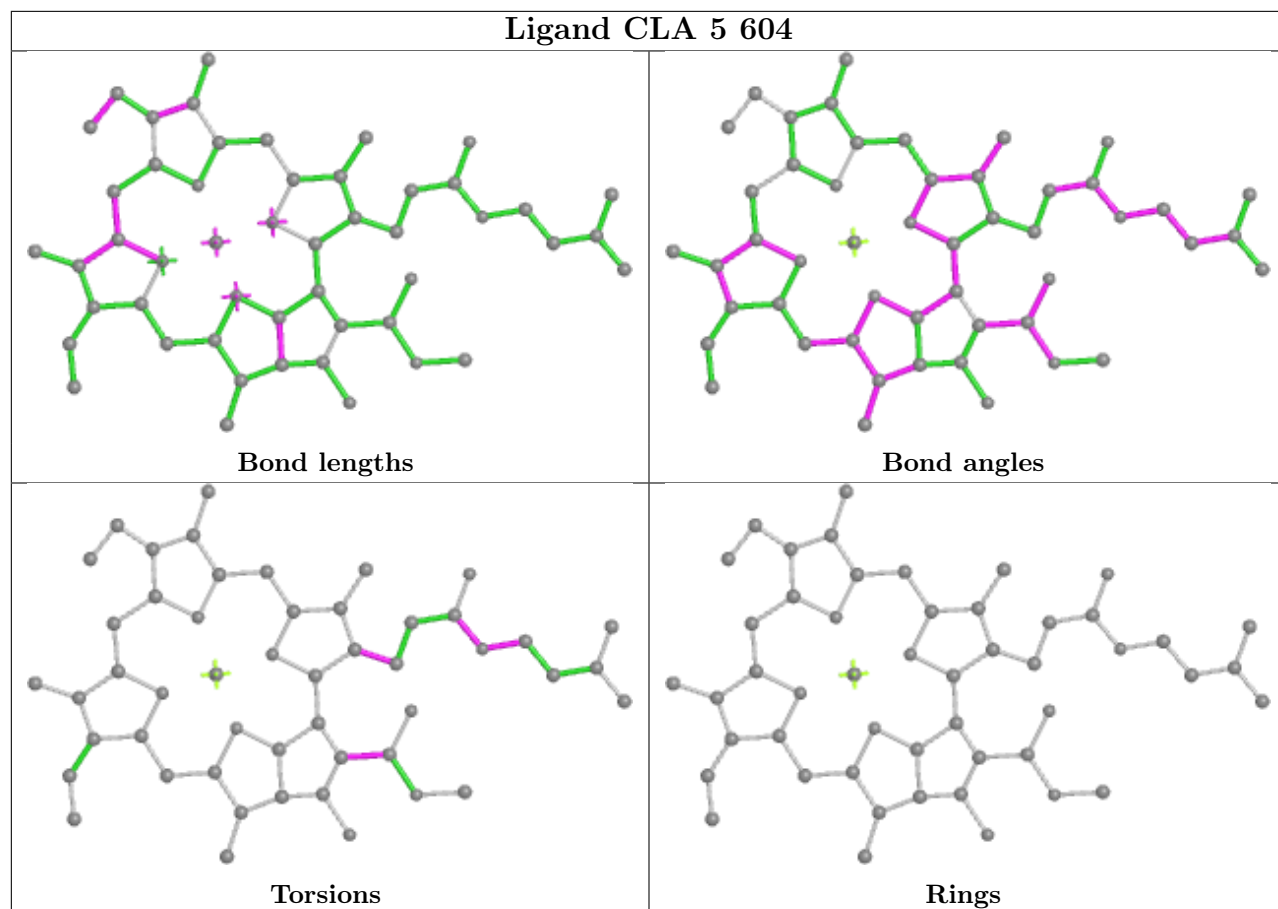


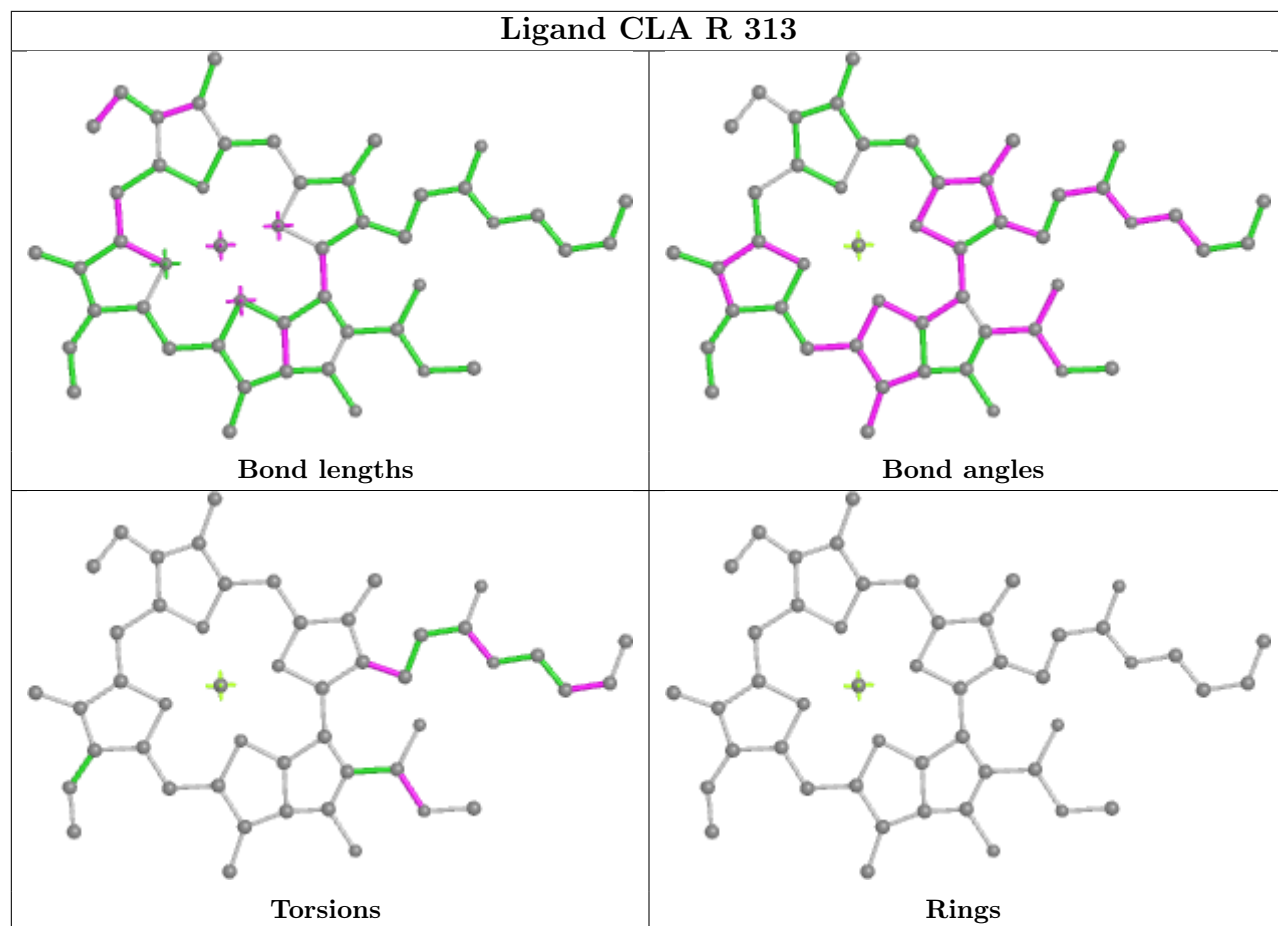


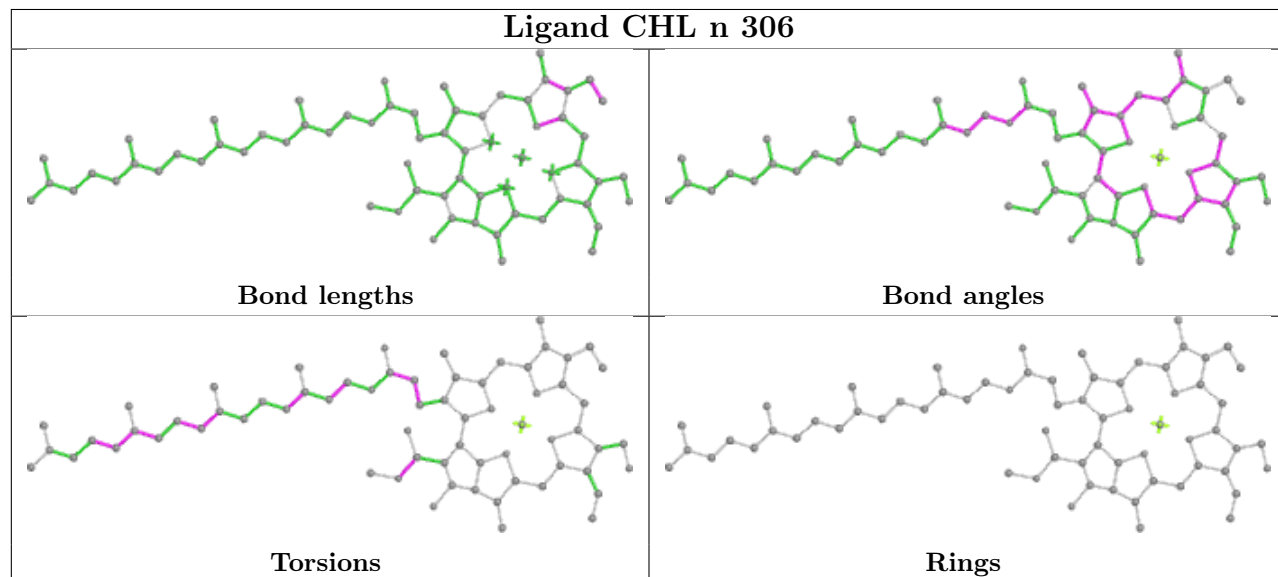
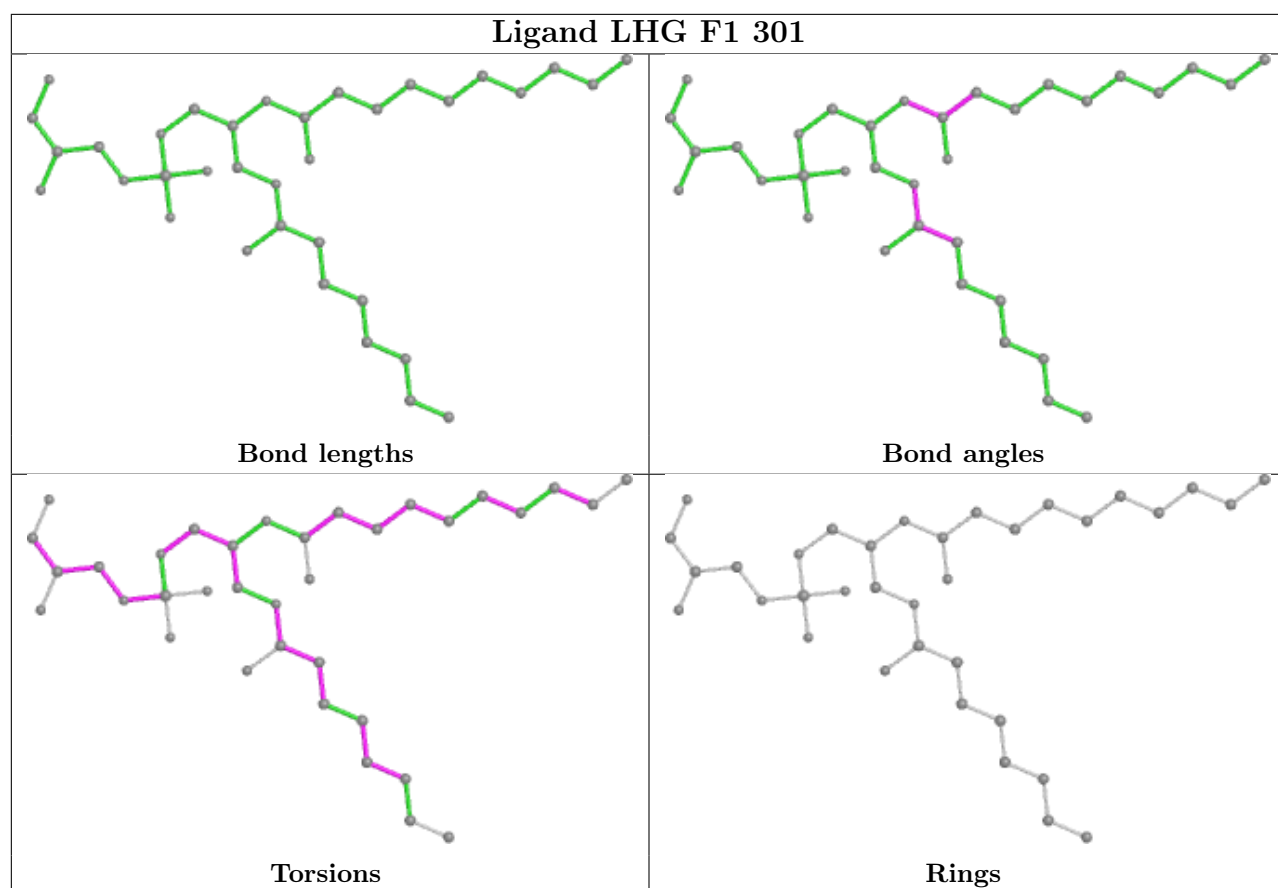


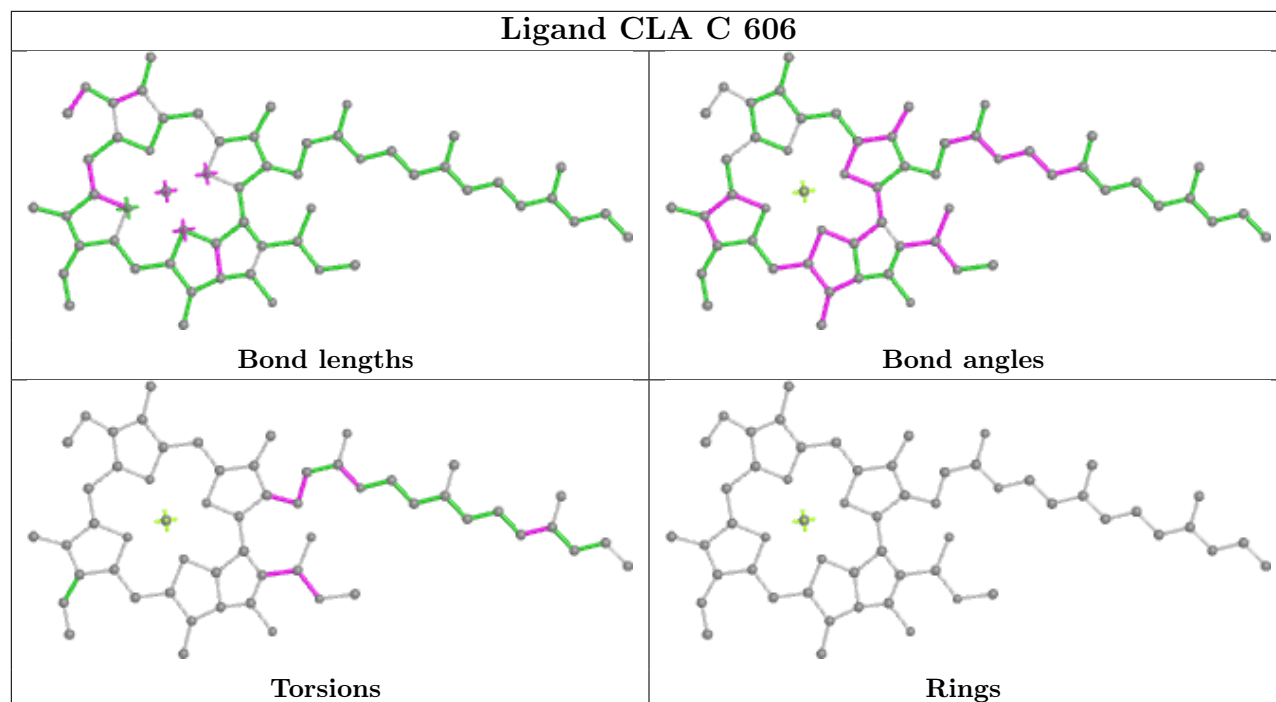
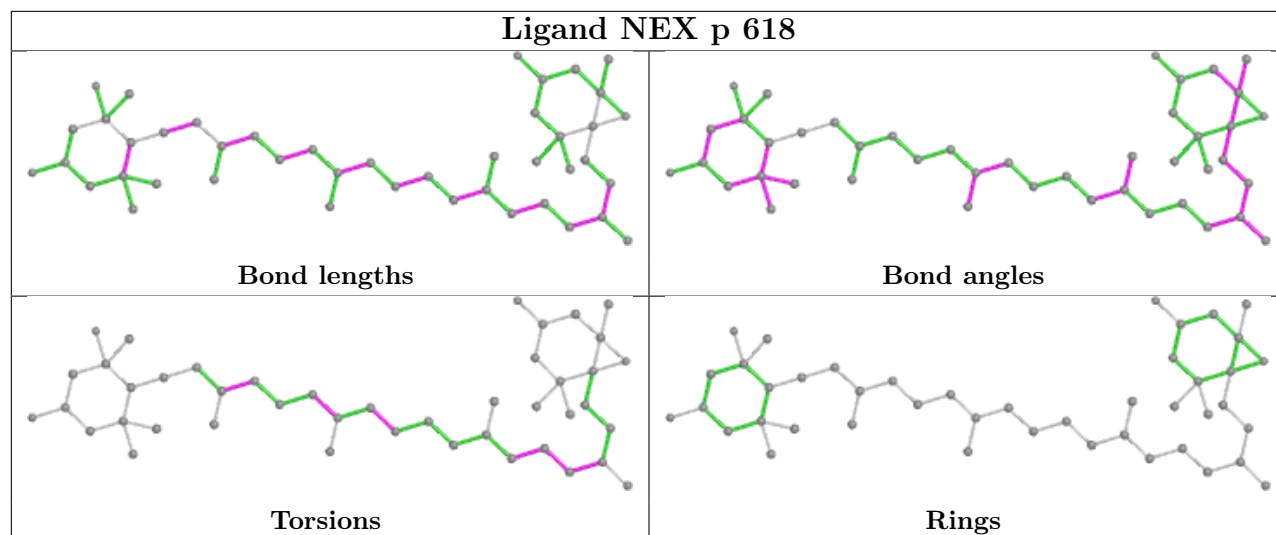
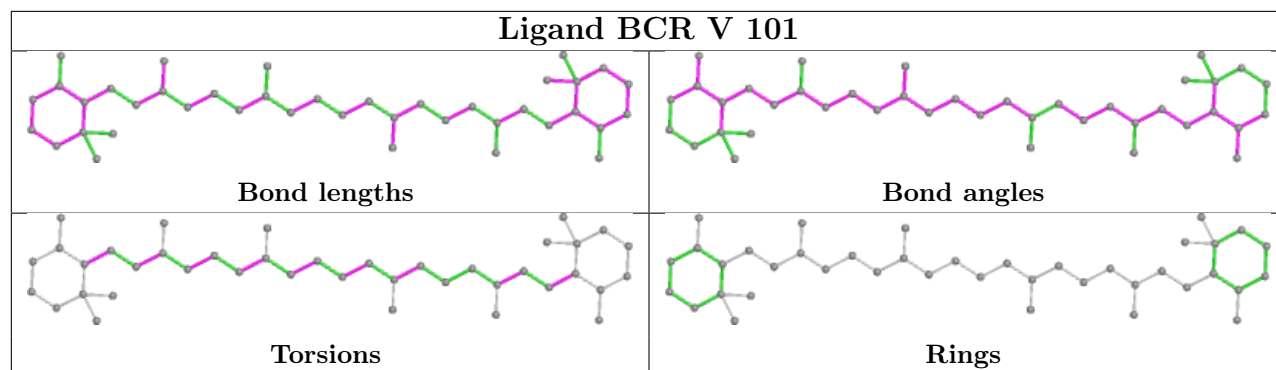


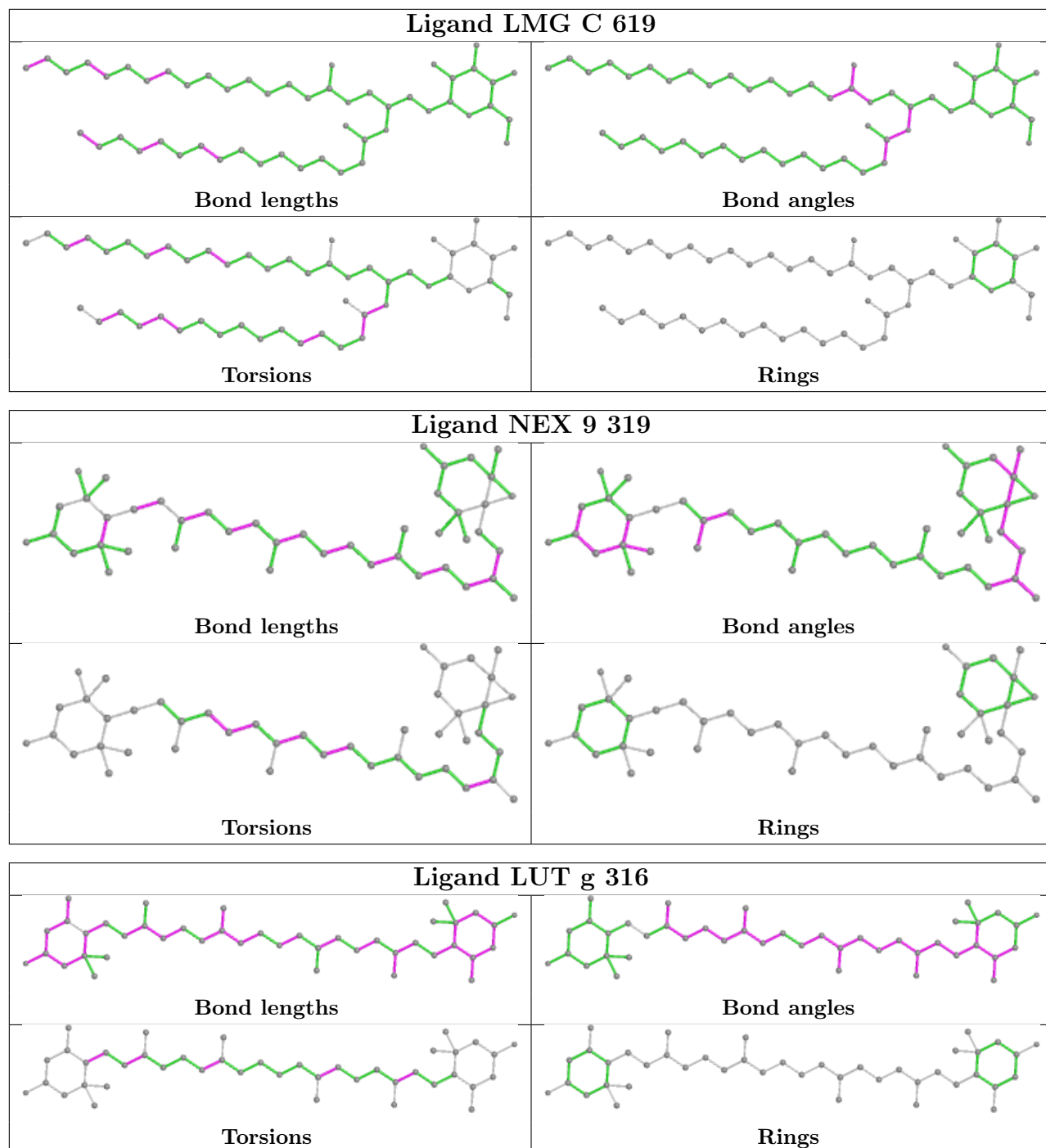


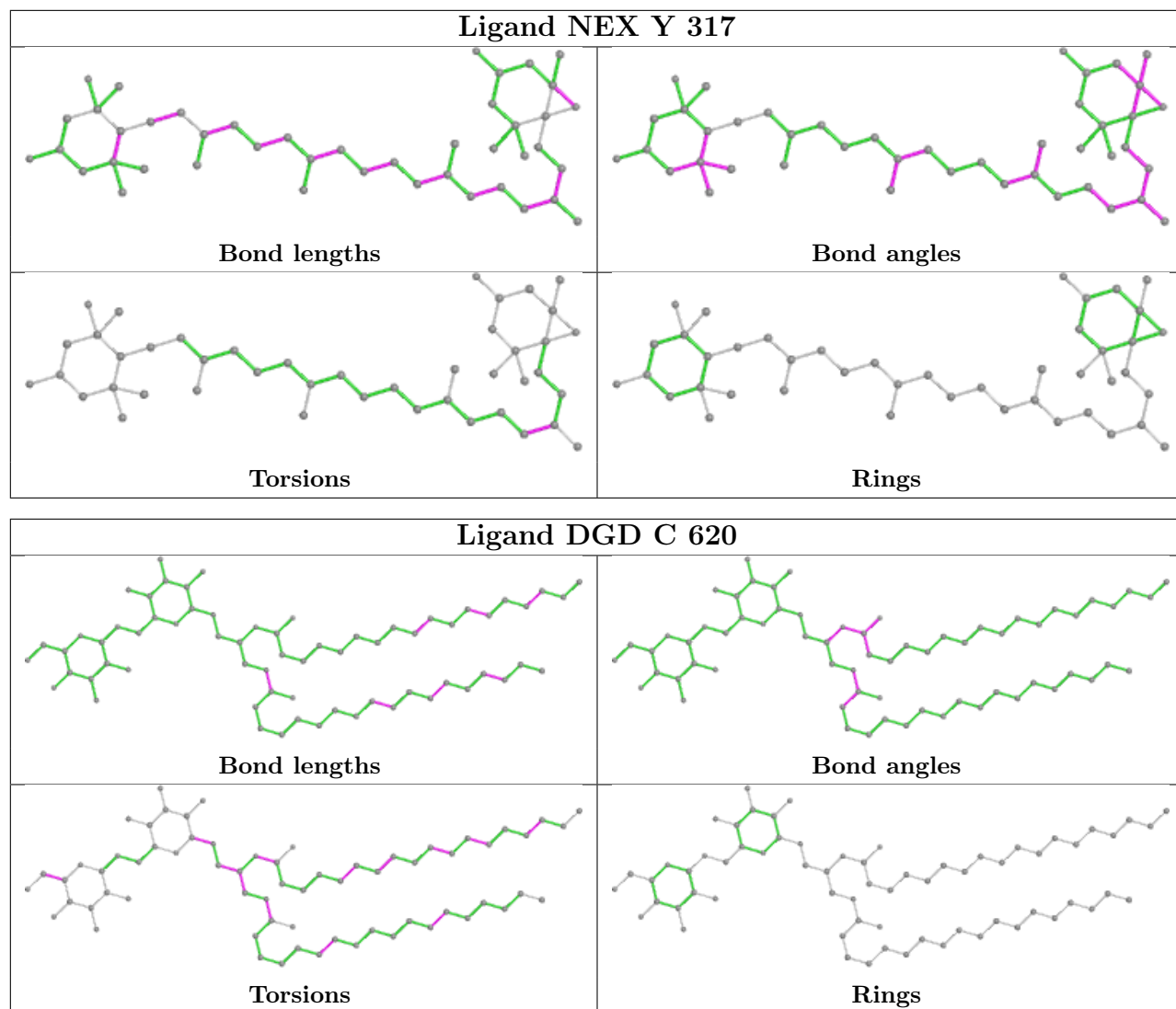


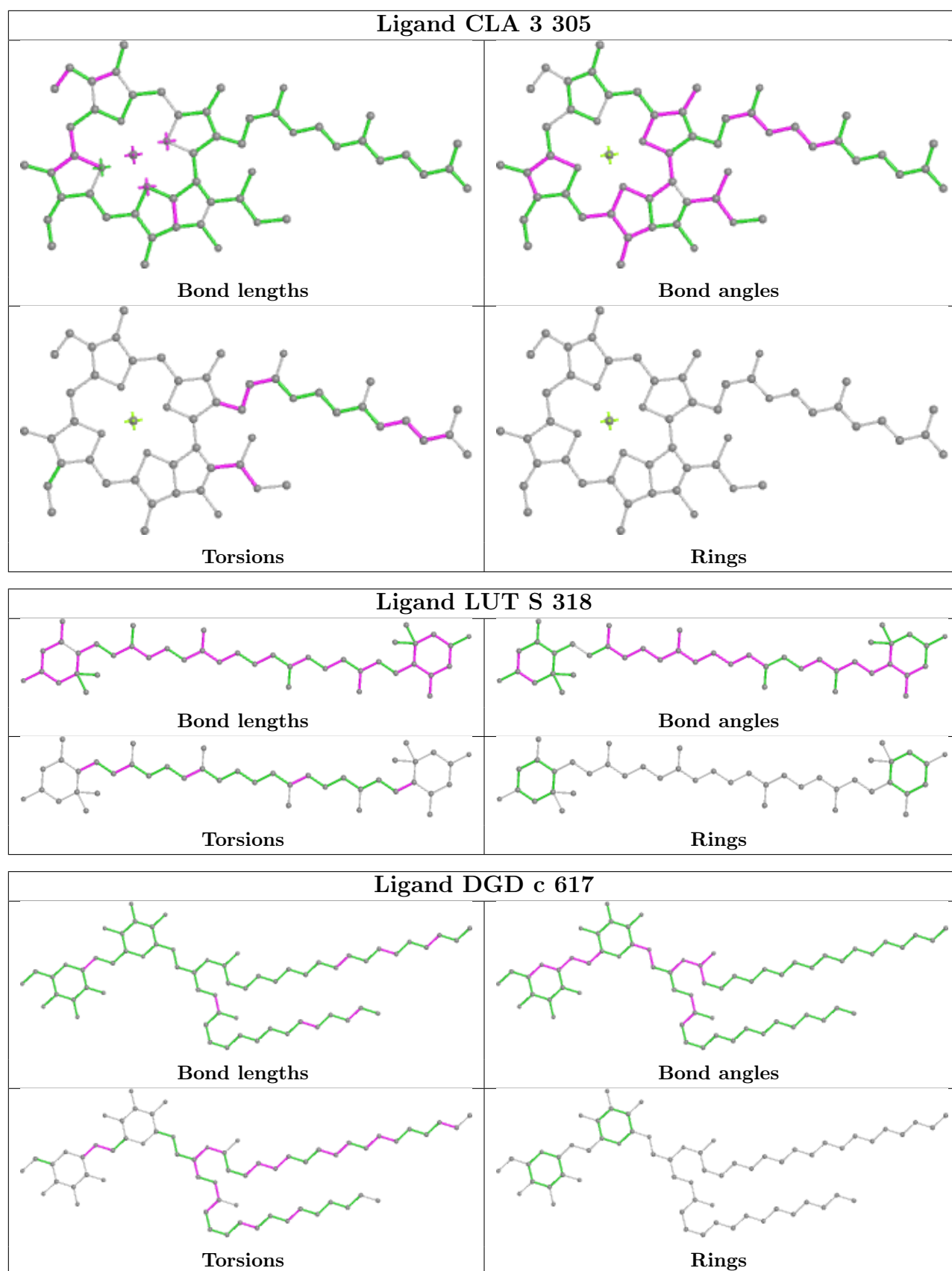


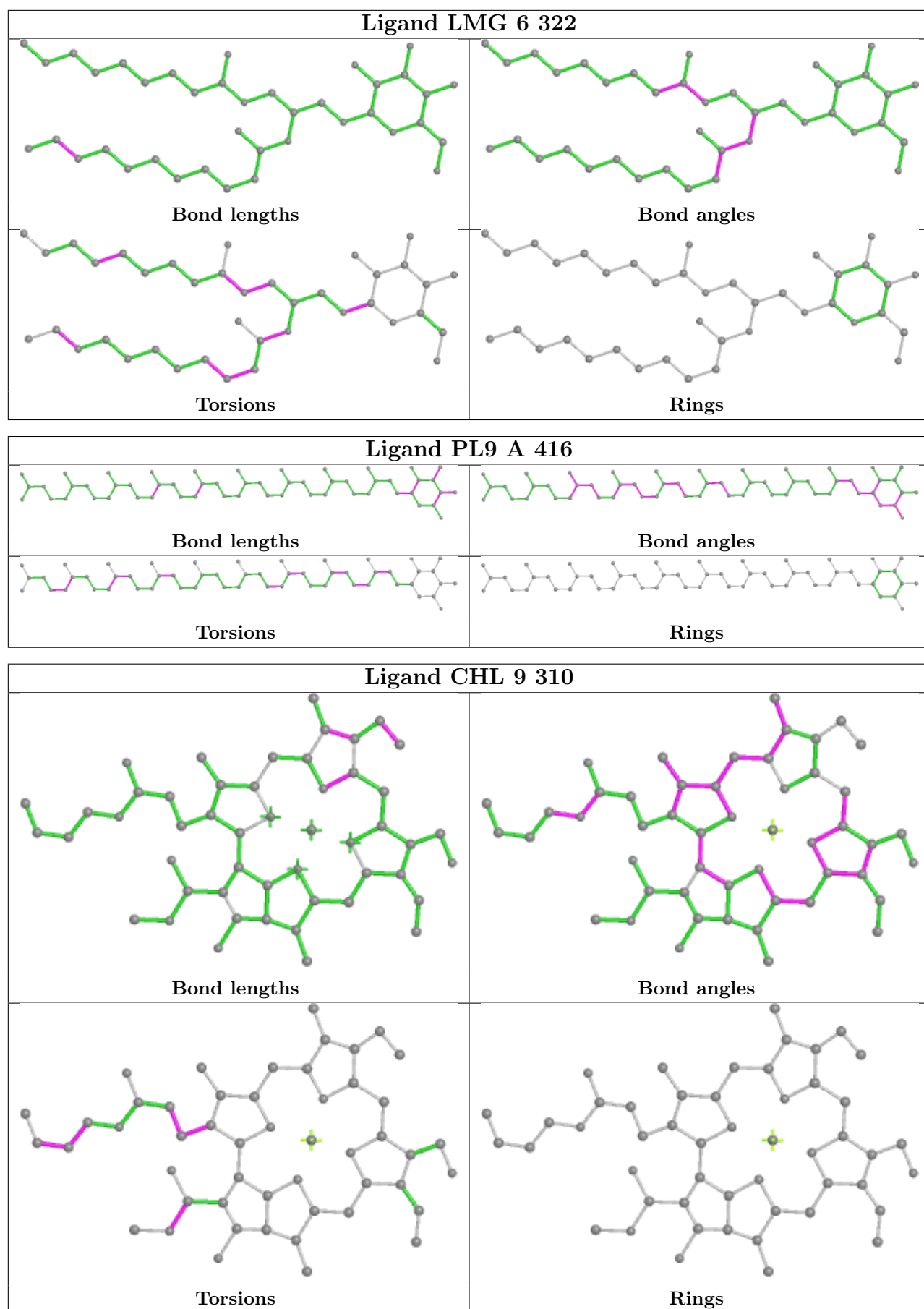


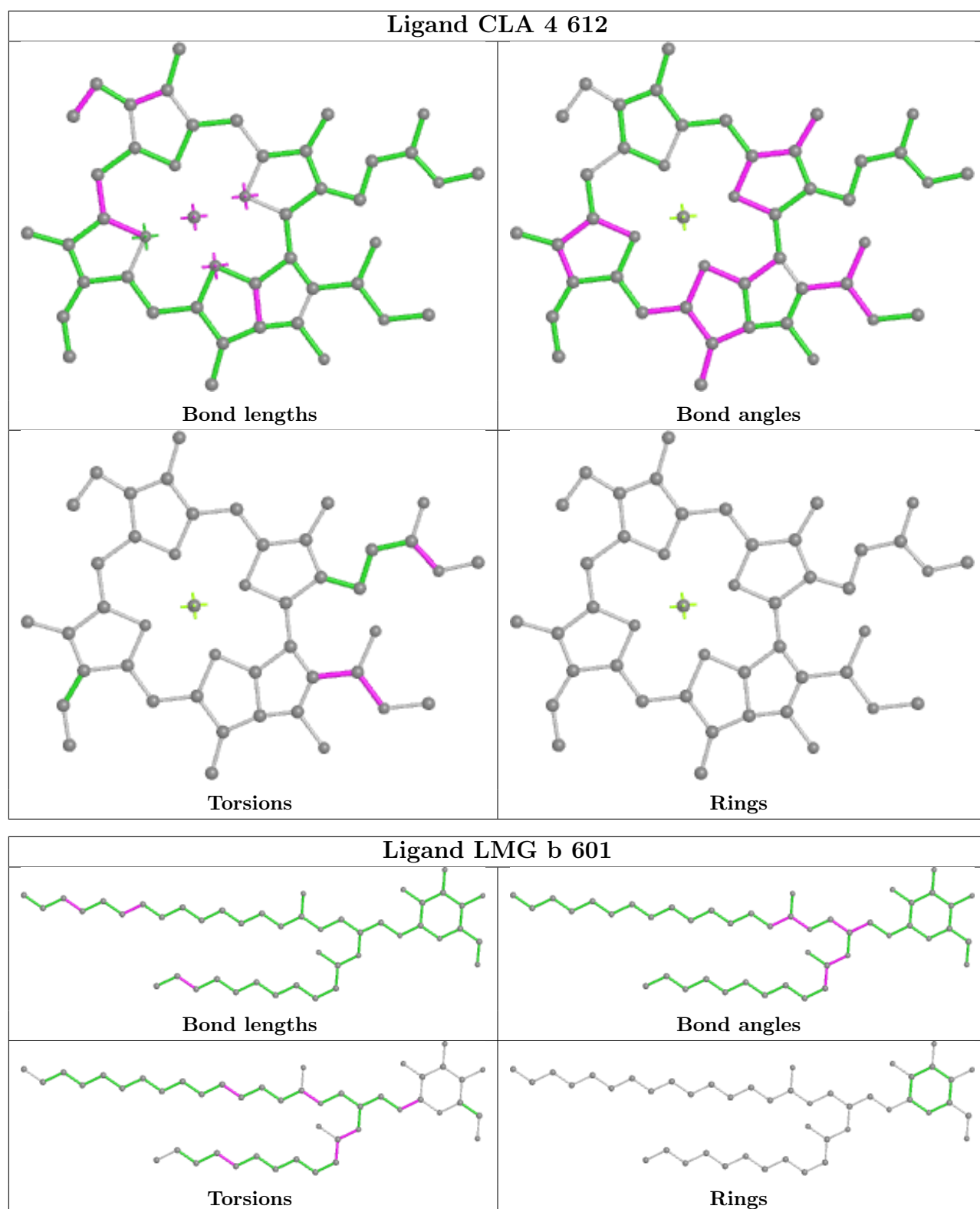


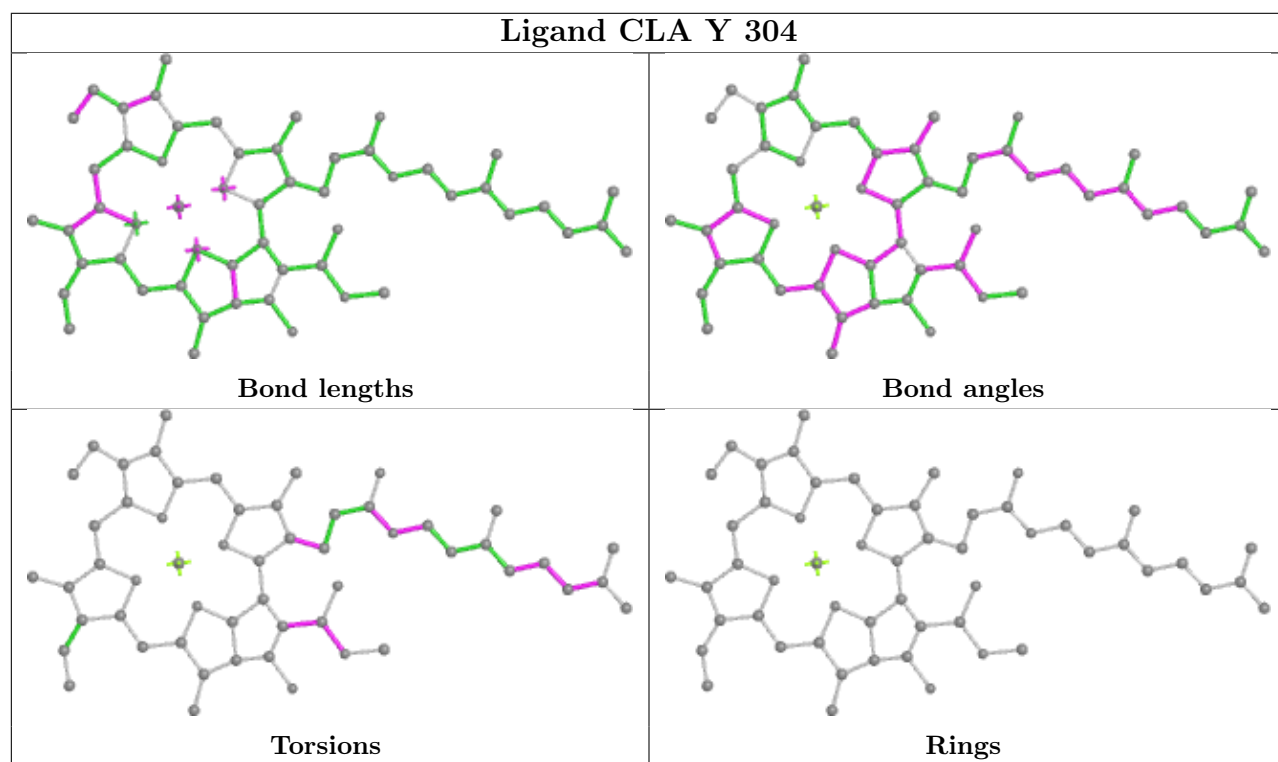
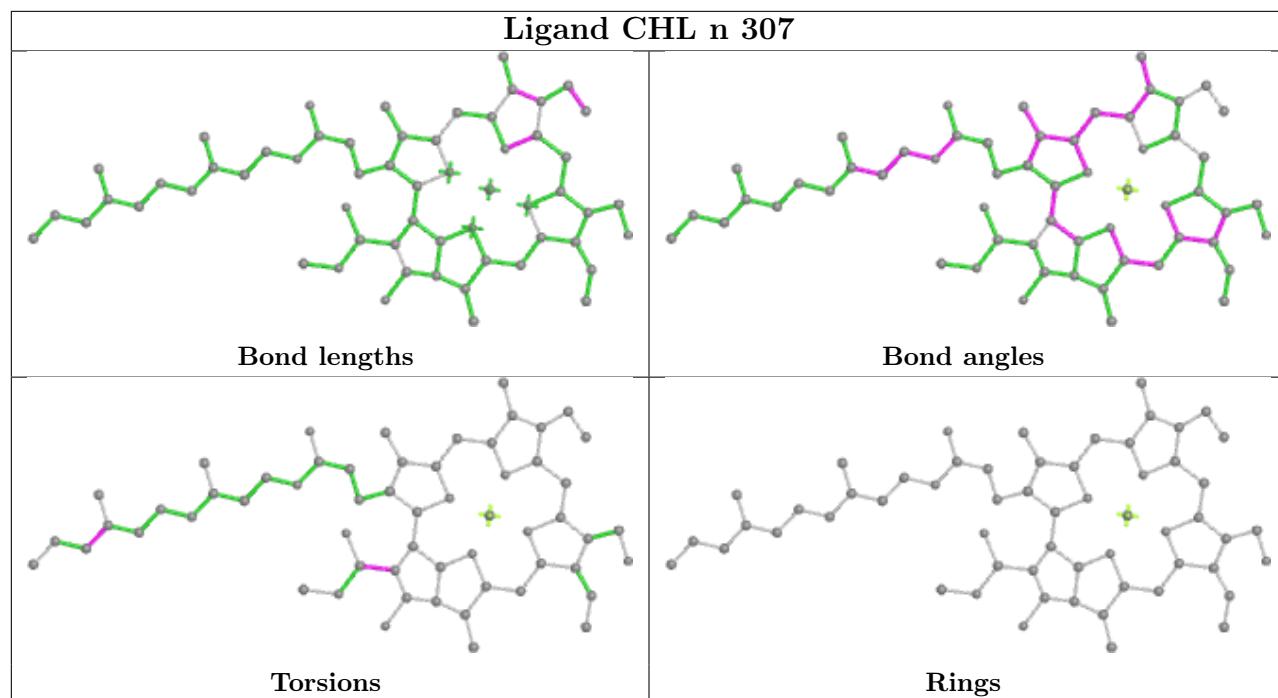


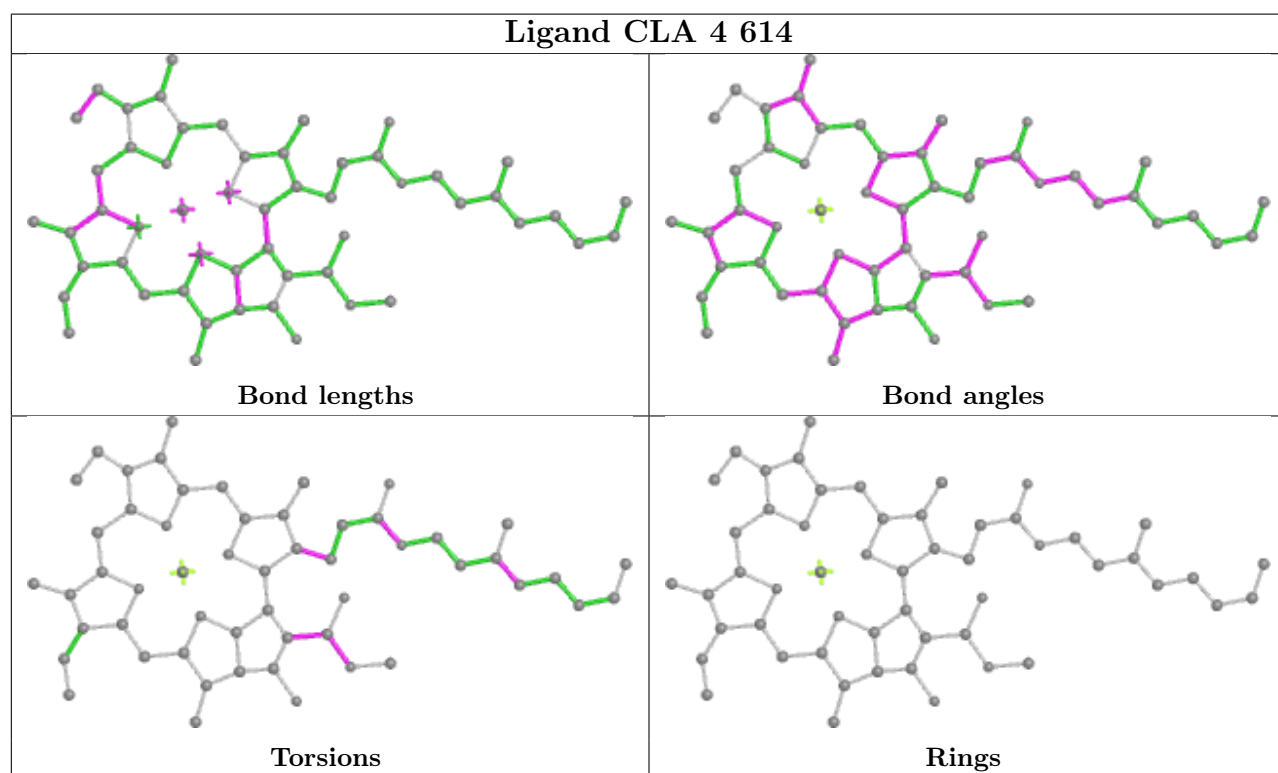
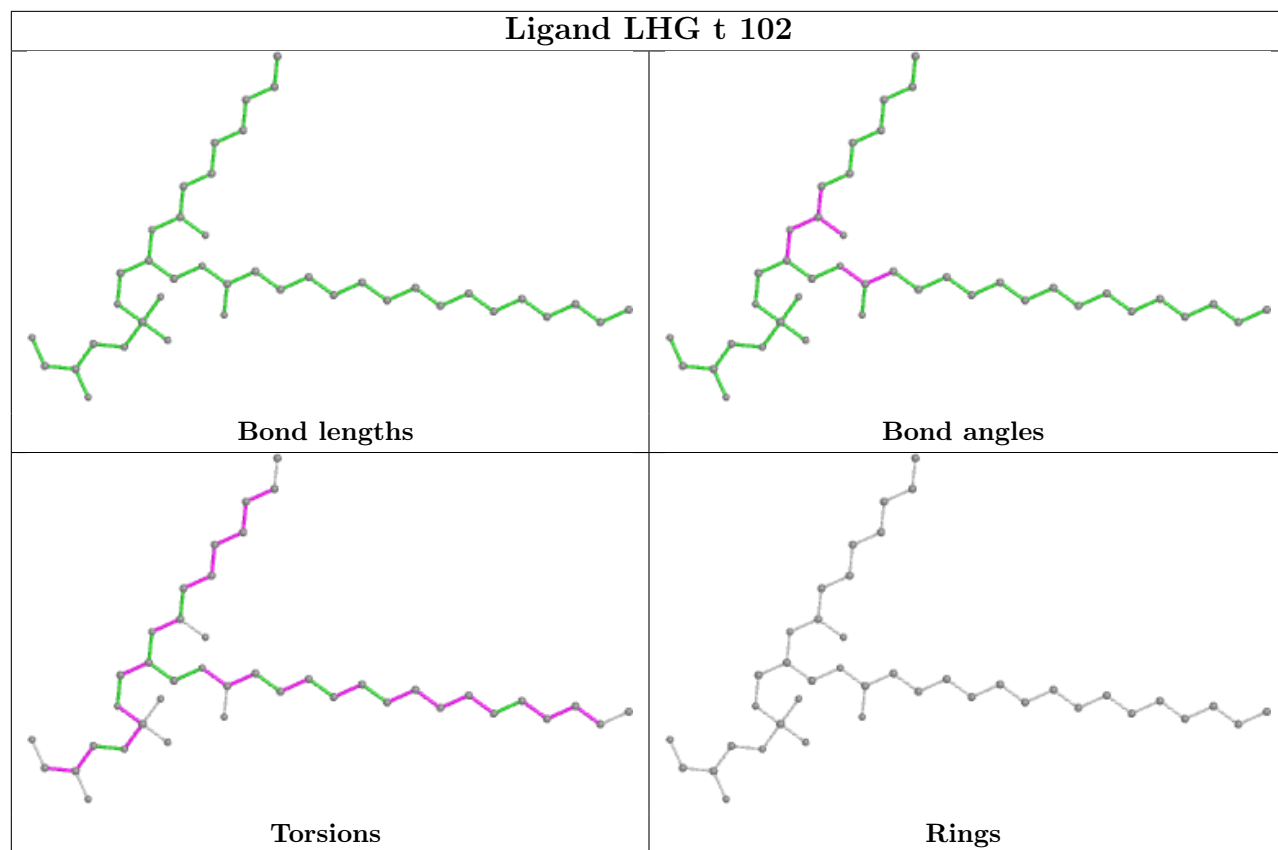


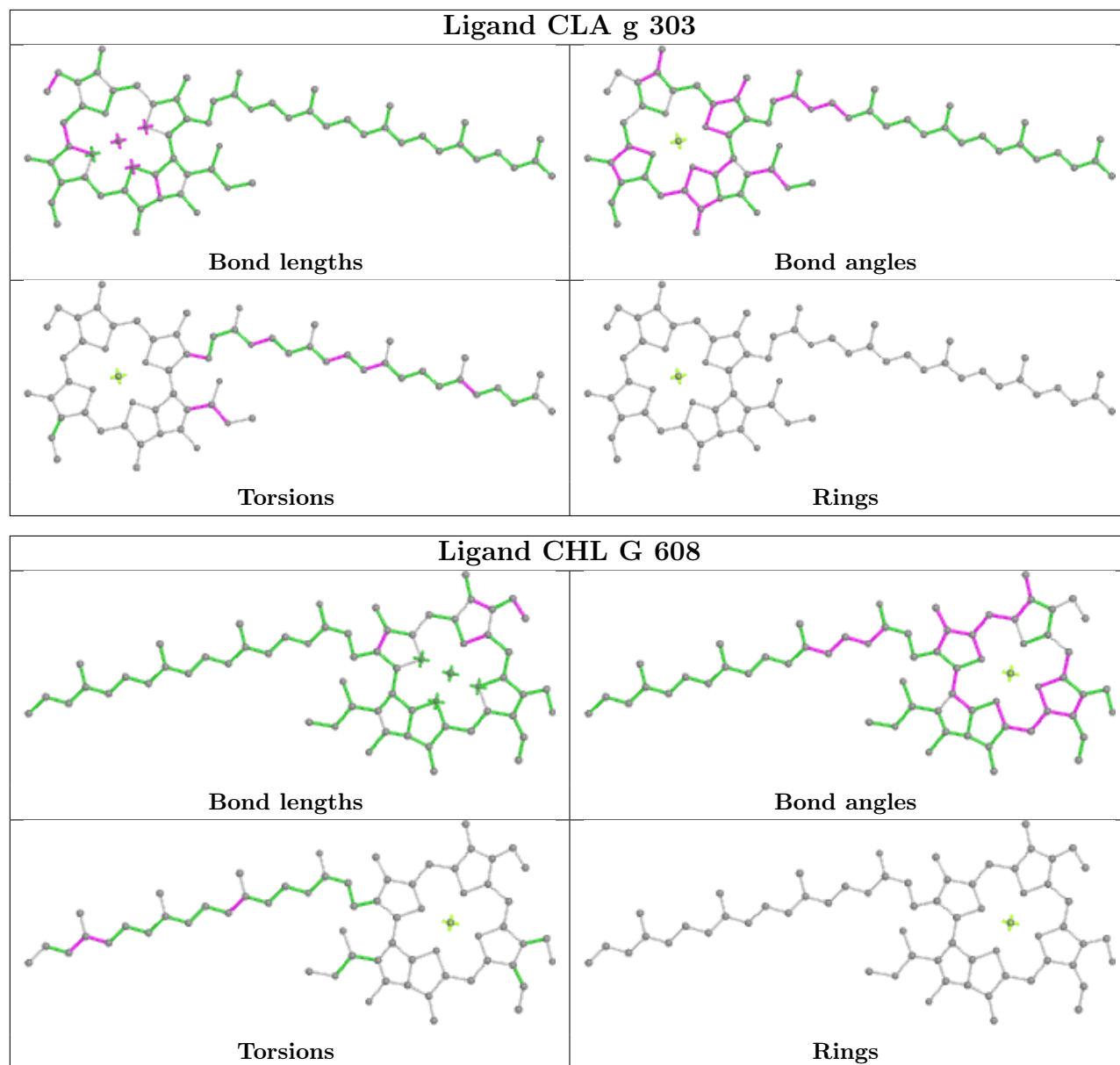


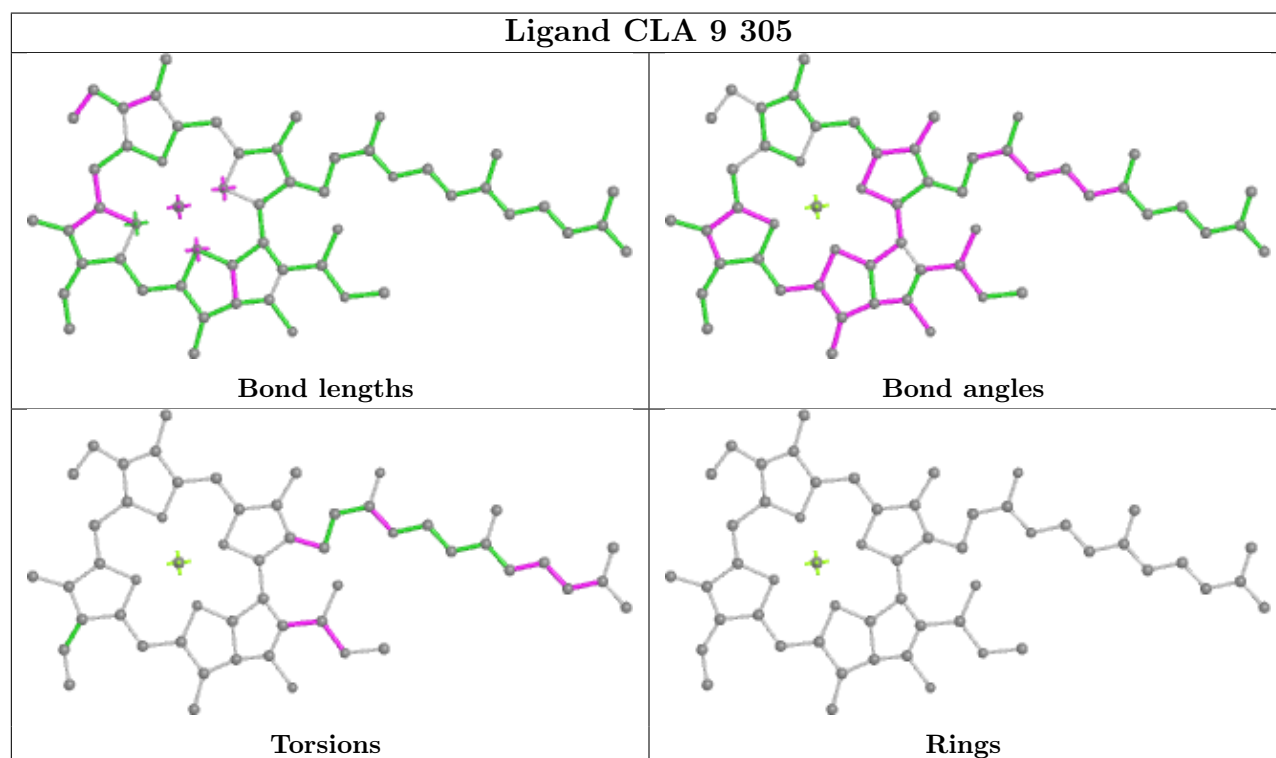
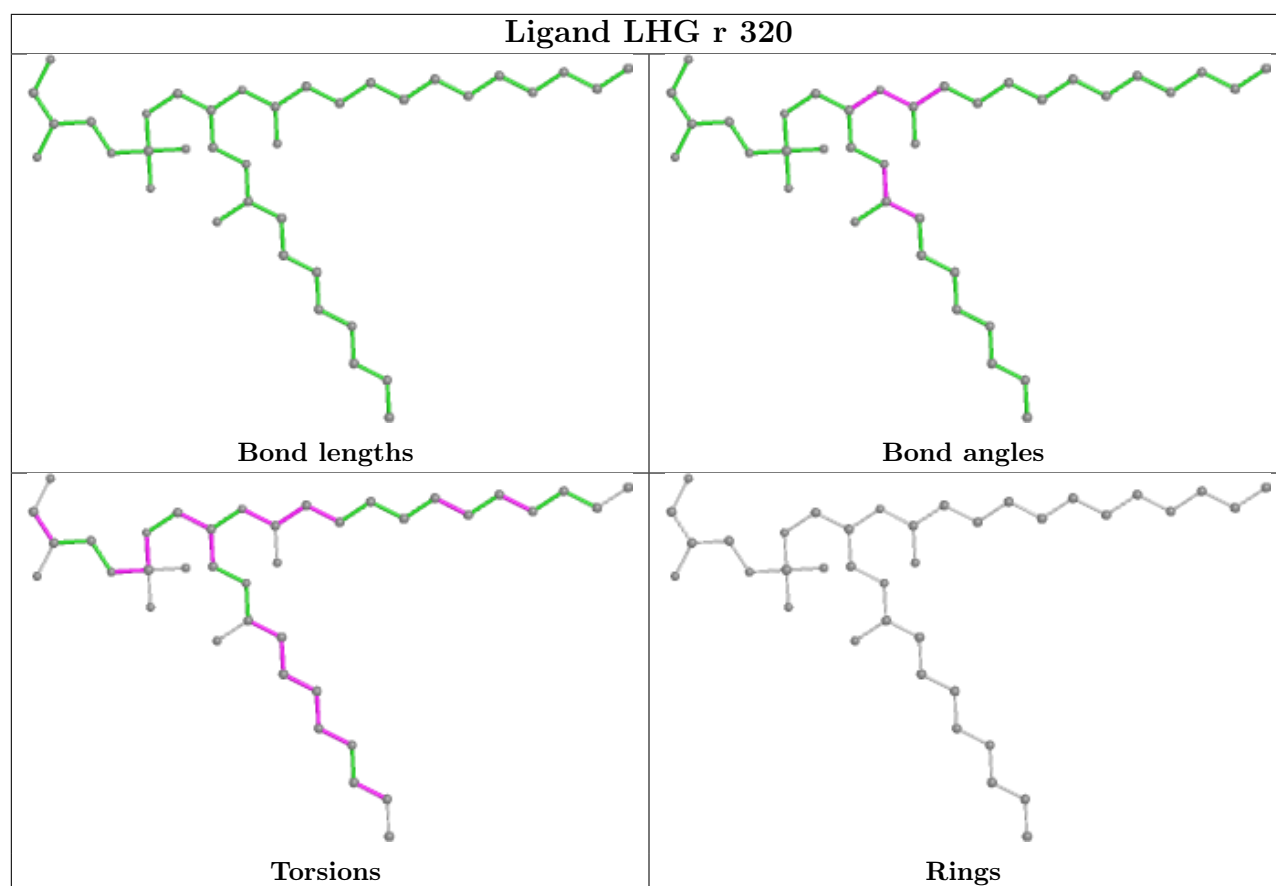


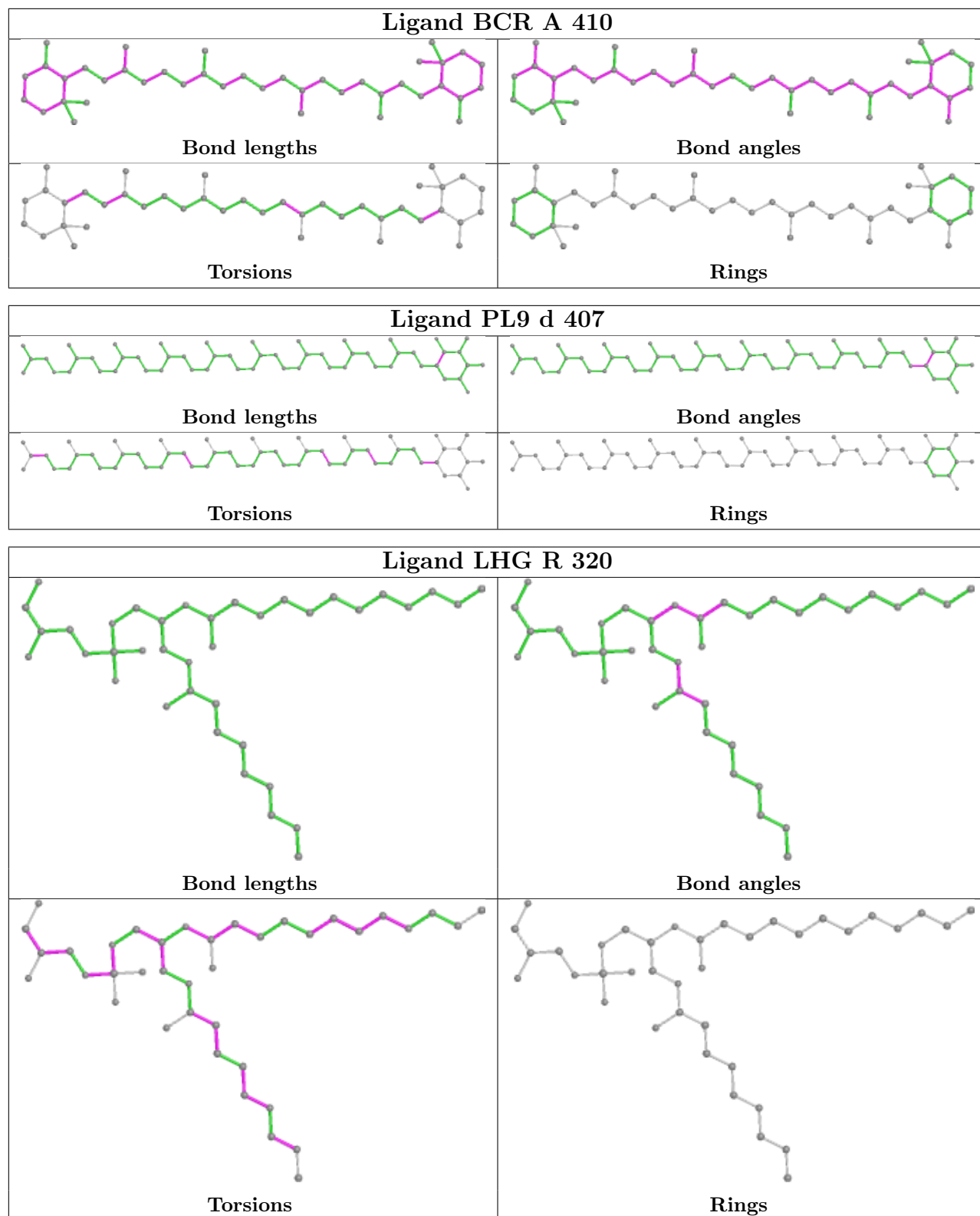


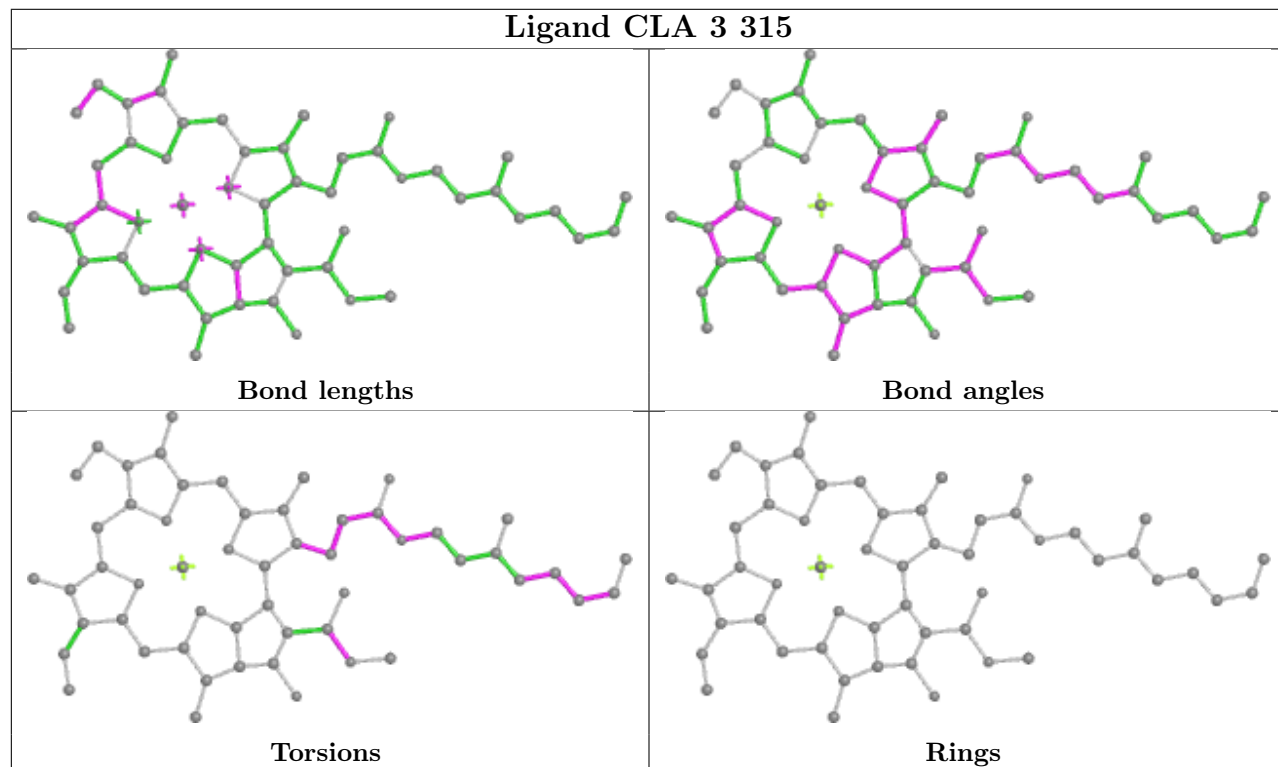
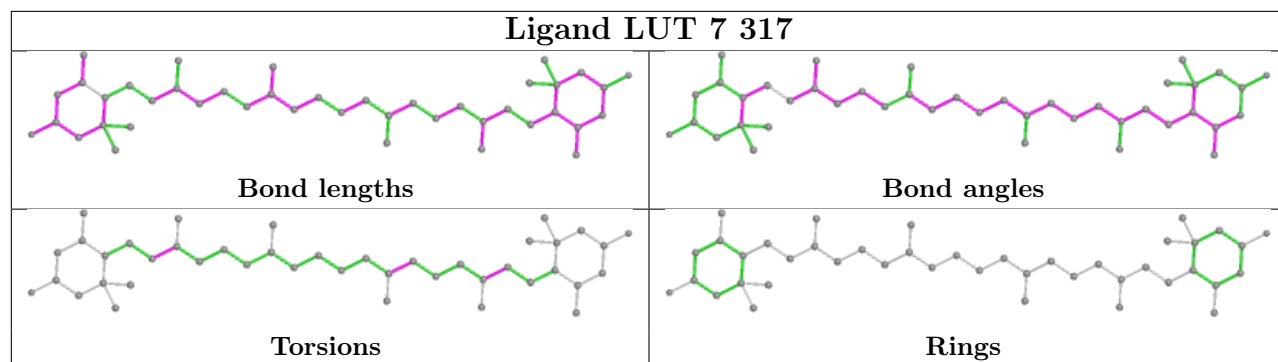


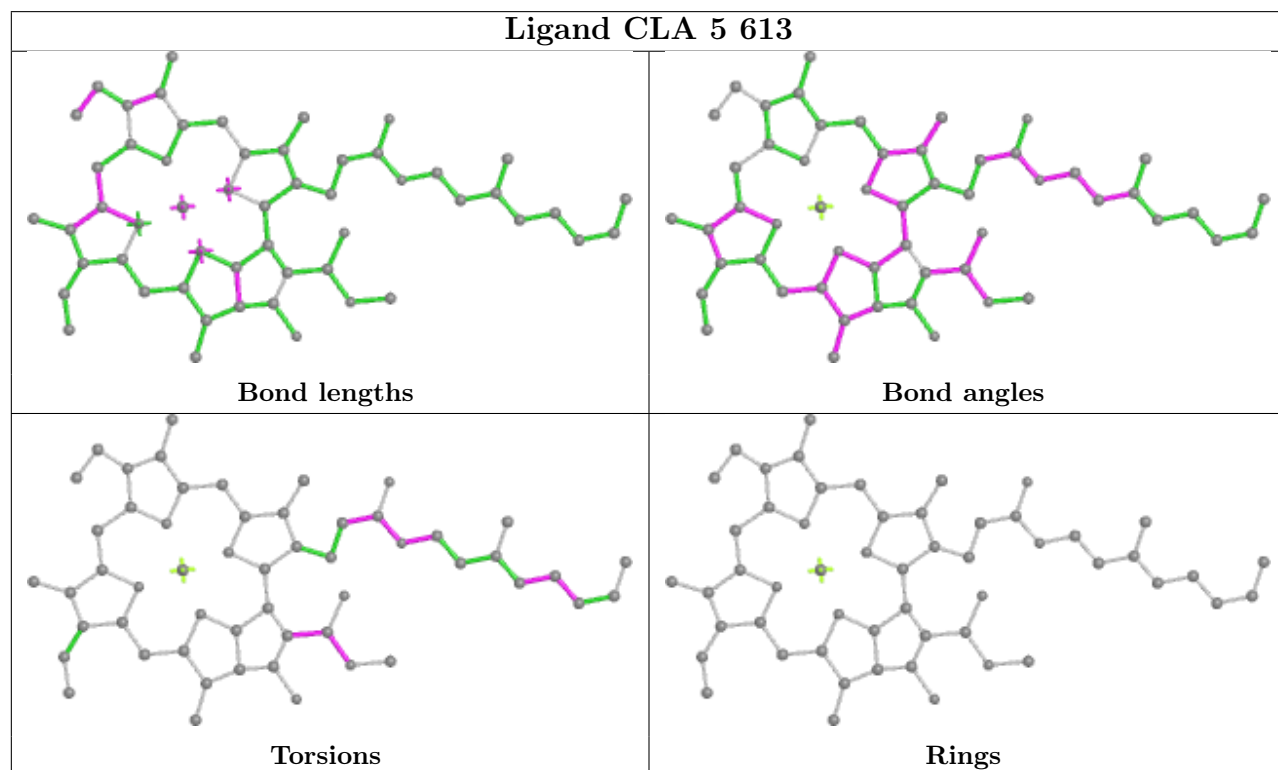
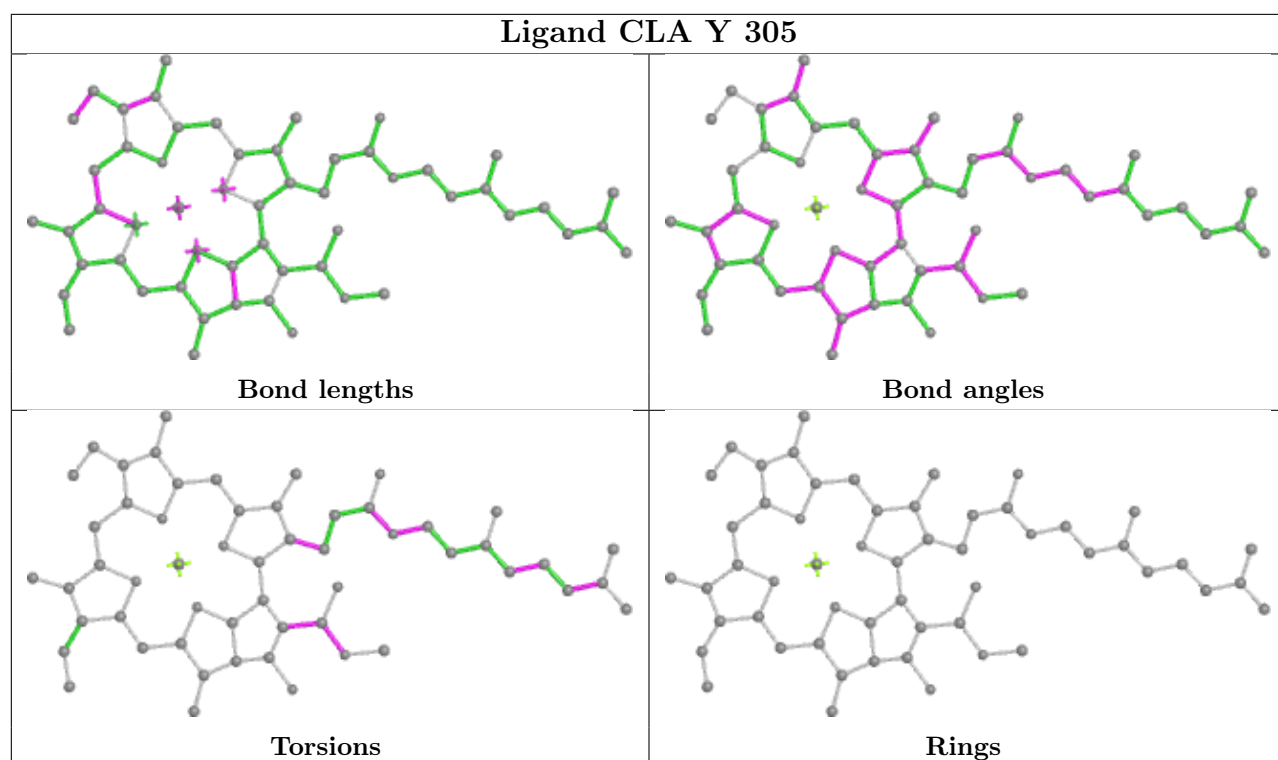


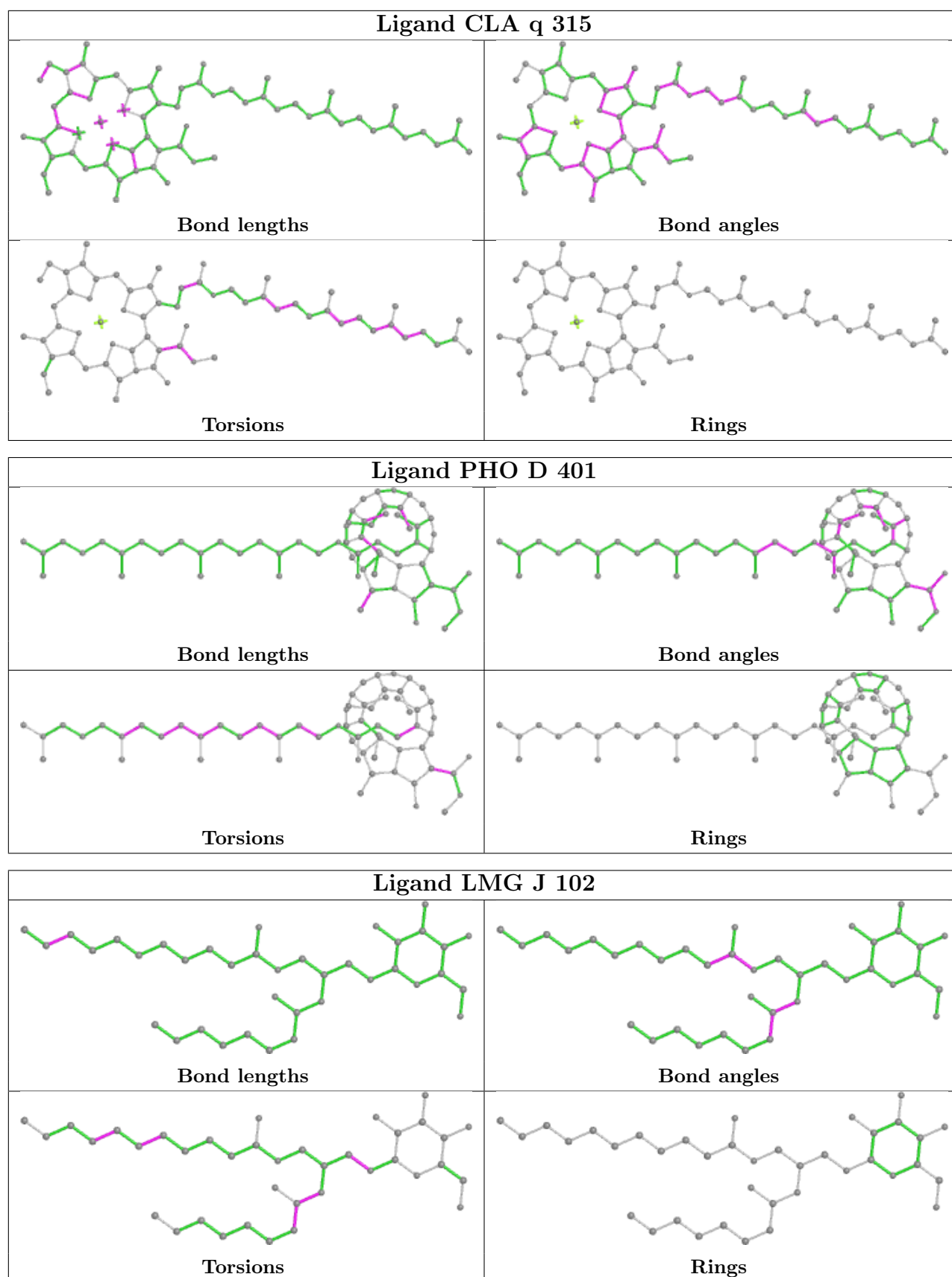


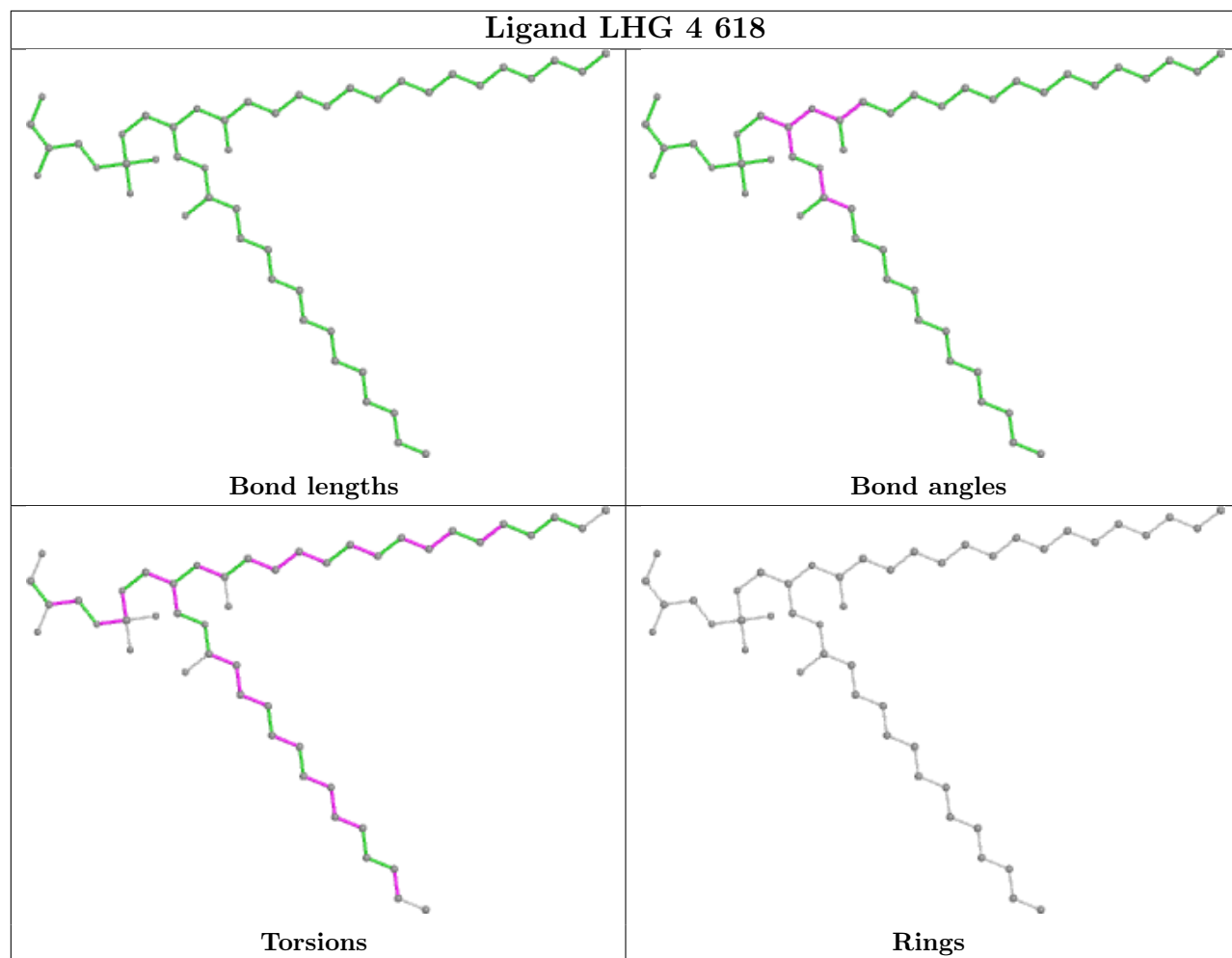


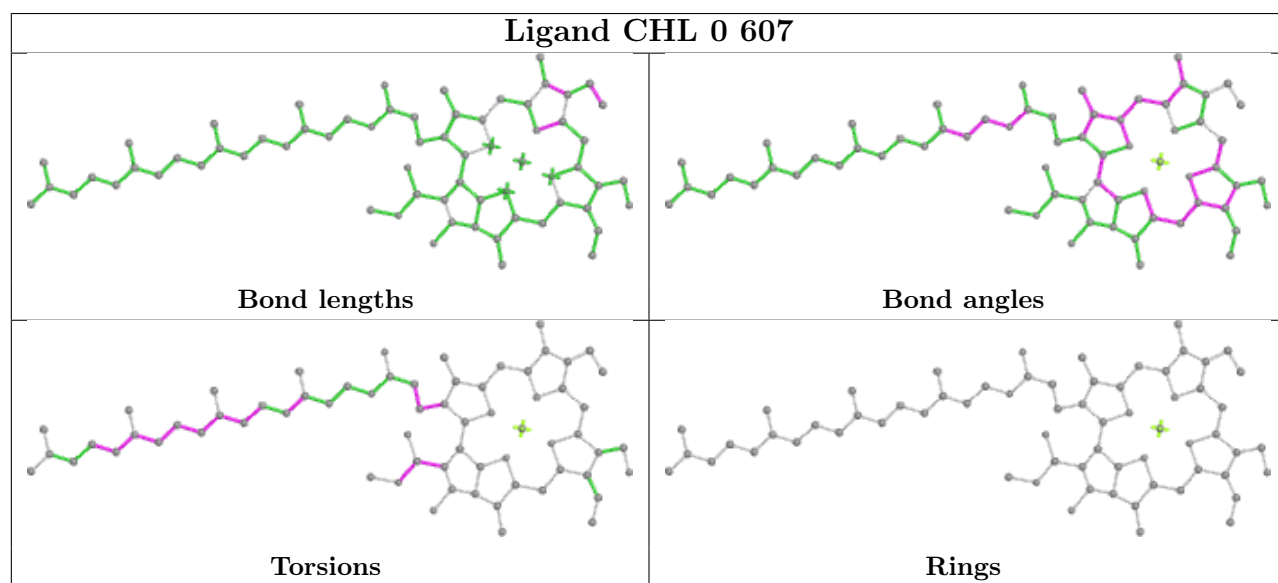
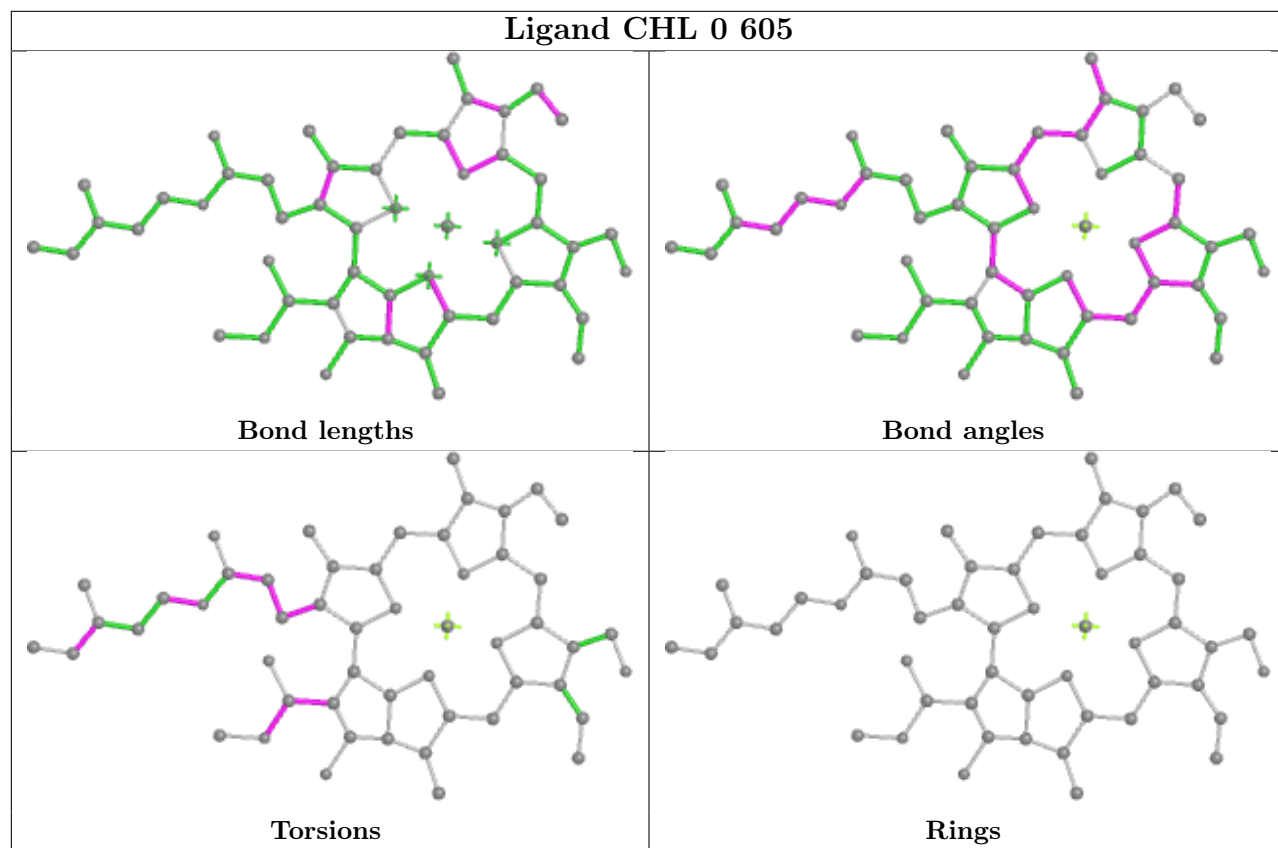


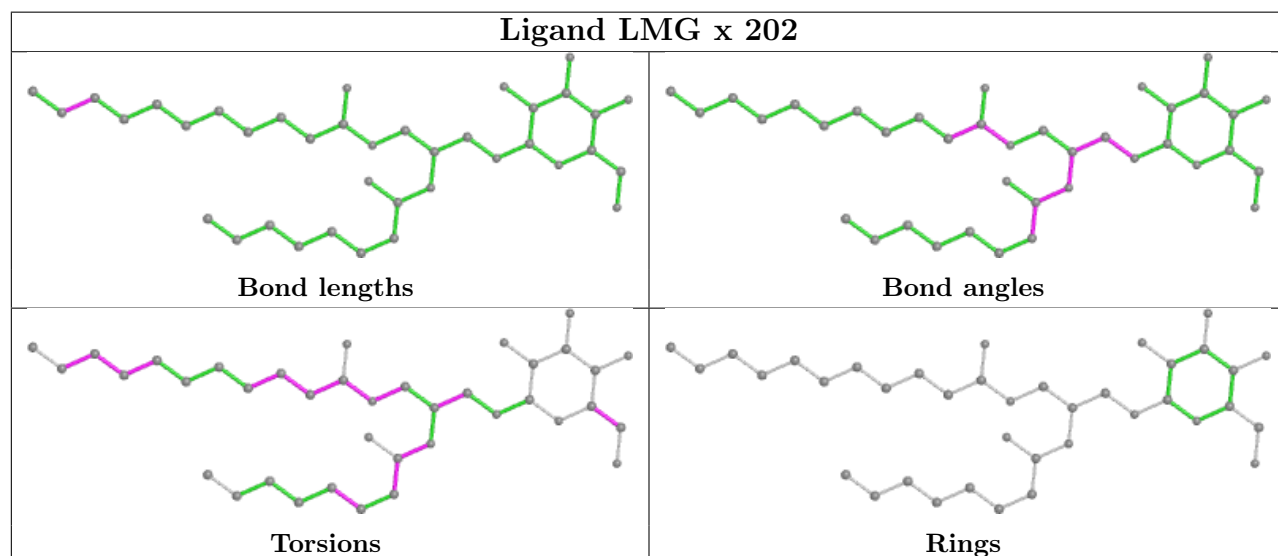
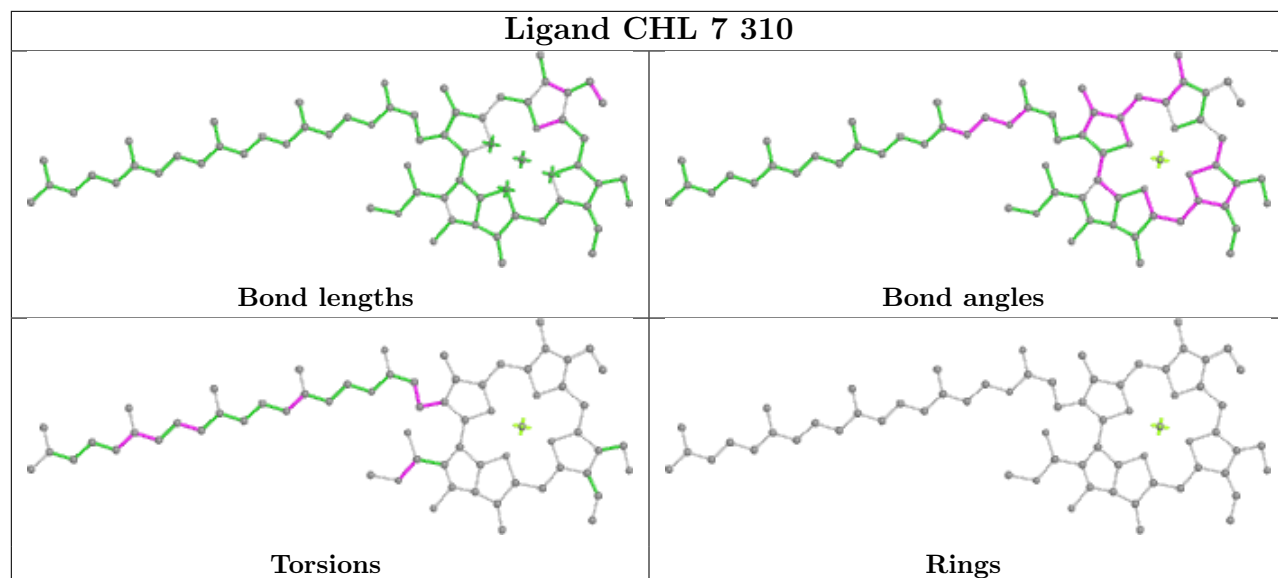


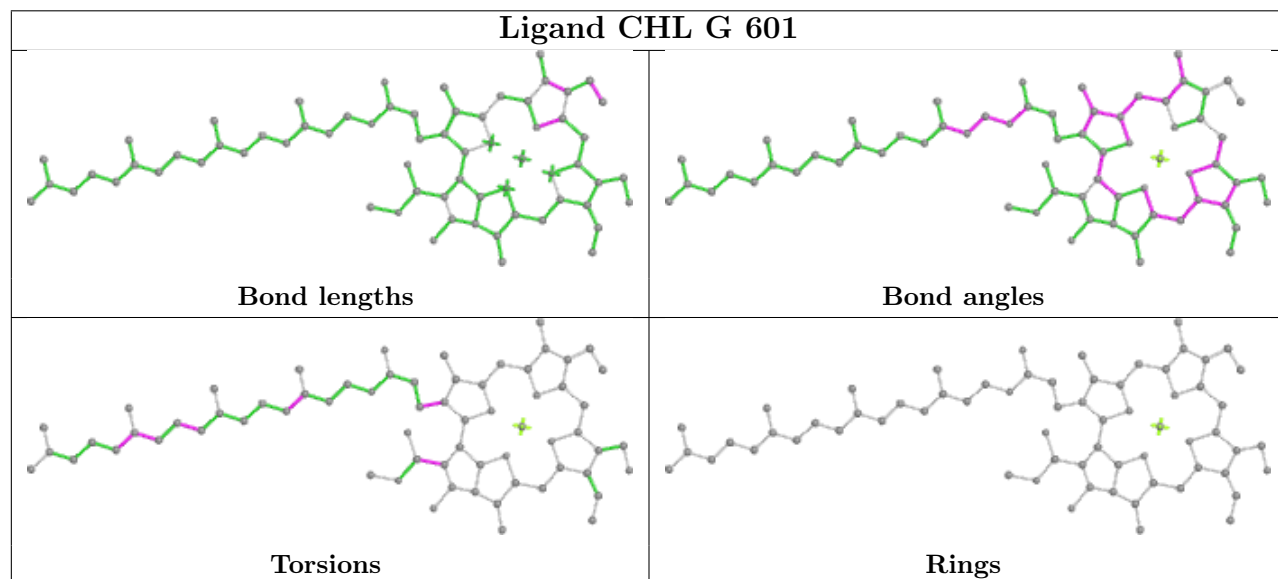
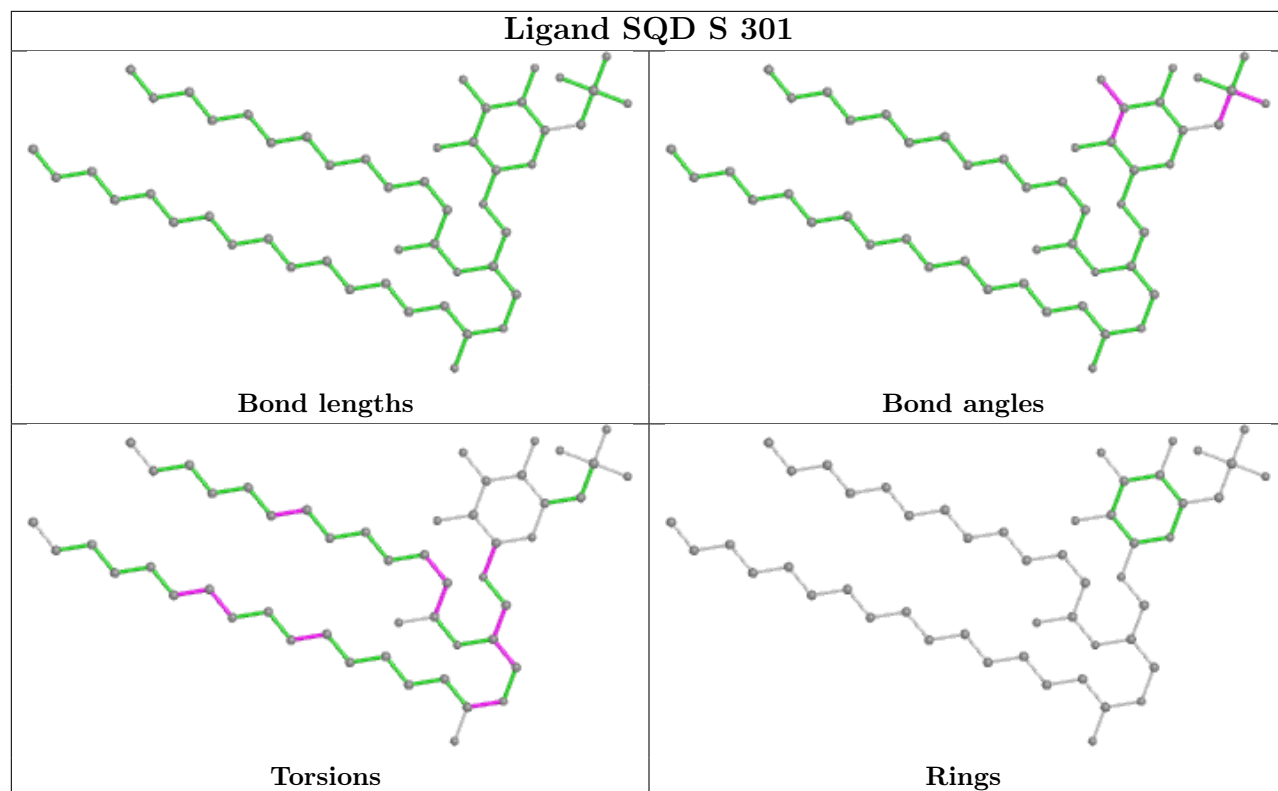


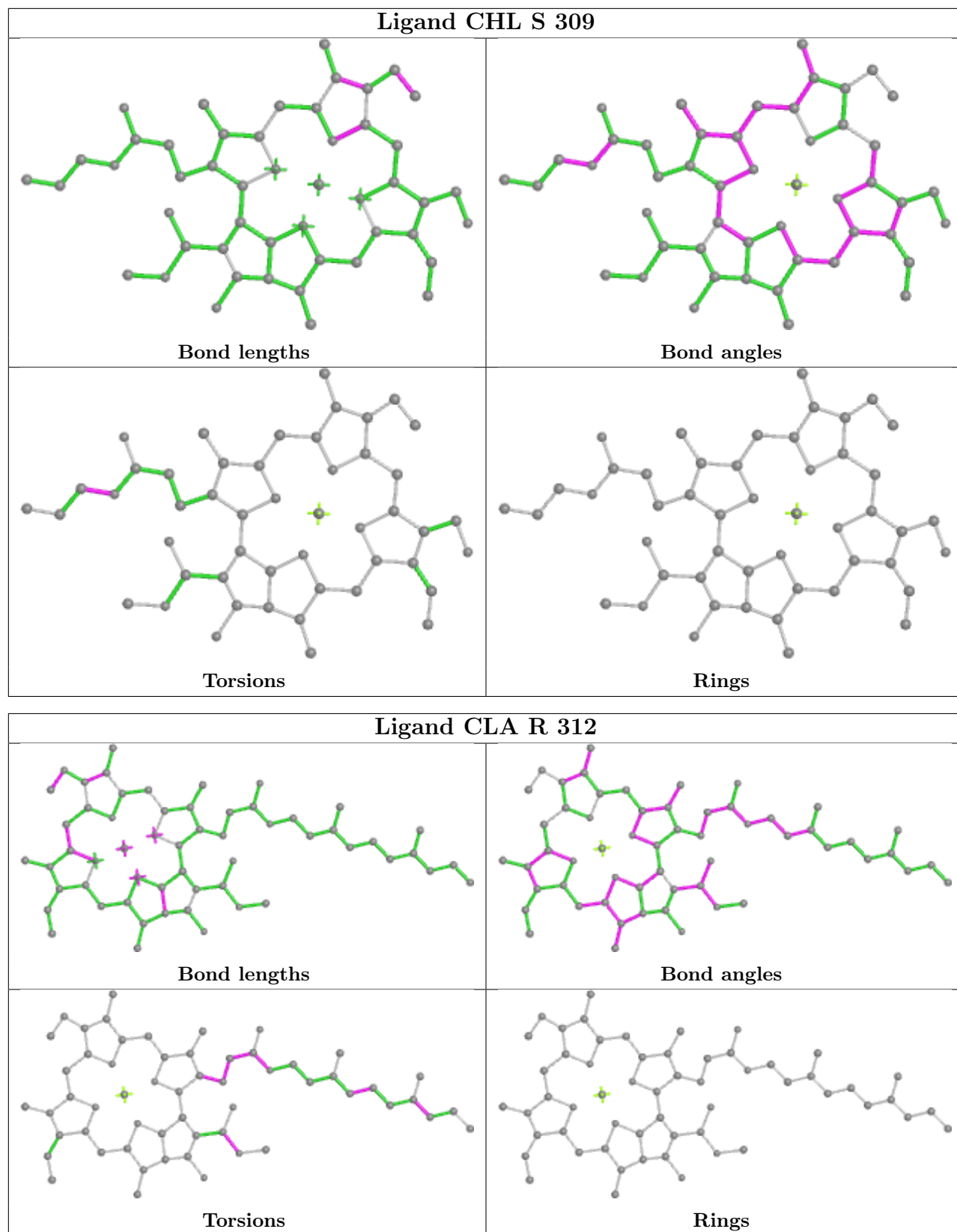


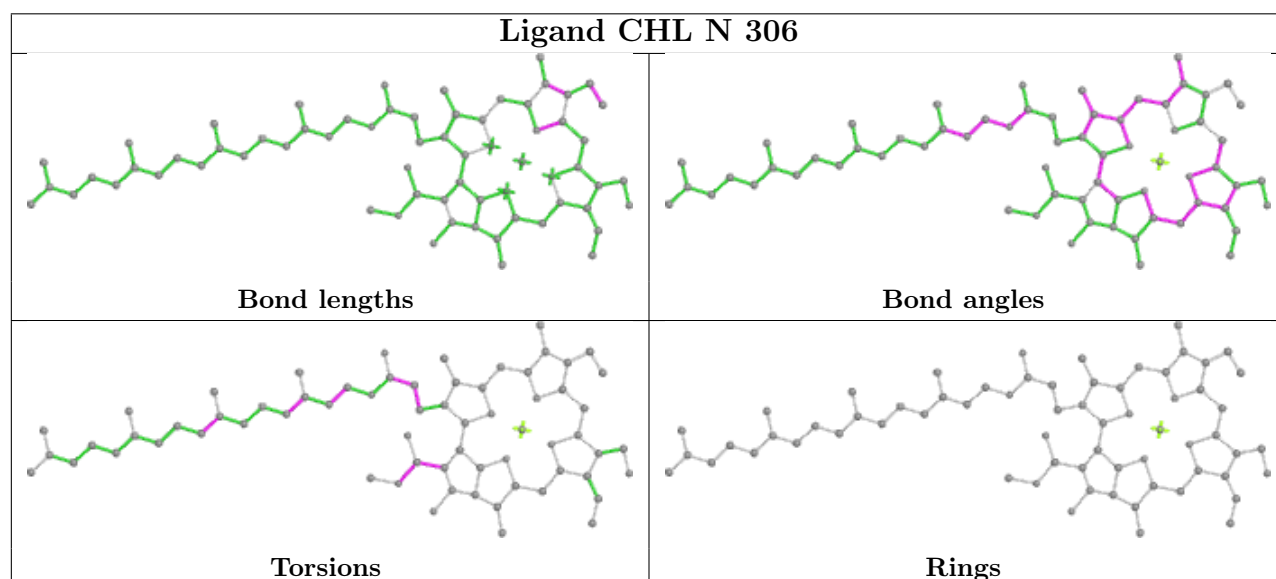
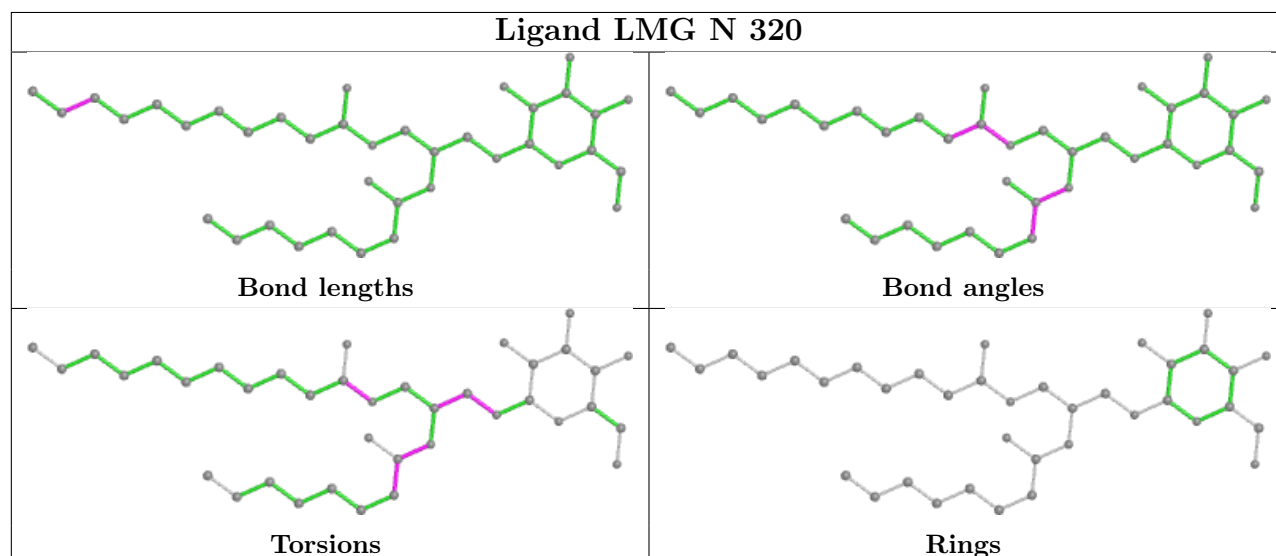
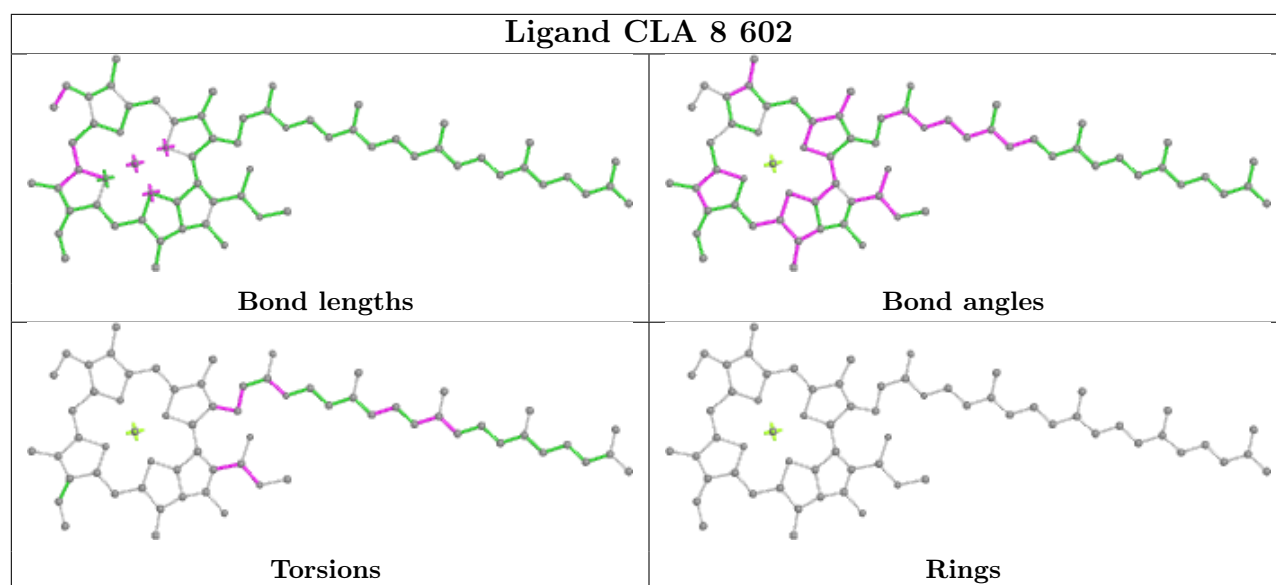


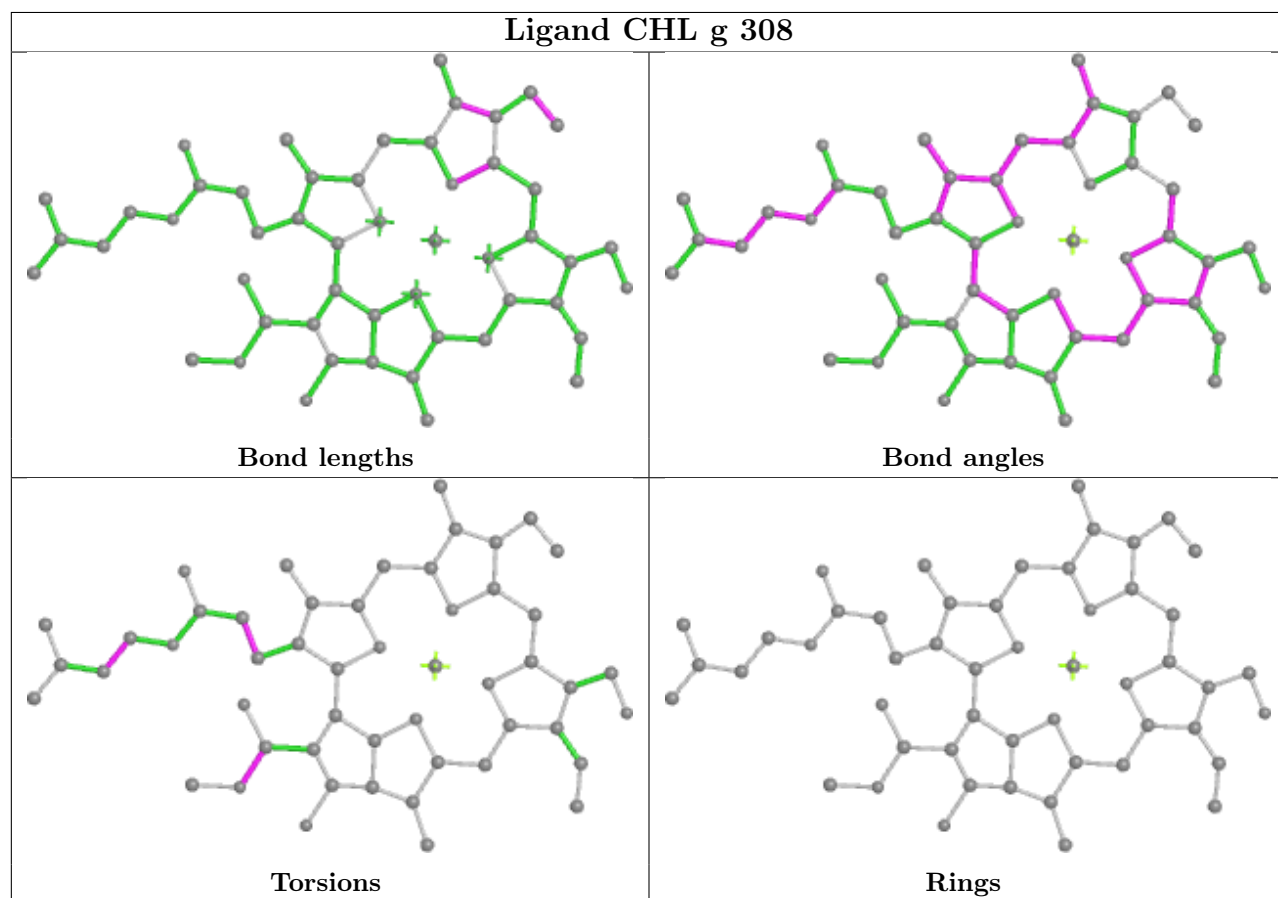
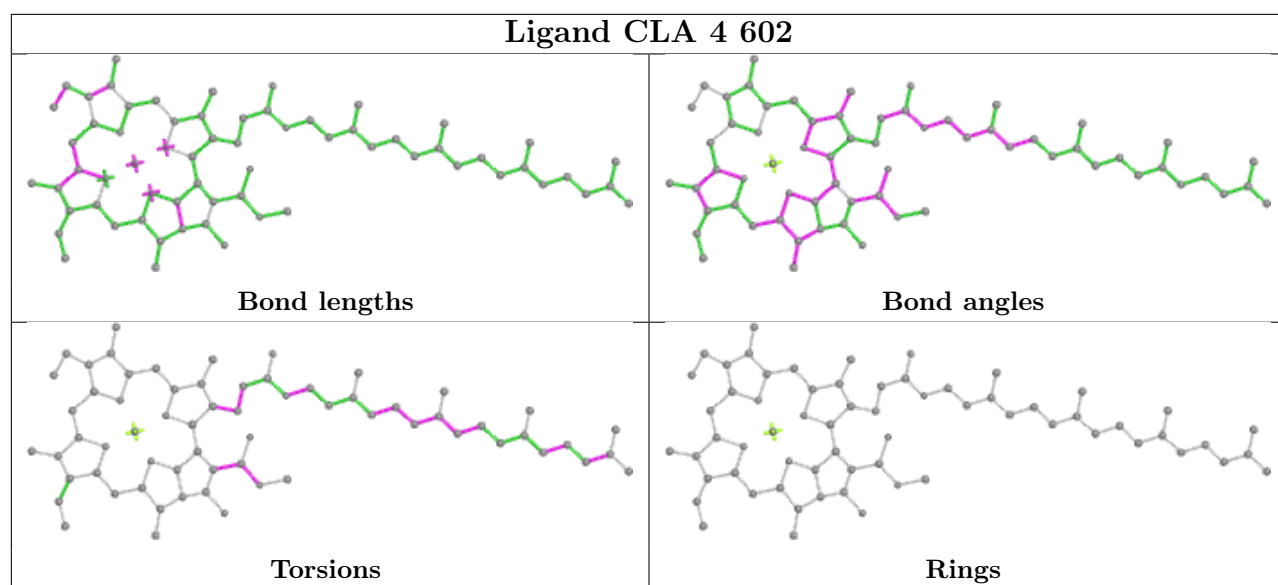


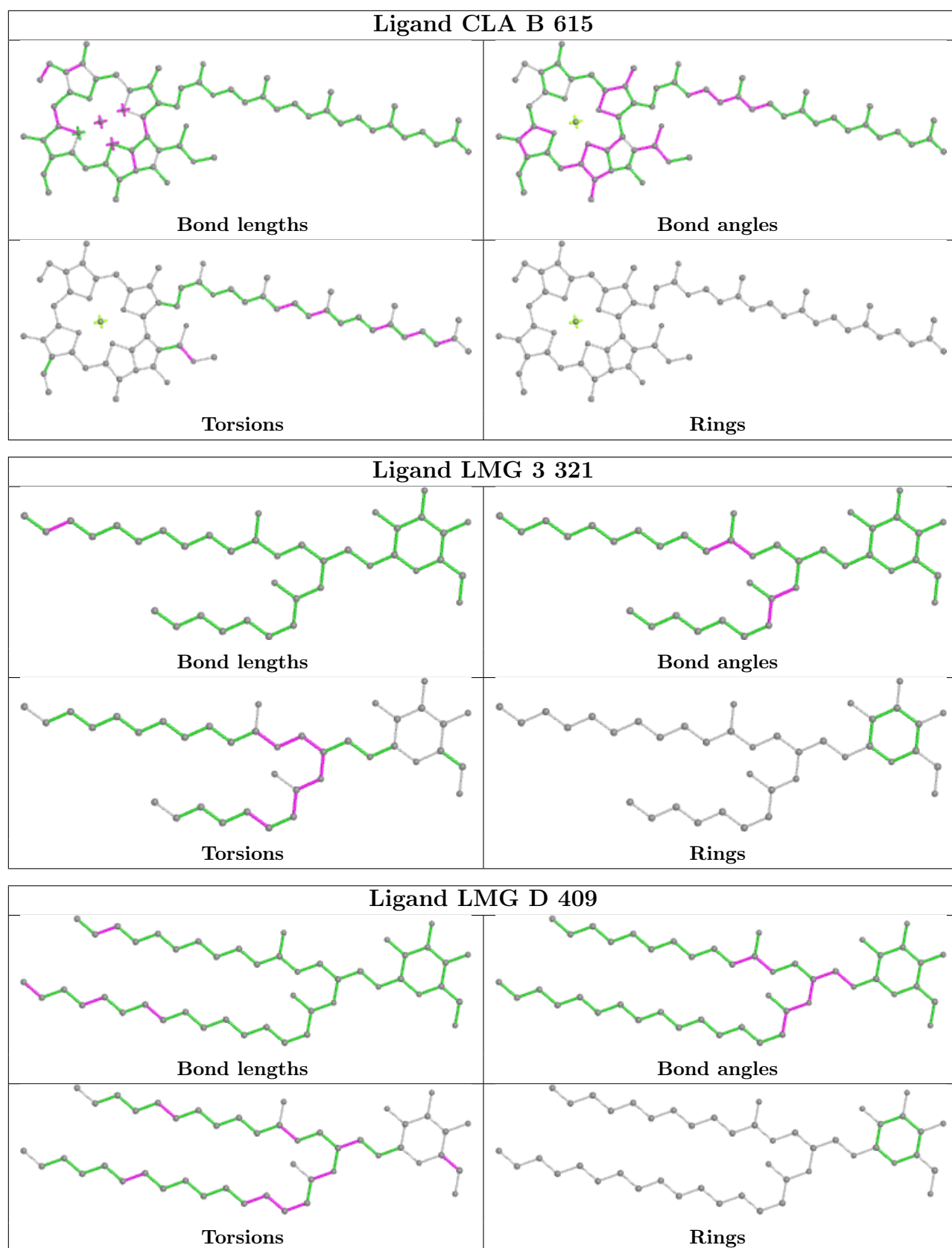


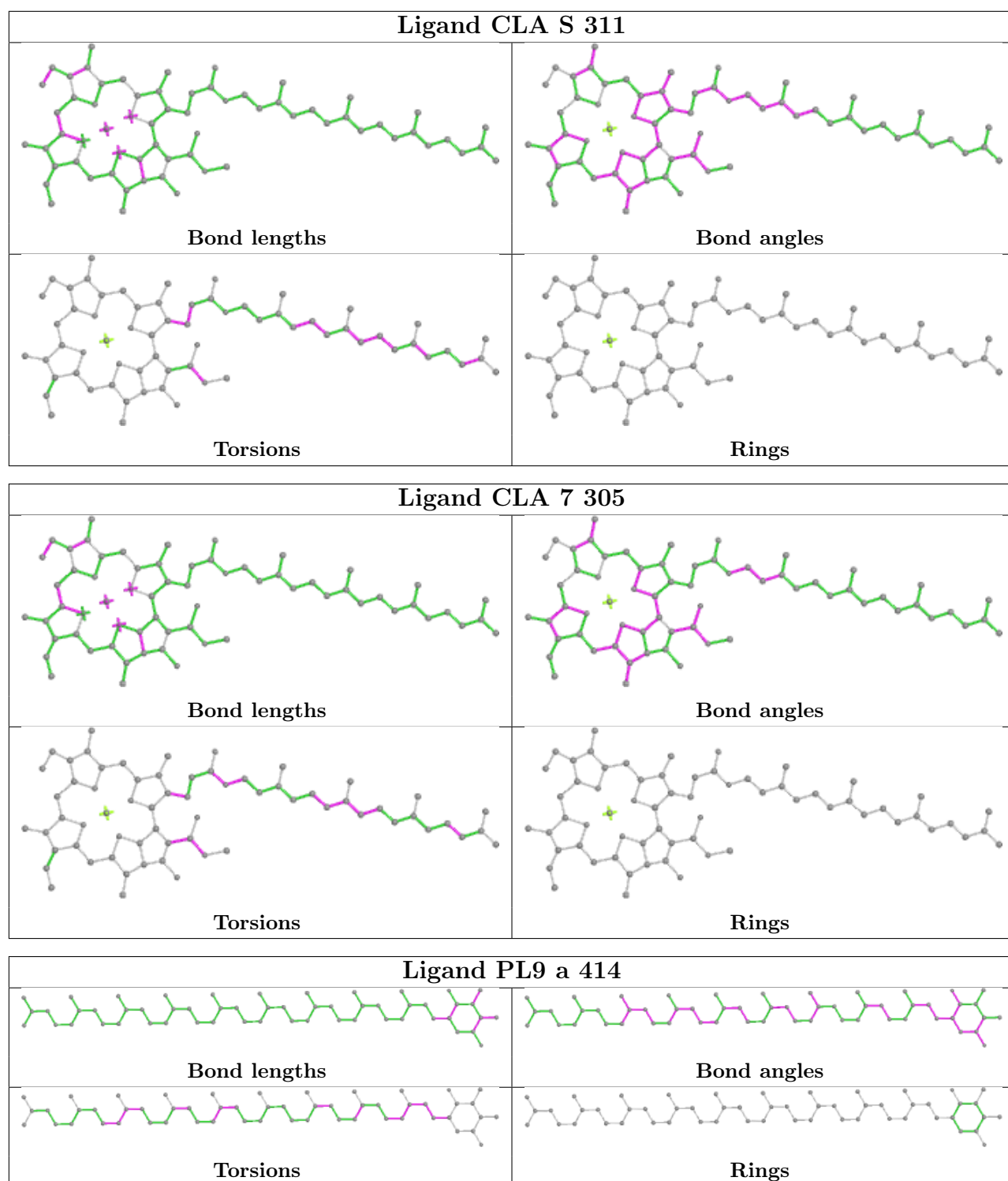


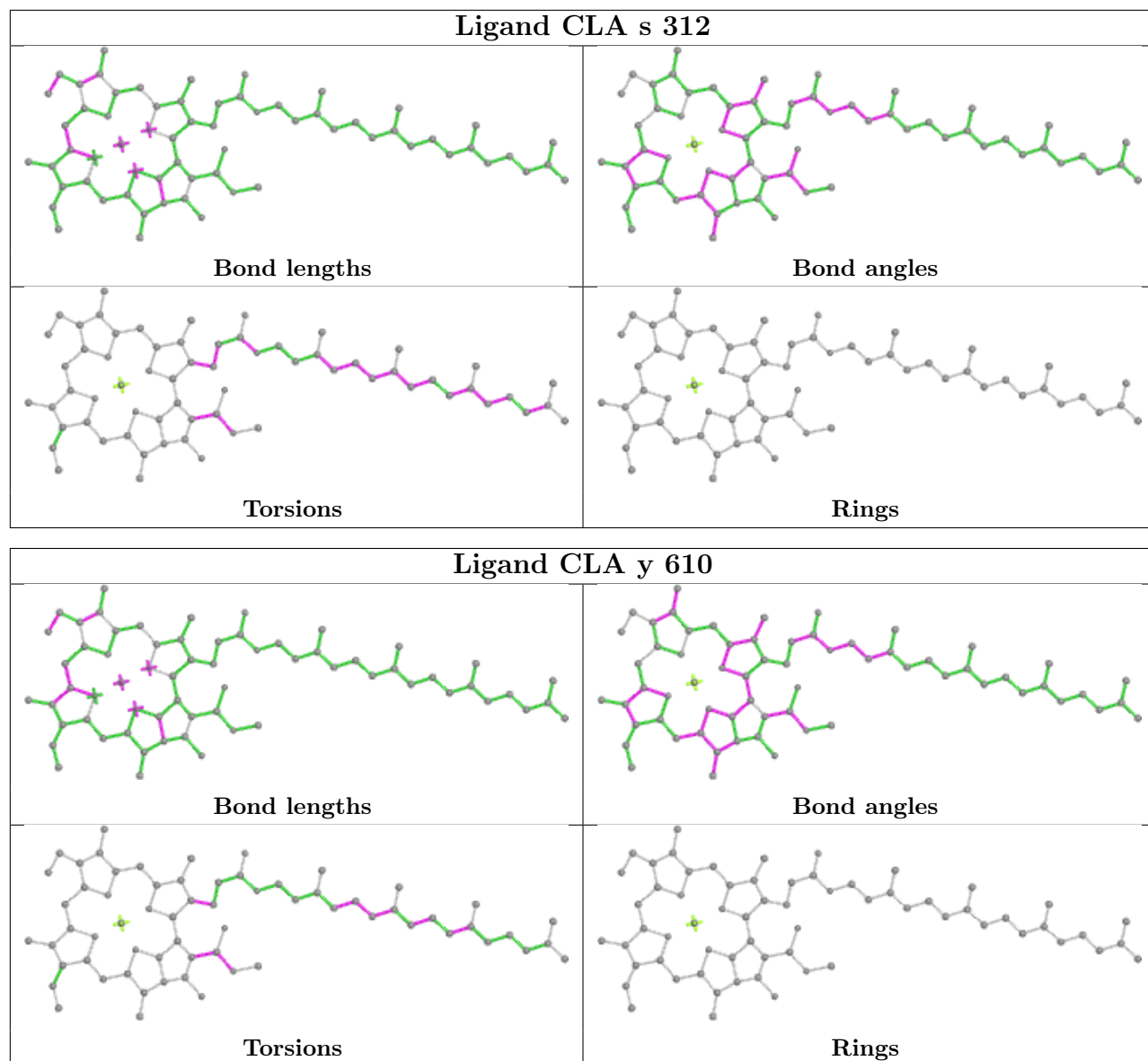


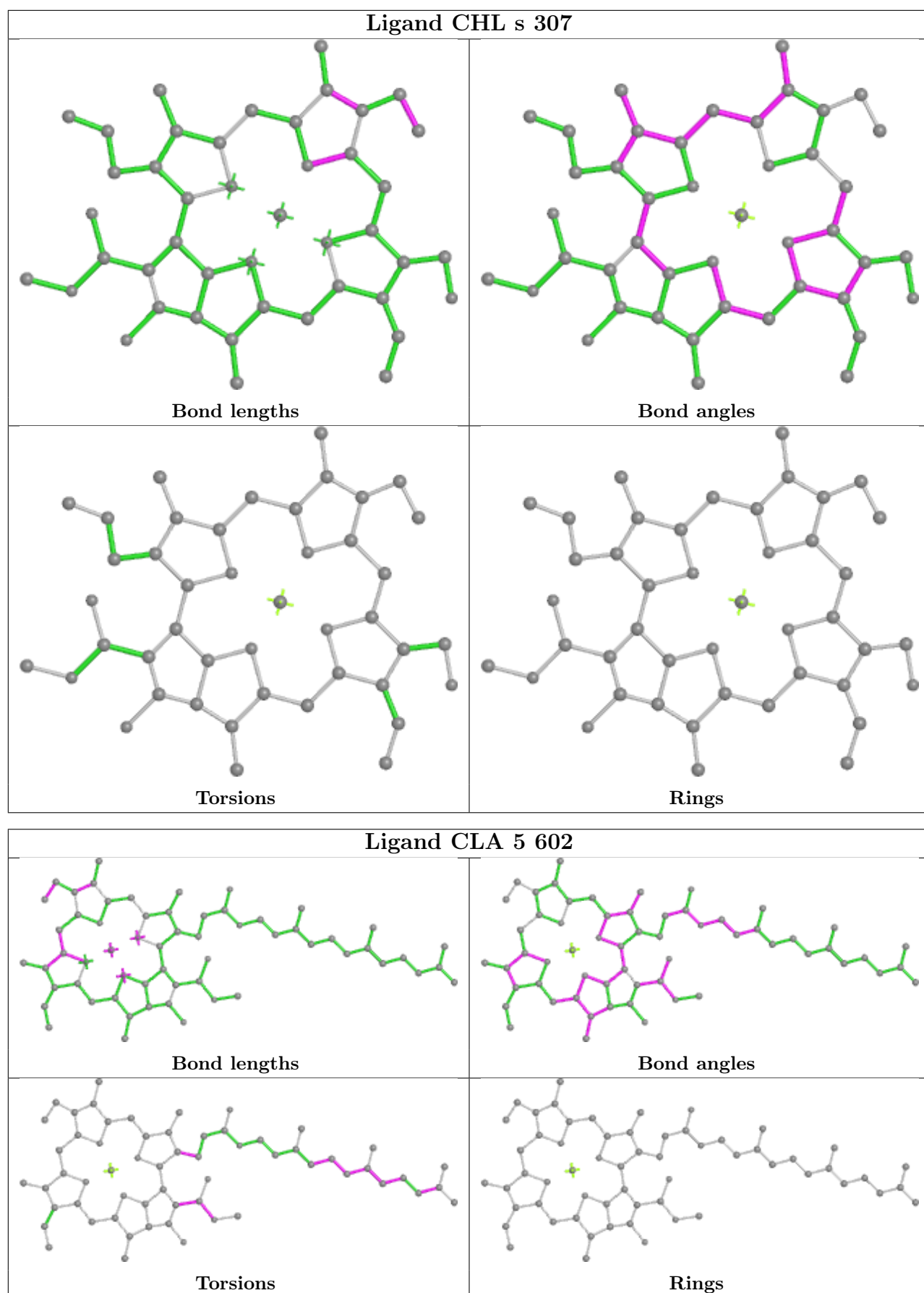


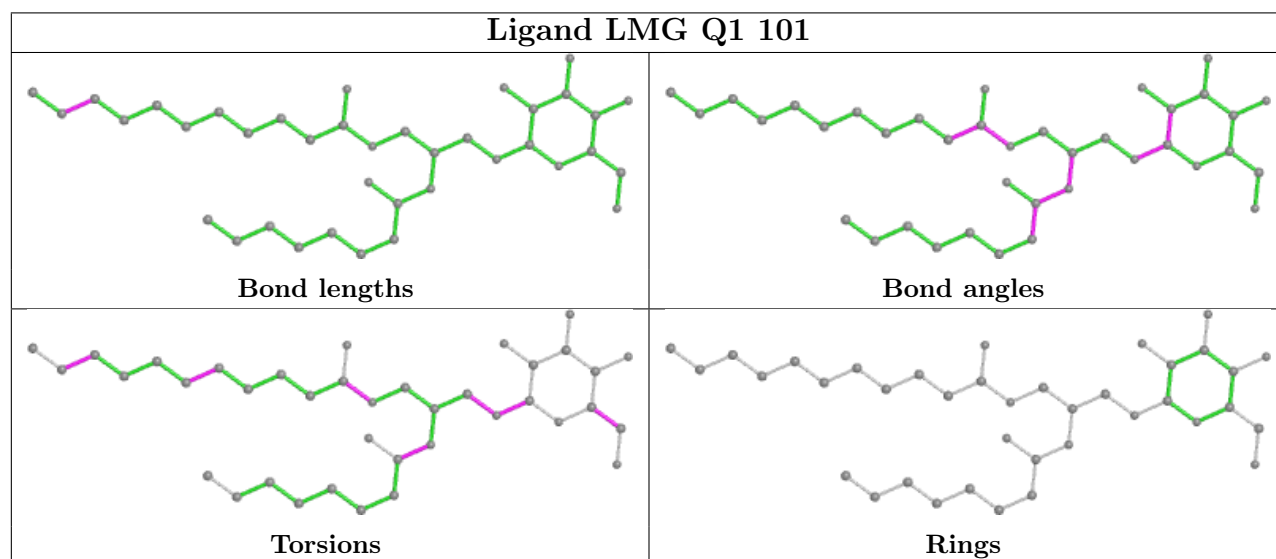
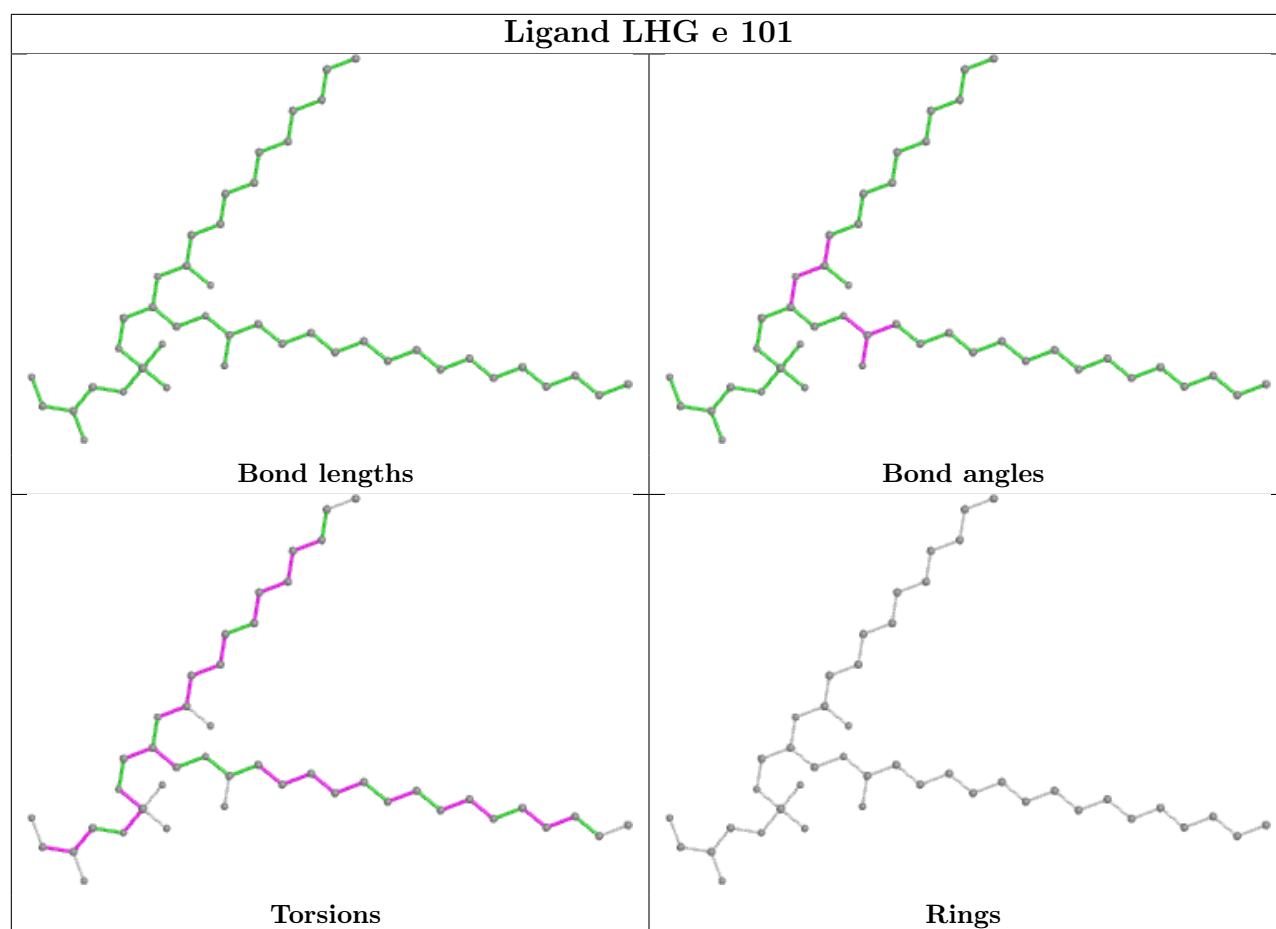


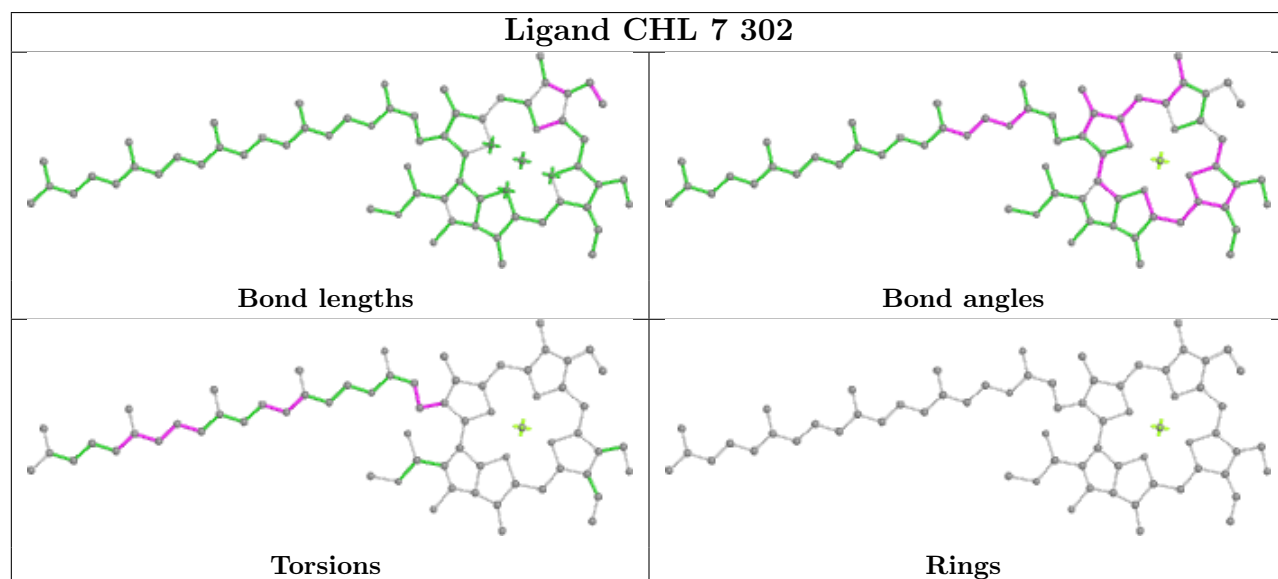
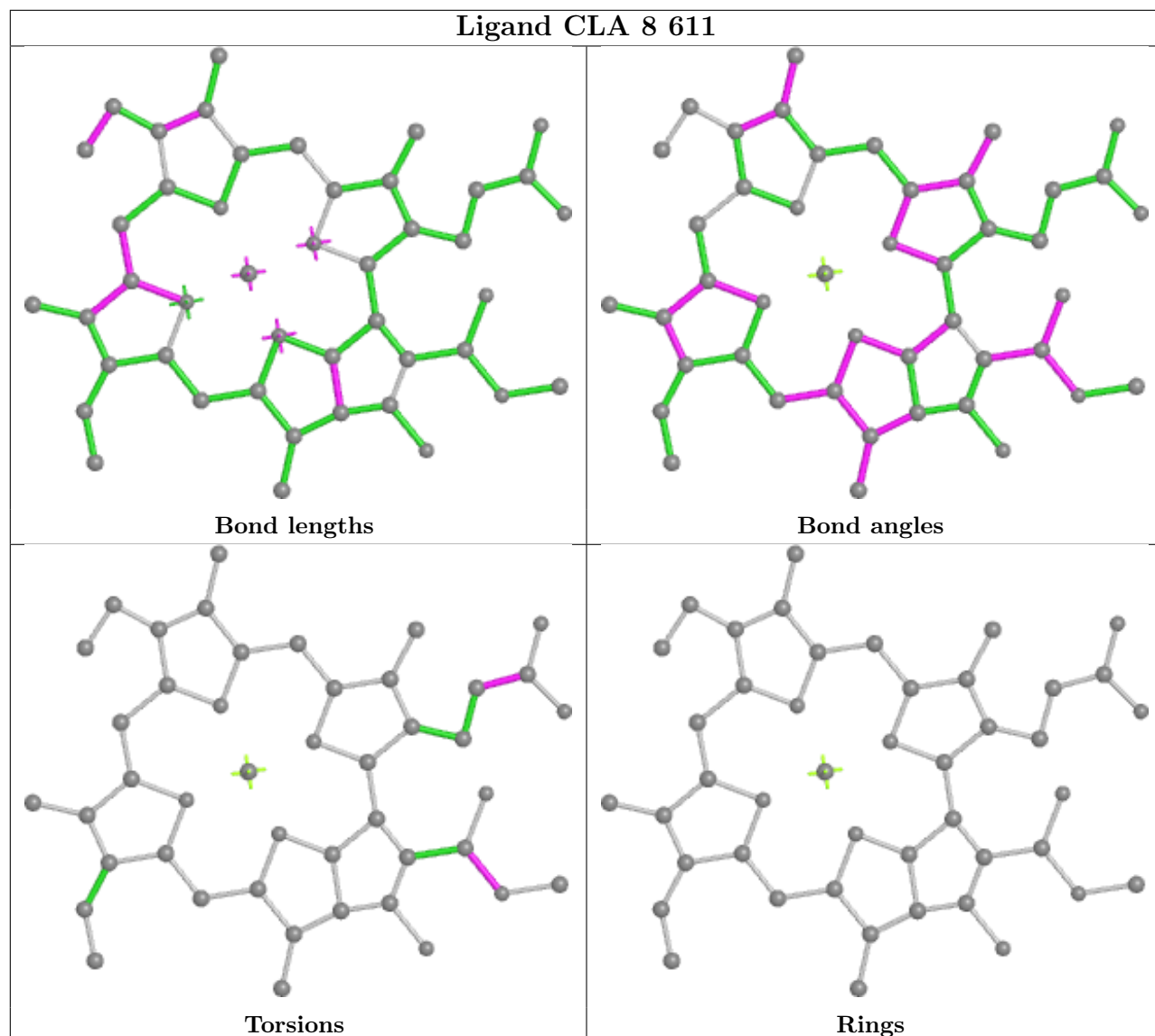


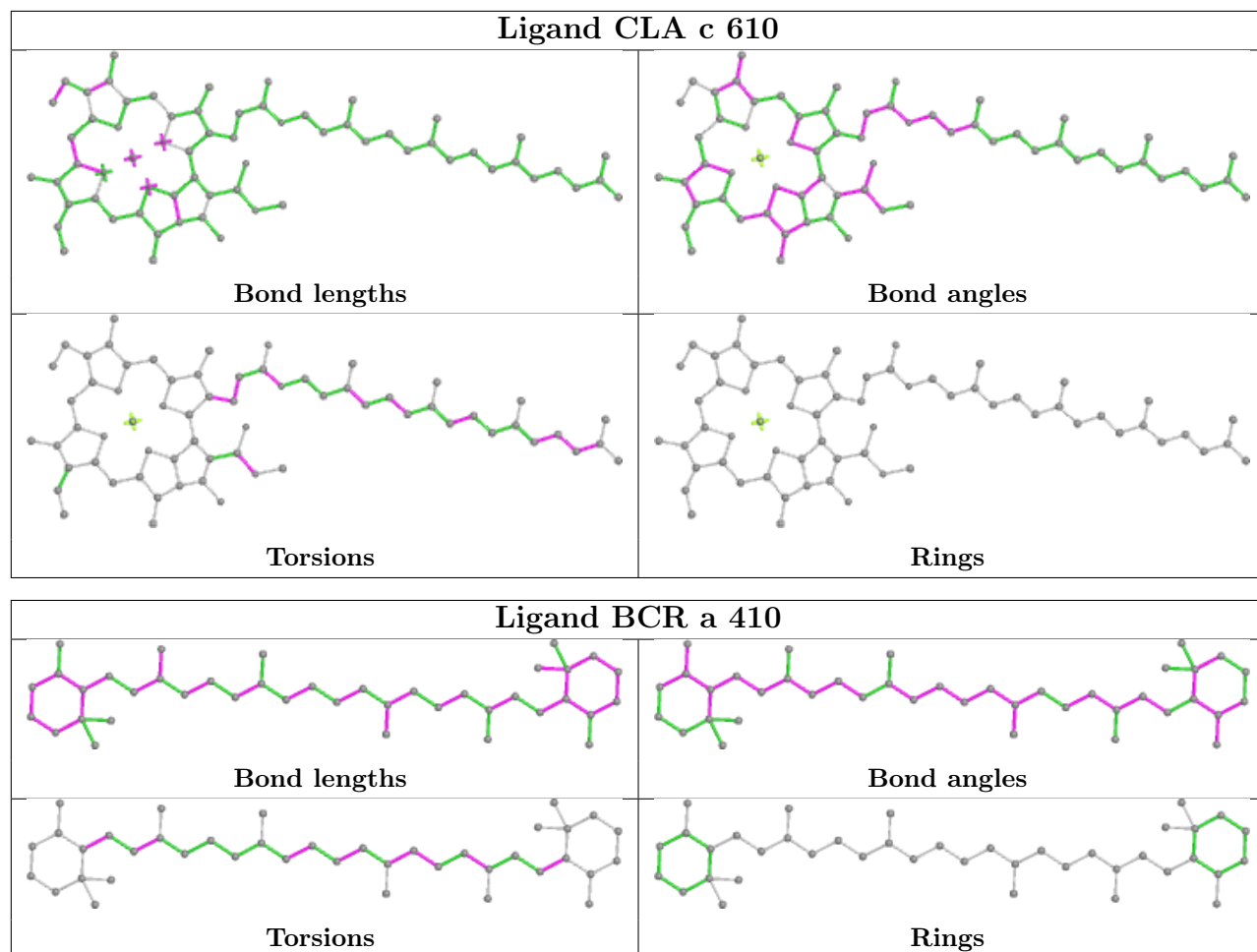


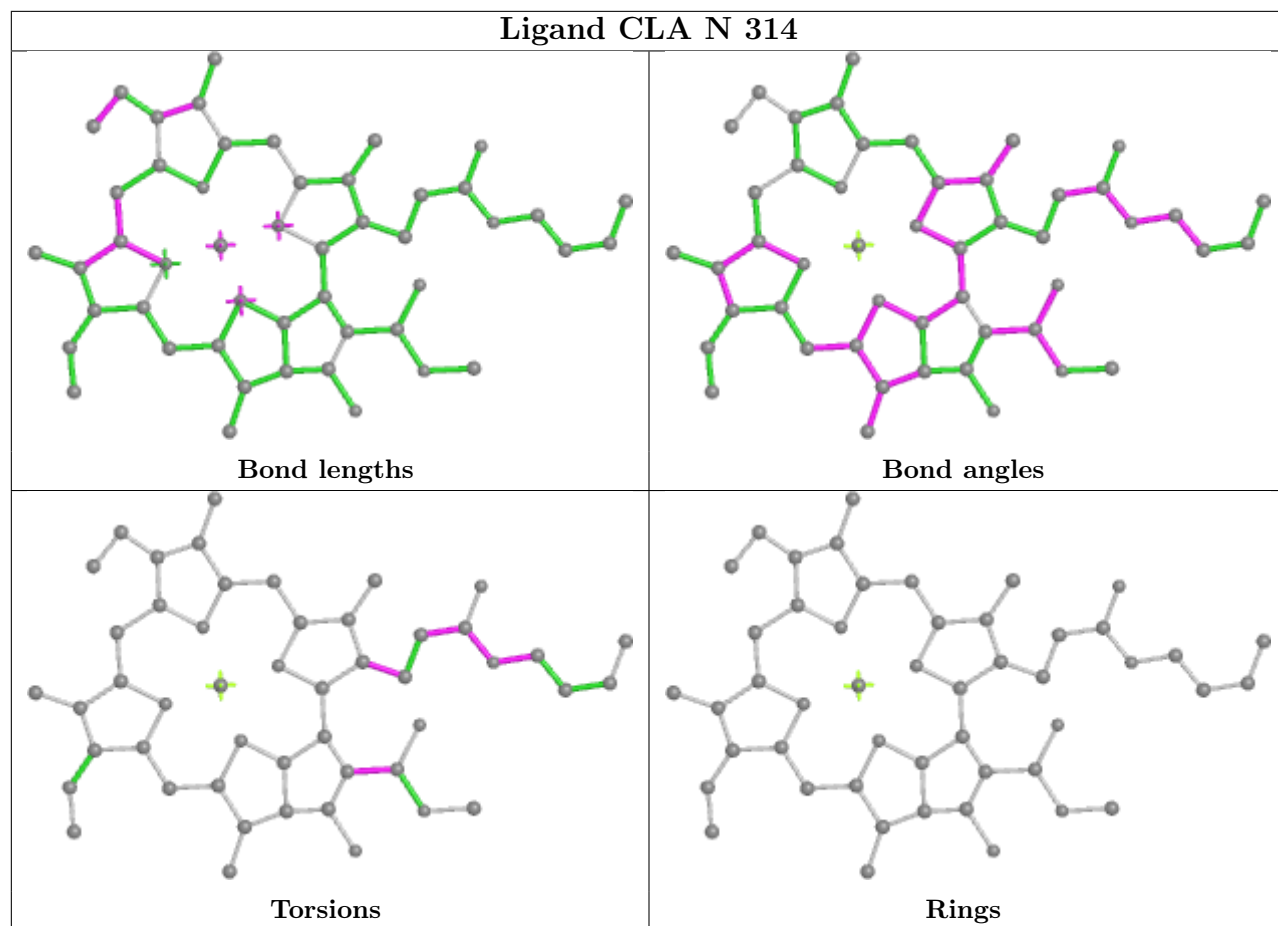


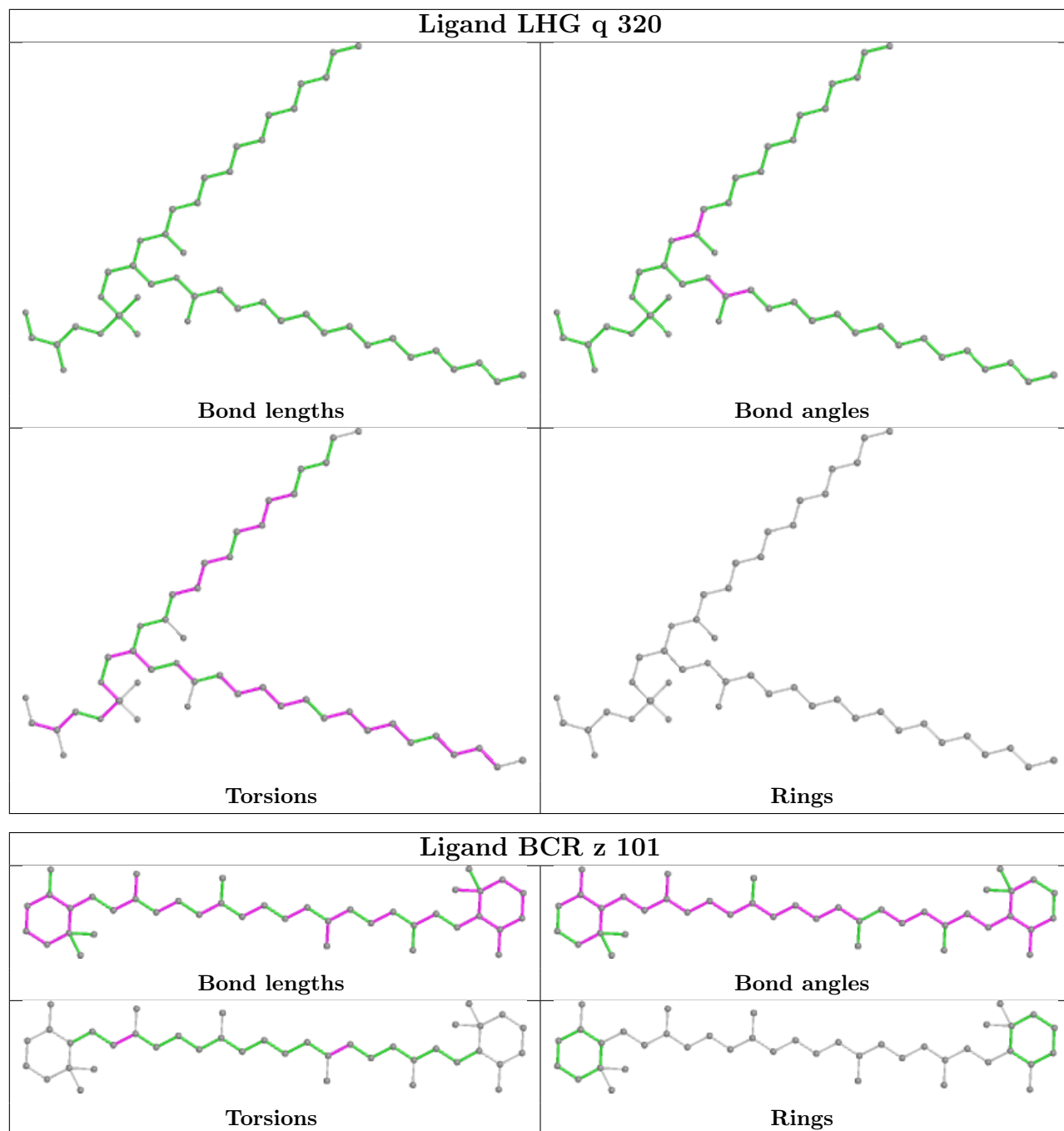


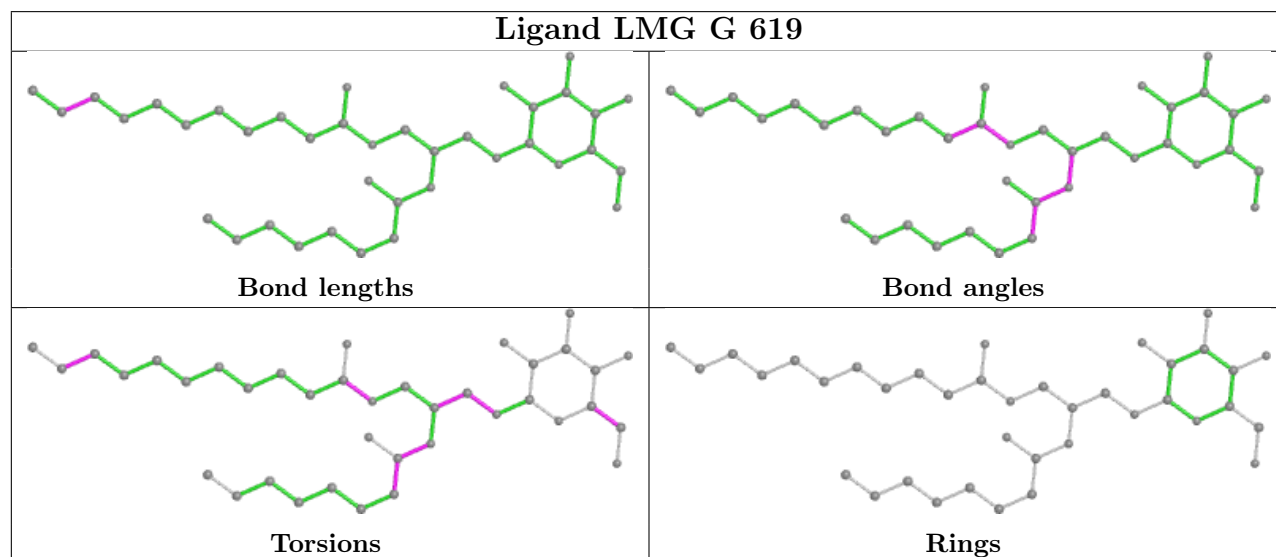
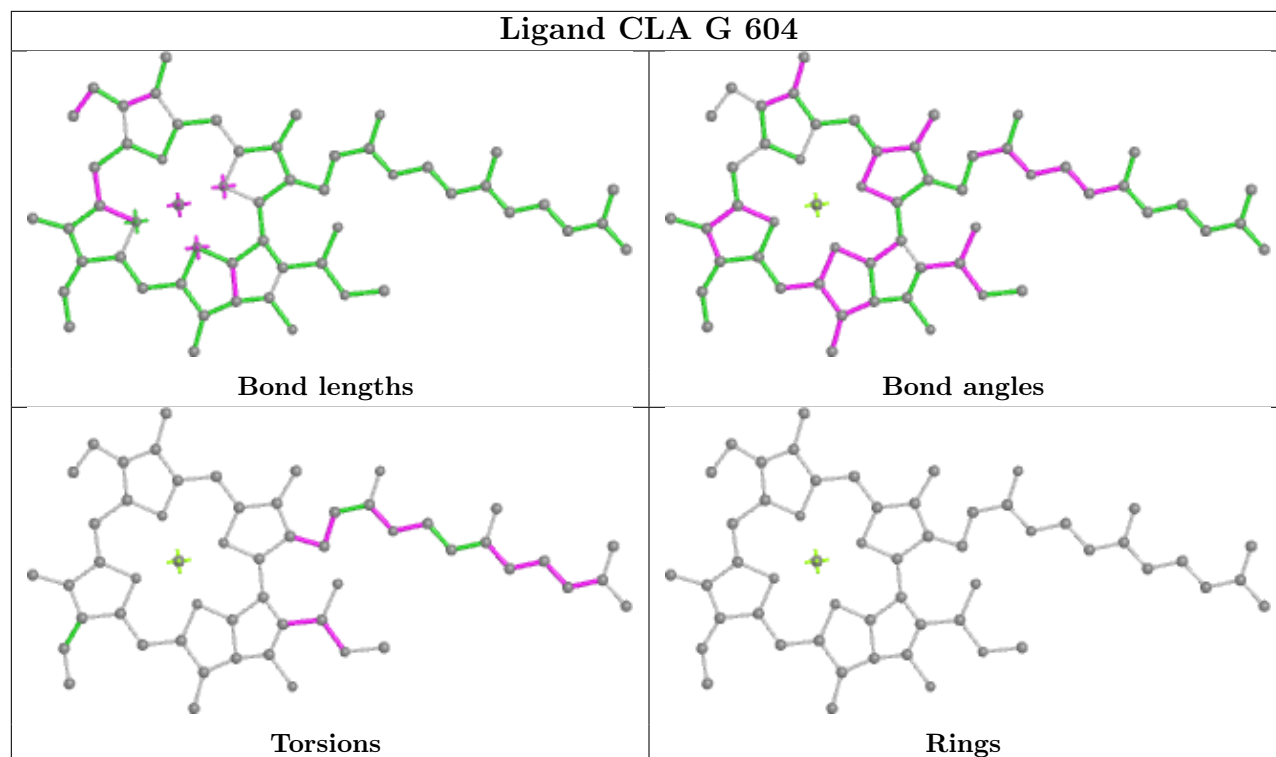


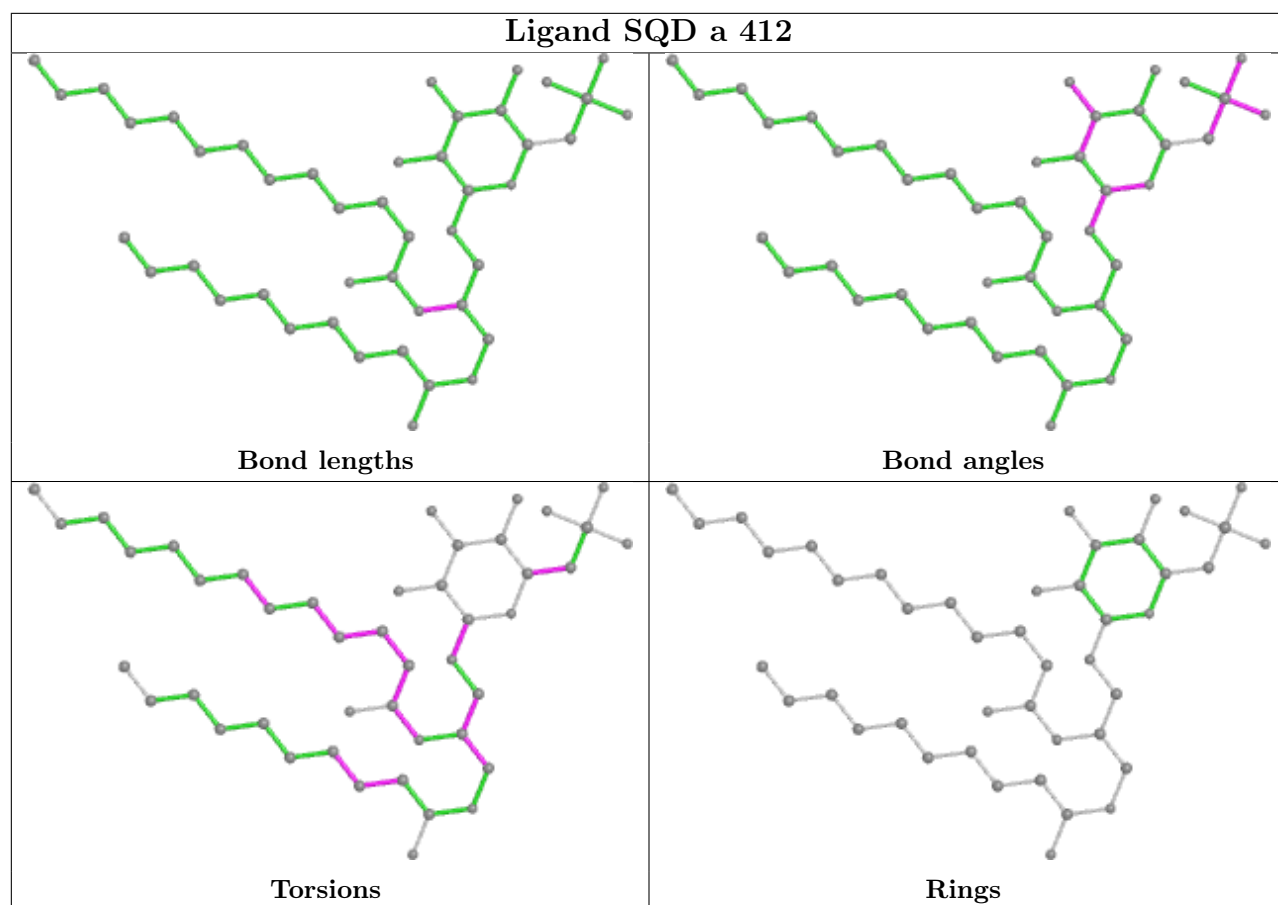
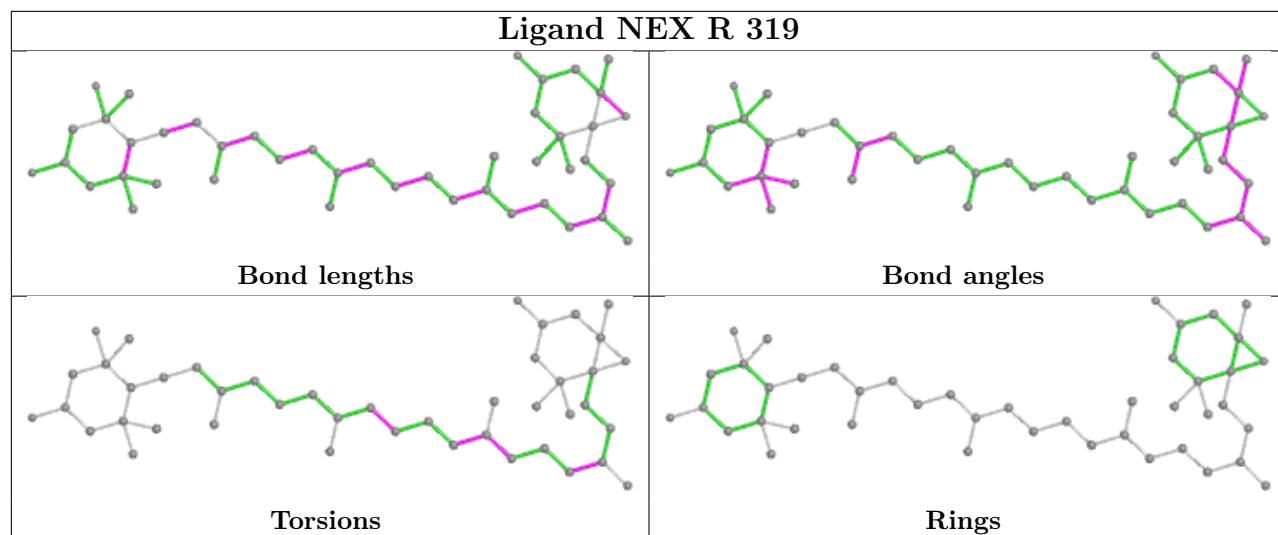


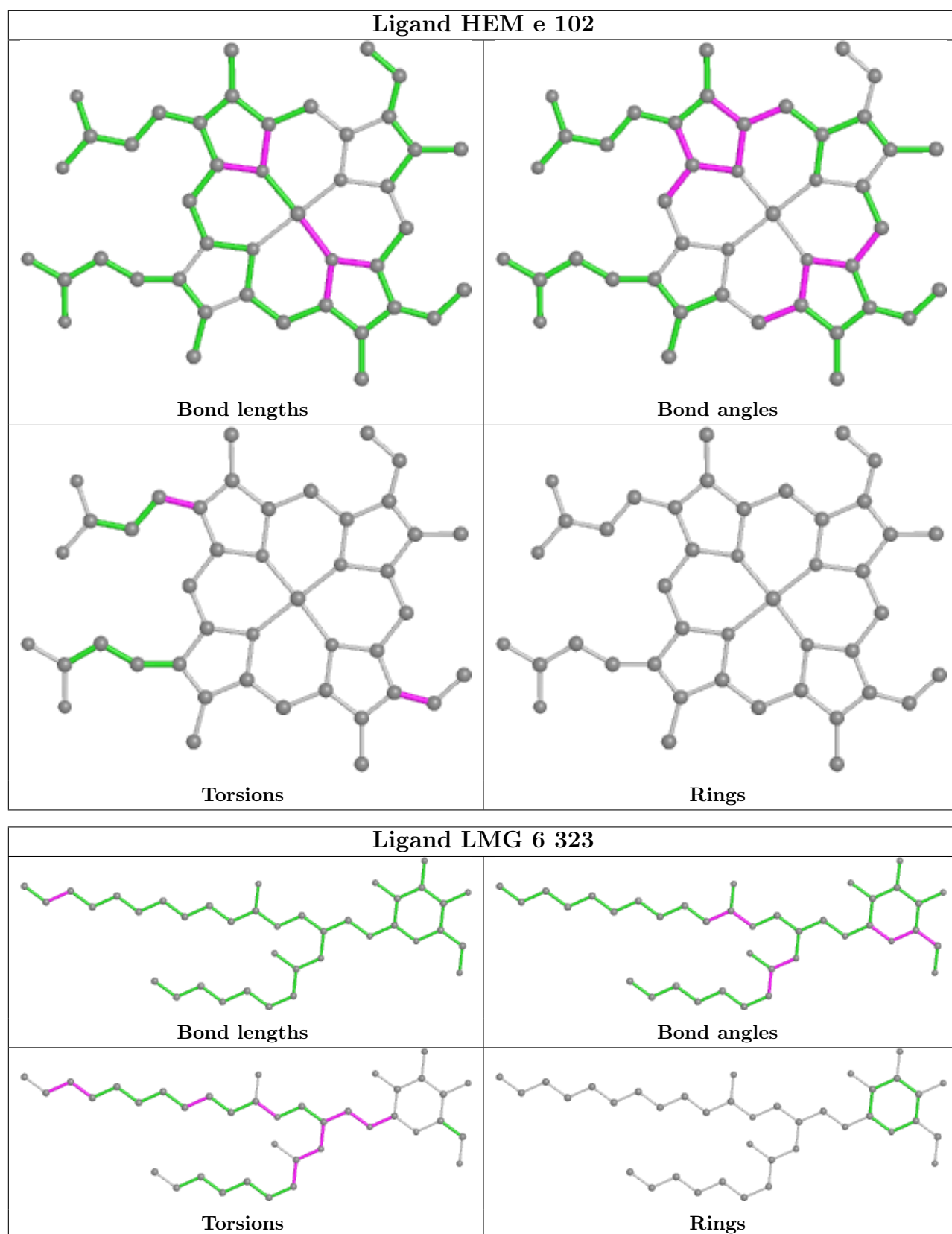


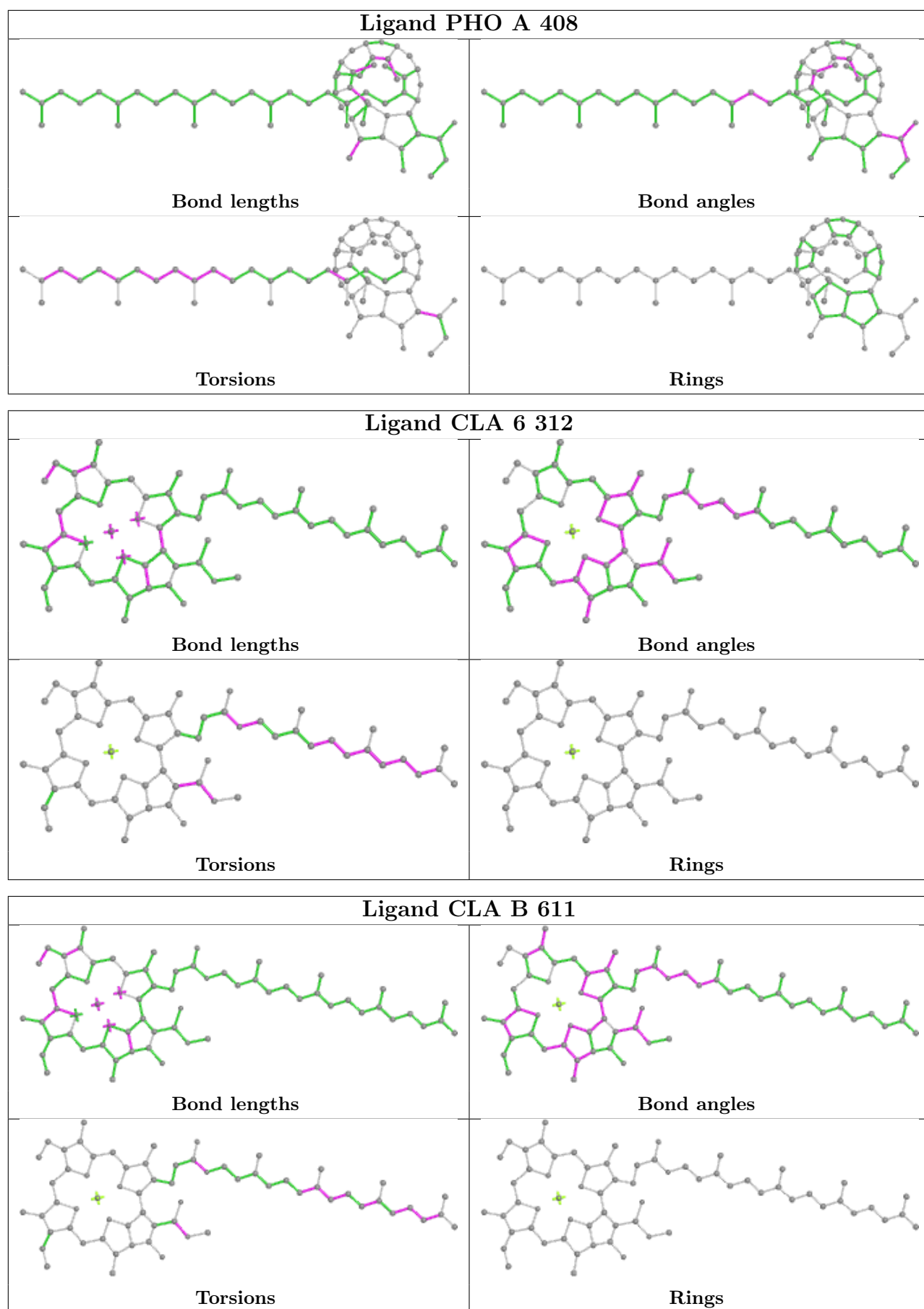


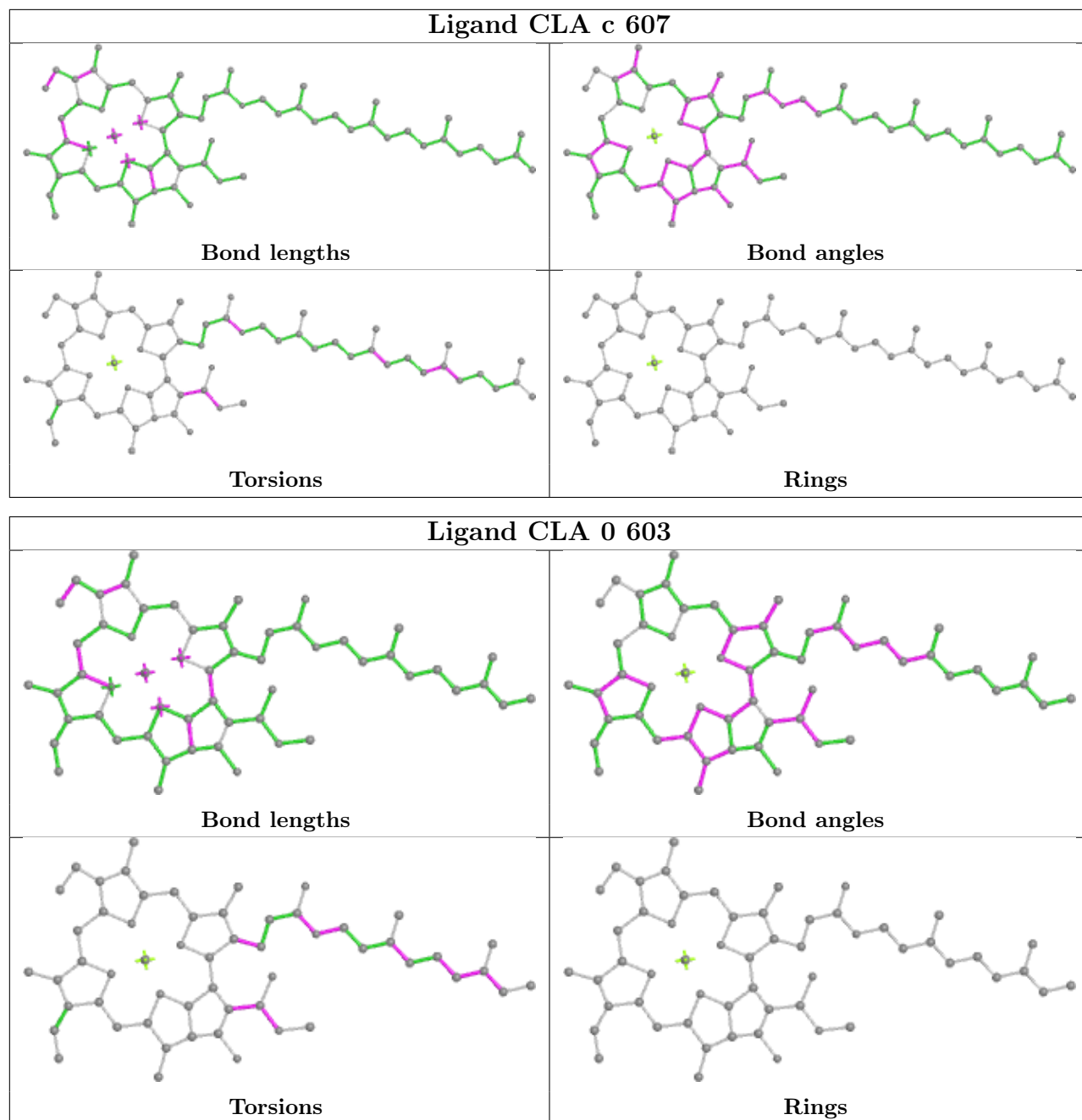


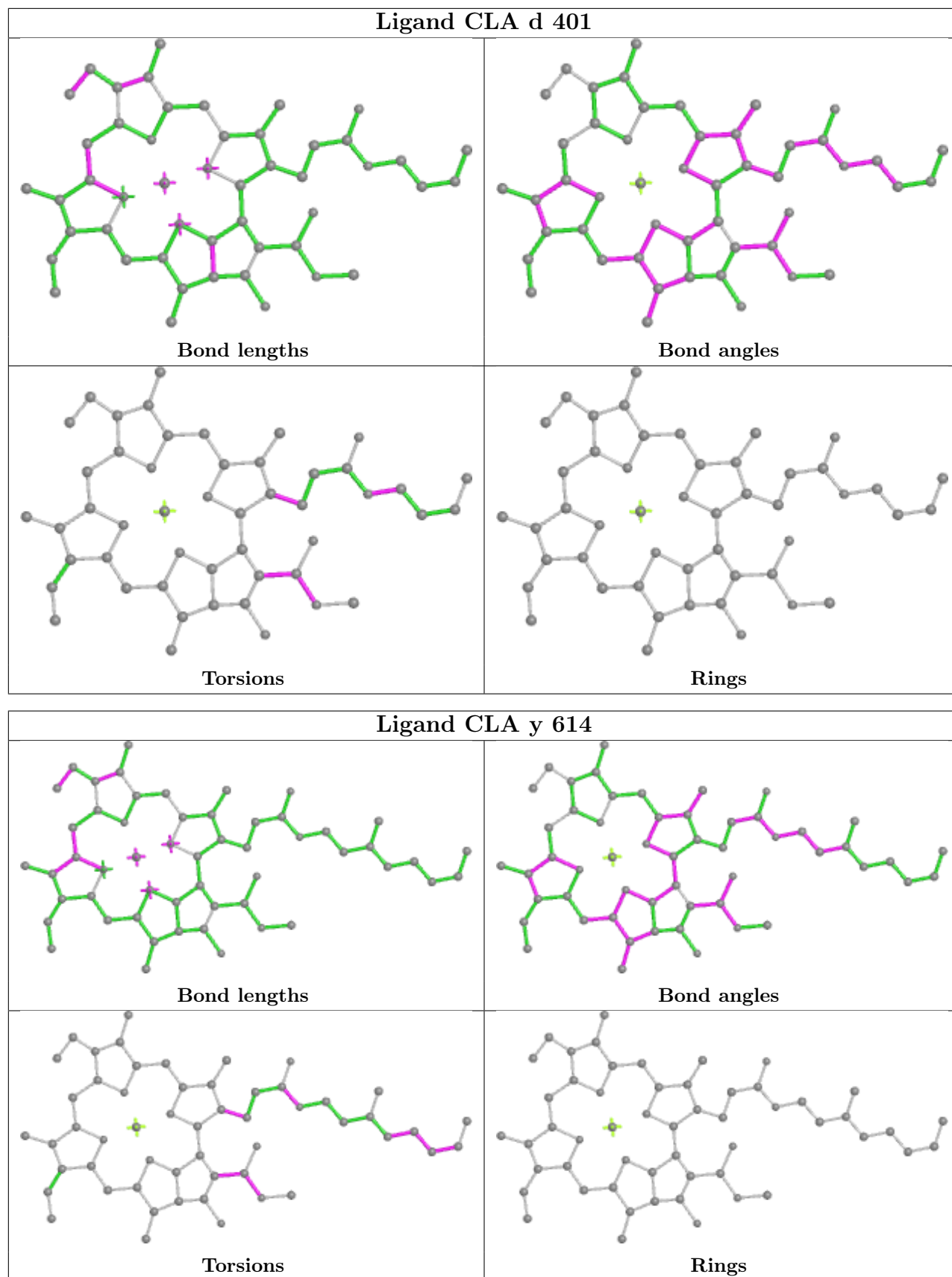


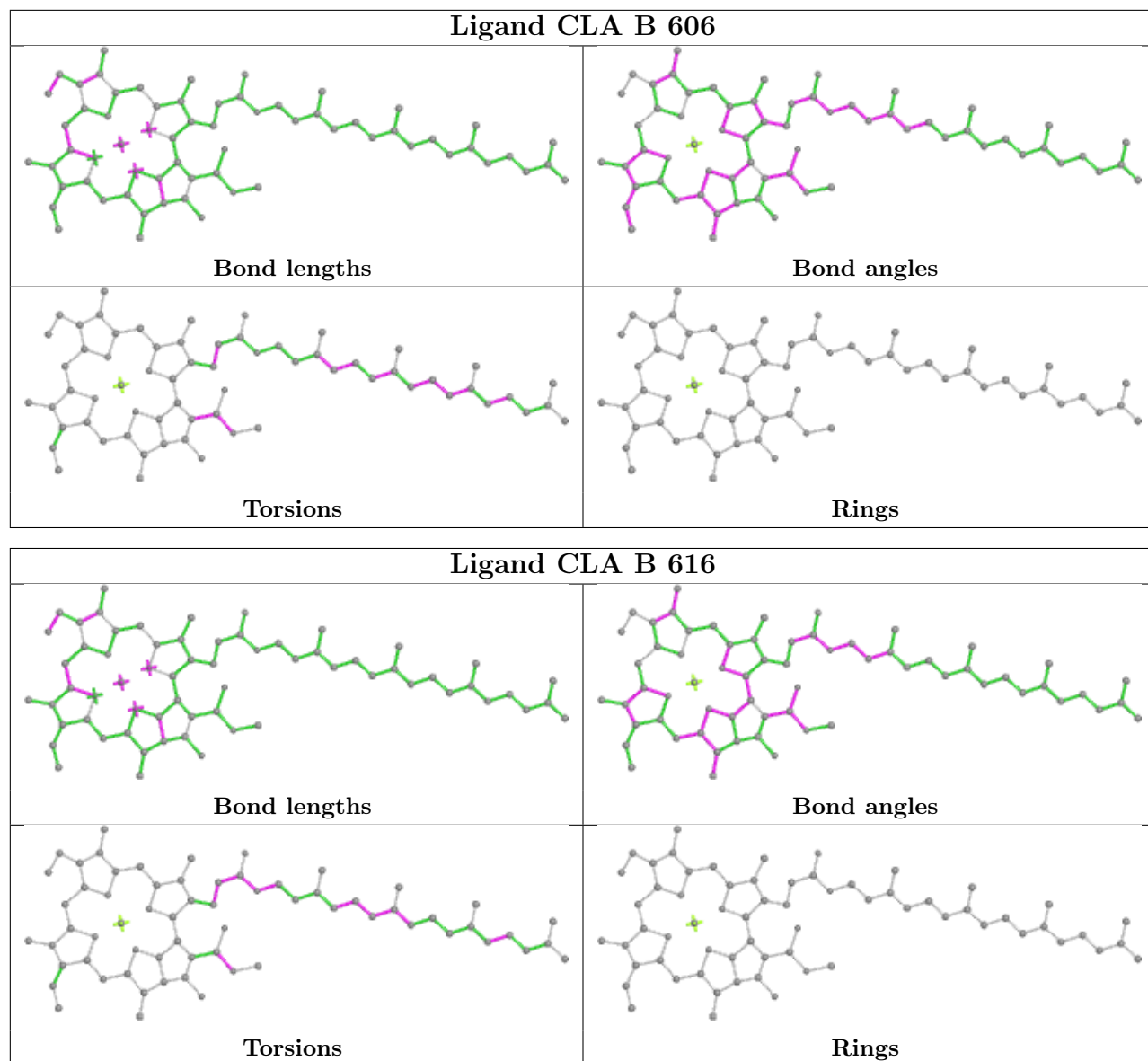


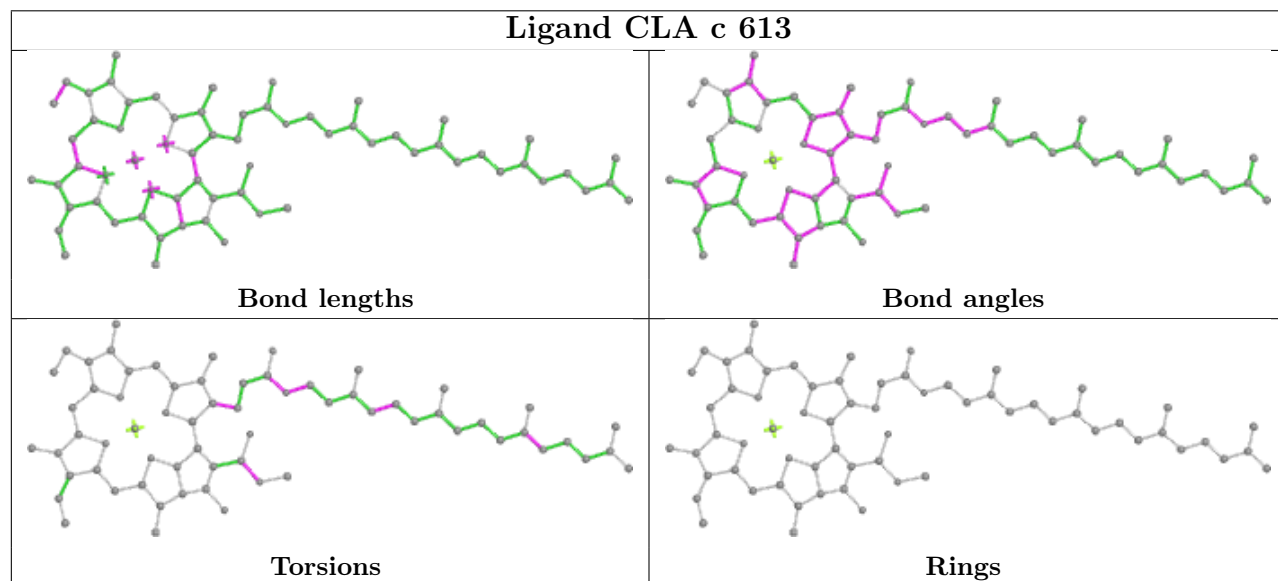
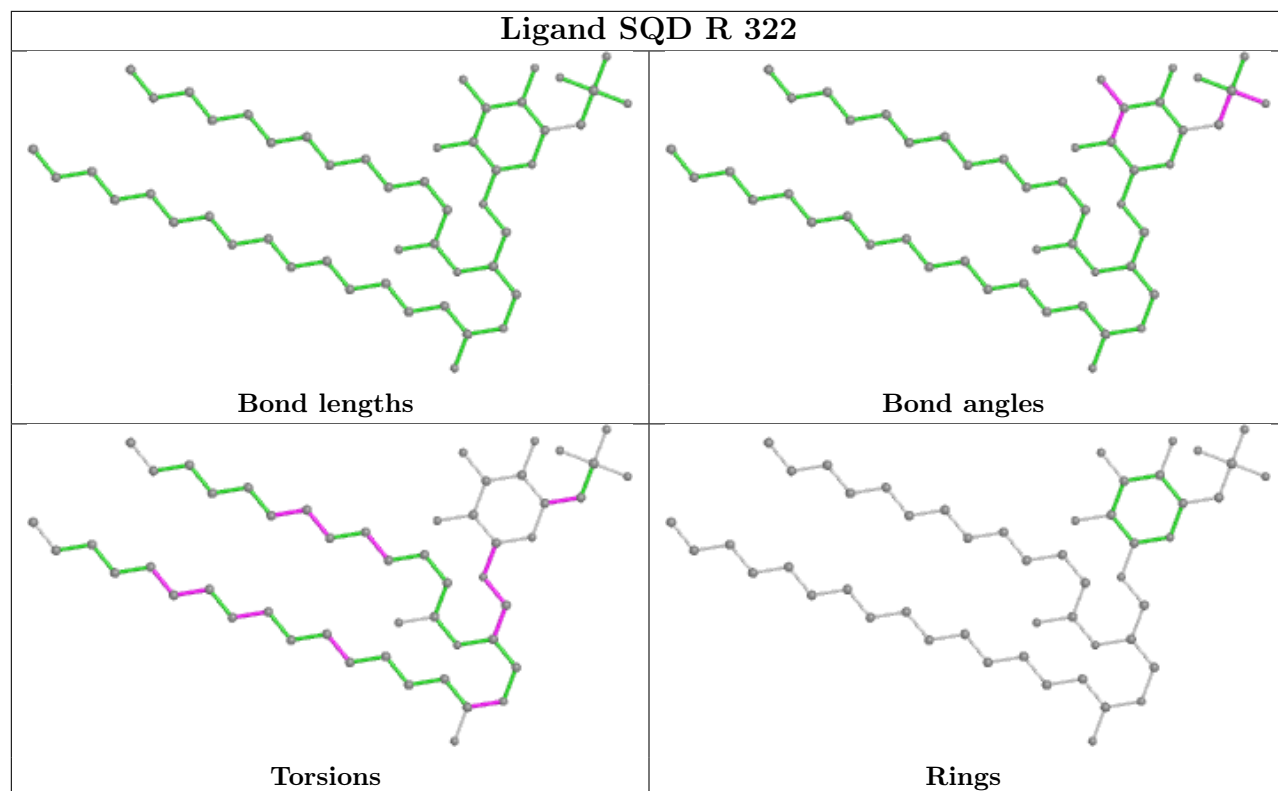


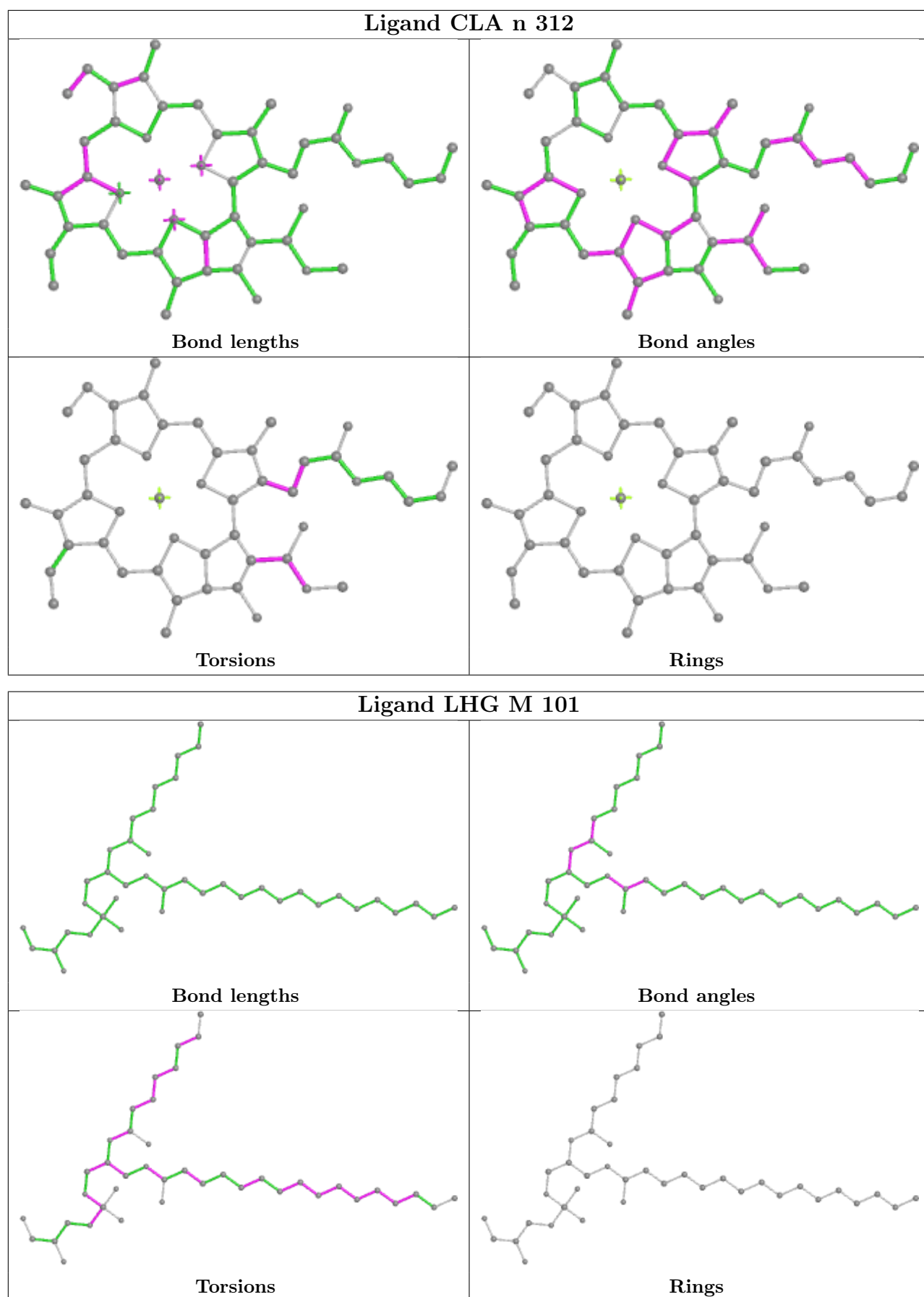


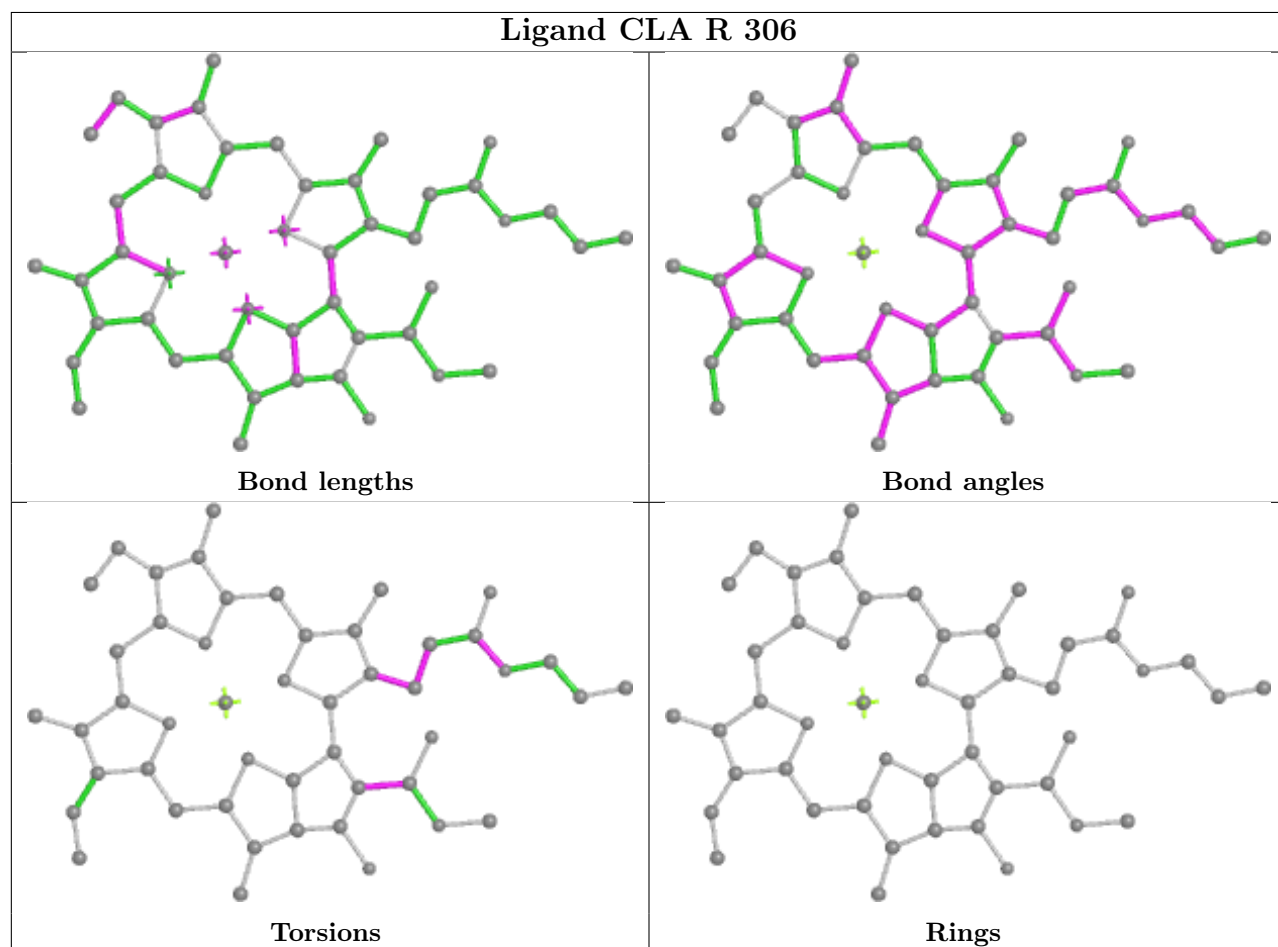
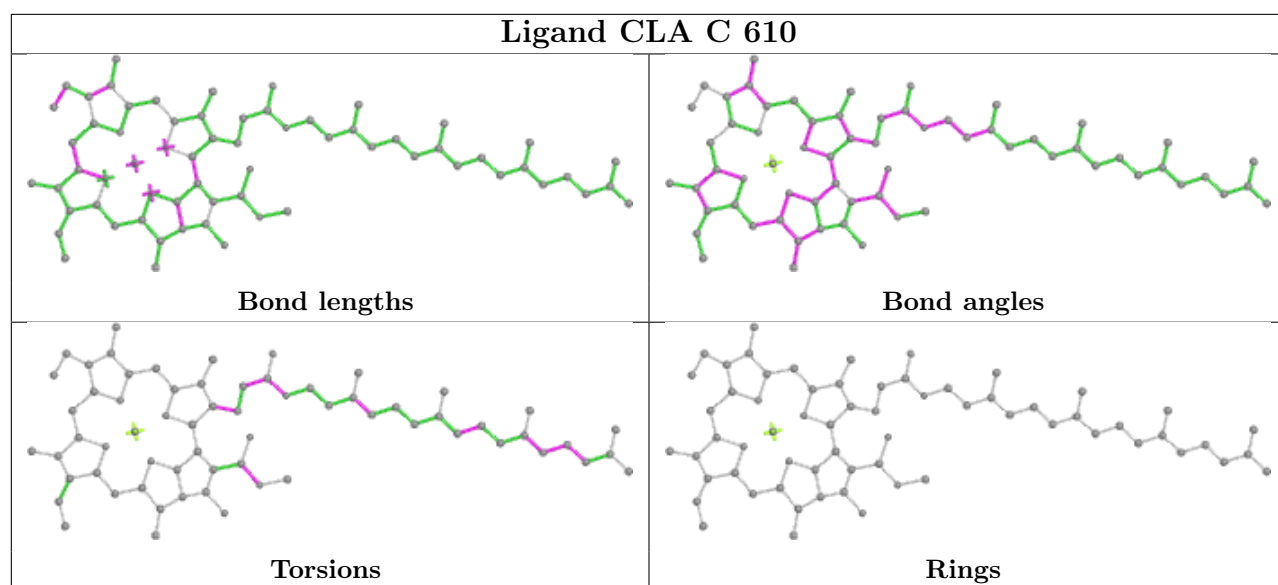


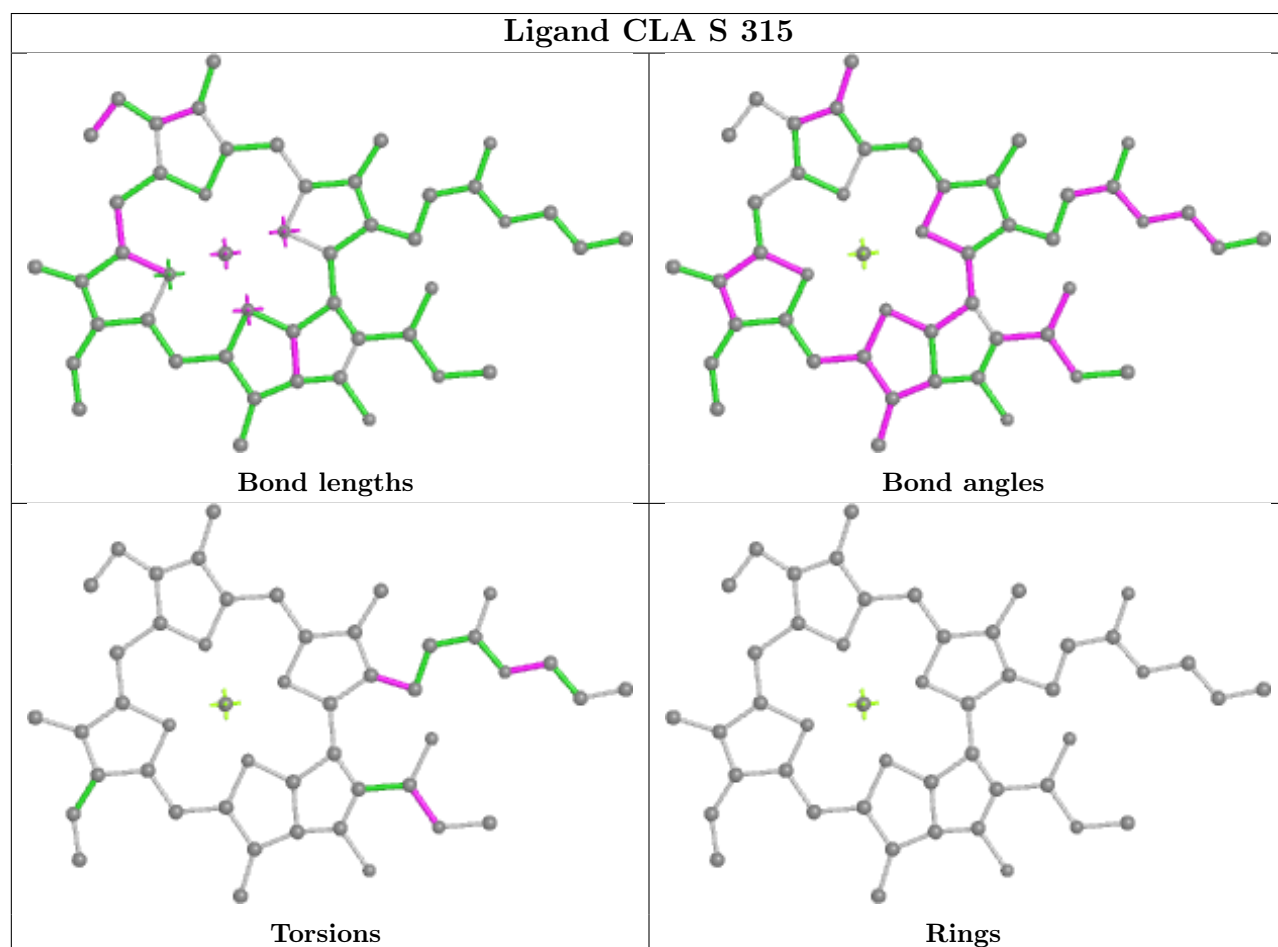
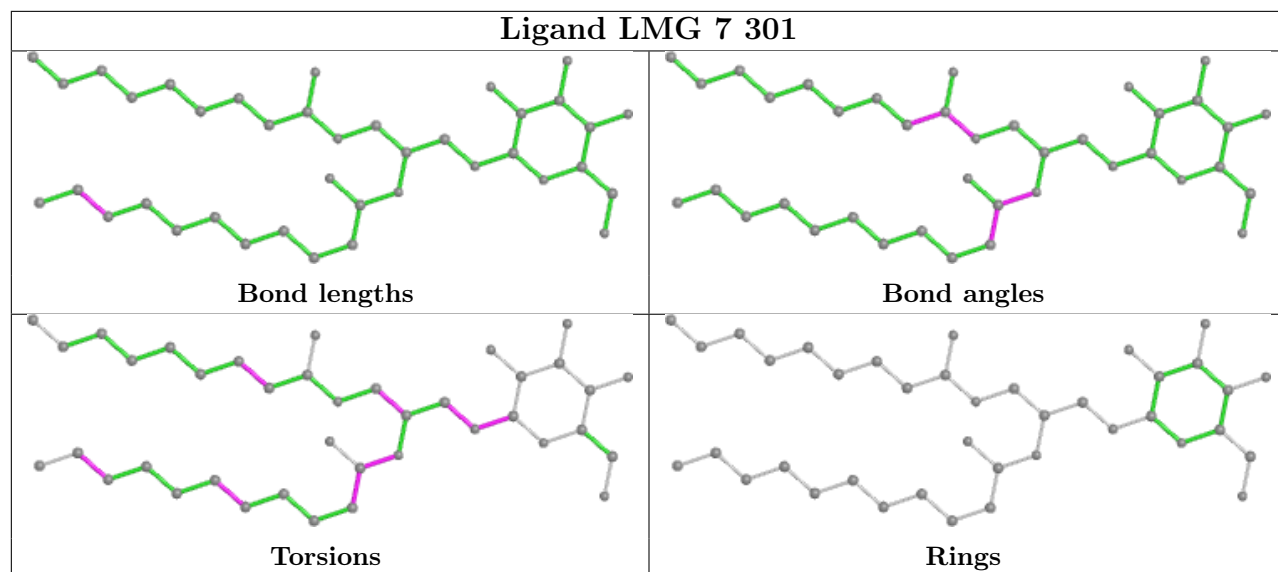


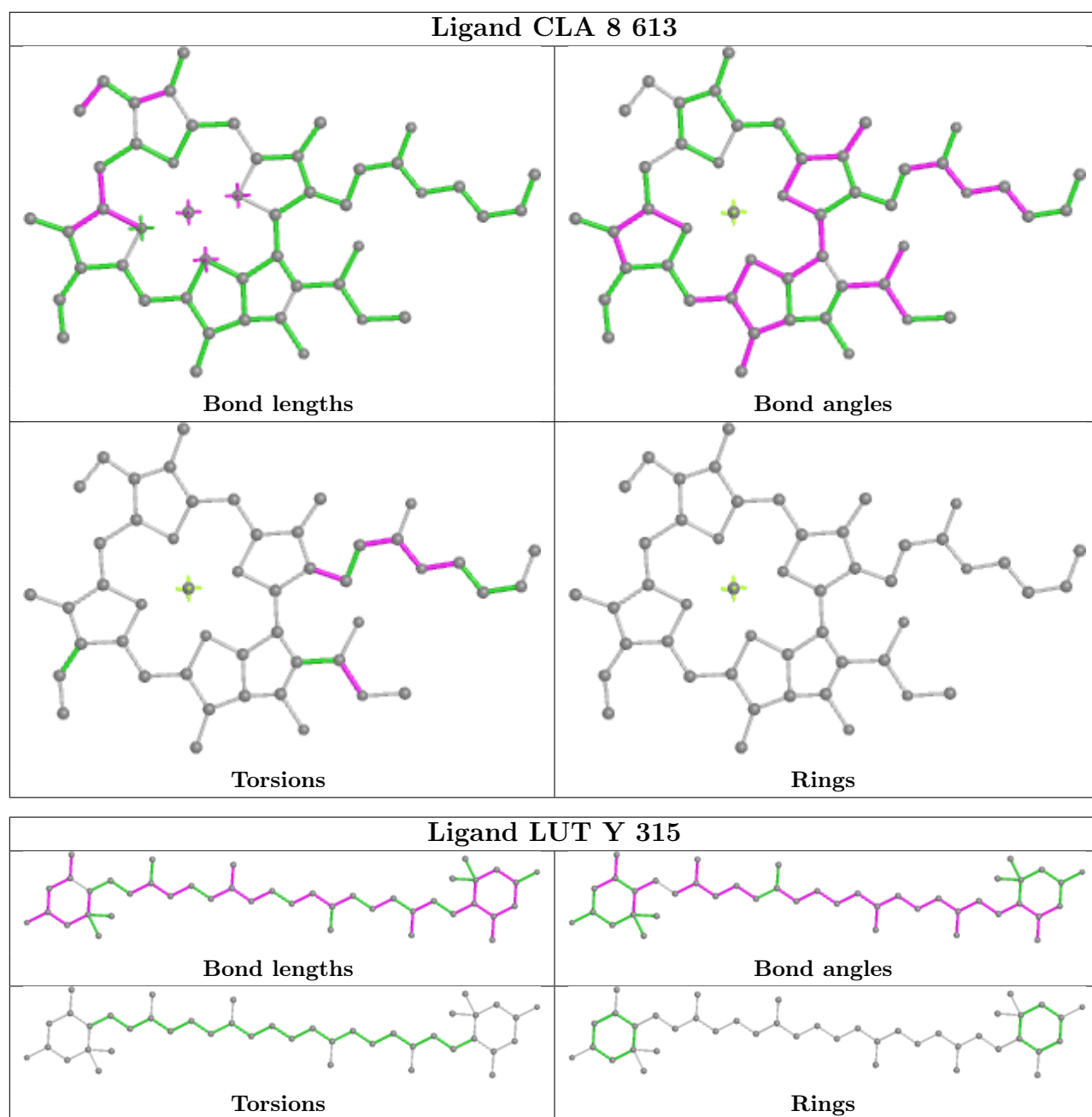


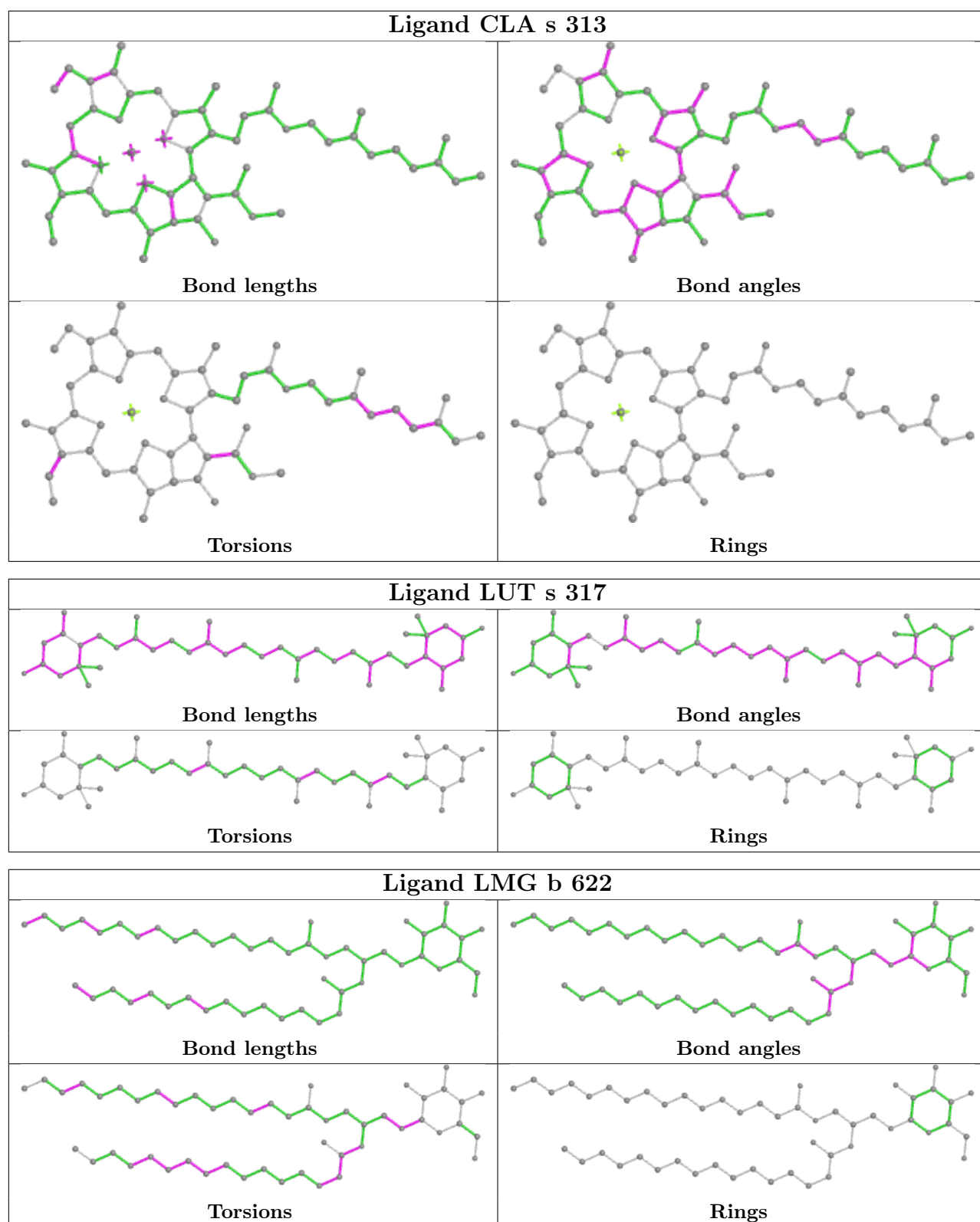


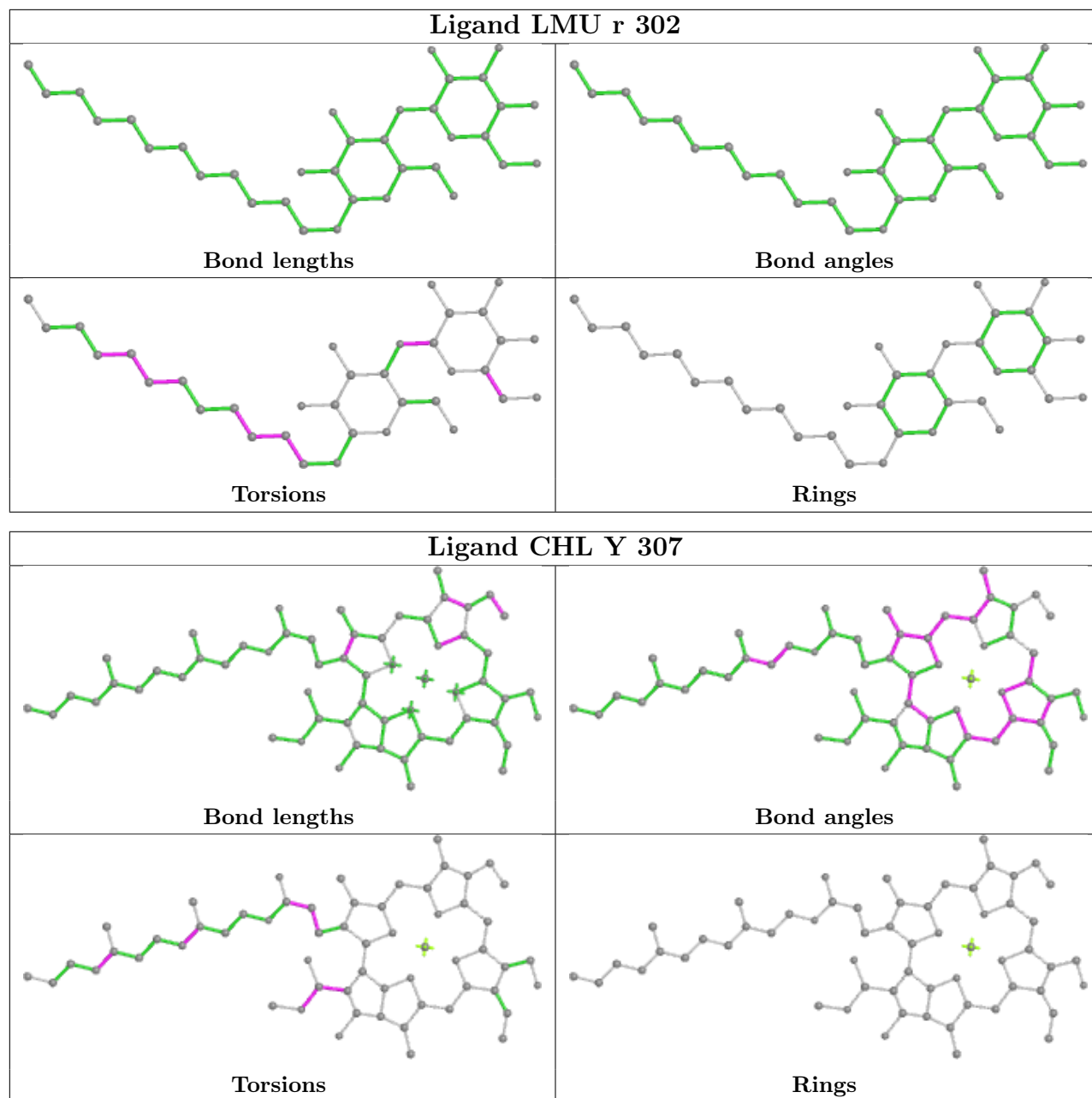


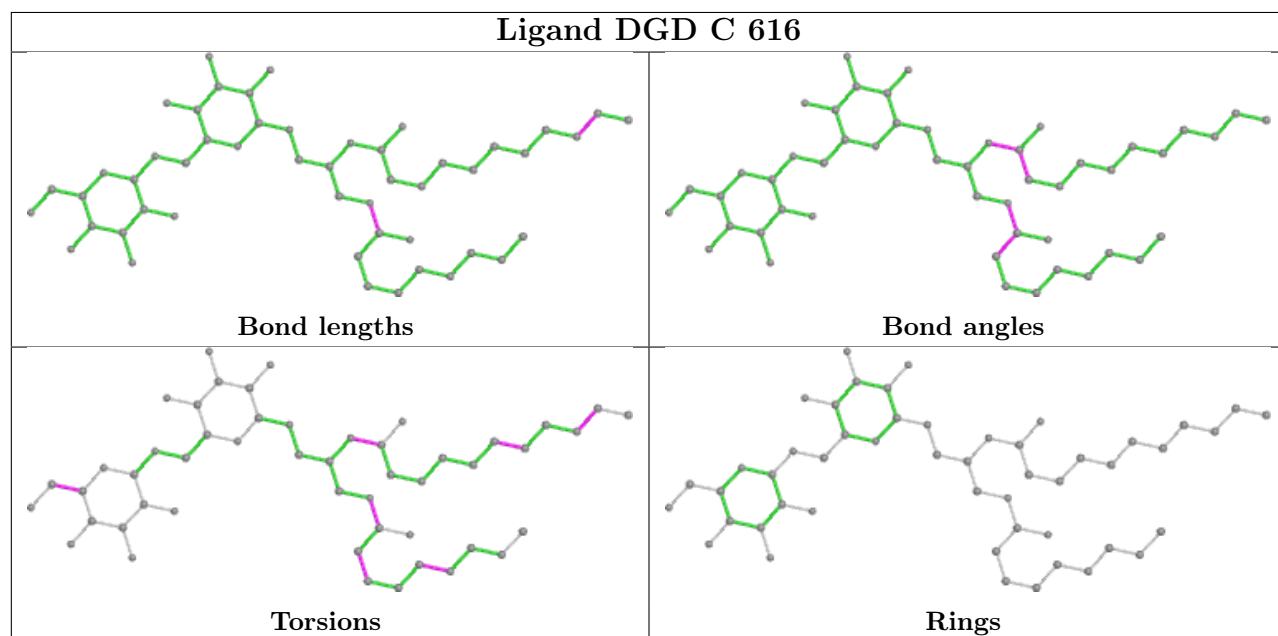
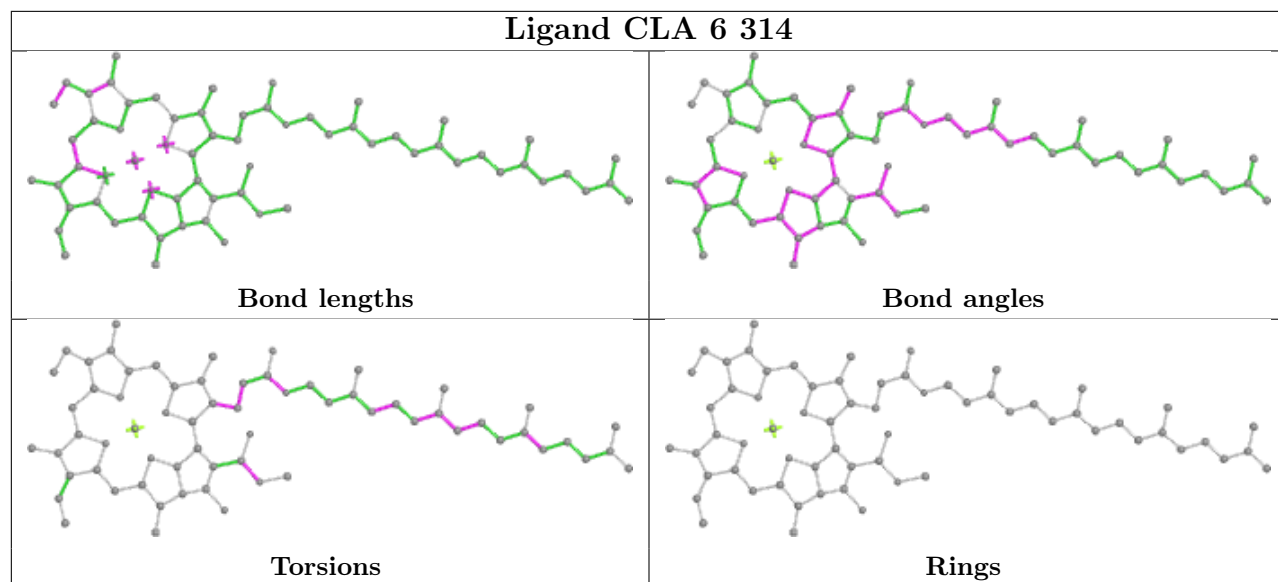


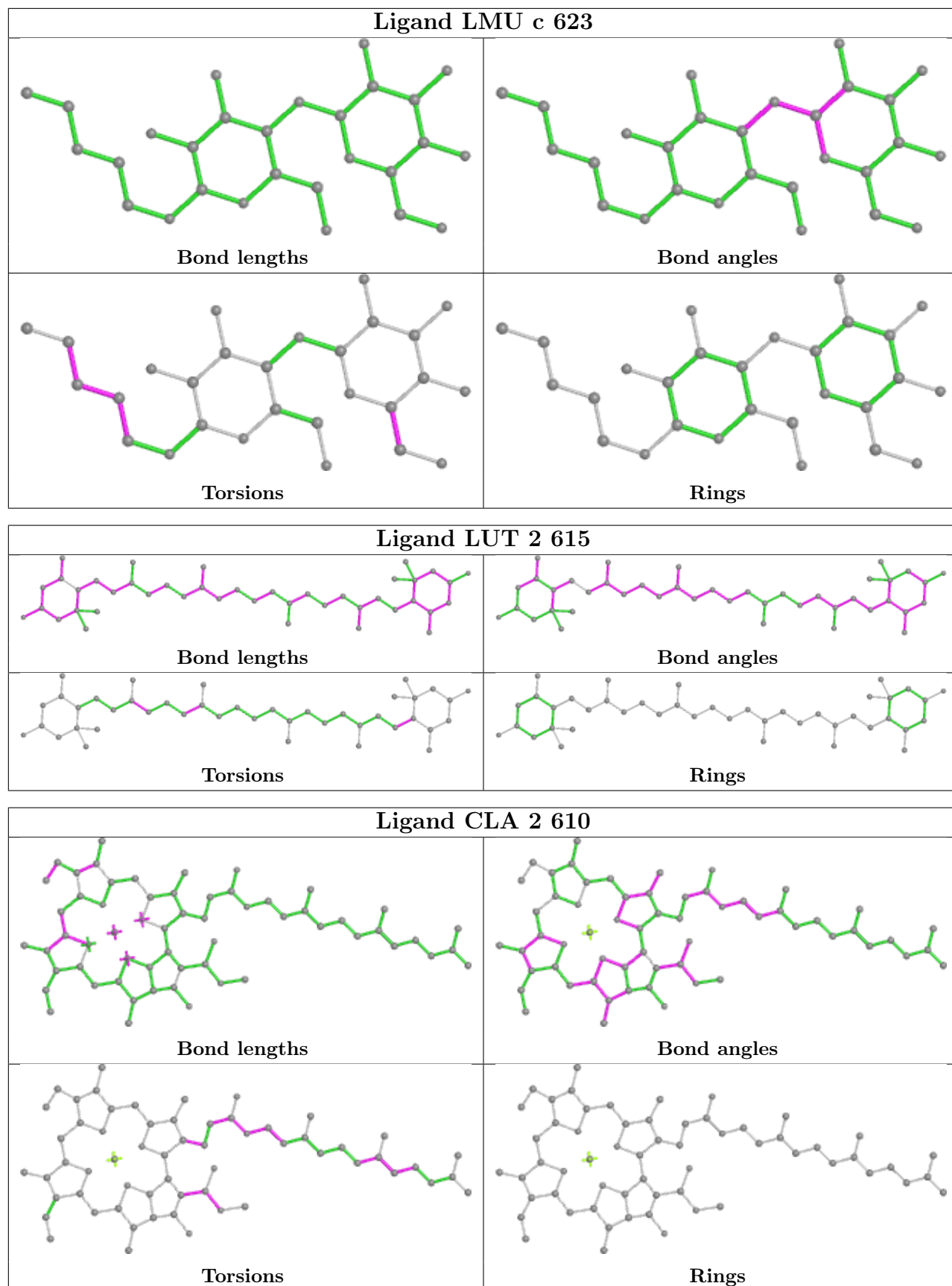


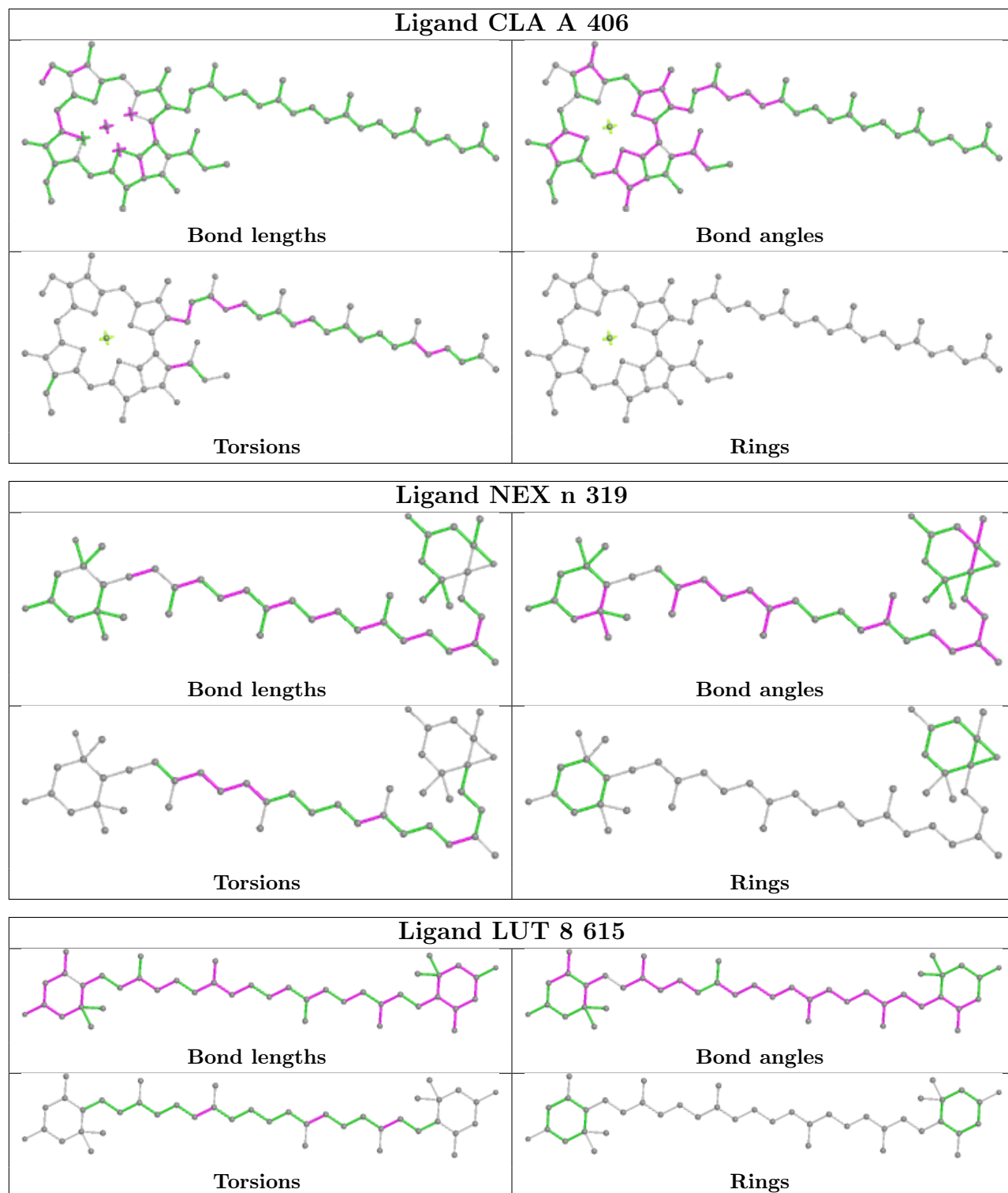


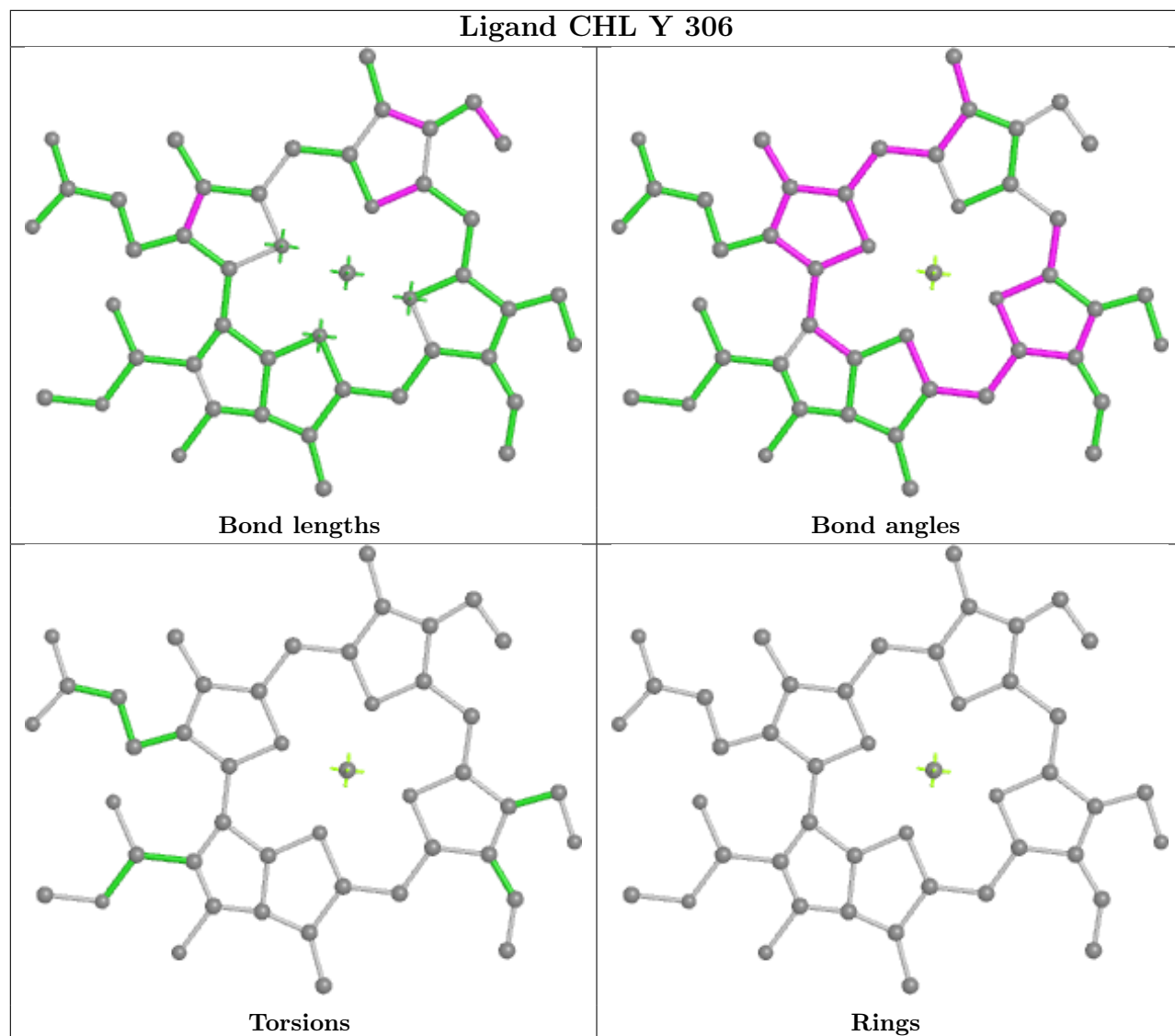


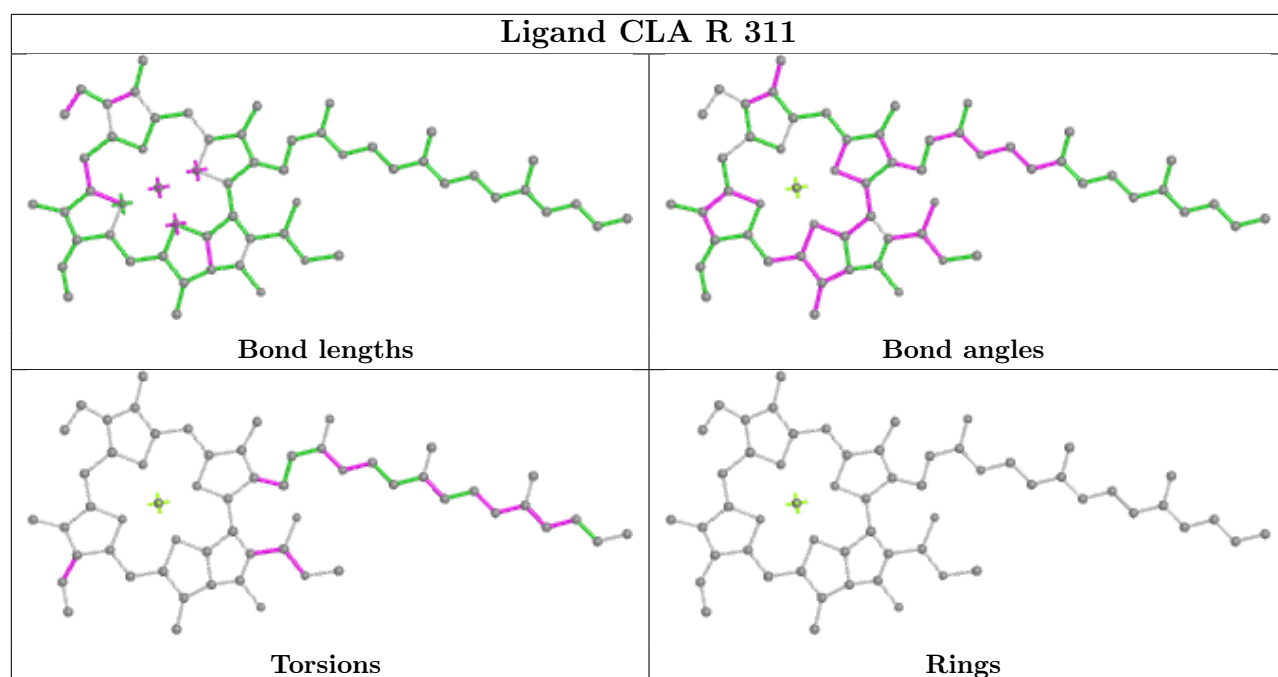
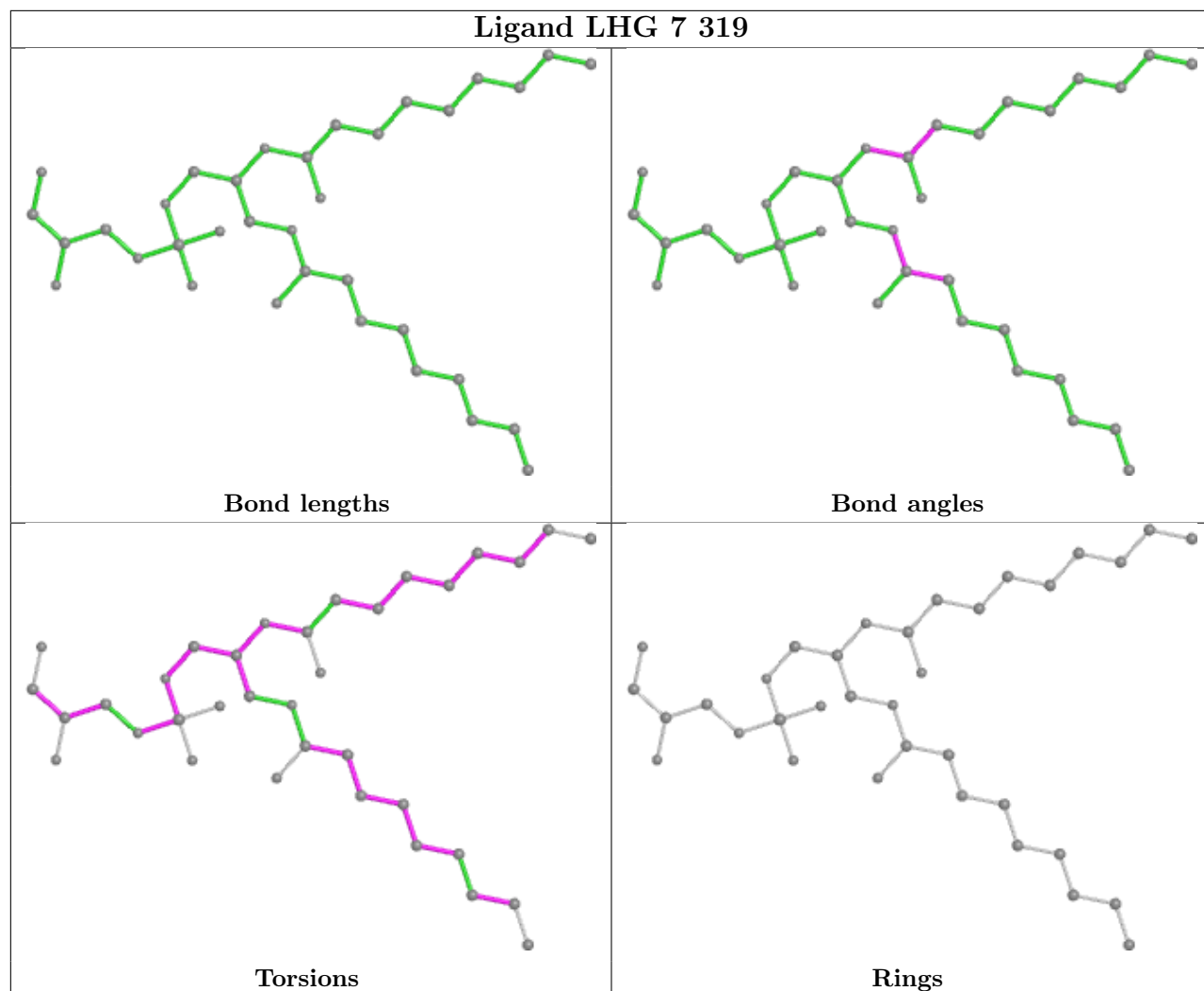


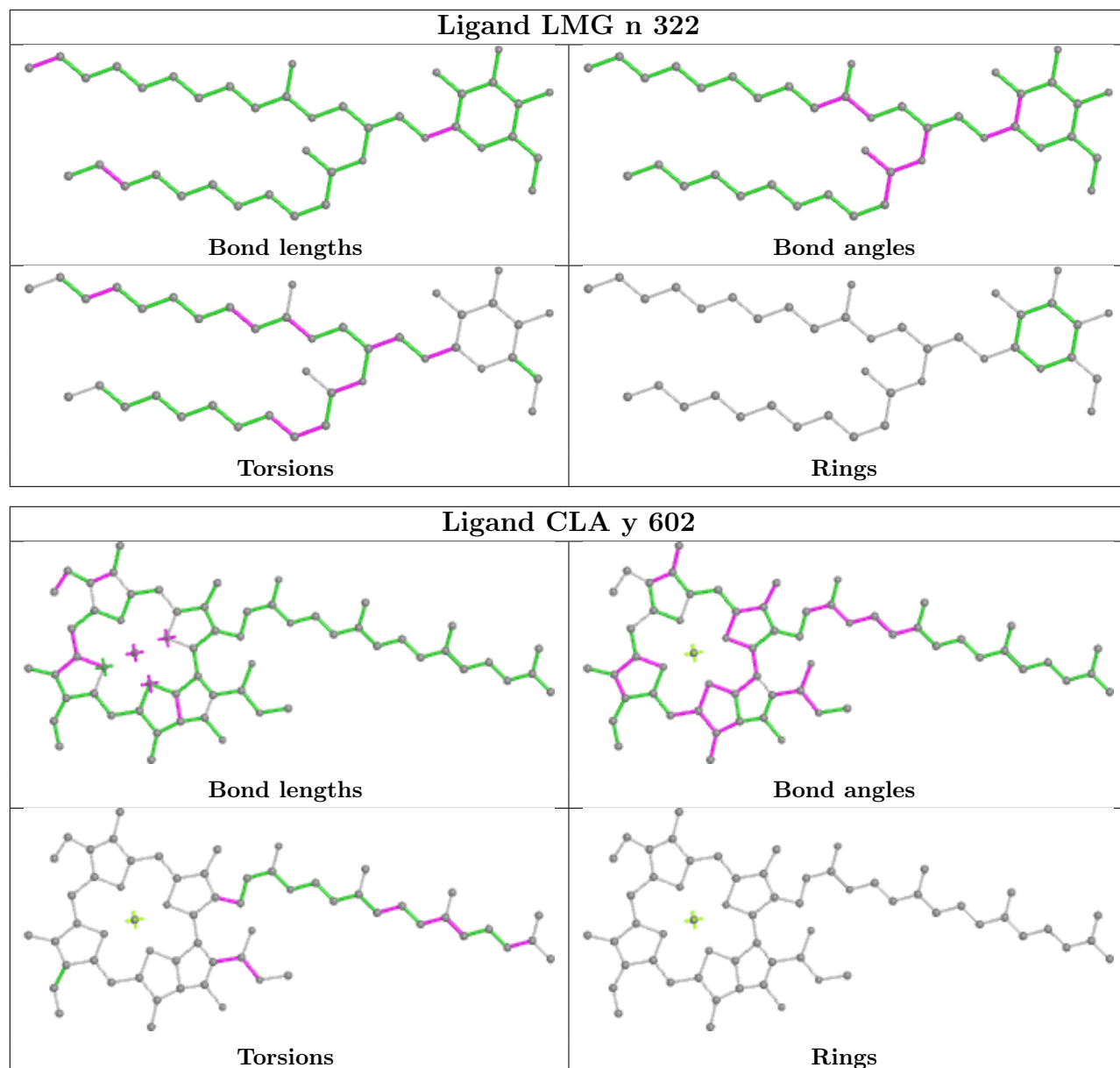


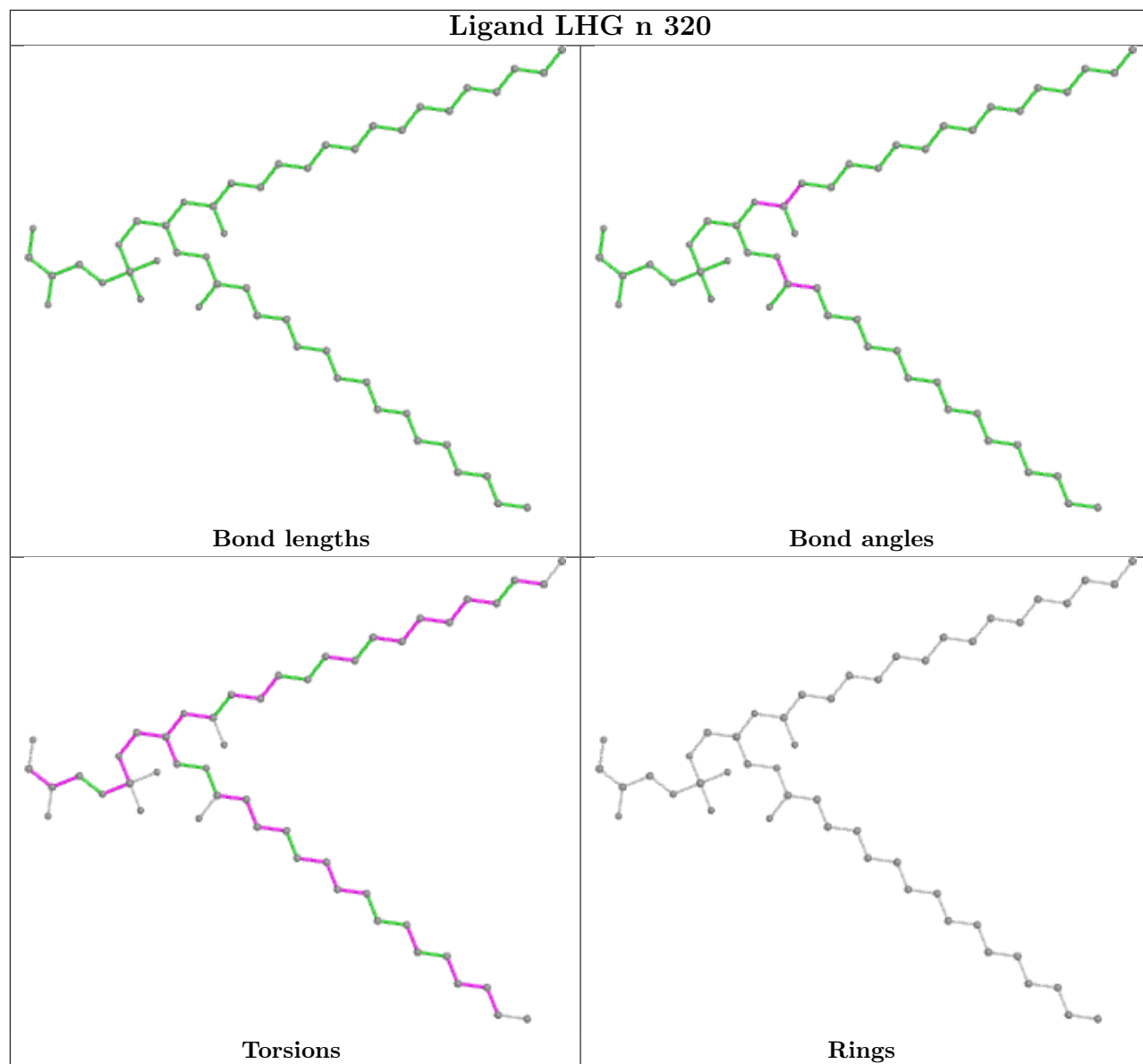


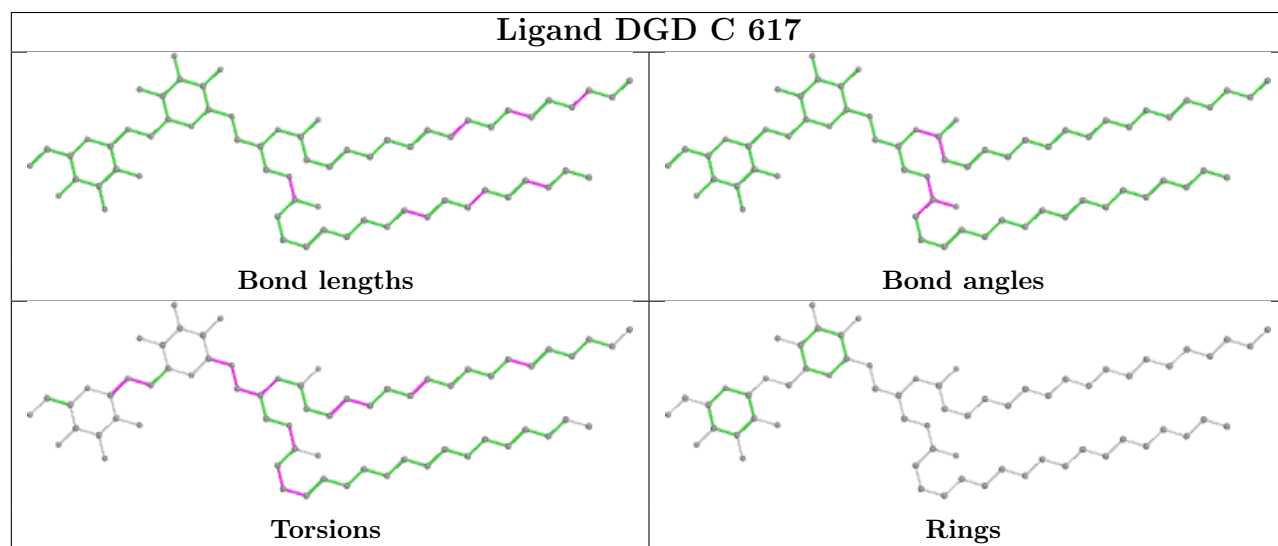
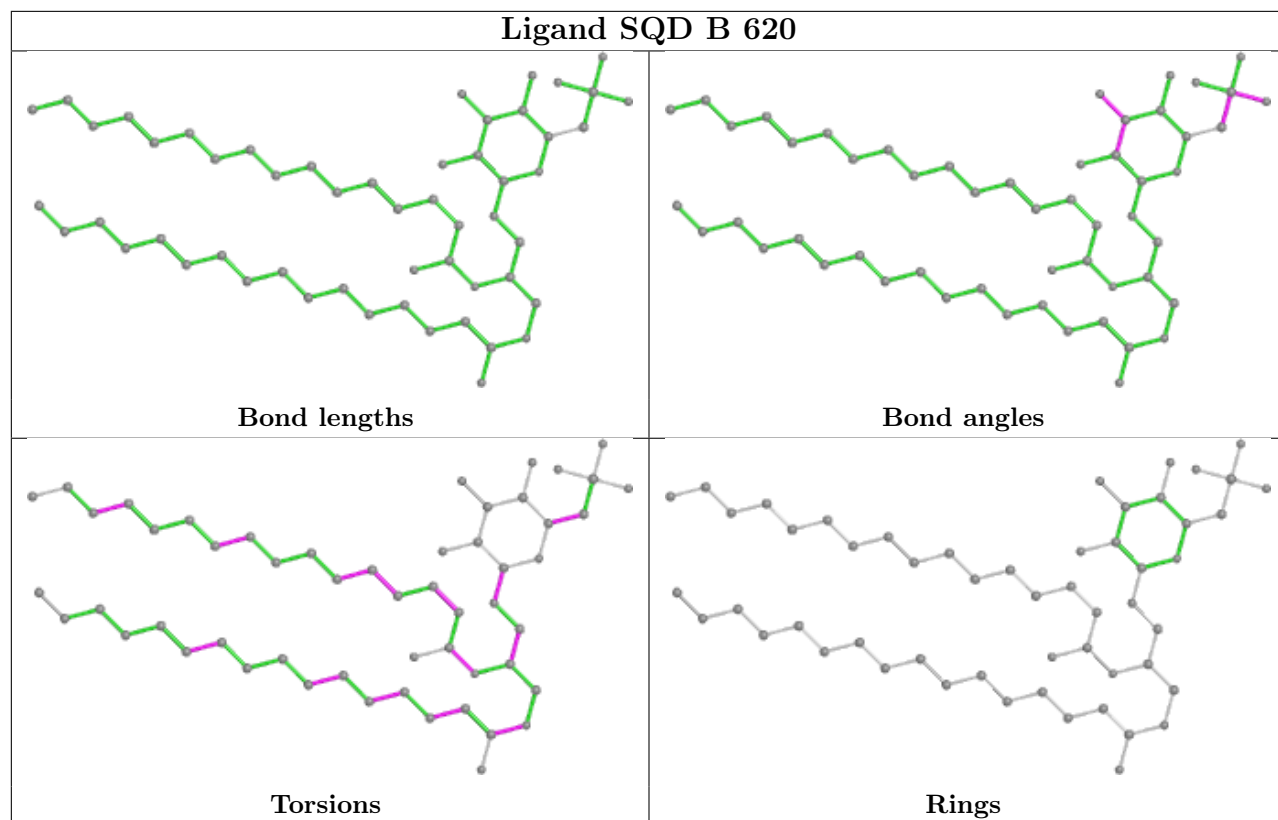


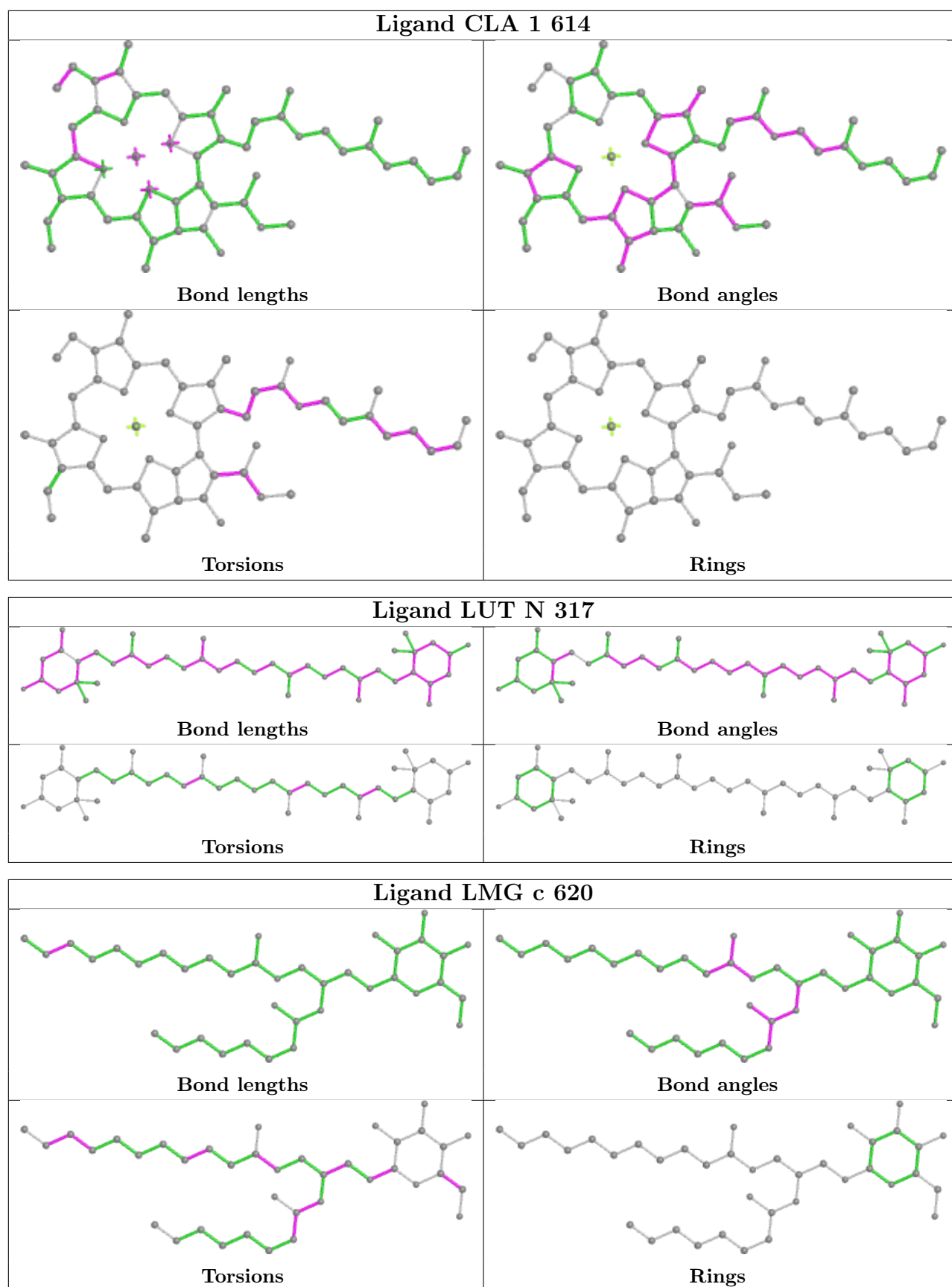


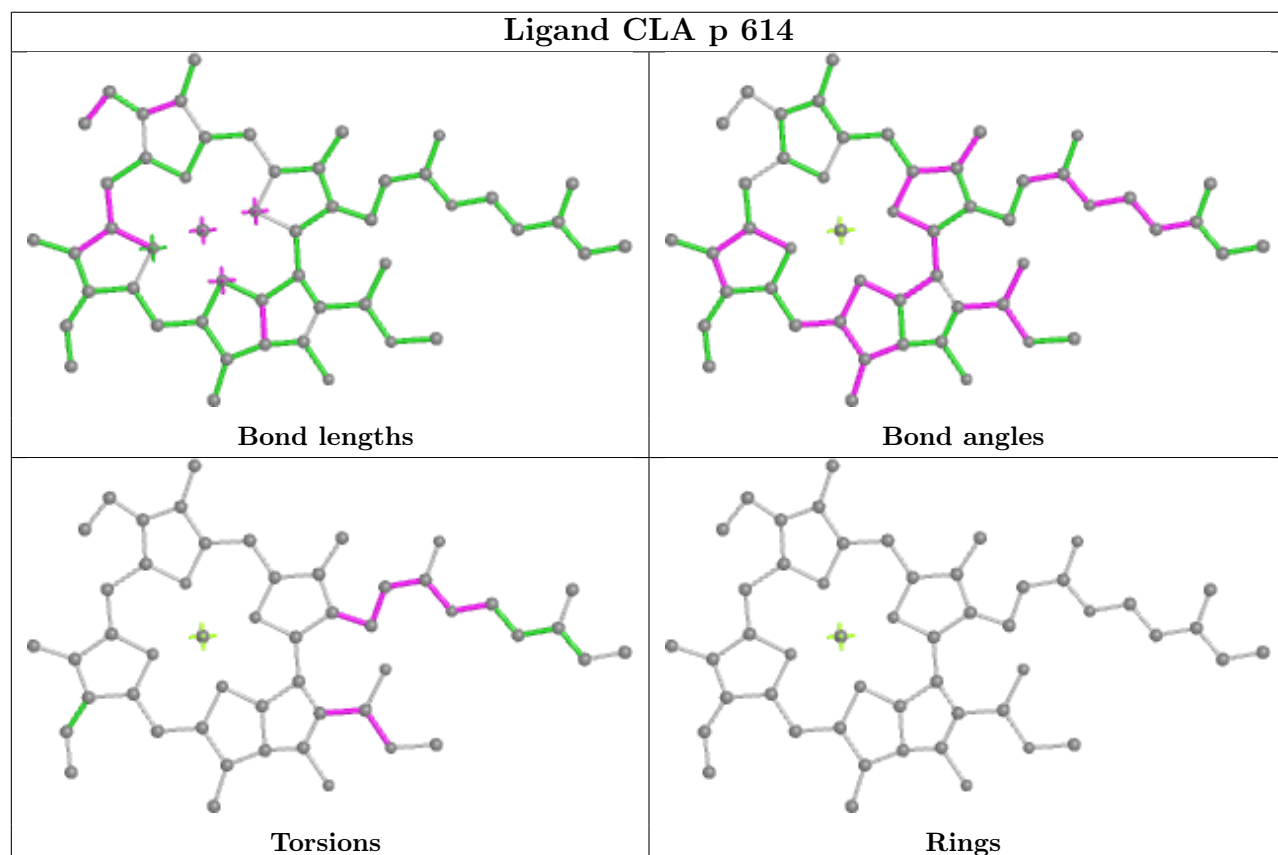
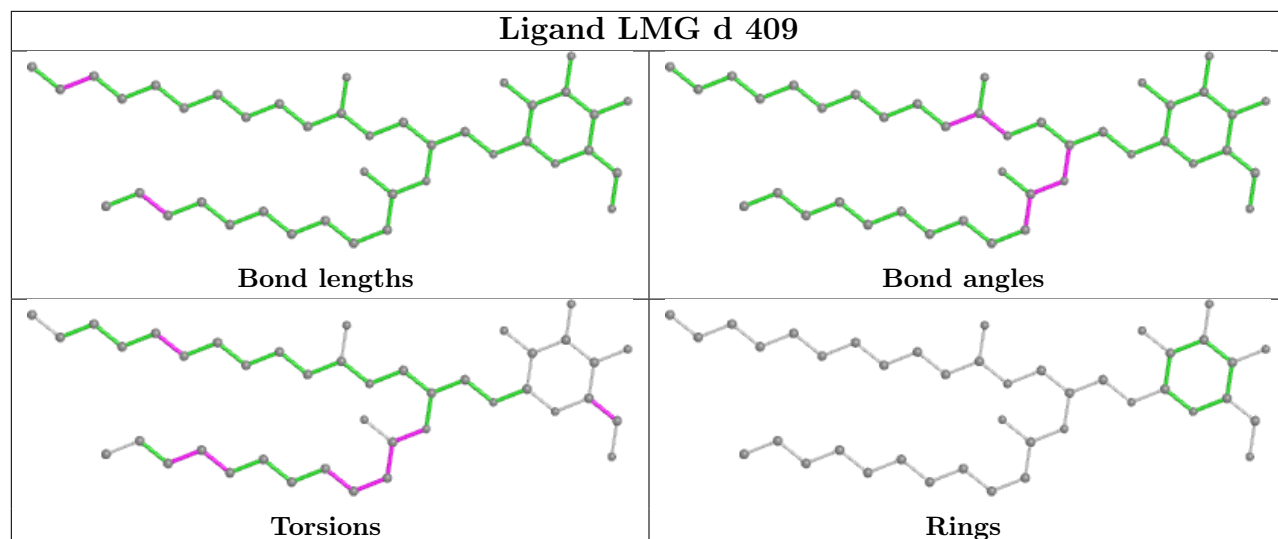


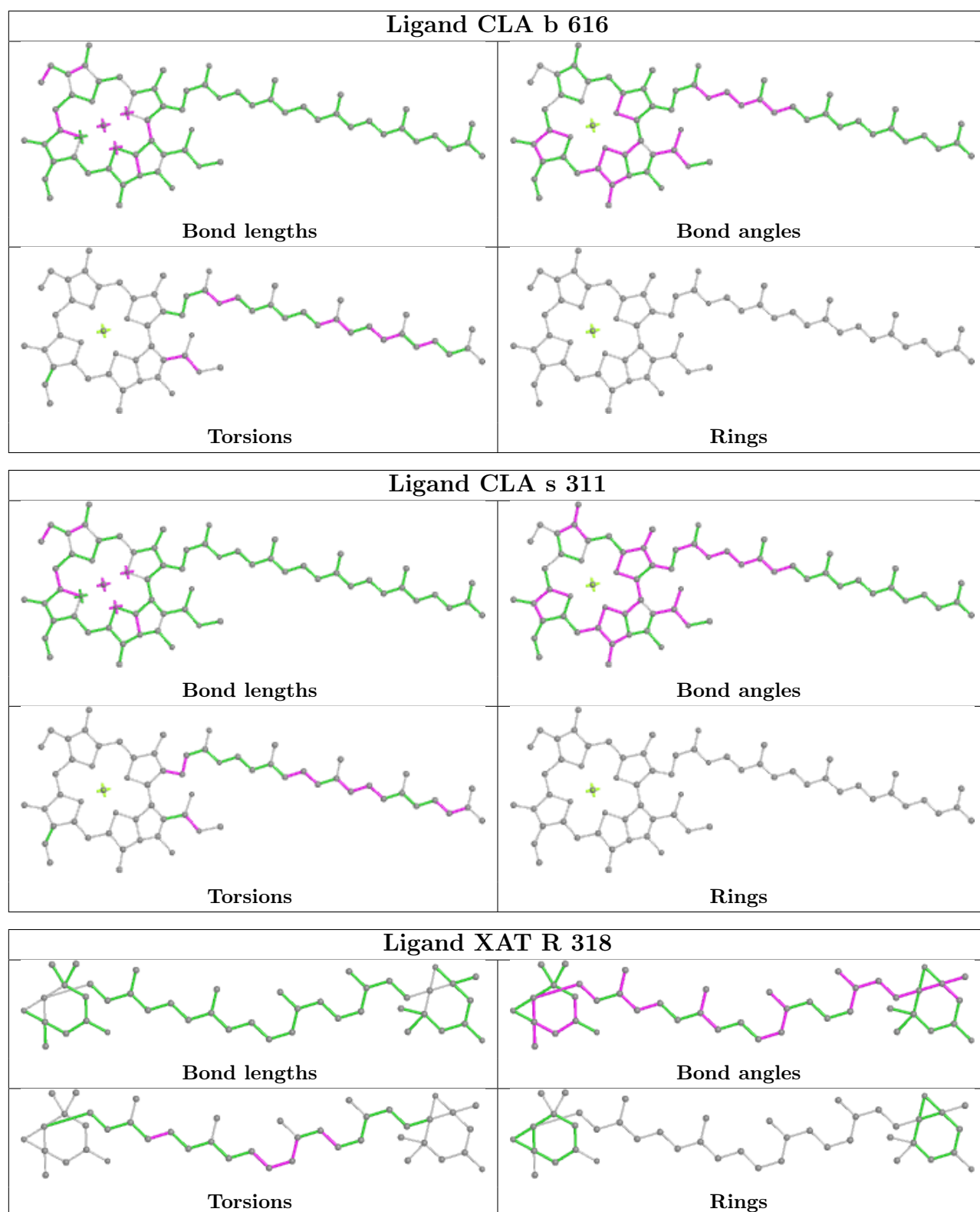


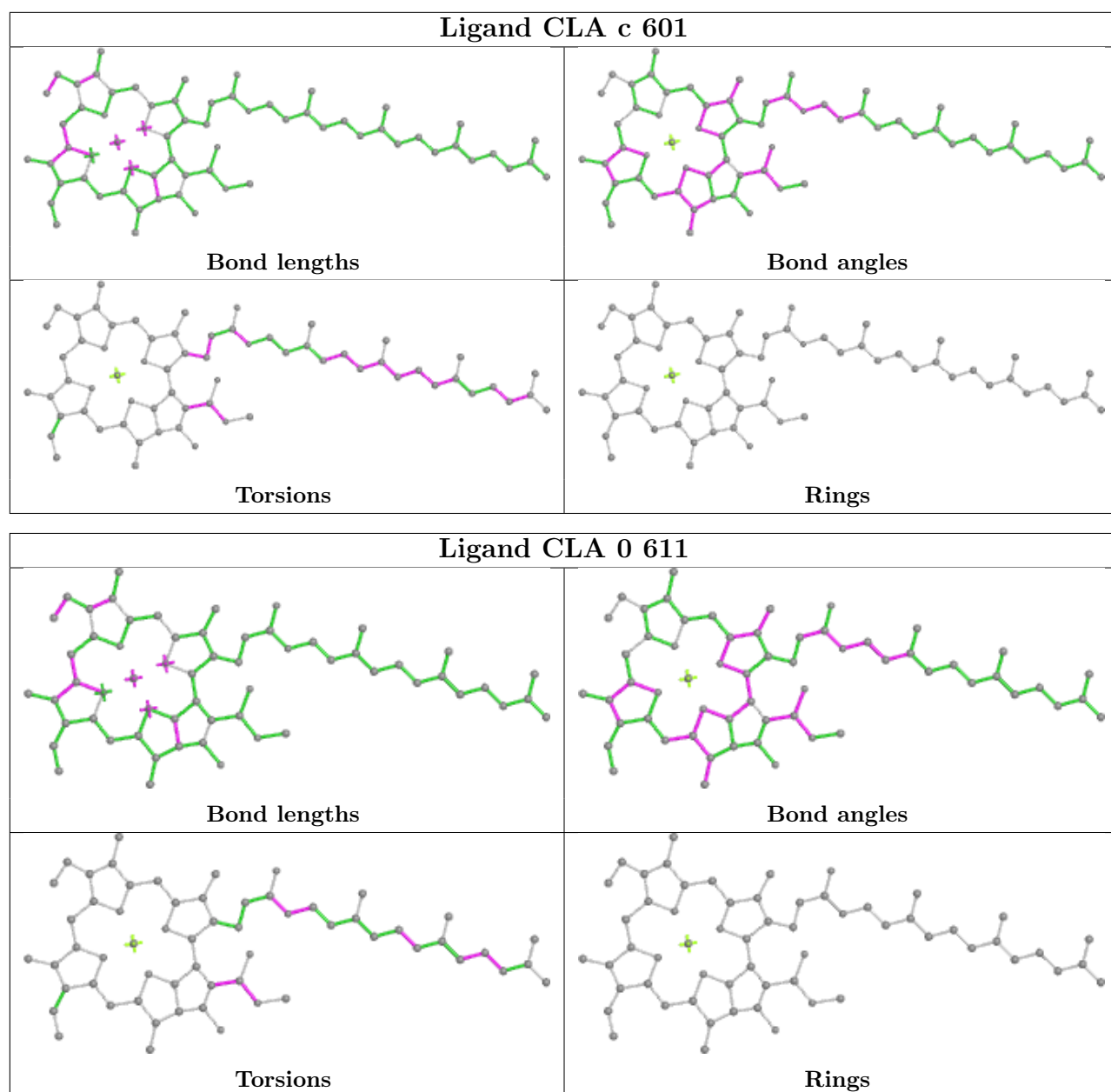


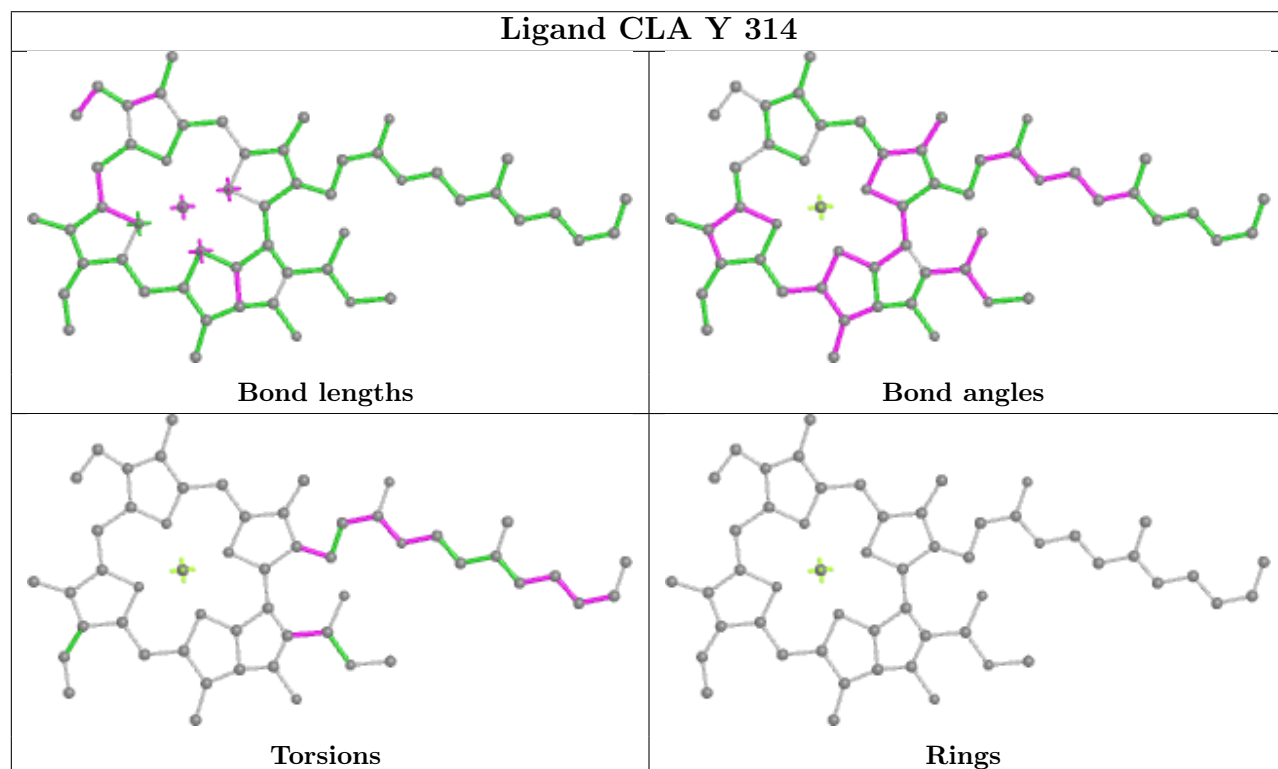
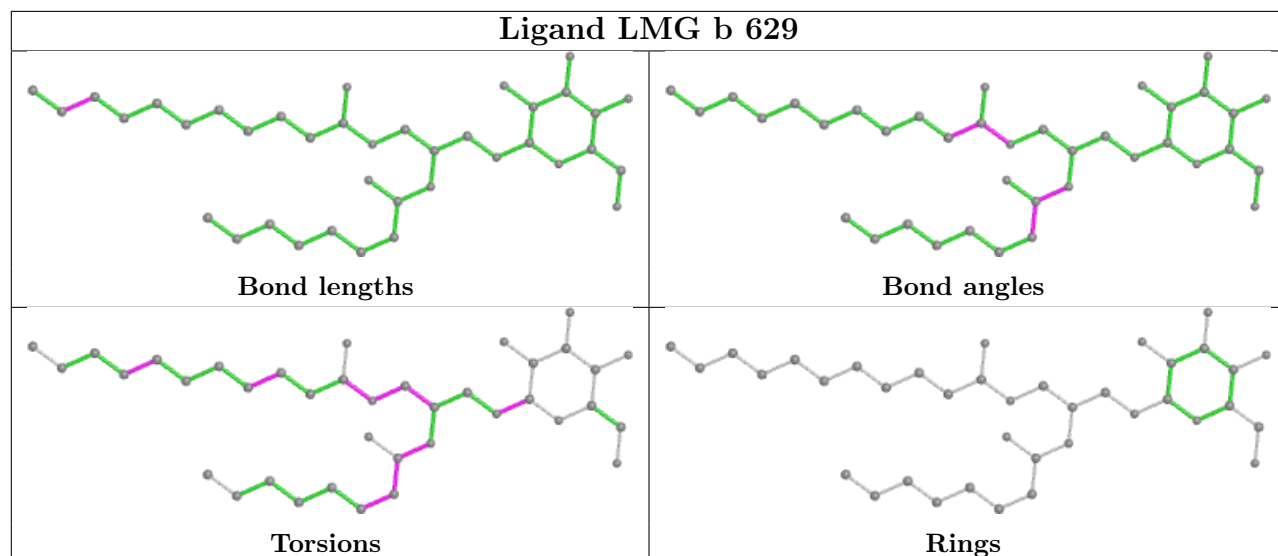


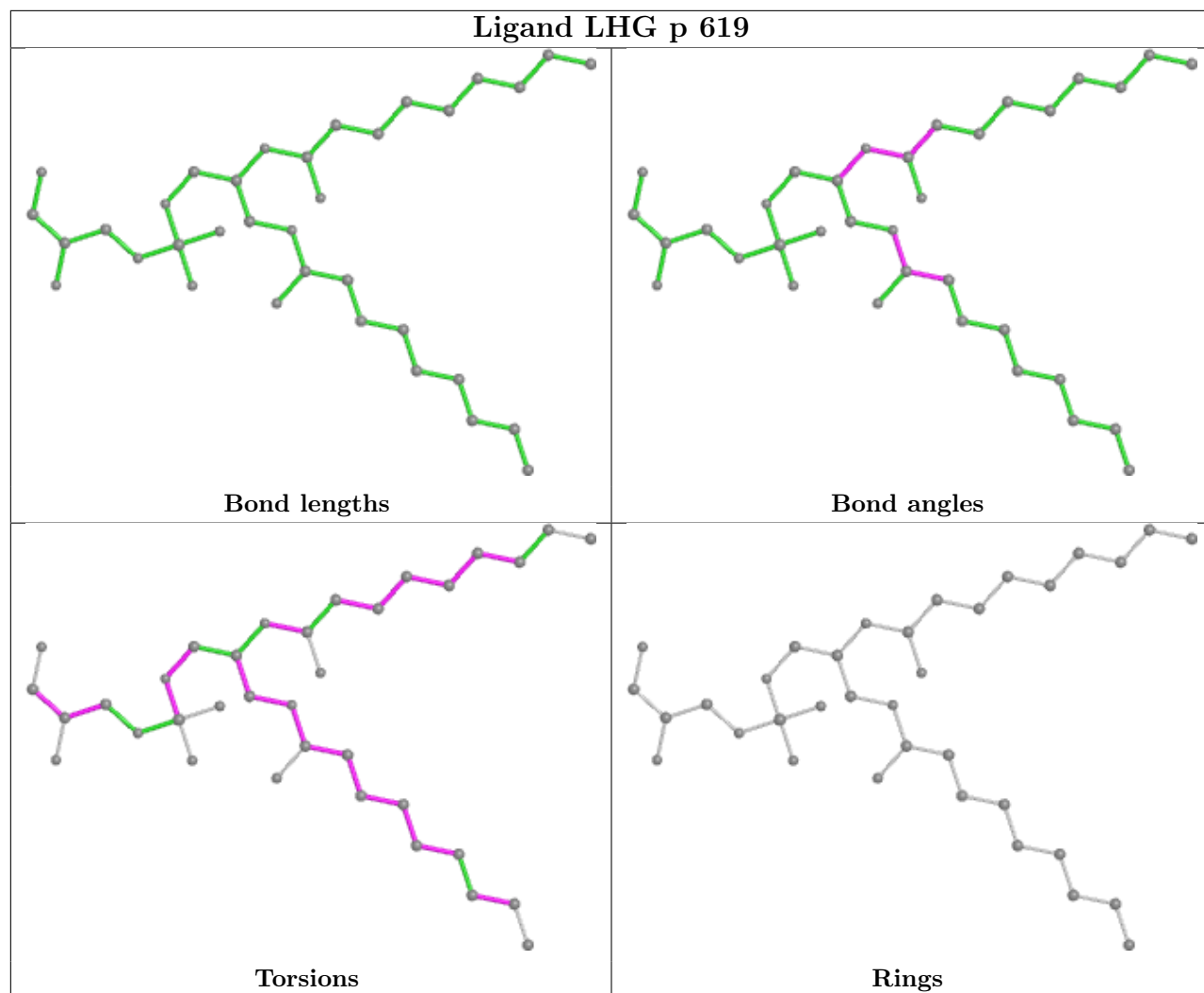


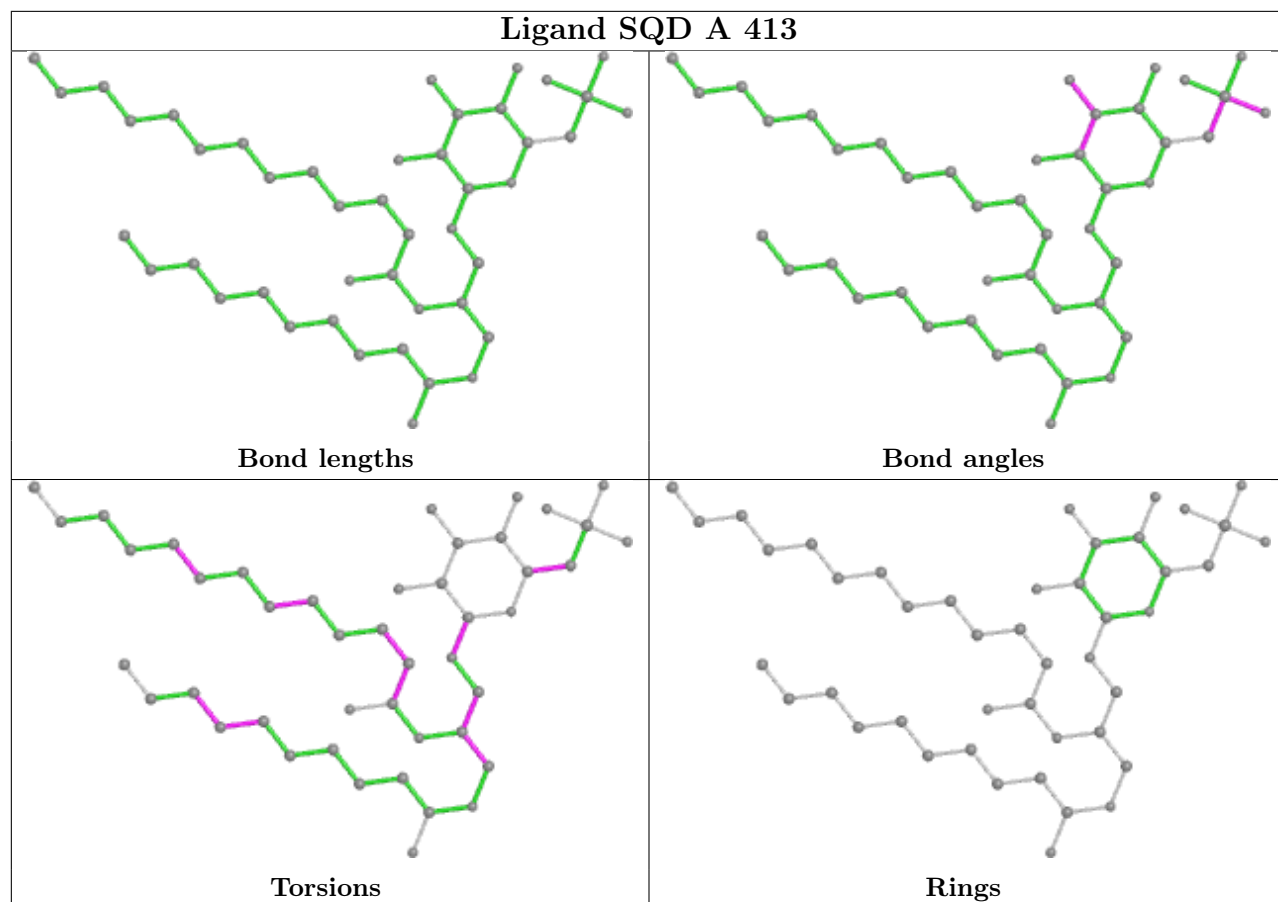


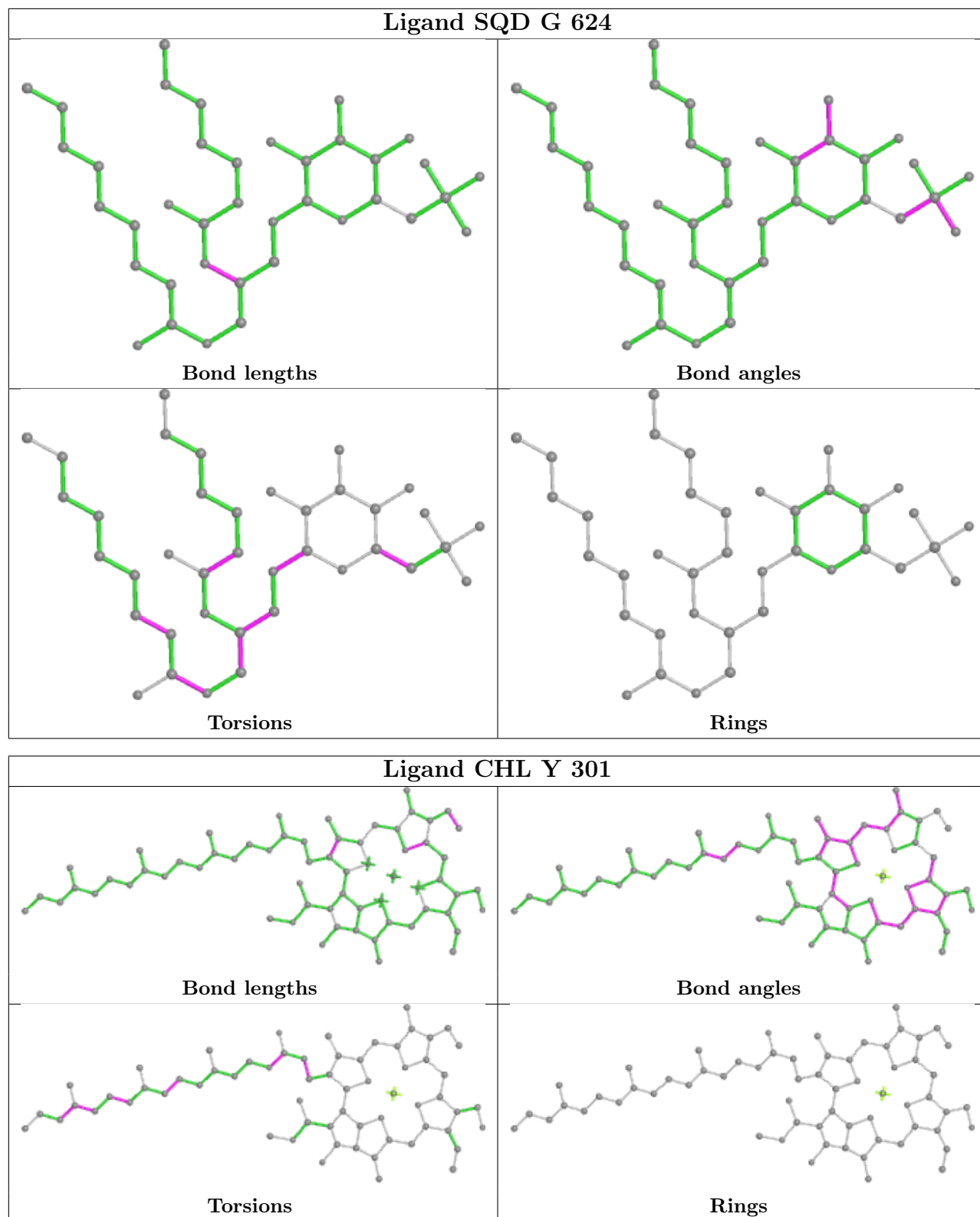


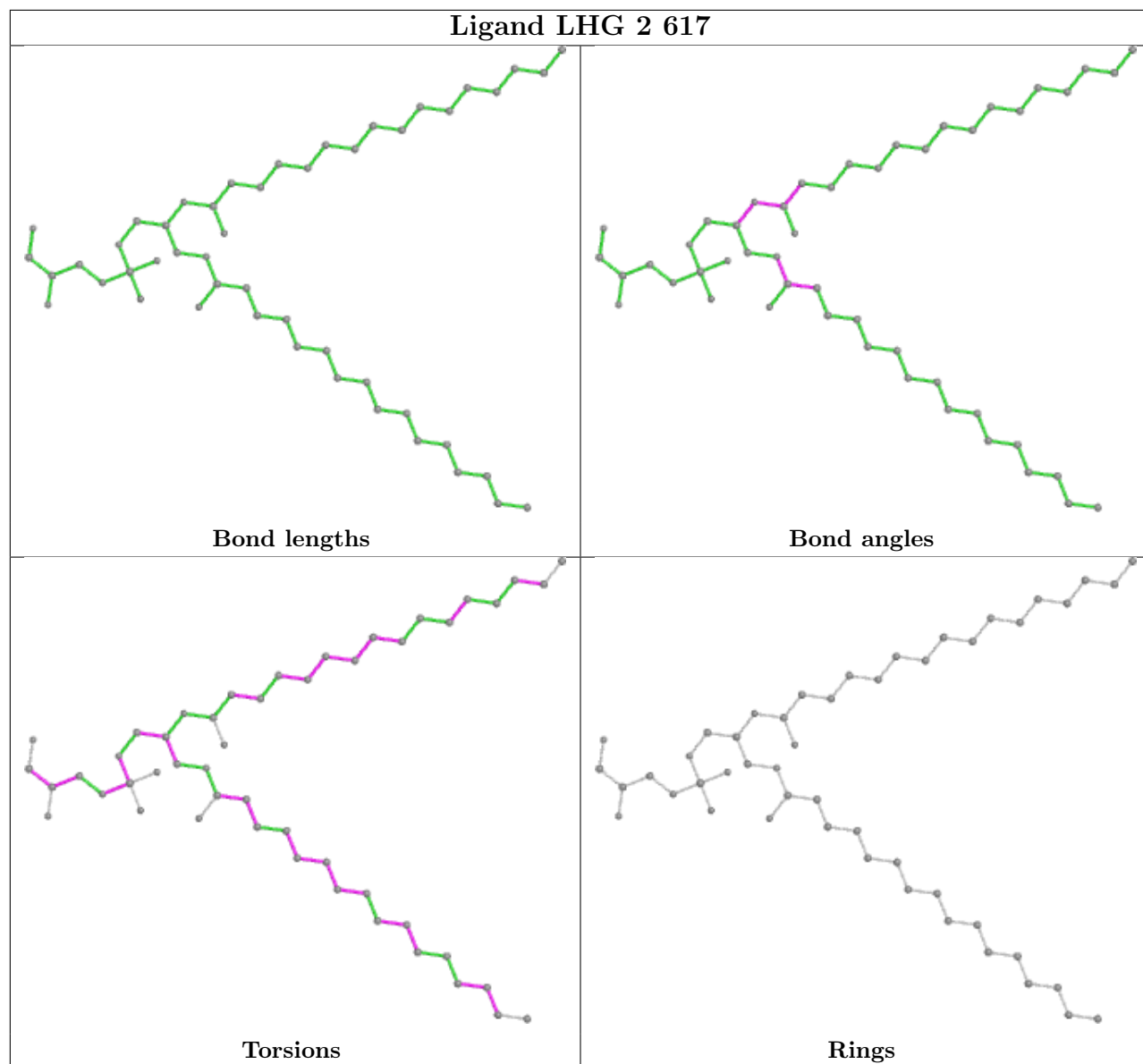


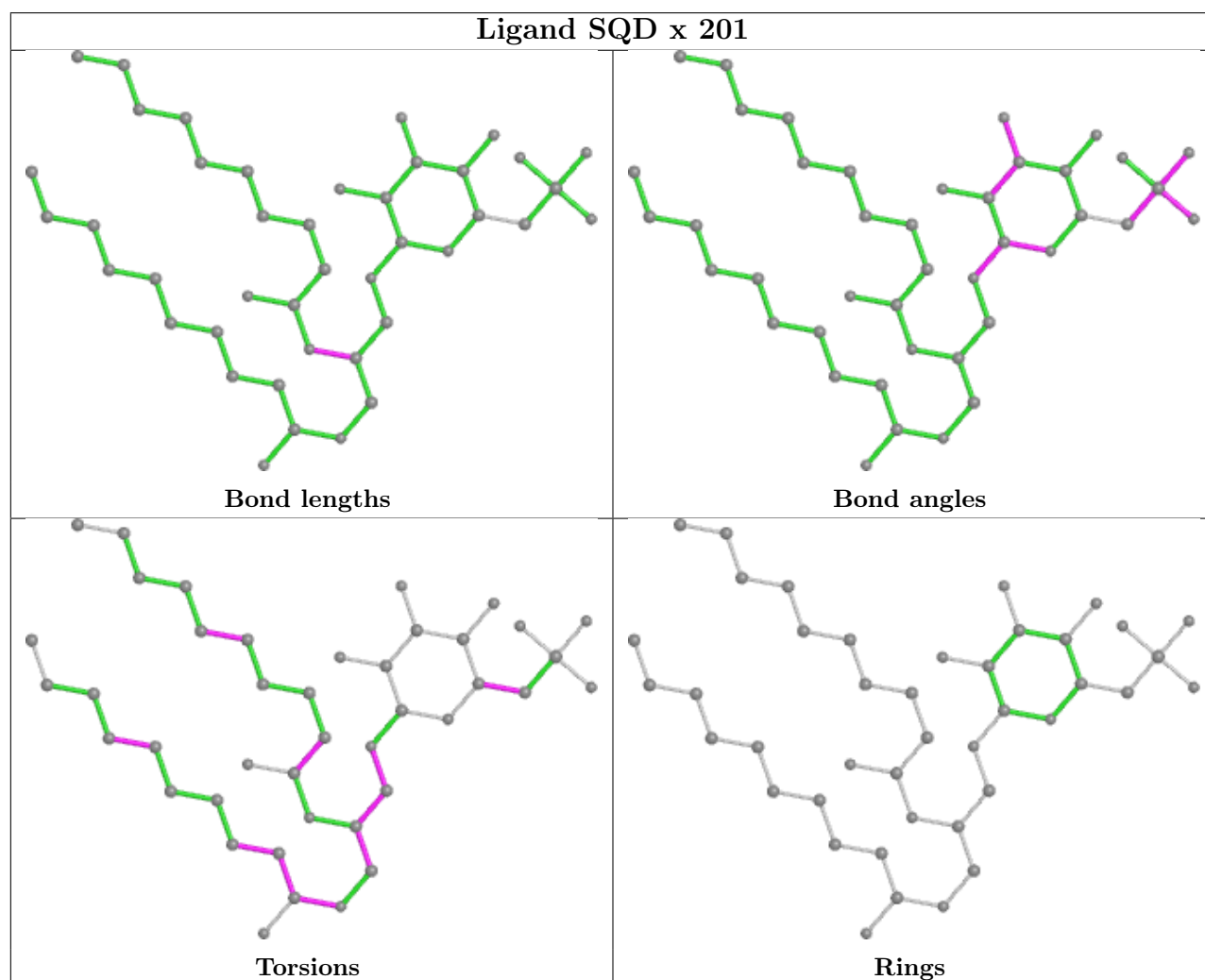
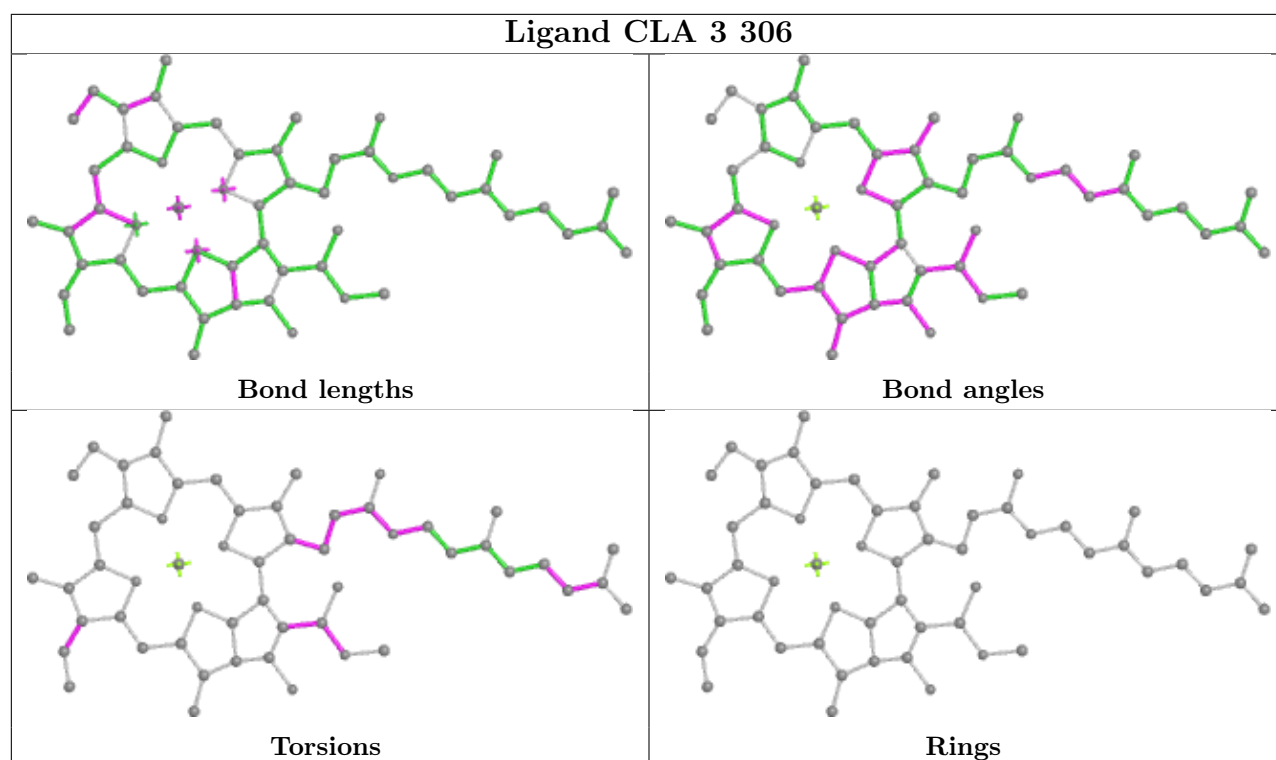


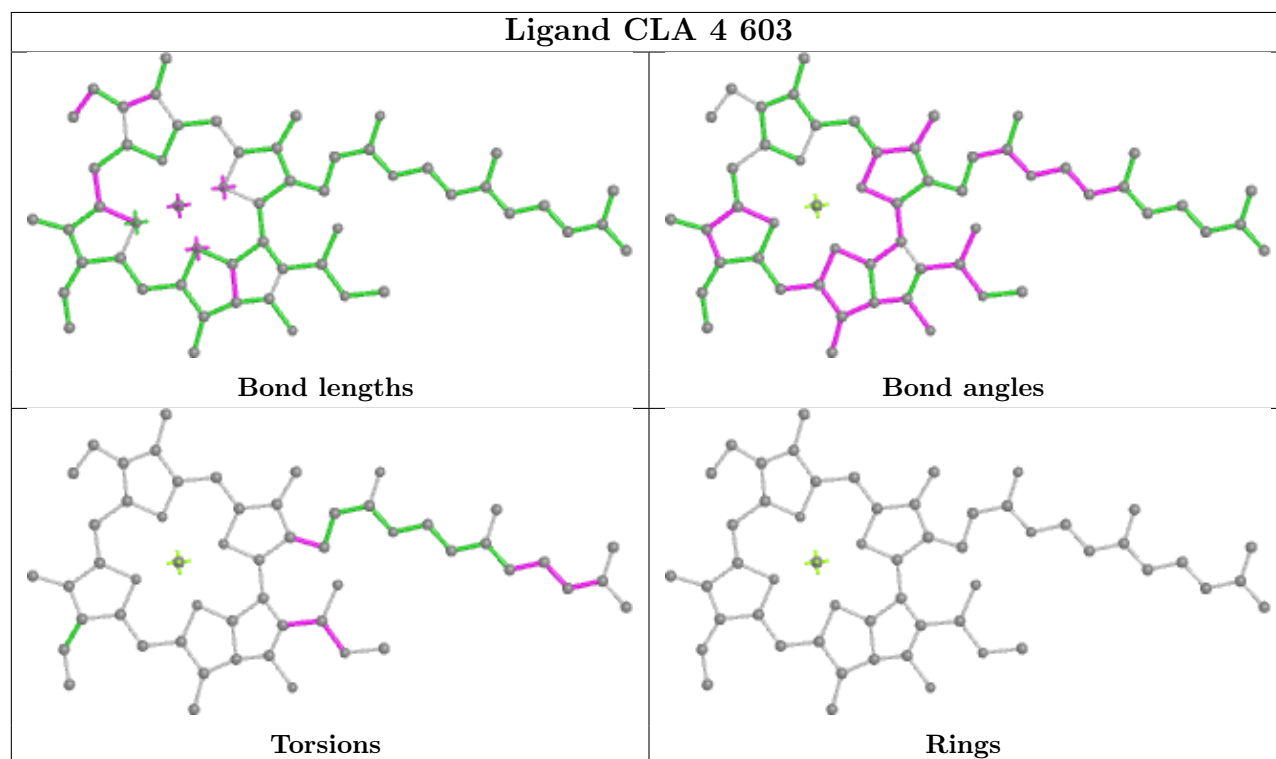
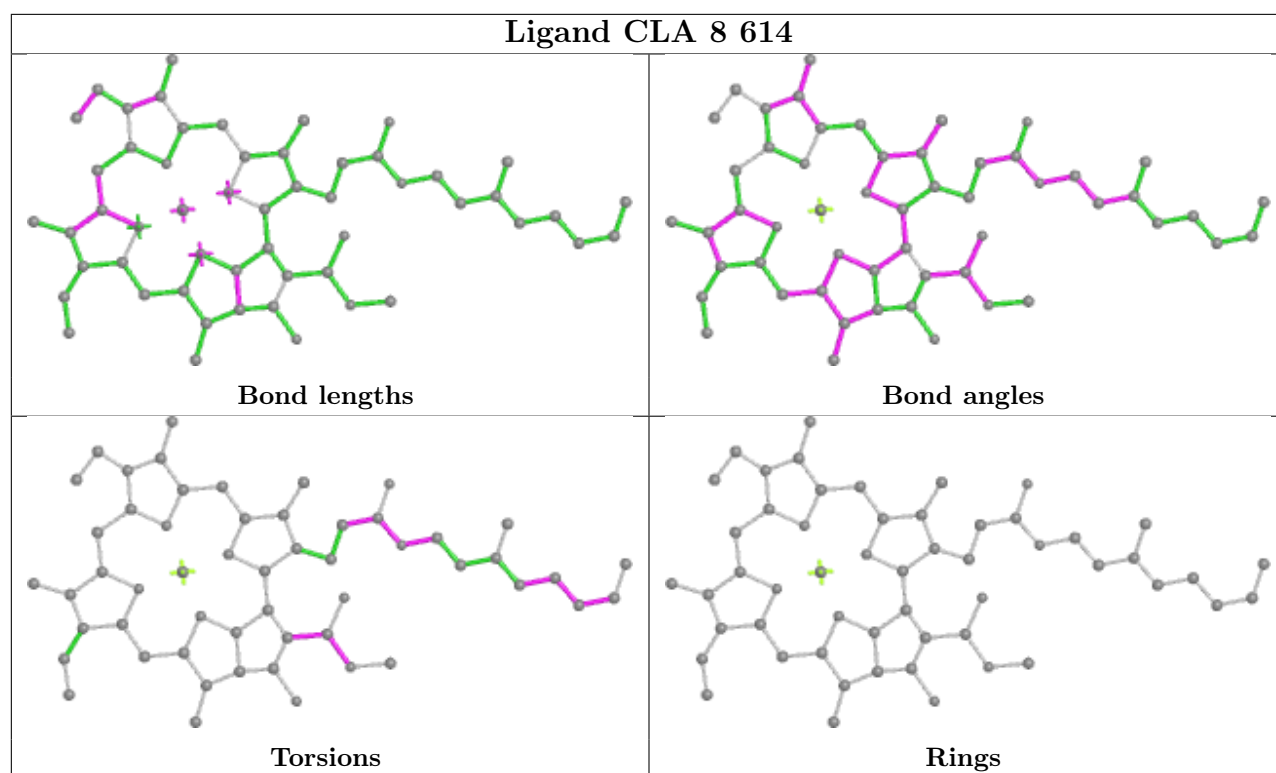


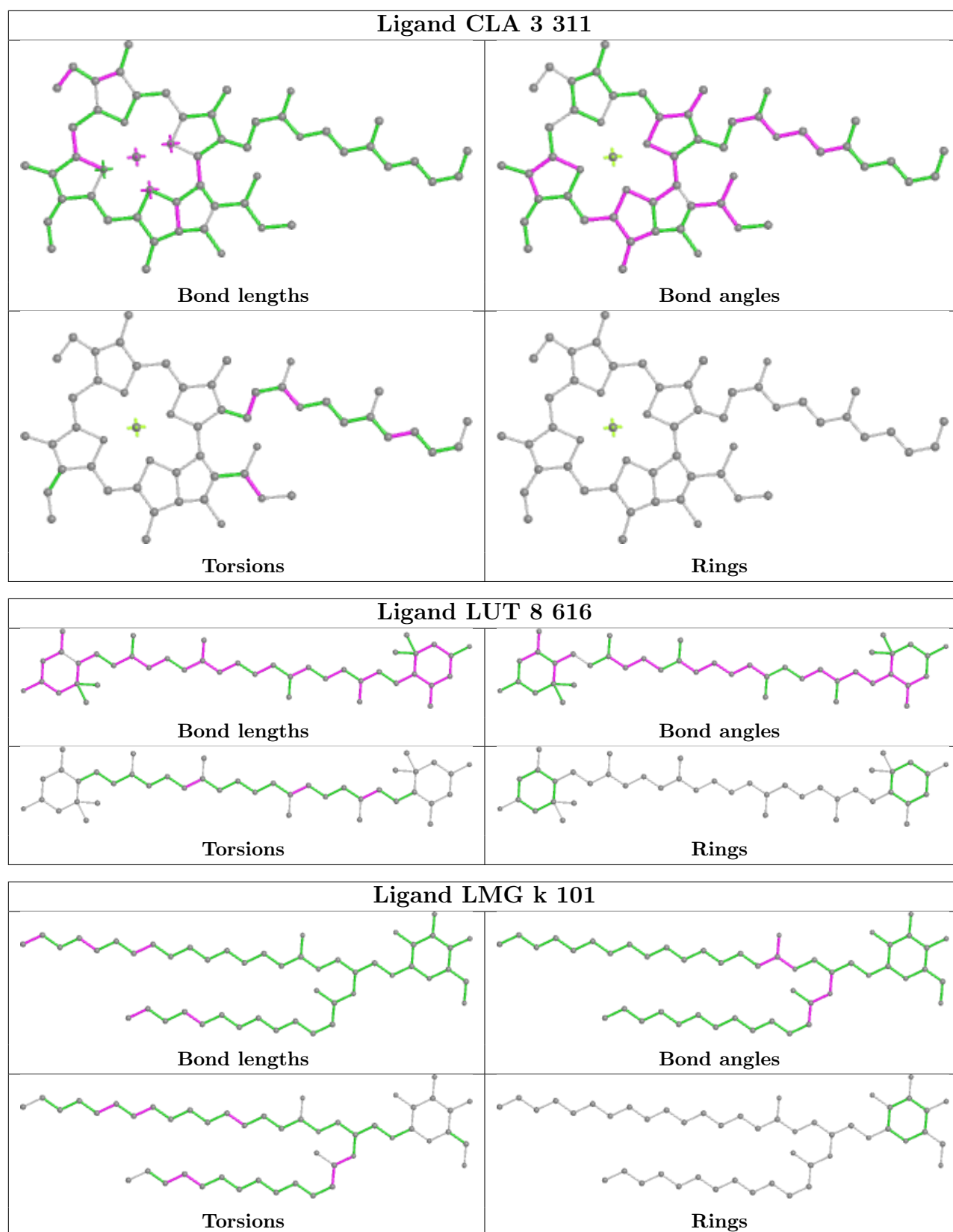


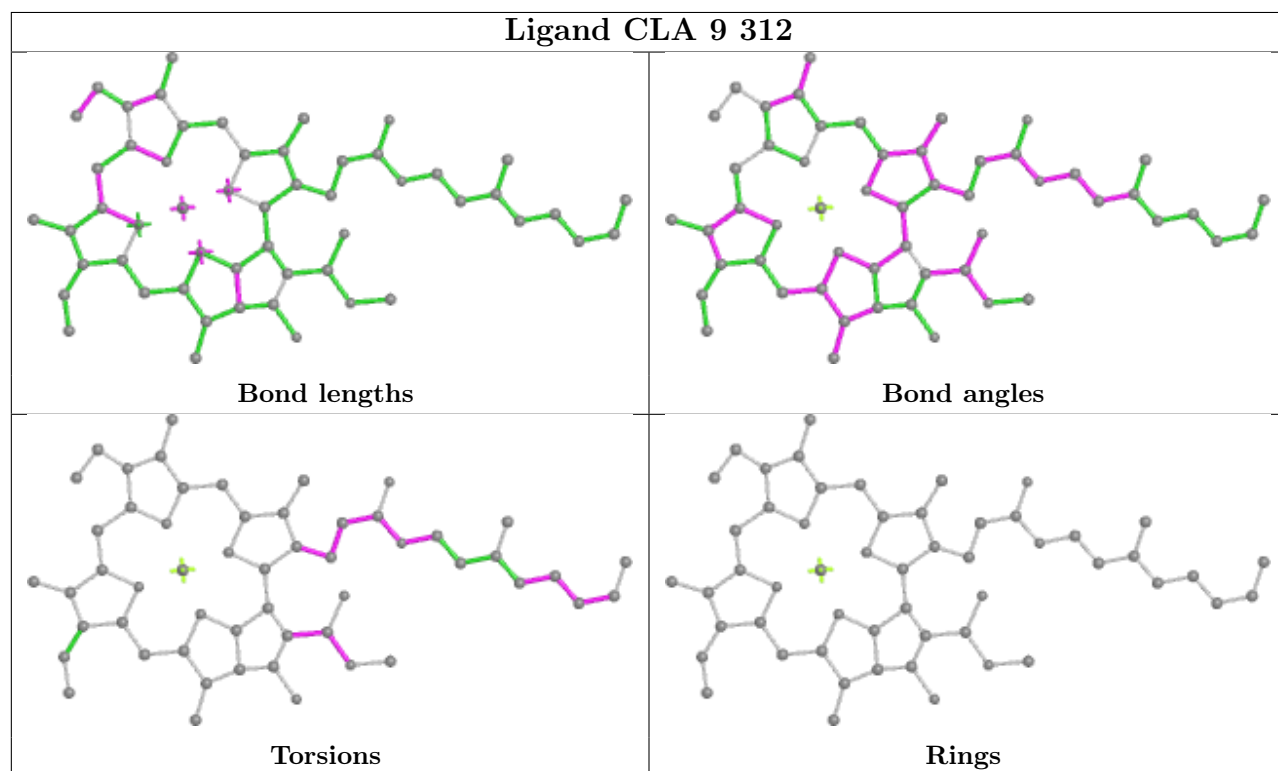
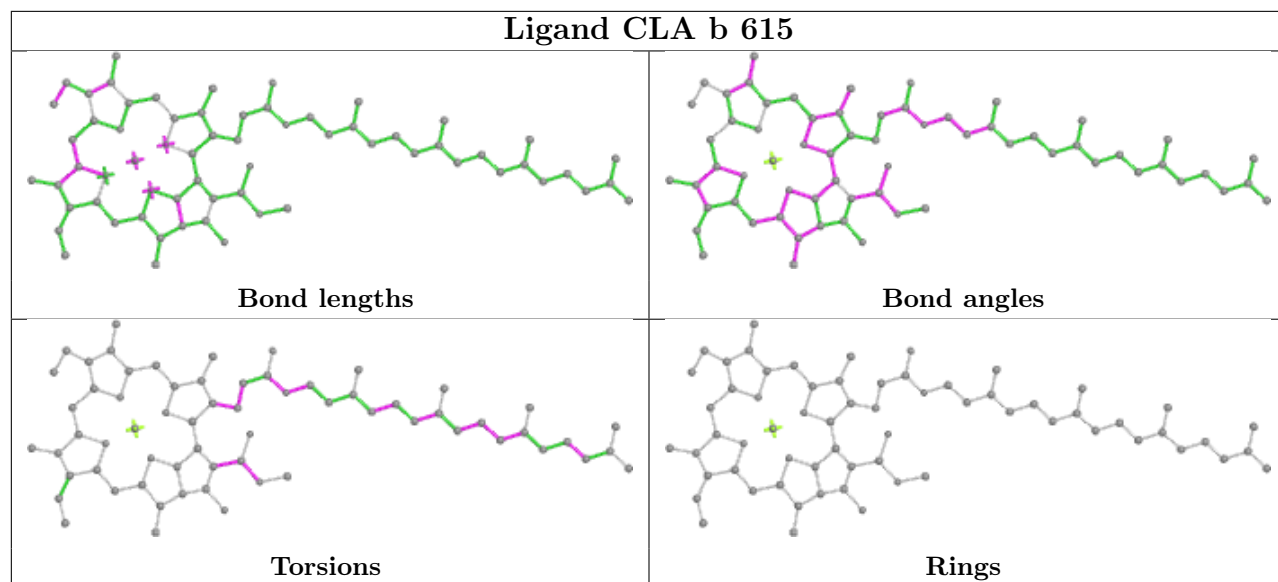


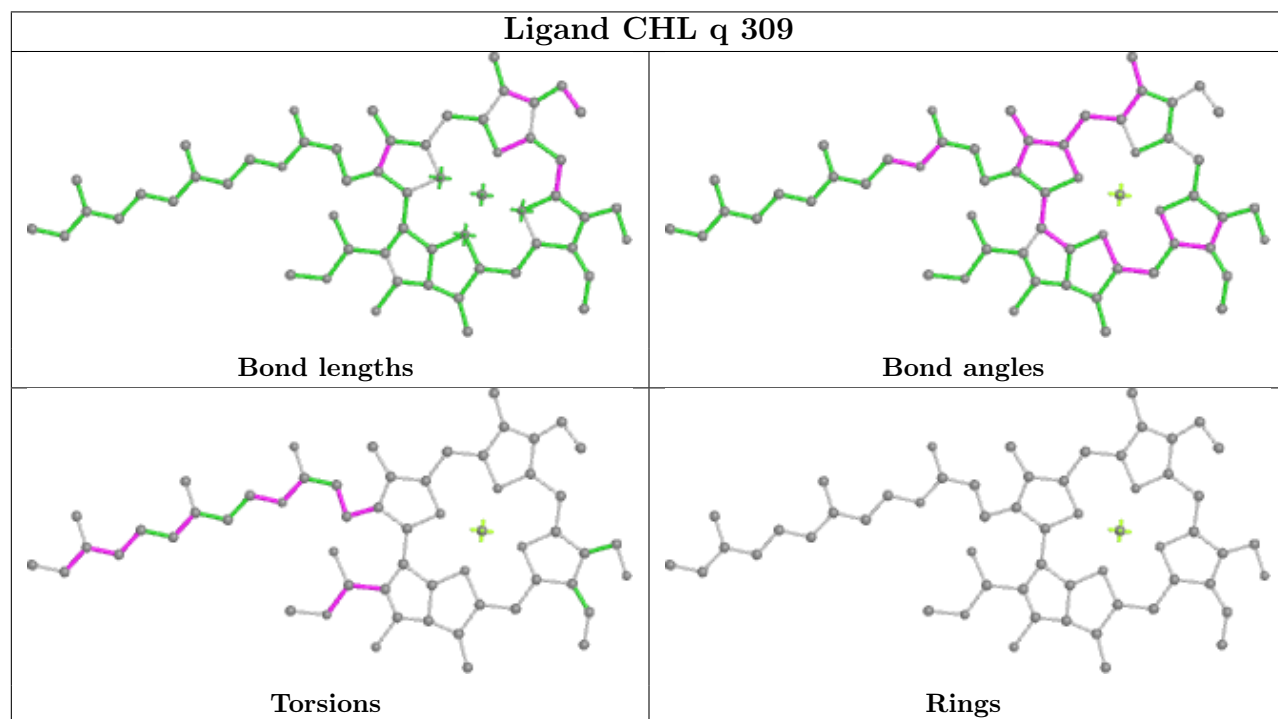
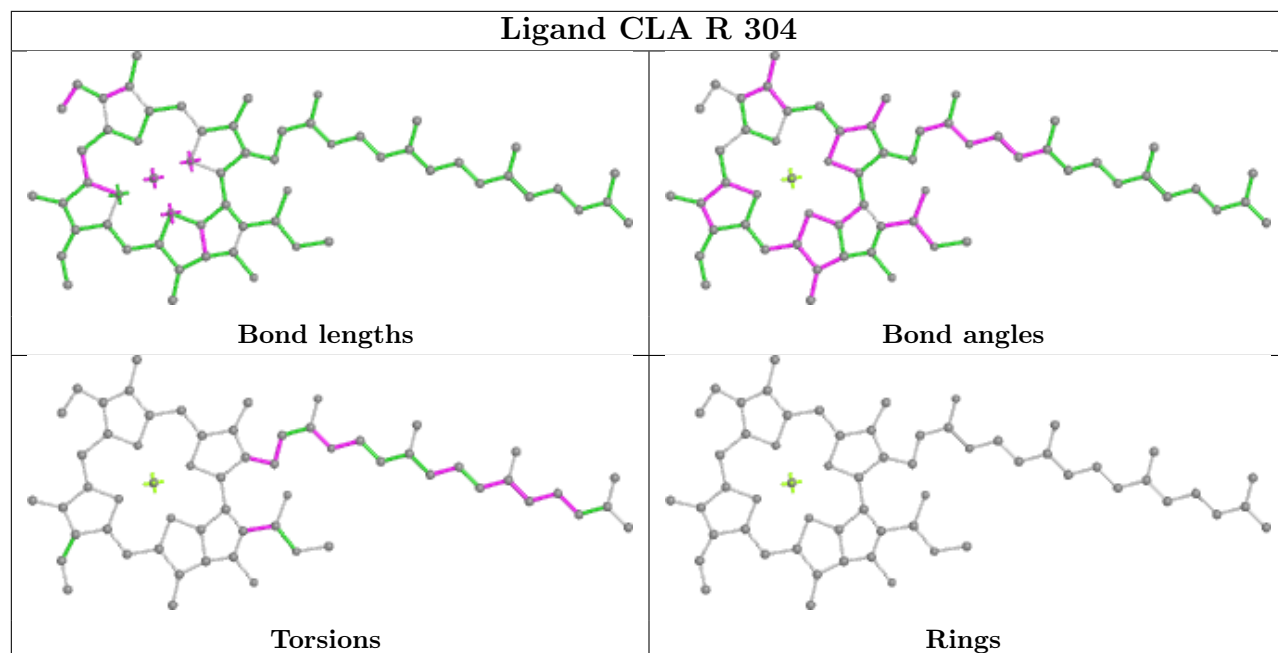


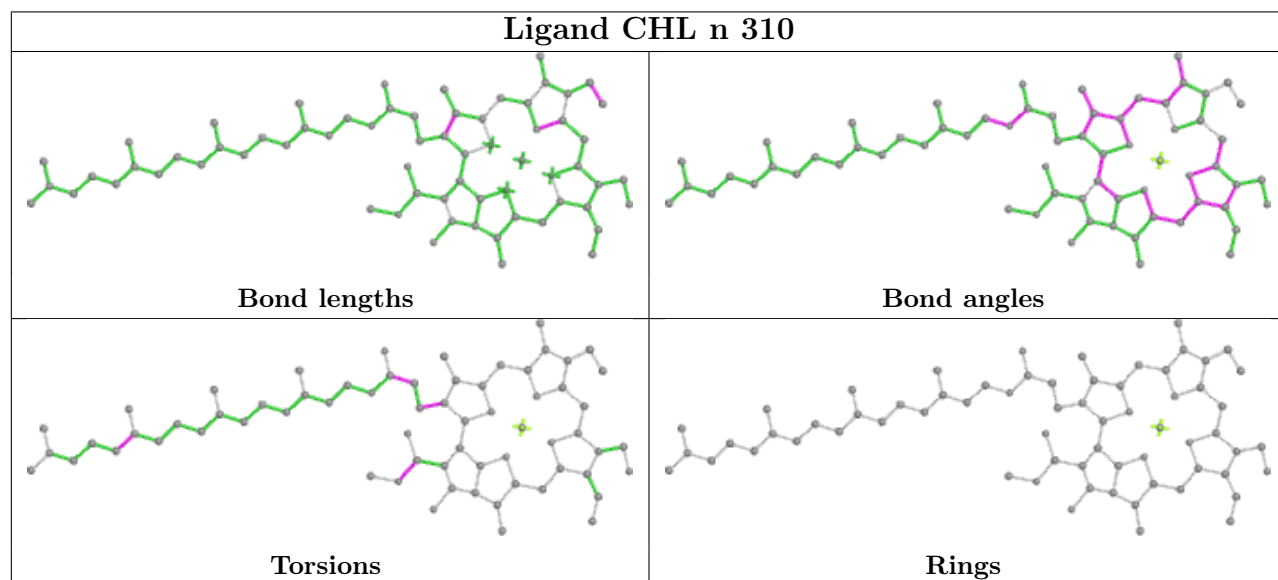
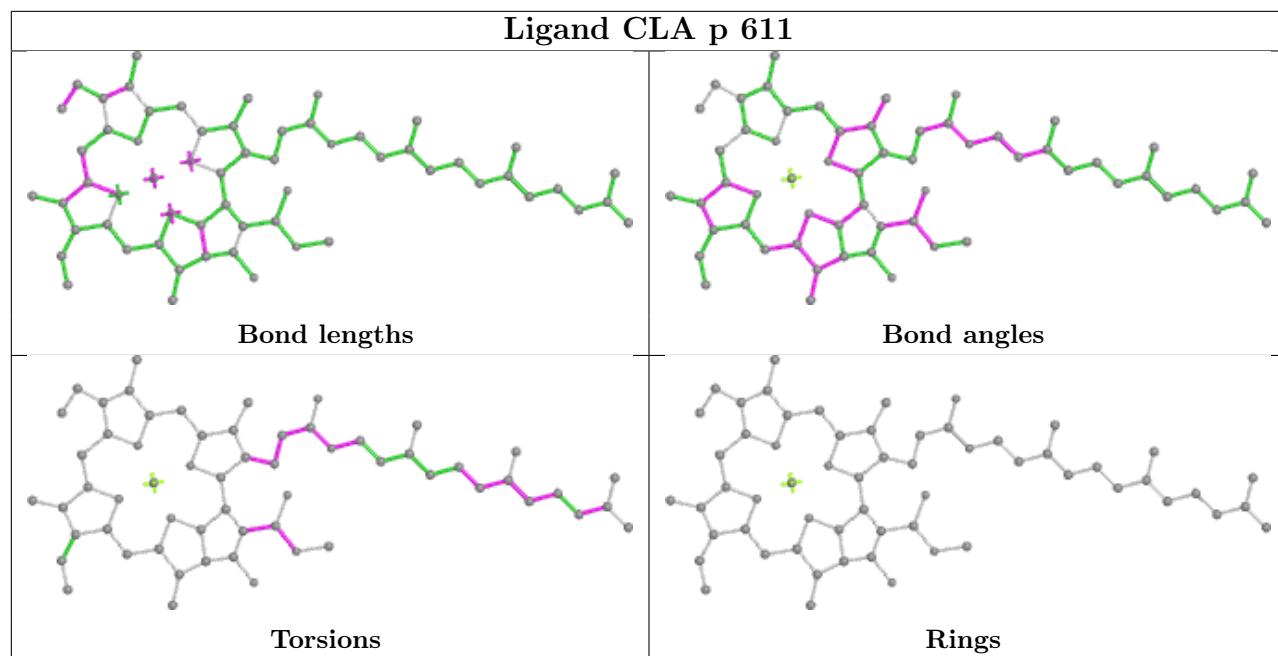


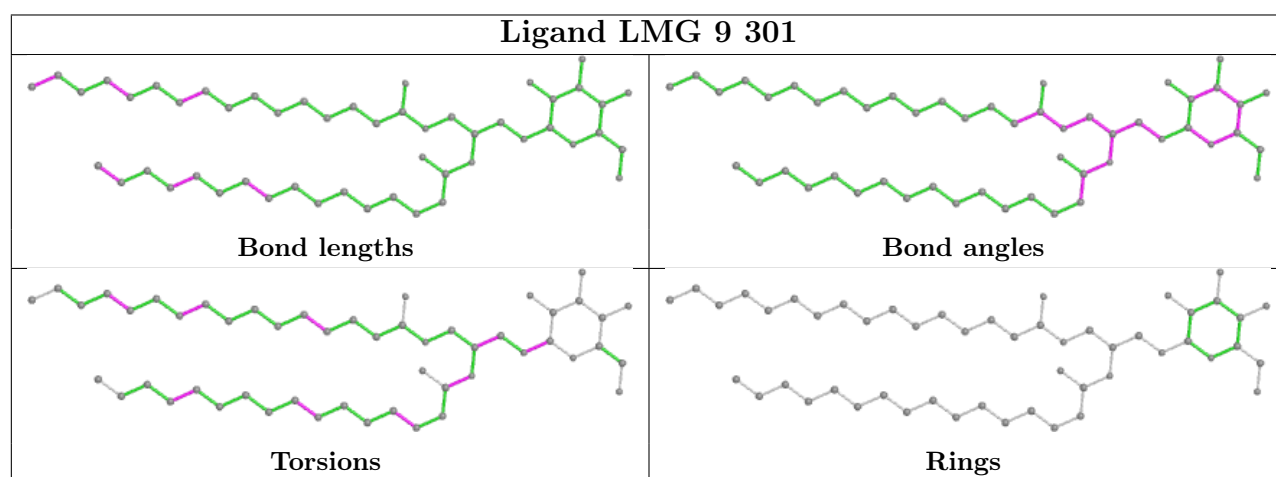
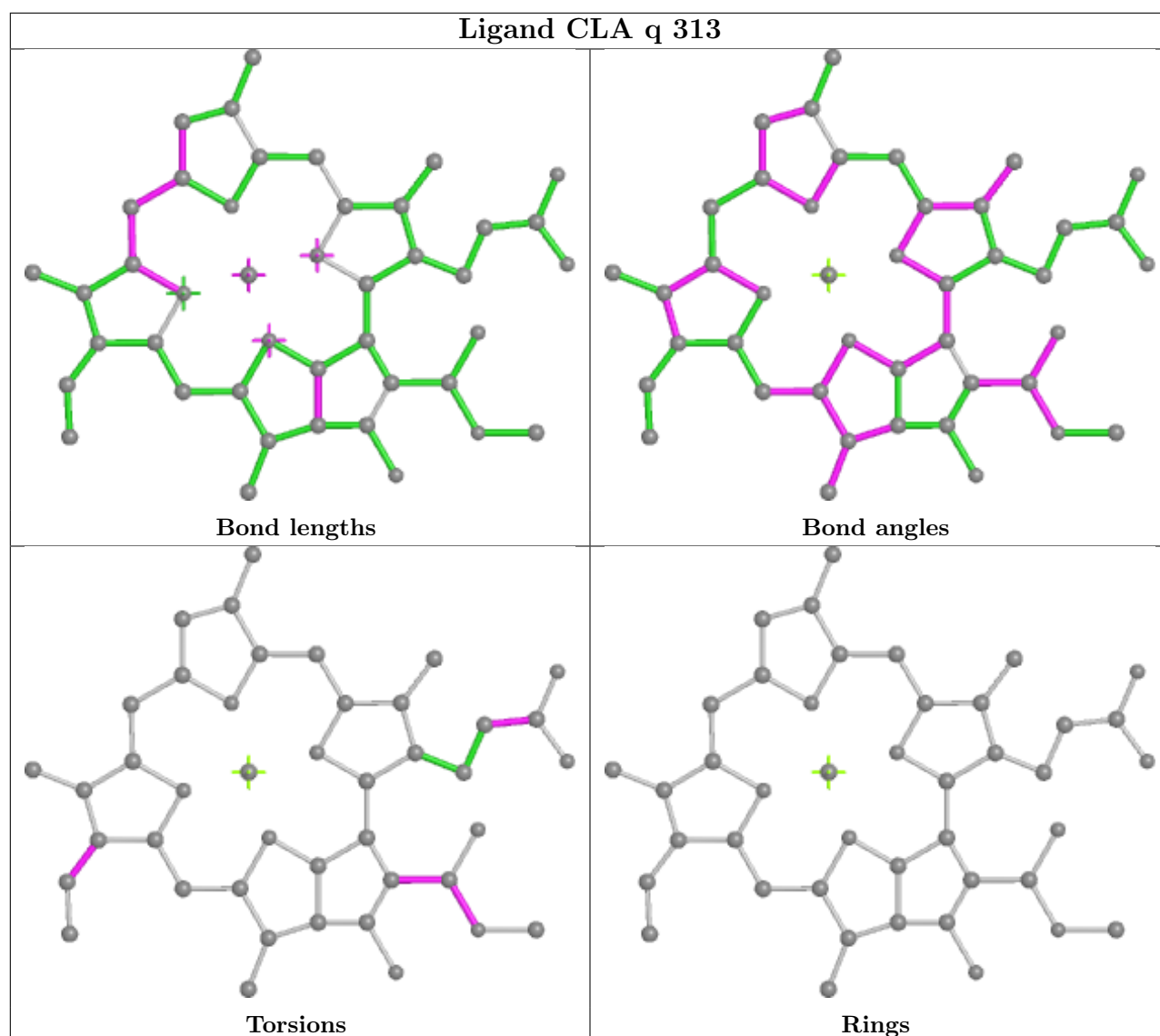


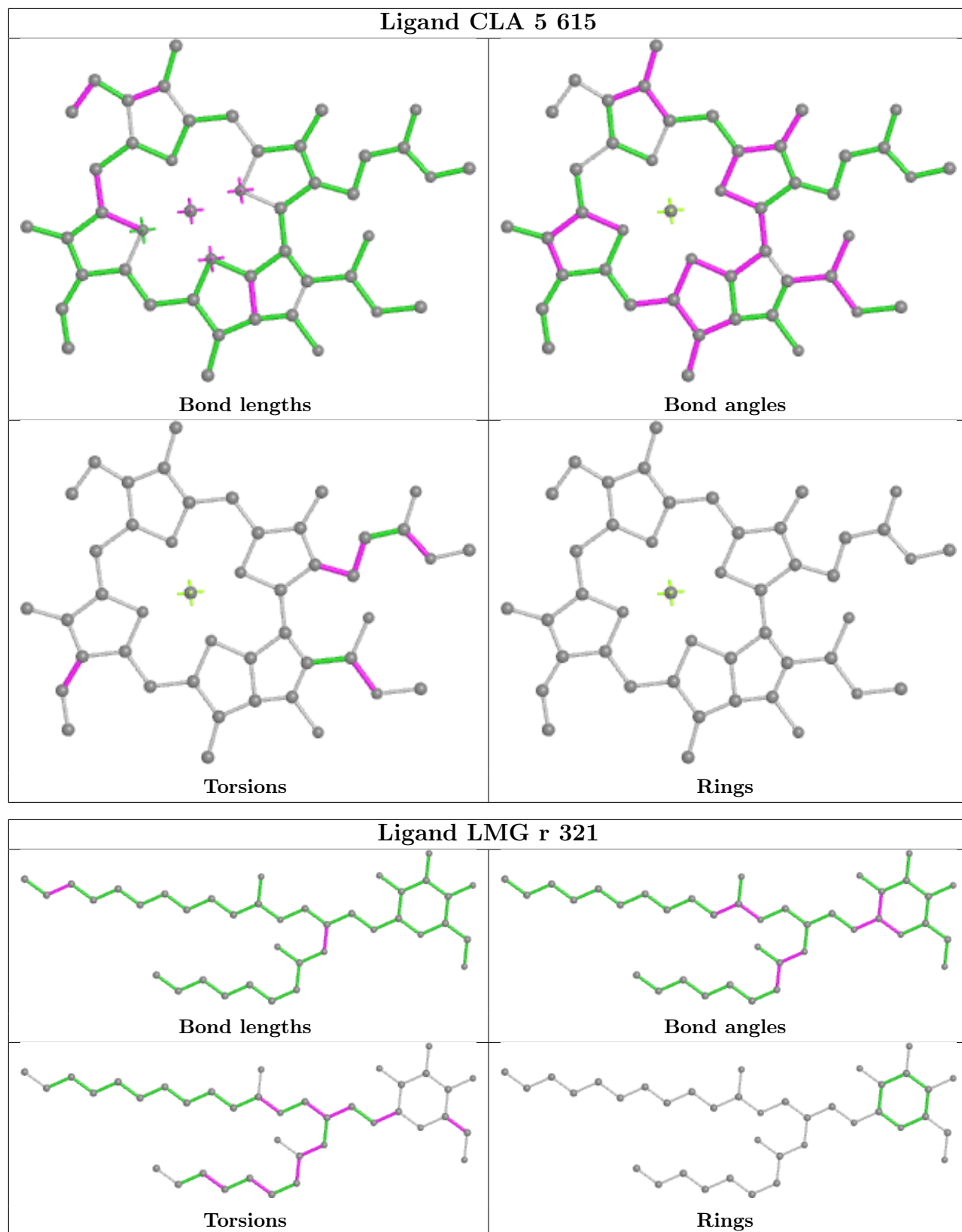


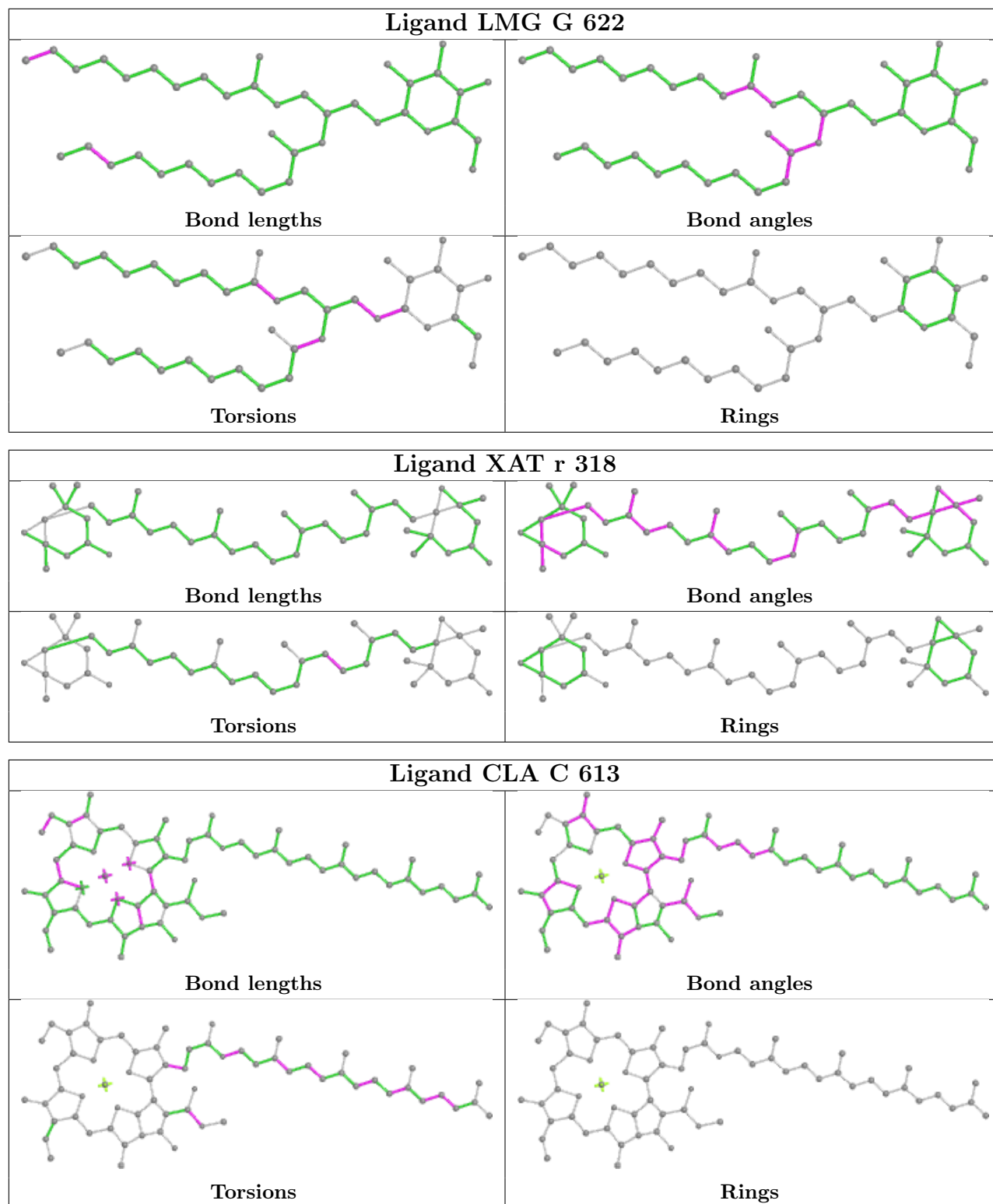


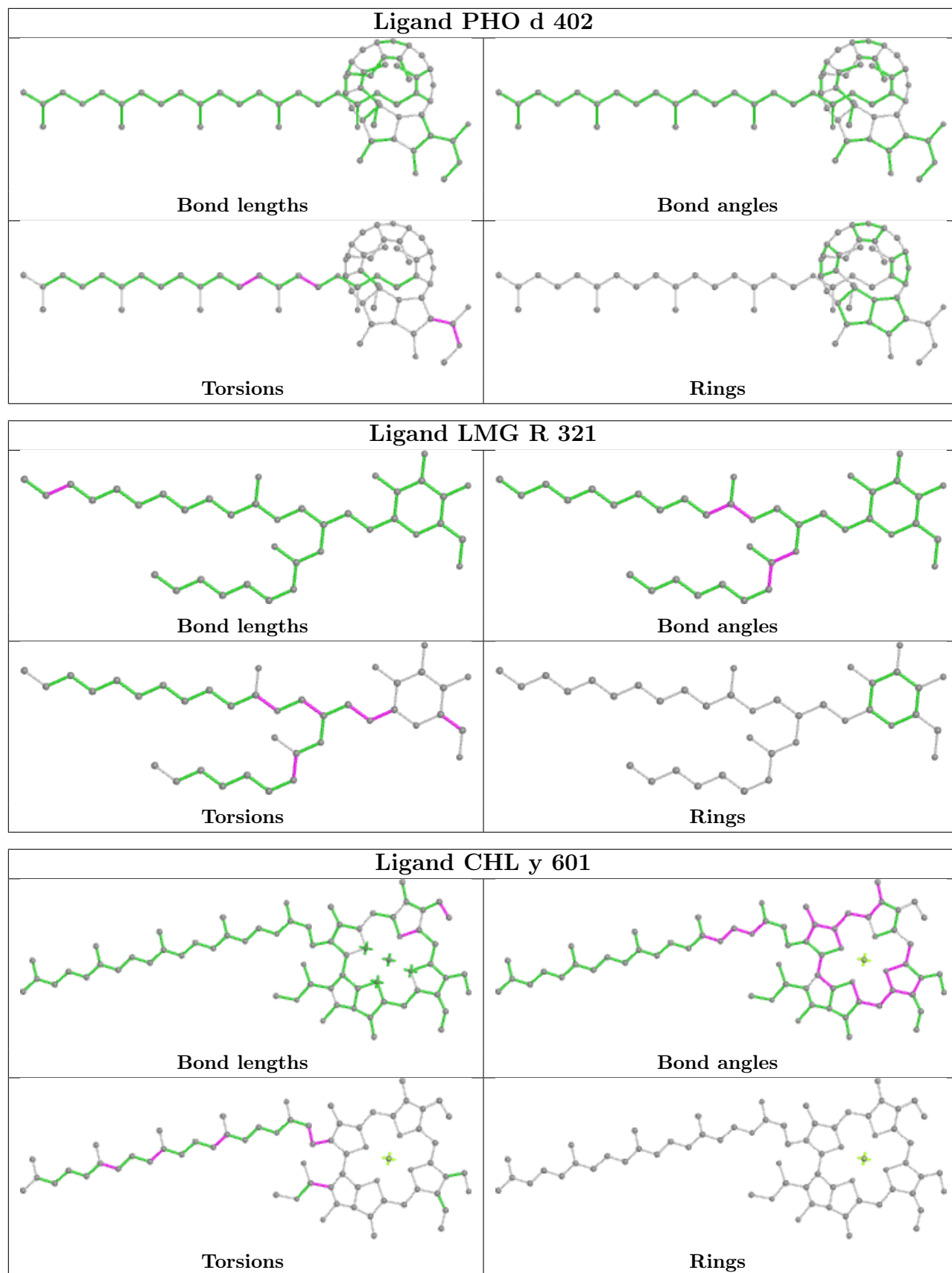


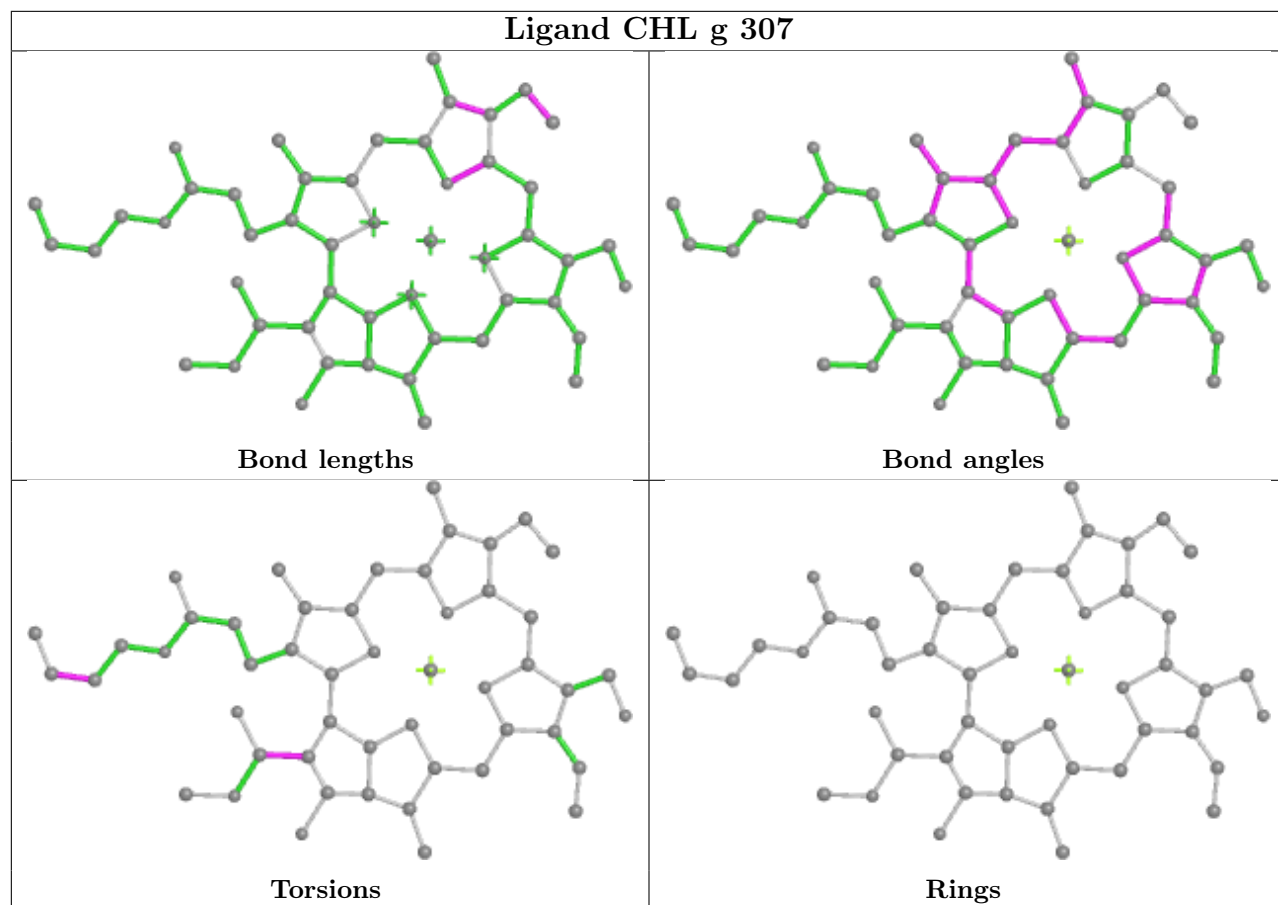
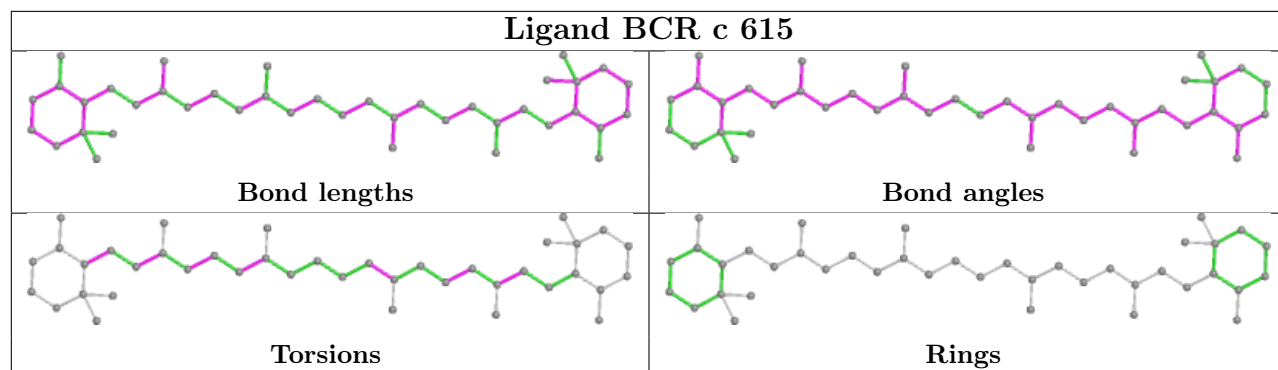


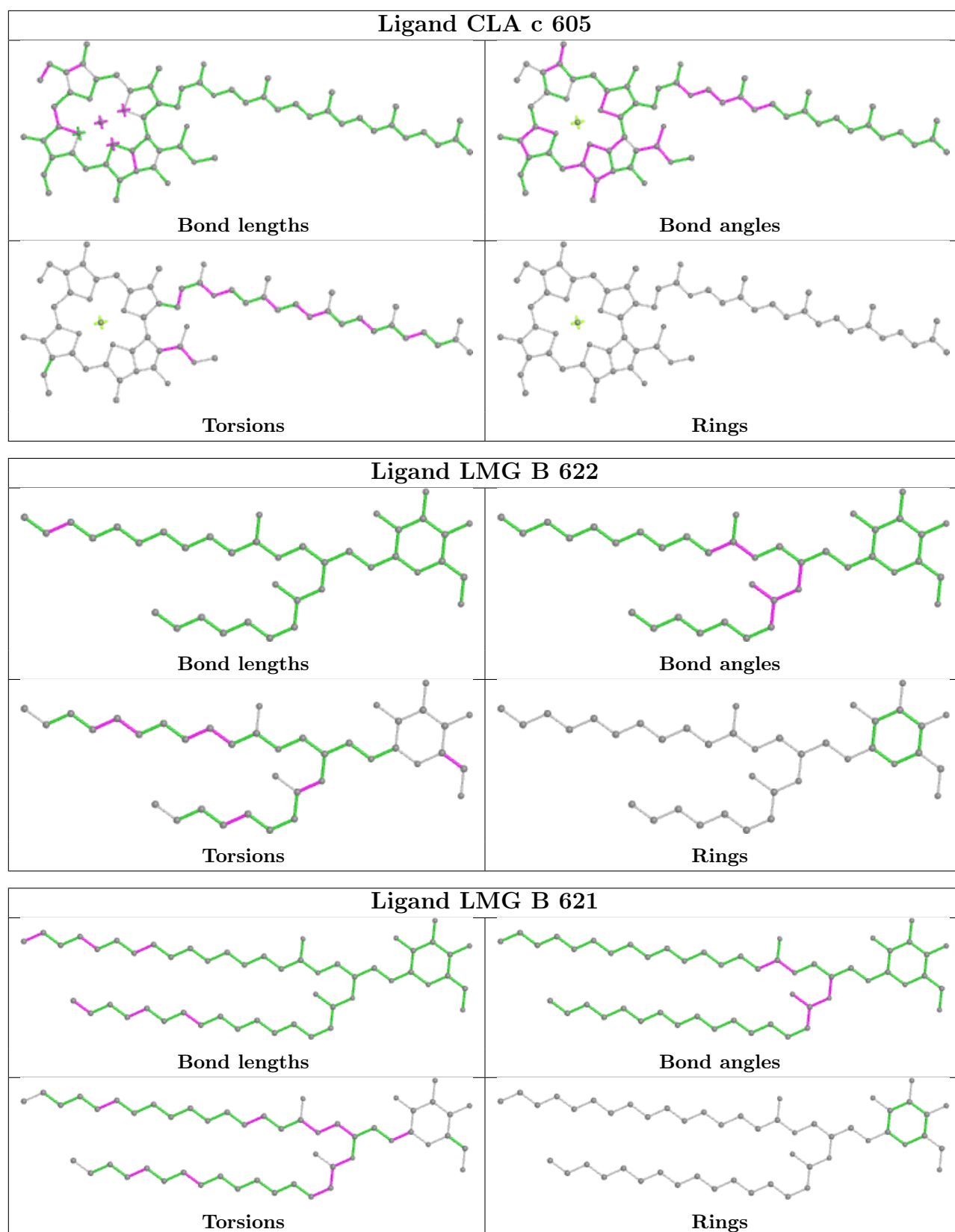


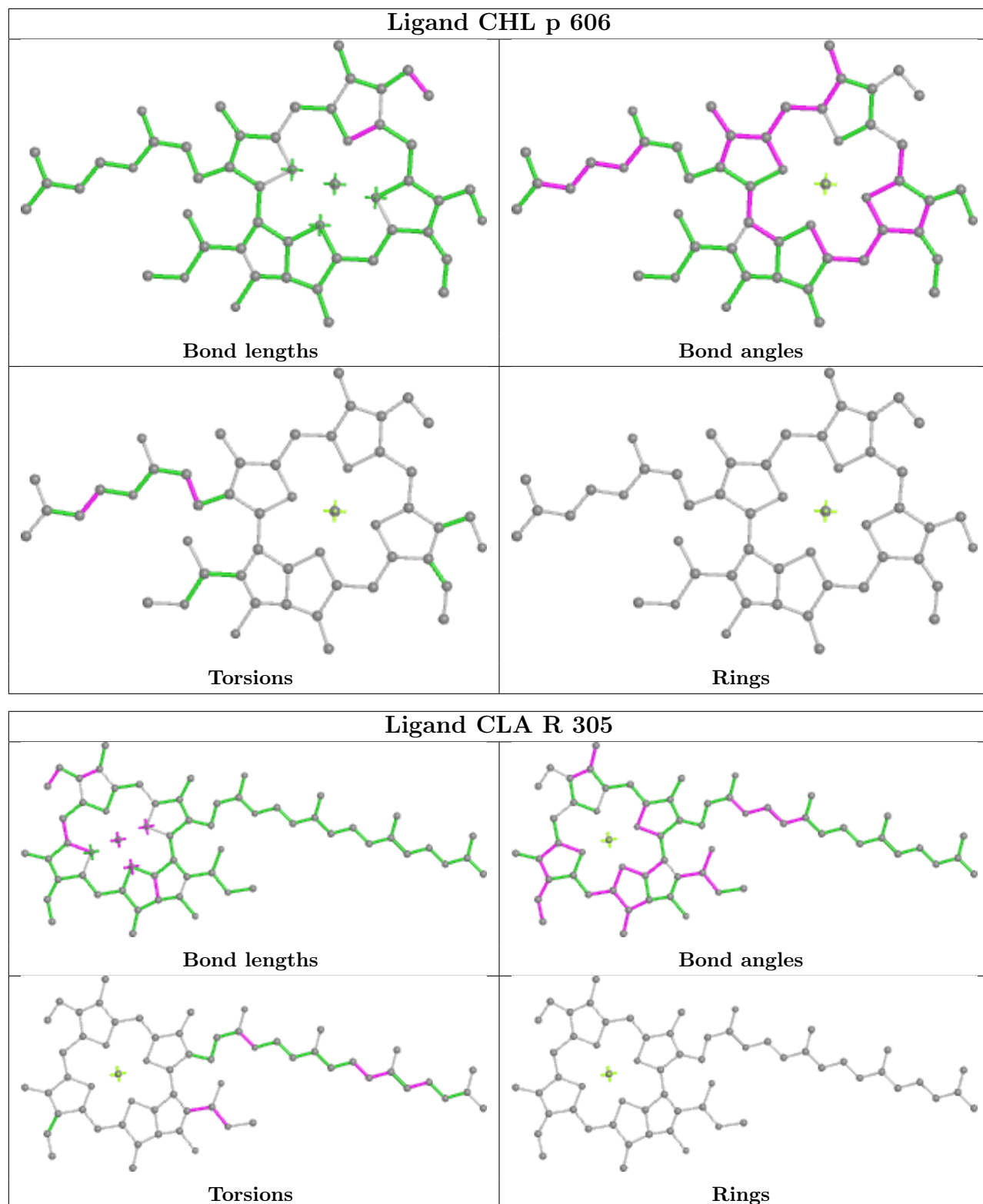


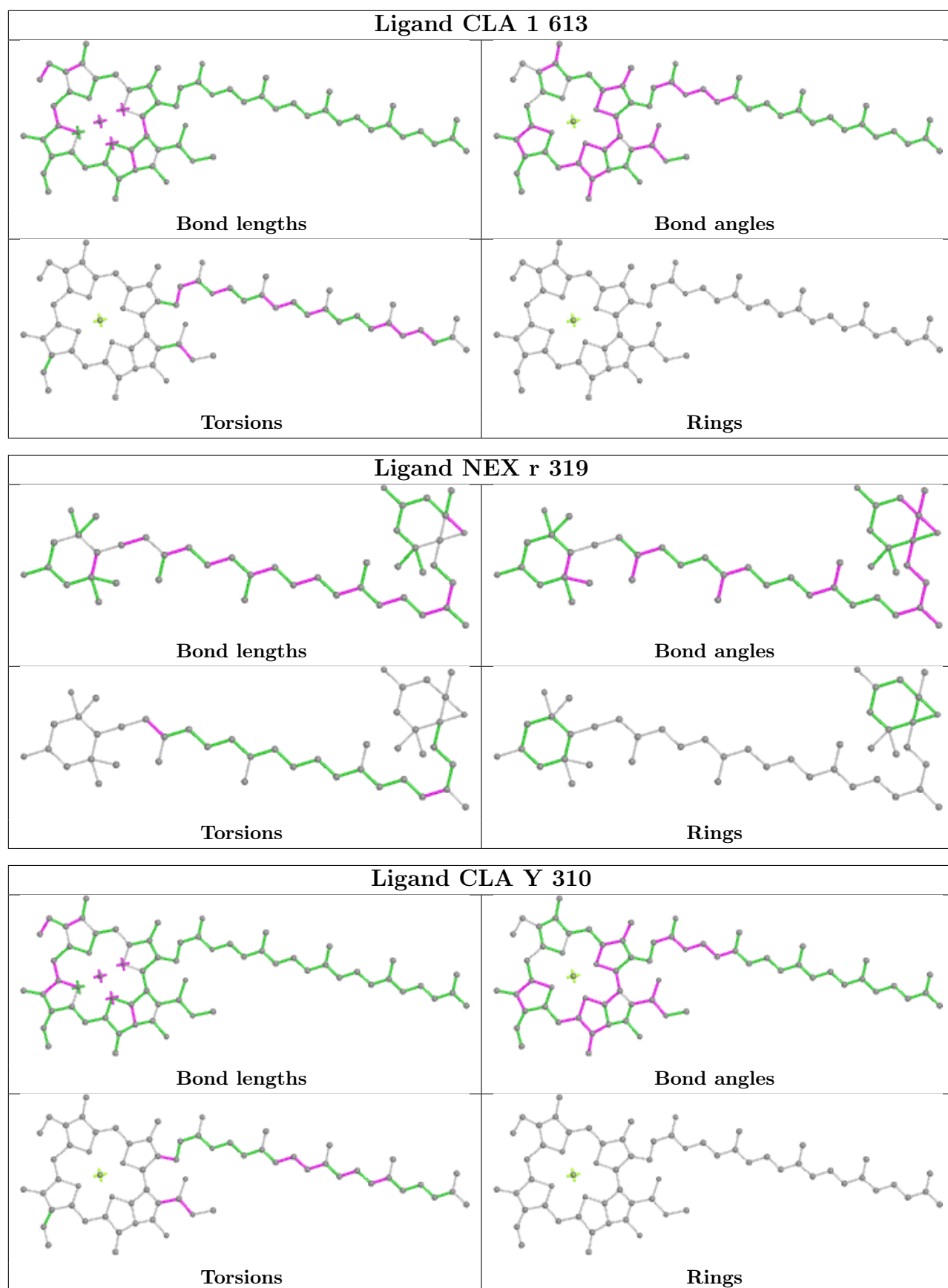


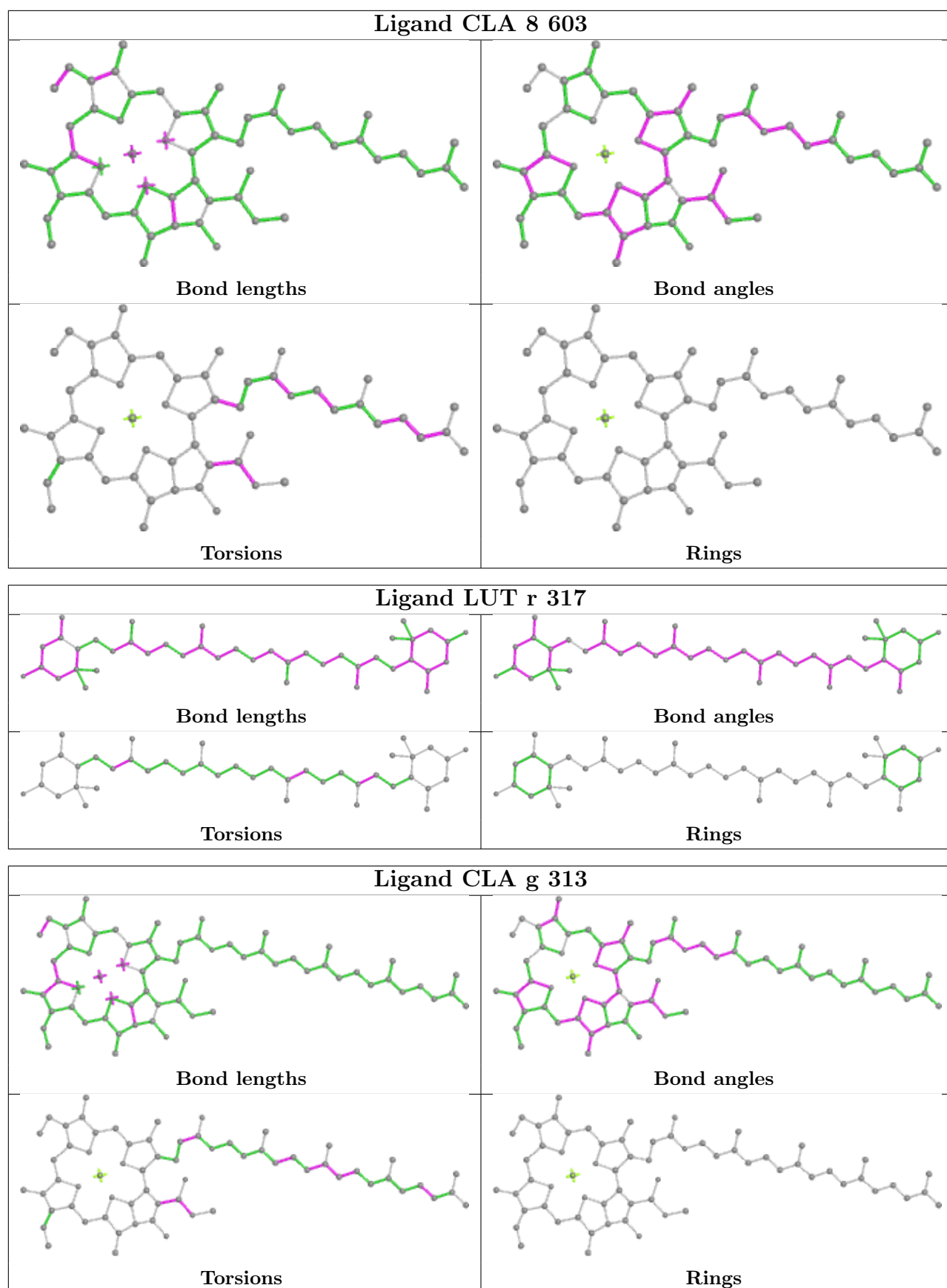


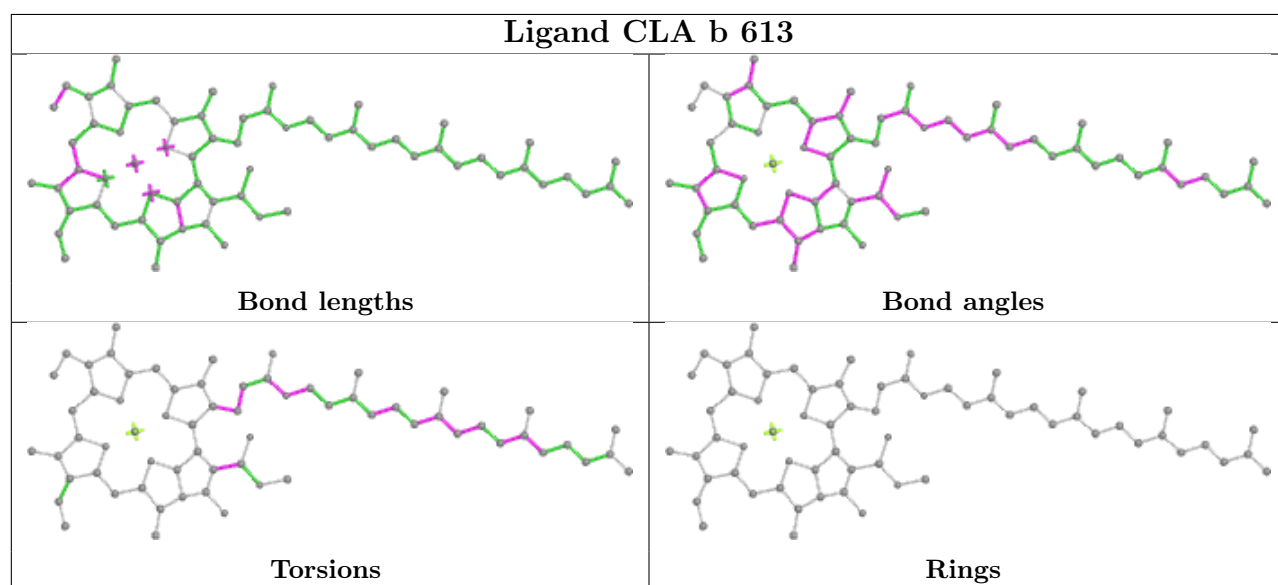
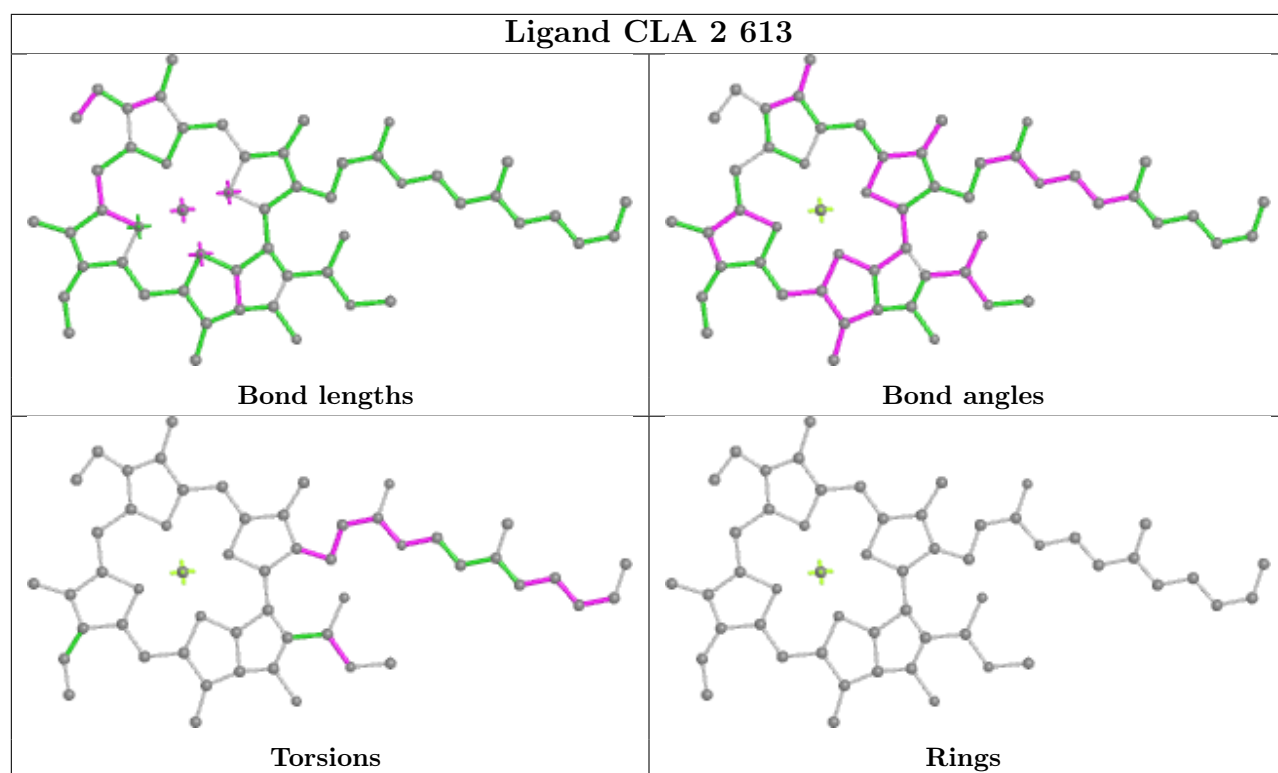


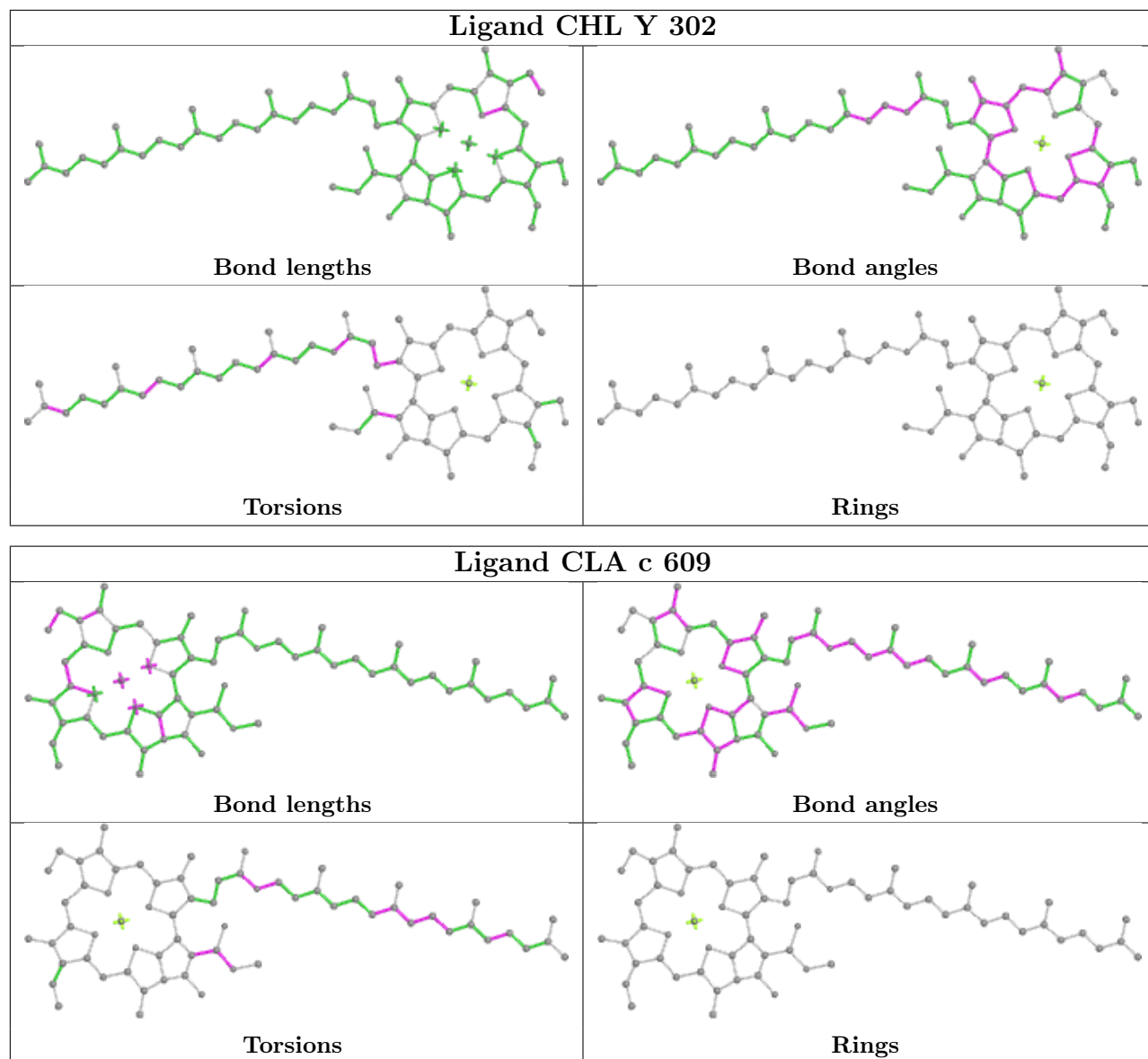


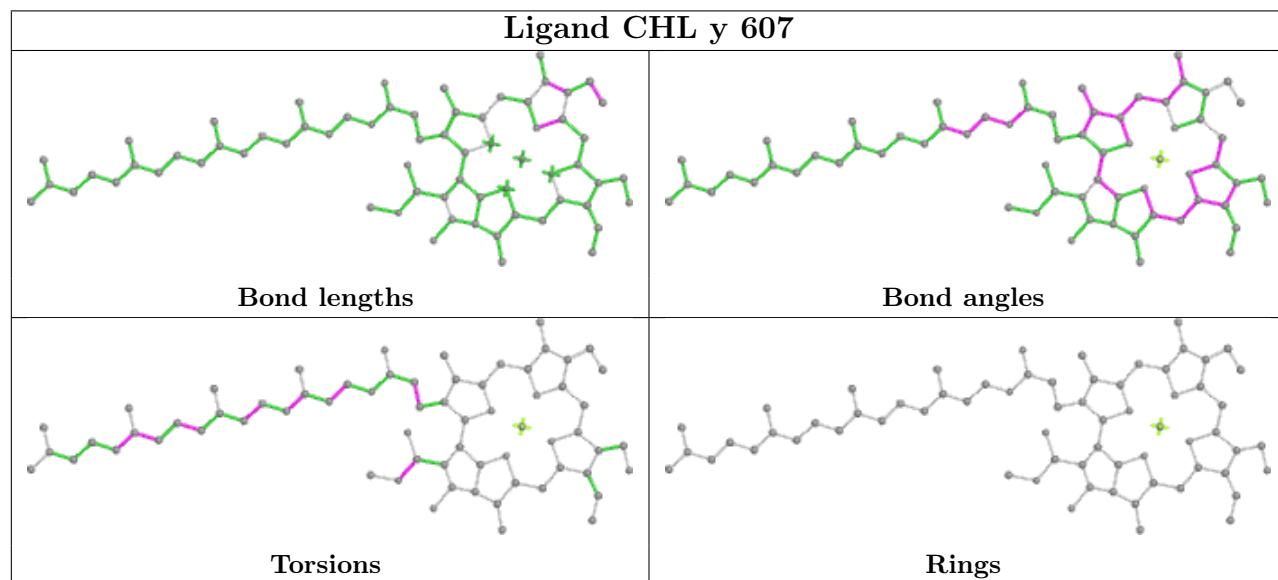
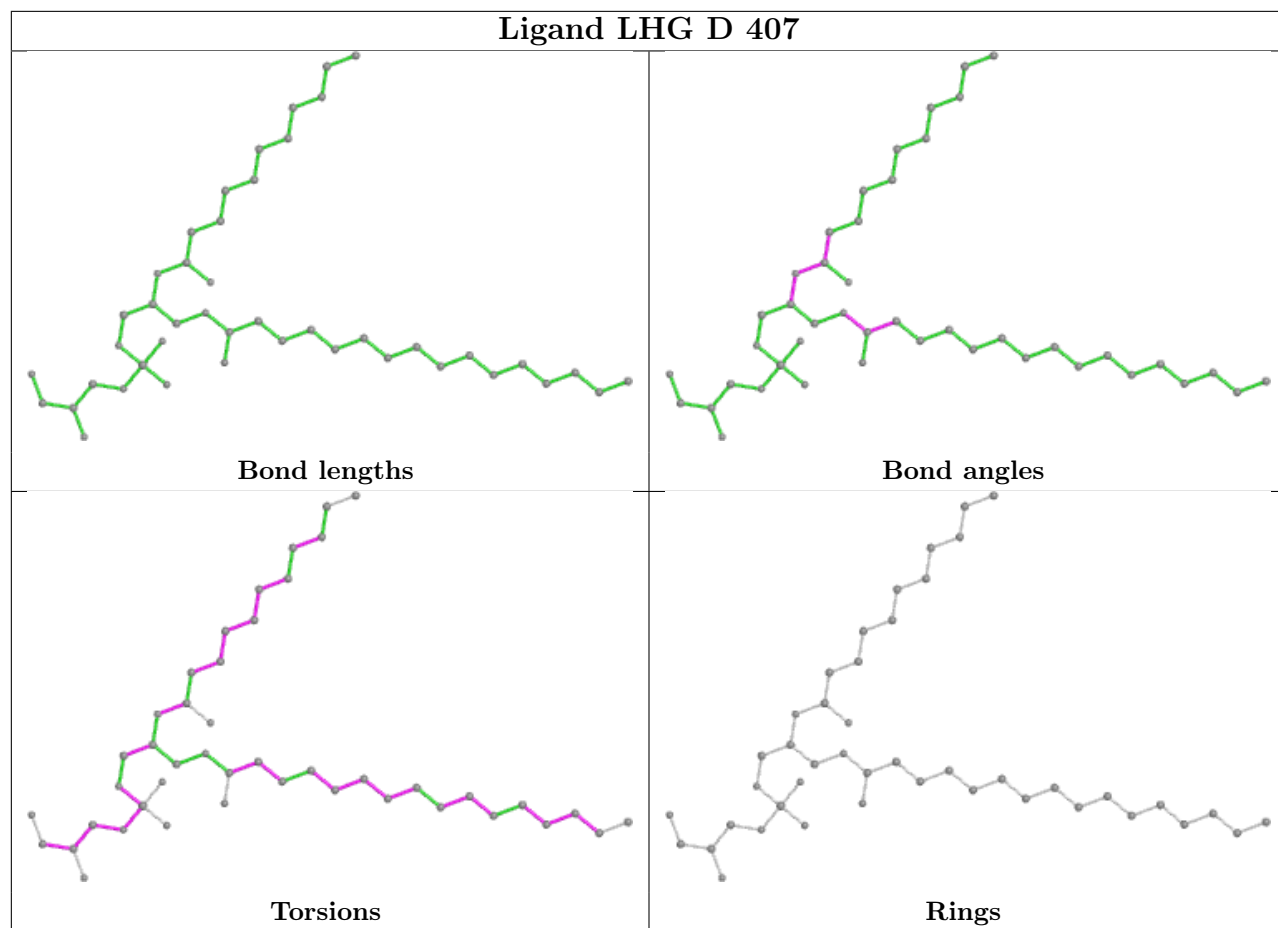


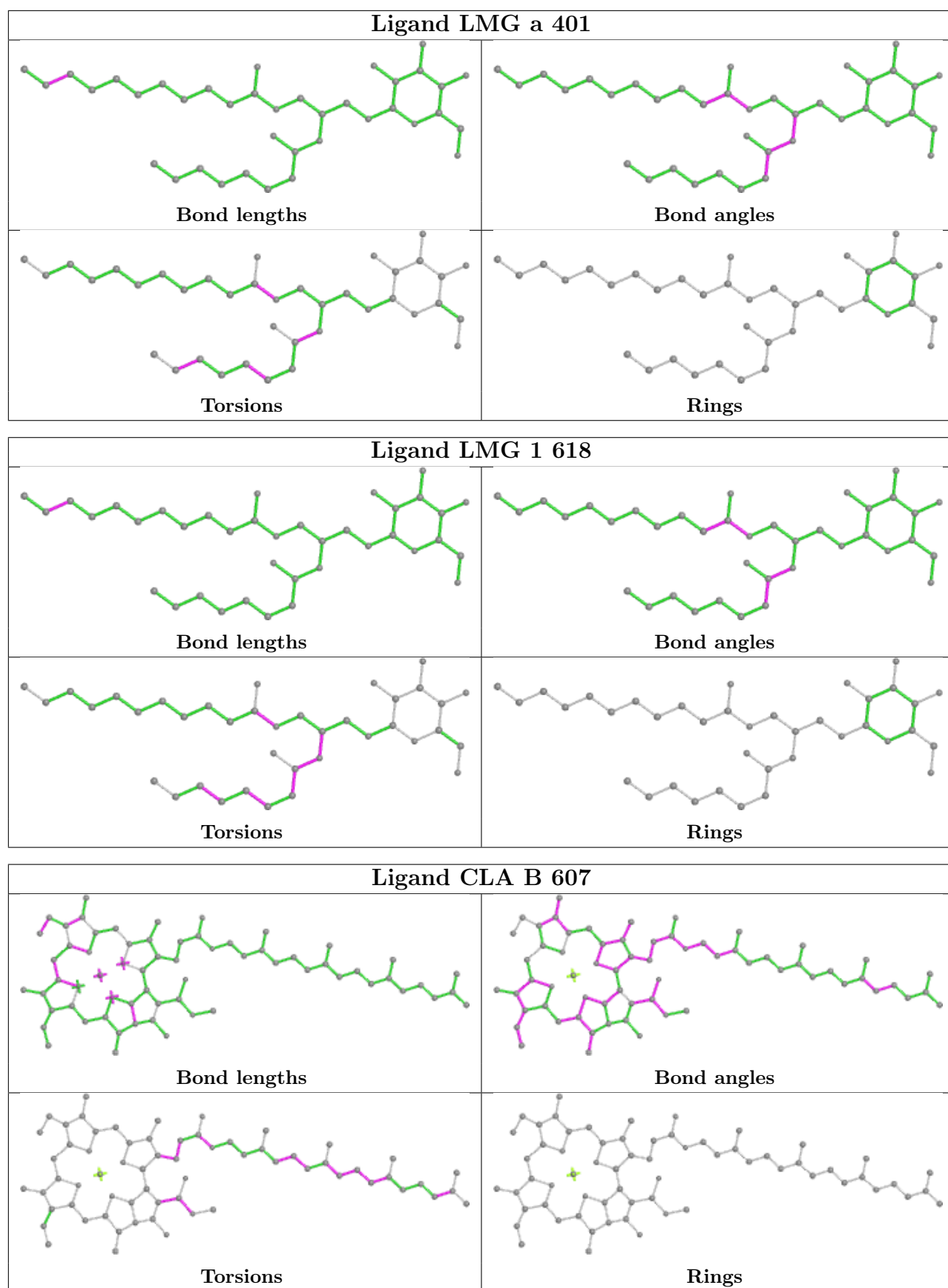


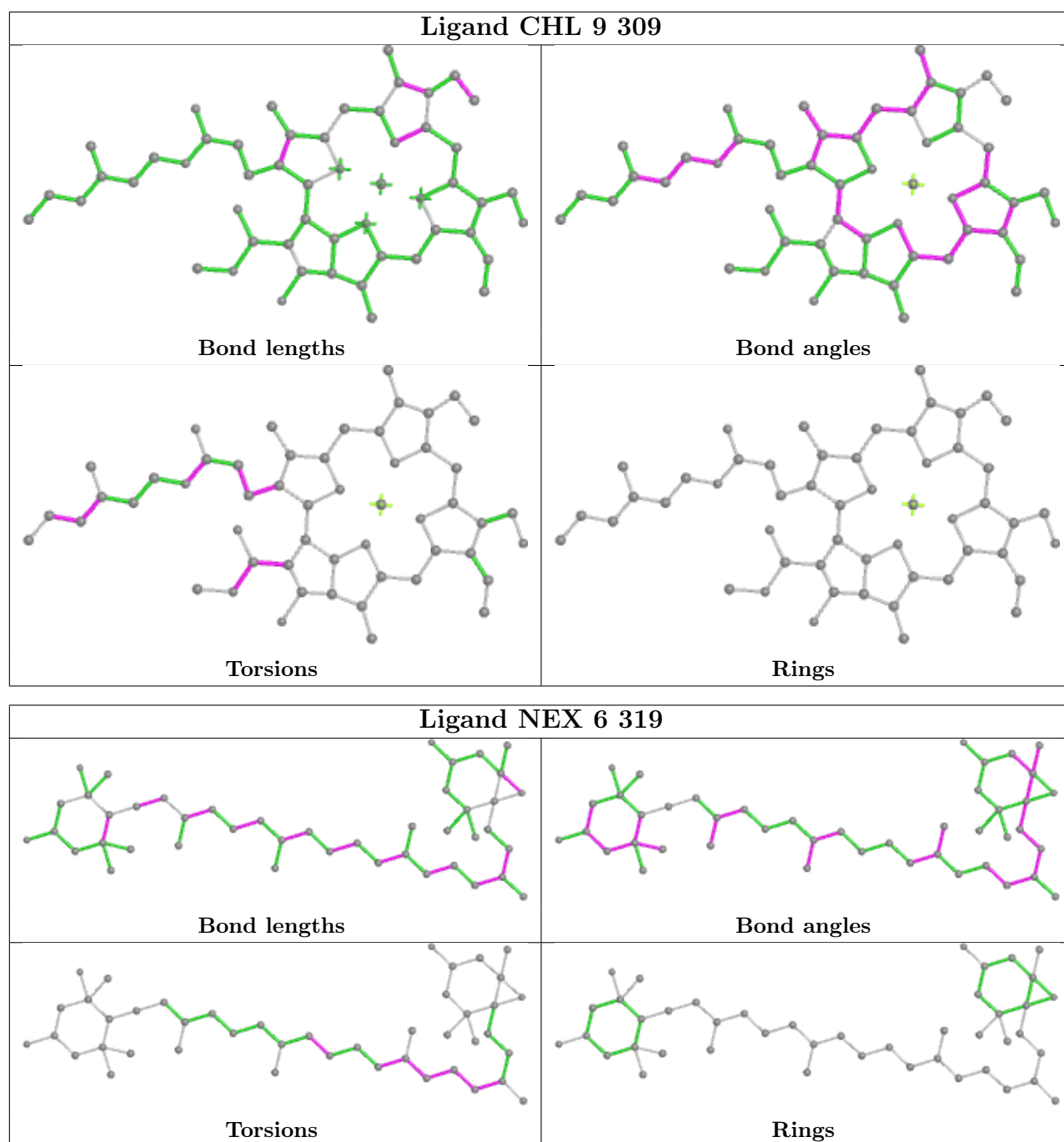


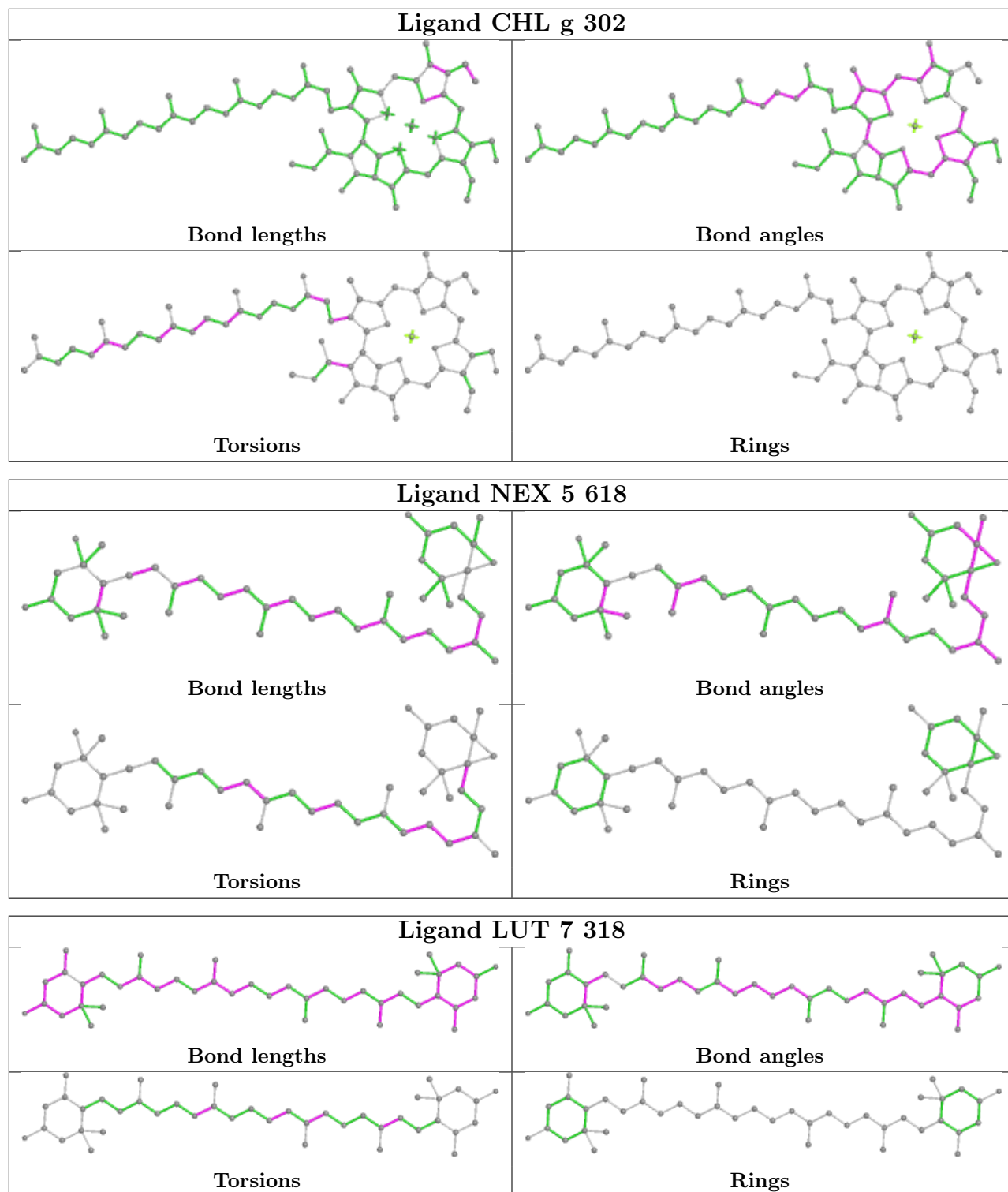


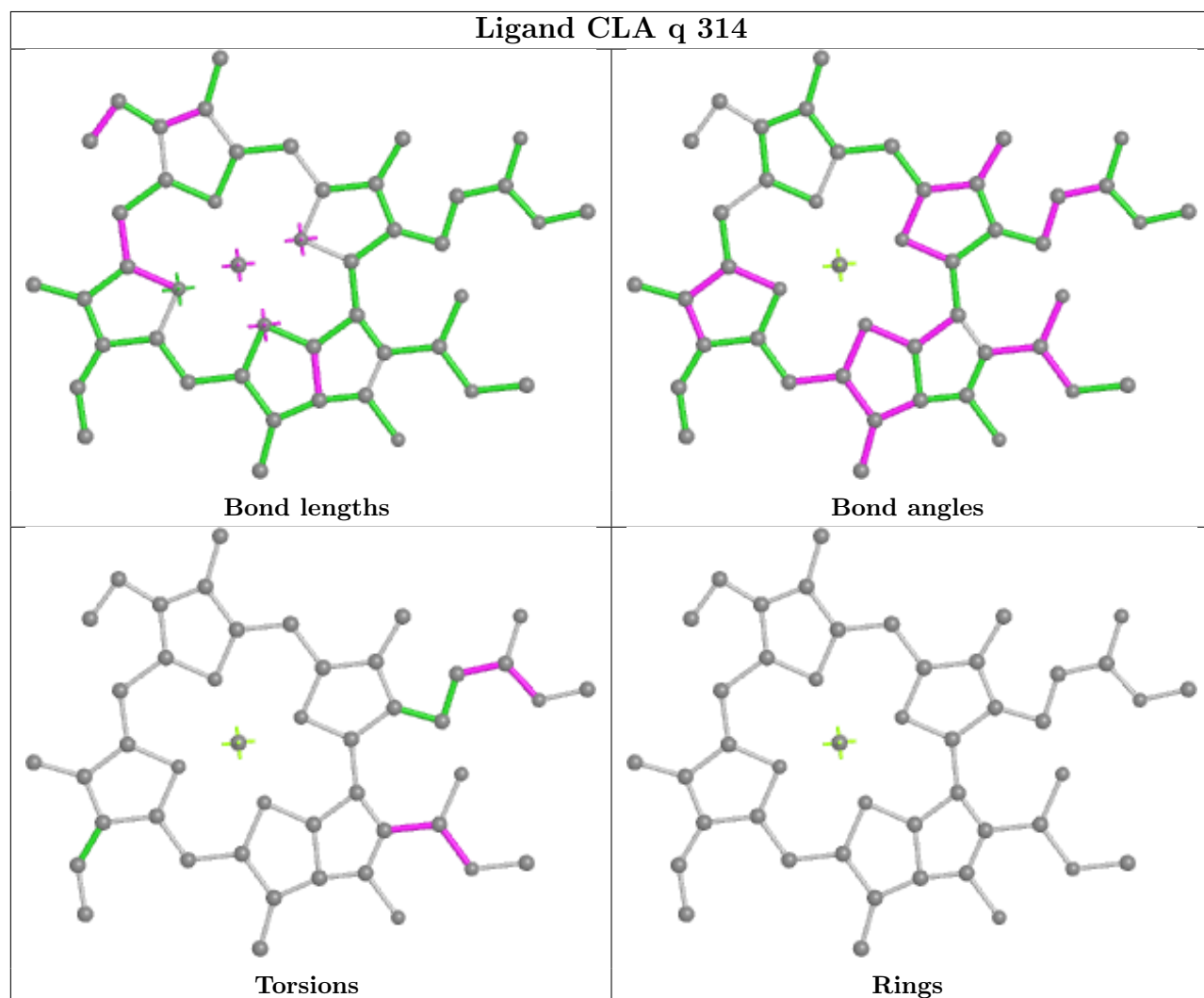
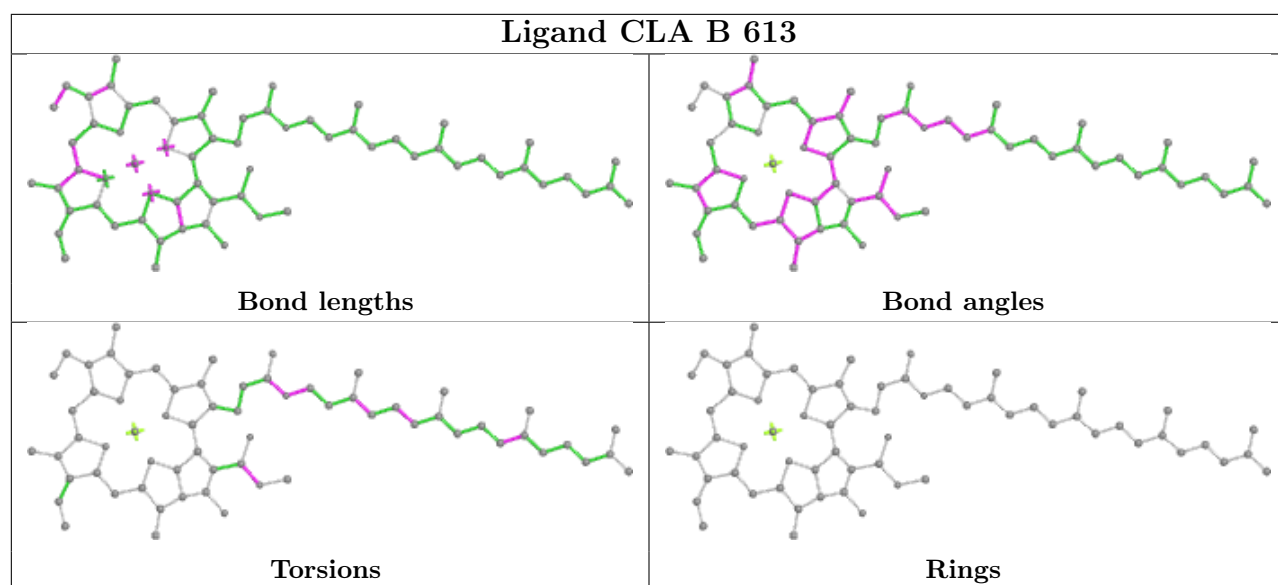


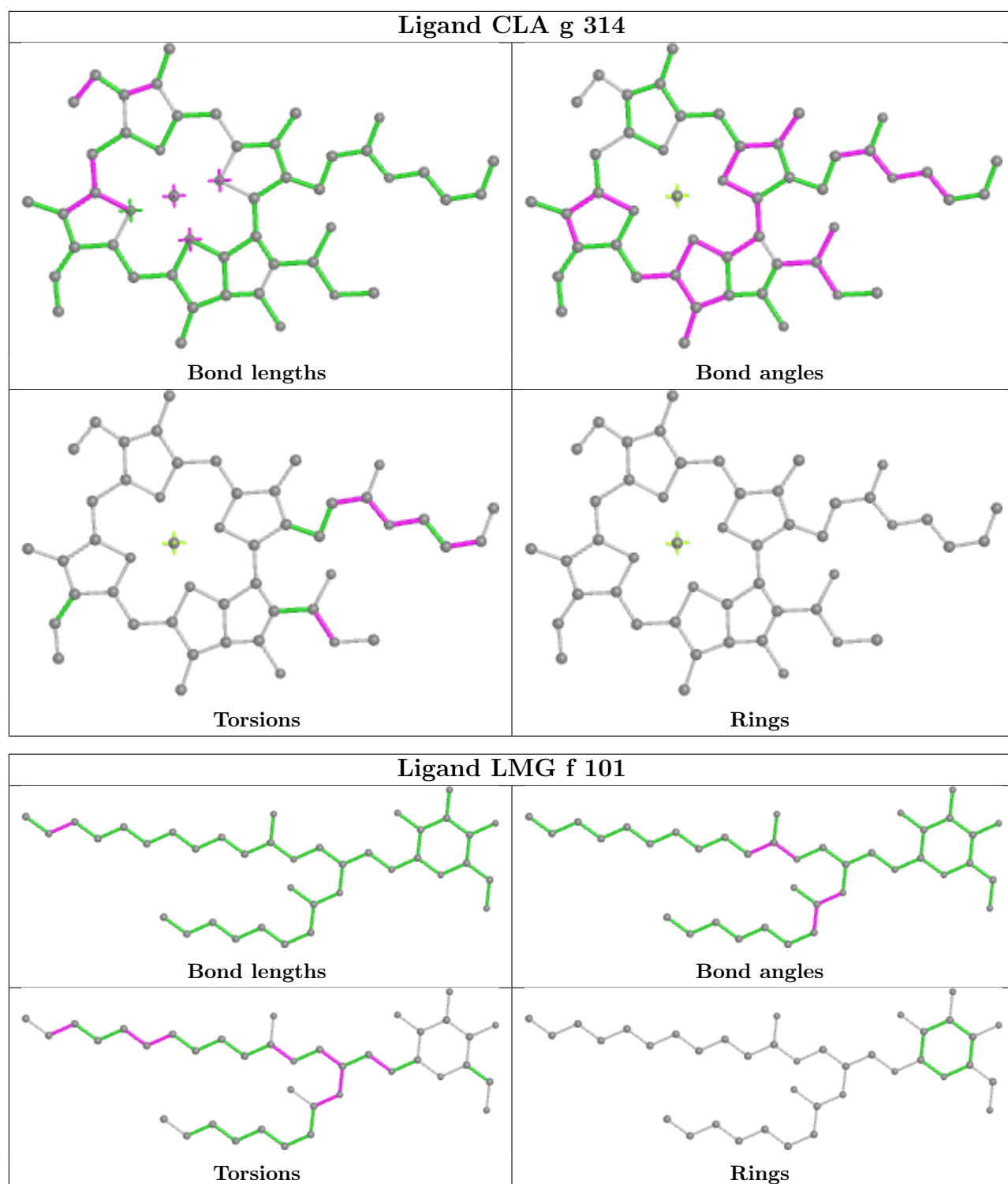


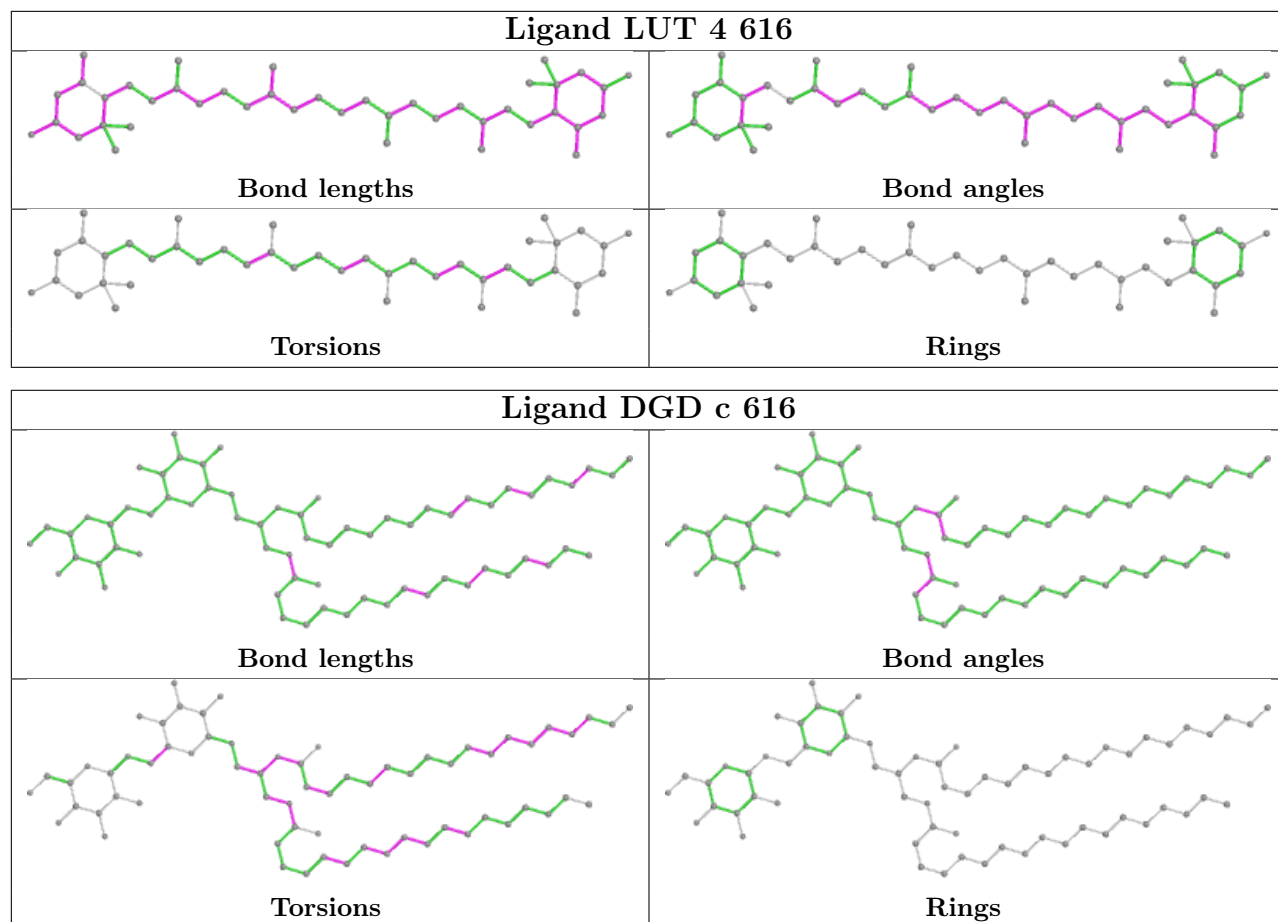


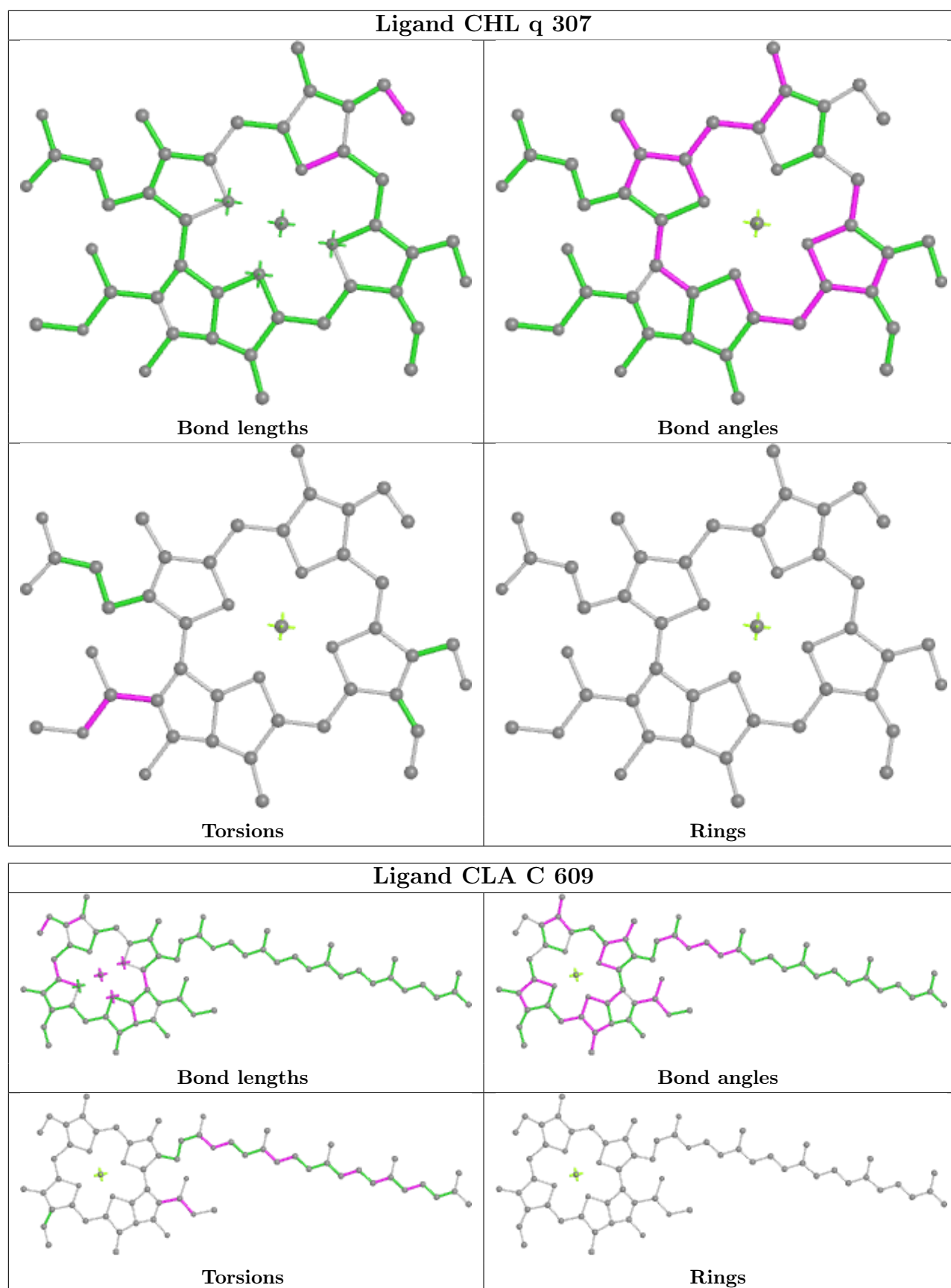


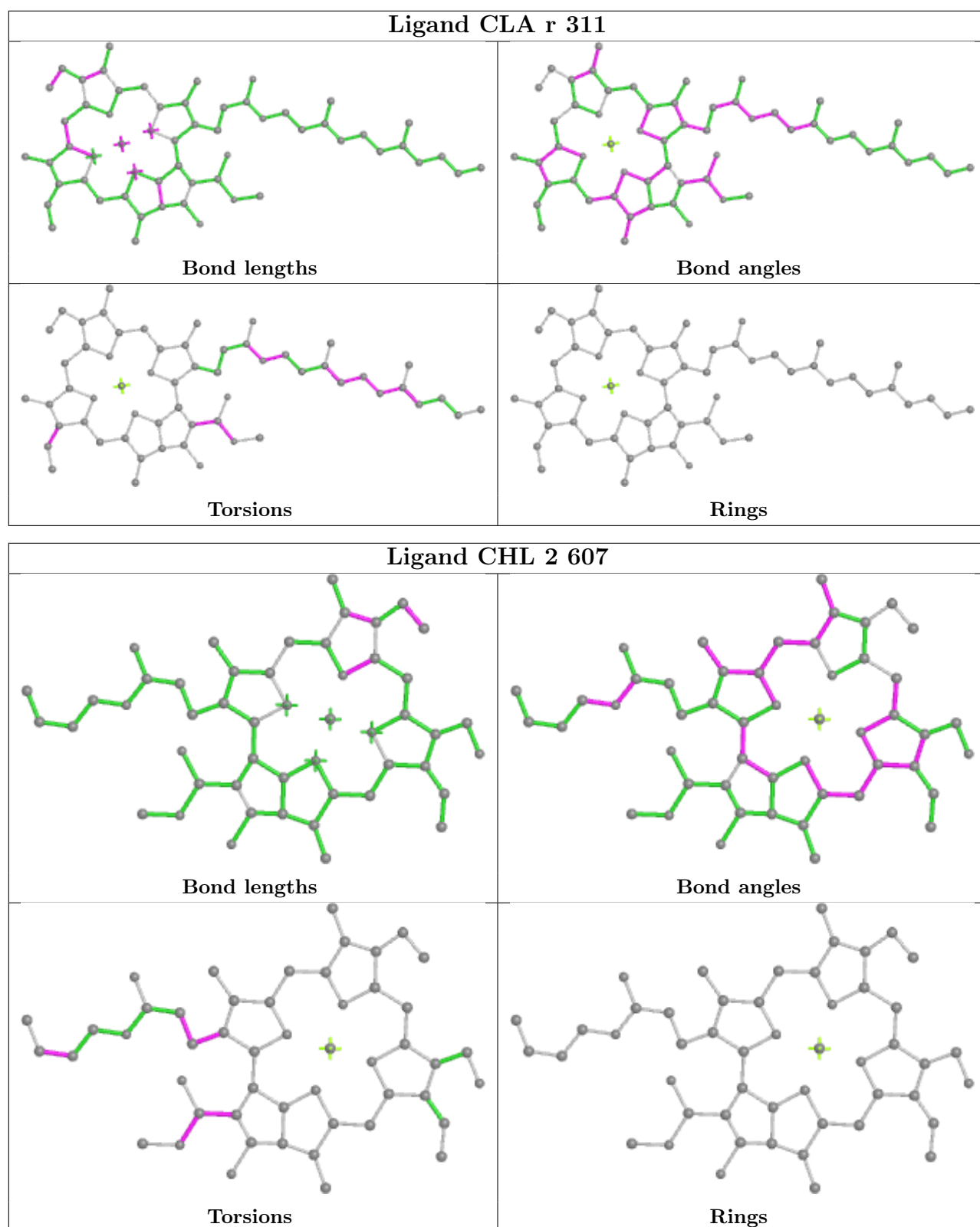


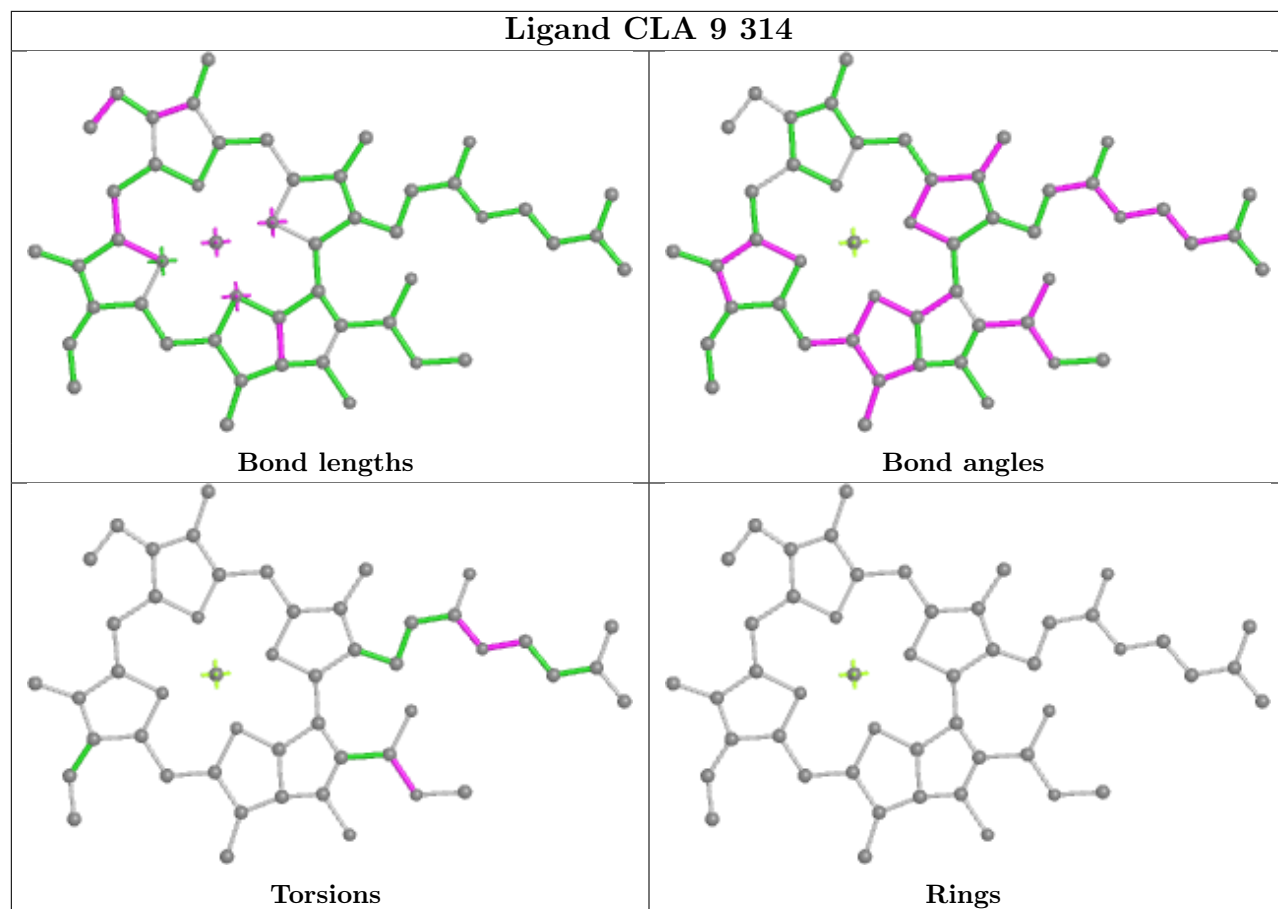


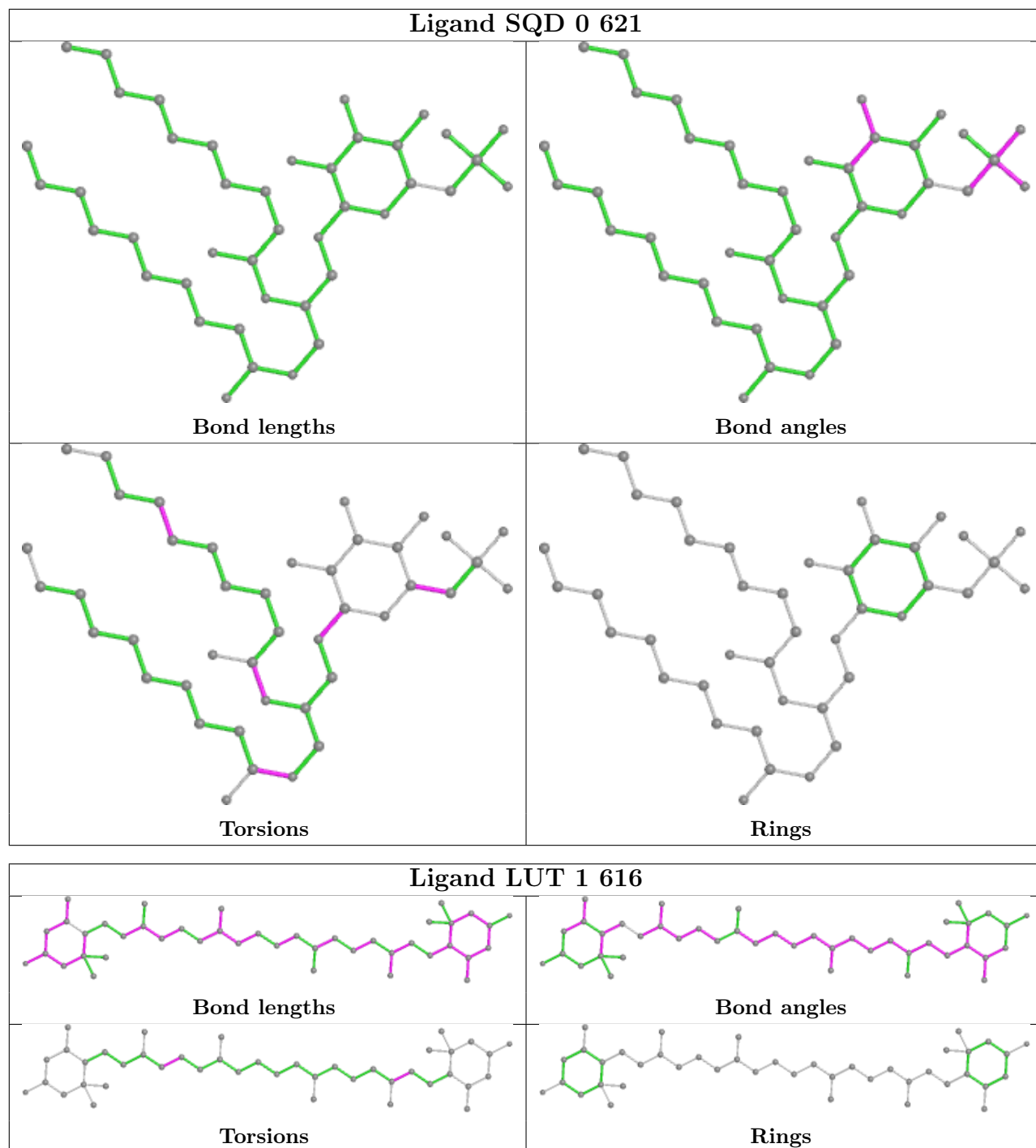


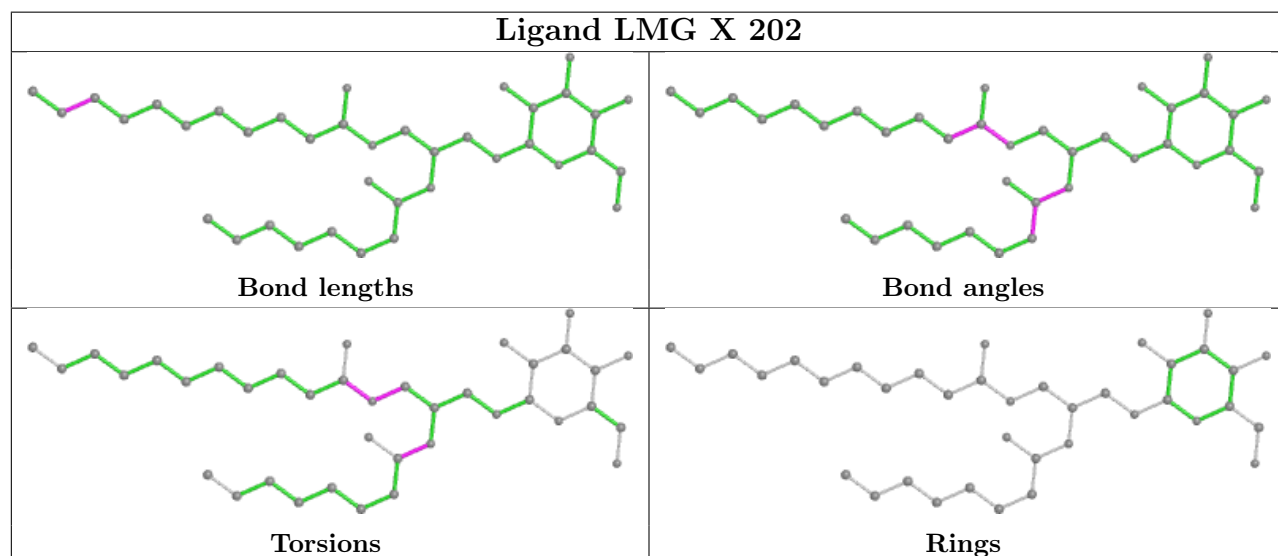
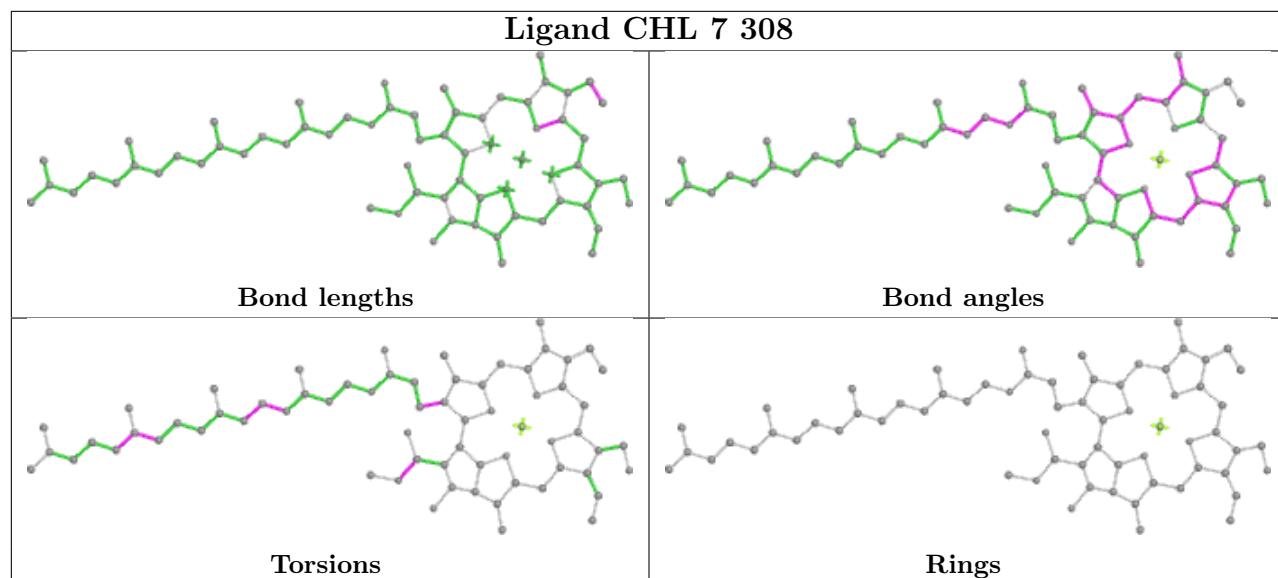


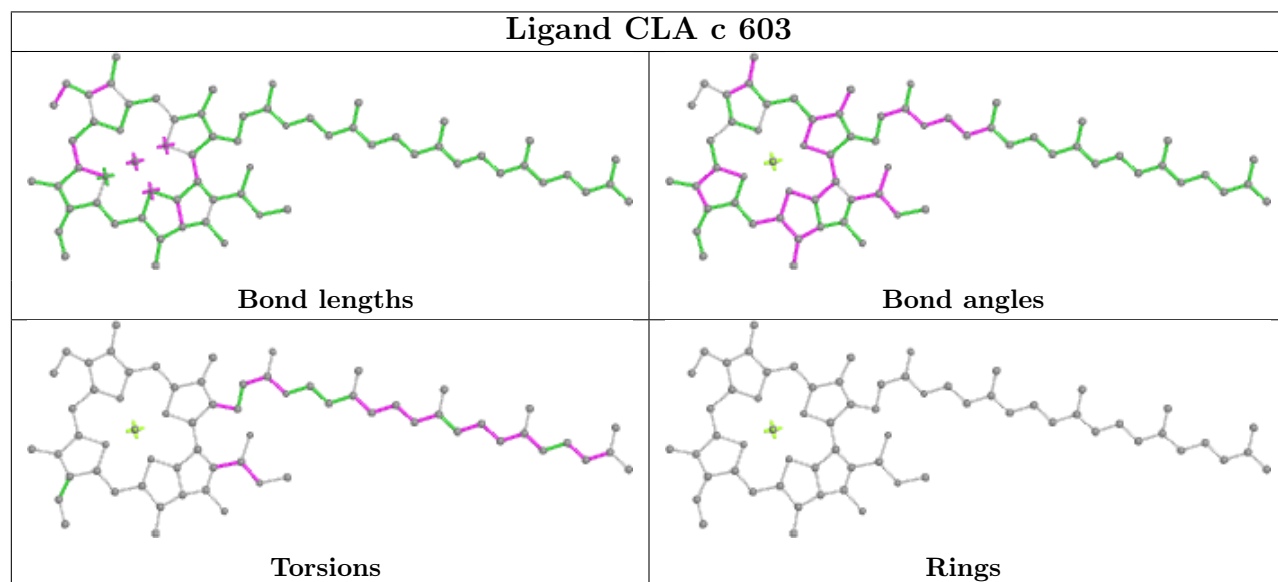
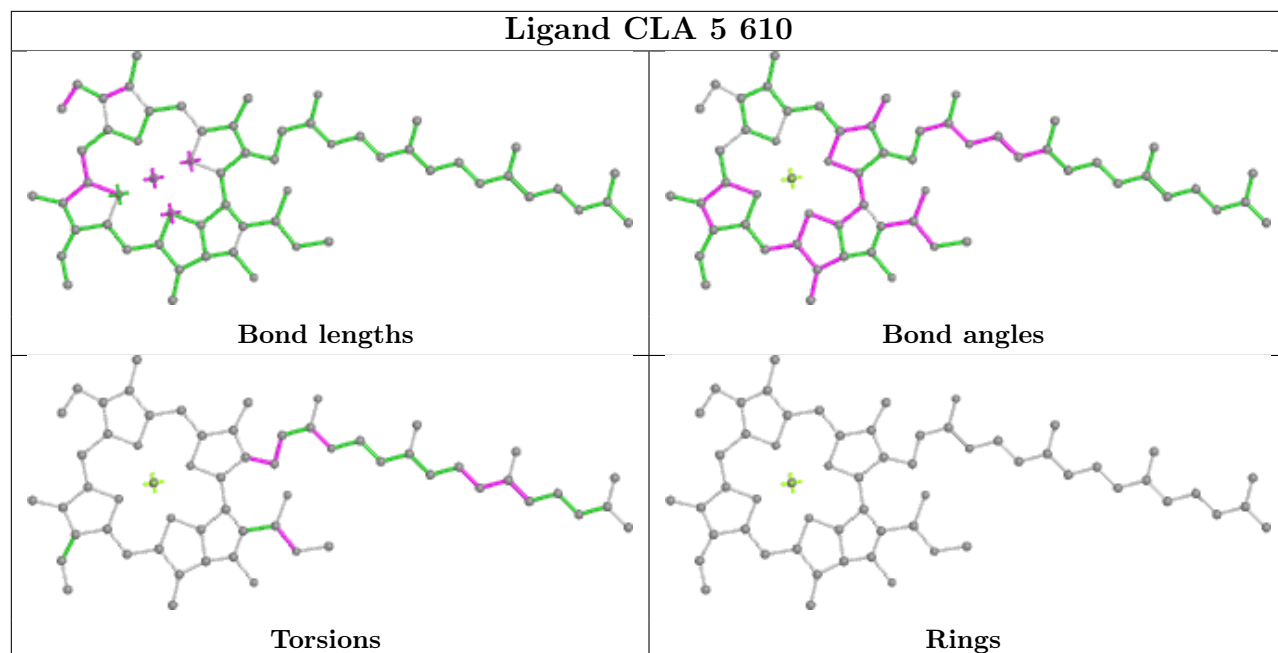


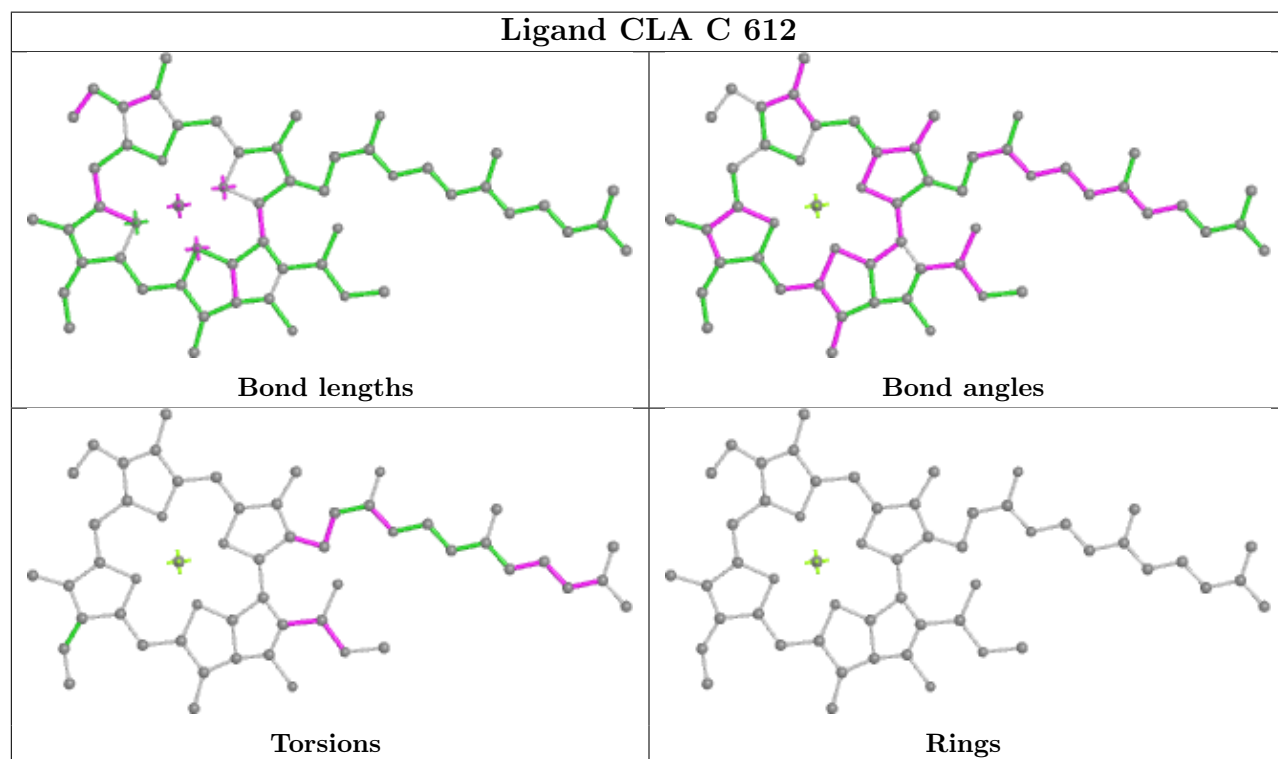
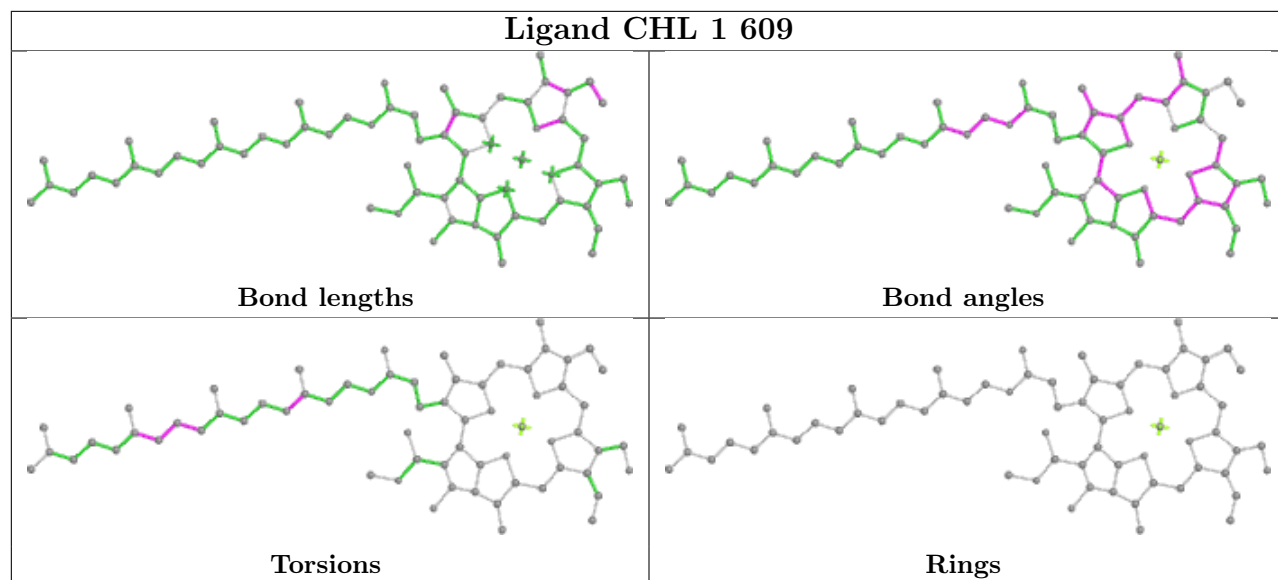


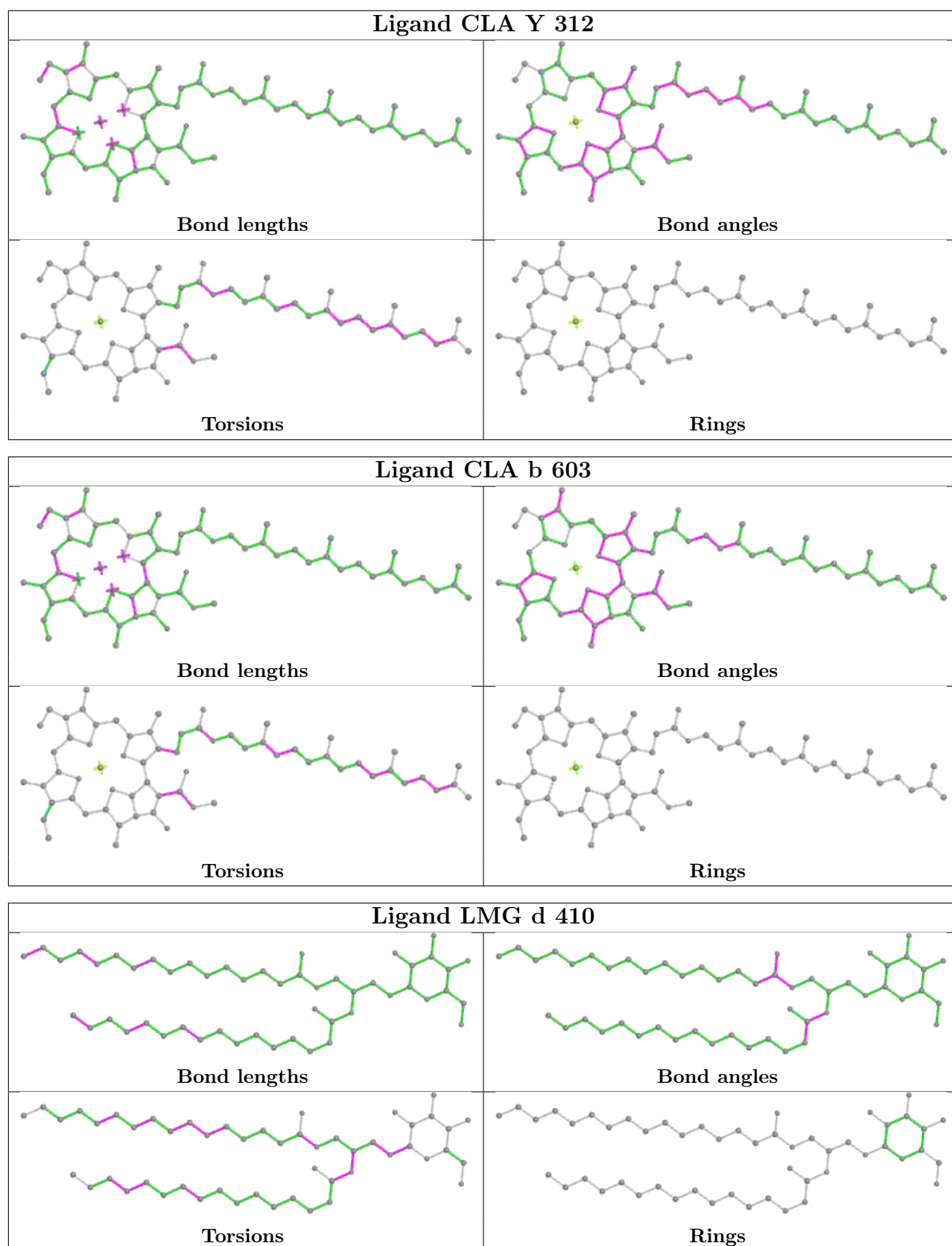


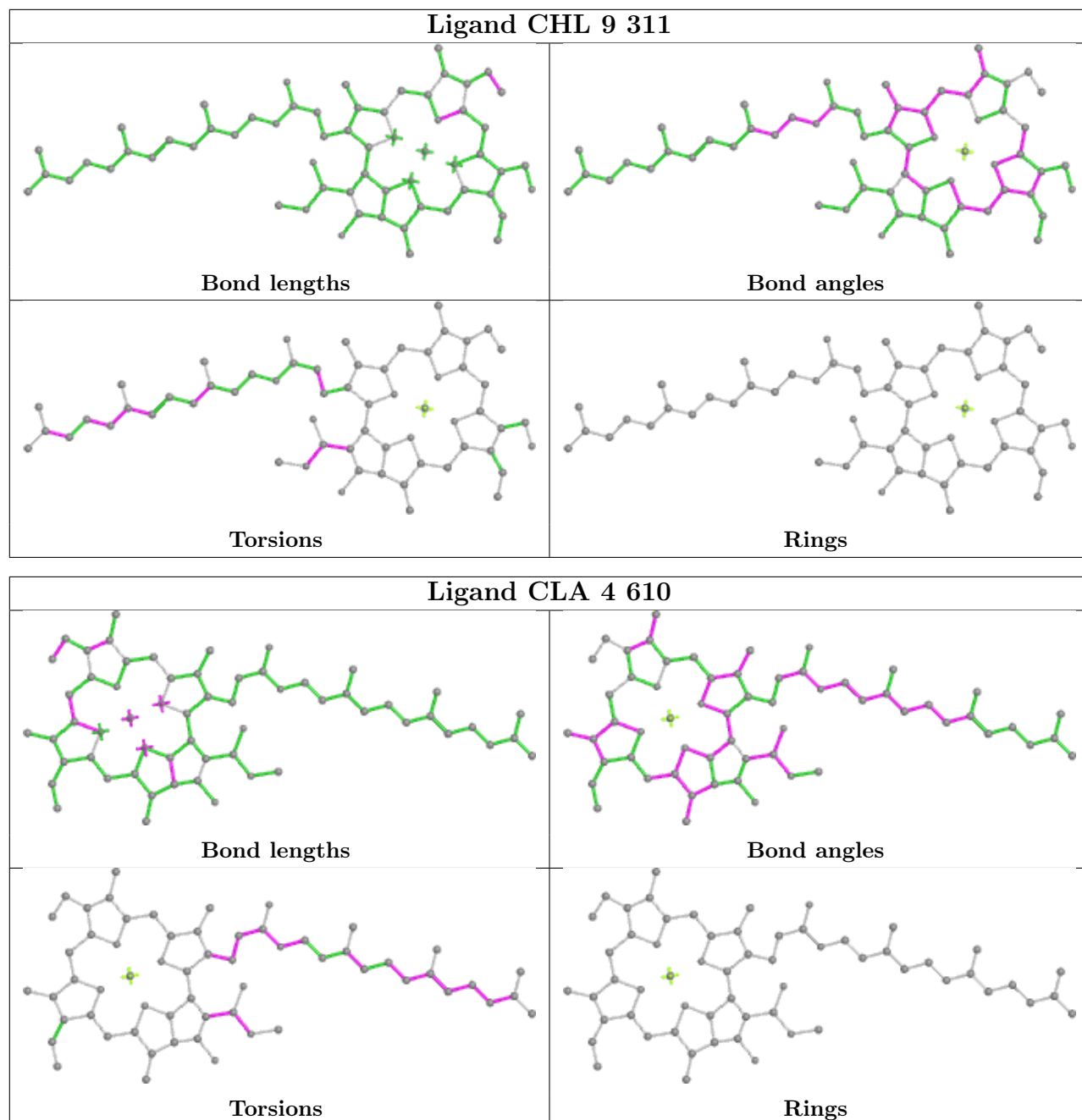


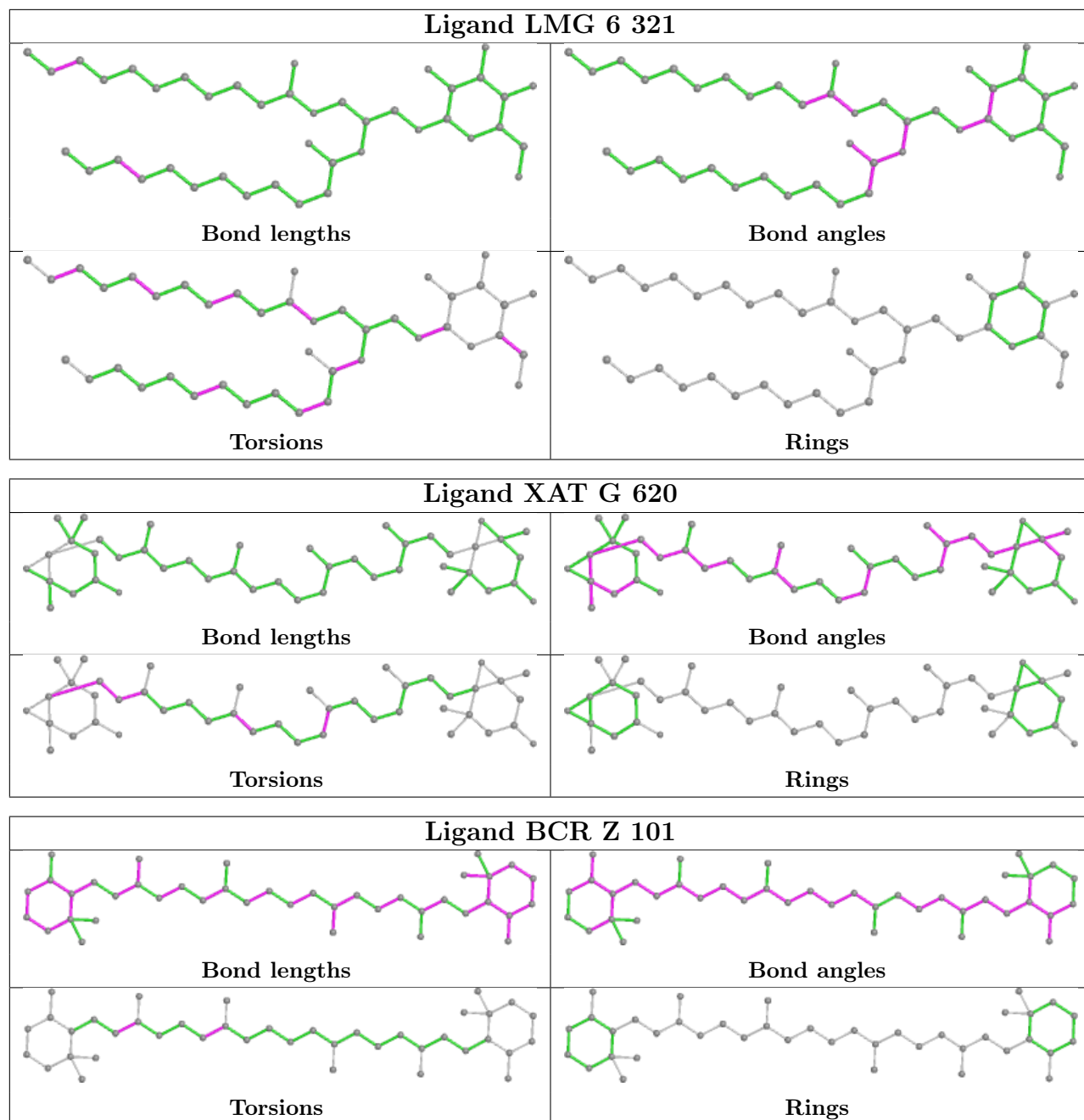


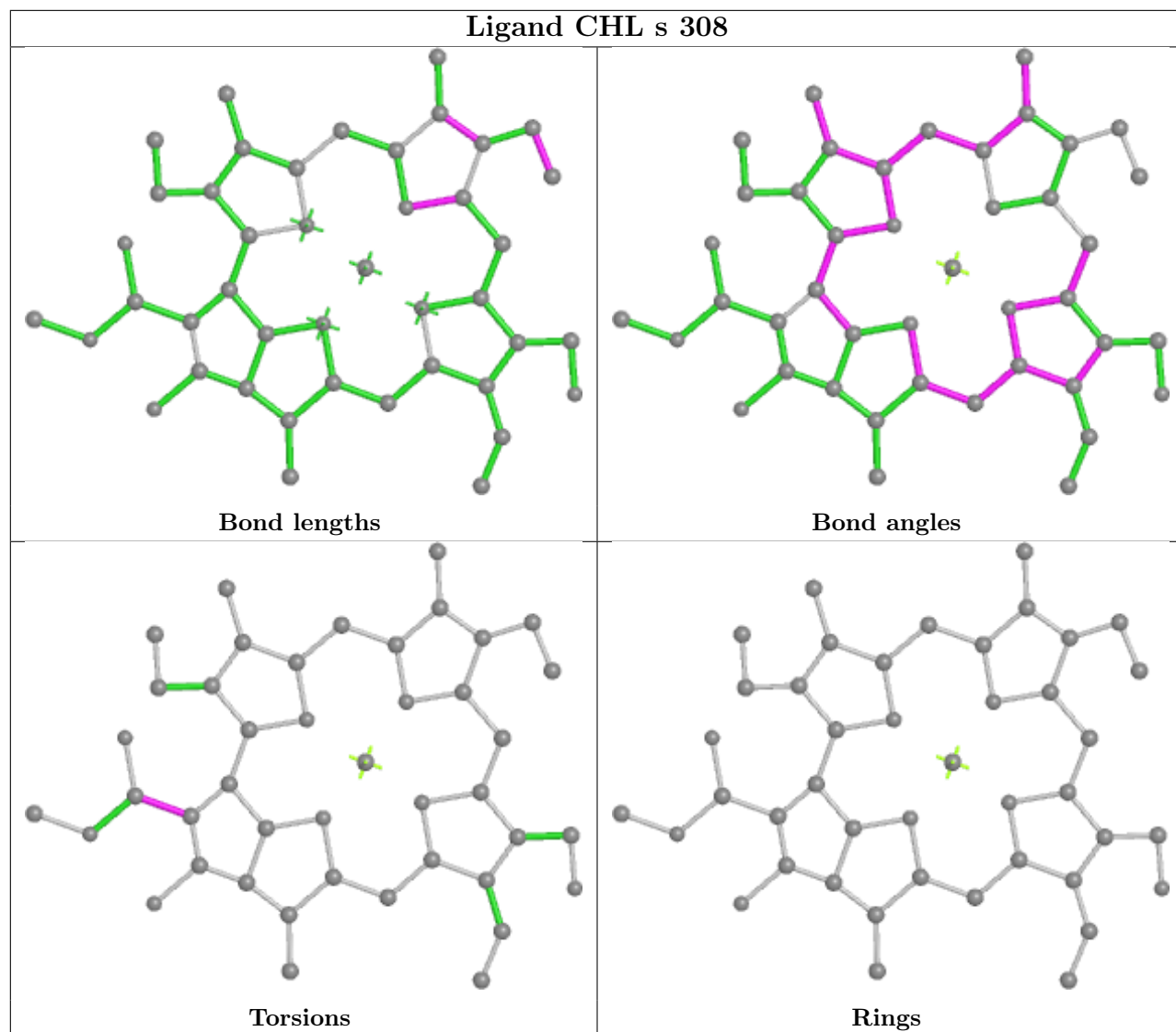


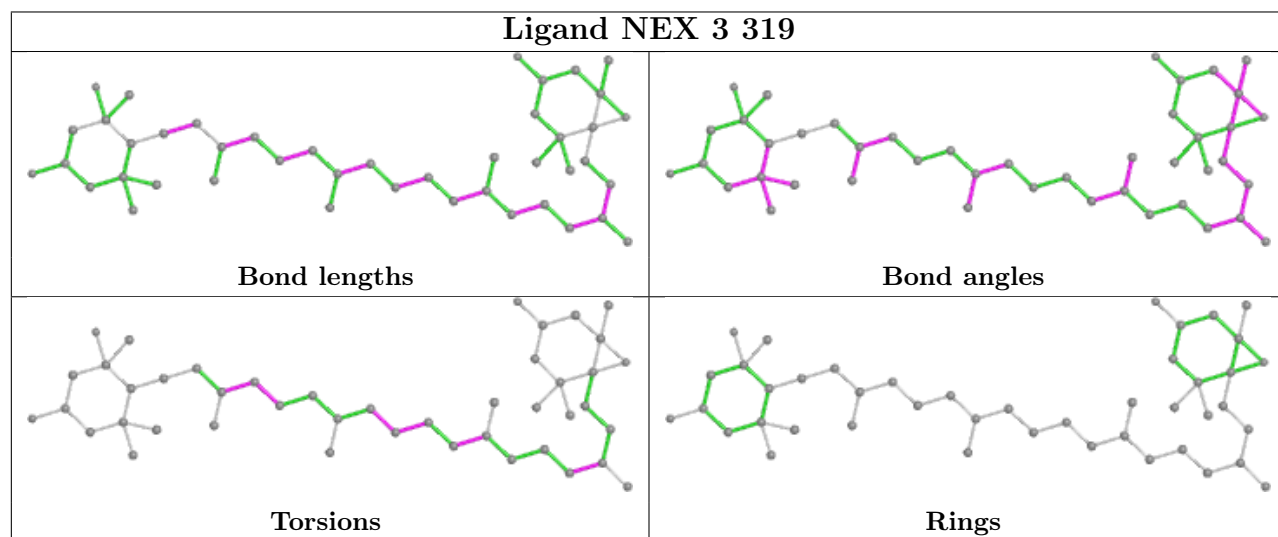
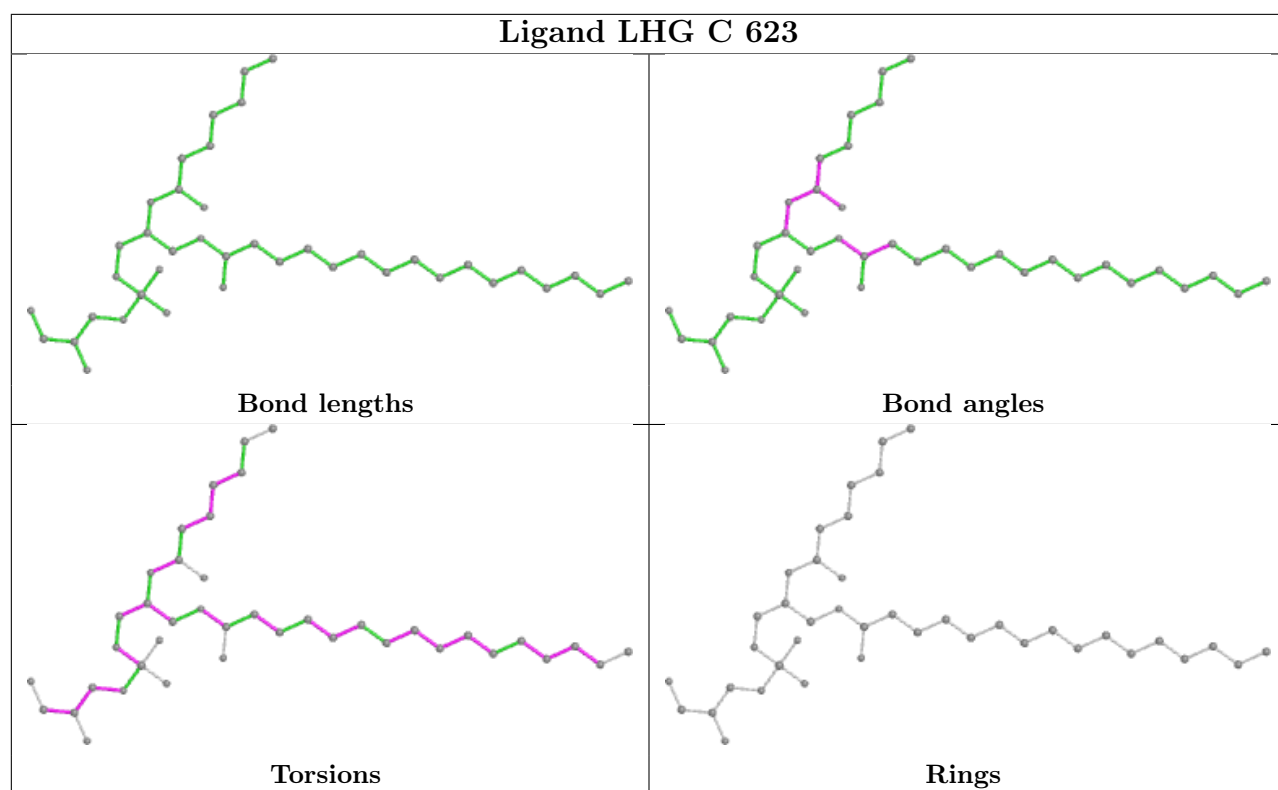


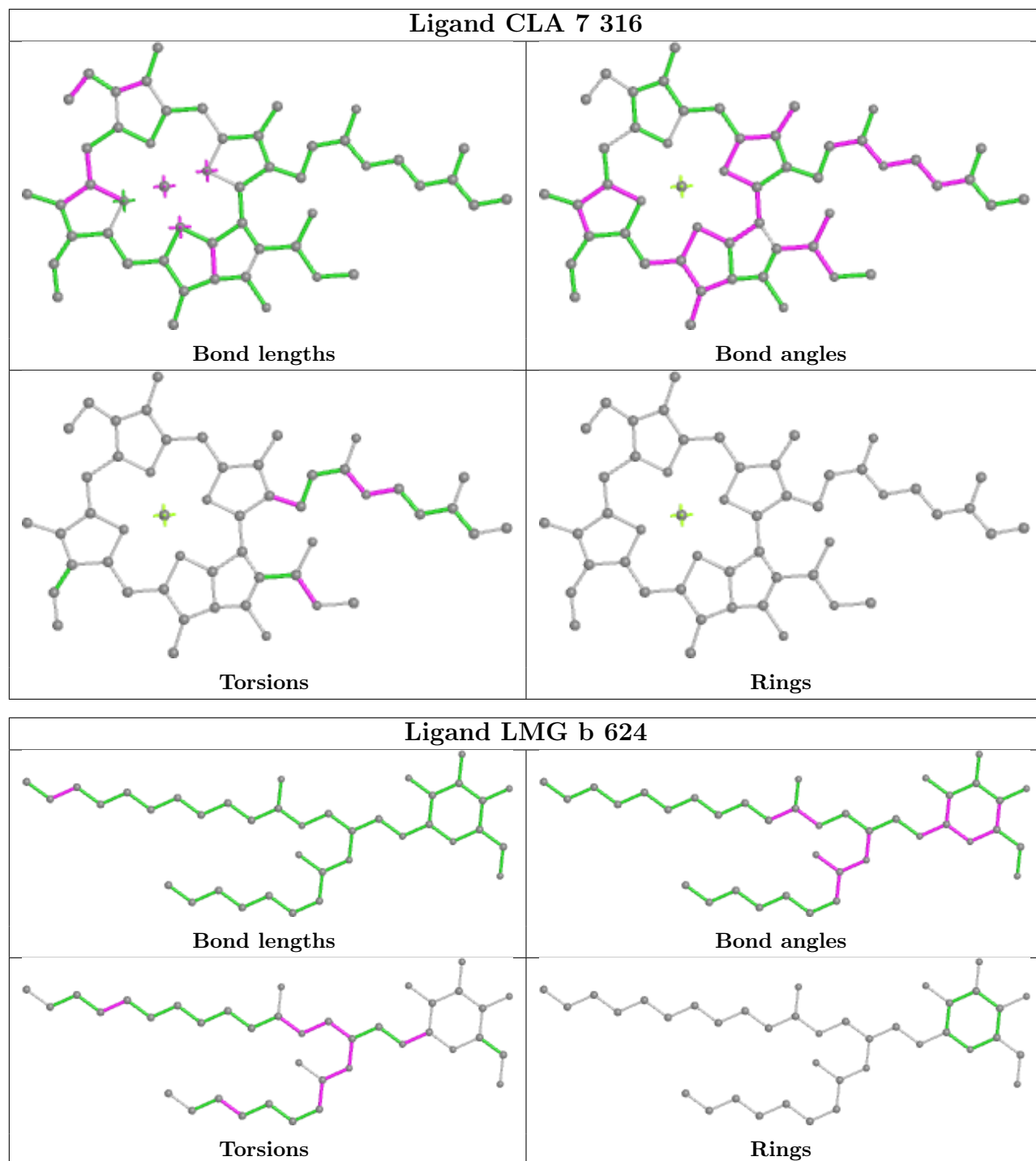


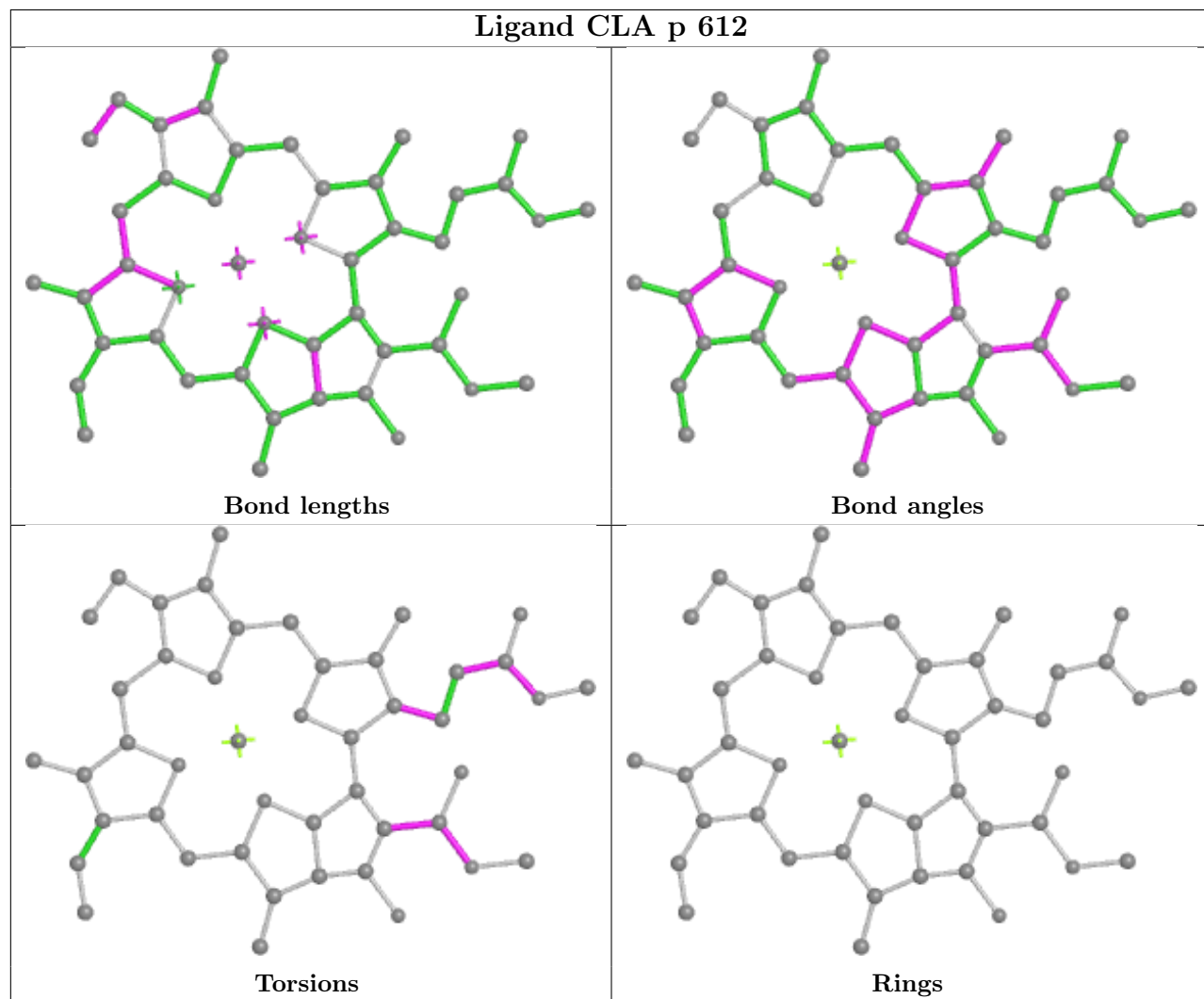
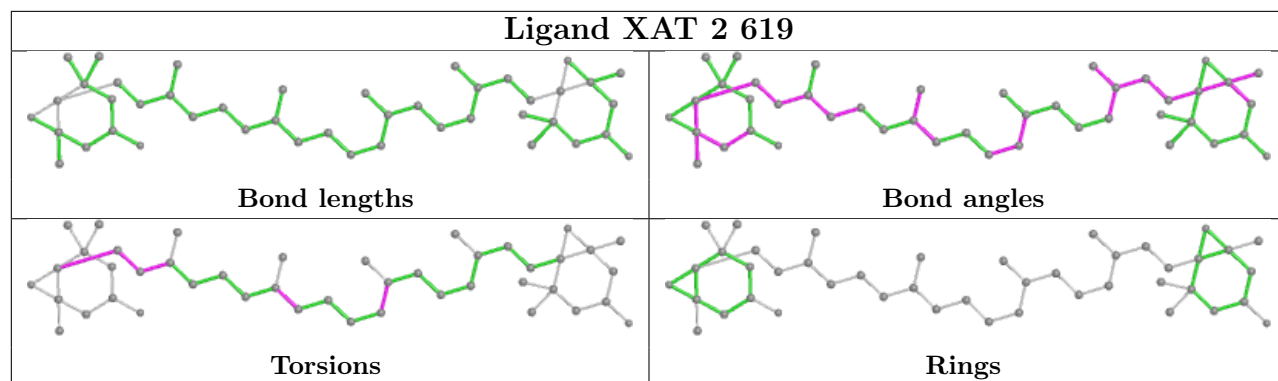


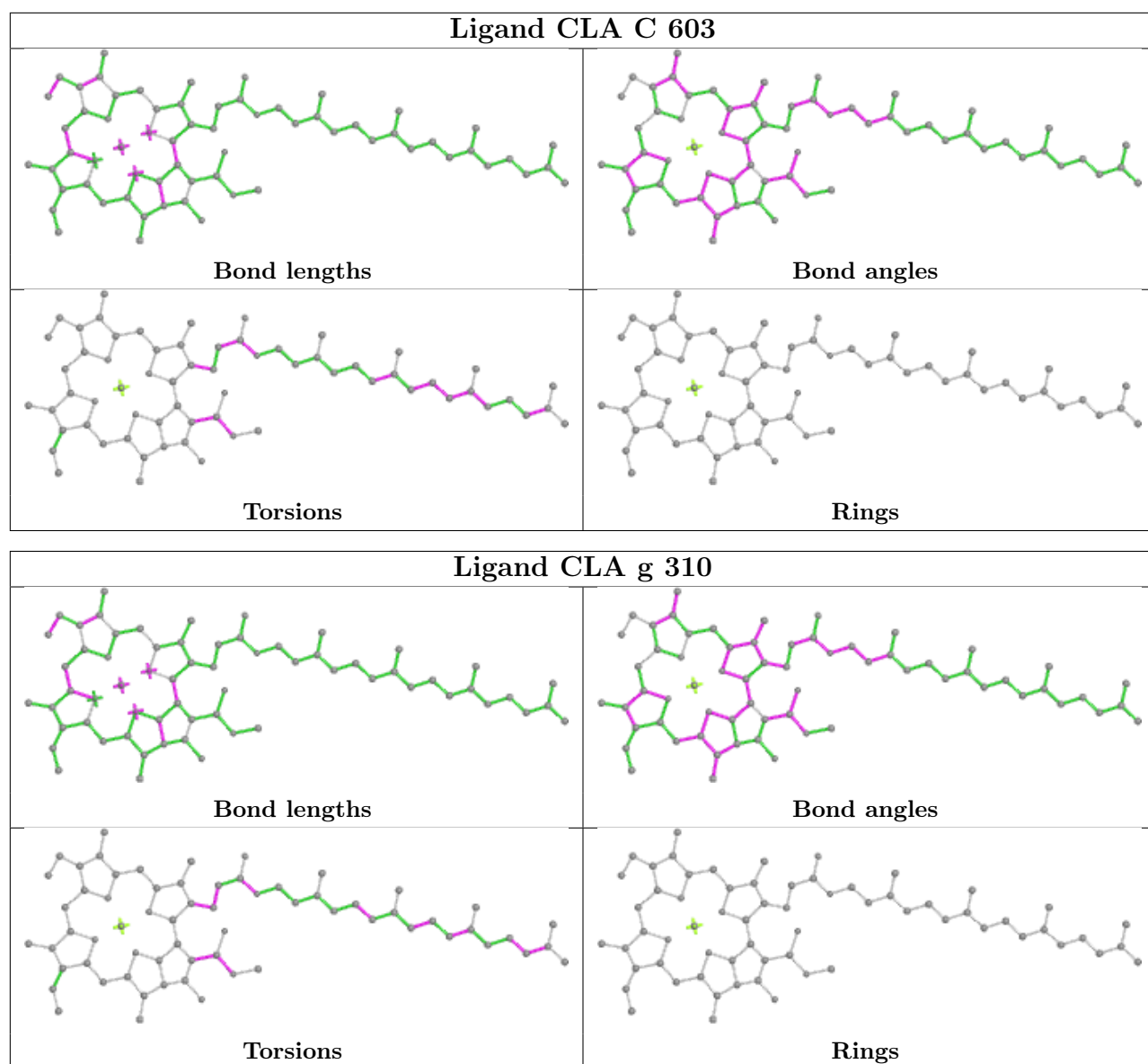


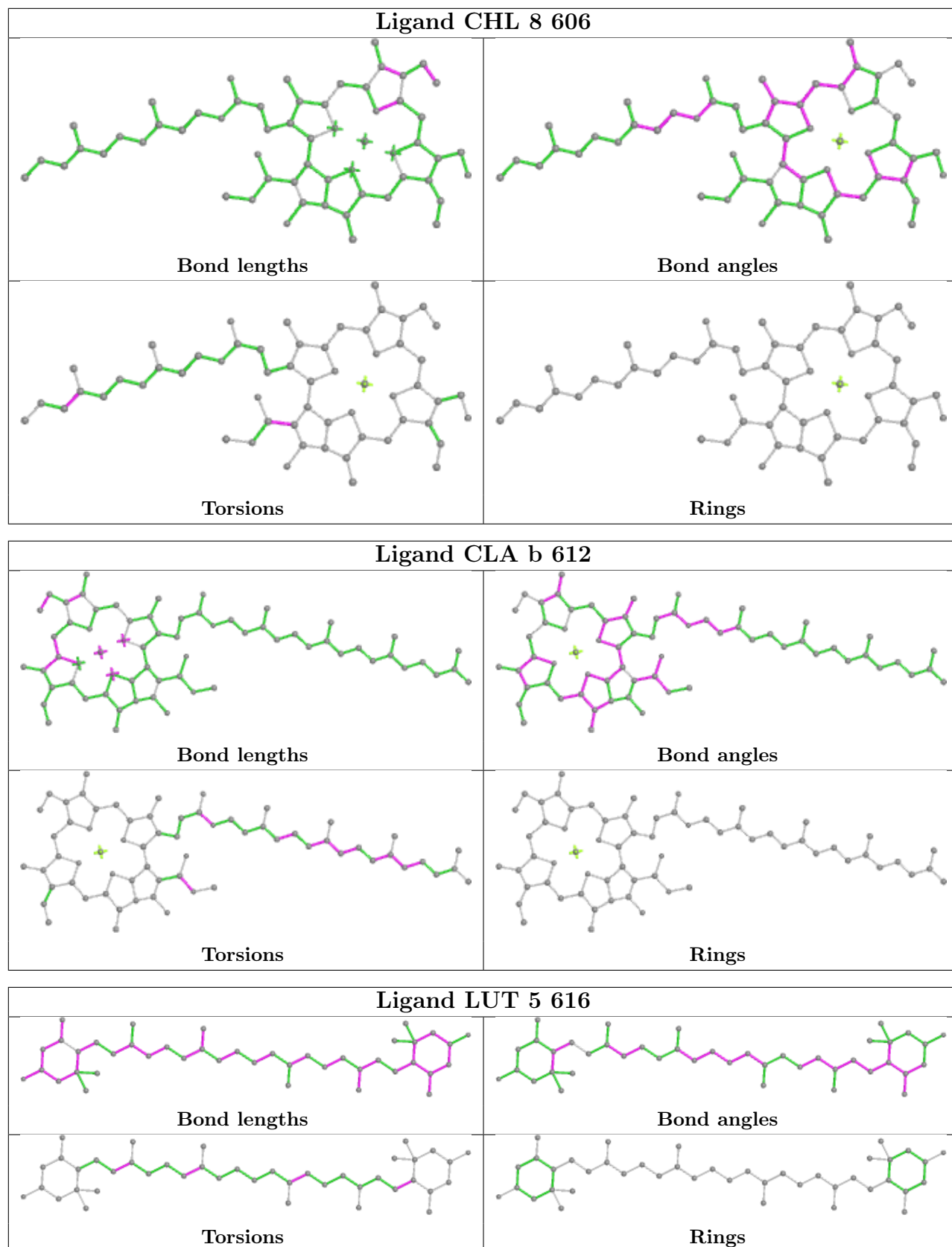


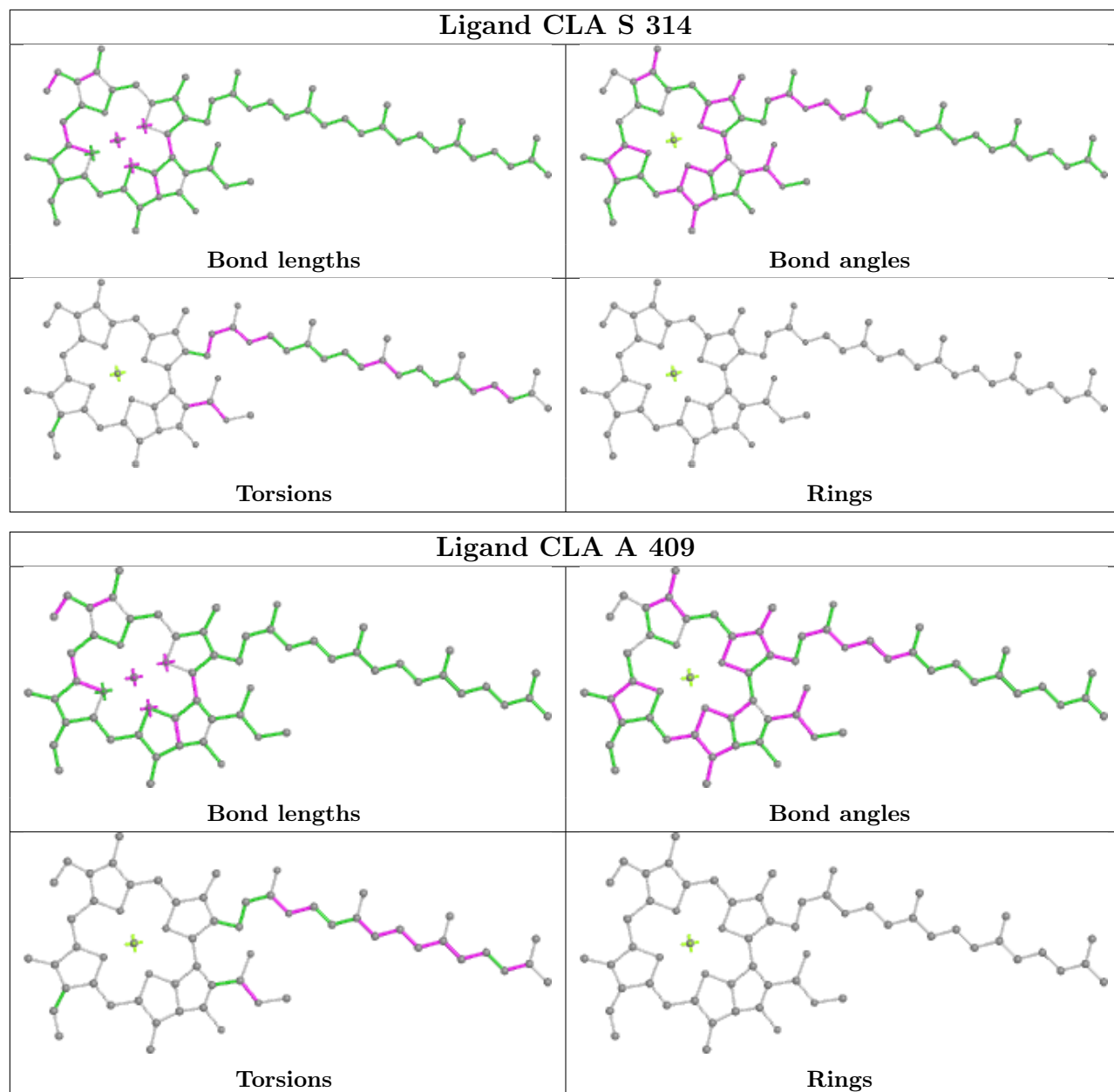


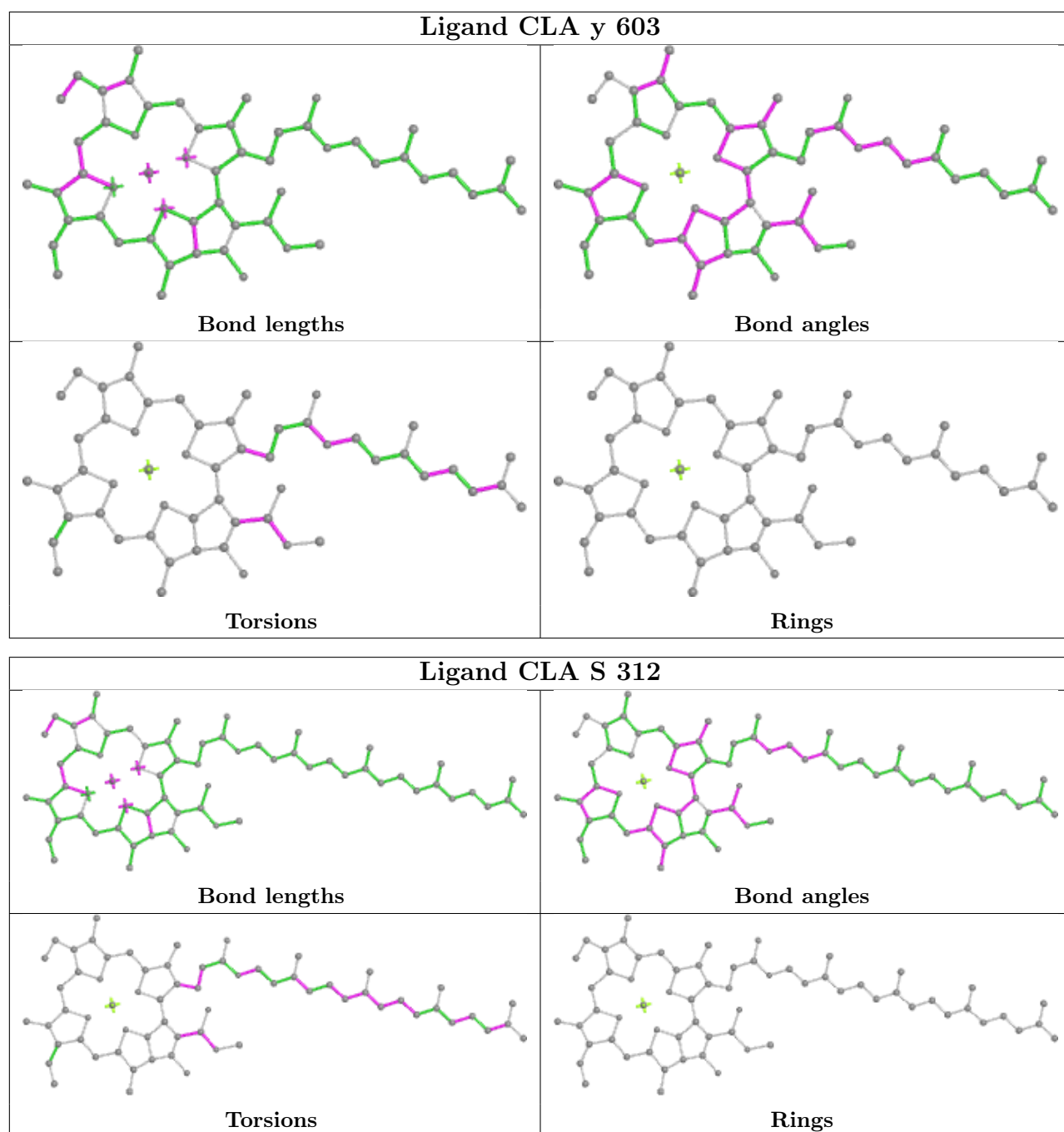


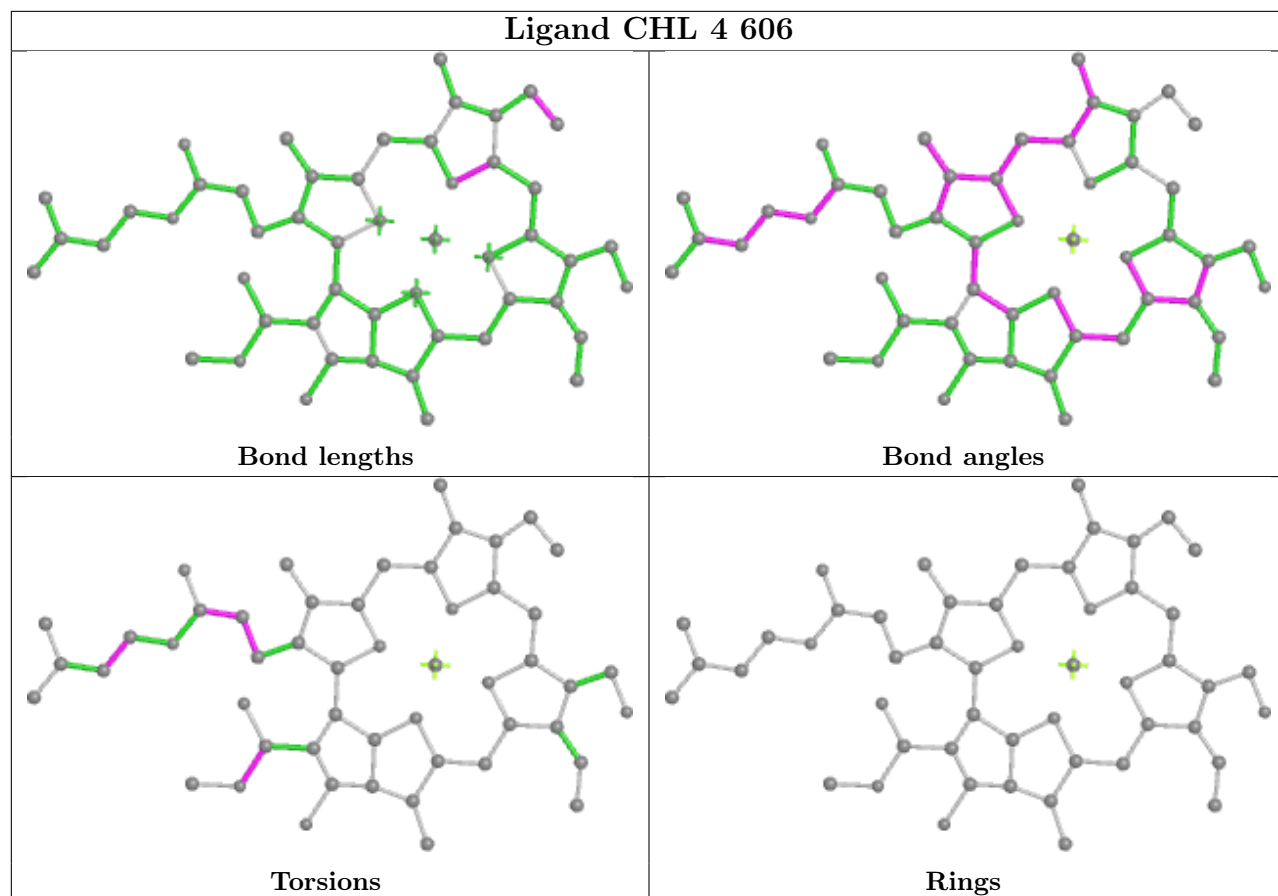


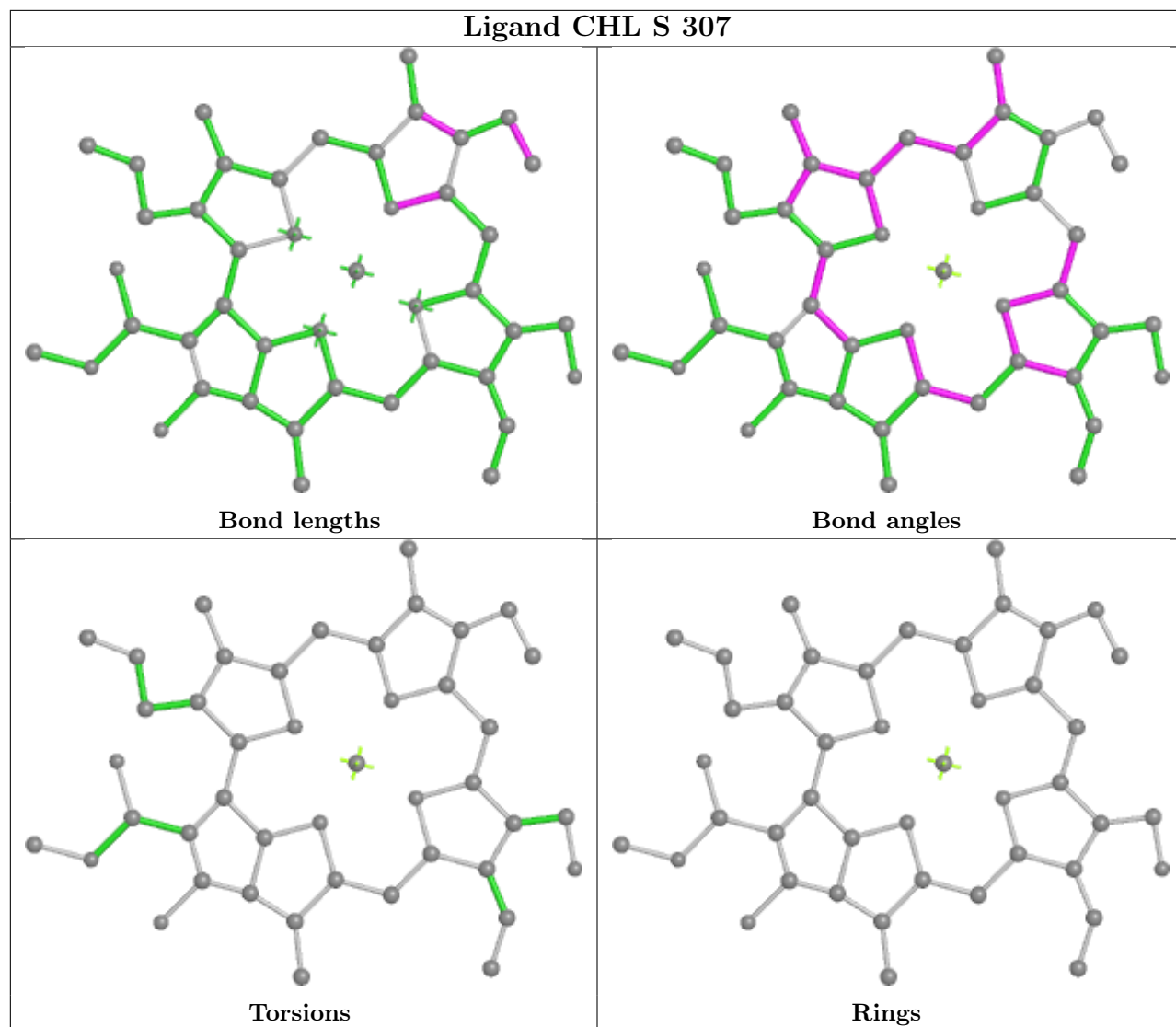


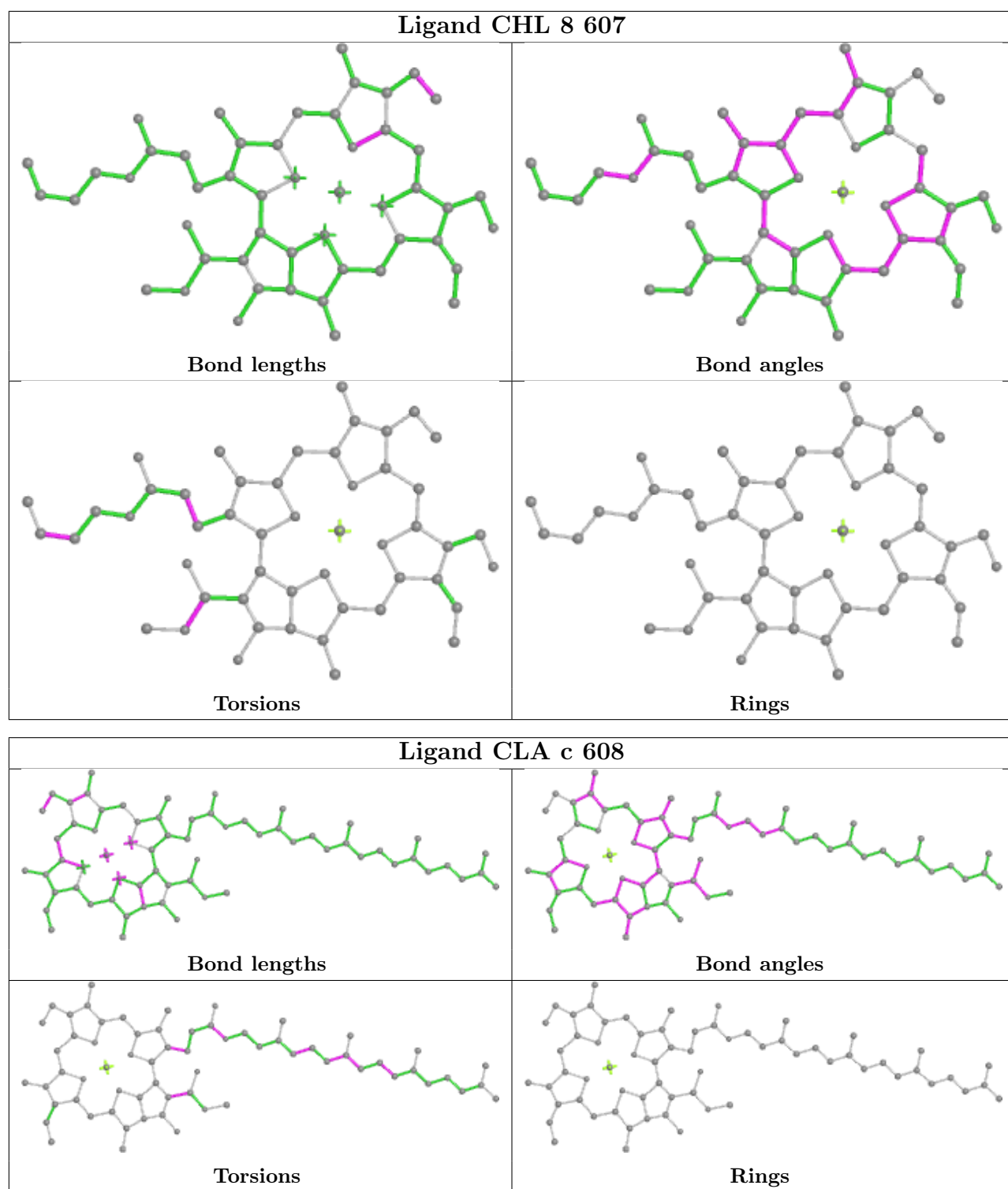


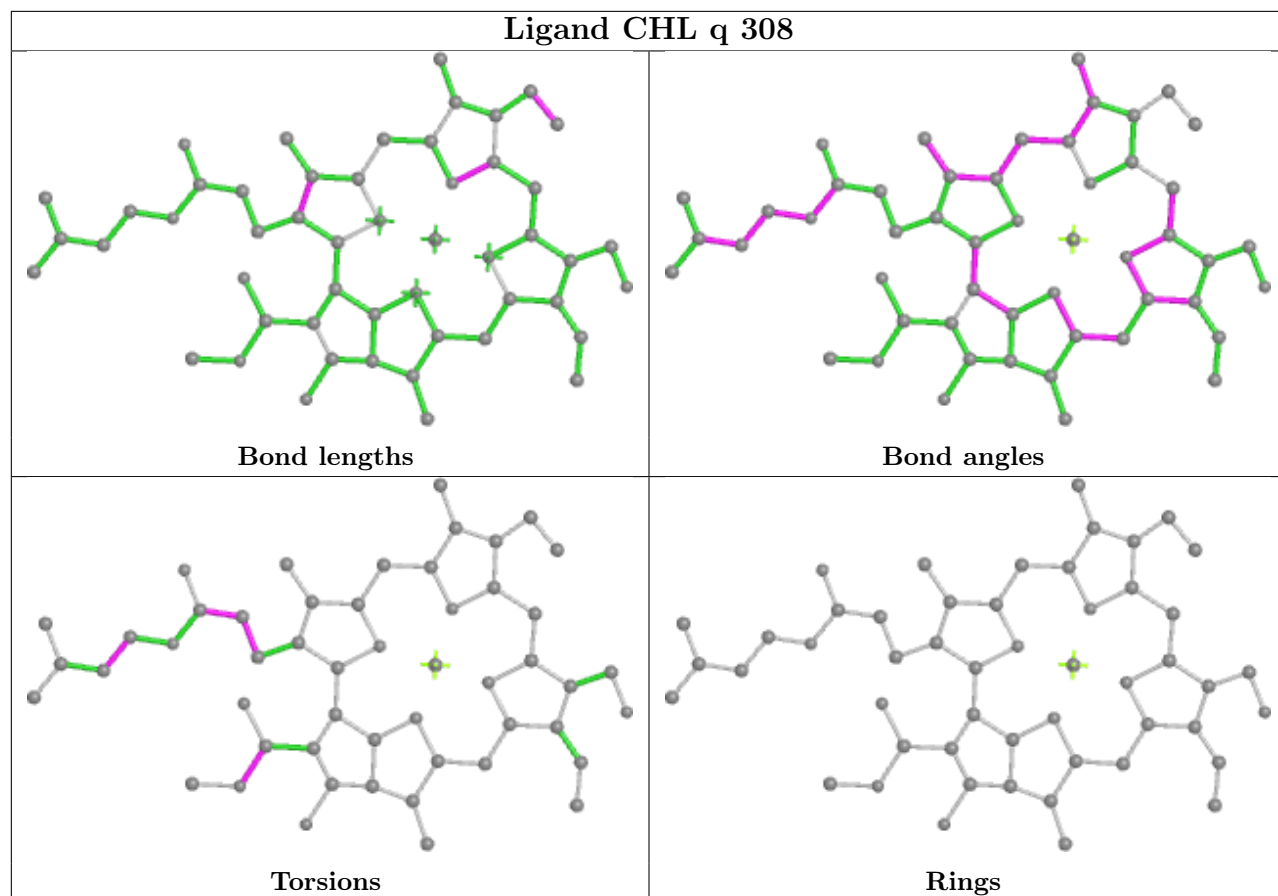


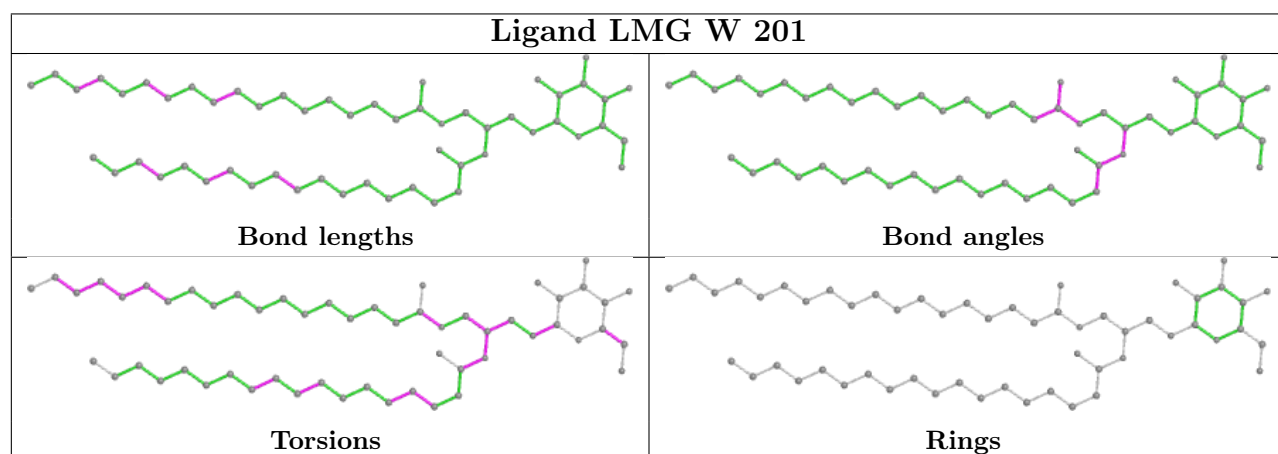
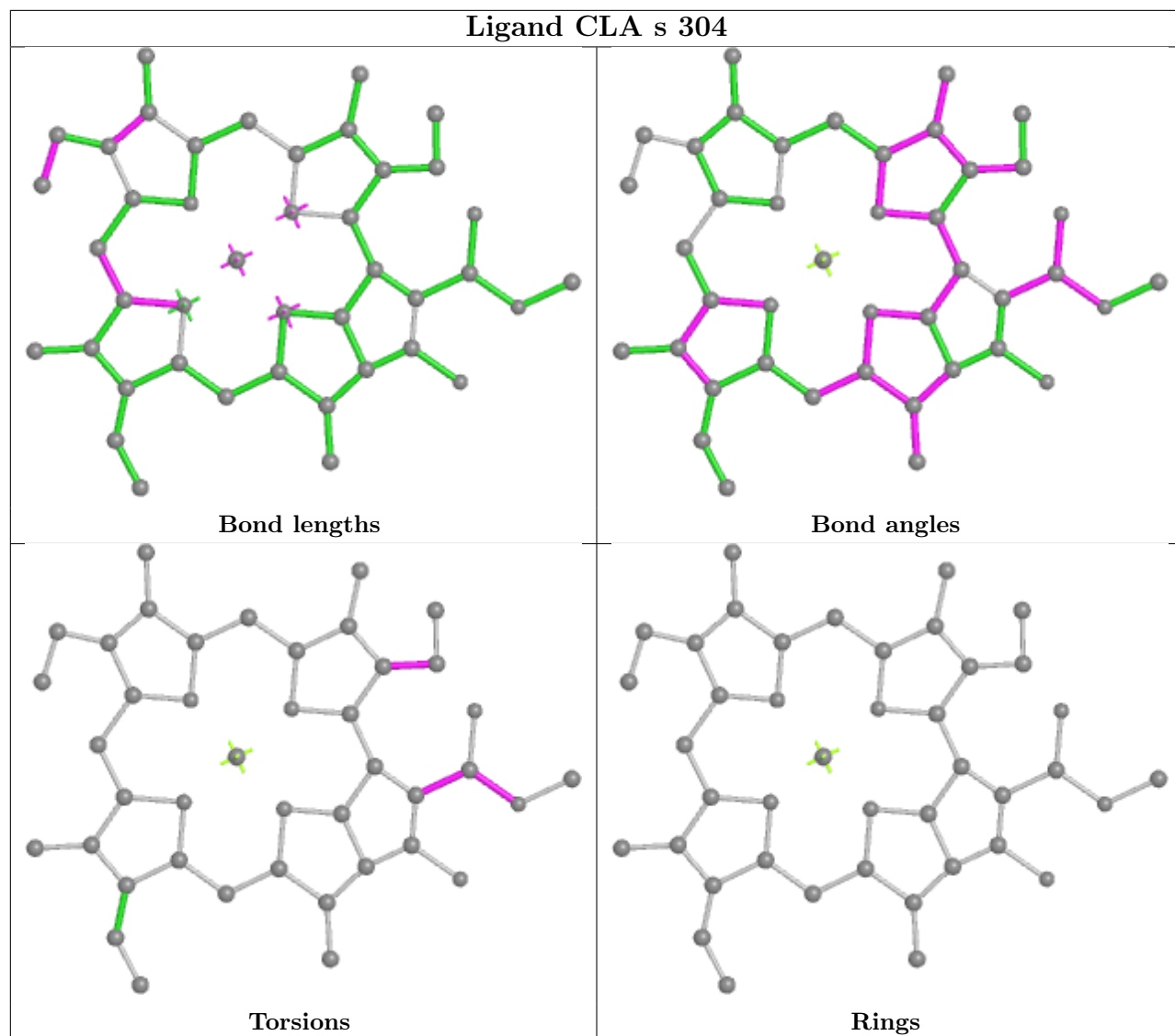


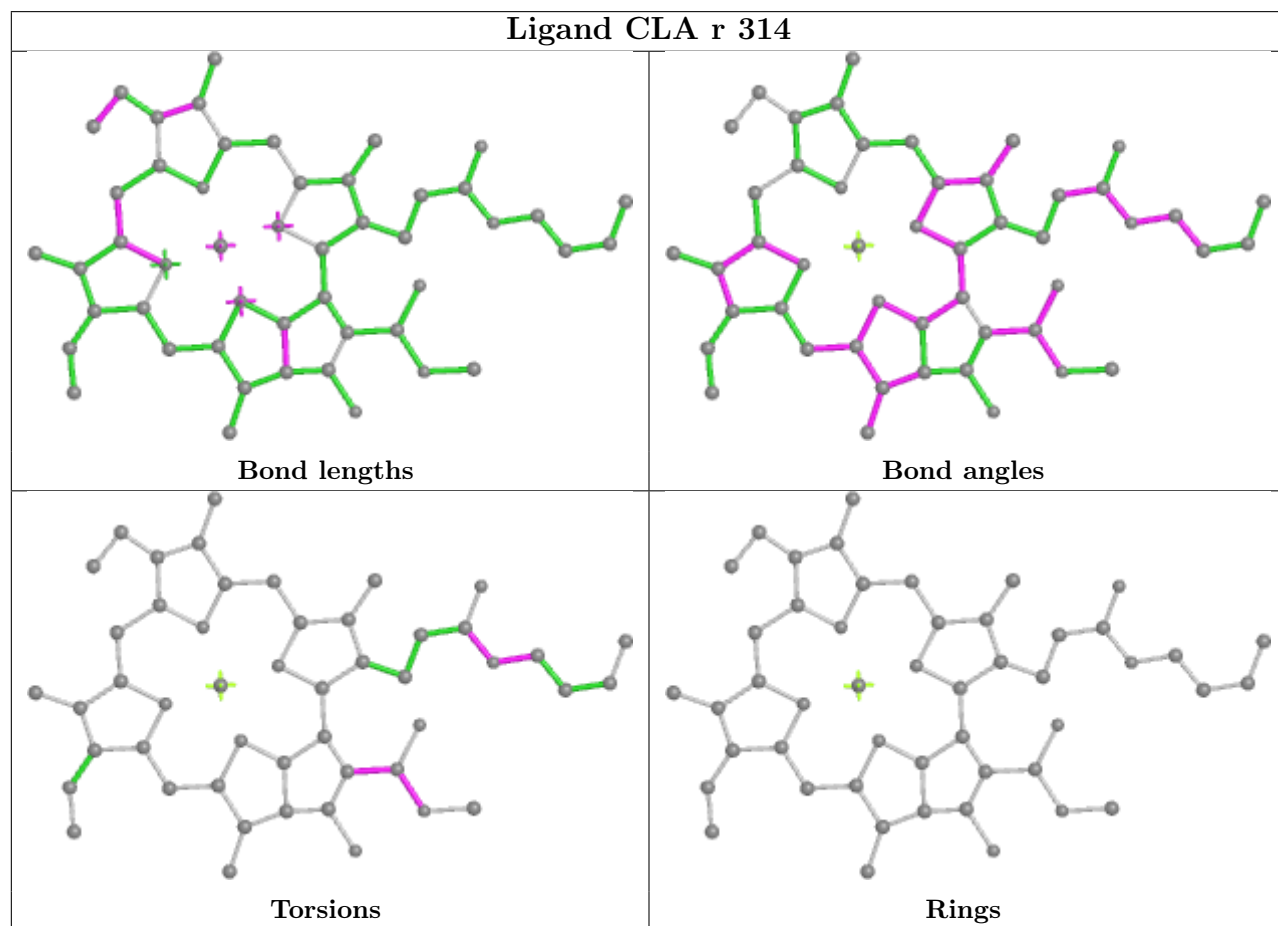
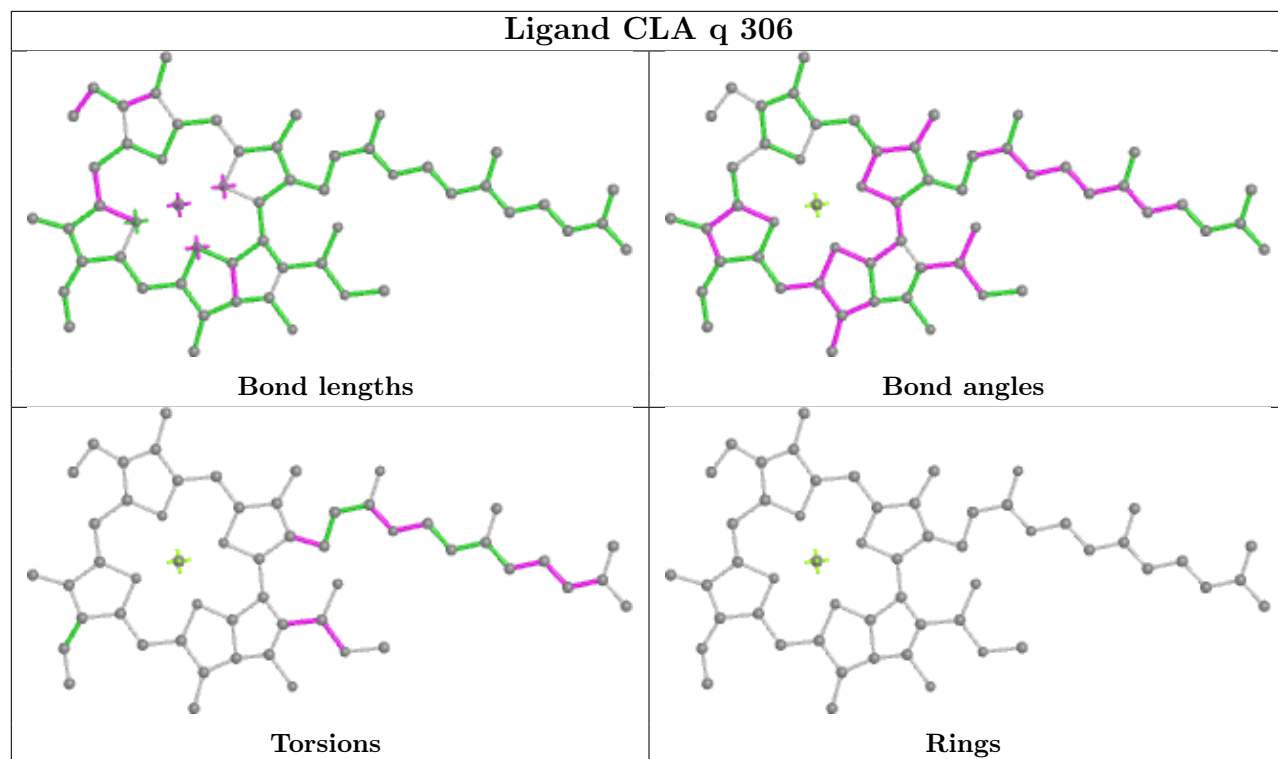


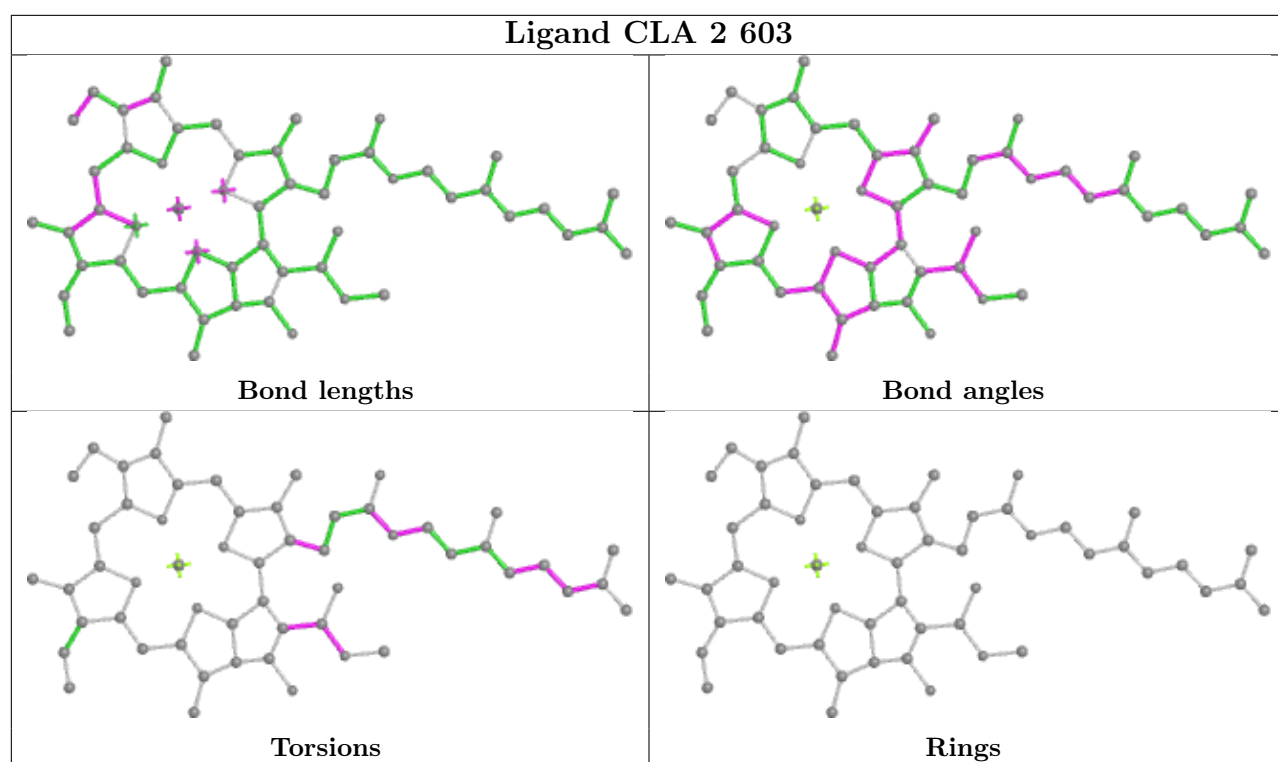
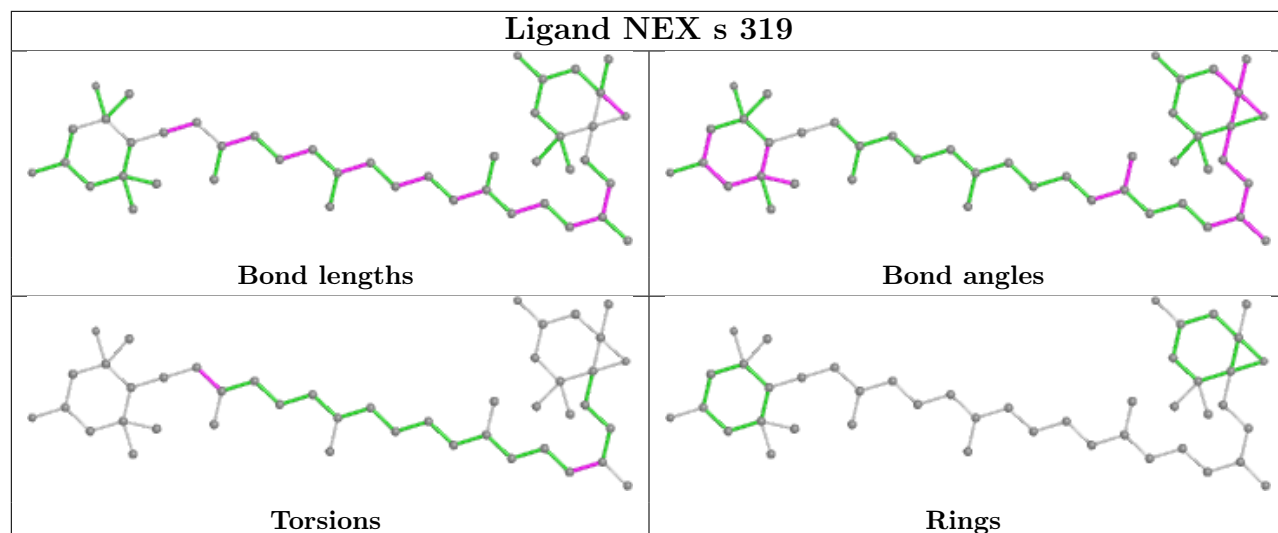


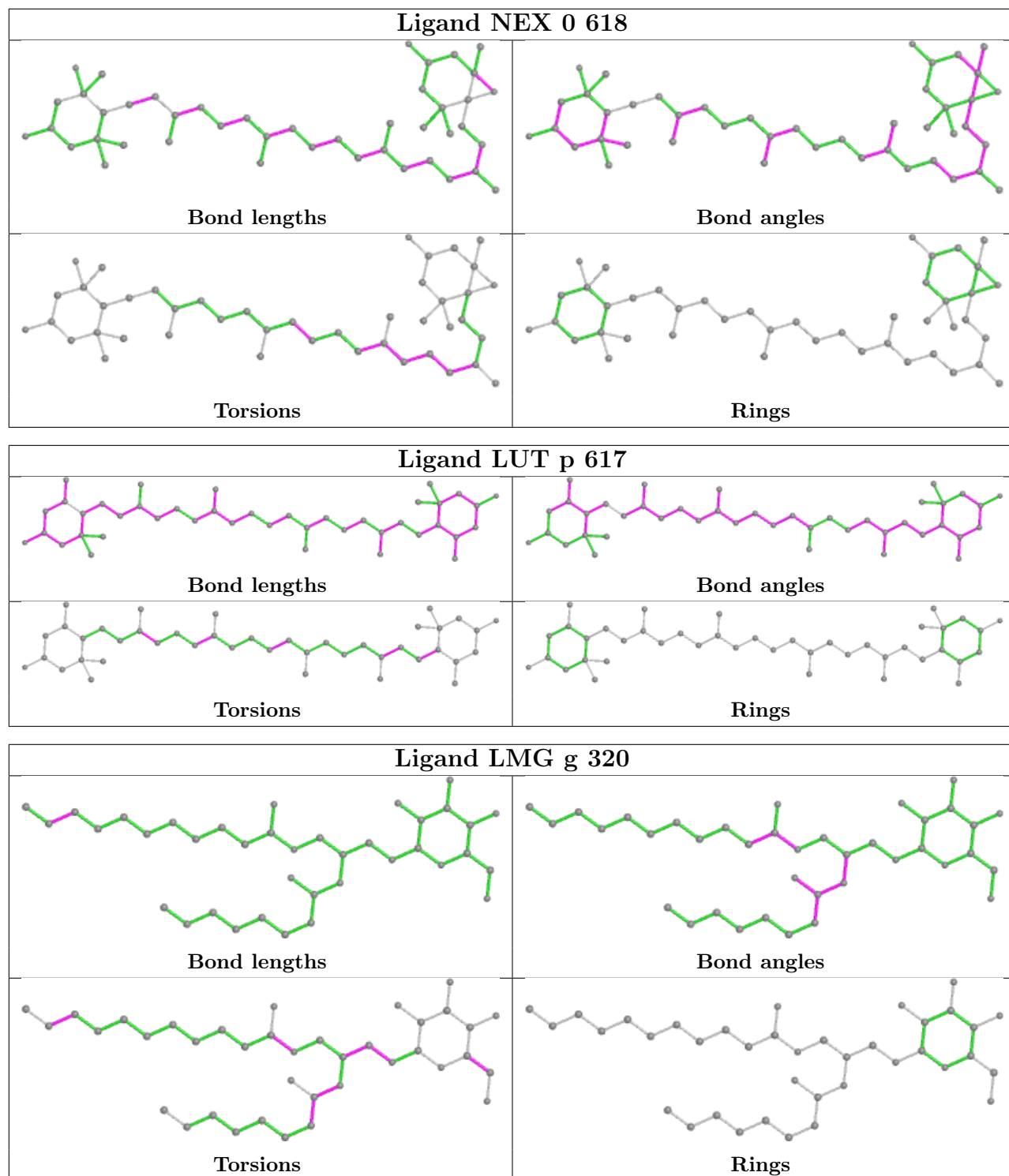


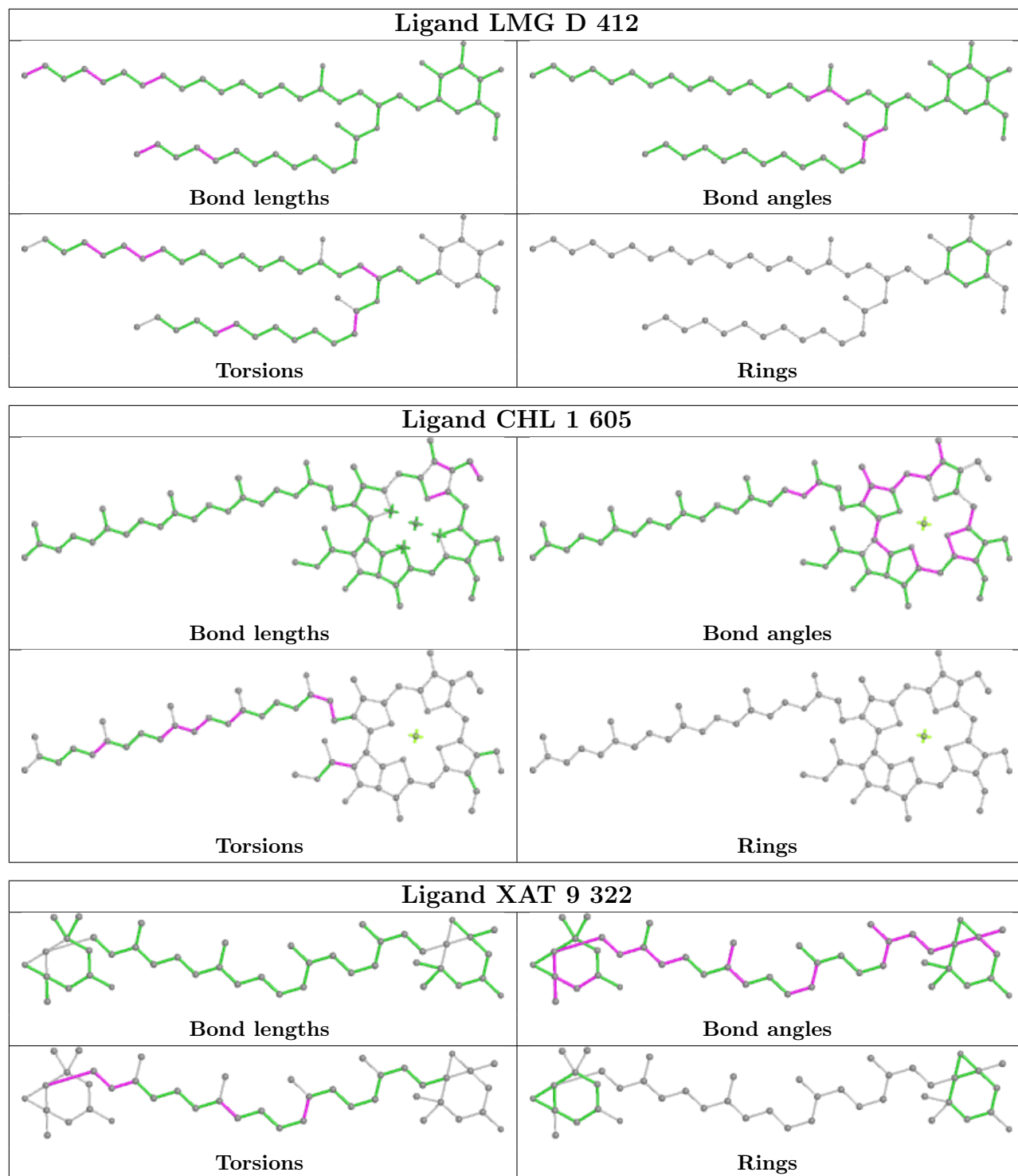


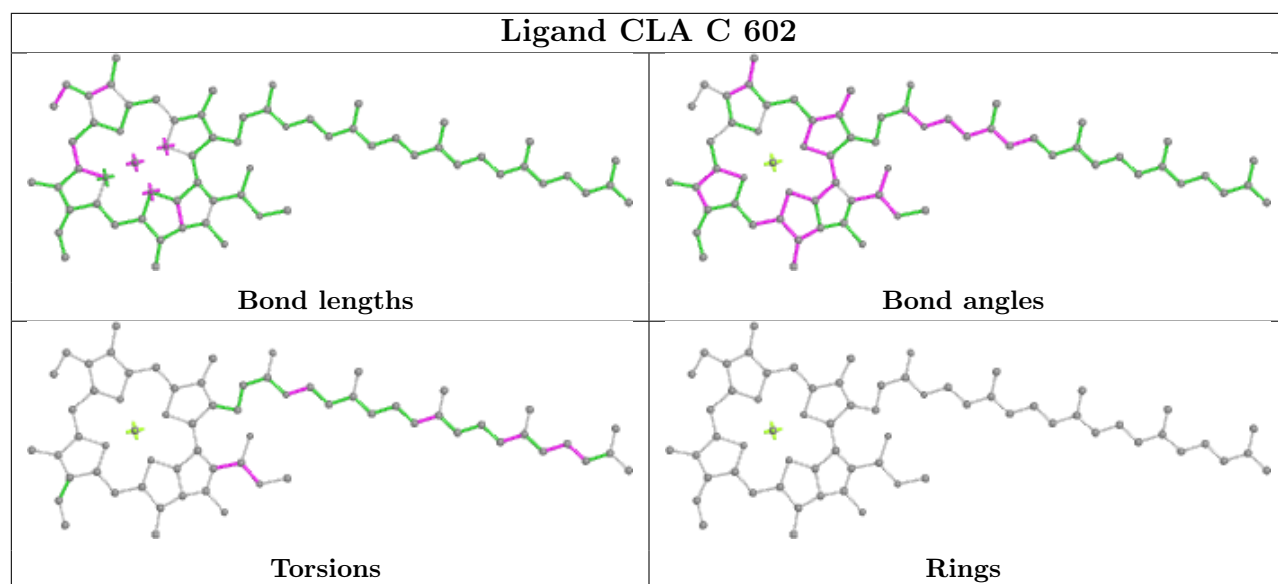
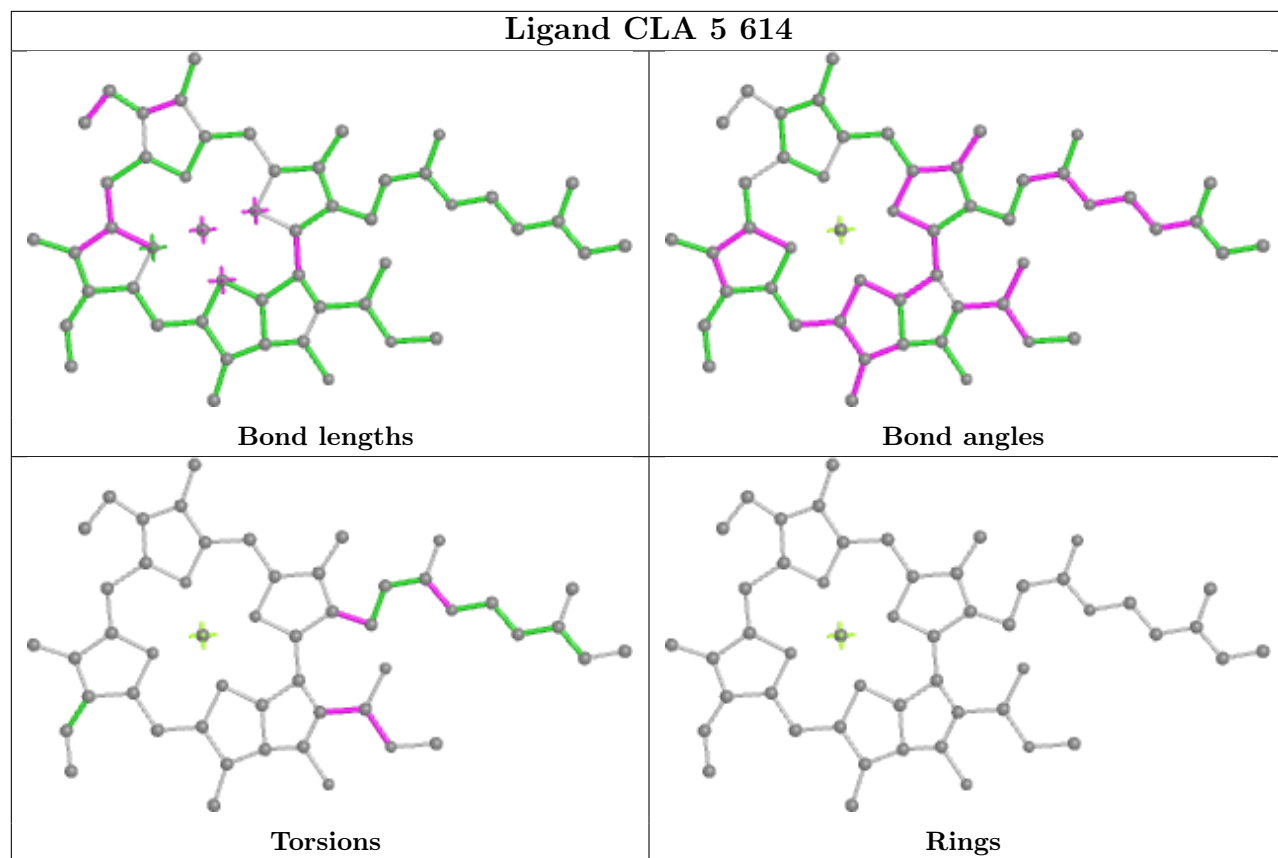


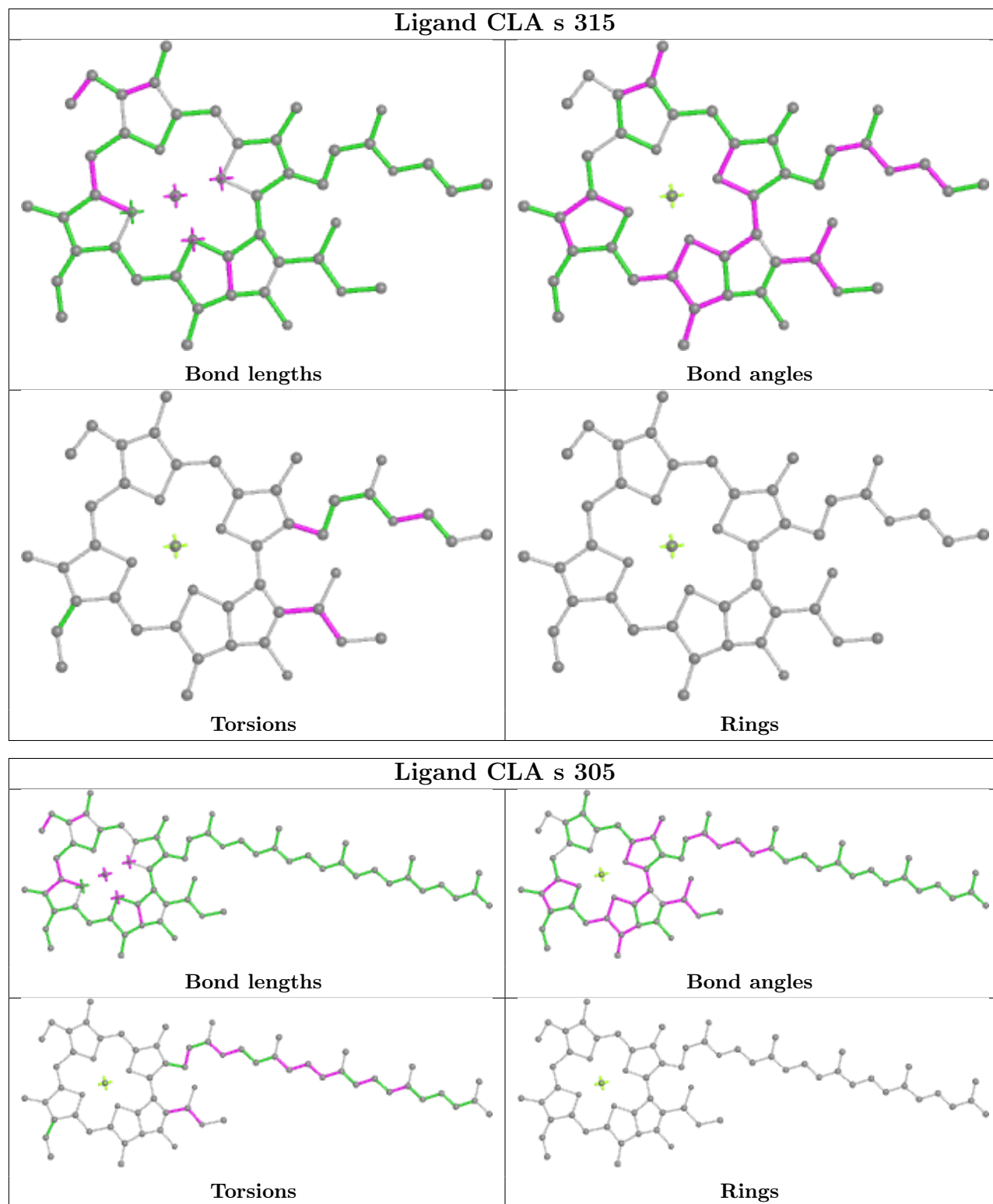


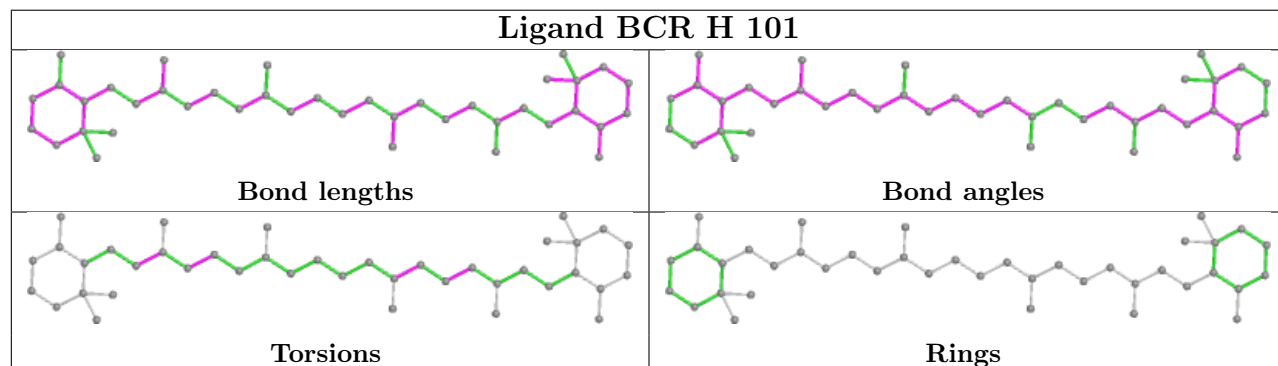
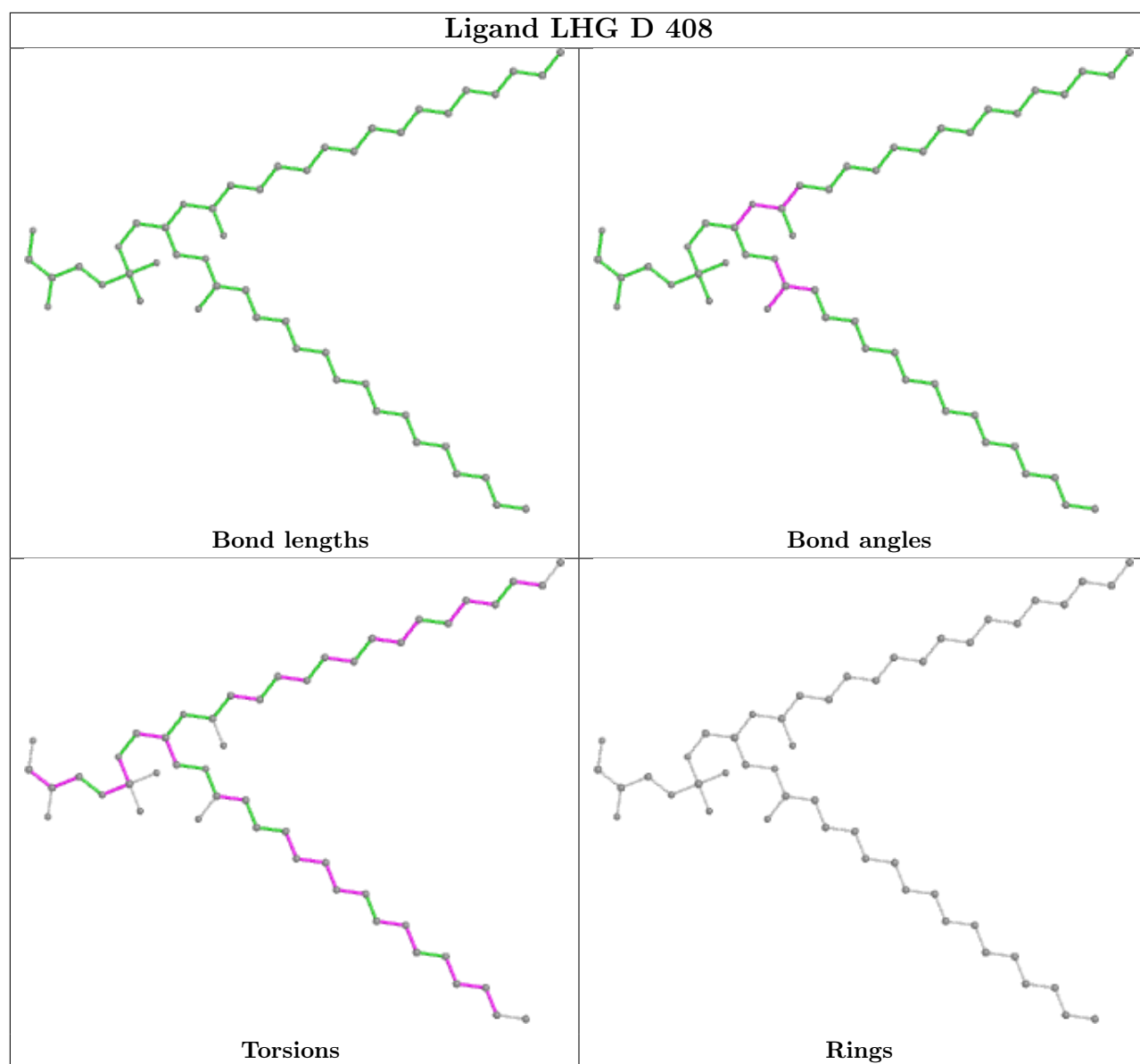


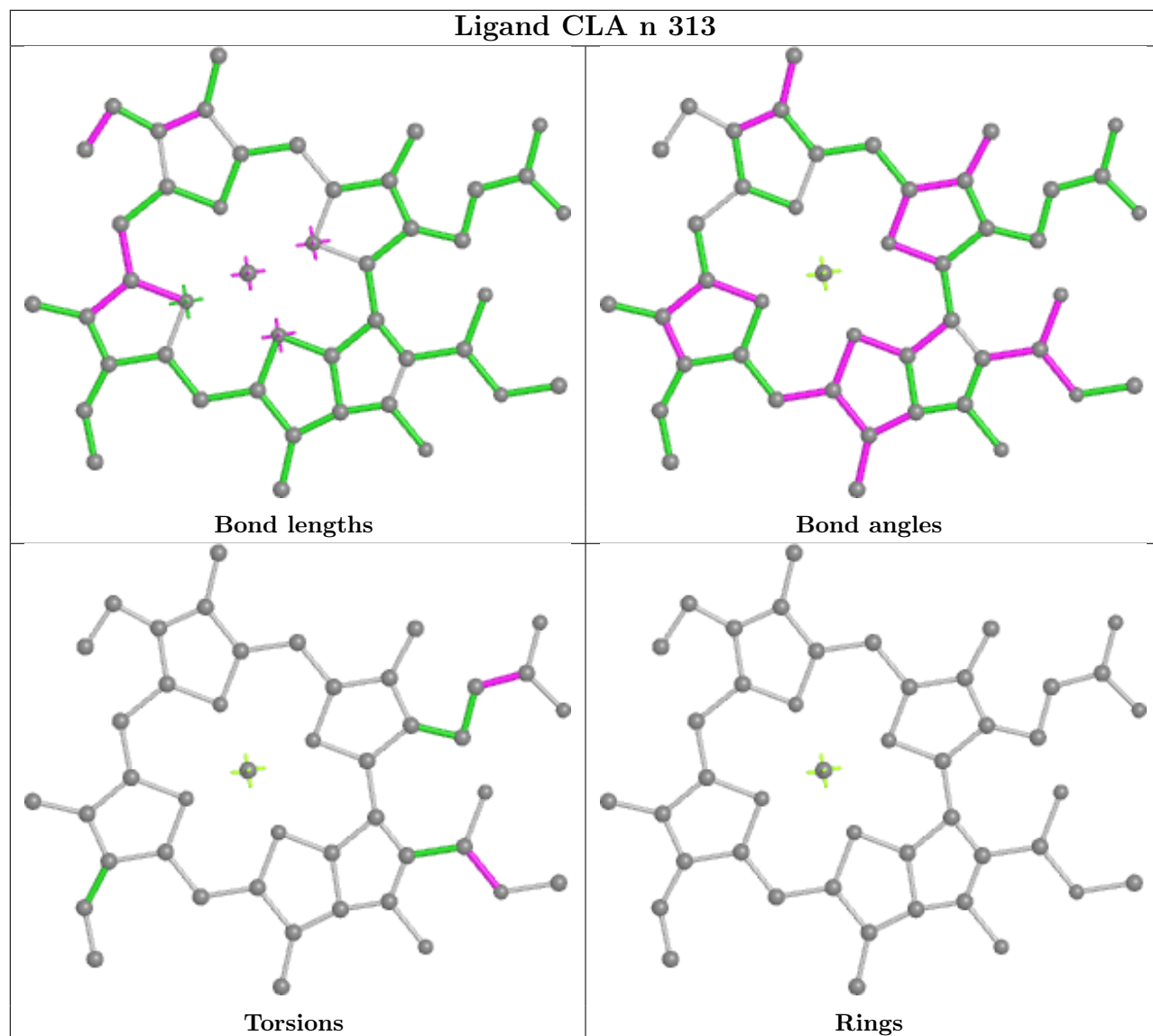


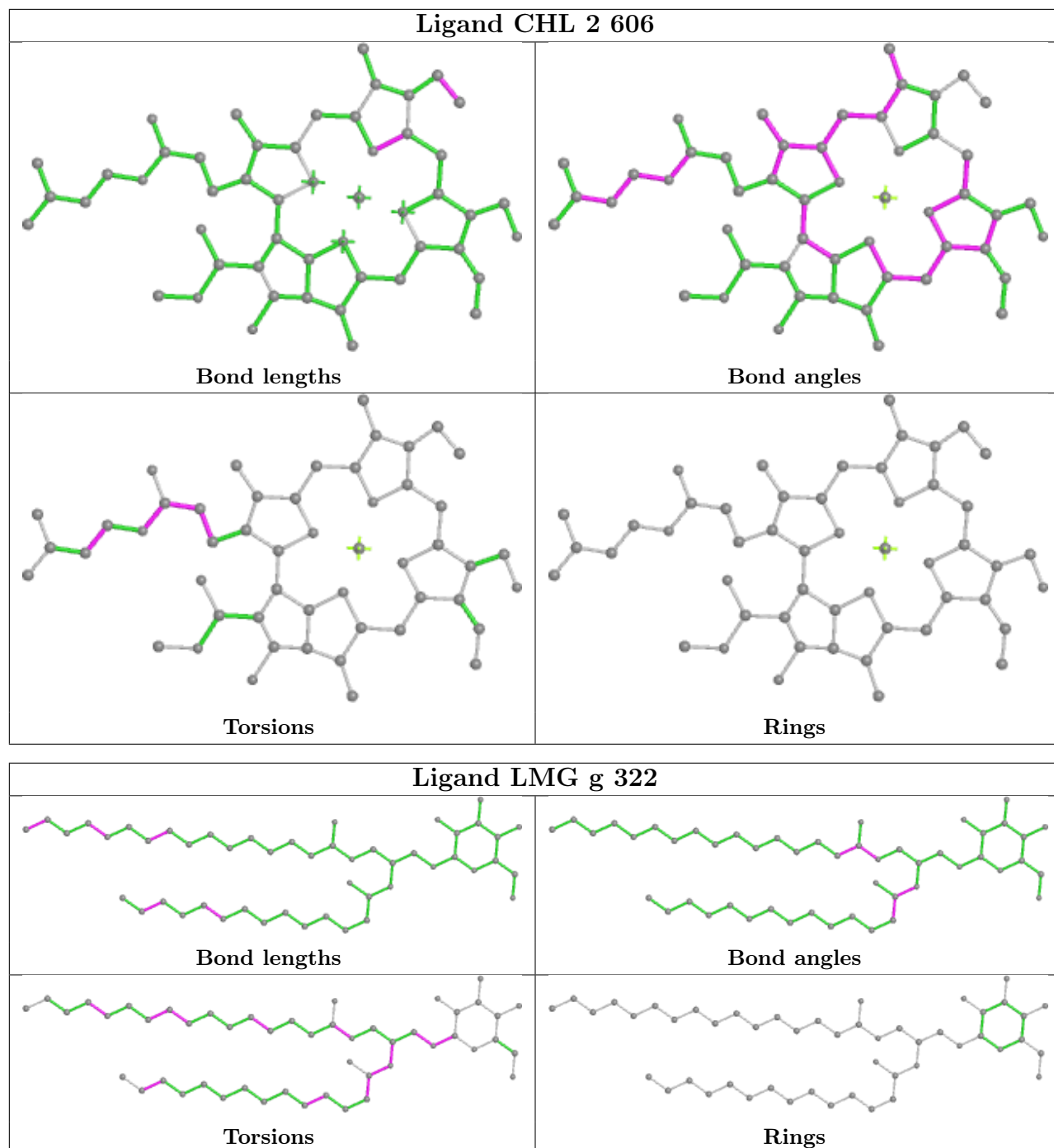


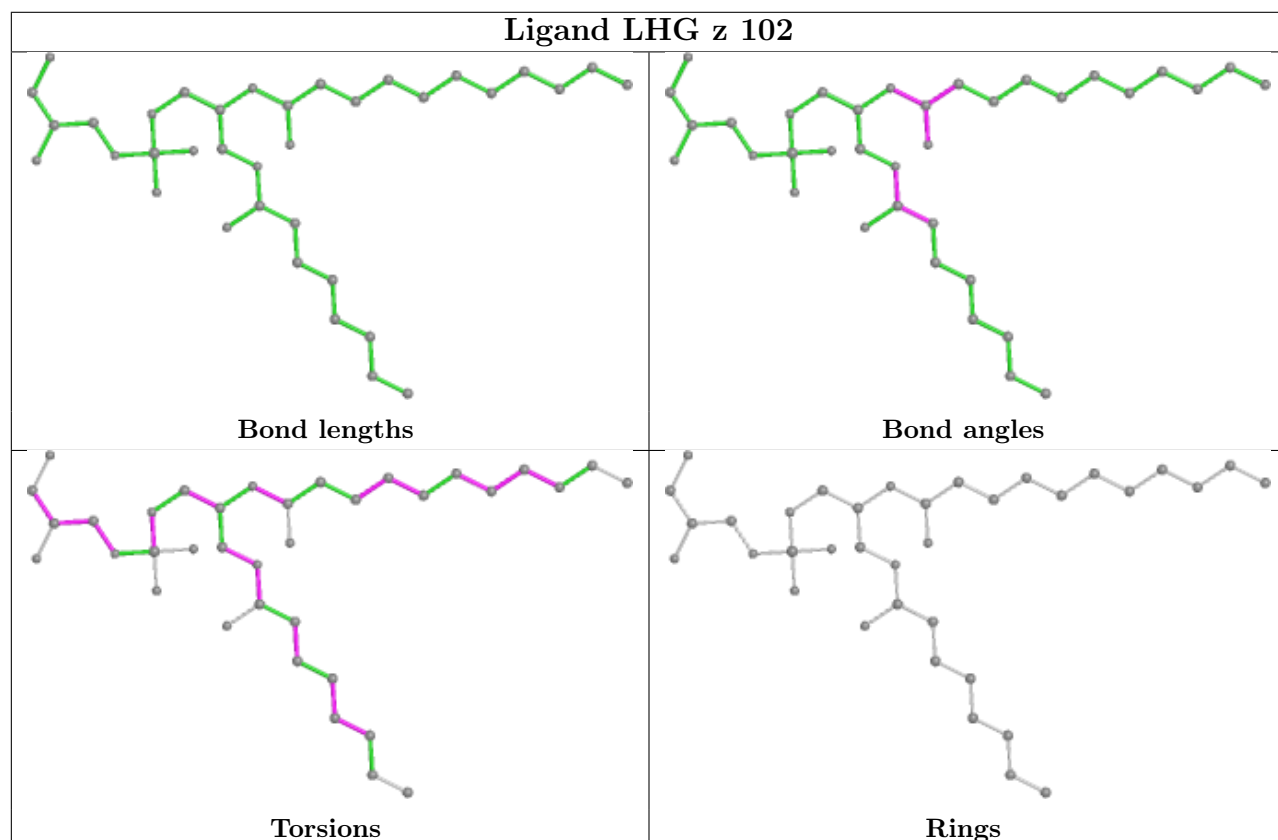
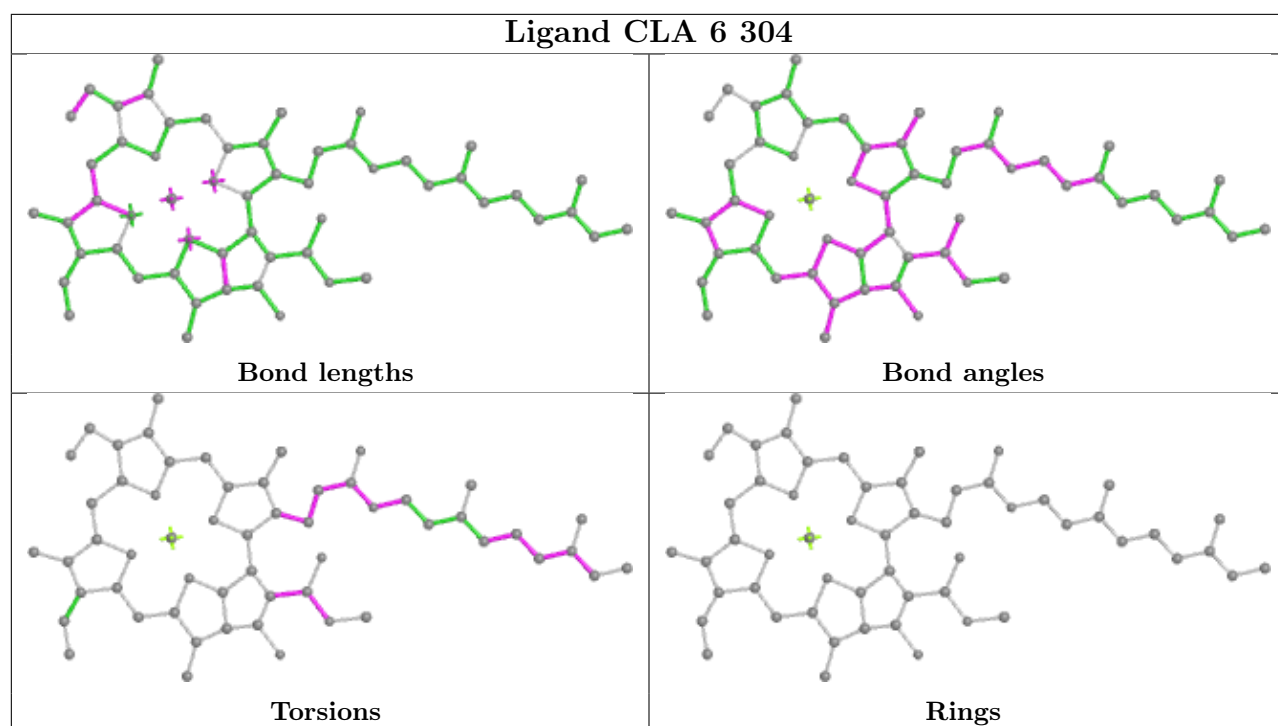


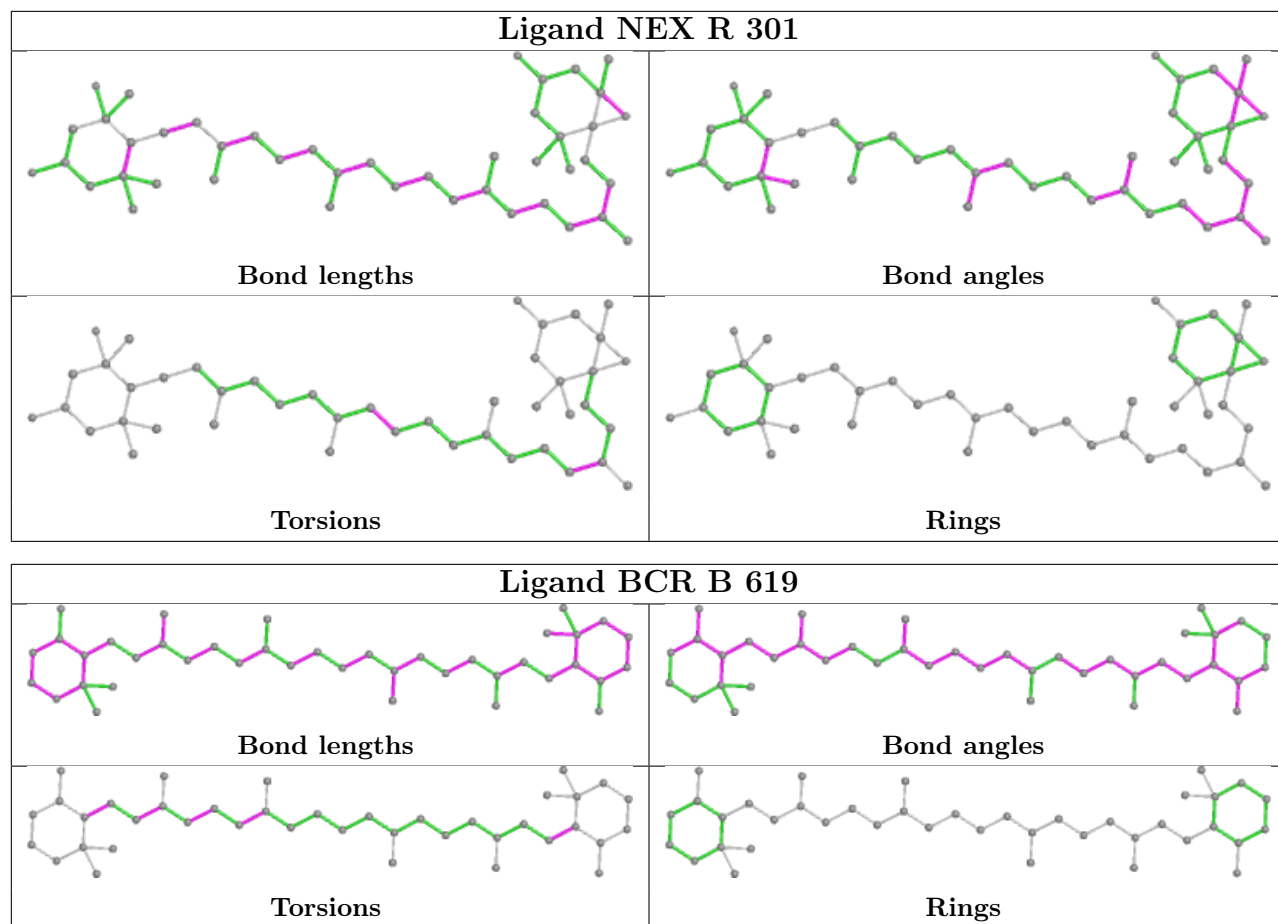


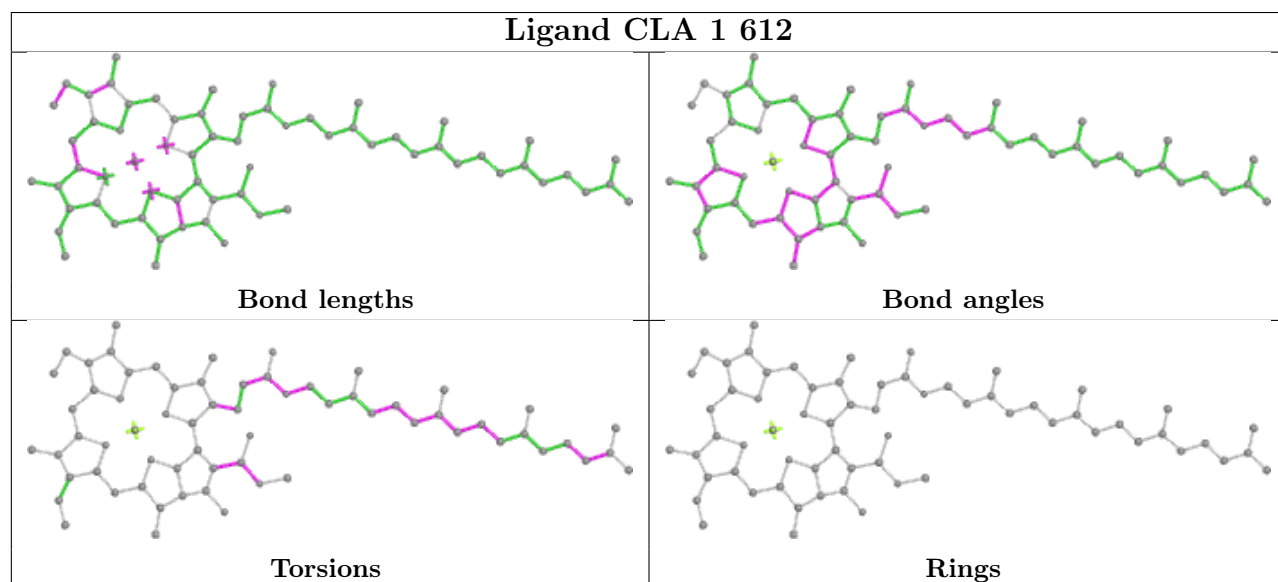
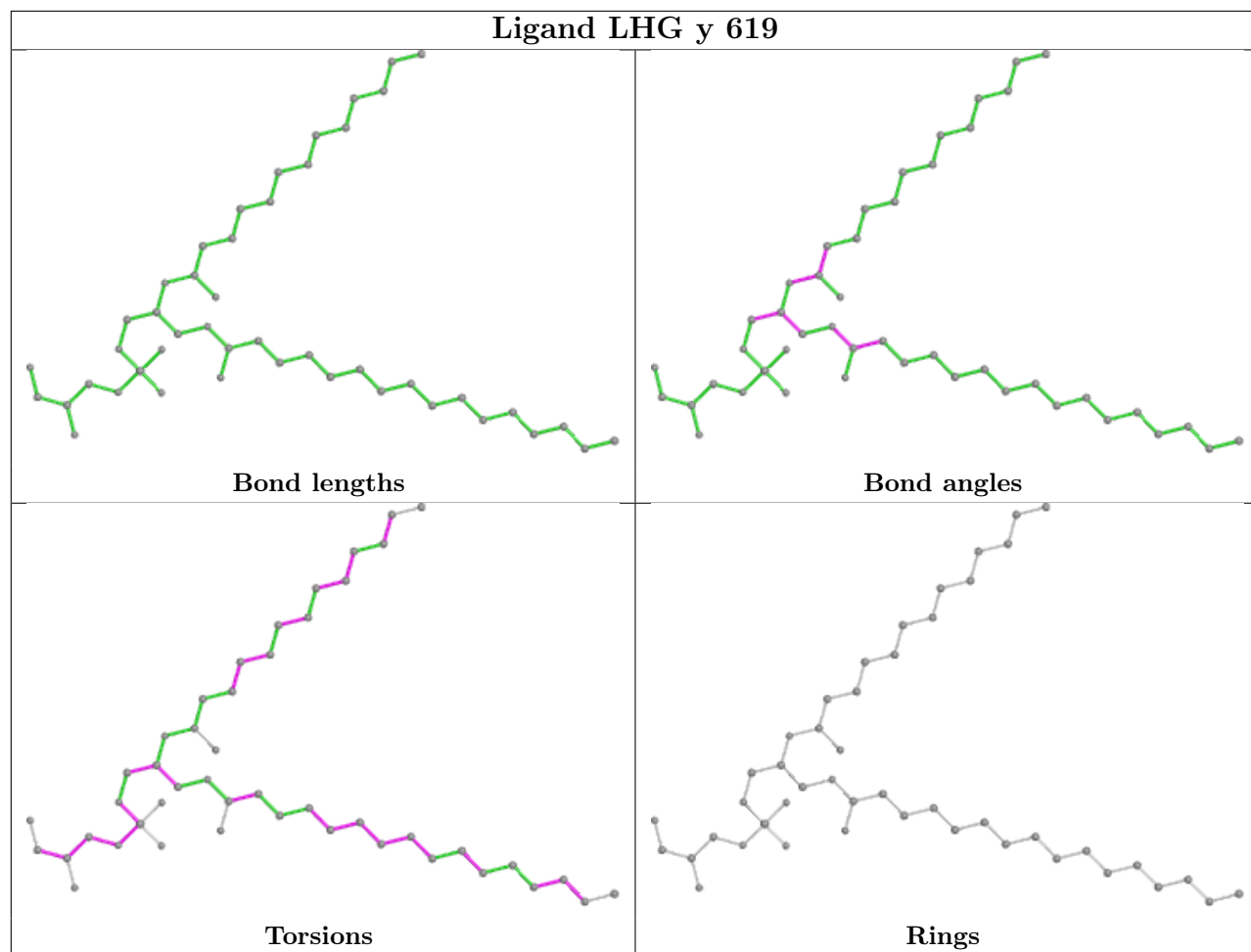


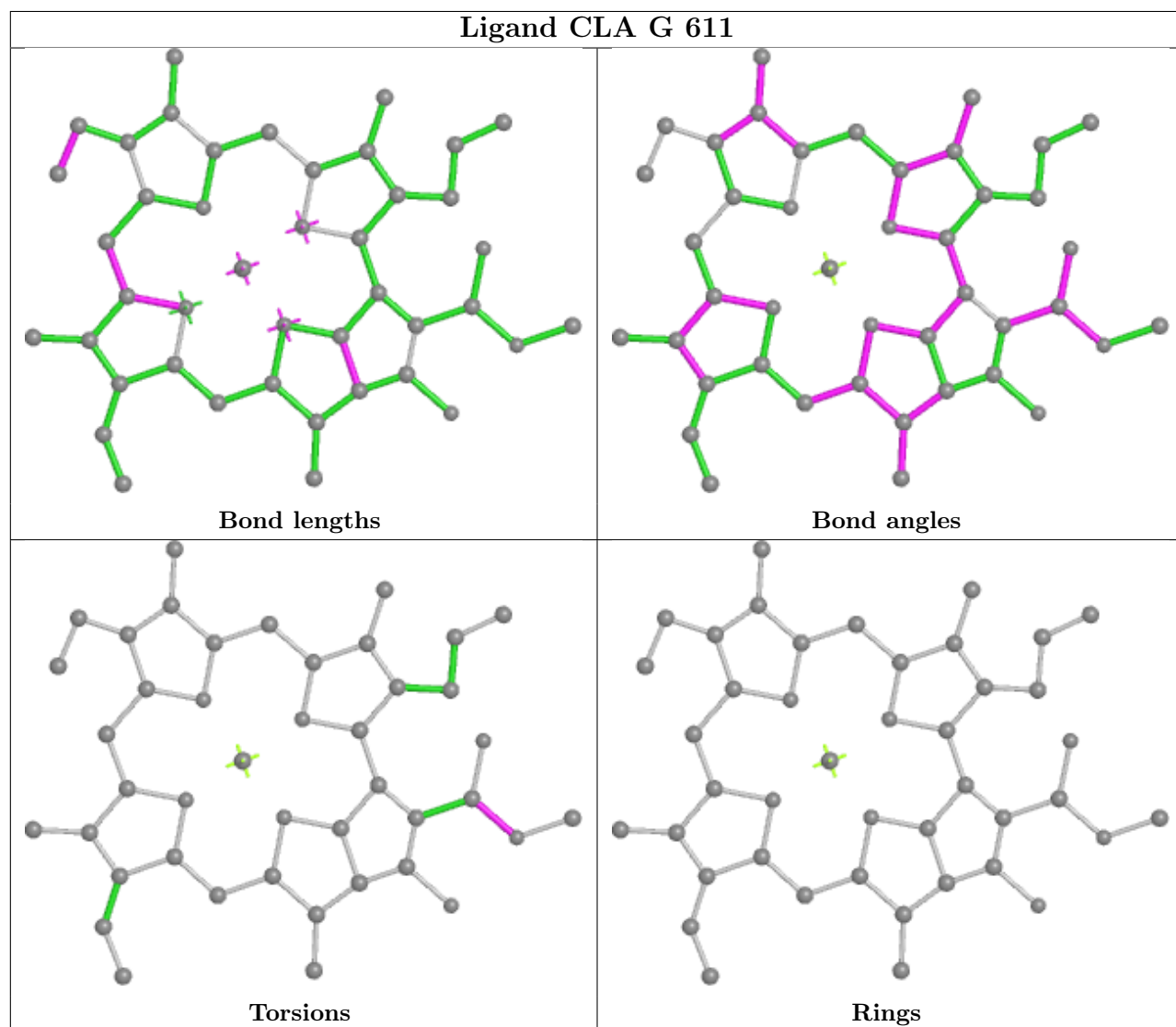
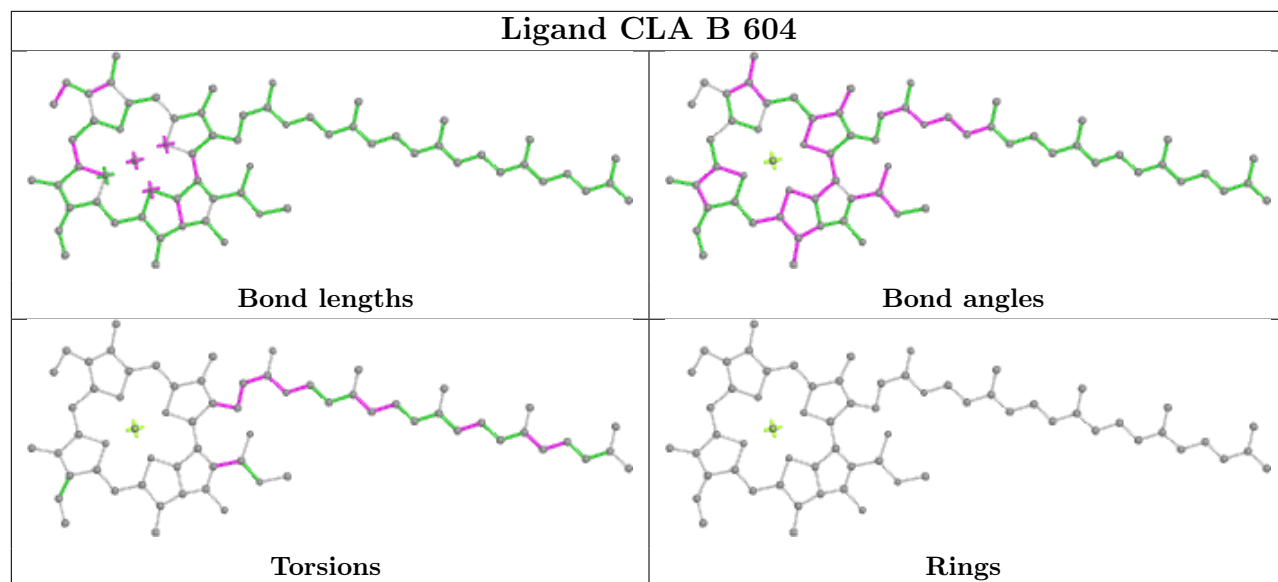


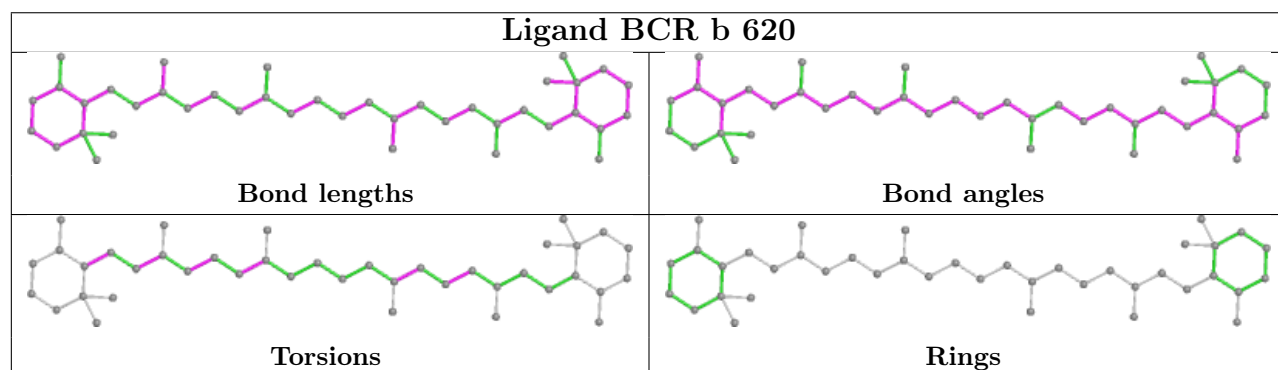
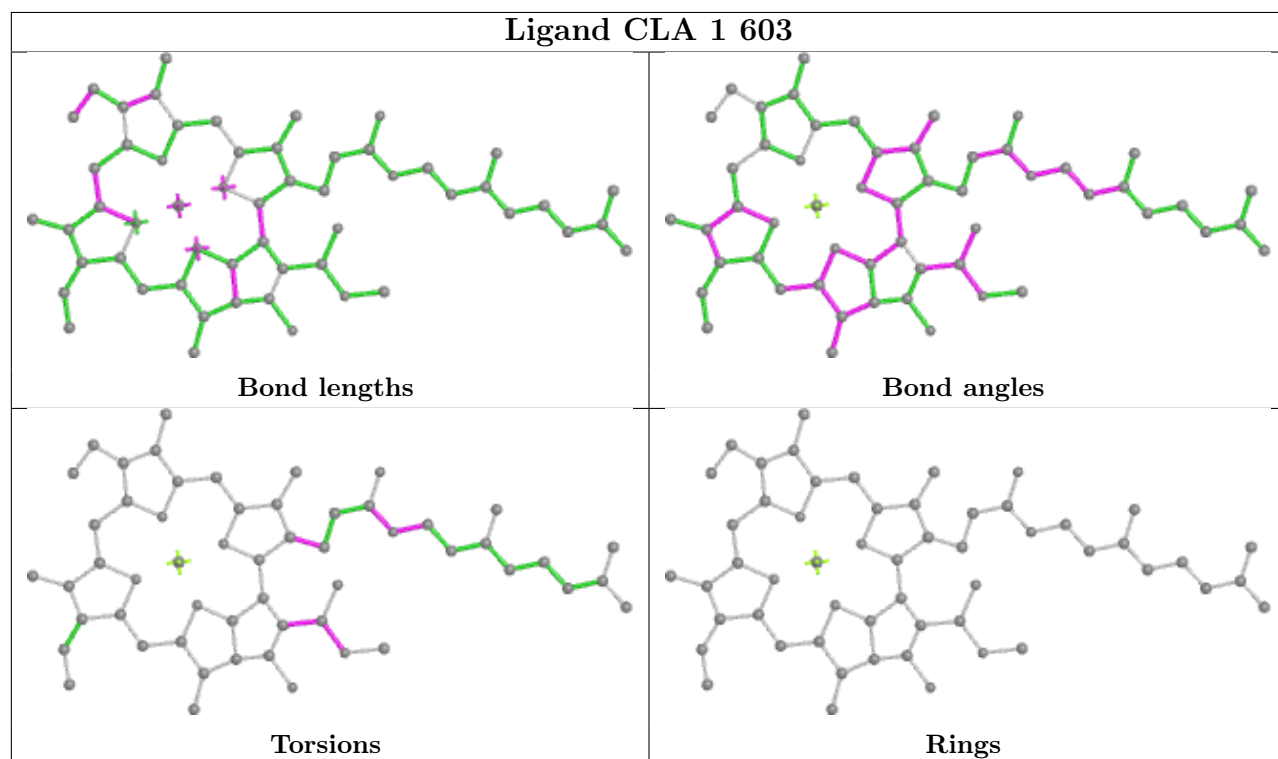
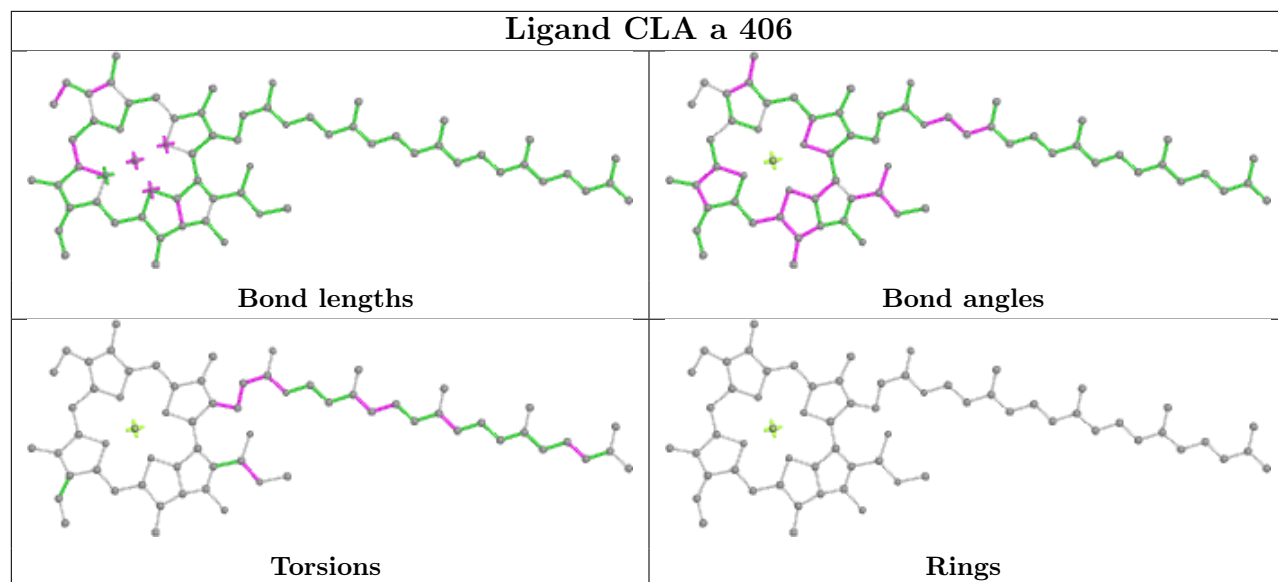


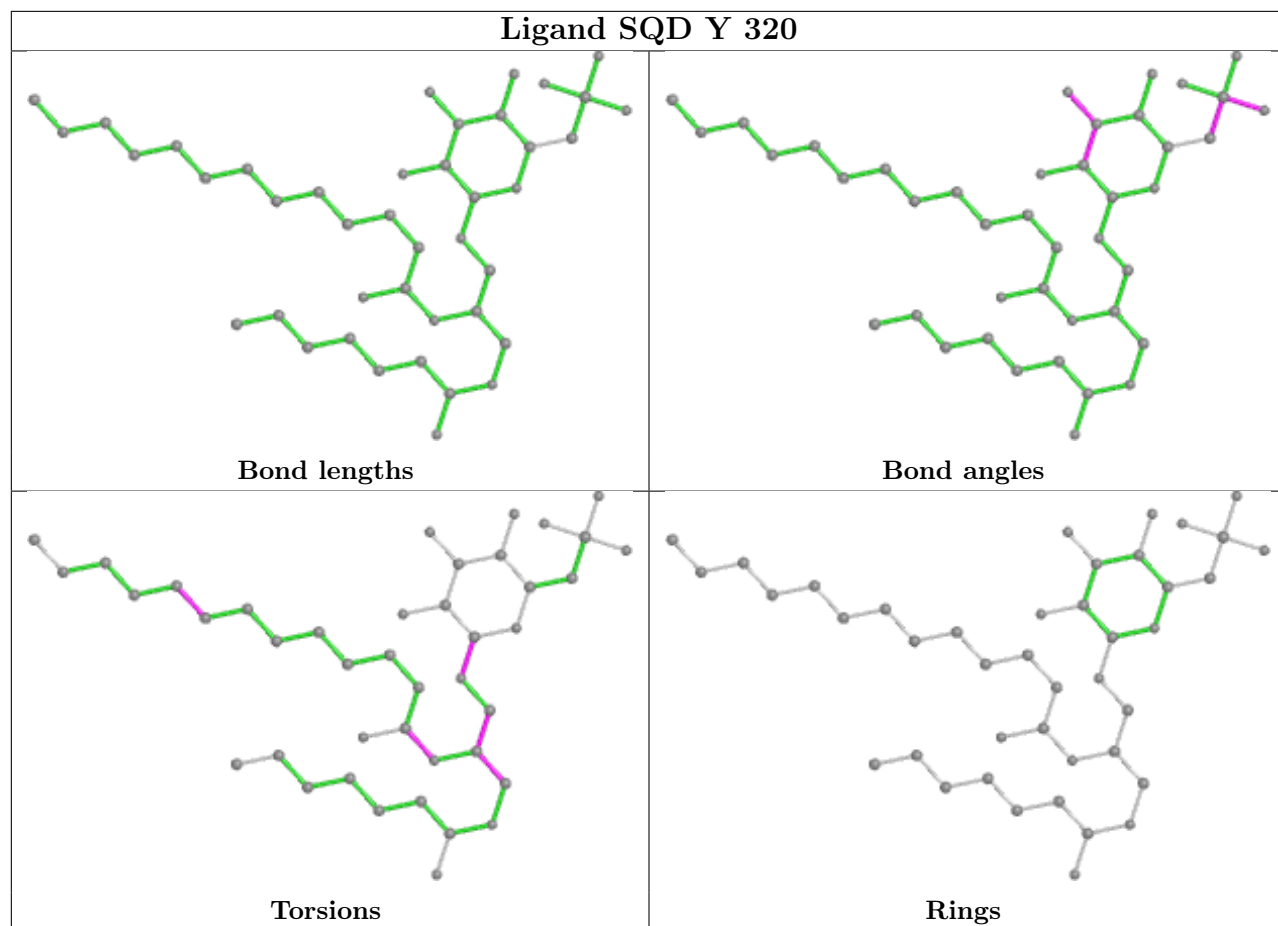


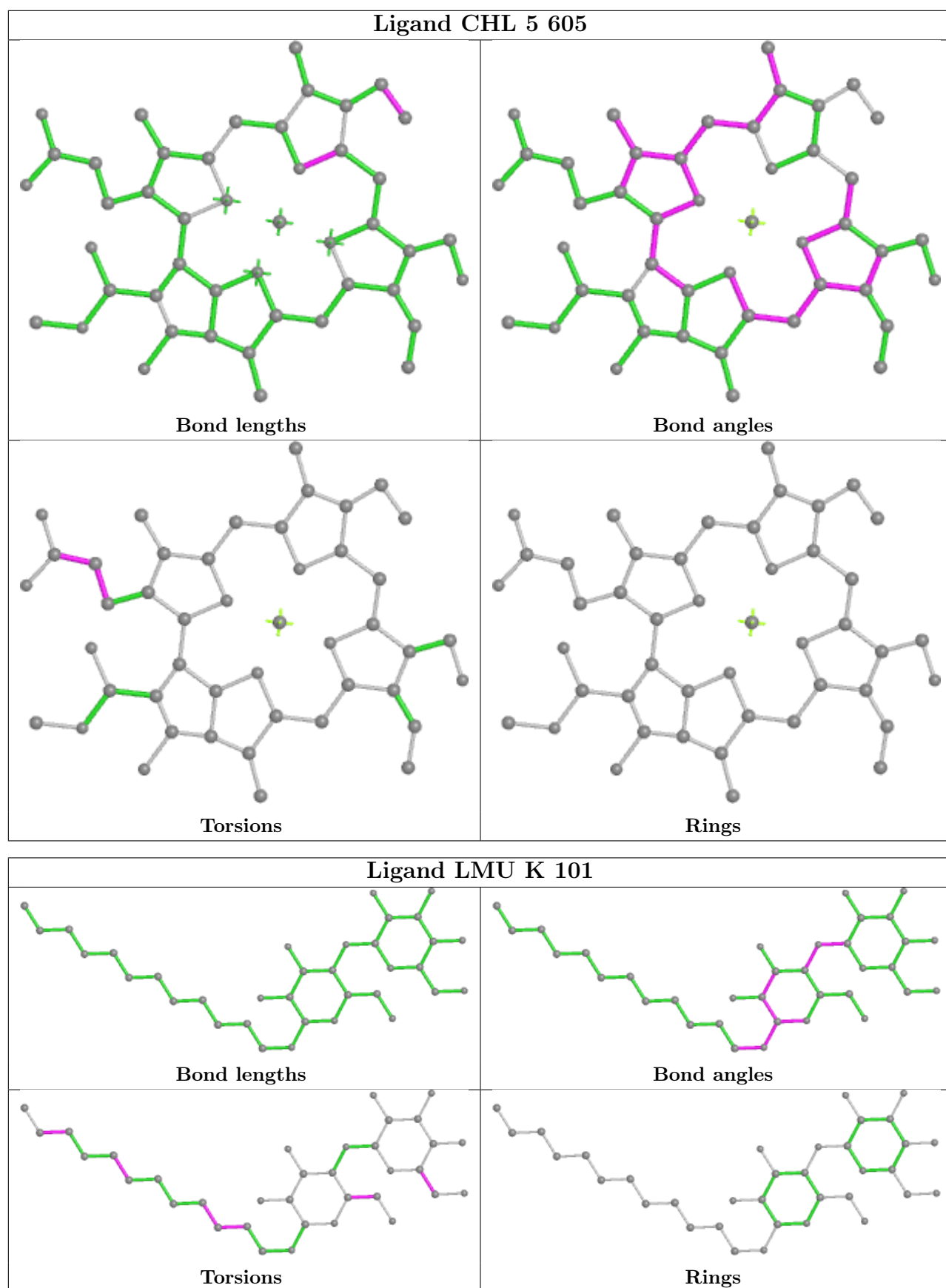


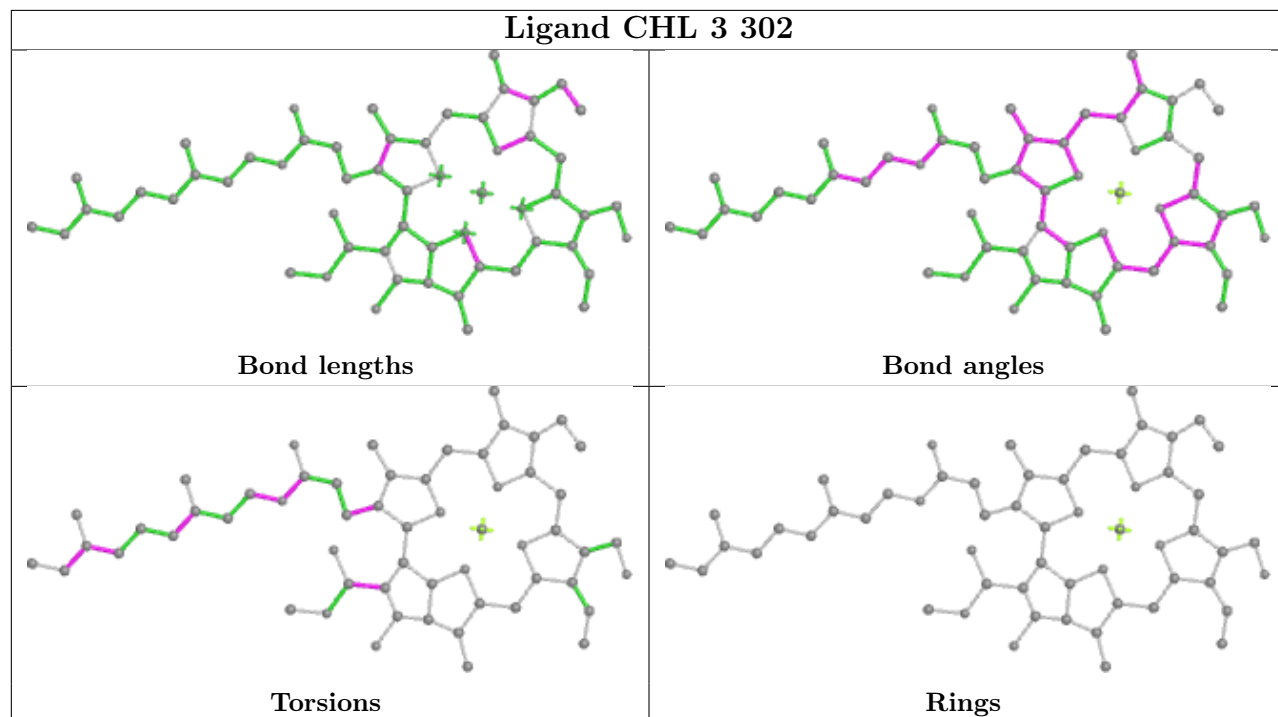
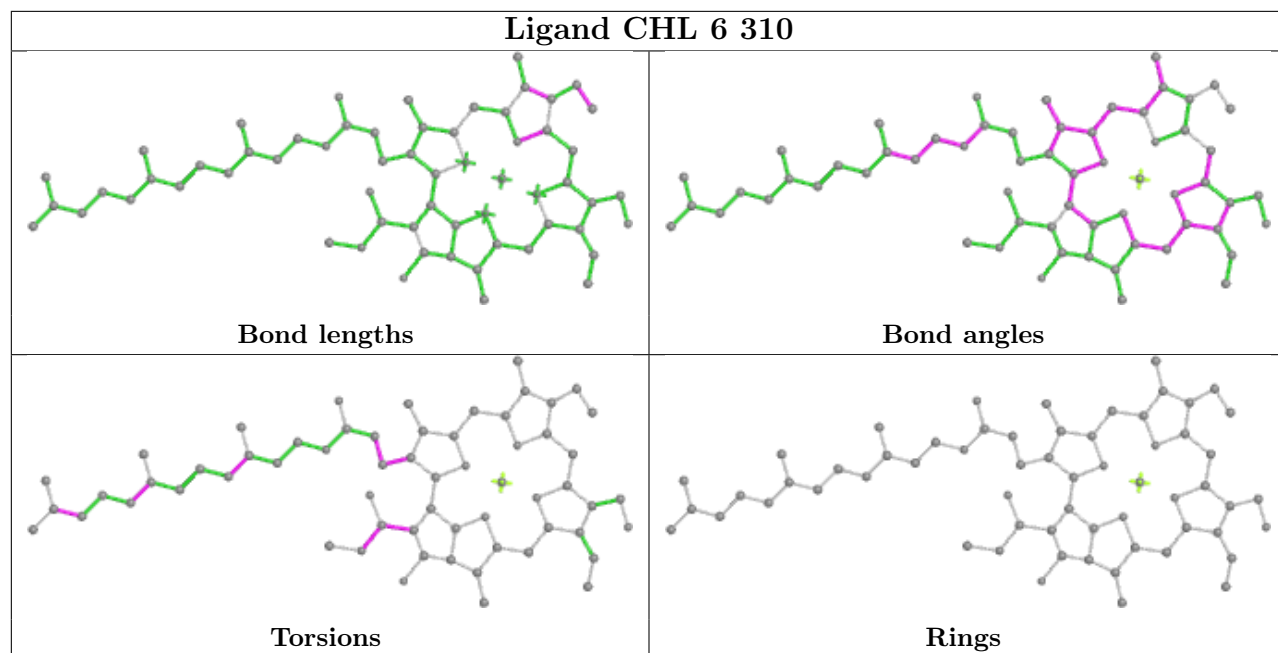


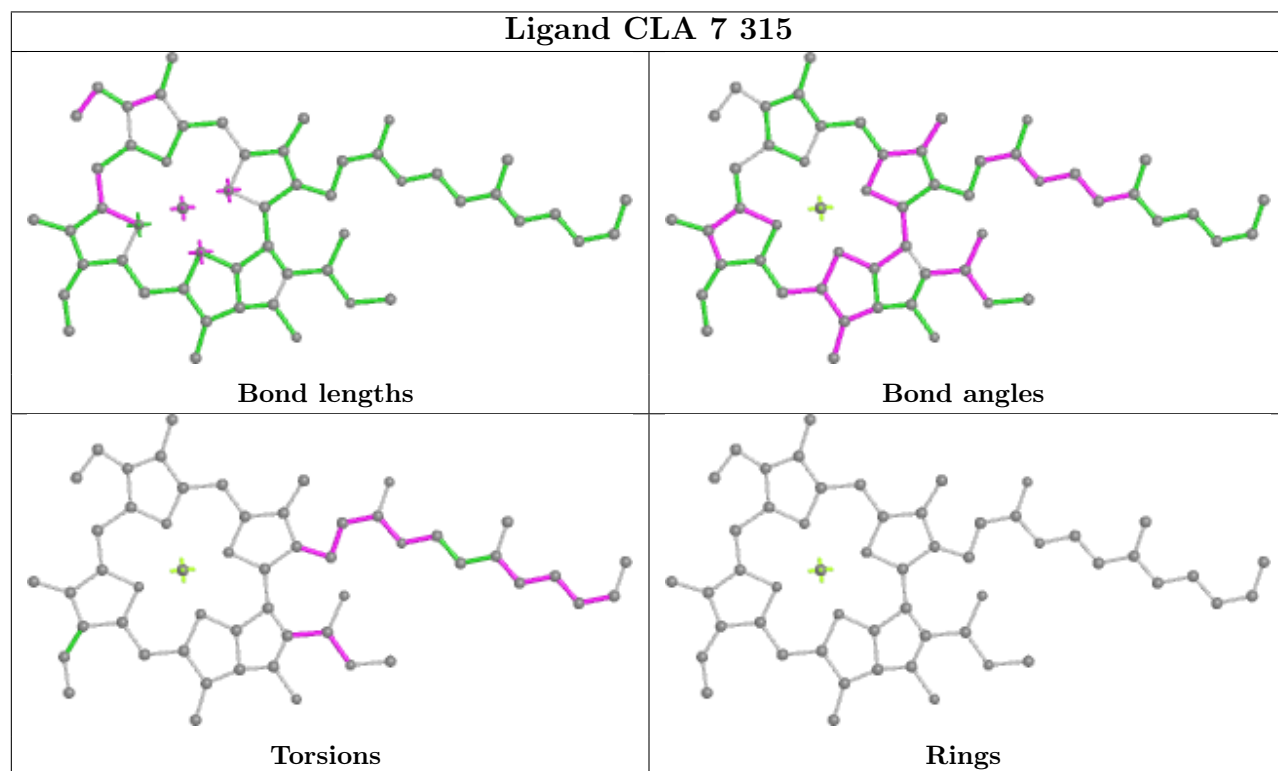
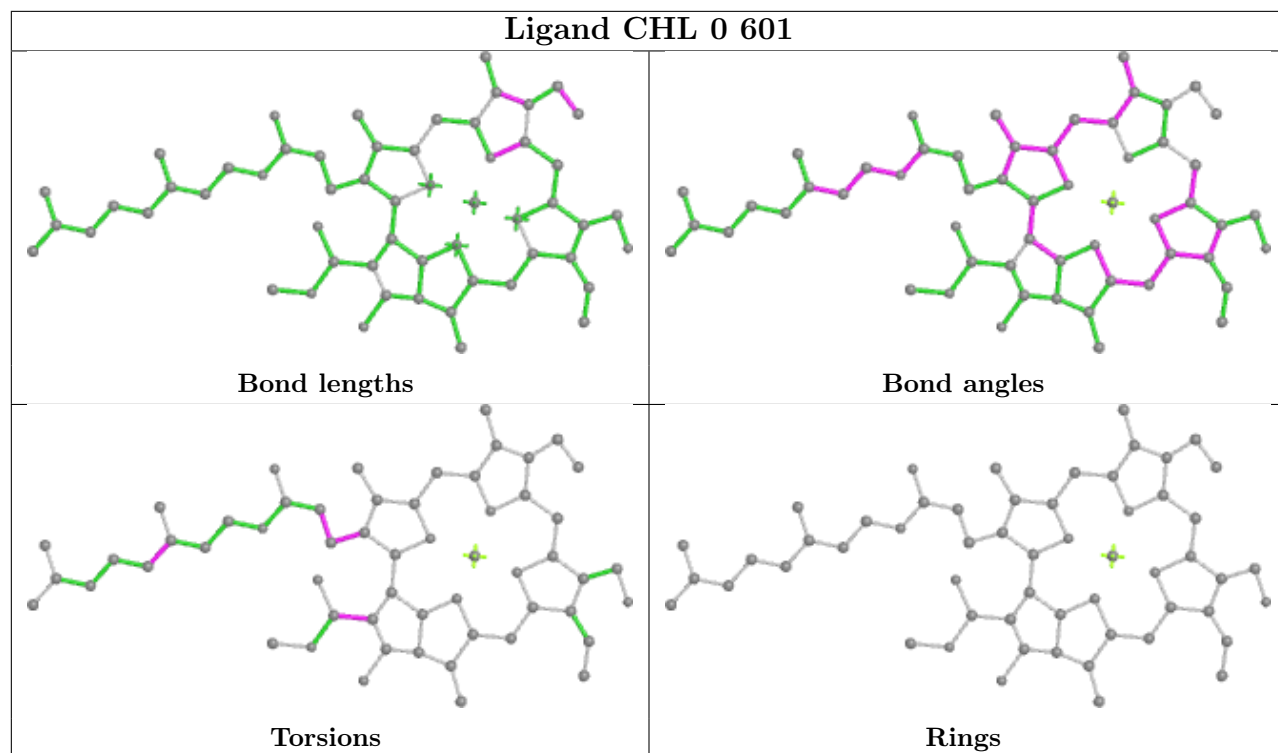


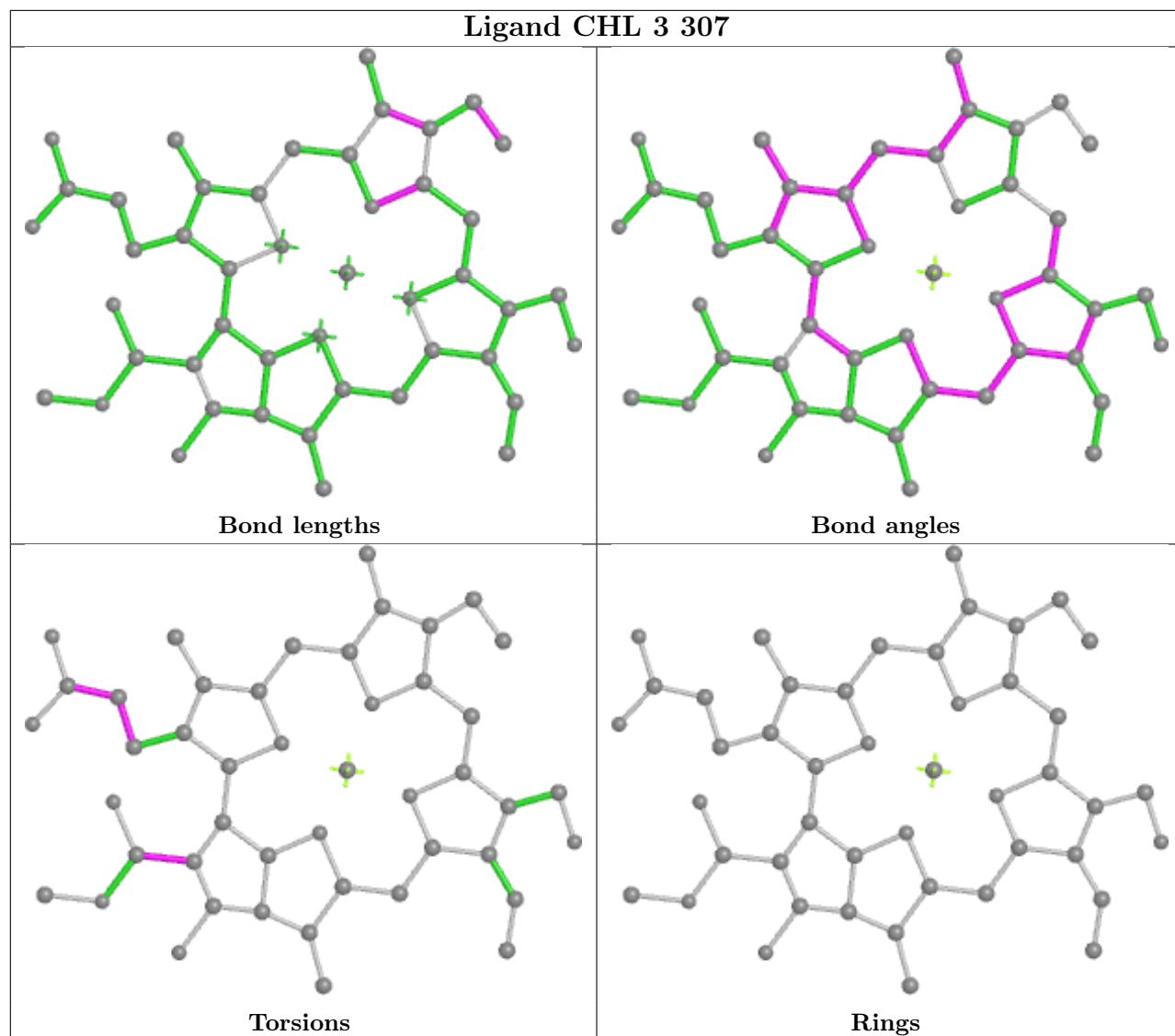


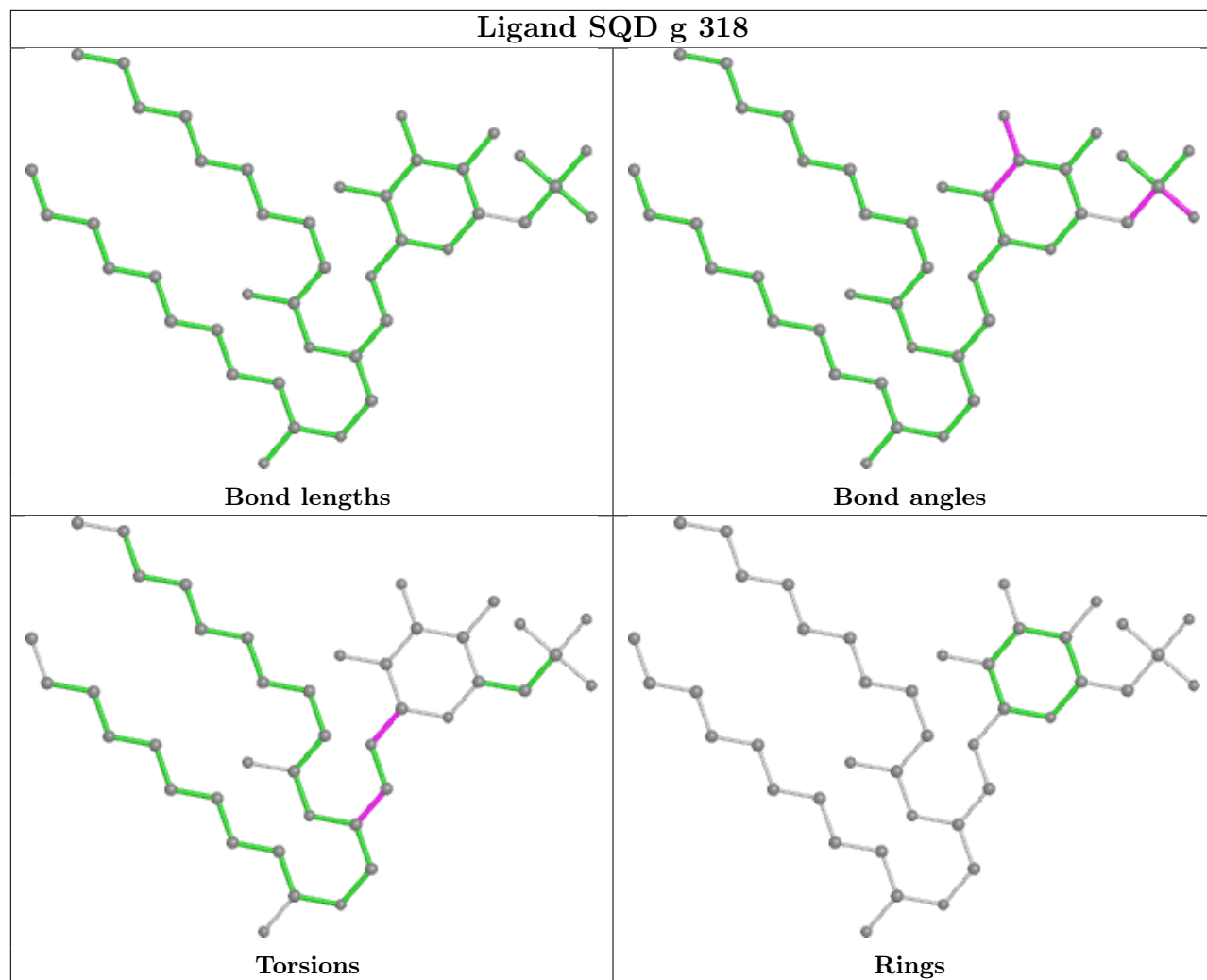


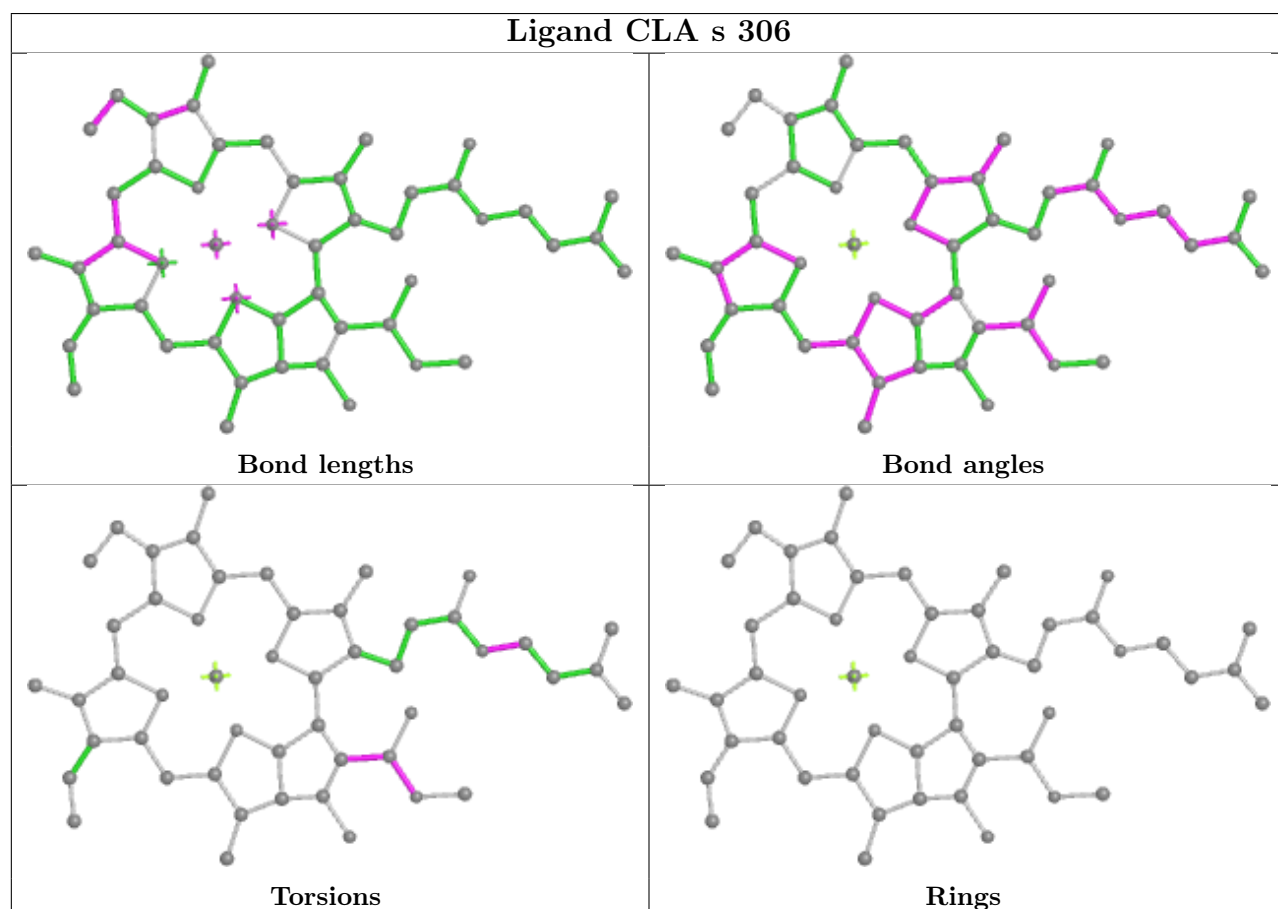
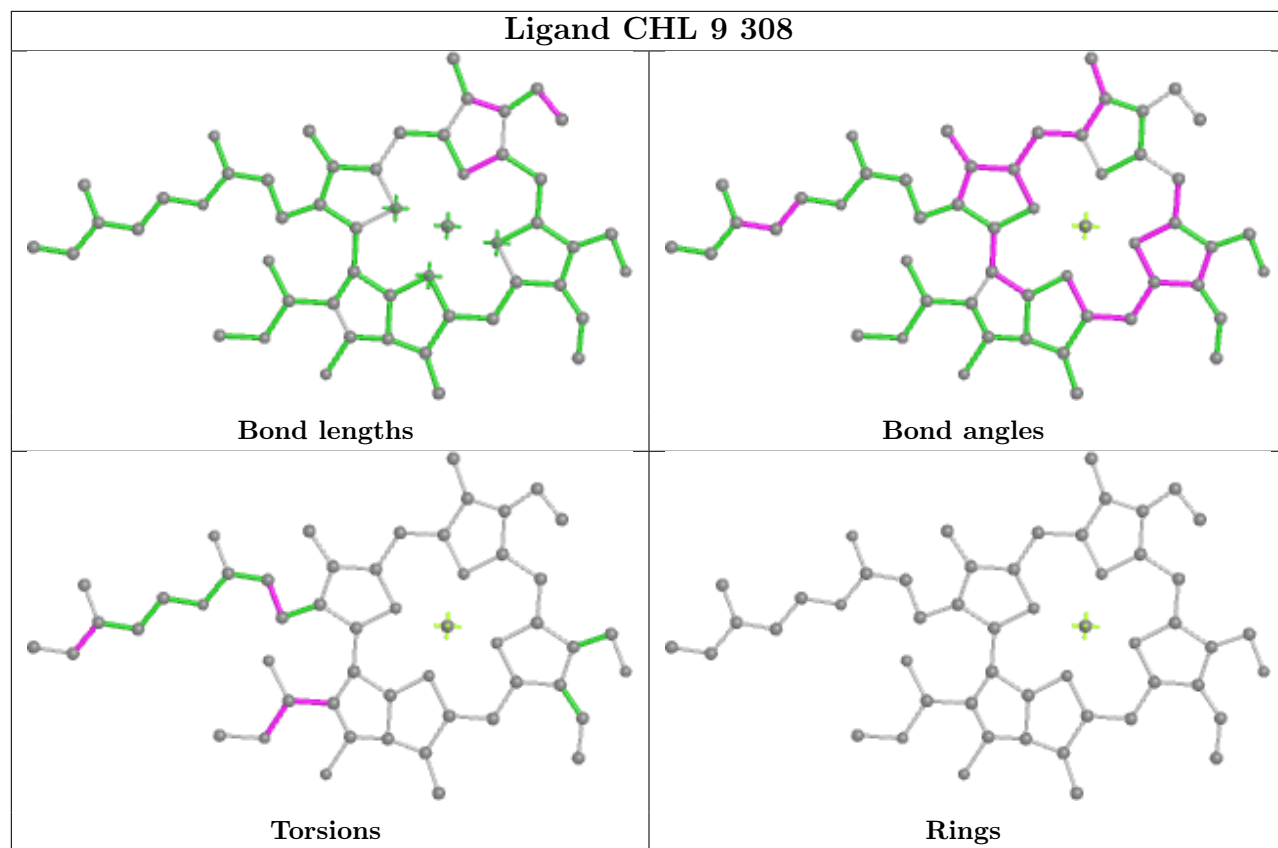


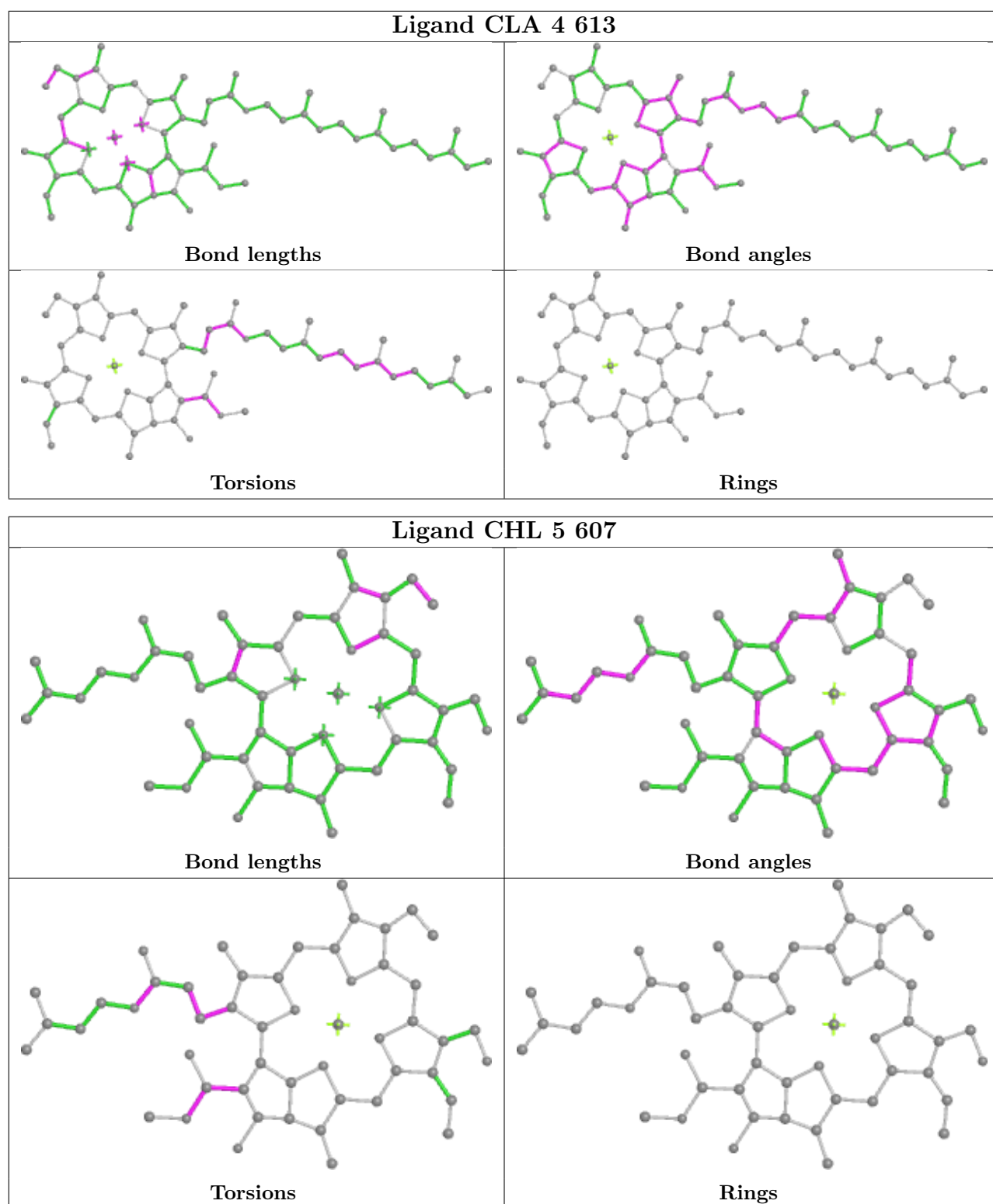


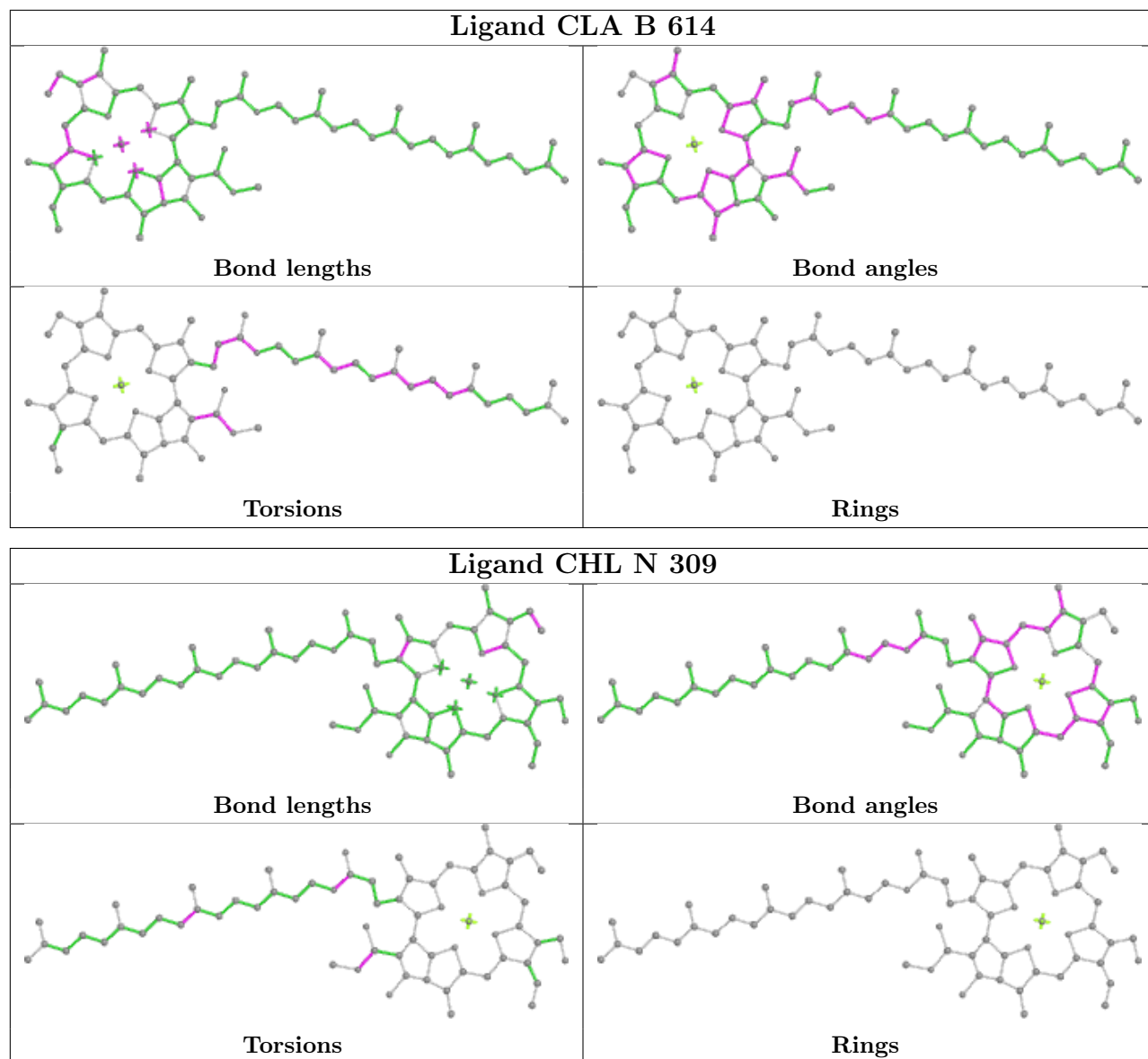


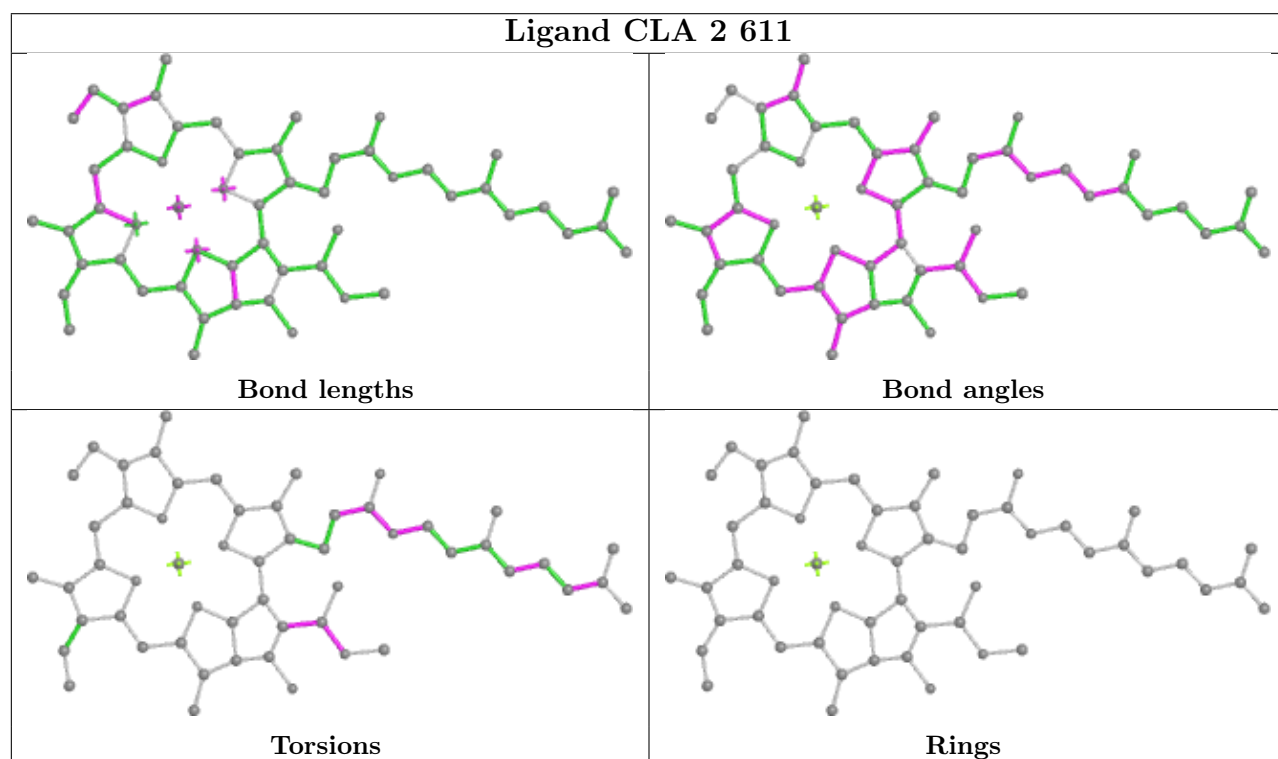
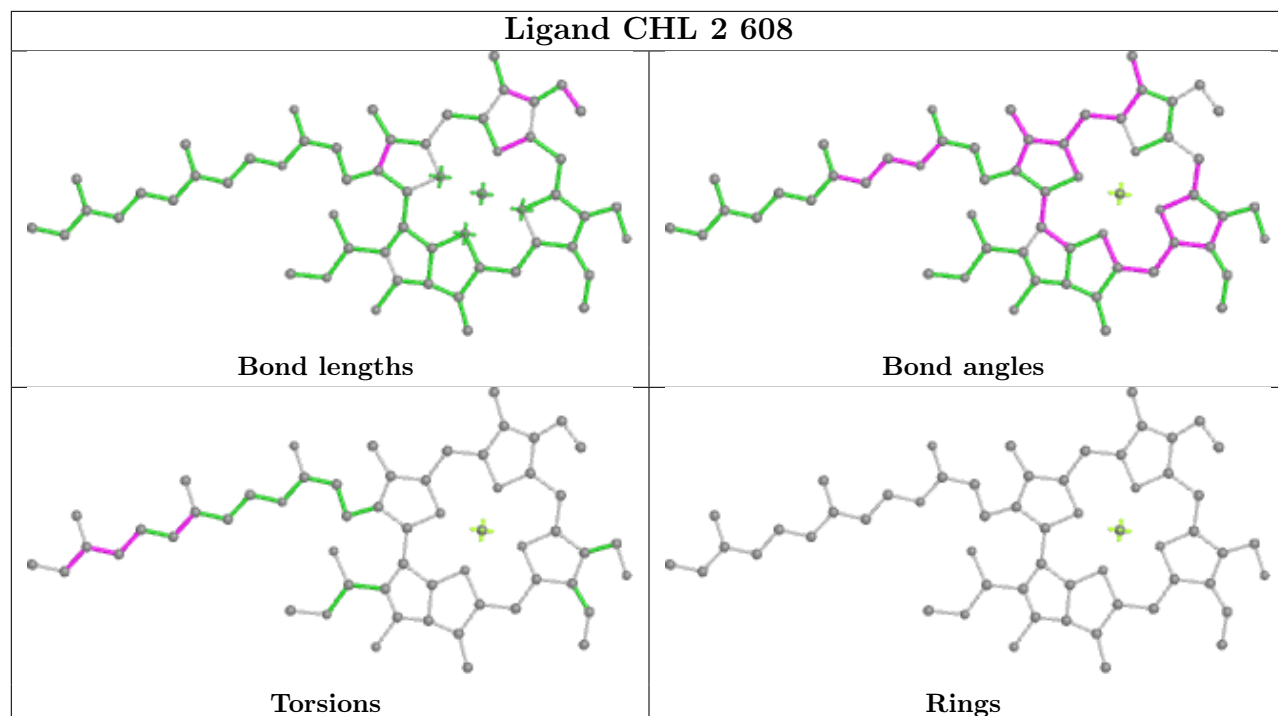


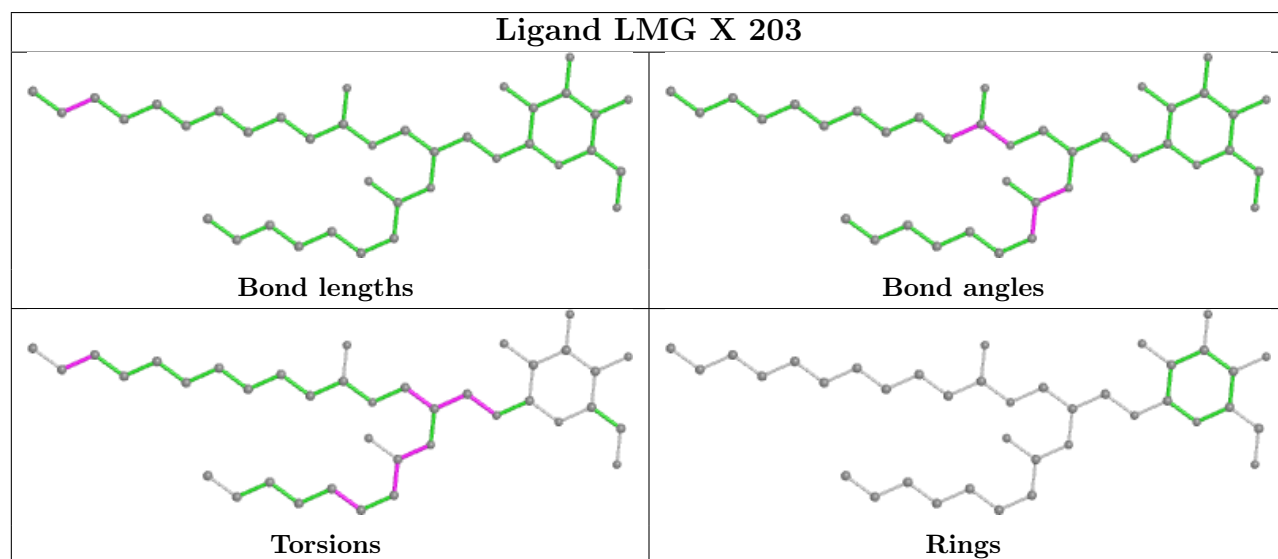
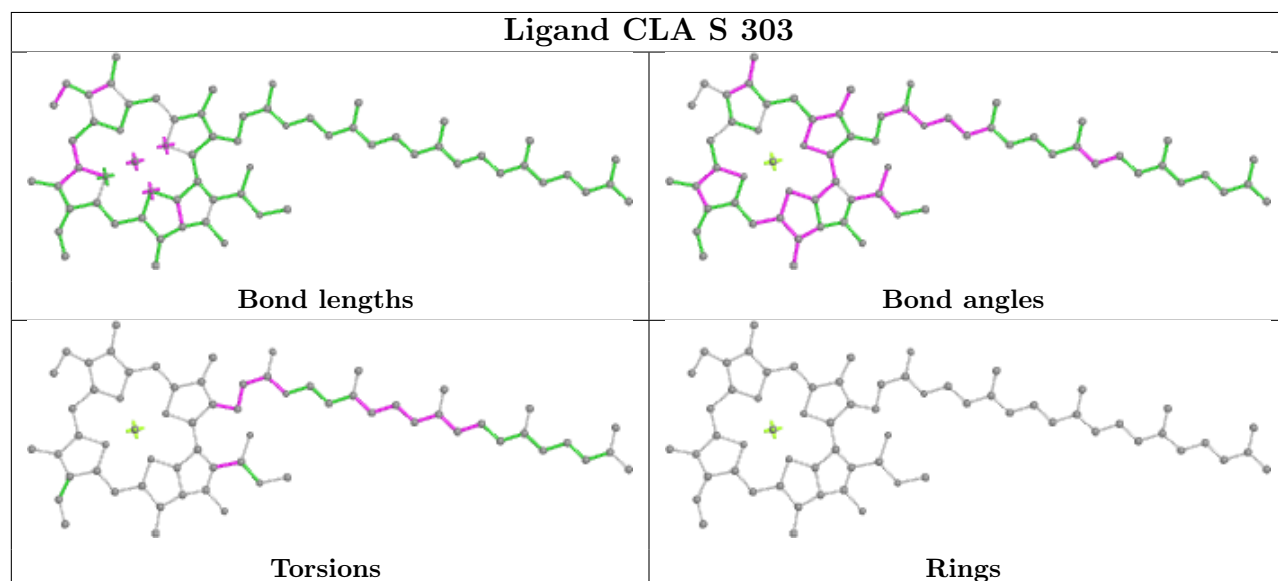
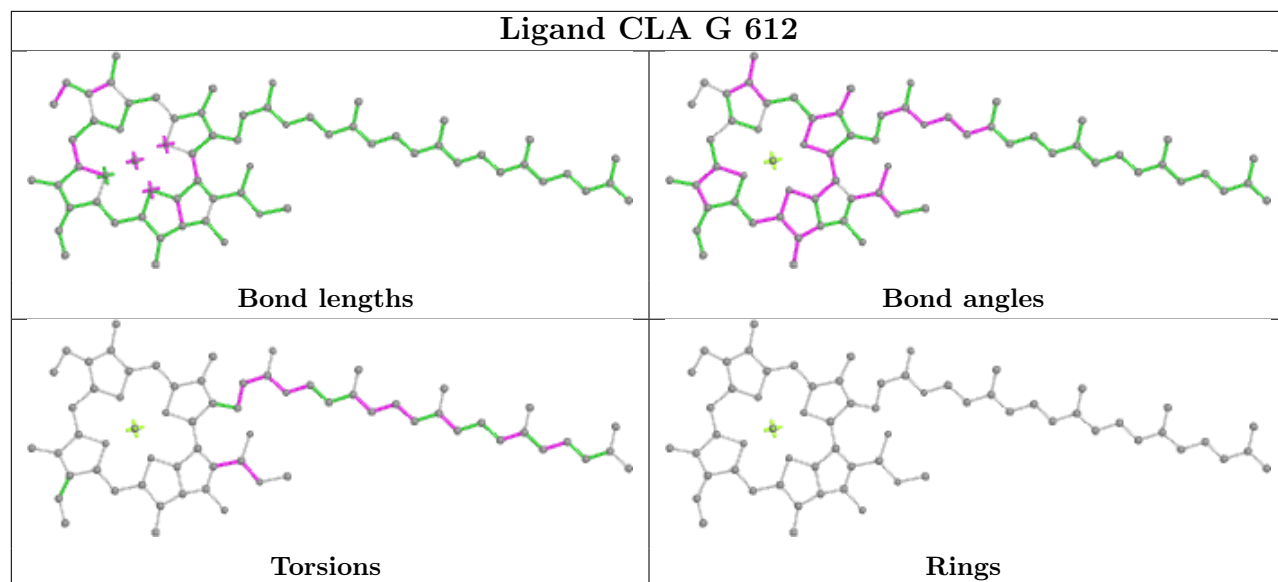


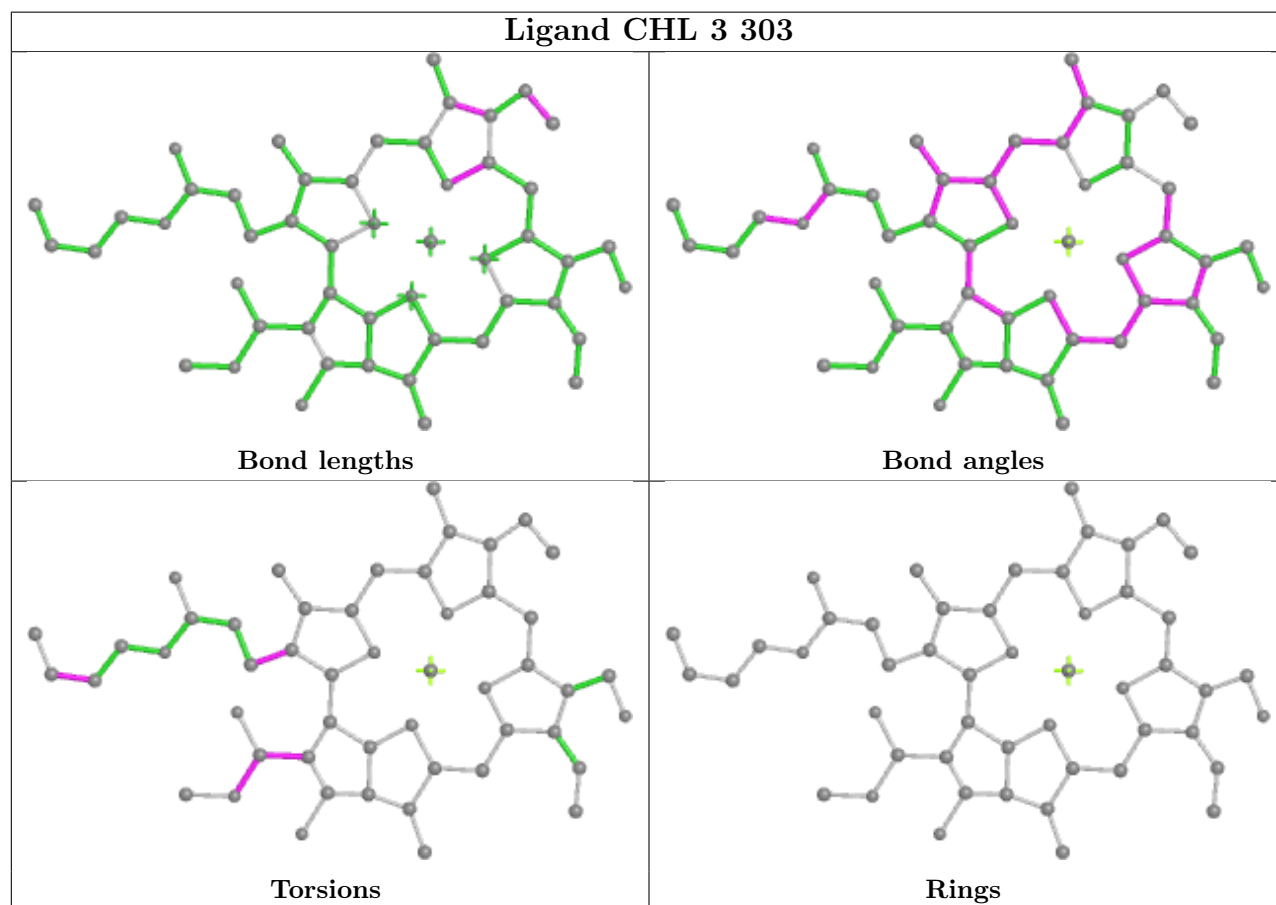
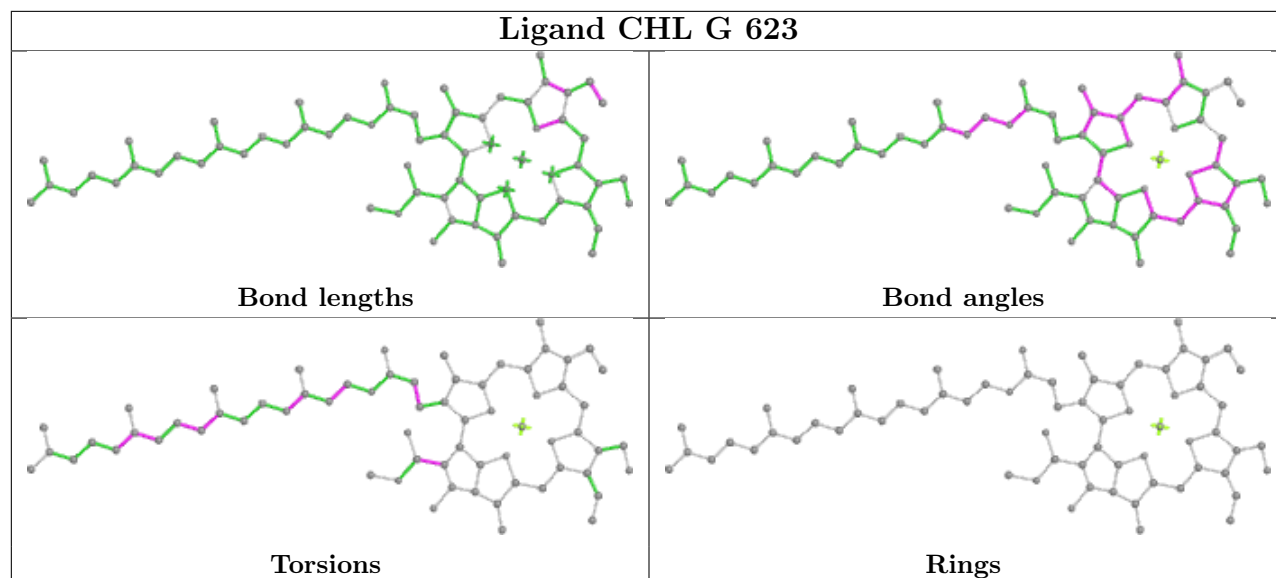


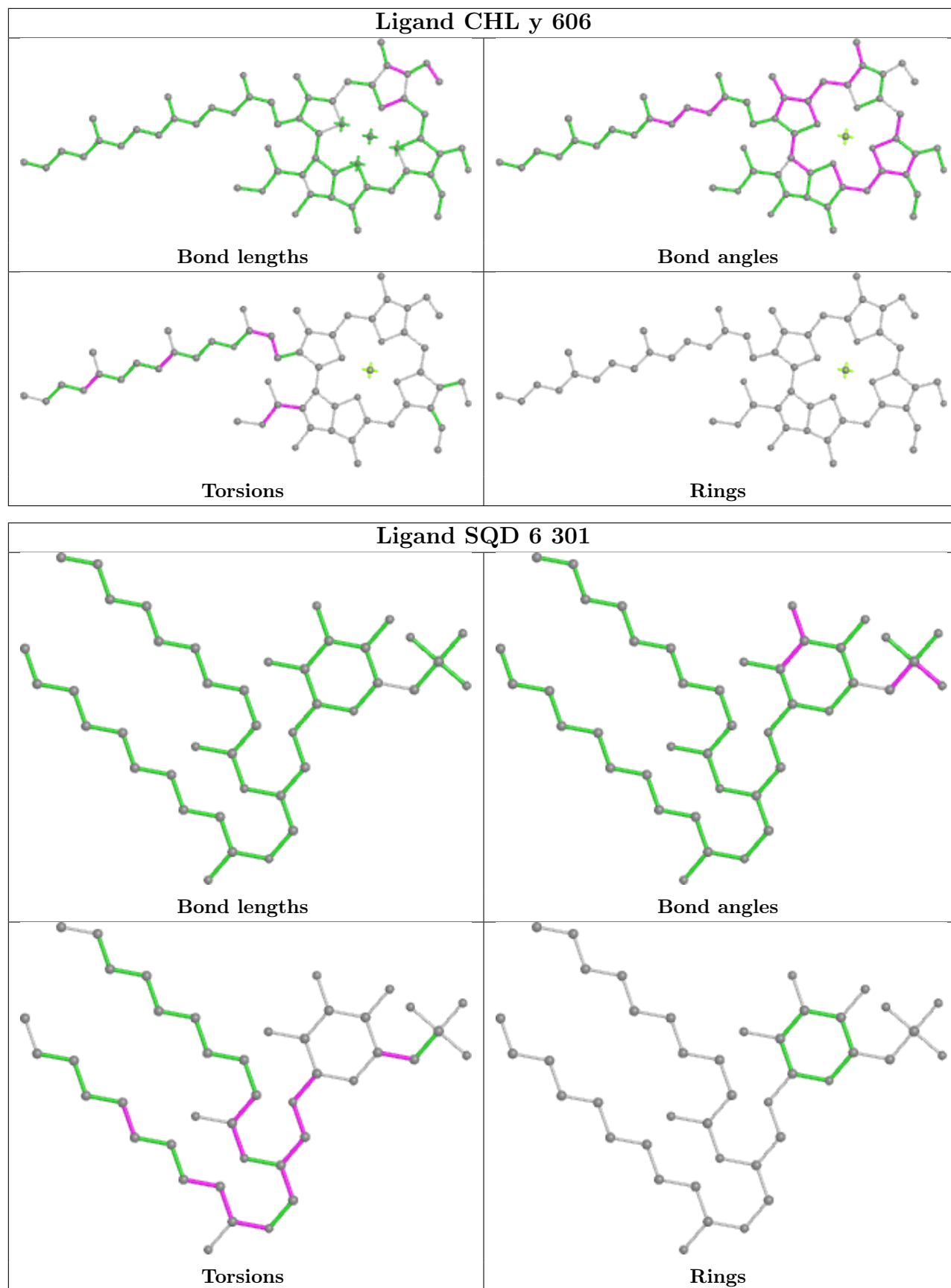


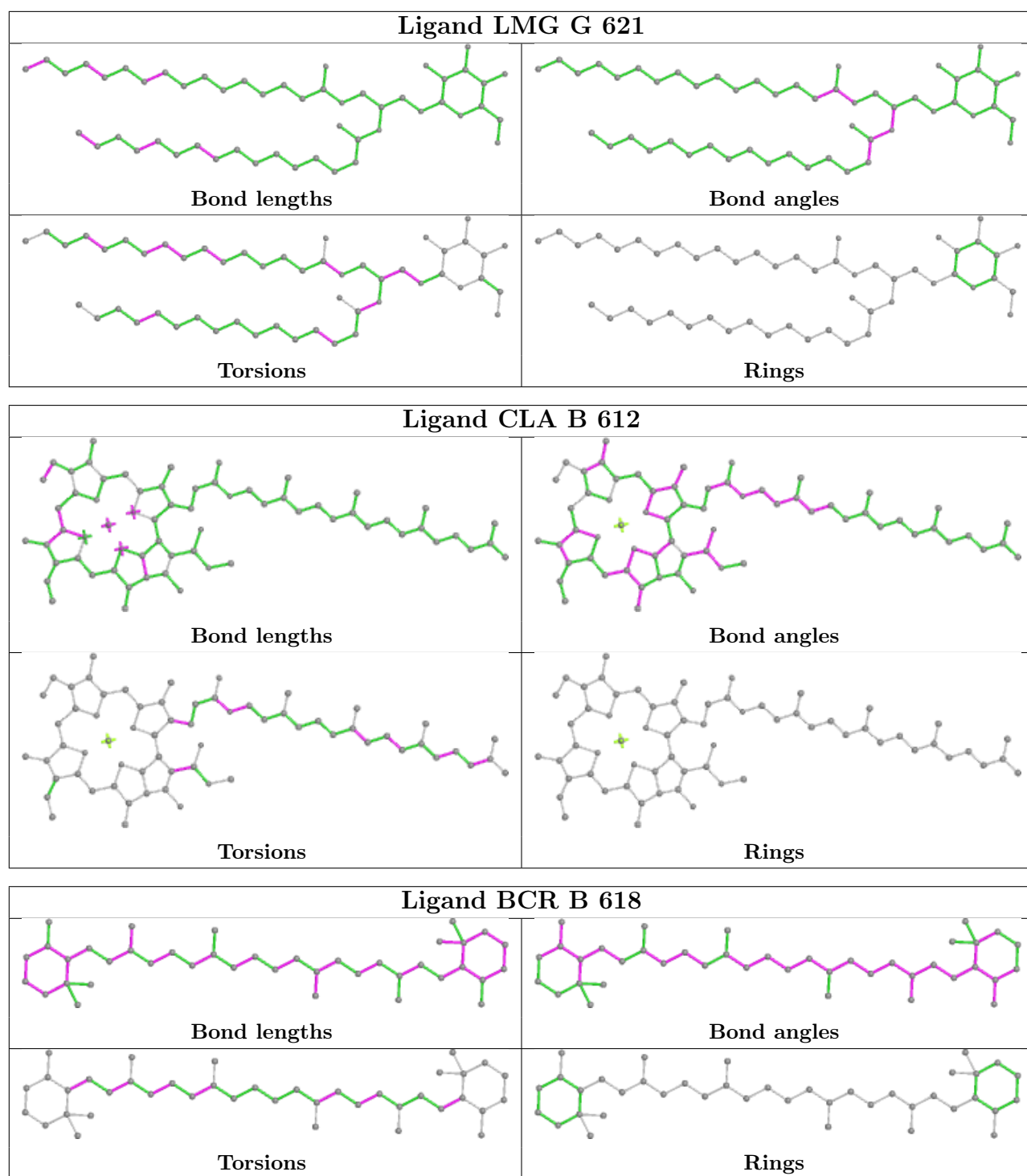


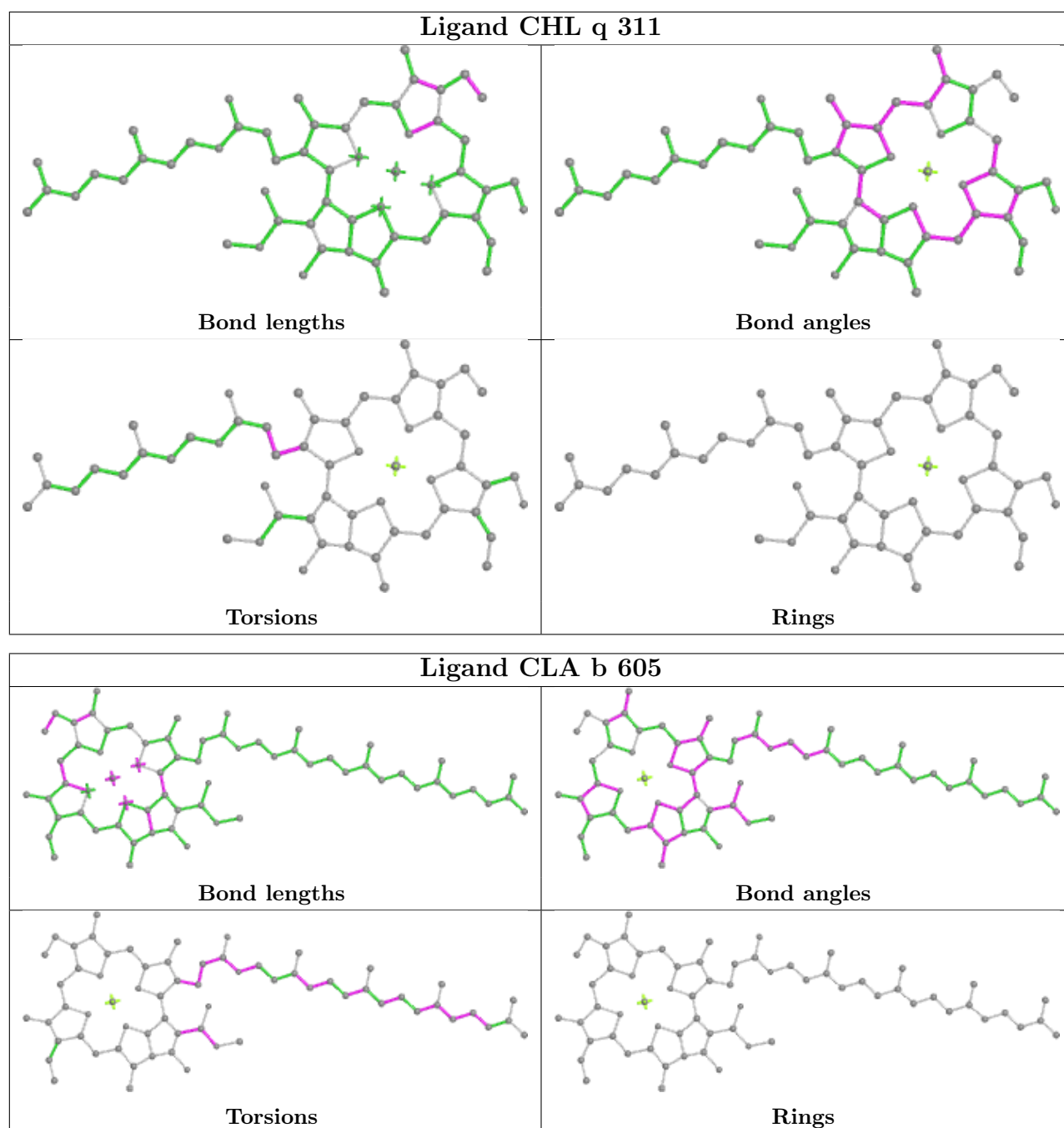


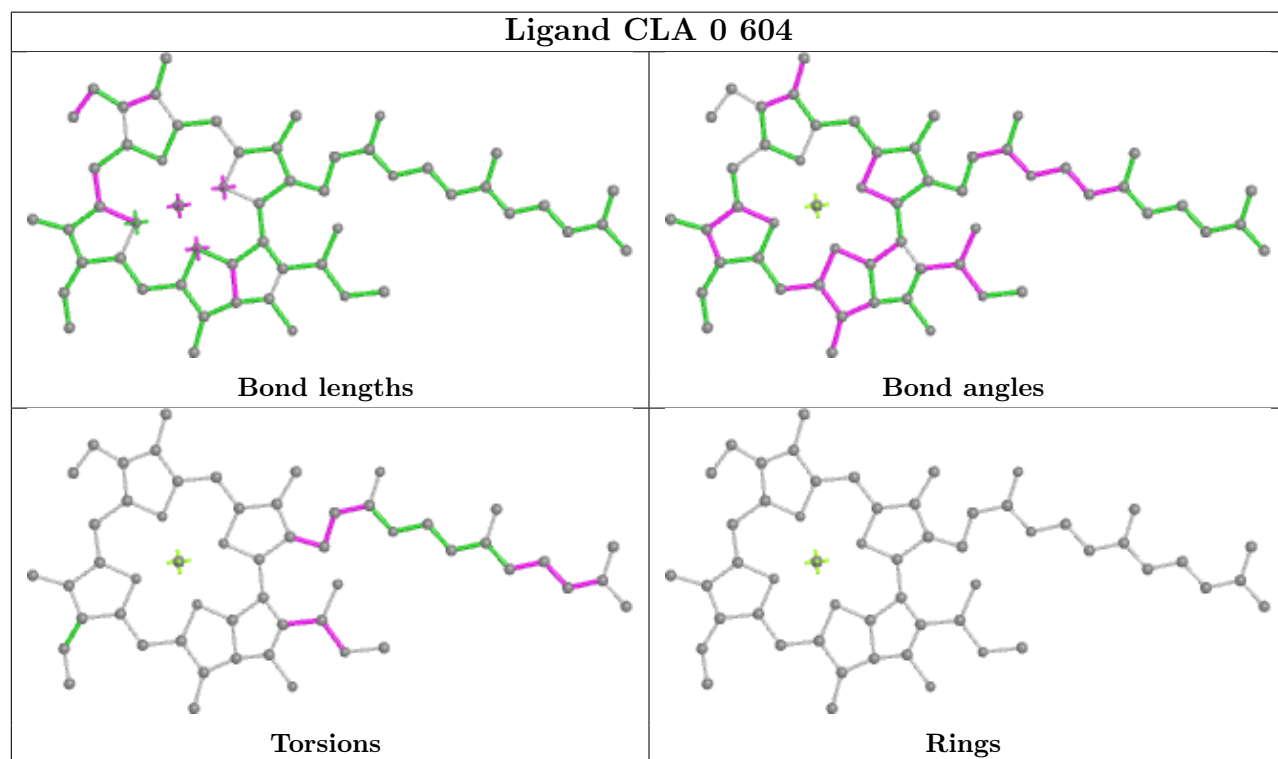
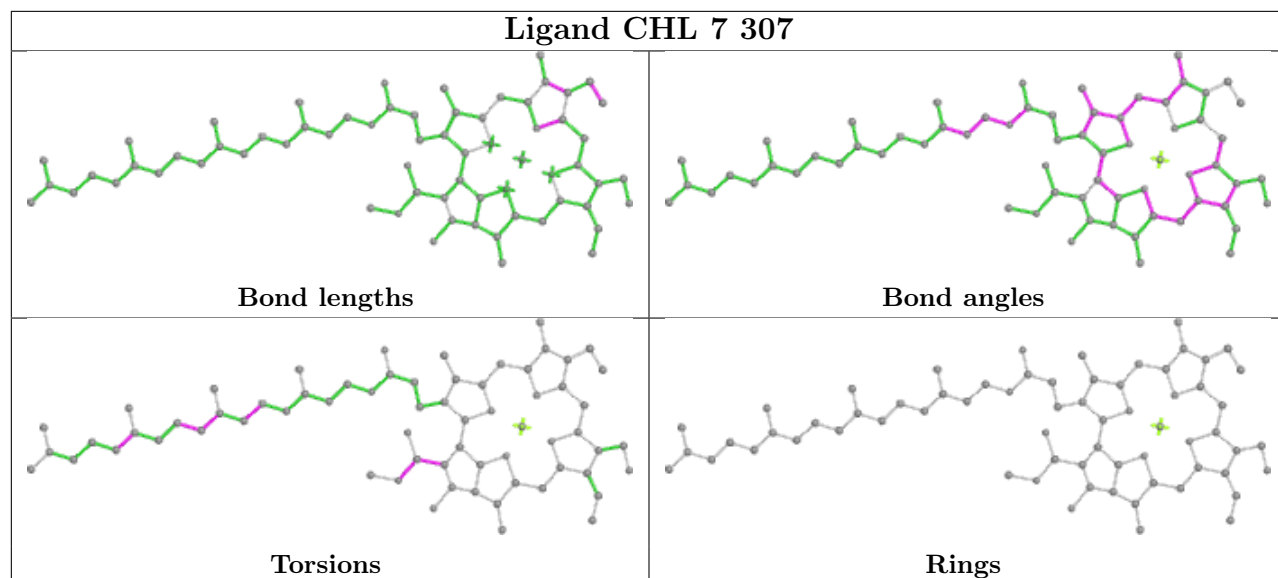


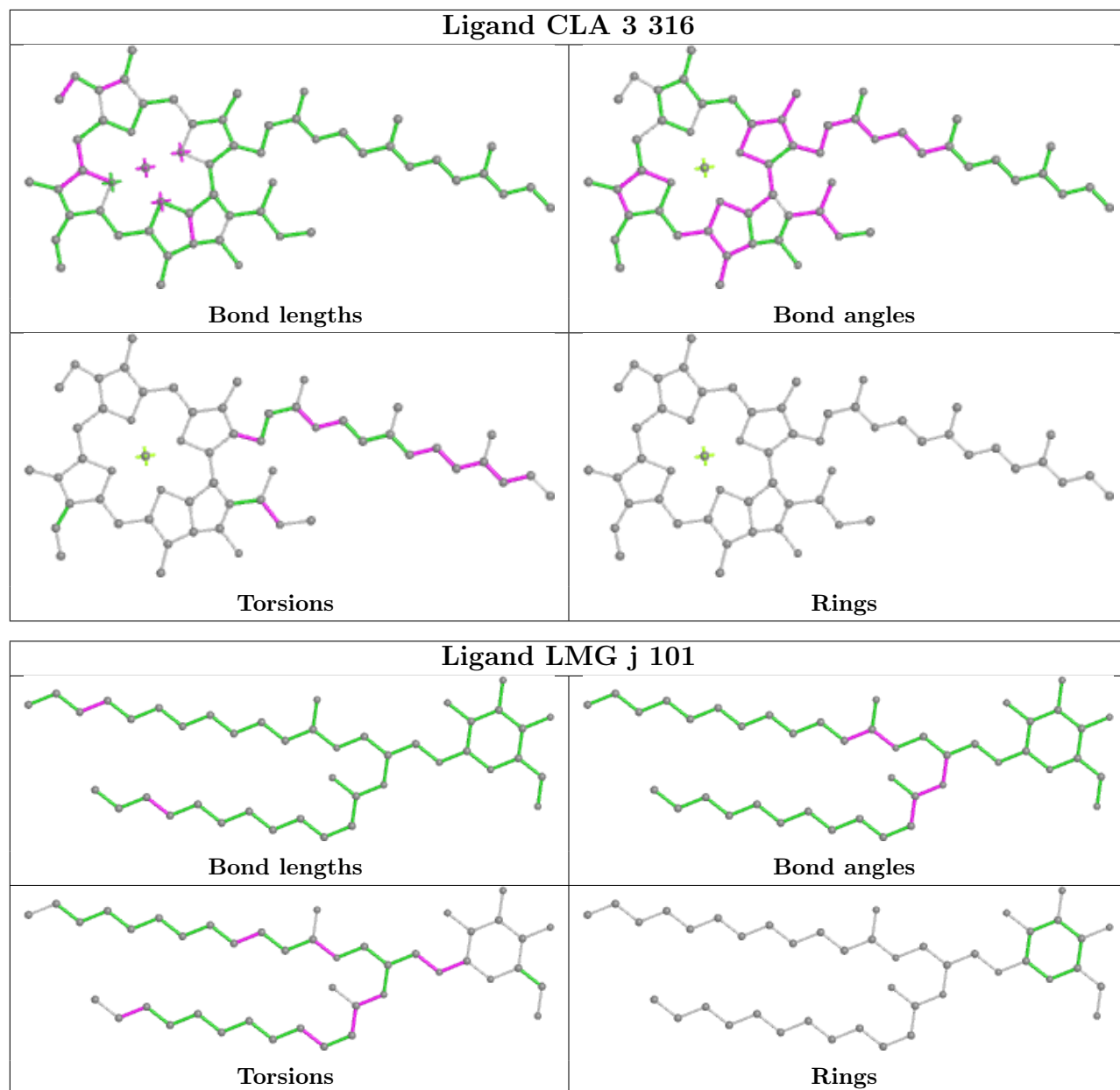


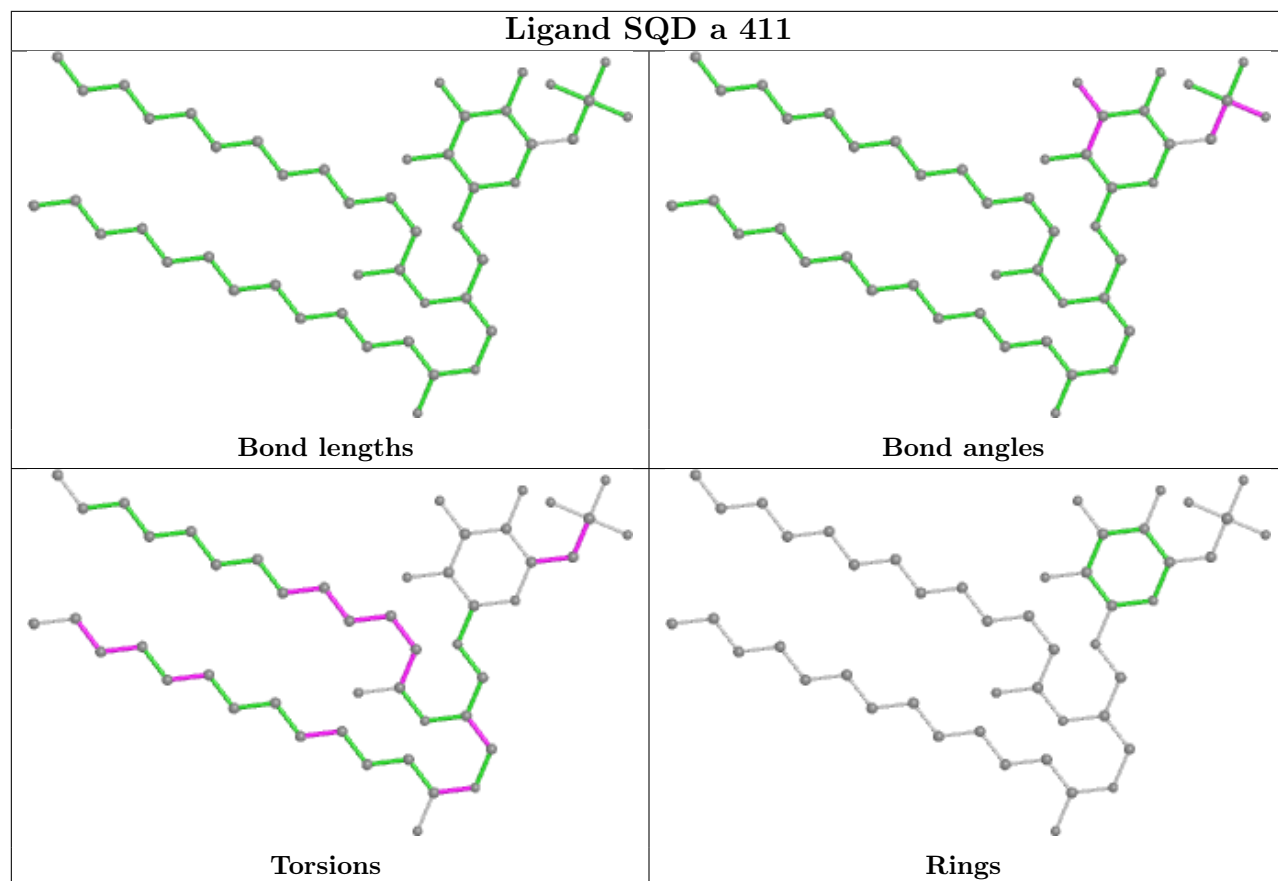


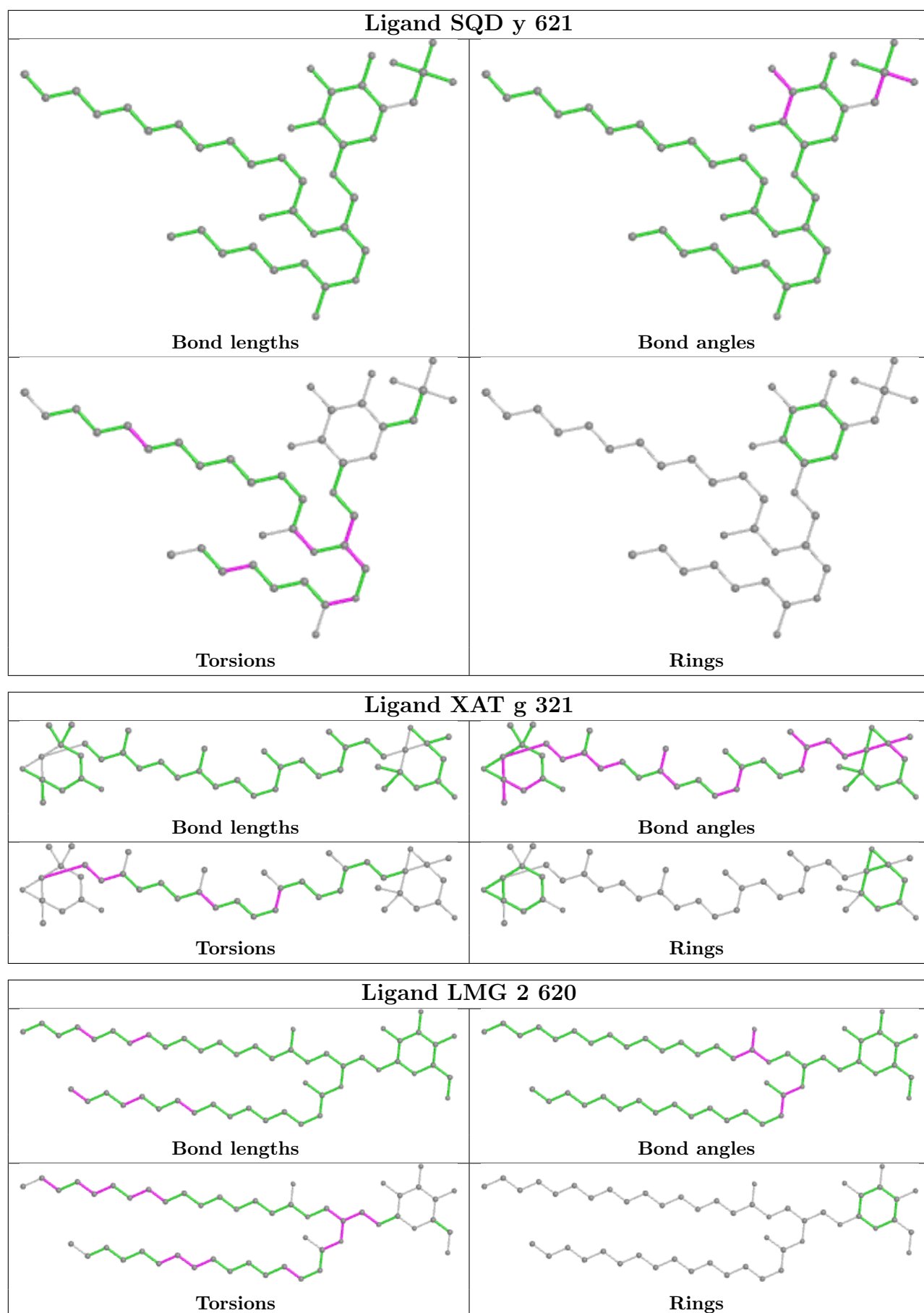


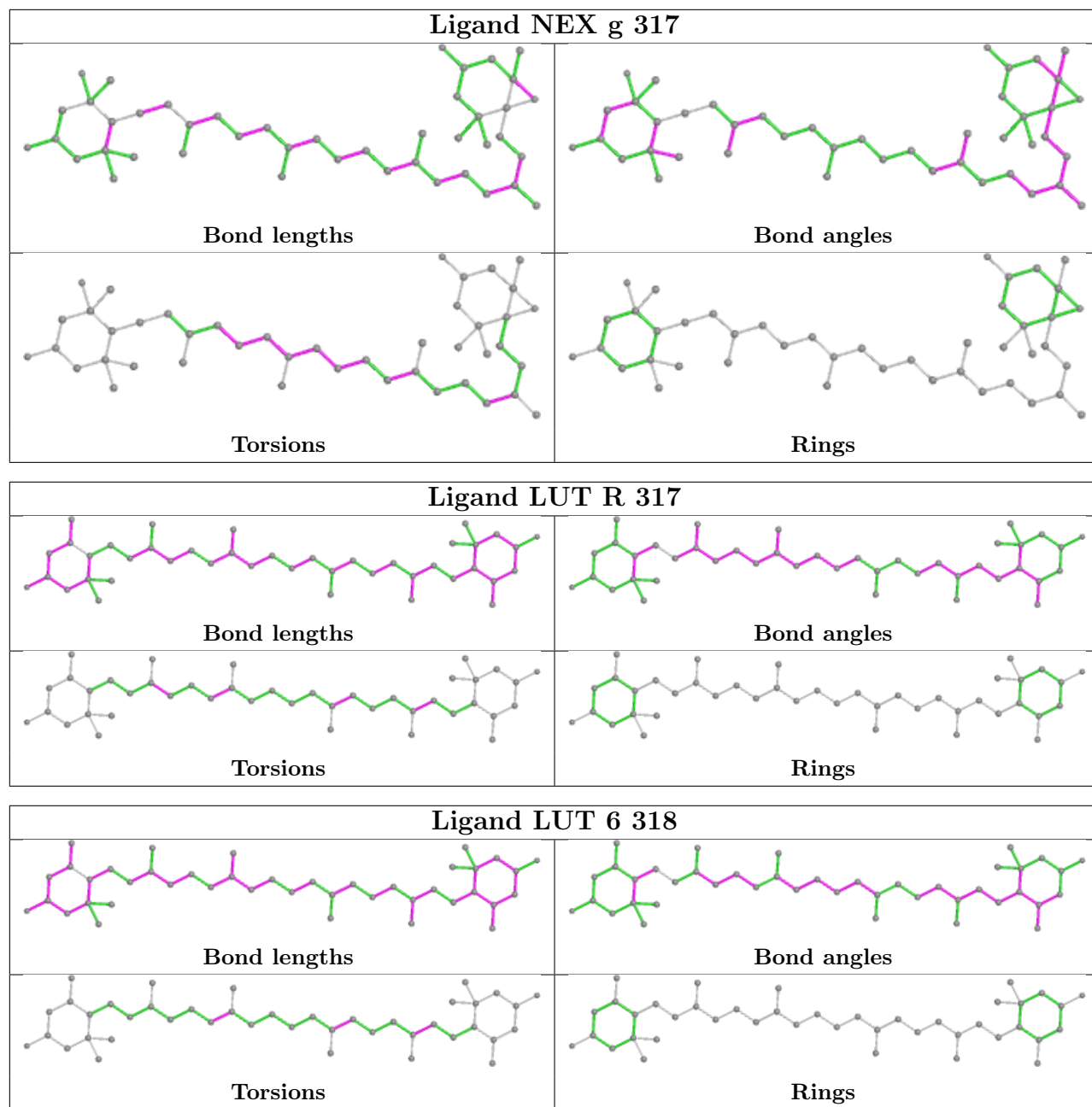


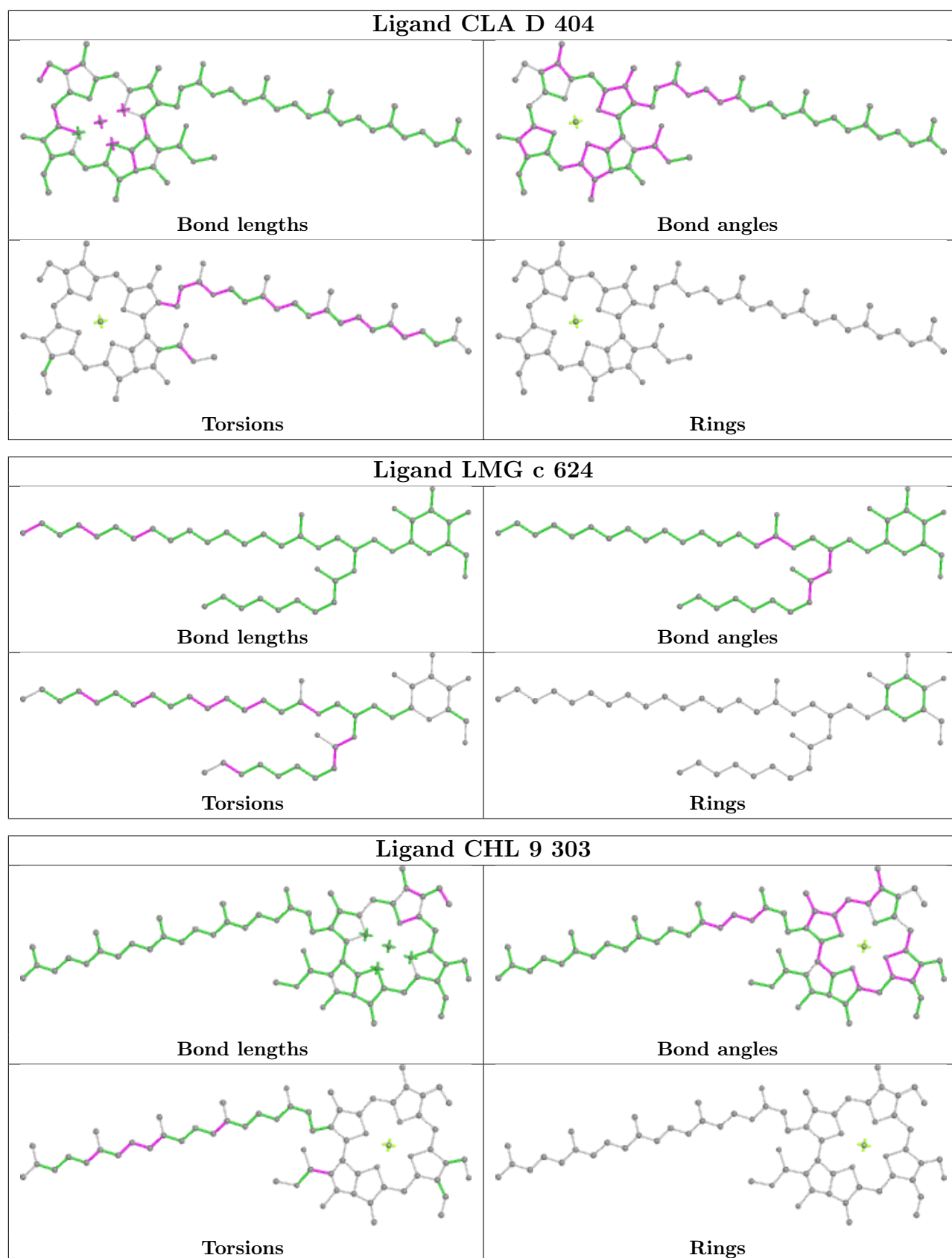


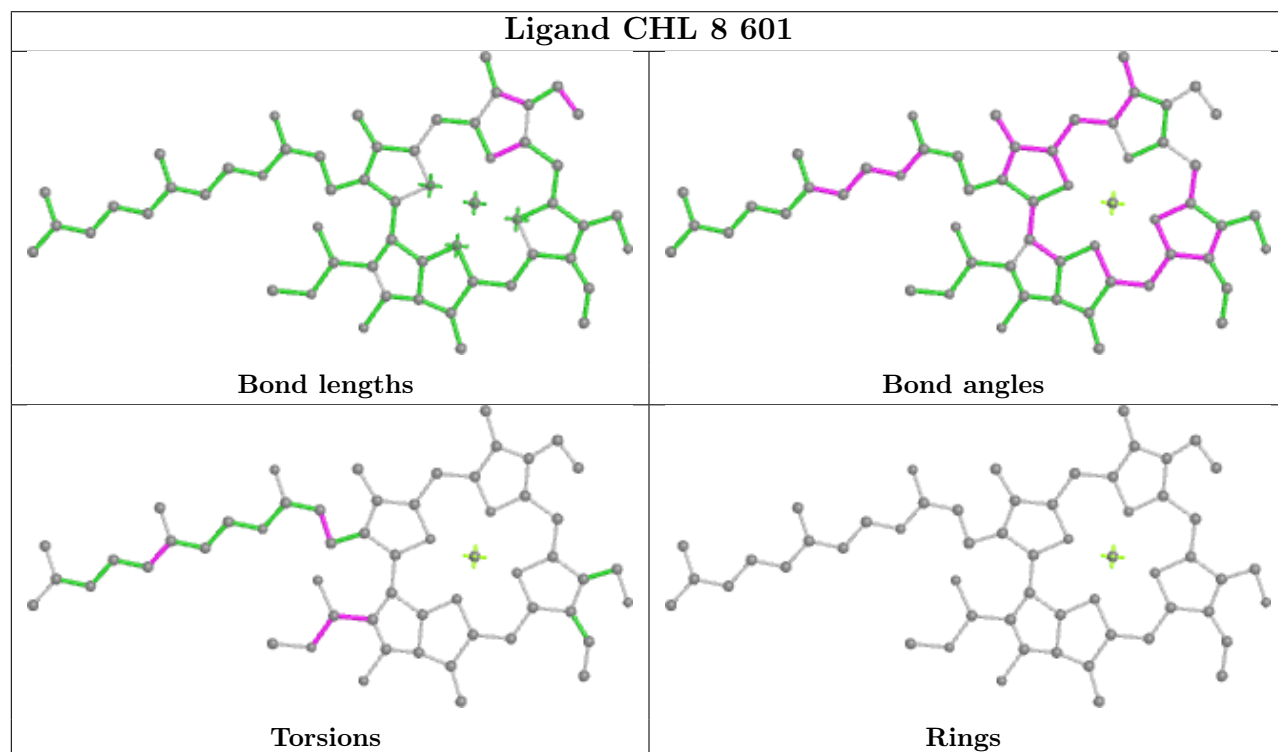
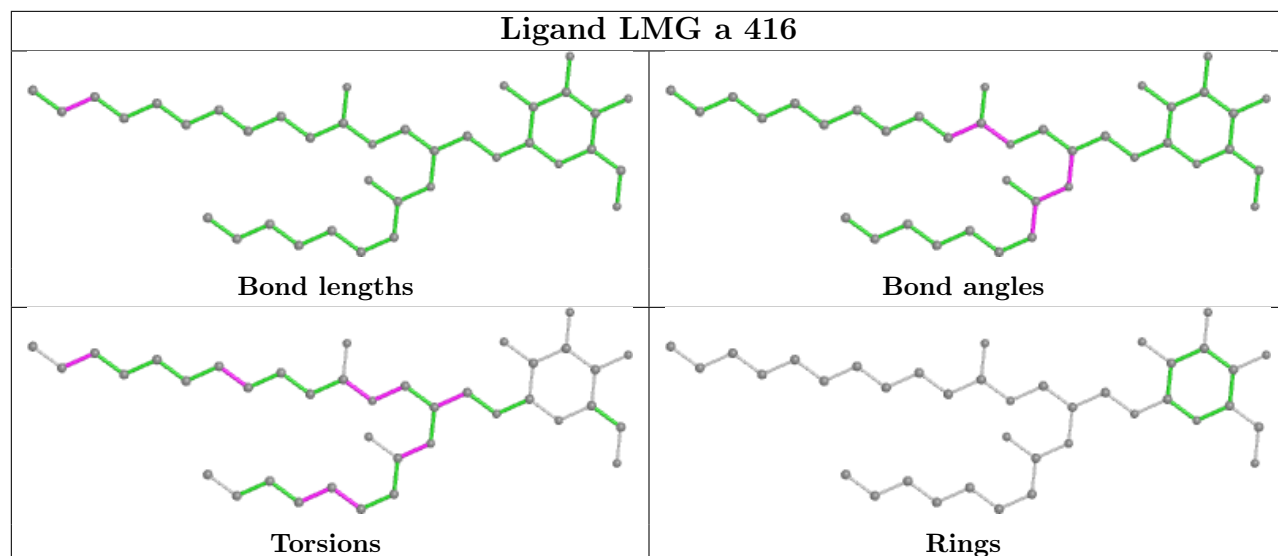


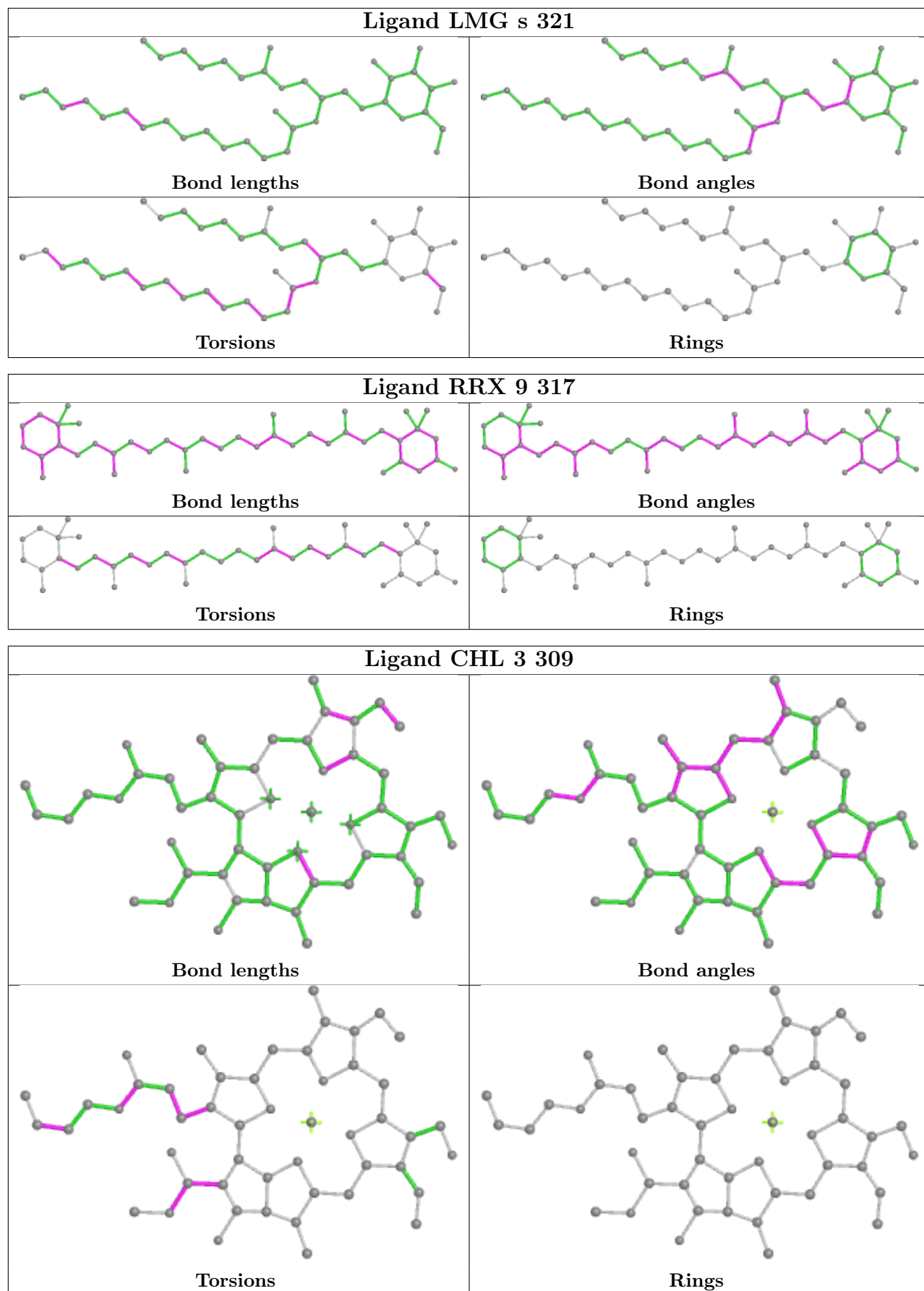


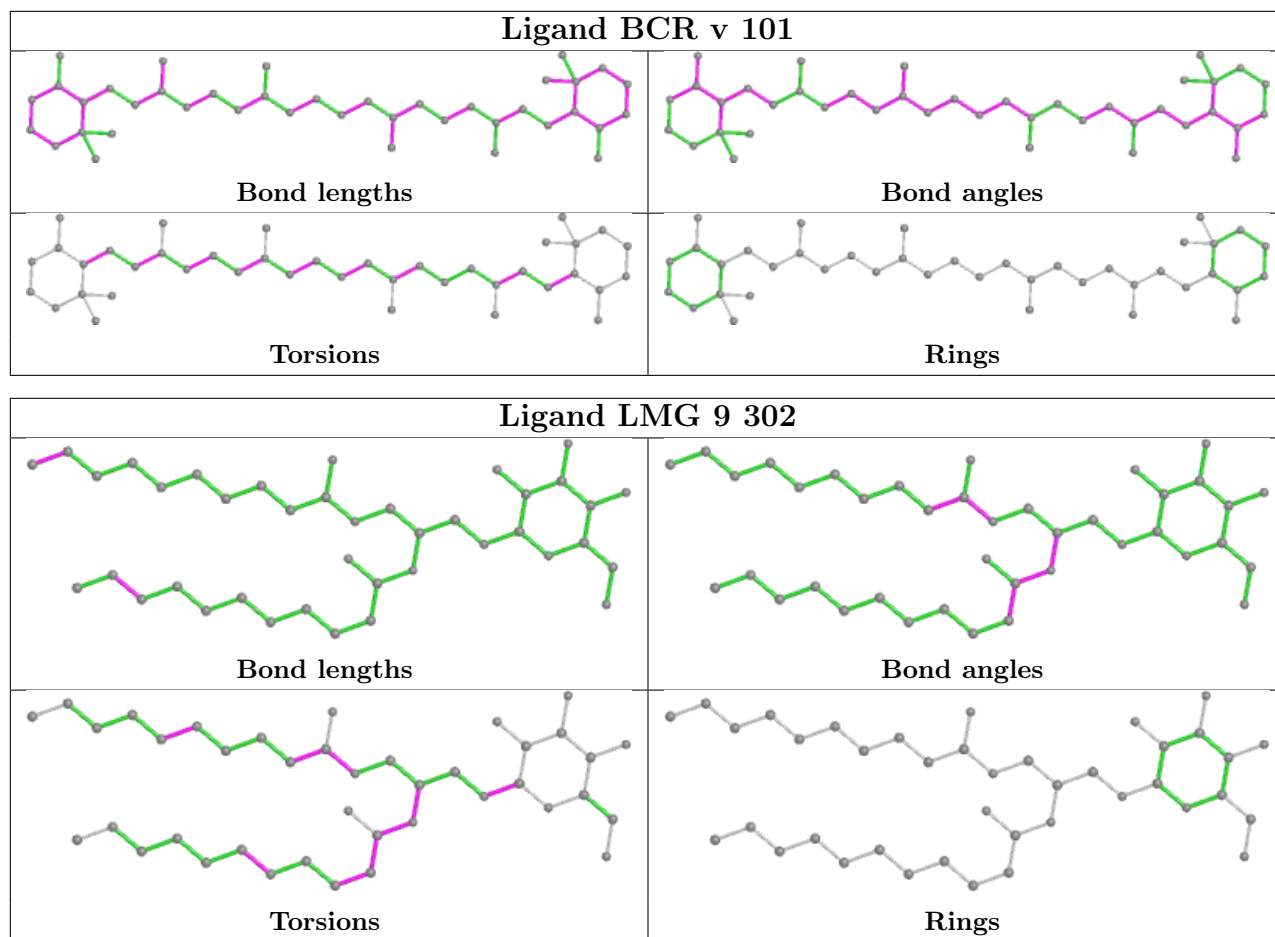


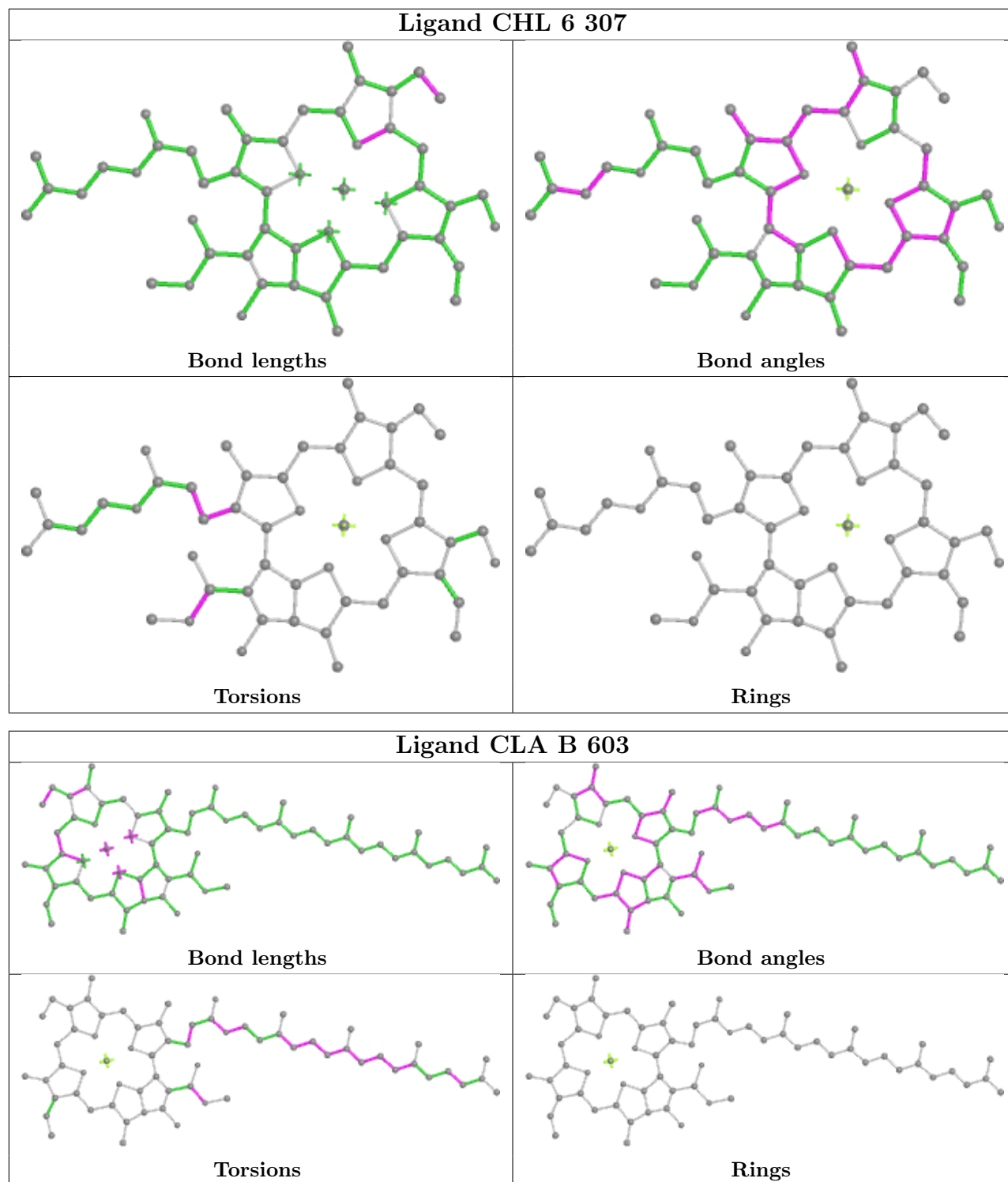


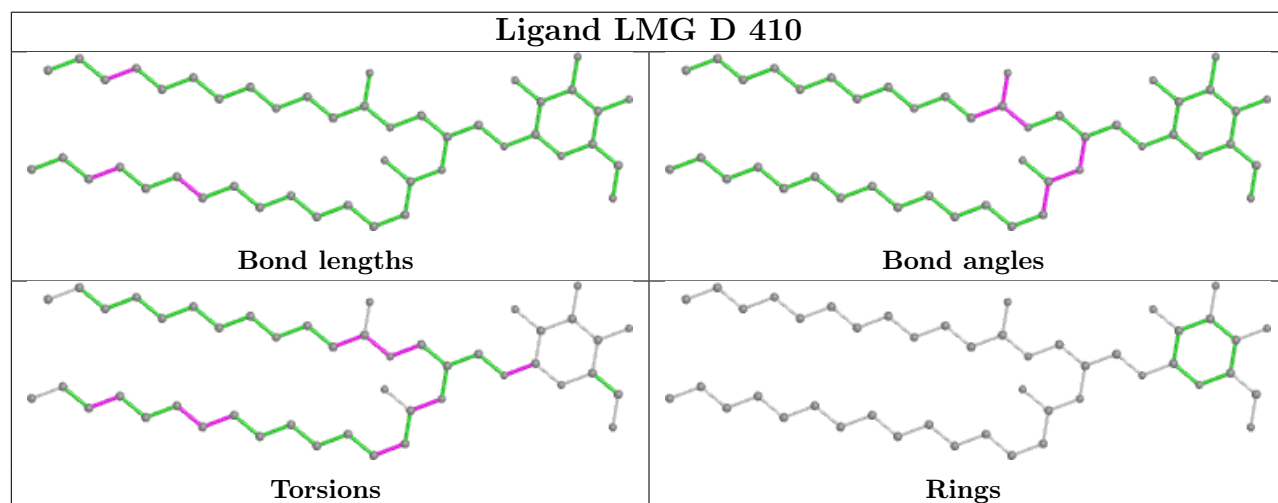
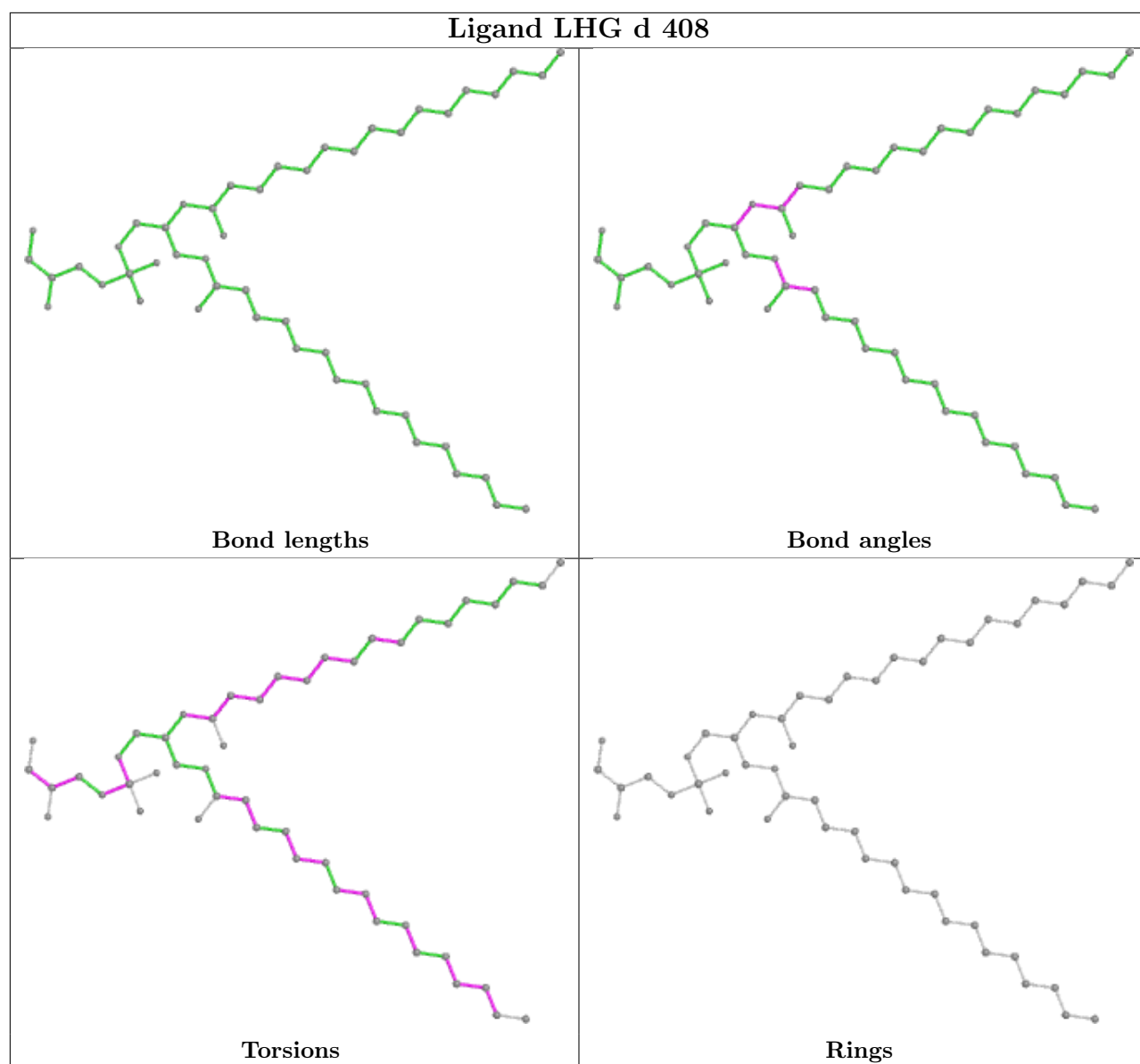


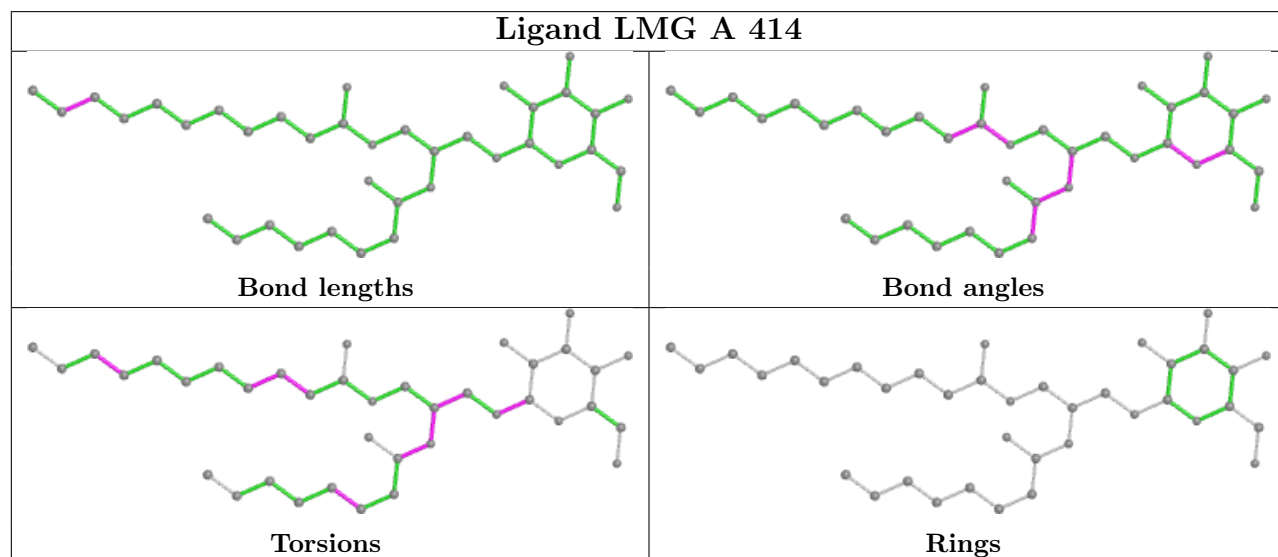
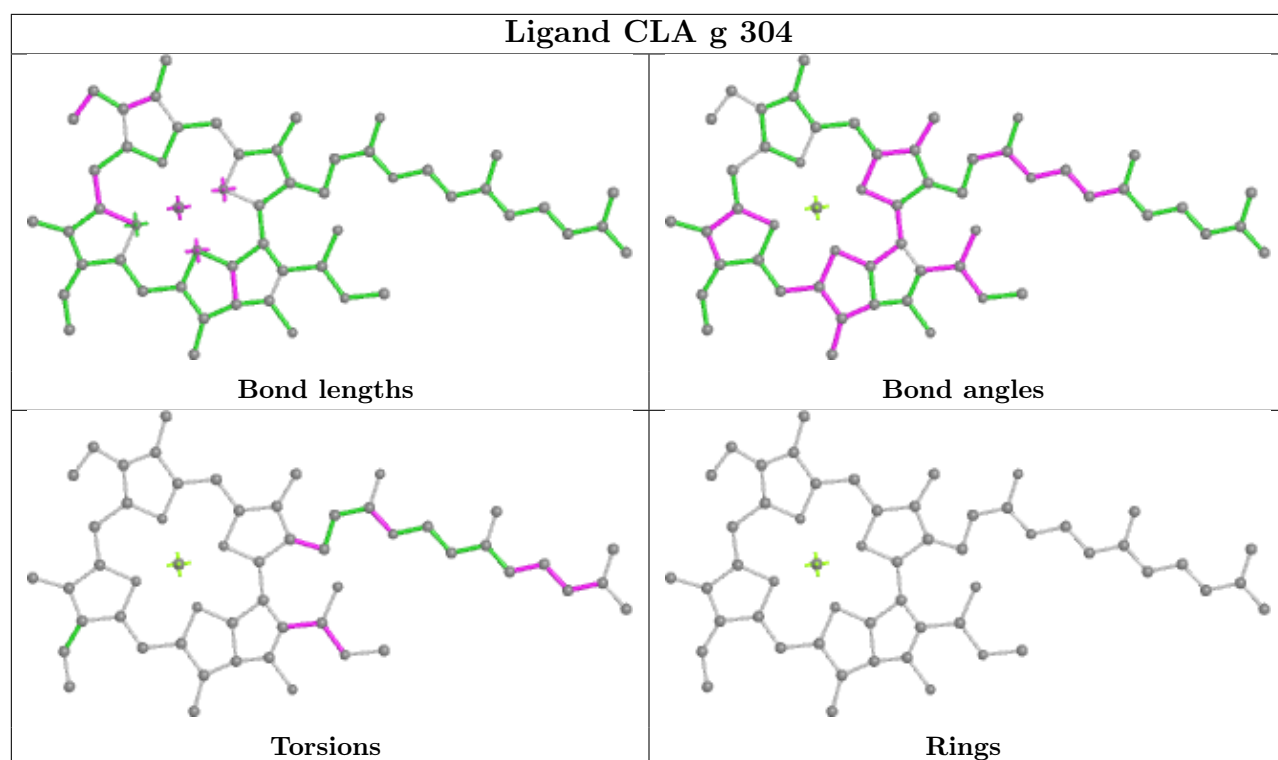


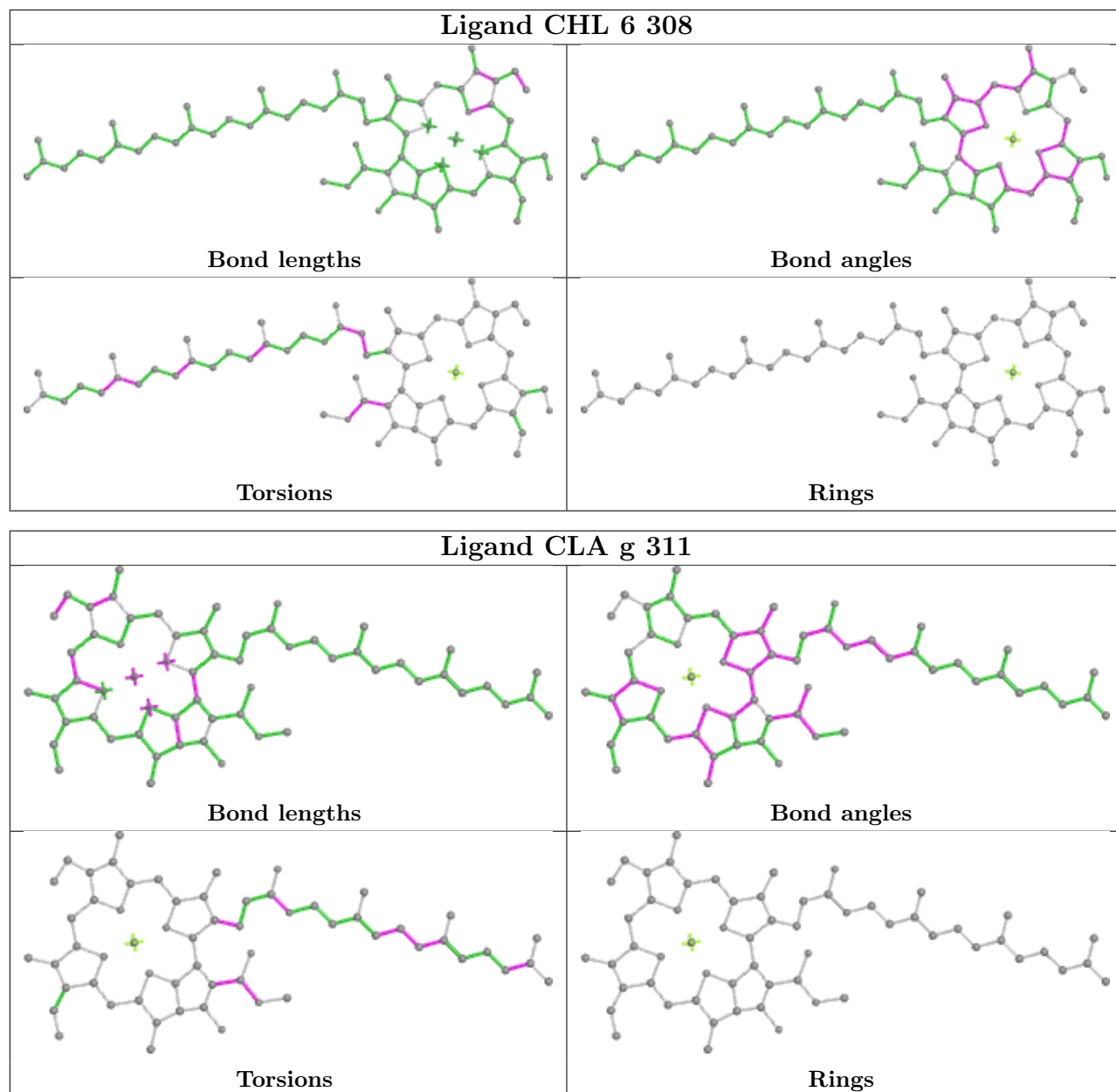


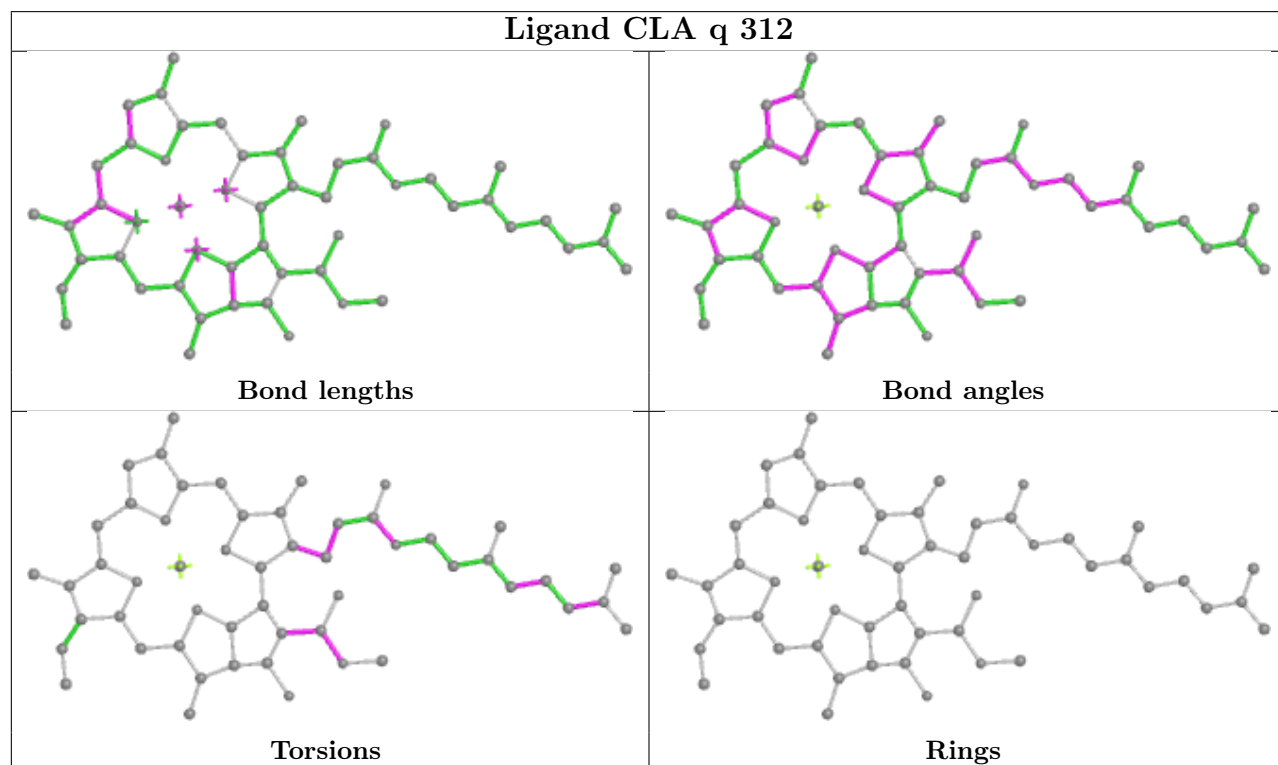
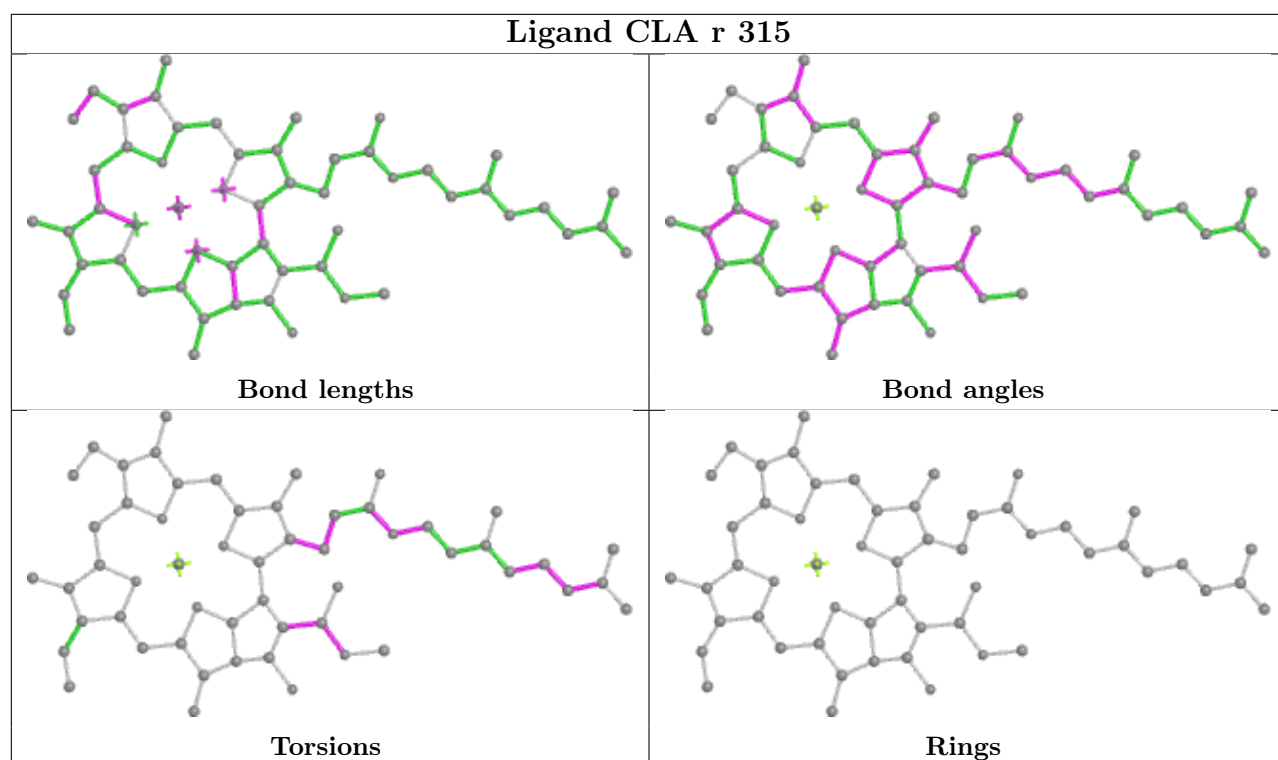


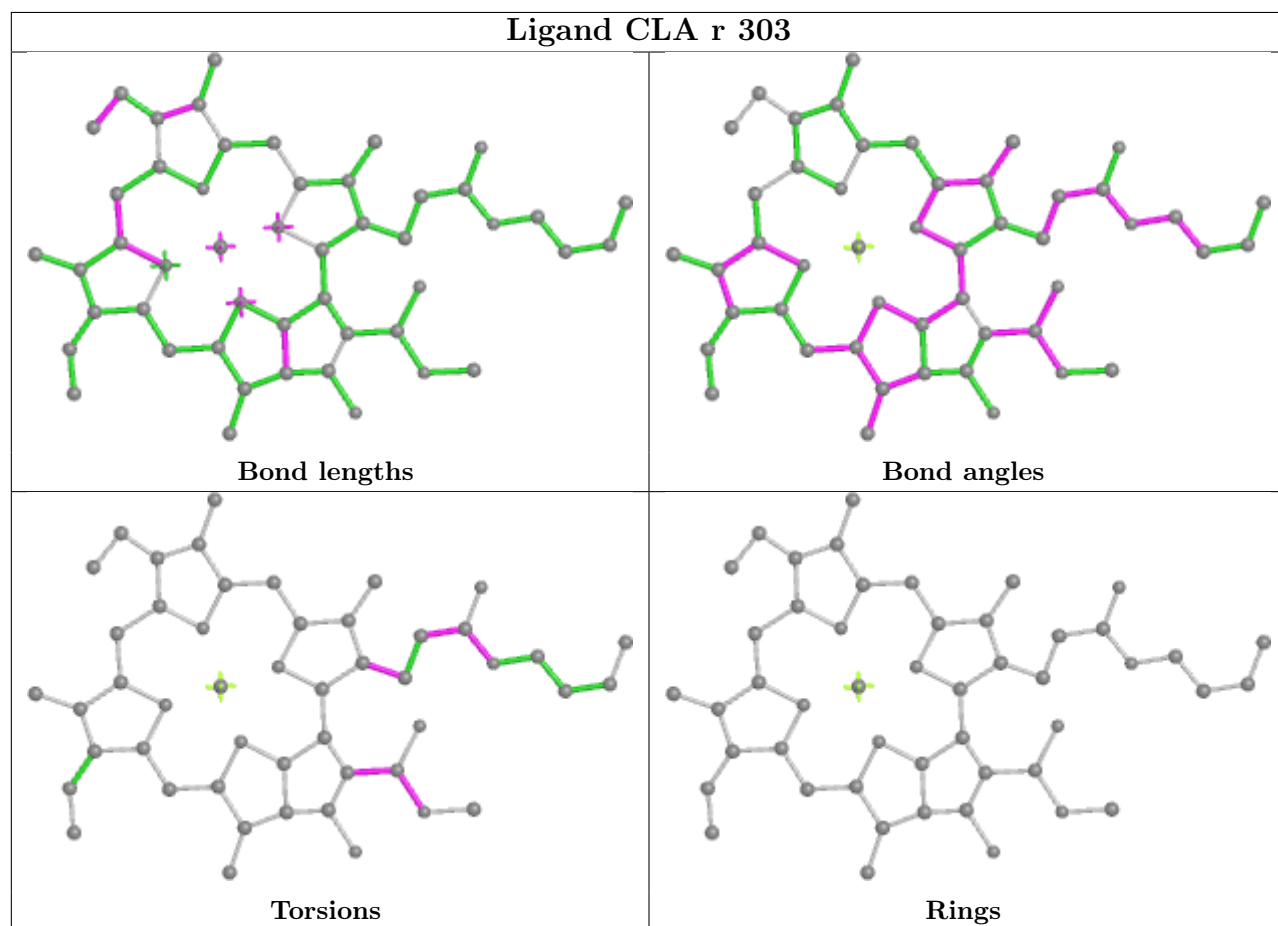
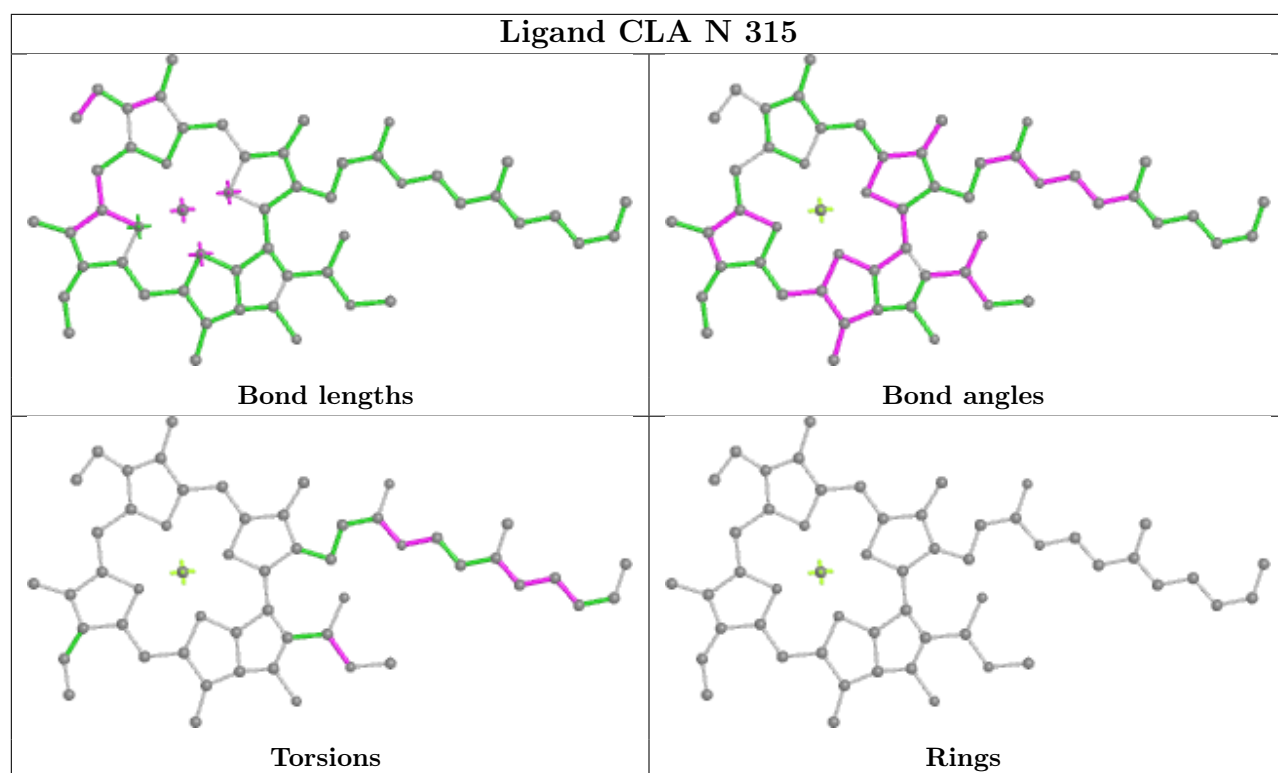


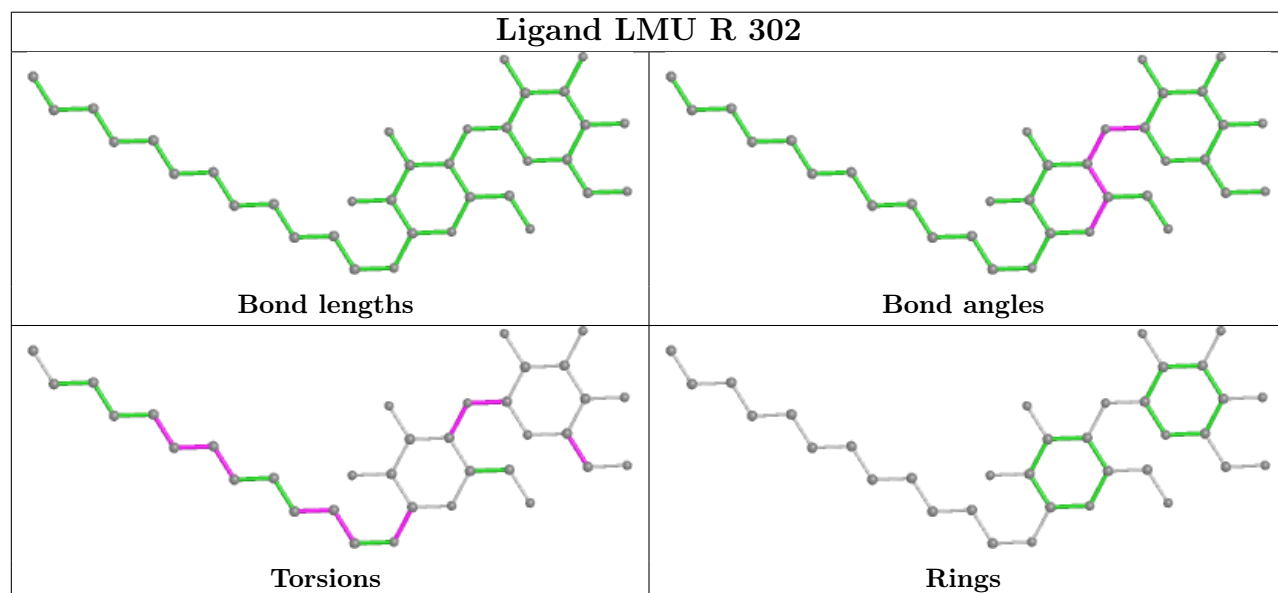
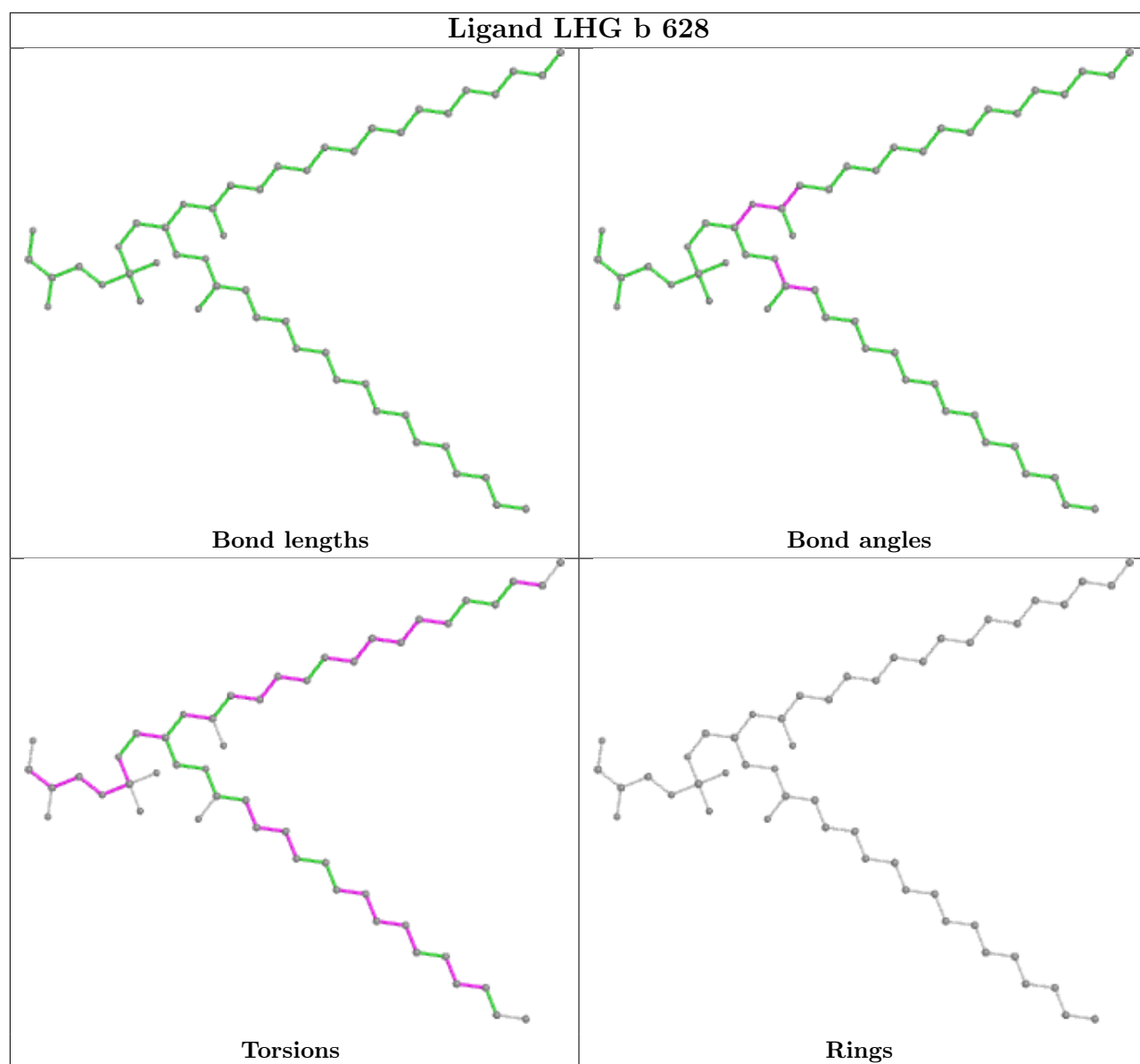


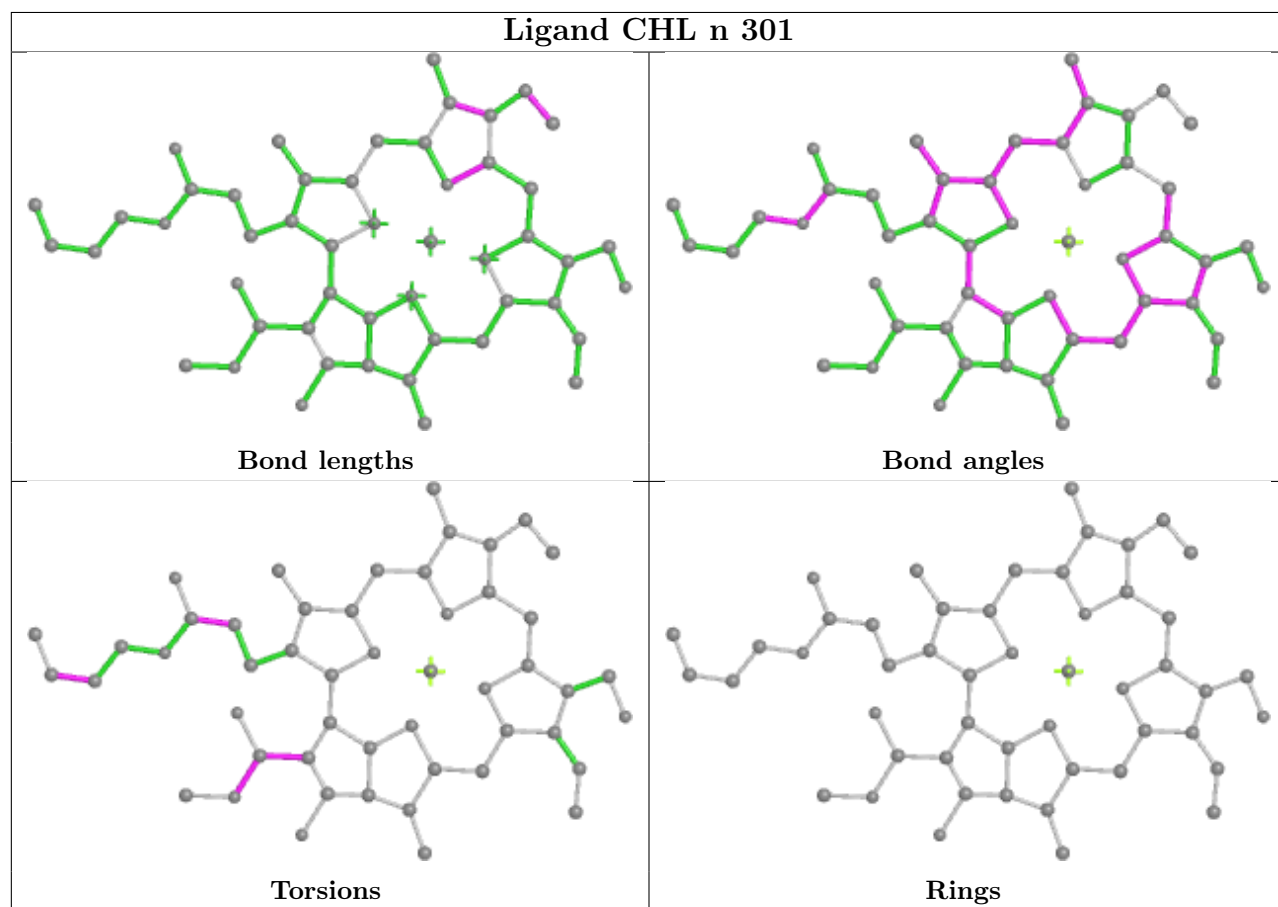
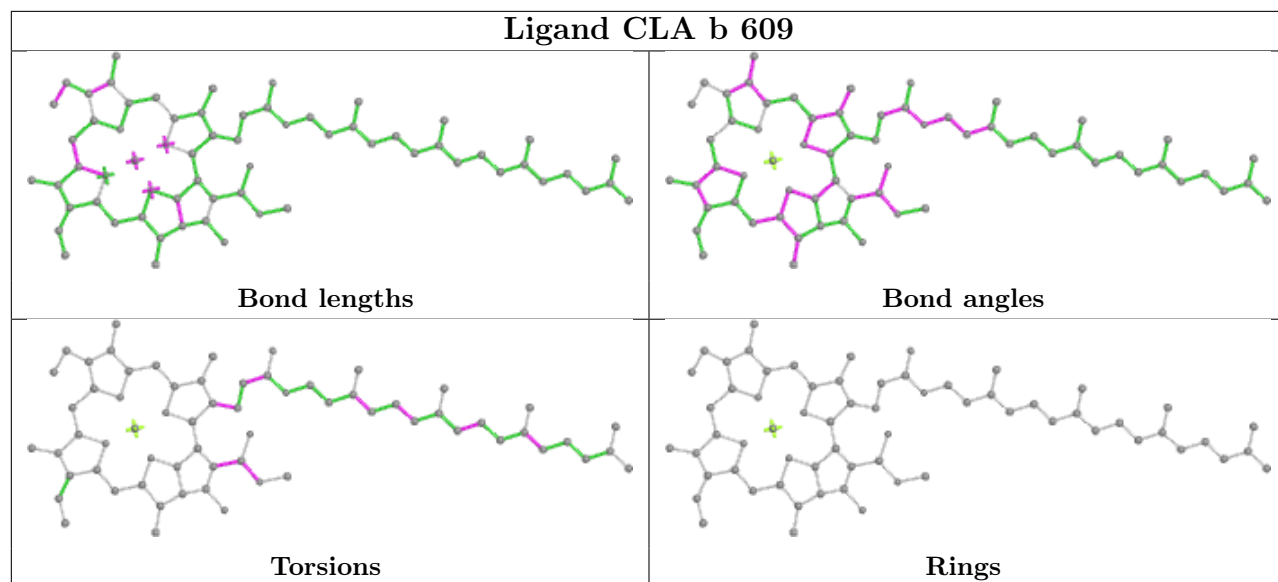


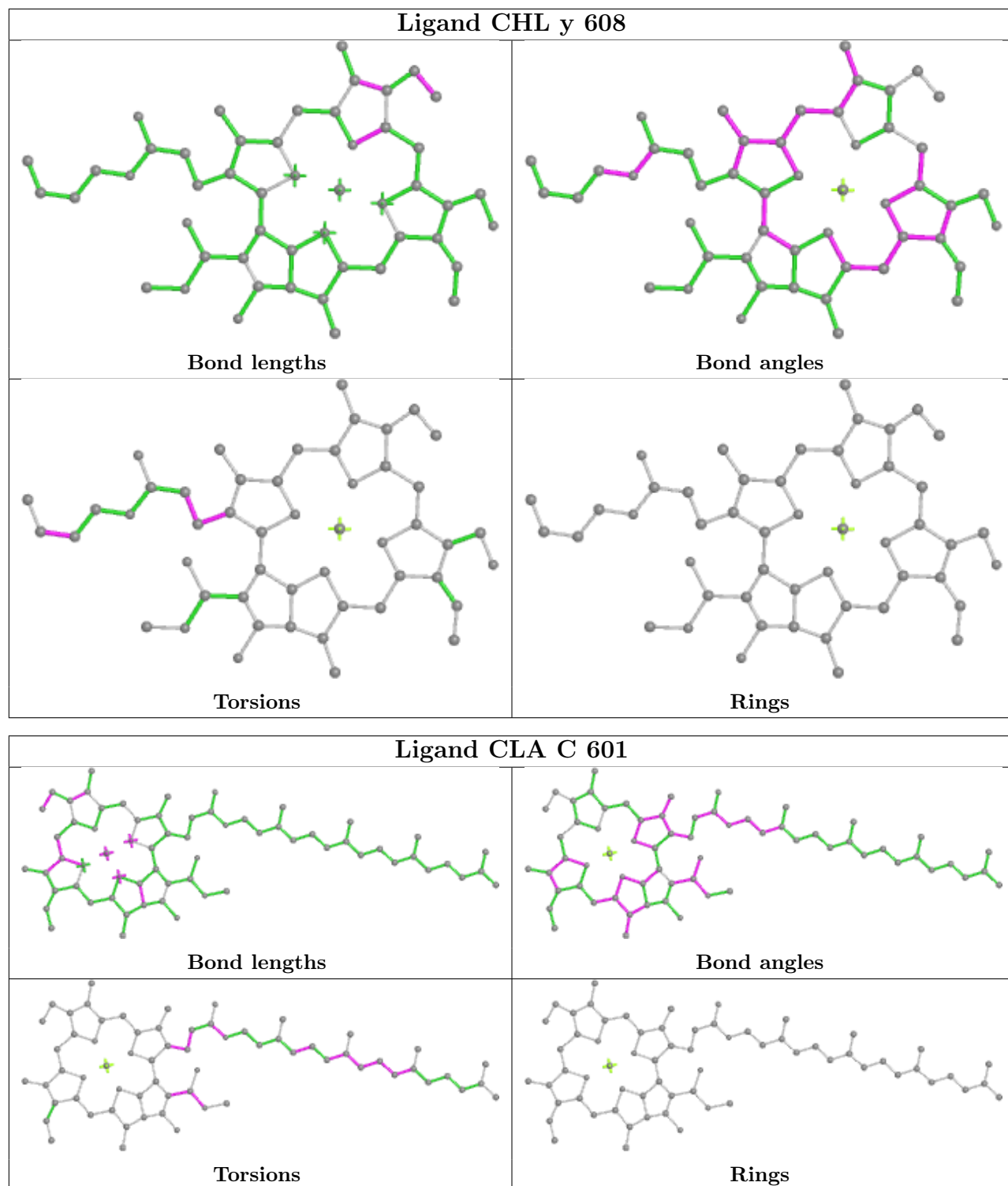


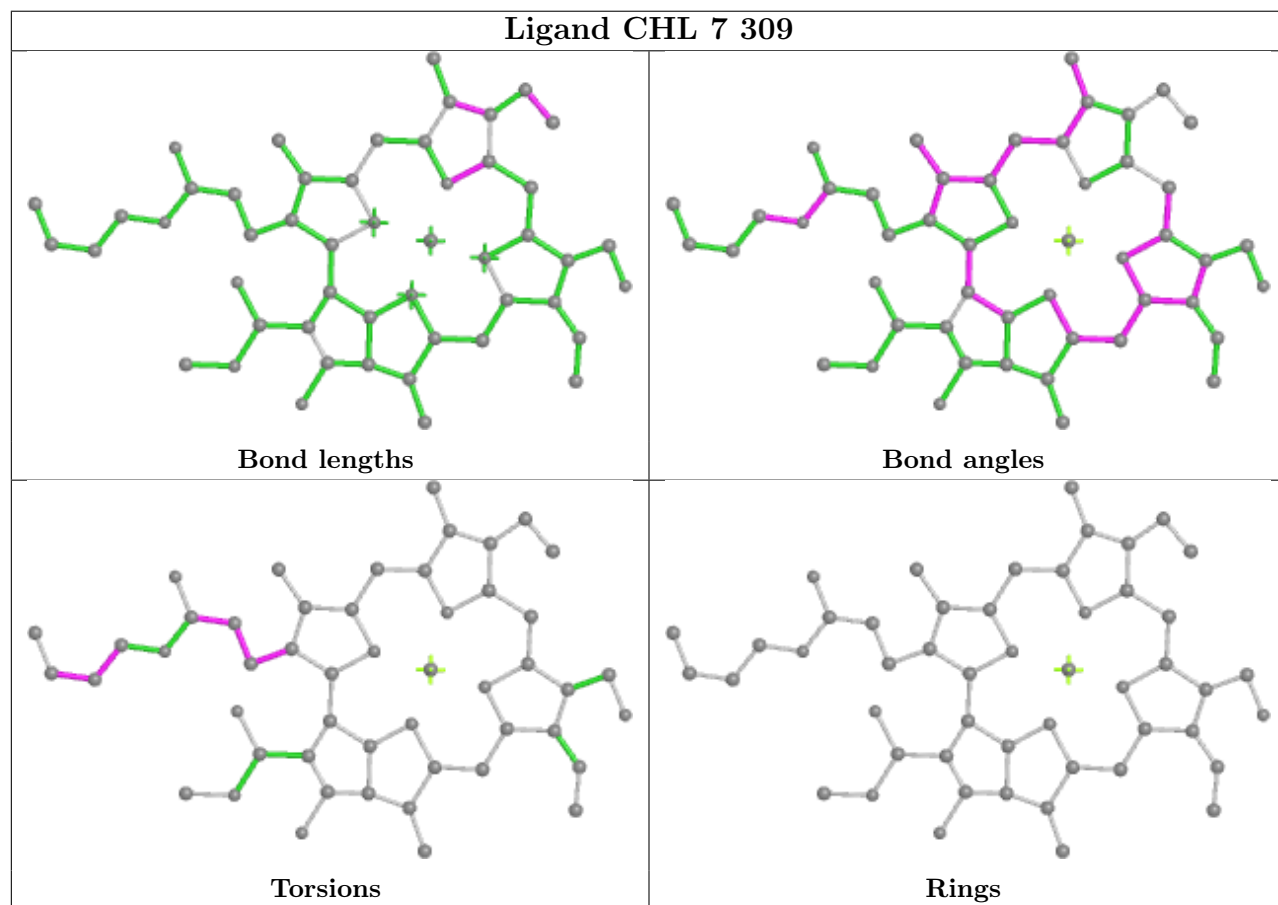
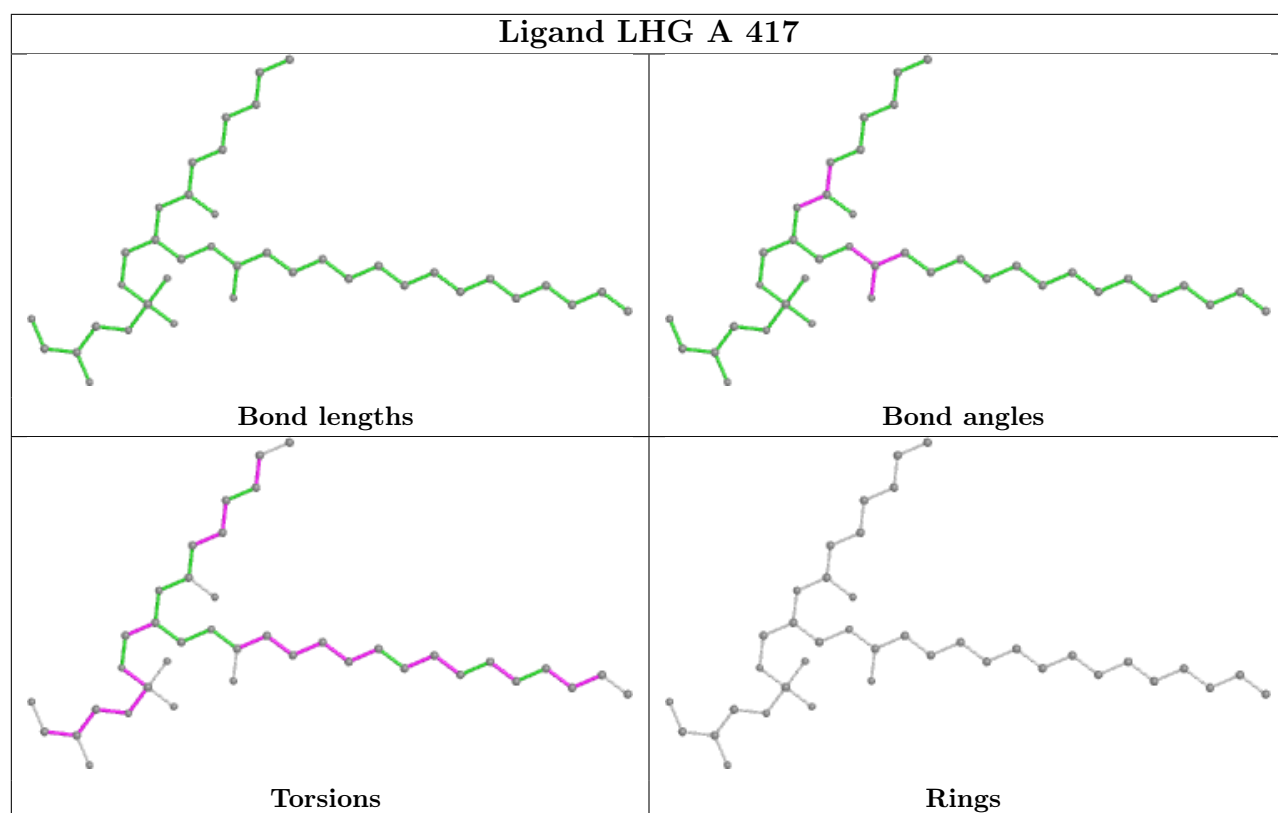


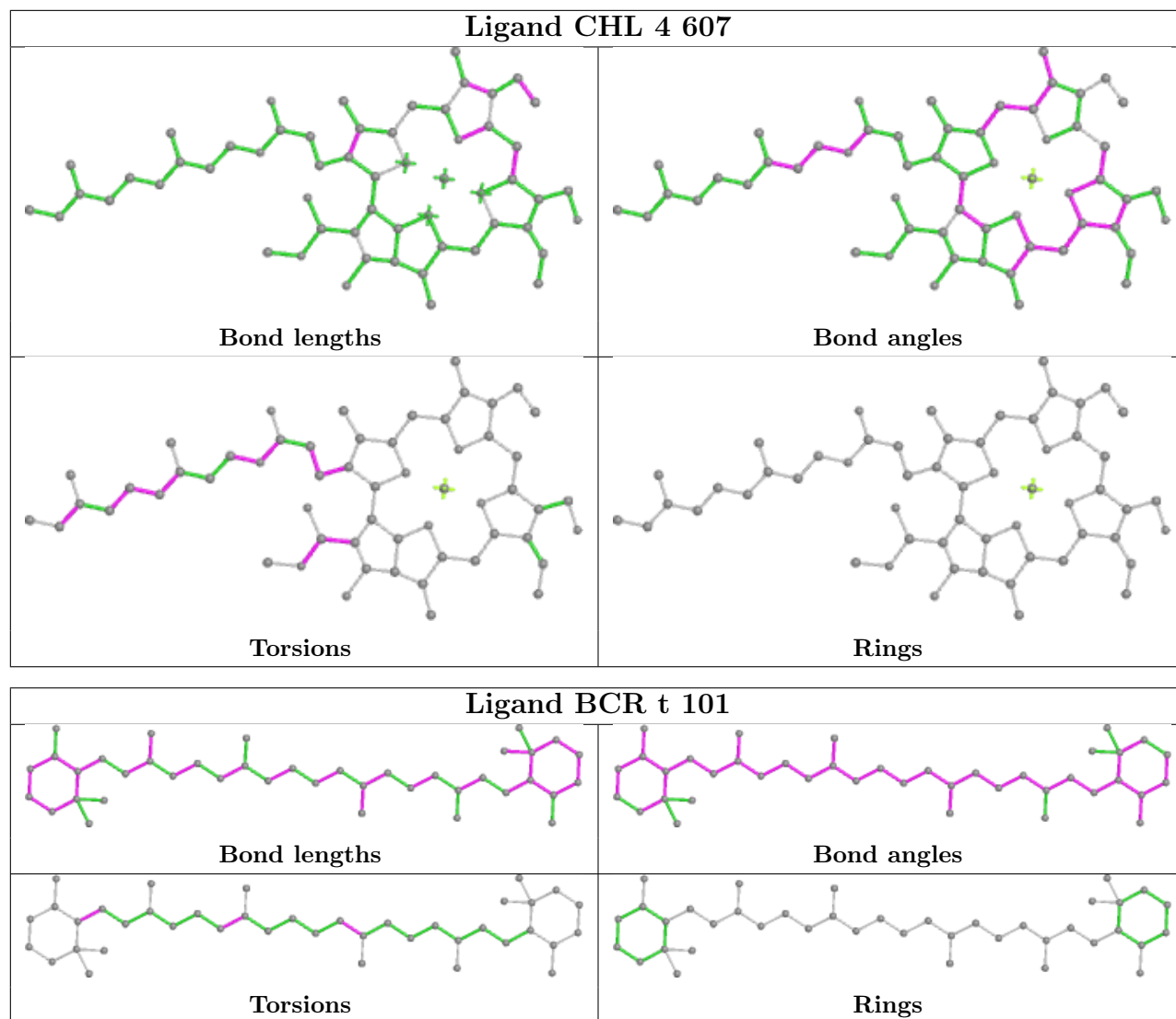


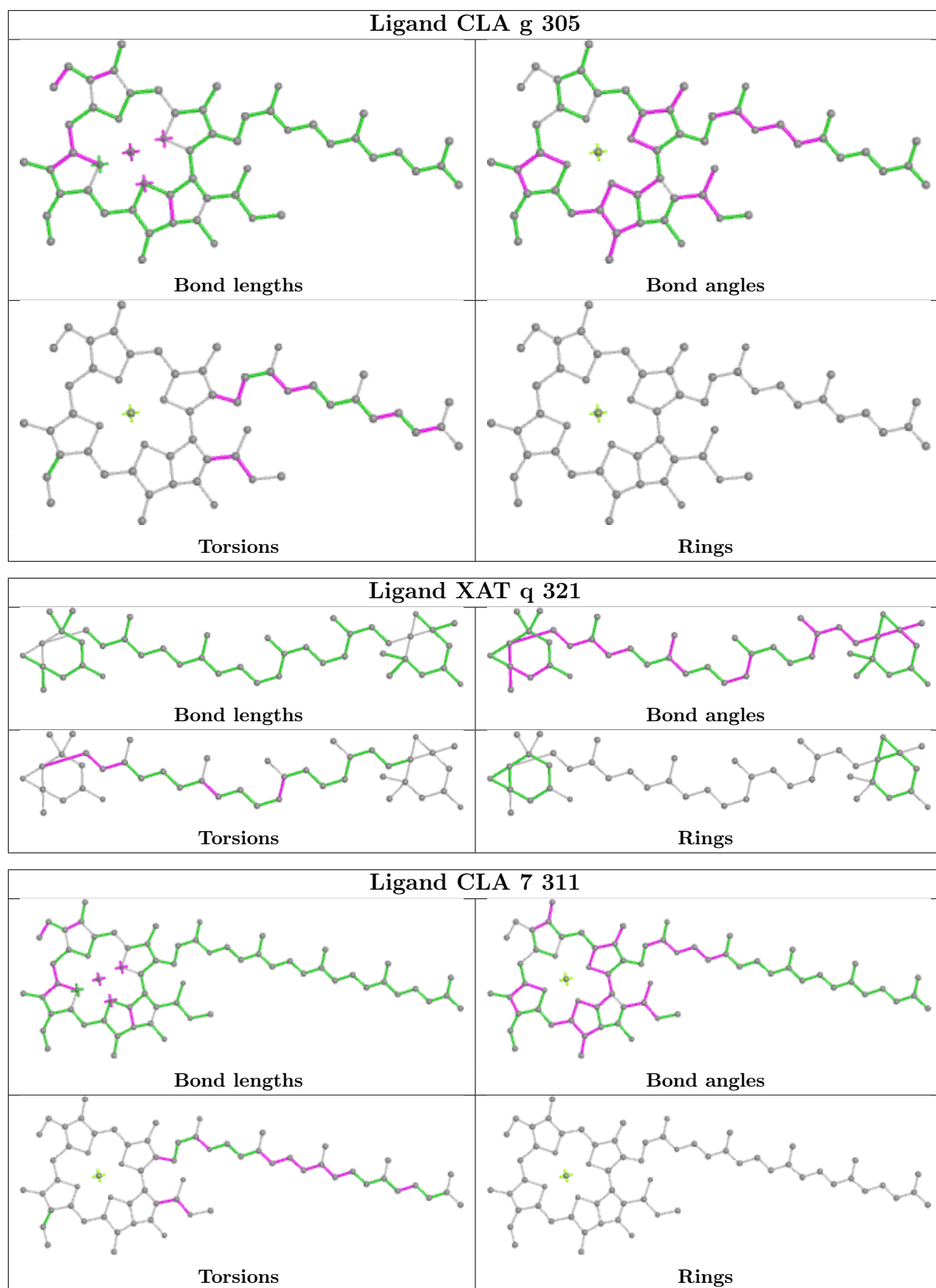


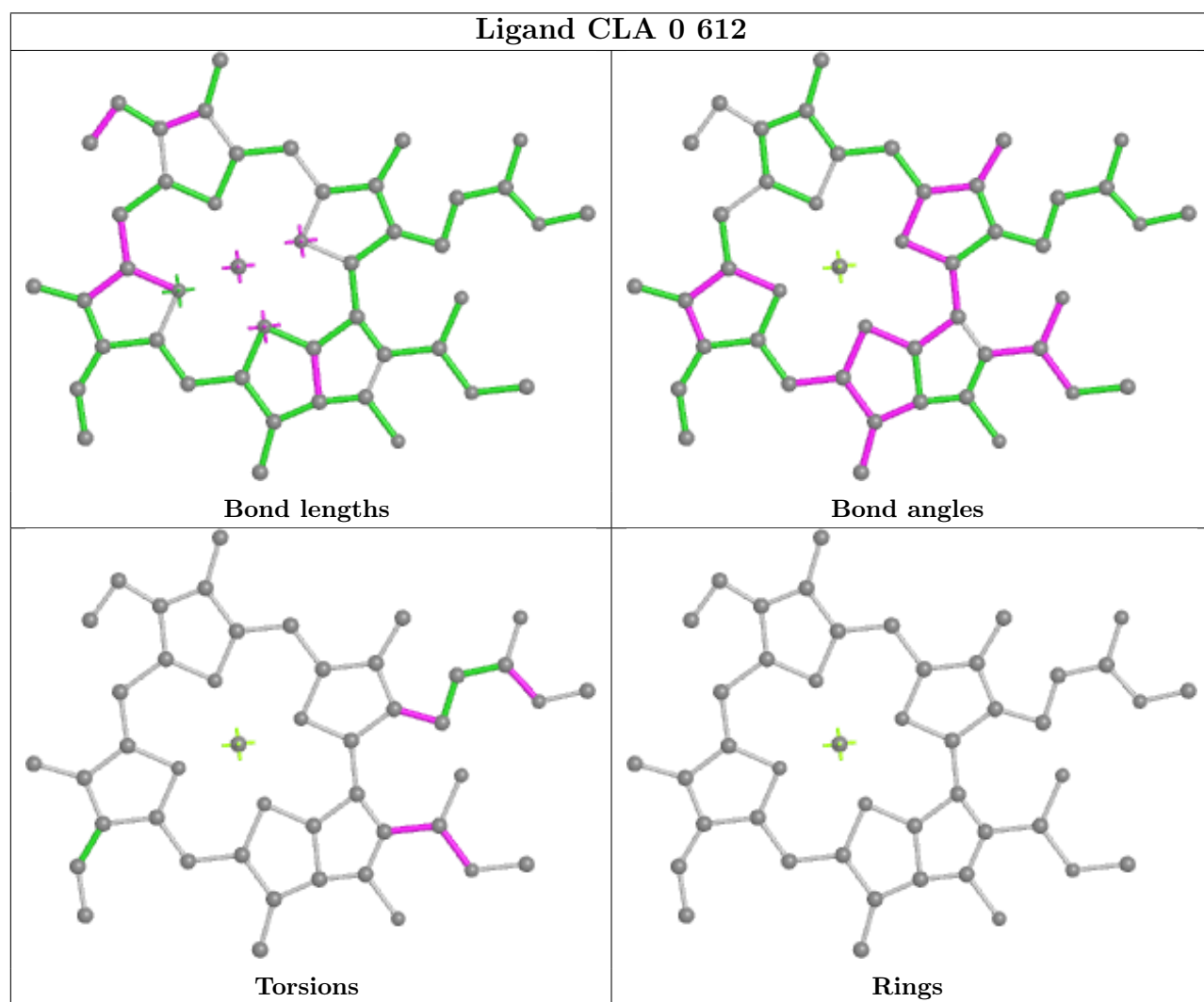
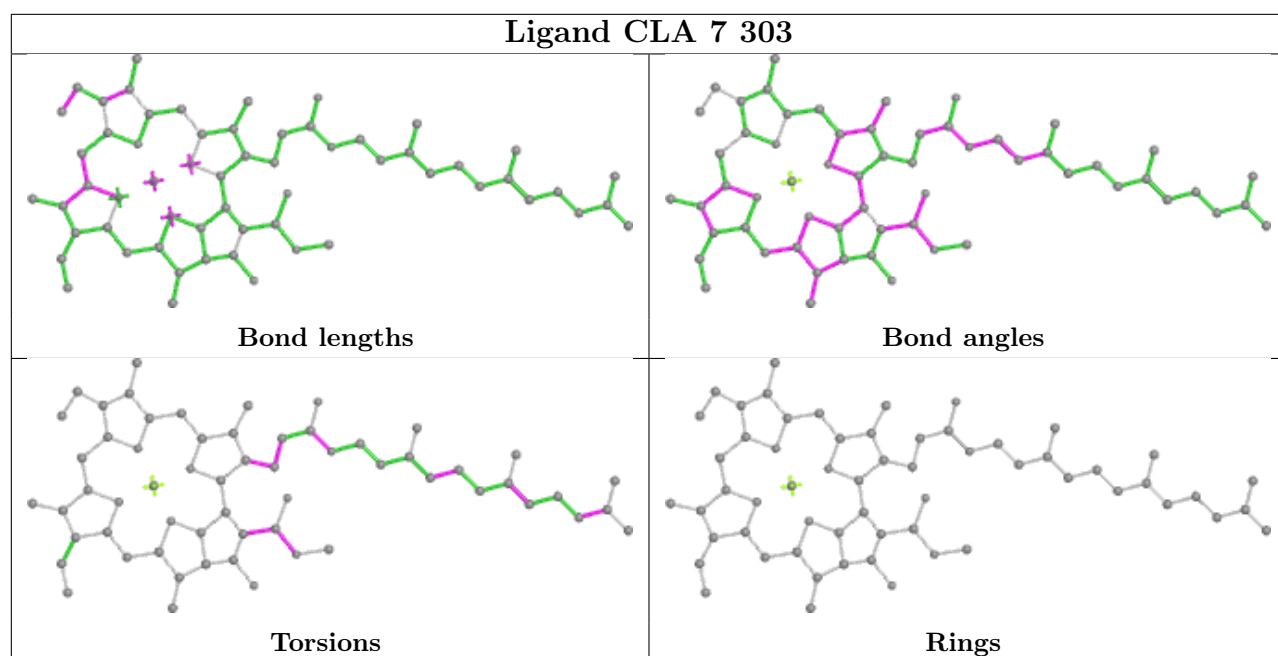


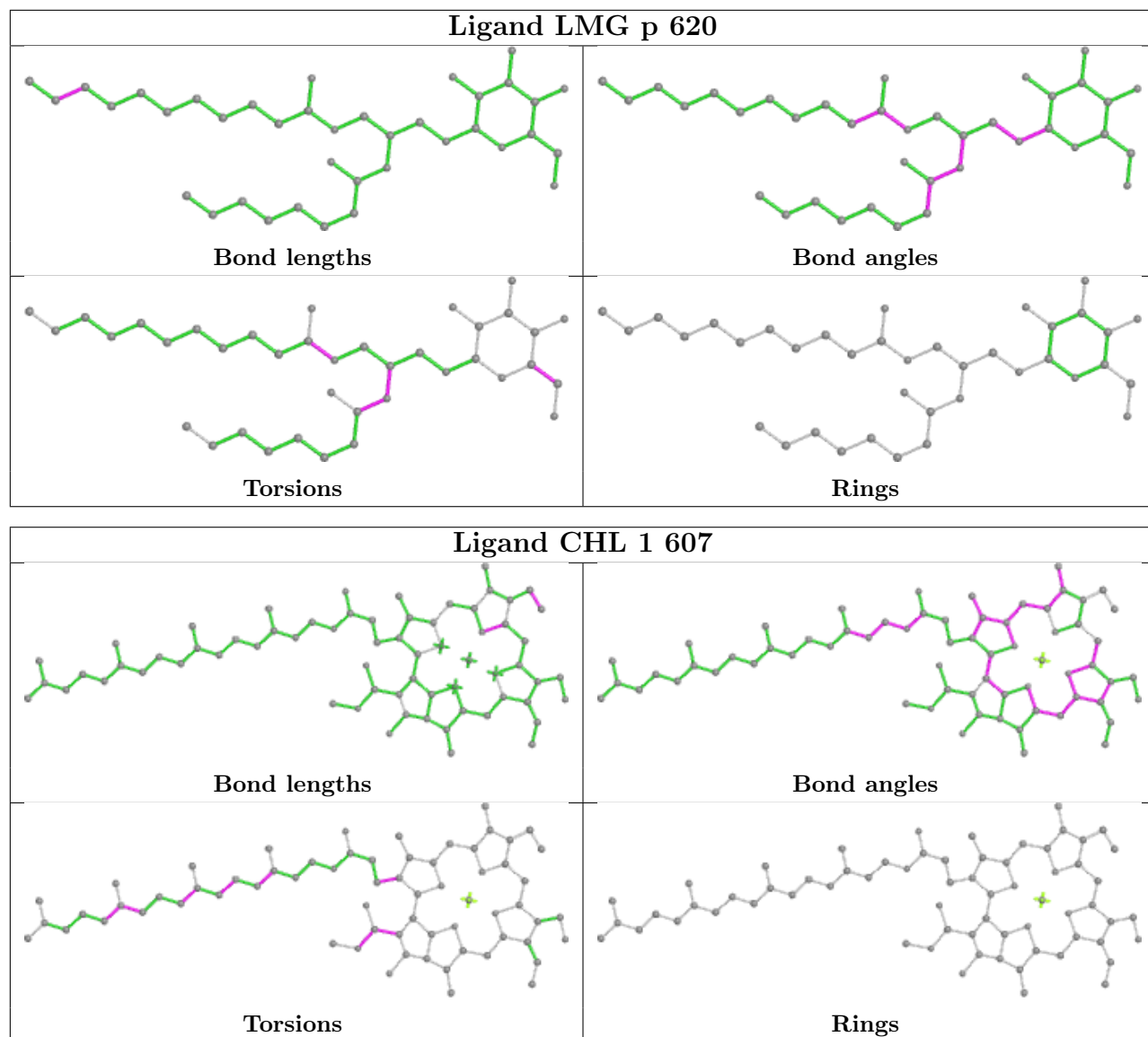


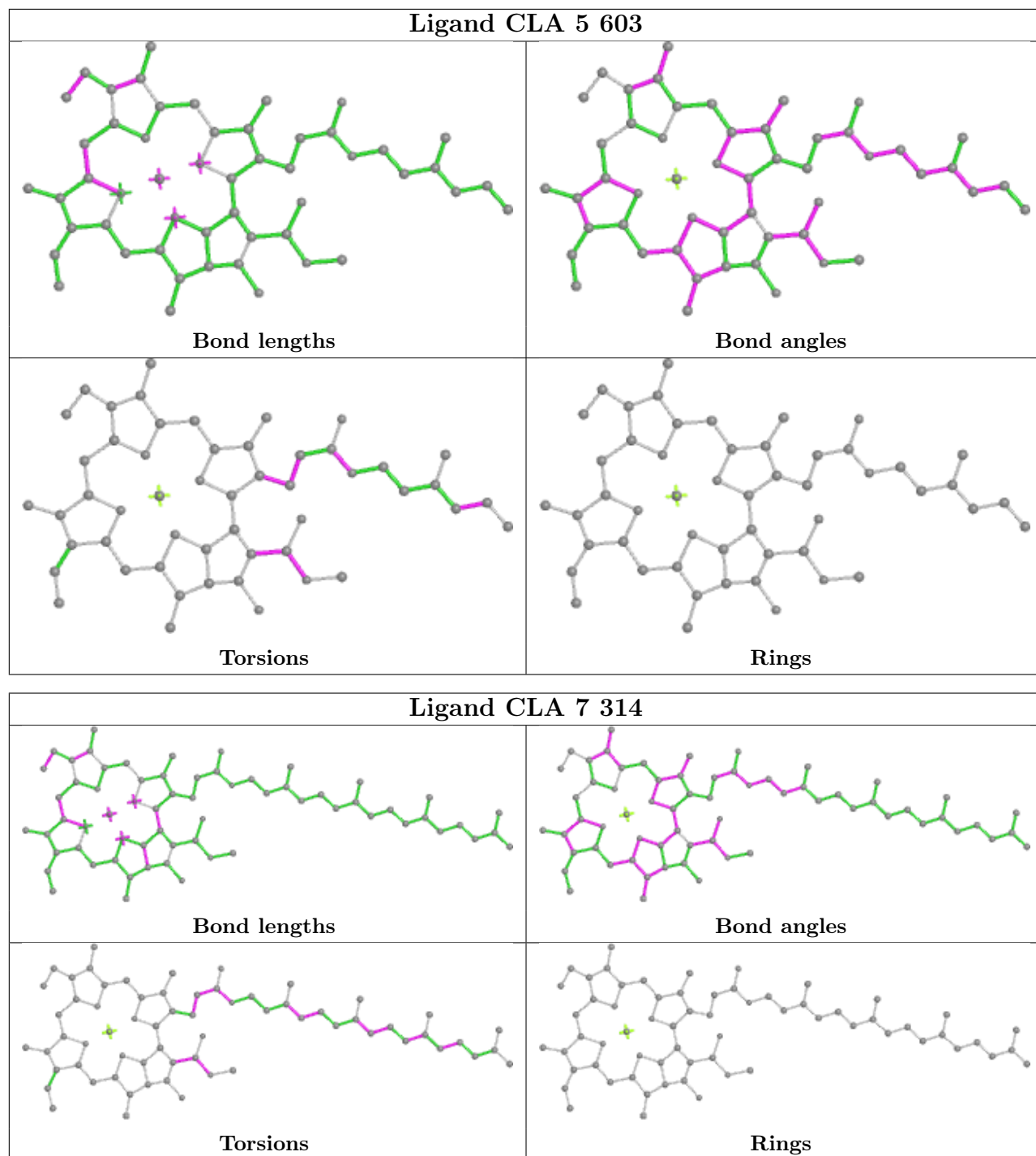


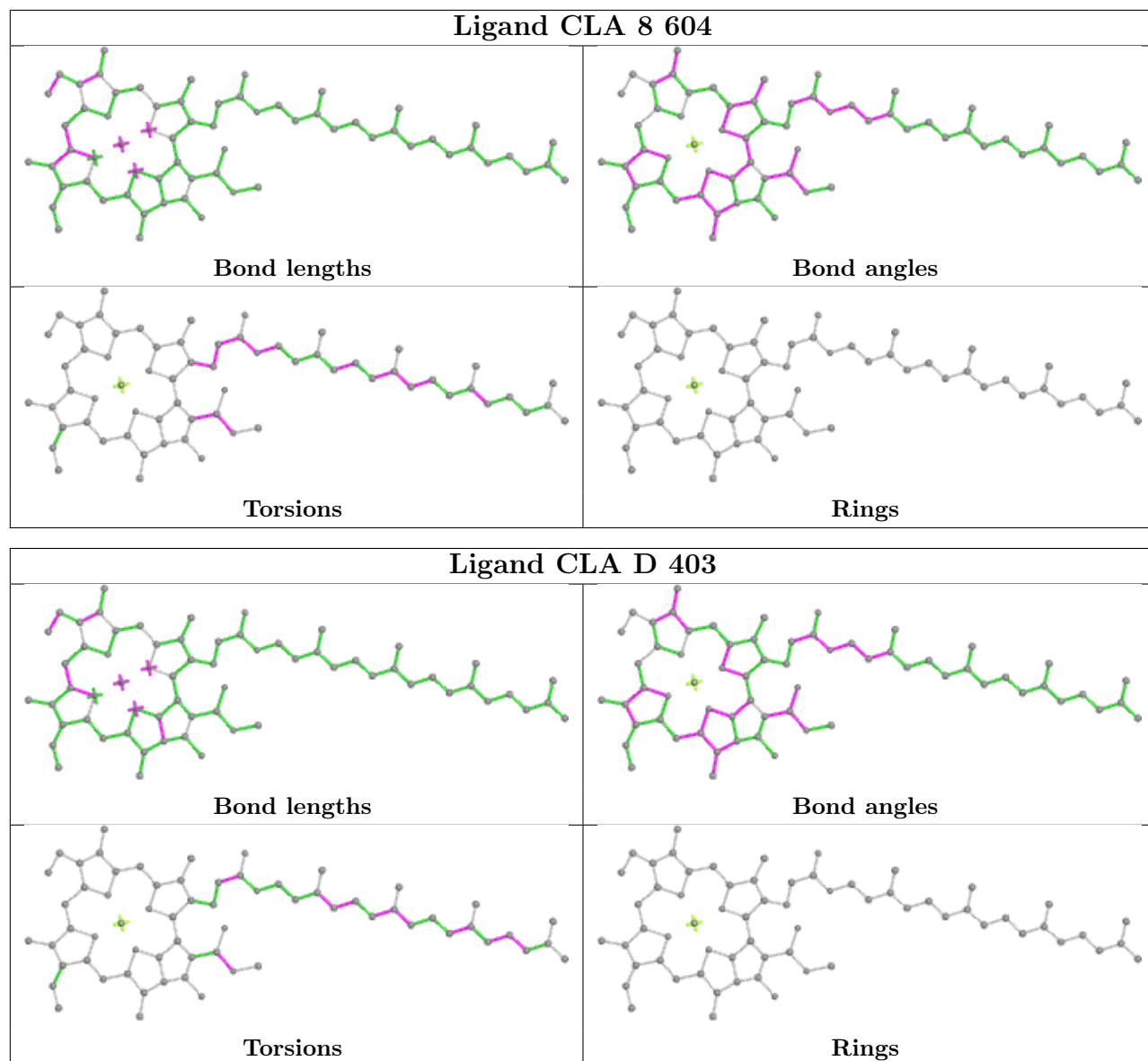


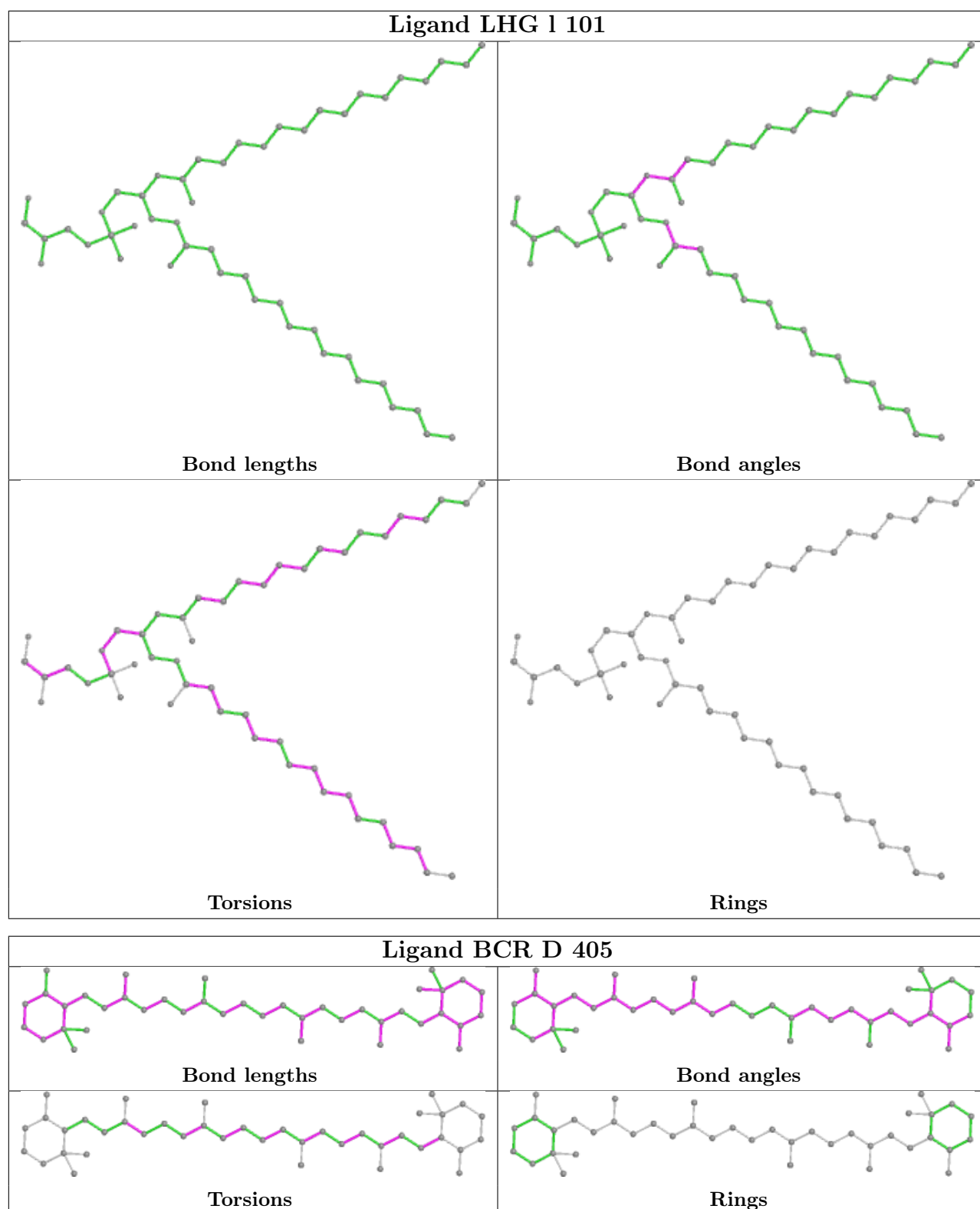


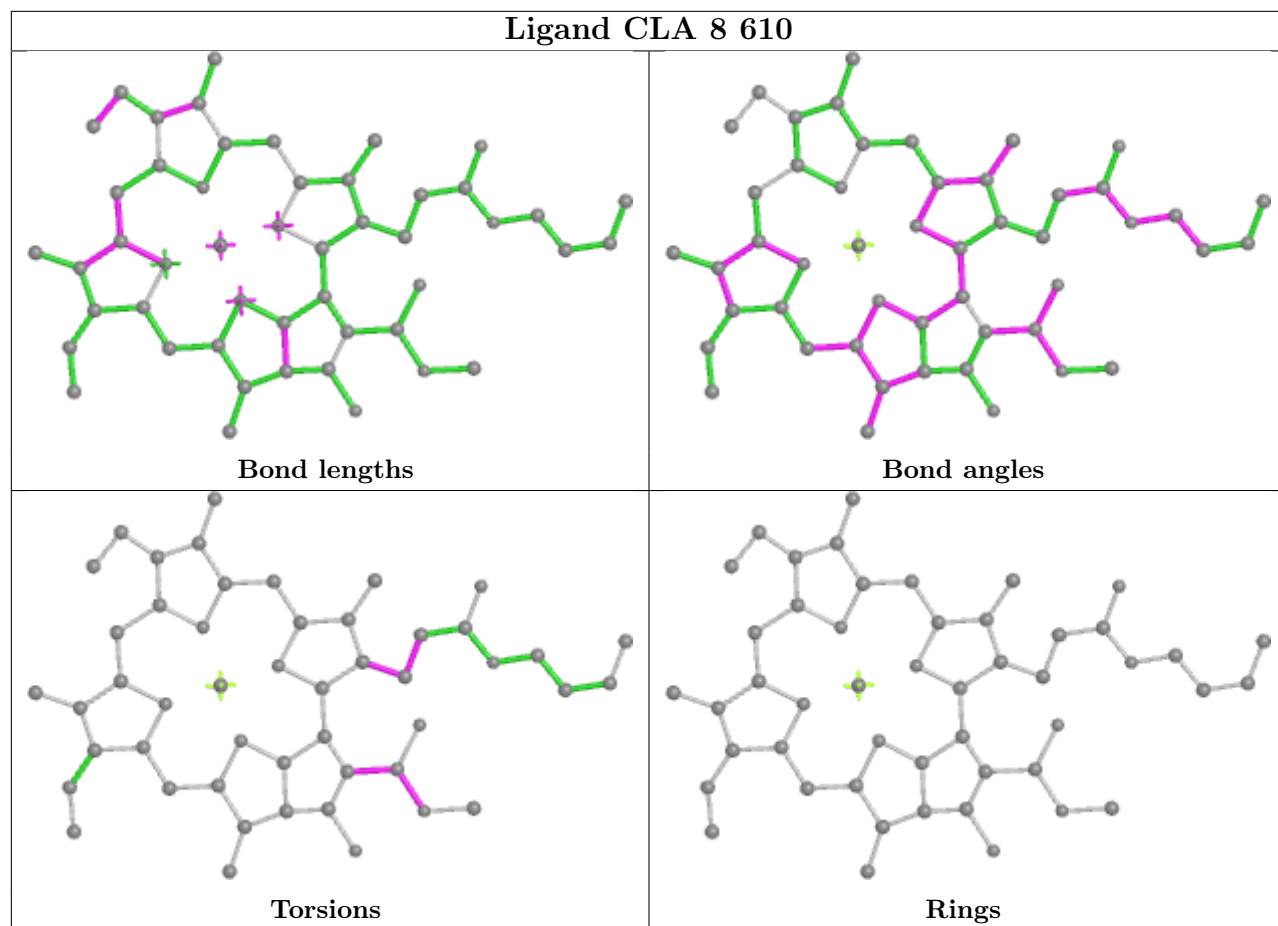


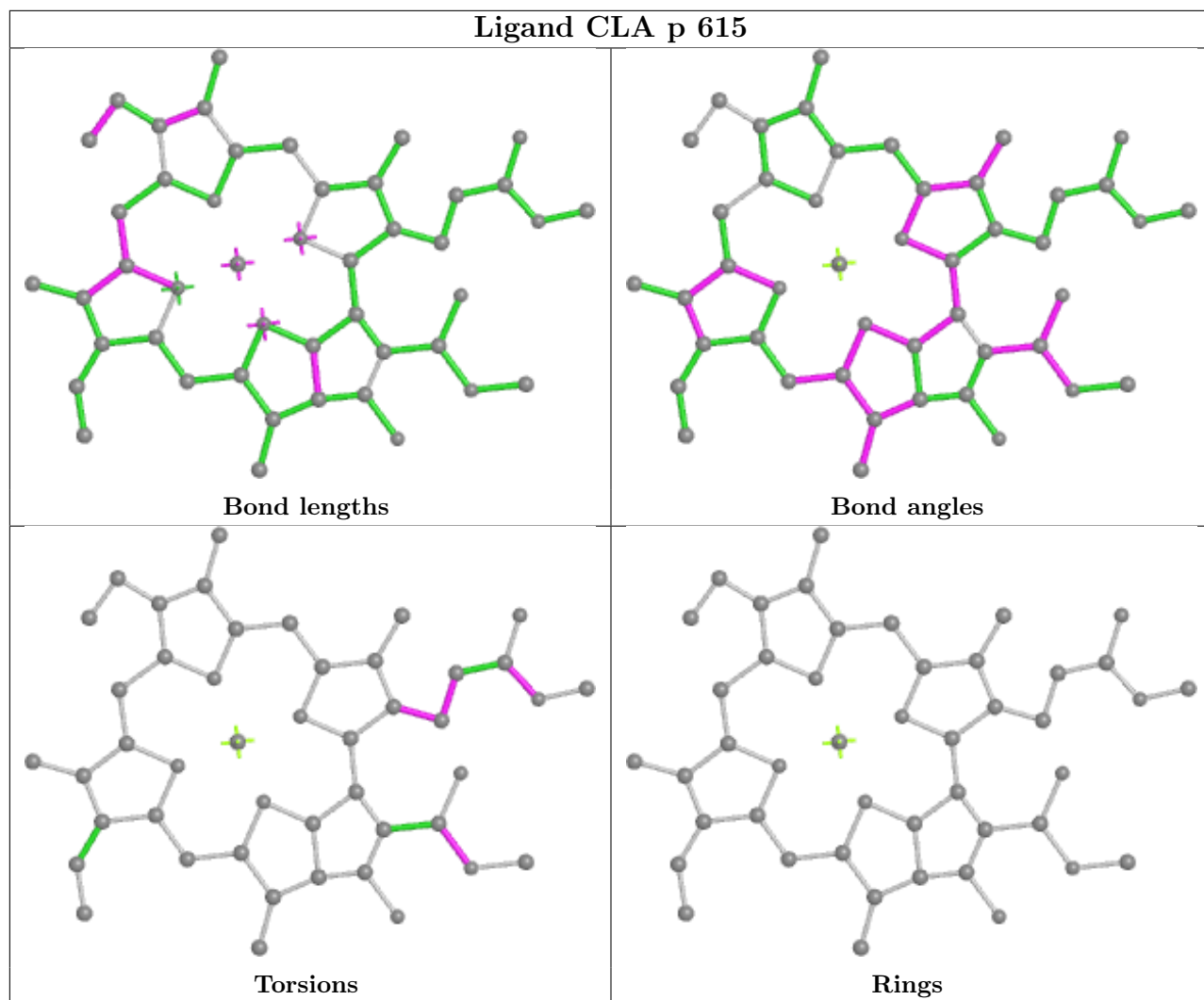


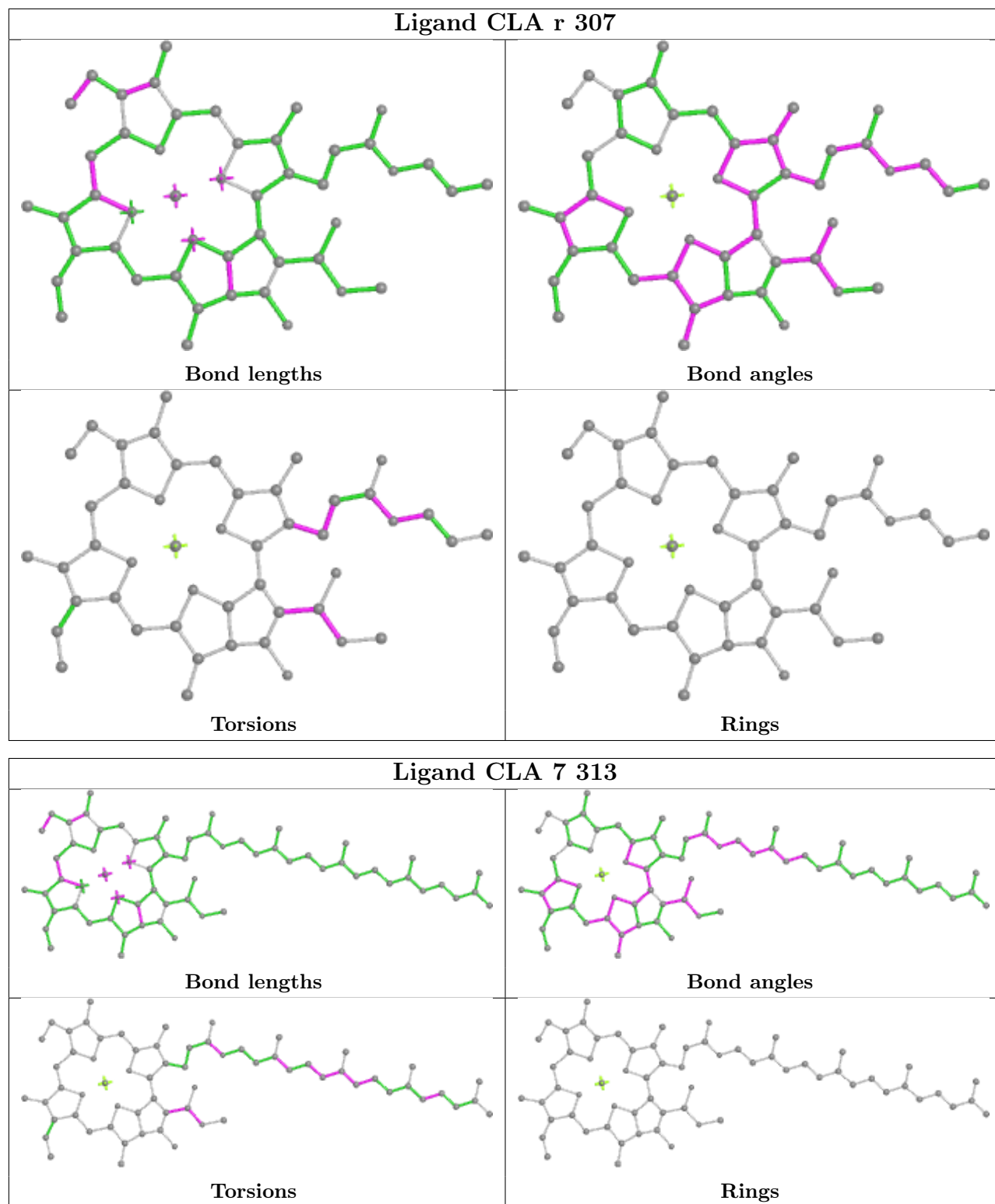


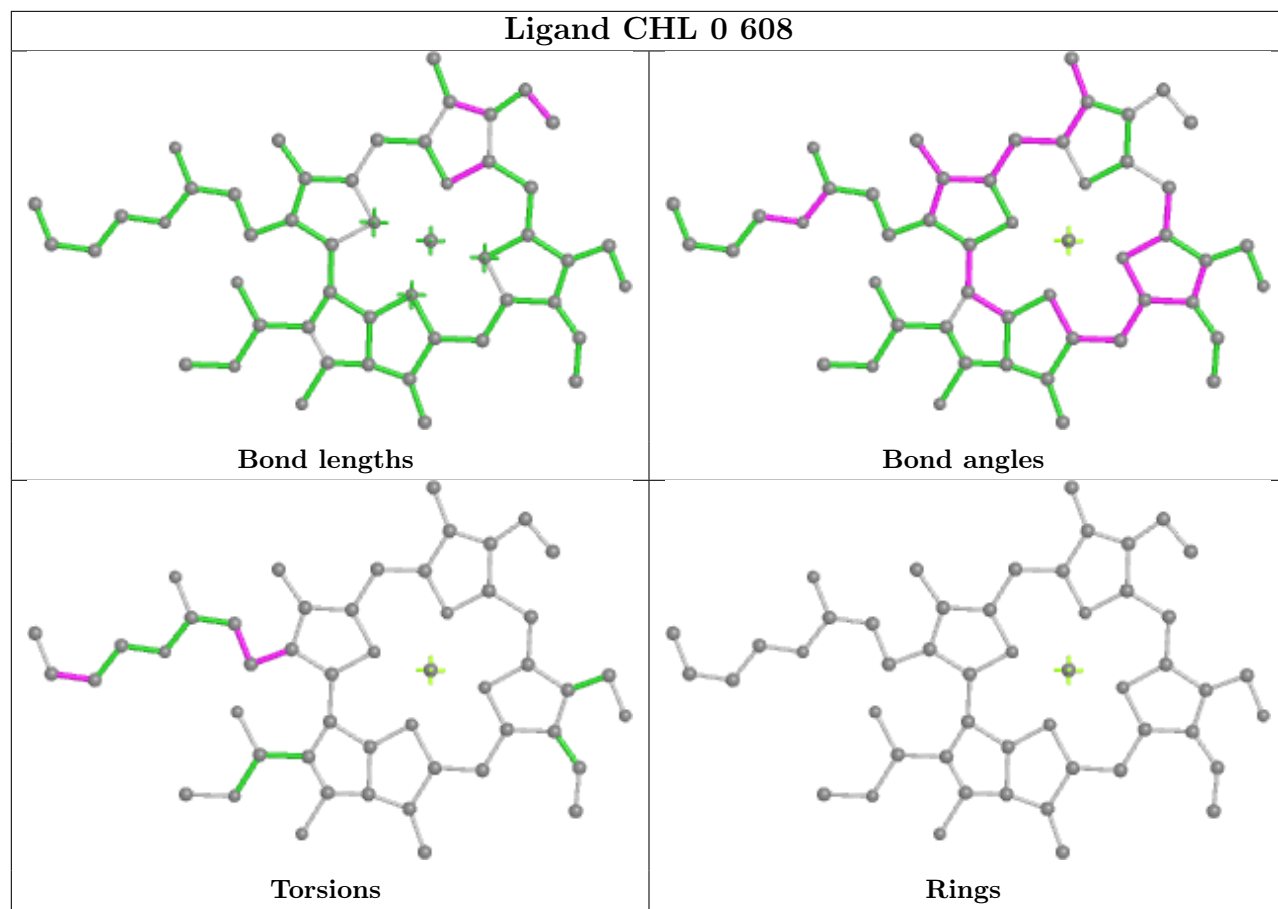


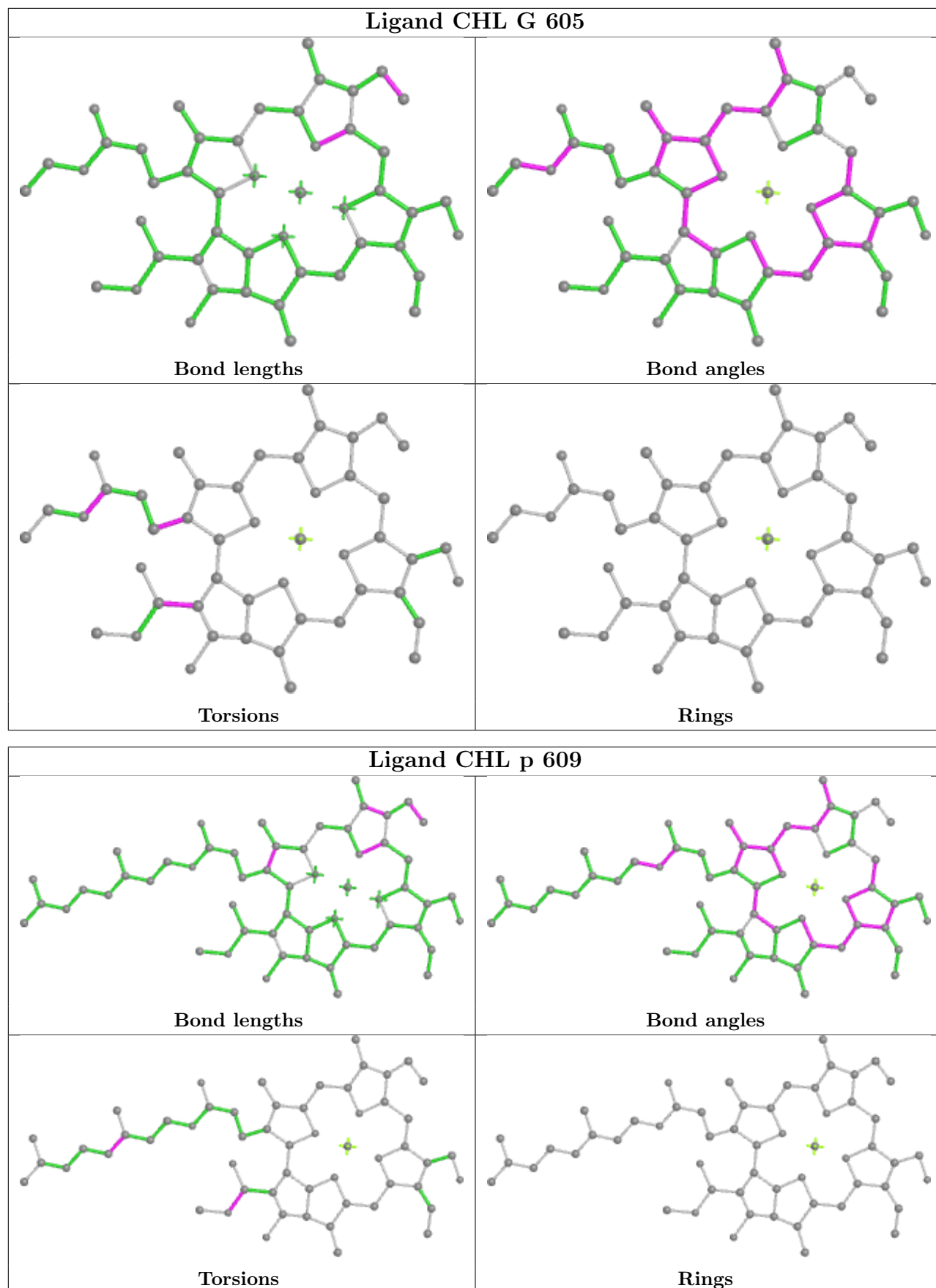


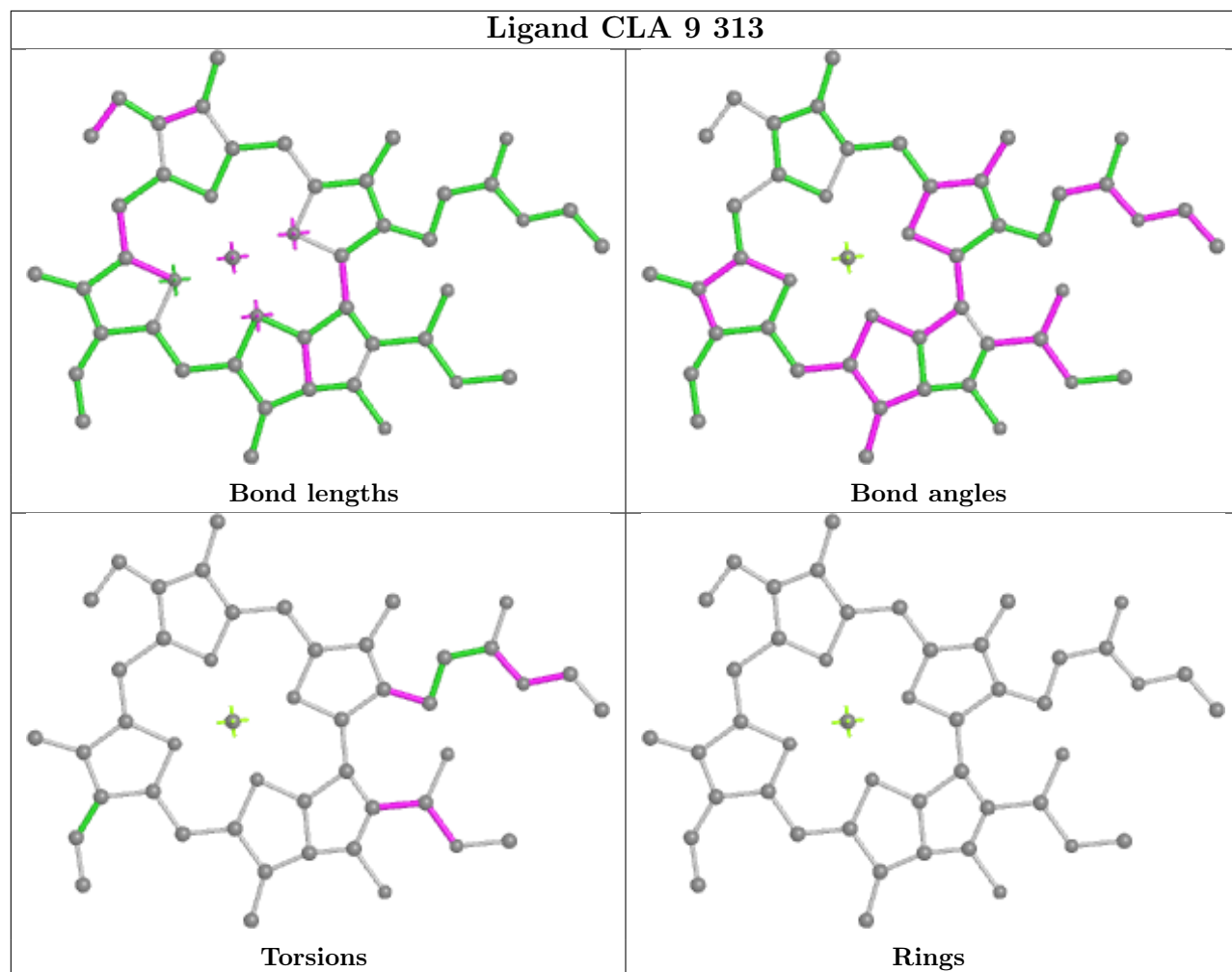


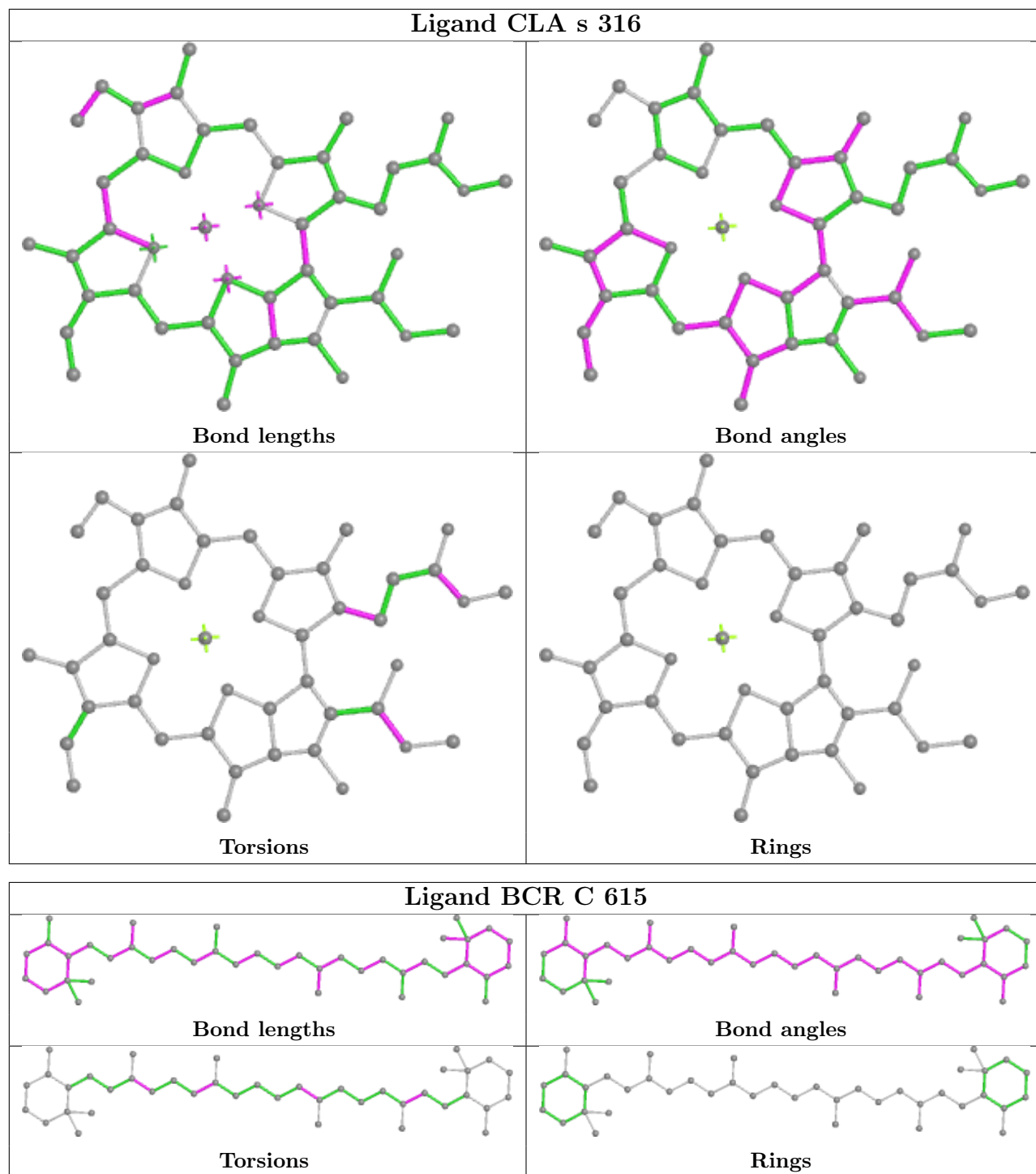


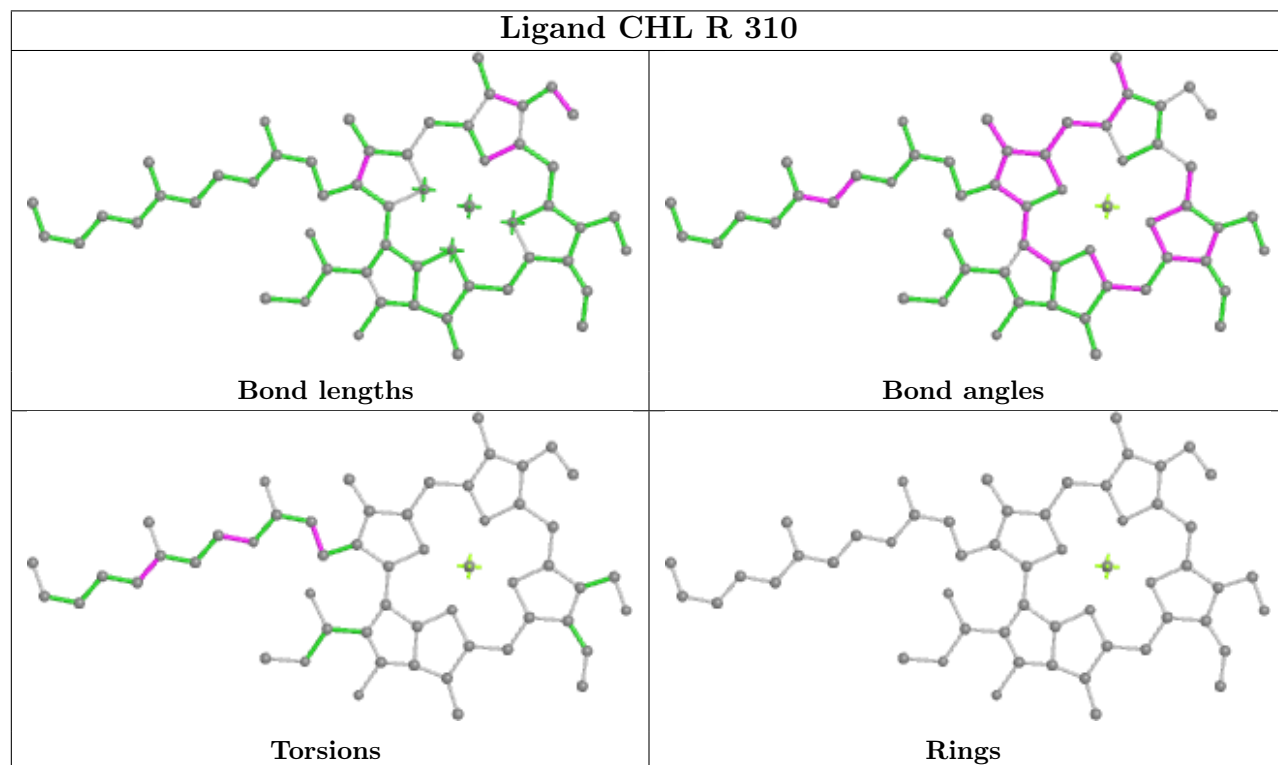
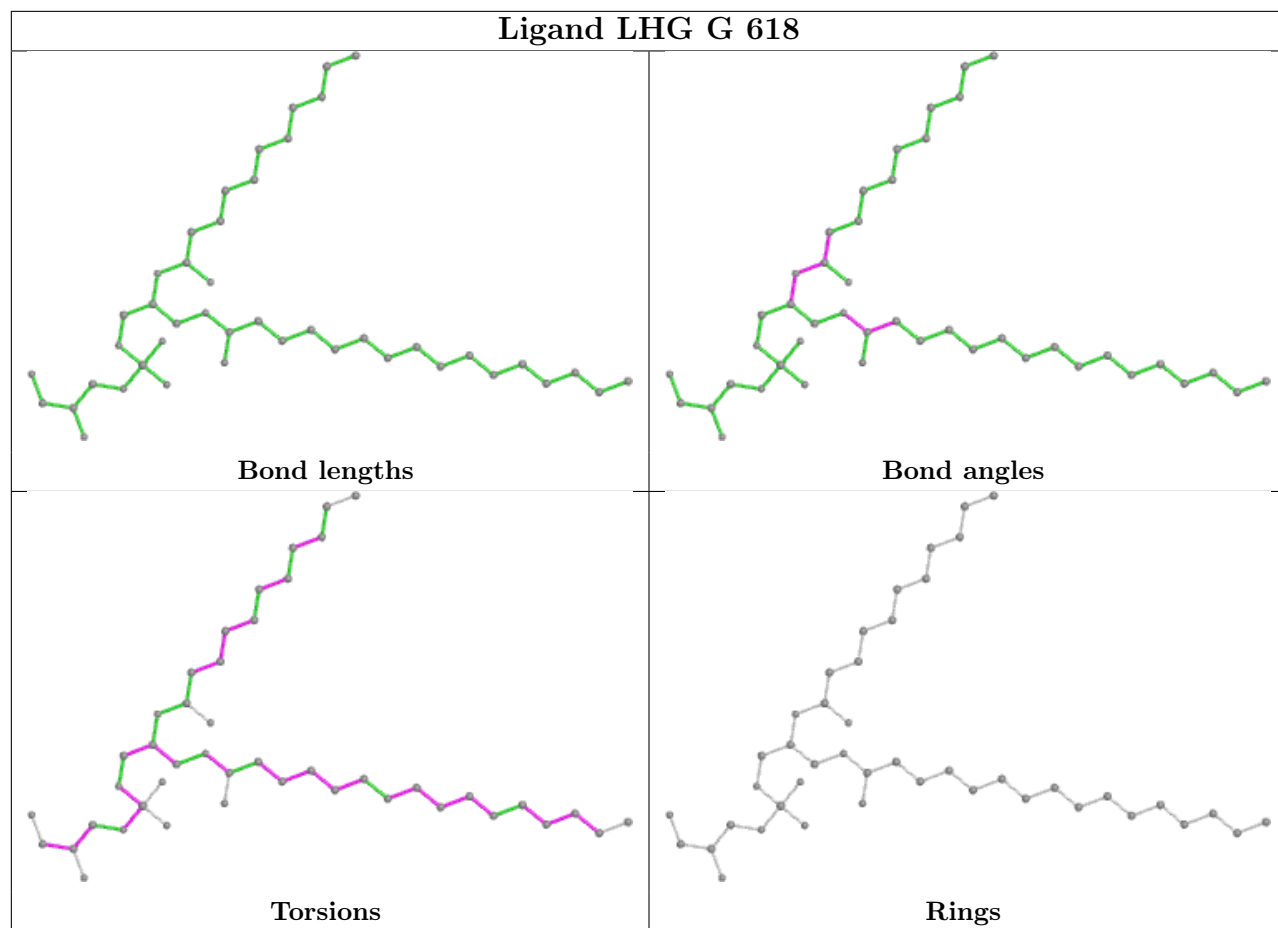


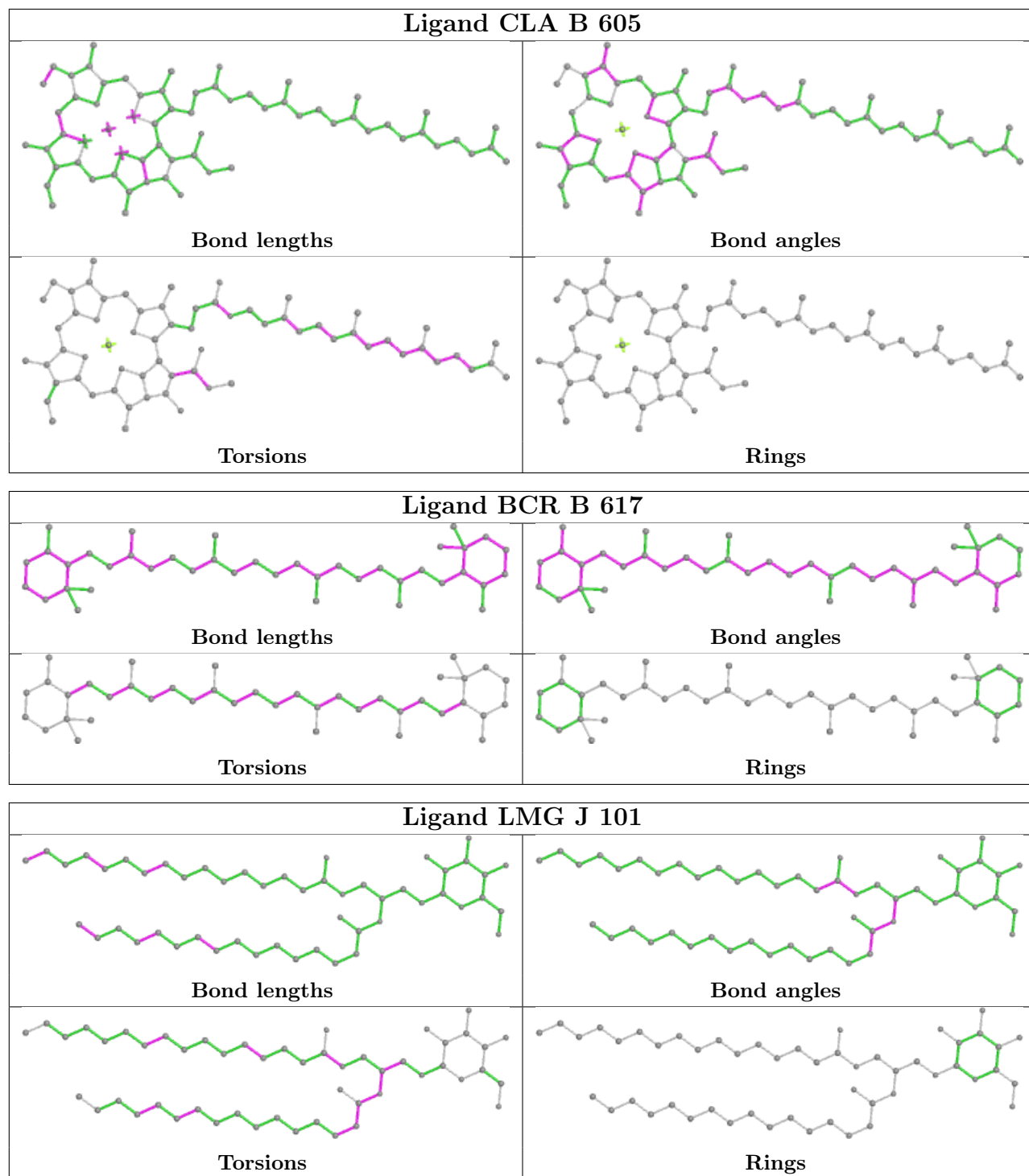


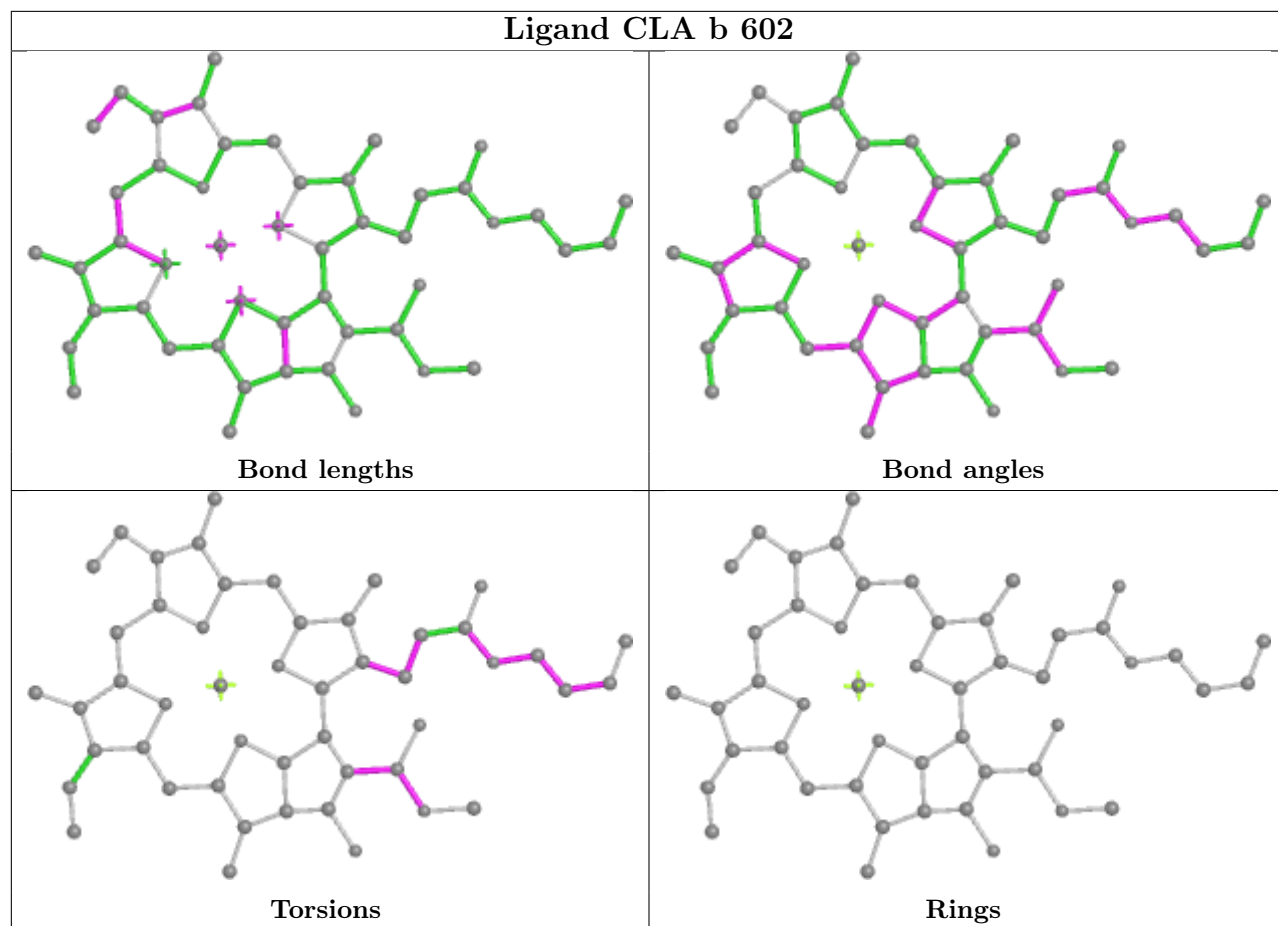


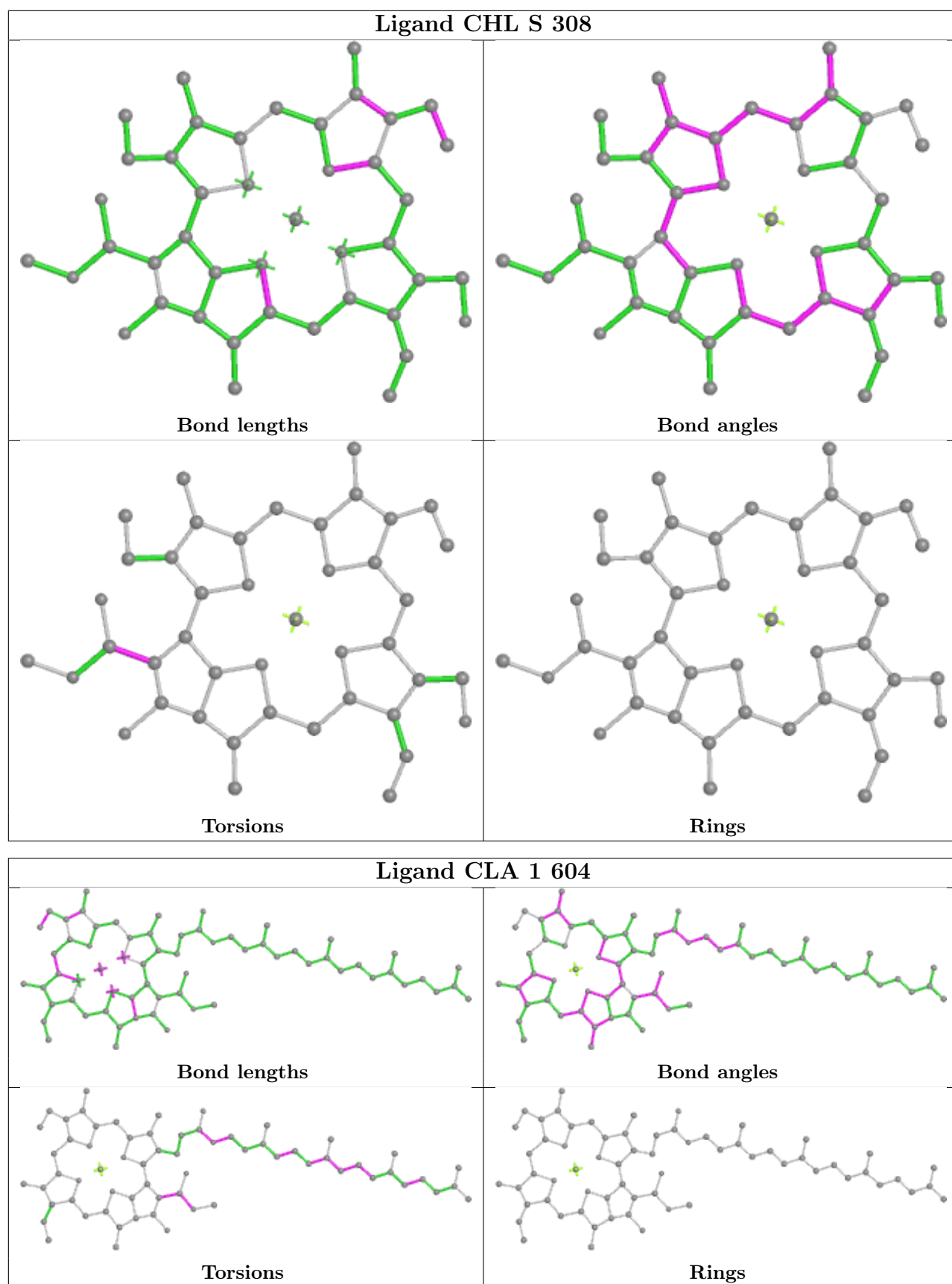


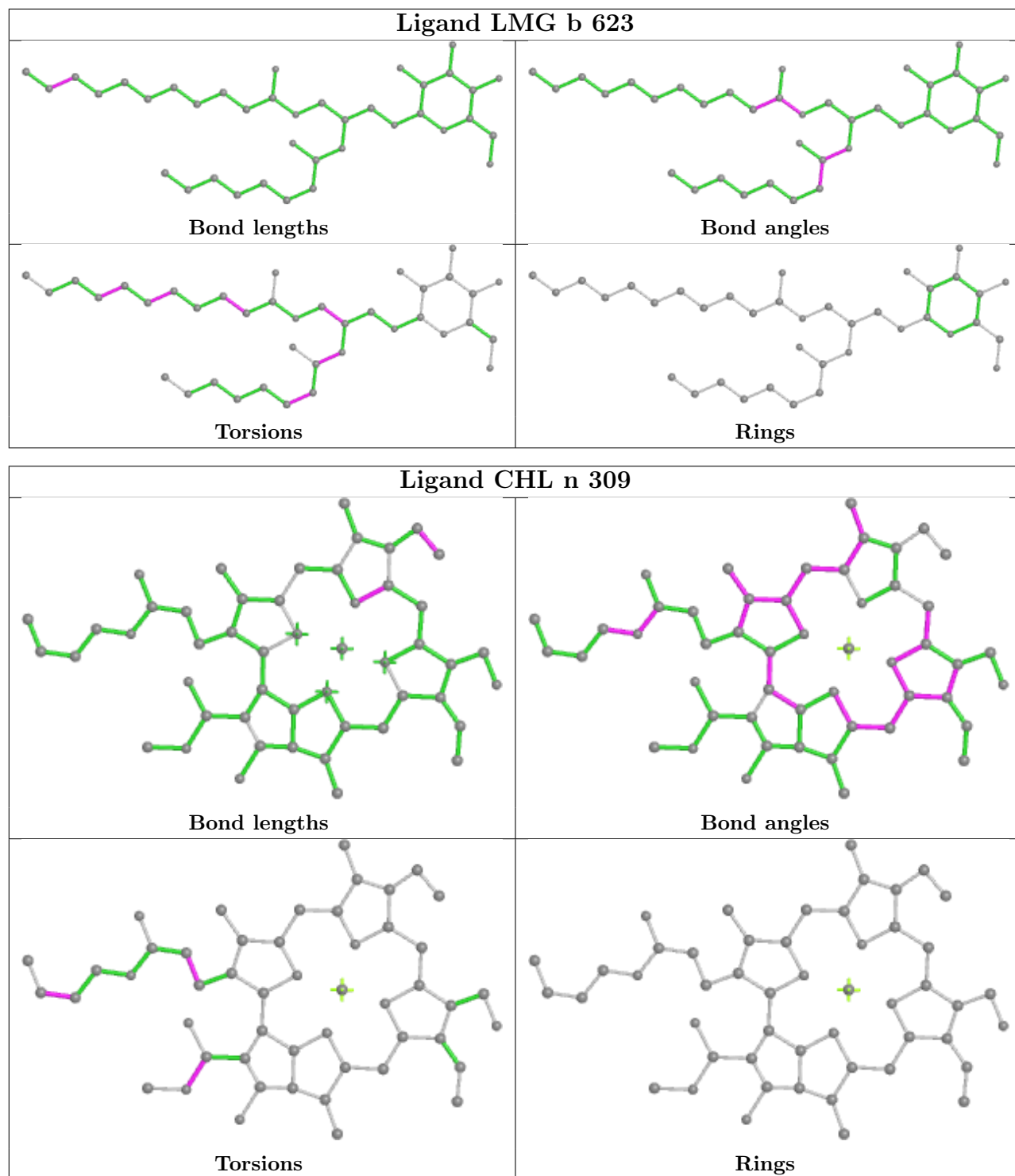


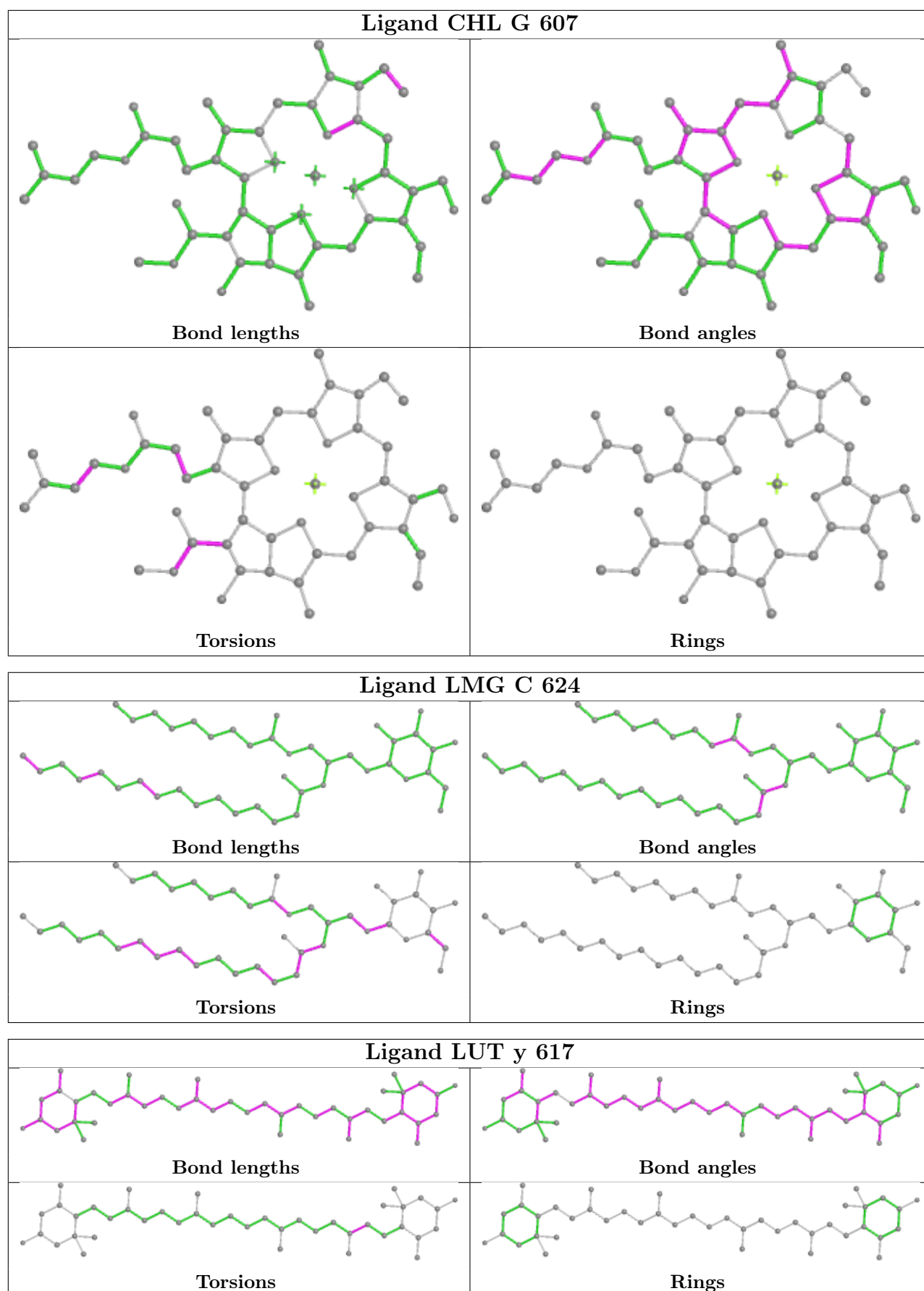


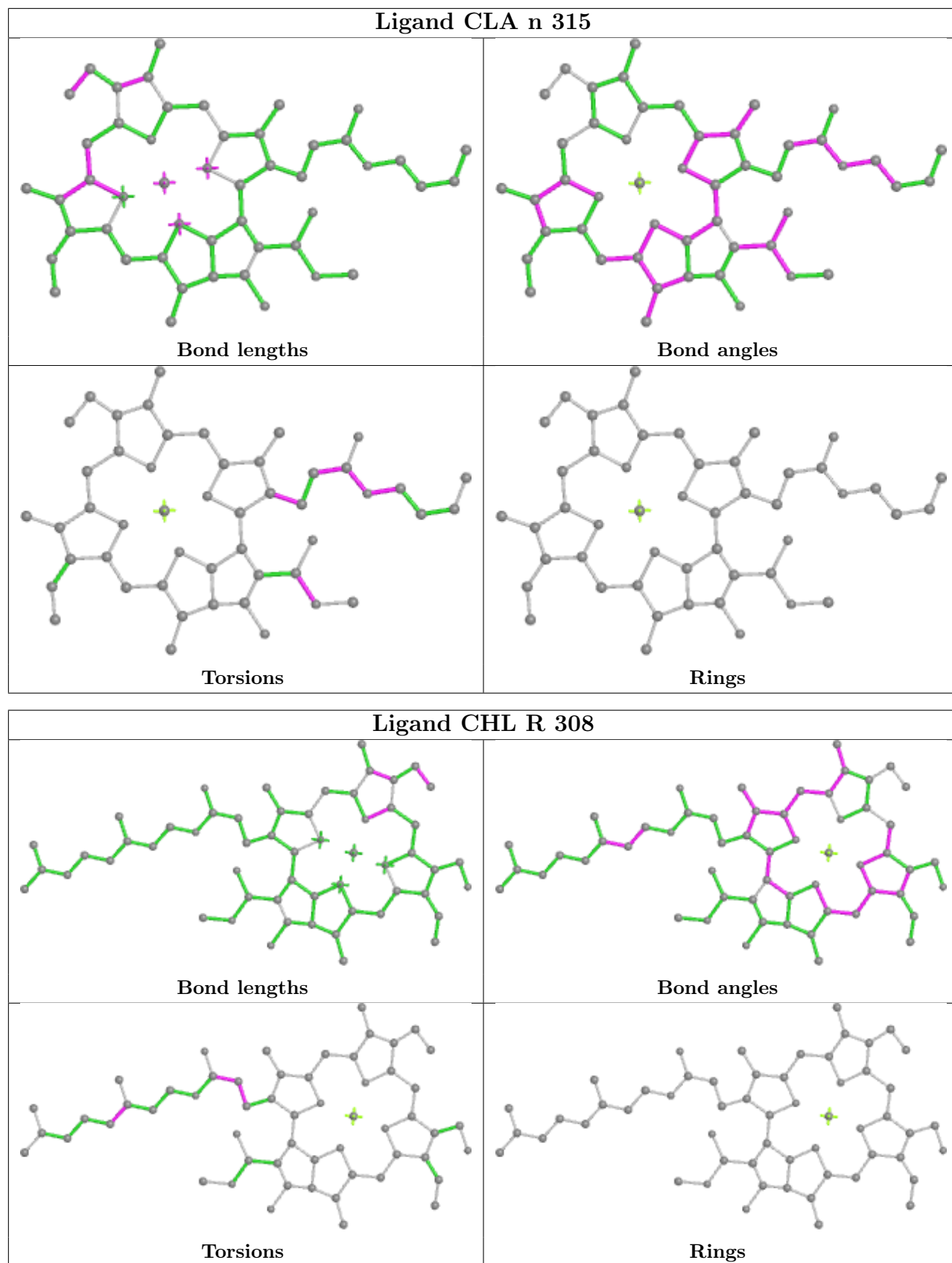


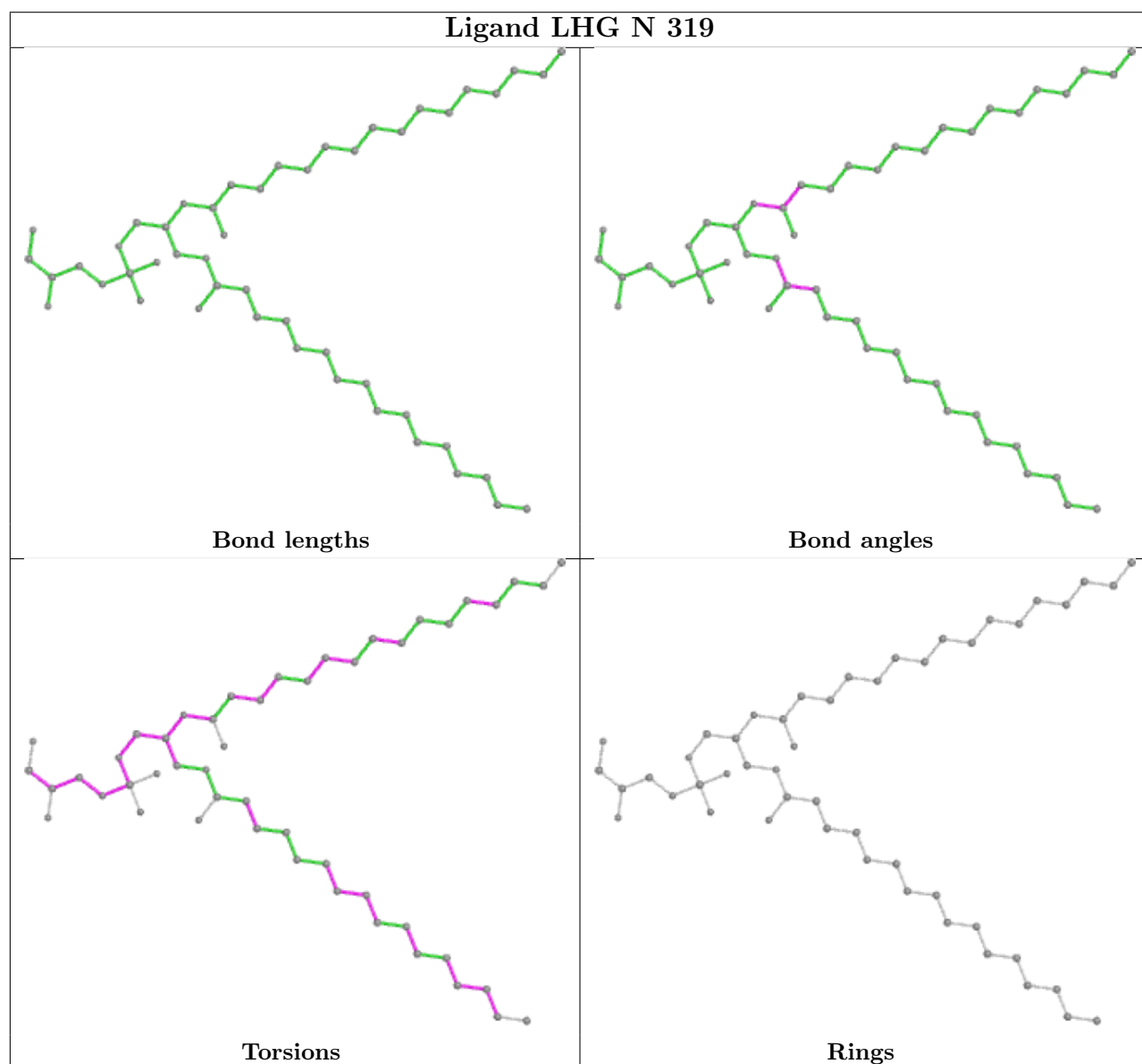
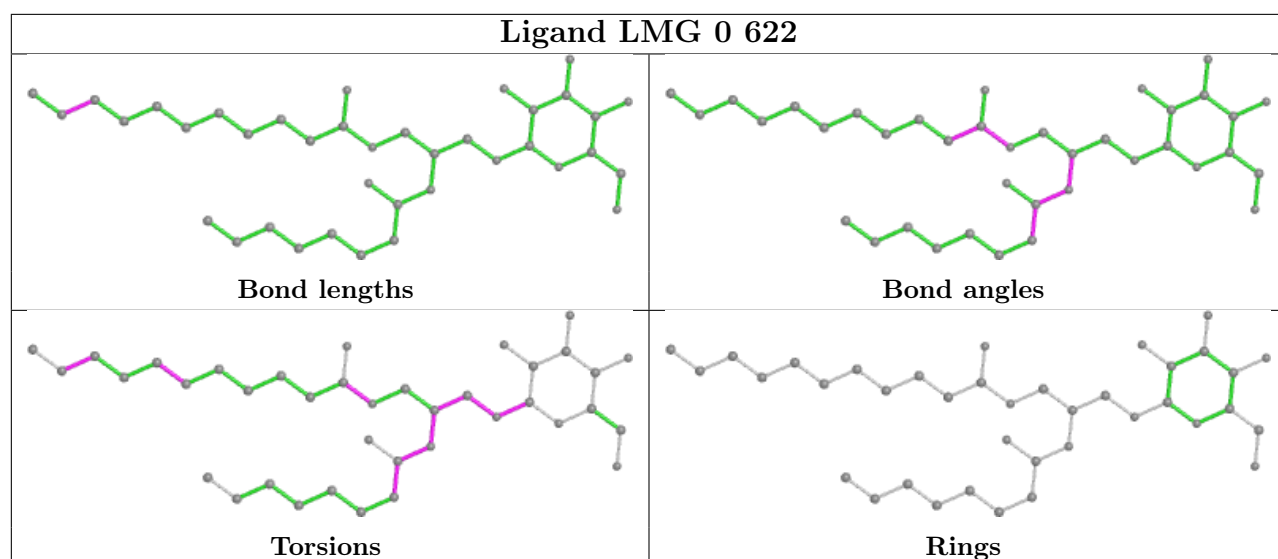


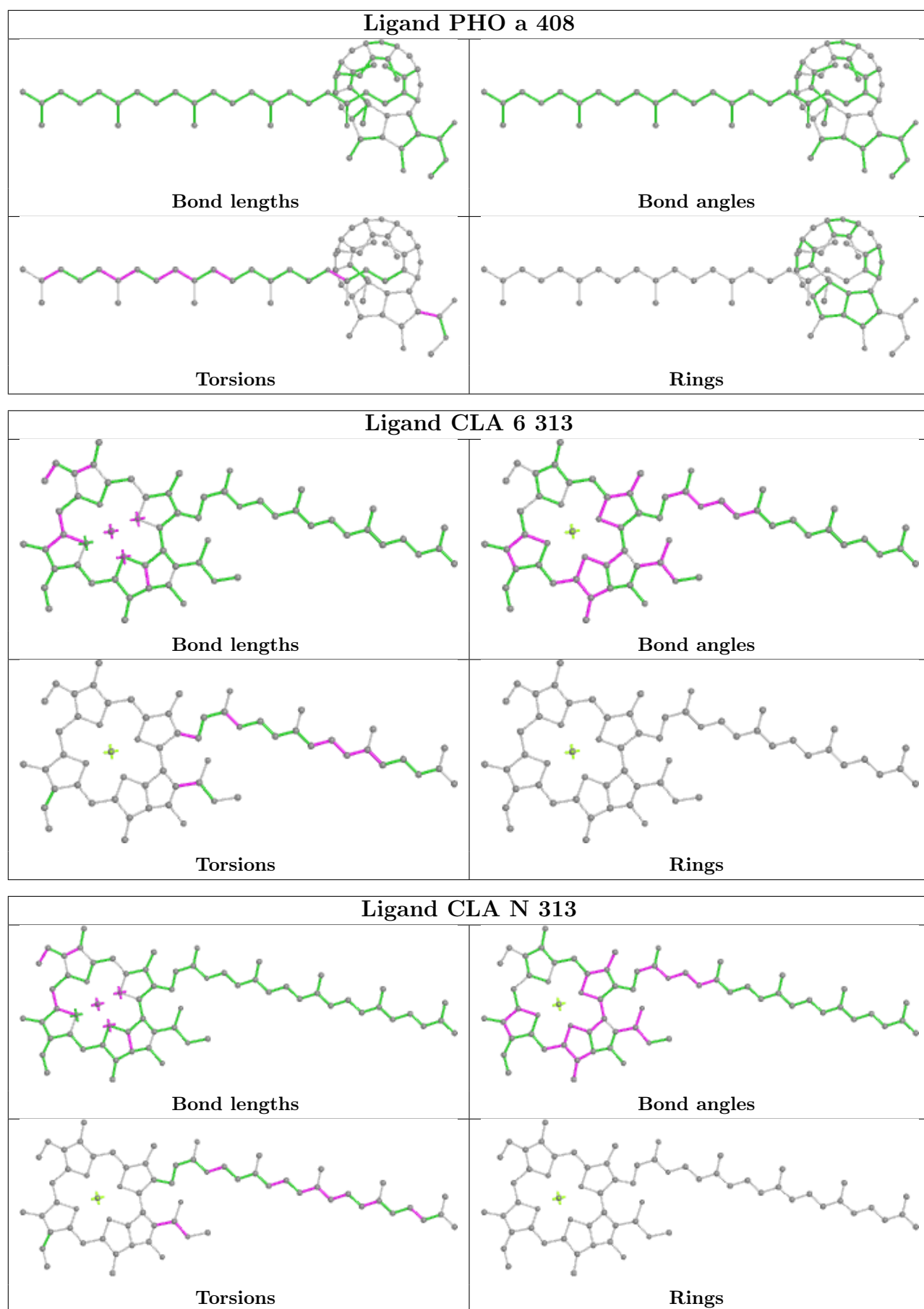


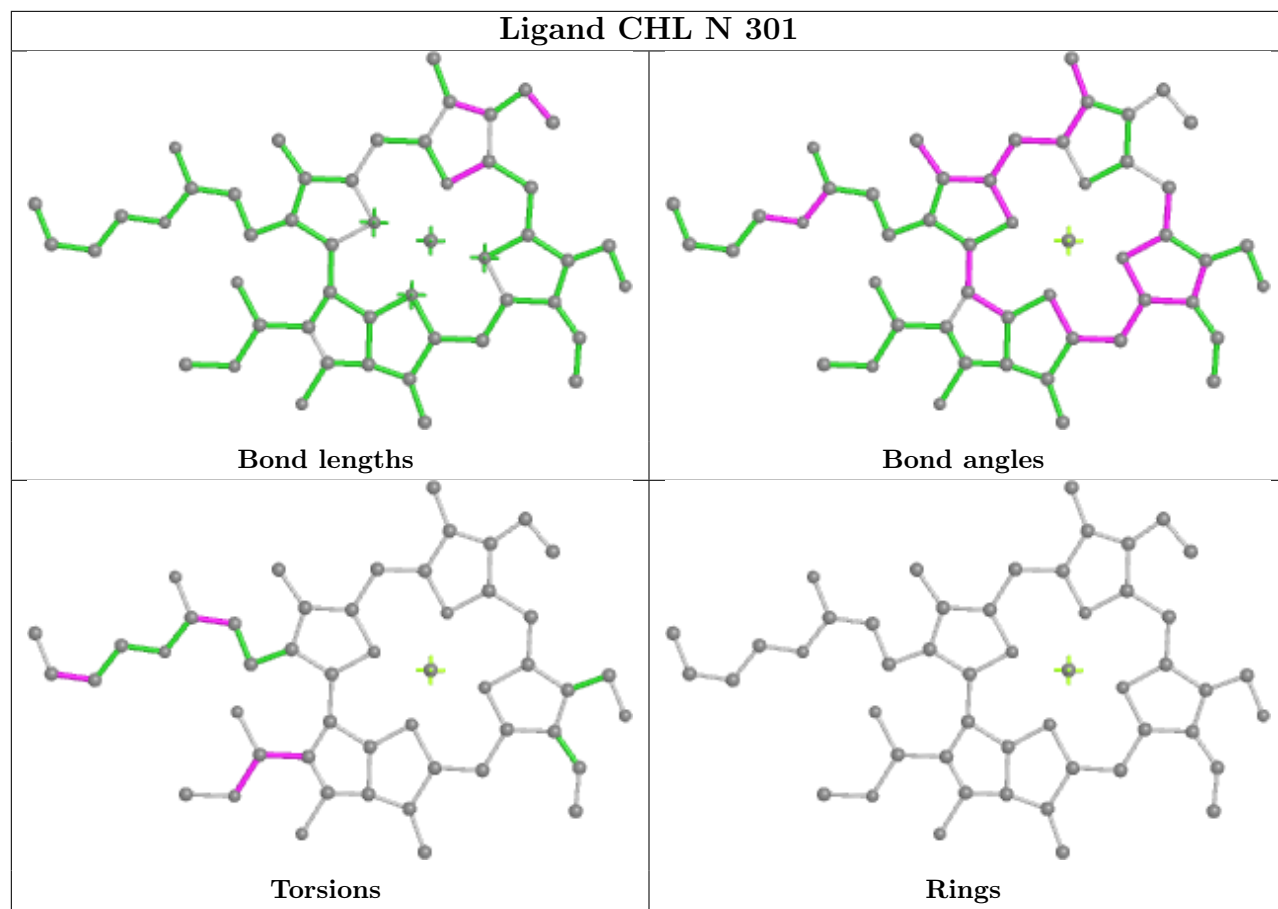


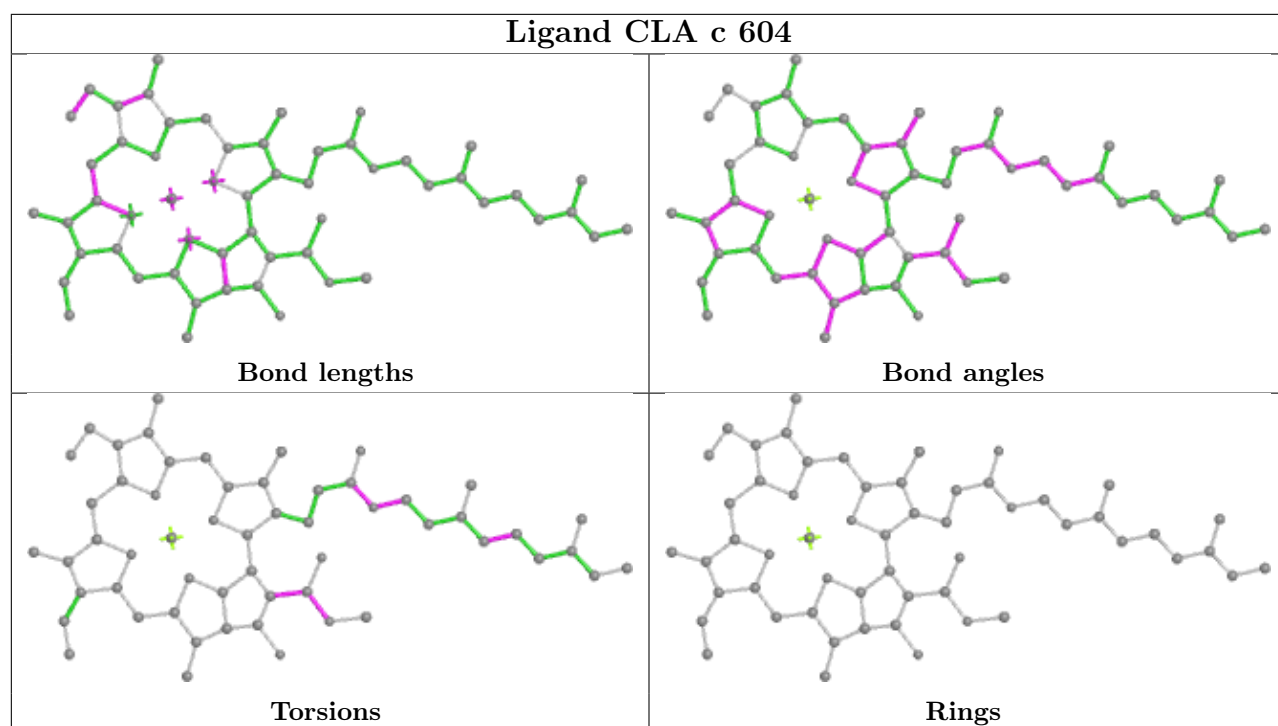
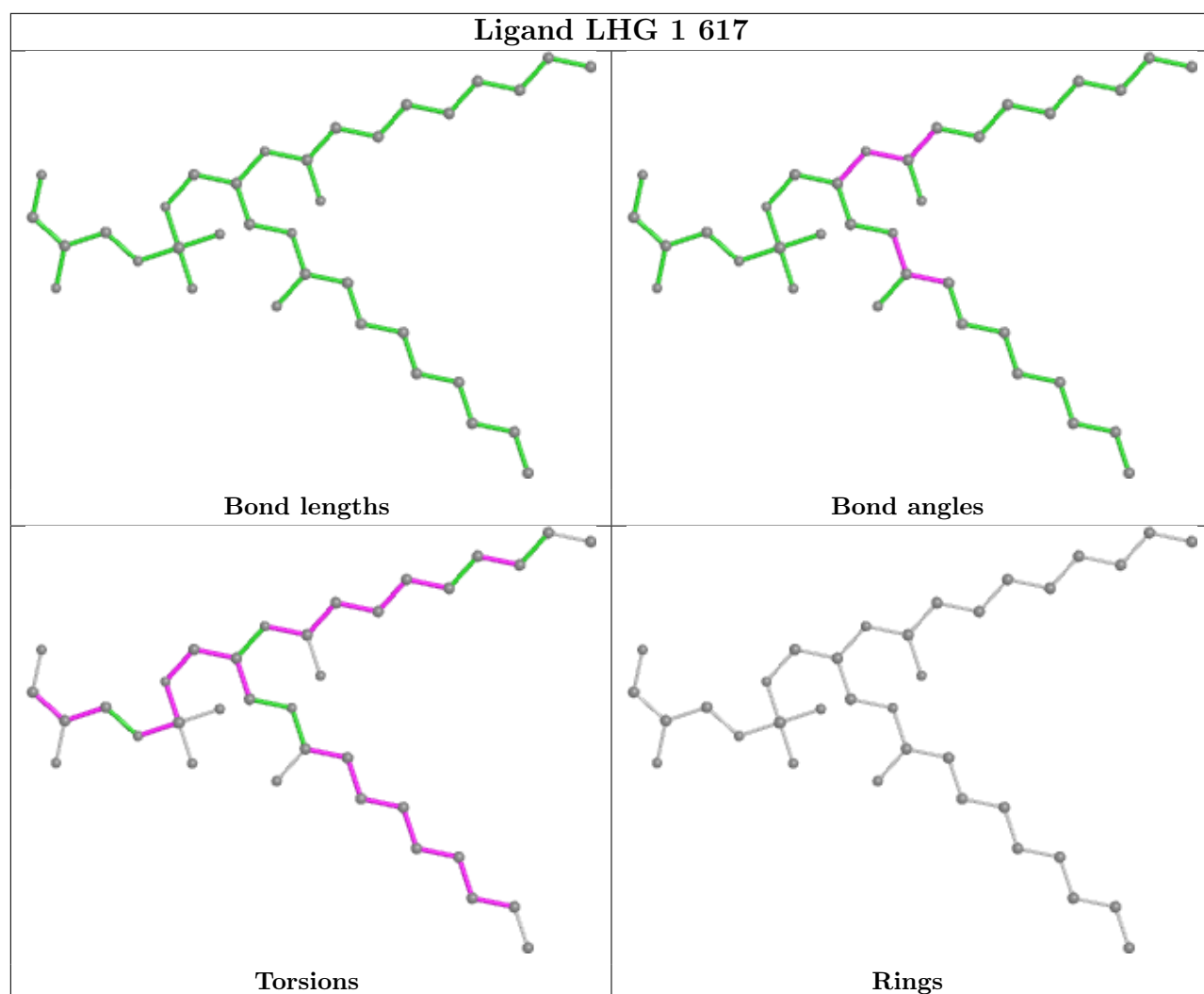


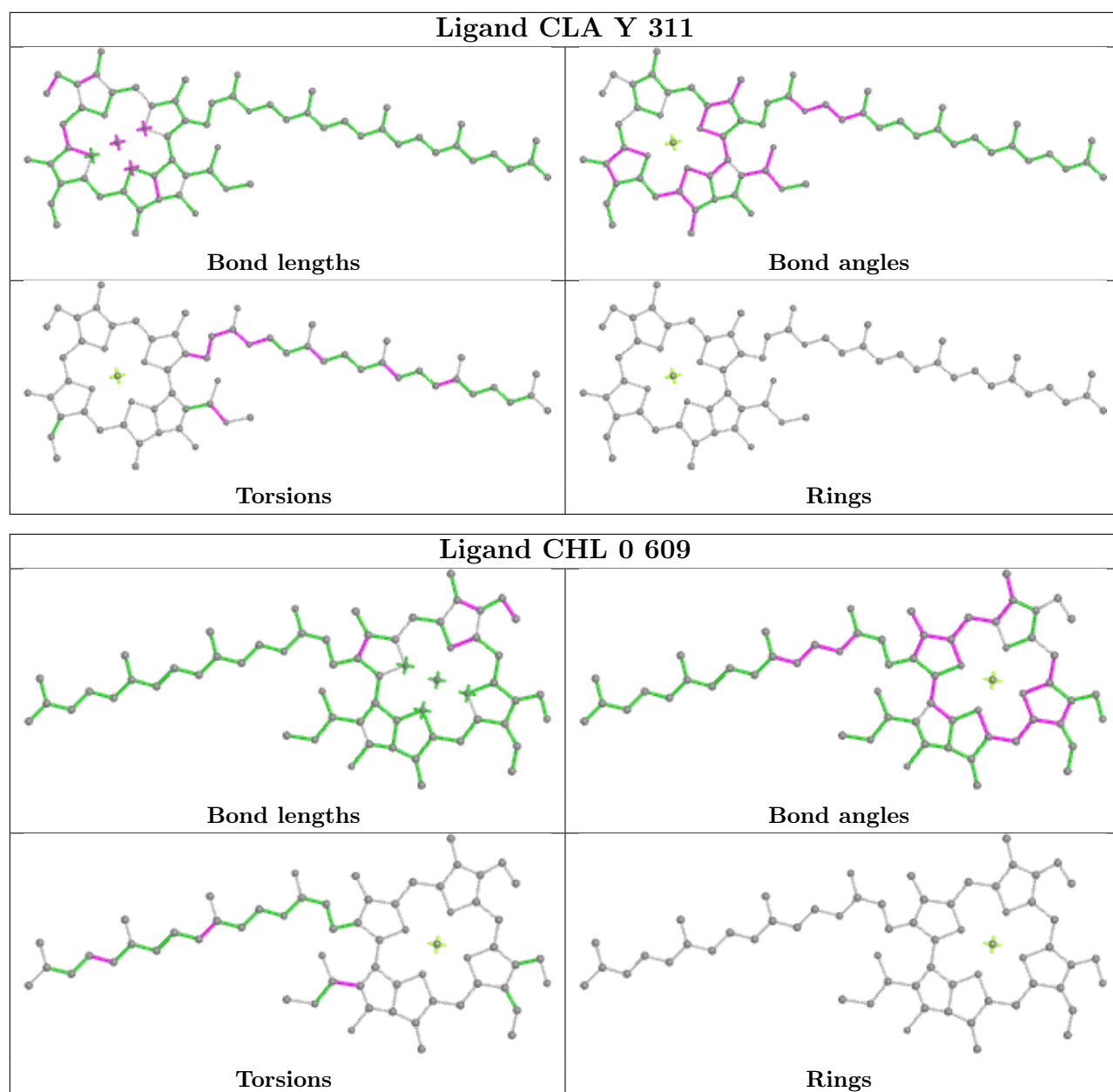


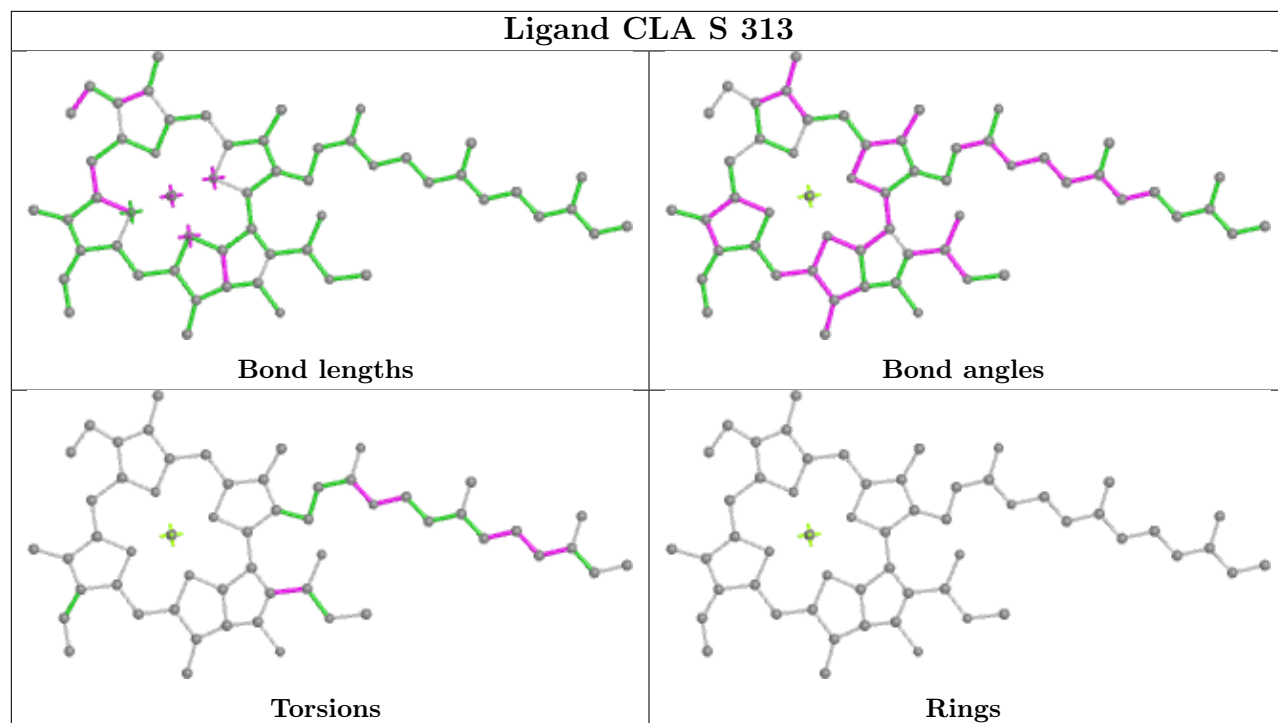


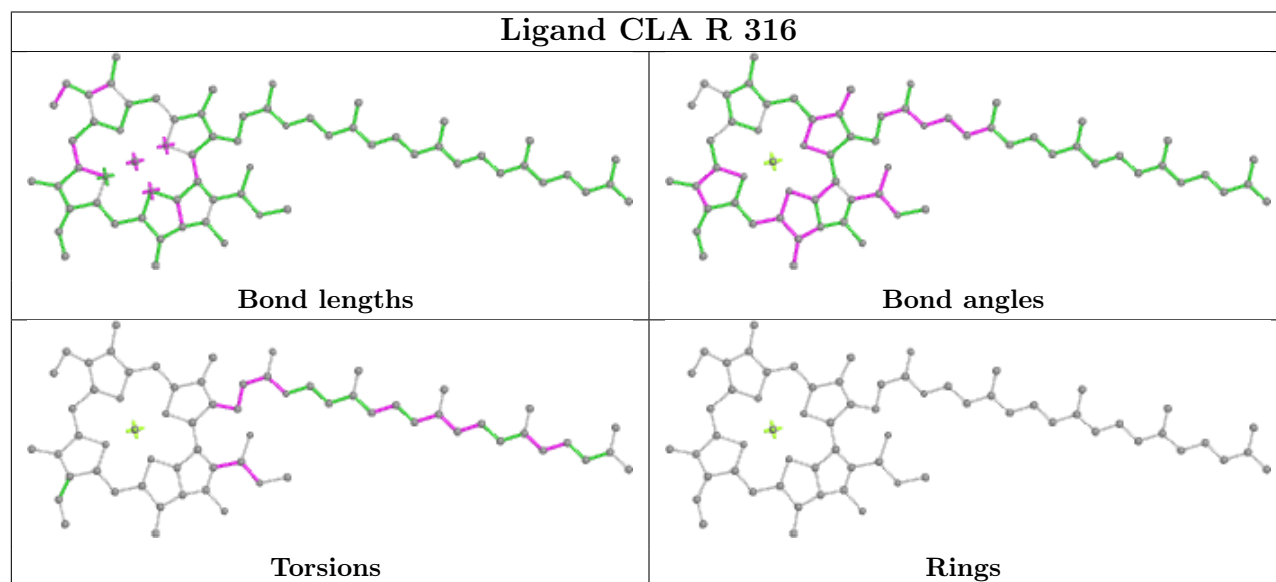
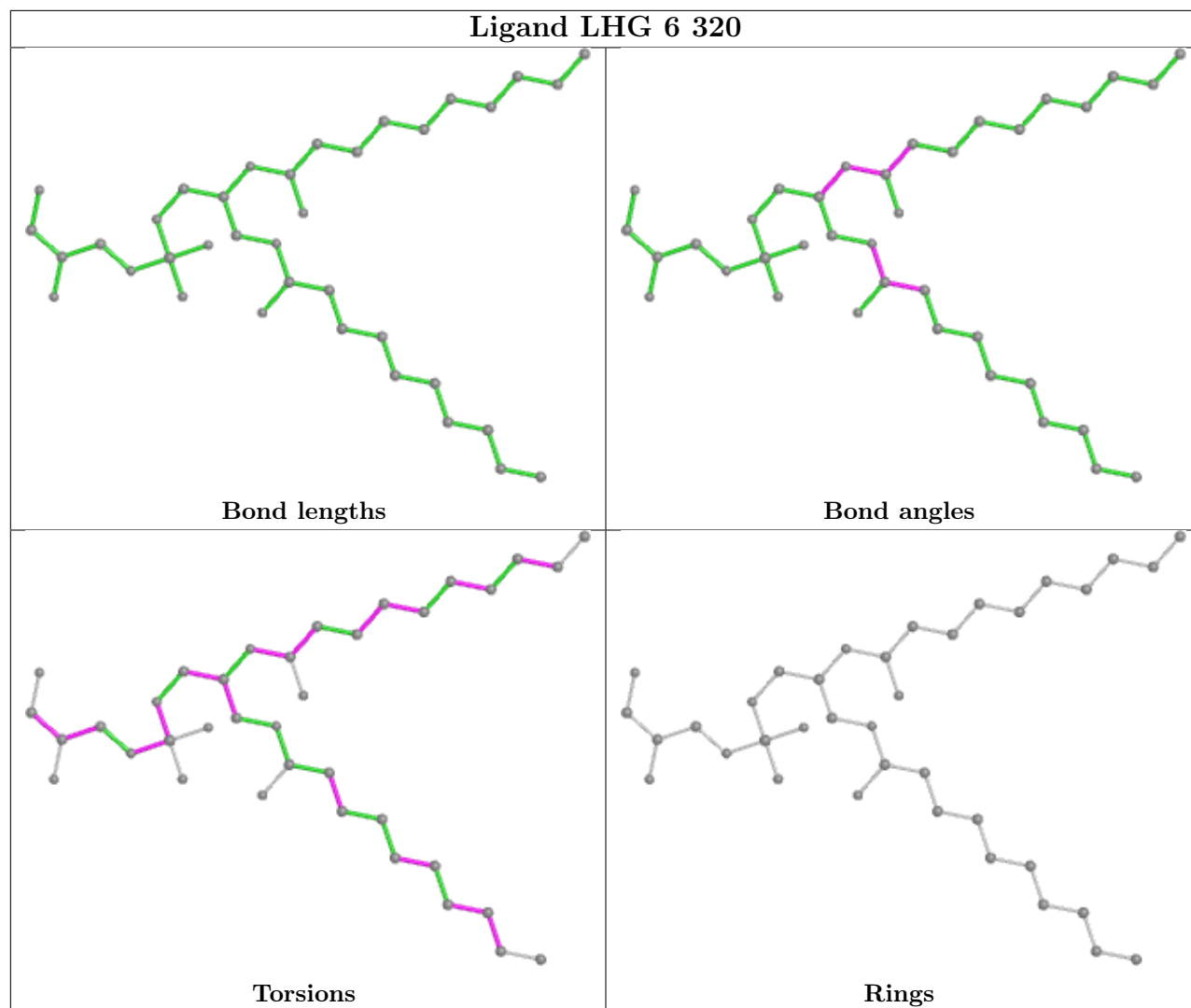


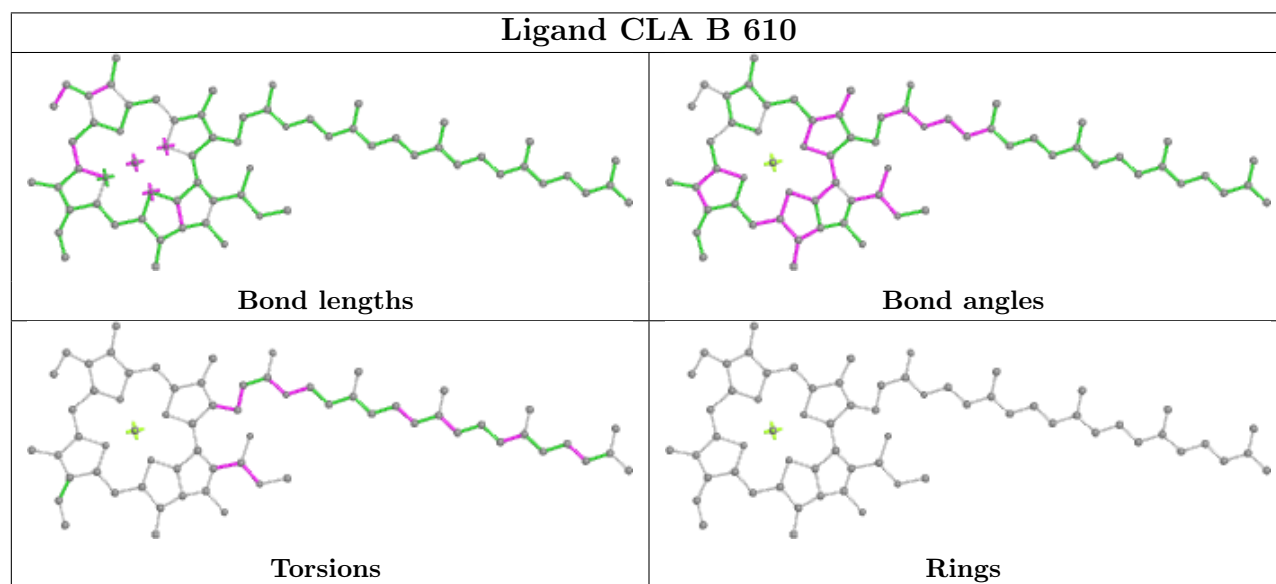
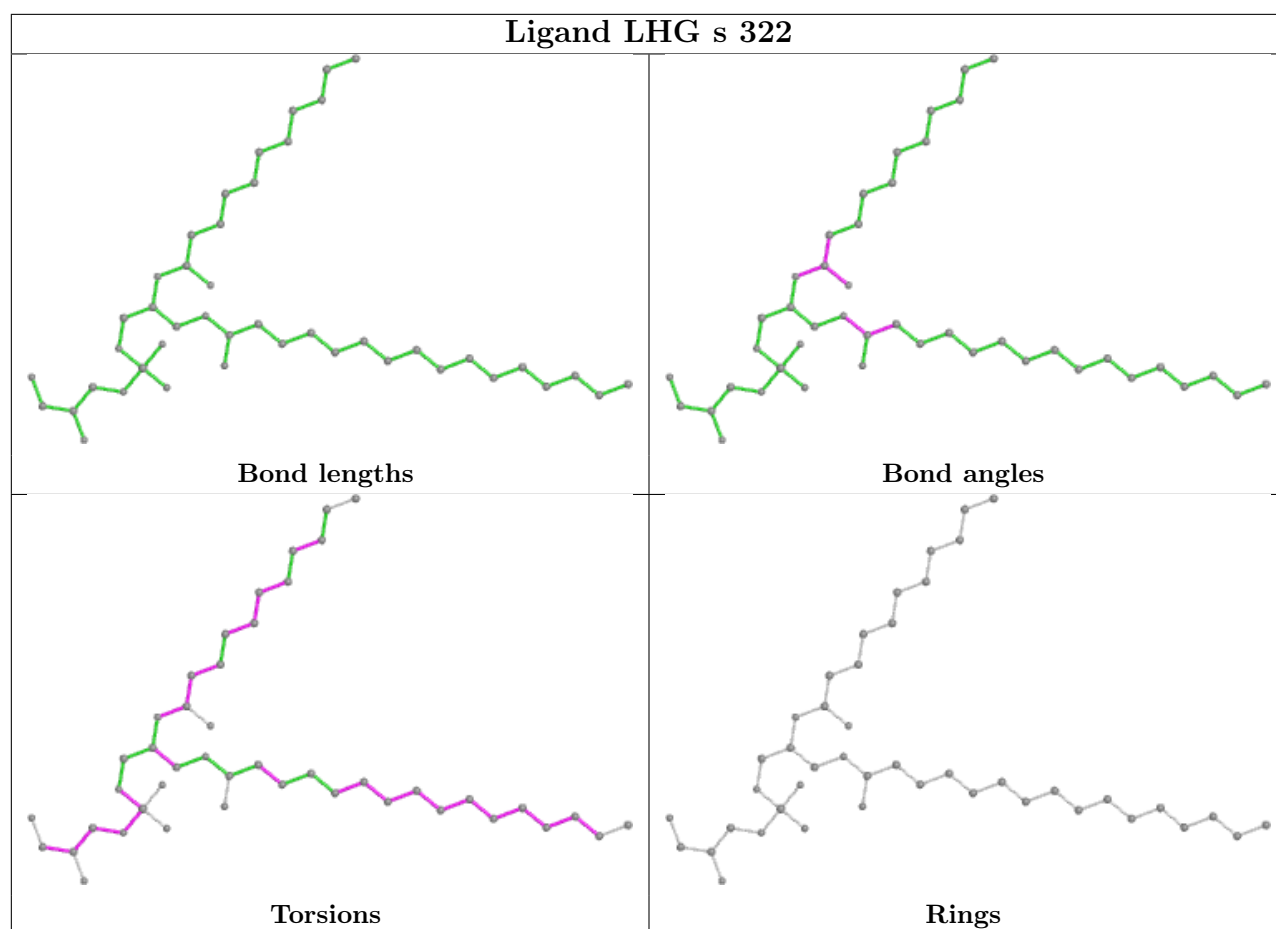


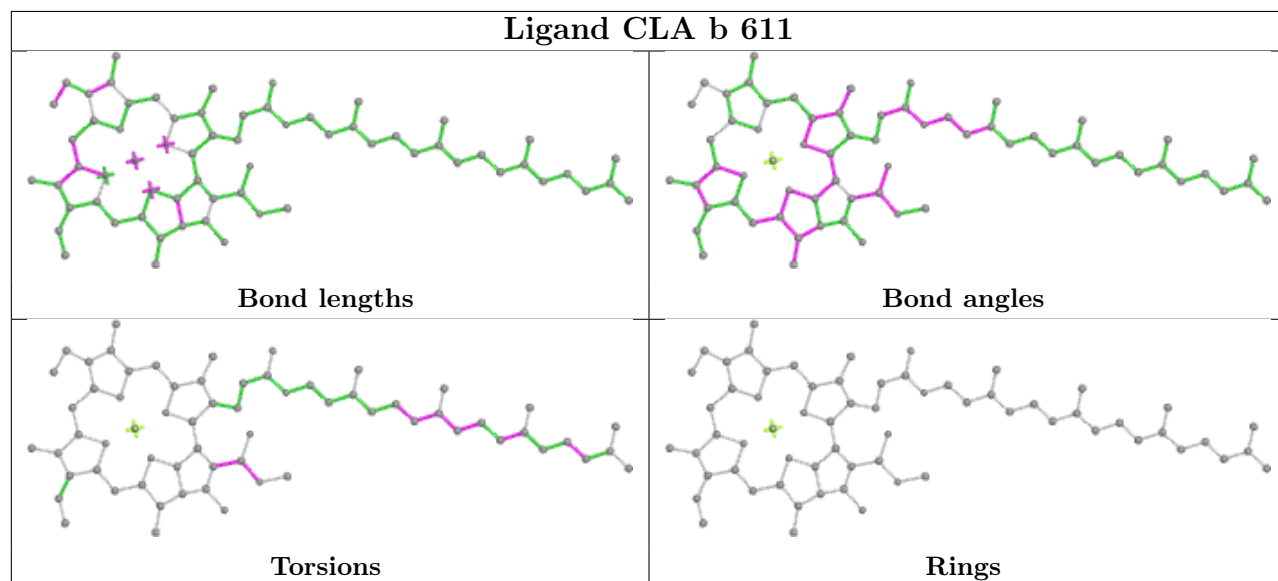
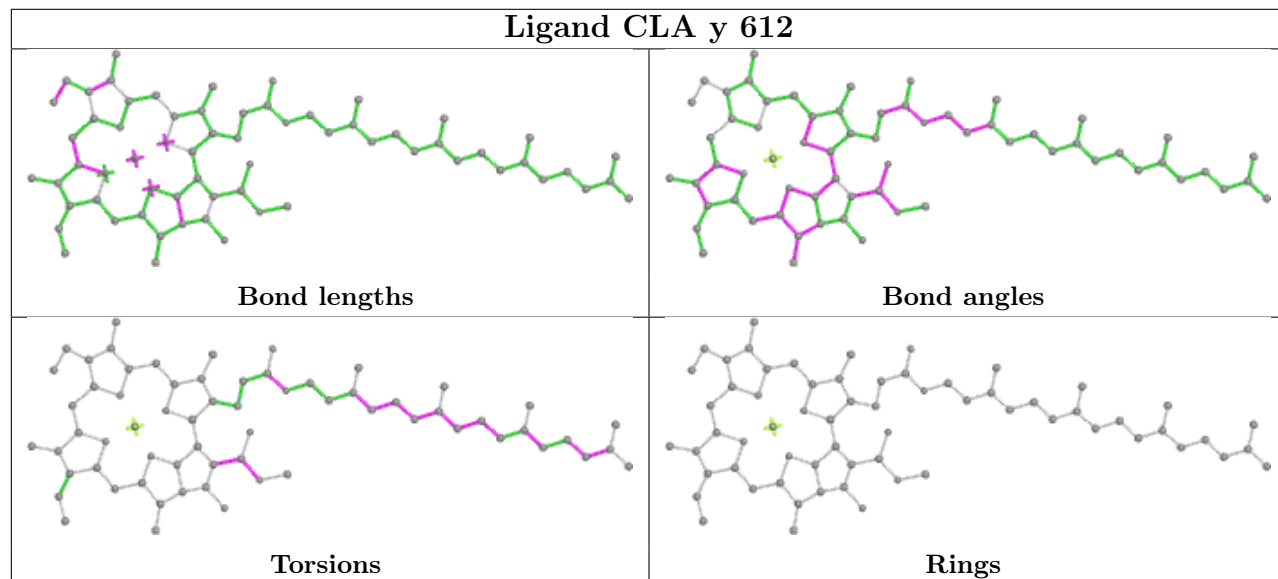
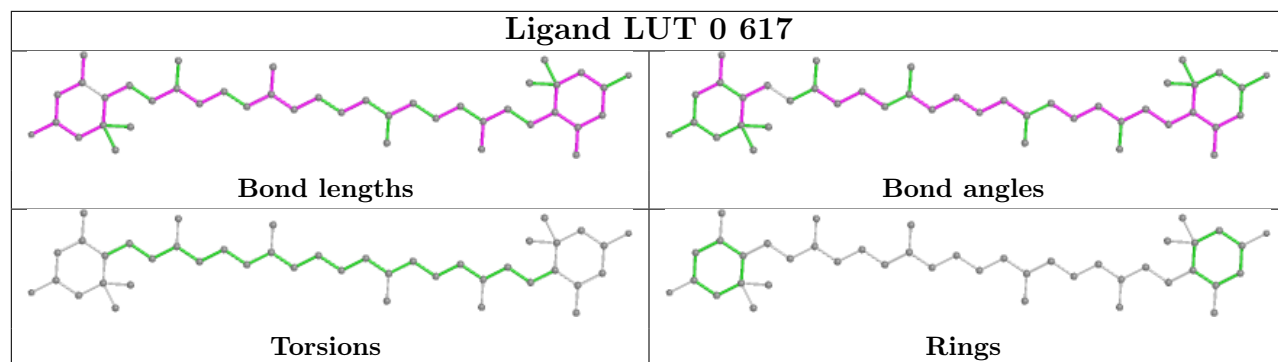


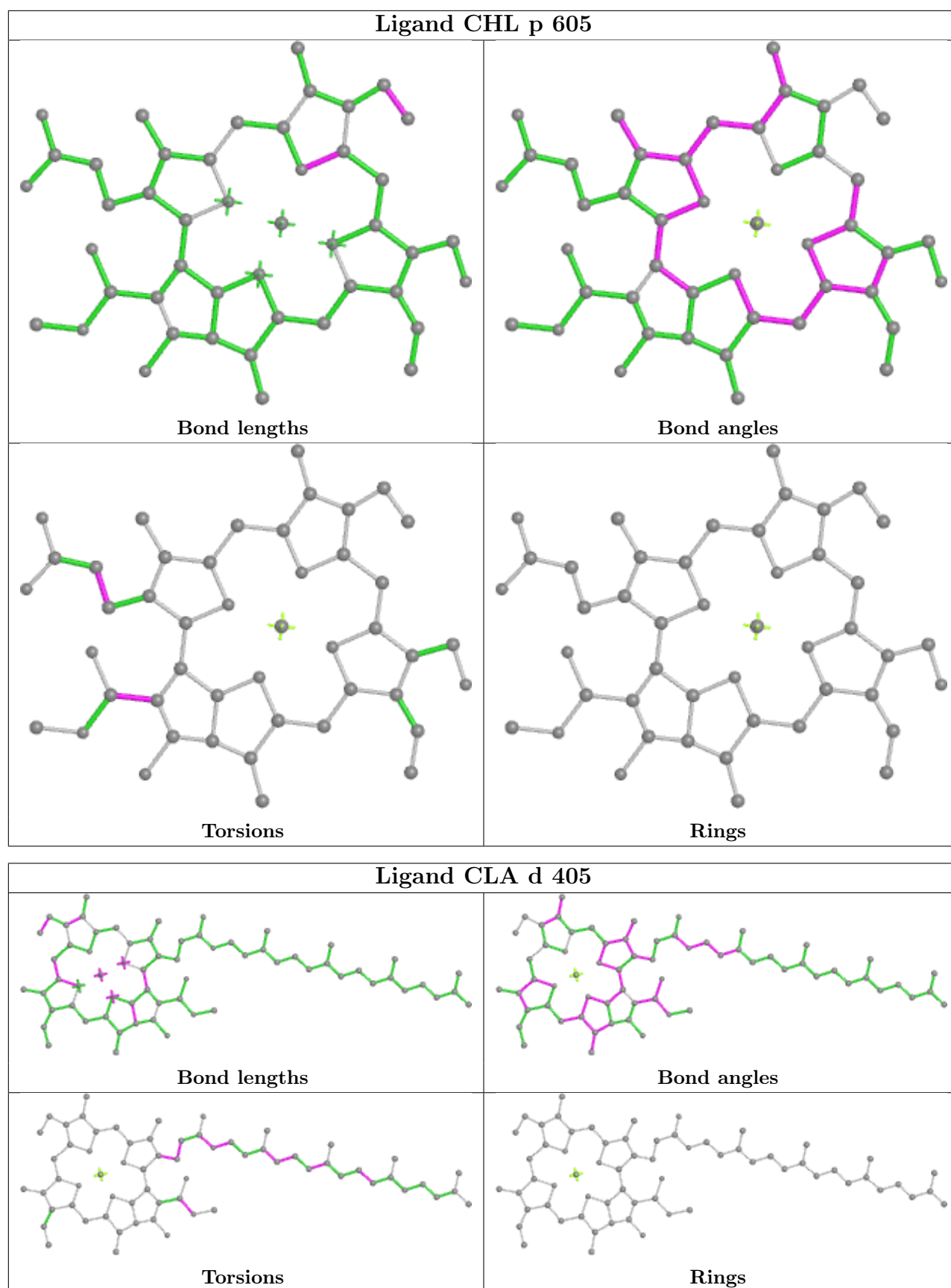


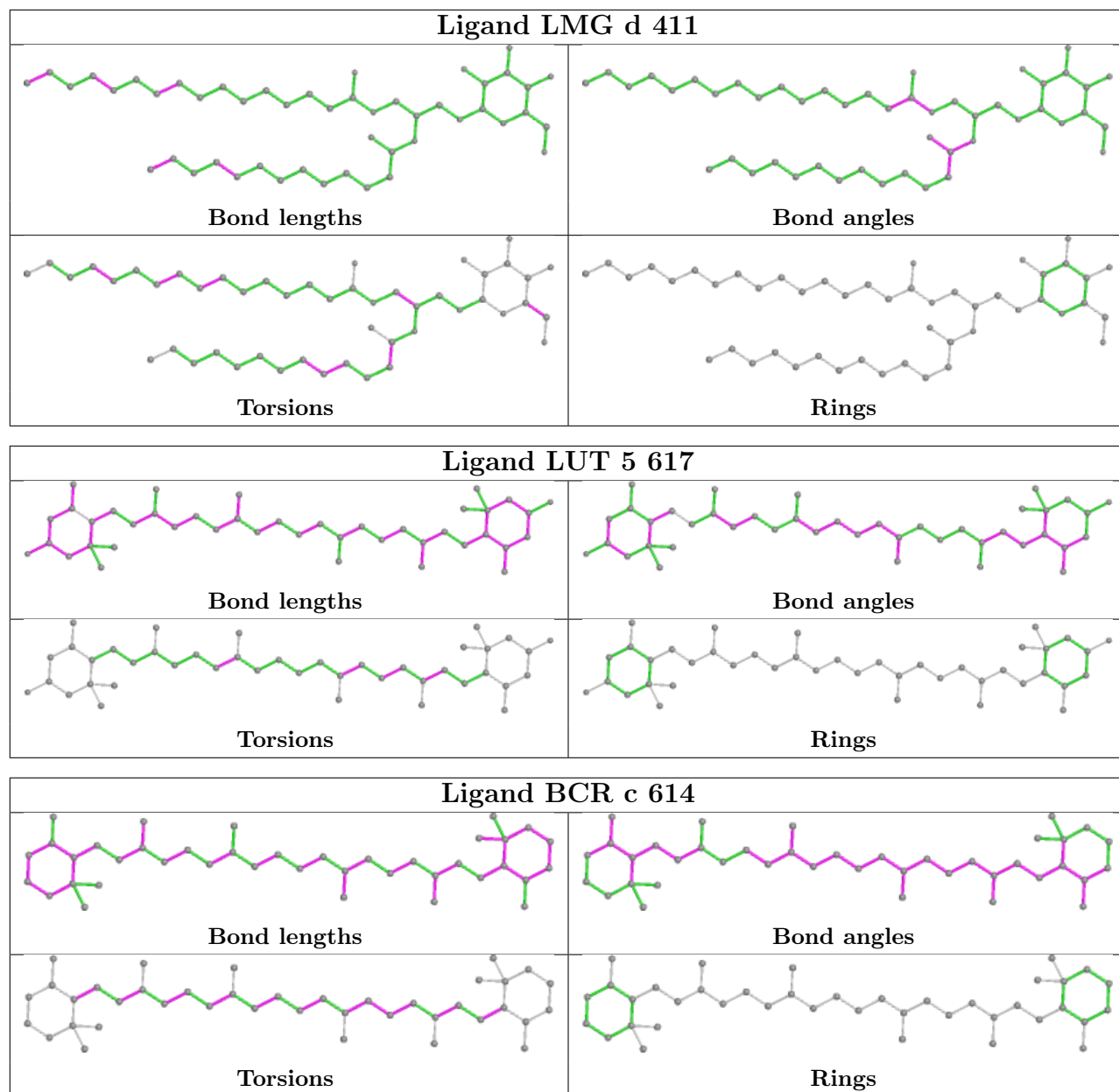


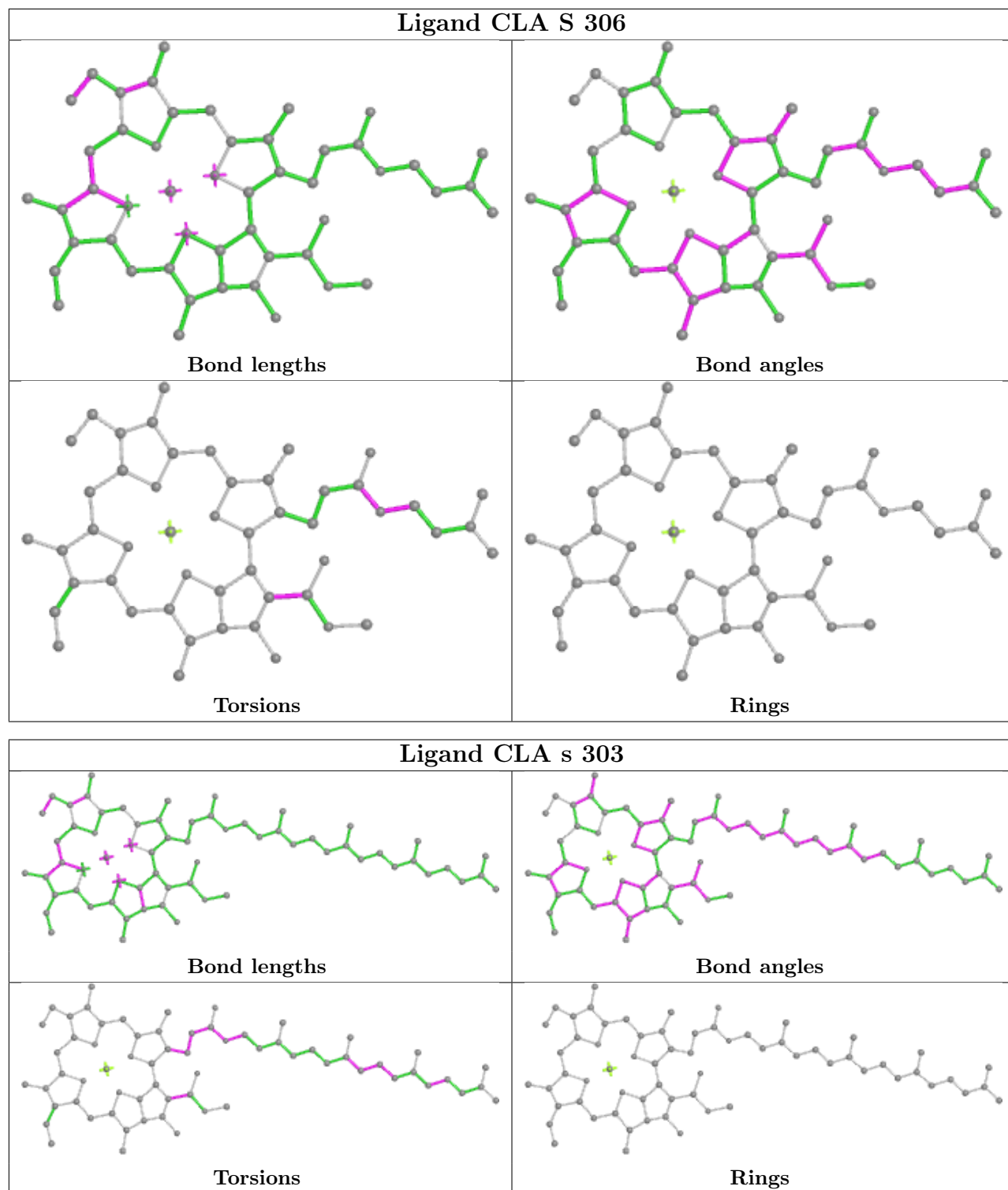


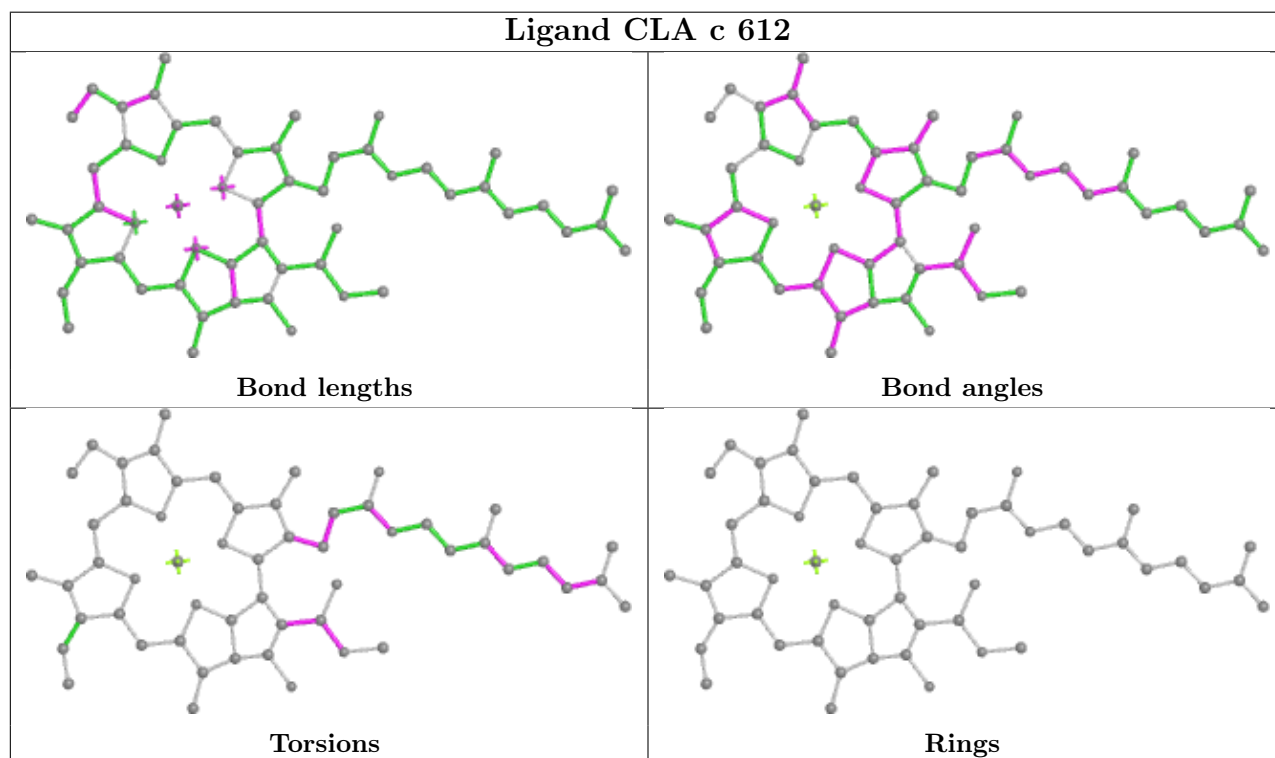
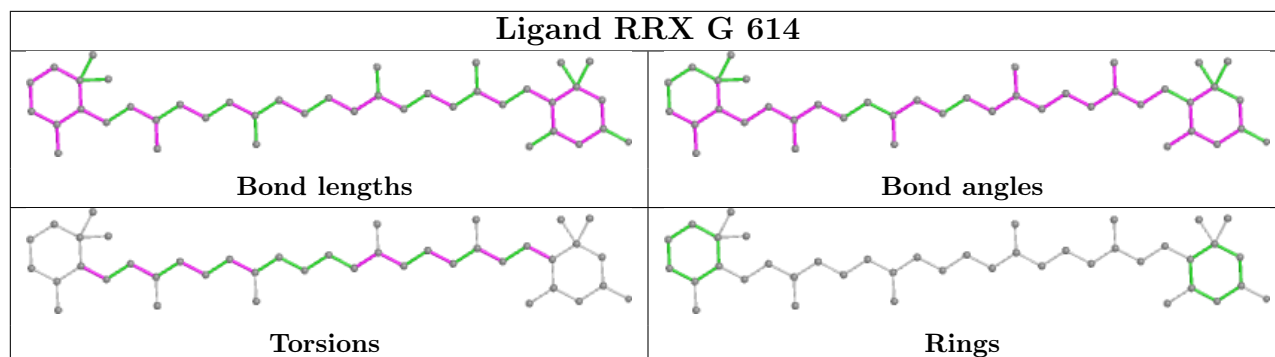


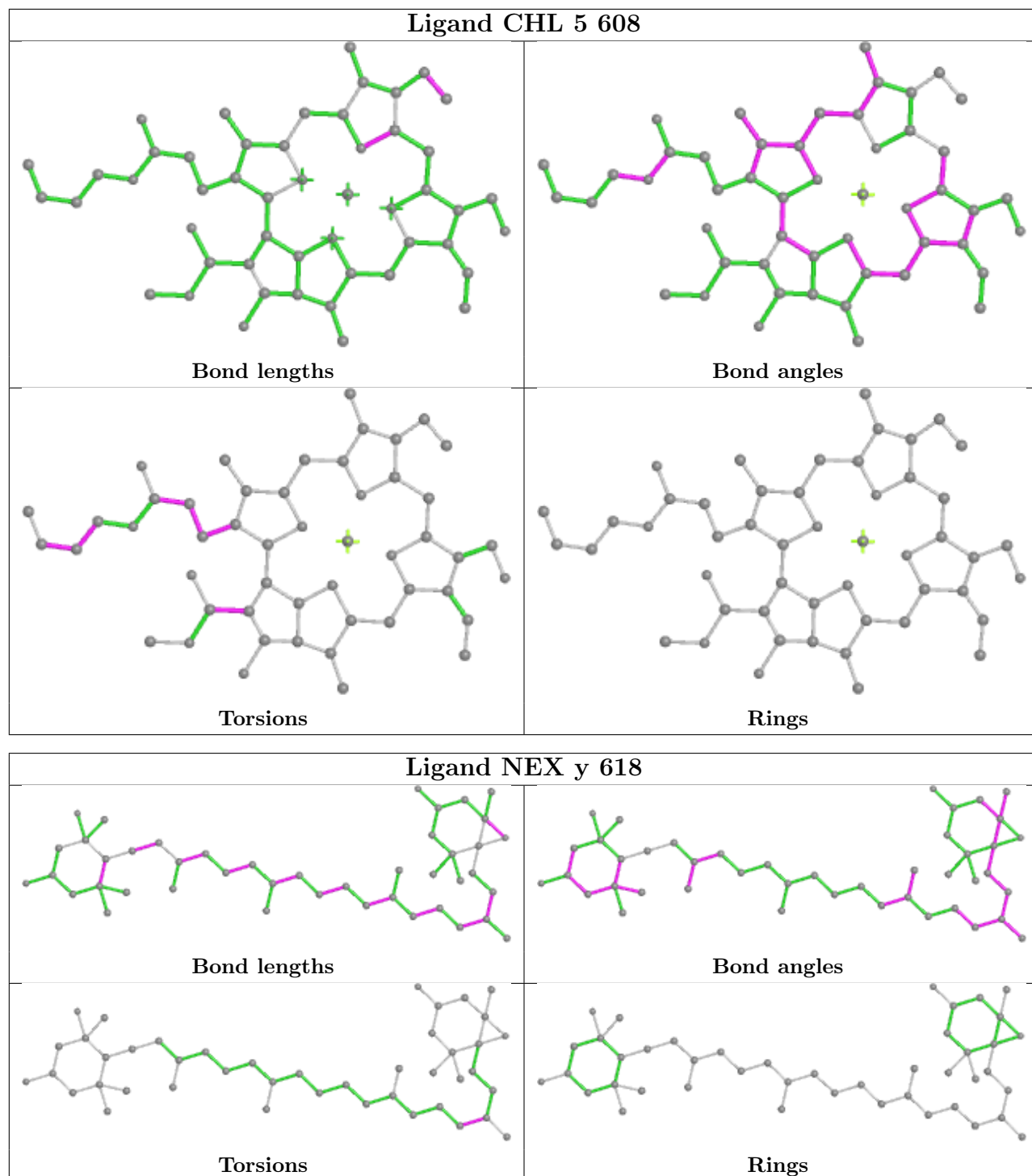


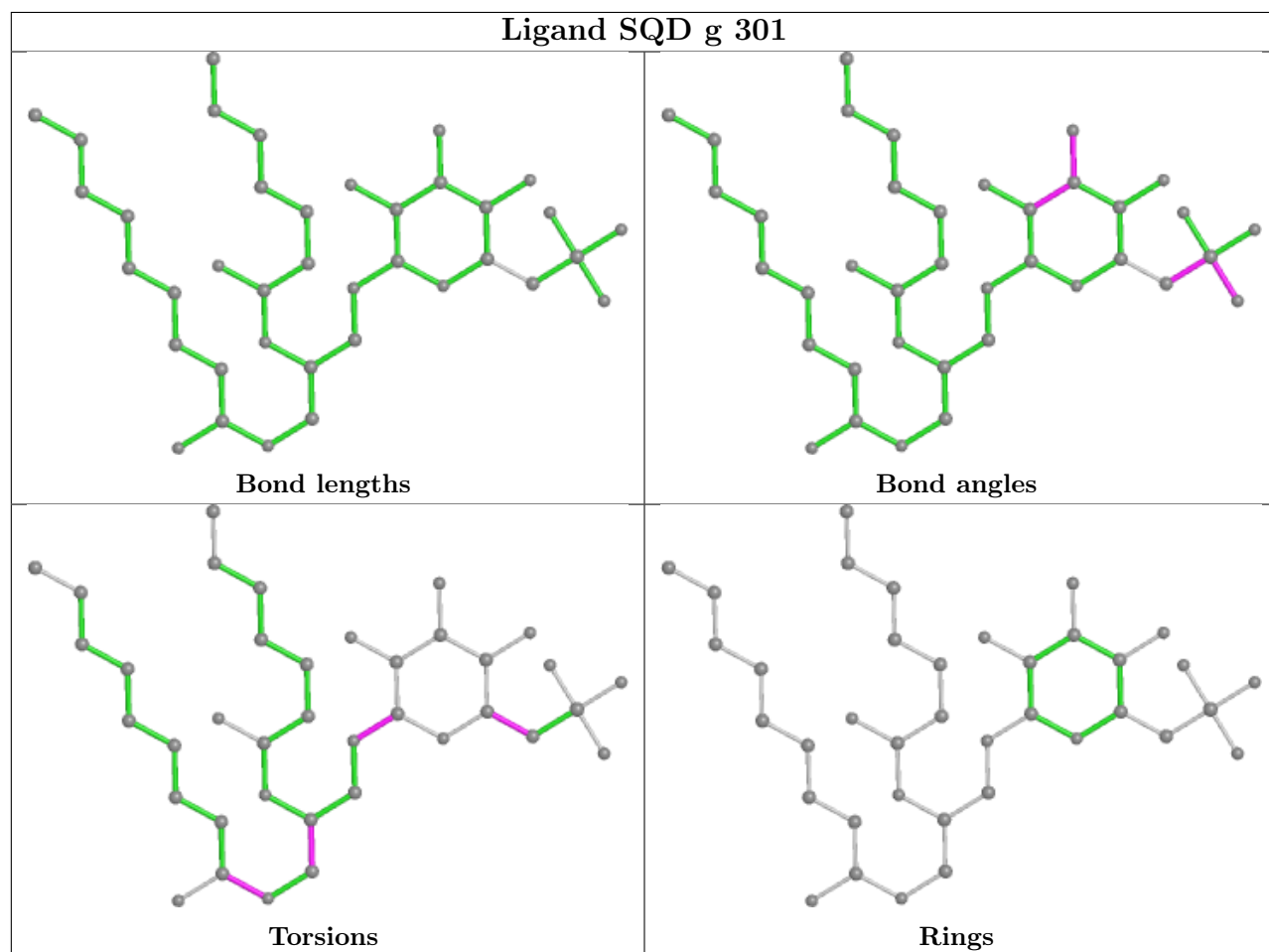
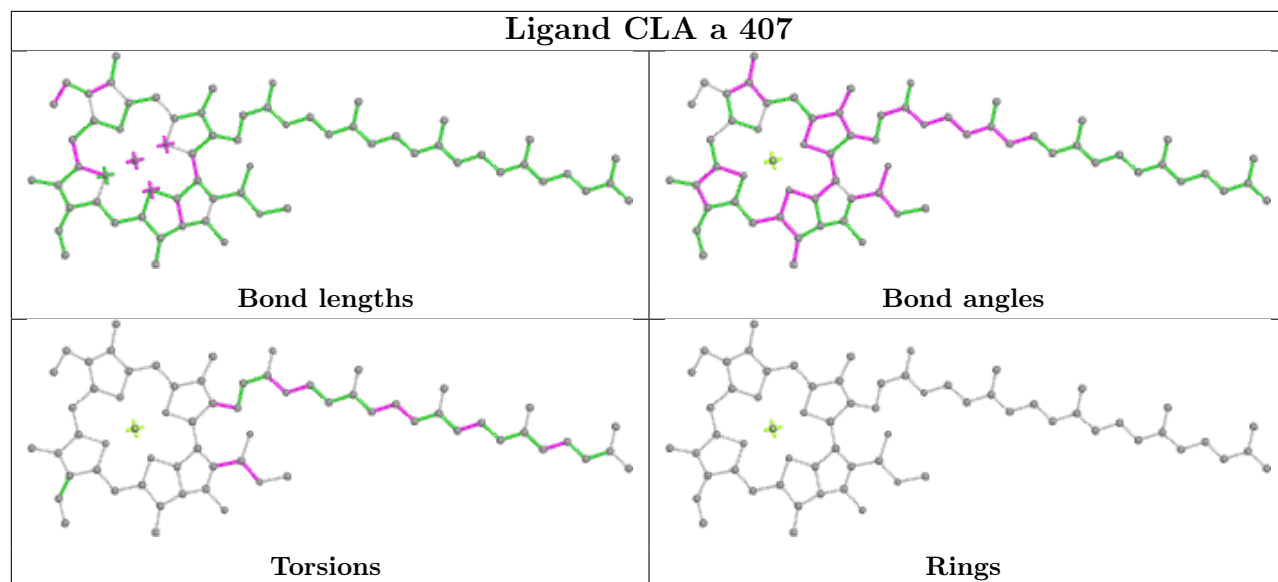


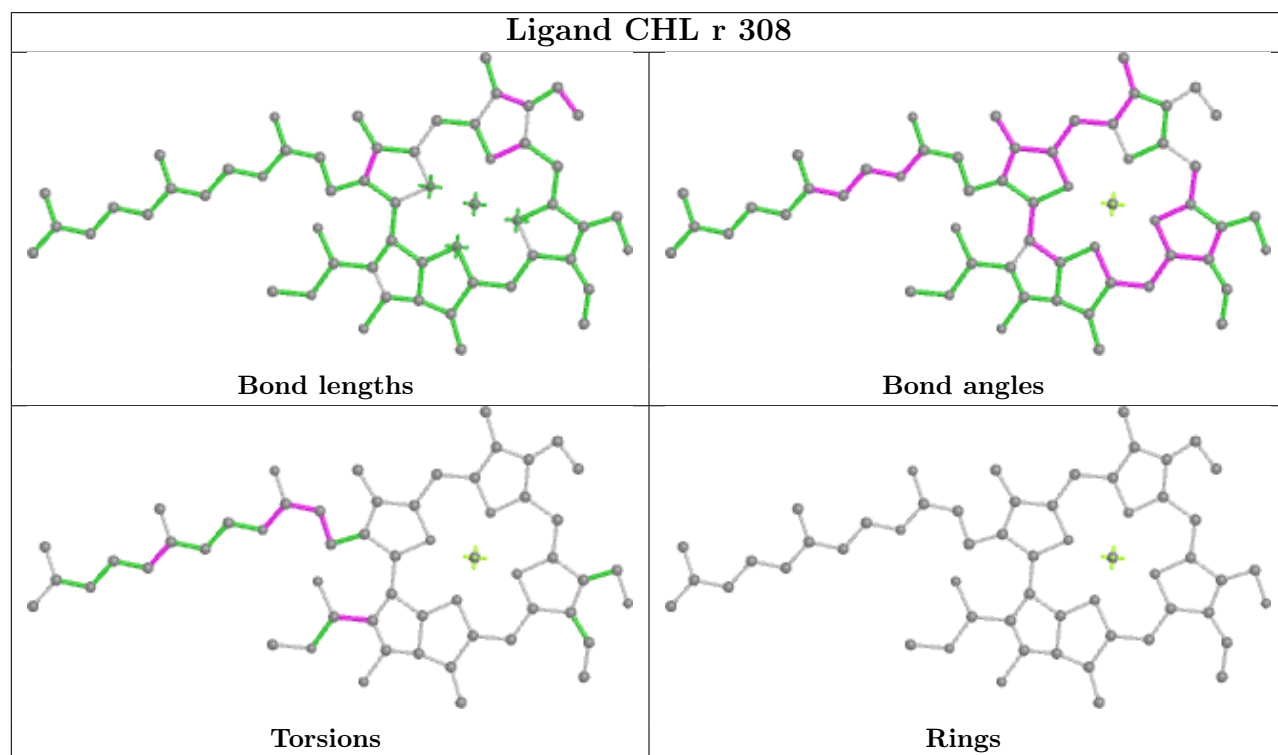
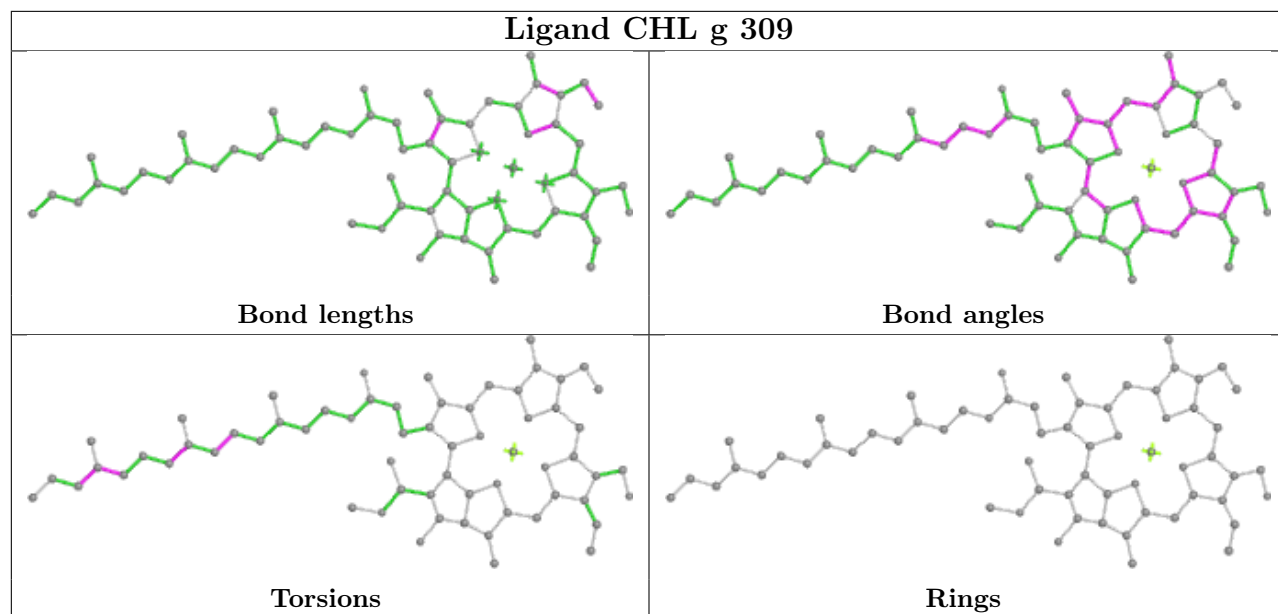


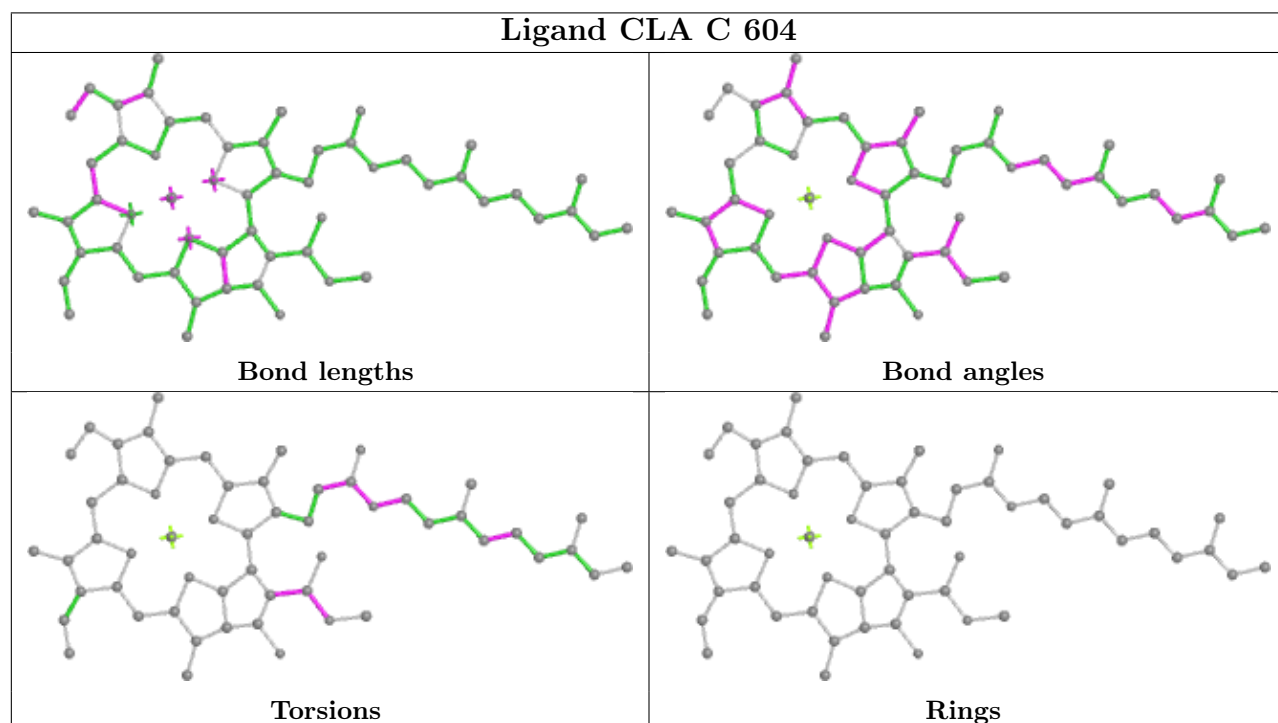
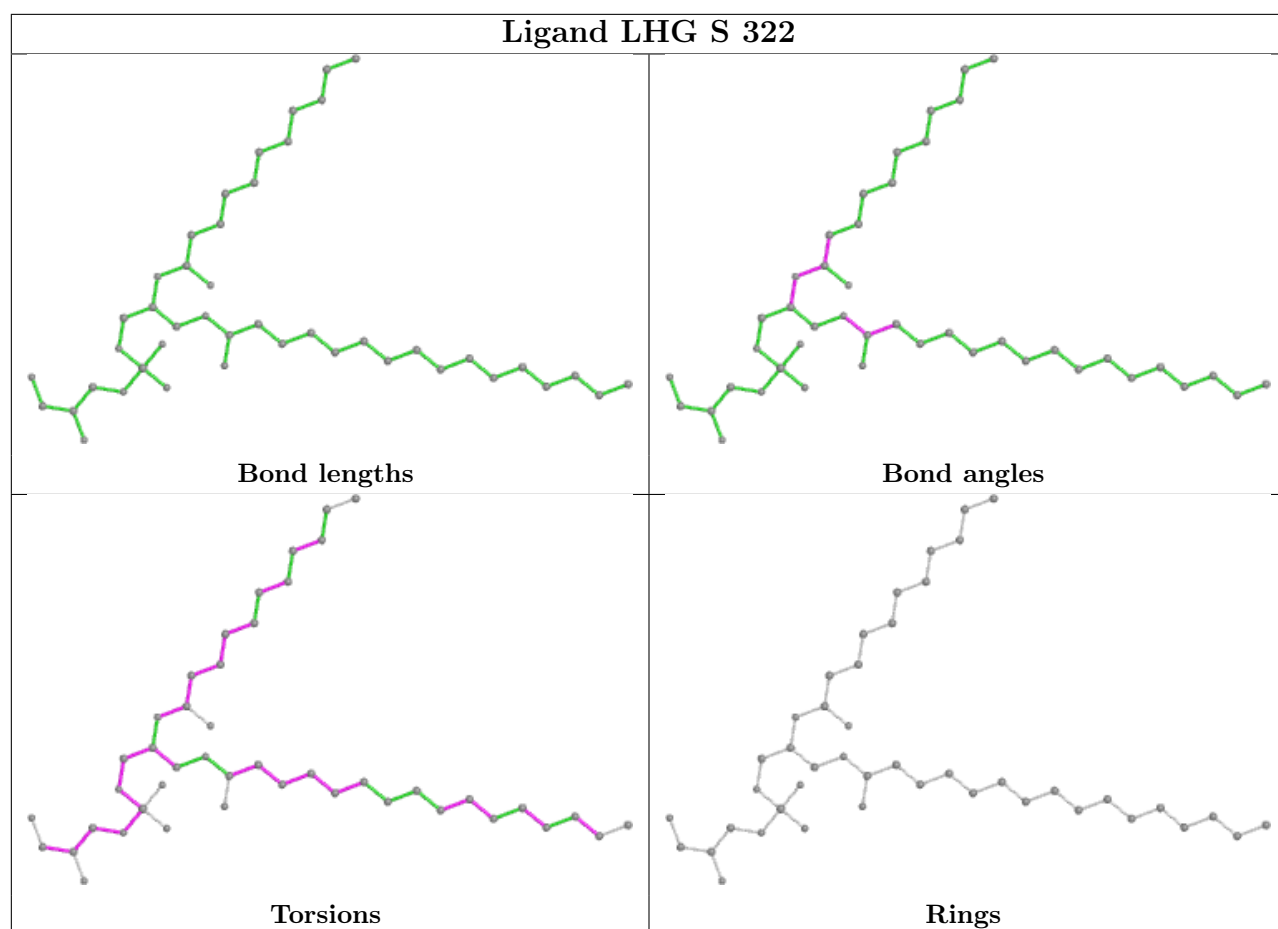


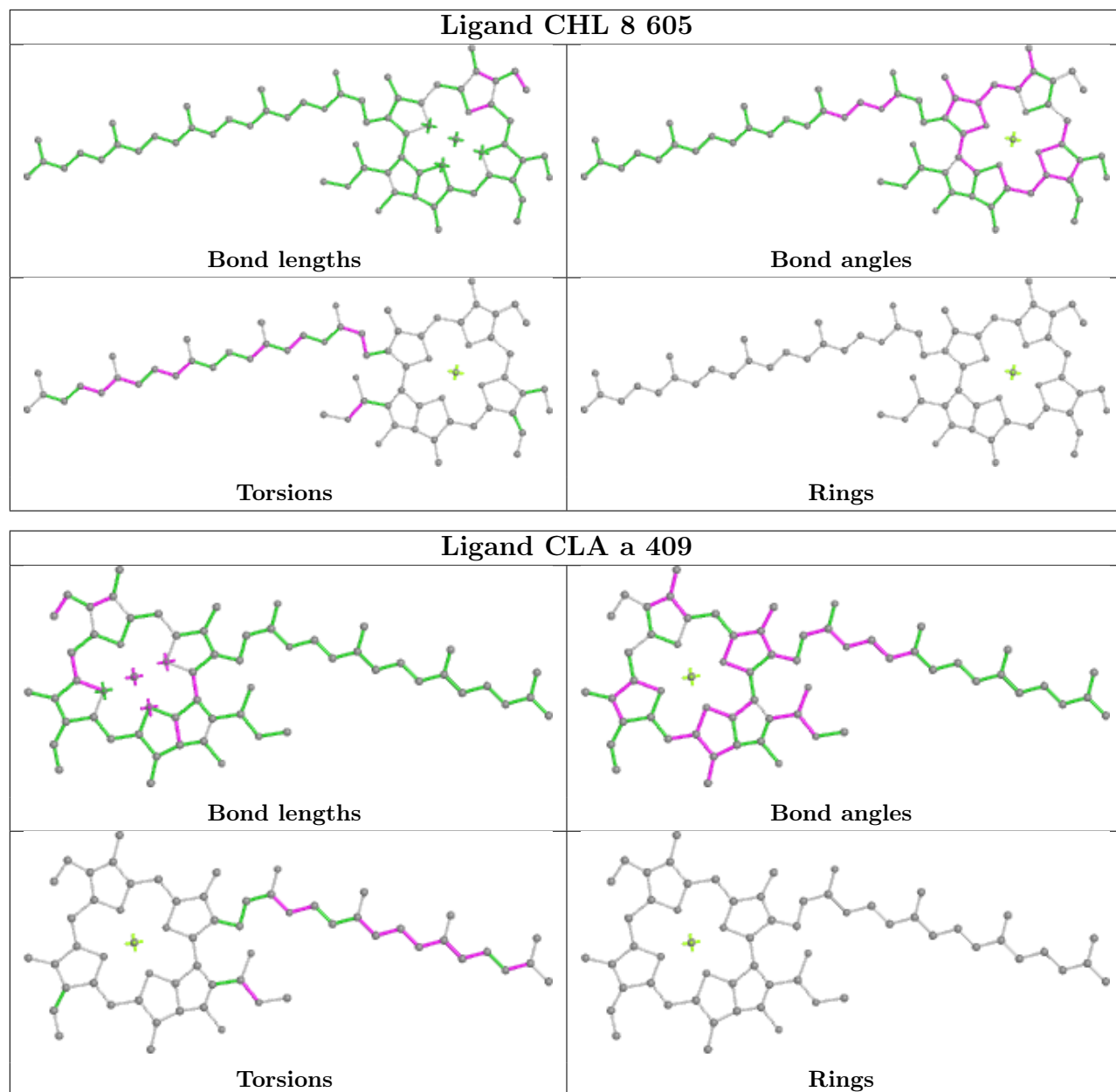


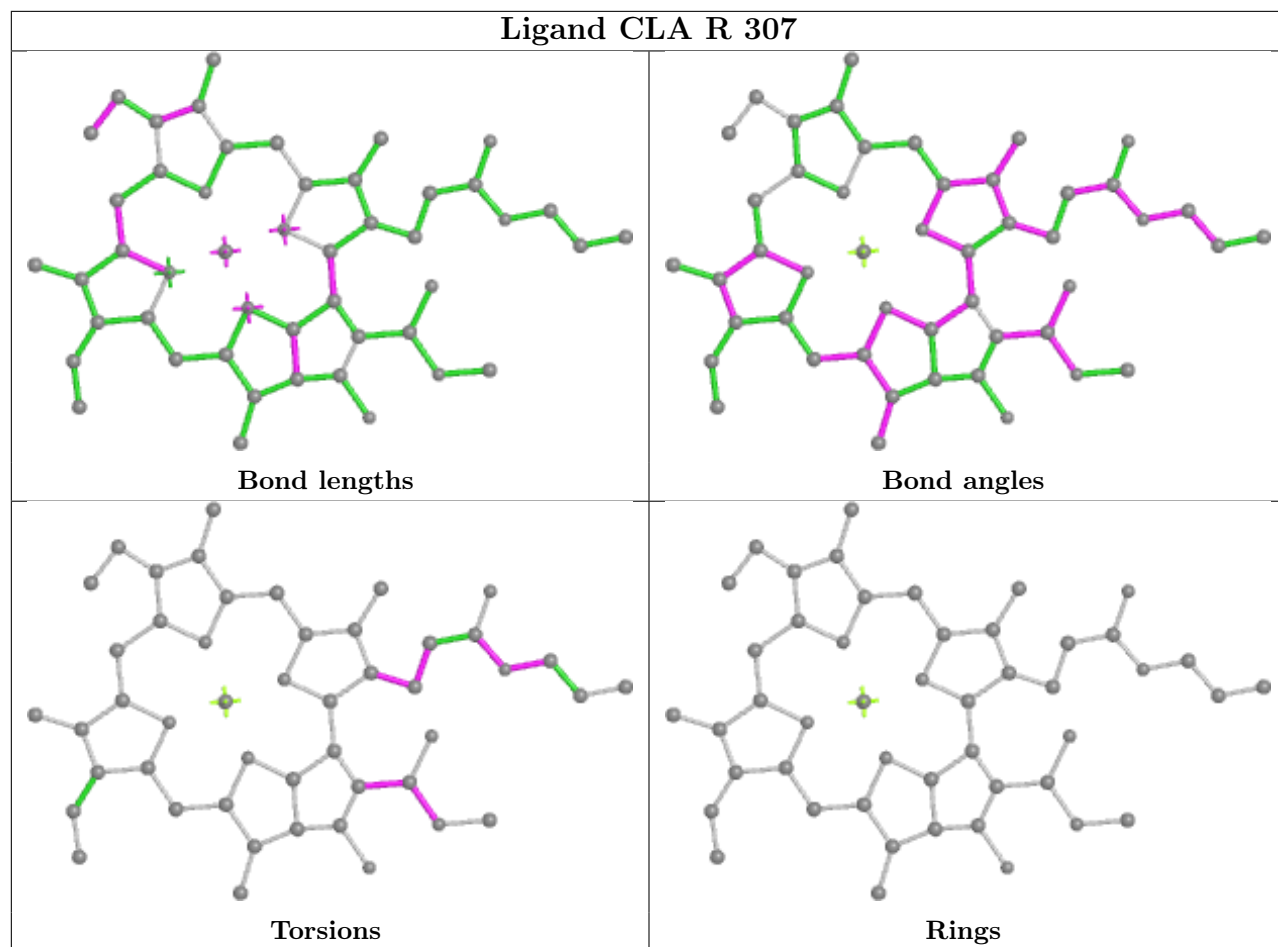


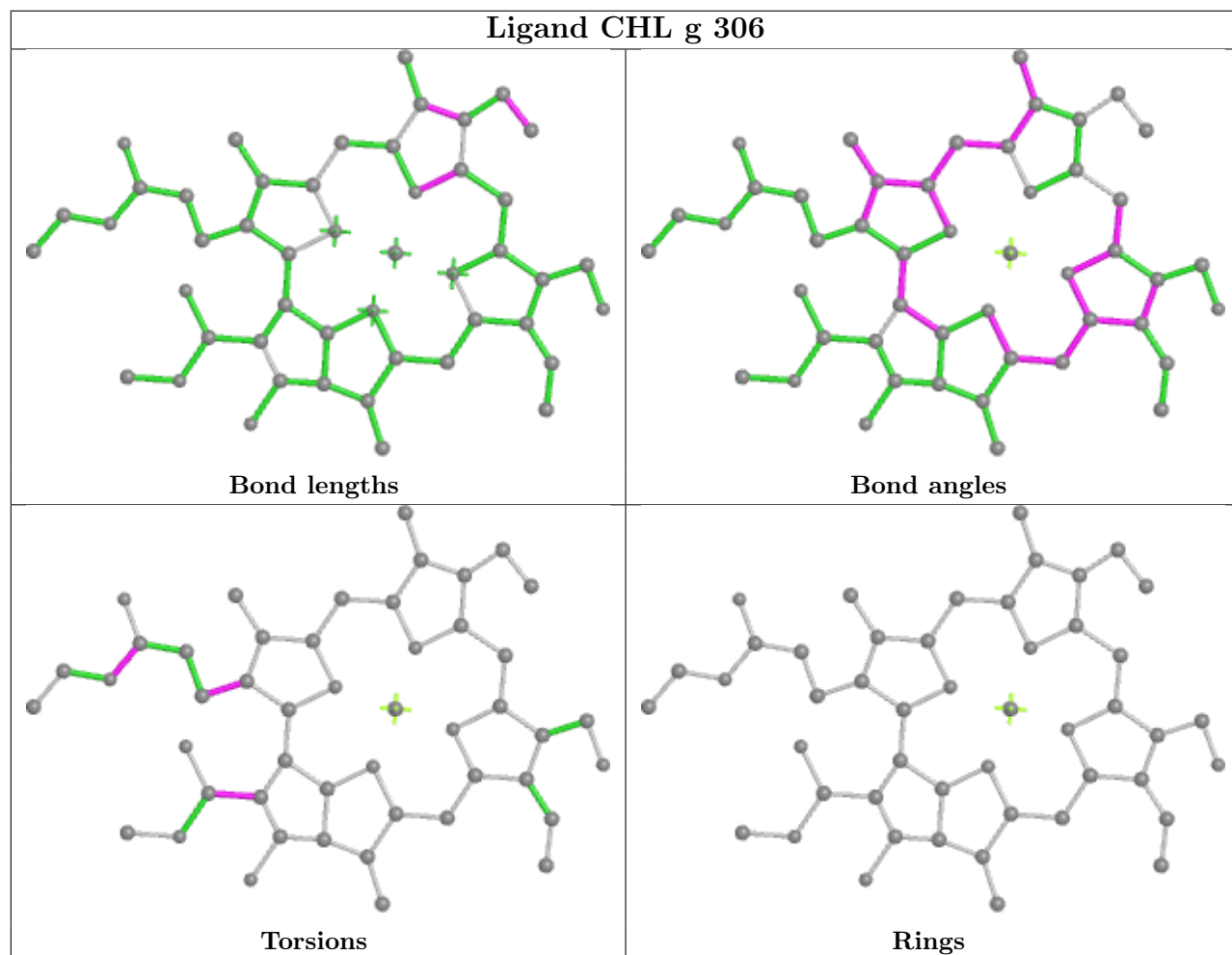


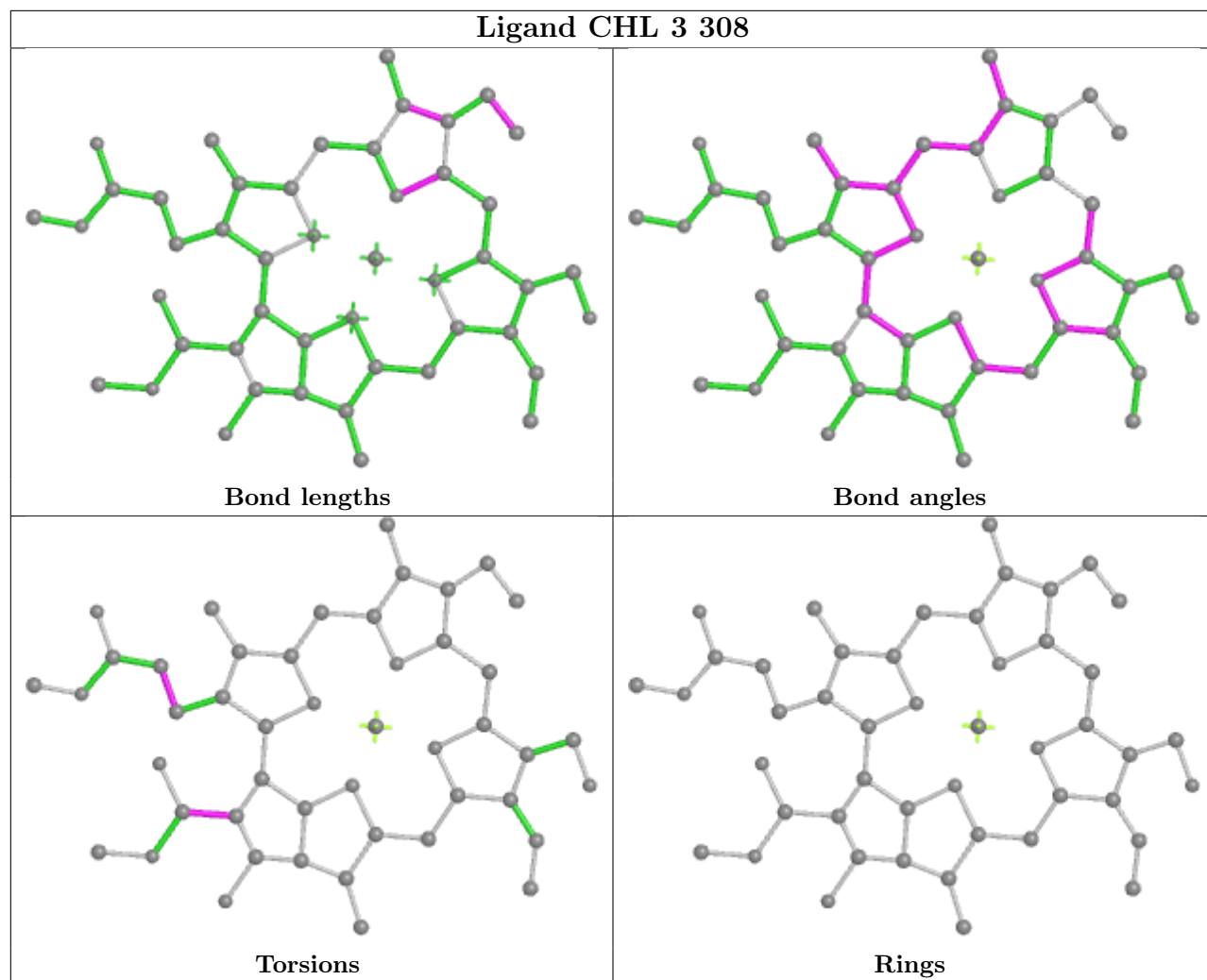


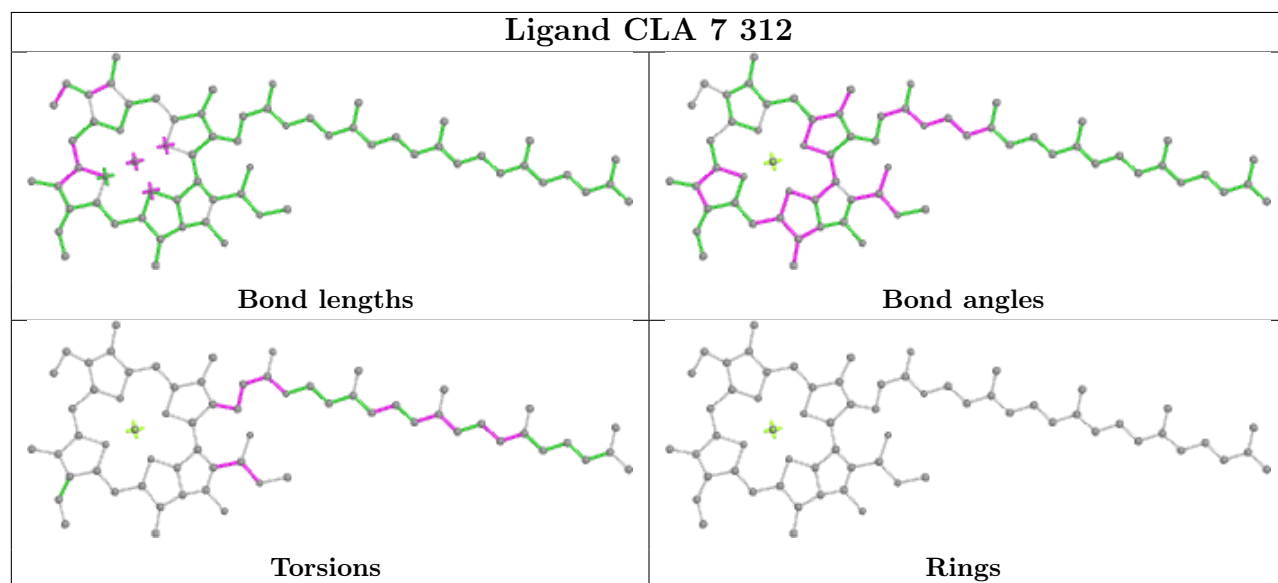
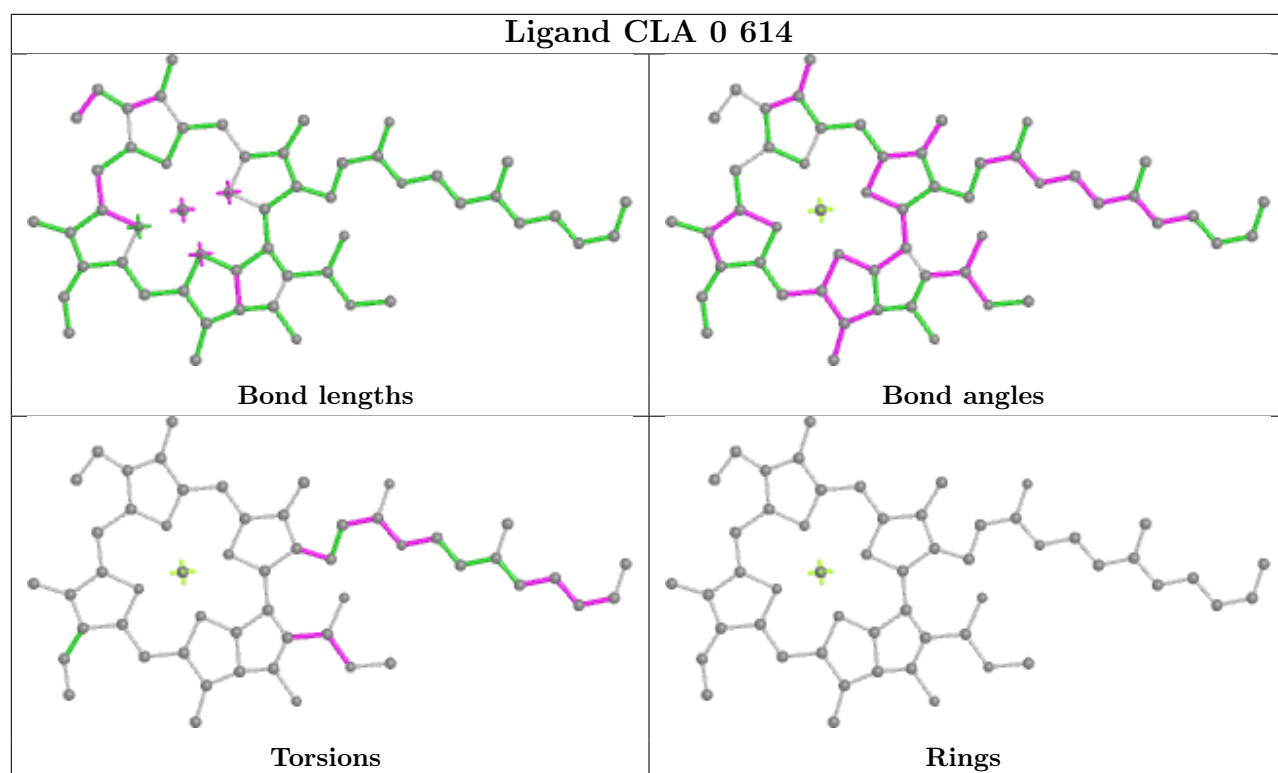


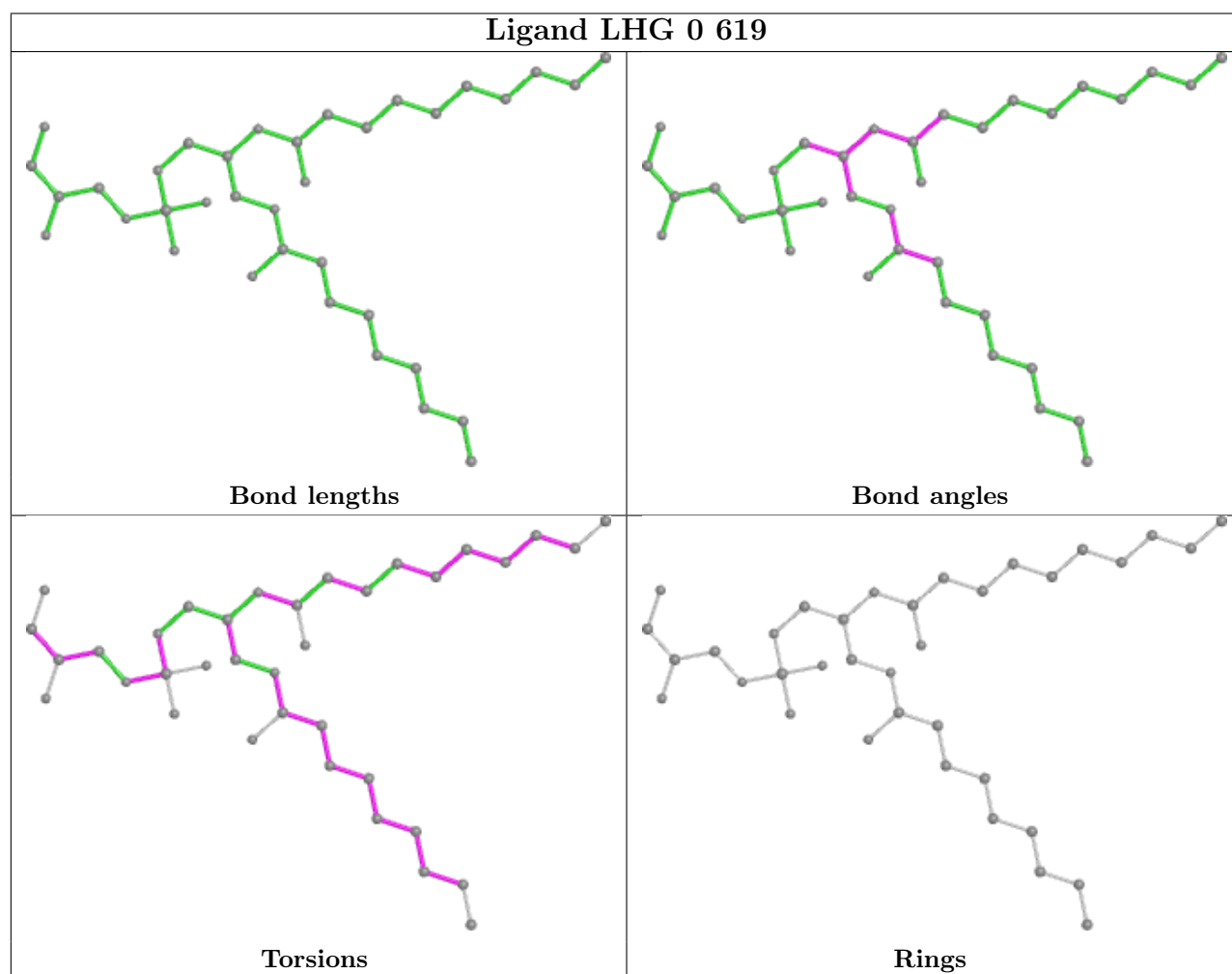
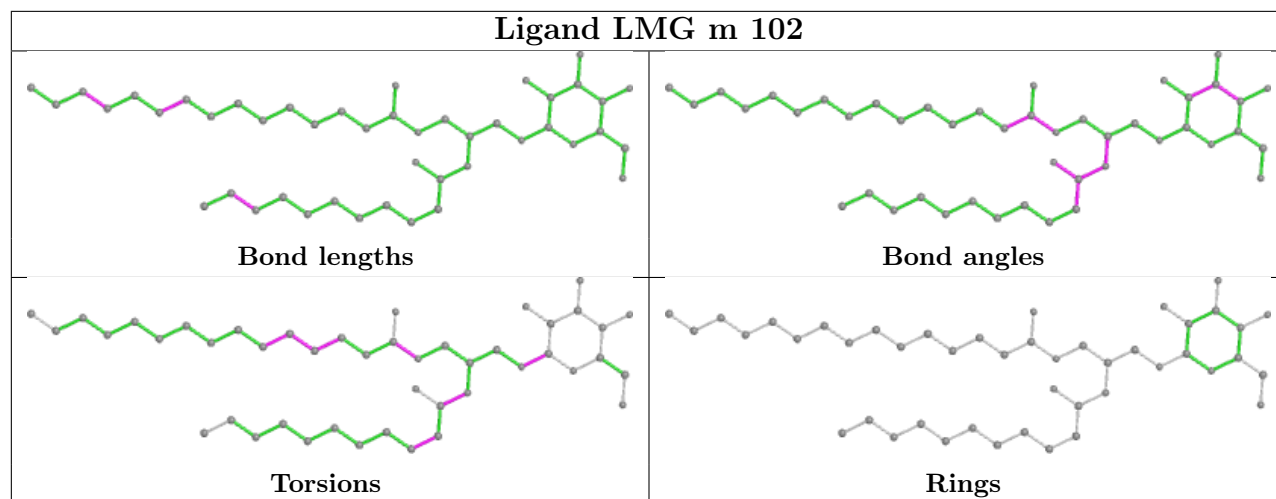


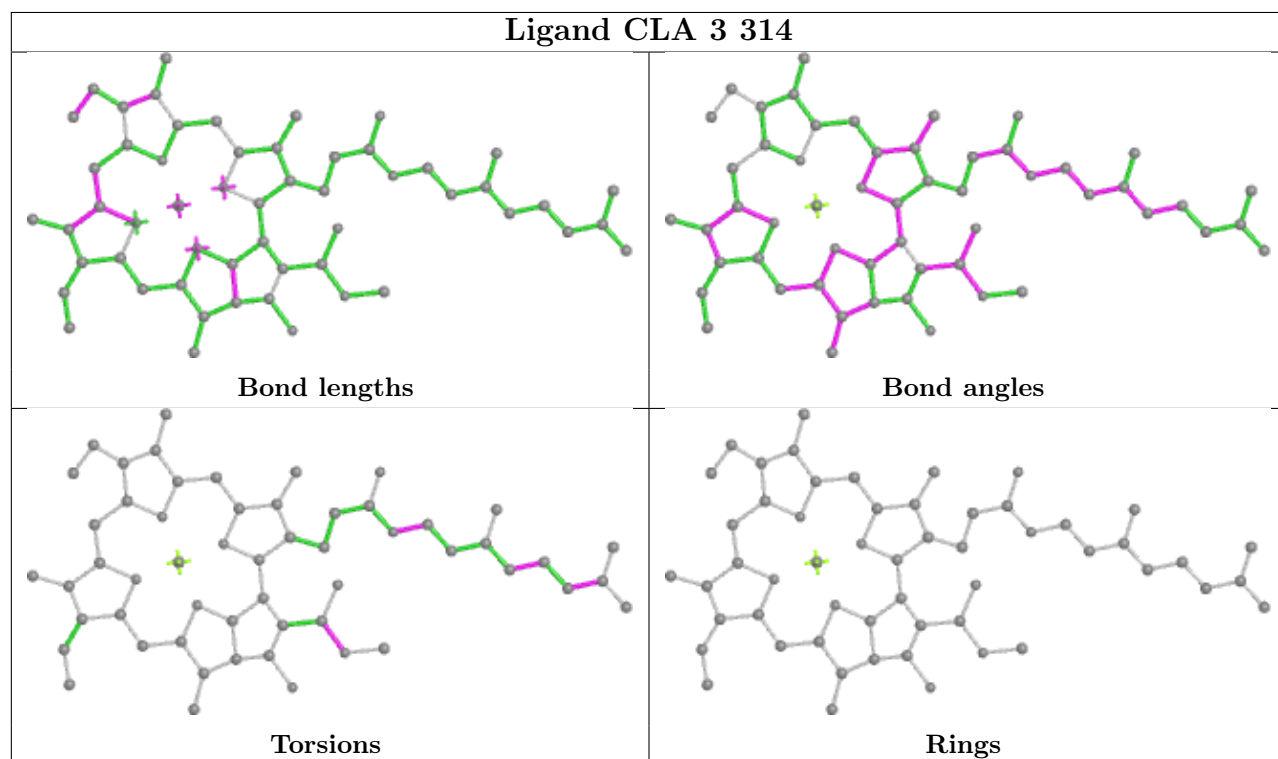
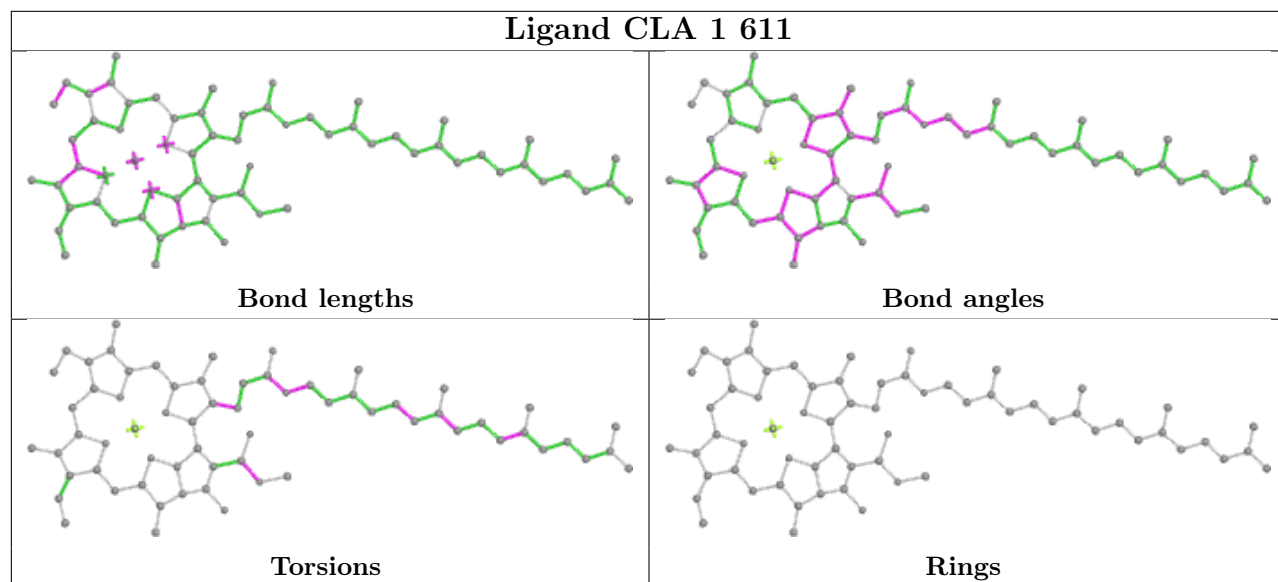


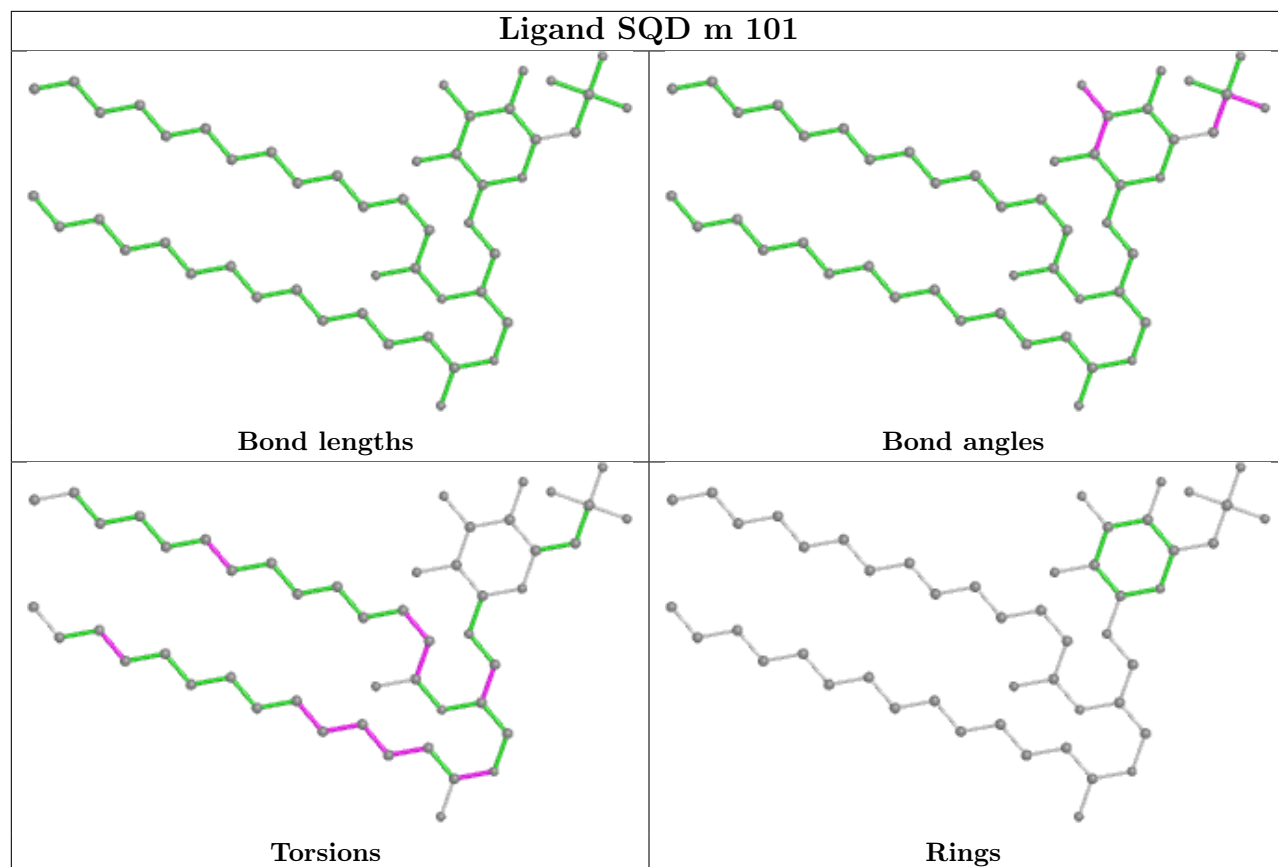


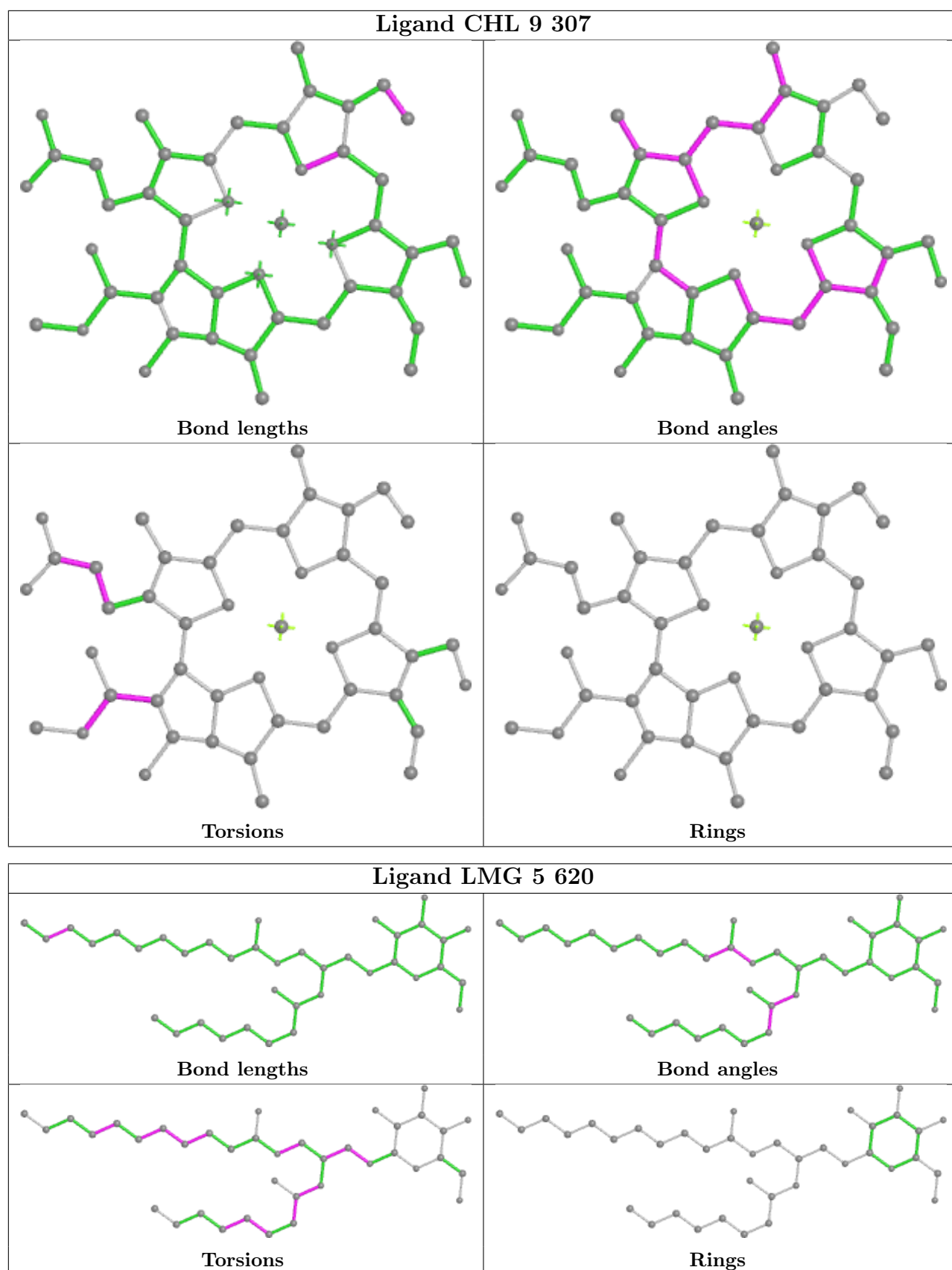


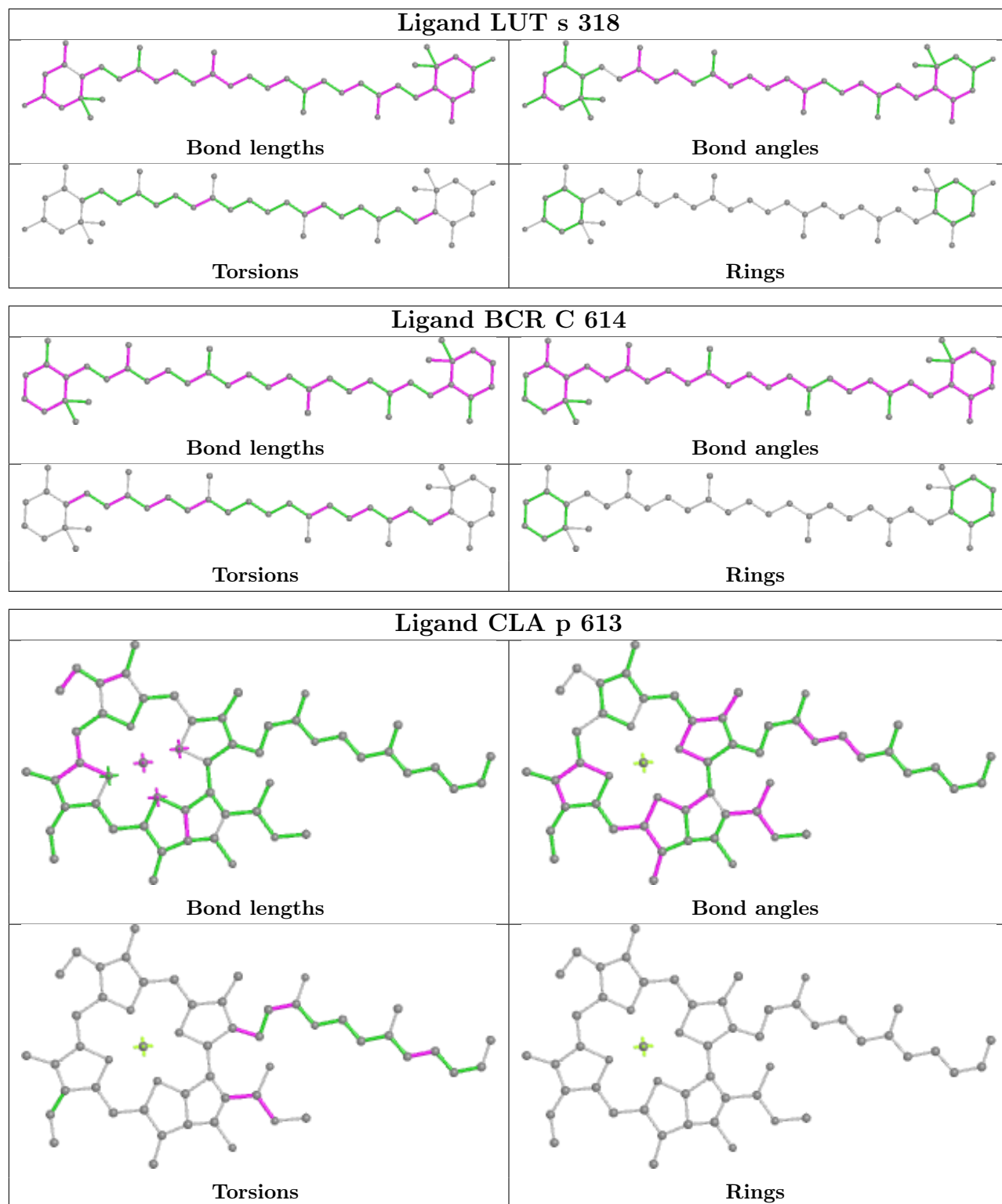


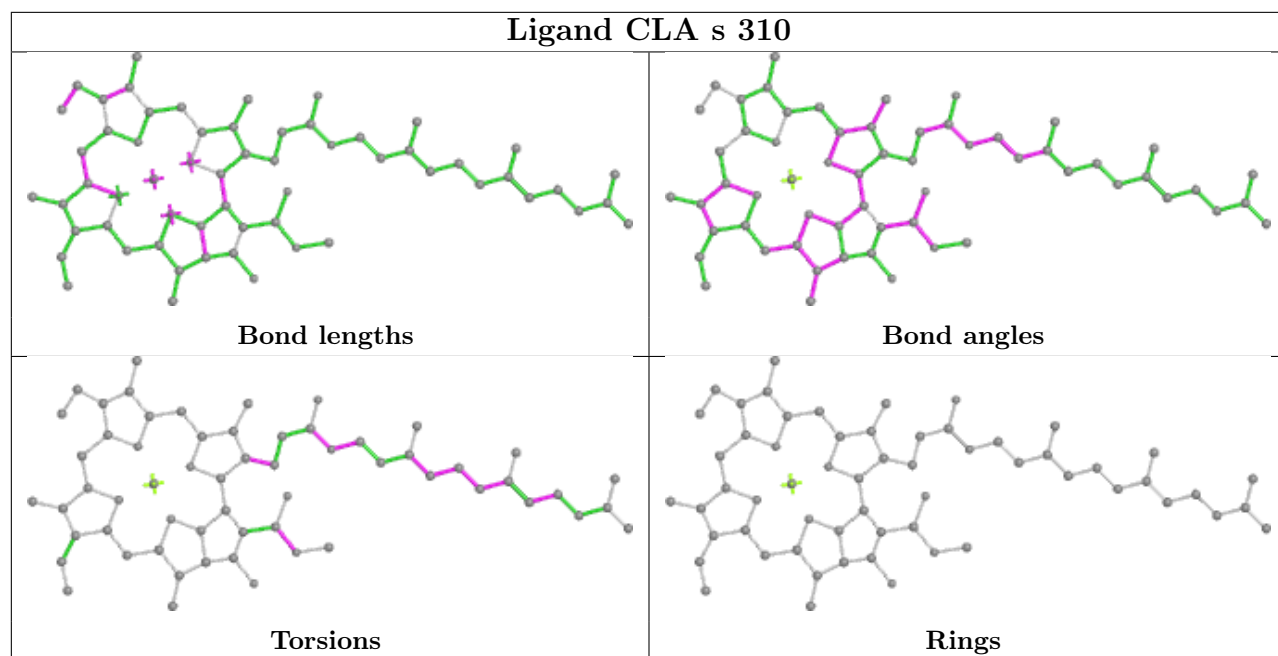
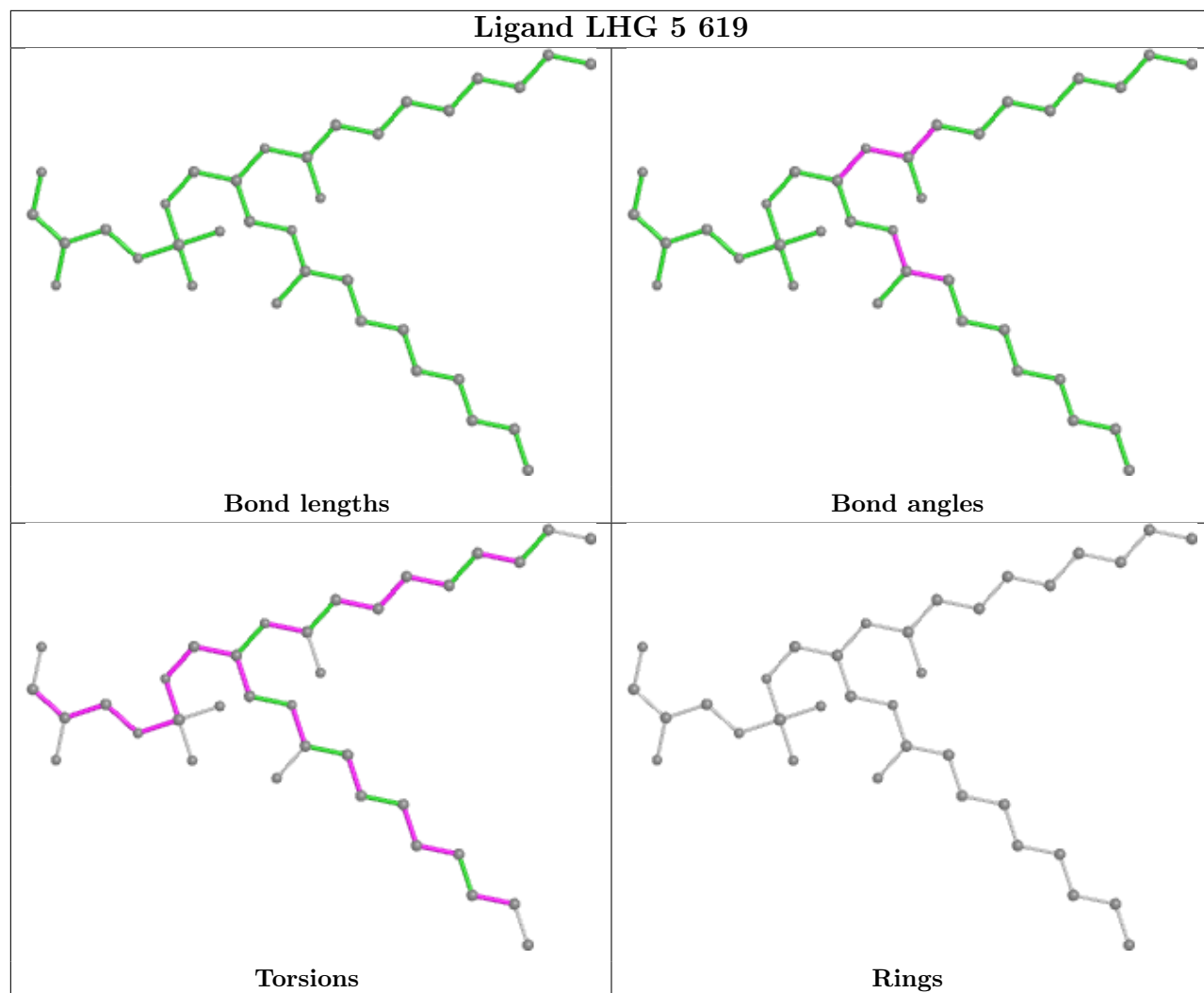


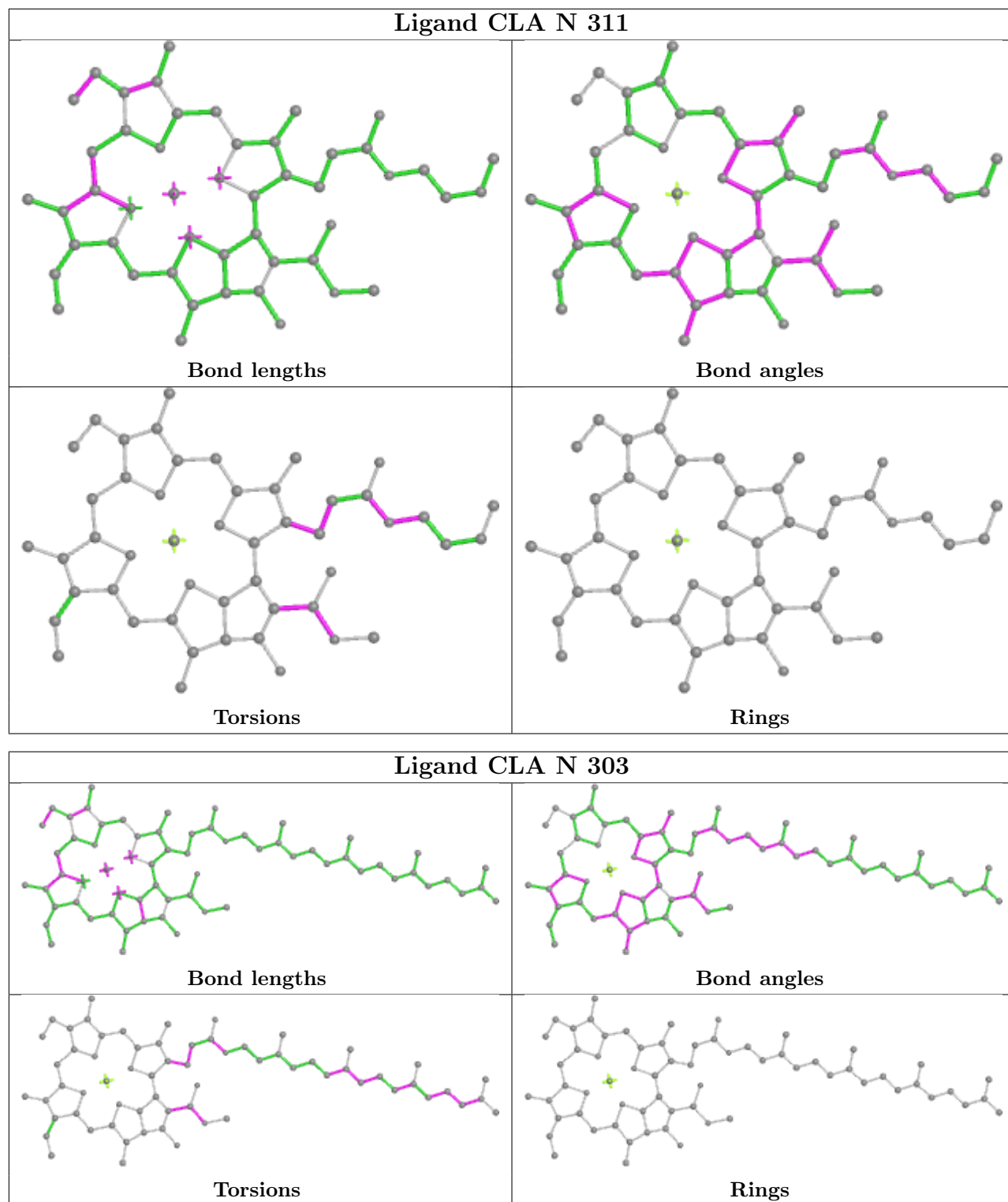


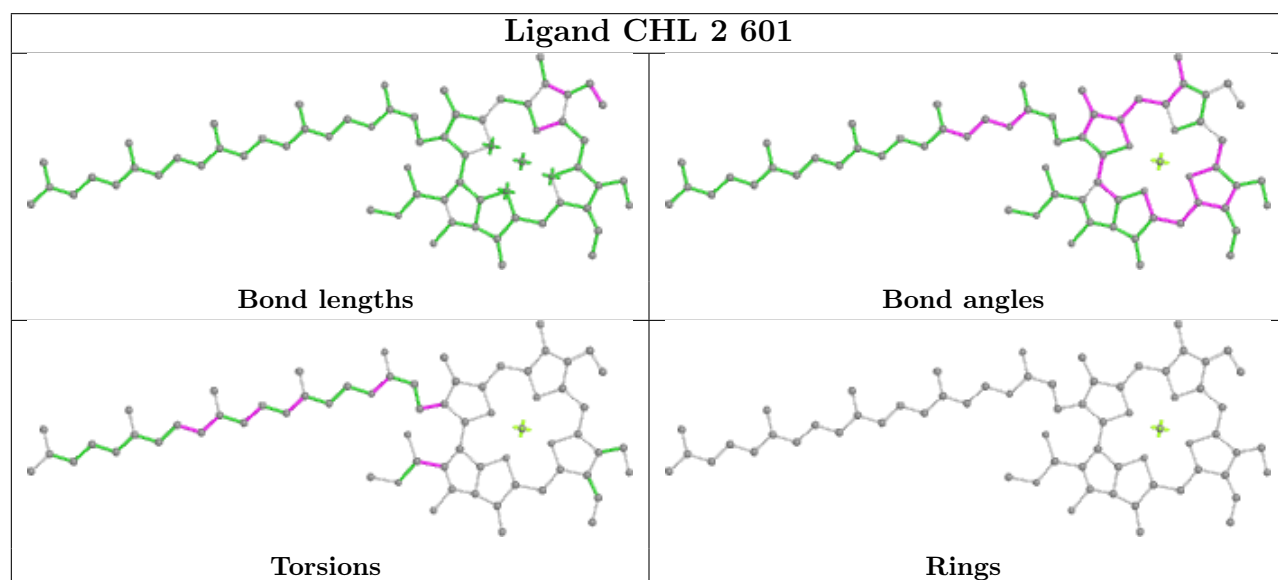
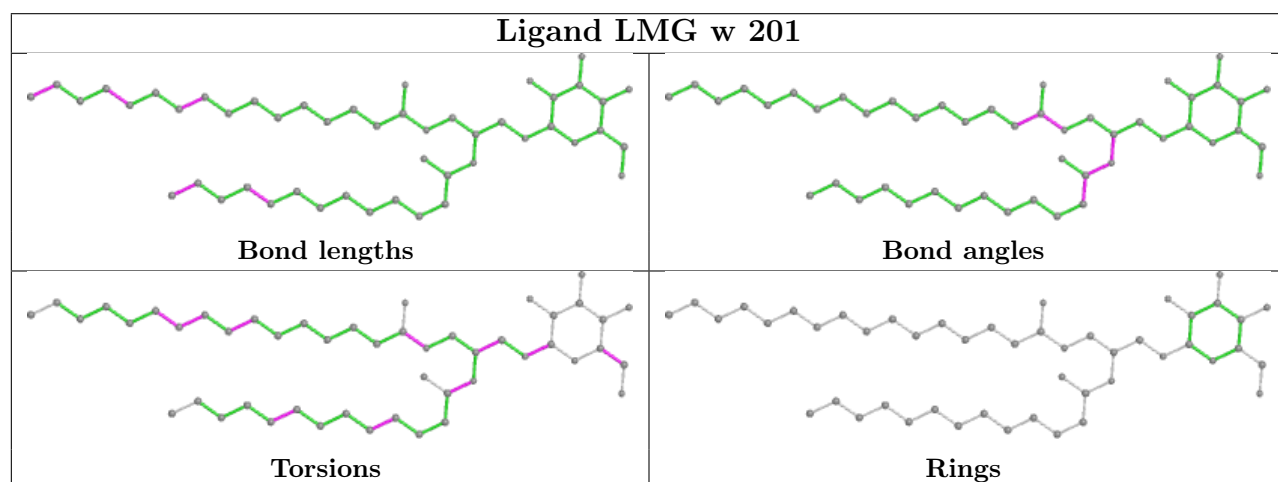
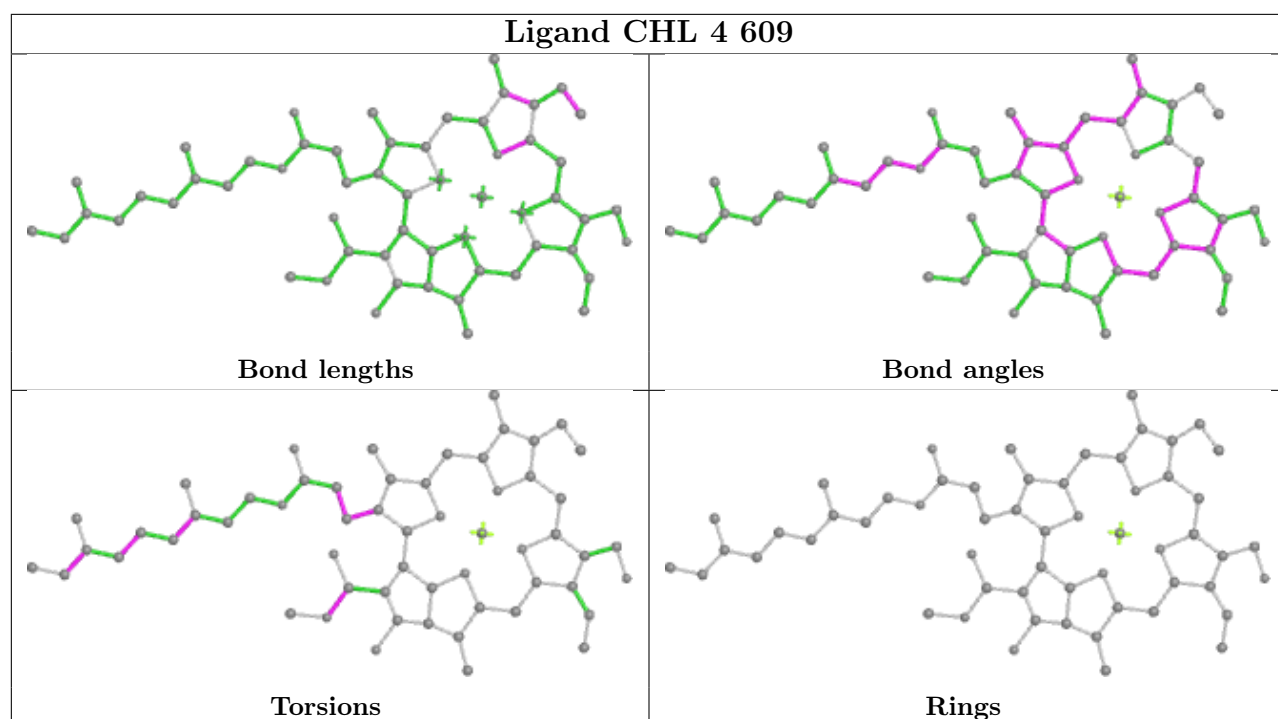


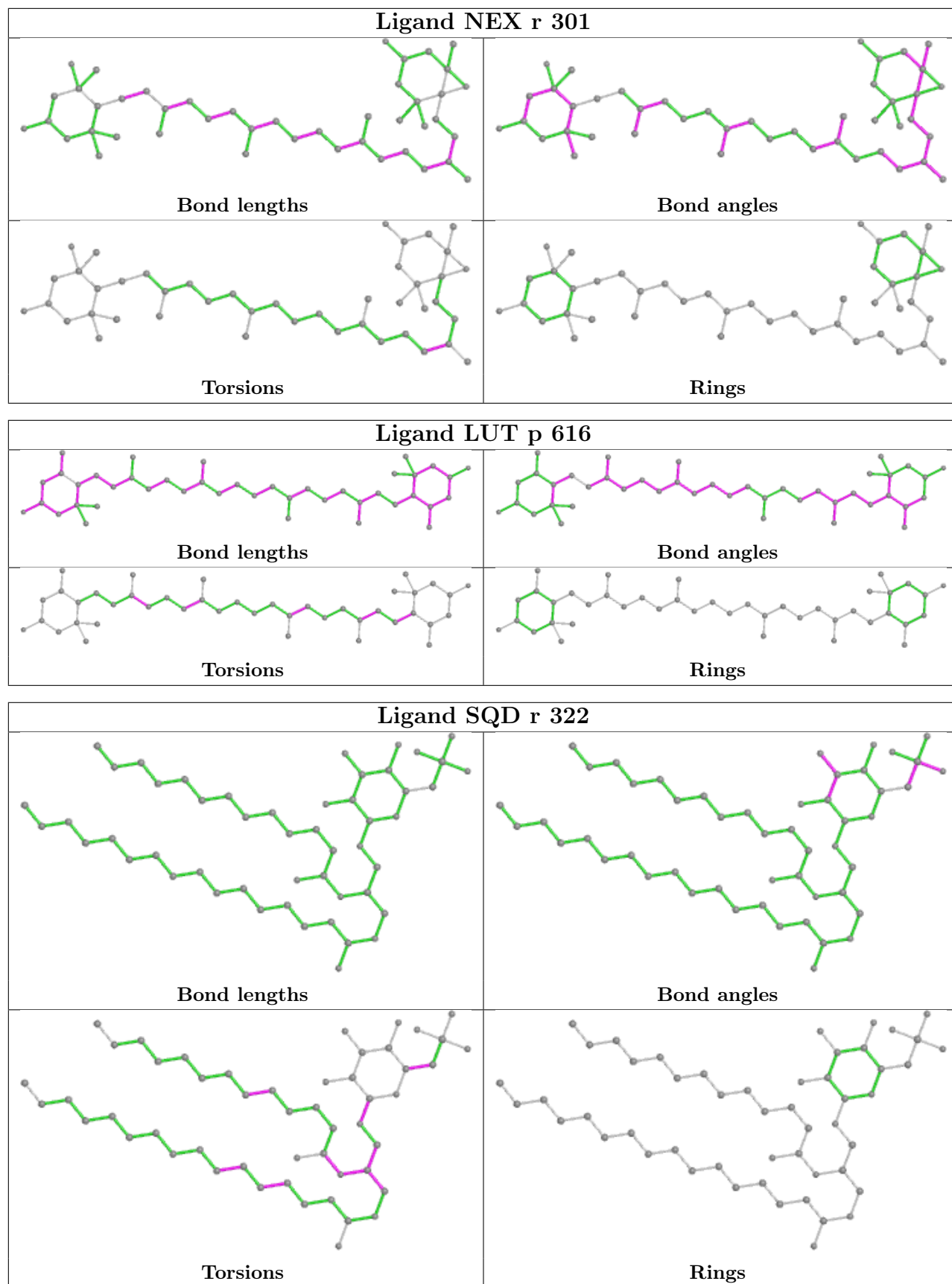


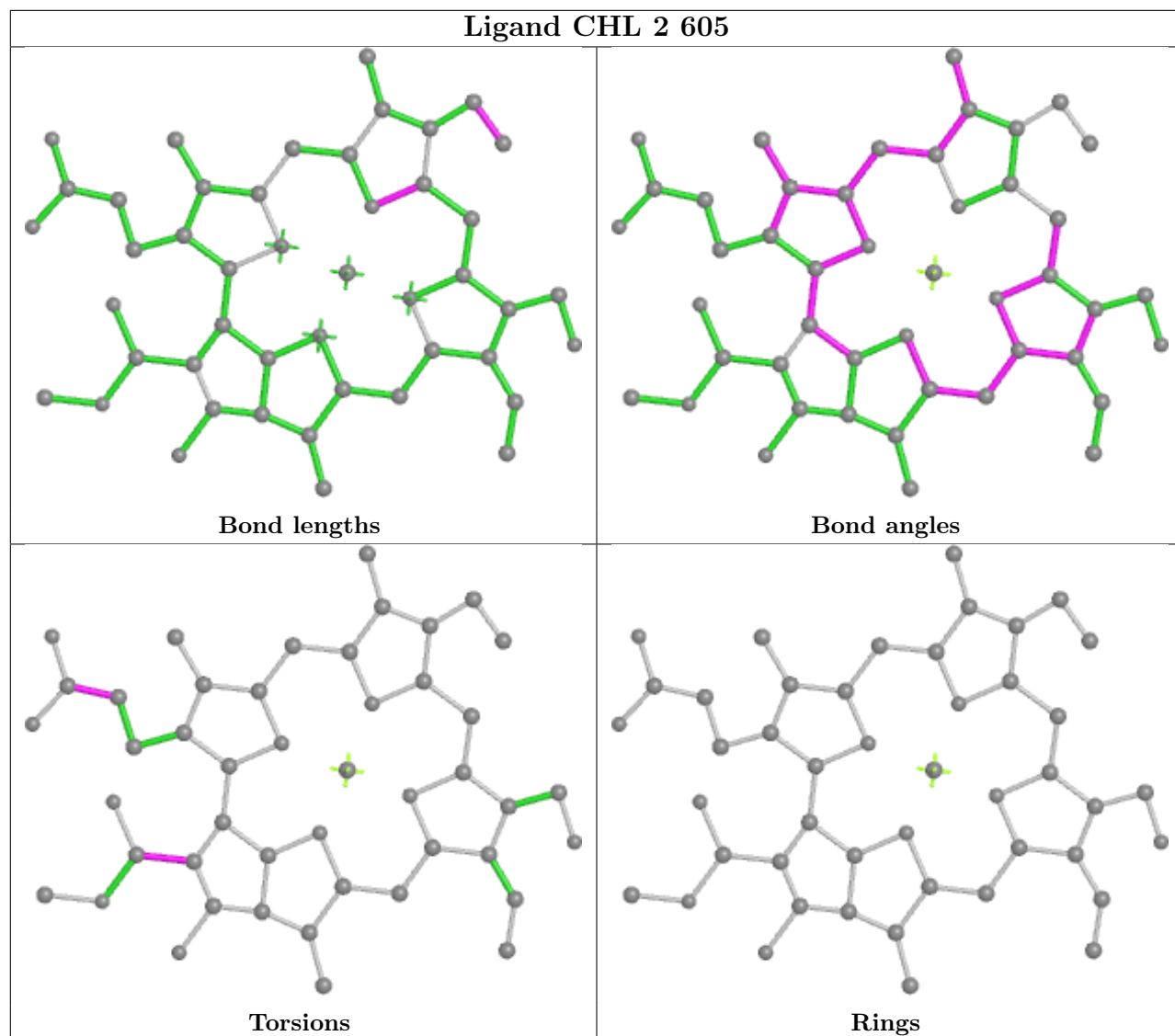


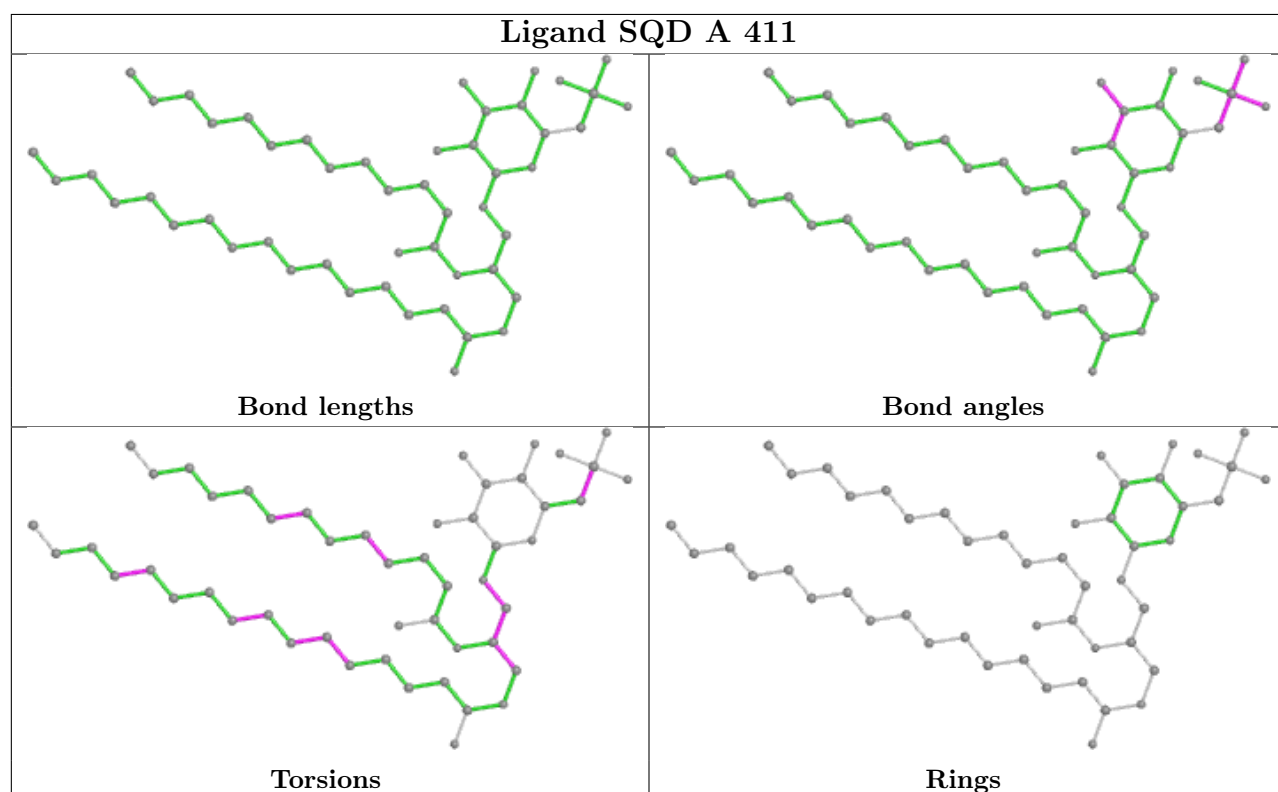
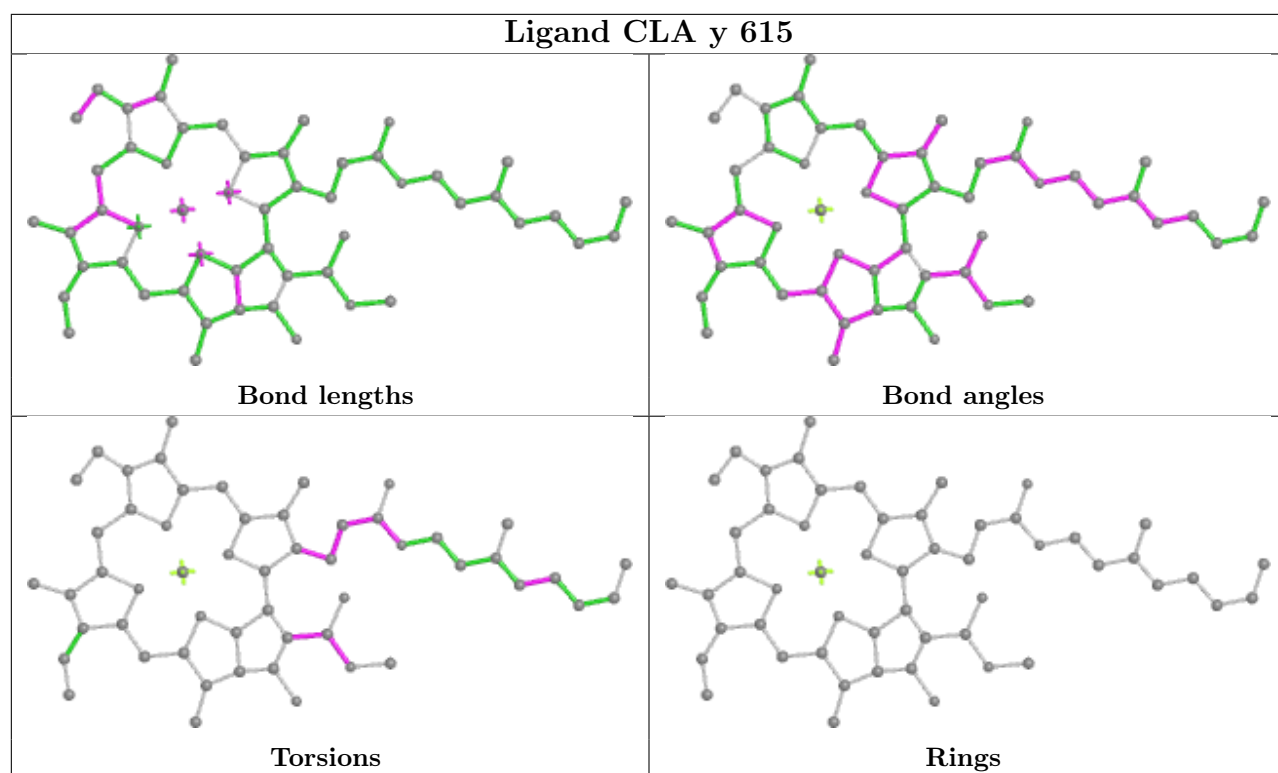


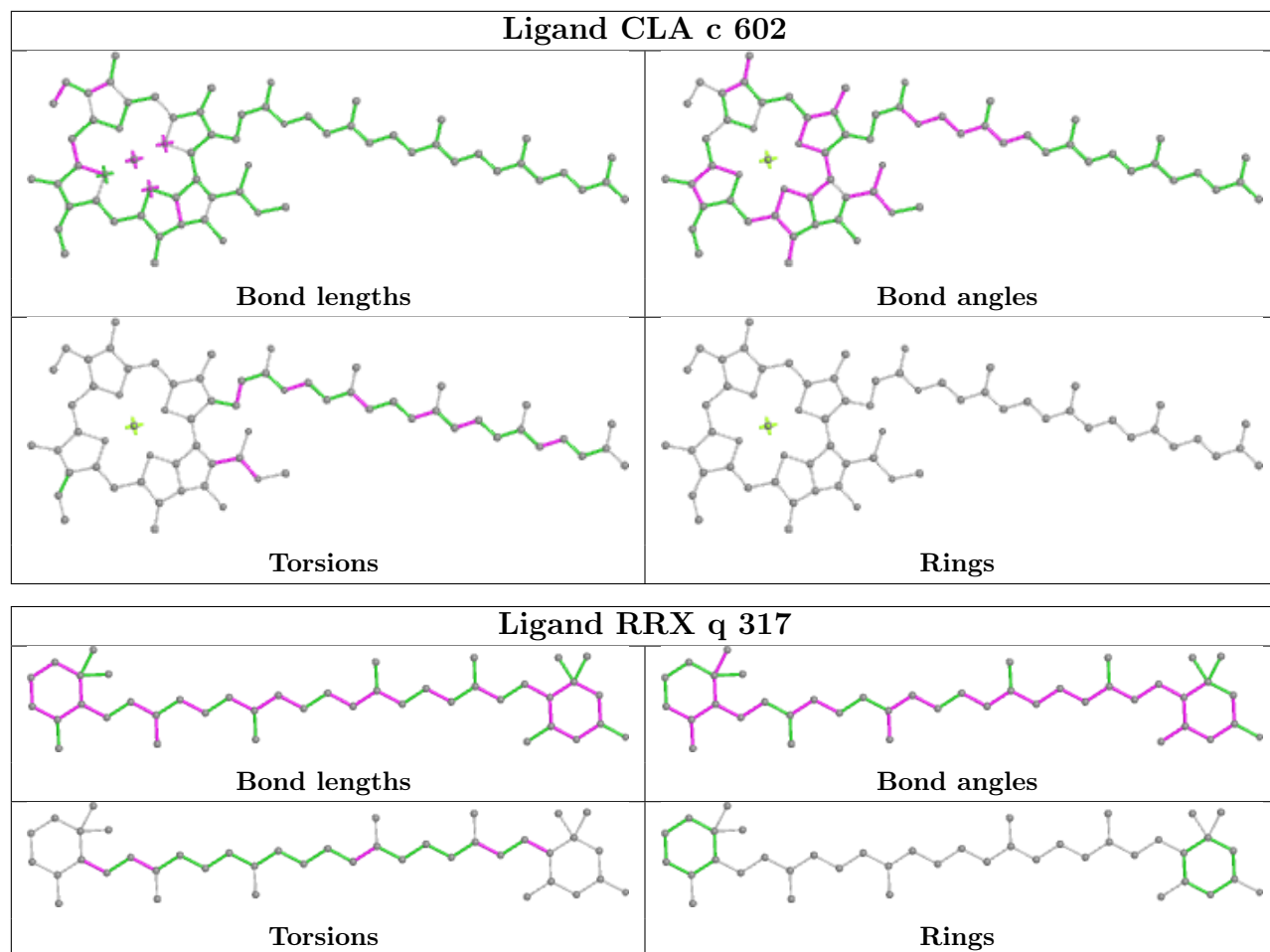


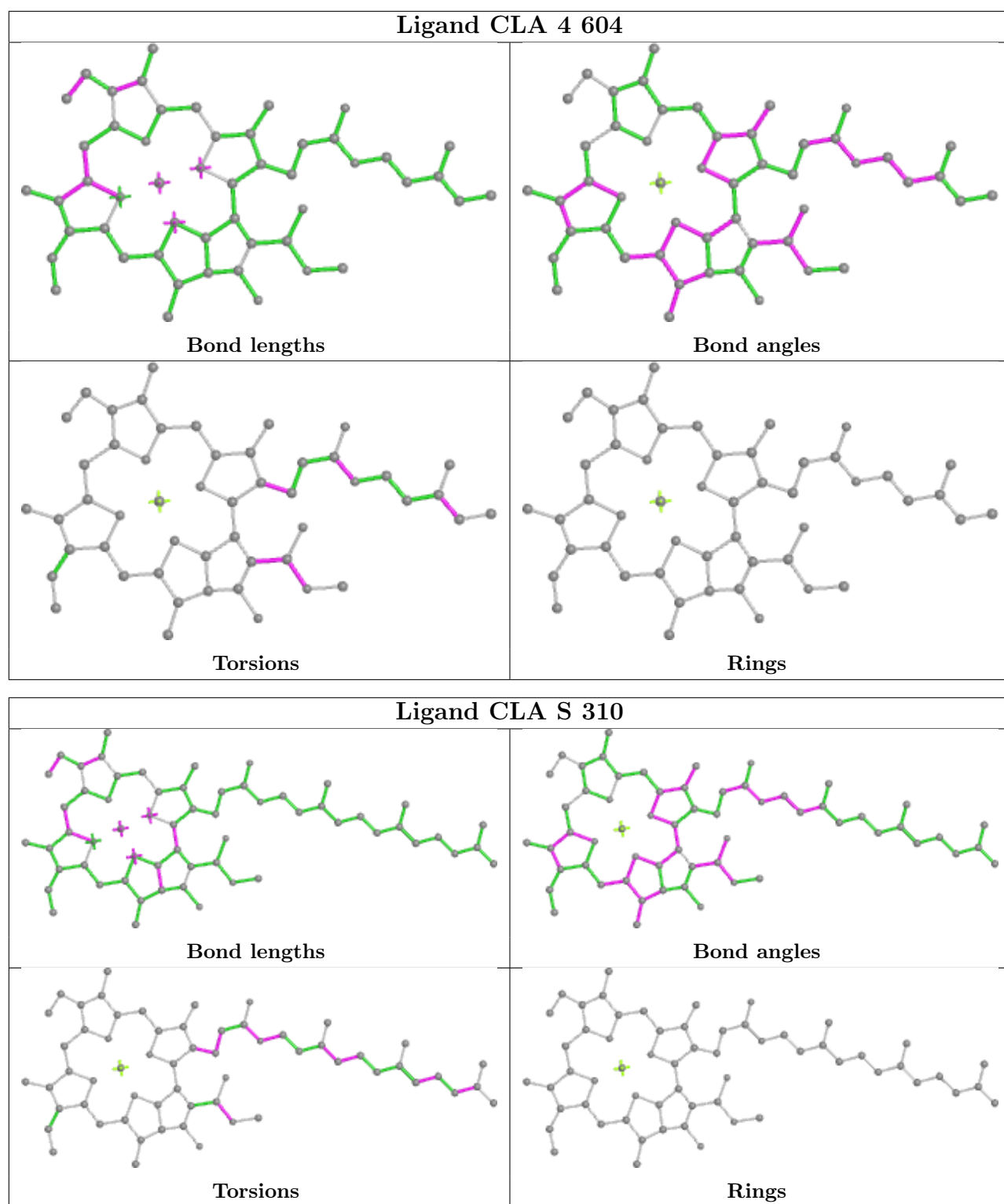


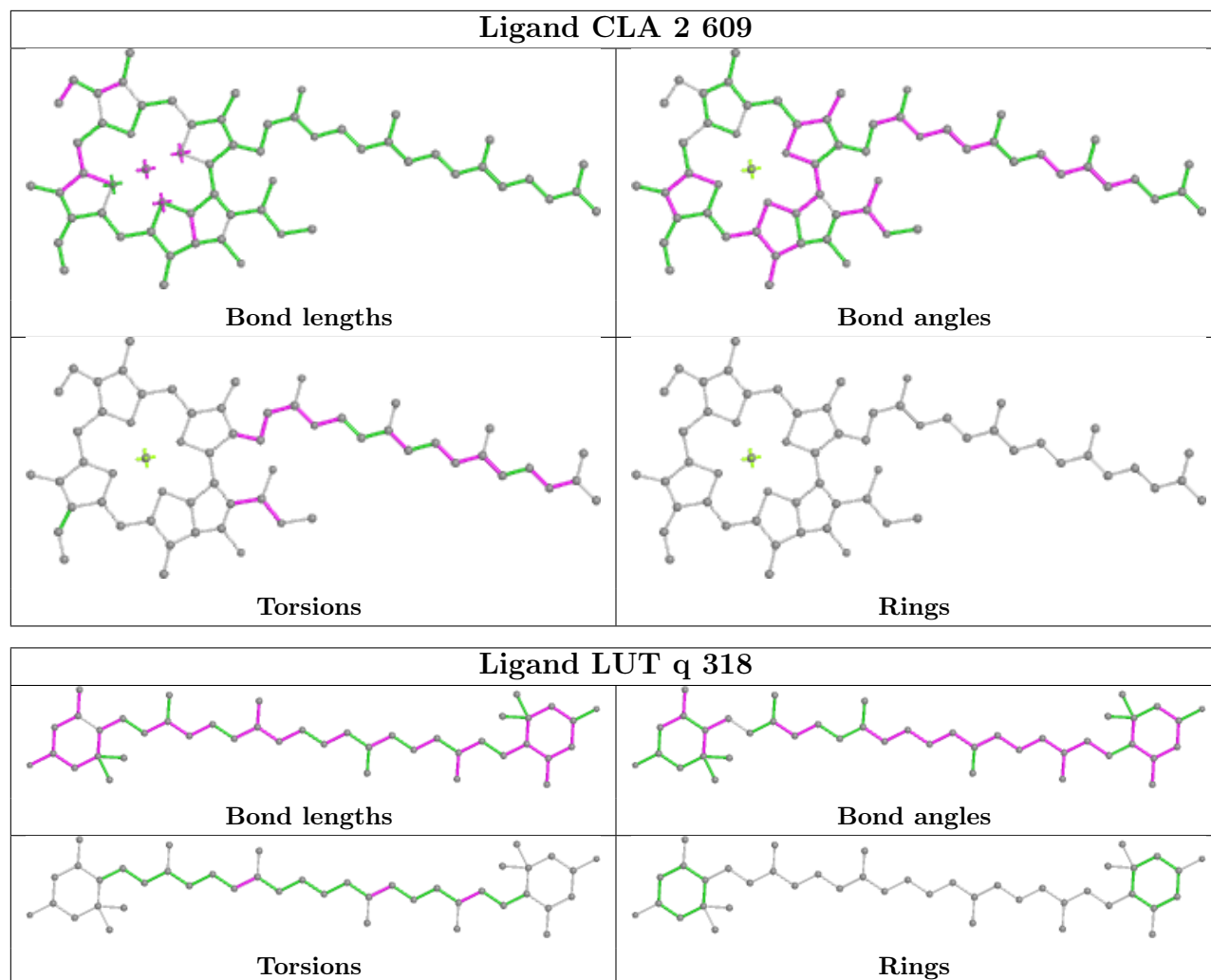


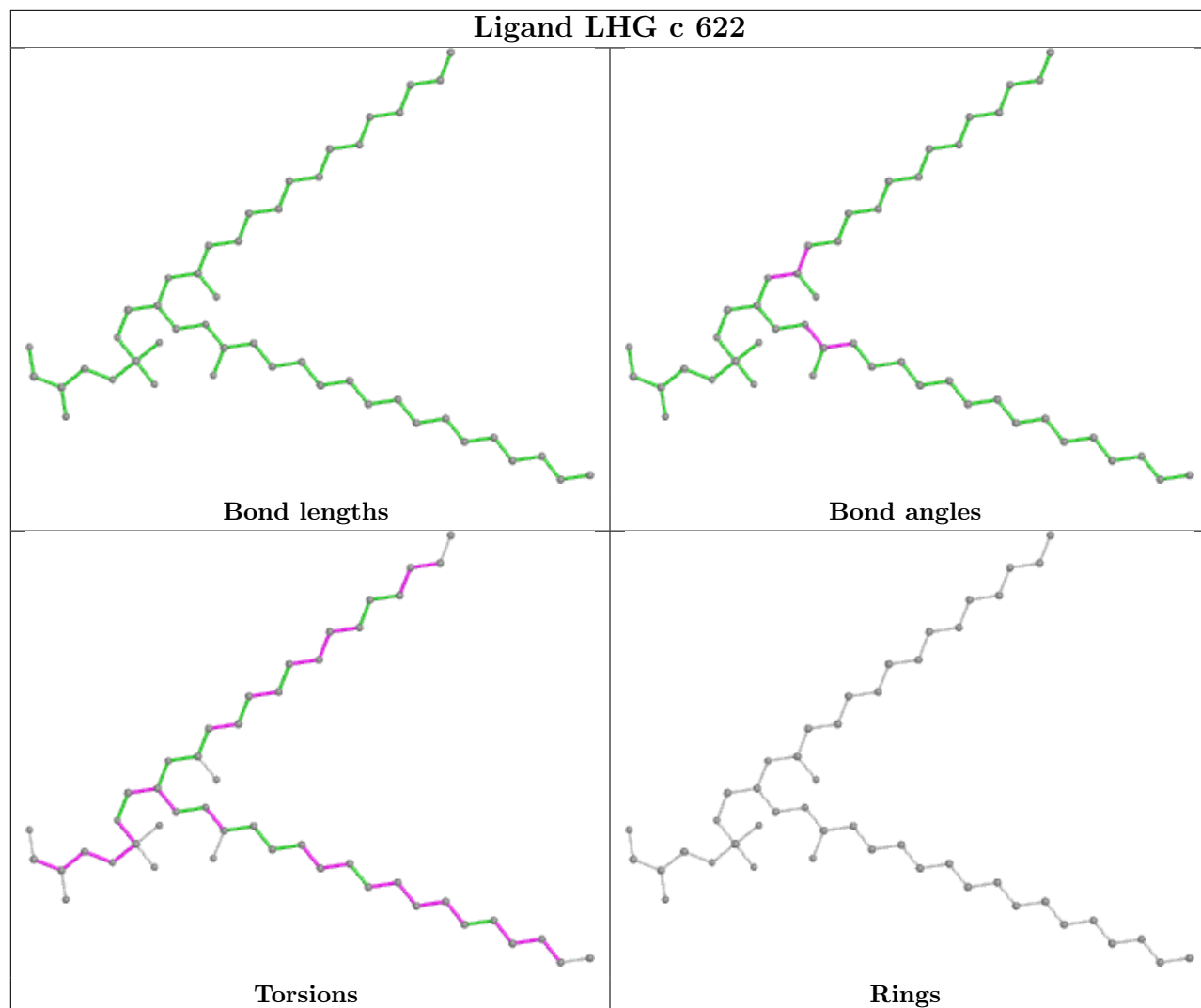


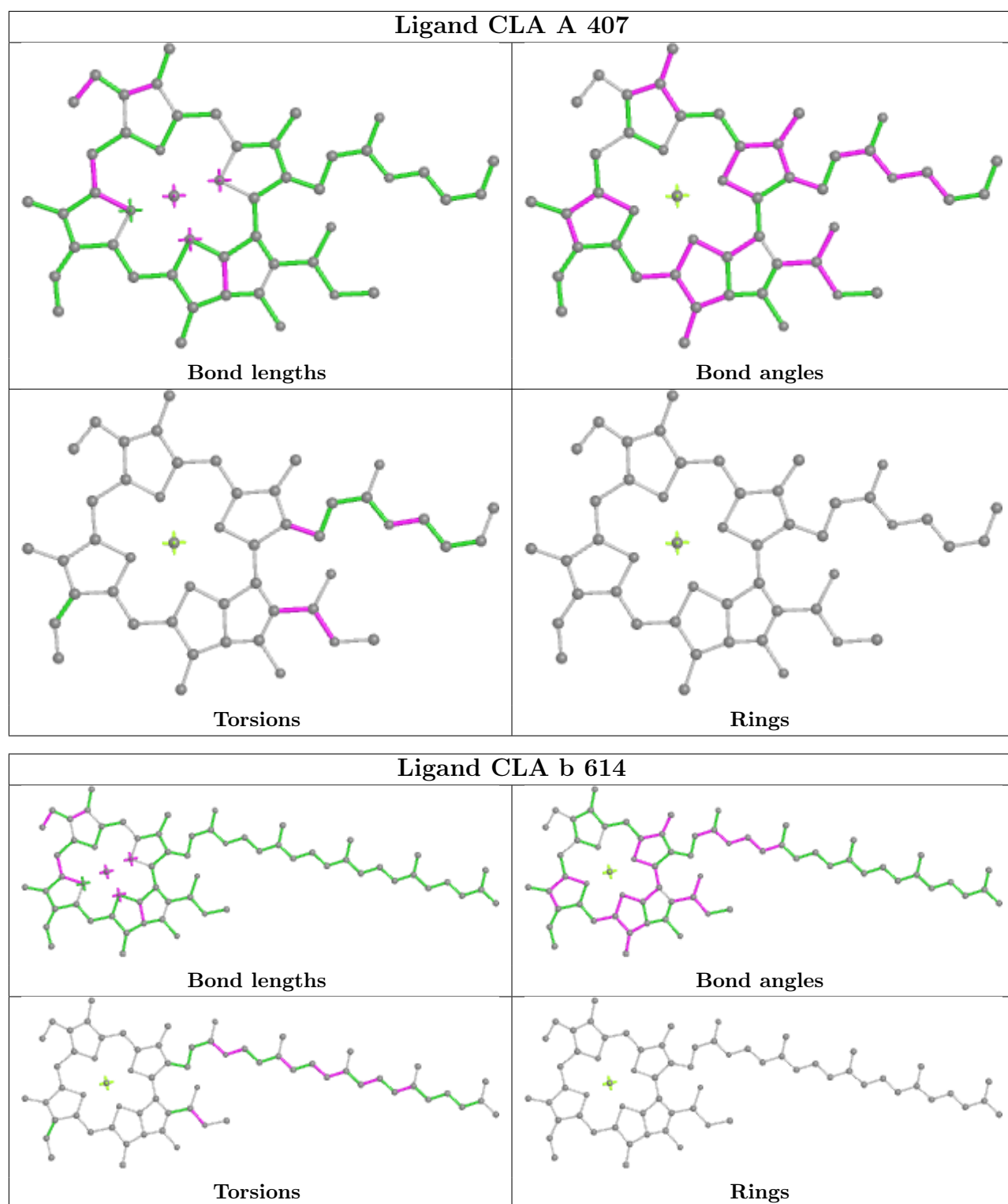


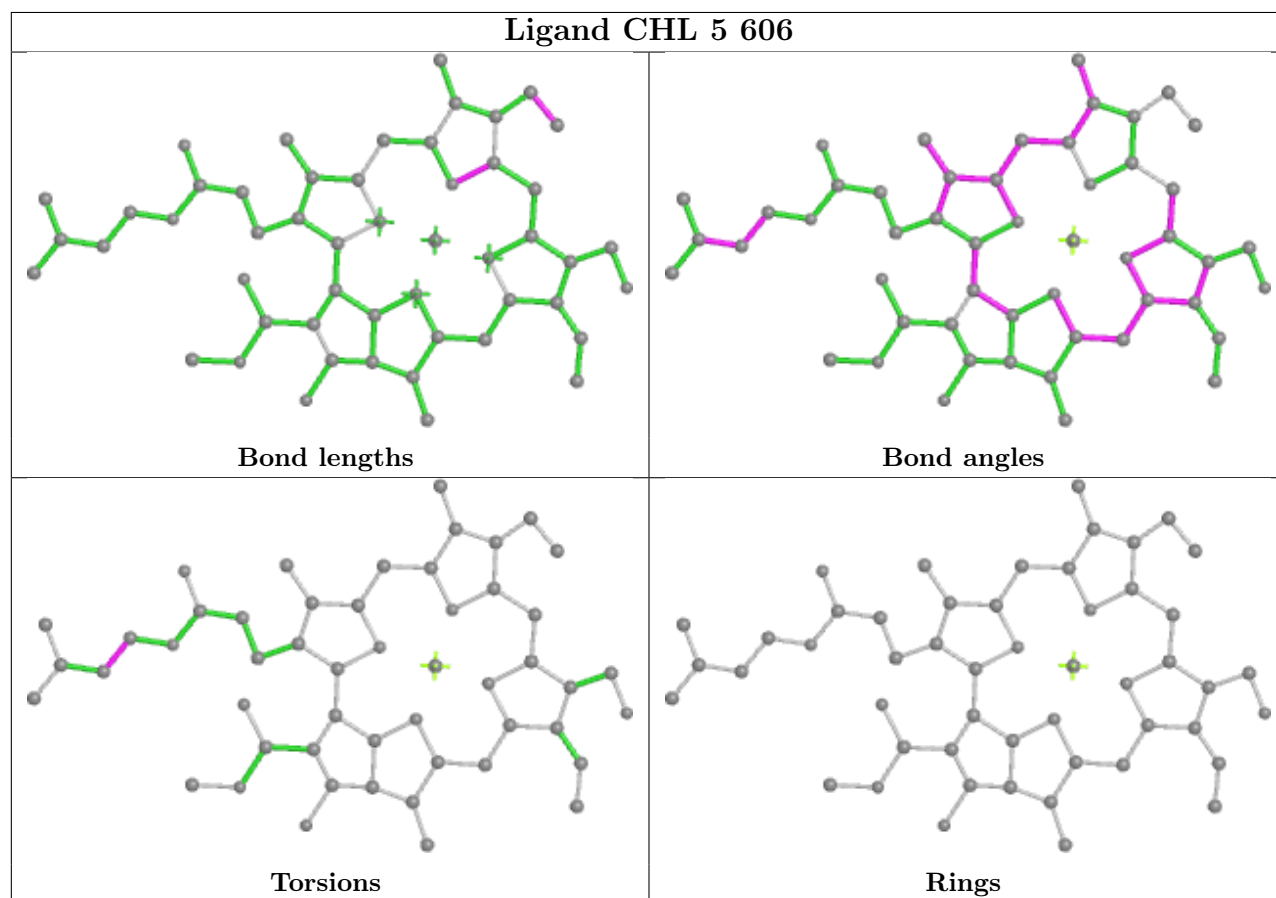
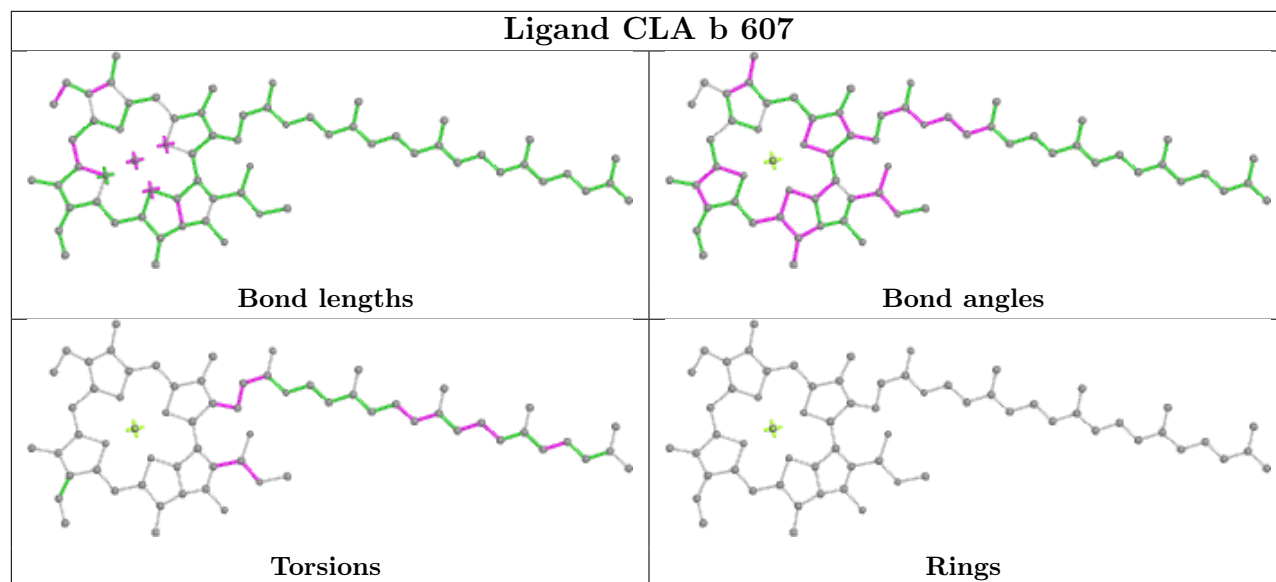


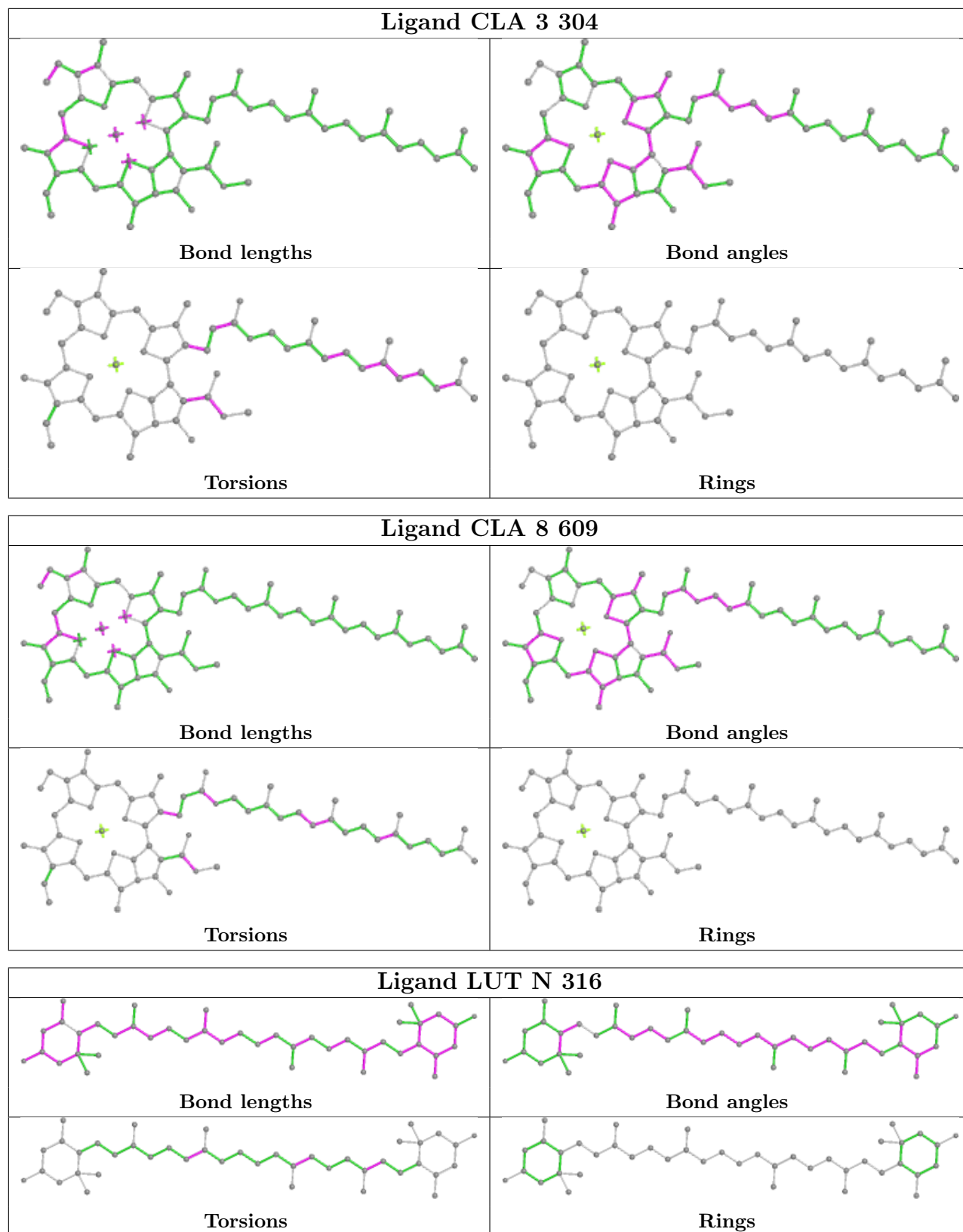


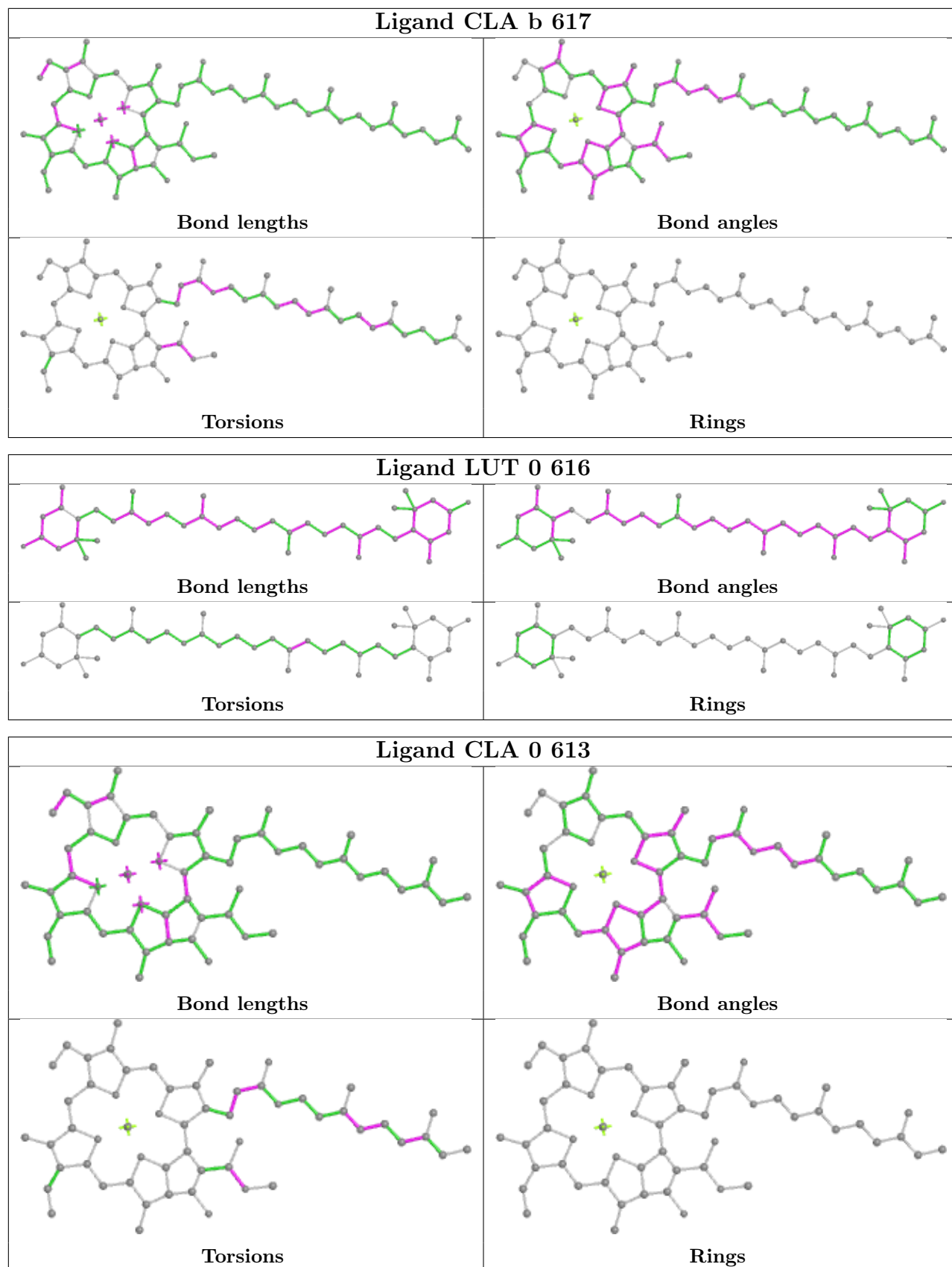


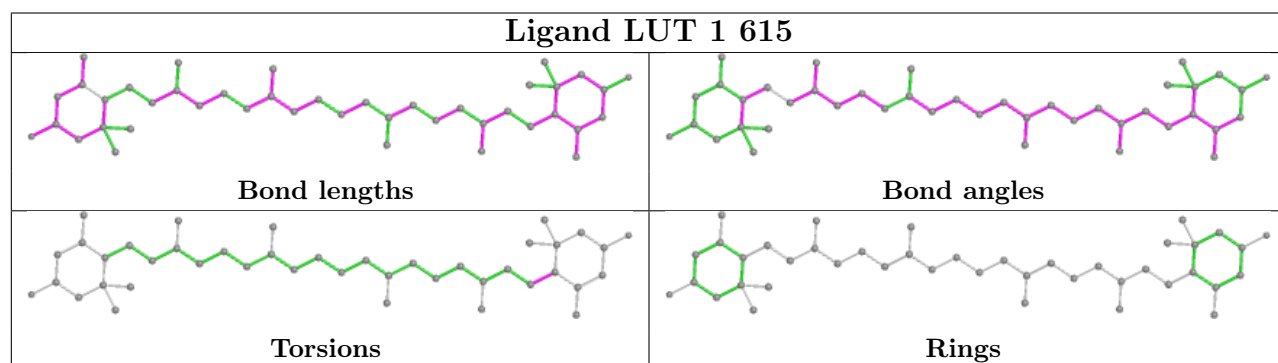
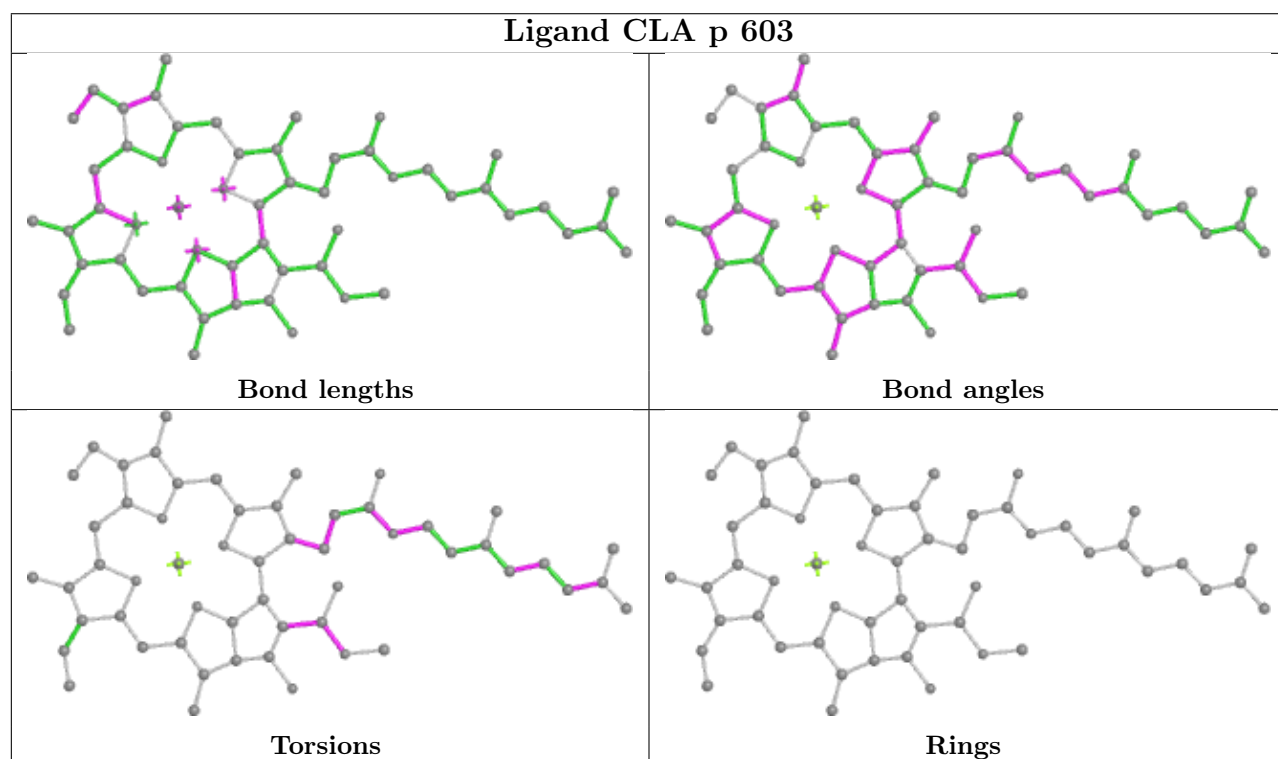
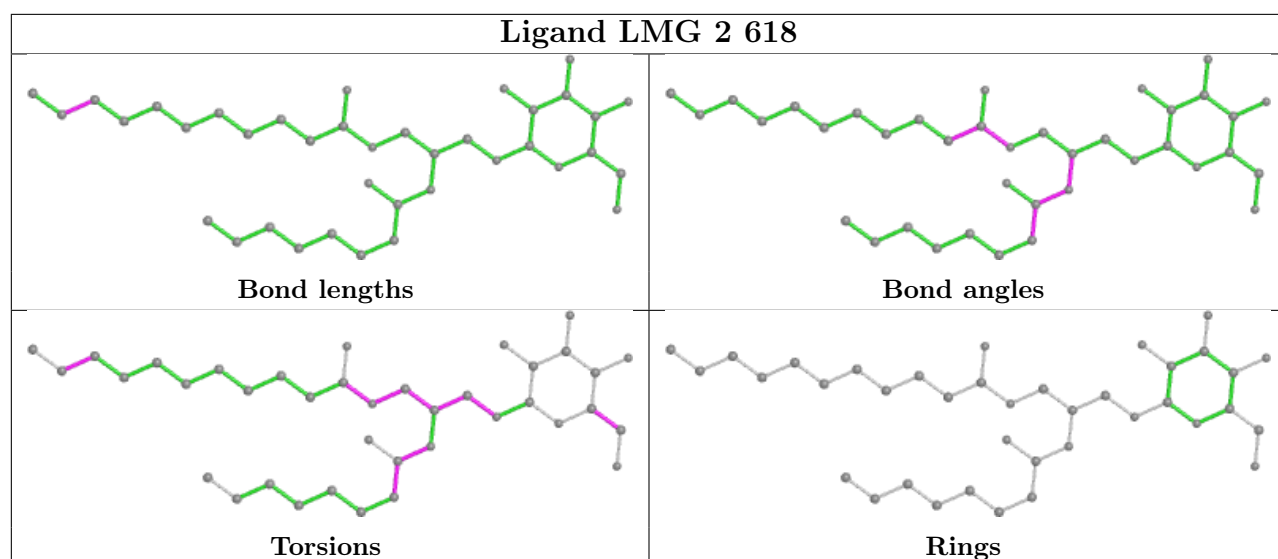


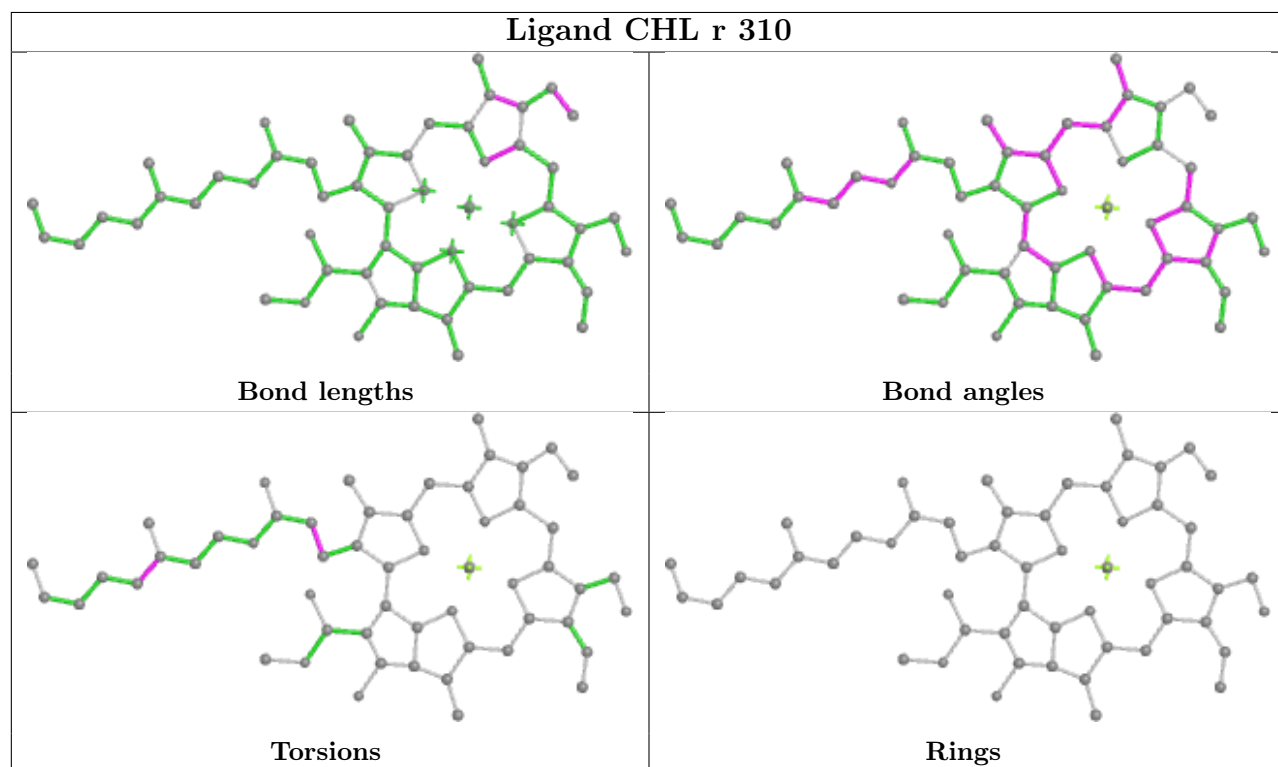
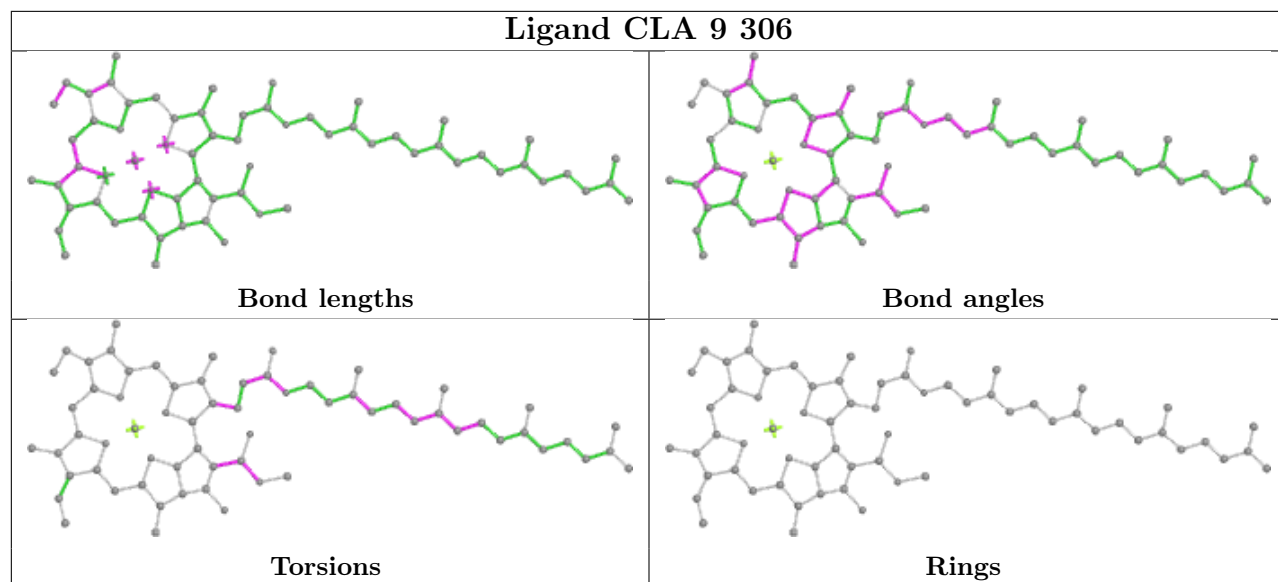


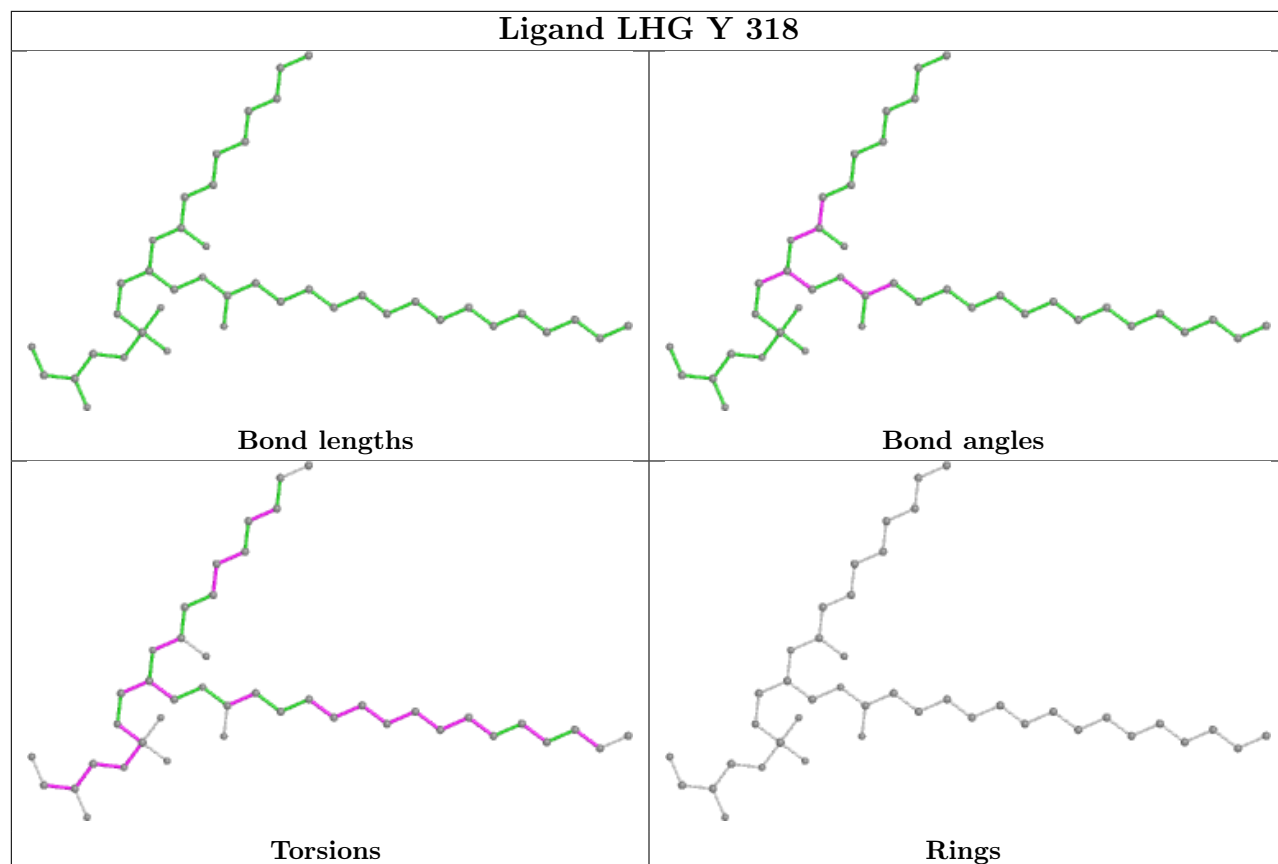


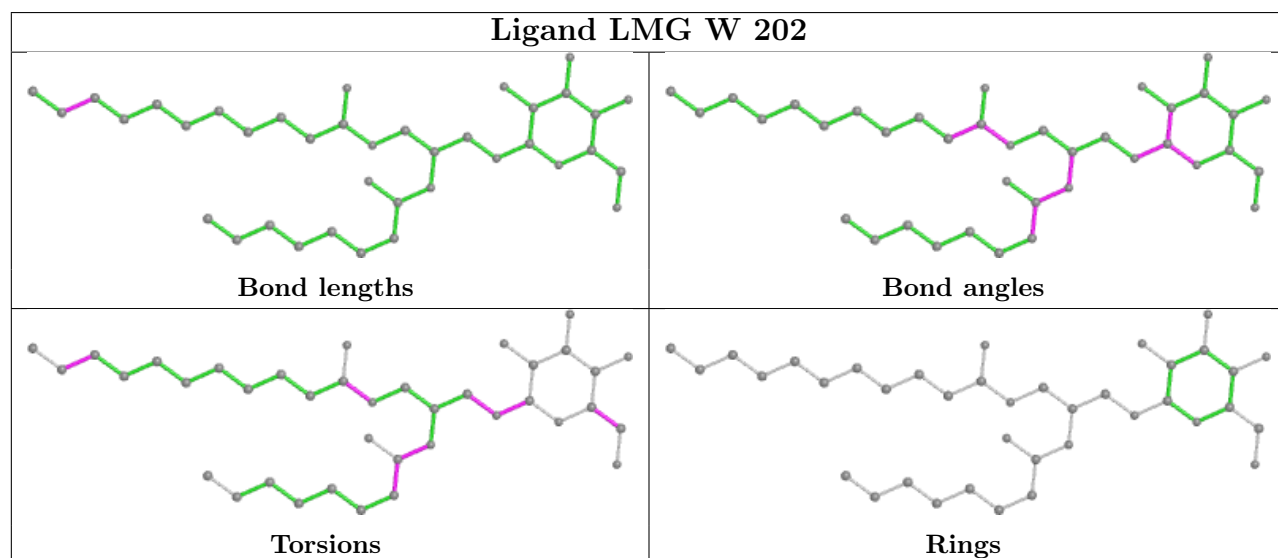
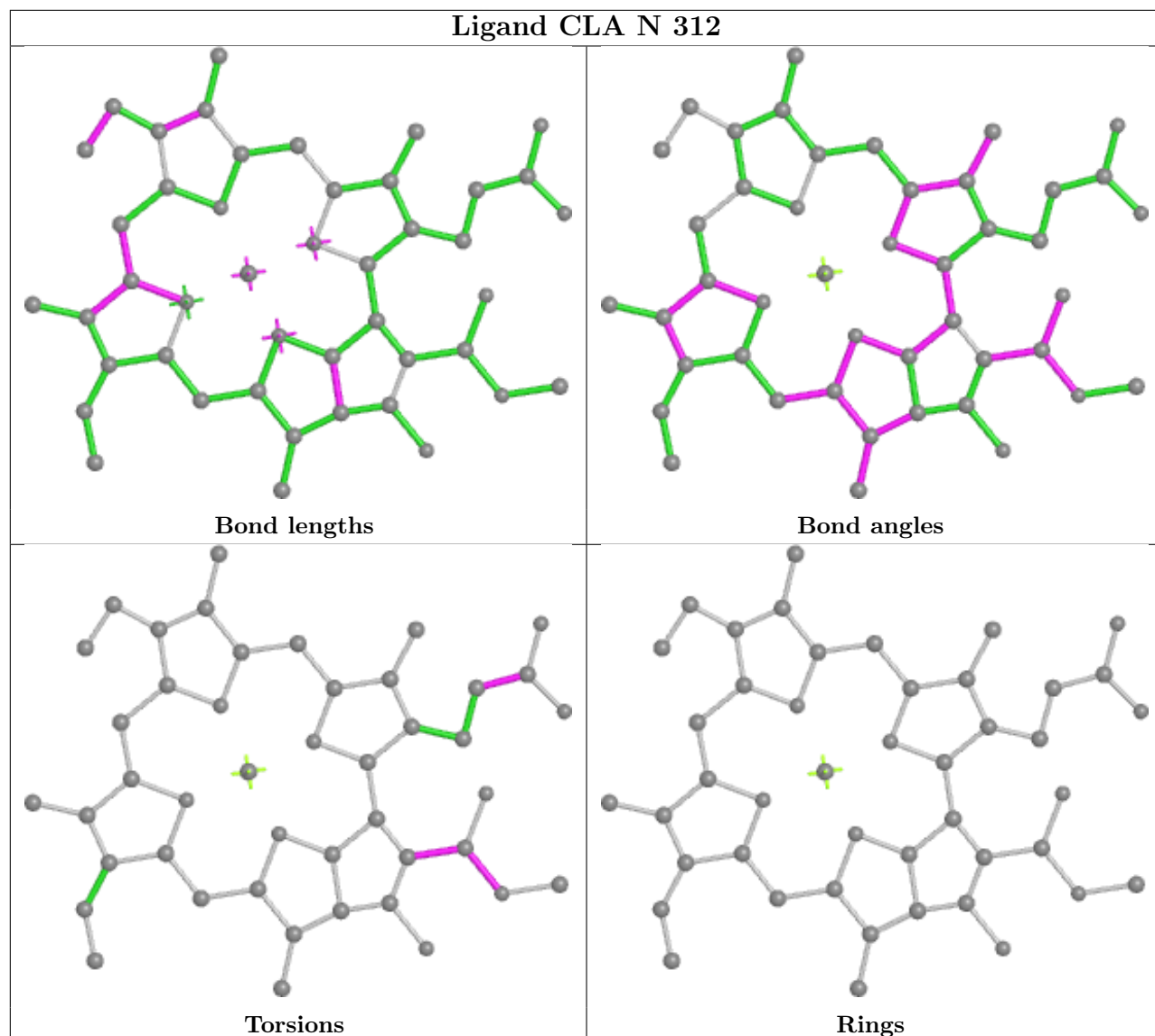


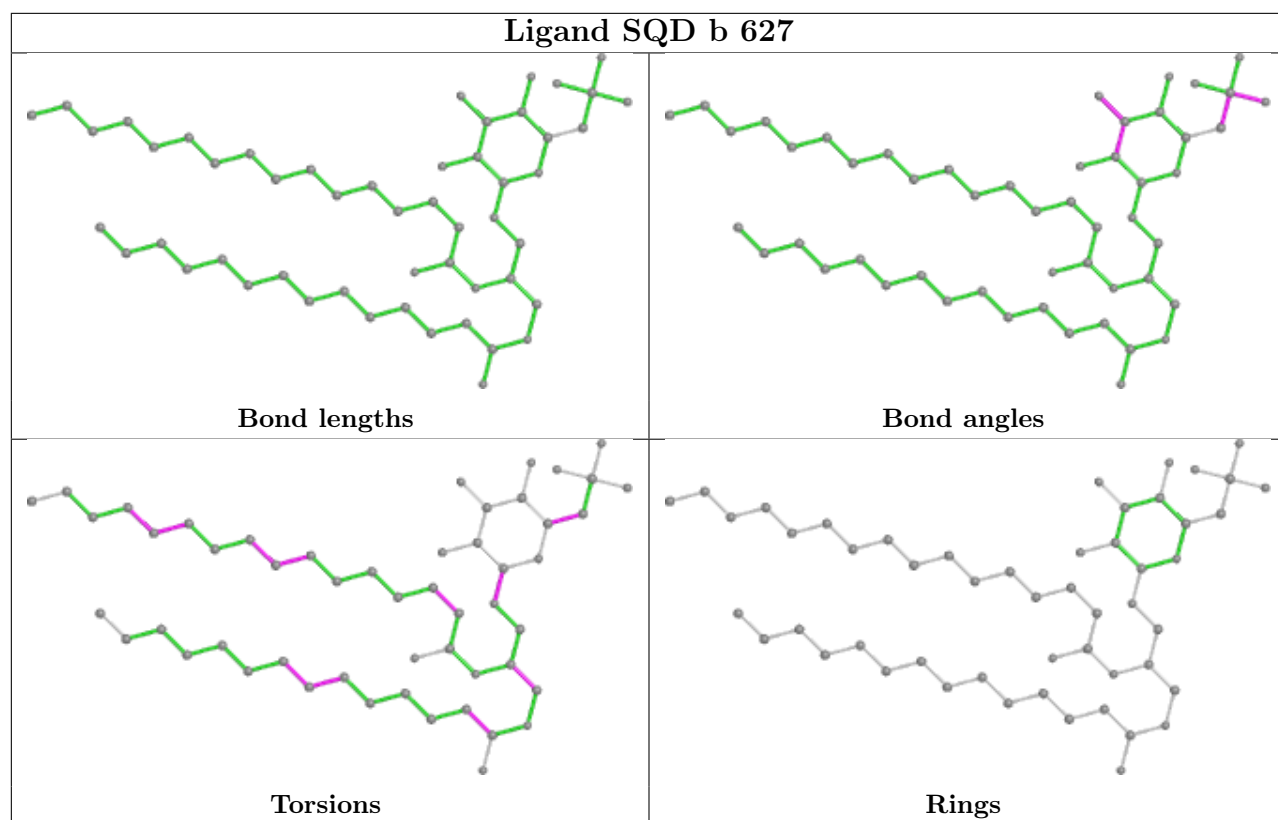
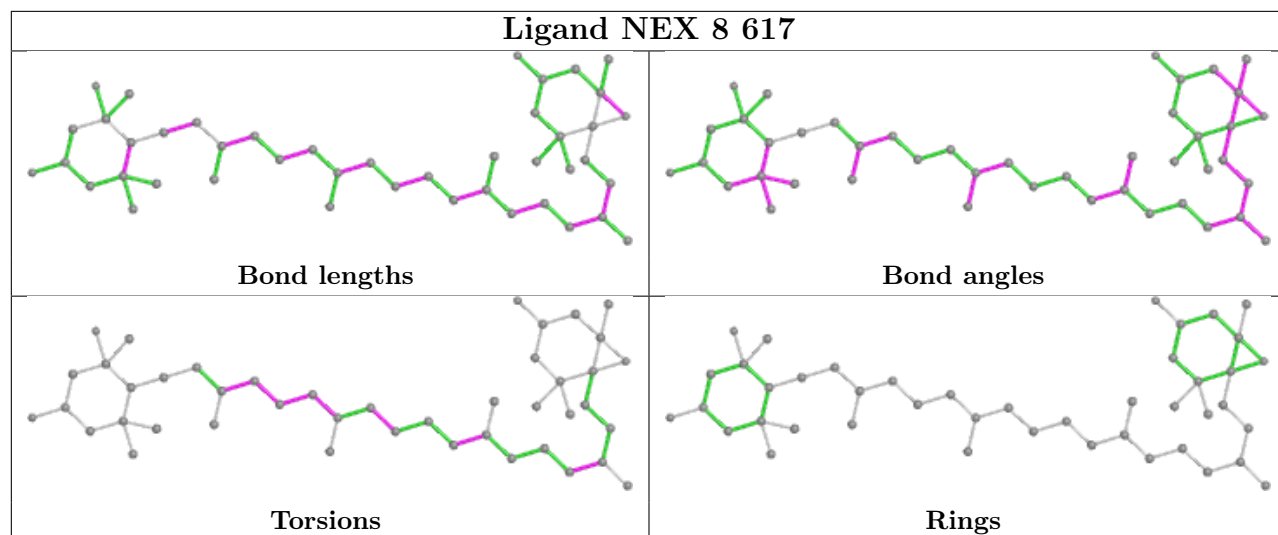


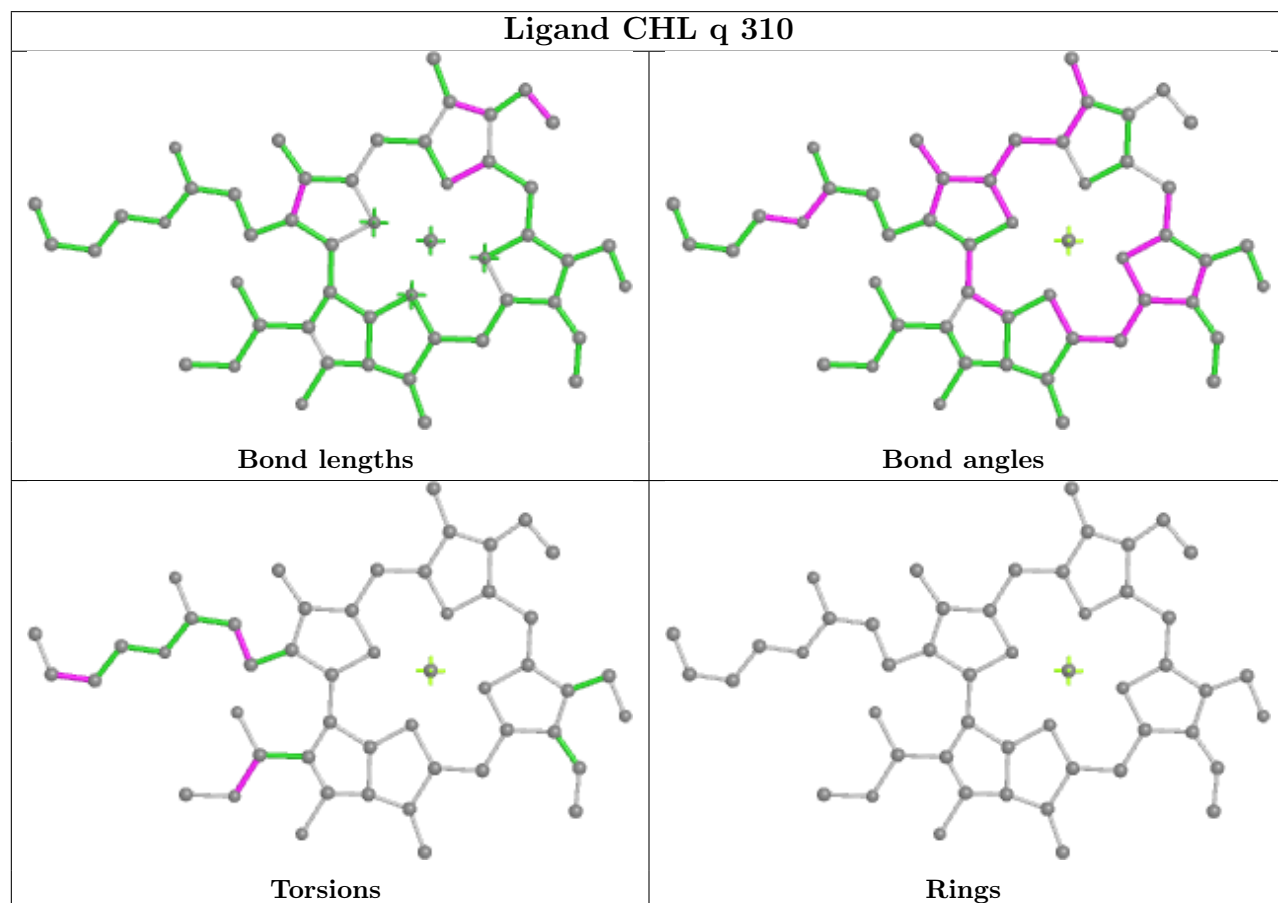
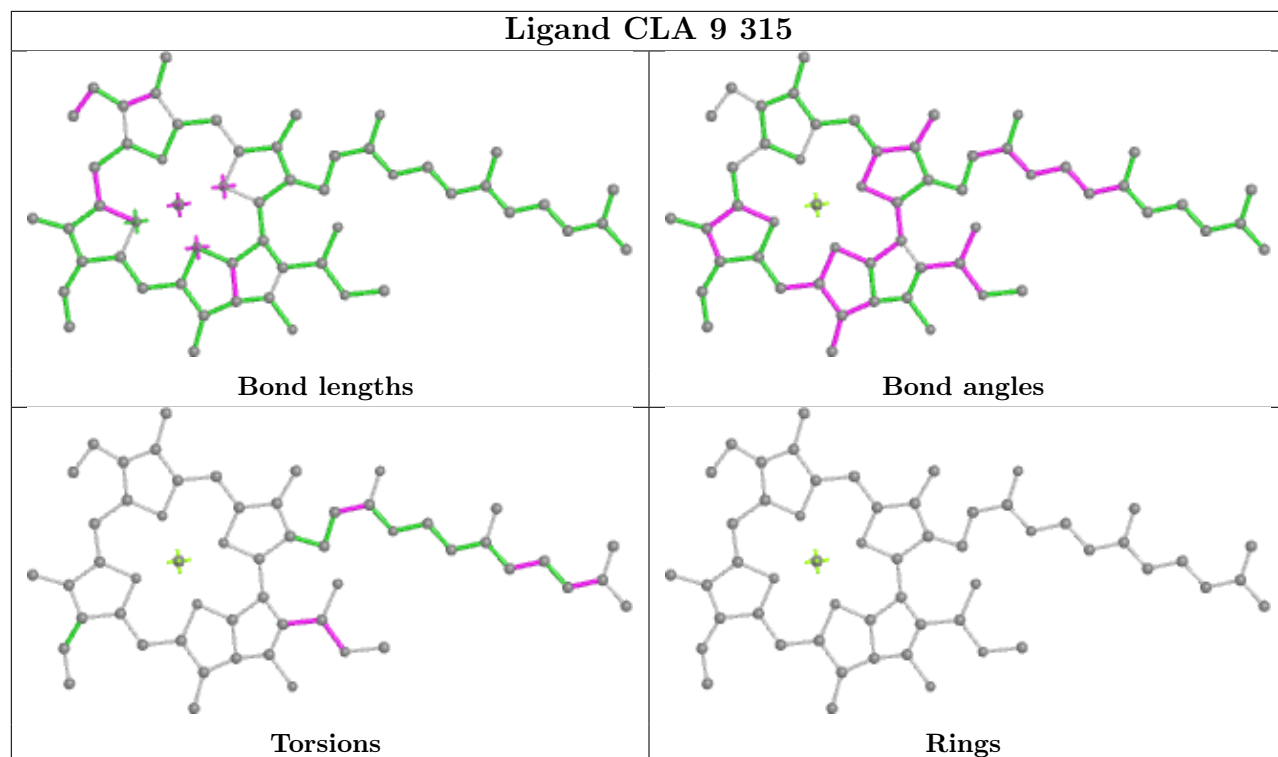


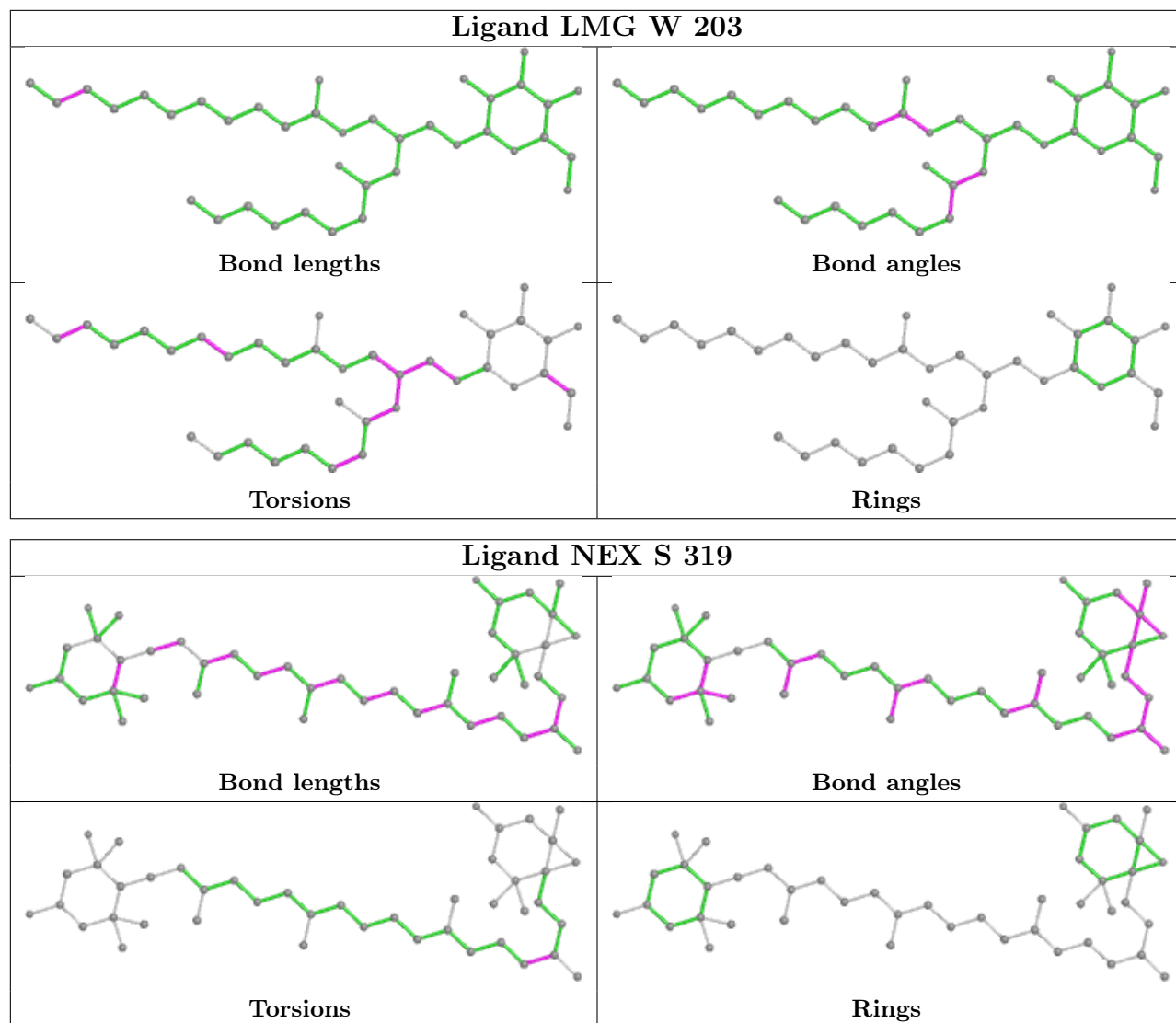


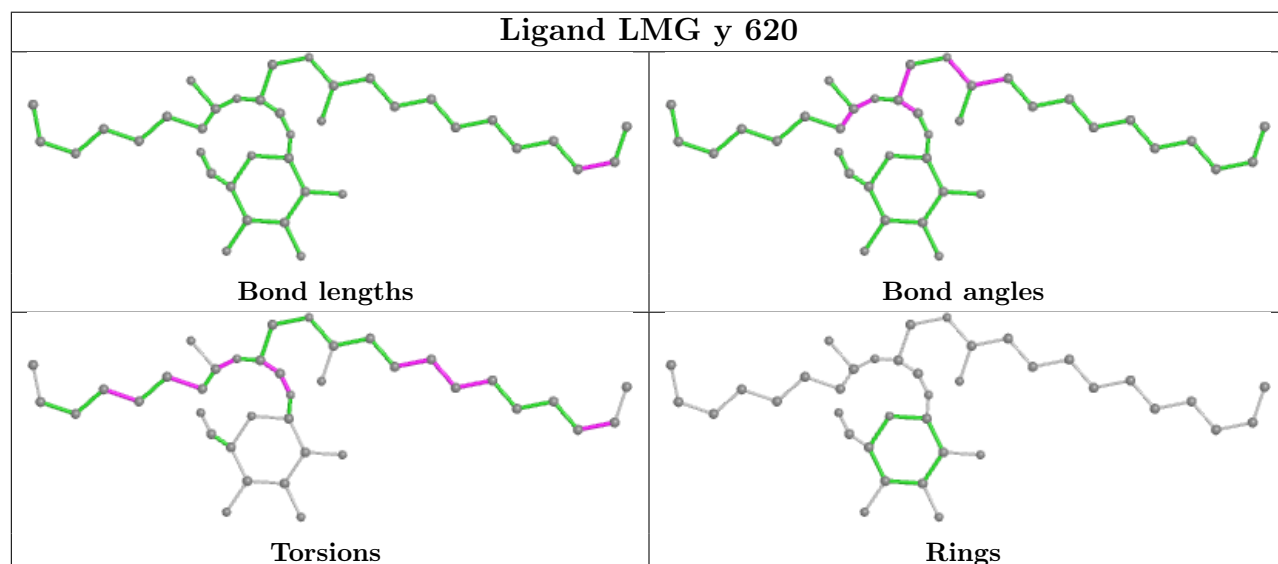
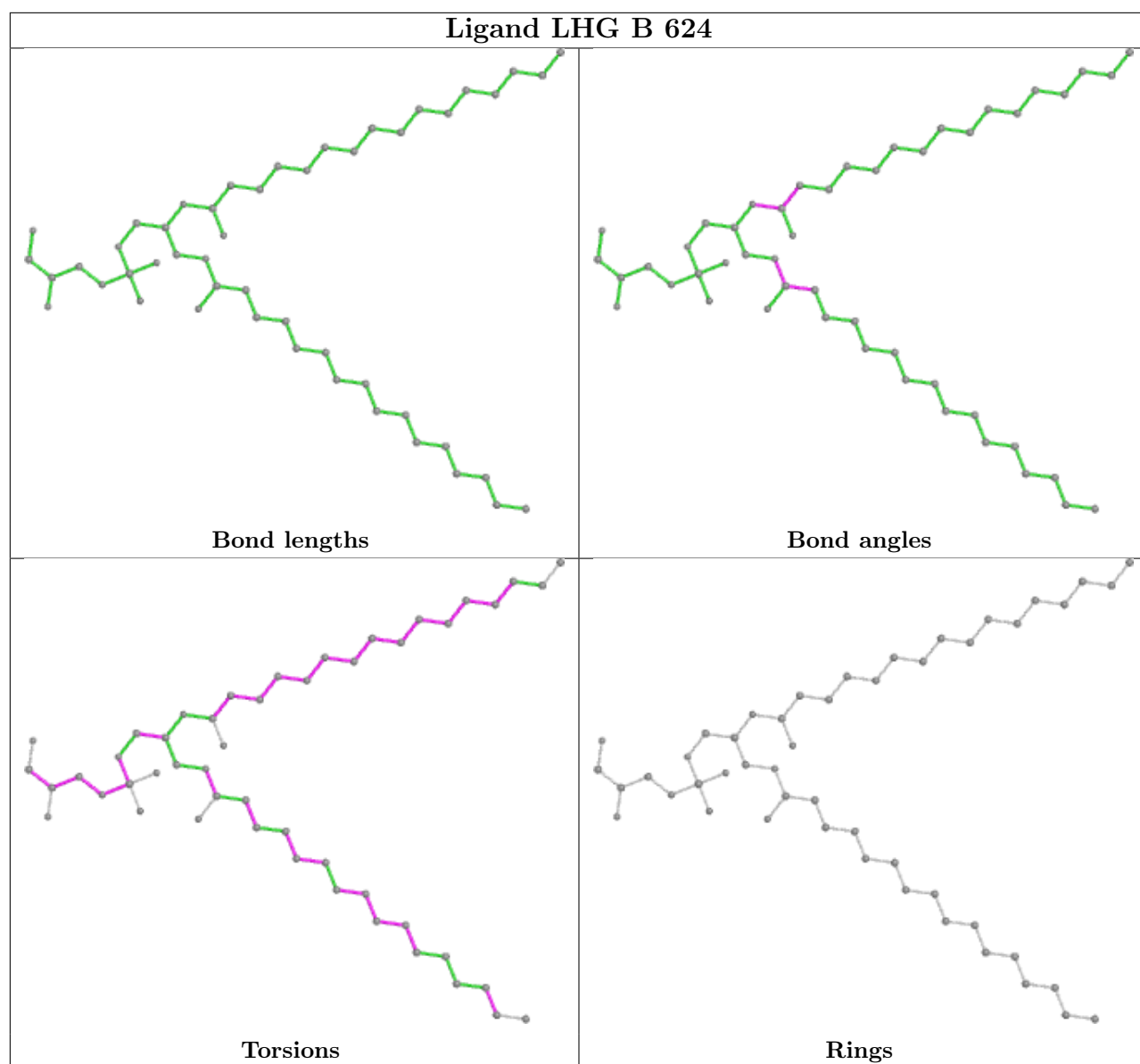


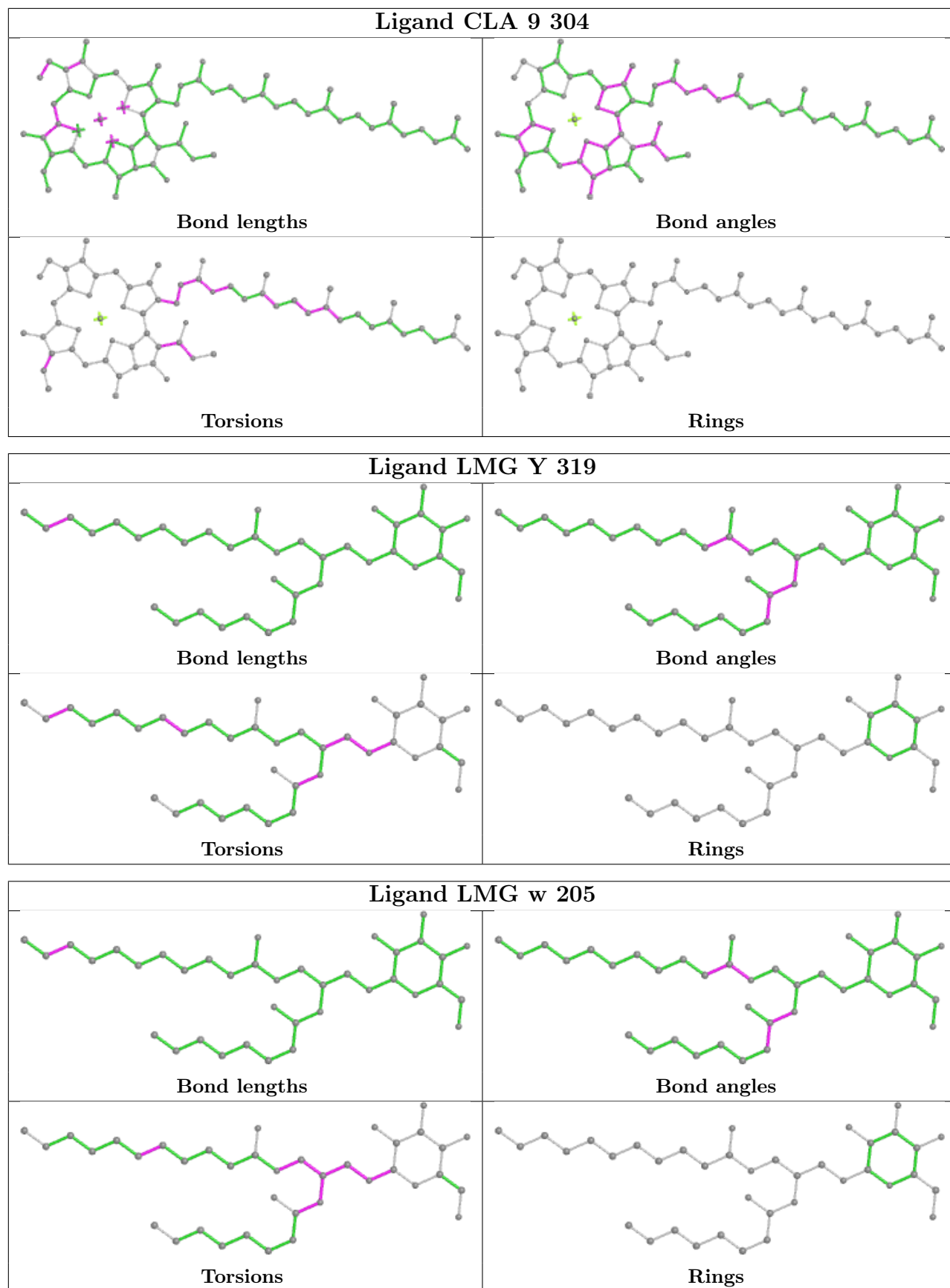


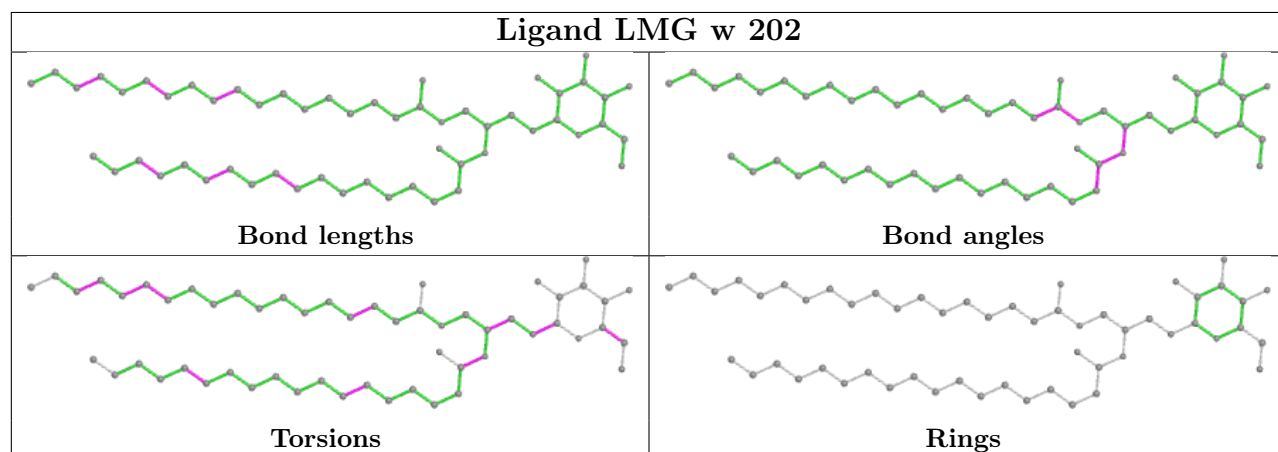
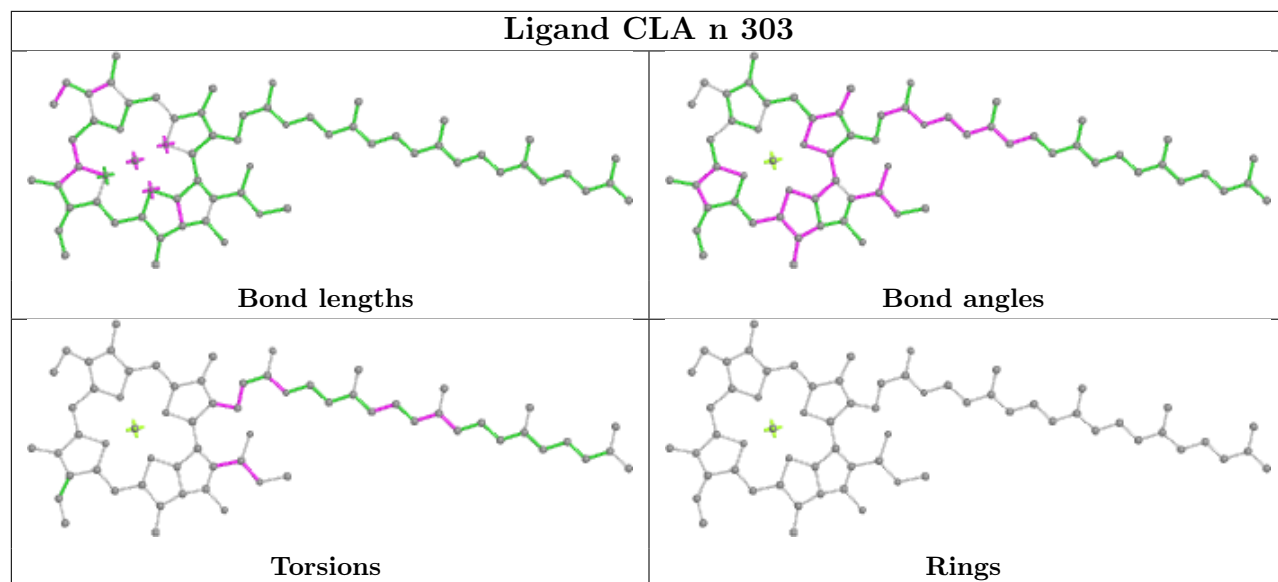


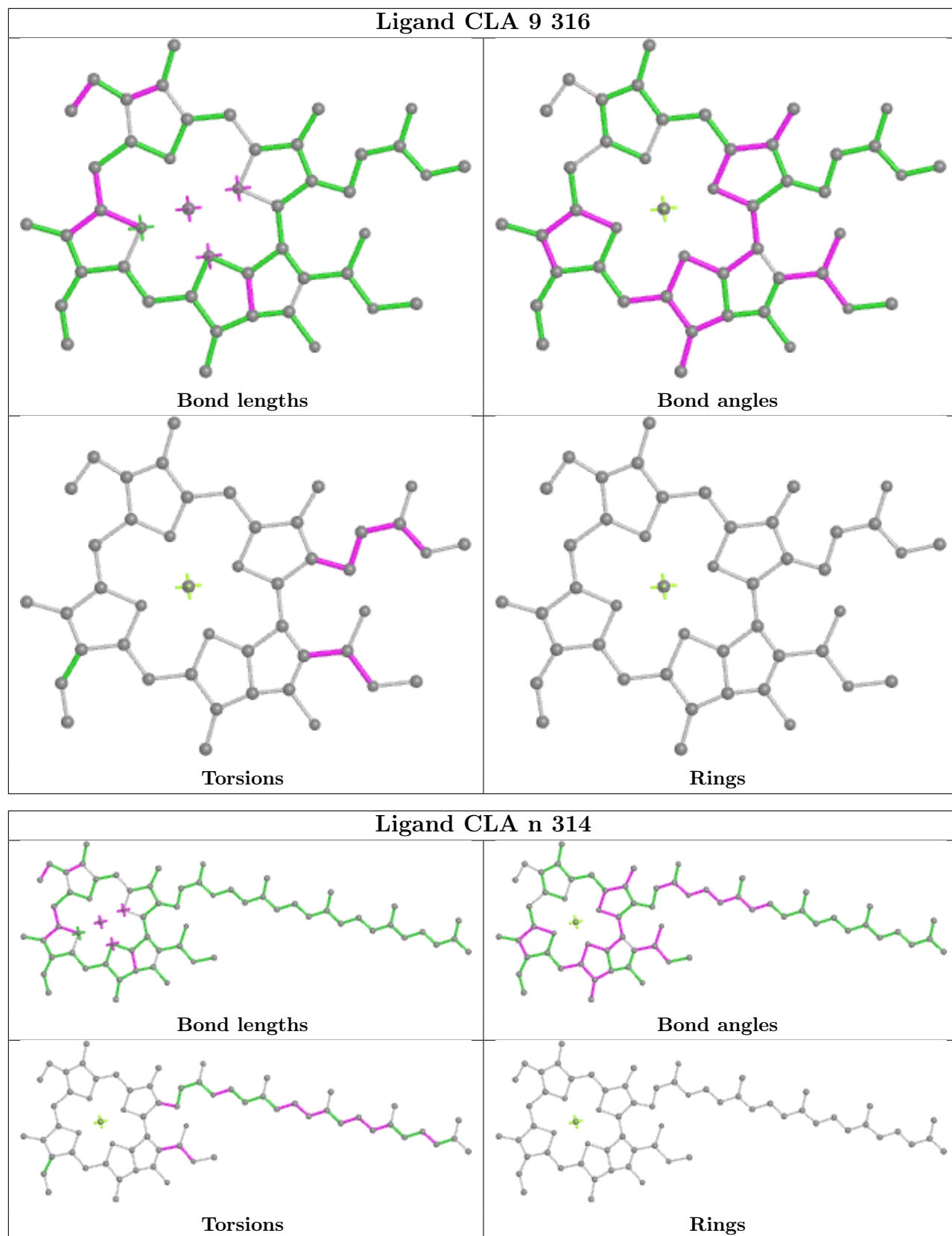


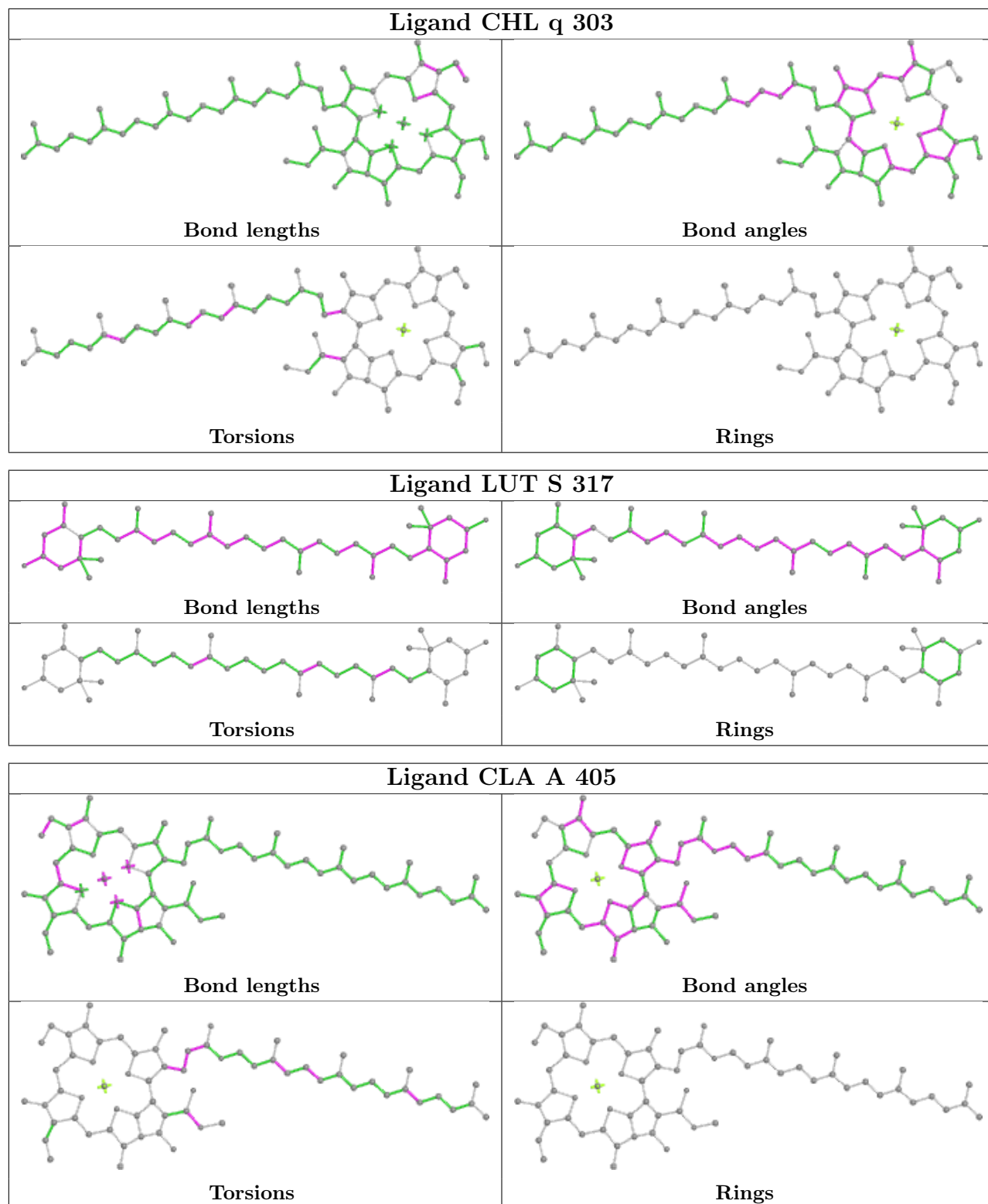


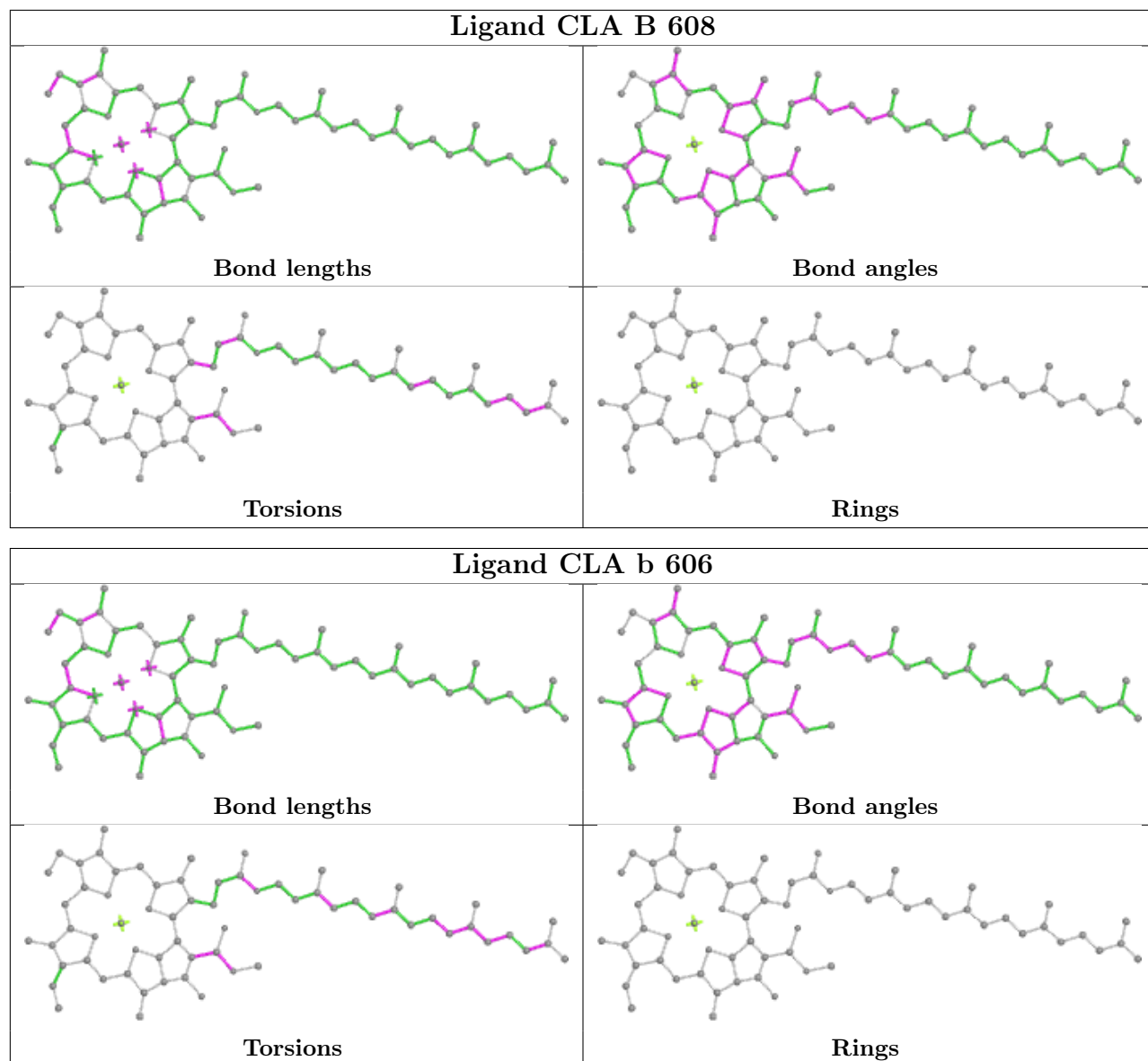


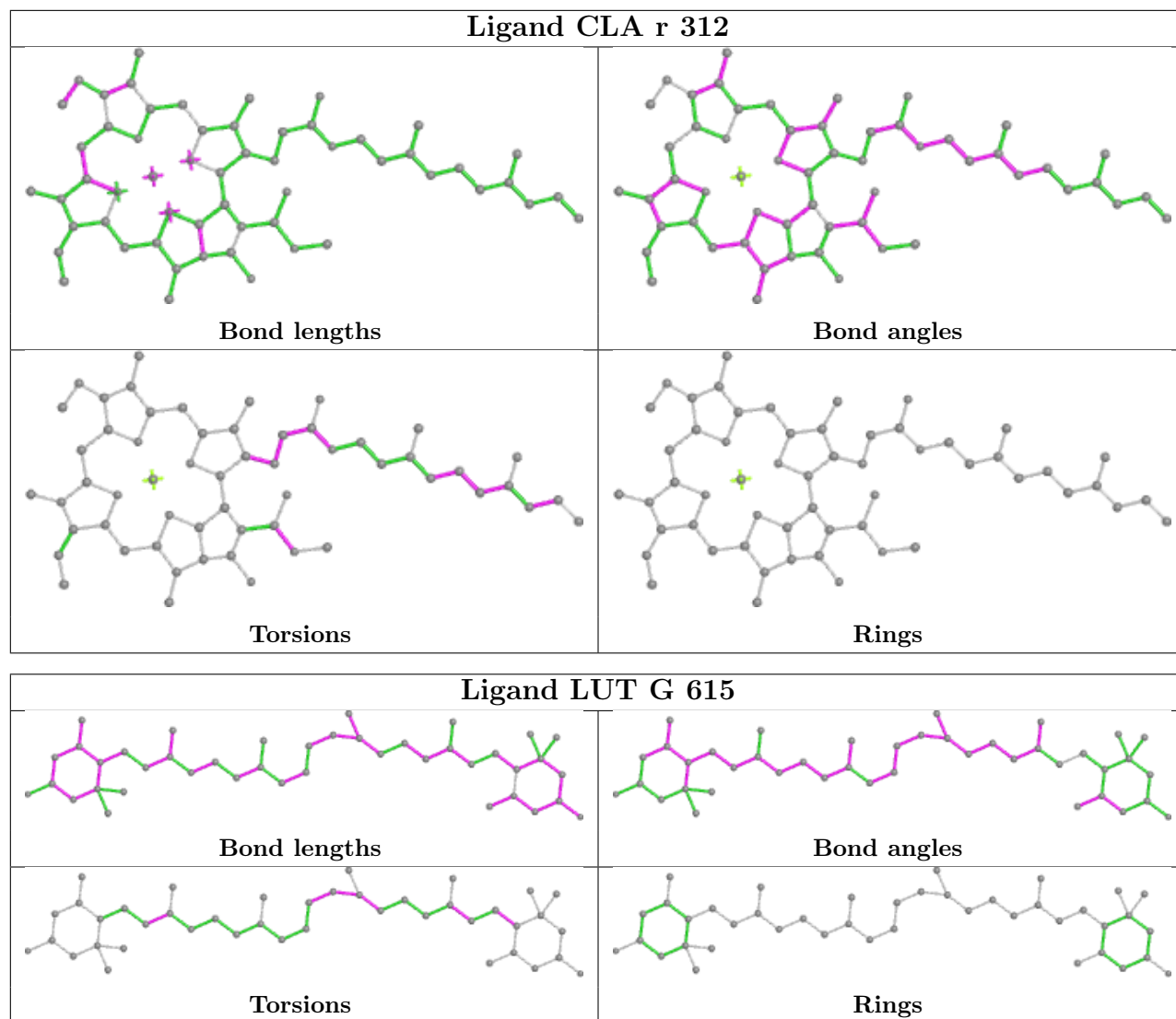


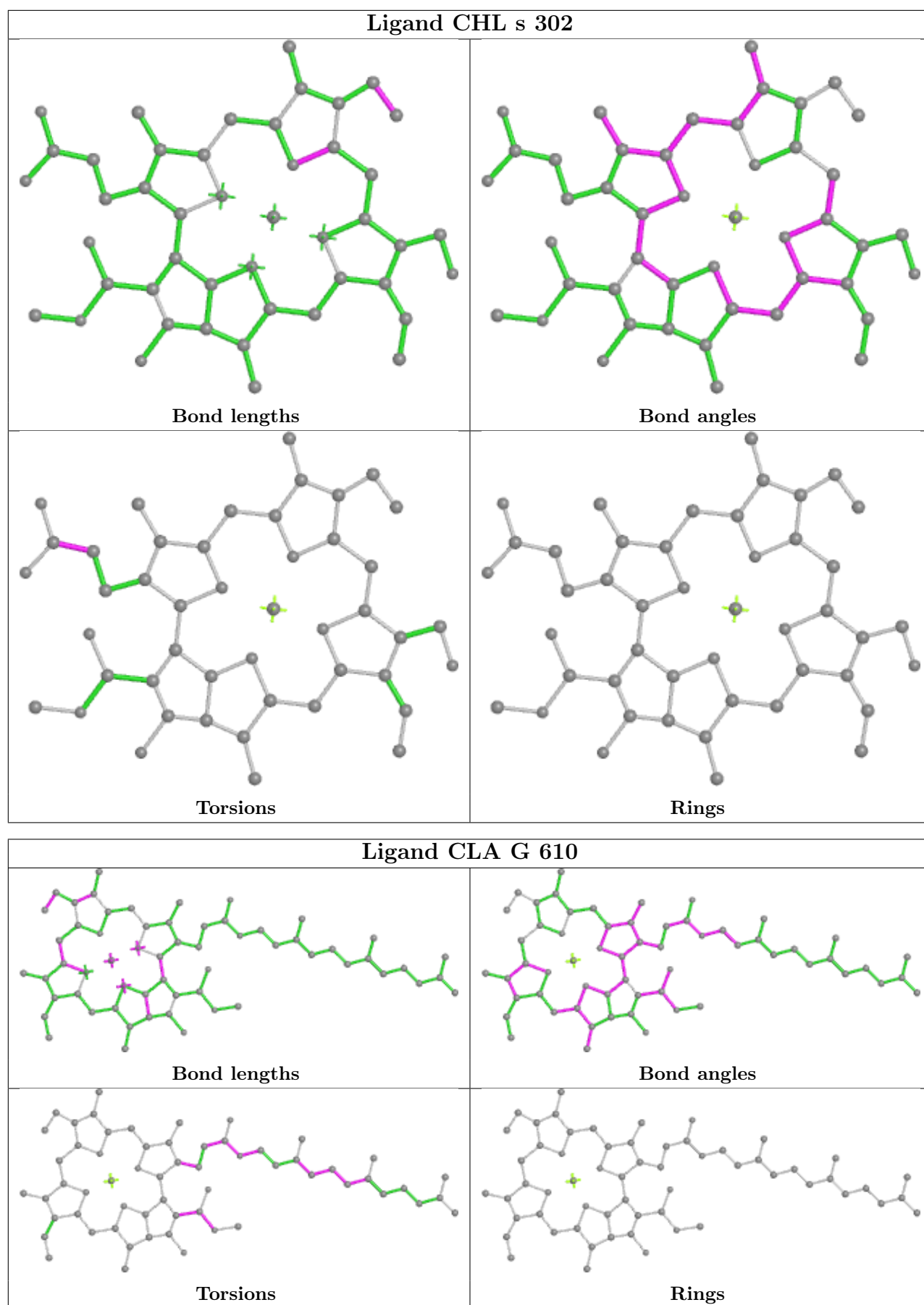


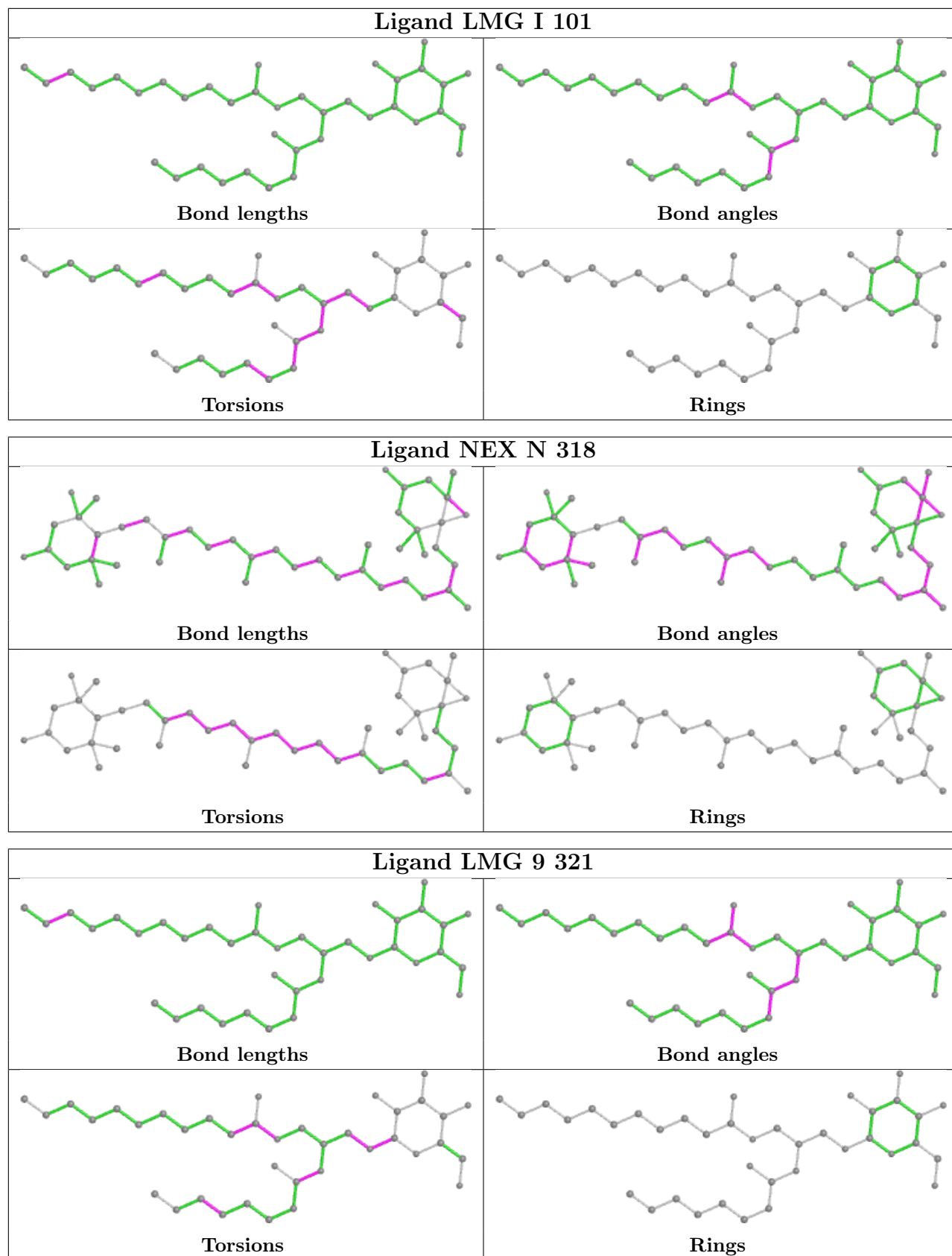


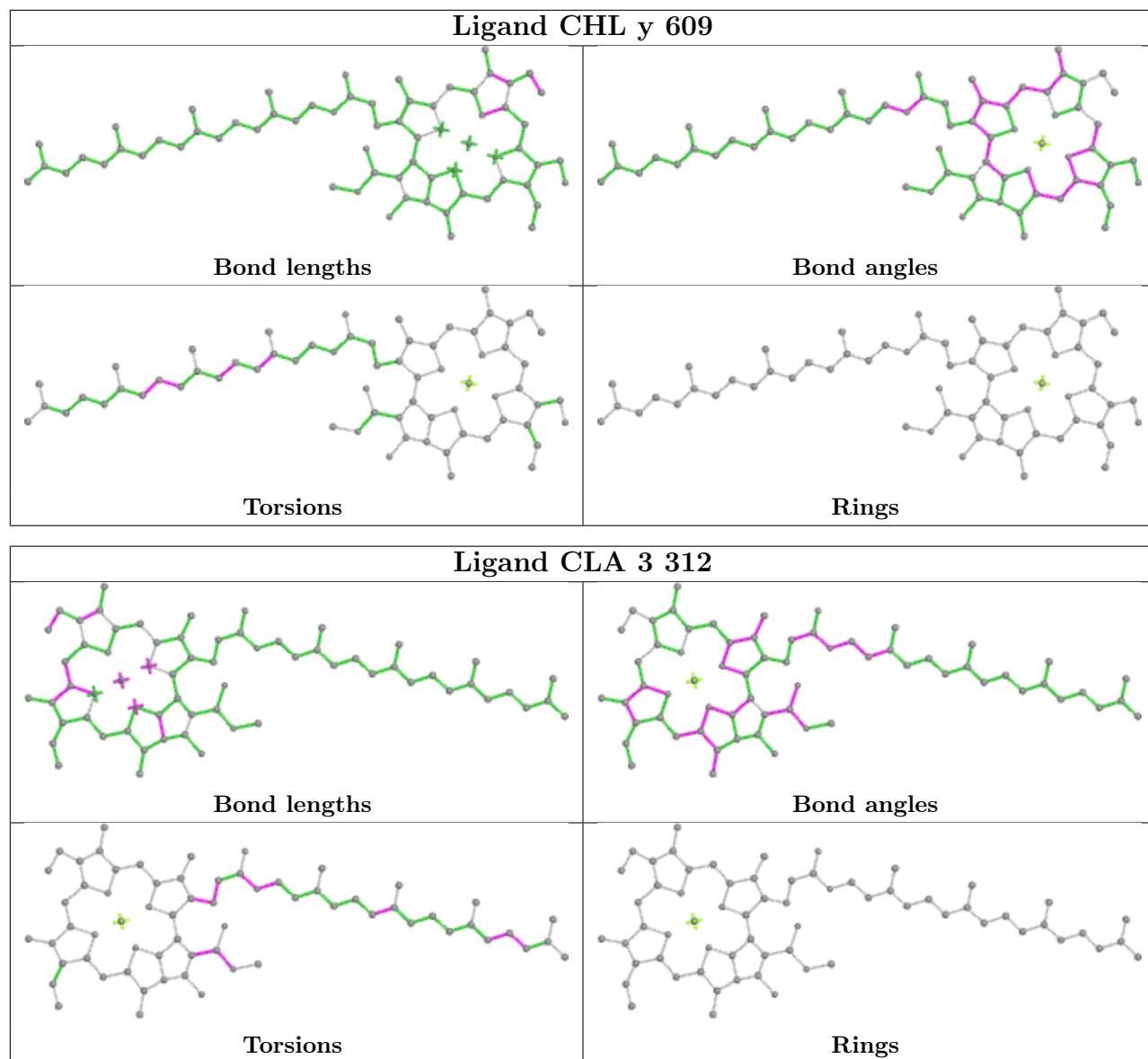


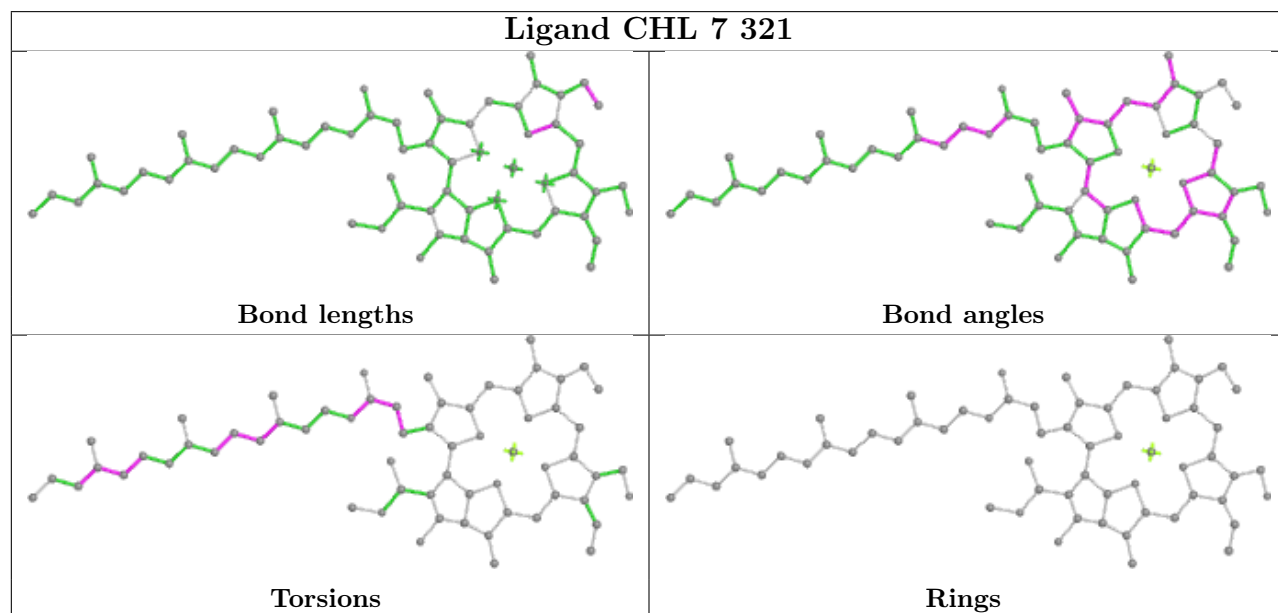
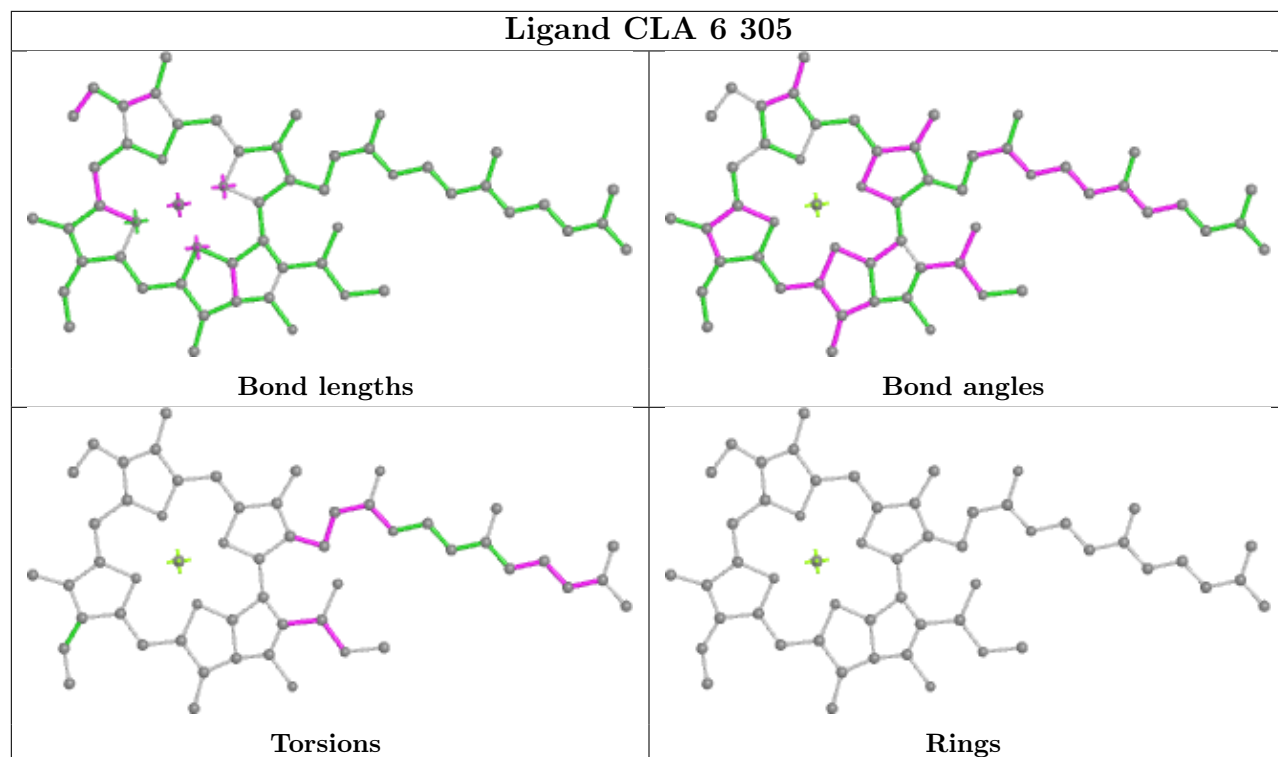


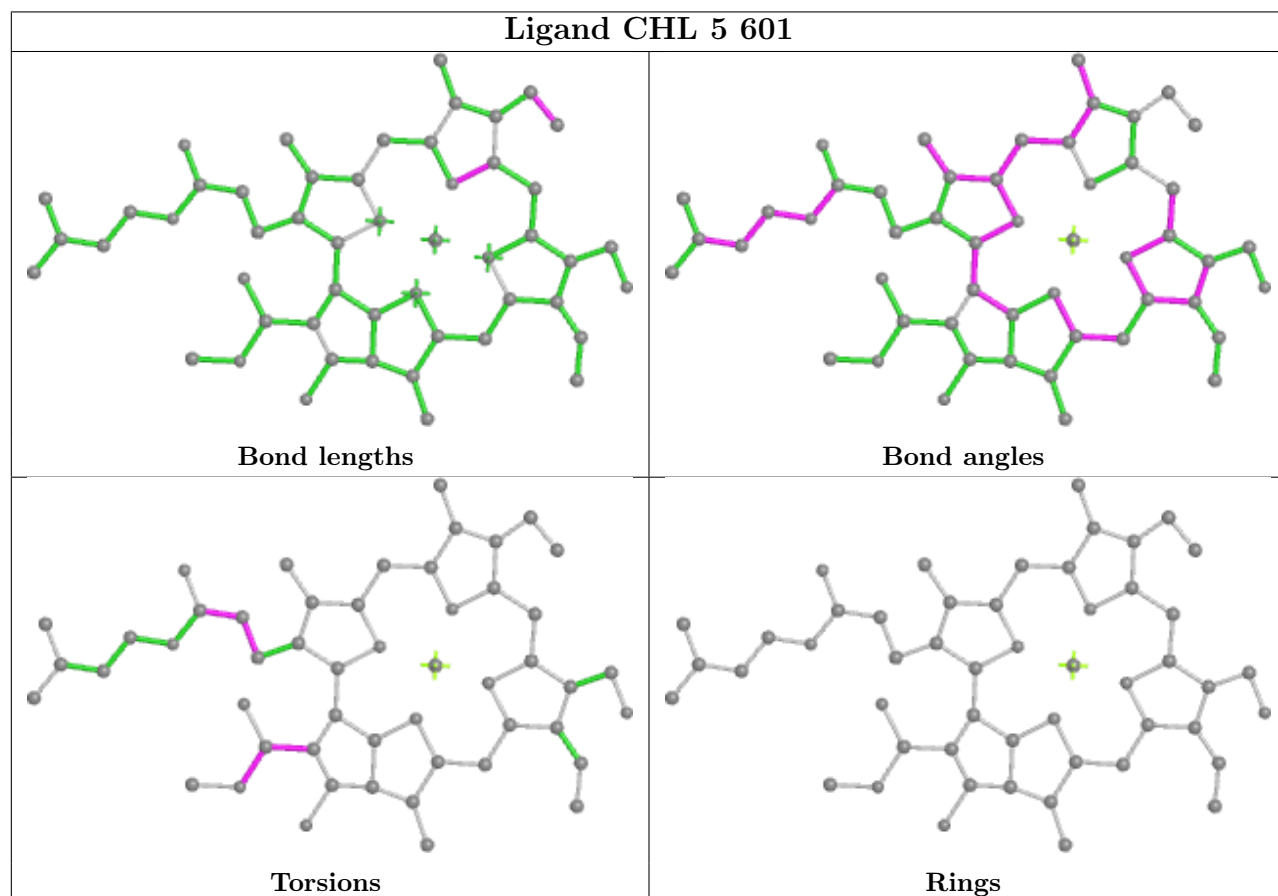
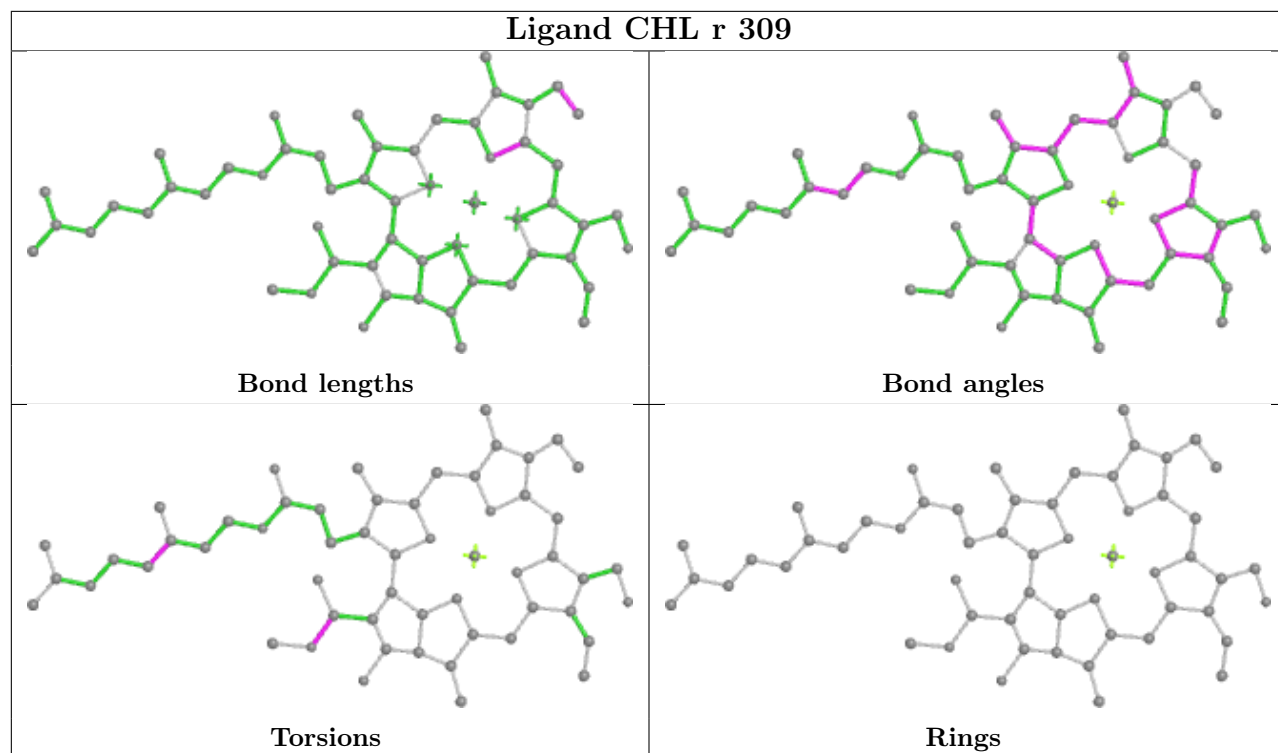


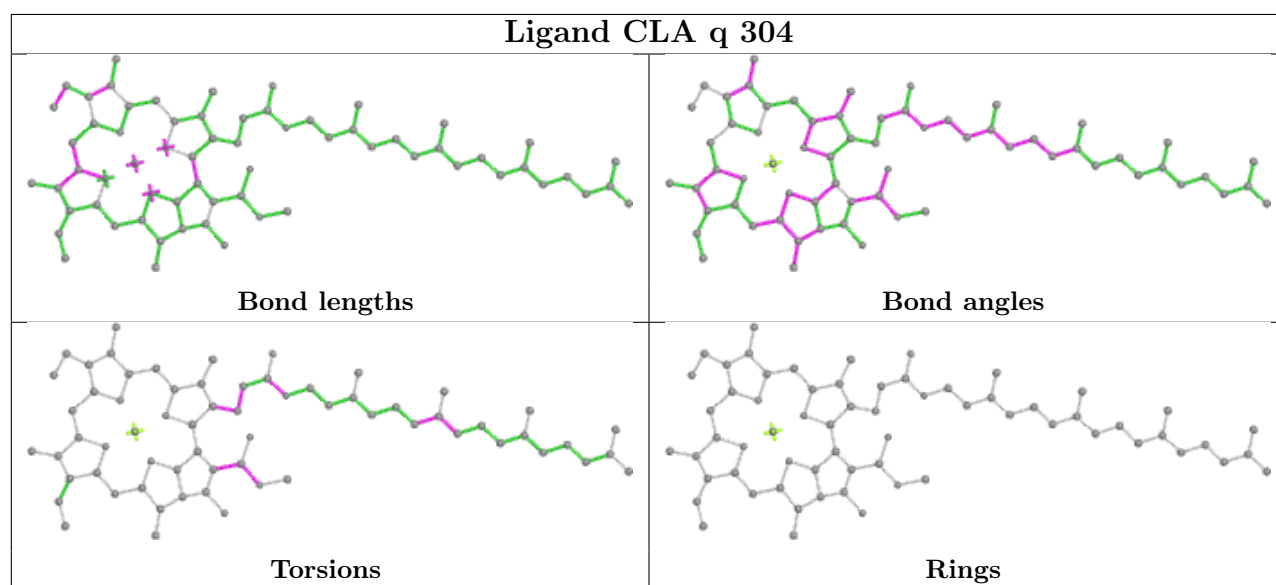
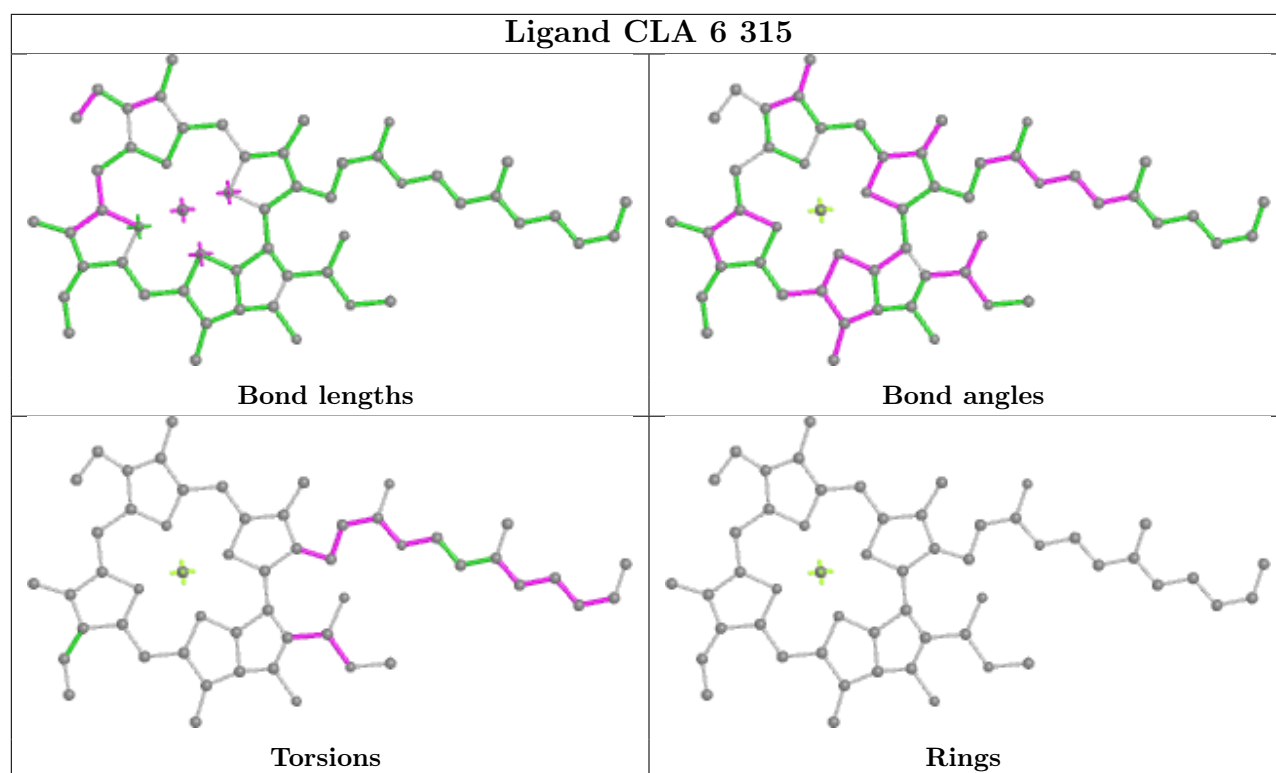


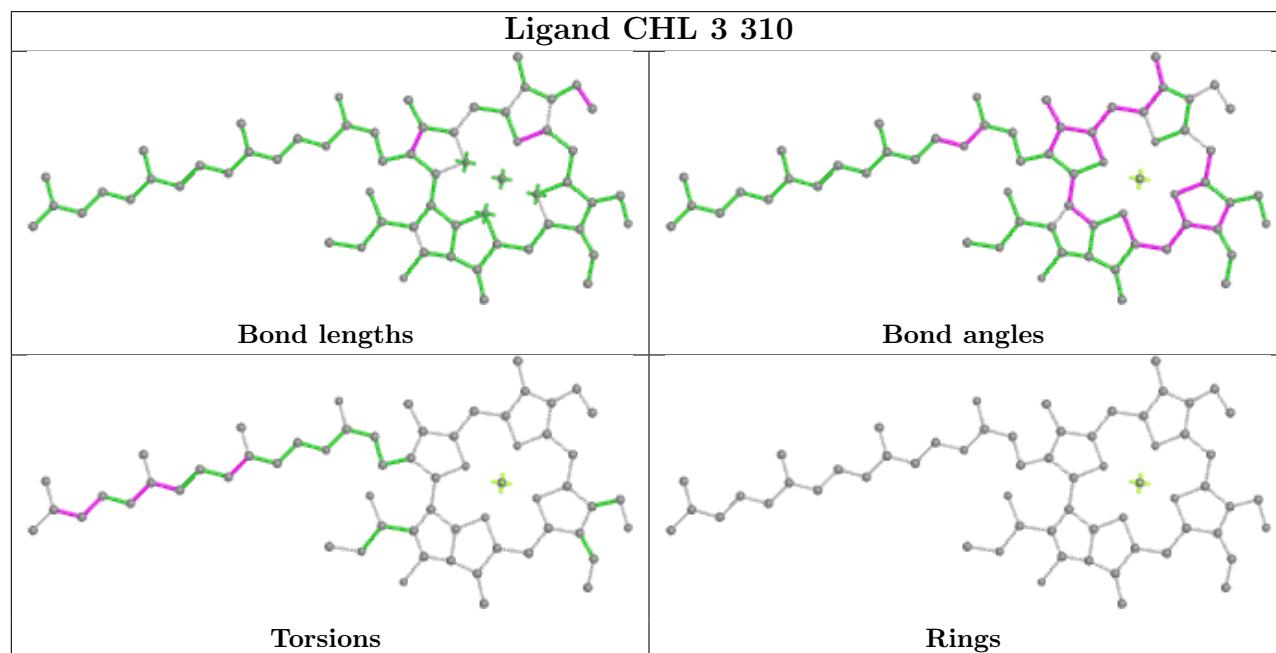
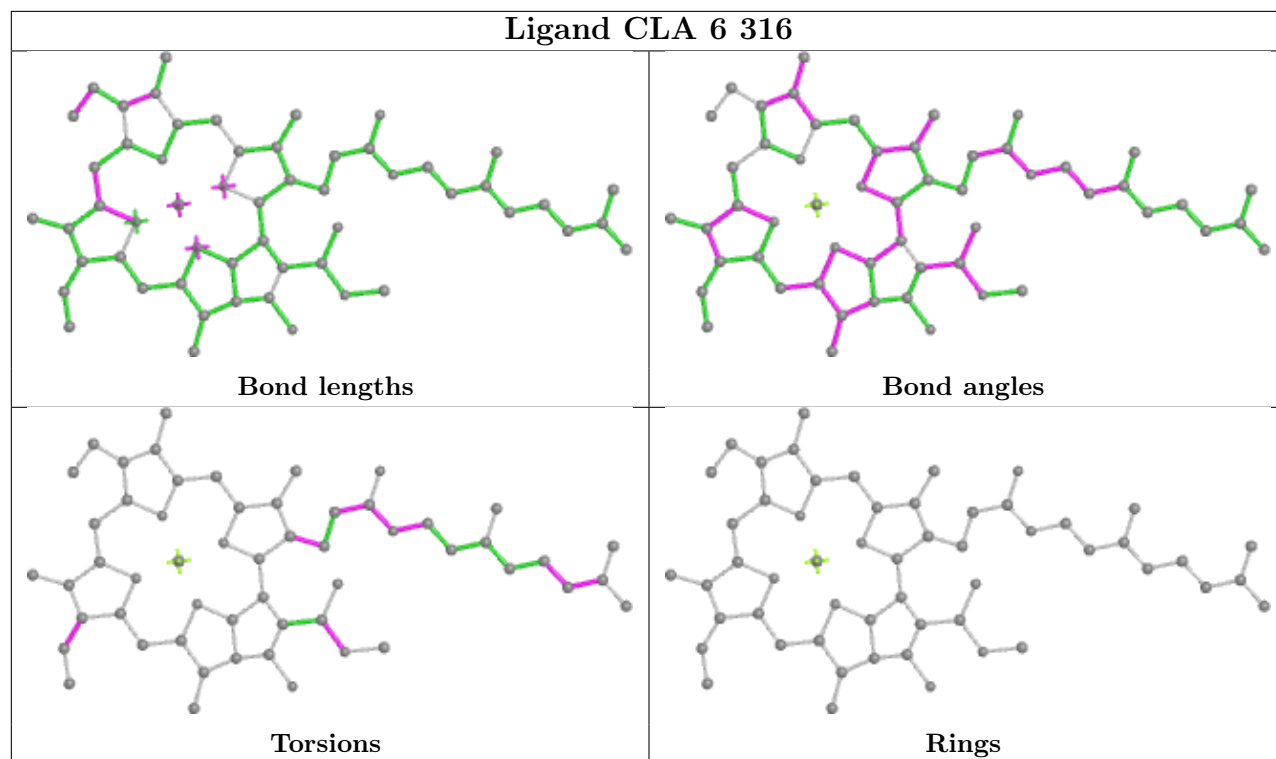


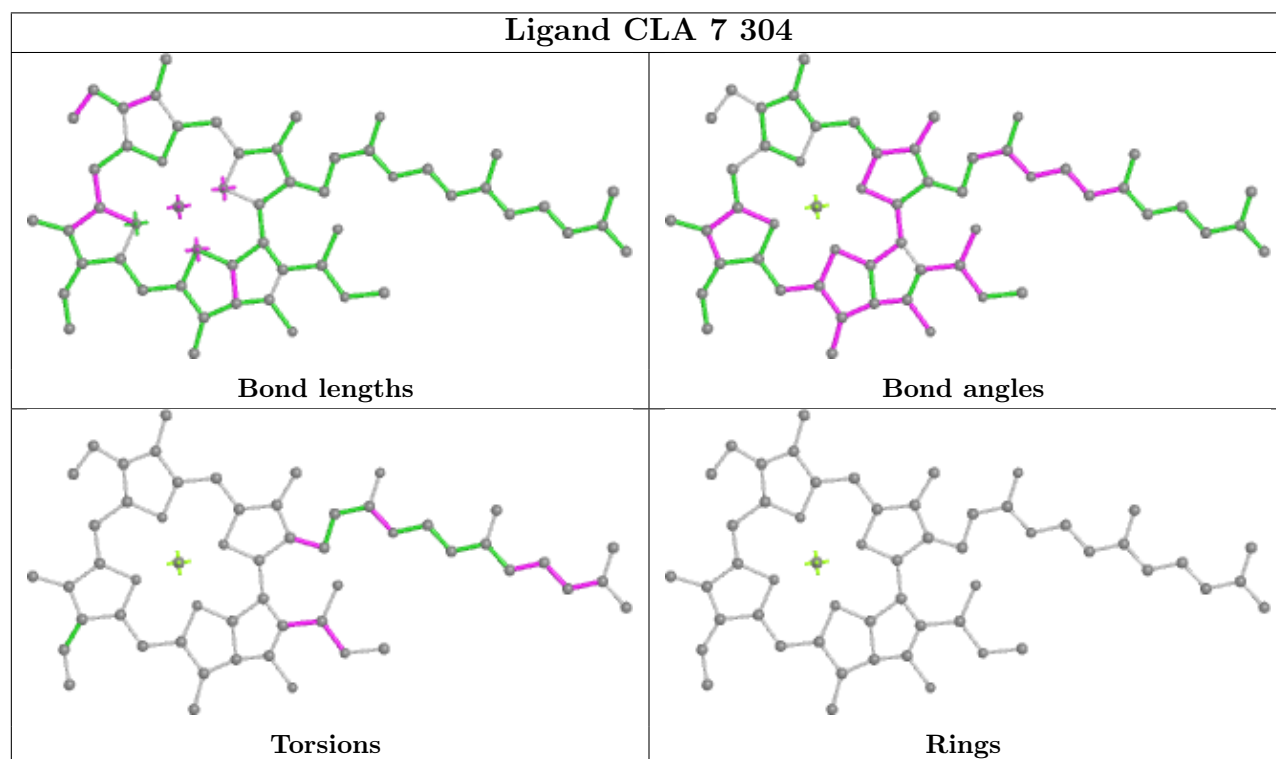
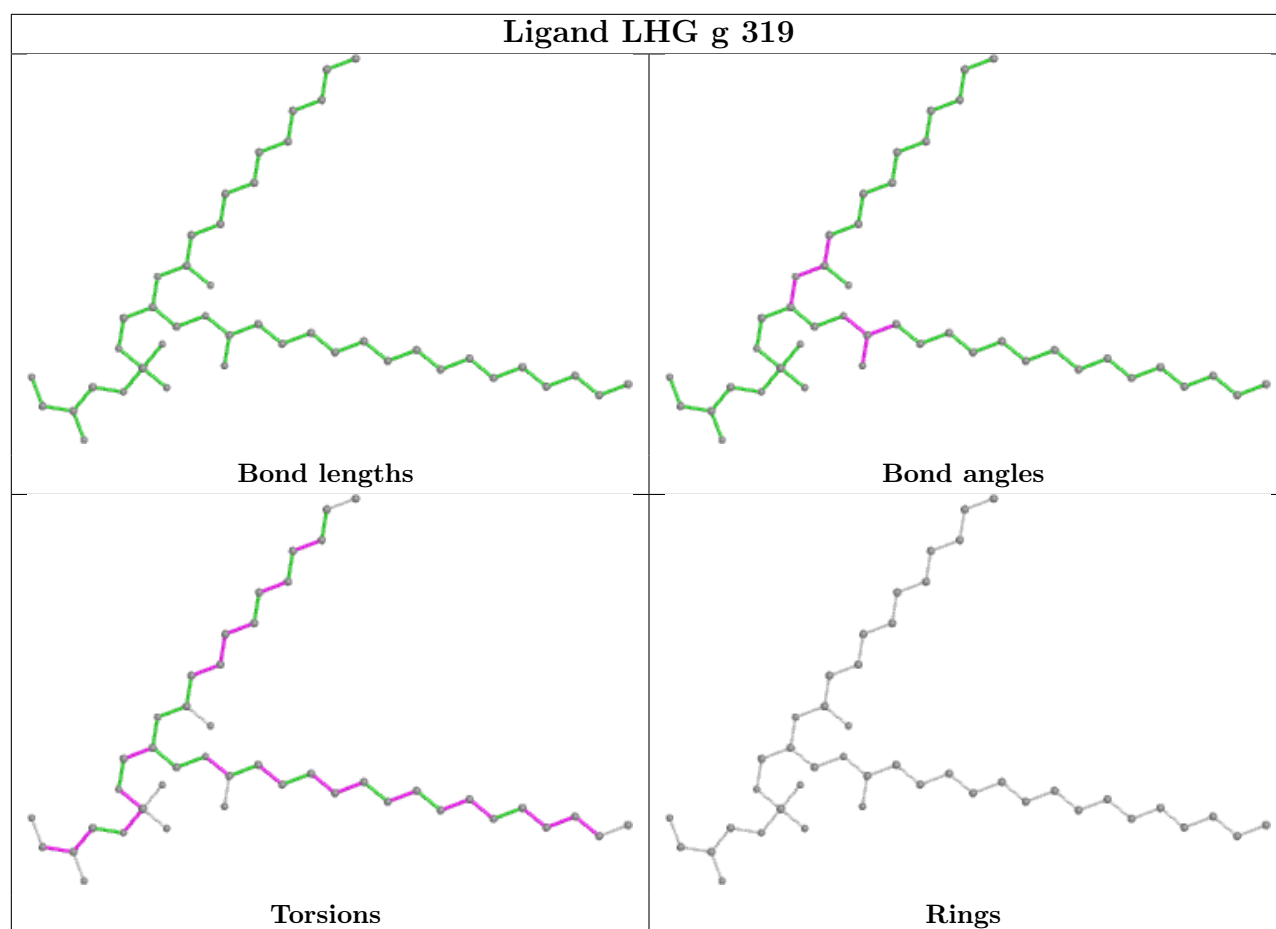


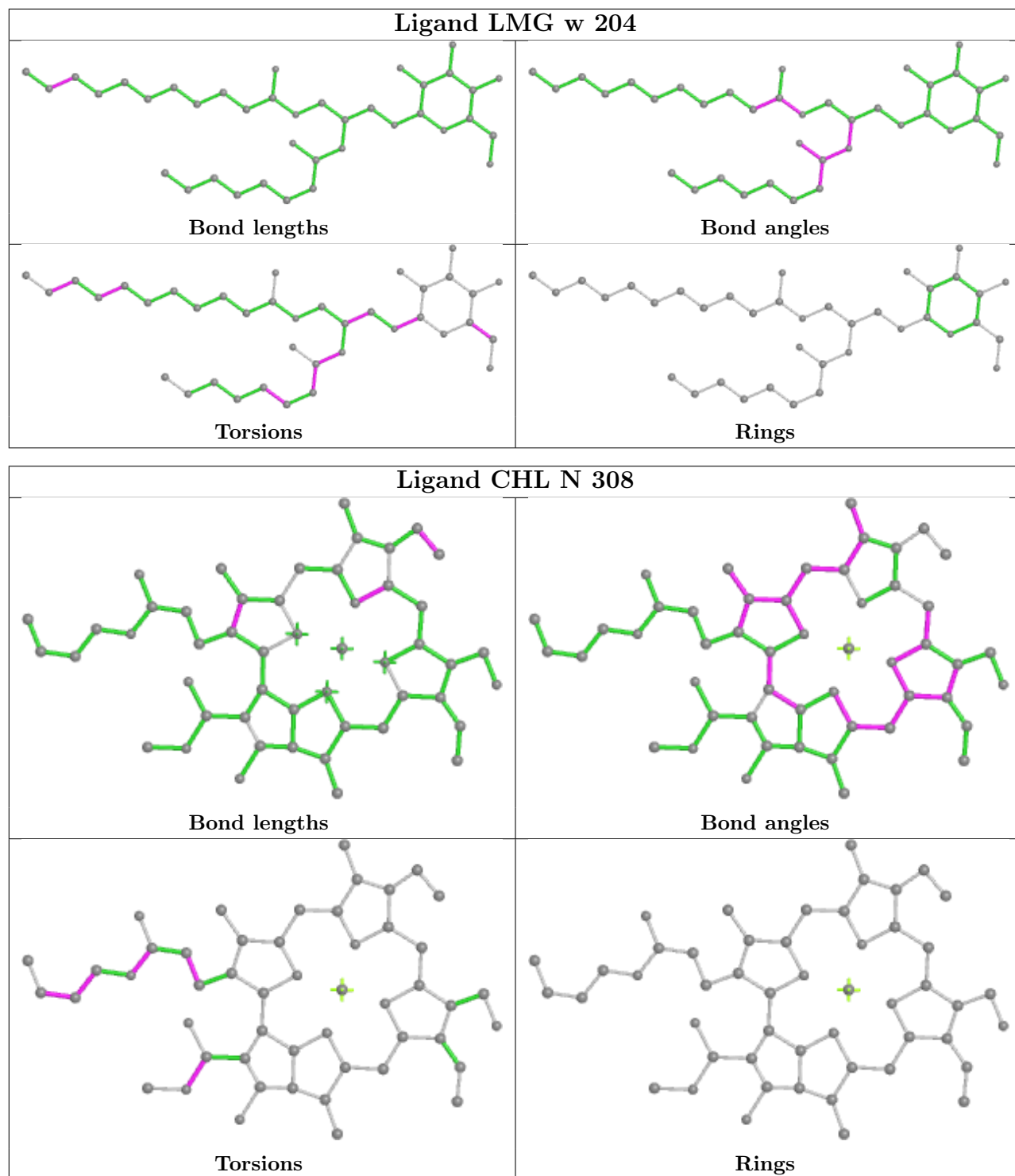


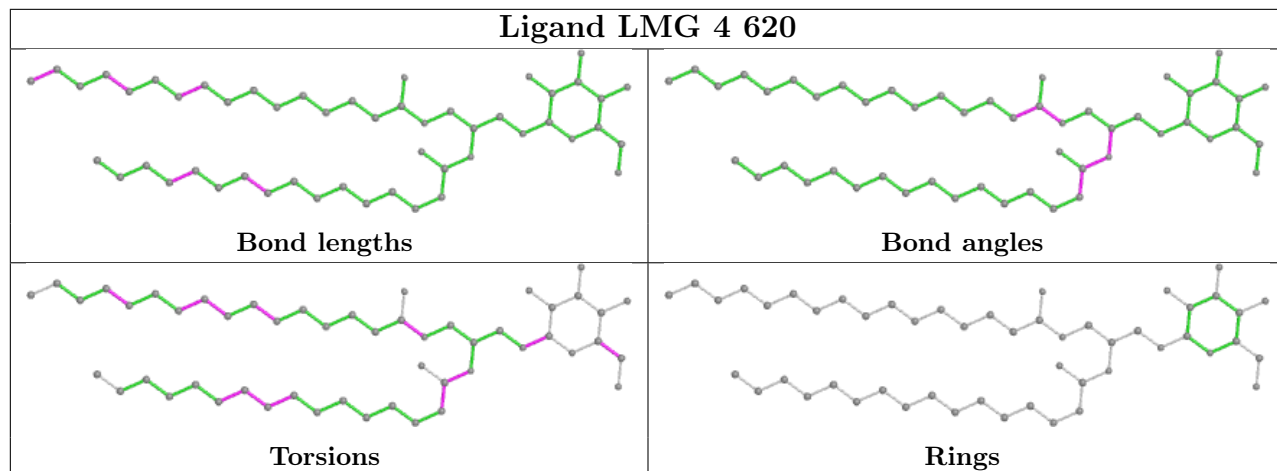
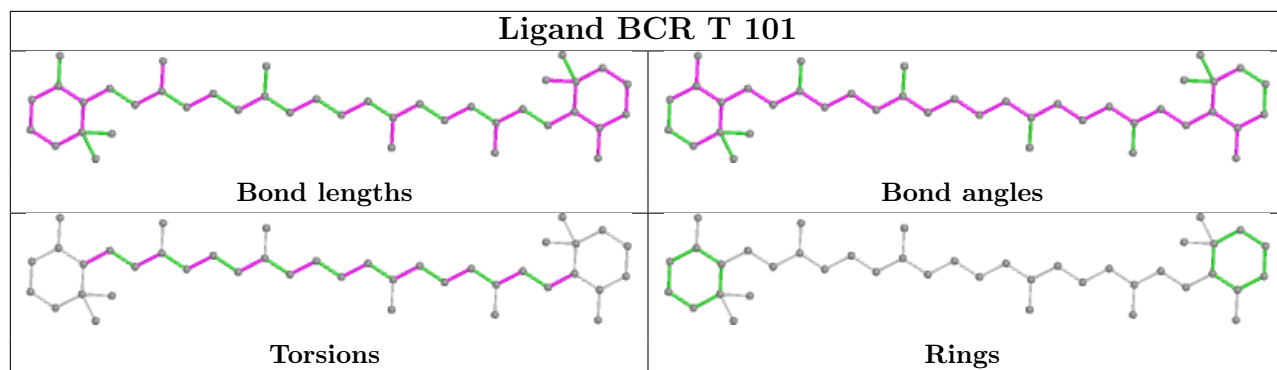


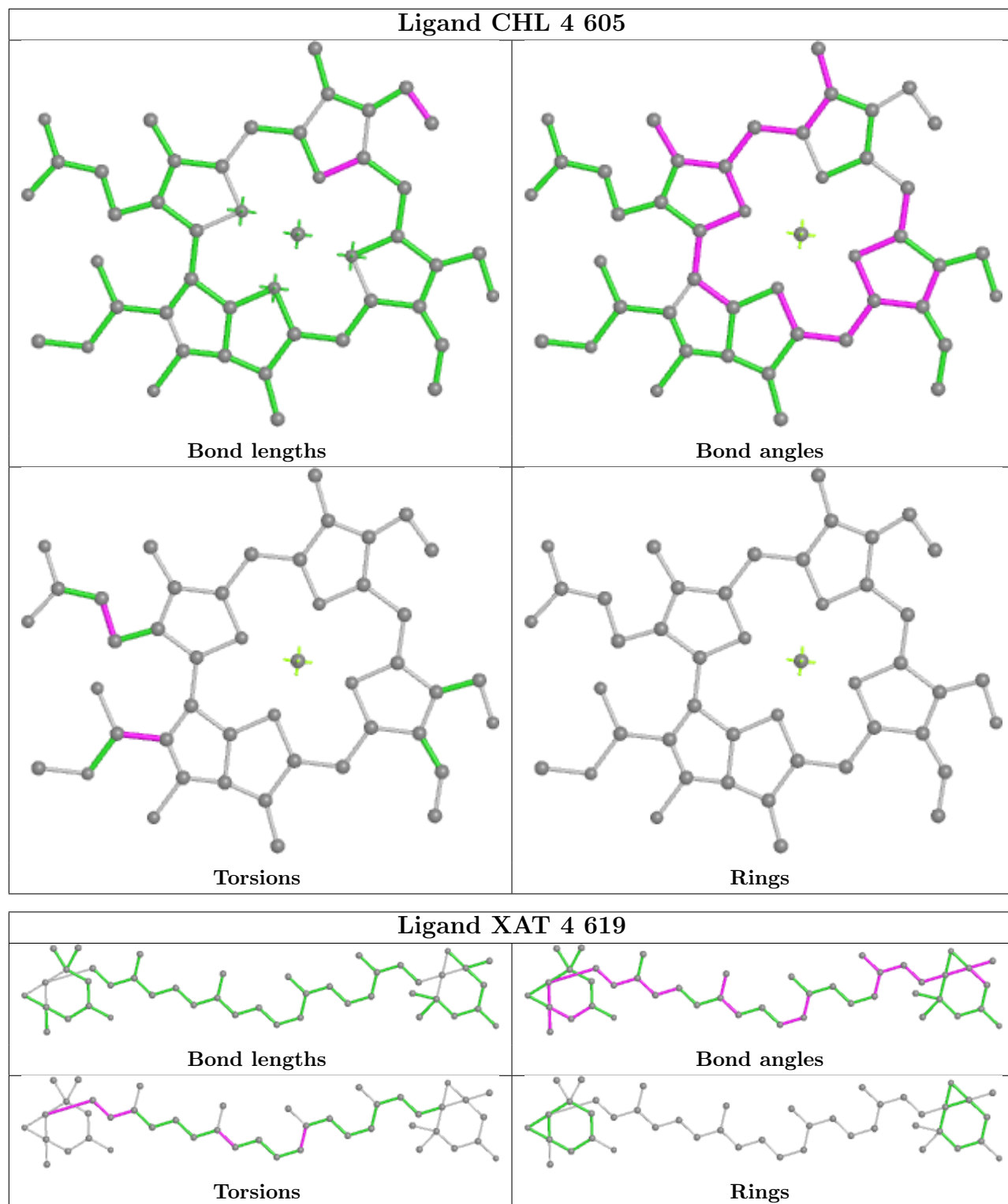


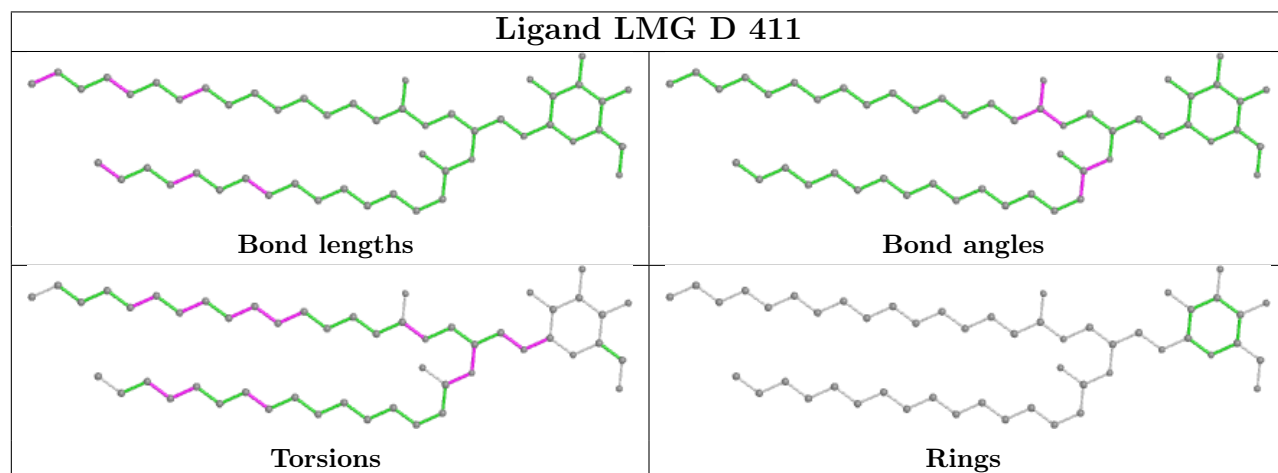
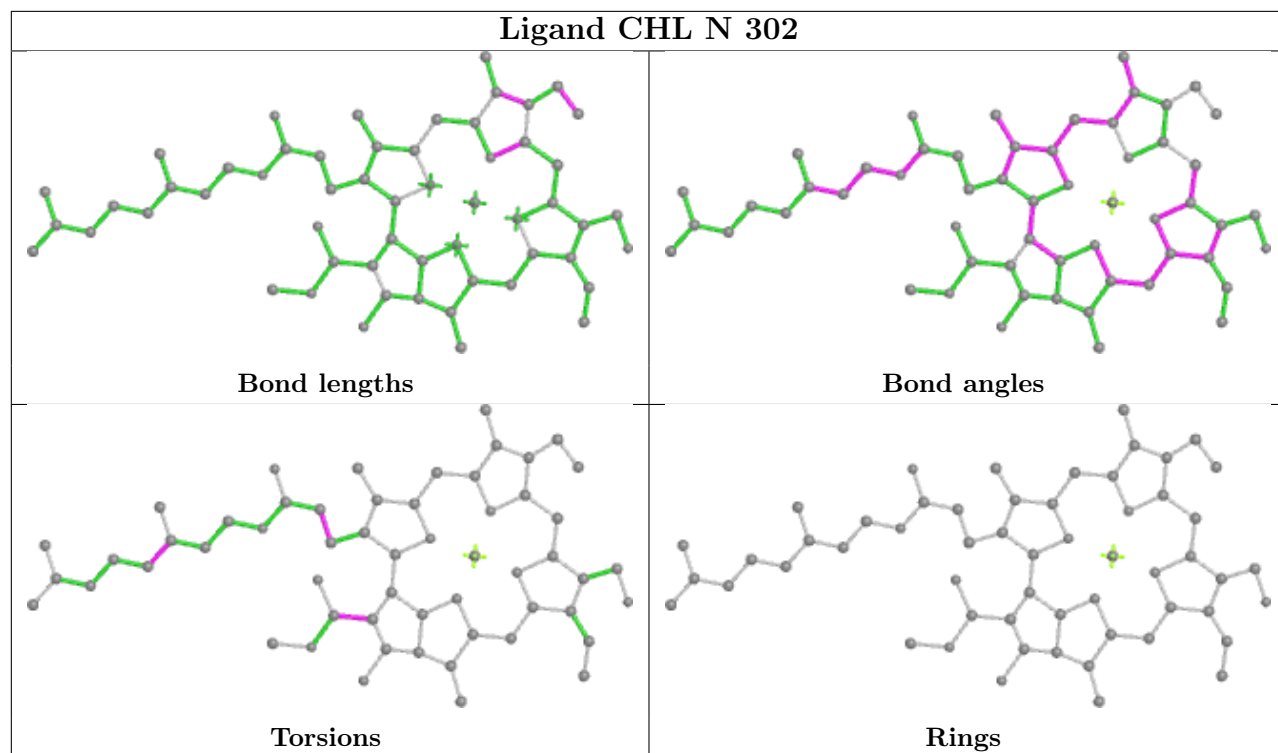


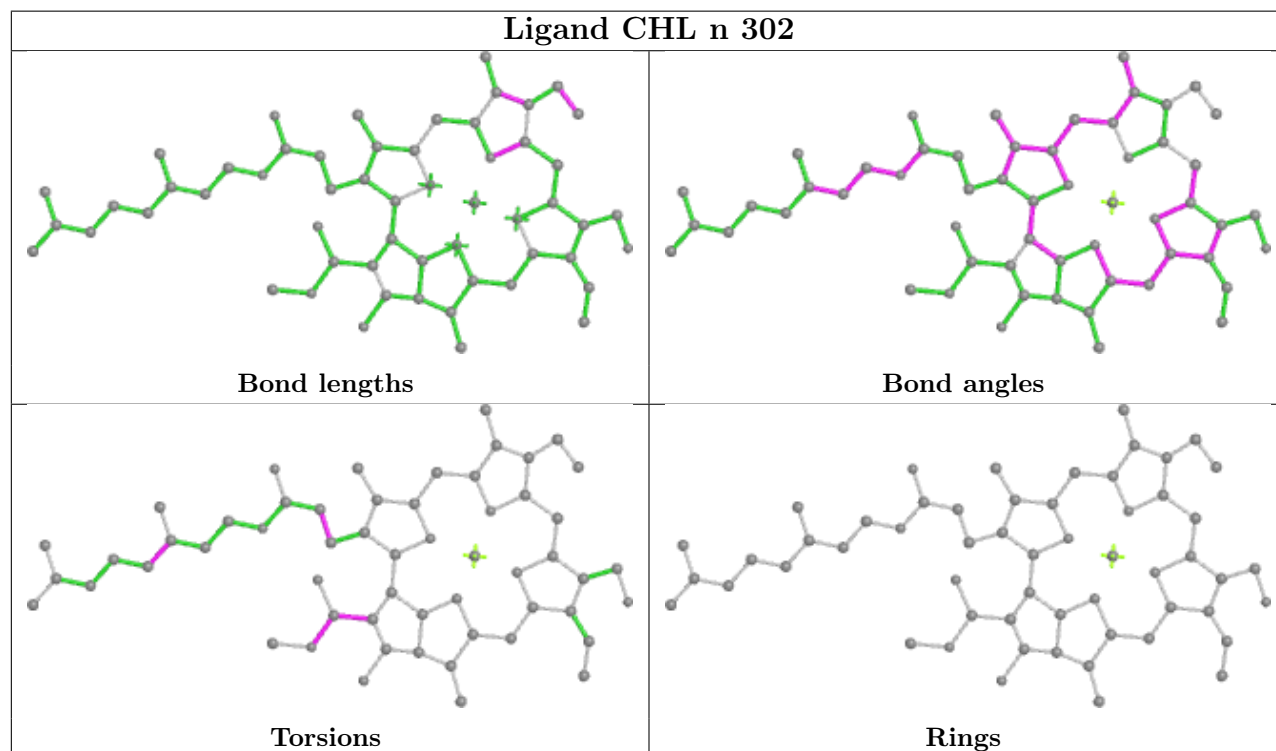
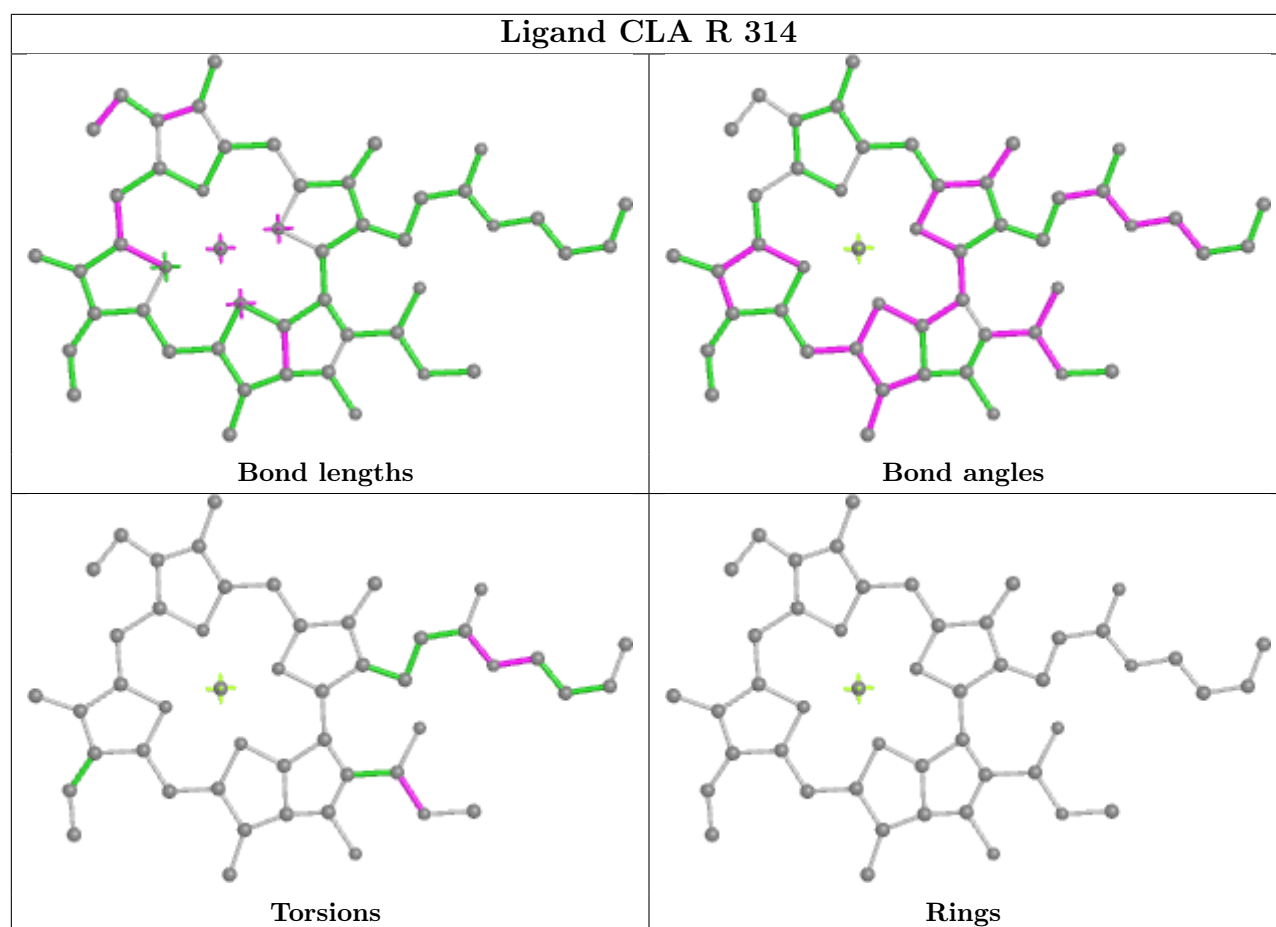


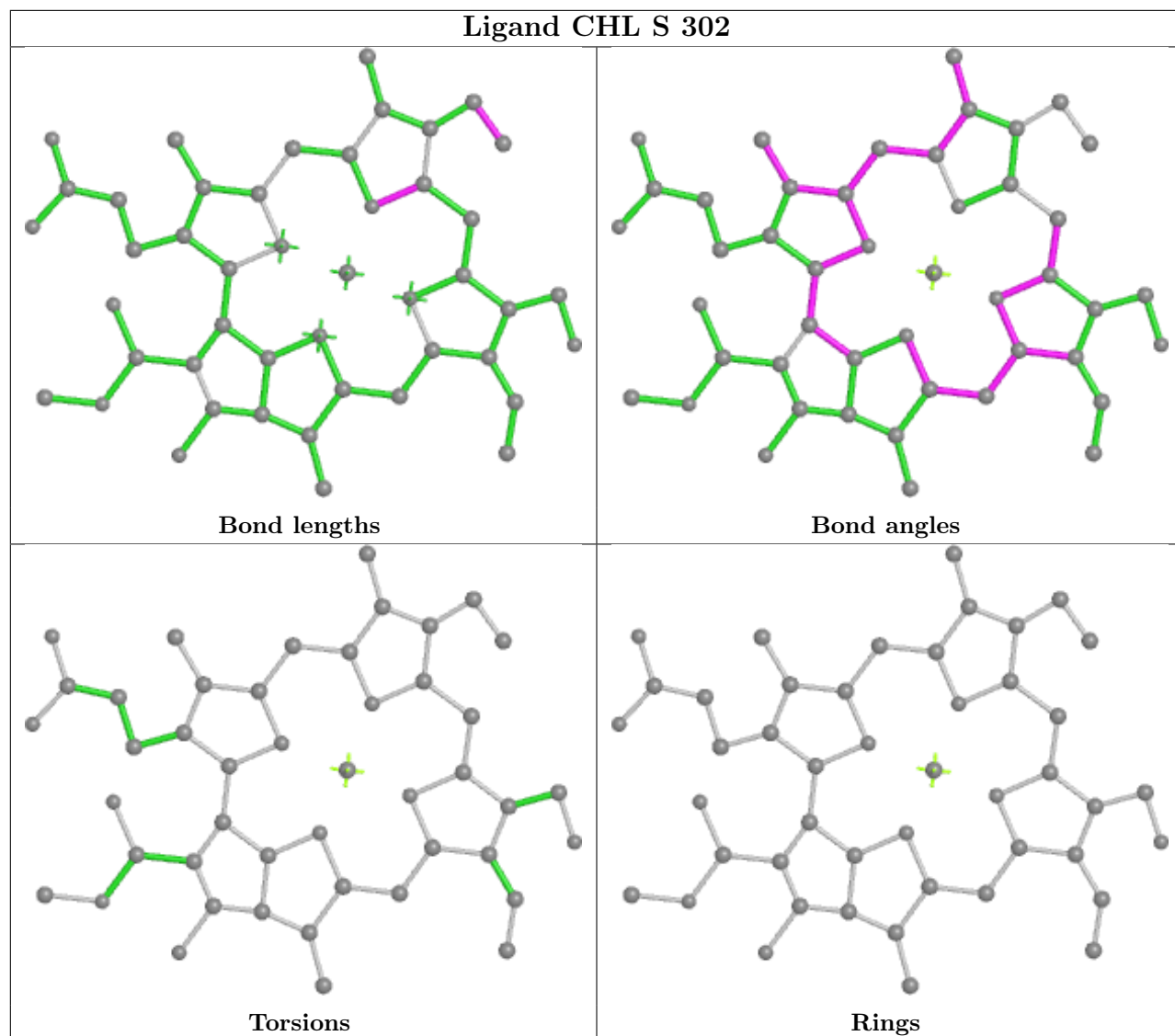


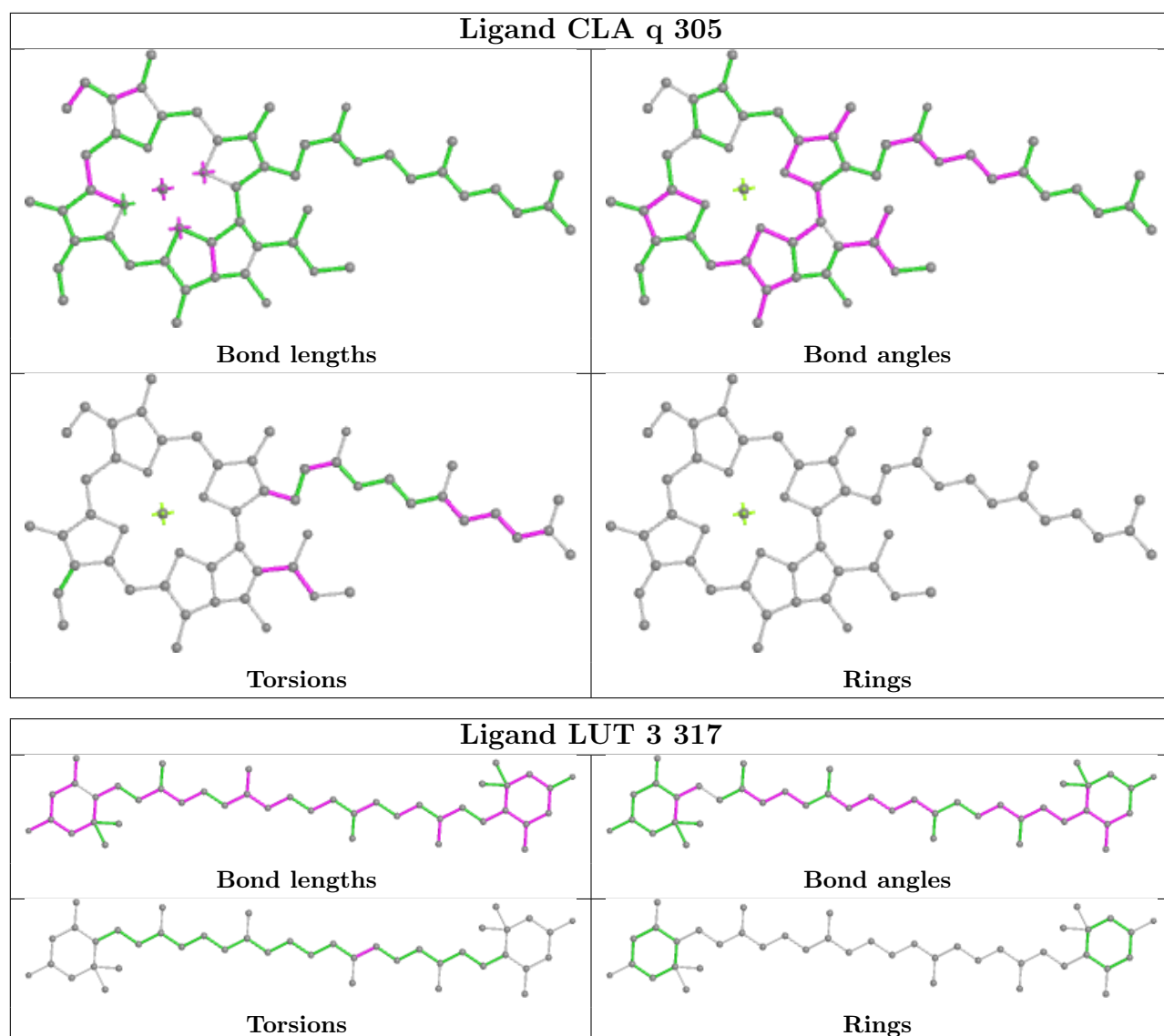


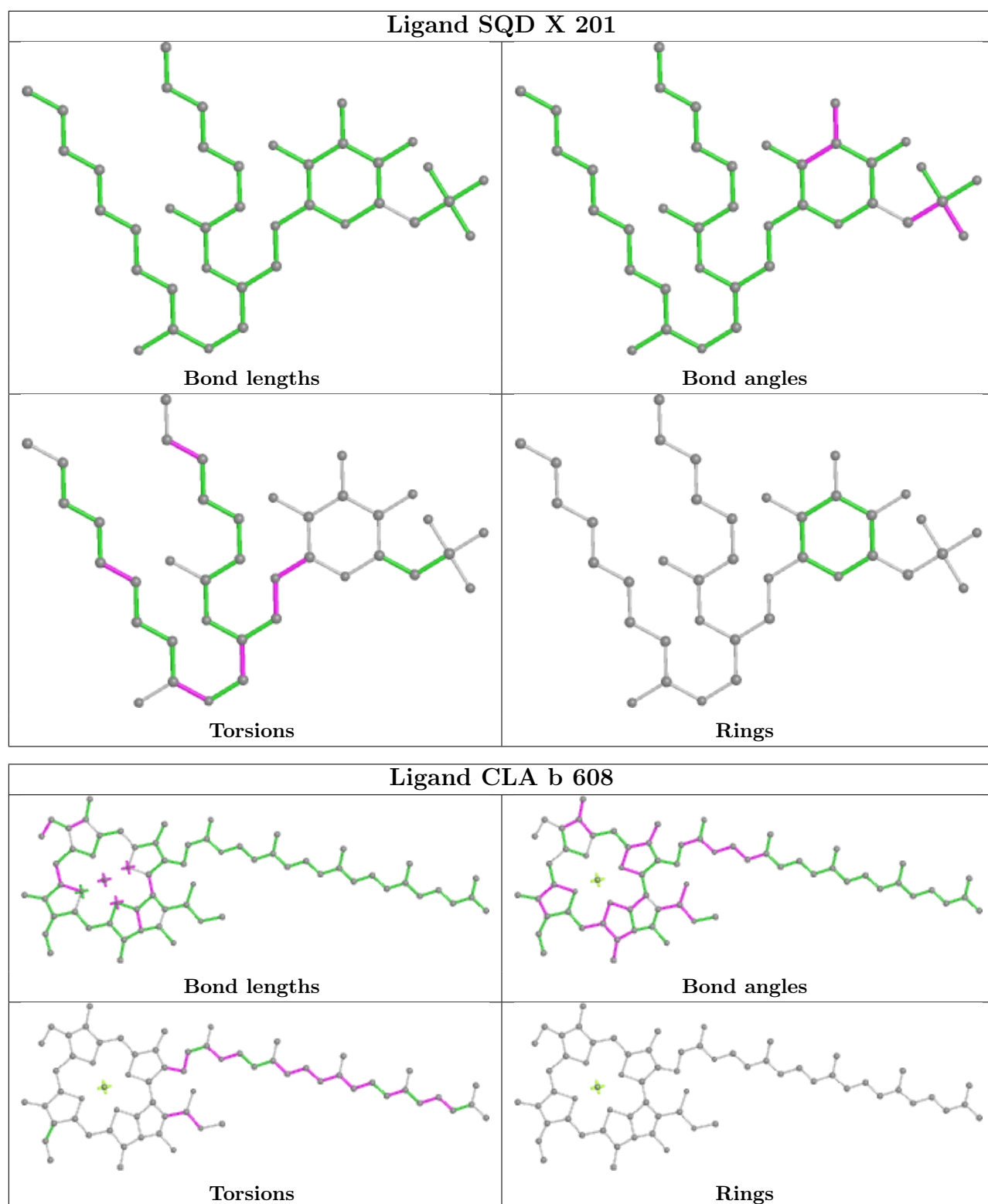


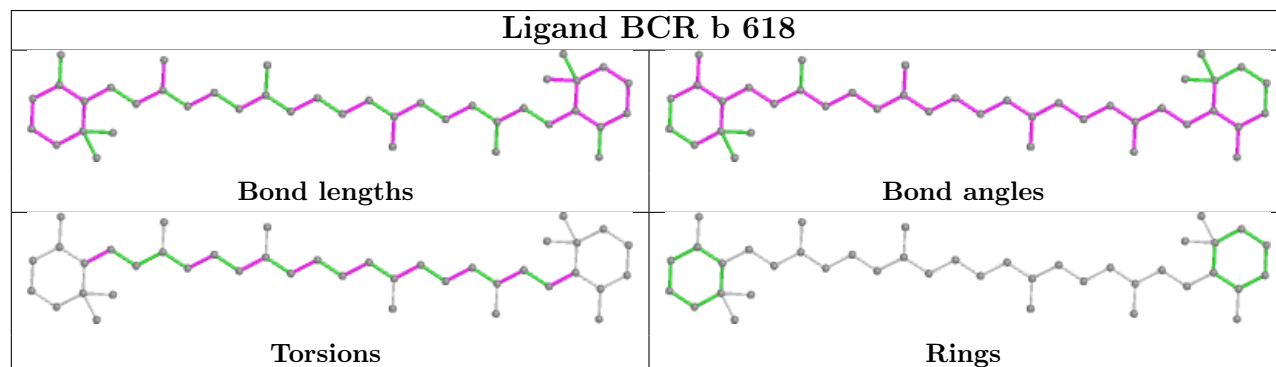
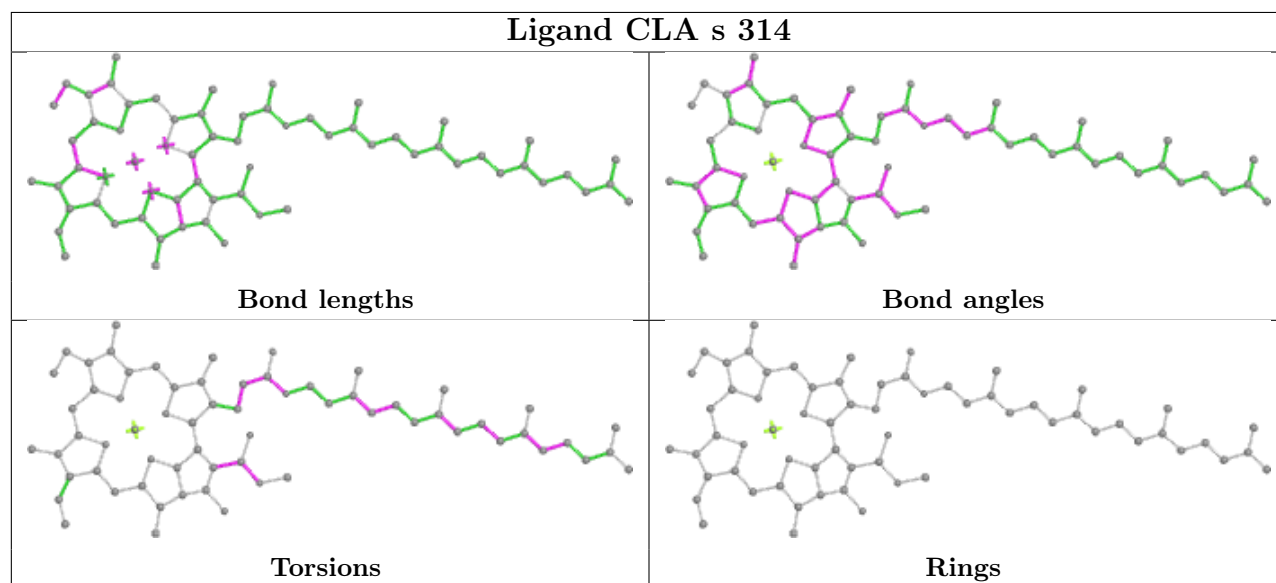
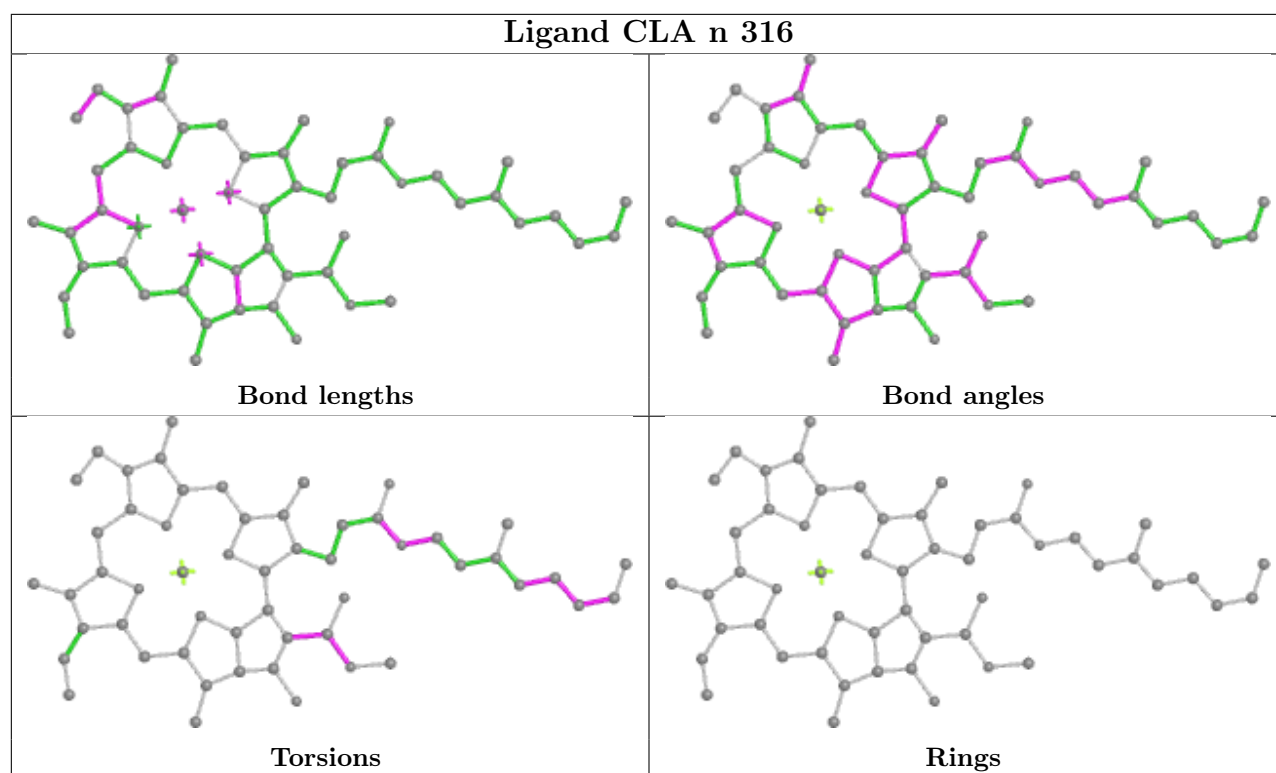


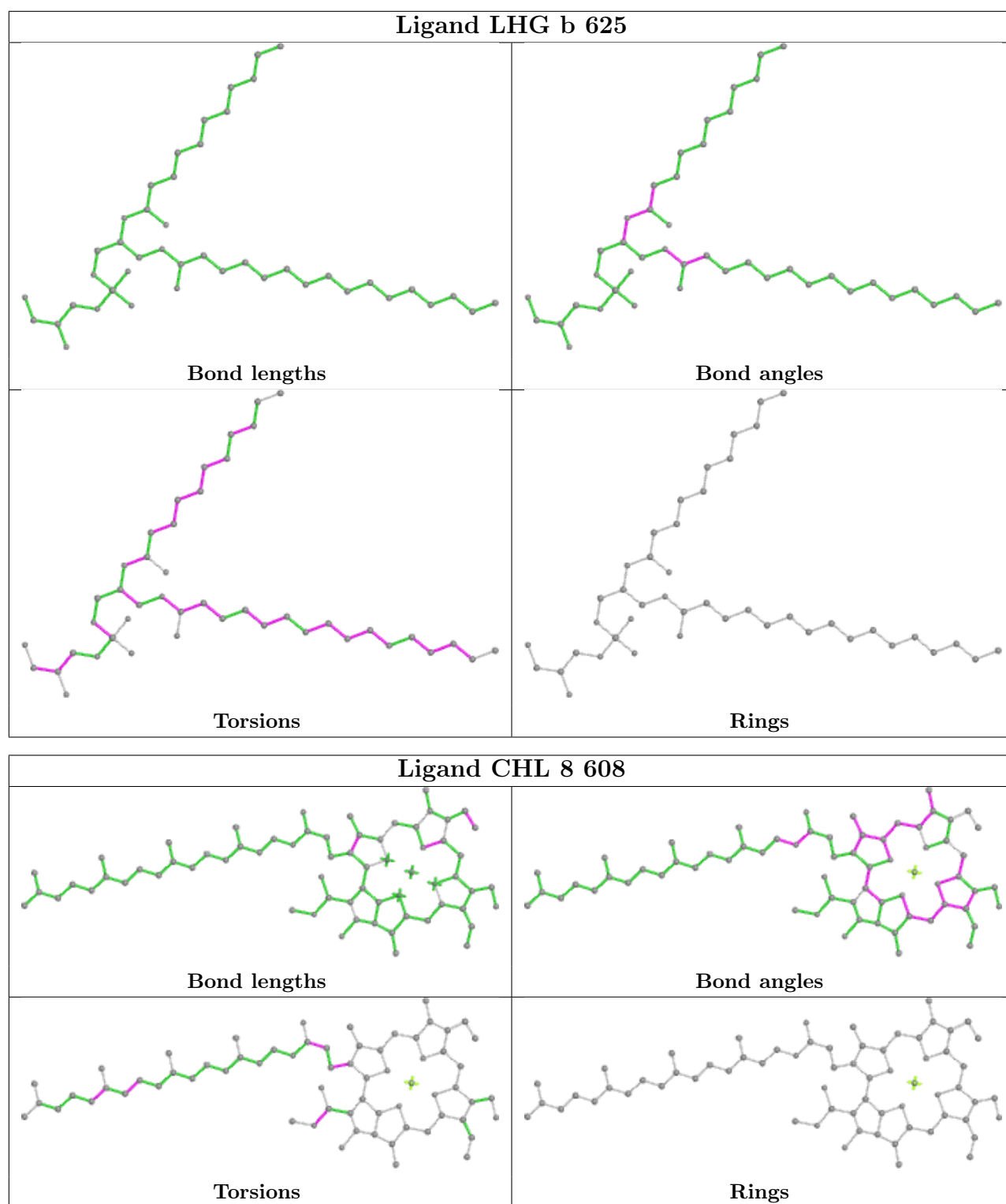


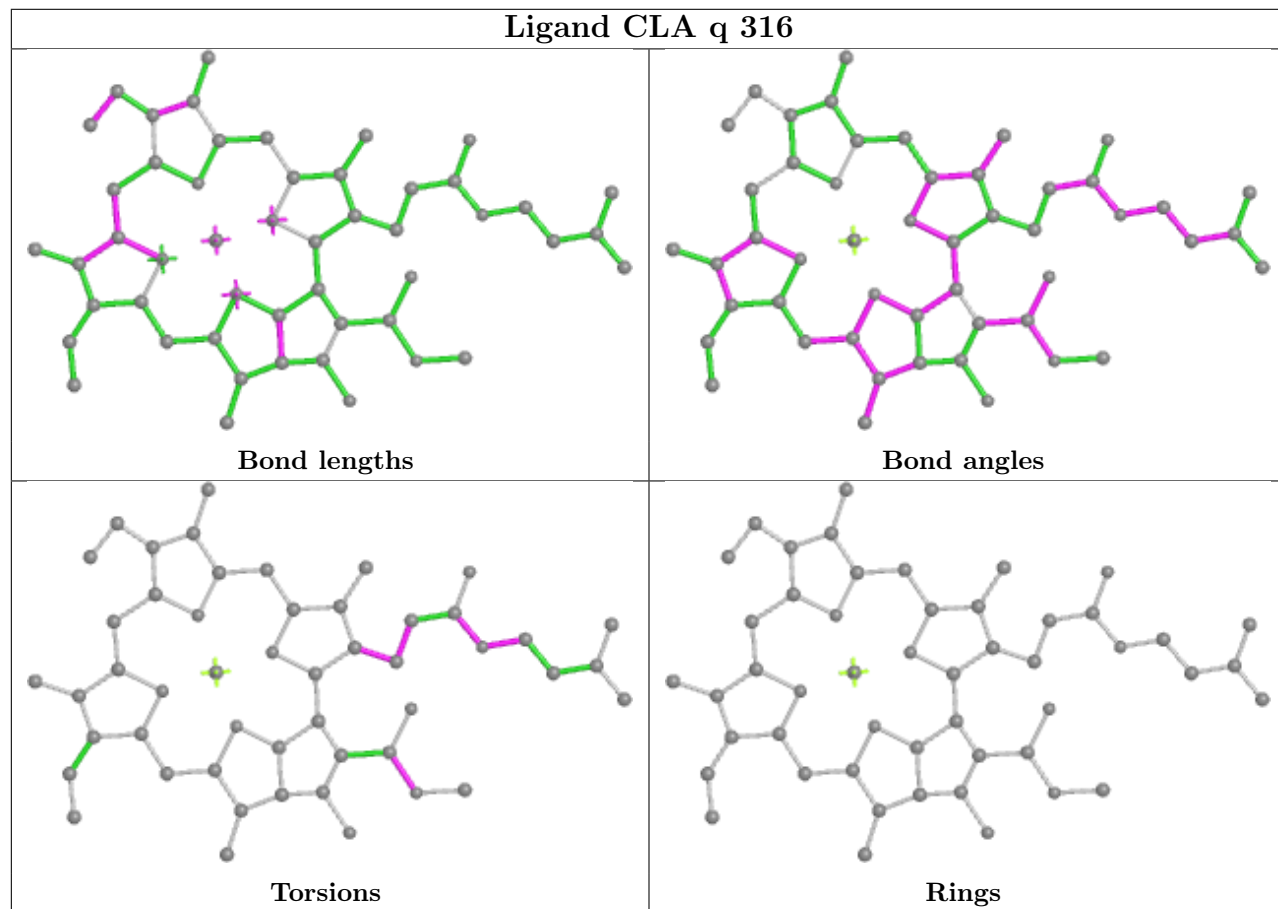
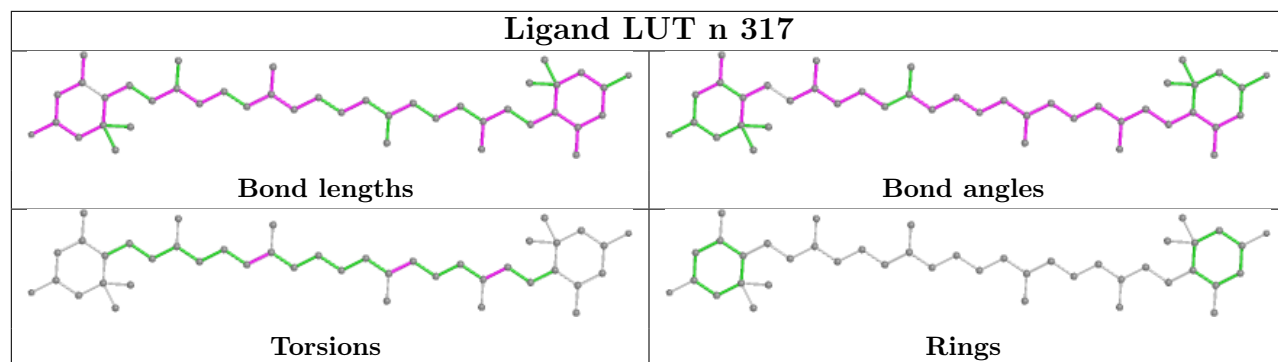


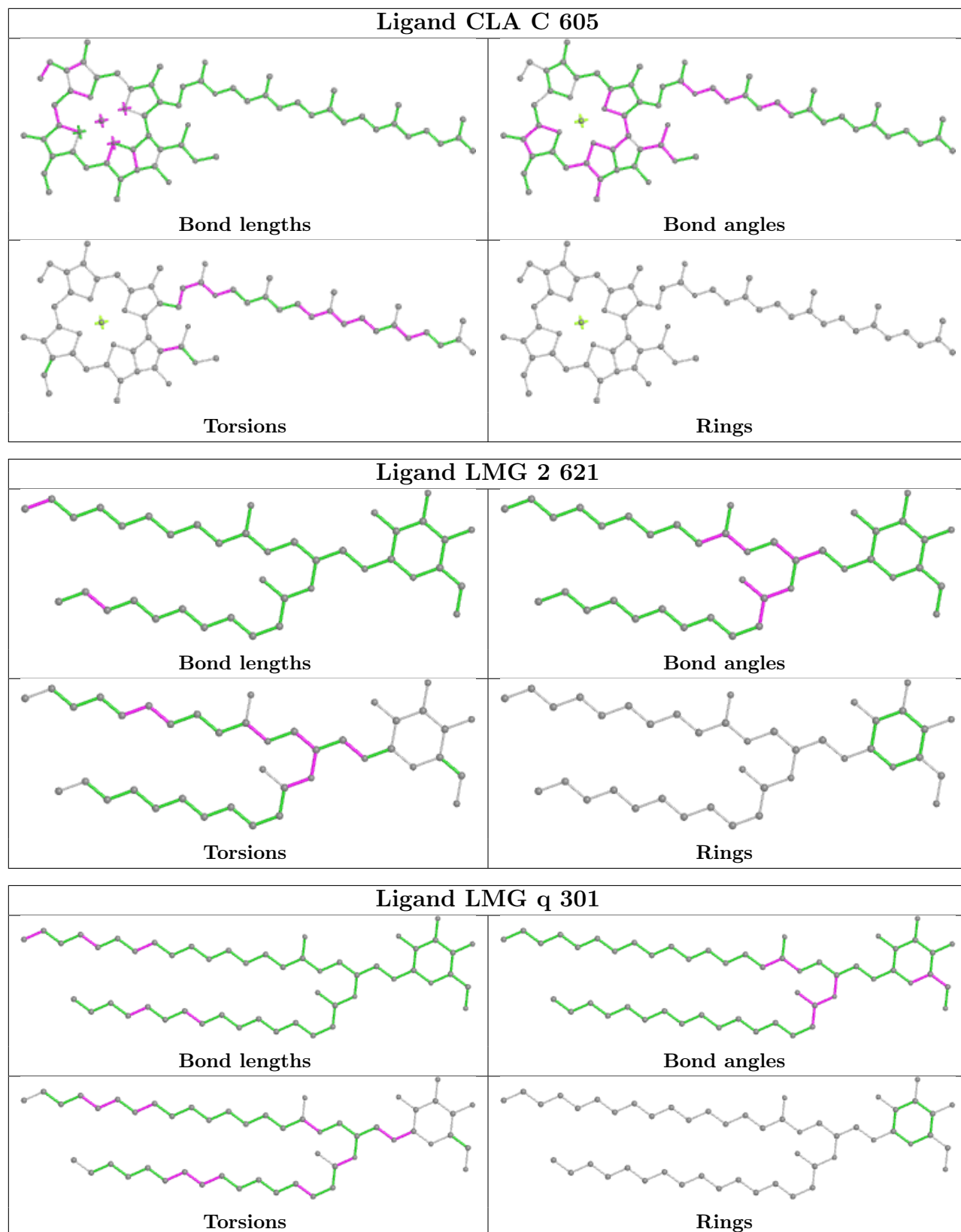


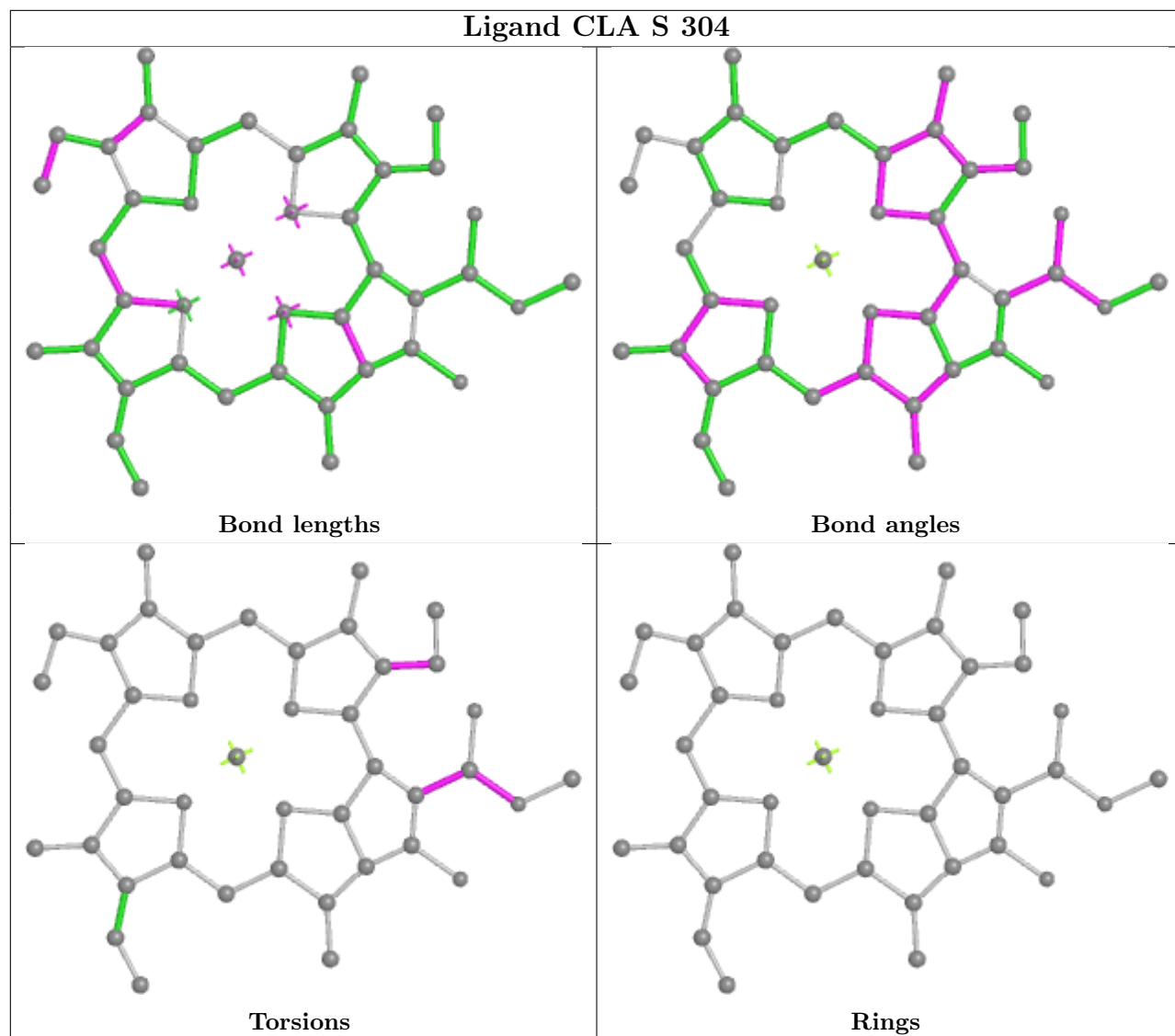


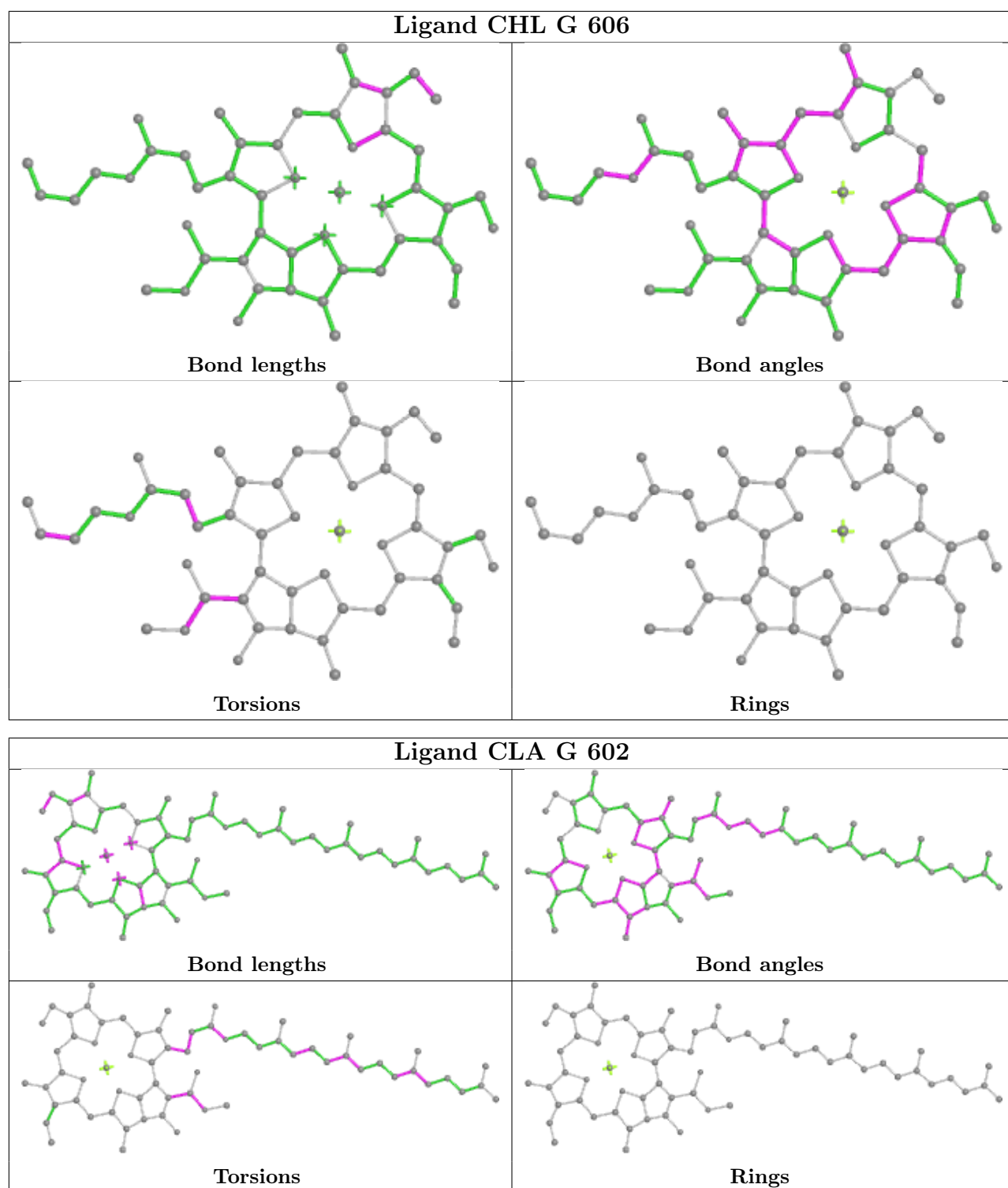


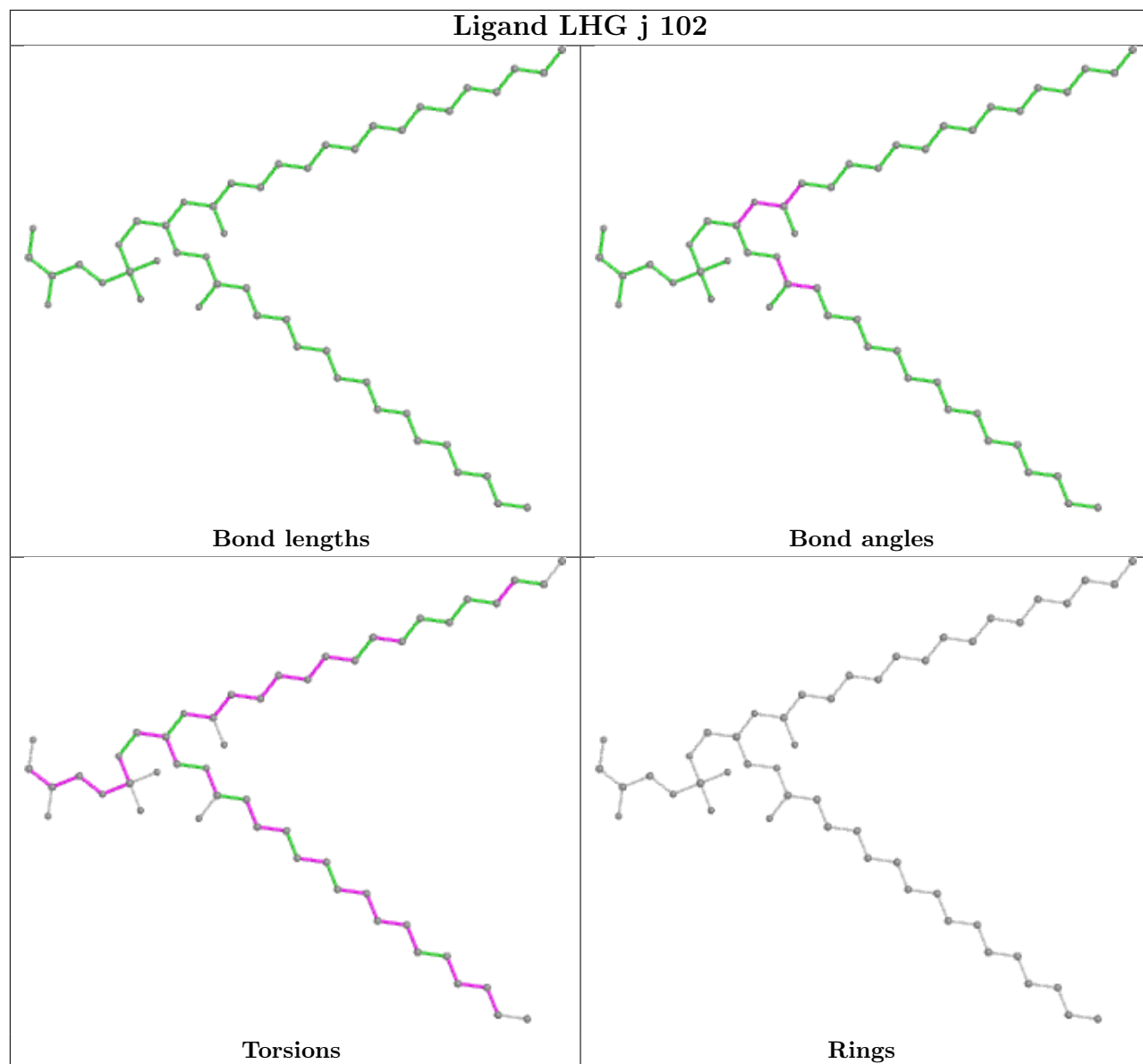


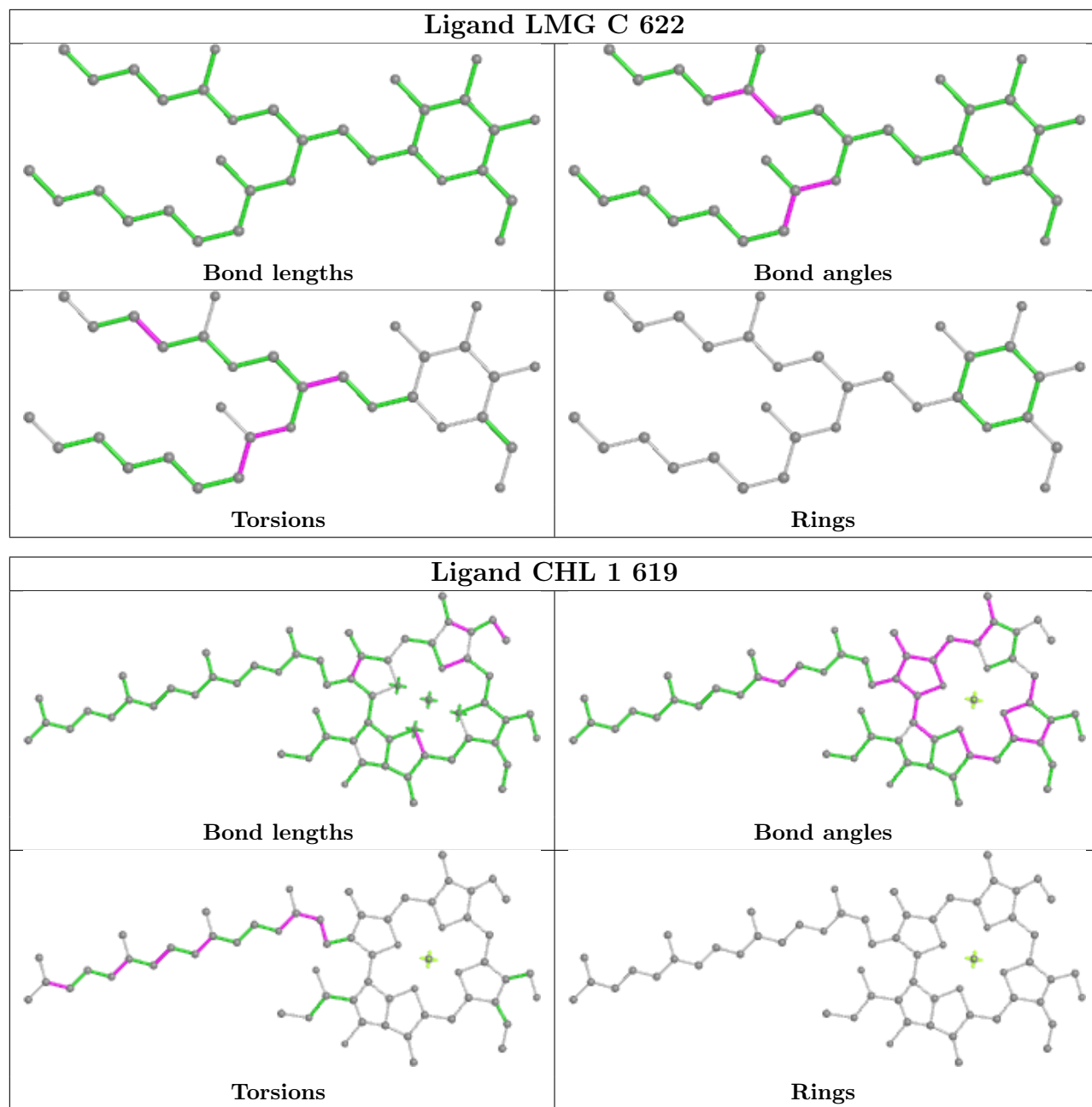


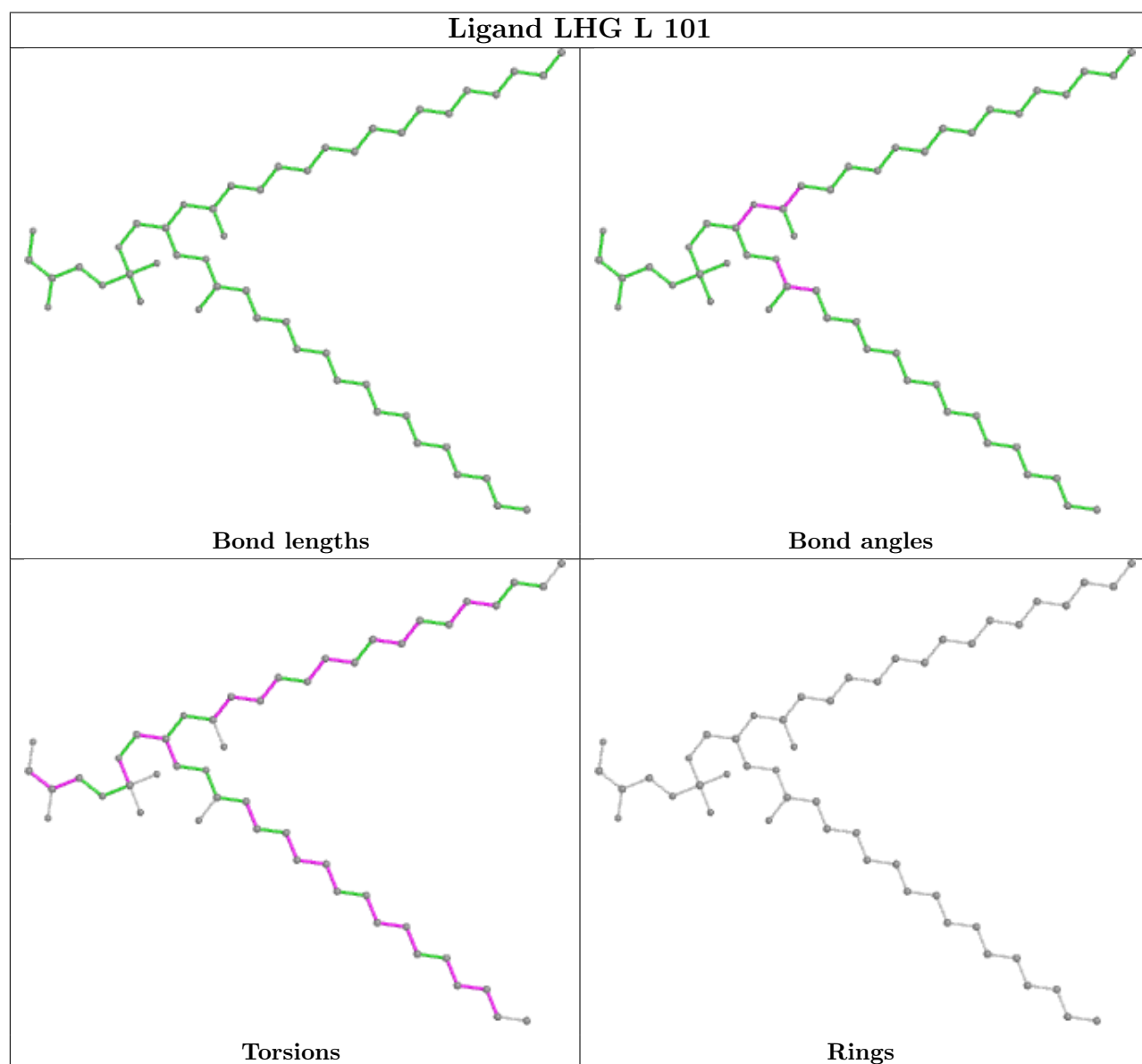
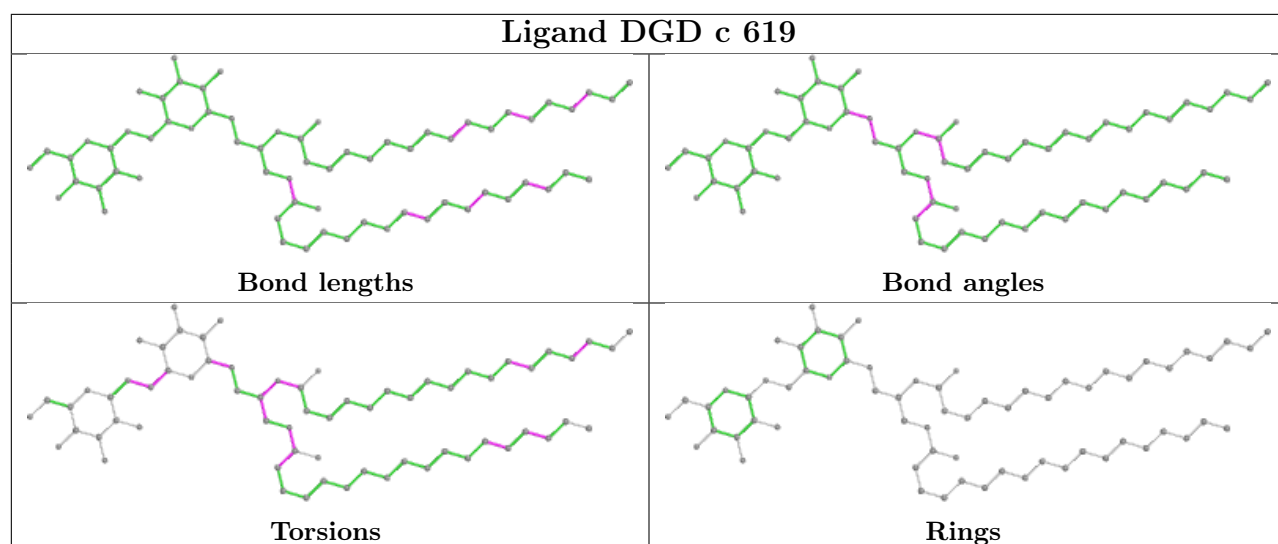


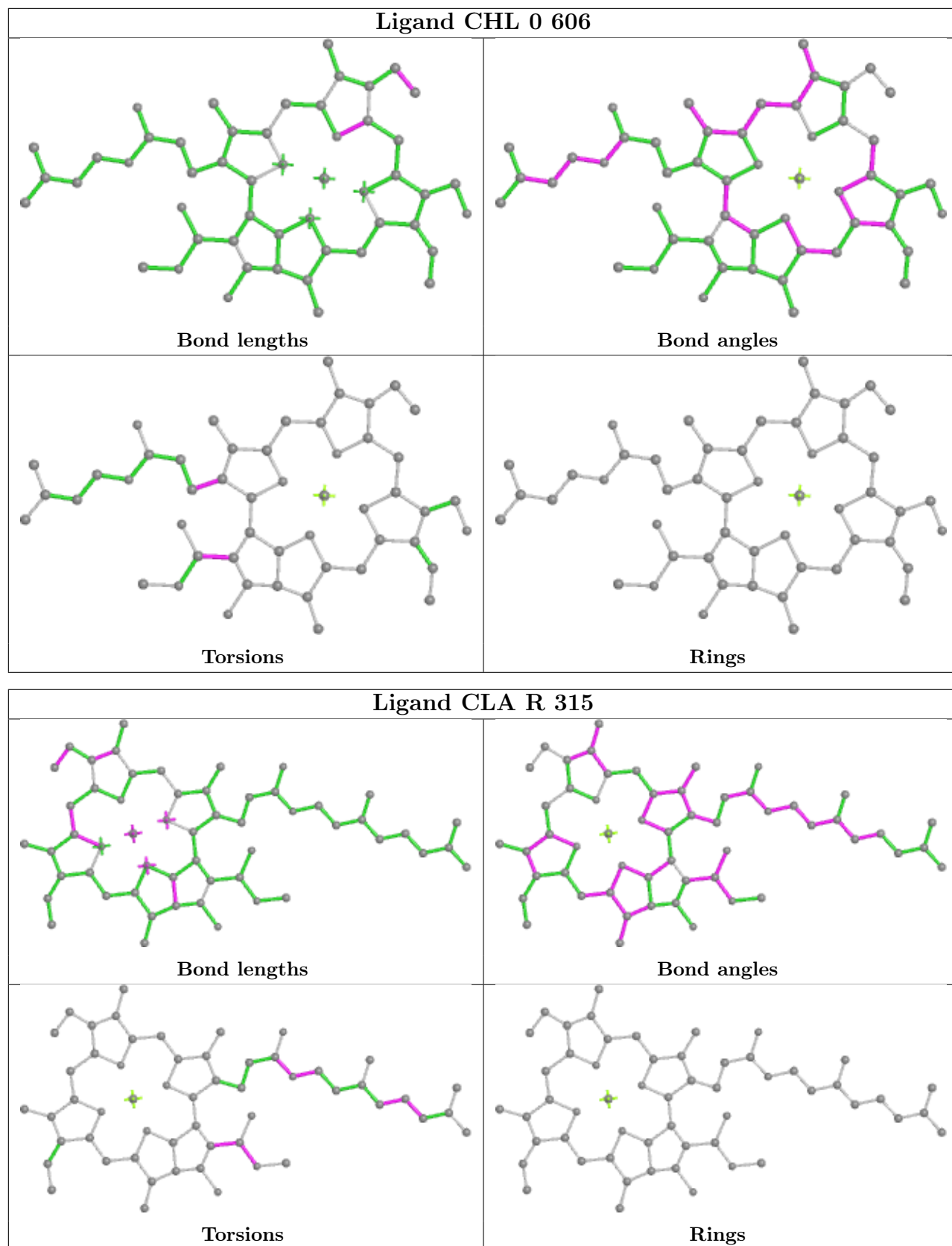


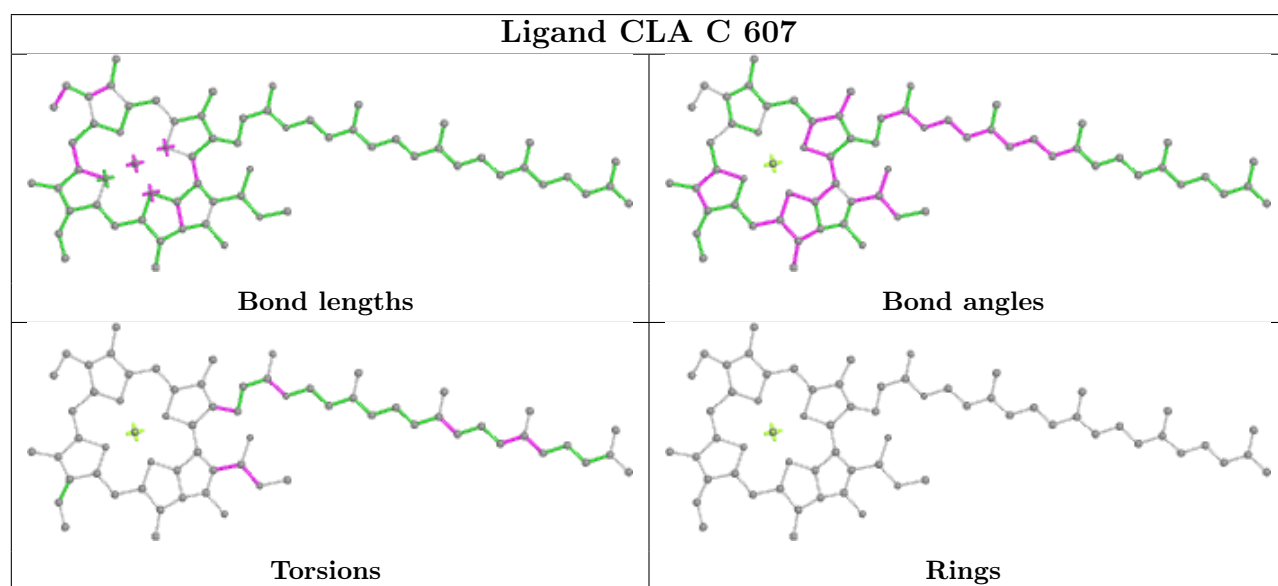
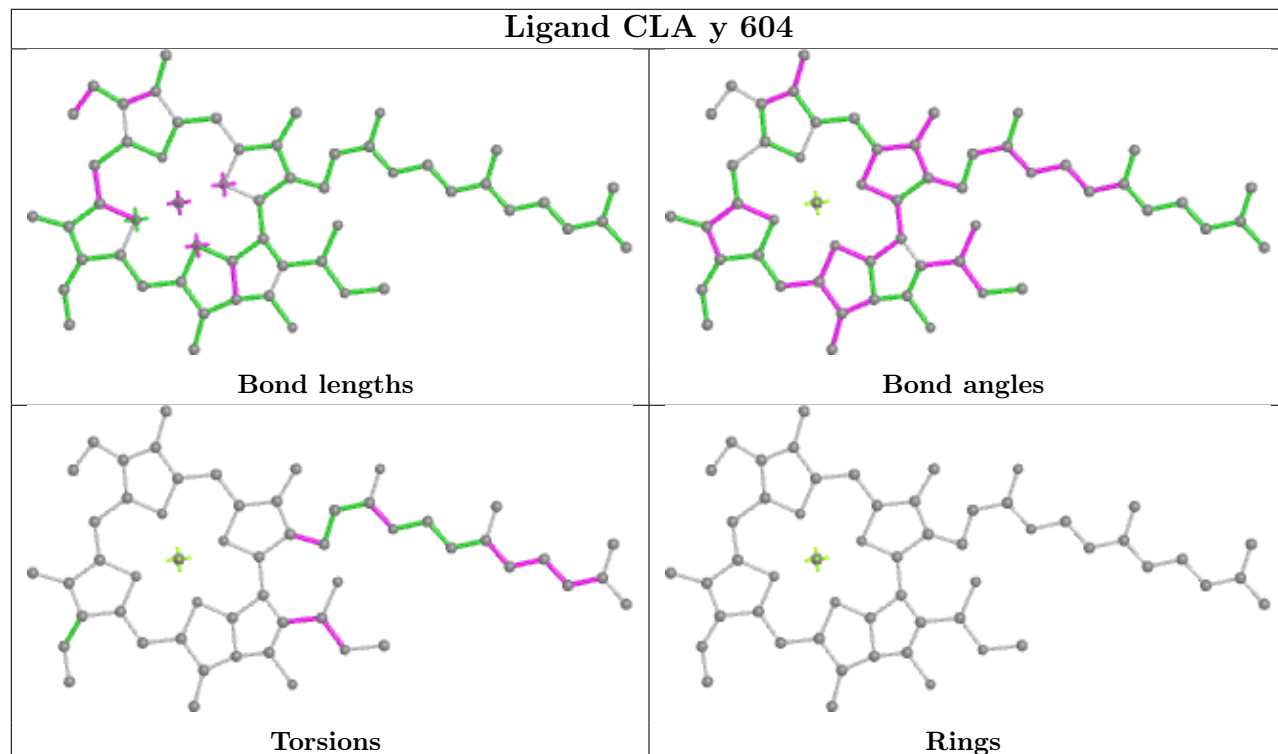
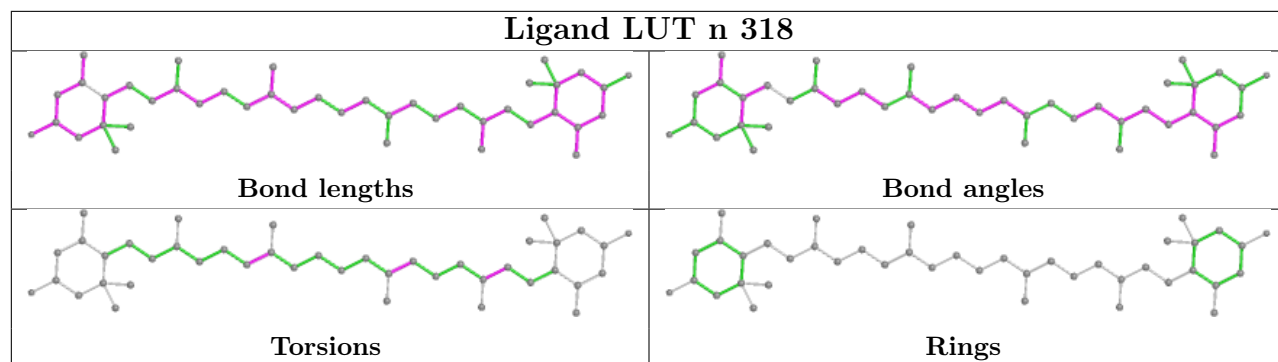


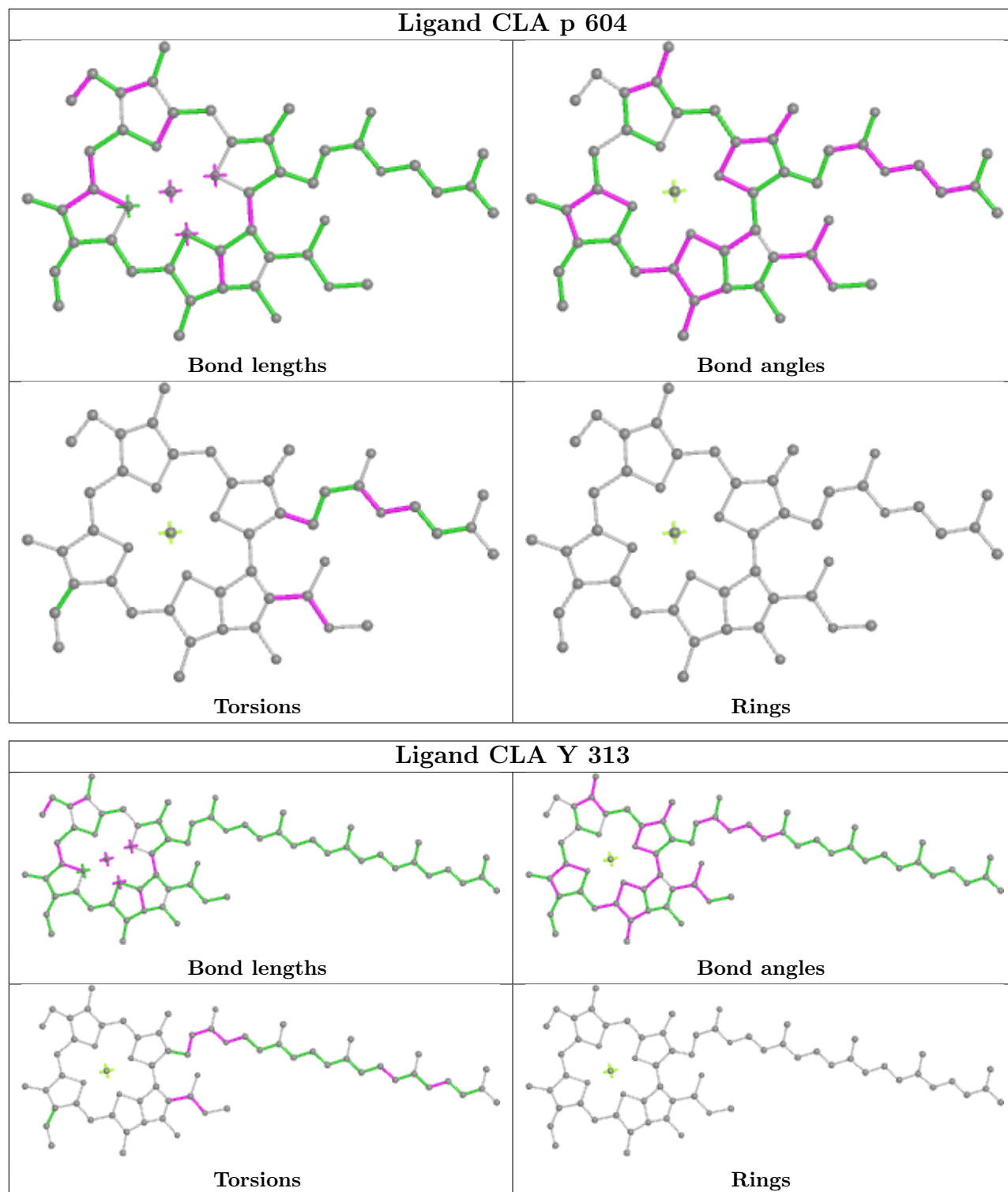


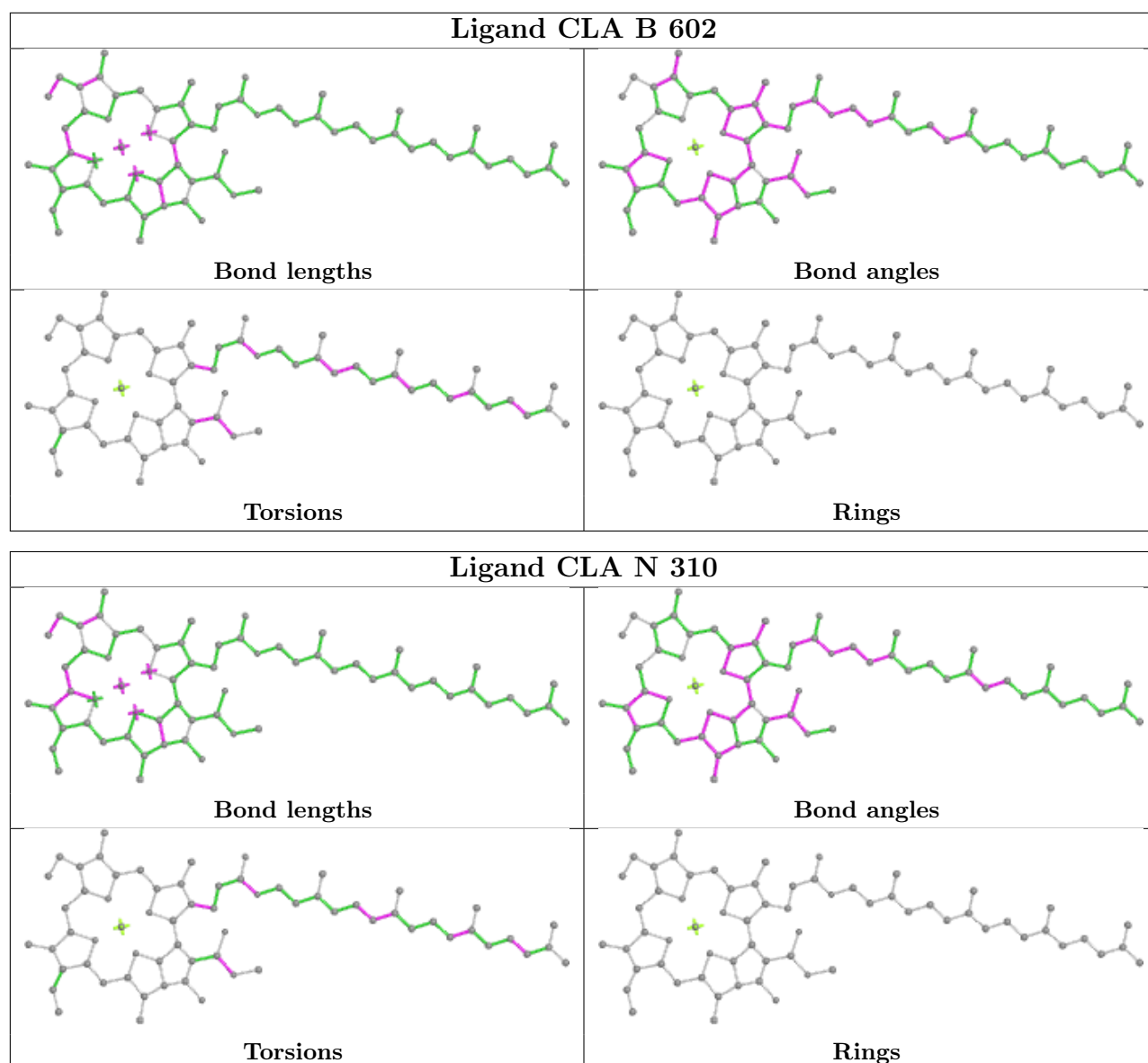












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

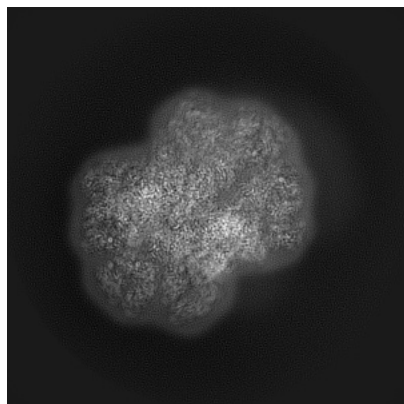
6 Map visualisation [i](#)

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.

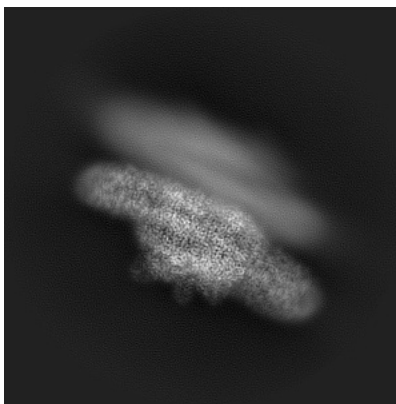
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

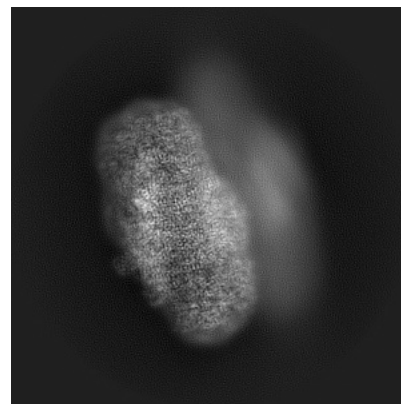
6.1.1 Primary map



X

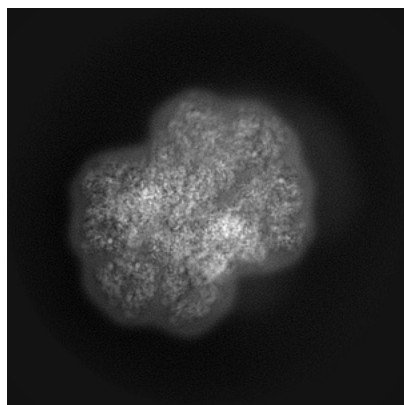


Y

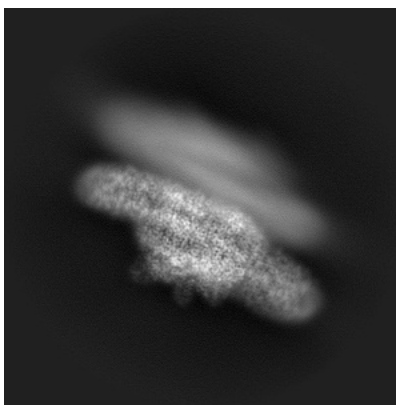


Z

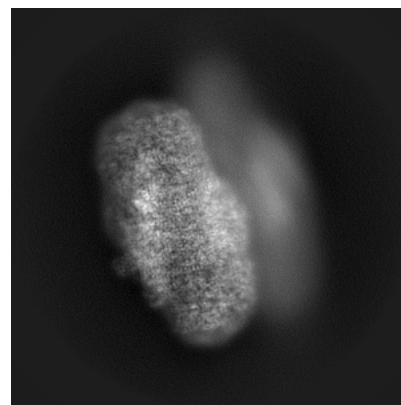
6.1.2 Raw map



X



Y

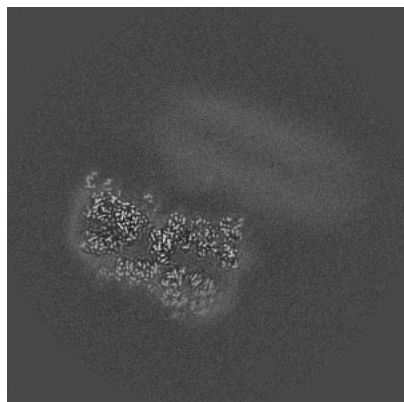


Z

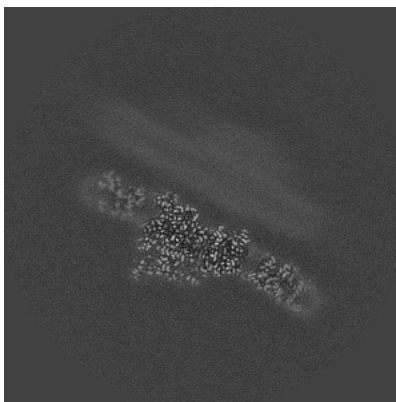
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

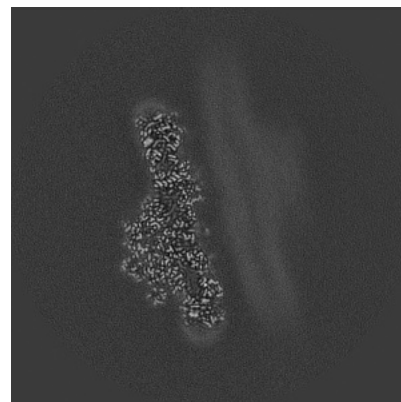
6.2.1 Primary map



X Index: 250

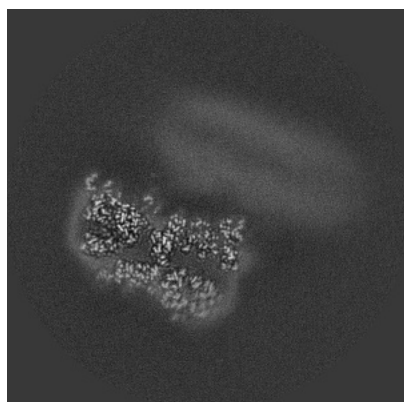


Y Index: 250

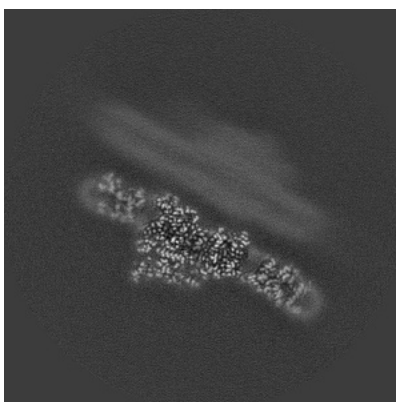


Z Index: 250

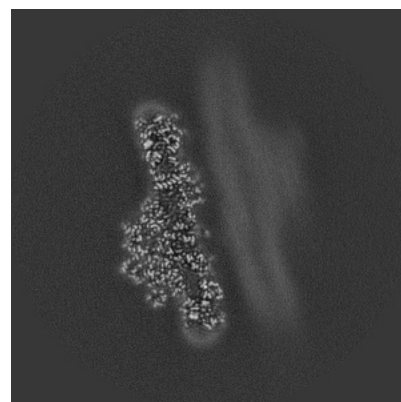
6.2.2 Raw map



X Index: 250



Y Index: 250

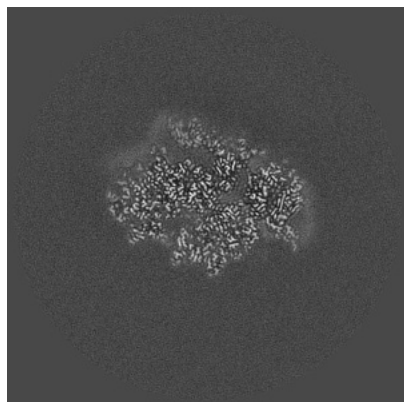


Z Index: 250

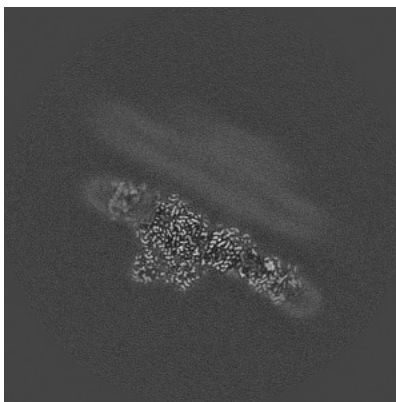
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

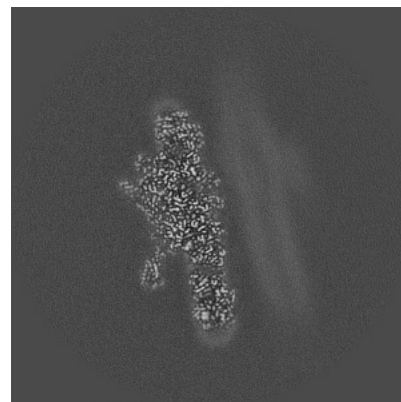
6.3.1 Primary map



X Index: 183

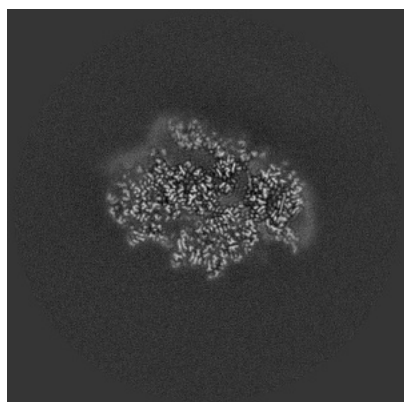


Y Index: 257

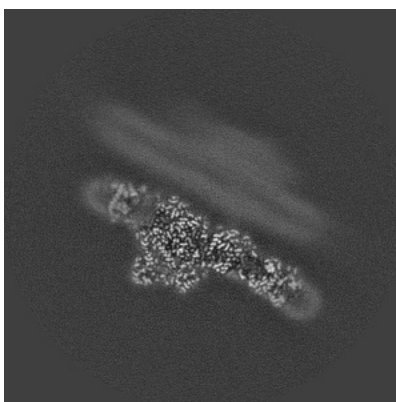


Z Index: 213

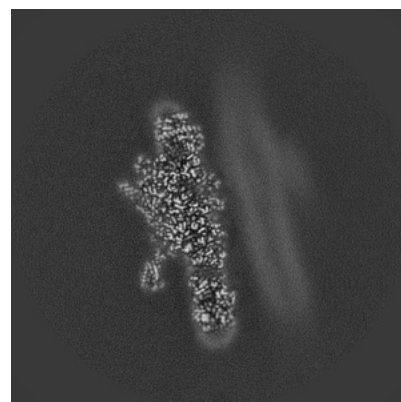
6.3.2 Raw map



X Index: 183



Y Index: 257

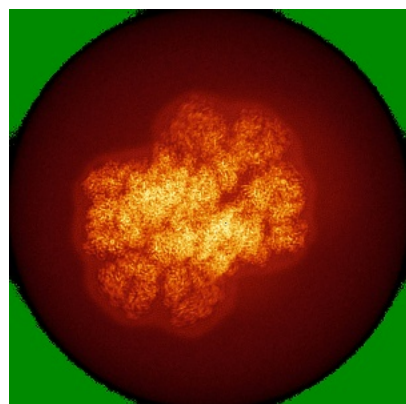


Z Index: 213

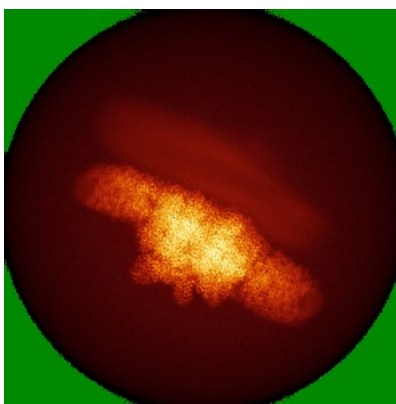
The images above show the largest variance slices of the map in three orthogonal directions.

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

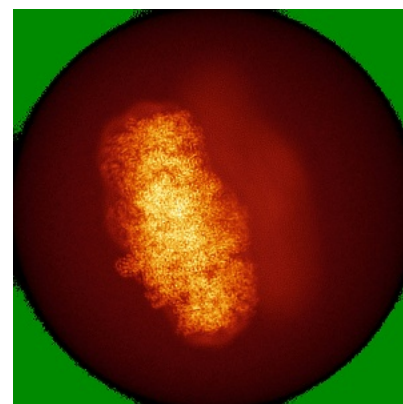
6.4.1 Primary map



X

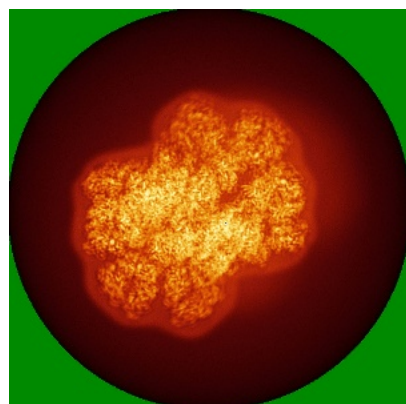


Y

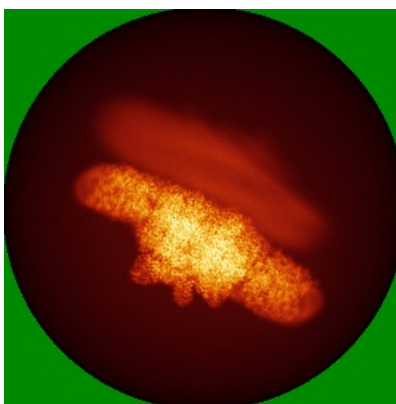


Z

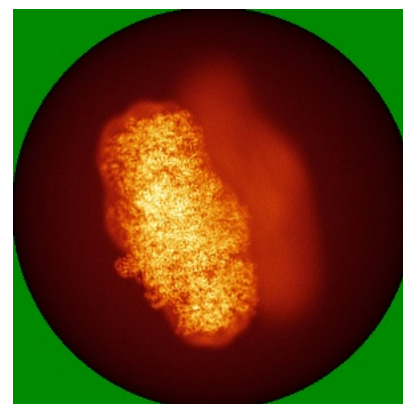
6.4.2 Raw map



X



Y

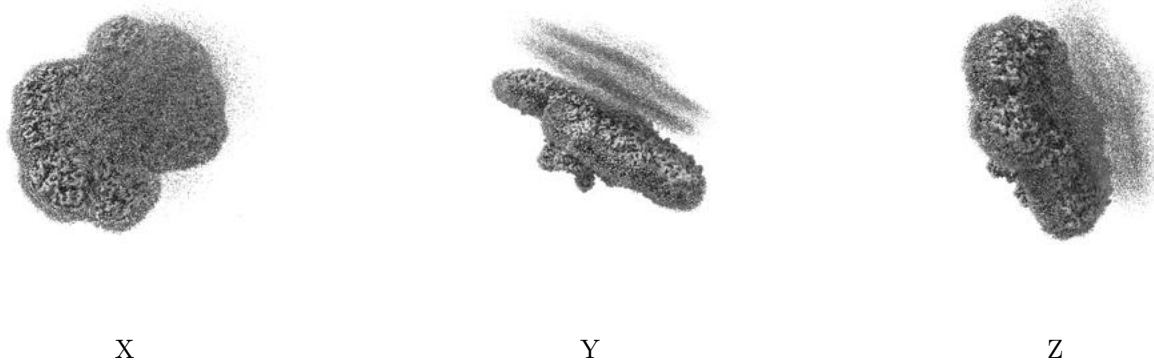


Z

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.

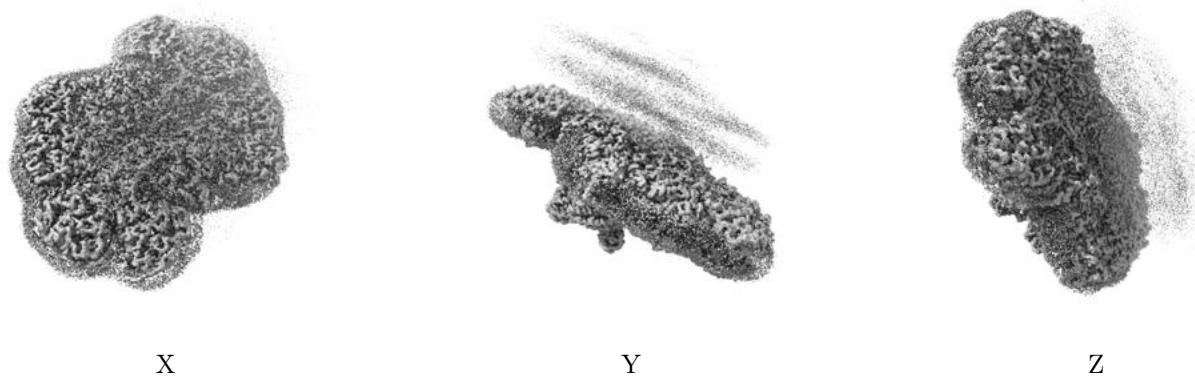
6.5 Orthogonal surface views [i](#)

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.

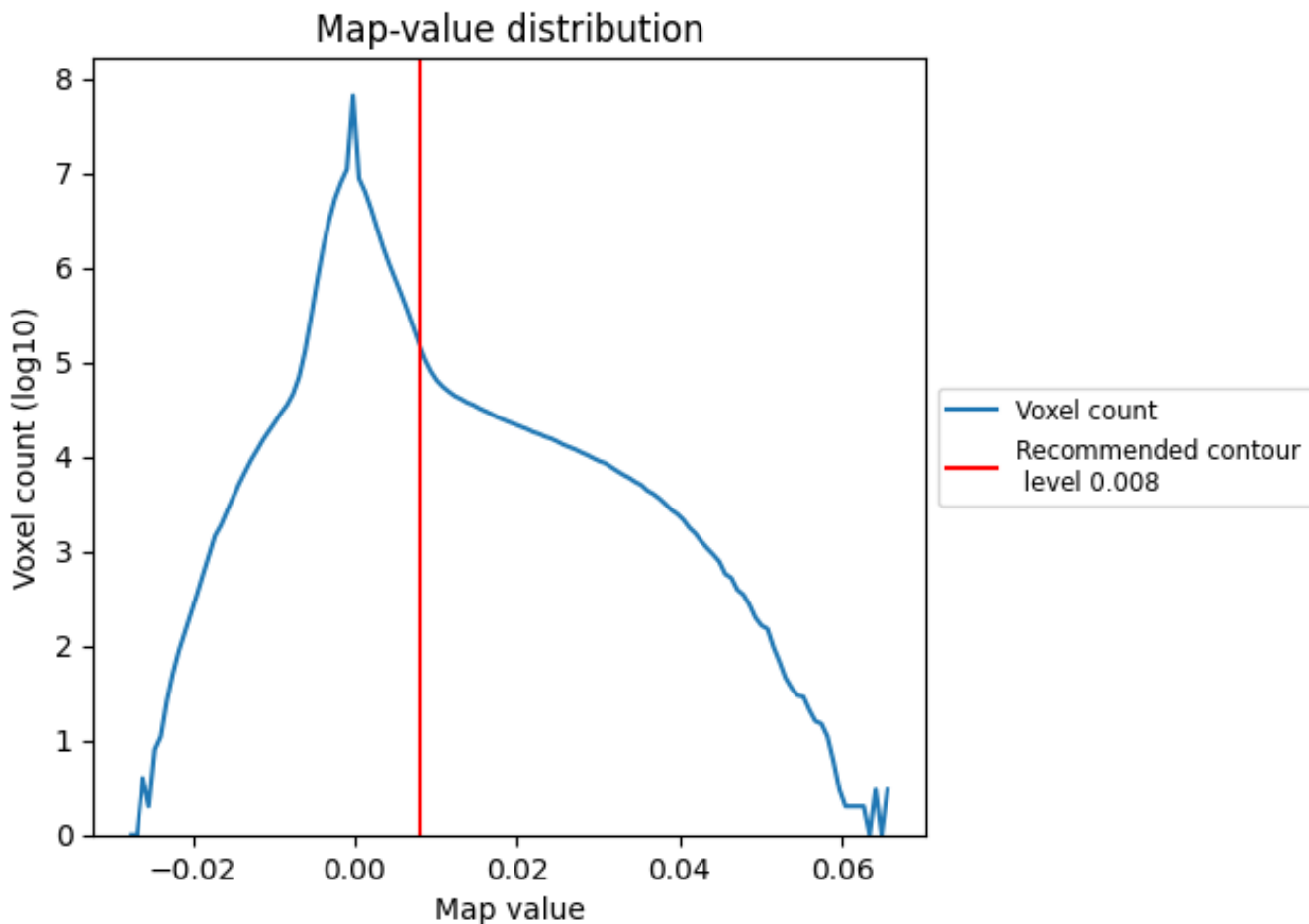
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

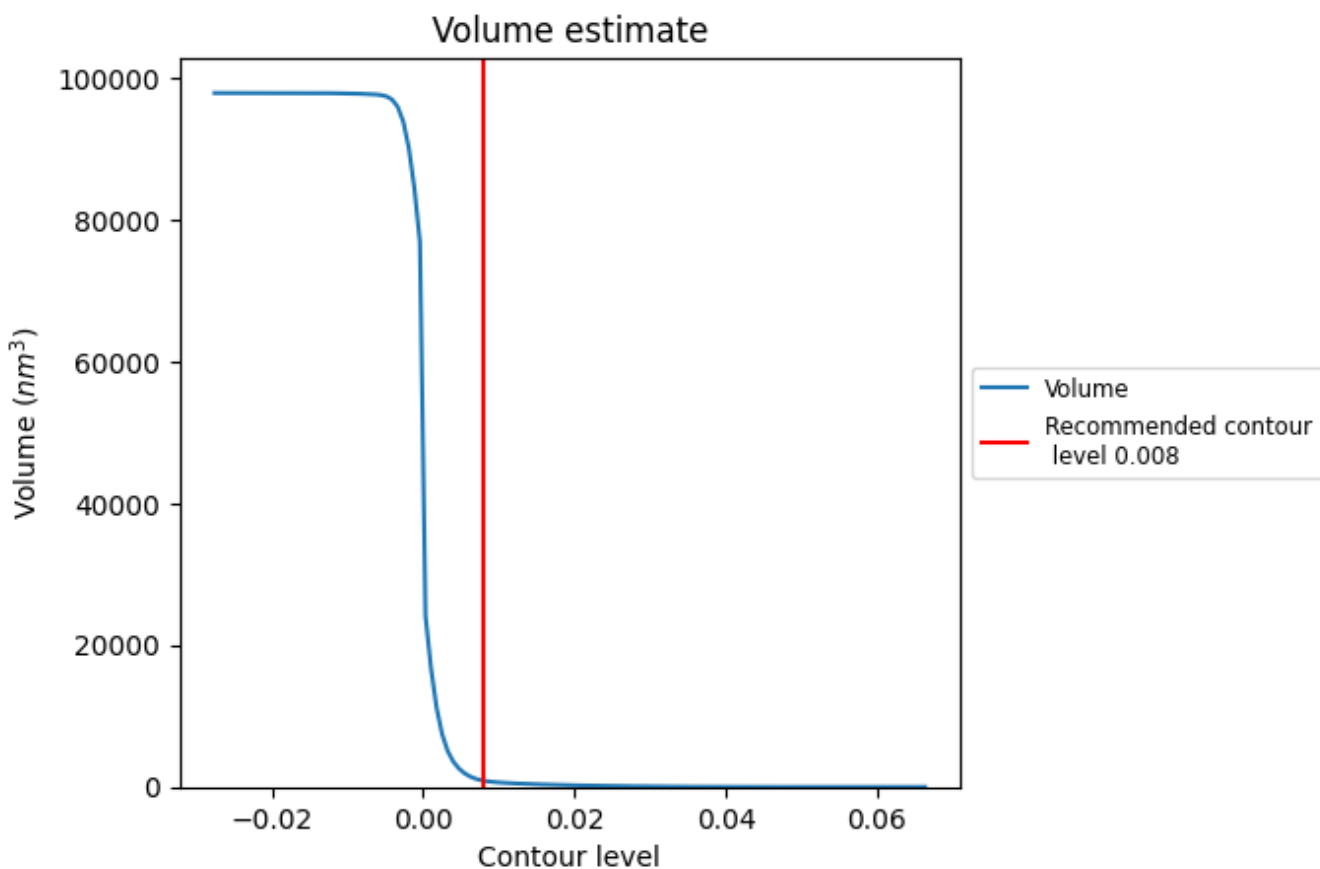
This section contains the results of statistical analysis of the map.

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.

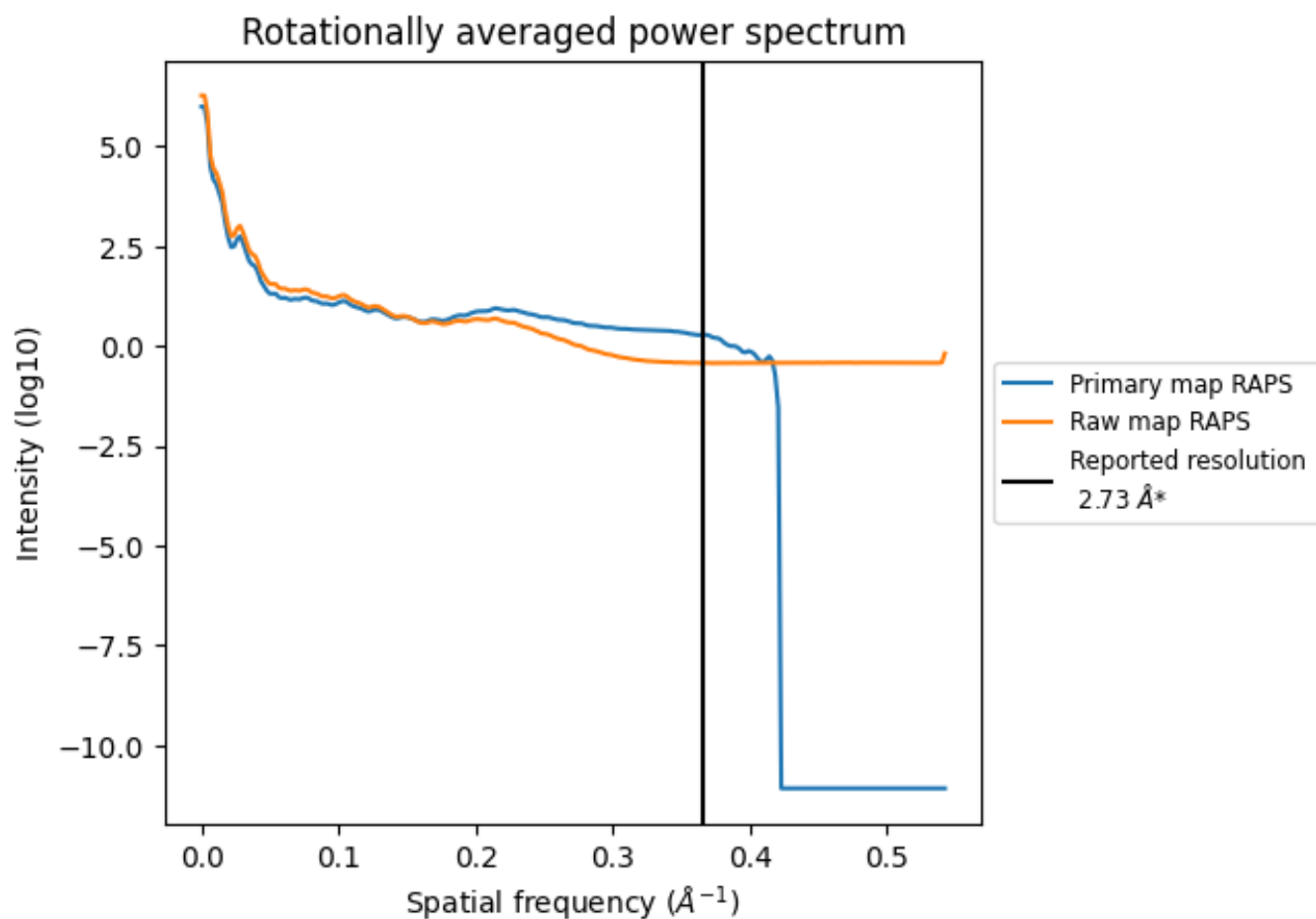
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 885 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](#)

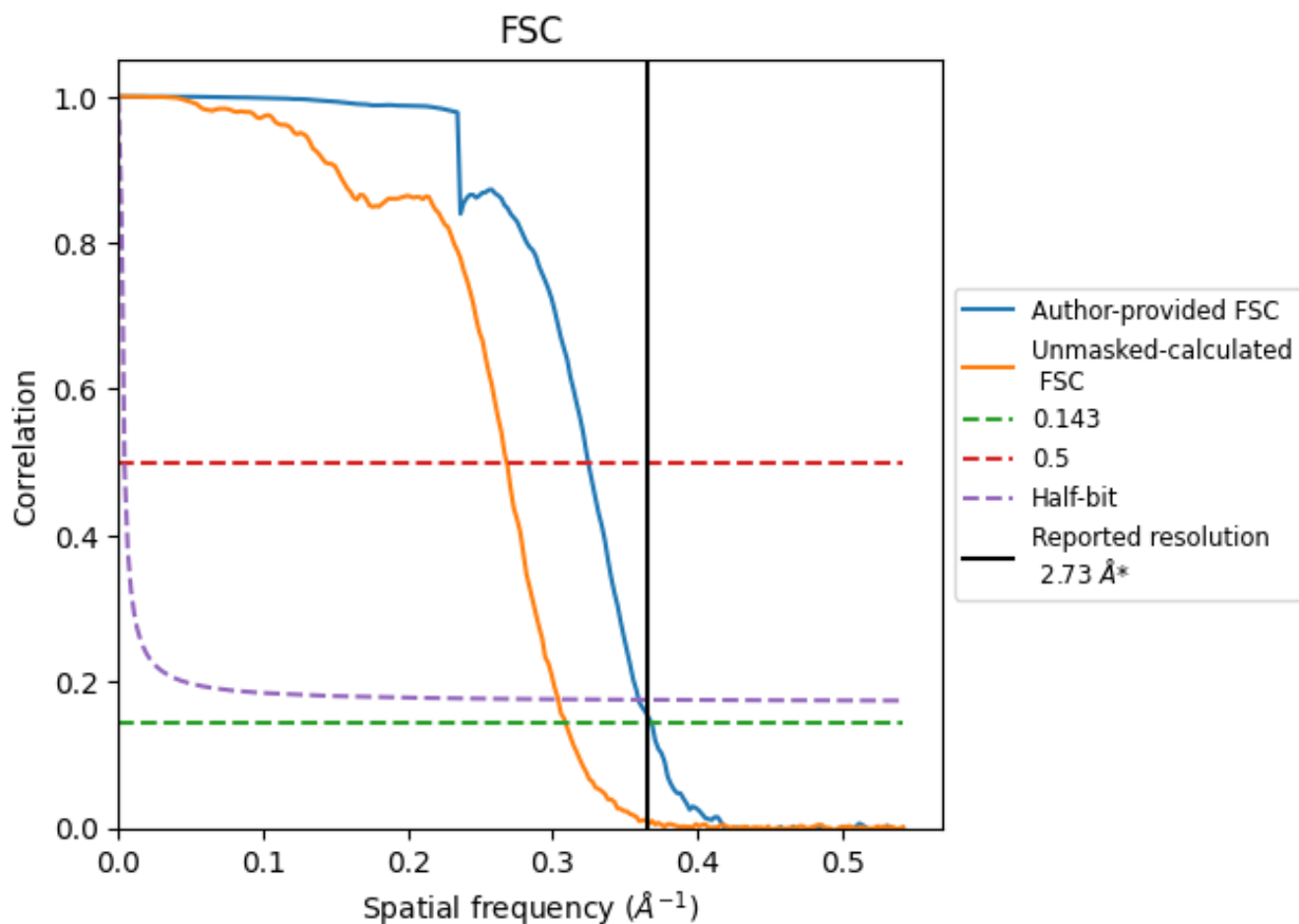


*Reported resolution corresponds to spatial frequency of 0.366 Å⁻¹

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⁻¹

8.2 Resolution estimates

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](#)

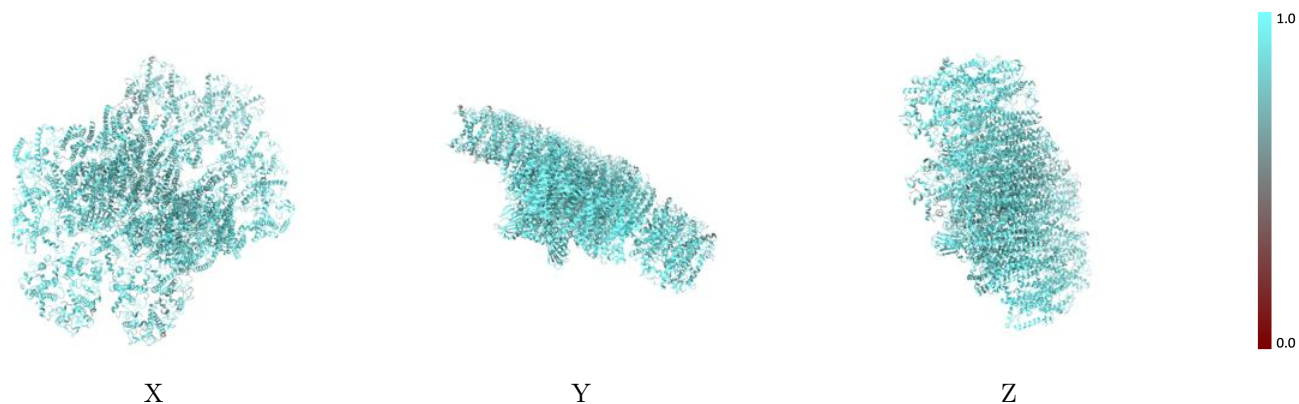


The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

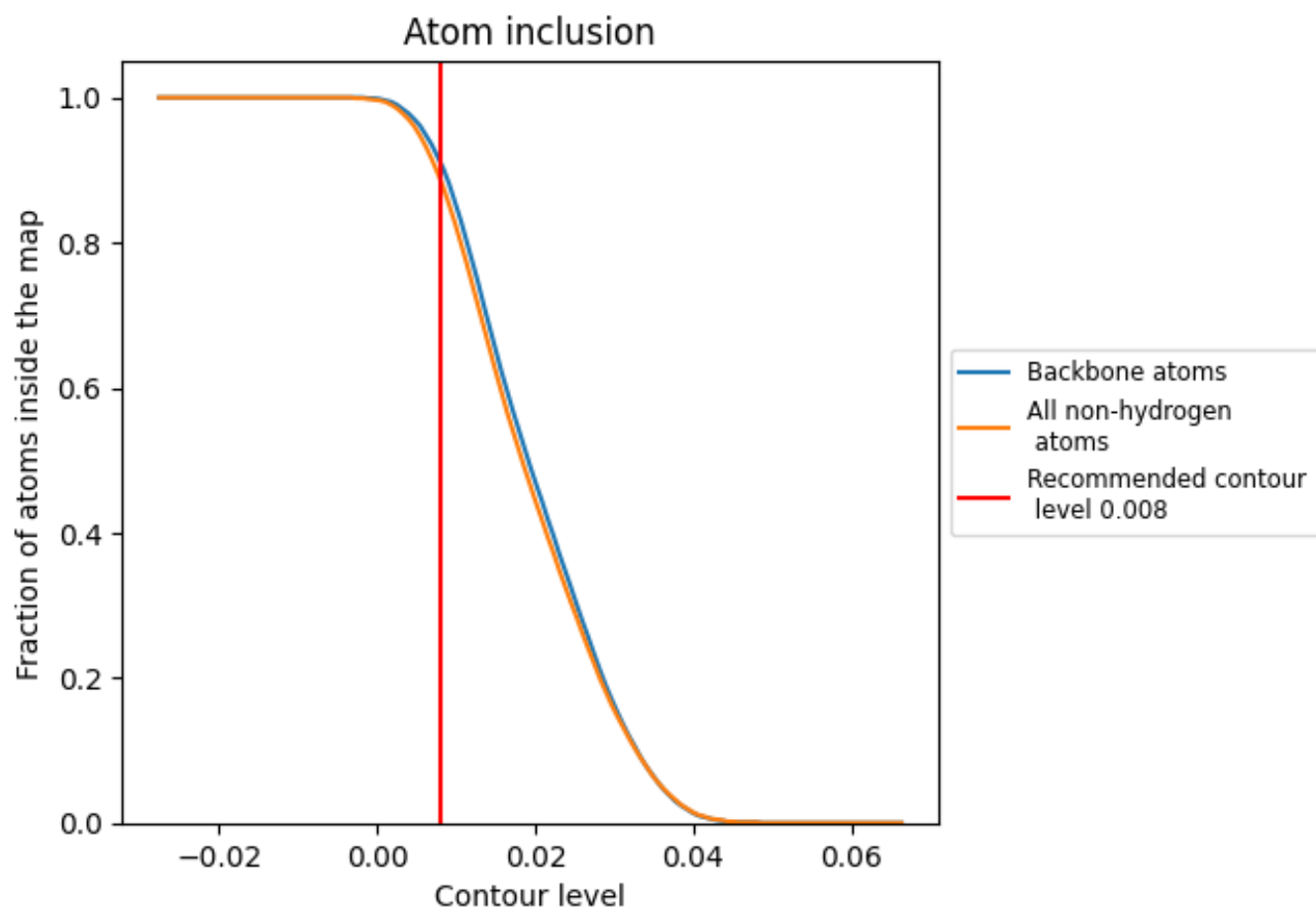
This section was not generated.

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

































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



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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