



Full wwPDB EM Validation Report ⓘ

Aug 8, 2023 – 12:50 PM JST

PDB ID : 7YMI
EMDB ID : EMD-33929
Title : PSII-Pcb Dimer of Acaryochloris Marina
Authors : Shen, L.L.; Gao, Y.Z.; Wang, W.D.; Zhang, X.; Shen, J.R.; Wang, P.Y.; Han, G.Y.
Deposited on : 2022-07-28
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

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:

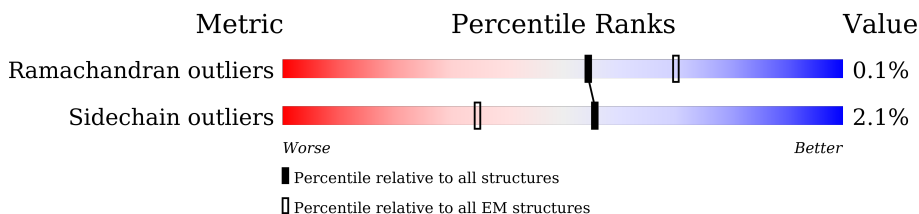
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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	A	360	
1	a	360	
2	B	506	
2	b	506	
3	C	490	
3	c	490	
4	D	351	
4	d	351	
5	E	83	

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Mol	Chain	Length	Quality of chain
5	e	83	47% 77% 22%
6	F	99	6% 30% 70%
6	f	99	6% 30% 70%
7	H	71	20% 94% ..
7	h	71	20% 94% ..
8	I	34	12% 97% .
8	i	34	12% 97% .
9	K	45	51% 80% 18%
9	k	45	51% 80% 18%
10	L	38	11% 95% 5%
10	l	38	11% 95% 5%
11	M	34	24% 91% 9%
11	m	34	24% 91% 9%
12	T	46	20% 61% 39%
12	t	46	20% 61% 39%
13	X	40	48% 88% 12%
13	x	40	48% 88% 12%
14	Y	39	59% 56% 41%
14	y	39	59% 56% 41%
15	Z	62	90% 94% 5%
15	z	62	90% 94% 5%
16	2	352	14% 97% ..
16	6	352	14% 97% ..
17	G	41	22% 100%
17	g	41	22% 100%

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Mol	Chain	Length	Quality of chain
18	1	356	
18	5	356	
19	3	349	
19	7	349	
20	4	353	
20	8	353	

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
21	CL7	1	402	X	-	-	-
21	CL7	1	403	X	-	-	-
21	CL7	1	404	X	-	-	-
21	CL7	1	405	X	-	-	-
21	CL7	1	406	X	-	-	-
21	CL7	1	407	X	-	-	-
21	CL7	1	408	X	-	-	-
21	CL7	1	409	X	-	-	-
21	CL7	1	410	X	-	-	-
21	CL7	1	411	X	-	-	-
21	CL7	1	412	X	-	-	-
21	CL7	1	413	X	-	-	-
21	CL7	1	414	X	-	-	-
21	CL7	1	415	X	-	-	-
21	CL7	1	416	X	-	-	-
21	CL7	1	417	X	-	-	-
21	CL7	1	418	X	-	-	-
21	CL7	1	419	X	-	-	-
21	CL7	1	420	X	-	-	-
21	CL7	2	501	X	-	-	-
21	CL7	2	502	X	-	-	-
21	CL7	2	503	X	-	-	-
21	CL7	2	504	X	-	-	-
21	CL7	2	505	X	-	-	-
21	CL7	2	506	X	-	-	-
21	CL7	2	507	X	-	-	-
21	CL7	2	508	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	2	509	X	-	-	-
21	CL7	2	510	X	-	-	-
21	CL7	2	511	X	-	-	-
21	CL7	2	512	X	-	-	-
21	CL7	2	513	X	-	-	-
21	CL7	2	514	X	-	-	-
21	CL7	2	515	X	-	-	-
21	CL7	2	516	X	-	-	-
21	CL7	2	517	X	-	-	-
21	CL7	2	518	X	-	-	-
21	CL7	3	501	X	-	-	-
21	CL7	3	502	X	-	-	-
21	CL7	3	503	X	-	-	-
21	CL7	3	504	X	-	-	-
21	CL7	3	505	X	-	-	-
21	CL7	3	506	X	-	-	-
21	CL7	3	507	X	-	-	-
21	CL7	3	508	X	-	-	-
21	CL7	3	509	X	-	-	-
21	CL7	3	510	X	-	-	-
21	CL7	3	511	X	-	-	-
21	CL7	3	512	X	-	-	-
21	CL7	3	513	X	-	-	-
21	CL7	3	514	X	-	-	-
21	CL7	3	515	X	-	-	-
21	CL7	3	516	X	-	-	-
21	CL7	3	517	X	-	-	-
21	CL7	3	518	X	-	-	-
21	CL7	4	404	X	-	-	-
21	CL7	4	405	X	-	-	-
21	CL7	4	406	X	-	-	-
21	CL7	4	407	X	-	-	-
21	CL7	4	408	X	-	-	-
21	CL7	4	409	X	-	-	-
21	CL7	4	410	X	-	-	-
21	CL7	4	411	X	-	-	-
21	CL7	4	412	X	-	-	-
21	CL7	4	413	X	-	-	-
21	CL7	4	414	X	-	-	-
21	CL7	4	415	X	-	-	-
21	CL7	4	416	X	-	-	-
21	CL7	4	417	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	5	402	X	-	-	-
21	CL7	5	403	X	-	-	-
21	CL7	5	404	X	-	-	-
21	CL7	5	405	X	-	-	-
21	CL7	5	406	X	-	-	-
21	CL7	5	407	X	-	-	-
21	CL7	5	408	X	-	-	-
21	CL7	5	409	X	-	-	-
21	CL7	5	410	X	-	-	-
21	CL7	5	411	X	-	-	-
21	CL7	5	412	X	-	-	-
21	CL7	5	413	X	-	-	-
21	CL7	5	414	X	-	-	-
21	CL7	5	415	X	-	-	-
21	CL7	5	416	X	-	-	-
21	CL7	5	417	X	-	-	-
21	CL7	5	418	X	-	-	-
21	CL7	5	419	X	-	-	-
21	CL7	5	420	X	-	-	-
21	CL7	6	501	X	-	-	-
21	CL7	6	502	X	-	-	-
21	CL7	6	503	X	-	-	-
21	CL7	6	504	X	-	-	-
21	CL7	6	505	X	-	-	-
21	CL7	6	506	X	-	-	-
21	CL7	6	507	X	-	-	-
21	CL7	6	508	X	-	-	-
21	CL7	6	509	X	-	-	-
21	CL7	6	510	X	-	-	-
21	CL7	6	511	X	-	-	-
21	CL7	6	512	X	-	-	-
21	CL7	6	513	X	-	-	-
21	CL7	6	514	X	-	-	-
21	CL7	6	515	X	-	-	-
21	CL7	6	516	X	-	-	-
21	CL7	6	517	X	-	-	-
21	CL7	6	518	X	-	-	-
21	CL7	7	501	X	-	-	-
21	CL7	7	502	X	-	-	-
21	CL7	7	503	X	-	-	-
21	CL7	7	504	X	-	-	-
21	CL7	7	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	7	506	X	-	-	-
21	CL7	7	507	X	-	-	-
21	CL7	7	508	X	-	-	-
21	CL7	7	509	X	-	-	-
21	CL7	7	510	X	-	-	-
21	CL7	7	511	X	-	-	-
21	CL7	7	512	X	-	-	-
21	CL7	7	513	X	-	-	-
21	CL7	7	514	X	-	-	-
21	CL7	7	515	X	-	-	-
21	CL7	7	516	X	-	-	-
21	CL7	7	517	X	-	-	-
21	CL7	7	518	X	-	-	-
21	CL7	8	404	X	-	-	-
21	CL7	8	405	X	-	-	-
21	CL7	8	406	X	-	-	-
21	CL7	8	407	X	-	-	-
21	CL7	8	408	X	-	-	-
21	CL7	8	409	X	-	-	-
21	CL7	8	410	X	-	-	-
21	CL7	8	411	X	-	-	-
21	CL7	8	412	X	-	-	-
21	CL7	8	413	X	-	-	-
21	CL7	8	414	X	-	-	-
21	CL7	8	415	X	-	-	-
21	CL7	8	416	X	-	-	-
21	CL7	8	417	X	-	-	-
21	CL7	A	401	X	-	-	-
21	CL7	A	403	X	-	-	-
21	CL7	A	406	X	-	-	-
21	CL7	B	601	X	-	-	-
21	CL7	B	602	X	-	-	-
21	CL7	B	603	X	-	-	-
21	CL7	B	604	X	-	-	-
21	CL7	B	605	X	-	-	-
21	CL7	B	606	X	-	-	-
21	CL7	B	607	X	-	-	-
21	CL7	B	608	X	-	-	-
21	CL7	B	609	X	-	-	-
21	CL7	B	610	X	-	-	-
21	CL7	B	611	X	-	-	-
21	CL7	B	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	B	613	X	-	-	-
21	CL7	B	614	X	-	-	-
21	CL7	B	615	X	-	-	-
21	CL7	B	616	X	-	-	-
21	CL7	B	622	X	-	-	-
21	CL7	C	502	X	-	-	-
21	CL7	C	503	X	-	-	-
21	CL7	C	504	X	-	-	-
21	CL7	C	505	X	-	-	-
21	CL7	C	506	X	-	-	-
21	CL7	C	507	X	-	-	-
21	CL7	C	508	X	-	-	-
21	CL7	C	509	X	-	-	-
21	CL7	C	510	X	-	-	-
21	CL7	C	511	X	-	-	-
21	CL7	C	512	X	-	-	-
21	CL7	C	513	X	-	-	-
21	CL7	C	514	X	-	-	-
21	CL7	C	518	X	-	-	-
21	CL7	D	402	X	-	-	-
21	CL7	D	404	X	-	-	-
21	CL7	D	405	X	-	-	-
21	CL7	a	401	X	-	-	-
21	CL7	a	403	X	-	-	-
21	CL7	a	405	X	-	-	-
21	CL7	b	602	X	-	-	-
21	CL7	b	603	X	-	-	-
21	CL7	b	604	X	-	-	-
21	CL7	b	605	X	-	-	-
21	CL7	b	606	X	-	-	-
21	CL7	b	607	X	-	-	-
21	CL7	b	608	X	-	-	-
21	CL7	b	609	X	-	-	-
21	CL7	b	610	X	-	-	-
21	CL7	b	611	X	-	-	-
21	CL7	b	612	X	-	-	-
21	CL7	b	613	X	-	-	-
21	CL7	b	614	X	-	-	-
21	CL7	b	615	X	-	-	-
21	CL7	b	616	X	-	-	-
21	CL7	b	617	X	-	-	-
21	CL7	b	623	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CL7	c	502	X	-	-	-
21	CL7	c	503	X	-	-	-
21	CL7	c	504	X	-	-	-
21	CL7	c	505	X	-	-	-
21	CL7	c	506	X	-	-	-
21	CL7	c	507	X	-	-	-
21	CL7	c	508	X	-	-	-
21	CL7	c	509	X	-	-	-
21	CL7	c	510	X	-	-	-
21	CL7	c	511	X	-	-	-
21	CL7	c	512	X	-	-	-
21	CL7	c	513	X	-	-	-
21	CL7	c	514	X	-	-	-
21	CL7	c	518	X	-	-	-
21	CL7	d	402	X	-	-	-
21	CL7	d	404	X	-	-	-
21	CL7	d	405	X	-	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 68428 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 Photosystem II protein D1 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		
1	a	284	Total	C	N	O	S	0	0
			2209	1450	361	381	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		
2	b	479	Total	C	N	O	S	0	0
			3794	2472	637	671	14		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		
3	c	420	Total	C	N	O	S	0	0
			3313	2173	556	570	14		

- Molecule 4 is a protein called Photosystem II D2 protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		
4	d	323	Total	C	N	O	S	0	0
			2583	1713	420	439	11		

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	65	Total	C	N	O	S	0	0
			538	354	87	96	1		
5	e	65	Total	C	N	O	S	0	0
			538	354	87	96	1		

- Molecule 6 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	30	Total	C	N	O	S	0	0
			242	166	39	36	1		
6	f	30	Total	C	N	O	S	0	0
			242	166	39	36	1		

- Molecule 7 is a protein called Photosystem II 10 kDa phosphoprotein PsbH.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	68	Total	C	N	O	S	0	0
			519	342	83	91	3		
7	h	68	Total	C	N	O	S	0	0
			519	342	83	91	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	34	Total	C	N	O	S	0	0
			281	194	41	45	1		
8	i	34	Total	C	N	O	S	0	0
			281	194	41	45	1		

- Molecule 9 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	37	Total	C	N	O	S	0	0
			292	205	41	45	1		
9	k	37	Total	C	N	O	S	0	0
			292	205	41	45	1		

- Molecule 10 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	L	36	Total	C	N	O	0	0
			288	194	45	49		

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Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	l	36	288	194	45	49	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	M	31	232	156	36	39	1	0	0
11	m	31	232	156	36	39	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	28	231	163	32	34	2	0	0
12	t	28	231	163	32	34	2	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	X	35	269	185	39	45	0	0
13	x	35	269	185	39	45	0	0

- Molecule 14 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Y	23	164	111	27	25	1	0	0
14	y	23	164	111	27	25	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Z	59	429	290	64	73	2	0	0
15	z	59	429	290	64	73	2	0	0

- Molecule 16 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	2	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		
16	6	349	Total	C	N	O	S	0	0
			2734	1811	442	473	8		

- Molecule 17 is a protein called Unknown protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	G	41	Total	C	N	O	0	0
			205	123	41	41		
17	g	41	Total	C	N	O	0	0
			205	123	41	41		

- Molecule 18 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		
18	5	329	Total	C	N	O	S	0	0
			2567	1715	400	445	7		

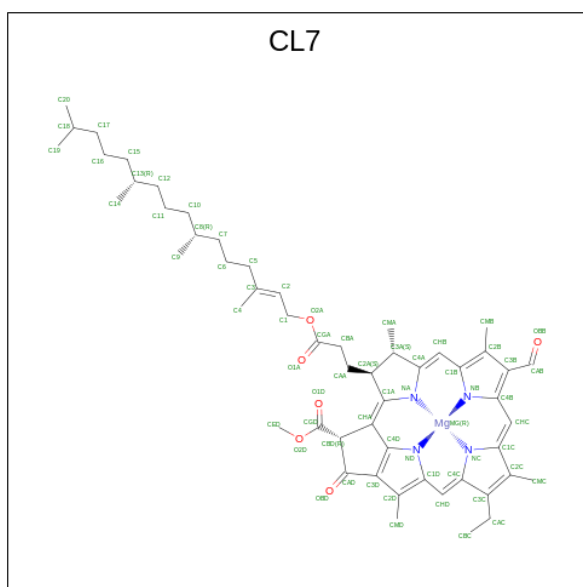
- Molecule 19 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	3	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		
19	7	344	Total	C	N	O	S	0	0
			2715	1794	444	468	9		

- Molecule 20 is a protein called High light inducible protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	4	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		
20	8	331	Total	C	N	O	S	0	0
			2514	1638	412	448	16		

- Molecule 21 is CHLOROPHYLL D (three-letter code: CL7) (formula: C₅₄H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
21	A	1	65	54	1	4	6	0
21	A	1	55	44	1	4	6	0
21	A	1	65	54	1	4	6	0
21	B	1	41	32	1	4	4	0
21	B	1	60	49	1	4	6	0
21	B	1	65	54	1	4	6	0
21	B	1	65	54	1	4	6	0
21	B	1	65	54	1	4	6	0
21	B	1	55	44	1	4	6	0
21	B	1	60	49	1	4	6	0
21	B	1	65	54	1	4	6	0
21	B	1	65	54	1	4	6	0
21	B	1	65	54	1	4	6	0
21	B	1	65	54	1	4	6	0

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
21	B	1	65	54	1	4	6	0
21	B	1	55	44	1	4	6	0
21	B	1	60	49	1	4	6	0
21	B	1	50	39	1	4	6	0
21	B	1	45	34	1	4	6	0
21	B	1	45	34	1	4	6	0
21	C	1	65	54	1	4	6	0
21	C	1	60	49	1	4	6	0
21	C	1	65	54	1	4	6	0
21	C	1	55	44	1	4	6	0
21	C	1	65	54	1	4	6	0
21	C	1	60	49	1	4	6	0
21	C	1	65	54	1	4	6	0
21	C	1	65	54	1	4	6	0
21	C	1	65	54	1	4	6	0
21	C	1	42	33	1	4	4	0
21	C	1	41	32	1	4	4	0
21	C	1	45	34	1	4	6	0
21	C	1	41	32	1	4	4	0
21	D	1	50	39	1	4	6	0

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
21	D	1	58	47	1	4	6	0
21	D	1	45	34	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	45	34	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	45	34	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	60	49	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	45	34	1	4	6	0
21	2	1	45	34	1	4	6	0
21	2	1	45	34	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	65	54	1	4	6	0
21	2	1	65	54	1	4	6	0
21	1	1	60	49	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	1	1	60	49	1	4	6	0
21	1	1	65	54	1	4	6	0
21	1	1	45	34	1	4	6	0
21	1	1	62	51	1	4	6	0
21	1	1	41	32	1	4	4	0
21	1	1	65	54	1	4	6	0
21	1	1	45	34	1	4	6	0
21	1	1	65	54	1	4	6	0
21	1	1	45	34	1	4	6	0
21	1	1	45	34	1	4	6	0
21	1	1	41	32	1	4	4	0
21	1	1	41	32	1	4	4	0
21	1	1	41	32	1	4	4	0
21	1	1	41	32	1	4	4	0
21	1	1	55	44	1	4	6	0
21	1	1	65	54	1	4	6	0
21	1	1	45	34	1	4	6	0
21	1	1	45	34	1	4	6	0
21	3	1	65	54	1	4	6	0
21	3	1	58	47	1	4	6	0
21	3	1	65	54	1	4	6	0

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Mol	Chain	Residues	Atoms				AltConf	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	3	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
21	3	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	4	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	4	1	Total	C	Mg	N	O	0
			60	49	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	4	1	45	34	1	4	6	0
21	4	1	65	54	1	4	6	0
21	4	1	65	54	1	4	6	0
21	4	1	60	49	1	4	6	0
21	4	1	53	42	1	4	6	0
21	4	1	45	34	1	4	6	0
21	4	1	41	32	1	4	4	0
21	4	1	42	33	1	4	4	0
21	a	1	65	54	1	4	6	0
21	a	1	55	44	1	4	6	0
21	a	1	65	54	1	4	6	0
21	b	1	41	32	1	4	4	0
21	b	1	60	49	1	4	6	0
21	b	1	65	54	1	4	6	0
21	b	1	65	54	1	4	6	0
21	b	1	55	44	1	4	6	0
21	b	1	60	49	1	4	6	0
21	b	1	65	54	1	4	6	0
21	b	1	65	54	1	4	6	0
21	b	1	65	54	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	b	1	65	54	1	4	6	0
21	b	1	65	54	1	4	6	0
21	b	1	55	44	1	4	6	0
21	b	1	60	49	1	4	6	0
21	b	1	50	39	1	4	6	0
21	b	1	45	34	1	4	6	0
21	b	1	45	34	1	4	6	0
21	c	1	65	54	1	4	6	0
21	c	1	60	49	1	4	6	0
21	c	1	65	54	1	4	6	0
21	c	1	55	44	1	4	6	0
21	c	1	65	54	1	4	6	0
21	c	1	60	49	1	4	6	0
21	c	1	65	54	1	4	6	0
21	c	1	65	54	1	4	6	0
21	c	1	65	54	1	4	6	0
21	c	1	42	33	1	4	4	0
21	c	1	41	32	1	4	4	0
21	c	1	45	34	1	4	6	0
21	c	1	41	32	1	4	4	0

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Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
21	d	1	50	39	1	4	6	0
21	d	1	58	47	1	4	6	0
21	d	1	45	34	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	45	34	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	60	49	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	45	34	1	4	6	0
21	6	1	45	34	1	4	6	0
21	6	1	45	34	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	65	54	1	4	6	0
21	6	1	65	54	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
21	5	1	60	49	1	4	6	0
21	5	1	60	49	1	4	6	0
21	5	1	65	54	1	4	6	0
21	5	1	45	34	1	4	6	0
21	5	1	62	51	1	4	6	0
21	5	1	41	32	1	4	4	0
21	5	1	65	54	1	4	6	0
21	5	1	45	34	1	4	6	0
21	5	1	65	54	1	4	6	0
21	5	1	45	34	1	4	6	0
21	5	1	45	34	1	4	6	0
21	5	1	41	32	1	4	4	0
21	5	1	41	32	1	4	4	0
21	5	1	41	32	1	4	4	0
21	5	1	41	32	1	4	4	0
21	5	1	41	32	1	4	4	0
21	5	1	55	44	1	4	6	0
21	5	1	65	54	1	4	6	0
21	5	1	45	34	1	4	6	0
21	5	1	45	34	1	4	6	0
21	7	1	65	54	1	4	6	0
21	7	1	58	47	1	4	6	0

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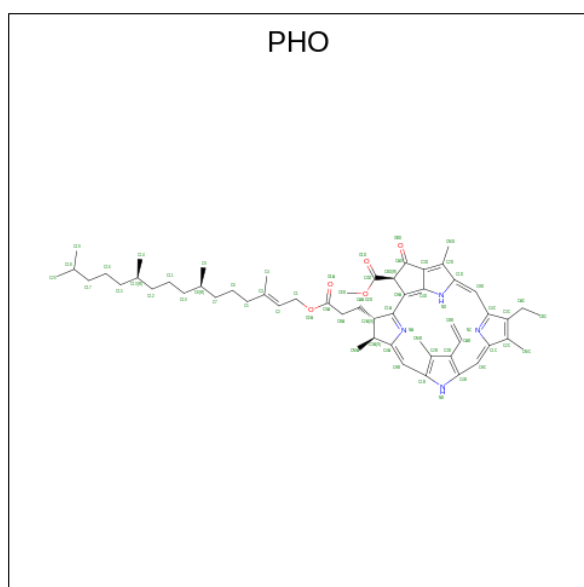
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N	O	
21	7	1	65	54	1	4	6	0
21	7	1	65	54	1	4	6	0
21	7	1	65	54	1	4	6	0
21	7	1	45	34	1	4	6	0
21	7	1	65	54	1	4	6	0
21	7	1	65	54	1	4	6	0
21	7	1	65	54	1	4	6	0
21	7	1	65	54	1	4	6	0
21	7	1	65	54	1	4	6	0
21	7	1	55	44	1	4	6	0
21	7	1	45	34	1	4	6	0
21	7	1	45	34	1	4	6	0
21	7	1	41	32	1	4	4	0
21	7	1	55	44	1	4	6	0
21	7	1	50	39	1	4	6	0
21	7	1	45	34	1	4	6	0
21	8	1	65	54	1	4	6	0
21	8	1	65	54	1	4	6	0
21	8	1	65	54	1	4	6	0
21	8	1	41	32	1	4	4	0
21	8	1	45	34	1	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
21	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			65	54	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			45	34	1	4	6	
21	8	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
21	8	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

- Molecule 22 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



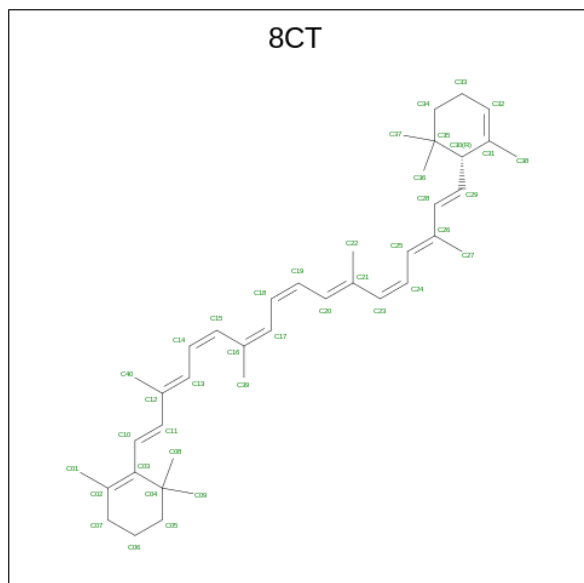
Mol	Chain	Residues	Atoms			AltConf	
22	A	1	Total	C	N	O	0
			64	55	4	5	
22	D	1	Total	C	N	O	0
			64	55	4	5	

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

- Molecule 23 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (three-letter code: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



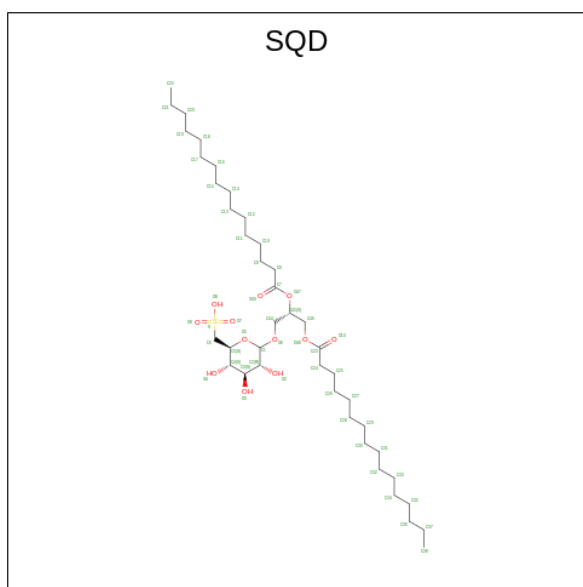
Mol	Chain	Residues	Atoms		AltConf
			Total	C	
23	A	1	40	40	0
23	B	1	40	40	0
23	B	1	40	40	0
23	B	1	40	40	0
23	B	1	40	40	0
23	C	1	40	40	0
23	C	1	40	40	0
23	C	1	40	40	0
23	D	1	40	40	0

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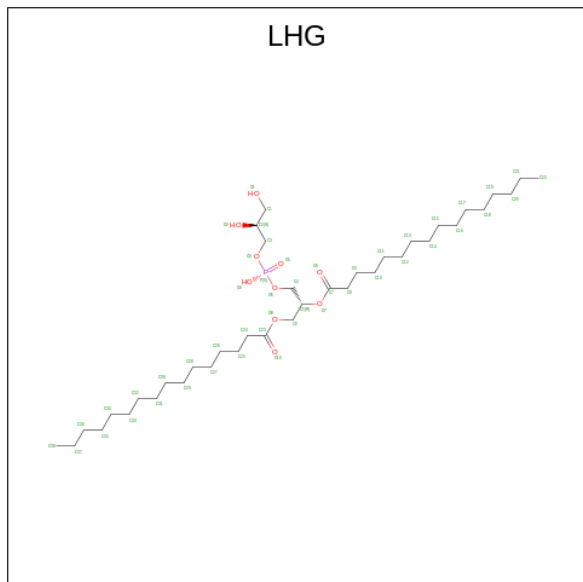
Mol	Chain	Residues	Atoms	AltConf
23	K	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	d	1	Total C 40 40	0
23	k	1	Total C 40 40	0
23	8	1	Total C 40 40	0

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



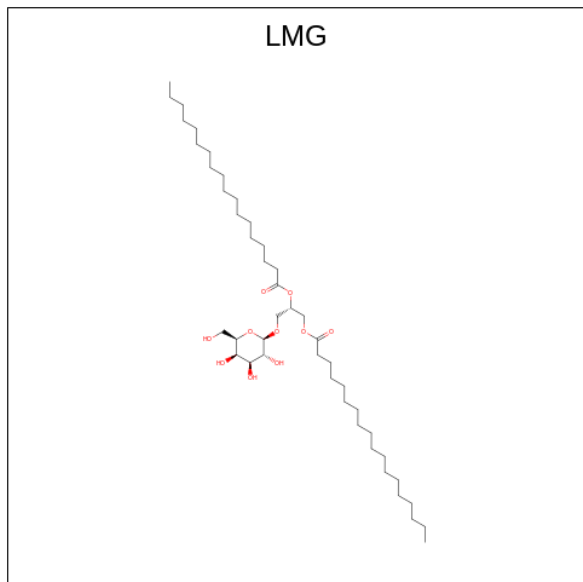
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		S
24	A	1	34	21	12	1	0
24	B	1	54	41	12	1	0
24	B	1	34	21	12	1	0
24	2	1	50	37	12	1	0
24	2	1	41	28	12	1	0
24	1	1	32	19	12	1	0
24	3	1	46	33	12	1	0
24	3	1	50	37	12	1	0
24	b	1	54	41	12	1	0
24	6	1	50	37	12	1	0
24	6	1	41	28	12	1	0
24	5	1	32	19	12	1	0
24	7	1	46	33	12	1	0
24	7	1	50	37	12	1	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



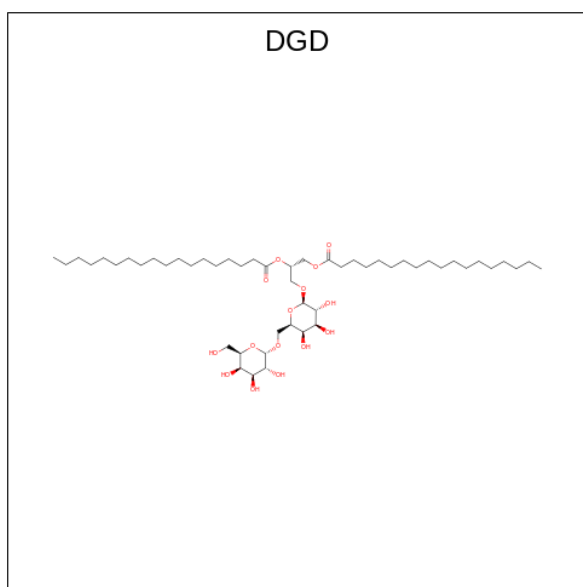
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
25	A	1	46	35	10	1	0
25	B	1	45	34	10	1	0
25	B	1	49	38	10	1	0
25	D	1	49	38	10	1	0
25	3	1	36	25	10	1	0
25	4	1	49	38	10	1	0
25	a	1	46	35	10	1	0
25	b	1	45	34	10	1	0
25	b	1	49	38	10	1	0
25	d	1	49	38	10	1	0
25	7	1	36	25	10	1	0
25	8	1	49	38	10	1	0

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
26	B	1	51	41	10	0
26	C	1	50	40	10	0
26	D	1	33	23	10	0
26	1	1	51	41	10	0
26	b	1	51	41	10	0
26	c	1	50	40	10	0
26	d	1	33	23	10	0
26	5	1	51	41	10	0

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

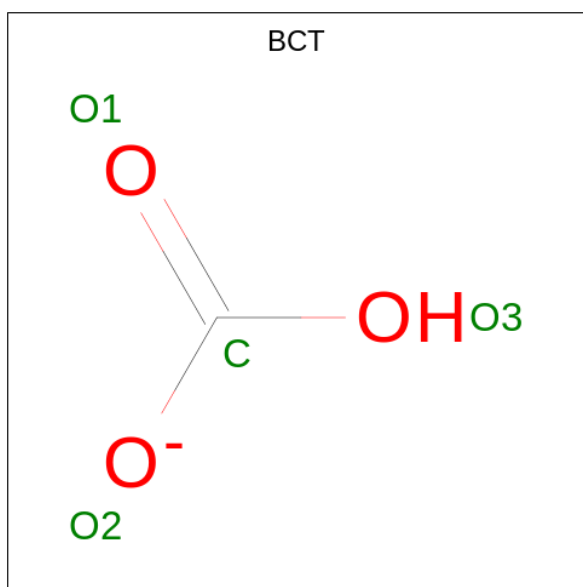


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	62	47	15	0
27	C	1	62	47	15	0
27	b	1	62	47	15	0
27	c	1	62	47	15	0

- Molecule 28 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

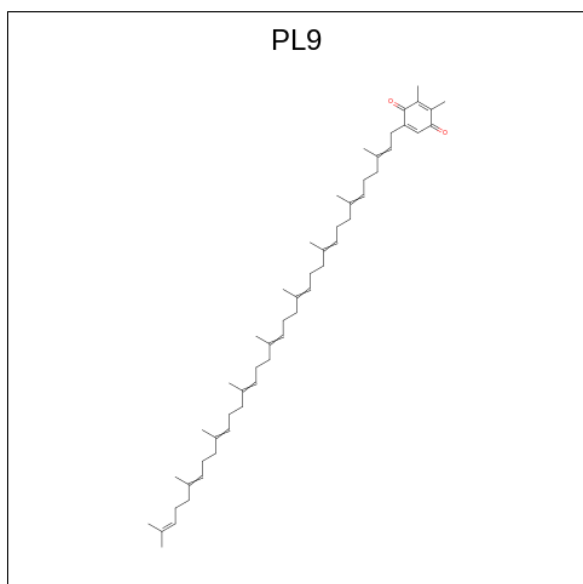
Mol	Chain	Residues	Atoms		AltConf
			Total	Fe	
28	D	1	1	1	0
28	d	1	1	1	0

- Molecule 29 is BICARBONATE ION (three-letter code: BCT) (formula: CHO₃) (labeled as "Ligand of Interest" by depositor).



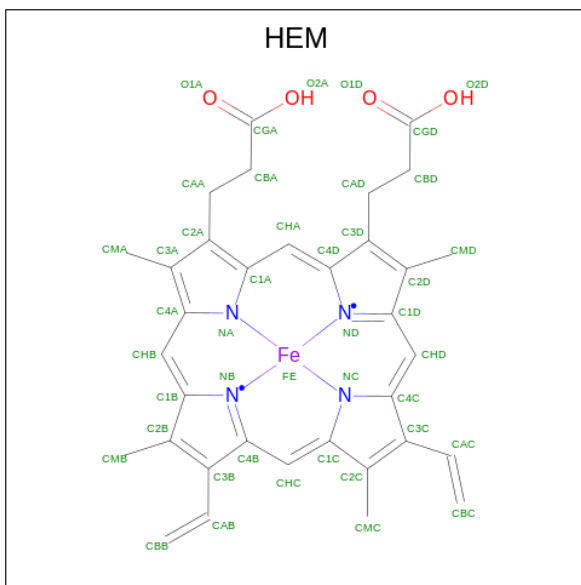
Mol	Chain	Residues	Atoms			AltConf
29	D	1	Total	C	O	0
			4	1	3	
29	d	1	Total	C	O	0
			4	1	3	

- Molecule 30 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) (labeled as "Ligand of Interest" by depositor).



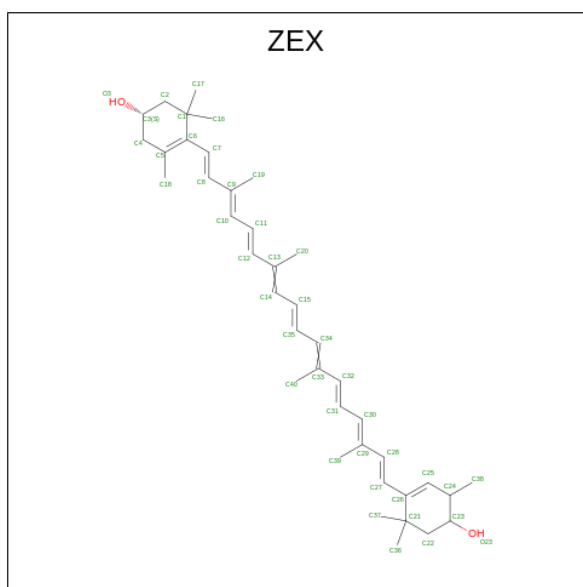
Mol	Chain	Residues	Atoms			AltConf
30	D	1	Total	C	O	0
			55	53	2	
30	d	1	Total	C	O	0
			55	53	2	

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
31	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
31	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 32 is (1R,2S)-4-[(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl]-2,5,5-trimethylcyclohex-3-en-1-ol (three-letter code: ZEX) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



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

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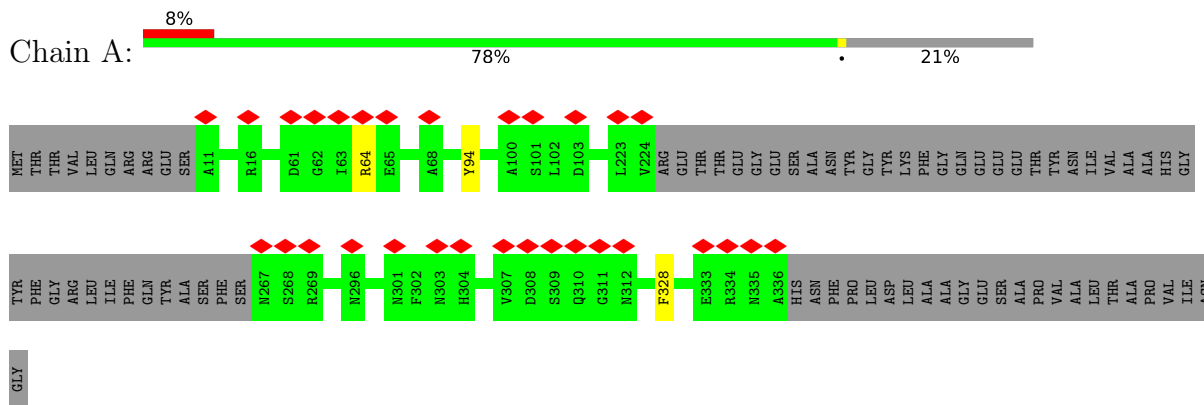
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Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
32	4	1	Total 42	C 40	O 2	0
32	6	1	Total 42	C 40	O 2	0
32	6	1	Total 42	C 40	O 2	0
32	6	1	Total 42	C 40	O 2	0
32	6	1	Total 42	C 40	O 2	0
32	5	1	Total 42	C 40	O 2	0
32	5	1	Total 42	C 40	O 2	0
32	7	1	Total 42	C 40	O 2	0
32	7	1	Total 42	C 40	O 2	0
32	7	1	Total 42	C 40	O 2	0
32	8	1	Total 42	C 40	O 2	0
32	8	1	Total 42	C 40	O 2	0
32	8	1	Total 42	C 40	O 2	0
32	8	1	Total 42	C 40	O 2	0

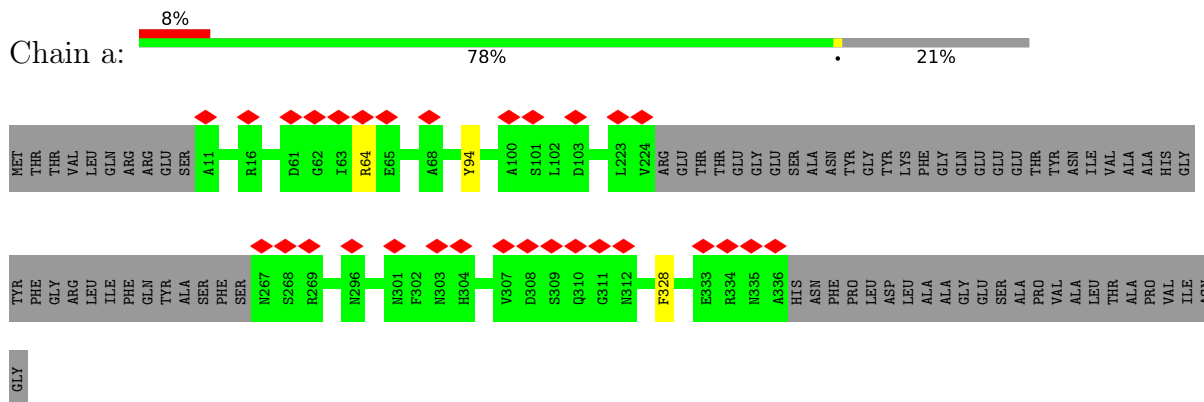
3 Residue-property plots

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.

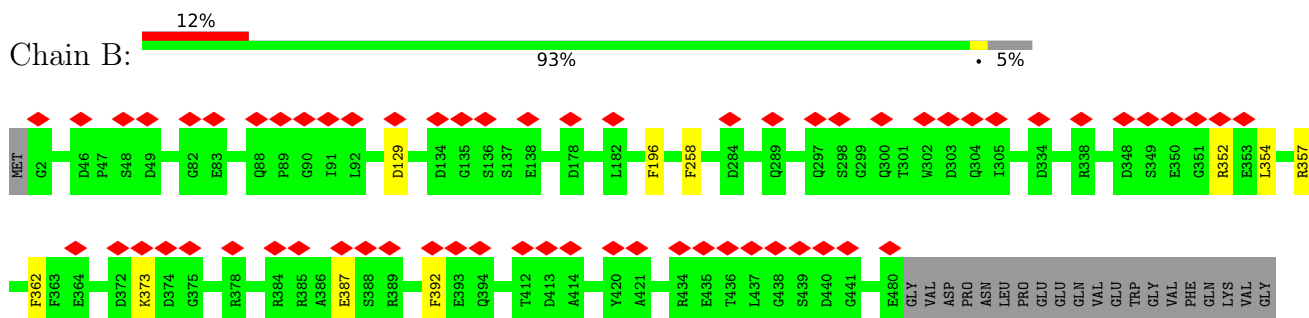
- Molecule 1: Photosystem II protein D1 2



- Molecule 1: Photosystem II protein D1 2

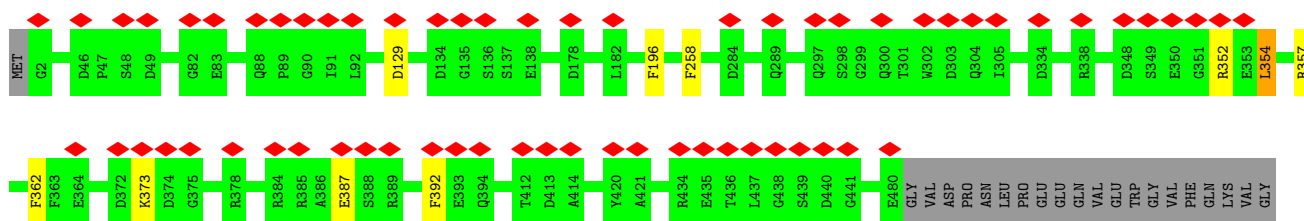


- Molecule 2: Photosystem II CP47 reaction center protein



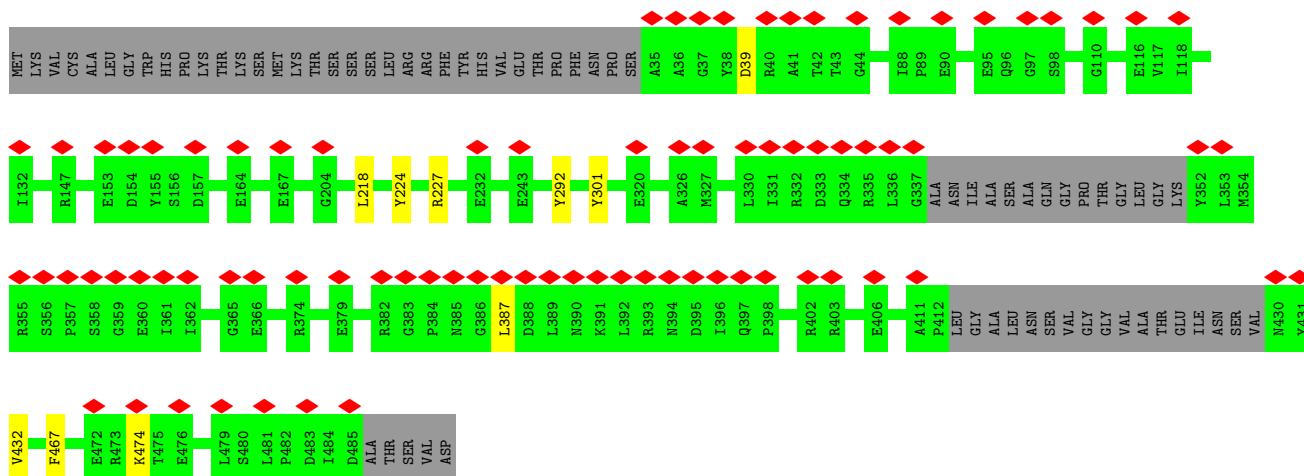
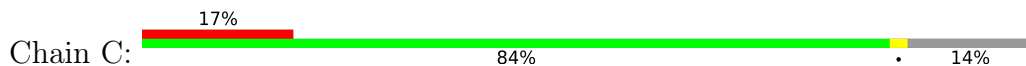
ASP
THR
THR
THR
ARG
ALA

• Molecule 2: Photosystem II CP47 reaction center protein

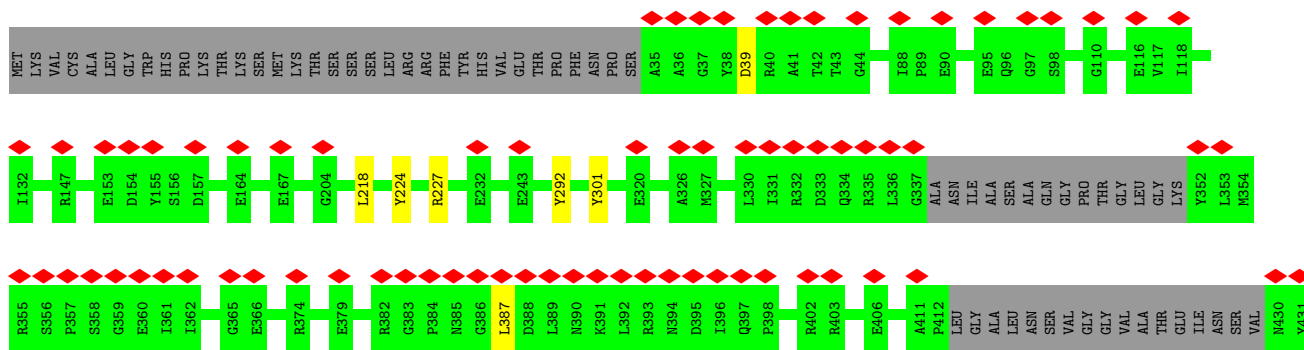
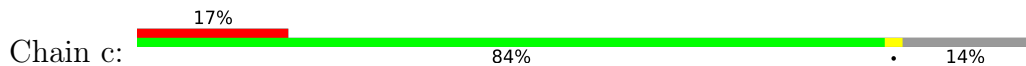


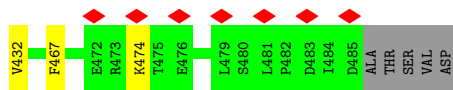
ASP
THR
THR
THR
ARG
ALA

• Molecule 3: Photosystem II CP43 reaction center protein

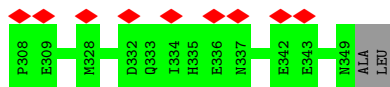
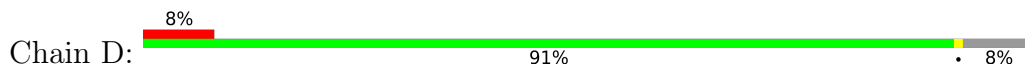


• Molecule 3: Photosystem II CP43 reaction center protein

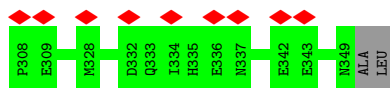
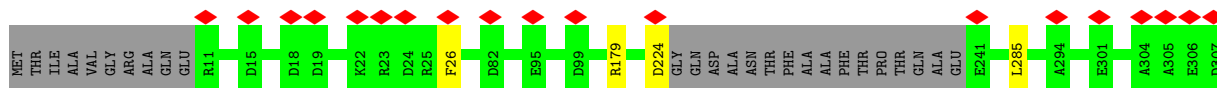
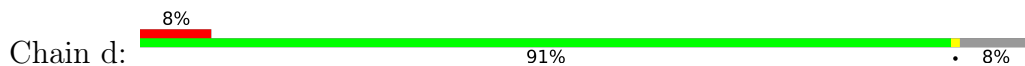




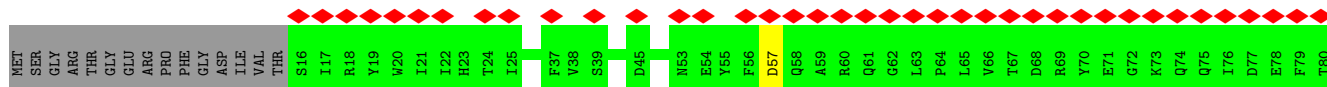
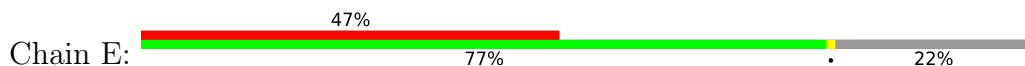
• Molecule 4: Photosystem II D2 protein 1



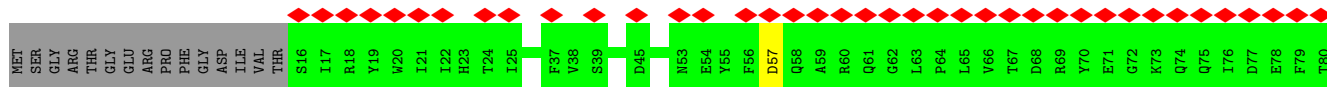
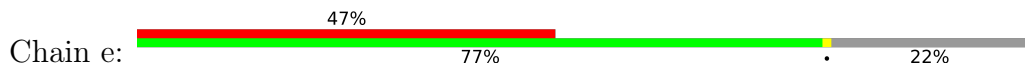
• Molecule 4: Photosystem II D2 protein 1



• Molecule 5: Cytochrome b559 subunit alpha

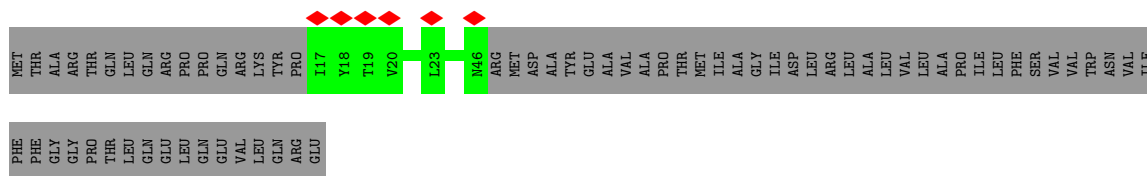


• Molecule 5: Cytochrome b559 subunit alpha

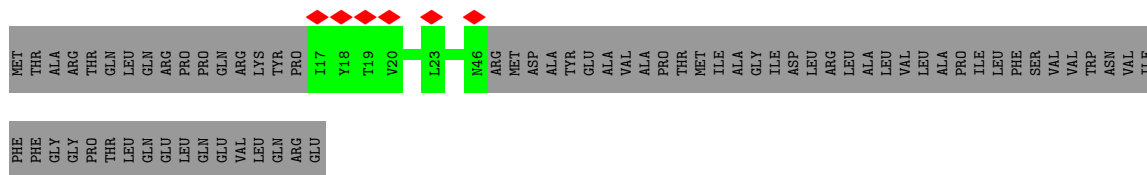


• Molecule 6: Photosystem II protein Y

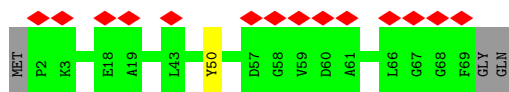




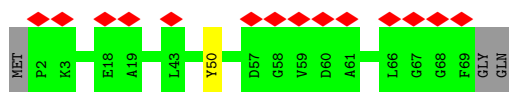
• Molecule 6: Photosystem II protein Y



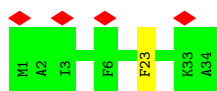
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



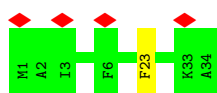
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



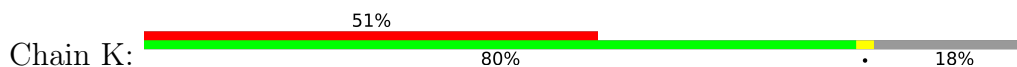
• Molecule 8: Photosystem II protein PsbI

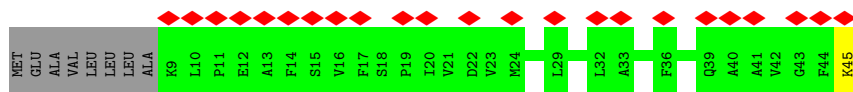


• Molecule 8: Photosystem II protein PsbI

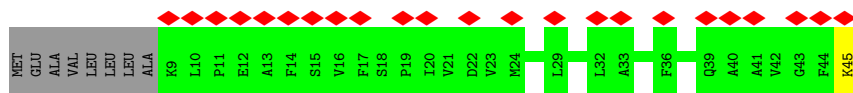
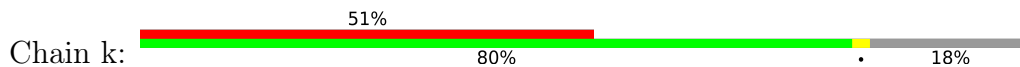


• Molecule 9: Photosystem II reaction center protein K

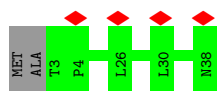




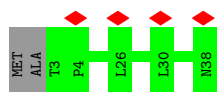
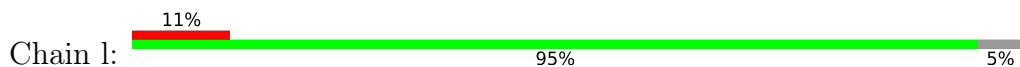
• Molecule 9: Photosystem II reaction center protein K



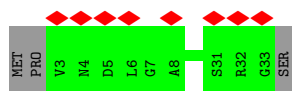
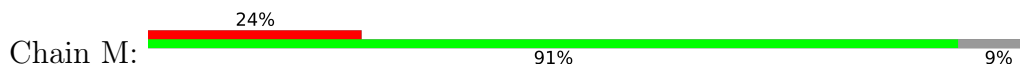
• Molecule 10: Photosystem II reaction center protein L



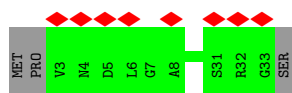
• Molecule 10: Photosystem II reaction center protein L



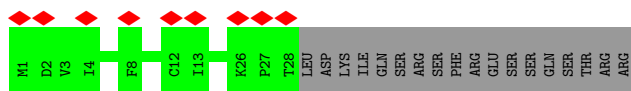
• Molecule 11: Photosystem II reaction center protein M



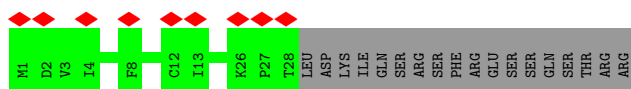
• Molecule 11: Photosystem II reaction center protein M



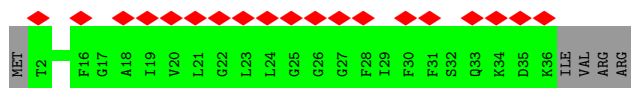
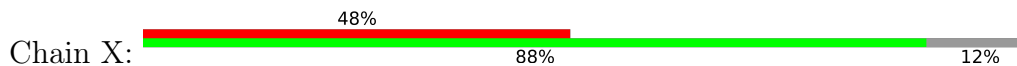
• Molecule 12: Photosystem II reaction center protein T



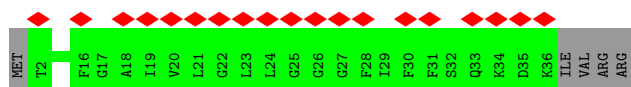
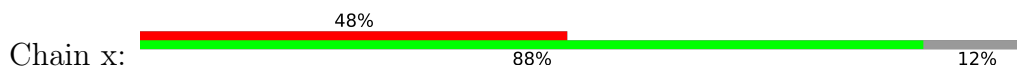
• Molecule 12: Photosystem II reaction center protein T



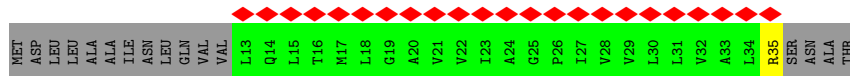
• Molecule 13: Photosystem II reaction center X protein



• Molecule 13: Photosystem II reaction center X protein



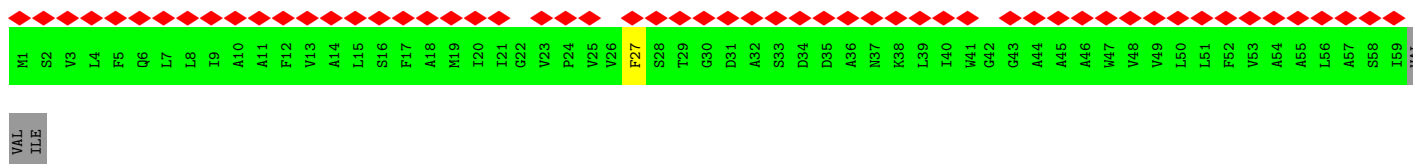
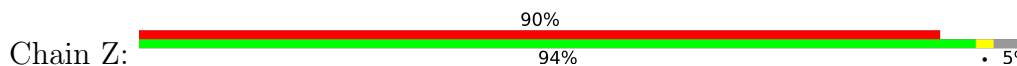
• Molecule 14: Photosystem II reaction center protein Ycf12



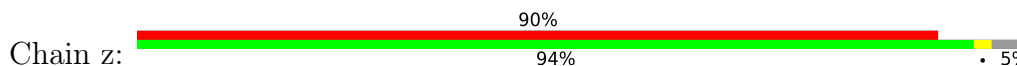
• Molecule 14: Photosystem II reaction center protein Ycf12



• Molecule 15: Photosystem II reaction center protein Z



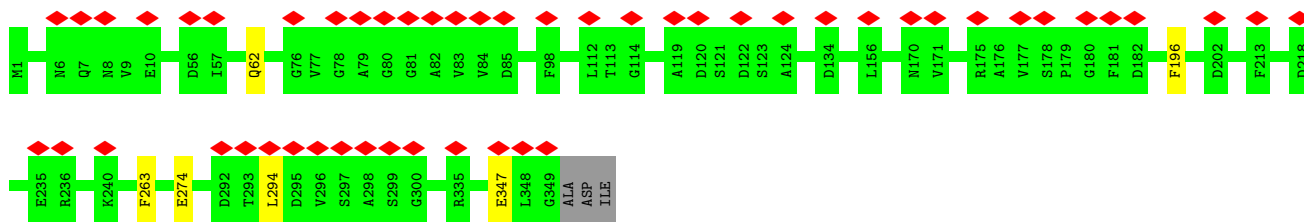
• Molecule 15: Photosystem II reaction center protein Z



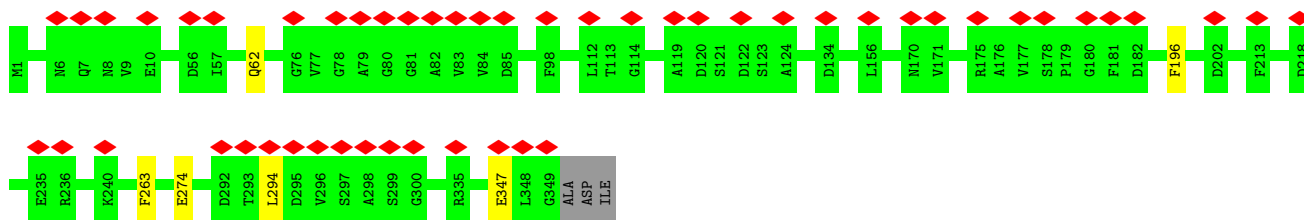


VAL
ILE

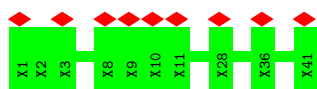
- Molecule 16: High light inducible protein



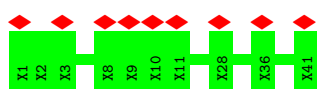
- Molecule 16: High light inducible protein



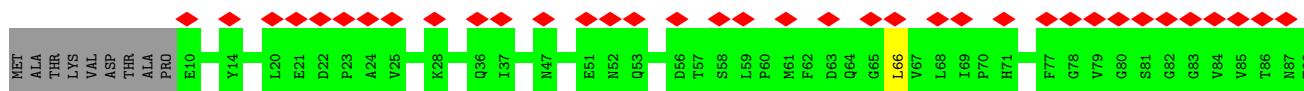
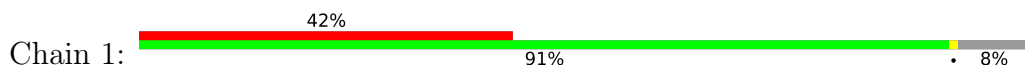
- Molecule 17: Unknown protein

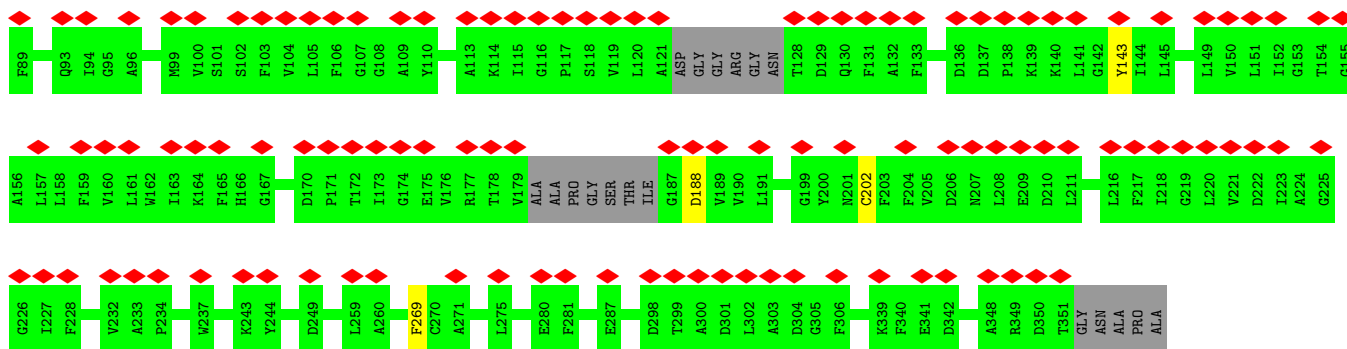


- Molecule 17: Unknown protein

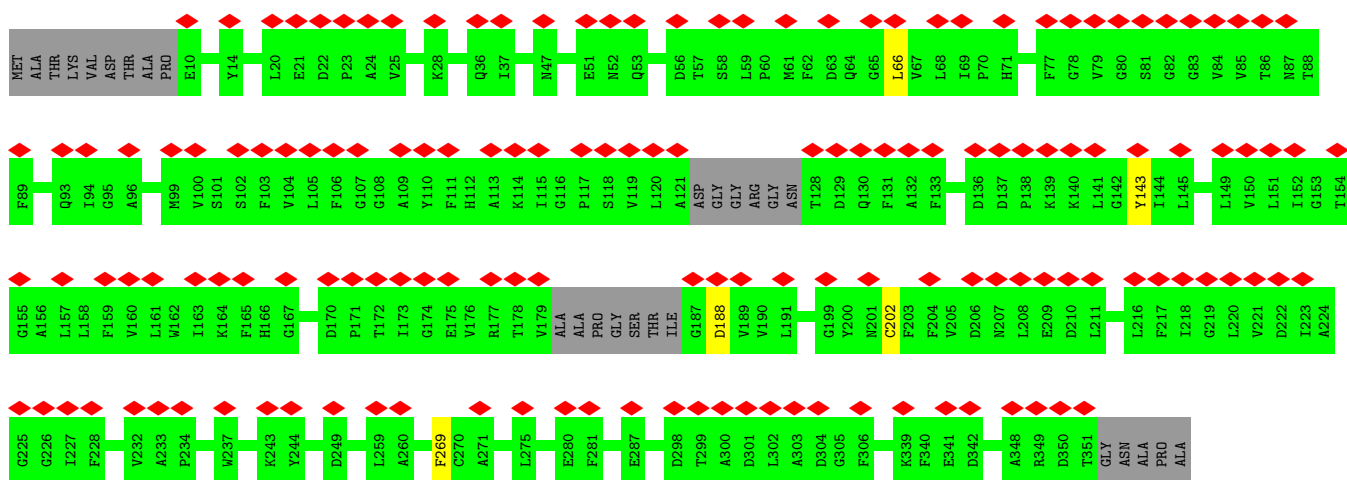
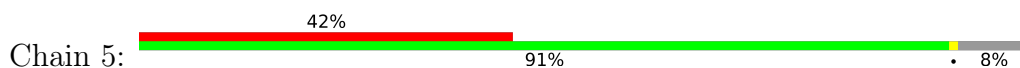


- Molecule 18: High light inducible protein

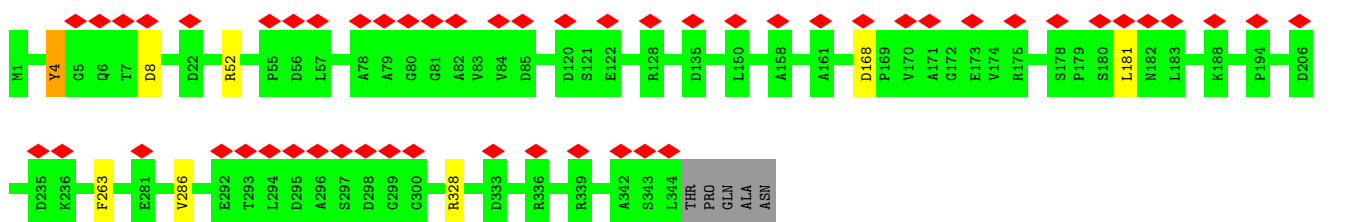




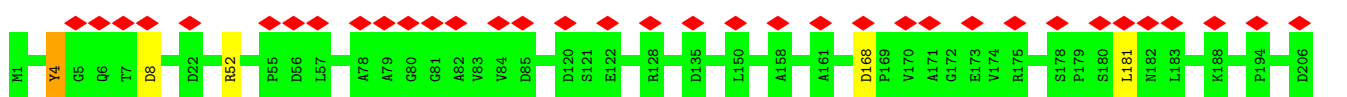
• Molecule 18: High light inducible protein

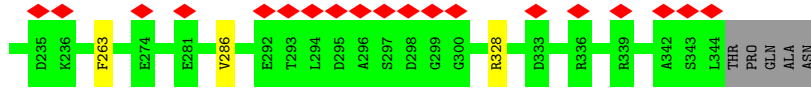


• Molecule 19: High light inducible protein

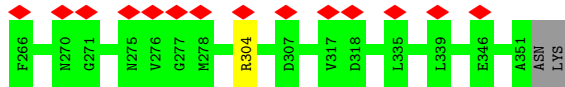
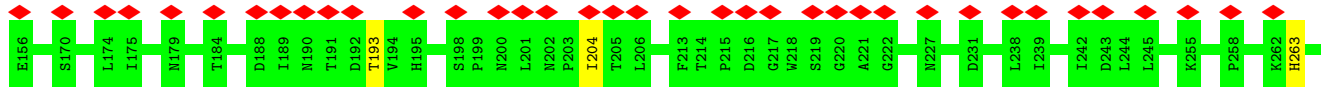
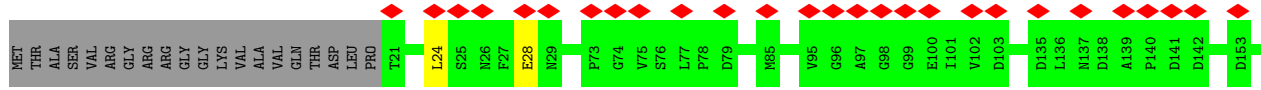
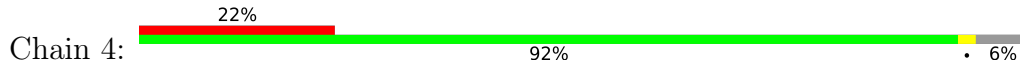


• Molecule 19: High light inducible protein

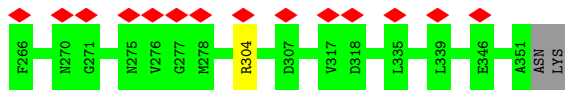
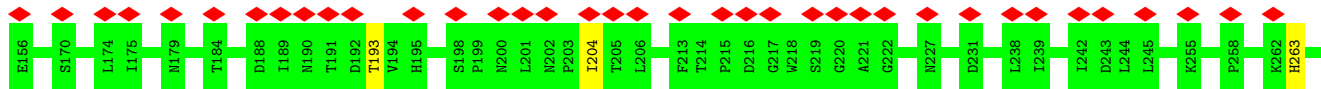
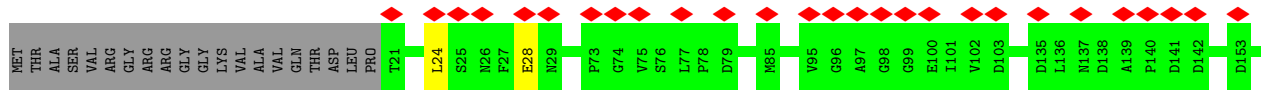
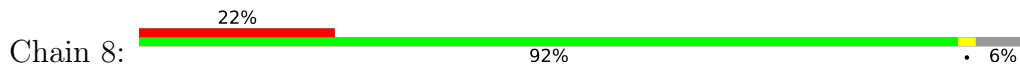




• Molecule 20: High light inducible protein



• Molecule 20: High light inducible protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132346	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)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.041	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0188	Depositor
Map size (\AA)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	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: BCT, SQD, ZEX, PL9, HEM, FE2, 8CT, PHO, CL7, LMG, DGD, LHG

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	A	0.47	0/2280	0.48	0/3112
1	a	0.47	0/2280	0.48	0/3112
2	B	0.46	0/3929	0.47	0/5360
2	b	0.46	0/3929	0.47	1/5360 (0.0%)
3	C	0.43	0/3431	0.48	1/4669 (0.0%)
3	c	0.43	0/3431	0.48	1/4669 (0.0%)
4	D	0.45	0/2672	0.47	0/3641
4	d	0.45	0/2672	0.47	0/3641
5	E	0.35	0/555	0.44	0/757
5	e	0.35	0/555	0.44	0/757
6	F	0.37	0/250	0.42	0/343
6	f	0.37	0/250	0.42	0/343
7	H	0.37	0/534	0.49	0/729
7	h	0.37	0/534	0.49	0/729
8	I	0.49	0/290	0.43	0/391
8	i	0.49	0/290	0.43	0/391
9	K	0.35	0/303	0.43	0/413
9	k	0.35	0/303	0.43	0/413
10	L	0.44	0/295	0.45	0/401
10	l	0.44	0/295	0.45	0/401
11	M	0.40	0/236	0.48	0/322
11	m	0.40	0/236	0.48	0/322
12	T	0.42	0/238	0.43	0/321
12	t	0.42	0/238	0.43	0/321
13	X	0.34	0/276	0.40	0/370
13	x	0.34	0/276	0.40	0/370
14	Y	0.26	0/164	0.42	0/224
14	y	0.26	0/164	0.42	0/224
15	Z	0.29	0/438	0.38	0/599
15	z	0.29	0/438	0.38	0/599
16	2	0.44	0/2830	0.47	0/3855
16	6	0.44	0/2830	0.47	0/3855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	1	0.37	0/2652	0.45	0/3618
18	5	0.37	0/2652	0.45	0/3618
19	3	0.46	0/2814	0.48	0/3841
19	7	0.46	0/2814	0.48	0/3841
20	4	0.38	0/2590	0.47	0/3537
20	8	0.39	0/2590	0.47	0/3537
All	All	0.43	0/53554	0.47	3/73006 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	387	LEU	CA-CB-CG	5.61	128.20	115.30
3	C	387	LEU	CA-CB-CG	5.59	128.16	115.30
2	b	354	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

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	A	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
1	a	280/360 (78%)	269 (96%)	11 (4%)	0	100	100
2	B	477/506 (94%)	452 (95%)	25 (5%)	0	100	100
2	b	477/506 (94%)	451 (94%)	26 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
3	c	414/490 (84%)	398 (96%)	16 (4%)	0	100	100
4	D	319/351 (91%)	309 (97%)	10 (3%)	0	100	100
4	d	319/351 (91%)	310 (97%)	9 (3%)	0	100	100
5	E	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
5	e	63/83 (76%)	59 (94%)	4 (6%)	0	100	100
6	F	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
6	f	28/99 (28%)	27 (96%)	1 (4%)	0	100	100
7	H	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
7	h	66/71 (93%)	62 (94%)	4 (6%)	0	100	100
8	I	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
8	i	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
9	K	35/45 (78%)	35 (100%)	0	0	100	100
9	k	35/45 (78%)	35 (100%)	0	0	100	100
10	L	34/38 (90%)	34 (100%)	0	0	100	100
10	l	34/38 (90%)	34 (100%)	0	0	100	100
11	M	29/34 (85%)	29 (100%)	0	0	100	100
11	m	29/34 (85%)	29 (100%)	0	0	100	100
12	T	26/46 (56%)	26 (100%)	0	0	100	100
12	t	26/46 (56%)	26 (100%)	0	0	100	100
13	X	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
13	x	33/40 (82%)	32 (97%)	1 (3%)	0	100	100
14	Y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
14	y	21/39 (54%)	20 (95%)	1 (5%)	0	100	100
15	Z	57/62 (92%)	57 (100%)	0	0	100	100
15	z	57/62 (92%)	57 (100%)	0	0	100	100
16	2	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
16	6	347/352 (99%)	325 (94%)	22 (6%)	0	100	100
18	1	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	41	71
18	5	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	41	71
19	3	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	41	71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	7	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	41	71
20	4	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
20	8	329/353 (93%)	306 (93%)	23 (7%)	0	100	100
All	All	6510/7416 (88%)	6206 (95%)	300 (5%)	4 (0%)	54	81

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	3	4	TYR
19	7	4	TYR
18	1	202	CYS
18	5	202	CYS

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	A	232/292 (80%)	229 (99%)	3 (1%)	69	82
1	a	232/292 (80%)	229 (99%)	3 (1%)	69	82
2	B	395/418 (94%)	385 (98%)	10 (2%)	47	72
2	b	395/418 (94%)	385 (98%)	10 (2%)	47	72
3	C	322/378 (85%)	313 (97%)	9 (3%)	43	70
3	c	322/378 (85%)	313 (97%)	9 (3%)	43	70
4	D	265/284 (93%)	261 (98%)	4 (2%)	65	81
4	d	265/284 (93%)	261 (98%)	4 (2%)	65	81
5	E	57/71 (80%)	56 (98%)	1 (2%)	59	78
5	e	57/71 (80%)	56 (98%)	1 (2%)	59	78
6	F	25/84 (30%)	25 (100%)	0	100	100
6	f	25/84 (30%)	25 (100%)	0	100	100
7	H	55/57 (96%)	54 (98%)	1 (2%)	59	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	h	55/57 (96%)	54 (98%)	1 (2%)	59	78
8	I	30/30 (100%)	29 (97%)	1 (3%)	38	66
8	i	30/30 (100%)	29 (97%)	1 (3%)	38	66
9	K	31/37 (84%)	30 (97%)	1 (3%)	39	67
9	k	31/37 (84%)	30 (97%)	1 (3%)	39	67
10	L	33/34 (97%)	33 (100%)	0	100	100
10	l	33/34 (97%)	33 (100%)	0	100	100
11	M	24/27 (89%)	24 (100%)	0	100	100
11	m	24/27 (89%)	24 (100%)	0	100	100
12	T	24/42 (57%)	24 (100%)	0	100	100
12	t	24/42 (57%)	24 (100%)	0	100	100
13	X	28/33 (85%)	28 (100%)	0	100	100
13	x	28/33 (85%)	28 (100%)	0	100	100
14	Y	18/31 (58%)	17 (94%)	1 (6%)	21	52
14	y	18/31 (58%)	17 (94%)	1 (6%)	21	52
15	Z	43/46 (94%)	42 (98%)	1 (2%)	50	73
15	z	43/46 (94%)	42 (98%)	1 (2%)	50	73
16	2	276/278 (99%)	270 (98%)	6 (2%)	52	74
16	6	276/278 (99%)	270 (98%)	6 (2%)	52	74
18	1	262/278 (94%)	258 (98%)	4 (2%)	65	81
18	5	262/278 (94%)	258 (98%)	4 (2%)	65	81
19	3	269/273 (98%)	261 (97%)	8 (3%)	41	68
19	7	269/273 (98%)	261 (97%)	8 (3%)	41	68
20	4	260/277 (94%)	254 (98%)	6 (2%)	50	73
20	8	260/277 (94%)	254 (98%)	6 (2%)	50	73
All	All	5298/5940 (89%)	5186 (98%)	112 (2%)	56	75

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	94	TYR
1	A	328	PHE

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Mol	Chain	Res	Type
2	B	129	ASP
2	B	196	PHE
2	B	258	PHE
2	B	352	ARG
2	B	354	LEU
2	B	357	ARG
2	B	362	PHE
2	B	373	LYS
2	B	387	GLU
2	B	392	PHE
3	C	39	ASP
3	C	218	LEU
3	C	224	TYR
3	C	227	ARG
3	C	292	TYR
3	C	301	TYR
3	C	432	VAL
3	C	467	PHE
3	C	474	LYS
4	D	26	PHE
4	D	179	ARG
4	D	224	ASP
4	D	285	LEU
5	E	57	ASP
7	H	50	TYR
8	I	23	PHE
9	K	45	LYS
14	Y	35	ARG
15	Z	27	PHE
16	2	62	GLN
16	2	196	PHE
16	2	263	PHE
16	2	274	GLU
16	2	294	LEU
16	2	347	GLU
18	1	66	LEU
18	1	143	TYR
18	1	188	ASP
18	1	269	PHE
19	3	4	TYR
19	3	8	ASP
19	3	52	ARG

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Mol	Chain	Res	Type
19	3	168	ASP
19	3	181	LEU
19	3	263	PHE
19	3	286	VAL
19	3	328	ARG
20	4	24	LEU
20	4	28	GLU
20	4	193	THR
20	4	204	ILE
20	4	263	HIS
20	4	304	ARG
1	a	64	ARG
1	a	94	TYR
1	a	328	PHE
2	b	129	ASP
2	b	196	PHE
2	b	258	PHE
2	b	352	ARG
2	b	354	LEU
2	b	357	ARG
2	b	362	PHE
2	b	373	LYS
2	b	387	GLU
2	b	392	PHE
3	c	39	ASP
3	c	218	LEU
3	c	224	TYR
3	c	227	ARG
3	c	292	TYR
3	c	301	TYR
3	c	432	VAL
3	c	467	PHE
3	c	474	LYS
4	d	26	PHE
4	d	179	ARG
4	d	224	ASP
4	d	285	LEU
5	e	57	ASP
7	h	50	TYR
8	i	23	PHE
9	k	45	LYS
14	y	35	ARG

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Mol	Chain	Res	Type
15	z	27	PHE
16	6	62	GLN
16	6	196	PHE
16	6	263	PHE
16	6	274	GLU
16	6	294	LEU
16	6	347	GLU
18	5	66	LEU
18	5	143	TYR
18	5	188	ASP
18	5	269	PHE
19	7	4	TYR
19	7	8	ASP
19	7	52	ARG
19	7	168	ASP
19	7	181	LEU
19	7	263	PHE
19	7	286	VAL
19	7	328	ARG
20	8	24	LEU
20	8	28	GLU
20	8	193	THR
20	8	204	ILE
20	8	263	HIS
20	8	304	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
5	E	23	HIS
16	2	62	GLN
18	1	215	HIS
20	4	195	HIS
20	4	280	ASN
5	e	23	HIS
16	6	62	GLN
18	5	215	HIS
19	7	34	GLN
20	8	195	HIS
20	8	280	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 2 are monoatomic - leaving 310 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
23	8CT	c	516	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
24	SQD	6	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	b	615	-	61,68,73	2.30	14 (22%)	59,107,113	2.37	18 (30%)
21	CL7	C	511	-	66,73,73	2.23	11 (16%)	65,113,113	2.19	17 (26%)
21	CL7	3	502	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
32	ZEX	8	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	8	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.88	15 (36%)
25	LHG	b	624	-	44,44,48	0.31	0	47,50,54	0.39	0
21	CL7	4	404	-	66,73,73	2.22	13 (19%)	65,113,113	2.21	16 (24%)
21	CL7	7	512	-	56,63,73	2.39	13 (23%)	53,101,113	2.45	18 (33%)
21	CL7	6	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	8	408	-	46,53,73	2.66	15 (32%)	41,89,113	2.66	13 (31%)
32	ZEX	3	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	6	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	D	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
25	LHG	7	524	-	35,35,48	0.34	0	38,41,54	0.47	0
25	LHG	3	524	-	35,35,48	0.34	0	38,41,54	0.47	0
32	ZEX	7	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)
21	CL7	5	418	18	66,73,73	2.18	12 (18%)	65,113,113	2.31	20 (30%)
21	CL7	6	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.68	12 (29%)
21	CL7	c	511	-	66,73,73	2.23	11 (16%)	65,113,113	2.20	17 (26%)
32	ZEX	7	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	c	504	-	66,73,73	2.20	14 (21%)	65,113,113	2.22	17 (26%)
21	CL7	2	510	16	66,73,73	2.18	13 (19%)	65,113,113	2.24	18 (27%)
24	SQD	A	405	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
23	8CT	C	516	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	7	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	3	501	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	5	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.76	14 (38%)
21	CL7	3	506	-	46,53,73	2.58	14 (30%)	41,89,113	2.72	14 (34%)
32	ZEX	8	419	-	42,43,43	0.99	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	3	508	-	66,73,73	2.20	14 (21%)	65,113,113	2.23	18 (27%)
26	LMG	B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
23	8CT	c	515	-	40,41,41	4.64	22 (55%)	50,56,56	2.40	23 (46%)
32	ZEX	6	524	-	42,43,43	1.03	4 (9%)	55,60,60	2.51	17 (30%)
21	CL7	1	406	-	63,70,73	2.26	12 (19%)	61,109,113	2.30	14 (22%)
21	CL7	5	420	18	46,53,73	2.63	12 (26%)	41,89,113	2.74	14 (34%)
21	CL7	3	514	-	46,53,73	2.63	14 (30%)	41,89,113	2.80	14 (34%)
21	CL7	5	406	-	63,70,73	2.26	12 (19%)	61,109,113	2.29	14 (22%)
21	CL7	b	608	-	61,68,73	2.30	13 (21%)	59,107,113	2.27	16 (27%)
25	LHG	a	406	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	C	509	-	66,73,73	2.22	13 (19%)	65,113,113	2.28	21 (32%)
21	CL7	4	406	-	66,73,73	2.21	12 (18%)	65,113,113	2.22	17 (26%)
32	ZEX	4	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	7	511	19	66,73,73	2.18	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	b	613	-	66,73,73	2.15	13 (19%)	65,113,113	2.28	18 (27%)
21	CL7	C	502	-	66,73,73	2.18	13 (19%)	65,113,113	2.19	15 (23%)
21	CL7	6	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
23	8CT	C	515	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)
25	LHG	4	401	-	48,48,48	0.28	0	51,54,54	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	2	502	-	66,73,73	2.19	13 (19%)	65,113,113	2.26	18 (27%)
32	ZEX	4	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	5	403	-	61,68,73	2.29	13 (21%)	59,107,113	2.38	15 (25%)
29	BCT	D	403	28	2,3,3	1.00	0	2,3,3	1.67	1 (50%)
21	CL7	6	511	16	61,68,73	2.33	11 (18%)	59,107,113	2.21	15 (25%)
25	LHG	b	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	6	504	-	46,53,73	2.62	13 (28%)	41,89,113	2.63	14 (34%)
21	CL7	3	518	19	46,53,73	2.68	12 (26%)	41,89,113	2.66	14 (34%)
21	CL7	3	512	-	56,63,73	2.38	13 (23%)	53,101,113	2.45	18 (33%)
21	CL7	b	614	-	56,63,73	2.38	14 (25%)	53,101,113	2.41	17 (32%)
24	SQD	B	626	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
32	ZEX	8	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
27	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
23	8CT	4	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	C	507	-	61,68,73	2.31	13 (21%)	59,107,113	2.39	18 (30%)
21	CL7	7	517	19	51,58,73	2.49	13 (25%)	47,95,113	2.55	14 (29%)
25	LHG	B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	2	517	16	66,73,73	2.18	12 (18%)	65,113,113	2.20	17 (26%)
32	ZEX	2	525	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
30	PL9	d	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.62	1 (1%)
21	CL7	b	612	-	66,73,73	2.19	14 (21%)	65,113,113	2.26	15 (23%)
21	CL7	7	507	-	66,73,73	2.16	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	2	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.31	17 (26%)
21	CL7	8	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.50	20 (33%)
32	ZEX	5	422	-	42,43,43	0.95	1 (2%)	55,60,60	2.24	18 (32%)
21	CL7	7	505	-	66,73,73	2.16	13 (19%)	65,113,113	2.34	15 (23%)
21	CL7	5	405	-	46,53,73	2.62	13 (28%)	41,89,113	2.59	12 (29%)
32	ZEX	8	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	1	403	-	61,68,73	2.29	13 (21%)	59,107,113	2.39	15 (25%)
21	CL7	d	402	-	51,58,73	2.55	12 (23%)	47,95,113	2.47	15 (31%)
21	CL7	B	610	-	66,73,73	2.16	13 (19%)	65,113,113	2.31	15 (23%)
26	LMG	b	622	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	3	516	19	56,63,73	2.42	13 (23%)	53,101,113	2.43	19 (35%)
21	CL7	5	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	c	510	-	66,73,73	2.22	14 (21%)	65,113,113	2.23	16 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	5	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	7	502	-	59,66,73	2.36	13 (22%)	56,104,113	2.26	17 (30%)
26	LMG	5	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
21	CL7	5	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	A	406	-	66,73,73	2.24	13 (19%)	65,113,113	2.30	16 (24%)
21	CL7	4	407	-	42,49,73	2.66	10 (23%)	36,84,113	2.86	14 (38%)
21	CL7	7	504	-	66,73,73	2.21	13 (19%)	65,113,113	2.24	17 (26%)
21	CL7	B	611	-	66,73,73	2.18	14 (21%)	65,113,113	2.26	16 (24%)
21	CL7	a	405	-	66,73,73	2.24	13 (19%)	65,113,113	2.29	16 (24%)
21	CL7	b	606	-	66,73,73	2.23	14 (21%)	65,113,113	2.22	15 (23%)
21	CL7	1	407	-	42,49,73	2.66	11 (26%)	36,84,113	2.81	15 (41%)
22	PHO	a	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
21	CL7	c	503	-	61,68,73	2.30	14 (22%)	59,107,113	2.30	15 (25%)
24	SQD	3	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	C	508	-	66,73,73	2.17	14 (21%)	65,113,113	2.26	18 (27%)
21	CL7	1	411	-	46,53,73	2.64	12 (26%)	41,89,113	2.61	14 (34%)
21	CL7	b	617	-	46,53,73	2.62	14 (30%)	41,89,113	2.60	16 (39%)
21	CL7	A	403	-	56,63,73	2.40	14 (25%)	53,101,113	2.59	18 (33%)
21	CL7	c	506	-	66,73,73	2.21	14 (21%)	65,113,113	2.25	17 (26%)
21	CL7	C	514	-	46,53,73	2.63	12 (26%)	41,89,113	2.69	14 (34%)
24	SQD	1	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
26	LMG	c	501	-	50,50,55	0.91	2 (4%)	58,58,63	1.21	5 (8%)
32	ZEX	1	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	B	622	-	46,53,73	2.67	12 (26%)	41,89,113	2.58	13 (31%)
24	SQD	5	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
21	CL7	8	410	-	46,53,73	2.61	12 (26%)	41,89,113	2.65	13 (31%)
24	SQD	2	524	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	7	501	-	66,73,73	2.22	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	2	501	-	66,73,73	2.17	12 (18%)	65,113,113	2.23	15 (23%)
21	CL7	D	402	-	51,58,73	2.55	12 (23%)	47,95,113	2.46	15 (31%)
21	CL7	7	508	-	66,73,73	2.20	14 (21%)	65,113,113	2.24	18 (27%)
21	CL7	3	517	19	51,58,73	2.49	13 (25%)	47,95,113	2.54	14 (29%)
21	CL7	8	405	-	66,73,73	2.21	14 (21%)	65,113,113	2.31	20 (30%)
27	DGD	b	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
23	8CT	B	627	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	ZEX	6	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	B	607	-	61,68,73	2.30	13 (21%)	59,107,113	2.27	16 (27%)
21	CL7	7	510	-	66,73,73	2.18	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	5	410	-	66,73,73	2.24	13 (19%)	65,113,113	2.17	16 (24%)
24	SQD	7	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	3	510	-	66,73,73	2.18	13 (19%)	65,113,113	2.22	18 (27%)
21	CL7	7	518	19	46,53,73	2.68	13 (28%)	41,89,113	2.66	14 (34%)
21	CL7	2	518	16	66,73,73	2.23	12 (18%)	65,113,113	2.17	17 (26%)
29	BCT	d	403	28	2,3,3	1.00	0	2,3,3	1.67	1 (50%)
21	CL7	7	509	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
31	HEM	F	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
32	ZEX	6	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	b	610	-	66,73,73	2.24	14 (21%)	65,113,113	2.15	15 (23%)
21	CL7	1	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.91	14 (38%)
32	ZEX	2	520	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	4	417	20	43,50,73	2.67	11 (25%)	36,85,113	2.89	13 (36%)
23	8CT	b	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
23	8CT	8	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
32	ZEX	7	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	4	409	-	61,68,73	2.27	14 (22%)	59,107,113	2.50	20 (33%)
23	8CT	b	619	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	3	509	-	66,73,73	2.20	11 (16%)	65,113,113	2.19	16 (24%)
21	CL7	4	413	20	61,68,73	2.27	14 (22%)	59,107,113	2.32	16 (27%)
21	CL7	1	418	18	66,73,73	2.17	12 (18%)	65,113,113	2.31	20 (30%)
21	CL7	C	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.25	17 (26%)
21	CL7	C	505	-	56,63,73	2.43	12 (21%)	53,101,113	2.38	14 (26%)
21	CL7	3	504	-	66,73,73	2.20	13 (19%)	65,113,113	2.24	17 (26%)
23	8CT	B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
32	ZEX	4	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	7	516	19	56,63,73	2.41	13 (23%)	53,101,113	2.42	19 (35%)
21	CL7	b	602	-	42,49,73	2.67	11 (26%)	36,84,113	2.82	12 (33%)
21	CL7	D	405	-	46,53,73	2.57	13 (28%)	41,89,113	2.73	16 (39%)
21	CL7	1	416	-	42,49,73	2.73	10 (23%)	36,84,113	2.76	14 (38%)
23	8CT	b	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	C	513	-	42,49,73	2.56	9 (21%)	36,84,113	2.89	14 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	6	503	-	66,73,73	2.19	15 (22%)	65,113,113	2.38	19 (29%)
26	LMG	C	501	-	50,50,55	0.92	2 (4%)	58,58,63	1.22	5 (8%)
21	CL7	b	611	-	66,73,73	2.15	13 (19%)	65,113,113	2.32	15 (23%)
21	CL7	B	606	-	56,63,73	2.43	14 (25%)	53,101,113	2.48	16 (30%)
21	CL7	1	414	-	42,49,73	2.73	10 (23%)	36,84,113	2.92	15 (41%)
21	CL7	c	509	-	66,73,73	2.21	13 (19%)	65,113,113	2.29	21 (32%)
21	CL7	5	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.71	14 (34%)
21	CL7	5	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.62	15 (36%)
21	CL7	2	516	-	66,73,73	2.20	13 (19%)	65,113,113	2.23	19 (29%)
21	CL7	1	408	-	66,73,73	2.19	13 (19%)	65,113,113	2.31	19 (29%)
21	CL7	B	615	-	51,58,73	2.44	14 (27%)	47,95,113	2.63	16 (34%)
21	CL7	1	420	18	46,53,73	2.63	12 (26%)	41,89,113	2.74	14 (34%)
21	CL7	B	605	-	66,73,73	2.24	14 (21%)	65,113,113	2.22	15 (23%)
23	8CT	k	101	-	40,41,41	4.75	24 (60%)	50,56,56	2.65	16 (32%)
25	LHG	B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
32	ZEX	1	422	-	42,43,43	0.95	1 (2%)	55,60,60	2.24	18 (32%)
21	CL7	5	417	18	56,63,73	2.42	14 (25%)	53,101,113	2.41	15 (28%)
24	SQD	6	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
31	HEM	f	101	-	41,50,50	1.41	6 (14%)	45,82,82	2.03	11 (24%)
21	CL7	8	406	-	66,73,73	2.21	13 (19%)	65,113,113	2.22	17 (26%)
32	ZEX	2	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)
21	CL7	b	607	-	56,63,73	2.43	14 (25%)	53,101,113	2.48	16 (30%)
24	SQD	3	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
21	CL7	a	403	-	56,63,73	2.40	14 (25%)	53,101,113	2.58	18 (33%)
23	8CT	c	519	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	2	503	-	66,73,73	2.18	15 (22%)	65,113,113	2.38	19 (29%)
21	CL7	1	413	-	42,49,73	2.64	10 (23%)	36,84,113	2.94	15 (41%)
21	CL7	B	603	-	66,73,73	2.22	13 (19%)	65,113,113	2.22	17 (26%)
21	CL7	6	505	-	66,73,73	2.22	13 (19%)	65,113,113	2.40	19 (29%)
23	8CT	b	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	5	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.25	16 (24%)
23	8CT	a	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	C	503	-	61,68,73	2.30	14 (22%)	59,107,113	2.30	15 (25%)
21	CL7	5	402	-	61,68,73	2.31	14 (22%)	59,107,113	2.37	15 (25%)
21	CL7	1	405	-	46,53,73	2.63	13 (28%)	41,89,113	2.59	12 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	8CT	B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
21	CL7	3	511	19	66,73,73	2.18	15 (22%)	65,113,113	2.43	19 (29%)
21	CL7	1	419	-	46,53,73	2.65	12 (26%)	41,89,113	2.58	13 (31%)
21	CL7	2	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.19	16 (24%)
21	CL7	1	410	-	66,73,73	2.24	13 (19%)	65,113,113	2.17	16 (24%)
21	CL7	4	412	-	66,73,73	2.22	12 (18%)	65,113,113	2.20	18 (27%)
22	PHO	d	408	-	51,69,69	1.68	7 (13%)	47,99,99	1.66	11 (23%)
21	CL7	4	405	-	66,73,73	2.21	14 (21%)	65,113,113	2.31	20 (30%)
21	CL7	b	623	-	46,53,73	2.67	12 (26%)	41,89,113	2.57	13 (31%)
21	CL7	2	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	15 (36%)
21	CL7	8	411	-	66,73,73	2.22	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	B	608	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	14 (21%)
21	CL7	c	508	-	66,73,73	2.17	14 (21%)	65,113,113	2.26	18 (27%)
21	CL7	5	414	-	42,49,73	2.74	10 (23%)	36,84,113	2.92	15 (41%)
21	CL7	3	513	-	46,53,73	2.66	15 (32%)	41,89,113	2.67	13 (31%)
21	CL7	d	405	-	46,53,73	2.57	13 (28%)	41,89,113	2.74	16 (39%)
21	CL7	b	605	-	66,73,73	2.15	13 (19%)	65,113,113	2.23	18 (27%)
21	CL7	B	602	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)
21	CL7	6	507	-	66,73,73	2.19	14 (21%)	65,113,113	2.31	17 (26%)
24	SQD	7	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	C	518	-	42,49,73	2.62	10 (23%)	36,84,113	2.83	14 (38%)
21	CL7	B	614	-	61,68,73	2.30	14 (22%)	59,107,113	2.37	18 (30%)
26	LMG	d	410	-	33,33,55	0.28	0	41,41,63	0.33	0
25	LHG	8	401	-	48,48,48	0.28	0	51,54,54	0.34	0
22	PHO	A	402	-	51,69,69	0.74	2 (3%)	47,99,99	0.74	1 (2%)
23	8CT	C	519	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
22	PHO	D	408	-	51,69,69	1.67	7 (13%)	47,99,99	1.66	11 (23%)
21	CL7	c	514	-	46,53,73	2.62	12 (26%)	41,89,113	2.68	14 (34%)
23	8CT	d	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
24	SQD	B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
32	ZEX	3	520	-	42,43,43	0.94	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	4	410	-	46,53,73	2.62	12 (26%)	41,89,113	2.64	13 (31%)
32	ZEX	3	519	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	6	518	16	66,73,73	2.23	12 (18%)	65,113,113	2.17	16 (24%)
21	CL7	b	603	-	61,68,73	2.32	12 (19%)	59,107,113	2.39	18 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	4	408	-	46,53,73	2.65	15 (32%)	41,89,113	2.67	13 (31%)
21	CL7	3	503	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
21	CL7	2	509	-	66,73,73	2.22	14 (21%)	65,113,113	2.17	15 (23%)
21	CL7	C	512	3	43,50,73	2.70	11 (25%)	36,85,113	2.79	12 (33%)
21	CL7	4	415	-	46,53,73	2.60	15 (32%)	41,89,113	2.88	14 (34%)
21	CL7	B	609	-	66,73,73	2.24	14 (21%)	65,113,113	2.15	15 (23%)
21	CL7	c	507	-	61,68,73	2.32	13 (21%)	59,107,113	2.40	18 (30%)
21	CL7	8	407	-	42,49,73	2.64	10 (23%)	36,84,113	2.85	14 (38%)
32	ZEX	2	523	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	16 (29%)
21	CL7	4	411	-	66,73,73	2.22	12 (18%)	65,113,113	2.20	17 (26%)
21	CL7	B	612	-	66,73,73	2.15	13 (19%)	65,113,113	2.28	18 (27%)
21	CL7	8	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.90	15 (41%)
21	CL7	c	512	3	43,50,73	2.69	11 (25%)	36,85,113	2.78	13 (36%)
32	ZEX	2	521	-	42,43,43	0.98	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	c	505	-	56,63,73	2.43	13 (23%)	53,101,113	2.38	14 (26%)
21	CL7	c	513	-	42,49,73	2.56	10 (23%)	36,84,113	2.89	14 (38%)
26	LMG	D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	A	401	-	66,73,73	2.27	15 (22%)	65,113,113	2.34	19 (29%)
21	CL7	6	508	-	46,53,73	2.59	14 (30%)	41,89,113	2.65	14 (34%)
21	CL7	4	414	-	54,61,73	2.39	13 (24%)	50,98,113	2.53	16 (32%)
21	CL7	B	616	-	46,53,73	2.62	14 (30%)	41,89,113	2.60	16 (39%)
23	8CT	D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	2	504	-	46,53,73	2.62	13 (28%)	41,89,113	2.63	14 (34%)
21	CL7	8	417	20	43,50,73	2.66	11 (25%)	36,85,113	2.89	13 (36%)
21	CL7	8	404	-	66,73,73	2.22	13 (19%)	65,113,113	2.20	16 (24%)
21	CL7	2	514	-	46,53,73	2.63	13 (28%)	41,89,113	2.68	12 (29%)
23	8CT	A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	c	502	-	66,73,73	2.18	13 (19%)	65,113,113	2.20	15 (23%)
27	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	2	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	17 (26%)
21	CL7	b	604	-	66,73,73	2.22	13 (19%)	65,113,113	2.22	17 (26%)
25	LHG	A	407	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	B	604	-	66,73,73	2.15	13 (19%)	65,113,113	2.23	18 (27%)
32	ZEX	3	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	5	415	-	42,49,73	2.70	12 (28%)	36,84,113	2.91	14 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	a	401	-	66,73,73	2.27	15 (22%)	65,113,113	2.34	19 (29%)
21	CL7	C	510	-	66,73,73	2.22	14 (21%)	65,113,113	2.23	16 (24%)
21	CL7	8	412	-	66,73,73	2.21	13 (19%)	65,113,113	2.20	18 (27%)
21	CL7	B	601	-	42,49,73	2.67	11 (26%)	36,84,113	2.81	12 (33%)
21	CL7	5	407	-	42,49,73	2.65	11 (26%)	36,84,113	2.81	16 (44%)
24	SQD	b	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
23	8CT	B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	2	511	16	61,68,73	2.33	12 (19%)	59,107,113	2.22	15 (25%)
21	CL7	5	411	-	46,53,73	2.64	12 (26%)	41,89,113	2.62	14 (34%)
27	DGD	B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	1	412	-	46,53,73	2.59	12 (26%)	41,89,113	2.70	14 (34%)
21	CL7	B	613	-	56,63,73	2.38	14 (25%)	53,101,113	2.42	17 (32%)
21	CL7	7	515	-	42,49,73	2.66	10 (23%)	36,84,113	2.86	15 (41%)
25	LHG	d	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	2	508	-	46,53,73	2.60	14 (30%)	41,89,113	2.65	14 (34%)
21	CL7	1	409	-	46,53,73	2.61	13 (28%)	41,89,113	2.61	15 (36%)
21	CL7	6	506	-	66,73,73	2.22	14 (21%)	65,113,113	2.19	16 (24%)
21	CL7	6	512	-	66,73,73	2.17	11 (16%)	65,113,113	2.28	17 (26%)
32	ZEX	4	419	-	42,43,43	0.99	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	1	402	-	61,68,73	2.31	14 (22%)	59,107,113	2.37	15 (25%)
21	CL7	1	417	18	56,63,73	2.42	14 (25%)	53,101,113	2.41	15 (28%)
21	CL7	3	505	-	66,73,73	2.16	13 (19%)	65,113,113	2.33	15 (23%)
21	CL7	6	510	16	66,73,73	2.18	13 (19%)	65,113,113	2.24	18 (27%)
21	CL7	6	515	-	46,53,73	2.62	12 (26%)	41,89,113	2.66	15 (36%)
21	CL7	d	404	-	59,66,73	2.33	14 (23%)	56,104,113	2.36	17 (30%)
21	CL7	7	506	-	46,53,73	2.59	14 (30%)	41,89,113	2.73	14 (34%)
25	LHG	D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
30	PL9	D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
21	CL7	7	503	-	66,73,73	2.19	14 (21%)	65,113,113	2.30	18 (27%)
21	CL7	c	518	-	42,49,73	2.62	10 (23%)	36,84,113	2.83	14 (38%)
21	CL7	2	505	-	66,73,73	2.22	13 (19%)	65,113,113	2.42	19 (29%)
21	CL7	7	513	-	46,53,73	2.66	15 (32%)	41,89,113	2.67	13 (31%)
21	CL7	2	513	-	46,53,73	2.65	13 (28%)	41,89,113	2.66	15 (36%)
24	SQD	2	522	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	C	504	-	66,73,73	2.20	14 (21%)	65,113,113	2.22	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	6	502	-	66,73,73	2.19	13 (19%)	65,113,113	2.26	17 (26%)
21	CL7	6	509	-	66,73,73	2.21	14 (21%)	65,113,113	2.17	15 (23%)
26	LMG	1	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
32	ZEX	5	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	3	507	-	66,73,73	2.16	13 (19%)	65,113,113	2.30	18 (27%)
21	CL7	b	616	-	51,58,73	2.44	14 (27%)	47,95,113	2.63	16 (34%)
21	CL7	8	414	-	54,61,73	2.39	14 (25%)	50,98,113	2.53	16 (32%)
32	ZEX	6	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	16 (29%)
21	CL7	6	513	-	46,53,73	2.65	13 (28%)	41,89,113	2.67	15 (36%)
21	CL7	1	404	-	66,73,73	2.27	12 (18%)	65,113,113	2.25	16 (24%)
21	CL7	4	416	-	42,49,73	2.69	10 (23%)	36,84,113	2.89	15 (41%)
21	CL7	b	609	-	66,73,73	2.19	13 (19%)	65,113,113	2.17	14 (21%)
21	CL7	3	515	-	42,49,73	2.65	10 (23%)	36,84,113	2.86	15 (41%)
23	8CT	K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.65	16 (32%)
21	CL7	8	413	20	61,68,73	2.27	14 (22%)	59,107,113	2.32	16 (27%)

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
23	8CT	c	516	-	-	10/29/63/63	0/2/2/2
24	SQD	6	521	-	-	7/45/65/69	0/1/1/1
21	CL7	b	615	-	2/2/14/20	12/31/109/115	-
21	CL7	C	511	-	2/2/15/20	20/37/115/115	-
21	CL7	3	502	-	2/2/13/20	10/29/107/115	-
32	ZEX	8	403	-	-	10/29/67/67	0/2/2/2
21	CL7	8	415	-	2/2/11/20	10/13/91/115	-
25	LHG	b	624	-	-	3/49/49/53	-
21	CL7	4	404	-	2/2/15/20	14/37/115/115	-
21	CL7	7	512	-	2/2/13/20	12/25/103/115	-
21	CL7	6	517	16	2/2/15/20	19/37/115/115	-
21	CL7	8	408	-	2/2/11/20	2/13/91/115	-
32	ZEX	3	522	-	-	5/29/67/67	0/2/2/2
21	CL7	6	501	-	2/2/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	D	404	-	2/2/13/20	11/29/107/115	-
25	LHG	7	524	-	-	3/40/40/53	-
25	LHG	3	524	-	-	3/40/40/53	-
32	ZEX	7	519	-	-	10/29/67/67	0/2/2/2
21	CL7	5	418	18	2/2/15/20	20/37/115/115	-
21	CL7	6	514	-	2/2/11/20	7/13/91/115	-
21	CL7	c	511	-	2/2/15/20	20/37/115/115	-
32	ZEX	7	520	-	-	10/29/67/67	0/2/2/2
21	CL7	c	504	-	2/2/15/20	17/37/115/115	-
21	CL7	2	510	16	2/2/15/20	20/37/115/115	-
24	SQD	A	405	-	-	3/29/49/69	0/1/1/1
23	8CT	C	516	-	-	10/29/63/63	0/2/2/2
21	CL7	7	514	-	2/2/11/20	5/13/91/115	-
21	CL7	3	501	-	2/2/15/20	19/37/115/115	-
21	CL7	5	416	-	2/2/10/20	2/8/86/115	-
21	CL7	3	506	-	2/2/11/20	11/13/91/115	-
32	ZEX	8	419	-	-	9/29/67/67	0/2/2/2
21	CL7	3	508	-	2/2/15/20	14/37/115/115	-
26	LMG	B	621	-	-	7/46/66/70	0/1/1/1
23	8CT	c	515	-	-	14/29/63/63	0/2/2/2
32	ZEX	6	524	-	-	11/29/67/67	0/2/2/2
21	CL7	1	406	-	2/2/14/20	11/34/112/115	-
21	CL7	5	420	18	2/2/11/20	4/13/91/115	-
21	CL7	3	514	-	2/2/11/20	5/13/91/115	-
21	CL7	5	406	-	2/2/14/20	11/34/112/115	-
21	CL7	b	608	-	2/2/14/20	9/31/109/115	-
25	LHG	a	406	-	-	5/50/50/53	-
21	CL7	C	509	-	2/2/15/20	15/37/115/115	-
21	CL7	4	406	-	2/2/15/20	22/37/115/115	-
32	ZEX	4	420	-	-	12/29/67/67	0/2/2/2
21	CL7	7	511	19	2/2/15/20	17/37/115/115	-
21	CL7	b	613	-	2/2/15/20	15/37/115/115	-
21	CL7	C	502	-	2/2/15/20	18/37/115/115	-
21	CL7	6	516	-	2/2/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	8CT	C	515	-	-	14/29/63/63	0/2/2/2
25	LHG	4	401	-	-	8/53/53/53	-
21	CL7	2	502	-	2/2/15/20	15/37/115/115	-
32	ZEX	4	418	-	-	9/29/67/67	0/2/2/2
21	CL7	5	403	-	2/2/14/20	9/31/109/115	-
21	CL7	6	511	16	2/2/14/20	14/31/109/115	-
25	LHG	b	626	-	-	6/53/53/53	-
21	CL7	6	504	-	2/2/11/20	4/13/91/115	-
21	CL7	3	518	19	2/2/11/20	5/13/91/115	-
21	CL7	3	512	-	2/2/13/20	12/25/103/115	-
21	CL7	b	614	-	2/2/13/20	4/25/103/115	-
24	SQD	B	626	-	-	3/29/49/69	0/1/1/1
32	ZEX	8	418	-	-	9/29/67/67	0/2/2/2
27	DGD	c	517	-	-	9/51/91/95	0/2/2/2
23	8CT	4	402	-	-	4/29/63/63	0/2/2/2
21	CL7	C	507	-	2/2/14/20	13/31/109/115	-
21	CL7	7	517	19	2/2/12/20	7/19/97/115	-
25	LHG	B	625	-	-	6/53/53/53	-
21	CL7	2	517	16	2/2/15/20	19/37/115/115	-
32	ZEX	2	525	-	-	11/29/67/67	0/2/2/2
30	PL9	d	407	-	-	9/53/73/73	0/1/1/1
21	CL7	b	612	-	2/2/15/20	15/37/115/115	-
21	CL7	7	507	-	2/2/15/20	13/37/115/115	-
21	CL7	2	507	-	2/2/15/20	18/37/115/115	-
21	CL7	8	409	-	2/2/14/20	15/31/109/115	-
32	ZEX	5	422	-	-	6/29/67/67	0/2/2/2
21	CL7	7	505	-	2/2/15/20	14/37/115/115	-
21	CL7	5	405	-	2/2/11/20	9/13/91/115	-
32	ZEX	8	420	-	-	12/29/67/67	0/2/2/2
21	CL7	1	403	-	2/2/14/20	9/31/109/115	-
21	CL7	d	402	-	2/2/12/20	7/19/97/115	-
21	CL7	B	610	-	2/2/15/20	11/37/115/115	-
26	LMG	b	622	-	-	7/46/66/70	0/1/1/1
21	CL7	3	516	19	2/2/13/20	14/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	5	408	-	2/2/15/20	14/37/115/115	-
21	CL7	c	510	-	2/2/15/20	18/37/115/115	-
21	CL7	5	419	-	2/2/11/20	7/13/91/115	-
21	CL7	7	502	-	2/2/13/20	10/29/107/115	-
26	LMG	5	401	-	-	5/46/66/70	0/1/1/1
21	CL7	5	413	-	2/2/10/20	2/8/86/115	-
21	CL7	A	406	-	2/2/15/20	14/37/115/115	-
21	CL7	4	407	-	2/2/10/20	1/8/86/115	-
21	CL7	7	504	-	2/2/15/20	14/37/115/115	-
21	CL7	B	611	-	2/2/15/20	15/37/115/115	-
21	CL7	a	405	-	2/2/15/20	14/37/115/115	-
21	CL7	b	606	-	2/2/15/20	16/37/115/115	-
21	CL7	1	407	-	2/2/10/20	2/8/86/115	-
22	PHO	a	402	-	-	3/37/103/103	0/5/6/6
21	CL7	c	503	-	2/2/14/20	10/31/109/115	-
24	SQD	3	521	-	-	3/41/61/69	0/1/1/1
21	CL7	C	508	-	2/2/15/20	15/37/115/115	-
21	CL7	1	411	-	2/2/11/20	5/13/91/115	-
21	CL7	b	617	-	2/2/11/20	4/13/91/115	-
21	CL7	A	403	-	2/2/13/20	9/25/103/115	-
21	CL7	c	506	-	2/2/15/20	14/37/115/115	-
21	CL7	C	514	-	2/2/11/20	6/13/91/115	-
24	SQD	1	423	-	-	3/27/47/69	0/1/1/1
26	LMG	c	501	-	-	16/45/65/70	0/1/1/1
32	ZEX	1	421	-	-	14/29/67/67	0/2/2/2
21	CL7	B	622	-	2/2/11/20	6/13/91/115	-
24	SQD	5	423	-	-	3/27/47/69	0/1/1/1
21	CL7	8	410	-	2/2/11/20	7/13/91/115	-
24	SQD	2	524	-	-	0/36/56/69	0/1/1/1
21	CL7	7	501	-	2/2/15/20	19/37/115/115	-
21	CL7	2	501	-	2/2/15/20	15/37/115/115	-
21	CL7	D	402	-	2/2/12/20	7/19/97/115	-
21	CL7	7	508	-	2/2/15/20	14/37/115/115	-
21	CL7	3	517	19	2/2/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	8	405	-	2/2/15/20	16/37/115/115	-
27	DGD	b	625	-	-	7/51/91/95	0/2/2/2
23	8CT	B	627	-	-	10/29/63/63	0/2/2/2
32	ZEX	6	519	-	-	11/29/67/67	0/2/2/2
21	CL7	B	607	-	2/2/14/20	9/31/109/115	-
21	CL7	7	510	-	2/2/15/20	13/37/115/115	-
21	CL7	5	410	-	2/2/15/20	15/37/115/115	-
24	SQD	7	523	-	-	7/45/65/69	0/1/1/1
21	CL7	3	510	-	2/2/15/20	13/37/115/115	-
21	CL7	7	518	19	2/2/11/20	5/13/91/115	-
21	CL7	2	518	16	2/2/15/20	10/37/115/115	-
21	CL7	7	509	-	2/2/15/20	15/37/115/115	-
31	HEM	F	101	-	-	6/12/54/54	-
32	ZEX	6	520	-	-	6/29/67/67	0/2/2/2
21	CL7	b	610	-	2/2/15/20	12/37/115/115	-
21	CL7	1	415	-	2/2/10/20	5/8/86/115	-
32	ZEX	2	520	-	-	7/29/67/67	0/2/2/2
21	CL7	4	417	20	2/2/10/20	4/10/88/115	-
23	8CT	b	620	-	-	4/29/63/63	0/2/2/2
23	8CT	8	402	-	-	4/29/63/63	0/2/2/2
32	ZEX	7	522	-	-	5/29/67/67	0/2/2/2
21	CL7	4	409	-	2/2/14/20	15/31/109/115	-
23	8CT	b	619	-	-	10/29/63/63	0/2/2/2
21	CL7	3	509	-	2/2/15/20	15/37/115/115	-
21	CL7	4	413	20	2/2/14/20	7/31/109/115	-
21	CL7	1	418	18	2/2/15/20	20/37/115/115	-
21	CL7	C	506	-	2/2/15/20	14/37/115/115	-
21	CL7	C	505	-	2/2/13/20	11/25/103/115	-
21	CL7	3	504	-	2/2/15/20	14/37/115/115	-
23	8CT	B	618	-	-	10/29/63/63	0/2/2/2
32	ZEX	4	403	-	-	10/29/67/67	0/2/2/2
21	CL7	7	516	19	2/2/13/20	14/25/103/115	-
21	CL7	b	602	-	2/2/10/20	4/8/86/115	-
21	CL7	D	405	-	2/2/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	1	416	-	2/2/10/20	2/8/86/115	-
23	8CT	b	601	-	-	10/29/63/63	0/2/2/2
21	CL7	C	513	-	2/2/10/20	2/8/86/115	-
21	CL7	6	503	-	2/2/15/20	17/37/115/115	-
26	LMG	C	501	-	-	16/45/65/70	0/1/1/1
21	CL7	b	611	-	2/2/15/20	11/37/115/115	-
21	CL7	B	606	-	2/2/13/20	4/25/103/115	-
21	CL7	1	414	-	2/2/10/20	1/8/86/115	-
21	CL7	c	509	-	2/2/15/20	15/37/115/115	-
21	CL7	5	412	-	2/2/11/20	8/13/91/115	-
21	CL7	5	409	-	2/2/11/20	4/13/91/115	-
21	CL7	2	516	-	2/2/15/20	14/37/115/115	-
21	CL7	1	408	-	2/2/15/20	14/37/115/115	-
21	CL7	B	615	-	2/2/12/20	8/19/97/115	-
21	CL7	1	420	18	2/2/11/20	4/13/91/115	-
21	CL7	B	605	-	2/2/15/20	16/37/115/115	-
23	8CT	k	101	-	-	10/29/63/63	0/2/2/2
25	LHG	B	623	-	-	3/49/49/53	-
32	ZEX	1	422	-	-	6/29/67/67	0/2/2/2
21	CL7	5	417	18	2/2/13/20	7/25/103/115	-
24	SQD	6	523	-	-	0/36/56/69	0/1/1/1
31	HEM	f	101	-	-	6/12/54/54	-
21	CL7	8	406	-	2/2/15/20	22/37/115/115	-
32	ZEX	2	519	-	-	11/29/67/67	0/2/2/2
21	CL7	b	607	-	2/2/13/20	4/25/103/115	-
24	SQD	3	523	-	-	7/45/65/69	0/1/1/1
21	CL7	a	403	-	2/2/13/20	9/25/103/115	-
23	8CT	c	519	-	-	8/29/63/63	0/2/2/2
21	CL7	2	503	-	2/2/15/20	17/37/115/115	-
21	CL7	1	413	-	2/2/10/20	2/8/86/115	-
21	CL7	B	603	-	2/2/15/20	12/37/115/115	-
21	CL7	6	505	-	2/2/15/20	16/37/115/115	-
23	8CT	b	618	-	-	7/29/63/63	0/2/2/2
21	CL7	5	404	-	2/2/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	8CT	a	404	-	-	5/29/63/63	0/2/2/2
21	CL7	C	503	-	2/2/14/20	10/31/109/115	-
21	CL7	5	402	-	2/2/14/20	14/31/109/115	-
21	CL7	1	405	-	2/2/11/20	9/13/91/115	-
23	8CT	B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	3	511	19	2/2/15/20	17/37/115/115	-
21	CL7	1	419	-	2/2/11/20	7/13/91/115	-
21	CL7	2	506	-	2/2/15/20	12/37/115/115	-
21	CL7	1	410	-	2/2/15/20	15/37/115/115	-
21	CL7	4	412	-	2/2/15/20	17/37/115/115	-
22	PHO	d	408	-	-	5/37/103/103	0/5/6/6
21	CL7	4	405	-	2/2/15/20	16/37/115/115	-
21	CL7	b	623	-	2/2/11/20	6/13/91/115	-
21	CL7	2	515	-	2/2/11/20	6/13/91/115	-
21	CL7	8	411	-	2/2/15/20	12/37/115/115	-
21	CL7	B	608	-	2/2/15/20	15/37/115/115	-
21	CL7	c	508	-	2/2/15/20	15/37/115/115	-
21	CL7	5	414	-	2/2/10/20	1/8/86/115	-
21	CL7	3	513	-	2/2/11/20	7/13/91/115	-
21	CL7	d	405	-	2/2/11/20	6/13/91/115	-
21	CL7	b	605	-	2/2/15/20	15/37/115/115	-
21	CL7	B	602	-	2/2/14/20	7/31/109/115	-
21	CL7	6	507	-	2/2/15/20	18/37/115/115	-
24	SQD	7	521	-	-	3/41/61/69	0/1/1/1
21	CL7	C	518	-	2/2/10/20	3/8/86/115	-
21	CL7	B	614	-	2/2/14/20	12/31/109/115	-
26	LMG	d	410	-	-	6/28/48/70	0/1/1/1
25	LHG	8	401	-	-	8/53/53/53	-
22	PHO	A	402	-	-	3/37/103/103	0/5/6/6
23	8CT	C	519	-	-	8/29/63/63	0/2/2/2
22	PHO	D	408	-	-	5/37/103/103	0/5/6/6
21	CL7	c	514	-	2/2/11/20	6/13/91/115	-
23	8CT	d	406	-	-	10/29/63/63	0/2/2/2
24	SQD	B	620	-	-	5/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	3	520	-	-	10/29/67/67	0/2/2/2
21	CL7	4	410	-	2/2/11/20	7/13/91/115	-
32	ZEX	3	519	-	-	10/29/67/67	0/2/2/2
21	CL7	6	518	16	2/2/15/20	10/37/115/115	-
21	CL7	b	603	-	2/2/14/20	7/31/109/115	-
21	CL7	4	408	-	2/2/11/20	2/13/91/115	-
21	CL7	3	503	-	2/2/15/20	18/37/115/115	-
21	CL7	2	509	-	2/2/15/20	14/37/115/115	-
21	CL7	C	512	3	2/2/10/20	3/10/88/115	-
21	CL7	4	415	-	2/2/11/20	10/13/91/115	-
21	CL7	B	609	-	2/2/15/20	12/37/115/115	-
21	CL7	c	507	-	2/2/14/20	13/31/109/115	-
21	CL7	8	407	-	2/2/10/20	1/8/86/115	-
32	ZEX	2	523	-	-	6/29/67/67	0/2/2/2
21	CL7	4	411	-	2/2/15/20	12/37/115/115	-
21	CL7	B	612	-	2/2/15/20	15/37/115/115	-
21	CL7	8	416	-	2/2/10/20	5/8/86/115	-
21	CL7	c	512	3	2/2/10/20	3/10/88/115	-
32	ZEX	2	521	-	-	6/29/67/67	0/2/2/2
21	CL7	c	505	-	2/2/13/20	11/25/103/115	-
21	CL7	c	513	-	2/2/10/20	2/8/86/115	-
26	LMG	D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	A	401	-	2/2/15/20	16/37/115/115	-
21	CL7	6	508	-	2/2/11/20	3/13/91/115	-
21	CL7	4	414	-	2/2/12/20	6/23/101/115	-
21	CL7	B	616	-	2/2/11/20	4/13/91/115	-
23	8CT	D	406	-	-	10/29/63/63	0/2/2/2
21	CL7	2	504	-	2/2/11/20	4/13/91/115	-
21	CL7	8	417	20	2/2/10/20	4/10/88/115	-
21	CL7	8	404	-	2/2/15/20	14/37/115/115	-
21	CL7	2	514	-	2/2/11/20	7/13/91/115	-
23	8CT	A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	c	502	-	2/2/15/20	18/37/115/115	-
27	DGD	C	517	-	-	9/51/91/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2	512	-	2/2/15/20	16/37/115/115	-
21	CL7	b	604	-	2/2/15/20	12/37/115/115	-
25	LHG	A	407	-	-	5/50/50/53	-
21	CL7	B	604	-	2/2/15/20	15/37/115/115	-
32	ZEX	3	525	-	-	7/29/67/67	0/2/2/2
21	CL7	5	415	-	2/2/10/20	5/8/86/115	-
21	CL7	a	401	-	2/2/15/20	16/37/115/115	-
21	CL7	C	510	-	2/2/15/20	18/37/115/115	-
21	CL7	8	412	-	2/2/15/20	17/37/115/115	-
21	CL7	B	601	-	2/2/10/20	4/8/86/115	-
21	CL7	5	407	-	2/2/10/20	2/8/86/115	-
24	SQD	b	621	-	-	5/49/69/69	0/1/1/1
23	8CT	B	617	-	-	7/29/63/63	0/2/2/2
21	CL7	2	511	16	2/2/14/20	14/31/109/115	-
21	CL7	5	411	-	2/2/11/20	5/13/91/115	-
27	DGD	B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	1	412	-	2/2/11/20	8/13/91/115	-
21	CL7	B	613	-	2/2/13/20	4/25/103/115	-
21	CL7	7	515	-	2/2/10/20	0/8/86/115	-
25	LHG	d	409	-	-	7/53/53/53	-
21	CL7	2	508	-	2/2/11/20	3/13/91/115	-
21	CL7	1	409	-	2/2/11/20	4/13/91/115	-
21	CL7	6	506	-	2/2/15/20	12/37/115/115	-
21	CL7	6	512	-	2/2/15/20	16/37/115/115	-
32	ZEX	4	419	-	-	9/29/67/67	0/2/2/2
21	CL7	1	402	-	2/2/14/20	14/31/109/115	-
21	CL7	1	417	18	2/2/13/20	7/25/103/115	-
21	CL7	3	505	-	2/2/15/20	14/37/115/115	-
21	CL7	6	510	16	2/2/15/20	20/37/115/115	-
21	CL7	6	515	-	2/2/11/20	6/13/91/115	-
21	CL7	d	404	-	2/2/13/20	11/29/107/115	-
21	CL7	7	506	-	2/2/11/20	11/13/91/115	-
25	LHG	D	409	-	-	7/53/53/53	-
30	PL9	D	407	-	-	9/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	7	503	-	2/2/15/20	18/37/115/115	-
21	CL7	c	518	-	2/2/10/20	3/8/86/115	-
21	CL7	2	505	-	2/2/15/20	16/37/115/115	-
21	CL7	7	513	-	2/2/11/20	7/13/91/115	-
21	CL7	2	513	-	2/2/11/20	6/13/91/115	-
24	SQD	2	522	-	-	7/45/65/69	0/1/1/1
21	CL7	C	504	-	2/2/15/20	17/37/115/115	-
21	CL7	6	502	-	2/2/15/20	15/37/115/115	-
21	CL7	6	509	-	2/2/15/20	14/37/115/115	-
26	LMG	1	401	-	-	5/46/66/70	0/1/1/1
32	ZEX	5	421	-	-	14/29/67/67	0/2/2/2
21	CL7	3	507	-	2/2/15/20	13/37/115/115	-
21	CL7	b	616	-	2/2/12/20	8/19/97/115	-
21	CL7	8	414	-	2/2/12/20	6/23/101/115	-
32	ZEX	6	522	-	-	6/29/67/67	0/2/2/2
21	CL7	6	513	-	2/2/11/20	6/13/91/115	-
21	CL7	1	404	-	2/2/15/20	13/37/115/115	-
21	CL7	4	416	-	2/2/10/20	5/8/86/115	-
21	CL7	b	609	-	2/2/15/20	15/37/115/115	-
21	CL7	3	515	-	2/2/10/20	0/8/86/115	-
23	8CT	K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	8	413	20	2/2/14/20	7/31/109/115	-

All (3338) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	627	8CT	C02-C03	14.81	1.60	1.34
23	b	601	8CT	C02-C03	14.81	1.60	1.34
23	B	618	8CT	C02-C03	14.76	1.60	1.34
23	b	619	8CT	C02-C03	14.76	1.60	1.34
23	C	519	8CT	C02-C03	14.59	1.59	1.34
23	c	519	8CT	C02-C03	14.59	1.59	1.34
23	A	404	8CT	C02-C03	14.51	1.59	1.34
23	a	404	8CT	C02-C03	14.51	1.59	1.34
23	C	515	8CT	C02-C03	14.50	1.59	1.34
23	c	515	8CT	C02-C03	14.50	1.59	1.34
23	K	101	8CT	C02-C03	14.49	1.59	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	k	101	8CT	C02-C03	14.49	1.59	1.34
23	8	402	8CT	C02-C03	14.44	1.59	1.34
23	4	402	8CT	C02-C03	14.43	1.59	1.34
23	b	618	8CT	C02-C03	14.26	1.59	1.34
23	B	617	8CT	C02-C03	14.25	1.59	1.34
23	B	619	8CT	C02-C03	14.25	1.59	1.34
23	b	620	8CT	C02-C03	14.25	1.59	1.34
23	D	406	8CT	C02-C03	14.24	1.59	1.34
23	d	406	8CT	C02-C03	14.24	1.59	1.34
23	C	516	8CT	C02-C03	14.04	1.58	1.34
23	c	516	8CT	C02-C03	14.04	1.58	1.34
23	K	101	8CT	C32-C31	13.72	1.59	1.32
23	k	101	8CT	C32-C31	13.70	1.59	1.32
23	D	406	8CT	C32-C31	13.46	1.59	1.32
23	a	404	8CT	C32-C31	13.45	1.59	1.32
23	B	618	8CT	C32-C31	13.44	1.59	1.32
23	b	619	8CT	C32-C31	13.44	1.59	1.32
23	d	406	8CT	C32-C31	13.43	1.59	1.32
23	c	519	8CT	C32-C31	13.42	1.59	1.32
23	C	519	8CT	C32-C31	13.42	1.59	1.32
23	A	404	8CT	C32-C31	13.41	1.59	1.32
23	B	627	8CT	C32-C31	13.35	1.59	1.32
23	b	601	8CT	C32-C31	13.33	1.58	1.32
23	C	515	8CT	C32-C31	13.32	1.58	1.32
23	c	515	8CT	C32-C31	13.32	1.58	1.32
23	C	516	8CT	C32-C31	13.30	1.58	1.32
23	c	516	8CT	C32-C31	13.30	1.58	1.32
23	B	617	8CT	C32-C31	13.27	1.58	1.32
23	b	618	8CT	C32-C31	13.25	1.58	1.32
23	B	619	8CT	C32-C31	13.20	1.58	1.32
23	b	620	8CT	C32-C31	13.20	1.58	1.32
23	4	402	8CT	C32-C31	13.19	1.58	1.32
23	8	402	8CT	C32-C31	13.16	1.58	1.32
23	B	617	8CT	C34-C35	-9.92	1.33	1.54
23	b	618	8CT	C34-C35	-9.92	1.33	1.54
23	C	516	8CT	C34-C35	-9.78	1.34	1.54
23	c	516	8CT	C34-C35	-9.78	1.34	1.54
23	C	515	8CT	C34-C35	-9.74	1.34	1.54
23	c	515	8CT	C34-C35	-9.74	1.34	1.54
21	B	606	CL7	CHD-C4C	9.59	1.48	1.35
21	b	607	CL7	CHD-C4C	9.59	1.48	1.35
21	5	414	CL7	CHD-C4C	9.56	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	404	8CT	C34-C35	-9.53	1.34	1.54
23	a	404	8CT	C34-C35	-9.52	1.34	1.54
21	1	414	CL7	CHD-C4C	9.51	1.48	1.35
21	d	402	CL7	CHD-C4C	9.48	1.48	1.35
21	D	402	CL7	CHD-C4C	9.46	1.48	1.35
23	b	620	8CT	C34-C35	-9.37	1.34	1.54
23	C	519	8CT	C34-C35	-9.36	1.34	1.54
23	c	519	8CT	C34-C35	-9.36	1.34	1.54
21	2	513	CL7	CHD-C4C	9.36	1.48	1.35
21	6	513	CL7	CHD-C4C	9.36	1.48	1.35
21	1	416	CL7	CHD-C4C	9.35	1.48	1.35
21	A	401	CL7	CHC-C1C	9.35	1.48	1.35
21	a	401	CL7	CHC-C1C	9.35	1.48	1.35
23	K	101	8CT	C34-C35	-9.33	1.35	1.54
23	b	601	8CT	C34-C35	-9.33	1.35	1.54
23	B	619	8CT	C34-C35	-9.32	1.35	1.54
21	5	416	CL7	CHD-C4C	9.32	1.48	1.35
23	B	627	8CT	C34-C35	-9.31	1.35	1.54
23	k	101	8CT	C34-C35	-9.29	1.35	1.54
23	B	618	8CT	C34-C35	-9.27	1.35	1.54
21	B	622	CL7	CHD-C4C	9.27	1.48	1.35
21	b	623	CL7	CHD-C4C	9.27	1.48	1.35
21	1	404	CL7	CHD-C4C	9.26	1.48	1.35
21	5	404	CL7	CHD-C4C	9.26	1.48	1.35
21	6	514	CL7	CHD-C4C	9.25	1.48	1.35
21	3	518	CL7	CHD-C4C	9.25	1.48	1.35
21	7	518	CL7	CHD-C4C	9.25	1.48	1.35
23	b	619	8CT	C34-C35	-9.24	1.35	1.54
21	4	411	CL7	CHD-C4C	9.23	1.48	1.35
21	2	515	CL7	CHD-C4C	9.23	1.48	1.35
21	B	622	CL7	CHC-C1C	9.23	1.48	1.35
21	3	506	CL7	CHD-C4C	9.23	1.48	1.35
21	7	506	CL7	CHD-C4C	9.23	1.48	1.35
21	5	419	CL7	CHC-C1C	9.22	1.48	1.35
21	3	516	CL7	CHD-C4C	9.21	1.48	1.35
21	3	517	CL7	CHD-C4C	9.21	1.48	1.35
21	7	516	CL7	CHD-C4C	9.21	1.48	1.35
21	7	517	CL7	CHD-C4C	9.20	1.48	1.35
21	8	411	CL7	CHD-C4C	9.20	1.48	1.35
21	6	515	CL7	CHD-C4C	9.20	1.48	1.35
23	D	406	8CT	C34-C35	-9.19	1.35	1.54
23	d	406	8CT	C34-C35	-9.19	1.35	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	514	CL7	CHD-C4C	9.19	1.48	1.35
21	3	518	CL7	CHC-C1C	9.19	1.48	1.35
23	8	402	8CT	C34-C35	-9.19	1.35	1.54
23	4	402	8CT	C34-C35	-9.19	1.35	1.54
21	1	419	CL7	CHC-C1C	9.19	1.48	1.35
21	a	401	CL7	CHD-C4C	9.18	1.48	1.35
21	1	408	CL7	CHD-C4C	9.18	1.48	1.35
21	5	408	CL7	CHD-C4C	9.18	1.48	1.35
21	b	623	CL7	CHC-C1C	9.17	1.48	1.35
21	A	401	CL7	CHD-C4C	9.17	1.48	1.35
21	1	411	CL7	CHD-C4C	9.17	1.48	1.35
21	1	410	CL7	CHD-C4C	9.16	1.48	1.35
21	B	601	CL7	CHD-C4C	9.16	1.48	1.35
21	C	518	CL7	CHD-C4C	9.16	1.48	1.35
21	b	602	CL7	CHD-C4C	9.16	1.48	1.35
21	c	518	CL7	CHD-C4C	9.16	1.48	1.35
21	B	609	CL7	CHD-C4C	9.15	1.48	1.35
21	b	610	CL7	CHD-C4C	9.15	1.48	1.35
21	7	518	CL7	CHC-C1C	9.15	1.48	1.35
21	1	420	CL7	CHC-C1C	9.15	1.48	1.35
21	5	420	CL7	CHC-C1C	9.15	1.48	1.35
21	3	502	CL7	CHD-C4C	9.14	1.48	1.35
21	7	502	CL7	CHD-C4C	9.14	1.48	1.35
21	1	415	CL7	CHC-C1C	9.14	1.48	1.35
21	5	415	CL7	CHC-C1C	9.14	1.48	1.35
21	1	419	CL7	CHD-C4C	9.13	1.48	1.35
21	2	518	CL7	CHD-C4C	9.13	1.48	1.35
21	6	518	CL7	CHD-C4C	9.13	1.48	1.35
21	1	417	CL7	CHD-C4C	9.12	1.48	1.35
21	5	417	CL7	CHD-C4C	9.12	1.48	1.35
21	5	411	CL7	CHD-C4C	9.12	1.48	1.35
21	1	415	CL7	CHD-C4C	9.11	1.48	1.35
21	5	415	CL7	CHD-C4C	9.11	1.48	1.35
21	C	511	CL7	CHD-C4C	9.10	1.48	1.35
21	c	511	CL7	CHD-C4C	9.10	1.48	1.35
21	5	410	CL7	CHD-C4C	9.10	1.48	1.35
21	4	412	CL7	CHD-C4C	9.09	1.47	1.35
21	a	405	CL7	CHD-C4C	9.08	1.47	1.35
21	C	506	CL7	CHD-C4C	9.08	1.47	1.35
21	C	512	CL7	CHC-C1C	9.07	1.47	1.35
21	1	416	CL7	CHC-C1C	9.07	1.47	1.35
21	5	416	CL7	CHC-C1C	9.07	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	419	CL7	CHD-C4C	9.07	1.47	1.35
21	2	504	CL7	CHD-C4C	9.07	1.47	1.35
21	4	408	CL7	CHD-C4C	9.07	1.47	1.35
21	8	408	CL7	CHD-C4C	9.07	1.47	1.35
21	4	416	CL7	CHC-C1C	9.06	1.47	1.35
21	6	504	CL7	CHD-C4C	9.06	1.47	1.35
21	8	412	CL7	CHD-C4C	9.06	1.47	1.35
21	8	416	CL7	CHC-C1C	9.06	1.47	1.35
21	1	405	CL7	CHD-C4C	9.06	1.47	1.35
21	B	607	CL7	CHD-C4C	9.06	1.47	1.35
21	b	608	CL7	CHD-C4C	9.06	1.47	1.35
21	c	507	CL7	CHD-C4C	9.06	1.47	1.35
21	3	501	CL7	CHD-C4C	9.05	1.47	1.35
21	7	501	CL7	CHD-C4C	9.05	1.47	1.35
21	5	417	CL7	CHC-C1C	9.04	1.47	1.35
21	c	512	CL7	CHC-C1C	9.04	1.47	1.35
21	C	505	CL7	CHD-C4C	9.04	1.47	1.35
21	1	417	CL7	CHC-C1C	9.04	1.47	1.35
21	c	505	CL7	CHD-C4C	9.04	1.47	1.35
21	C	514	CL7	CHD-C4C	9.03	1.47	1.35
21	c	514	CL7	CHD-C4C	9.03	1.47	1.35
21	A	406	CL7	CHD-C4C	9.03	1.47	1.35
21	4	409	CL7	CHD-C4C	9.03	1.47	1.35
21	8	409	CL7	CHD-C4C	9.03	1.47	1.35
21	C	507	CL7	CHD-C4C	9.03	1.47	1.35
21	1	414	CL7	CHC-C1C	9.02	1.47	1.35
21	5	414	CL7	CHC-C1C	9.02	1.47	1.35
21	1	404	CL7	CHC-C1C	9.02	1.47	1.35
21	5	404	CL7	CHC-C1C	9.02	1.47	1.35
21	c	506	CL7	CHD-C4C	9.02	1.47	1.35
21	3	513	CL7	CHD-C4C	9.02	1.47	1.35
21	5	405	CL7	CHD-C4C	9.00	1.47	1.35
21	2	507	CL7	CHD-C4C	8.99	1.47	1.35
21	6	507	CL7	CHD-C4C	8.99	1.47	1.35
21	C	505	CL7	CHC-C1C	8.98	1.47	1.35
21	c	505	CL7	CHC-C1C	8.98	1.47	1.35
21	3	514	CL7	CHD-C4C	8.98	1.47	1.35
21	4	405	CL7	CHD-C4C	8.98	1.47	1.35
21	8	405	CL7	CHD-C4C	8.98	1.47	1.35
21	2	508	CL7	CHD-C4C	8.98	1.47	1.35
21	6	508	CL7	CHD-C4C	8.98	1.47	1.35
21	B	616	CL7	CHD-C4C	8.98	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	617	CL7	CHD-C4C	8.98	1.47	1.35
21	7	502	CL7	CHC-C1C	8.98	1.47	1.35
21	7	513	CL7	CHD-C4C	8.97	1.47	1.35
21	1	411	CL7	CHC-C1C	8.96	1.47	1.35
21	5	411	CL7	CHC-C1C	8.96	1.47	1.35
21	4	417	CL7	CHC-C1C	8.96	1.47	1.35
21	8	417	CL7	CHC-C1C	8.96	1.47	1.35
21	1	409	CL7	CHD-C4C	8.95	1.47	1.35
21	5	409	CL7	CHD-C4C	8.95	1.47	1.35
21	B	616	CL7	CHC-C1C	8.95	1.47	1.35
21	1	402	CL7	CHD-C4C	8.95	1.47	1.35
21	3	509	CL7	CHC-C1C	8.95	1.47	1.35
21	b	617	CL7	CHC-C1C	8.95	1.47	1.35
21	7	509	CL7	CHC-C1C	8.95	1.47	1.35
21	7	514	CL7	CHD-C4C	8.95	1.47	1.35
21	4	416	CL7	CHD-C4C	8.95	1.47	1.35
21	7	515	CL7	CHD-C4C	8.95	1.47	1.35
21	5	402	CL7	CHD-C4C	8.94	1.47	1.35
21	C	511	CL7	CHC-C1C	8.94	1.47	1.35
21	c	511	CL7	CHC-C1C	8.94	1.47	1.35
21	2	518	CL7	CHC-C1C	8.93	1.47	1.35
21	6	518	CL7	CHC-C1C	8.93	1.47	1.35
21	1	407	CL7	CHD-C4C	8.92	1.47	1.35
21	5	407	CL7	CHD-C4C	8.92	1.47	1.35
21	B	613	CL7	CHD-C4C	8.92	1.47	1.35
21	b	614	CL7	CHD-C4C	8.92	1.47	1.35
21	D	404	CL7	CHD-C4C	8.91	1.47	1.35
21	d	404	CL7	CHD-C4C	8.91	1.47	1.35
21	6	506	CL7	CHD-C4C	8.91	1.47	1.35
21	3	502	CL7	CHC-C1C	8.91	1.47	1.35
21	3	508	CL7	CHD-C4C	8.91	1.47	1.35
21	7	508	CL7	CHD-C4C	8.91	1.47	1.35
21	5	410	CL7	CHC-C1C	8.91	1.47	1.35
21	2	506	CL7	CHD-C4C	8.91	1.47	1.35
21	B	601	CL7	CHC-C1C	8.91	1.47	1.35
21	b	602	CL7	CHC-C1C	8.91	1.47	1.35
21	5	418	CL7	CHD-C4C	8.91	1.47	1.35
21	8	416	CL7	CHD-C4C	8.90	1.47	1.35
21	1	418	CL7	CHD-C4C	8.90	1.47	1.35
21	3	515	CL7	CHD-C4C	8.90	1.47	1.35
21	C	514	CL7	CHC-C1C	8.90	1.47	1.35
21	2	501	CL7	CHD-C4C	8.90	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	403	CL7	CHC-C1C	8.89	1.47	1.35
21	2	511	CL7	CHD-C4C	8.89	1.47	1.35
21	a	403	CL7	CHC-C1C	8.89	1.47	1.35
21	6	511	CL7	CHD-C4C	8.89	1.47	1.35
21	5	412	CL7	CHD-C4C	8.89	1.47	1.35
21	3	515	CL7	CHC-C1C	8.89	1.47	1.35
21	7	515	CL7	CHC-C1C	8.89	1.47	1.35
21	4	408	CL7	CHC-C1C	8.89	1.47	1.35
21	2	509	CL7	CHC-C1C	8.88	1.47	1.35
21	8	408	CL7	CHC-C1C	8.88	1.47	1.35
21	1	420	CL7	CHD-C4C	8.88	1.47	1.35
21	5	420	CL7	CHD-C4C	8.88	1.47	1.35
21	6	501	CL7	CHD-C4C	8.88	1.47	1.35
21	C	512	CL7	CHD-C4C	8.88	1.47	1.35
21	1	409	CL7	CHC-C1C	8.88	1.47	1.35
21	5	409	CL7	CHC-C1C	8.88	1.47	1.35
21	3	513	CL7	CHC-C1C	8.88	1.47	1.35
21	b	604	CL7	CHC-C1C	8.87	1.47	1.35
21	1	412	CL7	CHD-C4C	8.87	1.47	1.35
21	1	410	CL7	CHC-C1C	8.86	1.47	1.35
21	7	513	CL7	CHC-C1C	8.86	1.47	1.35
21	B	603	CL7	CHD-C4C	8.86	1.47	1.35
21	1	402	CL7	CHC-C1C	8.86	1.47	1.35
21	b	604	CL7	CHD-C4C	8.86	1.47	1.35
21	c	512	CL7	CHD-C4C	8.86	1.47	1.35
21	5	402	CL7	CHC-C1C	8.86	1.47	1.35
21	4	417	CL7	CHD-C4C	8.86	1.47	1.35
21	8	417	CL7	CHD-C4C	8.86	1.47	1.35
21	c	514	CL7	CHC-C1C	8.85	1.47	1.35
21	B	608	CL7	CHD-C4C	8.85	1.47	1.35
21	b	609	CL7	CHD-C4C	8.85	1.47	1.35
21	1	413	CL7	CHD-C4C	8.85	1.47	1.35
21	5	413	CL7	CHD-C4C	8.85	1.47	1.35
21	4	404	CL7	CHD-C4C	8.85	1.47	1.35
21	4	406	CL7	CHC-C1C	8.85	1.47	1.35
21	4	404	CL7	CHC-C1C	8.84	1.47	1.35
21	8	404	CL7	CHC-C1C	8.84	1.47	1.35
21	5	403	CL7	CHD-C4C	8.84	1.47	1.35
21	8	411	CL7	CHC-C1C	8.84	1.47	1.35
21	8	404	CL7	CHD-C4C	8.83	1.47	1.35
21	B	603	CL7	CHC-C1C	8.83	1.47	1.35
21	C	508	CL7	CHD-C4C	8.83	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	508	CL7	CHD-C4C	8.83	1.47	1.35
21	4	413	CL7	CHD-C4C	8.82	1.47	1.35
21	8	413	CL7	CHD-C4C	8.82	1.47	1.35
21	2	502	CL7	CHD-C4C	8.82	1.47	1.35
21	6	502	CL7	CHD-C4C	8.82	1.47	1.35
21	6	509	CL7	CHC-C1C	8.82	1.47	1.35
21	2	510	CL7	CHD-C4C	8.81	1.47	1.35
21	6	510	CL7	CHD-C4C	8.81	1.47	1.35
21	4	407	CL7	CHC-C1C	8.81	1.47	1.35
21	3	503	CL7	CHC-C1C	8.81	1.47	1.35
21	1	403	CL7	CHD-C4C	8.81	1.47	1.35
21	1	408	CL7	CHC-C1C	8.81	1.47	1.35
21	5	408	CL7	CHC-C1C	8.81	1.47	1.35
21	B	614	CL7	CHD-C4C	8.81	1.47	1.35
21	b	615	CL7	CHD-C4C	8.81	1.47	1.35
21	C	502	CL7	CHC-C1C	8.80	1.47	1.35
21	c	502	CL7	CHC-C1C	8.80	1.47	1.35
21	C	507	CL7	CHC-C1C	8.80	1.47	1.35
21	2	509	CL7	CHD-C4C	8.80	1.47	1.35
21	2	512	CL7	CHC-C1C	8.80	1.47	1.35
21	c	507	CL7	CHC-C1C	8.80	1.47	1.35
21	6	509	CL7	CHD-C4C	8.80	1.47	1.35
21	6	512	CL7	CHC-C1C	8.80	1.47	1.35
21	B	602	CL7	CHD-C4C	8.80	1.47	1.35
21	3	504	CL7	CHC-C1C	8.80	1.47	1.35
21	b	603	CL7	CHD-C4C	8.80	1.47	1.35
21	7	504	CL7	CHC-C1C	8.80	1.47	1.35
21	c	503	CL7	CHD-C4C	8.79	1.47	1.35
21	1	407	CL7	CHC-C1C	8.79	1.47	1.35
21	4	415	CL7	CHC-C1C	8.79	1.47	1.35
21	8	415	CL7	CHC-C1C	8.79	1.47	1.35
21	8	406	CL7	CHC-C1C	8.79	1.47	1.35
21	2	511	CL7	CHC-C1C	8.79	1.47	1.35
21	6	511	CL7	CHC-C1C	8.79	1.47	1.35
21	3	512	CL7	CHD-C4C	8.79	1.47	1.35
21	7	512	CL7	CHD-C4C	8.79	1.47	1.35
21	C	503	CL7	CHD-C4C	8.78	1.47	1.35
21	1	405	CL7	CHC-C1C	8.78	1.47	1.35
21	1	412	CL7	CHC-C1C	8.78	1.47	1.35
21	3	507	CL7	CHD-C4C	8.78	1.47	1.35
21	4	411	CL7	CHC-C1C	8.78	1.47	1.35
21	5	405	CL7	CHC-C1C	8.78	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	412	CL7	CHC-C1C	8.78	1.47	1.35
21	7	507	CL7	CHD-C4C	8.78	1.47	1.35
21	A	406	CL7	CHC-C1C	8.78	1.47	1.35
21	B	615	CL7	CHD-C4C	8.78	1.47	1.35
21	a	405	CL7	CHC-C1C	8.78	1.47	1.35
21	b	616	CL7	CHD-C4C	8.78	1.47	1.35
21	c	504	CL7	CHC-C1C	8.78	1.47	1.35
21	2	503	CL7	CHC-C1C	8.77	1.47	1.35
21	6	503	CL7	CHC-C1C	8.77	1.47	1.35
21	2	504	CL7	CHC-C1C	8.77	1.47	1.35
21	6	504	CL7	CHC-C1C	8.77	1.47	1.35
21	4	405	CL7	CHC-C1C	8.77	1.47	1.35
21	2	517	CL7	CHC-C1C	8.77	1.47	1.35
21	6	517	CL7	CHC-C1C	8.77	1.47	1.35
21	2	516	CL7	CHC-C1C	8.76	1.47	1.35
21	6	516	CL7	CHC-C1C	8.76	1.47	1.35
21	8	407	CL7	CHC-C1C	8.76	1.47	1.35
21	C	504	CL7	CHD-C4C	8.75	1.47	1.35
21	B	602	CL7	CHC-C1C	8.75	1.47	1.35
21	b	603	CL7	CHC-C1C	8.75	1.47	1.35
21	7	503	CL7	CHC-C1C	8.75	1.47	1.35
21	D	402	CL7	CHC-C1C	8.74	1.47	1.35
21	B	614	CL7	CHC-C1C	8.74	1.47	1.35
21	C	503	CL7	CHC-C1C	8.74	1.47	1.35
21	b	615	CL7	CHC-C1C	8.74	1.47	1.35
21	c	503	CL7	CHC-C1C	8.74	1.47	1.35
21	3	501	CL7	CHC-C1C	8.74	1.47	1.35
21	7	501	CL7	CHC-C1C	8.74	1.47	1.35
21	5	407	CL7	CHC-C1C	8.73	1.47	1.35
21	7	514	CL7	CHC-C1C	8.73	1.47	1.35
21	c	504	CL7	CHD-C4C	8.73	1.47	1.35
21	C	504	CL7	CHC-C1C	8.72	1.47	1.35
21	B	611	CL7	CHD-C4C	8.72	1.47	1.35
21	D	405	CL7	CHD-C4C	8.72	1.47	1.35
21	b	612	CL7	CHD-C4C	8.72	1.47	1.35
21	d	405	CL7	CHD-C4C	8.72	1.47	1.35
21	8	405	CL7	CHC-C1C	8.72	1.47	1.35
21	3	510	CL7	CHD-C4C	8.72	1.47	1.35
21	3	516	CL7	CHC-C1C	8.72	1.47	1.35
21	4	412	CL7	CHC-C1C	8.72	1.47	1.35
21	7	510	CL7	CHD-C4C	8.72	1.47	1.35
21	8	412	CL7	CHC-C1C	8.72	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	406	CL7	CHD-C4C	8.72	1.47	1.35
21	8	406	CL7	CHD-C4C	8.72	1.47	1.35
21	B	605	CL7	CHD-C4C	8.71	1.47	1.35
21	C	509	CL7	CHD-C4C	8.71	1.47	1.35
21	c	509	CL7	CHD-C4C	8.71	1.47	1.35
21	2	516	CL7	CHD-C4C	8.71	1.47	1.35
21	b	605	CL7	CHD-C4C	8.71	1.47	1.35
21	6	516	CL7	CHD-C4C	8.71	1.47	1.35
21	1	413	CL7	CHC-C1C	8.71	1.47	1.35
21	4	415	CL7	CHD-C4C	8.71	1.47	1.35
21	d	402	CL7	CHC-C1C	8.71	1.47	1.35
21	4	410	CL7	CHD-C4C	8.71	1.47	1.35
21	B	604	CL7	CHD-C4C	8.70	1.47	1.35
21	B	607	CL7	CHC-C1C	8.70	1.47	1.35
21	B	606	CL7	CHC-C1C	8.70	1.47	1.35
21	b	607	CL7	CHC-C1C	8.70	1.47	1.35
21	4	407	CL7	CHD-C4C	8.70	1.47	1.35
21	C	510	CL7	CHD-C4C	8.69	1.47	1.35
21	c	510	CL7	CHD-C4C	8.69	1.47	1.35
21	8	415	CL7	CHD-C4C	8.69	1.47	1.35
21	2	513	CL7	CHC-C1C	8.69	1.47	1.35
21	2	505	CL7	CHC-C1C	8.69	1.47	1.35
21	6	505	CL7	CHC-C1C	8.69	1.47	1.35
21	5	413	CL7	CHC-C1C	8.69	1.47	1.35
21	3	517	CL7	CHC-C1C	8.69	1.47	1.35
21	7	517	CL7	CHC-C1C	8.69	1.47	1.35
21	1	406	CL7	CHC-C1C	8.69	1.47	1.35
21	5	406	CL7	CHC-C1C	8.69	1.47	1.35
21	b	606	CL7	CHD-C4C	8.68	1.47	1.35
21	B	605	CL7	CHC-C1C	8.68	1.47	1.35
21	4	414	CL7	CHD-C4C	8.67	1.47	1.35
21	8	414	CL7	CHD-C4C	8.67	1.47	1.35
21	3	514	CL7	CHC-C1C	8.67	1.47	1.35
21	1	406	CL7	CHD-C4C	8.67	1.47	1.35
21	3	505	CL7	CHC-C1C	8.67	1.47	1.35
21	b	608	CL7	CHC-C1C	8.67	1.47	1.35
21	7	505	CL7	CHC-C1C	8.67	1.47	1.35
21	3	510	CL7	CHC-C1C	8.66	1.47	1.35
21	5	406	CL7	CHD-C4C	8.66	1.47	1.35
21	7	510	CL7	CHC-C1C	8.66	1.47	1.35
21	8	410	CL7	CHC-C1C	8.66	1.47	1.35
21	B	613	CL7	CHC-C1C	8.65	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	517	CL7	CHD-C4C	8.65	1.47	1.35
21	7	516	CL7	CHC-C1C	8.65	1.47	1.35
21	C	513	CL7	CHD-C4C	8.65	1.47	1.35
21	c	513	CL7	CHD-C4C	8.65	1.47	1.35
21	8	410	CL7	CHD-C4C	8.65	1.47	1.35
21	4	410	CL7	CHC-C1C	8.65	1.47	1.35
21	3	504	CL7	CHD-C4C	8.65	1.47	1.35
21	7	504	CL7	CHD-C4C	8.65	1.47	1.35
21	8	407	CL7	CHD-C4C	8.64	1.47	1.35
21	6	513	CL7	CHC-C1C	8.64	1.47	1.35
21	3	511	CL7	CHD-C4C	8.64	1.47	1.35
21	7	511	CL7	CHD-C4C	8.64	1.47	1.35
21	3	509	CL7	CHD-C4C	8.64	1.47	1.35
21	7	509	CL7	CHD-C4C	8.64	1.47	1.35
21	6	517	CL7	CHD-C4C	8.64	1.47	1.35
21	b	606	CL7	CHC-C1C	8.63	1.47	1.35
21	b	614	CL7	CHC-C1C	8.63	1.47	1.35
21	B	612	CL7	CHD-C4C	8.62	1.47	1.35
21	b	613	CL7	CHD-C4C	8.62	1.47	1.35
21	b	610	CL7	CHC-C1C	8.61	1.47	1.35
21	4	413	CL7	CHC-C1C	8.60	1.47	1.35
21	8	413	CL7	CHC-C1C	8.60	1.47	1.35
21	c	508	CL7	CHC-C1C	8.60	1.47	1.35
21	3	503	CL7	CHD-C4C	8.60	1.47	1.35
21	7	503	CL7	CHD-C4C	8.60	1.47	1.35
21	3	511	CL7	CHC-C1C	8.59	1.47	1.35
21	3	512	CL7	CHC-C1C	8.59	1.47	1.35
21	7	512	CL7	CHC-C1C	8.59	1.47	1.35
21	C	509	CL7	CHC-C1C	8.58	1.47	1.35
21	2	506	CL7	CHC-C1C	8.58	1.47	1.35
21	6	506	CL7	CHC-C1C	8.58	1.47	1.35
21	3	505	CL7	CHD-C4C	8.58	1.47	1.35
21	7	505	CL7	CHD-C4C	8.58	1.47	1.35
21	B	610	CL7	CHC-C1C	8.58	1.47	1.35
21	2	501	CL7	CHC-C1C	8.58	1.47	1.35
21	6	501	CL7	CHC-C1C	8.58	1.47	1.35
21	2	510	CL7	CHC-C1C	8.58	1.47	1.35
21	7	511	CL7	CHC-C1C	8.57	1.47	1.35
21	6	510	CL7	CHC-C1C	8.56	1.47	1.35
21	c	509	CL7	CHC-C1C	8.56	1.47	1.35
21	C	508	CL7	CHC-C1C	8.55	1.47	1.35
21	C	510	CL7	CHC-C1C	8.54	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	510	CL7	CHC-C1C	8.54	1.47	1.35
21	B	609	CL7	CHC-C1C	8.54	1.47	1.35
21	5	418	CL7	CHC-C1C	8.53	1.47	1.35
21	2	515	CL7	CHC-C1C	8.53	1.47	1.35
21	6	515	CL7	CHC-C1C	8.53	1.47	1.35
21	B	610	CL7	CHD-C4C	8.53	1.47	1.35
21	b	611	CL7	CHC-C1C	8.53	1.47	1.35
21	2	505	CL7	CHD-C4C	8.53	1.47	1.35
21	a	403	CL7	CHD-C4C	8.52	1.47	1.35
21	b	611	CL7	CHD-C4C	8.52	1.47	1.35
21	B	608	CL7	CHC-C1C	8.52	1.47	1.35
21	b	609	CL7	CHC-C1C	8.52	1.47	1.35
21	A	403	CL7	CHD-C4C	8.51	1.47	1.35
21	6	503	CL7	CHD-C4C	8.51	1.47	1.35
21	1	403	CL7	CHC-C1C	8.49	1.47	1.35
21	5	403	CL7	CHC-C1C	8.49	1.47	1.35
21	4	414	CL7	CHC-C1C	8.48	1.47	1.35
21	C	506	CL7	CHC-C1C	8.48	1.47	1.35
21	c	506	CL7	CHC-C1C	8.48	1.47	1.35
21	6	505	CL7	CHD-C4C	8.47	1.47	1.35
21	1	418	CL7	CHC-C1C	8.47	1.47	1.35
21	2	502	CL7	CHC-C1C	8.45	1.47	1.35
21	2	503	CL7	CHD-C4C	8.45	1.47	1.35
21	6	502	CL7	CHC-C1C	8.45	1.47	1.35
21	C	513	CL7	CHC-C1C	8.44	1.47	1.35
21	c	513	CL7	CHC-C1C	8.44	1.47	1.35
21	c	502	CL7	CHD-C4C	8.44	1.47	1.35
21	2	514	CL7	CHC-C1C	8.43	1.47	1.35
21	C	518	CL7	CHC-C1C	8.42	1.47	1.35
21	c	518	CL7	CHC-C1C	8.42	1.47	1.35
21	D	405	CL7	CHC-C1C	8.42	1.47	1.35
21	d	405	CL7	CHC-C1C	8.42	1.47	1.35
21	3	508	CL7	CHC-C1C	8.42	1.47	1.35
21	7	508	CL7	CHC-C1C	8.42	1.47	1.35
21	8	414	CL7	CHC-C1C	8.42	1.47	1.35
21	6	514	CL7	CHC-C1C	8.42	1.47	1.35
21	C	502	CL7	CHD-C4C	8.40	1.47	1.35
21	4	409	CL7	CHC-C1C	8.39	1.47	1.35
21	8	409	CL7	CHC-C1C	8.39	1.47	1.35
21	2	507	CL7	CHC-C1C	8.36	1.46	1.35
21	6	507	CL7	CHC-C1C	8.36	1.46	1.35
21	7	507	CL7	CHC-C1C	8.36	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	507	CL7	CHC-C1C	8.34	1.46	1.35
21	2	508	CL7	CHC-C1C	8.32	1.46	1.35
21	6	508	CL7	CHC-C1C	8.32	1.46	1.35
21	2	512	CL7	CHD-C4C	8.32	1.46	1.35
21	6	512	CL7	CHD-C4C	8.32	1.46	1.35
21	D	404	CL7	CHC-C1C	8.30	1.46	1.35
21	d	404	CL7	CHC-C1C	8.30	1.46	1.35
21	B	611	CL7	CHC-C1C	8.29	1.46	1.35
21	b	612	CL7	CHC-C1C	8.29	1.46	1.35
21	B	604	CL7	CHC-C1C	8.24	1.46	1.35
21	b	605	CL7	CHC-C1C	8.24	1.46	1.35
21	B	612	CL7	CHC-C1C	8.16	1.46	1.35
21	b	613	CL7	CHC-C1C	8.16	1.46	1.35
21	7	506	CL7	CHC-C1C	8.04	1.46	1.35
21	3	506	CL7	CHC-C1C	8.04	1.46	1.35
23	C	516	8CT	C04-C03	-7.99	1.42	1.53
21	B	615	CL7	CHC-C1C	7.99	1.46	1.35
21	b	616	CL7	CHC-C1C	7.99	1.46	1.35
23	c	516	8CT	C04-C03	-7.99	1.42	1.53
23	B	618	8CT	C04-C03	-7.92	1.42	1.53
23	b	619	8CT	C04-C03	-7.92	1.42	1.53
23	4	402	8CT	C04-C03	-7.70	1.43	1.53
23	8	402	8CT	C04-C03	-7.70	1.43	1.53
23	A	404	8CT	C04-C03	-7.63	1.43	1.53
23	a	404	8CT	C04-C03	-7.63	1.43	1.53
23	B	617	8CT	C04-C03	-7.63	1.43	1.53
23	b	618	8CT	C04-C03	-7.63	1.43	1.53
23	C	519	8CT	C04-C03	-7.62	1.43	1.53
23	c	519	8CT	C04-C03	-7.62	1.43	1.53
23	B	619	8CT	C04-C03	-7.49	1.43	1.53
23	b	620	8CT	C04-C03	-7.49	1.43	1.53
23	K	101	8CT	C04-C03	-7.45	1.43	1.53
23	k	101	8CT	C04-C03	-7.45	1.43	1.53
23	C	515	8CT	C04-C03	-7.27	1.43	1.53
23	c	515	8CT	C04-C03	-7.27	1.43	1.53
23	D	406	8CT	C04-C03	-7.01	1.44	1.53
23	d	406	8CT	C04-C03	-7.01	1.44	1.53
23	B	627	8CT	C04-C03	-6.80	1.44	1.53
23	b	601	8CT	C04-C03	-6.80	1.44	1.53
23	8	402	8CT	C05-C06	-6.76	1.35	1.52
23	4	402	8CT	C05-C06	-6.72	1.36	1.52
21	B	605	CL7	C3D-C4D	-6.72	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	606	CL7	C3D-C4D	-6.72	1.34	1.40
21	3	509	CL7	C3D-C4D	-6.60	1.34	1.40
21	7	509	CL7	C3D-C4D	-6.60	1.34	1.40
21	2	505	CL7	C3D-C4D	-6.59	1.34	1.40
21	6	505	CL7	C3D-C4D	-6.59	1.34	1.40
23	b	620	8CT	C05-C06	-6.57	1.36	1.52
23	B	619	8CT	C05-C06	-6.54	1.36	1.52
21	C	510	CL7	C3D-C4D	-6.53	1.34	1.40
21	c	510	CL7	C3D-C4D	-6.53	1.34	1.40
23	C	515	8CT	C05-C06	-6.53	1.36	1.52
23	c	515	8CT	C05-C06	-6.53	1.36	1.52
21	B	609	CL7	C3D-C4D	-6.52	1.34	1.40
21	b	610	CL7	C3D-C4D	-6.52	1.34	1.40
23	C	516	8CT	C05-C06	-6.51	1.36	1.52
23	c	516	8CT	C05-C06	-6.51	1.36	1.52
23	a	404	8CT	C05-C06	-6.50	1.36	1.52
23	A	404	8CT	C05-C06	-6.50	1.36	1.52
23	B	627	8CT	C05-C06	-6.48	1.36	1.52
23	b	601	8CT	C05-C06	-6.48	1.36	1.52
23	B	618	8CT	C05-C06	-6.48	1.36	1.52
23	b	619	8CT	C05-C06	-6.48	1.36	1.52
23	D	406	8CT	C05-C06	-6.47	1.36	1.52
23	d	406	8CT	C05-C06	-6.47	1.36	1.52
21	a	405	CL7	C3D-C4D	-6.45	1.34	1.40
23	k	101	8CT	C05-C06	-6.45	1.36	1.52
23	B	617	8CT	C05-C06	-6.45	1.36	1.52
23	b	618	8CT	C05-C06	-6.45	1.36	1.52
23	K	101	8CT	C05-C06	-6.41	1.36	1.52
21	2	509	CL7	C3D-C4D	-6.40	1.34	1.40
21	6	509	CL7	C3D-C4D	-6.39	1.34	1.40
21	C	506	CL7	C3D-C4D	-6.39	1.34	1.40
21	A	406	CL7	C3D-C4D	-6.37	1.34	1.40
21	3	516	CL7	C3D-C4D	-6.37	1.34	1.40
21	7	516	CL7	C3D-C4D	-6.34	1.34	1.40
23	C	519	8CT	C05-C06	-6.33	1.36	1.52
21	B	608	CL7	C3D-C4D	-6.32	1.34	1.40
21	b	609	CL7	C3D-C4D	-6.32	1.34	1.40
21	c	506	CL7	C3D-C4D	-6.30	1.34	1.40
21	b	603	CL7	C3D-C4D	-6.30	1.34	1.40
21	b	614	CL7	C3D-C4D	-6.29	1.34	1.40
23	c	519	8CT	C05-C06	-6.29	1.37	1.52
21	B	612	CL7	C3D-C4D	-6.29	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	613	CL7	C3D-C4D	-6.29	1.34	1.40
21	B	603	CL7	C3D-C4D	-6.29	1.34	1.40
21	b	604	CL7	C3D-C4D	-6.29	1.34	1.40
21	D	404	CL7	C3D-C4D	-6.27	1.34	1.40
21	b	612	CL7	C3D-C4D	-6.27	1.34	1.40
21	1	406	CL7	C3D-C4D	-6.26	1.34	1.40
21	5	406	CL7	C3D-C4D	-6.26	1.34	1.40
21	B	613	CL7	C3D-C4D	-6.26	1.34	1.40
21	B	602	CL7	C3D-C4D	-6.24	1.34	1.40
21	d	404	CL7	C3D-C4D	-6.24	1.34	1.40
21	B	611	CL7	C3D-C4D	-6.23	1.34	1.40
21	3	502	CL7	C3D-C4D	-6.22	1.34	1.40
21	7	502	CL7	C3D-C4D	-6.22	1.34	1.40
21	C	511	CL7	C3D-C4D	-6.20	1.34	1.40
21	c	511	CL7	C3D-C4D	-6.20	1.34	1.40
21	4	411	CL7	C3D-C4D	-6.11	1.34	1.40
21	B	615	CL7	C3D-C4D	-6.11	1.34	1.40
21	b	616	CL7	C3D-C4D	-6.11	1.34	1.40
21	C	509	CL7	C3D-C4D	-6.10	1.34	1.40
21	c	509	CL7	C3D-C4D	-6.10	1.34	1.40
21	A	403	CL7	C3D-C4D	-6.10	1.34	1.40
21	a	403	CL7	C3D-C4D	-6.10	1.34	1.40
21	2	516	CL7	C3D-C4D	-6.08	1.34	1.40
21	6	516	CL7	C3D-C4D	-6.08	1.34	1.40
21	2	506	CL7	C3D-C4D	-6.06	1.34	1.40
21	3	507	CL7	C3D-C4D	-6.05	1.34	1.40
21	6	506	CL7	C3D-C4D	-6.05	1.34	1.40
21	7	507	CL7	C3D-C4D	-6.05	1.34	1.40
21	2	502	CL7	C3D-C4D	-6.04	1.34	1.40
21	b	607	CL7	C3D-C4D	-6.04	1.34	1.40
21	b	608	CL7	C3D-C4D	-6.04	1.34	1.40
21	6	502	CL7	C3D-C4D	-6.04	1.34	1.40
21	8	410	CL7	C3D-C4D	-6.03	1.34	1.40
21	8	411	CL7	C3D-C4D	-6.02	1.34	1.40
21	B	607	CL7	C3D-C4D	-6.02	1.34	1.40
21	7	512	CL7	C3D-C4D	-6.02	1.34	1.40
21	B	604	CL7	C3D-C4D	-6.01	1.34	1.40
21	b	605	CL7	C3D-C4D	-6.01	1.34	1.40
21	3	513	CL7	C3D-C4D	-6.01	1.34	1.40
21	C	507	CL7	C3D-C4D	-6.00	1.34	1.40
21	c	507	CL7	C3D-C4D	-6.00	1.34	1.40
21	4	412	CL7	C3D-C4D	-6.00	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	412	CL7	C3D-C4D	-6.00	1.34	1.40
21	2	511	CL7	C3D-C4D	-6.00	1.34	1.40
21	6	511	CL7	C3D-C4D	-6.00	1.34	1.40
21	B	606	CL7	C3D-C4D	-5.99	1.34	1.40
21	7	513	CL7	C3D-C4D	-5.99	1.34	1.40
21	4	417	CL7	C3D-C4D	-5.99	1.34	1.40
21	3	511	CL7	C3D-C4D	-5.99	1.34	1.40
21	7	511	CL7	C3D-C4D	-5.99	1.34	1.40
21	8	404	CL7	C3D-C4D	-5.99	1.34	1.40
21	4	413	CL7	C3D-C4D	-5.98	1.34	1.40
21	2	508	CL7	C3D-C4D	-5.98	1.34	1.40
21	2	510	CL7	C3D-C4D	-5.97	1.34	1.40
21	6	510	CL7	C3D-C4D	-5.97	1.34	1.40
21	7	504	CL7	C3D-C4D	-5.96	1.34	1.40
21	8	413	CL7	C3D-C4D	-5.96	1.34	1.40
21	6	508	CL7	C3D-C4D	-5.95	1.34	1.40
21	C	508	CL7	C3D-C4D	-5.95	1.34	1.40
21	c	508	CL7	C3D-C4D	-5.95	1.34	1.40
21	C	503	CL7	C3D-C4D	-5.95	1.34	1.40
21	1	403	CL7	C3D-C4D	-5.95	1.34	1.40
21	c	503	CL7	C3D-C4D	-5.95	1.34	1.40
21	5	403	CL7	C3D-C4D	-5.95	1.34	1.40
21	4	410	CL7	C3D-C4D	-5.95	1.34	1.40
21	3	510	CL7	C3D-C4D	-5.94	1.34	1.40
21	7	510	CL7	C3D-C4D	-5.94	1.34	1.40
23	k	101	8CT	C15-C16	5.94	1.58	1.45
21	3	508	CL7	C3D-C4D	-5.94	1.34	1.40
21	7	508	CL7	C3D-C4D	-5.94	1.34	1.40
23	K	101	8CT	C15-C16	5.94	1.58	1.45
21	6	514	CL7	C3D-C4D	-5.94	1.34	1.40
21	3	512	CL7	C3D-C4D	-5.93	1.34	1.40
21	4	407	CL7	C3D-C4D	-5.93	1.34	1.40
21	8	407	CL7	C3D-C4D	-5.93	1.34	1.40
21	3	501	CL7	C3D-C4D	-5.92	1.34	1.40
21	7	501	CL7	C3D-C4D	-5.92	1.34	1.40
21	2	507	CL7	C3D-C4D	-5.92	1.34	1.40
21	2	514	CL7	C3D-C4D	-5.92	1.34	1.40
21	3	504	CL7	C3D-C4D	-5.92	1.34	1.40
21	6	507	CL7	C3D-C4D	-5.92	1.34	1.40
21	8	417	CL7	C3D-C4D	-5.91	1.34	1.40
21	D	405	CL7	C3D-C4D	-5.91	1.34	1.40
21	d	405	CL7	C3D-C4D	-5.91	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	517	CL7	C3D-C4D	-5.90	1.34	1.40
21	6	517	CL7	C3D-C4D	-5.90	1.34	1.40
21	2	504	CL7	C3D-C4D	-5.90	1.34	1.40
21	6	504	CL7	C3D-C4D	-5.90	1.34	1.40
21	1	418	CL7	C3D-C4D	-5.89	1.34	1.40
21	5	418	CL7	C3D-C4D	-5.89	1.34	1.40
21	4	404	CL7	C3D-C4D	-5.89	1.34	1.40
21	4	415	CL7	C3D-C4D	-5.87	1.34	1.40
21	B	614	CL7	C3D-C4D	-5.87	1.34	1.40
21	1	417	CL7	C3D-C4D	-5.87	1.34	1.40
21	5	417	CL7	C3D-C4D	-5.87	1.34	1.40
21	8	415	CL7	C3D-C4D	-5.85	1.34	1.40
21	2	513	CL7	C3D-C4D	-5.84	1.34	1.40
21	6	513	CL7	C3D-C4D	-5.84	1.34	1.40
21	1	404	CL7	C3D-C4D	-5.84	1.34	1.40
21	5	404	CL7	C3D-C4D	-5.84	1.34	1.40
23	B	627	8CT	C15-C16	5.84	1.58	1.45
23	b	601	8CT	C15-C16	5.84	1.58	1.45
21	C	504	CL7	C3D-C4D	-5.84	1.34	1.40
21	c	504	CL7	C3D-C4D	-5.84	1.34	1.40
21	b	615	CL7	C3D-C4D	-5.83	1.34	1.40
21	8	414	CL7	C3D-C4D	-5.83	1.34	1.40
23	B	617	8CT	C15-C16	5.83	1.58	1.45
23	b	618	8CT	C15-C16	5.83	1.58	1.45
21	2	503	CL7	C3D-C4D	-5.82	1.34	1.40
21	6	503	CL7	C3D-C4D	-5.82	1.34	1.40
21	D	402	CL7	C3D-C4D	-5.81	1.34	1.40
21	d	402	CL7	C3D-C4D	-5.81	1.34	1.40
21	4	414	CL7	C3D-C4D	-5.80	1.34	1.40
21	B	610	CL7	C3D-C4D	-5.80	1.34	1.40
21	b	611	CL7	C3D-C4D	-5.80	1.34	1.40
21	3	514	CL7	C3D-C4D	-5.79	1.34	1.40
22	D	408	PHO	C3B-C2B	5.79	1.48	1.40
21	8	405	CL7	C3D-C4D	-5.79	1.34	1.40
21	B	616	CL7	C3D-C4D	-5.79	1.34	1.40
21	C	512	CL7	C3D-C4D	-5.79	1.34	1.40
21	b	617	CL7	C3D-C4D	-5.79	1.34	1.40
22	d	408	PHO	C3B-C2B	5.79	1.48	1.40
21	8	406	CL7	C3D-C4D	-5.78	1.34	1.40
21	4	409	CL7	C3D-C4D	-5.78	1.34	1.40
21	8	409	CL7	C3D-C4D	-5.78	1.34	1.40
21	4	406	CL7	C3D-C4D	-5.77	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	408	CL7	C3D-C4D	-5.76	1.34	1.40
21	3	505	CL7	C3D-C4D	-5.75	1.34	1.40
21	7	505	CL7	C3D-C4D	-5.75	1.34	1.40
21	4	405	CL7	C3D-C4D	-5.73	1.34	1.40
21	3	503	CL7	C3D-C4D	-5.73	1.34	1.40
21	7	503	CL7	C3D-C4D	-5.73	1.34	1.40
21	3	506	CL7	C3D-C4D	-5.72	1.34	1.40
21	c	512	CL7	C3D-C4D	-5.72	1.34	1.40
21	7	506	CL7	C3D-C4D	-5.72	1.34	1.40
21	1	410	CL7	C3D-C4D	-5.71	1.34	1.40
21	5	410	CL7	C3D-C4D	-5.71	1.34	1.40
21	C	502	CL7	C3D-C4D	-5.70	1.34	1.40
21	7	514	CL7	C3D-C4D	-5.69	1.34	1.40
23	C	516	8CT	C15-C16	5.69	1.58	1.45
21	c	502	CL7	C3D-C4D	-5.69	1.34	1.40
21	1	411	CL7	C3D-C4D	-5.69	1.34	1.40
21	5	411	CL7	C3D-C4D	-5.69	1.34	1.40
21	4	408	CL7	C3D-C4D	-5.68	1.34	1.40
21	2	515	CL7	C3D-C4D	-5.66	1.34	1.40
21	6	515	CL7	C3D-C4D	-5.66	1.34	1.40
23	c	516	8CT	C15-C16	5.66	1.58	1.45
23	b	619	8CT	C15-C16	5.65	1.58	1.45
21	B	622	CL7	C3D-C4D	-5.65	1.35	1.40
21	b	623	CL7	C3D-C4D	-5.65	1.35	1.40
21	3	517	CL7	C3D-C4D	-5.65	1.35	1.40
21	7	517	CL7	C3D-C4D	-5.65	1.35	1.40
21	1	407	CL7	C3D-C4D	-5.63	1.35	1.40
21	5	407	CL7	C3D-C4D	-5.63	1.35	1.40
23	C	515	8CT	C15-C16	5.62	1.58	1.45
23	c	515	8CT	C15-C16	5.62	1.58	1.45
21	5	414	CL7	C3D-C4D	-5.61	1.35	1.40
23	B	618	8CT	C15-C16	5.61	1.58	1.45
23	C	519	8CT	C15-C16	5.61	1.58	1.45
21	4	416	CL7	C3D-C4D	-5.60	1.35	1.40
21	8	416	CL7	C3D-C4D	-5.60	1.35	1.40
21	2	512	CL7	C3D-C4D	-5.59	1.35	1.40
21	6	512	CL7	C3D-C4D	-5.59	1.35	1.40
23	D	406	8CT	C15-C16	5.59	1.58	1.45
23	d	406	8CT	C15-C16	5.59	1.58	1.45
21	2	518	CL7	C3D-C4D	-5.59	1.35	1.40
21	6	518	CL7	C3D-C4D	-5.59	1.35	1.40
23	c	519	8CT	C15-C16	5.58	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	414	CL7	C3D-C4D	-5.58	1.35	1.40
23	B	619	8CT	C15-C16	5.58	1.57	1.45
23	b	620	8CT	C15-C16	5.58	1.57	1.45
21	1	405	CL7	C3D-C4D	-5.56	1.35	1.40
21	5	405	CL7	C3D-C4D	-5.56	1.35	1.40
21	C	518	CL7	C3D-C4D	-5.55	1.35	1.40
21	c	518	CL7	C3D-C4D	-5.55	1.35	1.40
21	2	501	CL7	C3D-C4D	-5.55	1.35	1.40
21	6	501	CL7	C3D-C4D	-5.55	1.35	1.40
21	3	518	CL7	C3D-C4D	-5.54	1.35	1.40
21	3	515	CL7	C3D-C4D	-5.52	1.35	1.40
21	7	515	CL7	C3D-C4D	-5.52	1.35	1.40
21	7	518	CL7	C3D-C4D	-5.51	1.35	1.40
21	1	409	CL7	C3D-C4D	-5.47	1.35	1.40
21	5	409	CL7	C3D-C4D	-5.47	1.35	1.40
21	B	601	CL7	C3D-C4D	-5.47	1.35	1.40
21	1	408	CL7	C3D-C4D	-5.46	1.35	1.40
21	5	408	CL7	C3D-C4D	-5.46	1.35	1.40
21	C	514	CL7	C3D-C4D	-5.45	1.35	1.40
21	c	514	CL7	C3D-C4D	-5.45	1.35	1.40
23	B	618	8CT	C11-C12	5.45	1.57	1.45
21	1	413	CL7	C3D-C4D	-5.43	1.35	1.40
21	5	413	CL7	C3D-C4D	-5.43	1.35	1.40
23	b	619	8CT	C11-C12	5.42	1.57	1.45
21	c	505	CL7	C3D-C4D	-5.42	1.35	1.40
23	A	404	8CT	C15-C16	5.40	1.57	1.45
23	a	404	8CT	C15-C16	5.40	1.57	1.45
21	b	602	CL7	C3D-C4D	-5.39	1.35	1.40
21	C	505	CL7	C3D-C4D	-5.38	1.35	1.40
21	1	416	CL7	C3D-C4D	-5.37	1.35	1.40
21	c	513	CL7	C3D-C4D	-5.37	1.35	1.40
23	8	402	8CT	C34-C33	5.37	1.65	1.52
21	5	416	CL7	C3D-C4D	-5.36	1.35	1.40
23	4	402	8CT	C34-C33	5.36	1.65	1.52
21	1	402	CL7	C3D-C4D	-5.35	1.35	1.40
21	C	513	CL7	C3D-C4D	-5.35	1.35	1.40
23	8	402	8CT	C15-C16	5.34	1.57	1.45
23	4	402	8CT	C15-C16	5.32	1.57	1.45
30	d	407	PL9	C3-C4	-5.29	1.40	1.49
23	B	627	8CT	C05-C04	5.29	1.66	1.54
23	b	601	8CT	C05-C04	5.29	1.66	1.54
23	K	101	8CT	C11-C12	5.27	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	k	101	8CT	C11-C12	5.27	1.57	1.45
30	D	407	PL9	C3-C4	-5.27	1.40	1.49
21	5	402	CL7	C3D-C4D	-5.26	1.35	1.40
21	1	420	CL7	C3D-C4D	-5.25	1.35	1.40
21	5	420	CL7	C3D-C4D	-5.25	1.35	1.40
23	B	627	8CT	C35-C30	5.23	1.71	1.56
23	b	601	8CT	C35-C30	5.23	1.71	1.56
23	k	101	8CT	C05-C04	5.19	1.66	1.54
21	D	404	CL7	C4D-CHA	-5.19	1.38	1.45
21	d	404	CL7	C4D-CHA	-5.19	1.38	1.45
23	B	618	8CT	C34-C33	5.17	1.64	1.52
23	b	619	8CT	C34-C33	5.17	1.64	1.52
23	K	101	8CT	C05-C04	5.17	1.66	1.54
21	1	419	CL7	C3D-C4D	-5.16	1.35	1.40
23	b	601	8CT	C11-C12	5.16	1.57	1.45
23	B	627	8CT	C11-C12	5.16	1.57	1.45
23	B	619	8CT	C34-C33	5.16	1.64	1.52
23	b	620	8CT	C34-C33	5.16	1.64	1.52
23	D	406	8CT	C34-C33	5.14	1.64	1.52
23	d	406	8CT	C34-C33	5.14	1.64	1.52
21	B	609	CL7	C4D-CHA	-5.14	1.38	1.45
21	b	610	CL7	C4D-CHA	-5.14	1.38	1.45
21	5	419	CL7	C3D-C4D	-5.14	1.35	1.40
21	C	509	CL7	C4D-CHA	-5.13	1.38	1.45
21	c	506	CL7	C4D-CHA	-5.11	1.38	1.45
21	A	406	CL7	C4D-CHA	-5.11	1.38	1.45
21	c	509	CL7	C4D-CHA	-5.07	1.38	1.45
21	B	605	CL7	C4D-CHA	-5.07	1.38	1.45
21	a	405	CL7	C4D-CHA	-5.07	1.38	1.45
21	C	506	CL7	C4D-CHA	-5.07	1.38	1.45
23	k	101	8CT	C35-C30	5.05	1.70	1.56
23	K	101	8CT	C35-C30	5.04	1.70	1.56
21	1	404	CL7	C4D-CHA	-5.03	1.38	1.45
21	5	404	CL7	C4D-CHA	-5.03	1.38	1.45
23	A	404	8CT	C34-C33	5.02	1.64	1.52
21	1	412	CL7	C3D-C4D	-5.02	1.35	1.40
21	5	412	CL7	C3D-C4D	-5.02	1.35	1.40
23	C	519	8CT	C11-C12	5.02	1.56	1.45
23	c	519	8CT	C11-C12	5.02	1.56	1.45
23	D	406	8CT	C05-C04	5.02	1.65	1.54
23	d	406	8CT	C05-C04	5.02	1.65	1.54
23	a	404	8CT	C34-C33	5.02	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	606	CL7	C4D-CHA	-5.00	1.38	1.45
23	B	617	8CT	C05-C04	5.00	1.65	1.54
23	b	618	8CT	C05-C04	5.00	1.65	1.54
21	C	511	CL7	C4D-CHA	-4.99	1.38	1.45
21	c	511	CL7	C4D-CHA	-4.99	1.38	1.45
21	C	510	CL7	C4D-CHA	-4.99	1.38	1.45
21	c	510	CL7	C4D-CHA	-4.99	1.38	1.45
21	B	612	CL7	C4D-CHA	-4.99	1.38	1.45
21	b	613	CL7	C4D-CHA	-4.99	1.38	1.45
23	b	620	8CT	C05-C04	4.98	1.65	1.54
23	K	101	8CT	C14-C13	4.98	1.58	1.43
23	k	101	8CT	C14-C13	4.97	1.58	1.43
23	B	619	8CT	C05-C04	4.97	1.65	1.54
23	C	519	8CT	C05-C04	4.96	1.65	1.54
21	B	611	CL7	C4D-CHA	-4.96	1.38	1.45
21	b	612	CL7	C4D-CHA	-4.96	1.38	1.45
21	2	509	CL7	C4D-CHA	-4.96	1.38	1.45
21	6	509	CL7	C4D-CHA	-4.96	1.38	1.45
23	B	627	8CT	C34-C33	4.94	1.64	1.52
23	b	601	8CT	C34-C33	4.94	1.64	1.52
23	c	519	8CT	C05-C04	4.93	1.65	1.54
21	3	501	CL7	C4D-CHA	-4.92	1.38	1.45
21	7	501	CL7	C4D-CHA	-4.92	1.38	1.45
21	6	505	CL7	C4D-CHA	-4.92	1.38	1.45
23	C	519	8CT	C34-C33	4.91	1.64	1.52
23	c	519	8CT	C34-C33	4.91	1.64	1.52
21	1	406	CL7	C4D-CHA	-4.91	1.38	1.45
21	5	406	CL7	C4D-CHA	-4.91	1.38	1.45
23	K	101	8CT	C28-C26	4.90	1.56	1.45
23	k	101	8CT	C28-C26	4.90	1.56	1.45
21	B	613	CL7	C4D-CHA	-4.90	1.38	1.45
23	8	402	8CT	C05-C04	4.89	1.65	1.54
21	2	502	CL7	C4D-CHA	-4.88	1.39	1.45
21	6	502	CL7	C4D-CHA	-4.88	1.39	1.45
23	4	402	8CT	C05-C04	4.88	1.65	1.54
23	B	618	8CT	C05-C04	4.87	1.65	1.54
23	b	619	8CT	C05-C04	4.87	1.65	1.54
23	A	404	8CT	C05-C04	4.87	1.65	1.54
23	a	404	8CT	C05-C04	4.87	1.65	1.54
23	B	617	8CT	C11-C12	4.87	1.56	1.45
21	b	609	CL7	C4D-CHA	-4.87	1.39	1.45
21	3	516	CL7	C4D-CHA	-4.87	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	505	CL7	C4D-CHA	-4.86	1.39	1.45
21	C	512	CL7	C4D-CHA	-4.86	1.39	1.45
21	b	614	CL7	C4D-CHA	-4.86	1.39	1.45
21	B	608	CL7	C4D-CHA	-4.85	1.39	1.45
23	B	627	8CT	C14-C13	4.85	1.58	1.43
23	b	601	8CT	C14-C13	4.85	1.58	1.43
21	8	411	CL7	C4D-CHA	-4.85	1.39	1.45
21	4	410	CL7	C4D-CHA	-4.84	1.39	1.45
21	8	410	CL7	C4D-CHA	-4.84	1.39	1.45
23	C	515	8CT	C05-C04	4.84	1.65	1.54
21	B	607	CL7	C4D-CHA	-4.84	1.39	1.45
21	7	516	CL7	C4D-CHA	-4.83	1.39	1.45
23	b	618	8CT	C11-C12	4.83	1.56	1.45
21	c	512	CL7	C4D-CHA	-4.83	1.39	1.45
23	c	515	8CT	C05-C04	4.83	1.65	1.54
21	3	503	CL7	C4D-CHA	-4.83	1.39	1.45
21	7	503	CL7	C4D-CHA	-4.83	1.39	1.45
21	D	402	CL7	C4D-CHA	-4.83	1.39	1.45
21	d	402	CL7	C4D-CHA	-4.83	1.39	1.45
21	4	411	CL7	C4D-CHA	-4.82	1.39	1.45
21	2	514	CL7	C4D-CHA	-4.82	1.39	1.45
21	6	514	CL7	C4D-CHA	-4.82	1.39	1.45
23	C	516	8CT	C05-C04	4.82	1.65	1.54
23	c	516	8CT	C05-C04	4.82	1.65	1.54
23	k	101	8CT	C34-C33	4.81	1.63	1.52
23	c	516	8CT	C14-C13	4.81	1.58	1.43
21	B	603	CL7	C4D-CHA	-4.81	1.39	1.45
21	b	604	CL7	C4D-CHA	-4.81	1.39	1.45
21	3	505	CL7	C4D-CHA	-4.80	1.39	1.45
21	7	505	CL7	C4D-CHA	-4.80	1.39	1.45
23	K	101	8CT	C34-C33	4.80	1.63	1.52
21	b	608	CL7	C4D-CHA	-4.80	1.39	1.45
21	3	508	CL7	C4D-CHA	-4.80	1.39	1.45
21	7	508	CL7	C4D-CHA	-4.80	1.39	1.45
21	3	513	CL7	C4D-CHA	-4.80	1.39	1.45
21	7	513	CL7	C4D-CHA	-4.80	1.39	1.45
23	C	516	8CT	C14-C13	4.79	1.58	1.43
21	1	403	CL7	C4D-CHA	-4.79	1.39	1.45
21	5	403	CL7	C4D-CHA	-4.79	1.39	1.45
21	2	503	CL7	C4D-CHA	-4.78	1.39	1.45
21	6	503	CL7	C4D-CHA	-4.78	1.39	1.45
23	C	516	8CT	C11-C12	4.78	1.56	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	516	8CT	C11-C12	4.78	1.56	1.45
23	d	406	8CT	C14-C13	4.78	1.58	1.43
21	C	507	CL7	C4D-CHA	-4.78	1.39	1.45
21	c	507	CL7	C4D-CHA	-4.78	1.39	1.45
23	C	519	8CT	C35-C30	4.78	1.69	1.56
23	c	519	8CT	C35-C30	4.78	1.69	1.56
23	B	617	8CT	C14-C13	4.77	1.58	1.43
23	b	618	8CT	C14-C13	4.77	1.58	1.43
23	D	406	8CT	C11-C12	4.77	1.56	1.45
23	B	617	8CT	C35-C30	4.76	1.69	1.56
23	b	618	8CT	C35-C30	4.76	1.69	1.56
23	D	406	8CT	C14-C13	4.76	1.58	1.43
23	C	515	8CT	C34-C33	4.76	1.63	1.52
23	c	515	8CT	C34-C33	4.76	1.63	1.52
23	c	519	8CT	C14-C13	4.76	1.58	1.43
21	C	502	CL7	C4D-CHA	-4.76	1.39	1.45
23	c	515	8CT	C11-C12	4.75	1.56	1.45
23	C	515	8CT	C35-C30	4.75	1.69	1.56
23	c	515	8CT	C35-C30	4.75	1.69	1.56
23	d	406	8CT	C11-C12	4.74	1.56	1.45
21	C	504	CL7	C4D-CHA	-4.74	1.39	1.45
21	c	504	CL7	C4D-CHA	-4.74	1.39	1.45
23	C	515	8CT	C11-C12	4.74	1.56	1.45
23	D	406	8CT	C35-C30	4.73	1.69	1.56
23	d	406	8CT	C35-C30	4.73	1.69	1.56
21	1	405	CL7	C4D-CHA	-4.73	1.39	1.45
21	5	405	CL7	C4D-CHA	-4.73	1.39	1.45
23	C	519	8CT	C14-C13	4.73	1.58	1.43
23	B	619	8CT	C11-C12	4.73	1.56	1.45
23	b	620	8CT	C11-C12	4.73	1.56	1.45
21	8	408	CL7	C4D-CHA	-4.73	1.39	1.45
21	2	515	CL7	C4D-CHA	-4.72	1.39	1.45
21	6	515	CL7	C4D-CHA	-4.72	1.39	1.45
21	3	504	CL7	C4D-CHA	-4.72	1.39	1.45
21	4	404	CL7	C4D-CHA	-4.72	1.39	1.45
21	3	511	CL7	C4D-CHA	-4.72	1.39	1.45
21	7	511	CL7	C4D-CHA	-4.72	1.39	1.45
21	3	509	CL7	C4D-CHA	-4.72	1.39	1.45
21	7	509	CL7	C4D-CHA	-4.72	1.39	1.45
21	4	408	CL7	C4D-CHA	-4.71	1.39	1.45
21	C	503	CL7	C4D-CHA	-4.71	1.39	1.45
21	c	503	CL7	C4D-CHA	-4.71	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	511	CL7	C4D-CHA	-4.70	1.39	1.45
21	7	504	CL7	C4D-CHA	-4.70	1.39	1.45
21	c	502	CL7	C4D-CHA	-4.69	1.39	1.45
23	A	404	8CT	C11-C12	4.69	1.56	1.45
21	3	502	CL7	C4D-CHA	-4.68	1.39	1.45
21	7	502	CL7	C4D-CHA	-4.68	1.39	1.45
21	4	406	CL7	C4D-CHA	-4.68	1.39	1.45
21	8	406	CL7	C4D-CHA	-4.68	1.39	1.45
21	6	510	CL7	C4D-CHA	-4.68	1.39	1.45
21	6	513	CL7	C4D-CHA	-4.68	1.39	1.45
22	d	408	PHO	OBD-CAD	4.67	1.28	1.22
21	2	507	CL7	C4D-CHA	-4.67	1.39	1.45
21	6	507	CL7	C4D-CHA	-4.67	1.39	1.45
21	2	511	CL7	C4D-CHA	-4.67	1.39	1.45
21	4	414	CL7	C4D-CHA	-4.67	1.39	1.45
21	8	414	CL7	C4D-CHA	-4.67	1.39	1.45
21	2	512	CL7	C4D-CHA	-4.66	1.39	1.45
21	6	512	CL7	C4D-CHA	-4.66	1.39	1.45
21	2	508	CL7	C4D-CHA	-4.66	1.39	1.45
21	B	602	CL7	C4D-CHA	-4.66	1.39	1.45
21	b	603	CL7	C4D-CHA	-4.66	1.39	1.45
21	1	415	CL7	C3D-C4D	-4.66	1.35	1.40
21	5	415	CL7	C3D-C4D	-4.66	1.35	1.40
21	4	412	CL7	C4D-CHA	-4.65	1.39	1.45
21	8	412	CL7	C4D-CHA	-4.65	1.39	1.45
23	a	404	8CT	C11-C12	4.65	1.55	1.45
23	K	101	8CT	C24-C25	4.65	1.57	1.43
23	k	101	8CT	C24-C25	4.65	1.57	1.43
22	D	408	PHO	OBD-CAD	4.65	1.28	1.22
21	2	506	CL7	C4D-CHA	-4.65	1.39	1.45
21	6	506	CL7	C4D-CHA	-4.65	1.39	1.45
21	6	508	CL7	C4D-CHA	-4.64	1.39	1.45
21	D	405	CL7	C4D-CHA	-4.64	1.39	1.45
21	d	405	CL7	C4D-CHA	-4.64	1.39	1.45
21	2	510	CL7	C4D-CHA	-4.64	1.39	1.45
23	C	516	8CT	C34-C33	4.63	1.63	1.52
23	c	516	8CT	C34-C33	4.63	1.63	1.52
23	C	516	8CT	C24-C25	4.63	1.57	1.43
23	c	516	8CT	C24-C25	4.63	1.57	1.43
21	A	403	CL7	C4D-CHA	-4.63	1.39	1.45
21	C	518	CL7	C4D-CHA	-4.63	1.39	1.45
21	c	518	CL7	C4D-CHA	-4.63	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	416	CL7	C4D-CHA	-4.63	1.39	1.45
21	8	416	CL7	C4D-CHA	-4.63	1.39	1.45
23	B	617	8CT	C34-C33	4.63	1.63	1.52
21	2	513	CL7	C4D-CHA	-4.63	1.39	1.45
21	7	512	CL7	C4D-CHA	-4.62	1.39	1.45
21	1	417	CL7	C4D-CHA	-4.62	1.39	1.45
21	5	417	CL7	C4D-CHA	-4.62	1.39	1.45
21	a	403	CL7	C4D-CHA	-4.61	1.39	1.45
21	8	404	CL7	C4D-CHA	-4.61	1.39	1.45
23	b	618	8CT	C34-C33	4.60	1.63	1.52
21	3	512	CL7	C4D-CHA	-4.60	1.39	1.45
21	C	508	CL7	C4D-CHA	-4.59	1.39	1.45
21	c	508	CL7	C4D-CHA	-4.59	1.39	1.45
21	B	610	CL7	C4D-CHA	-4.58	1.39	1.45
21	b	611	CL7	C4D-CHA	-4.58	1.39	1.45
21	B	616	CL7	C4D-CHA	-4.58	1.39	1.45
21	b	617	CL7	C4D-CHA	-4.58	1.39	1.45
23	A	404	8CT	C14-C13	4.58	1.57	1.43
23	a	404	8CT	C14-C13	4.58	1.57	1.43
23	B	618	8CT	C35-C30	4.58	1.69	1.56
23	b	619	8CT	C35-C30	4.58	1.69	1.56
21	5	410	CL7	C4D-CHA	-4.58	1.39	1.45
21	4	407	CL7	C4D-CHA	-4.58	1.39	1.45
23	b	619	8CT	C14-C13	4.57	1.57	1.43
23	C	515	8CT	C14-C13	4.57	1.57	1.43
23	c	515	8CT	C14-C13	4.57	1.57	1.43
21	5	416	CL7	C4D-CHA	-4.57	1.39	1.45
23	C	516	8CT	C35-C30	4.56	1.69	1.56
23	c	516	8CT	C35-C30	4.56	1.69	1.56
21	1	407	CL7	C4D-CHA	-4.56	1.39	1.45
21	5	407	CL7	C4D-CHA	-4.56	1.39	1.45
21	1	410	CL7	C4D-CHA	-4.56	1.39	1.45
21	1	411	CL7	C4D-CHA	-4.55	1.39	1.45
21	5	411	CL7	C4D-CHA	-4.55	1.39	1.45
23	A	404	8CT	C35-C30	4.55	1.69	1.56
23	B	618	8CT	C14-C13	4.55	1.57	1.43
23	a	404	8CT	C35-C30	4.54	1.69	1.56
23	4	402	8CT	C14-C13	4.54	1.57	1.43
23	8	402	8CT	C14-C13	4.54	1.57	1.43
21	8	407	CL7	C4D-CHA	-4.53	1.39	1.45
23	4	402	8CT	C35-C30	4.52	1.69	1.56
23	8	402	8CT	C35-C30	4.52	1.69	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	416	CL7	C4D-CHA	-4.52	1.39	1.45
21	1	418	CL7	C4D-CHA	-4.52	1.39	1.45
21	5	418	CL7	C4D-CHA	-4.52	1.39	1.45
23	k	101	8CT	C18-C17	4.51	1.57	1.43
21	2	516	CL7	C4D-CHA	-4.51	1.39	1.45
21	6	516	CL7	C4D-CHA	-4.51	1.39	1.45
23	b	620	8CT	C14-C13	4.51	1.57	1.43
21	2	517	CL7	C4D-CHA	-4.50	1.39	1.45
21	6	517	CL7	C4D-CHA	-4.50	1.39	1.45
23	B	619	8CT	C14-C13	4.50	1.57	1.43
21	3	514	CL7	C4D-CHA	-4.49	1.39	1.45
21	7	514	CL7	C4D-CHA	-4.49	1.39	1.45
21	B	615	CL7	C4D-CHA	-4.49	1.39	1.45
21	b	616	CL7	C4D-CHA	-4.49	1.39	1.45
23	K	101	8CT	C18-C17	4.49	1.57	1.43
21	4	415	CL7	C4D-CHA	-4.48	1.39	1.45
21	8	415	CL7	C4D-CHA	-4.48	1.39	1.45
23	B	627	8CT	C24-C25	4.48	1.57	1.43
23	b	601	8CT	C24-C25	4.48	1.57	1.43
21	3	507	CL7	C4D-CHA	-4.48	1.39	1.45
21	7	507	CL7	C4D-CHA	-4.47	1.39	1.45
21	4	417	CL7	C4D-CHA	-4.47	1.39	1.45
21	8	417	CL7	C4D-CHA	-4.47	1.39	1.45
21	a	401	CL7	O2D-CGD	4.47	1.44	1.33
21	C	514	CL7	C4D-CHA	-4.47	1.39	1.45
21	c	514	CL7	C4D-CHA	-4.47	1.39	1.45
21	A	401	CL7	O2D-CGD	4.46	1.44	1.33
23	4	402	8CT	C11-C12	4.45	1.55	1.45
23	8	402	8CT	C11-C12	4.45	1.55	1.45
21	4	405	CL7	C4D-CHA	-4.45	1.39	1.45
21	4	409	CL7	C4D-CHA	-4.45	1.39	1.45
21	8	409	CL7	C4D-CHA	-4.45	1.39	1.45
23	D	406	8CT	C24-C25	4.45	1.57	1.43
23	d	406	8CT	C24-C25	4.45	1.57	1.43
23	B	619	8CT	C35-C30	4.42	1.68	1.56
23	b	620	8CT	C35-C30	4.42	1.68	1.56
21	3	518	CL7	C4D-CHA	-4.42	1.39	1.45
21	7	518	CL7	C4D-CHA	-4.42	1.39	1.45
23	C	519	8CT	C24-C25	4.41	1.57	1.43
23	c	519	8CT	C24-C25	4.41	1.57	1.43
21	8	405	CL7	C4D-CHA	-4.41	1.39	1.45
21	3	517	CL7	C4D-CHA	-4.40	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	517	CL7	C4D-CHA	-4.40	1.39	1.45
21	2	518	CL7	C4D-CHA	-4.40	1.39	1.45
21	6	518	CL7	C4D-CHA	-4.40	1.39	1.45
23	D	406	8CT	C28-C26	4.40	1.55	1.45
23	d	406	8CT	C28-C26	4.40	1.55	1.45
21	b	602	CL7	C4D-CHA	-4.38	1.39	1.45
21	B	604	CL7	C4D-CHA	-4.38	1.39	1.45
21	b	605	CL7	C4D-CHA	-4.38	1.39	1.45
21	B	601	CL7	C4D-CHA	-4.36	1.39	1.45
23	B	627	8CT	C18-C17	4.36	1.57	1.43
23	b	601	8CT	C18-C17	4.36	1.57	1.43
21	1	413	CL7	C4D-CHA	-4.35	1.39	1.45
21	5	413	CL7	C4D-CHA	-4.35	1.39	1.45
21	b	623	CL7	C4D-CHA	-4.35	1.39	1.45
21	1	412	CL7	C4D-CHA	-4.35	1.39	1.45
21	5	412	CL7	C4D-CHA	-4.35	1.39	1.45
21	B	622	CL7	C4D-CHA	-4.34	1.39	1.45
21	1	414	CL7	C4D-CHA	-4.34	1.39	1.45
21	5	414	CL7	C4D-CHA	-4.34	1.39	1.45
21	C	505	CL7	C4D-CHA	-4.33	1.39	1.45
21	B	606	CL7	C4D-CHA	-4.33	1.39	1.45
21	b	607	CL7	C4D-CHA	-4.33	1.39	1.45
21	4	413	CL7	C4D-CHA	-4.33	1.39	1.45
21	8	413	CL7	C4D-CHA	-4.33	1.39	1.45
21	1	402	CL7	C4D-CHA	-4.33	1.39	1.45
21	5	402	CL7	C4D-CHA	-4.33	1.39	1.45
23	a	404	8CT	C24-C25	4.32	1.56	1.43
21	c	505	CL7	C4D-CHA	-4.31	1.39	1.45
23	A	404	8CT	C24-C25	4.31	1.56	1.43
23	4	402	8CT	C24-C25	4.31	1.56	1.43
23	8	402	8CT	C24-C25	4.31	1.56	1.43
21	2	501	CL7	C4D-CHA	-4.31	1.39	1.45
23	C	515	8CT	C24-C25	4.31	1.56	1.43
23	c	515	8CT	C24-C25	4.31	1.56	1.43
21	C	513	CL7	C4D-CHA	-4.29	1.39	1.45
21	c	513	CL7	C4D-CHA	-4.29	1.39	1.45
23	C	516	8CT	C28-C26	4.29	1.55	1.45
23	B	619	8CT	C24-C25	4.29	1.56	1.43
23	b	620	8CT	C24-C25	4.29	1.56	1.43
21	3	510	CL7	C4D-CHA	-4.29	1.39	1.45
23	B	618	8CT	C28-C26	4.28	1.55	1.45
23	b	619	8CT	C28-C26	4.28	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	515	CL7	C4D-CHA	-4.28	1.39	1.45
21	6	501	CL7	C4D-CHA	-4.28	1.39	1.45
21	7	515	CL7	C4D-CHA	-4.28	1.39	1.45
23	B	618	8CT	C24-C25	4.27	1.56	1.43
23	b	619	8CT	C24-C25	4.27	1.56	1.43
21	2	504	CL7	C4D-CHA	-4.27	1.39	1.45
21	6	504	CL7	C4D-CHA	-4.27	1.39	1.45
23	c	516	8CT	C18-C17	4.27	1.56	1.43
21	7	510	CL7	C4D-CHA	-4.26	1.39	1.45
21	7	506	CL7	C4D-CHA	-4.26	1.39	1.45
23	C	516	8CT	C18-C17	4.26	1.56	1.43
23	c	516	8CT	C28-C26	4.25	1.55	1.45
21	1	408	CL7	C4D-CHA	-4.24	1.39	1.45
23	B	627	8CT	C28-C26	4.24	1.55	1.45
23	b	601	8CT	C28-C26	4.24	1.55	1.45
23	B	617	8CT	C24-C25	4.24	1.56	1.43
23	b	618	8CT	C24-C25	4.24	1.56	1.43
21	3	506	CL7	C4D-CHA	-4.23	1.39	1.45
21	5	419	CL7	C4D-CHA	-4.23	1.39	1.45
21	1	419	CL7	C4D-CHA	-4.23	1.39	1.45
21	5	408	CL7	C4D-CHA	-4.22	1.39	1.45
21	B	614	CL7	C4D-CHA	-4.22	1.39	1.45
21	b	615	CL7	C4D-CHA	-4.22	1.39	1.45
23	D	406	8CT	C18-C17	4.22	1.56	1.43
23	B	618	8CT	C18-C17	4.20	1.56	1.43
23	b	619	8CT	C18-C17	4.20	1.56	1.43
21	1	409	CL7	C4D-CHA	-4.20	1.39	1.45
21	5	409	CL7	C4D-CHA	-4.20	1.39	1.45
23	d	406	8CT	C18-C17	4.20	1.56	1.43
23	8	402	8CT	C28-C26	4.19	1.54	1.45
23	C	519	8CT	C28-C26	4.18	1.54	1.45
23	c	519	8CT	C28-C26	4.18	1.54	1.45
23	C	515	8CT	C28-C26	4.18	1.54	1.45
23	c	515	8CT	C28-C26	4.18	1.54	1.45
23	4	402	8CT	C28-C26	4.18	1.54	1.45
23	B	617	8CT	C18-C17	4.17	1.56	1.43
23	b	618	8CT	C18-C17	4.17	1.56	1.43
21	A	401	CL7	C3D-C4D	-4.16	1.36	1.40
21	a	401	CL7	C3D-C4D	-4.16	1.36	1.40
23	c	519	8CT	C18-C17	4.16	1.56	1.43
23	c	515	8CT	C18-C17	4.14	1.56	1.43
23	C	515	8CT	C18-C17	4.14	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	519	8CT	C18-C17	4.14	1.56	1.43
26	C	501	LMG	O8-C28	4.14	1.45	1.33
23	a	404	8CT	C18-C17	4.11	1.56	1.43
23	B	617	8CT	C28-C26	4.11	1.54	1.45
23	b	618	8CT	C28-C26	4.11	1.54	1.45
23	C	519	8CT	C06-C07	4.11	1.65	1.52
23	c	519	8CT	C06-C07	4.11	1.65	1.52
23	B	619	8CT	C28-C26	4.11	1.54	1.45
23	b	620	8CT	C28-C26	4.11	1.54	1.45
21	1	420	CL7	C4D-CHA	-4.11	1.39	1.45
21	5	420	CL7	C4D-CHA	-4.11	1.39	1.45
23	A	404	8CT	C28-C26	4.10	1.54	1.45
23	a	404	8CT	C28-C26	4.10	1.54	1.45
23	A	404	8CT	C18-C17	4.09	1.56	1.43
23	4	402	8CT	C18-C17	4.09	1.56	1.43
23	8	402	8CT	C18-C17	4.09	1.56	1.43
26	c	501	LMG	O8-C28	4.07	1.45	1.33
27	B	624	DGD	O1G-C1A	4.07	1.45	1.33
27	b	625	DGD	O1G-C1A	4.07	1.45	1.33
23	b	620	8CT	C18-C17	4.04	1.56	1.43
21	1	415	CL7	C4D-CHA	-4.03	1.40	1.45
21	5	415	CL7	C4D-CHA	-4.03	1.40	1.45
23	B	619	8CT	C18-C17	4.03	1.55	1.43
27	c	517	DGD	O1G-C1A	4.00	1.45	1.33
27	C	517	DGD	O2G-C1B	3.99	1.45	1.34
27	c	517	DGD	O2G-C1B	3.99	1.45	1.34
27	C	517	DGD	O1G-C1A	3.98	1.45	1.33
23	A	404	8CT	C06-C07	3.96	1.64	1.52
23	a	404	8CT	C06-C07	3.95	1.64	1.52
21	b	603	CL7	O2A-CGA	3.93	1.44	1.33
23	b	618	8CT	C06-C07	3.93	1.64	1.52
22	D	408	PHO	C3D-C2D	3.92	1.46	1.39
22	d	408	PHO	C3D-C2D	3.91	1.46	1.39
23	c	516	8CT	C06-C07	3.91	1.64	1.52
21	B	602	CL7	O2A-CGA	3.91	1.44	1.33
23	C	516	8CT	C06-C07	3.91	1.64	1.52
23	K	101	8CT	C23-C21	3.90	1.54	1.45
23	B	617	8CT	C06-C07	3.90	1.64	1.52
23	B	618	8CT	C06-C07	3.88	1.64	1.52
23	k	101	8CT	C23-C21	3.88	1.54	1.45
23	B	627	8CT	C06-C07	3.87	1.64	1.52
23	b	601	8CT	C06-C07	3.87	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	516	8CT	C23-C21	3.87	1.54	1.45
23	c	516	8CT	C23-C21	3.87	1.54	1.45
23	D	406	8CT	C06-C07	3.86	1.64	1.52
23	d	406	8CT	C06-C07	3.86	1.64	1.52
23	b	619	8CT	C06-C07	3.86	1.64	1.52
21	A	401	CL7	O2A-CGA	3.85	1.44	1.33
21	a	401	CL7	O2A-CGA	3.85	1.44	1.33
22	d	408	PHO	O2D-CGD	3.85	1.42	1.33
23	K	101	8CT	C06-C07	3.85	1.64	1.52
23	k	101	8CT	C06-C07	3.85	1.64	1.52
22	D	408	PHO	O2D-CGD	3.84	1.42	1.33
23	b	620	8CT	C06-C07	3.83	1.64	1.52
21	A	401	CL7	C2A-C1A	3.82	1.56	1.50
21	a	401	CL7	C2A-C1A	3.82	1.56	1.50
26	C	501	LMG	O7-C10	3.81	1.45	1.34
23	4	402	8CT	C06-C07	3.80	1.64	1.52
23	8	402	8CT	C06-C07	3.80	1.64	1.52
23	c	515	8CT	C06-C07	3.80	1.64	1.52
21	C	505	CL7	C2A-C1A	3.79	1.56	1.50
23	B	619	8CT	C06-C07	3.79	1.64	1.52
23	b	601	8CT	C23-C21	3.78	1.54	1.45
23	C	515	8CT	C06-C07	3.78	1.64	1.52
26	c	501	LMG	O7-C10	3.77	1.44	1.34
23	B	627	8CT	C23-C21	3.77	1.54	1.45
31	F	101	HEM	C1B-NB	-3.76	1.33	1.40
31	f	101	HEM	C1B-NB	-3.76	1.33	1.40
23	d	406	8CT	C23-C21	3.74	1.54	1.45
21	c	505	CL7	C2A-C1A	3.73	1.56	1.50
23	4	402	8CT	C23-C21	3.72	1.53	1.45
23	8	402	8CT	C23-C21	3.72	1.53	1.45
27	B	624	DGD	O2G-C1B	3.71	1.44	1.34
23	D	406	8CT	C23-C21	3.71	1.53	1.45
31	f	101	HEM	C4D-ND	-3.69	1.33	1.40
27	b	625	DGD	O2G-C1B	3.68	1.44	1.34
31	F	101	HEM	C4D-ND	-3.68	1.34	1.40
21	1	411	CL7	O2A-CGA	3.68	1.43	1.30
21	5	411	CL7	O2A-CGA	3.67	1.43	1.30
21	1	420	CL7	O2A-CGA	3.63	1.42	1.30
21	5	420	CL7	O2A-CGA	3.63	1.42	1.30
21	5	402	CL7	C2A-C1A	3.62	1.56	1.50
21	A	401	CL7	C4D-CHA	-3.62	1.40	1.45
21	a	401	CL7	C4D-CHA	-3.62	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	623	CL7	O2A-CGA	3.61	1.42	1.30
21	3	518	CL7	O2A-CGA	3.61	1.42	1.30
21	1	419	CL7	O2A-CGA	3.60	1.42	1.30
21	5	419	CL7	O2A-CGA	3.60	1.42	1.30
21	7	518	CL7	O2A-CGA	3.60	1.42	1.30
21	1	412	CL7	O2A-CGA	3.60	1.42	1.30
21	5	412	CL7	O2A-CGA	3.60	1.42	1.30
21	1	402	CL7	C2A-C1A	3.59	1.56	1.50
21	B	614	CL7	O2A-CGA	3.59	1.43	1.33
21	b	615	CL7	O2A-CGA	3.59	1.43	1.33
21	2	515	CL7	O2A-CGA	3.59	1.42	1.30
21	6	515	CL7	O2A-CGA	3.59	1.42	1.30
21	B	622	CL7	O2A-CGA	3.59	1.42	1.30
21	2	514	CL7	O2A-CGA	3.58	1.42	1.30
21	6	514	CL7	O2A-CGA	3.58	1.42	1.30
21	2	508	CL7	O2A-CGA	3.58	1.42	1.30
23	C	519	8CT	C23-C21	3.58	1.53	1.45
23	c	519	8CT	C23-C21	3.58	1.53	1.45
21	7	514	CL7	O2A-CGA	3.57	1.42	1.30
21	3	513	CL7	O2A-CGA	3.57	1.42	1.30
21	7	513	CL7	O2A-CGA	3.57	1.42	1.30
21	1	405	CL7	O2A-CGA	3.57	1.42	1.30
21	5	405	CL7	O2A-CGA	3.57	1.42	1.30
21	4	408	CL7	O2A-CGA	3.56	1.42	1.30
21	8	408	CL7	O2A-CGA	3.56	1.42	1.30
21	6	508	CL7	O2A-CGA	3.56	1.42	1.30
21	3	514	CL7	O2A-CGA	3.56	1.42	1.30
23	C	515	8CT	C23-C21	3.55	1.53	1.45
23	c	515	8CT	C23-C21	3.55	1.53	1.45
21	2	504	CL7	O2A-CGA	3.54	1.42	1.30
21	6	504	CL7	O2A-CGA	3.54	1.42	1.30
21	1	409	CL7	O2A-CGA	3.53	1.42	1.30
21	5	409	CL7	O2A-CGA	3.53	1.42	1.30
21	B	616	CL7	O2A-CGA	3.53	1.42	1.30
21	4	410	CL7	O2A-CGA	3.53	1.42	1.30
21	8	410	CL7	O2A-CGA	3.53	1.42	1.30
23	A	404	8CT	C23-C21	3.52	1.53	1.45
23	a	404	8CT	C23-C21	3.52	1.53	1.45
21	4	417	CL7	O2D-CGD	3.52	1.41	1.33
21	D	405	CL7	O2A-CGA	3.52	1.42	1.30
21	d	405	CL7	O2A-CGA	3.52	1.42	1.30
21	b	617	CL7	O2A-CGA	3.51	1.42	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	403	CL7	O2A-CGA	3.51	1.43	1.33
21	a	403	CL7	O2A-CGA	3.51	1.43	1.33
21	1	419	CL7	O2D-CGD	3.50	1.41	1.33
21	5	419	CL7	O2D-CGD	3.50	1.41	1.33
21	8	417	CL7	O2D-CGD	3.50	1.41	1.33
21	C	514	CL7	O2A-CGA	3.50	1.42	1.30
21	c	514	CL7	O2A-CGA	3.50	1.42	1.30
21	4	415	CL7	O2A-CGA	3.49	1.42	1.30
21	8	415	CL7	O2A-CGA	3.49	1.42	1.30
21	3	514	CL7	C2A-C1A	3.49	1.56	1.50
21	7	514	CL7	C2A-C1A	3.49	1.56	1.50
21	1	412	CL7	C2A-C1A	3.48	1.56	1.50
21	4	408	CL7	C2A-C1A	3.47	1.56	1.50
21	8	408	CL7	C2A-C1A	3.47	1.56	1.50
21	3	506	CL7	O2A-CGA	3.47	1.42	1.30
21	5	412	CL7	C2A-C1A	3.47	1.56	1.50
21	B	614	CL7	C2A-C1A	3.46	1.56	1.50
21	b	615	CL7	C2A-C1A	3.46	1.56	1.50
21	4	417	CL7	C1B-CHB	3.46	1.50	1.41
21	8	417	CL7	C1B-CHB	3.46	1.50	1.41
21	5	415	CL7	O2D-CGD	3.46	1.41	1.33
21	4	416	CL7	O2D-CGD	3.46	1.41	1.33
21	8	416	CL7	O2D-CGD	3.46	1.41	1.33
21	1	416	CL7	O2D-CGD	3.45	1.41	1.33
21	5	416	CL7	O2D-CGD	3.45	1.41	1.33
21	7	506	CL7	O2A-CGA	3.45	1.42	1.30
21	1	415	CL7	O2D-CGD	3.44	1.41	1.33
21	1	411	CL7	O2D-CGD	3.44	1.41	1.33
21	5	411	CL7	O2D-CGD	3.44	1.41	1.33
21	C	509	CL7	O2A-CGA	3.44	1.43	1.33
21	c	509	CL7	O2A-CGA	3.44	1.43	1.33
21	2	513	CL7	O2A-CGA	3.44	1.42	1.30
21	7	513	CL7	C2A-C1A	3.43	1.56	1.50
21	6	513	CL7	O2A-CGA	3.42	1.42	1.30
21	6	512	CL7	C4C-C3C	-3.42	1.39	1.45
23	b	620	8CT	C23-C21	3.41	1.53	1.45
23	B	619	8CT	C23-C21	3.41	1.53	1.45
21	1	407	CL7	O2D-CGD	3.41	1.41	1.33
21	2	512	CL7	C4C-C3C	-3.40	1.39	1.45
32	4	420	ZEX	C21-C26	-3.40	1.49	1.53
23	B	618	8CT	C23-C21	3.40	1.53	1.45
23	b	619	8CT	C23-C21	3.40	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	601	CL7	O2D-CGD	3.39	1.41	1.33
21	3	513	CL7	C2A-C1A	3.39	1.55	1.50
21	b	602	CL7	O2D-CGD	3.38	1.41	1.33
21	1	412	CL7	O2D-CGD	3.38	1.41	1.33
21	5	407	CL7	O2D-CGD	3.38	1.41	1.33
21	5	412	CL7	O2D-CGD	3.38	1.41	1.33
21	5	402	CL7	O2A-CGA	3.38	1.43	1.33
21	3	518	CL7	O2D-CGD	3.37	1.41	1.33
21	7	518	CL7	O2D-CGD	3.37	1.41	1.33
21	1	402	CL7	O2A-CGA	3.36	1.43	1.33
21	C	514	CL7	O2D-CGD	3.36	1.41	1.33
21	5	417	CL7	O2A-CGA	3.36	1.43	1.33
32	8	420	ZEX	C21-C26	-3.36	1.49	1.53
21	c	514	CL7	O2D-CGD	3.36	1.41	1.33
21	2	514	CL7	O2D-CGD	3.36	1.41	1.33
21	6	514	CL7	O2D-CGD	3.36	1.41	1.33
21	1	417	CL7	O2A-CGA	3.35	1.43	1.33
21	3	506	CL7	C2A-C1A	3.35	1.55	1.50
21	7	506	CL7	C2A-C1A	3.35	1.55	1.50
21	1	414	CL7	O2D-CGD	3.35	1.41	1.33
21	5	414	CL7	O2D-CGD	3.35	1.41	1.33
21	5	415	CL7	C1B-CHB	3.34	1.50	1.41
21	1	415	CL7	C1B-CHB	3.34	1.50	1.41
21	5	413	CL7	C1B-CHB	3.34	1.50	1.41
21	4	413	CL7	C2A-C1A	3.33	1.55	1.50
21	c	505	CL7	O2D-CGD	3.33	1.41	1.33
21	B	612	CL7	C4C-C3C	-3.33	1.39	1.45
21	b	613	CL7	C4C-C3C	-3.33	1.39	1.45
21	1	413	CL7	O2D-CGD	3.33	1.41	1.33
21	1	413	CL7	C1B-CHB	3.33	1.50	1.41
21	1	412	CL7	C1B-CHB	3.33	1.50	1.41
21	C	505	CL7	O2D-CGD	3.32	1.41	1.33
21	2	511	CL7	O2A-CGA	3.32	1.43	1.33
21	6	511	CL7	O2A-CGA	3.32	1.43	1.33
21	7	512	CL7	C2A-C1A	3.32	1.55	1.50
21	3	517	CL7	O2D-CGD	3.32	1.41	1.33
21	7	517	CL7	O2D-CGD	3.32	1.41	1.33
21	5	420	CL7	O2D-CGD	3.31	1.41	1.33
21	3	512	CL7	O2A-CGA	3.31	1.43	1.33
21	7	512	CL7	O2A-CGA	3.31	1.43	1.33
21	B	622	CL7	O2D-CGD	3.31	1.41	1.33
21	b	623	CL7	O2D-CGD	3.31	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	405	CL7	O2A-CGA	3.31	1.43	1.33
21	8	405	CL7	O2A-CGA	3.31	1.43	1.33
21	2	501	CL7	O2D-CGD	3.31	1.41	1.33
21	6	501	CL7	O2D-CGD	3.31	1.41	1.33
21	3	510	CL7	O2D-CGD	3.31	1.41	1.33
21	7	510	CL7	O2D-CGD	3.31	1.41	1.33
21	2	518	CL7	O2A-CGA	3.30	1.43	1.33
21	6	518	CL7	O2A-CGA	3.30	1.43	1.33
21	4	409	CL7	C2A-C1A	3.30	1.55	1.50
21	8	409	CL7	C2A-C1A	3.30	1.55	1.50
21	1	402	CL7	O2D-CGD	3.30	1.41	1.33
21	5	402	CL7	O2D-CGD	3.30	1.41	1.33
21	5	412	CL7	C1B-CHB	3.30	1.50	1.41
21	1	410	CL7	O2D-CGD	3.30	1.41	1.33
21	5	410	CL7	O2D-CGD	3.30	1.41	1.33
21	4	404	CL7	O2A-CGA	3.30	1.43	1.33
21	8	404	CL7	O2A-CGA	3.30	1.43	1.33
21	6	510	CL7	O2D-CGD	3.30	1.41	1.33
21	5	413	CL7	O2D-CGD	3.30	1.41	1.33
21	8	413	CL7	O2D-CGD	3.30	1.41	1.33
21	4	413	CL7	O2D-CGD	3.29	1.41	1.33
21	3	503	CL7	C4C-C3C	-3.29	1.39	1.45
21	7	503	CL7	C4C-C3C	-3.29	1.39	1.45
21	3	512	CL7	C2A-C1A	3.29	1.55	1.50
21	2	506	CL7	O2D-CGD	3.29	1.41	1.33
21	2	502	CL7	C1B-CHB	3.29	1.50	1.41
21	6	502	CL7	C1B-CHB	3.29	1.50	1.41
21	1	420	CL7	O2D-CGD	3.29	1.41	1.33
21	C	503	CL7	O2D-CGD	3.29	1.41	1.33
21	c	503	CL7	O2D-CGD	3.29	1.41	1.33
21	6	506	CL7	O2D-CGD	3.29	1.41	1.33
21	8	413	CL7	C2A-C1A	3.29	1.55	1.50
21	6	505	CL7	C4C-C3C	-3.29	1.39	1.45
21	C	505	CL7	O2A-CGA	3.29	1.42	1.33
21	c	505	CL7	O2A-CGA	3.29	1.42	1.33
21	5	410	CL7	O2A-CGA	3.28	1.42	1.33
21	2	510	CL7	O2D-CGD	3.28	1.41	1.33
21	3	515	CL7	O2D-CGD	3.28	1.41	1.33
21	7	515	CL7	O2D-CGD	3.28	1.41	1.33
21	D	402	CL7	O2D-CGD	3.28	1.41	1.33
21	d	402	CL7	O2D-CGD	3.28	1.41	1.33
21	1	418	CL7	C4C-C3C	-3.28	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	418	CL7	C4C-C3C	-3.28	1.39	1.45
21	5	404	CL7	O2D-CGD	3.28	1.41	1.33
21	1	410	CL7	O2A-CGA	3.28	1.42	1.33
21	6	507	CL7	O2A-CGA	3.28	1.42	1.33
21	4	406	CL7	O2A-CGA	3.28	1.42	1.33
21	6	502	CL7	O2A-CGA	3.28	1.42	1.33
21	8	406	CL7	O2A-CGA	3.28	1.42	1.33
21	1	409	CL7	O2D-CGD	3.27	1.41	1.33
21	5	409	CL7	O2D-CGD	3.27	1.41	1.33
21	2	511	CL7	C2A-C1A	3.27	1.55	1.50
21	6	511	CL7	C2A-C1A	3.27	1.55	1.50
21	c	512	CL7	O2D-CGD	3.27	1.41	1.33
21	1	410	CL7	C2A-C1A	3.27	1.55	1.50
21	5	410	CL7	C2A-C1A	3.27	1.55	1.50
21	2	505	CL7	C4C-C3C	-3.27	1.39	1.45
21	4	404	CL7	O2D-CGD	3.27	1.41	1.33
21	8	404	CL7	O2D-CGD	3.27	1.41	1.33
21	C	504	CL7	O2A-CGA	3.26	1.42	1.33
21	c	504	CL7	O2A-CGA	3.26	1.42	1.33
21	8	406	CL7	C2A-C1A	3.26	1.55	1.50
21	3	518	CL7	C2A-C1A	3.26	1.55	1.50
21	7	518	CL7	C2A-C1A	3.26	1.55	1.50
21	2	502	CL7	O2A-CGA	3.26	1.42	1.33
21	1	405	CL7	O2D-CGD	3.26	1.41	1.33
21	5	405	CL7	O2D-CGD	3.26	1.41	1.33
23	B	617	8CT	C23-C21	3.26	1.52	1.45
23	b	618	8CT	C23-C21	3.26	1.52	1.45
21	2	507	CL7	O2A-CGA	3.26	1.42	1.33
21	C	512	CL7	O2D-CGD	3.26	1.41	1.33
21	3	509	CL7	O2D-CGD	3.26	1.41	1.33
21	4	407	CL7	O2D-CGD	3.26	1.41	1.33
21	7	509	CL7	O2D-CGD	3.26	1.41	1.33
21	8	407	CL7	O2D-CGD	3.26	1.41	1.33
32	2	523	ZEX	C1-C6	-3.26	1.49	1.53
32	6	522	ZEX	C1-C6	-3.26	1.49	1.53
21	D	402	CL7	C2A-C1A	3.25	1.55	1.50
21	d	402	CL7	C2A-C1A	3.25	1.55	1.50
21	C	511	CL7	O2D-CGD	3.25	1.41	1.33
21	c	511	CL7	O2D-CGD	3.25	1.41	1.33
21	2	513	CL7	C2A-C1A	3.25	1.55	1.50
21	3	504	CL7	C2A-C1A	3.25	1.55	1.50
21	7	504	CL7	C2A-C1A	3.25	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	404	CL7	O2D-CGD	3.25	1.41	1.33
21	2	511	CL7	O2D-CGD	3.25	1.41	1.33
21	6	511	CL7	O2D-CGD	3.25	1.41	1.33
21	6	513	CL7	C2A-C1A	3.25	1.55	1.50
21	1	420	CL7	C2A-C1A	3.24	1.55	1.50
21	2	504	CL7	O2D-CGD	3.24	1.41	1.33
21	6	504	CL7	O2D-CGD	3.24	1.41	1.33
21	c	511	CL7	O2A-CGA	3.24	1.42	1.33
21	2	517	CL7	O2A-CGA	3.24	1.42	1.33
21	6	517	CL7	O2A-CGA	3.23	1.42	1.33
21	4	405	CL7	O2D-CGD	3.23	1.41	1.33
21	8	405	CL7	O2D-CGD	3.23	1.41	1.33
21	5	416	CL7	C1B-CHB	3.23	1.50	1.41
21	C	511	CL7	O2A-CGA	3.23	1.42	1.33
21	2	518	CL7	O2D-CGD	3.23	1.41	1.33
21	6	518	CL7	O2D-CGD	3.23	1.41	1.33
21	C	503	CL7	O2A-CGA	3.23	1.42	1.33
21	c	503	CL7	O2A-CGA	3.23	1.42	1.33
21	3	506	CL7	O2D-CGD	3.23	1.41	1.33
21	7	506	CL7	O2D-CGD	3.23	1.41	1.33
21	C	508	CL7	C4C-C3C	-3.23	1.39	1.45
21	4	410	CL7	C2A-C1A	3.23	1.55	1.50
21	6	505	CL7	O2D-CGD	3.23	1.41	1.33
21	2	505	CL7	O2D-CGD	3.23	1.41	1.33
21	2	506	CL7	O2A-CGA	3.22	1.42	1.33
21	1	416	CL7	C1B-CHB	3.22	1.49	1.41
21	6	506	CL7	O2A-CGA	3.22	1.42	1.33
21	1	419	CL7	C1B-CHB	3.22	1.49	1.41
21	A	406	CL7	C4C-C3C	-3.22	1.39	1.45
21	a	405	CL7	C4C-C3C	-3.22	1.39	1.45
21	3	517	CL7	O2A-CGA	3.22	1.42	1.33
21	7	517	CL7	O2A-CGA	3.22	1.42	1.33
21	B	613	CL7	C4C-C3C	-3.22	1.39	1.45
21	b	614	CL7	C4C-C3C	-3.22	1.39	1.45
21	C	502	CL7	O2A-CGA	3.22	1.42	1.33
21	c	502	CL7	O2A-CGA	3.22	1.42	1.33
21	5	420	CL7	C2A-C1A	3.22	1.55	1.50
21	3	501	CL7	O2D-CGD	3.22	1.41	1.33
21	7	501	CL7	O2D-CGD	3.22	1.41	1.33
21	4	405	CL7	C1B-CHB	3.22	1.49	1.41
21	B	607	CL7	C4C-C3C	-3.21	1.39	1.45
21	b	608	CL7	C4C-C3C	-3.21	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	511	CL7	C4C-C3C	-3.21	1.39	1.45
21	5	419	CL7	C2A-C1A	3.21	1.55	1.50
21	B	622	CL7	C2A-C1A	3.21	1.55	1.50
21	b	623	CL7	C2A-C1A	3.21	1.55	1.50
21	B	610	CL7	O2A-CGA	3.21	1.42	1.33
21	b	611	CL7	O2A-CGA	3.21	1.42	1.33
21	5	419	CL7	C1B-CHB	3.21	1.49	1.41
21	C	506	CL7	O2D-CGD	3.21	1.41	1.33
21	c	506	CL7	O2D-CGD	3.21	1.41	1.33
21	2	503	CL7	C4C-C3C	-3.21	1.39	1.45
21	6	503	CL7	C4C-C3C	-3.21	1.39	1.45
21	2	511	CL7	C4C-C3C	-3.21	1.39	1.45
21	1	408	CL7	O2D-CGD	3.21	1.41	1.33
21	8	409	CL7	C1B-CHB	3.21	1.49	1.41
21	1	403	CL7	C2A-C1A	3.20	1.55	1.50
21	4	413	CL7	O2A-CGA	3.20	1.42	1.33
21	2	515	CL7	O2D-CGD	3.20	1.41	1.33
21	6	515	CL7	O2D-CGD	3.20	1.41	1.33
21	1	404	CL7	C1B-CHB	3.20	1.49	1.41
21	4	406	CL7	C2A-C1A	3.20	1.55	1.50
21	7	508	CL7	O2A-CGA	3.20	1.42	1.33
21	2	509	CL7	O2D-CGD	3.20	1.41	1.33
21	6	509	CL7	O2D-CGD	3.20	1.41	1.33
21	B	609	CL7	O2D-CGD	3.20	1.41	1.33
21	b	610	CL7	O2D-CGD	3.20	1.41	1.33
21	1	406	CL7	O2D-CGD	3.20	1.41	1.33
21	5	406	CL7	O2D-CGD	3.20	1.41	1.33
21	6	516	CL7	O2A-CGA	3.20	1.42	1.33
21	2	501	CL7	C2A-C1A	3.20	1.55	1.50
21	6	501	CL7	C2A-C1A	3.20	1.55	1.50
21	8	405	CL7	C1B-CHB	3.20	1.49	1.41
21	B	604	CL7	C4C-C3C	-3.20	1.39	1.45
21	b	605	CL7	C4C-C3C	-3.20	1.39	1.45
21	3	516	CL7	O2A-CGA	3.20	1.42	1.33
21	7	516	CL7	O2A-CGA	3.20	1.42	1.33
21	4	412	CL7	O2A-CGA	3.20	1.42	1.33
21	2	516	CL7	O2A-CGA	3.20	1.42	1.33
21	2	508	CL7	O2D-CGD	3.20	1.41	1.33
21	6	508	CL7	O2D-CGD	3.20	1.41	1.33
21	3	514	CL7	O2D-CGD	3.20	1.41	1.33
21	2	515	CL7	C1B-CHB	3.20	1.49	1.41
21	6	515	CL7	C1B-CHB	3.20	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	514	CL7	O2D-CGD	3.19	1.41	1.33
21	1	420	CL7	C1B-CHB	3.19	1.49	1.41
21	5	420	CL7	C1B-CHB	3.19	1.49	1.41
21	2	503	CL7	C2A-C1A	3.19	1.55	1.50
21	6	503	CL7	C2A-C1A	3.19	1.55	1.50
23	B	619	8CT	C07-C02	-3.19	1.44	1.51
23	b	620	8CT	C07-C02	-3.19	1.44	1.51
23	c	515	8CT	C07-C02	-3.19	1.44	1.51
21	2	505	CL7	C1B-CHB	3.19	1.49	1.41
21	C	518	CL7	O2D-CGD	3.19	1.41	1.33
21	2	513	CL7	O2D-CGD	3.19	1.41	1.33
21	6	513	CL7	O2D-CGD	3.19	1.41	1.33
21	4	409	CL7	C1B-CHB	3.19	1.49	1.41
21	5	408	CL7	O2D-CGD	3.19	1.41	1.33
21	B	610	CL7	C4C-C3C	-3.19	1.39	1.45
21	b	611	CL7	C4C-C3C	-3.19	1.39	1.45
21	c	508	CL7	C4C-C3C	-3.19	1.39	1.45
21	1	403	CL7	O2D-CGD	3.19	1.41	1.33
21	5	403	CL7	O2D-CGD	3.19	1.41	1.33
21	2	512	CL7	C1B-CHB	3.19	1.49	1.41
21	6	512	CL7	C1B-CHB	3.19	1.49	1.41
21	3	508	CL7	O2A-CGA	3.19	1.42	1.33
21	3	504	CL7	C4C-C3C	-3.19	1.39	1.45
21	7	504	CL7	C4C-C3C	-3.19	1.39	1.45
21	8	413	CL7	O2A-CGA	3.19	1.42	1.33
21	4	407	CL7	C1B-CHB	3.19	1.49	1.41
21	5	403	CL7	C2A-C1A	3.19	1.55	1.50
21	8	410	CL7	C2A-C1A	3.19	1.55	1.50
32	2	520	ZEX	C1-C6	-3.18	1.49	1.53
21	6	505	CL7	C1B-CHB	3.18	1.49	1.41
21	D	402	CL7	O2A-CGA	3.18	1.42	1.33
21	d	402	CL7	O2A-CGA	3.18	1.42	1.33
21	B	615	CL7	O2A-CGA	3.18	1.42	1.33
21	b	616	CL7	O2A-CGA	3.18	1.42	1.33
21	C	510	CL7	O2D-CGD	3.18	1.41	1.33
21	3	502	CL7	C2A-C1A	3.18	1.55	1.50
21	1	403	CL7	O2A-CGA	3.18	1.42	1.33
21	B	615	CL7	O2D-CGD	3.18	1.41	1.33
21	b	616	CL7	O2D-CGD	3.18	1.41	1.33
21	B	614	CL7	O2D-CGD	3.18	1.41	1.33
21	b	615	CL7	O2D-CGD	3.18	1.41	1.33
21	4	406	CL7	C1B-CHB	3.18	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	406	CL7	C1B-CHB	3.18	1.49	1.41
21	8	412	CL7	O2A-CGA	3.18	1.42	1.33
21	1	419	CL7	C2A-C1A	3.18	1.55	1.50
21	4	414	CL7	O2A-CGA	3.18	1.42	1.33
21	8	414	CL7	O2A-CGA	3.18	1.42	1.33
21	4	411	CL7	O2D-CGD	3.18	1.41	1.33
21	c	518	CL7	O2D-CGD	3.17	1.40	1.33
21	8	407	CL7	C1B-CHB	3.17	1.49	1.41
21	7	507	CL7	O2A-CGA	3.17	1.42	1.33
21	2	508	CL7	C1B-CHB	3.17	1.49	1.41
21	5	404	CL7	C1B-CHB	3.17	1.49	1.41
21	8	411	CL7	O2D-CGD	3.17	1.40	1.33
21	B	604	CL7	C1B-CHB	3.17	1.49	1.41
21	b	605	CL7	C1B-CHB	3.17	1.49	1.41
21	4	412	CL7	C4C-C3C	-3.16	1.39	1.45
21	8	412	CL7	C4C-C3C	-3.16	1.39	1.45
21	1	403	CL7	C1B-CHB	3.16	1.49	1.41
21	3	502	CL7	O2A-CGA	3.16	1.42	1.33
21	7	502	CL7	O2A-CGA	3.16	1.42	1.33
21	C	502	CL7	C4C-C3C	-3.16	1.39	1.45
21	B	608	CL7	O2A-CGA	3.16	1.42	1.33
21	b	609	CL7	O2A-CGA	3.16	1.42	1.33
21	B	605	CL7	O2D-CGD	3.16	1.40	1.33
21	1	408	CL7	O2A-CGA	3.16	1.42	1.33
21	5	408	CL7	O2A-CGA	3.16	1.42	1.33
21	5	403	CL7	O2A-CGA	3.16	1.42	1.33
21	A	406	CL7	O2D-CGD	3.16	1.40	1.33
21	a	405	CL7	O2D-CGD	3.16	1.40	1.33
21	3	507	CL7	O2A-CGA	3.16	1.42	1.33
21	B	601	CL7	C1B-CHB	3.16	1.49	1.41
21	b	602	CL7	C1B-CHB	3.16	1.49	1.41
21	1	406	CL7	O2A-CGA	3.16	1.42	1.33
21	5	406	CL7	O2A-CGA	3.16	1.42	1.33
23	C	515	8CT	C07-C02	-3.15	1.44	1.51
21	3	510	CL7	O2A-CGA	3.15	1.42	1.33
21	7	510	CL7	O2A-CGA	3.15	1.42	1.33
21	c	510	CL7	O2D-CGD	3.15	1.40	1.33
23	B	617	8CT	C07-C02	-3.15	1.44	1.51
23	b	618	8CT	C07-C02	-3.15	1.44	1.51
23	B	627	8CT	C19-C20	3.15	1.53	1.43
23	b	601	8CT	C19-C20	3.15	1.53	1.43
21	2	512	CL7	O2A-CGA	3.15	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	512	CL7	O2A-CGA	3.15	1.42	1.33
21	B	605	CL7	C4C-C3C	-3.15	1.39	1.45
21	b	606	CL7	C4C-C3C	-3.15	1.39	1.45
21	b	609	CL7	O2D-CGD	3.15	1.40	1.33
21	3	504	CL7	O2D-CGD	3.15	1.40	1.33
21	7	504	CL7	O2D-CGD	3.15	1.40	1.33
21	b	606	CL7	O2D-CGD	3.15	1.40	1.33
21	2	516	CL7	O2D-CGD	3.15	1.40	1.33
32	4	419	ZEX	C21-C26	-3.15	1.49	1.53
21	B	608	CL7	O2D-CGD	3.15	1.40	1.33
21	5	403	CL7	C1B-CHB	3.15	1.49	1.41
21	c	502	CL7	C4C-C3C	-3.14	1.39	1.45
21	c	506	CL7	O2A-CGA	3.14	1.42	1.33
21	C	506	CL7	O2A-CGA	3.14	1.42	1.33
21	2	514	CL7	C2A-C1A	3.14	1.55	1.50
21	3	515	CL7	C1B-CHB	3.14	1.49	1.41
21	7	515	CL7	C1B-CHB	3.14	1.49	1.41
21	1	404	CL7	O2A-CGA	3.14	1.42	1.33
21	4	416	CL7	C1B-CHB	3.14	1.49	1.41
21	8	416	CL7	C1B-CHB	3.14	1.49	1.41
21	1	406	CL7	C1B-CHB	3.14	1.49	1.41
21	5	406	CL7	C1B-CHB	3.14	1.49	1.41
21	c	502	CL7	C1B-CHB	3.14	1.49	1.41
21	3	514	CL7	C1B-CHB	3.14	1.49	1.41
21	7	514	CL7	C1B-CHB	3.14	1.49	1.41
21	B	615	CL7	C1B-CHB	3.14	1.49	1.41
21	b	616	CL7	C1B-CHB	3.14	1.49	1.41
21	4	414	CL7	C4C-C3C	-3.14	1.39	1.45
21	8	414	CL7	C4C-C3C	-3.14	1.39	1.45
21	6	508	CL7	C1B-CHB	3.14	1.49	1.41
21	5	417	CL7	O2D-CGD	3.13	1.40	1.33
21	2	518	CL7	C1B-CHB	3.13	1.49	1.41
21	6	518	CL7	C1B-CHB	3.13	1.49	1.41
21	5	404	CL7	O2A-CGA	3.13	1.42	1.33
21	C	504	CL7	O2D-CGD	3.13	1.40	1.33
21	c	504	CL7	O2D-CGD	3.13	1.40	1.33
21	B	602	CL7	O2D-CGD	3.13	1.40	1.33
21	d	402	CL7	C1B-CHB	3.13	1.49	1.41
21	7	502	CL7	C2A-C1A	3.13	1.55	1.50
21	B	607	CL7	O2A-CGA	3.13	1.42	1.33
21	b	608	CL7	O2A-CGA	3.13	1.42	1.33
21	A	401	CL7	C1B-CHB	3.13	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	502	CL7	C1B-CHB	3.13	1.49	1.41
21	a	401	CL7	C1B-CHB	3.13	1.49	1.41
21	3	510	CL7	C4C-C3C	-3.13	1.39	1.45
21	7	510	CL7	C4C-C3C	-3.13	1.39	1.45
21	1	417	CL7	O2D-CGD	3.13	1.40	1.33
21	6	516	CL7	O2D-CGD	3.13	1.40	1.33
21	1	402	CL7	C1B-CHB	3.13	1.49	1.41
21	5	402	CL7	C1B-CHB	3.13	1.49	1.41
32	3	525	ZEX	C1-C6	-3.13	1.49	1.53
21	1	418	CL7	O2A-CGA	3.13	1.42	1.33
21	5	418	CL7	O2A-CGA	3.13	1.42	1.33
21	C	514	CL7	C1B-CHB	3.13	1.49	1.41
21	c	514	CL7	C1B-CHB	3.13	1.49	1.41
21	c	518	CL7	C1B-CHB	3.12	1.49	1.41
21	B	614	CL7	C4C-C3C	-3.12	1.39	1.45
21	b	615	CL7	C4C-C3C	-3.12	1.39	1.45
21	D	402	CL7	C1B-CHB	3.12	1.49	1.41
21	7	501	CL7	C4C-C3C	-3.12	1.39	1.45
21	C	512	CL7	C1B-CHB	3.12	1.49	1.41
21	c	512	CL7	C1B-CHB	3.12	1.49	1.41
21	2	507	CL7	C1B-CHB	3.12	1.49	1.41
21	3	513	CL7	O2D-CGD	3.12	1.40	1.33
21	7	513	CL7	O2D-CGD	3.12	1.40	1.33
21	1	405	CL7	C1B-CHB	3.12	1.49	1.41
21	5	405	CL7	C1B-CHB	3.12	1.49	1.41
21	C	510	CL7	C4C-C3C	-3.12	1.39	1.45
21	c	510	CL7	C4C-C3C	-3.12	1.39	1.45
21	C	504	CL7	C1B-CHB	3.12	1.49	1.41
21	c	504	CL7	C1B-CHB	3.12	1.49	1.41
21	4	410	CL7	O2D-CGD	3.12	1.40	1.33
21	4	414	CL7	O2D-CGD	3.12	1.40	1.33
21	8	410	CL7	O2D-CGD	3.12	1.40	1.33
21	8	414	CL7	O2D-CGD	3.12	1.40	1.33
21	B	610	CL7	C4C-NC	-3.12	1.34	1.37
21	b	611	CL7	C4C-NC	-3.12	1.34	1.37
21	B	603	CL7	O2D-CGD	3.12	1.40	1.33
21	b	604	CL7	O2D-CGD	3.12	1.40	1.33
21	4	409	CL7	O2A-CGA	3.11	1.42	1.33
32	8	419	ZEX	C21-C26	-3.11	1.49	1.53
21	2	504	CL7	C2A-C1A	3.11	1.55	1.50
21	2	512	CL7	C2A-C1A	3.11	1.55	1.50
21	6	504	CL7	C2A-C1A	3.11	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	512	CL7	C2A-C1A	3.11	1.55	1.50
21	6	507	CL7	C1B-CHB	3.11	1.49	1.41
21	3	511	CL7	C4C-C3C	-3.11	1.39	1.45
21	7	511	CL7	C4C-C3C	-3.11	1.39	1.45
23	K	101	8CT	C19-C20	3.11	1.53	1.43
23	k	101	8CT	C19-C20	3.11	1.53	1.43
21	3	507	CL7	C1B-CHB	3.11	1.49	1.41
21	8	409	CL7	O2A-CGA	3.11	1.42	1.33
21	6	514	CL7	C2A-C1A	3.11	1.55	1.50
21	3	506	CL7	C1B-CHB	3.11	1.49	1.41
21	7	506	CL7	C1B-CHB	3.11	1.49	1.41
21	2	518	CL7	C2A-C1A	3.10	1.55	1.50
21	3	508	CL7	C1B-CHB	3.10	1.49	1.41
21	7	508	CL7	C1B-CHB	3.10	1.49	1.41
23	4	402	8CT	C07-C02	-3.10	1.44	1.51
23	8	402	8CT	C07-C02	-3.10	1.44	1.51
21	3	511	CL7	O2D-CGD	3.10	1.40	1.33
21	7	511	CL7	O2D-CGD	3.10	1.40	1.33
21	3	501	CL7	C4C-C3C	-3.10	1.39	1.45
21	b	612	CL7	C4C-C3C	-3.10	1.39	1.45
23	K	101	8CT	C07-C02	-3.10	1.44	1.51
23	k	101	8CT	C07-C02	-3.10	1.44	1.51
21	b	603	CL7	O2D-CGD	3.10	1.40	1.33
21	B	610	CL7	O2D-CGD	3.10	1.40	1.33
21	C	518	CL7	C1B-CHB	3.09	1.49	1.41
21	b	612	CL7	C4C-NC	-3.09	1.34	1.37
21	B	616	CL7	O2D-CGD	3.09	1.40	1.33
21	b	617	CL7	O2D-CGD	3.09	1.40	1.33
21	b	611	CL7	O2D-CGD	3.09	1.40	1.33
21	B	609	CL7	O2A-CGA	3.09	1.42	1.33
21	b	610	CL7	O2A-CGA	3.09	1.42	1.33
21	3	503	CL7	O2A-CGA	3.09	1.42	1.33
21	7	503	CL7	O2A-CGA	3.09	1.42	1.33
21	B	611	CL7	C1B-CHB	3.09	1.49	1.41
21	B	605	CL7	C1B-CHB	3.09	1.49	1.41
21	b	606	CL7	C1B-CHB	3.09	1.49	1.41
21	C	512	CL7	C4C-C3C	-3.09	1.39	1.45
21	c	512	CL7	C4C-C3C	-3.09	1.39	1.45
21	1	414	CL7	C1B-CHB	3.09	1.49	1.41
21	C	507	CL7	C4C-C3C	-3.09	1.39	1.45
21	c	507	CL7	C4C-C3C	-3.09	1.39	1.45
21	4	415	CL7	O2D-CGD	3.09	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	415	CL7	O2D-CGD	3.09	1.40	1.33
21	D	405	CL7	C1B-CHB	3.09	1.49	1.41
21	d	405	CL7	C1B-CHB	3.09	1.49	1.41
21	B	606	CL7	O2A-CGA	3.09	1.42	1.33
21	b	607	CL7	O2A-CGA	3.09	1.42	1.33
21	7	507	CL7	C1B-CHB	3.08	1.49	1.41
21	B	611	CL7	C4C-C3C	-3.08	1.39	1.45
21	C	509	CL7	C4C-C3C	-3.08	1.39	1.45
21	4	406	CL7	C4C-C3C	-3.08	1.39	1.45
21	c	509	CL7	C4C-C3C	-3.08	1.39	1.45
21	8	406	CL7	C4C-C3C	-3.08	1.39	1.45
21	5	406	CL7	C2A-C1A	3.08	1.55	1.50
21	4	410	CL7	C1B-CHB	3.08	1.49	1.41
21	b	612	CL7	C1B-CHB	3.08	1.49	1.41
21	8	410	CL7	C1B-CHB	3.08	1.49	1.41
21	3	511	CL7	O2A-CGA	3.08	1.42	1.33
21	7	511	CL7	O2A-CGA	3.08	1.42	1.33
21	C	502	CL7	O2D-CGD	3.08	1.40	1.33
21	3	502	CL7	O2D-CGD	3.08	1.40	1.33
21	c	502	CL7	O2D-CGD	3.08	1.40	1.33
21	7	502	CL7	O2D-CGD	3.08	1.40	1.33
21	2	517	CL7	O2D-CGD	3.08	1.40	1.33
21	6	517	CL7	O2D-CGD	3.08	1.40	1.33
21	5	414	CL7	C1B-CHB	3.08	1.49	1.41
21	c	513	CL7	O2D-CGD	3.08	1.40	1.33
21	4	414	CL7	C1B-CHB	3.08	1.49	1.41
21	8	414	CL7	C1B-CHB	3.08	1.49	1.41
21	2	516	CL7	C1B-CHB	3.08	1.49	1.41
21	6	516	CL7	C1B-CHB	3.08	1.49	1.41
21	2	506	CL7	C2A-C1A	3.08	1.55	1.50
21	6	506	CL7	C2A-C1A	3.08	1.55	1.50
21	6	506	CL7	C1B-CHB	3.07	1.49	1.41
21	3	503	CL7	C1B-CHB	3.07	1.49	1.41
21	7	503	CL7	C1B-CHB	3.07	1.49	1.41
21	5	411	CL7	C1B-CHB	3.07	1.49	1.41
21	4	408	CL7	C1B-CHB	3.07	1.49	1.41
21	8	408	CL7	C1B-CHB	3.07	1.49	1.41
21	D	404	CL7	C4C-C3C	-3.07	1.39	1.45
21	d	404	CL7	C4C-C3C	-3.07	1.39	1.45
21	B	603	CL7	O2A-CGA	3.07	1.42	1.33
21	b	604	CL7	O2A-CGA	3.07	1.42	1.33
21	B	611	CL7	C4C-NC	-3.07	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	409	CL7	C2A-C1A	3.07	1.55	1.50
21	5	409	CL7	C2A-C1A	3.07	1.55	1.50
21	A	406	CL7	C1B-CHB	3.07	1.49	1.41
23	C	516	8CT	C07-C02	-3.07	1.44	1.51
23	c	516	8CT	C07-C02	-3.07	1.44	1.51
21	1	409	CL7	C1B-CHB	3.07	1.49	1.41
21	5	409	CL7	C1B-CHB	3.07	1.49	1.41
21	3	509	CL7	O2A-CGA	3.07	1.42	1.33
21	7	509	CL7	O2A-CGA	3.07	1.42	1.33
21	3	505	CL7	C1B-CHB	3.07	1.49	1.41
21	7	505	CL7	C1B-CHB	3.07	1.49	1.41
21	4	410	CL7	C4C-C3C	-3.07	1.39	1.45
21	C	513	CL7	O2D-CGD	3.06	1.40	1.33
21	B	608	CL7	C1B-CHB	3.06	1.49	1.41
21	2	511	CL7	C1B-CHB	3.06	1.49	1.41
21	6	511	CL7	C1B-CHB	3.06	1.49	1.41
21	b	609	CL7	C1B-CHB	3.06	1.49	1.41
21	C	509	CL7	C1B-CHB	3.06	1.49	1.41
21	2	514	CL7	C1B-CHB	3.06	1.49	1.41
21	c	509	CL7	C1B-CHB	3.06	1.49	1.41
21	6	514	CL7	C1B-CHB	3.06	1.49	1.41
21	C	509	CL7	C4C-NC	-3.06	1.34	1.37
21	c	509	CL7	C4C-NC	-3.06	1.34	1.37
21	B	604	CL7	O2A-CGA	3.06	1.42	1.33
21	b	605	CL7	O2A-CGA	3.06	1.42	1.33
21	B	613	CL7	O2A-CGA	3.06	1.42	1.33
21	b	614	CL7	O2A-CGA	3.06	1.42	1.33
21	1	411	CL7	C1B-CHB	3.06	1.49	1.41
21	c	513	CL7	C1B-CHB	3.06	1.49	1.41
21	4	411	CL7	C4C-C3C	-3.06	1.39	1.45
21	8	411	CL7	C4C-C3C	-3.06	1.39	1.45
21	C	513	CL7	C1B-CHB	3.05	1.49	1.41
21	1	408	CL7	C1B-CHB	3.05	1.49	1.41
21	5	408	CL7	C1B-CHB	3.05	1.49	1.41
21	C	514	CL7	C2A-C1A	3.05	1.55	1.50
21	2	515	CL7	C2A-C1A	3.05	1.55	1.50
21	6	515	CL7	C2A-C1A	3.05	1.55	1.50
21	2	510	CL7	C4C-C3C	-3.05	1.39	1.45
21	6	510	CL7	C4C-C3C	-3.05	1.39	1.45
21	C	507	CL7	O2A-CGA	3.05	1.42	1.33
21	c	507	CL7	O2A-CGA	3.05	1.42	1.33
21	1	418	CL7	C1B-CHB	3.05	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	518	CL7	C2A-C1A	3.05	1.55	1.50
21	2	516	CL7	C4C-C3C	-3.05	1.39	1.45
21	3	512	CL7	C4C-C3C	-3.05	1.39	1.45
21	6	516	CL7	C4C-C3C	-3.05	1.39	1.45
21	7	512	CL7	C4C-C3C	-3.05	1.39	1.45
21	2	513	CL7	C1B-CHB	3.05	1.49	1.41
21	6	513	CL7	C1B-CHB	3.05	1.49	1.41
21	C	506	CL7	C1B-CHB	3.05	1.49	1.41
21	c	506	CL7	C1B-CHB	3.05	1.49	1.41
21	4	412	CL7	O2D-CGD	3.05	1.40	1.33
21	8	412	CL7	O2D-CGD	3.05	1.40	1.33
23	B	618	8CT	C07-C02	-3.05	1.45	1.51
21	4	415	CL7	C1B-CHB	3.05	1.49	1.41
21	8	415	CL7	C1B-CHB	3.05	1.49	1.41
21	C	510	CL7	O2A-CGA	3.05	1.42	1.33
21	c	510	CL7	O2A-CGA	3.05	1.42	1.33
21	c	514	CL7	C2A-C1A	3.05	1.55	1.50
21	4	408	CL7	O2D-CGD	3.04	1.40	1.33
21	8	408	CL7	O2D-CGD	3.04	1.40	1.33
21	C	511	CL7	C4C-C3C	-3.04	1.39	1.45
21	c	511	CL7	C4C-C3C	-3.04	1.39	1.45
21	B	602	CL7	C1B-CHB	3.04	1.49	1.41
21	b	603	CL7	C1B-CHB	3.04	1.49	1.41
21	2	506	CL7	C1B-CHB	3.04	1.49	1.41
21	B	605	CL7	O2A-CGA	3.04	1.42	1.33
21	5	418	CL7	C1B-CHB	3.04	1.49	1.41
22	A	402	PHO	C3A-C2A	-3.04	1.51	1.54
22	a	402	PHO	C3A-C2A	-3.04	1.51	1.54
21	1	406	CL7	C2A-C1A	3.03	1.55	1.50
21	2	517	CL7	C1B-CHB	3.03	1.49	1.41
21	6	517	CL7	C1B-CHB	3.03	1.49	1.41
21	a	403	CL7	O2D-CGD	3.03	1.40	1.33
23	C	516	8CT	C19-C20	3.03	1.52	1.43
23	c	516	8CT	C19-C20	3.03	1.52	1.43
21	a	405	CL7	C1B-CHB	3.03	1.49	1.41
21	C	505	CL7	C1B-CHB	3.03	1.49	1.41
21	c	505	CL7	C1B-CHB	3.03	1.49	1.41
21	3	504	CL7	O2A-CGA	3.03	1.42	1.33
21	7	504	CL7	O2A-CGA	3.03	1.42	1.33
21	3	503	CL7	C2A-C1A	3.03	1.55	1.50
21	3	501	CL7	C1B-CHB	3.03	1.49	1.41
21	7	501	CL7	C1B-CHB	3.03	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	412	CL7	C1B-CHB	3.03	1.49	1.41
21	8	412	CL7	C1B-CHB	3.03	1.49	1.41
21	B	612	CL7	O2A-CGA	3.03	1.42	1.33
21	B	606	CL7	O2D-CGD	3.03	1.40	1.33
21	8	406	CL7	O2D-CGD	3.03	1.40	1.33
21	B	613	CL7	O2D-CGD	3.03	1.40	1.33
32	2	519	ZEX	C1-C6	-3.03	1.49	1.53
32	6	519	ZEX	C1-C6	-3.03	1.49	1.53
21	C	507	CL7	O2D-CGD	3.03	1.40	1.33
21	c	507	CL7	O2D-CGD	3.03	1.40	1.33
23	B	618	8CT	C19-C20	3.02	1.52	1.43
23	b	619	8CT	C19-C20	3.02	1.52	1.43
21	7	503	CL7	C2A-C1A	3.02	1.55	1.50
21	D	404	CL7	C1B-CHB	3.02	1.49	1.41
21	d	404	CL7	C1B-CHB	3.02	1.49	1.41
21	6	505	CL7	O2A-CGA	3.02	1.42	1.33
21	C	503	CL7	C1B-CHB	3.02	1.49	1.41
21	c	503	CL7	C1B-CHB	3.02	1.49	1.41
21	c	511	CL7	C1B-CHB	3.02	1.49	1.41
21	2	510	CL7	O2A-CGA	3.02	1.42	1.33
21	6	510	CL7	O2A-CGA	3.02	1.42	1.33
21	b	610	CL7	C1B-CHB	3.02	1.49	1.41
21	3	518	CL7	C1B-CHB	3.02	1.49	1.41
21	7	518	CL7	C1B-CHB	3.02	1.49	1.41
21	2	509	CL7	O2A-CGA	3.02	1.42	1.33
21	6	509	CL7	O2A-CGA	3.02	1.42	1.33
21	4	407	CL7	C4C-C3C	-3.02	1.39	1.45
21	2	505	CL7	O2A-CGA	3.02	1.42	1.33
21	b	613	CL7	O2A-CGA	3.02	1.42	1.33
21	B	612	CL7	O2D-CGD	3.02	1.40	1.33
21	b	613	CL7	O2D-CGD	3.02	1.40	1.33
21	3	508	CL7	O2D-CGD	3.01	1.40	1.33
21	7	508	CL7	O2D-CGD	3.01	1.40	1.33
21	b	606	CL7	O2A-CGA	3.01	1.42	1.33
21	3	513	CL7	C1B-CHB	3.01	1.49	1.41
21	7	513	CL7	C1B-CHB	3.01	1.49	1.41
21	b	605	CL7	O2D-CGD	3.01	1.40	1.33
21	D	404	CL7	O2A-CGA	3.01	1.42	1.33
21	d	404	CL7	O2A-CGA	3.01	1.42	1.33
21	1	408	CL7	C2A-C1A	3.01	1.55	1.50
21	5	408	CL7	C2A-C1A	3.01	1.55	1.50
21	2	508	CL7	C4C-C3C	-3.01	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	6	508	CL7	C4C-C3C	-3.01	1.39	1.45
21	6	509	CL7	C4C-C3C	-3.01	1.39	1.45
21	3	507	CL7	C4C-C3C	-3.01	1.39	1.45
21	7	507	CL7	C4C-C3C	-3.01	1.39	1.45
21	3	505	CL7	O2A-CGA	3.01	1.42	1.33
21	7	505	CL7	O2A-CGA	3.01	1.42	1.33
21	3	504	CL7	C1B-CHB	3.01	1.49	1.41
21	7	504	CL7	C1B-CHB	3.01	1.49	1.41
21	3	505	CL7	O2D-CGD	3.01	1.40	1.33
21	7	505	CL7	O2D-CGD	3.01	1.40	1.33
21	2	504	CL7	C1B-CHB	3.01	1.49	1.41
21	6	504	CL7	C1B-CHB	3.01	1.49	1.41
21	3	507	CL7	C2A-C1A	3.01	1.55	1.50
21	7	507	CL7	C2A-C1A	3.01	1.55	1.50
21	2	501	CL7	O2A-CGA	3.01	1.42	1.33
21	6	501	CL7	O2A-CGA	3.01	1.42	1.33
21	2	501	CL7	C4C-C3C	-3.00	1.39	1.45
21	3	505	CL7	C4C-C3C	-3.00	1.39	1.45
21	6	501	CL7	C4C-C3C	-3.00	1.39	1.45
21	7	505	CL7	C4C-C3C	-3.00	1.39	1.45
21	4	409	CL7	O2D-CGD	3.00	1.40	1.33
21	2	507	CL7	C2A-C1A	3.00	1.55	1.50
21	6	507	CL7	C2A-C1A	3.00	1.55	1.50
21	2	503	CL7	C1B-CHB	3.00	1.49	1.41
21	6	503	CL7	C1B-CHB	3.00	1.49	1.41
23	b	619	8CT	C07-C02	-3.00	1.45	1.51
21	C	511	CL7	C1B-CHB	3.00	1.49	1.41
21	B	616	CL7	C4C-C3C	-3.00	1.39	1.45
21	b	617	CL7	C4C-C3C	-3.00	1.39	1.45
21	b	614	CL7	O2D-CGD	3.00	1.40	1.33
21	7	501	CL7	O2A-CGA	3.00	1.42	1.33
21	3	516	CL7	O2D-CGD	3.00	1.40	1.33
21	b	607	CL7	O2D-CGD	3.00	1.40	1.33
21	7	516	CL7	O2D-CGD	3.00	1.40	1.33
21	B	610	CL7	C1B-CHB	3.00	1.49	1.41
21	3	516	CL7	C4C-C3C	-3.00	1.39	1.45
21	7	516	CL7	C4C-C3C	-3.00	1.39	1.45
21	B	609	CL7	C1B-CHB	3.00	1.49	1.41
21	2	510	CL7	C1B-CHB	3.00	1.49	1.41
21	6	510	CL7	C1B-CHB	3.00	1.49	1.41
21	1	407	CL7	C1B-CHB	3.00	1.49	1.41
21	B	604	CL7	O2D-CGD	3.00	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	410	CL7	C1B-CHB	3.00	1.49	1.41
21	2	509	CL7	C4C-C3C	-3.00	1.39	1.45
21	8	409	CL7	O2D-CGD	2.99	1.40	1.33
21	A	403	CL7	O2D-CGD	2.99	1.40	1.33
21	2	509	CL7	C1B-CHB	2.99	1.49	1.41
21	6	509	CL7	C1B-CHB	2.99	1.49	1.41
21	2	502	CL7	C4C-C3C	-2.99	1.39	1.45
21	6	502	CL7	C4C-C3C	-2.99	1.39	1.45
21	4	413	CL7	C4C-C3C	-2.99	1.39	1.45
21	8	413	CL7	C4C-C3C	-2.99	1.39	1.45
21	4	411	CL7	O2A-CGA	2.99	1.42	1.33
21	8	411	CL7	O2A-CGA	2.99	1.42	1.33
21	b	617	CL7	C1B-CHB	2.99	1.49	1.41
21	B	607	CL7	O2D-CGD	2.99	1.40	1.33
21	b	608	CL7	O2D-CGD	2.99	1.40	1.33
21	A	403	CL7	C1B-CHB	2.99	1.49	1.41
21	a	403	CL7	C1B-CHB	2.99	1.49	1.41
21	8	410	CL7	C4C-C3C	-2.99	1.39	1.45
21	5	407	CL7	C1B-CHB	2.99	1.49	1.41
21	1	406	CL7	C4C-C3C	-2.99	1.39	1.45
21	5	406	CL7	C4C-C3C	-2.99	1.39	1.45
21	3	501	CL7	O2A-CGA	2.99	1.42	1.33
21	D	404	CL7	O2D-CGD	2.98	1.40	1.33
21	d	404	CL7	O2D-CGD	2.98	1.40	1.33
21	b	611	CL7	C1B-CHB	2.98	1.49	1.41
21	3	516	CL7	C1B-CHB	2.98	1.49	1.41
21	7	516	CL7	C1B-CHB	2.98	1.49	1.41
21	2	512	CL7	O2D-CGD	2.98	1.40	1.33
21	6	512	CL7	O2D-CGD	2.98	1.40	1.33
23	D	406	8CT	C19-C20	2.98	1.52	1.43
23	d	406	8CT	C19-C20	2.98	1.52	1.43
21	1	416	CL7	OBD-CAD	2.98	1.26	1.22
21	5	416	CL7	OBD-CAD	2.98	1.26	1.22
21	C	507	CL7	C1B-CHB	2.98	1.49	1.41
21	c	507	CL7	C1B-CHB	2.98	1.49	1.41
21	8	407	CL7	C4C-C3C	-2.98	1.39	1.45
21	C	512	CL7	C2A-C1A	2.98	1.55	1.50
21	c	512	CL7	C2A-C1A	2.98	1.55	1.50
21	8	405	CL7	C2A-C1A	2.98	1.55	1.50
21	8	414	CL7	C4C-NC	-2.98	1.34	1.37
21	4	406	CL7	O2D-CGD	2.98	1.40	1.33
21	1	418	CL7	O2D-CGD	2.97	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	418	CL7	O2D-CGD	2.97	1.40	1.33
21	C	510	CL7	C1B-CHB	2.97	1.49	1.41
21	c	510	CL7	C1B-CHB	2.97	1.49	1.41
23	D	406	8CT	C07-C02	-2.97	1.45	1.51
23	d	406	8CT	C07-C02	-2.97	1.45	1.51
21	3	512	CL7	O2D-CGD	2.97	1.40	1.33
21	7	512	CL7	O2D-CGD	2.97	1.40	1.33
21	2	501	CL7	C1B-CHB	2.97	1.49	1.41
21	6	501	CL7	C1B-CHB	2.97	1.49	1.41
21	d	405	CL7	O2D-CGD	2.97	1.40	1.33
21	B	616	CL7	C1B-CHB	2.97	1.49	1.41
21	D	405	CL7	O2D-CGD	2.97	1.40	1.33
21	3	509	CL7	C1B-CHB	2.97	1.49	1.41
21	A	403	CL7	C4C-C3C	-2.97	1.39	1.45
21	a	403	CL7	C4C-C3C	-2.97	1.39	1.45
21	A	401	CL7	OBD-CAD	2.97	1.26	1.22
21	1	404	CL7	C2A-C1A	2.97	1.55	1.50
21	5	404	CL7	C2A-C1A	2.97	1.55	1.50
21	B	615	CL7	C4C-NC	-2.97	1.34	1.37
21	b	616	CL7	C4C-NC	-2.97	1.34	1.37
21	5	410	CL7	C1B-CHB	2.97	1.49	1.41
21	B	604	CL7	C4C-NC	-2.96	1.34	1.37
21	b	605	CL7	C4C-NC	-2.96	1.34	1.37
21	2	507	CL7	O2D-CGD	2.96	1.40	1.33
21	6	507	CL7	O2D-CGD	2.96	1.40	1.33
21	C	503	CL7	C2A-C1A	2.96	1.55	1.50
21	c	503	CL7	C2A-C1A	2.96	1.55	1.50
21	b	612	CL7	O2A-CGA	2.95	1.42	1.33
21	3	511	CL7	C1B-CHB	2.95	1.49	1.41
21	B	611	CL7	O2D-CGD	2.95	1.40	1.33
21	1	405	CL7	C4C-C3C	-2.95	1.40	1.45
21	5	405	CL7	C4C-C3C	-2.95	1.40	1.45
21	1	417	CL7	C1B-CHB	2.95	1.49	1.41
21	5	417	CL7	C1B-CHB	2.95	1.49	1.41
21	B	611	CL7	O2A-CGA	2.95	1.42	1.33
21	2	506	CL7	C4C-C3C	-2.95	1.40	1.45
21	6	506	CL7	C4C-C3C	-2.95	1.40	1.45
21	3	512	CL7	C1B-CHB	2.95	1.49	1.41
21	7	509	CL7	C1B-CHB	2.95	1.49	1.41
21	C	505	CL7	C4C-C3C	-2.95	1.40	1.45
21	c	505	CL7	C4C-C3C	-2.95	1.40	1.45
21	a	401	CL7	OBD-CAD	2.95	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	B	606	CL7	C2A-C1A	2.95	1.55	1.50
21	b	607	CL7	C2A-C1A	2.95	1.55	1.50
21	3	508	CL7	C4C-C3C	-2.94	1.40	1.45
21	4	413	CL7	C1B-CHB	2.94	1.49	1.41
21	8	413	CL7	C1B-CHB	2.94	1.49	1.41
21	6	505	CL7	C4C-NC	-2.94	1.34	1.37
21	5	403	CL7	C4C-C3C	-2.94	1.40	1.45
21	A	403	CL7	C2A-C1A	2.94	1.55	1.50
21	a	403	CL7	C2A-C1A	2.94	1.55	1.50
21	C	504	CL7	C4C-C3C	-2.94	1.40	1.45
21	3	515	CL7	C4C-C3C	-2.94	1.40	1.45
21	c	504	CL7	C4C-C3C	-2.94	1.40	1.45
21	7	515	CL7	C4C-C3C	-2.94	1.40	1.45
21	7	517	CL7	C1B-CHB	2.94	1.49	1.41
21	4	405	CL7	C2A-C1A	2.94	1.55	1.50
21	B	603	CL7	C4C-C3C	-2.94	1.40	1.45
21	b	604	CL7	C4C-C3C	-2.94	1.40	1.45
21	C	509	CL7	O2D-CGD	2.94	1.40	1.33
21	4	417	CL7	C2A-C1A	2.94	1.55	1.50
21	8	417	CL7	C2A-C1A	2.94	1.55	1.50
21	4	404	CL7	C1B-CHB	2.94	1.49	1.41
21	8	404	CL7	C1B-CHB	2.94	1.49	1.41
21	2	512	CL7	C4C-NC	-2.93	1.34	1.37
21	6	512	CL7	C4C-NC	-2.93	1.34	1.37
21	C	513	CL7	C4C-C3C	-2.93	1.40	1.45
21	c	513	CL7	C4C-C3C	-2.93	1.40	1.45
21	b	612	CL7	O2D-CGD	2.93	1.40	1.33
21	c	508	CL7	C4C-NC	-2.93	1.34	1.37
23	B	627	8CT	C07-C02	-2.93	1.45	1.51
23	b	601	8CT	C07-C02	-2.93	1.45	1.51
21	2	502	CL7	O2D-CGD	2.93	1.40	1.33
21	6	502	CL7	O2D-CGD	2.93	1.40	1.33
21	3	517	CL7	C1B-CHB	2.93	1.49	1.41
21	1	402	CL7	C4C-C3C	-2.93	1.40	1.45
21	3	513	CL7	C4C-C3C	-2.93	1.40	1.45
21	5	402	CL7	C4C-C3C	-2.93	1.40	1.45
21	7	513	CL7	C4C-C3C	-2.93	1.40	1.45
21	2	505	CL7	C4C-NC	-2.93	1.34	1.37
21	2	517	CL7	C4C-C3C	-2.93	1.40	1.45
21	6	517	CL7	C4C-C3C	-2.93	1.40	1.45
21	3	510	CL7	C2A-C1A	2.93	1.55	1.50
21	7	510	CL7	C2A-C1A	2.93	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	508	CL7	C4C-C3C	-2.93	1.40	1.45
23	A	404	8CT	C19-C20	2.93	1.52	1.43
21	B	613	CL7	C4C-NC	-2.93	1.34	1.37
21	b	614	CL7	C4C-NC	-2.93	1.34	1.37
22	A	402	PHO	CBD-CGD	-2.93	1.48	1.52
22	a	402	PHO	CBD-CGD	-2.93	1.48	1.52
21	7	511	CL7	C1B-CHB	2.92	1.49	1.41
21	c	509	CL7	O2D-CGD	2.92	1.40	1.33
21	3	510	CL7	C4C-NC	-2.92	1.34	1.37
21	7	510	CL7	C4C-NC	-2.92	1.34	1.37
21	B	622	CL7	C1B-CHB	2.92	1.49	1.41
21	b	623	CL7	C1B-CHB	2.92	1.49	1.41
21	b	613	CL7	C1B-CHB	2.92	1.49	1.41
21	7	502	CL7	C1B-CHB	2.92	1.49	1.41
21	7	510	CL7	C1B-CHB	2.92	1.49	1.41
21	1	403	CL7	C4C-C3C	-2.92	1.40	1.45
21	D	404	CL7	C4C-NC	-2.92	1.34	1.37
21	d	404	CL7	C4C-NC	-2.92	1.34	1.37
23	a	404	8CT	C19-C20	2.92	1.52	1.43
21	4	414	CL7	C4C-NC	-2.92	1.34	1.37
21	B	615	CL7	C4C-C3C	-2.92	1.40	1.45
21	1	413	CL7	C4C-C3C	-2.92	1.40	1.45
21	b	616	CL7	C4C-C3C	-2.92	1.40	1.45
21	5	413	CL7	C4C-C3C	-2.92	1.40	1.45
21	7	512	CL7	C1B-CHB	2.92	1.49	1.41
21	c	518	CL7	C4C-C3C	-2.92	1.40	1.45
21	B	602	CL7	C4C-C3C	-2.91	1.40	1.45
21	b	603	CL7	C4C-C3C	-2.91	1.40	1.45
21	4	404	CL7	C4C-C3C	-2.91	1.40	1.45
21	8	404	CL7	C4C-C3C	-2.91	1.40	1.45
21	B	612	CL7	C1B-CHB	2.91	1.49	1.41
21	2	516	CL7	C4C-NC	-2.91	1.34	1.37
21	6	516	CL7	C4C-NC	-2.91	1.34	1.37
21	3	508	CL7	C2A-C1A	2.91	1.55	1.50
21	7	508	CL7	C2A-C1A	2.91	1.55	1.50
21	3	510	CL7	C1B-CHB	2.90	1.49	1.41
21	3	503	CL7	O2D-CGD	2.90	1.40	1.33
21	7	503	CL7	O2D-CGD	2.90	1.40	1.33
21	1	417	CL7	C4C-C3C	-2.90	1.40	1.45
21	5	417	CL7	C4C-C3C	-2.90	1.40	1.45
21	C	518	CL7	C4C-C3C	-2.90	1.40	1.45
32	2	525	ZEX	C21-C26	-2.90	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	6	524	ZEX	C21-C26	-2.90	1.49	1.53
21	D	405	CL7	C4C-C3C	-2.90	1.40	1.45
21	d	405	CL7	C4C-C3C	-2.90	1.40	1.45
21	B	607	CL7	C1B-CHB	2.90	1.49	1.41
21	b	608	CL7	C1B-CHB	2.90	1.49	1.41
21	1	415	CL7	OBD-CAD	2.89	1.26	1.22
21	A	406	CL7	C4C-NC	-2.89	1.34	1.37
21	a	405	CL7	C4C-NC	-2.89	1.34	1.37
22	d	408	PHO	O2A-CGA	2.89	1.41	1.33
21	1	418	CL7	C4C-NC	-2.89	1.34	1.37
21	B	603	CL7	C1B-CHB	2.89	1.49	1.41
21	C	508	CL7	O2A-CGA	2.88	1.41	1.33
23	C	519	8CT	C19-C20	2.88	1.52	1.43
23	c	519	8CT	C19-C20	2.88	1.52	1.43
21	2	502	CL7	C4C-NC	-2.88	1.34	1.37
21	6	502	CL7	C4C-NC	-2.88	1.34	1.37
21	c	508	CL7	O2A-CGA	2.88	1.41	1.33
21	7	505	CL7	C2A-C1A	2.88	1.55	1.50
21	2	510	CL7	C4C-NC	-2.88	1.34	1.37
21	6	510	CL7	C4C-NC	-2.88	1.34	1.37
21	8	416	CL7	OBD-CAD	2.88	1.26	1.22
21	3	502	CL7	C1B-CHB	2.87	1.49	1.41
21	C	502	CL7	C4C-NC	-2.87	1.34	1.37
21	c	502	CL7	C4C-NC	-2.87	1.34	1.37
21	C	510	CL7	C4C-NC	-2.87	1.34	1.37
21	c	510	CL7	C4C-NC	-2.87	1.34	1.37
21	3	517	CL7	C2A-C1A	2.87	1.55	1.50
21	7	517	CL7	C2A-C1A	2.87	1.55	1.50
21	8	408	CL7	C4C-C3C	-2.87	1.40	1.45
32	2	520	ZEX	C21-C26	-2.87	1.49	1.53
32	3	525	ZEX	C21-C26	-2.87	1.49	1.53
23	4	402	8CT	C19-C20	2.87	1.52	1.43
23	8	402	8CT	C19-C20	2.87	1.52	1.43
21	3	507	CL7	O2D-CGD	2.87	1.40	1.33
21	7	507	CL7	O2D-CGD	2.87	1.40	1.33
21	B	602	CL7	C4C-NC	-2.87	1.34	1.37
21	b	603	CL7	C4C-NC	-2.87	1.34	1.37
21	b	604	CL7	C1B-CHB	2.87	1.49	1.41
23	B	617	8CT	C19-C20	2.86	1.52	1.43
23	b	618	8CT	C19-C20	2.86	1.52	1.43
21	c	503	CL7	C4C-C3C	-2.86	1.40	1.45
22	D	408	PHO	O2A-CGA	2.86	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	515	8CT	C19-C20	2.86	1.52	1.43
23	c	515	8CT	C19-C20	2.86	1.52	1.43
21	C	508	CL7	C4C-NC	-2.86	1.34	1.37
21	C	508	CL7	O2D-CGD	2.86	1.40	1.33
21	c	508	CL7	O2D-CGD	2.86	1.40	1.33
21	d	405	CL7	C2A-C1A	2.86	1.55	1.50
21	3	517	CL7	C4C-C3C	-2.86	1.40	1.45
21	7	517	CL7	C4C-C3C	-2.86	1.40	1.45
21	4	408	CL7	C4C-C3C	-2.86	1.40	1.45
21	2	517	CL7	C2A-C1A	2.86	1.55	1.50
21	6	517	CL7	C2A-C1A	2.86	1.55	1.50
21	2	503	CL7	O2A-CGA	2.85	1.41	1.33
21	6	503	CL7	O2A-CGA	2.85	1.41	1.33
21	A	406	CL7	O2A-CGA	2.85	1.41	1.33
21	a	405	CL7	O2A-CGA	2.85	1.41	1.33
23	A	404	8CT	C07-C02	-2.85	1.45	1.51
23	a	404	8CT	C07-C02	-2.85	1.45	1.51
21	5	405	CL7	C2A-C1A	2.85	1.55	1.50
21	C	508	CL7	C1B-CHB	2.85	1.48	1.41
21	c	508	CL7	C1B-CHB	2.85	1.48	1.41
21	3	509	CL7	C4C-C3C	-2.85	1.40	1.45
21	3	511	CL7	C2A-C1A	2.85	1.55	1.50
21	4	416	CL7	OBD-CAD	2.85	1.26	1.22
21	4	405	CL7	C4C-C3C	-2.84	1.40	1.45
21	8	405	CL7	C4C-C3C	-2.84	1.40	1.45
21	B	606	CL7	C1B-CHB	2.84	1.48	1.41
21	b	607	CL7	C1B-CHB	2.84	1.48	1.41
21	3	516	CL7	C4C-NC	-2.84	1.34	1.37
21	7	516	CL7	C4C-NC	-2.84	1.34	1.37
21	5	418	CL7	C4C-NC	-2.84	1.34	1.37
21	A	401	CL7	C1D-ND	2.84	1.37	1.35
21	a	401	CL7	C1D-ND	2.84	1.37	1.35
21	5	415	CL7	OBD-CAD	2.84	1.26	1.22
21	C	510	CL7	C2A-C1A	2.84	1.55	1.50
21	D	405	CL7	C2A-C1A	2.84	1.55	1.50
21	4	406	CL7	C4C-NC	-2.84	1.34	1.37
21	B	615	CL7	C2A-C1A	2.84	1.55	1.50
21	3	505	CL7	C2A-C1A	2.84	1.55	1.50
21	b	616	CL7	C2A-C1A	2.84	1.55	1.50
21	B	613	CL7	C1B-CHB	2.83	1.48	1.41
21	b	614	CL7	C1B-CHB	2.83	1.48	1.41
21	C	502	CL7	C2A-C1A	2.83	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	502	CL7	C2A-C1A	2.83	1.55	1.50
21	C	503	CL7	C4C-C3C	-2.83	1.40	1.45
21	3	518	CL7	C4C-C3C	-2.83	1.40	1.45
21	7	518	CL7	C4C-C3C	-2.83	1.40	1.45
21	8	415	CL7	C4C-C3C	-2.83	1.40	1.45
23	B	619	8CT	C19-C20	2.82	1.52	1.43
21	1	405	CL7	C2A-C1A	2.82	1.55	1.50
21	7	511	CL7	C2A-C1A	2.82	1.55	1.50
21	c	510	CL7	C2A-C1A	2.82	1.55	1.50
23	b	620	8CT	C19-C20	2.82	1.52	1.43
21	8	415	CL7	C2A-C1A	2.82	1.55	1.50
21	B	614	CL7	C1B-CHB	2.81	1.48	1.41
21	b	615	CL7	C1B-CHB	2.81	1.48	1.41
21	B	608	CL7	C4C-C3C	-2.81	1.40	1.45
21	b	609	CL7	C4C-C3C	-2.81	1.40	1.45
21	B	603	CL7	C4C-NC	-2.81	1.34	1.37
21	b	604	CL7	C4C-NC	-2.81	1.34	1.37
21	3	508	CL7	C4C-NC	-2.80	1.34	1.37
21	7	508	CL7	C4C-NC	-2.80	1.34	1.37
21	B	606	CL7	C4C-C3C	-2.80	1.40	1.45
21	b	607	CL7	C4C-C3C	-2.80	1.40	1.45
21	1	420	CL7	C4C-C3C	-2.80	1.40	1.45
21	7	509	CL7	C4C-C3C	-2.80	1.40	1.45
21	4	410	CL7	C4C-NC	-2.80	1.34	1.37
21	8	410	CL7	C4C-NC	-2.80	1.34	1.37
21	1	407	CL7	C4C-C3C	-2.80	1.40	1.45
21	B	612	CL7	C4C-NC	-2.79	1.34	1.37
21	b	613	CL7	C4C-NC	-2.79	1.34	1.37
32	2	523	ZEX	C21-C26	-2.79	1.49	1.53
32	6	522	ZEX	C21-C26	-2.79	1.49	1.53
21	c	514	CL7	C4C-C3C	-2.79	1.40	1.45
21	4	415	CL7	C2A-C1A	2.79	1.55	1.50
21	4	404	CL7	C4C-NC	-2.79	1.34	1.37
21	8	404	CL7	C4C-NC	-2.79	1.34	1.37
21	6	504	CL7	C4C-C3C	-2.79	1.40	1.45
21	3	501	CL7	C4C-NC	-2.79	1.34	1.37
21	7	501	CL7	C4C-NC	-2.79	1.34	1.37
21	2	504	CL7	C4C-C3C	-2.78	1.40	1.45
21	d	402	CL7	OBD-CAD	2.78	1.26	1.22
21	C	504	CL7	C2A-C1A	2.78	1.55	1.50
21	c	504	CL7	C2A-C1A	2.78	1.55	1.50
21	1	409	CL7	C4C-C3C	-2.78	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	409	CL7	C4C-C3C	-2.78	1.40	1.45
21	1	411	CL7	C2A-C1A	2.78	1.55	1.50
21	2	501	CL7	C4C-NC	-2.78	1.34	1.37
21	6	501	CL7	C4C-NC	-2.78	1.34	1.37
21	6	503	CL7	C4C-NC	-2.78	1.34	1.37
21	7	504	CL7	C4C-NC	-2.78	1.34	1.37
21	3	511	CL7	C4C-NC	-2.78	1.34	1.37
21	7	511	CL7	C4C-NC	-2.78	1.34	1.37
21	1	419	CL7	OBD-CAD	2.78	1.26	1.22
21	5	419	CL7	OBD-CAD	2.78	1.26	1.22
21	4	415	CL7	C4C-C3C	-2.78	1.40	1.45
32	2	519	ZEX	C21-C26	-2.77	1.50	1.53
21	5	407	CL7	C4C-C3C	-2.77	1.40	1.45
21	4	412	CL7	C2A-C1A	2.77	1.55	1.50
21	8	412	CL7	C2A-C1A	2.77	1.55	1.50
21	C	514	CL7	C4C-C3C	-2.77	1.40	1.45
21	5	420	CL7	C4C-C3C	-2.77	1.40	1.45
21	3	502	CL7	C4C-C3C	-2.76	1.40	1.45
21	7	502	CL7	C4C-C3C	-2.76	1.40	1.45
21	B	622	CL7	C4C-C3C	-2.76	1.40	1.45
21	b	623	CL7	C4C-C3C	-2.76	1.40	1.45
21	3	517	CL7	C4C-NC	-2.76	1.34	1.37
21	6	517	CL7	C4C-NC	-2.76	1.34	1.37
21	b	610	CL7	C4C-C3C	-2.76	1.40	1.45
21	b	607	CL7	C4C-NC	-2.76	1.34	1.37
21	5	411	CL7	C2A-C1A	2.76	1.55	1.50
21	5	414	CL7	OBD-CAD	2.76	1.26	1.22
21	B	603	CL7	C2A-C1A	2.75	1.55	1.50
21	8	406	CL7	C4C-NC	-2.75	1.34	1.37
21	1	415	CL7	C1D-ND	2.75	1.37	1.35
21	5	415	CL7	C1D-ND	2.75	1.37	1.35
21	4	404	CL7	C2A-C1A	2.75	1.55	1.50
21	8	404	CL7	C2A-C1A	2.75	1.55	1.50
21	1	403	CL7	C4C-NC	-2.75	1.34	1.37
21	5	403	CL7	C4C-NC	-2.75	1.34	1.37
21	3	504	CL7	C4C-NC	-2.75	1.34	1.37
21	7	512	CL7	C4C-NC	-2.75	1.34	1.37
21	5	411	CL7	C4C-C3C	-2.74	1.40	1.45
21	4	411	CL7	C2A-C1A	2.74	1.55	1.50
21	8	411	CL7	C2A-C1A	2.74	1.55	1.50
23	C	519	8CT	C07-C02	-2.74	1.45	1.51
23	c	519	8CT	C07-C02	-2.74	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	C	503	CL7	C4C-NC	-2.74	1.34	1.37
21	c	503	CL7	C4C-NC	-2.74	1.34	1.37
21	1	414	CL7	OBD-CAD	2.74	1.26	1.22
21	D	405	CL7	C4C-NC	-2.74	1.34	1.37
21	d	405	CL7	C4C-NC	-2.74	1.34	1.37
21	7	517	CL7	C4C-NC	-2.74	1.34	1.37
21	D	402	CL7	OBD-CAD	2.74	1.26	1.22
21	C	512	CL7	OBD-CAD	2.74	1.26	1.22
21	c	512	CL7	OBD-CAD	2.74	1.26	1.22
21	C	504	CL7	C4C-NC	-2.74	1.34	1.37
21	c	504	CL7	C4C-NC	-2.74	1.34	1.37
21	4	415	CL7	C4C-NC	-2.74	1.34	1.37
21	8	415	CL7	C4C-NC	-2.74	1.34	1.37
21	2	517	CL7	C4C-NC	-2.74	1.34	1.37
21	B	609	CL7	C4C-C3C	-2.73	1.40	1.45
21	1	410	CL7	C4C-C3C	-2.73	1.40	1.45
21	5	410	CL7	C4C-C3C	-2.73	1.40	1.45
32	6	519	ZEX	C21-C26	-2.73	1.50	1.53
21	6	507	CL7	C4C-C3C	-2.73	1.40	1.45
21	b	612	CL7	C2A-C1A	2.73	1.54	1.50
21	C	506	CL7	C2A-C1A	2.73	1.54	1.50
21	2	515	CL7	OBD-CAD	2.72	1.26	1.22
21	6	515	CL7	OBD-CAD	2.72	1.26	1.22
21	5	409	CL7	OBD-CAD	2.72	1.26	1.22
21	B	605	CL7	C4C-NC	-2.72	1.34	1.37
21	b	606	CL7	C4C-NC	-2.72	1.34	1.37
21	1	411	CL7	C4C-C3C	-2.72	1.40	1.45
21	2	503	CL7	C4C-NC	-2.72	1.34	1.37
21	4	416	CL7	C4C-C3C	-2.72	1.40	1.45
21	8	416	CL7	C4C-C3C	-2.72	1.40	1.45
21	C	514	CL7	OBD-CAD	2.72	1.26	1.22
21	c	514	CL7	OBD-CAD	2.72	1.26	1.22
21	B	606	CL7	C4C-NC	-2.71	1.34	1.37
21	B	616	CL7	C4C-NC	-2.71	1.34	1.37
21	b	617	CL7	C4C-NC	-2.71	1.34	1.37
21	2	516	CL7	C2A-C1A	2.71	1.54	1.50
21	B	608	CL7	C2A-C1A	2.71	1.54	1.50
21	b	609	CL7	C2A-C1A	2.71	1.54	1.50
21	B	604	CL7	C2A-C1A	2.71	1.54	1.50
21	b	605	CL7	C2A-C1A	2.71	1.54	1.50
21	b	604	CL7	C2A-C1A	2.70	1.54	1.50
21	1	413	CL7	OBD-CAD	2.70	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	413	CL7	OBD-CAD	2.70	1.26	1.22
21	3	512	CL7	C4C-NC	-2.70	1.34	1.37
21	2	518	CL7	C4C-C3C	-2.70	1.40	1.45
21	6	518	CL7	C4C-C3C	-2.70	1.40	1.45
21	B	622	CL7	OBD-CAD	2.70	1.26	1.22
21	b	623	CL7	OBD-CAD	2.70	1.26	1.22
21	2	507	CL7	C4C-C3C	-2.70	1.40	1.45
21	1	409	CL7	OBD-CAD	2.70	1.26	1.22
21	1	405	CL7	C4C-NC	-2.69	1.34	1.37
21	2	508	CL7	C2A-C1A	2.69	1.54	1.50
21	6	508	CL7	C2A-C1A	2.69	1.54	1.50
21	7	505	CL7	C4C-NC	-2.69	1.34	1.37
21	C	507	CL7	C4C-NC	-2.69	1.34	1.37
21	1	407	CL7	C4C-NC	-2.69	1.34	1.37
21	A	403	CL7	C4C-NC	-2.69	1.34	1.37
21	C	506	CL7	C4C-NC	-2.69	1.34	1.37
21	c	506	CL7	C4C-NC	-2.69	1.34	1.37
21	6	509	CL7	C4C-NC	-2.69	1.34	1.37
21	3	503	CL7	C4C-NC	-2.69	1.34	1.37
21	7	503	CL7	C4C-NC	-2.69	1.34	1.37
21	C	511	CL7	C4C-NC	-2.69	1.34	1.37
21	6	518	CL7	C4C-NC	-2.69	1.34	1.37
21	4	417	CL7	C4C-C3C	-2.69	1.40	1.45
21	8	417	CL7	C4C-C3C	-2.69	1.40	1.45
21	1	411	CL7	OBD-CAD	2.68	1.26	1.22
21	5	411	CL7	OBD-CAD	2.68	1.26	1.22
21	B	611	CL7	C2A-C1A	2.68	1.54	1.50
21	6	516	CL7	C2A-C1A	2.68	1.54	1.50
21	c	506	CL7	C2A-C1A	2.68	1.54	1.50
21	1	406	CL7	OBD-CAD	2.67	1.26	1.22
21	5	406	CL7	OBD-CAD	2.67	1.26	1.22
21	4	414	CL7	C2A-C1A	2.67	1.54	1.50
21	8	414	CL7	C2A-C1A	2.67	1.54	1.50
21	2	506	CL7	OBD-CAD	2.67	1.26	1.22
21	c	511	CL7	C4C-NC	-2.67	1.34	1.37
21	4	412	CL7	C4C-NC	-2.67	1.34	1.37
21	2	508	CL7	C4C-NC	-2.66	1.34	1.37
21	6	508	CL7	C4C-NC	-2.66	1.34	1.37
21	C	505	CL7	OBD-CAD	2.66	1.26	1.22
21	1	410	CL7	OBD-CAD	2.66	1.26	1.22
21	c	505	CL7	OBD-CAD	2.66	1.26	1.22
21	5	410	CL7	OBD-CAD	2.66	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	c	507	CL7	C4C-NC	-2.66	1.34	1.37
21	a	403	CL7	C4C-NC	-2.66	1.34	1.37
21	6	506	CL7	OBD-CAD	2.66	1.26	1.22
21	1	406	CL7	C4C-NC	-2.66	1.34	1.37
21	5	406	CL7	C4C-NC	-2.66	1.34	1.37
21	1	412	CL7	OBD-CAD	2.65	1.26	1.22
21	5	412	CL7	OBD-CAD	2.65	1.26	1.22
21	1	413	CL7	C4C-NC	-2.65	1.34	1.37
21	5	413	CL7	C4C-NC	-2.65	1.34	1.37
21	C	506	CL7	C4C-C3C	-2.65	1.40	1.45
32	8	420	ZEX	C1-C6	-2.65	1.50	1.53
21	1	405	CL7	OBD-CAD	2.65	1.26	1.22
21	5	405	CL7	OBD-CAD	2.65	1.26	1.22
21	1	404	CL7	C4C-C3C	-2.65	1.40	1.45
21	5	404	CL7	C4C-C3C	-2.65	1.40	1.45
21	3	505	CL7	C4C-NC	-2.65	1.34	1.37
21	3	509	CL7	C2A-C1A	2.64	1.54	1.50
31	F	101	HEM	FE-NB	2.64	2.09	1.96
21	C	507	CL7	C2A-C1A	2.64	1.54	1.50
21	c	507	CL7	C2A-C1A	2.64	1.54	1.50
32	2	520	ZEX	C30-C29	-2.64	1.32	1.35
32	3	525	ZEX	C30-C29	-2.64	1.32	1.35
21	1	420	CL7	C1D-ND	2.64	1.37	1.35
21	5	420	CL7	C1D-ND	2.64	1.37	1.35
21	b	608	CL7	C4C-NC	-2.64	1.34	1.37
21	1	420	CL7	OBD-CAD	2.64	1.26	1.22
21	5	420	CL7	OBD-CAD	2.64	1.26	1.22
21	5	407	CL7	C4C-NC	-2.64	1.34	1.37
21	B	616	CL7	C2A-C1A	2.64	1.54	1.50
21	b	617	CL7	C2A-C1A	2.64	1.54	1.50
21	3	514	CL7	C4C-C3C	-2.63	1.40	1.45
21	7	514	CL7	C4C-C3C	-2.63	1.40	1.45
21	2	509	CL7	C4C-NC	-2.63	1.34	1.37
31	f	101	HEM	FE-NB	2.63	2.09	1.96
21	2	515	CL7	C4C-C3C	-2.63	1.40	1.45
21	6	515	CL7	C4C-C3C	-2.63	1.40	1.45
21	4	415	CL7	OBD-CAD	2.63	1.26	1.22
21	8	415	CL7	OBD-CAD	2.63	1.26	1.22
21	5	405	CL7	C4C-NC	-2.62	1.34	1.37
21	3	506	CL7	C4C-C3C	-2.62	1.40	1.45
21	7	506	CL7	C4C-C3C	-2.62	1.40	1.45
21	B	609	CL7	C4C-NC	-2.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	610	CL7	C4C-NC	-2.62	1.34	1.37
21	1	416	CL7	C1D-ND	2.62	1.37	1.35
21	5	416	CL7	C1D-ND	2.62	1.37	1.35
21	2	505	CL7	C2A-C1A	2.62	1.54	1.50
21	6	505	CL7	C2A-C1A	2.62	1.54	1.50
21	2	511	CL7	C4C-NC	-2.62	1.34	1.37
21	2	518	CL7	C4C-NC	-2.62	1.34	1.37
21	B	607	CL7	C4C-NC	-2.62	1.34	1.37
21	3	501	CL7	OBD-CAD	2.62	1.26	1.22
21	4	404	CL7	OBD-CAD	2.62	1.26	1.22
21	8	404	CL7	OBD-CAD	2.62	1.26	1.22
23	C	519	8CT	C01-C02	2.62	1.55	1.50
21	8	412	CL7	C4C-NC	-2.62	1.34	1.37
32	4	420	ZEX	C1-C6	-2.61	1.50	1.53
21	B	602	CL7	C2A-C1A	2.61	1.54	1.50
21	1	407	CL7	OBD-CAD	2.61	1.25	1.22
21	5	407	CL7	OBD-CAD	2.61	1.25	1.22
21	2	511	CL7	OBD-CAD	2.61	1.25	1.22
21	4	407	CL7	OBD-CAD	2.61	1.25	1.22
21	6	511	CL7	OBD-CAD	2.61	1.25	1.22
21	B	601	CL7	C4C-C3C	-2.61	1.40	1.45
21	b	602	CL7	C4C-C3C	-2.61	1.40	1.45
21	2	503	CL7	CBD-CGD	-2.61	1.44	1.52
21	6	503	CL7	CBD-CGD	-2.61	1.44	1.52
21	D	404	CL7	C2A-C1A	2.61	1.54	1.50
21	C	513	CL7	C4C-NC	-2.60	1.34	1.37
21	c	513	CL7	C4C-NC	-2.60	1.34	1.37
21	c	506	CL7	C4C-C3C	-2.60	1.40	1.45
21	1	415	CL7	C4C-C3C	-2.60	1.40	1.45
21	5	415	CL7	C4C-C3C	-2.60	1.40	1.45
32	3	519	ZEX	C21-C26	-2.60	1.50	1.53
21	4	413	CL7	C4C-NC	-2.60	1.34	1.37
21	8	413	CL7	C4C-NC	-2.60	1.34	1.37
23	B	627	8CT	C01-C02	2.60	1.55	1.50
23	b	601	8CT	C01-C02	2.60	1.55	1.50
21	2	513	CL7	C4C-C3C	-2.60	1.40	1.45
21	6	513	CL7	C4C-C3C	-2.60	1.40	1.45
21	5	412	CL7	C4C-NC	-2.59	1.34	1.37
21	b	603	CL7	C2A-C1A	2.59	1.54	1.50
21	4	411	CL7	C1B-CHB	2.59	1.48	1.41
21	8	411	CL7	C1B-CHB	2.59	1.48	1.41
21	1	418	CL7	C2A-C1A	2.59	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	418	CL7	C2A-C1A	2.59	1.54	1.50
21	2	504	CL7	C4C-NC	-2.59	1.34	1.37
21	6	504	CL7	C4C-NC	-2.59	1.34	1.37
21	3	507	CL7	C4C-NC	-2.58	1.34	1.37
21	7	507	CL7	C4C-NC	-2.58	1.34	1.37
21	B	607	CL7	C2A-C1A	2.58	1.54	1.50
21	b	608	CL7	C2A-C1A	2.58	1.54	1.50
21	1	419	CL7	C4C-C3C	-2.58	1.40	1.45
21	5	419	CL7	C4C-C3C	-2.58	1.40	1.45
21	3	518	CL7	OBD-CAD	2.58	1.25	1.22
21	7	518	CL7	OBD-CAD	2.58	1.25	1.22
21	4	411	CL7	C4C-NC	-2.58	1.34	1.37
21	6	511	CL7	C4C-NC	-2.58	1.34	1.37
21	8	411	CL7	C4C-NC	-2.58	1.34	1.37
21	7	509	CL7	C2A-C1A	2.58	1.54	1.50
21	1	412	CL7	C4C-NC	-2.58	1.34	1.37
21	c	512	CL7	C4C-NC	-2.58	1.34	1.37
23	K	101	8CT	C22-C21	2.58	1.56	1.50
21	A	401	CL7	C4C-C3C	-2.58	1.40	1.45
21	a	401	CL7	C4C-C3C	-2.58	1.40	1.45
23	k	101	8CT	C22-C21	2.58	1.56	1.50
21	3	513	CL7	OBD-CAD	2.58	1.25	1.22
21	7	513	CL7	OBD-CAD	2.58	1.25	1.22
22	d	408	PHO	CBD-CGD	-2.57	1.49	1.52
23	c	519	8CT	C01-C02	2.57	1.55	1.50
23	B	627	8CT	C22-C21	2.57	1.56	1.50
21	D	402	CL7	C4C-C3C	-2.57	1.40	1.45
21	C	505	CL7	C4C-NC	-2.57	1.34	1.37
21	c	505	CL7	C4C-NC	-2.57	1.34	1.37
21	C	508	CL7	C2A-C1A	2.57	1.54	1.50
21	c	508	CL7	C2A-C1A	2.57	1.54	1.50
21	7	501	CL7	OBD-CAD	2.57	1.25	1.22
21	4	414	CL7	OBD-CAD	2.57	1.25	1.22
21	8	414	CL7	OBD-CAD	2.57	1.25	1.22
21	C	518	CL7	C4C-NC	-2.57	1.34	1.37
21	c	518	CL7	C4C-NC	-2.57	1.34	1.37
32	3	520	ZEX	C21-C26	-2.57	1.50	1.53
21	4	417	CL7	OBD-CAD	2.57	1.25	1.22
21	8	417	CL7	OBD-CAD	2.57	1.25	1.22
21	1	412	CL7	C4C-C3C	-2.57	1.40	1.45
21	5	412	CL7	C4C-C3C	-2.57	1.40	1.45
21	1	404	CL7	OBD-CAD	2.57	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	404	CL7	OBD-CAD	2.57	1.25	1.22
22	D	408	PHO	CBD-CGD	-2.56	1.49	1.52
21	8	407	CL7	OBD-CAD	2.56	1.25	1.22
21	3	518	CL7	C4C-NC	-2.56	1.34	1.37
21	7	518	CL7	C4C-NC	-2.56	1.34	1.37
21	B	609	CL7	C2A-C1A	2.56	1.54	1.50
21	b	610	CL7	C2A-C1A	2.56	1.54	1.50
21	3	515	CL7	OBD-CAD	2.56	1.25	1.22
21	7	515	CL7	OBD-CAD	2.56	1.25	1.22
21	4	405	CL7	C4C-NC	-2.56	1.34	1.37
21	5	420	CL7	C4C-NC	-2.56	1.34	1.37
21	8	405	CL7	C4C-NC	-2.56	1.34	1.37
21	d	402	CL7	C4C-C3C	-2.56	1.40	1.45
32	4	419	ZEX	C1-C6	-2.56	1.50	1.53
21	D	405	CL7	OBD-CAD	2.56	1.25	1.22
21	d	405	CL7	OBD-CAD	2.56	1.25	1.22
21	2	510	CL7	C2A-C1A	2.56	1.54	1.50
21	6	510	CL7	C2A-C1A	2.56	1.54	1.50
21	2	502	CL7	C2A-C1A	2.55	1.54	1.50
21	6	502	CL7	C2A-C1A	2.55	1.54	1.50
21	B	622	CL7	C1D-ND	2.55	1.37	1.35
21	b	623	CL7	C1D-ND	2.55	1.37	1.35
21	1	417	CL7	C4C-NC	-2.55	1.34	1.37
21	5	417	CL7	C4C-NC	-2.55	1.34	1.37
21	6	506	CL7	C4C-NC	-2.55	1.34	1.37
21	5	416	CL7	C4C-C3C	-2.55	1.40	1.45
23	B	619	8CT	C01-C02	2.55	1.55	1.50
23	b	620	8CT	C01-C02	2.55	1.55	1.50
21	C	512	CL7	C4C-NC	-2.55	1.34	1.37
21	B	614	CL7	C4C-NC	-2.54	1.34	1.37
21	b	615	CL7	C4C-NC	-2.54	1.34	1.37
21	2	501	CL7	OBD-CAD	2.54	1.25	1.22
21	4	408	CL7	OBD-CAD	2.54	1.25	1.22
21	6	501	CL7	OBD-CAD	2.54	1.25	1.22
21	8	408	CL7	OBD-CAD	2.54	1.25	1.22
23	b	601	8CT	C22-C21	2.54	1.56	1.50
21	d	404	CL7	C2A-C1A	2.54	1.54	1.50
21	C	507	CL7	OBD-CAD	2.54	1.25	1.22
21	c	507	CL7	OBD-CAD	2.54	1.25	1.22
21	3	502	CL7	C4C-NC	-2.54	1.34	1.37
21	7	514	CL7	OBD-CAD	2.54	1.25	1.22
21	3	514	CL7	OBD-CAD	2.54	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	409	CL7	C4C-NC	-2.53	1.34	1.37
21	8	409	CL7	C4C-NC	-2.53	1.34	1.37
23	c	515	8CT	C01-C02	2.53	1.55	1.50
21	6	518	CL7	OBD-CAD	2.53	1.25	1.22
21	2	504	CL7	OBD-CAD	2.53	1.25	1.22
21	6	504	CL7	OBD-CAD	2.53	1.25	1.22
32	7	520	ZEX	C21-C26	-2.53	1.50	1.53
21	7	506	CL7	OBD-CAD	2.52	1.25	1.22
21	1	416	CL7	C4C-C3C	-2.52	1.40	1.45
32	5	421	ZEX	C21-C26	-2.52	1.50	1.53
21	3	509	CL7	C4C-NC	-2.52	1.34	1.37
21	7	509	CL7	C4C-NC	-2.52	1.34	1.37
21	3	517	CL7	OBD-CAD	2.52	1.25	1.22
21	7	517	CL7	OBD-CAD	2.52	1.25	1.22
21	3	506	CL7	OBD-CAD	2.52	1.25	1.22
21	3	505	CL7	OBD-CAD	2.52	1.25	1.22
21	7	505	CL7	OBD-CAD	2.52	1.25	1.22
21	3	501	CL7	C2A-C1A	2.52	1.54	1.50
21	7	501	CL7	C2A-C1A	2.52	1.54	1.50
21	2	506	CL7	C4C-NC	-2.52	1.34	1.37
21	C	509	CL7	OBD-CAD	2.52	1.25	1.22
21	1	403	CL7	OBD-CAD	2.52	1.25	1.22
21	c	509	CL7	OBD-CAD	2.52	1.25	1.22
21	5	403	CL7	OBD-CAD	2.52	1.25	1.22
21	b	602	CL7	OBD-CAD	2.52	1.25	1.22
23	B	627	8CT	C30-C29	2.52	1.54	1.50
23	b	601	8CT	C30-C29	2.52	1.54	1.50
32	8	419	ZEX	C1-C6	-2.52	1.50	1.53
21	4	408	CL7	C4C-NC	-2.52	1.34	1.37
21	8	408	CL7	C4C-NC	-2.52	1.34	1.37
21	B	612	CL7	C1C-NC	-2.51	1.34	1.37
21	b	613	CL7	C1C-NC	-2.51	1.34	1.37
32	1	421	ZEX	C21-C26	-2.51	1.50	1.53
32	7	519	ZEX	C21-C26	-2.51	1.50	1.53
21	1	411	CL7	C4C-NC	-2.51	1.34	1.37
21	5	411	CL7	C4C-NC	-2.51	1.34	1.37
32	8	403	ZEX	C21-C26	-2.50	1.50	1.53
21	1	420	CL7	C4C-NC	-2.50	1.34	1.37
21	1	419	CL7	C1D-ND	2.50	1.37	1.35
21	5	419	CL7	C1D-ND	2.50	1.37	1.35
21	1	414	CL7	C4C-C3C	-2.50	1.40	1.45
21	5	414	CL7	C4C-C3C	-2.50	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	518	CL7	OBD-CAD	2.50	1.25	1.22
21	B	606	CL7	C1C-NC	-2.50	1.34	1.37
21	b	607	CL7	C1C-NC	-2.50	1.34	1.37
21	2	514	CL7	C4C-NC	-2.50	1.34	1.37
21	6	514	CL7	C4C-NC	-2.50	1.34	1.37
21	4	409	CL7	C4C-C3C	-2.50	1.40	1.45
21	8	409	CL7	C4C-C3C	-2.50	1.40	1.45
23	C	515	8CT	C22-C21	2.50	1.56	1.50
23	c	515	8CT	C22-C21	2.50	1.56	1.50
21	1	402	CL7	OBD-CAD	2.49	1.25	1.22
21	5	402	CL7	OBD-CAD	2.49	1.25	1.22
21	B	608	CL7	C4C-NC	-2.49	1.34	1.37
21	b	609	CL7	C4C-NC	-2.49	1.34	1.37
21	A	406	CL7	C2A-C1A	2.49	1.54	1.50
21	a	405	CL7	C2A-C1A	2.49	1.54	1.50
21	C	505	CL7	C1D-ND	2.49	1.37	1.35
21	c	505	CL7	C1D-ND	2.49	1.37	1.35
21	C	511	CL7	C2A-C1A	2.49	1.54	1.50
21	2	503	CL7	OBD-CAD	2.49	1.25	1.22
32	1	422	ZEX	C21-C26	-2.49	1.50	1.53
32	3	520	ZEX	C1-C6	-2.49	1.50	1.53
21	D	404	CL7	C1C-C2C	-2.49	1.40	1.45
21	d	404	CL7	C1C-C2C	-2.49	1.40	1.45
21	7	502	CL7	C4C-NC	-2.48	1.34	1.37
21	1	408	CL7	OBD-CAD	2.48	1.25	1.22
21	5	408	CL7	OBD-CAD	2.48	1.25	1.22
21	B	616	CL7	OBD-CAD	2.48	1.25	1.22
21	b	617	CL7	OBD-CAD	2.48	1.25	1.22
21	B	615	CL7	OBD-CAD	2.48	1.25	1.22
21	2	513	CL7	OBD-CAD	2.48	1.25	1.22
21	b	616	CL7	OBD-CAD	2.48	1.25	1.22
21	6	513	CL7	OBD-CAD	2.48	1.25	1.22
32	4	403	ZEX	C21-C26	-2.48	1.50	1.53
21	3	505	CL7	C1C-NC	-2.48	1.34	1.37
21	7	505	CL7	C1C-NC	-2.48	1.34	1.37
21	6	513	CL7	C4C-NC	-2.48	1.34	1.37
21	C	511	CL7	OBD-CAD	2.48	1.25	1.22
21	1	417	CL7	OBD-CAD	2.48	1.25	1.22
21	c	511	CL7	OBD-CAD	2.48	1.25	1.22
21	5	417	CL7	OBD-CAD	2.48	1.25	1.22
23	C	515	8CT	C01-C02	2.47	1.55	1.50
21	B	601	CL7	OBD-CAD	2.47	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	1	410	CL7	C4C-NC	-2.47	1.34	1.37
21	5	410	CL7	C4C-NC	-2.47	1.34	1.37
21	1	402	CL7	C4C-NC	-2.47	1.34	1.37
21	5	402	CL7	C4C-NC	-2.47	1.34	1.37
21	2	507	CL7	C4C-NC	-2.47	1.34	1.37
21	3	513	CL7	C4C-NC	-2.47	1.34	1.37
21	6	507	CL7	C4C-NC	-2.47	1.34	1.37
21	7	513	CL7	C4C-NC	-2.47	1.34	1.37
21	6	503	CL7	OBD-CAD	2.46	1.25	1.22
21	4	406	CL7	OBD-CAD	2.46	1.25	1.22
21	8	406	CL7	OBD-CAD	2.46	1.25	1.22
21	6	503	CL7	O2D-CGD	2.46	1.39	1.33
21	B	607	CL7	OBD-CAD	2.46	1.25	1.22
21	b	608	CL7	OBD-CAD	2.46	1.25	1.22
21	d	402	CL7	C4C-NC	-2.46	1.34	1.37
21	3	516	CL7	C1C-NC	-2.46	1.34	1.37
21	7	516	CL7	C1C-NC	-2.46	1.34	1.37
22	d	408	PHO	C3C-C2C	2.46	1.44	1.37
21	6	514	CL7	OBD-CAD	2.45	1.25	1.22
21	c	511	CL7	C2A-C1A	2.45	1.54	1.50
21	1	408	CL7	C4C-C3C	-2.45	1.40	1.45
21	5	408	CL7	C4C-C3C	-2.45	1.40	1.45
21	2	514	CL7	C4C-C3C	-2.45	1.40	1.45
21	6	514	CL7	C4C-C3C	-2.45	1.40	1.45
21	B	606	CL7	C1D-ND	2.45	1.37	1.35
21	b	607	CL7	C1D-ND	2.45	1.37	1.35
21	A	403	CL7	C1C-NC	-2.45	1.34	1.37
21	a	403	CL7	C1C-NC	-2.45	1.34	1.37
32	7	520	ZEX	C1-C6	-2.45	1.50	1.53
21	B	611	CL7	C1C-C2C	-2.45	1.40	1.45
22	D	408	PHO	C3C-C2C	2.45	1.44	1.37
21	3	506	CL7	C4C-NC	-2.45	1.34	1.37
21	3	515	CL7	C4C-NC	-2.45	1.34	1.37
21	7	506	CL7	C4C-NC	-2.45	1.34	1.37
21	7	515	CL7	C4C-NC	-2.45	1.34	1.37
32	5	422	ZEX	C21-C26	-2.44	1.50	1.53
21	1	414	CL7	C1D-ND	2.44	1.37	1.35
21	5	414	CL7	C1D-ND	2.44	1.37	1.35
21	B	615	CL7	C1C-C2C	-2.44	1.40	1.45
21	b	616	CL7	C1C-C2C	-2.44	1.40	1.45
21	c	514	CL7	C4C-NC	-2.44	1.34	1.37
21	3	508	CL7	C1C-C2C	-2.44	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	7	506	CL7	C1C-C2C	-2.44	1.40	1.45
21	7	508	CL7	C1C-C2C	-2.44	1.40	1.45
23	K	101	8CT	C30-C29	2.44	1.53	1.50
23	k	101	8CT	C30-C29	2.44	1.53	1.50
21	4	410	CL7	OBD-CAD	2.44	1.25	1.22
21	8	410	CL7	OBD-CAD	2.44	1.25	1.22
21	B	601	CL7	C4C-NC	-2.44	1.34	1.37
21	b	602	CL7	C4C-NC	-2.44	1.34	1.37
21	2	513	CL7	C4C-NC	-2.43	1.34	1.37
21	2	503	CL7	O2D-CGD	2.43	1.39	1.33
32	3	522	ZEX	C21-C26	-2.43	1.50	1.53
32	7	522	ZEX	C21-C26	-2.43	1.50	1.53
21	3	503	CL7	OBD-CAD	2.43	1.25	1.22
21	7	503	CL7	OBD-CAD	2.43	1.25	1.22
21	1	410	CL7	C1D-ND	2.43	1.37	1.35
21	1	418	CL7	OBD-CAD	2.43	1.25	1.22
21	5	418	CL7	OBD-CAD	2.43	1.25	1.22
21	4	415	CL7	C1C-NC	-2.43	1.34	1.37
21	8	415	CL7	C1C-NC	-2.43	1.34	1.37
21	b	613	CL7	C2A-C1A	2.42	1.54	1.50
21	B	609	CL7	OBD-CAD	2.42	1.25	1.22
21	b	610	CL7	OBD-CAD	2.42	1.25	1.22
21	B	612	CL7	C2A-C1A	2.42	1.54	1.50
21	3	516	CL7	OBD-CAD	2.42	1.25	1.22
21	7	516	CL7	OBD-CAD	2.42	1.25	1.22
21	b	612	CL7	C1C-C2C	-2.42	1.40	1.45
21	B	614	CL7	OBD-CAD	2.42	1.25	1.22
21	b	615	CL7	OBD-CAD	2.42	1.25	1.22
21	3	506	CL7	C1C-C2C	-2.41	1.40	1.45
21	2	508	CL7	OBD-CAD	2.41	1.25	1.22
21	6	508	CL7	OBD-CAD	2.41	1.25	1.22
21	D	402	CL7	C4C-NC	-2.41	1.34	1.37
23	K	101	8CT	C28-C29	2.41	1.38	1.32
23	k	101	8CT	C28-C29	2.41	1.38	1.32
21	b	606	CL7	C1D-ND	2.41	1.37	1.35
21	C	518	CL7	OBD-CAD	2.41	1.25	1.22
21	c	518	CL7	OBD-CAD	2.41	1.25	1.22
21	2	510	CL7	OBD-CAD	2.41	1.25	1.22
21	6	510	CL7	OBD-CAD	2.41	1.25	1.22
21	B	603	CL7	OBD-CAD	2.41	1.25	1.22
21	b	604	CL7	OBD-CAD	2.41	1.25	1.22
21	6	507	CL7	OBD-CAD	2.41	1.25	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	8	402	8CT	C22-C21	2.40	1.55	1.50
21	c	504	CL7	OBD-CAD	2.40	1.25	1.22
21	B	605	CL7	C1C-NC	-2.40	1.34	1.37
21	b	606	CL7	C1C-NC	-2.40	1.34	1.37
21	B	605	CL7	OBD-CAD	2.40	1.25	1.22
21	b	606	CL7	OBD-CAD	2.40	1.25	1.22
21	2	508	CL7	C1C-C2C	-2.40	1.40	1.45
21	6	508	CL7	C1C-C2C	-2.40	1.40	1.45
21	2	514	CL7	OBD-CAD	2.40	1.25	1.22
23	K	101	8CT	C01-C02	2.40	1.54	1.50
23	k	101	8CT	C01-C02	2.40	1.54	1.50
21	C	514	CL7	C4C-NC	-2.40	1.34	1.37
23	A	404	8CT	C01-C02	2.40	1.54	1.50
21	2	516	CL7	OBD-CAD	2.40	1.25	1.22
21	6	516	CL7	OBD-CAD	2.40	1.25	1.22
21	B	613	CL7	C2A-C1A	2.39	1.54	1.50
21	b	614	CL7	C2A-C1A	2.39	1.54	1.50
21	4	413	CL7	OBD-CAD	2.39	1.25	1.22
21	8	413	CL7	OBD-CAD	2.39	1.25	1.22
21	C	503	CL7	OBD-CAD	2.39	1.25	1.22
21	c	503	CL7	OBD-CAD	2.39	1.25	1.22
21	C	512	CL7	C1D-ND	2.39	1.37	1.35
21	c	512	CL7	C1D-ND	2.39	1.37	1.35
21	5	418	CL7	C1C-NC	-2.39	1.34	1.37
21	6	505	CL7	OBD-CAD	2.39	1.25	1.22
21	4	407	CL7	C4C-NC	-2.39	1.34	1.37
21	8	407	CL7	C4C-NC	-2.39	1.34	1.37
21	B	601	CL7	C1D-ND	2.38	1.37	1.35
21	B	613	CL7	C1C-NC	-2.38	1.34	1.37
21	b	614	CL7	C1C-NC	-2.38	1.34	1.37
21	2	516	CL7	C1C-NC	-2.38	1.34	1.37
21	6	516	CL7	C1C-NC	-2.38	1.34	1.37
21	3	514	CL7	C4C-NC	-2.38	1.34	1.37
21	7	514	CL7	C4C-NC	-2.38	1.34	1.37
21	2	507	CL7	OBD-CAD	2.38	1.25	1.22
23	a	404	8CT	C01-C02	2.37	1.54	1.50
21	2	505	CL7	OBD-CAD	2.37	1.25	1.22
21	3	515	CL7	C1D-ND	2.37	1.37	1.35
21	7	515	CL7	C1D-ND	2.37	1.37	1.35
21	1	417	CL7	C2A-C1A	2.37	1.54	1.50
21	5	417	CL7	C2A-C1A	2.37	1.54	1.50
21	4	416	CL7	C4C-NC	-2.37	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	8	416	CL7	C4C-NC	-2.37	1.34	1.37
21	1	409	CL7	C4C-NC	-2.37	1.34	1.37
21	5	409	CL7	C4C-NC	-2.37	1.34	1.37
21	C	506	CL7	OBD-CAD	2.37	1.25	1.22
21	c	506	CL7	OBD-CAD	2.37	1.25	1.22
21	B	610	CL7	C2A-C1A	2.37	1.54	1.50
21	3	518	CL7	C1D-ND	2.37	1.37	1.35
21	7	518	CL7	C1D-ND	2.37	1.37	1.35
21	2	503	CL7	C1D-ND	2.37	1.37	1.35
21	6	503	CL7	C1D-ND	2.37	1.37	1.35
23	4	402	8CT	C01-C02	2.36	1.54	1.50
23	8	402	8CT	C01-C02	2.36	1.54	1.50
21	b	602	CL7	C1D-ND	2.36	1.37	1.35
21	A	406	CL7	OBD-CAD	2.36	1.25	1.22
21	a	405	CL7	OBD-CAD	2.36	1.25	1.22
21	2	503	CL7	C1C-NC	-2.36	1.34	1.37
21	b	603	CL7	OBD-CAD	2.36	1.25	1.22
23	4	402	8CT	C22-C21	2.36	1.55	1.50
21	b	609	CL7	OBD-CAD	2.36	1.25	1.22
21	b	611	CL7	C2A-C1A	2.36	1.54	1.50
21	5	410	CL7	C1D-ND	2.36	1.37	1.35
21	1	419	CL7	C4C-NC	-2.35	1.34	1.37
21	5	419	CL7	C4C-NC	-2.35	1.34	1.37
23	B	618	8CT	C22-C21	2.35	1.55	1.50
23	b	619	8CT	C22-C21	2.35	1.55	1.50
21	B	606	CL7	OBD-CAD	2.35	1.25	1.22
21	b	607	CL7	OBD-CAD	2.35	1.25	1.22
21	7	511	CL7	OBD-CAD	2.35	1.25	1.22
21	2	509	CL7	C2A-C1A	2.35	1.54	1.50
21	6	509	CL7	C2A-C1A	2.35	1.54	1.50
21	A	403	CL7	OBD-CAD	2.35	1.25	1.22
21	B	611	CL7	OBD-CAD	2.35	1.25	1.22
21	a	403	CL7	OBD-CAD	2.35	1.25	1.22
21	b	612	CL7	OBD-CAD	2.35	1.25	1.22
23	D	406	8CT	C22-C21	2.35	1.55	1.50
23	d	406	8CT	C22-C21	2.35	1.55	1.50
21	1	415	CL7	C4B-NB	2.35	1.37	1.35
21	5	415	CL7	C4B-NB	2.35	1.37	1.35
31	F	101	HEM	C4B-NB	-2.35	1.34	1.38
31	f	101	HEM	C4B-NB	-2.35	1.34	1.38
23	D	406	8CT	C01-C02	2.34	1.54	1.50
23	d	406	8CT	C01-C02	2.34	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	513	CL7	C1C-C2C	-2.34	1.40	1.45
21	6	513	CL7	C1C-C2C	-2.34	1.40	1.45
21	3	514	CL7	C1C-NC	-2.34	1.34	1.37
21	7	514	CL7	C1C-NC	-2.34	1.34	1.37
21	B	602	CL7	OBD-CAD	2.34	1.25	1.22
21	C	502	CL7	OBD-CAD	2.34	1.25	1.22
21	c	502	CL7	OBD-CAD	2.34	1.25	1.22
21	C	504	CL7	OBD-CAD	2.34	1.25	1.22
21	6	507	CL7	C1C-C2C	-2.34	1.40	1.45
21	1	409	CL7	C1D-ND	2.34	1.37	1.35
21	5	409	CL7	C1D-ND	2.34	1.37	1.35
21	3	511	CL7	OBD-CAD	2.33	1.25	1.22
21	C	508	CL7	C1C-C2C	-2.33	1.40	1.45
21	c	508	CL7	C1C-C2C	-2.33	1.40	1.45
21	B	608	CL7	OBD-CAD	2.33	1.25	1.22
21	2	509	CL7	OBD-CAD	2.33	1.25	1.22
21	6	509	CL7	OBD-CAD	2.33	1.25	1.22
23	B	617	8CT	C01-C02	2.33	1.54	1.50
21	C	503	CL7	C1C-C2C	-2.33	1.40	1.45
21	c	503	CL7	C1C-C2C	-2.33	1.40	1.45
21	2	515	CL7	C4C-NC	-2.33	1.34	1.37
21	6	515	CL7	C4C-NC	-2.33	1.34	1.37
21	6	503	CL7	C1C-NC	-2.33	1.34	1.37
23	b	618	8CT	C01-C02	2.32	1.54	1.50
21	2	515	CL7	C1D-ND	2.32	1.37	1.35
21	2	507	CL7	C1C-C2C	-2.32	1.40	1.45
21	1	418	CL7	C1C-NC	-2.32	1.34	1.37
21	5	404	CL7	C1D-ND	2.31	1.37	1.35
21	2	506	CL7	C1C-NC	-2.31	1.34	1.37
21	6	506	CL7	C1C-NC	-2.31	1.34	1.37
23	d	406	8CT	C38-C31	2.31	1.54	1.50
21	1	404	CL7	C1D-ND	2.31	1.37	1.35
21	C	503	CL7	C1C-NC	-2.31	1.34	1.37
21	c	503	CL7	C1C-NC	-2.31	1.34	1.37
32	3	522	ZEX	C1-C6	-2.30	1.50	1.53
32	7	522	ZEX	C1-C6	-2.30	1.50	1.53
21	B	604	CL7	C1C-C2C	-2.30	1.40	1.45
21	b	605	CL7	C1C-C2C	-2.30	1.40	1.45
21	2	514	CL7	C1C-C2C	-2.30	1.40	1.45
21	B	610	CL7	C1C-NC	-2.30	1.35	1.37
21	b	611	CL7	C1C-NC	-2.30	1.35	1.37
23	C	516	8CT	C22-C21	2.30	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	516	8CT	C22-C21	2.30	1.55	1.50
21	8	405	CL7	OBD-CAD	2.29	1.25	1.22
21	B	615	CL7	C1C-NC	-2.29	1.35	1.37
21	b	616	CL7	C1C-NC	-2.29	1.35	1.37
32	3	522	ZEX	C10-C9	-2.29	1.32	1.35
32	7	522	ZEX	C10-C9	-2.29	1.32	1.35
21	4	409	CL7	OBD-CAD	2.29	1.25	1.22
21	B	611	CL7	C1C-NC	-2.29	1.35	1.37
21	b	612	CL7	C1C-NC	-2.29	1.35	1.37
21	8	409	CL7	OBD-CAD	2.29	1.25	1.22
21	C	514	CL7	C1D-ND	2.29	1.37	1.35
21	c	514	CL7	C1D-ND	2.29	1.37	1.35
23	B	618	8CT	C01-C02	2.29	1.54	1.50
23	b	619	8CT	C01-C02	2.29	1.54	1.50
32	6	520	ZEX	C21-C26	-2.29	1.50	1.53
21	3	508	CL7	OBD-CAD	2.29	1.25	1.22
21	4	405	CL7	OBD-CAD	2.29	1.25	1.22
21	7	508	CL7	OBD-CAD	2.29	1.25	1.22
21	6	515	CL7	C1D-ND	2.29	1.37	1.35
21	C	513	CL7	OBD-CAD	2.28	1.25	1.22
21	c	513	CL7	OBD-CAD	2.28	1.25	1.22
21	B	605	CL7	C1D-ND	2.28	1.37	1.35
21	3	516	CL7	C2A-C1A	2.28	1.54	1.50
21	7	516	CL7	C2A-C1A	2.28	1.54	1.50
21	C	506	CL7	C1C-C2C	-2.28	1.40	1.45
21	c	506	CL7	C1C-C2C	-2.28	1.40	1.45
21	B	610	CL7	OBD-CAD	2.28	1.25	1.22
21	b	611	CL7	OBD-CAD	2.28	1.25	1.22
21	4	404	CL7	C1C-C2C	-2.28	1.40	1.45
21	8	404	CL7	C1C-C2C	-2.28	1.40	1.45
21	A	401	CL7	CAA-C2A	-2.28	1.49	1.54
21	3	511	CL7	C1C-C2C	-2.28	1.40	1.45
21	7	511	CL7	C1C-C2C	-2.28	1.40	1.45
21	A	406	CL7	C1C-NC	-2.28	1.35	1.37
21	a	405	CL7	C1C-NC	-2.28	1.35	1.37
21	a	401	CL7	CAA-C2A	-2.27	1.49	1.54
21	B	606	CL7	C1C-C2C	-2.27	1.40	1.45
21	b	607	CL7	C1C-C2C	-2.27	1.40	1.45
23	D	406	8CT	C38-C31	2.27	1.54	1.50
21	C	502	CL7	C1D-ND	2.27	1.37	1.35
21	3	516	CL7	C1C-C2C	-2.27	1.40	1.45
21	7	516	CL7	C1C-C2C	-2.27	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	510	CL7	C1C-NC	-2.27	1.35	1.37
32	3	519	ZEX	C10-C9	-2.27	1.32	1.35
32	7	519	ZEX	C10-C9	-2.27	1.32	1.35
21	B	605	CL7	C1C-C2C	-2.27	1.40	1.45
21	b	606	CL7	C1C-C2C	-2.27	1.40	1.45
21	C	507	CL7	C1C-NC	-2.26	1.35	1.37
21	1	409	CL7	C1C-C2C	-2.26	1.40	1.45
21	5	409	CL7	C1C-C2C	-2.26	1.40	1.45
21	1	413	CL7	C1D-ND	2.26	1.37	1.35
21	3	509	CL7	OBD-CAD	2.26	1.25	1.22
21	7	509	CL7	OBD-CAD	2.26	1.25	1.22
21	4	412	CL7	C1C-NC	-2.26	1.35	1.37
32	8	418	ZEX	C21-C26	-2.26	1.50	1.53
21	7	510	CL7	C1C-NC	-2.26	1.35	1.37
23	d	406	8CT	C30-C29	2.26	1.53	1.50
21	6	514	CL7	C1C-C2C	-2.26	1.40	1.45
21	B	605	CL7	C2A-C1A	2.26	1.54	1.50
21	b	606	CL7	C2A-C1A	2.26	1.54	1.50
21	1	414	CL7	C4C-NC	-2.26	1.35	1.37
21	5	414	CL7	C4C-NC	-2.26	1.35	1.37
21	A	401	CL7	C4B-NB	2.26	1.37	1.35
21	a	401	CL7	C4B-NB	2.26	1.37	1.35
21	2	509	CL7	C1C-NC	-2.26	1.35	1.37
21	3	504	CL7	C1C-NC	-2.25	1.35	1.37
21	3	506	CL7	C1C-NC	-2.25	1.35	1.37
21	7	504	CL7	C1C-NC	-2.25	1.35	1.37
21	7	506	CL7	C1C-NC	-2.25	1.35	1.37
21	4	412	CL7	OBD-CAD	2.25	1.25	1.22
21	8	412	CL7	OBD-CAD	2.25	1.25	1.22
21	3	501	CL7	C1C-NC	-2.25	1.35	1.37
21	B	614	CL7	C1C-C2C	-2.25	1.40	1.45
21	2	506	CL7	C1C-C2C	-2.25	1.40	1.45
21	6	506	CL7	C1C-C2C	-2.25	1.40	1.45
21	1	402	CL7	C1C-NC	-2.24	1.35	1.37
21	5	402	CL7	C1C-NC	-2.24	1.35	1.37
23	D	406	8CT	C30-C29	2.24	1.53	1.50
21	2	514	CL7	C1D-ND	2.24	1.37	1.35
21	4	408	CL7	C1D-ND	2.24	1.37	1.35
21	6	514	CL7	C1D-ND	2.24	1.37	1.35
21	8	408	CL7	C1D-ND	2.24	1.37	1.35
21	2	507	CL7	C1C-NC	-2.24	1.35	1.37
21	7	514	CL7	C1D-ND	2.24	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	512	CL7	C1C-NC	-2.24	1.35	1.37
21	7	512	CL7	C1C-NC	-2.24	1.35	1.37
32	2	521	ZEX	C21-C26	-2.23	1.50	1.53
21	2	502	CL7	OBD-CAD	2.23	1.25	1.22
21	6	502	CL7	OBD-CAD	2.23	1.25	1.22
32	2	520	ZEX	C14-C13	-2.23	1.32	1.35
32	3	525	ZEX	C14-C13	-2.23	1.32	1.35
21	4	404	CL7	C1C-NC	-2.23	1.35	1.37
21	8	404	CL7	C1C-NC	-2.23	1.35	1.37
23	c	519	8CT	C38-C31	2.23	1.54	1.50
21	8	417	CL7	C1D-ND	2.23	1.37	1.35
21	3	511	CL7	C1C-NC	-2.23	1.35	1.37
21	7	511	CL7	C1C-NC	-2.23	1.35	1.37
21	A	406	CL7	C1C-C2C	-2.23	1.40	1.45
21	a	405	CL7	C1C-C2C	-2.23	1.40	1.45
21	2	507	CL7	CBD-CGD	-2.22	1.45	1.52
21	6	507	CL7	CBD-CGD	-2.22	1.45	1.52
21	4	417	CL7	C1D-ND	2.22	1.37	1.35
23	B	619	8CT	C22-C21	2.22	1.55	1.50
23	b	620	8CT	C22-C21	2.22	1.55	1.50
21	c	502	CL7	C1D-ND	2.22	1.37	1.35
21	d	405	CL7	C1C-C2C	-2.22	1.40	1.45
21	7	504	CL7	C1C-C2C	-2.22	1.40	1.45
21	3	507	CL7	OBD-CAD	2.22	1.25	1.22
21	7	507	CL7	OBD-CAD	2.22	1.25	1.22
21	b	615	CL7	C1C-C2C	-2.22	1.41	1.45
23	A	404	8CT	C22-C21	2.21	1.55	1.50
21	B	614	CL7	C1C-NC	-2.21	1.35	1.37
21	C	510	CL7	C1C-NC	-2.21	1.35	1.37
21	b	615	CL7	C1C-NC	-2.21	1.35	1.37
21	c	510	CL7	C1C-NC	-2.21	1.35	1.37
32	4	418	ZEX	C21-C26	-2.21	1.50	1.53
21	c	507	CL7	C1C-NC	-2.21	1.35	1.37
21	2	516	CL7	C1C-C2C	-2.21	1.41	1.45
21	6	516	CL7	C1C-C2C	-2.21	1.41	1.45
21	7	501	CL7	C1C-NC	-2.21	1.35	1.37
21	3	502	CL7	OBD-CAD	2.21	1.25	1.22
21	7	502	CL7	OBD-CAD	2.21	1.25	1.22
21	2	504	CL7	C1C-C2C	-2.21	1.41	1.45
32	2	525	ZEX	C1-C6	-2.21	1.50	1.53
32	6	524	ZEX	C1-C6	-2.21	1.50	1.53
21	6	507	CL7	C1C-NC	-2.21	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	404	8CT	C22-C21	2.21	1.55	1.50
23	B	617	8CT	C22-C21	2.21	1.55	1.50
23	b	618	8CT	C22-C21	2.21	1.55	1.50
21	B	604	CL7	OBD-CAD	2.21	1.25	1.22
21	3	504	CL7	C1C-C2C	-2.20	1.41	1.45
21	2	510	CL7	C1C-NC	-2.20	1.35	1.37
21	6	510	CL7	C1C-NC	-2.20	1.35	1.37
21	1	408	CL7	C4C-NC	-2.20	1.35	1.37
21	5	408	CL7	C4C-NC	-2.20	1.35	1.37
23	C	519	8CT	C38-C31	2.20	1.54	1.50
21	b	605	CL7	OBD-CAD	2.20	1.25	1.22
21	8	412	CL7	C1C-NC	-2.20	1.35	1.37
21	3	510	CL7	C1C-C2C	-2.20	1.41	1.45
21	7	510	CL7	C1C-C2C	-2.20	1.41	1.45
21	3	510	CL7	OBD-CAD	2.20	1.25	1.22
21	7	510	CL7	OBD-CAD	2.20	1.25	1.22
21	D	405	CL7	C1C-NC	-2.20	1.35	1.37
21	1	416	CL7	C4C-NC	-2.20	1.35	1.37
21	2	502	CL7	C1C-C2C	-2.20	1.41	1.45
21	6	502	CL7	C1C-C2C	-2.20	1.41	1.45
21	4	410	CL7	C1C-C2C	-2.20	1.41	1.45
21	B	603	CL7	C1C-C2C	-2.20	1.41	1.45
21	b	604	CL7	C1C-C2C	-2.20	1.41	1.45
21	1	408	CL7	C1D-ND	2.19	1.37	1.35
21	5	408	CL7	C1D-ND	2.19	1.37	1.35
21	2	518	CL7	C1D-ND	2.19	1.37	1.35
21	6	518	CL7	C1D-ND	2.19	1.37	1.35
21	3	503	CL7	C1C-NC	-2.19	1.35	1.37
21	7	503	CL7	C1C-NC	-2.19	1.35	1.37
32	4	403	ZEX	C14-C13	-2.19	1.32	1.35
21	6	504	CL7	C1C-C2C	-2.19	1.41	1.45
21	b	609	CL7	C1C-C2C	-2.19	1.41	1.45
21	d	405	CL7	C1C-NC	-2.19	1.35	1.37
21	6	509	CL7	C1C-NC	-2.19	1.35	1.37
21	3	503	CL7	C1D-ND	2.19	1.37	1.35
21	7	503	CL7	C1D-ND	2.19	1.37	1.35
21	2	510	CL7	C1C-C2C	-2.19	1.41	1.45
21	6	510	CL7	C1C-C2C	-2.19	1.41	1.45
21	C	508	CL7	OBD-CAD	2.19	1.25	1.22
21	c	508	CL7	OBD-CAD	2.19	1.25	1.22
21	B	604	CL7	C1C-NC	-2.19	1.35	1.37
21	b	605	CL7	C1C-NC	-2.19	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	5	413	CL7	C1D-ND	2.18	1.37	1.35
21	4	409	CL7	C1C-C2C	-2.18	1.41	1.45
21	b	610	CL7	C1C-C2C	-2.18	1.41	1.45
21	8	409	CL7	C1C-C2C	-2.18	1.41	1.45
21	D	405	CL7	C1C-C2C	-2.18	1.41	1.45
21	3	512	CL7	OBD-CAD	2.18	1.25	1.22
21	7	512	CL7	OBD-CAD	2.18	1.25	1.22
21	C	509	CL7	C1C-C2C	-2.18	1.41	1.45
21	c	509	CL7	C1C-C2C	-2.18	1.41	1.45
21	B	608	CL7	C1C-C2C	-2.18	1.41	1.45
21	2	506	CL7	C1D-ND	2.18	1.37	1.35
31	F	101	HEM	C1D-ND	-2.18	1.34	1.38
21	B	616	CL7	C1C-NC	-2.18	1.35	1.37
21	b	617	CL7	C1C-NC	-2.18	1.35	1.37
21	B	612	CL7	C1C-C2C	-2.18	1.41	1.45
21	b	613	CL7	C1C-C2C	-2.18	1.41	1.45
21	4	413	CL7	C1C-NC	-2.17	1.35	1.37
21	8	413	CL7	C1C-NC	-2.17	1.35	1.37
21	D	402	CL7	C1D-ND	2.17	1.37	1.35
21	1	412	CL7	C1D-ND	2.17	1.37	1.35
21	d	402	CL7	C1D-ND	2.17	1.37	1.35
21	5	412	CL7	C1D-ND	2.17	1.37	1.35
21	1	407	CL7	C1D-ND	2.17	1.37	1.35
21	5	407	CL7	C1D-ND	2.17	1.37	1.35
23	C	516	8CT	C01-C02	2.17	1.54	1.50
23	c	516	8CT	C01-C02	2.17	1.54	1.50
21	6	513	CL7	C1D-ND	2.17	1.37	1.35
21	3	504	CL7	OBD-CAD	2.17	1.25	1.22
21	B	613	CL7	CBD-CGD	-2.17	1.45	1.52
21	b	614	CL7	CBD-CGD	-2.17	1.45	1.52
31	f	101	HEM	C1D-ND	-2.17	1.34	1.38
21	7	504	CL7	OBD-CAD	2.17	1.25	1.22
21	4	411	CL7	C1C-NC	-2.17	1.35	1.37
21	8	411	CL7	C1C-NC	-2.17	1.35	1.37
21	c	502	CL7	C1C-NC	-2.17	1.35	1.37
23	B	617	8CT	C39-C16	2.16	1.55	1.50
23	b	618	8CT	C39-C16	2.16	1.55	1.50
31	F	101	HEM	FE-ND	-2.16	1.86	1.96
31	f	101	HEM	FE-ND	-2.16	1.86	1.96
21	C	509	CL7	C2A-C1A	2.16	1.54	1.50
21	6	505	CL7	C1C-C2C	-2.16	1.41	1.45
23	K	101	8CT	C10-C03	2.16	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	k	101	8CT	C10-C03	2.16	1.52	1.45
21	7	505	CL7	C1C-C2C	-2.16	1.41	1.45
21	8	410	CL7	C1C-C2C	-2.16	1.41	1.45
21	A	401	CL7	C4D-ND	2.16	1.37	1.35
21	a	401	CL7	C4D-ND	2.16	1.37	1.35
21	3	514	CL7	C1D-ND	2.15	1.37	1.35
21	3	517	CL7	C1C-C2C	-2.15	1.41	1.45
21	7	517	CL7	C1C-C2C	-2.15	1.41	1.45
21	C	502	CL7	C1C-NC	-2.15	1.35	1.37
21	4	409	CL7	C1C-NC	-2.15	1.35	1.37
21	B	607	CL7	C1C-NC	-2.15	1.35	1.37
21	5	416	CL7	C4C-NC	-2.15	1.35	1.37
23	k	101	8CT	C39-C16	2.14	1.55	1.50
21	1	402	CL7	C1D-ND	2.14	1.37	1.35
21	5	402	CL7	C1D-ND	2.14	1.37	1.35
21	B	609	CL7	C1C-C2C	-2.14	1.41	1.45
23	b	618	8CT	C38-C31	2.14	1.54	1.50
23	K	101	8CT	C39-C16	2.14	1.55	1.50
21	3	505	CL7	C1C-C2C	-2.14	1.41	1.45
21	1	405	CL7	C1D-ND	2.14	1.37	1.35
21	5	405	CL7	C1D-ND	2.14	1.37	1.35
21	1	417	CL7	C1C-NC	-2.14	1.35	1.37
21	5	417	CL7	C1C-NC	-2.14	1.35	1.37
21	2	505	CL7	C1C-NC	-2.14	1.35	1.37
21	C	510	CL7	CBD-CGD	-2.14	1.45	1.52
21	c	510	CL7	CBD-CGD	-2.14	1.45	1.52
32	2	525	ZEX	C30-C29	-2.14	1.32	1.35
32	6	524	ZEX	C30-C29	-2.14	1.32	1.35
21	c	518	CL7	C1C-C2C	-2.14	1.41	1.45
21	B	622	CL7	C4C-NC	-2.14	1.35	1.37
23	B	617	8CT	C30-C29	2.14	1.53	1.50
23	b	618	8CT	C30-C29	2.14	1.53	1.50
21	b	608	CL7	C1C-NC	-2.14	1.35	1.37
21	B	613	CL7	C1C-C2C	-2.13	1.41	1.45
32	2	520	ZEX	C10-C9	-2.13	1.33	1.35
32	3	525	ZEX	C10-C9	-2.13	1.33	1.35
21	C	506	CL7	CBD-CGD	-2.13	1.45	1.52
21	c	506	CL7	CBD-CGD	-2.13	1.45	1.52
21	C	510	CL7	OBD-CAD	2.13	1.25	1.22
21	c	510	CL7	OBD-CAD	2.13	1.25	1.22
24	b	621	SQD	O8-S	2.13	1.55	1.47
21	2	505	CL7	C1C-C2C	-2.13	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	507	CL7	CBD-CGD	-2.13	1.45	1.52
21	7	507	CL7	CBD-CGD	-2.13	1.45	1.52
21	6	506	CL7	C1D-ND	2.13	1.37	1.35
21	C	518	CL7	C1C-C2C	-2.13	1.41	1.45
32	2	523	ZEX	C34-C33	-2.13	1.33	1.35
32	6	522	ZEX	C34-C33	-2.13	1.33	1.35
21	4	417	CL7	C4C-NC	-2.13	1.35	1.37
21	8	417	CL7	C4C-NC	-2.13	1.35	1.37
21	4	414	CL7	C1C-NC	-2.12	1.35	1.37
21	3	513	CL7	C1D-ND	2.12	1.37	1.35
21	7	513	CL7	C1D-ND	2.12	1.37	1.35
21	8	409	CL7	C1C-NC	-2.12	1.35	1.37
24	1	423	SQD	O8-S	2.12	1.55	1.47
21	3	501	CL7	C1C-C2C	-2.12	1.41	1.45
21	6	505	CL7	C1C-NC	-2.12	1.35	1.37
21	3	513	CL7	C1C-C2C	-2.12	1.41	1.45
21	7	513	CL7	C1C-C2C	-2.12	1.41	1.45
24	5	423	SQD	O8-S	2.12	1.55	1.47
21	7	501	CL7	C1C-C2C	-2.12	1.41	1.45
21	4	407	CL7	C1D-ND	2.12	1.37	1.35
21	2	502	CL7	C1C-NC	-2.11	1.35	1.37
21	6	502	CL7	C1C-NC	-2.11	1.35	1.37
24	B	620	SQD	O8-S	2.11	1.55	1.47
21	c	509	CL7	C2A-C1A	2.11	1.54	1.50
23	B	619	8CT	C38-C31	2.11	1.54	1.50
23	b	620	8CT	C38-C31	2.11	1.54	1.50
21	b	614	CL7	C1C-C2C	-2.11	1.41	1.45
21	2	509	CL7	C1C-C2C	-2.11	1.41	1.45
21	6	509	CL7	C1C-C2C	-2.11	1.41	1.45
23	B	627	8CT	C39-C16	2.11	1.55	1.50
21	d	404	CL7	C1C-NC	-2.11	1.35	1.37
21	4	408	CL7	CBD-CGD	-2.11	1.45	1.52
21	8	408	CL7	CBD-CGD	-2.11	1.45	1.52
21	2	504	CL7	C1C-NC	-2.11	1.35	1.37
21	6	504	CL7	C1C-NC	-2.11	1.35	1.37
21	B	611	CL7	CBD-CGD	-2.11	1.45	1.52
21	b	612	CL7	CBD-CGD	-2.11	1.45	1.52
21	1	406	CL7	C1C-C2C	-2.10	1.41	1.45
21	5	406	CL7	C1C-C2C	-2.10	1.41	1.45
21	C	506	CL7	C1C-NC	-2.10	1.35	1.37
21	c	506	CL7	C1C-NC	-2.10	1.35	1.37
23	B	627	8CT	C10-C03	2.10	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	4	415	CL7	CBD-CGD	-2.10	1.45	1.52
21	8	415	CL7	CBD-CGD	-2.10	1.45	1.52
32	8	403	ZEX	C14-C13	-2.10	1.33	1.35
21	b	623	CL7	C4C-NC	-2.10	1.35	1.37
21	7	506	CL7	C1D-ND	2.10	1.37	1.35
21	D	404	CL7	OBD-CAD	2.10	1.25	1.22
21	d	404	CL7	OBD-CAD	2.10	1.25	1.22
24	A	405	SQD	O8-S	2.10	1.55	1.47
24	B	626	SQD	O8-S	2.10	1.55	1.47
23	b	601	8CT	C39-C16	2.10	1.55	1.50
21	3	502	CL7	C1D-ND	2.10	1.37	1.35
21	7	502	CL7	C1D-ND	2.10	1.37	1.35
23	B	617	8CT	C38-C31	2.10	1.54	1.50
21	B	603	CL7	C1C-NC	-2.10	1.35	1.37
21	b	604	CL7	C1C-NC	-2.10	1.35	1.37
21	1	408	CL7	C1C-C2C	-2.10	1.41	1.45
21	3	514	CL7	C1C-C2C	-2.10	1.41	1.45
21	5	408	CL7	C1C-C2C	-2.10	1.41	1.45
21	7	514	CL7	C1C-C2C	-2.10	1.41	1.45
32	2	521	ZEX	C30-C29	-2.10	1.33	1.35
32	6	520	ZEX	C30-C29	-2.10	1.33	1.35
21	B	613	CL7	OBD-CAD	2.10	1.25	1.22
21	b	614	CL7	OBD-CAD	2.10	1.25	1.22
21	5	403	CL7	C1C-NC	-2.10	1.35	1.37
21	C	510	CL7	C1C-C2C	-2.09	1.41	1.45
21	c	510	CL7	C1C-C2C	-2.09	1.41	1.45
32	4	420	ZEX	C10-C9	-2.09	1.33	1.35
32	8	420	ZEX	C10-C9	-2.09	1.33	1.35
21	1	417	CL7	C1D-ND	2.09	1.37	1.35
21	5	417	CL7	C1D-ND	2.09	1.37	1.35
21	1	415	CL7	C4C-NC	-2.09	1.35	1.37
23	b	601	8CT	C10-C03	2.09	1.52	1.45
21	A	403	CL7	CBD-CGD	-2.09	1.45	1.52
21	C	508	CL7	C1C-NC	-2.09	1.35	1.37
21	2	508	CL7	C1C-NC	-2.09	1.35	1.37
21	c	508	CL7	C1C-NC	-2.09	1.35	1.37
21	6	508	CL7	C1C-NC	-2.09	1.35	1.37
21	3	502	CL7	C1C-C2C	-2.09	1.41	1.45
21	7	502	CL7	C1C-C2C	-2.09	1.41	1.45
21	1	415	CL7	C3A-C2A	2.09	1.56	1.54
21	5	415	CL7	C3A-C2A	2.09	1.56	1.54
21	7	512	CL7	C1C-C2C	-2.09	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	519	8CT	C22-C21	2.09	1.55	1.50
23	c	519	8CT	C22-C21	2.09	1.55	1.50
21	a	403	CL7	CBD-CGD	-2.09	1.45	1.52
21	3	511	CL7	C1D-ND	2.09	1.37	1.35
21	7	511	CL7	C1D-ND	2.09	1.37	1.35
32	2	521	ZEX	C1-C6	-2.09	1.50	1.53
32	6	520	ZEX	C1-C6	-2.09	1.50	1.53
32	4	403	ZEX	C34-C33	-2.09	1.33	1.35
32	8	403	ZEX	C34-C33	-2.09	1.33	1.35
21	2	512	CL7	OBD-CAD	2.09	1.25	1.22
21	6	512	CL7	OBD-CAD	2.09	1.25	1.22
21	1	407	CL7	C1C-C2C	-2.09	1.41	1.45
21	4	405	CL7	C1C-C2C	-2.09	1.41	1.45
21	5	407	CL7	C1C-C2C	-2.09	1.41	1.45
21	C	509	CL7	C1C-NC	-2.09	1.35	1.37
21	c	509	CL7	C1C-NC	-2.09	1.35	1.37
21	3	512	CL7	C1C-C2C	-2.09	1.41	1.45
21	2	513	CL7	C1D-ND	2.08	1.37	1.35
21	b	609	CL7	C1C-NC	-2.08	1.35	1.37
21	5	415	CL7	C4C-NC	-2.08	1.35	1.37
21	B	607	CL7	C1C-C2C	-2.08	1.41	1.45
21	b	608	CL7	C1C-C2C	-2.08	1.41	1.45
21	4	416	CL7	C1D-ND	2.08	1.37	1.35
21	8	416	CL7	C1D-ND	2.08	1.37	1.35
21	4	411	CL7	OBD-CAD	2.07	1.25	1.22
21	8	411	CL7	OBD-CAD	2.07	1.25	1.22
21	B	616	CL7	CBD-CGD	-2.07	1.45	1.52
21	b	617	CL7	CBD-CGD	-2.07	1.45	1.52
21	C	508	CL7	CBD-CGD	-2.07	1.45	1.52
21	c	508	CL7	CBD-CGD	-2.07	1.45	1.52
21	B	602	CL7	C1C-NC	-2.07	1.35	1.37
21	8	409	CL7	CBD-CGD	-2.07	1.45	1.52
32	4	403	ZEX	C1-C6	-2.07	1.50	1.53
32	8	403	ZEX	C1-C6	-2.07	1.50	1.53
21	3	506	CL7	C1D-ND	2.07	1.37	1.35
21	B	608	CL7	C1C-NC	-2.07	1.35	1.37
21	C	503	CL7	CBD-CGD	-2.07	1.45	1.52
21	c	503	CL7	CBD-CGD	-2.07	1.45	1.52
21	B	612	CL7	OBD-CAD	2.07	1.25	1.22
21	b	613	CL7	OBD-CAD	2.07	1.25	1.22
32	8	419	ZEX	C34-C33	-2.07	1.33	1.35
21	B	609	CL7	C1D-ND	2.06	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	b	610	CL7	C1D-ND	2.06	1.37	1.35
21	3	513	CL7	CBD-CGD	-2.06	1.45	1.52
21	7	513	CL7	CBD-CGD	-2.06	1.45	1.52
23	B	627	8CT	C28-C29	2.06	1.37	1.32
23	b	601	8CT	C28-C29	2.06	1.37	1.32
21	8	414	CL7	C1C-NC	-2.06	1.35	1.37
32	3	519	ZEX	C30-C29	-2.06	1.33	1.35
32	7	519	ZEX	C30-C29	-2.06	1.33	1.35
21	2	517	CL7	OBD-CAD	2.06	1.25	1.22
21	6	517	CL7	OBD-CAD	2.06	1.25	1.22
21	8	405	CL7	C1C-C2C	-2.06	1.41	1.45
23	B	617	8CT	C10-C03	2.06	1.52	1.45
23	b	618	8CT	C10-C03	2.06	1.52	1.45
21	4	414	CL7	C1C-C2C	-2.06	1.41	1.45
21	8	414	CL7	C1C-C2C	-2.06	1.41	1.45
24	2	524	SQD	O8-S	2.06	1.54	1.47
24	6	523	SQD	O8-S	2.06	1.54	1.47
21	4	405	CL7	C1D-ND	2.06	1.37	1.35
21	8	405	CL7	C1D-ND	2.06	1.37	1.35
21	1	404	CL7	C4C-NC	-2.06	1.35	1.37
21	5	404	CL7	C4C-NC	-2.06	1.35	1.37
23	C	515	8CT	C39-C16	2.06	1.55	1.50
23	c	515	8CT	C39-C16	2.06	1.55	1.50
21	4	415	CL7	C1D-ND	2.06	1.37	1.35
21	1	402	CL7	C1C-C2C	-2.06	1.41	1.45
21	5	402	CL7	C1C-C2C	-2.06	1.41	1.45
21	4	405	CL7	C1C-NC	-2.06	1.35	1.37
21	8	405	CL7	C1C-NC	-2.06	1.35	1.37
21	7	508	CL7	C1C-NC	-2.05	1.35	1.37
21	4	409	CL7	CBD-CGD	-2.05	1.46	1.52
21	5	411	CL7	C1D-ND	2.05	1.37	1.35
32	2	519	ZEX	C10-C9	-2.05	1.33	1.35
32	6	519	ZEX	C10-C9	-2.05	1.33	1.35
21	2	501	CL7	C1C-C2C	-2.05	1.41	1.45
21	6	501	CL7	C1C-C2C	-2.05	1.41	1.45
21	2	509	CL7	CBD-CGD	-2.05	1.46	1.52
21	1	405	CL7	C1C-C2C	-2.05	1.41	1.45
21	5	405	CL7	C1C-C2C	-2.05	1.41	1.45
21	B	616	CL7	C1C-C2C	-2.05	1.41	1.45
21	b	617	CL7	C1C-C2C	-2.05	1.41	1.45
21	4	408	CL7	C1C-C2C	-2.05	1.41	1.45
21	8	408	CL7	C1C-C2C	-2.05	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	3	508	CL7	CBD-CGD	-2.05	1.46	1.52
21	7	508	CL7	CBD-CGD	-2.05	1.46	1.52
21	B	610	CL7	C1C-C2C	-2.04	1.41	1.45
21	2	503	CL7	C1C-C2C	-2.04	1.41	1.45
21	b	611	CL7	C1C-C2C	-2.04	1.41	1.45
21	6	503	CL7	C1C-C2C	-2.04	1.41	1.45
21	8	415	CL7	C1C-C2C	-2.04	1.41	1.45
21	6	509	CL7	CBD-CGD	-2.04	1.46	1.52
21	D	404	CL7	C1C-NC	-2.04	1.35	1.37
21	1	411	CL7	C1D-ND	2.04	1.37	1.35
21	C	504	CL7	C1C-NC	-2.04	1.35	1.37
21	c	504	CL7	C1C-NC	-2.04	1.35	1.37
21	D	404	CL7	CBD-CGD	-2.04	1.46	1.52
21	d	404	CL7	CBD-CGD	-2.04	1.46	1.52
21	b	610	CL7	C1C-NC	-2.04	1.35	1.37
21	B	615	CL7	CBD-CGD	-2.04	1.46	1.52
21	b	616	CL7	CBD-CGD	-2.04	1.46	1.52
32	2	523	ZEX	C10-C9	-2.04	1.33	1.35
32	6	522	ZEX	C10-C9	-2.04	1.33	1.35
21	8	407	CL7	C1D-ND	2.04	1.37	1.35
21	3	517	CL7	C1C-NC	-2.04	1.35	1.37
21	1	403	CL7	C1C-NC	-2.04	1.35	1.37
23	B	618	8CT	C30-C29	2.03	1.53	1.50
21	4	408	CL7	C1C-NC	-2.03	1.35	1.37
21	3	508	CL7	C1C-NC	-2.03	1.35	1.37
21	3	503	CL7	CBD-CGD	-2.03	1.46	1.52
21	7	503	CL7	CBD-CGD	-2.03	1.46	1.52
21	7	517	CL7	C1C-NC	-2.03	1.35	1.37
21	c	504	CL7	CBD-CGD	-2.03	1.46	1.52
21	B	614	CL7	CBD-CGD	-2.03	1.46	1.52
21	b	615	CL7	CBD-CGD	-2.03	1.46	1.52
21	C	507	CL7	CBD-CGD	-2.03	1.46	1.52
21	C	504	CL7	C1D-ND	2.03	1.37	1.35
21	2	511	CL7	C1D-ND	2.03	1.37	1.35
21	c	504	CL7	C1D-ND	2.03	1.37	1.35
21	3	511	CL7	CBD-CGD	-2.03	1.46	1.52
21	7	511	CL7	CBD-CGD	-2.03	1.46	1.52
21	a	403	CL7	C1C-C2C	-2.03	1.41	1.45
21	c	507	CL7	CBD-CGD	-2.03	1.46	1.52
32	3	519	ZEX	C34-C33	-2.03	1.33	1.35
21	4	413	CL7	C1C-C2C	-2.03	1.41	1.45
21	8	413	CL7	C1C-C2C	-2.03	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	3	522	ZEX	C30-C29	-2.02	1.33	1.35
32	7	522	ZEX	C30-C29	-2.02	1.33	1.35
21	3	513	CL7	C1C-NC	-2.02	1.35	1.37
21	7	513	CL7	C1C-NC	-2.02	1.35	1.37
21	C	504	CL7	CBD-CGD	-2.02	1.46	1.52
21	B	601	CL7	C1C-C2C	-2.02	1.41	1.45
21	b	602	CL7	C1C-C2C	-2.02	1.41	1.45
21	b	603	CL7	C1C-NC	-2.02	1.35	1.37
21	6	514	CL7	C1C-NC	-2.02	1.35	1.37
21	1	410	CL7	C1C-C2C	-2.02	1.41	1.45
21	5	410	CL7	C1C-C2C	-2.02	1.41	1.45
21	3	507	CL7	C1C-C2C	-2.02	1.41	1.45
21	7	507	CL7	C1C-C2C	-2.02	1.41	1.45
21	2	508	CL7	C1D-ND	2.02	1.37	1.35
21	6	508	CL7	C1D-ND	2.02	1.37	1.35
21	8	412	CL7	C1C-C2C	-2.02	1.41	1.45
21	4	415	CL7	C1C-C2C	-2.02	1.41	1.45
21	A	403	CL7	C1C-C2C	-2.02	1.41	1.45
21	8	406	CL7	CBD-CGD	-2.02	1.46	1.52
21	c	505	CL7	C1C-C2C	-2.02	1.41	1.45
21	c	513	CL7	C1C-NC	-2.01	1.35	1.37
21	8	415	CL7	C1D-ND	2.01	1.37	1.35
24	2	522	SQD	O8-S	2.01	1.54	1.47
24	6	521	SQD	O8-S	2.01	1.54	1.47
21	1	417	CL7	CBD-CGD	-2.01	1.46	1.52
21	5	417	CL7	CBD-CGD	-2.01	1.46	1.52
32	6	524	ZEX	C14-C13	-2.01	1.33	1.35
23	D	406	8CT	C39-C16	2.01	1.55	1.50
23	d	406	8CT	C39-C16	2.01	1.55	1.50
21	A	401	CL7	C4C-NC	-2.01	1.35	1.37
21	a	401	CL7	C4C-NC	-2.01	1.35	1.37
23	B	619	8CT	C39-C16	2.01	1.55	1.50
23	b	620	8CT	C39-C16	2.01	1.55	1.50
21	7	518	CL7	C4B-NB	2.01	1.37	1.35
21	4	406	CL7	C1C-C2C	-2.01	1.41	1.45
32	4	419	ZEX	C34-C33	-2.01	1.33	1.35
21	8	408	CL7	C1C-NC	-2.01	1.35	1.37
21	2	517	CL7	C1C-NC	-2.01	1.35	1.37
21	6	517	CL7	C1C-NC	-2.01	1.35	1.37
23	c	515	8CT	C30-C29	2.00	1.53	1.50
21	8	413	CL7	CBD-CGD	-2.00	1.46	1.52
24	3	521	SQD	O8-S	2.00	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	7	521	SQD	O8-S	2.00	1.54	1.47
21	1	403	CL7	C1C-C2C	-2.00	1.41	1.45
21	5	403	CL7	C1C-C2C	-2.00	1.41	1.45
21	B	609	CL7	C1C-NC	-2.00	1.35	1.37
23	A	404	8CT	C39-C16	2.00	1.55	1.50
23	a	404	8CT	C39-C16	2.00	1.55	1.50
21	4	413	CL7	CBD-CGD	-2.00	1.46	1.52
21	8	406	CL7	C1C-C2C	-2.00	1.41	1.45
21	8	414	CL7	CBD-CGD	-2.00	1.46	1.52

All (4416) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	403	CL7	C3C-C4C-NC	10.55	117.83	110.18
21	a	403	CL7	C3C-C4C-NC	10.50	117.79	110.18
21	7	505	CL7	C3C-C4C-NC	10.29	117.64	110.18
21	3	505	CL7	C3C-C4C-NC	10.28	117.63	110.18
23	8	402	8CT	C33-C32-C31	-10.15	115.12	124.85
23	4	402	8CT	C33-C32-C31	-10.12	115.15	124.85
21	3	514	CL7	C3C-C4C-NC	10.01	117.43	110.18
21	7	514	CL7	C3C-C4C-NC	10.01	117.43	110.18
21	8	415	CL7	C3C-C4C-NC	9.96	117.40	110.18
21	4	415	CL7	C3C-C4C-NC	9.95	117.39	110.18
21	1	415	CL7	C3C-C4C-NC	9.82	117.29	110.18
21	3	511	CL7	C3C-C4C-NC	9.81	117.29	110.18
21	5	415	CL7	C3C-C4C-NC	9.81	117.29	110.18
21	7	511	CL7	C3C-C4C-NC	9.81	117.29	110.18
21	4	416	CL7	C3C-C4C-NC	9.76	117.25	110.18
21	8	416	CL7	C3C-C4C-NC	9.76	117.25	110.18
23	b	620	8CT	C33-C32-C31	-9.72	115.53	124.85
21	6	512	CL7	C3C-C4C-NC	9.71	117.22	110.18
21	1	414	CL7	C3C-C4C-NC	9.69	117.20	110.18
21	5	414	CL7	C3C-C4C-NC	9.69	117.20	110.18
21	2	512	CL7	C3C-C4C-NC	9.68	117.19	110.18
23	B	619	8CT	C33-C32-C31	-9.68	115.57	124.85
23	D	406	8CT	C33-C32-C31	-9.66	115.58	124.85
23	d	406	8CT	C33-C32-C31	-9.65	115.59	124.85
21	4	417	CL7	C3C-C4C-NC	9.65	117.17	110.18
21	5	420	CL7	C3C-C4C-NC	9.65	117.17	110.18
21	8	417	CL7	C3C-C4C-NC	9.65	117.17	110.18
21	1	420	CL7	C3C-C4C-NC	9.64	117.17	110.18
21	3	503	CL7	C3C-C4C-NC	9.62	117.15	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	503	CL7	C3C-C4C-NC	9.62	117.15	110.18
21	6	503	CL7	C3C-C4C-NC	9.58	117.12	110.18
21	2	503	CL7	C3C-C4C-NC	9.55	117.10	110.18
21	1	413	CL7	C3C-C4C-NC	9.54	117.09	110.18
21	5	413	CL7	C3C-C4C-NC	9.54	117.09	110.18
21	4	407	CL7	C3C-C4C-NC	9.53	117.09	110.18
23	a	404	8CT	C33-C32-C31	-9.52	115.72	124.85
23	A	404	8CT	C33-C32-C31	-9.50	115.74	124.85
21	8	407	CL7	C3C-C4C-NC	9.47	117.04	110.18
21	4	409	CL7	C3C-C4C-NC	9.47	117.04	110.18
21	8	409	CL7	C3C-C4C-NC	9.47	117.04	110.18
21	c	502	CL7	C3C-C4C-NC	9.44	117.02	110.18
21	7	512	CL7	C3C-C4C-NC	9.42	117.01	110.18
21	1	417	CL7	C3C-C4C-NC	9.41	117.00	110.18
21	5	417	CL7	C3C-C4C-NC	9.41	117.00	110.18
21	C	502	CL7	C3C-C4C-NC	9.39	116.99	110.18
21	B	610	CL7	C3C-C4C-NC	9.39	116.99	110.18
21	b	611	CL7	C3C-C4C-NC	9.39	116.99	110.18
21	3	512	CL7	C3C-C4C-NC	9.39	116.98	110.18
21	C	503	CL7	C3C-C4C-NC	9.36	116.96	110.18
21	3	515	CL7	C3C-C4C-NC	9.35	116.96	110.18
21	7	515	CL7	C3C-C4C-NC	9.35	116.96	110.18
21	c	503	CL7	C3C-C4C-NC	9.35	116.95	110.18
21	8	414	CL7	C3C-C4C-NC	9.29	116.91	110.18
21	4	413	CL7	C3C-C4C-NC	9.27	116.89	110.18
21	8	413	CL7	C3C-C4C-NC	9.27	116.89	110.18
21	4	408	CL7	C3C-C4C-NC	9.26	116.89	110.18
32	2	519	ZEX	C27-C28-C29	-9.26	112.24	126.23
32	6	519	ZEX	C27-C28-C29	-9.26	112.24	126.23
21	4	414	CL7	C3C-C4C-NC	9.25	116.88	110.18
21	3	513	CL7	C3C-C4C-NC	9.25	116.88	110.18
21	7	513	CL7	C3C-C4C-NC	9.25	116.88	110.18
21	1	402	CL7	C3C-C4C-NC	9.23	116.86	110.18
21	5	402	CL7	C3C-C4C-NC	9.23	116.86	110.18
21	B	613	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	b	614	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	2	517	CL7	C3C-C4C-NC	9.22	116.86	110.18
21	C	513	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	c	507	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	c	513	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	8	408	CL7	C3C-C4C-NC	9.21	116.85	110.18
21	6	517	CL7	C3C-C4C-NC	9.21	116.85	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	507	CL7	C3C-C4C-NC	9.19	116.84	110.18
21	7	507	CL7	C3C-C4C-NC	9.19	116.84	110.18
21	C	507	CL7	C3C-C4C-NC	9.16	116.82	110.18
21	1	406	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	5	406	CL7	C3C-C4C-NC	9.15	116.81	110.18
21	2	510	CL7	C3C-C4C-NC	9.13	116.80	110.18
21	6	510	CL7	C3C-C4C-NC	9.13	116.80	110.18
21	7	509	CL7	C3C-C4C-NC	9.13	116.79	110.18
21	A	401	CL7	C3C-C4C-NC	9.12	116.79	110.18
21	a	401	CL7	C3C-C4C-NC	9.12	116.79	110.18
21	C	510	CL7	C3C-C4C-NC	9.12	116.79	110.18
21	c	510	CL7	C3C-C4C-NC	9.12	116.79	110.18
21	2	514	CL7	C3C-C4C-NC	9.11	116.78	110.18
21	6	514	CL7	C3C-C4C-NC	9.11	116.78	110.18
21	1	418	CL7	C3C-C4C-NC	9.11	116.78	110.18
32	2	520	ZEX	C28-C27-C26	-9.11	111.53	127.09
32	3	525	ZEX	C28-C27-C26	-9.11	111.53	127.09
21	3	509	CL7	C3C-C4C-NC	9.11	116.78	110.18
21	B	612	CL7	C3C-C4C-NC	9.10	116.77	110.18
21	b	613	CL7	C3C-C4C-NC	9.10	116.77	110.18
21	5	403	CL7	C3C-C4C-NC	9.07	116.75	110.18
21	5	418	CL7	C3C-C4C-NC	9.06	116.75	110.18
21	1	403	CL7	C3C-C4C-NC	9.05	116.74	110.18
21	2	505	CL7	C3C-C4C-NC	9.05	116.73	110.18
23	B	627	8CT	C33-C32-C31	-9.04	116.18	124.85
21	1	404	CL7	C3C-C4C-NC	9.04	116.73	110.18
21	5	404	CL7	C3C-C4C-NC	9.04	116.73	110.18
21	B	602	CL7	C3C-C4C-NC	9.03	116.73	110.18
21	b	603	CL7	C3C-C4C-NC	9.03	116.73	110.18
21	5	411	CL7	C3C-C4C-NC	9.03	116.72	110.18
21	1	411	CL7	C3C-C4C-NC	9.02	116.71	110.18
23	b	601	8CT	C33-C32-C31	-9.01	116.21	124.85
21	B	614	CL7	C3C-C4C-NC	8.99	116.69	110.18
21	b	615	CL7	C3C-C4C-NC	8.99	116.69	110.18
21	8	406	CL7	C3C-C4C-NC	8.98	116.69	110.18
21	4	406	CL7	C3C-C4C-NC	8.96	116.67	110.18
21	7	504	CL7	C3C-C4C-NC	8.96	116.67	110.18
21	3	504	CL7	C3C-C4C-NC	8.96	116.67	110.18
21	2	502	CL7	C3C-C4C-NC	8.95	116.66	110.18
21	6	502	CL7	C3C-C4C-NC	8.95	116.66	110.18
21	5	412	CL7	C3C-C4C-NC	8.95	116.66	110.18
23	c	519	8CT	C33-C32-C31	-8.94	116.28	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	412	CL7	C3C-C4C-NC	8.94	116.66	110.18
21	6	505	CL7	C3C-C4C-NC	8.94	116.66	110.18
21	3	518	CL7	C3C-C4C-NC	8.93	116.65	110.18
21	7	518	CL7	C3C-C4C-NC	8.93	116.65	110.18
23	C	519	8CT	C33-C32-C31	-8.92	116.30	124.85
21	D	405	CL7	C3C-C4C-NC	8.91	116.64	110.18
21	d	405	CL7	C3C-C4C-NC	8.91	116.64	110.18
21	2	515	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	6	515	CL7	C3C-C4C-NC	8.90	116.63	110.18
21	C	504	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	C	514	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	c	504	CL7	C3C-C4C-NC	8.86	116.60	110.18
21	B	616	CL7	C3C-C4C-NC	8.85	116.59	110.18
21	b	617	CL7	C3C-C4C-NC	8.85	116.59	110.18
21	c	514	CL7	C3C-C4C-NC	8.84	116.59	110.18
21	B	615	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	b	616	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	2	511	CL7	C3C-C4C-NC	8.83	116.58	110.18
21	4	410	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	1	419	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	5	419	CL7	C3C-C4C-NC	8.82	116.57	110.18
21	B	608	CL7	C3C-C4C-NC	8.81	116.57	110.18
21	b	609	CL7	C3C-C4C-NC	8.81	116.57	110.18
21	3	510	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	7	510	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	7	517	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	8	410	CL7	C3C-C4C-NC	8.81	116.56	110.18
21	3	517	CL7	C3C-C4C-NC	8.80	116.56	110.18
21	6	511	CL7	C3C-C4C-NC	8.80	116.56	110.18
21	5	408	CL7	C3C-C4C-NC	8.80	116.56	110.18
21	B	609	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	b	608	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	6	507	CL7	C3C-C4C-NC	8.79	116.55	110.18
21	1	407	CL7	C3C-C4C-NC	8.78	116.54	110.18
21	2	501	CL7	C3C-C4C-NC	8.77	116.54	110.18
21	6	501	CL7	C3C-C4C-NC	8.77	116.54	110.18
21	1	408	CL7	C3C-C4C-NC	8.77	116.53	110.18
21	7	506	CL7	C2C-C1C-NC	8.77	116.56	110.10
21	2	507	CL7	C3C-C4C-NC	8.76	116.53	110.18
21	5	407	CL7	C3C-C4C-NC	8.75	116.52	110.18
21	b	610	CL7	C3C-C4C-NC	8.74	116.52	110.18
21	C	506	CL7	C3C-C4C-NC	8.74	116.51	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	416	CL7	C3C-C4C-NC	8.74	116.51	110.18
21	5	412	CL7	C2C-C1C-NC	8.73	116.54	110.10
21	B	607	CL7	C3C-C4C-NC	8.73	116.50	110.18
21	1	416	CL7	C3C-C4C-NC	8.73	116.50	110.18
21	2	518	CL7	C3C-C4C-NC	8.73	116.50	110.18
21	B	615	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	b	616	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	1	412	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	c	506	CL7	C3C-C4C-NC	8.72	116.50	110.18
21	3	506	CL7	C2C-C1C-NC	8.72	116.53	110.10
21	4	404	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	6	518	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	8	404	CL7	C3C-C4C-NC	8.71	116.49	110.18
21	3	501	CL7	C3C-C4C-NC	8.70	116.48	110.18
21	3	506	CL7	C3C-C4C-NC	8.69	116.47	110.18
21	7	506	CL7	C3C-C4C-NC	8.69	116.47	110.18
21	6	513	CL7	C3C-C4C-NC	8.69	116.47	110.18
21	B	622	CL7	C3C-C4C-NC	8.68	116.47	110.18
21	c	508	CL7	C3C-C4C-NC	8.67	116.47	110.18
21	C	512	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	2	516	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	c	512	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	6	516	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	A	406	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	a	405	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	2	506	CL7	C3C-C4C-NC	8.67	116.46	110.18
21	6	509	CL7	C3C-C4C-NC	8.66	116.46	110.18
21	C	505	CL7	C3C-C4C-NC	8.66	116.45	110.18
21	C	508	CL7	C3C-C4C-NC	8.66	116.45	110.18
21	c	505	CL7	C3C-C4C-NC	8.66	116.45	110.18
21	B	611	CL7	C2C-C1C-NC	8.66	116.48	110.10
21	2	513	CL7	C3C-C4C-NC	8.65	116.45	110.18
21	7	501	CL7	C3C-C4C-NC	8.65	116.45	110.18
21	b	623	CL7	C3C-C4C-NC	8.63	116.44	110.18
21	B	605	CL7	C3C-C4C-NC	8.63	116.43	110.18
21	b	606	CL7	C3C-C4C-NC	8.63	116.43	110.18
21	2	509	CL7	C3C-C4C-NC	8.62	116.43	110.18
21	6	506	CL7	C3C-C4C-NC	8.62	116.43	110.18
21	1	403	CL7	C2C-C1C-NC	8.60	116.44	110.10
21	b	612	CL7	C2C-C1C-NC	8.59	116.44	110.10
21	B	601	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	b	602	CL7	C3C-C4C-NC	8.59	116.40	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	409	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	5	409	CL7	C3C-C4C-NC	8.59	116.40	110.18
21	6	507	CL7	C2C-C1C-NC	8.58	116.43	110.10
21	2	507	CL7	C2C-C1C-NC	8.57	116.42	110.10
21	5	403	CL7	C2C-C1C-NC	8.57	116.42	110.10
21	4	412	CL7	C3C-C4C-NC	8.57	116.39	110.18
21	c	511	CL7	C3C-C4C-NC	8.56	116.39	110.18
21	7	508	CL7	C2C-C1C-NC	8.54	116.40	110.10
21	1	405	CL7	C3C-C4C-NC	8.53	116.36	110.18
21	8	412	CL7	C3C-C4C-NC	8.53	116.36	110.18
21	8	409	CL7	C2C-C1C-NC	8.52	116.38	110.10
21	2	508	CL7	C3C-C4C-NC	8.52	116.35	110.18
21	6	508	CL7	C3C-C4C-NC	8.52	116.35	110.18
21	4	409	CL7	C2C-C1C-NC	8.51	116.38	110.10
21	C	511	CL7	C3C-C4C-NC	8.51	116.35	110.18
21	5	405	CL7	C3C-C4C-NC	8.51	116.34	110.18
23	B	627	8CT	C19-C20-C21	-8.50	115.17	127.31
23	b	601	8CT	C19-C20-C21	-8.50	115.17	127.31
21	1	410	CL7	C3C-C4C-NC	8.50	116.34	110.18
21	5	410	CL7	C3C-C4C-NC	8.50	116.34	110.18
23	C	516	8CT	C33-C32-C31	-8.50	116.70	124.85
23	c	516	8CT	C33-C32-C31	-8.50	116.70	124.85
21	3	508	CL7	C2C-C1C-NC	8.49	116.36	110.10
21	4	411	CL7	C3C-C4C-NC	8.48	116.33	110.18
21	8	411	CL7	C3C-C4C-NC	8.48	116.33	110.18
21	C	509	CL7	C3C-C4C-NC	8.48	116.32	110.18
21	c	509	CL7	C3C-C4C-NC	8.48	116.32	110.18
21	B	606	CL7	C3C-C4C-NC	8.47	116.32	110.18
21	d	402	CL7	C3C-C4C-NC	8.47	116.32	110.18
21	B	603	CL7	C3C-C4C-NC	8.47	116.32	110.18
21	b	604	CL7	C3C-C4C-NC	8.47	116.32	110.18
21	B	601	CL7	C2C-C1C-NC	8.47	116.34	110.10
21	b	602	CL7	C2C-C1C-NC	8.47	116.34	110.10
23	b	618	8CT	C33-C32-C31	-8.46	116.74	124.85
21	D	402	CL7	C3C-C4C-NC	8.44	116.30	110.18
21	b	607	CL7	C3C-C4C-NC	8.44	116.30	110.18
21	B	611	CL7	C3C-C4C-NC	8.43	116.29	110.18
23	B	617	8CT	C33-C32-C31	-8.43	116.77	124.85
23	C	516	8CT	C14-C13-C12	-8.42	115.29	127.31
21	B	604	CL7	C3C-C4C-NC	8.42	116.28	110.18
21	b	605	CL7	C3C-C4C-NC	8.42	116.28	110.18
21	2	501	CL7	C2C-C1C-NC	8.42	116.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	501	CL7	C2C-C1C-NC	8.42	116.31	110.10
23	c	516	8CT	C14-C13-C12	-8.41	115.31	127.31
21	b	612	CL7	C3C-C4C-NC	8.40	116.27	110.18
23	B	627	8CT	C24-C25-C26	-8.39	115.33	127.31
21	2	514	CL7	C2C-C1C-NC	8.37	116.27	110.10
21	6	514	CL7	C2C-C1C-NC	8.37	116.27	110.10
23	D	406	8CT	C19-C20-C21	-8.37	115.37	127.31
23	b	601	8CT	C24-C25-C26	-8.37	115.37	127.31
21	7	508	CL7	C3C-C4C-NC	8.36	116.23	110.18
21	2	502	CL7	C2C-C1C-NC	8.35	116.26	110.10
21	6	502	CL7	C2C-C1C-NC	8.35	116.26	110.10
23	d	406	8CT	C19-C20-C21	-8.35	115.39	127.31
21	c	507	CL7	C2C-C1C-NC	8.35	116.25	110.10
21	c	518	CL7	C3C-C4C-NC	8.33	116.22	110.18
21	C	518	CL7	C3C-C4C-NC	8.33	116.22	110.18
21	C	507	CL7	C2C-C1C-NC	8.32	116.23	110.10
21	6	504	CL7	C3C-C4C-NC	8.31	116.20	110.18
21	3	508	CL7	C3C-C4C-NC	8.31	116.20	110.18
21	2	508	CL7	C2C-C1C-NC	8.30	116.22	110.10
21	6	508	CL7	C2C-C1C-NC	8.30	116.22	110.10
21	4	405	CL7	C3C-C4C-NC	8.30	116.19	110.18
21	8	405	CL7	C3C-C4C-NC	8.30	116.19	110.18
21	2	506	CL7	C2C-C1C-NC	8.29	116.22	110.10
21	6	506	CL7	C2C-C1C-NC	8.29	116.22	110.10
32	3	522	ZEX	C11-C10-C9	-8.29	115.48	127.31
32	7	522	ZEX	C11-C10-C9	-8.29	115.48	127.31
21	C	514	CL7	C2C-C1C-NC	8.27	116.20	110.10
21	2	504	CL7	C3C-C4C-NC	8.26	116.16	110.18
21	8	410	CL7	C2C-C1C-NC	8.23	116.17	110.10
21	B	605	CL7	C2C-C1C-NC	8.23	116.17	110.10
21	b	606	CL7	C2C-C1C-NC	8.23	116.17	110.10
21	C	506	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	c	506	CL7	C2C-C1C-NC	8.22	116.16	110.10
21	2	513	CL7	C2C-C1C-NC	8.22	116.16	110.10
23	C	515	8CT	C33-C32-C31	-8.21	116.97	124.85
23	c	515	8CT	C33-C32-C31	-8.21	116.97	124.85
21	1	402	CL7	C2C-C1C-NC	8.21	116.16	110.10
21	5	402	CL7	C2C-C1C-NC	8.21	116.16	110.10
21	c	514	CL7	C2C-C1C-NC	8.20	116.15	110.10
21	3	507	CL7	C2C-C1C-NC	8.20	116.15	110.10
21	D	404	CL7	C3C-C4C-NC	8.20	116.12	110.18
21	d	404	CL7	C3C-C4C-NC	8.20	116.12	110.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	513	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	C	512	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	1	413	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	5	413	CL7	C2C-C1C-NC	8.19	116.14	110.10
21	c	505	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	c	512	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	5	405	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	C	518	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	7	504	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	4	410	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	c	504	CL7	C2C-C1C-NC	8.16	116.12	110.10
21	c	518	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	3	502	CL7	C3C-C4C-NC	8.15	116.09	110.18
21	7	507	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	3	504	CL7	C2C-C1C-NC	8.15	116.11	110.10
21	7	517	CL7	C2C-C1C-NC	8.14	116.11	110.10
21	1	409	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	5	409	CL7	C2C-C1C-NC	8.14	116.10	110.10
21	3	517	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	2	510	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	1	406	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	6	510	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	5	406	CL7	C2C-C1C-NC	8.13	116.09	110.10
21	B	603	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	C	505	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	b	604	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	1	405	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	B	604	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	b	605	CL7	C2C-C1C-NC	8.12	116.09	110.10
21	D	402	CL7	C2C-C1C-NC	8.12	116.08	110.10
21	d	402	CL7	C2C-C1C-NC	8.12	116.08	110.10
21	C	504	CL7	C2C-C1C-NC	8.11	116.08	110.10
21	7	502	CL7	C3C-C4C-NC	8.11	116.06	110.18
21	7	515	CL7	C2C-C1C-NC	8.10	116.08	110.10
21	3	515	CL7	C2C-C1C-NC	8.09	116.07	110.10
21	c	513	CL7	C2C-C1C-NC	8.09	116.07	110.10
21	d	405	CL7	C2C-C1C-NC	8.09	116.06	110.10
21	4	416	CL7	C2C-C1C-NC	8.08	116.06	110.10
21	8	416	CL7	C2C-C1C-NC	8.08	116.06	110.10
21	C	513	CL7	C2C-C1C-NC	8.08	116.06	110.10
23	B	618	8CT	C33-C32-C31	-8.07	117.11	124.85
21	2	515	CL7	C2C-C1C-NC	8.06	116.04	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	515	CL7	C2C-C1C-NC	8.06	116.04	110.10
21	8	415	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	2	504	CL7	C2C-C1C-NC	8.05	116.04	110.10
21	D	405	CL7	C2C-C1C-NC	8.04	116.03	110.10
21	4	405	CL7	C2C-C1C-NC	8.03	116.03	110.10
23	b	619	8CT	C33-C32-C31	-8.03	117.15	124.85
21	1	407	CL7	C2C-C1C-NC	8.02	116.02	110.10
21	5	407	CL7	C2C-C1C-NC	8.02	116.02	110.10
21	3	516	CL7	C3C-C4C-NC	8.02	115.99	110.18
21	7	516	CL7	C3C-C4C-NC	8.02	115.99	110.18
21	4	413	CL7	C2C-C1C-NC	8.02	116.01	110.10
21	8	413	CL7	C2C-C1C-NC	8.02	116.01	110.10
21	8	405	CL7	C2C-C1C-NC	8.01	116.01	110.10
21	4	415	CL7	C2C-C1C-NC	8.01	116.01	110.10
21	6	504	CL7	C2C-C1C-NC	8.00	116.00	110.10
21	2	516	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	6	516	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	5	418	CL7	C2C-C1C-NC	7.99	115.99	110.10
21	3	501	CL7	C2C-C1C-NC	7.98	115.99	110.10
23	a	404	8CT	C24-C25-C26	-7.98	115.93	127.31
21	4	404	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	8	404	CL7	C2C-C1C-NC	7.97	115.98	110.10
21	1	418	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	3	518	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	7	518	CL7	C2C-C1C-NC	7.96	115.97	110.10
21	B	606	CL7	C2C-C1C-NC	7.94	115.96	110.10
21	b	607	CL7	C2C-C1C-NC	7.94	115.96	110.10
21	1	410	CL7	C2C-C1C-NC	7.94	115.96	110.10
21	5	410	CL7	C2C-C1C-NC	7.94	115.96	110.10
21	2	503	CL7	C2C-C1C-NC	7.94	115.95	110.10
21	5	408	CL7	C2C-C1C-NC	7.94	115.95	110.10
21	7	501	CL7	C2C-C1C-NC	7.93	115.95	110.10
23	A	404	8CT	C24-C25-C26	-7.93	116.00	127.31
21	B	612	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	b	613	CL7	C2C-C1C-NC	7.92	115.94	110.10
32	3	520	ZEX	C11-C10-C9	-7.92	116.01	127.31
32	7	520	ZEX	C11-C10-C9	-7.92	116.01	127.31
21	6	503	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	7	510	CL7	C2C-C1C-NC	7.92	115.94	110.10
21	1	408	CL7	C2C-C1C-NC	7.91	115.93	110.10
21	4	408	CL7	C2C-C1C-NC	7.89	115.92	110.10
21	C	510	CL7	C2C-C1C-NC	7.89	115.92	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	510	CL7	C2C-C1C-NC	7.89	115.92	110.10
21	3	510	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	4	417	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	8	417	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	B	602	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	b	615	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	A	406	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	4	414	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	a	405	CL7	C2C-C1C-NC	7.88	115.91	110.10
21	b	603	CL7	C2C-C1C-NC	7.87	115.90	110.10
21	5	416	CL7	C2C-C1C-NC	7.86	115.89	110.10
21	2	509	CL7	C2C-C1C-NC	7.85	115.89	110.10
21	8	414	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	B	614	CL7	C2C-C1C-NC	7.84	115.88	110.10
21	8	408	CL7	C2C-C1C-NC	7.84	115.88	110.10
32	5	421	ZEX	C31-C30-C29	-7.83	116.13	127.31
21	C	509	CL7	C2C-C1C-NC	7.83	115.87	110.10
21	c	509	CL7	C2C-C1C-NC	7.83	115.87	110.10
21	6	509	CL7	C2C-C1C-NC	7.82	115.87	110.10
21	1	416	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	1	419	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	5	419	CL7	C2C-C1C-NC	7.81	115.86	110.10
32	1	421	ZEX	C31-C30-C29	-7.81	116.17	127.31
21	1	415	CL7	C2C-C1C-NC	7.81	115.86	110.10
21	5	415	CL7	C2C-C1C-NC	7.80	115.85	110.10
21	b	609	CL7	C2C-C1C-NC	7.79	115.84	110.10
21	7	512	CL7	C2C-C1C-NC	7.78	115.84	110.10
21	4	407	CL7	C2C-C1C-NC	7.78	115.84	110.10
21	3	514	CL7	C2C-C1C-NC	7.77	115.83	110.10
21	7	514	CL7	C2C-C1C-NC	7.77	115.83	110.10
21	4	406	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	B	608	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	d	404	CL7	C2C-C1C-NC	7.76	115.82	110.10
21	D	404	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	3	513	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	7	513	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	8	407	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	3	512	CL7	C2C-C1C-NC	7.74	115.81	110.10
21	1	420	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	8	406	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	C	508	CL7	C2C-C1C-NC	7.73	115.80	110.10
21	c	508	CL7	C2C-C1C-NC	7.73	115.80	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	420	CL7	C2C-C1C-NC	7.71	115.79	110.10
21	2	505	CL7	C2C-C1C-NC	7.69	115.77	110.10
32	3	519	ZEX	C31-C30-C29	-7.69	116.34	127.31
32	7	519	ZEX	C31-C30-C29	-7.69	116.34	127.31
21	7	509	CL7	C2C-C1C-NC	7.68	115.76	110.10
21	c	511	CL7	C2C-C1C-NC	7.65	115.75	110.10
21	C	511	CL7	C2C-C1C-NC	7.62	115.72	110.10
21	b	610	CL7	C2C-C1C-NC	7.62	115.72	110.10
21	7	505	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	2	518	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	6	518	CL7	C2C-C1C-NC	7.61	115.71	110.10
21	B	609	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	3	516	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	7	516	CL7	C2C-C1C-NC	7.60	115.71	110.10
21	6	505	CL7	C2C-C1C-NC	7.60	115.70	110.10
21	7	502	CL7	C2C-C1C-NC	7.60	115.70	110.10
21	B	616	CL7	C2C-C1C-NC	7.59	115.70	110.10
21	b	617	CL7	C2C-C1C-NC	7.59	115.70	110.10
21	3	509	CL7	C2C-C1C-NC	7.59	115.69	110.10
21	3	505	CL7	C2C-C1C-NC	7.59	115.69	110.10
21	c	502	CL7	C2C-C1C-NC	7.56	115.68	110.10
21	2	517	CL7	C2C-C1C-NC	7.56	115.68	110.10
21	6	517	CL7	C2C-C1C-NC	7.56	115.68	110.10
21	3	503	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	3	511	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	7	503	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	7	511	CL7	C2C-C1C-NC	7.55	115.67	110.10
21	B	607	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	1	411	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	5	411	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	2	511	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	3	502	CL7	C2C-C1C-NC	7.53	115.65	110.10
21	C	502	CL7	C2C-C1C-NC	7.52	115.65	110.10
21	B	622	CL7	C2C-C1C-NC	7.52	115.64	110.10
21	6	511	CL7	C2C-C1C-NC	7.51	115.64	110.10
21	b	608	CL7	C2C-C1C-NC	7.50	115.63	110.10
21	C	503	CL7	C2C-C1C-NC	7.48	115.62	110.10
21	c	503	CL7	C2C-C1C-NC	7.48	115.62	110.10
21	B	610	CL7	C2C-C1C-NC	7.47	115.61	110.10
21	B	613	CL7	C2C-C1C-NC	7.47	115.61	110.10
21	b	611	CL7	C2C-C1C-NC	7.47	115.61	110.10
21	b	614	CL7	C2C-C1C-NC	7.46	115.61	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	623	CL7	C2C-C1C-NC	7.45	115.60	110.10
23	8	402	8CT	C30-C31-C32	-7.42	112.34	121.47
23	4	402	8CT	C30-C31-C32	-7.42	112.34	121.47
32	4	403	ZEX	C31-C30-C29	-7.42	116.72	127.31
32	8	403	ZEX	C31-C30-C29	-7.42	116.72	127.31
21	1	414	CL7	C2C-C1C-NC	7.41	115.57	110.10
21	5	414	CL7	C2C-C1C-NC	7.41	115.57	110.10
21	1	404	CL7	C2C-C1C-NC	7.41	115.56	110.10
21	5	404	CL7	C2C-C1C-NC	7.41	115.56	110.10
32	3	520	ZEX	C31-C30-C29	-7.33	116.84	127.31
32	2	519	ZEX	C31-C30-C29	-7.33	116.85	127.31
32	6	519	ZEX	C31-C30-C29	-7.33	116.85	127.31
32	7	520	ZEX	C31-C30-C29	-7.32	116.86	127.31
21	2	512	CL7	C2C-C1C-NC	7.31	115.49	110.10
21	A	403	CL7	C2C-C1C-NC	7.30	115.48	110.10
21	6	512	CL7	C2C-C1C-NC	7.29	115.48	110.10
21	4	412	CL7	C2C-C1C-NC	7.29	115.48	110.10
21	4	411	CL7	C2C-C1C-NC	7.27	115.46	110.10
21	8	411	CL7	C2C-C1C-NC	7.27	115.46	110.10
21	A	401	CL7	C2C-C1C-NC	7.26	115.45	110.10
21	a	401	CL7	C2C-C1C-NC	7.26	115.45	110.10
32	2	525	ZEX	C31-C30-C29	-7.25	116.97	127.31
32	6	524	ZEX	C31-C30-C29	-7.25	116.97	127.31
21	8	412	CL7	C2C-C1C-NC	7.25	115.44	110.10
21	a	403	CL7	C2C-C1C-NC	7.24	115.44	110.10
32	1	422	ZEX	C7-C8-C9	-7.20	115.35	126.23
32	5	422	ZEX	C7-C8-C9	-7.20	115.35	126.23
32	2	523	ZEX	C35-C34-C33	-7.16	117.09	127.31
32	6	522	ZEX	C35-C34-C33	-7.16	117.09	127.31
32	4	419	ZEX	C28-C27-C26	-7.16	114.86	127.09
32	8	419	ZEX	C28-C27-C26	-7.16	114.86	127.09
23	C	519	8CT	C24-C25-C26	-7.15	117.10	127.31
23	c	519	8CT	C24-C25-C26	-7.14	117.12	127.31
32	2	525	ZEX	C28-C27-C26	-7.07	115.01	127.09
32	6	524	ZEX	C28-C27-C26	-7.07	115.01	127.09
32	4	403	ZEX	C28-C27-C26	-7.01	115.11	127.09
32	2	525	ZEX	C7-C8-C9	-7.01	115.64	126.23
32	6	524	ZEX	C7-C8-C9	-7.01	115.64	126.23
32	8	403	ZEX	C28-C27-C26	-6.99	115.14	127.09
32	4	419	ZEX	C15-C14-C13	-6.99	117.34	127.31
32	4	418	ZEX	C31-C30-C29	-6.97	117.36	127.31
32	8	418	ZEX	C31-C30-C29	-6.97	117.36	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	8	419	ZEX	C15-C14-C13	-6.97	117.36	127.31
32	4	420	ZEX	C28-C27-C26	-6.90	115.29	127.09
32	8	420	ZEX	C28-C27-C26	-6.90	115.29	127.09
21	1	402	CL7	C1A-NA-C4A	6.86	110.46	106.30
21	5	402	CL7	C1A-NA-C4A	6.83	110.43	106.30
23	K	101	8CT	C33-C32-C31	-6.80	118.33	124.85
32	2	523	ZEX	C28-C27-C26	-6.76	115.54	127.09
23	k	101	8CT	C33-C32-C31	-6.76	118.37	124.85
23	B	619	8CT	C24-C25-C26	-6.75	117.67	127.31
23	b	620	8CT	C24-C25-C26	-6.75	117.67	127.31
32	6	522	ZEX	C28-C27-C26	-6.75	115.56	127.09
21	1	417	CL7	C2C-C1C-NC	6.73	115.06	110.10
21	5	417	CL7	C2C-C1C-NC	6.73	115.06	110.10
23	B	627	8CT	C14-C13-C12	-6.69	117.76	127.31
32	6	520	ZEX	C7-C8-C9	-6.68	116.14	126.23
32	2	521	ZEX	C7-C8-C9	-6.67	116.16	126.23
23	b	601	8CT	C14-C13-C12	-6.65	117.81	127.31
23	d	406	8CT	C19-C18-C17	-6.63	109.89	123.47
23	D	406	8CT	C19-C18-C17	-6.62	109.91	123.47
23	A	404	8CT	C19-C20-C21	-6.62	117.86	127.31
23	a	404	8CT	C19-C20-C21	-6.62	117.86	127.31
32	6	522	ZEX	C7-C8-C9	-6.56	116.33	126.23
23	C	516	8CT	C10-C11-C12	-6.56	116.33	126.23
23	c	516	8CT	C10-C11-C12	-6.56	116.33	126.23
21	B	615	CL7	C1A-NA-C4A	6.55	110.27	106.30
21	b	616	CL7	C1A-NA-C4A	6.55	110.27	106.30
32	2	523	ZEX	C7-C8-C9	-6.54	116.36	126.23
23	b	601	8CT	C10-C11-C12	-6.47	116.45	126.23
21	b	611	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	3	511	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	4	405	CL7	C1A-NA-C4A	6.47	110.22	106.30
21	8	405	CL7	C1A-NA-C4A	6.47	110.22	106.30
23	B	627	8CT	C10-C11-C12	-6.45	116.49	126.23
21	7	511	CL7	C1A-NA-C4A	6.44	110.20	106.30
21	2	503	CL7	C1A-NA-C4A	6.43	110.19	106.30
21	6	503	CL7	C1A-NA-C4A	6.43	110.19	106.30
21	2	505	CL7	C1A-NA-C4A	6.39	110.17	106.30
21	6	505	CL7	C1A-NA-C4A	6.39	110.17	106.30
32	4	418	ZEX	C15-C14-C13	-6.37	118.22	127.31
32	8	418	ZEX	C15-C14-C13	-6.37	118.22	127.31
21	3	503	CL7	C1A-NA-C4A	6.36	110.15	106.30
21	B	610	CL7	C1A-NA-C4A	6.35	110.15	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	503	CL7	C1A-NA-C4A	6.35	110.15	106.30
21	A	406	CL7	C1A-NA-C4A	6.35	110.15	106.30
32	2	520	ZEX	C31-C30-C29	-6.35	118.25	127.31
32	3	525	ZEX	C31-C30-C29	-6.35	118.25	127.31
21	1	413	CL7	C1A-NA-C4A	6.34	110.14	106.30
32	3	519	ZEX	C15-C14-C13	-6.32	118.29	127.31
32	7	519	ZEX	C15-C14-C13	-6.32	118.29	127.31
21	B	604	CL7	C1A-NA-C4A	6.32	110.13	106.30
21	b	605	CL7	C1A-NA-C4A	6.32	110.13	106.30
21	7	505	CL7	C1A-NA-C4A	6.31	110.12	106.30
21	3	505	CL7	C1A-NA-C4A	6.31	110.12	106.30
21	a	405	CL7	C1A-NA-C4A	6.30	110.11	106.30
21	4	417	CL7	C1A-NA-C4A	6.29	110.11	106.30
21	8	417	CL7	C1A-NA-C4A	6.29	110.11	106.30
21	5	413	CL7	C1A-NA-C4A	6.29	110.11	106.30
32	7	519	ZEX	C27-C28-C29	-6.28	116.74	126.23
32	3	519	ZEX	C27-C28-C29	-6.28	116.75	126.23
21	7	506	CL7	C1A-NA-C4A	6.27	110.10	106.30
32	4	403	ZEX	C7-C8-C9	-6.25	116.79	126.23
21	3	506	CL7	C1A-NA-C4A	6.23	110.07	106.30
32	8	403	ZEX	C7-C8-C9	-6.20	116.86	126.23
21	4	414	CL7	C1A-NA-C4A	6.19	110.05	106.30
21	8	414	CL7	C1A-NA-C4A	6.19	110.05	106.30
23	B	618	8CT	C30-C31-C32	-6.19	113.86	121.47
23	b	619	8CT	C30-C31-C32	-6.19	113.86	121.47
21	B	605	CL7	C1A-NA-C4A	6.13	110.01	106.30
21	b	606	CL7	C1A-NA-C4A	6.12	110.01	106.30
32	3	520	ZEX	C35-C34-C33	-6.11	118.58	127.31
32	7	520	ZEX	C35-C34-C33	-6.11	118.58	127.31
21	1	403	CL7	C1A-NA-C4A	6.10	109.99	106.30
32	2	525	ZEX	C11-C10-C9	-6.10	118.61	127.31
32	6	524	ZEX	C11-C10-C9	-6.10	118.61	127.31
23	b	619	8CT	C19-C18-C17	-6.09	111.00	123.47
23	B	618	8CT	C19-C18-C17	-6.08	111.03	123.47
21	5	403	CL7	C1A-NA-C4A	6.07	109.98	106.30
21	5	415	CL7	C1A-NA-C4A	6.07	109.97	106.30
21	1	415	CL7	C1A-NA-C4A	6.07	109.97	106.30
21	5	420	CL7	C1A-NA-C4A	6.06	109.97	106.30
32	3	519	ZEX	C11-C10-C9	-6.06	118.67	127.31
21	8	410	CL7	C1A-NA-C4A	6.04	109.96	106.30
32	7	519	ZEX	C11-C10-C9	-6.04	118.70	127.31
21	4	415	CL7	C1A-NA-C4A	6.02	109.94	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	410	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	C	502	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	c	502	CL7	C1A-NA-C4A	6.01	109.94	106.30
21	8	415	CL7	C1A-NA-C4A	6.00	109.94	106.30
21	1	420	CL7	C1A-NA-C4A	5.99	109.93	106.30
21	b	604	CL7	C1A-NA-C4A	5.97	109.91	106.30
21	B	603	CL7	C1A-NA-C4A	5.95	109.90	106.30
23	B	619	8CT	C19-C20-C21	-5.95	118.82	127.31
21	d	405	CL7	C1A-NA-C4A	5.94	109.90	106.30
21	3	504	CL7	C1A-NA-C4A	5.94	109.90	106.30
21	b	602	CL7	C1A-NA-C4A	5.94	109.89	106.30
21	D	404	CL7	C1A-NA-C4A	5.93	109.89	106.30
21	d	404	CL7	C1A-NA-C4A	5.93	109.89	106.30
23	b	620	8CT	C19-C20-C21	-5.93	118.85	127.31
21	1	406	CL7	C1A-NA-C4A	5.92	109.88	106.30
21	4	409	CL7	C1A-NA-C4A	5.92	109.88	106.30
21	8	409	CL7	C1A-NA-C4A	5.92	109.88	106.30
21	B	601	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	C	506	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	7	504	CL7	C1A-NA-C4A	5.90	109.87	106.30
21	6	501	CL7	C1A-NA-C4A	5.89	109.87	106.30
23	A	404	8CT	C10-C11-C12	-5.88	117.34	126.23
21	6	513	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	D	405	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	c	506	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	7	510	CL7	C1A-NA-C4A	5.88	109.86	106.30
21	1	412	CL7	C1A-NA-C4A	5.87	109.86	106.30
21	2	501	CL7	C1A-NA-C4A	5.87	109.85	106.30
21	5	412	CL7	C1A-NA-C4A	5.87	109.85	106.30
23	a	404	8CT	C10-C11-C12	-5.87	117.37	126.23
21	8	406	CL7	C1A-NA-C4A	5.86	109.85	106.30
21	5	406	CL7	C1A-NA-C4A	5.85	109.84	106.30
21	3	514	CL7	C1A-NA-C4A	5.84	109.84	106.30
21	7	514	CL7	C1A-NA-C4A	5.84	109.84	106.30
32	7	522	ZEX	C28-C27-C26	-5.83	117.13	127.09
21	7	513	CL7	C1A-NA-C4A	5.83	109.83	106.30
21	3	510	CL7	C1A-NA-C4A	5.82	109.82	106.30
32	3	522	ZEX	C28-C27-C26	-5.82	117.15	127.09
21	5	418	CL7	C1A-NA-C4A	5.81	109.82	106.30
23	c	516	8CT	C04-C03-C02	-5.81	114.43	122.61
21	3	516	CL7	C1A-NA-C4A	5.81	109.82	106.30
21	C	512	CL7	C1A-NA-C4A	5.80	109.81	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	406	CL7	C1A-NA-C4A	5.80	109.81	106.30
21	c	512	CL7	C1A-NA-C4A	5.80	109.81	106.30
23	C	516	8CT	C04-C03-C02	-5.80	114.44	122.61
21	C	505	CL7	C1A-NA-C4A	5.79	109.81	106.30
32	1	421	ZEX	C28-C27-C26	-5.79	117.20	127.09
32	5	421	ZEX	C28-C27-C26	-5.79	117.20	127.09
21	3	513	CL7	C1A-NA-C4A	5.78	109.80	106.30
21	1	418	CL7	C1A-NA-C4A	5.77	109.79	106.30
23	B	619	8CT	C14-C13-C12	-5.77	119.08	127.31
21	2	513	CL7	C1A-NA-C4A	5.76	109.79	106.30
21	C	509	CL7	C1A-NA-C4A	5.76	109.79	106.30
21	c	509	CL7	C1A-NA-C4A	5.76	109.79	106.30
21	6	502	CL7	C1A-NA-C4A	5.75	109.78	106.30
21	c	505	CL7	C1A-NA-C4A	5.74	109.78	106.30
31	f	101	HEM	CHC-C4B-NB	5.74	130.66	124.43
21	2	515	CL7	C1A-NA-C4A	5.74	109.77	106.30
21	6	515	CL7	C1A-NA-C4A	5.74	109.77	106.30
21	7	516	CL7	C1A-NA-C4A	5.74	109.77	106.30
31	F	101	HEM	CHC-C4B-NB	5.74	130.66	124.43
23	K	101	8CT	C19-C20-C21	-5.73	119.13	127.31
23	k	101	8CT	C19-C20-C21	-5.73	119.13	127.31
23	b	620	8CT	C14-C13-C12	-5.73	119.13	127.31
32	4	403	ZEX	C15-C14-C13	-5.73	119.13	127.31
21	C	513	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	c	513	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	B	614	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	2	508	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	b	615	CL7	C1A-NA-C4A	5.73	109.77	106.30
21	6	516	CL7	C1A-NA-C4A	5.73	109.77	106.30
23	b	619	8CT	C18-C17-C16	-5.73	119.14	127.31
21	6	508	CL7	C1A-NA-C4A	5.72	109.76	106.30
21	B	611	CL7	C1A-NA-C4A	5.71	109.76	106.30
32	8	403	ZEX	C15-C14-C13	-5.71	119.16	127.31
21	2	502	CL7	C1A-NA-C4A	5.71	109.75	106.30
23	B	618	8CT	C18-C17-C16	-5.70	119.17	127.31
21	8	413	CL7	C1A-NA-C4A	5.70	109.75	106.30
23	C	516	8CT	C35-C30-C29	-5.70	105.50	112.70
21	4	404	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	B	608	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	c	514	CL7	C1A-NA-C4A	5.70	109.75	106.30
21	4	413	CL7	C1A-NA-C4A	5.69	109.74	106.30
21	2	516	CL7	C1A-NA-C4A	5.68	109.74	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	508	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	7	508	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	2	505	CL7	C1-C2-C3	5.68	135.86	126.04
21	6	505	CL7	C1-C2-C3	5.68	135.86	126.04
21	B	612	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	3	507	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	b	613	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	7	507	CL7	C1A-NA-C4A	5.68	109.74	106.30
23	c	516	8CT	C35-C30-C29	-5.68	105.53	112.70
21	1	409	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	5	409	CL7	C1A-NA-C4A	5.68	109.74	106.30
21	c	508	CL7	C1A-NA-C4A	5.67	109.74	106.30
21	b	609	CL7	C1A-NA-C4A	5.67	109.73	106.30
21	b	612	CL7	C1A-NA-C4A	5.65	109.72	106.30
21	C	514	CL7	C1A-NA-C4A	5.64	109.72	106.30
21	1	407	CL7	C1A-NA-C4A	5.64	109.72	106.30
21	c	504	CL7	C1A-NA-C4A	5.64	109.72	106.30
21	6	507	CL7	C1A-NA-C4A	5.64	109.71	106.30
21	8	404	CL7	C1A-NA-C4A	5.64	109.71	106.30
21	C	508	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	2	512	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	6	512	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	2	514	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	6	514	CL7	C1A-NA-C4A	5.63	109.71	106.30
21	8	408	CL7	C1A-NA-C4A	5.62	109.71	106.30
21	2	504	CL7	C1A-NA-C4A	5.62	109.70	106.30
21	4	408	CL7	C1A-NA-C4A	5.62	109.70	106.30
32	2	523	ZEX	C27-C28-C29	-5.61	117.75	126.23
32	6	522	ZEX	C27-C28-C29	-5.61	117.75	126.23
23	B	617	8CT	C18-C17-C16	-5.61	119.30	127.31
23	b	618	8CT	C18-C17-C16	-5.61	119.30	127.31
21	C	504	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	1	408	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	5	407	CL7	C1A-NA-C4A	5.61	109.70	106.30
21	1	404	CL7	C1A-NA-C4A	5.60	109.69	106.30
21	6	504	CL7	C1A-NA-C4A	5.60	109.69	106.30
21	5	404	CL7	C1A-NA-C4A	5.60	109.69	106.30
21	2	507	CL7	C1A-NA-C4A	5.59	109.69	106.30
21	1	405	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	5	405	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	5	408	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	2	510	CL7	C1A-NA-C4A	5.58	109.68	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	510	CL7	C1A-NA-C4A	5.58	109.68	106.30
21	C	503	CL7	C1A-NA-C4A	5.56	109.67	106.30
21	c	503	CL7	C1A-NA-C4A	5.56	109.67	106.30
23	C	516	8CT	C24-C25-C26	-5.56	119.37	127.31
23	c	516	8CT	C24-C25-C26	-5.56	119.37	127.31
21	3	515	CL7	C1A-NA-C4A	5.52	109.64	106.30
21	5	416	CL7	C1A-NA-C4A	5.51	109.64	106.30
23	4	402	8CT	C19-C20-C21	-5.51	119.45	127.31
21	C	518	CL7	C1A-NA-C4A	5.50	109.63	106.30
21	c	518	CL7	C1A-NA-C4A	5.50	109.63	106.30
23	8	402	8CT	C19-C20-C21	-5.49	119.48	127.31
21	1	416	CL7	C1A-NA-C4A	5.48	109.62	106.30
21	3	509	CL7	C1A-NA-C4A	5.48	109.62	106.30
23	C	519	8CT	C19-C20-C21	-5.47	119.50	127.31
23	c	519	8CT	C19-C20-C21	-5.47	119.50	127.31
21	c	507	CL7	C1A-NA-C4A	5.47	109.61	106.30
21	1	410	CL7	C1A-NA-C4A	5.46	109.61	106.30
21	5	410	CL7	C1A-NA-C4A	5.46	109.61	106.30
21	7	509	CL7	C1A-NA-C4A	5.46	109.61	106.30
21	4	407	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	8	407	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	7	517	CL7	C1A-NA-C4A	5.45	109.60	106.30
21	2	511	CL7	C1A-NA-C4A	5.43	109.59	106.30
21	6	511	CL7	C1A-NA-C4A	5.43	109.59	106.30
23	K	101	8CT	C07-C02-C03	-5.43	114.85	122.73
23	k	101	8CT	C07-C02-C03	-5.43	114.85	122.73
21	2	506	CL7	C1A-NA-C4A	5.42	109.58	106.30
21	6	506	CL7	C1A-NA-C4A	5.42	109.58	106.30
21	C	507	CL7	C1A-NA-C4A	5.42	109.58	106.30
21	3	501	CL7	C1A-NA-C4A	5.40	109.57	106.30
21	4	416	CL7	C1A-NA-C4A	5.40	109.57	106.30
23	A	404	8CT	C14-C13-C12	-5.40	119.61	127.31
23	a	404	8CT	C14-C13-C12	-5.40	119.61	127.31
21	7	515	CL7	C1A-NA-C4A	5.40	109.57	106.30
21	8	416	CL7	C1A-NA-C4A	5.38	109.56	106.30
21	A	403	CL7	C1A-NA-C4A	5.38	109.56	106.30
21	a	403	CL7	C1A-NA-C4A	5.38	109.56	106.30
21	3	517	CL7	C1A-NA-C4A	5.38	109.56	106.30
23	k	101	8CT	C14-C13-C12	-5.37	119.64	127.31
21	B	606	CL7	C1A-NA-C4A	5.37	109.55	106.30
21	b	607	CL7	C1A-NA-C4A	5.37	109.55	106.30
21	a	401	CL7	C1A-NA-C4A	5.36	109.55	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	K	101	8CT	C14-C13-C12	-5.36	119.67	127.31
21	1	419	CL7	C1A-NA-C4A	5.35	109.54	106.30
21	5	419	CL7	C1A-NA-C4A	5.35	109.54	106.30
32	2	519	ZEX	C35-C34-C33	-5.35	119.67	127.31
32	6	519	ZEX	C35-C34-C33	-5.35	119.67	127.31
21	7	501	CL7	C1A-NA-C4A	5.34	109.53	106.30
23	D	406	8CT	C18-C17-C16	-5.33	119.70	127.31
21	c	510	CL7	C1A-NA-C4A	5.33	109.53	106.30
23	d	406	8CT	C18-C17-C16	-5.33	119.71	127.31
21	C	510	CL7	C1A-NA-C4A	5.32	109.52	106.30
32	2	520	ZEX	C35-C34-C33	-5.29	119.75	127.31
21	A	401	CL7	C1A-NA-C4A	5.29	109.50	106.30
32	3	525	ZEX	C35-C34-C33	-5.29	119.77	127.31
21	3	518	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	7	518	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	B	602	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	2	509	CL7	C1A-NA-C4A	5.28	109.50	106.30
23	D	406	8CT	C01-C02-C03	-5.28	118.60	124.53
23	d	406	8CT	C01-C02-C03	-5.28	118.60	124.53
21	b	603	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	B	616	CL7	C1A-NA-C4A	5.28	109.50	106.30
21	2	518	CL7	C1A-NA-C4A	5.28	109.50	106.30
23	B	617	8CT	C30-C31-C32	-5.27	114.99	121.47
21	B	609	CL7	C1A-NA-C4A	5.25	109.48	106.30
32	3	522	ZEX	C35-C34-C33	-5.24	119.83	127.31
32	7	522	ZEX	C35-C34-C33	-5.24	119.83	127.31
32	2	521	ZEX	C27-C28-C29	-5.24	118.32	126.23
32	6	520	ZEX	C27-C28-C29	-5.24	118.32	126.23
23	b	618	8CT	C30-C31-C32	-5.23	115.03	121.47
21	6	509	CL7	C1A-NA-C4A	5.23	109.47	106.30
32	2	519	ZEX	C15-C14-C13	-5.22	119.86	127.31
21	b	617	CL7	C1A-NA-C4A	5.22	109.46	106.30
21	6	518	CL7	C1A-NA-C4A	5.22	109.46	106.30
32	3	520	ZEX	C27-C28-C29	-5.21	118.37	126.23
32	7	520	ZEX	C27-C28-C29	-5.21	118.37	126.23
32	6	519	ZEX	C15-C14-C13	-5.20	119.88	127.31
21	2	517	CL7	C1A-NA-C4A	5.20	109.45	106.30
21	1	417	CL7	C1A-NA-C4A	5.20	109.45	106.30
21	4	412	CL7	C1A-NA-C4A	5.19	109.45	106.30
21	b	610	CL7	C1A-NA-C4A	5.19	109.45	106.30
21	8	412	CL7	C1A-NA-C4A	5.19	109.45	106.30
23	D	406	8CT	C30-C31-C32	-5.19	115.09	121.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	411	CL7	C1A-NA-C4A	5.18	109.44	106.30
21	6	517	CL7	C1A-NA-C4A	5.17	109.43	106.30
32	1	422	ZEX	C28-C27-C26	-5.15	118.28	127.09
21	B	607	CL7	C1A-NA-C4A	5.15	109.42	106.30
23	c	516	8CT	C18-C17-C16	-5.15	119.97	127.31
23	d	406	8CT	C30-C31-C32	-5.15	115.14	121.47
23	B	617	8CT	C01-C02-C03	-5.15	118.75	124.53
23	K	101	8CT	C04-C03-C02	-5.14	115.37	122.61
23	k	101	8CT	C04-C03-C02	-5.14	115.37	122.61
21	1	411	CL7	C1A-NA-C4A	5.14	109.42	106.30
32	5	422	ZEX	C28-C27-C26	-5.14	118.30	127.09
21	5	417	CL7	C1A-NA-C4A	5.13	109.41	106.30
23	C	516	8CT	C18-C17-C16	-5.13	119.99	127.31
21	B	613	CL7	C1A-NA-C4A	5.12	109.40	106.30
21	b	614	CL7	C1A-NA-C4A	5.12	109.40	106.30
32	8	403	ZEX	C35-C34-C33	-5.12	120.00	127.31
32	4	403	ZEX	C35-C34-C33	-5.12	120.00	127.31
21	8	411	CL7	C1A-NA-C4A	5.12	109.40	106.30
21	b	608	CL7	C1A-NA-C4A	5.11	109.40	106.30
32	3	519	ZEX	C7-C8-C9	-5.11	118.51	126.23
32	7	519	ZEX	C7-C8-C9	-5.11	118.51	126.23
21	4	411	CL7	C1A-NA-C4A	5.11	109.39	106.30
32	2	523	ZEX	C15-C14-C13	-5.10	120.03	127.31
23	b	618	8CT	C01-C02-C03	-5.09	118.81	124.53
32	6	522	ZEX	C15-C14-C13	-5.08	120.05	127.31
21	7	512	CL7	C1A-NA-C4A	5.07	109.37	106.30
21	3	512	CL7	C1A-NA-C4A	5.06	109.36	106.30
23	K	101	8CT	C01-C02-C03	-5.06	118.85	124.53
23	k	101	8CT	C01-C02-C03	-5.06	118.85	124.53
21	1	414	CL7	C1A-NA-C4A	5.04	109.35	106.30
21	5	414	CL7	C1A-NA-C4A	5.04	109.35	106.30
21	D	402	CL7	C1A-NA-C4A	5.03	109.35	106.30
21	d	402	CL7	C1A-NA-C4A	5.03	109.35	106.30
26	C	501	LMG	O7-C10-C11	5.02	122.32	111.50
32	8	420	ZEX	C15-C14-C13	-5.02	120.15	127.31
23	b	620	8CT	C18-C17-C16	-5.01	120.17	127.31
32	4	419	ZEX	C35-C34-C33	-5.00	120.18	127.31
32	4	420	ZEX	C15-C14-C13	-4.99	120.18	127.31
23	B	618	8CT	C14-C13-C12	-4.98	120.20	127.31
23	B	619	8CT	C18-C17-C16	-4.98	120.20	127.31
32	8	419	ZEX	C35-C34-C33	-4.98	120.21	127.31
32	7	519	ZEX	C28-C27-C26	-4.98	118.59	127.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	3	519	ZEX	C28-C27-C26	-4.97	118.60	127.09
32	4	418	ZEX	C27-C28-C29	-4.97	118.73	126.23
23	B	617	8CT	C24-C25-C26	-4.97	120.22	127.31
23	b	618	8CT	C24-C25-C26	-4.97	120.22	127.31
23	c	516	8CT	C19-C20-C21	-4.97	120.22	127.31
23	k	101	8CT	C35-C30-C29	-4.97	106.42	112.70
23	b	619	8CT	C14-C13-C12	-4.97	120.22	127.31
23	C	516	8CT	C19-C20-C21	-4.96	120.23	127.31
23	K	101	8CT	C10-C11-C12	-4.96	118.74	126.23
23	k	101	8CT	C10-C11-C12	-4.96	118.74	126.23
31	F	101	HEM	CBA-CAA-C2A	-4.96	104.16	112.62
31	f	101	HEM	CBA-CAA-C2A	-4.96	104.16	112.62
23	K	101	8CT	C35-C30-C29	-4.95	106.44	112.70
32	8	418	ZEX	C27-C28-C29	-4.94	118.77	126.23
26	c	501	LMG	O7-C10-C11	4.94	122.16	111.50
23	a	404	8CT	C18-C17-C16	-4.94	120.26	127.31
23	c	519	8CT	C14-C13-C12	-4.93	120.27	127.31
23	C	519	8CT	C14-C13-C12	-4.92	120.28	127.31
23	A	404	8CT	C18-C17-C16	-4.92	120.29	127.31
23	B	627	8CT	C19-C18-C17	-4.88	113.47	123.47
23	b	601	8CT	C19-C18-C17	-4.87	113.49	123.47
31	f	101	HEM	CHD-C1D-ND	4.84	129.69	124.43
31	F	101	HEM	CHD-C1D-ND	4.84	129.69	124.43
21	B	622	CL7	C1A-NA-C4A	4.82	109.22	106.30
21	b	623	CL7	C1A-NA-C4A	4.82	109.22	106.30
23	B	619	8CT	C30-C31-C32	-4.81	115.55	121.47
23	b	620	8CT	C30-C31-C32	-4.81	115.55	121.47
23	B	619	8CT	C10-C11-C12	-4.80	118.98	126.23
23	b	620	8CT	C10-C11-C12	-4.80	118.98	126.23
32	7	520	ZEX	C15-C14-C13	-4.79	120.47	127.31
32	3	520	ZEX	C15-C14-C13	-4.79	120.48	127.31
32	4	418	ZEX	C35-C34-C33	-4.76	120.52	127.31
32	8	418	ZEX	C35-C34-C33	-4.76	120.52	127.31
32	2	525	ZEX	C35-C34-C33	-4.75	120.53	127.31
32	6	524	ZEX	C35-C34-C33	-4.75	120.53	127.31
21	c	511	CL7	C1A-NA-C4A	4.75	109.17	106.30
21	C	511	CL7	C1A-NA-C4A	4.72	109.16	106.30
32	4	403	ZEX	C11-C10-C9	-4.71	120.58	127.31
32	1	422	ZEX	C27-C28-C29	-4.71	119.12	126.23
32	8	403	ZEX	C11-C10-C9	-4.70	120.60	127.31
32	5	422	ZEX	C27-C28-C29	-4.70	119.14	126.23
23	A	404	8CT	C01-C02-C03	-4.70	119.25	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	8CT	C01-C02-C03	-4.68	119.27	124.53
23	b	618	8CT	C07-C02-C03	-4.67	115.94	122.73
23	B	617	8CT	C07-C02-C03	-4.67	115.96	122.73
23	C	515	8CT	C01-C02-C03	-4.66	119.29	124.53
23	c	515	8CT	C01-C02-C03	-4.66	119.29	124.53
32	8	420	ZEX	C11-C10-C9	-4.65	120.67	127.31
32	4	420	ZEX	C11-C10-C9	-4.65	120.68	127.31
23	B	627	8CT	C01-C02-C03	-4.62	119.34	124.53
23	b	601	8CT	C01-C02-C03	-4.62	119.34	124.53
21	4	415	CL7	O2D-CGD-CBD	4.62	119.47	111.27
21	8	415	CL7	O2D-CGD-CBD	4.62	119.47	111.27
23	C	515	8CT	C19-C20-C21	-4.61	120.73	127.31
23	c	515	8CT	C19-C20-C21	-4.60	120.75	127.31
23	b	601	8CT	C24-C23-C21	-4.56	113.61	126.42
23	B	627	8CT	C24-C23-C21	-4.55	113.64	126.42
23	4	402	8CT	C01-C02-C03	-4.55	119.42	124.53
32	4	419	ZEX	C8-C7-C6	-4.54	114.44	127.20
23	8	402	8CT	C01-C02-C03	-4.53	119.44	124.53
32	8	419	ZEX	C8-C7-C6	-4.53	114.49	127.20
23	C	519	8CT	C01-C02-C03	-4.51	119.47	124.53
23	c	519	8CT	C01-C02-C03	-4.50	119.48	124.53
32	8	420	ZEX	C7-C8-C9	-4.50	119.44	126.23
32	6	519	ZEX	C7-C8-C9	-4.48	119.46	126.23
32	4	420	ZEX	C7-C8-C9	-4.48	119.46	126.23
32	7	522	ZEX	C15-C14-C13	-4.47	120.93	127.31
32	8	418	ZEX	C11-C10-C9	-4.47	120.93	127.31
32	3	522	ZEX	C15-C14-C13	-4.46	120.94	127.31
32	2	519	ZEX	C7-C8-C9	-4.46	119.49	126.23
21	2	505	CL7	O2A-C1-C2	-4.45	96.93	108.64
21	6	505	CL7	O2A-C1-C2	-4.45	96.93	108.64
32	4	418	ZEX	C11-C10-C9	-4.44	120.97	127.31
32	2	520	ZEX	C27-C26-C25	-4.41	115.71	122.84
32	3	525	ZEX	C27-C26-C25	-4.41	115.71	122.84
23	B	618	8CT	C04-C03-C02	-4.41	116.41	122.61
23	b	619	8CT	C04-C03-C02	-4.41	116.41	122.61
32	2	525	ZEX	C15-C14-C13	-4.40	121.04	127.31
21	3	511	CL7	CAA-CBA-CGA	-4.40	100.41	113.25
21	7	511	CL7	CAA-CBA-CGA	-4.40	100.41	113.25
21	a	401	CL7	C1-C2-C3	-4.39	118.45	126.04
32	1	422	ZEX	C11-C10-C9	-4.38	121.06	127.31
32	5	422	ZEX	C11-C10-C9	-4.38	121.06	127.31
21	A	401	CL7	C1-C2-C3	-4.36	118.50	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	1	421	ZEX	C35-C34-C33	-4.36	121.08	127.31
32	5	421	ZEX	C35-C34-C33	-4.36	121.08	127.31
32	6	524	ZEX	C15-C14-C13	-4.33	121.13	127.31
21	7	502	CL7	C1A-NA-C4A	4.33	108.92	106.30
21	8	409	CL7	O2D-CGD-CBD	4.31	118.93	111.27
32	3	519	ZEX	C18-C5-C6	-4.31	119.69	124.53
32	8	403	ZEX	C27-C28-C29	-4.30	119.73	126.23
21	4	409	CL7	O2D-CGD-CBD	4.29	118.89	111.27
32	4	418	ZEX	C28-C27-C26	-4.29	119.76	127.09
32	8	418	ZEX	C28-C27-C26	-4.29	119.76	127.09
32	7	519	ZEX	C18-C5-C6	-4.29	119.71	124.53
32	4	403	ZEX	C27-C28-C29	-4.29	119.76	126.23
21	3	507	CL7	O2D-CGD-CBD	4.29	118.89	111.27
21	7	507	CL7	O2D-CGD-CBD	4.29	118.89	111.27
21	1	420	CL7	O2D-CGD-CBD	4.28	118.87	111.27
21	3	502	CL7	C1A-NA-C4A	4.27	108.89	106.30
23	A	404	8CT	C30-C31-C32	-4.27	116.21	121.47
32	6	520	ZEX	C35-C34-C33	-4.27	121.22	127.31
21	8	411	CL7	C3A-C4A-CHB	-4.27	117.36	123.70
21	5	420	CL7	O2D-CGD-CBD	4.27	118.85	111.27
23	C	519	8CT	C18-C17-C16	-4.26	121.22	127.31
21	4	411	CL7	C3A-C4A-CHB	-4.26	117.37	123.70
23	a	404	8CT	C30-C31-C32	-4.26	116.22	121.47
23	c	519	8CT	C18-C17-C16	-4.25	121.24	127.31
32	2	521	ZEX	C35-C34-C33	-4.24	121.25	127.31
32	5	422	ZEX	C35-C34-C33	-4.24	121.26	127.31
21	2	507	CL7	O2D-CGD-CBD	4.24	118.80	111.27
21	6	507	CL7	O2D-CGD-CBD	4.24	118.80	111.27
23	4	402	8CT	C11-C10-C03	-4.24	115.31	127.20
32	7	520	ZEX	C18-C5-C6	-4.24	119.77	124.53
23	8	402	8CT	C11-C10-C03	-4.23	115.31	127.20
23	B	618	8CT	C01-C02-C03	-4.22	119.78	124.53
23	b	619	8CT	C01-C02-C03	-4.22	119.78	124.53
21	B	614	CL7	C3A-C4A-CHB	-4.22	117.43	123.70
21	b	615	CL7	C3A-C4A-CHB	-4.22	117.43	123.70
23	B	619	8CT	C35-C30-C29	-4.22	107.37	112.70
32	1	422	ZEX	C35-C34-C33	-4.22	121.29	127.31
32	3	520	ZEX	C18-C5-C6	-4.21	119.80	124.53
23	b	620	8CT	C35-C30-C29	-4.20	107.39	112.70
32	3	520	ZEX	C28-C27-C26	-4.18	119.95	127.09
32	7	520	ZEX	C28-C27-C26	-4.18	119.95	127.09
32	8	418	ZEX	C7-C8-C9	-4.17	119.94	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	7	522	ZEX	C27-C28-C29	-4.17	119.94	126.23
32	4	418	ZEX	C7-C8-C9	-4.16	119.95	126.23
23	4	402	8CT	C13-C14-C15	-4.15	110.25	123.22
23	8	402	8CT	C13-C14-C15	-4.15	110.25	123.22
32	3	522	ZEX	C27-C28-C29	-4.15	119.96	126.23
21	a	401	CL7	C3A-C4A-CHB	-4.15	117.55	123.70
21	A	401	CL7	C3A-C4A-CHB	-4.14	117.55	123.70
21	7	514	CL7	O2D-CGD-CBD	4.14	118.62	111.27
21	B	606	CL7	C3A-C4A-CHB	-4.13	117.58	123.70
21	b	607	CL7	C3A-C4A-CHB	-4.13	117.58	123.70
21	3	514	CL7	O2D-CGD-CBD	4.12	118.59	111.27
21	3	518	CL7	C3A-C4A-CHB	-4.11	117.60	123.70
32	6	520	ZEX	C28-C27-C26	-4.11	120.07	127.09
21	7	518	CL7	C3A-C4A-CHB	-4.10	117.61	123.70
21	2	505	CL7	O2D-CGD-CBD	4.10	118.55	111.27
21	6	505	CL7	O2D-CGD-CBD	4.10	118.55	111.27
32	2	521	ZEX	C28-C27-C26	-4.09	120.10	127.09
21	D	405	CL7	C3A-C4A-CHB	-4.09	117.64	123.70
23	b	619	8CT	C13-C14-C15	-4.08	110.49	123.22
23	B	618	8CT	C13-C14-C15	-4.08	110.49	123.22
32	3	522	ZEX	C18-C5-C6	-4.08	119.95	124.53
32	7	522	ZEX	C18-C5-C6	-4.08	119.95	124.53
21	A	401	CL7	CAA-C2A-C1A	-4.08	98.78	112.19
32	4	420	ZEX	C31-C30-C29	-4.07	121.50	127.31
32	8	420	ZEX	C31-C30-C29	-4.07	121.50	127.31
21	d	405	CL7	C3A-C4A-CHB	-4.07	117.66	123.70
21	1	418	CL7	O2D-CGD-CBD	4.07	118.50	111.27
21	5	418	CL7	O2D-CGD-CBD	4.07	118.50	111.27
23	8	402	8CT	C07-C02-C03	-4.07	116.83	122.73
23	B	617	8CT	C14-C13-C12	-4.06	121.51	127.31
23	b	618	8CT	C14-C13-C12	-4.06	121.51	127.31
21	a	401	CL7	CAA-C2A-C1A	-4.06	98.82	112.19
21	1	404	CL7	O2D-CGD-CBD	4.06	118.48	111.27
21	1	410	CL7	C3A-C4A-CHB	-4.05	117.69	123.70
21	5	410	CL7	C3A-C4A-CHB	-4.05	117.69	123.70
23	C	519	8CT	C04-C03-C02	-4.05	116.91	122.61
23	c	519	8CT	C04-C03-C02	-4.05	116.91	122.61
21	5	404	CL7	O2D-CGD-CBD	4.05	118.47	111.27
23	k	101	8CT	C19-C18-C17	-4.05	115.18	123.47
32	2	520	ZEX	C8-C7-C6	-4.05	115.83	127.20
32	3	525	ZEX	C8-C7-C6	-4.05	115.83	127.20
21	2	503	CL7	C3A-C4A-CHB	-4.05	117.69	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	402	8CT	C07-C02-C03	-4.05	116.86	122.73
21	6	503	CL7	C3A-C4A-CHB	-4.04	117.70	123.70
23	K	101	8CT	C19-C18-C17	-4.04	115.20	123.47
21	3	510	CL7	C3A-C4A-CHB	-4.04	117.71	123.70
21	7	510	CL7	C3A-C4A-CHB	-4.04	117.71	123.70
21	3	504	CL7	C3A-C4A-CHB	-4.02	117.73	123.70
23	C	519	8CT	C07-C02-C03	-4.02	116.90	122.73
23	c	519	8CT	C07-C02-C03	-4.02	116.90	122.73
21	7	504	CL7	C3A-C4A-CHB	-4.00	117.76	123.70
32	2	523	ZEX	C27-C26-C25	-4.00	116.37	122.84
23	D	406	8CT	C14-C13-C12	-4.00	121.60	127.31
21	3	505	CL7	O2D-CGD-CBD	4.00	118.37	111.27
21	7	505	CL7	O2D-CGD-CBD	3.99	118.37	111.27
32	7	519	ZEX	C35-C34-C33	-3.99	121.61	127.31
32	6	522	ZEX	C27-C26-C25	-3.99	116.39	122.84
32	8	403	ZEX	C27-C26-C25	-3.99	116.39	122.84
23	d	406	8CT	C14-C13-C12	-3.98	121.63	127.31
21	b	604	CL7	C3A-C4A-CHB	-3.97	117.80	123.70
32	3	519	ZEX	C35-C34-C33	-3.97	121.64	127.31
21	B	603	CL7	C3A-C4A-CHB	-3.97	117.81	123.70
21	1	408	CL7	O2D-CGD-CBD	3.96	118.30	111.27
23	A	404	8CT	C35-C30-C29	-3.96	107.70	112.70
21	B	606	CL7	O2D-CGD-CBD	3.95	118.29	111.27
32	4	403	ZEX	C27-C26-C25	-3.95	116.45	122.84
21	5	408	CL7	O2D-CGD-CBD	3.94	118.28	111.27
21	7	513	CL7	C3A-C4A-CHB	-3.94	117.85	123.70
23	a	404	8CT	C35-C30-C29	-3.93	107.73	112.70
21	B	610	CL7	CAA-CBA-CGA	-3.93	101.75	113.25
21	C	510	CL7	C3A-C4A-CHB	-3.93	117.86	123.70
21	c	510	CL7	C3A-C4A-CHB	-3.93	117.86	123.70
21	3	513	CL7	C3A-C4A-CHB	-3.93	117.87	123.70
21	b	611	CL7	CAA-CBA-CGA	-3.93	101.77	113.25
21	b	607	CL7	O2D-CGD-CBD	3.92	118.24	111.27
21	C	505	CL7	C3A-C4A-CHB	-3.92	117.88	123.70
21	c	505	CL7	C3A-C4A-CHB	-3.92	117.88	123.70
21	4	405	CL7	CAA-CBA-CGA	-3.92	101.81	113.25
21	8	405	CL7	CAA-CBA-CGA	-3.92	101.81	113.25
23	B	617	8CT	C10-C11-C12	-3.92	120.32	126.23
32	7	520	ZEX	C7-C8-C9	-3.91	120.32	126.23
32	2	523	ZEX	C1-C6-C5	-3.91	117.11	122.61
32	6	522	ZEX	C1-C6-C5	-3.91	117.11	122.61
21	C	511	CL7	CAA-CBA-CGA	-3.91	101.83	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	511	CL7	CAA-CBA-CGA	-3.91	101.83	113.25
23	b	618	8CT	C10-C11-C12	-3.91	120.33	126.23
21	3	511	CL7	O2D-CGD-CBD	3.90	118.21	111.27
21	7	511	CL7	O2D-CGD-CBD	3.90	118.21	111.27
21	2	504	CL7	C3A-C4A-CHB	-3.90	117.91	123.70
21	6	504	CL7	C3A-C4A-CHB	-3.90	117.91	123.70
32	1	421	ZEX	C27-C28-C29	-3.90	120.34	126.23
32	5	421	ZEX	C27-C28-C29	-3.90	120.34	126.23
32	2	523	ZEX	C31-C30-C29	-3.90	121.75	127.31
32	6	522	ZEX	C31-C30-C29	-3.90	121.75	127.31
32	3	520	ZEX	C7-C8-C9	-3.89	120.35	126.23
21	5	408	CL7	C3A-C4A-CHB	-3.88	117.94	123.70
21	6	512	CL7	CHD-C4C-C3C	-3.87	118.67	124.93
21	1	408	CL7	C3A-C4A-CHB	-3.87	117.96	123.70
21	a	403	CL7	CHD-C4C-C3C	-3.86	118.69	124.93
21	6	503	CL7	CED-O2D-CGD	-3.86	107.20	115.94
23	d	406	8CT	C25-C24-C23	-3.86	111.18	123.22
21	2	512	CL7	CHD-C4C-C3C	-3.86	118.70	124.93
23	D	406	8CT	C25-C24-C23	-3.86	111.18	123.22
21	3	512	CL7	C3A-C4A-CHB	-3.85	117.99	123.70
21	7	512	CL7	C3A-C4A-CHB	-3.85	117.99	123.70
21	c	509	CL7	O2D-CGD-CBD	3.84	118.10	111.27
21	7	506	CL7	C3A-C4A-CHB	-3.84	118.00	123.70
21	A	403	CL7	CHD-C4C-C3C	-3.84	118.72	124.93
21	B	614	CL7	CAA-C2A-C3A	-3.84	102.26	112.78
21	2	503	CL7	CED-O2D-CGD	-3.84	107.25	115.94
23	C	516	8CT	C14-C15-C16	-3.84	115.63	126.42
21	3	506	CL7	C3A-C4A-CHB	-3.84	118.01	123.70
21	2	512	CL7	O2D-CGD-CBD	3.84	118.08	111.27
21	6	512	CL7	O2D-CGD-CBD	3.84	118.08	111.27
21	b	615	CL7	CAA-C2A-C3A	-3.83	102.28	112.78
21	6	513	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
23	D	406	8CT	C10-C11-C12	-3.83	120.45	126.23
21	2	513	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
21	C	508	CL7	C3A-C4A-CHB	-3.83	118.02	123.70
23	d	406	8CT	C10-C11-C12	-3.82	120.46	126.23
23	c	516	8CT	C14-C15-C16	-3.82	115.69	126.42
21	C	503	CL7	C3A-C4A-CHB	-3.81	118.04	123.70
27	b	625	DGD	O2G-C1B-C2B	3.81	119.72	111.50
21	c	503	CL7	C3A-C4A-CHB	-3.81	118.04	123.70
32	2	520	ZEX	C15-C14-C13	-3.81	121.87	127.31
32	3	525	ZEX	C15-C14-C13	-3.81	121.87	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	509	CL7	O2D-CGD-CBD	3.81	118.04	111.27
21	C	508	CL7	O2D-CGD-CBD	3.81	118.04	111.27
21	c	508	CL7	O2D-CGD-CBD	3.81	118.04	111.27
32	5	422	ZEX	C15-C14-C13	-3.80	121.88	127.31
32	1	422	ZEX	C15-C14-C13	-3.80	121.88	127.31
23	B	617	8CT	C04-C03-C02	-3.80	117.26	122.61
21	c	508	CL7	C3A-C4A-CHB	-3.80	118.06	123.70
32	1	421	ZEX	C15-C14-C13	-3.80	121.89	127.31
21	B	622	CL7	C3A-C4A-CHB	-3.80	118.06	123.70
21	b	623	CL7	C3A-C4A-CHB	-3.80	118.06	123.70
27	B	624	DGD	O2G-C1B-C2B	3.80	119.68	111.50
21	6	507	CL7	C3A-C4A-CHB	-3.80	118.07	123.70
32	4	418	ZEX	C18-C5-C6	-3.79	120.27	124.53
32	8	418	ZEX	C18-C5-C6	-3.79	120.27	124.53
21	2	507	CL7	C3A-C4A-CHB	-3.79	118.08	123.70
32	5	421	ZEX	C15-C14-C13	-3.79	121.90	127.31
21	b	611	CL7	O2D-CGD-CBD	3.78	117.99	111.27
31	F	101	HEM	C1B-NB-C4B	3.78	108.98	105.07
31	f	101	HEM	C1B-NB-C4B	3.78	108.98	105.07
23	b	618	8CT	C04-C03-C02	-3.78	117.29	122.61
21	8	404	CL7	C3A-C4A-CHB	-3.78	118.09	123.70
32	3	519	ZEX	C15-C35-C34	-3.77	115.75	123.47
32	7	519	ZEX	C15-C35-C34	-3.77	115.75	123.47
21	3	502	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	7	502	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	3	503	CL7	CHD-C4C-C3C	-3.77	118.84	124.93
21	7	503	CL7	CHD-C4C-C3C	-3.77	118.84	124.93
21	6	518	CL7	C3A-C4A-CHB	-3.77	118.11	123.70
21	B	610	CL7	O2D-CGD-CBD	3.76	117.96	111.27
21	4	413	CL7	C3A-C4A-CHB	-3.76	118.11	123.70
21	8	413	CL7	C3A-C4A-CHB	-3.76	118.11	123.70
31	F	101	HEM	CHA-C4D-ND	3.76	129.03	124.38
31	f	101	HEM	CHA-C4D-ND	3.76	129.03	124.38
21	4	408	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	8	408	CL7	C3A-C4A-CHB	-3.76	118.12	123.70
21	4	404	CL7	C3A-C4A-CHB	-3.76	118.13	123.70
21	1	407	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
21	5	407	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
21	2	518	CL7	C3A-C4A-CHB	-3.75	118.13	123.70
32	4	420	ZEX	C35-C34-C33	-3.75	121.95	127.31
32	8	420	ZEX	C35-C34-C33	-3.75	121.95	127.31
21	1	404	CL7	C1-C2-C3	3.75	132.53	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	404	CL7	C1-C2-C3	3.75	132.53	126.04
21	B	604	CL7	O2D-CGD-CBD	3.75	117.93	111.27
23	B	627	8CT	C39-C16-C17	-3.75	117.67	122.92
23	b	620	8CT	C24-C23-C21	-3.74	115.90	126.42
21	1	414	CL7	C3A-C4A-CHB	-3.74	118.14	123.70
21	5	414	CL7	C3A-C4A-CHB	-3.74	118.14	123.70
21	b	605	CL7	O2D-CGD-CBD	3.74	117.91	111.27
21	4	405	CL7	C1-C2-C3	3.74	132.51	126.04
21	8	405	CL7	C1-C2-C3	3.74	132.51	126.04
23	c	515	8CT	C10-C11-C12	-3.74	120.59	126.23
21	1	402	CL7	C3A-C4A-CHB	-3.74	118.16	123.70
21	5	402	CL7	C3A-C4A-CHB	-3.74	118.16	123.70
21	2	503	CL7	CAA-CBA-CGA	-3.74	102.34	113.25
21	6	503	CL7	CAA-CBA-CGA	-3.74	102.34	113.25
23	B	619	8CT	C01-C02-C03	-3.73	120.33	124.53
23	b	620	8CT	C01-C02-C03	-3.73	120.33	124.53
21	6	503	CL7	CHD-C4C-C3C	-3.73	118.90	124.93
32	8	419	ZEX	C31-C30-C29	-3.73	121.99	127.31
32	4	419	ZEX	C31-C30-C29	-3.72	121.99	127.31
23	b	601	8CT	C39-C16-C17	-3.72	117.71	122.92
21	2	503	CL7	CHD-C4C-C3C	-3.72	118.91	124.93
21	C	507	CL7	C3A-C4A-CHB	-3.72	118.18	123.70
21	c	507	CL7	C3A-C4A-CHB	-3.72	118.18	123.70
23	C	515	8CT	C10-C11-C12	-3.72	120.61	126.23
23	K	101	8CT	C24-C25-C26	-3.72	122.00	127.31
23	k	101	8CT	C24-C25-C26	-3.72	122.00	127.31
23	B	619	8CT	C24-C23-C21	-3.72	115.97	126.42
32	2	521	ZEX	C15-C14-C13	-3.72	122.00	127.31
32	2	523	ZEX	C31-C32-C33	-3.72	115.98	126.42
21	C	504	CL7	C3A-C4A-CHB	-3.72	118.19	123.70
21	c	504	CL7	C3A-C4A-CHB	-3.72	118.19	123.70
21	B	609	CL7	C3A-C4A-CHB	-3.71	118.19	123.70
21	b	610	CL7	C3A-C4A-CHB	-3.71	118.19	123.70
32	6	522	ZEX	C31-C32-C33	-3.70	116.01	126.42
23	k	101	8CT	C18-C17-C16	-3.70	122.02	127.31
23	B	617	8CT	C19-C20-C21	-3.70	122.03	127.31
23	b	618	8CT	C19-C20-C21	-3.70	122.03	127.31
21	4	411	CL7	O2A-C1-C2	-3.70	98.91	108.64
21	8	411	CL7	O2A-C1-C2	-3.70	98.91	108.64
23	B	619	8CT	C11-C10-C03	-3.70	116.82	127.20
23	b	620	8CT	C11-C10-C03	-3.70	116.82	127.20
32	6	520	ZEX	C15-C14-C13	-3.69	122.04	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	612	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	B	622	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	b	613	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	b	623	CL7	O2D-CGD-CBD	3.69	117.83	111.27
21	2	517	CL7	C3A-C4A-CHB	-3.69	118.22	123.70
23	K	101	8CT	C18-C17-C16	-3.69	122.05	127.31
21	C	514	CL7	C3A-C4A-CHB	-3.69	118.23	123.70
21	C	502	CL7	CHD-C4C-C3C	-3.68	118.98	124.93
21	c	502	CL7	CHD-C4C-C3C	-3.68	118.98	124.93
21	4	409	CL7	C4D-C3D-CAD	-3.68	101.86	107.81
21	3	516	CL7	C7-C6-C5	-3.68	103.37	113.36
21	7	516	CL7	C7-C6-C5	-3.68	103.37	113.36
21	8	409	CL7	C4D-C3D-CAD	-3.68	101.86	107.81
21	3	511	CL7	CHD-C4C-C3C	-3.67	118.99	124.93
21	7	511	CL7	CHD-C4C-C3C	-3.67	118.99	124.93
21	c	514	CL7	C3A-C4A-CHB	-3.67	118.25	123.70
21	7	508	CL7	C1-C2-C3	3.67	132.39	126.04
21	6	506	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	4	409	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	8	409	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	1	411	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	6	517	CL7	C3A-C4A-CHB	-3.67	118.26	123.70
21	4	412	CL7	O2D-CGD-CBD	3.66	117.78	111.27
21	8	412	CL7	O2D-CGD-CBD	3.66	117.78	111.27
21	D	404	CL7	O2D-CGD-CBD	3.66	117.77	111.27
21	d	404	CL7	O2D-CGD-CBD	3.66	117.77	111.27
21	1	420	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
21	5	420	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
21	2	506	CL7	C3A-C4A-CHB	-3.65	118.28	123.70
32	2	521	ZEX	C11-C10-C9	-3.65	122.09	127.31
21	3	508	CL7	C1-C2-C3	3.65	132.36	126.04
21	5	411	CL7	C3A-C4A-CHB	-3.65	118.29	123.70
21	6	511	CL7	C3A-C4A-CHB	-3.65	118.29	123.70
32	6	520	ZEX	C11-C10-C9	-3.64	122.11	127.31
21	2	511	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	B	602	CL7	O2D-CGD-CBD	3.64	117.73	111.27
21	B	602	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	b	603	CL7	C3A-C4A-CHB	-3.64	118.30	123.70
21	C	508	CL7	C4D-C3D-CAD	-3.64	101.92	107.81
21	c	508	CL7	C4D-C3D-CAD	-3.64	101.92	107.81
21	b	603	CL7	O2D-CGD-CBD	3.64	117.73	111.27
27	C	517	DGD	O2G-C1B-C2B	3.64	119.34	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	c	517	DGD	O2G-C1B-C2B	3.64	119.34	111.50
23	c	519	8CT	C10-C11-C12	-3.63	120.74	126.23
21	3	517	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	7	517	CL7	C3A-C4A-CHB	-3.63	118.31	123.70
21	A	406	CL7	O2D-CGD-CBD	3.63	117.72	111.27
21	a	405	CL7	O2D-CGD-CBD	3.63	117.72	111.27
21	1	406	CL7	C3A-C4A-CHB	-3.63	118.32	123.70
21	5	406	CL7	C3A-C4A-CHB	-3.63	118.32	123.70
21	1	417	CL7	CHD-C4C-C3C	-3.62	119.08	124.93
21	5	417	CL7	CHD-C4C-C3C	-3.62	119.08	124.93
21	3	503	CL7	C3A-C4A-CHB	-3.62	118.33	123.70
21	7	503	CL7	C3A-C4A-CHB	-3.62	118.33	123.70
23	C	519	8CT	C10-C11-C12	-3.62	120.77	126.23
32	4	419	ZEX	C27-C28-C29	-3.61	120.78	126.23
32	8	419	ZEX	C27-C28-C29	-3.61	120.78	126.23
21	4	407	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	8	407	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	1	414	CL7	CAC-C3C-C4C	-3.61	119.00	124.68
21	5	414	CL7	CAC-C3C-C4C	-3.61	119.00	124.68
21	c	518	CL7	O2D-CGD-CBD	3.61	117.68	111.27
23	b	601	8CT	C30-C31-C32	-3.61	117.03	121.47
21	6	501	CL7	C3A-C4A-CHB	-3.61	118.34	123.70
21	8	406	CL7	C3A-C4A-CHB	-3.61	118.35	123.70
21	3	505	CL7	C7-C6-C5	-3.61	103.57	113.36
21	4	415	CL7	C3A-C4A-CHB	-3.60	118.35	123.70
21	D	404	CL7	C3A-C4A-CHB	-3.60	118.35	123.70
21	A	406	CL7	O2A-C1-C2	-3.60	99.17	108.64
21	C	518	CL7	O2D-CGD-CBD	3.60	117.66	111.27
21	d	404	CL7	C3A-C4A-CHB	-3.60	118.36	123.70
21	7	505	CL7	C7-C6-C5	-3.59	103.60	113.36
21	4	406	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
21	2	501	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
21	a	405	CL7	O2A-C1-C2	-3.59	99.20	108.64
21	5	418	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
23	4	402	8CT	C24-C25-C26	-3.59	122.19	127.31
23	8	402	8CT	C24-C25-C26	-3.59	122.19	127.31
21	8	415	CL7	C3A-C4A-CHB	-3.59	118.37	123.70
21	3	515	CL7	O2D-CGD-CBD	3.59	117.64	111.27
21	7	515	CL7	O2D-CGD-CBD	3.59	117.64	111.27
21	5	408	CL7	C4D-C3D-CAD	-3.58	102.01	107.81
23	B	627	8CT	C30-C31-C32	-3.58	117.06	121.47
21	1	418	CL7	C3A-C4A-CHB	-3.58	118.39	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	403	CL7	C4C-C3C-C2C	-3.58	102.46	107.13
21	a	403	CL7	C4C-C3C-C2C	-3.58	102.46	107.13
32	2	521	ZEX	C35-C15-C14	-3.58	116.14	123.47
21	D	402	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	d	402	CL7	C3A-C4A-CHB	-3.58	118.39	123.70
21	2	510	CL7	C3A-C4A-CHB	-3.57	118.39	123.70
21	6	510	CL7	C3A-C4A-CHB	-3.57	118.39	123.70
21	B	610	CL7	C3A-C4A-CHB	-3.57	118.40	123.70
32	2	520	ZEX	C10-C11-C12	-3.57	112.08	123.22
21	1	417	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
21	b	617	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
21	c	513	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
21	5	417	CL7	C3A-C4A-CHB	-3.57	118.41	123.70
21	5	420	CL7	CHD-C4C-C3C	-3.56	119.17	124.93
32	3	525	ZEX	C10-C11-C12	-3.56	112.09	123.22
21	C	513	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
23	C	516	8CT	C07-C02-C03	-3.56	117.56	122.73
23	c	516	8CT	C07-C02-C03	-3.56	117.56	122.73
32	6	520	ZEX	C35-C15-C14	-3.56	116.17	123.47
23	C	516	8CT	C01-C02-C07	3.56	120.46	113.62
23	c	516	8CT	C01-C02-C07	3.56	120.46	113.62
21	B	613	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	b	614	CL7	C3A-C4A-CHB	-3.56	118.41	123.70
21	1	416	CL7	O2D-CGD-CBD	3.56	117.60	111.27
21	5	416	CL7	O2D-CGD-CBD	3.56	117.60	111.27
21	B	616	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	3	507	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	7	507	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	C	502	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	c	502	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	b	611	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	1	409	CL7	C3A-C4A-CHB	-3.56	118.42	123.70
21	C	514	CL7	C4D-C3D-CAD	-3.55	102.06	107.81
21	1	408	CL7	C4D-C3D-CAD	-3.55	102.06	107.81
21	c	514	CL7	C4D-C3D-CAD	-3.55	102.06	107.81
21	3	512	CL7	O2D-CGD-CBD	3.55	117.58	111.27
21	7	512	CL7	O2D-CGD-CBD	3.55	117.58	111.27
21	1	415	CL7	CHD-C4C-C3C	-3.55	119.19	124.93
21	5	415	CL7	CHD-C4C-C3C	-3.55	119.19	124.93
21	1	416	CL7	C3A-C4A-CHB	-3.55	118.42	123.70
21	1	420	CL7	CHD-C4C-C3C	-3.55	119.19	124.93
21	3	505	CL7	CHD-C4C-C3C	-3.55	119.19	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	505	CL7	CHD-C4C-C3C	-3.55	119.19	124.93
23	b	619	8CT	C07-C02-C03	-3.55	117.57	122.73
21	4	412	CL7	C3A-C4A-CHB	-3.55	118.43	123.70
21	1	418	CL7	CHD-C4C-C3C	-3.55	119.19	124.93
21	5	409	CL7	C3A-C4A-CHB	-3.55	118.44	123.70
21	4	415	CL7	CHD-C4C-C3C	-3.54	119.20	124.93
21	4	410	CL7	C3A-C4A-CHB	-3.54	118.44	123.70
21	8	410	CL7	C3A-C4A-CHB	-3.54	118.44	123.70
21	c	518	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
23	B	618	8CT	C07-C02-C03	-3.54	117.59	122.73
21	A	403	CL7	CAC-C3C-C4C	-3.54	119.11	124.68
21	7	509	CL7	C3A-C4A-CHB	-3.54	118.45	123.70
21	5	418	CL7	CHD-C4C-C3C	-3.53	119.22	124.93
21	1	403	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	3	509	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	5	403	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	8	412	CL7	C3A-C4A-CHB	-3.53	118.46	123.70
21	C	518	CL7	C3A-C4A-CHB	-3.52	118.48	123.70
32	3	520	ZEX	C31-C32-C33	-3.52	116.53	126.42
32	7	520	ZEX	C31-C32-C33	-3.52	116.53	126.42
21	a	403	CL7	CAC-C3C-C4C	-3.52	119.14	124.68
21	7	515	CL7	C3A-C4A-CHB	-3.52	118.48	123.70
21	8	415	CL7	CHD-C4C-C3C	-3.51	119.25	124.93
21	3	515	CL7	C3A-C4A-CHB	-3.51	118.48	123.70
21	5	416	CL7	C3A-C4A-CHB	-3.51	118.48	123.70
32	2	519	ZEX	C18-C5-C6	-3.51	120.59	124.53
32	6	519	ZEX	C18-C5-C6	-3.51	120.59	124.53
21	4	414	CL7	CHD-C4C-C3C	-3.51	119.26	124.93
21	8	414	CL7	CHD-C4C-C3C	-3.51	119.26	124.93
21	C	518	CL7	CMA-C3A-C2A	-3.50	107.92	116.10
21	3	514	CL7	CHD-C4C-C3C	-3.50	119.27	124.93
21	4	416	CL7	CHD-C4C-C3C	-3.50	119.27	124.93
21	2	513	CL7	O2D-CGD-CBD	3.50	117.49	111.27
21	6	513	CL7	O2D-CGD-CBD	3.50	117.49	111.27
21	b	608	CL7	C3A-C4A-CHB	-3.50	118.50	123.70
21	7	501	CL7	C3A-C4A-CHB	-3.50	118.50	123.70
21	5	414	CL7	CHD-C4C-C3C	-3.50	119.27	124.93
21	7	511	CL7	C3A-C4A-CHB	-3.50	118.51	123.70
21	4	407	CL7	CMA-C3A-C2A	-3.50	107.93	116.10
21	8	407	CL7	CMA-C3A-C2A	-3.50	107.93	116.10
21	7	514	CL7	CHD-C4C-C3C	-3.50	119.28	124.93
22	d	408	PHO	C1-C2-C3	-3.50	119.99	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	2	525	ZEX	C27-C28-C29	-3.50	120.95	126.23
32	6	524	ZEX	C27-C28-C29	-3.50	120.95	126.23
21	8	416	CL7	CHD-C4C-C3C	-3.50	119.28	124.93
21	2	505	CL7	CHD-C4C-C3C	-3.49	119.29	124.93
21	3	511	CL7	C3A-C4A-CHB	-3.49	118.52	123.70
21	B	607	CL7	C3A-C4A-CHB	-3.49	118.52	123.70
21	c	518	CL7	CMA-C3A-C2A	-3.49	107.96	116.10
21	6	505	CL7	CHD-C4C-C3C	-3.49	119.30	124.93
21	1	414	CL7	CHD-C4C-C3C	-3.49	119.30	124.93
32	4	420	ZEX	C27-C28-C29	-3.48	120.97	126.23
32	8	420	ZEX	C27-C28-C29	-3.48	120.97	126.23
22	D	408	PHO	C1-C2-C3	-3.48	120.02	126.04
21	3	501	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	3	505	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
21	7	505	CL7	C3A-C4A-CHB	-3.48	118.53	123.70
22	d	408	PHO	O2D-CGD-CBD	3.48	115.40	111.00
22	D	408	PHO	O2D-CGD-CBD	3.48	115.40	111.00
21	4	407	CL7	CHD-C4C-C3C	-3.48	119.31	124.93
21	b	602	CL7	C3A-C4A-CHB	-3.47	118.55	123.70
21	B	608	CL7	O2D-CGD-CBD	3.47	117.43	111.27
21	B	601	CL7	C3A-C4A-CHB	-3.47	118.56	123.70
23	C	516	8CT	C01-C02-C03	-3.47	120.64	124.53
23	c	516	8CT	C01-C02-C03	-3.47	120.64	124.53
21	8	407	CL7	CHD-C4C-C3C	-3.46	119.33	124.93
21	3	514	CL7	C3A-C4A-CHB	-3.46	118.56	123.70
21	A	403	CL7	C3A-C4A-CHB	-3.46	118.57	123.70
21	a	403	CL7	C3A-C4A-CHB	-3.46	118.57	123.70
32	2	519	ZEX	C2-C3-C4	3.45	115.03	110.30
21	7	514	CL7	C3A-C4A-CHB	-3.45	118.58	123.70
21	1	413	CL7	CHD-C4C-C3C	-3.45	119.35	124.93
21	4	417	CL7	CHD-C4C-C3C	-3.45	119.35	124.93
21	5	413	CL7	CHD-C4C-C3C	-3.45	119.35	124.93
21	8	417	CL7	CHD-C4C-C3C	-3.45	119.35	124.93
21	b	609	CL7	O2D-CGD-CBD	3.45	117.40	111.27
21	4	414	CL7	CHC-C1C-NC	-3.45	121.29	124.45
32	6	519	ZEX	C2-C3-C4	3.44	115.02	110.30
21	C	511	CL7	CHC-C1C-NC	-3.44	121.29	124.45
21	c	511	CL7	CHC-C1C-NC	-3.44	121.29	124.45
32	8	403	ZEX	C18-C5-C6	-3.44	120.66	124.53
21	4	412	CL7	CHD-C4C-C3C	-3.44	119.37	124.93
21	2	511	CL7	CHD-C4C-C3C	-3.44	119.37	124.93
21	3	512	CL7	CHD-C4C-C3C	-3.44	119.37	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	512	CL7	CHD-C4C-C3C	-3.44	119.37	124.93
21	C	512	CL7	O2D-CGD-CBD	3.44	117.38	111.27
21	c	512	CL7	O2D-CGD-CBD	3.44	117.38	111.27
32	8	419	ZEX	C18-C5-C4	3.44	120.72	114.36
21	8	414	CL7	CHC-C1C-NC	-3.43	121.30	124.45
21	A	401	CL7	C4-C3-C5	3.43	121.05	115.27
21	a	401	CL7	C4-C3-C5	3.43	121.05	115.27
21	1	403	CL7	O2D-CGD-CBD	3.43	117.37	111.27
21	1	414	CL7	O2D-CGD-CBD	3.43	117.37	111.27
21	5	403	CL7	O2D-CGD-CBD	3.43	117.37	111.27
21	5	414	CL7	O2D-CGD-CBD	3.43	117.37	111.27
32	4	419	ZEX	C18-C5-C4	3.43	120.71	114.36
21	6	511	CL7	CHD-C4C-C3C	-3.43	119.39	124.93
21	8	412	CL7	CHD-C4C-C3C	-3.43	119.39	124.93
21	B	615	CL7	O2D-CGD-CBD	3.43	117.36	111.27
21	b	616	CL7	O2D-CGD-CBD	3.43	117.36	111.27
23	4	402	8CT	C18-C17-C16	-3.42	122.42	127.31
23	B	619	8CT	C01-C02-C07	3.42	120.19	113.62
23	b	620	8CT	C01-C02-C07	3.42	120.19	113.62
21	2	516	CL7	C3A-C4A-CHB	-3.42	118.62	123.70
21	b	612	CL7	O2D-CGD-CBD	3.42	117.35	111.27
23	A	404	8CT	C04-C03-C02	-3.42	117.80	122.61
23	a	404	8CT	C04-C03-C02	-3.42	117.80	122.61
32	4	403	ZEX	C18-C5-C6	-3.42	120.69	124.53
21	C	507	CL7	CHD-C4C-C3C	-3.42	119.40	124.93
21	B	615	CL7	C3A-C4A-CHB	-3.41	118.63	123.70
21	b	616	CL7	C3A-C4A-CHB	-3.41	118.63	123.70
32	7	520	ZEX	C11-C12-C13	-3.41	116.83	126.42
21	6	515	CL7	C3A-C4A-CHB	-3.41	118.64	123.70
21	1	415	CL7	C3A-C4A-CHB	-3.41	118.65	123.70
21	5	415	CL7	C3A-C4A-CHB	-3.41	118.65	123.70
32	3	520	ZEX	C11-C12-C13	-3.41	116.85	126.42
23	8	402	8CT	C18-C17-C16	-3.41	122.45	127.31
21	B	611	CL7	O2D-CGD-CBD	3.40	117.32	111.27
21	c	507	CL7	CHD-C4C-C3C	-3.40	119.43	124.93
21	6	516	CL7	C3A-C4A-CHB	-3.40	118.65	123.70
21	b	613	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	1	417	CL7	O2D-CGD-CBD	3.40	117.31	111.27
21	C	512	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	c	512	CL7	C3A-C4A-CHB	-3.40	118.66	123.70
21	1	402	CL7	CHD-C4C-C3C	-3.40	119.44	124.93
23	B	627	8CT	C15-C16-C17	3.39	124.15	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	8CT	C15-C16-C17	3.39	124.15	118.94
23	B	619	8CT	C07-C02-C03	-3.39	117.81	122.73
23	b	620	8CT	C07-C02-C03	-3.39	117.81	122.73
21	a	405	CL7	C3A-C4A-CHB	-3.39	118.68	123.70
23	B	617	8CT	C11-C10-C03	-3.38	117.70	127.20
23	b	618	8CT	C11-C10-C03	-3.38	117.70	127.20
21	8	413	CL7	CHD-C4C-C3C	-3.38	119.46	124.93
21	A	406	CL7	C3A-C4A-CHB	-3.38	118.68	123.70
21	D	405	CL7	O2D-CGD-CBD	3.38	117.28	111.27
21	5	402	CL7	CHD-C4C-C3C	-3.38	119.46	124.93
21	5	417	CL7	O2D-CGD-CBD	3.38	117.27	111.27
21	B	612	CL7	C3A-C4A-CHB	-3.38	118.69	123.70
23	b	601	8CT	C14-C15-C16	-3.37	116.94	126.42
32	3	522	ZEX	C19-C9-C10	-3.37	118.20	122.92
21	C	504	CL7	CHD-C4C-C3C	-3.37	119.48	124.93
21	D	404	CL7	CAA-CBA-CGA	-3.37	103.40	113.25
21	2	515	CL7	C3A-C4A-CHB	-3.37	118.70	123.70
21	3	517	CL7	O2D-CGD-CBD	3.37	117.26	111.27
21	7	517	CL7	O2D-CGD-CBD	3.37	117.26	111.27
21	4	413	CL7	CHD-C4C-C3C	-3.37	119.48	124.93
21	B	612	CL7	CHC-C1C-NC	-3.37	121.36	124.45
21	b	613	CL7	CHC-C1C-NC	-3.37	121.36	124.45
21	3	516	CL7	C3A-C4A-CHB	-3.37	118.70	123.70
21	c	504	CL7	CHD-C4C-C3C	-3.37	119.49	124.93
23	B	627	8CT	C14-C15-C16	-3.36	116.97	126.42
21	B	603	CL7	CMD-C2D-C1D	3.36	133.63	128.46
21	b	604	CL7	CMD-C2D-C1D	3.36	133.63	128.46
21	3	514	CL7	C4C-C3C-C2C	-3.36	102.75	107.13
21	7	514	CL7	C4C-C3C-C2C	-3.36	102.75	107.13
21	4	414	CL7	O2D-CGD-CBD	3.36	117.24	111.27
21	B	610	CL7	CHD-C4C-C3C	-3.36	119.50	124.93
21	3	503	CL7	C7-C6-C5	-3.36	104.24	113.36
21	7	503	CL7	C7-C6-C5	-3.36	104.24	113.36
32	1	422	ZEX	C18-C5-C4	3.36	120.57	114.36
32	5	422	ZEX	C18-C5-C4	3.36	120.57	114.36
32	7	522	ZEX	C19-C9-C10	-3.35	118.22	122.92
21	7	516	CL7	C3A-C4A-CHB	-3.35	118.72	123.70
21	d	404	CL7	CAA-CBA-CGA	-3.35	103.46	113.25
21	B	613	CL7	CHD-C4C-C3C	-3.35	119.51	124.93
21	b	614	CL7	CHD-C4C-C3C	-3.35	119.51	124.93
21	d	405	CL7	O2D-CGD-CBD	3.35	117.22	111.27
21	b	607	CL7	CMD-C2D-C1D	3.35	133.61	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	406	CL7	C7-C6-C5	-3.35	104.26	113.36
21	5	406	CL7	C7-C6-C5	-3.35	104.26	113.36
21	c	508	CL7	C7-C6-C5	-3.35	104.27	113.36
21	4	408	CL7	CHD-C4C-C3C	-3.35	119.52	124.93
21	B	612	CL7	CHD-C4C-C3C	-3.35	119.52	124.93
21	8	414	CL7	O2D-CGD-CBD	3.34	117.21	111.27
21	c	513	CL7	CHC-C1C-NC	-3.34	121.38	124.45
23	C	515	8CT	C01-C02-C07	3.34	120.03	113.62
21	2	509	CL7	C3A-C4A-CHB	-3.34	118.74	123.70
21	5	406	CL7	CHD-C4C-C3C	-3.34	119.53	124.93
32	2	521	ZEX	C18-C5-C6	-3.34	120.78	124.53
32	6	520	ZEX	C18-C5-C6	-3.34	120.78	124.53
21	b	613	CL7	CHD-C4C-C3C	-3.34	119.54	124.93
21	A	406	CL7	CHD-C4C-C3C	-3.34	119.54	124.93
23	c	515	8CT	C35-C30-C29	-3.34	108.48	112.70
21	1	406	CL7	CHD-C4C-C3C	-3.34	119.54	124.93
21	b	611	CL7	CHD-C4C-C3C	-3.33	119.54	124.93
21	8	405	CL7	C3A-C4A-CHB	-3.33	118.75	123.70
21	B	611	CL7	C3A-C4A-CHB	-3.33	118.75	123.70
21	b	612	CL7	C3A-C4A-CHB	-3.33	118.75	123.70
21	6	509	CL7	C3A-C4A-CHB	-3.33	118.76	123.70
21	C	503	CL7	CHD-C4C-C3C	-3.33	119.55	124.93
21	C	508	CL7	C7-C6-C5	-3.33	104.31	113.36
23	D	406	8CT	C01-C02-C07	3.33	120.01	113.62
23	d	406	8CT	C01-C02-C07	3.33	120.01	113.62
21	C	513	CL7	CHC-C1C-NC	-3.33	121.40	124.45
32	7	520	ZEX	C18-C5-C4	3.33	120.52	114.36
21	B	606	CL7	CMD-C2D-C1D	3.33	133.57	128.46
21	3	507	CL7	CHC-C1C-NC	-3.32	121.40	124.45
21	8	408	CL7	CHD-C4C-C3C	-3.32	119.56	124.93
21	1	413	CL7	CMA-C3A-C2A	-3.32	108.35	116.10
21	1	415	CL7	O2D-CGD-CBD	3.32	117.17	111.27
21	8	416	CL7	C3A-C4A-CHB	-3.32	118.77	123.70
21	a	405	CL7	CHD-C4C-C3C	-3.32	119.57	124.93
21	5	413	CL7	CMA-C3A-C2A	-3.32	108.35	116.10
23	C	515	8CT	C35-C30-C29	-3.32	108.51	112.70
21	B	610	CL7	C7-C6-C5	-3.32	104.35	113.36
21	b	611	CL7	C7-C6-C5	-3.32	104.35	113.36
21	5	403	CL7	CHD-C4C-C3C	-3.32	119.57	124.93
21	4	405	CL7	C3A-C4A-CHB	-3.31	118.78	123.70
21	1	403	CL7	CHD-C4C-C3C	-3.31	119.57	124.93
21	3	501	CL7	CHD-C4C-C3C	-3.31	119.57	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	f	101	HEM	CHB-C1B-NB	3.31	128.48	124.38
21	6	514	CL7	O2D-CGD-CBD	3.31	117.16	111.27
21	c	503	CL7	CHD-C4C-C3C	-3.31	119.58	124.93
32	3	520	ZEX	C18-C5-C4	3.31	120.49	114.36
21	B	608	CL7	C3A-C4A-CHB	-3.31	118.79	123.70
21	b	609	CL7	C3A-C4A-CHB	-3.31	118.79	123.70
21	5	419	CL7	C3A-C4A-CHB	-3.31	118.79	123.70
30	d	407	PL9	C7-C3-C4	3.31	119.56	116.88
21	4	406	CL7	CHD-C4C-C3C	-3.31	119.59	124.93
21	8	406	CL7	CHD-C4C-C3C	-3.31	119.59	124.93
21	2	516	CL7	C7-C6-C5	-3.31	104.38	113.36
23	D	406	8CT	C11-C10-C03	-3.31	117.92	127.20
23	d	406	8CT	C11-C10-C03	-3.31	117.92	127.20
21	2	504	CL7	O2D-CGD-CBD	3.30	117.14	111.27
21	6	504	CL7	O2D-CGD-CBD	3.30	117.14	111.27
21	6	516	CL7	C7-C6-C5	-3.30	104.39	113.36
21	2	501	CL7	CHC-C1C-NC	-3.30	121.42	124.45
21	6	501	CL7	CHC-C1C-NC	-3.30	121.42	124.45
21	4	416	CL7	C3A-C4A-CHB	-3.30	118.80	123.70
23	c	515	8CT	C01-C02-C07	3.30	119.96	113.62
21	5	415	CL7	O2D-CGD-CBD	3.30	117.13	111.27
21	1	404	CL7	CHD-C4C-C3C	-3.30	119.60	124.93
21	5	404	CL7	CHD-C4C-C3C	-3.30	119.60	124.93
21	7	513	CL7	CHD-C4C-C3C	-3.30	119.60	124.93
21	B	605	CL7	C3A-C4A-CHB	-3.30	118.81	123.70
21	b	606	CL7	C3A-C4A-CHB	-3.30	118.81	123.70
32	1	422	ZEX	C31-C30-C29	-3.30	122.60	127.31
21	2	514	CL7	O2D-CGD-CBD	3.29	117.12	111.27
21	7	501	CL7	CHD-C4C-C3C	-3.29	119.61	124.93
21	7	515	CL7	CHD-C4C-C3C	-3.29	119.61	124.93
23	A	404	8CT	C07-C02-C03	-3.29	117.95	122.73
23	a	404	8CT	C07-C02-C03	-3.29	117.95	122.73
30	D	407	PL9	C7-C3-C4	3.29	119.55	116.88
21	3	515	CL7	CHD-C4C-C3C	-3.29	119.61	124.93
21	2	508	CL7	C3A-C4A-CHB	-3.29	118.82	123.70
22	d	408	PHO	O2D-CGD-O1D	-3.29	117.41	123.84
31	F	101	HEM	CHB-C1B-NB	3.29	128.44	124.38
21	1	419	CL7	C3A-C4A-CHB	-3.28	118.83	123.70
21	3	505	CL7	C4C-C3C-C2C	-3.28	102.85	107.13
21	7	505	CL7	C4C-C3C-C2C	-3.28	102.85	107.13
22	D	408	PHO	O2D-CGD-O1D	-3.28	117.42	123.84
21	5	405	CL7	C3A-C4A-CHB	-3.28	118.83	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	407	CL7	CHC-C1C-NC	-3.28	121.44	124.45
21	A	406	CL7	C7-C6-C5	-3.28	104.44	113.36
21	a	405	CL7	C7-C6-C5	-3.28	104.44	113.36
21	3	513	CL7	CHD-C4C-C3C	-3.28	119.63	124.93
21	C	513	CL7	CHD-C4C-C3C	-3.28	119.63	124.93
21	c	513	CL7	CHD-C4C-C3C	-3.28	119.63	124.93
21	C	510	CL7	CHC-C1C-NC	-3.28	121.44	124.45
21	c	510	CL7	CHC-C1C-NC	-3.28	121.44	124.45
21	c	510	CL7	C7-C6-C5	-3.28	104.45	113.36
32	5	422	ZEX	C31-C30-C29	-3.28	122.63	127.31
22	d	408	PHO	C4-C3-C5	3.28	120.79	115.27
21	C	510	CL7	C7-C6-C5	-3.28	104.46	113.36
21	B	601	CL7	O2D-CGD-CBD	3.28	117.09	111.27
21	C	512	CL7	CHD-C4C-C3C	-3.28	119.63	124.93
23	B	627	8CT	C35-C30-C29	3.28	116.84	112.70
23	b	601	8CT	C35-C30-C29	3.28	116.84	112.70
32	7	522	ZEX	C35-C15-C14	-3.28	116.76	123.47
21	b	602	CL7	O2D-CGD-CBD	3.27	117.09	111.27
21	2	508	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	6	508	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	2	514	CL7	C3A-C4A-CHB	-3.27	118.84	123.70
21	C	510	CL7	CHD-C4C-C3C	-3.27	119.64	124.93
21	c	510	CL7	CHD-C4C-C3C	-3.27	119.64	124.93
21	3	502	CL7	O2D-CGD-CBD	3.27	117.08	111.27
21	7	502	CL7	O2D-CGD-CBD	3.27	117.08	111.27
32	4	418	ZEX	C39-C29-C30	-3.27	118.34	122.92
32	3	522	ZEX	C35-C15-C14	-3.27	116.78	123.47
32	8	418	ZEX	C39-C29-C30	-3.27	118.35	122.92
22	D	408	PHO	C4-C3-C5	3.27	120.77	115.27
21	1	405	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	6	508	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	D	402	CL7	O2D-CGD-CBD	3.26	117.06	111.27
21	d	402	CL7	O2D-CGD-CBD	3.26	117.06	111.27
21	7	507	CL7	CHC-C1C-NC	-3.26	121.46	124.45
23	C	515	8CT	C11-C10-C03	-3.26	118.04	127.20
23	c	515	8CT	C11-C10-C03	-3.26	118.04	127.20
21	c	506	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
32	2	520	ZEX	C27-C28-C29	-3.26	121.31	126.23
32	3	525	ZEX	C27-C28-C29	-3.26	121.31	126.23
21	7	508	CL7	C3A-C4A-CHB	-3.26	118.86	123.70
21	c	512	CL7	CHD-C4C-C3C	-3.26	119.67	124.93
21	D	405	CL7	CHD-C4C-C3C	-3.26	119.67	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	d	405	CL7	CHD-C4C-C3C	-3.26	119.67	124.93
21	B	622	CL7	CHD-C4C-C3C	-3.25	119.67	124.93
21	b	623	CL7	CHD-C4C-C3C	-3.25	119.67	124.93
21	3	504	CL7	CHD-C4C-C3C	-3.25	119.67	124.93
21	7	504	CL7	CHD-C4C-C3C	-3.25	119.67	124.93
21	C	506	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
21	b	606	CL7	CHD-C4C-C3C	-3.25	119.68	124.93
21	c	507	CL7	CHC-C1C-NC	-3.25	121.47	124.45
21	8	407	CL7	CHC-C1C-NC	-3.25	121.47	124.45
21	6	514	CL7	C3A-C4A-CHB	-3.25	118.88	123.70
32	2	521	ZEX	C31-C30-C29	-3.25	122.68	127.31
32	6	520	ZEX	C31-C30-C29	-3.25	122.68	127.31
22	D	408	PHO	CMB-C2B-C3B	3.24	130.75	124.68
21	C	514	CL7	O2D-CGD-CBD	3.24	117.03	111.27
21	C	505	CL7	CHD-C4C-C3C	-3.24	119.69	124.93
21	c	505	CL7	CHD-C4C-C3C	-3.24	119.69	124.93
21	C	506	CL7	O2D-CGD-CBD	3.24	117.03	111.27
21	c	506	CL7	O2D-CGD-CBD	3.24	117.03	111.27
22	d	408	PHO	CMB-C2B-C3B	3.24	130.74	124.68
21	B	607	CL7	CHD-C4C-C3C	-3.24	119.69	124.93
21	b	608	CL7	CHD-C4C-C3C	-3.24	119.69	124.93
21	a	401	CL7	CHD-C4C-C3C	-3.24	119.70	124.93
21	C	511	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	3	508	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	c	511	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	3	516	CL7	CMD-C2D-C1D	3.24	133.44	128.46
21	7	516	CL7	CMD-C2D-C1D	3.24	133.44	128.46
21	c	514	CL7	O2D-CGD-CBD	3.24	117.02	111.27
21	1	404	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	5	404	CL7	C3A-C4A-CHB	-3.24	118.90	123.70
21	4	414	CL7	C3A-C4A-CHB	-3.23	118.90	123.70
21	8	414	CL7	C3A-C4A-CHB	-3.23	118.90	123.70
21	A	406	CL7	CMD-C2D-C1D	3.23	133.43	128.46
21	a	405	CL7	CMD-C2D-C1D	3.23	133.43	128.46
21	a	405	CL7	CAA-CBA-CGA	-3.23	103.81	113.25
21	1	418	CL7	CHC-C1C-NC	-3.23	121.48	124.45
21	B	605	CL7	CHD-C4C-C3C	-3.23	119.71	124.93
21	8	412	CL7	CHC-C1C-NC	-3.23	121.49	124.45
21	3	518	CL7	CHD-C4C-C3C	-3.23	119.72	124.93
21	7	518	CL7	CHD-C4C-C3C	-3.23	119.72	124.93
21	1	411	CL7	O2D-CGD-CBD	3.23	117.00	111.27
21	4	404	CL7	O2D-CGD-CBD	3.23	117.00	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	411	CL7	O2D-CGD-CBD	3.23	117.00	111.27
21	8	404	CL7	O2D-CGD-CBD	3.23	117.00	111.27
21	4	411	CL7	CHC-C1C-NC	-3.23	121.49	124.45
32	3	522	ZEX	C1-C2-C3	-3.23	106.36	113.64
32	7	522	ZEX	C1-C2-C3	-3.23	106.36	113.64
21	C	507	CL7	CHC-C1C-NC	-3.23	121.49	124.45
21	5	418	CL7	CHC-C1C-NC	-3.23	121.49	124.45
21	A	406	CL7	CAA-CBA-CGA	-3.22	103.83	113.25
21	4	406	CL7	O2D-CGD-CBD	3.22	117.00	111.27
21	A	401	CL7	CAA-CBA-CGA	-3.22	103.84	113.25
21	a	401	CL7	CAA-CBA-CGA	-3.22	103.84	113.25
21	1	413	CL7	C3A-C4A-CHB	-3.22	118.92	123.70
21	5	413	CL7	C3A-C4A-CHB	-3.22	118.92	123.70
21	2	518	CL7	CHD-C4C-C3C	-3.22	119.73	124.93
21	6	518	CL7	CHD-C4C-C3C	-3.22	119.73	124.93
21	A	401	CL7	CHD-C4C-C3C	-3.21	119.74	124.93
23	B	617	8CT	C14-C15-C16	-3.21	117.39	126.42
23	b	618	8CT	C14-C15-C16	-3.21	117.39	126.42
21	1	411	CL7	CHD-C4C-C3C	-3.21	119.74	124.93
21	8	411	CL7	CHC-C1C-NC	-3.21	121.50	124.45
21	2	515	CL7	O2D-CGD-CBD	3.21	116.97	111.27
21	6	515	CL7	O2D-CGD-CBD	3.21	116.97	111.27
21	1	414	CL7	C4C-C3C-C2C	-3.21	102.94	107.13
21	5	414	CL7	C4C-C3C-C2C	-3.21	102.94	107.13
21	3	510	CL7	CHD-C4C-C3C	-3.21	119.75	124.93
21	7	510	CL7	CHD-C4C-C3C	-3.21	119.75	124.93
21	4	412	CL7	CAA-CBA-CGA	-3.21	103.88	113.25
21	8	412	CL7	CAA-CBA-CGA	-3.21	103.88	113.25
21	8	406	CL7	O2D-CGD-CBD	3.21	116.97	111.27
21	4	412	CL7	CHC-C1C-NC	-3.21	121.51	124.45
21	2	510	CL7	CHD-C4C-C3C	-3.21	119.75	124.93
21	6	510	CL7	CHD-C4C-C3C	-3.21	119.75	124.93
21	2	518	CL7	C7-C6-C5	-3.20	104.66	113.36
21	5	412	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
21	2	510	CL7	C7-C6-C5	-3.20	104.66	113.36
21	6	510	CL7	C7-C6-C5	-3.20	104.66	113.36
21	5	411	CL7	CHD-C4C-C3C	-3.20	119.76	124.93
21	C	509	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
21	c	509	CL7	C3A-C4A-CHB	-3.20	118.95	123.70
21	3	517	CL7	CHD-C4C-C3C	-3.20	119.76	124.93
21	C	509	CL7	CHD-C4C-C3C	-3.20	119.77	124.93
21	c	509	CL7	CHD-C4C-C3C	-3.20	119.77	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	512	CL7	C3A-C4A-CHB	-3.19	118.96	123.70
21	6	518	CL7	C7-C6-C5	-3.19	104.69	113.36
21	1	402	CL7	CHC-C1C-NC	-3.19	121.52	124.45
21	5	402	CL7	CHC-C1C-NC	-3.19	121.52	124.45
21	7	517	CL7	CHD-C4C-C3C	-3.19	119.77	124.93
21	1	412	CL7	C3A-C4A-CHB	-3.19	118.96	123.70
21	2	518	CL7	O2D-CGD-CBD	3.19	116.94	111.27
21	6	518	CL7	O2D-CGD-CBD	3.19	116.94	111.27
21	1	408	CL7	C7-C6-C5	-3.19	104.69	113.36
21	5	408	CL7	C7-C6-C5	-3.19	104.69	113.36
21	B	616	CL7	CHD-C4C-C3C	-3.19	119.78	124.93
21	b	617	CL7	CHD-C4C-C3C	-3.19	119.78	124.93
21	1	408	CL7	CAA-CBA-CGA	-3.19	103.94	113.25
21	5	408	CL7	CAA-CBA-CGA	-3.19	103.94	113.25
21	8	409	CL7	CHC-C1C-NC	-3.19	121.53	124.45
21	b	608	CL7	C7-C6-C5	-3.19	104.71	113.36
32	3	522	ZEX	C8-C7-C6	-3.18	118.26	127.20
21	C	511	CL7	CHD-C4C-C3C	-3.18	119.78	124.93
21	c	511	CL7	CHD-C4C-C3C	-3.18	119.78	124.93
23	B	627	8CT	C01-C02-C07	3.18	119.73	113.62
23	b	601	8CT	C01-C02-C07	3.18	119.73	113.62
21	2	517	CL7	CHD-C4C-C3C	-3.18	119.79	124.93
21	b	612	CL7	C7-C6-C5	-3.18	104.72	113.36
21	4	409	CL7	CHC-C1C-NC	-3.18	121.53	124.45
21	2	502	CL7	CHD-C4C-C3C	-3.18	119.79	124.93
21	3	507	CL7	CHD-C4C-C3C	-3.18	119.79	124.93
21	6	502	CL7	CHD-C4C-C3C	-3.18	119.79	124.93
21	7	507	CL7	CHD-C4C-C3C	-3.18	119.79	124.93
21	2	512	CL7	C3A-C4A-CHB	-3.18	118.98	123.70
21	B	607	CL7	C7-C6-C5	-3.18	104.73	113.36
21	B	611	CL7	C7-C6-C5	-3.18	104.73	113.36
32	7	522	ZEX	C8-C7-C6	-3.17	118.30	127.20
21	2	501	CL7	CHD-C4C-C3C	-3.17	119.81	124.93
21	6	517	CL7	CHD-C4C-C3C	-3.17	119.81	124.93
21	3	508	CL7	C7-C6-C5	-3.17	104.75	113.36
21	B	606	CL7	CHD-C4C-C3C	-3.16	119.82	124.93
21	b	607	CL7	CHD-C4C-C3C	-3.16	119.82	124.93
23	B	617	8CT	C18-C19-C20	-3.16	116.99	123.47
23	b	618	8CT	C18-C19-C20	-3.16	116.99	123.47
21	7	508	CL7	C7-C6-C5	-3.16	104.77	113.36
23	c	519	8CT	C24-C23-C21	-3.16	117.53	126.42
21	6	506	CL7	C7-C6-C5	-3.16	104.78	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	515	CL7	CHD-C4C-C3C	-3.16	119.83	124.93
23	C	519	8CT	C24-C23-C21	-3.15	117.55	126.42
21	6	501	CL7	CHD-C4C-C3C	-3.15	119.83	124.93
21	3	513	CL7	O2D-CGD-CBD	3.15	116.87	111.27
21	7	513	CL7	O2D-CGD-CBD	3.15	116.87	111.27
32	4	419	ZEX	C3-C4-C5	-3.15	105.58	111.85
21	2	506	CL7	C7-C6-C5	-3.15	104.80	113.36
21	3	516	CL7	O2D-CGD-CBD	3.15	116.87	111.27
21	1	419	CL7	C4D-C3D-CAD	-3.15	102.72	107.81
21	2	513	CL7	C4D-C3D-CAD	-3.14	102.72	107.81
21	7	516	CL7	O2D-CGD-CBD	3.14	116.85	111.27
21	2	515	CL7	CHD-C4C-C3C	-3.14	119.85	124.93
21	B	605	CL7	CMD-C2D-C1D	3.14	133.29	128.46
21	b	606	CL7	CMD-C2D-C1D	3.14	133.29	128.46
21	B	602	CL7	CHD-C4C-C3C	-3.14	119.86	124.93
21	b	603	CL7	CHD-C4C-C3C	-3.14	119.86	124.93
32	8	419	ZEX	C3-C4-C5	-3.14	105.61	111.85
21	3	501	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	7	501	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	3	518	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	7	518	CL7	O2D-CGD-CBD	3.13	116.83	111.27
21	4	410	CL7	CHD-C4C-C3C	-3.13	119.88	124.93
21	6	513	CL7	C4D-C3D-CAD	-3.13	102.75	107.81
21	b	623	CL7	C4D-C3D-CAD	-3.13	102.75	107.81
32	2	520	ZEX	C35-C15-C14	-3.13	117.07	123.47
23	B	618	8CT	C27-C26-C28	3.13	123.00	118.08
23	b	619	8CT	C27-C26-C28	3.13	123.00	118.08
21	2	509	CL7	CHC-C1C-NC	-3.12	121.58	124.45
21	c	508	CL7	CHD-C4C-C3C	-3.12	119.89	124.93
21	8	406	CL7	C7-C6-C5	-3.12	104.88	113.36
21	B	604	CL7	C3A-C4A-CHB	-3.12	119.07	123.70
21	4	410	CL7	O2D-CGD-CBD	3.12	116.81	111.27
21	1	403	CL7	CHC-C1C-NC	-3.12	121.59	124.45
21	4	406	CL7	C7-C6-C5	-3.12	104.89	113.36
21	6	509	CL7	CHC-C1C-NC	-3.12	121.59	124.45
21	2	503	CL7	CMD-C2D-C1D	3.12	133.25	128.46
21	6	503	CL7	CMD-C2D-C1D	3.12	133.25	128.46
32	3	519	ZEX	C27-C26-C25	-3.11	117.81	122.84
21	5	419	CL7	C4D-C3D-CAD	-3.11	102.77	107.81
21	7	509	CL7	CHD-C4C-C3C	-3.11	119.90	124.93
21	6	509	CL7	CHD-C4C-C3C	-3.11	119.90	124.93
21	8	410	CL7	CHD-C4C-C3C	-3.11	119.90	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	3	525	ZEX	C35-C15-C14	-3.11	117.10	123.47
32	2	519	ZEX	C11-C10-C9	-3.11	122.88	127.31
32	6	519	ZEX	C11-C10-C9	-3.11	122.88	127.31
21	B	622	CL7	C4D-C3D-CAD	-3.11	102.78	107.81
21	B	603	CL7	C7-C6-C5	-3.11	104.92	113.36
21	b	604	CL7	C7-C6-C5	-3.11	104.92	113.36
21	4	405	CL7	CHD-C4C-C3C	-3.11	119.91	124.93
21	8	405	CL7	CHD-C4C-C3C	-3.11	119.91	124.93
21	C	508	CL7	CHD-C4C-C3C	-3.11	119.91	124.93
21	3	511	CL7	O2A-C1-C2	-3.11	100.47	108.64
21	7	511	CL7	O2A-C1-C2	-3.11	100.47	108.64
21	b	605	CL7	C3A-C4A-CHB	-3.11	119.09	123.70
21	B	613	CL7	CHC-C1C-NC	-3.10	121.60	124.45
21	3	509	CL7	CHD-C4C-C3C	-3.10	119.91	124.93
21	4	411	CL7	CHD-C4C-C3C	-3.10	119.92	124.93
21	8	410	CL7	O2D-CGD-CBD	3.10	116.78	111.27
21	1	405	CL7	CHD-C4C-C3C	-3.10	119.92	124.93
32	8	418	ZEX	C15-C35-C34	-3.10	117.13	123.47
32	7	519	ZEX	C27-C26-C25	-3.10	117.83	122.84
21	2	505	CL7	C3A-C4A-CHB	-3.10	119.10	123.70
21	6	505	CL7	C3A-C4A-CHB	-3.10	119.10	123.70
21	5	412	CL7	CHD-C4C-C3C	-3.10	119.93	124.93
21	b	606	CL7	O2D-CGD-CBD	3.10	116.77	111.27
21	2	509	CL7	CHD-C4C-C3C	-3.10	119.93	124.93
21	1	412	CL7	CHD-C4C-C3C	-3.10	119.93	124.93
21	2	503	CL7	CHC-C1C-NC	-3.10	121.61	124.45
21	5	403	CL7	CHC-C1C-NC	-3.10	121.61	124.45
21	4	415	CL7	C4C-C3C-C2C	-3.09	103.09	107.13
32	4	418	ZEX	C15-C35-C34	-3.09	117.14	123.47
21	8	411	CL7	CHD-C4C-C3C	-3.09	119.93	124.93
21	b	614	CL7	CHC-C1C-NC	-3.09	121.61	124.45
21	5	405	CL7	CHD-C4C-C3C	-3.09	119.94	124.93
21	2	509	CL7	C7-C6-C5	-3.09	104.97	113.36
21	6	509	CL7	C7-C6-C5	-3.09	104.97	113.36
21	B	613	CL7	O2D-CGD-CBD	3.09	116.75	111.27
21	C	507	CL7	O2A-CGA-O1A	-3.09	115.81	123.59
21	c	507	CL7	O2A-CGA-O1A	-3.09	115.81	123.59
21	b	611	CL7	CHC-C1C-NC	-3.08	121.62	124.45
32	3	522	ZEX	C30-C31-C32	-3.08	113.60	123.22
32	7	522	ZEX	C30-C31-C32	-3.08	113.60	123.22
21	1	419	CL7	CHD-C4C-C3C	-3.08	119.95	124.93
21	8	415	CL7	C4C-C3C-C2C	-3.08	103.11	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	503	CL7	CHC-C1C-NC	-3.08	121.62	124.45
21	3	515	CL7	CHC-C1C-NC	-3.08	121.62	124.45
32	7	520	ZEX	C1-C2-C3	-3.08	106.69	113.64
26	C	501	LMG	C8-O7-C10	-3.08	110.21	117.79
21	B	605	CL7	O2D-CGD-CBD	3.08	116.74	111.27
32	3	520	ZEX	C1-C2-C3	-3.08	106.69	113.64
21	5	419	CL7	CHD-C4C-C3C	-3.08	119.96	124.93
21	2	502	CL7	C3A-C4A-CHB	-3.08	119.14	123.70
21	C	508	CL7	CAA-CBA-CGA	-3.08	104.27	113.25
21	c	508	CL7	CAA-CBA-CGA	-3.08	104.27	113.25
21	2	516	CL7	CHD-C4C-C3C	-3.07	119.96	124.93
21	6	516	CL7	CHD-C4C-C3C	-3.07	119.96	124.93
21	3	510	CL7	C7-C6-C5	-3.07	105.01	113.36
21	7	510	CL7	C7-C6-C5	-3.07	105.01	113.36
21	6	502	CL7	C3A-C4A-CHB	-3.07	119.14	123.70
21	6	516	CL7	O2D-CGD-CBD	3.07	116.73	111.27
32	4	403	ZEX	C31-C32-C33	-3.07	117.79	126.42
32	8	403	ZEX	C31-C32-C33	-3.07	117.79	126.42
21	8	413	CL7	O2D-CGD-CBD	3.07	116.72	111.27
32	4	419	ZEX	C11-C10-C9	-3.07	122.93	127.31
21	B	609	CL7	CMD-C2D-C1D	3.07	133.18	128.46
21	b	610	CL7	CMD-C2D-C1D	3.07	133.18	128.46
21	4	413	CL7	O2D-CGD-CBD	3.07	116.72	111.27
21	C	518	CL7	CHC-C1C-NC	-3.07	121.63	124.45
21	c	518	CL7	CHC-C1C-NC	-3.07	121.63	124.45
23	D	406	8CT	C07-C02-C03	-3.07	118.28	122.73
23	d	406	8CT	C07-C02-C03	-3.07	118.28	122.73
21	4	417	CL7	CHC-C1C-NC	-3.07	121.64	124.45
21	8	417	CL7	CHC-C1C-NC	-3.07	121.64	124.45
21	C	513	CL7	C4D-C3D-CAD	-3.07	102.85	107.81
21	B	614	CL7	CHD-C4C-C3C	-3.06	119.98	124.93
21	b	615	CL7	CHD-C4C-C3C	-3.06	119.98	124.93
21	b	614	CL7	O2D-CGD-CBD	3.06	116.71	111.27
23	4	402	8CT	C05-C04-C03	3.06	115.20	110.48
21	B	610	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	1	407	CL7	CHD-C4C-C3C	-3.06	119.98	124.93
21	7	515	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	1	415	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	5	415	CL7	CHC-C1C-NC	-3.06	121.64	124.45
21	C	513	CL7	O2D-CGD-CBD	3.06	116.70	111.27
21	C	514	CL7	CHD-C4C-C3C	-3.06	119.99	124.93
26	c	501	LMG	C8-O7-C10	-3.06	110.27	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	519	8CT	C11-C10-C03	-3.05	118.62	127.20
32	8	419	ZEX	C11-C10-C9	-3.05	122.95	127.31
21	C	502	CL7	O2D-CGD-CBD	3.05	116.69	111.27
23	C	515	8CT	C25-C24-C23	-3.05	113.70	123.22
32	3	522	ZEX	C11-C12-C13	-3.05	117.85	126.42
32	7	522	ZEX	C11-C12-C13	-3.05	117.85	126.42
21	B	604	CL7	CHD-C4C-C3C	-3.05	120.00	124.93
21	7	506	CL7	C3B-C4B-NB	3.05	113.15	109.21
21	2	504	CL7	CMD-C2D-C1D	3.05	133.15	128.46
21	6	504	CL7	CMD-C2D-C1D	3.05	133.15	128.46
21	2	516	CL7	O2D-CGD-CBD	3.05	116.68	111.27
21	B	608	CL7	CHD-C4C-C3C	-3.05	120.01	124.93
21	b	609	CL7	CHD-C4C-C3C	-3.05	120.01	124.93
21	5	407	CL7	CHD-C4C-C3C	-3.05	120.01	124.93
32	1	422	ZEX	C21-C22-C23	-3.05	107.09	113.69
21	C	509	CL7	CAA-CBA-CGA	-3.05	104.35	113.25
21	c	509	CL7	CAA-CBA-CGA	-3.05	104.35	113.25
21	3	509	CL7	C7-C6-C5	-3.05	105.09	113.36
21	7	509	CL7	C7-C6-C5	-3.05	105.09	113.36
21	d	404	CL7	CMD-C2D-C1D	3.04	133.14	128.46
32	4	420	ZEX	C30-C31-C32	-3.04	113.72	123.22
21	c	513	CL7	C4D-C3D-CAD	-3.04	102.88	107.81
21	3	501	CL7	CHC-C1C-NC	-3.04	121.66	124.45
23	8	402	8CT	C05-C04-C03	3.04	115.17	110.48
21	1	412	CL7	O2D-CGD-CBD	3.04	116.68	111.27
21	5	412	CL7	O2D-CGD-CBD	3.04	116.68	111.27
21	6	504	CL7	CAA-CBA-CGA	-3.04	104.43	112.51
23	c	515	8CT	C25-C24-C23	-3.04	113.72	123.22
21	b	603	CL7	O2A-CGA-CBA	3.04	121.45	111.91
21	c	513	CL7	O2D-CGD-CBD	3.04	116.67	111.27
21	c	514	CL7	CHD-C4C-C3C	-3.04	120.02	124.93
21	6	506	CL7	CHD-C4C-C3C	-3.04	120.02	124.93
21	3	506	CL7	C3B-C4B-NB	3.04	113.14	109.21
21	2	504	CL7	CAA-CBA-CGA	-3.04	104.45	112.51
23	C	519	8CT	C11-C10-C03	-3.04	118.67	127.20
26	C	501	LMG	O8-C28-C29	3.04	121.44	111.91
21	4	408	CL7	CHC-C1C-NC	-3.04	121.66	124.45
21	5	418	CL7	C7-C6-C5	-3.03	105.12	113.36
21	8	408	CL7	CHC-C1C-NC	-3.03	121.67	124.45
32	8	420	ZEX	C30-C31-C32	-3.03	113.75	123.22
21	B	602	CL7	O2A-CGA-CBA	3.03	121.43	111.91
21	b	605	CL7	CHD-C4C-C3C	-3.03	120.03	124.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	501	CL7	CHC-C1C-NC	-3.03	121.67	124.45
21	c	502	CL7	O2D-CGD-CBD	3.03	116.65	111.27
21	1	414	CL7	CHC-C1C-NC	-3.03	121.67	124.45
21	5	414	CL7	CHC-C1C-NC	-3.03	121.67	124.45
21	1	418	CL7	C7-C6-C5	-3.03	105.14	113.36
21	2	506	CL7	CHD-C4C-C3C	-3.03	120.04	124.93
21	c	506	CL7	CMD-C2D-C1D	3.03	133.11	128.46
21	D	404	CL7	CMD-C2D-C1D	3.02	133.11	128.46
32	2	521	ZEX	C30-C31-C32	-3.02	113.78	123.22
32	6	520	ZEX	C30-C31-C32	-3.02	113.78	123.22
21	2	509	CL7	CAA-CBA-CGA	-3.02	104.42	113.25
21	6	509	CL7	CAA-CBA-CGA	-3.02	104.42	113.25
32	8	420	ZEX	C10-C11-C12	-3.02	113.78	123.22
21	1	409	CL7	O2D-CGD-CBD	3.02	116.64	111.27
21	5	409	CL7	O2D-CGD-CBD	3.02	116.64	111.27
21	3	503	CL7	CHC-C1C-NC	-3.02	121.68	124.45
26	c	501	LMG	O8-C28-C29	3.02	121.38	111.91
21	1	417	CL7	CMD-C2D-C1D	3.02	133.10	128.46
21	5	417	CL7	CMD-C2D-C1D	3.02	133.10	128.46
32	4	420	ZEX	C10-C11-C12	-3.02	113.80	123.22
32	1	422	ZEX	C3-C4-C5	-3.02	105.84	111.85
32	5	422	ZEX	C3-C4-C5	-3.02	105.84	111.85
21	1	417	CL7	C4C-C3C-C2C	-3.02	103.19	107.13
21	5	417	CL7	C4C-C3C-C2C	-3.02	103.19	107.13
32	1	421	ZEX	C11-C10-C9	-3.02	123.00	127.31
32	5	421	ZEX	C11-C10-C9	-3.02	123.00	127.31
32	5	422	ZEX	C21-C22-C23	-3.02	107.16	113.69
21	6	514	CL7	CHD-C4C-C3C	-3.02	120.06	124.93
21	1	419	CL7	CHC-C1C-NC	-3.01	121.68	124.45
32	2	521	ZEX	C1-C2-C3	-3.01	106.84	113.64
21	B	603	CL7	CHD-C4C-C3C	-3.01	120.07	124.93
21	2	508	CL7	CHD-C4C-C3C	-3.01	120.07	124.93
21	b	604	CL7	CHD-C4C-C3C	-3.01	120.07	124.93
21	6	508	CL7	CHD-C4C-C3C	-3.01	120.07	124.93
23	4	402	8CT	C19-C18-C17	-3.01	117.31	123.47
23	8	402	8CT	C19-C18-C17	-3.01	117.31	123.47
21	B	601	CL7	CHD-C4C-C3C	-3.01	120.07	124.93
21	b	602	CL7	CHD-C4C-C3C	-3.01	120.07	124.93
21	B	613	CL7	CAA-CBA-CGA	-3.01	104.47	113.25
21	b	614	CL7	CAA-CBA-CGA	-3.01	104.47	113.25
21	7	510	CL7	CHC-C1C-NC	-3.01	121.69	124.45
32	6	520	ZEX	C1-C2-C3	-3.00	106.86	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	419	CL7	CHC-C1C-NC	-3.00	121.69	124.45
21	8	411	CL7	C1B-CHB-C4A	-3.00	124.17	130.12
21	7	511	CL7	C7-C6-C5	-3.00	105.20	113.36
21	c	518	CL7	CHD-C4C-C3C	-3.00	120.08	124.93
21	C	504	CL7	CHC-C1C-NC	-3.00	121.69	124.45
21	C	518	CL7	CHD-C4C-C3C	-3.00	120.08	124.93
21	2	514	CL7	CHD-C4C-C3C	-3.00	120.08	124.93
21	b	603	CL7	CAA-C2A-C1A	-3.00	102.32	112.19
32	2	521	ZEX	C3-C4-C5	-3.00	105.88	111.85
21	B	604	CL7	C4-C3-C5	3.00	120.31	115.27
21	b	605	CL7	C4-C3-C5	3.00	120.31	115.27
21	6	512	CL7	CHC-C1C-NC	-3.00	121.70	124.45
21	2	517	CL7	O2D-CGD-CBD	2.99	116.59	111.27
21	6	517	CL7	O2D-CGD-CBD	2.99	116.59	111.27
21	3	511	CL7	C7-C6-C5	-2.99	105.23	113.36
21	D	402	CL7	CHC-C1C-NC	-2.99	121.70	124.45
21	C	506	CL7	CMD-C2D-C1D	2.99	133.06	128.46
21	8	417	CL7	C4D-C3D-CAD	-2.99	102.97	107.81
21	B	609	CL7	CHD-C4C-C3C	-2.99	120.10	124.93
23	B	617	8CT	C01-C02-C07	2.99	119.36	113.62
21	8	417	CL7	O2D-CGD-CBD	2.99	116.58	111.27
21	B	602	CL7	CAA-C2A-C1A	-2.99	102.36	112.19
21	4	417	CL7	C4D-C3D-CAD	-2.99	102.97	107.81
21	4	411	CL7	C1B-CHB-C4A	-2.99	124.20	130.12
21	7	517	CL7	CHC-C1C-NC	-2.99	121.71	124.45
21	2	502	CL7	O2D-CGD-CBD	2.99	116.57	111.27
21	6	502	CL7	O2D-CGD-CBD	2.99	116.57	111.27
21	3	511	CL7	C4C-C3C-C2C	-2.99	103.24	107.13
21	7	511	CL7	C4C-C3C-C2C	-2.99	103.24	107.13
32	3	522	ZEX	C7-C8-C9	-2.98	121.72	126.23
32	7	522	ZEX	C7-C8-C9	-2.98	121.72	126.23
32	1	421	ZEX	C27-C26-C25	-2.98	118.02	122.84
32	5	421	ZEX	C27-C26-C25	-2.98	118.02	122.84
23	c	516	8CT	C40-C12-C13	-2.98	118.74	122.92
21	3	514	CL7	CHC-C1C-NC	-2.98	121.71	124.45
21	4	417	CL7	O2D-CGD-CBD	2.98	116.57	111.27
21	2	512	CL7	CHC-C1C-NC	-2.98	121.71	124.45
21	d	402	CL7	CHC-C1C-NC	-2.98	121.71	124.45
21	2	502	CL7	C7-C6-C5	-2.98	105.26	113.36
21	6	502	CL7	C7-C6-C5	-2.98	105.26	113.36
21	1	412	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	5	412	CL7	CHC-C1C-NC	-2.98	121.72	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	503	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	7	514	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	3	510	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	B	622	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	C	503	CL7	C4C-C3C-C2C	-2.98	103.25	107.13
21	3	512	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	7	512	CL7	CHC-C1C-NC	-2.98	121.72	124.45
21	3	517	CL7	CHC-C1C-NC	-2.97	121.72	124.45
21	7	504	CL7	O2D-CGD-CBD	2.97	116.55	111.27
23	b	618	8CT	C01-C02-C07	2.97	119.33	113.62
23	B	627	8CT	C07-C02-C03	-2.97	118.42	122.73
23	b	601	8CT	C07-C02-C03	-2.97	118.42	122.73
32	6	520	ZEX	C3-C4-C5	-2.97	105.94	111.85
21	1	410	CL7	CHD-C4C-C3C	-2.97	120.13	124.93
21	b	610	CL7	CHD-C4C-C3C	-2.97	120.13	124.93
21	B	613	CL7	OBD-CAD-CBD	-2.97	121.66	125.89
21	b	614	CL7	OBD-CAD-CBD	-2.97	121.66	125.89
21	1	416	CL7	CHD-C4C-C3C	-2.97	120.14	124.93
21	8	404	CL7	CHD-C4C-C3C	-2.97	120.14	124.93
21	8	411	CL7	O2D-CGD-CBD	2.97	116.54	111.27
23	C	516	8CT	C40-C12-C13	-2.96	118.77	122.92
21	5	410	CL7	CHD-C4C-C3C	-2.96	120.14	124.93
21	5	417	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	B	603	CL7	CHC-C1C-NC	-2.96	121.73	124.45
21	4	411	CL7	O2D-CGD-CBD	2.96	116.53	111.27
21	5	410	CL7	C7-C6-C5	-2.96	105.33	113.36
21	2	510	CL7	CHC-C1C-NC	-2.96	121.74	124.45
21	8	406	CL7	CAA-CBA-CGA	-2.96	104.61	113.25
21	b	604	CL7	CHC-C1C-NC	-2.96	121.74	124.45
21	2	501	CL7	O2D-CGD-CBD	2.96	116.52	111.27
21	3	504	CL7	O2D-CGD-CBD	2.96	116.52	111.27
21	c	504	CL7	CHC-C1C-NC	-2.95	121.74	124.45
21	4	404	CL7	CHD-C4C-C3C	-2.95	120.16	124.93
21	c	503	CL7	C4C-C3C-C2C	-2.95	103.28	107.13
21	B	615	CL7	CHD-C4C-C3C	-2.95	120.16	124.93
21	b	616	CL7	CHD-C4C-C3C	-2.95	120.16	124.93
21	B	611	CL7	CHC-C1C-NC	-2.95	121.74	124.45
21	b	612	CL7	CHC-C1C-NC	-2.95	121.74	124.45
21	1	410	CL7	CMD-C2D-C1D	2.95	133.00	128.46
21	5	410	CL7	CMD-C2D-C1D	2.95	133.00	128.46
21	C	509	CL7	O2A-CGA-CBA	2.95	121.16	111.91
21	c	509	CL7	O2A-CGA-CBA	2.95	121.16	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	a	401	CL7	O2D-CGD-CBD	2.95	116.51	111.27
21	4	406	CL7	CAA-CBA-CGA	-2.95	104.64	113.25
21	8	406	CL7	CHC-C1C-NC	-2.95	121.75	124.45
21	7	516	CL7	CHD-C4C-C3C	-2.95	120.17	124.93
21	2	507	CL7	C4D-C3D-CAD	-2.95	103.04	107.81
21	6	507	CL7	C4D-C3D-CAD	-2.95	103.04	107.81
21	1	410	CL7	C7-C6-C5	-2.94	105.36	113.36
21	B	615	CL7	C3B-C4B-NB	2.94	113.01	109.21
21	4	406	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	6	501	CL7	O2D-CGD-CBD	2.94	116.49	111.27
21	6	510	CL7	CHC-C1C-NC	-2.94	121.75	124.45
21	A	401	CL7	O2D-CGD-CBD	2.94	116.49	111.27
21	a	403	CL7	O2D-CGD-CBD	2.94	116.48	111.27
21	4	405	CL7	O2D-CGD-CBD	2.94	116.48	111.27
21	8	405	CL7	O2D-CGD-CBD	2.94	116.48	111.27
21	3	507	CL7	C7-C6-C5	-2.93	105.39	113.36
21	7	518	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	A	403	CL7	O2D-CGD-CBD	2.93	116.48	111.27
21	2	514	CL7	CMD-C2D-C1D	2.93	132.97	128.46
21	6	514	CL7	CMD-C2D-C1D	2.93	132.97	128.46
21	7	507	CL7	C7-C6-C5	-2.93	105.40	113.36
32	6	520	ZEX	C2-C3-C4	-2.93	106.29	110.30
21	b	616	CL7	C3B-C4B-NB	2.93	113.00	109.21
21	5	416	CL7	CHD-C4C-C3C	-2.93	120.20	124.93
21	3	516	CL7	CHD-C4C-C3C	-2.93	120.20	124.93
21	B	609	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	b	610	CL7	O2D-CGD-CBD	2.93	116.47	111.27
21	4	412	CL7	C7-C6-C5	-2.93	105.41	113.36
21	8	412	CL7	C7-C6-C5	-2.93	105.41	113.36
21	2	505	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	b	623	CL7	CHC-C1C-NC	-2.93	121.76	124.45
21	3	504	CL7	C7-C6-C5	-2.93	105.41	113.36
21	7	504	CL7	C7-C6-C5	-2.93	105.41	113.36
21	c	509	CL7	C1-C2-C3	2.93	131.10	126.04
21	B	607	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	B	616	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	b	617	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	5	407	CL7	O2D-CGD-CBD	2.92	116.46	111.27
32	2	521	ZEX	C2-C3-C4	-2.92	106.30	110.30
32	1	421	ZEX	C18-C5-C6	-2.92	121.25	124.53
32	5	421	ZEX	C18-C5-C6	-2.92	121.25	124.53
32	1	421	ZEX	C39-C29-C30	-2.92	118.83	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	417	CL7	CHC-C1C-NC	-2.92	121.77	124.45
21	1	407	CL7	O2D-CGD-CBD	2.92	116.46	111.27
21	7	513	CL7	CHC-C1C-NC	-2.92	121.77	124.45
23	b	619	8CT	C25-C24-C23	-2.92	114.11	123.22
21	c	506	CL7	CHD-C4C-C3C	-2.92	120.22	124.93
32	5	421	ZEX	C39-C29-C30	-2.92	118.84	122.92
21	4	405	CL7	CHC-C1C-NC	-2.92	121.77	124.45
23	b	620	8CT	C19-C18-C17	-2.91	117.50	123.47
21	C	506	CL7	CHD-C4C-C3C	-2.91	120.22	124.93
21	B	607	CL7	O2D-CGD-CBD	2.91	116.44	111.27
32	2	525	ZEX	C1-C6-C5	-2.91	118.51	122.61
31	F	101	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
31	f	101	HEM	CHD-C1D-C2D	-2.91	120.43	124.98
23	B	618	8CT	C25-C24-C23	-2.91	114.13	123.22
21	2	511	CL7	CHC-C1C-NC	-2.91	121.78	124.45
21	6	511	CL7	CHC-C1C-NC	-2.91	121.78	124.45
27	B	624	DGD	O1G-C1A-C2A	2.91	121.03	111.91
32	2	523	ZEX	C18-C5-C4	2.91	119.74	114.36
32	6	522	ZEX	C18-C5-C4	2.91	119.74	114.36
21	C	509	CL7	C1-C2-C3	2.91	131.07	126.04
21	6	511	CL7	CMD-C2D-C1D	2.91	132.93	128.46
21	8	405	CL7	CHC-C1C-NC	-2.91	121.78	124.45
32	6	524	ZEX	C1-C6-C5	-2.91	118.52	122.61
21	4	411	CL7	CMD-C2D-C1D	2.91	132.93	128.46
21	8	411	CL7	CMD-C2D-C1D	2.91	132.93	128.46
21	6	507	CL7	CHC-C1C-NC	-2.90	121.78	124.45
21	b	608	CL7	O2D-CGD-CBD	2.90	116.43	111.27
21	2	515	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	6	515	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	7	509	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	3	518	CL7	CHC-C1C-NC	-2.90	121.79	124.45
23	B	619	8CT	C19-C18-C17	-2.90	117.53	123.47
27	b	625	DGD	O1G-C1A-C2A	2.90	121.00	111.91
21	b	616	CL7	CAA-CBA-CGA	-2.90	104.79	113.25
21	2	511	CL7	CMD-C2D-C1D	2.90	132.92	128.46
21	C	511	CL7	C7-C6-C5	-2.90	105.49	113.36
21	1	410	CL7	O2D-CGD-CBD	2.90	116.41	111.27
21	3	513	CL7	CHC-C1C-NC	-2.90	121.79	124.45
21	6	510	CL7	O2D-CGD-CBD	2.89	116.41	111.27
21	B	615	CL7	CAA-CBA-CGA	-2.89	104.80	113.25
21	5	410	CL7	O2D-CGD-CBD	2.89	116.41	111.27
21	b	608	CL7	CHC-C1C-NC	-2.89	121.80	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	606	CL7	C1B-CHB-C4A	-2.89	124.39	130.12
21	b	607	CL7	C1B-CHB-C4A	-2.89	124.39	130.12
21	5	407	CL7	CHC-C1C-NC	-2.89	121.80	124.45
21	1	419	CL7	O2D-CGD-CBD	2.89	116.40	111.27
21	c	511	CL7	C7-C6-C5	-2.89	105.52	113.36
21	4	409	CL7	CHD-C4C-C3C	-2.89	120.27	124.93
21	8	409	CL7	CHD-C4C-C3C	-2.89	120.27	124.93
21	6	505	CL7	CHC-C1C-NC	-2.88	121.80	124.45
21	5	419	CL7	O2D-CGD-CBD	2.88	116.39	111.27
21	b	612	CL7	CHD-C4C-C3C	-2.88	120.27	124.93
21	2	517	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	6	517	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	2	504	CL7	C4D-C3D-CAD	-2.88	103.16	107.81
21	6	504	CL7	C4D-C3D-CAD	-2.88	103.16	107.81
21	1	407	CL7	CHC-C1C-NC	-2.88	121.81	124.45
21	4	416	CL7	CMA-C3A-C2A	-2.87	109.39	116.10
21	B	611	CL7	CHD-C4C-C3C	-2.87	120.29	124.93
32	4	403	ZEX	C15-C35-C34	-2.87	117.59	123.47
32	8	403	ZEX	C15-C35-C34	-2.87	117.59	123.47
21	2	510	CL7	O2D-CGD-CBD	2.87	116.37	111.27
21	b	608	CL7	C4D-C3D-CAD	-2.87	103.16	107.81
21	4	408	CL7	CAA-CBA-CGA	-2.87	104.89	112.51
21	8	408	CL7	CAA-CBA-CGA	-2.87	104.89	112.51
21	4	413	CL7	CHC-C1C-NC	-2.87	121.82	124.45
21	8	413	CL7	CHC-C1C-NC	-2.87	121.82	124.45
21	1	406	CL7	O2D-CGD-CBD	2.87	116.36	111.27
21	5	406	CL7	O2D-CGD-CBD	2.87	116.36	111.27
21	1	409	CL7	CHD-C4C-C3C	-2.87	120.30	124.93
21	5	409	CL7	CHD-C4C-C3C	-2.87	120.30	124.93
21	7	508	CL7	CHD-C4C-C3C	-2.86	120.30	124.93
21	2	507	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	A	403	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	a	403	CL7	CHC-C1C-NC	-2.86	121.82	124.45
21	3	511	CL7	O2A-CGA-O1A	-2.86	116.37	123.59
21	7	511	CL7	O2A-CGA-O1A	-2.86	116.37	123.59
21	3	508	CL7	O2D-CGD-CBD	2.86	116.35	111.27
21	7	508	CL7	O2D-CGD-CBD	2.86	116.35	111.27
21	5	405	CL7	O2D-CGD-CBD	2.86	116.35	111.27
21	4	416	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	8	416	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	8	416	CL7	CMA-C3A-C2A	-2.86	109.42	116.10
32	4	420	ZEX	C1-C6-C5	-2.86	118.58	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	8CT	C35-C30-C29	-2.86	109.09	112.70
23	b	618	8CT	C35-C30-C29	-2.86	109.09	112.70
21	3	512	CL7	C7-C6-C5	-2.86	105.59	113.36
21	7	512	CL7	C7-C6-C5	-2.86	105.59	113.36
21	6	507	CL7	C1B-CHB-C4A	-2.86	124.46	130.12
21	2	502	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	6	502	CL7	CHC-C1C-NC	-2.86	121.83	124.45
32	4	419	ZEX	C27-C26-C25	-2.86	118.22	122.84
21	3	505	CL7	CHC-C1C-NC	-2.86	121.83	124.45
21	7	505	CL7	CHC-C1C-NC	-2.86	121.83	124.45
32	8	420	ZEX	C1-C6-C5	-2.86	118.59	122.61
21	2	503	CL7	C7-C6-C5	-2.85	105.61	113.36
27	B	624	DGD	C2G-O2G-C1B	-2.85	110.76	117.79
21	1	404	CL7	C7-C6-C5	-2.85	105.61	113.36
21	B	614	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	b	615	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	2	507	CL7	C1B-CHB-C4A	-2.85	124.47	130.12
32	8	419	ZEX	C27-C26-C25	-2.85	118.24	122.84
27	b	625	DGD	C2G-O2G-C1B	-2.85	110.78	117.79
21	2	509	CL7	O2D-CGD-CBD	2.85	116.33	111.27
21	d	402	CL7	CHD-C4C-C3C	-2.84	120.33	124.93
21	3	508	CL7	CHD-C4C-C3C	-2.84	120.34	124.93
21	6	503	CL7	C7-C6-C5	-2.84	105.64	113.36
21	5	404	CL7	C7-C6-C5	-2.84	105.64	113.36
21	6	509	CL7	O2D-CGD-CBD	2.84	116.32	111.27
21	3	508	CL7	OBD-CAD-CBD	-2.84	121.84	125.89
21	7	508	CL7	OBD-CAD-CBD	-2.84	121.84	125.89
21	1	405	CL7	O2D-CGD-CBD	2.84	116.31	111.27
32	1	422	ZEX	C30-C31-C32	-2.84	114.36	123.22
23	C	516	8CT	C30-C31-C32	-2.84	117.98	121.47
23	c	516	8CT	C30-C31-C32	-2.84	117.98	121.47
23	d	406	8CT	C22-C21-C20	-2.84	118.95	122.92
32	4	420	ZEX	C35-C15-C14	-2.84	117.66	123.47
32	8	420	ZEX	C35-C15-C14	-2.84	117.66	123.47
21	B	607	CL7	C4D-C3D-CAD	-2.84	103.22	107.81
21	5	413	CL7	C3B-C4B-NB	2.84	112.88	109.21
23	C	515	8CT	C19-C18-C17	-2.83	117.67	123.47
21	C	512	CL7	CHC-C1C-NC	-2.83	121.85	124.45
21	c	510	CL7	O2D-CGD-CBD	2.83	116.31	111.27
32	5	422	ZEX	C30-C31-C32	-2.83	114.37	123.22
21	B	602	CL7	CHC-C1C-NC	-2.83	121.85	124.45
32	3	520	ZEX	C19-C9-C10	-2.83	118.96	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	7	520	ZEX	C19-C9-C10	-2.83	118.96	122.92
21	4	417	CL7	C4C-C3C-C2C	-2.83	103.44	107.13
21	8	417	CL7	C4C-C3C-C2C	-2.83	103.44	107.13
21	C	510	CL7	O2D-CGD-CBD	2.83	116.29	111.27
21	2	516	CL7	CHC-C1C-NC	-2.83	121.86	124.45
21	3	509	CL7	CHC-C1C-NC	-2.83	121.86	124.45
21	6	516	CL7	CHC-C1C-NC	-2.83	121.86	124.45
21	b	603	CL7	CHC-C1C-NC	-2.82	121.86	124.45
23	c	515	8CT	C19-C18-C17	-2.82	117.69	123.47
21	C	509	CL7	O2A-CGA-O1A	-2.82	116.47	123.59
21	c	509	CL7	O2A-CGA-O1A	-2.82	116.47	123.59
32	4	419	ZEX	C18-C5-C6	-2.82	121.36	124.53
21	1	411	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	5	411	CL7	CHC-C1C-NC	-2.82	121.86	124.45
21	c	504	CL7	C7-C6-C5	-2.82	105.70	113.36
21	D	402	CL7	CHD-C4C-C3C	-2.82	120.37	124.93
21	4	416	CL7	O2D-CGD-CBD	2.82	116.28	111.27
21	8	416	CL7	O2D-CGD-CBD	2.82	116.28	111.27
21	c	510	CL7	CMD-C2D-C1D	2.82	132.80	128.46
23	D	406	8CT	C22-C21-C20	-2.82	118.97	122.92
21	B	609	CL7	C7-C6-C5	-2.82	105.71	113.36
21	C	511	CL7	C4D-C3D-CAD	-2.82	103.25	107.81
21	b	602	CL7	C3B-C4B-NB	2.82	112.85	109.21
21	c	511	CL7	C4D-C3D-CAD	-2.82	103.25	107.81
21	3	509	CL7	O2D-CGD-CBD	2.82	116.27	111.27
21	7	509	CL7	O2D-CGD-CBD	2.82	116.27	111.27
21	C	504	CL7	C7-C6-C5	-2.82	105.71	113.36
21	b	605	CL7	CMD-C2D-C1D	2.81	132.79	128.46
21	3	506	CL7	CHD-C4C-C3C	-2.81	120.38	124.93
21	7	506	CL7	CHD-C4C-C3C	-2.81	120.38	124.93
21	C	510	CL7	CMD-C2D-C1D	2.81	132.79	128.46
21	b	610	CL7	C7-C6-C5	-2.81	105.72	113.36
21	3	502	CL7	CHD-C4C-C3C	-2.81	120.39	124.93
21	7	502	CL7	CHD-C4C-C3C	-2.81	120.39	124.93
21	1	404	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	5	404	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	1	413	CL7	C3B-C4B-NB	2.81	112.84	109.21
23	D	406	8CT	C04-C03-C02	-2.81	118.66	122.61
23	d	406	8CT	C04-C03-C02	-2.81	118.66	122.61
21	C	514	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	c	512	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	b	613	CL7	CAA-CBA-CGA	-2.81	105.05	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	406	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	5	406	CL7	CHC-C1C-NC	-2.81	121.87	124.45
21	1	406	CL7	C4-C3-C5	2.81	119.99	115.27
21	C	507	CL7	C1B-CHB-C4A	-2.80	124.56	130.12
21	c	507	CL7	C1B-CHB-C4A	-2.80	124.56	130.12
32	3	520	ZEX	C8-C7-C6	-2.80	119.33	127.20
32	7	520	ZEX	C8-C7-C6	-2.80	119.33	127.20
21	B	601	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	b	602	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	2	514	CL7	C4C-C3C-C2C	-2.80	103.48	107.13
21	6	514	CL7	C4C-C3C-C2C	-2.80	103.48	107.13
21	C	504	CL7	O2D-CGD-CBD	2.80	116.24	111.27
21	D	404	CL7	CHD-C4C-C3C	-2.80	120.41	124.93
21	d	404	CL7	CHD-C4C-C3C	-2.80	120.41	124.93
21	C	505	CL7	O2D-CGD-CBD	2.80	116.24	111.27
21	5	406	CL7	C4-C3-C5	2.80	119.98	115.27
21	B	604	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	b	605	CL7	CHC-C1C-NC	-2.80	121.88	124.45
21	1	418	CL7	C4D-C3D-CAD	-2.80	103.29	107.81
21	5	418	CL7	C4D-C3D-CAD	-2.80	103.29	107.81
21	8	408	CL7	C1B-CHB-C4A	-2.79	124.58	130.12
21	c	504	CL7	O2D-CGD-CBD	2.79	116.23	111.27
23	B	627	8CT	C23-C21-C20	2.79	123.23	118.94
32	3	519	ZEX	C19-C9-C10	-2.79	119.01	122.92
32	7	519	ZEX	C19-C9-C10	-2.79	119.01	122.92
21	1	407	CL7	C1B-CHB-C4A	-2.79	124.59	130.12
21	4	409	CL7	C4C-C3C-C2C	-2.79	103.49	107.13
21	2	502	CL7	CAA-CBA-CGA	-2.79	105.09	113.25
21	6	502	CL7	CAA-CBA-CGA	-2.79	105.09	113.25
21	3	511	CL7	O2A-CGA-CBA	2.79	120.67	111.91
21	7	511	CL7	O2A-CGA-CBA	2.79	120.67	111.91
21	b	609	CL7	CHC-C1C-NC	-2.79	121.89	124.45
21	B	601	CL7	C3B-C4B-NB	2.79	112.81	109.21
23	4	402	8CT	C14-C13-C12	-2.79	123.33	127.31
23	8	402	8CT	C14-C13-C12	-2.79	123.33	127.31
21	B	604	CL7	CMD-C2D-C1D	2.79	132.75	128.46
23	b	601	8CT	C27-C26-C25	-2.78	119.02	122.92
23	C	515	8CT	C18-C17-C16	-2.78	123.34	127.31
21	3	510	CL7	O2D-CGD-CBD	2.78	116.22	111.27
21	7	510	CL7	O2D-CGD-CBD	2.78	116.22	111.27
32	8	419	ZEX	C18-C5-C6	-2.78	121.40	124.53
21	7	503	CL7	CAA-CBA-CGA	-2.78	105.12	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	409	CL7	C4C-C3C-C2C	-2.78	103.50	107.13
21	B	612	CL7	CAA-CBA-CGA	-2.78	105.12	113.25
21	6	507	CL7	CAA-CBA-CGA	-2.78	105.12	113.25
21	1	417	CL7	C1B-CHB-C4A	-2.78	124.61	130.12
21	5	417	CL7	C1B-CHB-C4A	-2.78	124.61	130.12
21	7	502	CL7	CHC-C1C-NC	-2.78	121.90	124.45
21	5	407	CL7	C1B-CHB-C4A	-2.78	124.61	130.12
21	B	606	CL7	CAA-C2A-C3A	-2.78	105.17	112.78
21	b	607	CL7	CAA-C2A-C3A	-2.78	105.17	112.78
23	b	601	8CT	C23-C21-C20	2.78	123.21	118.94
21	B	608	CL7	CHC-C1C-NC	-2.78	121.90	124.45
21	4	408	CL7	C1B-CHB-C4A	-2.78	124.62	130.12
21	c	505	CL7	O2D-CGD-CBD	2.78	116.20	111.27
21	6	512	CL7	CAC-C3C-C2C	2.78	132.28	127.53
21	6	501	CL7	C4D-C3D-CAD	-2.78	103.32	107.81
32	1	422	ZEX	C35-C15-C14	-2.77	117.79	123.47
23	C	515	8CT	C07-C02-C03	-2.77	118.70	122.73
32	5	422	ZEX	C35-C15-C14	-2.77	117.79	123.47
21	2	512	CL7	CAC-C3C-C2C	2.77	132.27	127.53
21	2	506	CL7	O2D-CGD-CBD	2.77	116.19	111.27
21	2	507	CL7	CAA-CBA-CGA	-2.77	105.15	113.25
21	3	503	CL7	CAA-CBA-CGA	-2.77	105.15	113.25
21	1	403	CL7	C7-C6-C5	-2.77	105.83	113.36
21	5	403	CL7	C7-C6-C5	-2.77	105.83	113.36
21	5	420	CL7	CHC-C1C-NC	-2.77	121.91	124.45
21	4	408	CL7	O2D-CGD-CBD	2.77	116.19	111.27
21	8	408	CL7	O2D-CGD-CBD	2.77	116.19	111.27
21	6	506	CL7	C4-C3-C5	2.77	119.93	115.27
21	1	420	CL7	CHC-C1C-NC	-2.77	121.91	124.45
21	B	611	CL7	C1B-CHB-C4A	-2.76	124.65	130.12
21	c	514	CL7	CHC-C1C-NC	-2.76	121.92	124.45
21	3	501	CL7	C1B-CHB-C4A	-2.76	124.65	130.12
21	7	501	CL7	C1B-CHB-C4A	-2.76	124.65	130.12
21	2	501	CL7	C4D-C3D-CAD	-2.76	103.34	107.81
21	1	404	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	5	404	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	3	503	CL7	O2D-CGD-CBD	2.76	116.17	111.27
21	7	503	CL7	O2D-CGD-CBD	2.76	116.17	111.27
21	4	417	CL7	C3A-C4A-CHB	-2.76	119.61	123.70
21	8	417	CL7	C3A-C4A-CHB	-2.76	119.61	123.70
23	B	627	8CT	C27-C26-C25	-2.76	119.06	122.92
23	B	627	8CT	C05-C04-C03	2.76	114.73	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	601	8CT	C05-C04-C03	2.76	114.73	110.48
23	A	404	8CT	C24-C23-C21	-2.76	118.67	126.42
23	a	404	8CT	C24-C23-C21	-2.76	118.67	126.42
21	1	415	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	4	416	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	5	415	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	8	416	CL7	C4C-C3C-C2C	-2.76	103.53	107.13
21	6	501	CL7	CMD-C2D-C1D	2.76	132.70	128.46
23	B	617	8CT	C25-C24-C23	-2.75	114.62	123.22
21	1	416	CL7	CHC-C1C-NC	-2.75	121.92	124.45
21	5	416	CL7	CHC-C1C-NC	-2.75	121.92	124.45
23	b	618	8CT	C25-C24-C23	-2.75	114.63	123.22
21	C	510	CL7	C1B-CHB-C4A	-2.75	124.67	130.12
21	c	510	CL7	C1B-CHB-C4A	-2.75	124.67	130.12
21	4	415	CL7	CHC-C1C-NC	-2.75	121.93	124.45
21	8	415	CL7	CHC-C1C-NC	-2.75	121.93	124.45
21	6	506	CL7	O2D-CGD-CBD	2.75	116.15	111.27
21	2	506	CL7	C4-C3-C5	2.75	119.89	115.27
21	2	512	CL7	C7-C6-C5	-2.74	105.90	113.36
21	6	512	CL7	C7-C6-C5	-2.74	105.90	113.36
21	B	610	CL7	CMD-C2D-C1D	2.74	132.68	128.46
21	b	611	CL7	CMD-C2D-C1D	2.74	132.68	128.46
21	b	612	CL7	C1B-CHB-C4A	-2.74	124.68	130.12
21	1	417	CL7	C7-C6-C5	-2.74	105.91	113.36
21	5	417	CL7	C7-C6-C5	-2.74	105.91	113.36
21	6	507	CL7	CHD-C4C-C3C	-2.74	120.50	124.93
23	c	515	8CT	C18-C17-C16	-2.74	123.40	127.31
21	3	502	CL7	CHC-C1C-NC	-2.74	121.93	124.45
21	c	502	CL7	CHC-C1C-NC	-2.74	121.94	124.45
21	2	518	CL7	CHC-C1C-NC	-2.74	121.94	124.45
21	6	518	CL7	CHC-C1C-NC	-2.74	121.94	124.45
21	B	616	CL7	CAA-CBA-CGA	-2.74	105.24	112.51
21	b	617	CL7	CAA-CBA-CGA	-2.74	105.24	112.51
21	4	412	CL7	C1B-CHB-C4A	-2.74	124.69	130.12
21	3	501	CL7	C3B-C4B-NB	2.74	112.75	109.21
21	7	501	CL7	C3B-C4B-NB	2.74	112.75	109.21
23	C	519	8CT	C19-C18-C17	-2.74	117.87	123.47
21	a	401	CL7	CAA-C2A-C3A	-2.74	105.29	112.78
21	5	411	CL7	CMD-C2D-C1D	2.73	132.67	128.46
21	C	503	CL7	C1B-CHB-C4A	-2.73	124.70	130.12
21	c	503	CL7	C1B-CHB-C4A	-2.73	124.70	130.12
21	c	505	CL7	C7-C6-C5	-2.73	105.94	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	515	8CT	C07-C02-C03	-2.73	118.76	122.73
21	2	501	CL7	CMD-C2D-C1D	2.73	132.66	128.46
32	4	419	ZEX	C15-C35-C34	-2.73	117.88	123.47
32	8	419	ZEX	C15-C35-C34	-2.73	117.88	123.47
21	1	402	CL7	O2D-CGD-CBD	2.73	116.12	111.27
21	5	402	CL7	O2D-CGD-CBD	2.73	116.12	111.27
21	2	507	CL7	CHD-C4C-C3C	-2.73	120.52	124.93
21	1	411	CL7	CMD-C2D-C1D	2.73	132.66	128.46
21	7	517	CL7	C1B-CHB-C4A	-2.73	124.71	130.12
21	A	406	CL7	CHC-C1C-NC	-2.73	121.95	124.45
21	a	405	CL7	CHC-C1C-NC	-2.73	121.95	124.45
21	2	513	CL7	CHD-C4C-C3C	-2.73	120.52	124.93
21	6	513	CL7	CHD-C4C-C3C	-2.73	120.52	124.93
21	A	401	CL7	CAA-C2A-C3A	-2.73	105.31	112.78
23	c	519	8CT	C19-C18-C17	-2.73	117.89	123.47
23	C	515	8CT	C39-C16-C15	2.72	122.37	118.08
23	c	515	8CT	C39-C16-C15	2.72	122.37	118.08
21	3	501	CL7	C7-C6-C5	-2.72	105.96	113.36
21	C	505	CL7	C7-C6-C5	-2.72	105.96	113.36
21	2	509	CL7	C1B-CHB-C4A	-2.72	124.72	130.12
21	6	509	CL7	C1B-CHB-C4A	-2.72	124.72	130.12
21	A	401	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	a	401	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	8	412	CL7	C1B-CHB-C4A	-2.72	124.73	130.12
21	B	614	CL7	C7-C6-C5	-2.72	105.97	113.36
21	C	508	CL7	CHC-C1C-NC	-2.72	121.95	124.45
21	B	616	CL7	CMD-C2D-C1D	2.72	132.64	128.46
21	b	617	CL7	CMD-C2D-C1D	2.72	132.64	128.46
21	3	516	CL7	C1B-CHB-C4A	-2.72	124.74	130.12
21	6	510	CL7	O2A-C1-C2	-2.71	101.50	108.64
32	1	421	ZEX	C18-C5-C4	2.71	119.38	114.36
32	5	421	ZEX	C18-C5-C4	2.71	119.38	114.36
21	C	509	CL7	C7-C6-C5	-2.71	105.99	113.36
21	b	615	CL7	C7-C6-C5	-2.71	105.99	113.36
24	3	523	SQD	O8-S-C6	-2.71	101.42	105.74
24	7	523	SQD	O8-S-C6	-2.71	101.42	105.74
32	2	525	ZEX	C18-C5-C4	2.71	119.38	114.36
32	6	524	ZEX	C18-C5-C4	2.71	119.38	114.36
21	B	614	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	4	404	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	b	615	CL7	CHC-C1C-NC	-2.71	121.96	124.45
21	8	404	CL7	CHC-C1C-NC	-2.71	121.96	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	501	CL7	C7-C6-C5	-2.71	105.99	113.36
21	3	517	CL7	C1B-CHB-C4A	-2.71	124.75	130.12
21	7	516	CL7	C1B-CHB-C4A	-2.71	124.75	130.12
21	1	410	CL7	C1B-CHB-C4A	-2.71	124.75	130.12
26	C	501	LMG	O7-C10-O9	-2.71	117.16	123.70
21	5	405	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	5	408	CL7	CHD-C4C-C3C	-2.71	120.56	124.93
21	C	502	CL7	CHC-C1C-NC	-2.71	121.97	124.45
21	c	509	CL7	C7-C6-C5	-2.70	106.01	113.36
21	C	506	CL7	CHC-C1C-NC	-2.70	121.97	124.45
21	c	506	CL7	CHC-C1C-NC	-2.70	121.97	124.45
21	5	410	CL7	C1B-CHB-C4A	-2.70	124.77	130.12
32	7	522	ZEX	C27-C26-C25	-2.70	118.48	122.84
21	c	507	CL7	O2D-CGD-CBD	2.70	116.06	111.27
23	b	619	8CT	C40-C12-C13	-2.70	119.15	122.92
21	2	510	CL7	O2A-C1-C2	-2.70	101.55	108.64
21	1	408	CL7	CHD-C4C-C3C	-2.69	120.58	124.93
21	4	404	CL7	C1B-CHB-C4A	-2.69	124.79	130.12
21	8	404	CL7	C1B-CHB-C4A	-2.69	124.79	130.12
21	B	603	CL7	O2D-CGD-CBD	2.69	116.05	111.27
23	c	516	8CT	C19-C18-C17	-2.69	117.97	123.47
21	A	406	CL7	C1B-CHB-C4A	-2.69	124.80	130.12
21	5	413	CL7	CHC-C1C-NC	-2.69	121.99	124.45
21	b	604	CL7	O2D-CGD-CBD	2.69	116.04	111.27
21	c	511	CL7	C1B-CHB-C4A	-2.68	124.80	130.12
21	3	512	CL7	C4C-C3C-C2C	-2.68	103.63	107.13
21	7	512	CL7	C4C-C3C-C2C	-2.68	103.63	107.13
21	C	507	CL7	O2D-CGD-CBD	2.68	116.03	111.27
32	3	522	ZEX	C27-C26-C25	-2.68	118.51	122.84
21	C	511	CL7	C1B-CHB-C4A	-2.68	124.81	130.12
21	7	502	CL7	C1B-CHB-C4A	-2.68	124.81	130.12
21	2	502	CL7	C3B-C4B-NB	2.67	112.67	109.21
21	6	502	CL7	C3B-C4B-NB	2.67	112.67	109.21
21	7	518	CL7	CAA-CBA-CGA	-2.67	105.41	112.51
21	4	415	CL7	CAC-C3C-C4C	-2.67	120.47	124.68
21	1	405	CL7	CHC-C1C-NC	-2.67	122.00	124.45
21	a	405	CL7	C1B-CHB-C4A	-2.67	124.82	130.12
21	5	412	CL7	C1C-C2C-C3C	-2.67	103.04	106.94
23	C	516	8CT	C19-C18-C17	-2.67	118.00	123.47
21	D	402	CL7	C3B-C4B-NB	2.67	112.66	109.21
21	d	402	CL7	C3B-C4B-NB	2.67	112.66	109.21
21	1	413	CL7	CHC-C1C-NC	-2.67	122.00	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	618	8CT	C40-C12-C13	-2.67	119.19	122.92
21	a	403	CL7	C7-C6-C5	-2.67	106.11	113.36
21	7	502	CL7	CMD-C2D-C1D	2.67	132.56	128.46
21	7	516	CL7	CHC-C1C-NC	-2.67	122.00	124.45
21	3	502	CL7	C1B-CHB-C4A	-2.67	124.84	130.12
21	3	516	CL7	C3B-C4B-NB	2.67	112.66	109.21
21	7	516	CL7	C3B-C4B-NB	2.67	112.66	109.21
21	C	503	CL7	O2D-CGD-CBD	2.67	116.00	111.27
21	c	503	CL7	O2D-CGD-CBD	2.67	116.00	111.27
21	1	412	CL7	C1C-C2C-C3C	-2.67	103.05	106.94
21	c	508	CL7	CHC-C1C-NC	-2.66	122.00	124.45
21	3	516	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	6	504	CL7	CHD-C4C-C3C	-2.66	120.63	124.93
21	3	518	CL7	CAA-CBA-CGA	-2.66	105.44	112.51
21	2	508	CL7	C1B-CHB-C4A	-2.66	124.85	130.12
21	b	612	CL7	OBD-CAD-CBD	-2.66	122.09	125.89
21	B	606	CL7	C3B-C4B-NB	2.66	112.65	109.21
21	b	607	CL7	C3B-C4B-NB	2.66	112.65	109.21
21	C	504	CL7	C1B-CHB-C4A	-2.66	124.85	130.12
21	c	504	CL7	C1B-CHB-C4A	-2.66	124.85	130.12
22	d	408	PHO	CBA-CAA-C2A	-2.66	106.04	113.81
32	2	523	ZEX	C7-C6-C5	2.66	127.90	121.46
32	6	522	ZEX	C7-C6-C5	2.66	127.90	121.46
21	B	612	CL7	C7-C6-C5	-2.66	106.14	113.36
21	b	613	CL7	C7-C6-C5	-2.66	106.14	113.36
32	6	524	ZEX	C11-C12-C13	-2.66	118.95	126.42
32	8	418	ZEX	C27-C26-C25	-2.66	118.55	122.84
21	3	505	CL7	CAA-CBA-CGA	-2.66	105.49	113.25
21	B	602	CL7	C7-C6-C5	-2.66	106.14	113.36
21	b	603	CL7	C7-C6-C5	-2.66	106.14	113.36
21	B	605	CL7	CHC-C1C-NC	-2.66	122.01	124.45
21	1	403	CL7	C3B-C4B-NB	2.66	112.64	109.21
21	5	403	CL7	C3B-C4B-NB	2.66	112.64	109.21
22	D	408	PHO	CBA-CAA-C2A	-2.66	106.05	113.81
21	3	502	CL7	CMD-C2D-C1D	2.66	132.54	128.46
21	8	406	CL7	CMD-C2D-C1D	2.66	132.54	128.46
21	A	403	CL7	C7-C6-C5	-2.65	106.15	113.36
23	b	601	8CT	C28-C26-C25	2.65	123.01	118.94
21	8	415	CL7	CAC-C3C-C4C	-2.65	120.50	124.68
32	6	519	ZEX	C28-C29-C30	2.65	123.01	118.94
21	b	606	CL7	CHC-C1C-NC	-2.65	122.02	124.45
32	2	525	ZEX	C11-C12-C13	-2.65	118.97	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	506	CL7	CHC-C1C-NC	-2.65	122.02	124.45
21	C	512	CL7	C1C-C2C-C3C	-2.65	103.07	106.94
21	c	512	CL7	C1C-C2C-C3C	-2.65	103.07	106.94
32	2	519	ZEX	C28-C29-C30	2.65	123.01	118.94
23	A	404	8CT	C13-C14-C15	-2.65	114.95	123.22
23	a	404	8CT	C13-C14-C15	-2.65	114.95	123.22
21	4	411	CL7	CAA-C2A-C3A	-2.65	105.53	112.78
21	8	411	CL7	CAA-C2A-C3A	-2.65	105.53	112.78
21	C	508	CL7	C1B-CHB-C4A	-2.65	124.87	130.12
21	7	505	CL7	CAA-CBA-CGA	-2.65	105.52	113.25
21	D	405	CL7	O2D-CGD-O1D	-2.65	118.66	123.84
21	1	414	CL7	C1B-CHB-C4A	-2.65	124.87	130.12
21	7	511	CL7	CHC-C1C-NC	-2.65	122.02	124.45
21	6	508	CL7	C1B-CHB-C4A	-2.65	124.87	130.12
21	3	511	CL7	CMD-C2D-C1D	2.65	132.53	128.46
21	B	611	CL7	OBD-CAD-CBD	-2.65	122.11	125.89
22	D	408	PHO	CED-O2D-CGD	2.65	121.92	115.94
21	2	504	CL7	CHD-C4C-C3C	-2.65	120.66	124.93
21	C	518	CL7	C4D-C3D-CAD	-2.65	103.53	107.81
21	c	518	CL7	C4D-C3D-CAD	-2.65	103.53	107.81
32	4	418	ZEX	C27-C26-C25	-2.65	118.56	122.84
21	4	415	CL7	CMD-C2D-C1D	2.64	132.53	128.46
21	8	415	CL7	CMD-C2D-C1D	2.64	132.53	128.46
21	D	405	CL7	C3B-C4B-NB	2.64	112.63	109.21
21	d	405	CL7	C3B-C4B-NB	2.64	112.63	109.21
32	4	419	ZEX	C7-C8-C9	-2.64	122.25	126.23
21	3	511	CL7	CHC-C1C-NC	-2.64	122.03	124.45
21	5	407	CL7	CMA-C3A-C2A	-2.64	109.94	116.10
21	2	501	CL7	C1B-CHB-C4A	-2.64	124.89	130.12
21	6	501	CL7	C1B-CHB-C4A	-2.64	124.89	130.12
22	d	408	PHO	CED-O2D-CGD	2.64	121.90	115.94
23	c	519	8CT	C01-C02-C07	2.64	118.68	113.62
21	B	604	CL7	C3B-C4B-NB	2.64	112.62	109.21
21	b	605	CL7	C3B-C4B-NB	2.64	112.62	109.21
32	8	419	ZEX	C7-C8-C9	-2.64	122.25	126.23
23	C	519	8CT	C01-C02-C07	2.64	118.68	113.62
21	7	511	CL7	CMD-C2D-C1D	2.64	132.51	128.46
21	2	508	CL7	C3B-C4B-NB	2.63	112.62	109.21
21	6	508	CL7	C3B-C4B-NB	2.63	112.62	109.21
21	4	415	CL7	OBD-CAD-CBD	-2.63	122.13	125.89
21	4	406	CL7	CMD-C2D-C1D	2.63	132.51	128.46
21	D	405	CL7	C1B-CHB-C4A	-2.63	124.90	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	407	CL7	CMA-C3A-C2A	-2.63	109.95	116.10
21	b	612	CL7	C1C-C2C-C3C	-2.63	103.10	106.94
21	7	510	CL7	CMD-C2D-C1D	2.63	132.51	128.46
21	1	420	CL7	C4C-C3C-C2C	-2.63	103.70	107.13
21	5	414	CL7	C1B-CHB-C4A	-2.63	124.91	130.12
23	B	627	8CT	C28-C26-C25	2.63	122.97	118.94
21	4	414	CL7	CAC-C3C-C2C	2.63	132.03	127.53
21	c	508	CL7	C1B-CHB-C4A	-2.63	124.91	130.12
21	8	414	CL7	CAC-C3C-C2C	2.63	132.02	127.53
32	4	418	ZEX	C11-C12-C13	-2.63	119.03	126.42
32	8	418	ZEX	C11-C12-C13	-2.63	119.03	126.42
23	c	515	8CT	C40-C12-C11	2.63	122.22	118.08
27	c	517	DGD	C3G-C2G-C1G	-2.63	105.58	111.79
21	B	611	CL7	C1C-C2C-C3C	-2.63	103.11	106.94
21	C	506	CL7	C3B-C4B-NB	2.63	112.61	109.21
21	c	506	CL7	C3B-C4B-NB	2.63	112.61	109.21
21	b	610	CL7	C1B-CHB-C4A	-2.63	124.92	130.12
26	c	501	LMG	O7-C10-O9	-2.63	117.36	123.70
21	B	609	CL7	C1B-CHB-C4A	-2.62	124.92	130.12
21	2	505	CL7	C7-C6-C5	-2.62	106.23	113.36
21	6	505	CL7	C7-C6-C5	-2.62	106.23	113.36
21	3	510	CL7	CMD-C2D-C1D	2.62	132.50	128.46
21	5	420	CL7	C4C-C3C-C2C	-2.62	103.71	107.13
21	B	603	CL7	C1B-CHB-C4A	-2.62	124.92	130.12
21	A	403	CL7	C1-C2-C3	2.62	130.58	126.04
21	B	601	CL7	CMD-C2D-C1D	2.62	132.49	128.46
21	1	404	CL7	C1B-CHB-C4A	-2.62	124.93	130.12
21	d	405	CL7	C1B-CHB-C4A	-2.62	124.93	130.12
21	4	408	CL7	C4C-C3C-C2C	-2.62	103.71	107.13
21	1	413	CL7	CMD-C2D-C1D	2.62	132.49	128.46
21	5	413	CL7	CMD-C2D-C1D	2.62	132.49	128.46
21	3	509	CL7	C4-C3-C5	2.62	119.68	115.27
21	3	507	CL7	OBD-CAD-CBD	-2.62	122.15	125.89
23	C	515	8CT	C18-C19-C20	-2.62	118.11	123.47
23	c	515	8CT	C18-C19-C20	-2.62	118.11	123.47
21	b	604	CL7	C1B-CHB-C4A	-2.62	124.93	130.12
21	5	404	CL7	C1B-CHB-C4A	-2.62	124.93	130.12
32	2	525	ZEX	C27-C26-C25	-2.62	118.61	122.84
32	6	524	ZEX	C27-C26-C25	-2.62	118.61	122.84
27	C	517	DGD	C3G-C2G-C1G	-2.62	105.60	111.79
21	d	404	CL7	C7-C6-C5	-2.62	106.25	113.36
21	c	505	CL7	CMD-C2D-C1D	2.62	132.48	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	4	419	ZEX	C30-C31-C32	-2.62	115.06	123.22
21	C	505	CL7	CMD-C2D-C1D	2.61	132.48	128.46
21	a	403	CL7	C1-C2-C3	2.61	130.56	126.04
32	2	519	ZEX	C10-C11-C12	-2.61	115.06	123.22
32	6	519	ZEX	C10-C11-C12	-2.61	115.06	123.22
21	3	518	CL7	C1B-CHB-C4A	-2.61	124.94	130.12
21	d	402	CL7	C1B-CHB-C4A	-2.61	124.94	130.12
21	7	518	CL7	C1B-CHB-C4A	-2.61	124.94	130.12
32	8	419	ZEX	C30-C31-C32	-2.61	115.06	123.22
21	4	404	CL7	CMD-C2D-C1D	2.61	132.48	128.46
21	8	404	CL7	CMD-C2D-C1D	2.61	132.48	128.46
21	4	407	CL7	O2D-CGD-CBD	2.61	115.91	111.27
21	8	407	CL7	O2D-CGD-CBD	2.61	115.91	111.27
21	4	409	CL7	C7-C6-C5	-2.61	106.27	113.36
21	8	409	CL7	C7-C6-C5	-2.61	106.27	113.36
21	8	415	CL7	OBD-CAD-CBD	-2.61	122.17	125.89
21	B	604	CL7	C1B-CHB-C4A	-2.61	124.95	130.12
21	3	513	CL7	C4C-C3C-C2C	-2.61	103.72	107.13
21	7	513	CL7	C4C-C3C-C2C	-2.61	103.72	107.13
21	5	410	CL7	C3B-C4B-NB	2.61	112.58	109.21
21	d	405	CL7	O2D-CGD-O1D	-2.61	118.74	123.84
21	4	412	CL7	C3B-C4B-NB	2.61	112.58	109.21
21	8	412	CL7	C3B-C4B-NB	2.61	112.58	109.21
21	2	506	CL7	C3B-C4B-NB	2.61	112.58	109.21
21	6	506	CL7	C3B-C4B-NB	2.61	112.58	109.21
21	C	503	CL7	C4D-C3D-CAD	-2.61	103.59	107.81
21	c	503	CL7	C4D-C3D-CAD	-2.61	103.59	107.81
21	5	408	CL7	CHC-C1C-NC	-2.61	122.06	124.45
21	2	506	CL7	C4D-C3D-CAD	-2.61	103.59	107.81
21	B	609	CL7	CAA-CBA-CGA	-2.60	105.64	113.25
23	C	515	8CT	C40-C12-C11	2.60	122.18	118.08
21	D	404	CL7	C7-C6-C5	-2.60	106.29	113.36
21	2	501	CL7	C1C-C2C-C3C	-2.60	103.14	106.94
21	6	501	CL7	C1C-C2C-C3C	-2.60	103.14	106.94
32	2	519	ZEX	C8-C7-C6	-2.60	119.89	127.20
32	6	519	ZEX	C8-C7-C6	-2.60	119.89	127.20
21	3	504	CL7	CHC-C1C-NC	-2.60	122.06	124.45
21	7	504	CL7	CHC-C1C-NC	-2.60	122.06	124.45
21	b	602	CL7	CMD-C2D-C1D	2.60	132.46	128.46
21	1	419	CL7	CMD-C2D-C1D	2.60	132.46	128.46
21	b	610	CL7	CAA-CBA-CGA	-2.60	105.65	113.25
21	7	509	CL7	C4-C3-C5	2.60	119.65	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	518	CL7	C1B-CHB-C4A	-2.60	124.97	130.12
21	2	503	CL7	C1B-CHB-C4A	-2.60	124.97	130.12
21	C	508	CL7	OBD-CAD-CBD	-2.60	122.18	125.89
21	c	508	CL7	OBD-CAD-CBD	-2.60	122.18	125.89
21	b	605	CL7	C1B-CHB-C4A	-2.60	124.97	130.12
21	5	412	CL7	CAA-CBA-CGA	-2.60	105.61	112.51
21	2	510	CL7	CAA-CBA-CGA	-2.60	105.67	113.25
21	6	510	CL7	CAA-CBA-CGA	-2.60	105.67	113.25
21	7	507	CL7	OBD-CAD-CBD	-2.60	122.19	125.89
21	5	408	CL7	C4C-C3C-C2C	-2.60	103.74	107.13
21	6	503	CL7	C1B-CHB-C4A	-2.59	124.98	130.12
21	3	506	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	c	518	CL7	C1B-CHB-C4A	-2.59	124.98	130.12
21	4	409	CL7	OBD-CAD-CBD	-2.59	122.19	125.89
21	1	412	CL7	CAA-CBA-CGA	-2.59	105.63	112.51
21	8	408	CL7	C4C-C3C-C2C	-2.59	103.75	107.13
21	B	606	CL7	C7-C6-C5	-2.59	106.32	113.36
21	b	607	CL7	C7-C6-C5	-2.59	106.32	113.36
21	2	506	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	6	506	CL7	CHC-C1C-NC	-2.59	122.07	124.45
21	6	511	CL7	O2D-CGD-CBD	2.59	115.87	111.27
21	7	516	CL7	C4-C3-C5	2.59	119.63	115.27
21	B	603	CL7	O2A-C1-C2	-2.59	101.83	108.64
21	b	604	CL7	O2A-C1-C2	-2.59	101.83	108.64
21	C	514	CL7	C1B-CHB-C4A	-2.59	124.99	130.12
21	c	514	CL7	C1B-CHB-C4A	-2.59	124.99	130.12
21	1	410	CL7	C3B-C4B-NB	2.59	112.56	109.21
21	D	402	CL7	C1B-CHB-C4A	-2.59	124.99	130.12
21	2	511	CL7	O2D-CGD-CBD	2.59	115.86	111.27
21	1	403	CL7	C1C-C2C-C3C	-2.59	103.17	106.94
21	1	408	CL7	CHC-C1C-NC	-2.59	122.08	124.45
21	3	503	CL7	C4C-C3C-C2C	-2.59	103.76	107.13
21	7	503	CL7	C4C-C3C-C2C	-2.59	103.76	107.13
21	5	416	CL7	C4D-C3D-CAD	-2.59	103.63	107.81
21	5	419	CL7	CMD-C2D-C1D	2.58	132.44	128.46
32	2	525	ZEX	C39-C29-C30	-2.58	119.31	122.92
32	6	524	ZEX	C39-C29-C30	-2.58	119.31	122.92
21	6	506	CL7	C4D-C3D-CAD	-2.58	103.63	107.81
21	b	613	CL7	C1B-CHB-C4A	-2.58	125.00	130.12
21	3	510	CL7	CAA-C2A-C3A	-2.58	105.71	112.78
21	2	503	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	1	402	CL7	C4C-C3C-C2C	-2.58	103.77	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	408	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	5	402	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
23	4	402	8CT	C35-C30-C29	-2.58	109.44	112.70
23	8	402	8CT	C35-C30-C29	-2.58	109.44	112.70
21	B	622	CL7	C1B-CHB-C4A	-2.58	125.01	130.12
21	b	623	CL7	C1B-CHB-C4A	-2.58	125.01	130.12
21	B	612	CL7	C1B-CHB-C4A	-2.58	125.01	130.12
21	C	504	CL7	CAA-CBA-CGA	-2.58	105.72	113.25
21	c	504	CL7	CAA-CBA-CGA	-2.58	105.72	113.25
21	6	503	CL7	C4C-C3C-C2C	-2.58	103.77	107.13
21	3	516	CL7	C4-C3-C5	2.58	119.60	115.27
21	B	613	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
21	1	405	CL7	C3B-C4B-NB	2.57	112.54	109.21
21	8	412	CL7	CMD-C2D-C1D	2.57	132.42	128.46
21	3	509	CL7	C4C-C3C-C2C	-2.57	103.77	107.13
21	7	506	CL7	C4D-C3D-CAD	-2.57	103.65	107.81
21	C	503	CL7	CMD-C2D-C1D	2.57	132.42	128.46
21	c	503	CL7	CMD-C2D-C1D	2.57	132.42	128.46
21	5	403	CL7	C1C-C2C-C3C	-2.57	103.19	106.94
21	7	510	CL7	CAA-C2A-C3A	-2.57	105.74	112.78
21	1	416	CL7	C4D-C3D-CAD	-2.57	103.65	107.81
23	K	101	8CT	C40-C12-C13	-2.57	119.33	122.92
21	1	411	CL7	C4C-C3C-C2C	-2.57	103.78	107.13
21	3	506	CL7	C4D-C3D-CAD	-2.57	103.66	107.81
21	6	515	CL7	C1B-CHB-C4A	-2.57	125.03	130.12
21	C	509	CL7	C1B-CHB-C4A	-2.56	125.04	130.12
21	c	509	CL7	C1B-CHB-C4A	-2.56	125.04	130.12
21	2	508	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	6	508	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	1	408	CL7	C1B-CHB-C4A	-2.56	125.04	130.12
21	6	518	CL7	C1B-CHB-C4A	-2.56	125.04	130.12
21	5	408	CL7	C1B-CHB-C4A	-2.56	125.04	130.12
21	B	616	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	b	617	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	4	412	CL7	CMD-C2D-C1D	2.56	132.40	128.46
21	4	405	CL7	C4D-C3D-CAD	-2.56	103.66	107.81
21	3	502	CL7	C4-C3-C5	2.56	119.58	115.27
21	7	502	CL7	C4-C3-C5	2.56	119.58	115.27
21	B	615	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	b	616	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	c	502	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	2	508	CL7	OBD-CAD-CBD	-2.56	122.23	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	508	CL7	OBD-CAD-CBD	-2.56	122.23	125.89
21	4	415	CL7	C3B-C4B-NB	2.56	112.52	109.21
21	5	411	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	4	410	CL7	C1B-CHB-C4A	-2.56	125.05	130.12
21	8	410	CL7	C1B-CHB-C4A	-2.56	125.05	130.12
21	1	412	CL7	C3B-C4B-NB	2.56	112.52	109.21
21	5	412	CL7	C3B-C4B-NB	2.56	112.52	109.21
21	B	610	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	4	407	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	b	611	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	b	614	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	B	613	CL7	C1B-CHB-C4A	-2.56	125.05	130.12
21	b	614	CL7	C1B-CHB-C4A	-2.56	125.05	130.12
21	C	518	CL7	C3B-C4B-NB	2.56	112.52	109.21
21	c	518	CL7	C3B-C4B-NB	2.56	112.52	109.21
21	2	517	CL7	C4C-C3C-C2C	-2.56	103.79	107.13
21	4	410	CL7	CHC-C1C-NC	-2.56	122.10	124.45
21	1	404	CL7	CMD-C2D-C1D	2.56	132.40	128.46
21	5	404	CL7	CMD-C2D-C1D	2.56	132.40	128.46
21	6	518	CL7	CMD-C2D-C1D	2.56	132.40	128.46
21	2	514	CL7	C3B-C4B-NB	2.56	112.52	109.21
21	6	514	CL7	C3B-C4B-NB	2.56	112.52	109.21
21	5	409	CL7	C3B-C4B-NB	2.56	112.52	109.21
21	2	518	CL7	C1B-CHB-C4A	-2.56	125.05	130.12
32	3	519	ZEX	C11-C12-C13	-2.56	119.23	126.42
21	2	504	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	6	504	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	4	410	CL7	CMD-C2D-C1D	2.55	132.39	128.46
21	8	410	CL7	CMD-C2D-C1D	2.55	132.39	128.46
21	8	410	CL7	CHC-C1C-NC	-2.55	122.11	124.45
21	C	502	CL7	CAA-CBA-CGA	-2.55	105.79	113.25
21	7	509	CL7	C4C-C3C-C2C	-2.55	103.80	107.13
21	6	511	CL7	C7-C6-C5	-2.55	106.43	113.36
21	3	507	CL7	C4D-C3D-CAD	-2.55	103.68	107.81
21	8	405	CL7	C4D-C3D-CAD	-2.55	103.68	107.81
21	7	508	CL7	O2A-C1-C2	-2.55	101.93	108.64
21	d	404	CL7	C3B-C4B-NB	2.55	112.51	109.21
21	7	507	CL7	C4D-C3D-CAD	-2.55	103.68	107.81
21	D	402	CL7	CMD-C2D-C1D	2.55	132.38	128.46
21	7	508	CL7	C1B-CHB-C4A	-2.55	125.07	130.12
21	8	415	CL7	C3B-C4B-NB	2.55	112.51	109.21
32	7	519	ZEX	C11-C12-C13	-2.55	119.25	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	407	CL7	C4C-C3C-C2C	-2.55	103.80	107.13
21	3	518	CL7	CMD-C2D-C1D	2.55	132.38	128.46
21	7	518	CL7	CMD-C2D-C1D	2.55	132.38	128.46
21	c	502	CL7	CAA-CBA-CGA	-2.55	105.80	113.25
21	2	518	CL7	CMD-C2D-C1D	2.55	132.38	128.46
21	6	517	CL7	C4C-C3C-C2C	-2.55	103.81	107.13
32	1	421	ZEX	C7-C8-C9	-2.55	122.39	126.23
32	5	421	ZEX	C7-C8-C9	-2.55	122.39	126.23
21	c	509	CL7	CHC-C1C-NC	-2.55	122.11	124.45
23	C	515	8CT	C35-C30-C31	2.55	115.98	111.42
23	c	515	8CT	C35-C30-C31	2.55	115.98	111.42
21	c	505	CL7	C3B-C4B-NB	2.54	112.50	109.21
21	5	405	CL7	C3B-C4B-NB	2.54	112.50	109.21
21	3	505	CL7	C4-C3-C5	2.54	119.55	115.27
23	k	101	8CT	C40-C12-C13	-2.54	119.36	122.92
21	c	513	CL7	CMA-C3A-C2A	-2.54	110.16	116.10
27	C	517	DGD	C4E-C3E-C2E	-2.54	106.39	110.82
21	1	402	CL7	C1B-CHB-C4A	-2.54	125.08	130.12
21	5	402	CL7	C1B-CHB-C4A	-2.54	125.08	130.12
21	4	405	CL7	O2A-CGA-CBA	2.54	119.88	111.91
21	8	405	CL7	O2A-CGA-CBA	2.54	119.88	111.91
21	8	409	CL7	OBD-CAD-CBD	-2.54	122.26	125.89
21	2	507	CL7	CED-O2D-CGD	-2.54	110.19	115.94
21	6	507	CL7	CED-O2D-CGD	-2.54	110.19	115.94
21	B	614	CL7	C1B-CHB-C4A	-2.54	125.09	130.12
21	b	615	CL7	C1B-CHB-C4A	-2.54	125.09	130.12
21	4	409	CL7	C1-C2-C3	-2.54	121.65	126.04
21	8	409	CL7	C1-C2-C3	-2.54	121.65	126.04
21	C	502	CL7	C4C-C3C-C2C	-2.54	103.82	107.13
21	C	502	CL7	C7-C6-C5	-2.54	106.46	113.36
21	7	506	CL7	C1B-CHB-C4A	-2.54	125.09	130.12
21	2	511	CL7	C7-C6-C5	-2.54	106.47	113.36
21	4	408	CL7	CMD-C2D-C1D	2.54	132.36	128.46
21	8	408	CL7	CMD-C2D-C1D	2.54	132.36	128.46
21	2	515	CL7	C1B-CHB-C4A	-2.54	125.09	130.12
24	b	621	SQD	O8-S-C6	-2.54	101.70	105.74
21	1	413	CL7	C4C-C3C-C2C	-2.54	103.82	107.13
21	5	413	CL7	C4C-C3C-C2C	-2.54	103.82	107.13
21	D	404	CL7	C3B-C4B-NB	2.54	112.49	109.21
21	2	517	CL7	CAA-CBA-CGA	-2.54	105.84	113.25
21	3	508	CL7	C1B-CHB-C4A	-2.53	125.10	130.12
21	4	408	CL7	C3B-C4B-NB	2.53	112.49	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	408	CL7	C3B-C4B-NB	2.53	112.49	109.21
23	b	619	8CT	C01-C02-C07	2.53	118.48	113.62
21	d	402	CL7	CMD-C2D-C1D	2.53	132.36	128.46
32	4	420	ZEX	C15-C35-C34	-2.53	118.29	123.47
32	8	420	ZEX	C15-C35-C34	-2.53	118.29	123.47
21	a	403	CL7	C3B-C4B-NB	2.53	112.48	109.21
21	C	503	CL7	CHC-C1C-NC	-2.53	122.13	124.45
21	c	503	CL7	CHC-C1C-NC	-2.53	122.13	124.45
21	B	609	CL7	C4C-C3C-C2C	-2.53	103.83	107.13
21	3	508	CL7	O2A-C1-C2	-2.53	101.98	108.64
24	B	620	SQD	O8-S-C6	-2.53	101.71	105.74
21	C	513	CL7	CMA-C3A-C2A	-2.53	110.19	116.10
21	3	506	CL7	C1B-CHB-C4A	-2.53	125.11	130.12
21	c	502	CL7	C7-C6-C5	-2.53	106.49	113.36
21	5	408	CL7	CMD-C2D-C1D	2.53	132.35	128.46
23	D	406	8CT	C13-C14-C15	-2.53	115.33	123.22
21	C	507	CL7	C4D-C3D-CAD	-2.53	103.72	107.81
21	c	507	CL7	C4D-C3D-CAD	-2.53	103.72	107.81
21	C	505	CL7	C3B-C4B-NB	2.53	112.48	109.21
21	C	513	CL7	C3B-C4B-NB	2.53	112.48	109.21
21	B	606	CL7	C4C-C3C-C2C	-2.53	103.83	107.13
21	7	505	CL7	C4-C3-C5	2.52	119.52	115.27
21	C	512	CL7	CMD-C2D-C1D	2.52	132.34	128.46
21	c	512	CL7	CMD-C2D-C1D	2.52	132.34	128.46
21	6	517	CL7	CAA-CBA-CGA	-2.52	105.88	113.25
23	B	618	8CT	C01-C02-C07	2.52	118.46	113.62
21	1	409	CL7	C3B-C4B-NB	2.52	112.47	109.21
32	2	520	ZEX	C7-C8-C9	-2.52	122.42	126.23
32	3	525	ZEX	C7-C8-C9	-2.52	122.42	126.23
27	c	517	DGD	C4E-C3E-C2E	-2.52	106.42	110.82
21	B	622	CL7	CMD-C2D-C1D	2.52	132.34	128.46
21	b	623	CL7	CMD-C2D-C1D	2.52	132.34	128.46
21	2	514	CL7	CHC-C1C-NC	-2.52	122.14	124.45
21	b	603	CL7	CMD-C2D-C1D	2.52	132.34	128.46
21	B	616	CL7	OBD-CAD-CBD	-2.52	122.30	125.89
21	b	617	CL7	OBD-CAD-CBD	-2.52	122.30	125.89
23	d	406	8CT	C13-C14-C15	-2.52	115.35	123.22
21	4	416	CL7	C1B-CHB-C4A	-2.52	125.13	130.12
21	8	416	CL7	C1B-CHB-C4A	-2.52	125.13	130.12
21	b	610	CL7	C4C-C3C-C2C	-2.52	103.84	107.13
21	4	413	CL7	CMD-C2D-C1D	2.52	132.34	128.46
21	8	413	CL7	CMD-C2D-C1D	2.52	132.34	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	405	CL7	C3B-C4B-NB	2.52	112.47	109.21
21	c	513	CL7	C3B-C4B-NB	2.52	112.46	109.21
21	C	505	CL7	C1C-C2C-C3C	-2.52	103.27	106.94
21	7	517	CL7	C3B-C4B-NB	2.52	112.46	109.21
21	2	517	CL7	OBD-CAD-CBD	-2.52	122.30	125.89
21	6	517	CL7	OBD-CAD-CBD	-2.52	122.30	125.89
21	2	518	CL7	C3B-C4B-NB	2.52	112.46	109.21
21	B	602	CL7	C1B-CHB-C4A	-2.52	125.14	130.12
21	b	603	CL7	C1B-CHB-C4A	-2.52	125.14	130.12
21	B	602	CL7	CMD-C2D-C1D	2.51	132.33	128.46
21	4	413	CL7	C3B-C4B-NB	2.51	112.46	109.21
21	b	610	CL7	CHC-C1C-NC	-2.51	122.14	124.45
21	1	415	CL7	C4D-C3D-CAD	-2.51	103.74	107.81
21	5	415	CL7	C4D-C3D-CAD	-2.51	103.74	107.81
21	3	509	CL7	CMD-C2D-C1D	2.51	132.33	128.46
21	3	506	CL7	O2D-CGD-CBD	2.51	115.73	111.27
21	7	506	CL7	O2D-CGD-CBD	2.51	115.73	111.27
21	d	405	CL7	CHC-C1C-NC	-2.51	122.14	124.45
21	c	505	CL7	C1C-C2C-C3C	-2.51	103.27	106.94
21	6	518	CL7	C3B-C4B-NB	2.51	112.46	109.21
21	D	405	CL7	CMD-C2D-C1D	2.51	132.32	128.46
21	d	405	CL7	CMD-C2D-C1D	2.51	132.32	128.46
23	C	515	8CT	C13-C14-C15	-2.51	115.38	123.22
23	c	515	8CT	C13-C14-C15	-2.51	115.38	123.22
23	C	516	8CT	C11-C10-C03	-2.51	120.15	127.20
23	c	516	8CT	C11-C10-C03	-2.51	120.15	127.20
21	B	609	CL7	CHC-C1C-NC	-2.51	122.15	124.45
21	B	608	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	b	609	CL7	C4C-C3C-C2C	-2.51	103.86	107.13
21	3	504	CL7	C1B-CHB-C4A	-2.51	125.15	130.12
21	3	502	CL7	C7-C6-C5	-2.51	106.54	113.36
21	A	403	CL7	C1B-CHB-C4A	-2.51	125.15	130.12
21	a	403	CL7	C1B-CHB-C4A	-2.51	125.15	130.12
21	3	508	CL7	C1C-C2C-C3C	-2.51	103.28	106.94
21	7	508	CL7	C1C-C2C-C3C	-2.51	103.28	106.94
21	5	410	CL7	CHC-C1C-NC	-2.51	122.15	124.45
21	A	403	CL7	C3B-C4B-NB	2.51	112.45	109.21
21	5	418	CL7	CMD-C2D-C1D	2.51	132.32	128.46
21	3	501	CL7	OBD-CAD-CBD	-2.51	122.31	125.89
21	A	401	CL7	C6-C5-C3	-2.51	106.89	113.45
21	7	509	CL7	CMD-C2D-C1D	2.50	132.31	128.46
21	2	507	CL7	C7-C6-C5	-2.50	106.56	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	502	CL7	C7-C6-C5	-2.50	106.56	113.36
21	4	410	CL7	C3B-C4B-NB	2.50	112.44	109.21
21	8	410	CL7	C3B-C4B-NB	2.50	112.44	109.21
21	7	504	CL7	C1B-CHB-C4A	-2.50	125.16	130.12
21	b	607	CL7	C4C-C3C-C2C	-2.50	103.87	107.13
21	6	507	CL7	C7-C6-C5	-2.50	106.58	113.36
21	b	609	CL7	C7-C6-C5	-2.50	106.58	113.36
21	4	413	CL7	C4C-C3C-C2C	-2.50	103.87	107.13
21	8	413	CL7	C4C-C3C-C2C	-2.50	103.87	107.13
21	8	413	CL7	C3B-C4B-NB	2.50	112.44	109.21
21	B	607	CL7	C1B-CHB-C4A	-2.50	125.17	130.12
21	b	608	CL7	C1B-CHB-C4A	-2.50	125.17	130.12
21	4	404	CL7	C3B-C4B-NB	2.50	112.44	109.21
21	8	404	CL7	C3B-C4B-NB	2.50	112.44	109.21
21	2	513	CL7	C3B-C4B-NB	2.49	112.44	109.21
21	C	509	CL7	CHC-C1C-NC	-2.49	122.16	124.45
21	6	514	CL7	CHC-C1C-NC	-2.49	122.16	124.45
21	1	408	CL7	CMD-C2D-C1D	2.49	132.30	128.46
21	B	615	CL7	CMD-C2D-C1D	2.49	132.30	128.46
21	b	616	CL7	CMD-C2D-C1D	2.49	132.30	128.46
21	2	502	CL7	OBD-CAD-CBD	-2.49	122.33	125.89
21	6	502	CL7	OBD-CAD-CBD	-2.49	122.33	125.89
21	6	506	CL7	C1B-CHB-C4A	-2.49	125.18	130.12
21	7	510	CL7	C1B-CHB-C4A	-2.49	125.18	130.12
21	8	405	CL7	C3B-C4B-NB	2.49	112.43	109.21
21	B	608	CL7	C7-C6-C5	-2.49	106.59	113.36
21	c	505	CL7	CHC-C1C-NC	-2.49	122.17	124.45
23	k	101	8CT	C22-C21-C20	-2.49	119.44	122.92
21	2	501	CL7	C3B-C4B-NB	2.49	112.43	109.21
21	4	404	CL7	OBD-CAD-CBD	-2.49	122.34	125.89
21	8	404	CL7	OBD-CAD-CBD	-2.49	122.34	125.89
21	a	401	CL7	C6-C5-C3	-2.49	106.93	113.45
21	c	506	CL7	C4C-C3C-C2C	-2.49	103.88	107.13
21	1	414	CL7	CMD-C2D-C1D	2.49	132.29	128.46
21	1	418	CL7	CMD-C2D-C1D	2.49	132.29	128.46
21	5	414	CL7	CMD-C2D-C1D	2.49	132.29	128.46
21	1	410	CL7	CHC-C1C-NC	-2.49	122.17	124.45
21	5	414	CL7	CMA-C3A-C2A	-2.49	110.29	116.10
21	b	603	CL7	O2A-CGA-O1A	-2.49	117.31	123.59
21	B	614	CL7	C3B-C4B-NB	2.49	112.42	109.21
21	2	513	CL7	C4C-C3C-C2C	-2.49	103.89	107.13
21	6	513	CL7	C4C-C3C-C2C	-2.49	103.89	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	513	CL7	C1B-CHB-C4A	-2.49	125.19	130.12
21	3	517	CL7	C3B-C4B-NB	2.49	112.42	109.21
21	b	611	CL7	C4-C3-C5	2.49	119.45	115.27
21	7	517	CL7	C4-C3-C5	2.49	120.09	114.60
21	3	514	CL7	C1B-CHB-C4A	-2.49	125.19	130.12
21	D	405	CL7	C4C-C3C-C2C	-2.49	103.89	107.13
21	d	405	CL7	C4C-C3C-C2C	-2.49	103.89	107.13
21	B	603	CL7	C1-C2-C3	2.48	130.34	126.04
21	b	604	CL7	C1-C2-C3	2.48	130.34	126.04
21	4	415	CL7	C1B-CHB-C4A	-2.48	125.20	130.12
21	7	501	CL7	OBD-CAD-CBD	-2.48	122.35	125.89
21	1	403	CL7	C4-C3-C5	2.48	119.45	115.27
21	5	403	CL7	C4-C3-C5	2.48	119.45	115.27
21	7	514	CL7	C1B-CHB-C4A	-2.48	125.20	130.12
21	1	409	CL7	C1B-CHB-C4A	-2.48	125.20	130.12
21	4	409	CL7	C3B-C4B-NB	2.48	112.42	109.21
21	3	510	CL7	C1B-CHB-C4A	-2.48	125.20	130.12
21	1	418	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	5	418	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	B	610	CL7	C4-C3-C5	2.48	119.44	115.27
21	2	506	CL7	C1B-CHB-C4A	-2.48	125.20	130.12
21	D	405	CL7	CHC-C1C-NC	-2.48	122.17	124.45
21	7	518	CL7	C3B-C4B-NB	2.48	112.42	109.21
23	B	618	8CT	C19-C20-C21	-2.48	123.77	127.31
21	C	507	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	c	507	CL7	C1C-C2C-C3C	-2.48	103.32	106.94
21	1	420	CL7	CMD-C2D-C1D	2.48	132.27	128.46
21	5	420	CL7	CMD-C2D-C1D	2.48	132.27	128.46
26	1	401	LMG	O1-C7-C8	-2.48	104.92	110.90
26	5	401	LMG	O1-C7-C8	-2.48	104.92	110.90
21	A	403	CL7	CAA-CBA-CGA	-2.48	106.01	113.25
21	a	403	CL7	CAA-CBA-CGA	-2.48	106.01	113.25
21	C	506	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
21	6	512	CL7	C4C-C3C-C2C	-2.48	103.90	107.13
21	2	514	CL7	C1B-CHB-C4A	-2.48	125.21	130.12
32	4	419	ZEX	C38-C24-C25	-2.48	106.93	110.87
21	b	615	CL7	C3B-C4B-NB	2.48	112.41	109.21
21	5	409	CL7	C1B-CHB-C4A	-2.47	125.22	130.12
21	c	505	CL7	C4D-C3D-CAD	-2.47	103.81	107.81
21	1	414	CL7	CMA-C3A-C2A	-2.47	110.32	116.10
21	B	602	CL7	O2A-CGA-O1A	-2.47	117.35	123.59
21	b	611	CL7	C1B-CHB-C4A	-2.47	125.22	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	8	419	ZEX	C38-C24-C25	-2.47	106.93	110.87
21	8	415	CL7	C1B-CHB-C4A	-2.47	125.22	130.12
21	3	518	CL7	C3B-C4B-NB	2.47	112.41	109.21
21	6	501	CL7	C3B-C4B-NB	2.47	112.41	109.21
21	4	409	CL7	CAA-CBA-CGA	-2.47	106.03	113.25
21	B	614	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
21	C	505	CL7	C4D-C3D-CAD	-2.47	103.81	107.81
21	c	513	CL7	C1B-CHB-C4A	-2.47	125.22	130.12
21	1	408	CL7	C4-C3-C5	2.47	119.43	115.27
21	5	408	CL7	C4-C3-C5	2.47	119.43	115.27
32	7	520	ZEX	C2-C3-C4	-2.47	106.92	110.30
21	6	503	CL7	C3B-C4B-NB	2.47	112.40	109.21
21	3	517	CL7	C4-C3-C5	2.47	120.06	114.60
21	1	405	CL7	CMD-C2D-C1D	2.47	132.26	128.46
21	5	405	CL7	CMD-C2D-C1D	2.47	132.26	128.46
21	b	614	CL7	C7-C6-C5	-2.47	106.65	113.36
21	4	417	CL7	C1B-CHB-C4A	-2.47	125.23	130.12
21	8	417	CL7	C1B-CHB-C4A	-2.47	125.23	130.12
21	3	509	CL7	O2A-CGA-O1A	-2.47	117.36	123.59
21	7	509	CL7	O2A-CGA-O1A	-2.47	117.36	123.59
21	B	613	CL7	C7-C6-C5	-2.47	106.66	113.36
23	C	515	8CT	C27-C26-C28	2.47	121.97	118.08
23	c	515	8CT	C27-C26-C28	2.47	121.97	118.08
21	8	409	CL7	CAA-CBA-CGA	-2.47	106.04	113.25
21	7	506	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
32	4	419	ZEX	C11-C12-C13	-2.47	119.49	126.42
32	8	419	ZEX	C11-C12-C13	-2.47	119.49	126.42
21	6	513	CL7	C3B-C4B-NB	2.47	112.40	109.21
21	2	507	CL7	C4C-C3C-C2C	-2.47	103.91	107.13
21	c	504	CL7	C1C-C2C-C3C	-2.47	103.34	106.94
23	b	601	8CT	C22-C21-C20	-2.47	119.47	122.92
21	C	511	CL7	CMD-C2D-C1D	2.46	132.25	128.46
23	B	627	8CT	C22-C21-C20	-2.46	119.47	122.92
21	5	412	CL7	C1B-CHB-C4A	-2.46	125.24	130.12
21	B	610	CL7	C1B-CHB-C4A	-2.46	125.24	130.12
21	c	511	CL7	CMD-C2D-C1D	2.46	132.25	128.46
23	D	406	8CT	C05-C04-C03	2.46	114.27	110.48
23	d	406	8CT	C05-C04-C03	2.46	114.27	110.48
21	5	405	CL7	C1C-C2C-C3C	-2.46	103.35	106.94
21	2	502	CL7	C4-C3-C5	2.46	119.41	115.27
21	6	502	CL7	C4-C3-C5	2.46	119.41	115.27
32	3	520	ZEX	C2-C3-C4	-2.46	106.94	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	420	CL7	C3B-C4B-NB	2.46	112.39	109.21
23	b	619	8CT	C19-C20-C21	-2.46	123.80	127.31
21	C	510	CL7	C1-C2-C3	2.46	130.30	126.04
21	c	510	CL7	C1-C2-C3	2.46	130.30	126.04
21	8	411	CL7	C4-C3-C5	2.46	119.41	115.27
21	3	506	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	4	414	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	8	414	CL7	C4C-C3C-C2C	-2.46	103.92	107.13
21	3	512	CL7	CMD-C2D-C1D	2.46	132.24	128.46
21	7	512	CL7	CMD-C2D-C1D	2.46	132.24	128.46
21	6	514	CL7	C1B-CHB-C4A	-2.46	125.25	130.12
21	1	402	CL7	CMD-C2D-C1D	2.46	132.24	128.46
21	5	402	CL7	CMD-C2D-C1D	2.46	132.24	128.46
23	K	101	8CT	C22-C21-C20	-2.46	119.48	122.92
21	1	405	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	8	405	CL7	C1B-CHB-C4A	-2.45	125.25	130.12
21	C	511	CL7	O2D-CGD-CBD	2.45	115.63	111.27
21	c	511	CL7	O2D-CGD-CBD	2.45	115.63	111.27
21	2	512	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	2	504	CL7	C1B-CHB-C4A	-2.45	125.26	130.12
21	6	504	CL7	C1B-CHB-C4A	-2.45	125.26	130.12
21	B	601	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	b	602	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	a	403	CL7	OBD-CAD-CBD	-2.45	122.39	125.89
21	8	411	CL7	C7-C6-C5	-2.45	106.70	113.36
21	D	405	CL7	OBD-CAD-CBD	-2.45	122.39	125.89
21	d	405	CL7	OBD-CAD-CBD	-2.45	122.39	125.89
21	6	507	CL7	C4C-C3C-C2C	-2.45	103.93	107.13
21	1	412	CL7	C1B-CHB-C4A	-2.45	125.26	130.12
21	7	504	CL7	OBD-CAD-CBD	-2.45	122.39	125.89
21	a	403	CL7	CMD-C2D-C1D	2.45	132.23	128.46
21	C	518	CL7	C1C-C2C-C3C	-2.45	103.36	106.94
21	A	401	CL7	C4C-C3C-C2C	-2.45	103.94	107.13
21	a	401	CL7	C4C-C3C-C2C	-2.45	103.94	107.13
21	1	407	CL7	C3B-C4B-NB	2.45	112.38	109.21
21	5	407	CL7	C3B-C4B-NB	2.45	112.38	109.21
21	8	409	CL7	C3B-C4B-NB	2.45	112.38	109.21
21	2	510	CL7	C1B-CHB-C4A	-2.45	125.27	130.12
21	6	510	CL7	C1B-CHB-C4A	-2.45	125.27	130.12
21	C	504	CL7	C1C-C2C-C3C	-2.45	103.37	106.94
21	B	605	CL7	C3B-C4B-NB	2.45	112.37	109.21
21	b	606	CL7	C3B-C4B-NB	2.45	112.37	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	503	CL7	CMD-C2D-C1D	2.45	132.22	128.46
21	7	503	CL7	CMD-C2D-C1D	2.45	132.22	128.46
21	2	503	CL7	C3B-C4B-NB	2.45	112.37	109.21
21	b	615	CL7	C4C-C3C-C2C	-2.45	103.94	107.13
21	7	501	CL7	C4-C3-C5	2.45	119.39	115.27
32	3	520	ZEX	C35-C15-C14	-2.45	118.47	123.47
21	3	515	CL7	CMD-C2D-C1D	2.45	132.22	128.46
21	7	515	CL7	CMD-C2D-C1D	2.45	132.22	128.46
21	c	518	CL7	C1C-C2C-C3C	-2.44	103.37	106.94
22	D	408	PHO	C16-C15-C13	-2.44	108.02	115.92
21	b	617	CL7	C1B-CHB-C4A	-2.44	125.28	130.12
21	4	405	CL7	C1B-CHB-C4A	-2.44	125.28	130.12
21	3	504	CL7	OBD-CAD-CBD	-2.44	122.40	125.89
21	b	609	CL7	C1B-CHB-C4A	-2.44	125.28	130.12
21	8	416	CL7	CMD-C2D-C1D	2.44	132.22	128.46
21	D	405	CL7	CAA-CBA-CGA	-2.44	106.02	112.51
21	d	405	CL7	CAA-CBA-CGA	-2.44	106.02	112.51
21	C	506	CL7	C1B-CHB-C4A	-2.44	125.28	130.12
21	c	506	CL7	C1B-CHB-C4A	-2.44	125.28	130.12
21	2	516	CL7	C3B-C4B-NB	2.44	112.37	109.21
21	4	411	CL7	C7-C6-C5	-2.44	106.73	113.36
21	C	505	CL7	CHC-C1C-NC	-2.44	122.21	124.45
23	A	404	8CT	C11-C10-C03	-2.44	120.35	127.20
21	2	515	CL7	C3B-C4B-NB	2.44	112.36	109.21
21	B	616	CL7	C1B-CHB-C4A	-2.44	125.28	130.12
21	5	420	CL7	C3B-C4B-NB	2.44	112.36	109.21
21	1	415	CL7	C3B-C4B-NB	2.44	112.36	109.21
21	6	505	CL7	C3B-C4B-NB	2.44	112.36	109.21
21	5	415	CL7	C3B-C4B-NB	2.44	112.36	109.21
21	2	512	CL7	O2D-CGD-O1D	-2.44	119.07	123.84
21	6	512	CL7	O2D-CGD-O1D	-2.44	119.07	123.84
21	2	516	CL7	C1B-CHB-C4A	-2.44	125.29	130.12
21	3	507	CL7	C1B-CHB-C4A	-2.44	125.29	130.12
21	6	516	CL7	C1B-CHB-C4A	-2.44	125.29	130.12
21	4	411	CL7	C4-C3-C5	2.44	119.37	115.27
23	b	601	8CT	C40-C12-C13	-2.44	119.51	122.92
21	4	413	CL7	C7-C6-C5	-2.44	106.74	113.36
21	8	413	CL7	C7-C6-C5	-2.44	106.74	113.36
21	7	509	CL7	C1B-CHB-C4A	-2.44	125.29	130.12
22	d	408	PHO	C16-C15-C13	-2.44	108.04	115.92
21	6	517	CL7	C7-C6-C5	-2.44	106.74	113.36
21	2	515	CL7	C4C-C3C-C2C	-2.44	103.95	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	515	CL7	C4C-C3C-C2C	-2.44	103.95	107.13
21	2	517	CL7	C7-C6-C5	-2.44	106.75	113.36
21	8	410	CL7	C1C-C2C-C3C	-2.44	103.39	106.94
21	B	604	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	C	509	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	b	605	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	c	509	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
32	3	525	ZEX	C31-C32-C33	-2.43	119.58	126.42
32	7	520	ZEX	C35-C15-C14	-2.43	118.49	123.47
23	C	515	8CT	C14-C13-C12	-2.43	123.84	127.31
23	c	515	8CT	C14-C13-C12	-2.43	123.84	127.31
21	B	615	CL7	C4-C3-C5	2.43	119.98	114.60
21	b	616	CL7	C4-C3-C5	2.43	119.98	114.60
21	B	615	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	b	616	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
32	3	522	ZEX	C31-C30-C29	-2.43	123.84	127.31
32	7	522	ZEX	C31-C30-C29	-2.43	123.84	127.31
21	3	501	CL7	C4-C3-C5	2.43	119.36	115.27
21	6	503	CL7	C4-C3-C5	2.43	119.36	115.27
21	1	402	CL7	C3B-C4B-NB	2.43	112.35	109.21
32	6	519	ZEX	C28-C27-C26	-2.43	122.93	127.09
21	2	510	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	6	510	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	3	503	CL7	C1B-CHB-C4A	-2.43	125.30	130.12
21	7	503	CL7	C1B-CHB-C4A	-2.43	125.30	130.12
21	2	512	CL7	C4-C3-C5	2.43	119.36	115.27
21	C	504	CL7	C3B-C4B-NB	2.43	112.35	109.21
21	A	403	CL7	CMD-C2D-C1D	2.43	132.20	128.46
21	C	504	CL7	CMD-C2D-C1D	2.43	132.20	128.46
21	c	504	CL7	CMD-C2D-C1D	2.43	132.20	128.46
21	6	516	CL7	C3B-C4B-NB	2.43	112.35	109.21
21	c	513	CL7	C4C-C3C-C2C	-2.43	103.96	107.13
21	7	507	CL7	C1B-CHB-C4A	-2.43	125.31	130.12
21	B	605	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	b	606	CL7	C1C-C2C-C3C	-2.43	103.39	106.94
21	2	517	CL7	C1B-CHB-C4A	-2.43	125.31	130.12
21	4	409	CL7	O2A-C1-C2	2.43	115.02	108.64
21	8	409	CL7	O2A-C1-C2	2.43	115.02	108.64
21	A	403	CL7	OBD-CAD-CBD	-2.43	122.43	125.89
21	4	404	CL7	C7-C6-C5	-2.43	106.77	113.36
32	2	520	ZEX	C31-C32-C33	-2.43	119.60	126.42
32	4	403	ZEX	C39-C29-C30	-2.43	119.52	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	8	403	ZEX	C39-C29-C30	-2.43	119.52	122.92
23	a	404	8CT	C11-C10-C03	-2.43	120.39	127.20
32	1	421	ZEX	C8-C7-C6	-2.43	120.39	127.20
32	5	421	ZEX	C8-C7-C6	-2.43	120.39	127.20
21	6	515	CL7	C3B-C4B-NB	2.43	112.35	109.21
21	3	509	CL7	C1B-CHB-C4A	-2.43	125.31	130.12
21	1	408	CL7	O2D-CGD-O1D	-2.43	119.10	123.84
21	2	510	CL7	C4-C3-C5	2.43	119.35	115.27
21	6	510	CL7	C4-C3-C5	2.43	119.35	115.27
21	B	608	CL7	C1B-CHB-C4A	-2.42	125.31	130.12
21	1	411	CL7	C1B-CHB-C4A	-2.42	125.32	130.12
23	A	404	8CT	C22-C21-C20	-2.42	119.53	122.92
21	C	513	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
21	8	404	CL7	C7-C6-C5	-2.42	106.78	113.36
21	B	605	CL7	C1B-CHB-C4A	-2.42	125.32	130.12
21	b	606	CL7	C1B-CHB-C4A	-2.42	125.32	130.12
21	6	516	CL7	CMD-C2D-C1D	2.42	132.18	128.46
32	1	421	ZEX	C31-C32-C33	-2.42	119.62	126.42
32	5	421	ZEX	C31-C32-C33	-2.42	119.62	126.42
21	C	510	CL7	CAA-CBA-CGA	-2.42	106.18	113.25
21	2	503	CL7	C4-C3-C5	2.42	119.34	115.27
21	b	602	CL7	C1B-CHB-C4A	-2.42	125.33	130.12
21	C	514	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	c	514	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	4	407	CL7	C1B-CHB-C4A	-2.42	125.33	130.12
21	2	516	CL7	CAA-CBA-CGA	-2.42	106.19	113.25
21	3	501	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	7	501	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	4	404	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
21	8	404	CL7	C4C-C3C-C2C	-2.42	103.97	107.13
21	3	506	CL7	CMD-C2D-C1D	2.42	132.18	128.46
21	7	506	CL7	CMD-C2D-C1D	2.42	132.18	128.46
21	2	506	CL7	CMD-C2D-C1D	2.42	132.18	128.46
21	6	506	CL7	CMD-C2D-C1D	2.42	132.18	128.46
21	C	509	CL7	OBD-CAD-CBD	-2.42	122.44	125.89
21	c	509	CL7	OBD-CAD-CBD	-2.42	122.44	125.89
21	2	505	CL7	CGD-CBD-CAD	2.42	118.56	110.73
21	4	416	CL7	CMD-C2D-C1D	2.42	132.18	128.46
32	2	519	ZEX	C28-C27-C26	-2.42	122.96	127.09
21	4	410	CL7	C1C-C2C-C3C	-2.42	103.41	106.94
21	B	601	CL7	C1B-CHB-C4A	-2.42	125.33	130.12
21	B	611	CL7	C4-C3-C5	2.41	119.33	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	612	CL7	C4-C3-C5	2.41	119.33	115.27
21	c	510	CL7	CAA-CBA-CGA	-2.41	106.20	113.25
21	2	505	CL7	C3B-C4B-NB	2.41	112.33	109.21
21	2	503	CL7	O2D-CGD-CBD	2.41	115.55	111.27
21	6	513	CL7	C1B-CHB-C4A	-2.41	125.34	130.12
21	1	416	CL7	C4C-C3C-C2C	-2.41	103.98	107.13
21	6	505	CL7	CGD-CBD-CAD	2.41	118.55	110.73
21	2	502	CL7	C1C-C2C-C3C	-2.41	103.42	106.94
21	6	502	CL7	C1C-C2C-C3C	-2.41	103.42	106.94
21	b	609	CL7	C3B-C4B-NB	2.41	112.33	109.21
21	5	408	CL7	O2D-CGD-O1D	-2.41	119.12	123.84
23	B	627	8CT	C40-C12-C13	-2.41	119.55	122.92
21	6	517	CL7	C1B-CHB-C4A	-2.41	125.34	130.12
21	2	516	CL7	CMD-C2D-C1D	2.41	132.17	128.46
21	6	512	CL7	C4-C3-C5	2.41	119.32	115.27
23	B	618	8CT	C28-C26-C25	-2.41	115.25	118.94
23	b	619	8CT	C28-C26-C25	-2.41	115.25	118.94
21	1	413	CL7	O2D-CGD-CBD	2.41	115.55	111.27
21	3	513	CL7	CMD-C2D-C1D	2.41	132.16	128.46
21	1	411	CL7	C3B-C4B-NB	2.41	112.32	109.21
21	1	418	CL7	C3B-C4B-NB	2.41	112.32	109.21
21	5	411	CL7	C3B-C4B-NB	2.41	112.32	109.21
21	5	418	CL7	C3B-C4B-NB	2.41	112.32	109.21
21	8	407	CL7	C1B-CHB-C4A	-2.41	125.35	130.12
21	6	516	CL7	CAA-CBA-CGA	-2.41	106.22	113.25
21	5	411	CL7	C1B-CHB-C4A	-2.41	125.35	130.12
21	5	403	CL7	C4D-C3D-CAD	-2.41	103.92	107.81
32	7	520	ZEX	C1-C6-C5	-2.40	119.23	122.61
21	1	418	CL7	C1B-CHB-C4A	-2.40	125.36	130.12
23	C	519	8CT	C18-C19-C20	-2.40	118.55	123.47
23	c	519	8CT	C18-C19-C20	-2.40	118.55	123.47
21	b	612	CL7	CMD-C2D-C1D	2.40	132.16	128.46
21	5	402	CL7	C3B-C4B-NB	2.40	112.32	109.21
21	3	506	CL7	OBD-CAD-CBD	-2.40	122.46	125.89
21	1	418	CL7	CAC-C3C-C2C	2.40	131.64	127.53
21	5	418	CL7	CAC-C3C-C2C	2.40	131.64	127.53
21	A	403	CL7	O2A-CGA-CBA	2.40	119.45	111.91
21	a	403	CL7	O2A-CGA-CBA	2.40	119.45	111.91
21	B	611	CL7	CMD-C2D-C1D	2.40	132.16	128.46
21	c	504	CL7	C3B-C4B-NB	2.40	112.31	109.21
21	B	603	CL7	C1C-C2C-C3C	-2.40	103.44	106.94
21	b	604	CL7	C1C-C2C-C3C	-2.40	103.44	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	3	519	ZEX	C39-C29-C30	-2.40	119.56	122.92
32	7	519	ZEX	C39-C29-C30	-2.40	119.56	122.92
21	C	503	CL7	C7-C6-C5	-2.40	106.84	113.36
21	5	418	CL7	C1B-CHB-C4A	-2.40	125.36	130.12
32	4	419	ZEX	C1-C6-C5	-2.40	119.23	122.61
21	c	511	CL7	C1C-C2C-C3C	-2.40	103.44	106.94
21	2	513	CL7	C1B-CHB-C4A	-2.40	125.37	130.12
32	8	419	ZEX	C1-C6-C5	-2.40	119.24	122.61
21	1	412	CL7	C4D-C3D-CAD	-2.40	103.93	107.81
21	5	412	CL7	C4D-C3D-CAD	-2.40	103.93	107.81
21	5	413	CL7	O2D-CGD-CBD	2.40	115.52	111.27
21	3	516	CL7	CAA-C2A-C1A	-2.39	104.31	112.19
21	5	416	CL7	C1B-CHB-C4A	-2.39	125.37	130.12
21	7	506	CL7	OBD-CAD-CBD	-2.39	122.47	125.89
32	3	520	ZEX	C1-C6-C5	-2.39	119.24	122.61
21	4	412	CL7	C4D-C3D-CAD	-2.39	103.94	107.81
21	8	412	CL7	C4D-C3D-CAD	-2.39	103.94	107.81
21	3	508	CL7	C3B-C4B-NB	2.39	112.31	109.21
21	3	503	CL7	C4-C3-C5	2.39	119.30	115.27
21	B	612	CL7	C3B-C4B-NB	2.39	112.30	109.21
21	C	514	CL7	C3B-C4B-NB	2.39	112.30	109.21
21	b	613	CL7	C3B-C4B-NB	2.39	112.30	109.21
21	1	406	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	5	406	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	4	406	CL7	C3B-C4B-NB	2.39	112.30	109.21
21	8	406	CL7	C3B-C4B-NB	2.39	112.30	109.21
23	a	404	8CT	C22-C21-C20	-2.39	119.57	122.92
21	7	516	CL7	CAA-C2A-C1A	-2.39	104.32	112.19
21	7	513	CL7	CMD-C2D-C1D	2.39	132.14	128.46
23	C	516	8CT	C27-C26-C25	-2.39	119.57	122.92
23	c	516	8CT	C27-C26-C25	-2.39	119.57	122.92
21	3	518	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	7	518	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	B	604	CL7	C7-C6-C5	-2.39	106.87	113.36
21	b	605	CL7	C7-C6-C5	-2.39	106.87	113.36
21	3	508	CL7	CBA-CAA-C2A	-2.39	106.81	113.86
21	7	508	CL7	CBA-CAA-C2A	-2.39	106.81	113.86
21	1	419	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	5	419	CL7	C4C-C3C-C2C	-2.39	104.01	107.13
21	4	406	CL7	C1B-CHB-C4A	-2.39	125.39	130.12
21	6	511	CL7	C1B-CHB-C4A	-2.39	125.39	130.12
21	8	406	CL7	C1B-CHB-C4A	-2.39	125.39	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	416	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
21	4	414	CL7	C3B-C4B-NB	2.39	112.30	109.21
21	8	414	CL7	CAA-CBA-CGA	-2.39	106.28	113.25
21	c	503	CL7	C7-C6-C5	-2.39	106.88	113.36
21	B	602	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
21	3	515	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
21	7	515	CL7	C4C-C3C-C2C	-2.39	104.02	107.13
21	B	615	CL7	C1B-CHB-C4A	-2.39	125.39	130.12
21	b	616	CL7	C1B-CHB-C4A	-2.39	125.39	130.12
21	2	518	CL7	OBD-CAD-CBD	-2.39	122.49	125.89
21	4	417	CL7	CAA-C2A-C3A	2.39	120.22	114.26
21	8	417	CL7	CAA-C2A-C3A	2.39	120.22	114.26
21	c	507	CL7	C7-C6-C5	-2.39	106.88	113.36
21	1	416	CL7	CMA-C3A-C2A	-2.39	110.53	116.10
21	5	416	CL7	CMA-C3A-C2A	-2.39	110.53	116.10
21	1	409	CL7	C4D-C3D-CAD	-2.38	103.95	107.81
21	5	409	CL7	C4D-C3D-CAD	-2.38	103.95	107.81
21	3	515	CL7	C3B-C4B-NB	2.38	112.29	109.21
21	5	419	CL7	C3B-C4B-NB	2.38	112.29	109.21
21	7	515	CL7	C3B-C4B-NB	2.38	112.29	109.21
21	1	403	CL7	C4D-C3D-CAD	-2.38	103.95	107.81
21	c	502	CL7	C1B-CHB-C4A	-2.38	125.40	130.12
21	6	503	CL7	O2D-CGD-CBD	2.38	115.50	111.27
21	6	507	CL7	C3B-C4B-NB	2.38	112.29	109.21
21	6	511	CL7	C3B-C4B-NB	2.38	112.29	109.21
21	7	508	CL7	C3B-C4B-NB	2.38	112.29	109.21
21	C	511	CL7	C1C-C2C-C3C	-2.38	103.46	106.94
21	B	608	CL7	C3B-C4B-NB	2.38	112.29	109.21
21	C	512	CL7	C1B-CHB-C4A	-2.38	125.40	130.12
21	c	512	CL7	C1B-CHB-C4A	-2.38	125.40	130.12
21	8	414	CL7	C3B-C4B-NB	2.38	112.29	109.21
21	2	511	CL7	C1B-CHB-C4A	-2.38	125.40	130.12
21	3	512	CL7	C1B-CHB-C4A	-2.38	125.40	130.12
21	3	501	CL7	CAA-C2A-C1A	-2.38	104.36	112.19
21	7	501	CL7	CAA-C2A-C1A	-2.38	104.36	112.19
21	4	405	CL7	CMD-C2D-C1D	2.38	132.12	128.46
23	A	404	8CT	C18-C19-C20	-2.38	118.60	123.47
21	1	416	CL7	C1B-CHB-C4A	-2.38	125.40	130.12
21	B	607	CL7	CMD-C2D-C1D	2.38	132.12	128.46
21	b	608	CL7	CMD-C2D-C1D	2.38	132.12	128.46
32	2	523	ZEX	C21-C26-C27	2.38	122.51	115.78
21	b	603	CL7	C4C-C3C-C2C	-2.38	104.03	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	414	CL7	CAA-CBA-CGA	-2.38	106.30	113.25
21	4	405	CL7	O2A-CGA-O1A	-2.38	117.59	123.59
21	8	405	CL7	O2A-CGA-O1A	-2.38	117.59	123.59
21	C	514	CL7	CAA-CBA-CGA	-2.38	106.20	112.51
21	c	514	CL7	CAA-CBA-CGA	-2.38	106.20	112.51
21	7	504	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	B	615	CL7	OBD-CAD-CBD	-2.38	122.50	125.89
21	b	616	CL7	OBD-CAD-CBD	-2.38	122.50	125.89
21	C	507	CL7	C7-C6-C5	-2.38	106.91	113.36
23	a	404	8CT	C18-C19-C20	-2.38	118.61	123.47
21	4	405	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	8	405	CL7	C1C-C2C-C3C	-2.38	103.47	106.94
21	6	518	CL7	OBD-CAD-CBD	-2.37	122.50	125.89
21	7	514	CL7	C3B-C4B-NB	2.37	112.28	109.21
21	D	402	CL7	C4D-C3D-CAD	-2.37	103.97	107.81
21	d	402	CL7	C4D-C3D-CAD	-2.37	103.97	107.81
21	7	508	CL7	CHC-C1C-NC	-2.37	122.27	124.45
21	1	419	CL7	C3B-C4B-NB	2.37	112.28	109.21
21	2	516	CL7	C4D-C3D-CAD	-2.37	103.97	107.81
21	6	516	CL7	C4D-C3D-CAD	-2.37	103.97	107.81
21	D	404	CL7	C1B-CHB-C4A	-2.37	125.42	130.12
21	B	602	CL7	C3B-C4B-NB	2.37	112.28	109.21
21	b	603	CL7	C3B-C4B-NB	2.37	112.28	109.21
21	B	606	CL7	CHC-C1C-NC	-2.37	122.27	124.45
21	b	607	CL7	CHC-C1C-NC	-2.37	122.27	124.45
21	6	505	CL7	CMD-C2D-C1D	2.37	132.11	128.46
21	d	404	CL7	C1B-CHB-C4A	-2.37	125.42	130.12
21	2	518	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
32	1	421	ZEX	C1-C6-C5	-2.37	119.27	122.61
32	5	421	ZEX	C1-C6-C5	-2.37	119.27	122.61
21	8	407	CL7	CMD-C2D-C1D	2.37	132.11	128.46
32	6	522	ZEX	C21-C26-C27	2.37	122.48	115.78
21	a	401	CL7	C1B-CHB-C4A	-2.37	125.42	130.12
21	2	513	CL7	CHC-C1C-NC	-2.37	122.28	124.45
21	C	502	CL7	C1B-CHB-C4A	-2.37	125.42	130.12
21	C	510	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	c	510	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	4	414	CL7	C1B-CHB-C4A	-2.37	125.43	130.12
21	8	414	CL7	C1B-CHB-C4A	-2.37	125.43	130.12
32	3	525	ZEX	C1-C6-C5	-2.37	119.28	122.61
31	f	101	HEM	C4D-ND-C1D	2.37	107.52	105.07
21	3	504	CL7	C1C-C2C-C3C	-2.37	103.48	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	505	CL7	C1B-CHB-C4A	-2.37	125.43	130.12
21	7	505	CL7	C1B-CHB-C4A	-2.37	125.43	130.12
21	A	403	CL7	O2A-CGA-O1A	-2.37	117.62	123.59
21	a	403	CL7	O2A-CGA-O1A	-2.37	117.62	123.59
21	B	614	CL7	CMD-C2D-C1D	2.37	132.10	128.46
23	B	617	8CT	C04-C03-C10	2.37	122.47	115.78
23	b	618	8CT	C04-C03-C10	2.37	122.47	115.78
31	F	101	HEM	C4D-ND-C1D	2.37	107.52	105.07
21	7	503	CL7	C4-C3-C5	2.37	119.25	115.27
21	A	401	CL7	C1B-CHB-C4A	-2.37	125.43	130.12
21	1	418	CL7	C4-C3-C5	2.37	119.25	115.27
21	5	418	CL7	C4-C3-C5	2.37	119.25	115.27
21	b	613	CL7	O2D-CGD-O1D	-2.37	119.21	123.84
21	B	612	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	b	613	CL7	C4C-C3C-C2C	-2.37	104.04	107.13
21	C	507	CL7	CMD-C2D-C1D	2.36	132.10	128.46
21	c	507	CL7	CMD-C2D-C1D	2.36	132.10	128.46
21	2	507	CL7	C3B-C4B-NB	2.36	112.27	109.21
21	3	514	CL7	C3B-C4B-NB	2.36	112.27	109.21
21	6	513	CL7	CHC-C1C-NC	-2.36	122.28	124.45
21	c	514	CL7	C3B-C4B-NB	2.36	112.27	109.21
21	7	511	CL7	C1B-CHB-C4A	-2.36	125.44	130.12
21	7	512	CL7	C1B-CHB-C4A	-2.36	125.44	130.12
21	b	615	CL7	CMD-C2D-C1D	2.36	132.09	128.46
21	8	405	CL7	CMD-C2D-C1D	2.36	132.09	128.46
21	4	405	CL7	C7-C6-C5	-2.36	106.95	113.36
21	8	405	CL7	C7-C6-C5	-2.36	106.95	113.36
21	2	505	CL7	CMD-C2D-C1D	2.36	132.09	128.46
21	1	420	CL7	C1B-CHB-C4A	-2.36	125.44	130.12
21	5	420	CL7	C1B-CHB-C4A	-2.36	125.44	130.12
21	1	414	CL7	C3B-C4B-NB	2.36	112.26	109.21
21	5	414	CL7	C3B-C4B-NB	2.36	112.26	109.21
21	3	511	CL7	C1B-CHB-C4A	-2.36	125.44	130.12
21	2	511	CL7	C3B-C4B-NB	2.36	112.26	109.21
32	2	520	ZEX	C1-C6-C5	-2.36	119.29	122.61
21	4	413	CL7	C1B-CHB-C4A	-2.36	125.45	130.12
21	8	413	CL7	C1B-CHB-C4A	-2.36	125.45	130.12
23	K	101	8CT	C27-C26-C25	-2.36	119.62	122.92
23	k	101	8CT	C27-C26-C25	-2.36	119.62	122.92
21	1	404	CL7	C3B-C4B-NB	2.35	112.25	109.21
21	3	515	CL7	C4D-C3D-CAD	-2.35	104.00	107.81
21	7	515	CL7	C4D-C3D-CAD	-2.35	104.00	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	404	8CT	C19-C18-C17	-2.35	118.65	123.47
21	5	403	CL7	C1B-CHB-C4A	-2.35	125.46	130.12
21	A	406	CL7	OBD-CAD-CBD	-2.35	122.53	125.89
21	B	616	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	b	617	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	1	403	CL7	C1B-CHB-C4A	-2.35	125.46	130.12
32	6	520	ZEX	C17-C1-C6	-2.35	106.49	110.30
21	1	409	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	5	409	CL7	C4C-C3C-C2C	-2.35	104.06	107.13
21	3	511	CL7	C3B-C4B-NB	2.35	112.25	109.21
21	7	511	CL7	C3B-C4B-NB	2.35	112.25	109.21
21	B	609	CL7	C4-C3-C5	2.35	119.22	115.27
21	b	610	CL7	C4-C3-C5	2.35	119.22	115.27
21	A	406	CL7	C1C-C2C-C3C	-2.35	103.51	106.94
21	a	405	CL7	C1C-C2C-C3C	-2.35	103.51	106.94
21	6	518	CL7	C4C-C3C-C2C	-2.35	104.07	107.13
21	B	607	CL7	C4-C3-C5	2.35	119.22	115.27
21	8	413	CL7	CAA-CBA-CGA	-2.35	106.40	113.25
21	a	405	CL7	C3B-C4B-NB	2.34	112.24	109.21
21	8	411	CL7	CAA-CBA-CGA	-2.34	106.40	113.25
21	2	502	CL7	C1B-CHB-C4A	-2.34	125.47	130.12
21	6	502	CL7	C1B-CHB-C4A	-2.34	125.47	130.12
21	4	407	CL7	CMD-C2D-C1D	2.34	132.07	128.46
21	3	504	CL7	C3B-C4B-NB	2.34	112.24	109.21
21	7	504	CL7	C3B-C4B-NB	2.34	112.24	109.21
23	B	619	8CT	C14-C15-C16	-2.34	119.83	126.42
23	b	620	8CT	C14-C15-C16	-2.34	119.83	126.42
21	C	507	CL7	C4-C3-C5	2.34	119.21	115.27
21	1	406	CL7	C3B-C4B-NB	2.34	112.24	109.21
21	5	406	CL7	C3B-C4B-NB	2.34	112.24	109.21
23	C	516	8CT	C35-C30-C31	2.34	115.61	111.42
23	c	516	8CT	C35-C30-C31	2.34	115.61	111.42
23	A	404	8CT	C19-C18-C17	-2.34	118.68	123.47
21	B	605	CL7	OBD-CAD-CBD	-2.34	122.55	125.89
21	b	606	CL7	OBD-CAD-CBD	-2.34	122.55	125.89
21	5	407	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	2	516	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
21	6	516	CL7	C1C-C2C-C3C	-2.34	103.52	106.94
21	B	612	CL7	O2D-CGD-O1D	-2.34	119.26	123.84
32	2	521	ZEX	C17-C1-C6	-2.34	106.50	110.30
21	7	513	CL7	C1B-CHB-C4A	-2.34	125.48	130.12
21	3	507	CL7	C4-C3-C5	2.34	119.20	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	413	CL7	C4-C3-C5	2.34	119.20	115.27
21	8	413	CL7	C4-C3-C5	2.34	119.20	115.27
21	2	508	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	3	507	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	6	508	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	7	515	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	c	507	CL7	O2A-CGA-CBA	2.34	119.24	111.91
21	4	413	CL7	CAA-CBA-CGA	-2.34	106.42	113.25
21	C	507	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	c	507	CL7	C4C-C3C-C2C	-2.34	104.08	107.13
21	c	511	CL7	C4-C3-C5	2.34	119.20	115.27
21	C	513	CL7	C1C-C2C-C3C	-2.34	103.53	106.94
21	2	504	CL7	C3B-C4B-NB	2.34	112.23	109.21
21	6	504	CL7	C3B-C4B-NB	2.34	112.23	109.21
21	4	411	CL7	CAA-CBA-CGA	-2.33	106.43	113.25
21	C	513	CL7	CMD-C2D-C1D	2.33	132.05	128.46
21	3	508	CL7	CHC-C1C-NC	-2.33	122.31	124.45
21	7	515	CL7	C1B-CHB-C4A	-2.33	125.49	130.12
21	7	501	CL7	CMD-C2D-C1D	2.33	132.05	128.46
21	1	407	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
32	7	522	ZEX	C21-C22-C23	-2.33	108.64	113.69
21	c	507	CL7	C4-C3-C5	2.33	119.19	115.27
21	3	515	CL7	C1B-CHB-C4A	-2.33	125.50	130.12
21	7	510	CL7	C4-C3-C5	2.33	119.19	115.27
21	B	614	CL7	OBD-CAD-CBD	-2.33	122.56	125.89
21	3	513	CL7	C1B-CHB-C4A	-2.33	125.50	130.12
21	c	513	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
32	2	519	ZEX	C15-C35-C34	-2.33	118.70	123.47
32	6	519	ZEX	C15-C35-C34	-2.33	118.70	123.47
21	1	409	CL7	CMD-C2D-C1D	2.33	132.04	128.46
21	4	414	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	8	414	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	c	510	CL7	C3B-C4B-NB	2.33	112.22	109.21
21	3	517	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
21	7	517	CL7	C4C-C3C-C2C	-2.33	104.09	107.13
21	3	514	CL7	CMD-C2D-C1D	2.33	132.04	128.46
21	3	517	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	7	517	CL7	C1C-C2C-C3C	-2.33	103.54	106.94
21	3	511	CL7	C4D-C3D-CAD	-2.33	104.04	107.81
21	7	511	CL7	C4D-C3D-CAD	-2.33	104.04	107.81
21	c	518	CL7	CMD-C2D-C1D	2.33	132.04	128.46
21	a	405	CL7	OBD-CAD-CBD	-2.33	122.57	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	C	507	CL7	O2A-CGA-CBA	2.33	119.21	111.91
21	b	608	CL7	C4-C3-C5	2.33	119.18	115.27
21	1	413	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	5	413	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	3	510	CL7	C4-C3-C5	2.32	119.18	115.27
21	1	404	CL7	OBD-CAD-CBD	-2.32	122.57	125.89
21	5	404	CL7	OBD-CAD-CBD	-2.32	122.57	125.89
32	2	525	ZEX	C1-C6-C7	2.32	122.35	115.78
32	6	524	ZEX	C1-C6-C7	2.32	122.35	115.78
22	D	408	PHO	C4C-NC-C1C	-2.32	102.32	107.09
21	6	506	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	5	404	CL7	C3B-C4B-NB	2.32	112.21	109.21
21	B	611	CL7	C3B-C4B-NB	2.32	112.21	109.21
21	3	515	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
21	4	406	CL7	C1C-C2C-C3C	-2.32	103.55	106.94
27	c	517	DGD	O3G-C3G-C2G	-2.32	105.30	110.90
21	2	505	CL7	C4C-C3C-C2C	-2.32	104.10	107.13
21	5	409	CL7	CMD-C2D-C1D	2.32	132.03	128.46
21	1	406	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
21	5	406	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
27	C	517	DGD	O3G-C3G-C2G	-2.32	105.31	110.90
32	8	419	ZEX	C1-C6-C7	2.32	122.34	115.78
32	7	520	ZEX	C39-C29-C30	-2.32	119.68	122.92
32	3	522	ZEX	C21-C22-C23	-2.32	108.67	113.69
32	2	523	ZEX	C39-C29-C28	2.32	121.73	118.08
32	6	522	ZEX	C39-C29-C28	2.32	121.73	118.08
32	1	422	ZEX	C15-C35-C34	-2.32	118.73	123.47
32	5	422	ZEX	C15-C35-C34	-2.32	118.73	123.47
21	2	506	CL7	C4C-C3C-C2C	-2.32	104.11	107.13
21	C	510	CL7	C3B-C4B-NB	2.32	112.20	109.21
21	1	407	CL7	C1C-C2C-C3C	-2.32	103.56	106.94
21	2	512	CL7	OBD-CAD-CBD	-2.31	122.59	125.89
21	6	512	CL7	OBD-CAD-CBD	-2.31	122.59	125.89
23	4	402	8CT	C25-C24-C23	-2.31	116.00	123.22
23	8	402	8CT	C25-C24-C23	-2.31	116.00	123.22
32	4	419	ZEX	C1-C6-C7	2.31	122.33	115.78
21	4	416	CL7	C4D-C3D-CAD	-2.31	104.06	107.81
21	8	416	CL7	C4D-C3D-CAD	-2.31	104.06	107.81
21	A	406	CL7	C3B-C4B-NB	2.31	112.20	109.21
21	b	603	CL7	C1C-C2C-C3C	-2.31	103.56	106.94
21	C	511	CL7	C4-C3-C5	2.31	119.16	115.27
23	c	519	8CT	C27-C26-C25	-2.31	119.68	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	3	501	CL7	CMD-C2D-C1D	2.31	132.02	128.46
21	7	507	CL7	C1C-C2C-C3C	-2.31	103.56	106.94
22	d	408	PHO	C4C-NC-C1C	-2.31	102.35	107.09
21	C	509	CL7	C3B-C4B-NB	2.31	112.20	109.21
21	c	509	CL7	C3B-C4B-NB	2.31	112.20	109.21
21	2	516	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
21	6	516	CL7	C4C-C3C-C2C	-2.31	104.11	107.13
21	3	512	CL7	C3B-C4B-NB	2.31	112.20	109.21
21	8	416	CL7	OBD-CAD-CBD	-2.31	122.59	125.89
21	c	513	CL7	CMD-C2D-C1D	2.31	132.01	128.46
32	2	525	ZEX	C15-C35-C34	-2.31	118.74	123.47
32	6	524	ZEX	C15-C35-C34	-2.31	118.74	123.47
21	2	517	CL7	C1-C2-C3	2.31	130.04	126.04
21	5	414	CL7	C4D-C3D-CAD	-2.31	104.07	107.81
21	2	510	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	6	510	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	3	507	CL7	CAA-CBA-CGA	-2.31	106.51	113.25
21	C	518	CL7	CMD-C2D-C1D	2.31	132.01	128.46
21	3	504	CL7	CMD-C2D-C1D	2.31	132.01	128.46
21	7	504	CL7	CMD-C2D-C1D	2.31	132.01	128.46
32	4	419	ZEX	C40-C33-C32	2.31	121.71	118.08
32	8	419	ZEX	C40-C33-C32	2.31	121.71	118.08
21	7	507	CL7	C4-C3-C5	2.31	119.15	115.27
21	b	615	CL7	OBD-CAD-CBD	-2.31	122.60	125.89
23	b	620	8CT	C05-C04-C03	2.31	114.03	110.48
32	3	520	ZEX	C39-C29-C30	-2.31	119.69	122.92
21	B	602	CL7	C1C-C2C-C3C	-2.31	103.57	106.94
21	7	514	CL7	CMD-C2D-C1D	2.31	132.01	128.46
23	C	519	8CT	C27-C26-C25	-2.30	119.69	122.92
21	2	512	CL7	C3B-C4B-NB	2.30	112.19	109.21
21	6	512	CL7	C3B-C4B-NB	2.30	112.19	109.21
21	3	504	CL7	C4C-C3C-C2C	-2.30	104.12	107.13
21	7	504	CL7	C4C-C3C-C2C	-2.30	104.12	107.13
21	7	507	CL7	C4C-C3C-C2C	-2.30	104.12	107.13
32	4	420	ZEX	C20-C13-C12	2.30	121.70	118.08
32	8	420	ZEX	C20-C13-C12	2.30	121.70	118.08
21	C	505	CL7	C4-C3-C5	2.30	119.14	115.27
21	7	507	CL7	CAA-CBA-CGA	-2.30	106.53	113.25
21	1	414	CL7	C4D-C3D-CAD	-2.30	104.08	107.81
21	C	502	CL7	C3B-C4B-NB	2.30	112.19	109.21
21	c	502	CL7	C3B-C4B-NB	2.30	112.19	109.21
23	B	619	8CT	C05-C04-C03	2.30	114.02	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	404	8CT	C27-C26-C25	-2.30	119.70	122.92
21	5	415	CL7	C1B-CHB-C4A	-2.30	125.56	130.12
21	1	406	CL7	C1B-CHB-C4A	-2.30	125.56	130.12
21	5	406	CL7	C1B-CHB-C4A	-2.30	125.56	130.12
21	C	507	CL7	C3B-C4B-NB	2.30	112.18	109.21
21	2	506	CL7	C1C-C2C-C3C	-2.30	103.58	106.94
21	1	410	CL7	C1C-C2C-C3C	-2.30	103.59	106.94
21	5	410	CL7	C1C-C2C-C3C	-2.30	103.59	106.94
21	1	409	CL7	CAA-CBA-CGA	-2.30	106.41	112.51
21	D	404	CL7	OBD-CAD-CBD	-2.30	122.61	125.89
21	3	503	CL7	C4D-C3D-CAD	-2.30	104.09	107.81
21	7	503	CL7	C4D-C3D-CAD	-2.30	104.09	107.81
21	3	505	CL7	C3B-C4B-NB	2.30	112.18	109.21
21	7	505	CL7	C3B-C4B-NB	2.30	112.18	109.21
21	1	415	CL7	C1B-CHB-C4A	-2.30	125.57	130.12
21	3	517	CL7	C4D-C3D-CAD	-2.30	104.09	107.81
21	7	517	CL7	C4D-C3D-CAD	-2.30	104.09	107.81
21	2	509	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	b	609	CL7	O2D-CGD-O1D	-2.29	119.35	123.84
32	3	519	ZEX	C2-C3-C4	-2.29	107.17	110.30
21	6	505	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	4	405	CL7	O2A-C1-C2	-2.29	102.61	108.64
21	8	405	CL7	O2A-C1-C2	-2.29	102.61	108.64
21	C	506	CL7	C7-C6-C5	-2.29	107.13	113.36
21	c	506	CL7	C7-C6-C5	-2.29	107.13	113.36
21	1	405	CL7	C1B-CHB-C4A	-2.29	125.58	130.12
21	5	407	CL7	C1C-C2C-C3C	-2.29	103.59	106.94
21	c	505	CL7	C4-C3-C5	2.29	119.12	115.27
21	C	514	CL7	CMD-C2D-C1D	2.29	131.99	128.46
21	2	504	CL7	C1C-C2C-C3C	-2.29	103.60	106.94
21	4	412	CL7	CAC-C3C-C2C	2.29	131.45	127.53
21	8	412	CL7	CAC-C3C-C2C	2.29	131.45	127.53
21	6	509	CL7	C3B-C4B-NB	2.29	112.17	109.21
21	B	608	CL7	O2D-CGD-O1D	-2.29	119.36	123.84
21	6	506	CL7	C4C-C3C-C2C	-2.29	104.14	107.13
21	5	405	CL7	C1B-CHB-C4A	-2.29	125.59	130.12
21	2	515	CL7	CMD-C2D-C1D	2.29	131.98	128.46
21	6	515	CL7	CMD-C2D-C1D	2.29	131.98	128.46
21	5	409	CL7	CAA-CBA-CGA	-2.29	106.44	112.51
21	6	517	CL7	C1-C2-C3	2.29	130.00	126.04
21	4	411	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	4	412	CL7	C4C-C3C-C2C	-2.28	104.15	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	509	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	8	411	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	8	412	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	2	510	CL7	C3B-C4B-NB	2.28	112.16	109.21
21	d	404	CL7	OBD-CAD-CBD	-2.28	122.63	125.89
21	3	513	CL7	CAA-CBA-CGA	-2.28	106.45	112.51
21	3	518	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
21	7	518	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
21	4	416	CL7	OBD-CAD-CBD	-2.28	122.64	125.89
21	c	514	CL7	CMD-C2D-C1D	2.28	131.97	128.46
21	b	612	CL7	C3B-C4B-NB	2.28	112.16	109.21
21	B	615	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	b	616	CL7	C4C-C3C-C2C	-2.28	104.15	107.13
21	2	509	CL7	C3B-C4B-NB	2.28	112.16	109.21
21	7	512	CL7	C3B-C4B-NB	2.28	112.16	109.21
21	6	511	CL7	C1C-C2C-C3C	-2.28	103.61	106.94
23	D	406	8CT	C18-C19-C20	2.28	128.14	123.47
23	d	406	8CT	C18-C19-C20	2.28	128.14	123.47
21	8	409	CL7	C1B-CHB-C4A	-2.28	125.60	130.12
21	7	510	CL7	C4D-C3D-CAD	-2.28	104.12	107.81
21	4	417	CL7	C3B-C4B-NB	2.28	112.15	109.21
21	C	506	CL7	OBD-CAD-CBD	-2.28	122.64	125.89
21	c	506	CL7	OBD-CAD-CBD	-2.28	122.64	125.89
21	b	608	CL7	C4C-C3C-C2C	-2.28	104.16	107.13
21	B	612	CL7	CAC-C3C-C2C	2.28	131.42	127.53
21	b	613	CL7	CAC-C3C-C2C	2.28	131.42	127.53
21	4	409	CL7	C1B-CHB-C4A	-2.28	125.61	130.12
21	8	406	CL7	C1C-C2C-C3C	-2.28	103.62	106.94
21	3	507	CL7	C4C-C3C-C2C	-2.27	104.16	107.13
23	4	402	8CT	C01-C02-C07	2.27	117.98	113.62
23	8	402	8CT	C01-C02-C07	2.27	117.98	113.62
21	7	510	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
23	B	619	8CT	C04-C03-C02	-2.27	119.41	122.61
23	b	620	8CT	C04-C03-C02	-2.27	119.41	122.61
21	2	505	CL7	C1C-C2C-C3C	-2.27	103.62	106.94
21	c	507	CL7	C3B-C4B-NB	2.27	112.15	109.21
21	c	511	CL7	C3B-C4B-NB	2.27	112.15	109.21
21	1	407	CL7	CMD-C2D-C1D	2.27	131.96	128.46
21	5	407	CL7	CMD-C2D-C1D	2.27	131.96	128.46
21	1	417	CL7	CAC-C3C-C4C	-2.27	121.10	124.68
21	5	417	CL7	CAC-C3C-C4C	-2.27	121.10	124.68
21	B	603	CL7	C3B-C4B-NB	2.27	112.15	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	604	CL7	C3B-C4B-NB	2.27	112.15	109.21
21	7	502	CL7	C3B-C4B-NB	2.27	112.14	109.21
21	7	513	CL7	CAA-CBA-CGA	-2.27	106.48	112.51
21	6	510	CL7	C3B-C4B-NB	2.27	112.14	109.21
21	1	415	CL7	CMA-C3A-C2A	-2.27	110.80	116.10
21	5	415	CL7	CMA-C3A-C2A	-2.27	110.80	116.10
21	C	503	CL7	C3B-C4B-NB	2.27	112.14	109.21
21	1	416	CL7	C3B-C4B-NB	2.27	112.14	109.21
21	c	503	CL7	C3B-C4B-NB	2.27	112.14	109.21
21	5	416	CL7	C3B-C4B-NB	2.27	112.14	109.21
21	C	504	CL7	OBD-CAD-CBD	-2.27	122.65	125.89
21	b	613	CL7	O2A-CGA-O1A	-2.27	117.87	123.59
21	D	402	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
21	d	402	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
21	3	510	CL7	C4D-C3D-CAD	-2.27	104.14	107.81
21	5	419	CL7	C1B-CHB-C4A	-2.27	125.63	130.12
21	6	504	CL7	C1C-C2C-C3C	-2.27	103.63	106.94
32	7	519	ZEX	C2-C3-C4	-2.27	107.20	110.30
21	b	605	CL7	CAA-CBA-CGA	-2.26	106.64	113.25
21	d	402	CL7	OBD-CAD-CBD	-2.26	122.66	125.89
21	2	511	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
22	A	402	PHO	CMA-C3A-C4A	-2.26	109.42	114.38
32	1	422	ZEX	C18-C5-C6	-2.26	121.99	124.53
21	6	509	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
21	1	417	CL7	C3B-C4B-NB	2.26	112.13	109.21
21	8	417	CL7	C3B-C4B-NB	2.26	112.13	109.21
21	3	510	CL7	C4C-C3C-C2C	-2.26	104.18	107.13
23	D	406	8CT	C24-C25-C26	-2.26	124.08	127.31
23	d	406	8CT	C24-C25-C26	-2.26	124.08	127.31
21	5	417	CL7	C3B-C4B-NB	2.26	112.13	109.21
32	4	418	ZEX	C20-C13-C14	-2.26	119.76	122.92
32	8	418	ZEX	C20-C13-C14	-2.26	119.76	122.92
21	6	507	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
21	3	510	CL7	C1C-C2C-C3C	-2.26	103.64	106.94
21	1	407	CL7	C4D-C3D-CAD	-2.26	104.15	107.81
21	6	507	CL7	CMD-C2D-C1D	2.26	131.94	128.46
21	B	614	CL7	C4D-C3D-CAD	-2.26	104.15	107.81
21	c	504	CL7	OBD-CAD-CBD	-2.26	122.67	125.89
32	3	520	ZEX	C3-C4-C5	-2.26	107.36	111.85
21	2	503	CL7	CAA-C2A-C1A	2.26	119.61	112.19
21	6	503	CL7	CAA-C2A-C1A	2.26	119.61	112.19
21	3	501	CL7	C4C-C3C-C2C	-2.26	104.18	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	618	8CT	C24-C25-C26	-2.26	124.09	127.31
23	b	619	8CT	C24-C25-C26	-2.26	124.09	127.31
32	8	419	ZEX	C35-C15-C14	-2.26	118.85	123.47
21	1	402	CL7	C1C-C2C-C3C	-2.26	103.65	106.94
21	5	402	CL7	C1C-C2C-C3C	-2.26	103.65	106.94
21	2	510	CL7	C4D-C3D-CAD	-2.26	104.16	107.81
21	6	510	CL7	C4D-C3D-CAD	-2.26	104.16	107.81
22	a	402	PHO	CMA-C3A-C4A	-2.26	109.44	114.38
21	C	514	CL7	C4C-C3C-C2C	-2.26	104.19	107.13
23	c	519	8CT	C40-C12-C13	-2.26	119.76	122.92
32	2	520	ZEX	C19-C9-C8	2.26	121.63	118.08
32	3	525	ZEX	C19-C9-C8	2.26	121.63	118.08
21	C	511	CL7	C3B-C4B-NB	2.25	112.12	109.21
21	C	512	CL7	C3B-C4B-NB	2.25	112.12	109.21
23	C	519	8CT	C40-C12-C13	-2.25	119.77	122.92
32	4	403	ZEX	C35-C15-C14	-2.25	118.86	123.47
32	8	403	ZEX	C35-C15-C14	-2.25	118.86	123.47
23	B	619	8CT	C18-C19-C20	-2.25	118.86	123.47
21	2	507	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
21	6	505	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
21	B	604	CL7	CAA-CBA-CGA	-2.25	106.67	113.25
21	2	509	CL7	C1C-C2C-C3C	-2.25	103.65	106.94
21	3	502	CL7	CGD-CBD-CAD	2.25	118.03	110.73
21	7	502	CL7	CGD-CBD-CAD	2.25	118.03	110.73
31	f	101	HEM	CHA-C4D-C3D	-2.25	121.10	125.33
21	7	512	CL7	OBD-CAD-CBD	-2.25	122.68	125.89
21	C	509	CL7	CMD-C2D-C1D	2.25	131.93	128.46
21	c	509	CL7	CMD-C2D-C1D	2.25	131.93	128.46
32	4	419	ZEX	C35-C15-C14	-2.25	118.86	123.47
31	F	101	HEM	CHA-C4D-C3D	-2.25	121.10	125.33
21	2	506	CL7	CAA-CBA-CGA	-2.25	106.68	113.25
21	6	506	CL7	CAA-CBA-CGA	-2.25	106.68	113.25
21	B	606	CL7	O2D-CGD-O1D	-2.25	119.44	123.84
23	a	404	8CT	C27-C26-C25	-2.25	119.77	122.92
21	B	607	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
27	c	517	DGD	O1G-C1A-C2A	2.25	118.96	111.91
21	1	419	CL7	C1B-CHB-C4A	-2.25	125.66	130.12
21	4	409	CL7	C4-C3-C5	2.25	119.05	115.27
27	C	517	DGD	O1G-C1A-C2A	2.25	118.96	111.91
21	B	622	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
21	3	515	CL7	CAC-C3C-C2C	2.25	131.37	127.53
21	7	515	CL7	CAC-C3C-C2C	2.25	131.37	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	510	CL7	C4C-C3C-C2C	-2.25	104.20	107.13
26	c	501	LMG	C30-C29-C28	-2.25	105.45	113.62
21	5	407	CL7	C4D-C3D-CAD	-2.25	104.17	107.81
32	2	525	ZEX	C35-C15-C14	-2.25	118.87	123.47
32	1	421	ZEX	C3-C4-C5	-2.25	107.38	111.85
32	5	421	ZEX	C3-C4-C5	-2.25	107.38	111.85
23	C	516	8CT	C22-C21-C20	-2.24	119.78	122.92
21	d	405	CL7	C1C-C2C-C3C	-2.24	103.66	106.94
21	3	502	CL7	C3B-C4B-NB	2.24	112.11	109.21
21	8	409	CL7	C4-C3-C5	2.24	119.05	115.27
21	3	511	CL7	C1-C2-C3	2.24	129.92	126.04
21	2	507	CL7	CMD-C2D-C1D	2.24	131.91	128.46
21	c	508	CL7	C4C-C3C-C2C	-2.24	104.20	107.13
21	2	509	CL7	CMD-C2D-C1D	2.24	131.91	128.46
21	6	509	CL7	CMD-C2D-C1D	2.24	131.91	128.46
21	b	613	CL7	C4D-C3D-CAD	-2.24	104.18	107.81
21	2	513	CL7	OBD-CAD-CBD	-2.24	122.69	125.89
21	6	513	CL7	OBD-CAD-CBD	-2.24	122.69	125.89
21	C	510	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	c	510	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
21	3	517	CL7	CMD-C2D-C1D	2.24	131.91	128.46
21	B	612	CL7	O2A-CGA-O1A	-2.24	117.94	123.59
21	D	405	CL7	C1C-C2C-C3C	-2.24	103.67	106.94
23	b	620	8CT	C18-C19-C20	-2.24	118.89	123.47
21	D	402	CL7	OBD-CAD-CBD	-2.24	122.70	125.89
21	B	612	CL7	C4D-C3D-CAD	-2.24	104.19	107.81
21	b	607	CL7	C4D-C3D-CAD	-2.24	104.19	107.81
23	c	516	8CT	C22-C21-C20	-2.24	119.79	122.92
21	8	406	CL7	C4C-C3C-C2C	-2.24	104.21	107.13
21	b	615	CL7	C4D-C3D-CAD	-2.24	104.19	107.81
21	3	504	CL7	C4D-C3D-CAD	-2.24	104.19	107.81
21	b	607	CL7	O2D-CGD-O1D	-2.24	119.47	123.84
32	4	403	ZEX	C10-C11-C12	-2.23	116.25	123.22
32	8	403	ZEX	C10-C11-C12	-2.23	116.25	123.22
21	3	516	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	7	506	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	7	516	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	3	503	CL7	CED-O2D-CGD	-2.23	110.89	115.94
21	2	502	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	6	502	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	1	419	CL7	C1C-C2C-C3C	-2.23	103.68	106.94
21	5	419	CL7	C1C-C2C-C3C	-2.23	103.68	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	514	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	1	403	CL7	CAA-CBA-CGA	-2.23	106.73	113.25
21	3	512	CL7	OBD-CAD-CBD	-2.23	122.71	125.89
21	B	605	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	b	606	CL7	C4C-C3C-C2C	-2.23	104.22	107.13
21	2	517	CL7	CMD-C2D-C1D	2.23	131.89	128.46
21	6	517	CL7	CMD-C2D-C1D	2.23	131.89	128.46
21	7	511	CL7	C1-C2-C3	2.23	129.90	126.04
32	6	524	ZEX	C35-C15-C14	-2.23	118.91	123.47
32	5	422	ZEX	C18-C5-C6	-2.23	122.02	124.53
21	7	504	CL7	C4D-C3D-CAD	-2.23	104.20	107.81
21	2	501	CL7	C1-C2-C3	2.23	129.90	126.04
21	5	403	CL7	CAA-CBA-CGA	-2.23	106.74	113.25
32	7	520	ZEX	C3-C4-C5	-2.23	107.42	111.85
21	6	501	CL7	C1-C2-C3	2.23	129.90	126.04
21	b	614	CL7	CMD-C2D-C1D	2.23	131.89	128.46
21	7	503	CL7	CED-O2D-CGD	-2.23	110.90	115.94
21	4	413	CL7	OBD-CAD-CBD	-2.23	122.71	125.89
21	8	413	CL7	OBD-CAD-CBD	-2.23	122.71	125.89
21	B	606	CL7	C4D-C3D-CAD	-2.23	104.20	107.81
21	C	508	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
21	c	508	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
21	B	612	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
21	b	613	CL7	C1C-C2C-C3C	-2.23	103.69	106.94
26	C	501	LMG	C30-C29-C28	-2.23	105.52	113.62
21	c	512	CL7	C3B-C4B-NB	2.23	112.09	109.21
21	2	516	CL7	C1-C2-C3	2.23	129.89	126.04
21	6	516	CL7	C1-C2-C3	2.23	129.89	126.04
21	7	517	CL7	CMD-C2D-C1D	2.23	131.88	128.46
21	7	504	CL7	CAA-CBA-CGA	-2.23	106.75	113.25
21	3	504	CL7	CAA-CBA-CGA	-2.22	106.76	113.25
21	C	508	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	b	623	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	d	402	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	1	410	CL7	O2A-CGA-O1A	-2.22	117.98	123.59
21	3	508	CL7	C4D-C3D-CAD	-2.22	104.21	107.81
21	7	508	CL7	C4D-C3D-CAD	-2.22	104.21	107.81
21	B	622	CL7	C1C-C2C-C3C	-2.22	103.70	106.94
21	1	410	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	5	410	CL7	C4C-C3C-C2C	-2.22	104.23	107.13
21	4	411	CL7	C3B-C4B-NB	2.22	112.08	109.21
21	8	411	CL7	C3B-C4B-NB	2.22	112.08	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	6	519	ZEX	C39-C29-C30	-2.22	119.81	122.92
21	B	613	CL7	CMD-C2D-C1D	2.22	131.88	128.46
21	3	511	CL7	C4-C3-C5	2.22	119.01	115.27
21	7	511	CL7	C4-C3-C5	2.22	119.01	115.27
21	1	408	CL7	C3B-C4B-NB	2.22	112.08	109.21
21	5	408	CL7	C3B-C4B-NB	2.22	112.08	109.21
21	b	606	CL7	CAA-CBA-CGA	-2.22	106.77	113.25
32	2	519	ZEX	C39-C29-C30	-2.22	119.81	122.92
23	4	402	8CT	C10-C11-C12	-2.22	122.88	126.23
23	C	519	8CT	C13-C14-C15	-2.22	116.30	123.22
32	2	519	ZEX	C31-C32-C33	-2.22	120.19	126.42
32	6	519	ZEX	C31-C32-C33	-2.22	120.19	126.42
32	2	521	ZEX	C40-C33-C32	2.22	121.57	118.08
21	4	407	CL7	C3B-C4B-NB	2.22	112.08	109.21
21	3	506	CL7	C1C-C2C-C3C	-2.22	103.70	106.94
21	5	410	CL7	O2A-CGA-O1A	-2.22	118.00	123.59
23	b	619	8CT	C40-C12-C11	2.22	121.57	118.08
21	3	513	CL7	C3B-C4B-NB	2.22	112.07	109.21
21	3	503	CL7	C3B-C4B-NB	2.21	112.07	109.21
21	7	501	CL7	C4C-C3C-C2C	-2.21	104.24	107.13
23	K	101	8CT	C25-C24-C23	-2.21	116.31	123.22
23	k	101	8CT	C25-C24-C23	-2.21	116.31	123.22
21	B	605	CL7	CAA-CBA-CGA	-2.21	106.79	113.25
21	C	505	CL7	C1B-CHB-C4A	-2.21	125.73	130.12
21	c	505	CL7	C1B-CHB-C4A	-2.21	125.73	130.12
23	c	519	8CT	C13-C14-C15	-2.21	116.31	123.22
21	3	501	CL7	C4D-C3D-CAD	-2.21	104.23	107.81
21	7	501	CL7	C4D-C3D-CAD	-2.21	104.23	107.81
23	B	618	8CT	C40-C12-C11	2.21	121.56	118.08
21	5	403	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
21	2	503	CL7	CAA-C2A-C3A	2.21	118.83	112.78
21	6	503	CL7	CAA-C2A-C3A	2.21	118.83	112.78
21	6	504	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
21	b	623	CL7	C1C-C2C-C3C	-2.21	103.71	106.94
21	b	607	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
21	D	402	CL7	C4C-C3C-C2C	-2.21	104.25	107.13
21	D	402	CL7	C4-C3-C5	2.21	119.48	114.60
21	d	402	CL7	C4-C3-C5	2.21	119.48	114.60
23	A	404	8CT	C14-C15-C16	-2.21	120.22	126.42
23	a	404	8CT	C14-C15-C16	-2.21	120.22	126.42
21	D	404	CL7	C1C-C2C-C3C	-2.21	103.72	106.94
21	4	406	CL7	C4C-C3C-C2C	-2.21	104.25	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	402	8CT	C18-C19-C20	-2.21	118.95	123.47
23	8	402	8CT	C18-C19-C20	-2.21	118.95	123.47
21	8	407	CL7	C3B-C4B-NB	2.21	112.06	109.21
32	5	421	ZEX	C10-C11-C12	-2.20	116.34	123.22
21	2	508	CL7	CMD-C2D-C1D	2.20	131.85	128.46
21	6	508	CL7	CMD-C2D-C1D	2.20	131.85	128.46
21	8	410	CL7	OBD-CAD-CBD	-2.20	122.75	125.89
21	2	512	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
29	D	403	BCT	O2-C-O1	2.20	125.26	119.55
29	d	403	BCT	O2-C-O1	2.20	125.26	119.55
21	4	404	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
21	8	404	CL7	C1C-C2C-C3C	-2.20	103.72	106.94
32	1	421	ZEX	C10-C11-C12	-2.20	116.34	123.22
21	1	411	CL7	C4D-C3D-CAD	-2.20	104.24	107.81
21	5	411	CL7	C4D-C3D-CAD	-2.20	104.24	107.81
21	2	513	CL7	CMD-C2D-C1D	2.20	131.85	128.46
21	C	506	CL7	CBA-CAA-C2A	-2.20	107.36	113.86
32	6	520	ZEX	C40-C33-C32	2.20	121.55	118.08
32	3	520	ZEX	C40-C33-C34	-2.20	119.84	122.92
32	7	520	ZEX	C40-C33-C34	-2.20	119.84	122.92
21	2	515	CL7	C1C-C2C-C3C	-2.20	103.73	106.94
21	6	515	CL7	C1C-C2C-C3C	-2.20	103.73	106.94
21	4	404	CL7	CAC-C3C-C2C	2.20	131.29	127.53
32	6	524	ZEX	C30-C31-C32	-2.20	116.36	123.22
21	4	410	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	1	418	CL7	OBD-CAD-CBD	-2.20	122.75	125.89
21	5	418	CL7	OBD-CAD-CBD	-2.20	122.75	125.89
23	C	515	8CT	C22-C21-C23	2.20	121.54	118.08
23	c	515	8CT	C22-C21-C23	2.20	121.54	118.08
21	1	418	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	5	418	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	7	503	CL7	C3B-C4B-NB	2.20	112.05	109.21
21	d	404	CL7	C1C-C2C-C3C	-2.20	103.73	106.94
23	C	516	8CT	C24-C23-C21	-2.20	120.25	126.42
23	c	516	8CT	C24-C23-C21	-2.20	120.25	126.42
21	A	406	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
21	a	405	CL7	C4C-C3C-C2C	-2.20	104.26	107.13
23	8	402	8CT	C10-C11-C12	-2.20	122.92	126.23
21	8	404	CL7	CAC-C3C-C2C	2.19	131.28	127.53
32	2	525	ZEX	C30-C31-C32	-2.19	116.37	123.22
21	C	512	CL7	CAC-C3C-C2C	2.19	131.28	127.53
21	c	512	CL7	CAC-C3C-C2C	2.19	131.28	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	513	CL7	C3B-C4B-NB	2.19	112.05	109.21
21	8	416	CL7	C3B-C4B-NB	2.19	112.05	109.21
21	c	506	CL7	CBA-CAA-C2A	-2.19	107.39	113.86
21	1	415	CL7	CMD-C2D-C1D	2.19	131.83	128.46
21	6	513	CL7	CMD-C2D-C1D	2.19	131.83	128.46
21	5	415	CL7	CMD-C2D-C1D	2.19	131.83	128.46
21	4	414	CL7	C4-C3-C5	2.19	118.95	115.27
21	8	414	CL7	C4-C3-C5	2.19	118.95	115.27
21	4	413	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
21	8	413	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
32	3	520	ZEX	C27-C26-C25	-2.19	119.31	122.84
32	7	520	ZEX	C27-C26-C25	-2.19	119.31	122.84
32	3	520	ZEX	C1-C6-C7	2.19	121.97	115.78
21	4	410	CL7	OBD-CAD-CBD	-2.19	122.77	125.89
21	c	508	CL7	CED-O2D-CGD	-2.19	110.99	115.94
21	1	410	CL7	C4-C3-C5	2.19	118.95	115.27
21	5	410	CL7	C4-C3-C5	2.19	118.95	115.27
21	c	504	CL7	C4C-C3C-C2C	-2.19	104.28	107.13
21	8	410	CL7	C4C-C3C-C2C	-2.19	104.28	107.13
21	B	606	CL7	C1C-C2C-C3C	-2.19	103.75	106.94
21	4	406	CL7	OBD-CAD-CBD	-2.18	122.77	125.89
21	8	406	CL7	OBD-CAD-CBD	-2.18	122.77	125.89
21	3	516	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	7	516	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	1	403	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	3	516	CL7	OBD-CAD-CBD	-2.18	122.78	125.89
21	7	516	CL7	OBD-CAD-CBD	-2.18	122.78	125.89
21	A	401	CL7	CMD-C2D-C1D	2.18	131.82	128.46
21	a	401	CL7	CMD-C2D-C1D	2.18	131.82	128.46
21	6	512	CL7	C1C-C2C-C3C	-2.18	103.75	106.94
31	f	101	HEM	CHC-C4B-C3B	-2.18	121.23	124.57
21	C	508	CL7	CED-O2D-CGD	-2.18	111.00	115.94
31	F	101	HEM	CHC-C4B-C3B	-2.18	121.23	124.57
32	2	520	ZEX	C8-C9-C10	-2.18	115.59	118.94
32	3	525	ZEX	C8-C9-C10	-2.18	115.59	118.94
21	C	504	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	1	409	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	4	416	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	5	409	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	8	416	CL7	C1C-C2C-C3C	-2.18	103.76	106.94
21	2	504	CL7	C4C-C3C-C2C	-2.18	104.28	107.13
21	7	510	CL7	C3B-C4B-NB	2.18	112.03	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	613	CL7	C3B-C4B-NB	2.18	112.03	109.21
23	B	617	8CT	C39-C16-C17	-2.18	119.87	122.92
23	b	618	8CT	C39-C16-C17	-2.18	119.87	122.92
21	C	508	CL7	O2D-CGD-O1D	-2.18	119.58	123.84
21	c	508	CL7	O2D-CGD-O1D	-2.18	119.58	123.84
21	2	511	CL7	C4C-C3C-C2C	-2.18	104.29	107.13
21	4	416	CL7	C3B-C4B-NB	2.18	112.02	109.21
21	5	417	CL7	C4-C3-C5	2.18	118.93	115.27
21	2	508	CL7	C4C-C3C-C2C	-2.18	104.29	107.13
21	6	508	CL7	C4C-C3C-C2C	-2.18	104.29	107.13
23	C	515	8CT	C15-C16-C17	-2.18	115.60	118.94
21	6	505	CL7	C1B-CHB-C4A	-2.17	125.81	130.12
21	3	502	CL7	C4C-C3C-C2C	-2.17	104.29	107.13
21	B	607	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
21	3	510	CL7	C3B-C4B-NB	2.17	112.02	109.21
32	7	520	ZEX	C1-C6-C7	2.17	121.93	115.78
21	2	505	CL7	C1B-CHB-C4A	-2.17	125.81	130.12
21	A	401	CL7	O2A-CGA-CBA	2.17	118.73	111.91
21	a	401	CL7	O2A-CGA-CBA	2.17	118.73	111.91
21	1	416	CL7	CMD-C2D-C1D	2.17	131.80	128.46
32	2	520	ZEX	C23-C24-C25	-2.17	106.24	109.33
21	1	402	CL7	OBD-CAD-CBD	-2.17	122.79	125.89
21	5	402	CL7	OBD-CAD-CBD	-2.17	122.79	125.89
23	B	618	8CT	C08-C04-C03	-2.17	106.78	110.30
23	b	619	8CT	C08-C04-C03	-2.17	106.78	110.30
21	C	506	CL7	C1C-C2C-C3C	-2.17	103.77	106.94
21	7	507	CL7	CAC-C3C-C2C	2.17	131.24	127.53
21	5	402	CL7	C4D-C3D-CAD	-2.17	104.30	107.81
21	B	611	CL7	O2A-CGA-O1A	-2.17	118.12	123.59
32	5	422	ZEX	C27-C26-C25	-2.17	119.34	122.84
23	B	617	8CT	C36-C35-C30	2.16	112.82	109.55
23	b	618	8CT	C36-C35-C30	2.16	112.82	109.55
21	4	412	CL7	C1C-C2C-C3C	-2.16	103.78	106.94
21	3	514	CL7	C4D-C3D-CAD	-2.16	104.31	107.81
21	C	503	CL7	C4-C3-C5	2.16	118.91	115.27
21	c	503	CL7	C4-C3-C5	2.16	118.91	115.27
21	8	407	CL7	CAC-C3C-C2C	2.16	131.23	127.53
21	b	612	CL7	O2A-CGA-O1A	-2.16	118.13	123.59
23	A	404	8CT	C01-C02-C07	2.16	117.77	113.62
21	1	413	CL7	C1B-CHB-C4A	-2.16	125.83	130.12
23	a	404	8CT	C01-C02-C07	2.16	117.77	113.62
21	4	409	CL7	CMD-C2D-C1D	2.16	131.79	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	8	409	CL7	CMD-C2D-C1D	2.16	131.79	128.46
21	3	509	CL7	C3B-C4B-NB	2.16	112.00	109.21
21	D	404	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
21	d	404	CL7	O2A-CGA-O1A	-2.16	118.14	123.59
21	6	518	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
32	4	403	ZEX	C1-C6-C7	2.16	121.89	115.78
32	8	403	ZEX	C1-C6-C7	2.16	121.89	115.78
21	B	609	CL7	C4D-C3D-CAD	-2.16	104.31	107.81
21	b	610	CL7	C4D-C3D-CAD	-2.16	104.31	107.81
23	c	515	8CT	C15-C16-C17	-2.16	115.63	118.94
23	c	519	8CT	C39-C16-C15	2.16	121.48	118.08
21	6	503	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
21	7	514	CL7	C4D-C3D-CAD	-2.16	104.32	107.81
21	2	505	CL7	CAC-C3C-C2C	2.16	131.22	127.53
21	B	622	CL7	C3B-C4B-NB	2.16	112.00	109.21
21	2	503	CL7	C1C-C2C-C3C	-2.16	103.79	106.94
21	7	502	CL7	C4C-C3C-C2C	-2.16	104.32	107.13
32	4	419	ZEX	C21-C26-C27	2.16	121.88	115.78
32	8	403	ZEX	C20-C13-C12	2.16	121.47	118.08
23	4	402	8CT	C40-C12-C11	2.15	121.47	118.08
23	8	402	8CT	C40-C12-C11	2.15	121.47	118.08
21	5	420	CL7	C1C-C2C-C3C	-2.15	103.80	106.94
21	1	417	CL7	C4-C3-C5	2.15	118.89	115.27
21	7	502	CL7	C4D-C3D-CAD	-2.15	104.33	107.81
21	3	515	CL7	CMA-C3A-C2A	-2.15	111.07	116.10
21	7	502	CL7	C1C-C2C-C3C	-2.15	103.80	106.94
32	8	403	ZEX	C20-C13-C14	-2.15	119.91	122.92
21	5	416	CL7	CMD-C2D-C1D	2.15	131.77	128.46
21	7	515	CL7	CMA-C3A-C2A	-2.15	111.08	116.10
32	3	525	ZEX	C23-C24-C25	-2.15	106.27	109.33
21	b	608	CL7	C1C-C2C-C3C	-2.15	103.80	106.94
21	c	506	CL7	C1C-C2C-C3C	-2.15	103.81	106.94
23	4	402	8CT	C22-C21-C23	2.15	121.46	118.08
32	1	422	ZEX	C27-C26-C25	-2.15	119.37	122.84
21	3	507	CL7	CAC-C3C-C2C	2.15	131.20	127.53
31	F	101	HEM	CBD-CAD-C3D	-2.15	106.67	112.63
31	f	101	HEM	CBD-CAD-C3D	-2.15	106.67	112.63
21	b	614	CL7	C3B-C4B-NB	2.15	111.98	109.21
21	5	413	CL7	C1B-CHB-C4A	-2.15	125.87	130.12
21	1	420	CL7	C1C-C2C-C3C	-2.15	103.81	106.94
21	4	407	CL7	CAC-C3C-C2C	2.15	131.20	127.53
32	8	419	ZEX	C21-C26-C27	2.14	121.84	115.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	501	CL7	C4-C3-C5	2.14	118.88	115.27
21	A	401	CL7	C3B-C4B-NB	2.14	111.98	109.21
21	a	401	CL7	C3B-C4B-NB	2.14	111.98	109.21
32	4	403	ZEX	C20-C13-C12	2.14	121.45	118.08
21	B	601	CL7	C4C-C3C-C2C	-2.14	104.33	107.13
21	b	602	CL7	C4C-C3C-C2C	-2.14	104.33	107.13
21	B	616	CL7	C4D-C3D-CAD	-2.14	104.34	107.81
21	3	502	CL7	C4D-C3D-CAD	-2.14	104.34	107.81
21	b	617	CL7	C4D-C3D-CAD	-2.14	104.34	107.81
21	C	503	CL7	OBD-CAD-CBD	-2.14	122.83	125.89
21	c	503	CL7	OBD-CAD-CBD	-2.14	122.83	125.89
21	1	402	CL7	CAA-C2A-C3A	-2.14	106.91	112.78
21	B	607	CL7	C3B-C4B-NB	2.14	111.98	109.21
21	b	608	CL7	C3B-C4B-NB	2.14	111.98	109.21
32	4	419	ZEX	C10-C11-C12	-2.14	116.54	123.22
32	8	419	ZEX	C10-C11-C12	-2.14	116.54	123.22
21	b	609	CL7	OBD-CAD-CBD	-2.14	122.84	125.89
21	6	515	CL7	CAA-CBA-CGA	-2.14	106.83	112.51
21	7	514	CL7	O2D-CGD-O1D	-2.14	119.66	123.84
23	8	402	8CT	C22-C21-C23	2.14	121.45	118.08
21	7	509	CL7	C3B-C4B-NB	2.14	111.97	109.21
21	6	511	CL7	C4C-C3C-C2C	-2.14	104.34	107.13
21	6	505	CL7	CAC-C3C-C2C	2.14	131.19	127.53
21	2	518	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	b	615	CL7	CBA-CAA-C2A	2.14	120.17	113.86
21	4	414	CL7	C4D-C3D-CAD	-2.14	104.35	107.81
21	C	502	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	c	502	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	3	502	CL7	C1C-C2C-C3C	-2.14	103.82	106.94
21	6	507	CL7	OBD-CAD-CBD	-2.13	122.85	125.89
32	7	519	ZEX	C21-C26-C27	2.13	121.81	115.78
21	2	501	CL7	C4-C3-C5	2.13	118.86	115.27
21	3	512	CL7	CED-O2D-CGD	-2.13	111.11	115.94
21	1	408	CL7	OBD-CAD-CBD	-2.13	122.85	125.89
32	8	418	ZEX	C31-C32-C33	-2.13	120.42	126.42
21	1	402	CL7	C4D-C3D-CAD	-2.13	104.36	107.81
21	b	609	CL7	CAA-CBA-CGA	-2.13	107.02	113.25
21	5	409	CL7	OBD-CAD-CBD	-2.13	122.85	125.89
21	3	512	CL7	C4-C3-C5	2.13	118.86	115.27
21	5	402	CL7	CAA-C2A-C3A	-2.13	106.94	112.78
23	C	519	8CT	C39-C16-C15	2.13	121.43	118.08
21	B	614	CL7	CBA-CAA-C2A	2.13	120.15	113.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	4	403	ZEX	C20-C13-C14	-2.13	119.94	122.92
21	b	623	CL7	C3B-C4B-NB	2.13	111.96	109.21
21	2	507	CL7	OBD-CAD-CBD	-2.13	122.85	125.89
21	2	515	CL7	CAA-CBA-CGA	-2.13	106.86	112.51
21	8	406	CL7	C4-C3-C5	2.13	118.85	115.27
21	c	502	CL7	CAC-C3C-C2C	2.13	131.17	127.53
21	4	406	CL7	C4-C3-C5	2.13	118.85	115.27
21	8	412	CL7	C1C-C2C-C3C	-2.13	103.83	106.94
21	B	616	CL7	CMB-C2B-C3B	2.13	128.66	124.68
21	1	411	CL7	CAA-CBA-CGA	-2.13	106.87	112.51
21	5	411	CL7	CAA-CBA-CGA	-2.13	106.87	112.51
24	2	524	SQD	O8-S-C6	-2.13	102.35	105.74
21	7	512	CL7	C4-C3-C5	2.13	118.85	115.27
21	b	615	CL7	C1C-C2C-C3C	-2.13	103.84	106.94
23	C	515	8CT	C05-C04-C03	2.12	113.75	110.48
32	3	519	ZEX	C21-C26-C27	2.12	121.79	115.78
23	8	402	8CT	C39-C16-C15	2.12	121.42	118.08
21	B	608	CL7	OBD-CAD-CBD	-2.12	122.86	125.89
21	2	511	CL7	CAC-C3C-C2C	2.12	131.16	127.53
21	c	504	CL7	C4-C3-C5	2.12	118.84	115.27
21	d	404	CL7	C4C-C3C-C2C	-2.12	104.36	107.13
21	2	517	CL7	C4D-C3D-CAD	-2.12	104.37	107.81
21	6	517	CL7	C4D-C3D-CAD	-2.12	104.37	107.81
32	4	418	ZEX	C31-C32-C33	-2.12	120.45	126.42
32	3	519	ZEX	C20-C13-C14	-2.12	119.95	122.92
32	7	519	ZEX	C20-C13-C14	-2.12	119.95	122.92
21	3	513	CL7	OBD-CAD-CBD	-2.12	122.86	125.89
21	8	414	CL7	C4D-C3D-CAD	-2.12	104.38	107.81
21	B	608	CL7	CAA-CBA-CGA	-2.12	107.06	113.25
21	3	514	CL7	O2D-CGD-O1D	-2.12	119.69	123.84
21	7	512	CL7	CED-O2D-CGD	-2.12	111.14	115.94
21	1	409	CL7	CHC-C1C-NC	-2.12	122.51	124.45
21	5	409	CL7	CHC-C1C-NC	-2.12	122.51	124.45
21	5	408	CL7	OBD-CAD-CBD	-2.12	122.87	125.89
23	C	516	8CT	C11-C12-C13	2.12	122.19	118.94
23	c	516	8CT	C11-C12-C13	2.12	122.19	118.94
23	C	519	8CT	C22-C21-C20	-2.12	119.96	122.92
23	c	519	8CT	C22-C21-C20	-2.12	119.96	122.92
24	6	523	SQD	O8-S-C6	-2.12	102.36	105.74
23	4	402	8CT	C39-C16-C15	2.12	121.41	118.08
21	3	510	CL7	CAC-C3C-C2C	2.12	131.15	127.53
21	B	602	CL7	OBD-CAD-CBD	-2.12	122.87	125.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	6	512	CL7	C1B-CHB-C4A	-2.12	125.92	130.12
21	b	617	CL7	CMB-C2B-C3B	2.12	128.64	124.68
21	1	404	CL7	C4D-C3D-CAD	-2.12	104.39	107.81
21	5	404	CL7	C4D-C3D-CAD	-2.12	104.39	107.81
22	D	408	PHO	O2A-CGA-O1A	-2.11	118.26	123.59
21	5	418	CL7	CAA-CBA-CGA	-2.11	107.08	113.25
21	B	603	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
21	b	604	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
21	D	404	CL7	C4C-C3C-C2C	-2.11	104.37	107.13
32	2	520	ZEX	C20-C13-C12	2.11	121.40	118.08
32	3	525	ZEX	C20-C13-C12	2.11	121.40	118.08
22	d	408	PHO	O2A-CGA-O1A	-2.11	118.26	123.59
21	d	404	CL7	CHC-C1C-NC	-2.11	122.51	124.45
21	5	413	CL7	C4D-C3D-CAD	-2.11	104.39	107.81
21	C	502	CL7	CAC-C3C-C2C	2.11	131.14	127.53
21	3	509	CL7	C4D-C3D-CAD	-2.11	104.39	107.81
21	7	509	CL7	C4D-C3D-CAD	-2.11	104.39	107.81
21	4	411	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
21	8	411	CL7	C1C-C2C-C3C	-2.11	103.86	106.94
21	1	418	CL7	CAA-CBA-CGA	-2.11	107.09	113.25
21	7	516	CL7	CBC-CAC-C3C	-2.11	106.61	112.43
21	b	610	CL7	C3B-C4B-NB	2.11	111.94	109.21
32	2	520	ZEX	C18-C5-C4	2.11	118.26	114.36
32	3	525	ZEX	C18-C5-C4	2.11	118.26	114.36
21	B	603	CL7	OBD-CAD-CBD	-2.11	122.88	125.89
21	b	604	CL7	OBD-CAD-CBD	-2.11	122.88	125.89
21	2	512	CL7	C1B-CHB-C4A	-2.11	125.94	130.12
21	1	413	CL7	C4D-C3D-CAD	-2.11	104.40	107.81
21	B	603	CL7	C4-C3-C5	2.11	118.81	115.27
21	1	409	CL7	OBD-CAD-CBD	-2.11	122.89	125.89
21	7	510	CL7	CAC-C3C-C2C	2.11	131.13	127.53
21	C	509	CL7	C4C-C3C-C2C	-2.11	104.38	107.13
21	c	509	CL7	C4C-C3C-C2C	-2.11	104.38	107.13
21	b	603	CL7	OBD-CAD-CBD	-2.11	122.89	125.89
21	1	418	CL7	CED-O2D-CGD	-2.11	111.17	115.94
21	5	418	CL7	CED-O2D-CGD	-2.11	111.17	115.94
23	c	515	8CT	C05-C04-C03	2.10	113.72	110.48
21	C	504	CL7	C4-C3-C5	2.10	118.81	115.27
21	1	417	CL7	C4D-C3D-CAD	-2.10	104.40	107.81
21	5	417	CL7	C4D-C3D-CAD	-2.10	104.40	107.81
21	C	511	CL7	C2A-C1A-CHA	-2.10	122.16	126.36
23	d	406	8CT	C27-C26-C28	2.10	121.39	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	c	511	CL7	C2A-C1A-CHA	-2.10	122.16	126.36
21	D	404	CL7	CHC-C1C-NC	-2.10	122.52	124.45
21	B	604	CL7	O2D-CGD-O1D	-2.10	119.73	123.84
21	B	609	CL7	C3B-C4B-NB	2.10	111.93	109.21
21	b	604	CL7	C4-C3-C5	2.10	118.80	115.27
21	6	517	CL7	C3B-C4B-NB	2.10	111.92	109.21
21	2	516	CL7	OBD-CAD-CBD	-2.10	122.89	125.89
21	6	516	CL7	OBD-CAD-CBD	-2.10	122.89	125.89
21	6	511	CL7	CAC-C3C-C2C	2.10	131.12	127.53
21	1	408	CL7	C1-O2A-CGA	-2.10	110.94	116.44
21	3	507	CL7	C3D-CAD-CBD	2.10	110.37	107.61
32	3	522	ZEX	C8-C9-C10	2.10	122.16	118.94
32	7	522	ZEX	C8-C9-C10	2.10	122.16	118.94
21	7	513	CL7	OBD-CAD-CBD	-2.10	122.90	125.89
21	4	404	CL7	C4D-C3D-CAD	-2.10	104.42	107.81
21	5	407	CL7	OBD-CAD-CBD	-2.10	122.90	125.89
21	3	505	CL7	CED-O2D-CGD	-2.10	111.20	115.94
21	7	505	CL7	CED-O2D-CGD	-2.10	111.20	115.94
21	4	407	CL7	C1C-C2C-C3C	-2.10	103.88	106.94
21	B	607	CL7	CED-O2D-CGD	-2.10	111.20	115.94
21	C	510	CL7	OBD-CAD-CBD	-2.10	122.90	125.89
21	c	510	CL7	OBD-CAD-CBD	-2.10	122.90	125.89
32	4	420	ZEX	C18-C5-C4	2.10	118.24	114.36
32	8	420	ZEX	C18-C5-C4	2.10	118.24	114.36
32	4	403	ZEX	C7-C6-C5	-2.10	116.39	121.46
32	8	403	ZEX	C7-C6-C5	-2.10	116.39	121.46
21	2	513	CL7	C1C-C2C-C3C	-2.09	103.88	106.94
21	6	513	CL7	C1C-C2C-C3C	-2.09	103.88	106.94
21	1	407	CL7	OBD-CAD-CBD	-2.09	122.90	125.89
32	1	421	ZEX	C15-C35-C34	-2.09	119.18	123.47
32	5	421	ZEX	C15-C35-C34	-2.09	119.18	123.47
21	4	405	CL7	C4C-C3C-C2C	-2.09	104.40	107.13
21	3	516	CL7	CBC-CAC-C3C	-2.09	106.66	112.43
21	3	514	CL7	CAC-C3C-C4C	-2.09	121.38	124.68
21	7	514	CL7	CAC-C3C-C4C	-2.09	121.38	124.68
21	b	605	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	c	509	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	8	404	CL7	C4D-C3D-CAD	-2.09	104.43	107.81
32	1	421	ZEX	C37-C21-C26	-2.09	106.91	110.30
32	5	421	ZEX	C37-C21-C26	-2.09	106.91	110.30
21	B	615	CL7	C4D-C3D-CAD	-2.09	104.43	107.81
21	b	616	CL7	C4D-C3D-CAD	-2.09	104.43	107.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	502	CL7	CMD-C2D-C1D	2.09	131.68	128.46
21	6	502	CL7	CMD-C2D-C1D	2.09	131.68	128.46
21	2	505	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
32	4	403	ZEX	C40-C33-C34	-2.09	120.00	122.92
32	4	420	ZEX	C38-C24-C23	-2.09	108.97	112.20
21	2	513	CL7	O2D-CGD-O1D	-2.09	119.75	123.84
21	B	616	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	b	617	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	7	512	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
32	8	403	ZEX	C40-C33-C34	-2.09	120.00	122.92
32	2	523	ZEX	C4-C5-C6	-2.09	116.20	120.85
32	6	522	ZEX	C4-C5-C6	-2.09	116.20	120.85
21	4	412	CL7	C4-C3-C5	2.09	118.78	115.27
21	8	412	CL7	C4-C3-C5	2.09	118.78	115.27
21	B	610	CL7	C3B-C4B-NB	2.09	111.91	109.21
21	b	611	CL7	C3B-C4B-NB	2.09	111.91	109.21
21	B	610	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	b	611	CL7	C1C-C2C-C3C	-2.09	103.89	106.94
21	1	410	CL7	CAA-CBA-CGA	-2.09	107.16	113.25
21	B	605	CL7	C4D-C3D-CAD	-2.09	104.43	107.81
21	b	606	CL7	C4D-C3D-CAD	-2.09	104.43	107.81
21	c	507	CL7	C1-C2-C3	2.08	129.65	126.04
23	D	406	8CT	C27-C26-C28	2.08	121.36	118.08
21	b	608	CL7	CED-O2D-CGD	-2.08	111.22	115.94
21	5	408	CL7	C1-O2A-CGA	-2.08	110.98	116.44
21	C	506	CL7	C1-O2A-CGA	-2.08	110.98	116.44
21	3	505	CL7	OBD-CAD-CBD	-2.08	122.92	125.89
21	7	505	CL7	OBD-CAD-CBD	-2.08	122.92	125.89
21	B	614	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	2	511	CL7	C4D-C3D-CAD	-2.08	104.44	107.81
21	6	511	CL7	C4D-C3D-CAD	-2.08	104.44	107.81
32	8	418	ZEX	C1-C2-C3	-2.08	108.94	113.64
21	A	401	CL7	CAC-C3C-C2C	2.08	131.09	127.53
21	a	401	CL7	CAC-C3C-C2C	2.08	131.09	127.53
21	7	508	CL7	C4C-C3C-C2C	-2.08	104.41	107.13
24	5	423	SQD	O8-S-C6	-2.08	102.42	105.74
21	5	416	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	8	405	CL7	C4C-C3C-C2C	-2.08	104.42	107.13
21	3	512	CL7	O2D-CGD-O1D	-2.08	119.77	123.84
21	7	512	CL7	O2D-CGD-O1D	-2.08	119.77	123.84
21	5	411	CL7	C1C-C2C-C3C	-2.08	103.90	106.94
21	1	404	CL7	CAA-CBA-CGA	-2.08	107.18	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	5	404	CL7	CAA-CBA-CGA	-2.08	107.18	113.25
32	8	420	ZEX	C38-C24-C23	-2.08	108.99	112.20
21	4	408	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	8	408	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	1	420	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	5	410	CL7	CAA-CBA-CGA	-2.08	107.18	113.25
21	C	509	CL7	CAC-C3C-C2C	2.08	131.08	127.53
21	c	509	CL7	CAC-C3C-C2C	2.08	131.08	127.53
32	4	418	ZEX	C19-C9-C10	-2.08	120.01	122.92
21	3	516	CL7	CBA-CAA-C2A	-2.08	107.73	113.86
21	d	405	CL7	CED-O2D-CGD	-2.08	111.24	115.94
23	B	618	8CT	C18-C19-C20	2.08	127.73	123.47
21	6	513	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	2	510	CL7	OBD-CAD-CBD	-2.08	122.93	125.89
21	3	503	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
21	7	503	CL7	C1C-C2C-C3C	-2.08	103.91	106.94
32	5	422	ZEX	C1-C2-C3	-2.08	108.95	113.64
21	2	518	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	6	518	CL7	O2D-CGD-O1D	-2.08	119.78	123.84
21	7	516	CL7	CBA-CAA-C2A	-2.08	107.74	113.86
21	1	406	CL7	CMD-C2D-C1D	2.07	131.65	128.46
21	5	406	CL7	CMD-C2D-C1D	2.07	131.65	128.46
21	7	507	CL7	C3D-CAD-CBD	2.07	110.33	107.61
21	8	407	CL7	C1C-C2C-C3C	-2.07	103.91	106.94
21	c	506	CL7	C1-O2A-CGA	-2.07	111.00	116.44
21	C	509	CL7	O2D-CGD-O1D	-2.07	119.78	123.84
21	2	510	CL7	CMD-C2D-C1D	2.07	131.65	128.46
21	6	510	CL7	CMD-C2D-C1D	2.07	131.65	128.46
21	2	515	CL7	C4D-C3D-CAD	-2.07	104.46	107.81
21	6	515	CL7	C4D-C3D-CAD	-2.07	104.46	107.81
21	6	517	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	b	605	CL7	OBD-CAD-CBD	-2.07	122.94	125.89
21	b	615	CL7	C4-C3-C5	2.07	118.75	115.27
32	4	418	ZEX	C1-C2-C3	-2.07	108.97	113.64
21	1	415	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	8	406	CL7	CED-O2D-CGD	-2.07	111.25	115.94
32	8	418	ZEX	C19-C9-C10	-2.07	120.02	122.92
21	2	502	CL7	C4D-C3D-CAD	-2.07	104.46	107.81
21	6	502	CL7	C4D-C3D-CAD	-2.07	104.46	107.81
32	1	421	ZEX	C1-C2-C3	-2.07	108.97	113.64
32	5	421	ZEX	C1-C2-C3	-2.07	108.97	113.64
21	1	411	CL7	C1C-C2C-C3C	-2.07	103.92	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	4	417	CL7	CMD-C2D-C1D	2.07	131.64	128.46
21	8	417	CL7	CMD-C2D-C1D	2.07	131.64	128.46
21	6	510	CL7	OBD-CAD-CBD	-2.07	122.94	125.89
21	6	514	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
21	5	415	CL7	C1C-C2C-C3C	-2.07	103.92	106.94
32	1	422	ZEX	C1-C2-C3	-2.07	108.97	113.64
24	2	522	SQD	O8-S-C6	-2.07	102.45	105.74
24	6	521	SQD	O8-S-C6	-2.07	102.45	105.74
32	4	420	ZEX	C40-C33-C32	2.07	121.33	118.08
32	8	420	ZEX	C40-C33-C32	2.07	121.33	118.08
21	4	415	CL7	O1D-CGD-CBD	-2.07	120.26	124.48
32	2	525	ZEX	C21-C26-C27	2.07	121.62	115.78
32	6	524	ZEX	C21-C26-C27	2.07	121.62	115.78
21	5	420	CL7	O2D-CGD-O1D	-2.07	119.80	123.84
21	1	412	CL7	C4C-C3C-C2C	-2.07	104.43	107.13
21	5	412	CL7	C4C-C3C-C2C	-2.07	104.43	107.13
21	2	517	CL7	C3B-C4B-NB	2.07	111.88	109.21
21	3	512	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
32	4	420	ZEX	C39-C29-C28	2.06	121.33	118.08
32	8	420	ZEX	C39-C29-C28	2.06	121.33	118.08
21	1	412	CL7	CMD-C2D-C1D	2.06	131.63	128.46
21	5	412	CL7	CMD-C2D-C1D	2.06	131.63	128.46
21	C	506	CL7	C9-C8-C7	-2.06	103.82	111.29
21	2	517	CL7	C1C-C2C-C3C	-2.06	103.93	106.94
21	b	617	CL7	C3B-C4B-NB	2.06	111.88	109.21
23	b	619	8CT	C18-C19-C20	2.06	127.69	123.47
21	2	515	CL7	OBD-CAD-CBD	-2.06	122.95	125.89
21	6	515	CL7	OBD-CAD-CBD	-2.06	122.95	125.89
21	6	505	CL7	O2D-CGD-O1D	-2.06	119.81	123.84
21	D	405	CL7	CED-O2D-CGD	-2.06	111.28	115.94
23	4	402	8CT	C08-C04-C03	-2.06	106.96	110.30
21	C	509	CL7	CED-O2D-CGD	-2.06	111.28	115.94
21	d	404	CL7	C4-C3-C5	2.06	118.73	115.27
24	1	423	SQD	O8-S-C6	-2.06	102.46	105.74
21	1	416	CL7	C1C-C2C-C3C	-2.06	103.94	106.94
21	3	512	CL7	C4D-C3D-CAD	-2.06	104.48	107.81
21	7	501	CL7	C2A-C1A-CHA	-2.06	122.25	126.36
23	C	519	8CT	C35-C30-C31	2.06	115.10	111.42
21	3	508	CL7	C4C-C3C-C2C	-2.06	104.45	107.13
23	c	515	8CT	C11-C12-C13	-2.05	115.79	118.94
21	2	501	CL7	C4C-C3C-C2C	-2.05	104.45	107.13
21	6	501	CL7	C4C-C3C-C2C	-2.05	104.45	107.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	619	8CT	C11-C10-C03	-2.05	121.44	127.20
22	D	408	PHO	C1B-NB-C4B	-2.05	102.88	107.09
21	2	514	CL7	C1C-C2C-C3C	-2.05	103.94	106.94
21	7	516	CL7	CED-O2D-CGD	-2.05	111.29	115.94
21	C	507	CL7	C1-C2-C3	2.05	129.59	126.04
21	c	506	CL7	C9-C8-C7	-2.05	103.86	111.29
21	B	613	CL7	C4D-C3D-CAD	-2.05	104.49	107.81
21	7	512	CL7	C4D-C3D-CAD	-2.05	104.49	107.81
21	B	604	CL7	OBD-CAD-CBD	-2.05	122.97	125.89
21	5	408	CL7	O2A-CGA-O1A	-2.05	118.42	123.59
22	d	408	PHO	C1B-NB-C4B	-2.05	102.88	107.09
21	4	409	CL7	CBC-CAC-C3C	-2.05	106.78	112.43
21	8	409	CL7	CBC-CAC-C3C	-2.05	106.78	112.43
21	3	516	CL7	CED-O2D-CGD	-2.05	111.30	115.94
21	b	614	CL7	C1C-C2C-C3C	-2.05	103.95	106.94
21	8	415	CL7	O1D-CGD-CBD	-2.05	120.29	124.48
21	3	501	CL7	C2A-C1A-CHA	-2.05	122.27	126.36
21	4	406	CL7	CED-O2D-CGD	-2.05	111.31	115.94
32	4	419	ZEX	C20-C13-C14	-2.05	120.06	122.92
32	8	419	ZEX	C20-C13-C14	-2.05	120.06	122.92
32	4	419	ZEX	C1-C2-C3	-2.05	109.02	113.64
21	3	508	CL7	CMD-C2D-C1D	2.04	131.61	128.46
23	8	402	8CT	C08-C04-C03	-2.04	106.98	110.30
21	2	518	CL7	C4-C3-C5	2.04	118.71	115.27
21	8	405	CL7	OBD-CAD-CBD	-2.04	122.98	125.89
21	1	408	CL7	O2A-CGA-O1A	-2.04	118.44	123.59
21	b	614	CL7	C4D-C3D-CAD	-2.04	104.50	107.81
23	C	515	8CT	C24-C25-C26	-2.04	124.40	127.31
23	c	515	8CT	C24-C25-C26	-2.04	124.40	127.31
21	C	502	CL7	CMD-C2D-C1D	2.04	131.60	128.46
21	c	502	CL7	CMD-C2D-C1D	2.04	131.60	128.46
21	2	516	CL7	CAC-C3C-C2C	2.04	131.02	127.53
21	6	516	CL7	CAC-C3C-C2C	2.04	131.02	127.53
32	2	521	ZEX	C11-C12-C13	-2.04	120.69	126.42
32	6	520	ZEX	C11-C12-C13	-2.04	120.69	126.42
23	c	519	8CT	C35-C30-C31	2.04	115.07	111.42
21	B	613	CL7	C1C-C2C-C3C	-2.04	103.97	106.94
21	6	503	CL7	OBD-CAD-CBD	-2.04	122.98	125.89
21	7	510	CL7	O2A-CGA-CBA	2.04	118.30	111.91
21	B	614	CL7	C4-C3-C5	2.04	118.70	115.27
21	D	404	CL7	C4-C3-C5	2.04	118.70	115.27
21	6	516	CL7	O2A-C1-C2	-2.04	103.28	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	7	509	CL7	C1C-C2C-C3C	-2.04	103.97	106.94
21	4	412	CL7	O2D-CGD-O1D	-2.04	119.86	123.84
21	c	509	CL7	CED-O2D-CGD	-2.03	111.34	115.94
21	2	508	CL7	C4D-C3D-CAD	-2.03	104.52	107.81
23	K	101	8CT	C05-C04-C03	2.03	113.61	110.48
21	7	508	CL7	CMD-C2D-C1D	2.03	131.59	128.46
23	C	515	8CT	C11-C12-C13	-2.03	115.82	118.94
23	k	101	8CT	C05-C04-C03	2.03	113.61	110.48
23	B	618	8CT	C11-C10-C03	-2.03	121.50	127.20
21	B	616	CL7	C3B-C4B-NB	2.03	111.84	109.21
21	2	503	CL7	OBD-CAD-CBD	-2.03	122.99	125.89
32	8	419	ZEX	C1-C2-C3	-2.03	109.06	113.64
21	1	413	CL7	O2D-CGD-O1D	-2.03	119.87	123.84
21	3	502	CL7	C1-C2-C3	2.03	129.55	126.04
21	7	502	CL7	C1-C2-C3	2.03	129.55	126.04
21	7	503	CL7	CAC-C3C-C2C	2.03	131.00	127.53
21	2	516	CL7	O2A-C1-C2	-2.03	103.31	108.64
21	3	518	CL7	OBD-CAD-CBD	-2.03	123.00	125.89
21	c	518	CL7	OBD-CAD-CBD	-2.03	123.00	125.89
21	7	518	CL7	OBD-CAD-CBD	-2.03	123.00	125.89
21	3	507	CL7	O2D-CGD-O1D	-2.03	119.87	123.84
21	7	507	CL7	O2D-CGD-O1D	-2.03	119.87	123.84
21	C	518	CL7	OBD-CAD-CBD	-2.03	123.00	125.89
21	3	510	CL7	O2A-CGA-CBA	2.03	118.27	111.91
21	B	612	CL7	OBD-CAD-CBD	-2.03	123.00	125.89
21	C	511	CL7	OBD-CAD-CBD	-2.03	123.00	125.89
21	b	613	CL7	OBD-CAD-CBD	-2.03	123.00	125.89
21	c	511	CL7	OBD-CAD-CBD	-2.03	123.00	125.89
32	2	519	ZEX	C18-C5-C4	2.03	118.11	114.36
32	6	519	ZEX	C18-C5-C4	2.03	118.11	114.36
21	6	508	CL7	C4D-C3D-CAD	-2.03	104.53	107.81
21	6	518	CL7	C4-C3-C5	2.03	118.68	115.27
21	1	405	CL7	C4C-C3C-C2C	-2.03	104.49	107.13
32	2	520	ZEX	C21-C26-C27	2.02	121.51	115.78
32	3	525	ZEX	C21-C26-C27	2.02	121.51	115.78
21	4	414	CL7	CMD-C2D-C1D	2.02	131.57	128.46
21	1	420	CL7	CAA-CBA-CGA	-2.02	107.14	112.51
32	1	422	ZEX	C10-C11-C12	-2.02	116.91	123.22
21	b	605	CL7	CED-O2D-CGD	-2.02	111.36	115.94
32	2	521	ZEX	C10-C11-C12	-2.02	116.91	123.22
21	2	509	CL7	C4D-C3D-CAD	-2.02	104.54	107.81
21	B	613	CL7	CMB-C2B-C3B	2.02	128.46	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	614	CL7	CMB-C2B-C3B	2.02	128.46	124.68
32	6	520	ZEX	C10-C11-C12	-2.02	116.91	123.22
21	2	505	CL7	C4-C3-C2	-2.02	118.50	123.68
21	8	412	CL7	O2D-CGD-O1D	-2.02	119.89	123.84
32	8	419	ZEX	C19-C9-C8	2.02	121.26	118.08
21	3	504	CL7	CBA-CAA-C2A	2.02	119.82	113.86
21	7	504	CL7	CBA-CAA-C2A	2.02	119.82	113.86
21	2	512	CL7	C4D-C3D-CAD	-2.02	104.54	107.81
21	6	512	CL7	C4D-C3D-CAD	-2.02	104.54	107.81
32	1	422	ZEX	C1-C6-C7	2.02	121.49	115.78
32	5	422	ZEX	C1-C6-C7	2.02	121.49	115.78
21	5	413	CL7	O2D-CGD-O1D	-2.02	119.89	123.84
21	2	518	CL7	CAC-C3C-C2C	2.02	130.98	127.53
21	3	503	CL7	CAC-C3C-C2C	2.02	130.98	127.53
21	5	405	CL7	C4C-C3C-C2C	-2.02	104.50	107.13
23	C	519	8CT	C35-C30-C29	-2.02	110.15	112.70
23	c	519	8CT	C35-C30-C29	-2.02	110.15	112.70
21	C	508	CL7	CMD-C2D-C1D	2.02	131.56	128.46
21	c	508	CL7	CMD-C2D-C1D	2.02	131.56	128.46
32	3	519	ZEX	C31-C32-C33	-2.02	120.75	126.42
27	B	624	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
21	8	415	CL7	C1C-C2C-C3C	-2.02	104.00	106.94
32	5	422	ZEX	C10-C11-C12	-2.02	116.93	123.22
21	C	508	CL7	C4-C3-C5	2.02	118.66	115.27
21	c	508	CL7	C4-C3-C5	2.02	118.66	115.27
32	4	419	ZEX	C19-C9-C8	2.02	121.25	118.08
21	5	420	CL7	CAA-CBA-CGA	-2.01	107.16	112.51
21	4	405	CL7	OBD-CAD-CBD	-2.01	123.02	125.89
21	C	504	CL7	C4D-C3D-CAD	-2.01	104.55	107.81
21	c	504	CL7	C4D-C3D-CAD	-2.01	104.55	107.81
21	c	512	CL7	OBD-CAD-CBD	-2.01	123.02	125.89
21	5	407	CL7	CAC-C3C-C2C	2.01	130.97	127.53
32	8	420	ZEX	C37-C21-C26	-2.01	107.03	110.30
21	B	602	CL7	O2D-CGD-O1D	-2.01	119.90	123.84
21	6	509	CL7	C4D-C3D-CAD	-2.01	104.55	107.81
21	8	409	CL7	C1C-C2C-C3C	-2.01	104.00	106.94
32	4	420	ZEX	C37-C21-C26	-2.01	107.04	110.30
32	2	523	ZEX	C10-C11-C12	-2.01	116.94	123.22
32	6	522	ZEX	C10-C11-C12	-2.01	116.94	123.22
21	b	603	CL7	O2D-CGD-O1D	-2.01	119.91	123.84
21	B	604	CL7	CED-O2D-CGD	-2.01	111.39	115.94
32	4	420	ZEX	C1-C2-C3	-2.01	109.11	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	8	420	ZEX	C1-C2-C3	-2.01	109.11	113.64
21	3	509	CL7	C1C-C2C-C3C	-2.01	104.01	106.94
21	B	604	CL7	C4D-C3D-CAD	-2.01	104.56	107.81
21	b	605	CL7	C4D-C3D-CAD	-2.01	104.56	107.81
21	6	505	CL7	C4-C3-C2	-2.01	118.53	123.68
32	7	519	ZEX	C31-C32-C33	-2.01	120.78	126.42
21	5	414	CL7	CGD-CBD-CAD	2.01	117.23	110.73
21	2	502	CL7	CAC-C3C-C2C	2.01	130.96	127.53
32	2	523	ZEX	C28-C29-C30	-2.01	115.86	118.94
32	6	522	ZEX	C28-C29-C30	-2.01	115.86	118.94
32	1	421	ZEX	C40-C33-C34	-2.00	120.11	122.92
32	5	421	ZEX	C40-C33-C34	-2.00	120.11	122.92
27	b	625	DGD	O1G-C1A-O1A	-2.00	118.54	123.59
21	4	409	CL7	C1C-C2C-C3C	-2.00	104.02	106.94
21	B	611	CL7	C4C-C3C-C2C	-2.00	104.52	107.13
21	1	418	CL7	C3D-CAD-CBD	2.00	110.24	107.61
21	5	418	CL7	C3D-CAD-CBD	2.00	110.24	107.61
21	8	414	CL7	CMD-C2D-C1D	2.00	131.54	128.46
21	1	414	CL7	CGD-CBD-CAD	2.00	117.22	110.73

All (424) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	401	CL7	NA
21	A	401	CL7	NC
21	A	403	CL7	NA
21	A	403	CL7	NC
21	A	406	CL7	NA
21	A	406	CL7	NC
21	B	601	CL7	NA
21	B	601	CL7	NC
21	B	602	CL7	NA
21	B	602	CL7	NC
21	B	603	CL7	NA
21	B	603	CL7	NC
21	B	604	CL7	NA
21	B	604	CL7	NC
21	B	605	CL7	NA
21	B	605	CL7	NC
21	B	606	CL7	NA
21	B	606	CL7	NC
21	B	607	CL7	NA

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Mol	Chain	Res	Type	Atom
21	B	607	CL7	NC
21	B	608	CL7	NA
21	B	608	CL7	NC
21	B	609	CL7	NA
21	B	609	CL7	NC
21	B	610	CL7	NA
21	B	610	CL7	NC
21	B	611	CL7	NA
21	B	611	CL7	NC
21	B	612	CL7	NA
21	B	612	CL7	NC
21	B	613	CL7	NA
21	B	613	CL7	NC
21	B	614	CL7	NA
21	B	614	CL7	NC
21	B	615	CL7	NA
21	B	615	CL7	NC
21	B	616	CL7	NA
21	B	616	CL7	NC
21	B	622	CL7	NA
21	B	622	CL7	NC
21	C	502	CL7	NA
21	C	502	CL7	NC
21	C	503	CL7	NA
21	C	503	CL7	NC
21	C	504	CL7	NA
21	C	504	CL7	NC
21	C	505	CL7	NA
21	C	505	CL7	NC
21	C	506	CL7	NA
21	C	506	CL7	NC
21	C	507	CL7	NA
21	C	507	CL7	NC
21	C	508	CL7	NA
21	C	508	CL7	NC
21	C	509	CL7	NA
21	C	509	CL7	NC
21	C	510	CL7	NA
21	C	510	CL7	NC
21	C	511	CL7	NA
21	C	511	CL7	NC
21	C	512	CL7	NA

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Mol	Chain	Res	Type	Atom
21	C	512	CL7	NC
21	C	513	CL7	NA
21	C	513	CL7	NC
21	C	514	CL7	NA
21	C	514	CL7	NC
21	C	518	CL7	NA
21	C	518	CL7	NC
21	D	402	CL7	NA
21	D	402	CL7	NC
21	D	404	CL7	NA
21	D	404	CL7	NC
21	D	405	CL7	NA
21	D	405	CL7	NC
21	2	501	CL7	NA
21	2	501	CL7	NC
21	2	502	CL7	NA
21	2	502	CL7	NC
21	2	503	CL7	NA
21	2	503	CL7	NC
21	2	504	CL7	NA
21	2	504	CL7	NC
21	2	505	CL7	NA
21	2	505	CL7	NC
21	2	506	CL7	NA
21	2	506	CL7	NC
21	2	507	CL7	NA
21	2	507	CL7	NC
21	2	508	CL7	NA
21	2	508	CL7	NC
21	2	509	CL7	NA
21	2	509	CL7	NC
21	2	510	CL7	NA
21	2	510	CL7	NC
21	2	511	CL7	NA
21	2	511	CL7	NC
21	2	512	CL7	NA
21	2	512	CL7	NC
21	2	513	CL7	NA
21	2	513	CL7	NC
21	2	514	CL7	NA
21	2	514	CL7	NC
21	2	515	CL7	NA

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Mol	Chain	Res	Type	Atom
21	2	515	CL7	NC
21	2	516	CL7	NA
21	2	516	CL7	NC
21	2	517	CL7	NA
21	2	517	CL7	NC
21	2	518	CL7	NA
21	2	518	CL7	NC
21	1	402	CL7	NA
21	1	402	CL7	NC
21	1	403	CL7	NA
21	1	403	CL7	NC
21	1	404	CL7	NA
21	1	404	CL7	NC
21	1	405	CL7	NA
21	1	405	CL7	NC
21	1	406	CL7	NA
21	1	406	CL7	NC
21	1	407	CL7	NA
21	1	407	CL7	NC
21	1	408	CL7	NA
21	1	408	CL7	NC
21	1	409	CL7	NA
21	1	409	CL7	NC
21	1	410	CL7	NA
21	1	410	CL7	NC
21	1	411	CL7	NA
21	1	411	CL7	NC
21	1	412	CL7	NA
21	1	412	CL7	NC
21	1	413	CL7	NA
21	1	413	CL7	NC
21	1	414	CL7	NA
21	1	414	CL7	NC
21	1	415	CL7	NA
21	1	415	CL7	NC
21	1	416	CL7	NA
21	1	416	CL7	NC
21	1	417	CL7	NA
21	1	417	CL7	NC
21	1	418	CL7	NA
21	1	418	CL7	NC
21	1	419	CL7	NA

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Mol	Chain	Res	Type	Atom
21	1	419	CL7	NC
21	1	420	CL7	NA
21	1	420	CL7	NC
21	3	501	CL7	NA
21	3	501	CL7	NC
21	3	502	CL7	NA
21	3	502	CL7	NC
21	3	503	CL7	NA
21	3	503	CL7	NC
21	3	504	CL7	NA
21	3	504	CL7	NC
21	3	505	CL7	NA
21	3	505	CL7	NC
21	3	506	CL7	NA
21	3	506	CL7	NC
21	3	507	CL7	NA
21	3	507	CL7	NC
21	3	508	CL7	NA
21	3	508	CL7	NC
21	3	509	CL7	NA
21	3	509	CL7	NC
21	3	510	CL7	NA
21	3	510	CL7	NC
21	3	511	CL7	NA
21	3	511	CL7	NC
21	3	512	CL7	NA
21	3	512	CL7	NC
21	3	513	CL7	NA
21	3	513	CL7	NC
21	3	514	CL7	NA
21	3	514	CL7	NC
21	3	515	CL7	NA
21	3	515	CL7	NC
21	3	516	CL7	NA
21	3	516	CL7	NC
21	3	517	CL7	NA
21	3	517	CL7	NC
21	3	518	CL7	NA
21	3	518	CL7	NC
21	4	404	CL7	NA
21	4	404	CL7	NC
21	4	405	CL7	NA

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Mol	Chain	Res	Type	Atom
21	4	405	CL7	NC
21	4	406	CL7	NA
21	4	406	CL7	NC
21	4	407	CL7	NA
21	4	407	CL7	NC
21	4	408	CL7	NA
21	4	408	CL7	NC
21	4	409	CL7	NA
21	4	409	CL7	NC
21	4	410	CL7	NA
21	4	410	CL7	NC
21	4	411	CL7	NA
21	4	411	CL7	NC
21	4	412	CL7	NA
21	4	412	CL7	NC
21	4	413	CL7	NA
21	4	413	CL7	NC
21	4	414	CL7	NA
21	4	414	CL7	NC
21	4	415	CL7	NA
21	4	415	CL7	NC
21	4	416	CL7	NA
21	4	416	CL7	NC
21	4	417	CL7	NA
21	4	417	CL7	NC
21	a	401	CL7	NA
21	a	401	CL7	NC
21	a	403	CL7	NA
21	a	403	CL7	NC
21	a	405	CL7	NA
21	a	405	CL7	NC
21	b	602	CL7	NA
21	b	602	CL7	NC
21	b	603	CL7	NA
21	b	603	CL7	NC
21	b	604	CL7	NA
21	b	604	CL7	NC
21	b	605	CL7	NA
21	b	605	CL7	NC
21	b	606	CL7	NA
21	b	606	CL7	NC
21	b	607	CL7	NA

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Mol	Chain	Res	Type	Atom
21	b	607	CL7	NC
21	b	608	CL7	NA
21	b	608	CL7	NC
21	b	609	CL7	NA
21	b	609	CL7	NC
21	b	610	CL7	NA
21	b	610	CL7	NC
21	b	611	CL7	NA
21	b	611	CL7	NC
21	b	612	CL7	NA
21	b	612	CL7	NC
21	b	613	CL7	NA
21	b	613	CL7	NC
21	b	614	CL7	NA
21	b	614	CL7	NC
21	b	615	CL7	NA
21	b	615	CL7	NC
21	b	616	CL7	NA
21	b	616	CL7	NC
21	b	617	CL7	NA
21	b	617	CL7	NC
21	b	623	CL7	NA
21	b	623	CL7	NC
21	c	502	CL7	NA
21	c	502	CL7	NC
21	c	503	CL7	NA
21	c	503	CL7	NC
21	c	504	CL7	NA
21	c	504	CL7	NC
21	c	505	CL7	NA
21	c	505	CL7	NC
21	c	506	CL7	NA
21	c	506	CL7	NC
21	c	507	CL7	NA
21	c	507	CL7	NC
21	c	508	CL7	NA
21	c	508	CL7	NC
21	c	509	CL7	NA
21	c	509	CL7	NC
21	c	510	CL7	NA
21	c	510	CL7	NC
21	c	511	CL7	NA

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Mol	Chain	Res	Type	Atom
21	c	511	CL7	NC
21	c	512	CL7	NA
21	c	512	CL7	NC
21	c	513	CL7	NA
21	c	513	CL7	NC
21	c	514	CL7	NA
21	c	514	CL7	NC
21	c	518	CL7	NA
21	c	518	CL7	NC
21	d	402	CL7	NA
21	d	402	CL7	NC
21	d	404	CL7	NA
21	d	404	CL7	NC
21	d	405	CL7	NA
21	d	405	CL7	NC
21	6	501	CL7	NA
21	6	501	CL7	NC
21	6	502	CL7	NA
21	6	502	CL7	NC
21	6	503	CL7	NA
21	6	503	CL7	NC
21	6	504	CL7	NA
21	6	504	CL7	NC
21	6	505	CL7	NA
21	6	505	CL7	NC
21	6	506	CL7	NA
21	6	506	CL7	NC
21	6	507	CL7	NA
21	6	507	CL7	NC
21	6	508	CL7	NA
21	6	508	CL7	NC
21	6	509	CL7	NA
21	6	509	CL7	NC
21	6	510	CL7	NA
21	6	510	CL7	NC
21	6	511	CL7	NA
21	6	511	CL7	NC
21	6	512	CL7	NA
21	6	512	CL7	NC
21	6	513	CL7	NA
21	6	513	CL7	NC
21	6	514	CL7	NA

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Mol	Chain	Res	Type	Atom
21	6	514	CL7	NC
21	6	515	CL7	NA
21	6	515	CL7	NC
21	6	516	CL7	NA
21	6	516	CL7	NC
21	6	517	CL7	NA
21	6	517	CL7	NC
21	6	518	CL7	NA
21	6	518	CL7	NC
21	5	402	CL7	NA
21	5	402	CL7	NC
21	5	403	CL7	NA
21	5	403	CL7	NC
21	5	404	CL7	NA
21	5	404	CL7	NC
21	5	405	CL7	NA
21	5	405	CL7	NC
21	5	406	CL7	NA
21	5	406	CL7	NC
21	5	407	CL7	NA
21	5	407	CL7	NC
21	5	408	CL7	NA
21	5	408	CL7	NC
21	5	409	CL7	NA
21	5	409	CL7	NC
21	5	410	CL7	NA
21	5	410	CL7	NC
21	5	411	CL7	NA
21	5	411	CL7	NC
21	5	412	CL7	NA
21	5	412	CL7	NC
21	5	413	CL7	NA
21	5	413	CL7	NC
21	5	414	CL7	NA
21	5	414	CL7	NC
21	5	415	CL7	NA
21	5	415	CL7	NC
21	5	416	CL7	NA
21	5	416	CL7	NC
21	5	417	CL7	NA
21	5	417	CL7	NC
21	5	418	CL7	NA

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Mol	Chain	Res	Type	Atom
21	5	418	CL7	NC
21	5	419	CL7	NA
21	5	419	CL7	NC
21	5	420	CL7	NA
21	5	420	CL7	NC
21	7	501	CL7	NA
21	7	501	CL7	NC
21	7	502	CL7	NA
21	7	502	CL7	NC
21	7	503	CL7	NA
21	7	503	CL7	NC
21	7	504	CL7	NA
21	7	504	CL7	NC
21	7	505	CL7	NA
21	7	505	CL7	NC
21	7	506	CL7	NA
21	7	506	CL7	NC
21	7	507	CL7	NA
21	7	507	CL7	NC
21	7	508	CL7	NA
21	7	508	CL7	NC
21	7	509	CL7	NA
21	7	509	CL7	NC
21	7	510	CL7	NA
21	7	510	CL7	NC
21	7	511	CL7	NA
21	7	511	CL7	NC
21	7	512	CL7	NA
21	7	512	CL7	NC
21	7	513	CL7	NA
21	7	513	CL7	NC
21	7	514	CL7	NA
21	7	514	CL7	NC
21	7	515	CL7	NA
21	7	515	CL7	NC
21	7	516	CL7	NA
21	7	516	CL7	NC
21	7	517	CL7	NA
21	7	517	CL7	NC
21	7	518	CL7	NA
21	7	518	CL7	NC
21	8	404	CL7	NA

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Mol	Chain	Res	Type	Atom
21	8	404	CL7	NC
21	8	405	CL7	NA
21	8	405	CL7	NC
21	8	406	CL7	NA
21	8	406	CL7	NC
21	8	407	CL7	NA
21	8	407	CL7	NC
21	8	408	CL7	NA
21	8	408	CL7	NC
21	8	409	CL7	NA
21	8	409	CL7	NC
21	8	410	CL7	NA
21	8	410	CL7	NC
21	8	411	CL7	NA
21	8	411	CL7	NC
21	8	412	CL7	NA
21	8	412	CL7	NC
21	8	413	CL7	NA
21	8	413	CL7	NC
21	8	414	CL7	NA
21	8	414	CL7	NC
21	8	415	CL7	NA
21	8	415	CL7	NC
21	8	416	CL7	NA
21	8	416	CL7	NC
21	8	417	CL7	NA
21	8	417	CL7	NC

All (2944) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	403	CL7	O1A-CGA-O2A-C1
21	A	403	CL7	CBA-CGA-O2A-C1
21	A	403	CL7	C1A-C2A-CAA-CBA
21	A	403	CL7	C3A-C2A-CAA-CBA
21	A	406	CL7	C1A-C2A-CAA-CBA
21	A	406	CL7	C3A-C2A-CAA-CBA
21	B	602	CL7	O1A-CGA-O2A-C1
21	B	602	CL7	CBA-CGA-O2A-C1
21	B	602	CL7	C2-C3-C5-C6
21	B	602	CL7	C4-C3-C5-C6
21	B	604	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	B	604	CL7	C3A-C2A-CAA-CBA
21	B	605	CL7	C1A-C2A-CAA-CBA
21	B	605	CL7	C3A-C2A-CAA-CBA
21	B	607	CL7	C1A-C2A-CAA-CBA
21	B	607	CL7	C3A-C2A-CAA-CBA
21	B	607	CL7	CBD-CGD-O2D-CED
21	B	608	CL7	C4-C3-C5-C6
21	B	608	CL7	C1A-C2A-CAA-CBA
21	B	608	CL7	C3A-C2A-CAA-CBA
21	B	609	CL7	C3A-C2A-CAA-CBA
21	B	610	CL7	O1A-CGA-O2A-C1
21	B	610	CL7	CBA-CGA-O2A-C1
21	B	612	CL7	C6-C7-C8-C10
21	B	612	CL7	C3A-C2A-CAA-CBA
21	B	614	CL7	C4-C3-C5-C6
21	B	614	CL7	CHA-CBD-CGD-O2D
21	B	614	CL7	CHA-CBD-CGD-O1D
21	B	614	CL7	CAD-CBD-CGD-O1D
21	B	615	CL7	O1A-CGA-O2A-C1
21	B	615	CL7	CBA-CGA-O2A-C1
21	B	615	CL7	C1A-C2A-CAA-CBA
21	B	615	CL7	C3A-C2A-CAA-CBA
21	B	622	CL7	CBD-CGD-O2D-CED
21	C	502	CL7	C1A-C2A-CAA-CBA
21	C	502	CL7	C3A-C2A-CAA-CBA
21	C	503	CL7	C2-C3-C5-C6
21	C	503	CL7	C4-C3-C5-C6
21	C	503	CL7	CBD-CGD-O2D-CED
21	C	504	CL7	C2-C3-C5-C6
21	C	504	CL7	C4-C3-C5-C6
21	C	504	CL7	C1A-C2A-CAA-CBA
21	C	505	CL7	C1A-C2A-CAA-CBA
21	C	506	CL7	C14-C13-C15-C16
21	C	507	CL7	O1A-CGA-O2A-C1
21	C	507	CL7	CBA-CGA-O2A-C1
21	C	507	CL7	C1A-C2A-CAA-CBA
21	C	507	CL7	C3A-C2A-CAA-CBA
21	C	507	CL7	CHA-CBD-CGD-O2D
21	C	507	CL7	CHA-CBD-CGD-O1D
21	C	508	CL7	C2-C3-C5-C6
21	C	508	CL7	C4-C3-C5-C6
21	C	509	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	C	509	CL7	CBA-CGA-O2A-C1
21	C	510	CL7	O2A-C1-C2-C3
21	C	510	CL7	C2-C3-C5-C6
21	C	510	CL7	C4-C3-C5-C6
21	C	510	CL7	C14-C13-C15-C16
21	C	510	CL7	C1A-C2A-CAA-CBA
21	C	511	CL7	C3A-C2A-CAA-CBA
21	C	512	CL7	C1A-C2A-CAA-CBA
21	C	513	CL7	CBD-CGD-O2D-CED
21	C	514	CL7	CHA-CBD-CGD-O2D
21	C	514	CL7	CHA-CBD-CGD-O1D
21	C	514	CL7	CBD-CGD-O2D-CED
21	D	402	CL7	CHA-CBD-CGD-O2D
21	D	402	CL7	CHA-CBD-CGD-O1D
21	D	404	CL7	C2-C3-C5-C6
21	D	404	CL7	C4-C3-C5-C6
21	D	405	CL7	C1A-C2A-CAA-CBA
21	D	405	CL7	C3A-C2A-CAA-CBA
21	D	405	CL7	CAD-CBD-CGD-O2D
21	D	405	CL7	CAD-CBD-CGD-O1D
21	2	502	CL7	C1A-C2A-CAA-CBA
21	2	502	CL7	C3A-C2A-CAA-CBA
21	2	503	CL7	C1A-C2A-CAA-CBA
21	2	504	CL7	C1A-C2A-CAA-CBA
21	2	504	CL7	CBD-CGD-O2D-CED
21	2	509	CL7	C11-C12-C13-C15
21	2	510	CL7	C2-C3-C5-C6
21	2	510	CL7	C4-C3-C5-C6
21	2	511	CL7	C2-C3-C5-C6
21	2	511	CL7	C4-C3-C5-C6
21	2	511	CL7	CBD-CGD-O2D-CED
21	2	513	CL7	C1A-C2A-CAA-CBA
21	2	513	CL7	CHA-CBD-CGD-O1D
21	2	514	CL7	C1A-C2A-CAA-CBA
21	2	514	CL7	C3A-C2A-CAA-CBA
21	2	514	CL7	CBD-CGD-O2D-CED
21	2	515	CL7	CHA-CBD-CGD-O2D
21	2	515	CL7	CHA-CBD-CGD-O1D
21	2	515	CL7	CAD-CBD-CGD-O1D
21	2	516	CL7	O1A-CGA-O2A-C1
21	2	516	CL7	CBA-CGA-O2A-C1
21	2	516	CL7	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	2	517	CL7	C1A-C2A-CAA-CBA
21	2	517	CL7	C3A-C2A-CAA-CBA
21	2	518	CL7	C1A-C2A-CAA-CBA
21	2	518	CL7	C3A-C2A-CAA-CBA
21	1	402	CL7	C1A-C2A-CAA-CBA
21	1	402	CL7	C3A-C2A-CAA-CBA
21	1	404	CL7	O2A-C1-C2-C3
21	1	404	CL7	C2-C3-C5-C6
21	1	404	CL7	C4-C3-C5-C6
21	1	408	CL7	C1A-C2A-CAA-CBA
21	1	408	CL7	C3A-C2A-CAA-CBA
21	1	409	CL7	CBD-CGD-O2D-CED
21	1	410	CL7	O1A-CGA-O2A-C1
21	1	410	CL7	CBA-CGA-O2A-C1
21	1	410	CL7	C1A-C2A-CAA-CBA
21	1	410	CL7	C3A-C2A-CAA-CBA
21	1	411	CL7	CBD-CGD-O2D-CED
21	1	412	CL7	C1A-C2A-CAA-CBA
21	1	413	CL7	CAD-CBD-CGD-O2D
21	1	413	CL7	CAD-CBD-CGD-O1D
21	1	415	CL7	CHA-CBD-CGD-O2D
21	1	415	CL7	CHA-CBD-CGD-O1D
21	1	416	CL7	CBD-CGD-O2D-CED
21	1	417	CL7	O1A-CGA-O2A-C1
21	1	417	CL7	CBA-CGA-O2A-C1
21	1	417	CL7	C3A-C2A-CAA-CBA
21	1	418	CL7	CHA-CBD-CGD-O2D
21	1	418	CL7	CHA-CBD-CGD-O1D
21	1	419	CL7	CBD-CGD-O2D-CED
21	3	501	CL7	C1A-C2A-CAA-CBA
21	3	502	CL7	CBD-CGD-O2D-CED
21	3	503	CL7	CBD-CGD-O2D-CED
21	3	504	CL7	C1A-C2A-CAA-CBA
21	3	506	CL7	C1A-C2A-CAA-CBA
21	3	506	CL7	C3A-C2A-CAA-CBA
21	3	506	CL7	CHA-CBD-CGD-O1D
21	3	506	CL7	CAD-CBD-CGD-O2D
21	3	506	CL7	CAD-CBD-CGD-O1D
21	3	507	CL7	C2-C3-C5-C6
21	3	507	CL7	C4-C3-C5-C6
21	3	508	CL7	C2-C3-C5-C6
21	3	508	CL7	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	3	509	CL7	O1A-CGA-O2A-C1
21	3	509	CL7	CBA-CGA-O2A-C1
21	3	510	CL7	C1A-C2A-CAA-CBA
21	3	510	CL7	CBD-CGD-O2D-CED
21	3	511	CL7	O1A-CGA-O2A-C1
21	3	511	CL7	CBA-CGA-O2A-C1
21	3	513	CL7	C1A-C2A-CAA-CBA
21	3	516	CL7	O1A-CGA-O2A-C1
21	3	516	CL7	CBA-CGA-O2A-C1
21	3	516	CL7	C3A-C2A-CAA-CBA
21	3	517	CL7	C1A-C2A-CAA-CBA
21	3	517	CL7	C3A-C2A-CAA-CBA
21	4	404	CL7	C3A-C2A-CAA-CBA
21	4	405	CL7	O1A-CGA-O2A-C1
21	4	405	CL7	CBA-CGA-O2A-C1
21	4	405	CL7	C2-C3-C5-C6
21	4	405	CL7	C4-C3-C5-C6
21	4	406	CL7	C1A-C2A-CAA-CBA
21	4	406	CL7	C3A-C2A-CAA-CBA
21	4	409	CL7	C1A-C2A-CAA-CBA
21	4	409	CL7	C3A-C2A-CAA-CBA
21	4	410	CL7	C1A-C2A-CAA-CBA
21	4	411	CL7	C1A-C2A-CAA-CBA
21	4	411	CL7	CBD-CGD-O2D-CED
21	4	412	CL7	C1A-C2A-CAA-CBA
21	4	415	CL7	C1A-C2A-CAA-CBA
21	4	415	CL7	C3A-C2A-CAA-CBA
21	4	415	CL7	CAD-CBD-CGD-O2D
21	4	416	CL7	CHA-CBD-CGD-O2D
21	4	416	CL7	CHA-CBD-CGD-O1D
21	4	417	CL7	C1A-C2A-CAA-CBA
21	a	403	CL7	O1A-CGA-O2A-C1
21	a	403	CL7	CBA-CGA-O2A-C1
21	a	403	CL7	C1A-C2A-CAA-CBA
21	a	403	CL7	C3A-C2A-CAA-CBA
21	a	405	CL7	C1A-C2A-CAA-CBA
21	a	405	CL7	C3A-C2A-CAA-CBA
21	b	603	CL7	O1A-CGA-O2A-C1
21	b	603	CL7	CBA-CGA-O2A-C1
21	b	603	CL7	C2-C3-C5-C6
21	b	603	CL7	C4-C3-C5-C6
21	b	605	CL7	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	b	605	CL7	C3A-C2A-CAA-CBA
21	b	606	CL7	C1A-C2A-CAA-CBA
21	b	606	CL7	C3A-C2A-CAA-CBA
21	b	608	CL7	C1A-C2A-CAA-CBA
21	b	608	CL7	C3A-C2A-CAA-CBA
21	b	608	CL7	CBD-CGD-O2D-CED
21	b	609	CL7	C4-C3-C5-C6
21	b	609	CL7	C1A-C2A-CAA-CBA
21	b	609	CL7	C3A-C2A-CAA-CBA
21	b	610	CL7	C3A-C2A-CAA-CBA
21	b	611	CL7	O1A-CGA-O2A-C1
21	b	611	CL7	CBA-CGA-O2A-C1
21	b	613	CL7	C6-C7-C8-C10
21	b	613	CL7	C3A-C2A-CAA-CBA
21	b	615	CL7	C4-C3-C5-C6
21	b	615	CL7	CHA-CBD-CGD-O2D
21	b	615	CL7	CHA-CBD-CGD-O1D
21	b	615	CL7	CAD-CBD-CGD-O1D
21	b	616	CL7	O1A-CGA-O2A-C1
21	b	616	CL7	CBA-CGA-O2A-C1
21	b	616	CL7	C1A-C2A-CAA-CBA
21	b	616	CL7	C3A-C2A-CAA-CBA
21	b	623	CL7	CBD-CGD-O2D-CED
21	c	502	CL7	C1A-C2A-CAA-CBA
21	c	502	CL7	C3A-C2A-CAA-CBA
21	c	503	CL7	C2-C3-C5-C6
21	c	503	CL7	C4-C3-C5-C6
21	c	503	CL7	CBD-CGD-O2D-CED
21	c	504	CL7	C2-C3-C5-C6
21	c	504	CL7	C4-C3-C5-C6
21	c	504	CL7	C1A-C2A-CAA-CBA
21	c	505	CL7	C1A-C2A-CAA-CBA
21	c	506	CL7	C14-C13-C15-C16
21	c	507	CL7	O1A-CGA-O2A-C1
21	c	507	CL7	CBA-CGA-O2A-C1
21	c	507	CL7	C1A-C2A-CAA-CBA
21	c	507	CL7	C3A-C2A-CAA-CBA
21	c	507	CL7	CHA-CBD-CGD-O2D
21	c	507	CL7	CHA-CBD-CGD-O1D
21	c	508	CL7	C2-C3-C5-C6
21	c	508	CL7	C4-C3-C5-C6
21	c	509	CL7	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
21	c	509	CL7	CBA-CGA-O2A-C1
21	c	510	CL7	O2A-C1-C2-C3
21	c	510	CL7	C2-C3-C5-C6
21	c	510	CL7	C4-C3-C5-C6
21	c	510	CL7	C14-C13-C15-C16
21	c	510	CL7	C1A-C2A-CAA-CBA
21	c	511	CL7	C3A-C2A-CAA-CBA
21	c	512	CL7	C1A-C2A-CAA-CBA
21	c	513	CL7	CBD-CGD-O2D-CED
21	c	514	CL7	CHA-CBD-CGD-O2D
21	c	514	CL7	CHA-CBD-CGD-O1D
21	c	514	CL7	CBD-CGD-O2D-CED
21	d	402	CL7	CHA-CBD-CGD-O2D
21	d	402	CL7	CHA-CBD-CGD-O1D
21	d	404	CL7	C2-C3-C5-C6
21	d	404	CL7	C4-C3-C5-C6
21	d	405	CL7	C1A-C2A-CAA-CBA
21	d	405	CL7	C3A-C2A-CAA-CBA
21	d	405	CL7	CAD-CBD-CGD-O2D
21	d	405	CL7	CAD-CBD-CGD-O1D
21	6	502	CL7	C1A-C2A-CAA-CBA
21	6	502	CL7	C3A-C2A-CAA-CBA
21	6	503	CL7	C1A-C2A-CAA-CBA
21	6	504	CL7	C1A-C2A-CAA-CBA
21	6	504	CL7	CBD-CGD-O2D-CED
21	6	509	CL7	C11-C12-C13-C15
21	6	510	CL7	C2-C3-C5-C6
21	6	510	CL7	C4-C3-C5-C6
21	6	511	CL7	C2-C3-C5-C6
21	6	511	CL7	C4-C3-C5-C6
21	6	511	CL7	CBD-CGD-O2D-CED
21	6	513	CL7	C1A-C2A-CAA-CBA
21	6	513	CL7	CHA-CBD-CGD-O1D
21	6	514	CL7	C1A-C2A-CAA-CBA
21	6	514	CL7	C3A-C2A-CAA-CBA
21	6	514	CL7	CBD-CGD-O2D-CED
21	6	515	CL7	CHA-CBD-CGD-O2D
21	6	515	CL7	CHA-CBD-CGD-O1D
21	6	515	CL7	CAD-CBD-CGD-O1D
21	6	516	CL7	O1A-CGA-O2A-C1
21	6	516	CL7	CBA-CGA-O2A-C1
21	6	516	CL7	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
21	6	517	CL7	C1A-C2A-CAA-CBA
21	6	517	CL7	C3A-C2A-CAA-CBA
21	6	518	CL7	C1A-C2A-CAA-CBA
21	6	518	CL7	C3A-C2A-CAA-CBA
21	5	402	CL7	C1A-C2A-CAA-CBA
21	5	402	CL7	C3A-C2A-CAA-CBA
21	5	404	CL7	O2A-C1-C2-C3
21	5	404	CL7	C2-C3-C5-C6
21	5	404	CL7	C4-C3-C5-C6
21	5	408	CL7	C1A-C2A-CAA-CBA
21	5	408	CL7	C3A-C2A-CAA-CBA
21	5	409	CL7	CBD-CGD-O2D-CED
21	5	410	CL7	O1A-CGA-O2A-C1
21	5	410	CL7	CBA-CGA-O2A-C1
21	5	410	CL7	C1A-C2A-CAA-CBA
21	5	410	CL7	C3A-C2A-CAA-CBA
21	5	411	CL7	CBD-CGD-O2D-CED
21	5	412	CL7	C1A-C2A-CAA-CBA
21	5	413	CL7	CAD-CBD-CGD-O2D
21	5	413	CL7	CAD-CBD-CGD-O1D
21	5	415	CL7	CHA-CBD-CGD-O2D
21	5	415	CL7	CHA-CBD-CGD-O1D
21	5	416	CL7	CBD-CGD-O2D-CED
21	5	417	CL7	O1A-CGA-O2A-C1
21	5	417	CL7	CBA-CGA-O2A-C1
21	5	417	CL7	C3A-C2A-CAA-CBA
21	5	418	CL7	CHA-CBD-CGD-O2D
21	5	418	CL7	CHA-CBD-CGD-O1D
21	5	419	CL7	CBD-CGD-O2D-CED
21	7	501	CL7	C1A-C2A-CAA-CBA
21	7	502	CL7	CBD-CGD-O2D-CED
21	7	503	CL7	CBD-CGD-O2D-CED
21	7	504	CL7	C1A-C2A-CAA-CBA
21	7	506	CL7	C1A-C2A-CAA-CBA
21	7	506	CL7	C3A-C2A-CAA-CBA
21	7	506	CL7	CHA-CBD-CGD-O1D
21	7	506	CL7	CAD-CBD-CGD-O2D
21	7	506	CL7	CAD-CBD-CGD-O1D
21	7	507	CL7	C2-C3-C5-C6
21	7	507	CL7	C4-C3-C5-C6
21	7	508	CL7	C2-C3-C5-C6
21	7	508	CL7	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	7	509	CL7	O1A-CGA-O2A-C1
21	7	509	CL7	CBA-CGA-O2A-C1
21	7	510	CL7	C1A-C2A-CAA-CBA
21	7	510	CL7	CBD-CGD-O2D-CED
21	7	511	CL7	O1A-CGA-O2A-C1
21	7	511	CL7	CBA-CGA-O2A-C1
21	7	513	CL7	C1A-C2A-CAA-CBA
21	7	516	CL7	O1A-CGA-O2A-C1
21	7	516	CL7	CBA-CGA-O2A-C1
21	7	516	CL7	C3A-C2A-CAA-CBA
21	7	517	CL7	C1A-C2A-CAA-CBA
21	7	517	CL7	C3A-C2A-CAA-CBA
21	8	404	CL7	C3A-C2A-CAA-CBA
21	8	405	CL7	O1A-CGA-O2A-C1
21	8	405	CL7	CBA-CGA-O2A-C1
21	8	405	CL7	C2-C3-C5-C6
21	8	405	CL7	C4-C3-C5-C6
21	8	406	CL7	C1A-C2A-CAA-CBA
21	8	406	CL7	C3A-C2A-CAA-CBA
21	8	409	CL7	C1A-C2A-CAA-CBA
21	8	409	CL7	C3A-C2A-CAA-CBA
21	8	410	CL7	C1A-C2A-CAA-CBA
21	8	411	CL7	C1A-C2A-CAA-CBA
21	8	411	CL7	CBD-CGD-O2D-CED
21	8	412	CL7	C1A-C2A-CAA-CBA
21	8	415	CL7	C1A-C2A-CAA-CBA
21	8	415	CL7	C3A-C2A-CAA-CBA
21	8	415	CL7	CAD-CBD-CGD-O2D
21	8	416	CL7	CHA-CBD-CGD-O2D
21	8	416	CL7	CHA-CBD-CGD-O1D
21	8	417	CL7	C1A-C2A-CAA-CBA
23	A	404	8CT	C25-C26-C28-C29
23	A	404	8CT	C27-C26-C28-C29
23	B	617	8CT	C14-C15-C16-C17
23	B	617	8CT	C14-C15-C16-C39
23	B	618	8CT	C25-C26-C28-C29
23	B	618	8CT	C27-C26-C28-C29
23	B	619	8CT	C10-C11-C12-C13
23	B	619	8CT	C10-C11-C12-C40
23	B	627	8CT	C14-C15-C16-C17
23	B	627	8CT	C14-C15-C16-C39
23	B	627	8CT	C28-C29-C30-C35

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Mol	Chain	Res	Type	Atoms
23	C	515	8CT	C02-C03-C10-C11
23	C	515	8CT	C10-C11-C12-C13
23	C	515	8CT	C10-C11-C12-C40
23	C	515	8CT	C16-C17-C18-C19
23	C	515	8CT	C27-C26-C28-C29
23	C	515	8CT	C28-C29-C30-C35
23	C	516	8CT	C02-C03-C10-C11
23	C	516	8CT	C10-C11-C12-C13
23	C	516	8CT	C10-C11-C12-C40
23	C	516	8CT	C14-C15-C16-C17
23	C	516	8CT	C14-C15-C16-C39
23	C	516	8CT	C27-C26-C28-C29
23	C	519	8CT	C25-C26-C28-C29
23	C	519	8CT	C27-C26-C28-C29
23	C	519	8CT	C28-C29-C30-C31
23	C	519	8CT	C28-C29-C30-C35
23	D	406	8CT	C10-C11-C12-C13
23	D	406	8CT	C10-C11-C12-C40
23	D	406	8CT	C16-C17-C18-C19
23	D	406	8CT	C25-C26-C28-C29
23	D	406	8CT	C27-C26-C28-C29
23	K	101	8CT	C20-C21-C23-C24
23	K	101	8CT	C22-C21-C23-C24
23	K	101	8CT	C25-C26-C28-C29
23	K	101	8CT	C27-C26-C28-C29
23	K	101	8CT	C28-C29-C30-C35
23	a	404	8CT	C25-C26-C28-C29
23	a	404	8CT	C27-C26-C28-C29
23	b	601	8CT	C14-C15-C16-C17
23	b	601	8CT	C14-C15-C16-C39
23	b	601	8CT	C28-C29-C30-C35
23	b	618	8CT	C14-C15-C16-C17
23	b	618	8CT	C14-C15-C16-C39
23	b	619	8CT	C25-C26-C28-C29
23	b	619	8CT	C27-C26-C28-C29
23	b	620	8CT	C10-C11-C12-C13
23	b	620	8CT	C10-C11-C12-C40
23	c	515	8CT	C02-C03-C10-C11
23	c	515	8CT	C10-C11-C12-C13
23	c	515	8CT	C10-C11-C12-C40
23	c	515	8CT	C16-C17-C18-C19
23	c	515	8CT	C27-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
23	c	515	8CT	C28-C29-C30-C35
23	c	516	8CT	C02-C03-C10-C11
23	c	516	8CT	C10-C11-C12-C13
23	c	516	8CT	C10-C11-C12-C40
23	c	516	8CT	C14-C15-C16-C17
23	c	516	8CT	C14-C15-C16-C39
23	c	516	8CT	C27-C26-C28-C29
23	c	519	8CT	C04-C03-C10-C11
23	c	519	8CT	C25-C26-C28-C29
23	c	519	8CT	C27-C26-C28-C29
23	c	519	8CT	C28-C29-C30-C31
23	c	519	8CT	C28-C29-C30-C35
23	d	406	8CT	C10-C11-C12-C13
23	d	406	8CT	C10-C11-C12-C40
23	d	406	8CT	C16-C17-C18-C19
23	d	406	8CT	C25-C26-C28-C29
23	d	406	8CT	C27-C26-C28-C29
23	k	101	8CT	C20-C21-C23-C24
23	k	101	8CT	C22-C21-C23-C24
23	k	101	8CT	C25-C26-C28-C29
23	k	101	8CT	C27-C26-C28-C29
23	k	101	8CT	C28-C29-C30-C35
24	2	522	SQD	O49-C7-O47-C45
24	2	522	SQD	C8-C7-O47-C45
24	2	522	SQD	O5-C5-C6-S
24	3	521	SQD	O49-C7-O47-C45
24	3	521	SQD	C8-C7-O47-C45
24	3	523	SQD	O5-C5-C6-S
24	6	521	SQD	O49-C7-O47-C45
24	6	521	SQD	C8-C7-O47-C45
24	6	521	SQD	O5-C5-C6-S
24	7	521	SQD	O49-C7-O47-C45
24	7	521	SQD	C8-C7-O47-C45
24	7	523	SQD	O5-C5-C6-S
25	A	407	LHG	C2-C3-O3-P
25	D	409	LHG	C3-O3-P-O6
25	D	409	LHG	C4-O6-P-O3
25	4	401	LHG	C2-C3-O3-P
25	4	401	LHG	C4-O6-P-O3
25	a	406	LHG	C2-C3-O3-P
25	d	409	LHG	C3-O3-P-O6
25	d	409	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
25	8	401	LHG	C2-C3-O3-P
25	8	401	LHG	C4-O6-P-O3
26	B	621	LMG	C29-C28-O8-C9
26	C	501	LMG	O6-C1-O1-C7
26	b	622	LMG	C29-C28-O8-C9
26	c	501	LMG	O6-C1-O1-C7
30	D	407	PL9	C39-C41-C42-C43
30	d	407	PL9	C39-C41-C42-C43
31	F	101	HEM	C2B-C3B-CAB-CBB
31	f	101	HEM	C2B-C3B-CAB-CBB
32	2	519	ZEX	C1-C6-C7-C8
32	2	519	ZEX	C25-C26-C27-C28
32	2	519	ZEX	C7-C8-C9-C19
32	2	519	ZEX	C7-C8-C9-C10
32	2	519	ZEX	C11-C12-C13-C20
32	2	519	ZEX	C11-C12-C13-C14
32	2	519	ZEX	C27-C28-C29-C30
32	2	519	ZEX	C27-C28-C29-C39
32	2	520	ZEX	C31-C32-C33-C34
32	2	520	ZEX	C31-C32-C33-C40
32	2	520	ZEX	C27-C28-C29-C30
32	2	520	ZEX	C27-C28-C29-C39
32	2	521	ZEX	C25-C26-C27-C28
32	2	523	ZEX	C25-C26-C27-C28
32	2	523	ZEX	C31-C32-C33-C40
32	2	523	ZEX	C27-C28-C29-C30
32	2	523	ZEX	C27-C28-C29-C39
32	2	525	ZEX	C25-C26-C27-C28
32	2	525	ZEX	C31-C32-C33-C34
32	2	525	ZEX	C31-C32-C33-C40
32	2	525	ZEX	C27-C28-C29-C30
32	1	421	ZEX	C25-C26-C27-C28
32	1	421	ZEX	C7-C8-C9-C19
32	1	421	ZEX	C7-C8-C9-C10
32	1	421	ZEX	C11-C12-C13-C20
32	1	421	ZEX	C11-C12-C13-C14
32	1	421	ZEX	C31-C32-C33-C34
32	1	421	ZEX	C31-C32-C33-C40
32	1	421	ZEX	C27-C28-C29-C30
32	1	421	ZEX	C27-C28-C29-C39
32	1	422	ZEX	C25-C26-C27-C28
32	1	422	ZEX	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
32	3	519	ZEX	C25-C26-C27-C28
32	3	519	ZEX	C31-C32-C33-C34
32	3	519	ZEX	C31-C32-C33-C40
32	3	520	ZEX	C25-C26-C27-C28
32	3	522	ZEX	C1-C6-C7-C8
32	3	522	ZEX	C25-C26-C27-C28
32	3	525	ZEX	C31-C32-C33-C34
32	3	525	ZEX	C31-C32-C33-C40
32	3	525	ZEX	C27-C28-C29-C30
32	3	525	ZEX	C27-C28-C29-C39
32	4	403	ZEX	C5-C6-C7-C8
32	4	403	ZEX	C7-C8-C9-C19
32	4	403	ZEX	C7-C8-C9-C10
32	4	418	ZEX	C7-C8-C9-C19
32	4	418	ZEX	C7-C8-C9-C10
32	4	419	ZEX	C13-C14-C15-C35
32	4	419	ZEX	C27-C28-C29-C30
32	4	419	ZEX	C27-C28-C29-C39
32	4	420	ZEX	C27-C28-C29-C30
32	4	420	ZEX	C27-C28-C29-C39
32	6	519	ZEX	C1-C6-C7-C8
32	6	519	ZEX	C25-C26-C27-C28
32	6	519	ZEX	C7-C8-C9-C19
32	6	519	ZEX	C7-C8-C9-C10
32	6	519	ZEX	C11-C12-C13-C20
32	6	519	ZEX	C11-C12-C13-C14
32	6	519	ZEX	C27-C28-C29-C30
32	6	519	ZEX	C27-C28-C29-C39
32	6	520	ZEX	C25-C26-C27-C28
32	6	522	ZEX	C25-C26-C27-C28
32	6	522	ZEX	C31-C32-C33-C40
32	6	522	ZEX	C27-C28-C29-C30
32	6	522	ZEX	C27-C28-C29-C39
32	6	524	ZEX	C25-C26-C27-C28
32	6	524	ZEX	C31-C32-C33-C34
32	6	524	ZEX	C31-C32-C33-C40
32	6	524	ZEX	C27-C28-C29-C30
32	5	421	ZEX	C25-C26-C27-C28
32	5	421	ZEX	C7-C8-C9-C19
32	5	421	ZEX	C7-C8-C9-C10
32	5	421	ZEX	C11-C12-C13-C20
32	5	421	ZEX	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
32	5	421	ZEX	C31-C32-C33-C34
32	5	421	ZEX	C31-C32-C33-C40
32	5	421	ZEX	C27-C28-C29-C30
32	5	421	ZEX	C27-C28-C29-C39
32	5	422	ZEX	C25-C26-C27-C28
32	5	422	ZEX	C9-C10-C11-C12
32	7	519	ZEX	C25-C26-C27-C28
32	7	519	ZEX	C31-C32-C33-C34
32	7	519	ZEX	C31-C32-C33-C40
32	7	520	ZEX	C25-C26-C27-C28
32	7	522	ZEX	C1-C6-C7-C8
32	7	522	ZEX	C25-C26-C27-C28
32	8	403	ZEX	C5-C6-C7-C8
32	8	403	ZEX	C7-C8-C9-C19
32	8	403	ZEX	C7-C8-C9-C10
32	8	418	ZEX	C7-C8-C9-C19
32	8	418	ZEX	C7-C8-C9-C10
32	8	419	ZEX	C13-C14-C15-C35
32	8	419	ZEX	C27-C28-C29-C30
32	8	419	ZEX	C27-C28-C29-C39
32	8	420	ZEX	C27-C28-C29-C30
32	8	420	ZEX	C27-C28-C29-C39
21	A	401	CL7	O1D-CGD-O2D-CED
21	B	601	CL7	O1D-CGD-O2D-CED
21	B	607	CL7	O1D-CGD-O2D-CED
21	2	502	CL7	O1D-CGD-O2D-CED
21	2	514	CL7	O1D-CGD-O2D-CED
21	3	503	CL7	O1D-CGD-O2D-CED
21	a	401	CL7	O1D-CGD-O2D-CED
21	b	602	CL7	O1D-CGD-O2D-CED
21	b	608	CL7	O1D-CGD-O2D-CED
21	6	502	CL7	O1D-CGD-O2D-CED
21	6	514	CL7	O1D-CGD-O2D-CED
21	7	503	CL7	O1D-CGD-O2D-CED
21	A	403	CL7	C4C-C3C-CAC-CBC
21	a	403	CL7	C4C-C3C-CAC-CBC
21	C	503	CL7	O1D-CGD-O2D-CED
21	2	511	CL7	O1D-CGD-O2D-CED
21	1	409	CL7	O1D-CGD-O2D-CED
21	1	416	CL7	O1D-CGD-O2D-CED
21	1	419	CL7	O1D-CGD-O2D-CED
21	3	502	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	4	417	CL7	O1D-CGD-O2D-CED
21	c	503	CL7	O1D-CGD-O2D-CED
21	6	511	CL7	O1D-CGD-O2D-CED
21	5	409	CL7	O1D-CGD-O2D-CED
21	5	416	CL7	O1D-CGD-O2D-CED
21	5	419	CL7	O1D-CGD-O2D-CED
21	7	502	CL7	O1D-CGD-O2D-CED
21	8	417	CL7	O1D-CGD-O2D-CED
21	A	401	CL7	CBD-CGD-O2D-CED
21	A	403	CL7	CBD-CGD-O2D-CED
21	B	601	CL7	CBD-CGD-O2D-CED
21	B	605	CL7	CBD-CGD-O2D-CED
21	C	518	CL7	CBD-CGD-O2D-CED
21	2	502	CL7	CBD-CGD-O2D-CED
21	1	405	CL7	CBD-CGD-O2D-CED
21	1	407	CL7	CBD-CGD-O2D-CED
21	1	420	CL7	CBD-CGD-O2D-CED
21	3	506	CL7	CBD-CGD-O2D-CED
21	4	417	CL7	CBD-CGD-O2D-CED
21	a	401	CL7	CBD-CGD-O2D-CED
21	a	403	CL7	CBD-CGD-O2D-CED
21	b	602	CL7	CBD-CGD-O2D-CED
21	b	606	CL7	CBD-CGD-O2D-CED
21	c	518	CL7	CBD-CGD-O2D-CED
21	6	502	CL7	CBD-CGD-O2D-CED
21	5	405	CL7	CBD-CGD-O2D-CED
21	5	407	CL7	CBD-CGD-O2D-CED
21	5	420	CL7	CBD-CGD-O2D-CED
21	7	506	CL7	CBD-CGD-O2D-CED
21	8	417	CL7	CBD-CGD-O2D-CED
26	B	621	LMG	O10-C28-O8-C9
26	b	622	LMG	O10-C28-O8-C9
21	C	514	CL7	O1D-CGD-O2D-CED
21	1	407	CL7	O1D-CGD-O2D-CED
21	3	510	CL7	O1D-CGD-O2D-CED
21	c	514	CL7	O1D-CGD-O2D-CED
21	5	407	CL7	O1D-CGD-O2D-CED
21	7	510	CL7	O1D-CGD-O2D-CED
21	1	414	CL7	C4C-C3C-CAC-CBC
21	4	415	CL7	C4C-C3C-CAC-CBC
21	4	416	CL7	C4C-C3C-CAC-CBC
21	5	414	CL7	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
21	8	415	CL7	C4C-C3C-CAC-CBC
21	8	416	CL7	C4C-C3C-CAC-CBC
21	B	622	CL7	O1D-CGD-O2D-CED
21	4	411	CL7	O1D-CGD-O2D-CED
21	b	623	CL7	O1D-CGD-O2D-CED
21	8	411	CL7	O1D-CGD-O2D-CED
21	C	504	CL7	CBD-CGD-O2D-CED
21	C	510	CL7	CBD-CGD-O2D-CED
21	C	512	CL7	CBD-CGD-O2D-CED
21	2	510	CL7	CBD-CGD-O2D-CED
21	2	517	CL7	CBD-CGD-O2D-CED
21	1	403	CL7	CBD-CGD-O2D-CED
21	1	410	CL7	CBD-CGD-O2D-CED
21	1	412	CL7	CBD-CGD-O2D-CED
21	1	418	CL7	CBD-CGD-O2D-CED
21	3	508	CL7	CBD-CGD-O2D-CED
21	3	509	CL7	CBD-CGD-O2D-CED
21	3	516	CL7	CBD-CGD-O2D-CED
21	3	518	CL7	CBD-CGD-O2D-CED
21	4	409	CL7	CBD-CGD-O2D-CED
21	4	410	CL7	CBD-CGD-O2D-CED
21	c	504	CL7	CBD-CGD-O2D-CED
21	c	510	CL7	CBD-CGD-O2D-CED
21	c	512	CL7	CBD-CGD-O2D-CED
21	6	510	CL7	CBD-CGD-O2D-CED
21	6	517	CL7	CBD-CGD-O2D-CED
21	5	403	CL7	CBD-CGD-O2D-CED
21	5	410	CL7	CBD-CGD-O2D-CED
21	5	412	CL7	CBD-CGD-O2D-CED
21	5	418	CL7	CBD-CGD-O2D-CED
21	7	508	CL7	CBD-CGD-O2D-CED
21	7	509	CL7	CBD-CGD-O2D-CED
21	7	516	CL7	CBD-CGD-O2D-CED
21	7	518	CL7	CBD-CGD-O2D-CED
21	8	409	CL7	CBD-CGD-O2D-CED
21	8	410	CL7	CBD-CGD-O2D-CED
21	C	513	CL7	O1D-CGD-O2D-CED
21	2	504	CL7	O1D-CGD-O2D-CED
21	c	513	CL7	O1D-CGD-O2D-CED
21	6	504	CL7	O1D-CGD-O2D-CED
21	1	411	CL7	O1D-CGD-O2D-CED
21	5	411	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	B	611	CL7	CBD-CGD-O2D-CED
21	C	505	CL7	CBD-CGD-O2D-CED
21	2	509	CL7	CBD-CGD-O2D-CED
21	b	612	CL7	CBD-CGD-O2D-CED
21	c	505	CL7	CBD-CGD-O2D-CED
21	6	509	CL7	CBD-CGD-O2D-CED
21	1	404	CL7	C10-C11-C12-C13
21	5	404	CL7	C10-C11-C12-C13
21	B	602	CL7	C3-C5-C6-C7
21	B	605	CL7	C3-C5-C6-C7
21	B	609	CL7	C3-C5-C6-C7
21	B	613	CL7	C3-C5-C6-C7
21	B	614	CL7	C3-C5-C6-C7
21	C	502	CL7	C3-C5-C6-C7
21	C	508	CL7	C3-C5-C6-C7
21	C	509	CL7	C3-C5-C6-C7
21	C	510	CL7	C3-C5-C6-C7
21	2	506	CL7	C3-C5-C6-C7
21	2	507	CL7	C3-C5-C6-C7
21	2	516	CL7	C3-C5-C6-C7
21	1	408	CL7	C3-C5-C6-C7
21	3	501	CL7	C3-C5-C6-C7
21	3	504	CL7	C3-C5-C6-C7
21	3	505	CL7	C3-C5-C6-C7
21	3	508	CL7	C3-C5-C6-C7
21	4	404	CL7	C3-C5-C6-C7
21	4	405	CL7	C3-C5-C6-C7
21	4	413	CL7	C3-C5-C6-C7
21	b	603	CL7	C3-C5-C6-C7
21	b	606	CL7	C3-C5-C6-C7
21	b	610	CL7	C3-C5-C6-C7
21	b	614	CL7	C3-C5-C6-C7
21	b	615	CL7	C3-C5-C6-C7
21	c	502	CL7	C3-C5-C6-C7
21	c	508	CL7	C3-C5-C6-C7
21	c	509	CL7	C3-C5-C6-C7
21	c	510	CL7	C3-C5-C6-C7
21	6	506	CL7	C3-C5-C6-C7
21	6	507	CL7	C3-C5-C6-C7
21	6	516	CL7	C3-C5-C6-C7
21	5	408	CL7	C3-C5-C6-C7
21	7	501	CL7	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	7	504	CL7	C3-C5-C6-C7
21	7	505	CL7	C3-C5-C6-C7
21	7	508	CL7	C3-C5-C6-C7
21	8	404	CL7	C3-C5-C6-C7
21	8	405	CL7	C3-C5-C6-C7
21	8	413	CL7	C3-C5-C6-C7
21	C	518	CL7	O1D-CGD-O2D-CED
21	1	420	CL7	O1D-CGD-O2D-CED
21	c	518	CL7	O1D-CGD-O2D-CED
21	5	420	CL7	O1D-CGD-O2D-CED
21	D	402	CL7	C2C-C3C-CAC-CBC
21	2	514	CL7	C4C-C3C-CAC-CBC
21	d	402	CL7	C2C-C3C-CAC-CBC
21	6	514	CL7	C4C-C3C-CAC-CBC
21	B	606	CL7	C4-C3-C5-C6
21	C	502	CL7	C4-C3-C5-C6
21	1	410	CL7	C4-C3-C5-C6
21	3	512	CL7	C4-C3-C5-C6
21	4	412	CL7	C4-C3-C5-C6
21	b	607	CL7	C4-C3-C5-C6
21	c	502	CL7	C4-C3-C5-C6
21	5	410	CL7	C4-C3-C5-C6
21	7	512	CL7	C4-C3-C5-C6
21	8	412	CL7	C4-C3-C5-C6
21	B	606	CL7	C2-C3-C5-C6
21	C	502	CL7	C2-C3-C5-C6
21	4	412	CL7	C2-C3-C5-C6
21	b	607	CL7	C2-C3-C5-C6
21	c	502	CL7	C2-C3-C5-C6
21	8	412	CL7	C2-C3-C5-C6
21	2	506	CL7	CBD-CGD-O2D-CED
21	3	514	CL7	CBD-CGD-O2D-CED
21	6	506	CL7	CBD-CGD-O2D-CED
21	7	514	CL7	CBD-CGD-O2D-CED
21	B	604	CL7	C2A-CAA-CBA-CGA
21	B	607	CL7	C2A-CAA-CBA-CGA
21	B	610	CL7	C2A-CAA-CBA-CGA
21	C	514	CL7	C2A-CAA-CBA-CGA
21	2	502	CL7	C2A-CAA-CBA-CGA
21	1	409	CL7	C2A-CAA-CBA-CGA
21	3	516	CL7	C2A-CAA-CBA-CGA
21	3	518	CL7	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	4	409	CL7	C2A-CAA-CBA-CGA
21	b	605	CL7	C2A-CAA-CBA-CGA
21	b	608	CL7	C2A-CAA-CBA-CGA
21	b	611	CL7	C2A-CAA-CBA-CGA
21	c	514	CL7	C2A-CAA-CBA-CGA
21	6	502	CL7	C2A-CAA-CBA-CGA
21	5	409	CL7	C2A-CAA-CBA-CGA
21	7	516	CL7	C2A-CAA-CBA-CGA
21	7	518	CL7	C2A-CAA-CBA-CGA
21	8	409	CL7	C2A-CAA-CBA-CGA
21	C	505	CL7	C3-C5-C6-C7
21	C	506	CL7	C3-C5-C6-C7
21	2	512	CL7	C3-C5-C6-C7
21	4	406	CL7	C3-C5-C6-C7
21	c	505	CL7	C3-C5-C6-C7
21	c	506	CL7	C3-C5-C6-C7
21	6	512	CL7	C3-C5-C6-C7
21	8	406	CL7	C3-C5-C6-C7
21	B	605	CL7	O1D-CGD-O2D-CED
21	1	405	CL7	O1D-CGD-O2D-CED
21	3	506	CL7	O1D-CGD-O2D-CED
21	b	606	CL7	O1D-CGD-O2D-CED
21	5	405	CL7	O1D-CGD-O2D-CED
21	7	506	CL7	O1D-CGD-O2D-CED
23	C	515	8CT	C12-C13-C14-C15
23	c	515	8CT	C12-C13-C14-C15
32	2	519	ZEX	C29-C30-C31-C32
32	2	521	ZEX	C9-C10-C11-C12
32	4	418	ZEX	C9-C10-C11-C12
32	6	519	ZEX	C29-C30-C31-C32
32	6	520	ZEX	C9-C10-C11-C12
32	8	418	ZEX	C9-C10-C11-C12
21	A	406	CL7	CBD-CGD-O2D-CED
21	C	506	CL7	CBD-CGD-O2D-CED
21	D	402	CL7	CBD-CGD-O2D-CED
21	2	503	CL7	CBD-CGD-O2D-CED
21	a	405	CL7	CBD-CGD-O2D-CED
21	c	506	CL7	CBD-CGD-O2D-CED
21	d	402	CL7	CBD-CGD-O2D-CED
21	6	503	CL7	CBD-CGD-O2D-CED
25	B	625	LHG	O2-C2-C3-O3
25	b	626	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
21	A	401	CL7	C3-C5-C6-C7
21	C	504	CL7	C3-C5-C6-C7
21	1	406	CL7	C3-C5-C6-C7
21	1	417	CL7	C3-C5-C6-C7
21	1	418	CL7	C3-C5-C6-C7
21	a	401	CL7	C3-C5-C6-C7
21	c	504	CL7	C3-C5-C6-C7
21	5	406	CL7	C3-C5-C6-C7
21	5	417	CL7	C3-C5-C6-C7
21	5	418	CL7	C3-C5-C6-C7
26	c	501	LMG	C29-C28-O8-C9
21	C	511	CL7	C13-C15-C16-C17
21	C	511	CL7	CBD-CGD-O2D-CED
21	2	507	CL7	CBD-CGD-O2D-CED
21	4	412	CL7	CBD-CGD-O2D-CED
21	c	511	CL7	CBD-CGD-O2D-CED
21	6	507	CL7	CBD-CGD-O2D-CED
21	8	412	CL7	CBD-CGD-O2D-CED
21	3	514	CL7	C4C-C3C-CAC-CBC
21	7	514	CL7	C4C-C3C-CAC-CBC
21	3	509	CL7	C8-C10-C11-C12
21	c	511	CL7	C13-C15-C16-C17
21	7	509	CL7	C8-C10-C11-C12
21	A	403	CL7	O1D-CGD-O2D-CED
21	a	403	CL7	O1D-CGD-O2D-CED
21	C	503	CL7	C3-C5-C6-C7
21	c	503	CL7	C3-C5-C6-C7
26	C	501	LMG	C29-C28-O8-C9
21	A	401	CL7	C4-C3-C5-C6
21	B	603	CL7	C4-C3-C5-C6
21	C	509	CL7	C4-C3-C5-C6
21	2	505	CL7	C4-C3-C5-C6
21	2	516	CL7	C4-C3-C5-C6
21	2	517	CL7	C4-C3-C5-C6
21	1	403	CL7	C4-C3-C5-C6
21	3	504	CL7	C4-C3-C5-C6
21	3	510	CL7	C4-C3-C5-C6
21	3	511	CL7	C4-C3-C5-C6
21	4	406	CL7	C4-C3-C5-C6
21	a	401	CL7	C4-C3-C5-C6
21	b	604	CL7	C4-C3-C5-C6
21	c	509	CL7	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
21	6	505	CL7	C4-C3-C5-C6
21	6	516	CL7	C4-C3-C5-C6
21	6	517	CL7	C4-C3-C5-C6
21	5	403	CL7	C4-C3-C5-C6
21	7	504	CL7	C4-C3-C5-C6
21	7	510	CL7	C4-C3-C5-C6
21	7	511	CL7	C4-C3-C5-C6
21	8	406	CL7	C4-C3-C5-C6
21	A	401	CL7	C2-C3-C5-C6
21	B	603	CL7	C2-C3-C5-C6
21	B	608	CL7	C2-C3-C5-C6
21	B	614	CL7	C2-C3-C5-C6
21	C	509	CL7	C2-C3-C5-C6
21	2	505	CL7	C2-C3-C5-C6
21	2	516	CL7	C2-C3-C5-C6
21	2	517	CL7	C2-C3-C5-C6
21	1	403	CL7	C2-C3-C5-C6
21	3	504	CL7	C2-C3-C5-C6
21	3	510	CL7	C2-C3-C5-C6
21	3	511	CL7	C2-C3-C5-C6
21	4	406	CL7	C2-C3-C5-C6
21	a	401	CL7	C2-C3-C5-C6
21	b	604	CL7	C2-C3-C5-C6
21	b	609	CL7	C2-C3-C5-C6
21	b	615	CL7	C2-C3-C5-C6
21	c	509	CL7	C2-C3-C5-C6
21	6	505	CL7	C2-C3-C5-C6
21	6	516	CL7	C2-C3-C5-C6
21	6	517	CL7	C2-C3-C5-C6
21	5	403	CL7	C2-C3-C5-C6
21	7	504	CL7	C2-C3-C5-C6
21	7	510	CL7	C2-C3-C5-C6
21	7	511	CL7	C2-C3-C5-C6
21	8	406	CL7	C2-C3-C5-C6
21	B	622	CL7	C2A-CAA-CBA-CGA
21	1	405	CL7	C2A-CAA-CBA-CGA
21	3	503	CL7	C2A-CAA-CBA-CGA
21	3	512	CL7	C2A-CAA-CBA-CGA
21	4	404	CL7	C2A-CAA-CBA-CGA
21	b	623	CL7	C2A-CAA-CBA-CGA
21	5	405	CL7	C2A-CAA-CBA-CGA
21	7	503	CL7	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	7	512	CL7	C2A-CAA-CBA-CGA
21	8	404	CL7	C2A-CAA-CBA-CGA
21	A	406	CL7	C2C-C3C-CAC-CBC
21	a	405	CL7	C2C-C3C-CAC-CBC
21	4	414	CL7	CBD-CGD-O2D-CED
21	8	414	CL7	CBD-CGD-O2D-CED
26	c	501	LMG	O10-C28-O8-C9
21	1	410	CL7	O1D-CGD-O2D-CED
21	3	509	CL7	O1D-CGD-O2D-CED
21	3	516	CL7	O1D-CGD-O2D-CED
21	5	410	CL7	O1D-CGD-O2D-CED
21	7	509	CL7	O1D-CGD-O2D-CED
21	7	516	CL7	O1D-CGD-O2D-CED
21	C	510	CL7	O1D-CGD-O2D-CED
26	C	501	LMG	O10-C28-O8-C9
21	2	510	CL7	C3-C5-C6-C7
21	6	510	CL7	C3-C5-C6-C7
21	C	504	CL7	O1D-CGD-O2D-CED
21	c	504	CL7	O1D-CGD-O2D-CED
21	c	510	CL7	O1D-CGD-O2D-CED
21	c	510	CL7	C13-C15-C16-C17
21	A	401	CL7	C2C-C3C-CAC-CBC
21	a	401	CL7	C2C-C3C-CAC-CBC
21	C	510	CL7	C13-C15-C16-C17
21	2	510	CL7	C8-C10-C11-C12
21	3	503	CL7	C5-C6-C7-C8
21	6	510	CL7	C8-C10-C11-C12
21	7	503	CL7	C5-C6-C7-C8
27	C	517	DGD	C4B-C5B-C6B-C7B
27	c	517	DGD	C4B-C5B-C6B-C7B
21	2	512	CL7	C5-C6-C7-C8
21	3	504	CL7	C8-C10-C11-C12
21	3	504	CL7	C13-C15-C16-C17
21	3	505	CL7	C15-C16-C17-C18
21	3	510	CL7	C5-C6-C7-C8
21	3	510	CL7	C10-C11-C12-C13
21	4	412	CL7	C10-C11-C12-C13
21	6	512	CL7	C5-C6-C7-C8
21	7	504	CL7	C8-C10-C11-C12
21	7	504	CL7	C13-C15-C16-C17
21	7	505	CL7	C15-C16-C17-C18
21	7	510	CL7	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	7	510	CL7	C10-C11-C12-C13
21	8	412	CL7	C10-C11-C12-C13
25	A	407	LHG	O2-C2-C3-O3
25	a	406	LHG	O2-C2-C3-O3
21	1	410	CL7	C2-C3-C5-C6
21	5	410	CL7	C2-C3-C5-C6
21	B	603	CL7	C11-C10-C8-C9
21	B	603	CL7	C14-C13-C15-C16
21	B	608	CL7	C11-C10-C8-C9
21	B	611	CL7	C11-C10-C8-C9
21	B	611	CL7	C11-C12-C13-C14
21	B	612	CL7	C11-C12-C13-C14
21	C	507	CL7	C11-C10-C8-C9
21	C	509	CL7	C11-C10-C8-C9
21	C	511	CL7	C11-C12-C13-C14
21	D	404	CL7	C11-C10-C8-C9
21	2	505	CL7	C14-C13-C15-C16
21	2	510	CL7	C11-C10-C8-C9
21	2	510	CL7	C11-C12-C13-C14
21	1	408	CL7	C11-C10-C8-C9
21	3	501	CL7	C11-C10-C8-C9
21	3	501	CL7	C11-C12-C13-C14
21	3	504	CL7	C11-C10-C8-C9
21	3	507	CL7	C11-C10-C8-C9
21	3	509	CL7	C14-C13-C15-C16
21	3	511	CL7	C11-C10-C8-C9
21	4	404	CL7	C11-C10-C8-C9
21	4	404	CL7	C14-C13-C15-C16
21	4	406	CL7	C11-C10-C8-C9
21	b	604	CL7	C11-C10-C8-C9
21	b	604	CL7	C14-C13-C15-C16
21	b	609	CL7	C11-C10-C8-C9
21	b	612	CL7	C11-C10-C8-C9
21	b	612	CL7	C11-C12-C13-C14
21	b	613	CL7	C11-C12-C13-C14
21	c	507	CL7	C11-C10-C8-C9
21	c	509	CL7	C11-C10-C8-C9
21	c	511	CL7	C11-C12-C13-C14
21	d	404	CL7	C11-C10-C8-C9
21	6	505	CL7	C14-C13-C15-C16
21	6	510	CL7	C11-C10-C8-C9
21	6	510	CL7	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	5	408	CL7	C11-C10-C8-C9
21	7	501	CL7	C11-C10-C8-C9
21	7	501	CL7	C11-C12-C13-C14
21	7	504	CL7	C11-C10-C8-C9
21	7	507	CL7	C11-C10-C8-C9
21	7	509	CL7	C14-C13-C15-C16
21	7	511	CL7	C11-C10-C8-C9
21	8	404	CL7	C11-C10-C8-C9
21	8	404	CL7	C14-C13-C15-C16
21	8	406	CL7	C11-C10-C8-C9
21	C	512	CL7	O1D-CGD-O2D-CED
21	3	518	CL7	O1D-CGD-O2D-CED
21	c	512	CL7	O1D-CGD-O2D-CED
21	7	518	CL7	O1D-CGD-O2D-CED
21	D	404	CL7	CBD-CGD-O2D-CED
21	d	404	CL7	CBD-CGD-O2D-CED
21	5	419	CL7	C2A-CAA-CBA-CGA
23	B	618	8CT	C10-C11-C12-C40
23	C	515	8CT	C14-C15-C16-C39
23	C	515	8CT	C22-C21-C23-C24
23	C	519	8CT	C14-C15-C16-C39
23	b	619	8CT	C10-C11-C12-C40
23	c	515	8CT	C14-C15-C16-C39
23	c	515	8CT	C22-C21-C23-C24
23	c	519	8CT	C14-C15-C16-C39
32	2	525	ZEX	C27-C28-C29-C39
32	3	519	ZEX	C7-C8-C9-C19
32	3	519	ZEX	C27-C28-C29-C39
32	3	520	ZEX	C27-C28-C29-C39
32	3	522	ZEX	C7-C8-C9-C19
32	4	403	ZEX	C27-C28-C29-C39
32	4	418	ZEX	C27-C28-C29-C39
32	6	524	ZEX	C27-C28-C29-C39
32	7	519	ZEX	C7-C8-C9-C19
32	7	519	ZEX	C27-C28-C29-C39
32	7	520	ZEX	C27-C28-C29-C39
32	7	522	ZEX	C7-C8-C9-C19
32	8	403	ZEX	C27-C28-C29-C39
32	8	418	ZEX	C27-C28-C29-C39
23	B	618	8CT	C10-C11-C12-C13
23	C	515	8CT	C14-C15-C16-C17
23	C	519	8CT	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
23	b	619	8CT	C10-C11-C12-C13
23	c	515	8CT	C14-C15-C16-C17
23	c	519	8CT	C14-C15-C16-C17
32	2	521	ZEX	C7-C8-C9-C10
32	2	523	ZEX	C31-C32-C33-C34
32	1	422	ZEX	C7-C8-C9-C10
32	3	519	ZEX	C7-C8-C9-C10
32	3	519	ZEX	C27-C28-C29-C30
32	3	520	ZEX	C27-C28-C29-C30
32	3	522	ZEX	C7-C8-C9-C10
32	4	403	ZEX	C27-C28-C29-C30
32	4	418	ZEX	C27-C28-C29-C30
32	4	419	ZEX	C7-C8-C9-C10
32	6	520	ZEX	C7-C8-C9-C10
32	6	522	ZEX	C31-C32-C33-C34
32	5	422	ZEX	C7-C8-C9-C10
32	7	519	ZEX	C7-C8-C9-C10
32	7	519	ZEX	C27-C28-C29-C30
32	7	520	ZEX	C27-C28-C29-C30
32	7	522	ZEX	C7-C8-C9-C10
32	8	403	ZEX	C27-C28-C29-C30
32	8	418	ZEX	C27-C28-C29-C30
32	8	419	ZEX	C7-C8-C9-C10
21	2	510	CL7	C13-C15-C16-C17
21	2	511	CL7	C8-C10-C11-C12
21	1	404	CL7	C13-C15-C16-C17
21	1	408	CL7	C15-C16-C17-C18
21	3	501	CL7	C15-C16-C17-C18
21	6	510	CL7	C13-C15-C16-C17
21	6	511	CL7	C8-C10-C11-C12
21	5	404	CL7	C13-C15-C16-C17
21	5	408	CL7	C15-C16-C17-C18
21	7	501	CL7	C15-C16-C17-C18
21	1	418	CL7	O1D-CGD-O2D-CED
21	3	508	CL7	O1D-CGD-O2D-CED
21	5	418	CL7	O1D-CGD-O2D-CED
21	7	508	CL7	O1D-CGD-O2D-CED
21	1	419	CL7	C4C-C3C-CAC-CBC
21	5	419	CL7	C4C-C3C-CAC-CBC
21	6	510	CL7	O1D-CGD-O2D-CED
21	B	604	CL7	C3-C5-C6-C7
21	2	505	CL7	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	b	605	CL7	C3-C5-C6-C7
21	6	505	CL7	C3-C5-C6-C7
21	B	604	CL7	C15-C16-C17-C18
21	B	611	CL7	C5-C6-C7-C8
21	C	510	CL7	C5-C6-C7-C8
21	2	517	CL7	C5-C6-C7-C8
21	1	406	CL7	C10-C11-C12-C13
21	3	504	CL7	C5-C6-C7-C8
21	4	406	CL7	C13-C15-C16-C17
21	4	409	CL7	C8-C10-C11-C12
21	4	412	CL7	C8-C10-C11-C12
21	4	412	CL7	C15-C16-C17-C18
21	b	605	CL7	C15-C16-C17-C18
21	b	612	CL7	C5-C6-C7-C8
21	6	517	CL7	C5-C6-C7-C8
21	5	406	CL7	C10-C11-C12-C13
21	7	504	CL7	C5-C6-C7-C8
21	8	406	CL7	C13-C15-C16-C17
21	8	409	CL7	C8-C10-C11-C12
21	8	412	CL7	C8-C10-C11-C12
21	8	412	CL7	C15-C16-C17-C18
21	2	510	CL7	O1D-CGD-O2D-CED
21	A	401	CL7	C8-C10-C11-C12
21	B	605	CL7	C5-C6-C7-C8
21	B	608	CL7	C15-C16-C17-C18
21	C	502	CL7	C15-C16-C17-C18
21	C	510	CL7	C10-C11-C12-C13
21	2	502	CL7	C8-C10-C11-C12
21	2	510	CL7	C5-C6-C7-C8
21	1	404	CL7	C15-C16-C17-C18
21	3	511	CL7	C10-C11-C12-C13
21	3	512	CL7	C5-C6-C7-C8
21	4	405	CL7	C13-C15-C16-C17
21	4	409	CL7	C10-C11-C12-C13
21	a	401	CL7	C8-C10-C11-C12
21	b	606	CL7	C5-C6-C7-C8
21	b	609	CL7	C15-C16-C17-C18
21	c	502	CL7	C15-C16-C17-C18
21	c	510	CL7	C5-C6-C7-C8
21	c	510	CL7	C10-C11-C12-C13
21	6	502	CL7	C8-C10-C11-C12
21	6	510	CL7	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	5	404	CL7	C15-C16-C17-C18
21	7	511	CL7	C10-C11-C12-C13
21	7	512	CL7	C5-C6-C7-C8
21	8	405	CL7	C13-C15-C16-C17
21	8	409	CL7	C10-C11-C12-C13
21	1	412	CL7	O1D-CGD-O2D-CED
21	4	410	CL7	O1D-CGD-O2D-CED
21	5	412	CL7	O1D-CGD-O2D-CED
21	8	410	CL7	O1D-CGD-O2D-CED
24	2	522	SQD	C7-C8-C9-C10
24	6	521	SQD	C7-C8-C9-C10
21	3	517	CL7	CBD-CGD-O2D-CED
21	7	517	CL7	CBD-CGD-O2D-CED
21	A	406	CL7	C5-C6-C7-C8
21	B	603	CL7	C5-C6-C7-C8
21	B	605	CL7	C13-C15-C16-C17
21	2	503	CL7	C8-C10-C11-C12
21	2	512	CL7	C13-C15-C16-C17
21	3	509	CL7	C5-C6-C7-C8
21	3	509	CL7	C10-C11-C12-C13
21	a	405	CL7	C5-C6-C7-C8
21	b	604	CL7	C5-C6-C7-C8
21	b	606	CL7	C13-C15-C16-C17
21	6	503	CL7	C8-C10-C11-C12
21	6	512	CL7	C13-C15-C16-C17
21	7	509	CL7	C5-C6-C7-C8
21	7	509	CL7	C10-C11-C12-C13
21	B	608	CL7	C5-C6-C7-C8
21	3	505	CL7	C8-C10-C11-C12
21	4	406	CL7	C15-C16-C17-C18
21	b	609	CL7	C5-C6-C7-C8
21	7	505	CL7	C8-C10-C11-C12
21	8	406	CL7	C15-C16-C17-C18
21	1	415	CL7	CBD-CGD-O2D-CED
21	5	415	CL7	CBD-CGD-O2D-CED
21	1	406	CL7	C13-C15-C16-C17
21	5	406	CL7	C13-C15-C16-C17
21	2	501	CL7	C15-C16-C17-C18
21	6	501	CL7	C15-C16-C17-C18
21	B	603	CL7	C12-C13-C15-C16
21	C	504	CL7	C11-C12-C13-C15
21	C	508	CL7	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	2	512	CL7	C11-C12-C13-C15
21	1	406	CL7	C12-C13-C15-C16
21	1	408	CL7	C12-C13-C15-C16
21	1	418	CL7	C12-C13-C15-C16
21	3	501	CL7	C11-C10-C8-C7
21	3	503	CL7	C11-C10-C8-C7
21	3	503	CL7	C12-C13-C15-C16
21	3	508	CL7	C6-C7-C8-C10
21	3	510	CL7	C6-C7-C8-C10
21	3	511	CL7	C12-C13-C15-C16
21	4	406	CL7	C6-C7-C8-C10
21	4	406	CL7	C11-C10-C8-C7
21	4	406	CL7	C12-C13-C15-C16
21	b	604	CL7	C12-C13-C15-C16
21	c	504	CL7	C11-C12-C13-C15
21	c	508	CL7	C11-C10-C8-C7
21	6	512	CL7	C11-C12-C13-C15
21	5	406	CL7	C12-C13-C15-C16
21	5	408	CL7	C12-C13-C15-C16
21	5	418	CL7	C12-C13-C15-C16
21	7	501	CL7	C11-C10-C8-C7
21	7	503	CL7	C11-C10-C8-C7
21	7	503	CL7	C12-C13-C15-C16
21	7	508	CL7	C6-C7-C8-C10
21	7	510	CL7	C6-C7-C8-C10
21	7	511	CL7	C12-C13-C15-C16
21	8	406	CL7	C6-C7-C8-C10
21	8	406	CL7	C11-C10-C8-C7
21	8	406	CL7	C12-C13-C15-C16
21	B	610	CL7	C3-C5-C6-C7
21	2	509	CL7	C3-C5-C6-C7
21	3	502	CL7	C3-C5-C6-C7
21	b	611	CL7	C3-C5-C6-C7
21	6	509	CL7	C3-C5-C6-C7
21	7	502	CL7	C3-C5-C6-C7
23	B	617	8CT	C12-C13-C14-C15
23	B	618	8CT	C12-C13-C14-C15
23	B	618	8CT	C16-C17-C18-C19
23	B	618	8CT	C18-C19-C20-C21
23	C	516	8CT	C23-C24-C25-C26
23	C	519	8CT	C12-C13-C14-C15
23	b	618	8CT	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	b	619	8CT	C12-C13-C14-C15
23	b	619	8CT	C16-C17-C18-C19
23	b	619	8CT	C18-C19-C20-C21
23	c	516	8CT	C23-C24-C25-C26
23	c	519	8CT	C12-C13-C14-C15
32	2	520	ZEX	C33-C34-C35-C15
32	2	525	ZEX	C9-C10-C11-C12
32	3	519	ZEX	C29-C30-C31-C32
32	3	525	ZEX	C33-C34-C35-C15
32	4	420	ZEX	C29-C30-C31-C32
32	6	524	ZEX	C9-C10-C11-C12
32	7	519	ZEX	C29-C30-C31-C32
32	8	420	ZEX	C29-C30-C31-C32
21	1	419	CL7	C2A-CAA-CBA-CGA
21	4	406	CL7	C2A-CAA-CBA-CGA
21	8	406	CL7	C2A-CAA-CBA-CGA
21	C	505	CL7	O1D-CGD-O2D-CED
21	2	509	CL7	O1D-CGD-O2D-CED
21	2	517	CL7	O1D-CGD-O2D-CED
21	1	403	CL7	O1D-CGD-O2D-CED
21	4	409	CL7	O1D-CGD-O2D-CED
21	c	505	CL7	O1D-CGD-O2D-CED
21	6	509	CL7	O1D-CGD-O2D-CED
21	6	517	CL7	O1D-CGD-O2D-CED
21	5	403	CL7	O1D-CGD-O2D-CED
21	8	409	CL7	O1D-CGD-O2D-CED
21	C	506	CL7	C5-C6-C7-C8
21	C	508	CL7	C5-C6-C7-C8
21	C	511	CL7	C10-C11-C12-C13
21	1	403	CL7	C5-C6-C7-C8
21	1	404	CL7	C8-C10-C11-C12
21	c	506	CL7	C5-C6-C7-C8
21	c	508	CL7	C5-C6-C7-C8
21	c	511	CL7	C10-C11-C12-C13
21	5	403	CL7	C5-C6-C7-C8
21	5	404	CL7	C8-C10-C11-C12
21	1	410	CL7	C8-C10-C11-C12
21	4	404	CL7	C5-C6-C7-C8
21	5	410	CL7	C8-C10-C11-C12
21	8	404	CL7	C5-C6-C7-C8
21	1	402	CL7	C3-C5-C6-C7
21	5	402	CL7	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
21	B	610	CL7	C8-C10-C11-C12
21	C	509	CL7	C5-C6-C7-C8
21	2	509	CL7	C13-C15-C16-C17
21	2	511	CL7	C5-C6-C7-C8
21	1	402	CL7	C10-C11-C12-C13
21	1	404	CL7	C5-C6-C7-C8
21	b	611	CL7	C8-C10-C11-C12
21	c	509	CL7	C5-C6-C7-C8
21	6	509	CL7	C13-C15-C16-C17
21	6	511	CL7	C5-C6-C7-C8
21	5	402	CL7	C10-C11-C12-C13
21	5	404	CL7	C5-C6-C7-C8
21	B	611	CL7	O1D-CGD-O2D-CED
21	b	612	CL7	O1D-CGD-O2D-CED
21	B	603	CL7	C8-C10-C11-C12
21	B	614	CL7	C8-C10-C11-C12
21	C	503	CL7	C8-C10-C11-C12
21	C	511	CL7	C8-C10-C11-C12
21	2	501	CL7	C8-C10-C11-C12
21	2	509	CL7	C5-C6-C7-C8
21	1	403	CL7	C8-C10-C11-C12
21	1	406	CL7	C8-C10-C11-C12
21	3	501	CL7	C13-C15-C16-C17
21	4	405	CL7	C5-C6-C7-C8
21	b	604	CL7	C8-C10-C11-C12
21	b	615	CL7	C8-C10-C11-C12
21	c	503	CL7	C8-C10-C11-C12
21	c	511	CL7	C8-C10-C11-C12
21	6	501	CL7	C8-C10-C11-C12
21	6	509	CL7	C5-C6-C7-C8
21	5	403	CL7	C8-C10-C11-C12
21	5	406	CL7	C8-C10-C11-C12
21	7	501	CL7	C13-C15-C16-C17
21	8	405	CL7	C5-C6-C7-C8
21	C	507	CL7	C5-C6-C7-C8
21	C	509	CL7	C15-C16-C17-C18
21	2	505	CL7	C15-C16-C17-C18
21	2	510	CL7	C15-C16-C17-C18
21	4	404	CL7	C8-C10-C11-C12
21	c	507	CL7	C5-C6-C7-C8
21	c	509	CL7	C15-C16-C17-C18
21	6	505	CL7	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
21	6	510	CL7	C15-C16-C17-C18
21	8	404	CL7	C8-C10-C11-C12
25	3	524	LHG	C3-O3-P-O6
25	7	524	LHG	C3-O3-P-O6
21	B	608	CL7	C3-C5-C6-C7
21	b	609	CL7	C3-C5-C6-C7
21	B	616	CL7	CBD-CGD-O2D-CED
21	b	617	CL7	CBD-CGD-O2D-CED
21	B	602	CL7	C5-C6-C7-C8
21	C	504	CL7	C10-C11-C12-C13
21	2	516	CL7	C15-C16-C17-C18
21	2	517	CL7	C8-C10-C11-C12
21	b	603	CL7	C5-C6-C7-C8
21	c	504	CL7	C10-C11-C12-C13
21	6	516	CL7	C15-C16-C17-C18
21	6	517	CL7	C8-C10-C11-C12
32	2	520	ZEX	C25-C26-C27-C28
32	3	525	ZEX	C25-C26-C27-C28
32	4	403	ZEX	C25-C26-C27-C28
32	4	418	ZEX	C25-C26-C27-C28
32	4	420	ZEX	C25-C26-C27-C28
32	8	403	ZEX	C25-C26-C27-C28
32	8	418	ZEX	C25-C26-C27-C28
32	8	420	ZEX	C25-C26-C27-C28
25	A	407	LHG	C1-C2-C3-O3
25	a	406	LHG	C1-C2-C3-O3
21	3	501	CL7	C4-C3-C5-C6
21	3	505	CL7	C4-C3-C5-C6
21	6	503	CL7	C4-C3-C5-C6
21	7	501	CL7	C4-C3-C5-C6
21	7	505	CL7	C4-C3-C5-C6
21	3	512	CL7	C2-C3-C5-C6
21	7	512	CL7	C2-C3-C5-C6
21	C	511	CL7	C15-C16-C17-C18
21	3	507	CL7	C13-C15-C16-C17
21	4	411	CL7	C13-C15-C16-C17
21	c	511	CL7	C15-C16-C17-C18
21	7	507	CL7	C13-C15-C16-C17
21	8	411	CL7	C13-C15-C16-C17
21	D	402	CL7	C2A-CAA-CBA-CGA
21	d	402	CL7	C2A-CAA-CBA-CGA
21	2	518	CL7	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
21	6	518	CL7	C16-C17-C18-C19
21	B	607	CL7	C3-C5-C6-C7
21	B	612	CL7	C3-C5-C6-C7
21	2	517	CL7	C3-C5-C6-C7
21	b	608	CL7	C3-C5-C6-C7
21	b	613	CL7	C3-C5-C6-C7
21	6	517	CL7	C3-C5-C6-C7
23	4	402	8CT	C12-C13-C14-C15
23	8	402	8CT	C12-C13-C14-C15
32	2	523	ZEX	C29-C30-C31-C32
32	4	403	ZEX	C29-C30-C31-C32
32	6	522	ZEX	C29-C30-C31-C32
32	8	403	ZEX	C29-C30-C31-C32
21	1	420	CL7	C4C-C3C-CAC-CBC
21	5	420	CL7	C4C-C3C-CAC-CBC
21	2	517	CL7	C10-C11-C12-C13
21	6	517	CL7	C10-C11-C12-C13
21	2	506	CL7	O1D-CGD-O2D-CED
21	6	506	CL7	O1D-CGD-O2D-CED
21	2	517	CL7	C15-C16-C17-C18
21	6	517	CL7	C15-C16-C17-C18
22	D	408	PHO	O1D-CGD-O2D-CED
22	d	408	PHO	O1D-CGD-O2D-CED
27	C	517	DGD	C3B-C4B-C5B-C6B
21	3	511	CL7	C3-C5-C6-C7
21	7	511	CL7	C3-C5-C6-C7
27	c	517	DGD	C3B-C4B-C5B-C6B
21	2	501	CL7	C5-C6-C7-C8
21	6	501	CL7	C5-C6-C7-C8
21	3	514	CL7	O1D-CGD-O2D-CED
21	7	514	CL7	O1D-CGD-O2D-CED
21	B	611	CL7	C4-C3-C5-C6
21	b	612	CL7	C4-C3-C5-C6
21	B	604	CL7	C11-C12-C13-C14
21	B	608	CL7	C6-C7-C8-C9
21	B	611	CL7	C6-C7-C8-C9
21	2	501	CL7	C11-C12-C13-C14
21	2	509	CL7	C6-C7-C8-C9
21	3	508	CL7	C11-C10-C8-C9
21	b	605	CL7	C11-C12-C13-C14
21	b	609	CL7	C6-C7-C8-C9
21	b	612	CL7	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	6	501	CL7	C11-C12-C13-C14
21	6	509	CL7	C6-C7-C8-C9
21	7	508	CL7	C11-C10-C8-C9
21	2	509	CL7	C8-C10-C11-C12
21	6	509	CL7	C8-C10-C11-C12
26	C	501	LMG	O6-C5-C6-O5
26	c	501	LMG	O6-C5-C6-O5
21	B	615	CL7	C2A-CAA-CBA-CGA
21	b	616	CL7	C2A-CAA-CBA-CGA
23	B	618	8CT	C14-C15-C16-C39
23	B	627	8CT	C10-C11-C12-C40
23	D	406	8CT	C22-C21-C23-C24
23	b	601	8CT	C10-C11-C12-C40
23	b	619	8CT	C14-C15-C16-C39
23	d	406	8CT	C22-C21-C23-C24
32	2	521	ZEX	C7-C8-C9-C19
32	1	422	ZEX	C7-C8-C9-C19
32	4	419	ZEX	C7-C8-C9-C19
32	4	420	ZEX	C31-C32-C33-C40
32	6	520	ZEX	C7-C8-C9-C19
32	5	422	ZEX	C7-C8-C9-C19
32	8	419	ZEX	C7-C8-C9-C19
32	8	420	ZEX	C31-C32-C33-C40
23	B	618	8CT	C14-C15-C16-C17
23	B	627	8CT	C10-C11-C12-C13
23	C	515	8CT	C25-C26-C28-C29
23	D	406	8CT	C20-C21-C23-C24
23	b	601	8CT	C10-C11-C12-C13
23	b	619	8CT	C14-C15-C16-C17
23	c	515	8CT	C25-C26-C28-C29
23	d	406	8CT	C20-C21-C23-C24
32	3	520	ZEX	C7-C8-C9-C10
32	4	420	ZEX	C31-C32-C33-C34
32	7	520	ZEX	C7-C8-C9-C10
32	8	420	ZEX	C31-C32-C33-C34
21	2	518	CL7	C16-C17-C18-C20
21	6	518	CL7	C16-C17-C18-C20
21	B	605	CL7	C10-C11-C12-C13
21	D	402	CL7	O1D-CGD-O2D-CED
21	4	406	CL7	CBD-CGD-O2D-CED
21	8	406	CL7	CBD-CGD-O2D-CED
21	A	406	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	2	503	CL7	O1D-CGD-O2D-CED
21	a	405	CL7	O1D-CGD-O2D-CED
21	d	402	CL7	O1D-CGD-O2D-CED
21	B	612	CL7	C13-C15-C16-C17
21	1	402	CL7	C8-C10-C11-C12
21	b	606	CL7	C10-C11-C12-C13
21	b	613	CL7	C13-C15-C16-C17
21	5	402	CL7	C8-C10-C11-C12
21	C	506	CL7	O1D-CGD-O2D-CED
21	c	506	CL7	O1D-CGD-O2D-CED
21	6	503	CL7	O1D-CGD-O2D-CED
21	B	614	CL7	C3A-C2A-CAA-CBA
21	C	504	CL7	C3A-C2A-CAA-CBA
21	C	505	CL7	C3A-C2A-CAA-CBA
21	2	507	CL7	C3A-C2A-CAA-CBA
21	2	510	CL7	C3A-C2A-CAA-CBA
21	2	512	CL7	C3A-C2A-CAA-CBA
21	2	513	CL7	C3A-C2A-CAA-CBA
21	3	504	CL7	C3A-C2A-CAA-CBA
21	3	512	CL7	C3A-C2A-CAA-CBA
21	4	412	CL7	C3A-C2A-CAA-CBA
21	4	414	CL7	C3A-C2A-CAA-CBA
21	b	615	CL7	C3A-C2A-CAA-CBA
21	c	504	CL7	C3A-C2A-CAA-CBA
21	c	505	CL7	C3A-C2A-CAA-CBA
21	6	507	CL7	C3A-C2A-CAA-CBA
21	6	510	CL7	C3A-C2A-CAA-CBA
21	6	512	CL7	C3A-C2A-CAA-CBA
21	6	513	CL7	C3A-C2A-CAA-CBA
21	7	504	CL7	C3A-C2A-CAA-CBA
21	7	512	CL7	C3A-C2A-CAA-CBA
21	8	412	CL7	C3A-C2A-CAA-CBA
21	8	414	CL7	C3A-C2A-CAA-CBA
23	C	516	8CT	C12-C13-C14-C15
23	c	516	8CT	C12-C13-C14-C15
21	C	502	CL7	C16-C17-C18-C19
21	c	502	CL7	C16-C17-C18-C19
27	C	517	DGD	CCB-CDB-CEB-CFB
27	c	517	DGD	CCB-CDB-CEB-CFB
21	C	507	CL7	O2A-C1-C2-C3
21	C	508	CL7	O2A-C1-C2-C3
21	c	507	CL7	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
21	c	508	CL7	O2A-C1-C2-C3
21	A	406	CL7	C3-C5-C6-C7
21	a	405	CL7	C3-C5-C6-C7
21	C	506	CL7	C10-C11-C12-C13
21	c	506	CL7	C10-C11-C12-C13
21	2	503	CL7	C4-C3-C5-C6
26	C	501	LMG	C4-C5-C6-O5
26	C	501	LMG	C11-C10-O7-C8
26	c	501	LMG	C11-C10-O7-C8
27	C	517	DGD	C8A-C9A-CAA-CBA
27	c	517	DGD	C8A-C9A-CAA-CBA
21	4	405	CL7	C10-C11-C12-C13
21	8	405	CL7	C10-C11-C12-C13
21	6	503	CL7	C3-C5-C6-C7
26	c	501	LMG	C4-C5-C6-O5
21	A	401	CL7	C4C-C3C-CAC-CBC
21	a	401	CL7	C4C-C3C-CAC-CBC
27	C	517	DGD	O6E-C5E-C6E-O5E
27	c	517	DGD	O6E-C5E-C6E-O5E
26	C	501	LMG	O9-C10-O7-C8
26	c	501	LMG	O9-C10-O7-C8
21	2	518	CL7	C10-C11-C12-C13
21	6	518	CL7	C10-C11-C12-C13
21	2	503	CL7	C3-C5-C6-C7
23	B	627	8CT	C02-C03-C10-C11
23	C	515	8CT	C04-C03-C10-C11
23	C	519	8CT	C04-C03-C10-C11
23	D	406	8CT	C02-C03-C10-C11
23	K	101	8CT	C04-C03-C10-C11
23	b	601	8CT	C02-C03-C10-C11
23	c	515	8CT	C04-C03-C10-C11
23	d	406	8CT	C02-C03-C10-C11
23	k	101	8CT	C04-C03-C10-C11
32	2	519	ZEX	C5-C6-C7-C8
32	2	521	ZEX	C5-C6-C7-C8
32	2	525	ZEX	C1-C6-C7-C8
32	2	525	ZEX	C5-C6-C7-C8
32	1	421	ZEX	C1-C6-C7-C8
32	1	421	ZEX	C5-C6-C7-C8
32	1	422	ZEX	C1-C6-C7-C8
32	1	422	ZEX	C5-C6-C7-C8
32	3	519	ZEX	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
32	3	519	ZEX	C5-C6-C7-C8
32	3	522	ZEX	C5-C6-C7-C8
32	4	403	ZEX	C1-C6-C7-C8
32	6	519	ZEX	C5-C6-C7-C8
32	6	520	ZEX	C5-C6-C7-C8
32	6	524	ZEX	C1-C6-C7-C8
32	6	524	ZEX	C5-C6-C7-C8
32	5	421	ZEX	C1-C6-C7-C8
32	5	421	ZEX	C5-C6-C7-C8
32	5	422	ZEX	C1-C6-C7-C8
32	5	422	ZEX	C5-C6-C7-C8
32	7	519	ZEX	C1-C6-C7-C8
32	7	519	ZEX	C5-C6-C7-C8
32	7	522	ZEX	C5-C6-C7-C8
32	8	403	ZEX	C1-C6-C7-C8
21	3	508	CL7	C5-C6-C7-C8
21	4	406	CL7	C10-C11-C12-C13
21	8	406	CL7	C10-C11-C12-C13
21	A	406	CL7	C10-C11-C12-C13
21	a	405	CL7	C10-C11-C12-C13
21	7	508	CL7	C5-C6-C7-C8
21	B	608	CL7	C6-C7-C8-C10
21	B	611	CL7	C2-C3-C5-C6
21	B	611	CL7	C6-C7-C8-C10
21	B	612	CL7	C12-C13-C15-C16
21	C	509	CL7	C11-C10-C8-C7
21	C	511	CL7	C6-C7-C8-C10
21	C	511	CL7	C11-C10-C8-C7
21	2	505	CL7	C11-C12-C13-C15
21	2	505	CL7	C12-C13-C15-C16
21	2	511	CL7	C6-C7-C8-C10
21	2	517	CL7	C12-C13-C15-C16
21	1	418	CL7	C11-C10-C8-C7
21	3	504	CL7	C11-C10-C8-C7
21	3	508	CL7	C11-C10-C8-C7
21	b	609	CL7	C6-C7-C8-C10
21	b	612	CL7	C2-C3-C5-C6
21	b	612	CL7	C6-C7-C8-C10
21	b	613	CL7	C12-C13-C15-C16
21	c	509	CL7	C11-C10-C8-C7
21	c	511	CL7	C6-C7-C8-C10
21	c	511	CL7	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
21	6	505	CL7	C11-C12-C13-C15
21	6	505	CL7	C12-C13-C15-C16
21	6	511	CL7	C6-C7-C8-C10
21	6	517	CL7	C12-C13-C15-C16
21	5	418	CL7	C11-C10-C8-C7
21	7	504	CL7	C11-C10-C8-C7
21	7	508	CL7	C11-C10-C8-C7
21	2	506	CL7	C8-C10-C11-C12
21	2	507	CL7	C8-C10-C11-C12
21	6	506	CL7	C8-C10-C11-C12
32	2	525	ZEX	C29-C30-C31-C32
32	4	420	ZEX	C33-C34-C35-C15
32	6	524	ZEX	C29-C30-C31-C32
32	8	420	ZEX	C33-C34-C35-C15
21	C	511	CL7	O1D-CGD-O2D-CED
21	c	511	CL7	O1D-CGD-O2D-CED
21	2	513	CL7	C2A-CAA-CBA-CGA
21	4	410	CL7	C2A-CAA-CBA-CGA
21	4	415	CL7	C2A-CAA-CBA-CGA
21	6	513	CL7	C2A-CAA-CBA-CGA
21	8	410	CL7	C2A-CAA-CBA-CGA
21	8	415	CL7	C2A-CAA-CBA-CGA
21	B	603	CL7	C10-C11-C12-C13
21	C	502	CL7	C13-C15-C16-C17
21	1	403	CL7	C10-C11-C12-C13
21	b	604	CL7	C10-C11-C12-C13
21	c	502	CL7	C13-C15-C16-C17
21	5	403	CL7	C10-C11-C12-C13
21	C	507	CL7	C10-C11-C12-C13
21	c	507	CL7	C10-C11-C12-C13
21	4	412	CL7	O1D-CGD-O2D-CED
21	8	412	CL7	O1D-CGD-O2D-CED
21	1	418	CL7	C15-C16-C17-C18
21	6	507	CL7	C8-C10-C11-C12
21	5	418	CL7	C15-C16-C17-C18
21	2	507	CL7	O1D-CGD-O2D-CED
21	6	507	CL7	O1D-CGD-O2D-CED
31	F	101	HEM	C4B-C3B-CAB-CBB
31	f	101	HEM	C4B-C3B-CAB-CBB
21	4	412	CL7	C13-C15-C16-C17
21	4	416	CL7	CBD-CGD-O2D-CED
21	8	416	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	8	412	CL7	C13-C15-C16-C17
21	4	414	CL7	O1D-CGD-O2D-CED
21	8	414	CL7	O1D-CGD-O2D-CED
21	2	505	CL7	C10-C11-C12-C13
21	2	516	CL7	C5-C6-C7-C8
21	3	510	CL7	C8-C10-C11-C12
21	6	505	CL7	C10-C11-C12-C13
21	6	516	CL7	C5-C6-C7-C8
21	7	510	CL7	C8-C10-C11-C12
21	3	501	CL7	C2-C3-C5-C6
21	3	505	CL7	C2-C3-C5-C6
21	7	501	CL7	C2-C3-C5-C6
21	7	505	CL7	C2-C3-C5-C6
21	A	406	CL7	C11-C10-C8-C9
21	B	605	CL7	C14-C13-C15-C16
21	B	612	CL7	C6-C7-C8-C9
21	C	504	CL7	C11-C10-C8-C9
21	2	505	CL7	C11-C12-C13-C14
21	2	509	CL7	C11-C12-C13-C14
21	2	510	CL7	C14-C13-C15-C16
21	1	408	CL7	C14-C13-C15-C16
21	3	507	CL7	C14-C13-C15-C16
21	a	405	CL7	C11-C10-C8-C9
21	b	606	CL7	C14-C13-C15-C16
21	b	613	CL7	C6-C7-C8-C9
21	c	504	CL7	C11-C10-C8-C9
21	6	505	CL7	C11-C12-C13-C14
21	6	509	CL7	C11-C12-C13-C14
21	6	510	CL7	C14-C13-C15-C16
21	5	408	CL7	C14-C13-C15-C16
21	7	507	CL7	C14-C13-C15-C16
21	3	512	CL7	C3-C5-C6-C7
21	7	512	CL7	C3-C5-C6-C7
21	3	501	CL7	C2A-CAA-CBA-CGA
21	7	501	CL7	C2A-CAA-CBA-CGA
21	B	608	CL7	C2C-C3C-CAC-CBC
21	b	609	CL7	C2C-C3C-CAC-CBC
32	3	520	ZEX	C7-C8-C9-C19
32	7	520	ZEX	C7-C8-C9-C19
21	1	410	CL7	C5-C6-C7-C8
21	5	410	CL7	C5-C6-C7-C8
23	C	516	8CT	C25-C26-C28-C29

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Mol	Chain	Res	Type	Atoms
23	c	516	8CT	C25-C26-C28-C29
21	B	609	CL7	C1A-C2A-CAA-CBA
21	B	612	CL7	C1A-C2A-CAA-CBA
21	B	614	CL7	C1A-C2A-CAA-CBA
21	C	509	CL7	C1A-C2A-CAA-CBA
21	C	511	CL7	C1A-C2A-CAA-CBA
21	C	514	CL7	C1A-C2A-CAA-CBA
21	D	402	CL7	C1A-C2A-CAA-CBA
21	2	501	CL7	C1A-C2A-CAA-CBA
21	2	507	CL7	C1A-C2A-CAA-CBA
21	2	510	CL7	C1A-C2A-CAA-CBA
21	2	511	CL7	C1A-C2A-CAA-CBA
21	2	512	CL7	C1A-C2A-CAA-CBA
21	2	516	CL7	C1A-C2A-CAA-CBA
21	1	417	CL7	C1A-C2A-CAA-CBA
21	1	418	CL7	C1A-C2A-CAA-CBA
21	3	503	CL7	C1A-C2A-CAA-CBA
21	3	514	CL7	C1A-C2A-CAA-CBA
21	3	516	CL7	C1A-C2A-CAA-CBA
21	4	404	CL7	C1A-C2A-CAA-CBA
21	4	414	CL7	C1A-C2A-CAA-CBA
21	b	610	CL7	C1A-C2A-CAA-CBA
21	b	613	CL7	C1A-C2A-CAA-CBA
21	b	615	CL7	C1A-C2A-CAA-CBA
21	c	511	CL7	C1A-C2A-CAA-CBA
21	c	514	CL7	C1A-C2A-CAA-CBA
21	d	402	CL7	C1A-C2A-CAA-CBA
21	6	501	CL7	C1A-C2A-CAA-CBA
21	6	507	CL7	C1A-C2A-CAA-CBA
21	6	510	CL7	C1A-C2A-CAA-CBA
21	6	511	CL7	C1A-C2A-CAA-CBA
21	6	512	CL7	C1A-C2A-CAA-CBA
21	6	516	CL7	C1A-C2A-CAA-CBA
21	5	417	CL7	C1A-C2A-CAA-CBA
21	5	418	CL7	C1A-C2A-CAA-CBA
21	7	503	CL7	C1A-C2A-CAA-CBA
21	7	514	CL7	C1A-C2A-CAA-CBA
21	7	516	CL7	C1A-C2A-CAA-CBA
21	8	404	CL7	C1A-C2A-CAA-CBA
21	8	414	CL7	C1A-C2A-CAA-CBA
21	C	504	CL7	C16-C17-C18-C20
21	c	504	CL7	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
25	B	625	LHG	C15-C16-C17-C18
25	b	626	LHG	C15-C16-C17-C18
23	K	101	8CT	C18-C19-C20-C21
23	k	101	8CT	C18-C19-C20-C21
21	1	408	CL7	C4C-C3C-CAC-CBC
21	5	408	CL7	C4C-C3C-CAC-CBC
21	C	511	CL7	C3-C5-C6-C7
21	c	511	CL7	C3-C5-C6-C7
21	3	507	CL7	C5-C6-C7-C8
21	7	507	CL7	C5-C6-C7-C8
26	D	410	LMG	O6-C5-C6-O5
26	d	410	LMG	O6-C5-C6-O5
32	4	419	ZEX	C25-C26-C27-C28
32	8	419	ZEX	C25-C26-C27-C28
26	b	622	LMG	C38-C39-C40-C41
26	B	621	LMG	C38-C39-C40-C41
27	B	624	DGD	C2A-C1A-O1G-C1G
27	b	625	DGD	C2A-C1A-O1G-C1G
21	1	402	CL7	C4-C3-C5-C6
21	5	402	CL7	C4-C3-C5-C6
21	2	503	CL7	C2-C3-C5-C6
21	4	417	CL7	C3A-C2A-CAA-CBA
21	6	503	CL7	C2-C3-C5-C6
21	8	417	CL7	C3A-C2A-CAA-CBA
21	2	517	CL7	C2A-CAA-CBA-CGA
21	6	517	CL7	C2A-CAA-CBA-CGA
21	3	507	CL7	C3-C5-C6-C7
26	B	621	LMG	C7-C8-C9-O8
26	b	622	LMG	C7-C8-C9-O8
24	3	523	SQD	C45-C44-O6-C1
24	7	523	SQD	C45-C44-O6-C1
21	1	415	CL7	C4C-C3C-CAC-CBC
21	5	415	CL7	C4C-C3C-CAC-CBC
21	4	414	CL7	C5-C6-C7-C8
21	8	414	CL7	C5-C6-C7-C8
21	d	404	CL7	O1D-CGD-O2D-CED
26	1	401	LMG	O6-C5-C6-O5
26	5	401	LMG	O6-C5-C6-O5
21	7	507	CL7	C3-C5-C6-C7
21	2	503	CL7	C10-C11-C12-C13
21	6	503	CL7	C10-C11-C12-C13
21	D	404	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	2	512	CL7	C10-C11-C12-C13
21	6	512	CL7	C10-C11-C12-C13
21	4	415	CL7	CBD-CGD-O2D-CED
21	8	415	CL7	CBD-CGD-O2D-CED
21	B	609	CL7	C13-C15-C16-C17
21	b	610	CL7	C13-C15-C16-C17
21	1	410	CL7	C15-C16-C17-C18
21	5	410	CL7	C15-C16-C17-C18
26	C	501	LMG	C12-C13-C14-C15
21	4	409	CL7	C5-C6-C7-C8
21	8	409	CL7	C5-C6-C7-C8
25	D	409	LHG	O6-C4-C5-O7
25	d	409	LHG	O6-C4-C5-O7
21	B	609	CL7	C16-C17-C18-C20
21	C	504	CL7	C16-C17-C18-C19
21	b	610	CL7	C16-C17-C18-C20
21	c	504	CL7	C16-C17-C18-C19
21	7	512	CL7	CBD-CGD-O2D-CED
21	B	607	CL7	C8-C10-C11-C12
21	b	608	CL7	C8-C10-C11-C12
21	1	415	CL7	O1D-CGD-O2D-CED
27	B	624	DGD	O1A-C1A-O1G-C1G
27	b	625	DGD	O1A-C1A-O1G-C1G
24	b	621	SQD	C32-C33-C34-C35
21	3	512	CL7	CBD-CGD-O2D-CED
21	5	410	CL7	C10-C11-C12-C13
26	C	501	LMG	C2-C1-O1-C7
26	1	401	LMG	C2-C1-O1-C7
26	c	501	LMG	C2-C1-O1-C7
26	5	401	LMG	C2-C1-O1-C7
24	B	620	SQD	C32-C33-C34-C35
21	A	401	CL7	C10-C11-C12-C13
21	B	604	CL7	C8-C10-C11-C12
21	1	410	CL7	C10-C11-C12-C13
21	a	401	CL7	C10-C11-C12-C13
21	b	605	CL7	C8-C10-C11-C12
21	B	609	CL7	C16-C17-C18-C19
21	b	610	CL7	C16-C17-C18-C19
22	A	402	PHO	CHA-CBD-CGD-O1D
22	A	402	PHO	CHA-CBD-CGD-O2D
22	a	402	PHO	CHA-CBD-CGD-O1D
22	a	402	PHO	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	5	415	CL7	O1D-CGD-O2D-CED
21	2	507	CL7	C4-C3-C5-C6
21	6	507	CL7	C4-C3-C5-C6
21	7	502	CL7	C4-C3-C5-C6
21	B	603	CL7	C11-C10-C8-C7
21	B	604	CL7	C12-C13-C15-C16
21	B	605	CL7	C12-C13-C15-C16
21	B	609	CL7	C6-C7-C8-C10
21	B	612	CL7	C11-C10-C8-C7
21	C	504	CL7	C11-C10-C8-C7
21	C	506	CL7	C12-C13-C15-C16
21	C	507	CL7	C11-C10-C8-C7
21	C	511	CL7	C12-C13-C15-C16
21	2	503	CL7	C12-C13-C15-C16
21	2	507	CL7	C11-C10-C8-C7
21	2	510	CL7	C6-C7-C8-C10
21	2	510	CL7	C11-C10-C8-C7
21	1	408	CL7	C11-C10-C8-C7
21	3	501	CL7	C12-C13-C15-C16
21	3	507	CL7	C6-C7-C8-C10
21	4	411	CL7	C11-C12-C13-C15
21	b	604	CL7	C11-C10-C8-C7
21	b	605	CL7	C12-C13-C15-C16
21	b	606	CL7	C12-C13-C15-C16
21	b	610	CL7	C6-C7-C8-C10
21	b	613	CL7	C11-C10-C8-C7
21	c	504	CL7	C11-C10-C8-C7
21	c	506	CL7	C12-C13-C15-C16
21	c	507	CL7	C11-C10-C8-C7
21	c	511	CL7	C12-C13-C15-C16
21	6	503	CL7	C12-C13-C15-C16
21	6	507	CL7	C11-C10-C8-C7
21	6	510	CL7	C6-C7-C8-C10
21	6	510	CL7	C11-C10-C8-C7
21	5	408	CL7	C11-C10-C8-C7
21	7	501	CL7	C12-C13-C15-C16
21	7	507	CL7	C6-C7-C8-C10
21	8	411	CL7	C11-C12-C13-C15
21	3	516	CL7	C4C-C3C-CAC-CBC
21	B	612	CL7	C11-C10-C8-C9
21	C	511	CL7	C14-C13-C15-C16
21	2	501	CL7	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	2	503	CL7	C14-C13-C15-C16
21	2	505	CL7	C11-C10-C8-C9
21	2	512	CL7	C11-C10-C8-C9
21	1	402	CL7	C6-C7-C8-C9
21	1	406	CL7	C14-C13-C15-C16
21	1	418	CL7	C14-C13-C15-C16
21	3	501	CL7	C14-C13-C15-C16
21	3	503	CL7	C6-C7-C8-C9
21	3	503	CL7	C11-C10-C8-C9
21	3	504	CL7	C11-C12-C13-C14
21	3	509	CL7	C11-C10-C8-C9
21	3	511	CL7	C14-C13-C15-C16
21	b	613	CL7	C11-C10-C8-C9
21	c	511	CL7	C14-C13-C15-C16
21	6	501	CL7	C6-C7-C8-C9
21	6	503	CL7	C14-C13-C15-C16
21	6	505	CL7	C11-C10-C8-C9
21	6	512	CL7	C11-C10-C8-C9
21	5	402	CL7	C6-C7-C8-C9
21	5	406	CL7	C14-C13-C15-C16
21	5	418	CL7	C14-C13-C15-C16
21	7	501	CL7	C14-C13-C15-C16
21	7	503	CL7	C6-C7-C8-C9
21	7	503	CL7	C11-C10-C8-C9
21	7	504	CL7	C11-C12-C13-C14
21	7	509	CL7	C11-C10-C8-C9
21	7	511	CL7	C14-C13-C15-C16
21	7	516	CL7	C4C-C3C-CAC-CBC
21	1	402	CL7	C5-C6-C7-C8
21	4	413	CL7	C10-C11-C12-C13
21	5	402	CL7	C5-C6-C7-C8
21	8	413	CL7	C10-C11-C12-C13
21	3	517	CL7	O1D-CGD-O2D-CED
21	7	517	CL7	O1D-CGD-O2D-CED
23	K	101	8CT	C10-C11-C12-C40
23	k	101	8CT	C10-C11-C12-C40
32	3	520	ZEX	C31-C32-C33-C40
32	4	420	ZEX	C11-C12-C13-C20
32	7	520	ZEX	C31-C32-C33-C40
32	8	420	ZEX	C11-C12-C13-C20
23	B	619	8CT	C25-C26-C28-C29
23	K	101	8CT	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
23	b	620	8CT	C25-C26-C28-C29
23	k	101	8CT	C10-C11-C12-C13
32	2	525	ZEX	C7-C8-C9-C10
32	6	524	ZEX	C7-C8-C9-C10
21	3	504	CL7	C4C-C3C-CAC-CBC
21	7	504	CL7	C4C-C3C-CAC-CBC
21	3	502	CL7	C4-C3-C5-C6
21	2	518	CL7	C15-C16-C17-C18
21	6	518	CL7	C15-C16-C17-C18
26	c	501	LMG	C12-C13-C14-C15
21	B	616	CL7	O1D-CGD-O2D-CED
21	b	617	CL7	O1D-CGD-O2D-CED
21	C	506	CL7	C3A-C2A-CAA-CBA
21	C	510	CL7	C3A-C2A-CAA-CBA
21	2	503	CL7	C3A-C2A-CAA-CBA
21	2	515	CL7	C3A-C2A-CAA-CBA
21	1	405	CL7	C3A-C2A-CAA-CBA
21	1	418	CL7	C3A-C2A-CAA-CBA
21	3	501	CL7	C3A-C2A-CAA-CBA
21	3	503	CL7	C3A-C2A-CAA-CBA
21	4	411	CL7	C3A-C2A-CAA-CBA
21	c	506	CL7	C3A-C2A-CAA-CBA
21	c	510	CL7	C3A-C2A-CAA-CBA
21	6	503	CL7	C3A-C2A-CAA-CBA
21	6	515	CL7	C3A-C2A-CAA-CBA
21	5	405	CL7	C3A-C2A-CAA-CBA
21	5	418	CL7	C3A-C2A-CAA-CBA
21	7	501	CL7	C3A-C2A-CAA-CBA
21	7	503	CL7	C3A-C2A-CAA-CBA
21	8	411	CL7	C3A-C2A-CAA-CBA
23	A	404	8CT	C23-C24-C25-C26
23	a	404	8CT	C23-C24-C25-C26
21	C	502	CL7	CBD-CGD-O2D-CED
21	3	505	CL7	C2C-C3C-CAC-CBC
21	7	505	CL7	C2C-C3C-CAC-CBC
21	C	505	CL7	C6-C7-C8-C10
21	c	505	CL7	C6-C7-C8-C10
27	B	624	DGD	C6B-C7B-C8B-C9B
27	b	625	DGD	C6B-C7B-C8B-C9B
21	B	612	CL7	C10-C11-C12-C13
21	b	613	CL7	C10-C11-C12-C13
21	c	502	CL7	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
22	A	402	PHO	O2A-C1-C2-C3
22	a	402	PHO	O2A-C1-C2-C3
21	3	503	CL7	C10-C11-C12-C13
21	7	503	CL7	C8-C10-C11-C12
21	7	503	CL7	C10-C11-C12-C13
21	2	511	CL7	C3-C5-C6-C7
21	6	511	CL7	C3-C5-C6-C7
21	3	503	CL7	C8-C10-C11-C12
21	B	613	CL7	C4-C3-C5-C6
21	b	614	CL7	C4-C3-C5-C6
25	A	407	LHG	C3-O3-P-O6
25	a	406	LHG	C3-O3-P-O6
21	C	503	CL7	C10-C11-C12-C13
21	c	503	CL7	C10-C11-C12-C13
21	C	506	CL7	C4C-C3C-CAC-CBC
21	c	506	CL7	C4C-C3C-CAC-CBC
25	B	625	LHG	C1-C2-C3-O3
25	b	626	LHG	C1-C2-C3-O3
21	2	501	CL7	C2-C1-O2A-CGA
21	2	509	CL7	C2-C1-O2A-CGA
21	1	402	CL7	C2-C1-O2A-CGA
21	1	417	CL7	C2-C1-O2A-CGA
21	6	501	CL7	C2-C1-O2A-CGA
21	6	509	CL7	C2-C1-O2A-CGA
21	5	402	CL7	C2-C1-O2A-CGA
21	5	417	CL7	C2-C1-O2A-CGA
21	B	604	CL7	C13-C15-C16-C17
21	B	607	CL7	C11-C10-C8-C9
21	C	508	CL7	C6-C7-C8-C9
21	C	508	CL7	C14-C13-C15-C16
21	2	503	CL7	C11-C10-C8-C9
21	2	509	CL7	C14-C13-C15-C16
21	2	511	CL7	C11-C10-C8-C9
21	2	518	CL7	C14-C13-C15-C16
21	3	503	CL7	C14-C13-C15-C16
21	3	508	CL7	C6-C7-C8-C9
21	3	508	CL7	C14-C13-C15-C16
21	b	608	CL7	C11-C10-C8-C9
21	c	508	CL7	C6-C7-C8-C9
21	c	508	CL7	C14-C13-C15-C16
21	6	503	CL7	C11-C10-C8-C9
21	6	509	CL7	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
21	6	511	CL7	C11-C10-C8-C9
21	6	518	CL7	C14-C13-C15-C16
21	7	503	CL7	C14-C13-C15-C16
21	7	508	CL7	C6-C7-C8-C9
21	7	508	CL7	C14-C13-C15-C16
26	c	501	LMG	C38-C39-C40-C41
27	B	624	DGD	CBB-CCB-CDB-CEB
27	b	625	DGD	CBB-CCB-CDB-CEB
21	1	408	CL7	C13-C15-C16-C17
21	b	605	CL7	C13-C15-C16-C17
21	5	408	CL7	C13-C15-C16-C17
32	4	403	ZEX	C21-C26-C27-C28
32	8	403	ZEX	C21-C26-C27-C28
26	C	501	LMG	C38-C39-C40-C41
21	C	502	CL7	C16-C17-C18-C20
21	c	502	CL7	C16-C17-C18-C20
23	B	618	8CT	C02-C03-C10-C11
23	B	627	8CT	C04-C03-C10-C11
23	4	402	8CT	C02-C03-C10-C11
23	b	601	8CT	C04-C03-C10-C11
23	b	619	8CT	C02-C03-C10-C11
23	8	402	8CT	C02-C03-C10-C11
32	2	521	ZEX	C1-C6-C7-C8
32	3	520	ZEX	C1-C6-C7-C8
32	3	520	ZEX	C5-C6-C7-C8
32	4	418	ZEX	C1-C6-C7-C8
32	4	418	ZEX	C5-C6-C7-C8
32	4	420	ZEX	C1-C6-C7-C8
32	4	420	ZEX	C5-C6-C7-C8
32	6	520	ZEX	C1-C6-C7-C8
32	7	520	ZEX	C1-C6-C7-C8
32	7	520	ZEX	C5-C6-C7-C8
32	8	418	ZEX	C1-C6-C7-C8
32	8	418	ZEX	C5-C6-C7-C8
32	8	420	ZEX	C1-C6-C7-C8
32	8	420	ZEX	C5-C6-C7-C8
21	8	406	CL7	O1D-CGD-O2D-CED
23	B	619	8CT	C27-C26-C28-C29
23	b	620	8CT	C27-C26-C28-C29
21	4	406	CL7	O1D-CGD-O2D-CED
21	4	416	CL7	O1D-CGD-O2D-CED
21	8	416	CL7	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	515	8CT	C20-C21-C23-C24
23	c	515	8CT	C20-C21-C23-C24
21	3	511	CL7	C5-C6-C7-C8
21	7	511	CL7	C5-C6-C7-C8
30	d	407	PL9	C17-C18-C19-C20
21	4	405	CL7	C16-C17-C18-C19
21	8	405	CL7	C16-C17-C18-C19
25	4	401	LHG	O6-C4-C5-C6
25	8	401	LHG	O6-C4-C5-C6
21	B	608	CL7	C11-C10-C8-C7
21	C	502	CL7	C12-C13-C15-C16
21	C	510	CL7	C12-C13-C15-C16
21	D	404	CL7	C11-C10-C8-C7
21	2	512	CL7	C11-C10-C8-C7
21	1	402	CL7	C6-C7-C8-C10
21	1	404	CL7	C11-C12-C13-C15
21	3	503	CL7	C6-C7-C8-C10
21	3	508	CL7	C12-C13-C15-C16
21	3	509	CL7	C11-C10-C8-C7
21	3	511	CL7	C11-C10-C8-C7
21	4	404	CL7	C11-C10-C8-C7
21	b	609	CL7	C11-C10-C8-C7
21	c	502	CL7	C12-C13-C15-C16
21	c	510	CL7	C12-C13-C15-C16
21	d	404	CL7	C11-C10-C8-C7
21	6	512	CL7	C11-C10-C8-C7
21	5	402	CL7	C6-C7-C8-C10
21	5	404	CL7	C11-C12-C13-C15
21	7	503	CL7	C6-C7-C8-C10
21	7	508	CL7	C12-C13-C15-C16
21	7	509	CL7	C11-C10-C8-C7
21	7	511	CL7	C11-C10-C8-C7
21	8	404	CL7	C11-C10-C8-C7
21	4	406	CL7	C5-C6-C7-C8
21	8	406	CL7	C5-C6-C7-C8
23	C	516	8CT	C16-C17-C18-C19
23	c	516	8CT	C16-C17-C18-C19
21	2	517	CL7	C16-C17-C18-C19
21	6	517	CL7	C16-C17-C18-C19
21	3	516	CL7	C5-C6-C7-C8
21	7	516	CL7	C5-C6-C7-C8
21	1	403	CL7	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	3	514	CL7	C2A-CAA-CBA-CGA
21	5	403	CL7	C2A-CAA-CBA-CGA
21	7	514	CL7	C2A-CAA-CBA-CGA
27	C	517	DGD	C2A-C1A-O1G-C1G
27	c	517	DGD	C2A-C1A-O1G-C1G
26	C	501	LMG	C39-C40-C41-C42
21	B	603	CL7	CAD-CBD-CGD-O2D
21	B	604	CL7	CAD-CBD-CGD-O2D
21	B	612	CL7	CAD-CBD-CGD-O2D
21	B	613	CL7	CAD-CBD-CGD-O2D
21	B	622	CL7	CAD-CBD-CGD-O2D
21	C	502	CL7	CAD-CBD-CGD-O2D
21	C	503	CL7	CAD-CBD-CGD-O2D
21	C	506	CL7	CAD-CBD-CGD-O2D
21	2	505	CL7	CAD-CBD-CGD-O2D
21	2	509	CL7	CAD-CBD-CGD-O2D
21	2	515	CL7	CAD-CBD-CGD-O2D
21	1	404	CL7	CAD-CBD-CGD-O2D
21	1	410	CL7	CAD-CBD-CGD-O2D
21	1	411	CL7	CAD-CBD-CGD-O2D
21	1	412	CL7	CAD-CBD-CGD-O2D
21	3	504	CL7	CAD-CBD-CGD-O2D
21	3	509	CL7	CAD-CBD-CGD-O2D
21	3	510	CL7	CAD-CBD-CGD-O2D
21	4	411	CL7	CAD-CBD-CGD-O2D
21	a	401	CL7	CAD-CBD-CGD-O2D
21	b	604	CL7	CAD-CBD-CGD-O2D
21	b	605	CL7	CAD-CBD-CGD-O2D
21	b	613	CL7	CAD-CBD-CGD-O2D
21	b	614	CL7	CAD-CBD-CGD-O2D
21	b	623	CL7	CAD-CBD-CGD-O2D
21	c	502	CL7	CAD-CBD-CGD-O2D
21	c	503	CL7	CAD-CBD-CGD-O2D
21	c	506	CL7	CAD-CBD-CGD-O2D
21	6	505	CL7	CAD-CBD-CGD-O2D
21	6	509	CL7	CAD-CBD-CGD-O2D
21	6	515	CL7	CAD-CBD-CGD-O2D
21	5	404	CL7	CAD-CBD-CGD-O2D
21	5	410	CL7	CAD-CBD-CGD-O2D
21	5	411	CL7	CAD-CBD-CGD-O2D
21	5	412	CL7	CAD-CBD-CGD-O2D
21	7	504	CL7	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	7	509	CL7	CAD-CBD-CGD-O2D
21	7	510	CL7	CAD-CBD-CGD-O2D
21	8	411	CL7	CAD-CBD-CGD-O2D
22	D	408	PHO	CAD-CBD-CGD-O2D
22	d	408	PHO	CAD-CBD-CGD-O2D
30	D	407	PL9	C17-C18-C19-C20
21	B	606	CL7	C5-C6-C7-C8
21	3	507	CL7	C15-C16-C17-C18
21	4	406	CL7	C8-C10-C11-C12
21	b	607	CL7	C5-C6-C7-C8
21	7	507	CL7	C15-C16-C17-C18
21	8	406	CL7	C8-C10-C11-C12
21	C	505	CL7	C6-C7-C8-C9
21	2	507	CL7	C16-C17-C18-C19
21	c	505	CL7	C6-C7-C8-C9
21	6	507	CL7	C16-C17-C18-C19
26	D	410	LMG	O6-C1-O1-C7
26	d	410	LMG	O6-C1-O1-C7
21	3	507	CL7	C10-C11-C12-C13
21	7	507	CL7	C10-C11-C12-C13
25	3	524	LHG	C2-C3-O3-P
25	7	524	LHG	C2-C3-O3-P
25	4	401	LHG	O6-C4-C5-O7
25	8	401	LHG	O6-C4-C5-O7
21	1	418	CL7	C8-C10-C11-C12
21	5	418	CL7	C8-C10-C11-C12
21	B	616	CL7	C2A-CAA-CBA-CGA
21	b	617	CL7	C2A-CAA-CBA-CGA
21	B	605	CL7	CHA-CBD-CGD-O1D
21	B	608	CL7	CHA-CBD-CGD-O1D
21	B	610	CL7	CHA-CBD-CGD-O1D
21	B	615	CL7	CHA-CBD-CGD-O2D
21	B	615	CL7	CHA-CBD-CGD-O1D
21	C	505	CL7	CHA-CBD-CGD-O1D
21	C	510	CL7	CHA-CBD-CGD-O2D
21	C	510	CL7	CHA-CBD-CGD-O1D
21	2	502	CL7	CHA-CBD-CGD-O1D
21	2	506	CL7	CHA-CBD-CGD-O2D
21	2	506	CL7	CHA-CBD-CGD-O1D
21	2	513	CL7	CHA-CBD-CGD-O2D
21	1	408	CL7	CHA-CBD-CGD-O2D
21	1	408	CL7	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	3	502	CL7	CHA-CBD-CGD-O1D
21	3	506	CL7	CHA-CBD-CGD-O2D
21	4	409	CL7	CHA-CBD-CGD-O2D
21	4	409	CL7	CHA-CBD-CGD-O1D
21	b	606	CL7	CHA-CBD-CGD-O1D
21	b	609	CL7	CHA-CBD-CGD-O1D
21	b	611	CL7	CHA-CBD-CGD-O1D
21	b	616	CL7	CHA-CBD-CGD-O2D
21	b	616	CL7	CHA-CBD-CGD-O1D
21	c	505	CL7	CHA-CBD-CGD-O1D
21	c	510	CL7	CHA-CBD-CGD-O2D
21	c	510	CL7	CHA-CBD-CGD-O1D
21	6	502	CL7	CHA-CBD-CGD-O1D
21	6	506	CL7	CHA-CBD-CGD-O2D
21	6	506	CL7	CHA-CBD-CGD-O1D
21	6	513	CL7	CHA-CBD-CGD-O2D
21	5	408	CL7	CHA-CBD-CGD-O2D
21	5	408	CL7	CHA-CBD-CGD-O1D
21	7	502	CL7	CHA-CBD-CGD-O1D
21	7	506	CL7	CHA-CBD-CGD-O2D
21	8	409	CL7	CHA-CBD-CGD-O2D
21	8	409	CL7	CHA-CBD-CGD-O1D
21	4	415	CL7	O1D-CGD-O2D-CED
21	8	415	CL7	O1D-CGD-O2D-CED
21	A	401	CL7	O1A-CGA-O2A-C1
21	a	401	CL7	O1A-CGA-O2A-C1
26	c	501	LMG	C39-C40-C41-C42
21	4	404	CL7	C16-C17-C18-C20
21	8	404	CL7	C16-C17-C18-C20
21	7	512	CL7	O1D-CGD-O2D-CED
21	C	508	CL7	C11-C10-C8-C9
21	C	511	CL7	C6-C7-C8-C9
21	c	508	CL7	C11-C10-C8-C9
21	c	511	CL7	C6-C7-C8-C9
21	3	512	CL7	O1D-CGD-O2D-CED
21	B	601	CL7	C4C-C3C-CAC-CBC
21	b	602	CL7	C4C-C3C-CAC-CBC
21	2	505	CL7	C8-C10-C11-C12
21	6	505	CL7	C8-C10-C11-C12
21	C	506	CL7	C2A-CAA-CBA-CGA
21	c	506	CL7	C2A-CAA-CBA-CGA
23	A	404	8CT	C22-C21-C23-C24

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Mol	Chain	Res	Type	Atoms
23	B	617	8CT	C10-C11-C12-C40
23	a	404	8CT	C22-C21-C23-C24
23	b	618	8CT	C10-C11-C12-C40
32	2	525	ZEX	C7-C8-C9-C19
32	6	524	ZEX	C7-C8-C9-C19
23	B	617	8CT	C10-C11-C12-C13
23	b	618	8CT	C10-C11-C12-C13
21	1	404	CL7	C1A-C2A-CAA-CBA
21	c	509	CL7	C1A-C2A-CAA-CBA
21	5	404	CL7	C1A-C2A-CAA-CBA
21	2	512	CL7	C16-C17-C18-C20
21	6	512	CL7	C16-C17-C18-C20
21	b	612	CL7	C10-C11-C12-C13
21	B	614	CL7	C2-C1-O2A-CGA
21	4	409	CL7	C2-C1-O2A-CGA
21	b	615	CL7	C2-C1-O2A-CGA
21	8	409	CL7	C2-C1-O2A-CGA
21	B	611	CL7	C10-C11-C12-C13
21	2	512	CL7	C4-C3-C5-C6
21	6	512	CL7	C4-C3-C5-C6
21	1	402	CL7	C2-C3-C5-C6
21	5	402	CL7	C2-C3-C5-C6
25	D	409	LHG	C3-O3-P-O4
25	D	409	LHG	C4-O6-P-O4
25	3	524	LHG	C3-O3-P-O5
25	4	401	LHG	C4-O6-P-O4
25	d	409	LHG	C3-O3-P-O4
25	d	409	LHG	C4-O6-P-O4
25	7	524	LHG	C3-O3-P-O5
25	8	401	LHG	C4-O6-P-O4
25	b	624	LHG	C10-C11-C12-C13
21	C	506	CL7	C8-C10-C11-C12
21	c	506	CL7	C8-C10-C11-C12
21	2	508	CL7	C2A-CAA-CBA-CGA
21	6	508	CL7	C2A-CAA-CBA-CGA
25	B	623	LHG	C10-C11-C12-C13
21	2	503	CL7	C16-C17-C18-C19
21	6	503	CL7	C16-C17-C18-C19
21	B	601	CL7	CAD-CBD-CGD-O1D
21	2	502	CL7	CAD-CBD-CGD-O1D
21	2	506	CL7	CAD-CBD-CGD-O1D
21	2	511	CL7	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
21	2	513	CL7	CAD-CBD-CGD-O1D
21	1	409	CL7	CAD-CBD-CGD-O1D
21	b	602	CL7	CAD-CBD-CGD-O1D
21	6	502	CL7	CAD-CBD-CGD-O1D
21	6	506	CL7	CAD-CBD-CGD-O1D
21	6	511	CL7	CAD-CBD-CGD-O1D
21	6	513	CL7	CAD-CBD-CGD-O1D
21	5	409	CL7	CAD-CBD-CGD-O1D
24	B	620	SQD	O5-C5-C6-S
24	b	621	SQD	O5-C5-C6-S
21	2	505	CL7	C4C-C3C-CAC-CBC
21	6	505	CL7	C4C-C3C-CAC-CBC
21	C	510	CL7	C16-C17-C18-C19
21	c	510	CL7	C16-C17-C18-C19
21	B	604	CL7	CBD-CGD-O2D-CED
21	3	516	CL7	C4-C3-C5-C6
21	7	516	CL7	C4-C3-C5-C6
21	B	605	CL7	C6-C7-C8-C10
21	B	611	CL7	C11-C10-C8-C7
21	B	611	CL7	C11-C12-C13-C15
21	C	502	CL7	C11-C10-C8-C7
21	C	511	CL7	C11-C12-C13-C15
21	2	506	CL7	C11-C12-C13-C15
21	2	508	CL7	C3A-C2A-CAA-CBA
21	1	412	CL7	C3A-C2A-CAA-CBA
21	3	501	CL7	C6-C7-C8-C10
21	3	501	CL7	C11-C12-C13-C15
21	3	509	CL7	C12-C13-C15-C16
21	3	510	CL7	C3A-C2A-CAA-CBA
21	3	513	CL7	C3A-C2A-CAA-CBA
21	4	404	CL7	C6-C7-C8-C10
21	4	409	CL7	C11-C10-C8-C7
21	b	606	CL7	C6-C7-C8-C10
21	b	612	CL7	C11-C10-C8-C7
21	b	612	CL7	C11-C12-C13-C15
21	c	502	CL7	C11-C10-C8-C7
21	c	511	CL7	C11-C12-C13-C15
21	6	506	CL7	C11-C12-C13-C15
21	6	508	CL7	C3A-C2A-CAA-CBA
21	5	412	CL7	C3A-C2A-CAA-CBA
21	7	501	CL7	C6-C7-C8-C10
21	7	501	CL7	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
21	7	509	CL7	C12-C13-C15-C16
21	7	510	CL7	C3A-C2A-CAA-CBA
21	7	513	CL7	C3A-C2A-CAA-CBA
21	8	404	CL7	C6-C7-C8-C10
21	8	409	CL7	C11-C10-C8-C7
23	B	627	8CT	C28-C29-C30-C31
23	C	515	8CT	C28-C29-C30-C31
23	4	402	8CT	C28-C29-C30-C31
23	b	601	8CT	C28-C29-C30-C31
23	c	515	8CT	C28-C29-C30-C31
23	8	402	8CT	C28-C29-C30-C31
23	B	617	8CT	C16-C17-C18-C19
23	b	618	8CT	C16-C17-C18-C19
32	4	419	ZEX	C33-C34-C35-C15
32	8	419	ZEX	C33-C34-C35-C15
21	b	605	CL7	CBD-CGD-O2D-CED
24	7	523	SQD	C9-C10-C11-C12
21	4	411	CL7	C5-C6-C7-C8
21	4	412	CL7	C5-C6-C7-C8
21	8	412	CL7	C5-C6-C7-C8
24	3	523	SQD	C9-C10-C11-C12
27	c	517	DGD	O1A-C1A-O1G-C1G
21	8	411	CL7	C5-C6-C7-C8
21	A	406	CL7	C16-C17-C18-C19
21	2	517	CL7	C16-C17-C18-C20
21	a	405	CL7	C16-C17-C18-C19
27	C	517	DGD	O1A-C1A-O1G-C1G
24	2	522	SQD	O47-C45-C46-O48
24	6	521	SQD	O47-C45-C46-O48
26	B	621	LMG	O7-C8-C9-O8
26	b	622	LMG	O7-C8-C9-O8
24	2	522	SQD	C45-C44-O6-C1
24	3	521	SQD	C45-C44-O6-C1
24	6	521	SQD	C45-C44-O6-C1
24	7	521	SQD	C45-C44-O6-C1
21	B	614	CL7	C11-C12-C13-C15
21	b	615	CL7	C11-C12-C13-C15
21	6	517	CL7	C16-C17-C18-C20
21	6	503	CL7	C13-C15-C16-C17
21	C	502	CL7	O1D-CGD-O2D-CED
21	c	502	CL7	O1D-CGD-O2D-CED
21	2	503	CL7	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
30	D	407	PL9	C35-C34-C36-C37
30	D	407	PL9	C45-C44-C46-C47
30	d	407	PL9	C35-C34-C36-C37
30	d	407	PL9	C45-C44-C46-C47
21	A	401	CL7	CBA-CGA-O2A-C1
21	a	401	CL7	CBA-CGA-O2A-C1
24	B	620	SQD	C17-C18-C19-C20
24	A	405	SQD	C9-C10-C11-C12
24	B	626	SQD	C9-C10-C11-C12
24	b	621	SQD	C17-C18-C19-C20
21	B	609	CL7	C6-C7-C8-C9
21	C	502	CL7	C11-C10-C8-C9
21	C	502	CL7	C14-C13-C15-C16
21	C	503	CL7	C6-C7-C8-C9
21	2	501	CL7	C11-C10-C8-C9
21	2	502	CL7	C11-C10-C8-C9
21	2	507	CL7	C11-C10-C8-C9
21	2	507	CL7	C11-C12-C13-C14
21	2	511	CL7	C6-C7-C8-C9
21	1	404	CL7	C11-C12-C13-C14
21	3	509	CL7	C11-C12-C13-C14
21	3	510	CL7	C6-C7-C8-C9
21	3	511	CL7	C6-C7-C8-C9
21	4	405	CL7	C11-C12-C13-C14
21	4	406	CL7	C6-C7-C8-C9
21	4	409	CL7	C11-C10-C8-C9
21	4	411	CL7	C11-C12-C13-C14
21	b	610	CL7	C6-C7-C8-C9
21	c	502	CL7	C11-C10-C8-C9
21	c	502	CL7	C14-C13-C15-C16
21	c	503	CL7	C6-C7-C8-C9
21	6	501	CL7	C11-C10-C8-C9
21	6	502	CL7	C11-C10-C8-C9
21	6	507	CL7	C11-C10-C8-C9
21	6	507	CL7	C11-C12-C13-C14
21	6	511	CL7	C6-C7-C8-C9
21	5	404	CL7	C11-C12-C13-C14
21	7	509	CL7	C11-C12-C13-C14
21	7	510	CL7	C6-C7-C8-C9
21	7	511	CL7	C6-C7-C8-C9
21	8	405	CL7	C11-C12-C13-C14
21	8	406	CL7	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
21	8	409	CL7	C11-C10-C8-C9
21	8	411	CL7	C11-C12-C13-C14
21	3	505	CL7	C16-C17-C18-C19
21	7	505	CL7	C16-C17-C18-C19
32	3	520	ZEX	C31-C32-C33-C34
32	7	520	ZEX	C31-C32-C33-C34
21	3	510	CL7	CAA-CBA-CGA-O2A
21	7	510	CL7	CAA-CBA-CGA-O2A
21	B	608	CL7	C8-C10-C11-C12
21	4	405	CL7	C16-C17-C18-C20
27	C	517	DGD	CDB-CEB-CFB-CGB
27	c	517	DGD	CDB-CEB-CFB-CGB
21	B	611	CL7	C13-C15-C16-C17
21	b	609	CL7	C8-C10-C11-C12
21	b	612	CL7	C13-C15-C16-C17
21	2	516	CL7	C2A-CAA-CBA-CGA
21	6	516	CL7	C2A-CAA-CBA-CGA
21	B	602	CL7	C2-C1-O2A-CGA
21	2	516	CL7	C2-C1-O2A-CGA
21	1	410	CL7	C2-C1-O2A-CGA
21	3	517	CL7	C2-C1-O2A-CGA
21	4	405	CL7	C2-C1-O2A-CGA
21	b	603	CL7	C2-C1-O2A-CGA
21	6	516	CL7	C2-C1-O2A-CGA
21	5	410	CL7	C2-C1-O2A-CGA
21	7	517	CL7	C2-C1-O2A-CGA
21	8	405	CL7	C2-C1-O2A-CGA
25	b	624	LHG	C28-C29-C30-C31
26	1	401	LMG	C37-C38-C39-C40
26	5	401	LMG	C37-C38-C39-C40
21	8	405	CL7	C16-C17-C18-C20
25	B	623	LHG	C28-C29-C30-C31
32	2	520	ZEX	C21-C26-C27-C28
32	3	525	ZEX	C21-C26-C27-C28
25	B	625	LHG	C11-C12-C13-C14
21	1	418	CL7	C4-C3-C5-C6
21	5	418	CL7	C4-C3-C5-C6
21	2	507	CL7	C2-C3-C5-C6
21	6	507	CL7	C2-C3-C5-C6
24	B	620	SQD	C14-C15-C16-C17
25	b	626	LHG	C11-C12-C13-C14
24	b	621	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	2	518	CL7	C2A-CAA-CBA-CGA
21	6	518	CL7	C2A-CAA-CBA-CGA
24	3	523	SQD	O47-C45-C46-O48
24	7	523	SQD	O47-C45-C46-O48
22	D	408	PHO	CHA-CBD-CGD-O1D
22	d	408	PHO	CHA-CBD-CGD-O1D
21	C	508	CL7	C12-C13-C15-C16
21	2	501	CL7	C11-C10-C8-C7
21	2	502	CL7	C6-C7-C8-C10
21	2	502	CL7	C11-C10-C8-C7
21	2	516	CL7	C12-C13-C15-C16
21	3	502	CL7	C2-C3-C5-C6
21	3	507	CL7	C11-C10-C8-C7
21	3	507	CL7	C12-C13-C15-C16
21	c	508	CL7	C12-C13-C15-C16
21	6	501	CL7	C11-C10-C8-C7
21	6	502	CL7	C6-C7-C8-C10
21	6	502	CL7	C11-C10-C8-C7
21	6	516	CL7	C12-C13-C15-C16
21	7	502	CL7	C2-C3-C5-C6
21	7	507	CL7	C11-C10-C8-C7
21	7	507	CL7	C12-C13-C15-C16
21	B	605	CL7	C6-C7-C8-C9
21	2	502	CL7	C6-C7-C8-C9
21	2	506	CL7	C11-C12-C13-C14
21	2	512	CL7	C11-C12-C13-C14
21	3	501	CL7	C6-C7-C8-C9
21	4	404	CL7	C6-C7-C8-C9
21	b	606	CL7	C6-C7-C8-C9
21	6	502	CL7	C6-C7-C8-C9
21	6	506	CL7	C11-C12-C13-C14
21	6	512	CL7	C11-C12-C13-C14
21	7	501	CL7	C6-C7-C8-C9
21	8	404	CL7	C6-C7-C8-C9
21	B	611	CL7	C15-C16-C17-C18
21	b	612	CL7	C15-C16-C17-C18
32	1	421	ZEX	C9-C10-C11-C12
32	5	421	ZEX	C9-C10-C11-C12
21	B	603	CL7	C16-C17-C18-C20
21	b	604	CL7	C16-C17-C18-C20
27	B	624	DGD	CCA-CDA-CEA-CFA
21	3	505	CL7	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	7	505	CL7	C2A-CAA-CBA-CGA
26	B	621	LMG	C36-C37-C38-C39
27	b	625	DGD	CCA-CDA-CEA-CFA
26	b	622	LMG	C36-C37-C38-C39
21	3	503	CL7	C13-C15-C16-C17
21	7	503	CL7	C13-C15-C16-C17
21	4	404	CL7	C16-C17-C18-C19
21	8	404	CL7	C16-C17-C18-C19
27	B	624	DGD	C8B-C9B-CAB-CBB
27	b	625	DGD	C8B-C9B-CAB-CBB
21	C	504	CL7	CAA-CBA-CGA-O2A
21	1	418	CL7	CAA-CBA-CGA-O2A
21	c	504	CL7	CAA-CBA-CGA-O2A
21	5	418	CL7	CAA-CBA-CGA-O2A
21	3	509	CL7	C15-C16-C17-C18
21	7	509	CL7	C15-C16-C17-C18
21	1	402	CL7	CBD-CGD-O2D-CED
21	5	402	CL7	CBD-CGD-O2D-CED
21	4	411	CL7	C16-C17-C18-C20
21	8	411	CL7	C16-C17-C18-C20
32	1	421	ZEX	C33-C34-C35-C15
32	4	419	ZEX	C9-C10-C11-C12
32	4	420	ZEX	C9-C10-C11-C12
32	5	421	ZEX	C33-C34-C35-C15
32	8	419	ZEX	C9-C10-C11-C12
32	8	420	ZEX	C9-C10-C11-C12
30	D	407	PL9	C16-C17-C18-C19
30	d	407	PL9	C16-C17-C18-C19
21	4	408	CL7	CAA-CBA-CGA-O2A
21	8	408	CL7	CAA-CBA-CGA-O2A
21	C	503	CL7	C2-C1-O2A-CGA
21	1	403	CL7	C2-C1-O2A-CGA
21	4	412	CL7	C2-C1-O2A-CGA
21	c	503	CL7	C2-C1-O2A-CGA
21	5	403	CL7	C2-C1-O2A-CGA
21	8	412	CL7	C2-C1-O2A-CGA
21	D	405	CL7	C4C-C3C-CAC-CBC
21	d	405	CL7	C4C-C3C-CAC-CBC
21	B	614	CL7	C11-C12-C13-C14
21	2	507	CL7	C16-C17-C18-C20
21	b	615	CL7	C11-C12-C13-C14
21	6	507	CL7	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	3	513	CL7	C2A-CAA-CBA-CGA
21	7	513	CL7	C2A-CAA-CBA-CGA
21	b	605	CL7	O1D-CGD-O2D-CED
21	3	505	CL7	C3A-C2A-CAA-CBA
21	7	505	CL7	C3A-C2A-CAA-CBA
21	B	604	CL7	O1D-CGD-O2D-CED
21	B	606	CL7	C6-C7-C8-C9
21	1	418	CL7	C16-C17-C18-C19
21	5	418	CL7	C16-C17-C18-C19
32	4	403	ZEX	C33-C34-C35-C15
32	8	403	ZEX	C33-C34-C35-C15
21	3	506	CL7	C2C-C3C-CAC-CBC
21	A	401	CL7	C11-C10-C8-C9
21	B	611	CL7	C14-C13-C15-C16
21	2	506	CL7	C11-C10-C8-C9
21	1	406	CL7	C11-C12-C13-C14
21	3	502	CL7	C11-C10-C8-C9
21	4	406	CL7	C14-C13-C15-C16
21	4	413	CL7	C11-C10-C8-C9
21	a	401	CL7	C11-C10-C8-C9
21	b	612	CL7	C14-C13-C15-C16
21	6	506	CL7	C11-C10-C8-C9
21	5	406	CL7	C11-C12-C13-C14
21	7	502	CL7	C11-C10-C8-C9
21	8	406	CL7	C14-C13-C15-C16
21	8	413	CL7	C11-C10-C8-C9
21	1	417	CL7	C6-C7-C8-C9
21	1	418	CL7	C16-C17-C18-C20
21	b	607	CL7	C6-C7-C8-C9
21	5	417	CL7	C6-C7-C8-C9
21	5	418	CL7	C16-C17-C18-C20
21	7	506	CL7	C2C-C3C-CAC-CBC
21	3	506	CL7	CAA-CBA-CGA-O1A
21	7	506	CL7	CAA-CBA-CGA-O1A
21	2	505	CL7	C13-C15-C16-C17
21	6	505	CL7	C13-C15-C16-C17
23	B	627	8CT	C39-C16-C17-C18
23	b	601	8CT	C39-C16-C17-C18
31	F	101	HEM	CAA-CBA-CGA-O1A
31	f	101	HEM	CAA-CBA-CGA-O1A
21	C	509	CL7	C16-C17-C18-C20
21	c	509	CL7	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
21	A	406	CL7	O2A-C1-C2-C3
21	C	511	CL7	O2A-C1-C2-C3
21	2	509	CL7	O2A-C1-C2-C3
21	a	405	CL7	O2A-C1-C2-C3
21	c	511	CL7	O2A-C1-C2-C3
21	6	509	CL7	O2A-C1-C2-C3
21	B	615	CL7	C2C-C3C-CAC-CBC
21	b	616	CL7	C2C-C3C-CAC-CBC
31	F	101	HEM	CAD-CBD-CGD-O1D
31	f	101	HEM	CAD-CBD-CGD-O1D
24	B	620	SQD	C46-C45-O47-C7
24	b	621	SQD	C46-C45-O47-C7
21	2	506	CL7	C1A-C2A-CAA-CBA
21	2	515	CL7	C1A-C2A-CAA-CBA
21	4	405	CL7	C1A-C2A-CAA-CBA
21	6	506	CL7	C1A-C2A-CAA-CBA
21	6	515	CL7	C1A-C2A-CAA-CBA
21	8	405	CL7	C1A-C2A-CAA-CBA
21	c	509	CL7	C16-C17-C18-C19
21	A	406	CL7	C11-C10-C8-C7
21	B	612	CL7	C11-C12-C13-C15
21	2	501	CL7	C11-C12-C13-C15
21	3	503	CL7	C11-C12-C13-C15
21	3	511	CL7	C11-C12-C13-C15
21	4	404	CL7	C12-C13-C15-C16
21	4	412	CL7	C12-C13-C15-C16
21	a	405	CL7	C11-C10-C8-C7
21	b	613	CL7	C11-C12-C13-C15
21	6	501	CL7	C11-C12-C13-C15
21	7	503	CL7	C11-C12-C13-C15
21	7	511	CL7	C11-C12-C13-C15
21	8	404	CL7	C12-C13-C15-C16
21	8	412	CL7	C12-C13-C15-C16
21	2	514	CL7	CAA-CBA-CGA-O2A
21	6	514	CL7	CAA-CBA-CGA-O2A
21	2	514	CL7	CAA-CBA-CGA-O1A
21	6	514	CL7	CAA-CBA-CGA-O1A
21	B	612	CL7	C5-C6-C7-C8
21	b	613	CL7	C5-C6-C7-C8
21	C	509	CL7	C16-C17-C18-C19
21	A	401	CL7	C2A-CAA-CBA-CGA
21	2	501	CL7	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
21	1	402	CL7	C2A-CAA-CBA-CGA
21	4	405	CL7	C2A-CAA-CBA-CGA
21	a	401	CL7	C2A-CAA-CBA-CGA
21	6	501	CL7	C2A-CAA-CBA-CGA
21	5	402	CL7	C2A-CAA-CBA-CGA
21	8	405	CL7	C2A-CAA-CBA-CGA
26	c	501	LMG	C33-C34-C35-C36
26	C	501	LMG	C33-C34-C35-C36
26	c	501	LMG	C11-C12-C13-C14
21	3	506	CL7	CAA-CBA-CGA-O2A
21	7	506	CL7	CAA-CBA-CGA-O2A
21	C	508	CL7	C8-C10-C11-C12
21	c	508	CL7	C8-C10-C11-C12
21	2	518	CL7	C3-C5-C6-C7
21	6	518	CL7	C3-C5-C6-C7
23	B	627	8CT	C15-C16-C17-C18
23	b	601	8CT	C15-C16-C17-C18
25	4	401	LHG	O7-C5-C6-O8
25	8	401	LHG	O7-C5-C6-O8
26	1	401	LMG	O7-C8-C9-O8
26	5	401	LMG	O7-C8-C9-O8
21	C	508	CL7	C13-C15-C16-C17
21	1	402	CL7	O1D-CGD-O2D-CED
21	4	410	CL7	CAA-CBA-CGA-O1A
21	8	410	CL7	CAA-CBA-CGA-O1A
31	F	101	HEM	CAA-CBA-CGA-O2A
21	c	508	CL7	C13-C15-C16-C17
21	5	402	CL7	O1D-CGD-O2D-CED
21	3	504	CL7	C16-C17-C18-C19
31	f	101	HEM	CAA-CBA-CGA-O2A
21	4	411	CL7	C4-C3-C5-C6
21	8	411	CL7	C4-C3-C5-C6
21	C	509	CL7	C2-C1-O2A-CGA
21	3	508	CL7	C2-C1-O2A-CGA
21	3	511	CL7	C2-C1-O2A-CGA
21	c	509	CL7	C2-C1-O2A-CGA
21	7	508	CL7	C2-C1-O2A-CGA
21	7	511	CL7	C2-C1-O2A-CGA
21	7	504	CL7	C16-C17-C18-C19
21	C	502	CL7	C11-C12-C13-C14
21	1	418	CL7	C11-C10-C8-C9
21	c	502	CL7	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	5	418	CL7	C11-C10-C8-C9
21	2	517	CL7	C13-C15-C16-C17
21	6	517	CL7	C13-C15-C16-C17
32	3	520	ZEX	C21-C26-C27-C28
32	7	520	ZEX	C21-C26-C27-C28
21	C	508	CL7	C15-C16-C17-C18
21	c	508	CL7	C15-C16-C17-C18
21	4	410	CL7	CAA-CBA-CGA-O2A
21	8	410	CL7	CAA-CBA-CGA-O2A
23	D	406	8CT	C04-C03-C10-C11
23	d	406	8CT	C04-C03-C10-C11
21	C	510	CL7	CAA-CBA-CGA-O2A
21	c	510	CL7	CAA-CBA-CGA-O2A
21	4	408	CL7	CAA-CBA-CGA-O1A
21	8	408	CL7	CAA-CBA-CGA-O1A
32	1	421	ZEX	C29-C30-C31-C32
32	4	418	ZEX	C29-C30-C31-C32
32	5	421	ZEX	C29-C30-C31-C32
32	8	418	ZEX	C29-C30-C31-C32
21	B	604	CL7	C4-C3-C5-C6
21	b	605	CL7	C4-C3-C5-C6
32	4	420	ZEX	C11-C12-C13-C14
32	8	420	ZEX	C11-C12-C13-C14
21	A	403	CL7	C6-C7-C8-C9
21	a	403	CL7	C6-C7-C8-C9
30	D	407	PL9	C33-C34-C36-C37
30	D	407	PL9	C43-C44-C46-C47
30	d	407	PL9	C33-C34-C36-C37
30	d	407	PL9	C43-C44-C46-C47
21	1	410	CL7	C3-C5-C6-C7
21	5	410	CL7	C3-C5-C6-C7
21	3	513	CL7	CAA-CBA-CGA-O2A
21	7	513	CL7	CAA-CBA-CGA-O2A
25	a	406	LHG	C9-C10-C11-C12
21	4	406	CL7	C16-C17-C18-C20
21	8	406	CL7	C16-C17-C18-C20
25	A	407	LHG	C9-C10-C11-C12
21	3	518	CL7	CAA-CBA-CGA-O2A
21	7	518	CL7	CAA-CBA-CGA-O2A
21	4	405	CL7	C8-C10-C11-C12
21	8	405	CL7	C8-C10-C11-C12
25	D	409	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
25	d	409	LHG	O6-C4-C5-C6
27	B	624	DGD	O2G-C1B-C2B-C3B
27	b	625	DGD	O2G-C1B-C2B-C3B
21	2	506	CL7	C4-C3-C5-C6
21	4	414	CL7	C4-C3-C5-C6
21	6	506	CL7	C4-C3-C5-C6
21	8	414	CL7	C4-C3-C5-C6
21	B	609	CL7	C12-C13-C15-C16
21	2	505	CL7	C6-C7-C8-C10
21	3	516	CL7	C2-C3-C5-C6
21	4	411	CL7	C2-C3-C5-C6
21	b	610	CL7	C12-C13-C15-C16
21	6	505	CL7	C6-C7-C8-C10
21	7	516	CL7	C2-C3-C5-C6
21	8	411	CL7	C2-C3-C5-C6
23	D	406	8CT	C18-C19-C20-C21
23	d	406	8CT	C18-C19-C20-C21
21	A	401	CL7	CAA-CBA-CGA-O2A
21	a	401	CL7	CAA-CBA-CGA-O2A
21	D	404	CL7	C2A-CAA-CBA-CGA
21	1	412	CL7	C2A-CAA-CBA-CGA
21	d	404	CL7	C2A-CAA-CBA-CGA
21	5	412	CL7	C2A-CAA-CBA-CGA
21	B	622	CL7	CAA-CBA-CGA-O2A
21	b	623	CL7	CAA-CBA-CGA-O2A
22	D	408	PHO	C4C-C3C-CAC-CBC
22	d	408	PHO	C4C-C3C-CAC-CBC
21	7	513	CL7	C2C-C3C-CAC-CBC
21	B	605	CL7	C4-C3-C5-C6
21	C	507	CL7	C4-C3-C5-C6
21	C	511	CL7	C4-C3-C5-C6
21	2	502	CL7	C4-C3-C5-C6
21	b	606	CL7	C4-C3-C5-C6
21	c	507	CL7	C4-C3-C5-C6
21	c	511	CL7	C4-C3-C5-C6
21	6	502	CL7	C4-C3-C5-C6
30	D	407	PL9	C20-C19-C21-C22
30	d	407	PL9	C20-C19-C21-C22
21	3	513	CL7	C2C-C3C-CAC-CBC
21	4	415	CL7	CAA-CBA-CGA-O2A
21	5	412	CL7	CAA-CBA-CGA-O2A
21	8	415	CL7	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	B	613	CL7	C2-C3-C5-C6
21	2	512	CL7	C2-C3-C5-C6
21	b	614	CL7	C2-C3-C5-C6
21	6	512	CL7	C2-C3-C5-C6
21	B	605	CL7	C11-C12-C13-C14
21	C	504	CL7	C11-C12-C13-C14
21	2	507	CL7	C14-C13-C15-C16
21	4	412	CL7	C11-C10-C8-C9
21	4	412	CL7	C14-C13-C15-C16
21	b	606	CL7	C11-C12-C13-C14
21	c	504	CL7	C11-C12-C13-C14
21	6	507	CL7	C14-C13-C15-C16
21	8	412	CL7	C11-C10-C8-C9
21	8	412	CL7	C14-C13-C15-C16
21	1	412	CL7	CAA-CBA-CGA-O2A
21	2	504	CL7	C3A-C2A-CAA-CBA
21	1	419	CL7	C3A-C2A-CAA-CBA
21	6	504	CL7	C3A-C2A-CAA-CBA
21	5	419	CL7	C3A-C2A-CAA-CBA
21	1	411	CL7	CAA-CBA-CGA-O2A
21	5	411	CL7	CAA-CBA-CGA-O2A
21	A	401	CL7	CAD-CBD-CGD-O2D
21	B	609	CL7	CAD-CBD-CGD-O2D
21	C	504	CL7	CAD-CBD-CGD-O2D
21	C	509	CL7	CAD-CBD-CGD-O2D
21	C	518	CL7	CAD-CBD-CGD-O2D
21	D	404	CL7	CAD-CBD-CGD-O2D
21	2	508	CL7	CAD-CBD-CGD-O2D
21	1	420	CL7	CAD-CBD-CGD-O2D
21	3	501	CL7	CAD-CBD-CGD-O2D
21	3	503	CL7	CAD-CBD-CGD-O2D
21	3	507	CL7	CAD-CBD-CGD-O2D
21	3	508	CL7	CAD-CBD-CGD-O2D
21	3	511	CL7	CAD-CBD-CGD-O2D
21	3	512	CL7	CAD-CBD-CGD-O2D
21	3	513	CL7	CAD-CBD-CGD-O2D
21	b	610	CL7	CAD-CBD-CGD-O2D
21	c	504	CL7	CAD-CBD-CGD-O2D
21	c	509	CL7	CAD-CBD-CGD-O2D
21	c	518	CL7	CAD-CBD-CGD-O2D
21	d	404	CL7	CAD-CBD-CGD-O2D
21	6	508	CL7	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	5	420	CL7	CAD-CBD-CGD-O2D
21	7	501	CL7	CAD-CBD-CGD-O2D
21	7	503	CL7	CAD-CBD-CGD-O2D
21	7	507	CL7	CAD-CBD-CGD-O2D
21	7	508	CL7	CAD-CBD-CGD-O2D
21	7	511	CL7	CAD-CBD-CGD-O2D
21	7	512	CL7	CAD-CBD-CGD-O2D
21	7	513	CL7	CAD-CBD-CGD-O2D
26	C	501	LMG	C19-C20-C21-C22
21	1	419	CL7	CAA-CBA-CGA-O2A
21	5	419	CL7	CAA-CBA-CGA-O2A
31	F	101	HEM	CAD-CBD-CGD-O2D
31	f	101	HEM	CAD-CBD-CGD-O2D
26	C	501	LMG	C29-C30-C31-C32
21	4	406	CL7	CAA-CBA-CGA-O2A
21	8	406	CL7	CAA-CBA-CGA-O2A
21	C	504	CL7	C8-C10-C11-C12
21	c	504	CL7	C8-C10-C11-C12
21	2	516	CL7	C16-C17-C18-C19
21	6	516	CL7	C16-C17-C18-C19
21	1	405	CL7	CAA-CBA-CGA-O2A
21	3	513	CL7	CAA-CBA-CGA-O1A
21	5	405	CL7	CAA-CBA-CGA-O1A
21	5	405	CL7	CAA-CBA-CGA-O2A
21	7	513	CL7	CAA-CBA-CGA-O1A
21	2	501	CL7	CAA-CBA-CGA-O2A
21	6	501	CL7	CAA-CBA-CGA-O2A
23	A	404	8CT	C20-C21-C23-C24
23	a	404	8CT	C20-C21-C23-C24
22	D	408	PHO	C2C-C3C-CAC-CBC
22	d	408	PHO	C2C-C3C-CAC-CBC
24	2	522	SQD	C44-C45-C46-O48
24	6	521	SQD	C44-C45-C46-O48
21	1	405	CL7	CAA-CBA-CGA-O1A
26	c	501	LMG	C29-C30-C31-C32
21	6	503	CL7	C5-C6-C7-C8
21	B	609	CL7	CAA-CBA-CGA-O2A
21	3	518	CL7	CAA-CBA-CGA-O1A
21	B	610	CL7	O2A-C1-C2-C3
21	C	506	CL7	O2A-C1-C2-C3
21	4	413	CL7	O2A-C1-C2-C3
21	b	611	CL7	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
21	c	506	CL7	O2A-C1-C2-C3
21	8	413	CL7	O2A-C1-C2-C3
25	D	409	LHG	C31-C32-C33-C34
25	d	409	LHG	C31-C32-C33-C34
21	b	610	CL7	CAA-CBA-CGA-O2A
21	1	411	CL7	CAA-CBA-CGA-O1A
21	1	412	CL7	CAA-CBA-CGA-O1A
21	5	411	CL7	CAA-CBA-CGA-O1A
21	5	412	CL7	CAA-CBA-CGA-O1A
21	7	518	CL7	CAA-CBA-CGA-O1A
25	B	623	LHG	C25-C26-C27-C28
25	b	624	LHG	C25-C26-C27-C28
21	7	501	CL7	C5-C6-C7-C8
26	C	501	LMG	C11-C12-C13-C14
21	A	406	CL7	CHA-CBD-CGD-O2D
21	B	605	CL7	CHA-CBD-CGD-O2D
21	B	608	CL7	CHA-CBD-CGD-O2D
21	B	610	CL7	CHA-CBD-CGD-O2D
21	B	616	CL7	CHA-CBD-CGD-O2D
21	C	505	CL7	CHA-CBD-CGD-O2D
21	C	511	CL7	CHA-CBD-CGD-O1D
21	2	502	CL7	CHA-CBD-CGD-O2D
21	2	507	CL7	CHA-CBD-CGD-O2D
21	2	517	CL7	CHA-CBD-CGD-O2D
21	2	517	CL7	CHA-CBD-CGD-O1D
21	1	405	CL7	CHA-CBD-CGD-O2D
21	1	405	CL7	CHA-CBD-CGD-O1D
21	3	502	CL7	CHA-CBD-CGD-O2D
21	3	505	CL7	CHA-CBD-CGD-O2D
21	3	505	CL7	CHA-CBD-CGD-O1D
21	3	512	CL7	CHA-CBD-CGD-O1D
21	3	516	CL7	CHA-CBD-CGD-O2D
21	3	516	CL7	CHA-CBD-CGD-O1D
21	a	405	CL7	CHA-CBD-CGD-O2D
21	b	606	CL7	CHA-CBD-CGD-O2D
21	b	609	CL7	CHA-CBD-CGD-O2D
21	b	611	CL7	CHA-CBD-CGD-O2D
21	b	617	CL7	CHA-CBD-CGD-O2D
21	c	505	CL7	CHA-CBD-CGD-O2D
21	c	511	CL7	CHA-CBD-CGD-O1D
21	6	502	CL7	CHA-CBD-CGD-O2D
21	6	507	CL7	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
21	6	517	CL7	CHA-CBD-CGD-O2D
21	6	517	CL7	CHA-CBD-CGD-O1D
21	5	405	CL7	CHA-CBD-CGD-O2D
21	5	405	CL7	CHA-CBD-CGD-O1D
21	7	502	CL7	CHA-CBD-CGD-O2D
21	7	505	CL7	CHA-CBD-CGD-O2D
21	7	505	CL7	CHA-CBD-CGD-O1D
21	7	512	CL7	CHA-CBD-CGD-O1D
21	7	516	CL7	CHA-CBD-CGD-O2D
21	7	516	CL7	CHA-CBD-CGD-O1D
21	1	419	CL7	CAA-CBA-CGA-O1A
21	5	419	CL7	CAA-CBA-CGA-O1A
30	D	407	PL9	C17-C18-C19-C21
30	d	407	PL9	C17-C18-C19-C21
21	2	503	CL7	C5-C6-C7-C8
21	3	501	CL7	C5-C6-C7-C8
21	2	510	CL7	CAA-CBA-CGA-O2A
21	2	512	CL7	CAA-CBA-CGA-O2A
21	6	510	CL7	CAA-CBA-CGA-O2A
21	6	512	CL7	CAA-CBA-CGA-O2A
21	8	412	CL7	CAA-CBA-CGA-O2A
26	c	501	LMG	C28-C29-C30-C31
21	1	406	CL7	O1D-CGD-O2D-CED
21	5	406	CL7	O1D-CGD-O2D-CED
21	4	413	CL7	C8-C10-C11-C12
21	c	509	CL7	C8-C10-C11-C12
21	8	413	CL7	C8-C10-C11-C12
21	d	404	CL7	C3-C5-C6-C7
21	C	509	CL7	C8-C10-C11-C12
21	3	501	CL7	CAA-CBA-CGA-O2A
21	7	501	CL7	CAA-CBA-CGA-O2A
21	2	511	CL7	C11-C12-C13-C14
21	6	511	CL7	C11-C12-C13-C14
21	D	404	CL7	C3-C5-C6-C7
26	D	410	LMG	C11-C10-O7-C8
26	d	410	LMG	C11-C10-O7-C8
21	4	409	CL7	CAA-CBA-CGA-O2A
21	4	412	CL7	CAA-CBA-CGA-O2A
21	8	409	CL7	CAA-CBA-CGA-O2A
21	1	418	CL7	C6-C7-C8-C10
21	5	418	CL7	C6-C7-C8-C10
26	D	410	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
26	d	410	LMG	O7-C10-C11-C12
21	B	604	CL7	C14-C13-C15-C16
21	B	612	CL7	C14-C13-C15-C16
21	2	517	CL7	C14-C13-C15-C16
21	1	408	CL7	C11-C12-C13-C14
21	3	503	CL7	C11-C12-C13-C14
21	3	511	CL7	C11-C12-C13-C14
21	b	605	CL7	C14-C13-C15-C16
21	b	613	CL7	C14-C13-C15-C16
21	6	517	CL7	C14-C13-C15-C16
21	5	408	CL7	C11-C12-C13-C14
21	7	503	CL7	C11-C12-C13-C14
21	7	511	CL7	C11-C12-C13-C14
23	4	402	8CT	C23-C24-C25-C26
23	8	402	8CT	C23-C24-C25-C26
25	4	401	LHG	C15-C16-C17-C18
25	8	401	LHG	C15-C16-C17-C18
21	B	622	CL7	CAA-CBA-CGA-O1A
21	b	623	CL7	CAA-CBA-CGA-O1A
24	A	405	SQD	C4-C5-C6-S
24	B	626	SQD	C4-C5-C6-S
24	1	423	SQD	C4-C5-C6-S
24	5	423	SQD	C4-C5-C6-S
21	3	505	CL7	C16-C17-C18-C20
21	7	505	CL7	C16-C17-C18-C20
21	4	415	CL7	CAA-CBA-CGA-O1A
21	8	415	CL7	CAA-CBA-CGA-O1A
21	a	401	CL7	CAA-CBA-CGA-O1A
21	3	517	CL7	CAA-CBA-CGA-O2A
21	7	517	CL7	CAA-CBA-CGA-O2A
21	A	401	CL7	CAA-CBA-CGA-O1A
21	b	610	CL7	CAA-CBA-CGA-O1A
21	1	408	CL7	C10-C11-C12-C13
21	5	408	CL7	C10-C11-C12-C13
21	2	512	CL7	C16-C17-C18-C19
21	6	512	CL7	C16-C17-C18-C19
21	1	406	CL7	CBD-CGD-O2D-CED
21	5	406	CL7	CBD-CGD-O2D-CED
26	c	501	LMG	C19-C20-C21-C22
21	2	501	CL7	CAA-CBA-CGA-O1A
21	6	501	CL7	CAA-CBA-CGA-O1A
21	4	413	CL7	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	8	413	CL7	C5-C6-C7-C8
21	1	405	CL7	C1A-C2A-CAA-CBA
21	3	505	CL7	C1A-C2A-CAA-CBA
21	3	512	CL7	C1A-C2A-CAA-CBA
21	5	405	CL7	C1A-C2A-CAA-CBA
21	7	505	CL7	C1A-C2A-CAA-CBA
21	7	512	CL7	C1A-C2A-CAA-CBA
21	B	609	CL7	CAA-CBA-CGA-O1A
25	b	626	LHG	C14-C15-C16-C17
21	3	511	CL7	C15-C16-C17-C18
21	7	511	CL7	C15-C16-C17-C18
25	B	625	LHG	C14-C15-C16-C17
25	b	626	LHG	C17-C18-C19-C20
21	2	503	CL7	C2A-CAA-CBA-CGA
21	6	503	CL7	C2A-CAA-CBA-CGA
21	B	607	CL7	C11-C12-C13-C14
21	C	508	CL7	C16-C17-C18-C20
21	2	501	CL7	C16-C17-C18-C19
21	b	608	CL7	C11-C12-C13-C14
21	c	508	CL7	C16-C17-C18-C20
21	6	501	CL7	C16-C17-C18-C19
21	6	502	CL7	C10-C11-C12-C13
25	B	625	LHG	C17-C18-C19-C20
21	2	507	CL7	CAA-CBA-CGA-O2A
21	6	507	CL7	CAA-CBA-CGA-O2A
21	2	502	CL7	C10-C11-C12-C13
32	4	419	ZEX	C21-C26-C27-C28
32	8	419	ZEX	C21-C26-C27-C28
21	1	418	CL7	C2-C3-C5-C6
21	5	418	CL7	C2-C3-C5-C6
25	4	401	LHG	C3-O3-P-O5
25	8	401	LHG	C3-O3-P-O5
21	B	604	CL7	C16-C17-C18-C20
21	2	503	CL7	C16-C17-C18-C20
21	3	509	CL7	C16-C17-C18-C20
21	b	605	CL7	C16-C17-C18-C20
21	6	503	CL7	C16-C17-C18-C20
21	7	509	CL7	C16-C17-C18-C20
21	3	517	CL7	CAA-CBA-CGA-O1A
21	7	517	CL7	CAA-CBA-CGA-O1A
21	C	511	CL7	CAA-CBA-CGA-O2A
21	c	511	CL7	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
21	d	404	CL7	C10-C11-C12-C13
21	2	507	CL7	C13-C15-C16-C17
21	2	516	CL7	C13-C15-C16-C17
21	6	507	CL7	C13-C15-C16-C17
21	6	516	CL7	C13-C15-C16-C17
21	2	512	CL7	CAA-CBA-CGA-O1A
21	6	512	CL7	CAA-CBA-CGA-O1A
21	8	406	CL7	CAA-CBA-CGA-O1A
21	D	404	CL7	C10-C11-C12-C13
21	B	610	CL7	C16-C17-C18-C20
21	b	611	CL7	C16-C17-C18-C20
21	A	406	CL7	C2A-CAA-CBA-CGA
21	4	406	CL7	CAA-CBA-CGA-O1A
21	4	409	CL7	CAA-CBA-CGA-O1A
21	8	409	CL7	CAA-CBA-CGA-O1A
26	D	410	LMG	O9-C10-C11-C12
26	d	410	LMG	O9-C10-C11-C12
21	1	418	CL7	C10-C11-C12-C13
21	5	418	CL7	C10-C11-C12-C13
21	3	516	CL7	C6-C7-C8-C9
21	7	516	CL7	C6-C7-C8-C9
21	A	403	CL7	CAD-CBD-CGD-O1D
21	C	505	CL7	CAD-CBD-CGD-O1D
21	C	507	CL7	CAD-CBD-CGD-O1D
21	2	510	CL7	CAD-CBD-CGD-O1D
21	2	518	CL7	CAD-CBD-CGD-O1D
21	3	502	CL7	CAD-CBD-CGD-O1D
21	4	407	CL7	CAD-CBD-CGD-O1D
21	4	410	CL7	CAD-CBD-CGD-O1D
21	4	413	CL7	CAD-CBD-CGD-O1D
21	4	415	CL7	CAD-CBD-CGD-O1D
21	a	403	CL7	CAD-CBD-CGD-O1D
21	c	505	CL7	CAD-CBD-CGD-O1D
21	c	507	CL7	CAD-CBD-CGD-O1D
21	6	510	CL7	CAD-CBD-CGD-O1D
21	6	518	CL7	CAD-CBD-CGD-O1D
21	7	502	CL7	CAD-CBD-CGD-O1D
21	8	407	CL7	CAD-CBD-CGD-O1D
21	8	410	CL7	CAD-CBD-CGD-O1D
21	8	413	CL7	CAD-CBD-CGD-O1D
21	8	415	CL7	CAD-CBD-CGD-O1D
24	A	405	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
24	B	626	SQD	O5-C5-C6-S
24	1	423	SQD	O5-C5-C6-S
24	3	523	SQD	C46-C45-O47-C7
24	5	423	SQD	O5-C5-C6-S
24	7	523	SQD	C46-C45-O47-C7
26	B	621	LMG	C35-C36-C37-C38
26	b	622	LMG	C35-C36-C37-C38
21	B	610	CL7	C14-C13-C15-C16
21	C	506	CL7	C11-C12-C13-C14
21	4	405	CL7	C6-C7-C8-C9
21	b	611	CL7	C14-C13-C15-C16
21	c	506	CL7	C11-C12-C13-C14
21	8	405	CL7	C6-C7-C8-C9
27	C	517	DGD	C1A-C2A-C3A-C4A
27	c	517	DGD	C1A-C2A-C3A-C4A
21	D	404	CL7	CAA-CBA-CGA-O2A
26	1	401	LMG	O7-C10-C11-C12
26	5	401	LMG	O7-C10-C11-C12
21	D	405	CL7	C2A-CAA-CBA-CGA
21	a	405	CL7	C2A-CAA-CBA-CGA
21	d	405	CL7	C2A-CAA-CBA-CGA
21	C	502	CL7	CAA-CBA-CGA-O2A
21	1	406	CL7	CAA-CBA-CGA-O2A
21	3	512	CL7	CAA-CBA-CGA-O2A
21	c	502	CL7	CAA-CBA-CGA-O2A
21	d	404	CL7	CAA-CBA-CGA-O2A
21	5	406	CL7	CAA-CBA-CGA-O2A
21	7	512	CL7	CAA-CBA-CGA-O2A
26	D	410	LMG	O9-C10-O7-C8
26	d	410	LMG	O9-C10-O7-C8
21	C	510	CL7	C16-C17-C18-C20
21	c	510	CL7	C16-C17-C18-C20
21	2	509	CL7	C4-C3-C5-C6
21	6	509	CL7	C4-C3-C5-C6
21	B	610	CL7	C11-C12-C13-C15
21	C	508	CL7	C11-C12-C13-C15
21	2	501	CL7	C6-C7-C8-C10
21	2	505	CL7	C11-C10-C8-C7
21	2	510	CL7	C11-C12-C13-C15
21	2	511	CL7	C11-C10-C8-C7
21	1	404	CL7	C12-C13-C15-C16
21	3	502	CL7	C11-C10-C8-C7

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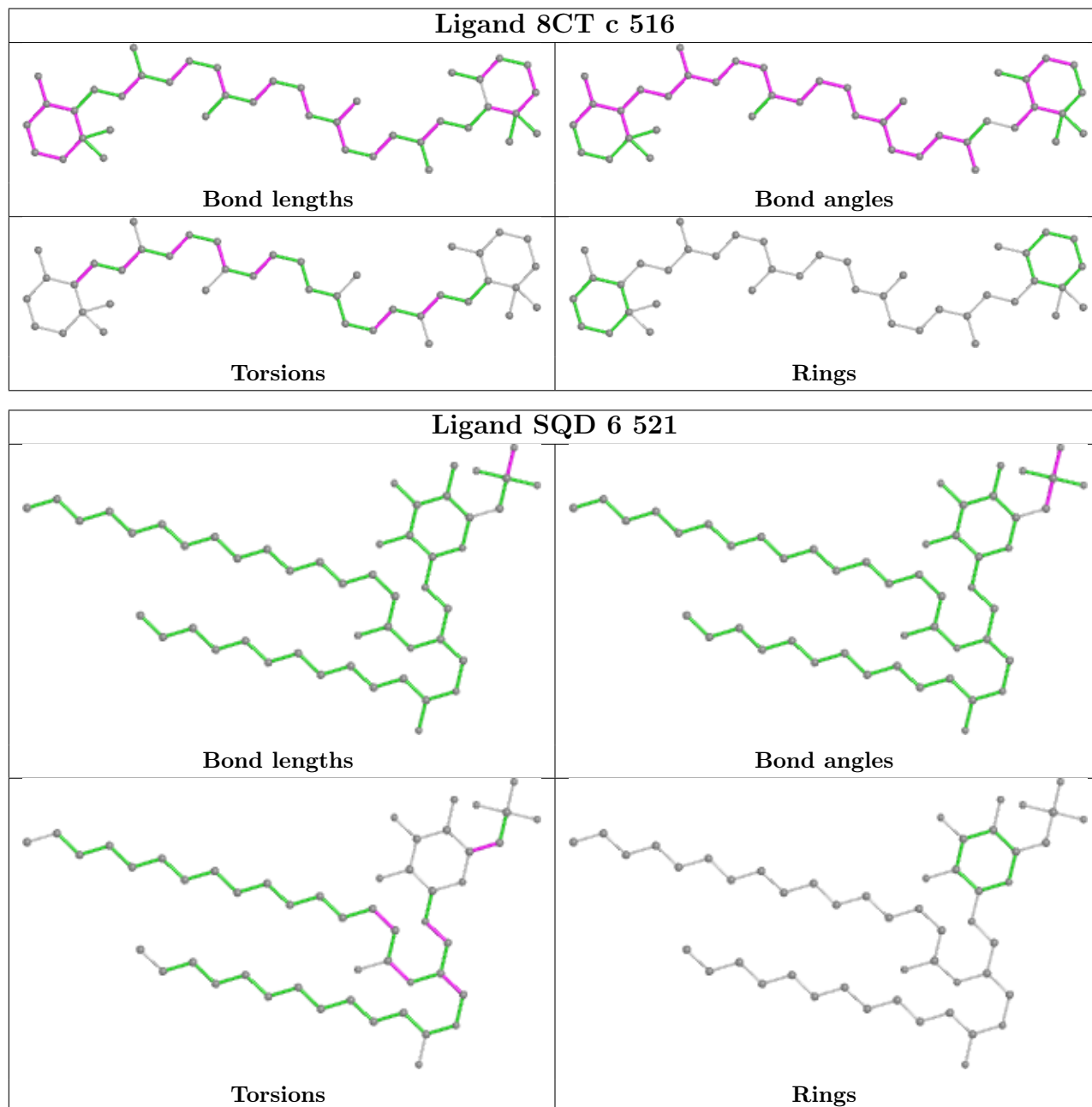
Mol	Chain	Res	Type	Atoms
21	b	611	CL7	C11-C12-C13-C15
21	c	508	CL7	C11-C12-C13-C15
21	6	501	CL7	C6-C7-C8-C10
21	6	505	CL7	C11-C10-C8-C7
21	6	510	CL7	C11-C12-C13-C15
21	6	511	CL7	C11-C10-C8-C7
21	5	404	CL7	C12-C13-C15-C16
21	7	502	CL7	C11-C10-C8-C7
23	B	617	8CT	C28-C29-C30-C31
23	K	101	8CT	C28-C29-C30-C31
23	b	618	8CT	C28-C29-C30-C31
23	k	101	8CT	C28-C29-C30-C31
21	6	507	CL7	CAA-CBA-CGA-O1A
24	3	523	SQD	C11-C12-C13-C14
24	7	523	SQD	C11-C12-C13-C14
21	2	507	CL7	CAA-CBA-CGA-O1A
21	1	406	CL7	CAA-CBA-CGA-O1A
21	5	406	CL7	CAA-CBA-CGA-O1A
32	2	519	ZEX	C33-C34-C35-C15
32	6	519	ZEX	C33-C34-C35-C15
24	3	523	SQD	C13-C14-C15-C16
24	7	523	SQD	C13-C14-C15-C16
21	B	603	CL7	C16-C17-C18-C19
21	b	604	CL7	C16-C17-C18-C19
26	C	501	LMG	C32-C33-C34-C35
21	2	510	CL7	CAA-CBA-CGA-O1A
21	4	412	CL7	CAA-CBA-CGA-O1A
21	6	510	CL7	CAA-CBA-CGA-O1A
21	8	412	CL7	CAA-CBA-CGA-O1A
21	C	505	CL7	C4C-C3C-CAC-CBC
21	c	505	CL7	C4C-C3C-CAC-CBC
24	1	423	SQD	O48-C23-C24-C25
24	5	423	SQD	O48-C23-C24-C25
21	3	505	CL7	CAA-CBA-CGA-O2A
21	7	505	CL7	CAA-CBA-CGA-O2A

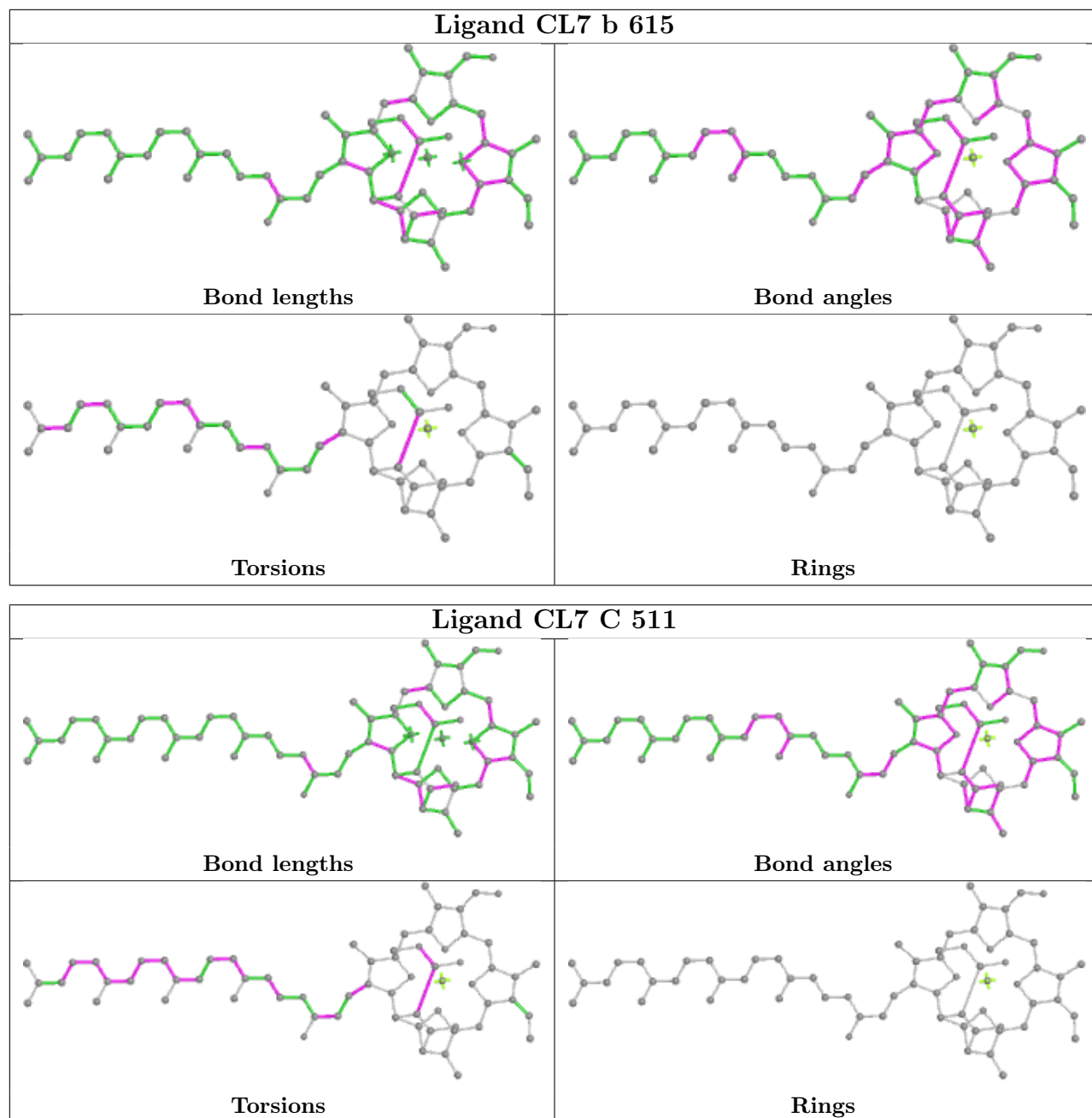
There are no ring outliers.

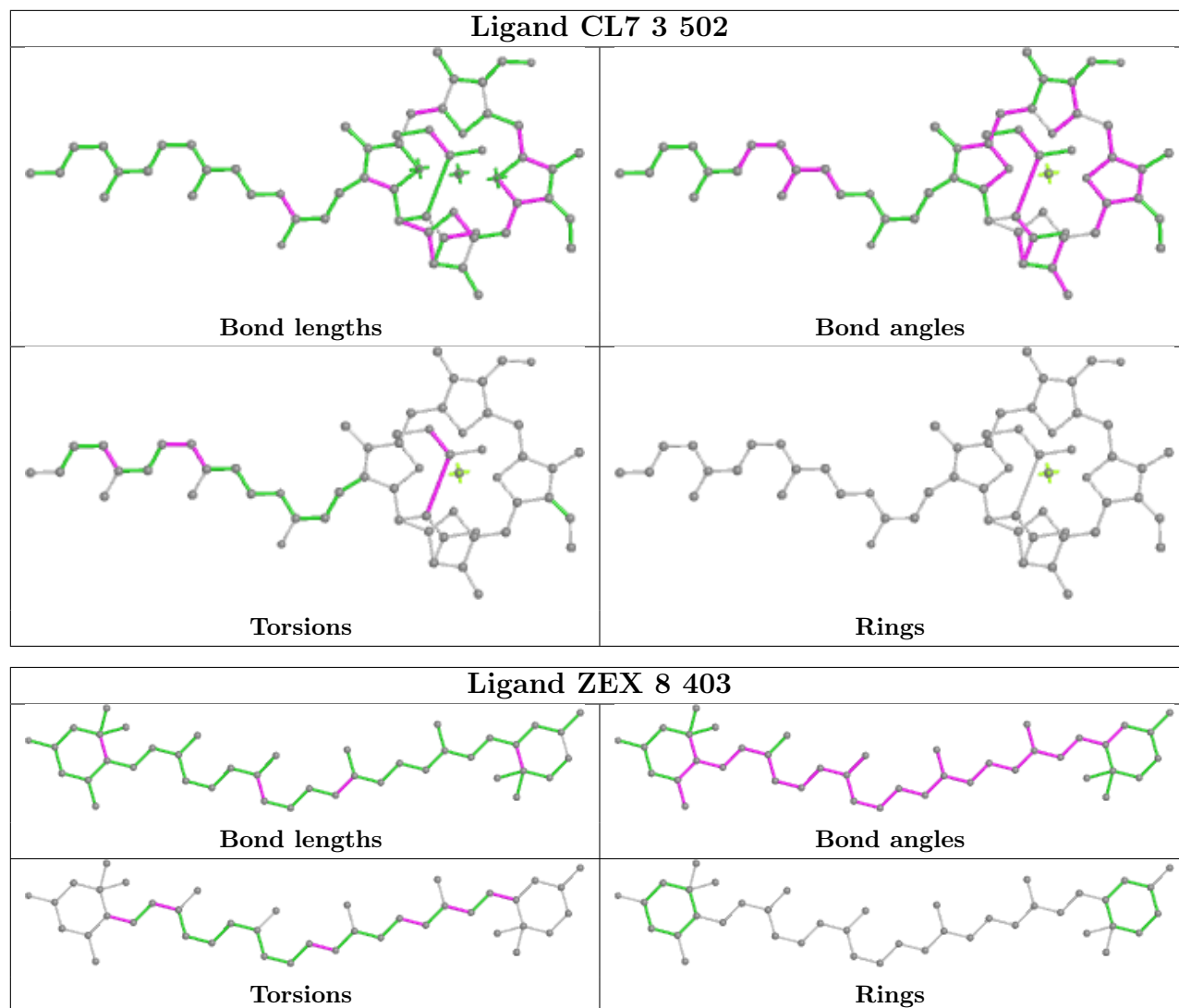
No monomer is involved in short contacts.

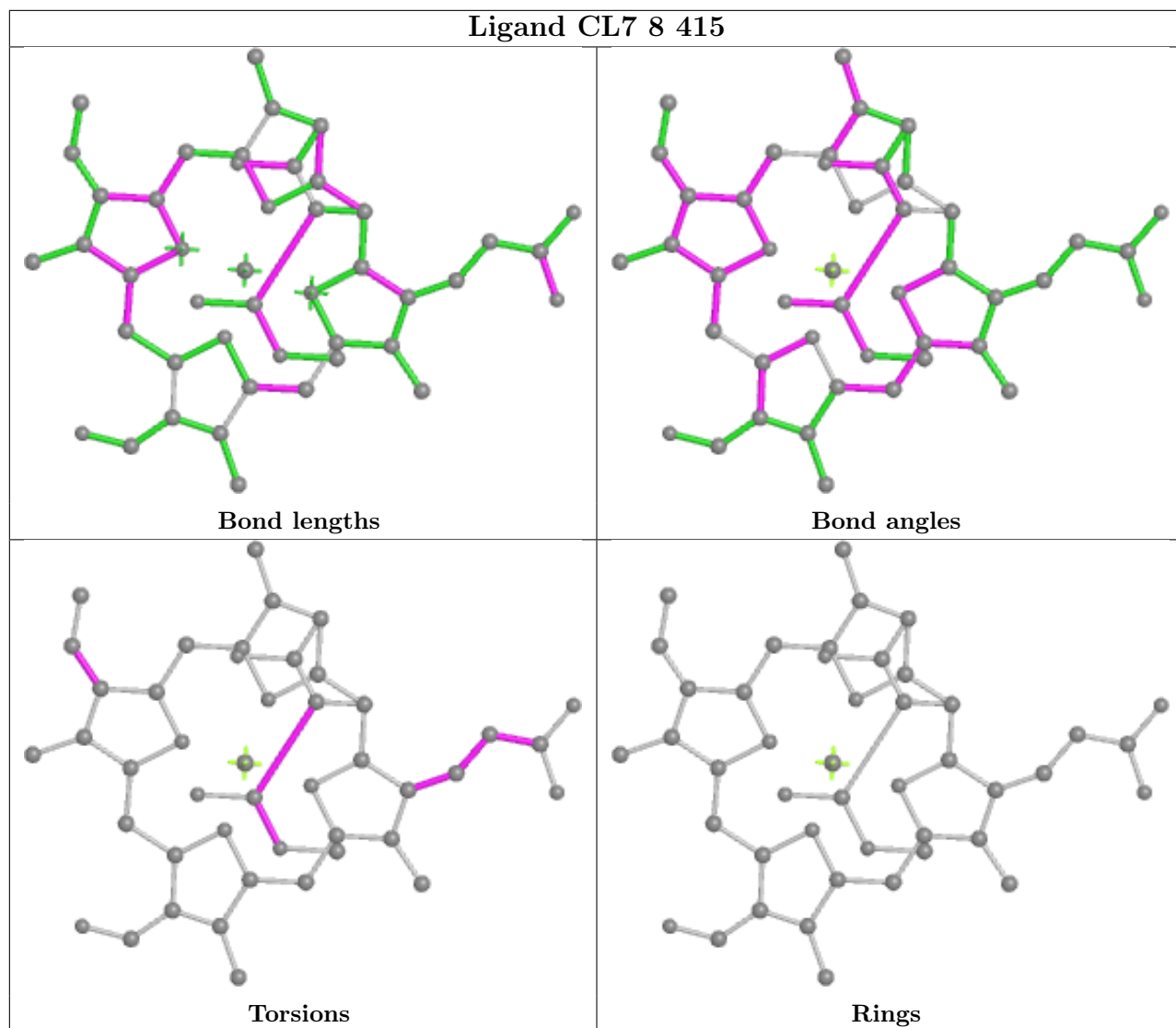
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

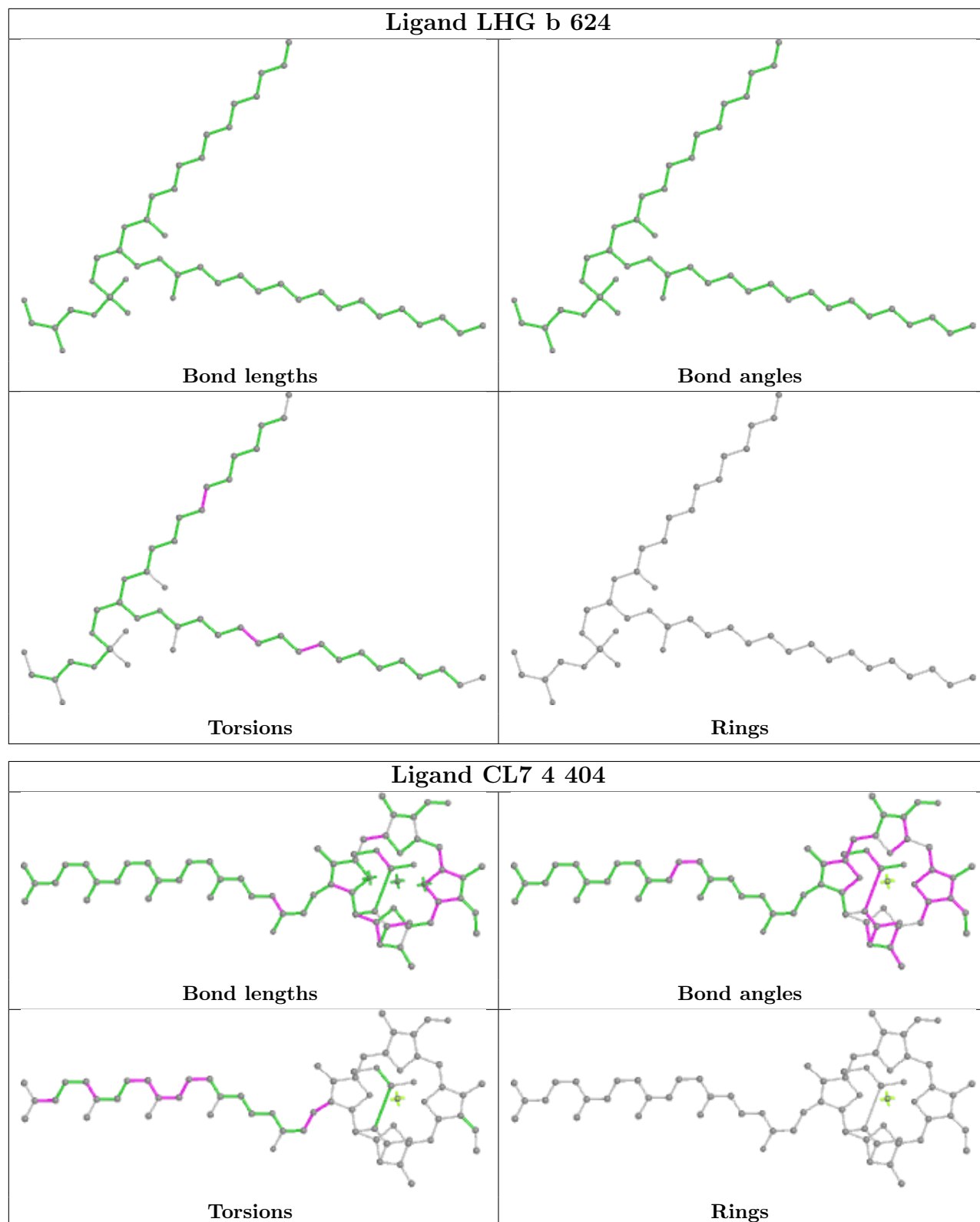
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

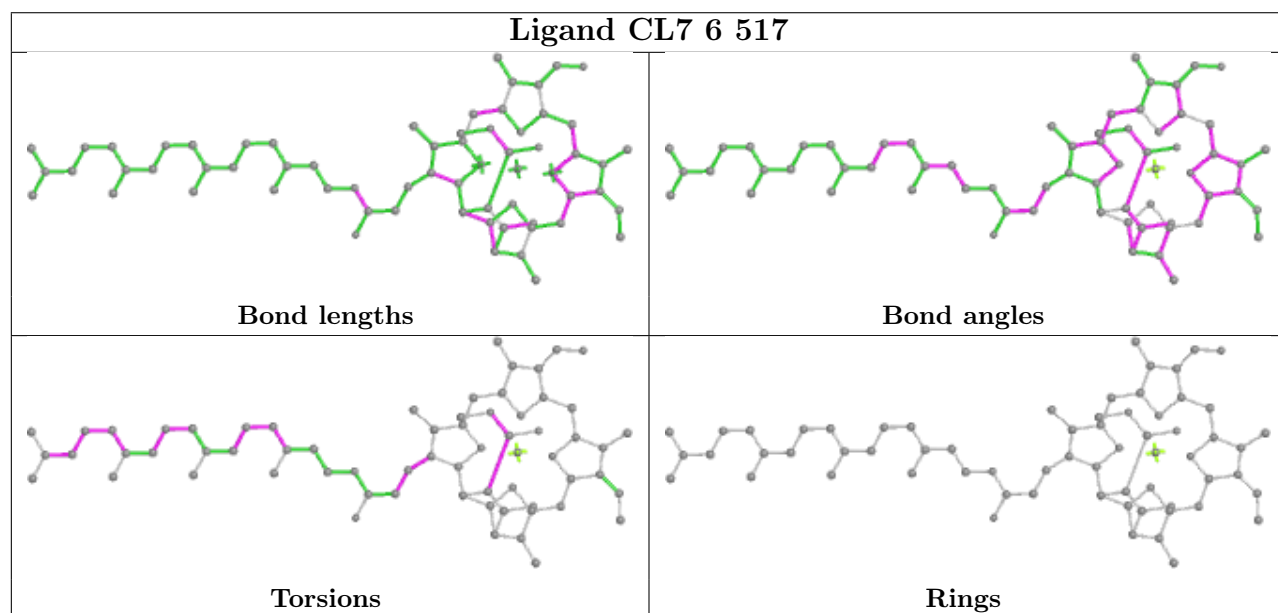
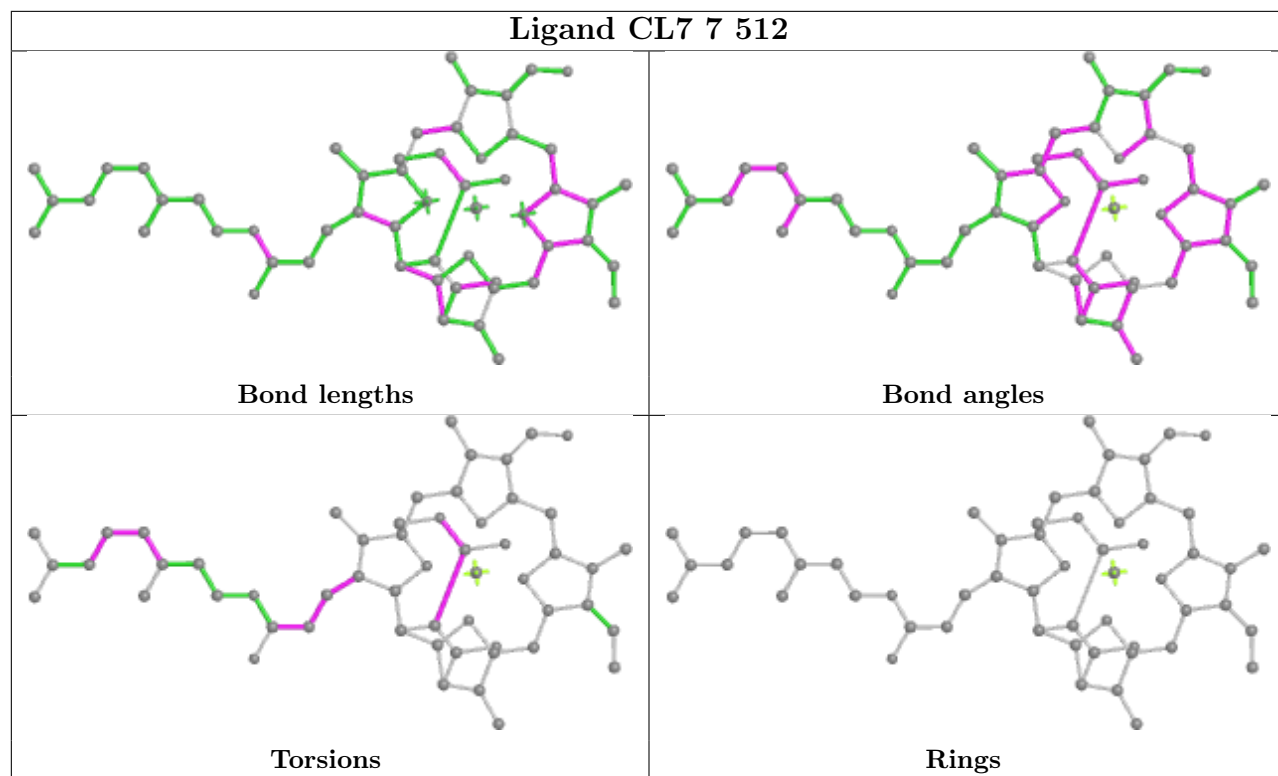


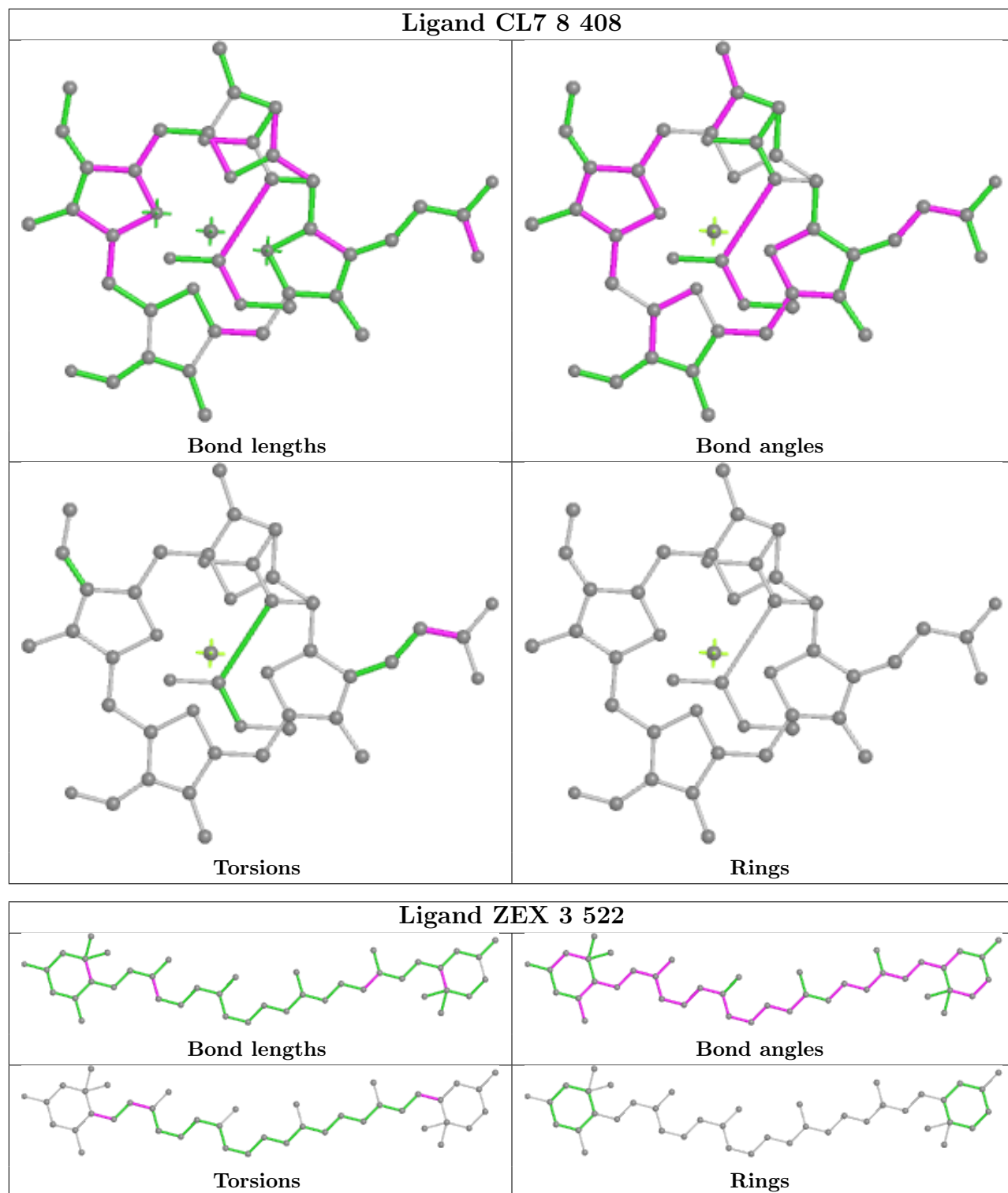


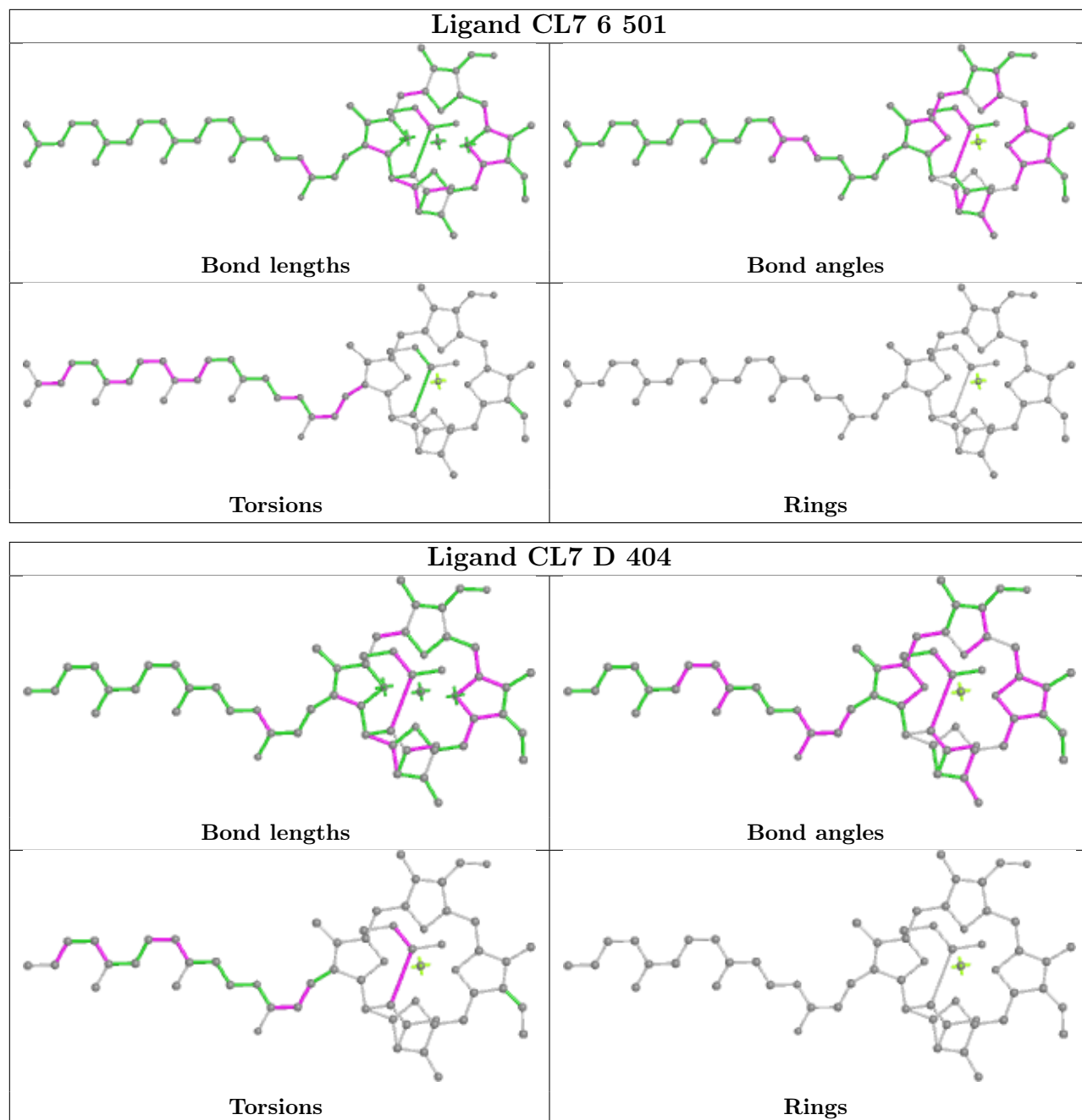


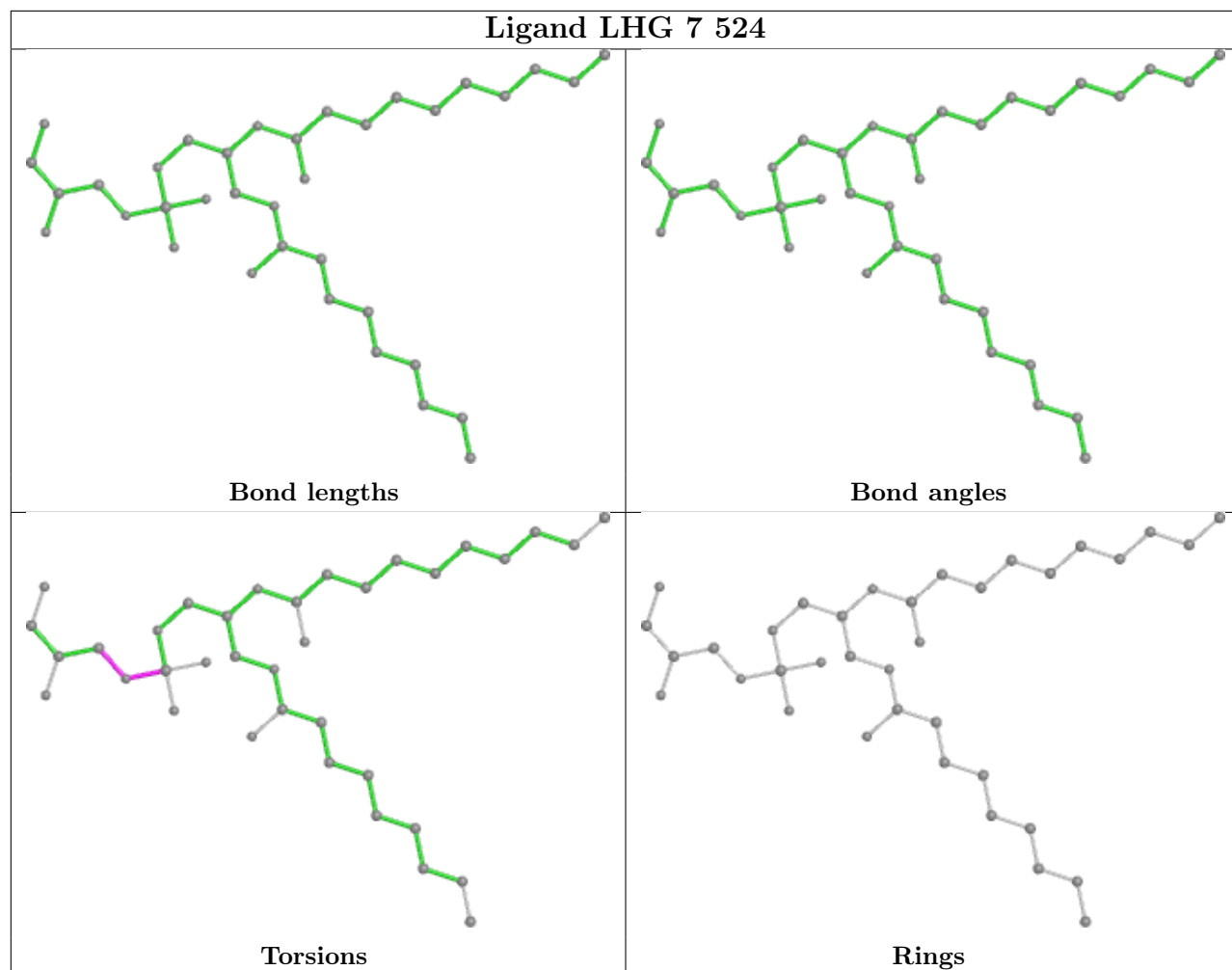


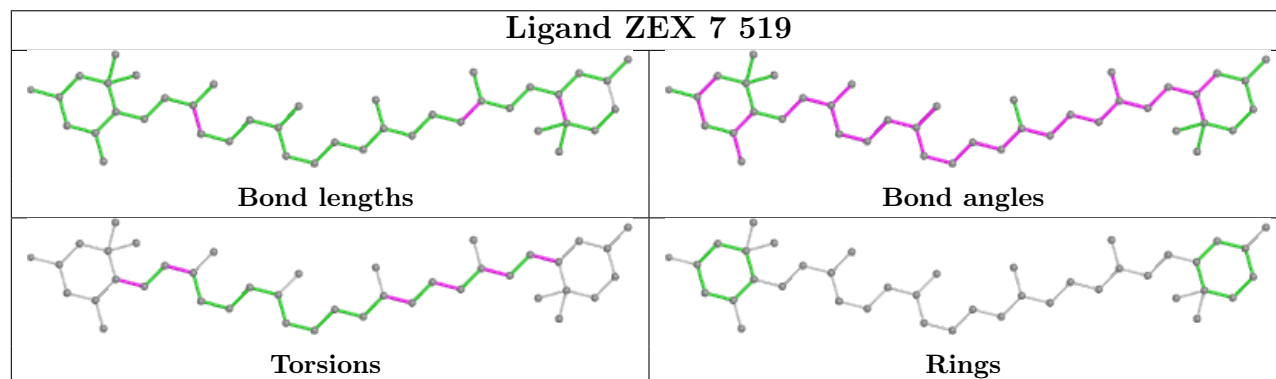
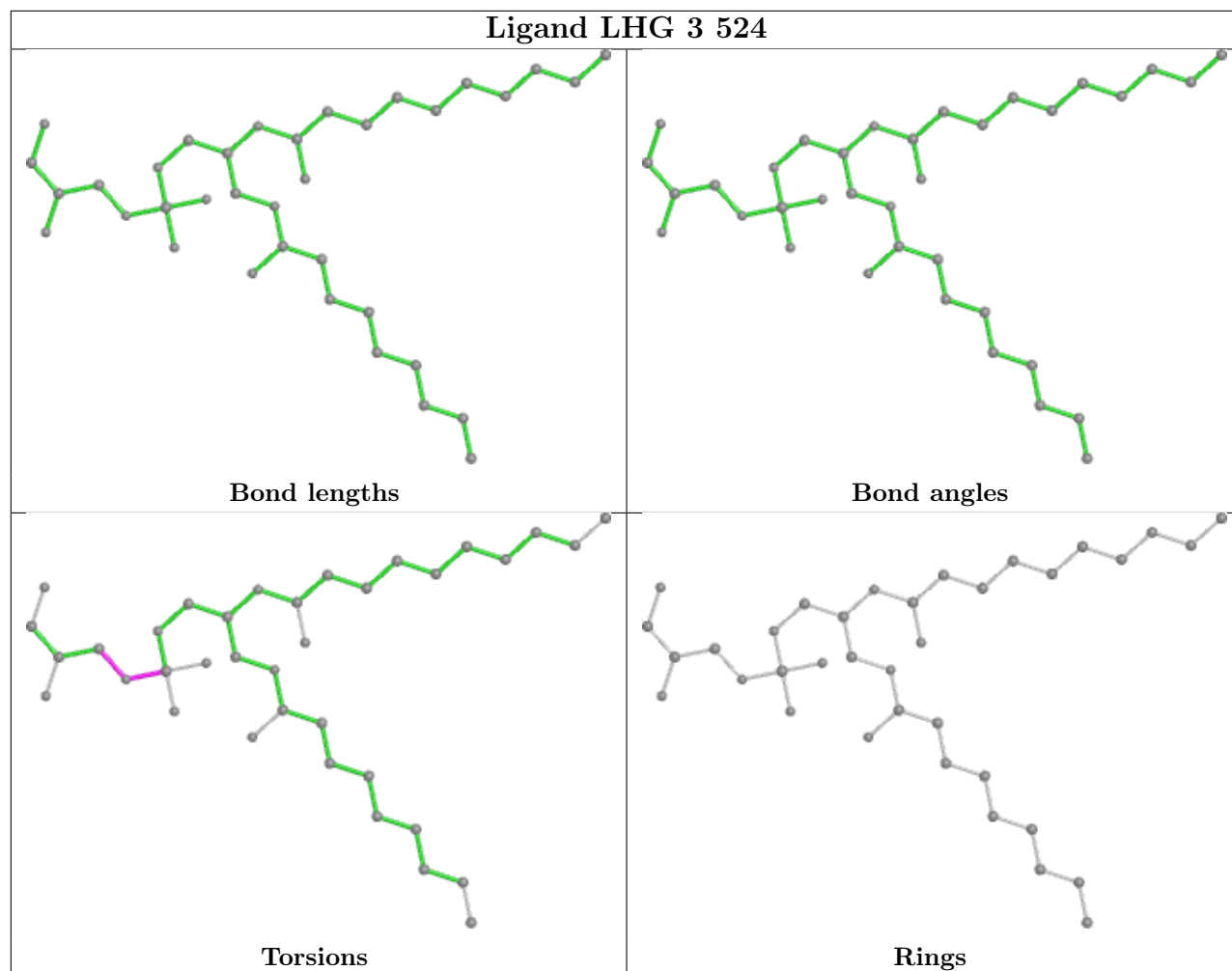


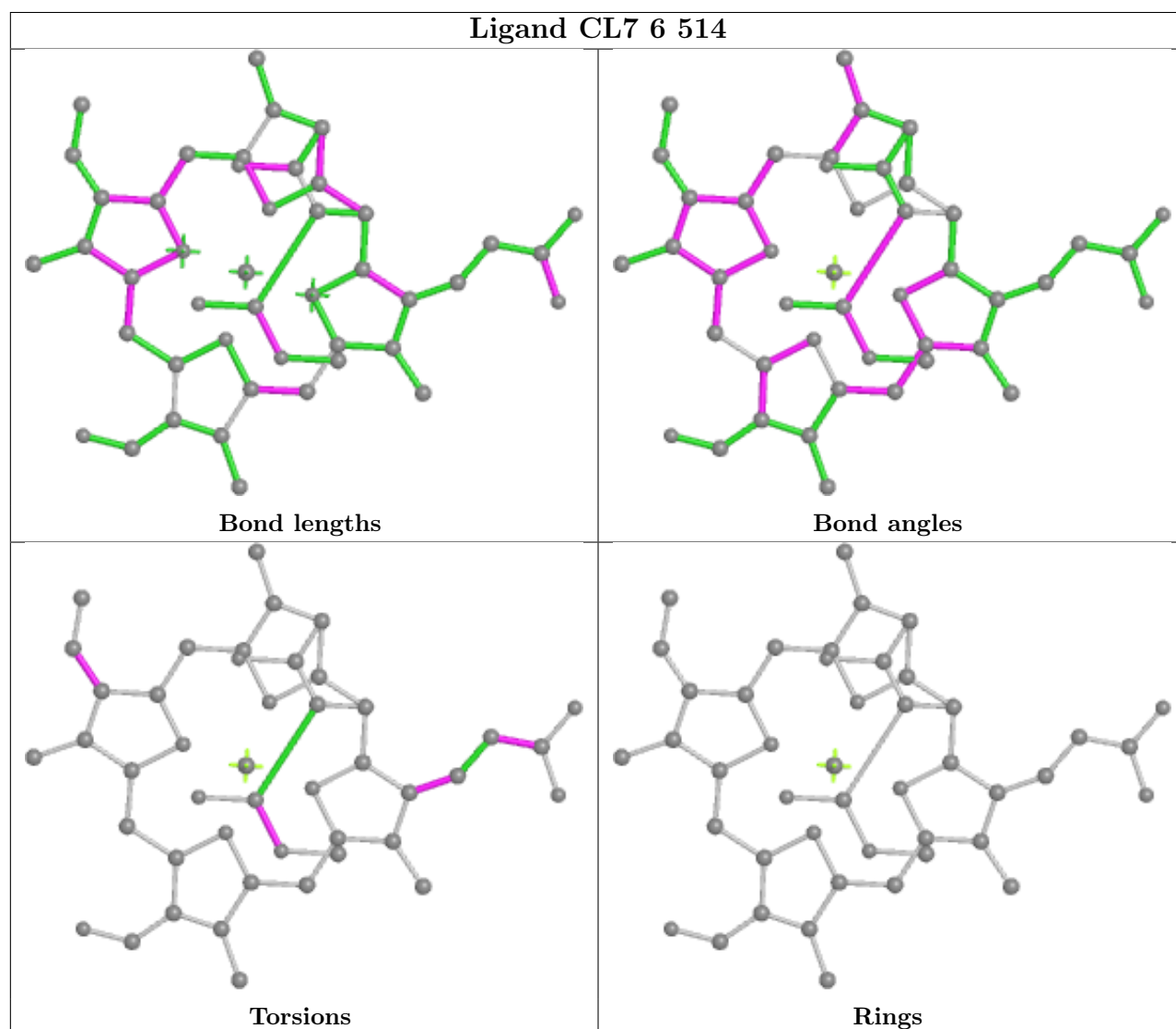
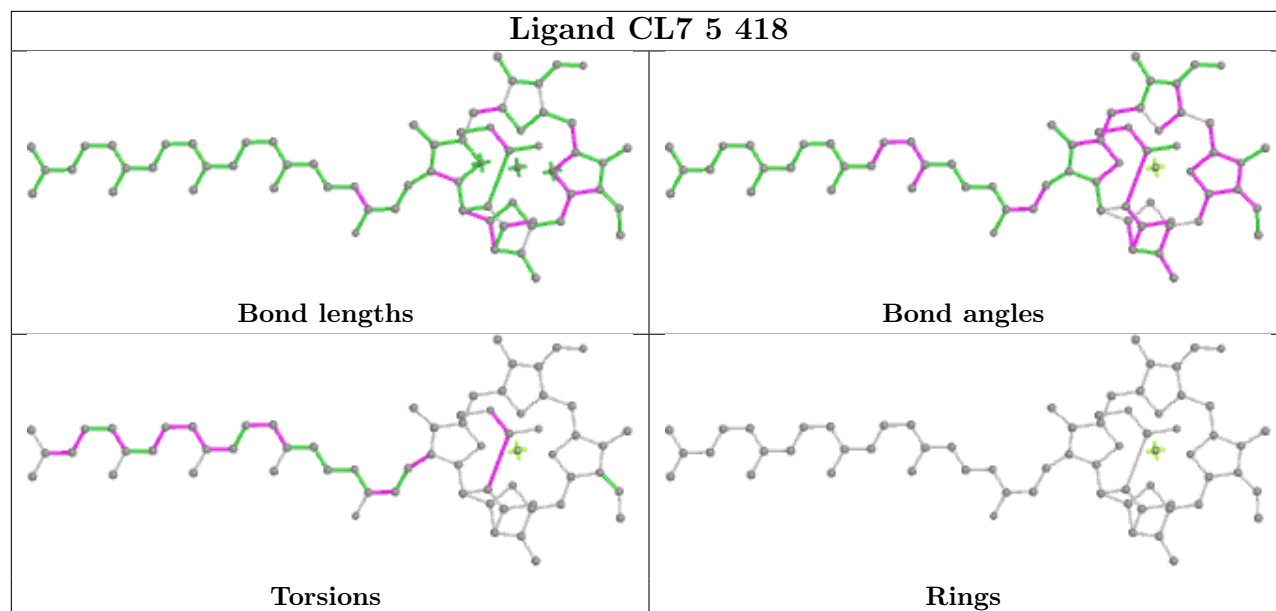


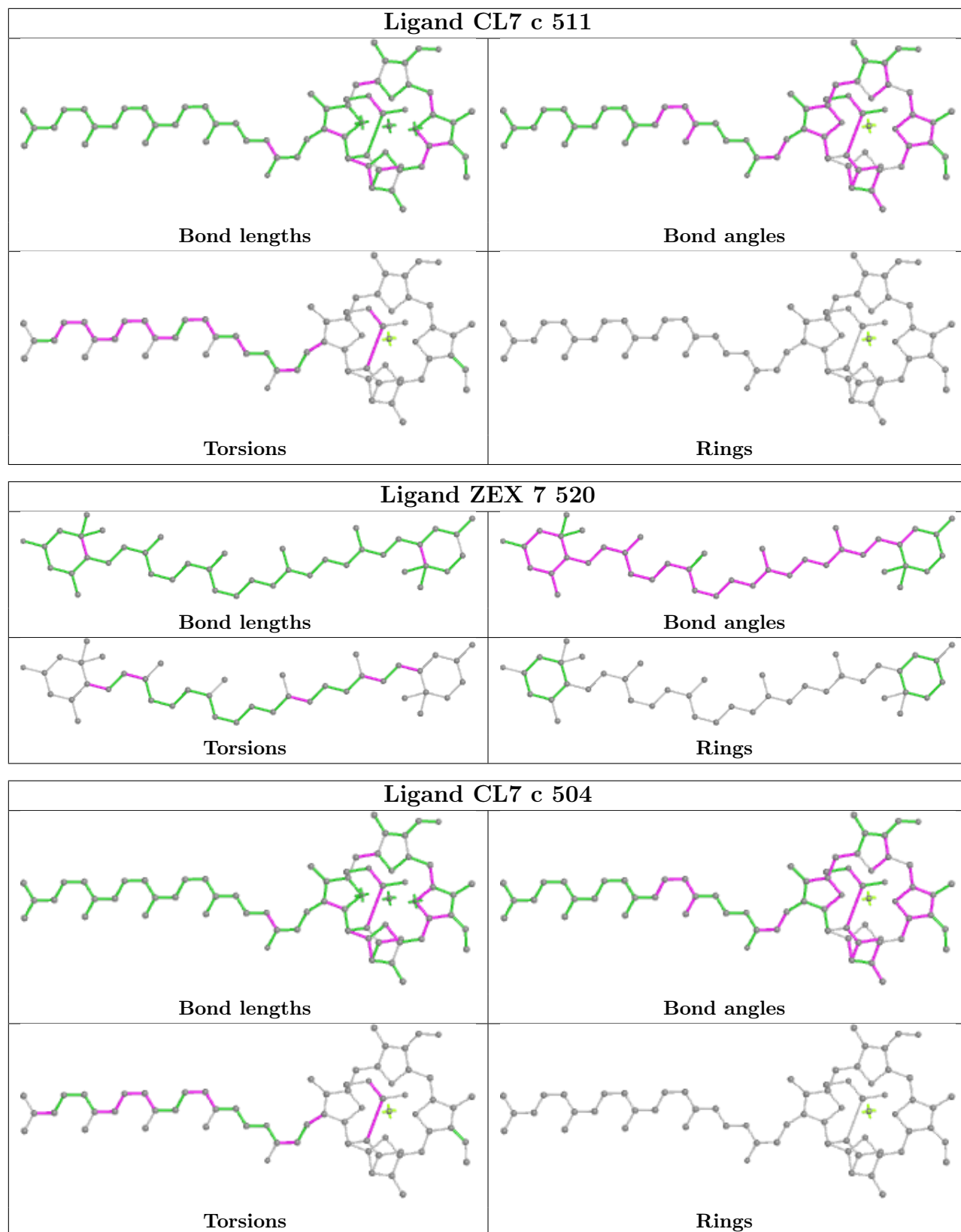


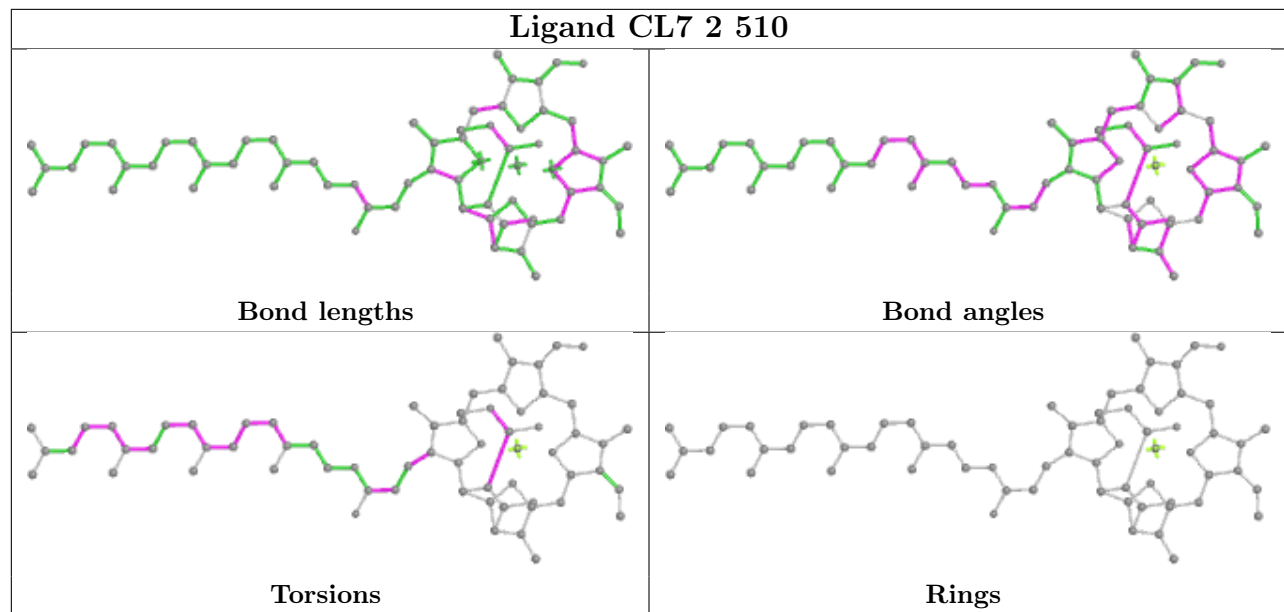


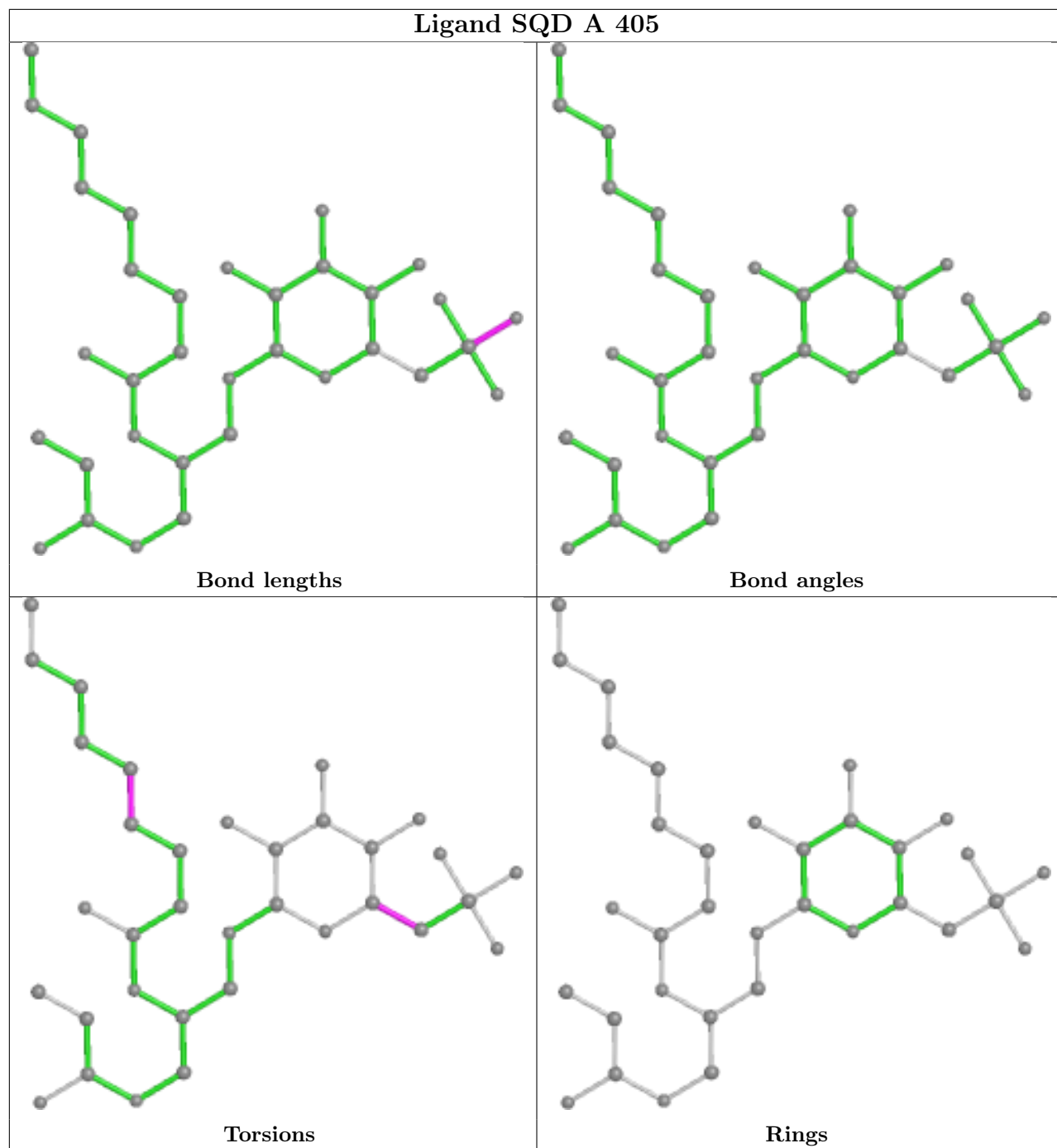


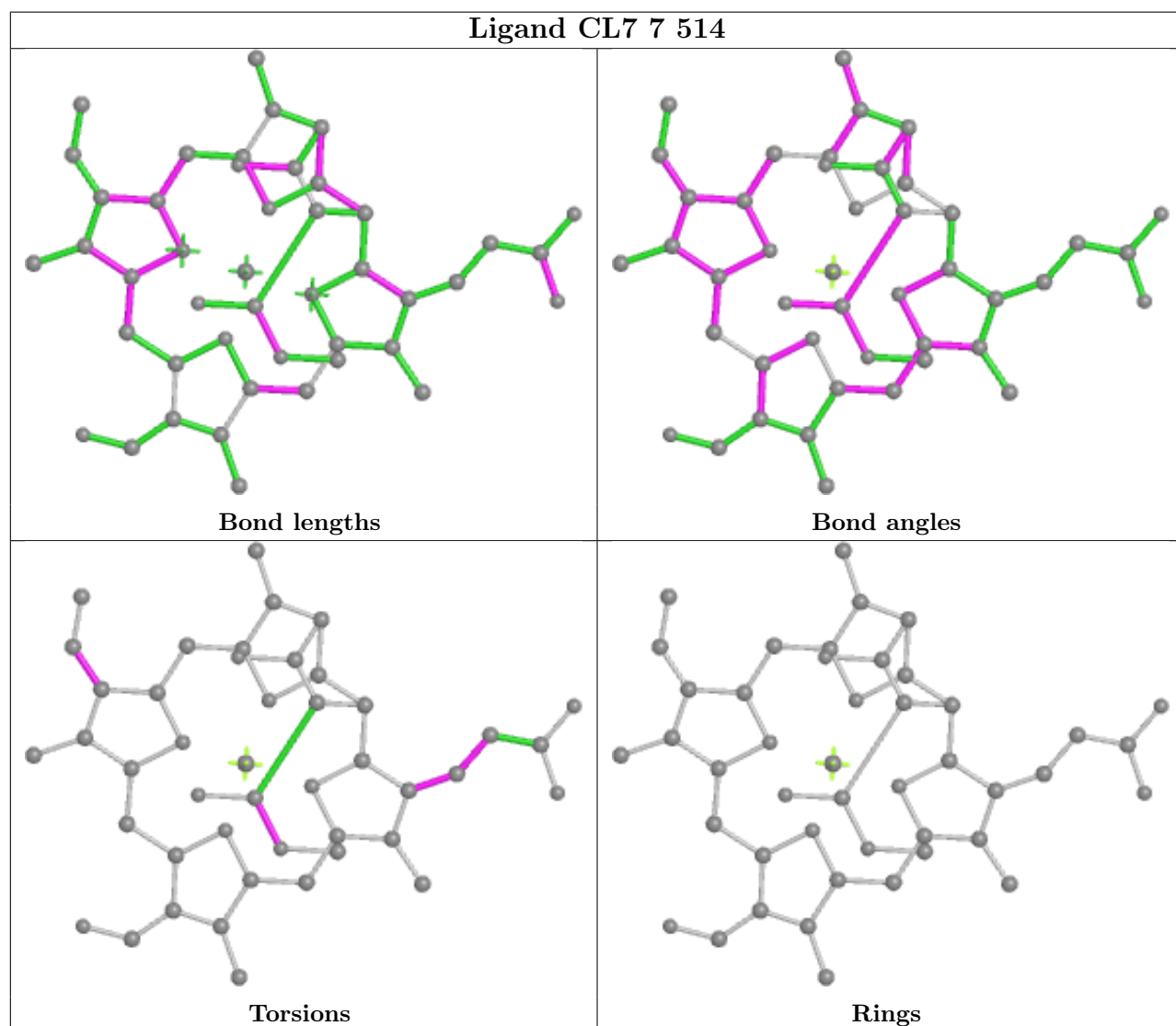
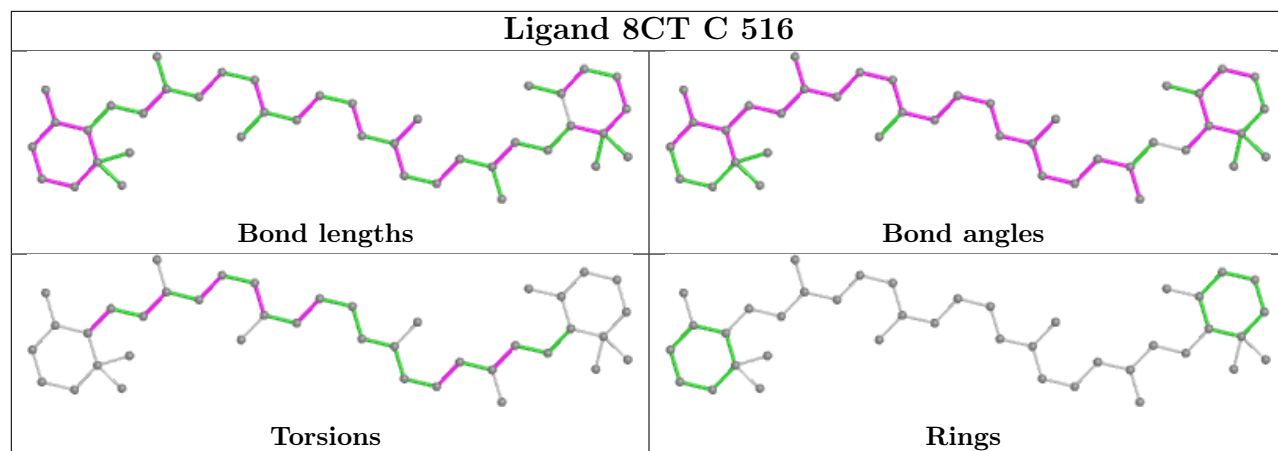


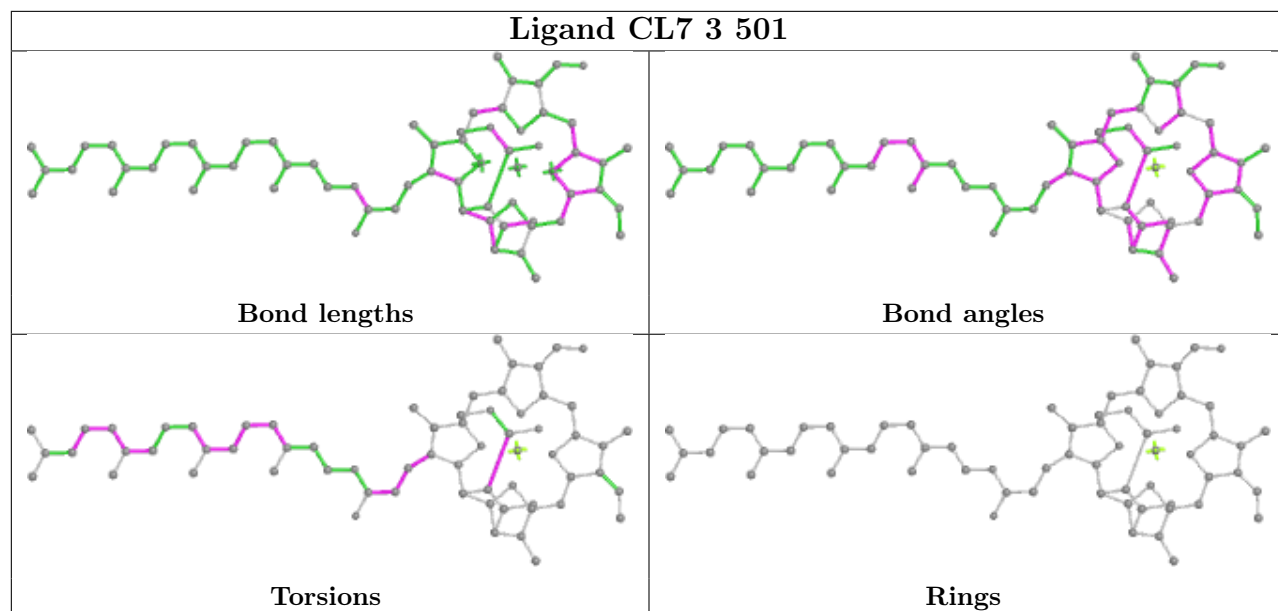




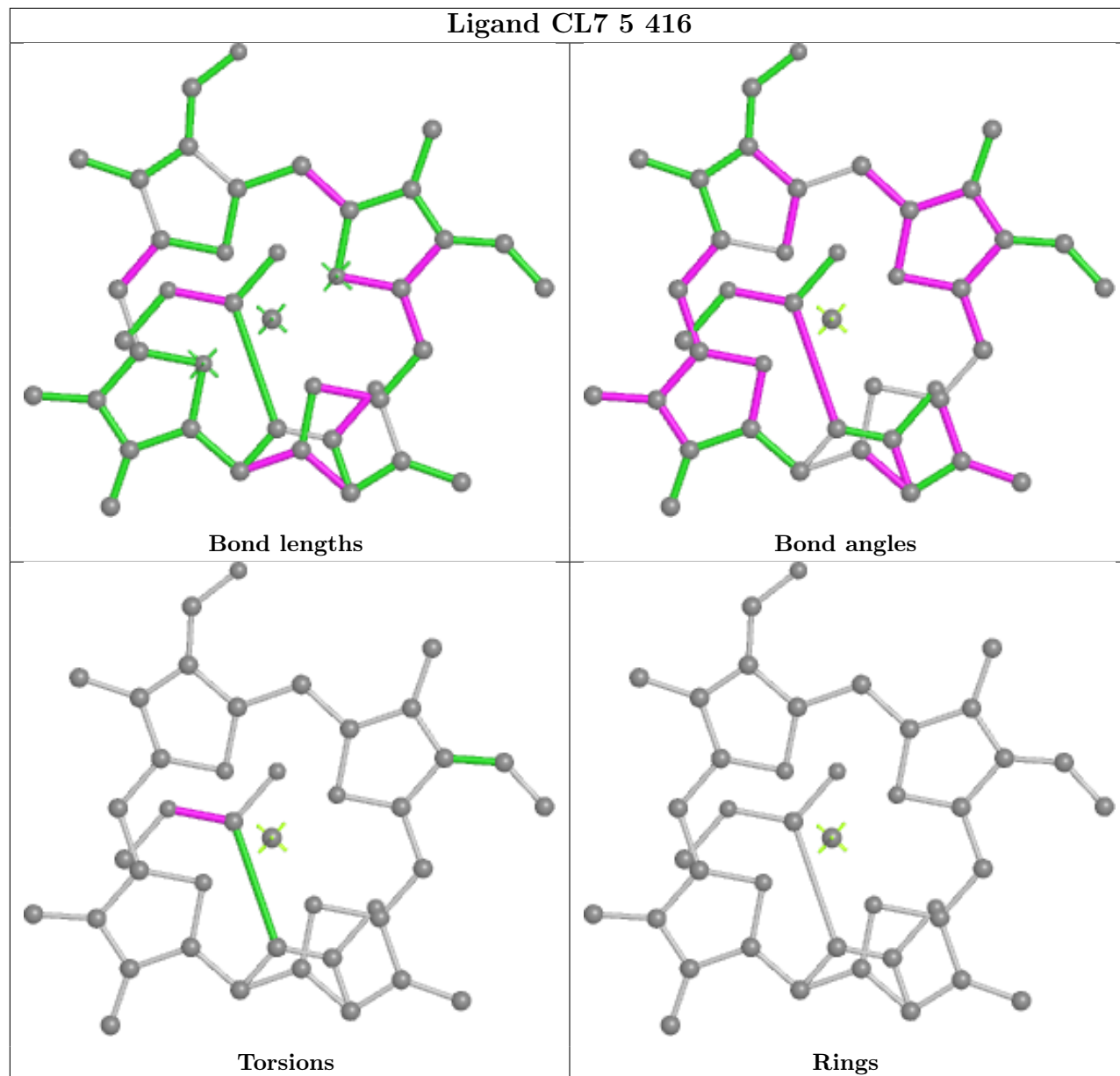


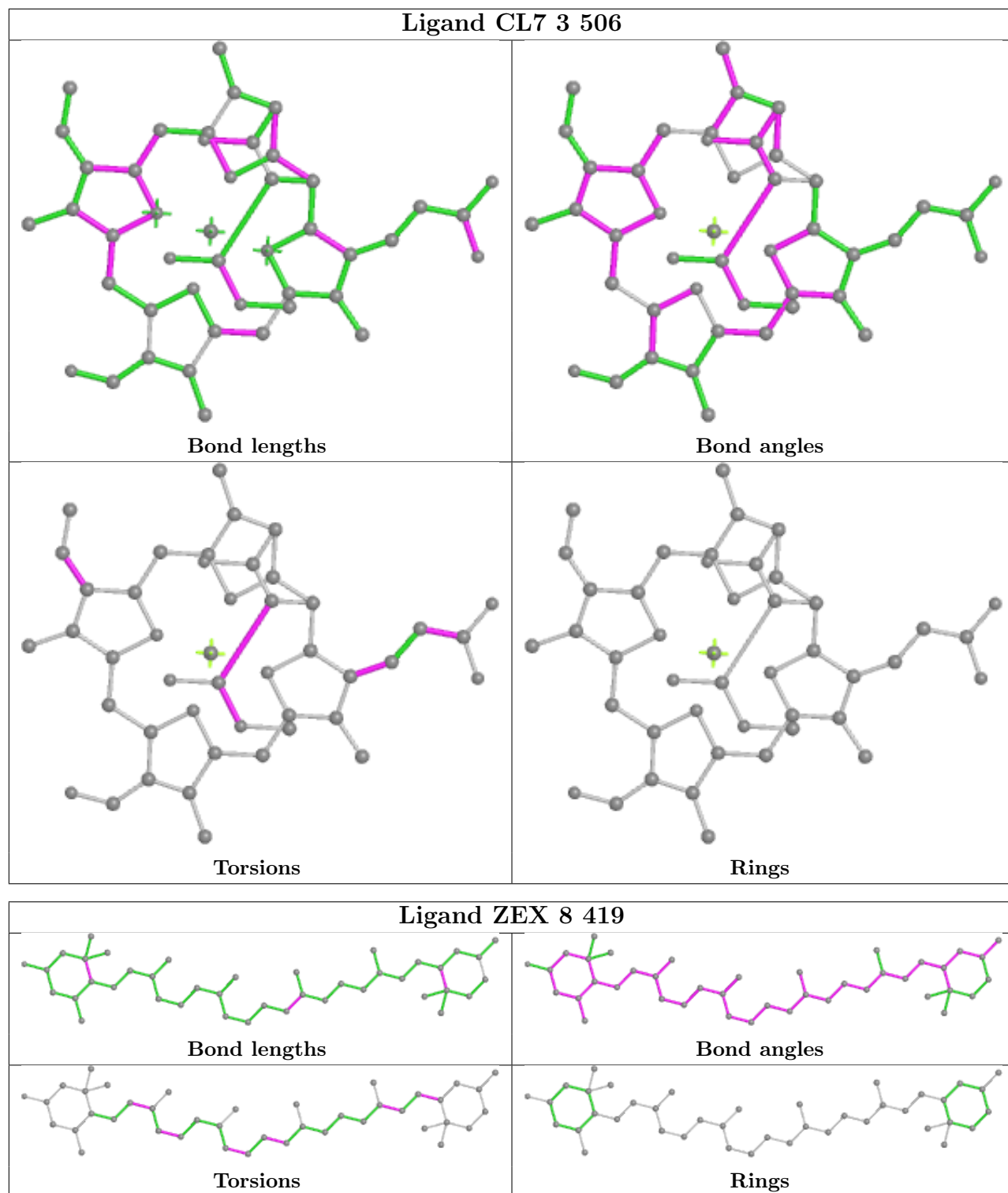


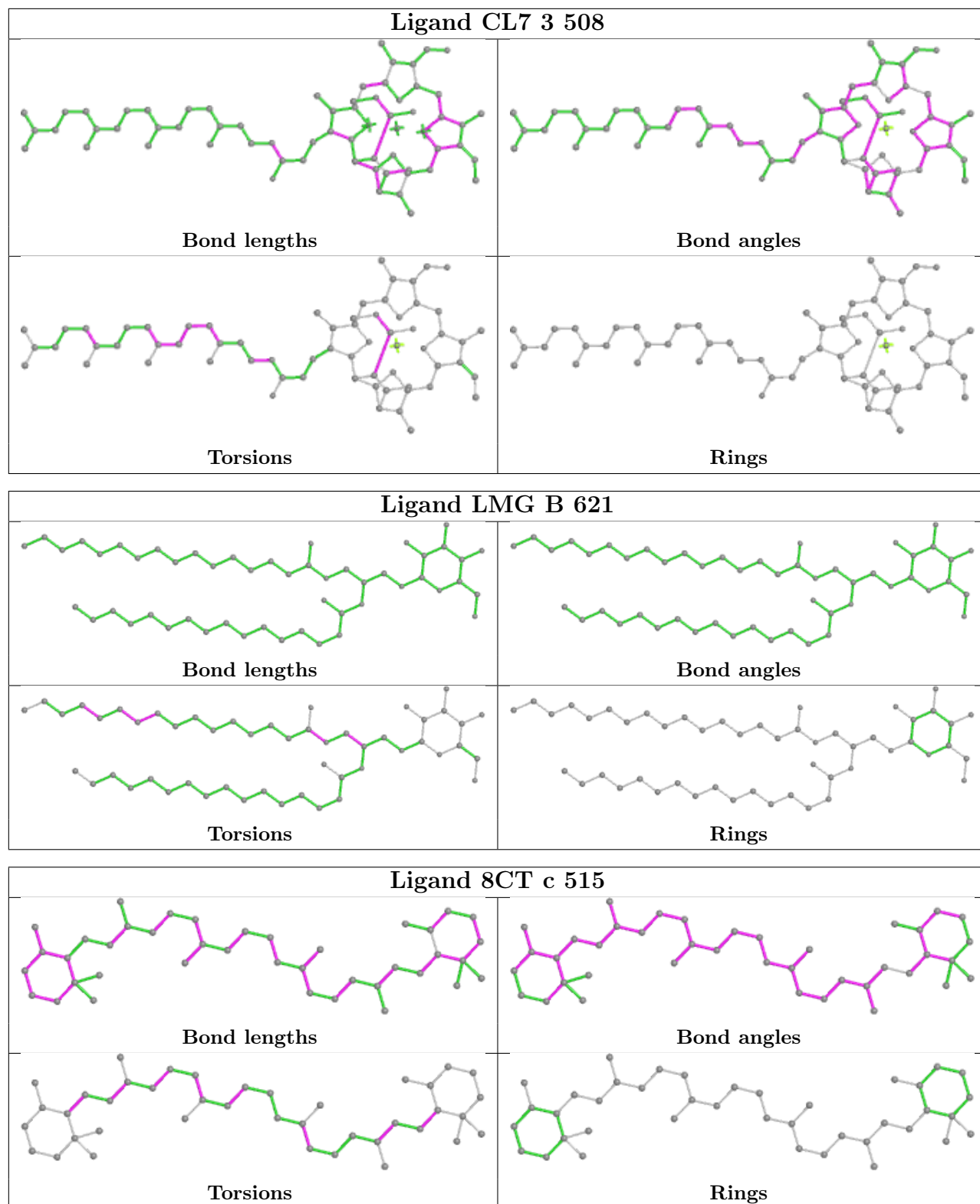


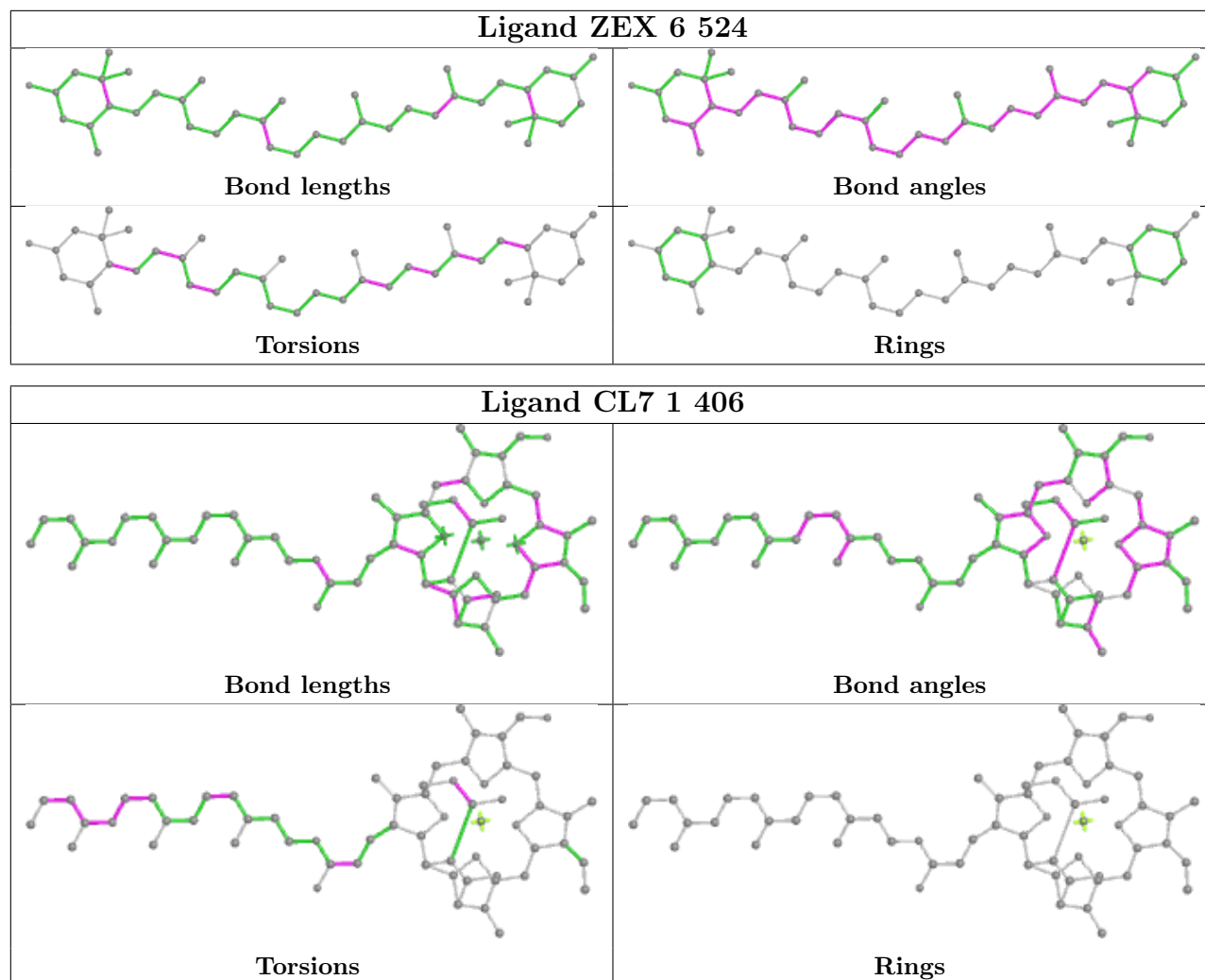


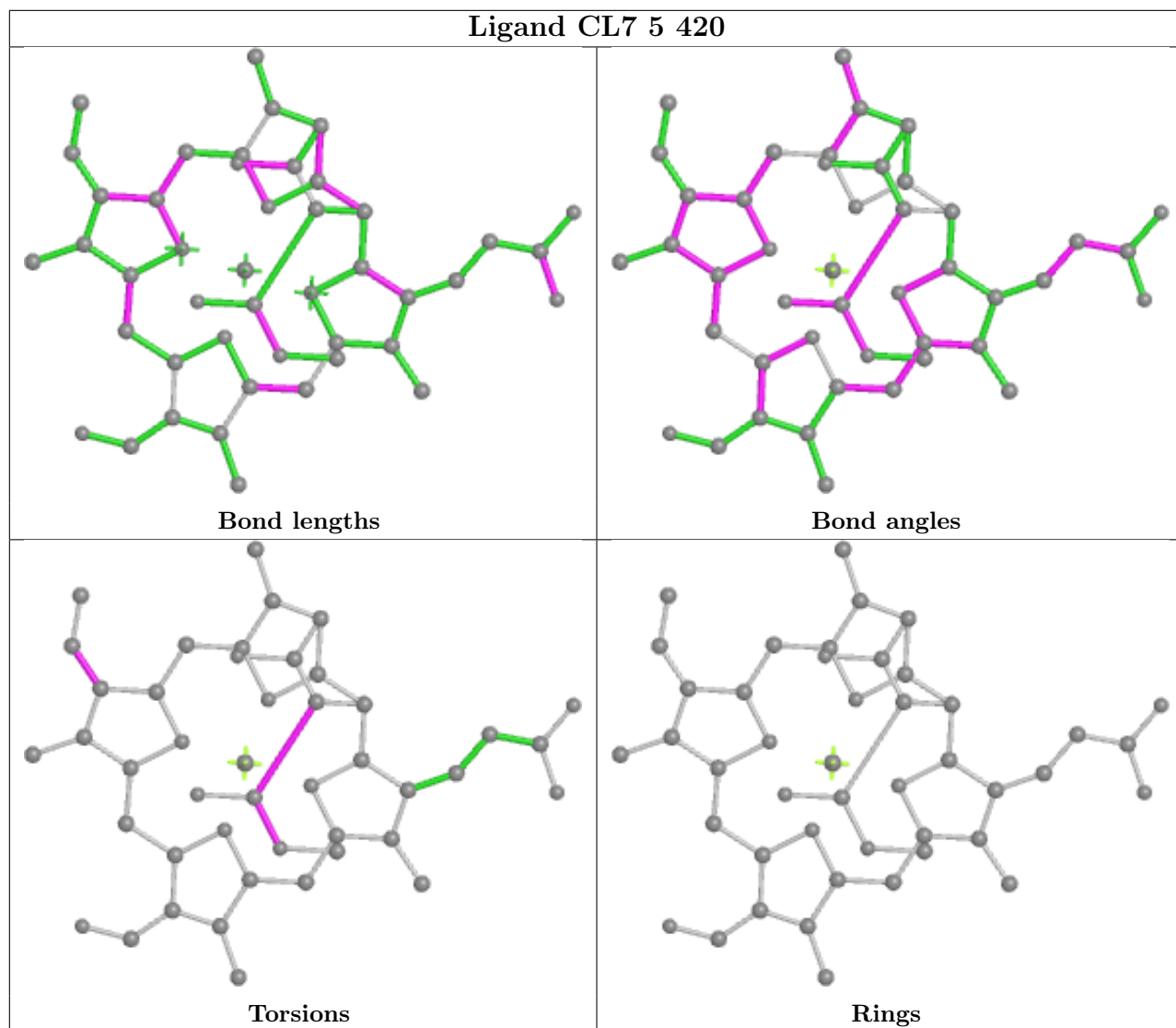
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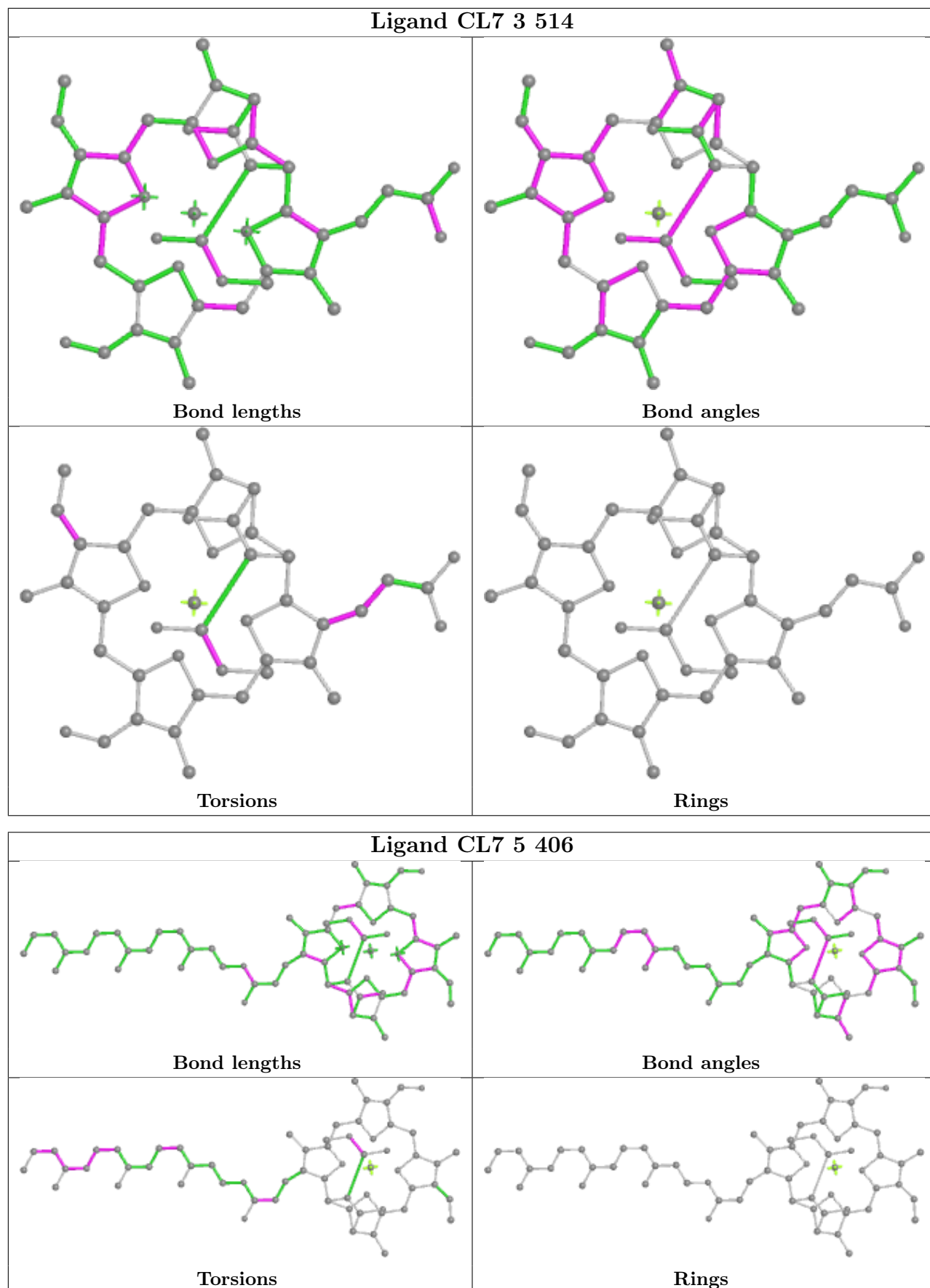


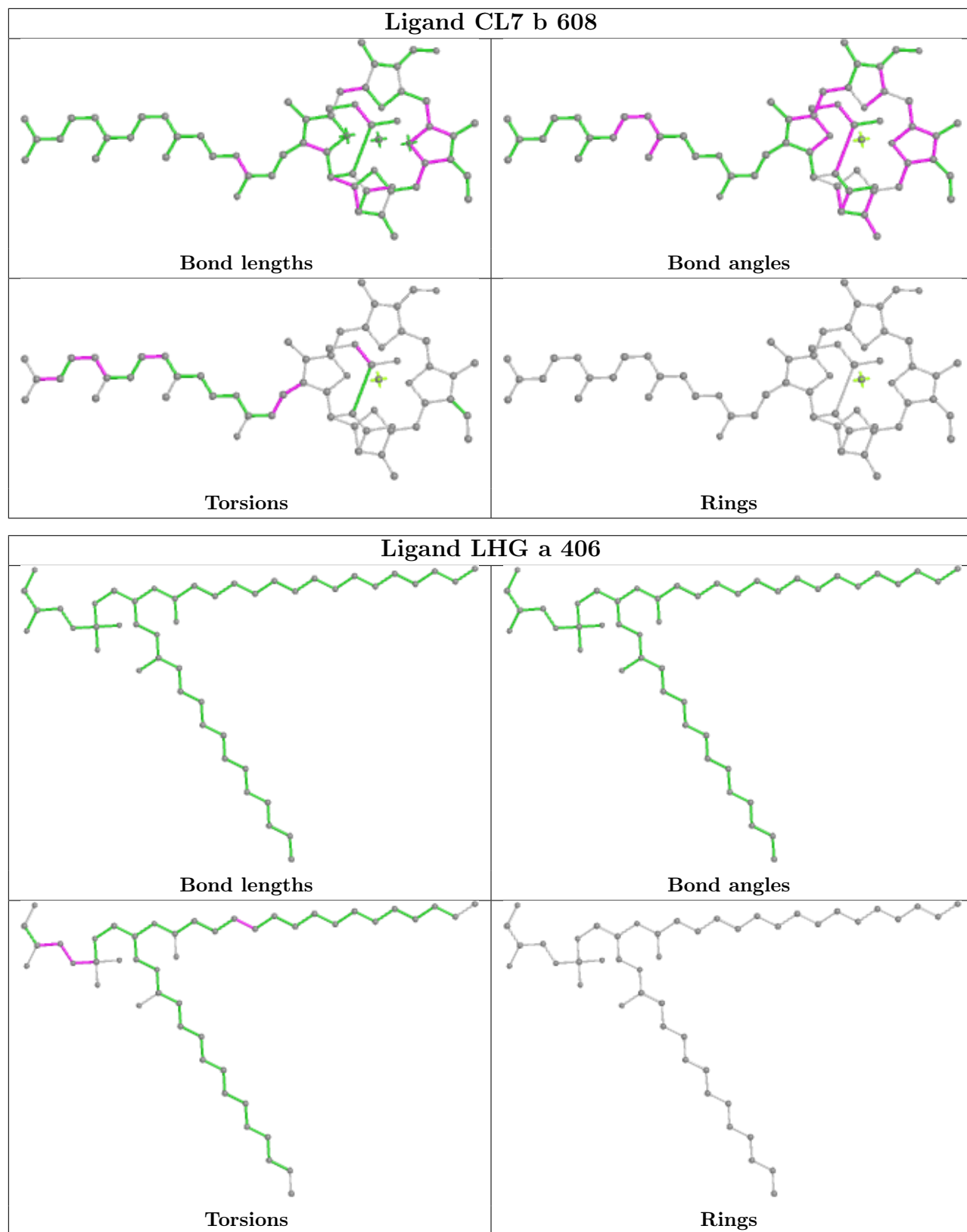


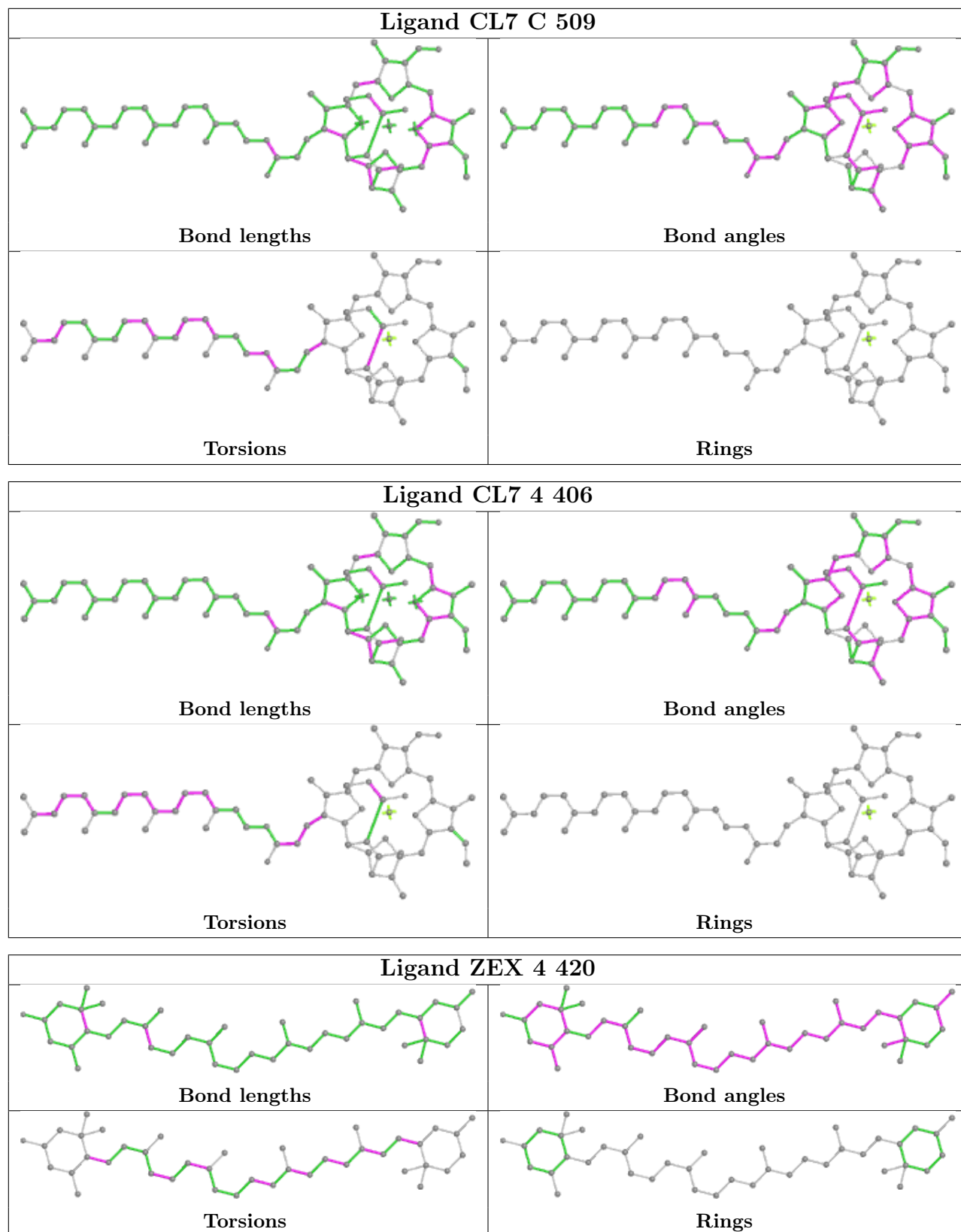


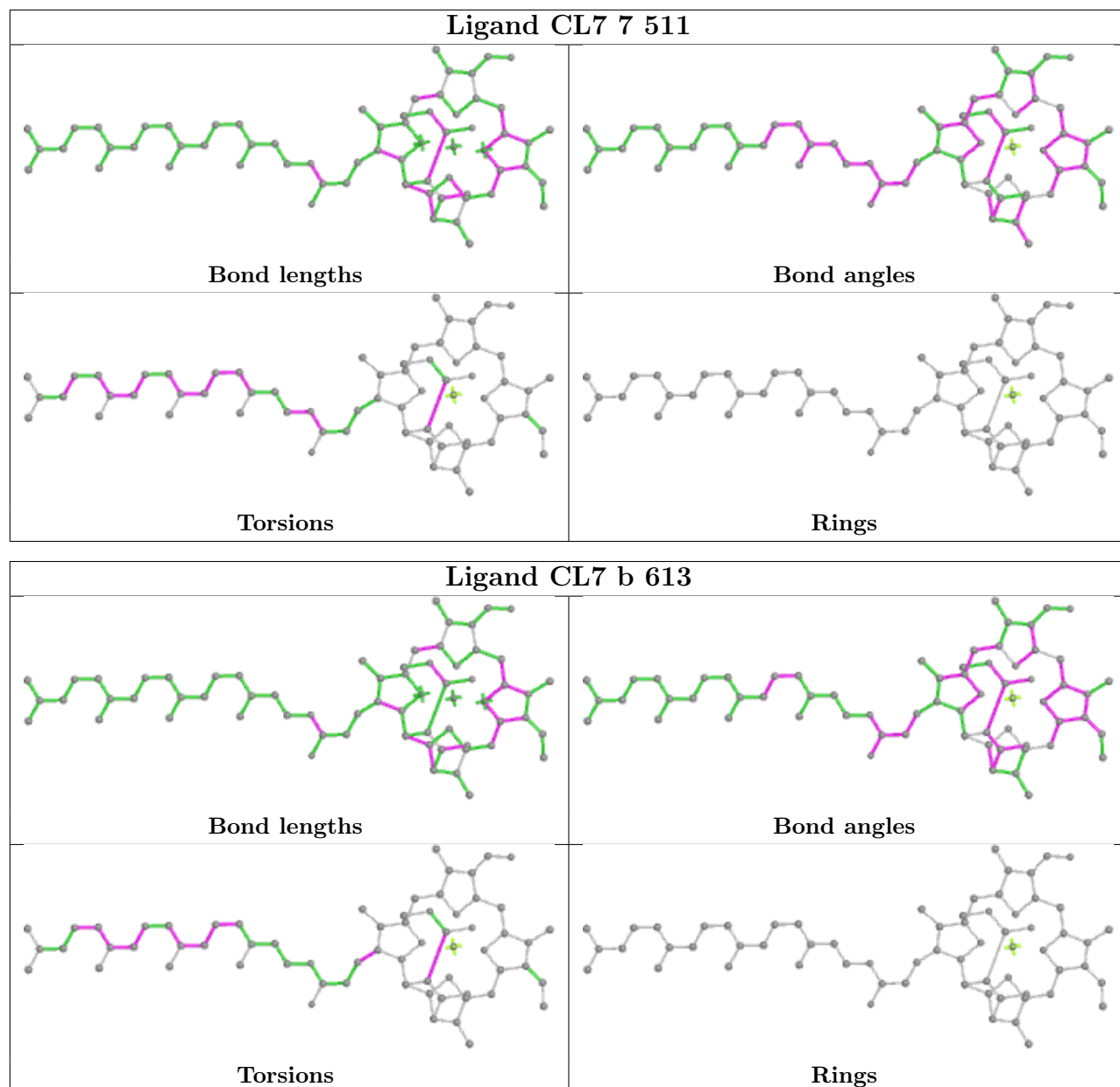


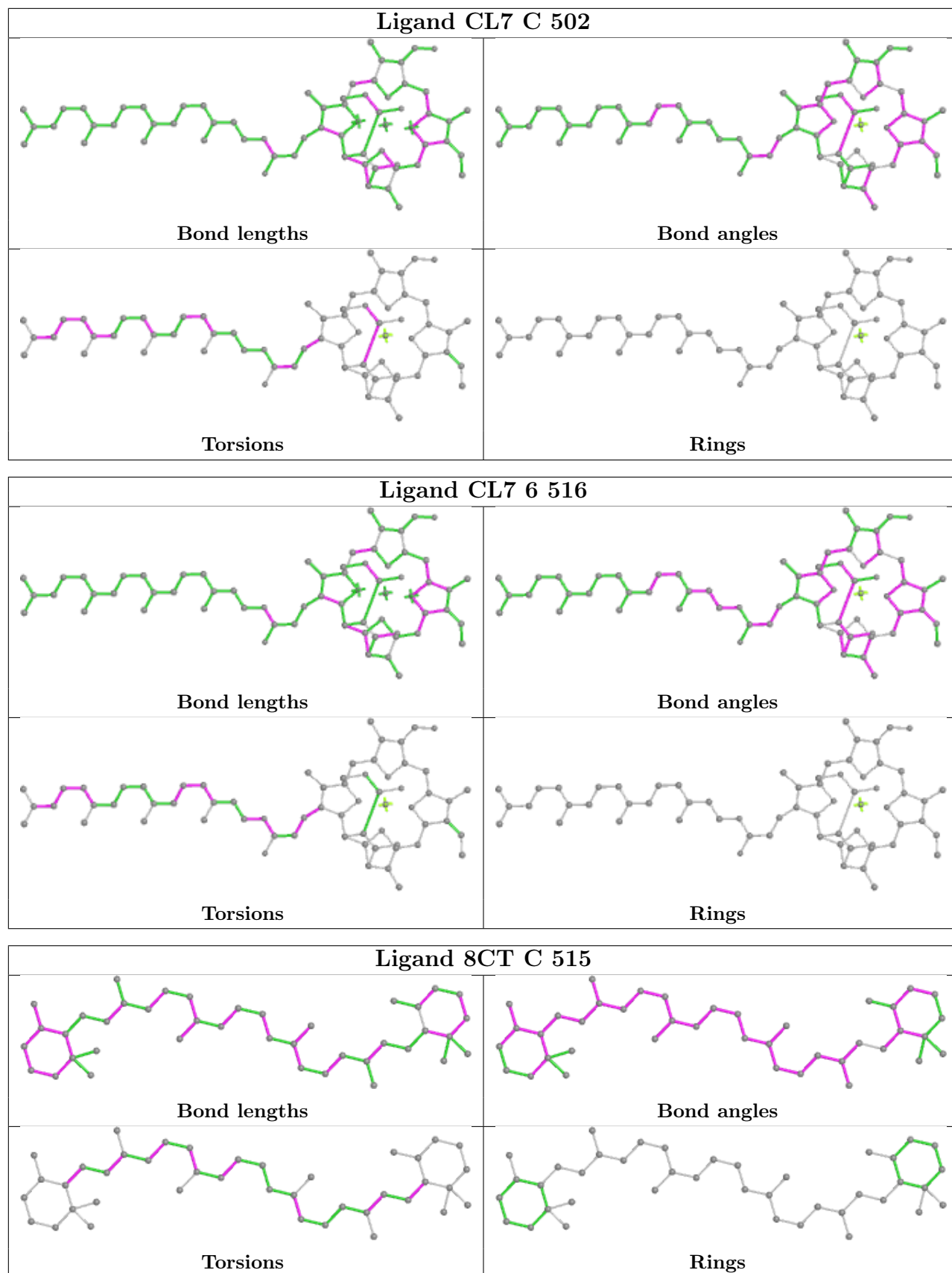


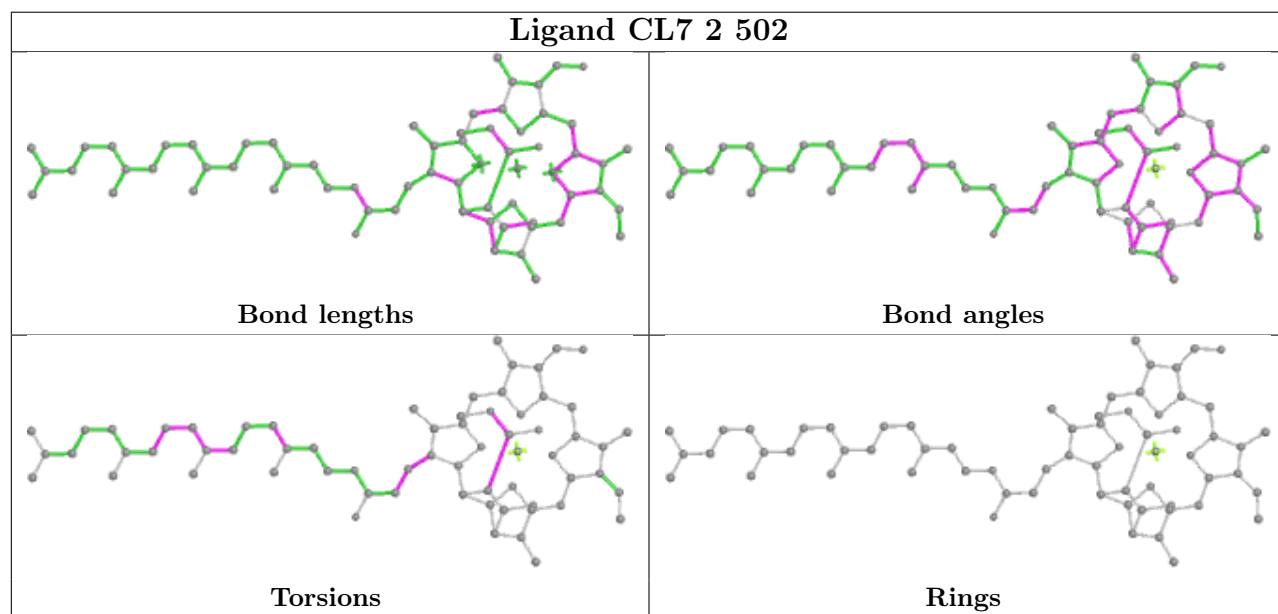
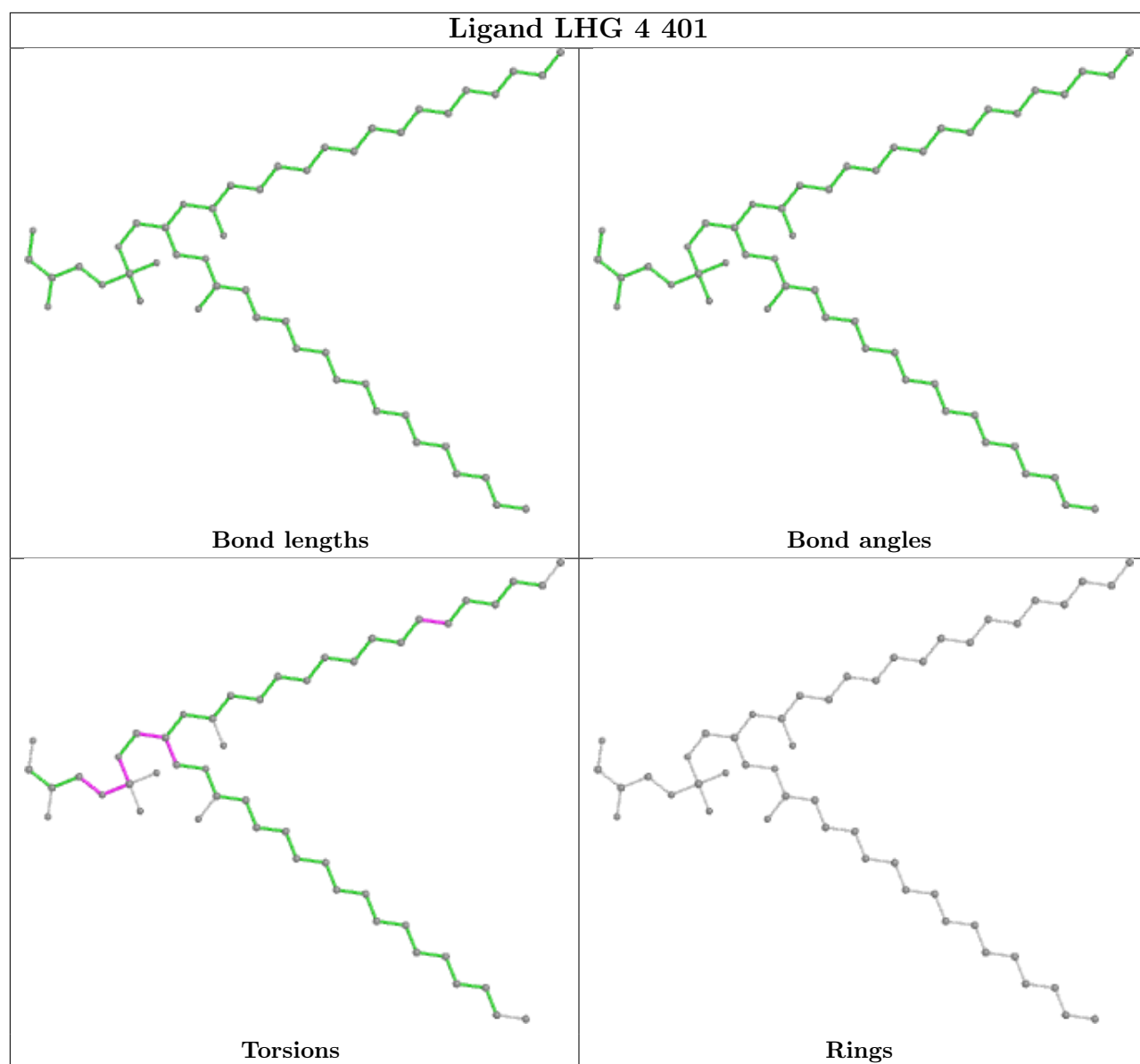


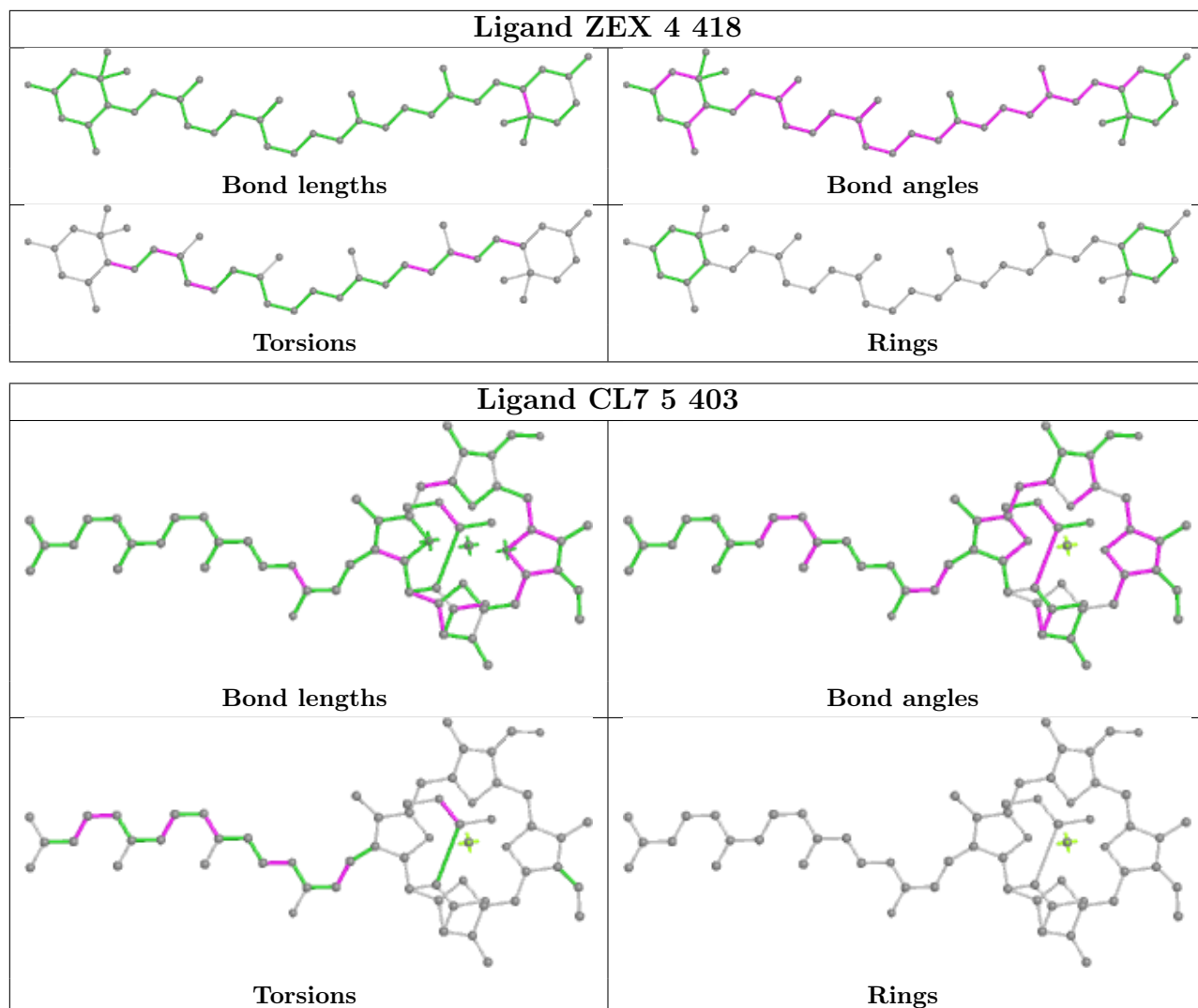


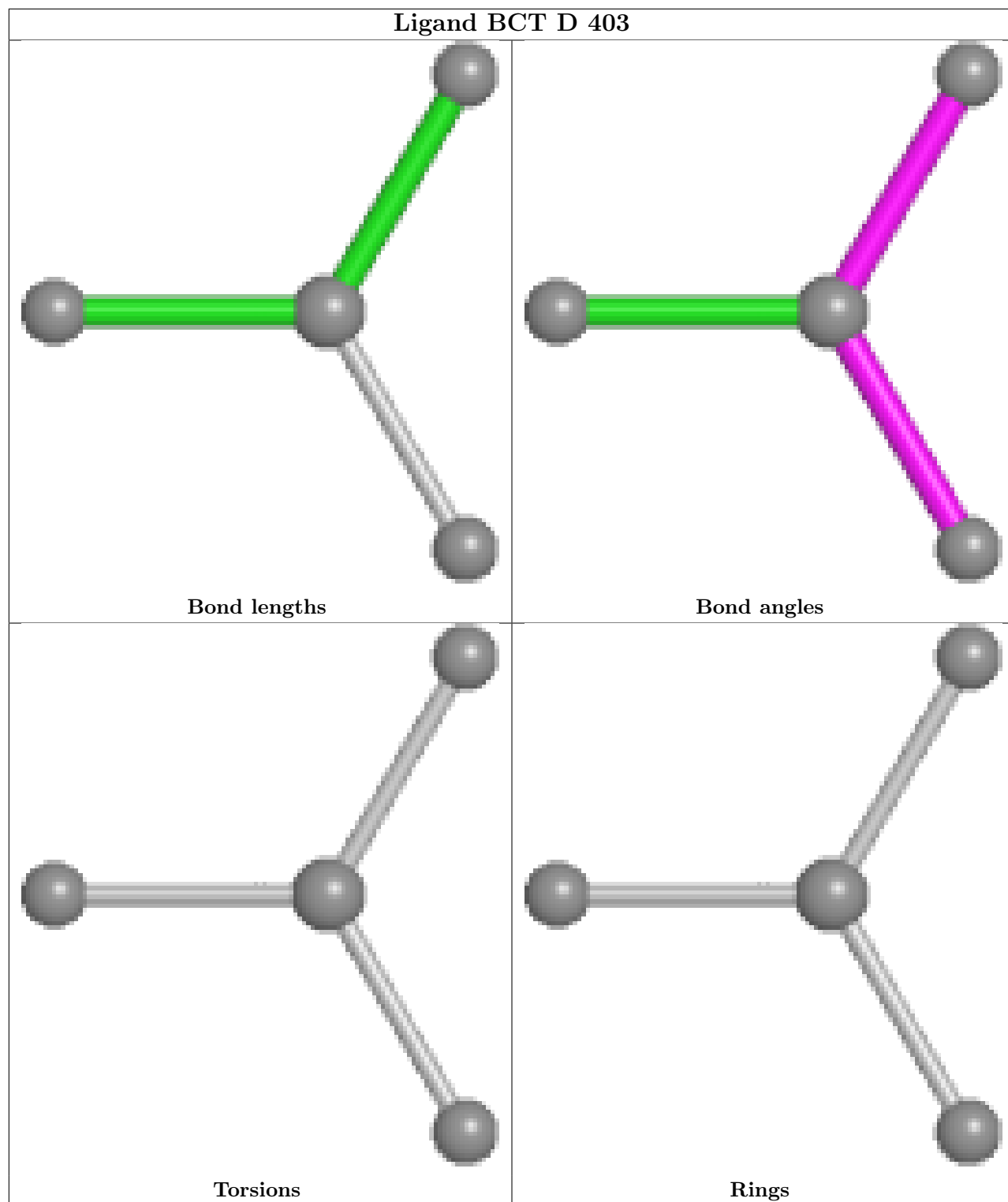


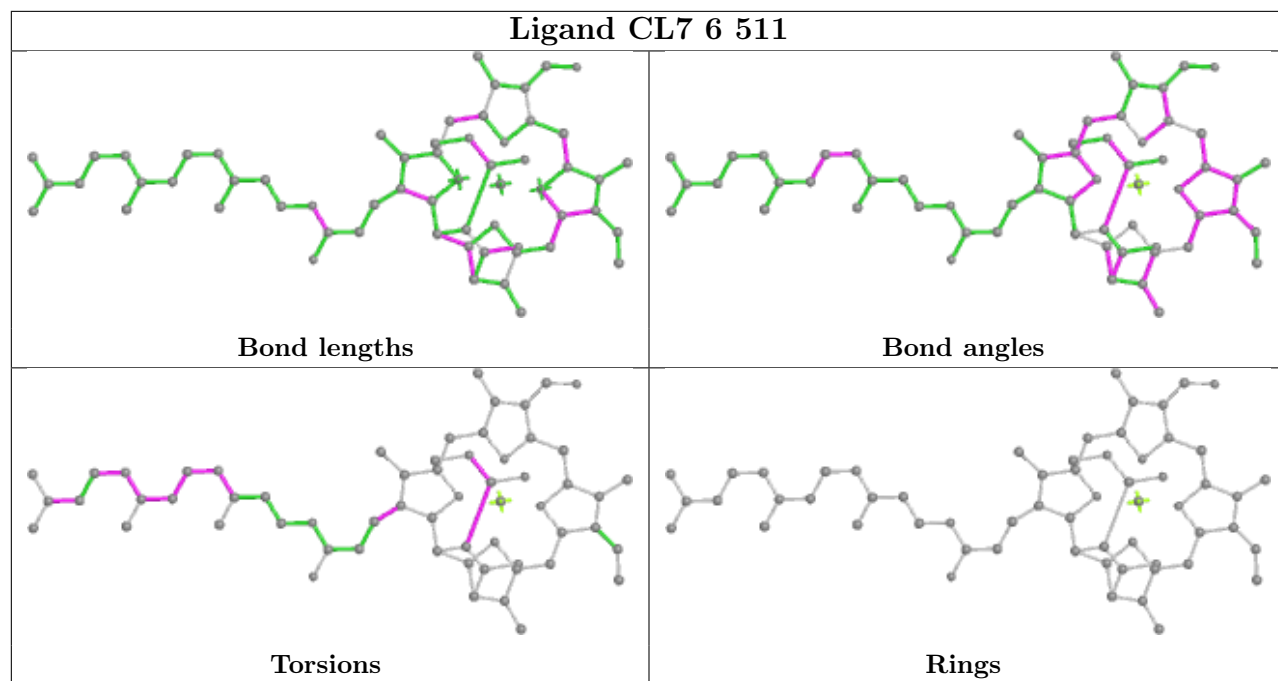


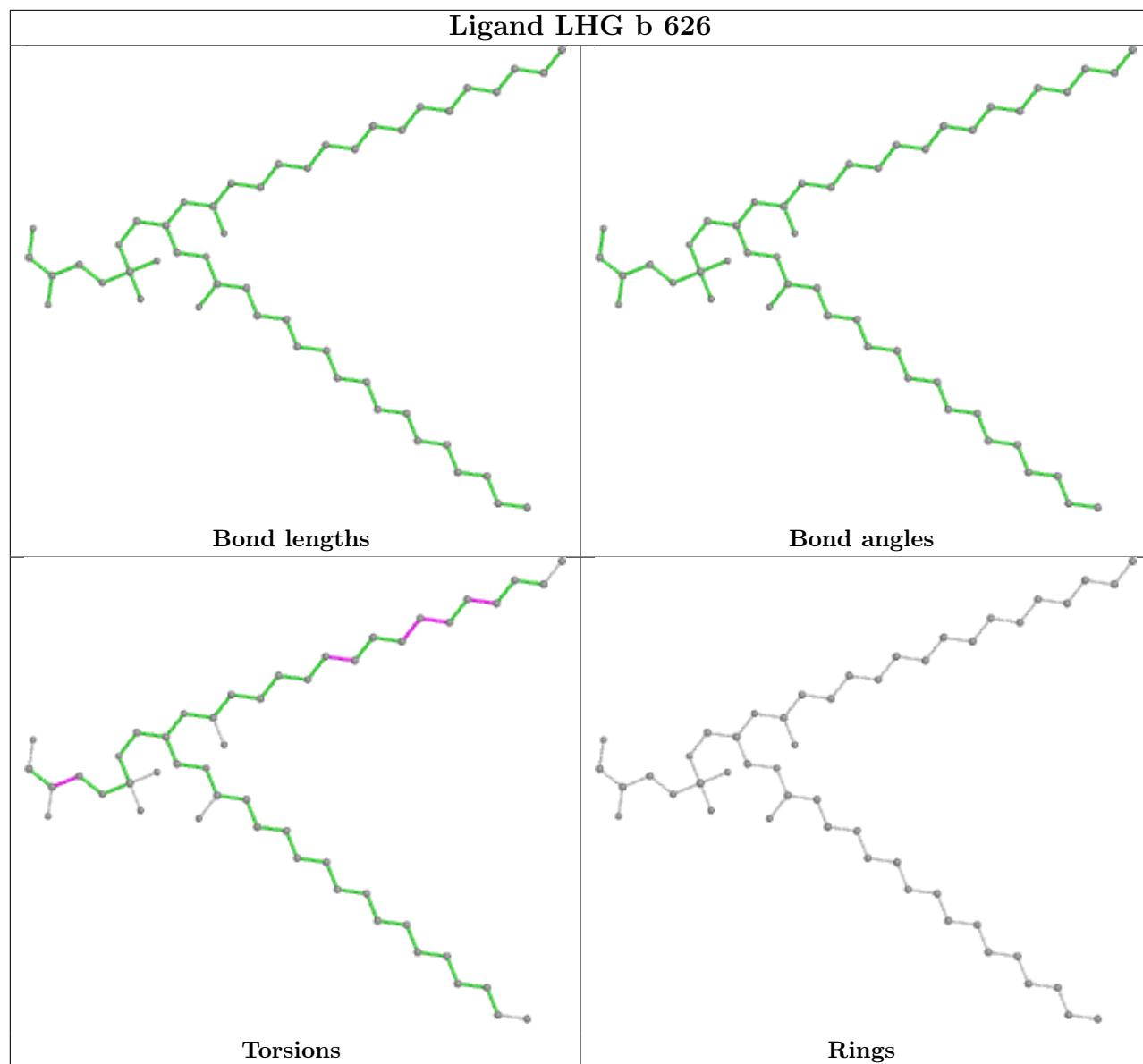


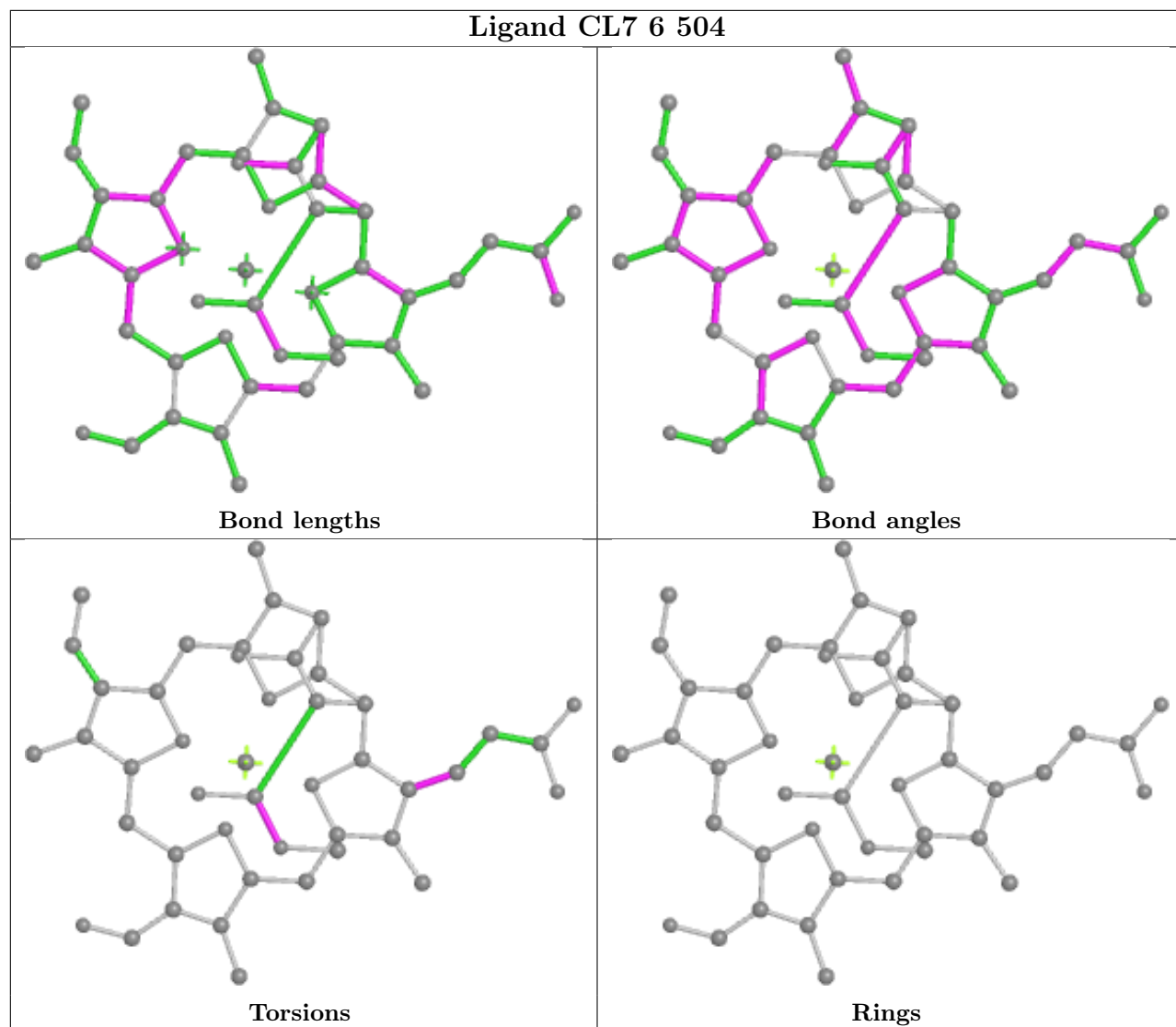


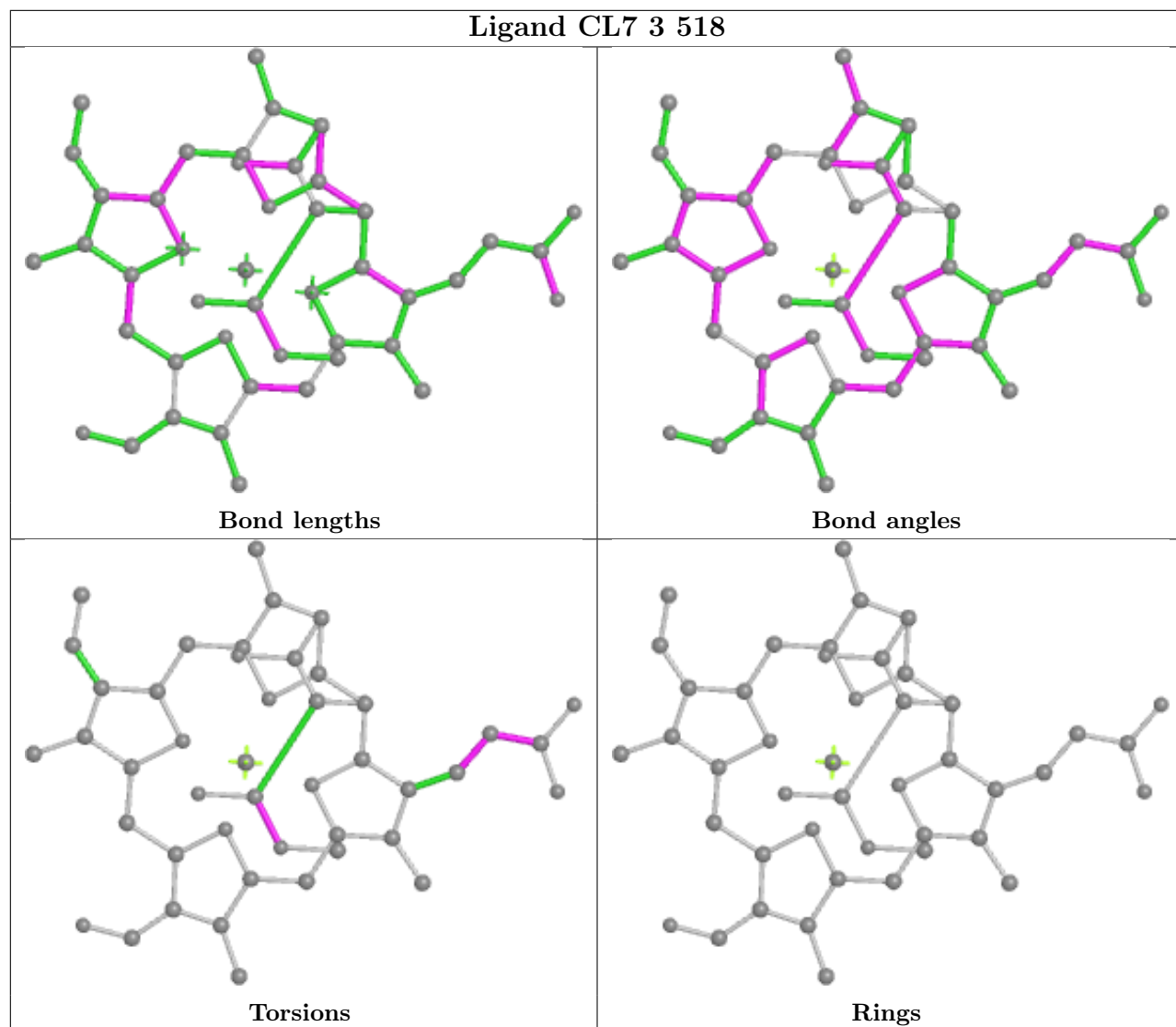


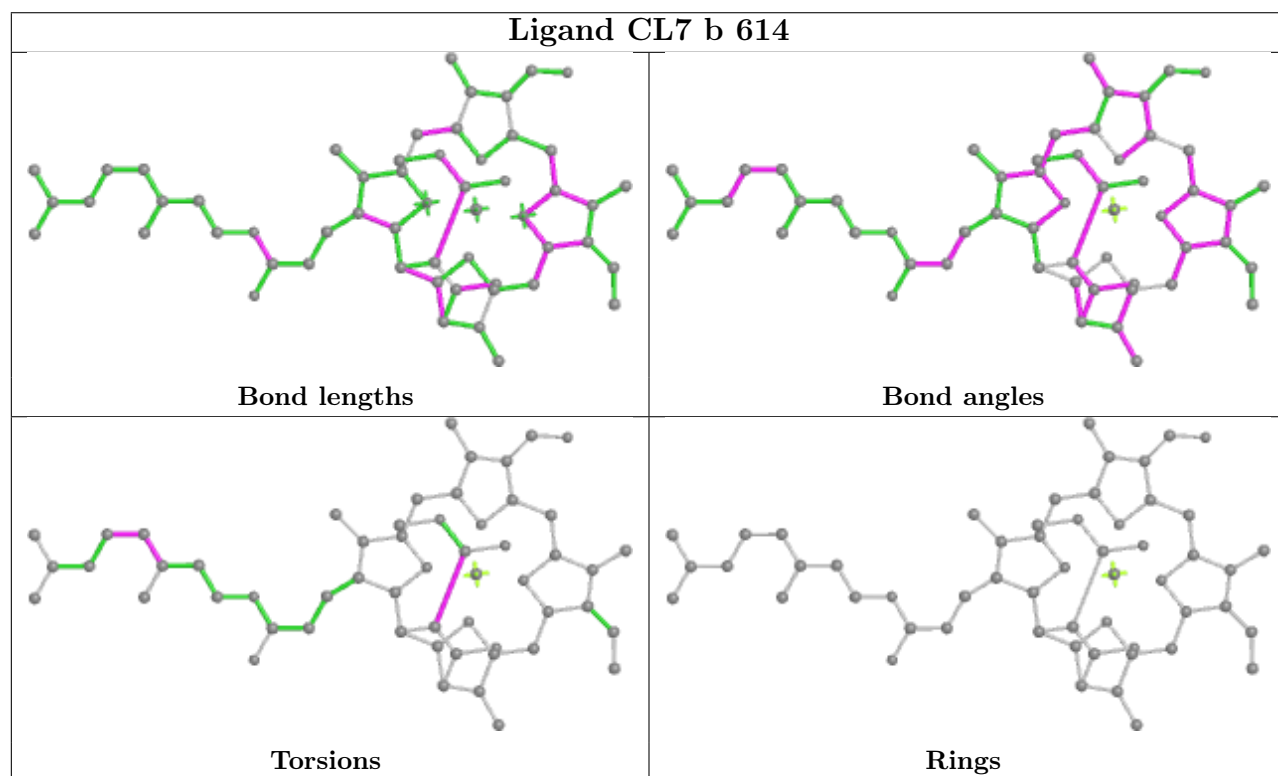
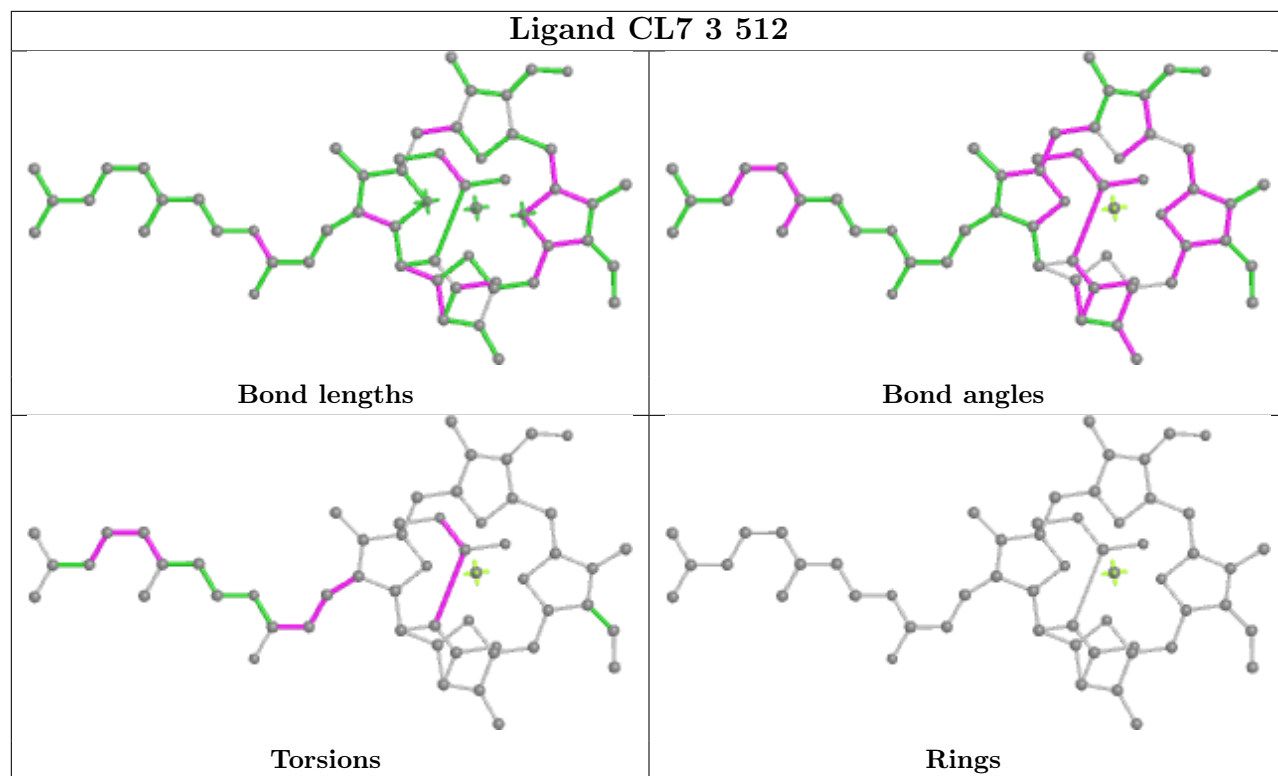


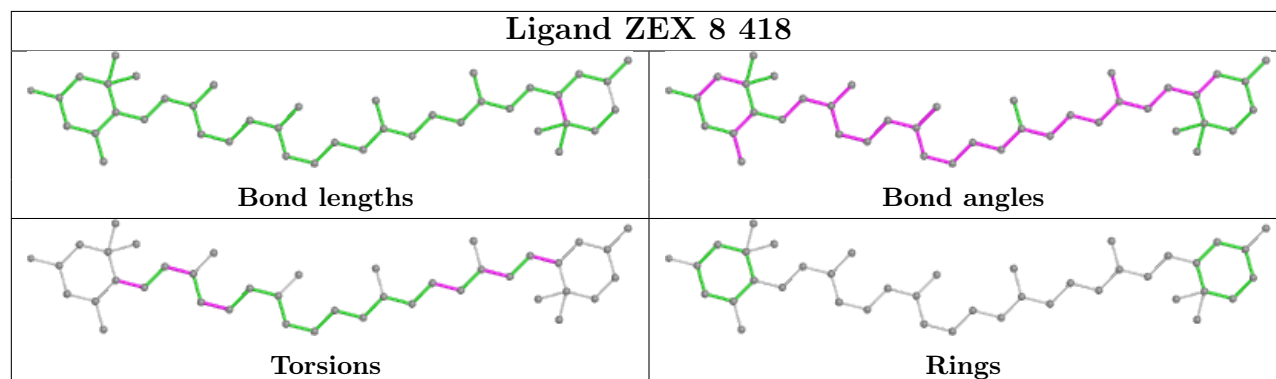
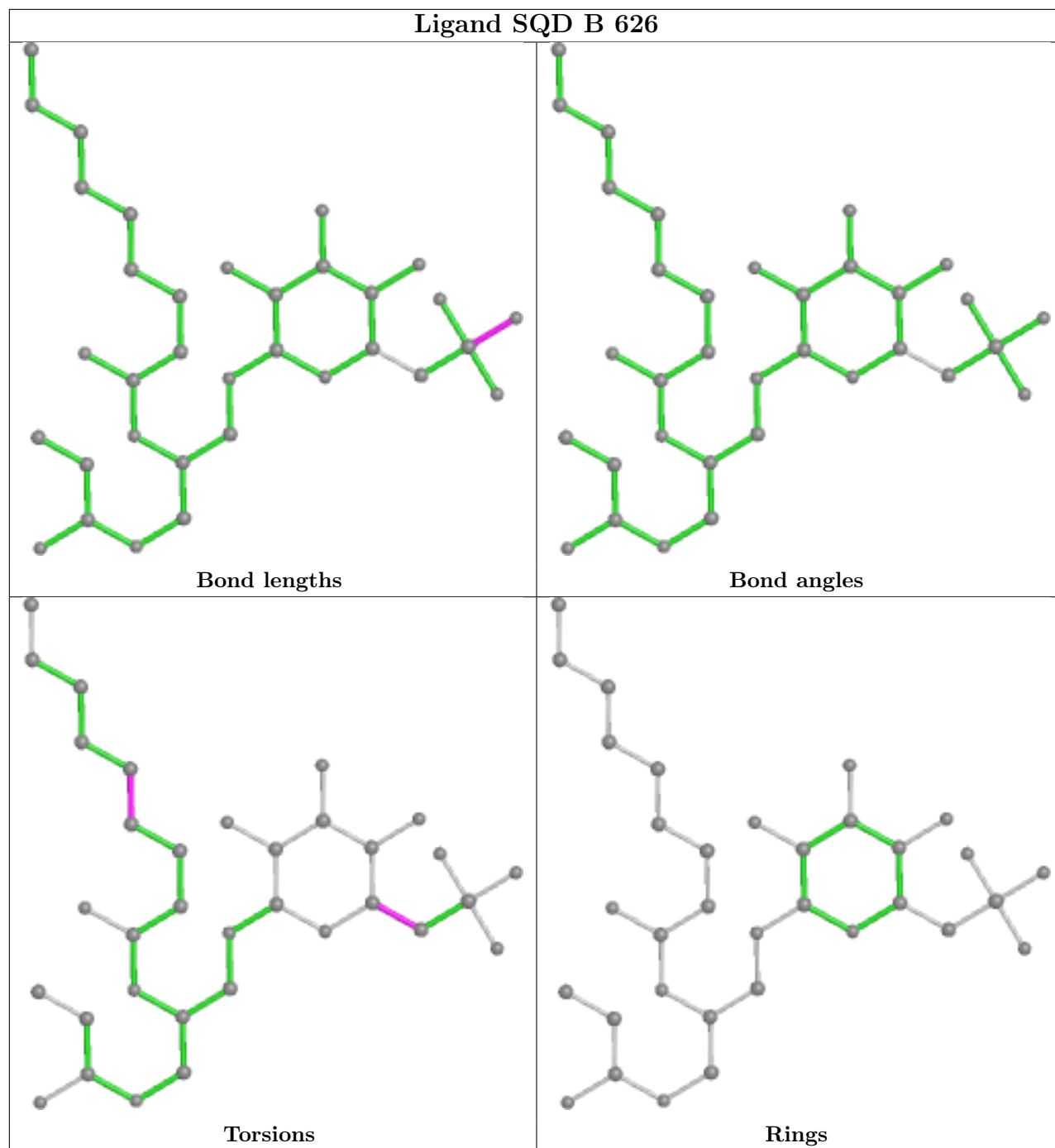


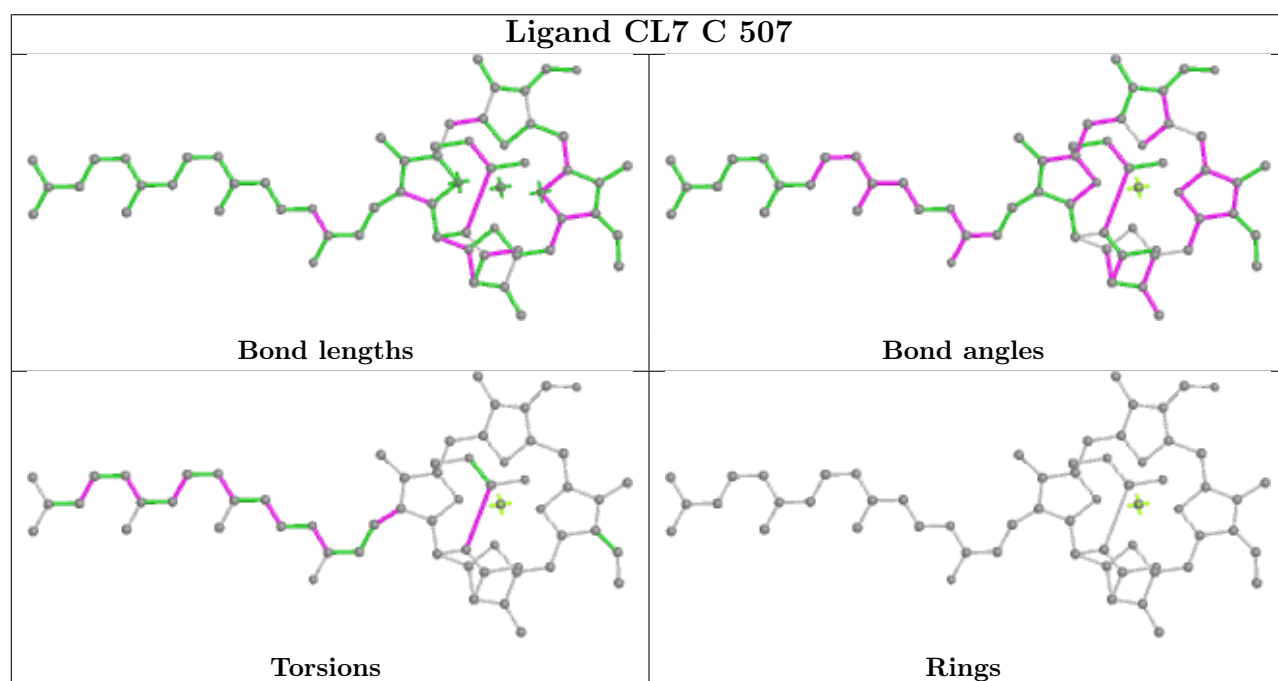
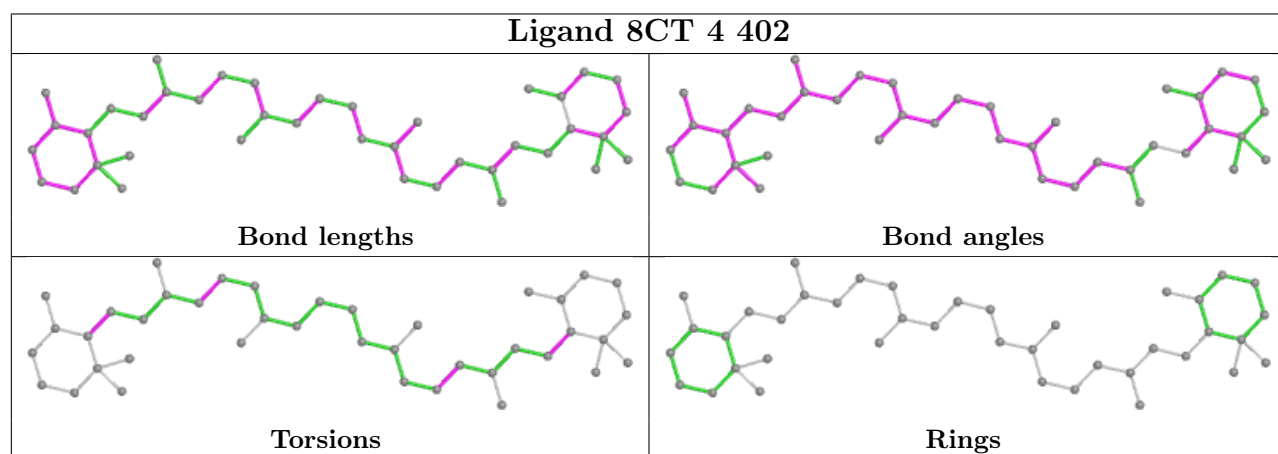
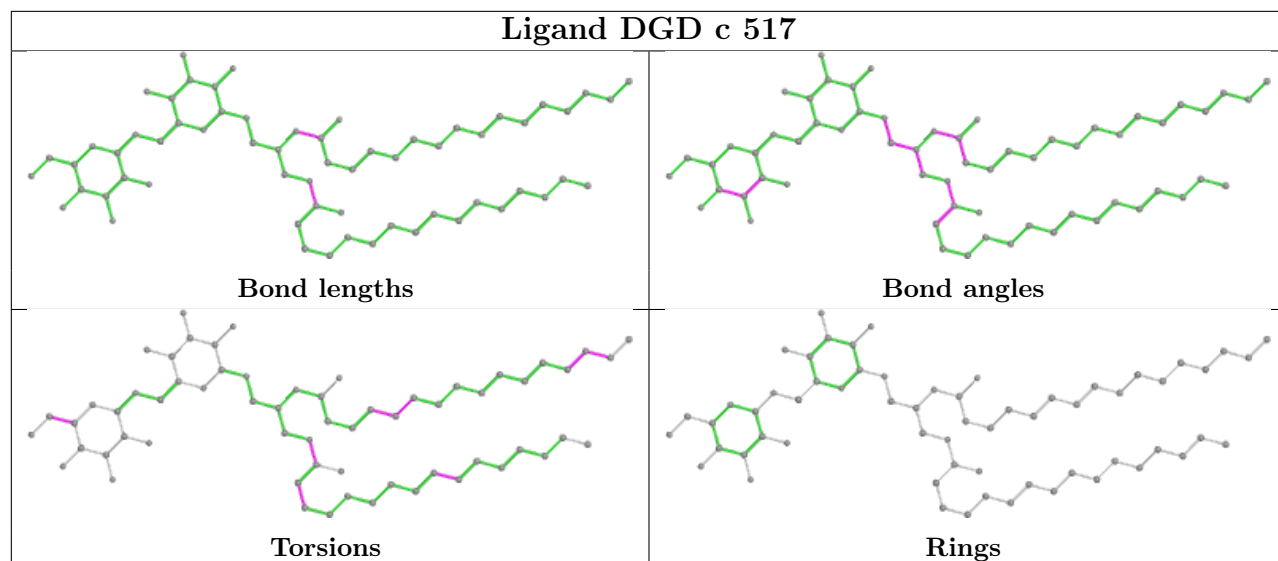


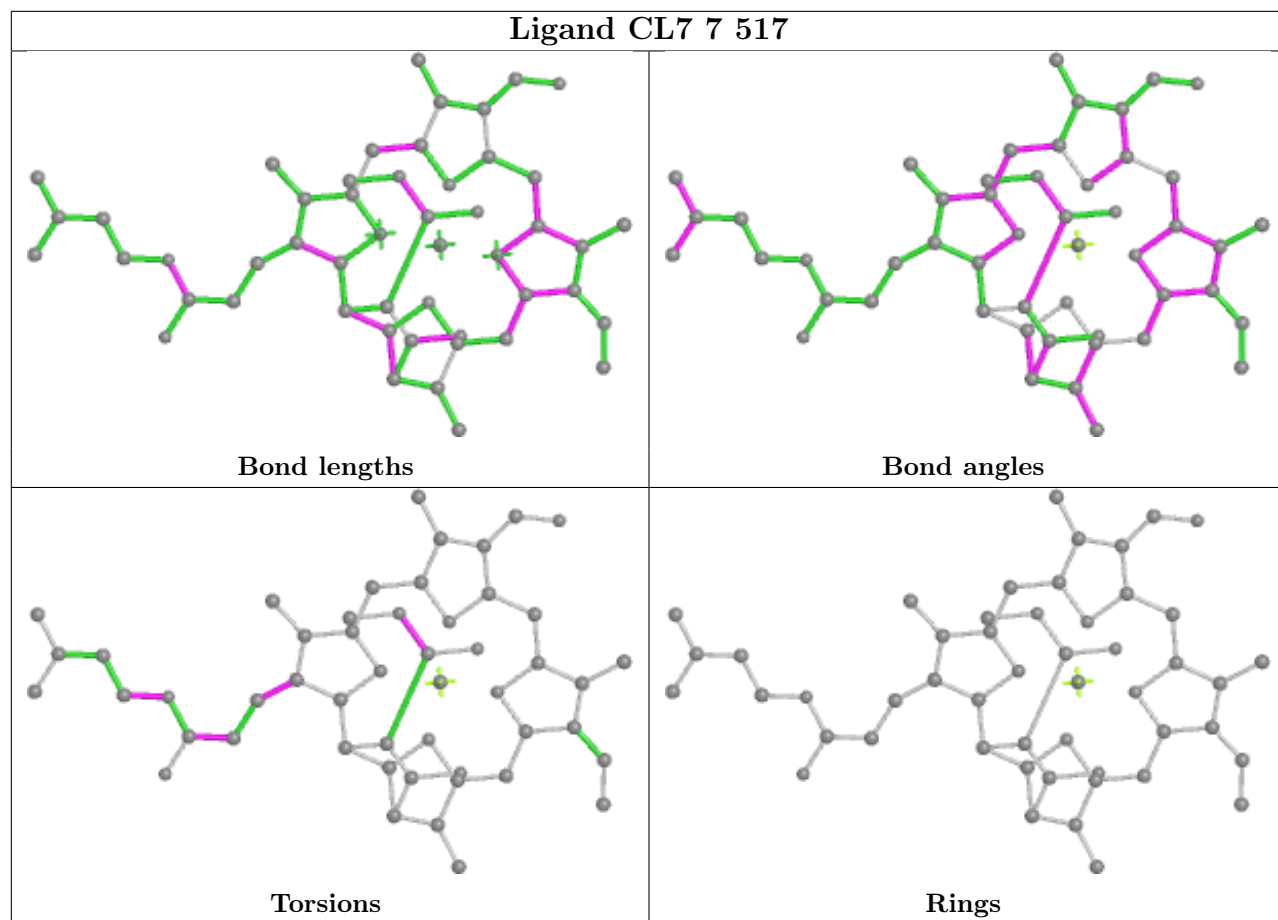


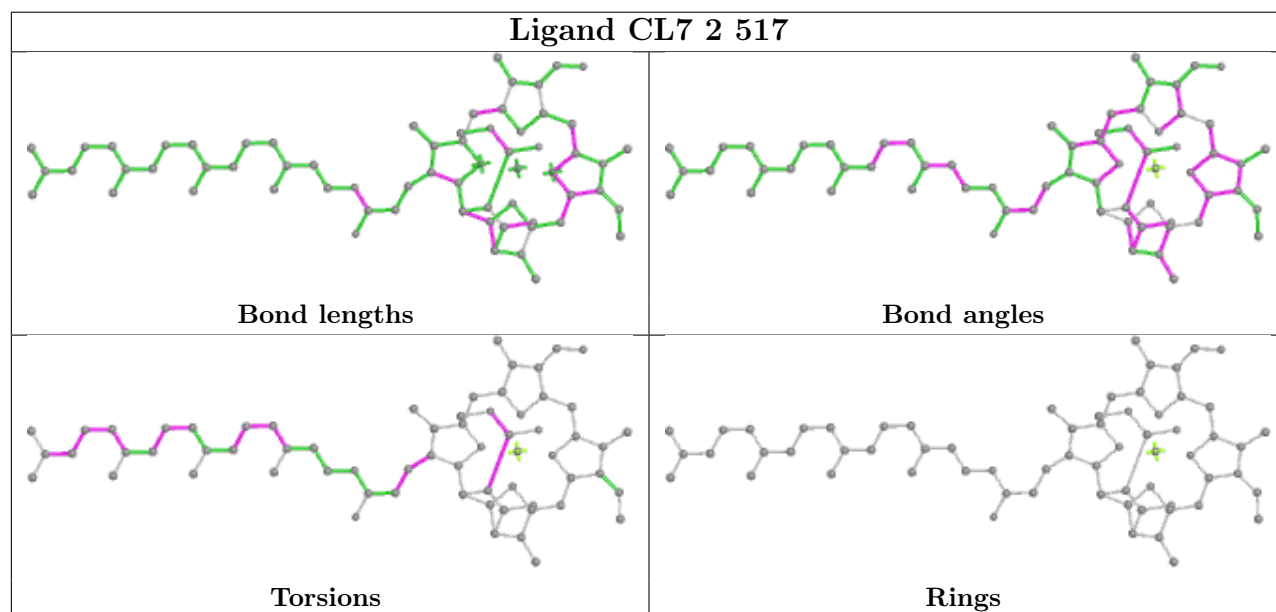
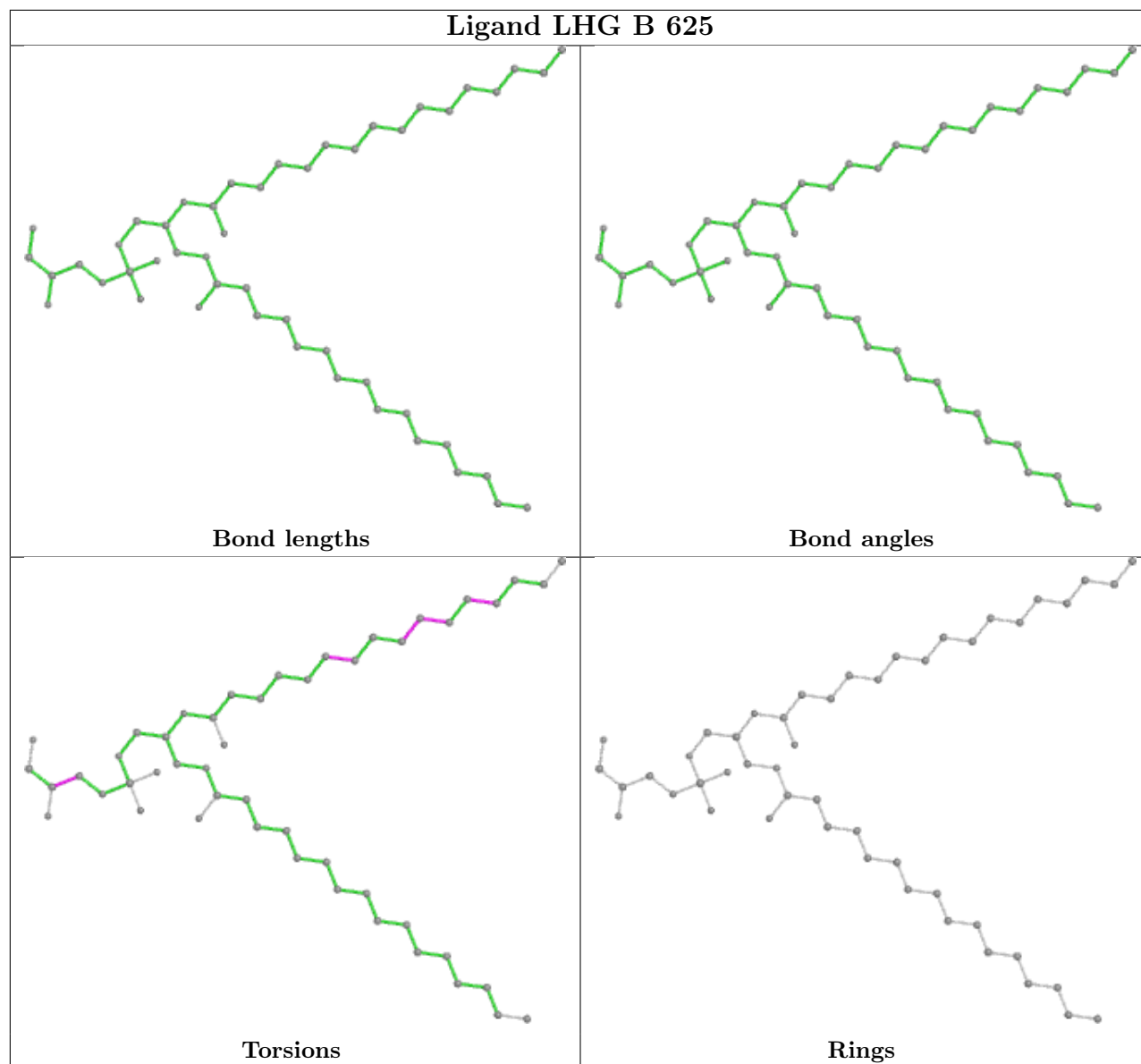


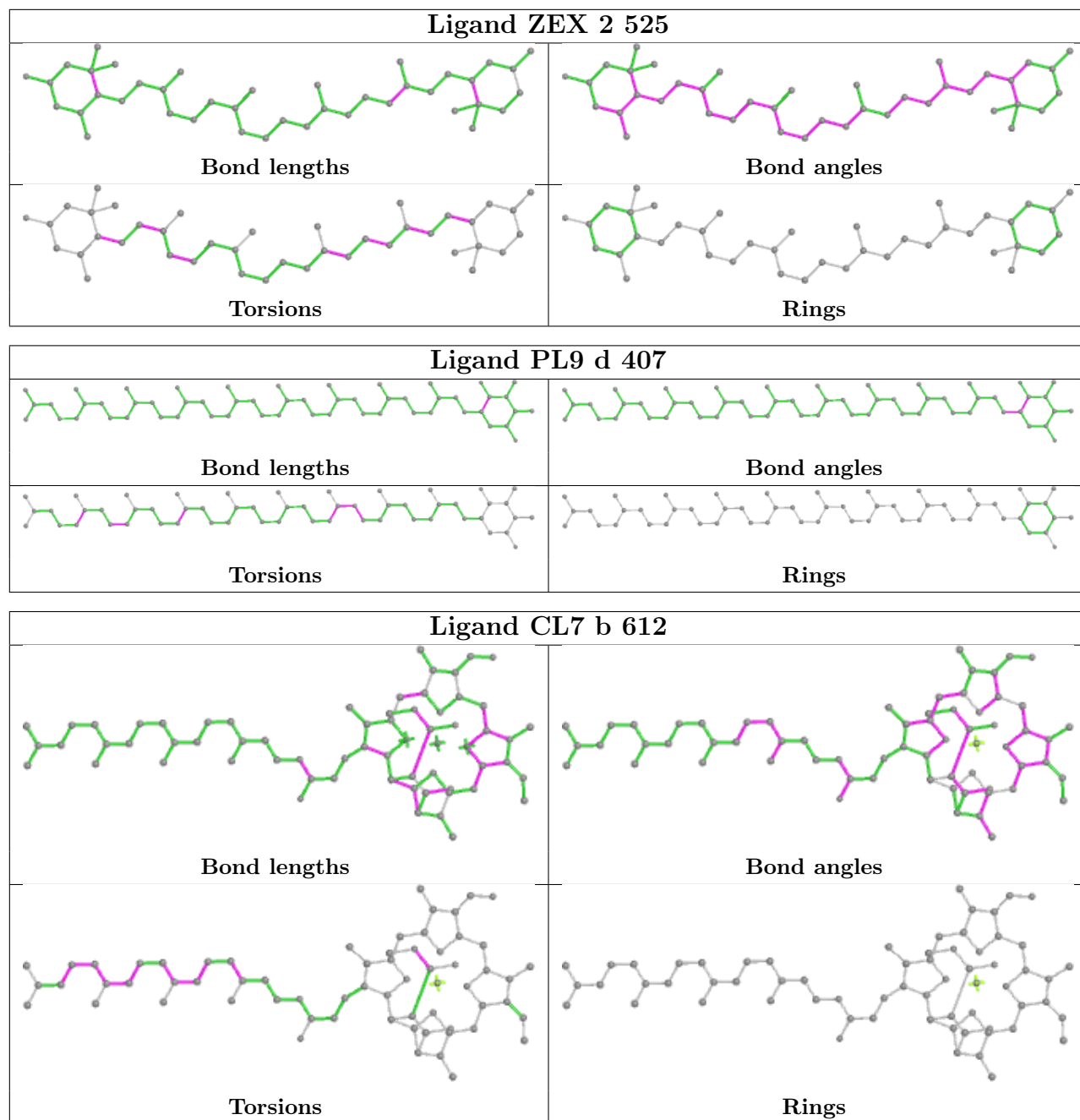


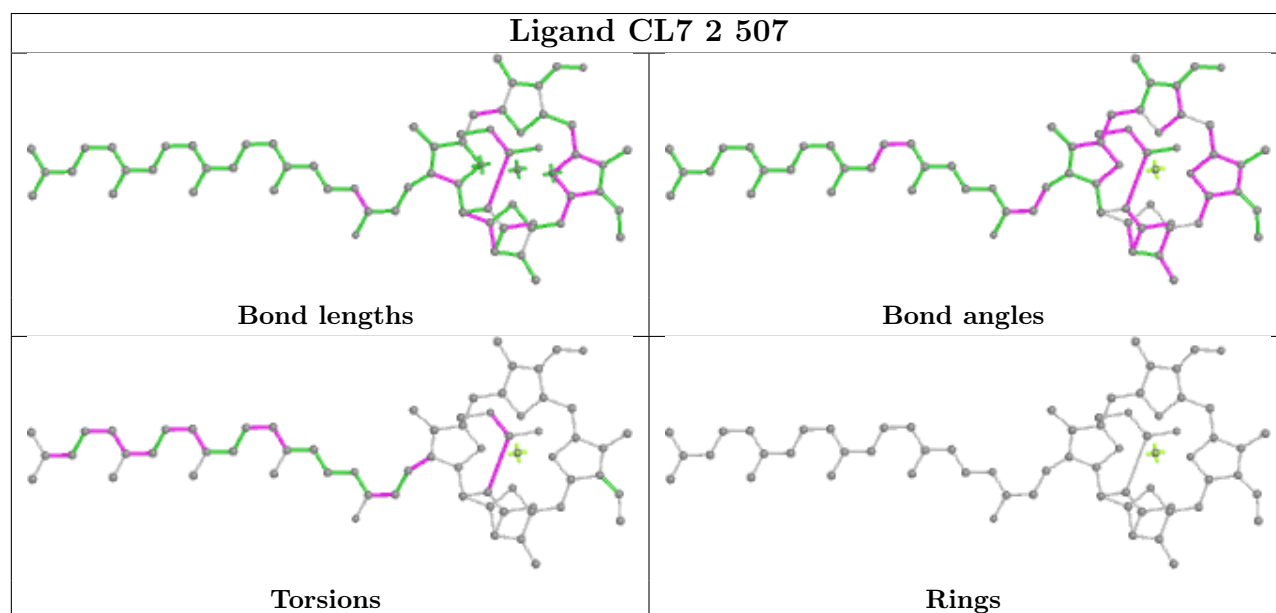
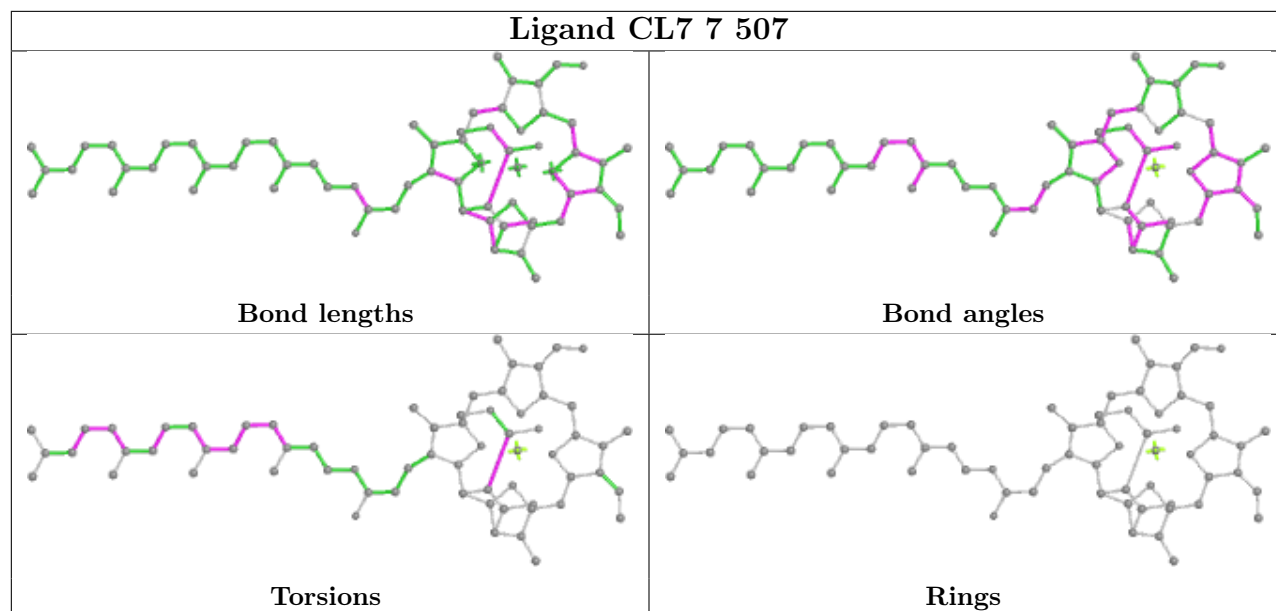


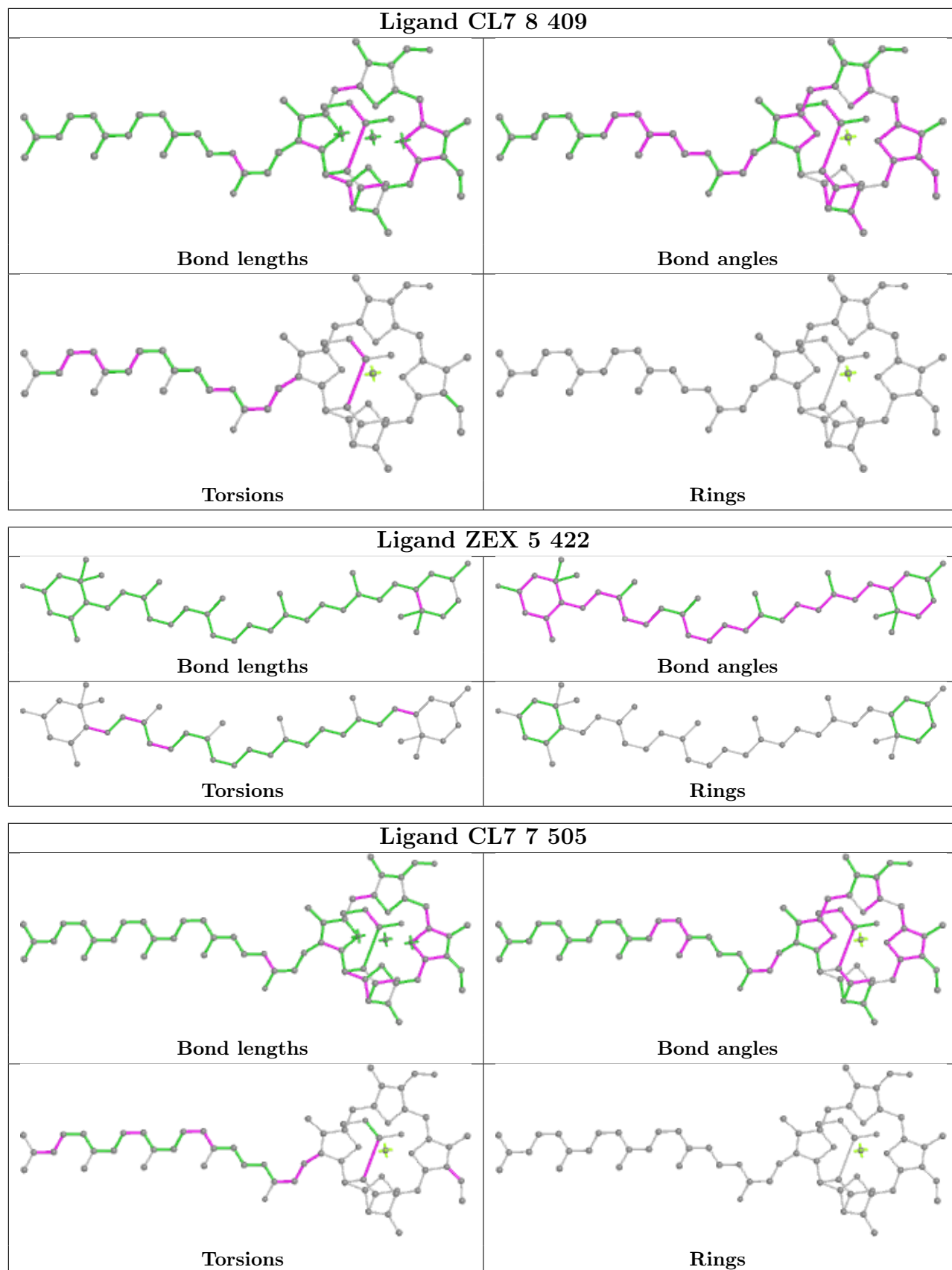


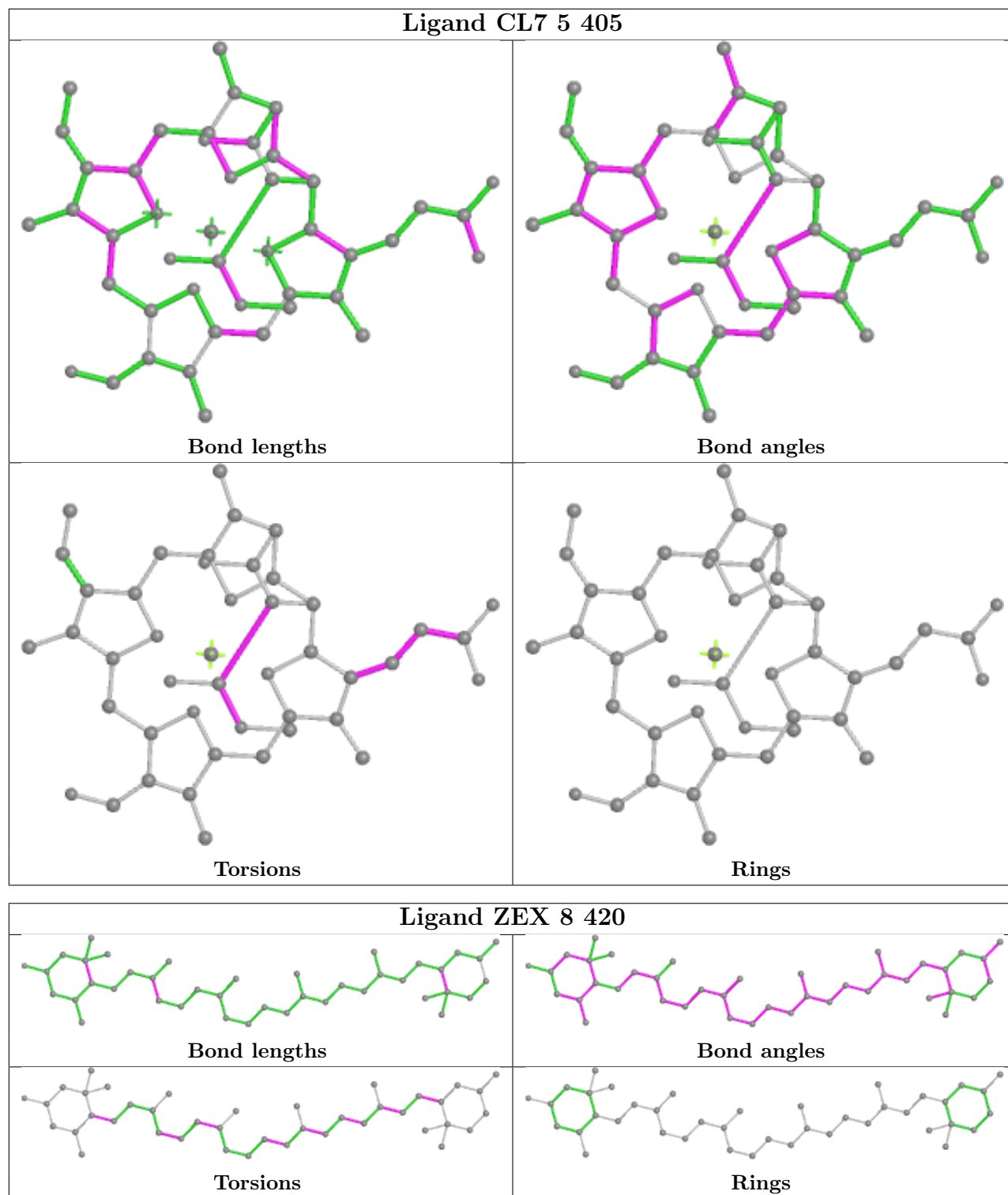


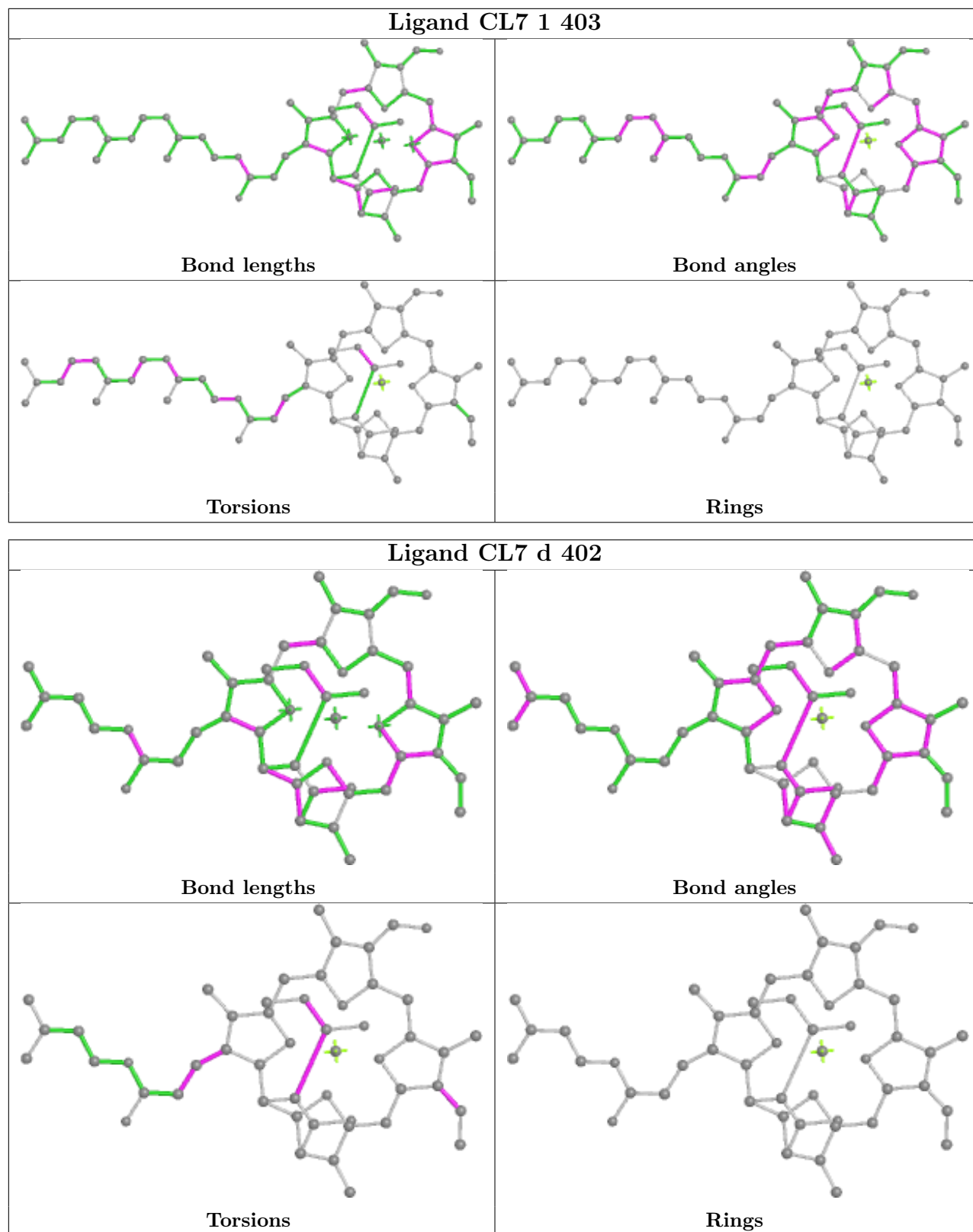


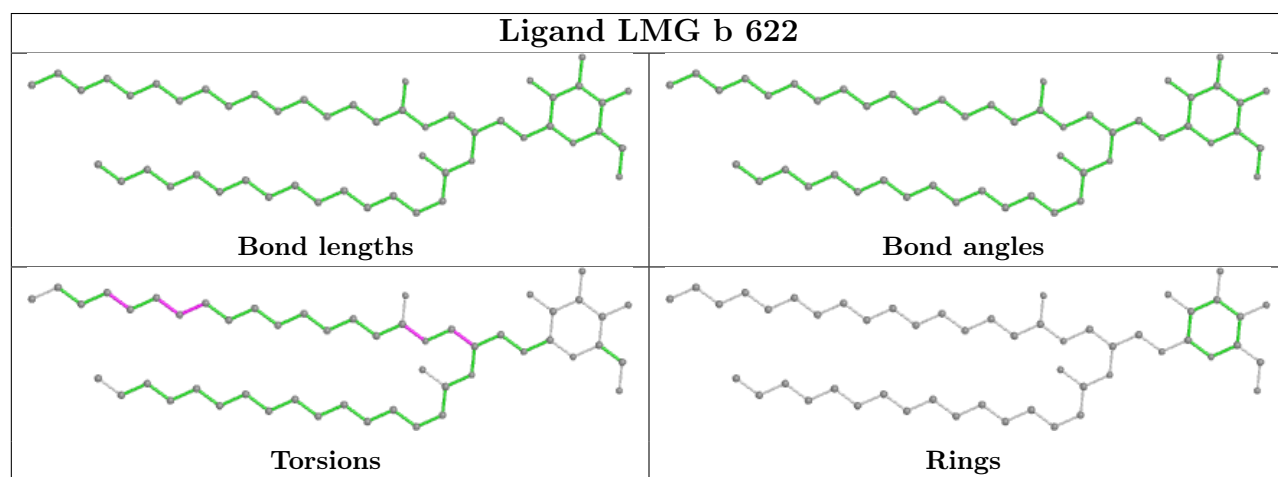
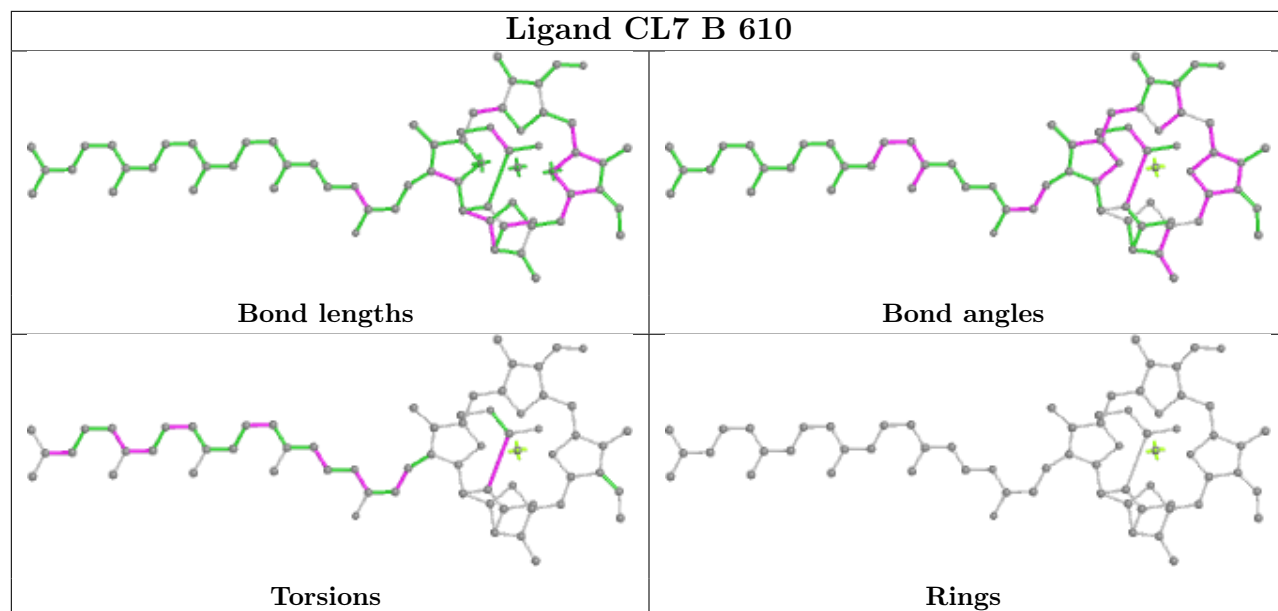


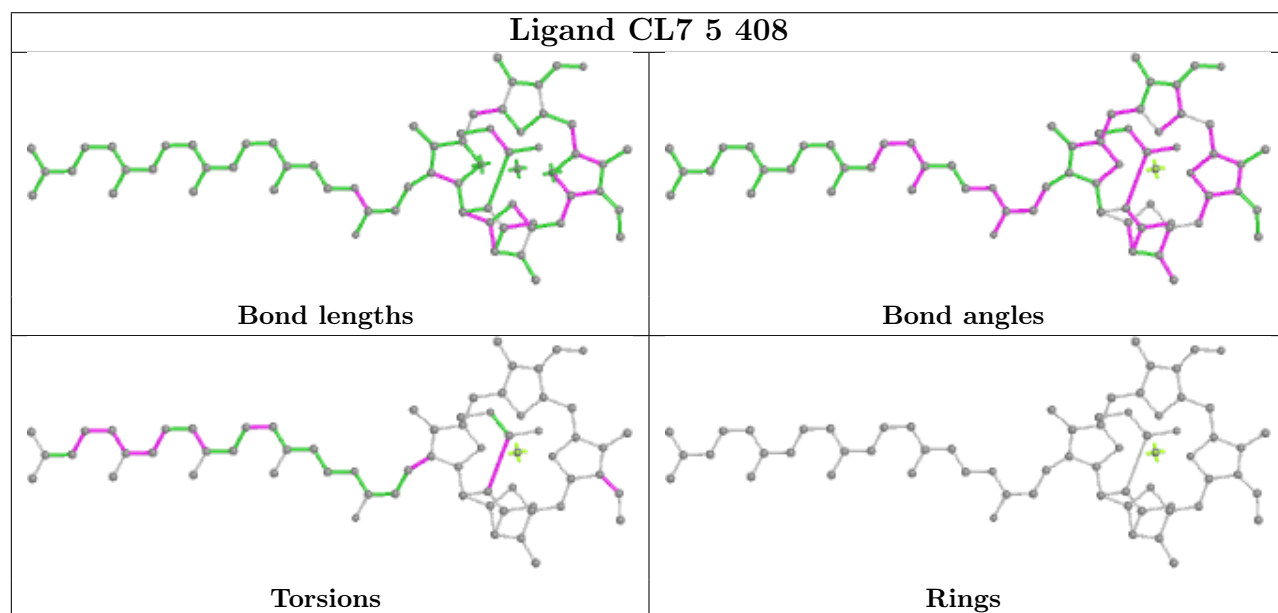
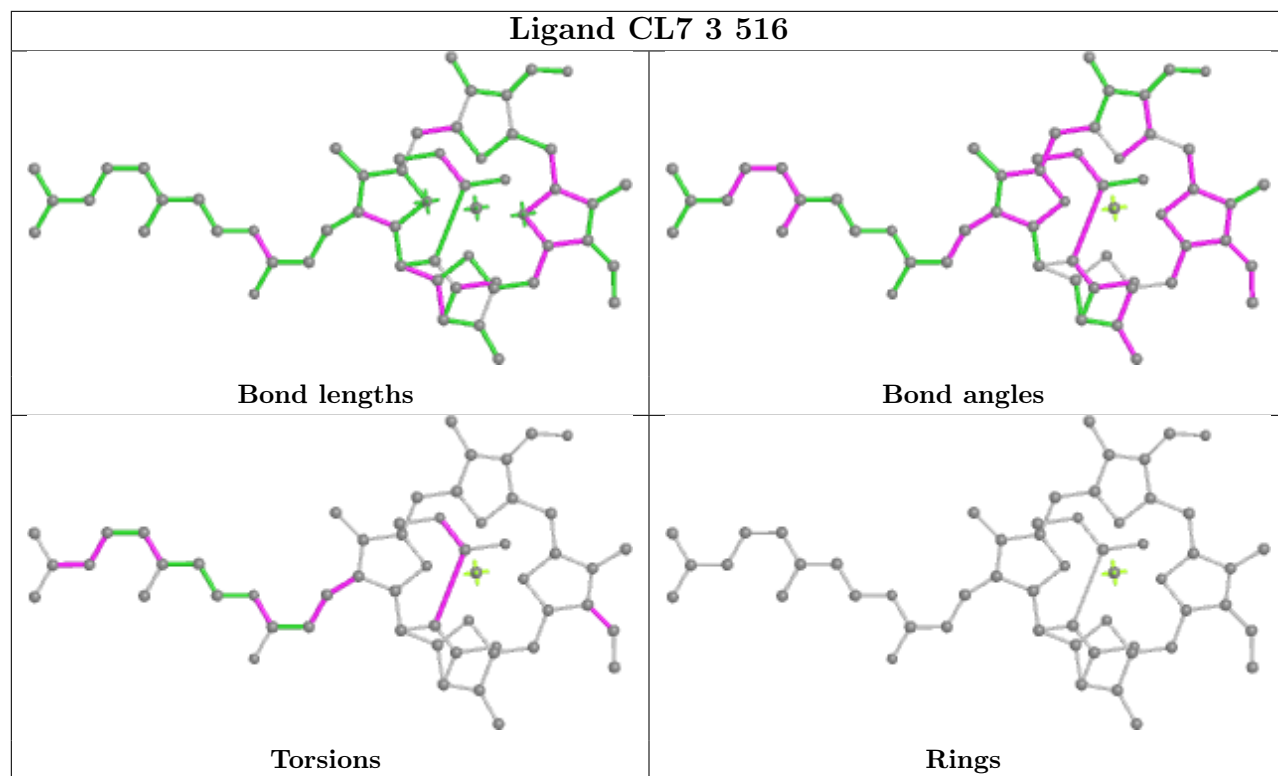


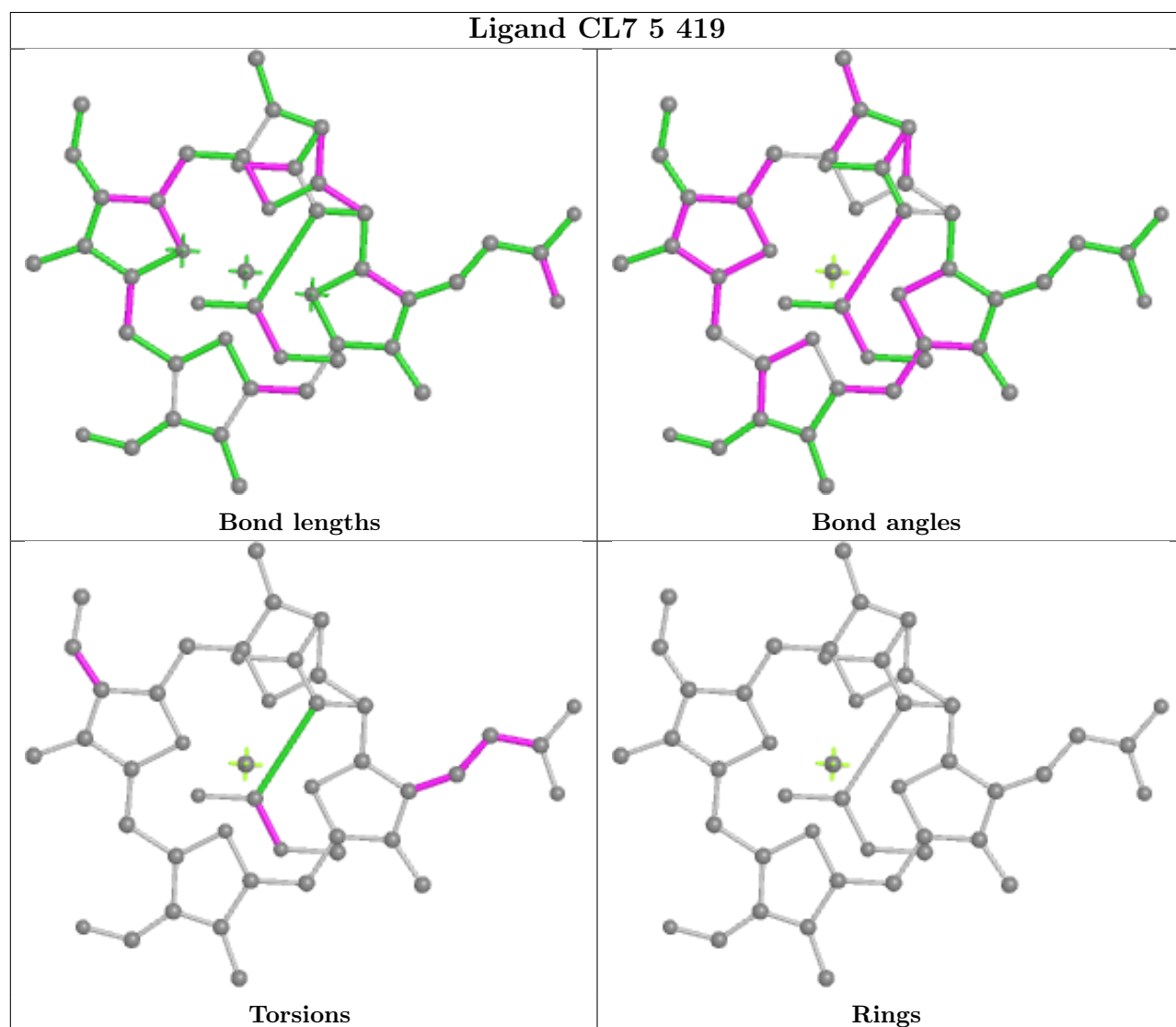
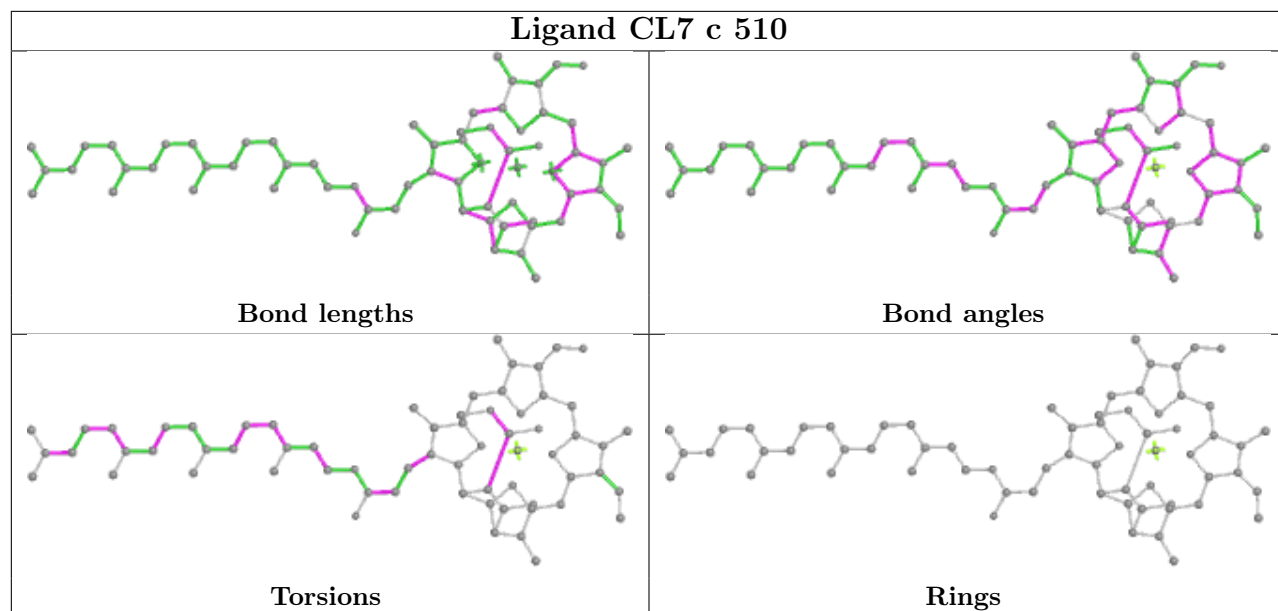


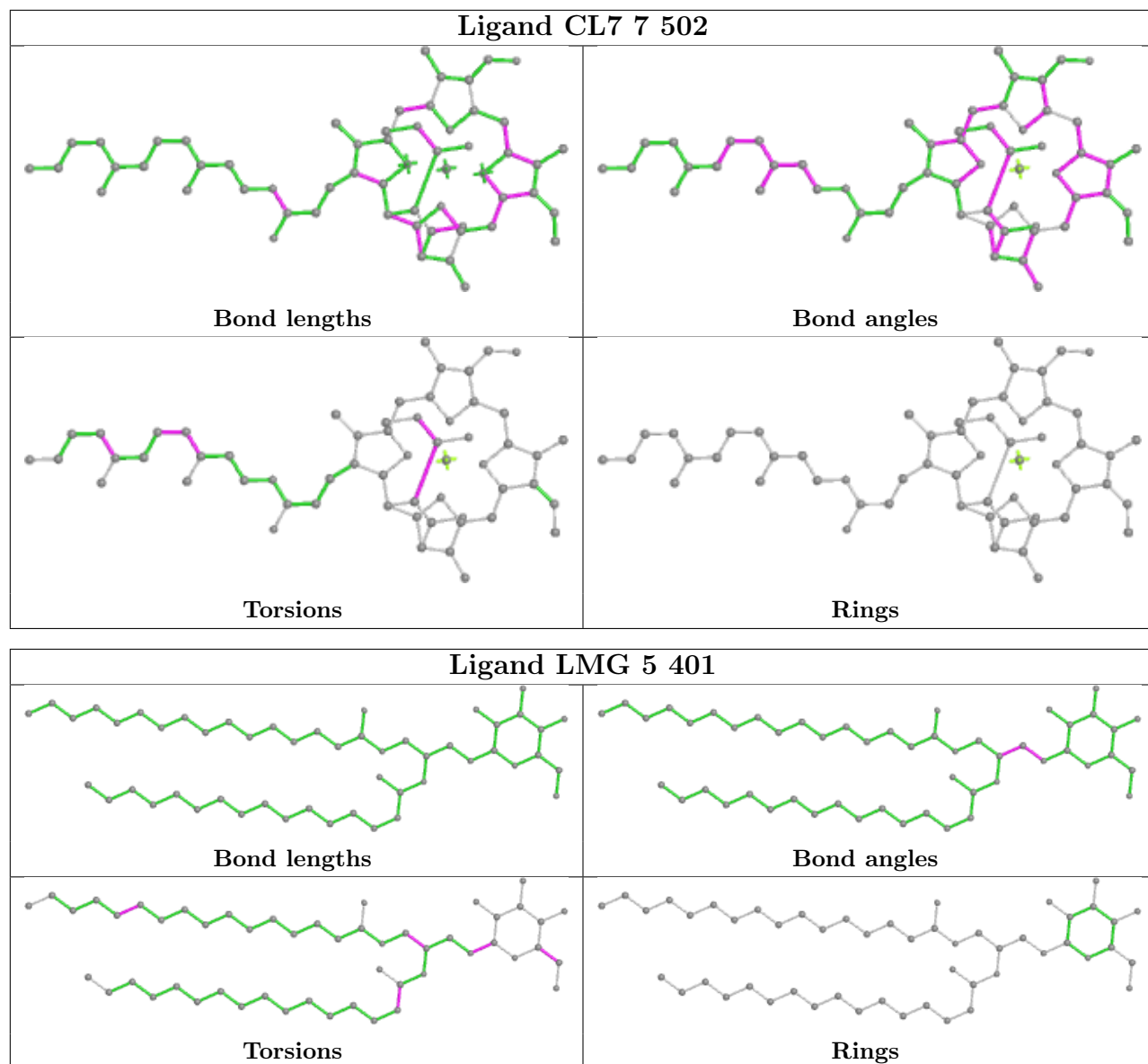


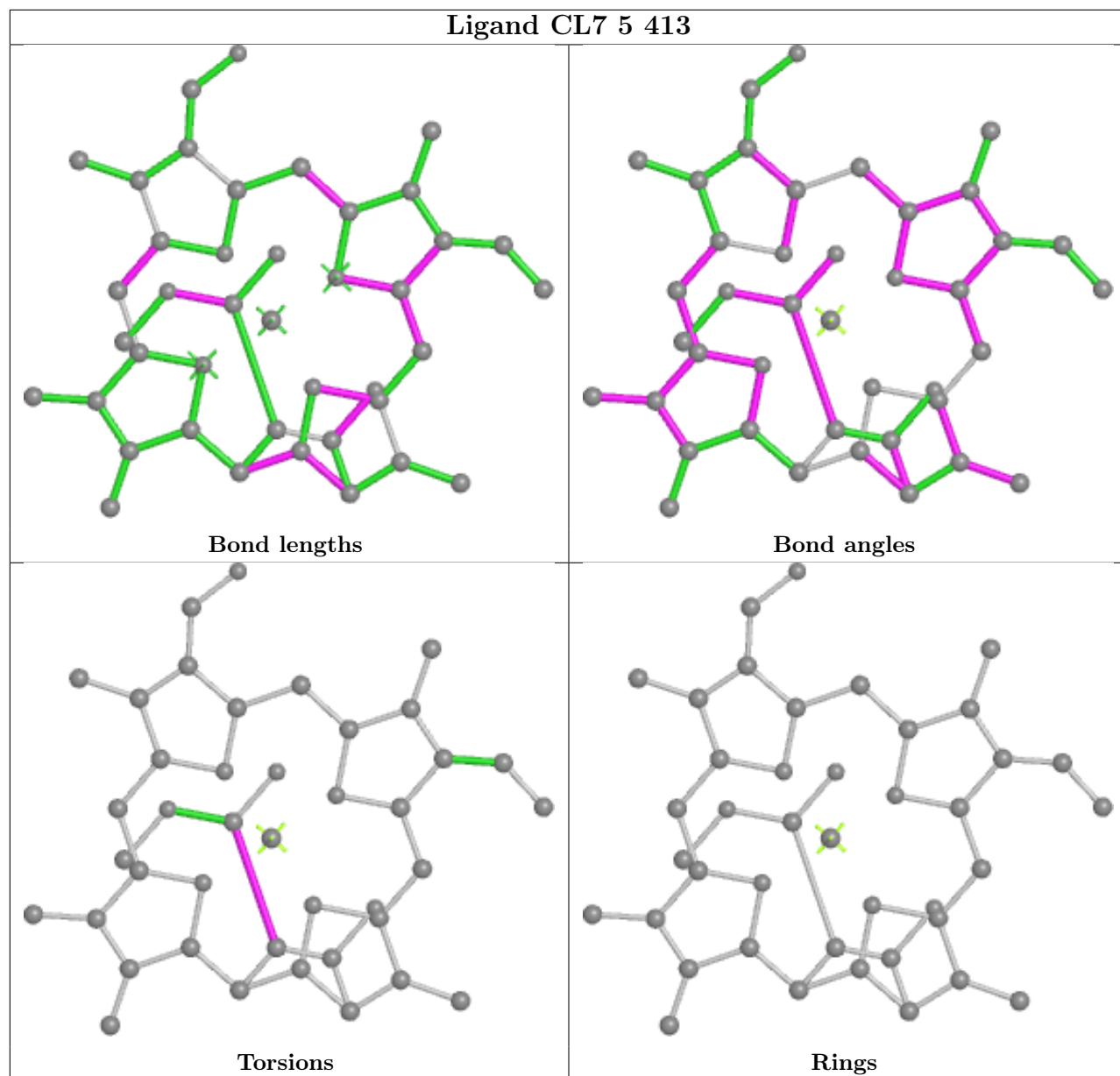


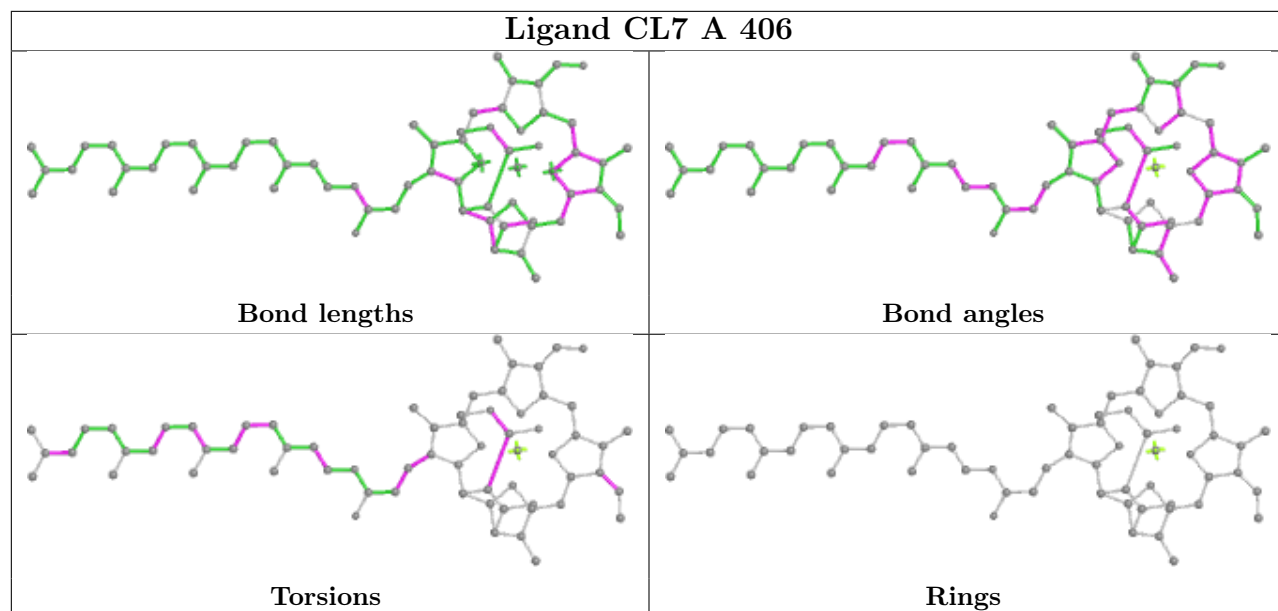


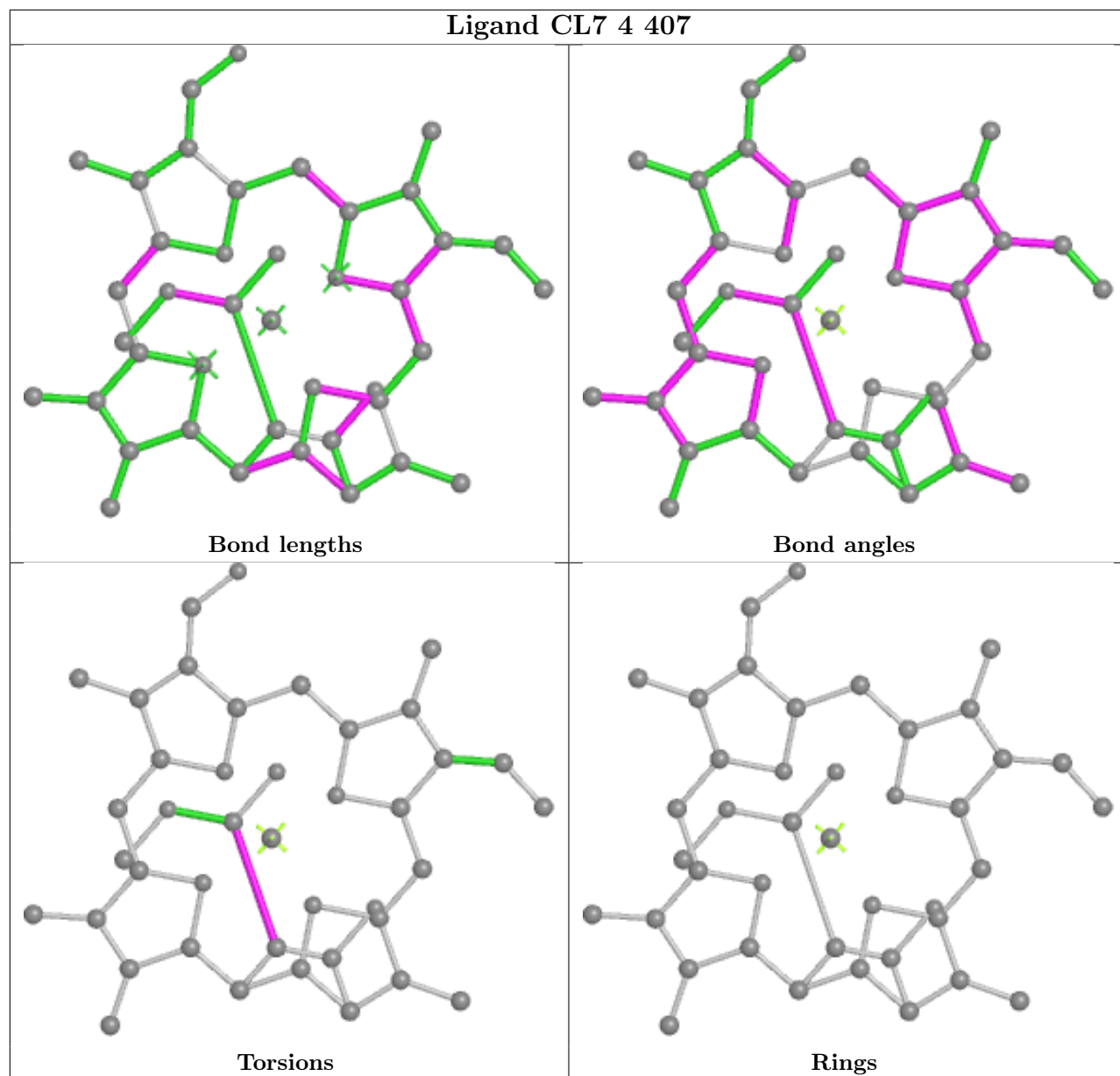


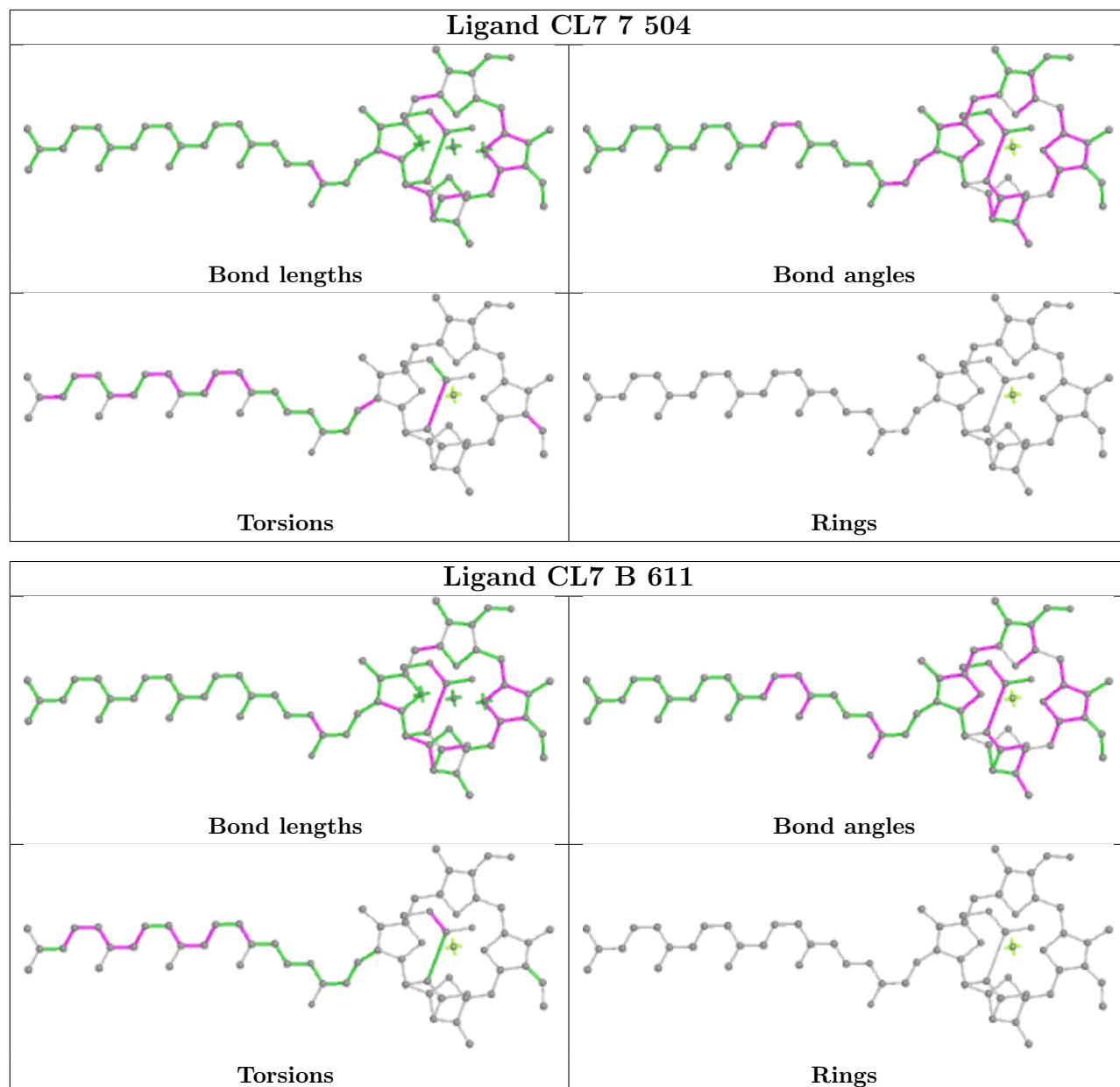


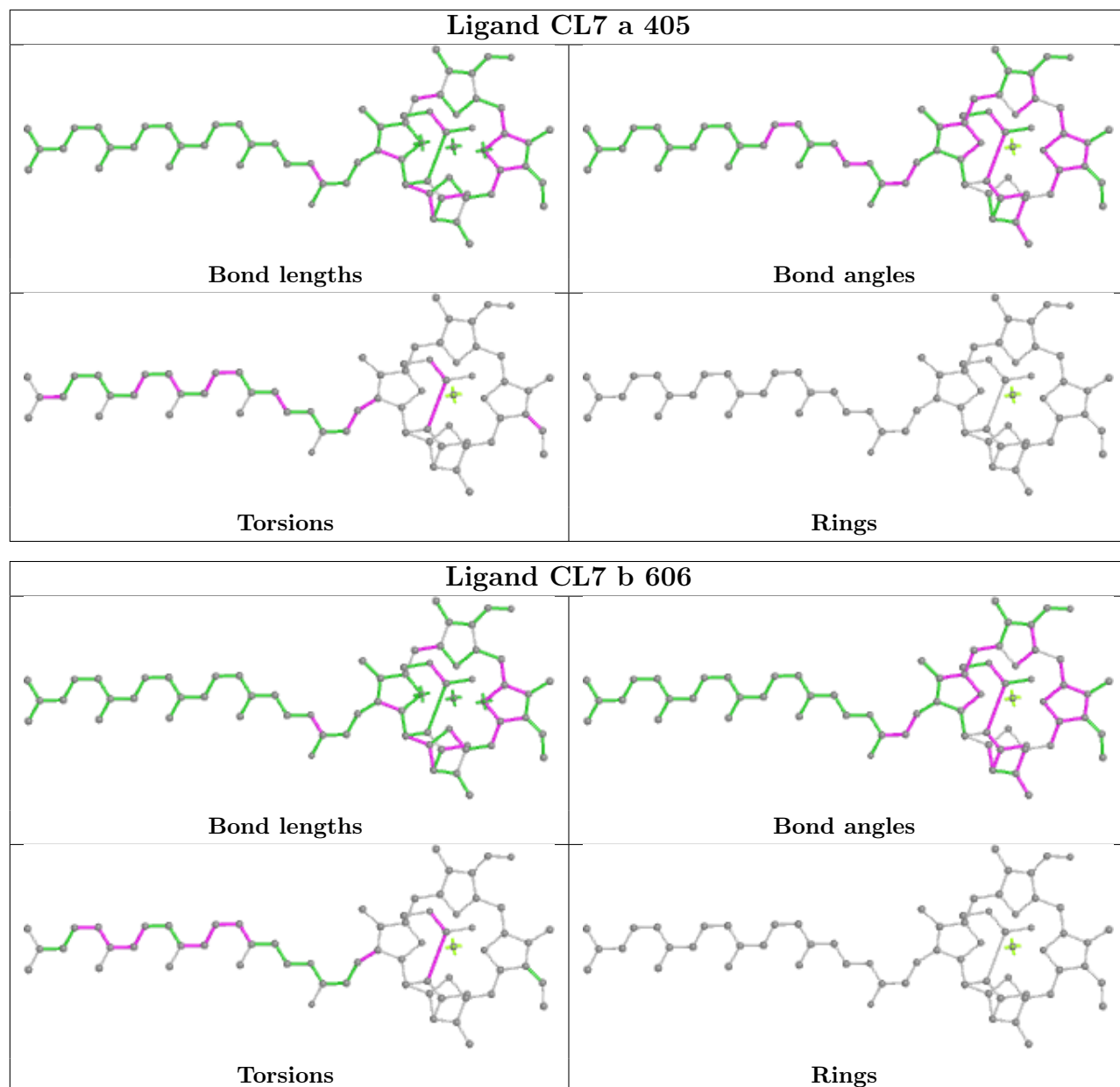


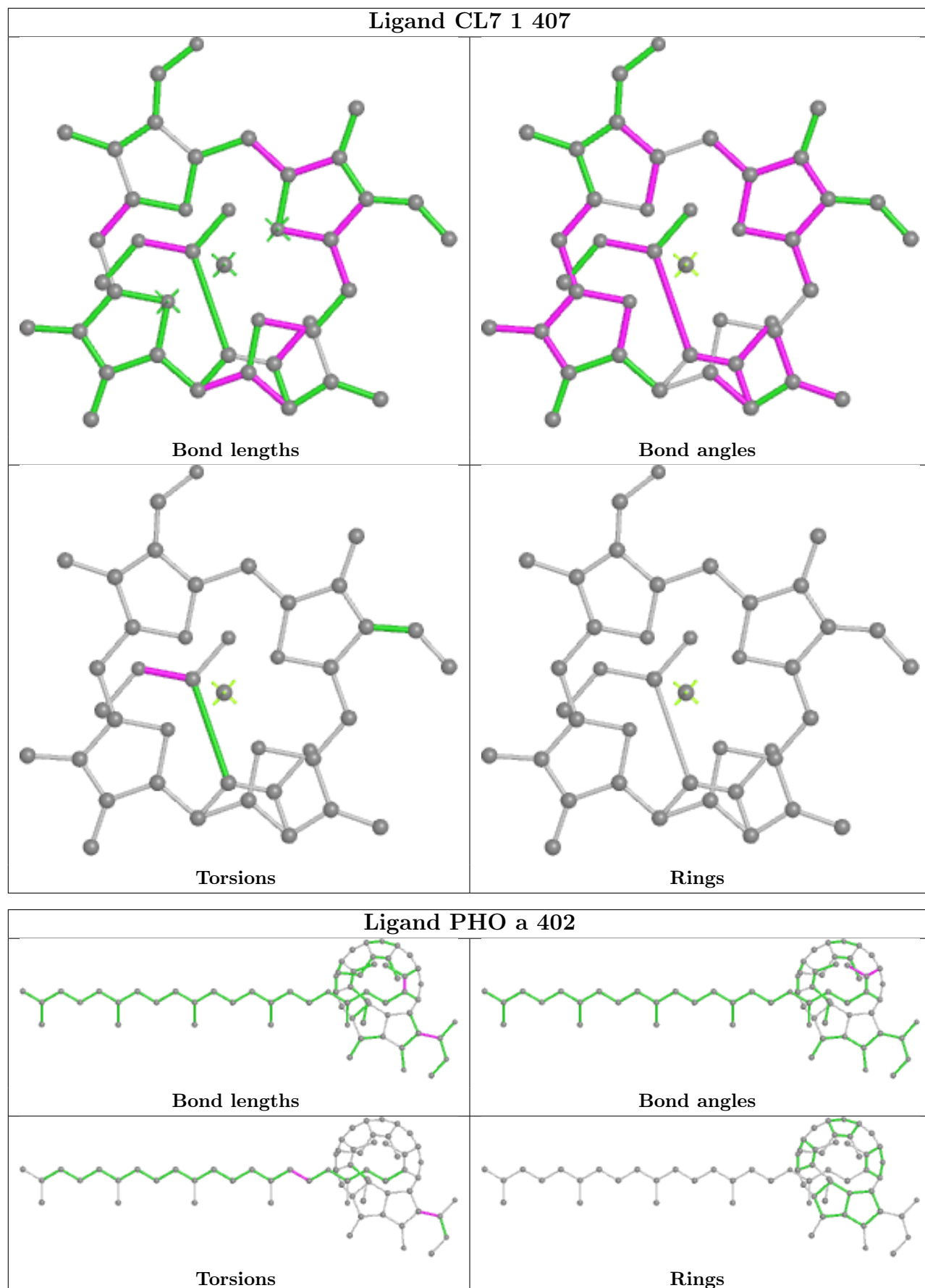


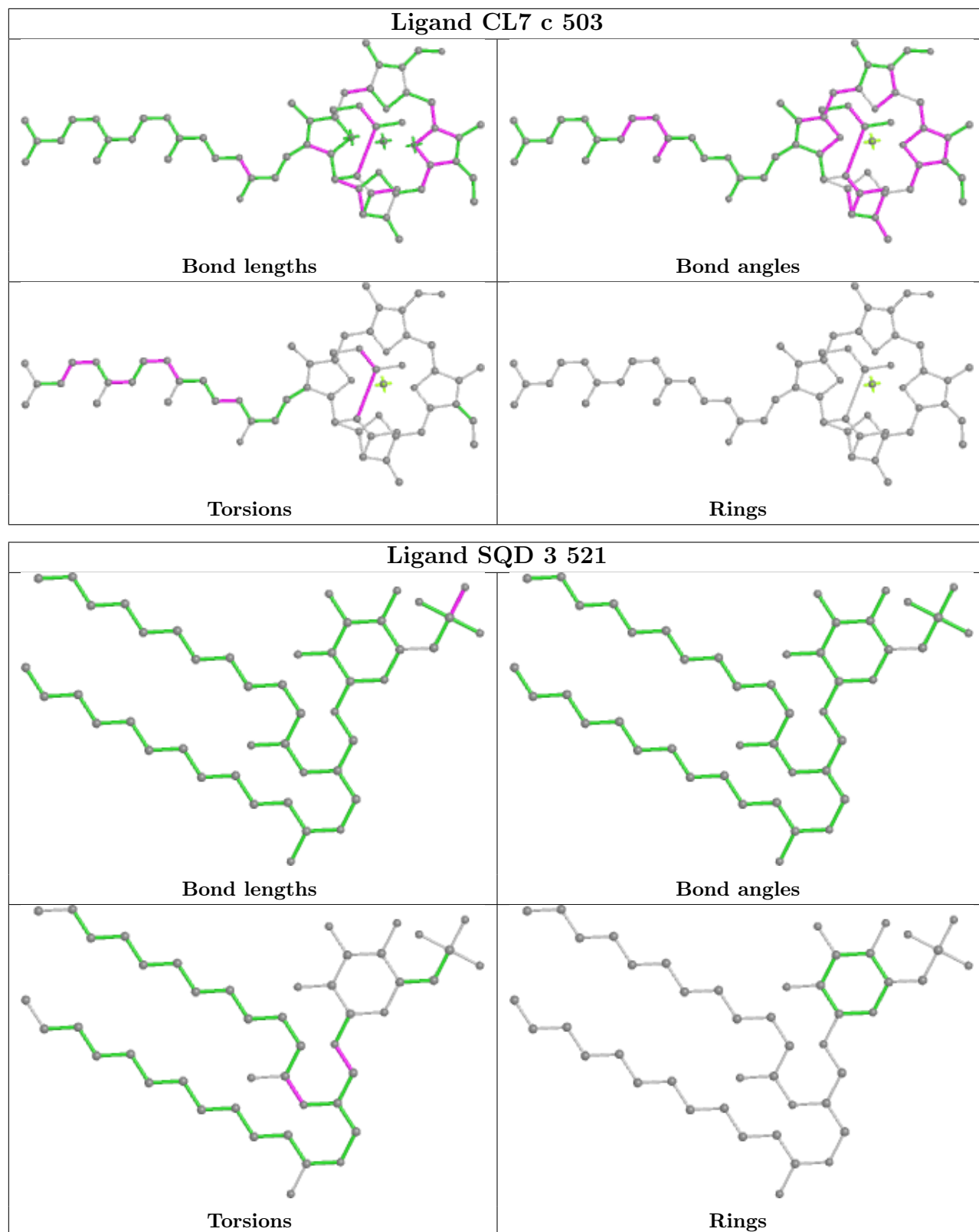


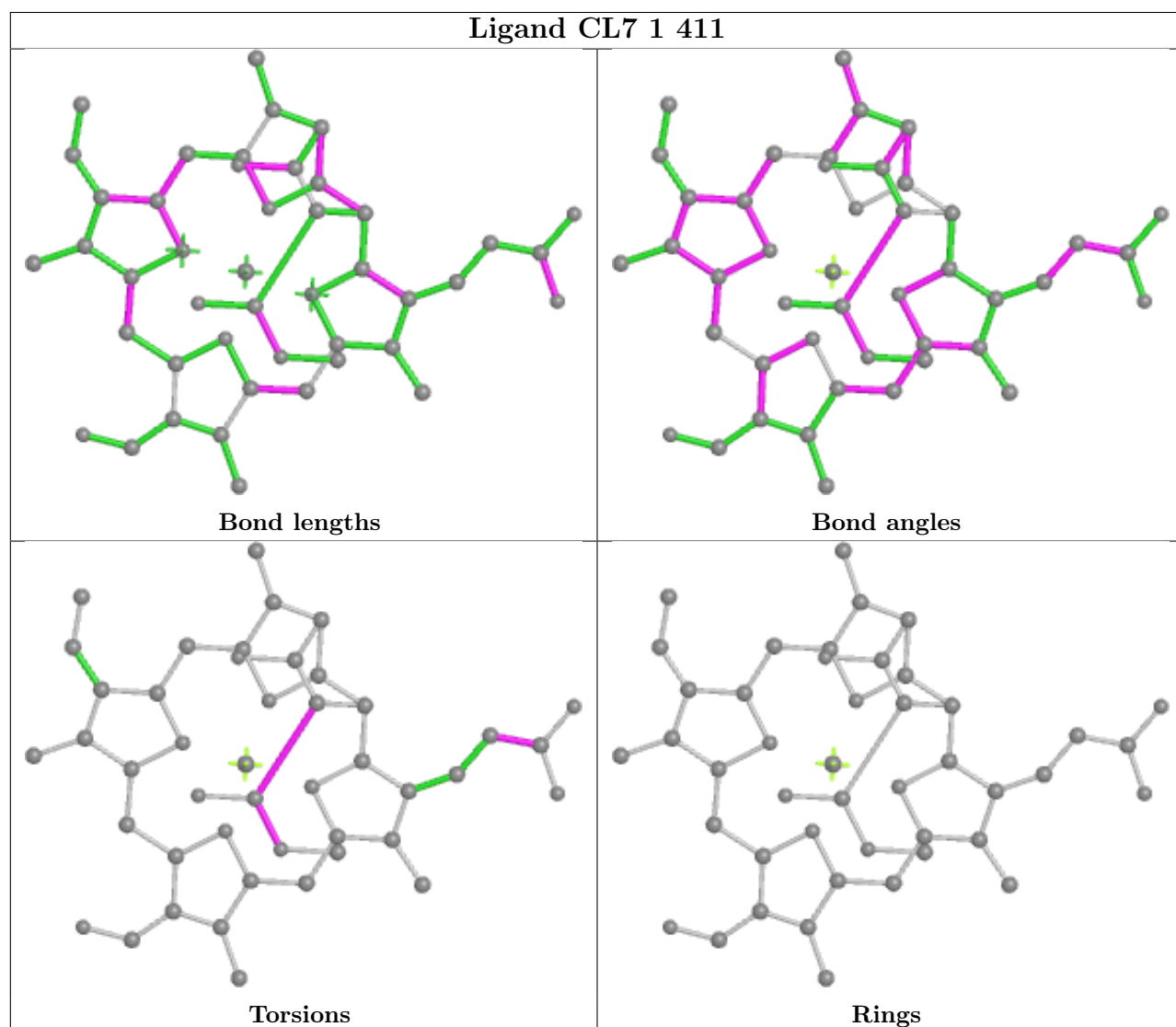
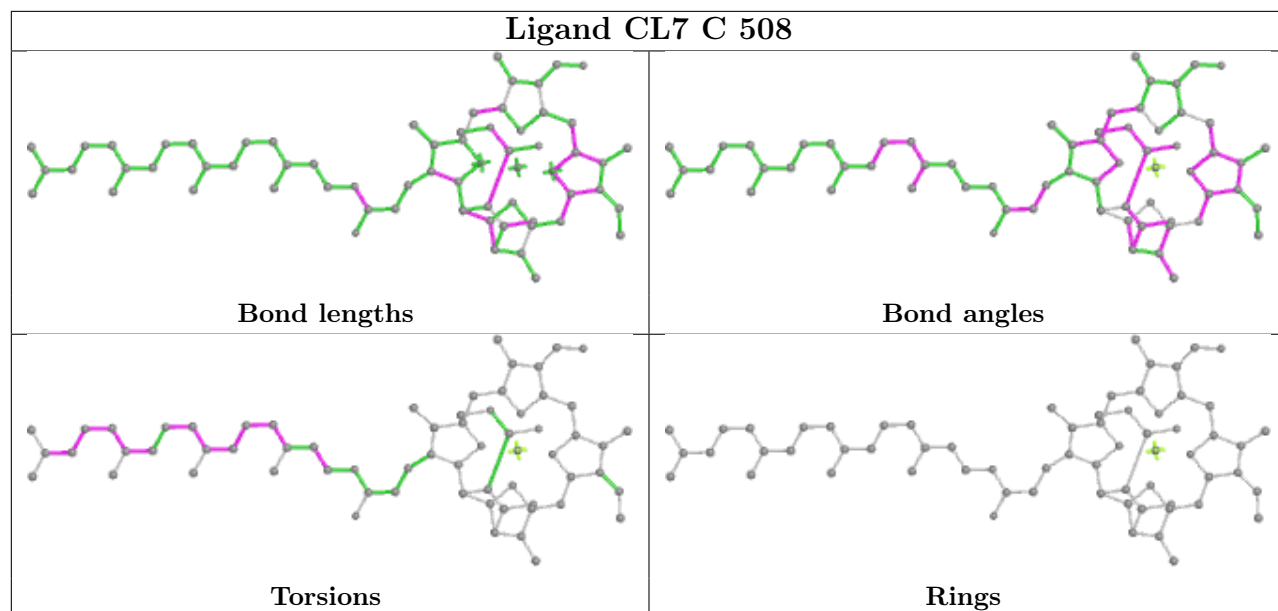


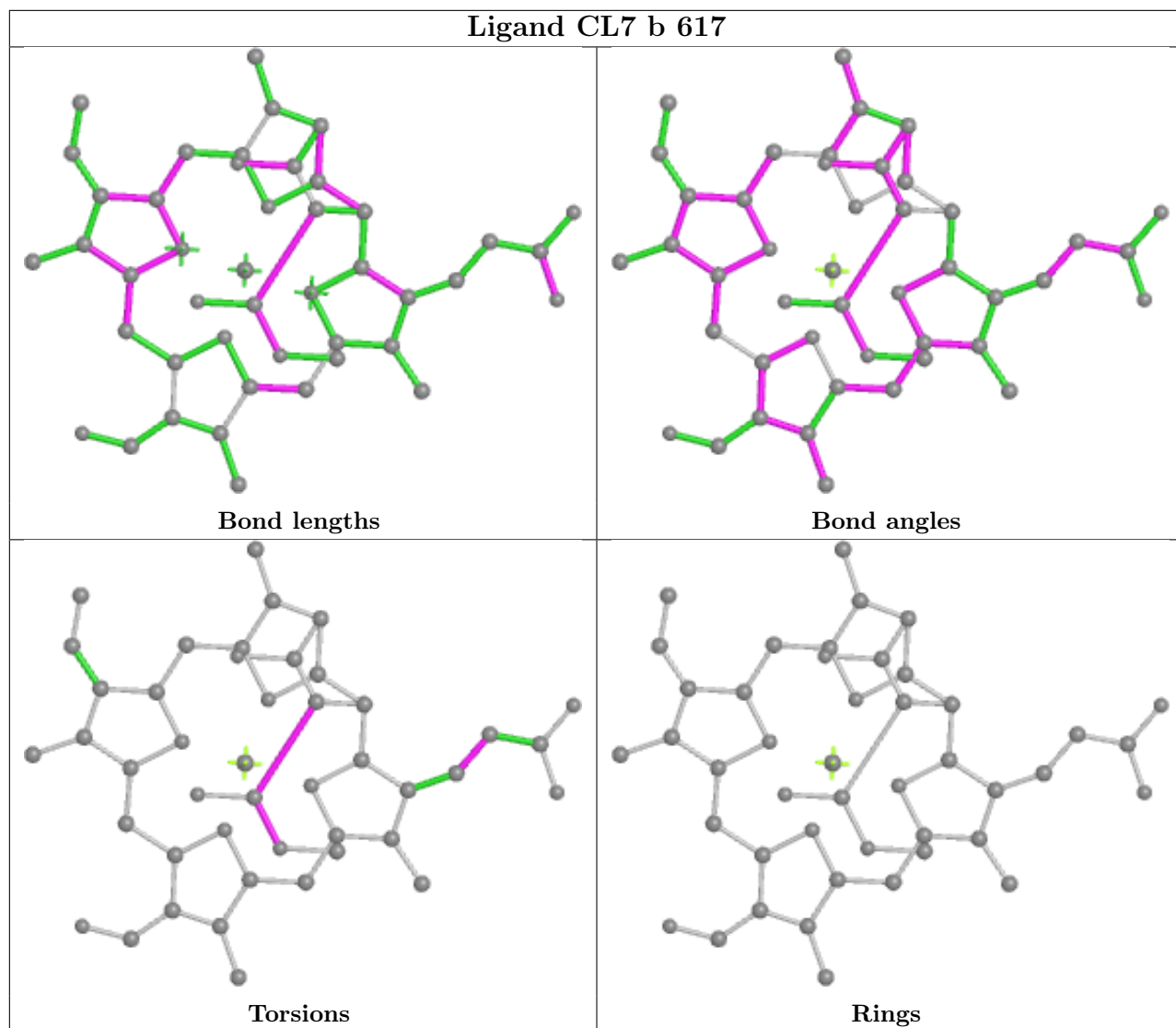


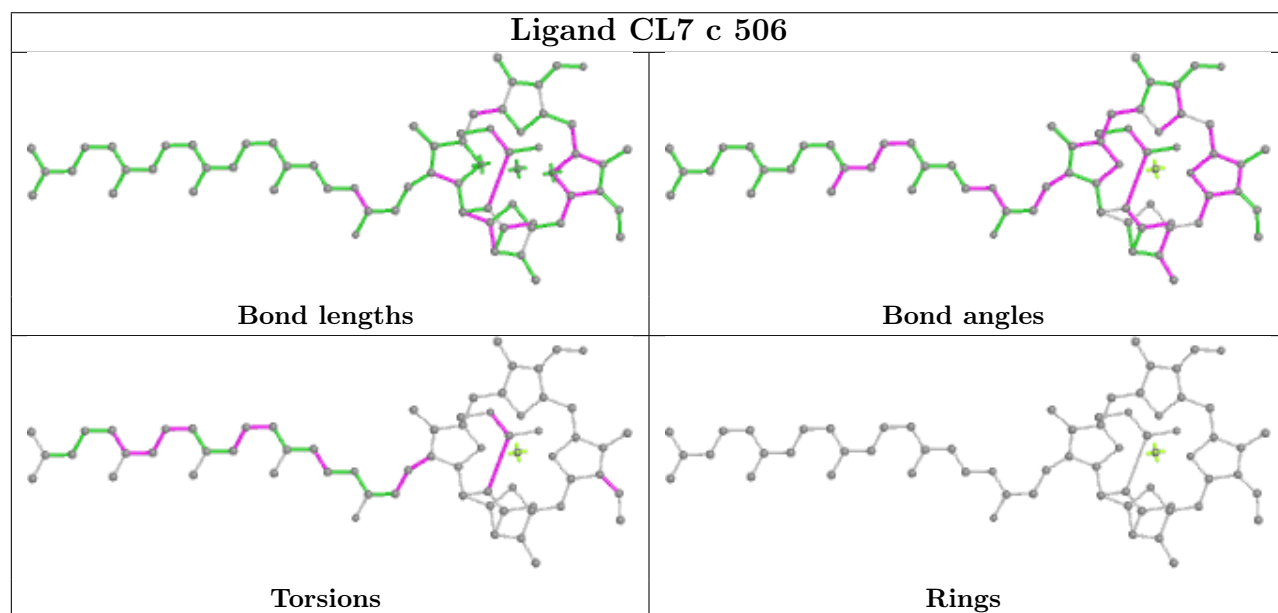
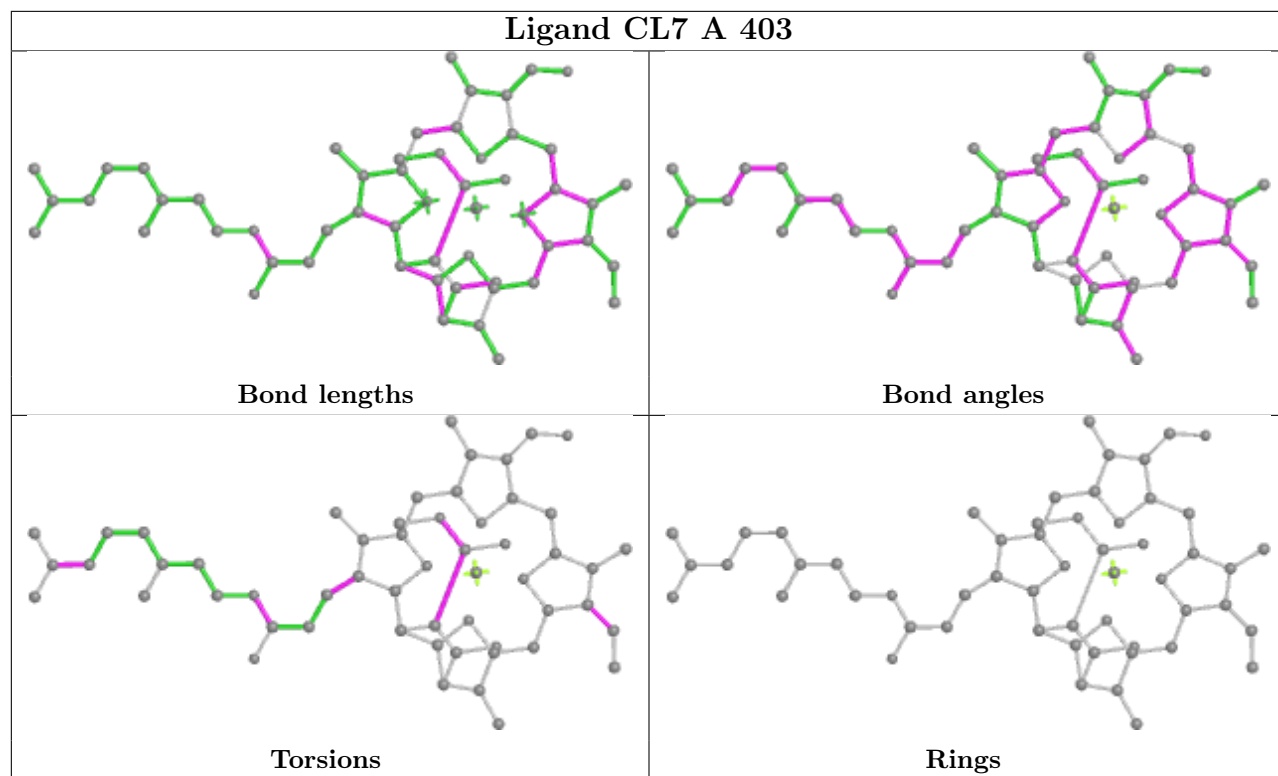


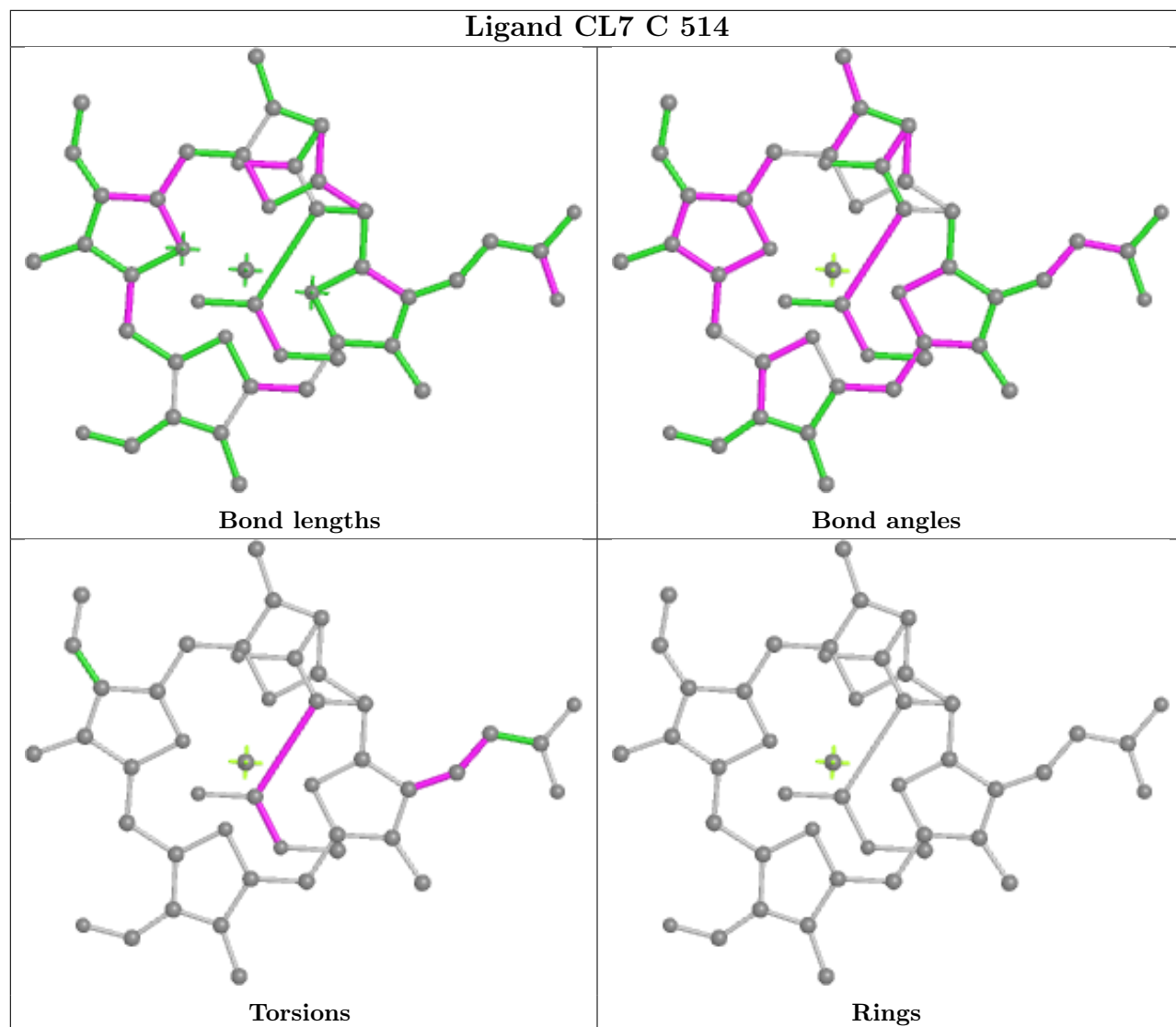


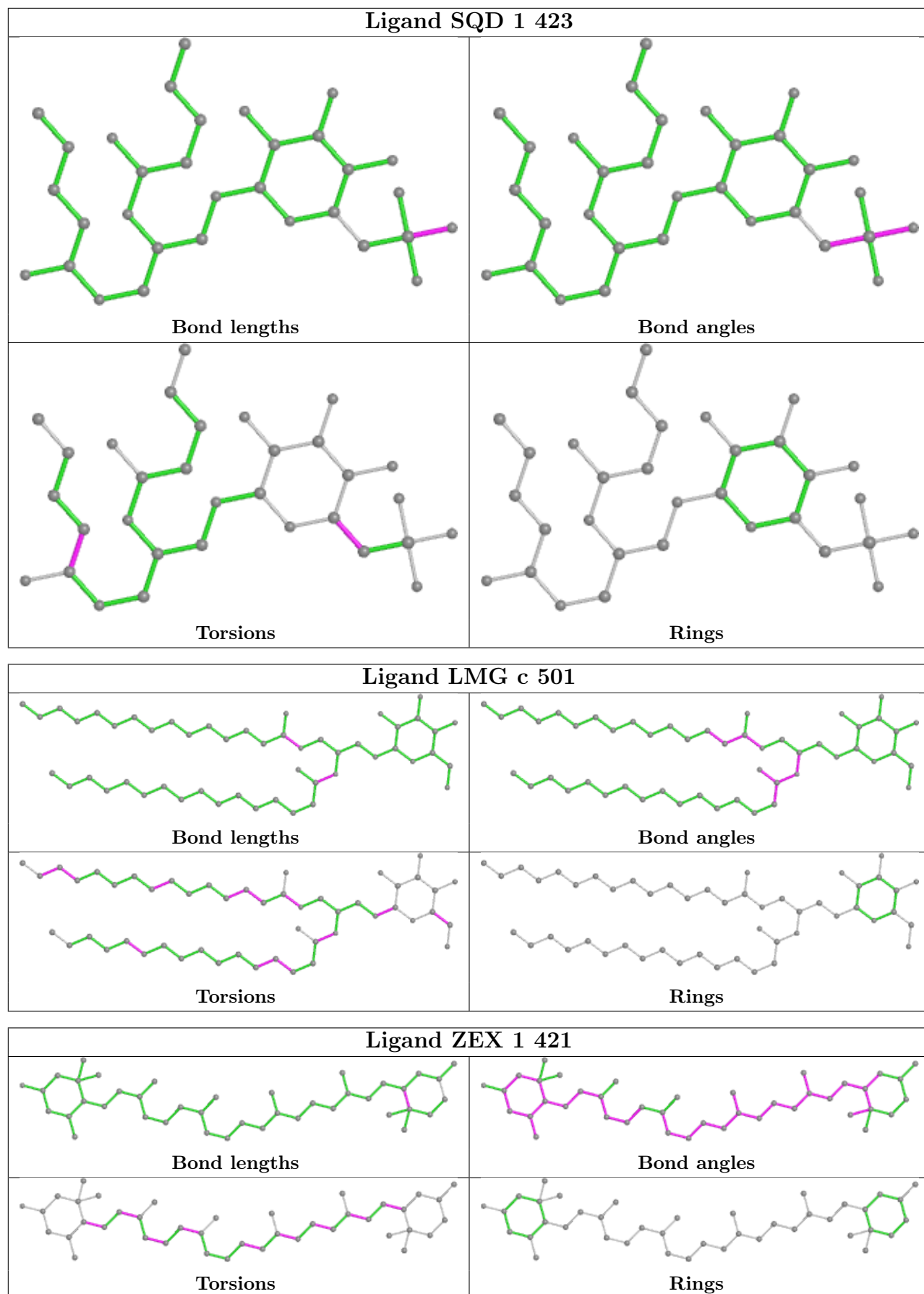


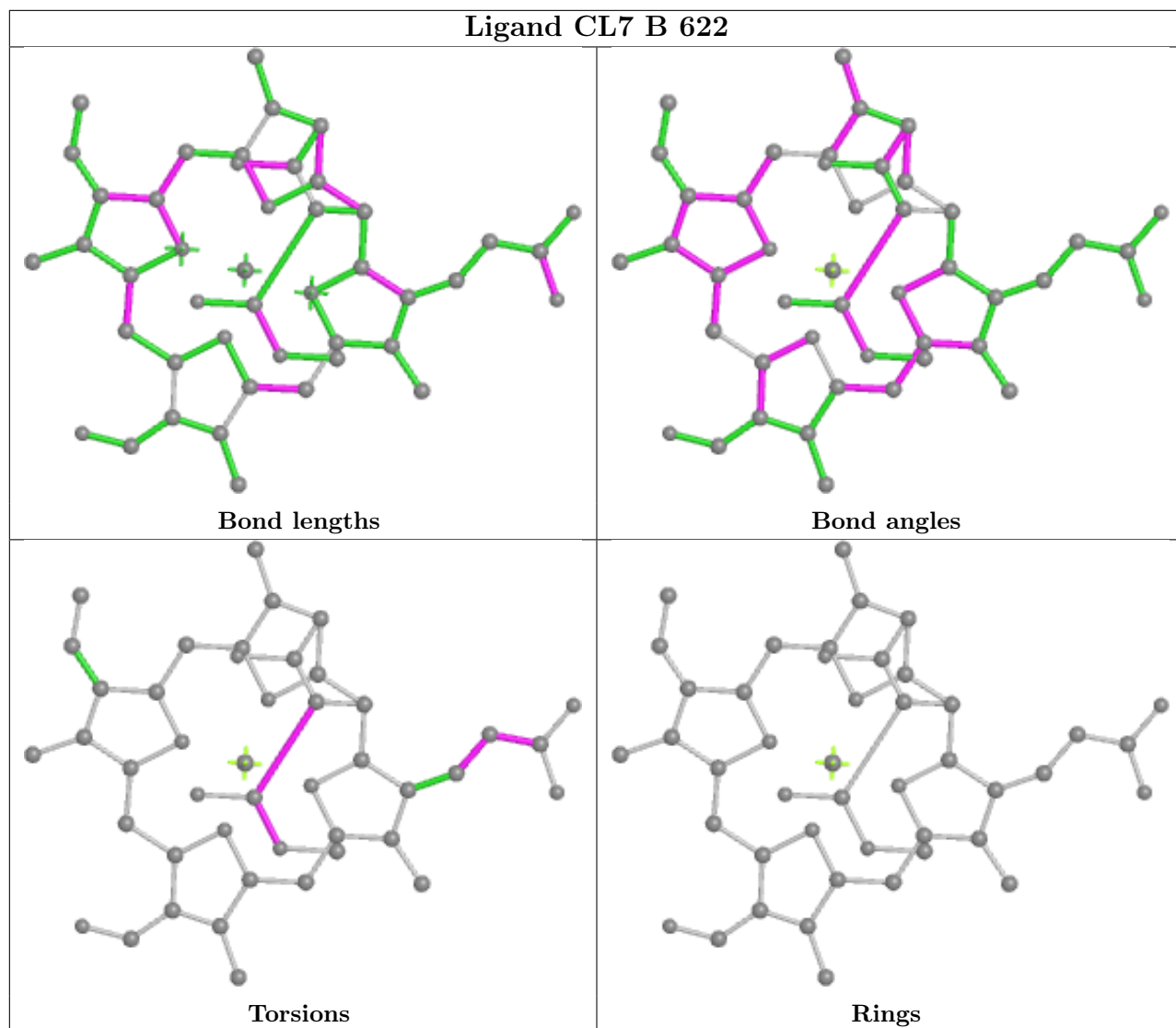


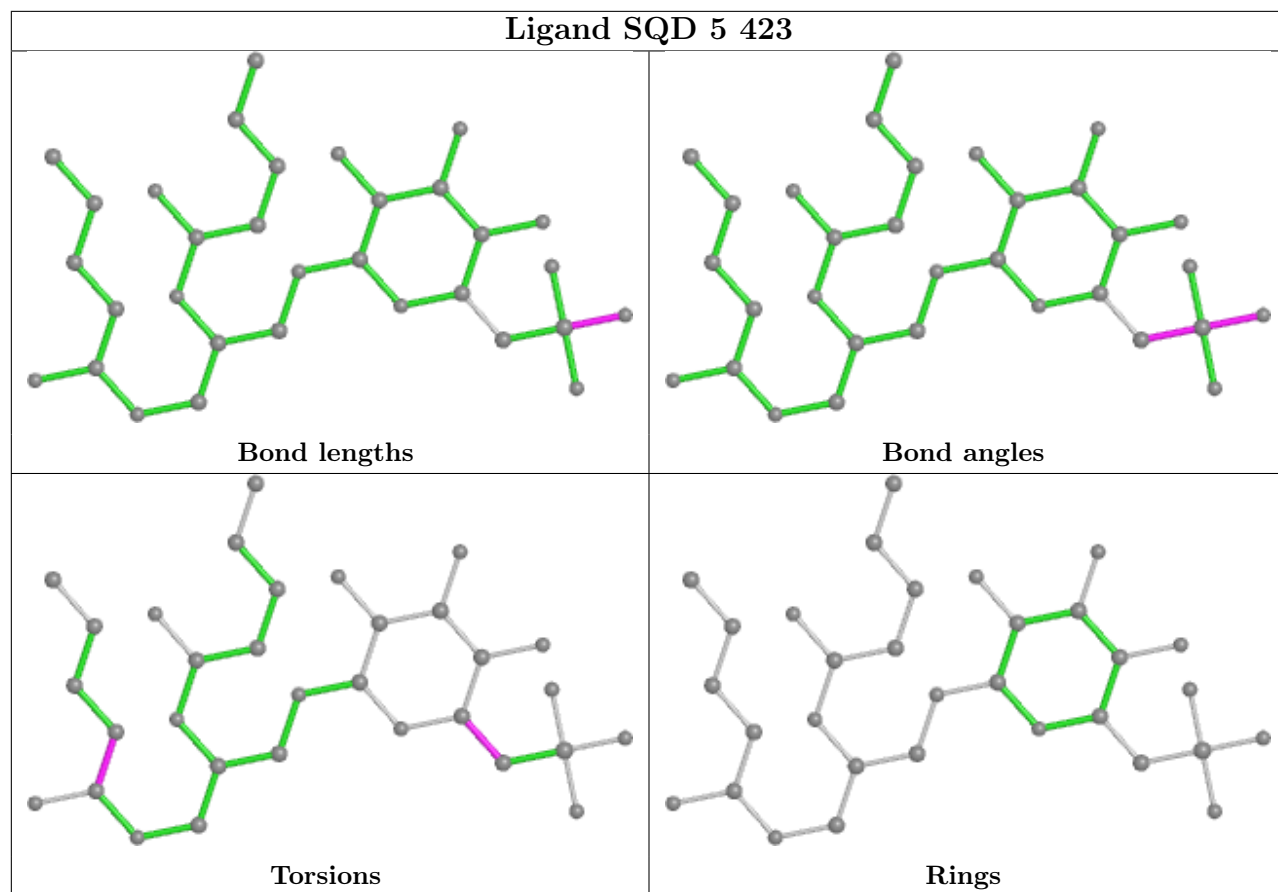


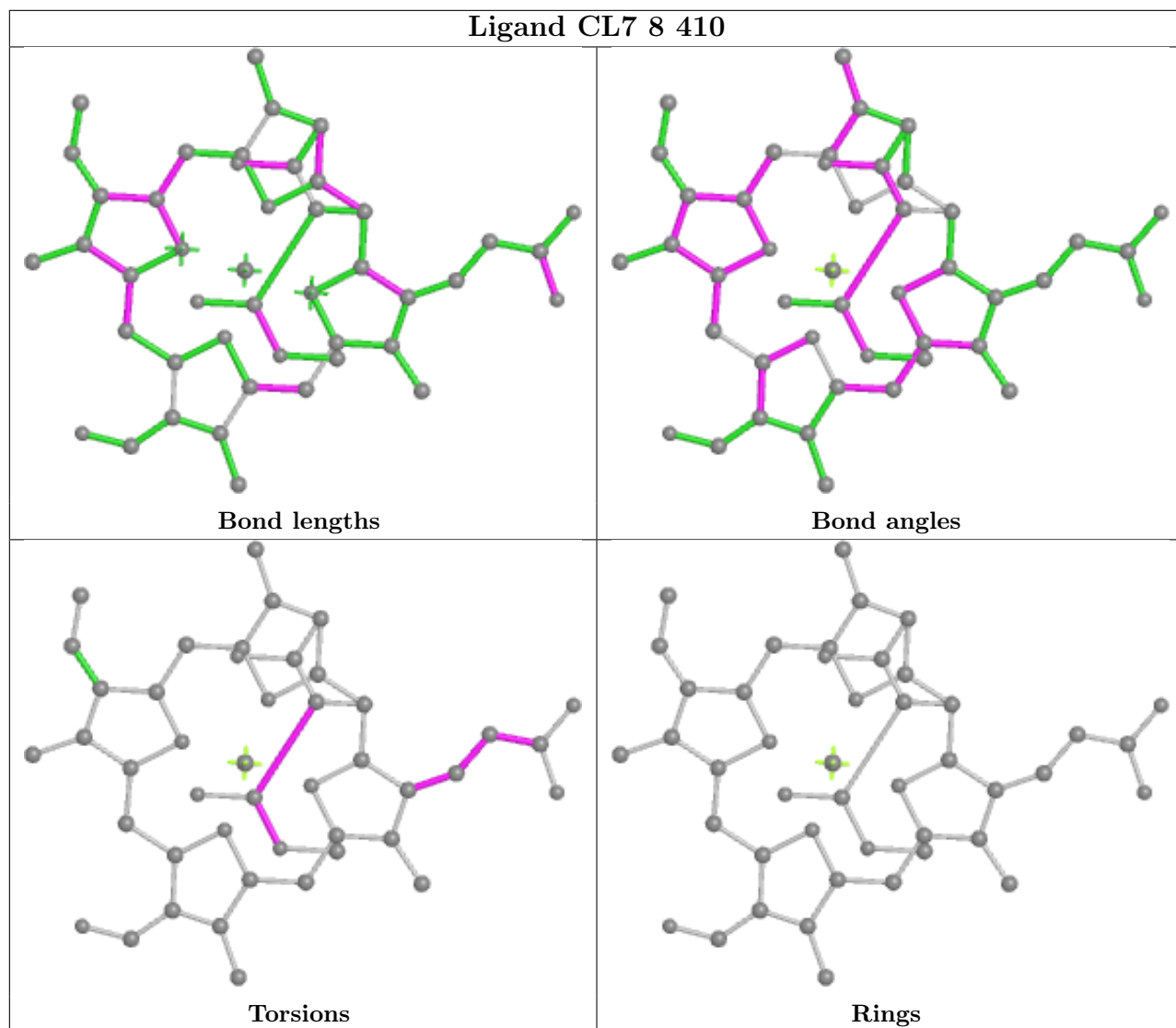


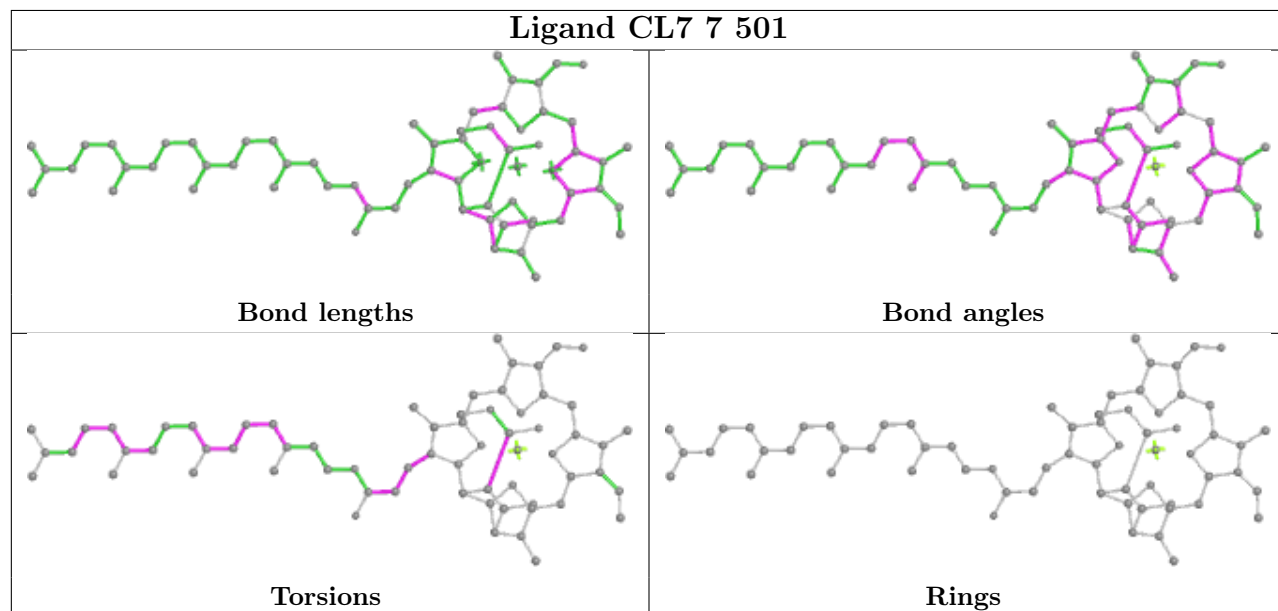
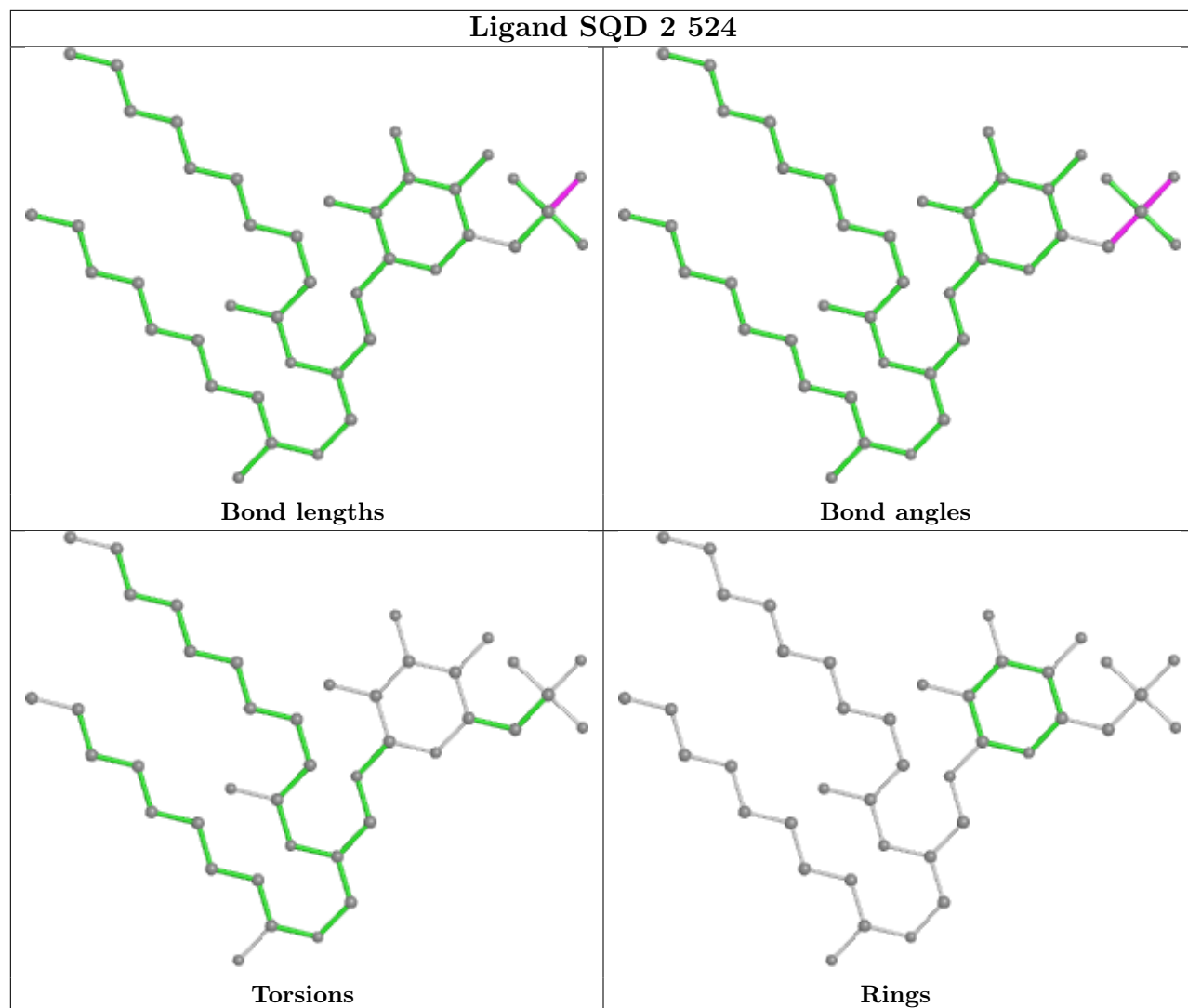


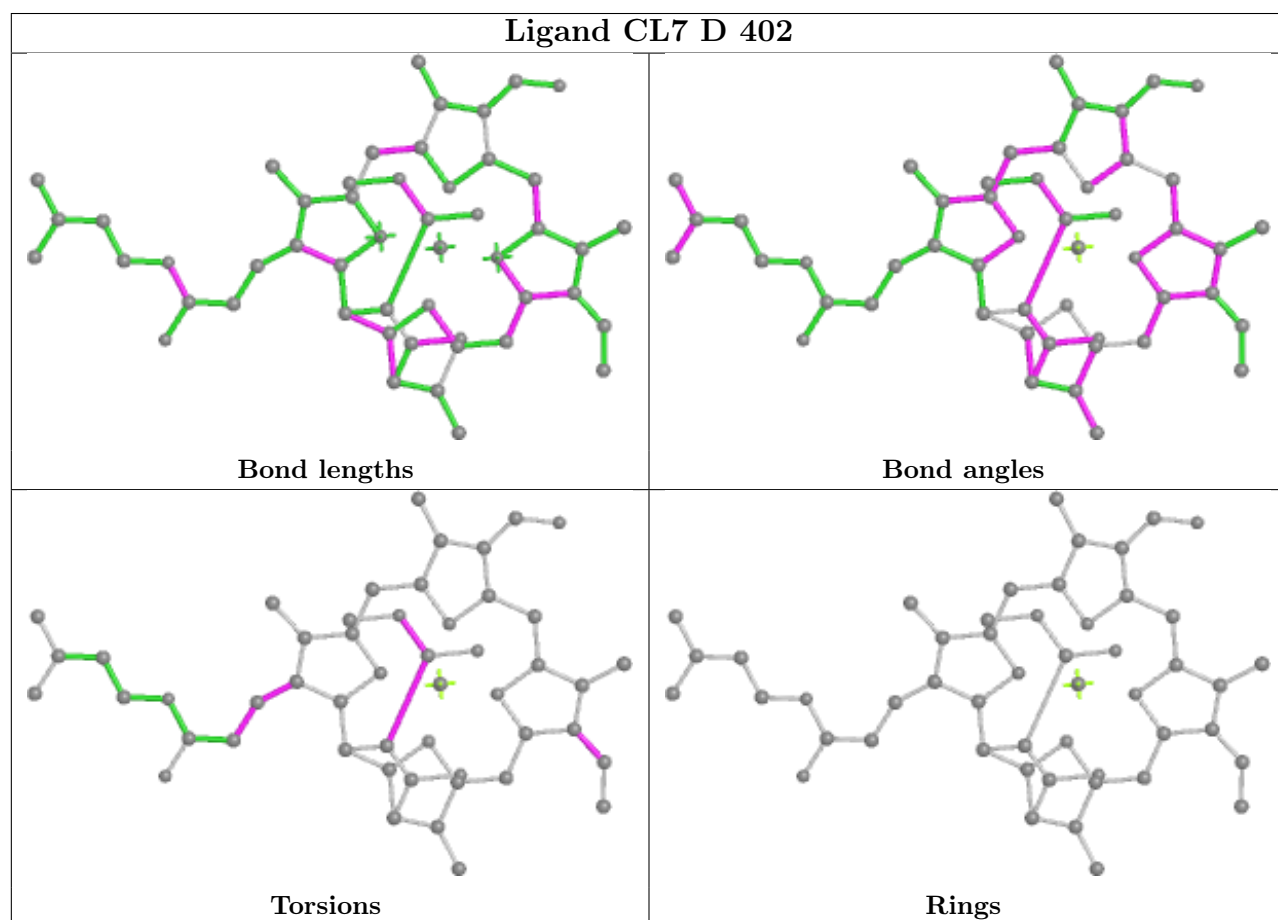
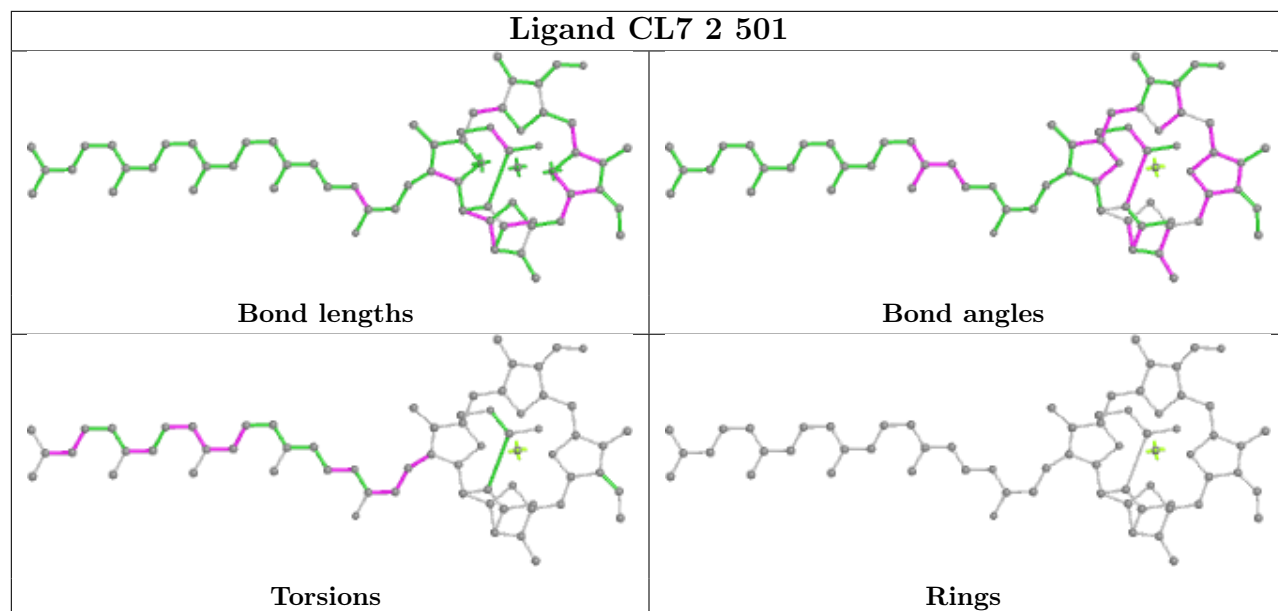


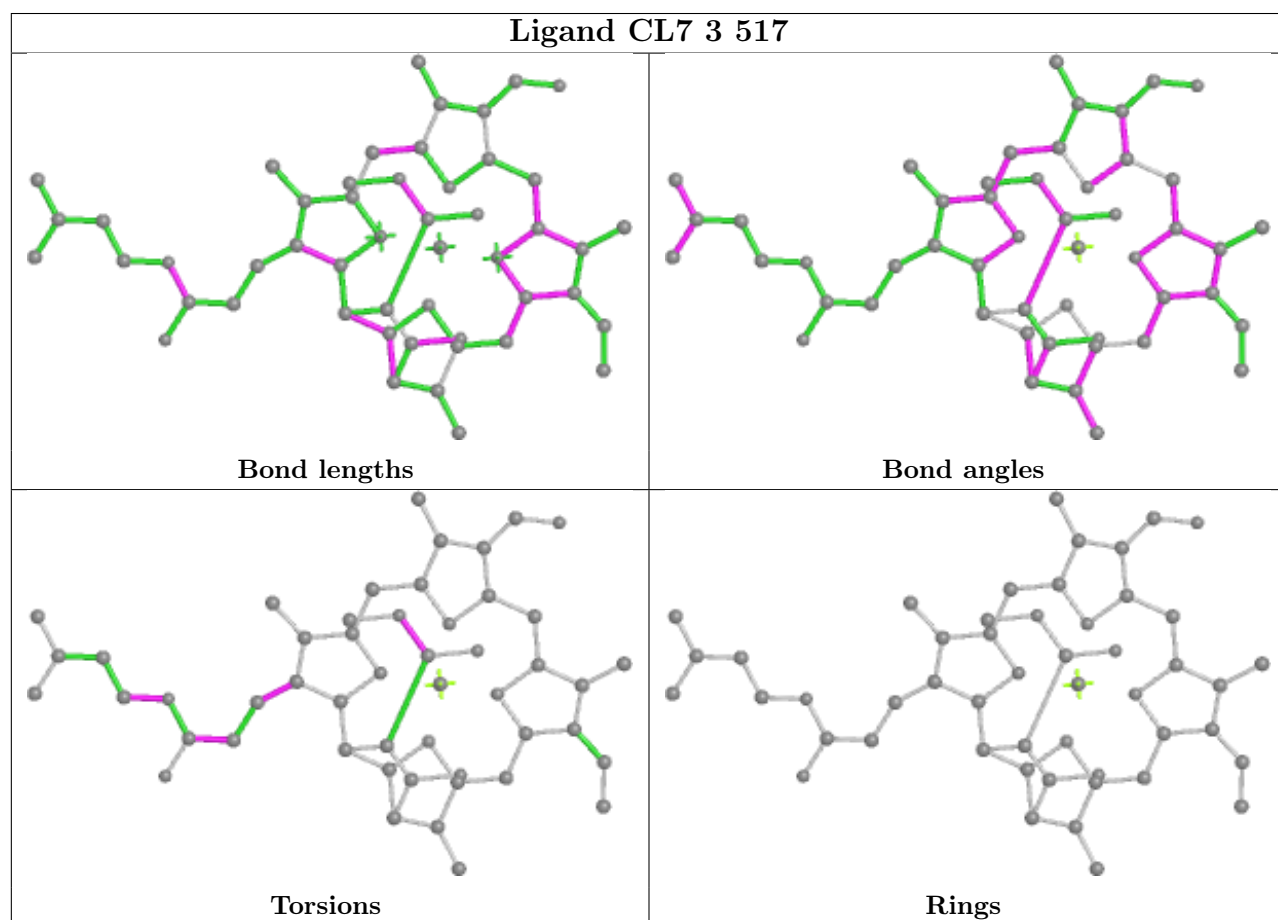
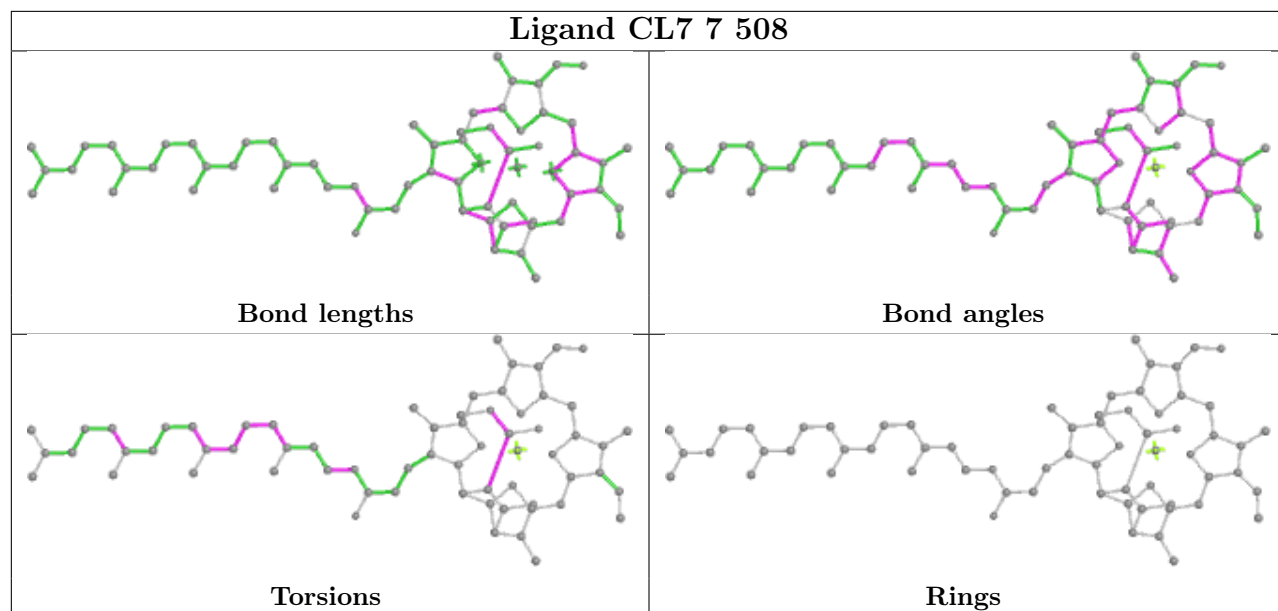


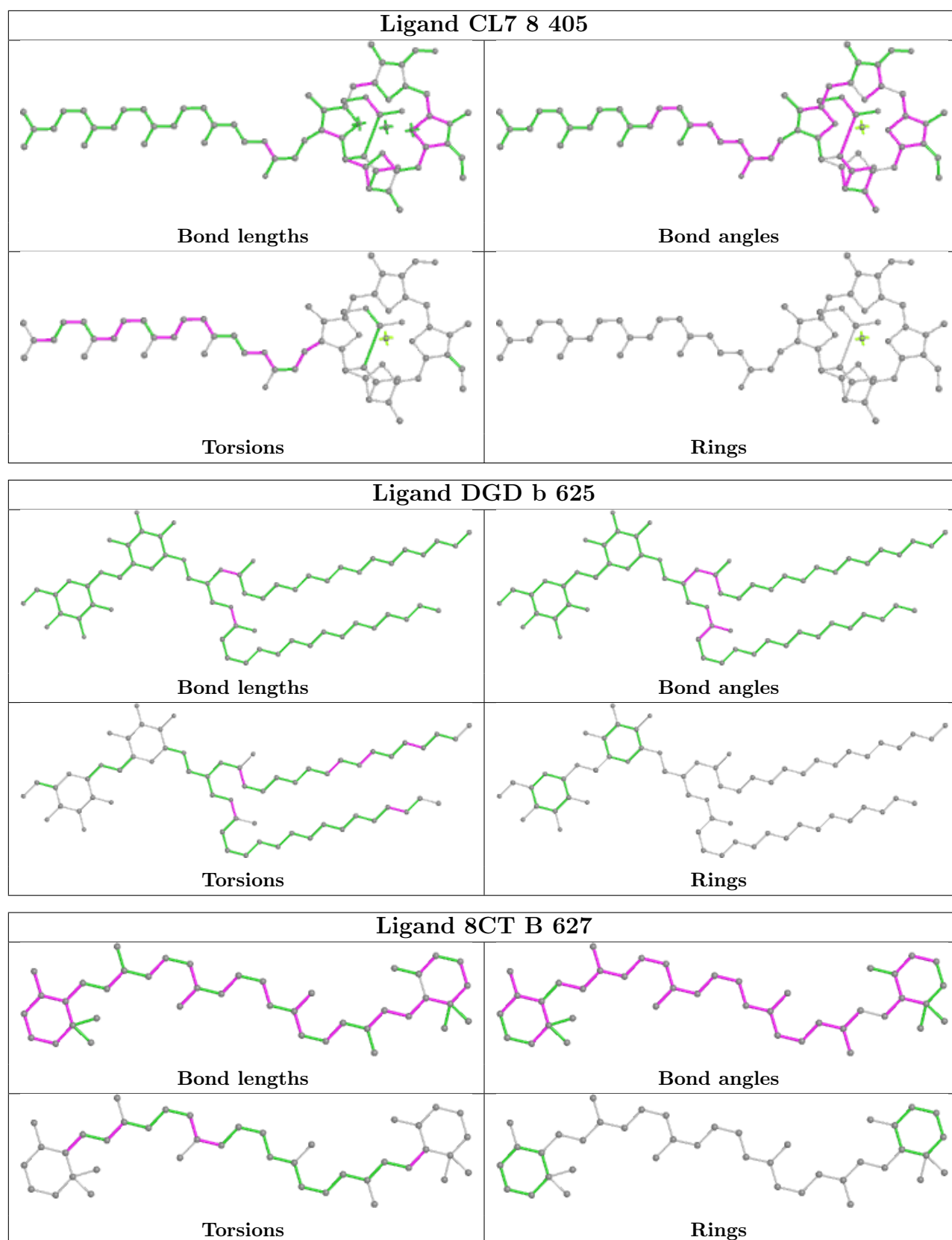


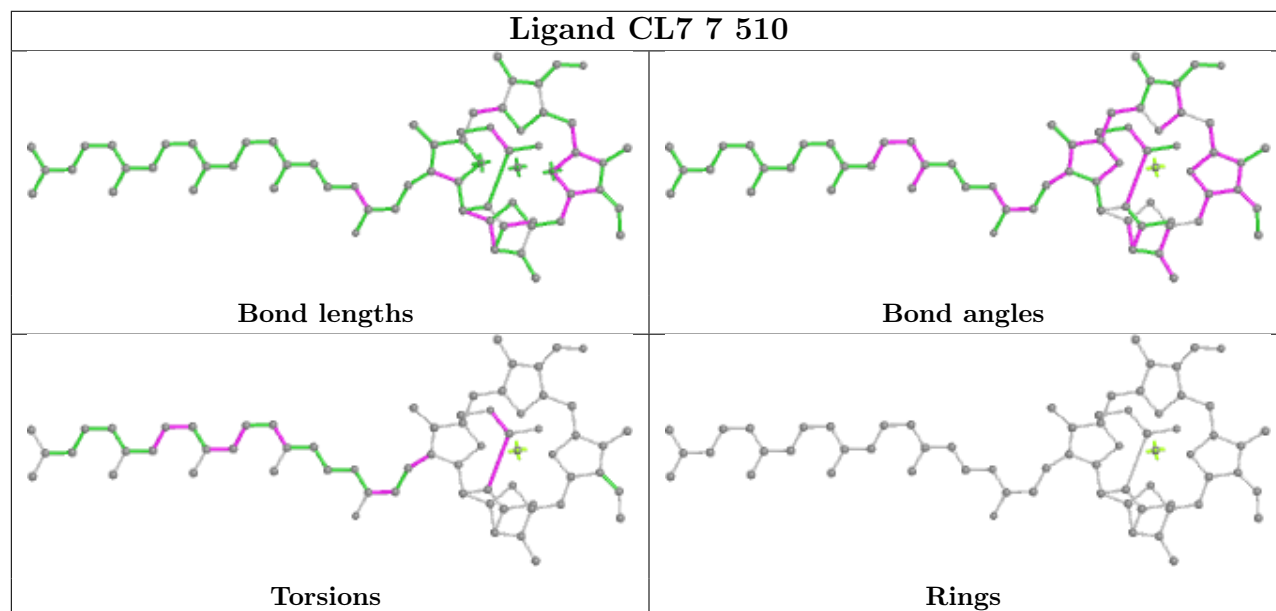
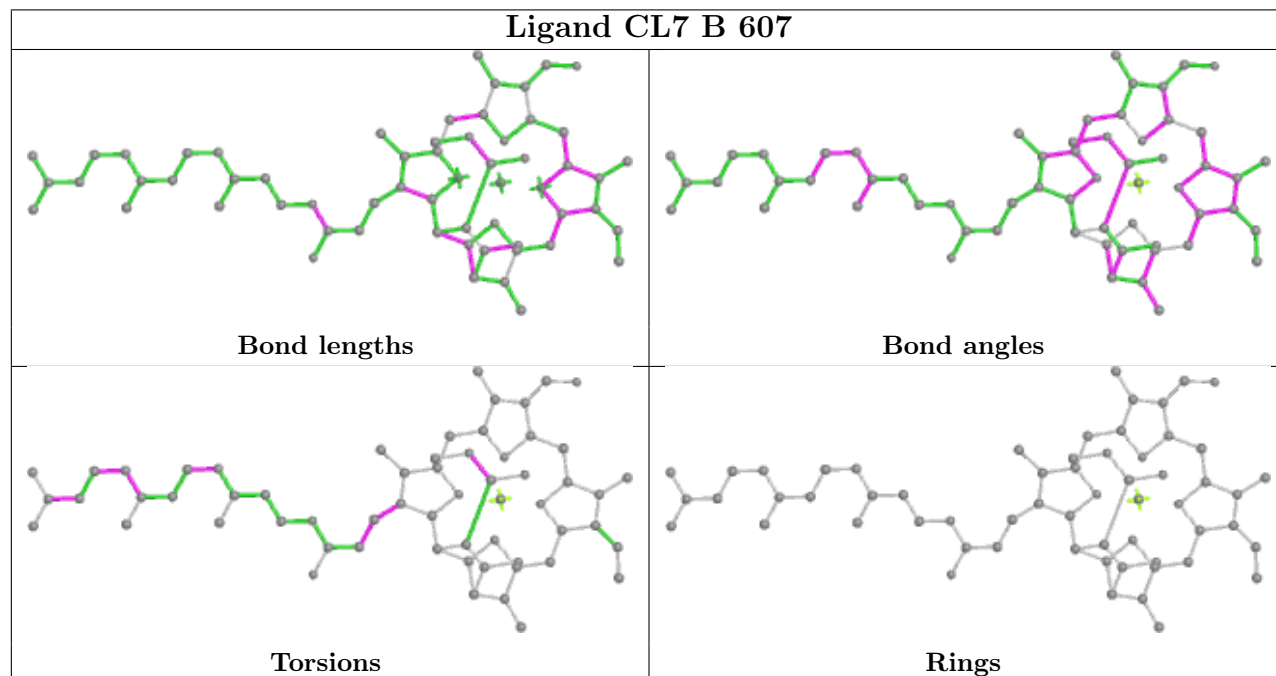
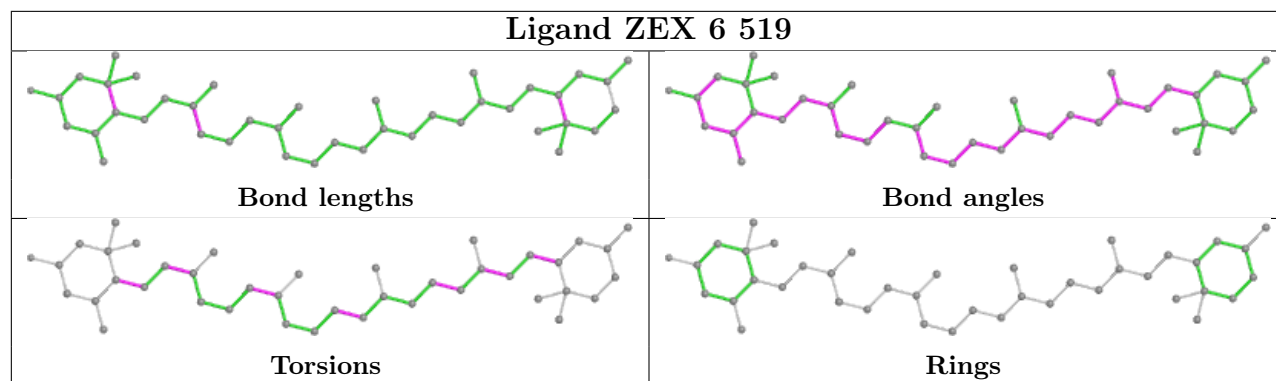


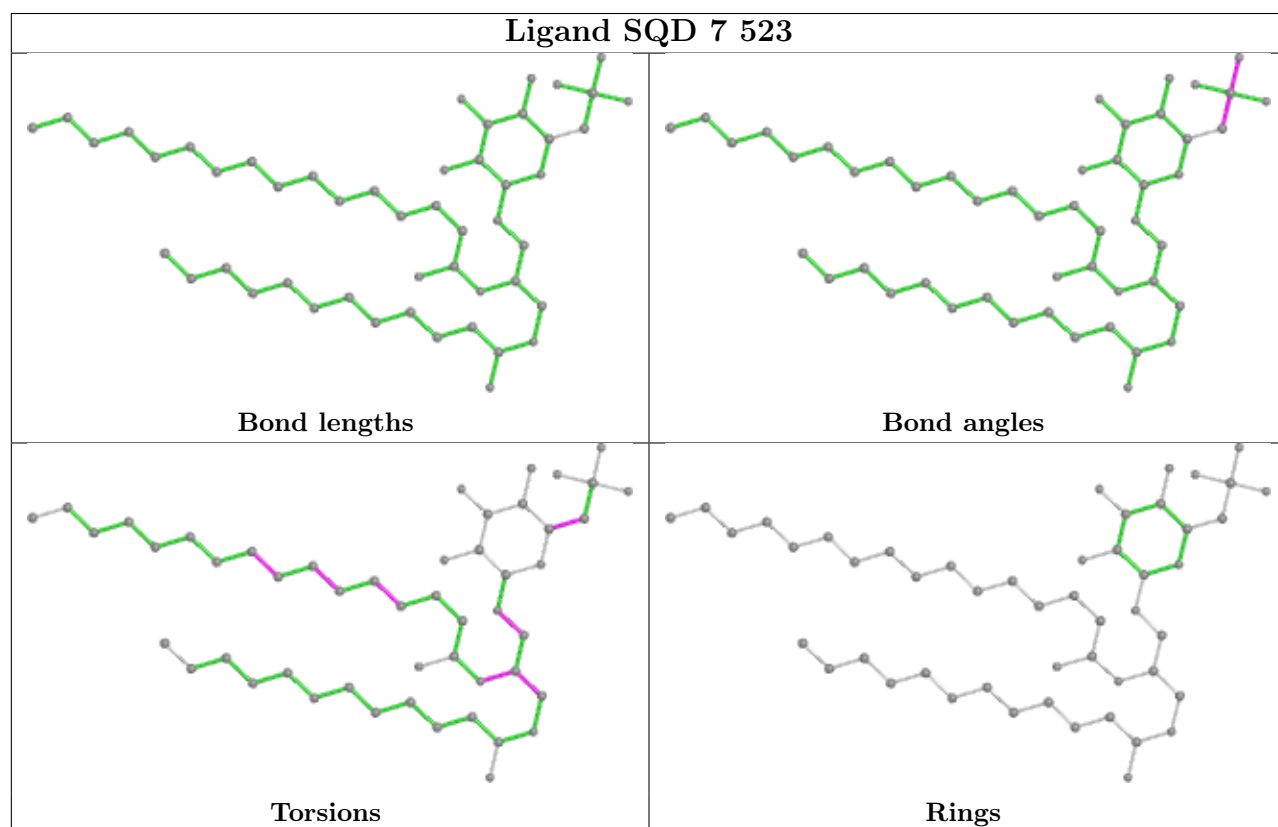
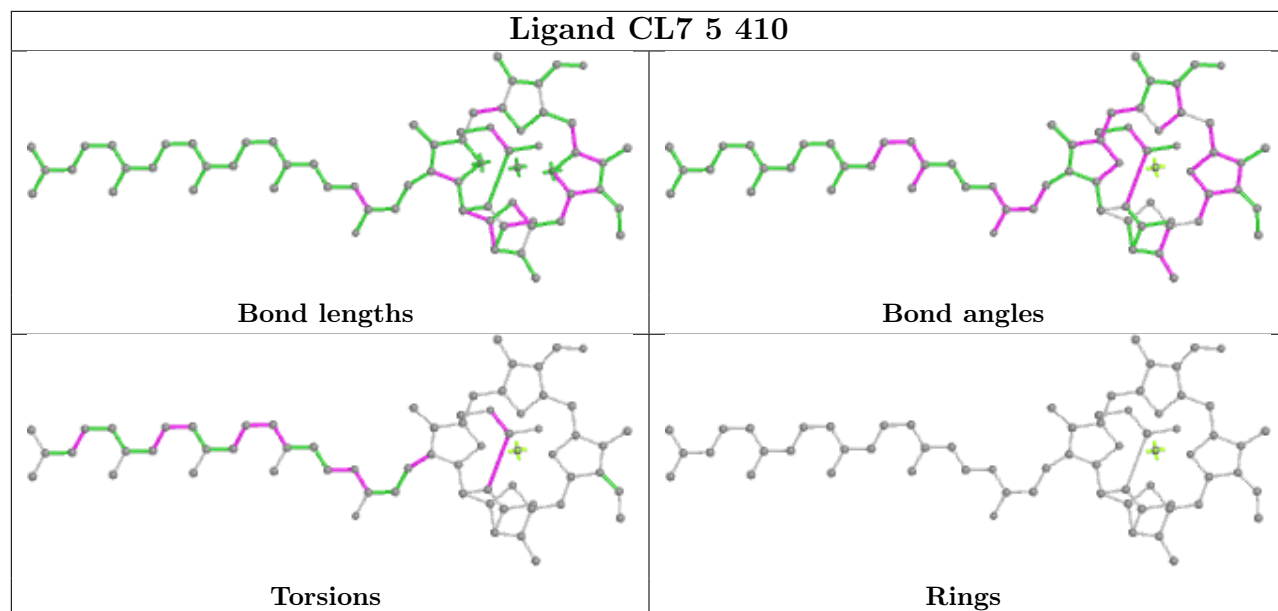


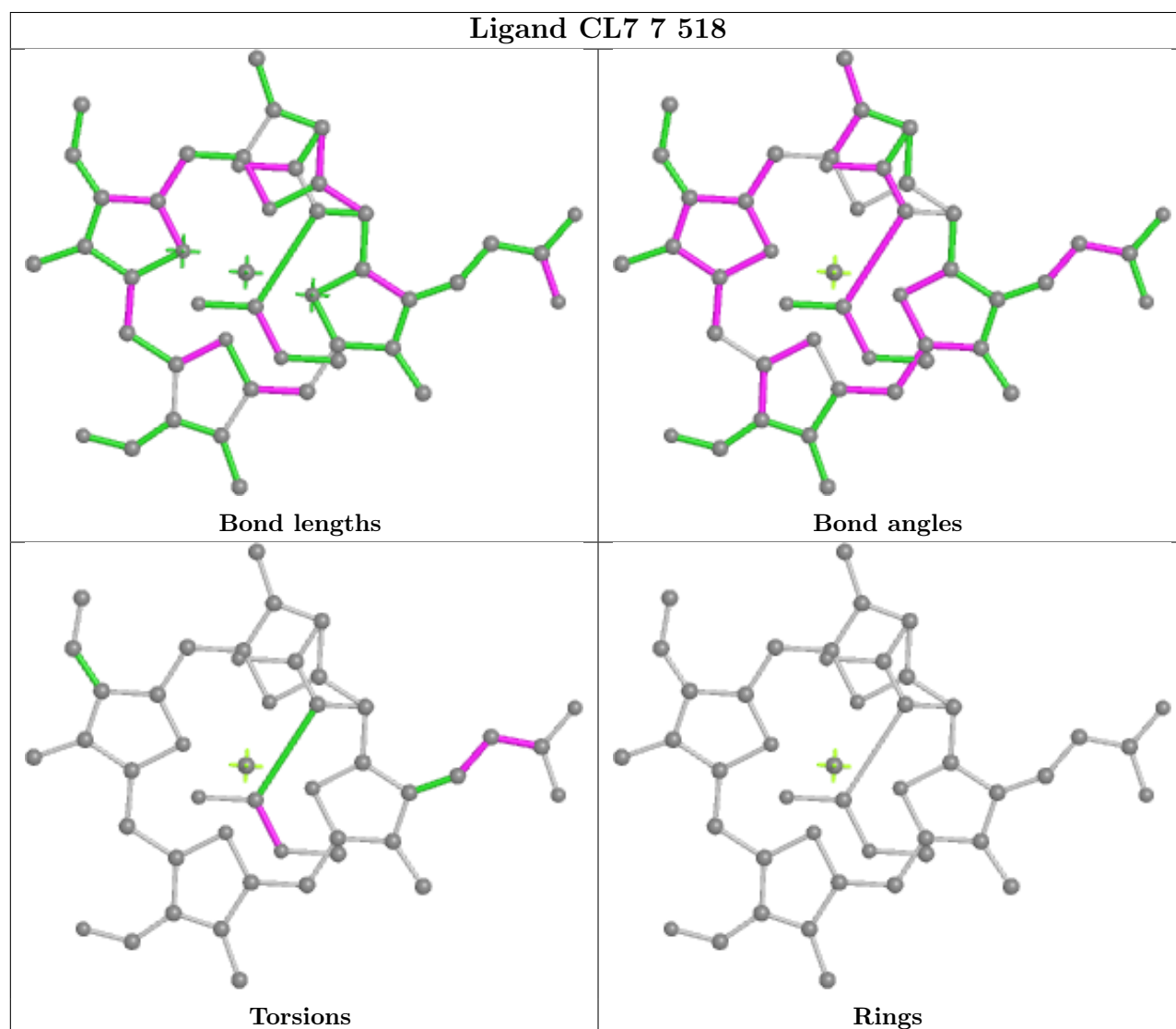
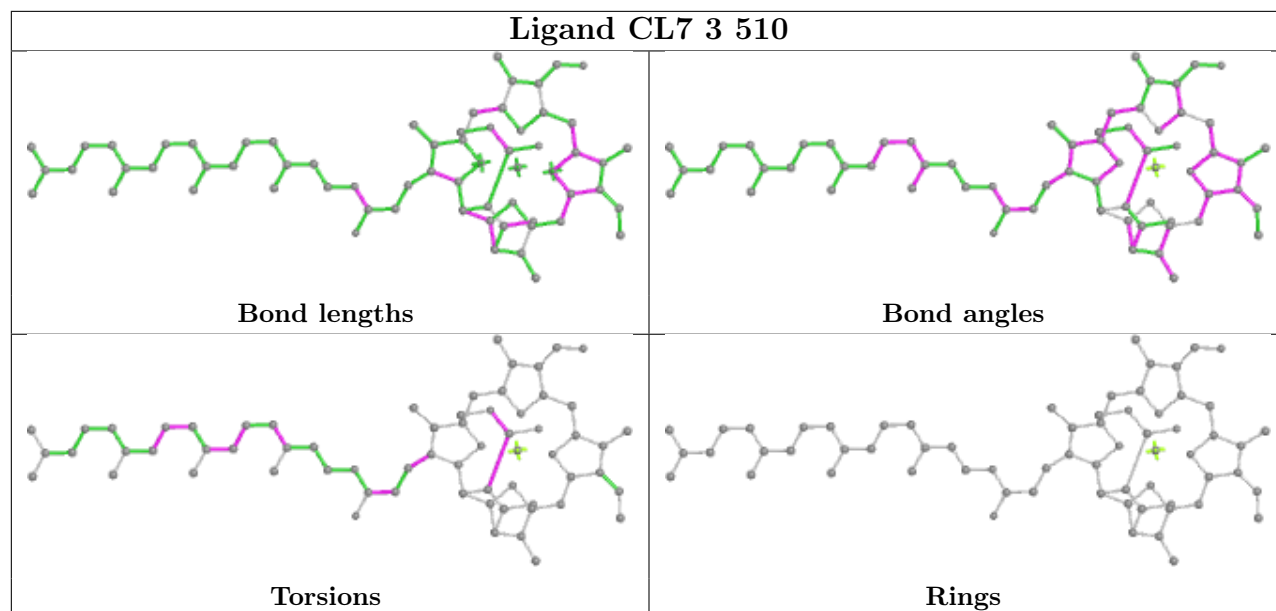


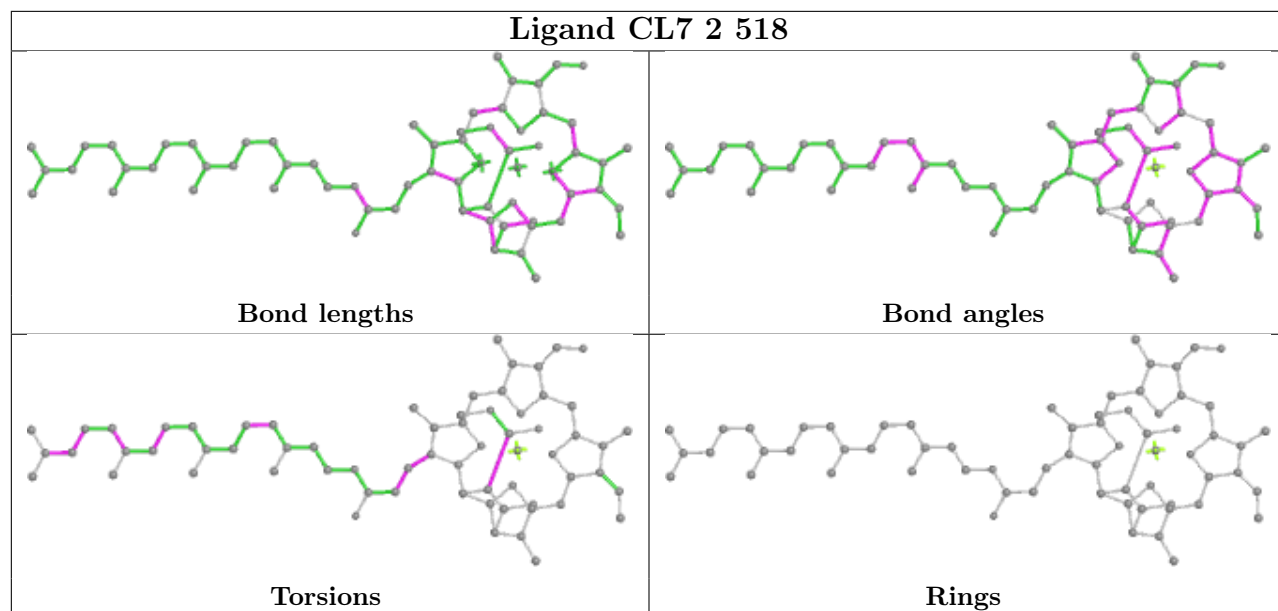


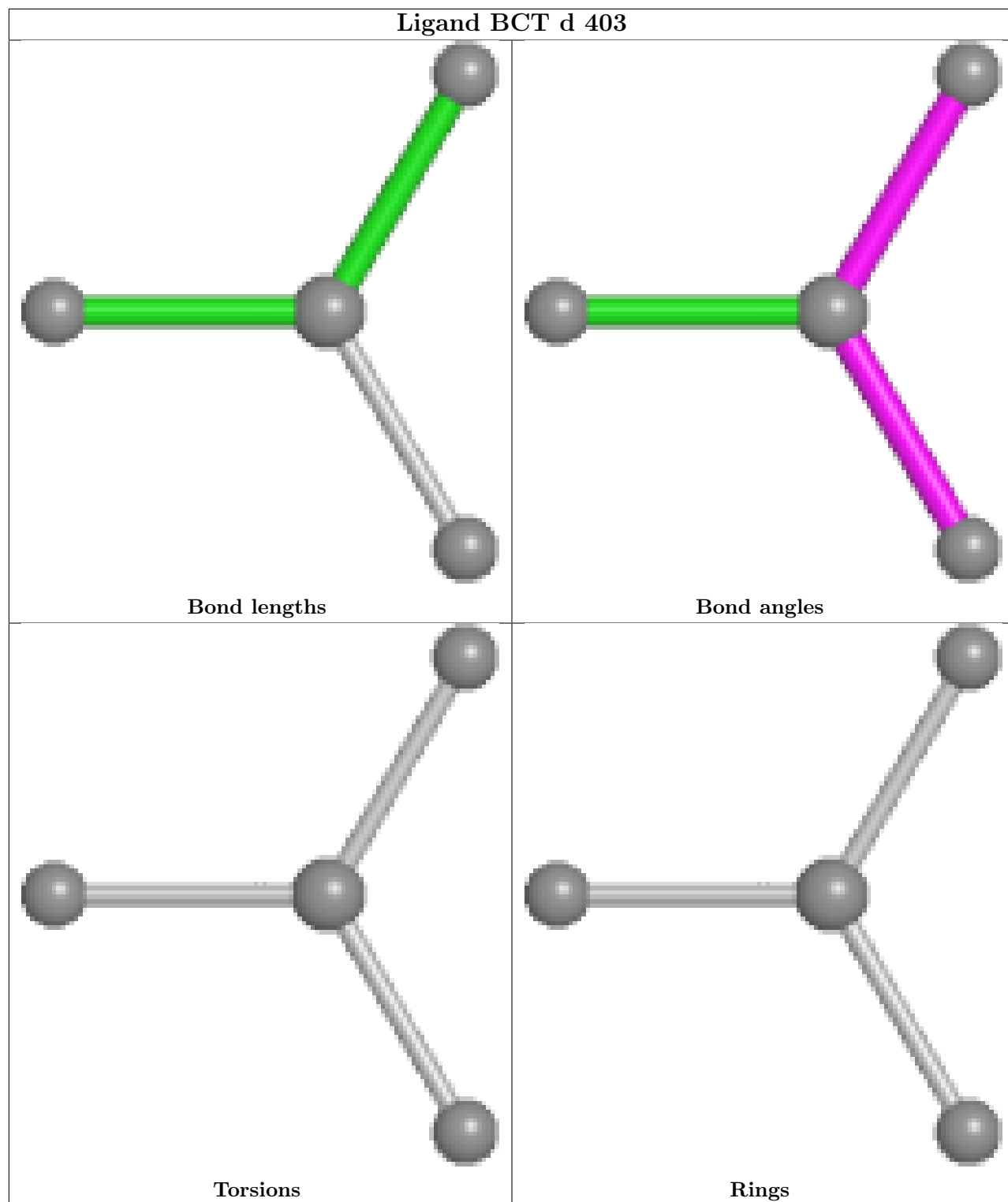


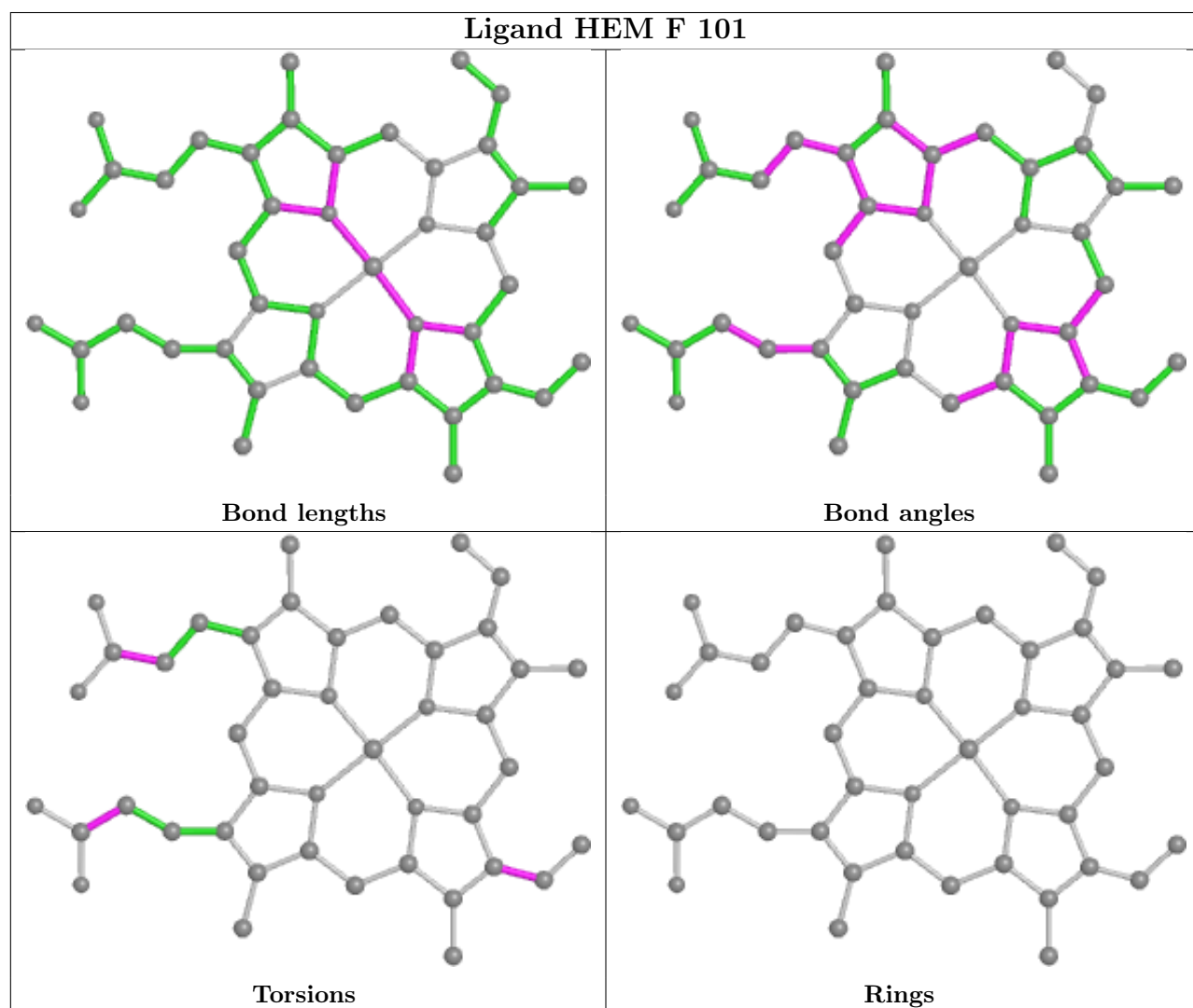
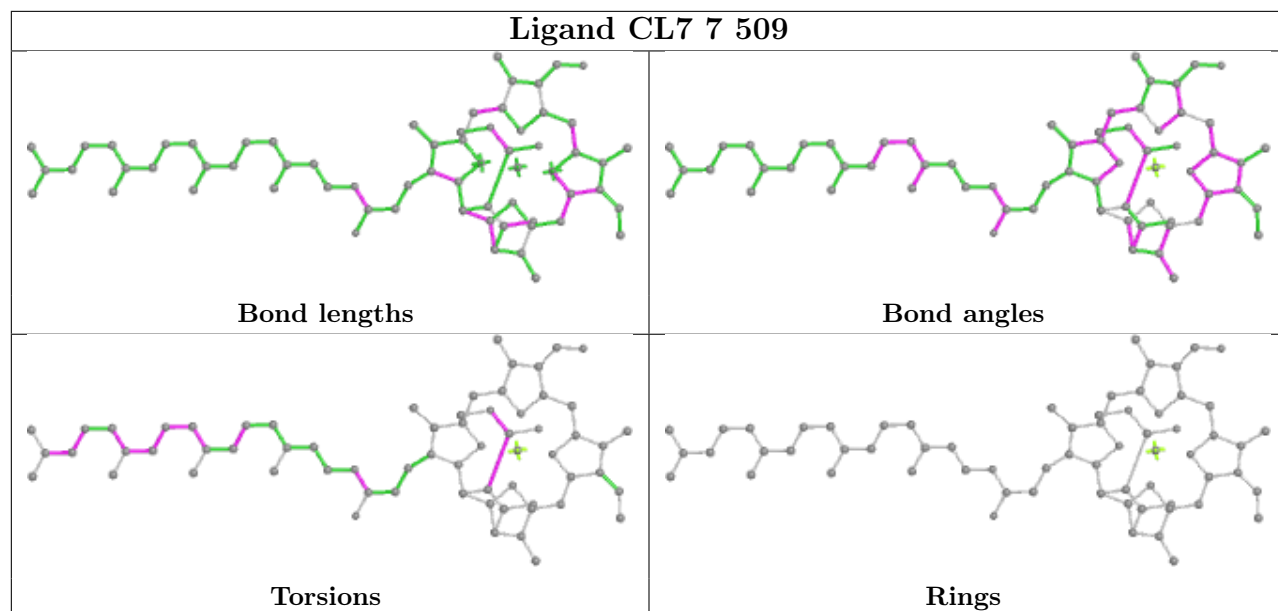


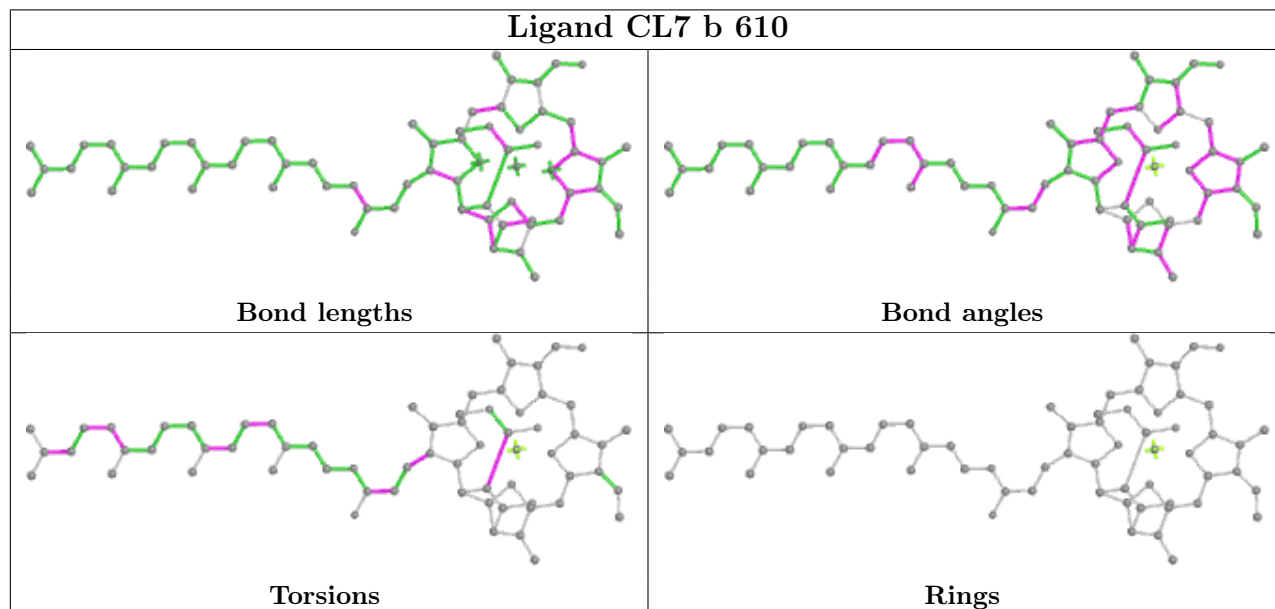
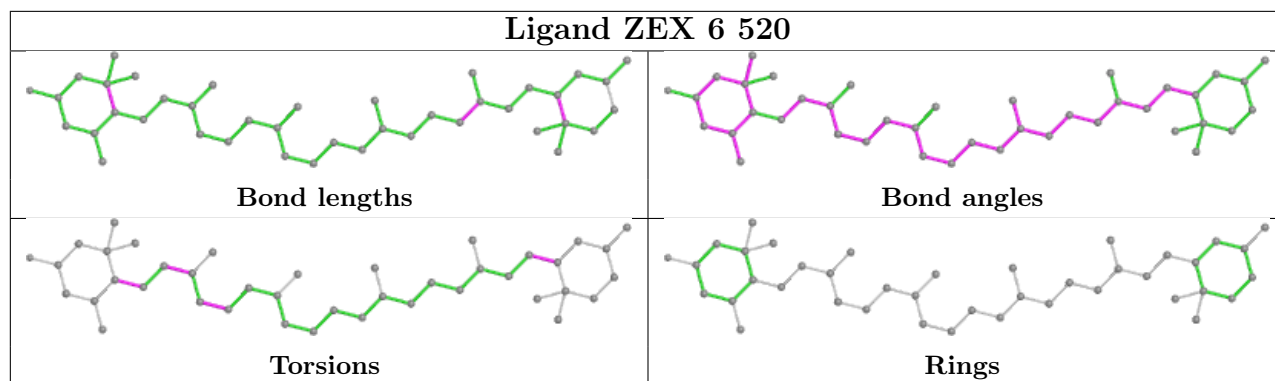


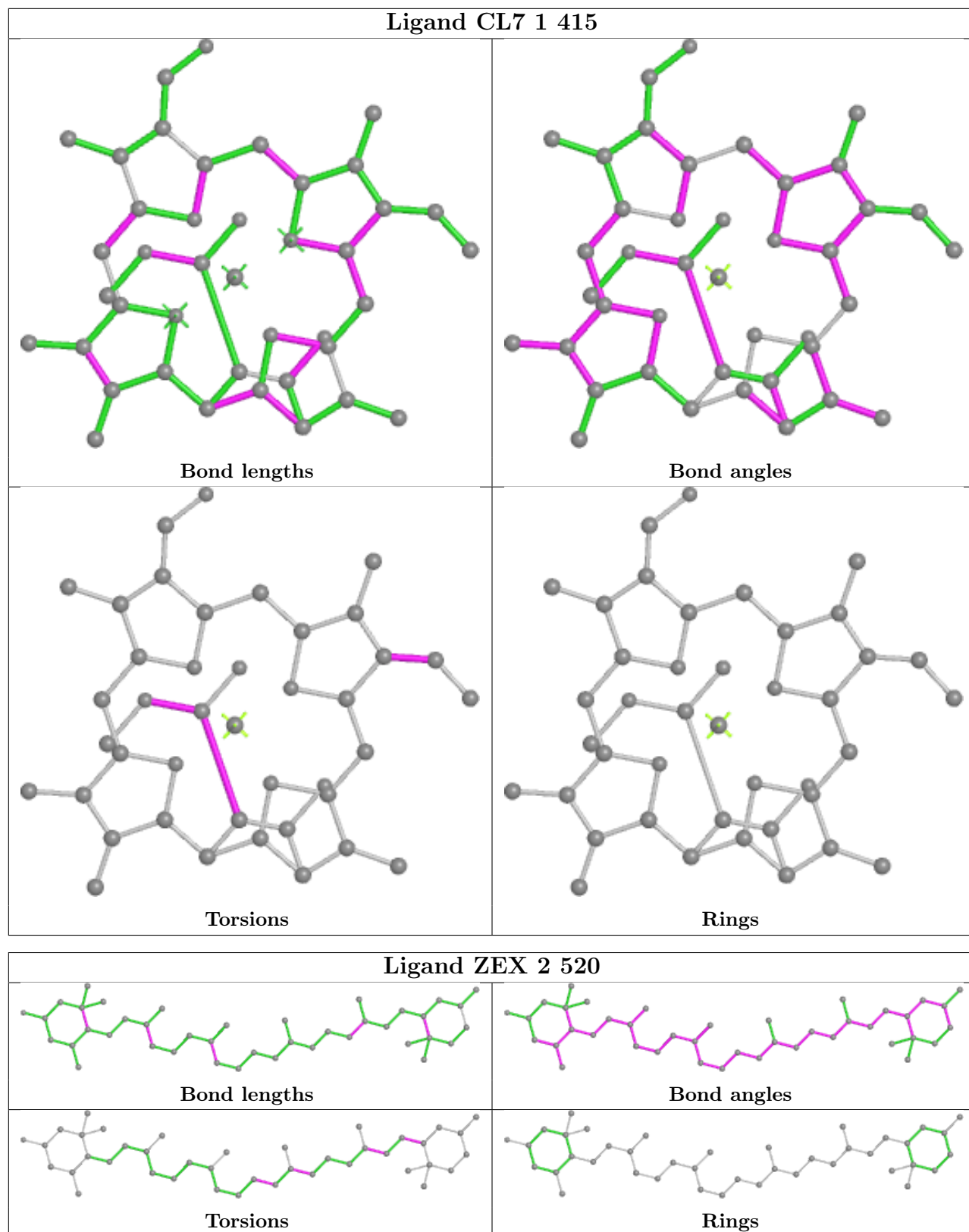


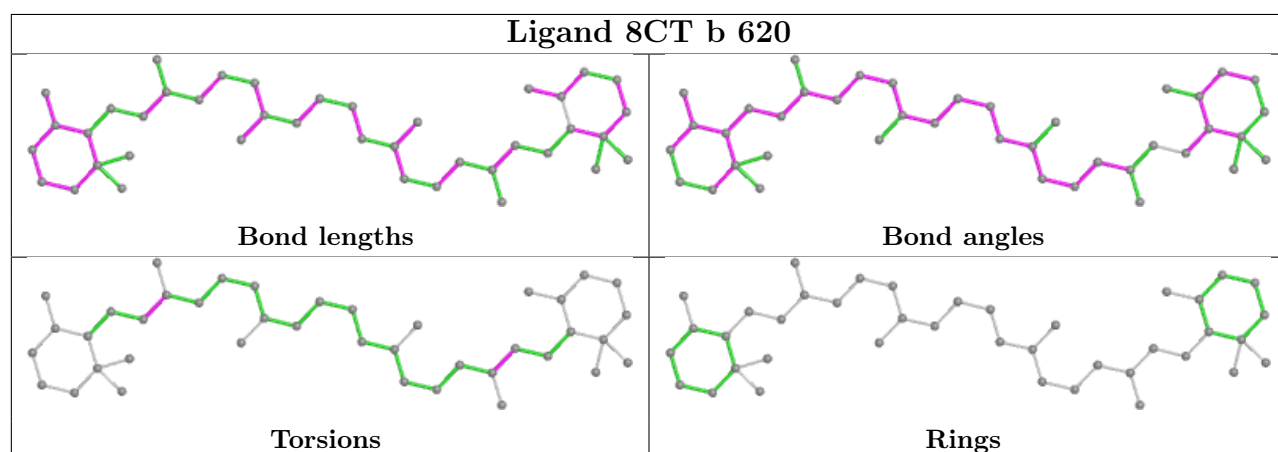
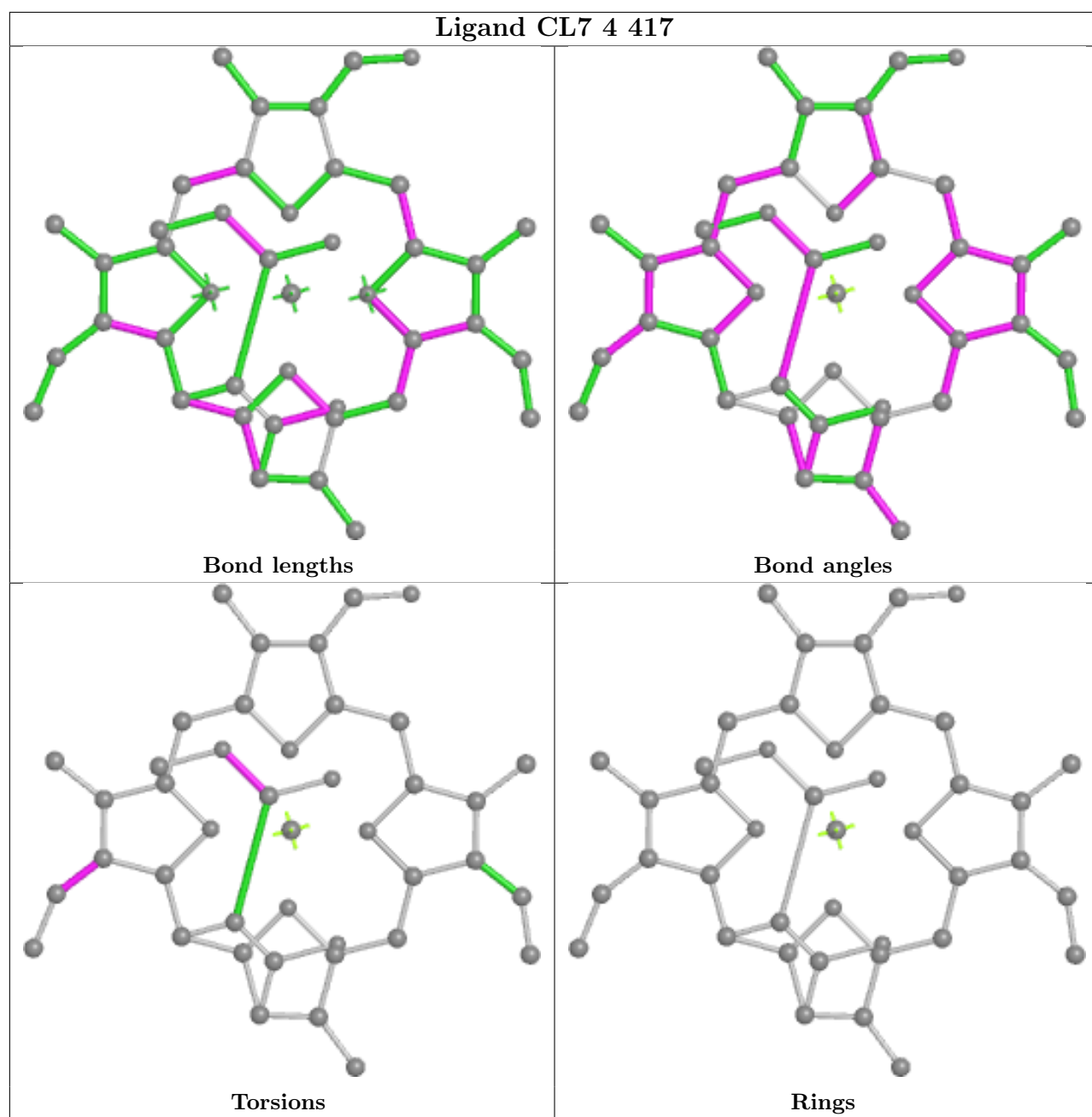


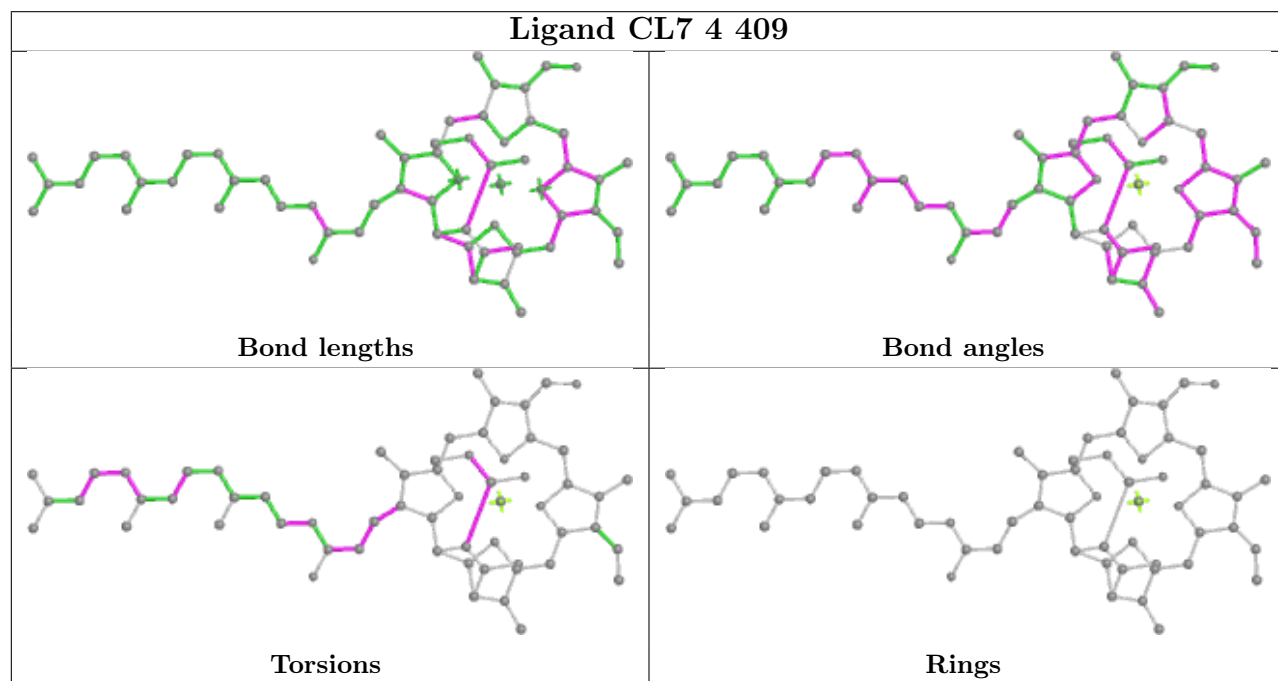
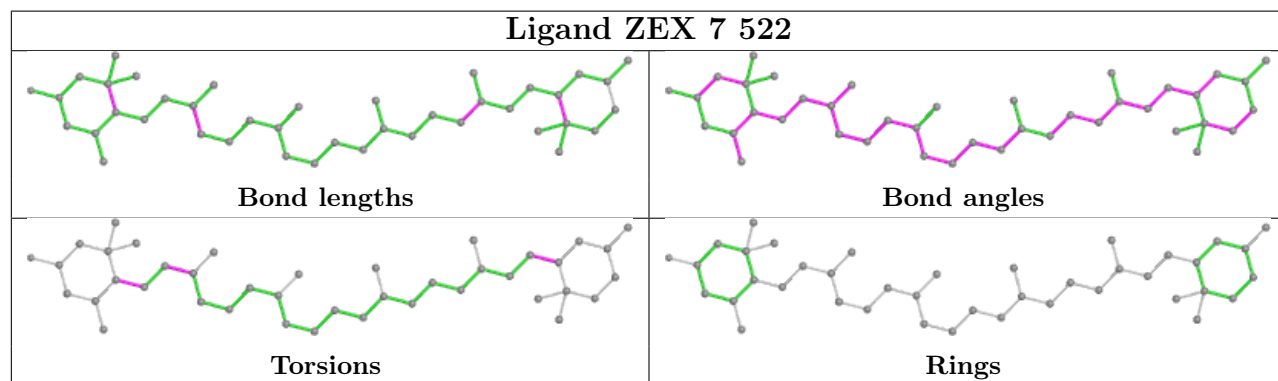
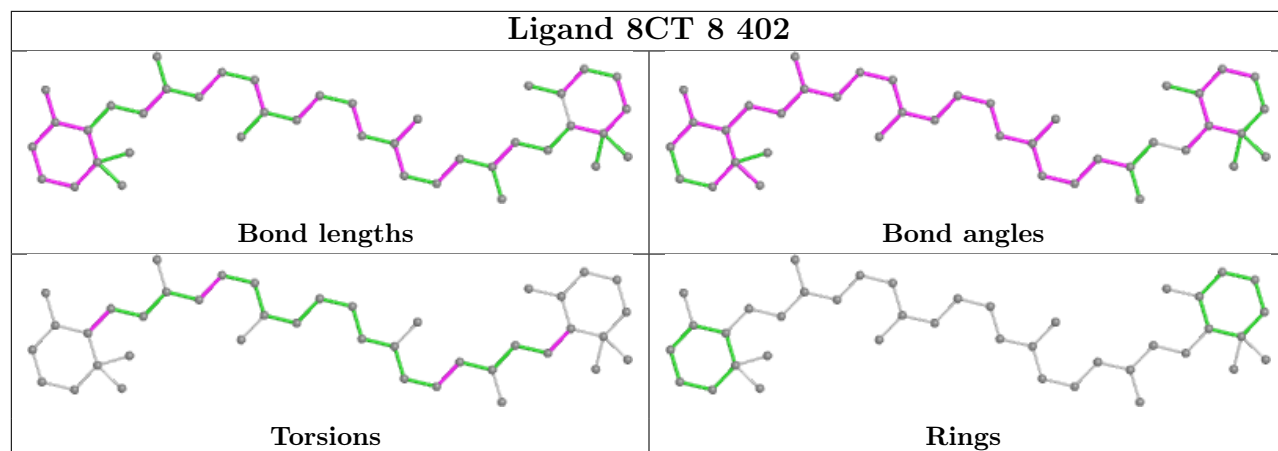


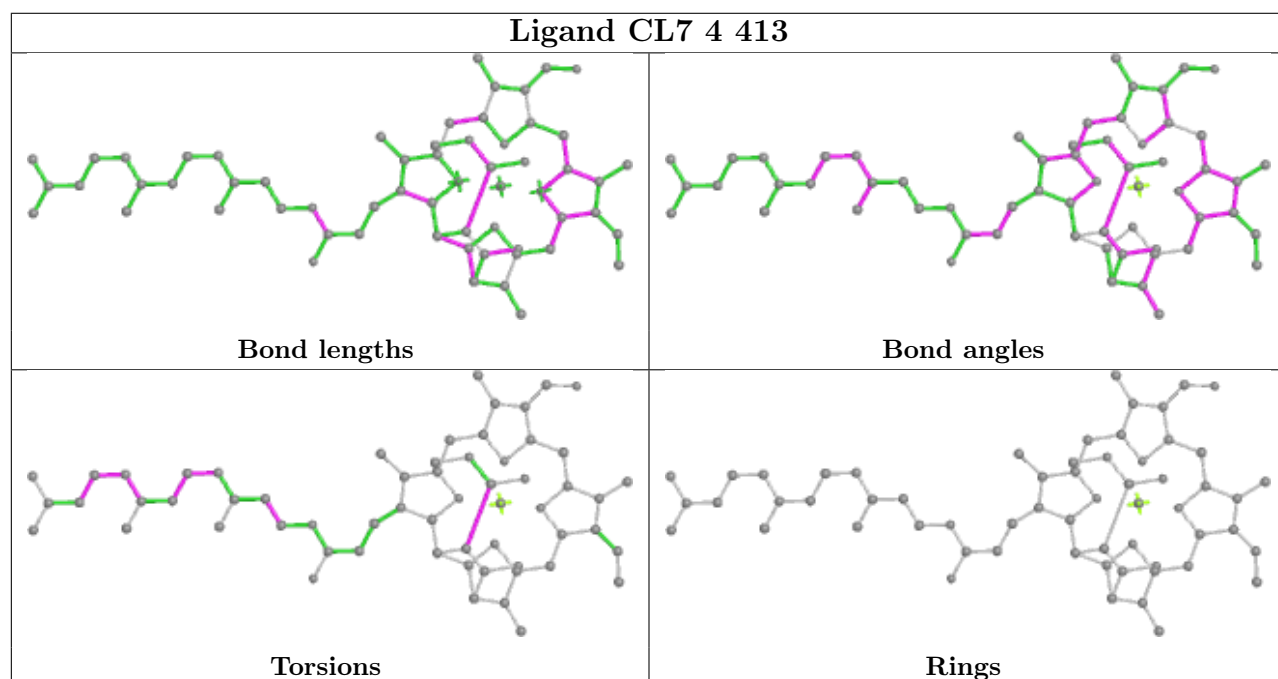
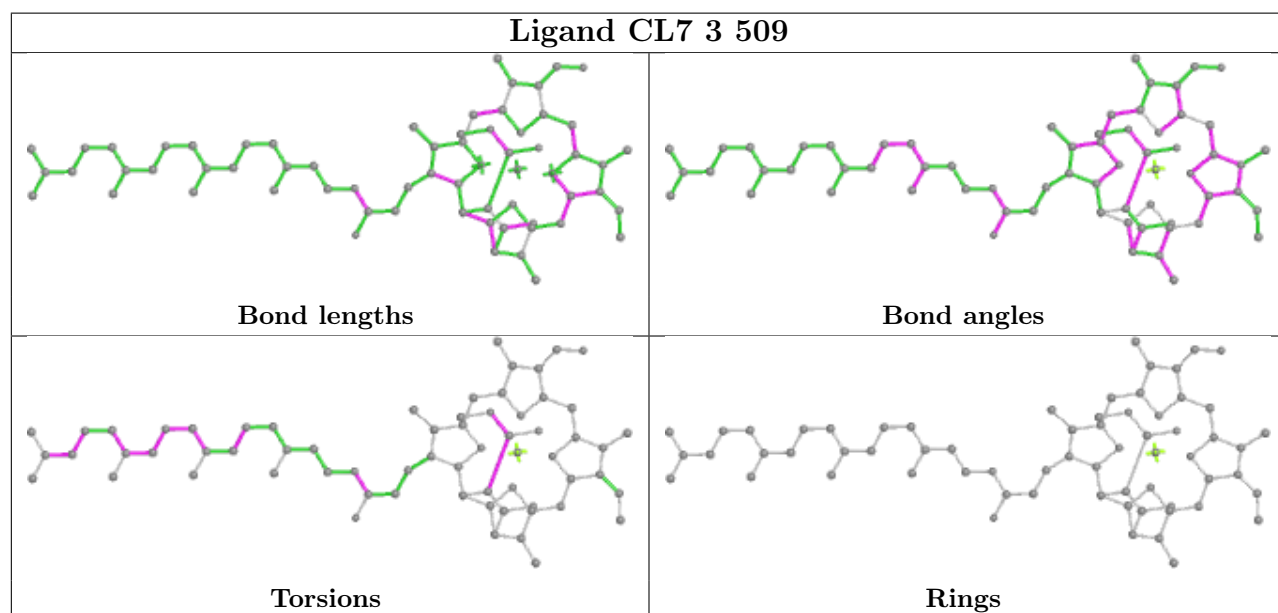
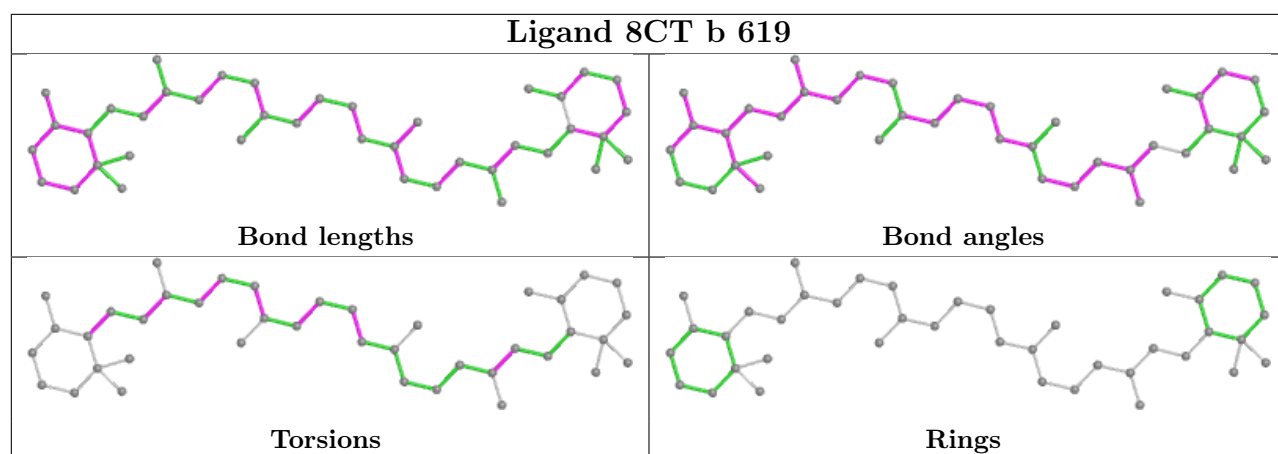


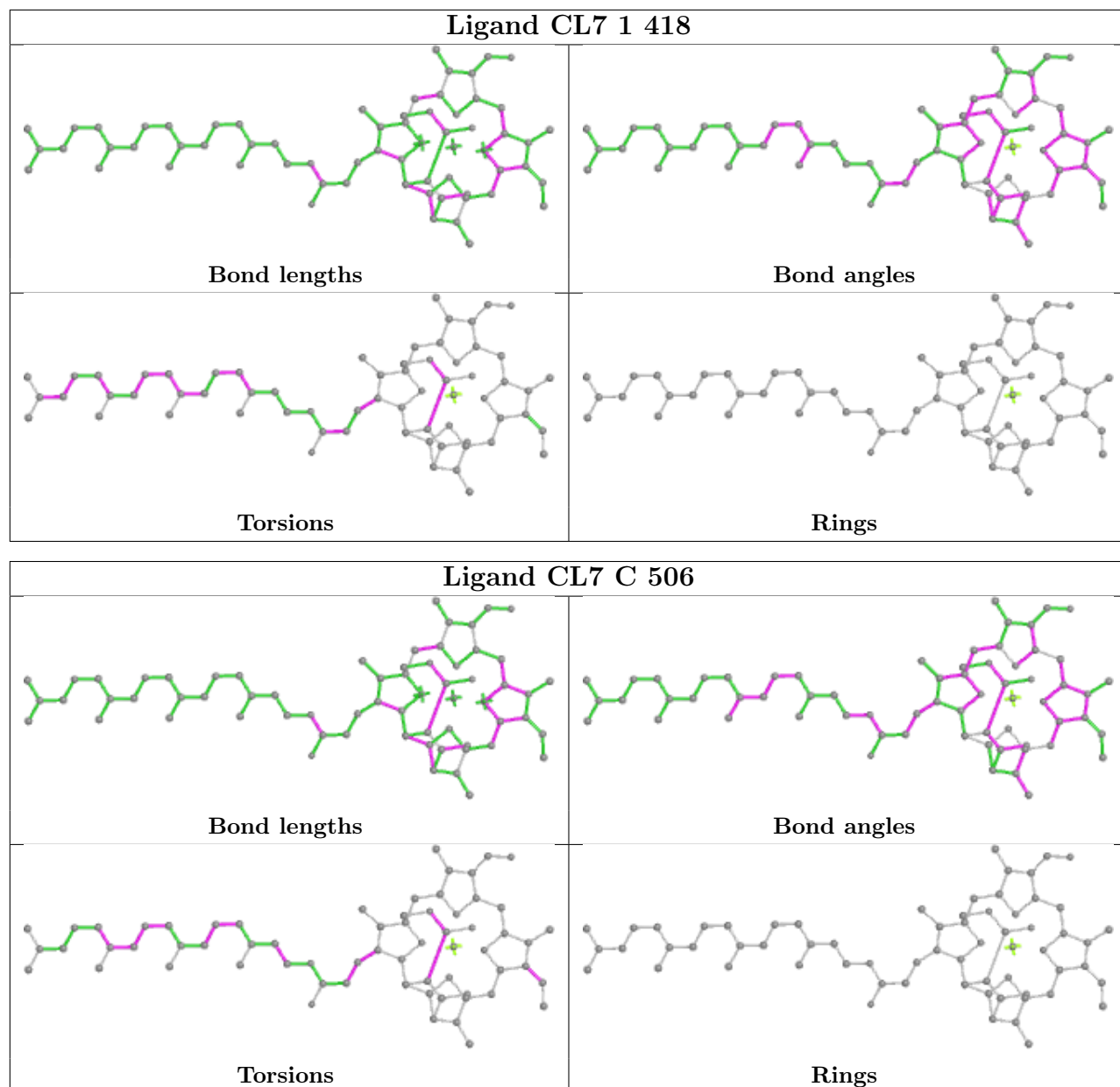


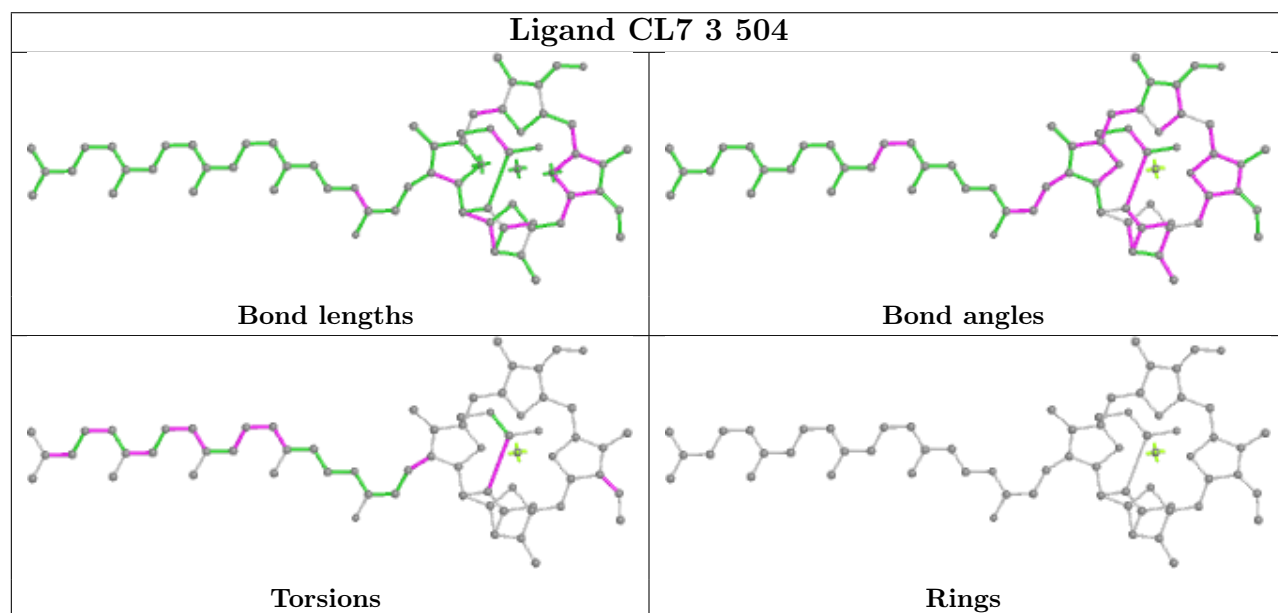
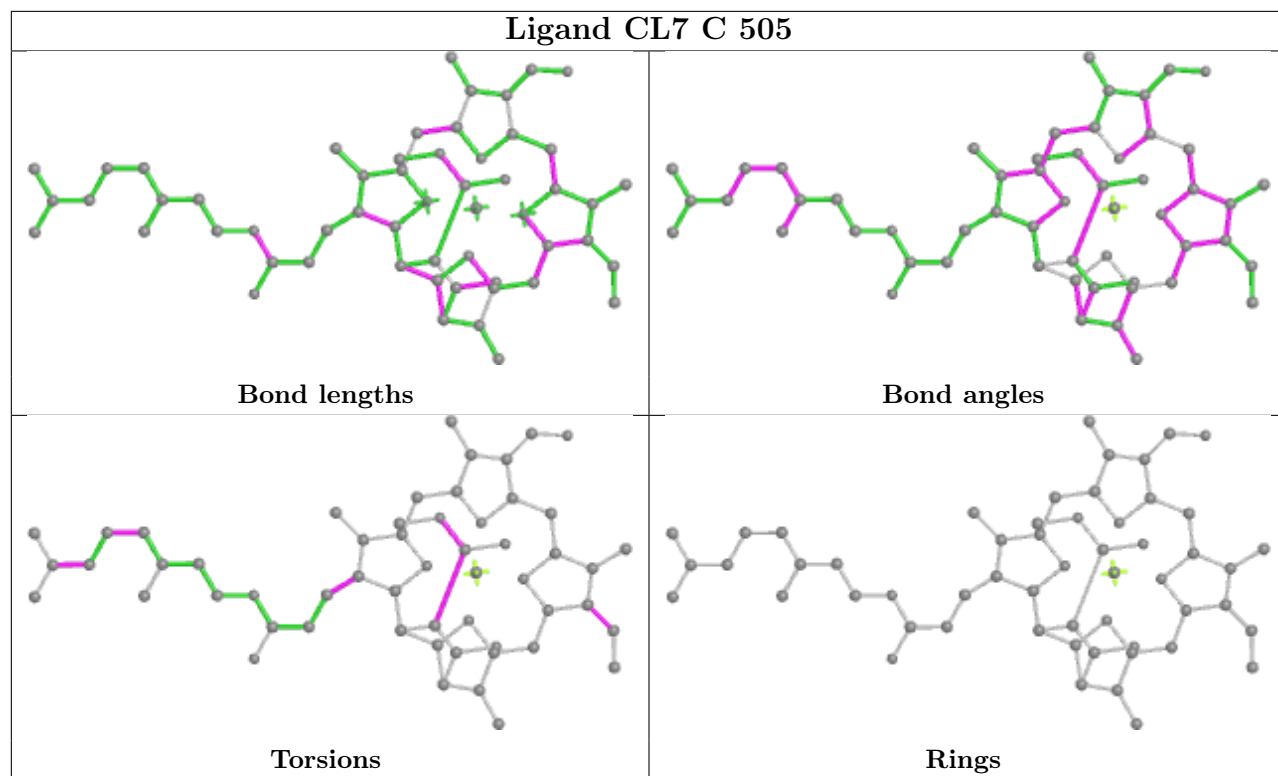


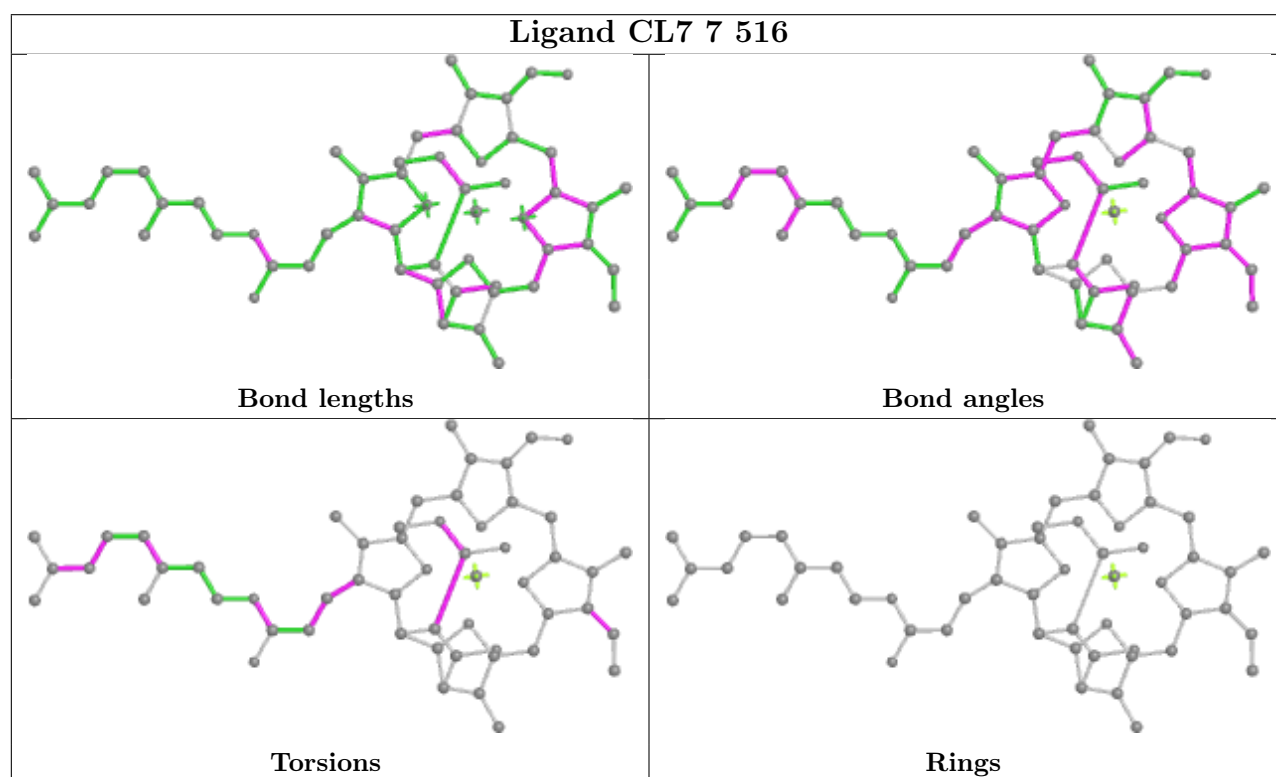
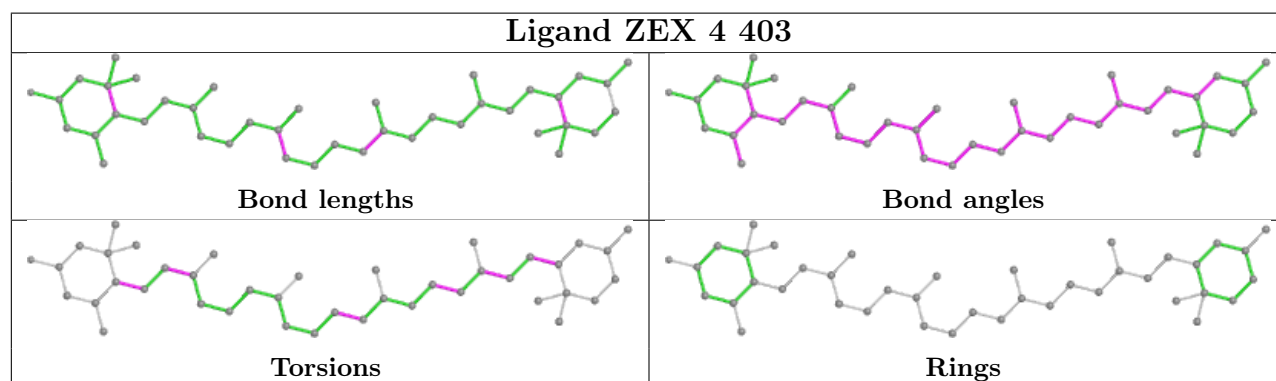
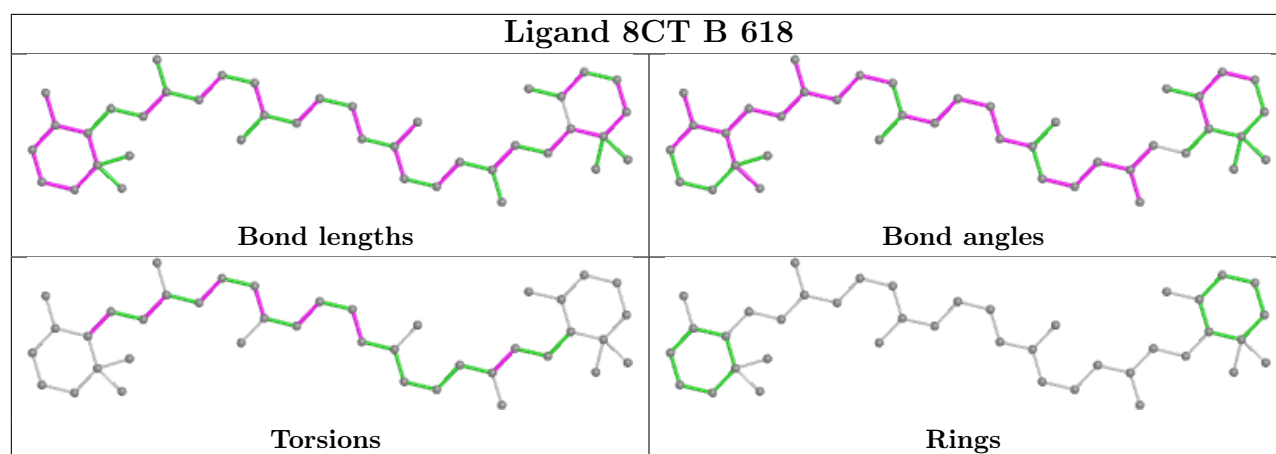


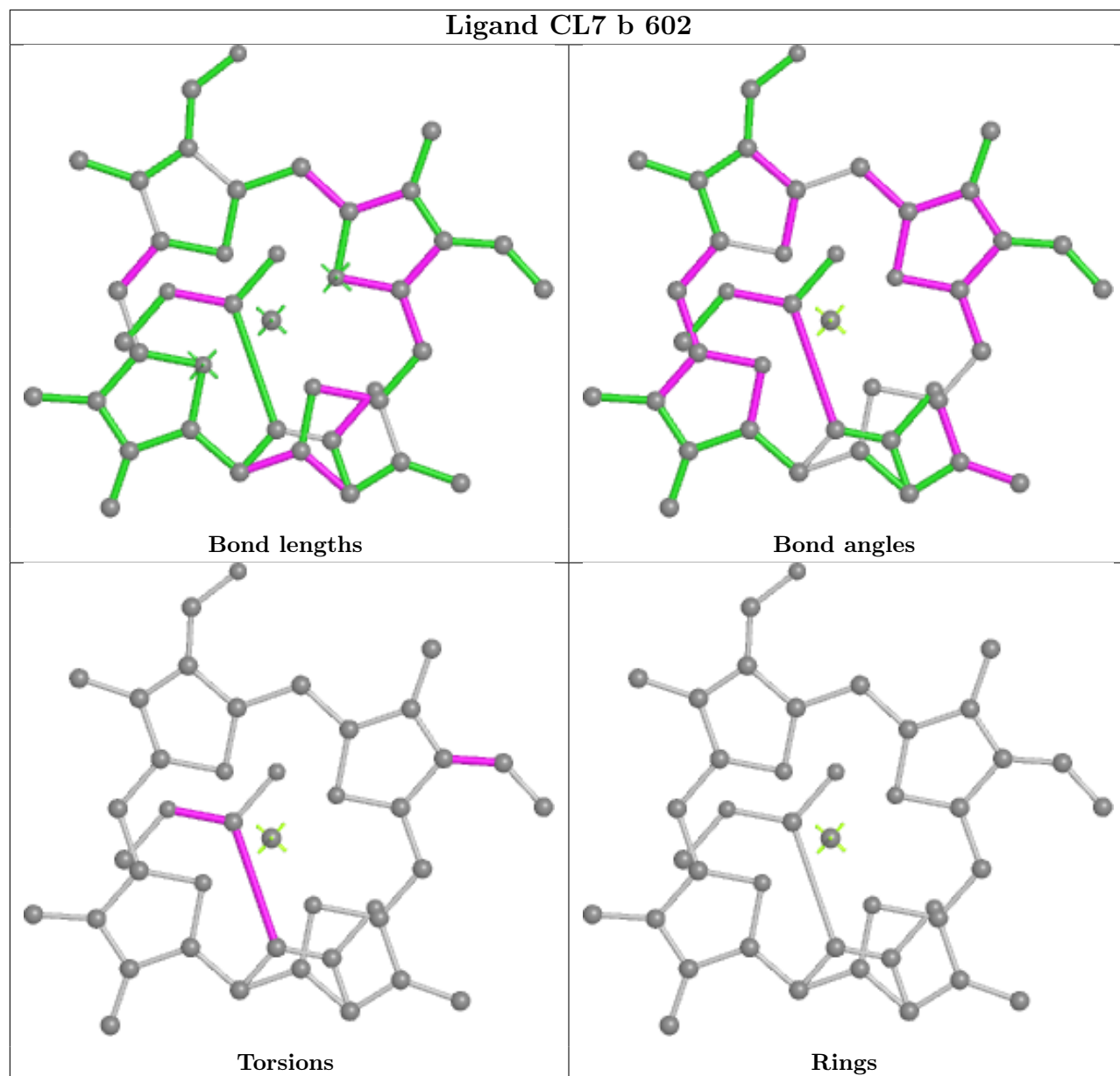


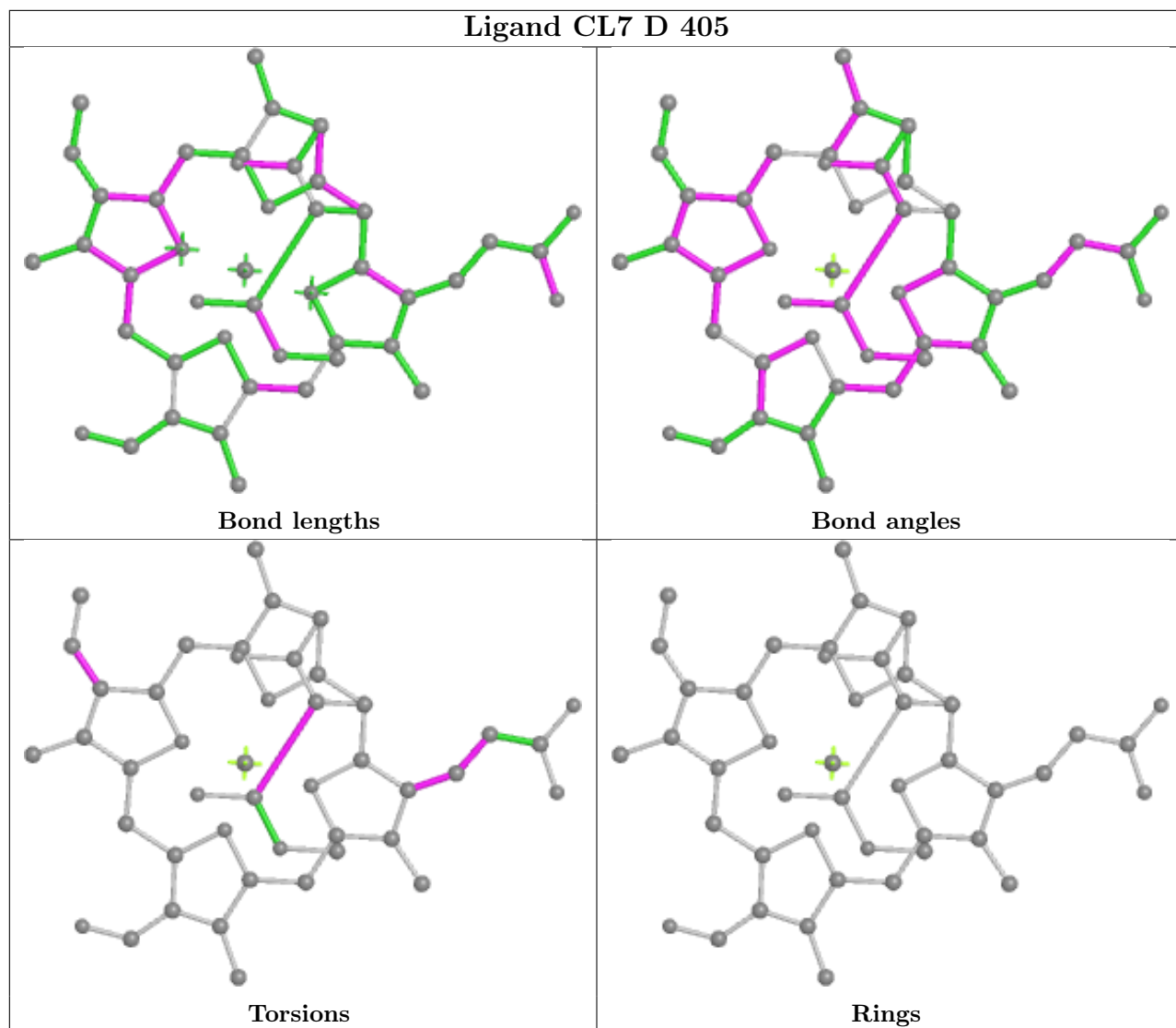


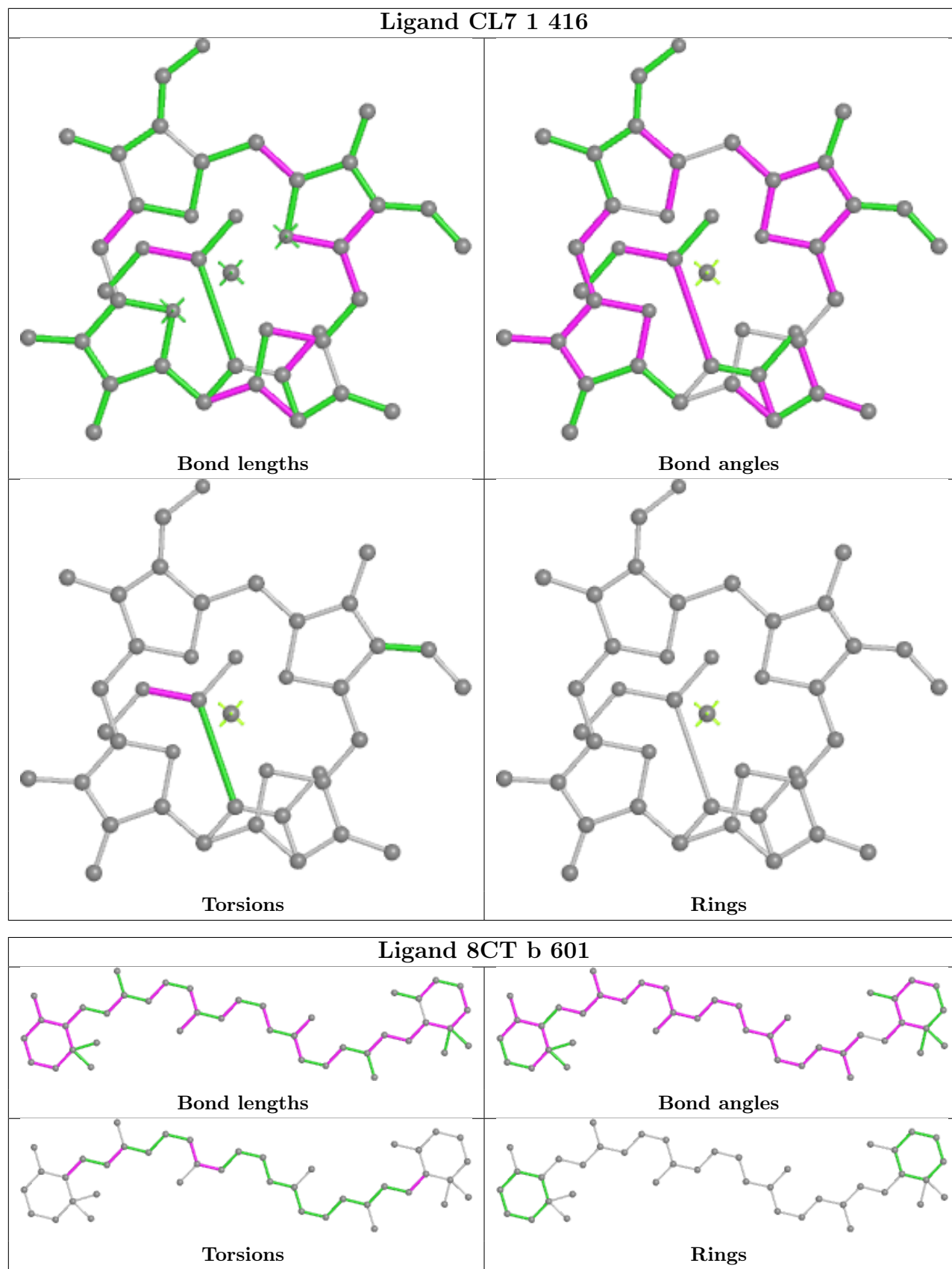


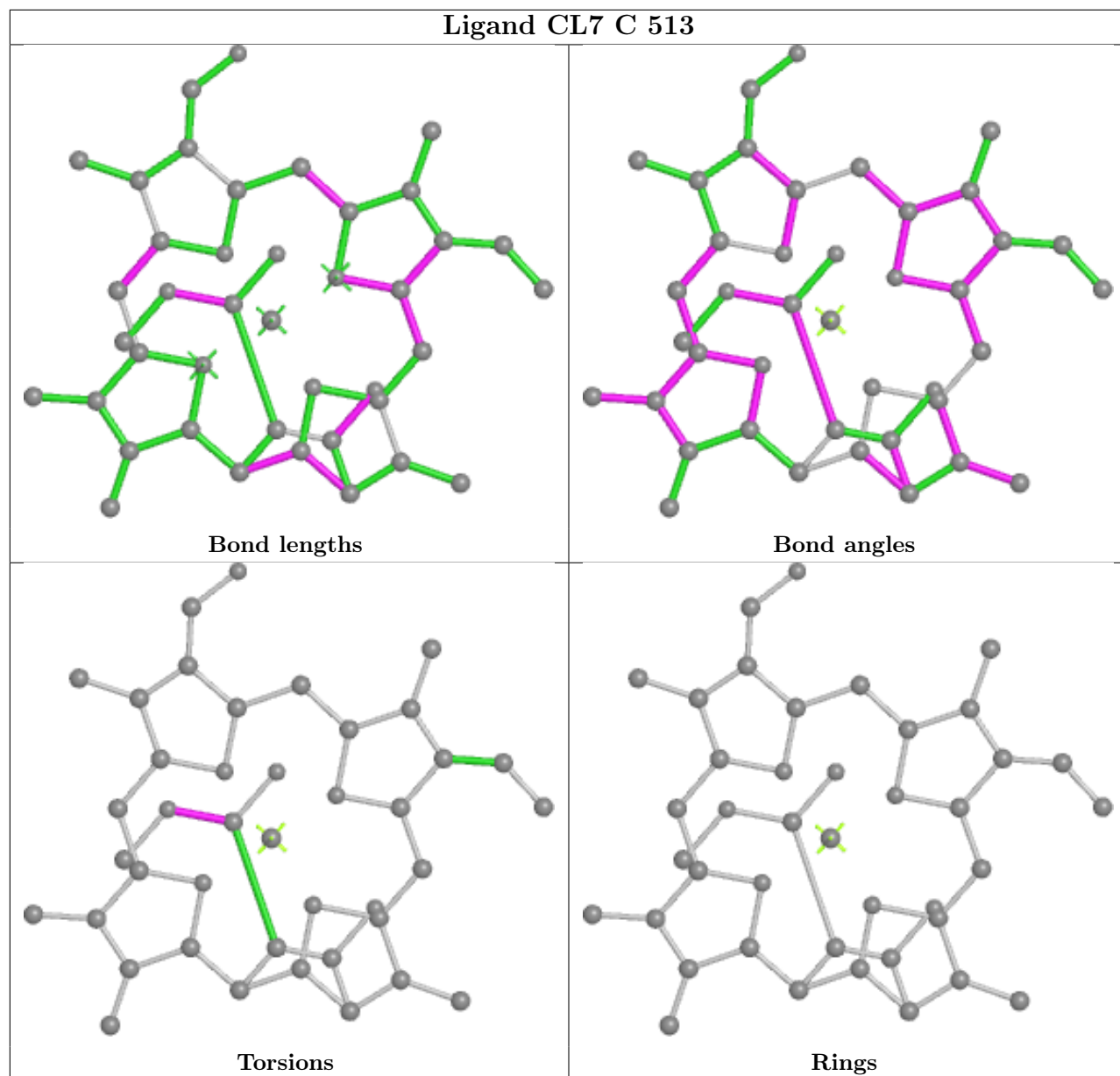


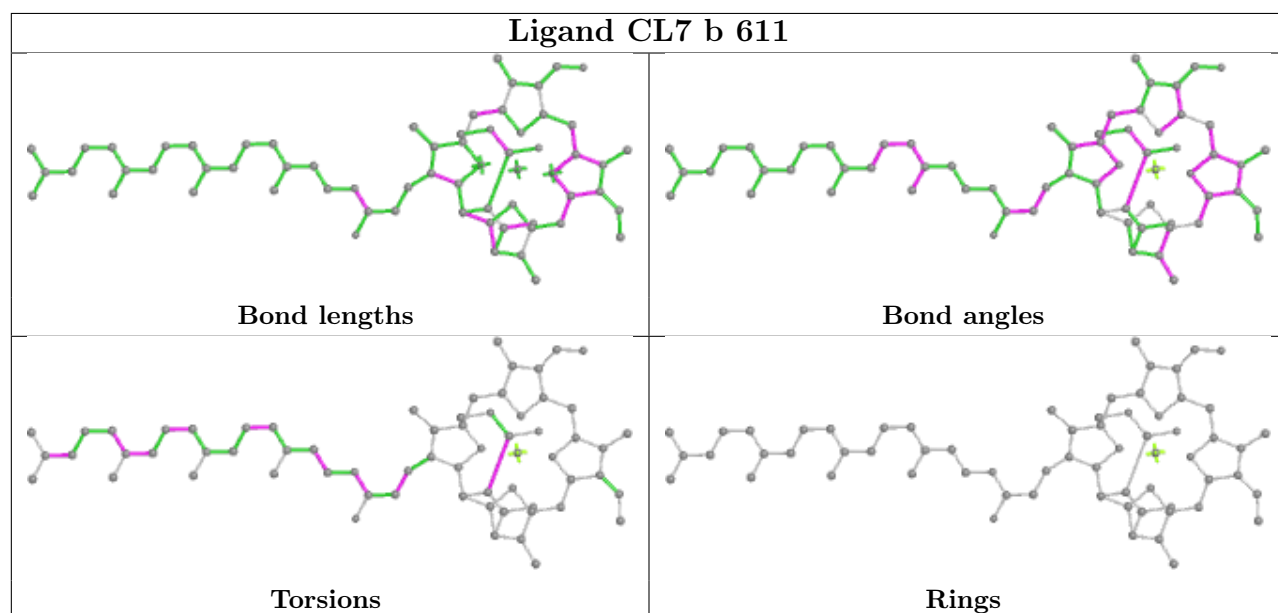
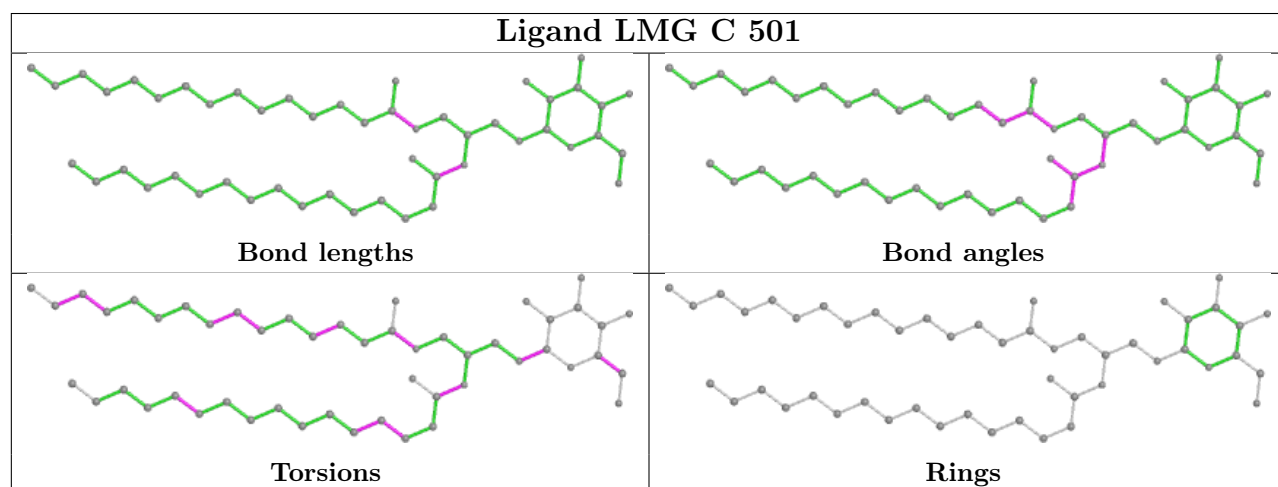
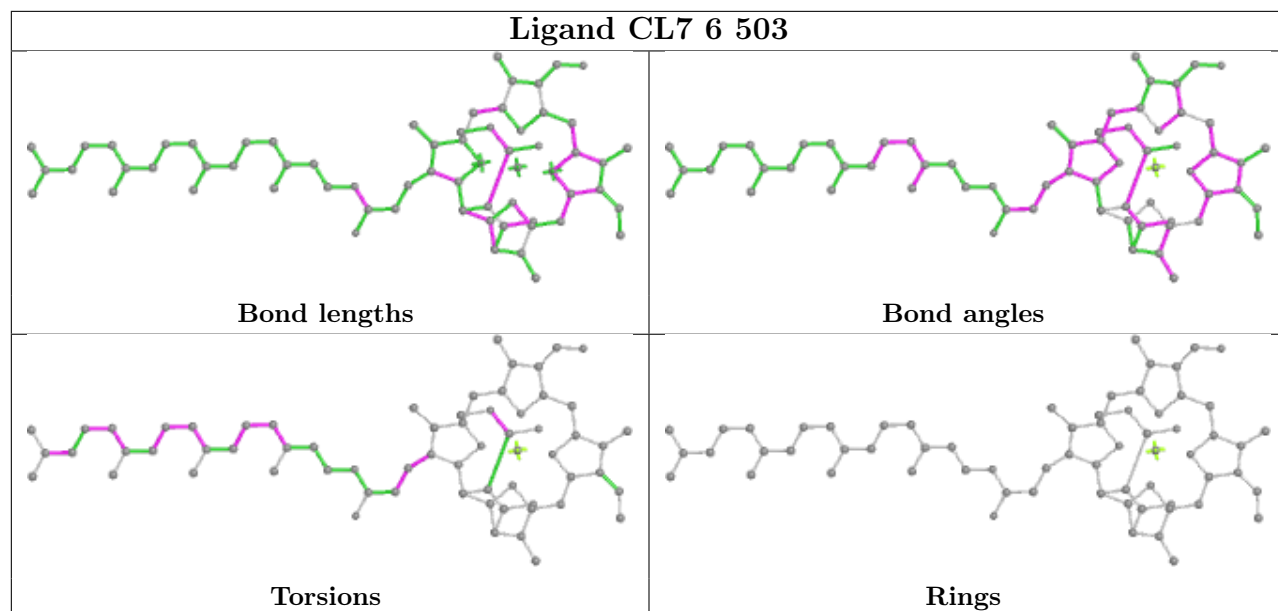


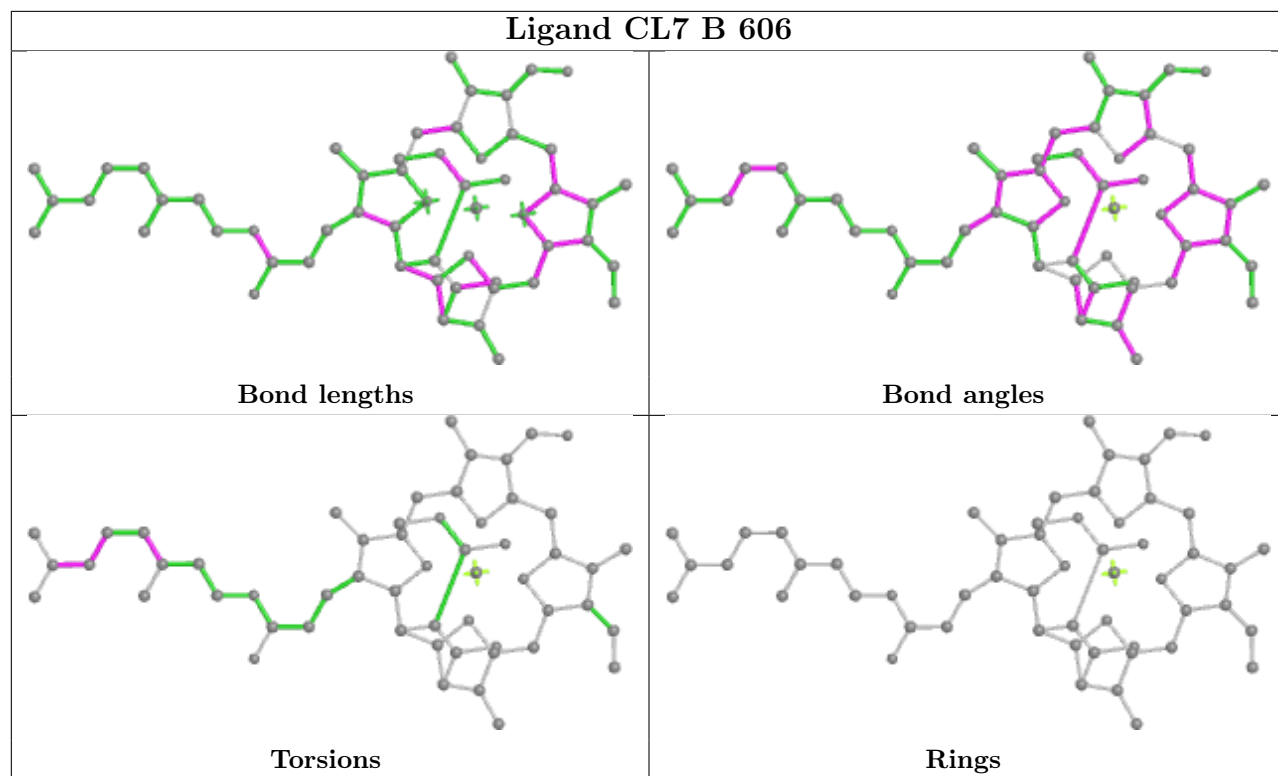


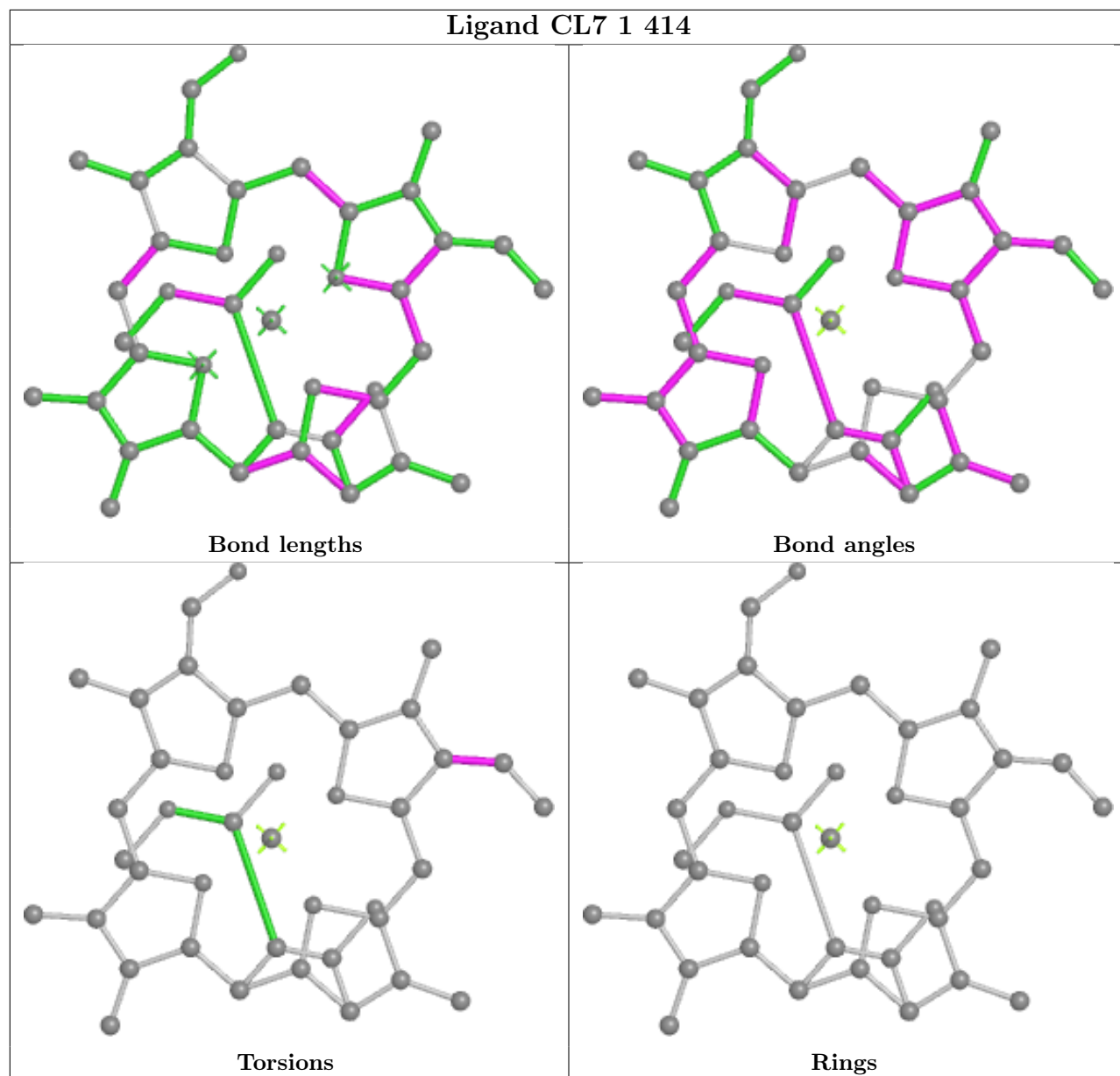


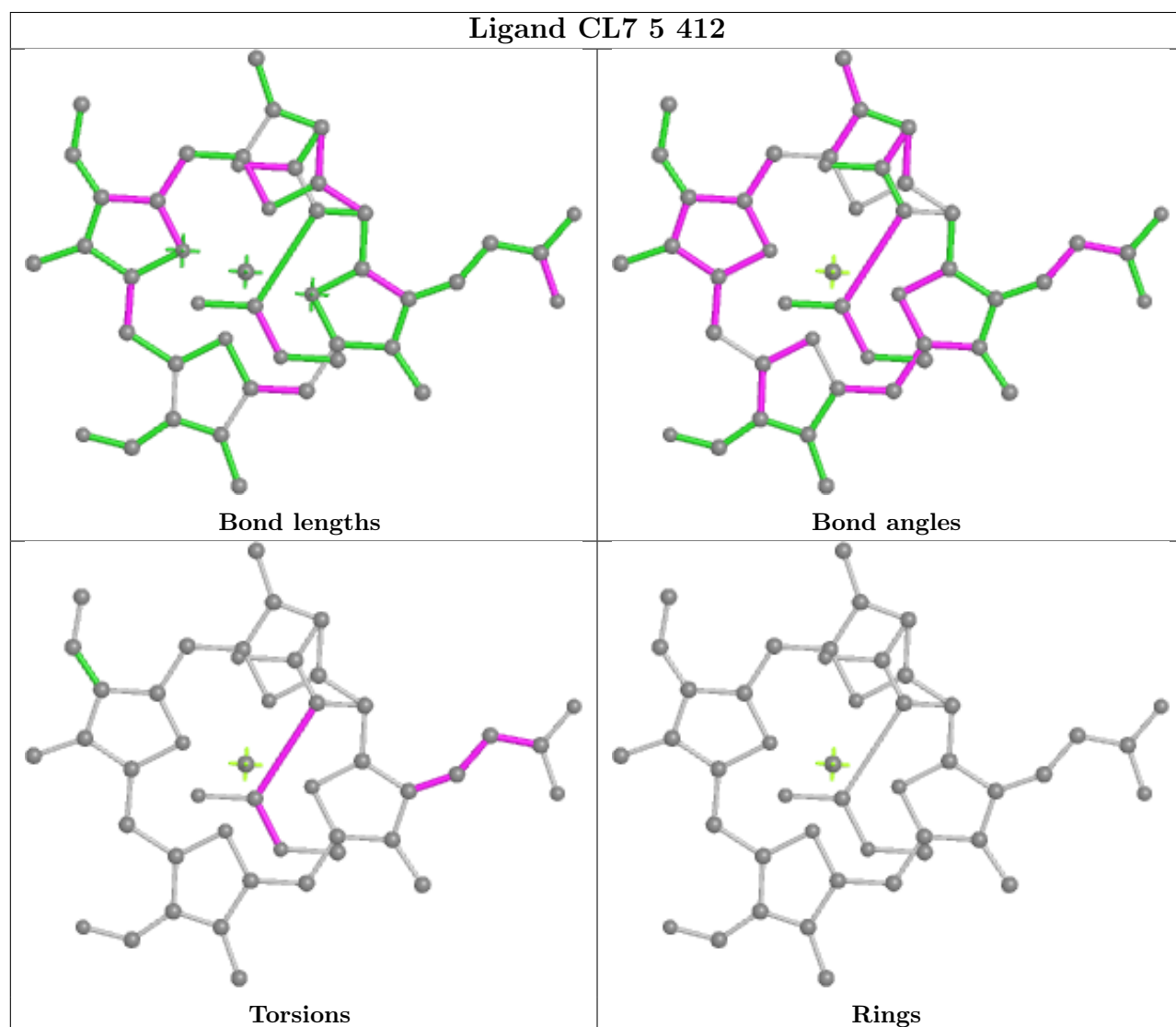
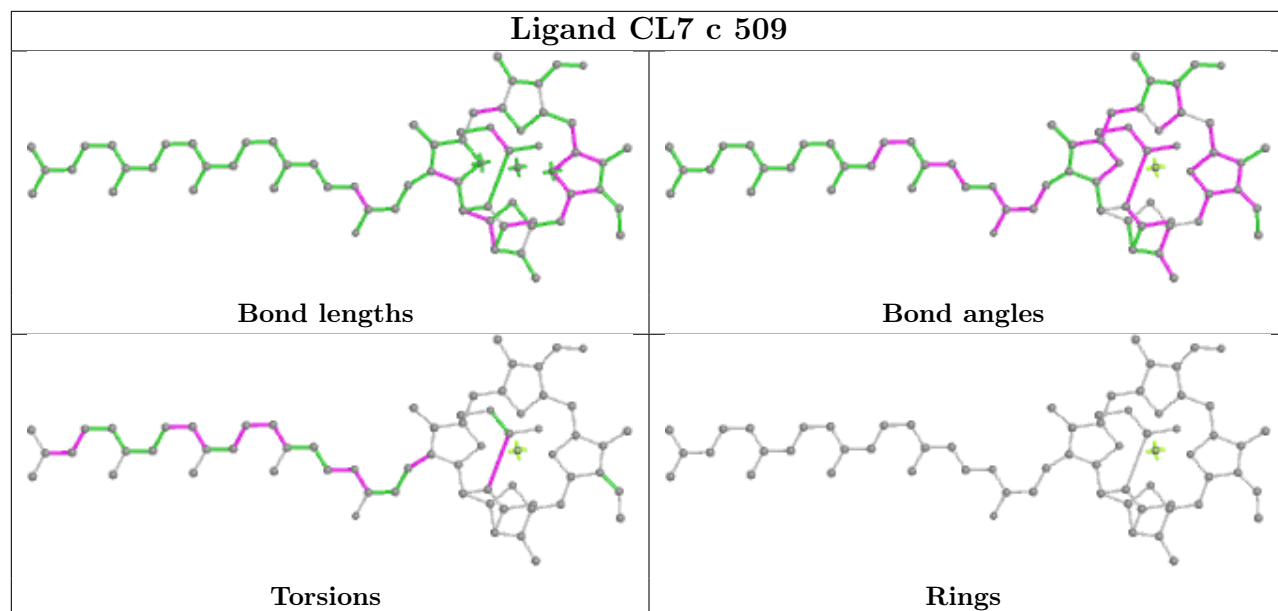


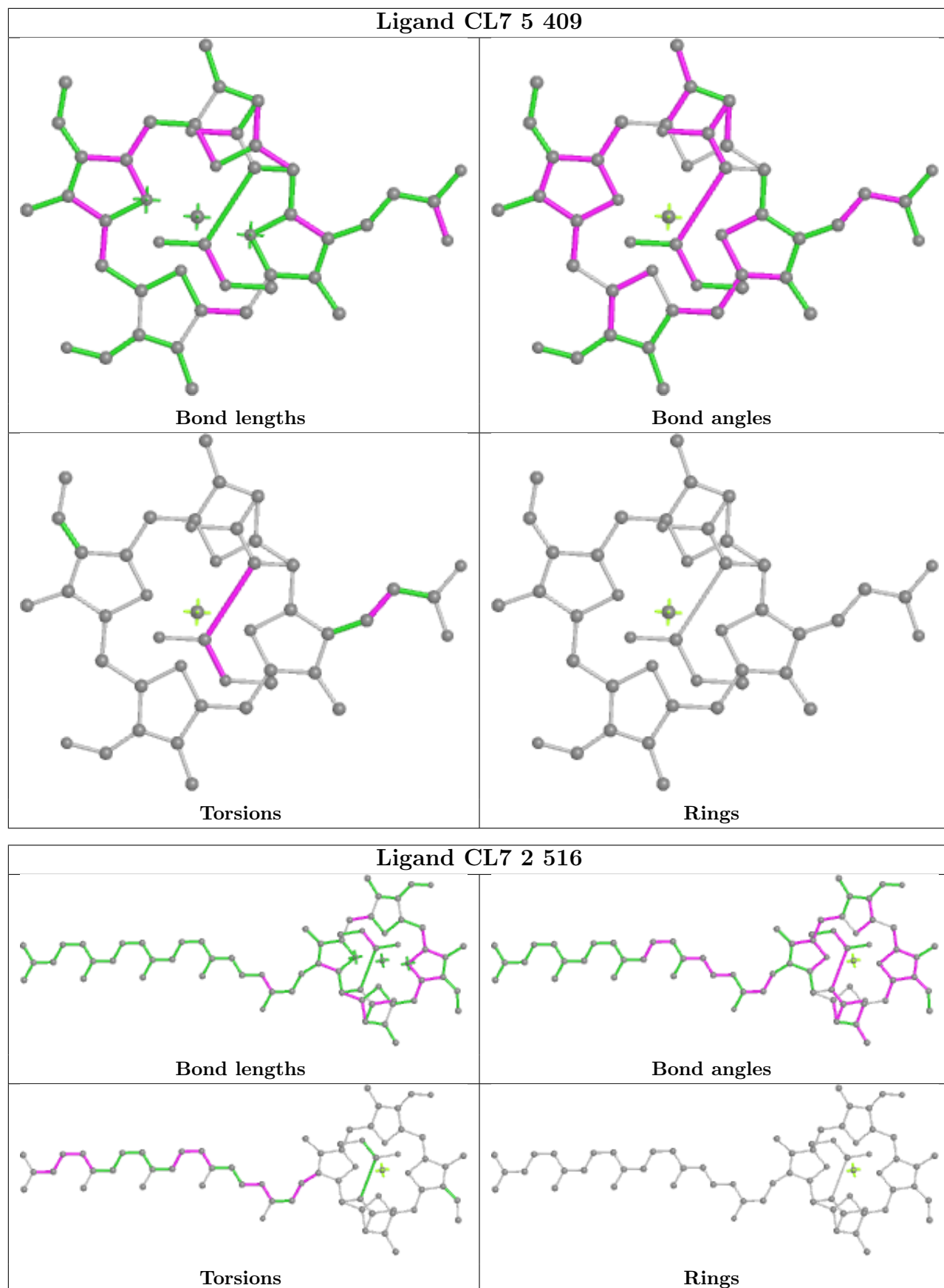


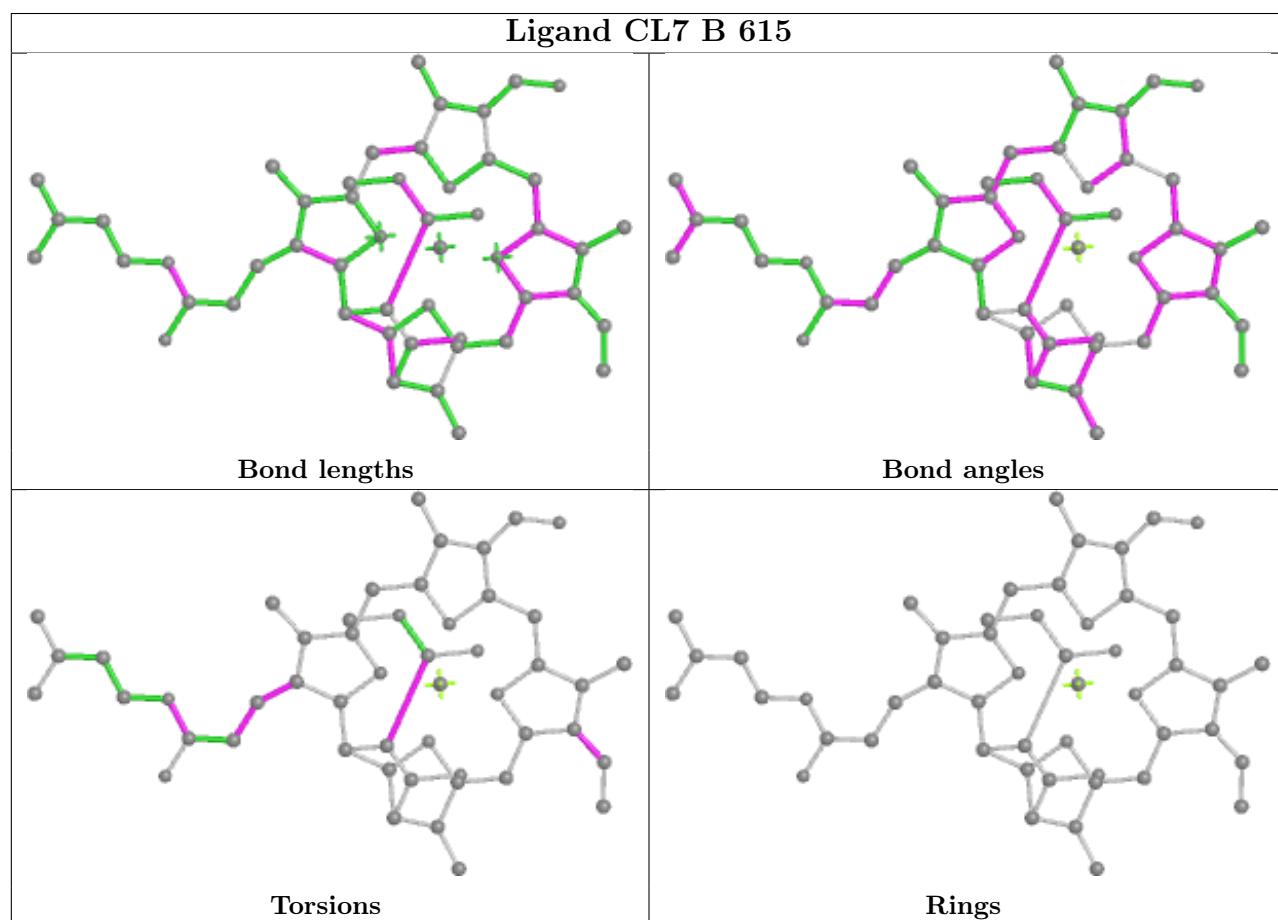
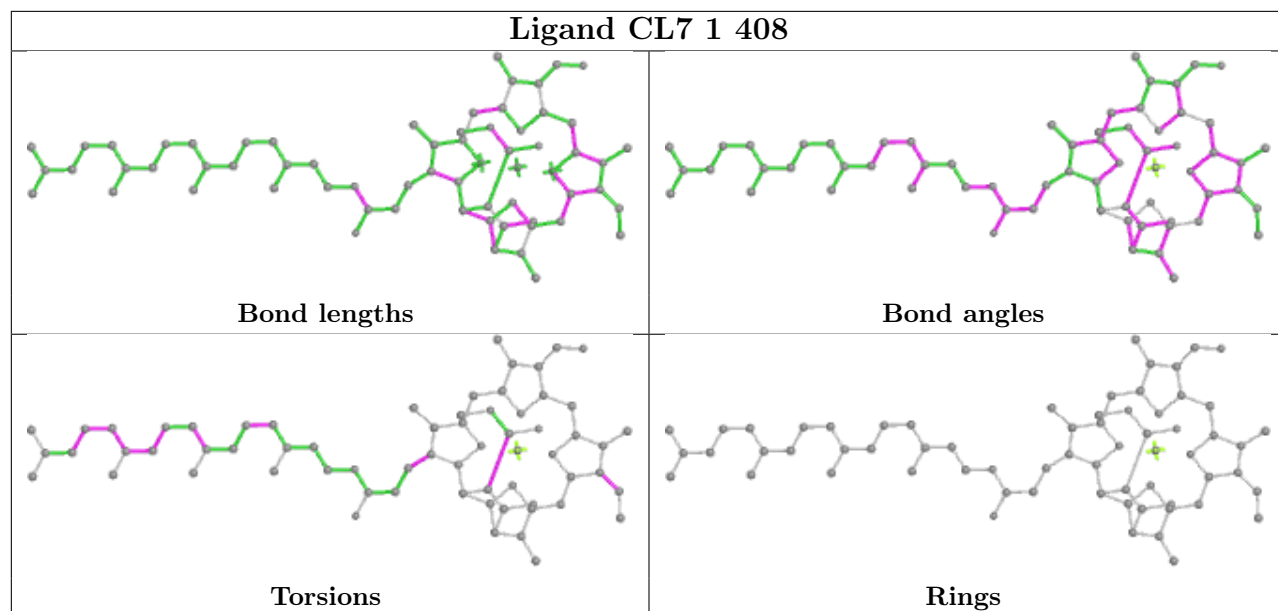


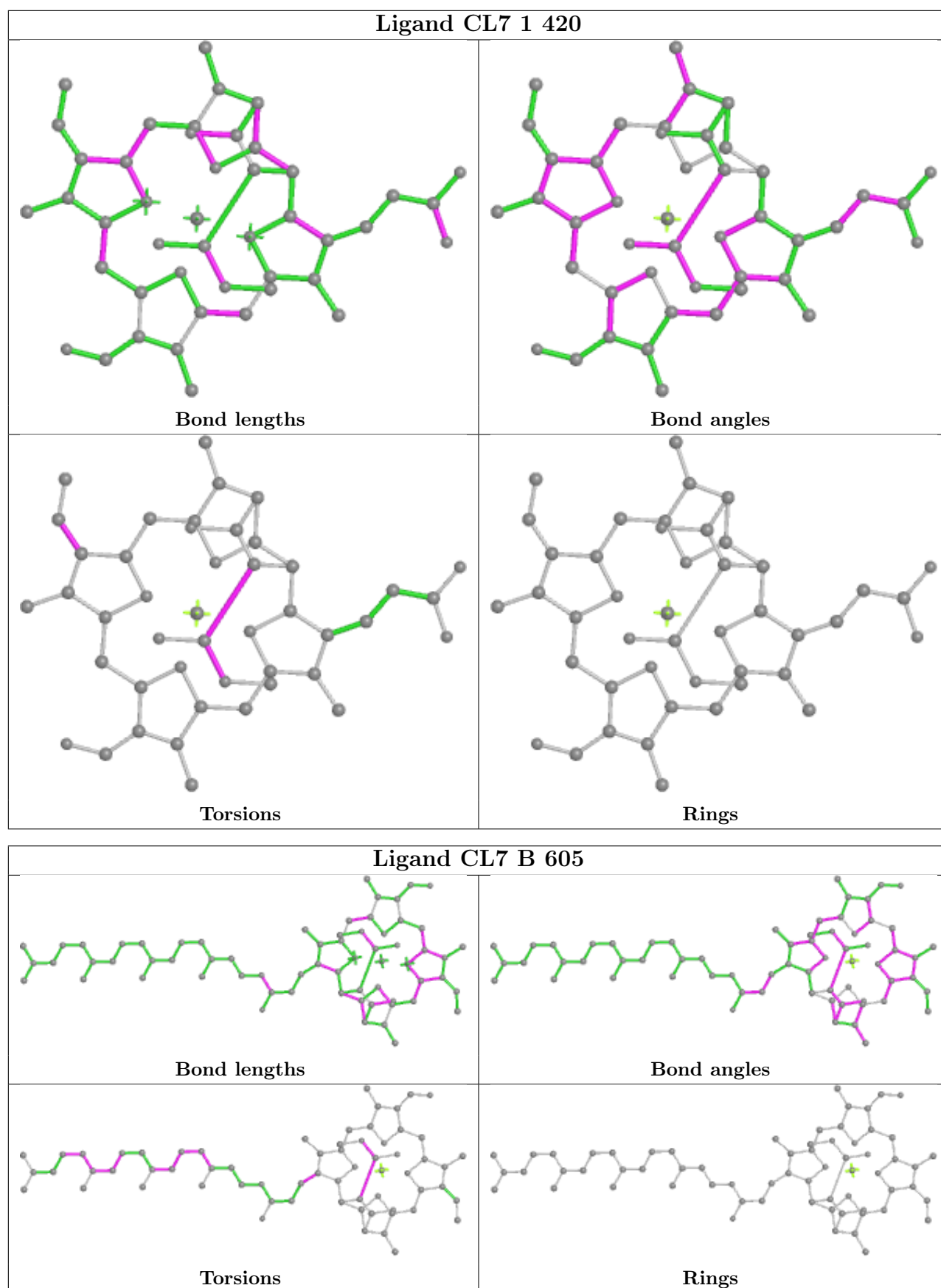


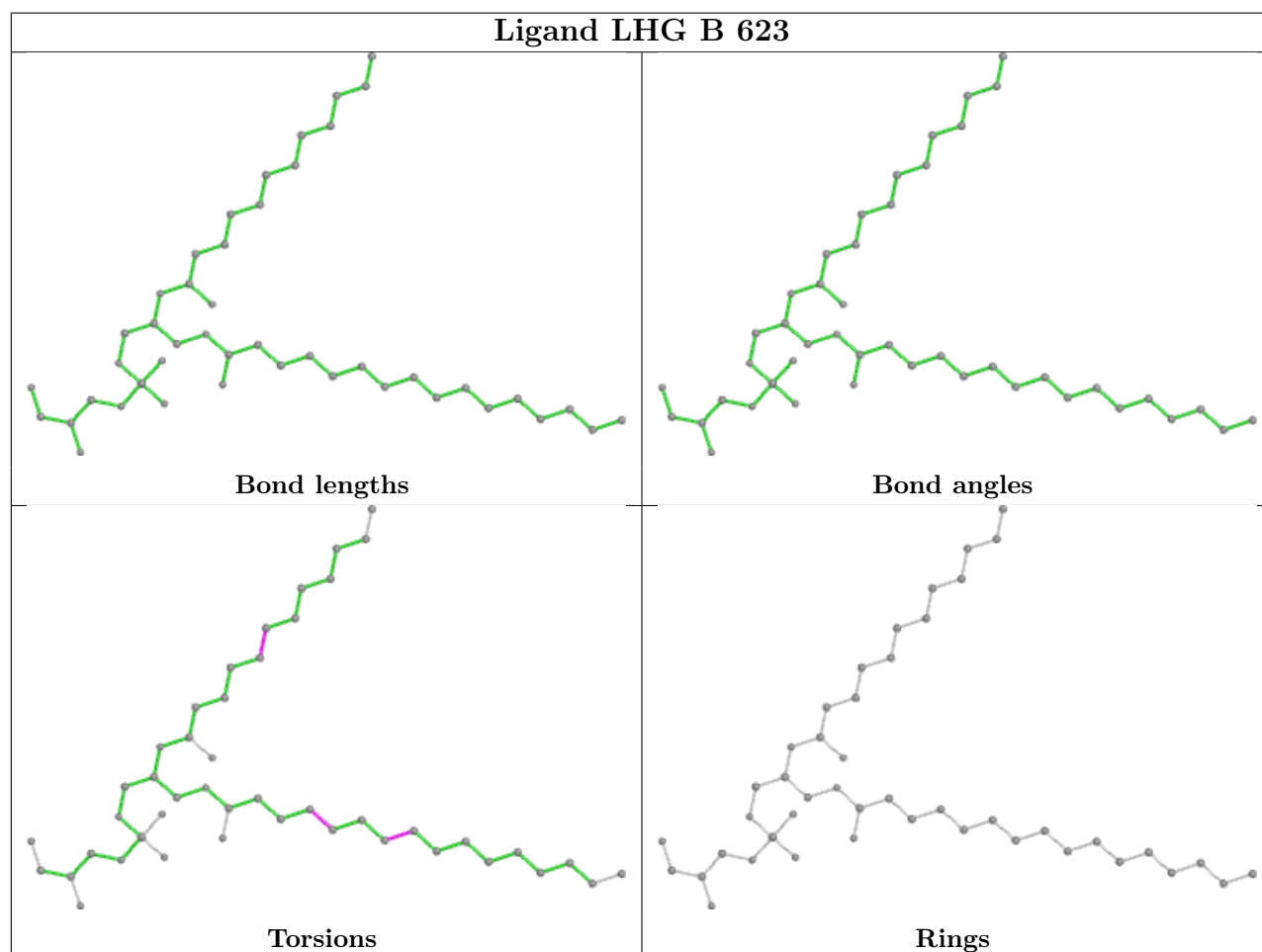
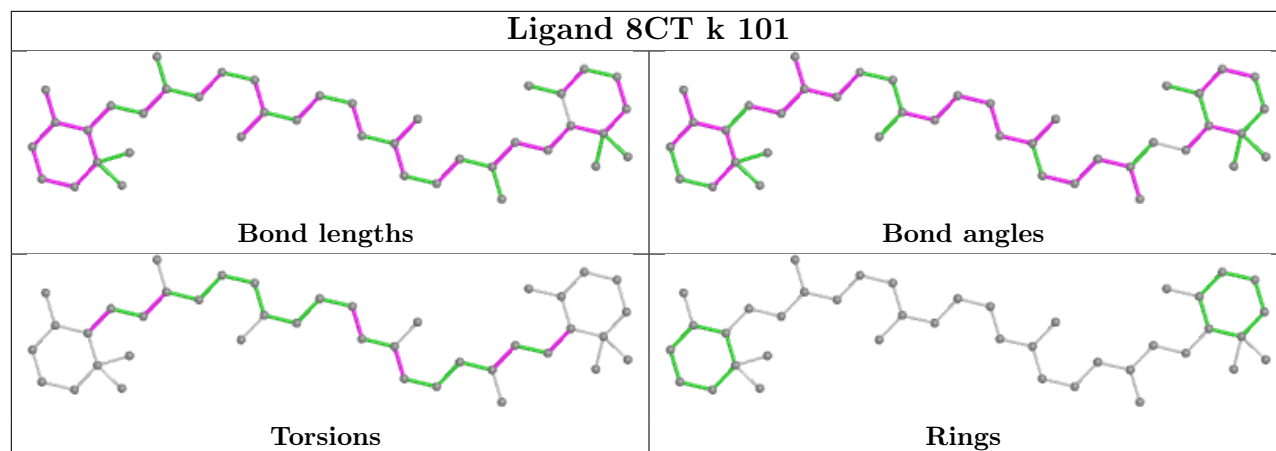


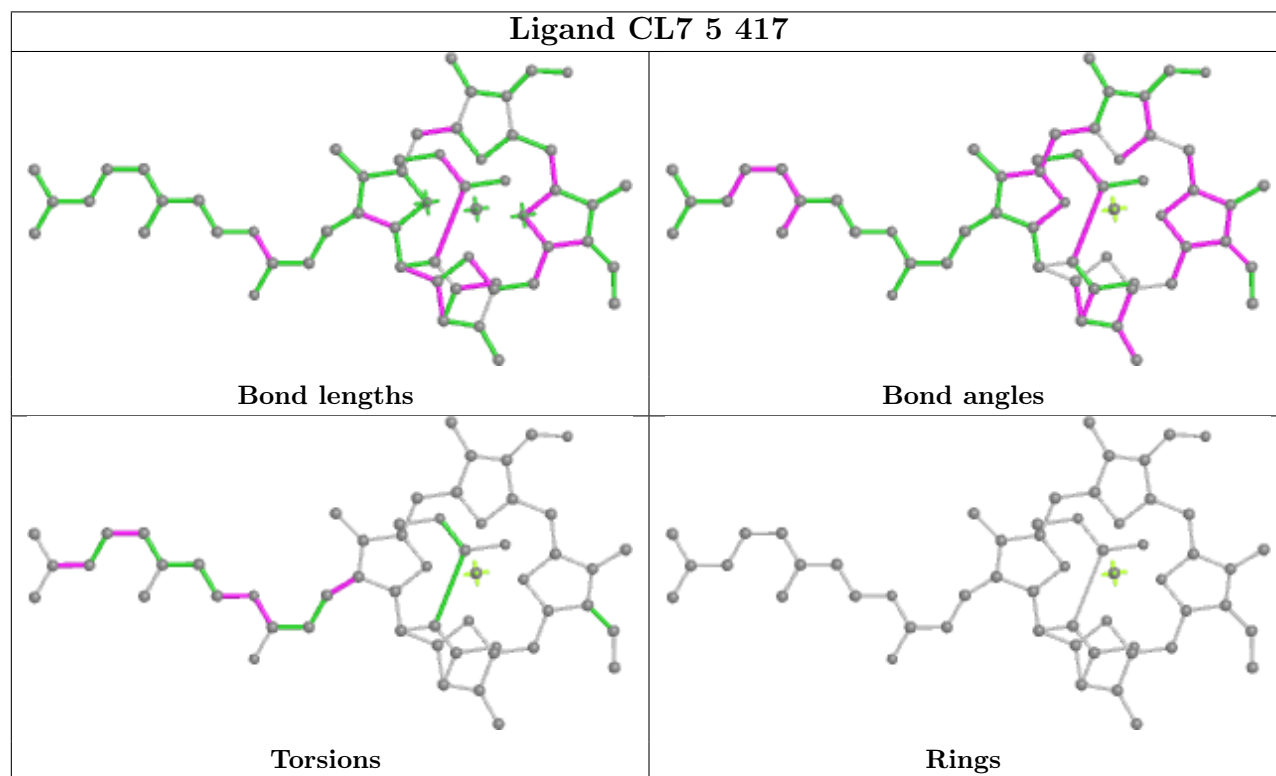
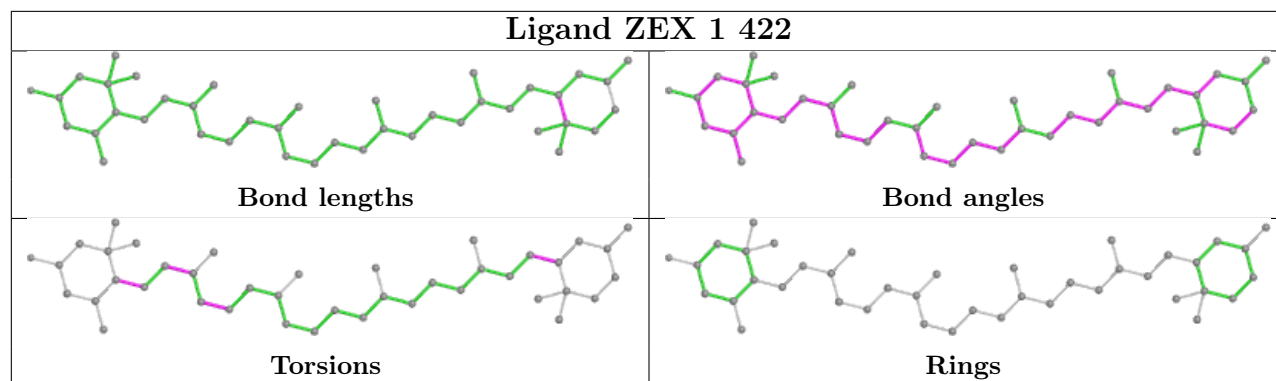


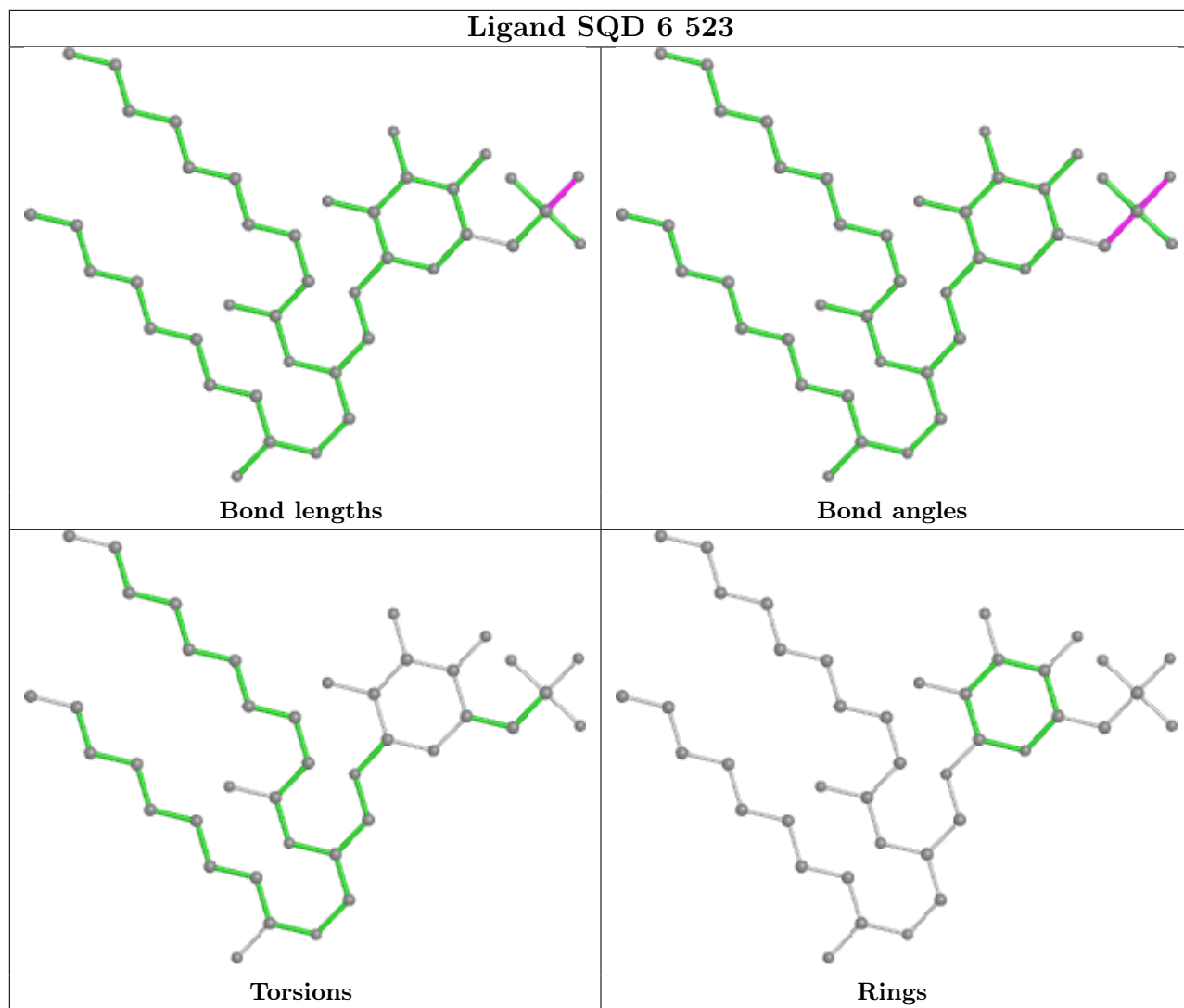


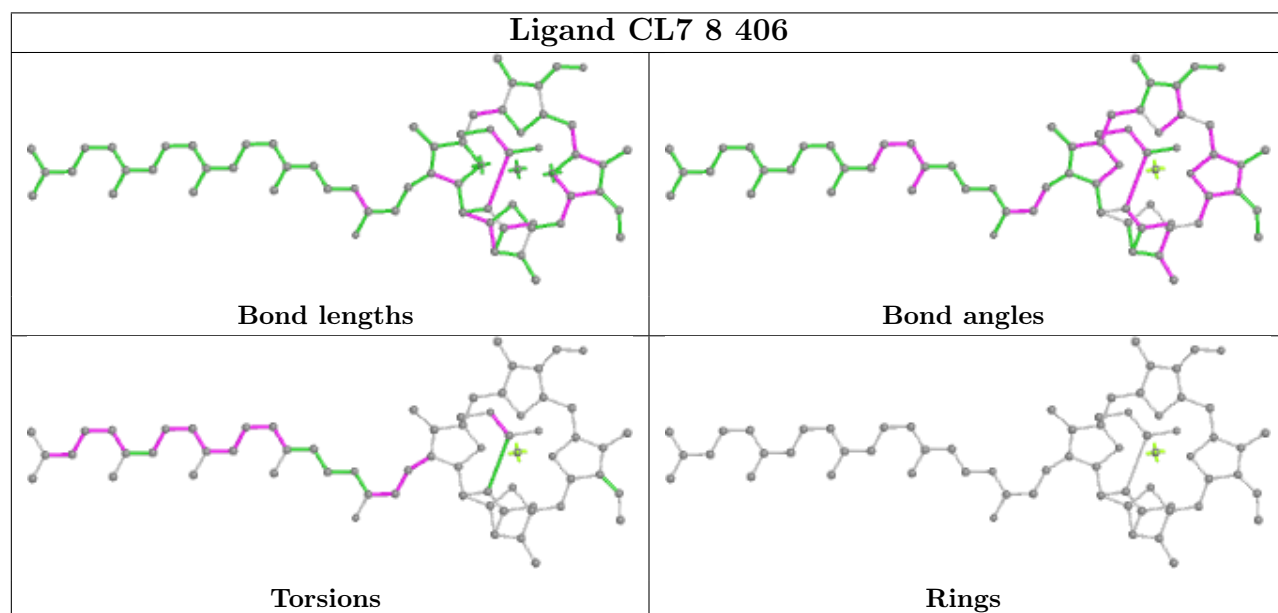
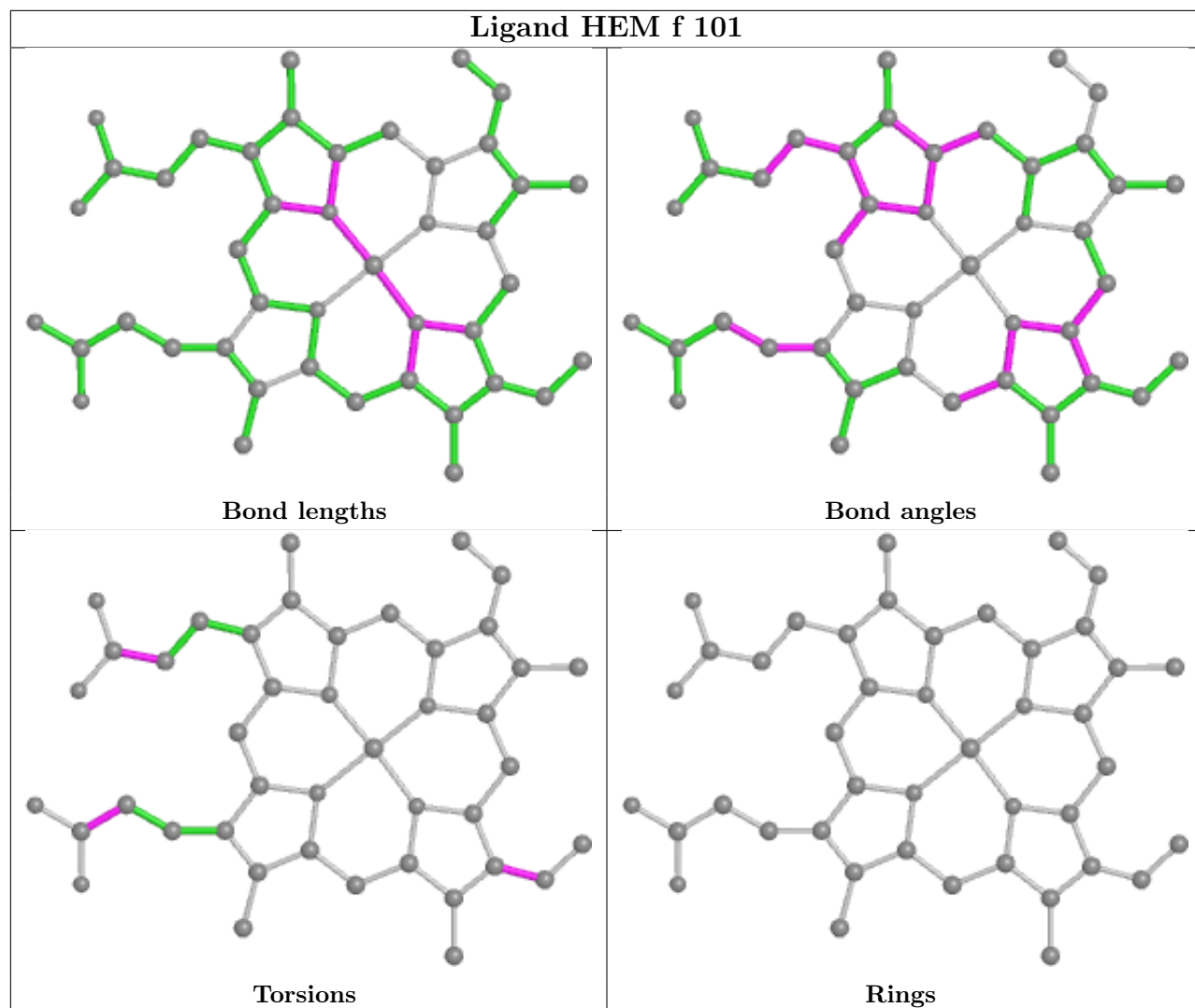


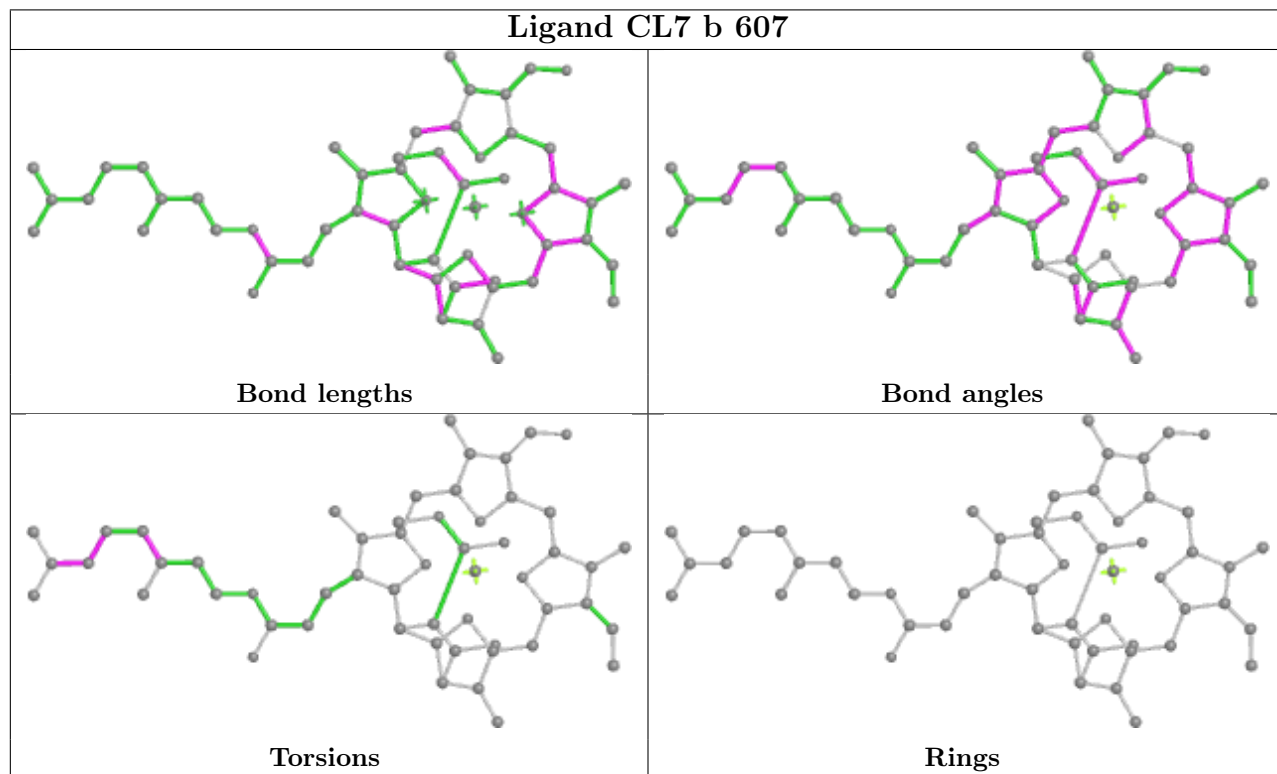
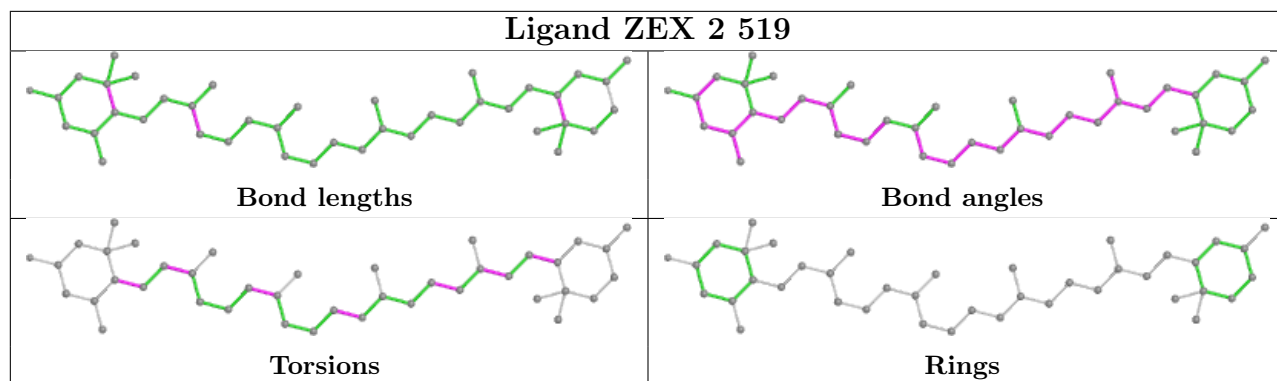


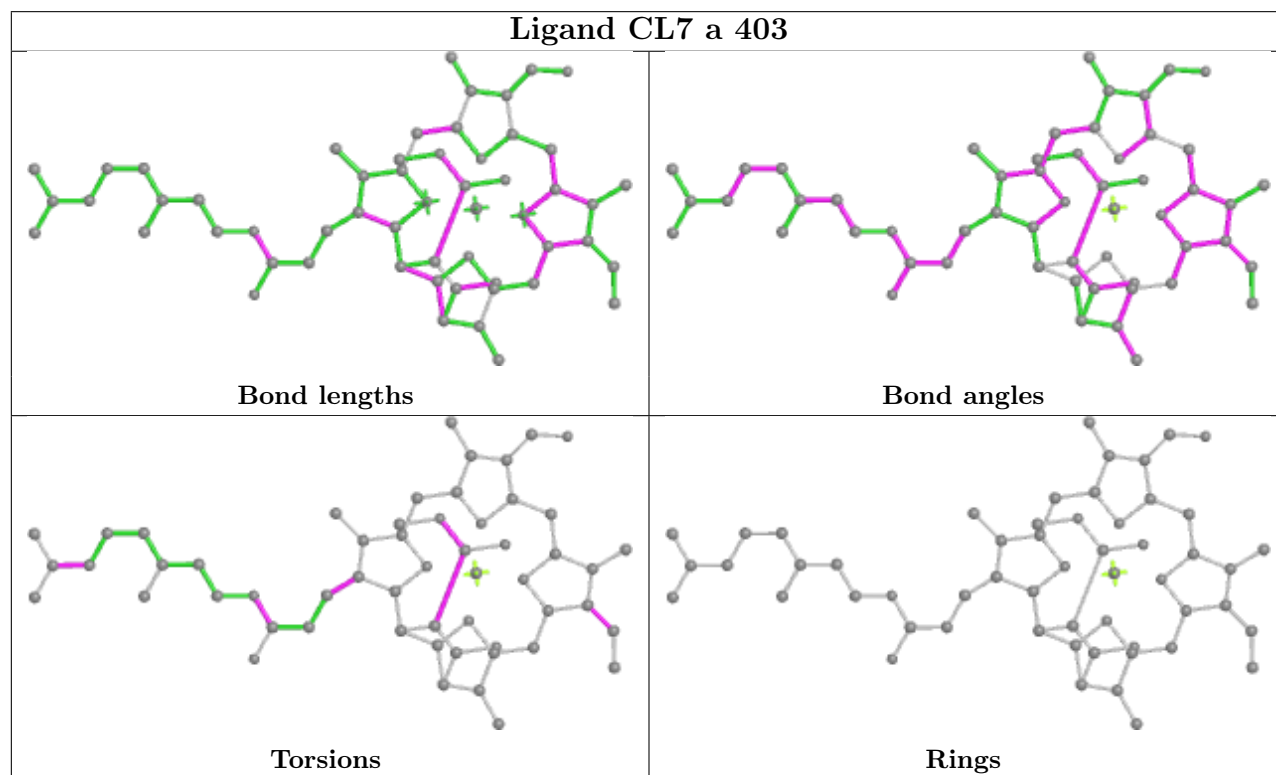
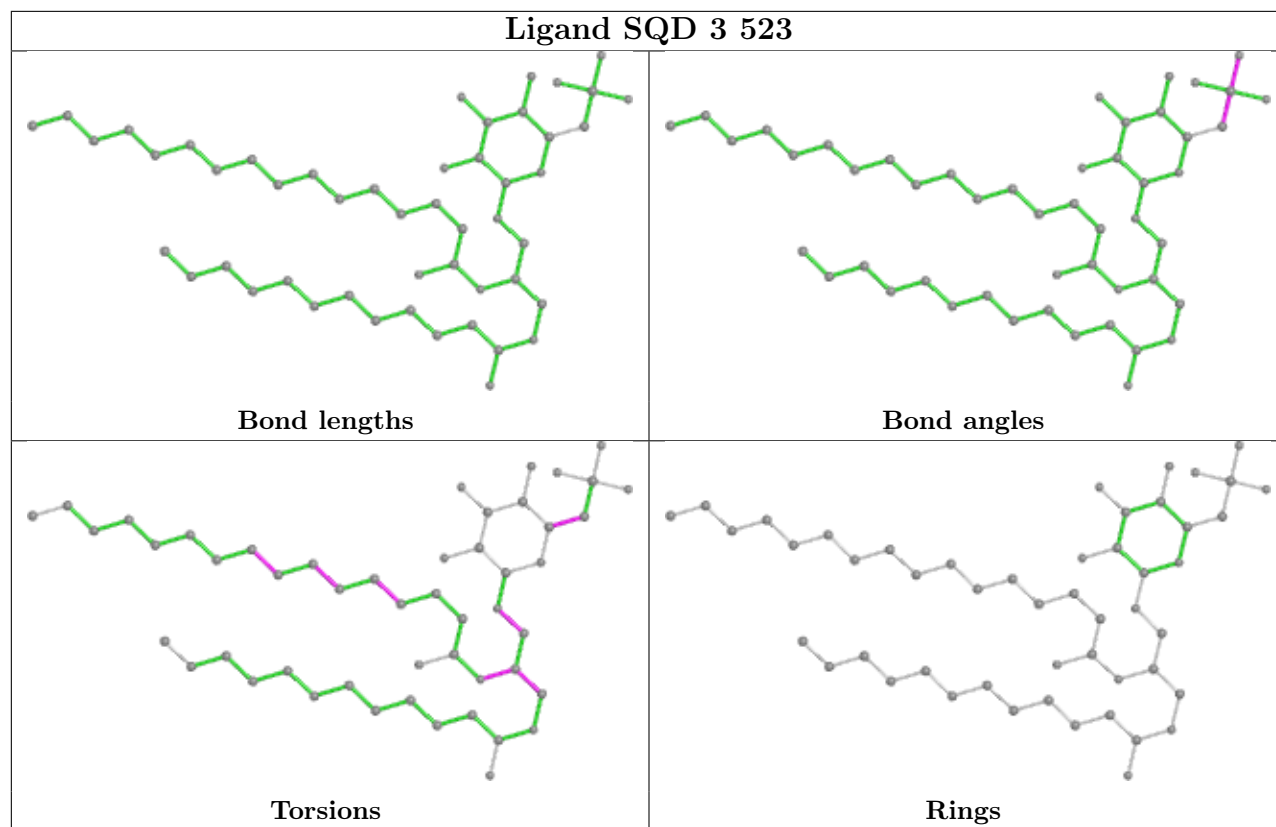


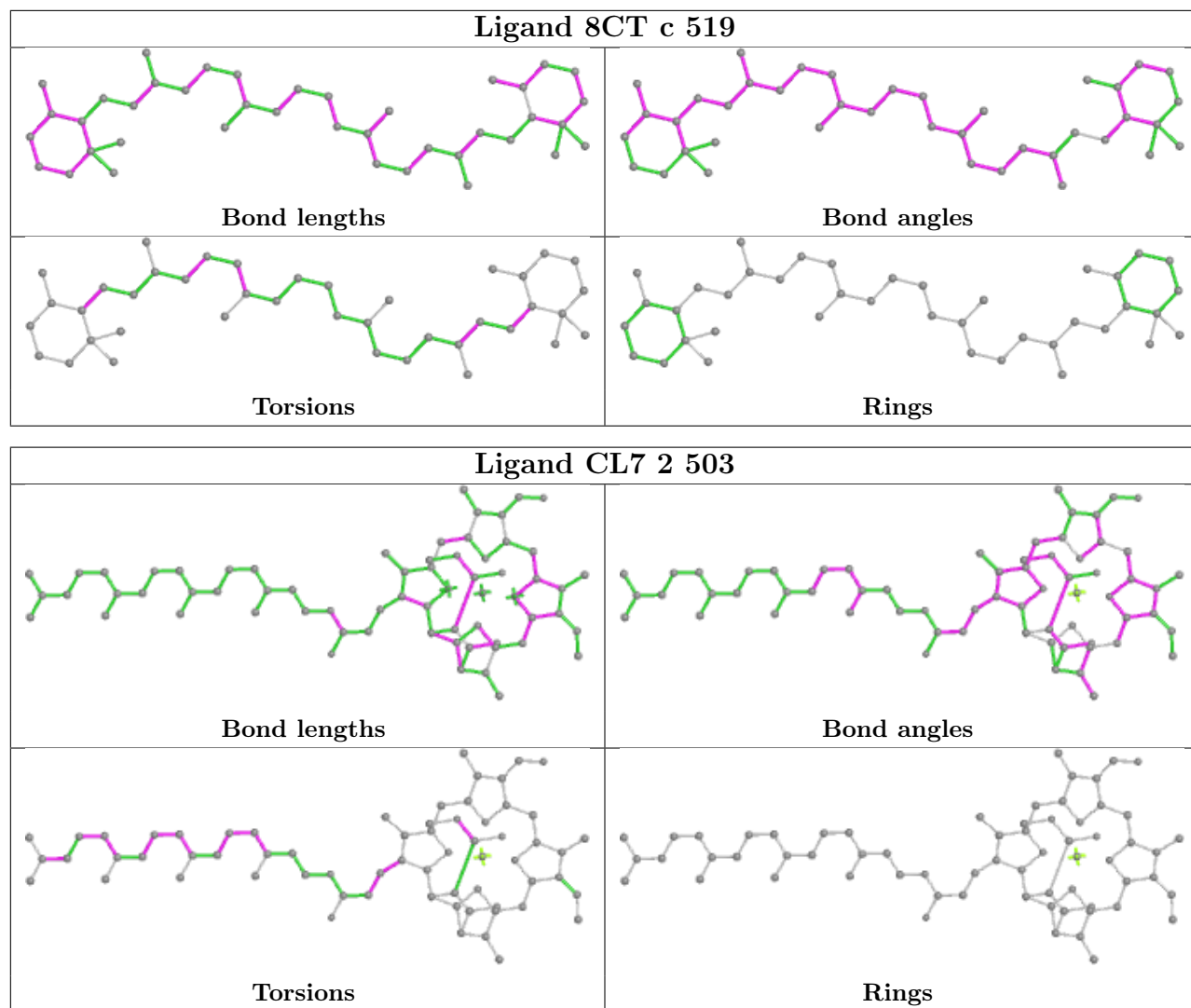


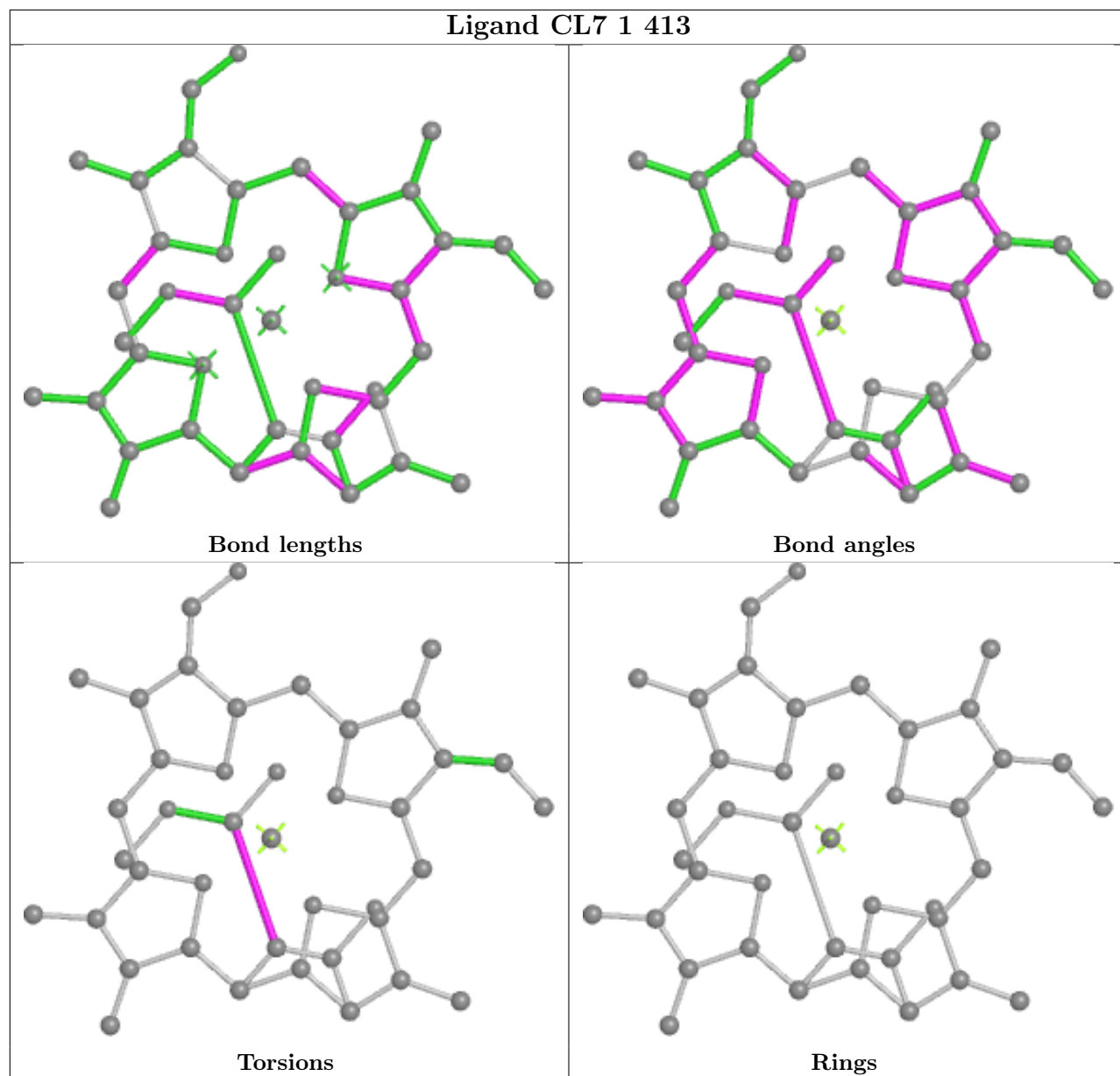


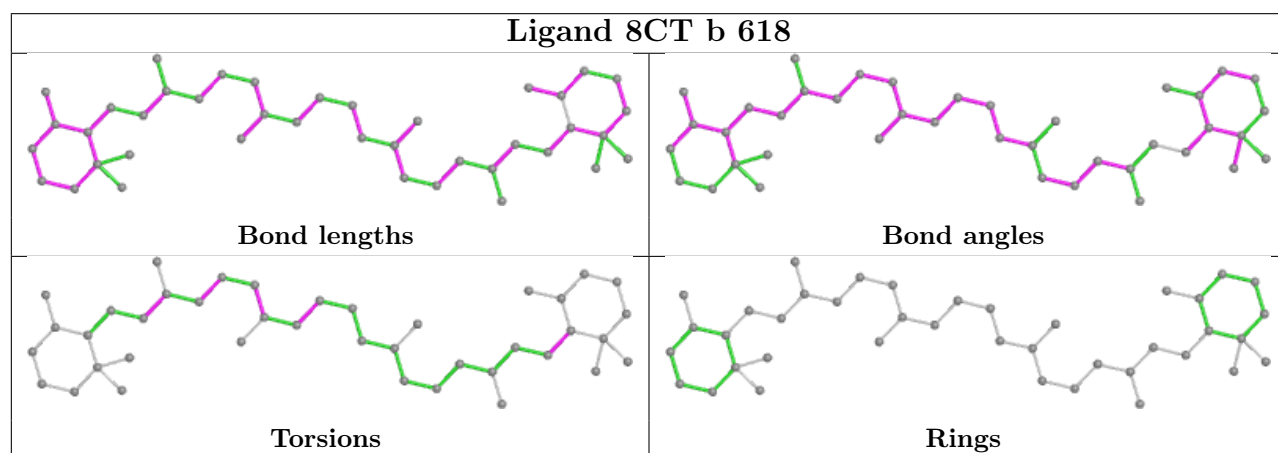
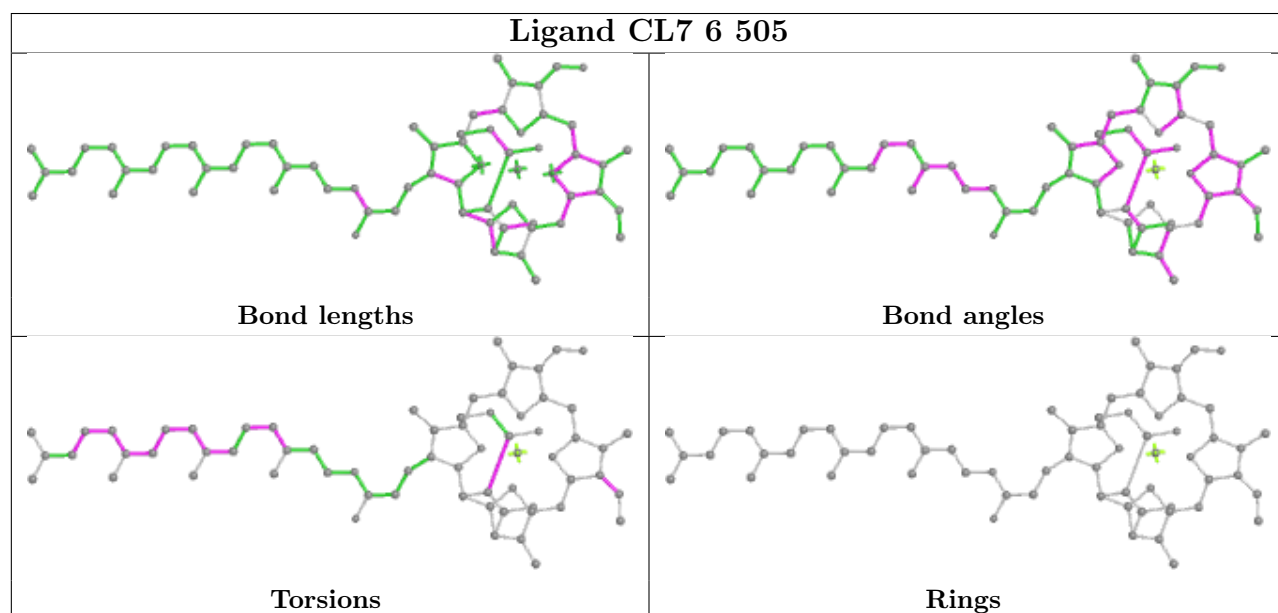
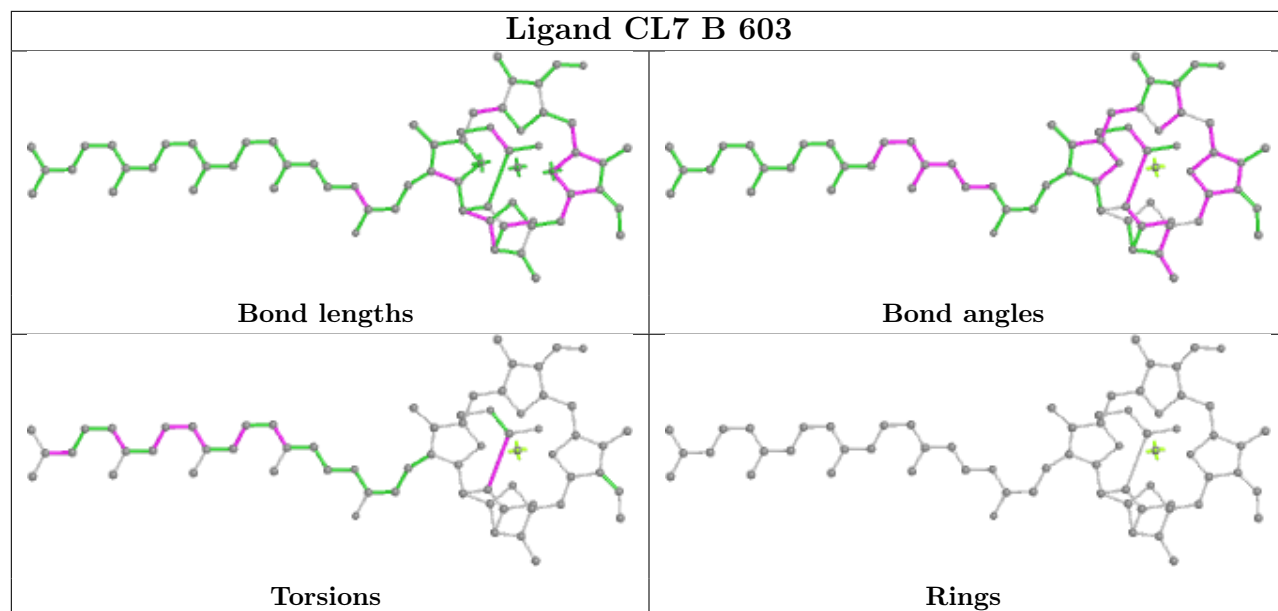


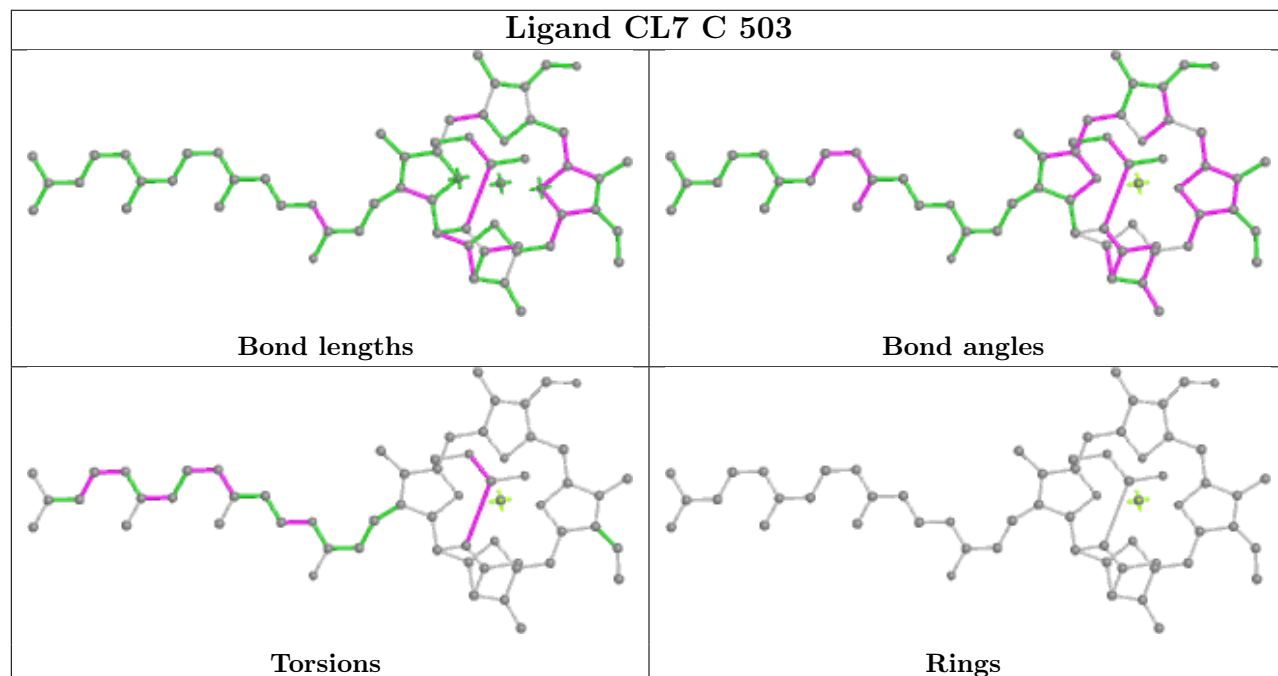
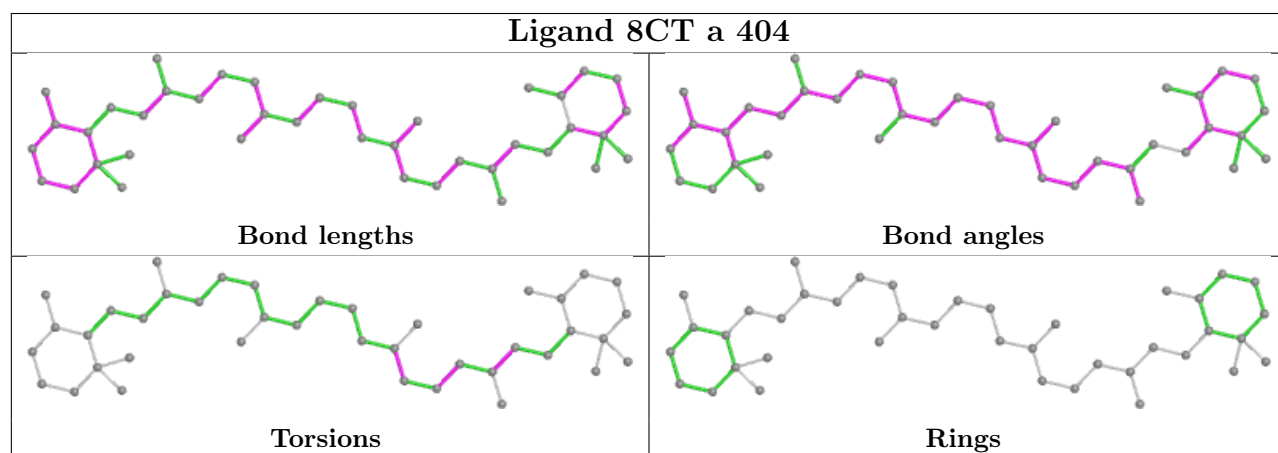
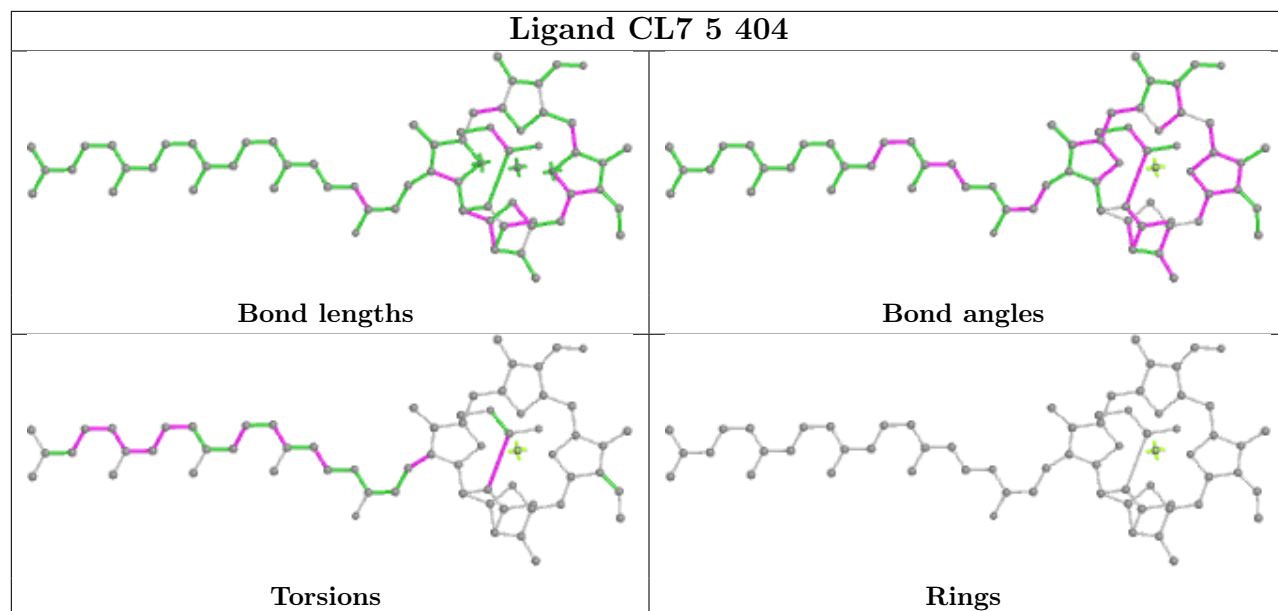


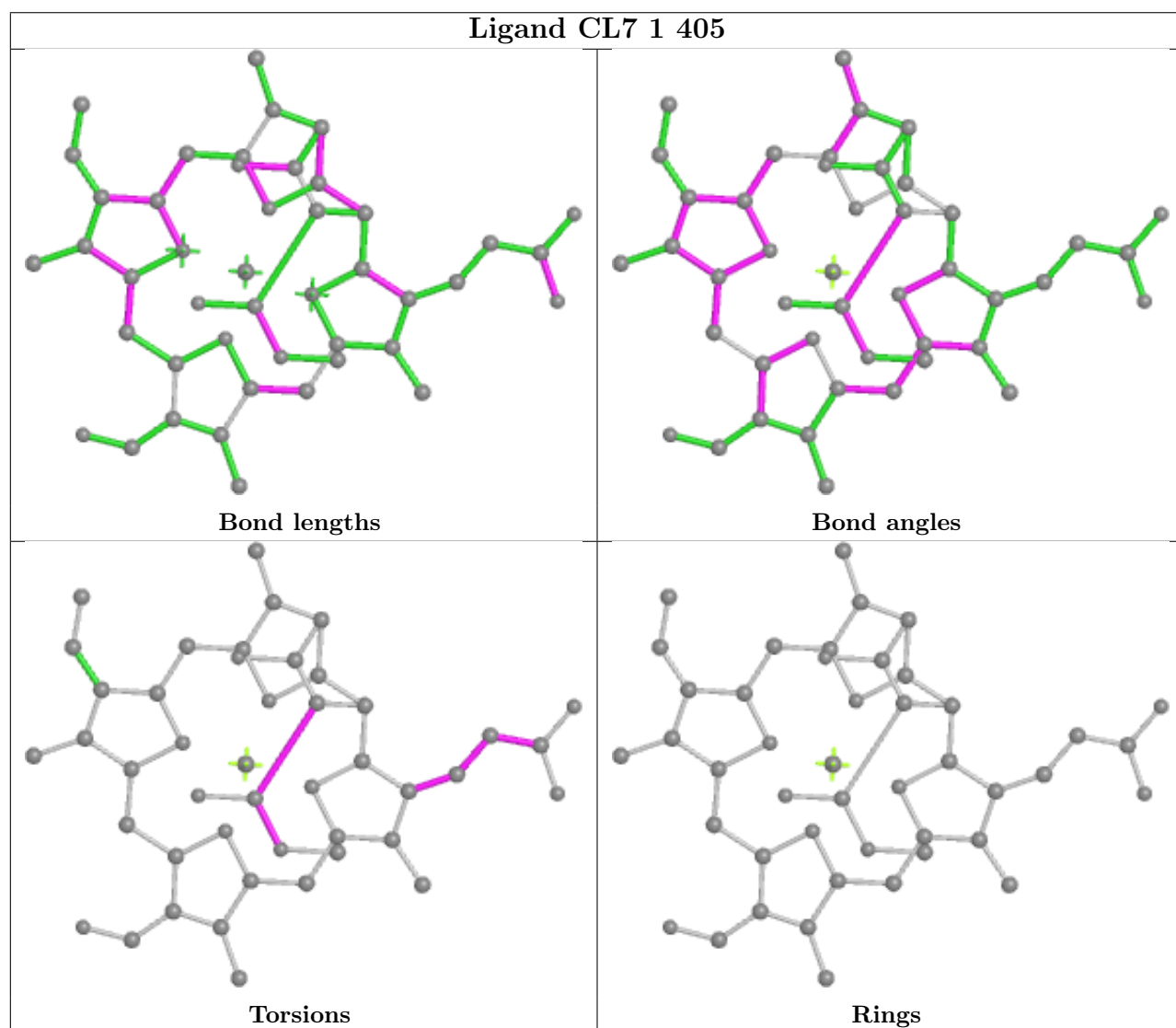
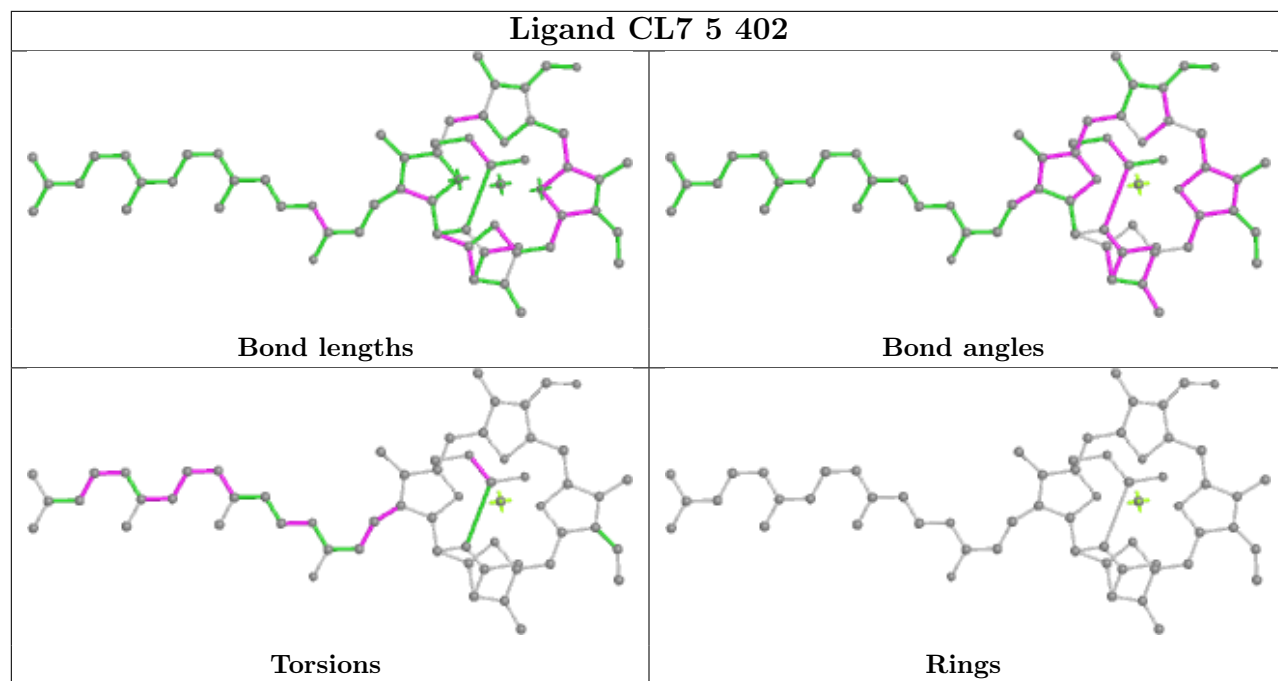


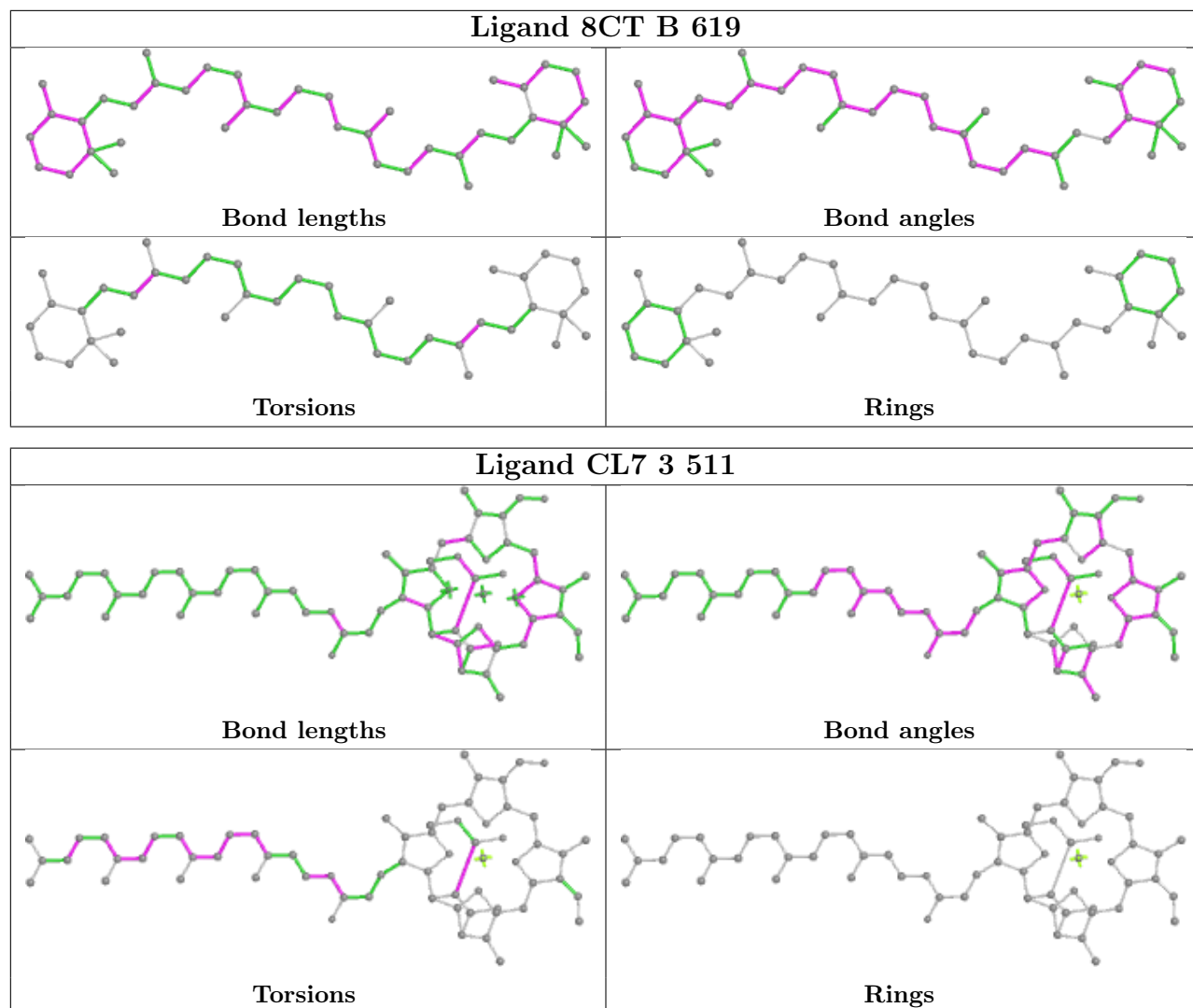


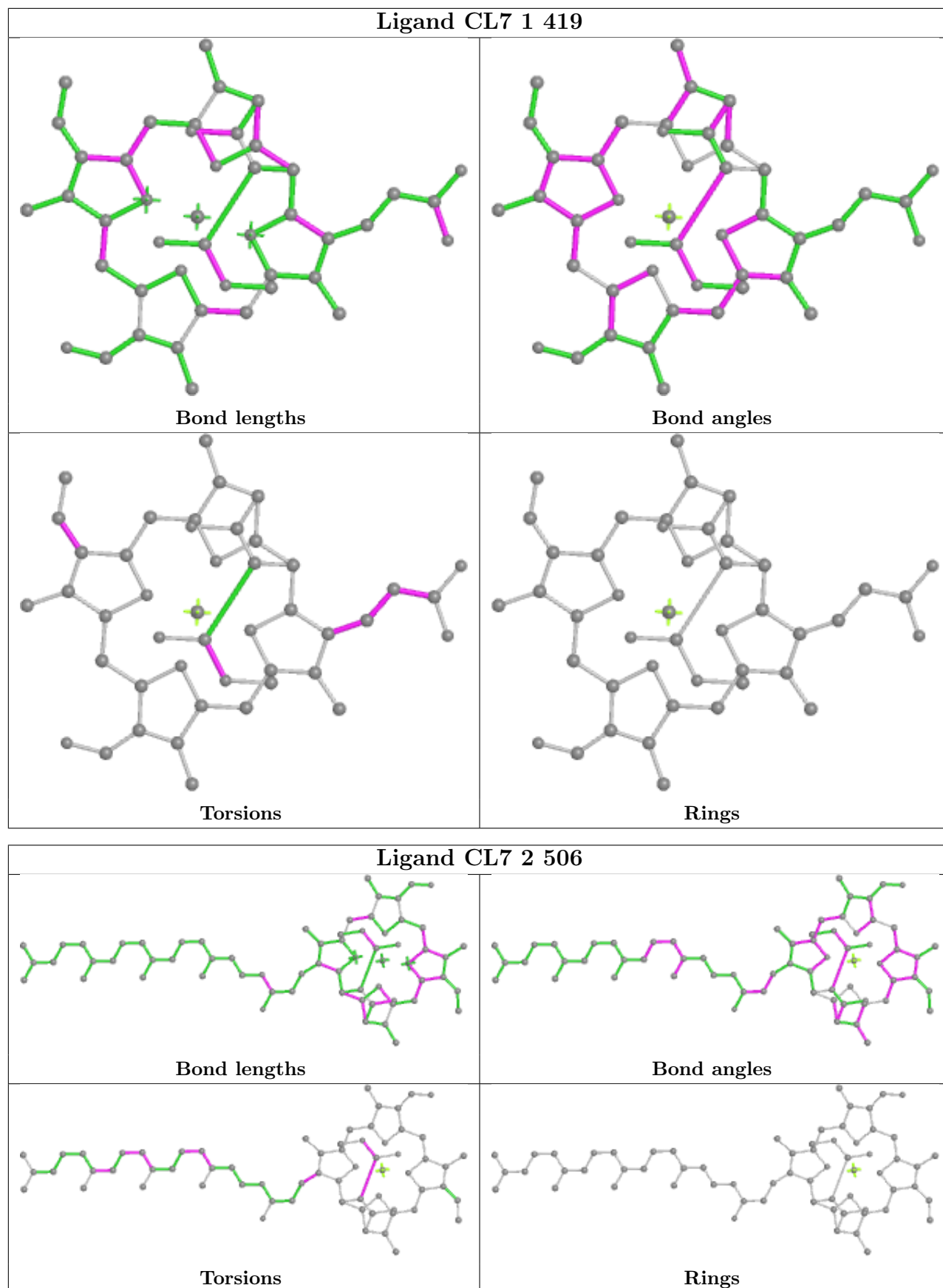


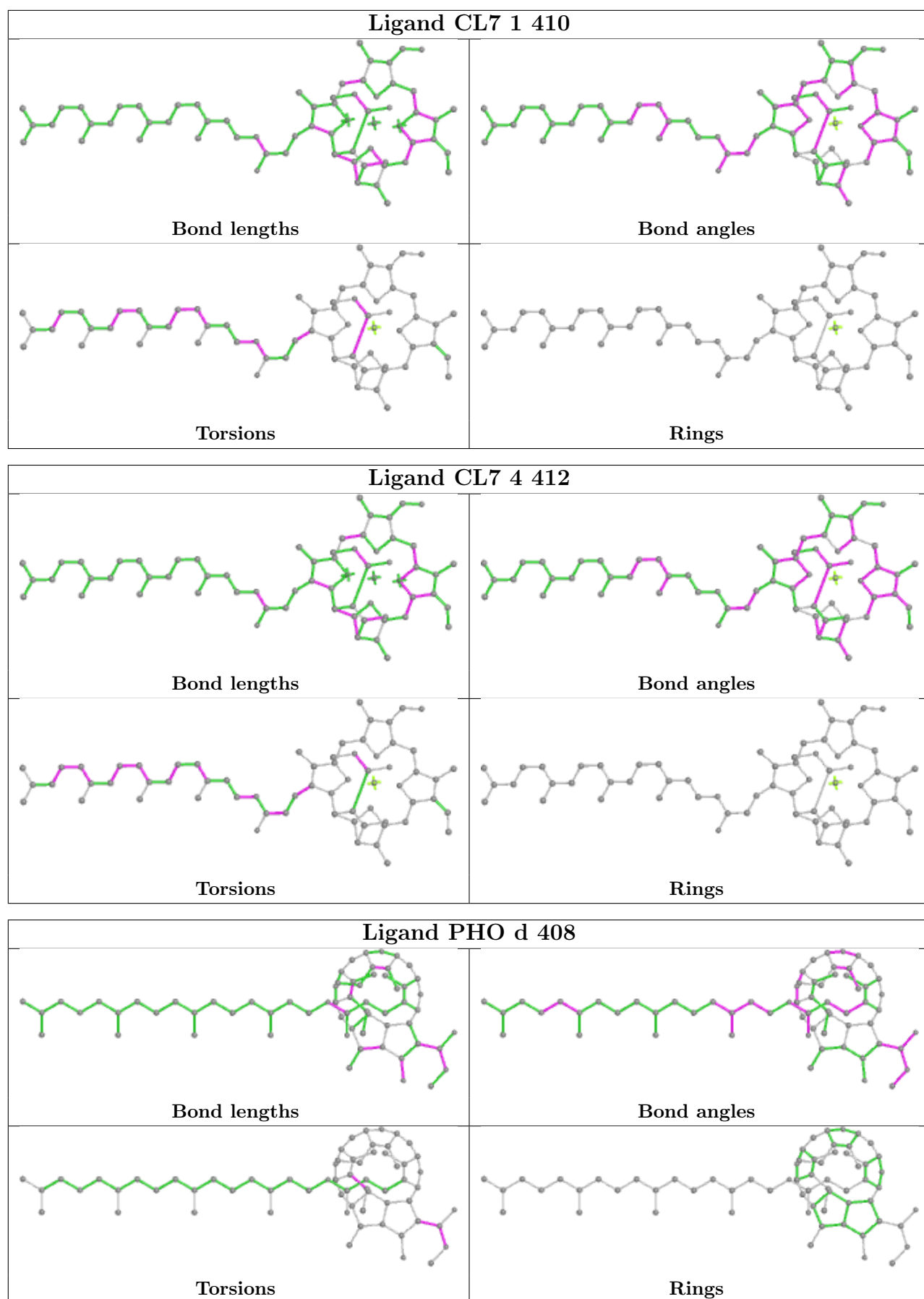


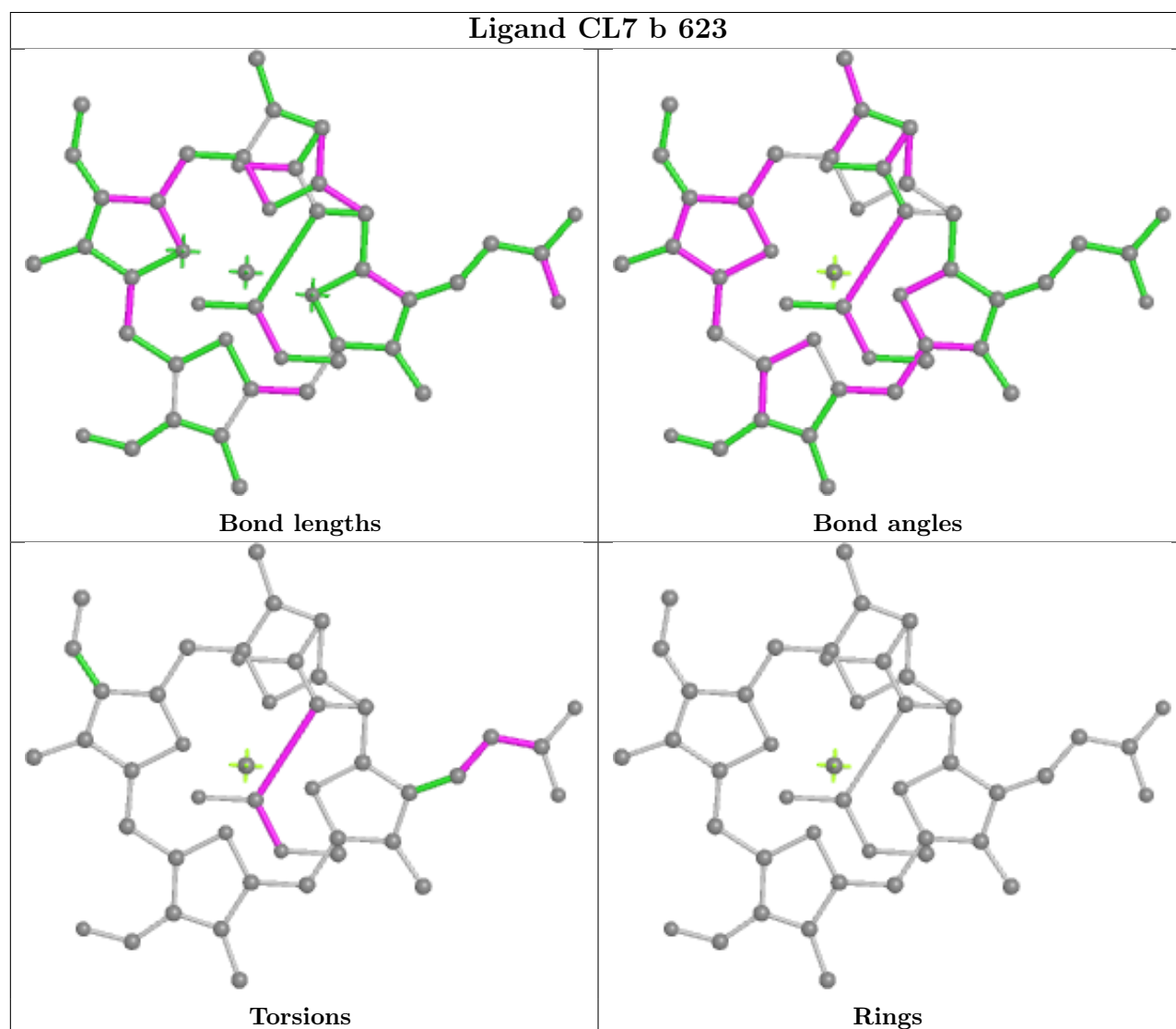
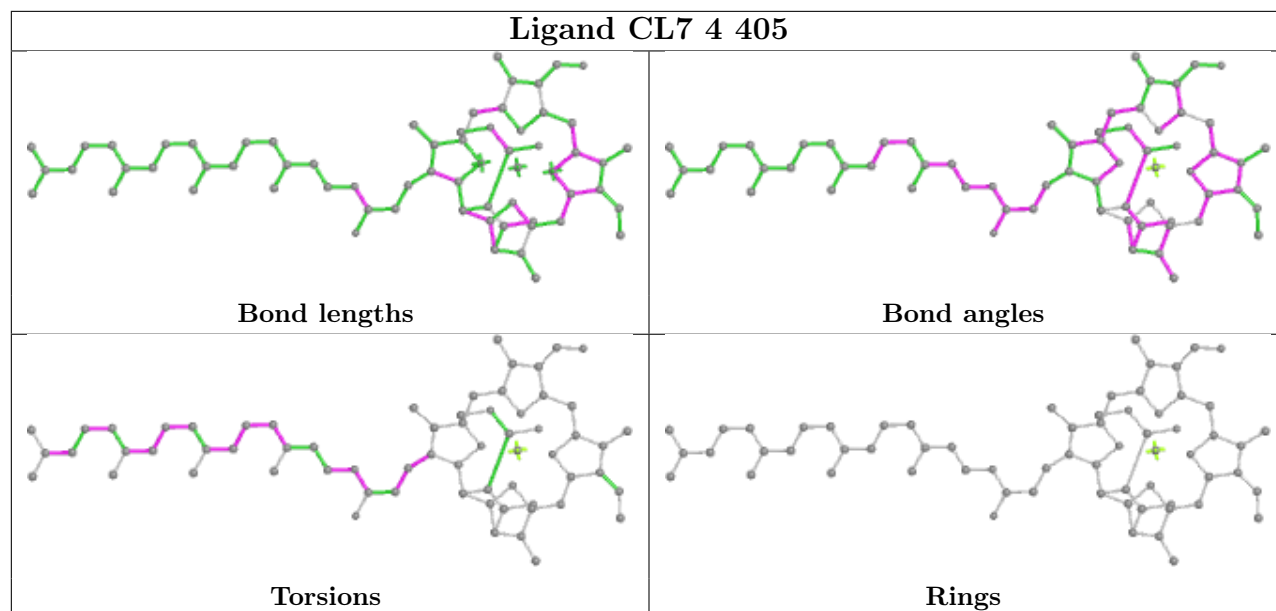


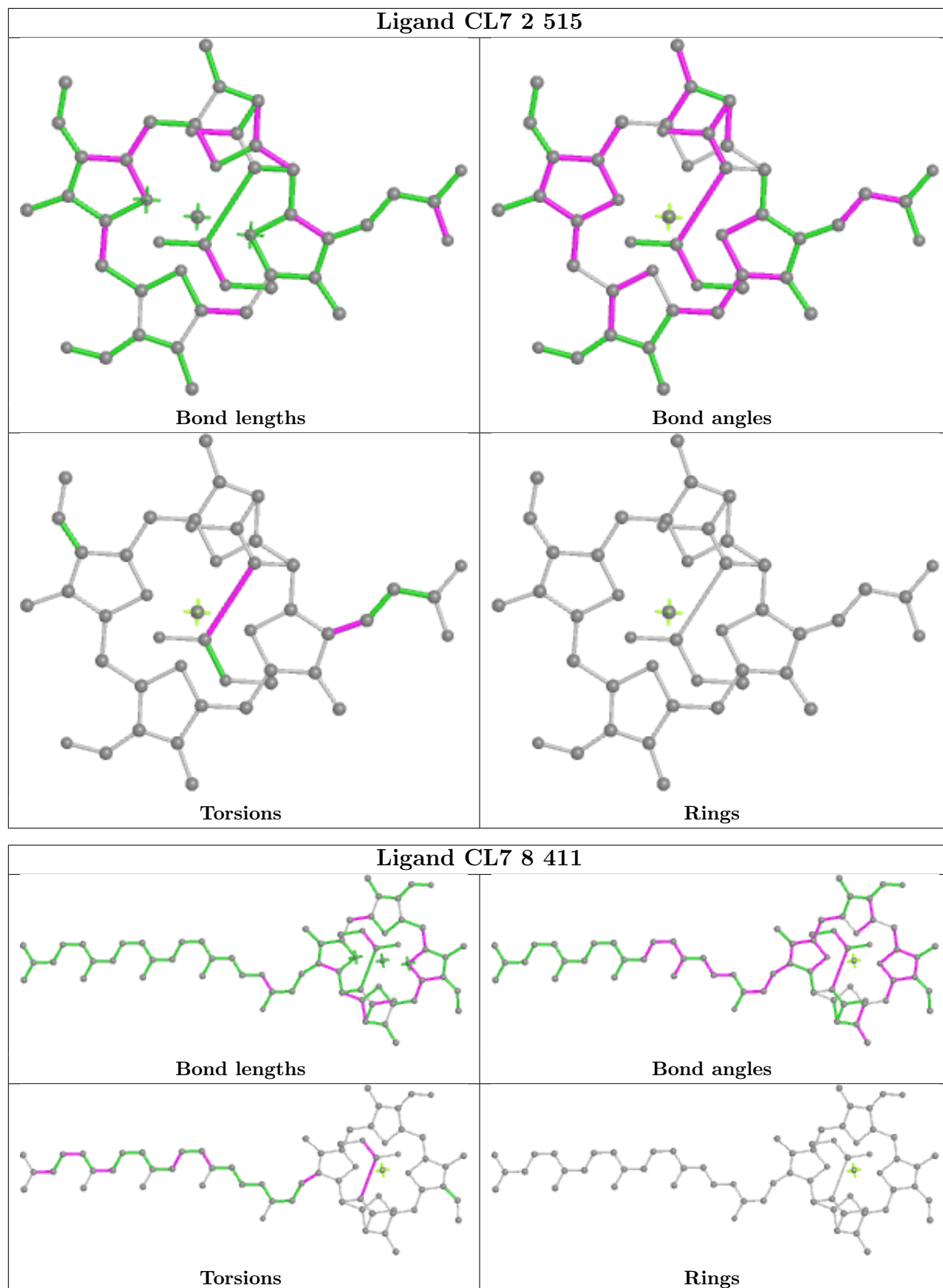


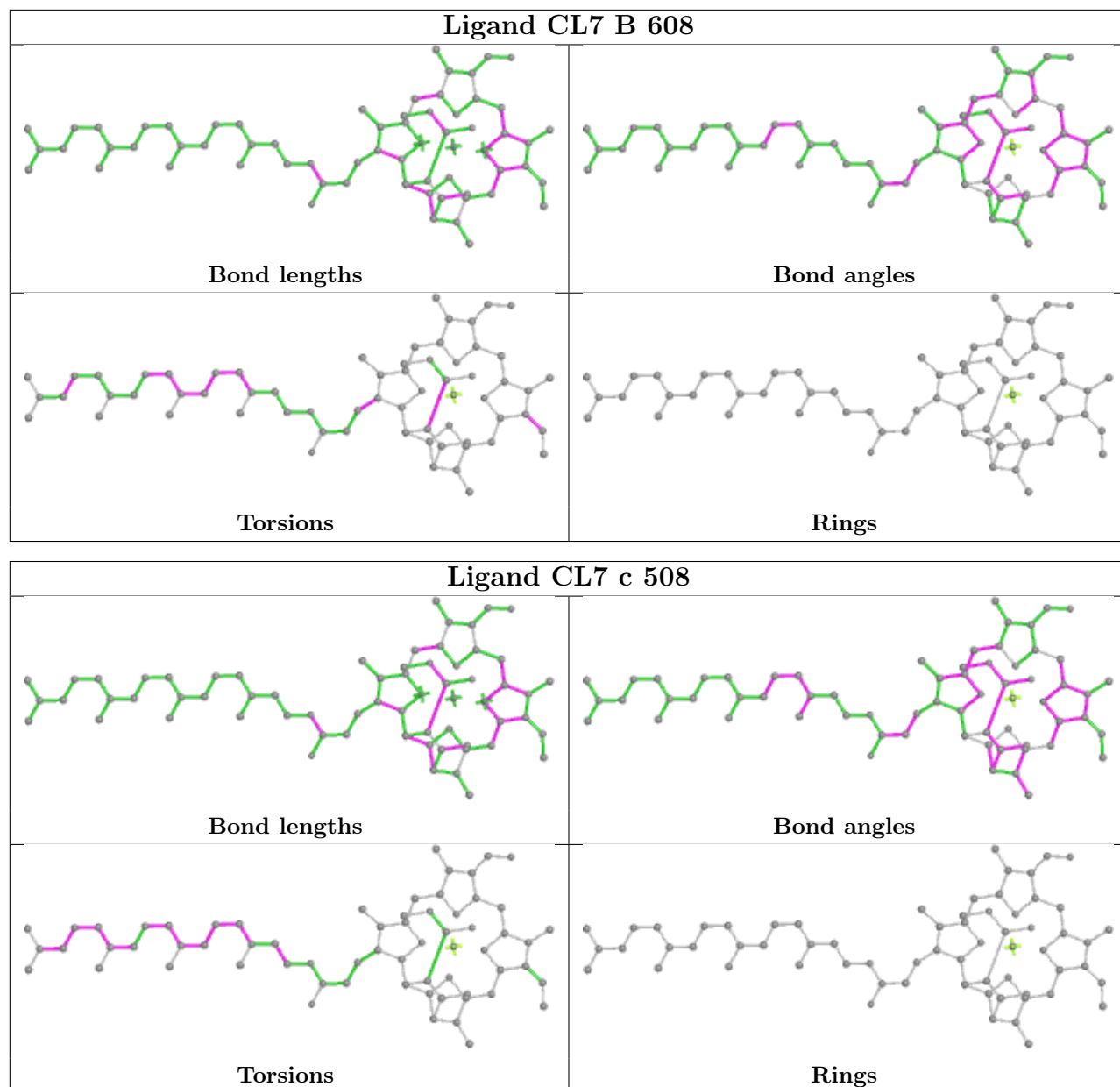


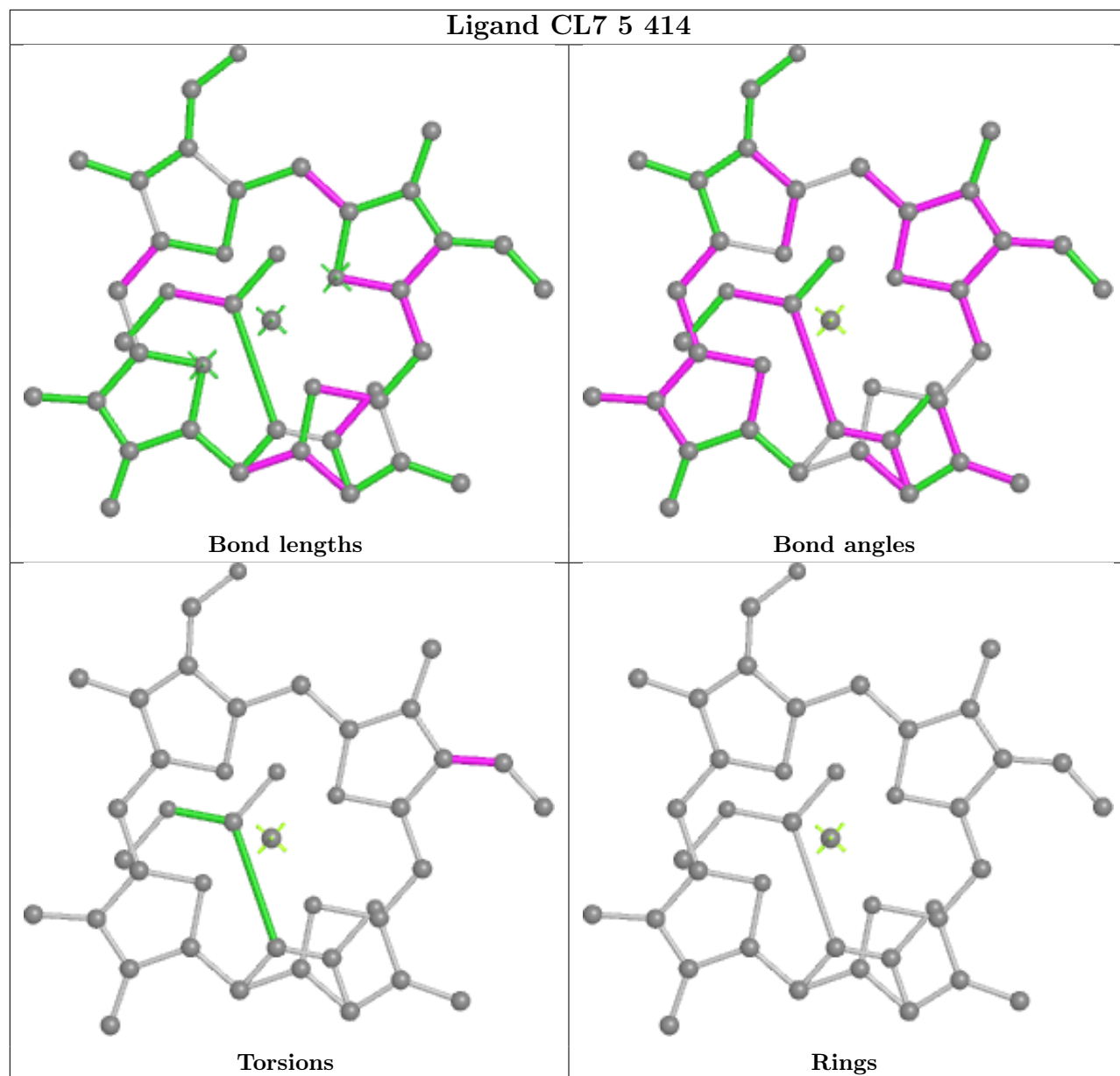


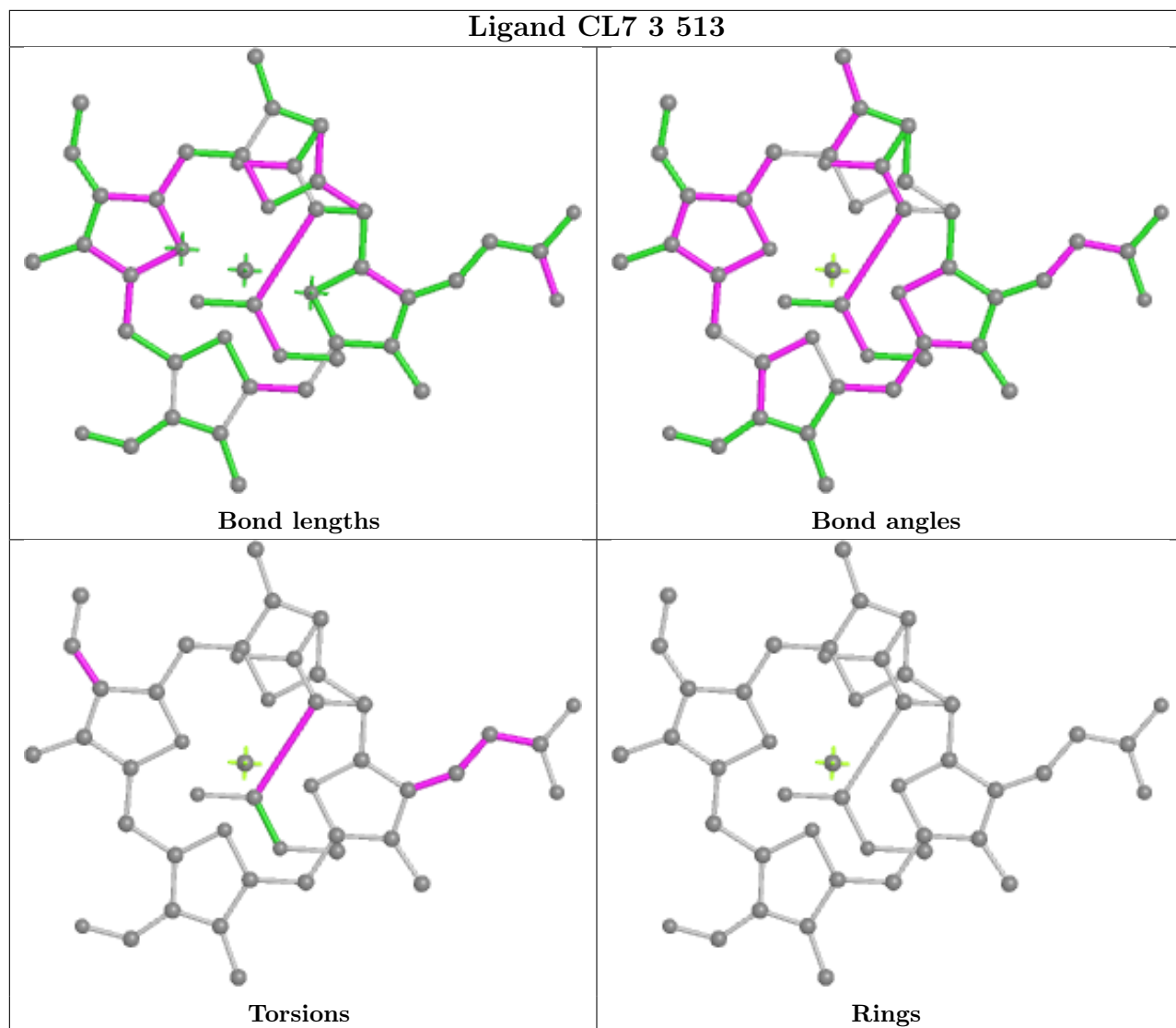


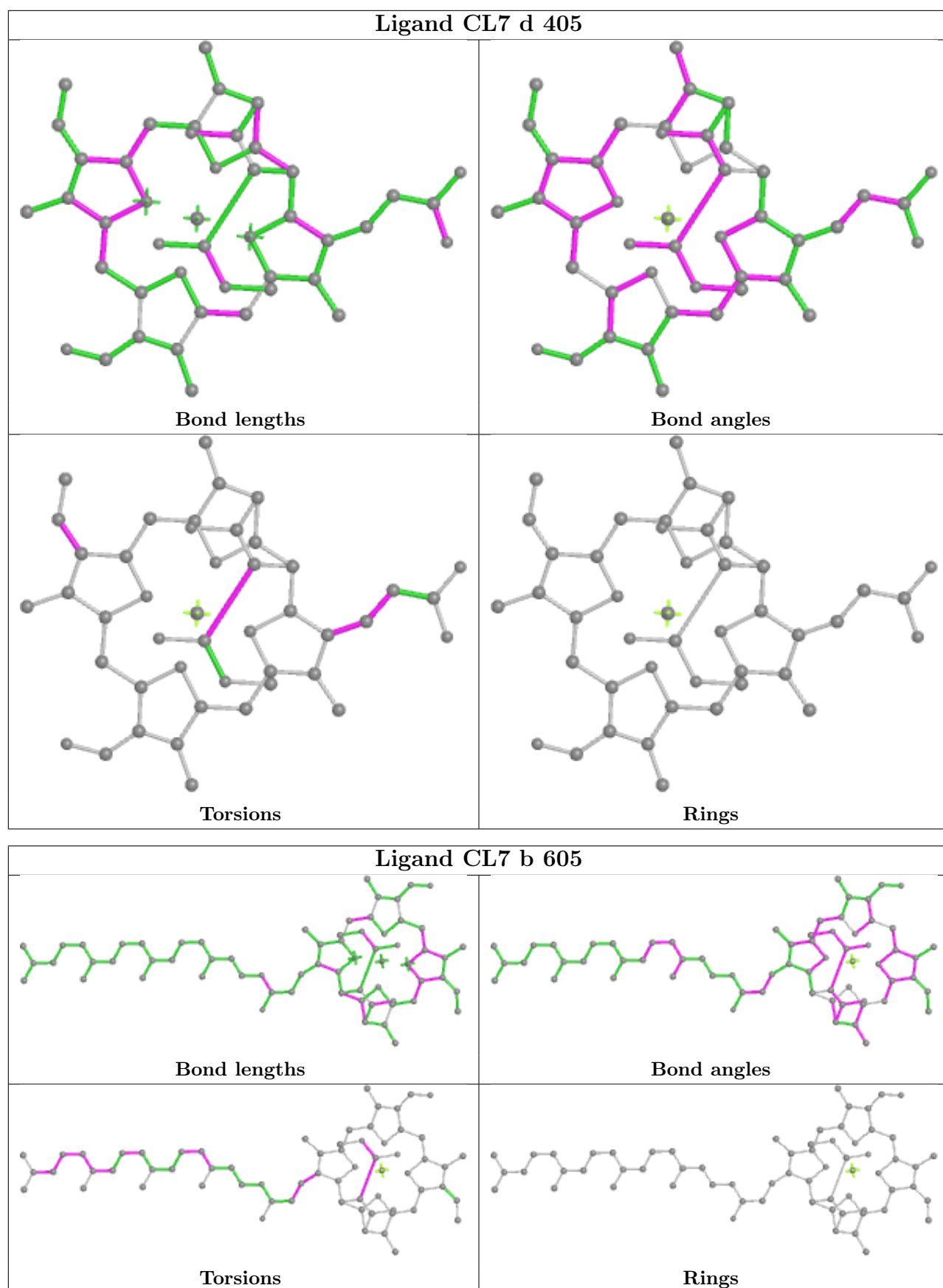


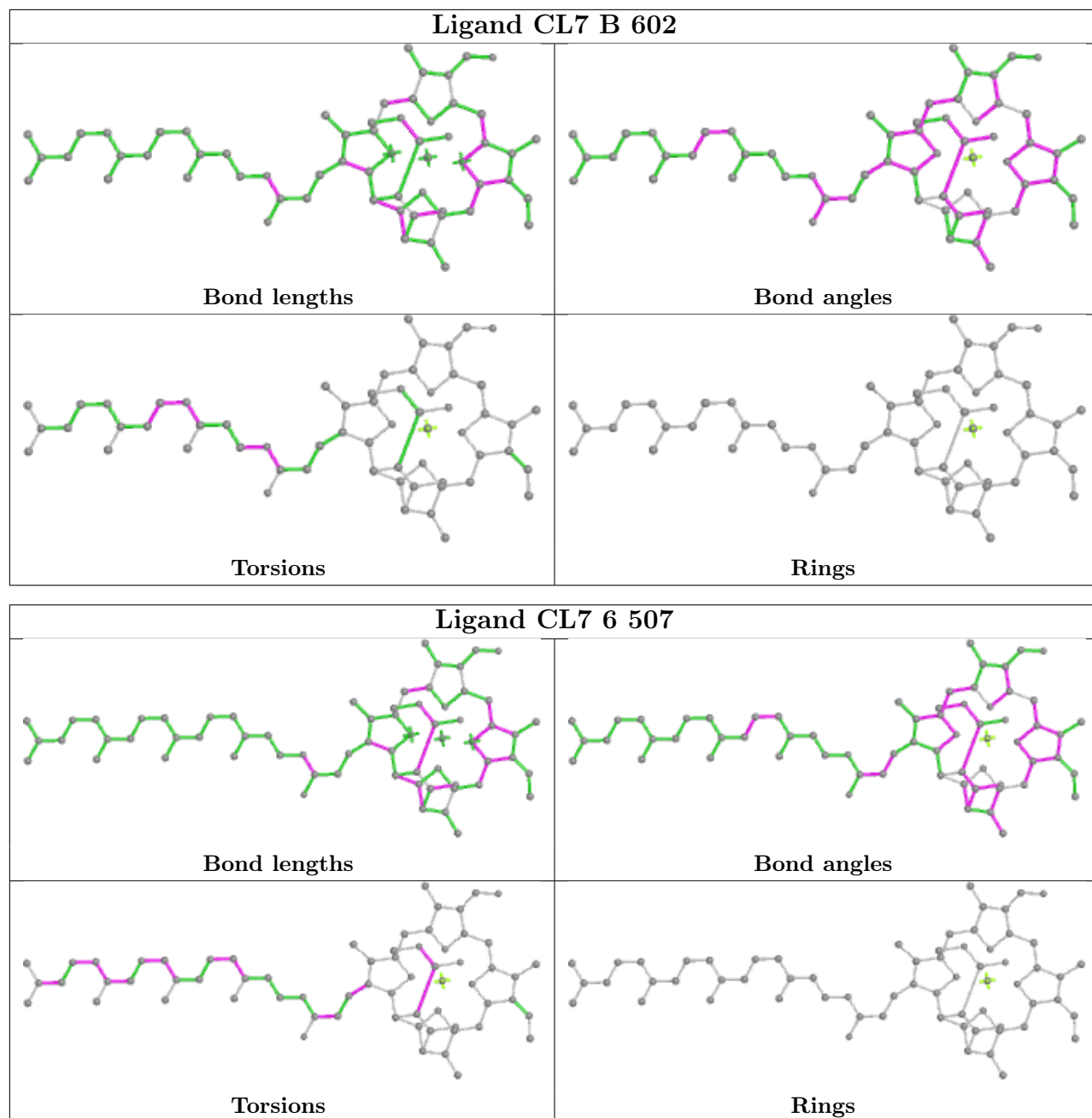


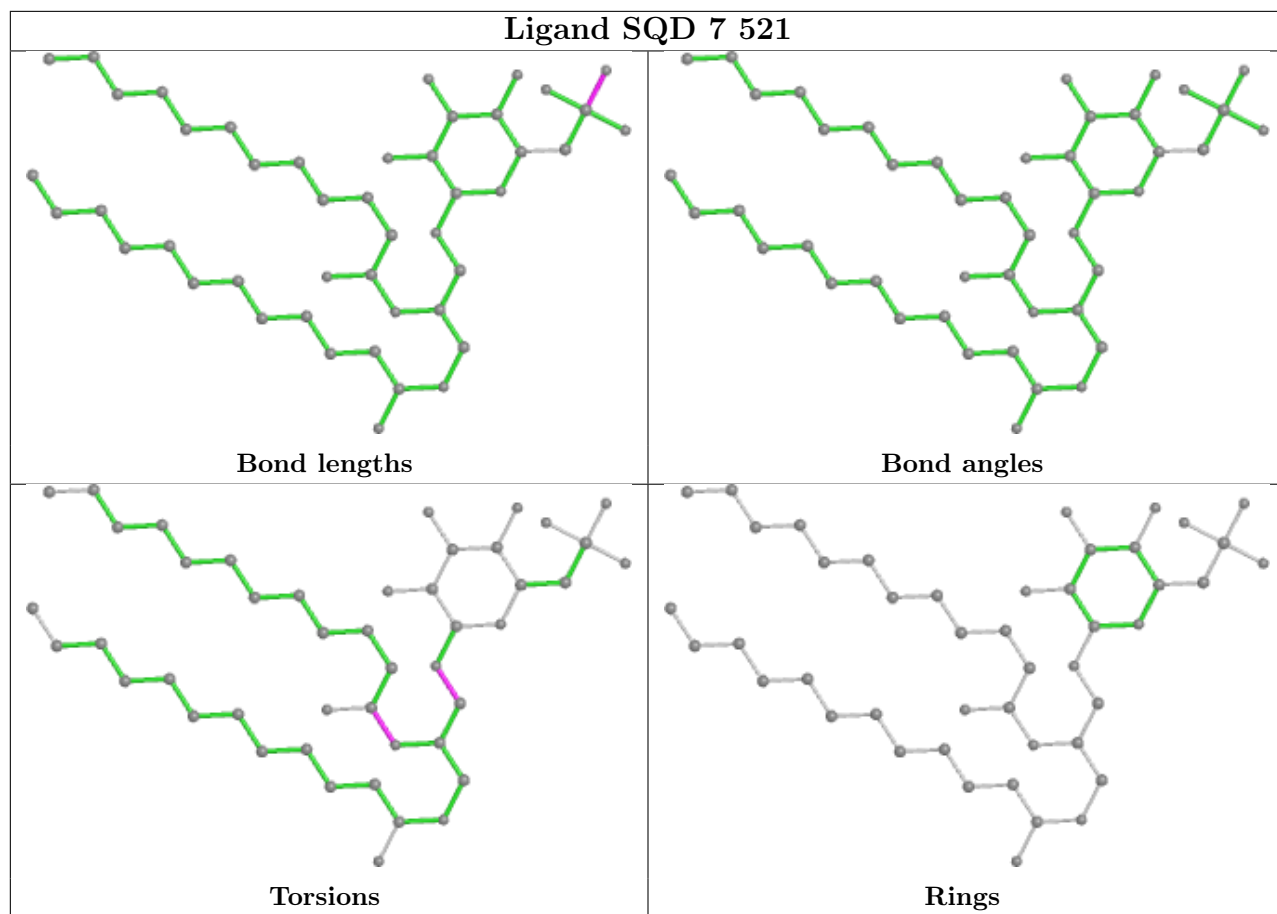


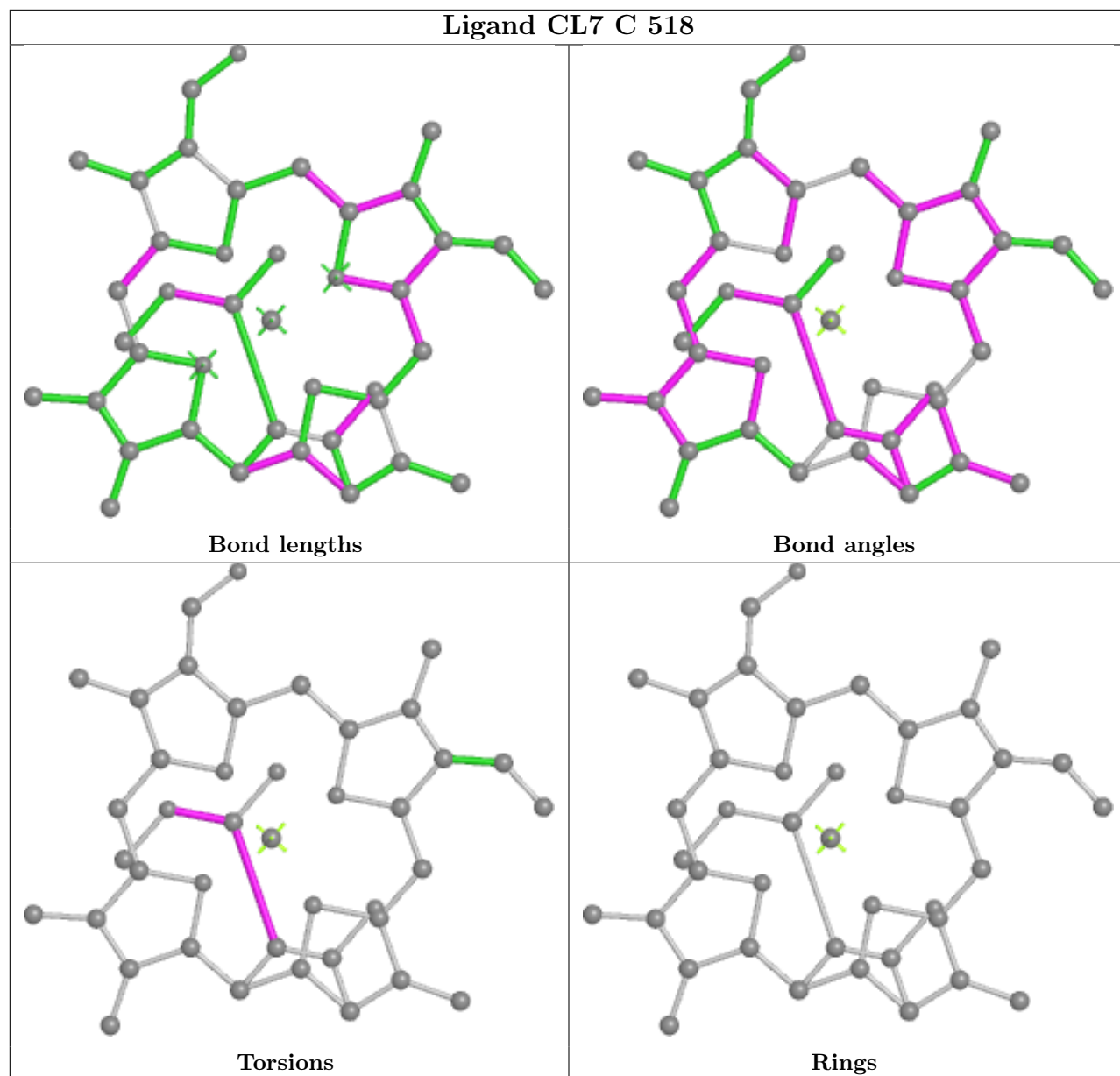


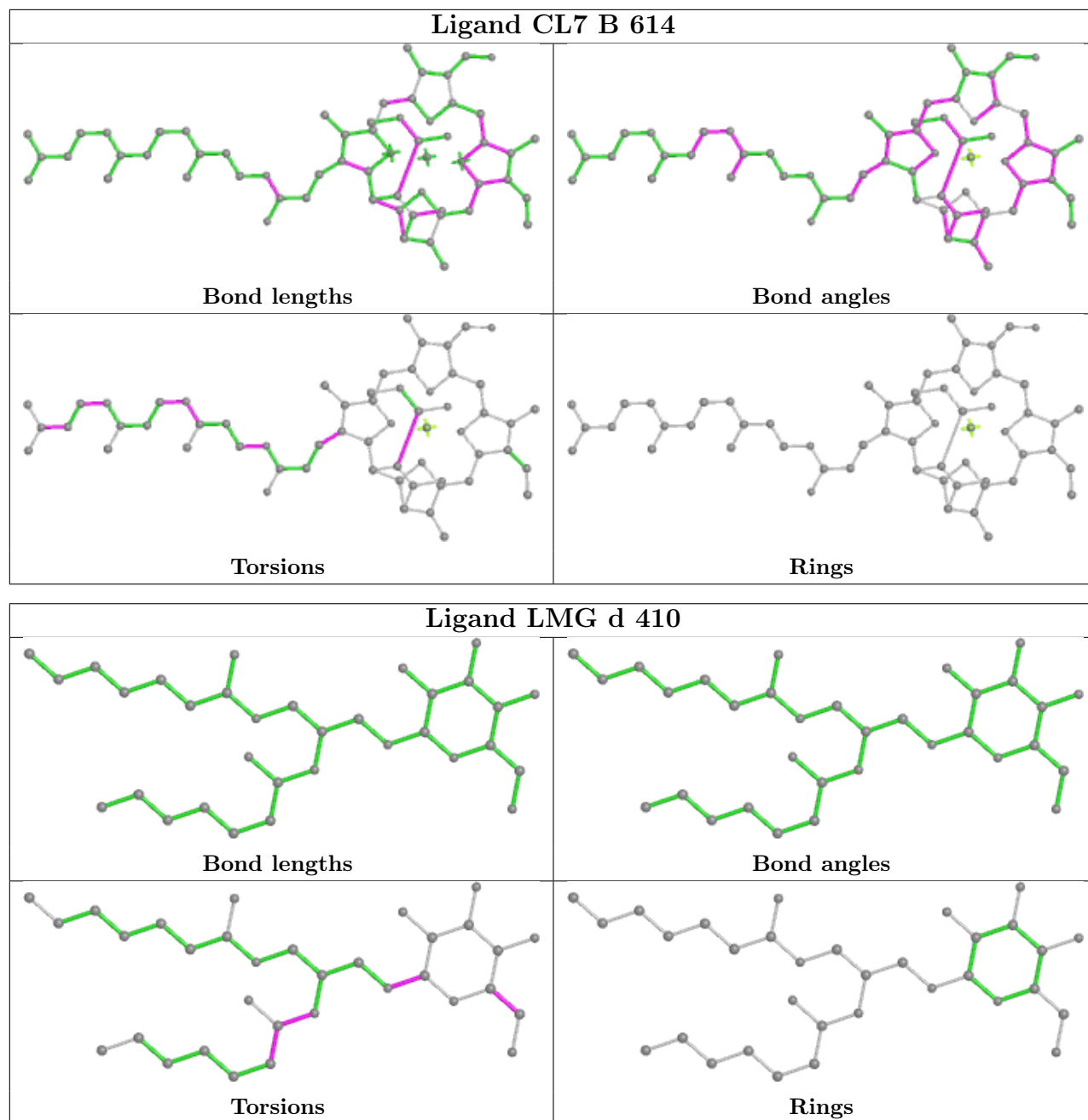


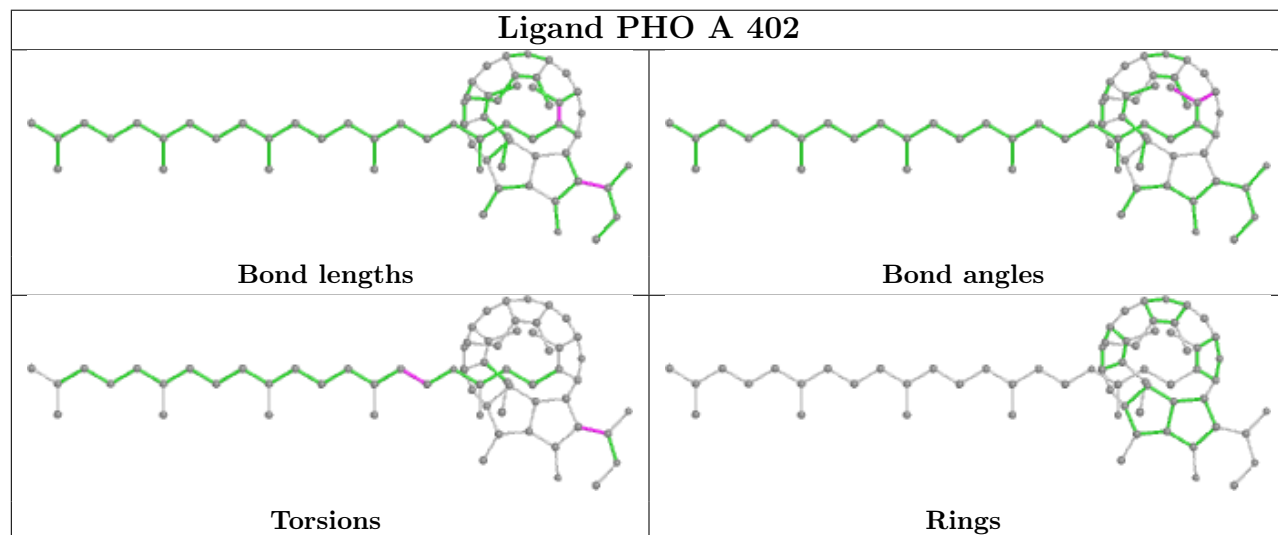
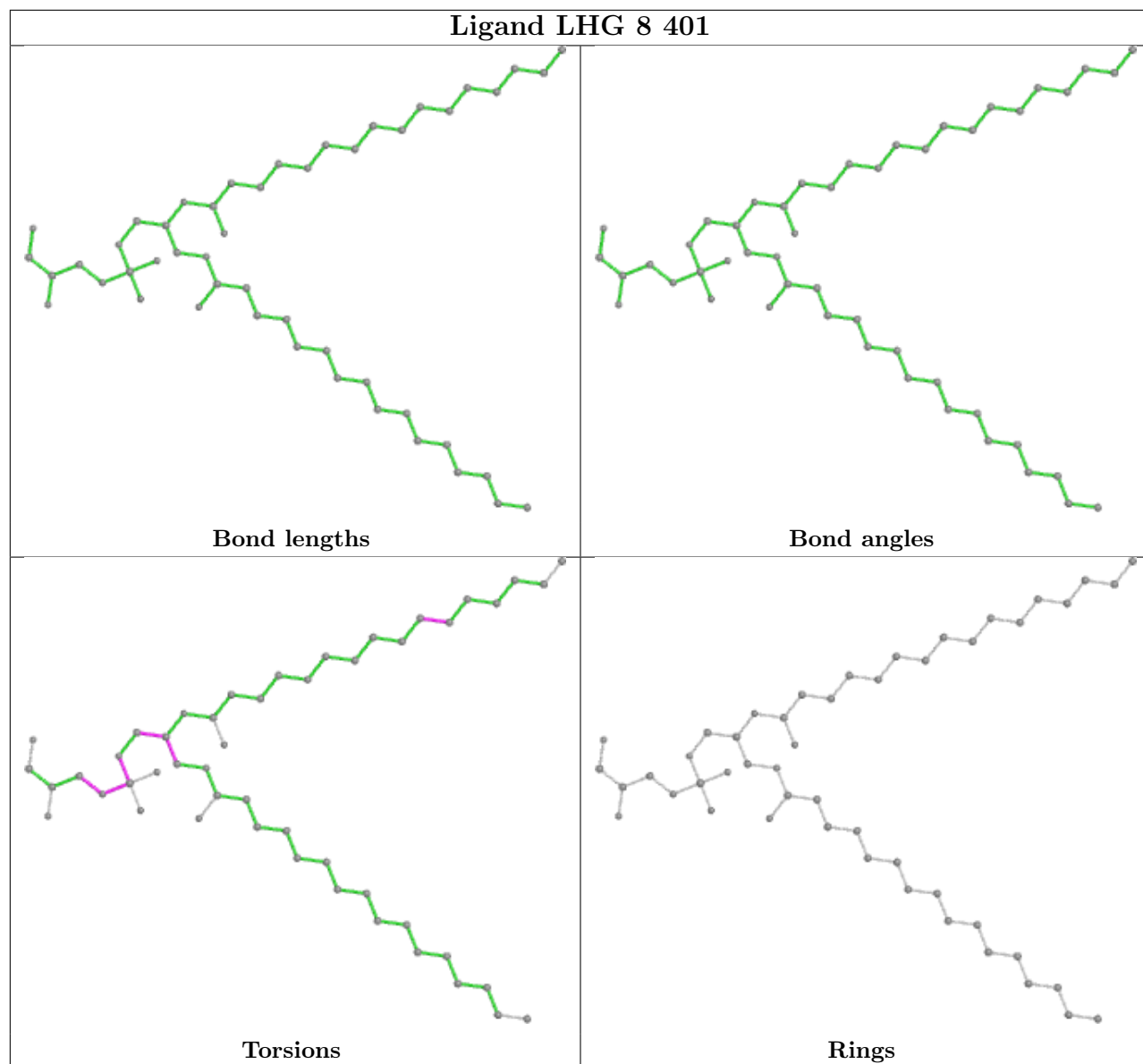


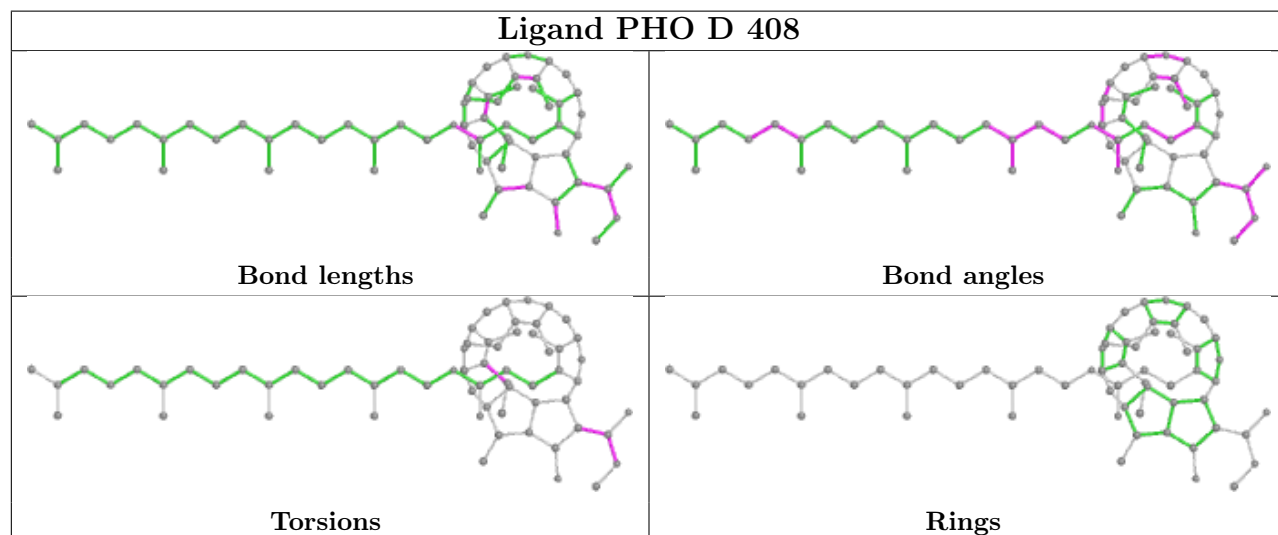
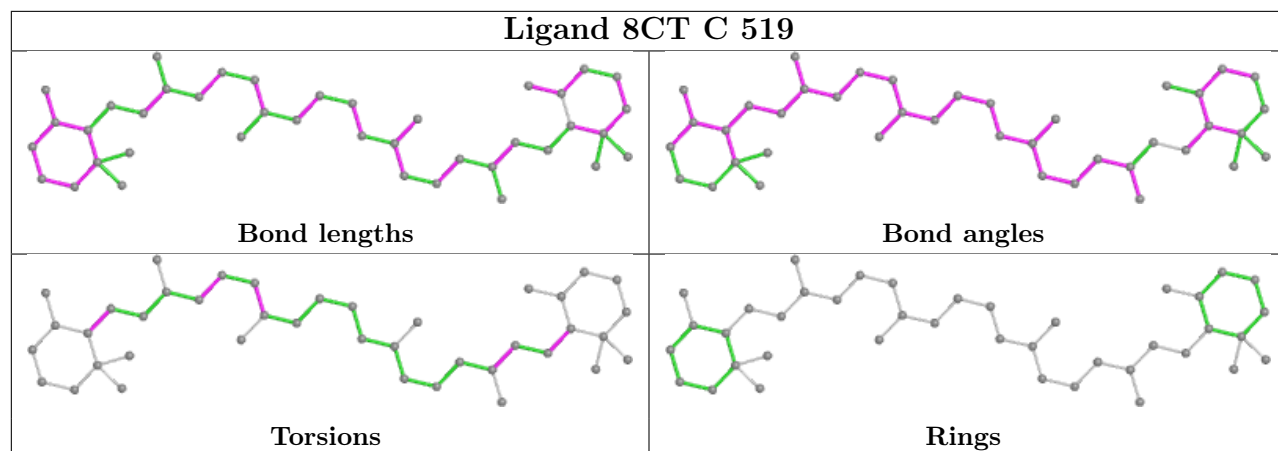


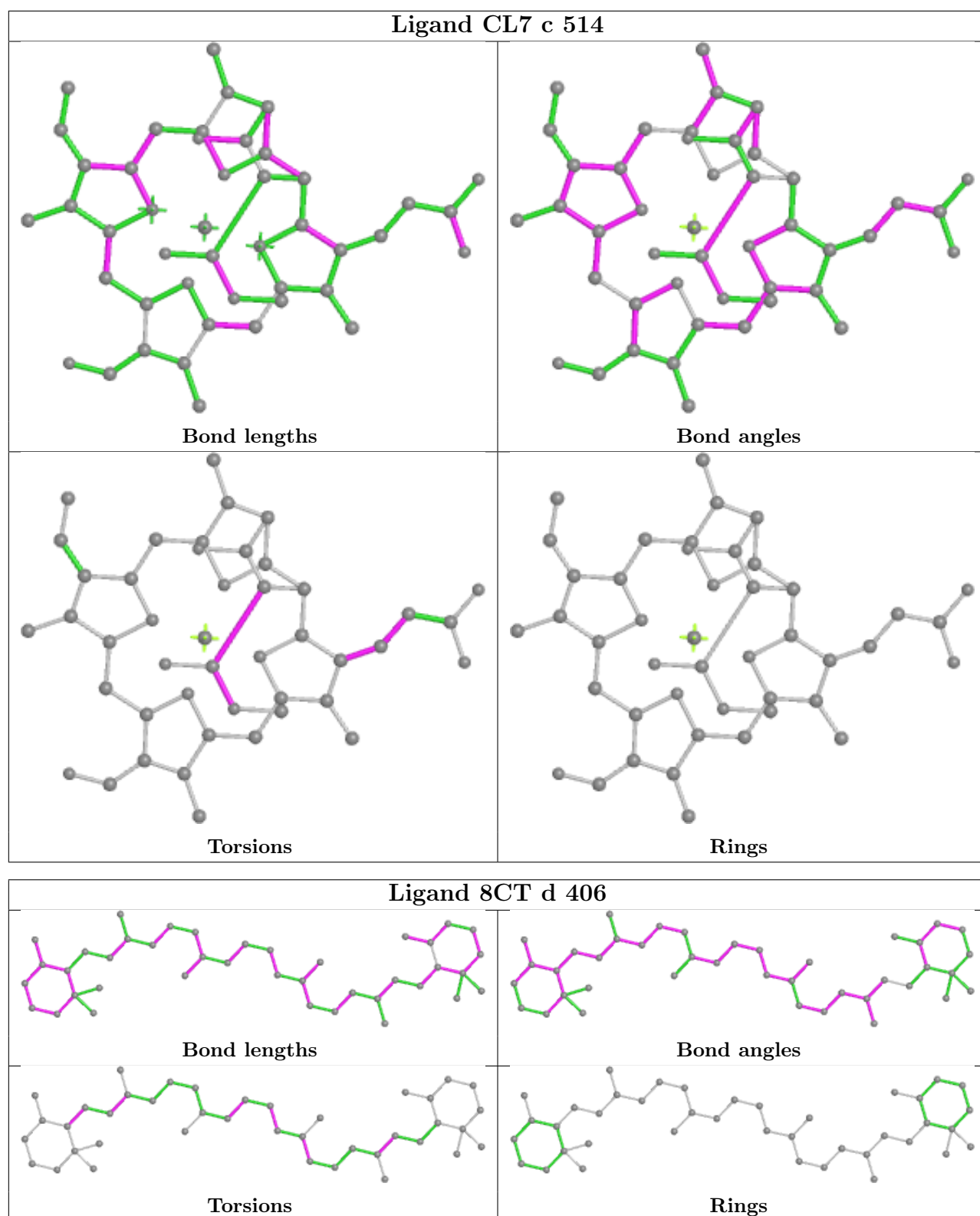


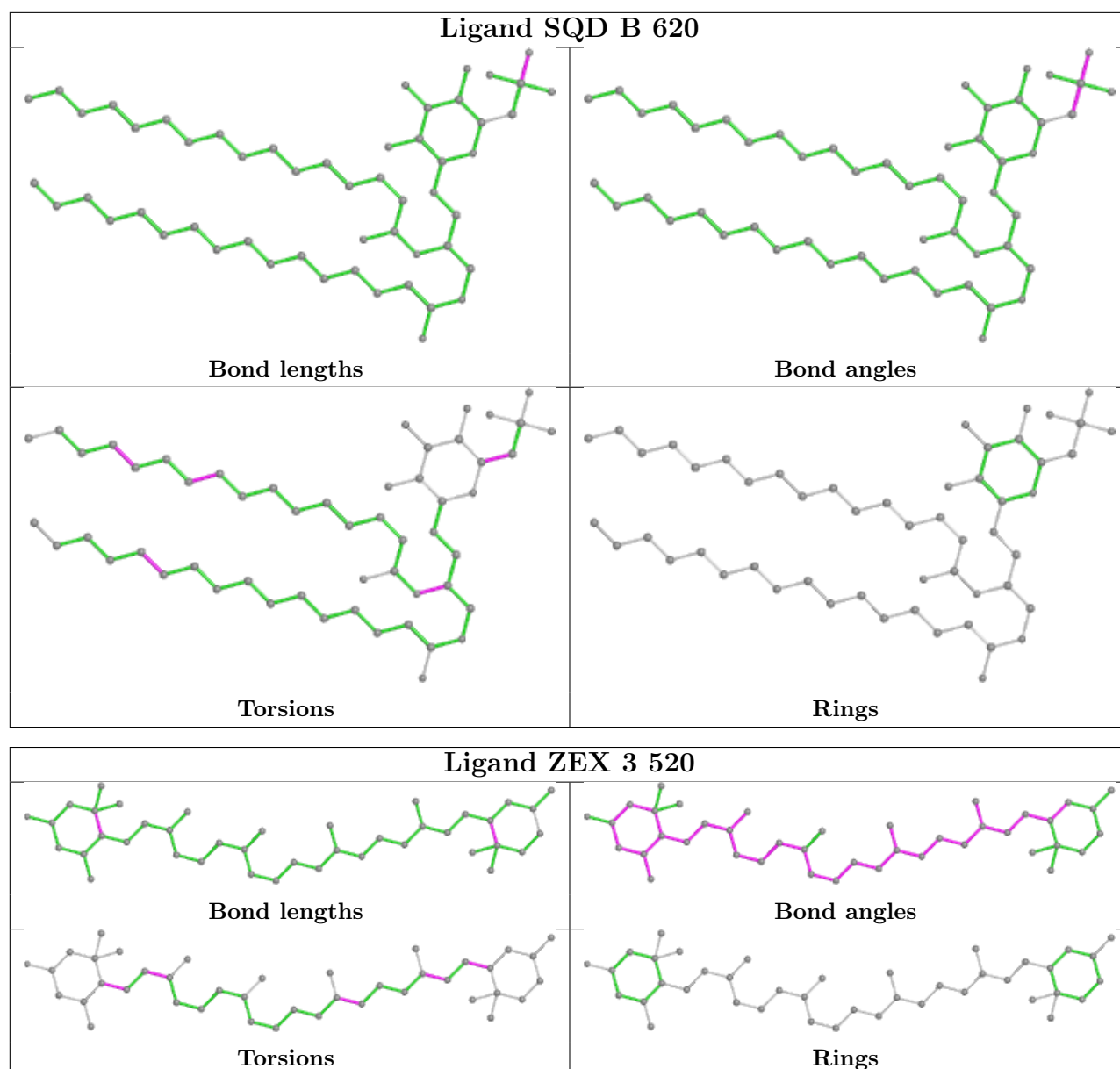


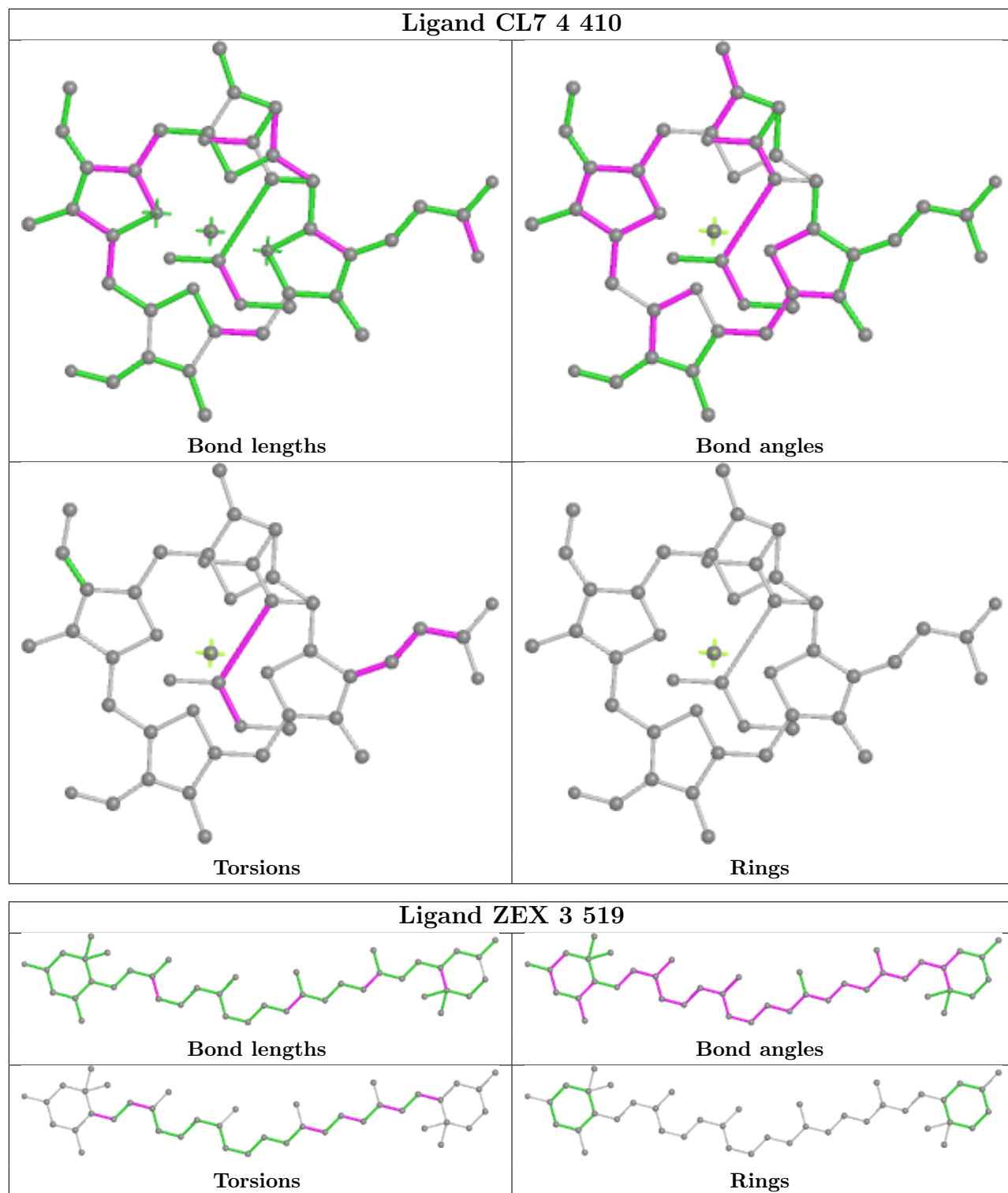


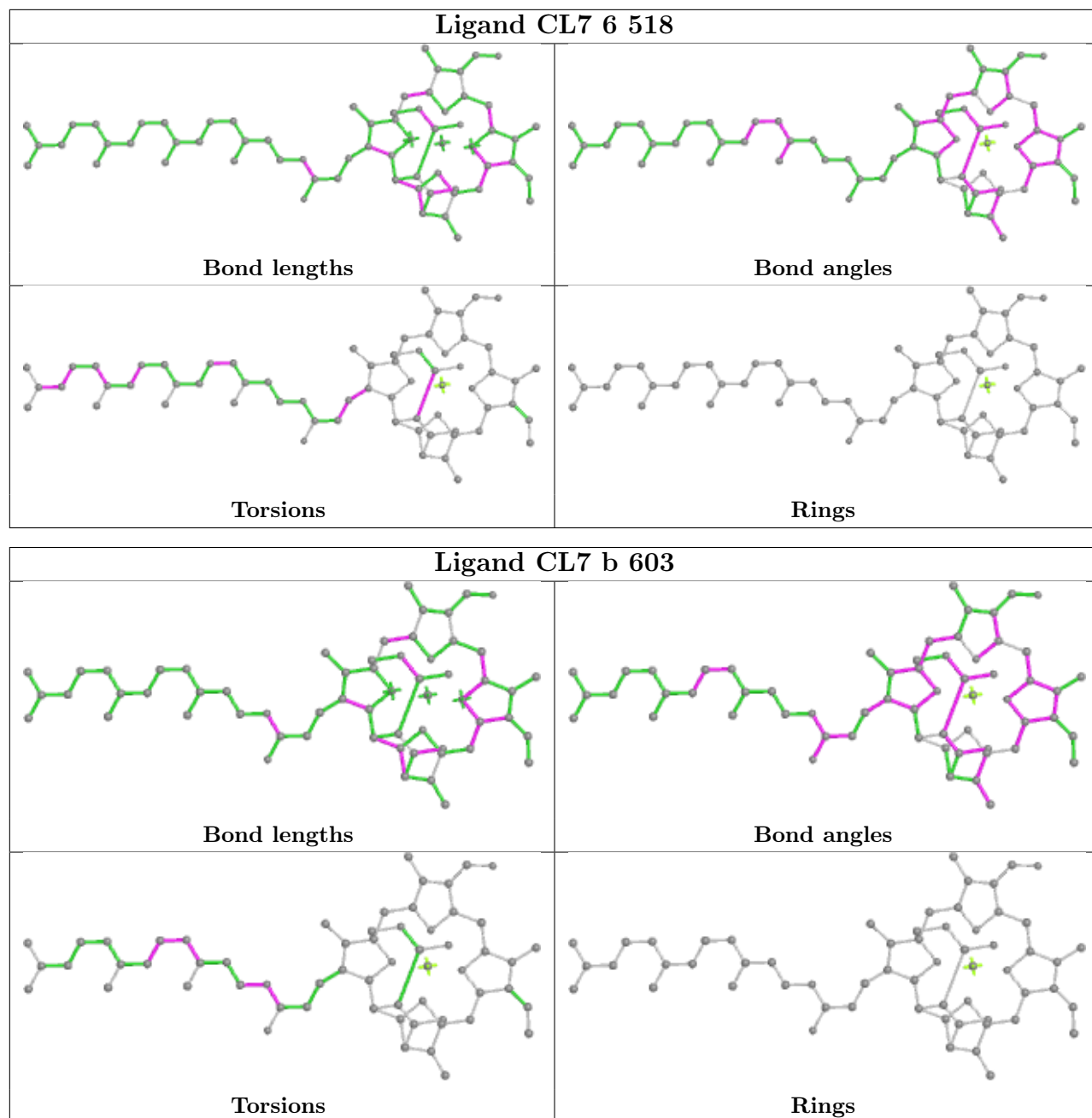


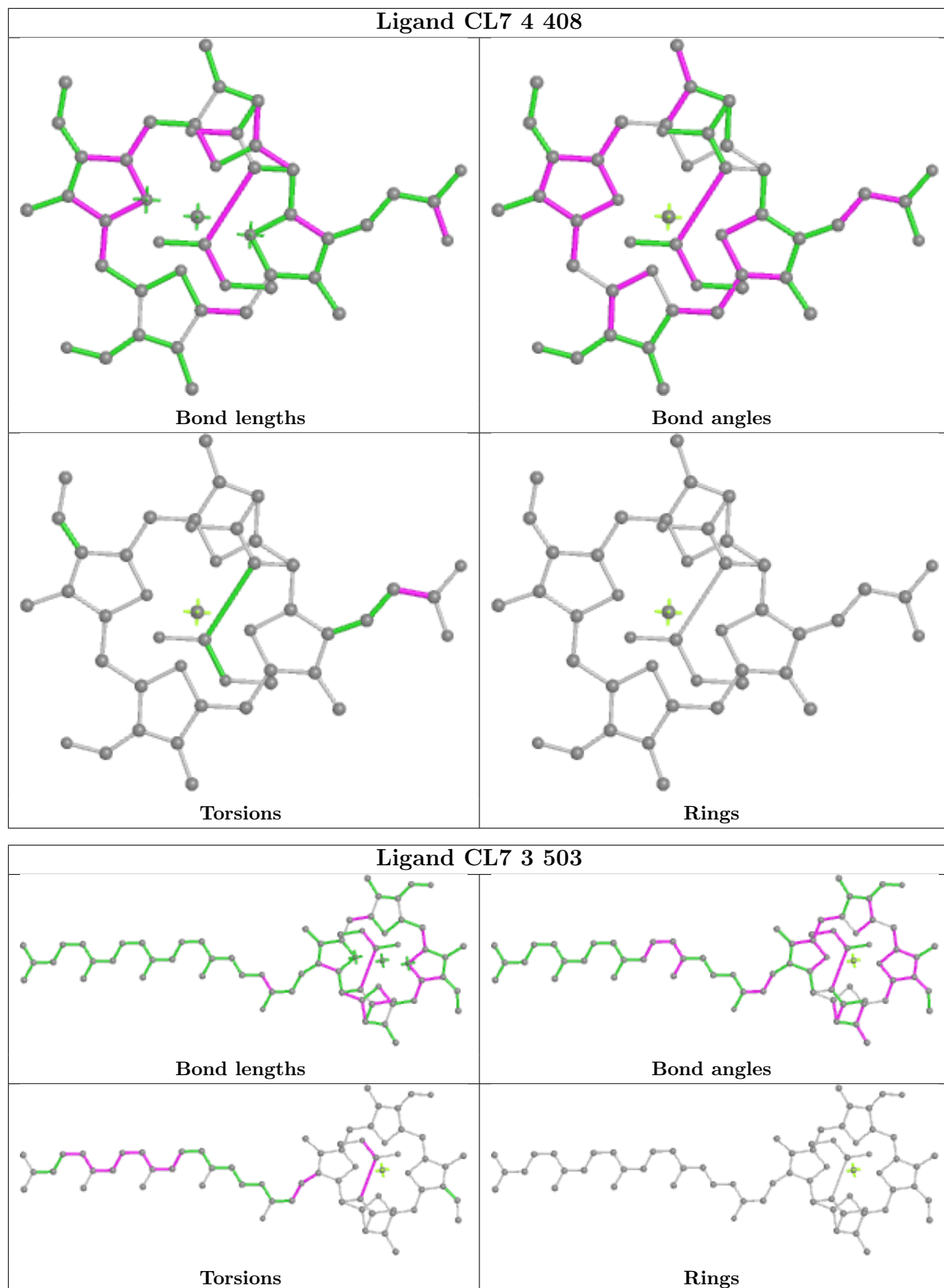


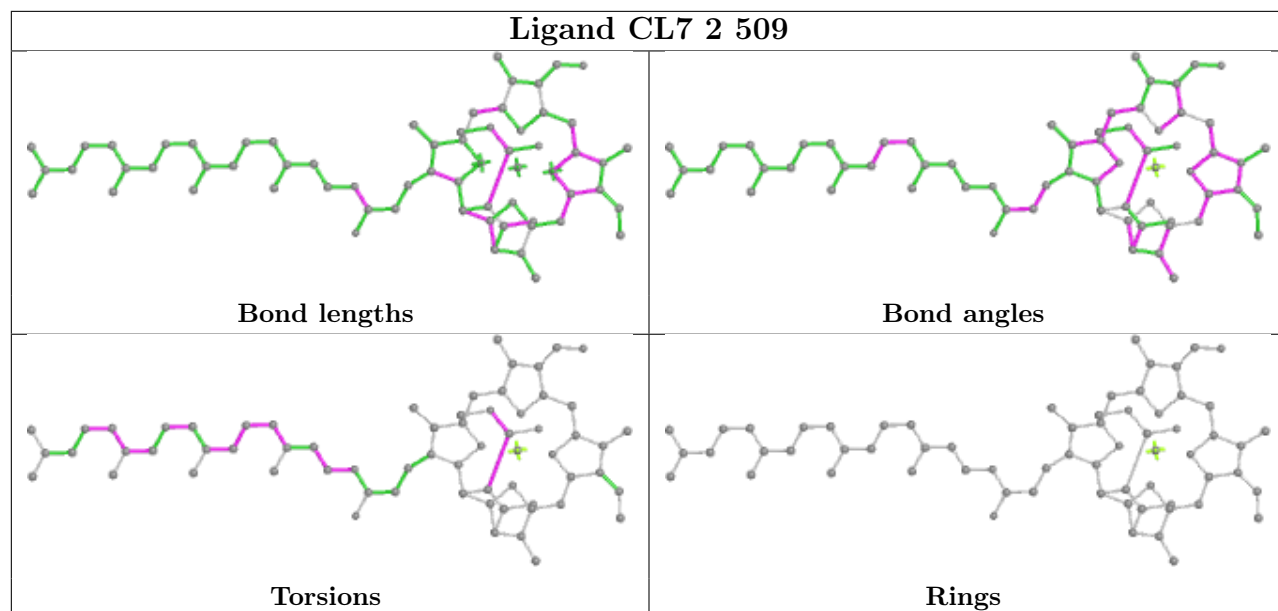


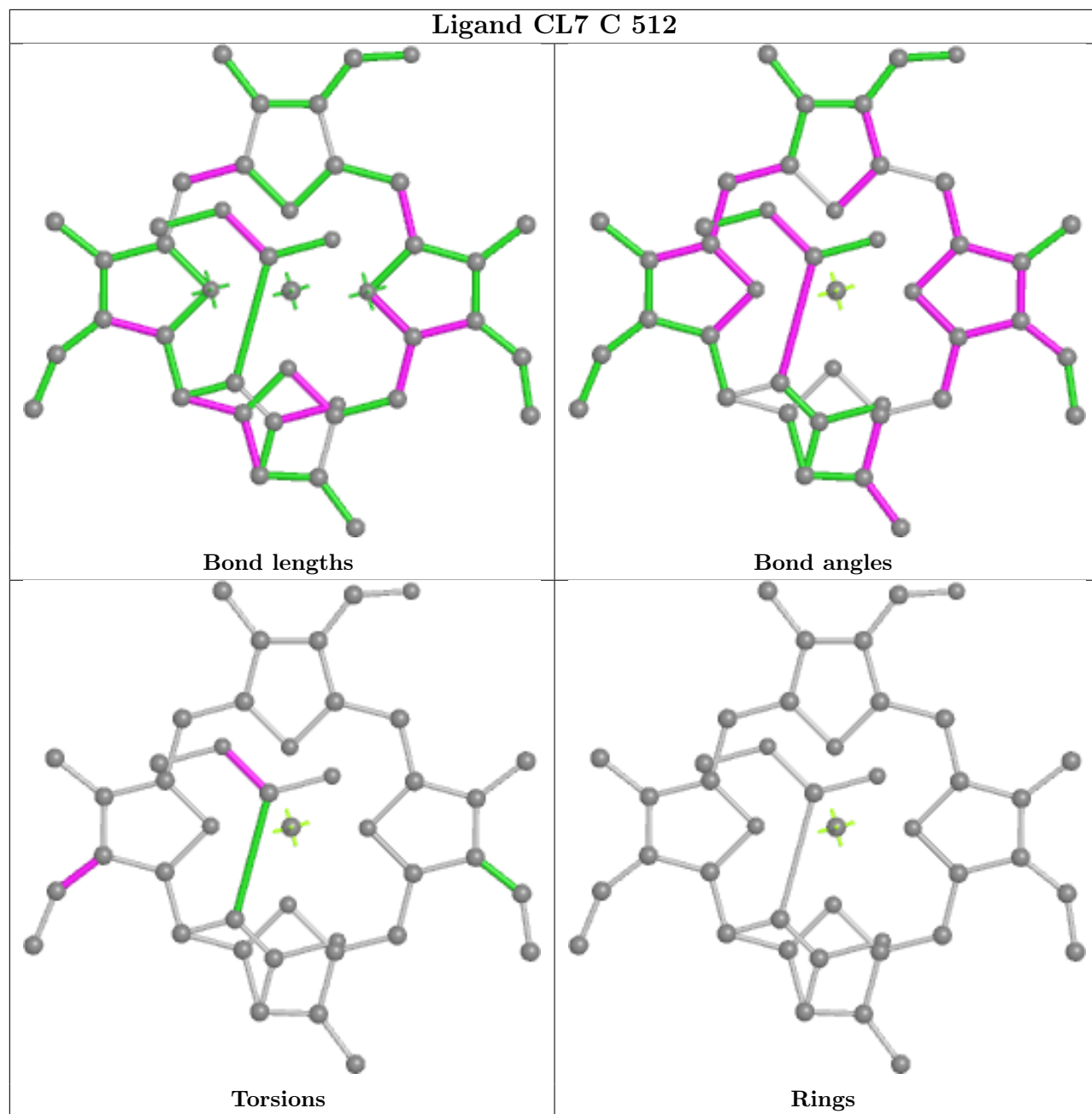


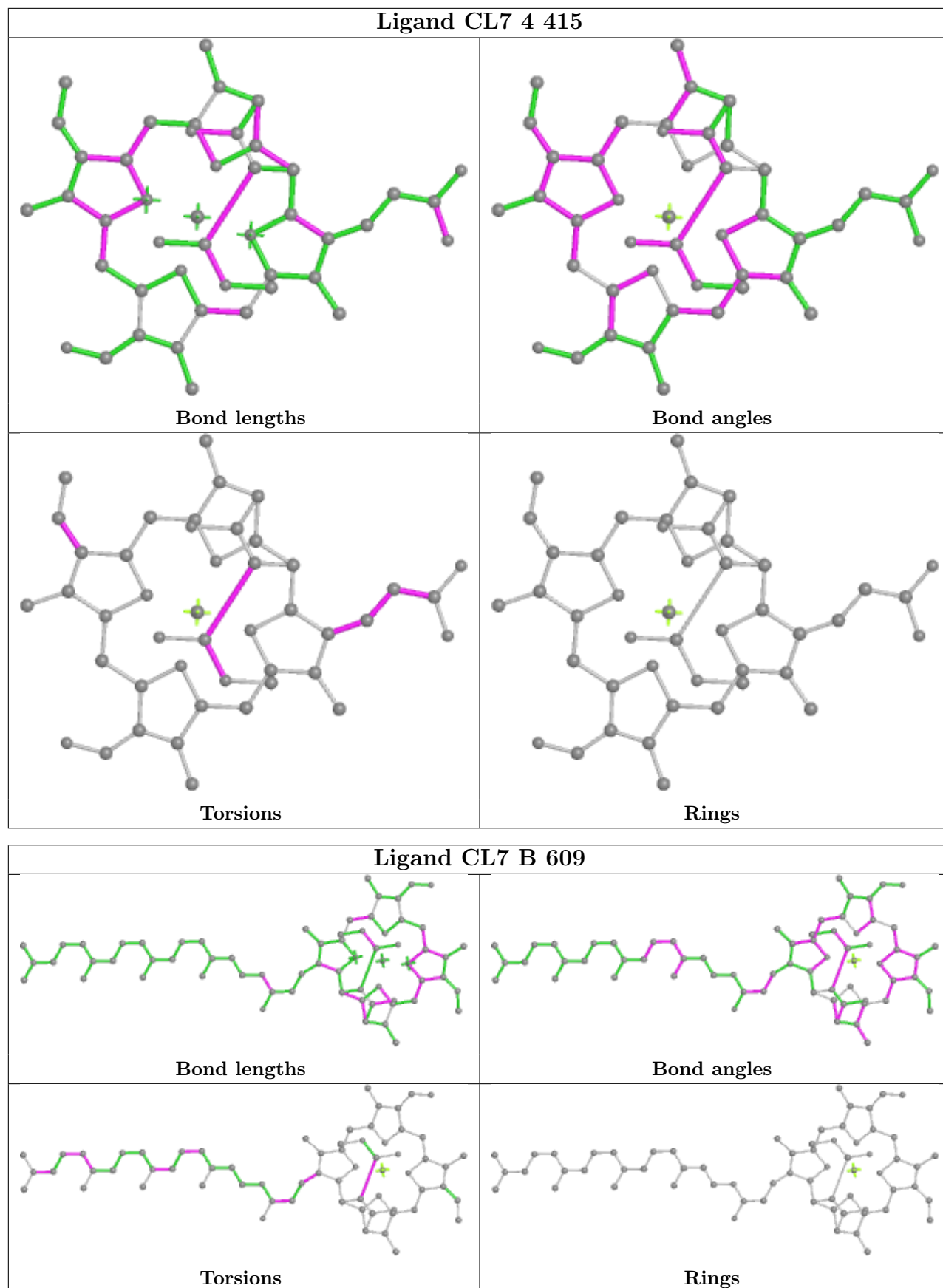


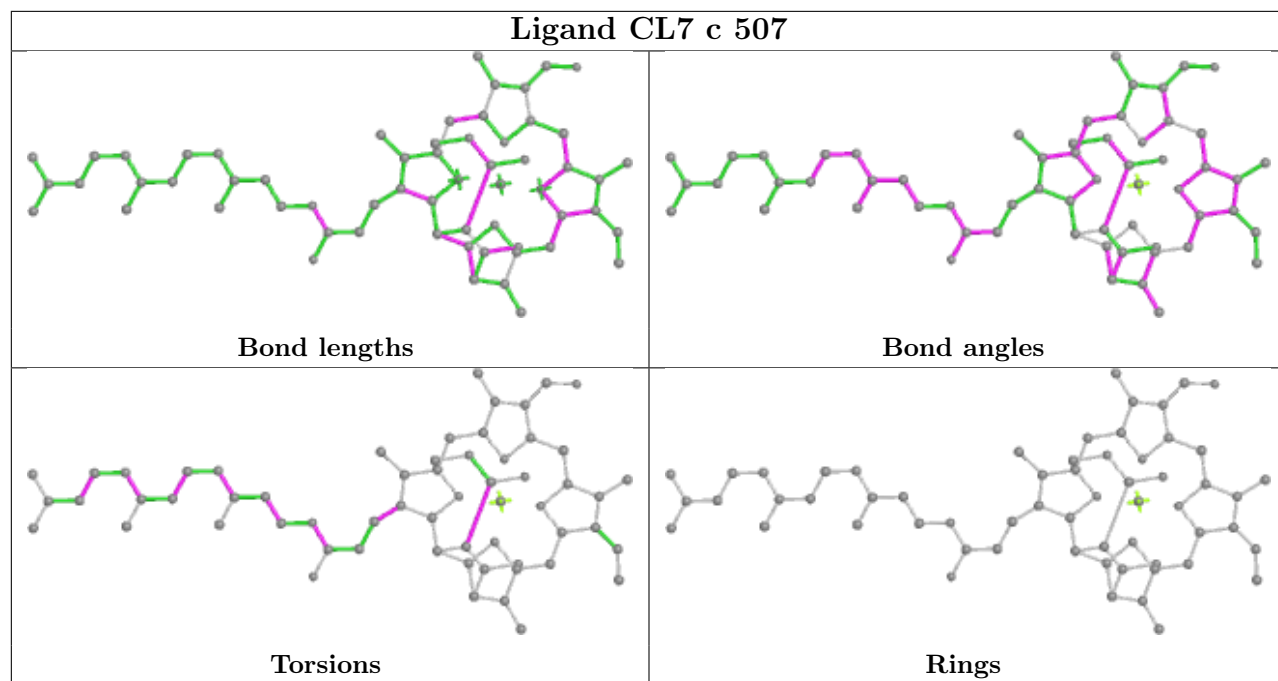


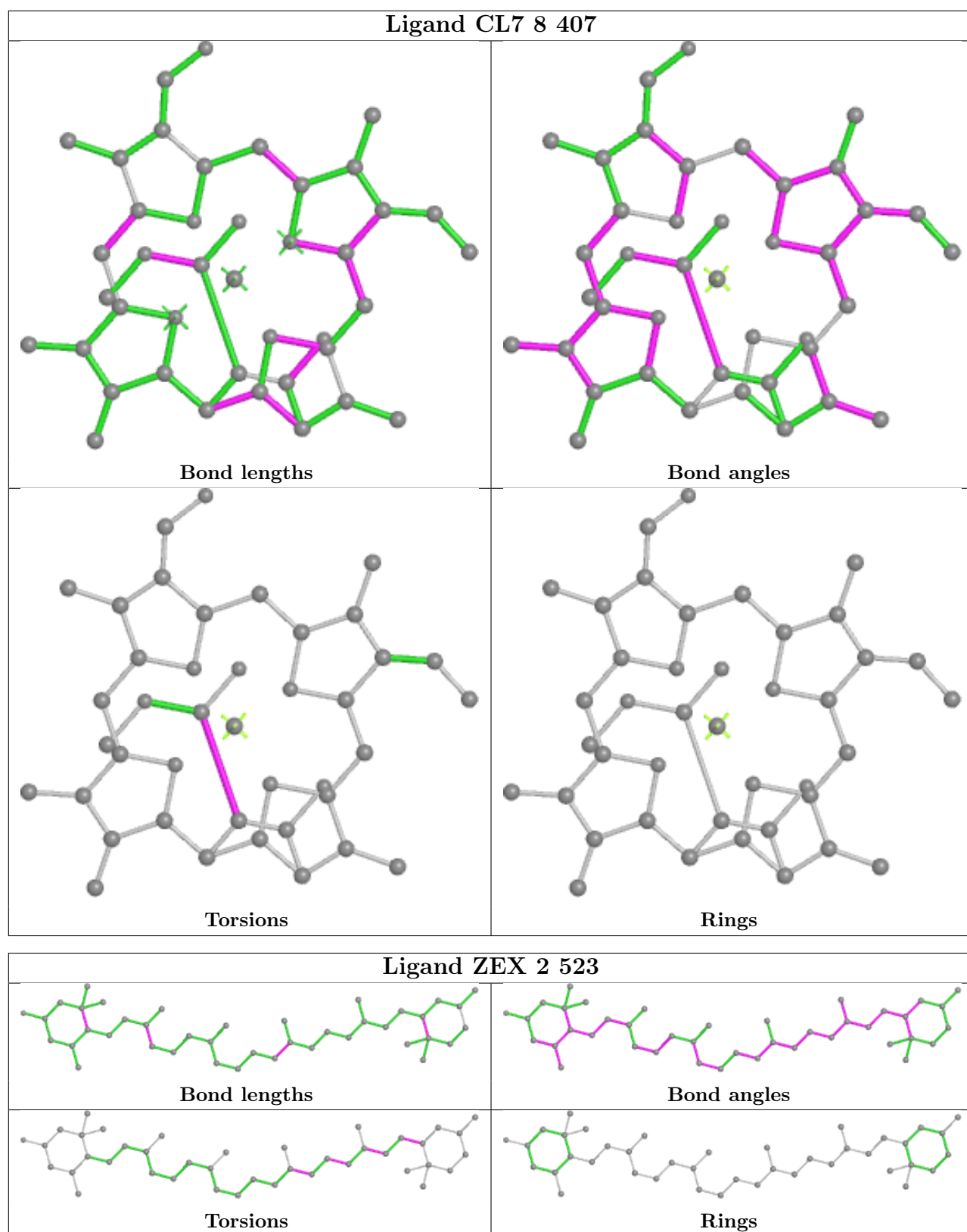


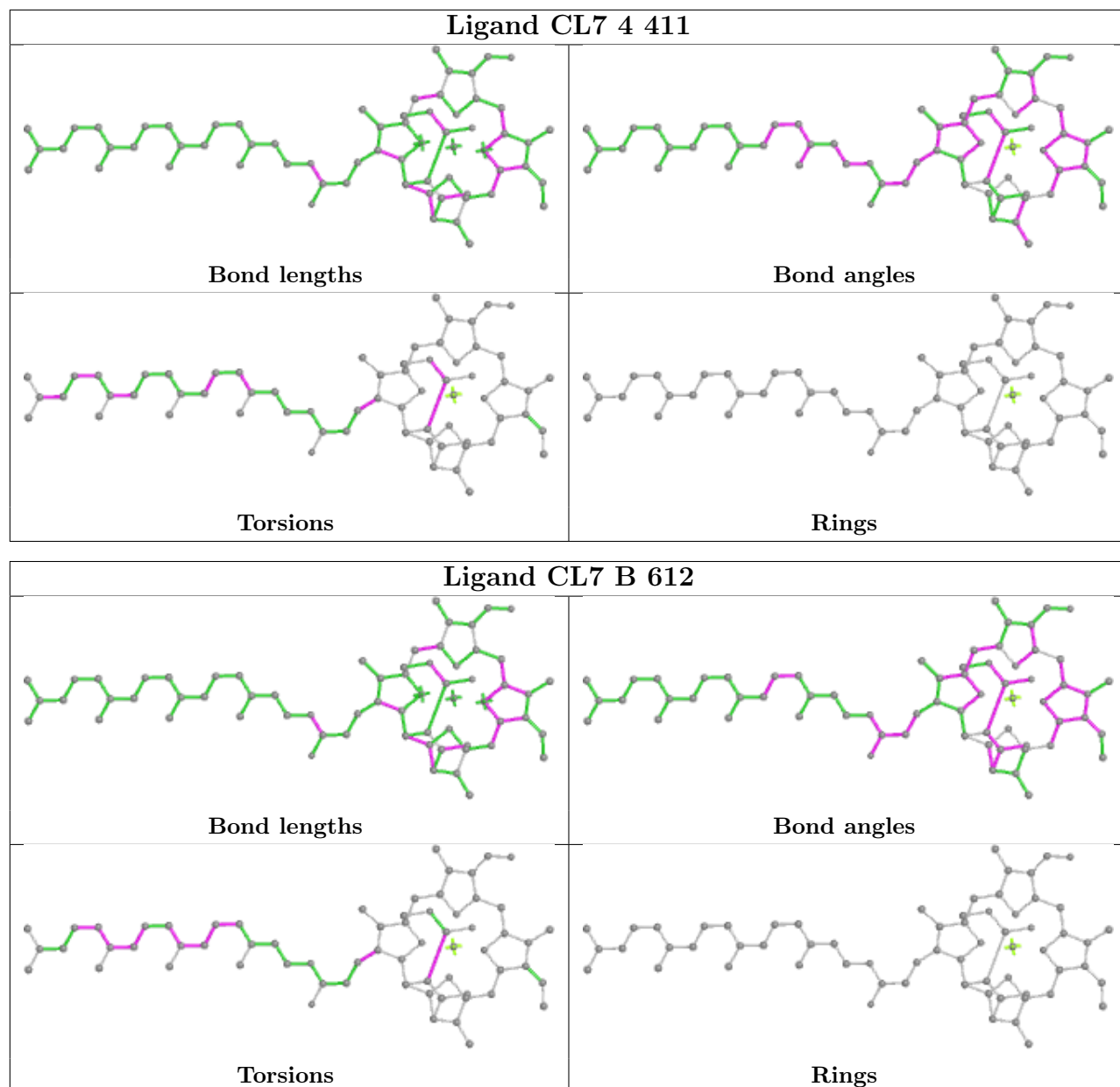




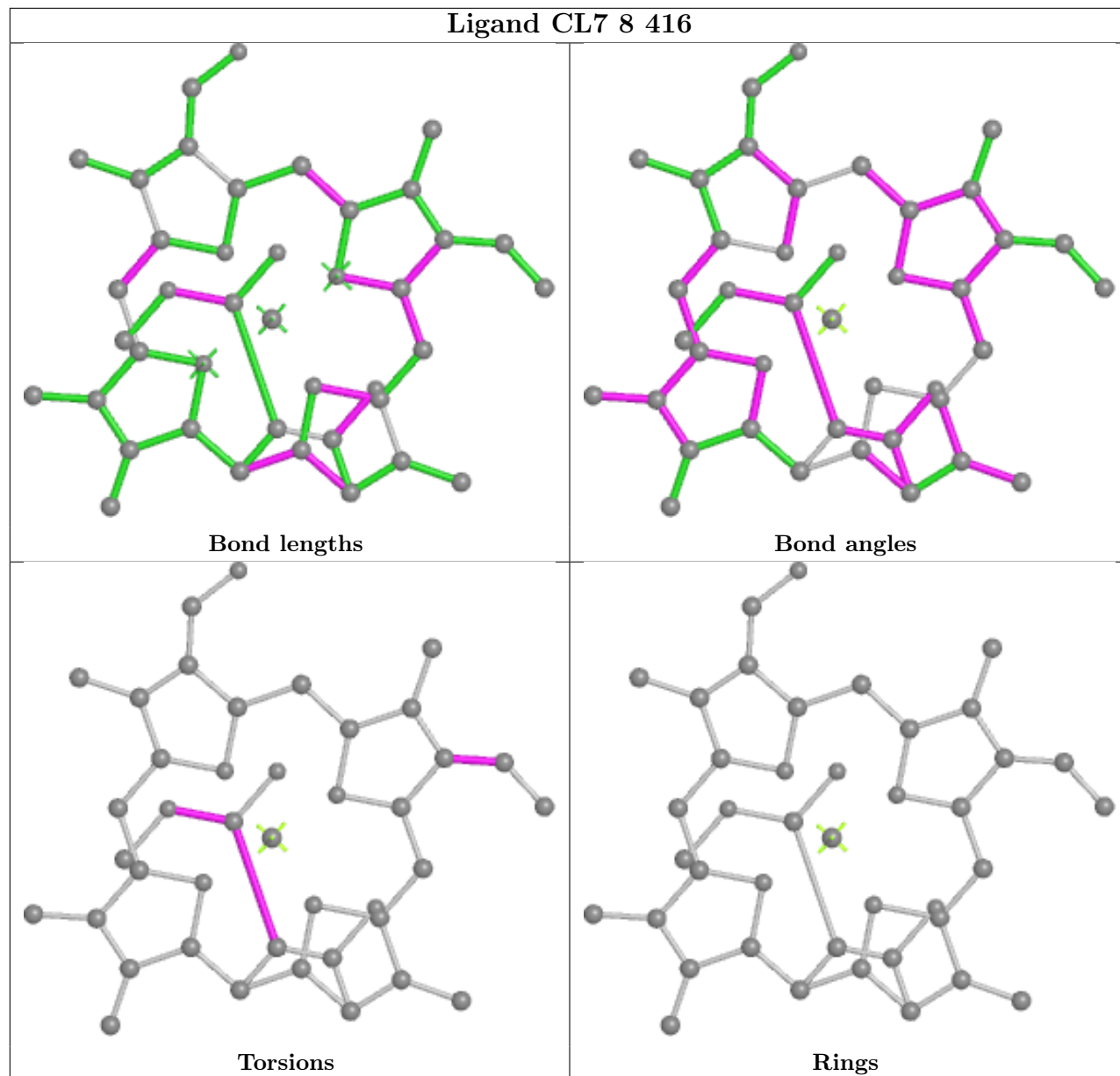


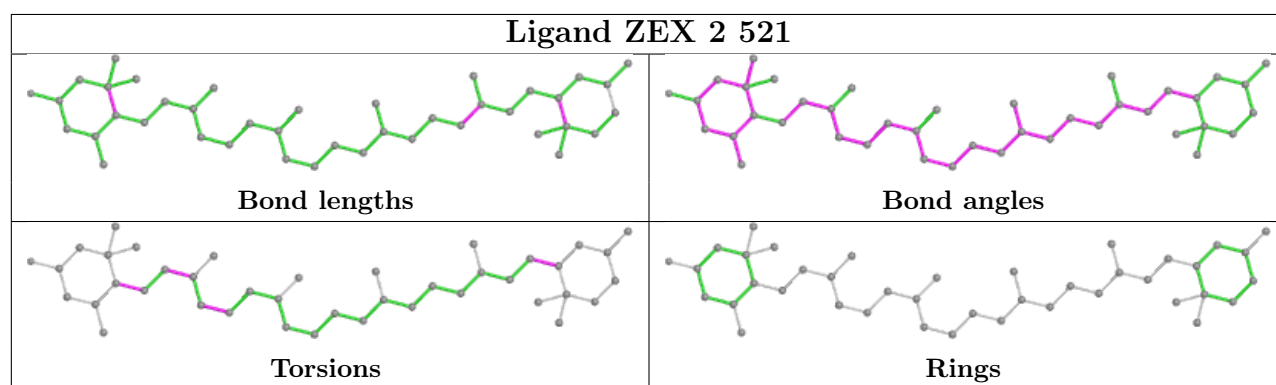
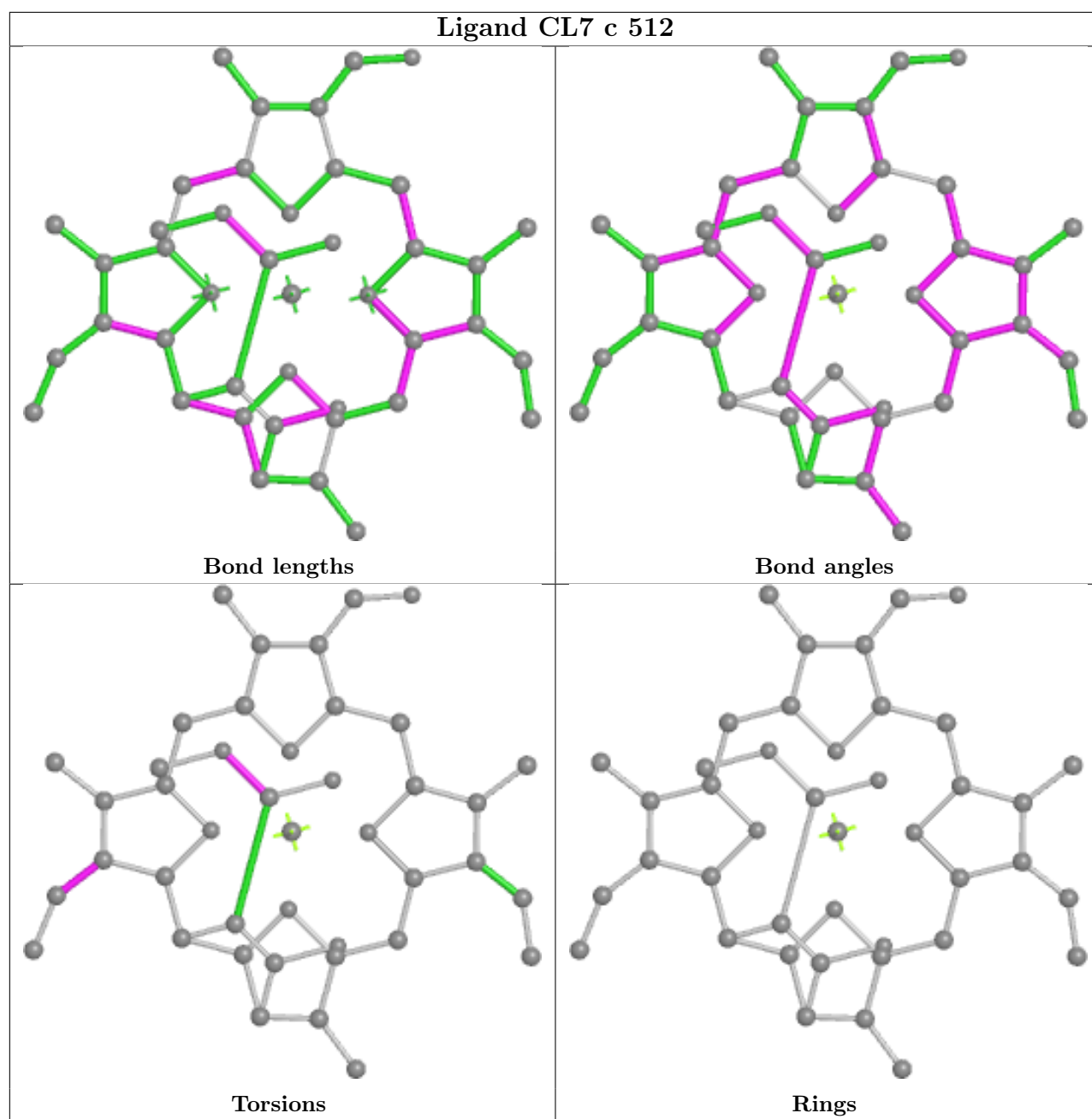


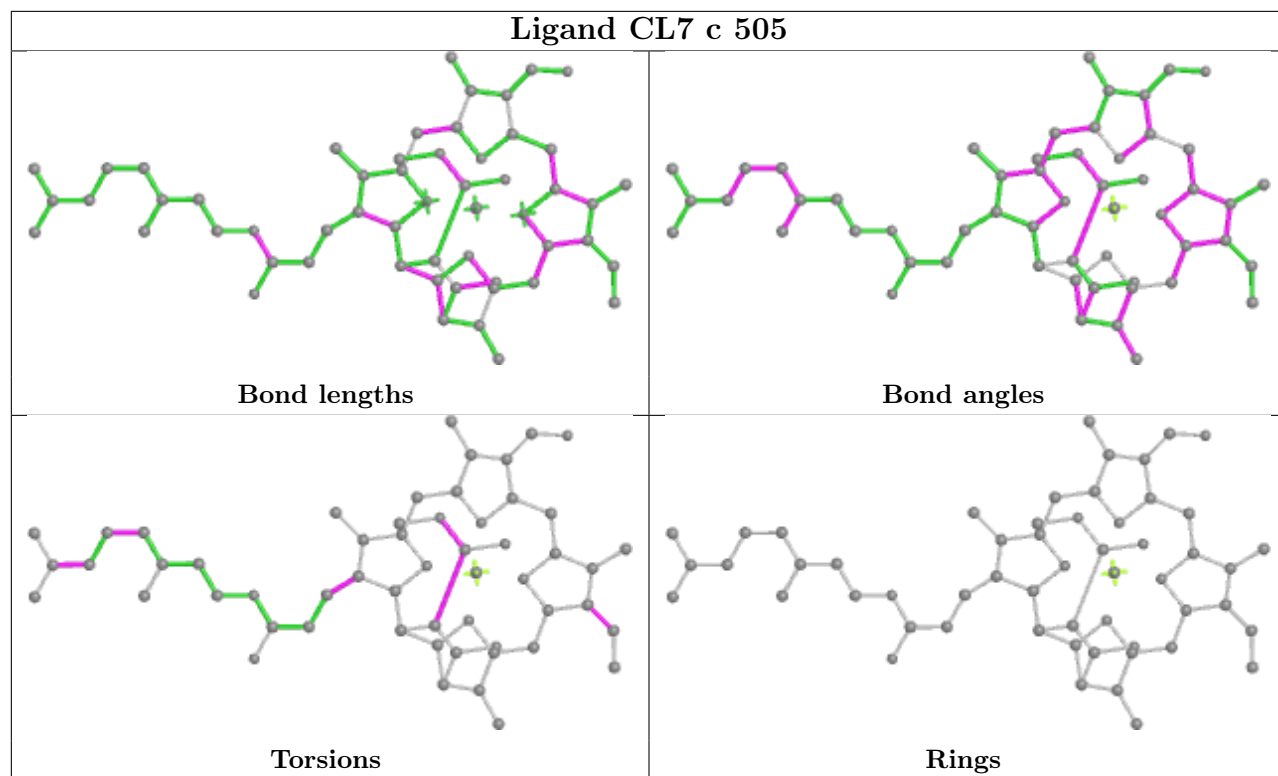




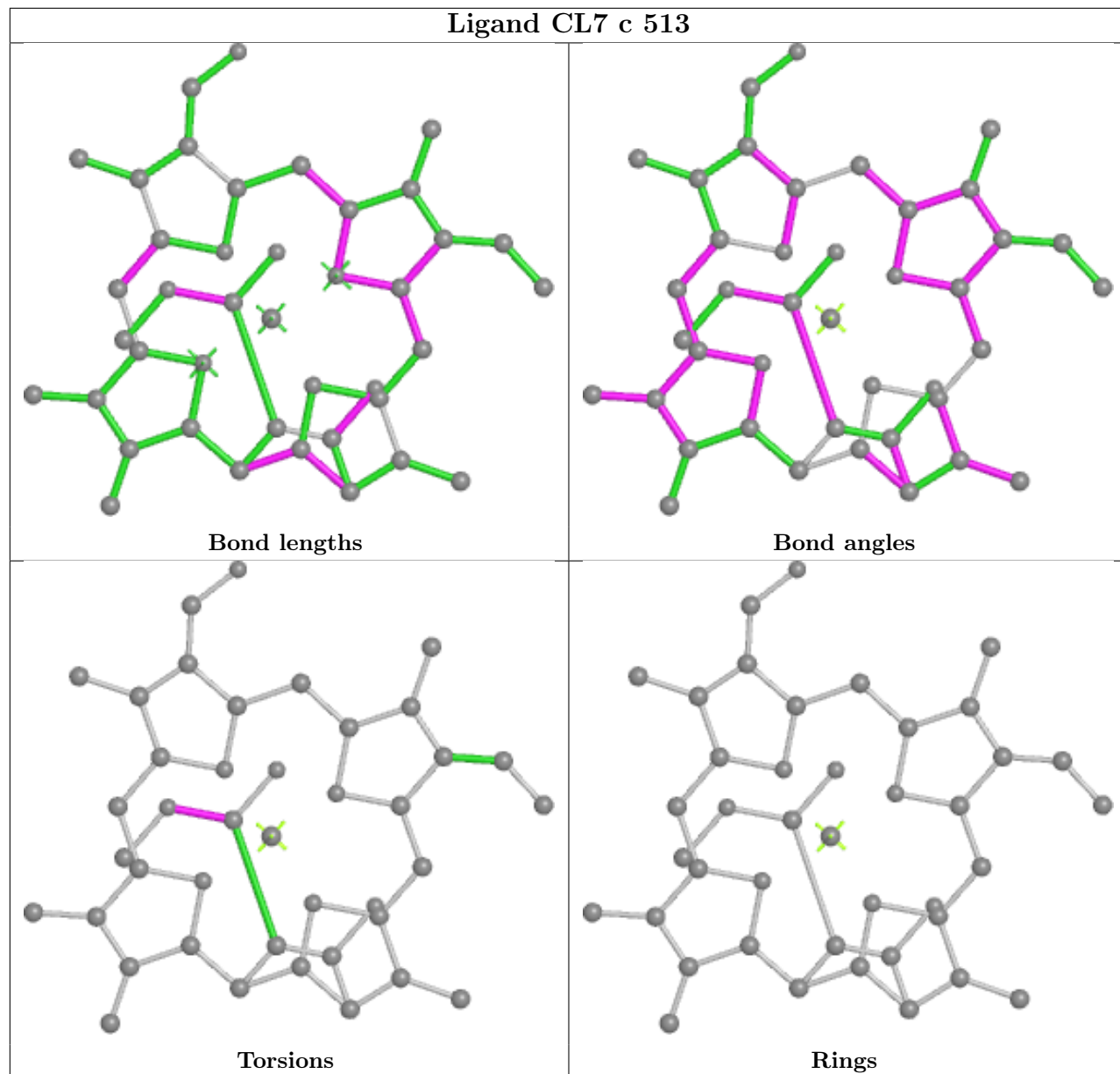
Ligand CL7 8 416

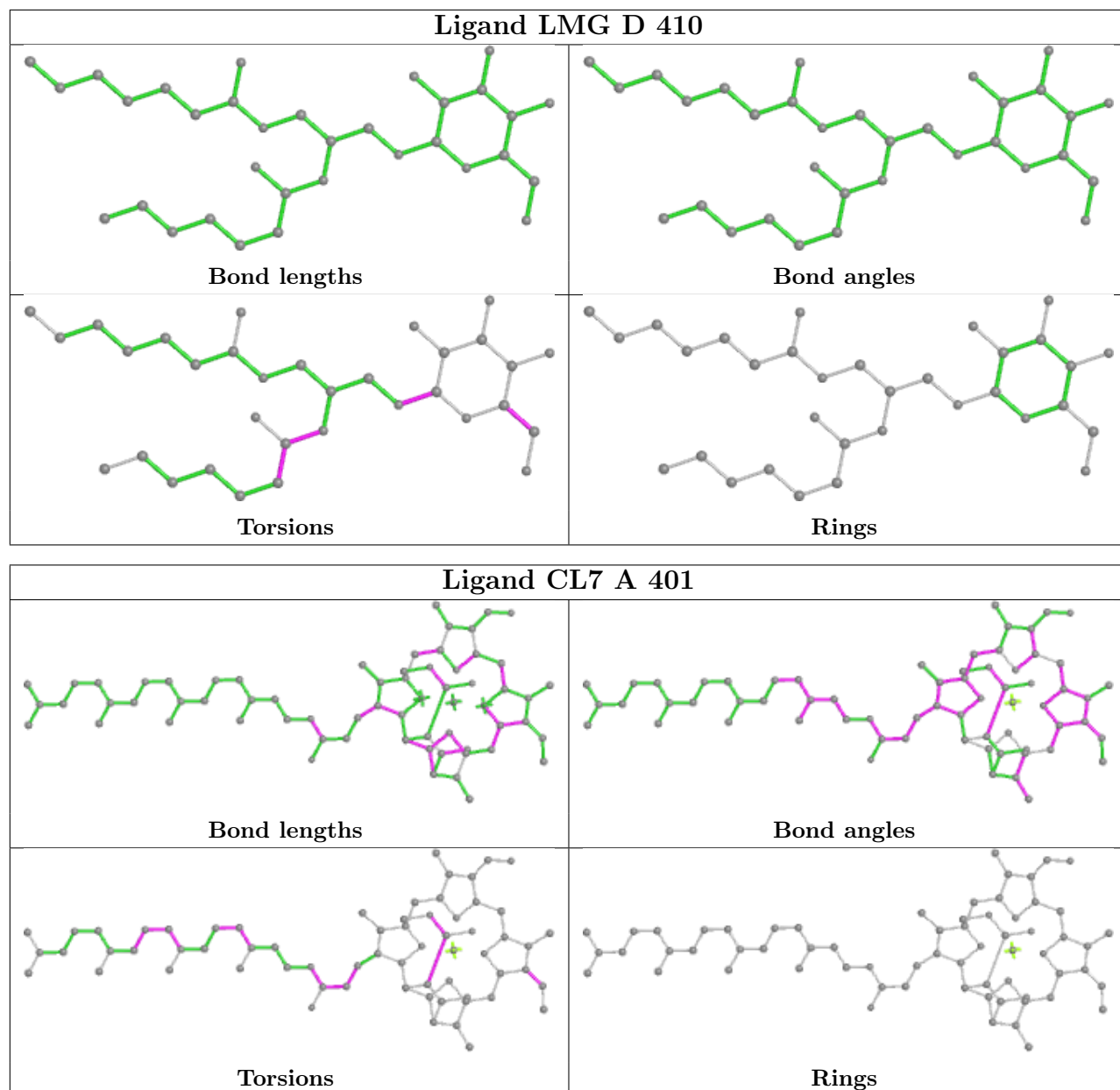


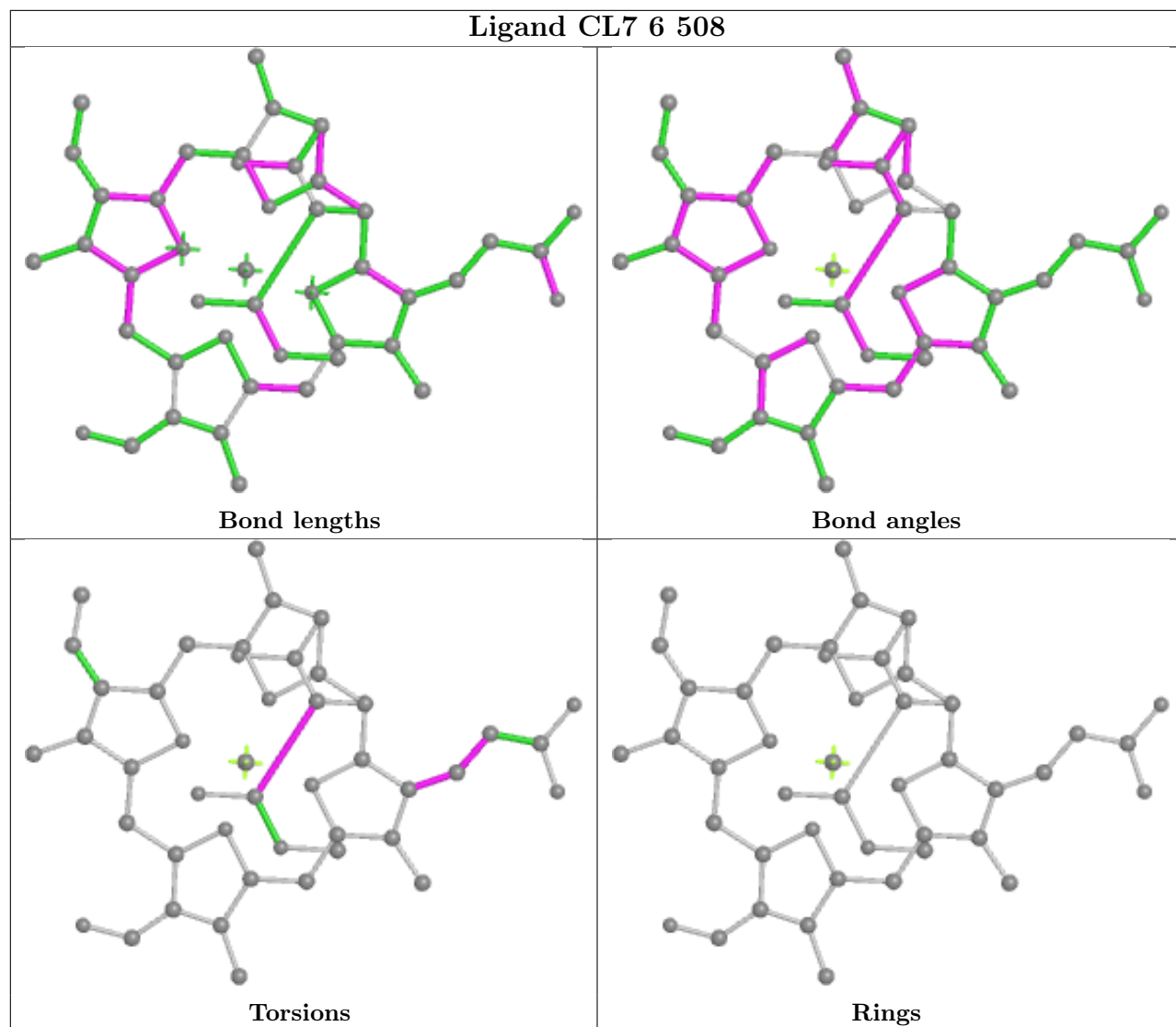


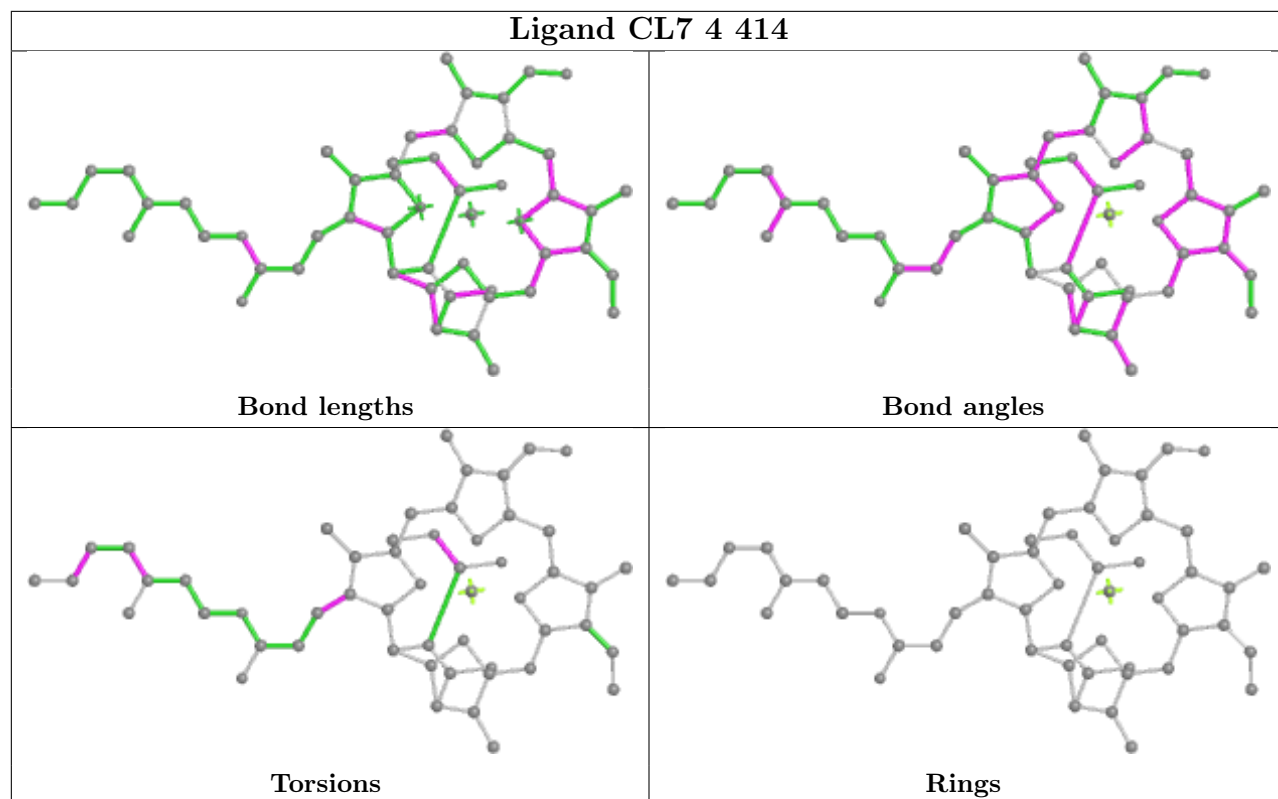


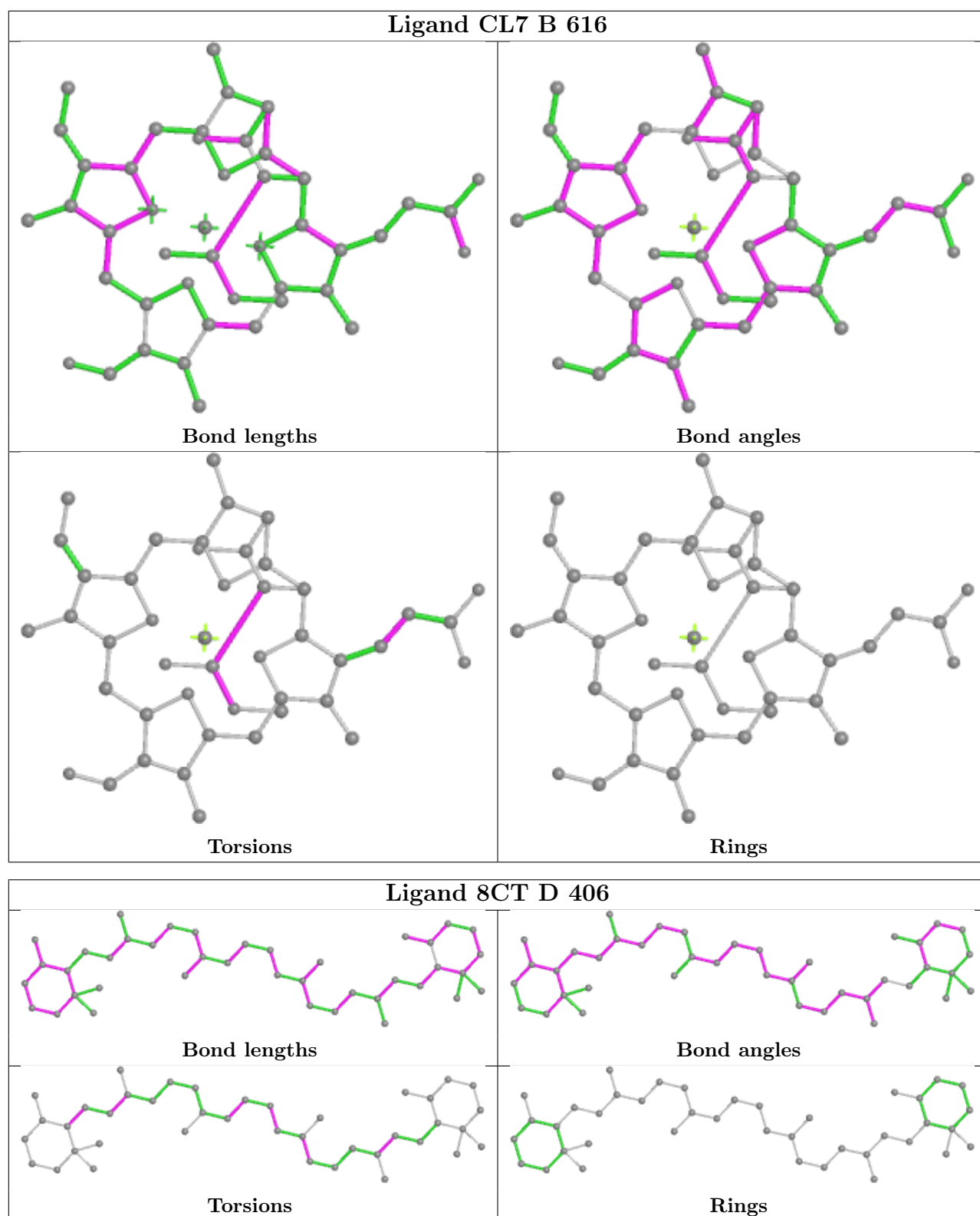
Ligand CL7 c 513

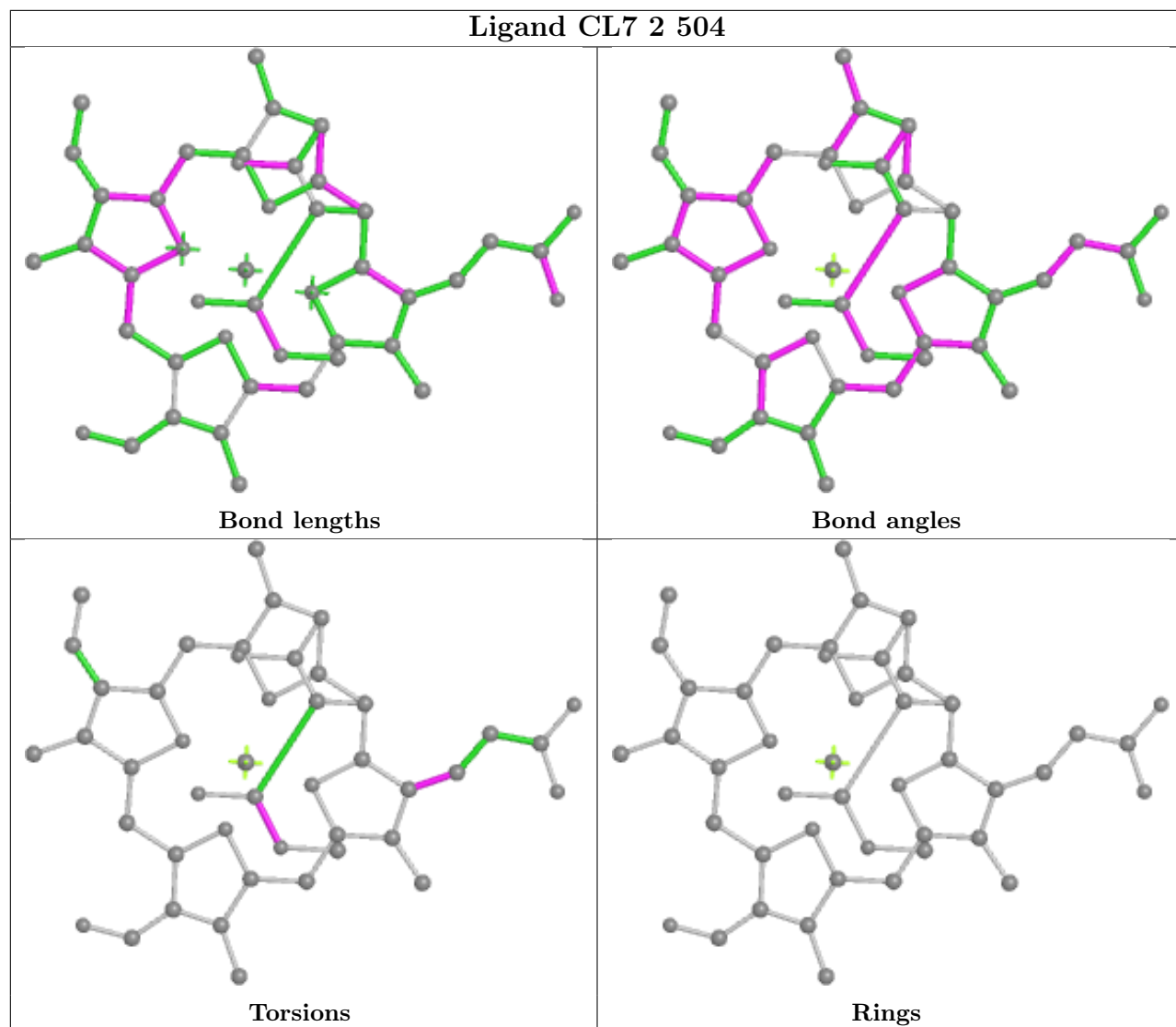


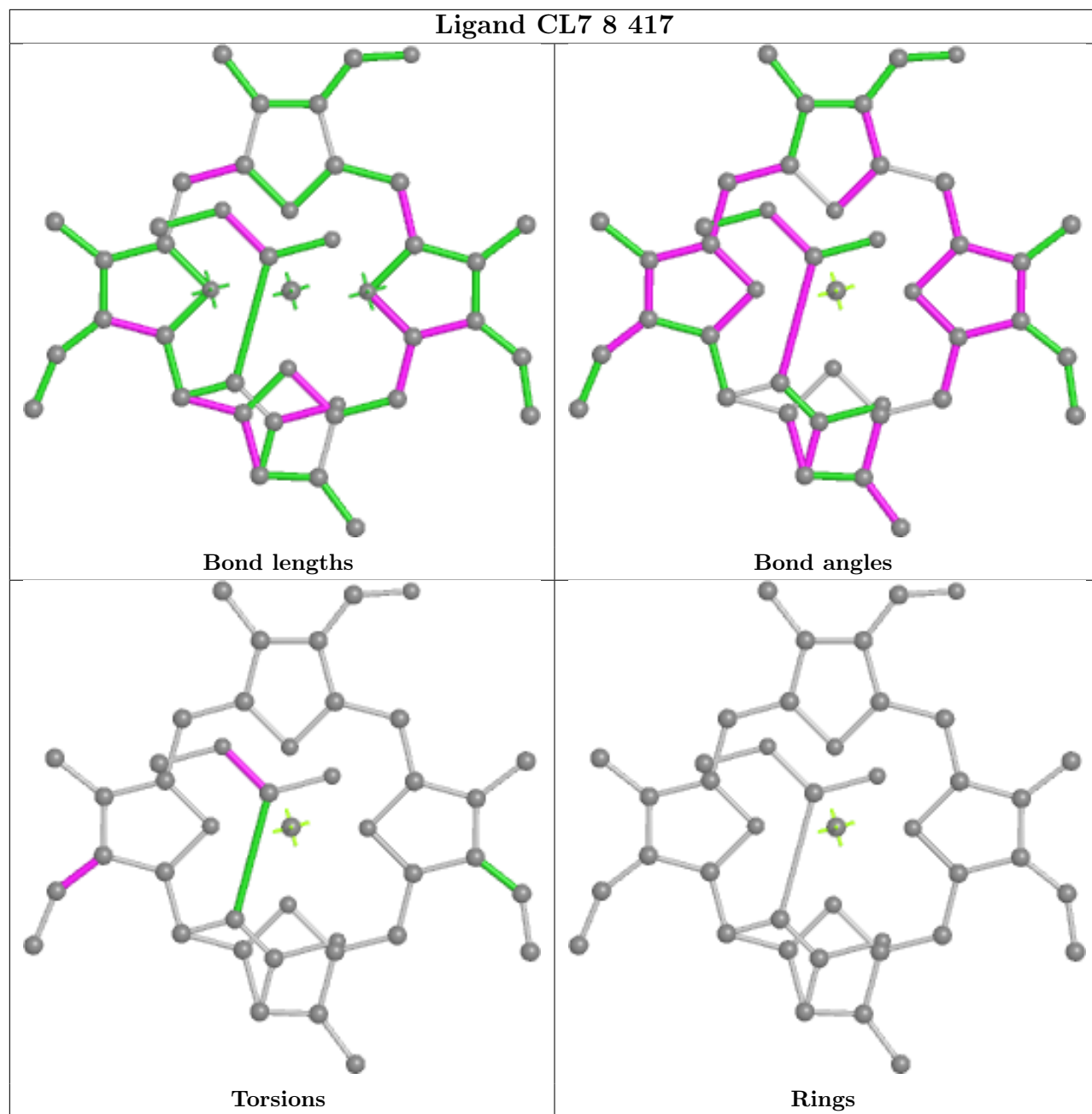


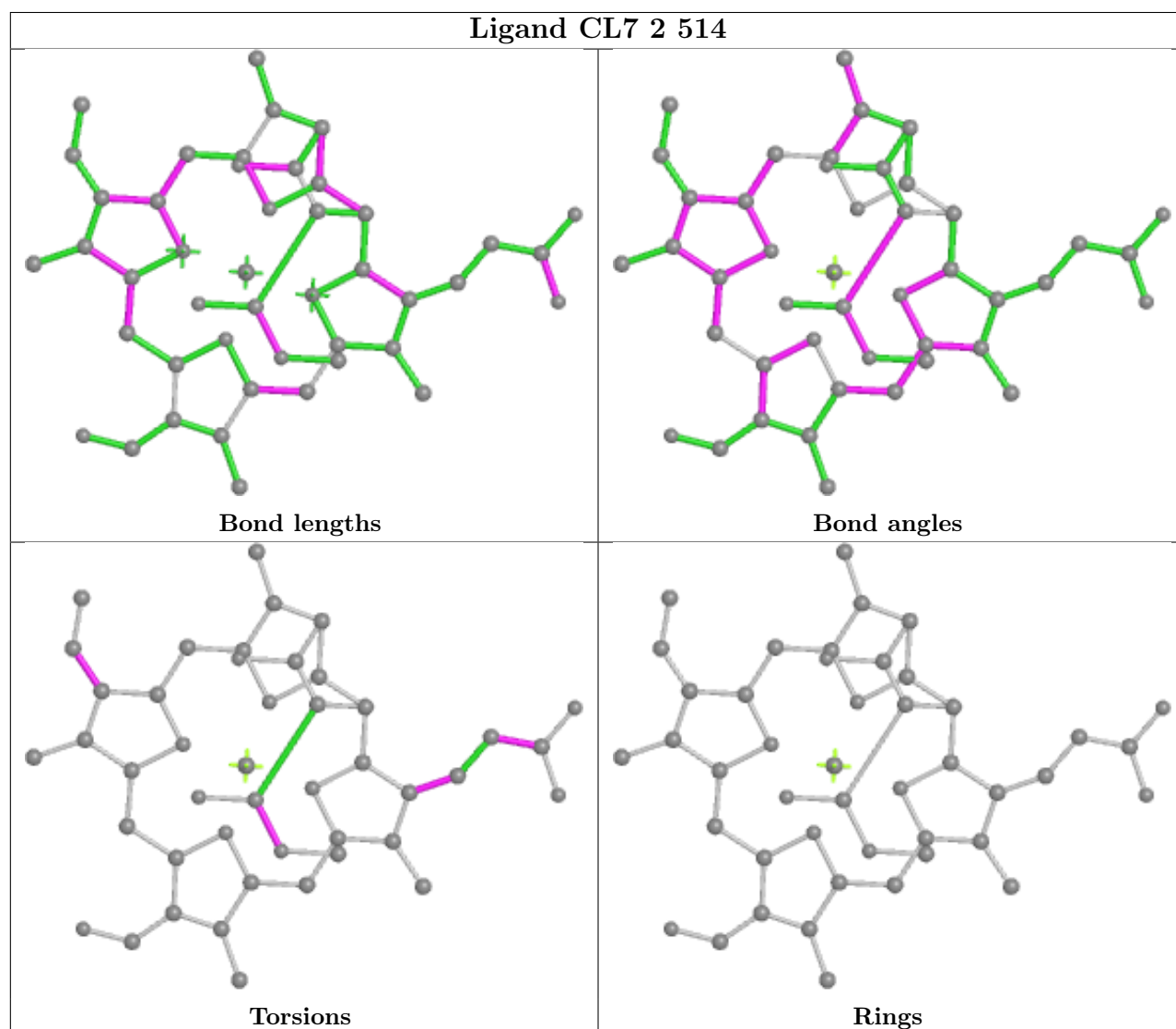
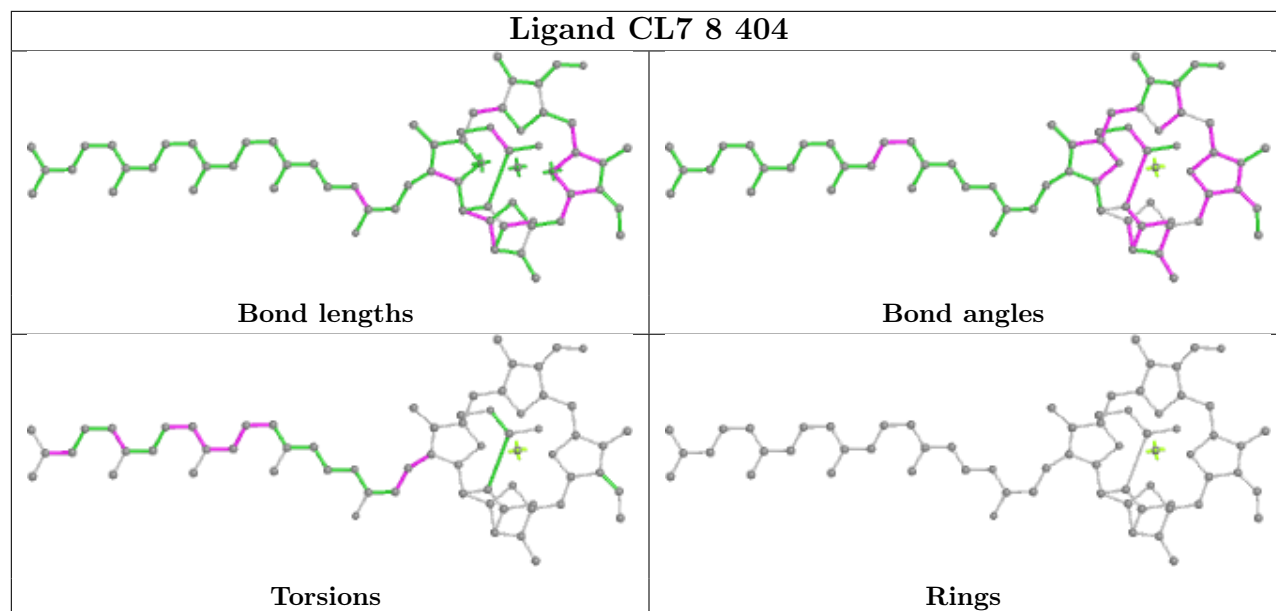


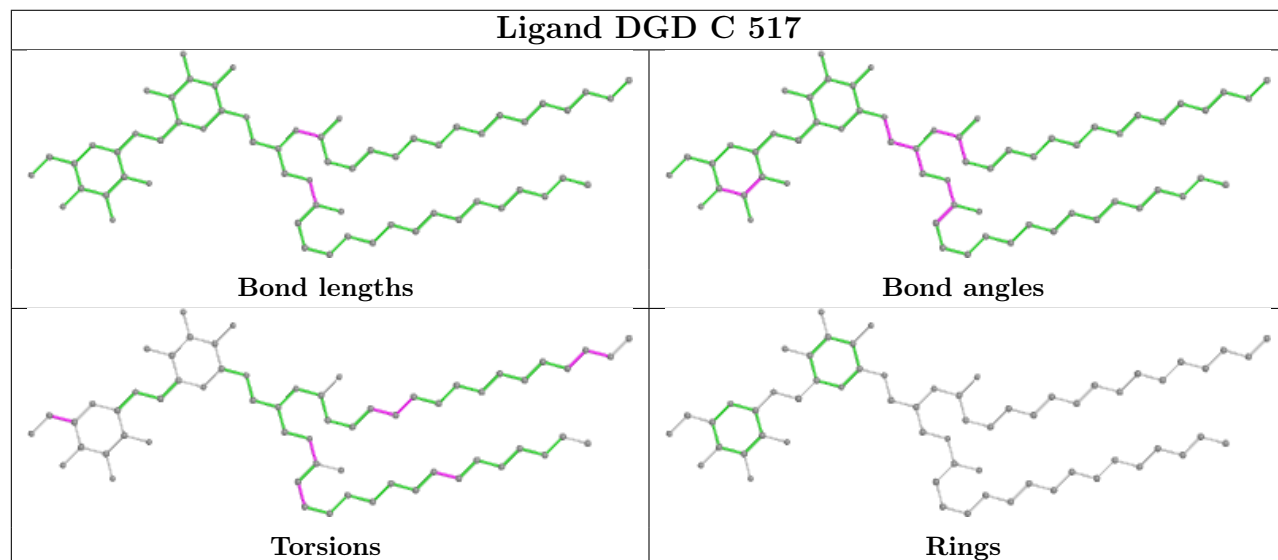
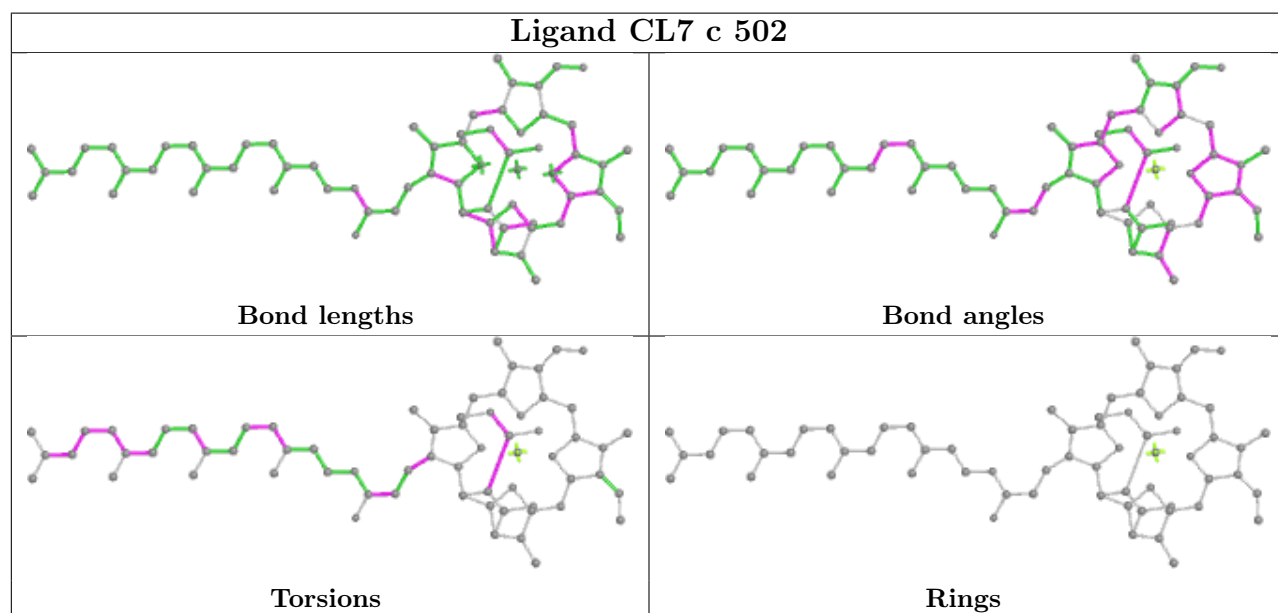
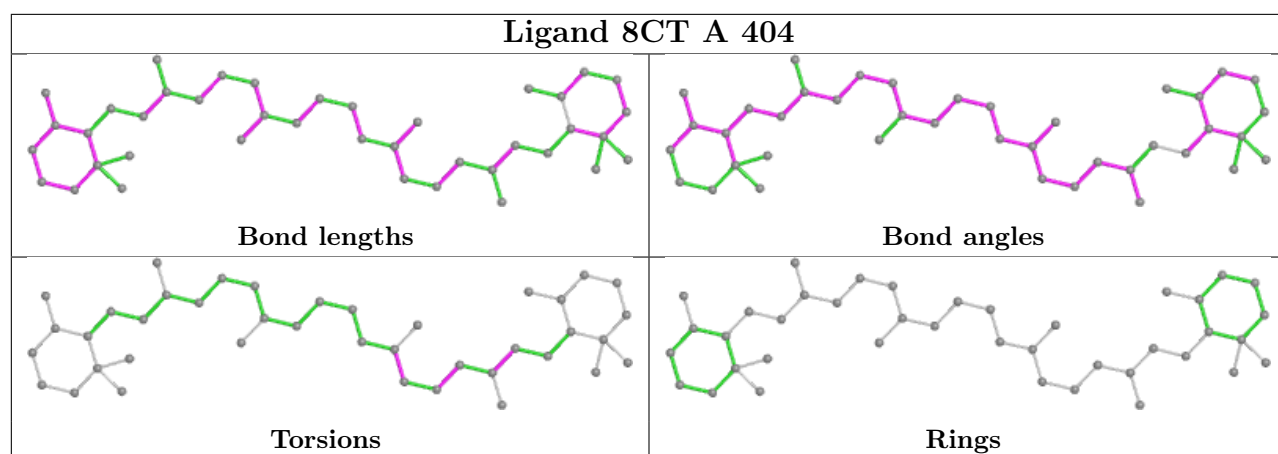


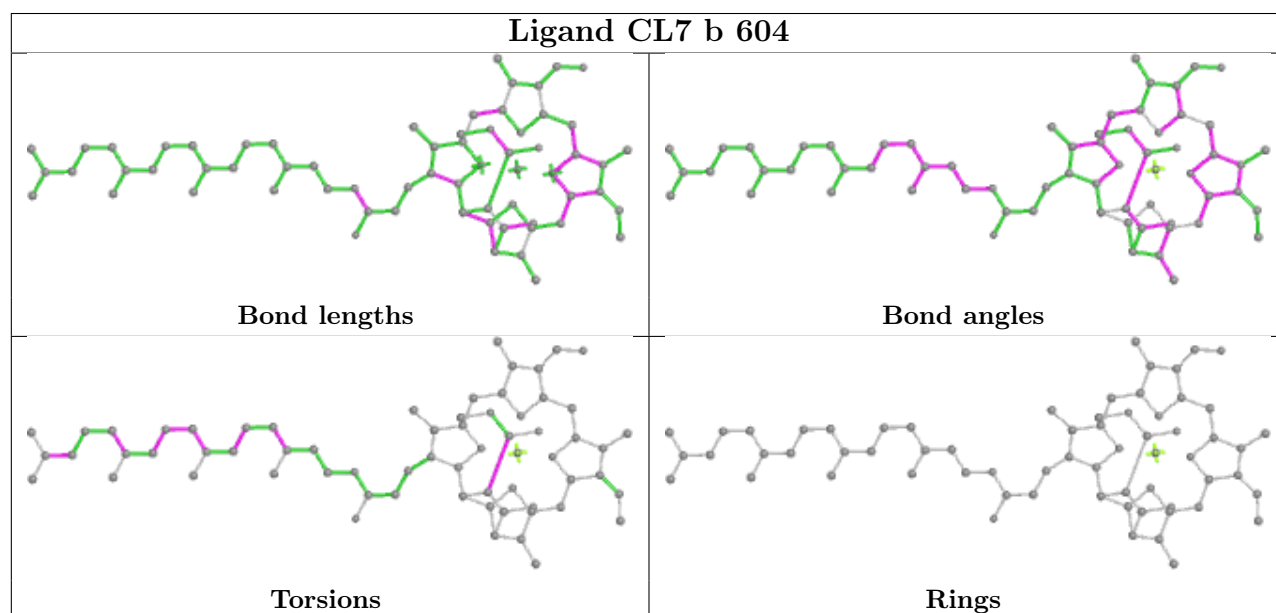
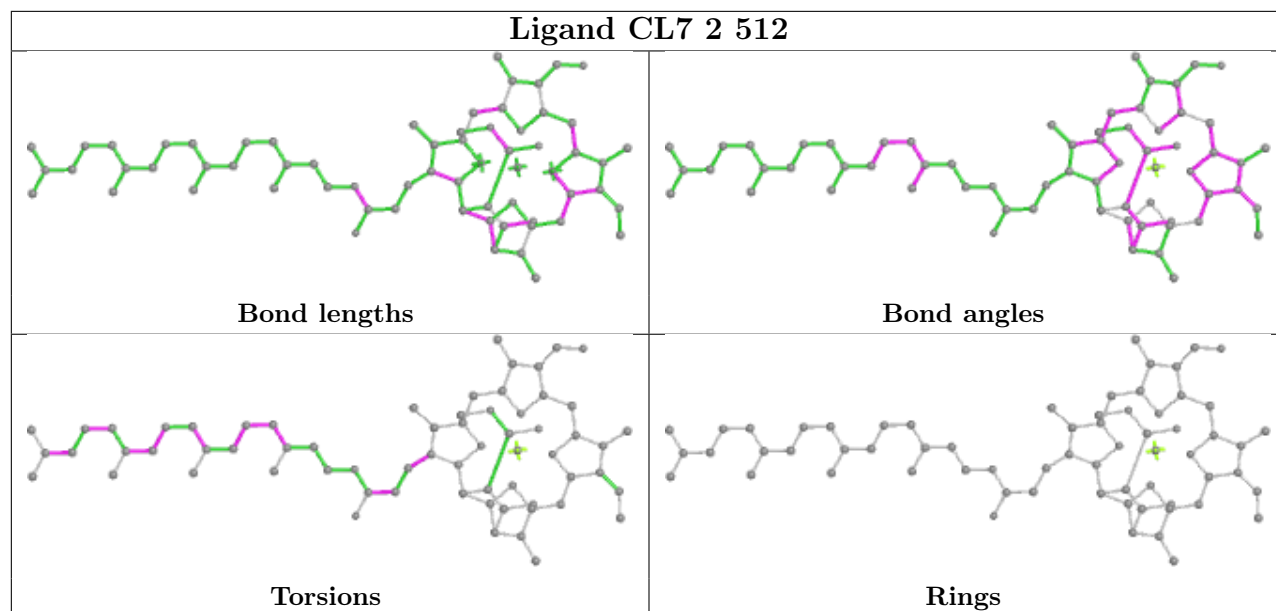


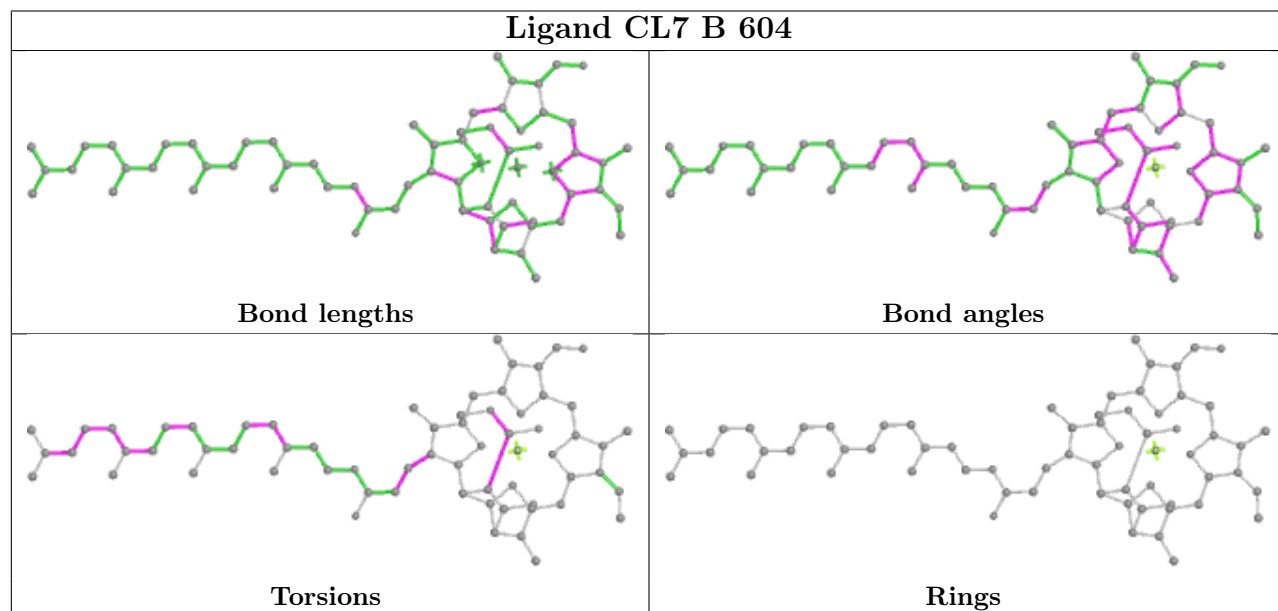
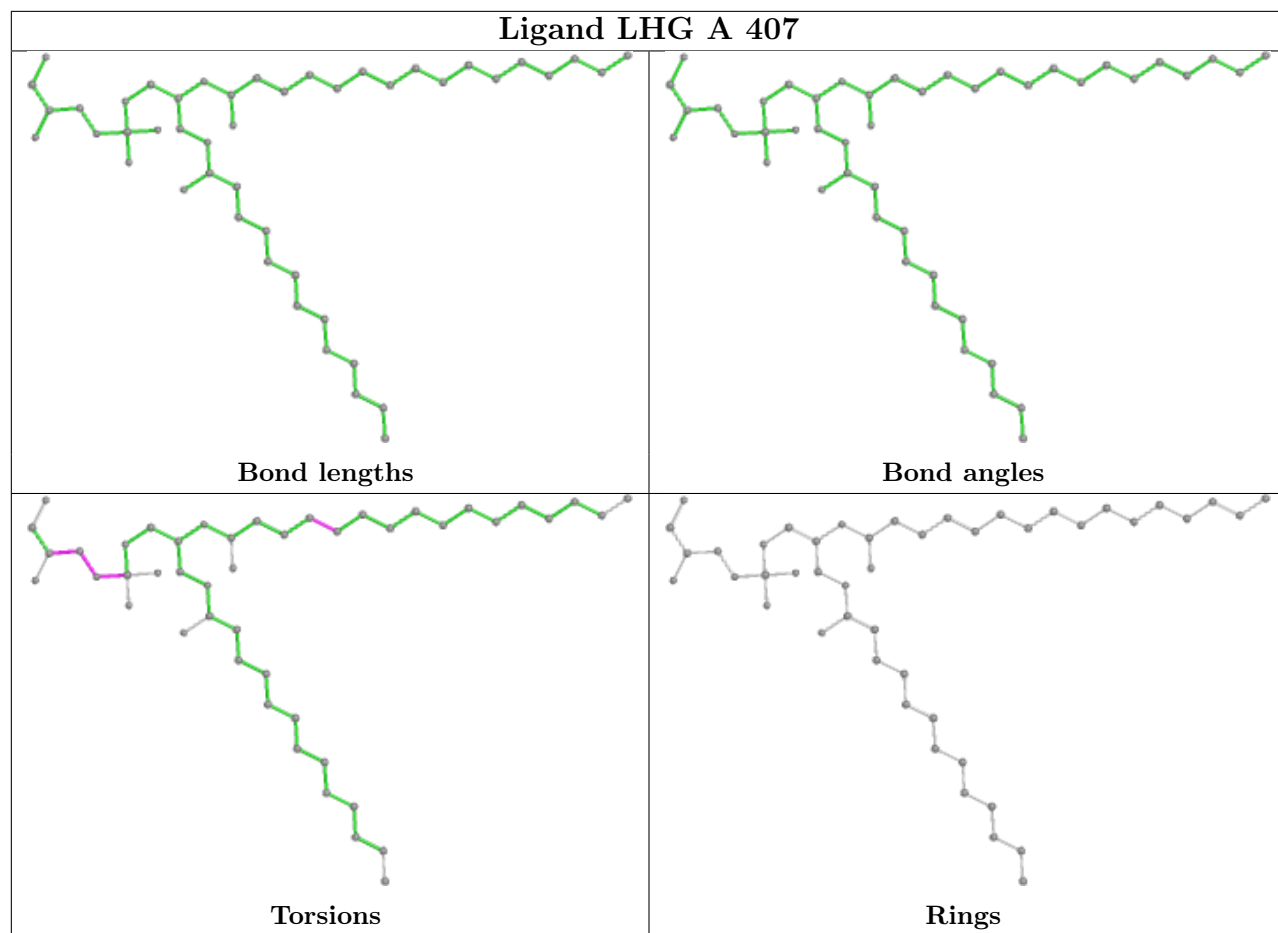


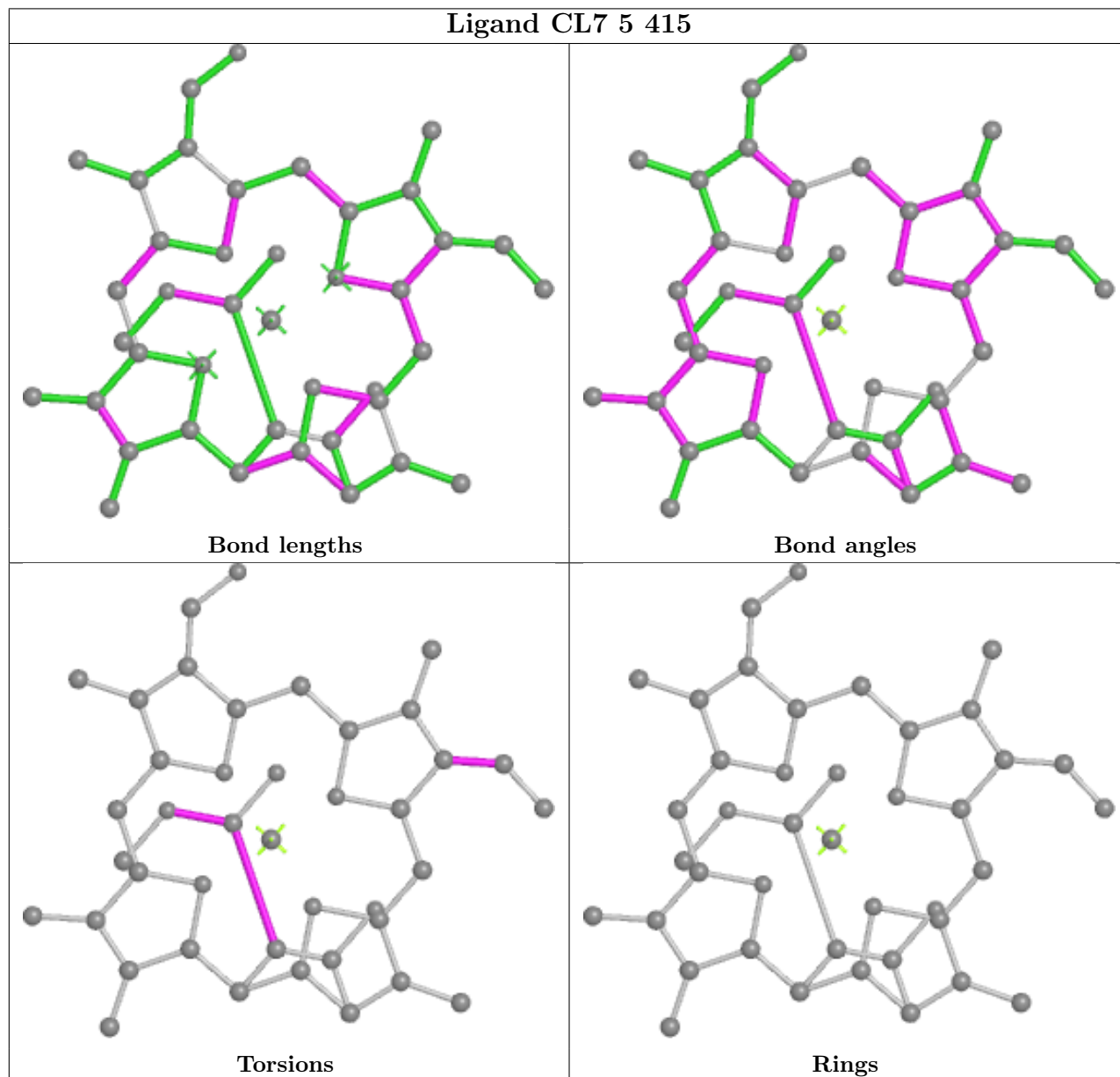
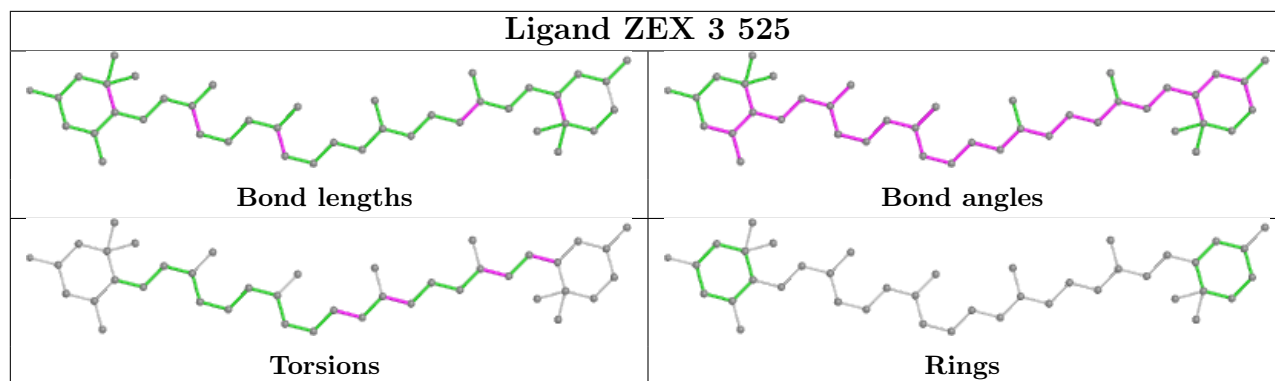


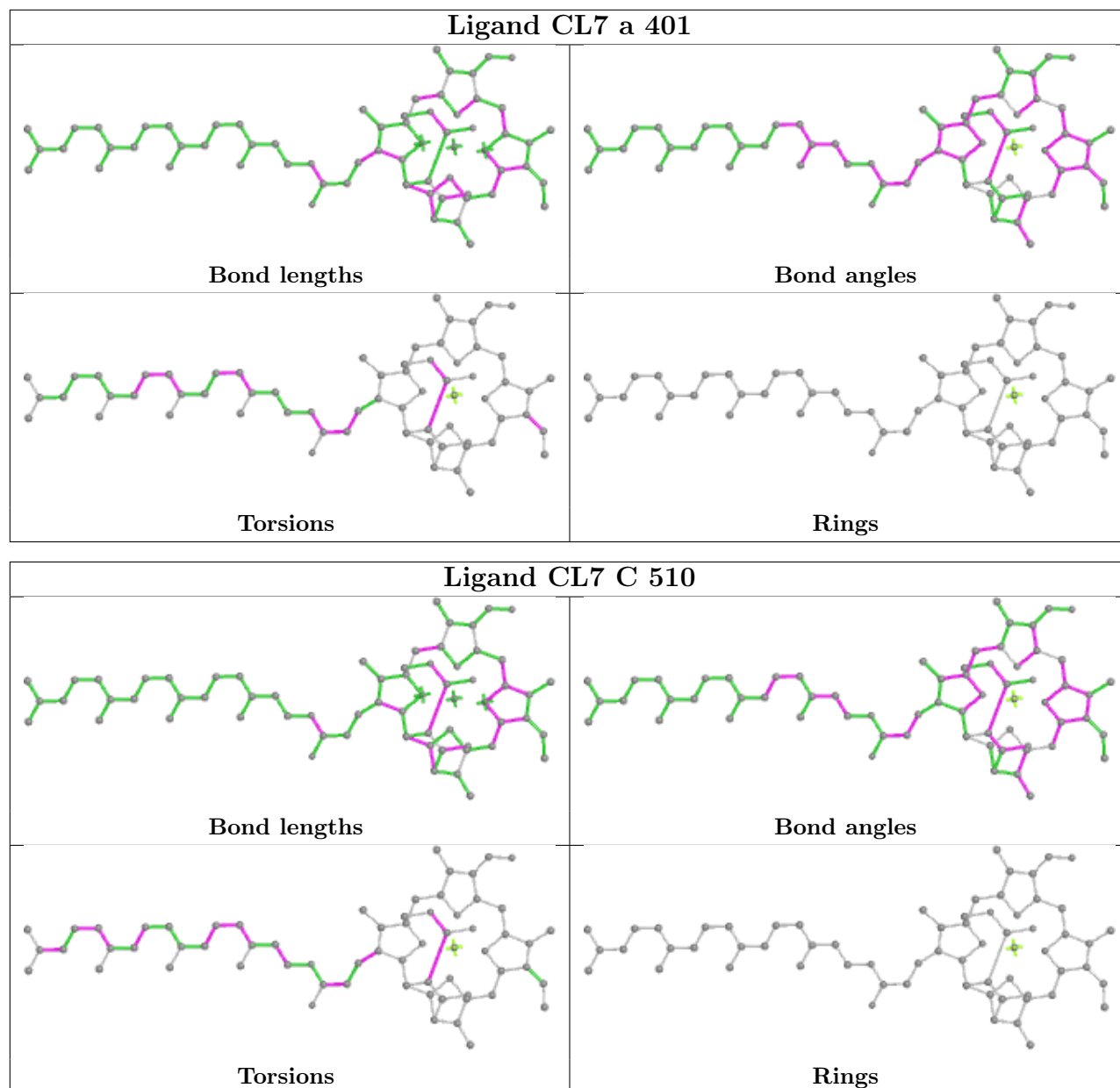


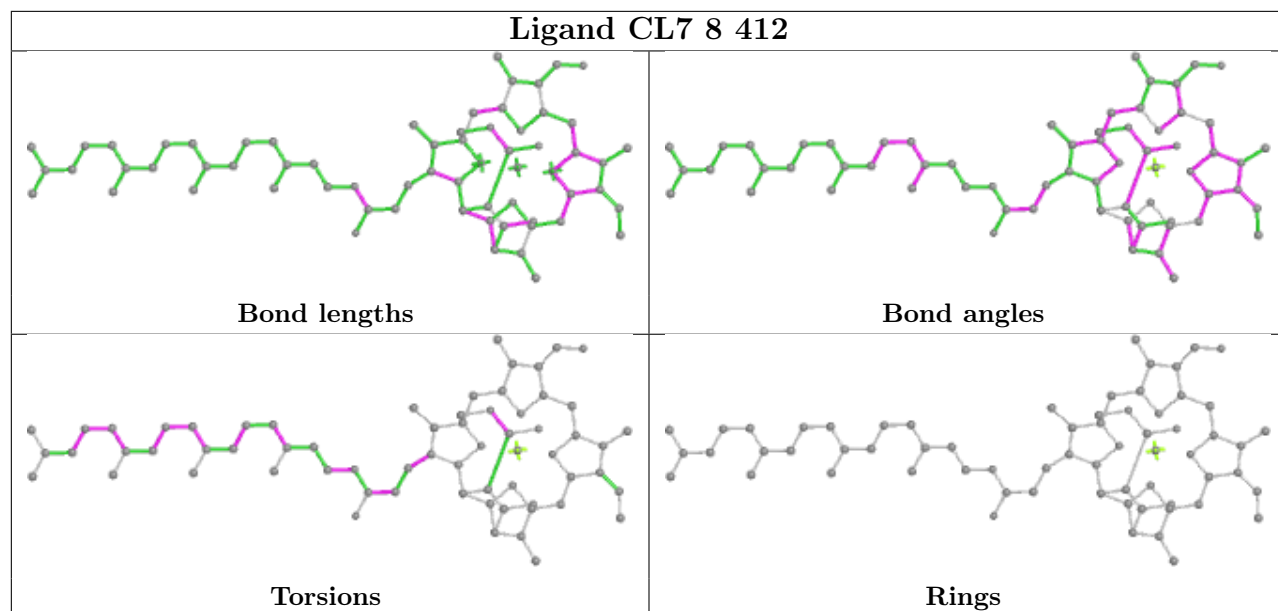


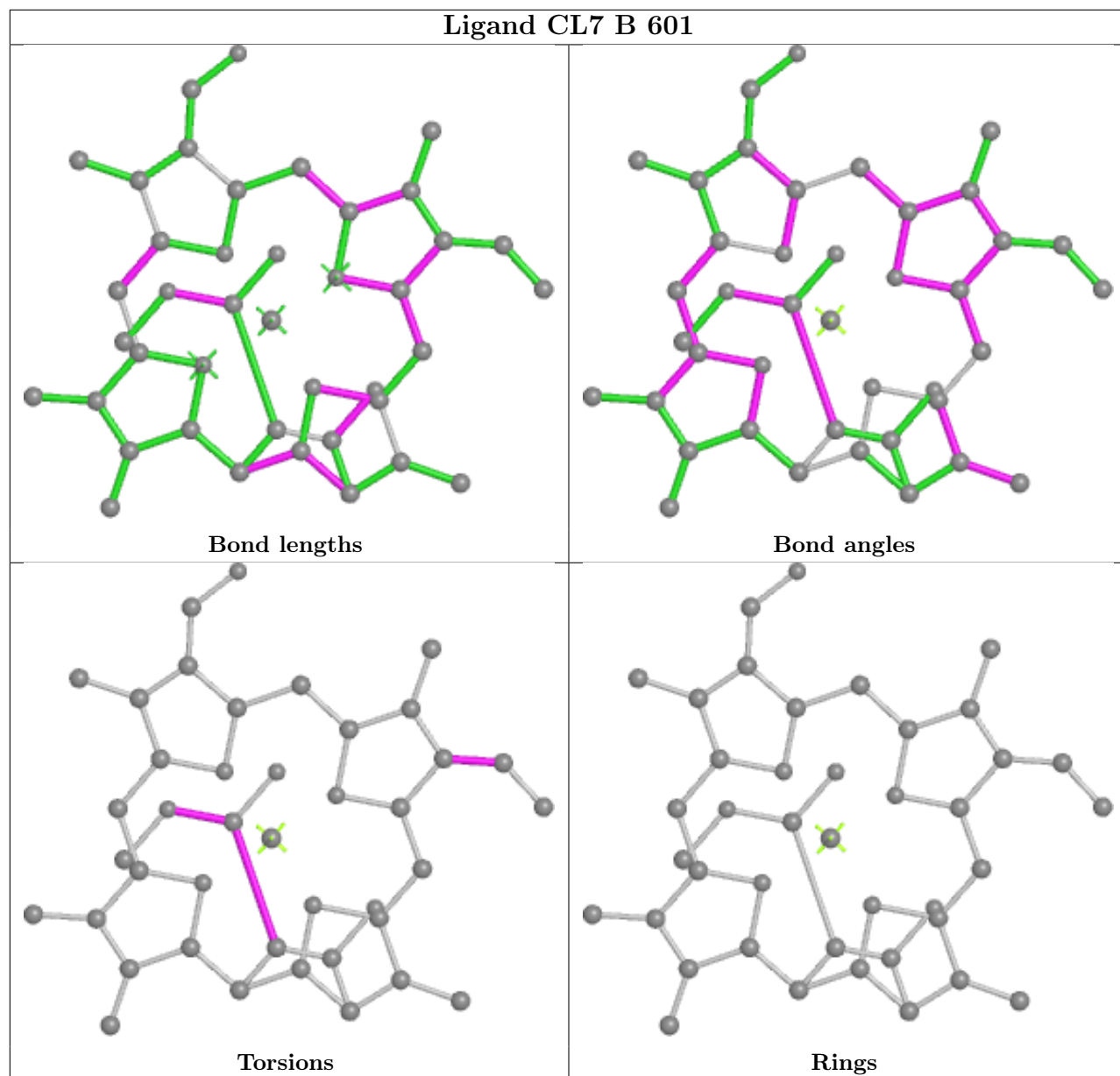


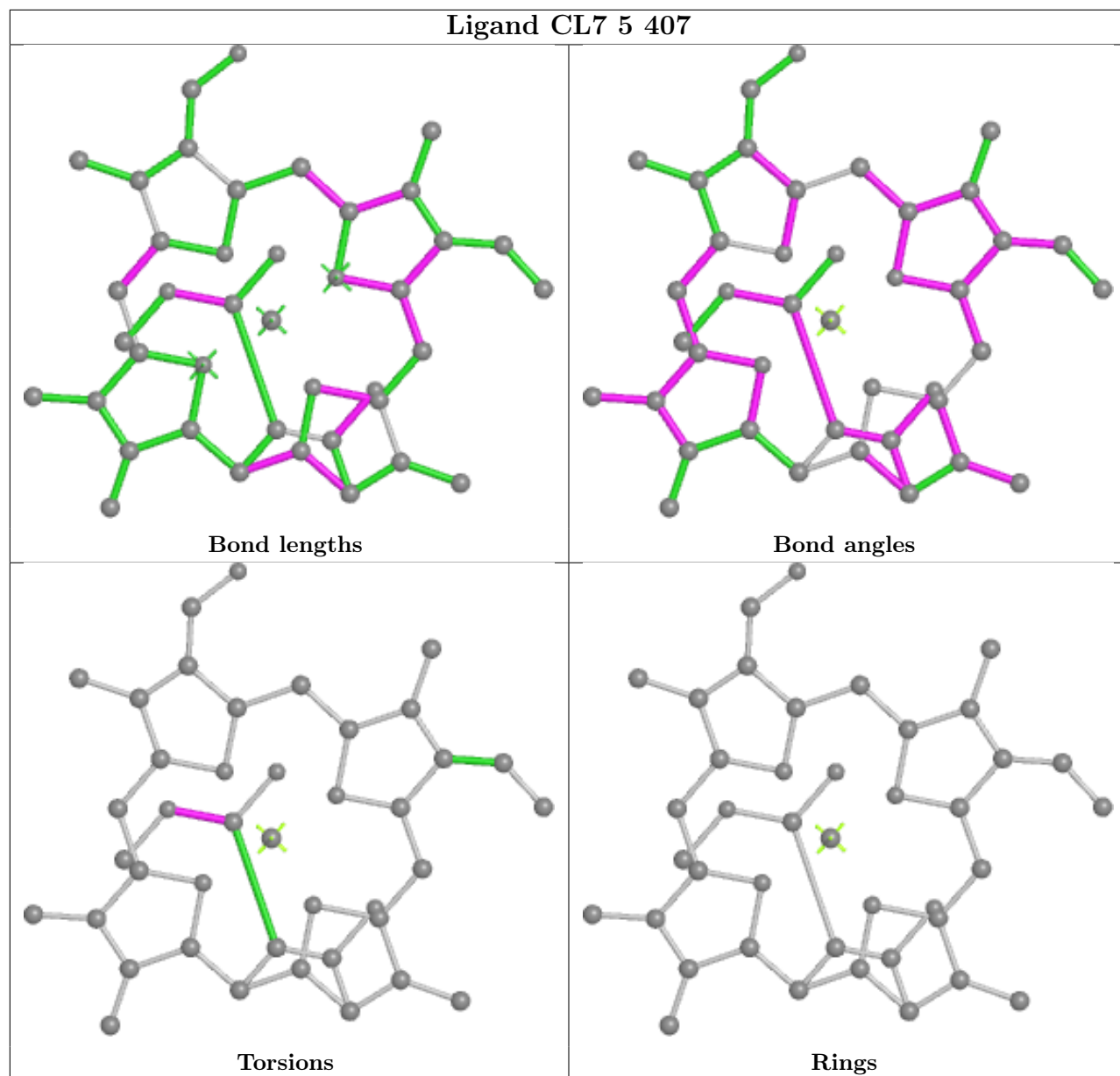


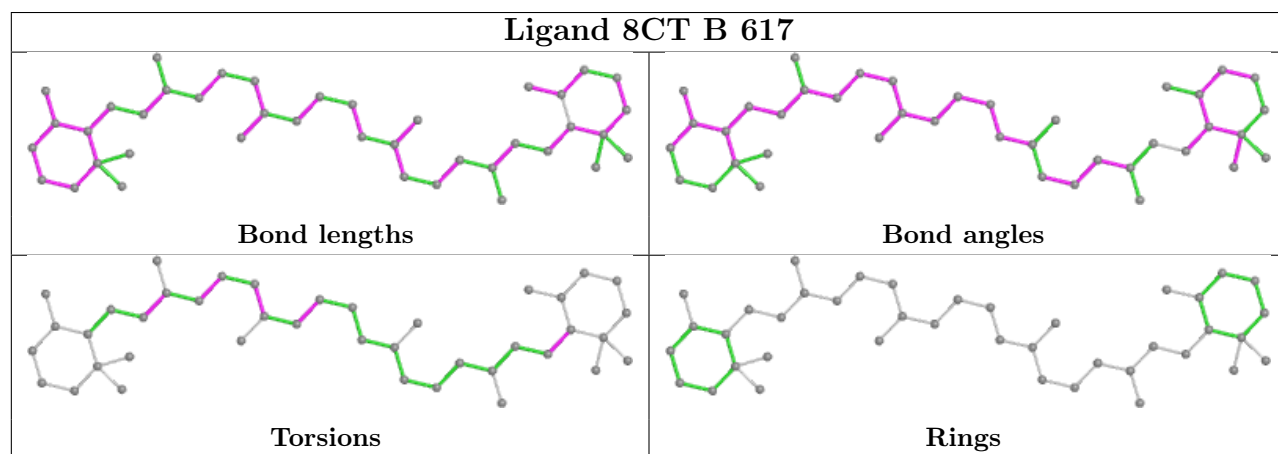
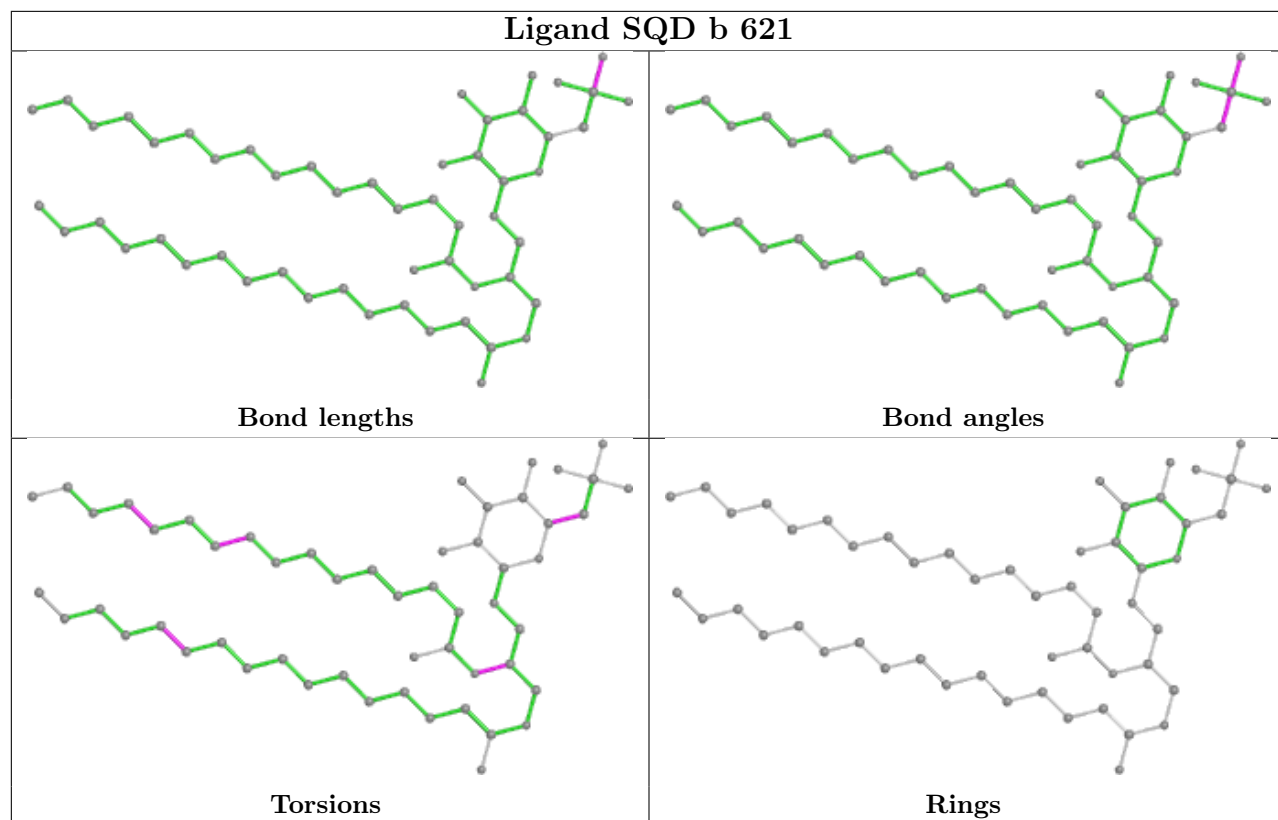


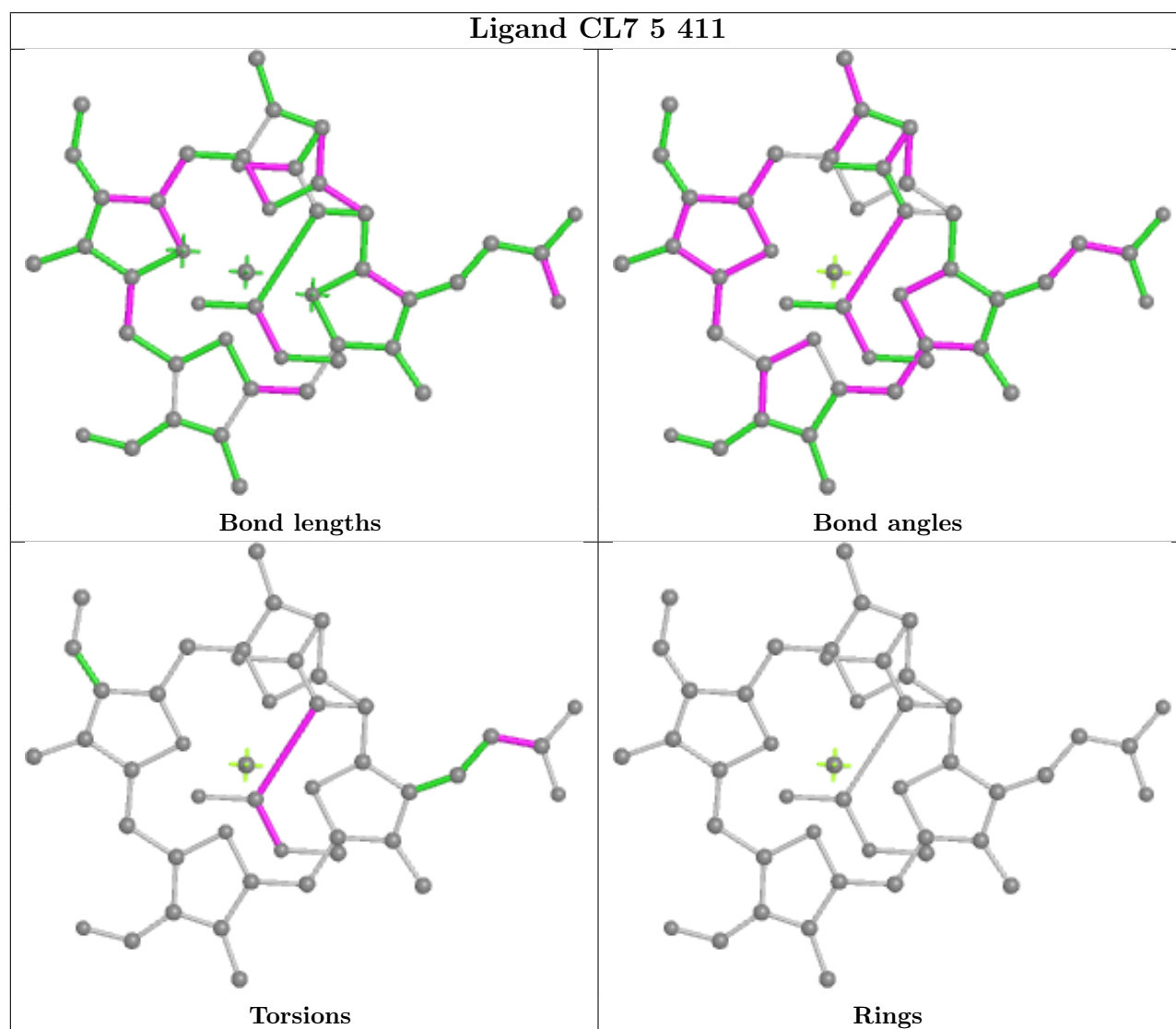
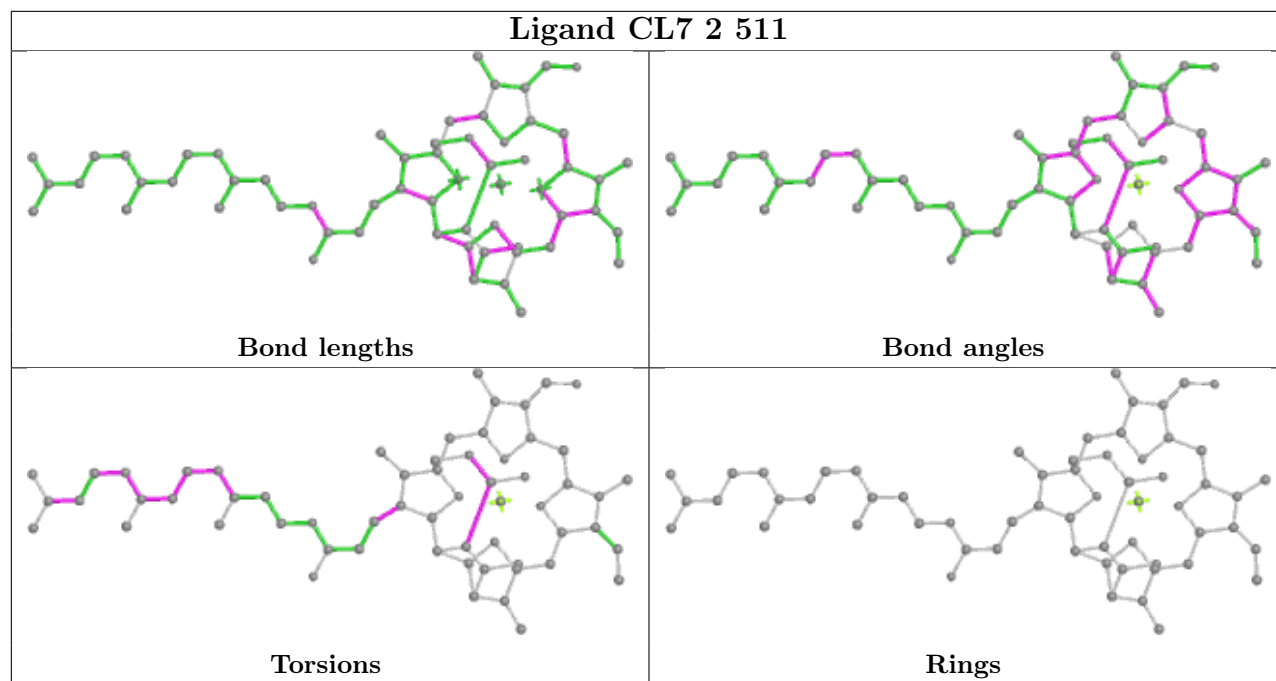


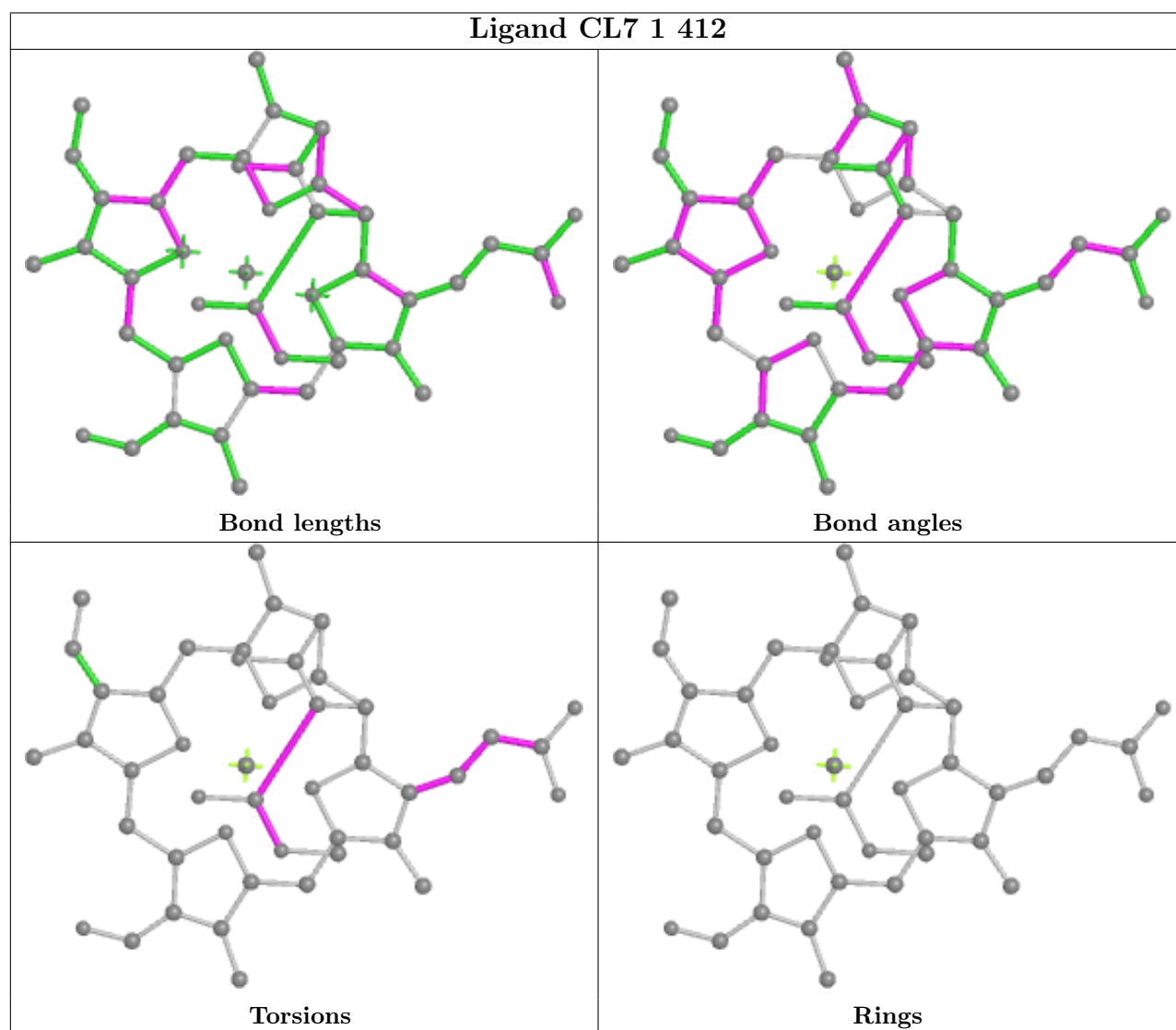
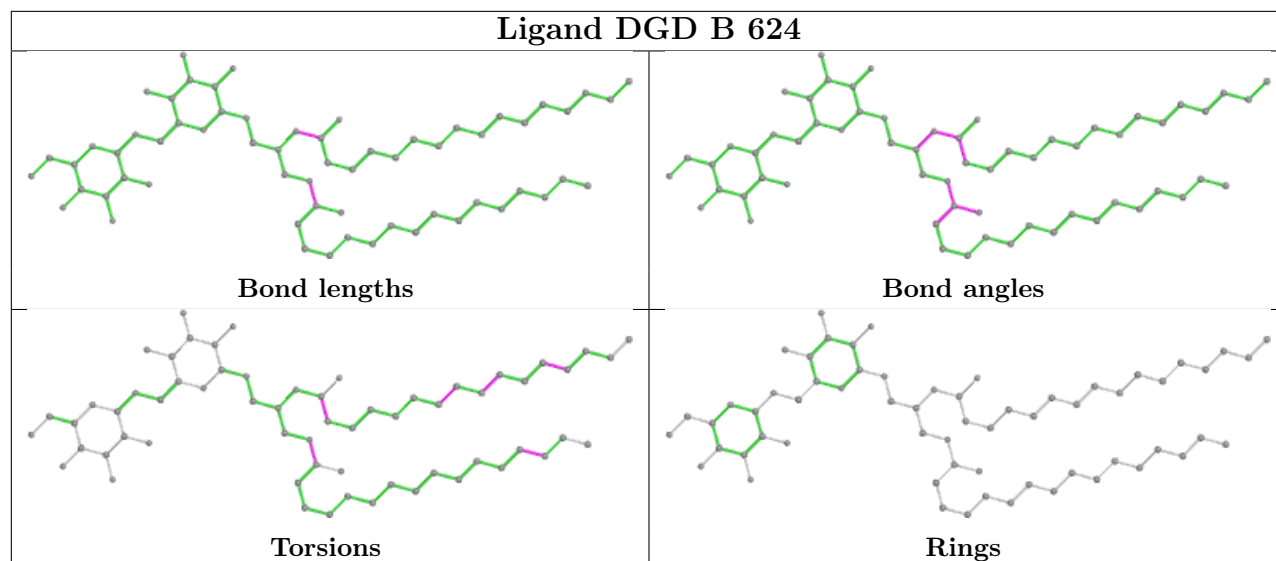


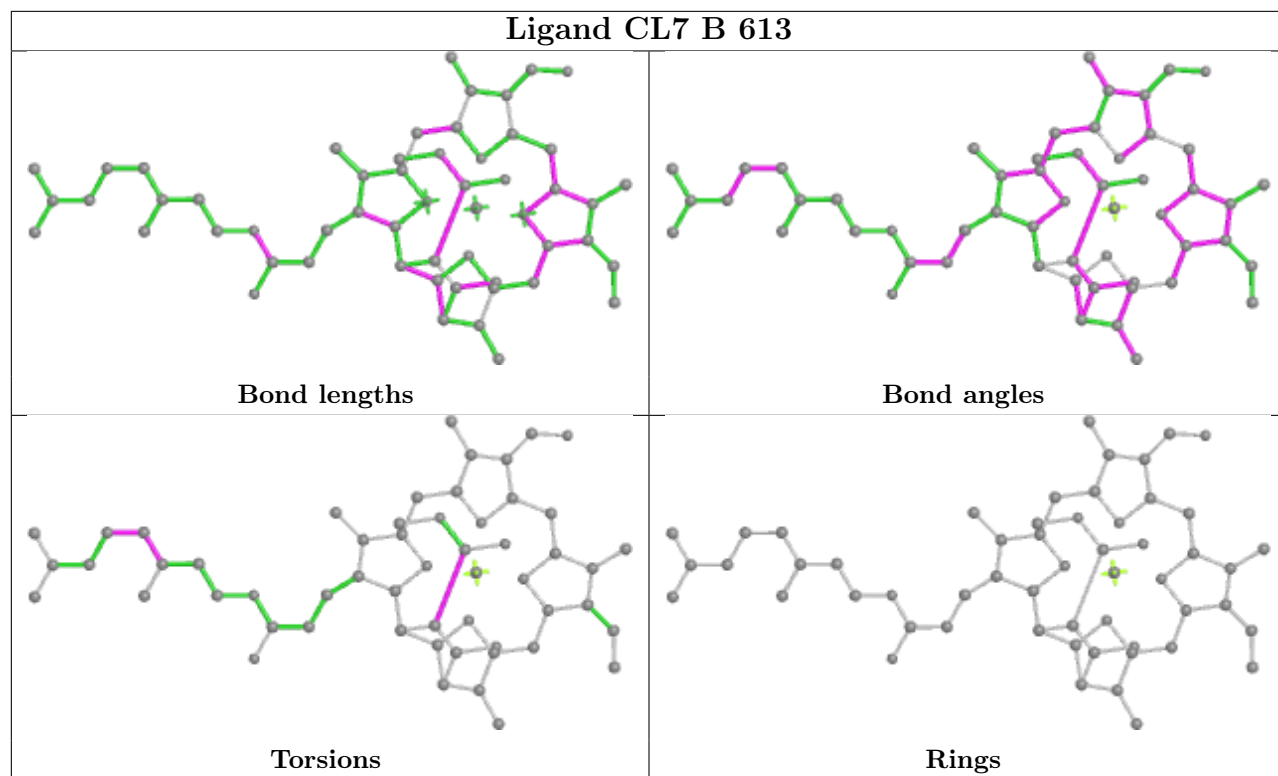


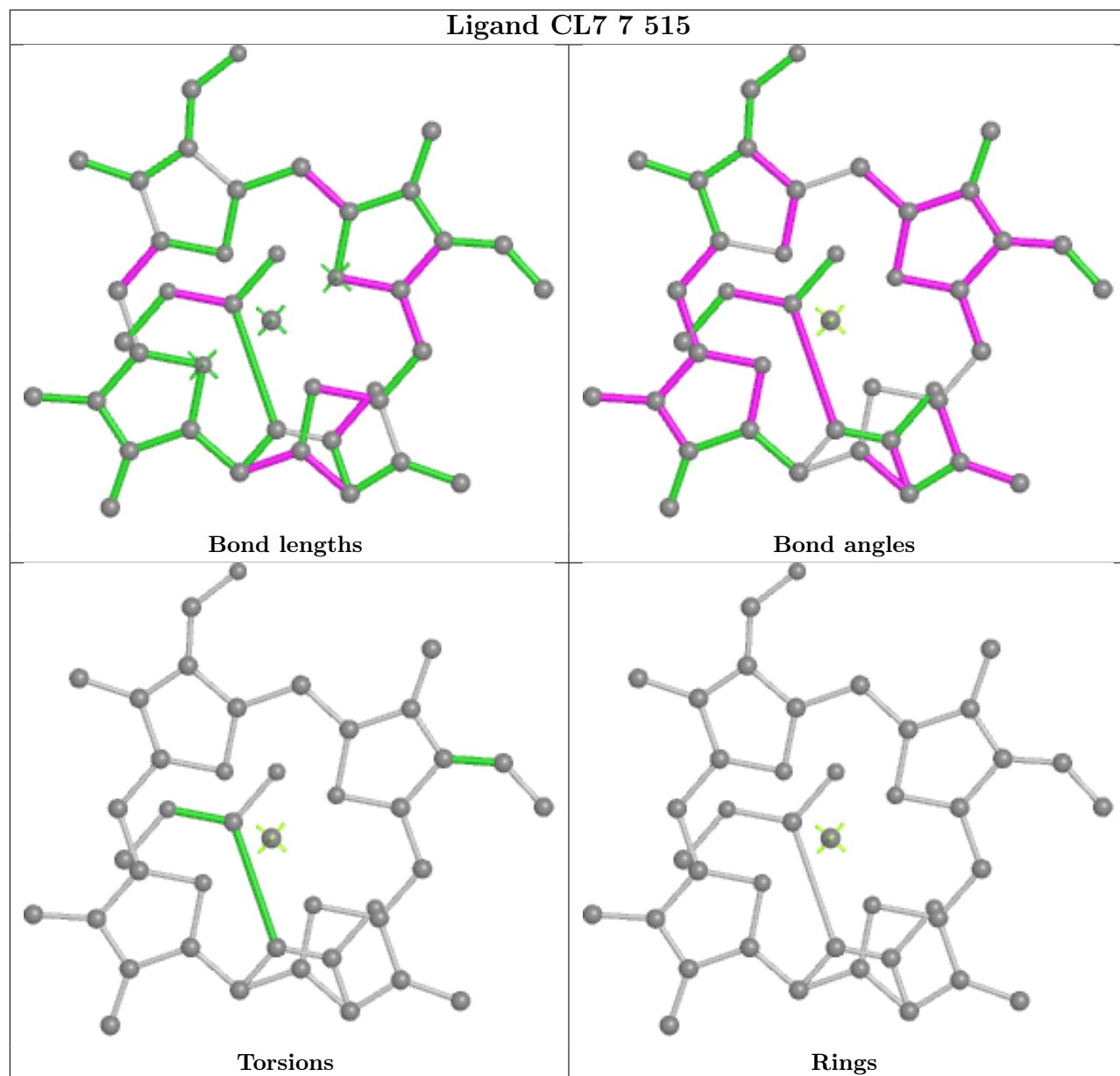


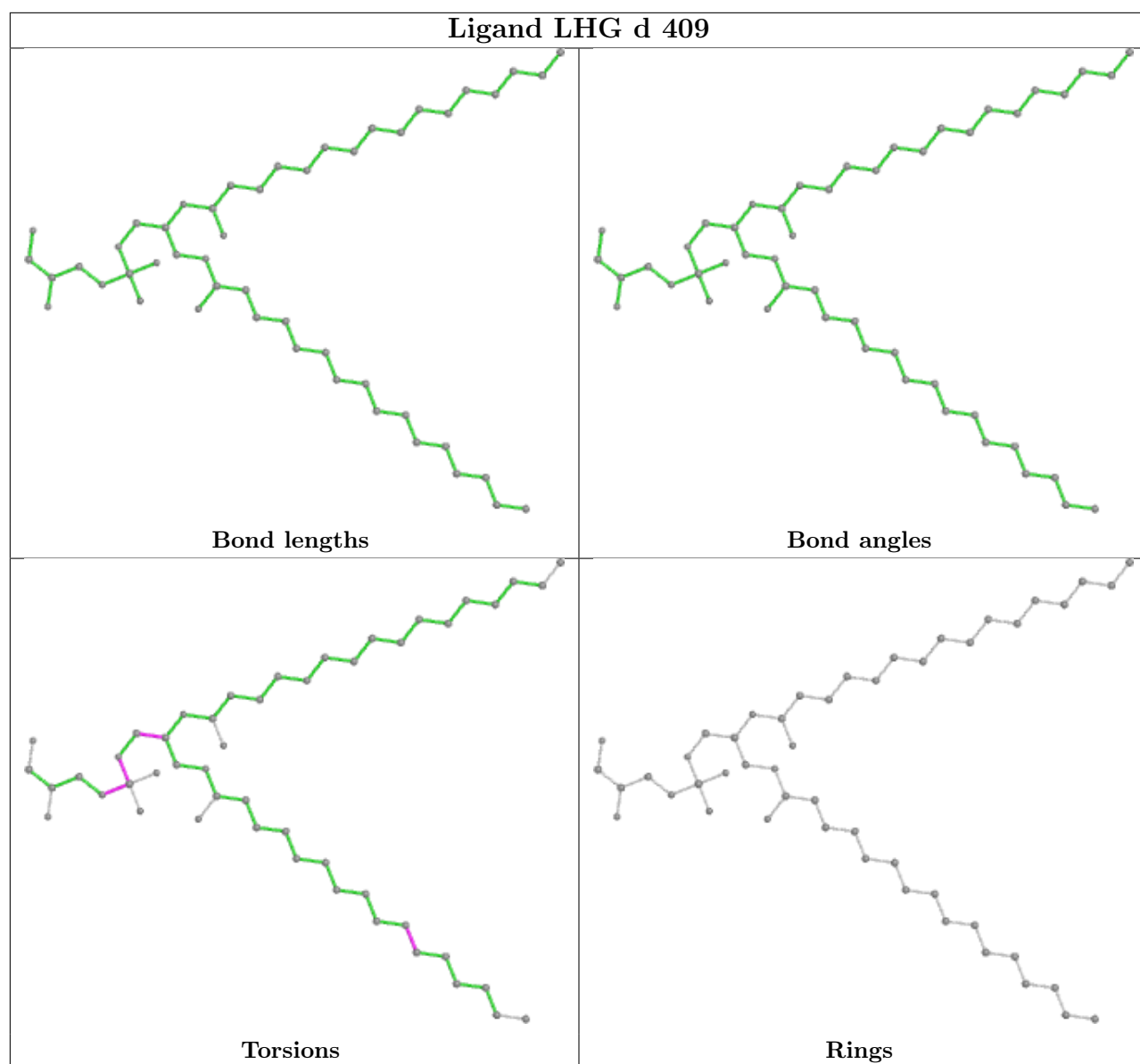


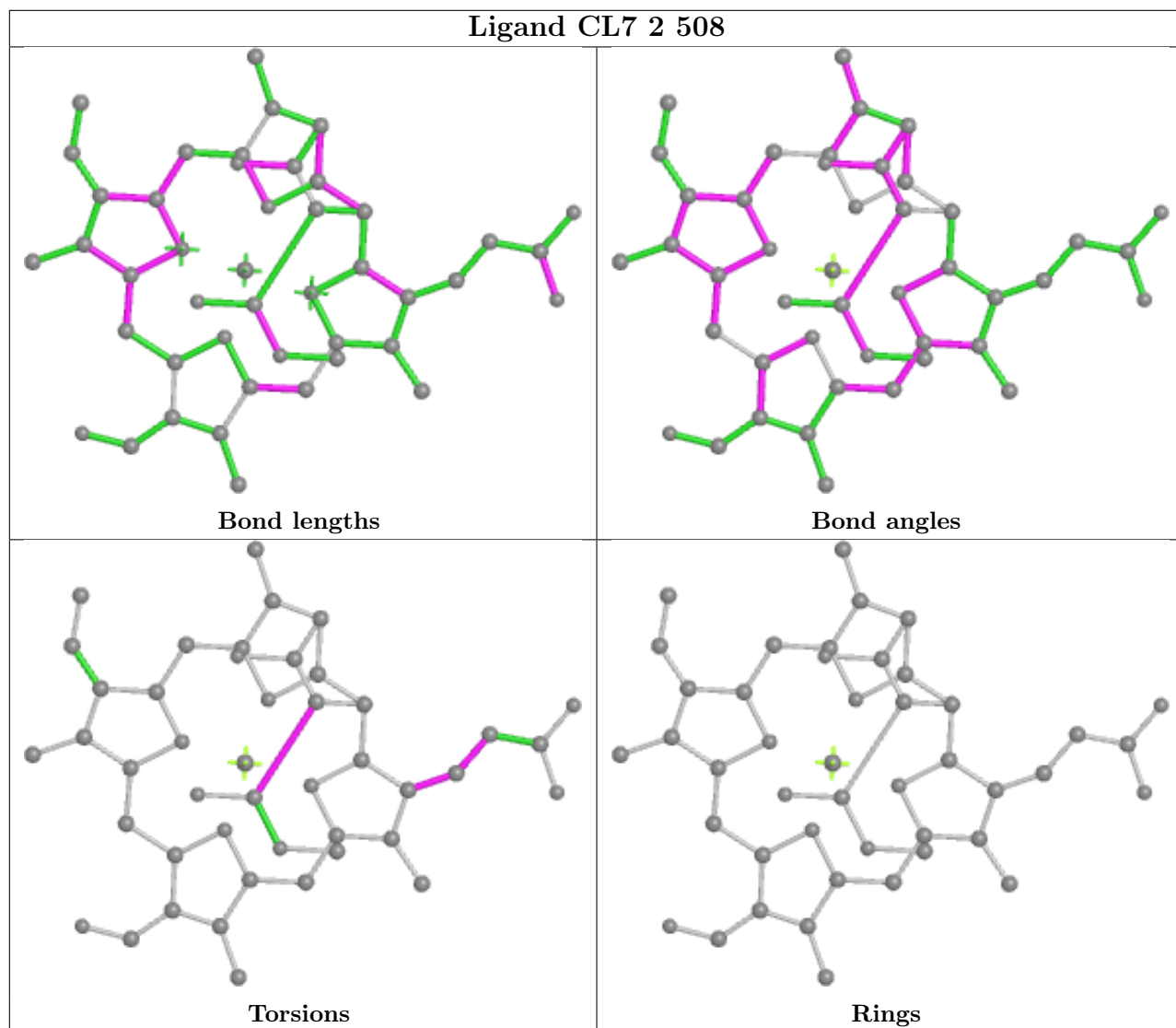


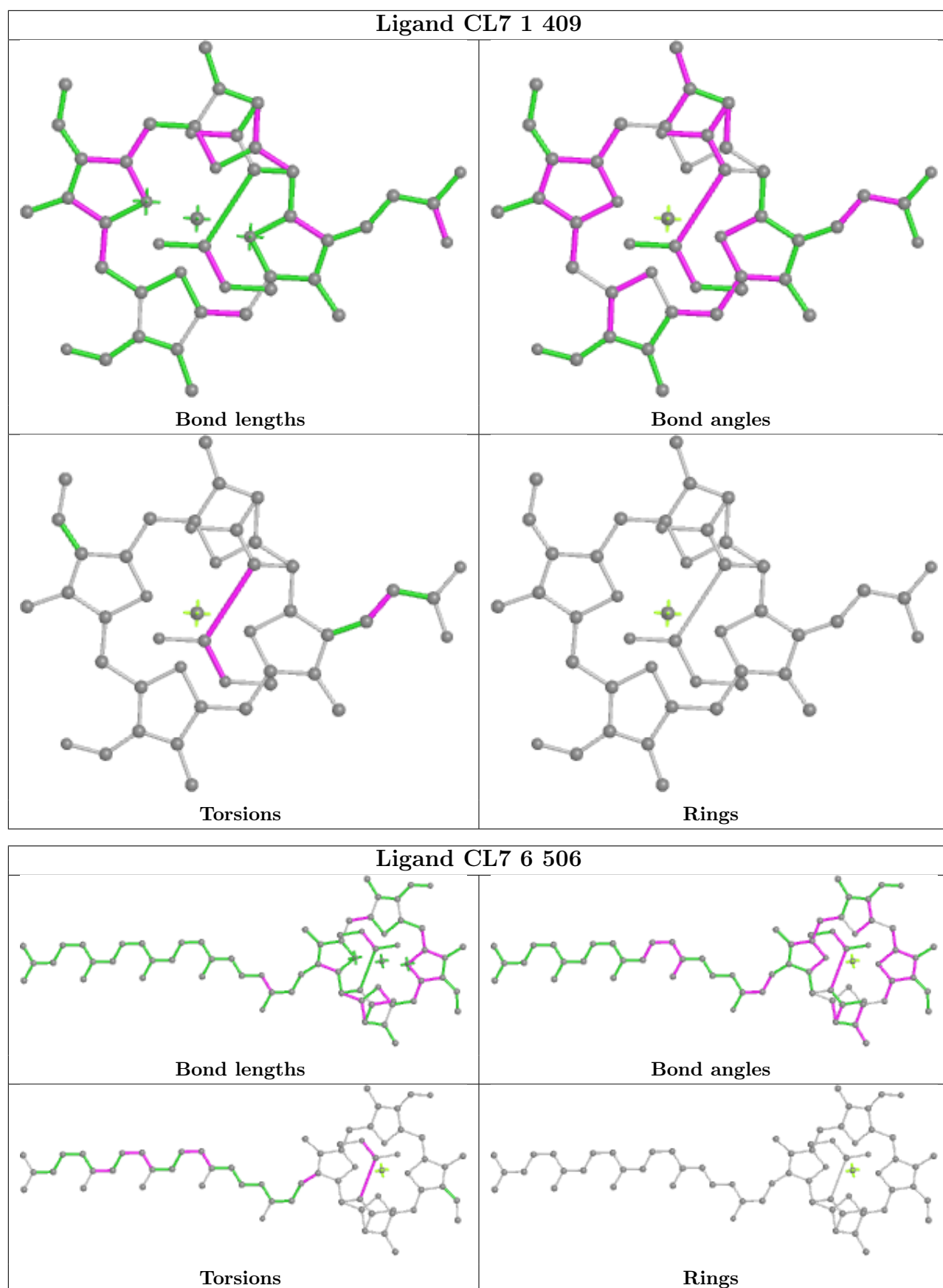


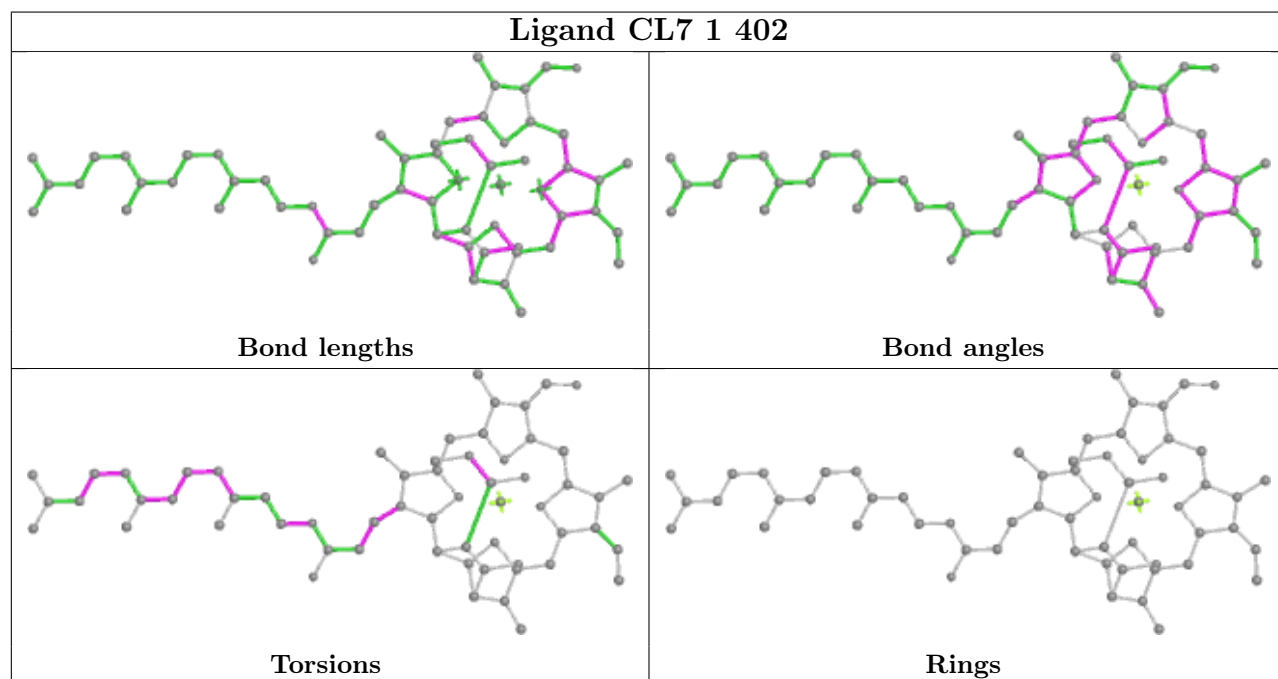
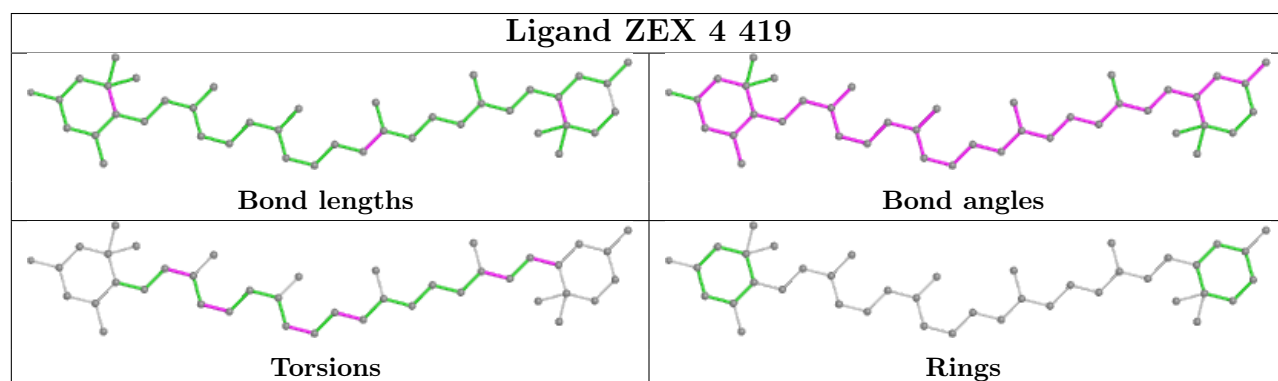
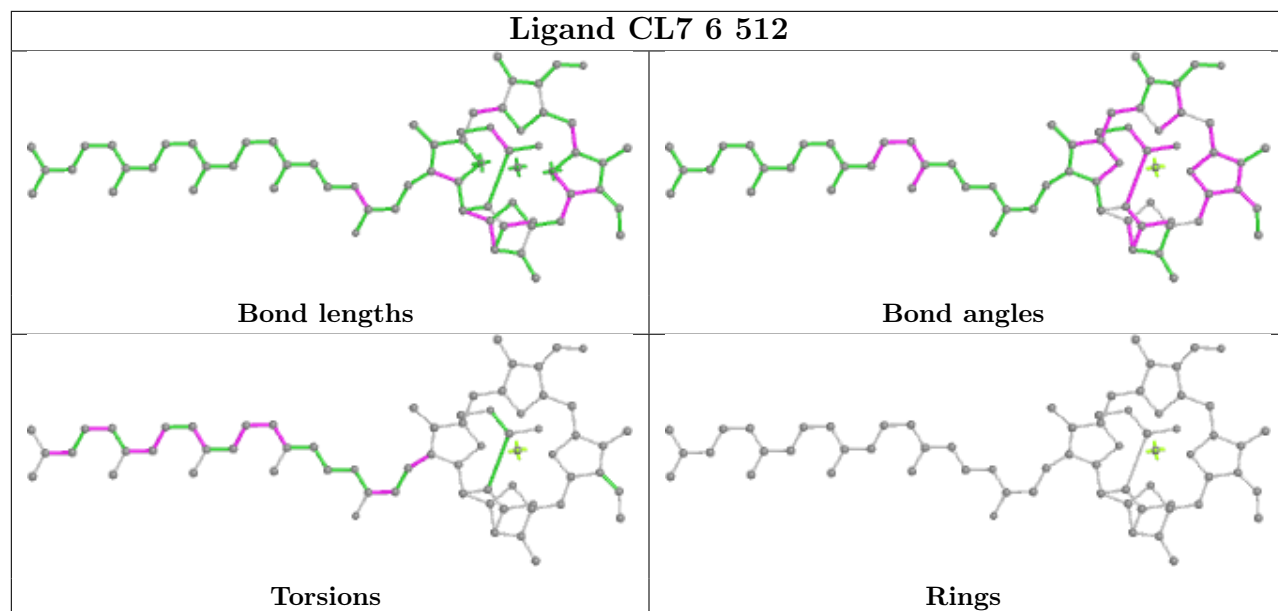


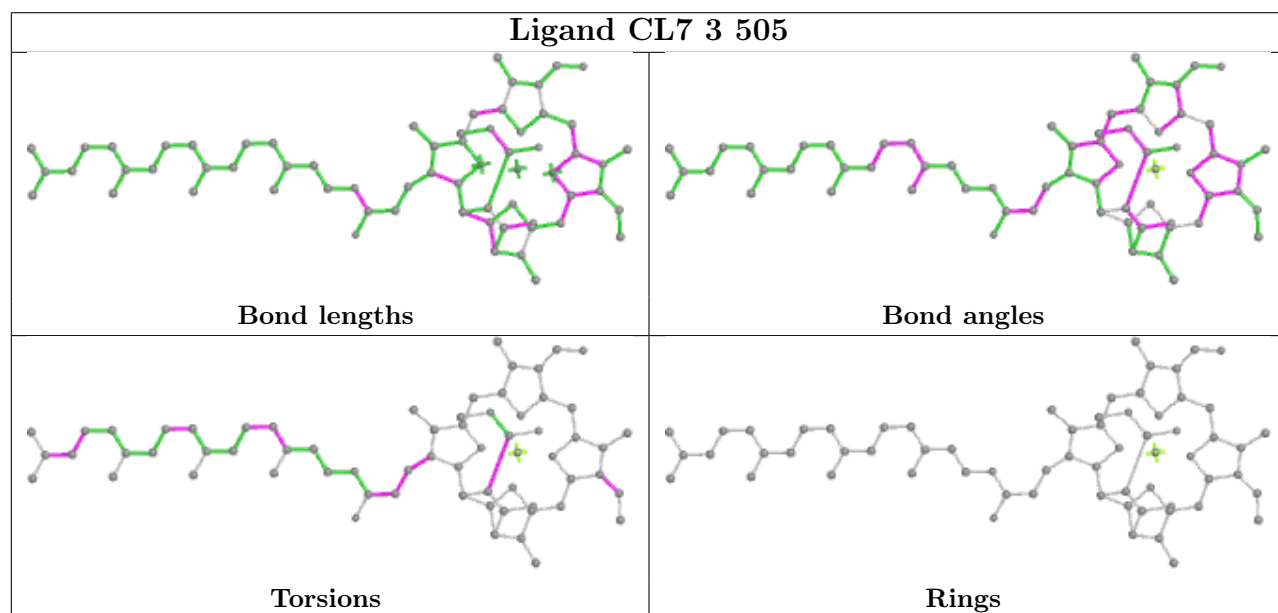
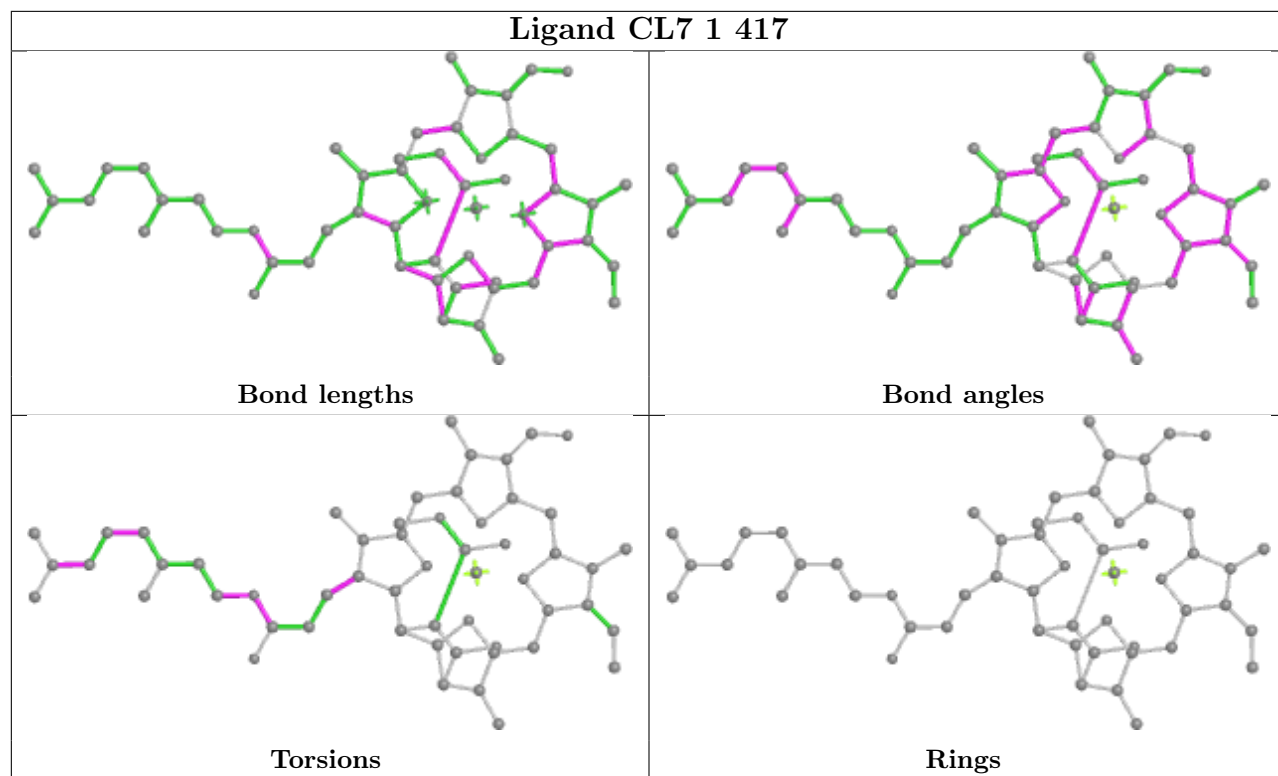


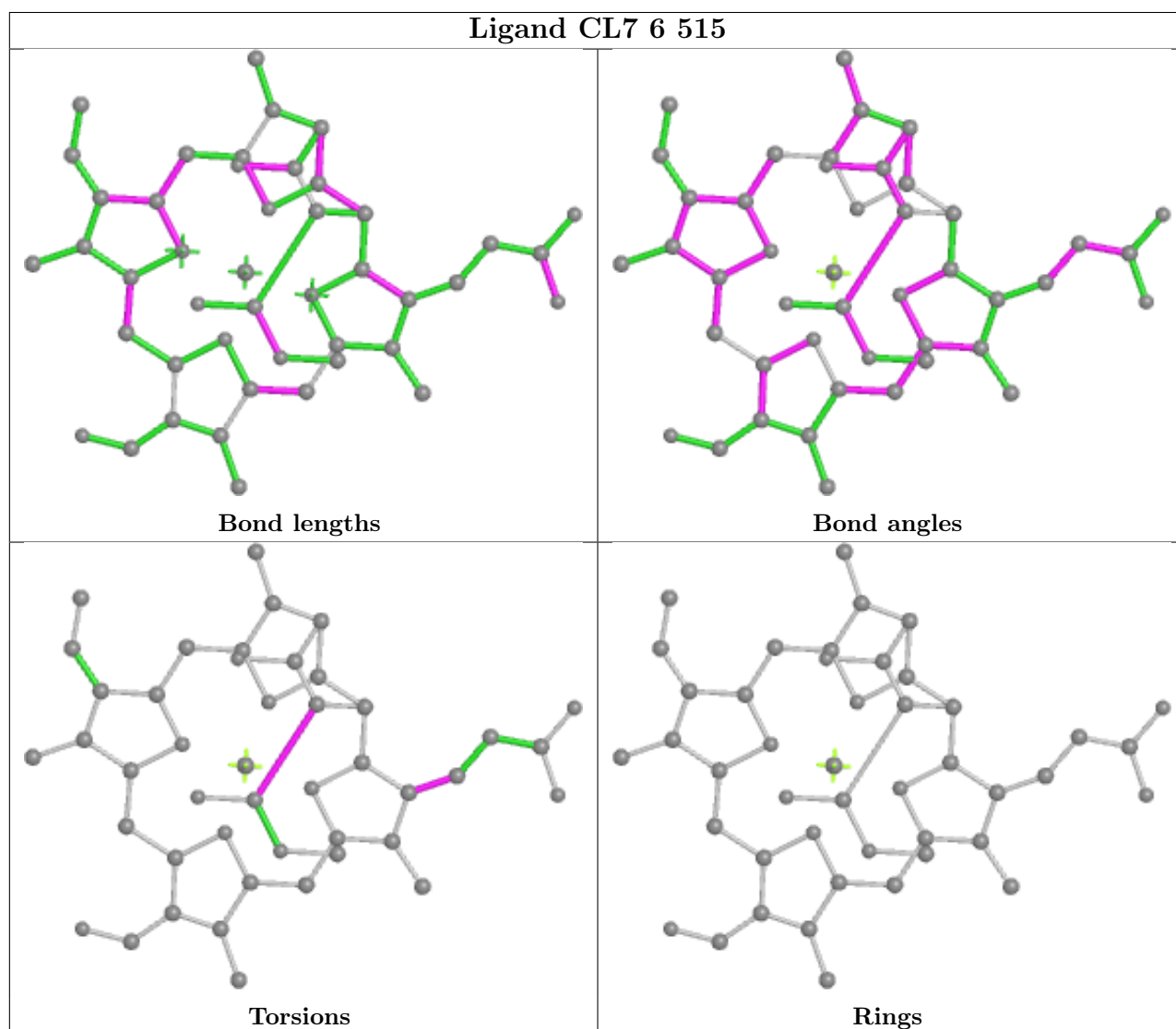
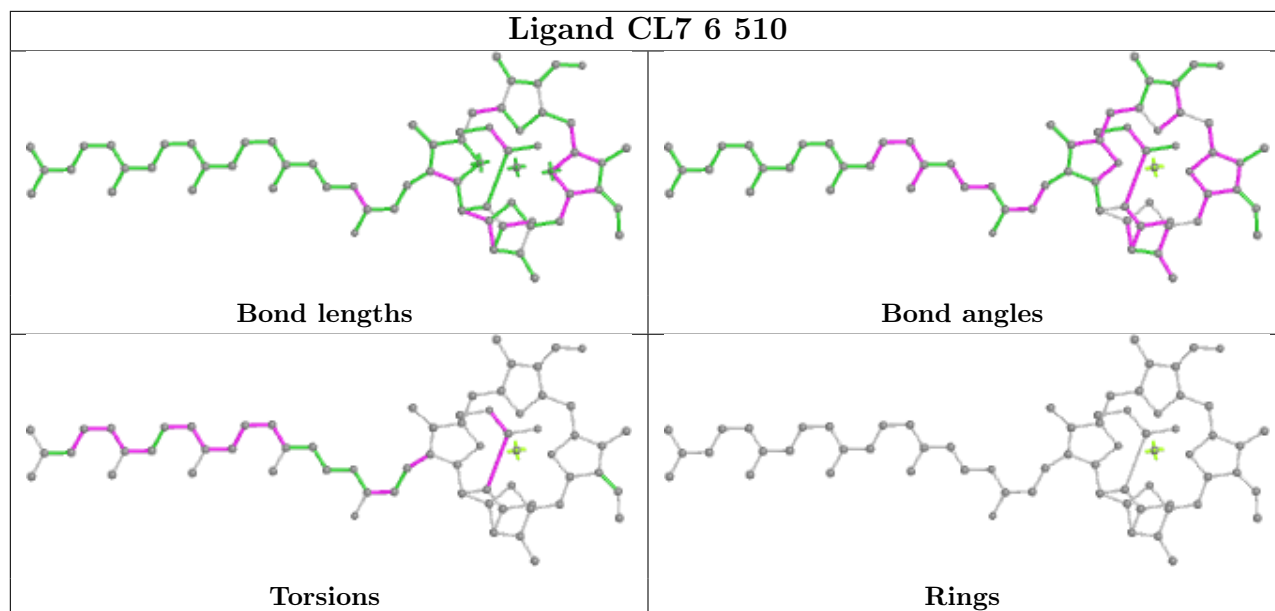


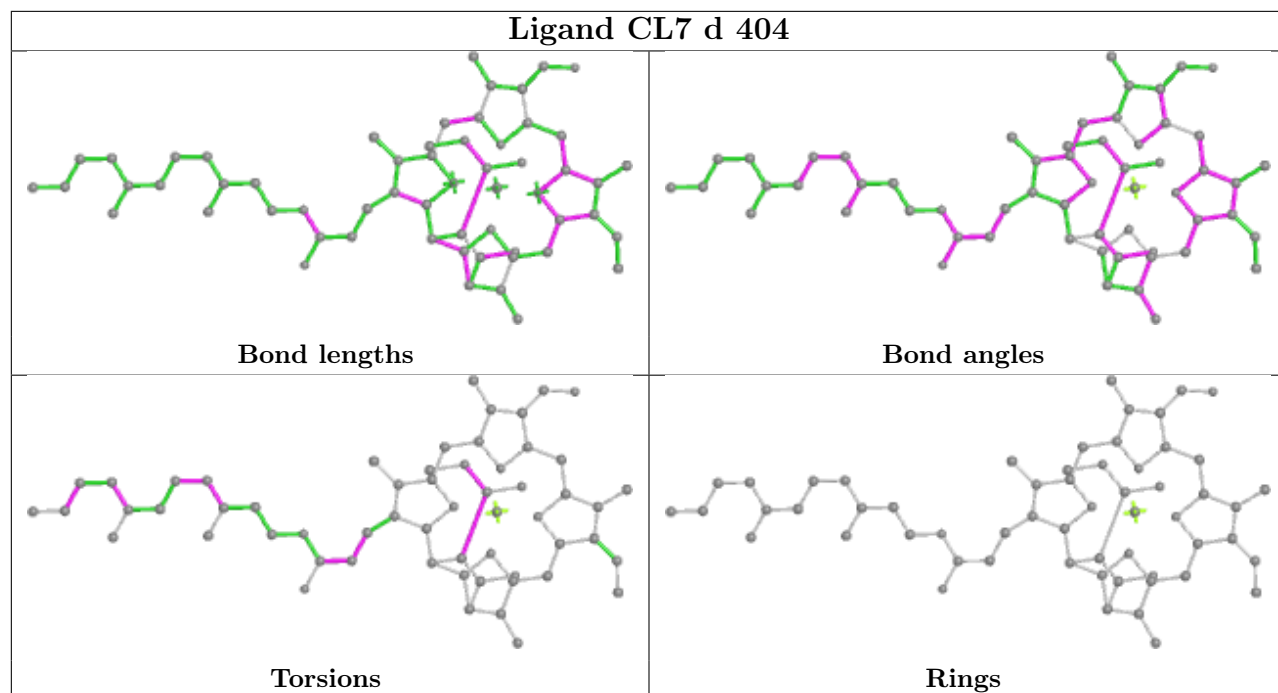


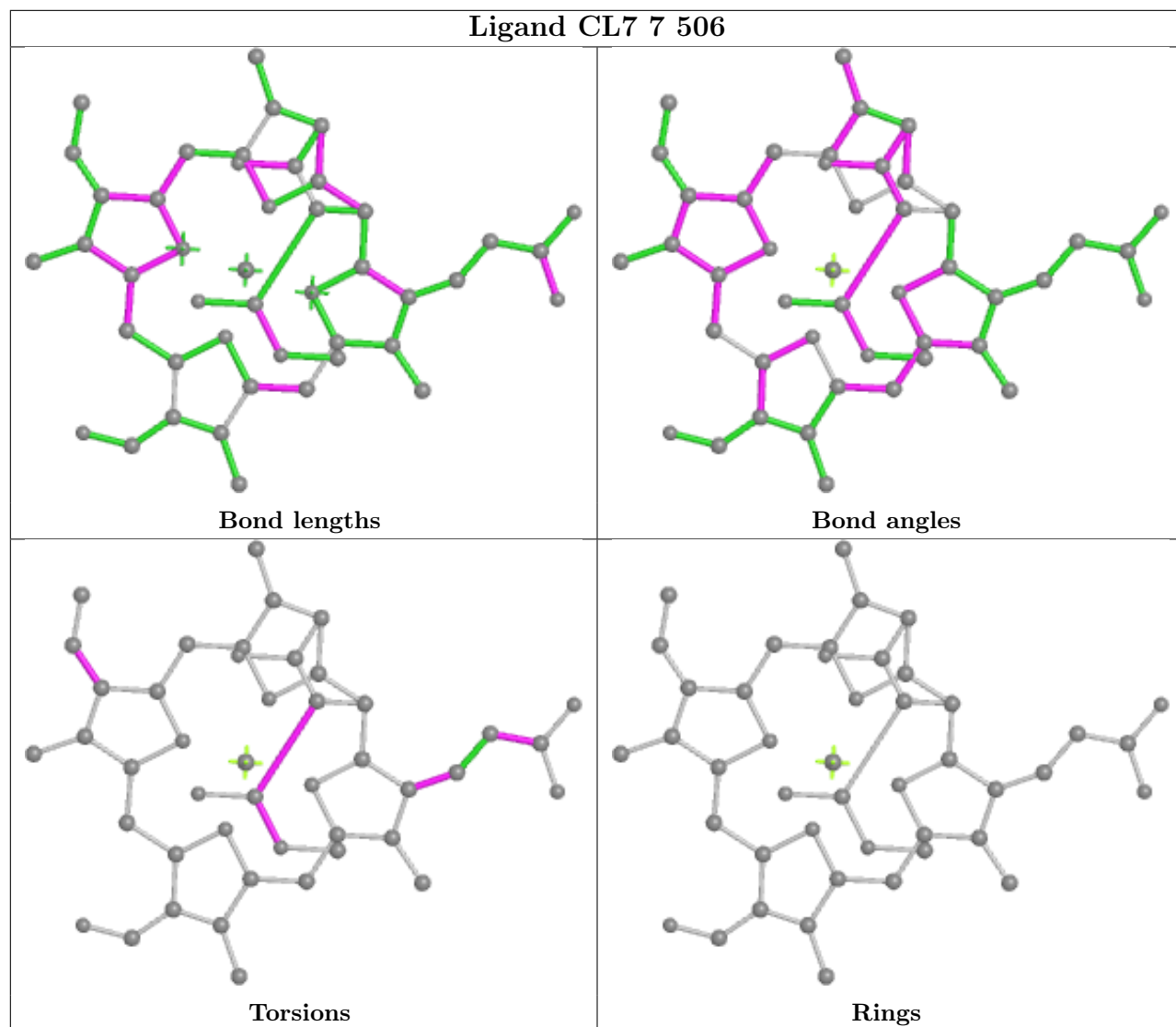


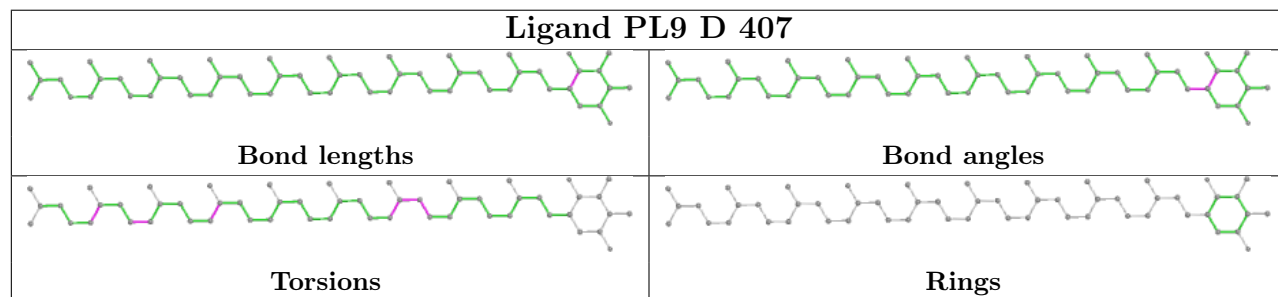
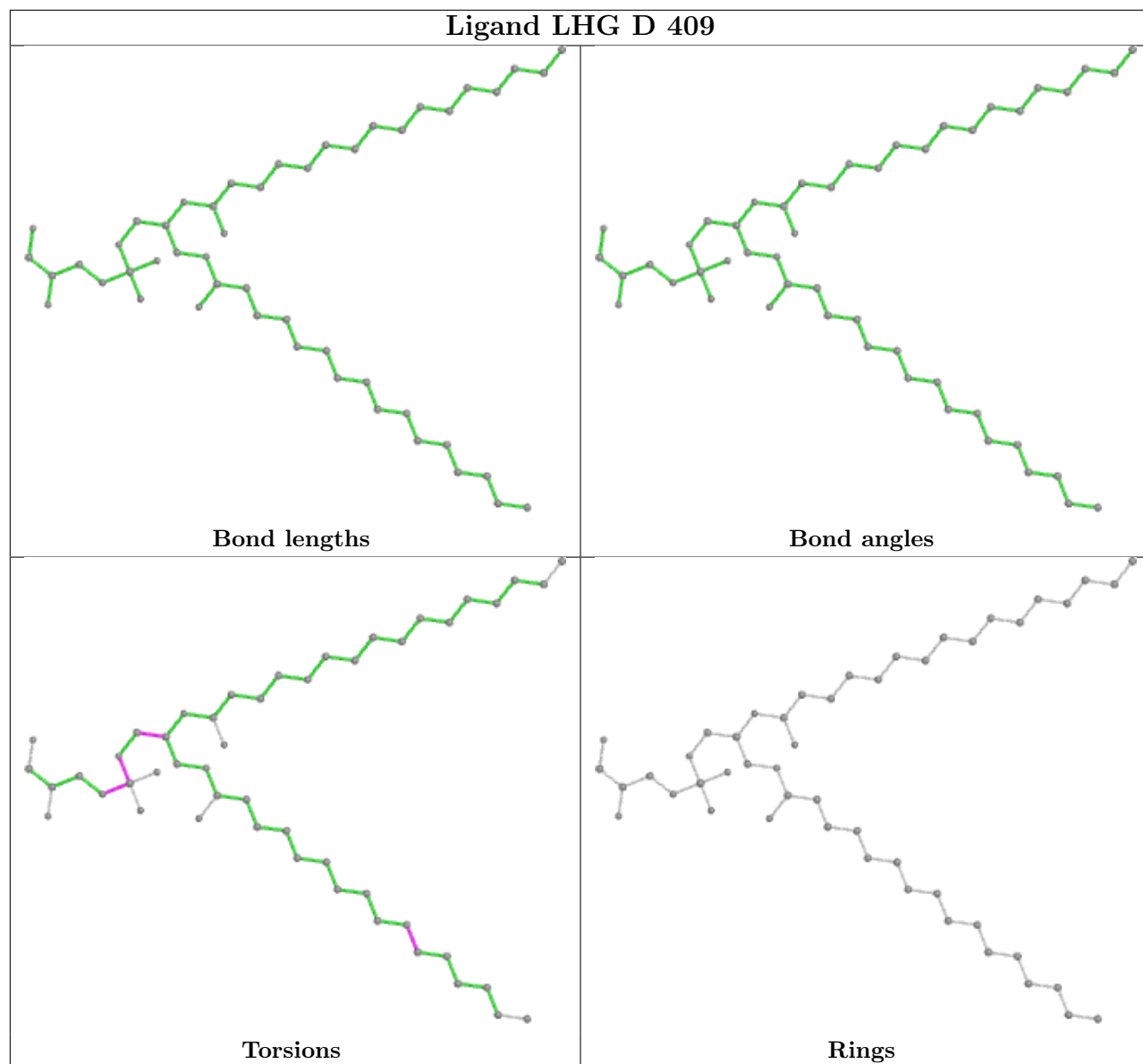


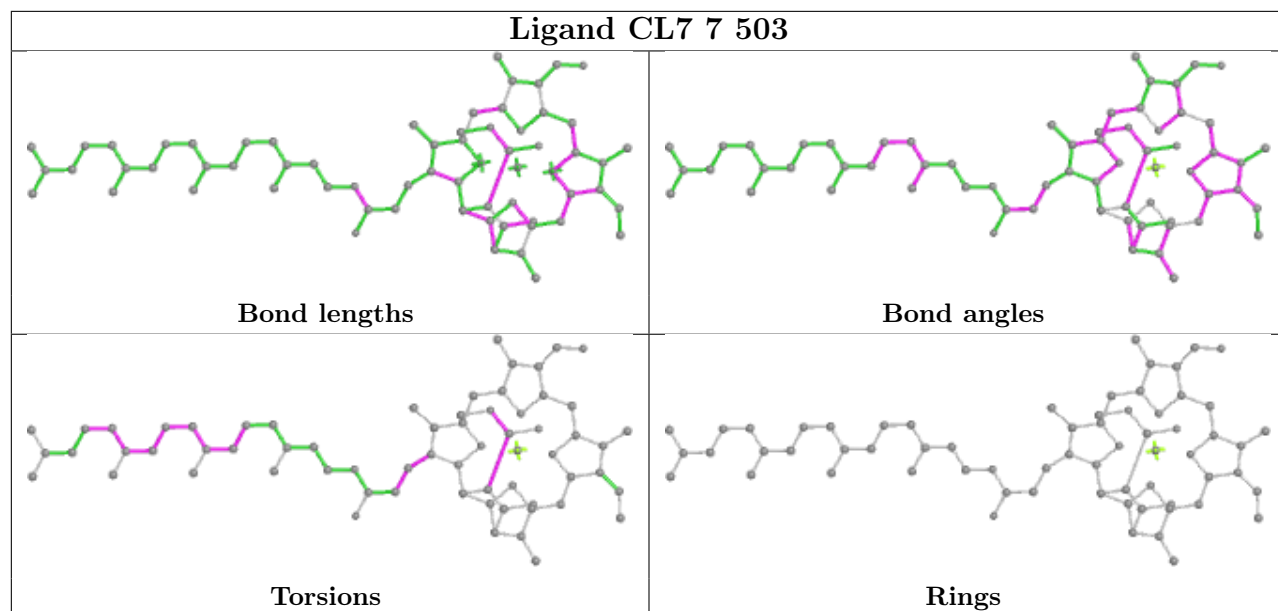


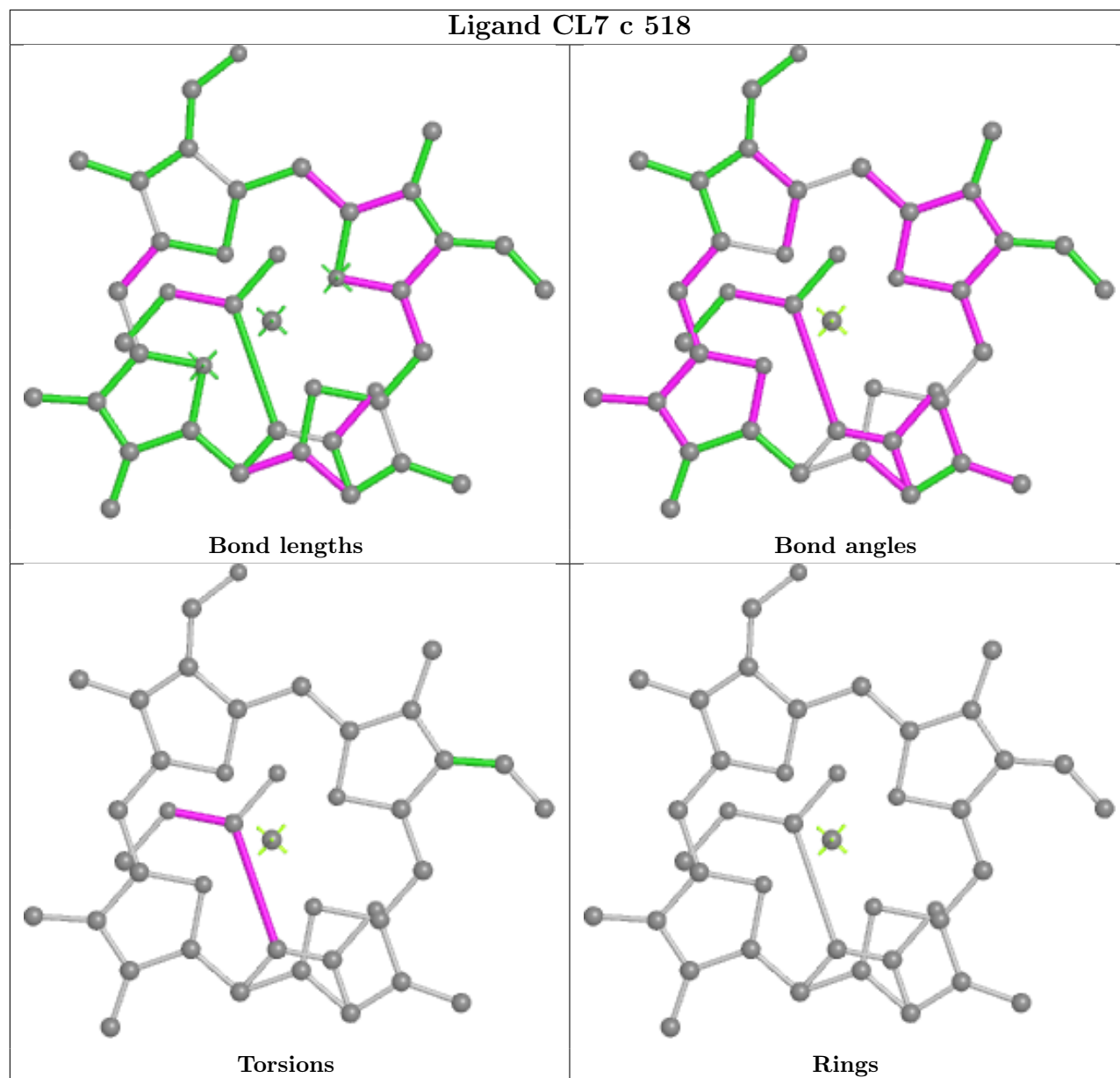


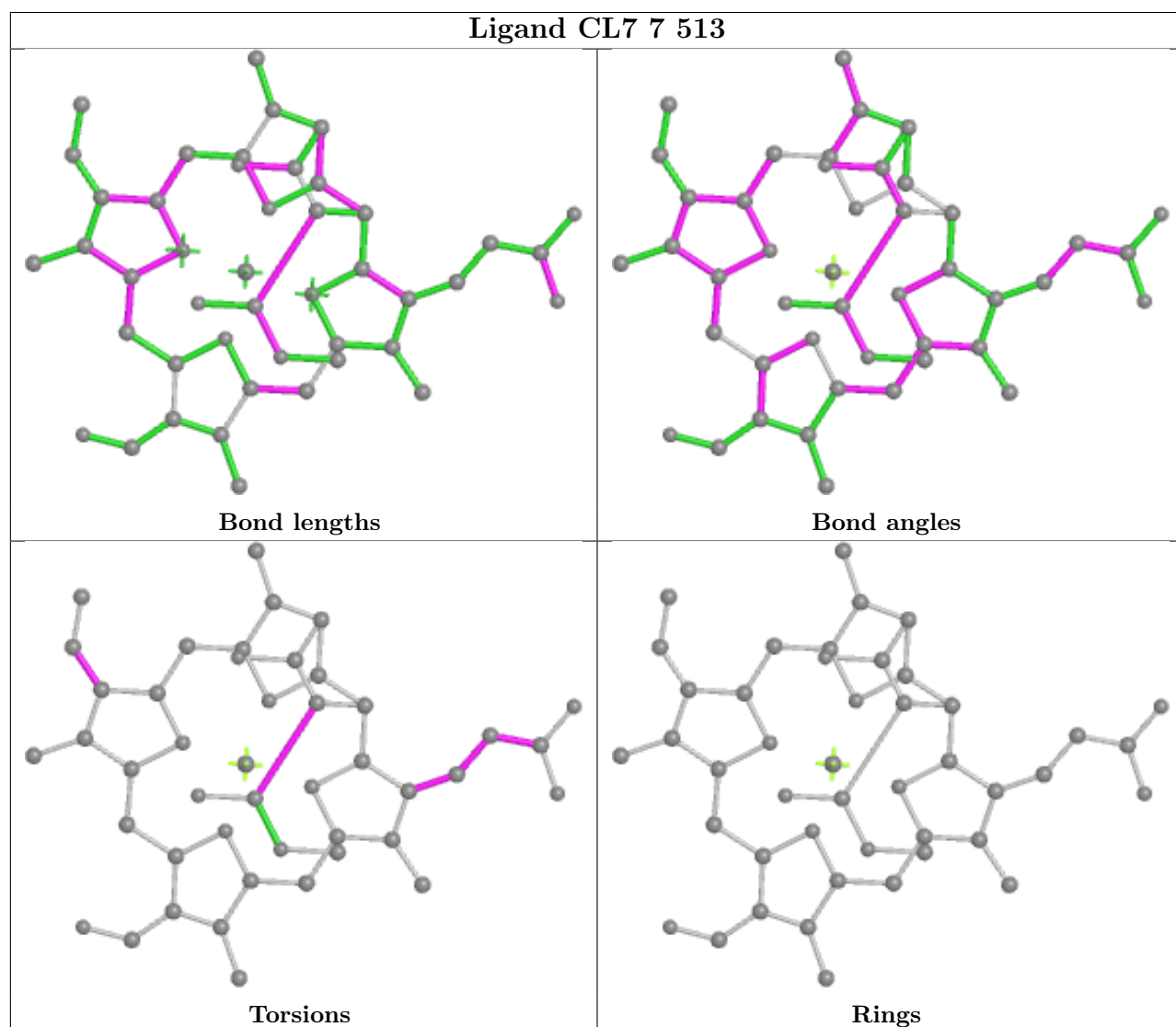
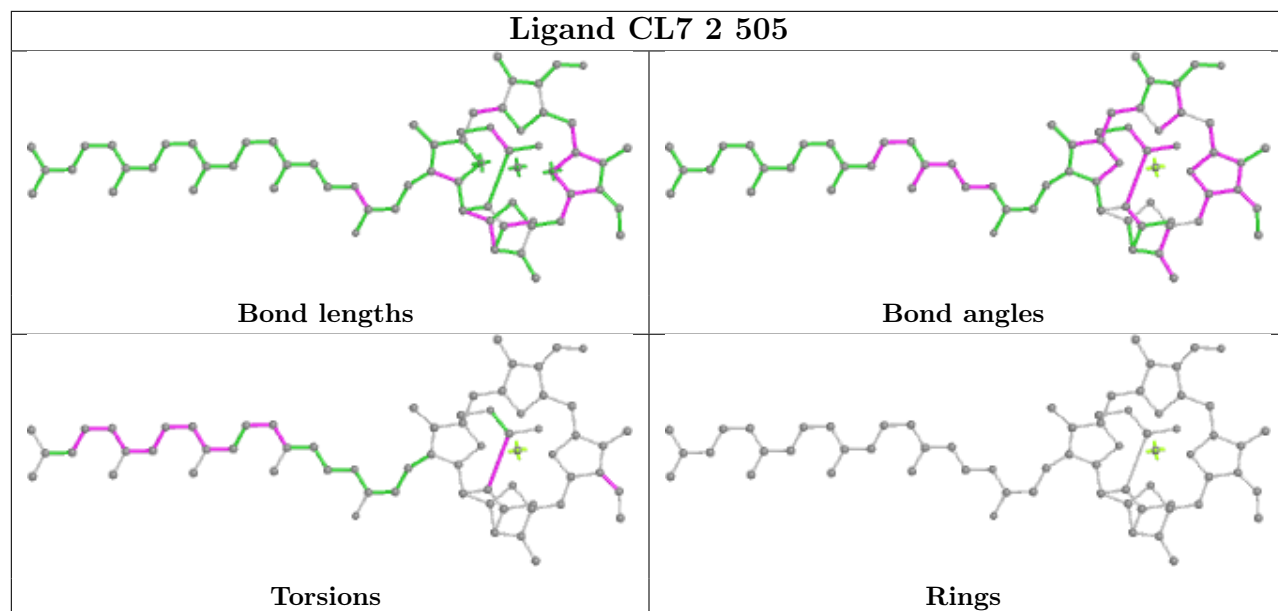


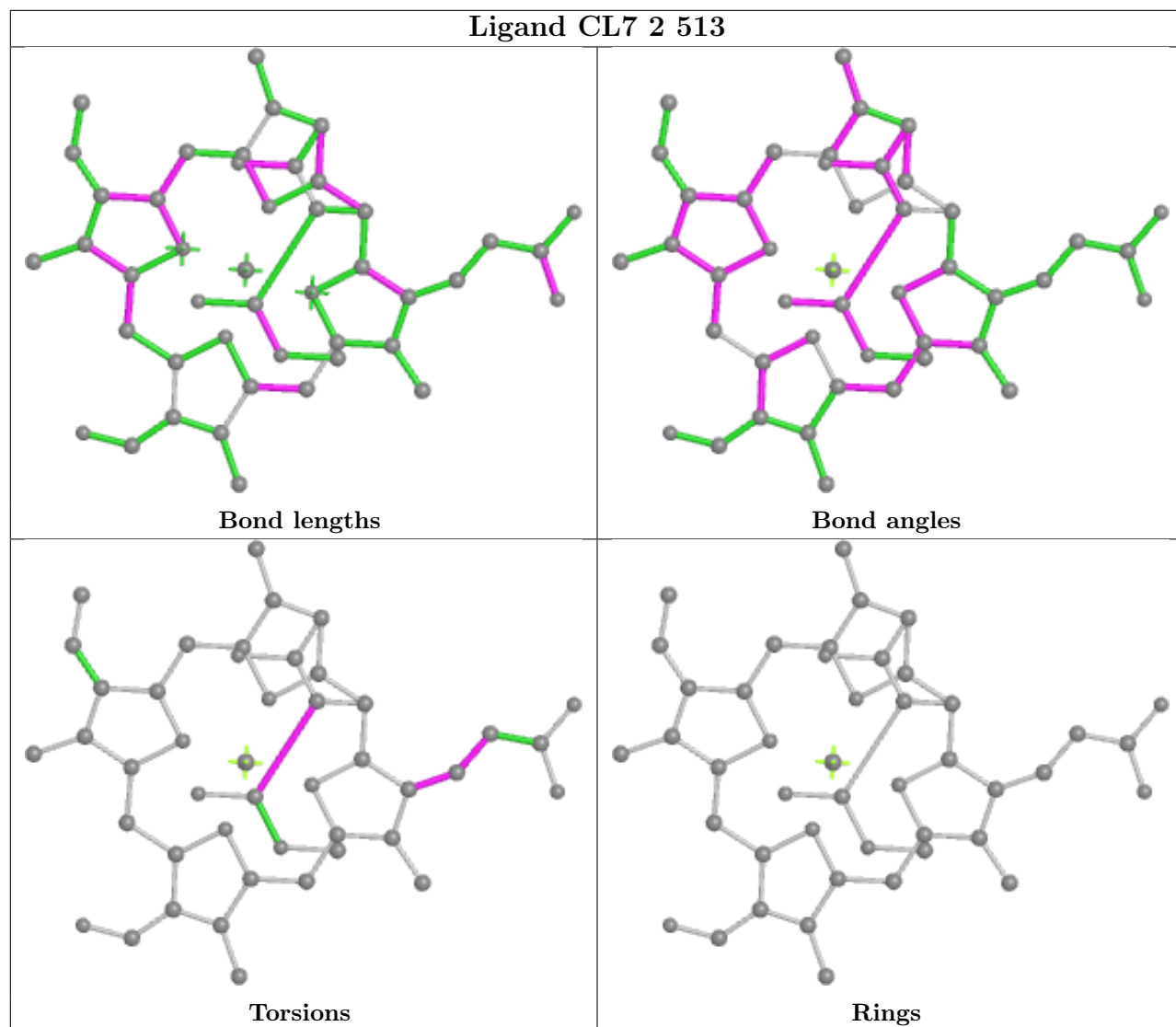


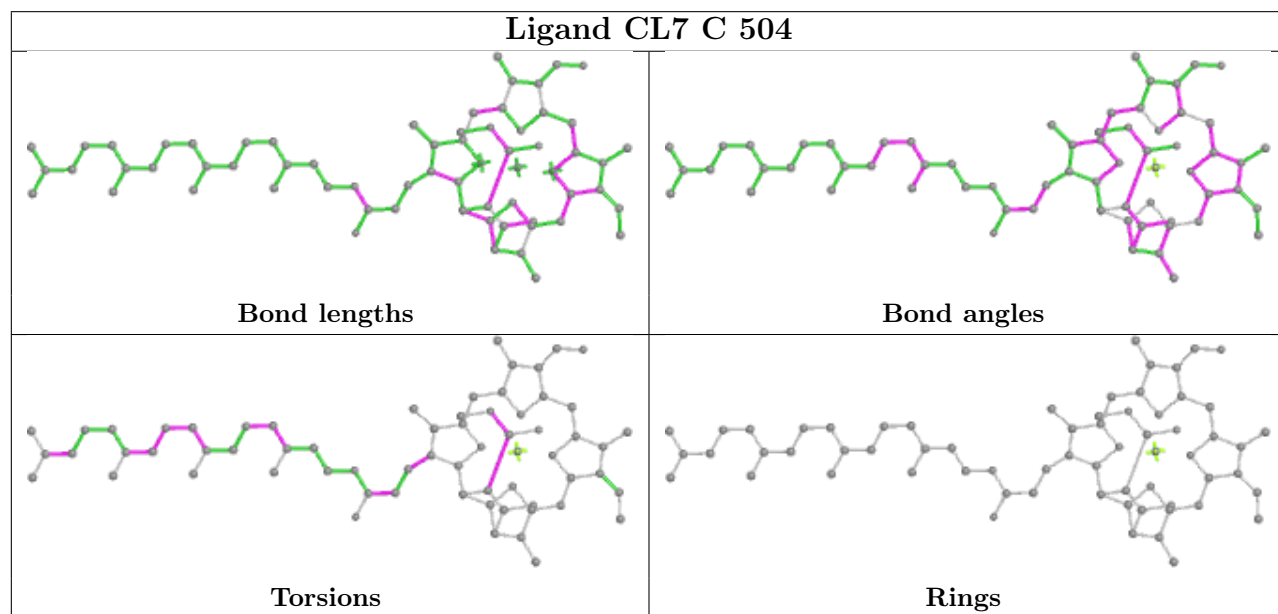
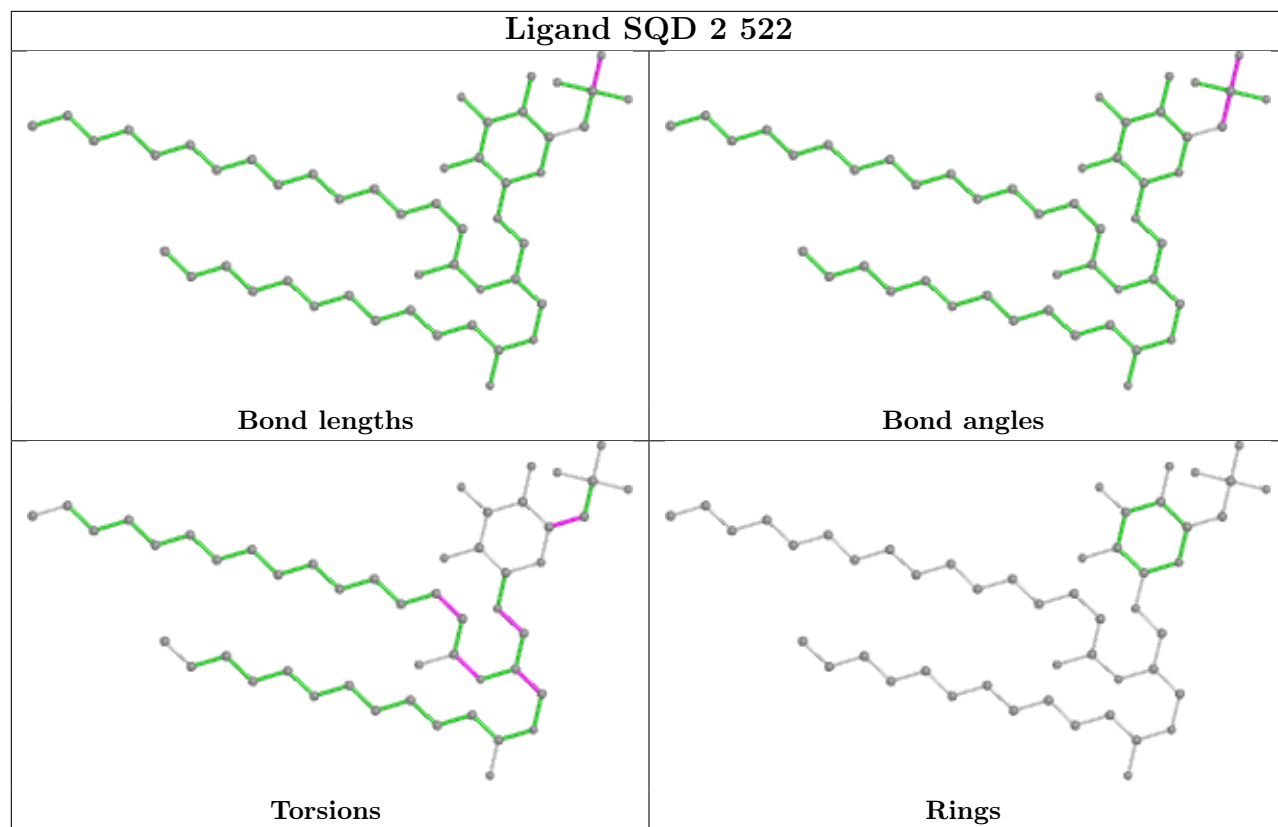


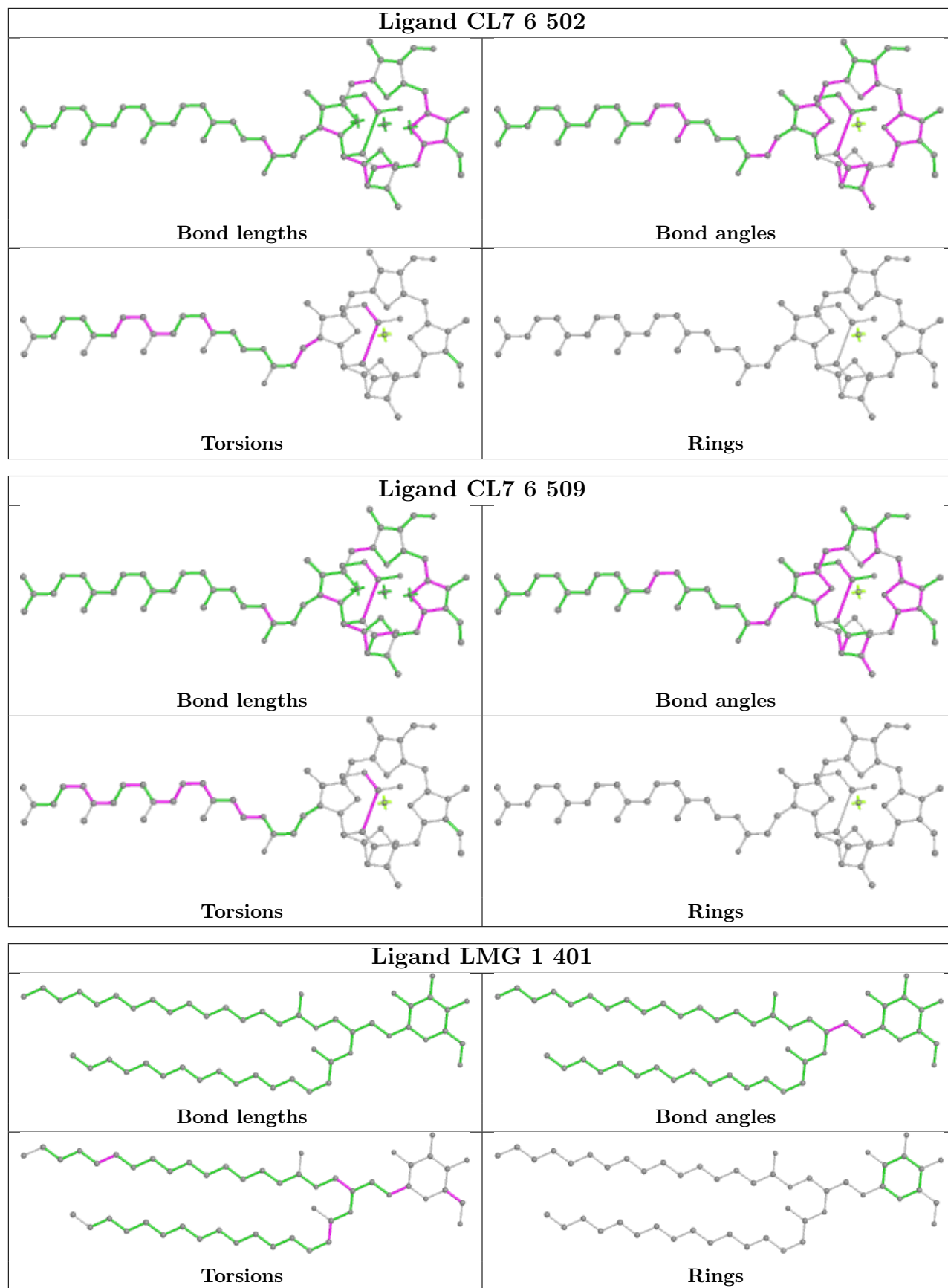


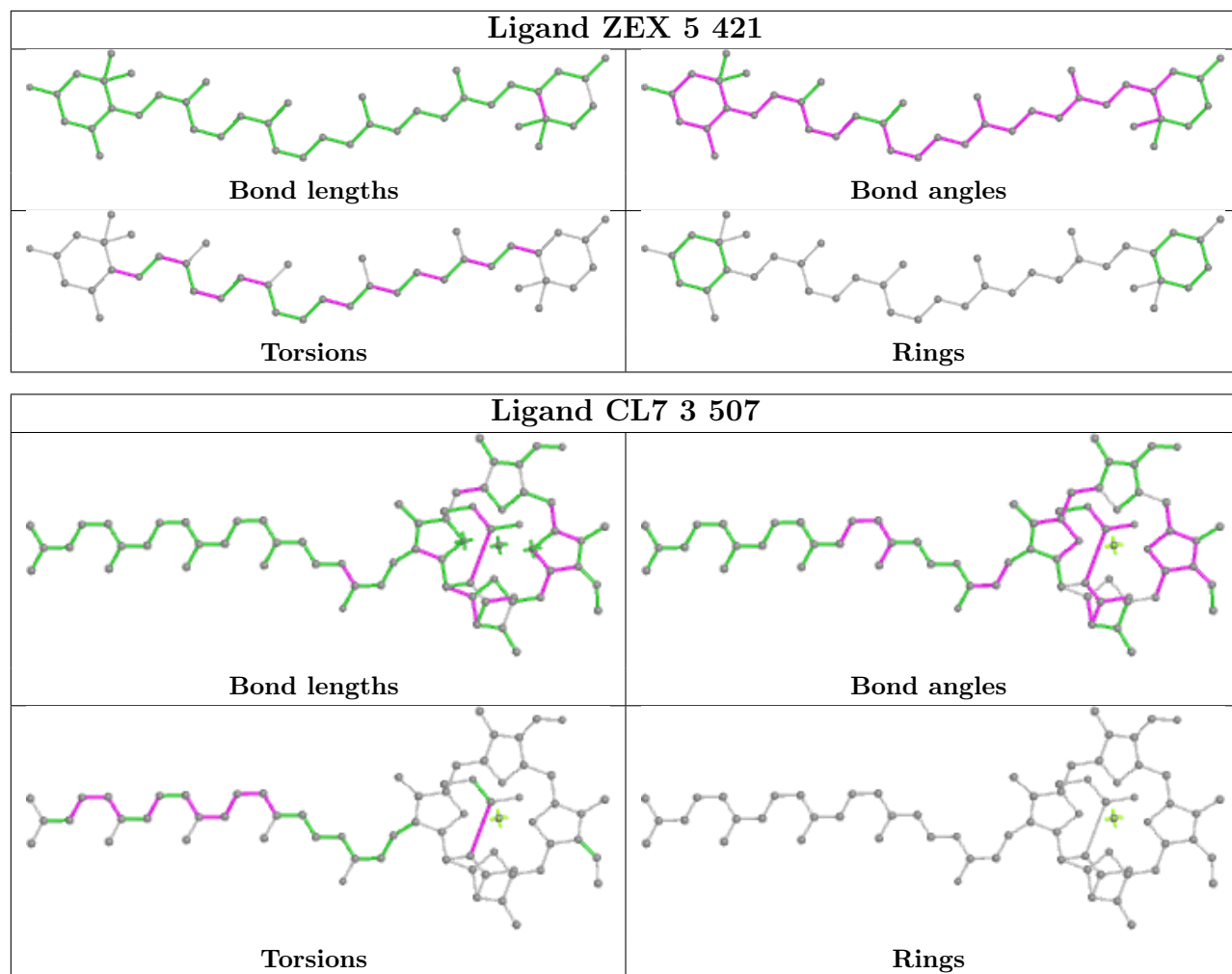


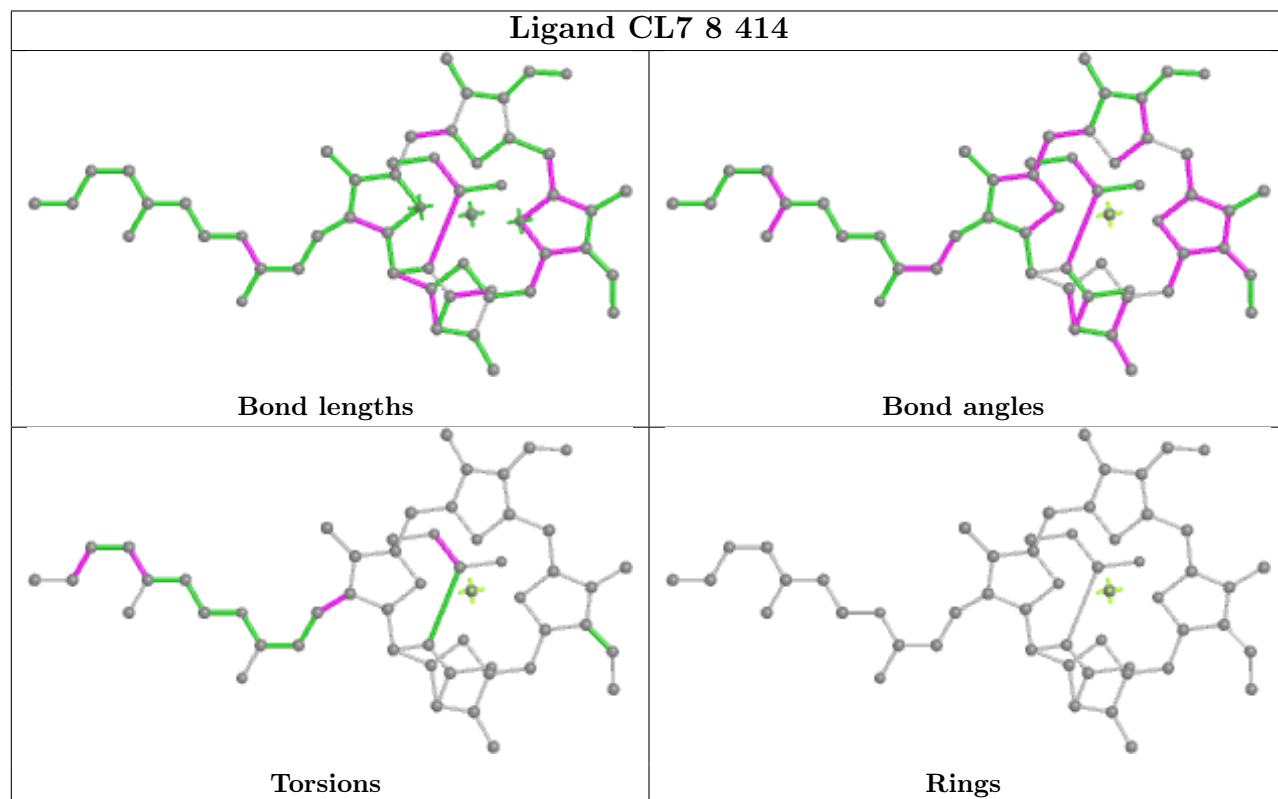
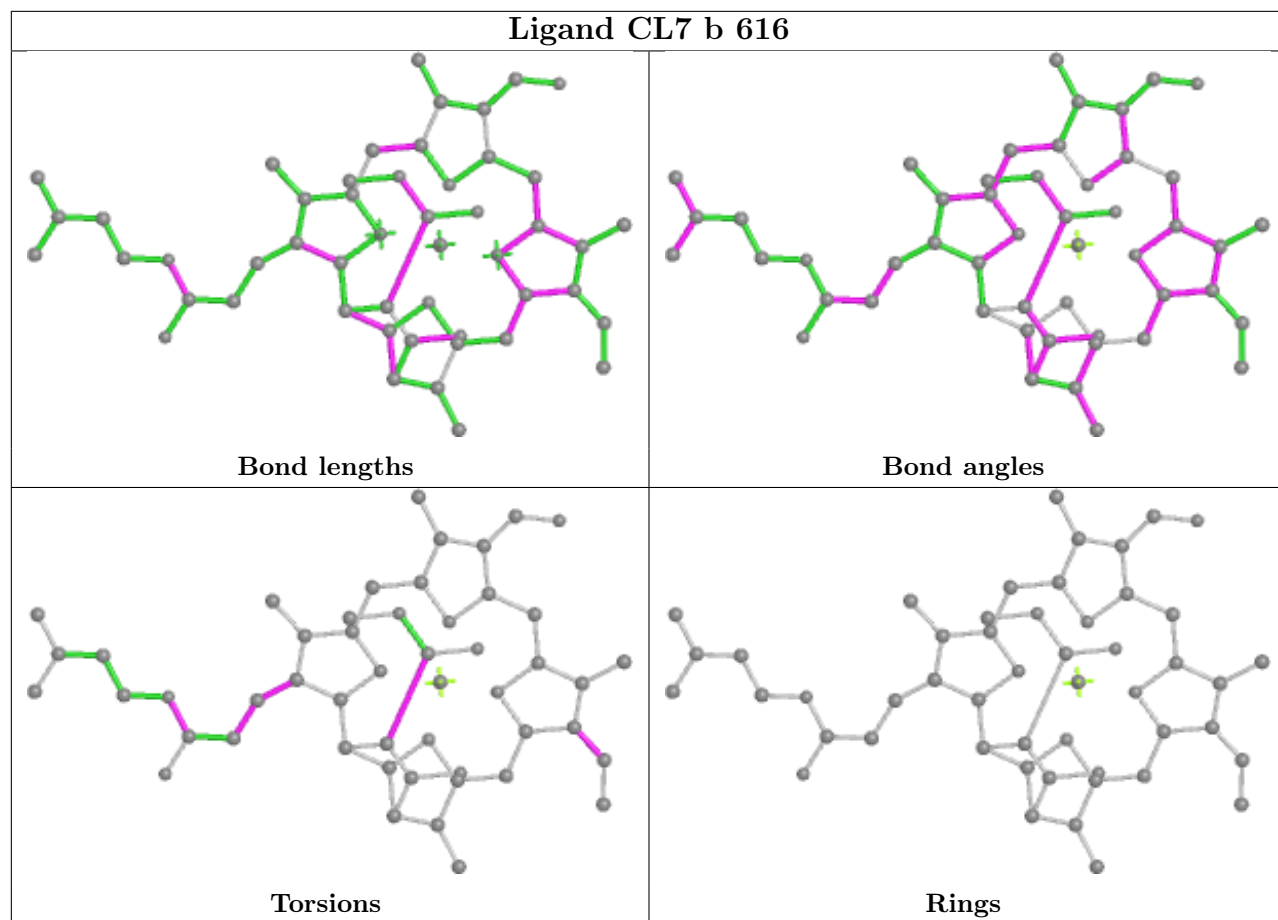


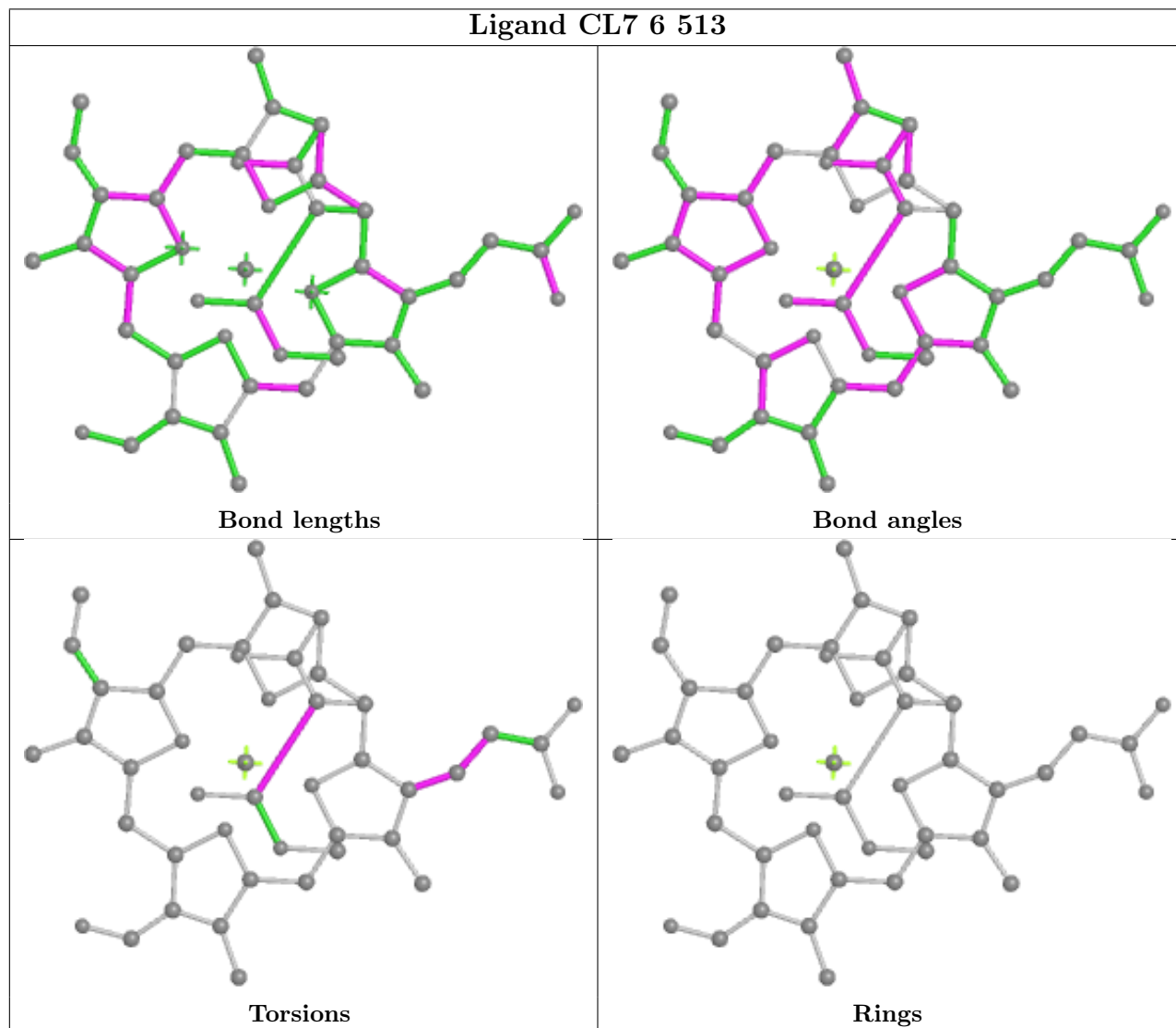
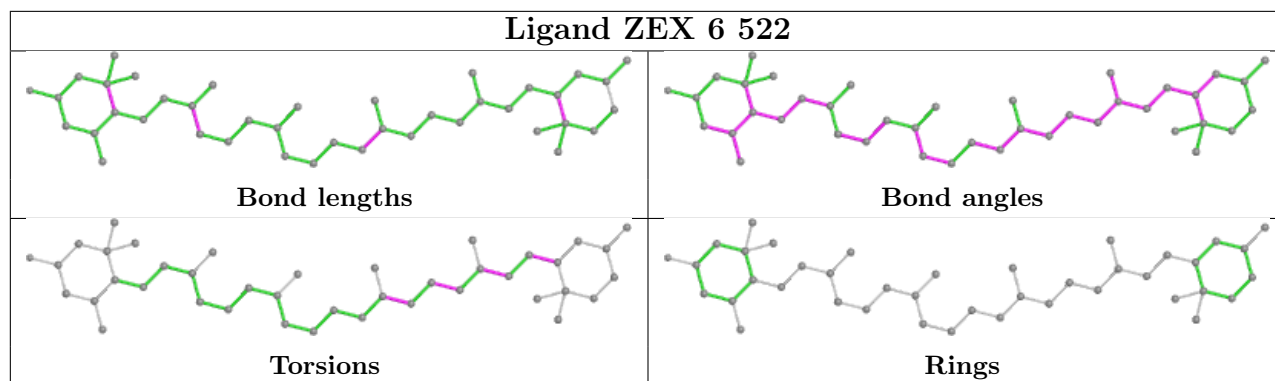


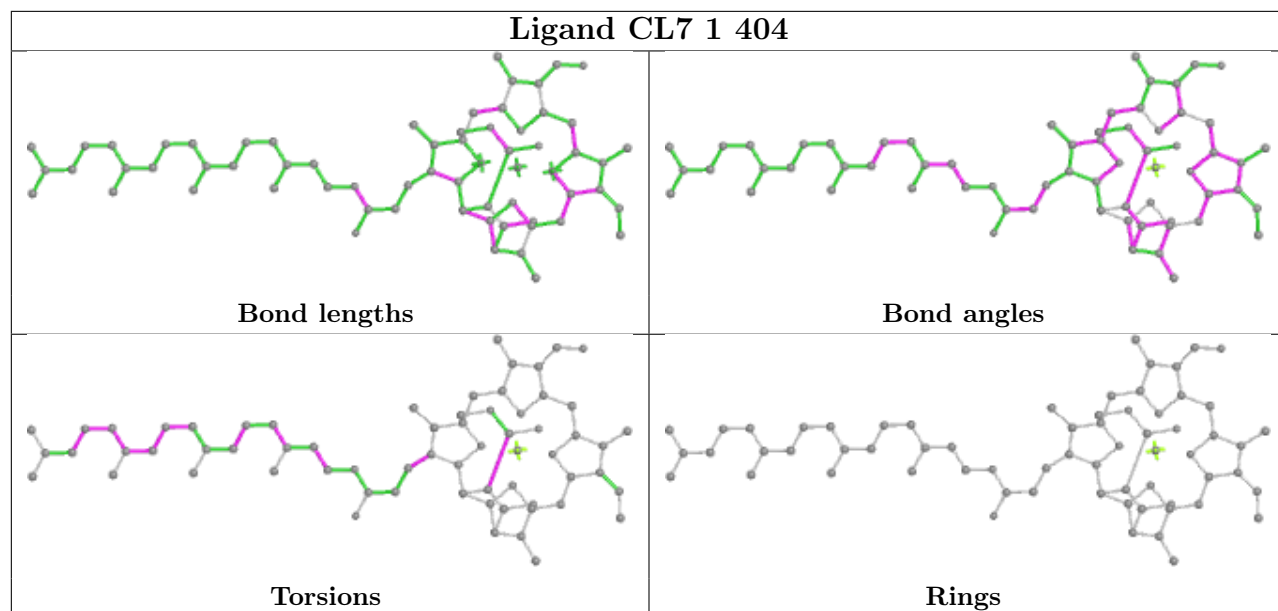


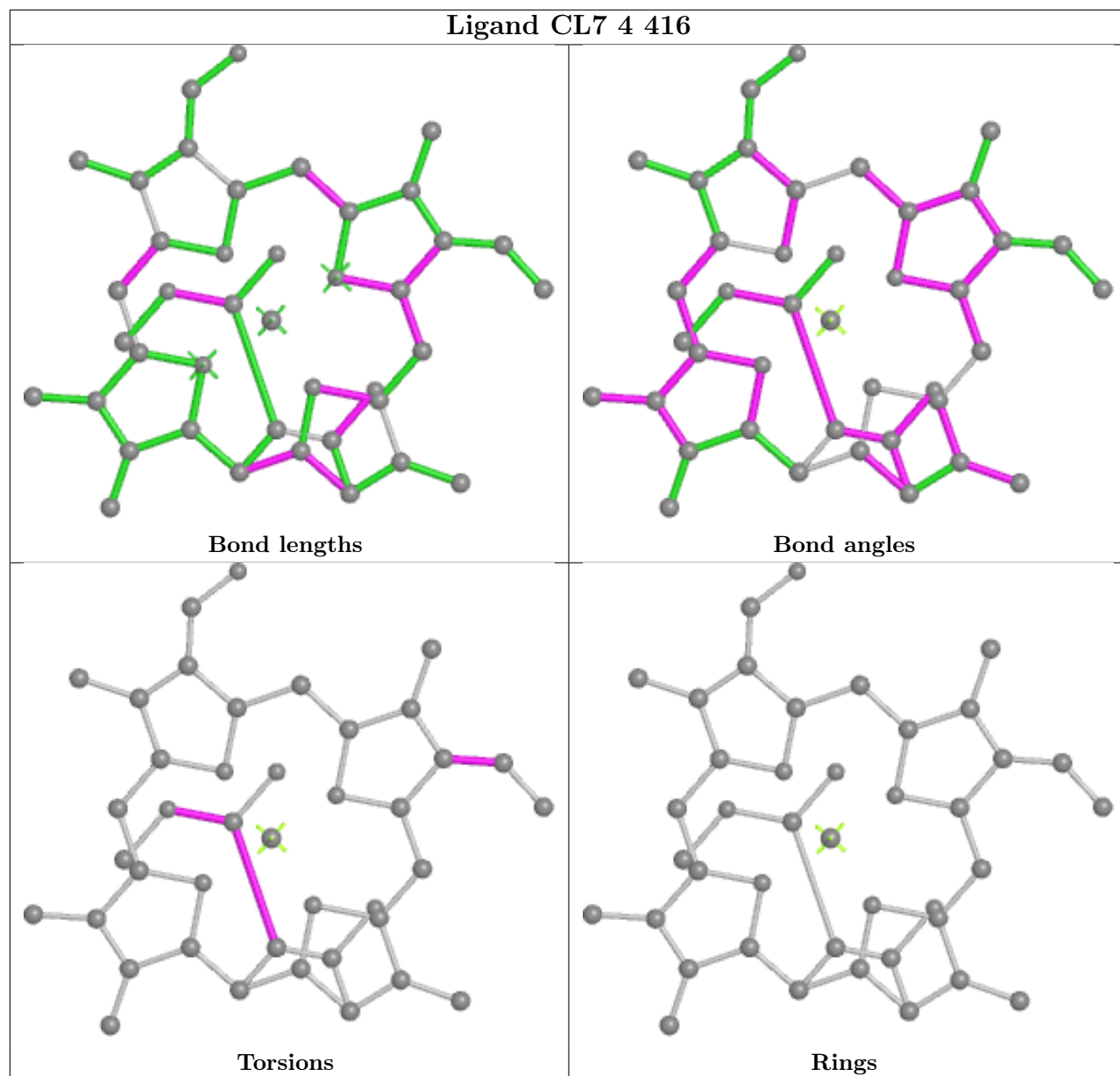


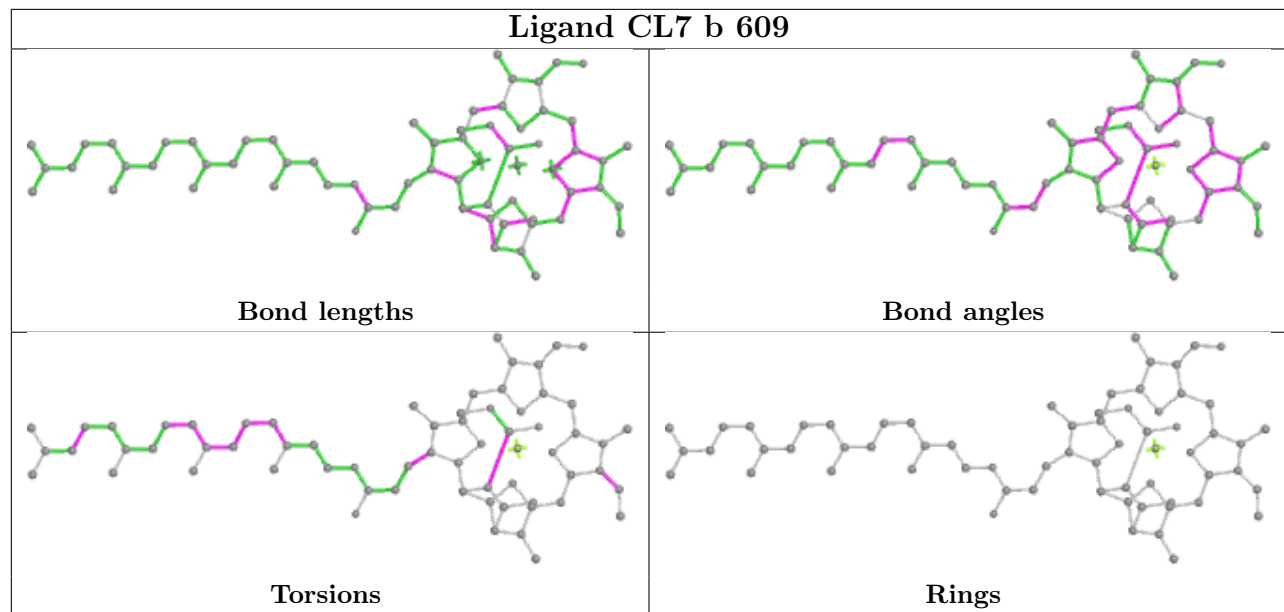


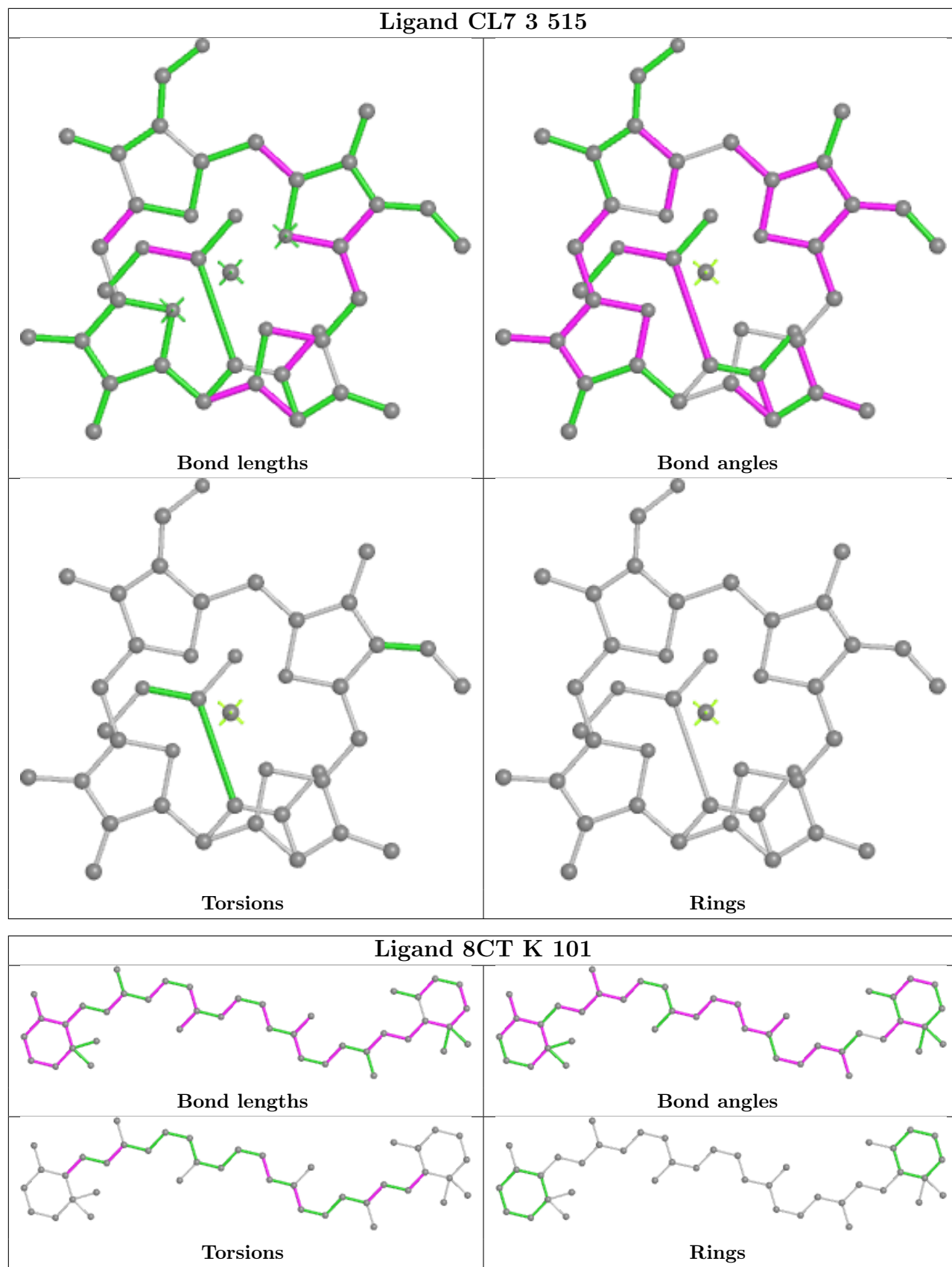


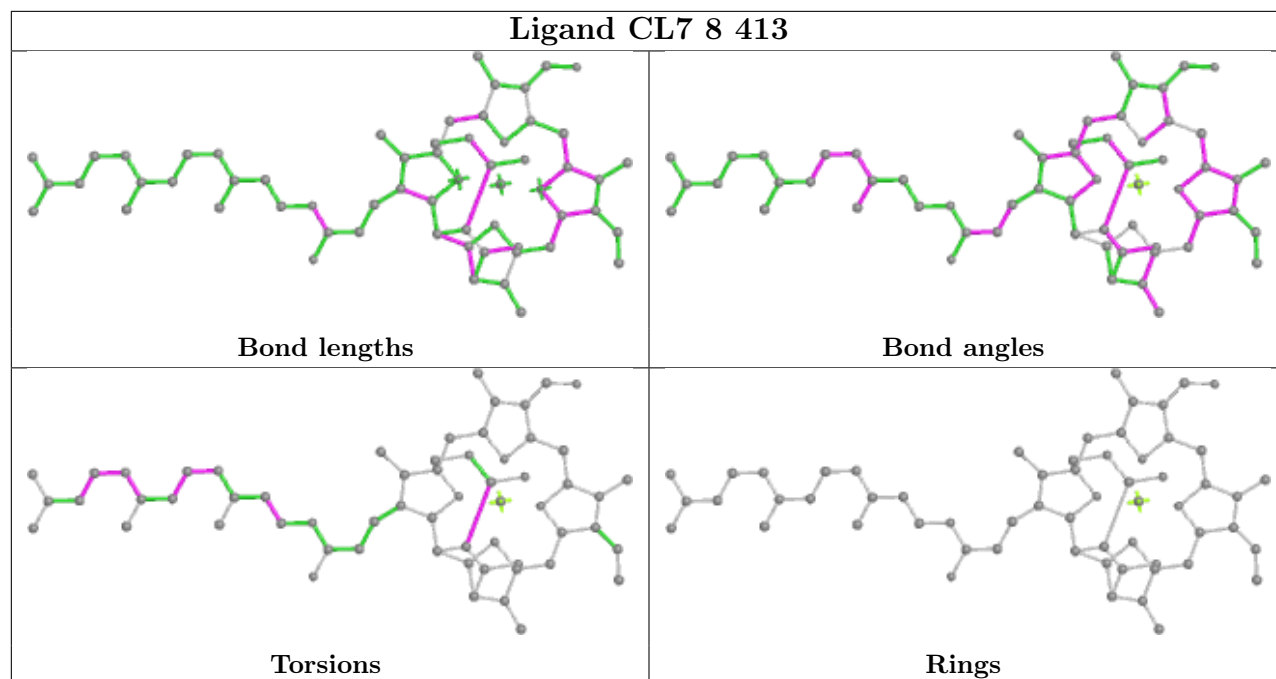












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

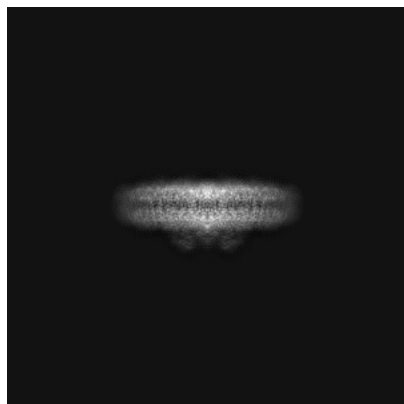
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33929. These allow visual inspection of the internal detail of the map and identification of artifacts.

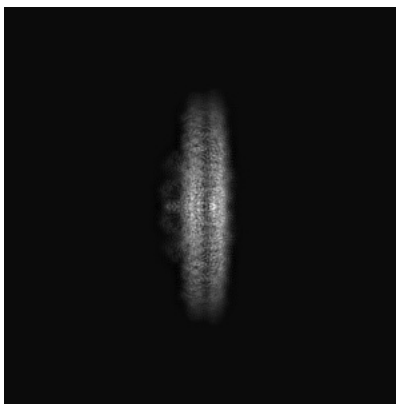
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

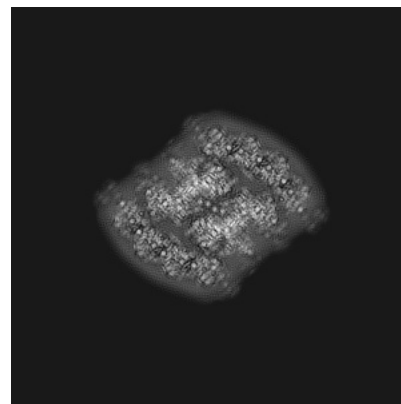
6.1.1 Primary map



X

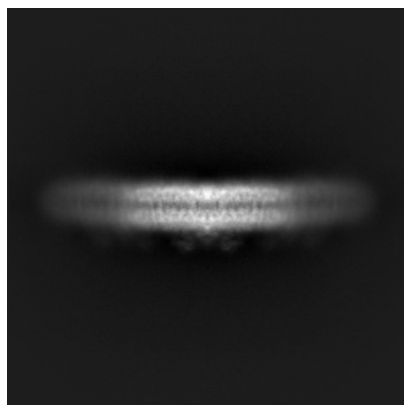


Y

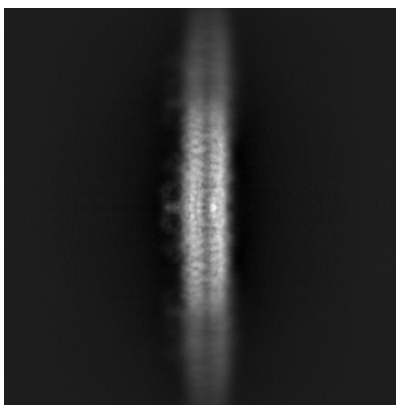


Z

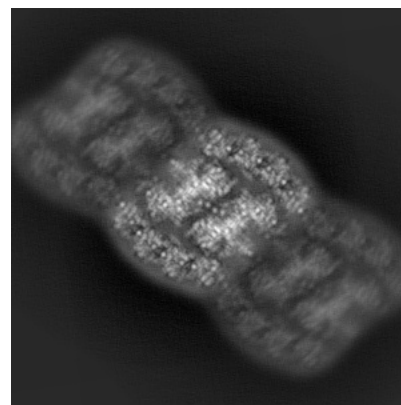
6.1.2 Raw map



X



Y

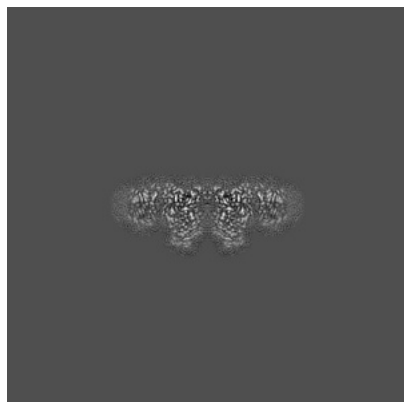


Z

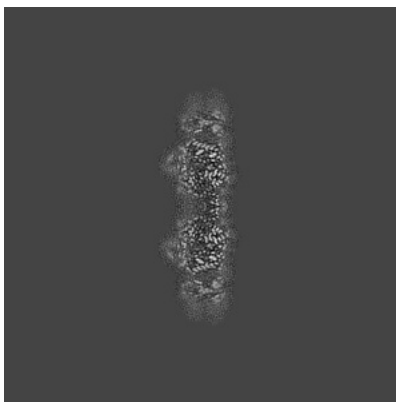
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

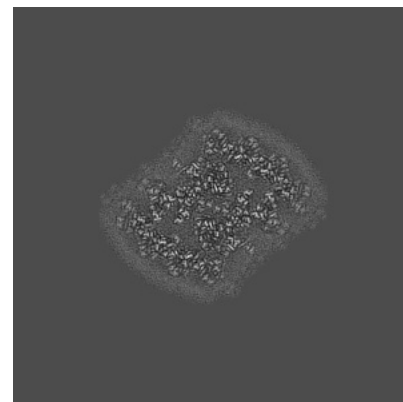
6.2.1 Primary map



X Index: 240

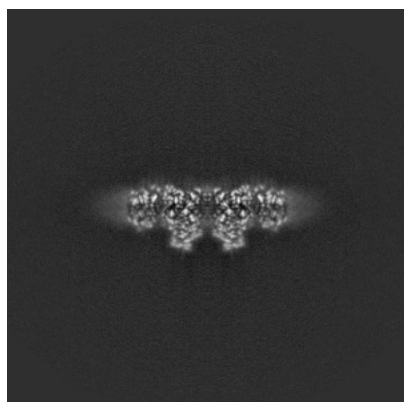


Y Index: 240

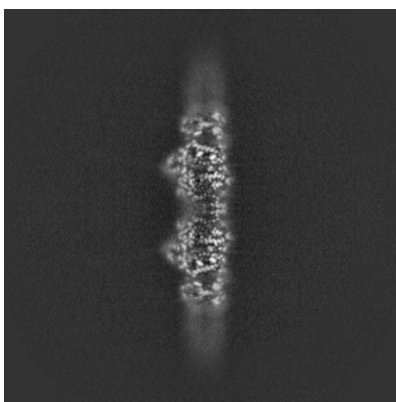


Z Index: 240

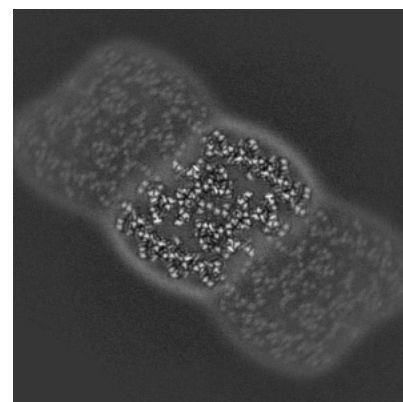
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

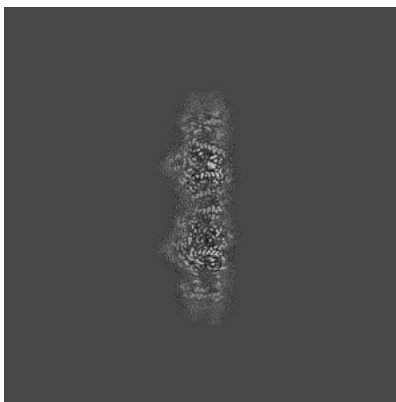
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

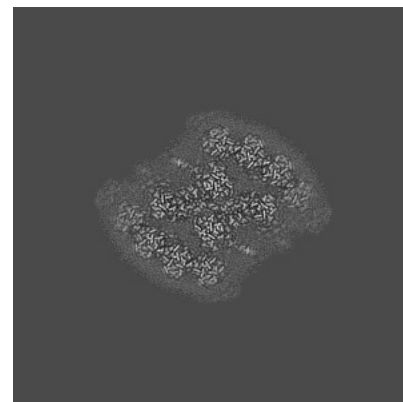
6.3.1 Primary map



X Index: 237



Y Index: 242

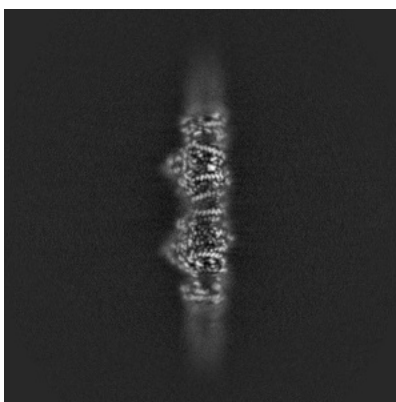


Z Index: 251

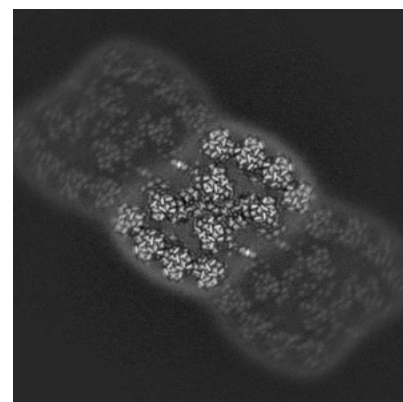
6.3.2 Raw map



X Index: 237



Y Index: 242

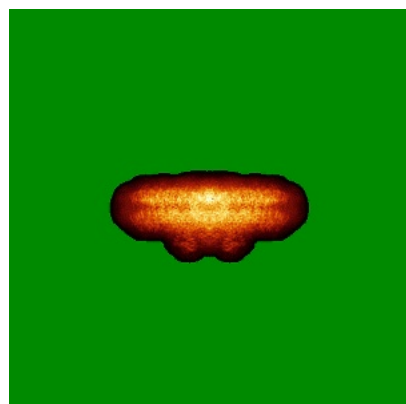


Z Index: 251

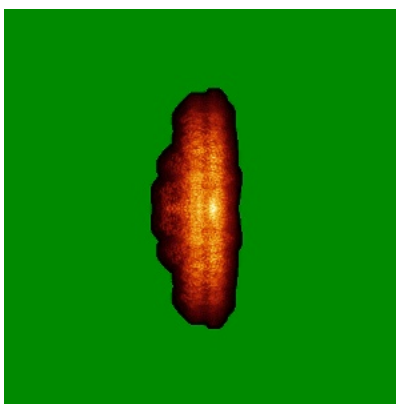
The images above show the largest variance slices of the map in three orthogonal directions.

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

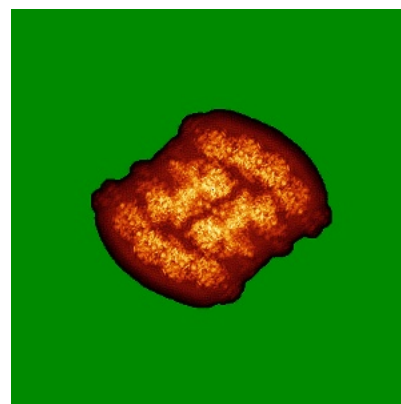
6.4.1 Primary map



X

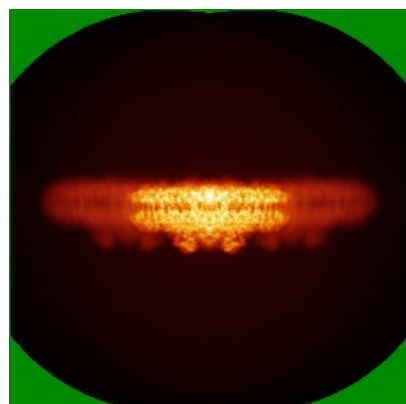


Y

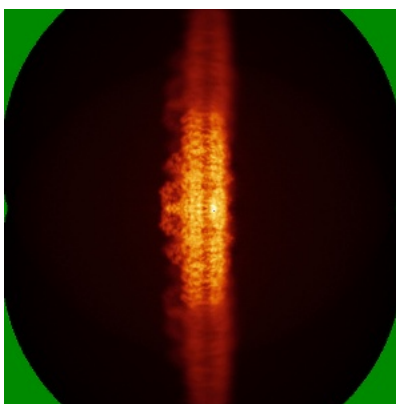


Z

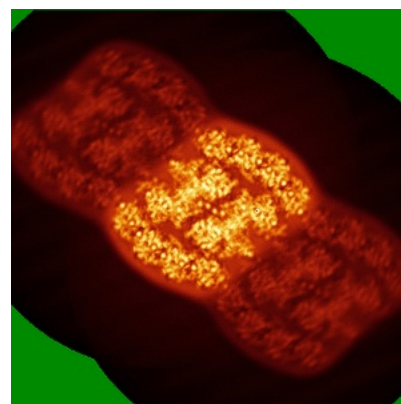
6.4.2 Raw map



X



Y

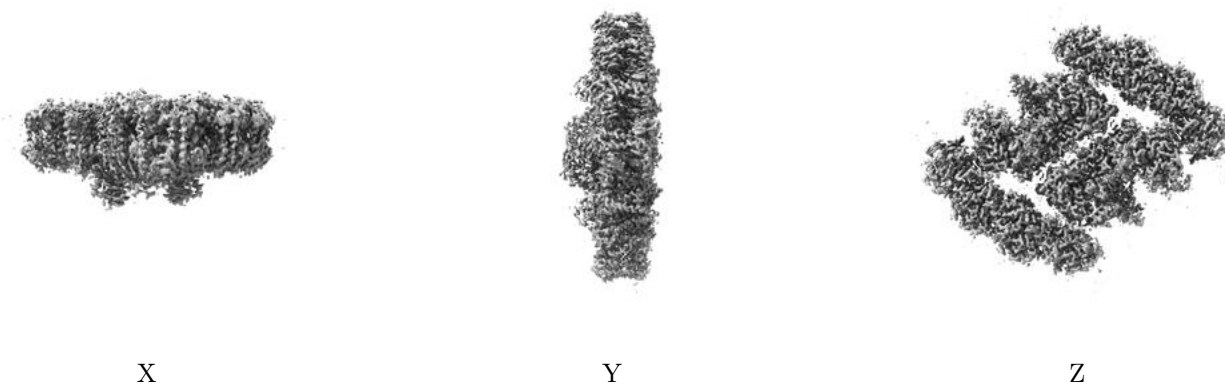


Z

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 0.0188. 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.

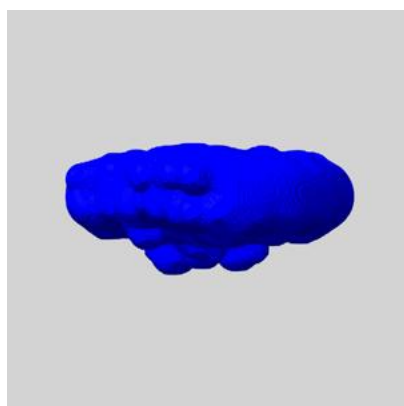
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

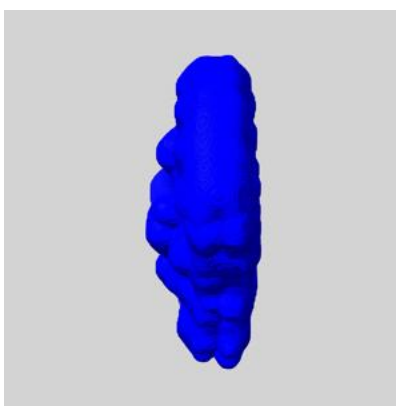
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

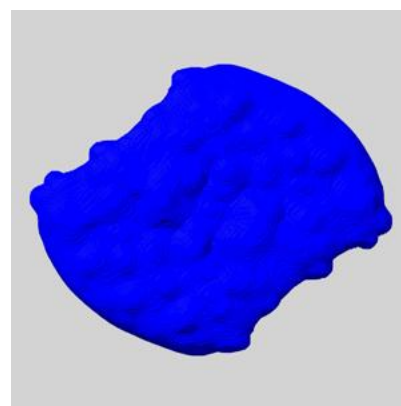
6.6.1 emd_33929_msk_1.map [i](#)



X



Y

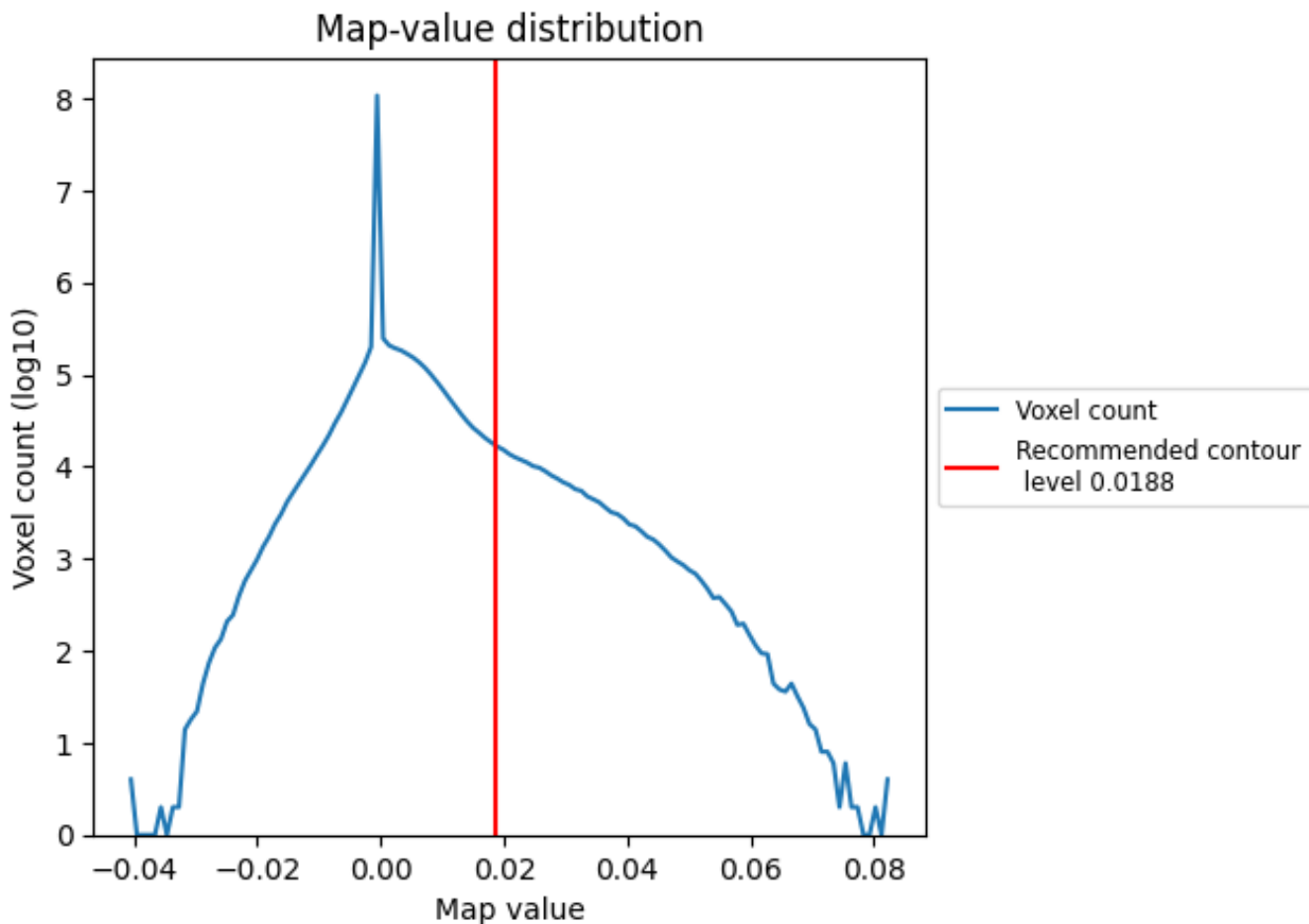


Z

7 Map analysis [i](#)

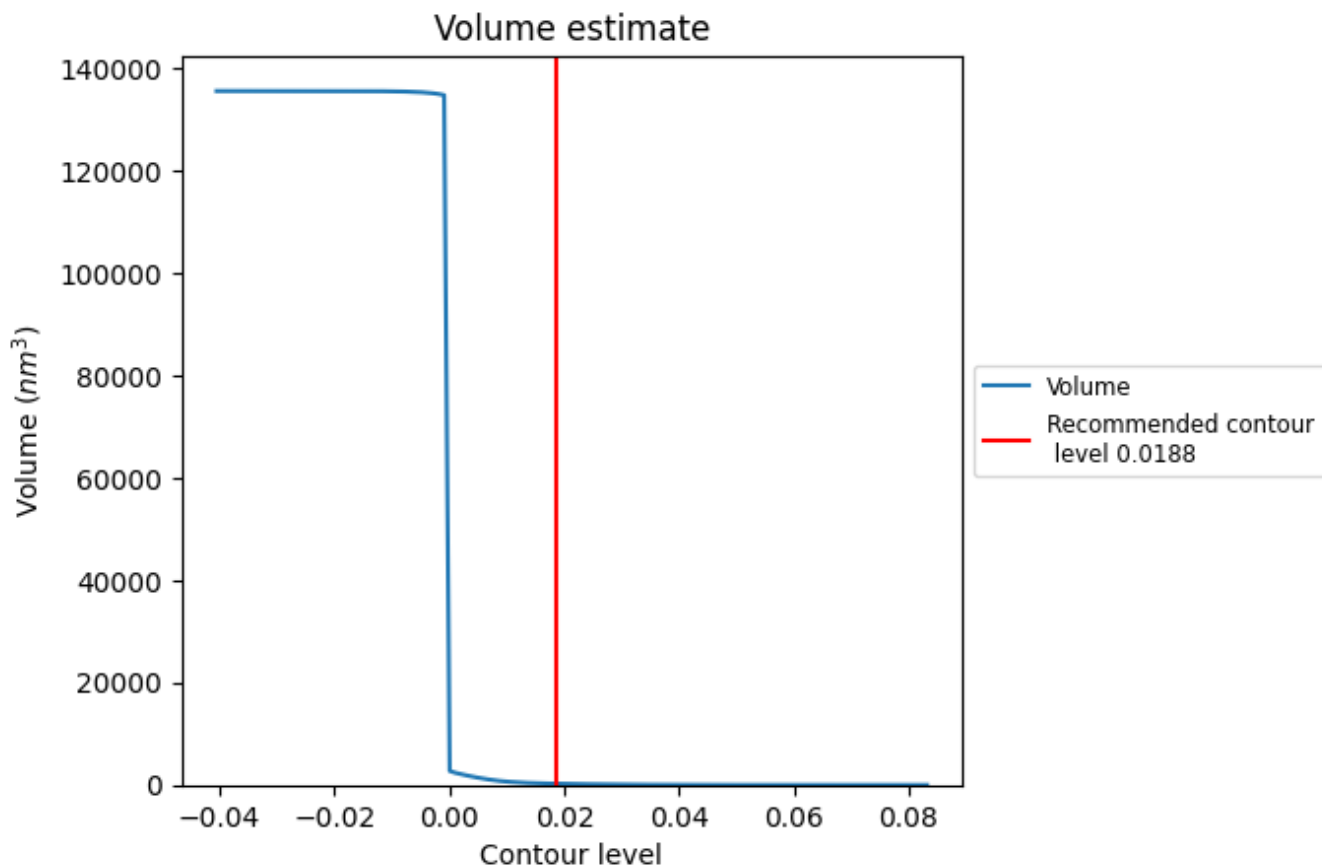
This section contains the results of statistical analysis of the map.

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.

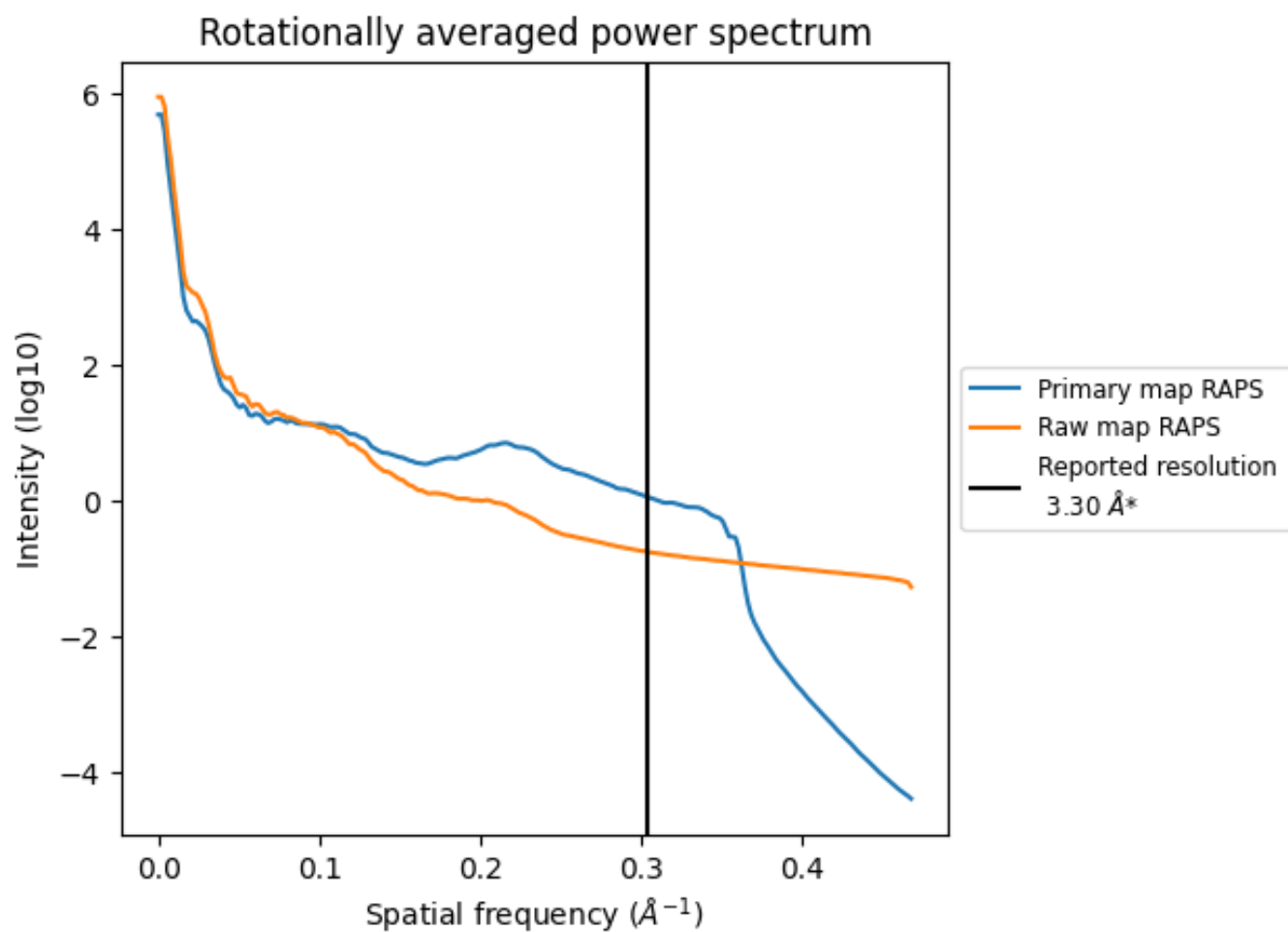
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 243 nm³; this corresponds to an approximate mass of 219 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](#)

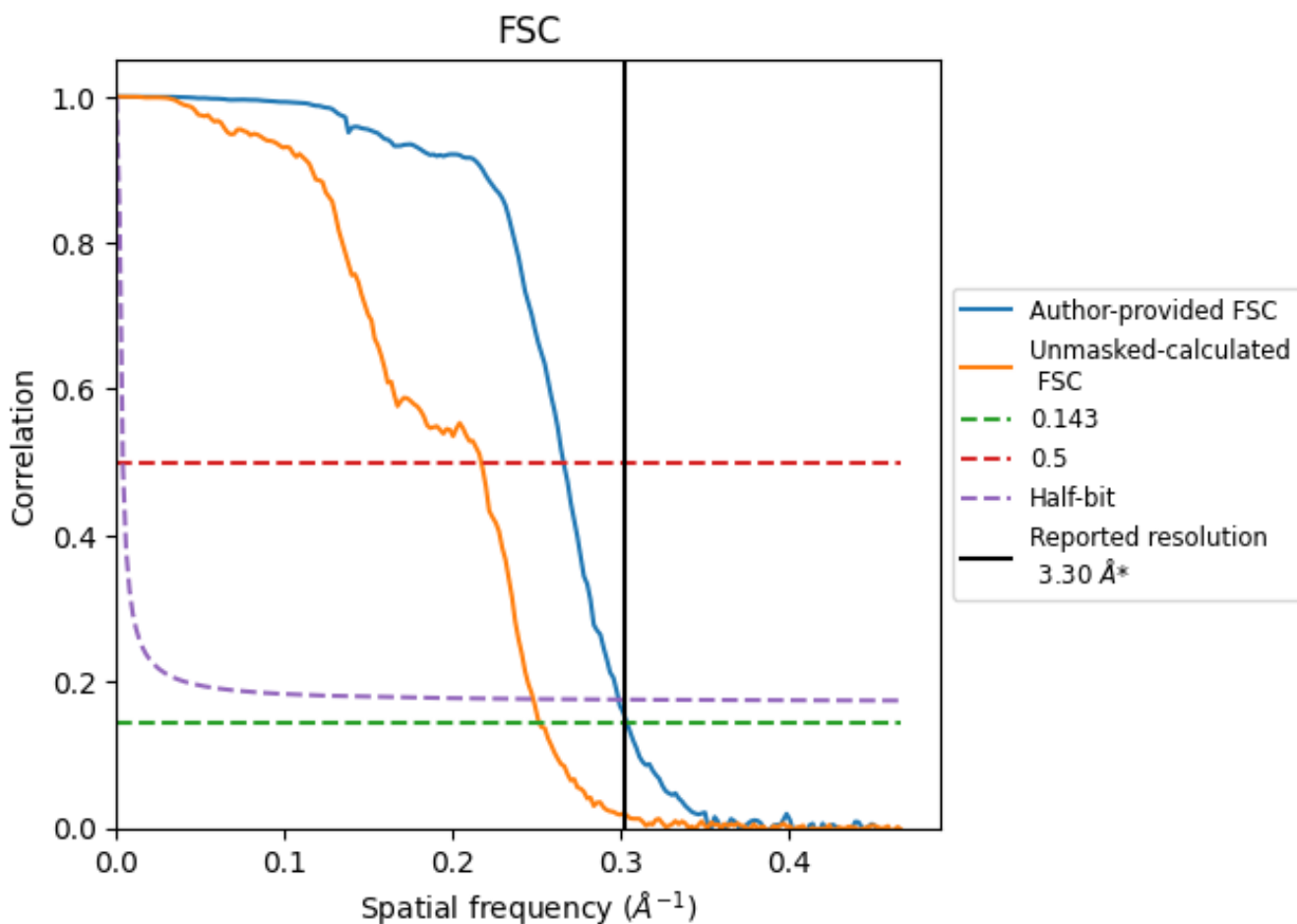


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

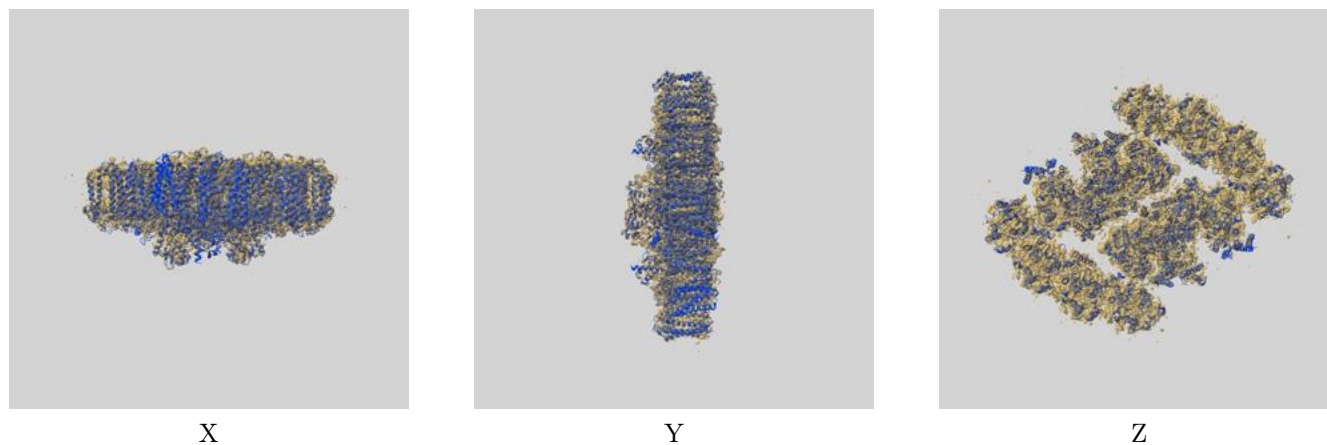
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.76	3.34
Unmasked-calculated*	3.97	4.60	4.03

*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 3.97 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

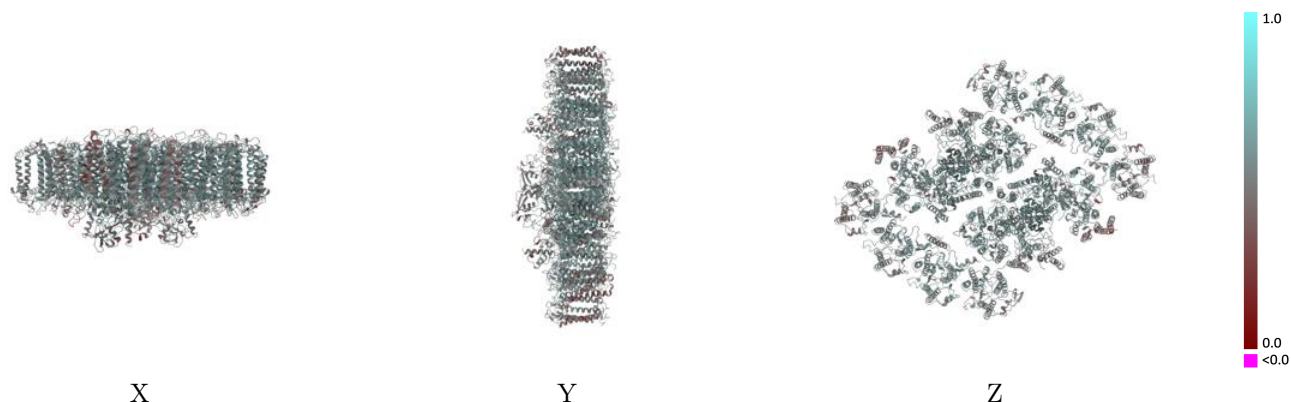
This section contains information regarding the fit between EMDB map EMD-33929 and PDB model 7YMI. Per-residue inclusion information can be found in section 3 on page 35.

9.1 Map-model overlay [i](#)



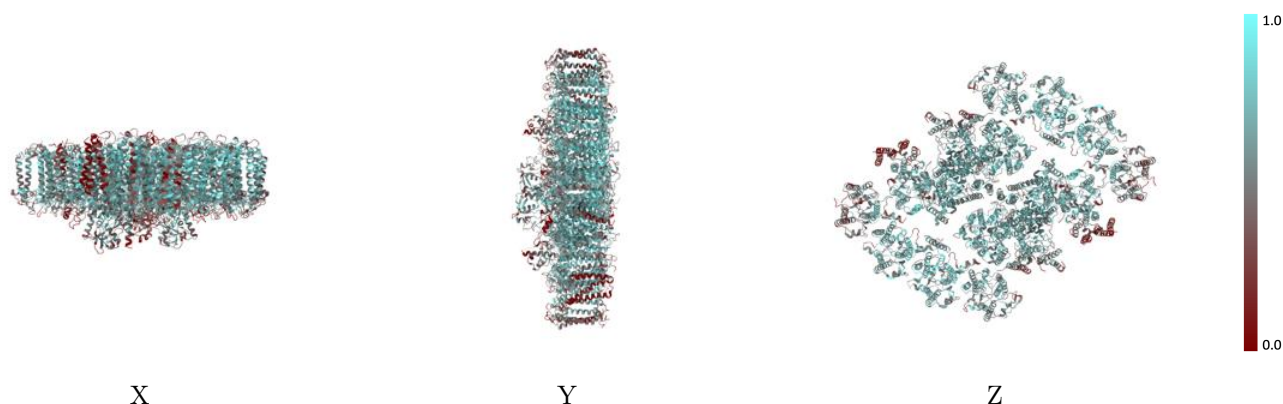
The images above show the 3D surface view of the map at the recommended contour level 0.0188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



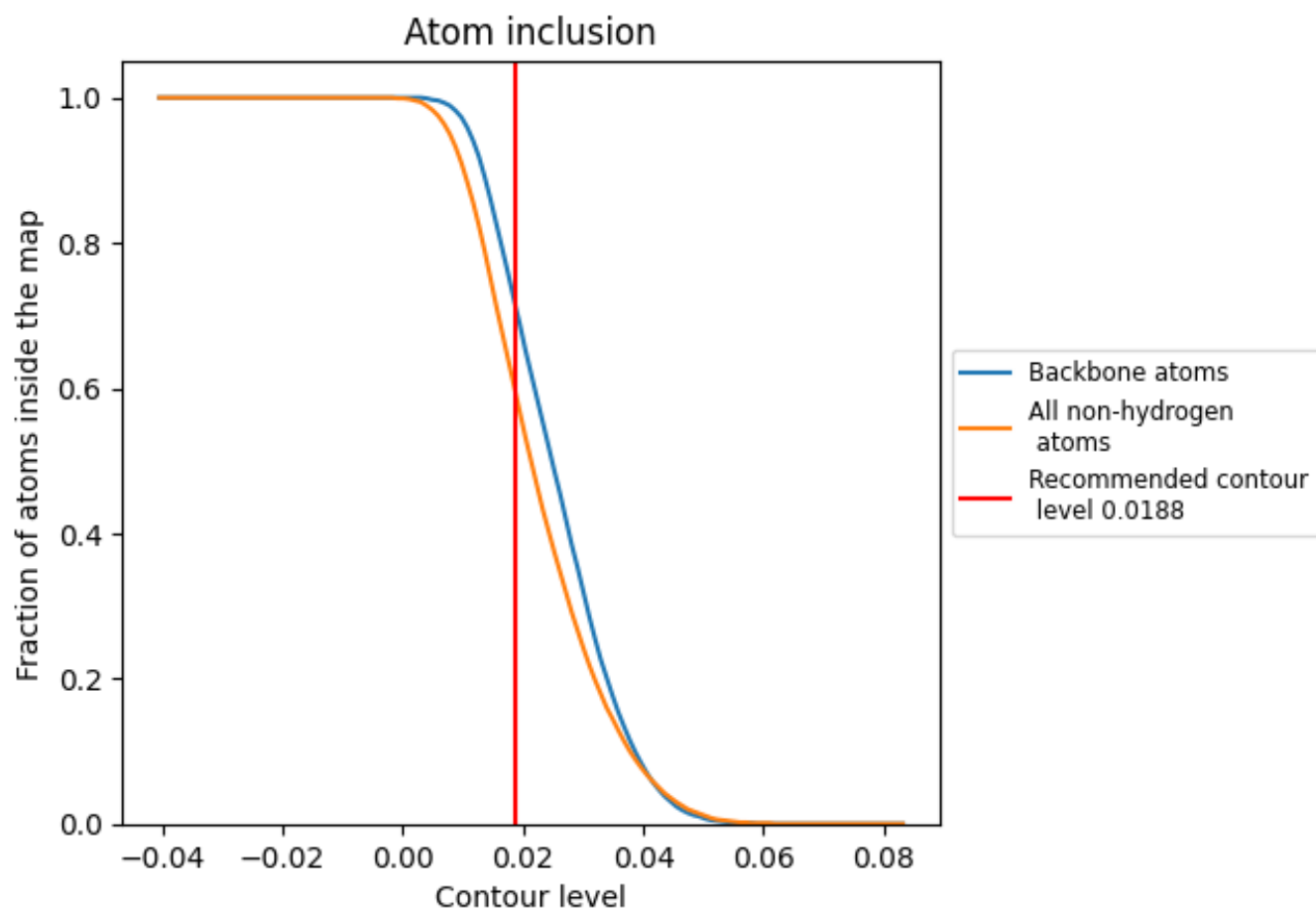
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

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 (0.0188).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 59% 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 (0.0188) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5910	 0.5380
1	 0.4760	 0.5010
2	 0.6300	 0.5500
3	 0.6430	 0.5510
4	 0.5670	 0.5290
5	 0.4770	 0.5000
6	 0.6280	 0.5490
7	 0.6410	 0.5510
8	 0.5670	 0.5310
A	 0.6660	 0.5610
B	 0.6550	 0.5590
C	 0.5910	 0.5410
D	 0.6720	 0.5710
E	 0.3170	 0.4380
F	 0.4820	 0.4780
G	 0.5660	 0.4670
H	 0.5860	 0.5430
I	 0.6350	 0.5470
K	 0.3050	 0.4820
L	 0.6320	 0.5700
M	 0.5240	 0.5200
T	 0.5130	 0.5430
X	 0.3360	 0.4910
Y	 0.0560	 0.4000
Z	 0.1340	 0.3830
a	 0.6740	 0.5610
b	 0.6590	 0.5590
c	 0.5920	 0.5410
d	 0.6720	 0.5700
e	 0.3190	 0.4380
f	 0.4820	 0.4720
g	 0.5660	 0.4590
h	 0.5880	 0.5420
i	 0.6350	 0.5490
k	 0.3050	 0.4810



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Chain	Atom inclusion	Q-score
l	 0.6280	 0.5630
m	 0.5240	 0.5180
t	 0.5130	 0.5400
x	 0.3360	 0.4860
y	 0.0560	 0.3990
z	 0.1340	 0.3810