



wwPDB EM Validation Summary Report ⓘ

Sep 14, 2026 – 01:54 PM JST

PDB ID : 7YMI / pdb_00007ymi
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 wwPDB EM Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

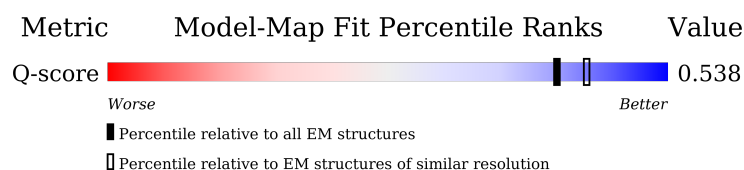
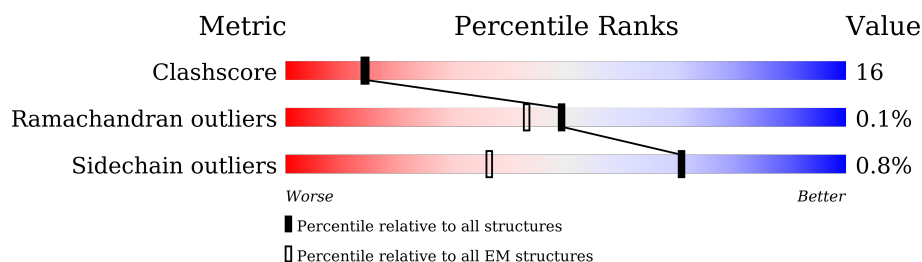
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	8% 61% 18% 21%
1	a	360	8% 59% 20% 21%
2	B	506	12% 77% 18% 5%
2	b	506	12% 77% 17% 5%

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Mol	Chain	Length	Quality of chain
3	C	490	
3	c	490	
4	D	351	
4	d	351	
5	E	83	
5	e	83	
6	F	99	
6	f	99	
7	H	71	
7	h	71	
8	I	34	
8	i	34	
9	K	45	
9	k	45	
10	L	38	
10	l	38	
11	M	34	
11	m	34	
12	T	46	
12	t	46	
13	X	40	
13	x	40	
14	Y	39	
14	y	39	
15	Z	62	

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Mol	Chain	Length	Quality of chain
15	z	62	
16	2	352	
16	6	352	
17	G	41	
17	g	41	
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-
32	ZEX	1	422	-	-	X	-
32	ZEX	2	520	-	-	X	-
32	ZEX	2	521	-	-	X	-
32	ZEX	3	522	-	-	X	-
32	ZEX	3	525	-	-	X	-
32	ZEX	4	403	-	-	X	-
32	ZEX	5	422	-	-	X	-
32	ZEX	6	520	-	-	X	-
32	ZEX	7	522	-	-	X	-
32	ZEX	8	403	-	-	X	-

2 Entry composition

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
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
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
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
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
10	l	36	Total	C	N	O	0	0
			288	194	45	49		

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

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

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

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

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

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

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

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

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

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

- 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 (CCD ID: CL7) (formula: $C_{54}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



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

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

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	1	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	1	1	Total 62	C 51	Mg 1	N 4	O 6	0
21	1	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	1	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	1	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	1	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	1	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	1	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	1	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	1	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	1	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	1	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	1	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	1	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	3	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	3	1	Total 58	C 47	Mg 1	N 4	O 6	0
21	3	1	Total 65	C 54	Mg 1	N 4	O 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
			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
21	4	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	4	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	4	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	4	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	4	1	Total 53	C 42	Mg 1	N 4	O 6	0
21	4	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	4	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	4	1	Total 42	C 33	Mg 1	N 4	O 4	0
21	a	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	a	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	a	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	b	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	b	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	b	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	b	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	b	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	b	1	Total 60	C 49	Mg 1	N 4	O 6	0
21	b	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	b	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	b	1	Total 65	C 54	Mg 1	N 4	O 6	0

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

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

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

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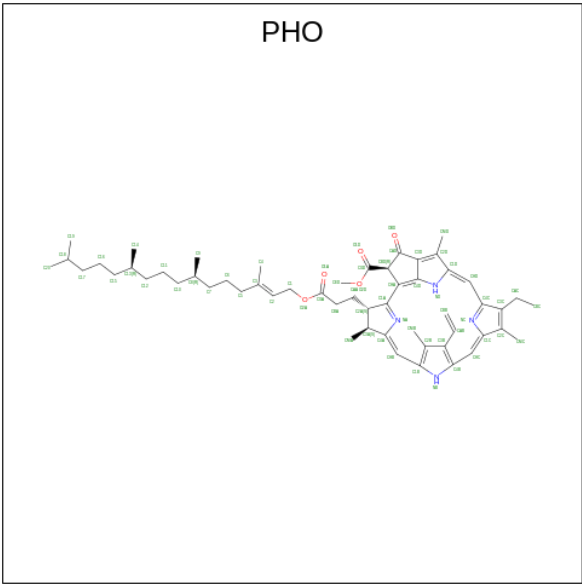
Mol	Chain	Residues	Atoms					AltConf
21	7	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	7	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	7	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	7	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	7	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	7	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	7	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	7	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	7	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	7	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	7	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	7	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	7	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	7	1	Total 55	C 44	Mg 1	N 4	O 6	0
21	7	1	Total 50	C 39	Mg 1	N 4	O 6	0
21	7	1	Total 45	C 34	Mg 1	N 4	O 6	0
21	8	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	8	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	8	1	Total 65	C 54	Mg 1	N 4	O 6	0
21	8	1	Total 41	C 32	Mg 1	N 4	O 4	0
21	8	1	Total 45	C 34	Mg 1	N 4	O 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 (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Ligand of Interest" by depositor).



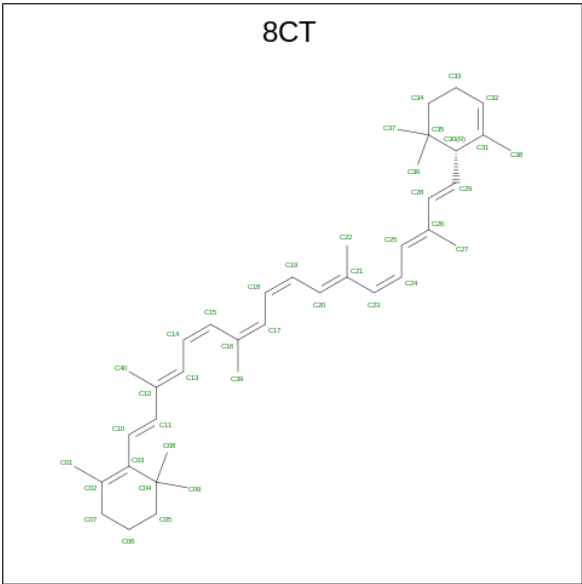
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	N	O	0
			64	55	4	5	
22	D	1	Total	C	N	O	0
			64	55	4	5	

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

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



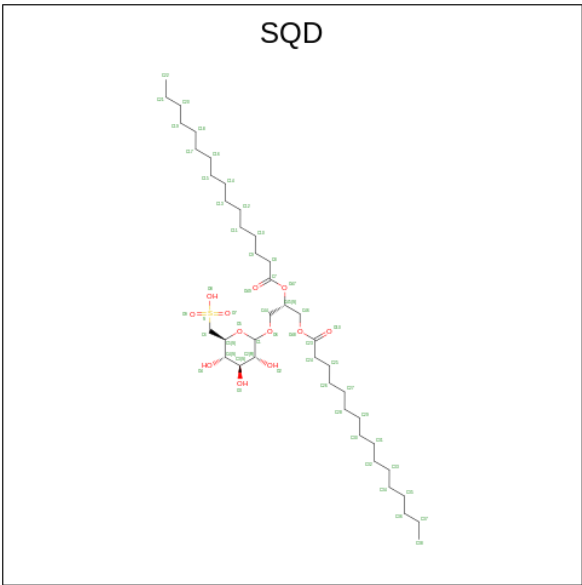
Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	B	1	Total	C	0
			40	40	
23	C	1	Total	C	0
			40	40	
23	C	1	Total	C	0
			40	40	
23	C	1	Total	C	0
			40	40	
23	D	1	Total	C	0
			40	40	

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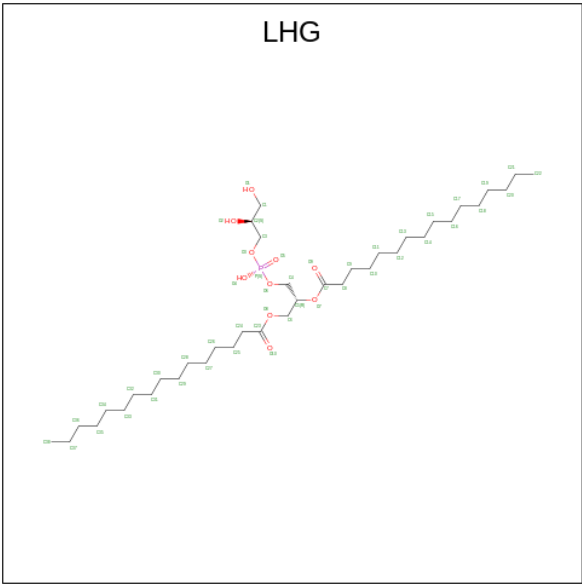
Mol	Chain	Residues	Atoms	AltConf
23	K	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	a	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	b	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	c	1	Total C 40 40	0
23	d	1	Total C 40 40	0
23	k	1	Total C 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 (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



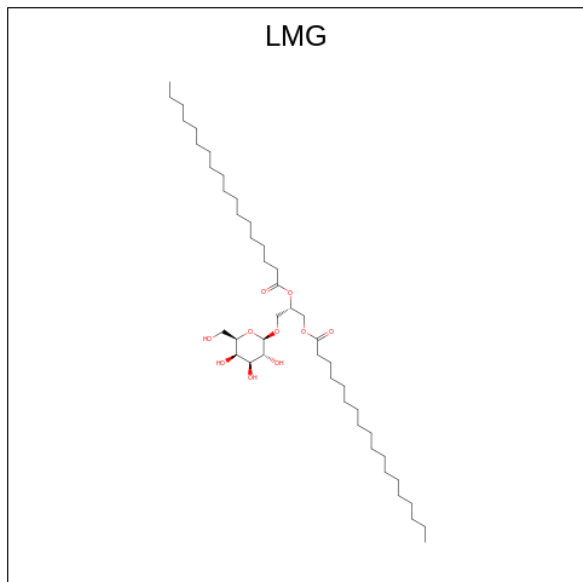
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	S	0
			34	21	12	1	
24	B	1	Total	C	O	S	0
			54	41	12	1	
24	B	1	Total	C	O	S	0
			34	21	12	1	
24	2	1	Total	C	O	S	0
			50	37	12	1	
24	2	1	Total	C	O	S	0
			41	28	12	1	
24	1	1	Total	C	O	S	0
			32	19	12	1	
24	3	1	Total	C	O	S	0
			46	33	12	1	
24	3	1	Total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

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



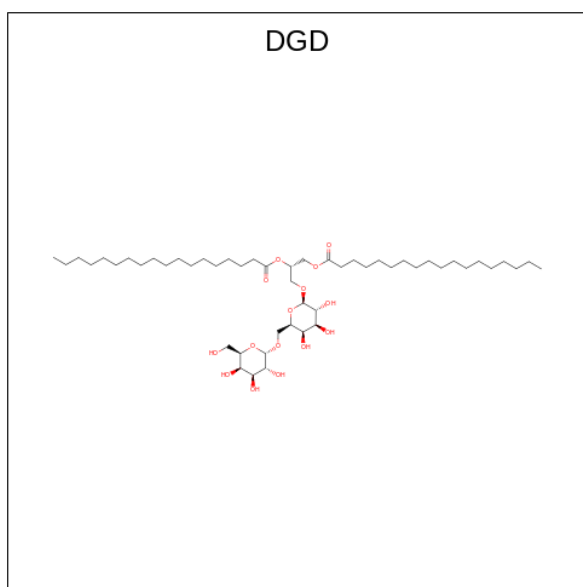
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			46	35	10	1	
25	B	1	Total	C	O	P	0
			45	34	10	1	
25	B	1	Total	C	O	P	0
			49	38	10	1	
25	D	1	Total	C	O	P	0
			49	38	10	1	
25	3	1	Total	C	O	P	0
			36	25	10	1	
25	4	1	Total	C	O	P	0
			49	38	10	1	
25	a	1	Total	C	O	P	0
			46	35	10	1	
25	b	1	Total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

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



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

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

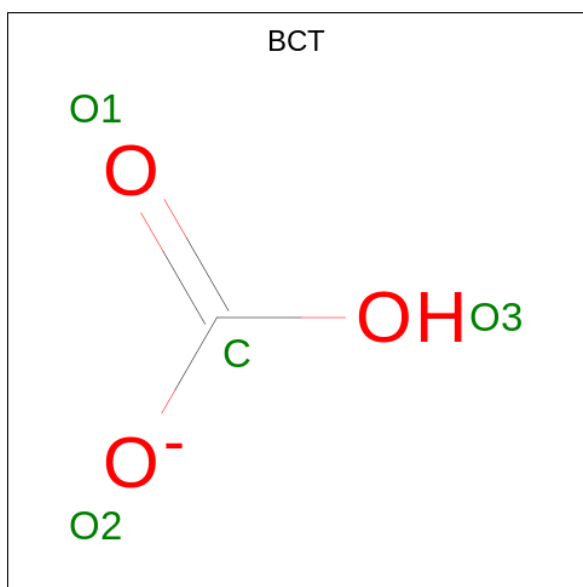


Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			62	47	15	
27	C	1	Total	C	O	0
			62	47	15	
27	b	1	Total	C	O	0
			62	47	15	
27	c	1	Total	C	O	0
			62	47	15	

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

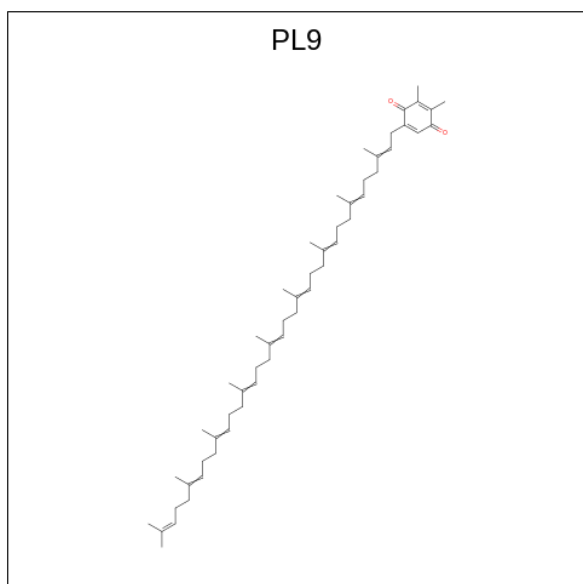
Mol	Chain	Residues	Atoms		AltConf
28	D	1	Total	Fe	0
			1	1	
28	d	1	Total	Fe	0
			1	1	

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



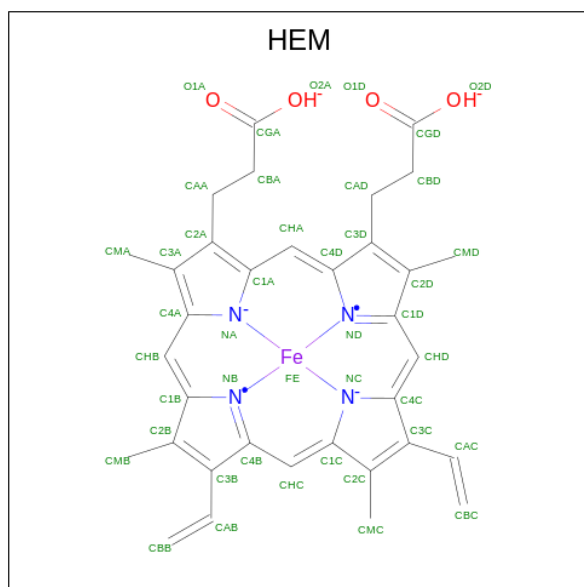
Mol	Chain	Residues	Atoms			AltConf
29	D	1	Total	C	O	0
			4	1	3	
29	d	1	Total	C	O	0
			4	1	3	

- 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 (CCD ID: PL9) (formula: C₅₃H₈₀O₂) (labeled as "Ligand of Interest" by depositor).



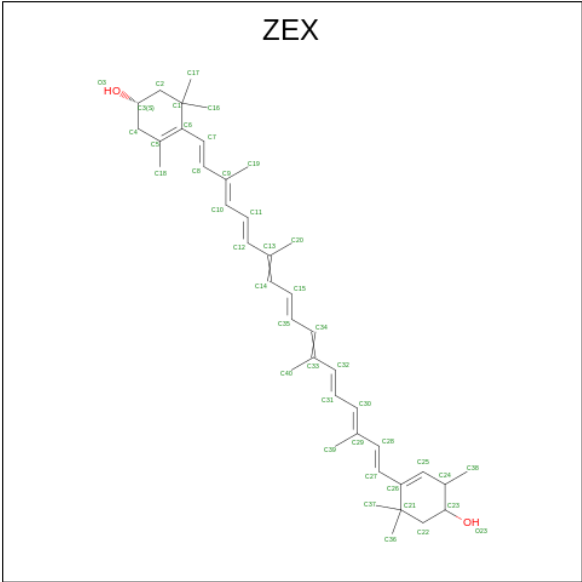
Mol	Chain	Residues	Atoms			AltConf
30	D	1	Total 55	C 53	O 2	0
30	d	1	Total 55	C 53	O 2	0

- Molecule 31 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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 43	C 34	Fe 1	N 4	O 4	0
31	f	1	Total 43	C 34	Fe 1	N 4	O 4	0

- 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 (CCD ID: ZEX) (formula: C₄₀H₅₆O₂) (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	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	

Continued on next page...

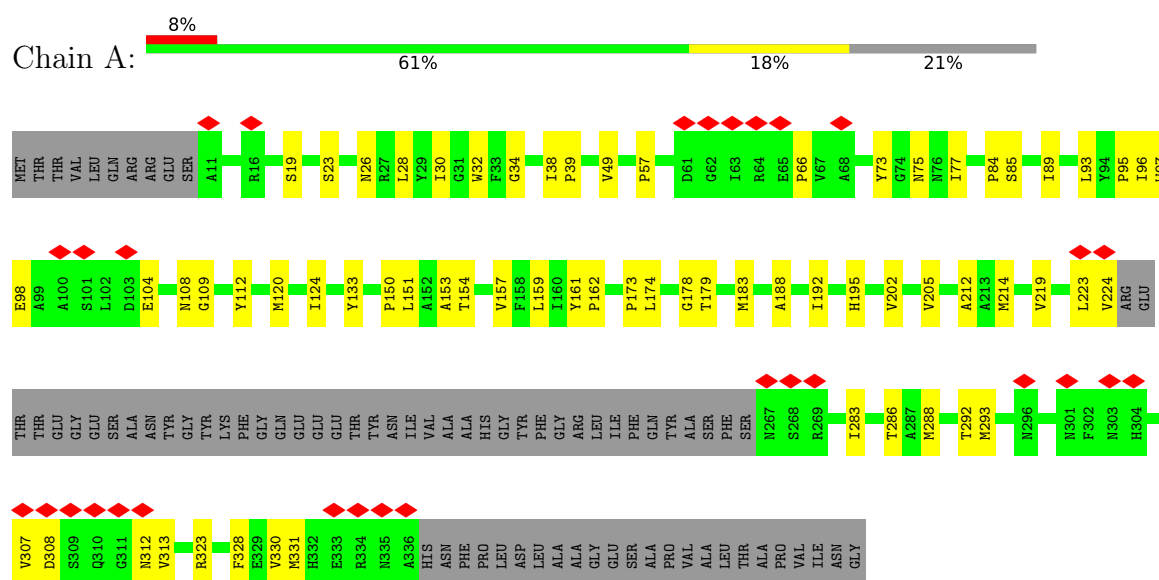
Continued from previous page...

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

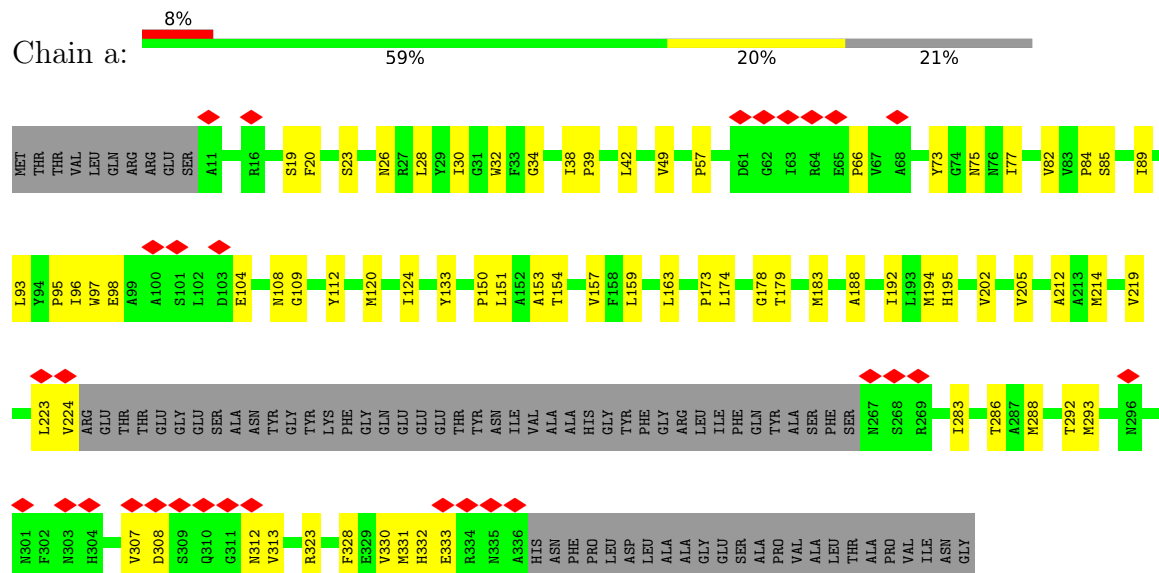
3 Residue-property plots

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.

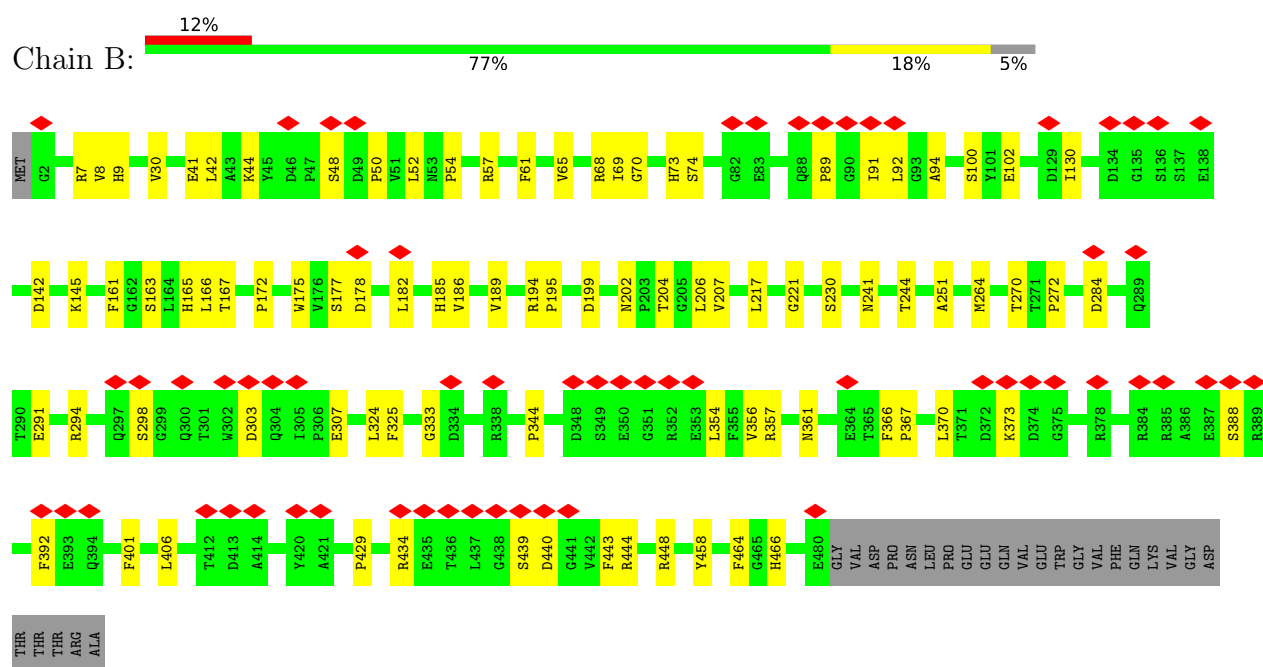
• Molecule 1: Photosystem II protein D1 2



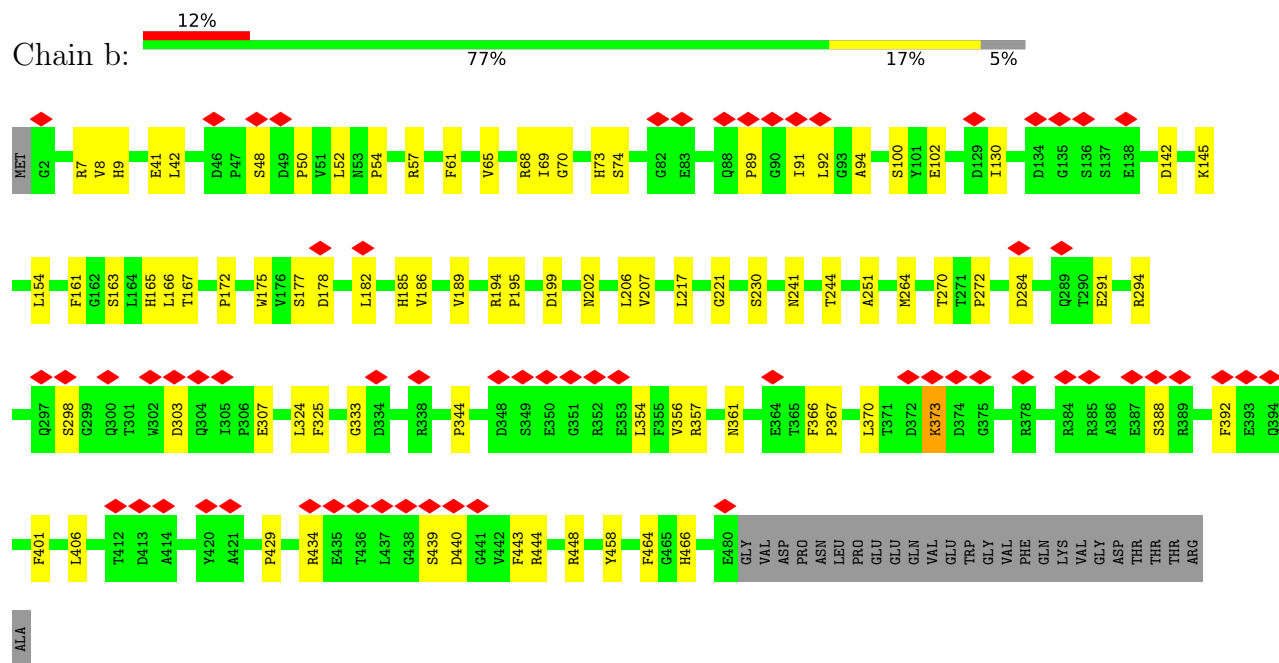
• Molecule 1: Photosystem II protein D1 2



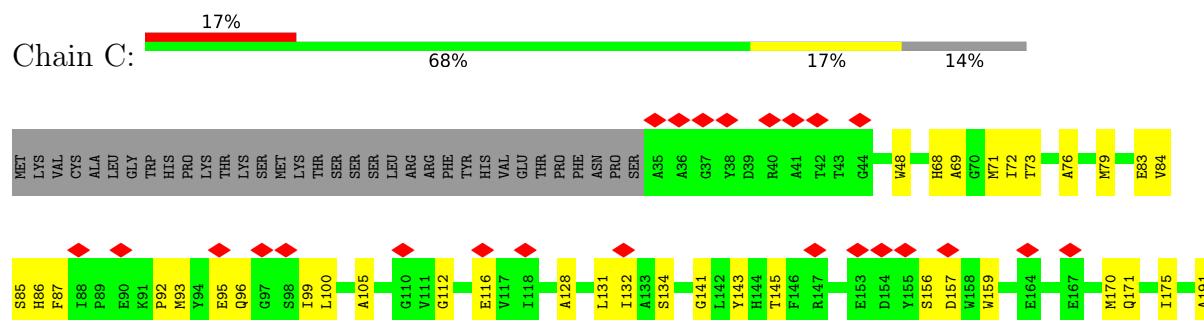
• Molecule 2: Photosystem II CP47 reaction center protein

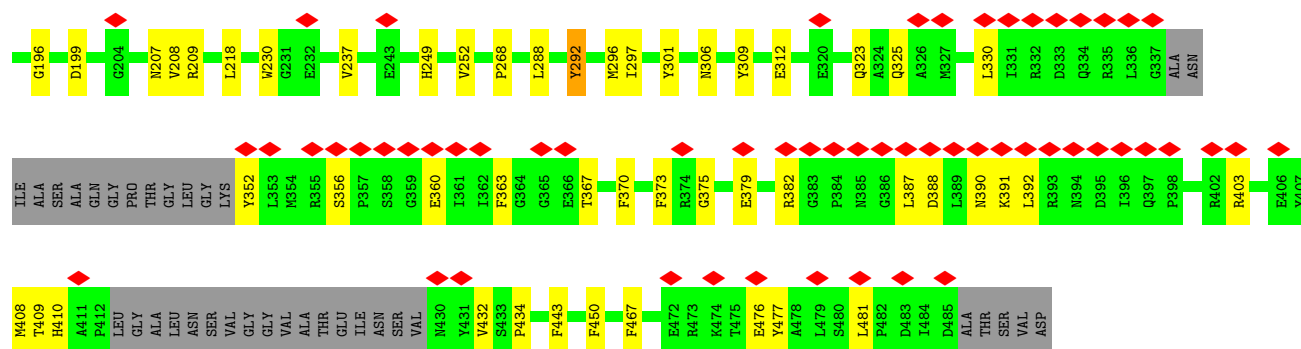


- Molecule 2: Photosystem II CP47 reaction center protein

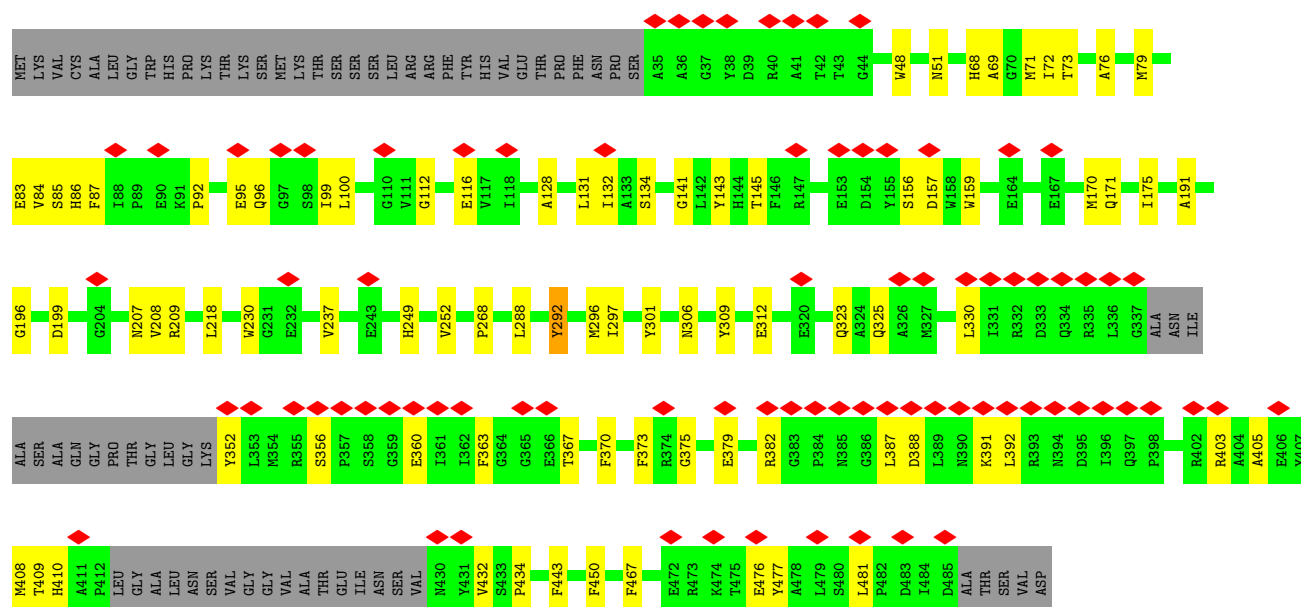


- Molecule 3: Photosystem II CP43 reaction center protein

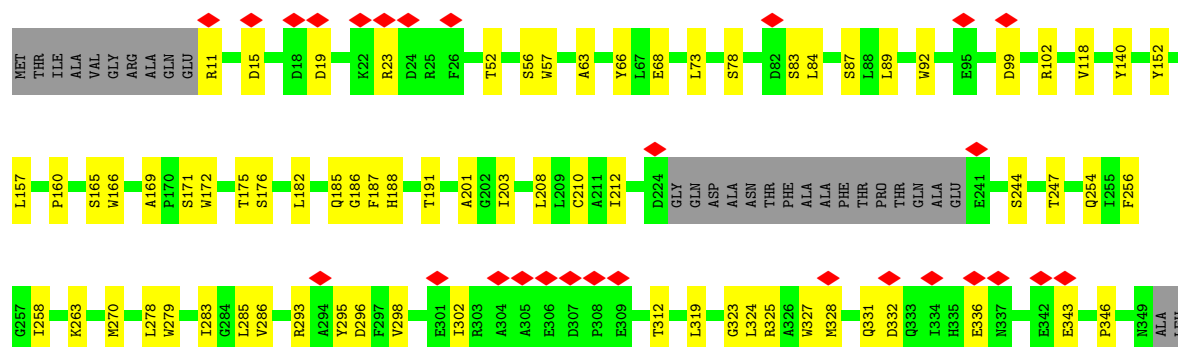




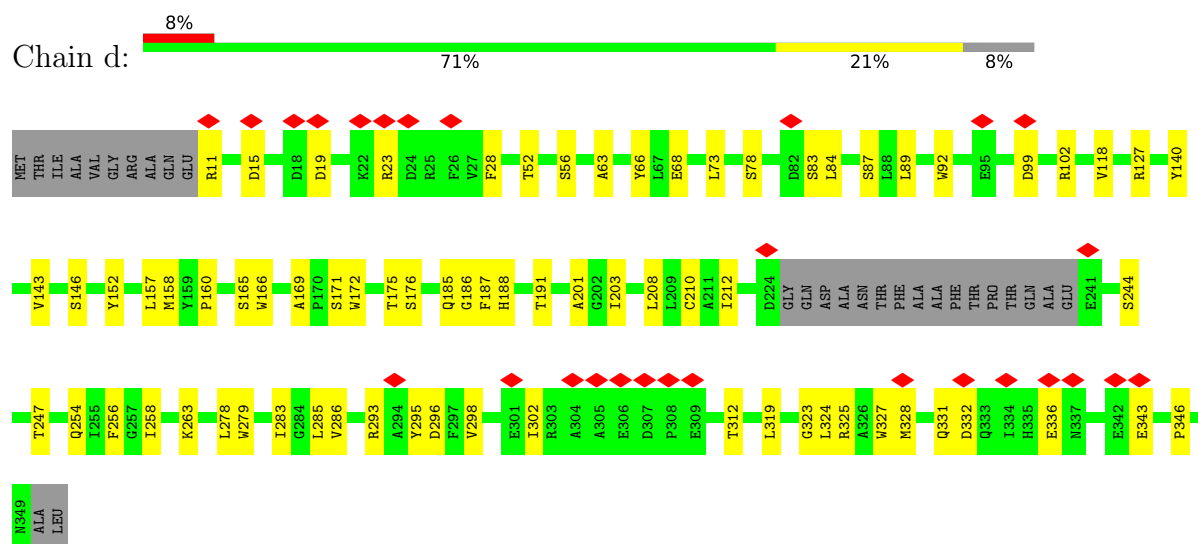
• Molecule 3: Photosystem II CP43 reaction center protein



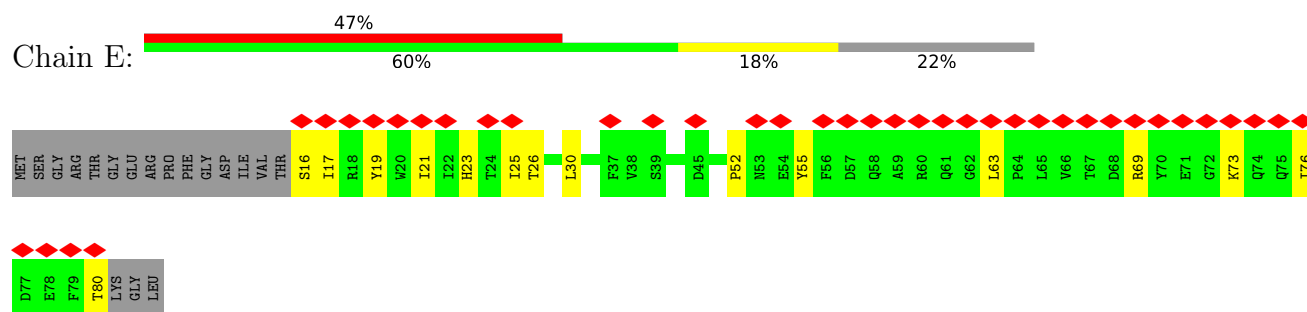
• Molecule 4: Photosystem II D2 protein 1



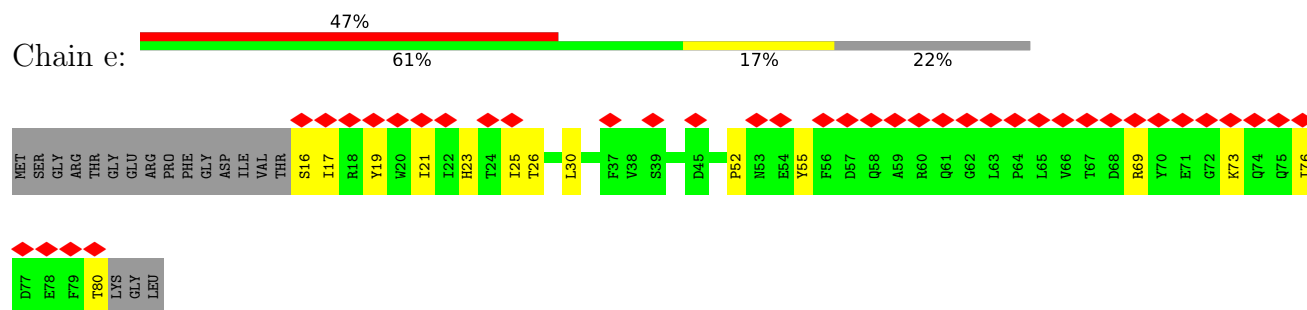
• Molecule 4: Photosystem II D2 protein 1



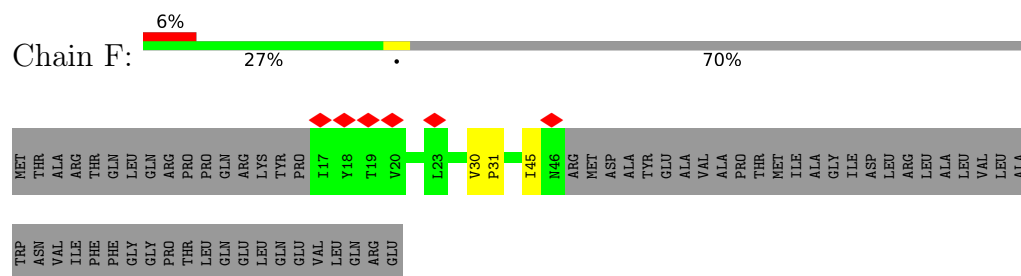
• Molecule 5: Cytochrome b559 subunit alpha



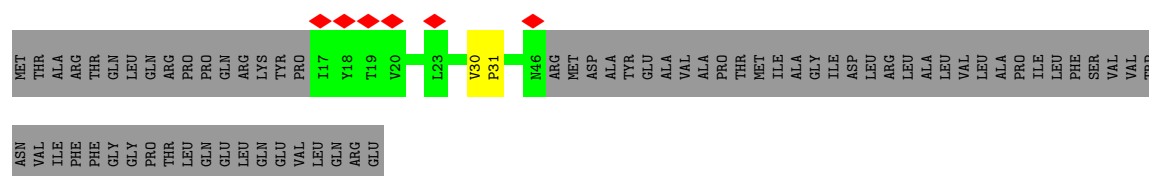
• Molecule 5: Cytochrome b559 subunit alpha



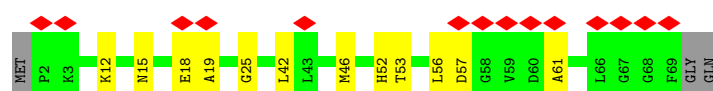
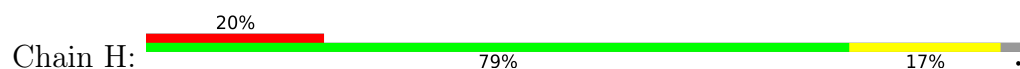
• Molecule 6: Photosystem II protein Y



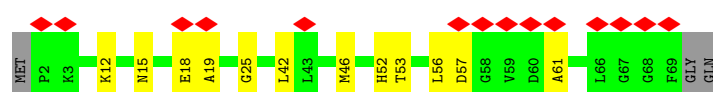
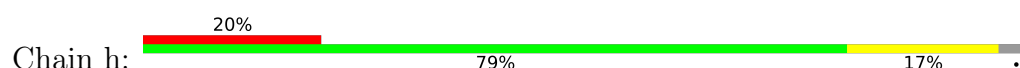
• Molecule 6: Photosystem II protein Y



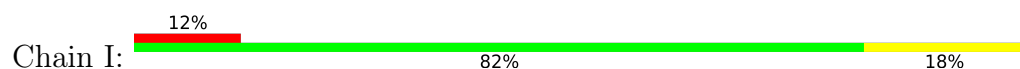
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



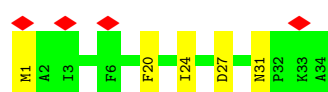
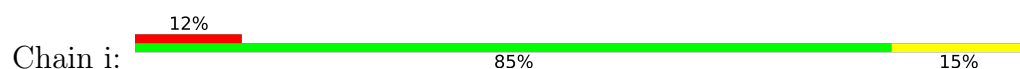
• Molecule 7: Photosystem II 10 kDa phosphoprotein PsbH



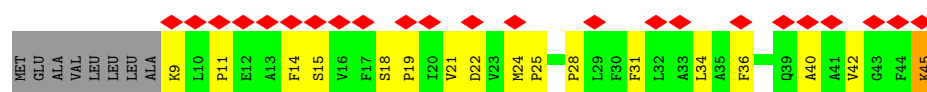
• Molecule 8: Photosystem II protein PsbI



• Molecule 8: Photosystem II protein PsbI



• Molecule 9: Photosystem II reaction center protein K

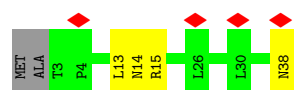
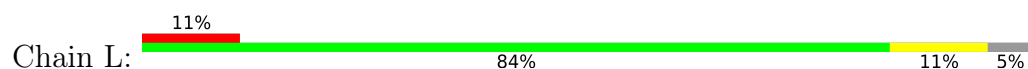


• Molecule 9: Photosystem II reaction center protein K

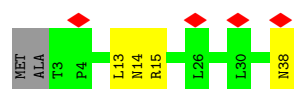
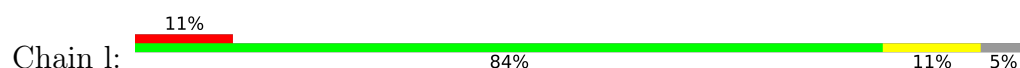




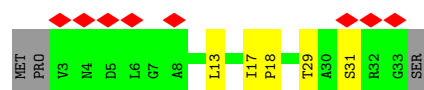
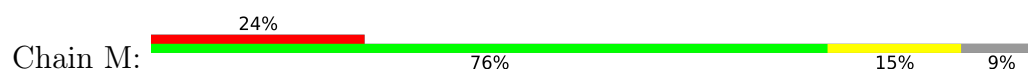
- Molecule 10: Photosystem II reaction center protein L



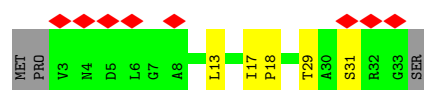
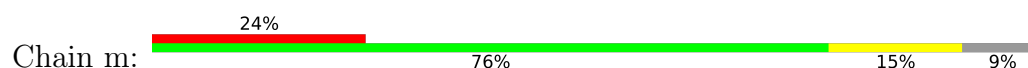
- Molecule 10: Photosystem II reaction center protein L



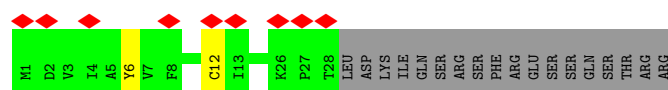
- Molecule 11: Photosystem II reaction center protein M



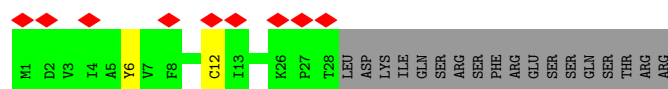
- Molecule 11: Photosystem II reaction center protein M



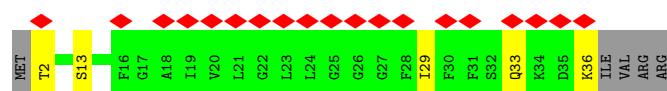
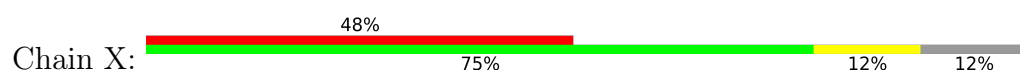
- Molecule 12: Photosystem II reaction center protein T



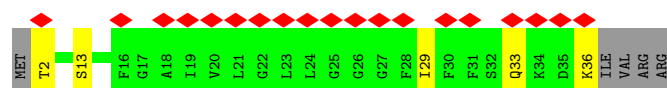
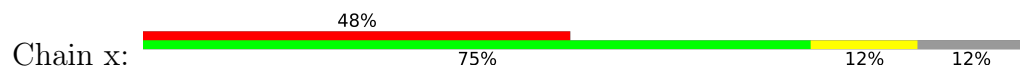
- Molecule 12: Photosystem II reaction center protein T



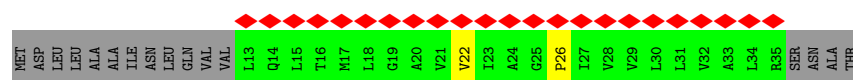
- Molecule 13: Photosystem II reaction center X protein



- Molecule 13: Photosystem II reaction center X protein



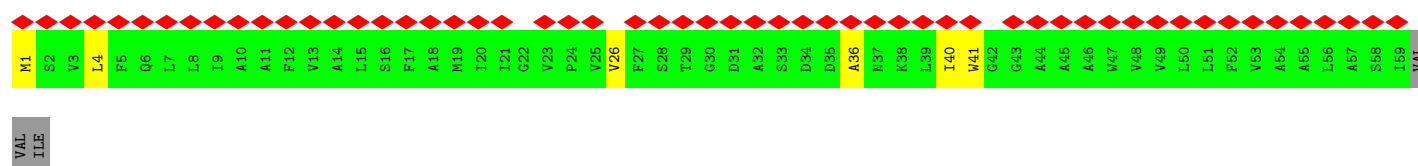
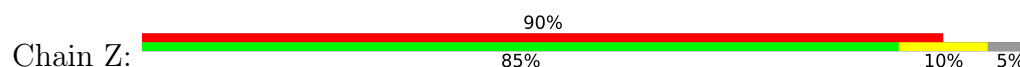
- Molecule 14: Photosystem II reaction center protein Ycf12



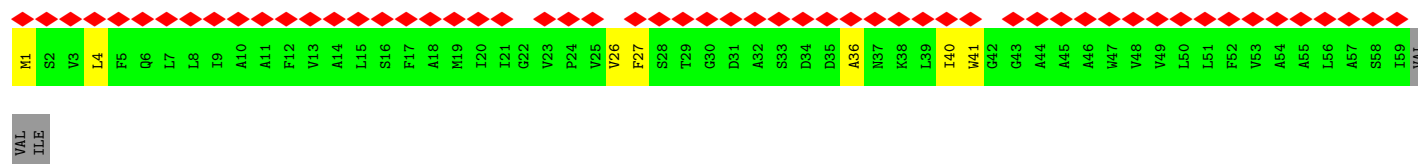
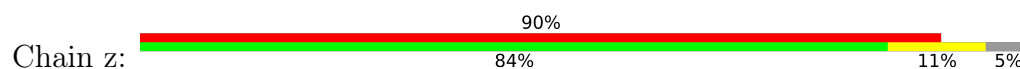
- Molecule 14: Photosystem II reaction center protein Ycf12



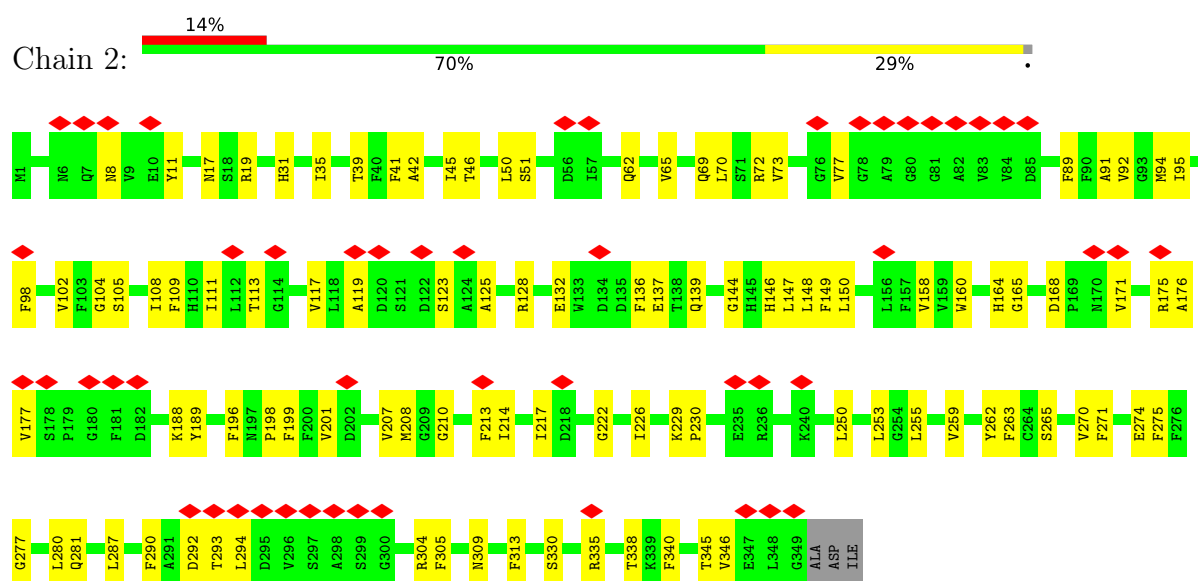
- Molecule 15: Photosystem II reaction center protein Z



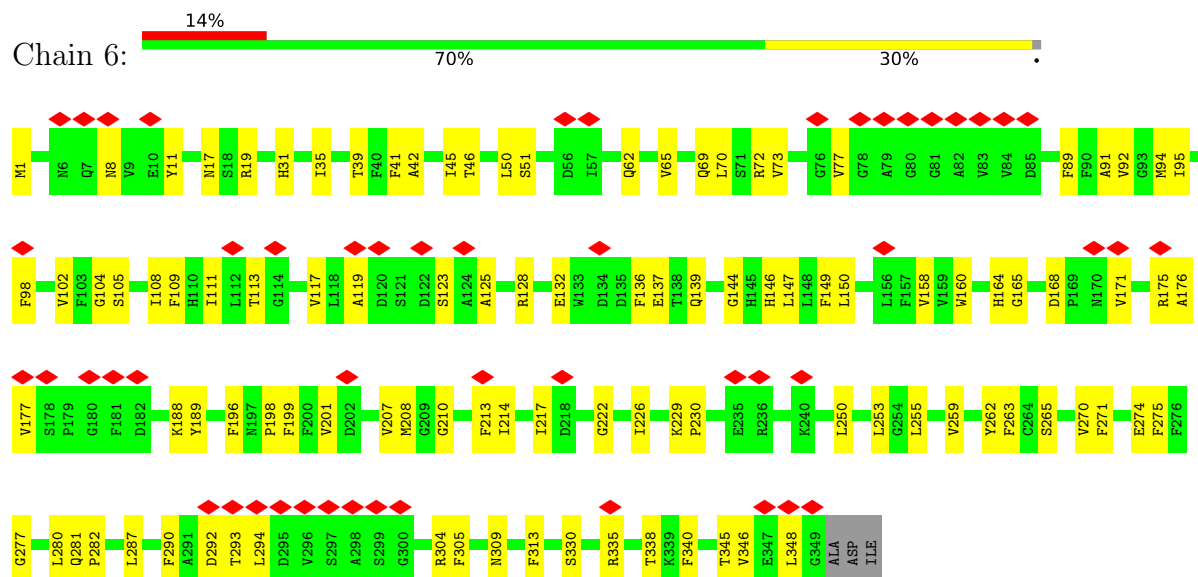
- Molecule 15: Photosystem II reaction center protein Z



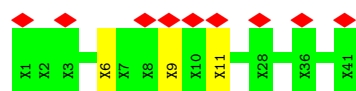
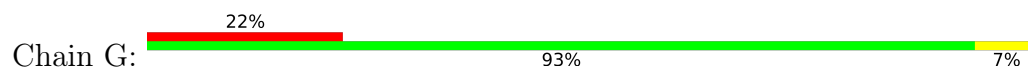
- Molecule 16: High light inducible protein



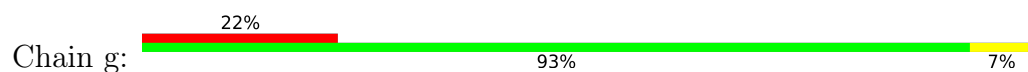
- Molecule 16: High light inducible protein



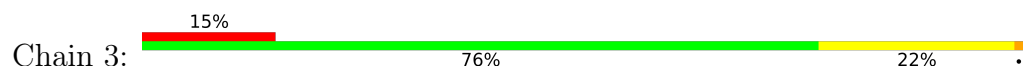
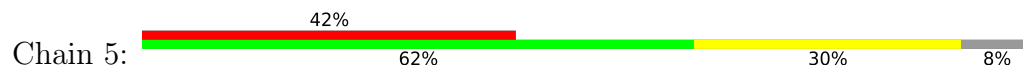
- Molecule 17: Unknown protein

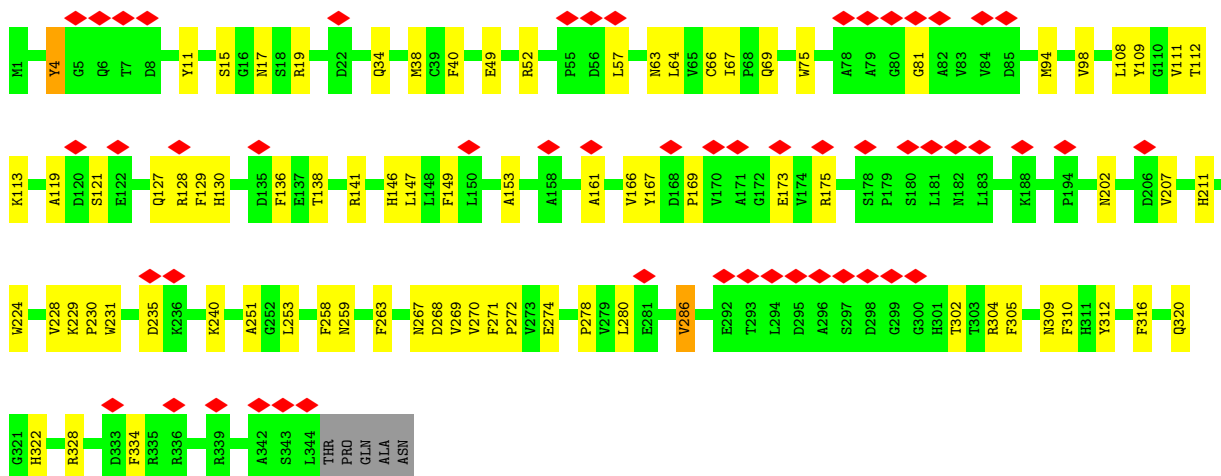


- Molecule 17: Unknown protein

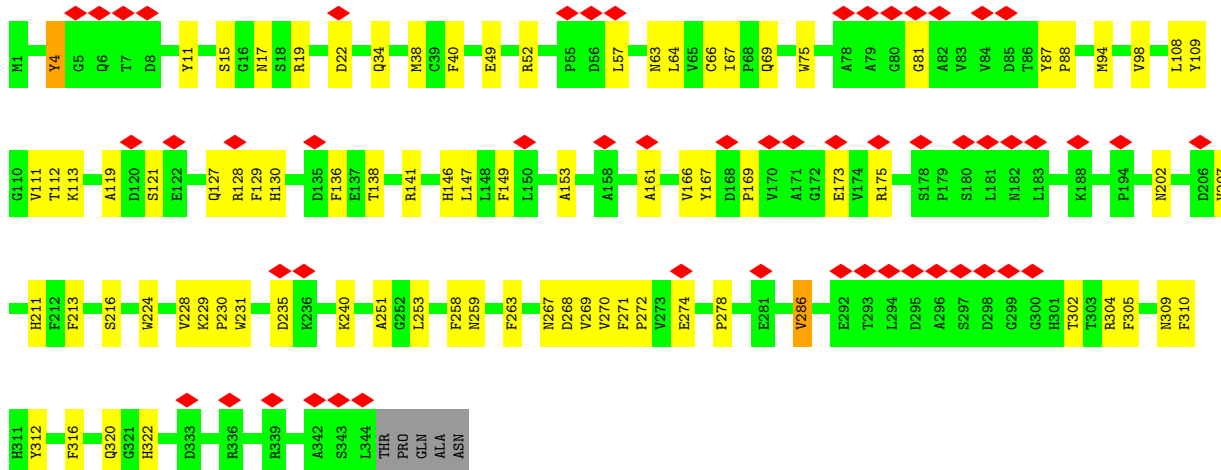
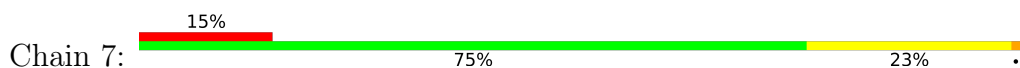


Chain 1:

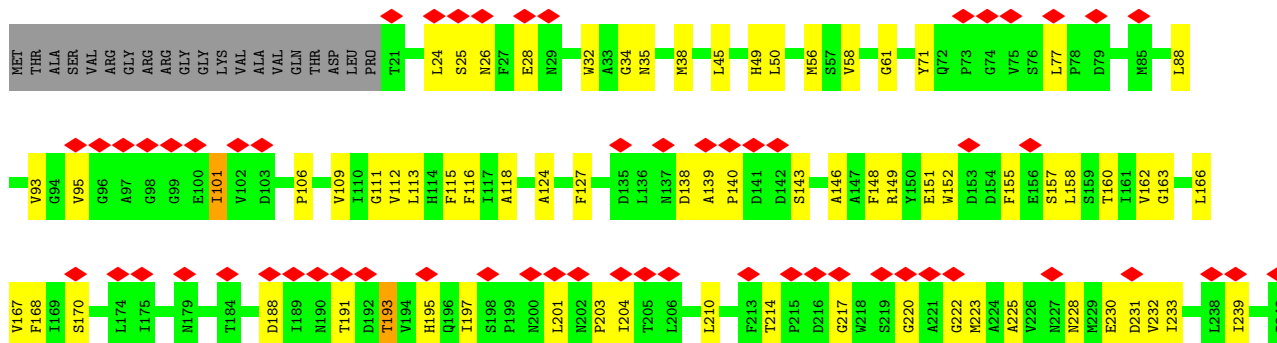




• Molecule 19: High light inducible protein

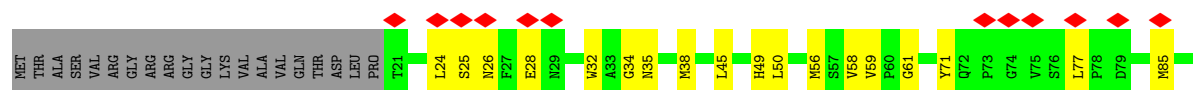


• Molecule 20: High light inducible protein





- 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 (Å)	513.60004, 513.60004, 513.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, FE2, CL7, LMG, 8CT, DGD, PL9, PHO, BCT, ZEX, SQD, HEM

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	0.39	0/2280	0.41	0/3112
1	a	0.39	0/2280	0.41	0/3112
2	B	0.37	0/3929	0.42	0/5360
2	b	0.37	0/3929	0.42	0/5360
3	C	0.34	0/3431	0.41	0/4669
3	c	0.34	0/3431	0.41	0/4669
4	D	0.38	0/2672	0.40	0/3641
4	d	0.38	0/2672	0.40	0/3641
5	E	0.25	0/555	0.38	0/757
5	e	0.25	0/555	0.38	0/757
6	F	0.33	0/250	0.39	0/343
6	f	0.33	0/250	0.39	0/343
7	H	0.32	0/534	0.49	1/729 (0.1%)
7	h	0.32	0/534	0.49	1/729 (0.1%)
8	I	0.39	0/290	0.37	0/391
8	i	0.39	0/290	0.37	0/391
9	K	0.26	0/303	0.39	0/413
9	k	0.26	0/303	0.39	0/413
10	L	0.37	0/295	0.38	0/401
10	l	0.37	0/295	0.38	0/401
11	M	0.33	0/236	0.44	0/322
11	m	0.33	0/236	0.44	0/322
12	T	0.31	0/238	0.35	0/321
12	t	0.31	0/238	0.35	0/321
13	X	0.25	0/276	0.29	0/370
13	x	0.25	0/276	0.29	0/370
14	Y	0.17	0/164	0.33	0/224
14	y	0.17	0/164	0.33	0/224
15	Z	0.19	0/438	0.29	0/599
15	z	0.20	0/438	0.29	0/599
16	2	0.35	0/2830	0.42	0/3855
16	6	0.35	0/2830	0.42	0/3855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	1	0.28	0/2652	0.41	0/3618
18	5	0.28	0/2652	0.41	0/3618
19	3	0.38	0/2814	0.46	1/3841 (0.0%)
19	7	0.38	0/2814	0.46	1/3841 (0.0%)
20	4	0.33	0/2590	0.43	0/3537
20	8	0.33	0/2590	0.43	0/3537
All	All	0.35	0/53554	0.42	4/73006 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	53	THR	N-CA-C	-7.25	101.89	111.24
7	h	53	THR	N-CA-C	-7.25	101.89	111.24
19	3	286	VAL	N-CA-C	-6.78	102.78	112.35
19	7	286	VAL	N-CA-C	-6.78	102.78	112.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2209	0	2142	60	0
1	a	2209	0	2142	65	0
2	B	3794	0	3626	65	0
2	b	3794	0	3626	66	0
3	C	3313	0	3162	58	0
3	c	3313	0	3162	58	0
4	D	2583	0	2493	65	0
4	d	2583	0	2493	66	0
5	E	538	0	520	14	0
5	e	538	0	520	13	0
6	F	242	0	249	2	0
6	f	242	0	249	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	519	0	518	10	0
7	h	519	0	518	10	0
8	I	281	0	289	6	0
8	i	281	0	289	5	0
9	K	292	0	302	9	0
9	k	292	0	302	9	0
10	L	288	0	301	7	0
10	l	288	0	301	7	0
11	M	232	0	243	4	0
11	m	232	0	243	4	0
12	T	231	0	240	2	0
12	t	231	0	240	2	0
13	X	269	0	275	4	0
13	x	269	0	275	4	0
14	Y	164	0	197	1	0
14	y	164	0	197	2	0
15	Z	429	0	450	3	0
15	z	429	0	450	4	0
16	2	2734	0	2611	105	0
16	6	2734	0	2611	106	0
17	G	205	0	46	2	0
17	g	205	0	46	2	0
18	1	2567	0	2508	100	0
18	5	2567	0	2508	104	0
19	3	2715	0	2580	80	0
19	7	2715	0	2580	83	0
20	4	2514	0	2436	76	0
20	8	2514	0	2436	76	0
21	1	972	0	822	80	0
21	2	1065	0	1050	104	0
21	3	1024	0	962	118	0
21	4	757	0	681	60	0
21	5	972	0	822	83	0
21	6	1065	0	1050	110	0
21	7	1024	0	962	118	0
21	8	757	0	681	64	0
21	A	185	0	187	24	0
21	B	991	0	947	59	0
21	C	799	0	763	39	0
21	D	153	0	121	8	0
21	a	185	0	187	26	0
21	b	991	0	947	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	c	799	0	763	38	0
21	d	153	0	121	8	0
22	A	64	0	74	2	0
22	D	64	0	74	7	0
22	a	64	0	74	2	0
22	d	64	0	74	7	0
23	4	40	0	0	0	0
23	8	40	0	0	0	0
23	A	40	0	0	0	0
23	B	160	0	0	0	0
23	C	120	0	0	2	0
23	D	40	0	0	0	0
23	K	40	0	0	0	0
23	a	40	0	0	0	0
23	b	160	0	0	0	0
23	c	120	0	0	2	0
23	d	40	0	0	0	0
23	k	40	0	0	0	0
24	1	32	0	28	1	0
24	2	91	0	113	2	0
24	3	96	0	123	6	0
24	5	32	0	28	1	0
24	6	91	0	113	1	0
24	7	96	0	123	6	0
24	A	34	0	32	2	0
24	B	88	0	110	5	0
24	b	54	0	78	3	0
25	3	36	0	42	1	0
25	4	49	0	74	2	0
25	7	36	0	42	1	0
25	8	49	0	74	2	0
25	A	46	0	65	0	0
25	B	94	0	137	8	0
25	D	49	0	74	3	0
25	a	46	0	65	0	0
25	b	94	0	137	7	0
25	d	49	0	74	4	0
26	1	51	0	72	2	0
26	5	51	0	72	2	0
26	B	51	0	72	6	0
26	C	50	0	70	0	0
26	D	33	0	36	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	b	51	0	72	6	0
26	c	50	0	70	0	0
26	d	33	0	36	1	0
27	B	62	0	82	2	0
27	C	62	0	82	4	0
27	b	62	0	82	2	0
27	c	62	0	82	4	0
28	D	1	0	0	0	0
28	d	1	0	0	0	0
29	D	4	0	0	0	0
29	d	4	0	0	0	0
30	D	55	0	80	7	0
30	d	55	0	80	6	0
31	F	43	0	30	3	0
31	f	43	0	30	3	0
32	1	84	0	112	35	0
32	2	210	0	280	91	0
32	3	168	0	224	78	0
32	4	168	0	224	47	0
32	5	84	0	112	36	0
32	6	168	0	224	69	0
32	7	126	0	168	52	0
32	8	168	0	224	51	0
All	All	68428	0	65886	2083	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 2083 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:5:315:ASN:HB3	32:5:421:ZEX:C36	1.32	1.59
18:1:315:ASN:HB3	32:1:421:ZEX:C36	1.32	1.59
18:5:315:ASN:CB	32:5:421:ZEX:C36	1.81	1.58
18:1:315:ASN:CB	32:1:421:ZEX:C36	1.81	1.58
21:3:508:CL7:H42C	32:3:519:ZEX:C17	1.38	1.53

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	65
18	5	323/356 (91%)	307 (95%)	15 (5%)	1 (0%)	36	65
19	3	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
19	7	342/349 (98%)	325 (95%)	16 (5%)	1 (0%)	36	65
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%)	49	75

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 ⓘ

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%)	232 (100%)	0	100	100
1	a	232/292 (80%)	232 (100%)	0	100	100
2	B	395/418 (94%)	392 (99%)	3 (1%)	73	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	395/418 (94%)	392 (99%)	3 (1%)	73	79
3	C	322/378 (85%)	319 (99%)	3 (1%)	70	78
3	c	322/378 (85%)	319 (99%)	3 (1%)	70	78
4	D	265/284 (93%)	264 (100%)	1 (0%)	84	84
4	d	265/284 (93%)	264 (100%)	1 (0%)	84	84
5	E	57/71 (80%)	57 (100%)	0	100	100
5	e	57/71 (80%)	57 (100%)	0	100	100
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%)	55 (100%)	0	100	100
7	h	55/57 (96%)	55 (100%)	0	100	100
8	I	30/30 (100%)	30 (100%)	0	100	100
8	i	30/30 (100%)	30 (100%)	0	100	100
9	K	31/37 (84%)	30 (97%)	1 (3%)	34	60
9	k	31/37 (84%)	30 (97%)	1 (3%)	34	60
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%)	18 (100%)	0	100	100
14	y	18/31 (58%)	18 (100%)	0	100	100
15	Z	43/46 (94%)	43 (100%)	0	100	100
15	z	43/46 (94%)	43 (100%)	0	100	100
16	2	276/278 (99%)	272 (99%)	4 (1%)	59	73
16	6	276/278 (99%)	272 (99%)	4 (1%)	59	73
18	1	262/278 (94%)	259 (99%)	3 (1%)	65	76
18	5	262/278 (94%)	259 (99%)	3 (1%)	65	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	3	269/273 (98%)	266 (99%)	3 (1%)	65	76
19	7	269/273 (98%)	266 (99%)	3 (1%)	65	76
20	4	260/277 (94%)	256 (98%)	4 (2%)	57	72
20	8	260/277 (94%)	256 (98%)	4 (2%)	57	72
All	All	5298/5940 (89%)	5254 (99%)	44 (1%)	70	79

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	d	285	LEU
18	5	143	TYR
9	k	45	LYS
16	6	274	GLU
19	7	4	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	a	335	ASN
3	c	68	HIS
2	b	9	HIS
2	b	224	HIS
4	d	337	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
24	SQD	B	626	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	8	405	-	71,73,73	1.69	16 (22%)	80,113,113	2.45	25 (31%)
21	CL7	2	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	19 (33%)
21	CL7	1	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.79	22 (39%)
21	CL7	3	501	19	71,73,73	1.69	18 (25%)	80,113,113	2.39	23 (28%)
21	CL7	2	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.72	19 (33%)
25	LHG	8	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	6	503	-	71,73,73	1.69	18 (25%)	80,113,113	2.51	25 (31%)
21	CL7	b	605	2	71,73,73	1.68	18 (25%)	80,113,113	2.33	23 (28%)
21	CL7	C	502	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	22 (27%)
21	CL7	2	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.33	23 (28%)
32	ZEX	4	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	7	512	19	61,63,73	1.84	18 (29%)	68,101,113	2.59	23 (33%)
32	ZEX	5	422	-	42,43,43	0.95	1 (2%)	55,60,60	2.24	18 (32%)
21	CL7	4	406	20	71,73,73	1.70	15 (21%)	80,113,113	2.35	21 (26%)
21	CL7	4	412	20	71,73,73	1.69	16 (22%)	80,113,113	2.38	24 (30%)
21	CL7	2	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	7	508	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	21 (26%)
24	SQD	5	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
23	8CT	C	515	-	40,41,41	4.64	21 (52%)	50,56,56	2.40	23 (46%)
21	CL7	5	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
21	CL7	2	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.77	19 (33%)
21	CL7	2	516	16	71,73,73	1.69	17 (23%)	80,113,113	2.39	23 (28%)
24	SQD	2	522	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	8	412	20	71,73,73	1.69	17 (23%)	80,113,113	2.37	25 (31%)
21	CL7	3	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	c	504	3	71,73,73	1.68	16 (22%)	80,113,113	2.40	21 (26%)
21	CL7	4	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
23	8CT	c	515	-	40,41,41	4.64	22 (55%)	50,56,56	2.40	23 (46%)
21	CL7	1	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	23 (28%)
21	CL7	1	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	C	504	3	71,73,73	1.68	16 (22%)	80,113,113	2.39	21 (26%)
21	CL7	3	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.40	23 (28%)
26	LMG	D	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	b	615	2	66,68,73	1.79	18 (27%)	74,107,113	2.50	24 (32%)
21	CL7	b	603	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
21	CL7	b	614	2	61,63,73	1.83	19 (31%)	68,101,113	2.47	18 (26%)
24	SQD	6	523	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	4	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.69	19 (33%)
24	SQD	7	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	a	405	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	2	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	23 (28%)
21	CL7	7	510	-	71,73,73	1.68	17 (23%)	80,113,113	2.38	24 (30%)
21	CL7	b	608	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
21	CL7	3	505	19	71,73,73	1.69	16 (22%)	80,113,113	2.39	21 (26%)
21	CL7	c	506	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)
32	ZEX	1	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
25	LHG	b	626	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	5	420	18	51,53,73	1.95	14 (27%)	56,89,113	2.80	21 (37%)
32	ZEX	2	521	-	42,43,43	0.98	3 (7%)	55,60,60	2.19	17 (30%)
21	CL7	3	510	-	71,73,73	1.68	17 (23%)	80,113,113	2.37	24 (30%)
21	CL7	5	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.76	20 (35%)
21	CL7	b	611	-	71,73,73	1.68	17 (23%)	80,113,113	2.46	22 (27%)
32	ZEX	8	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
32	ZEX	8	419	-	42,43,43	0.99	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	5	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.97	22 (43%)
21	CL7	4	414	20	59,61,73	1.84	17 (28%)	65,98,113	2.66	21 (32%)
23	8CT	8	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
25	LHG	A	407	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	B	610	-	71,73,73	1.69	17 (23%)	80,113,113	2.46	22 (27%)
21	CL7	2	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	6	509	-	71,73,73	1.69	18 (25%)	80,113,113	2.31	20 (25%)
21	CL7	6	513	16	51,53,73	1.96	14 (27%)	56,89,113	2.84	21 (37%)
32	ZEX	7	520	-	42,43,43	0.93	2 (4%)	55,60,60	2.65	22 (40%)
26	LMG	c	501	-	50,50,55	0.91	2 (4%)	58,58,63	1.21	5 (8%)
21	CL7	8	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.43	21 (28%)
21	CL7	6	515	-	51,53,73	1.94	16 (31%)	56,89,113	2.71	19 (33%)
26	LMG	C	501	-	50,50,55	0.92	2 (4%)	58,58,63	1.22	5 (8%)
25	LHG	d	409	-	48,48,48	0.30	0	51,54,54	0.37	0
32	ZEX	6	522	-	42,43,43	1.05	4 (9%)	55,60,60	2.47	16 (29%)
25	LHG	7	524	-	35,35,48	0.34	0	38,41,54	0.47	0
32	ZEX	3	519	-	42,43,43	1.02	4 (9%)	55,60,60	2.58	17 (30%)
21	CL7	4	415	-	51,53,73	1.96	20 (39%)	56,89,113	2.88	21 (37%)
32	ZEX	8	403	-	42,43,43	1.01	4 (9%)	55,60,60	2.56	19 (34%)
21	CL7	4	407	-	47,49,73	1.95	14 (29%)	51,84,113	2.82	20 (39%)
21	CL7	4	409	-	66,68,73	1.77	19 (28%)	74,107,113	2.67	25 (33%)
21	CL7	2	512	16	71,73,73	1.68	14 (19%)	80,113,113	2.42	21 (26%)
23	8CT	d	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
21	CL7	1	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.71	19 (33%)
21	CL7	A	403	1	61,63,73	1.86	19 (31%)	68,101,113	2.62	23 (33%)
21	CL7	3	512	19	61,63,73	1.84	18 (29%)	68,101,113	2.59	23 (33%)
21	CL7	8	416	20	47,49,73	1.97	14 (29%)	51,84,113	2.85	18 (35%)
21	CL7	3	504	-	71,73,73	1.69	17 (23%)	80,113,113	2.40	21 (26%)
21	CL7	6	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	C	518	3	47,49,73	1.92	13 (27%)	51,84,113	2.87	19 (37%)
24	SQD	3	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
32	ZEX	3	520	-	42,43,43	0.94	2 (4%)	55,60,60	2.65	22 (40%)
21	CL7	d	402	-	56,58,73	1.89	15 (26%)	62,95,113	2.59	20 (32%)
21	CL7	C	509	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
22	PHO	D	408	-	58,69,69	2.52	12 (20%)	56,99,99	2.99	16 (28%)
21	CL7	4	405	-	71,73,73	1.69	16 (22%)	80,113,113	2.46	25 (31%)
21	CL7	5	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
32	ZEX	6	524	-	42,43,43	1.03	4 (9%)	55,60,60	2.51	17 (30%)
21	CL7	2	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.36	23 (28%)
21	CL7	6	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)
32	ZEX	7	519	-	42,43,43	1.02	3 (7%)	55,60,60	2.58	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	c	511	3	71,73,73	1.69	15 (21%)	80,113,113	2.38	20 (25%)
23	8CT	c	519	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	1	416	-	47,49,73	1.95	12 (25%)	51,84,113	2.87	19 (37%)
21	CL7	4	413	20	66,68,73	1.77	18 (27%)	74,107,113	2.43	21 (28%)
23	8CT	c	516	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	c	509	3	71,73,73	1.70	16 (22%)	80,113,113	2.38	26 (32%)
21	CL7	1	407	18	47,49,73	1.94	15 (31%)	51,84,113	2.87	20 (39%)
26	LMG	B	621	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	7	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
21	CL7	b	623	2	51,53,73	1.97	15 (29%)	56,89,113	2.78	17 (30%)
32	ZEX	5	421	-	42,43,43	0.92	1 (2%)	55,60,60	2.23	20 (36%)
21	CL7	B	605	2	71,73,73	1.67	18 (25%)	80,113,113	2.40	20 (25%)
21	CL7	1	403	-	66,68,73	1.75	17 (25%)	74,107,113	2.52	22 (29%)
21	CL7	C	511	3	71,73,73	1.69	15 (21%)	80,113,113	2.38	20 (25%)
21	CL7	4	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.94	18 (35%)
22	PHO	a	402	-	58,69,69	0.84	3 (5%)	56,99,99	1.08	4 (7%)
32	ZEX	3	525	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	1	404	-	71,73,73	1.70	14 (19%)	80,113,113	2.39	21 (26%)
32	ZEX	3	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
23	8CT	C	516	-	40,41,41	4.65	20 (50%)	50,56,56	3.06	21 (42%)
21	CL7	b	606	2	71,73,73	1.67	18 (25%)	80,113,113	2.40	21 (26%)
23	8CT	B	627	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
21	CL7	2	505	16	71,73,73	1.72	18 (25%)	80,113,113	2.48	25 (31%)
27	DGD	B	624	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
21	CL7	2	503	-	71,73,73	1.68	18 (25%)	80,113,113	2.50	25 (31%)
23	8CT	B	617	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
27	DGD	C	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
21	CL7	B	612	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
21	CL7	B	616	2	51,53,73	1.97	18 (35%)	56,89,113	2.70	18 (32%)
21	CL7	1	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	4	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.34	21 (26%)
23	8CT	a	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)
21	CL7	b	616	2	56,58,73	1.89	17 (30%)	62,95,113	2.69	20 (32%)
21	CL7	B	615	2	56,58,73	1.89	17 (30%)	62,95,113	2.69	20 (32%)
21	CL7	C	506	3	71,73,73	1.70	19 (26%)	80,113,113	2.36	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	c	518	3	47,49,73	1.92	13 (27%)	51,84,113	2.88	19 (37%)
25	LHG	b	624	-	44,44,48	0.31	0	47,50,54	0.39	0
21	CL7	C	514	3	51,53,73	1.95	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	C	503	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
24	SQD	7	523	-	49,50,54	0.40	0	58,61,65	0.54	1 (1%)
23	8CT	B	618	-	40,41,41	4.69	21 (52%)	50,56,56	2.67	20 (40%)
21	CL7	b	604	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
21	CL7	1	408	-	71,73,73	1.67	15 (21%)	80,113,113	2.50	23 (28%)
32	ZEX	2	523	-	42,43,43	1.04	4 (9%)	55,60,60	2.47	16 (29%)
31	HEM	F	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)
21	CL7	D	402	-	56,58,73	1.88	15 (26%)	62,95,113	2.60	20 (32%)
21	CL7	7	501	19	71,73,73	1.69	17 (23%)	80,113,113	2.38	23 (28%)
23	8CT	b	619	-	40,41,41	4.69	20 (50%)	50,56,56	2.67	20 (40%)
21	CL7	B	613	2	61,63,73	1.83	19 (31%)	68,101,113	2.48	18 (26%)
21	CL7	2	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.42	21 (26%)
21	CL7	1	419	-	51,53,73	1.97	15 (29%)	56,89,113	2.78	18 (32%)
21	CL7	5	407	18	47,49,73	1.94	15 (31%)	51,84,113	2.86	21 (41%)
21	CL7	8	409	-	66,68,73	1.77	18 (27%)	74,107,113	2.67	25 (33%)
21	CL7	8	417	20	48,50,73	1.93	13 (27%)	51,85,113	2.94	18 (35%)
21	CL7	7	502	19	64,66,73	1.78	17 (26%)	71,104,113	2.41	22 (30%)
21	CL7	1	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.71	20 (35%)
26	LMG	d	410	-	33,33,55	0.28	0	41,41,63	0.33	0
21	CL7	2	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
32	ZEX	4	418	-	42,43,43	0.85	1 (2%)	55,60,60	2.33	16 (29%)
21	CL7	6	511	16	66,68,73	1.78	17 (25%)	74,107,113	2.40	21 (28%)
21	CL7	B	604	2	71,73,73	1.68	18 (25%)	80,113,113	2.33	23 (28%)
21	CL7	c	508	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	6	516	16	71,73,73	1.69	17 (23%)	80,113,113	2.39	23 (28%)
21	CL7	d	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.49	22 (30%)
23	8CT	b	618	-	40,41,41	4.65	24 (60%)	50,56,56	2.75	19 (38%)
21	CL7	1	412	18	51,53,73	1.96	16 (31%)	56,89,113	2.76	20 (35%)
21	CL7	C	512	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
21	CL7	C	508	-	71,73,73	1.68	18 (25%)	80,113,113	2.47	23 (28%)
21	CL7	1	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.33	23 (28%)
21	CL7	7	504	-	71,73,73	1.69	16 (22%)	80,113,113	2.40	21 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	7	517	19	56,58,73	1.89	16 (28%)	62,95,113	2.65	20 (32%)
26	LMG	b	622	-	51,51,55	0.25	0	59,59,63	0.33	0
21	CL7	8	404	20	71,73,73	1.71	19 (26%)	80,113,113	2.33	21 (26%)
26	LMG	1	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
25	LHG	D	409	-	48,48,48	0.30	0	51,54,54	0.37	0
21	CL7	c	512	3	48,50,73	1.95	14 (29%)	51,85,113	2.84	18 (35%)
21	CL7	2	513	16	51,53,73	1.96	14 (27%)	56,89,113	2.84	21 (37%)
21	CL7	6	506	16	71,73,73	1.71	19 (26%)	80,113,113	2.38	22 (27%)
21	CL7	7	514	-	51,53,73	1.98	16 (31%)	56,89,113	2.83	19 (33%)
21	CL7	c	513	3	47,49,73	1.92	14 (29%)	51,84,113	2.98	20 (39%)
27	DGD	c	517	-	63,63,67	0.84	2 (3%)	77,77,81	1.03	5 (6%)
32	ZEX	2	520	-	42,43,43	1.17	5 (11%)	55,60,60	2.43	18 (32%)
21	CL7	8	406	20	71,73,73	1.70	16 (22%)	80,113,113	2.35	21 (26%)
24	SQD	3	521	-	45,46,54	0.42	1 (2%)	54,57,65	0.48	0
21	CL7	2	511	16	66,68,73	1.78	17 (25%)	74,107,113	2.40	21 (28%)
21	CL7	7	507	-	71,73,73	1.68	15 (21%)	80,113,113	2.39	23 (28%)
21	CL7	3	517	19	56,58,73	1.88	16 (28%)	62,95,113	2.65	20 (32%)
23	8CT	k	101	-	40,41,41	4.75	24 (60%)	50,56,56	2.65	16 (32%)
21	CL7	1	411	-	51,53,73	1.97	16 (31%)	56,89,113	2.72	18 (32%)
21	CL7	b	612	2	71,73,73	1.69	18 (25%)	80,113,113	2.35	20 (25%)
21	CL7	6	505	16	71,73,73	1.72	19 (26%)	80,113,113	2.47	25 (31%)
21	CL7	C	510	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	8	414	20	59,61,73	1.84	19 (32%)	65,98,113	2.66	21 (32%)
21	CL7	c	502	3	71,73,73	1.68	16 (22%)	80,113,113	2.36	21 (26%)
21	CL7	B	609	2	71,73,73	1.69	17 (23%)	80,113,113	2.32	20 (25%)
21	CL7	3	511	19	71,73,73	1.69	17 (23%)	80,113,113	2.55	24 (30%)
21	CL7	a	401	1	71,73,73	1.73	14 (19%)	80,113,113	2.47	25 (31%)
21	CL7	2	507	-	71,73,73	1.71	17 (23%)	80,113,113	2.43	21 (26%)
21	CL7	1	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.97	20 (39%)
32	ZEX	4	419	-	42,43,43	0.99	3 (7%)	55,60,60	2.43	25 (45%)
21	CL7	4	411	20	71,73,73	1.68	14 (19%)	80,113,113	2.40	23 (28%)
32	ZEX	6	519	-	42,43,43	1.05	3 (7%)	55,60,60	2.50	16 (29%)
23	8CT	b	601	-	40,41,41	4.70	24 (60%)	50,56,56	3.25	21 (42%)
25	LHG	B	625	-	48,48,48	0.30	0	51,54,54	0.34	0
21	CL7	5	418	18	71,73,73	1.67	16 (22%)	80,113,113	2.46	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	8	407	-	47,49,73	1.94	13 (27%)	51,84,113	2.81	20 (39%)
21	CL7	3	509	19	71,73,73	1.69	15 (21%)	80,113,113	2.33	22 (27%)
21	CL7	D	404	4	64,66,73	1.78	20 (31%)	71,104,113	2.48	22 (30%)
24	SQD	b	621	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
21	CL7	6	501	16	71,73,73	1.68	16 (22%)	80,113,113	2.42	21 (26%)
24	SQD	1	423	-	31,32,54	0.48	1 (3%)	40,43,65	0.60	1 (2%)
32	ZEX	8	418	-	42,43,43	0.86	1 (2%)	55,60,60	2.33	16 (29%)
32	ZEX	2	525	-	42,43,43	1.02	3 (7%)	55,60,60	2.51	17 (30%)
21	CL7	5	403	-	66,68,73	1.75	17 (25%)	74,107,113	2.51	22 (29%)
30	PL9	D	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.61	1 (1%)
32	ZEX	1	422	-	42,43,43	0.95	1 (2%)	55,60,60	2.24	18 (32%)
21	CL7	3	515	-	47,49,73	1.94	11 (23%)	51,84,113	2.93	21 (41%)
21	CL7	8	415	-	51,53,73	1.97	20 (39%)	56,89,113	2.88	22 (39%)
27	DGD	b	625	-	63,63,67	0.82	2 (3%)	77,77,81	1.00	4 (5%)
25	LHG	3	524	-	35,35,48	0.34	0	38,41,54	0.47	0
23	8CT	b	620	-	40,41,41	4.59	22 (55%)	50,56,56	2.92	18 (36%)
21	CL7	B	601	-	47,49,73	1.94	13 (27%)	51,84,113	2.86	18 (35%)
21	CL7	5	402	18	66,68,73	1.78	15 (22%)	74,107,113	2.50	19 (25%)
21	CL7	6	508	16	51,53,73	1.97	18 (35%)	56,89,113	2.64	19 (33%)
21	CL7	6	514	-	51,53,73	1.98	17 (33%)	56,89,113	2.72	19 (33%)
21	CL7	a	403	1	61,63,73	1.87	19 (31%)	68,101,113	2.61	23 (33%)
21	CL7	b	609	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	19 (23%)
32	ZEX	2	519	-	42,43,43	1.06	3 (7%)	55,60,60	2.50	16 (29%)
23	8CT	K	101	-	40,41,41	4.76	24 (60%)	50,56,56	2.65	16 (32%)
21	CL7	c	507	3	66,68,73	1.76	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	C	505	-	61,63,73	1.85	17 (27%)	68,101,113	2.54	19 (27%)
21	CL7	A	401	1	71,73,73	1.74	14 (19%)	80,113,113	2.47	25 (31%)
22	PHO	d	408	-	58,69,69	2.53	12 (20%)	56,99,99	2.99	16 (28%)
21	CL7	5	406	18	68,70,73	1.73	18 (26%)	76,109,113	2.42	20 (26%)
21	CL7	C	513	3	47,49,73	1.92	13 (27%)	51,84,113	2.98	20 (39%)
21	CL7	1	402	18	66,68,73	1.78	15 (22%)	74,107,113	2.50	19 (25%)
21	CL7	c	503	3	66,68,73	1.77	17 (25%)	74,107,113	2.45	19 (25%)
21	CL7	B	603	2	71,73,73	1.69	18 (25%)	80,113,113	2.36	21 (26%)
21	CL7	3	518	19	51,53,73	1.98	13 (25%)	56,89,113	2.74	20 (35%)
23	8CT	A	404	-	40,41,41	4.63	21 (52%)	50,56,56	2.97	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CL7	6	512	16	71,73,73	1.68	14 (19%)	80,113,113	2.43	21 (26%)
29	BCT	D	403	28	2,3,3	1.00	0	2,3,3	1.67	1 (50%)
21	CL7	d	405	4	51,53,73	1.95	17 (33%)	56,89,113	2.77	22 (39%)
21	CL7	5	416	-	47,49,73	1.95	12 (25%)	51,84,113	2.88	19 (37%)
21	CL7	c	505	-	61,63,73	1.85	18 (29%)	68,101,113	2.54	19 (27%)
24	SQD	6	521	-	49,50,54	0.41	1 (2%)	58,61,65	0.54	1 (1%)
21	CL7	7	515	-	47,49,73	1.94	12 (25%)	51,84,113	2.93	21 (41%)
21	CL7	6	510	16	71,73,73	1.68	17 (23%)	80,113,113	2.38	22 (27%)
21	CL7	3	502	19	64,66,73	1.77	16 (25%)	71,104,113	2.41	22 (30%)
21	CL7	b	610	2	71,73,73	1.69	17 (23%)	80,113,113	2.32	20 (25%)
21	CL7	1	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.57	20 (29%)
25	LHG	B	623	-	44,44,48	0.32	0	47,50,54	0.39	0
32	ZEX	4	420	-	42,43,43	1.02	3 (7%)	55,60,60	2.20	19 (34%)
21	CL7	A	406	-	71,73,73	1.68	17 (23%)	80,113,113	2.44	21 (26%)
21	CL7	3	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
23	8CT	4	402	-	40,41,41	4.61	20 (50%)	50,56,56	2.78	21 (42%)
21	CL7	8	411	20	71,73,73	1.68	15 (21%)	80,113,113	2.40	23 (28%)
21	CL7	8	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	21 (37%)
21	CL7	5	419	-	51,53,73	1.98	15 (29%)	56,89,113	2.77	18 (32%)
21	CL7	B	611	2	71,73,73	1.69	18 (25%)	80,113,113	2.35	21 (26%)
21	CL7	1	413	-	47,49,73	1.94	12 (25%)	51,84,113	2.98	22 (43%)
21	CL7	7	509	19	71,73,73	1.68	15 (21%)	80,113,113	2.33	22 (27%)
21	CL7	7	513	-	51,53,73	1.98	18 (35%)	56,89,113	2.72	18 (32%)
21	CL7	7	506	19	51,53,73	1.97	17 (33%)	56,89,113	2.76	19 (33%)
21	CL7	7	511	19	71,73,73	1.69	17 (23%)	80,113,113	2.55	24 (30%)
23	8CT	B	619	-	40,41,41	4.59	22 (55%)	50,56,56	2.91	18 (36%)
21	CL7	5	417	18	61,63,73	1.81	16 (26%)	68,101,113	2.56	20 (29%)
23	8CT	D	406	-	40,41,41	4.62	23 (57%)	50,56,56	2.99	19 (38%)
29	BCT	d	403	28	2,3,3	1.00	0	2,3,3	1.67	1 (50%)
21	CL7	2	517	16	71,73,73	1.69	15 (21%)	80,113,113	2.36	21 (26%)
21	CL7	B	608	2	71,73,73	1.69	18 (25%)	80,113,113	2.30	19 (23%)
21	CL7	7	516	19	61,63,73	1.81	17 (27%)	68,101,113	2.56	25 (36%)
24	SQD	A	405	-	33,34,54	0.46	1 (3%)	42,45,65	0.52	0
21	CL7	3	508	19	71,73,73	1.70	18 (25%)	80,113,113	2.31	21 (26%)
31	HEM	f	101	-	50,50,50	1.62	9 (18%)	66,82,82	1.82	15 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	ZEX	6	520	-	42,43,43	0.98	3 (7%)	55,60,60	2.19	17 (30%)
32	ZEX	7	522	-	42,43,43	1.00	4 (9%)	55,60,60	2.40	17 (30%)
21	CL7	c	514	3	51,53,73	1.95	14 (27%)	56,89,113	2.90	19 (33%)
21	CL7	b	602	-	47,49,73	1.94	13 (27%)	51,84,113	2.87	18 (35%)
25	LHG	a	406	-	45,45,48	0.31	0	48,51,54	0.43	0
21	CL7	3	506	19	51,53,73	1.97	17 (33%)	56,89,113	2.75	19 (33%)
21	CL7	B	607	-	66,68,73	1.76	17 (25%)	74,107,113	2.48	20 (27%)
23	8CT	C	519	-	40,41,41	4.66	21 (52%)	50,56,56	2.71	21 (42%)
21	CL7	7	518	19	51,53,73	1.98	13 (25%)	56,89,113	2.74	20 (35%)
21	CL7	3	503	-	71,73,73	1.68	15 (21%)	80,113,113	2.47	24 (30%)
30	PL9	d	407	-	55,55,55	0.83	1 (1%)	68,69,69	0.62	1 (1%)
21	CL7	5	408	-	71,73,73	1.66	15 (21%)	80,113,113	2.51	23 (28%)
24	SQD	B	620	-	53,54,54	0.39	1 (1%)	62,65,65	0.54	1 (1%)
26	LMG	5	401	-	51,51,55	0.22	0	59,59,63	0.41	1 (1%)
22	PHO	A	402	-	58,69,69	0.84	3 (5%)	56,99,99	1.07	4 (7%)
25	LHG	4	401	-	48,48,48	0.28	0	51,54,54	0.34	0
21	CL7	6	504	-	51,53,73	1.98	17 (33%)	56,89,113	2.77	19 (33%)
21	CL7	6	502	16	71,73,73	1.68	17 (23%)	80,113,113	2.36	22 (27%)
21	CL7	B	606	2	61,63,73	1.81	16 (26%)	68,101,113	2.64	21 (30%)
21	CL7	3	513	-	51,53,73	1.98	18 (35%)	56,89,113	2.73	18 (32%)
21	CL7	8	410	20	51,53,73	1.98	17 (33%)	56,89,113	2.70	19 (33%)
21	CL7	B	614	2	66,68,73	1.79	18 (27%)	74,107,113	2.50	24 (32%)
21	CL7	c	510	3	71,73,73	1.72	19 (26%)	80,113,113	2.35	21 (26%)
21	CL7	4	408	20	51,53,73	1.97	17 (33%)	56,89,113	2.70	20 (35%)
21	CL7	5	414	18	47,49,73	1.95	12 (25%)	51,84,113	2.97	20 (39%)
21	CL7	5	410	-	71,73,73	1.70	17 (23%)	80,113,113	2.33	23 (28%)
21	CL7	5	415	-	47,49,73	1.94	11 (23%)	51,84,113	2.97	19 (37%)
21	CL7	B	602	2	66,68,73	1.78	17 (25%)	74,107,113	2.51	22 (29%)
21	CL7	b	613	2	71,73,73	1.68	18 (25%)	80,113,113	2.38	23 (28%)
21	CL7	5	409	18	51,53,73	1.95	16 (31%)	56,89,113	2.72	20 (35%)
21	CL7	5	405	-	51,53,73	1.97	18 (35%)	56,89,113	2.71	19 (33%)
21	CL7	D	405	4	51,53,73	1.95	17 (33%)	56,89,113	2.77	22 (39%)
21	CL7	C	507	3	66,68,73	1.77	17 (25%)	74,107,113	2.51	23 (31%)
21	CL7	7	505	19	71,73,73	1.70	17 (23%)	80,113,113	2.39	21 (26%)
21	CL7	b	607	2	61,63,73	1.81	16 (26%)	68,101,113	2.64	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	SQD	2	524	-	40,41,54	0.45	1 (2%)	49,52,65	0.52	1 (2%)
21	CL7	B	622	2	51,53,73	1.97	15 (29%)	56,89,113	2.79	17 (30%)
21	CL7	b	617	2	51,53,73	1.97	18 (35%)	56,89,113	2.70	18 (32%)
21	CL7	6	518	16	71,73,73	1.68	13 (18%)	80,113,113	2.33	22 (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
24	SQD	B	626	-	-	3/29/49/69	0/1/1/1
21	CL7	8	405	-	2/2/15/20	18/39/115/115	-
21	CL7	2	515	-	2/2/11/20	8/15/91/115	-
21	CL7	1	420	18	2/2/11/20	6/15/91/115	-
21	CL7	3	501	19	2/2/15/20	21/39/115/115	-
21	CL7	2	514	-	2/2/11/20	9/15/91/115	-
25	LHG	8	401	-	-	8/53/53/53	-
21	CL7	6	503	-	2/2/15/20	17/39/115/115	-
21	CL7	b	605	2	2/2/15/20	17/39/115/115	-
21	CL7	C	502	3	2/2/15/20	20/39/115/115	-
21	CL7	2	518	16	2/2/15/20	12/39/115/115	-
32	ZEX	4	403	-	-	10/29/67/67	0/2/2/2
21	CL7	7	512	19	2/2/13/20	12/27/103/115	-
32	ZEX	5	422	-	-	6/29/67/67	0/2/2/2
21	CL7	4	406	20	2/2/15/20	24/39/115/115	-
21	CL7	4	412	20	2/2/15/20	17/39/115/115	-
21	CL7	2	509	-	2/2/15/20	16/39/115/115	-
21	CL7	7	508	19	2/2/15/20	16/39/115/115	-
24	SQD	5	423	-	-	3/27/47/69	0/1/1/1
23	8CT	C	515	-	-	14/29/63/63	0/2/2/2
21	CL7	5	404	-	2/2/15/20	15/39/115/115	-
21	CL7	2	504	-	2/2/11/20	6/15/91/115	-
21	CL7	2	516	16	2/2/15/20	16/39/115/115	-
24	SQD	2	522	-	-	7/45/65/69	0/1/1/1
21	CL7	8	412	20	2/2/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	3	514	-	2/2/11/20	5/15/91/115	-
21	CL7	c	504	3	2/2/15/20	19/39/115/115	-
21	CL7	4	416	20	2/2/10/20	7/10/86/115	-
23	8CT	c	515	-	-	14/29/63/63	0/2/2/2
21	CL7	1	418	18	2/2/15/20	22/39/115/115	-
21	CL7	1	406	18	2/2/14/20	13/36/112/115	-
21	CL7	C	504	3	2/2/15/20	19/39/115/115	-
21	CL7	3	507	-	2/2/15/20	15/39/115/115	-
26	LMG	D	410	-	-	6/28/48/70	0/1/1/1
21	CL7	b	615	2	2/2/14/20	14/33/109/115	-
21	CL7	b	603	2	2/2/14/20	9/33/109/115	-
21	CL7	b	614	2	2/2/13/20	5/27/103/115	-
24	SQD	6	523	-	-	0/36/56/69	0/1/1/1
21	CL7	4	410	20	2/2/11/20	9/15/91/115	-
24	SQD	7	521	-	-	3/41/61/69	0/1/1/1
21	CL7	a	405	-	2/2/15/20	16/39/115/115	-
21	CL7	2	506	16	2/2/15/20	14/39/115/115	-
21	CL7	7	510	-	2/2/15/20	15/39/115/115	-
21	CL7	b	608	-	2/2/14/20	11/33/109/115	-
21	CL7	3	505	19	2/2/15/20	14/39/115/115	-
21	CL7	c	506	3	2/2/15/20	16/39/115/115	-
32	ZEX	1	421	-	-	14/29/67/67	0/2/2/2
25	LHG	b	626	-	-	6/53/53/53	-
21	CL7	5	420	18	2/2/11/20	6/15/91/115	-
32	ZEX	2	521	-	-	6/29/67/67	0/2/2/2
21	CL7	3	510	-	2/2/15/20	15/39/115/115	-
21	CL7	5	412	18	2/2/11/20	10/15/91/115	-
21	CL7	b	611	-	2/2/15/20	11/39/115/115	-
32	ZEX	8	420	-	-	12/29/67/67	0/2/2/2
32	ZEX	8	419	-	-	9/29/67/67	0/2/2/2
21	CL7	5	413	-	2/2/10/20	2/10/86/115	-
21	CL7	4	414	20	2/2/12/20	8/25/101/115	-
23	8CT	8	402	-	-	4/29/63/63	0/2/2/2
25	LHG	A	407	-	-	5/50/50/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	B	610	-	2/2/15/20	11/39/115/115	-
21	CL7	2	510	16	2/2/15/20	20/39/115/115	-
21	CL7	6	509	-	2/2/15/20	16/39/115/115	-
21	CL7	6	513	16	2/2/11/20	8/15/91/115	-
32	ZEX	7	520	-	-	10/29/67/67	0/2/2/2
26	LMG	c	501	-	-	16/45/65/70	0/1/1/1
21	CL7	8	413	20	2/2/14/20	7/33/109/115	-
21	CL7	6	515	-	2/2/11/20	8/15/91/115	-
26	LMG	C	501	-	-	16/45/65/70	0/1/1/1
25	LHG	d	409	-	-	7/53/53/53	-
32	ZEX	6	522	-	-	6/29/67/67	0/2/2/2
25	LHG	7	524	-	-	3/40/40/53	-
32	ZEX	3	519	-	-	10/29/67/67	0/2/2/2
21	CL7	4	415	-	2/2/11/20	11/15/91/115	-
32	ZEX	8	403	-	-	10/29/67/67	0/2/2/2
21	CL7	4	407	-	2/2/10/20	3/10/86/115	-
21	CL7	4	409	-	2/2/14/20	17/33/109/115	-
21	CL7	2	512	16	2/2/15/20	18/39/115/115	-
23	8CT	d	406	-	-	10/29/63/63	0/2/2/2
21	CL7	1	405	-	2/2/11/20	10/15/91/115	-
21	CL7	A	403	1	2/2/13/20	9/27/103/115	-
21	CL7	3	512	19	2/2/13/20	12/27/103/115	-
21	CL7	8	416	20	2/2/10/20	7/10/86/115	-
21	CL7	3	504	-	2/2/15/20	16/39/115/115	-
21	CL7	6	507	-	2/2/15/20	20/39/115/115	-
21	CL7	C	518	3	2/2/10/20	5/10/86/115	-
24	SQD	3	523	-	-	7/45/65/69	0/1/1/1
32	ZEX	3	520	-	-	10/29/67/67	0/2/2/2
21	CL7	d	402	-	2/2/12/20	9/21/97/115	-
21	CL7	C	509	3	2/2/15/20	17/39/115/115	-
22	PHO	D	408	-	-	4/37/103/103	0/5/6/6
21	CL7	4	405	-	2/2/15/20	18/39/115/115	-
21	CL7	5	411	-	2/2/11/20	7/15/91/115	-
32	ZEX	6	524	-	-	11/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2	502	16	2/2/15/20	17/39/115/115	-
21	CL7	6	517	16	2/2/15/20	21/39/115/115	-
32	ZEX	7	519	-	-	10/29/67/67	0/2/2/2
21	CL7	c	511	3	2/2/15/20	22/39/115/115	-
23	8CT	c	519	-	-	8/29/63/63	0/2/2/2
21	CL7	1	416	-	2/2/10/20	4/10/86/115	-
21	CL7	4	413	20	2/2/14/20	7/33/109/115	-
23	8CT	c	516	-	-	10/29/63/63	0/2/2/2
21	CL7	c	509	3	2/2/15/20	17/39/115/115	-
21	CL7	1	407	18	2/2/10/20	4/10/86/115	-
26	LMG	B	621	-	-	7/46/66/70	0/1/1/1
21	CL7	7	503	-	2/2/15/20	20/39/115/115	-
21	CL7	b	623	2	2/2/11/20	8/15/91/115	-
32	ZEX	5	421	-	-	14/29/67/67	0/2/2/2
21	CL7	B	605	2	2/2/15/20	18/39/115/115	-
21	CL7	1	403	-	2/2/14/20	11/33/109/115	-
21	CL7	C	511	3	2/2/15/20	22/39/115/115	-
21	CL7	4	417	20	2/2/10/20	6/12/88/115	-
22	PHO	a	402	-	-	3/37/103/103	0/5/6/6
32	ZEX	3	525	-	-	7/29/67/67	0/2/2/2
21	CL7	1	404	-	2/2/15/20	15/39/115/115	-
32	ZEX	3	522	-	-	5/29/67/67	0/2/2/2
23	8CT	C	516	-	-	10/29/63/63	0/2/2/2
21	CL7	b	606	2	2/2/15/20	18/39/115/115	-
23	8CT	B	627	-	-	10/29/63/63	0/2/2/2
21	CL7	2	505	16	2/2/15/20	18/39/115/115	-
27	DGD	B	624	-	-	7/51/91/95	0/2/2/2
21	CL7	2	503	-	2/2/15/20	17/39/115/115	-
23	8CT	B	617	-	-	7/29/63/63	0/2/2/2
27	DGD	C	517	-	-	9/51/91/95	0/2/2/2
21	CL7	B	612	2	2/2/15/20	17/39/115/115	-
21	CL7	B	616	2	2/2/11/20	4/15/91/115	-
21	CL7	1	415	-	2/2/10/20	7/10/86/115	-
21	CL7	4	404	20	2/2/15/20	14/39/115/115	-

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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	b	616	2	2/2/12/20	8/21/97/115	-
21	CL7	B	615	2	2/2/12/20	8/21/97/115	-
21	CL7	C	506	3	2/2/15/20	16/39/115/115	-
21	CL7	c	518	3	2/2/10/20	5/10/86/115	-
25	LHG	b	624	-	-	3/49/49/53	-
21	CL7	C	514	3	2/2/11/20	8/15/91/115	-
21	CL7	C	503	3	2/2/14/20	12/33/109/115	-
24	SQD	7	523	-	-	7/45/65/69	0/1/1/1
23	8CT	B	618	-	-	10/29/63/63	0/2/2/2
21	CL7	b	604	2	2/2/15/20	12/39/115/115	-
21	CL7	1	408	-	2/2/15/20	16/39/115/115	-
32	ZEX	2	523	-	-	6/29/67/67	0/2/2/2
31	HEM	F	101	-	-	8/14/54/54	-
21	CL7	D	402	-	2/2/12/20	9/21/97/115	-
21	CL7	7	501	19	2/2/15/20	21/39/115/115	-
23	8CT	b	619	-	-	10/29/63/63	0/2/2/2
21	CL7	B	613	2	2/2/13/20	5/27/103/115	-
21	CL7	2	501	16	2/2/15/20	17/39/115/115	-
21	CL7	1	419	-	2/2/11/20	9/15/91/115	-
21	CL7	5	407	18	2/2/10/20	4/10/86/115	-
21	CL7	8	409	-	2/2/14/20	17/33/109/115	-
21	CL7	8	417	20	2/2/10/20	6/12/88/115	-
21	CL7	7	502	19	2/2/13/20	12/31/107/115	-
21	CL7	1	409	18	2/2/11/20	6/15/91/115	-
26	LMG	d	410	-	-	6/28/48/70	0/1/1/1
21	CL7	2	508	16	2/2/11/20	5/15/91/115	-
32	ZEX	4	418	-	-	9/29/67/67	0/2/2/2
21	CL7	6	511	16	2/2/14/20	16/33/109/115	-
21	CL7	B	604	2	2/2/15/20	17/39/115/115	-
21	CL7	c	508	-	2/2/15/20	17/39/115/115	-
21	CL7	6	516	16	2/2/15/20	16/39/115/115	-
21	CL7	d	404	4	2/2/13/20	13/31/107/115	-
23	8CT	b	618	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	1	412	18	2/2/11/20	10/15/91/115	-
21	CL7	C	512	3	2/2/10/20	5/12/88/115	-
21	CL7	C	508	-	2/2/15/20	17/39/115/115	-
21	CL7	1	410	-	2/2/15/20	17/39/115/115	-
21	CL7	7	504	-	2/2/15/20	16/39/115/115	-
21	CL7	7	517	19	2/2/12/20	9/21/97/115	-
26	LMG	b	622	-	-	7/46/66/70	0/1/1/1
21	CL7	8	404	20	2/2/15/20	14/39/115/115	-
26	LMG	1	401	-	-	5/46/66/70	0/1/1/1
25	LHG	D	409	-	-	7/53/53/53	-
21	CL7	c	512	3	2/2/10/20	5/12/88/115	-
21	CL7	2	513	16	2/2/11/20	8/15/91/115	-
21	CL7	6	506	16	2/2/15/20	14/39/115/115	-
21	CL7	7	514	-	2/2/11/20	5/15/91/115	-
21	CL7	c	513	3	2/2/10/20	4/10/86/115	-
27	DGD	c	517	-	-	9/51/91/95	0/2/2/2
32	ZEX	2	520	-	-	7/29/67/67	0/2/2/2
21	CL7	8	406	20	2/2/15/20	24/39/115/115	-
24	SQD	3	521	-	-	3/41/61/69	0/1/1/1
21	CL7	2	511	16	2/2/14/20	16/33/109/115	-
21	CL7	7	507	-	2/2/15/20	15/39/115/115	-
21	CL7	3	517	19	2/2/12/20	9/21/97/115	-
23	8CT	k	101	-	-	10/29/63/63	0/2/2/2
21	CL7	1	411	-	2/2/11/20	7/15/91/115	-
21	CL7	b	612	2	2/2/15/20	17/39/115/115	-
21	CL7	6	505	16	2/2/15/20	18/39/115/115	-
21	CL7	C	510	3	2/2/15/20	20/39/115/115	-
21	CL7	8	414	20	2/2/12/20	8/25/101/115	-
21	CL7	c	502	3	2/2/15/20	20/39/115/115	-
21	CL7	B	609	2	2/2/15/20	14/39/115/115	-
21	CL7	3	511	19	2/2/15/20	19/39/115/115	-
21	CL7	a	401	1	2/2/15/20	18/39/115/115	-
21	CL7	2	507	-	2/2/15/20	20/39/115/115	-
21	CL7	1	414	18	2/2/10/20	3/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	ZEX	4	419	-	-	9/29/67/67	0/2/2/2
21	CL7	4	411	20	2/2/15/20	14/39/115/115	-
32	ZEX	6	519	-	-	11/29/67/67	0/2/2/2
23	8CT	b	601	-	-	10/29/63/63	0/2/2/2
25	LHG	B	625	-	-	6/53/53/53	-
21	CL7	5	418	18	2/2/15/20	22/39/115/115	-
21	CL7	8	407	-	2/2/10/20	3/10/86/115	-
21	CL7	3	509	19	2/2/15/20	17/39/115/115	-
21	CL7	D	404	4	2/2/13/20	13/31/107/115	-
24	SQD	b	621	-	-	5/49/69/69	0/1/1/1
21	CL7	6	501	16	2/2/15/20	17/39/115/115	-
24	SQD	1	423	-	-	3/27/47/69	0/1/1/1
32	ZEX	8	418	-	-	9/29/67/67	0/2/2/2
32	ZEX	2	525	-	-	11/29/67/67	0/2/2/2
21	CL7	5	403	-	2/2/14/20	11/33/109/115	-
30	PL9	D	407	-	-	9/53/73/73	0/1/1/1
32	ZEX	1	422	-	-	6/29/67/67	0/2/2/2
21	CL7	3	515	-	2/2/10/20	0/10/86/115	-
21	CL7	8	415	-	2/2/11/20	11/15/91/115	-
27	DGD	b	625	-	-	7/51/91/95	0/2/2/2
25	LHG	3	524	-	-	3/40/40/53	-
23	8CT	b	620	-	-	4/29/63/63	0/2/2/2
21	CL7	B	601	-	2/2/10/20	4/10/86/115	-
21	CL7	5	402	18	2/2/14/20	16/33/109/115	-
21	CL7	6	508	16	2/2/11/20	5/15/91/115	-
21	CL7	6	514	-	2/2/11/20	9/15/91/115	-
21	CL7	a	403	1	2/2/13/20	9/27/103/115	-
21	CL7	b	609	2	2/2/15/20	15/39/115/115	-
32	ZEX	2	519	-	-	11/29/67/67	0/2/2/2
23	8CT	K	101	-	-	10/29/63/63	0/2/2/2
21	CL7	c	507	3	2/2/14/20	15/33/109/115	-
21	CL7	C	505	-	2/2/13/20	13/27/103/115	-
21	CL7	A	401	1	2/2/15/20	18/39/115/115	-
22	PHO	d	408	-	-	4/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	5	406	18	2/2/14/20	13/36/112/115	-
21	CL7	C	513	3	2/2/10/20	4/10/86/115	-
21	CL7	1	402	18	2/2/14/20	16/33/109/115	-
21	CL7	c	503	3	2/2/14/20	12/33/109/115	-
21	CL7	B	603	2	2/2/15/20	12/39/115/115	-
21	CL7	3	518	19	2/2/11/20	7/15/91/115	-
23	8CT	A	404	-	-	5/29/63/63	0/2/2/2
21	CL7	6	512	16	2/2/15/20	18/39/115/115	-
21	CL7	d	405	4	2/2/11/20	8/15/91/115	-
21	CL7	5	416	-	2/2/10/20	4/10/86/115	-
21	CL7	c	505	-	2/2/13/20	13/27/103/115	-
24	SQD	6	521	-	-	7/45/65/69	0/1/1/1
21	CL7	7	515	-	2/2/10/20	0/10/86/115	-
21	CL7	6	510	16	2/2/15/20	20/39/115/115	-
21	CL7	3	502	19	2/2/13/20	12/31/107/115	-
21	CL7	b	610	2	2/2/15/20	14/39/115/115	-
21	CL7	1	417	18	2/2/13/20	9/27/103/115	-
25	LHG	B	623	-	-	3/49/49/53	-
32	ZEX	4	420	-	-	12/29/67/67	0/2/2/2
21	CL7	A	406	-	2/2/15/20	16/39/115/115	-
21	CL7	3	516	19	2/2/13/20	16/27/103/115	-
23	8CT	4	402	-	-	4/29/63/63	0/2/2/2
21	CL7	8	411	20	2/2/15/20	14/39/115/115	-
21	CL7	8	408	20	2/2/11/20	4/15/91/115	-
21	CL7	5	419	-	2/2/11/20	9/15/91/115	-
21	CL7	B	611	2	2/2/15/20	17/39/115/115	-
21	CL7	1	413	-	2/2/10/20	2/10/86/115	-
21	CL7	7	509	19	2/2/15/20	17/39/115/115	-
21	CL7	7	513	-	2/2/11/20	9/15/91/115	-
21	CL7	7	506	19	2/2/11/20	13/15/91/115	-
21	CL7	7	511	19	2/2/15/20	19/39/115/115	-
23	8CT	B	619	-	-	4/29/63/63	0/2/2/2
21	CL7	5	417	18	2/2/13/20	9/27/103/115	-
23	8CT	D	406	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	2	517	16	2/2/15/20	21/39/115/115	-
21	CL7	B	608	2	2/2/15/20	15/39/115/115	-
21	CL7	7	516	19	2/2/13/20	16/27/103/115	-
24	SQD	A	405	-	-	3/29/49/69	0/1/1/1
21	CL7	3	508	19	2/2/15/20	16/39/115/115	-
31	HEM	f	101	-	-	8/14/54/54	-
32	ZEX	6	520	-	-	6/29/67/67	0/2/2/2
32	ZEX	7	522	-	-	5/29/67/67	0/2/2/2
21	CL7	c	514	3	2/2/11/20	8/15/91/115	-
21	CL7	b	602	-	2/2/10/20	4/10/86/115	-
25	LHG	a	406	-	-	5/50/50/53	-
21	CL7	3	506	19	2/2/11/20	13/15/91/115	-
21	CL7	B	607	-	2/2/14/20	11/33/109/115	-
23	8CT	C	519	-	-	8/29/63/63	0/2/2/2
21	CL7	7	518	19	2/2/11/20	7/15/91/115	-
21	CL7	3	503	-	2/2/15/20	20/39/115/115	-
30	PL9	d	407	-	-	9/53/73/73	0/1/1/1
21	CL7	5	408	-	2/2/15/20	16/39/115/115	-
24	SQD	B	620	-	-	5/49/69/69	0/1/1/1
26	LMG	5	401	-	-	5/46/66/70	0/1/1/1
22	PHO	A	402	-	-	3/37/103/103	0/5/6/6
25	LHG	4	401	-	-	8/53/53/53	-
21	CL7	6	504	-	2/2/11/20	6/15/91/115	-
21	CL7	6	502	16	2/2/15/20	17/39/115/115	-
21	CL7	B	606	2	2/2/13/20	5/27/103/115	-
21	CL7	3	513	-	2/2/11/20	9/15/91/115	-
21	CL7	8	410	20	2/2/11/20	9/15/91/115	-
21	CL7	B	614	2	2/2/14/20	14/33/109/115	-
21	CL7	c	510	3	2/2/15/20	20/39/115/115	-
21	CL7	4	408	20	2/2/11/20	4/15/91/115	-
21	CL7	5	414	18	2/2/10/20	3/10/86/115	-
21	CL7	5	410	-	2/2/15/20	17/39/115/115	-
21	CL7	5	415	-	2/2/10/20	7/10/86/115	-
21	CL7	B	602	2	2/2/14/20	9/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CL7	b	613	2	2/2/15/20	17/39/115/115	-
21	CL7	5	409	18	2/2/11/20	6/15/91/115	-
21	CL7	5	405	-	2/2/11/20	10/15/91/115	-
21	CL7	D	405	4	2/2/11/20	8/15/91/115	-
21	CL7	C	507	3	2/2/14/20	15/33/109/115	-
21	CL7	7	505	19	2/2/15/20	14/39/115/115	-
21	CL7	b	607	2	2/2/13/20	5/27/103/115	-
24	SQD	2	524	-	-	0/36/56/69	0/1/1/1
21	CL7	B	622	2	2/2/11/20	8/15/91/115	-
21	CL7	b	617	2	2/2/11/20	4/15/91/115	-
21	CL7	6	518	16	2/2/15/20	12/39/115/115	-

The worst 5 of 4084 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

The worst 5 of 5533 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	d	408	PHO	C2D-C1D-ND	10.75	116.95	109.53
22	D	408	PHO	C2D-C1D-ND	10.73	116.94	109.53
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
22	D	408	PHO	C2B-C1B-NB	10.40	116.71	109.53

5 of 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

5 of 3294 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	401	CL7	C2B-C3B-CAB-OBB
21	A	401	CL7	C4B-C3B-CAB-OBB
21	A	403	CL7	O1A-CGA-O2A-C1
21	A	403	CL7	CBA-CGA-O2A-C1
21	A	403	CL7	C1A-C2A-CAA-CBA

There are no ring outliers.

269 monomers are involved in 1314 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	626	SQD	2	0
21	8	405	CL7	6	0
21	2	515	CL7	2	0
21	1	420	CL7	6	0
21	3	501	CL7	9	0
21	2	514	CL7	2	0
25	8	401	LHG	2	0
21	6	503	CL7	10	0
21	b	605	CL7	9	0
21	C	502	CL7	4	0
21	2	518	CL7	11	0
32	4	403	ZEX	22	0
21	7	512	CL7	6	0
32	5	422	ZEX	21	0
21	4	406	CL7	13	0
21	4	412	CL7	4	0
21	2	509	CL7	7	0
21	7	508	CL7	14	0
24	5	423	SQD	1	0
21	5	404	CL7	7	0
21	2	504	CL7	3	0
21	2	516	CL7	5	0
24	2	522	SQD	2	0
21	8	412	CL7	5	0
21	3	514	CL7	2	0
21	c	504	CL7	7	0
21	4	416	CL7	1	0
21	1	418	CL7	7	0
21	1	406	CL7	12	0
21	C	504	CL7	7	0
21	3	507	CL7	8	0
26	D	410	LMG	1	0
21	b	615	CL7	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	b	603	CL7	4	0
21	b	614	CL7	2	0
21	4	410	CL7	2	0
24	7	521	SQD	4	0
21	a	405	CL7	13	0
21	2	506	CL7	2	0
21	7	510	CL7	4	0
21	b	608	CL7	7	0
21	3	505	CL7	17	0
21	c	506	CL7	5	0
32	1	421	ZEX	13	0
25	b	626	LHG	1	0
21	5	420	CL7	6	0
32	2	521	ZEX	29	0
21	3	510	CL7	6	0
21	5	412	CL7	2	0
21	b	611	CL7	1	0
32	8	420	ZEX	13	0
32	8	419	ZEX	7	0
21	5	413	CL7	6	0
21	4	414	CL7	3	0
21	B	610	CL7	3	0
21	2	510	CL7	6	0
21	6	509	CL7	6	0
21	6	513	CL7	6	0
32	7	520	ZEX	10	0
21	8	413	CL7	4	0
21	6	515	CL7	2	0
25	d	409	LHG	4	0
32	6	522	ZEX	19	0
25	7	524	LHG	1	0
32	3	519	ZEX	17	0
21	4	415	CL7	4	0
32	8	403	ZEX	21	0
21	4	407	CL7	6	0
21	4	409	CL7	2	0
21	2	512	CL7	7	0
21	1	405	CL7	5	0
21	A	403	CL7	2	0
21	3	512	CL7	8	0
21	3	504	CL7	9	0
21	6	507	CL7	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	3	523	SQD	2	0
32	3	520	ZEX	11	0
21	C	509	CL7	3	0
22	D	408	PHO	7	0
21	4	405	CL7	7	0
21	5	411	CL7	2	0
32	6	524	ZEX	17	0
21	2	502	CL7	9	0
21	6	517	CL7	9	0
32	7	519	ZEX	17	0
21	c	511	CL7	3	0
23	c	519	8CT	1	0
21	1	416	CL7	1	0
21	4	413	CL7	4	0
23	c	516	8CT	1	0
21	c	509	CL7	4	0
21	1	407	CL7	3	0
26	B	621	LMG	6	0
21	7	503	CL7	11	0
32	5	421	ZEX	15	0
21	B	605	CL7	7	0
21	1	403	CL7	4	0
21	C	511	CL7	3	0
21	4	417	CL7	4	0
22	a	402	PHO	2	0
32	3	525	ZEX	23	0
21	1	404	CL7	7	0
32	3	522	ZEX	27	0
23	C	516	8CT	1	0
21	b	606	CL7	6	0
21	2	505	CL7	14	0
27	B	624	DGD	2	0
21	2	503	CL7	10	0
27	C	517	DGD	4	0
21	B	612	CL7	7	0
21	4	404	CL7	7	0
21	b	616	CL7	4	0
21	B	615	CL7	3	0
21	C	506	CL7	5	0
25	b	624	LHG	6	0
21	C	514	CL7	3	0
21	C	503	CL7	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7	523	SQD	2	0
21	b	604	CL7	9	0
21	1	408	CL7	7	0
32	2	523	ZEX	19	0
31	F	101	HEM	3	0
21	7	501	CL7	8	0
21	B	613	CL7	2	0
21	2	501	CL7	5	0
21	5	407	CL7	3	0
21	8	409	CL7	2	0
21	8	417	CL7	4	0
21	7	502	CL7	7	0
21	1	409	CL7	3	0
26	d	410	LMG	1	0
21	2	508	CL7	3	0
32	4	418	ZEX	9	0
21	6	511	CL7	9	0
21	B	604	CL7	9	0
21	c	508	CL7	4	0
21	6	516	CL7	6	0
21	d	404	CL7	6	0
21	1	412	CL7	2	0
21	C	512	CL7	1	0
21	C	508	CL7	4	0
21	1	410	CL7	7	0
21	7	504	CL7	9	0
21	7	517	CL7	2	0
26	b	622	LMG	6	0
21	8	404	CL7	8	0
26	1	401	LMG	2	0
25	D	409	LHG	3	0
21	c	512	CL7	1	0
21	2	513	CL7	6	0
21	6	506	CL7	2	0
21	7	514	CL7	2	0
21	c	513	CL7	1	0
27	c	517	DGD	4	0
32	2	520	ZEX	24	0
21	8	406	CL7	14	0
24	3	521	SQD	4	0
21	2	511	CL7	8	0
21	7	507	CL7	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	517	CL7	1	0
21	1	411	CL7	2	0
21	b	612	CL7	5	0
21	6	505	CL7	17	0
21	C	510	CL7	4	0
21	8	414	CL7	4	0
21	c	502	CL7	5	0
21	B	609	CL7	4	0
21	3	511	CL7	5	0
21	a	401	CL7	18	0
21	2	507	CL7	5	0
21	1	414	CL7	2	0
32	4	419	ZEX	7	0
21	4	411	CL7	7	0
32	6	519	ZEX	2	0
25	B	625	LHG	2	0
21	5	418	CL7	8	0
21	8	407	CL7	6	0
21	3	509	CL7	9	0
21	D	404	CL7	6	0
24	b	621	SQD	3	0
21	6	501	CL7	7	0
24	1	423	SQD	1	0
32	8	418	ZEX	10	0
32	2	525	ZEX	17	0
21	5	403	CL7	5	0
30	D	407	PL9	7	0
32	1	422	ZEX	22	0
21	3	515	CL7	2	0
21	8	415	CL7	5	0
27	b	625	DGD	2	0
25	3	524	LHG	1	0
21	5	402	CL7	10	0
21	6	508	CL7	4	0
21	6	514	CL7	2	0
21	a	403	CL7	1	0
21	b	609	CL7	3	0
32	2	519	ZEX	2	0
21	c	507	CL7	3	0
21	C	505	CL7	3	0
21	A	401	CL7	16	0
22	d	408	PHO	7	0

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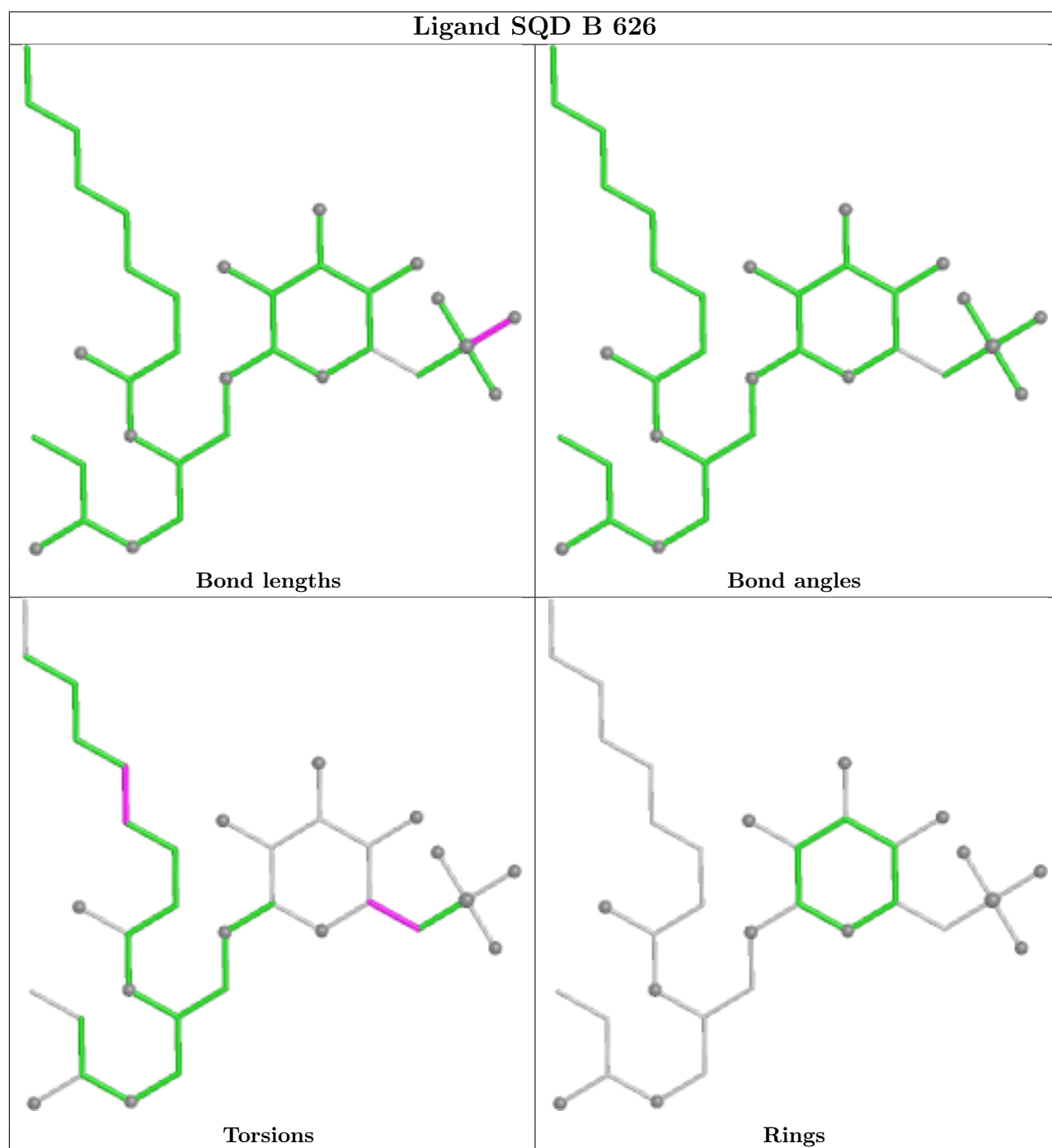
Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	5	406	CL7	12	0
21	C	513	CL7	1	0
21	1	402	CL7	10	0
21	c	503	CL7	4	0
21	B	603	CL7	8	0
21	3	518	CL7	3	0
21	6	512	CL7	8	0
21	d	405	CL7	2	0
21	5	416	CL7	1	0
21	c	505	CL7	3	0
24	6	521	SQD	1	0
21	7	515	CL7	2	0
21	6	510	CL7	6	0
21	3	502	CL7	7	0
21	b	610	CL7	4	0
21	1	417	CL7	4	0
25	B	623	LHG	6	0
32	4	420	ZEX	9	0
21	A	406	CL7	12	0
21	3	516	CL7	5	0
21	8	411	CL7	8	0
21	8	408	CL7	4	0
21	B	611	CL7	4	0
21	1	413	CL7	6	0
21	7	509	CL7	8	0
21	7	513	CL7	12	0
21	7	506	CL7	5	0
21	7	511	CL7	5	0
21	5	417	CL7	5	0
21	2	517	CL7	9	0
21	B	608	CL7	3	0
21	7	516	CL7	6	0
24	A	405	SQD	2	0
21	3	508	CL7	13	0
31	f	101	HEM	3	0
32	6	520	ZEX	31	0
32	7	522	ZEX	25	0
21	c	514	CL7	3	0
21	3	506	CL7	5	0
21	B	607	CL7	7	0
23	C	519	8CT	1	0
21	7	518	CL7	3	0

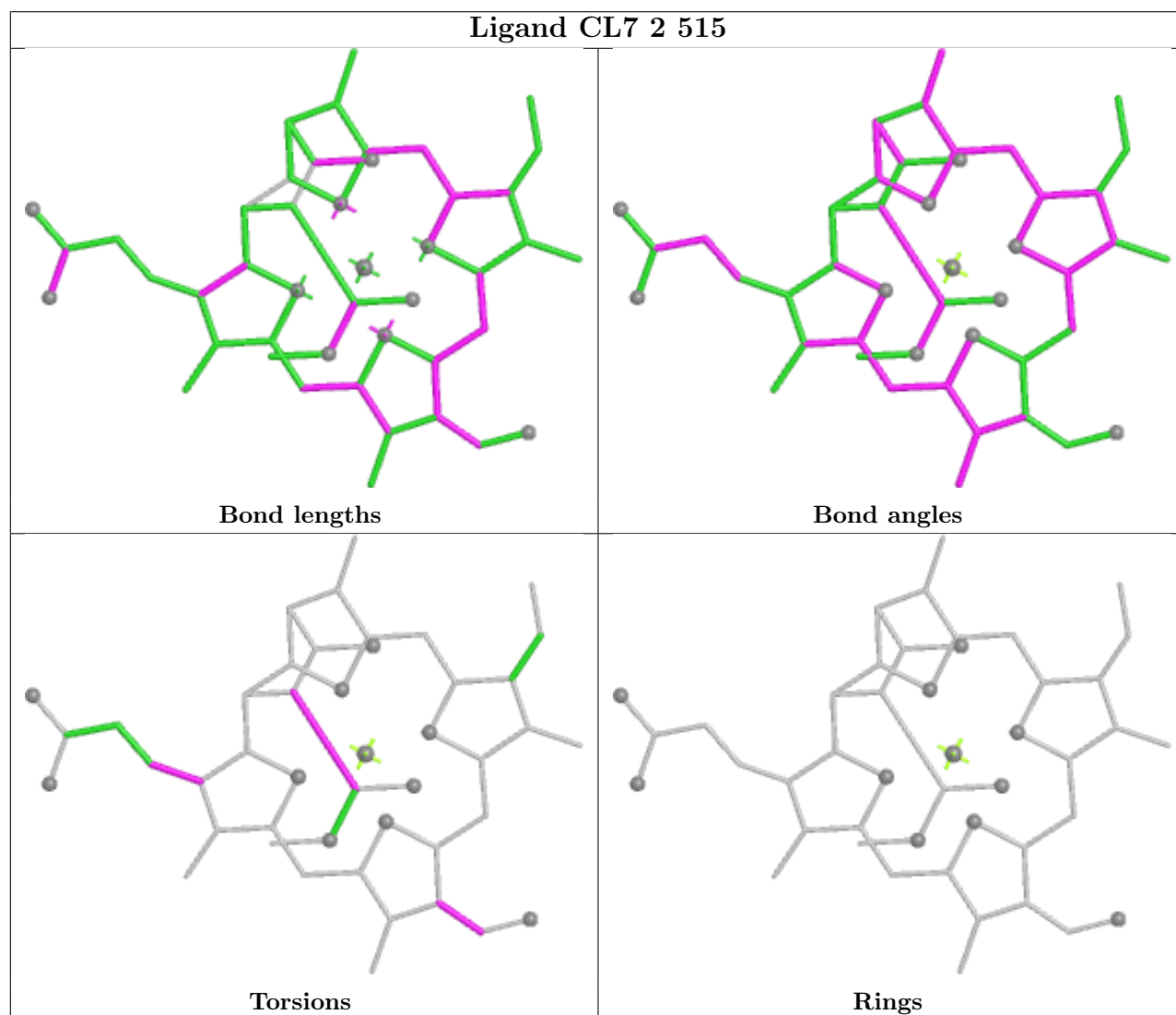
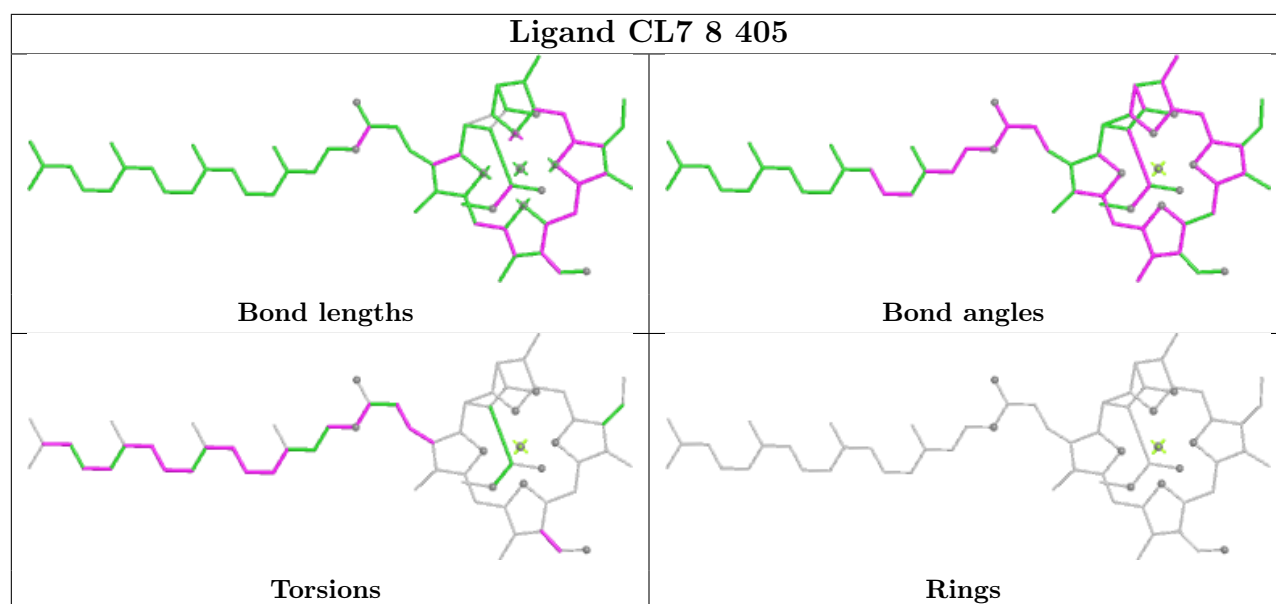
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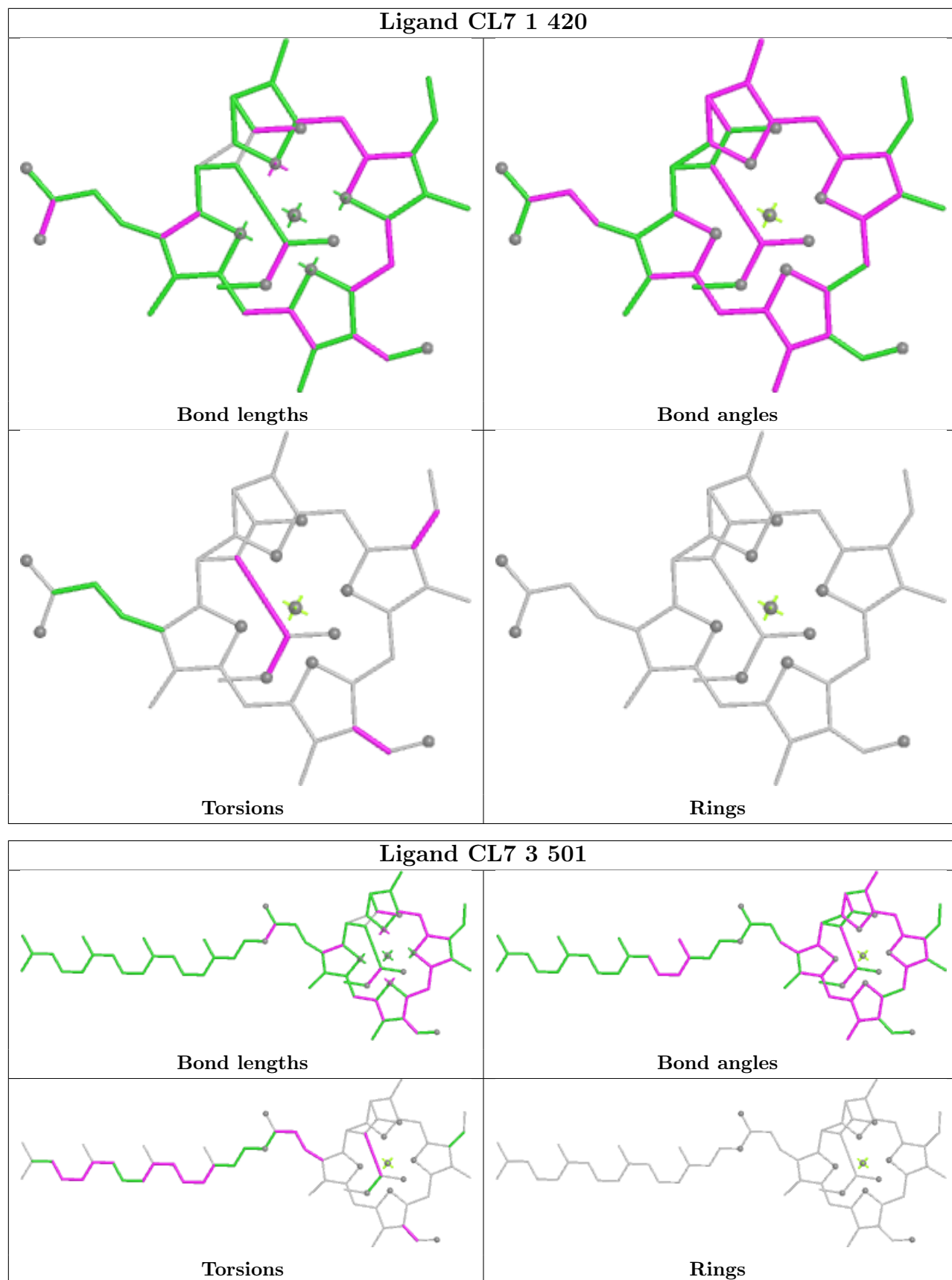
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	3	503	CL7	11	0
30	d	407	PL9	6	0
21	5	408	CL7	7	0
24	B	620	SQD	3	0
26	5	401	LMG	2	0
22	A	402	PHO	2	0
25	4	401	LHG	2	0
21	6	504	CL7	3	0
21	6	502	CL7	8	0
21	B	606	CL7	4	0
21	3	513	CL7	13	0
21	8	410	CL7	2	0
21	B	614	CL7	2	0
21	c	510	CL7	3	0
21	4	408	CL7	4	0
21	5	414	CL7	2	0
21	5	410	CL7	6	0
21	B	602	CL7	4	0
21	b	613	CL7	6	0
21	5	409	CL7	4	0
21	5	405	CL7	5	0
21	D	405	CL7	2	0
21	C	507	CL7	5	0
21	7	505	CL7	19	0
21	b	607	CL7	5	0
21	6	518	CL7	10	0

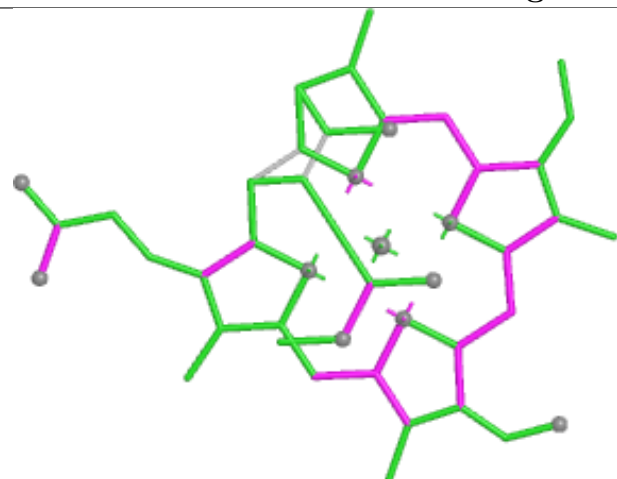
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



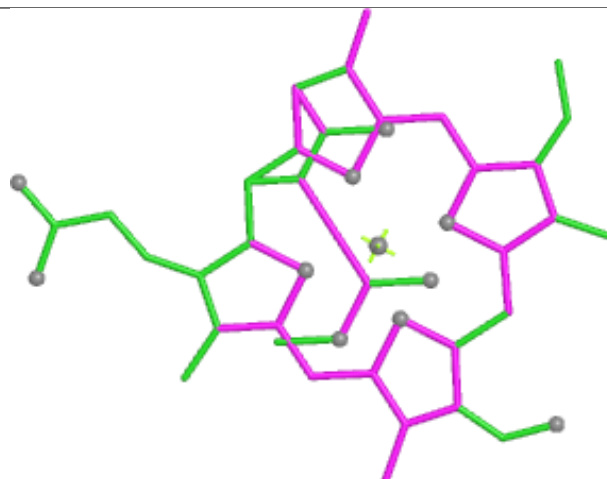




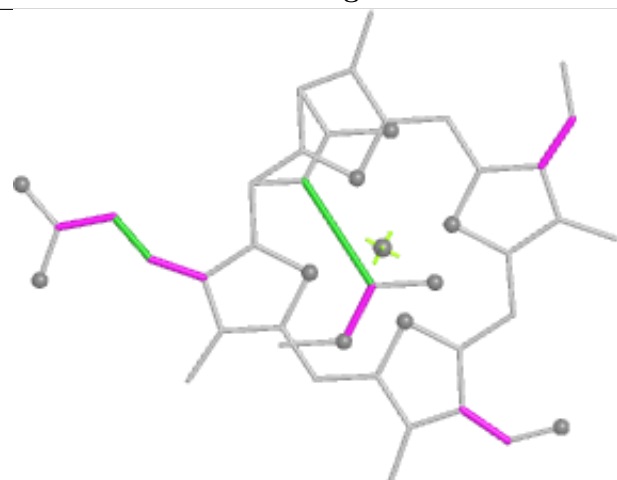
Ligand CL7 2 514



Bond lengths



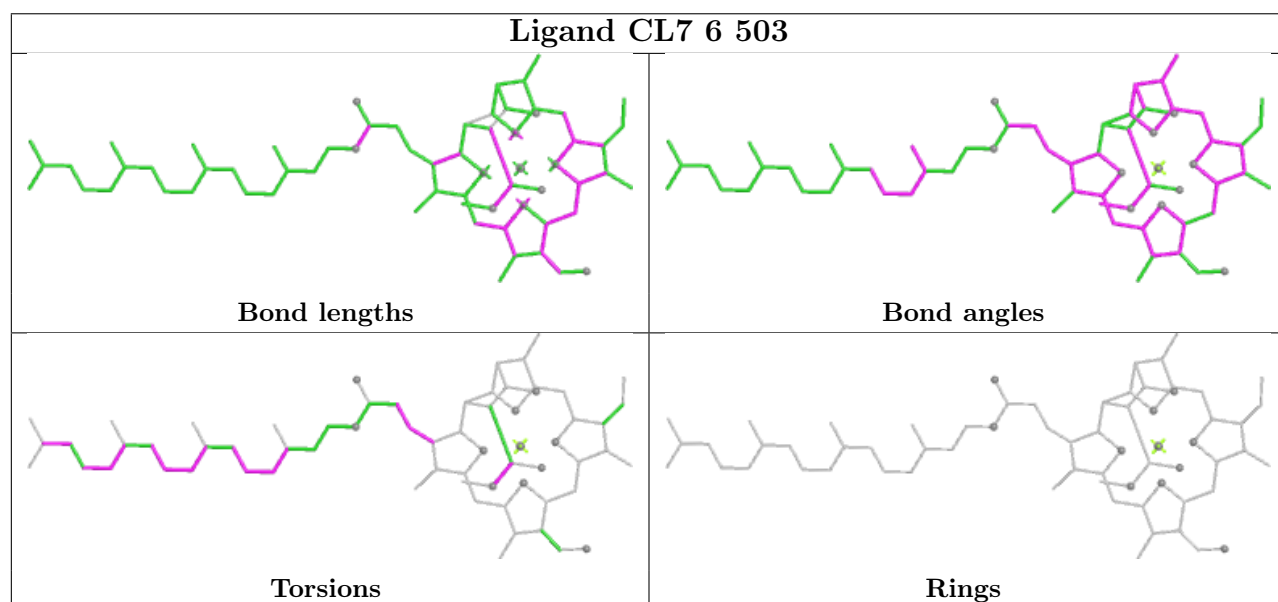
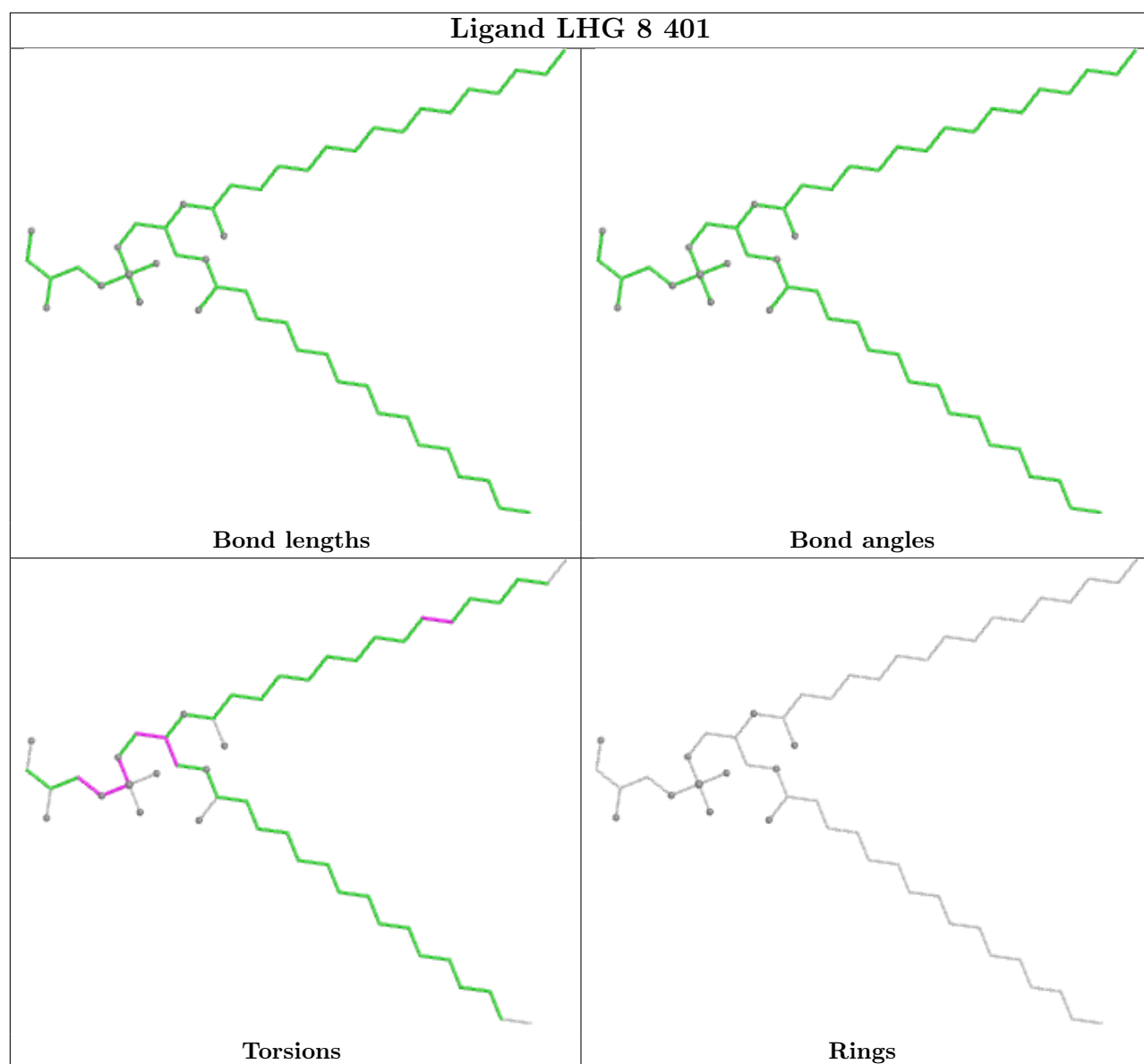
Bond angles

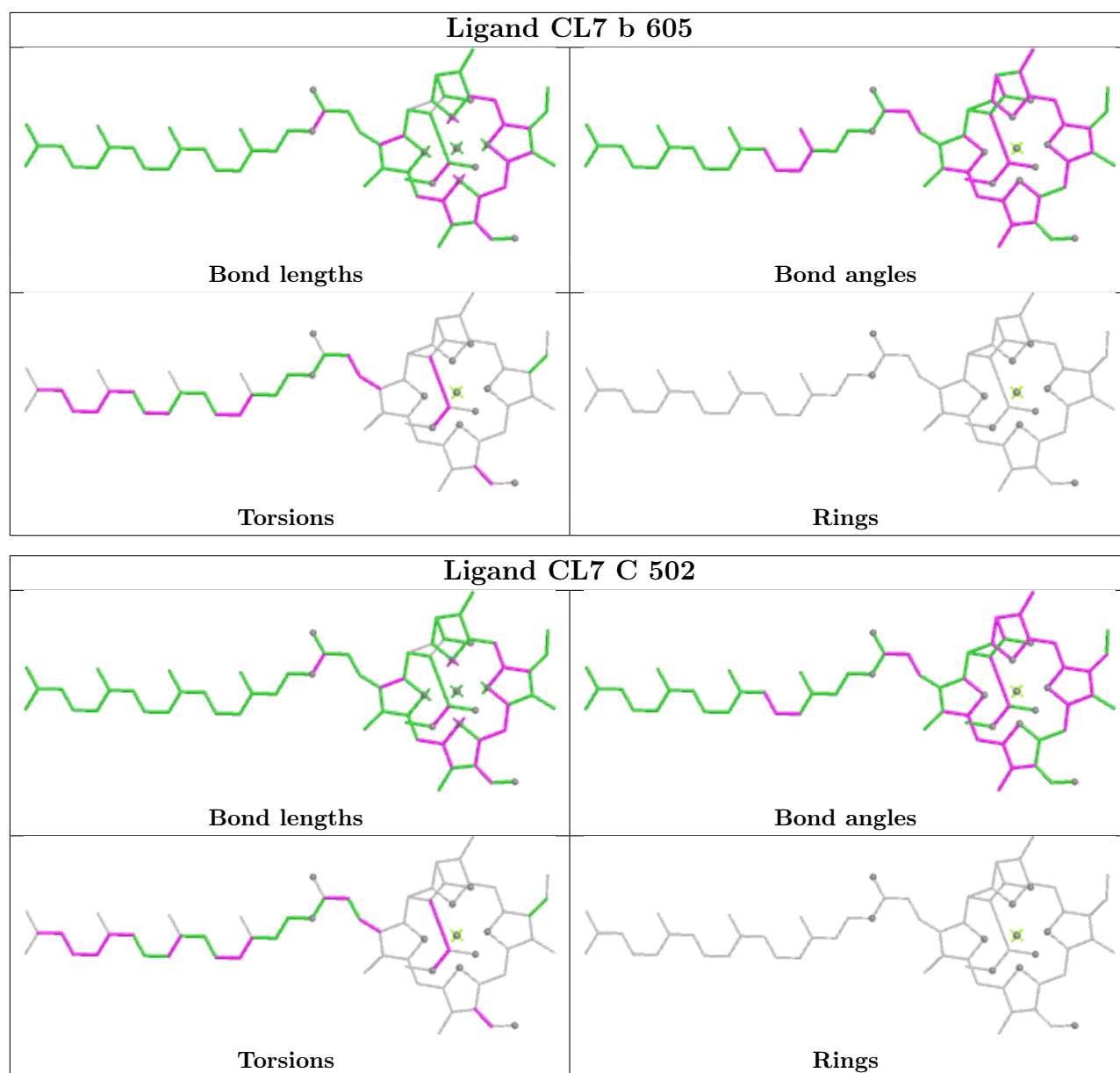


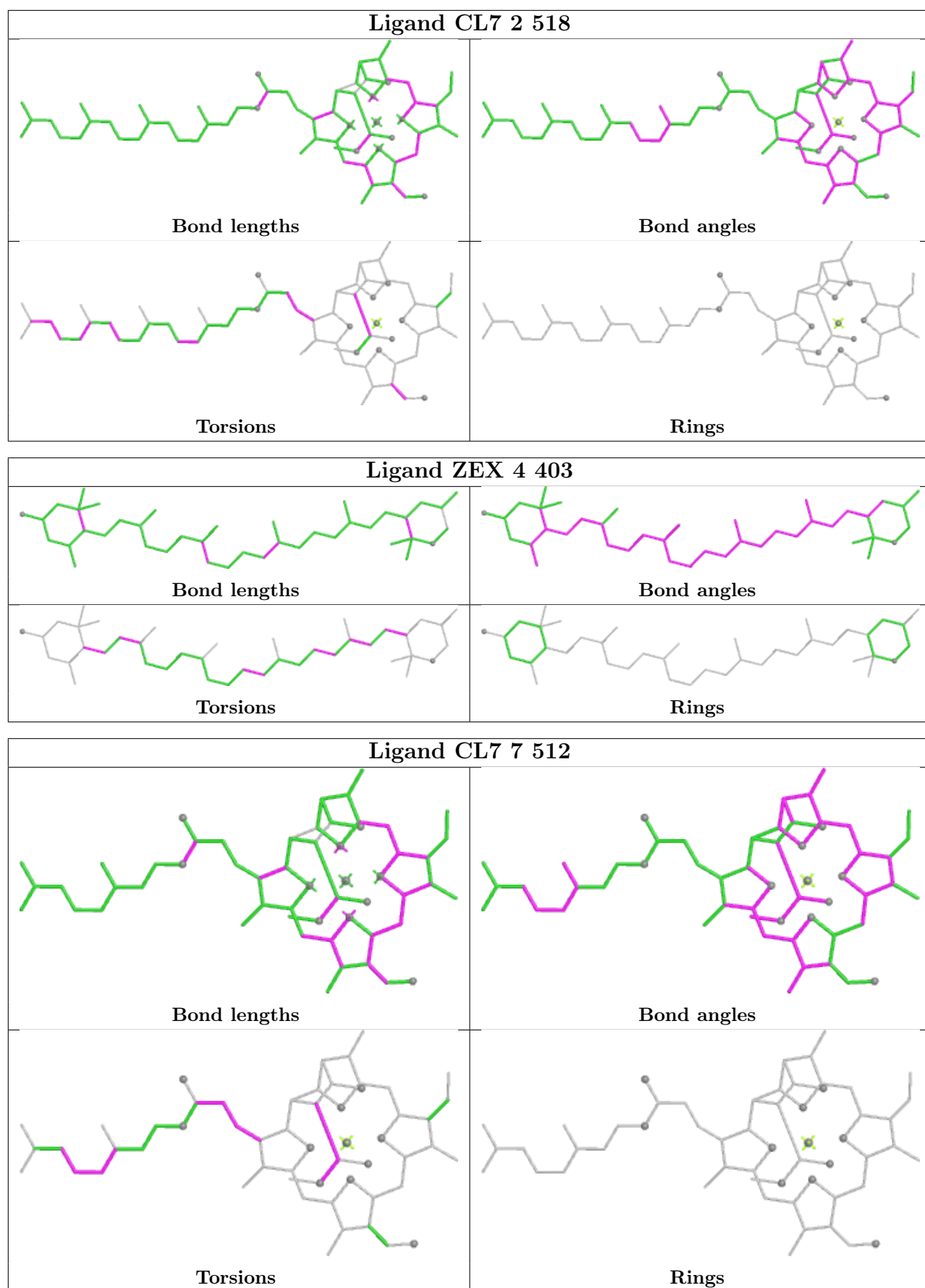
Torsions

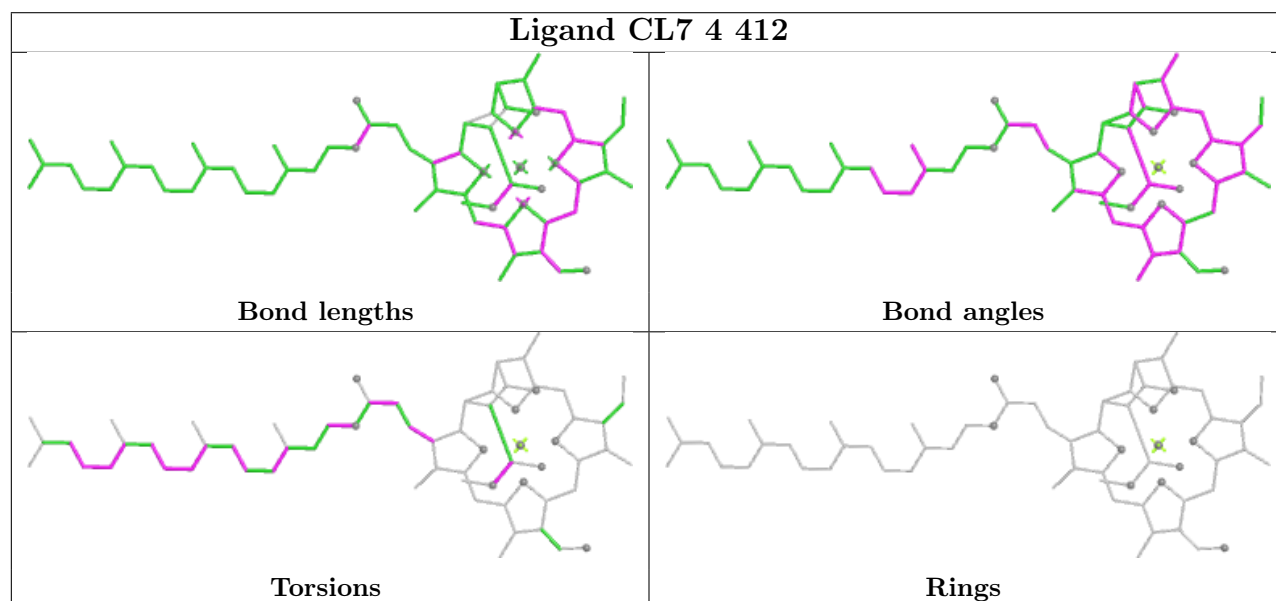
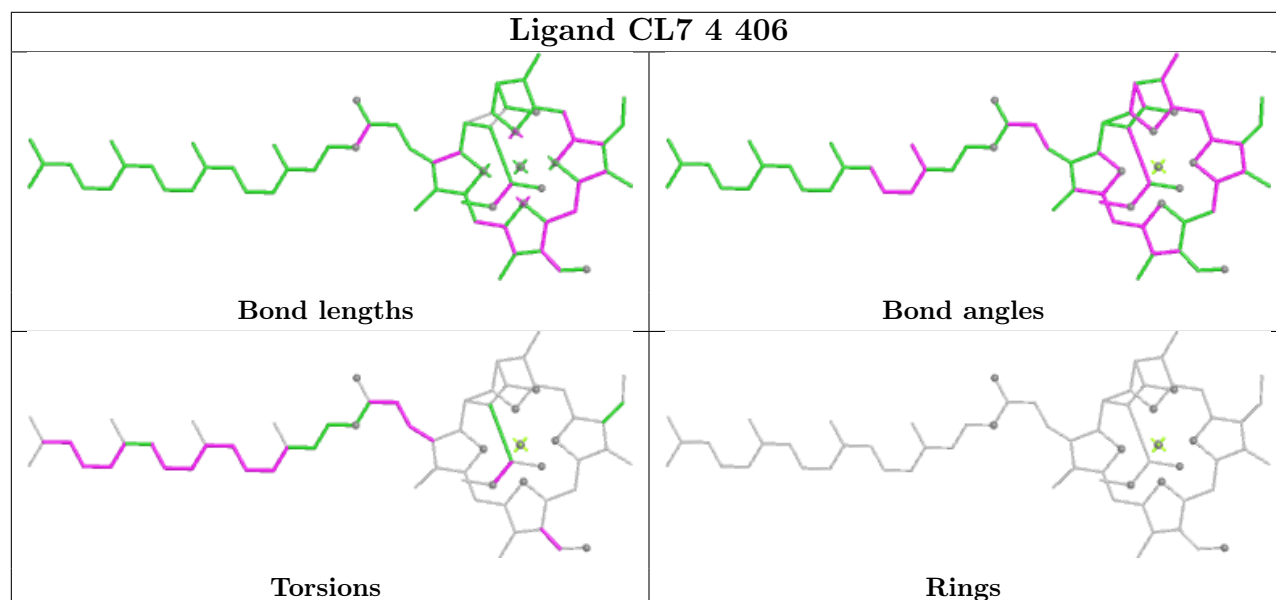
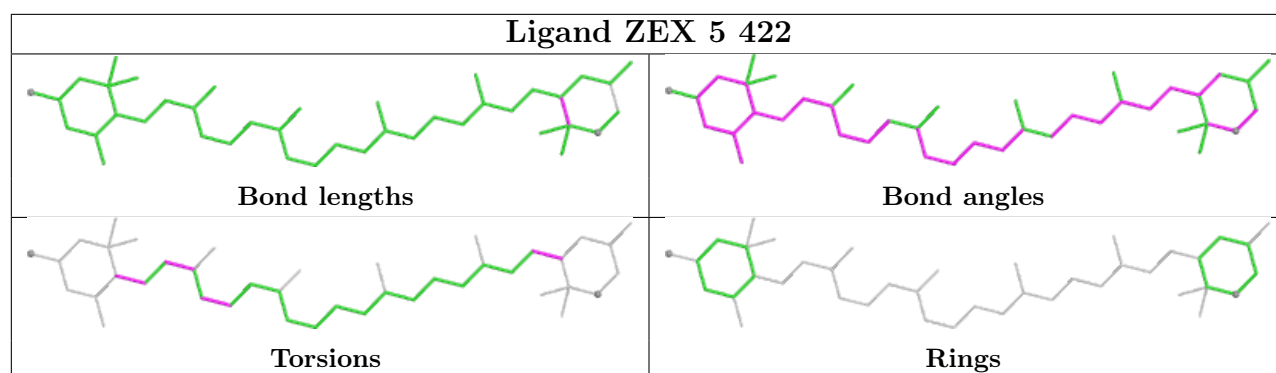


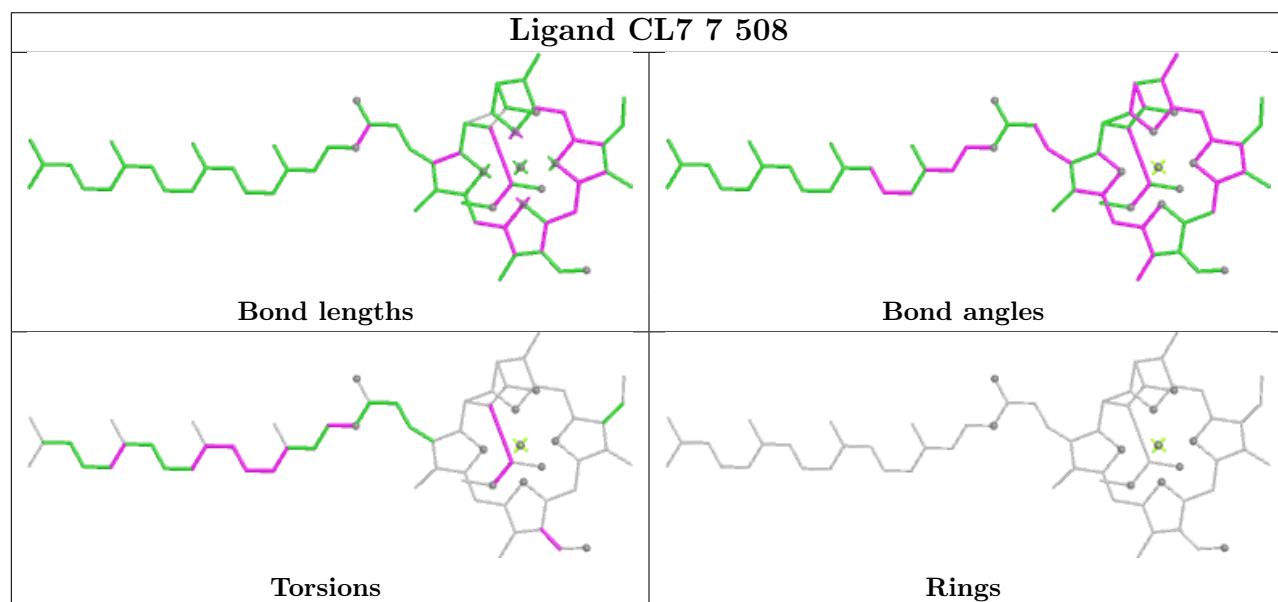
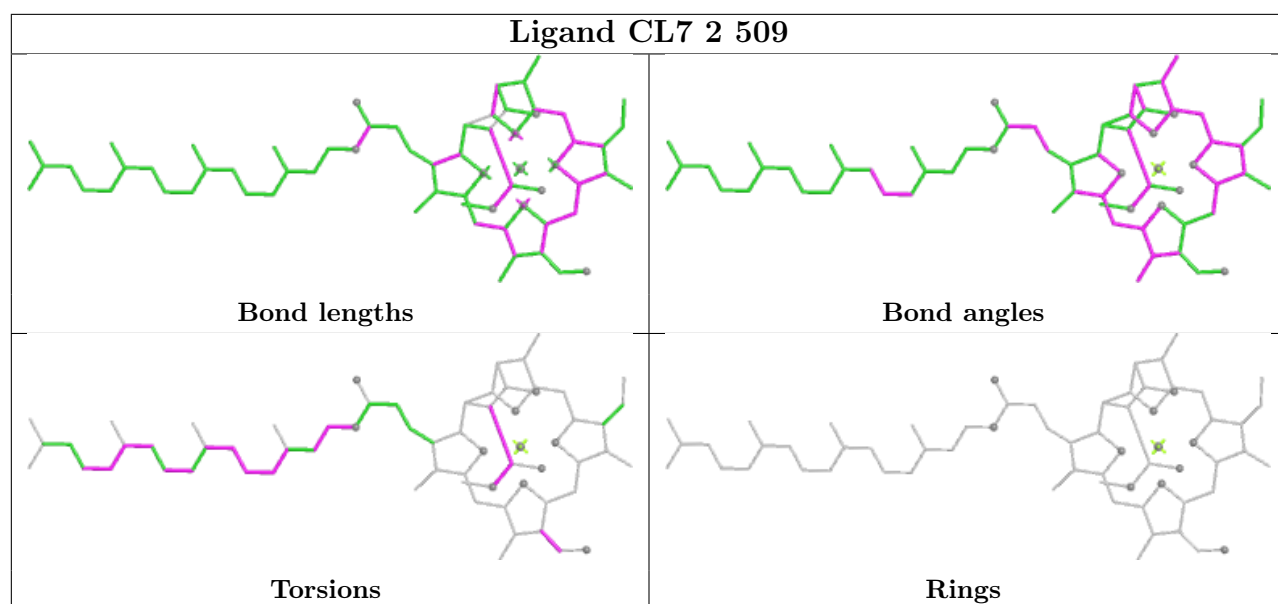
Rings

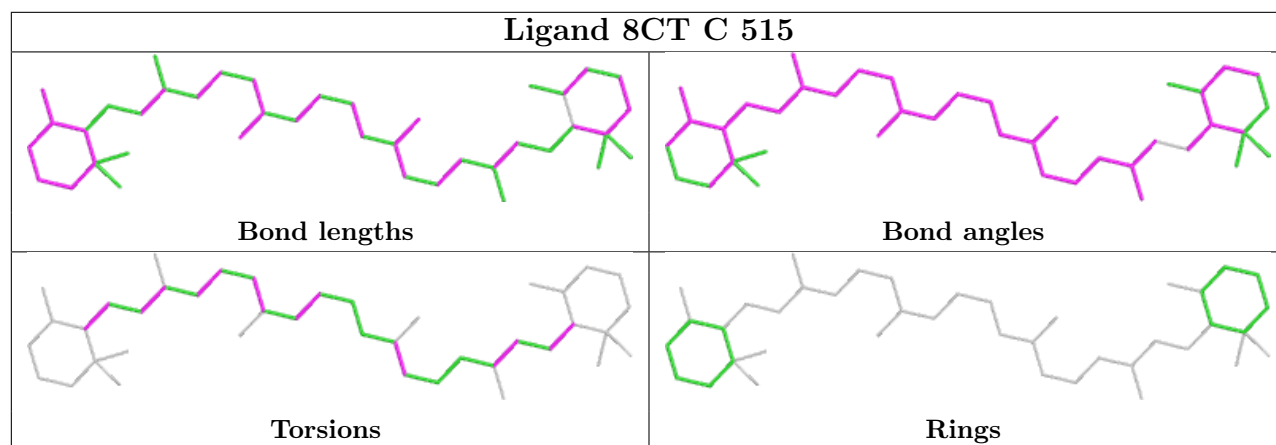
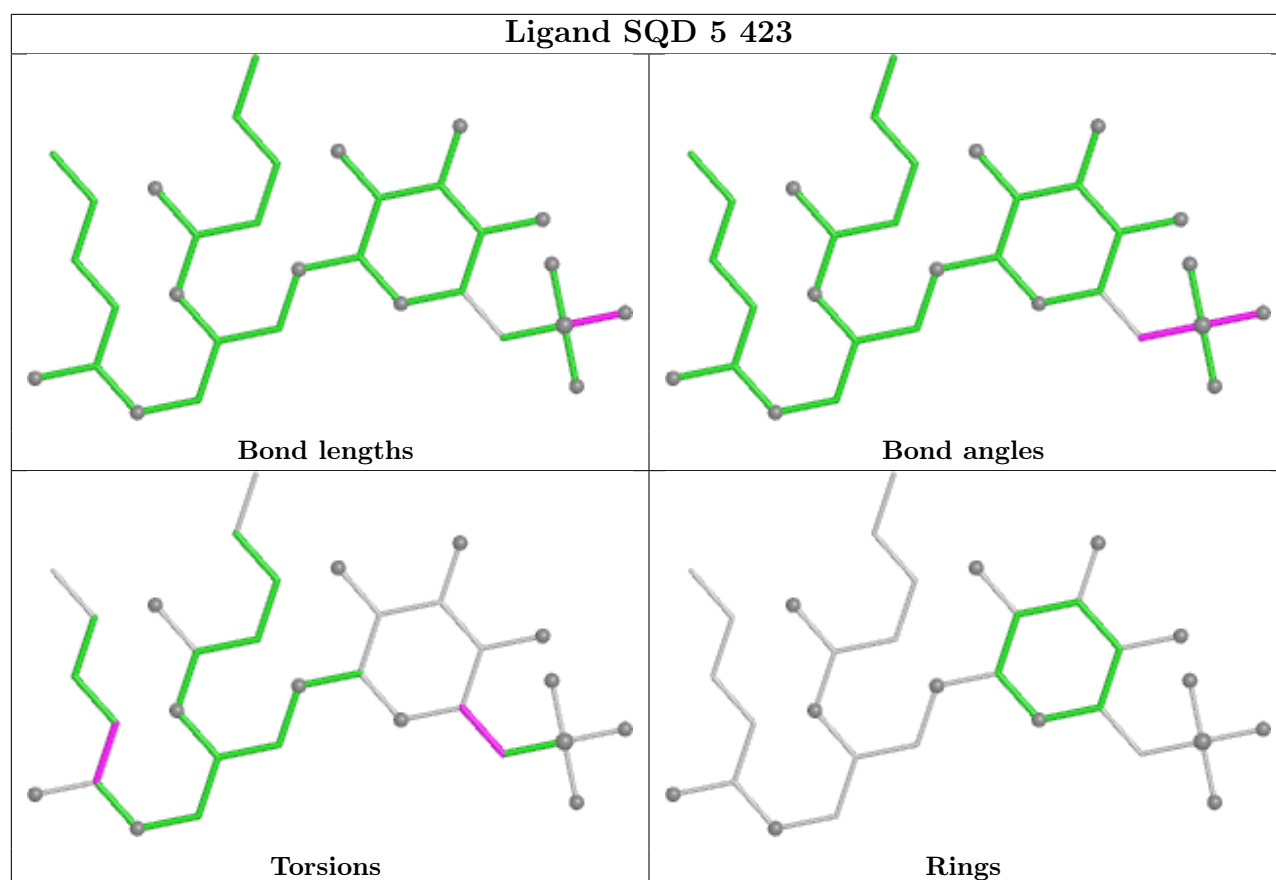


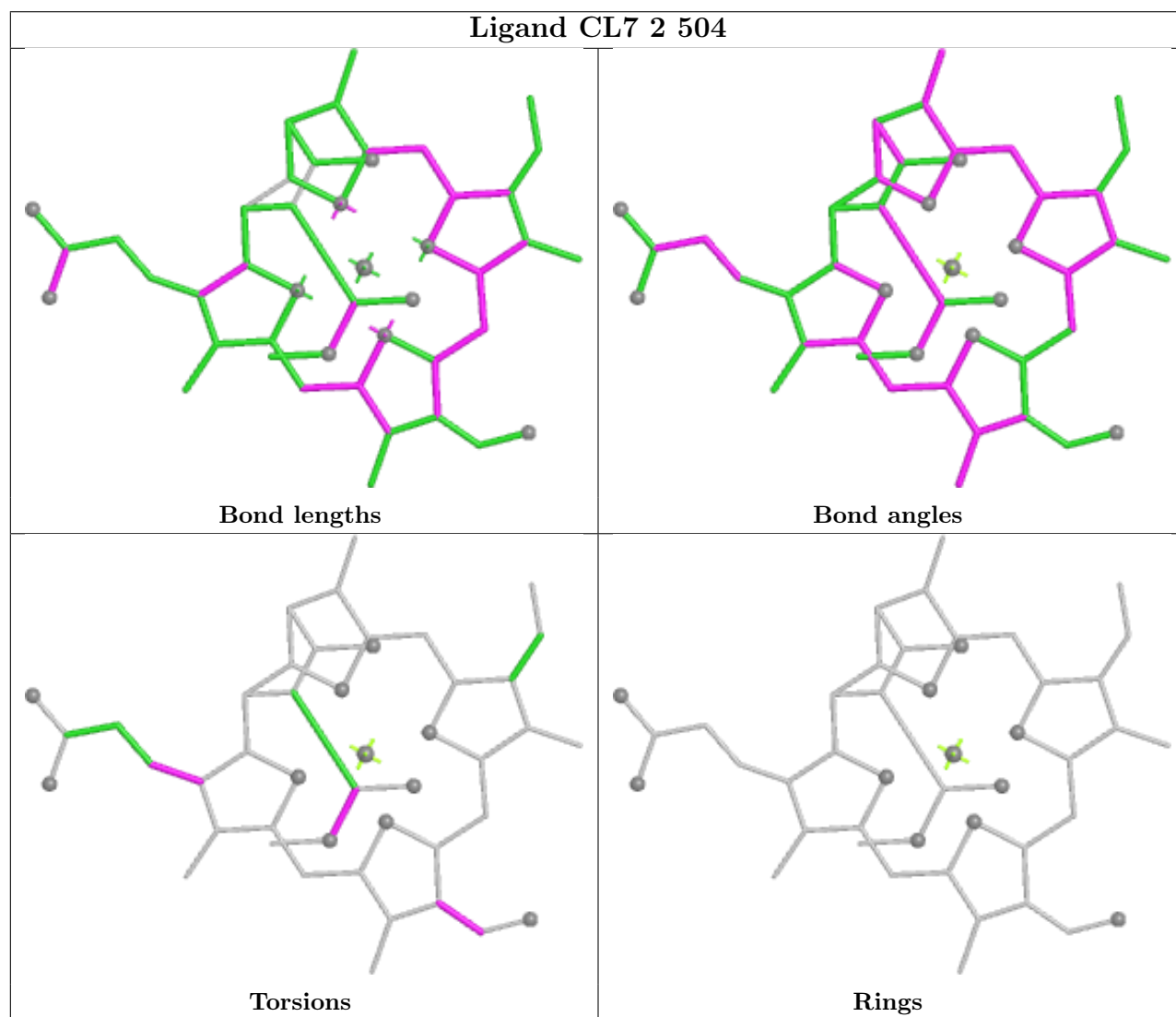
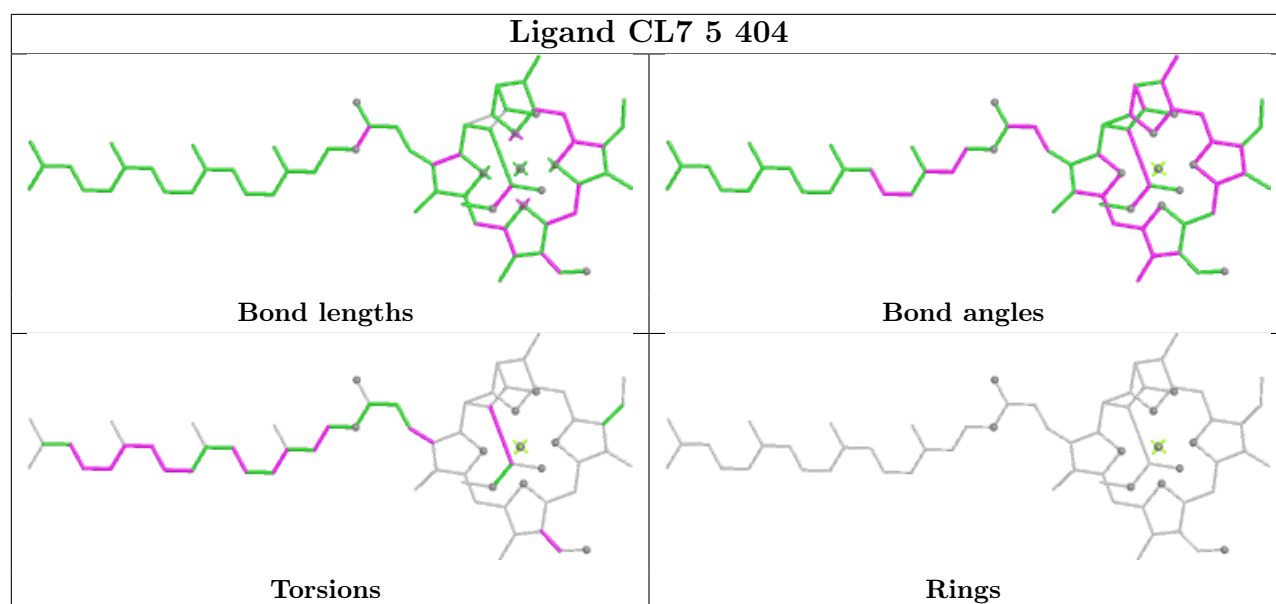


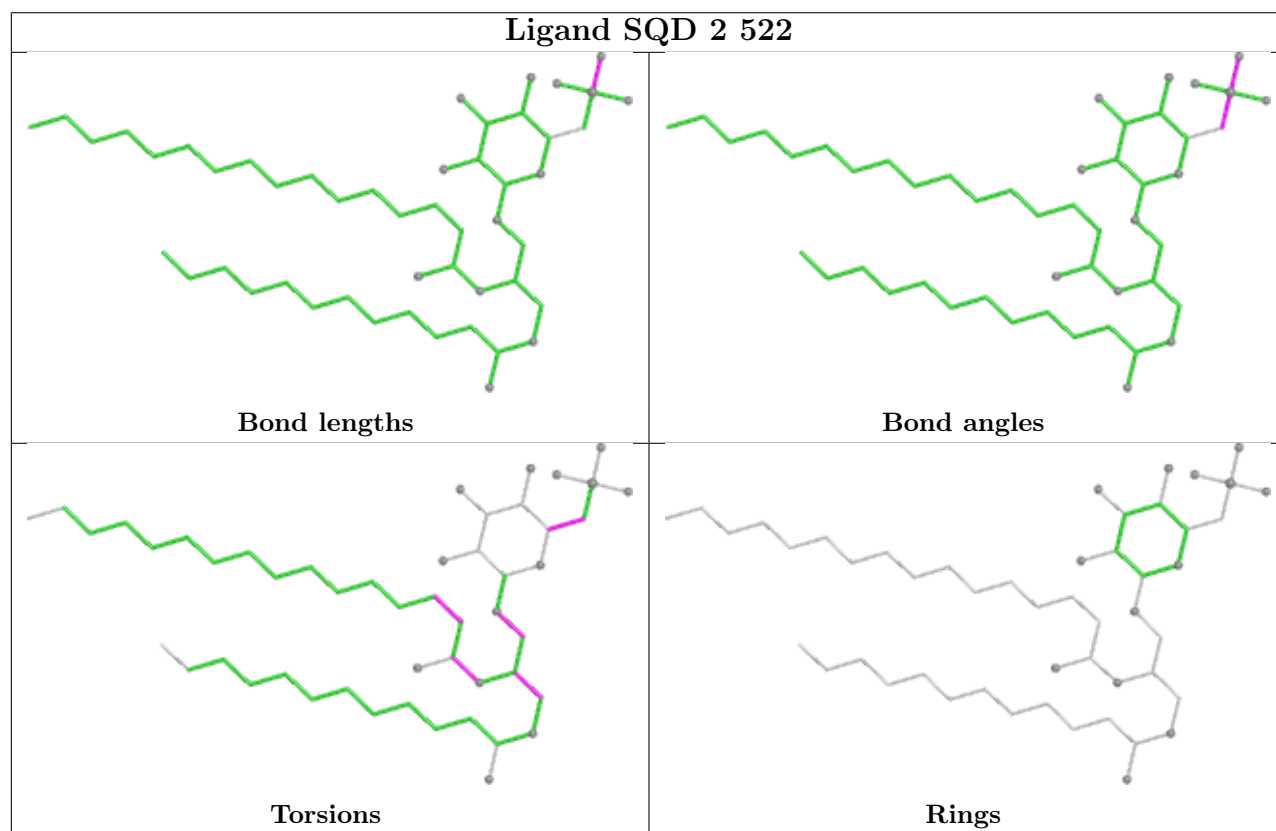
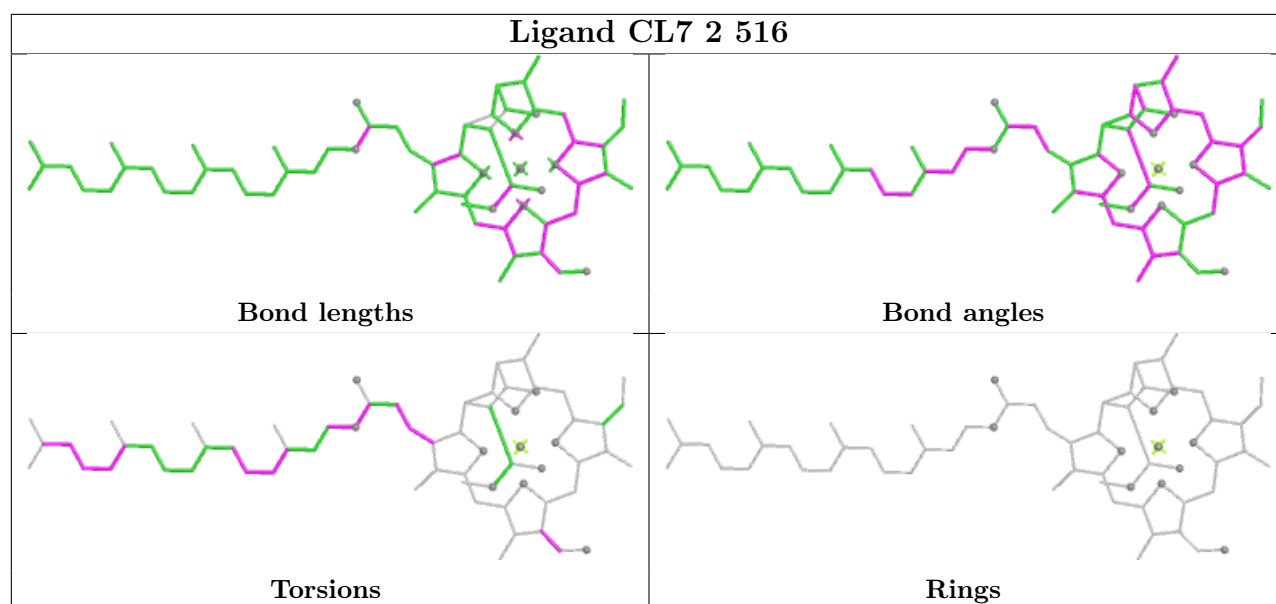


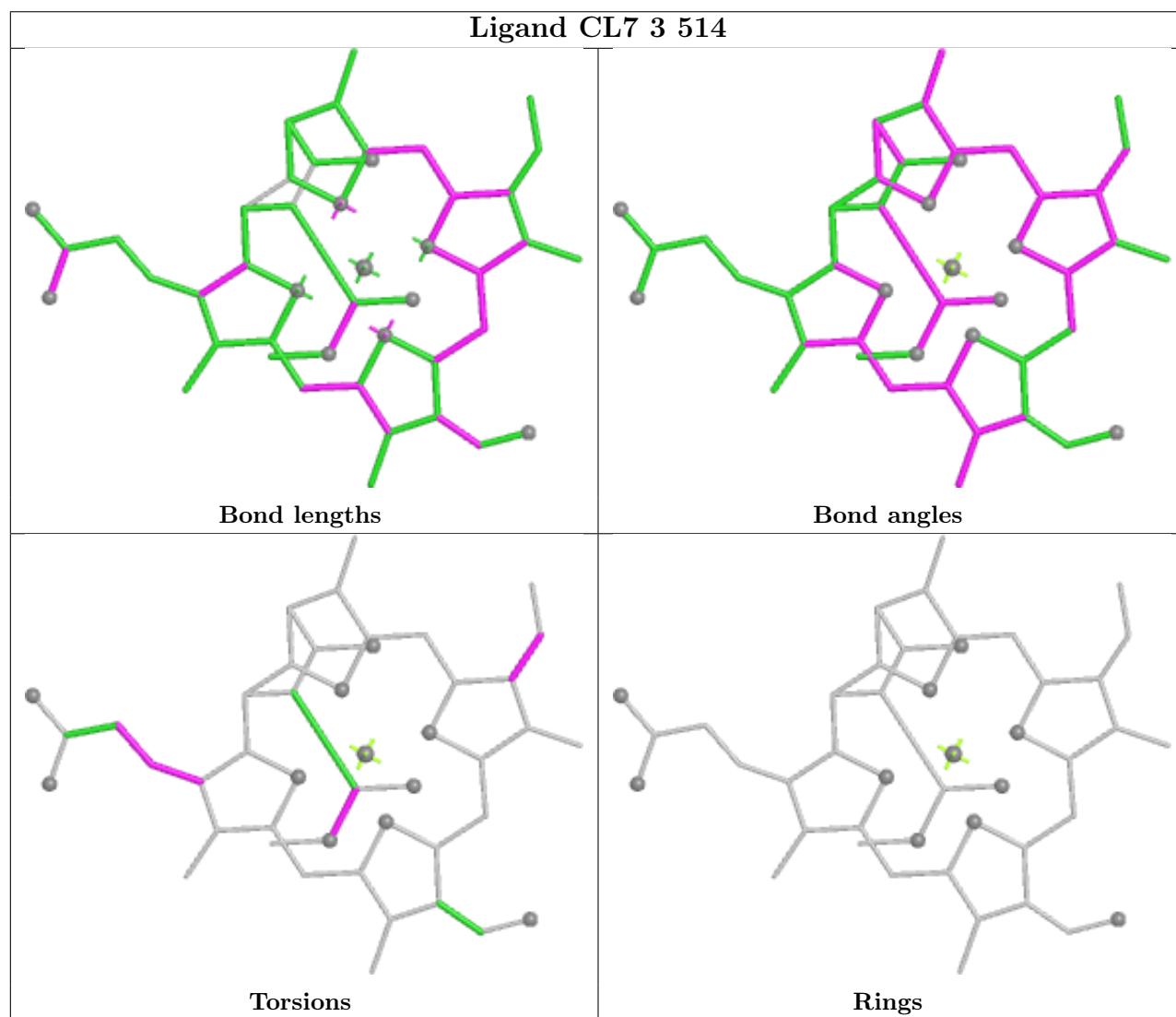
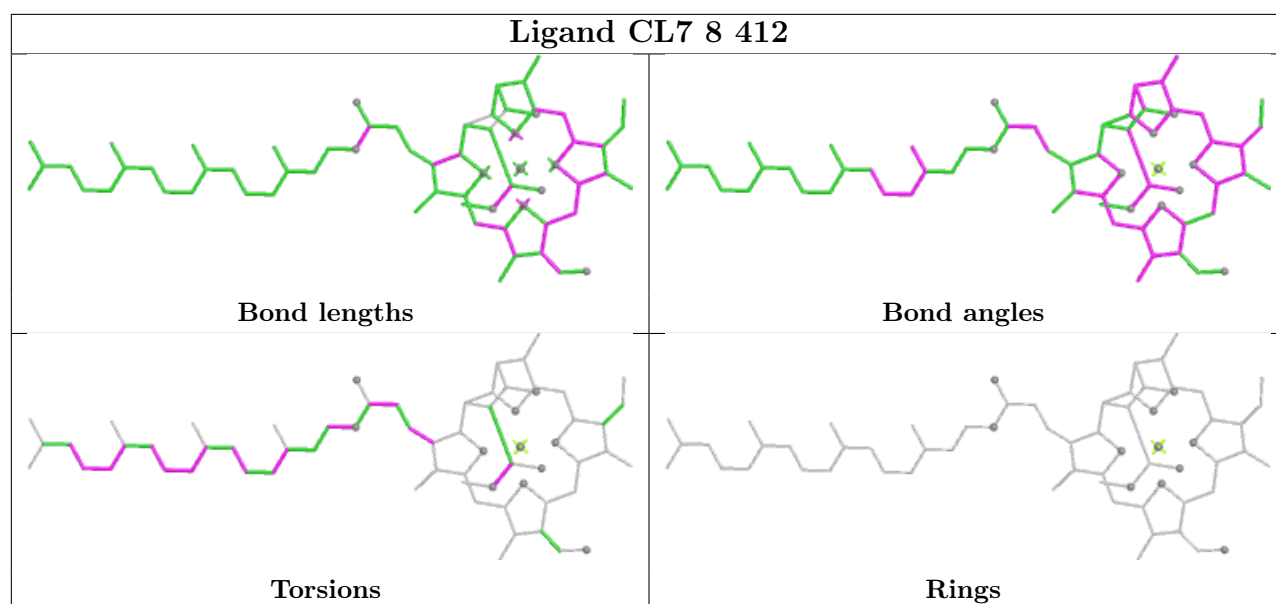


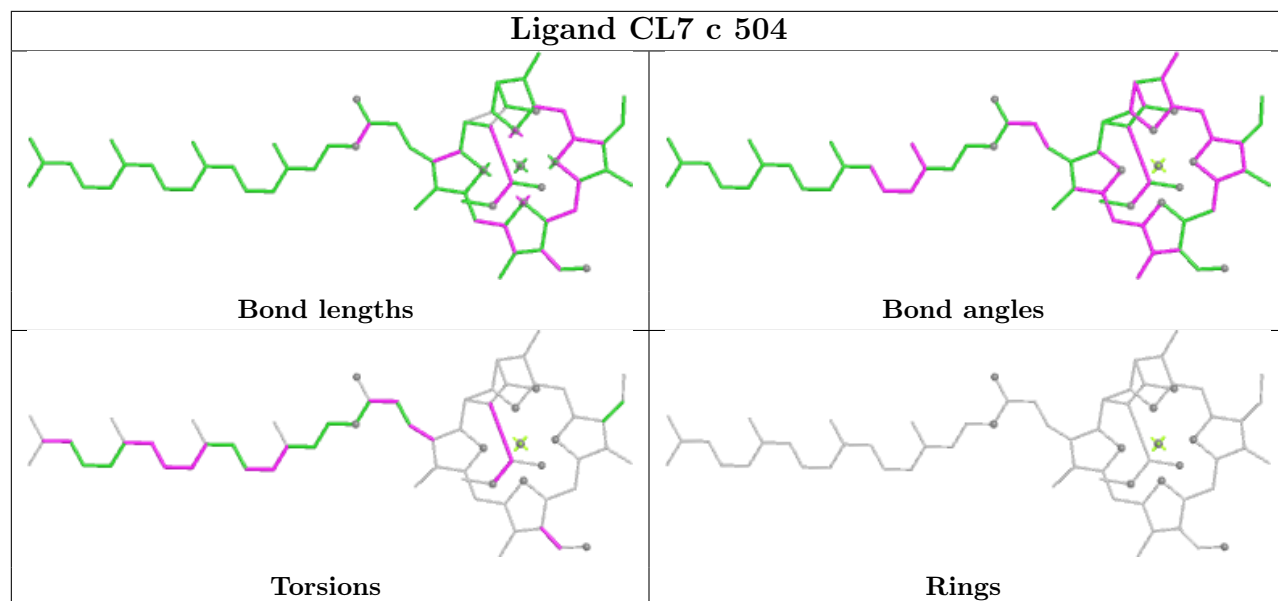




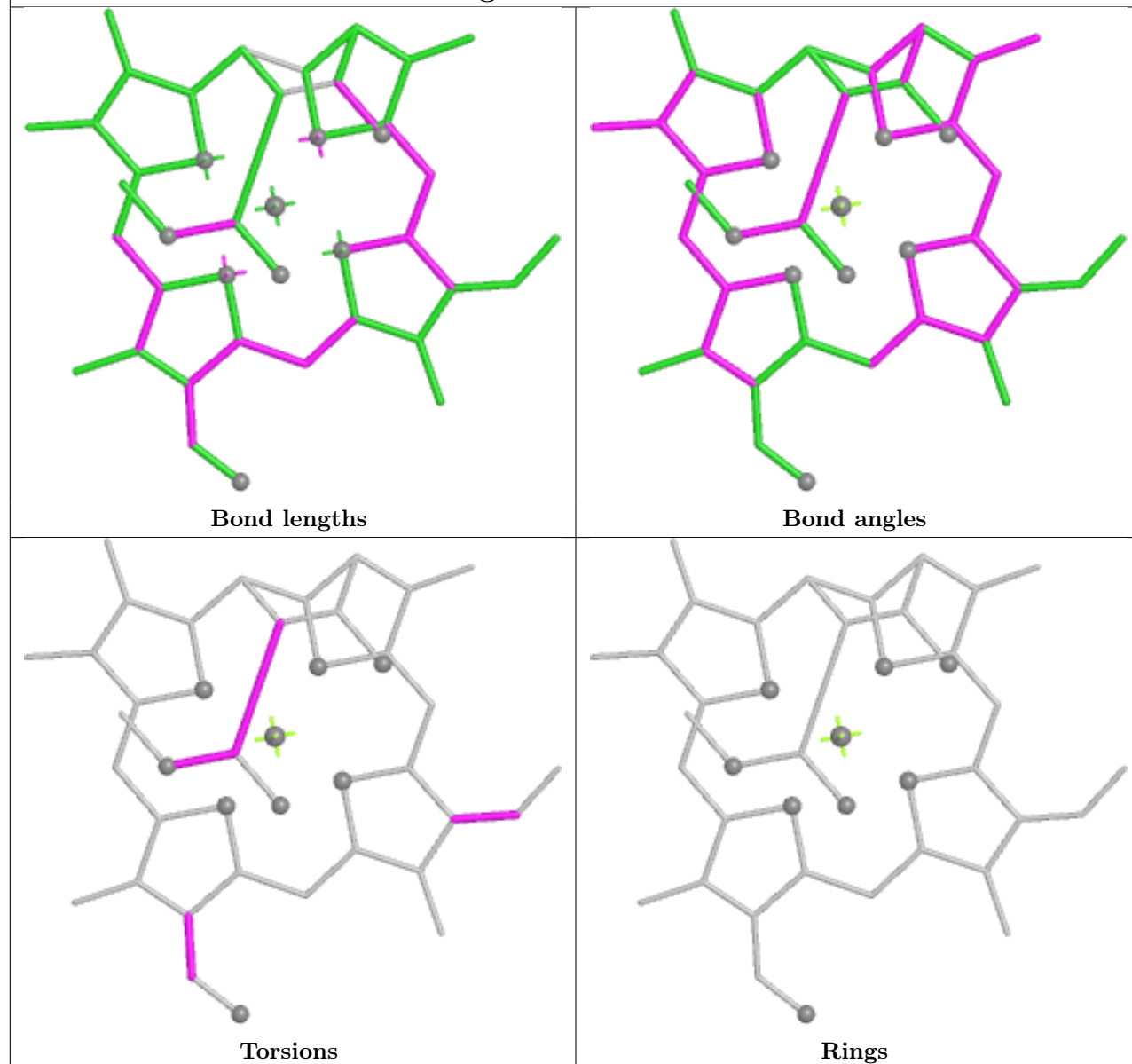




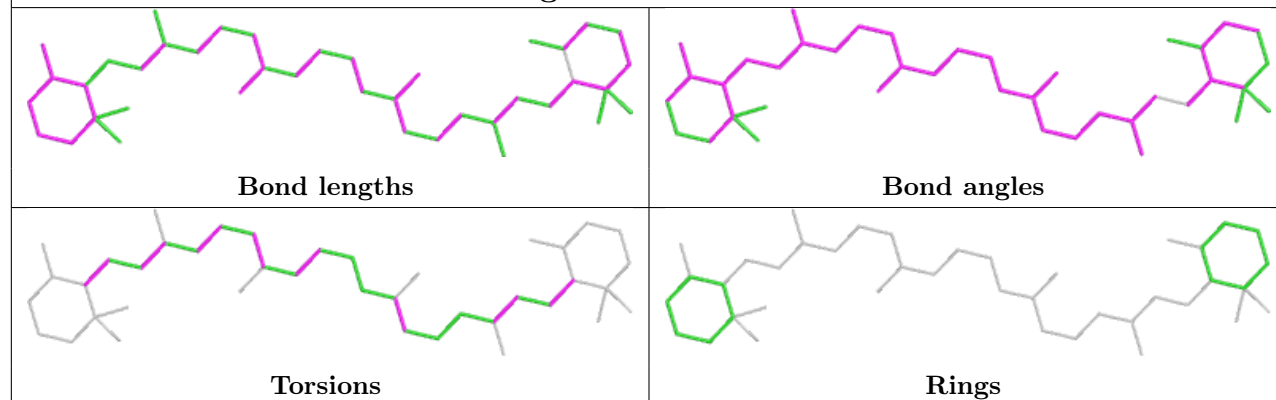


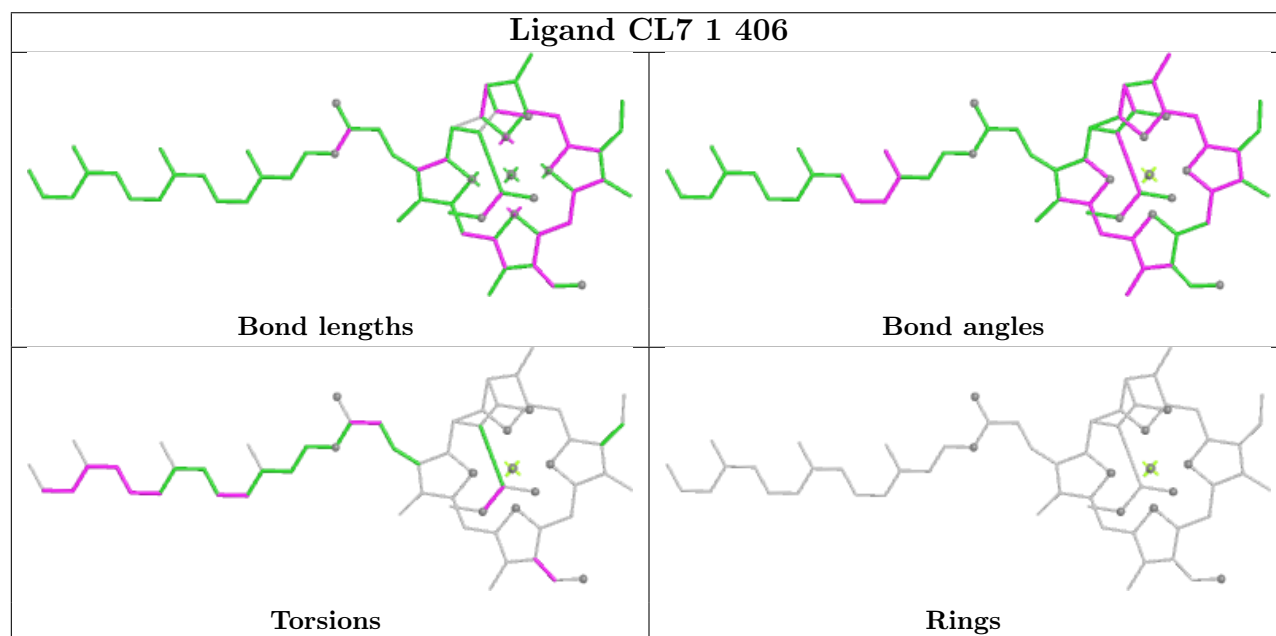
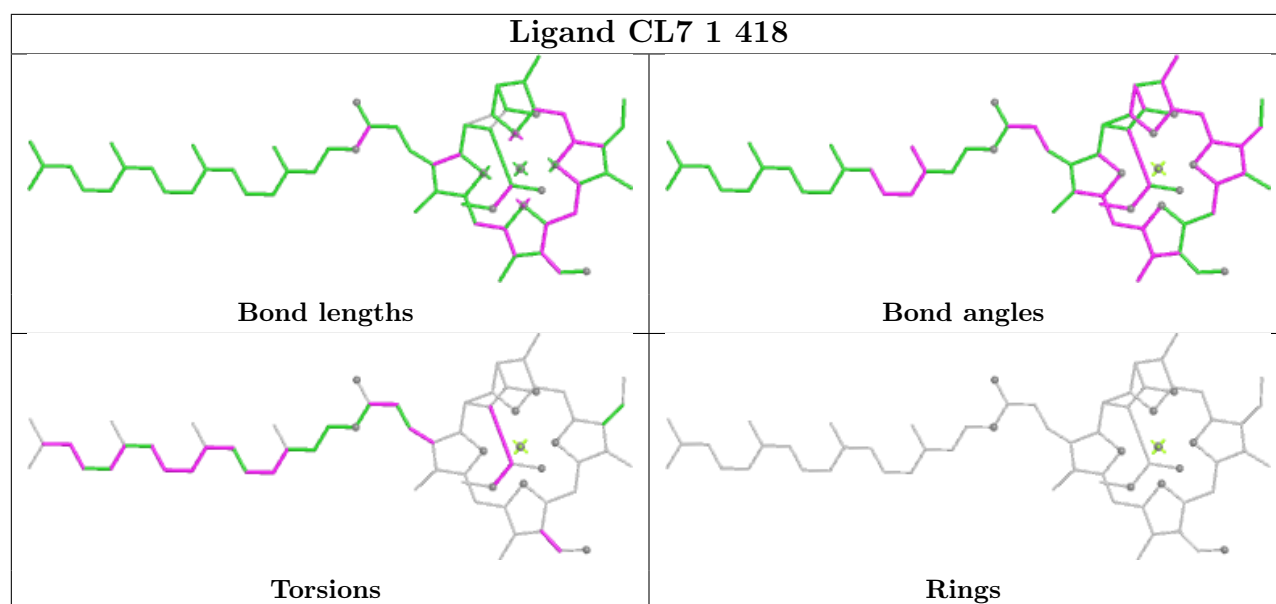


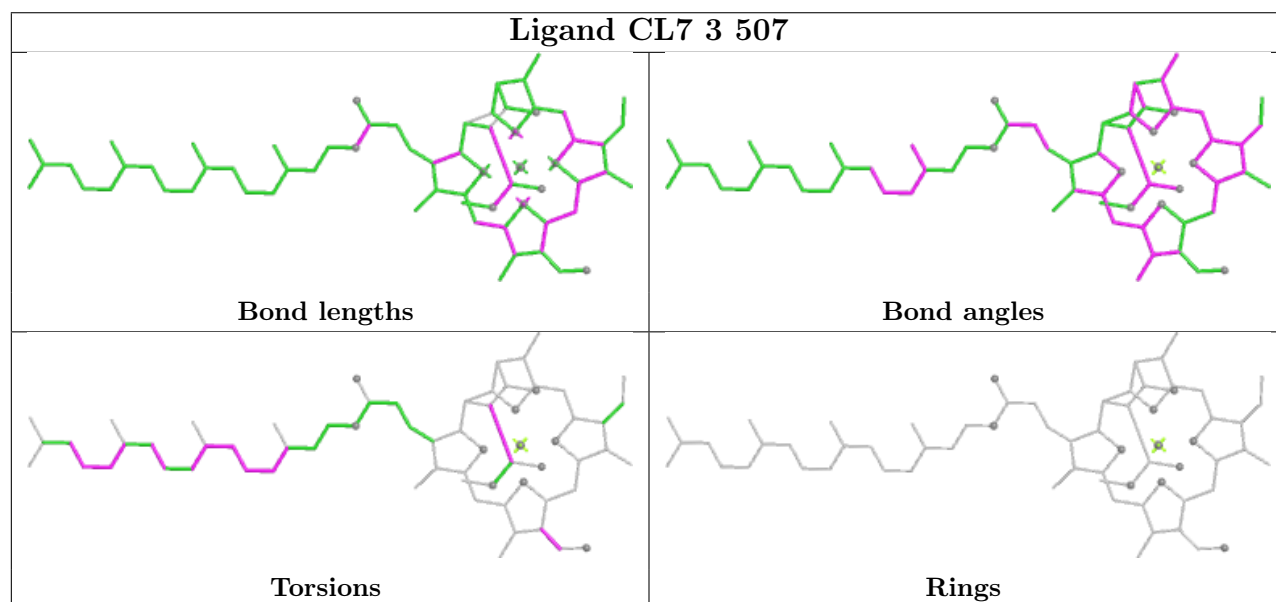
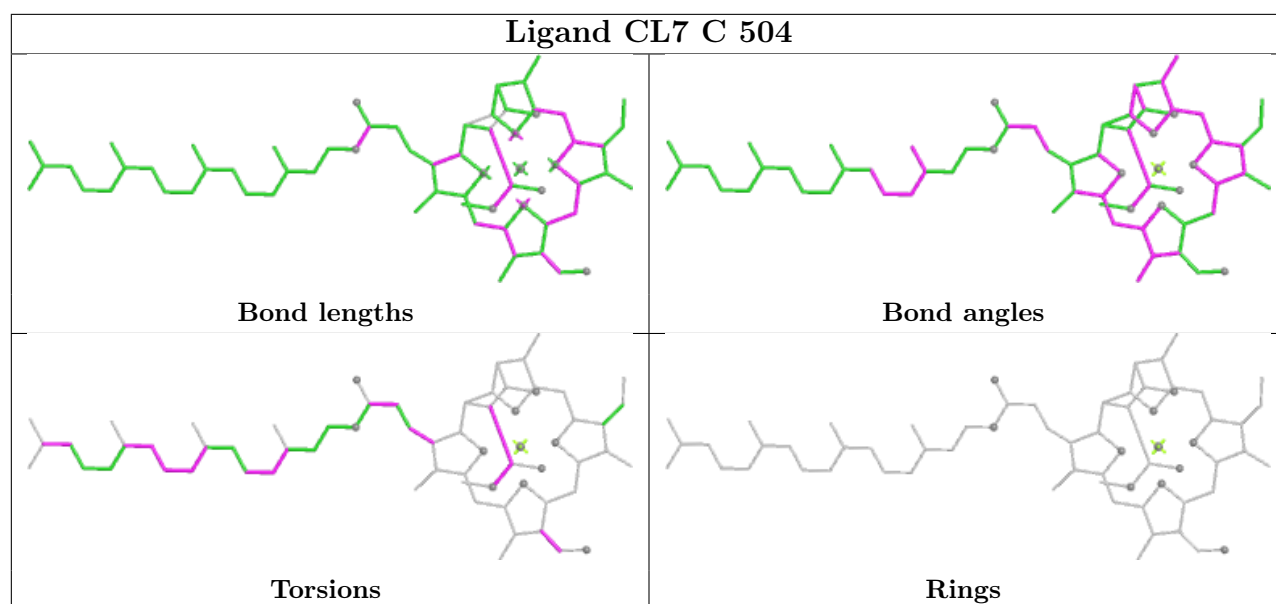
Ligand CL7 4 416

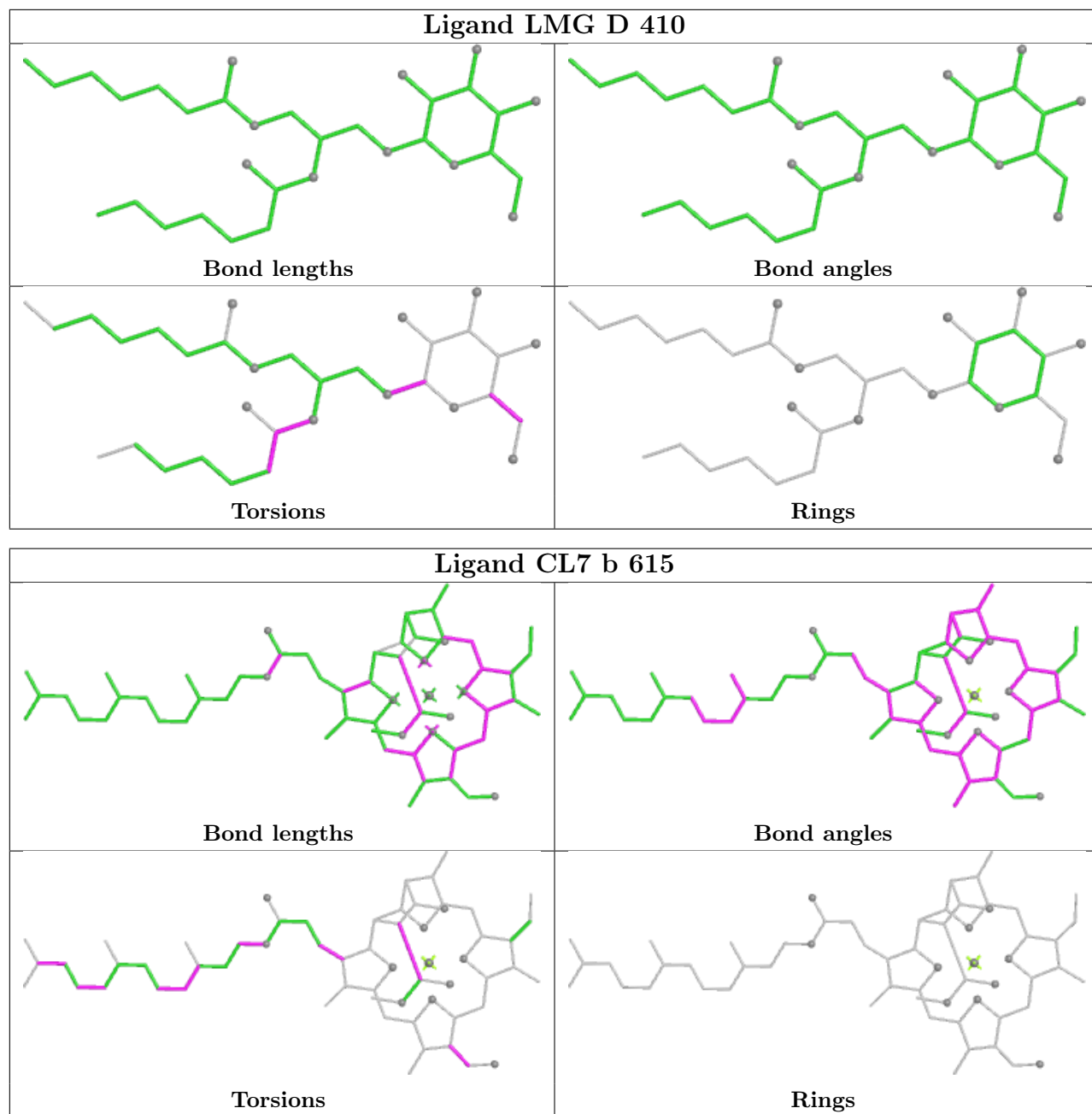


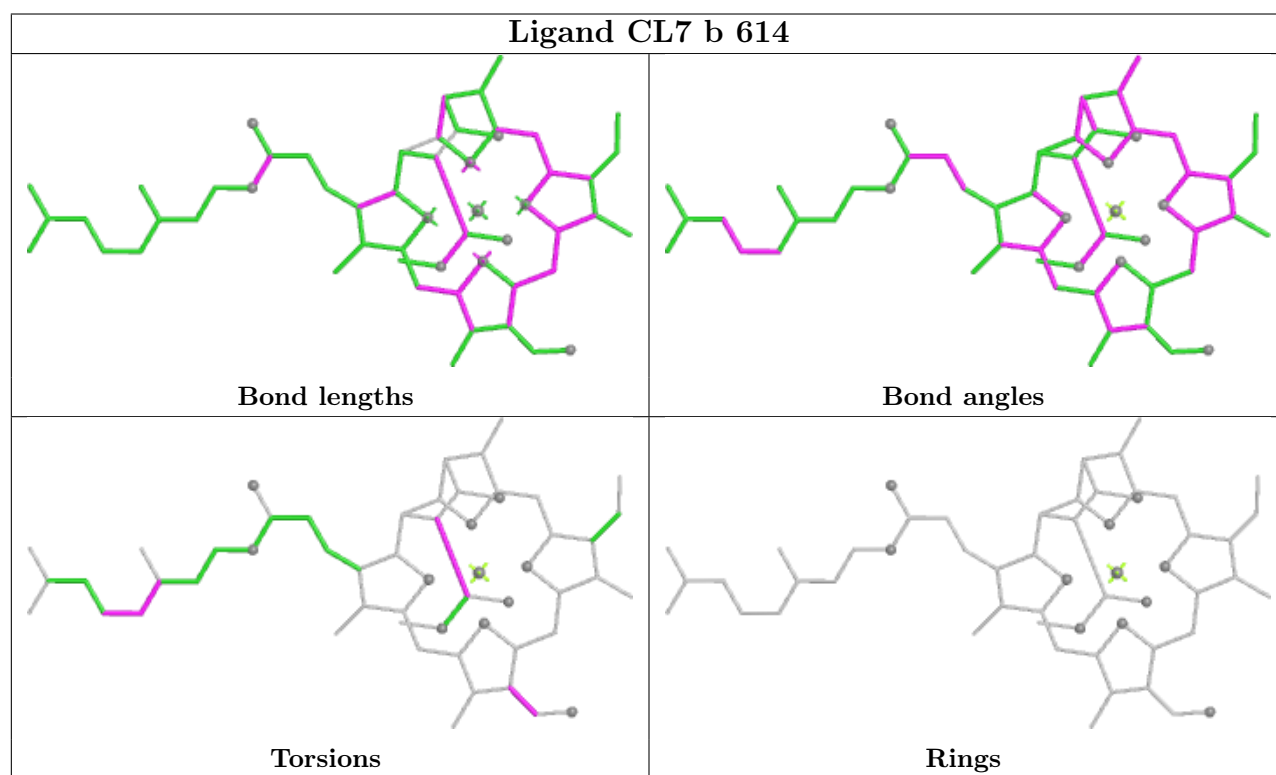
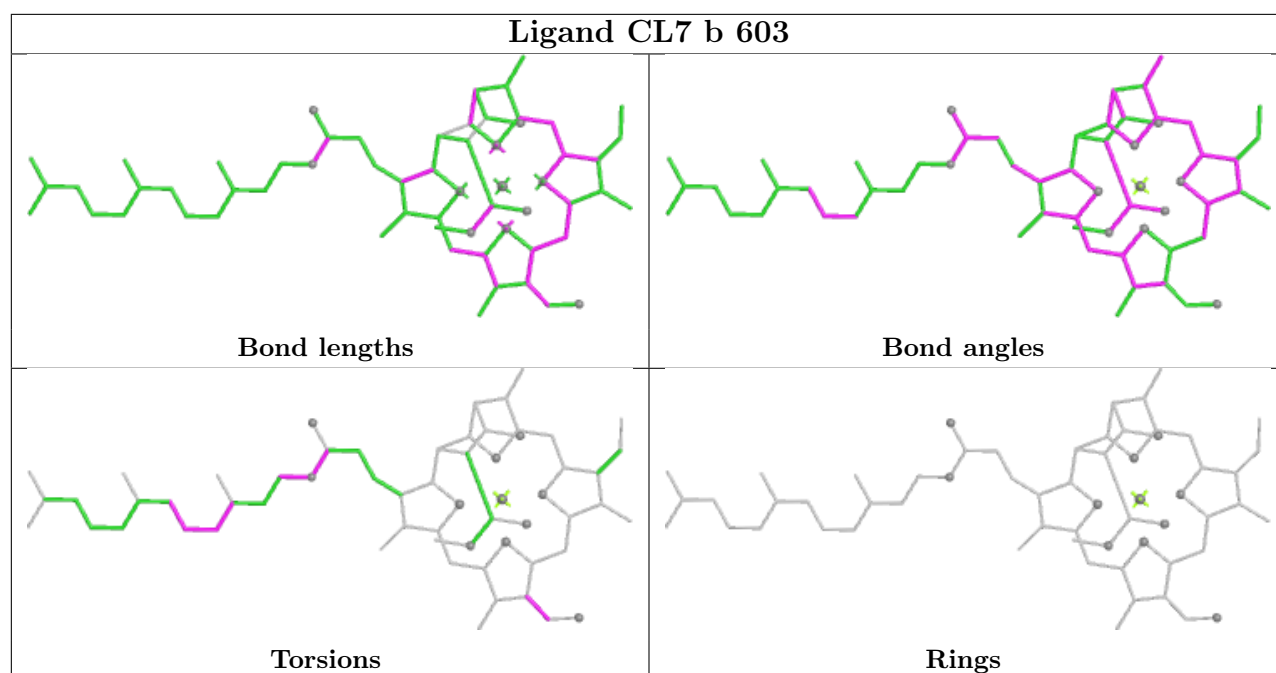
Ligand 8CT c 515

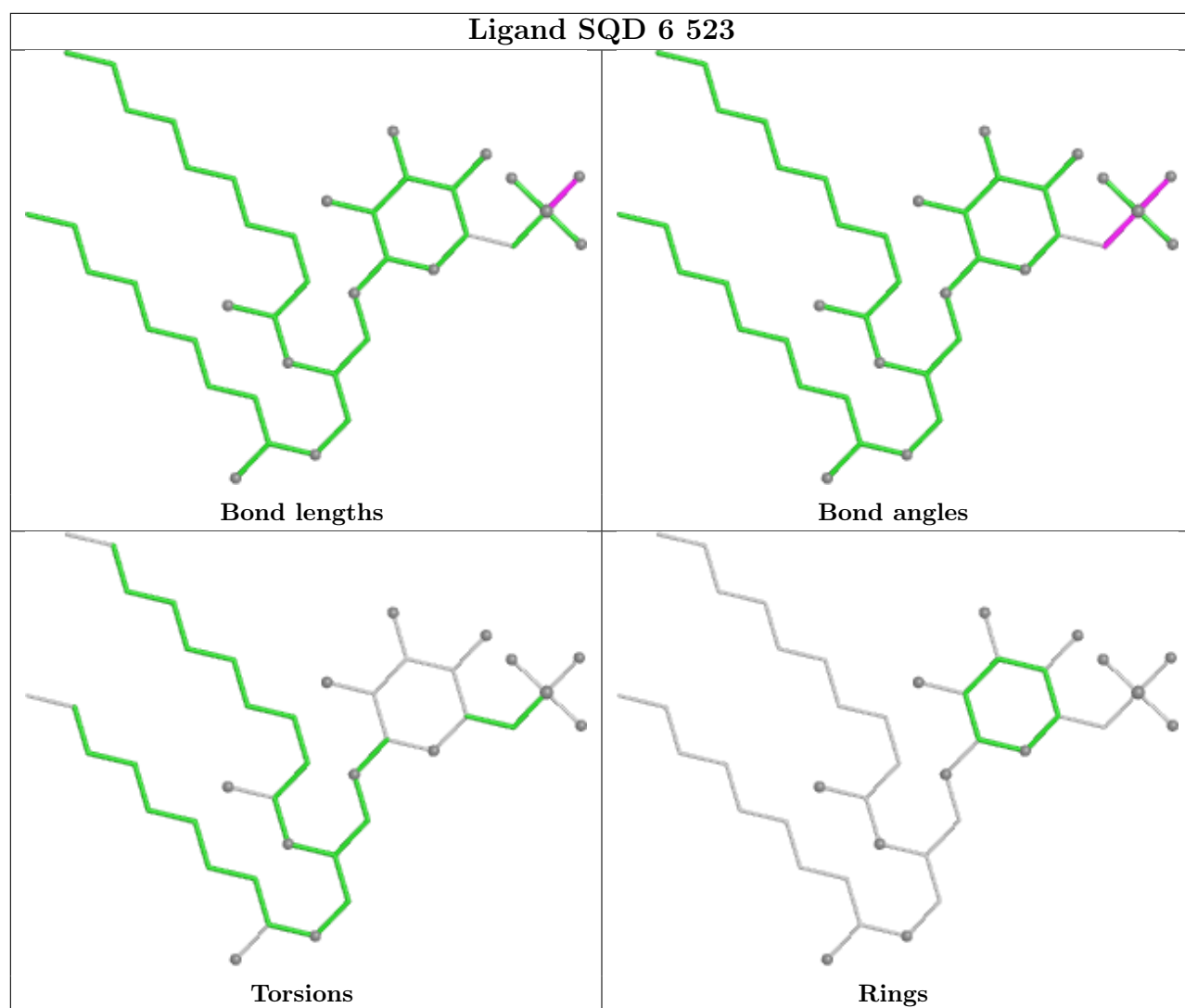




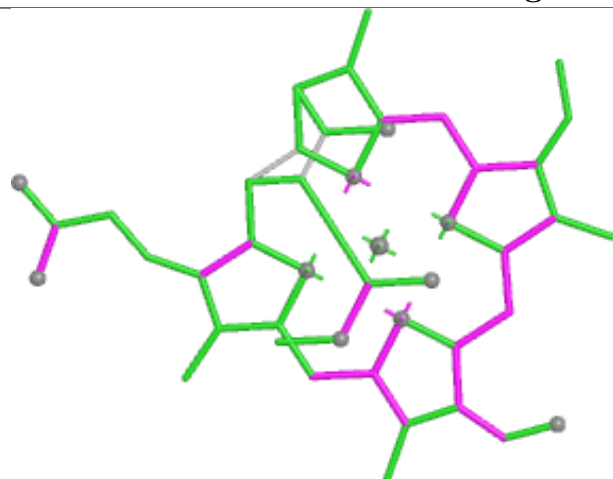




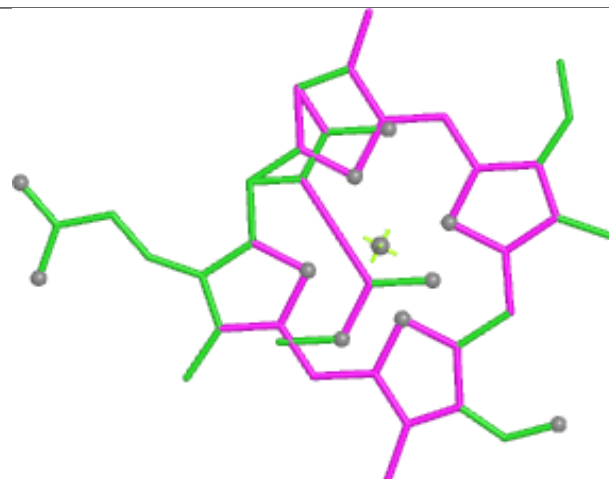




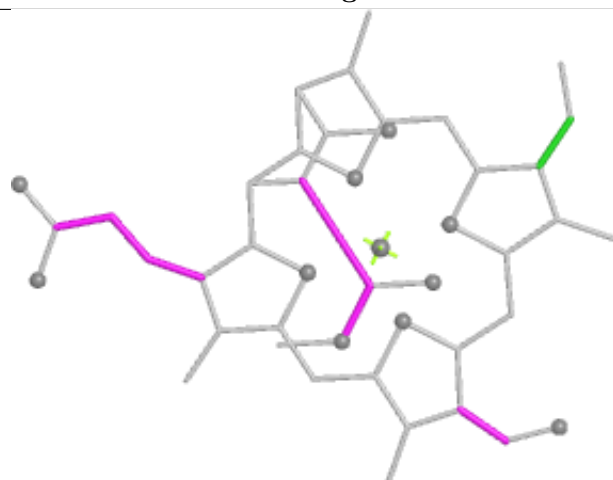
Ligand CL7 4 410



Bond lengths



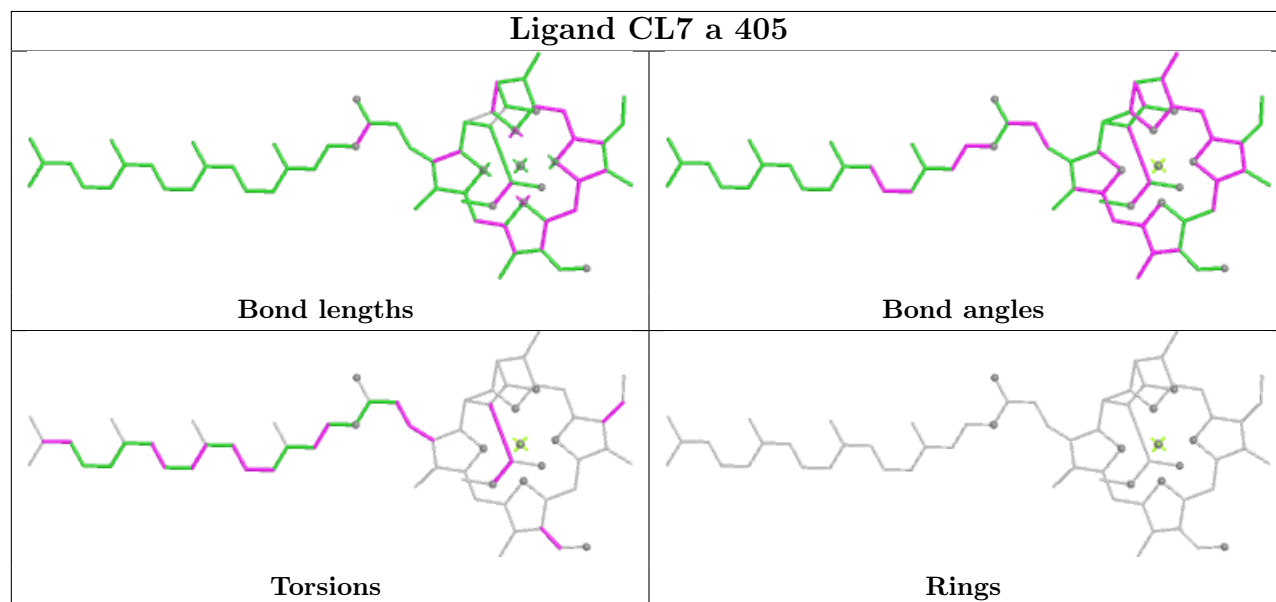
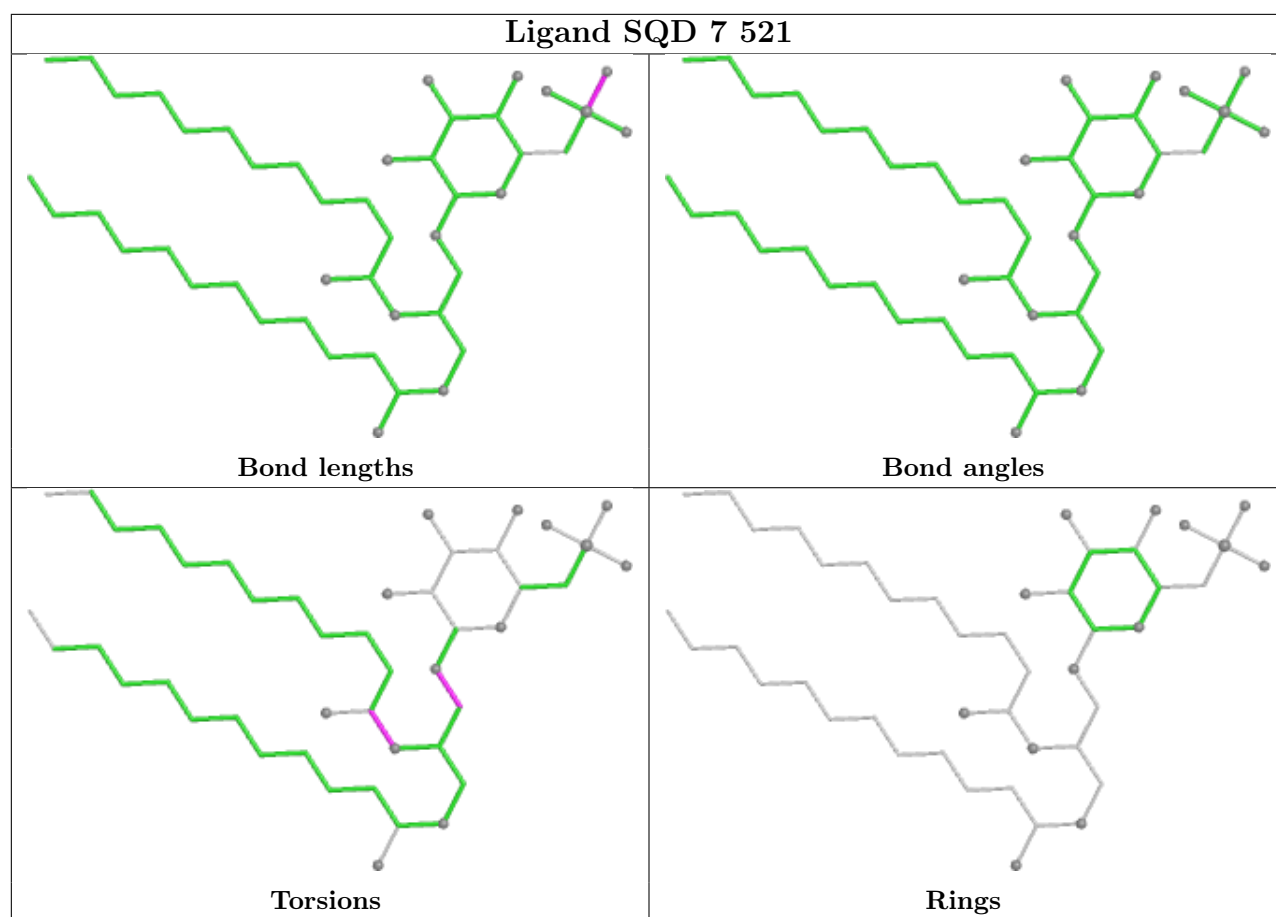
Bond angles

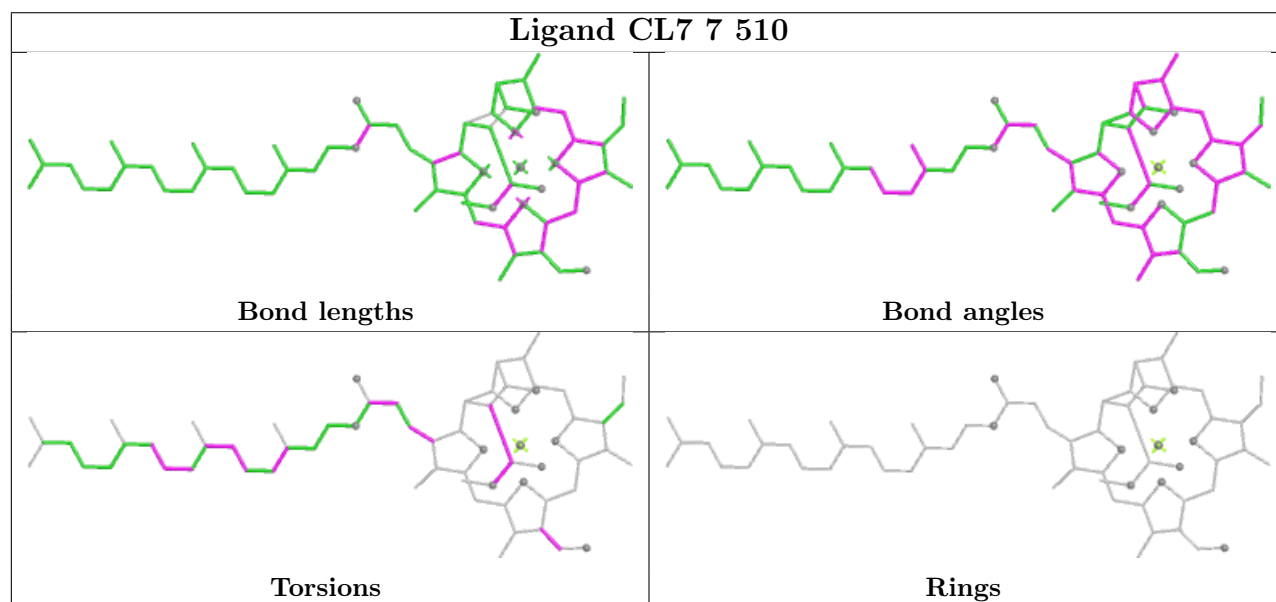
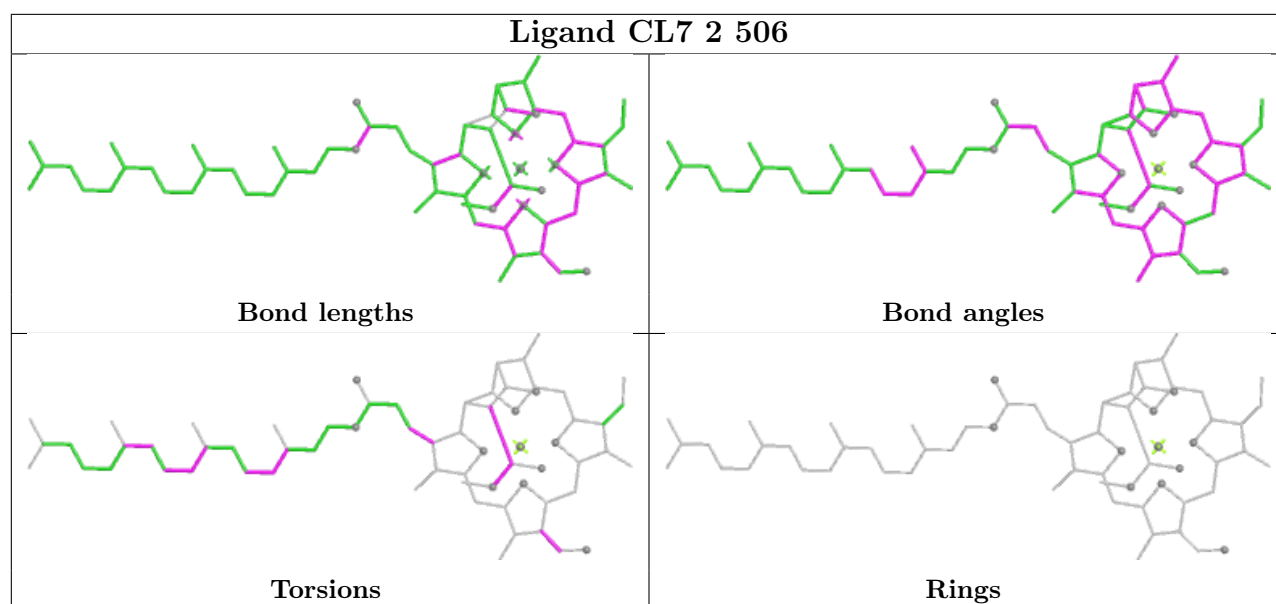


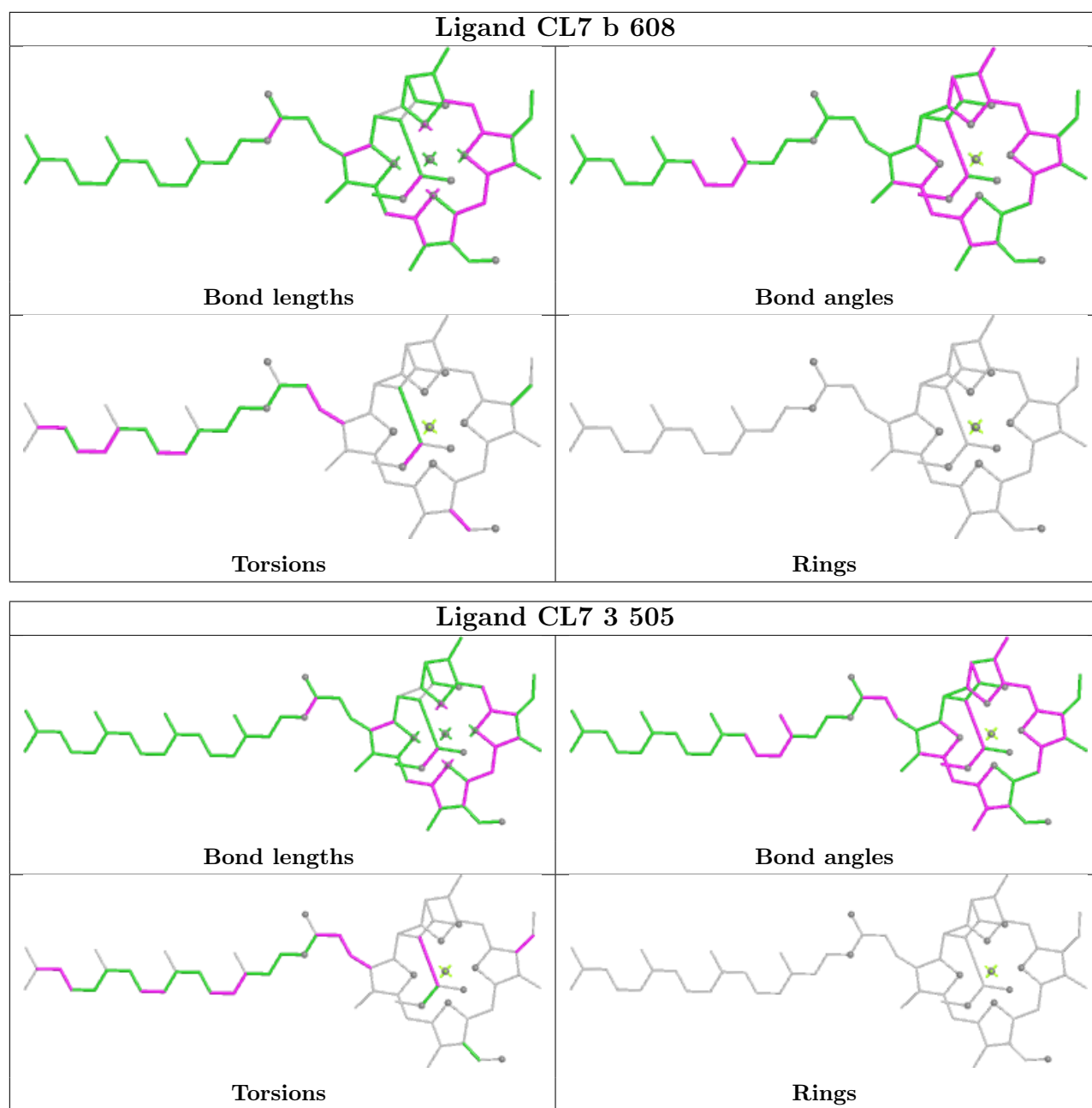
Torsions

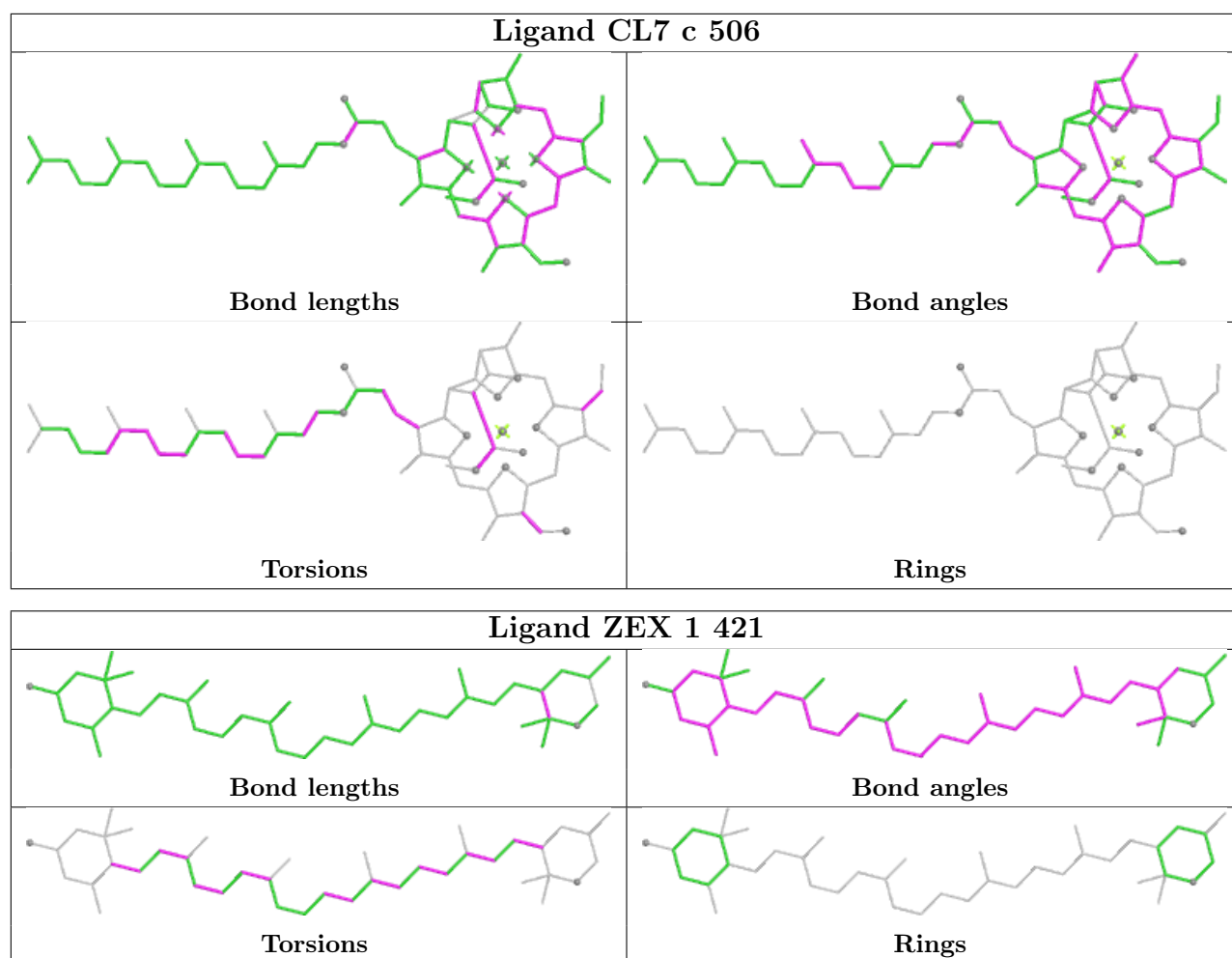


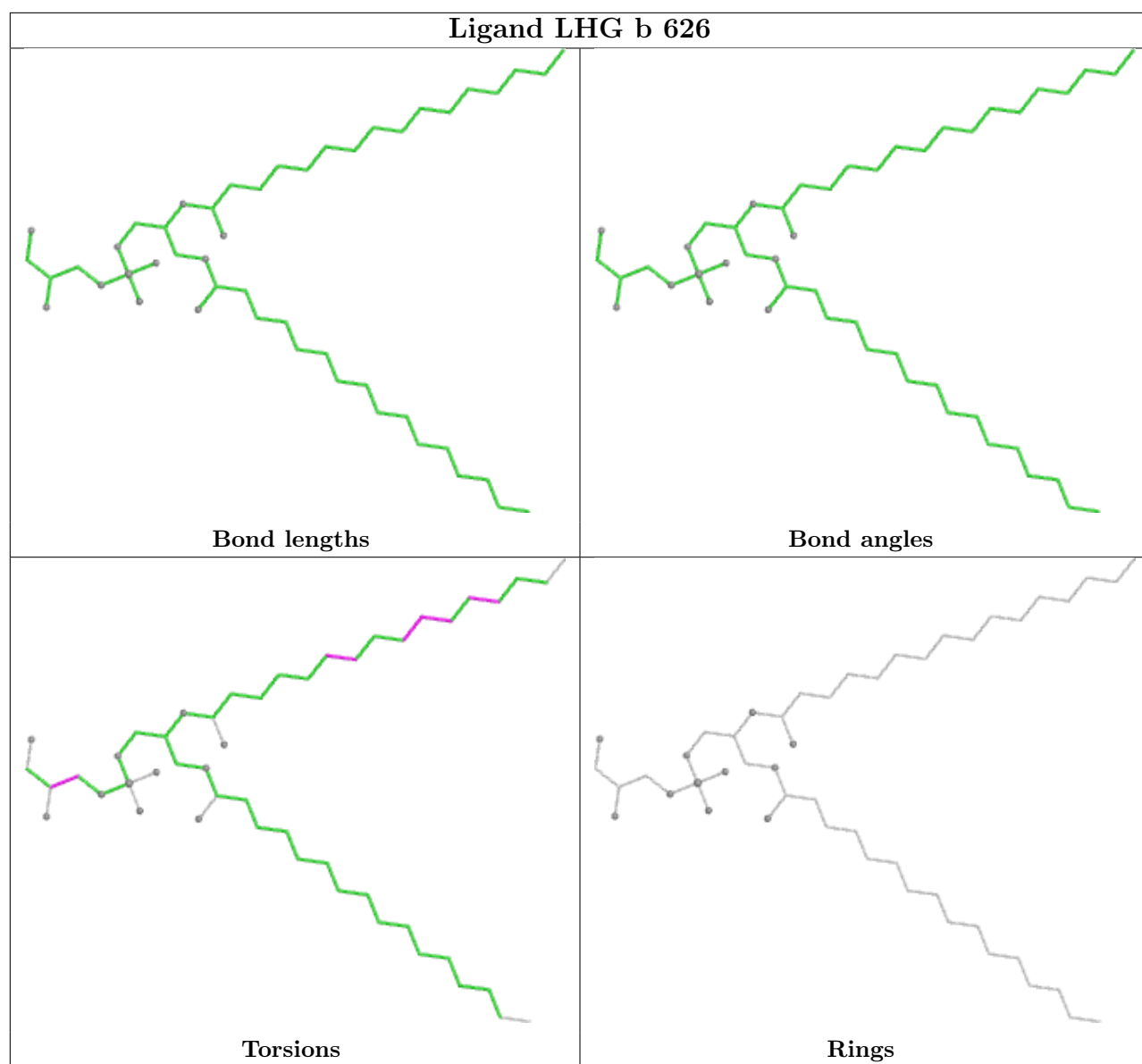
Rings



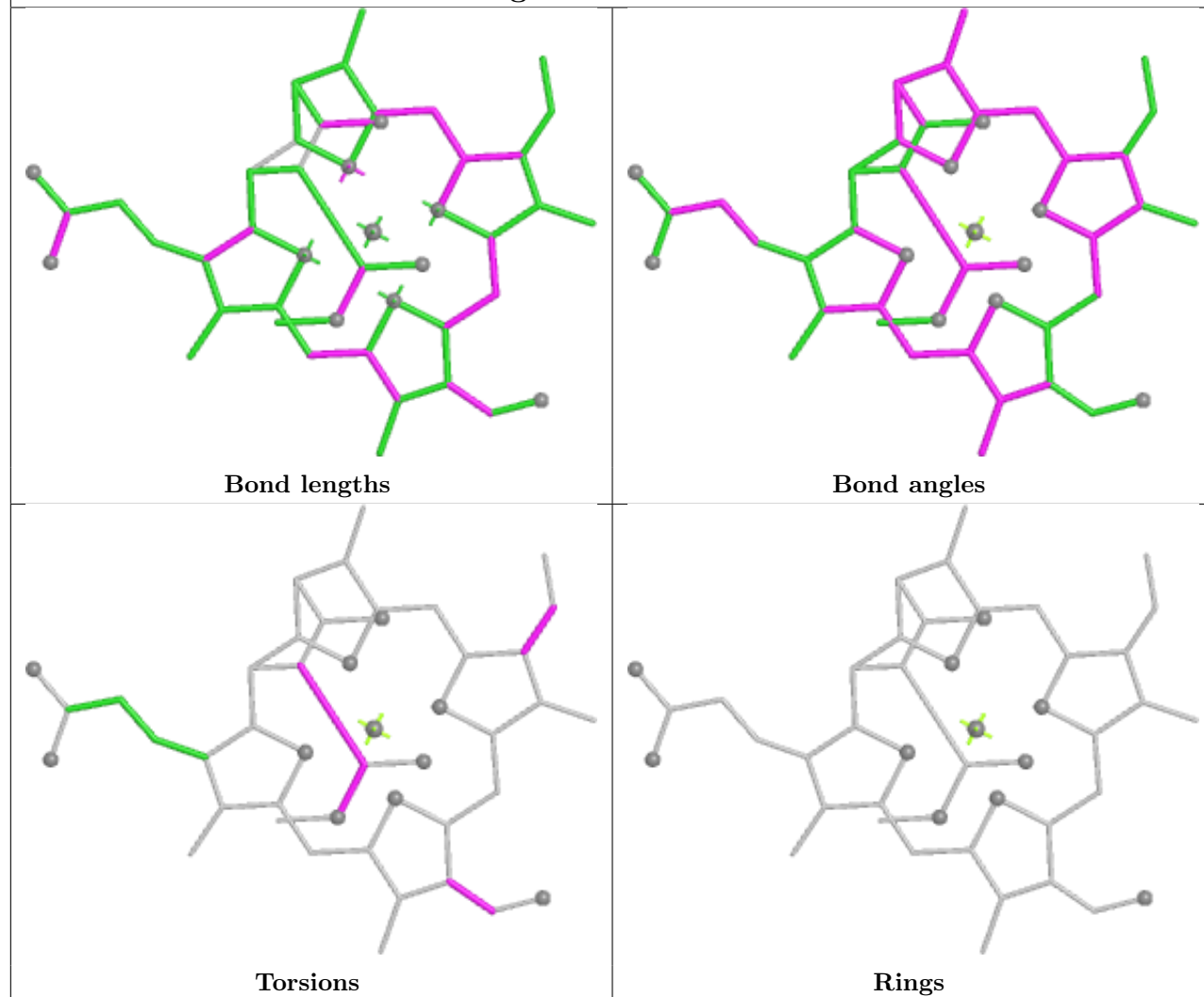




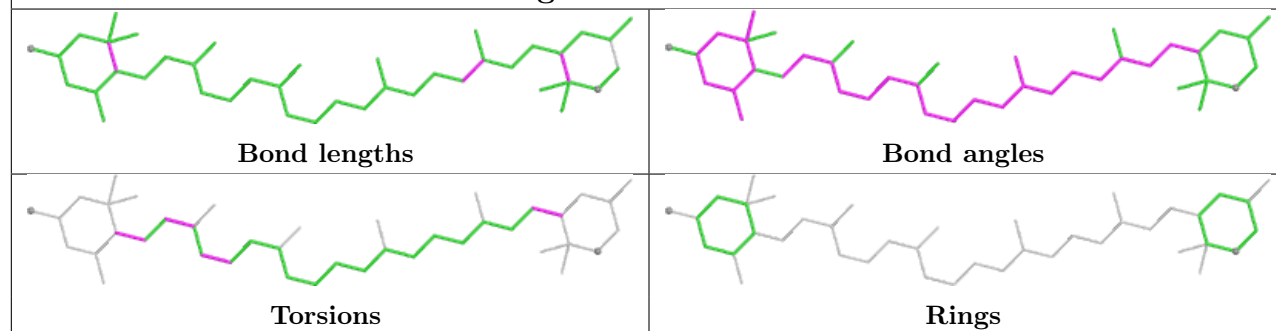


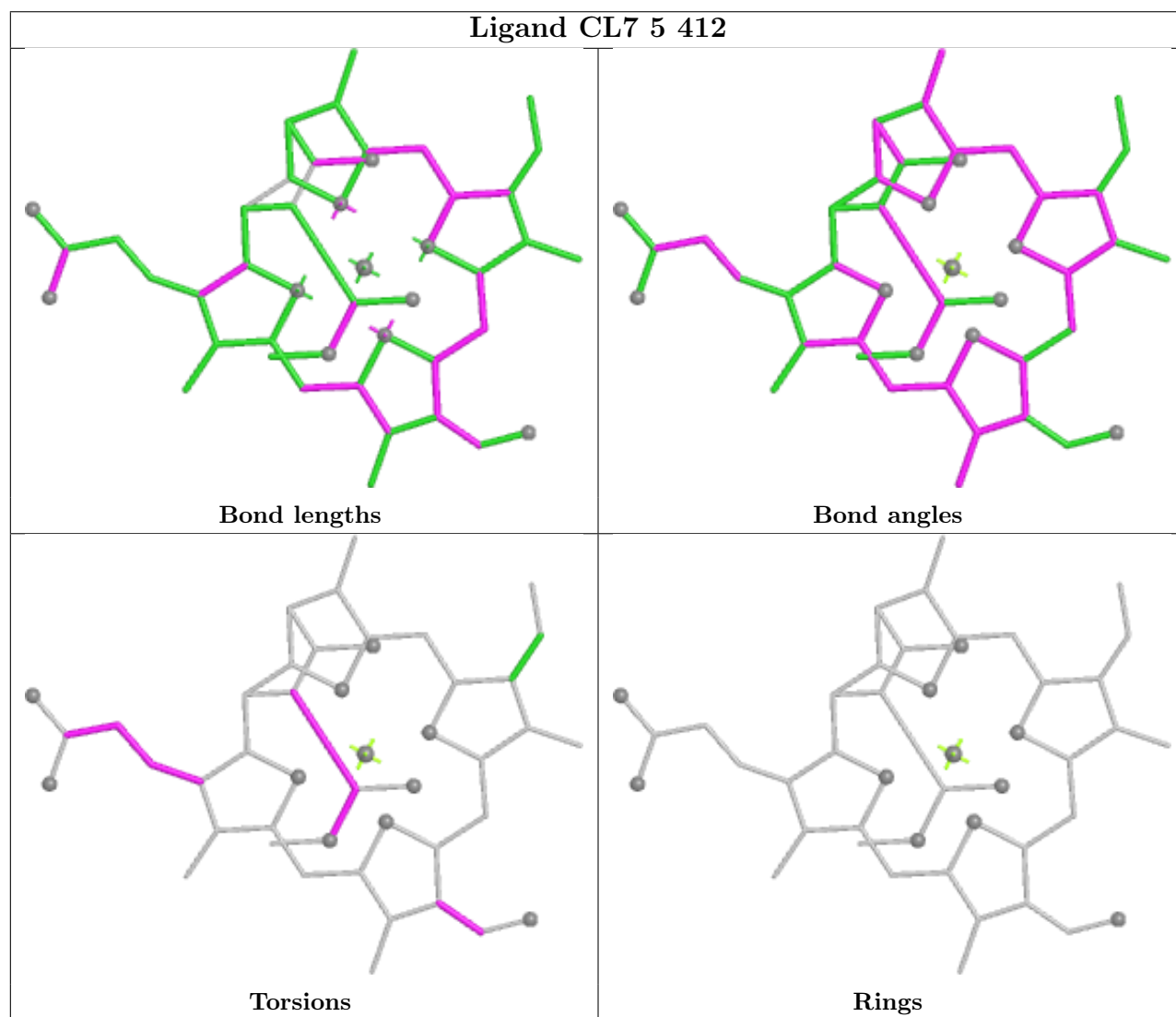
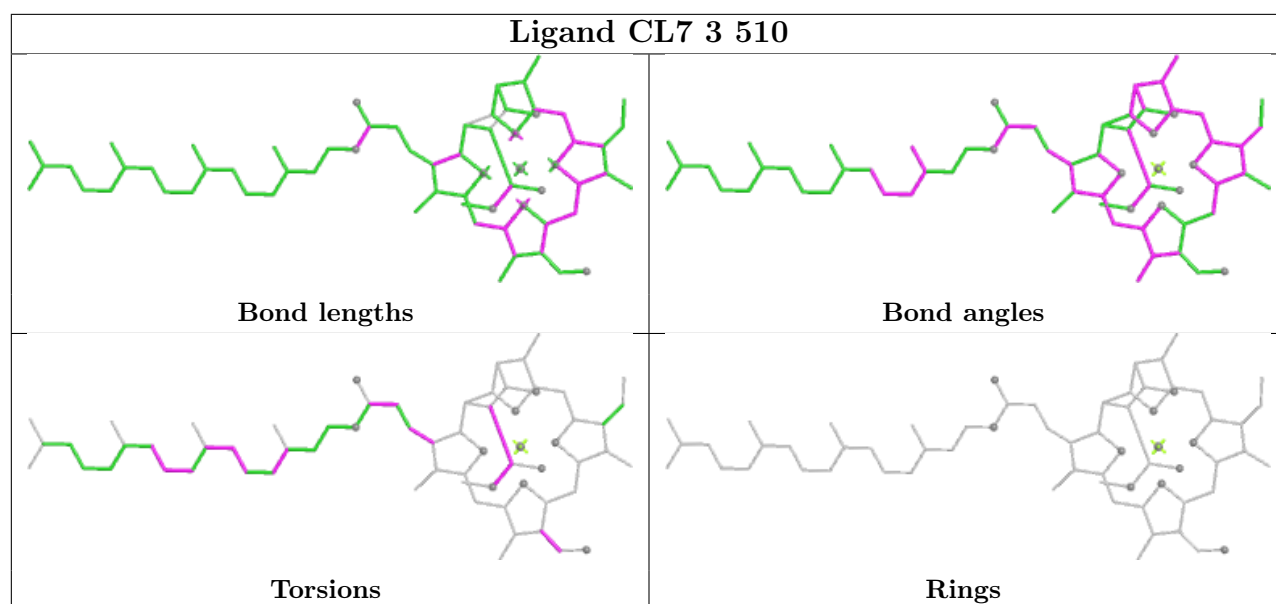


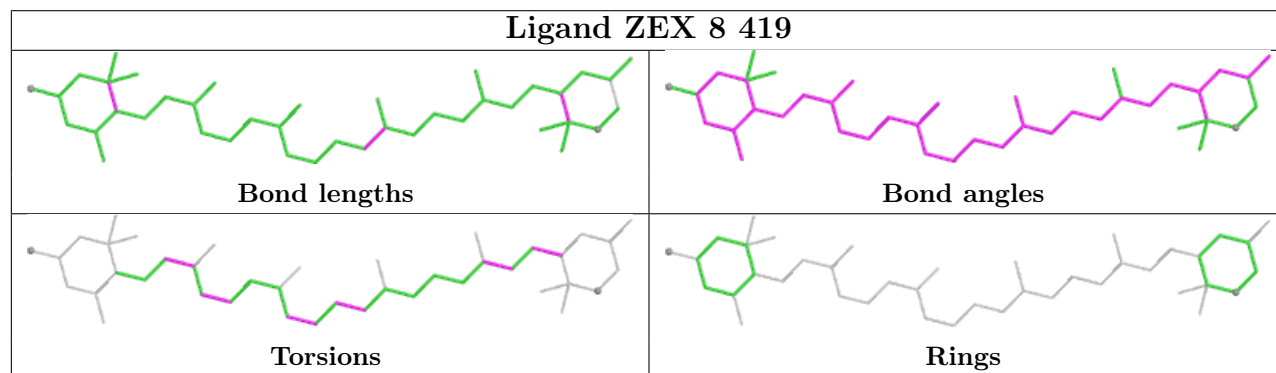
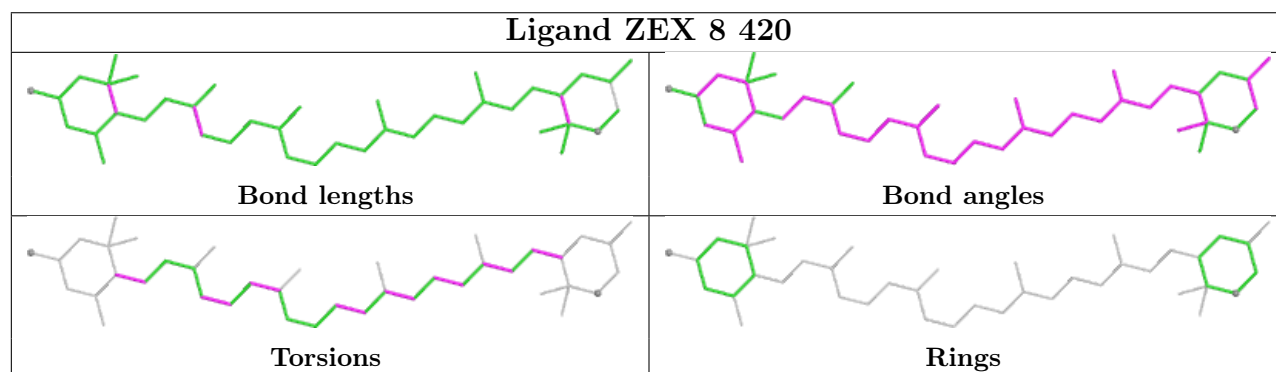
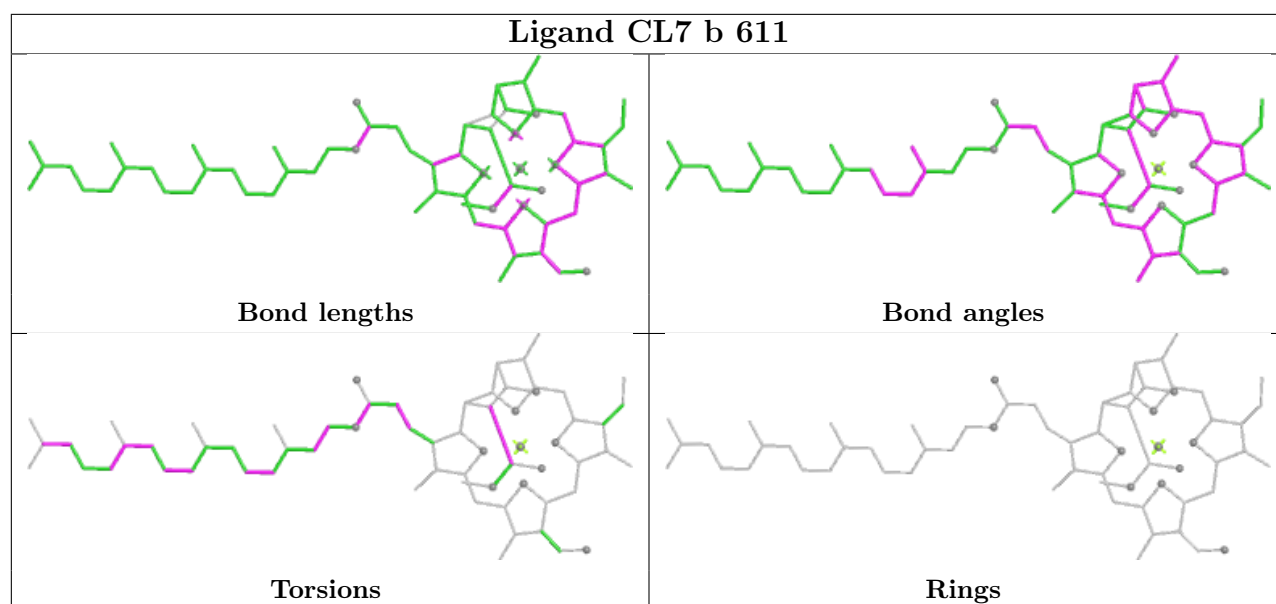
Ligand CL7 5 420



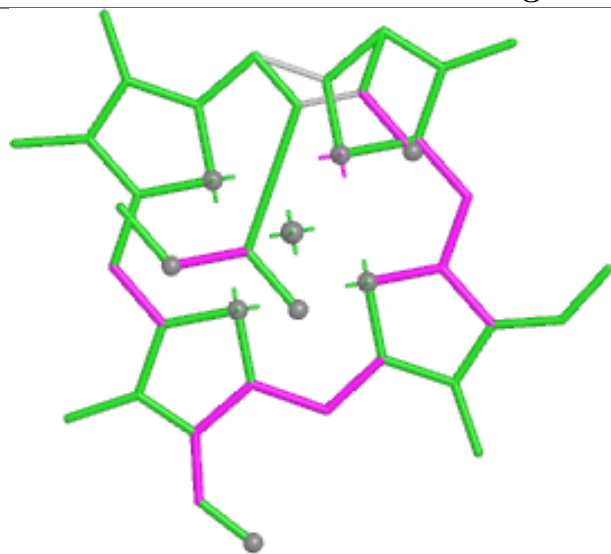
Ligand ZEX 2 521



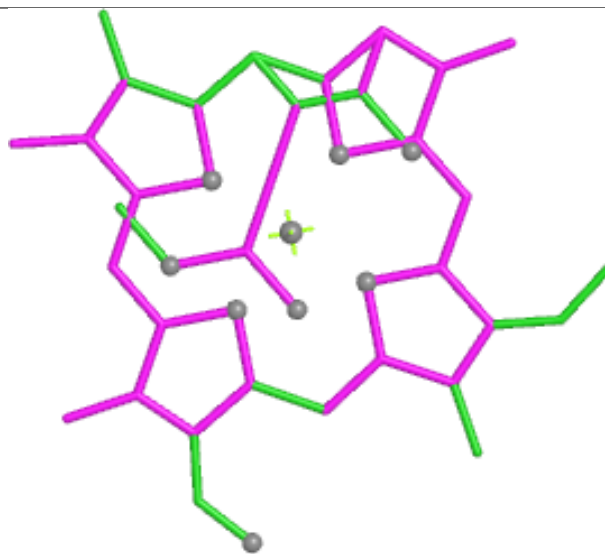




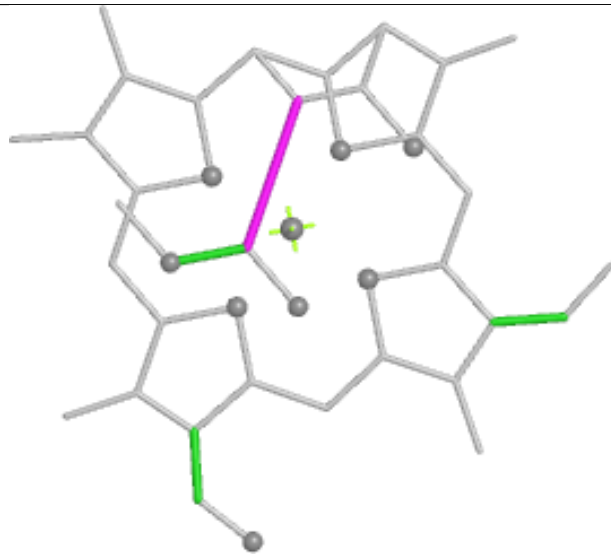
Ligand CL7 5 413



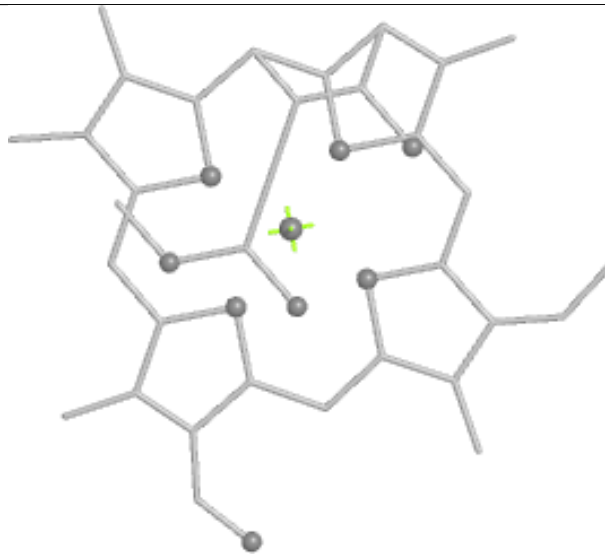
Bond lengths



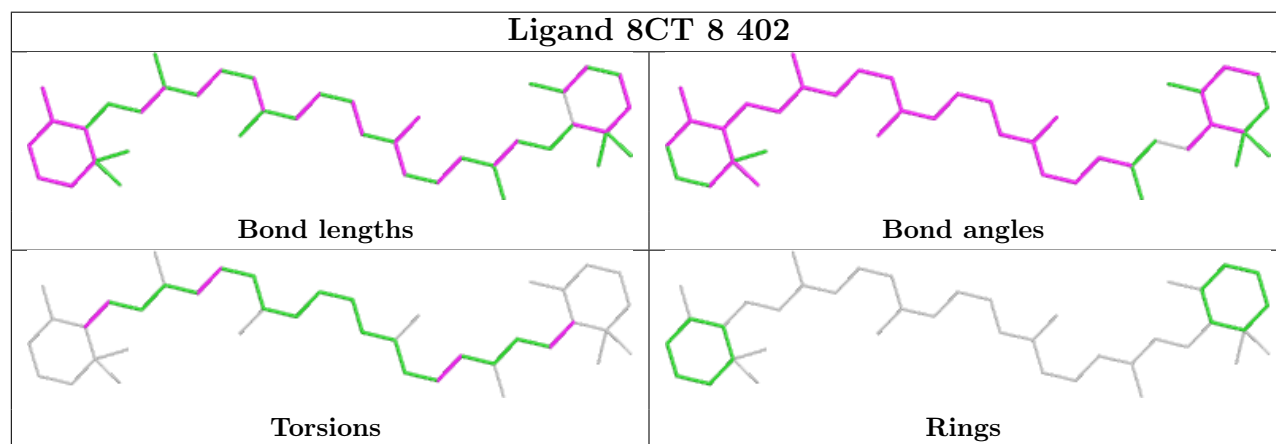
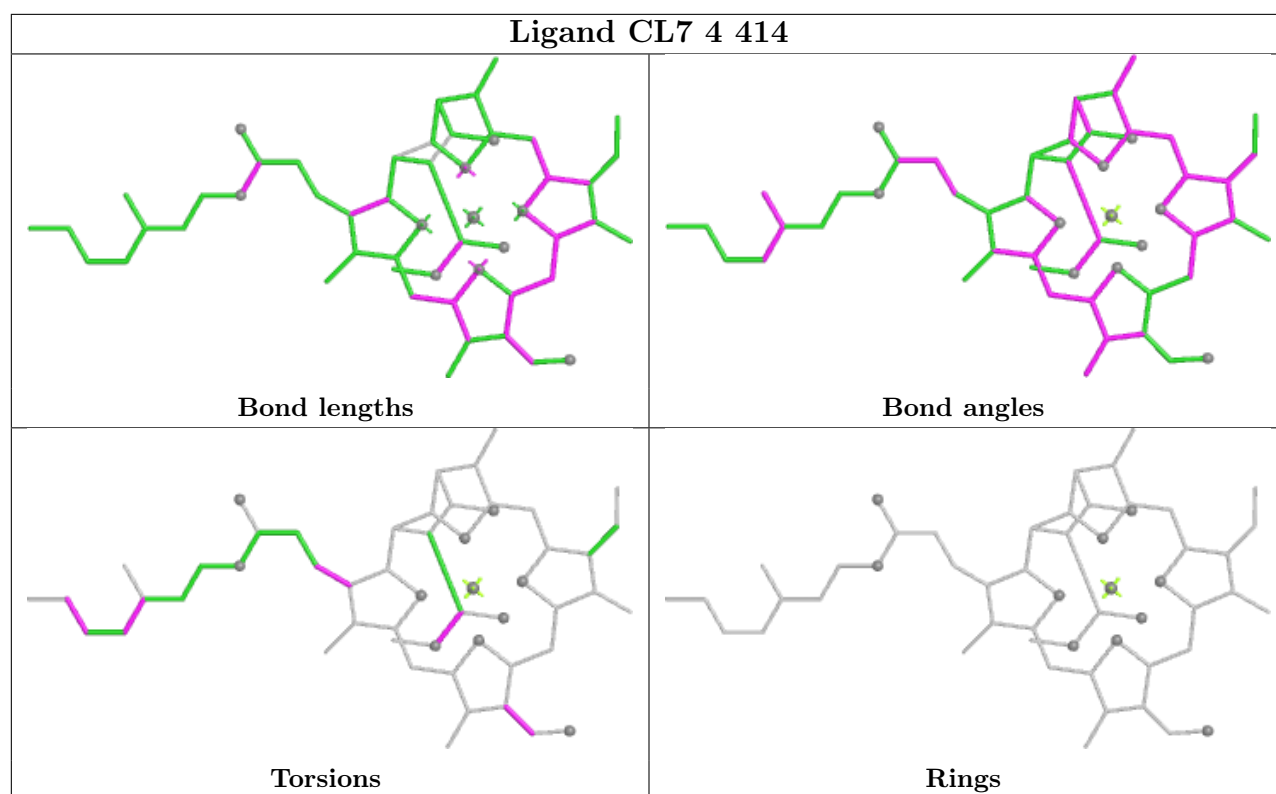
Bond angles

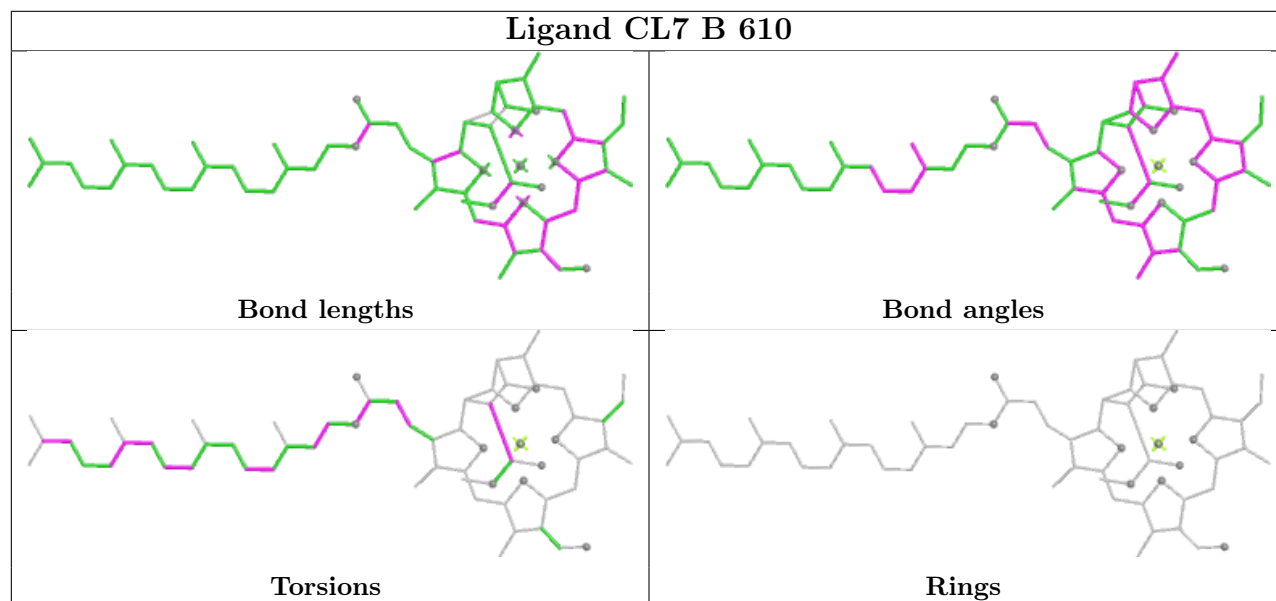
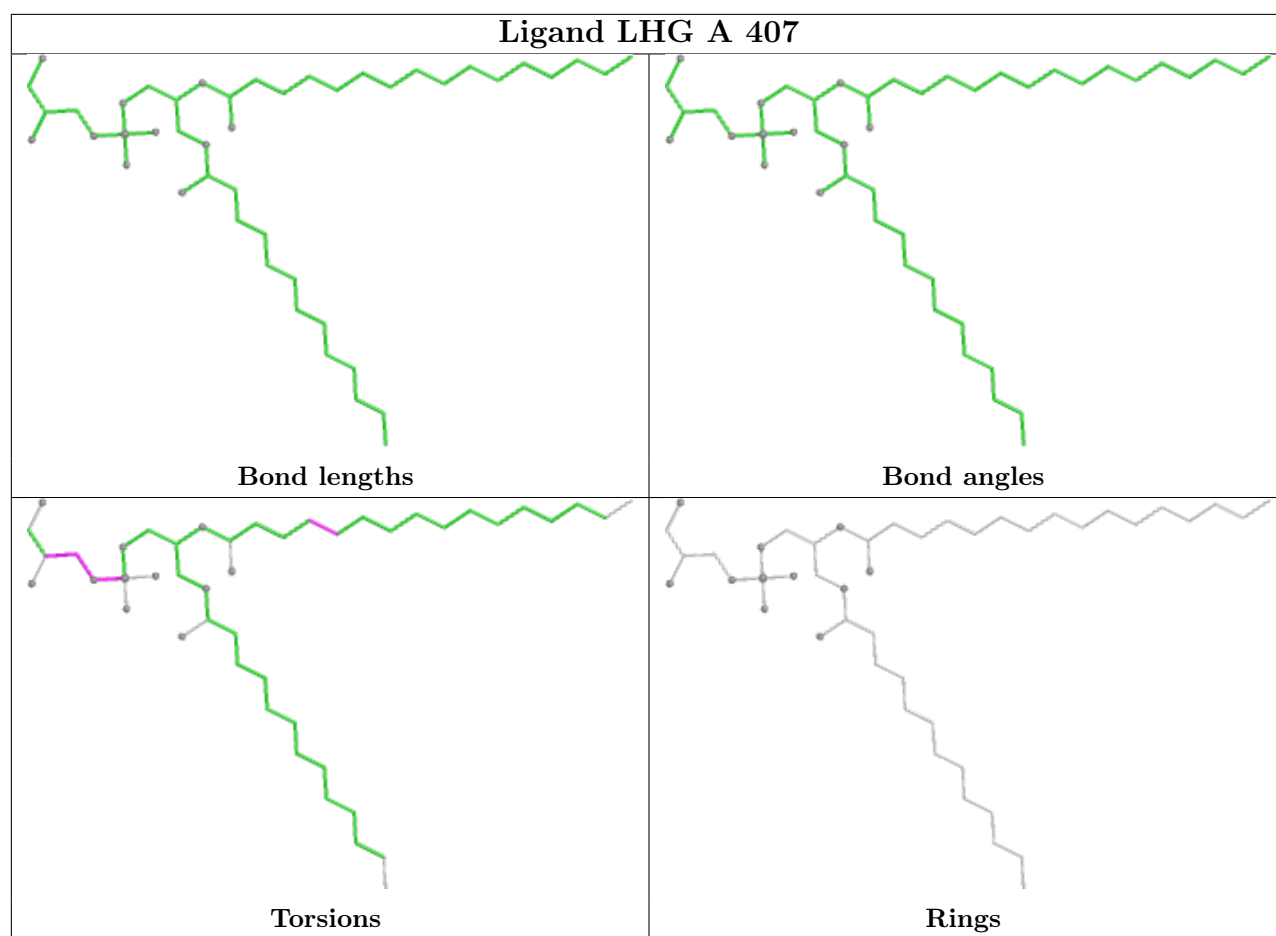


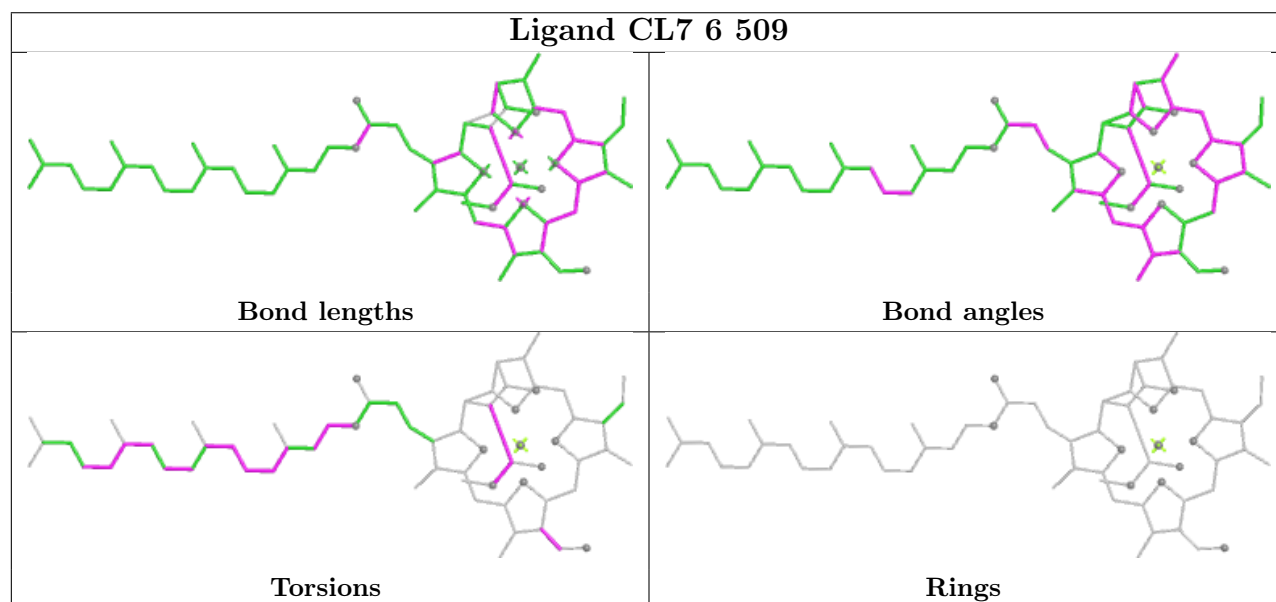
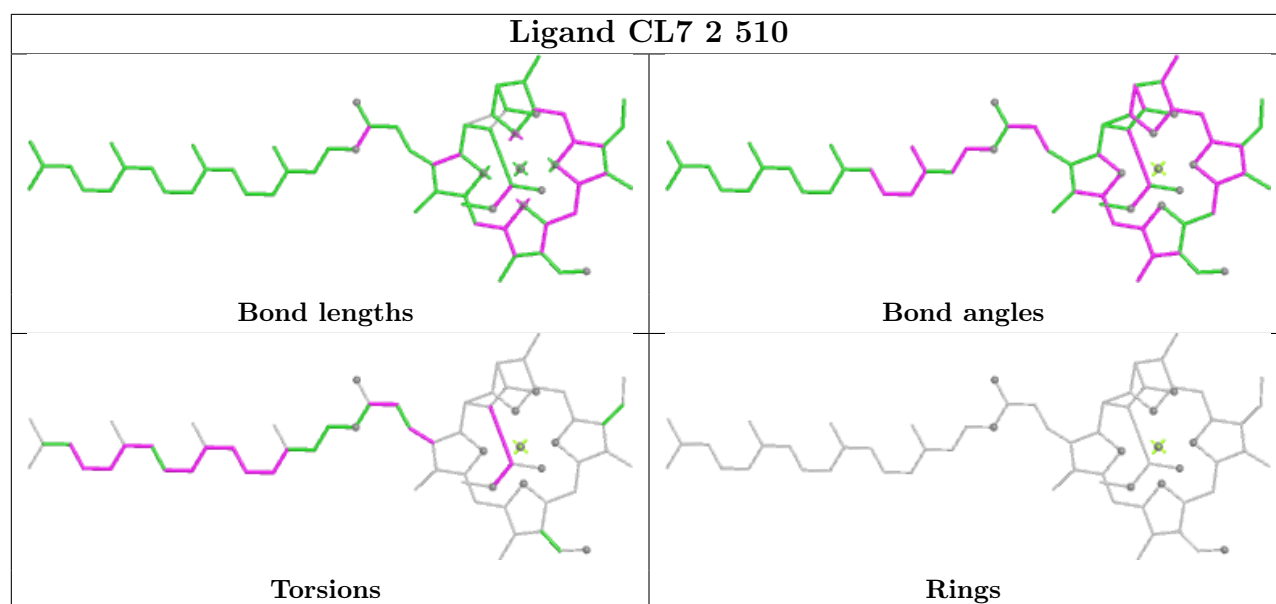
Torsions



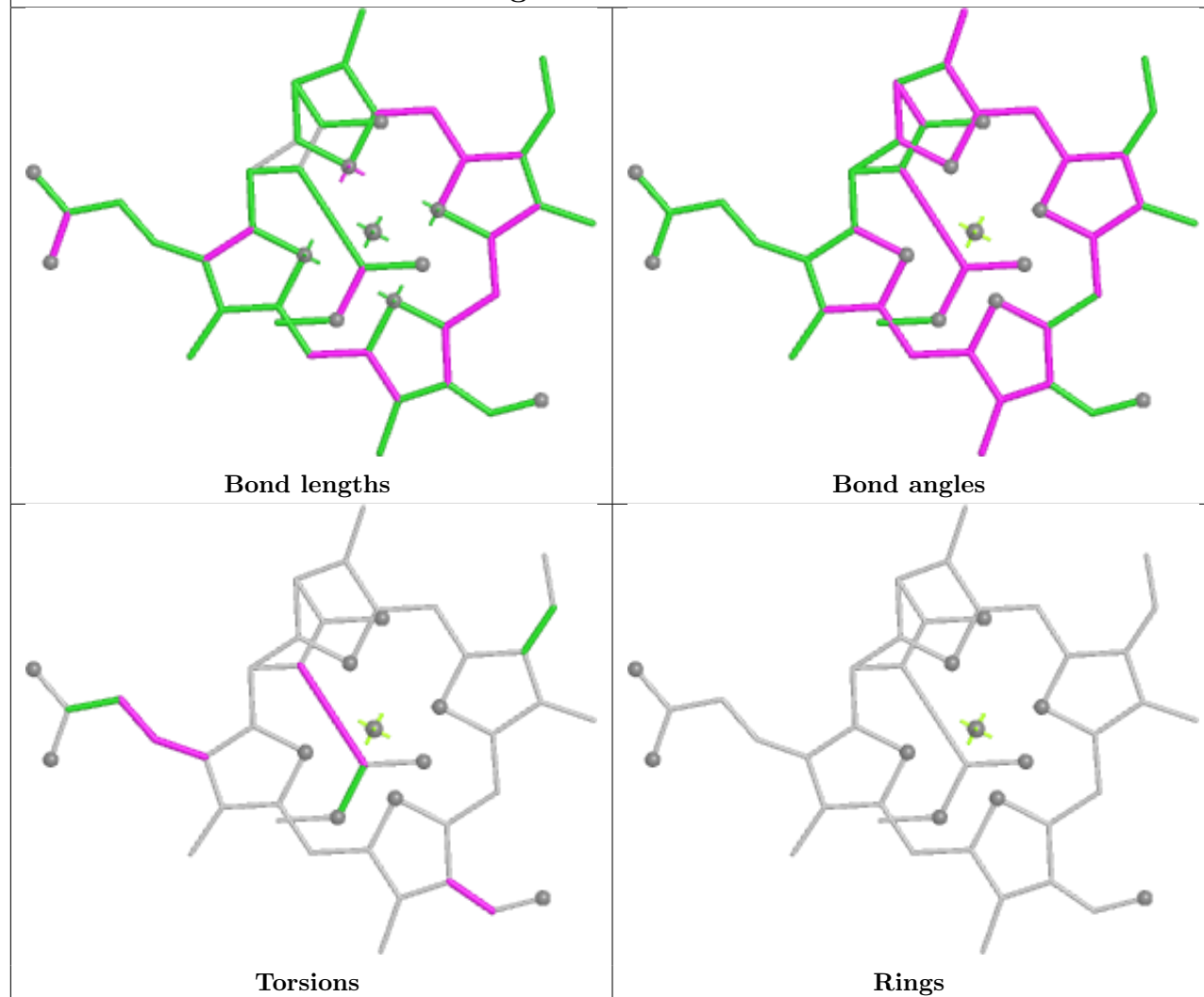
Rings



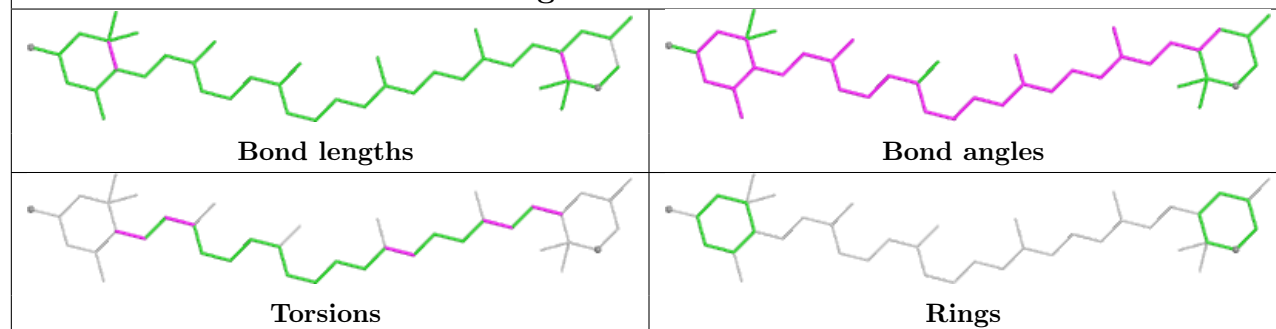


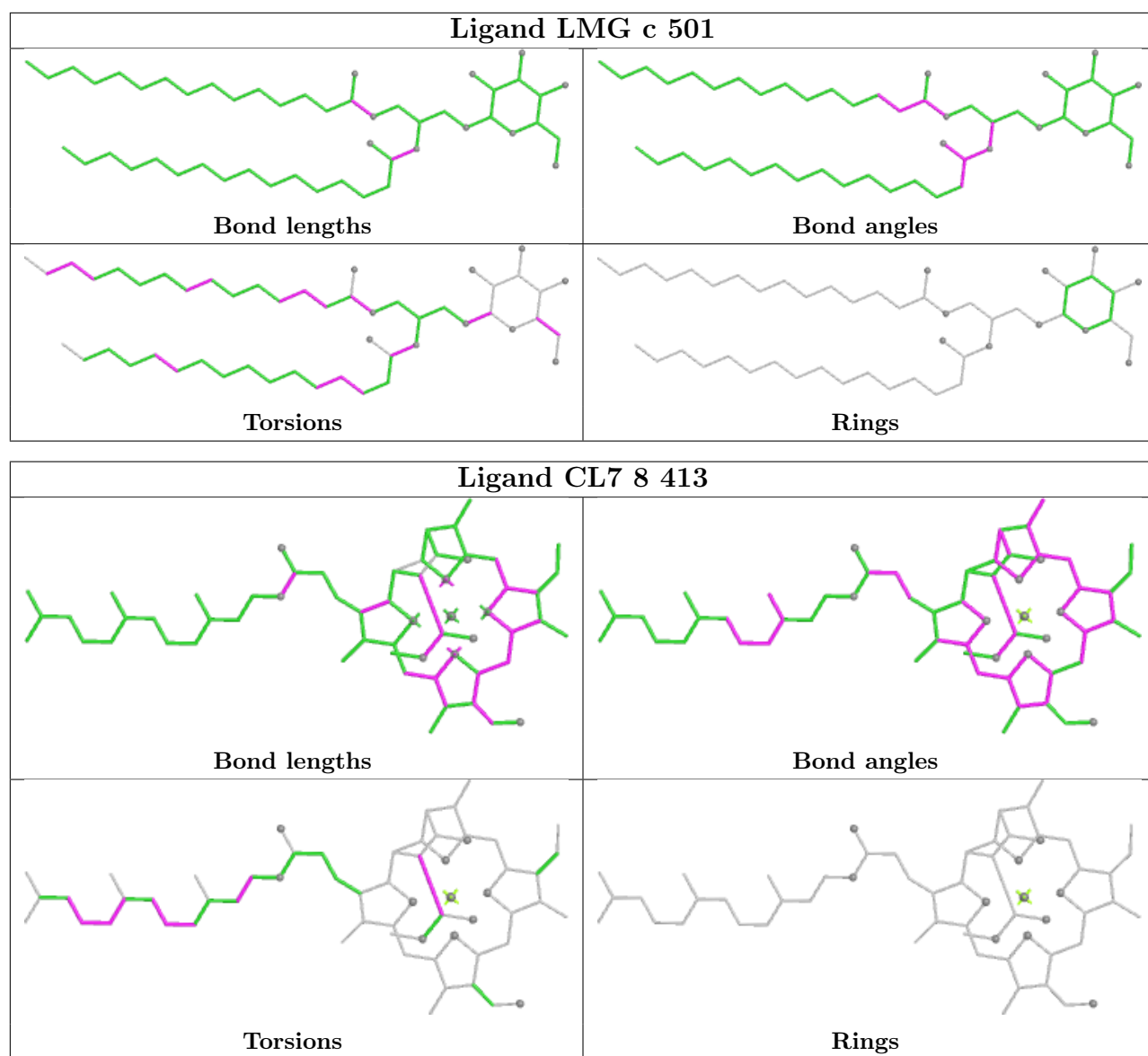


Ligand CL7 6 513

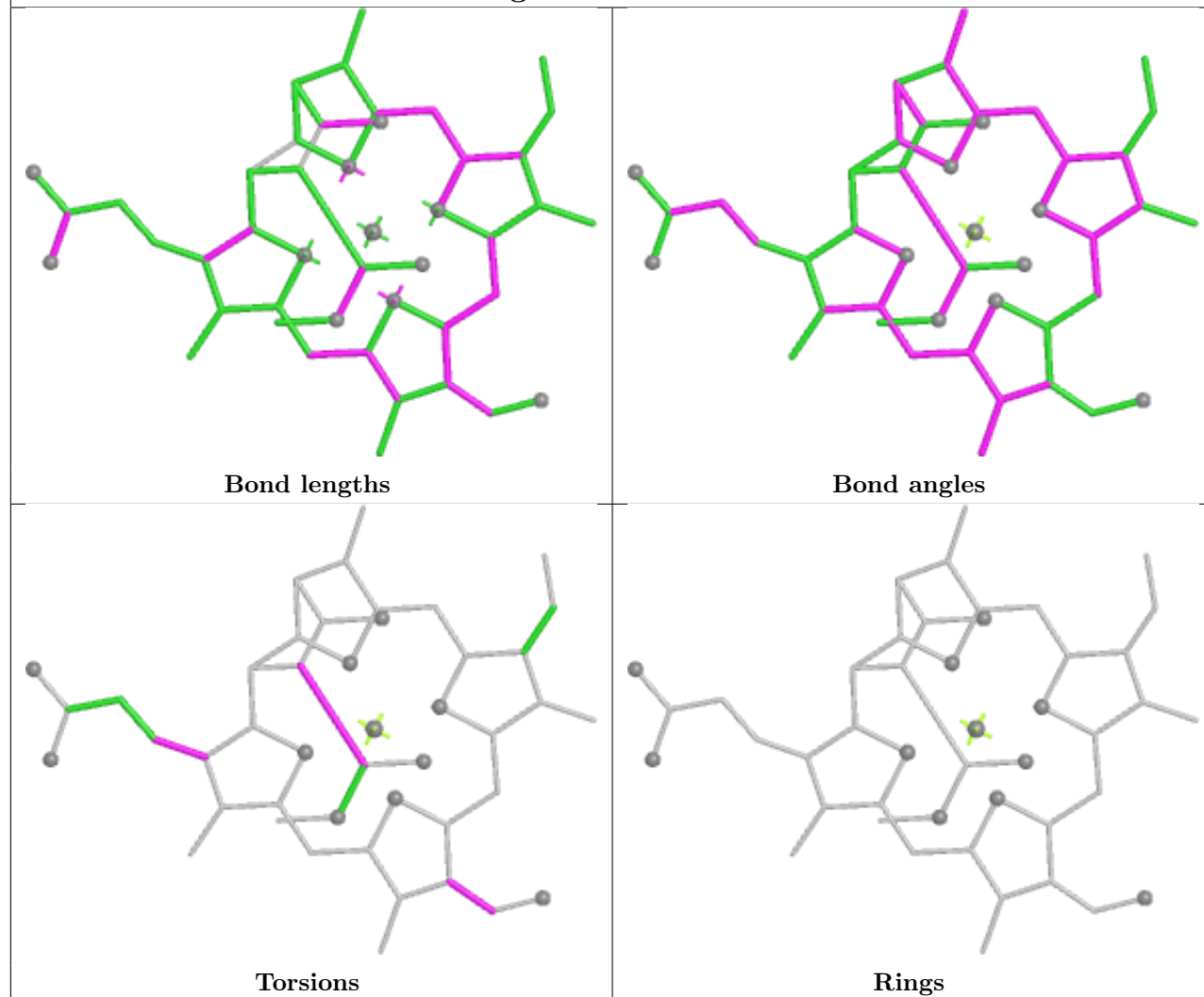


Ligand ZEX 7 520

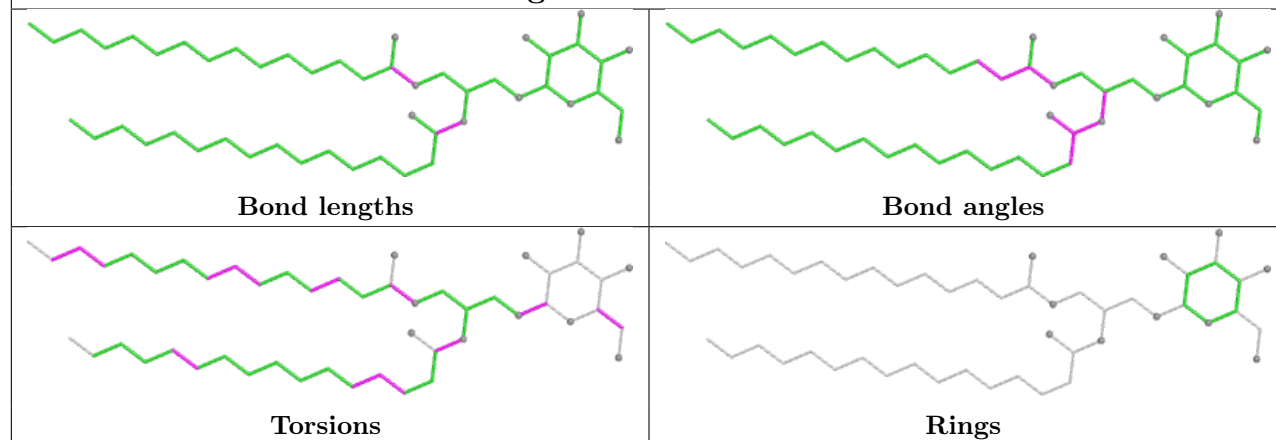


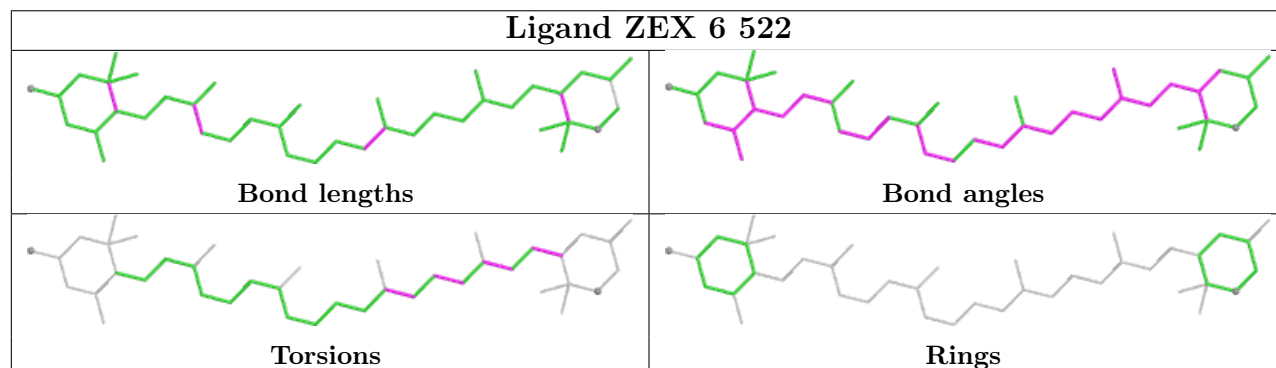
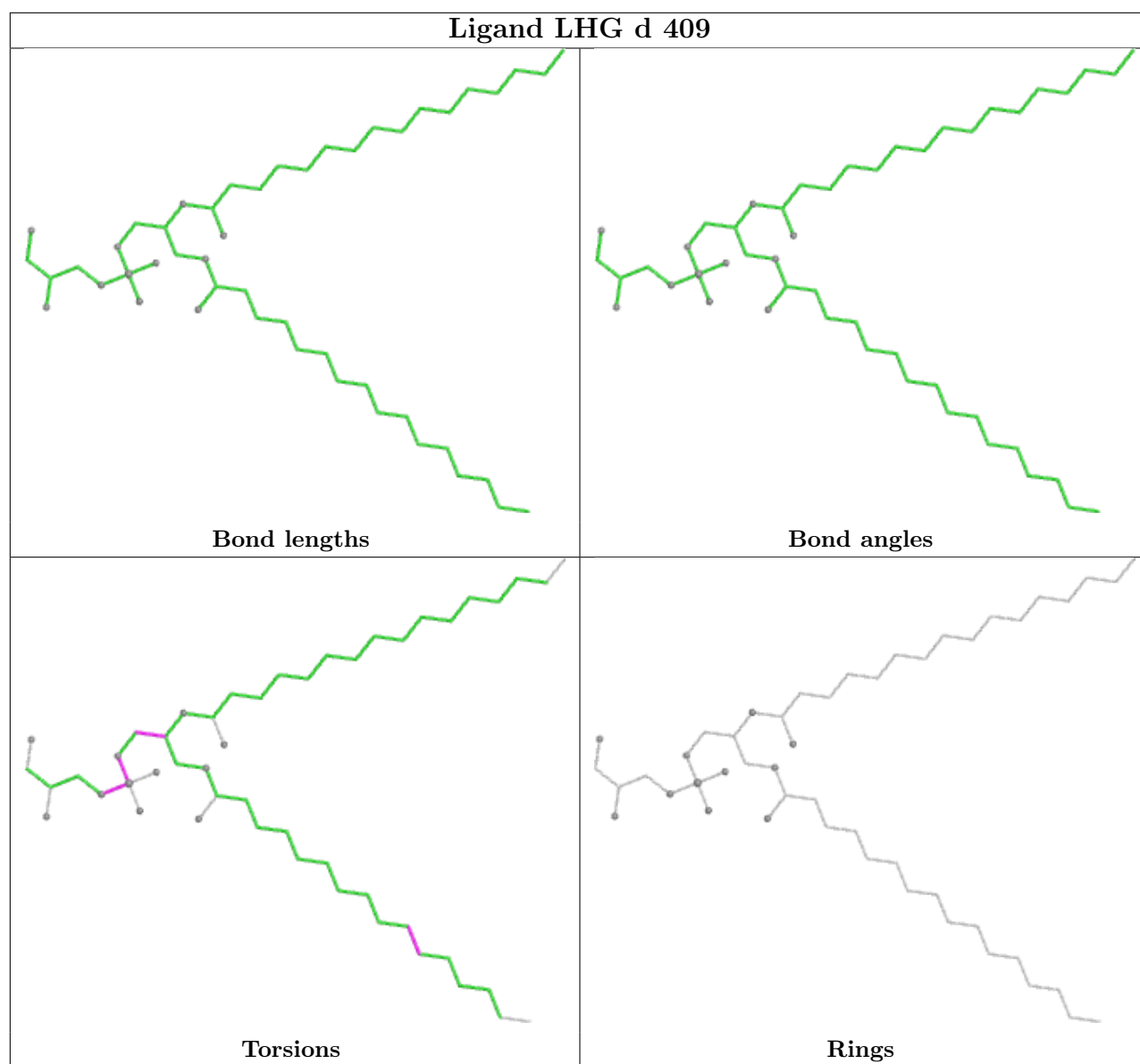


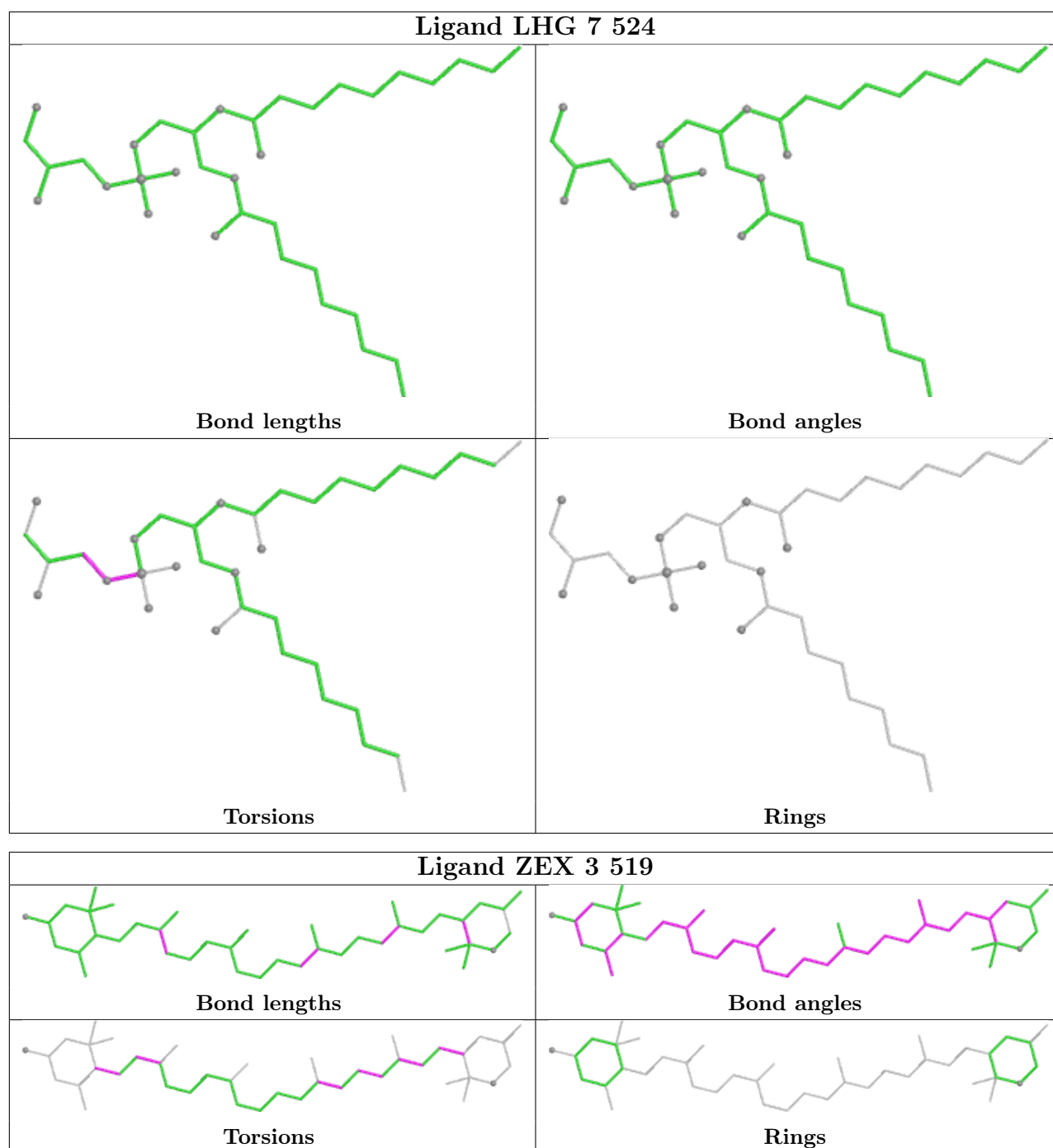
Ligand CL7 6 515



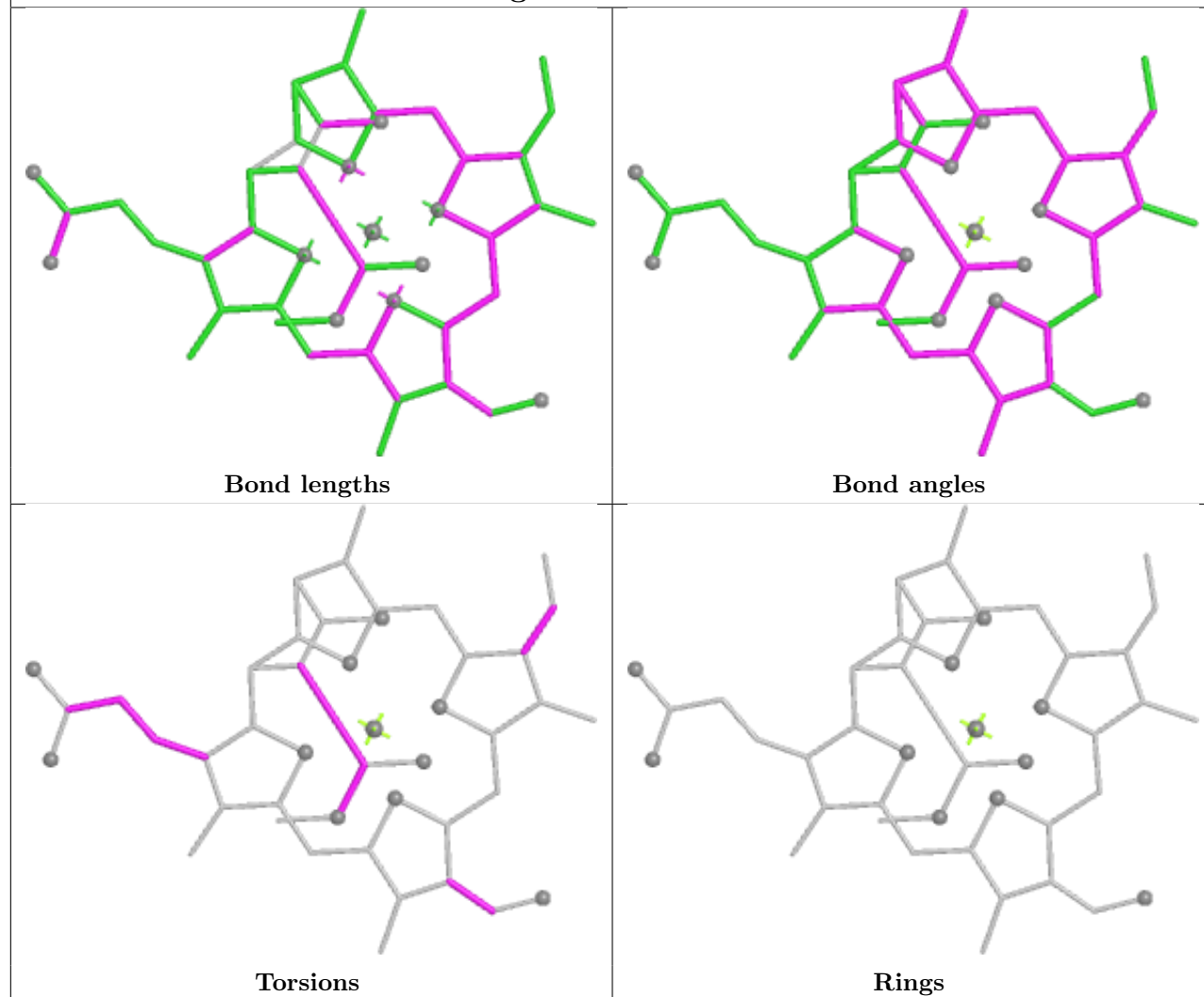
Ligand LMG C 501



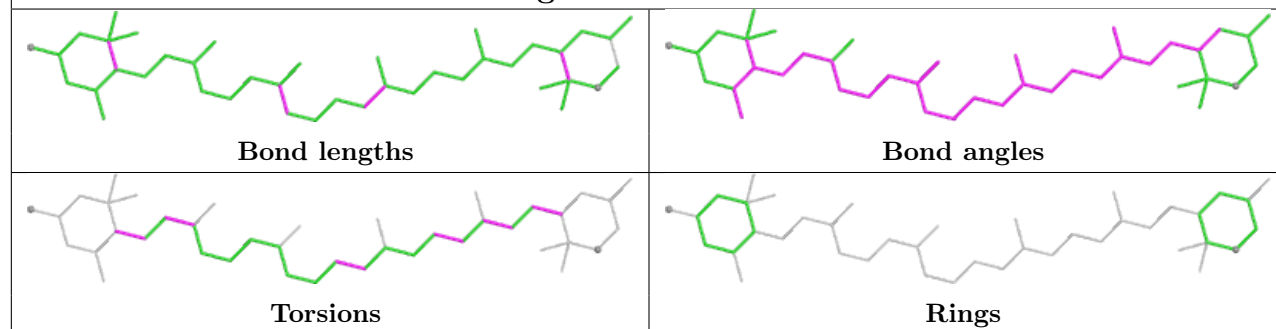




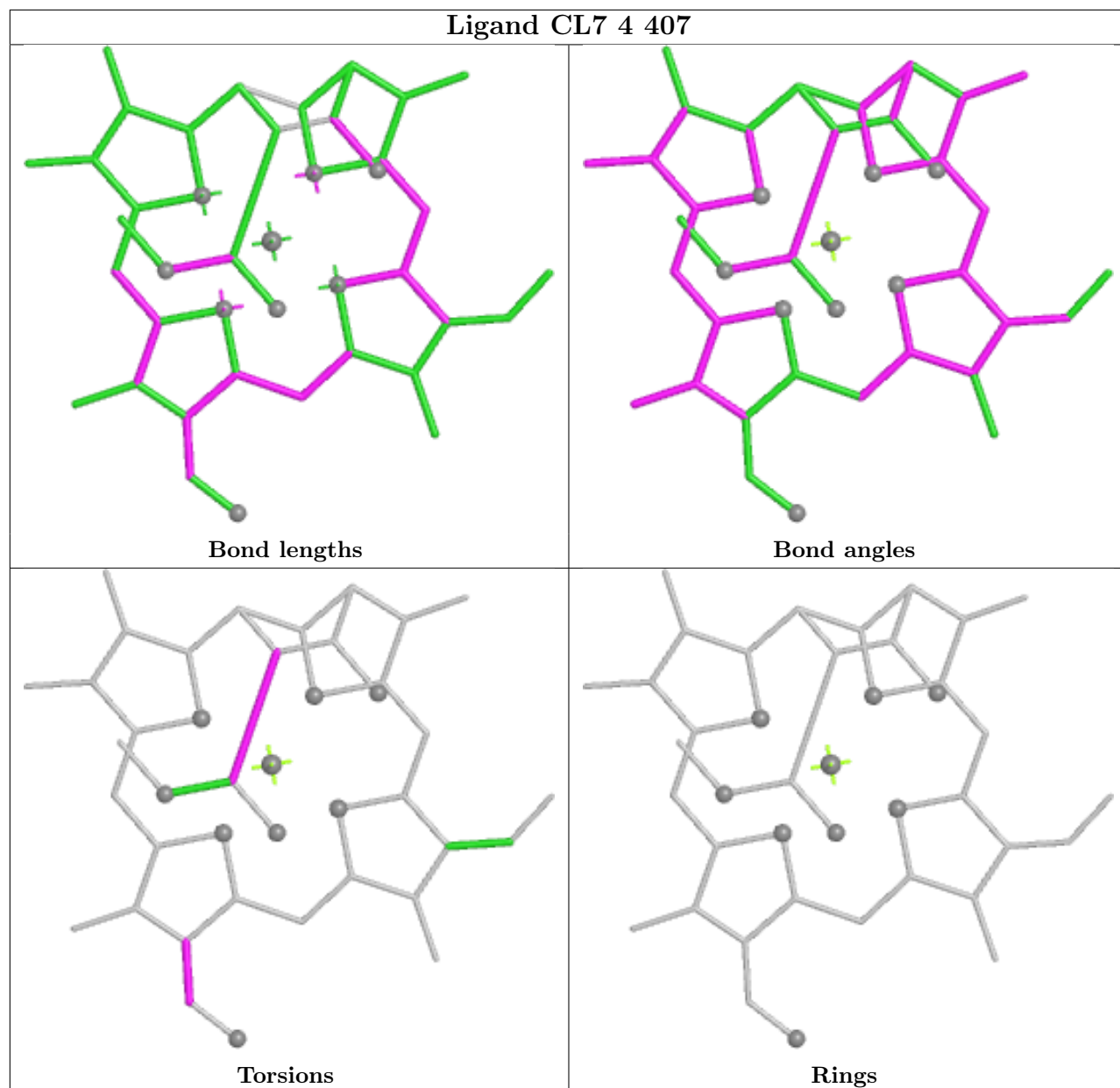
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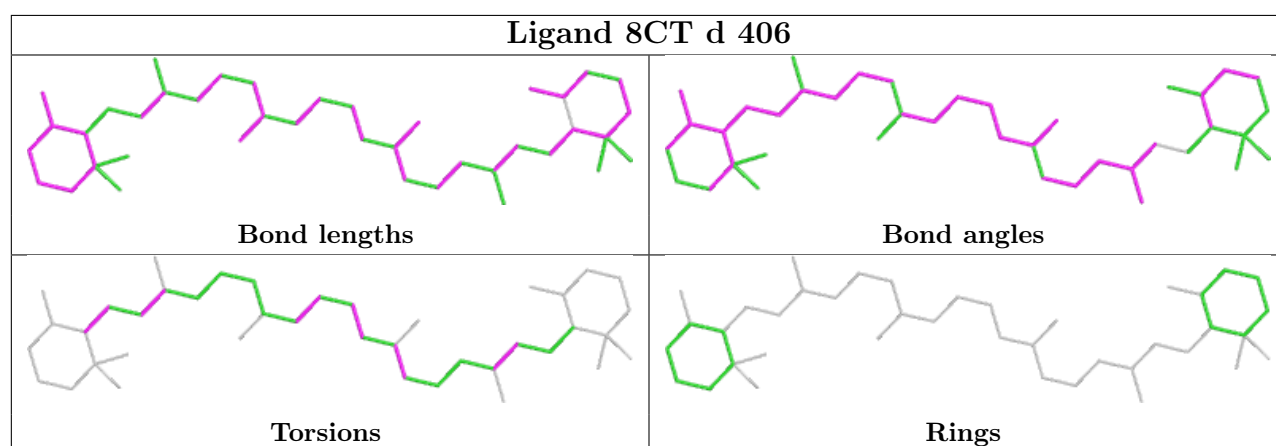
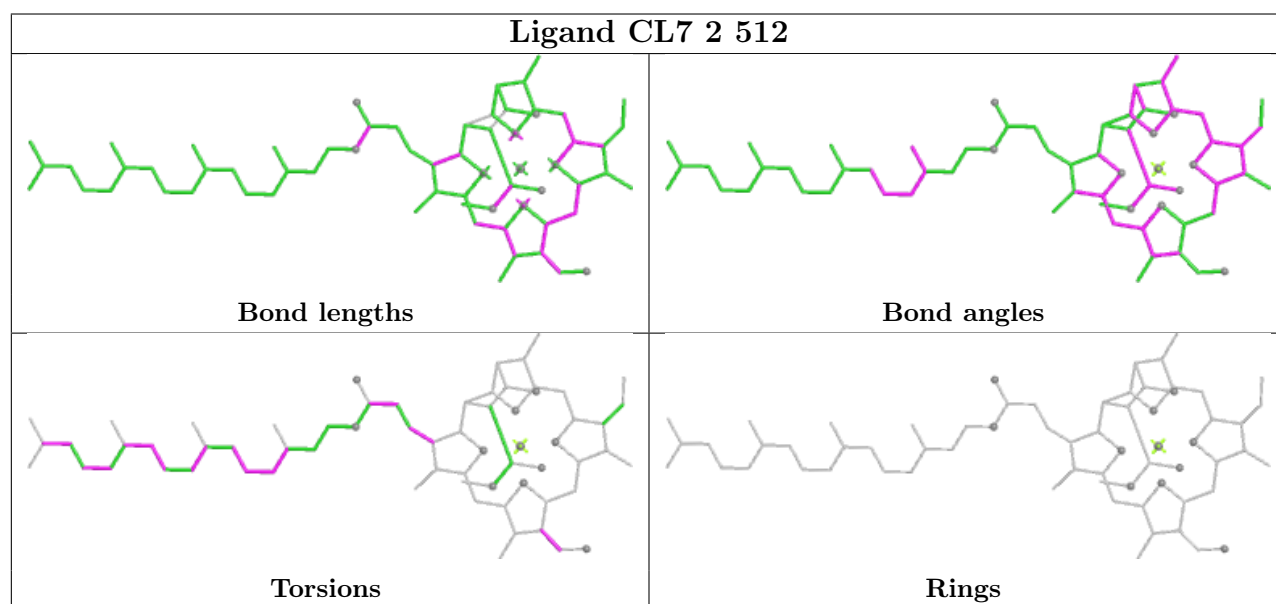
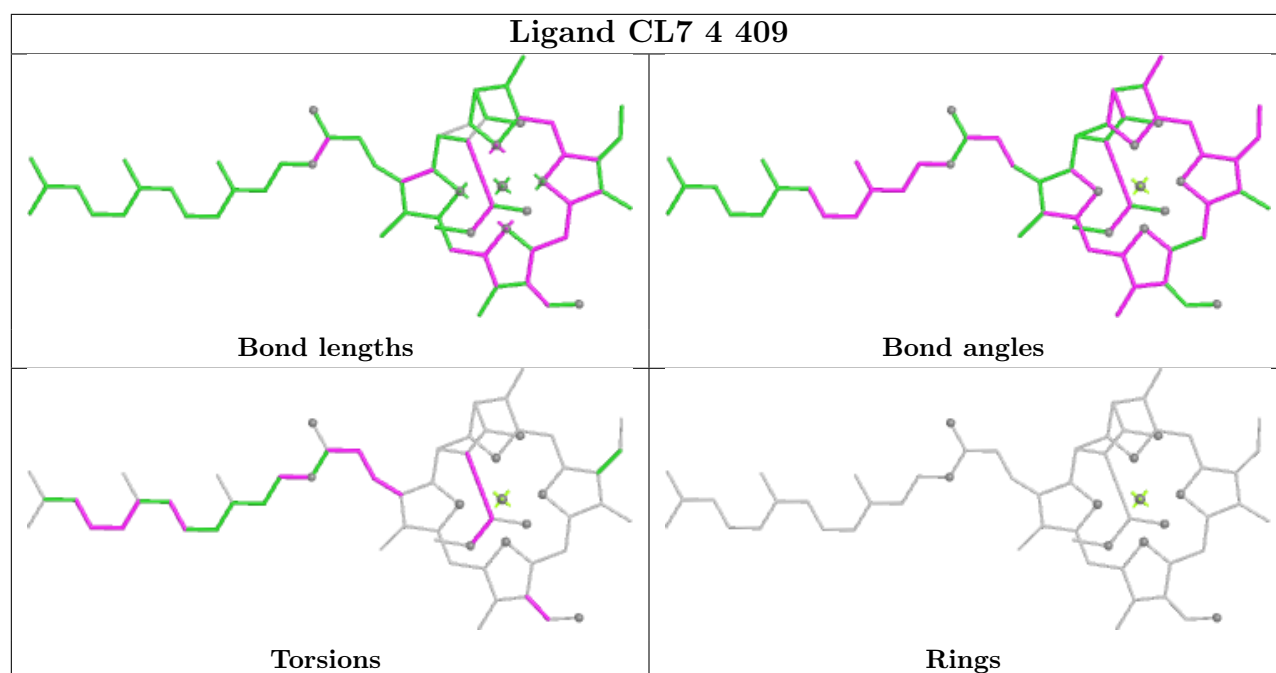


Ligand ZEX 8 403

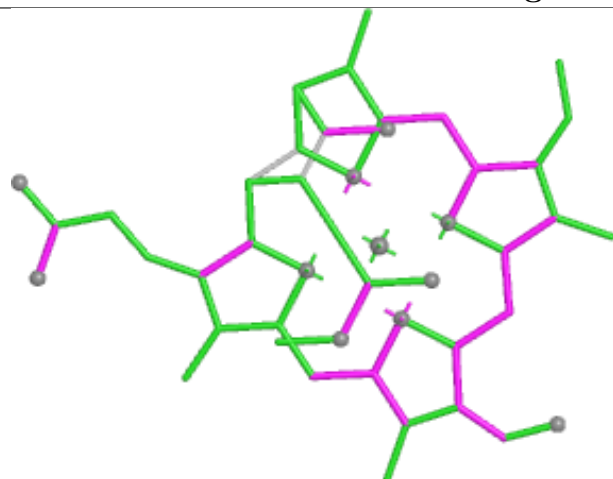


Ligand CL7 4 407

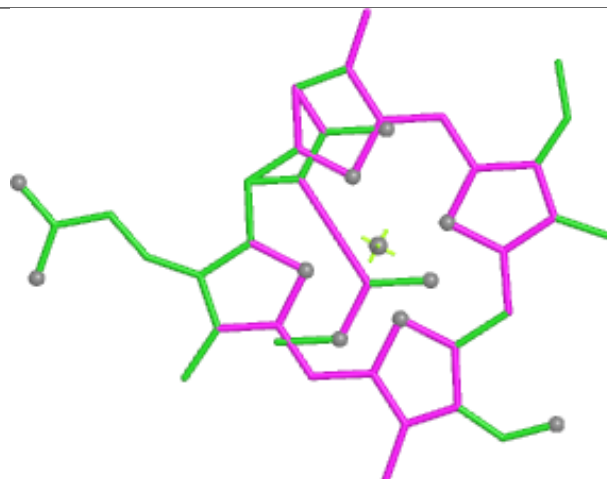




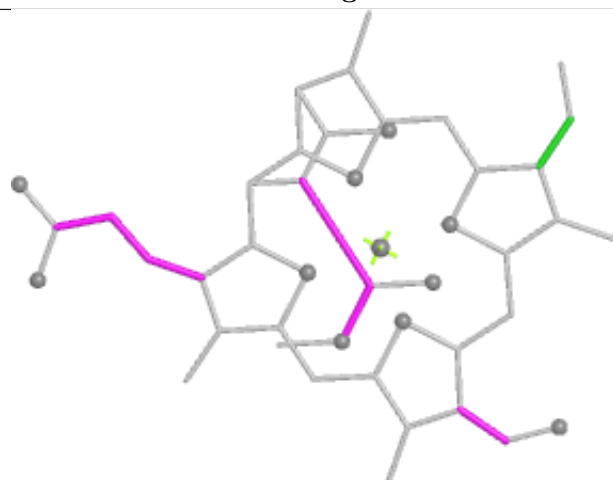
Ligand CL7 1 405



Bond lengths



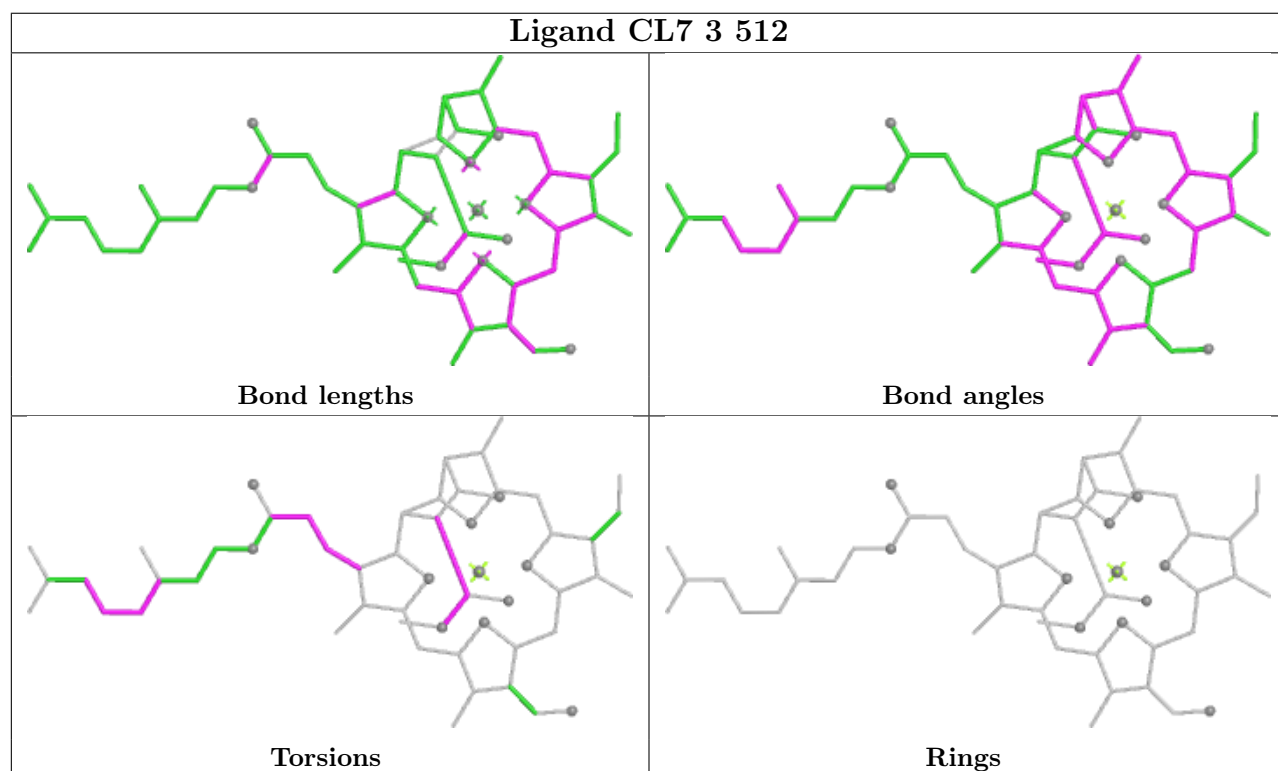
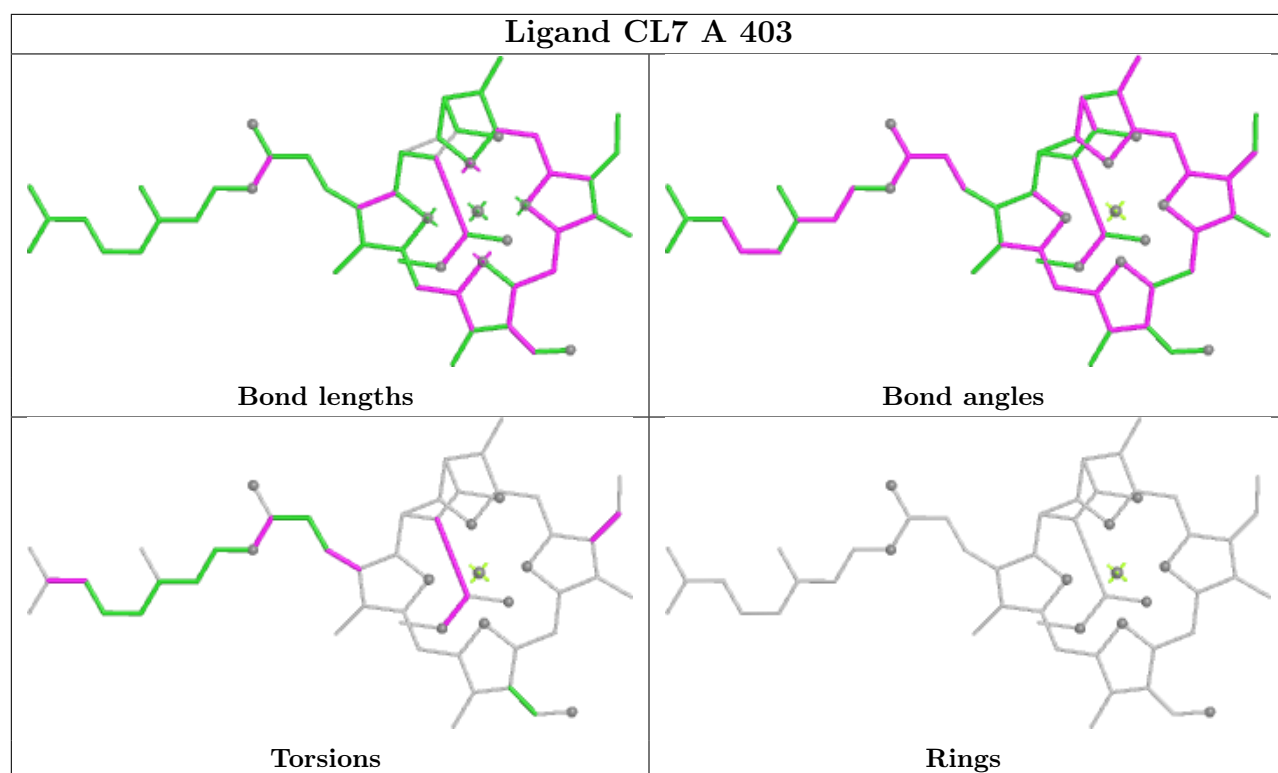
Bond angles



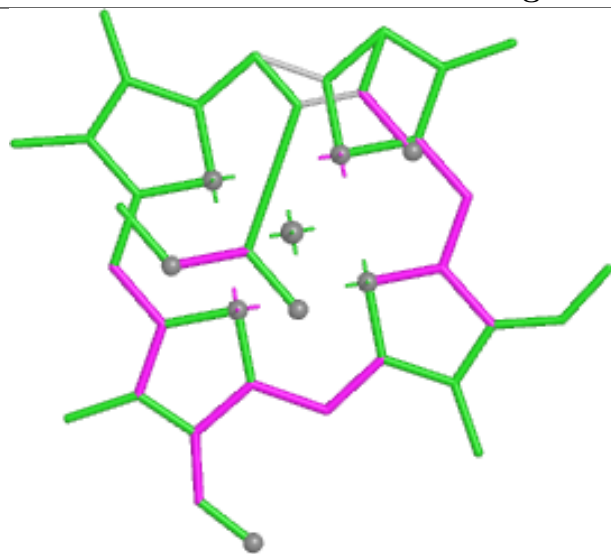
Torsions



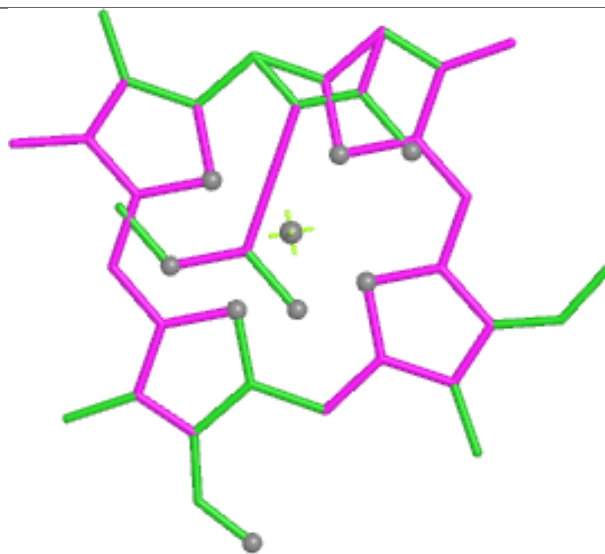
Rings



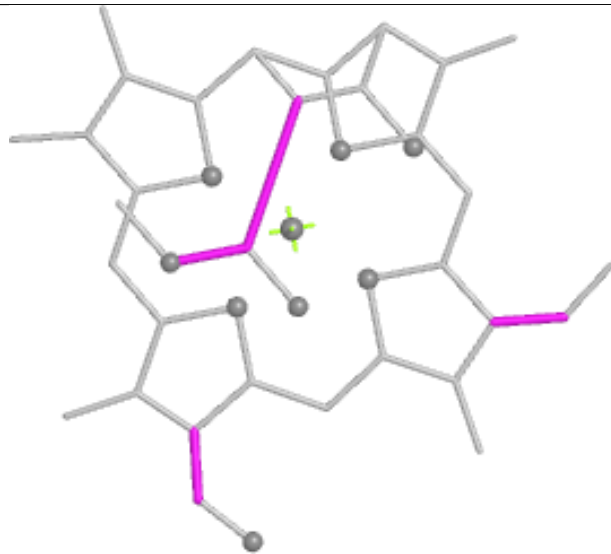
Ligand CL7 8 416



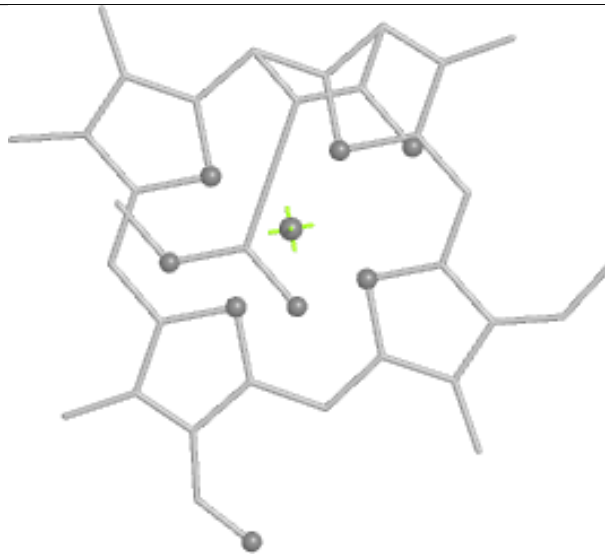
Bond lengths



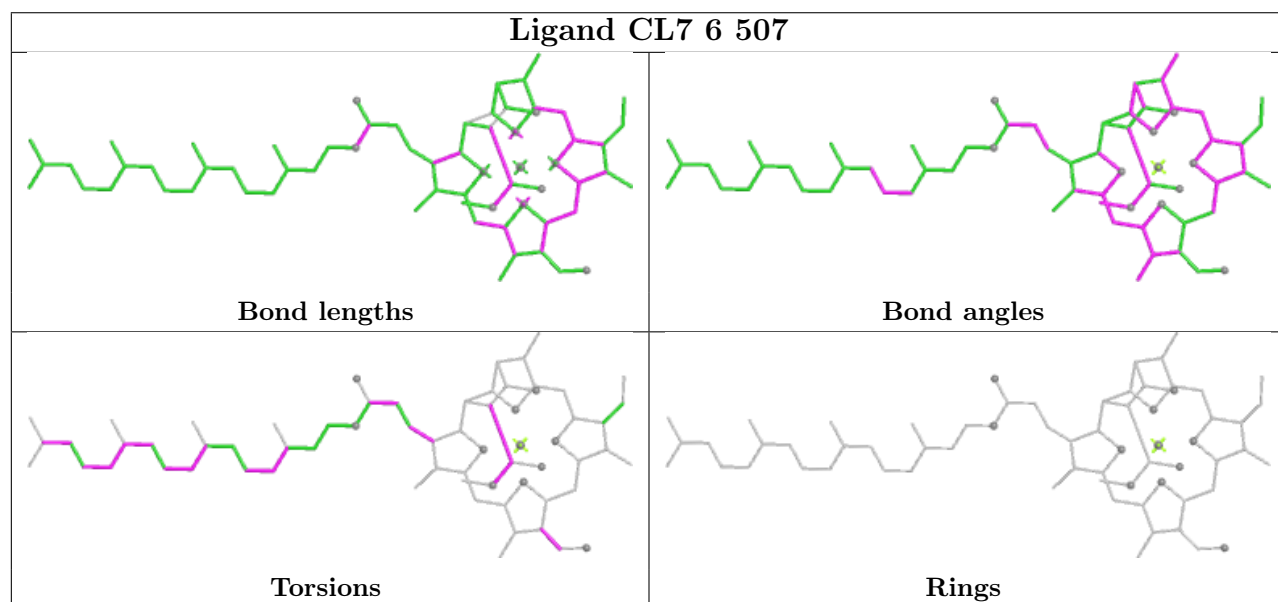
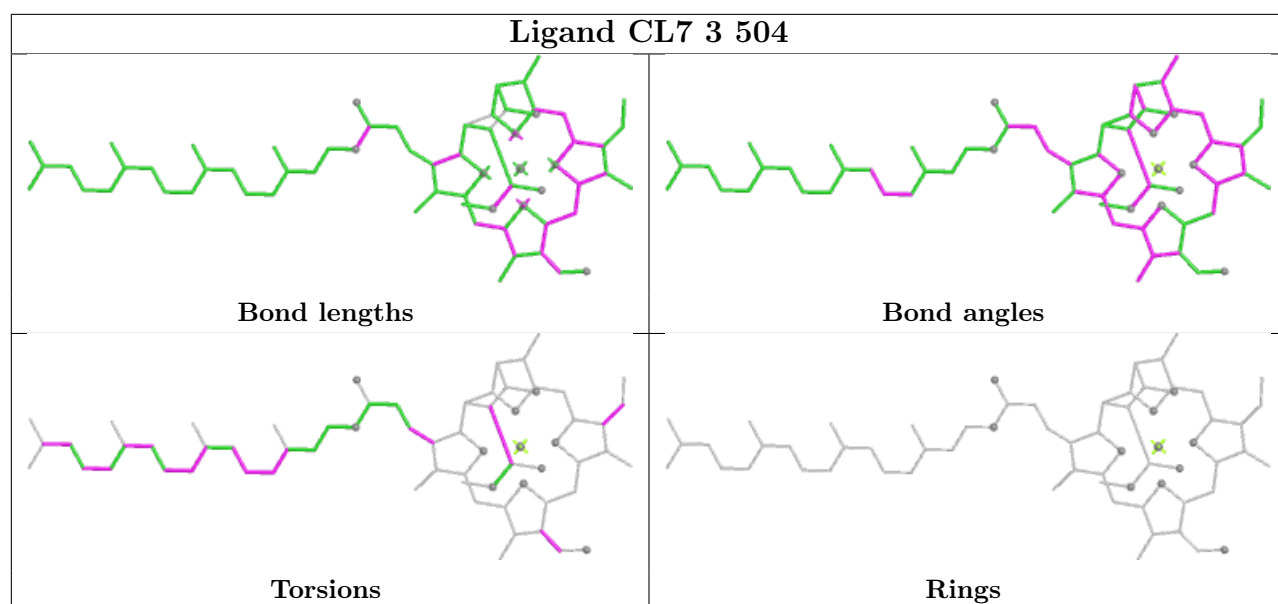
Bond angles



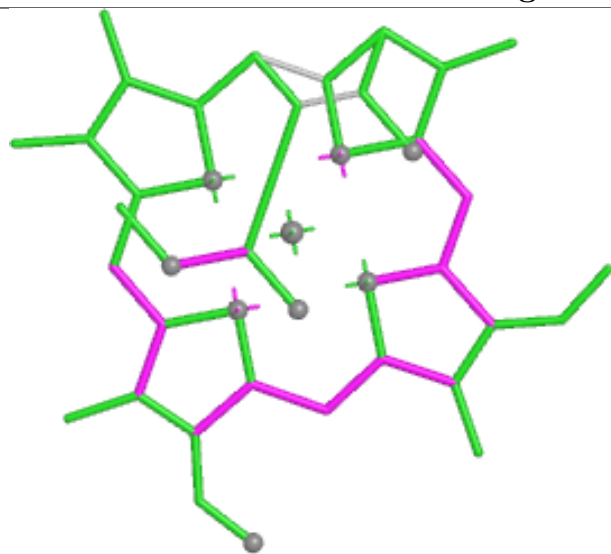
Torsions



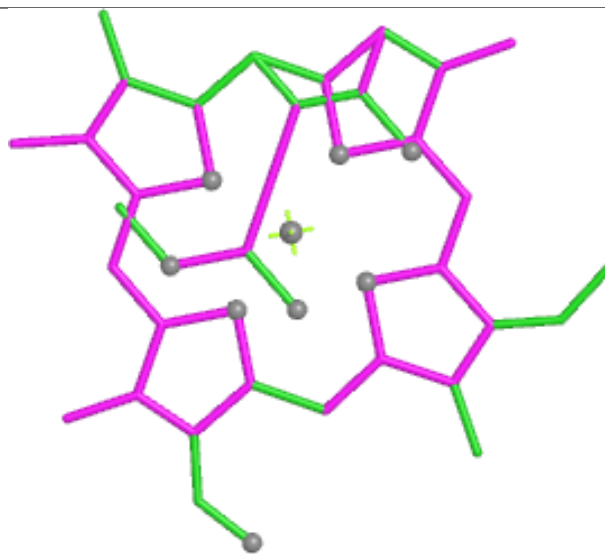
Rings



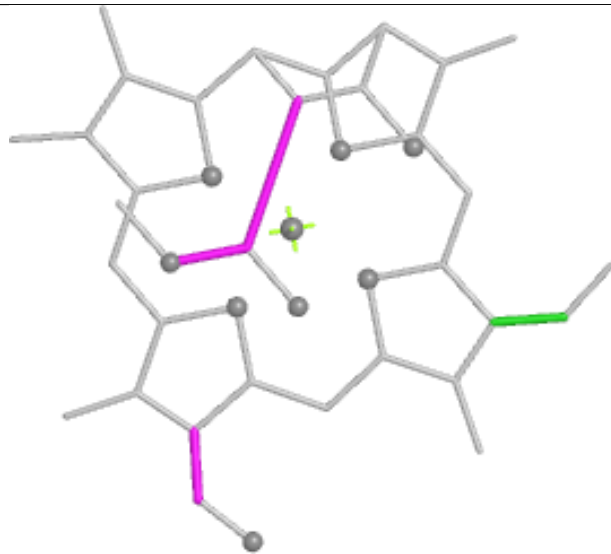
Ligand CL7 C 518



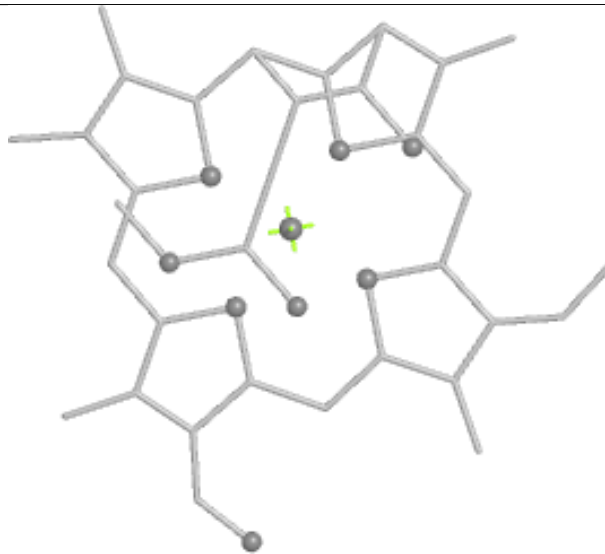
Bond lengths



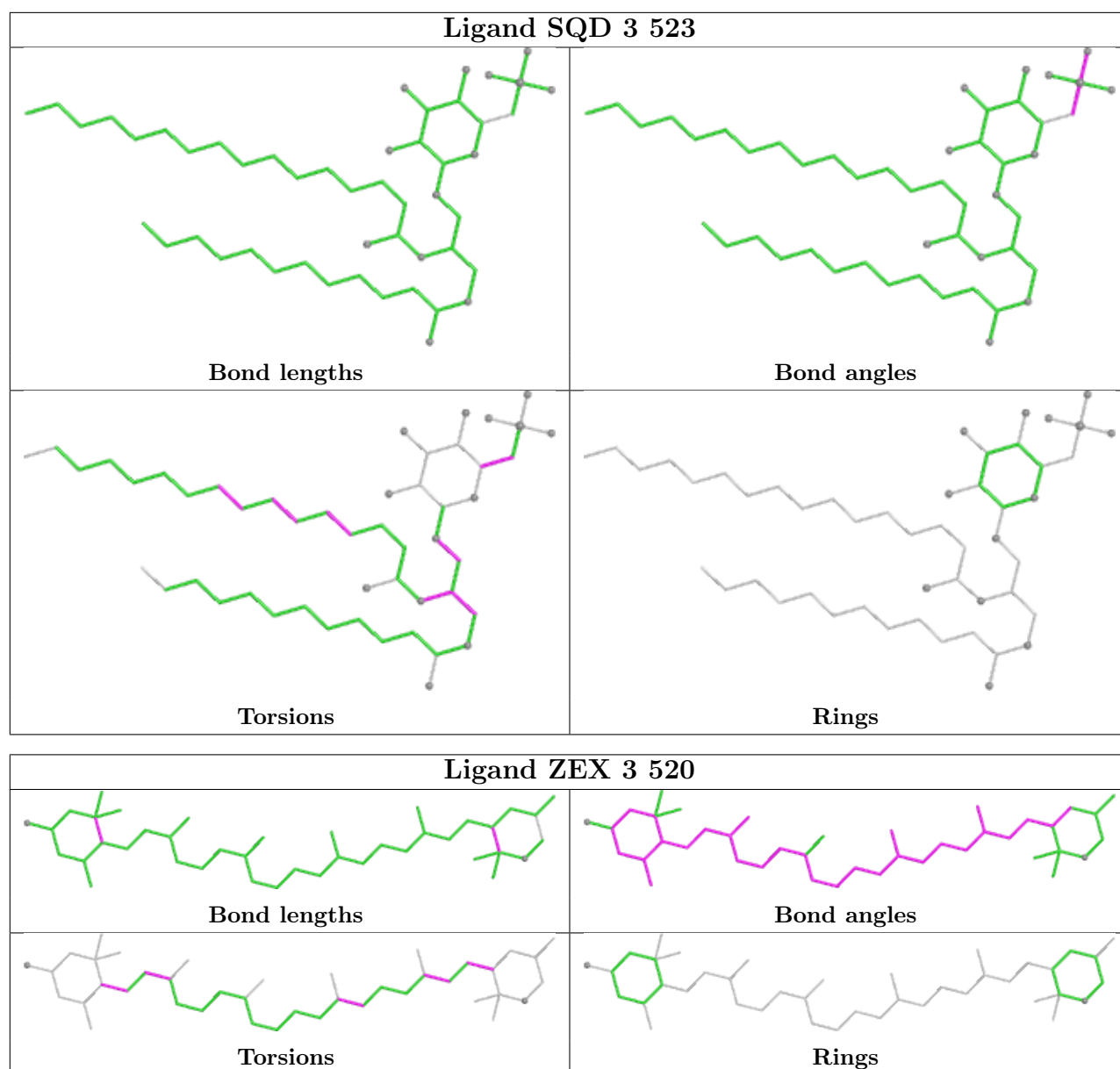
Bond angles

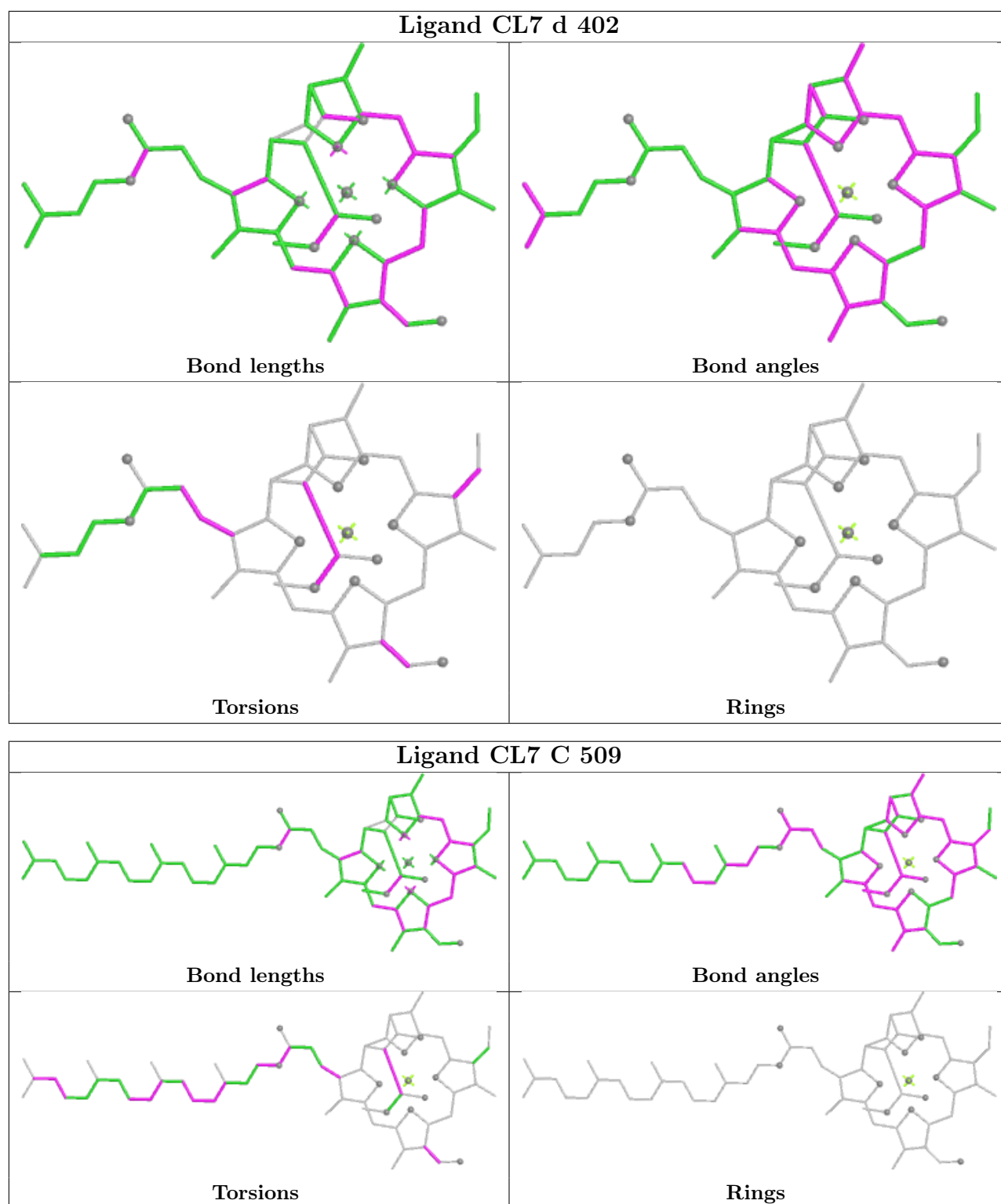


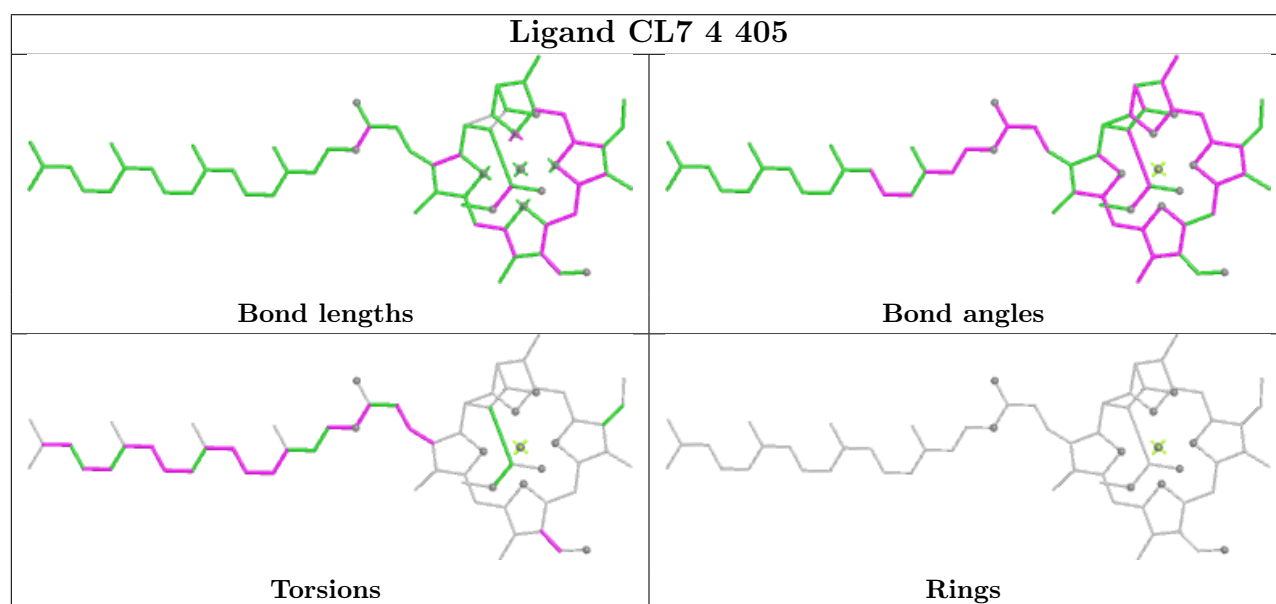
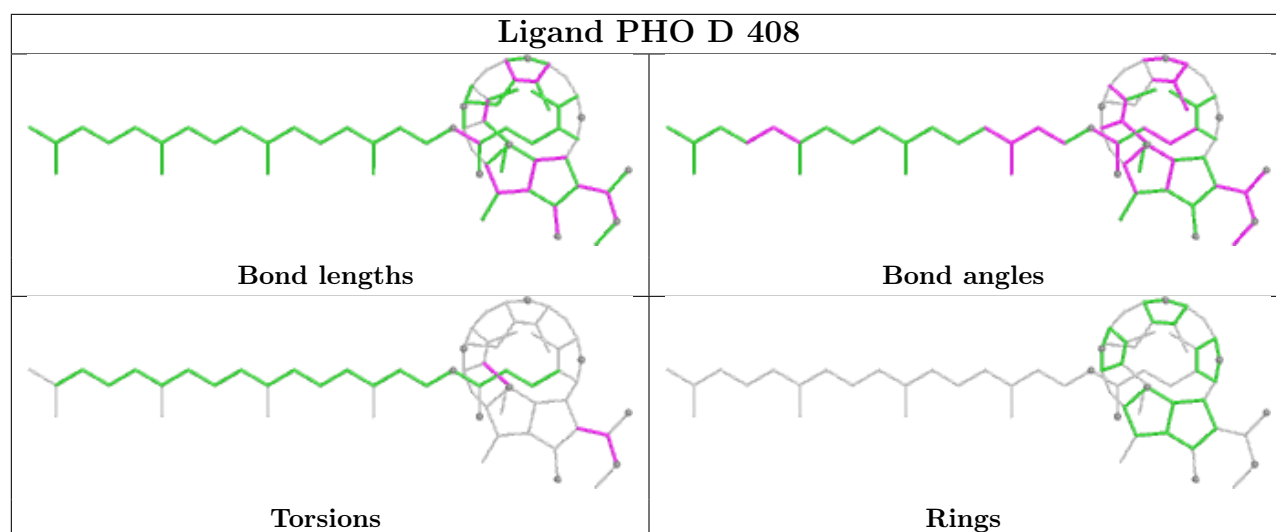
Torsions



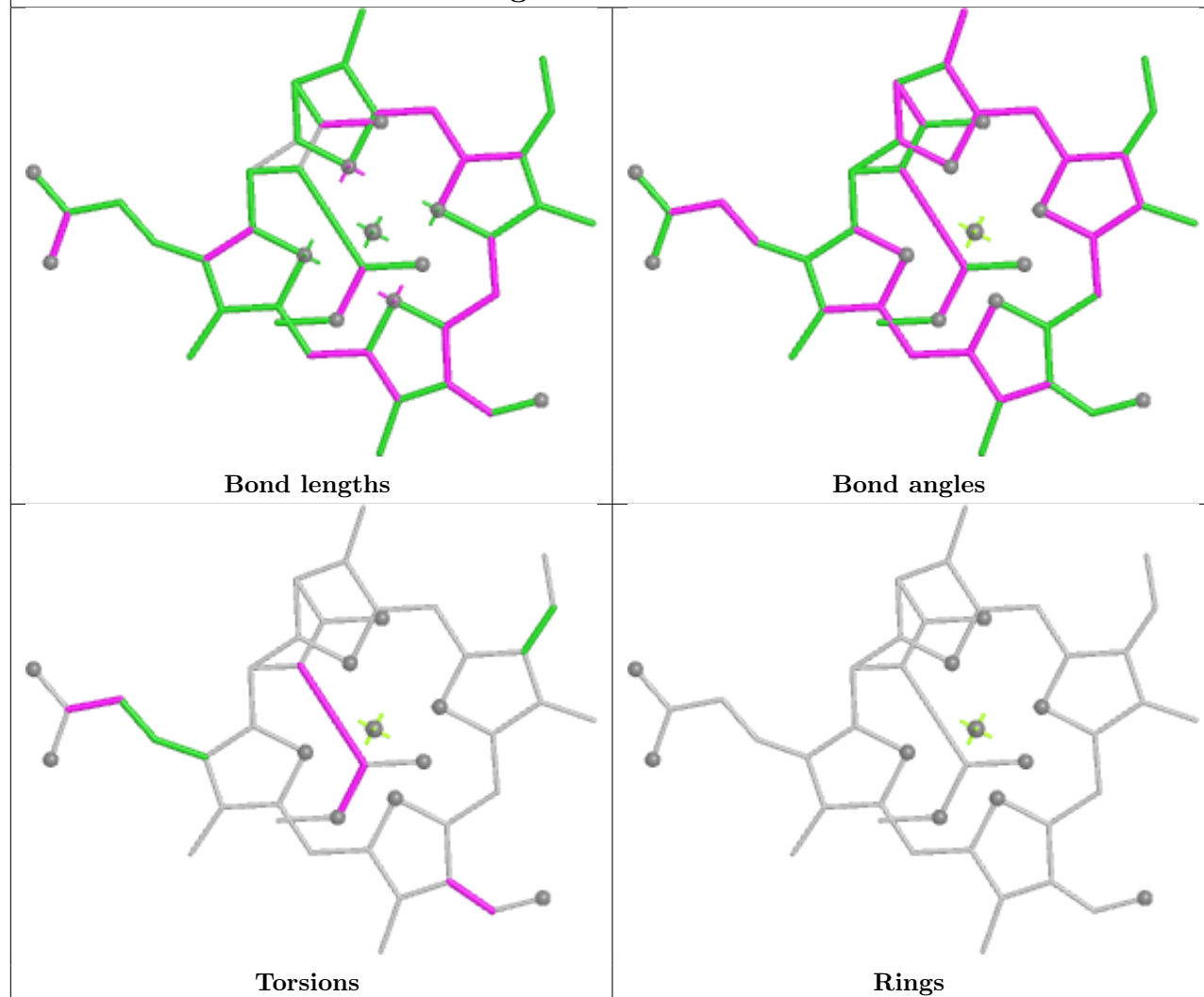
Rings



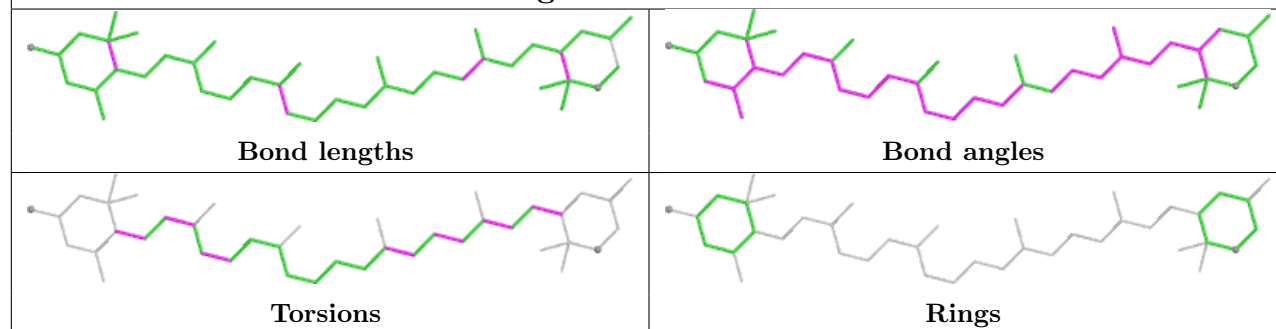


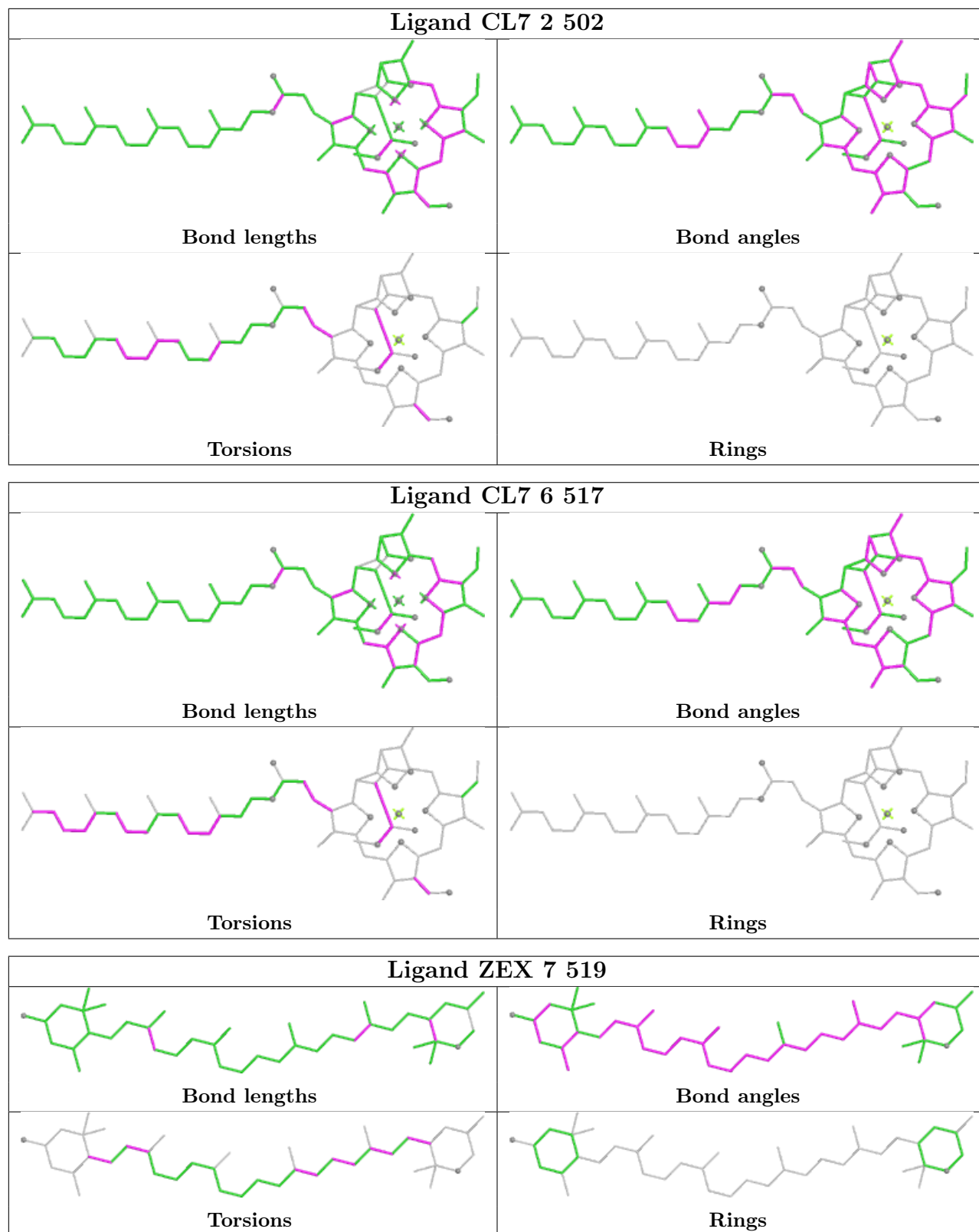


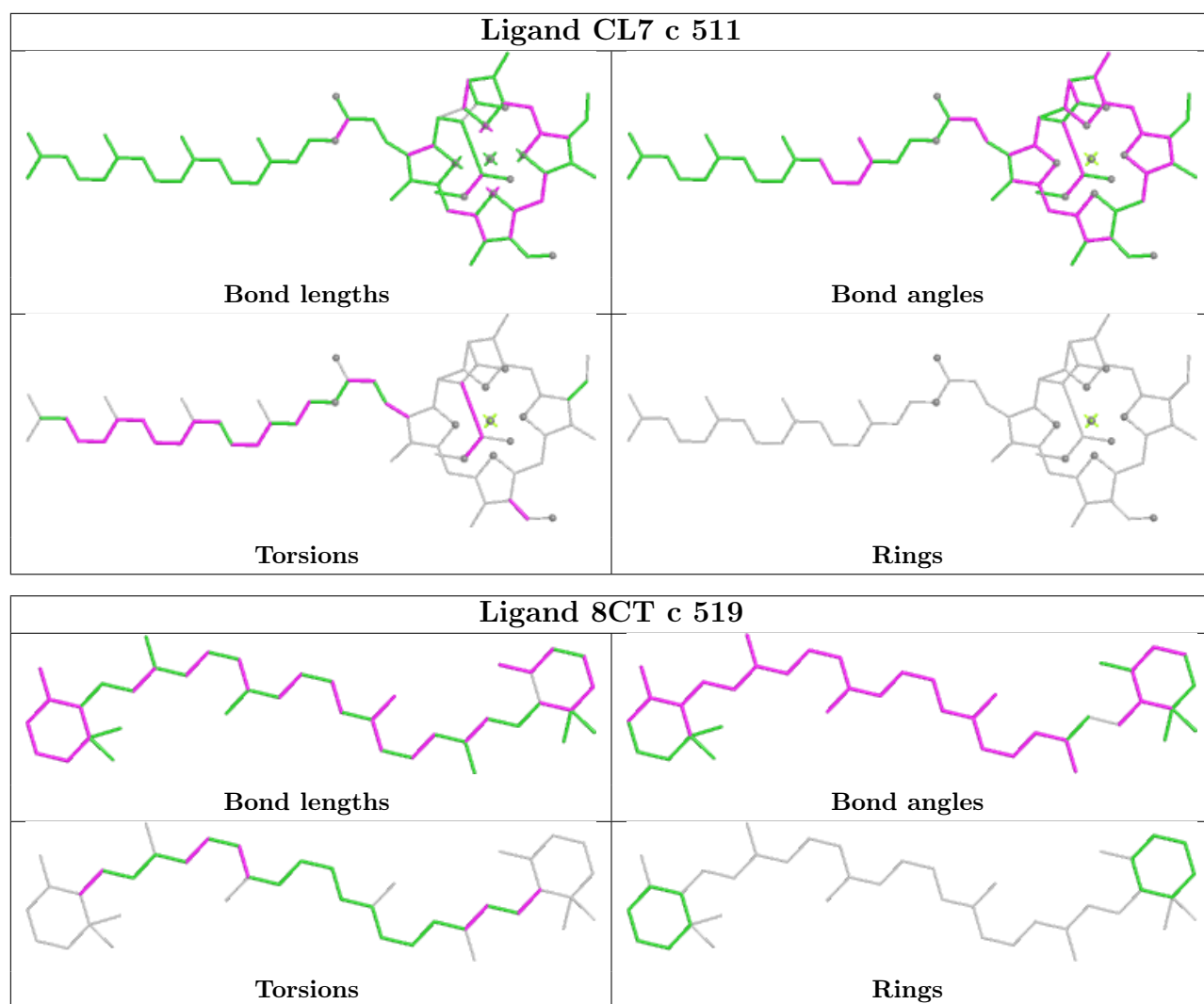
Ligand CL7 5 411



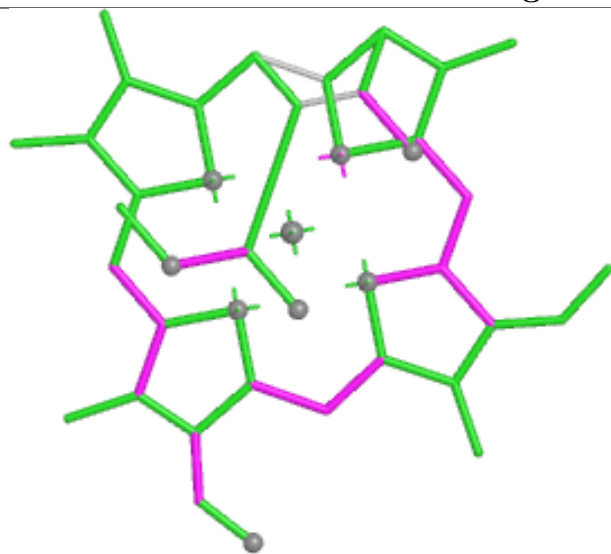
Ligand ZEX 6 524



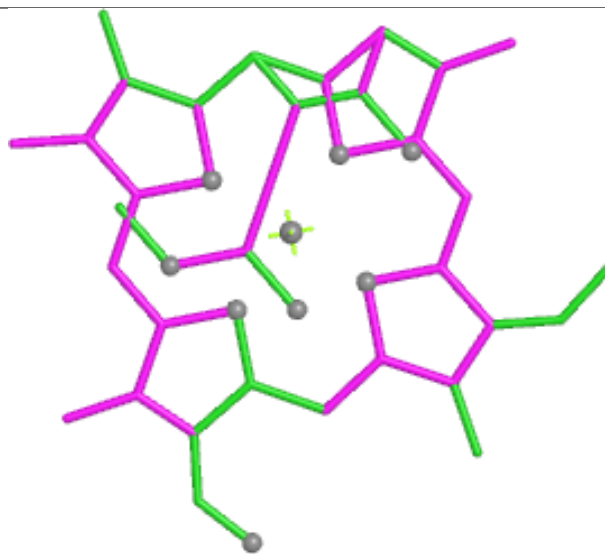




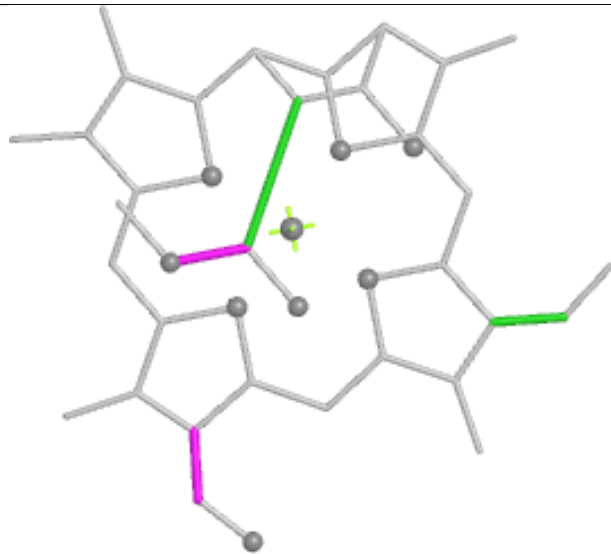
Ligand CL7 1 416



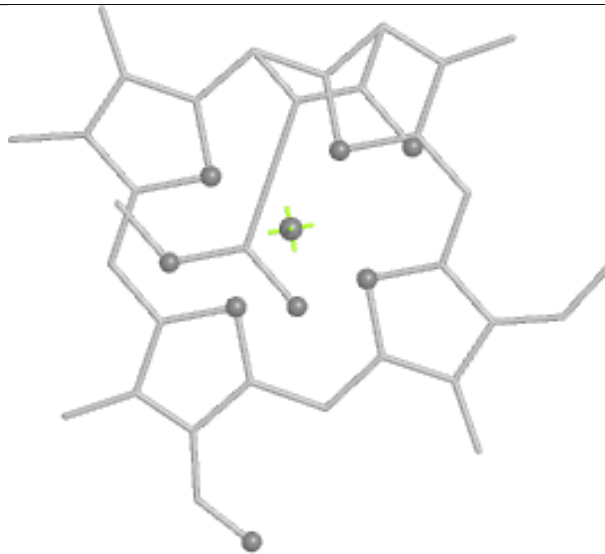
Bond lengths



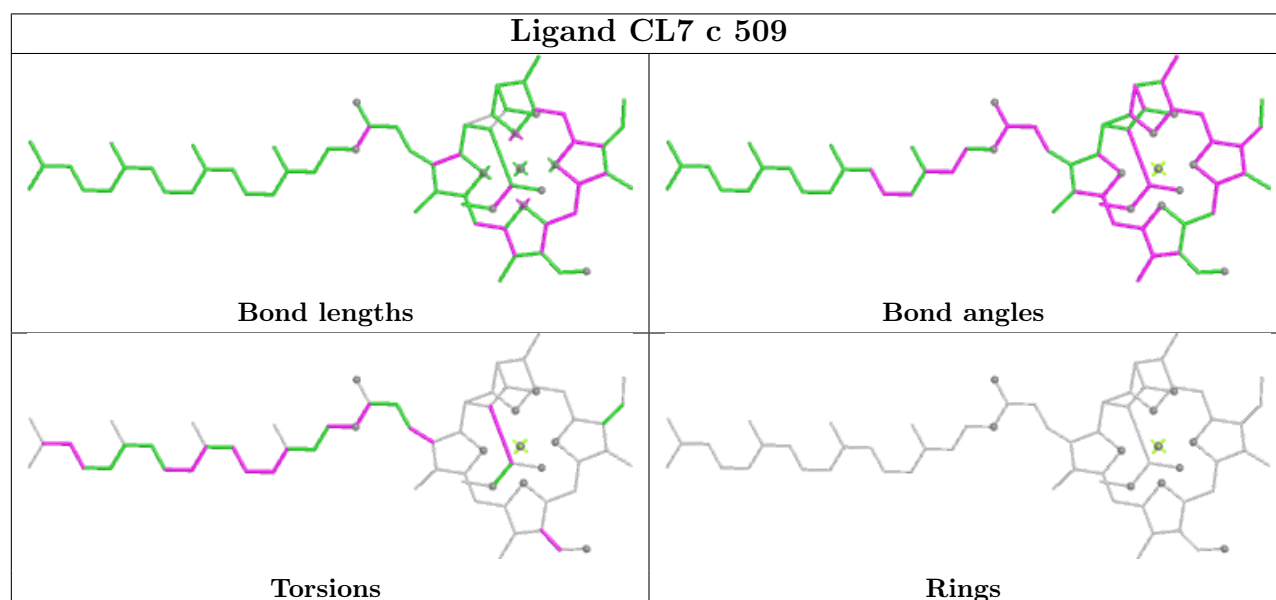
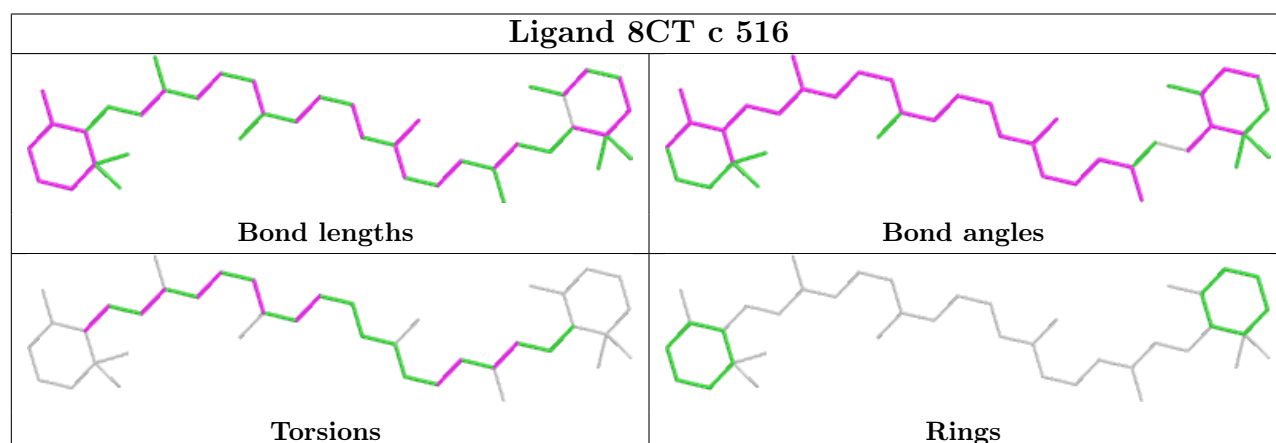
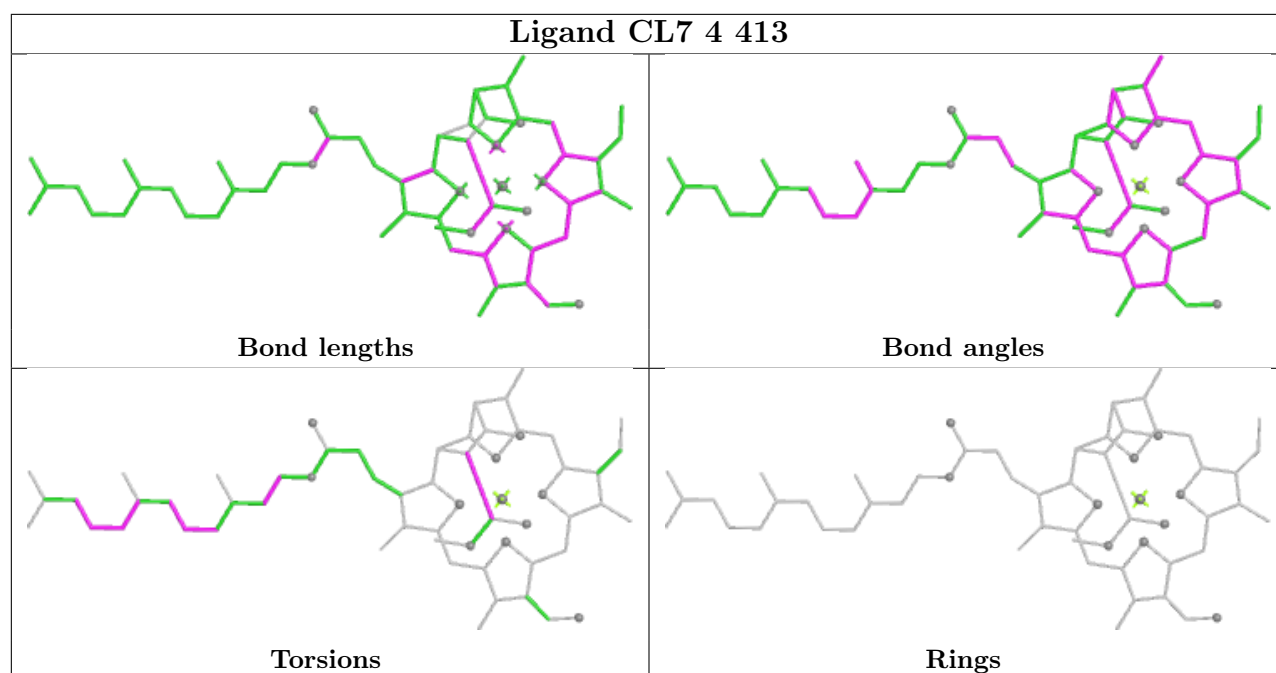
Bond angles

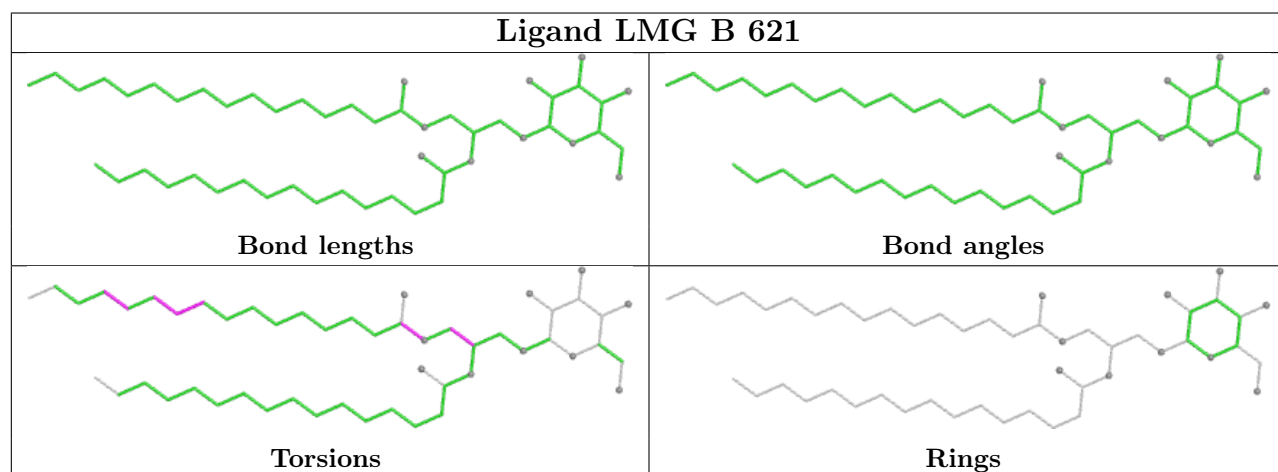
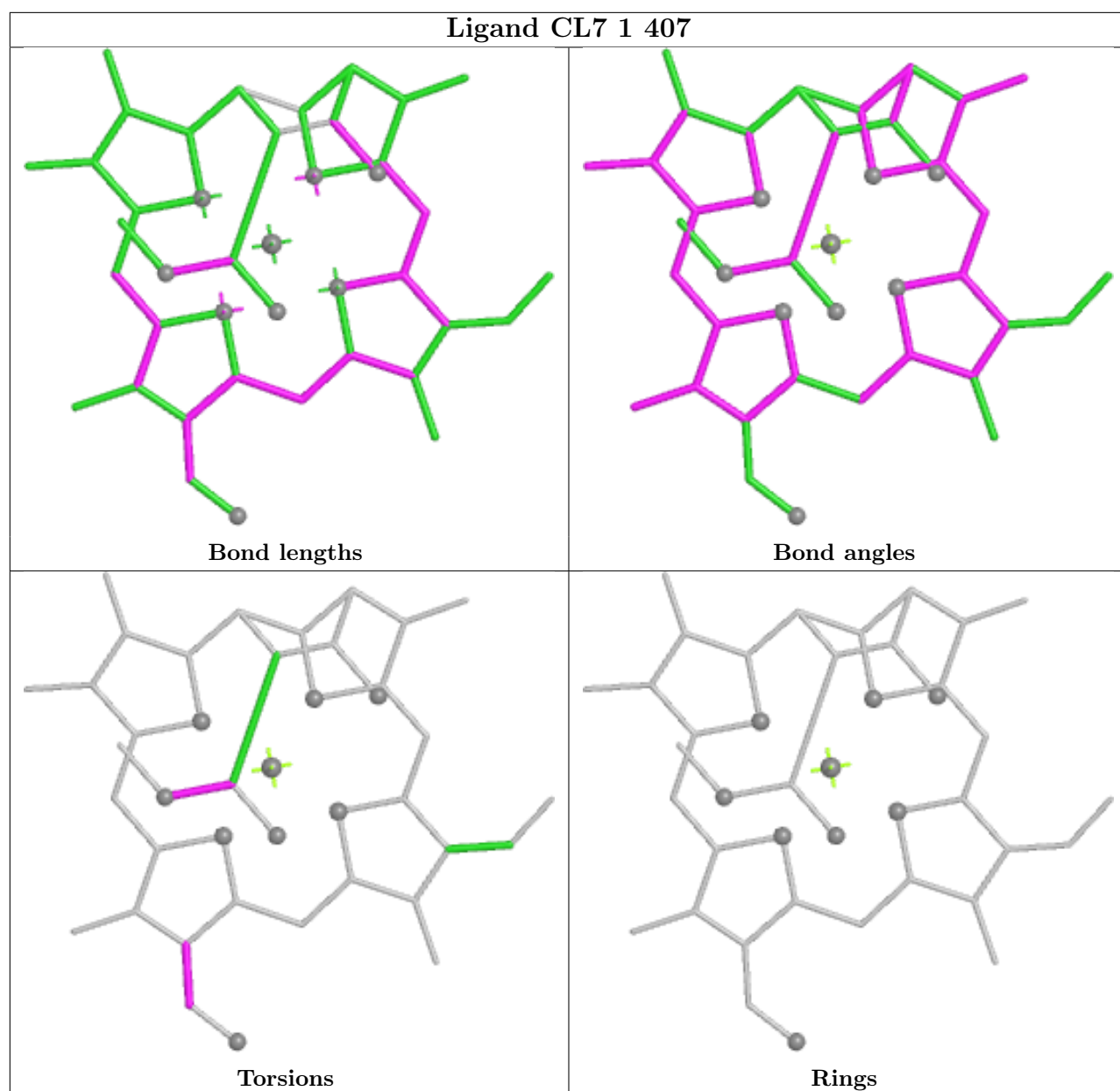


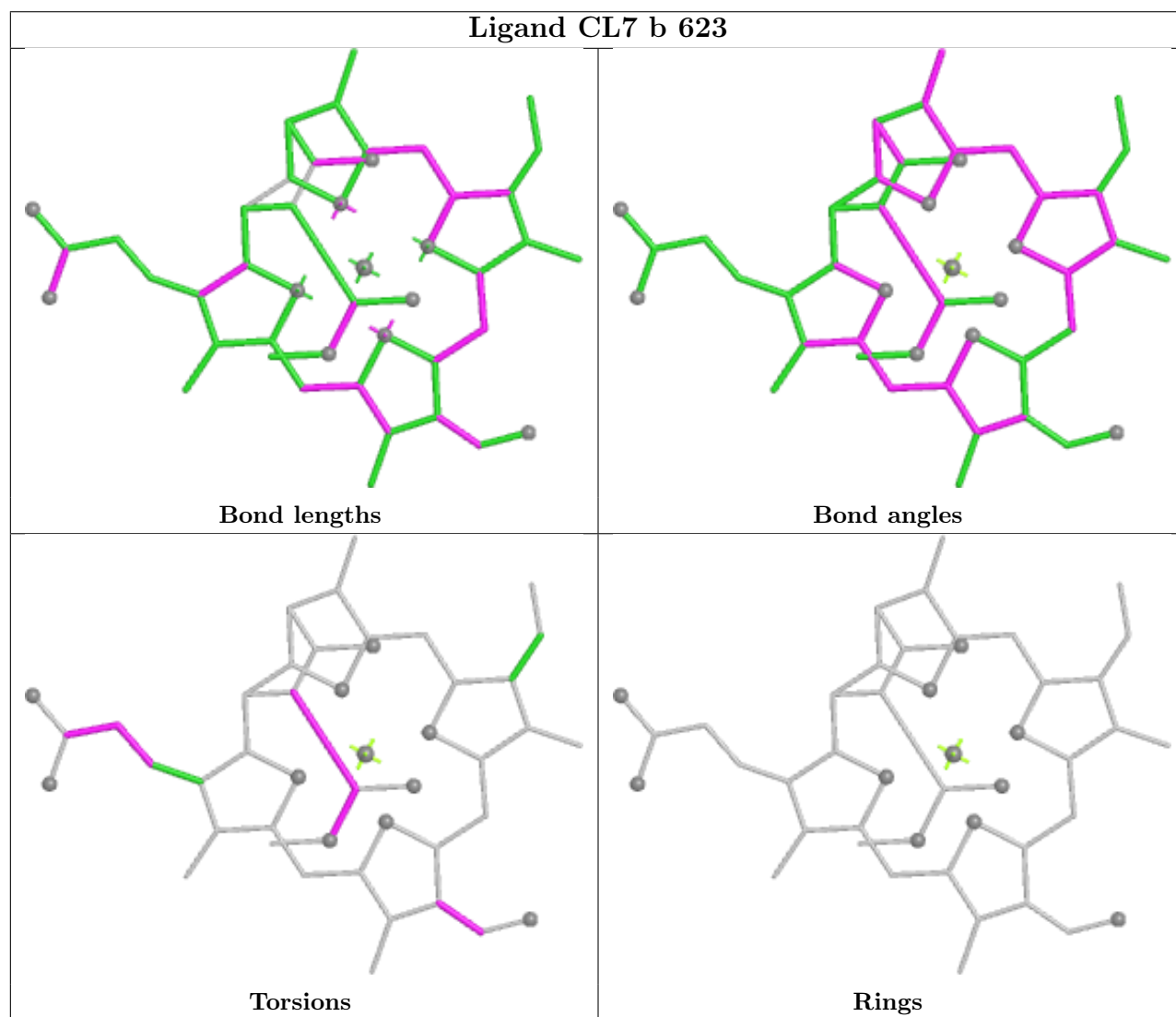
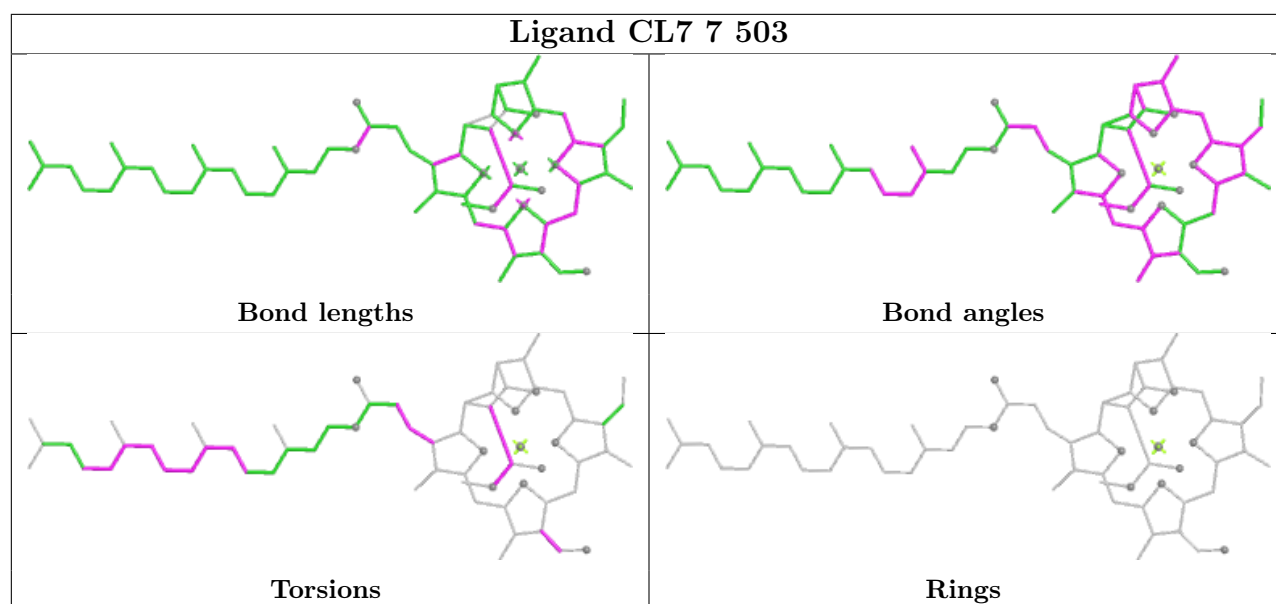
Torsions

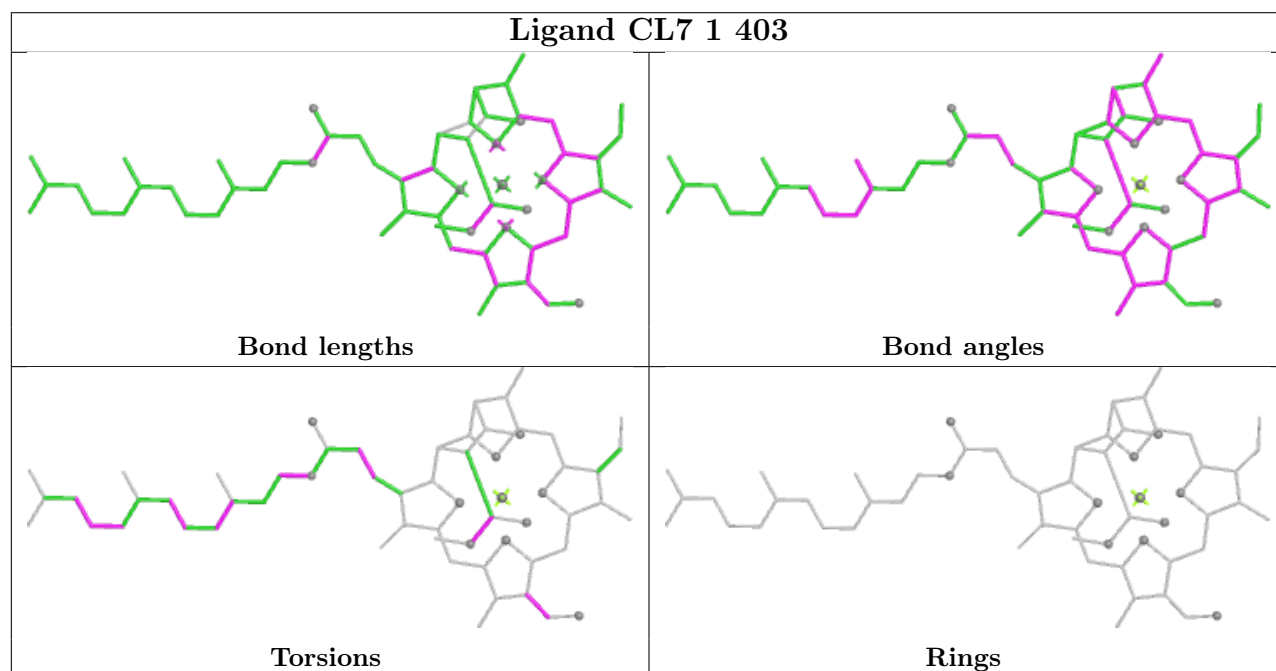
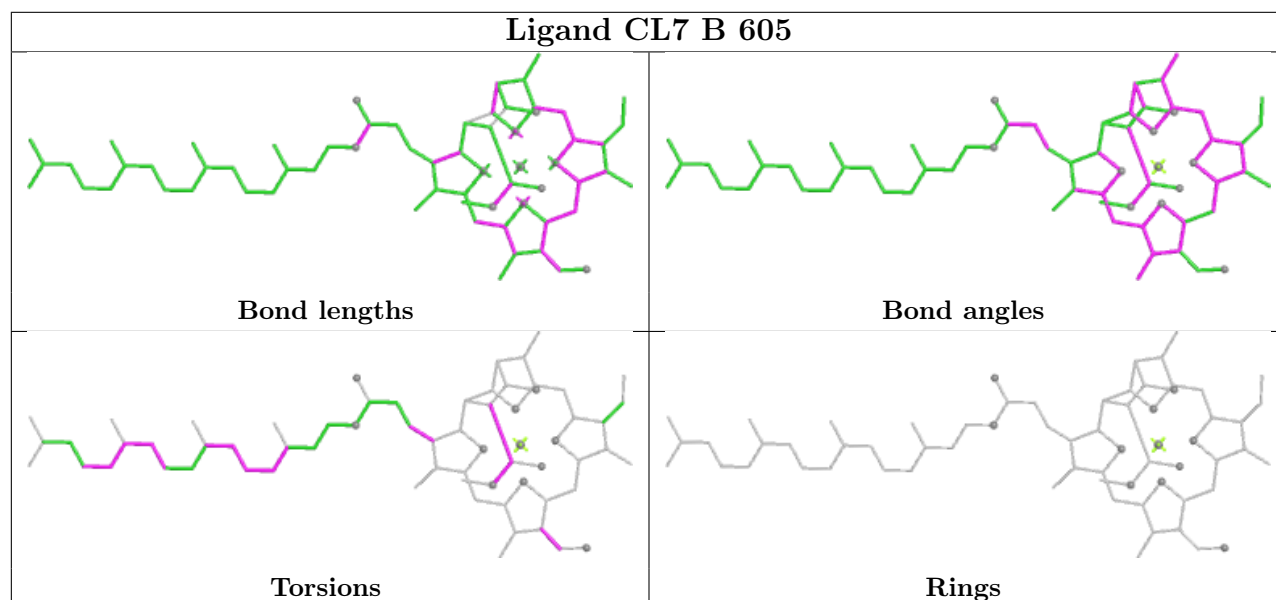
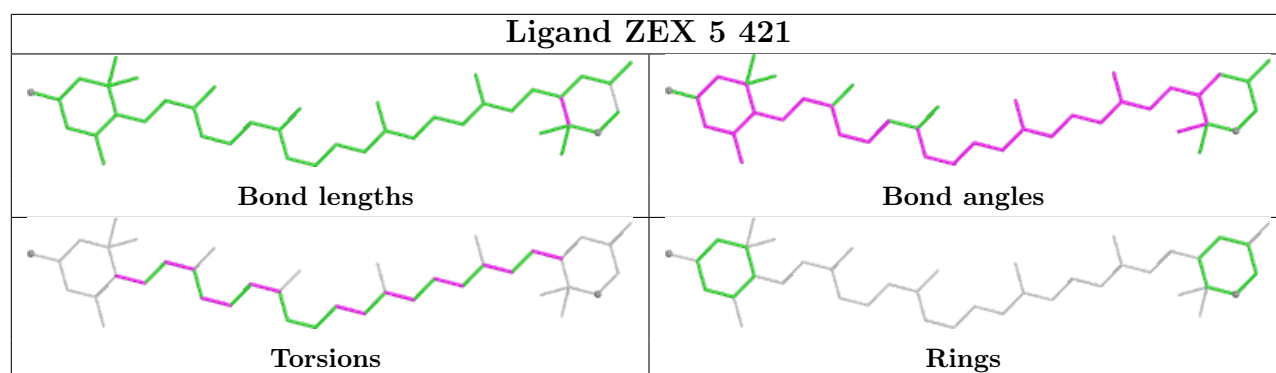


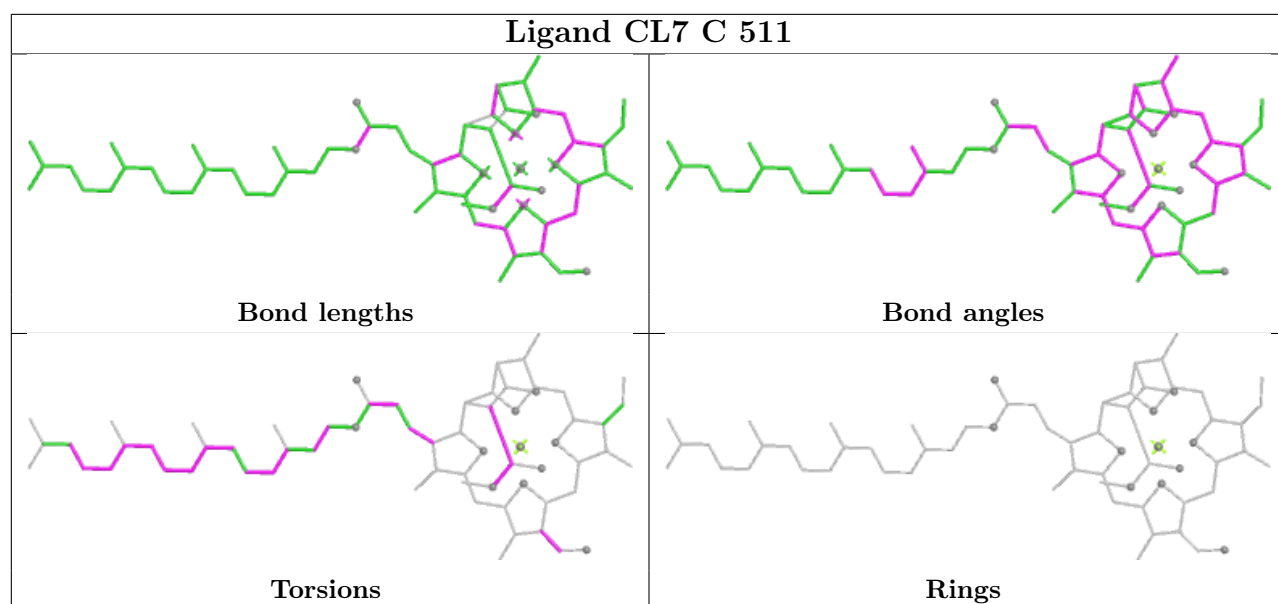
Rings



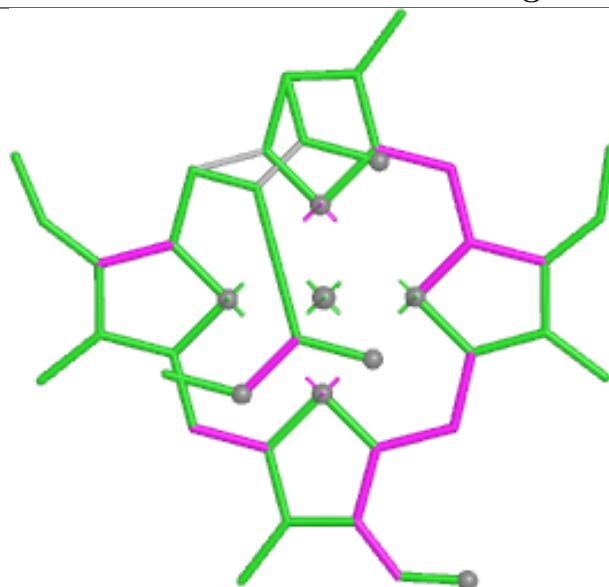




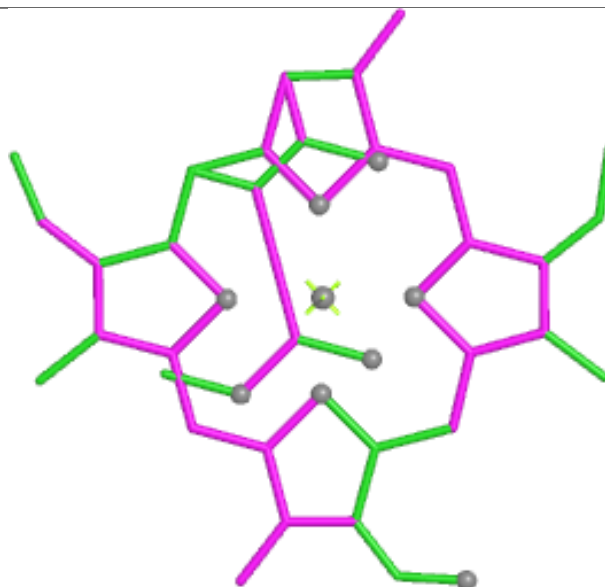




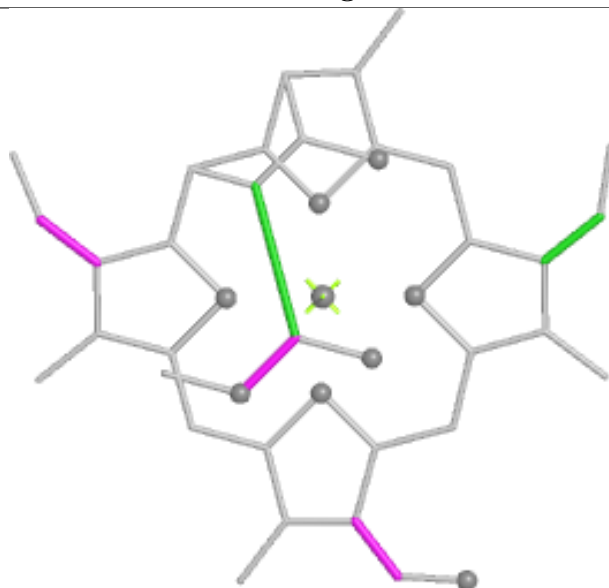
Ligand CL7 4 417



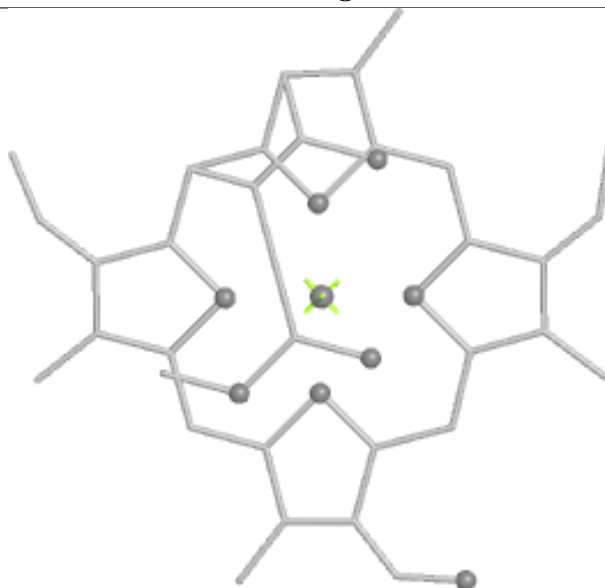
Bond lengths



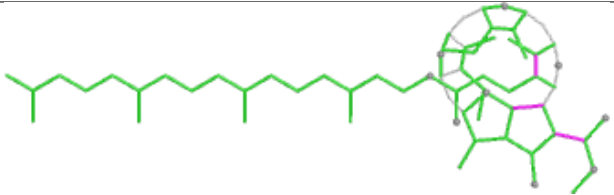
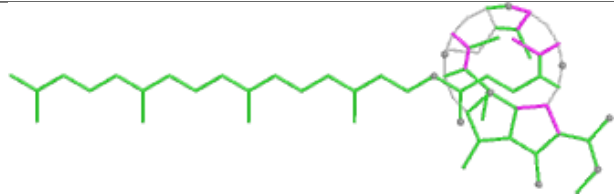
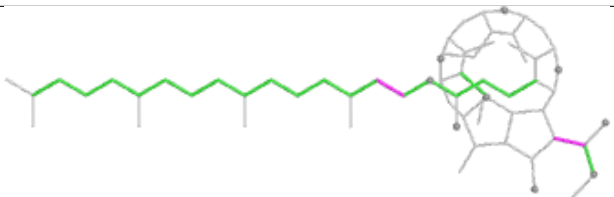
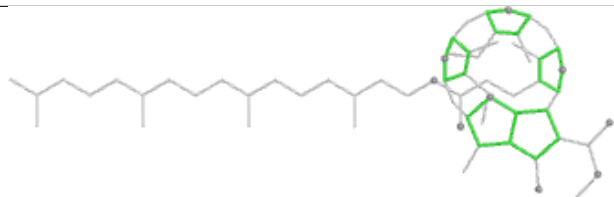
Bond angles

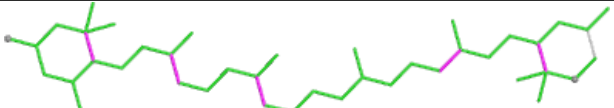
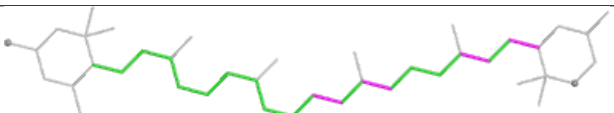
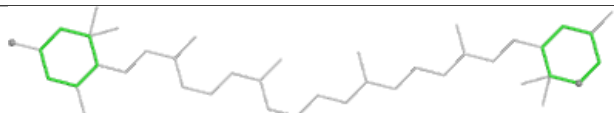


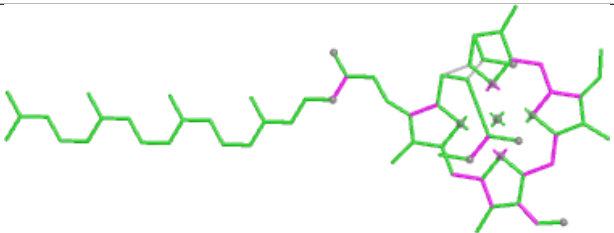
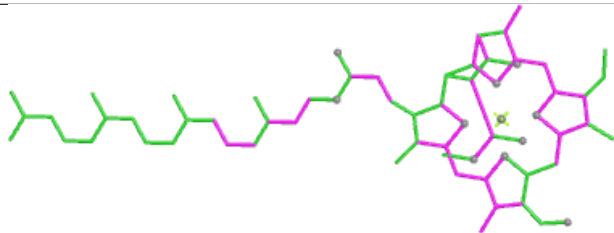
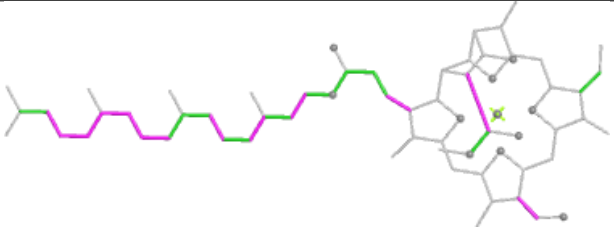
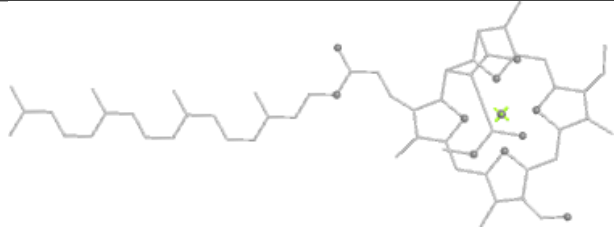
Torsions

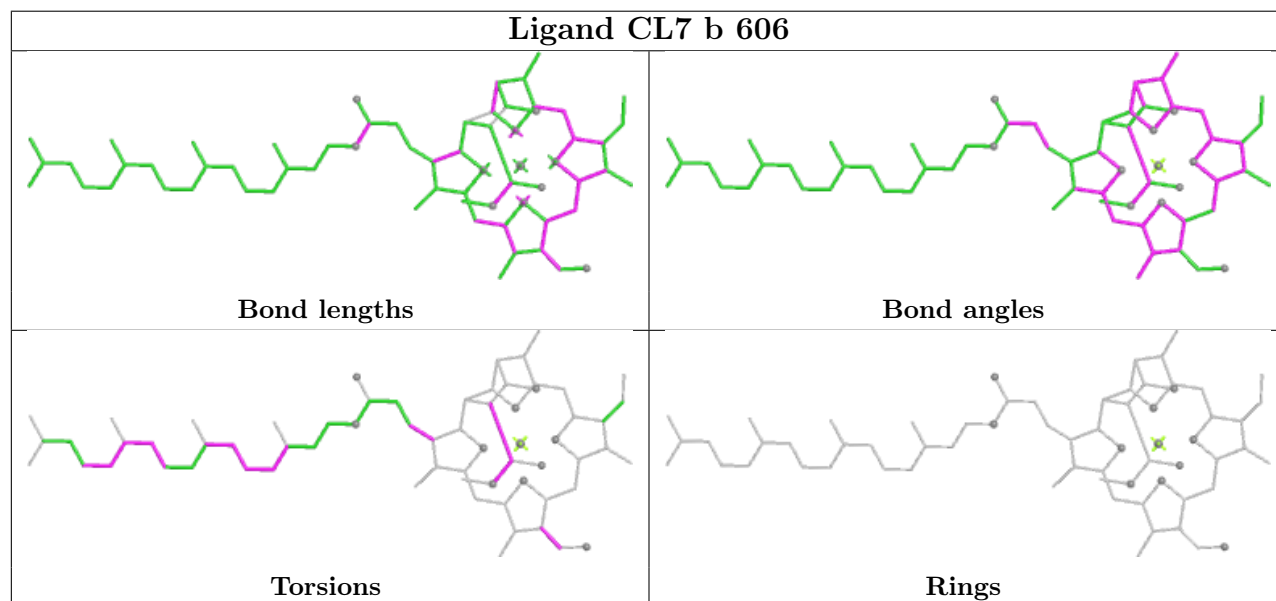
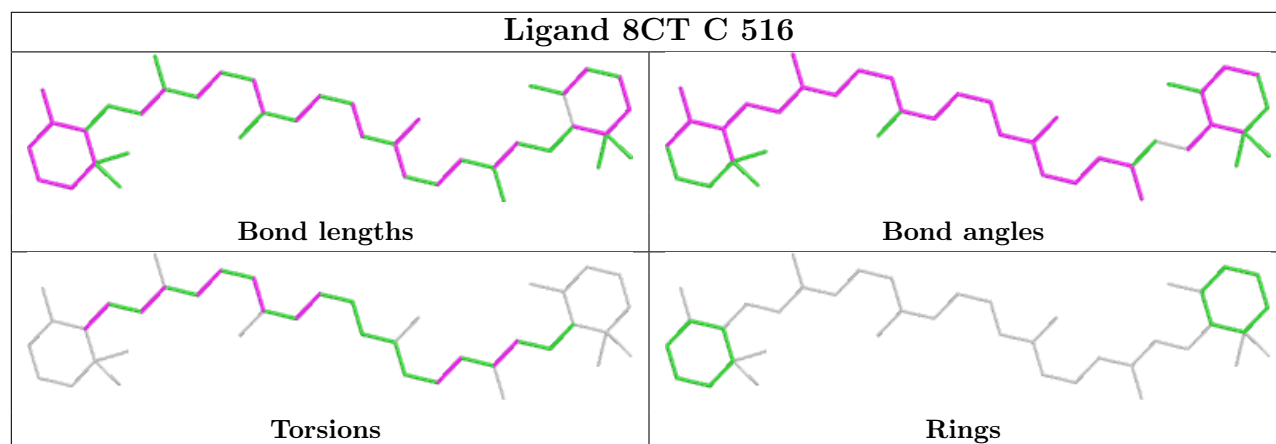
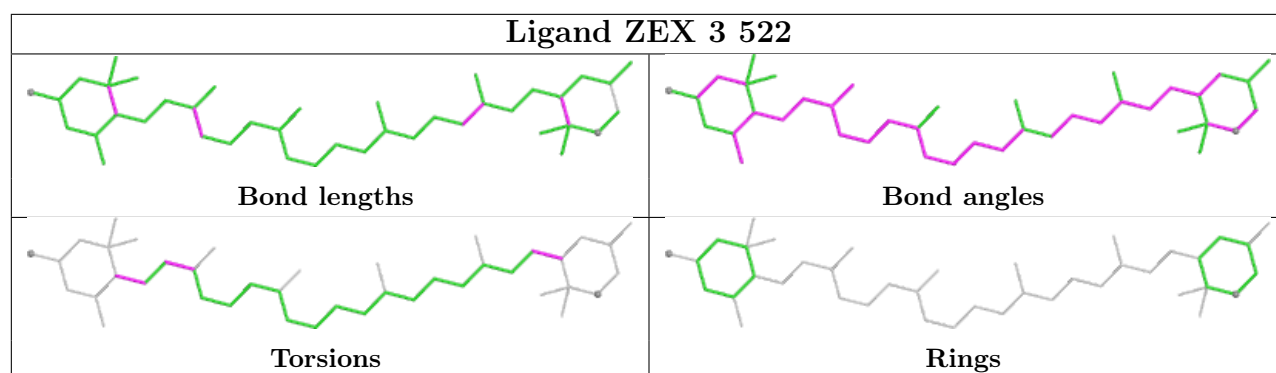


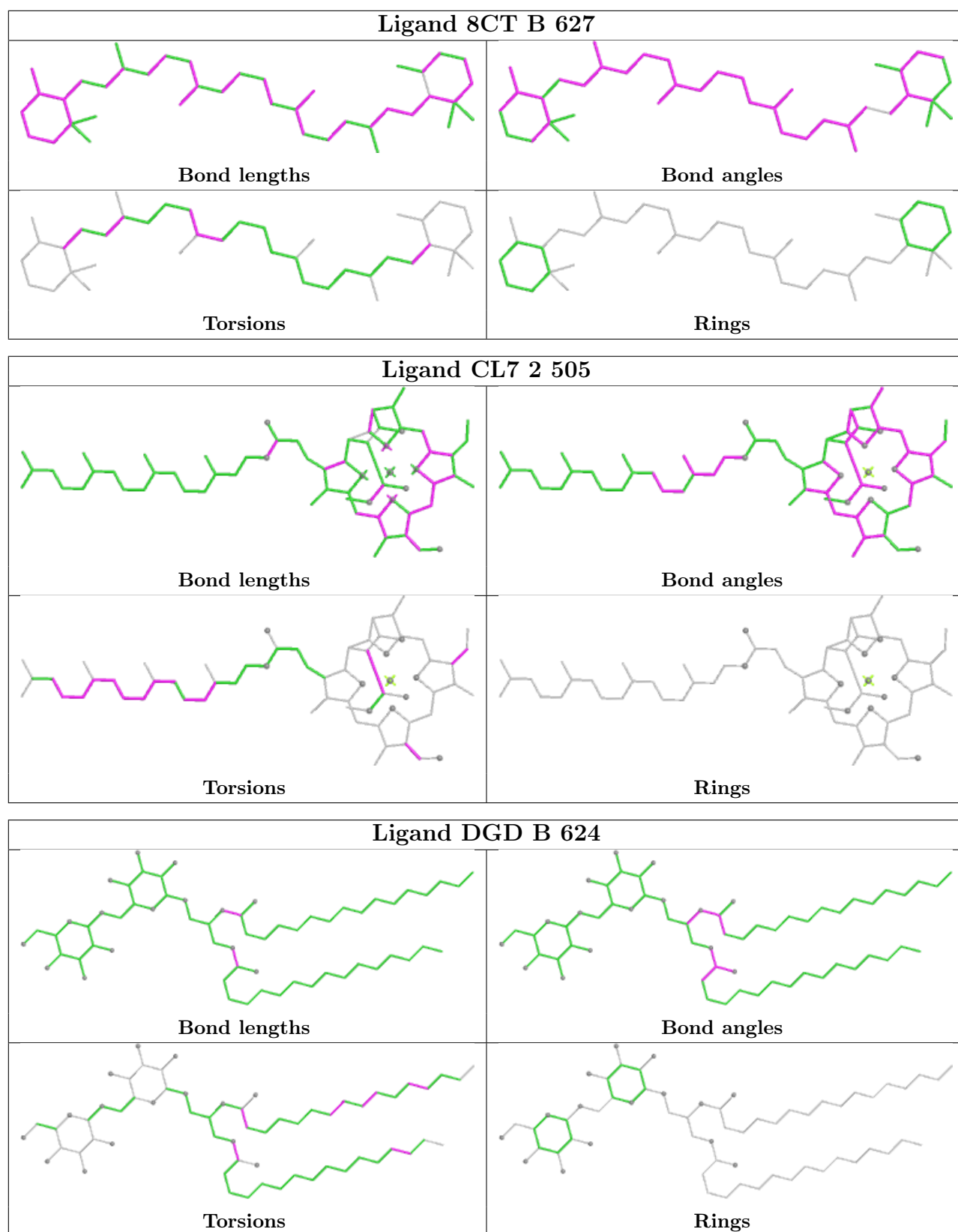
Rings

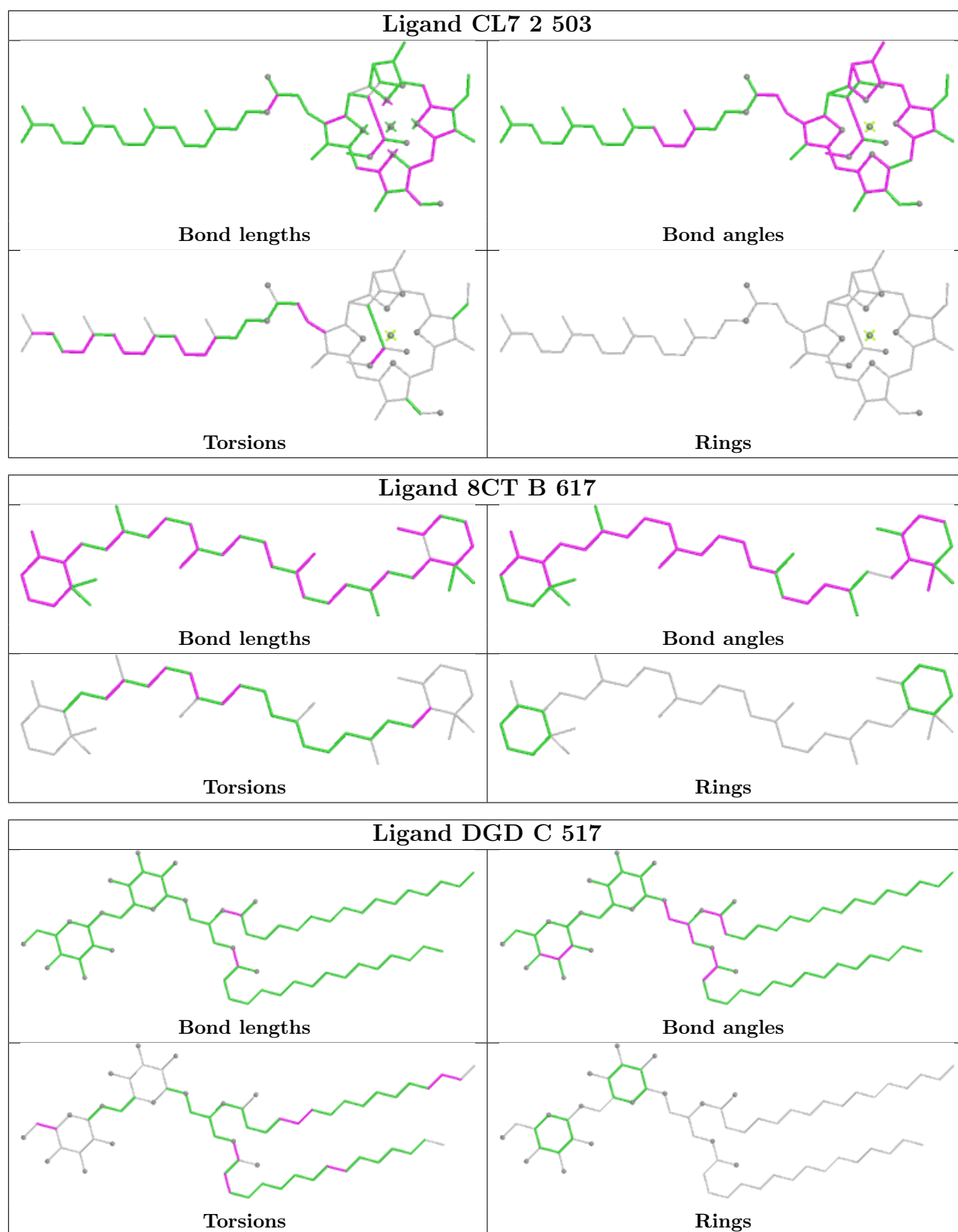
Ligand PHO a 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

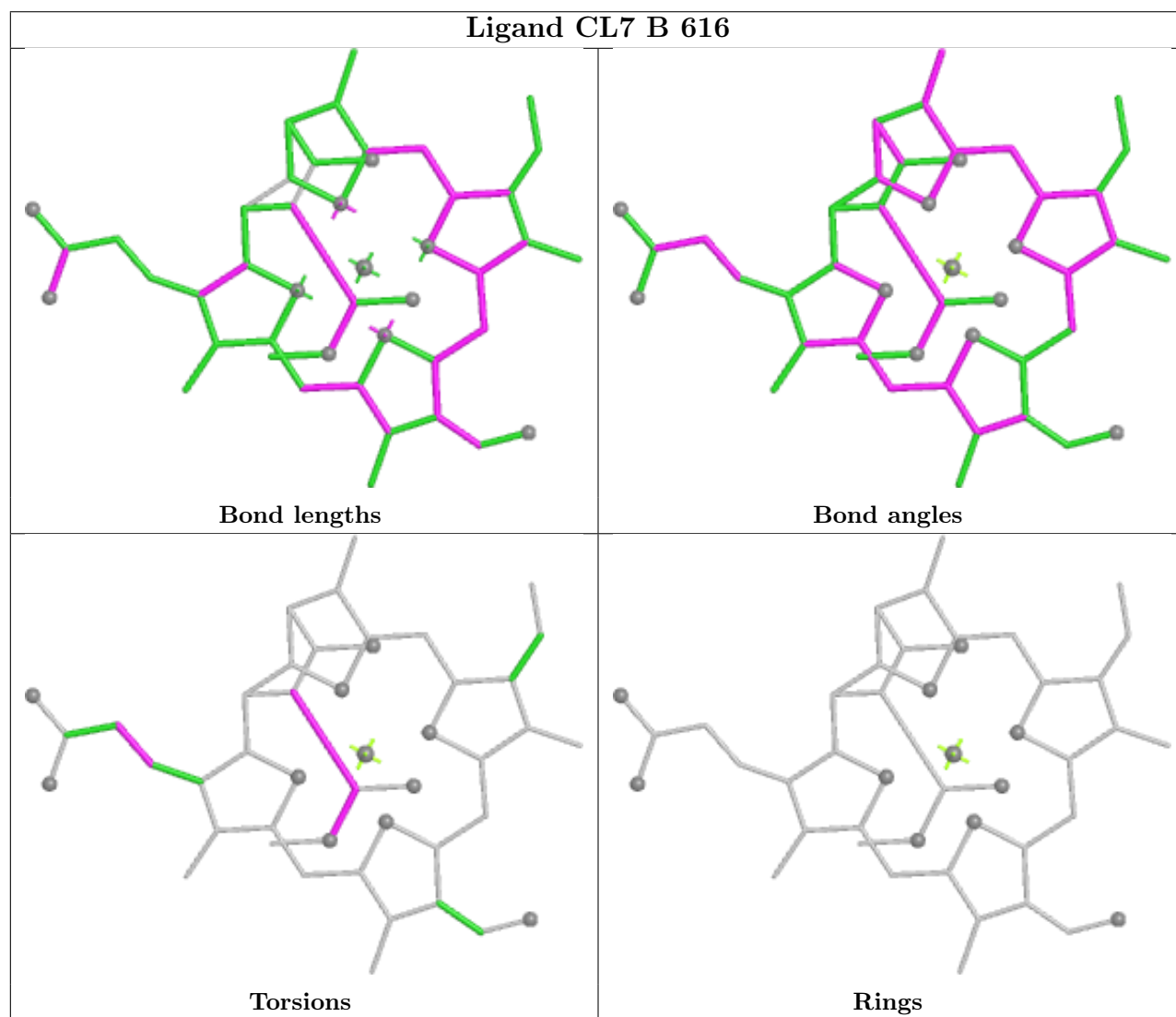
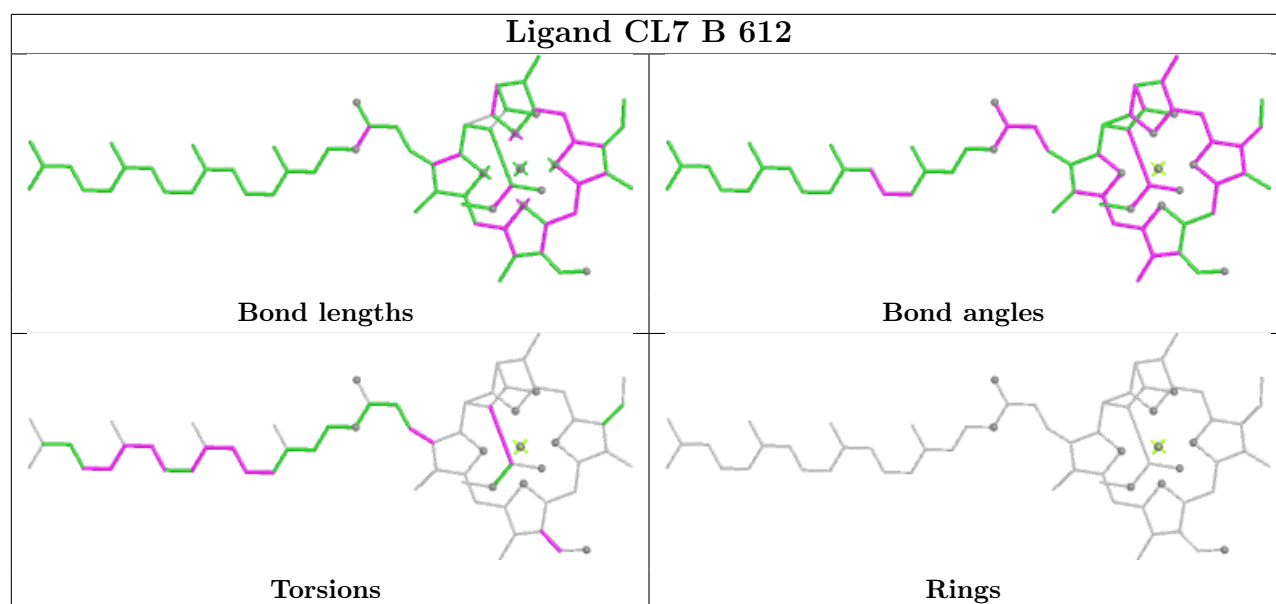
Ligand ZEX 3 525	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL7 1 404	
	
Bond lengths	Bond angles
	
Torsions	Rings

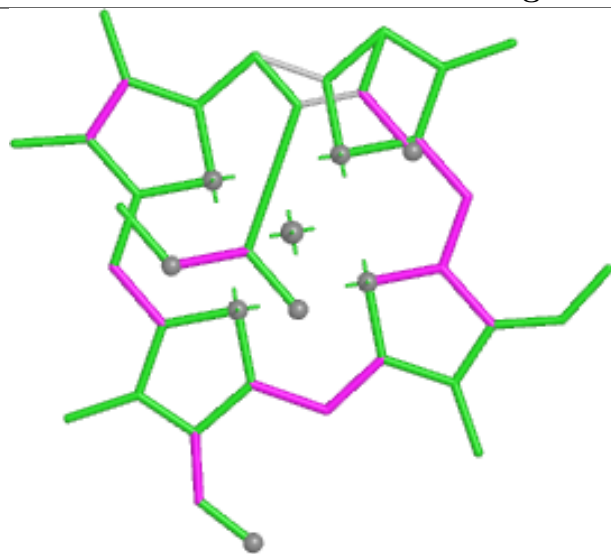




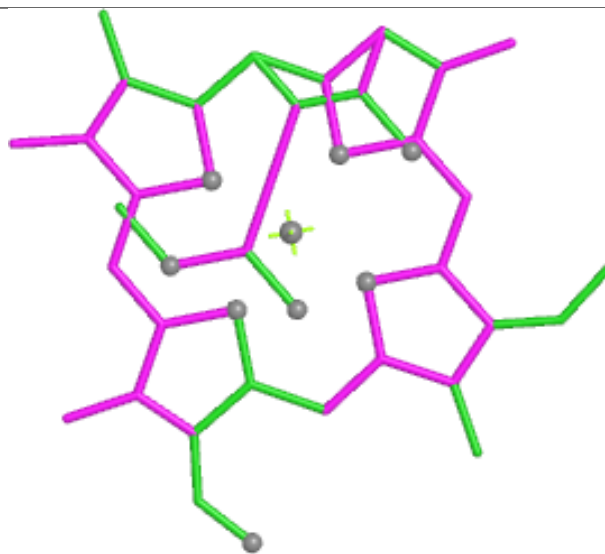




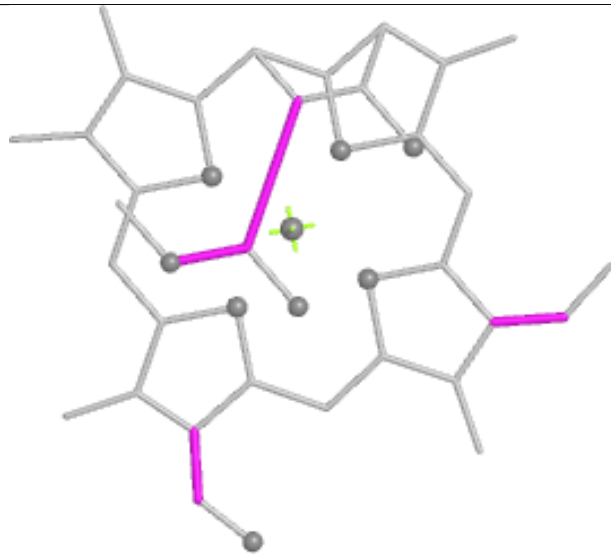
Ligand CL7 1 415



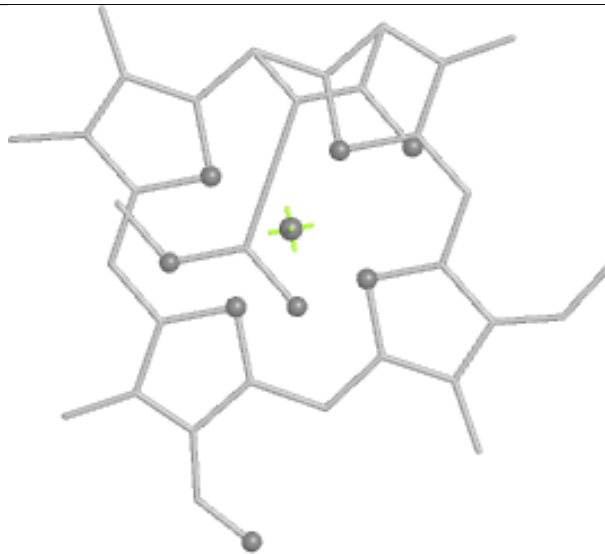
Bond lengths



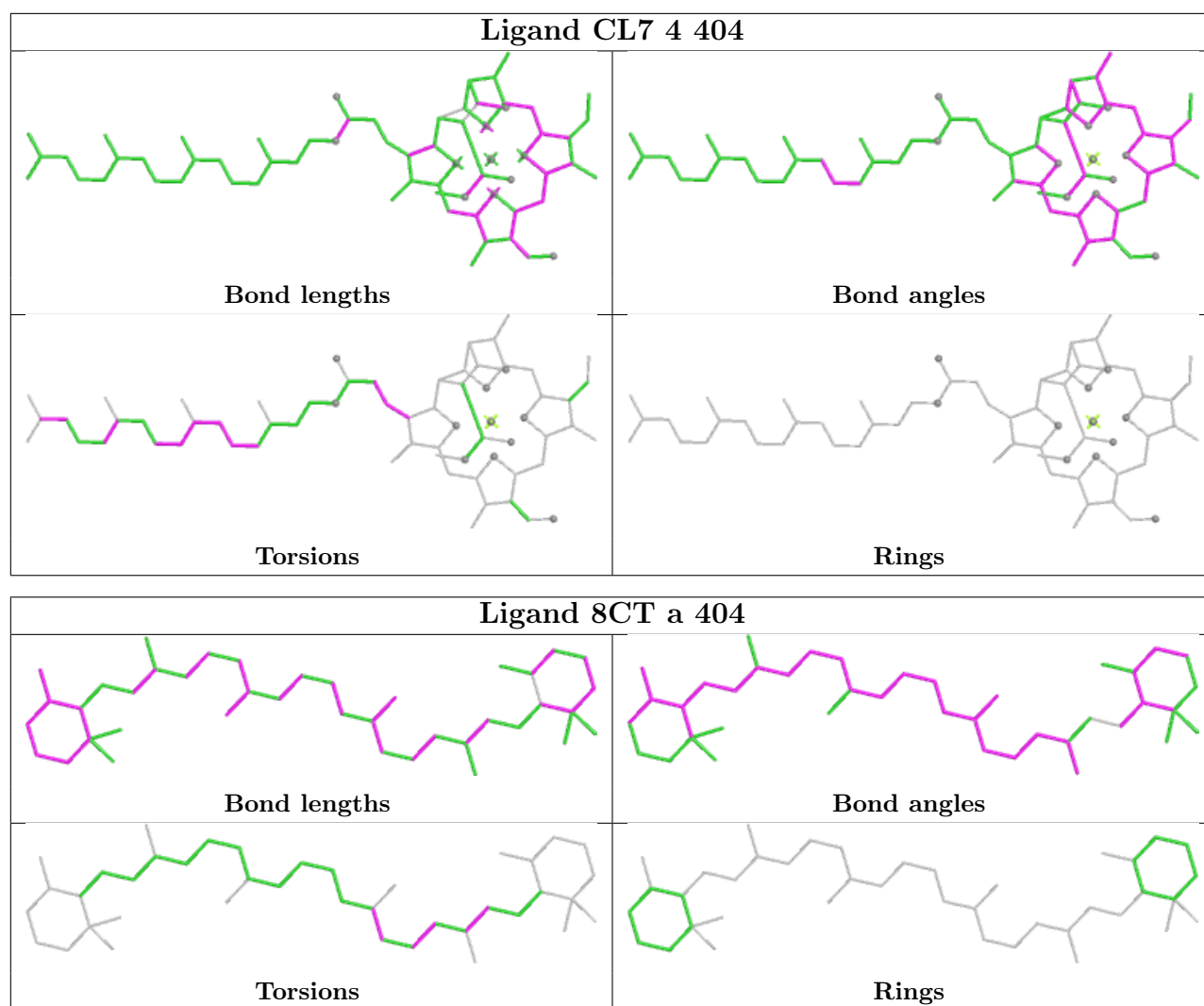
Bond angles

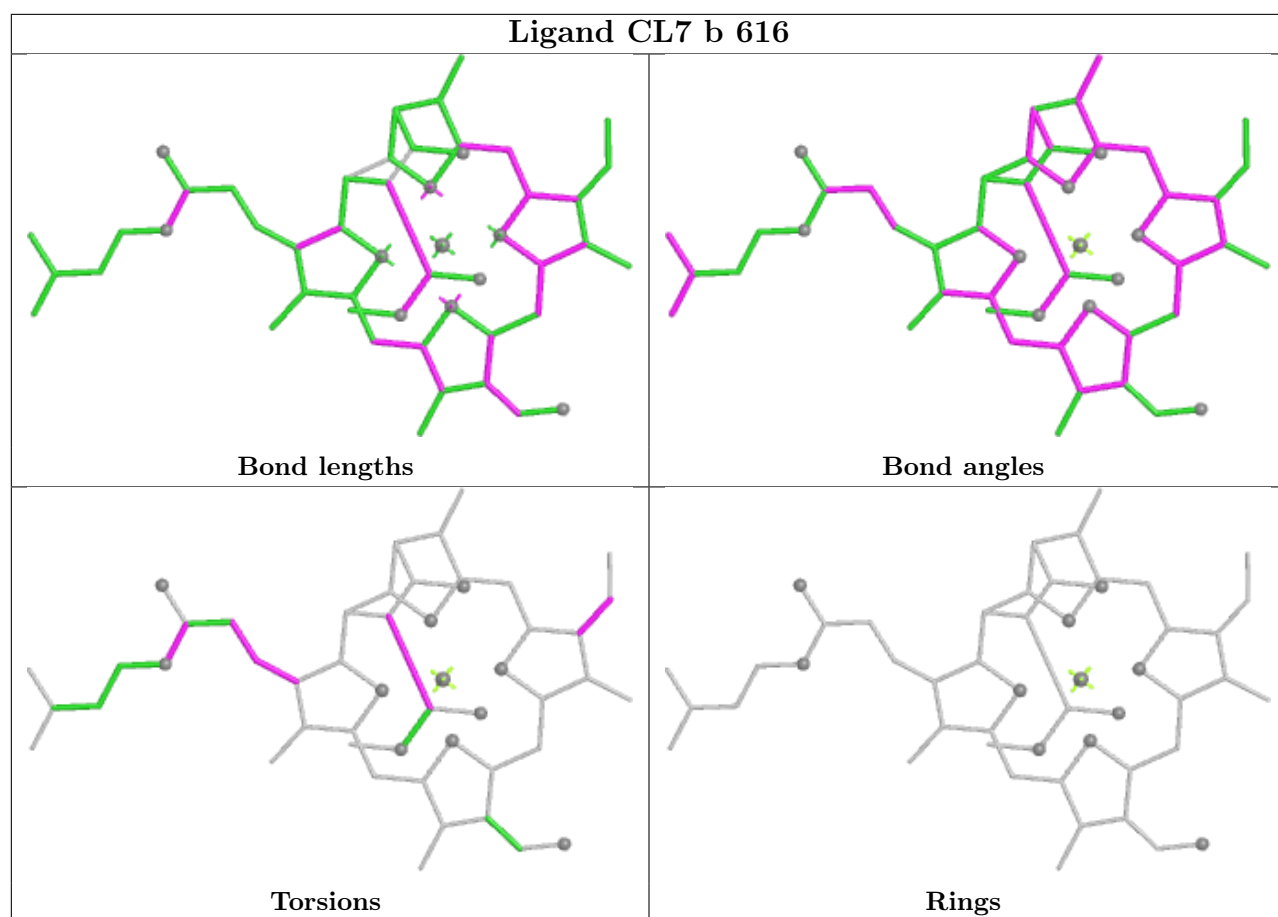


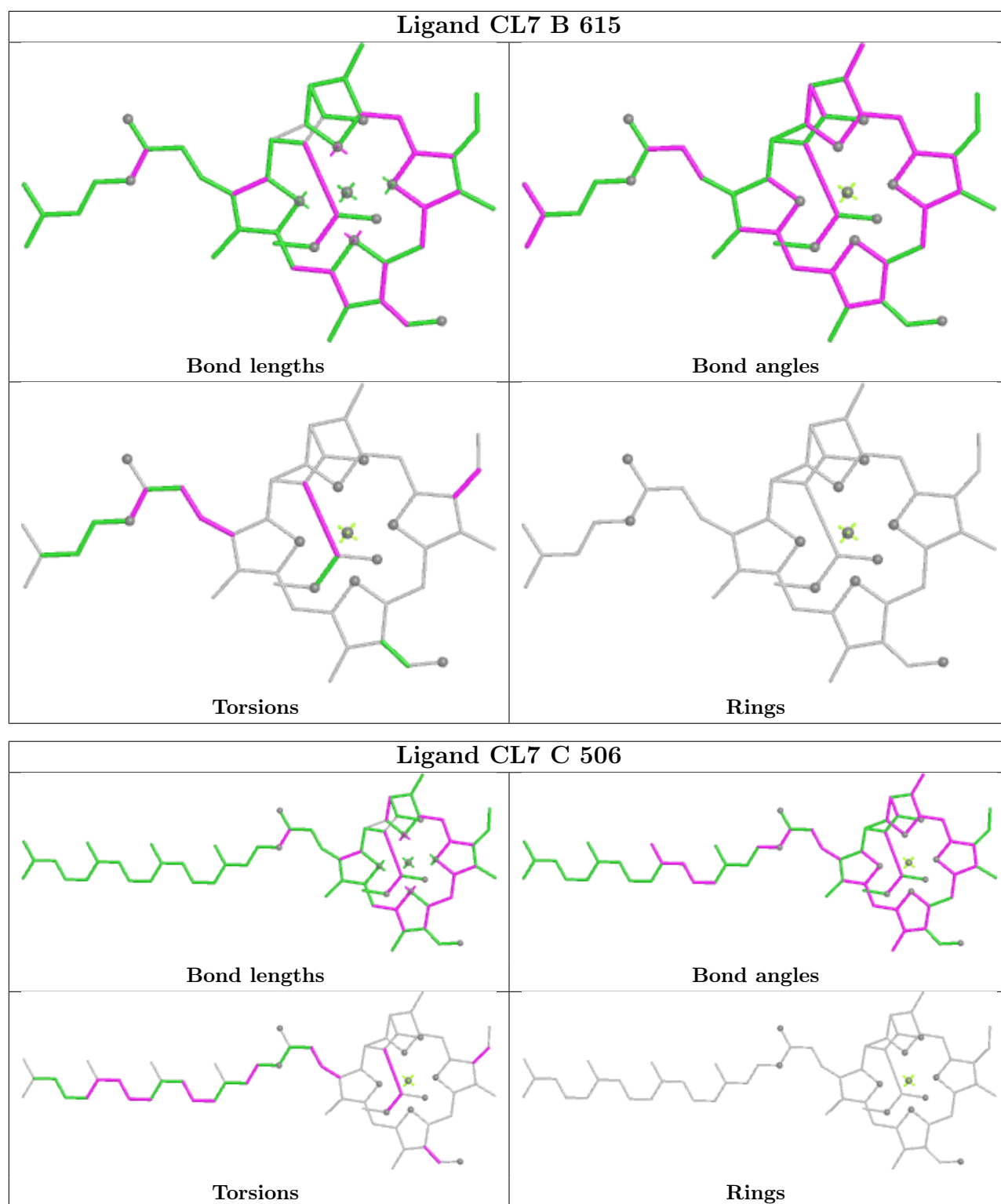
Torsions



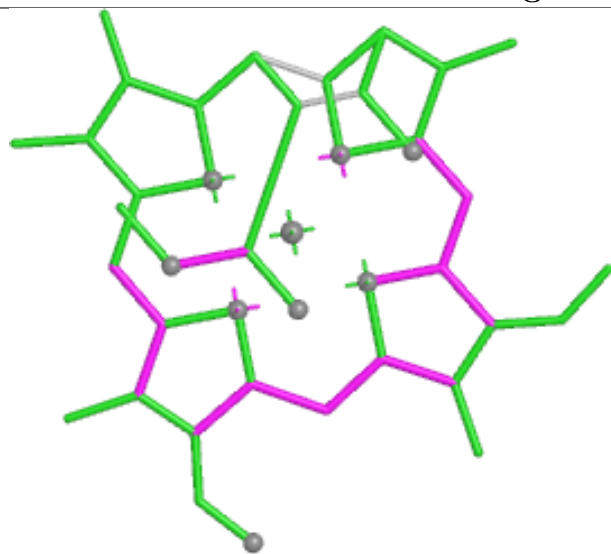
Rings



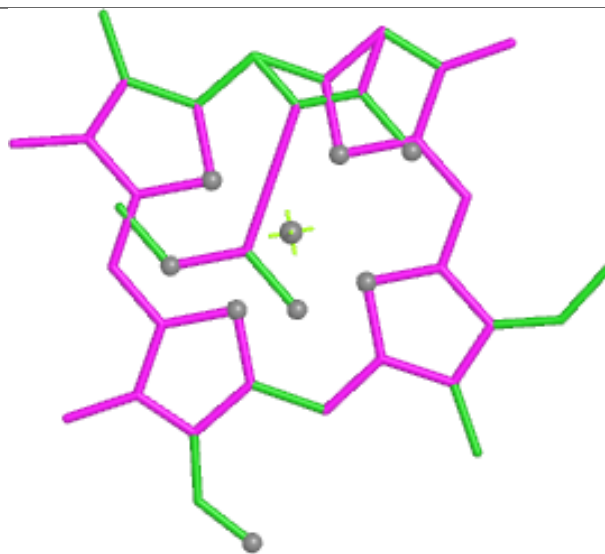




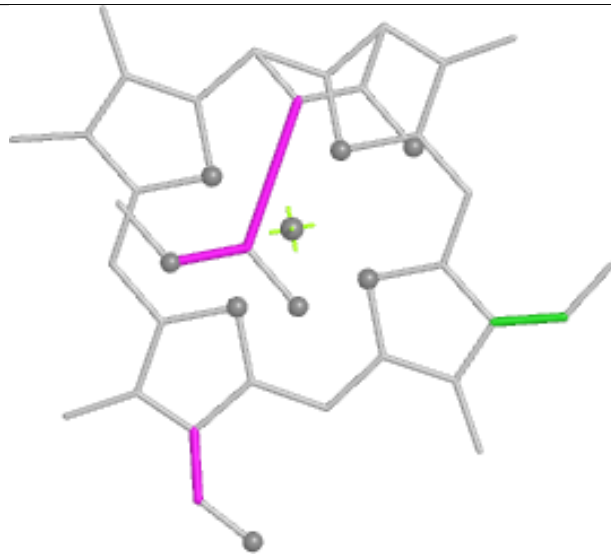
Ligand CL7 c 518



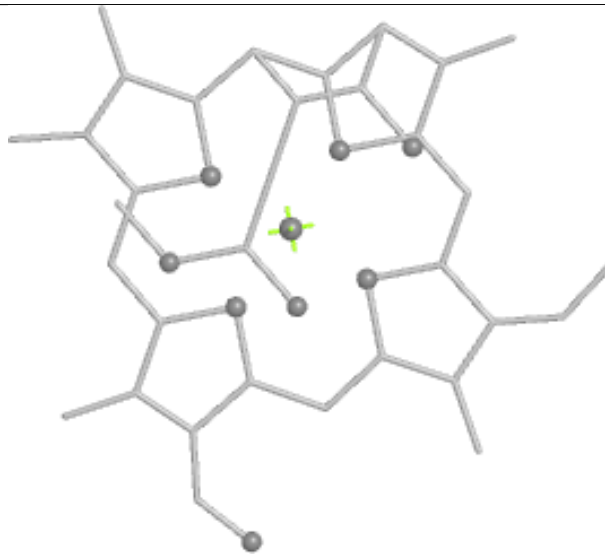
Bond lengths



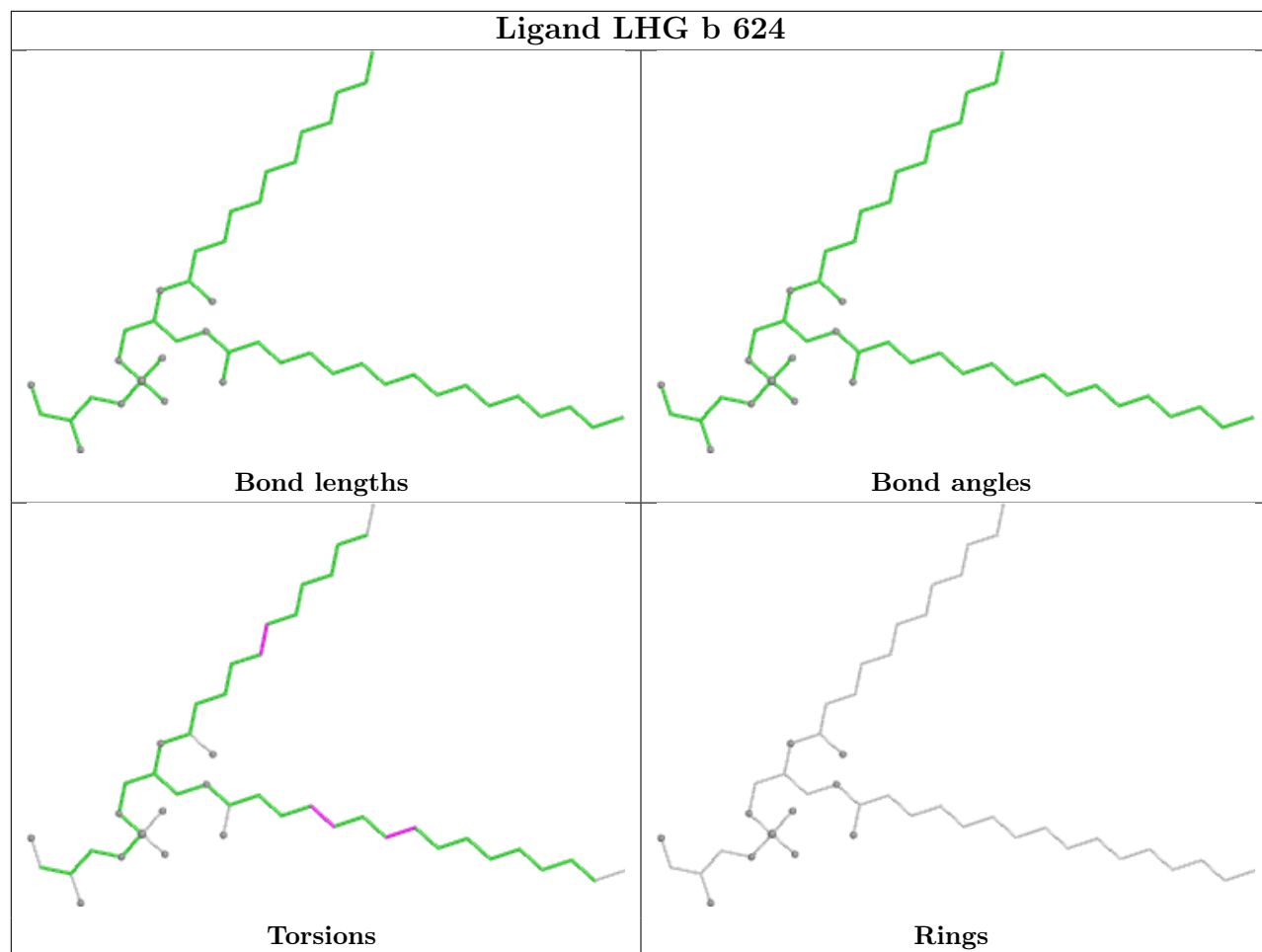
Bond angles



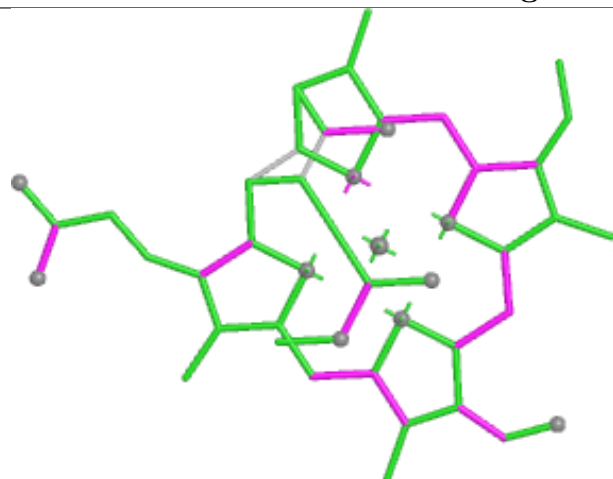
Torsions



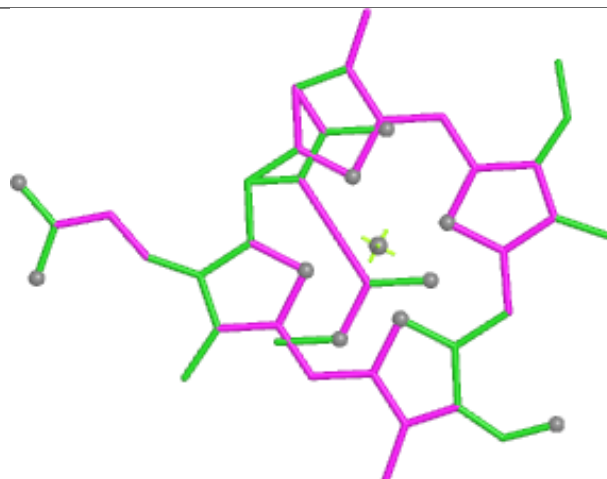
Rings



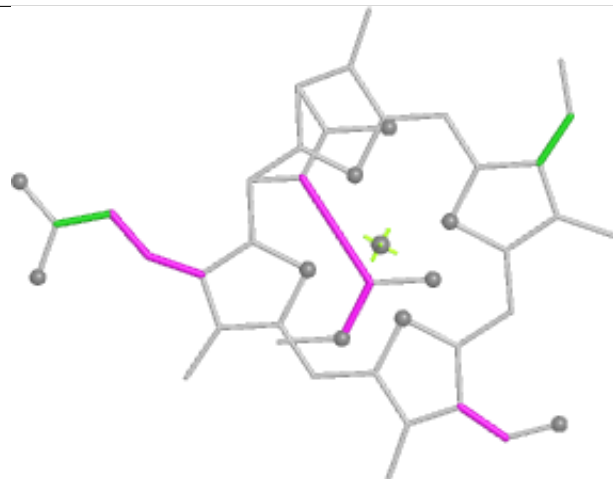
Ligand CL7 C 514



Bond lengths



Bond angles

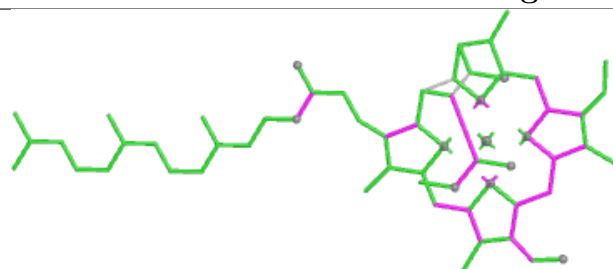


Torsions

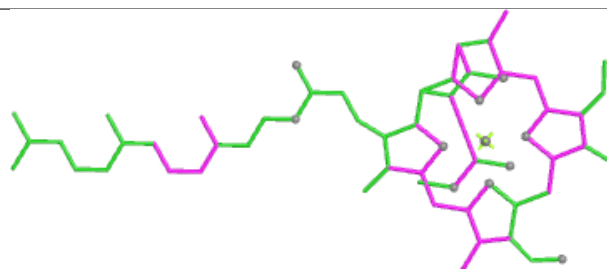


Rings

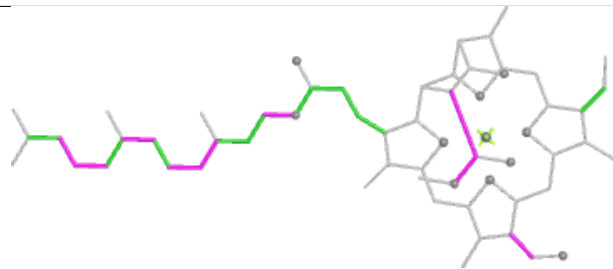
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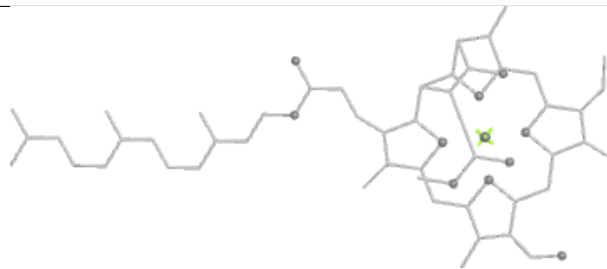
Bond lengths



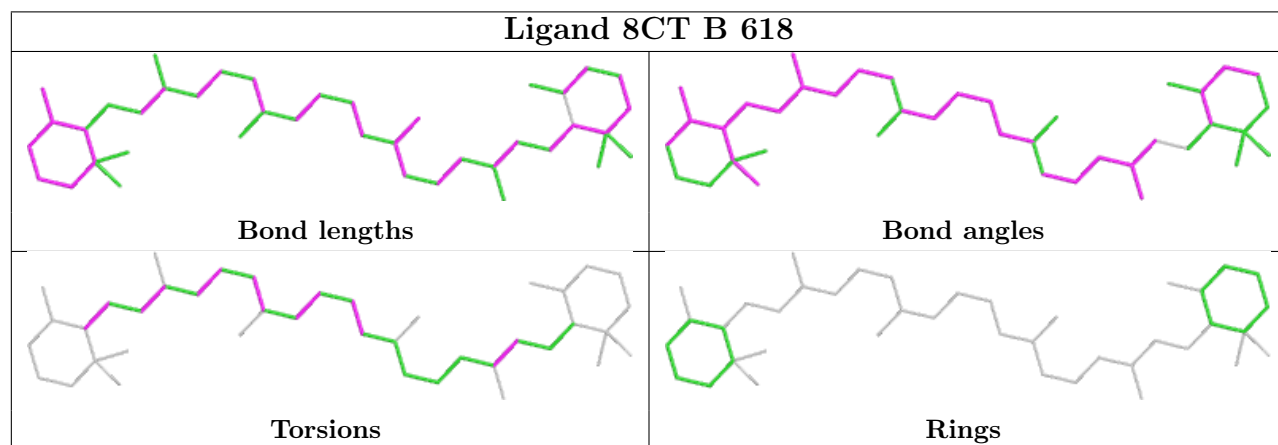
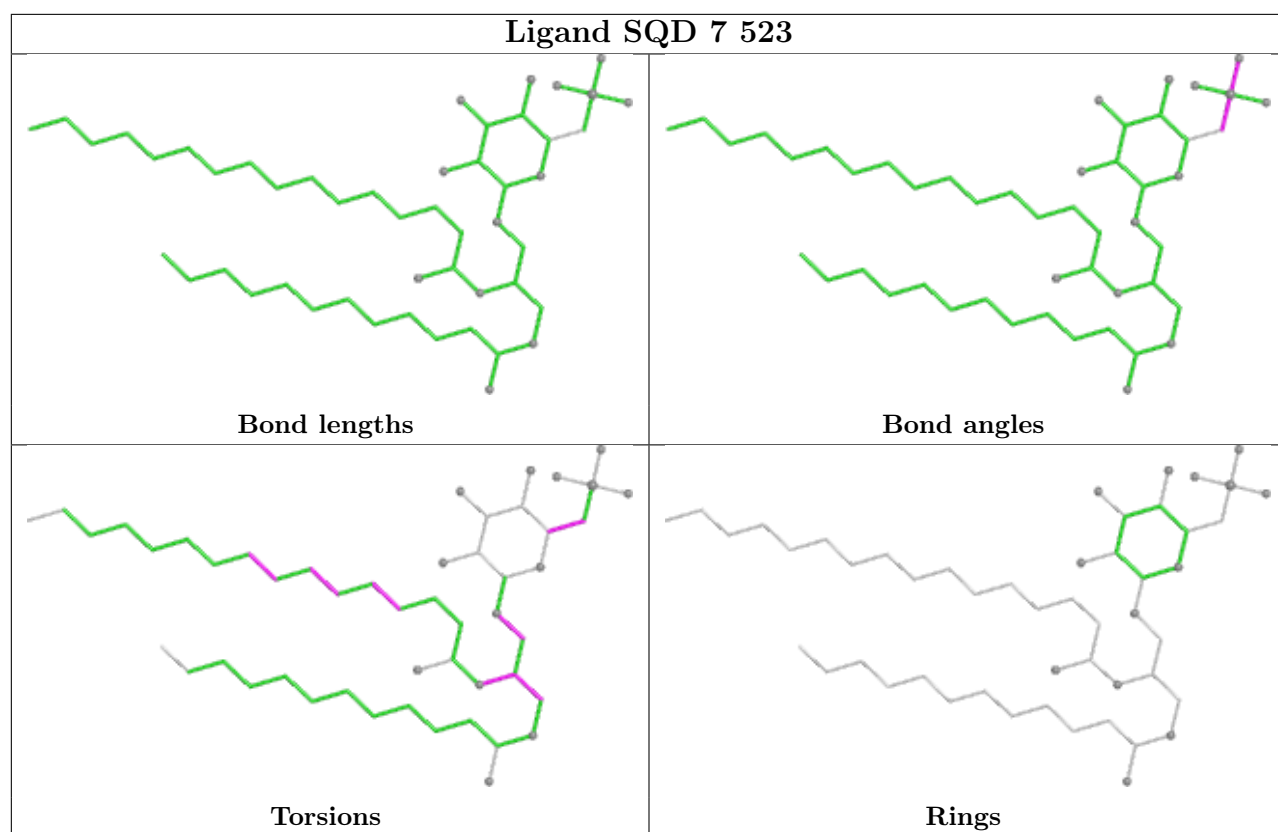
Bond angles

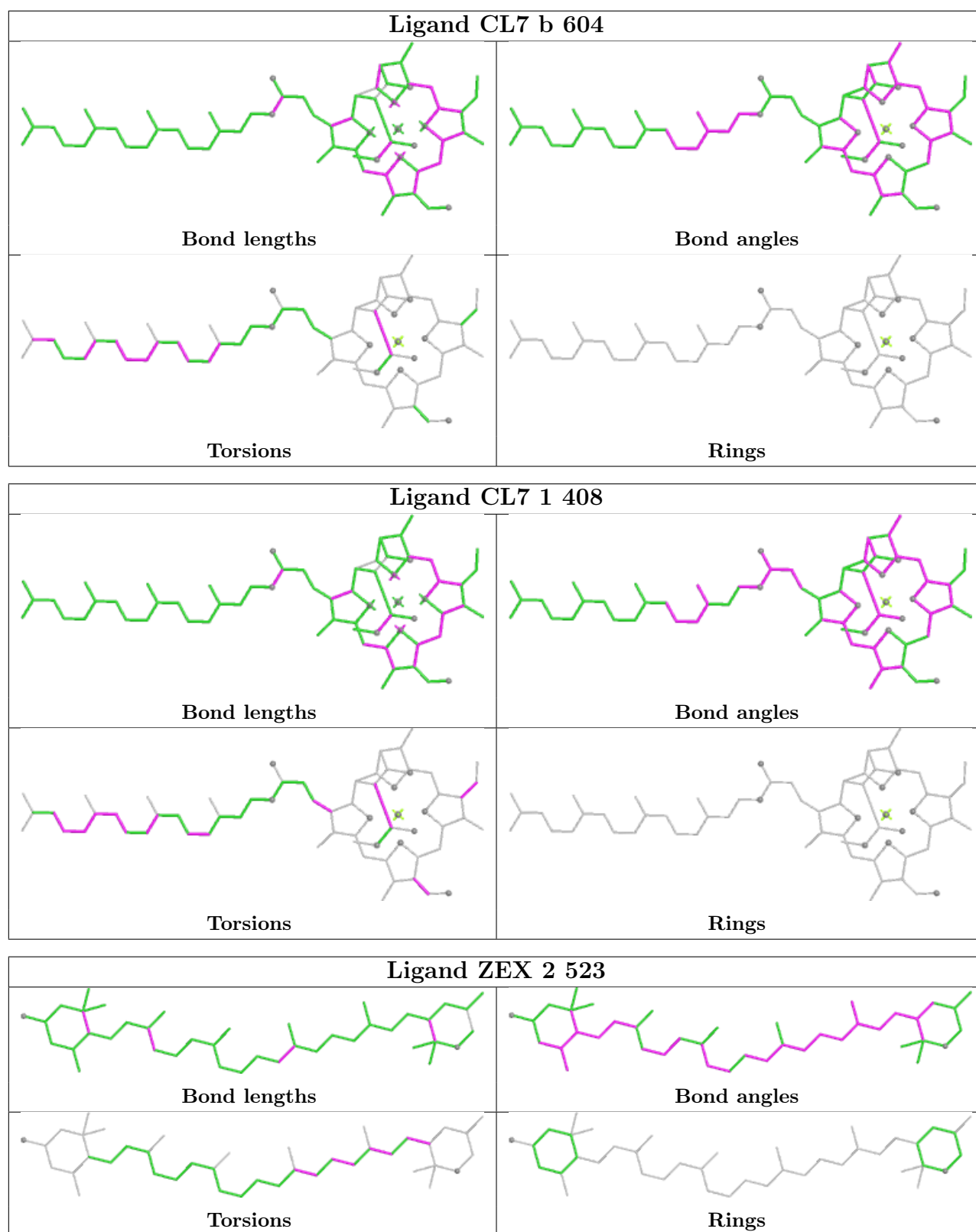


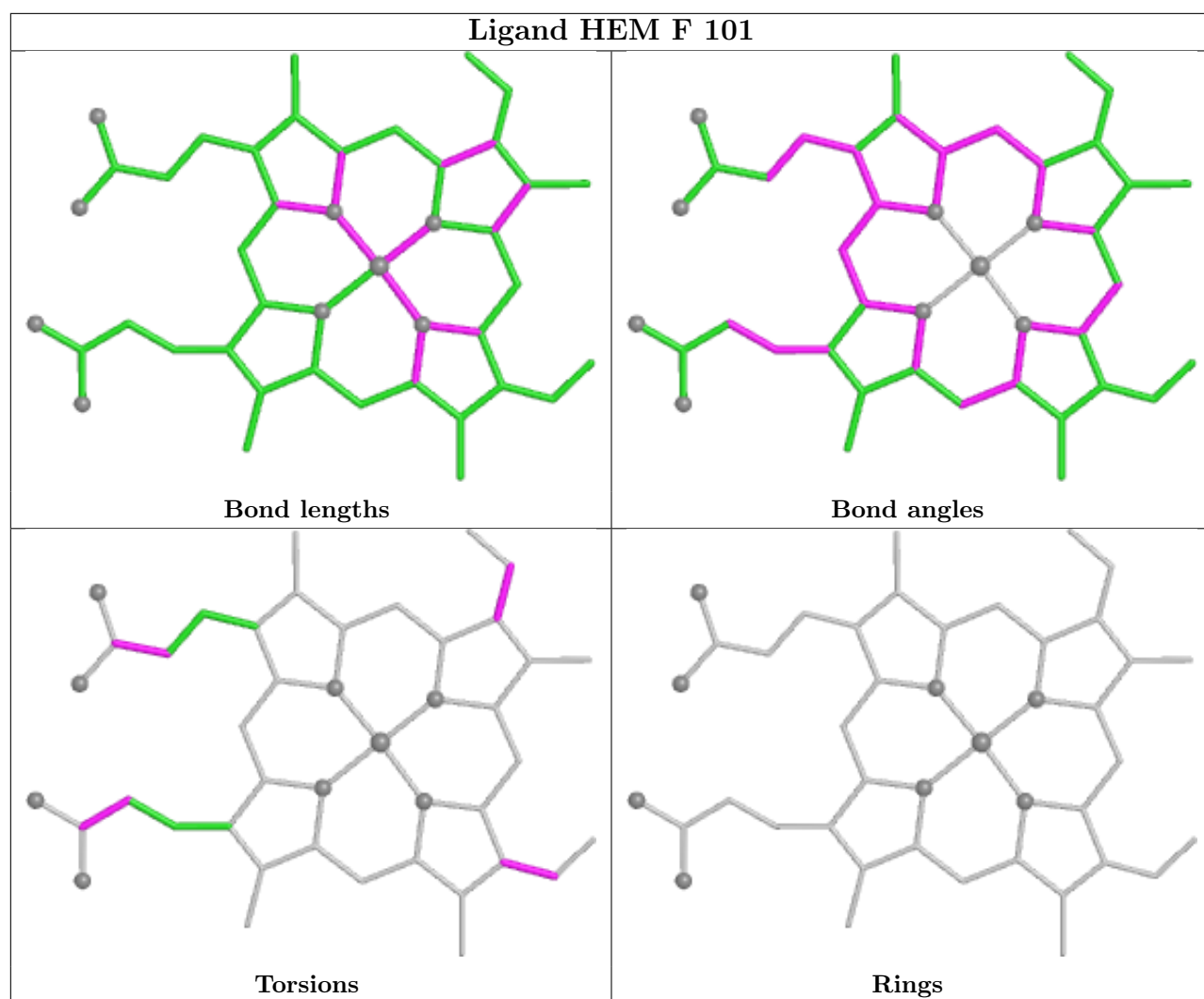
Torsions



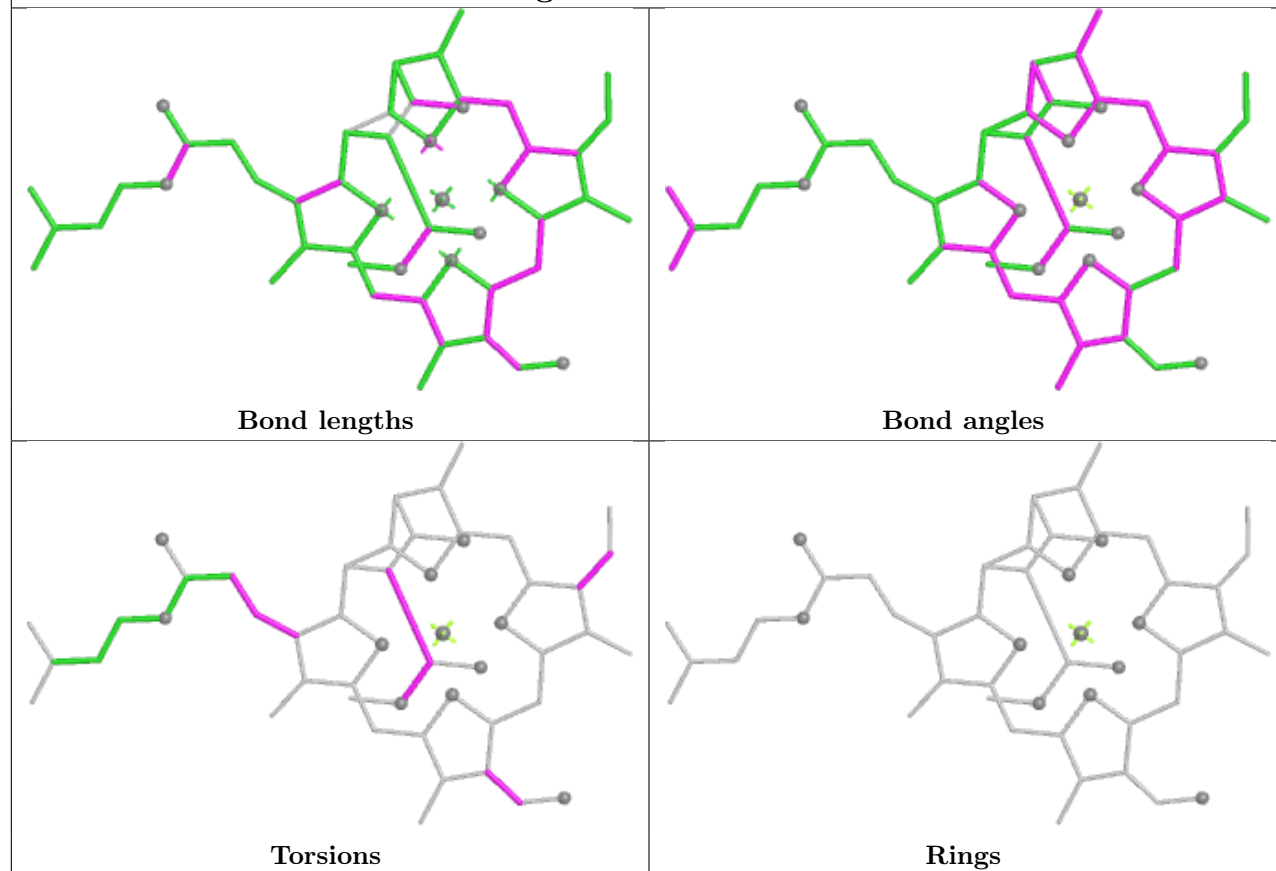
Rings



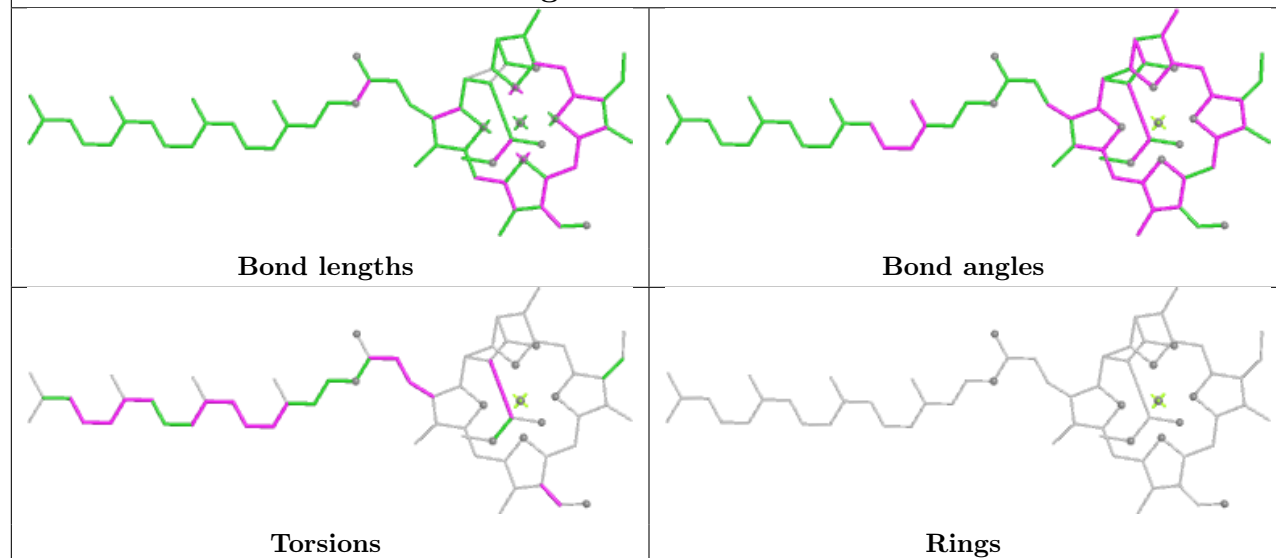


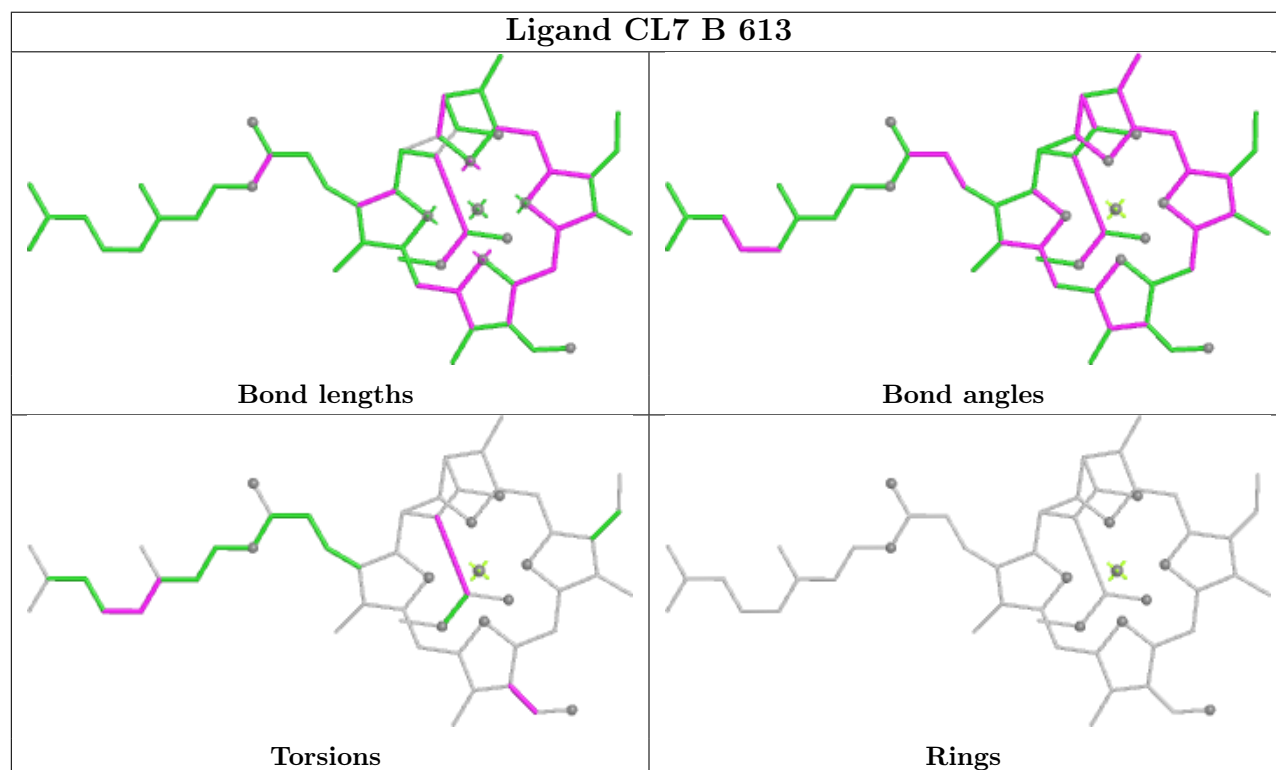
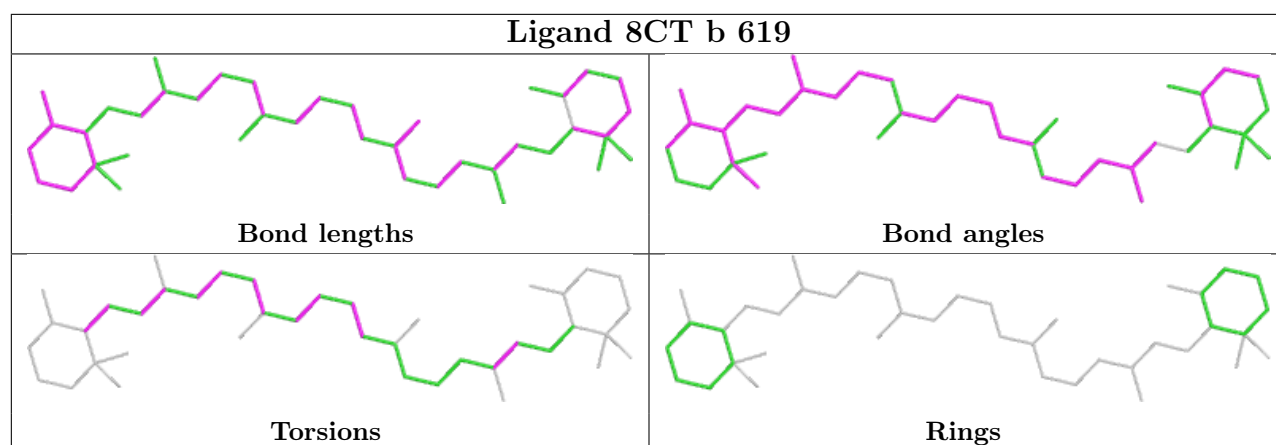


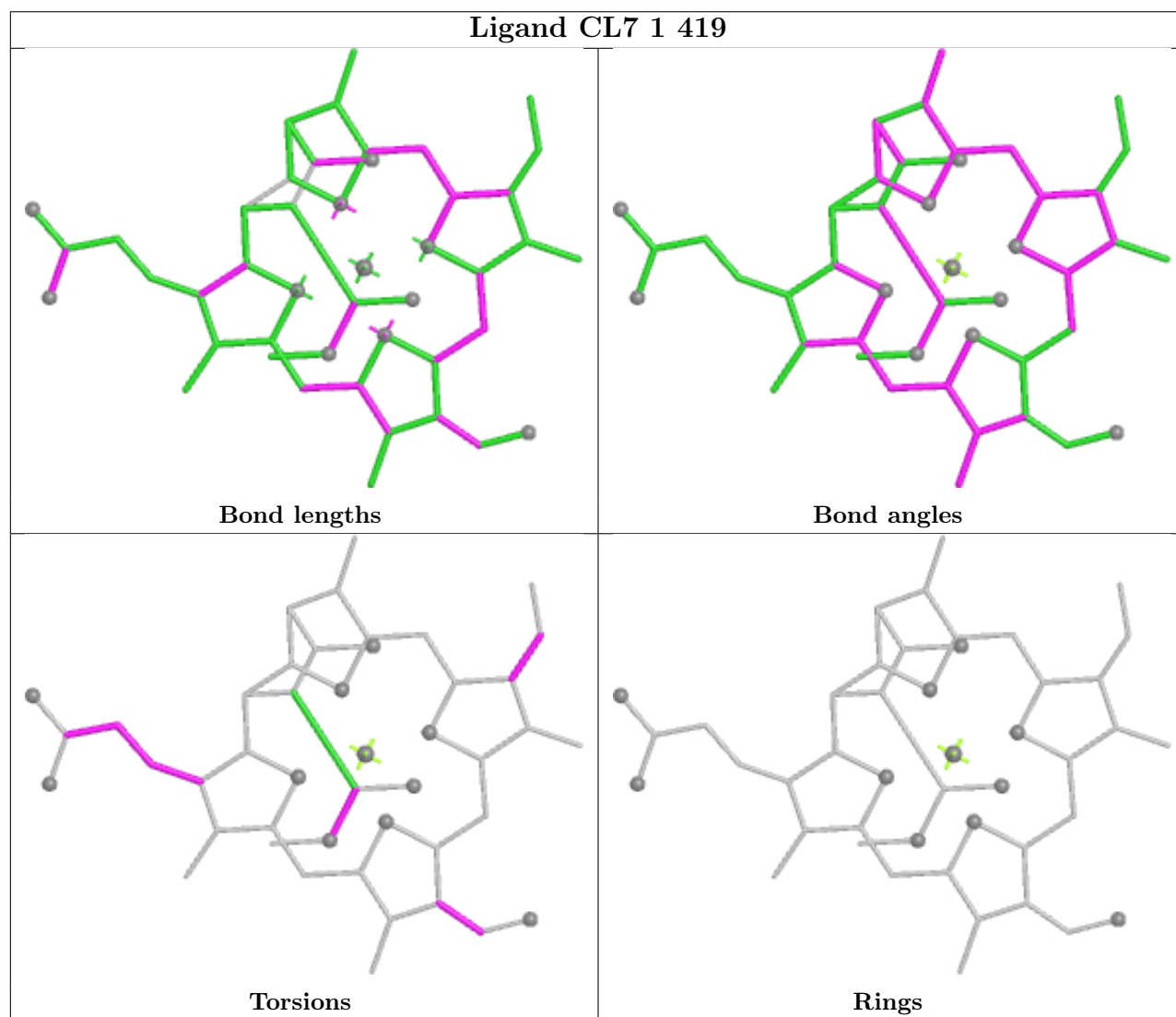
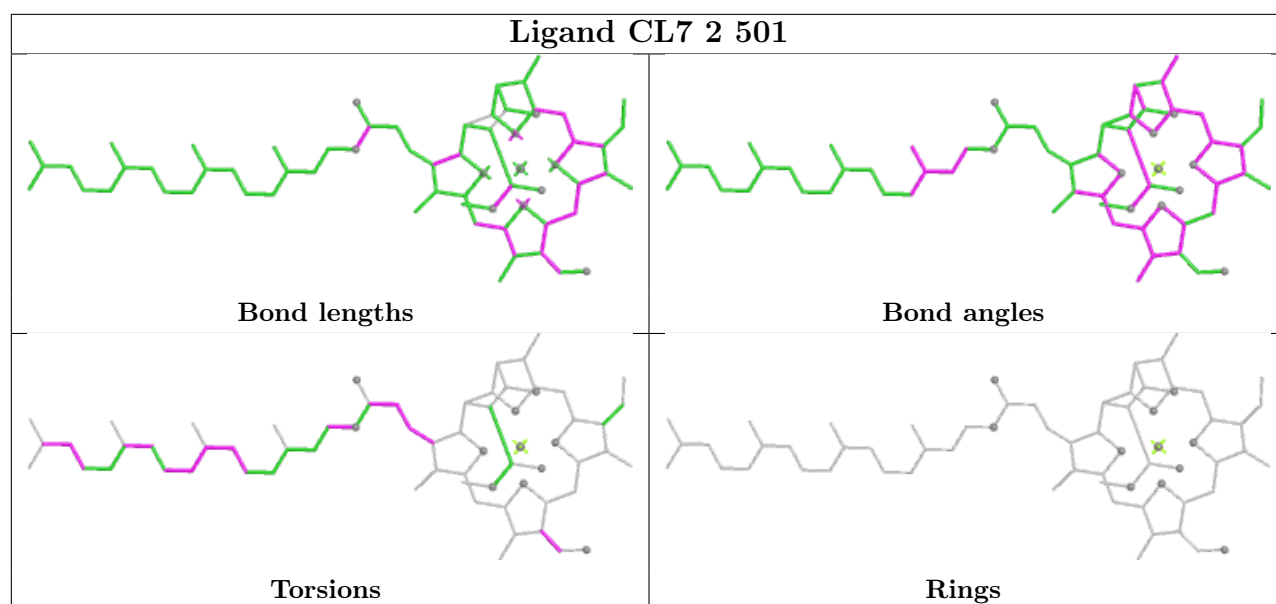
Ligand CL7 D 402



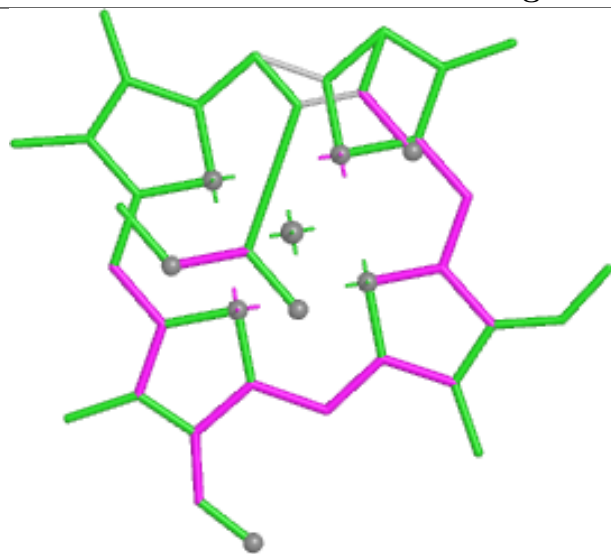
Ligand CL7 7 501



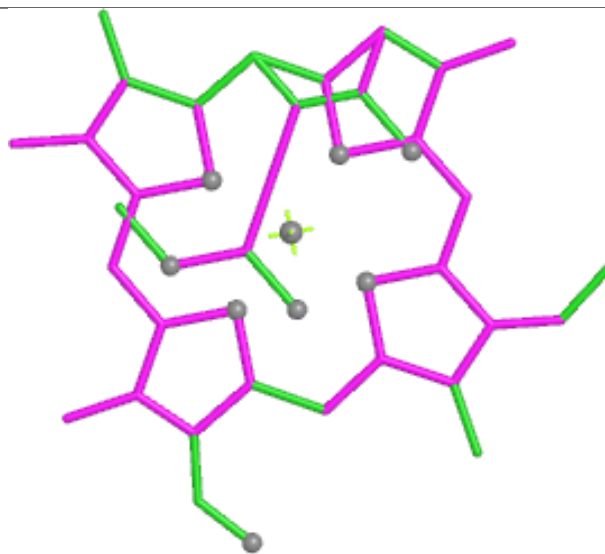




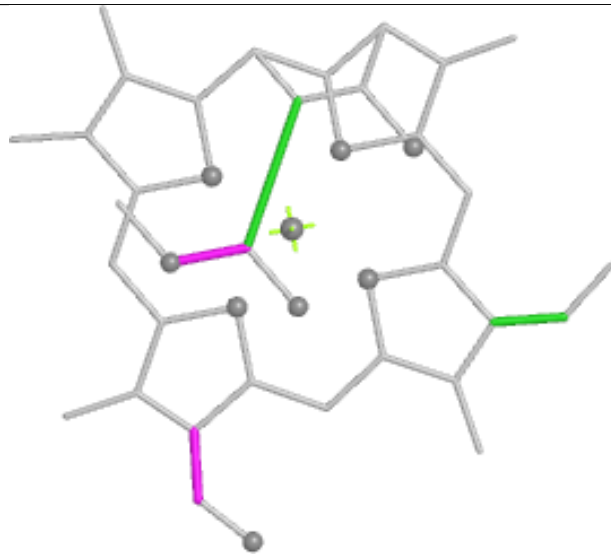
Ligand CL7 5 407



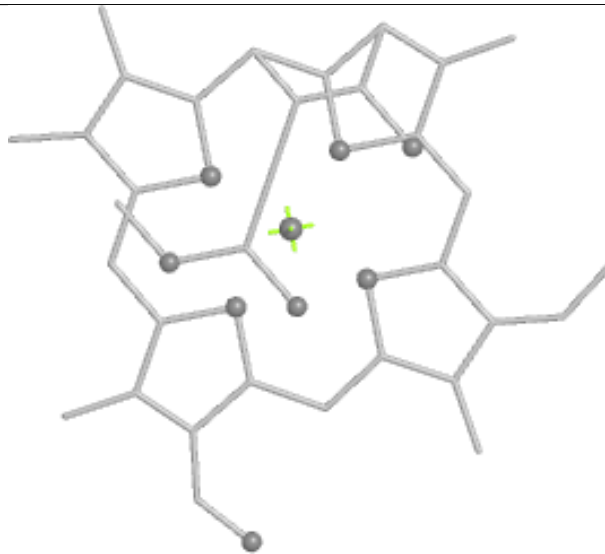
Bond lengths



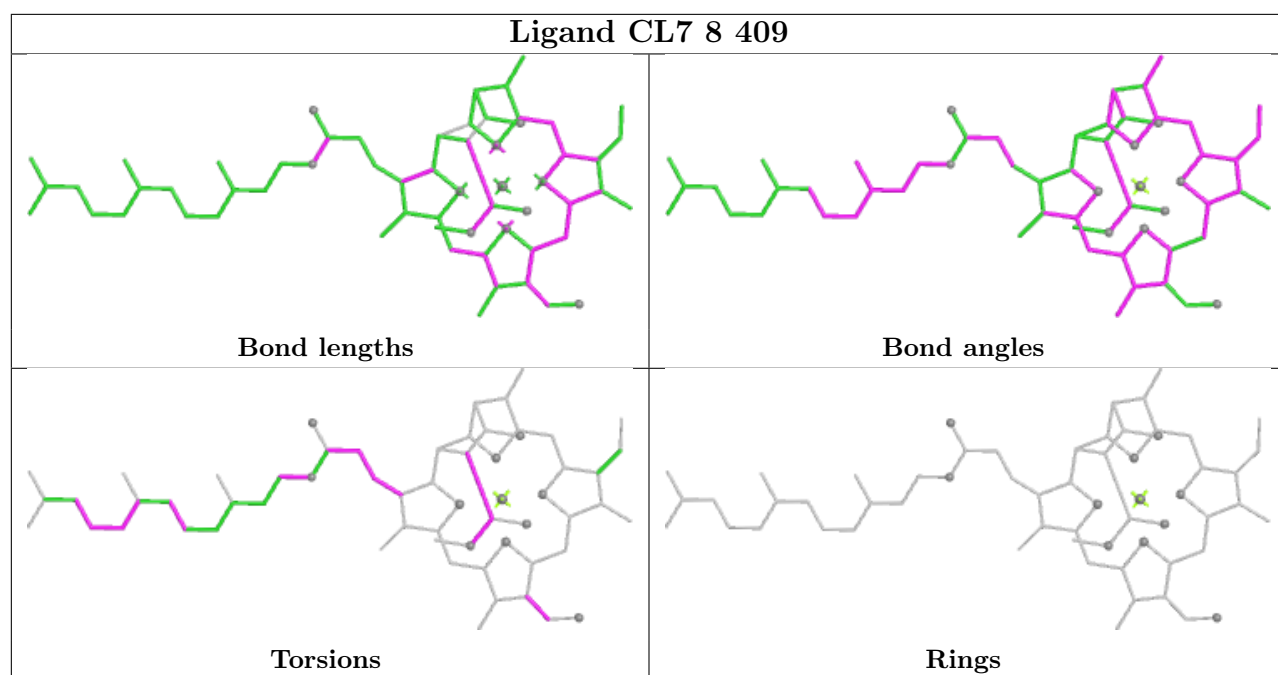
Bond angles



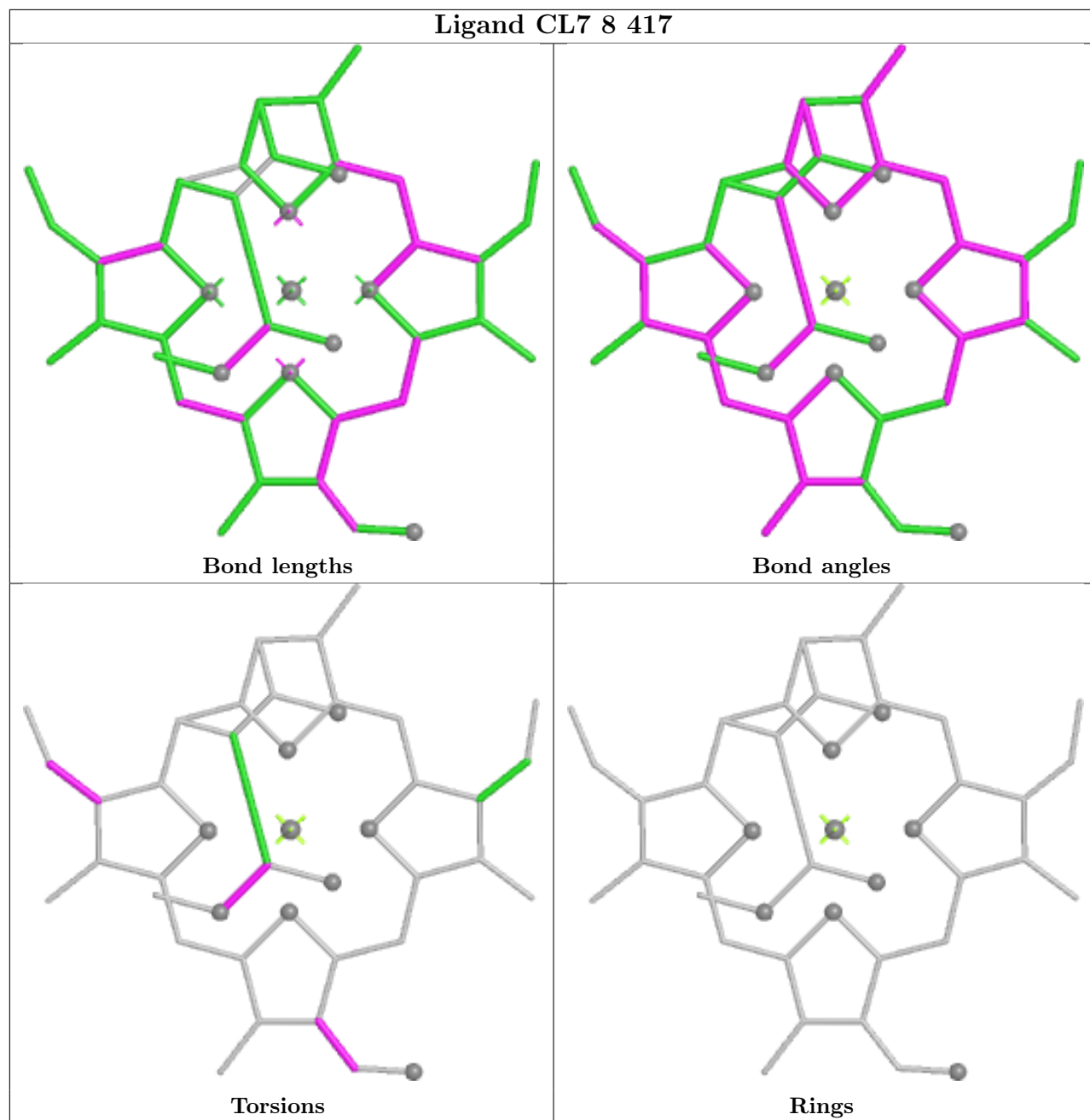
Torsions

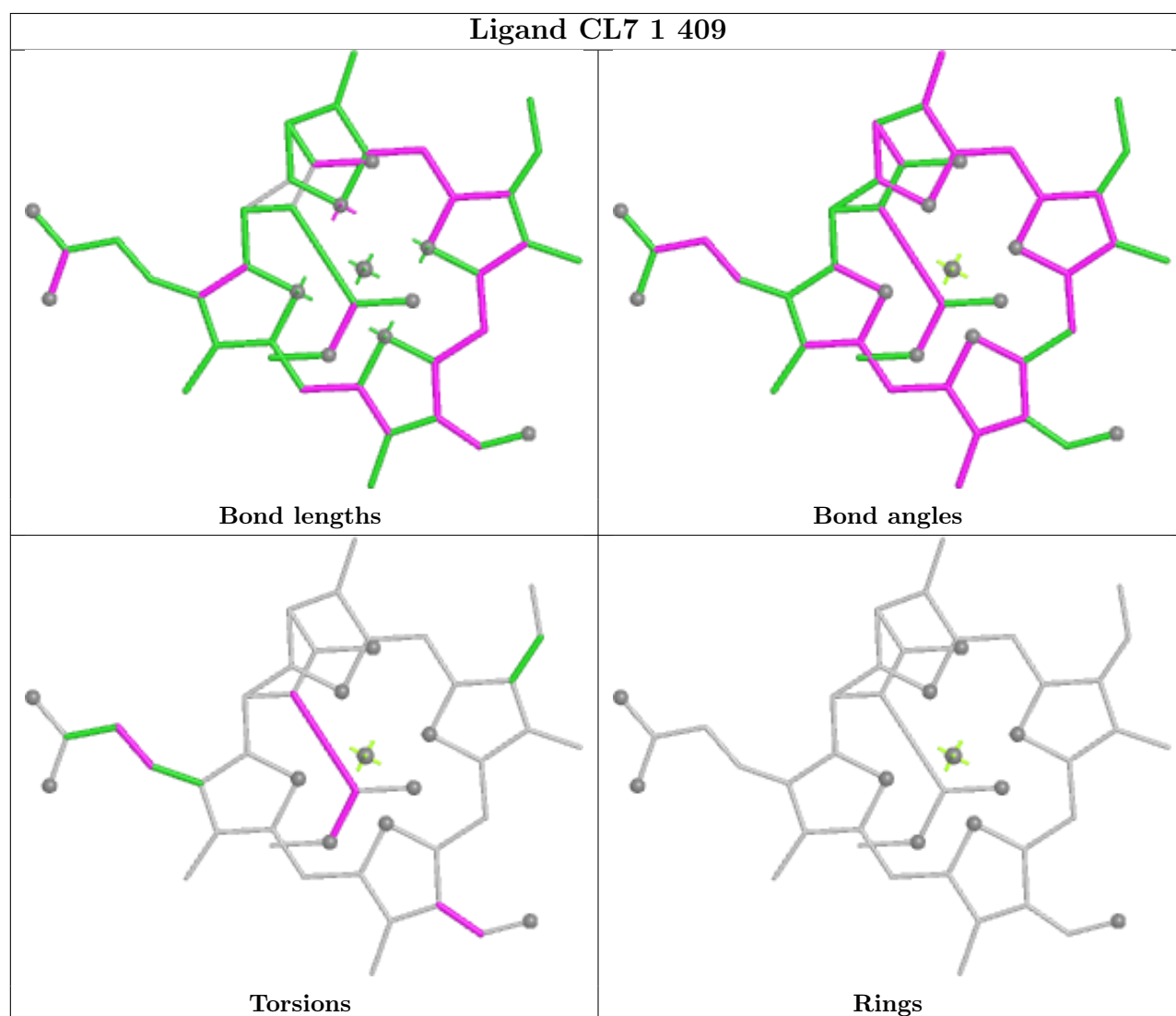
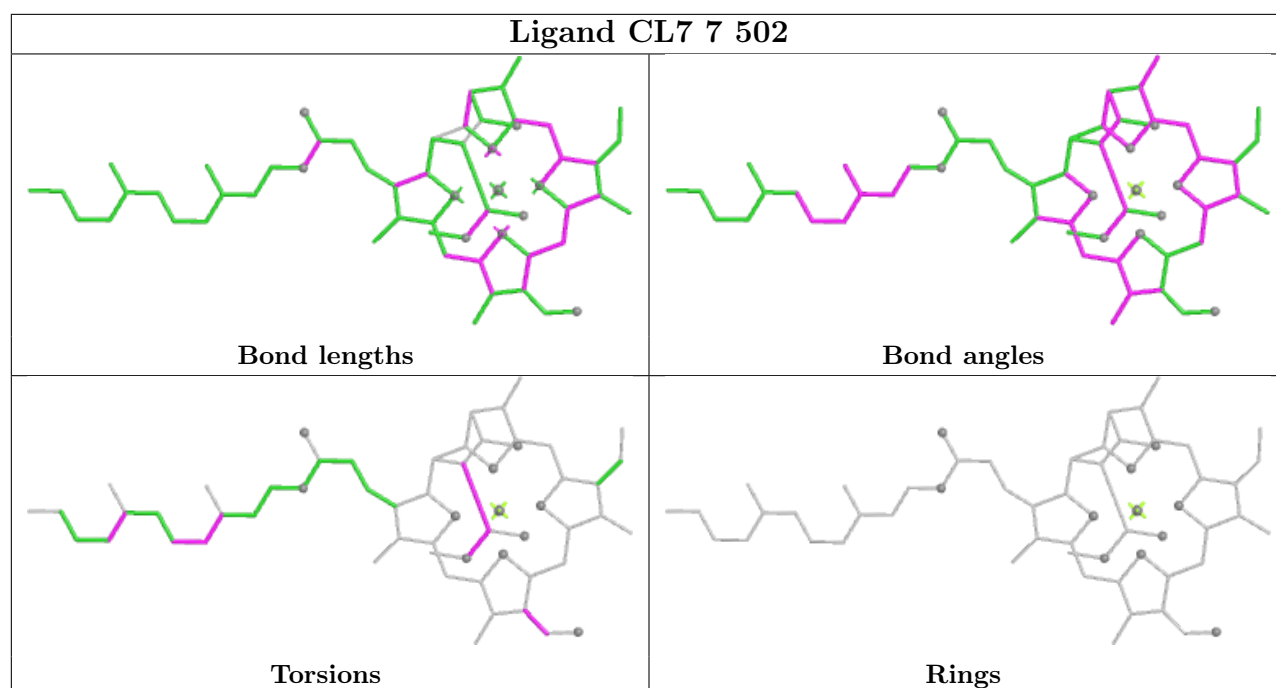


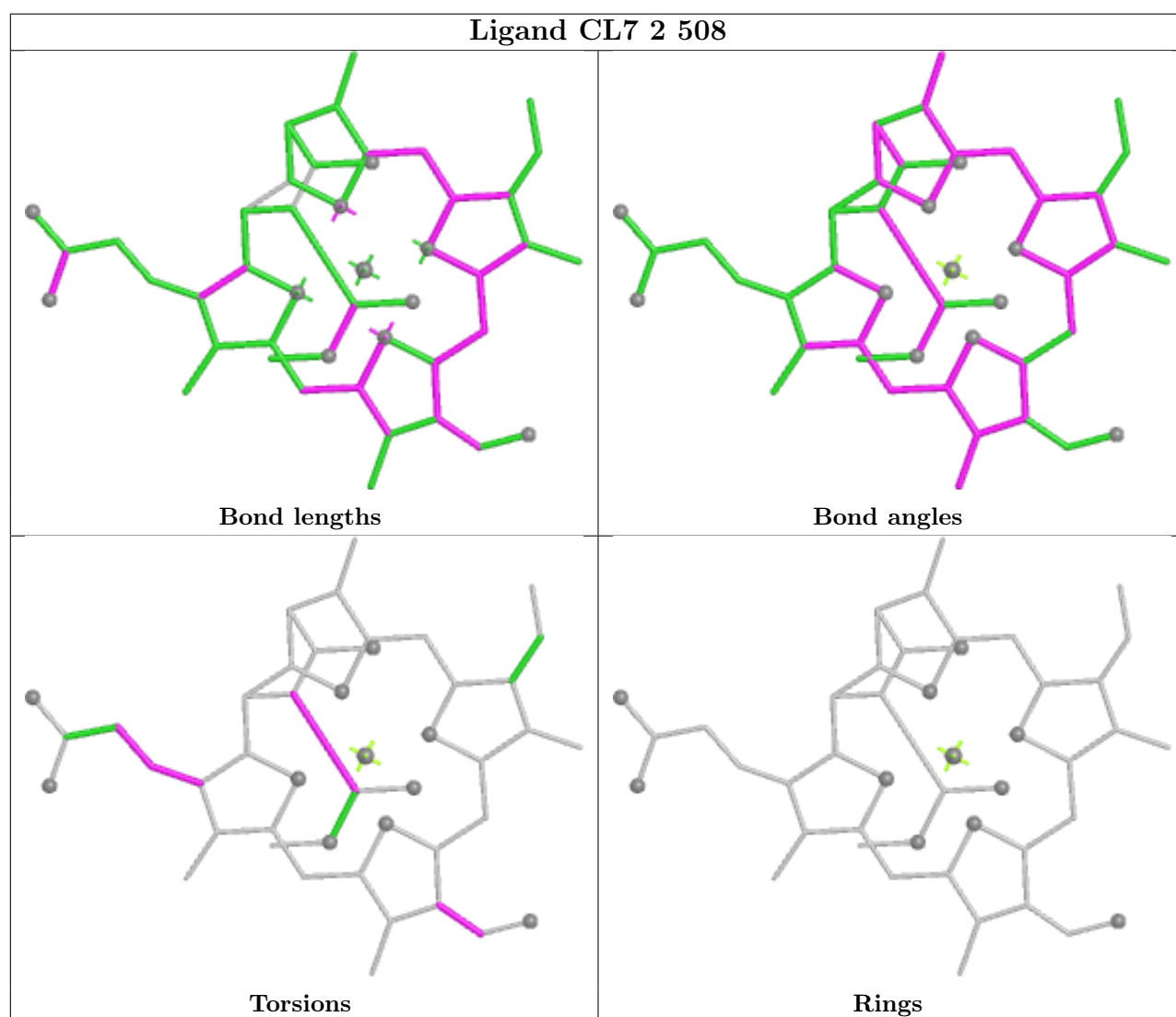
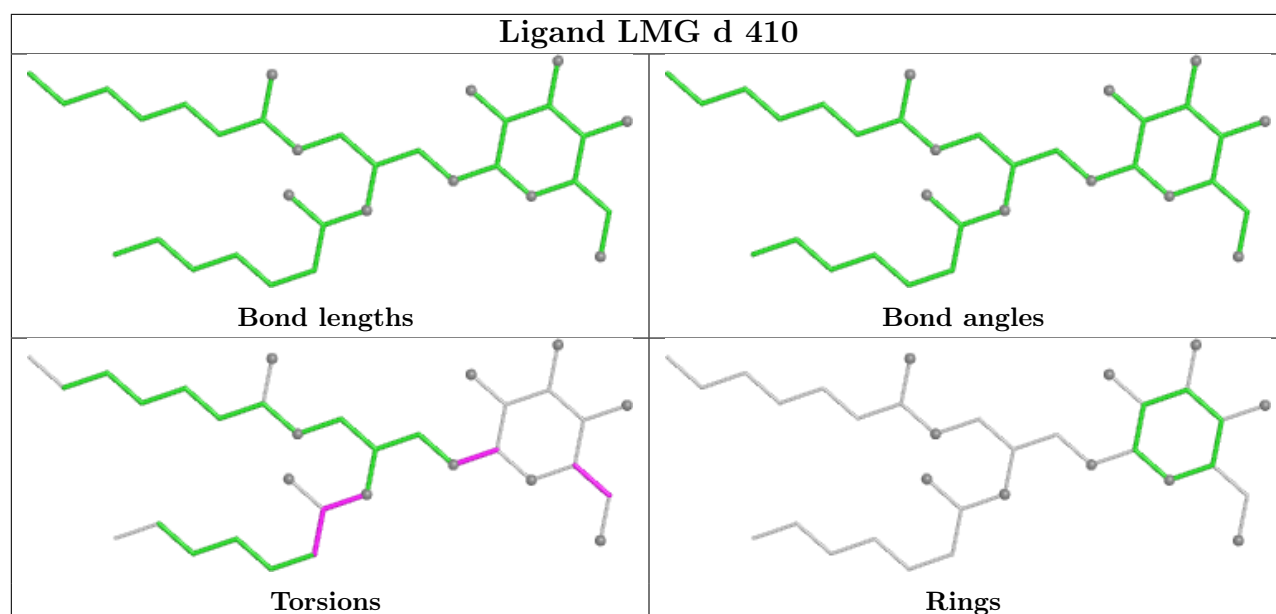
Rings

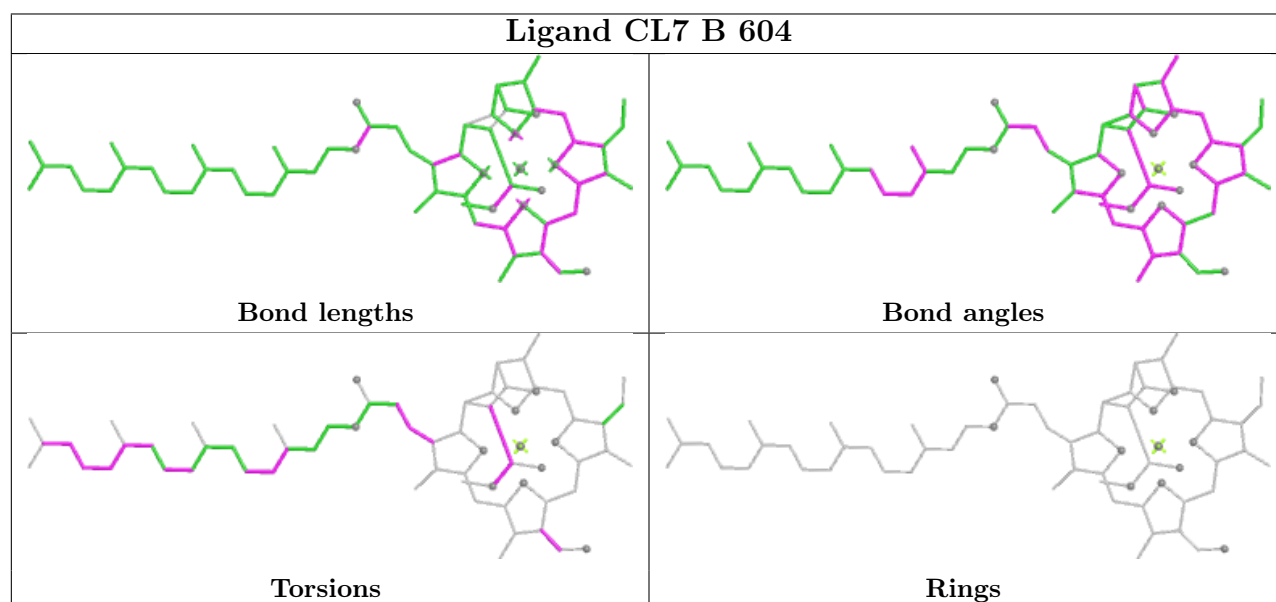
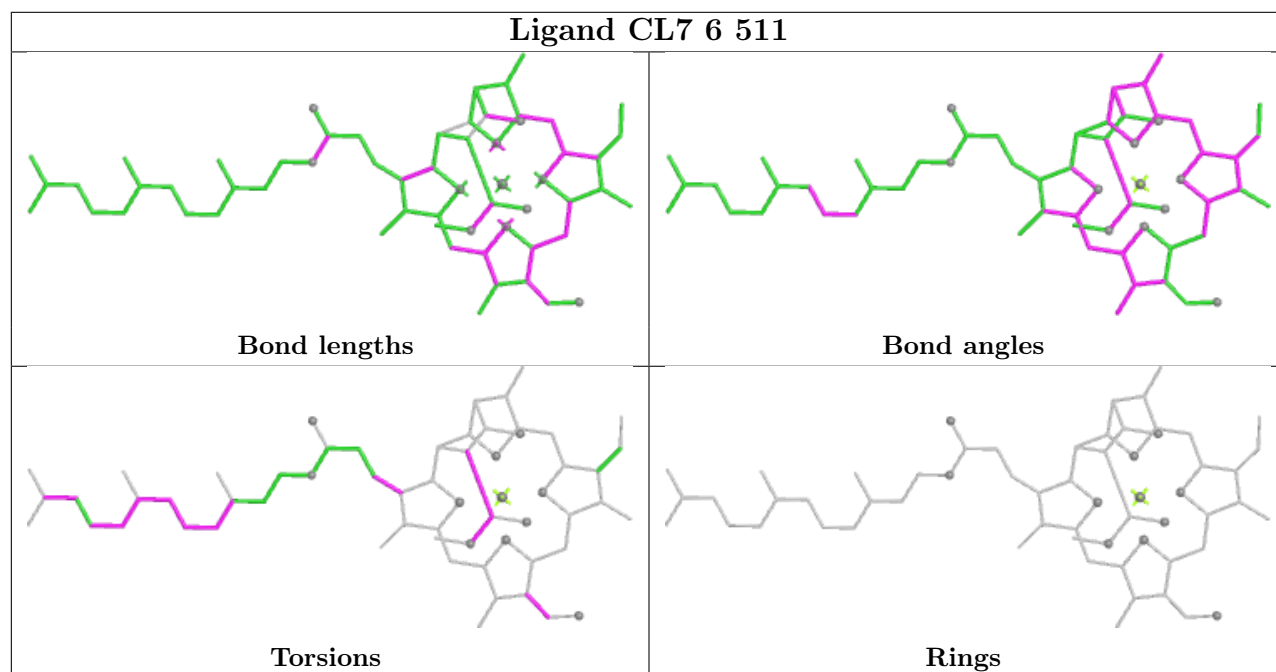
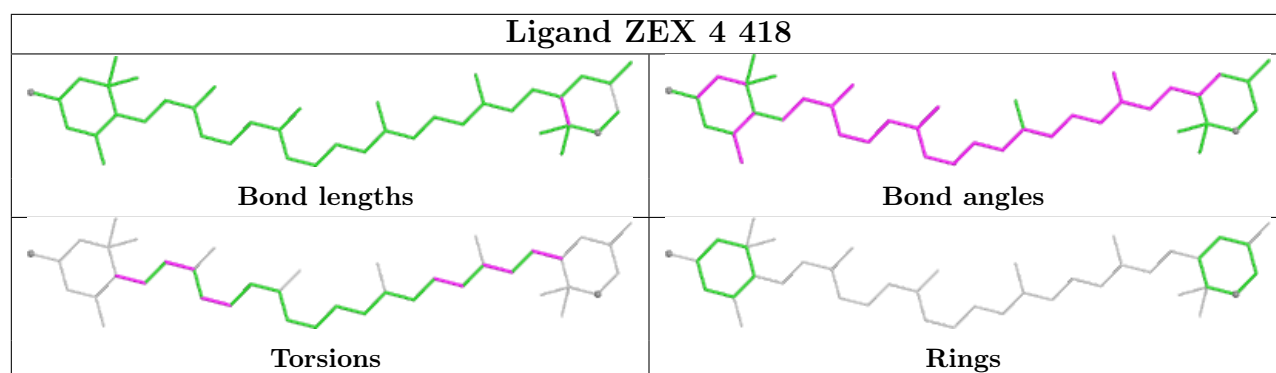


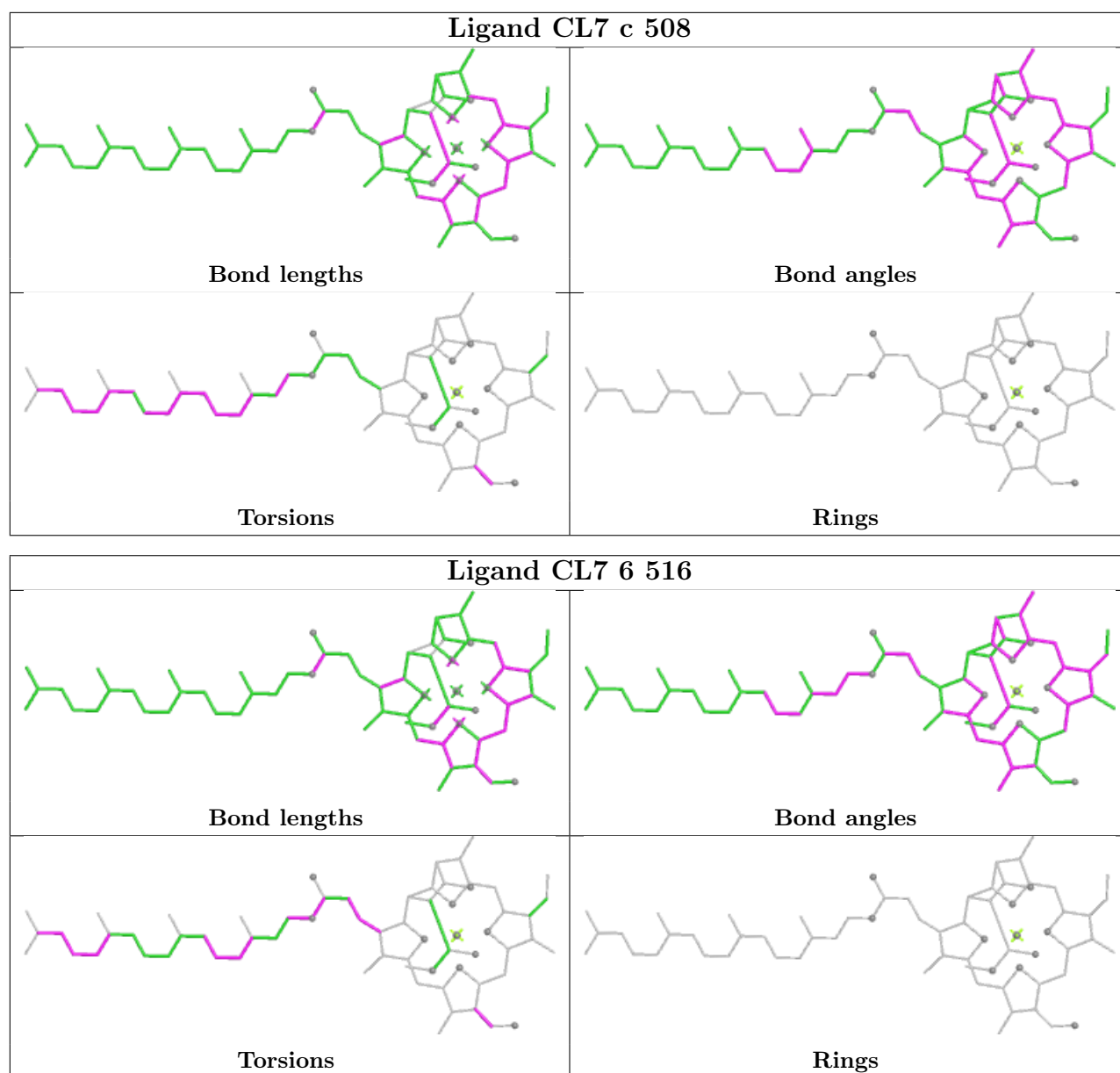
Ligand CL7 8 417

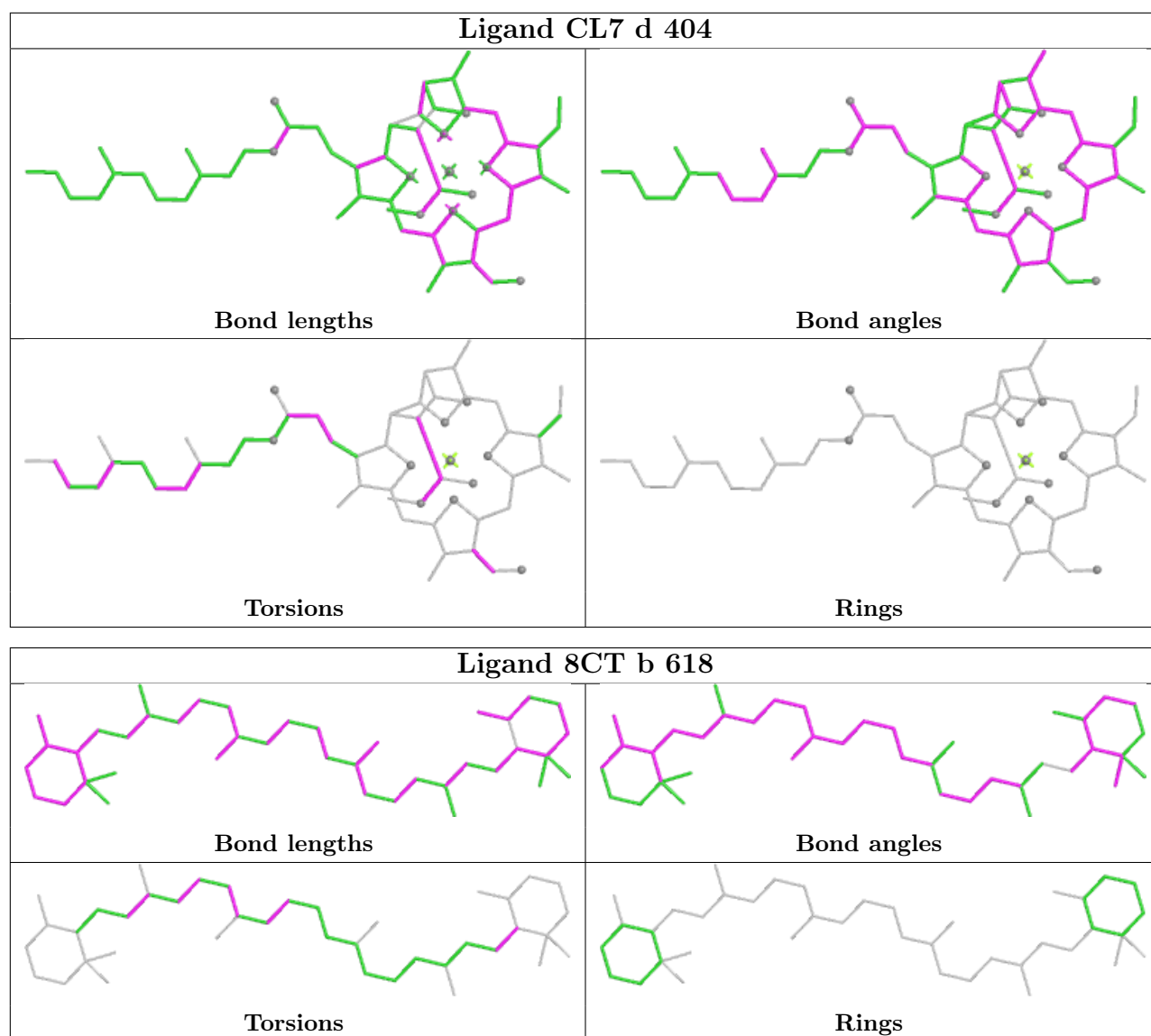




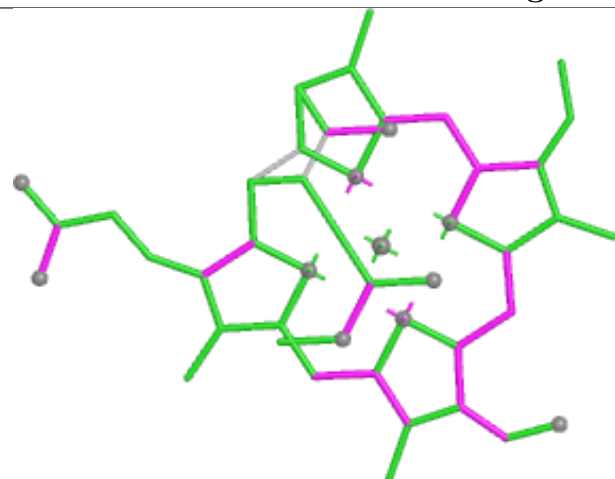




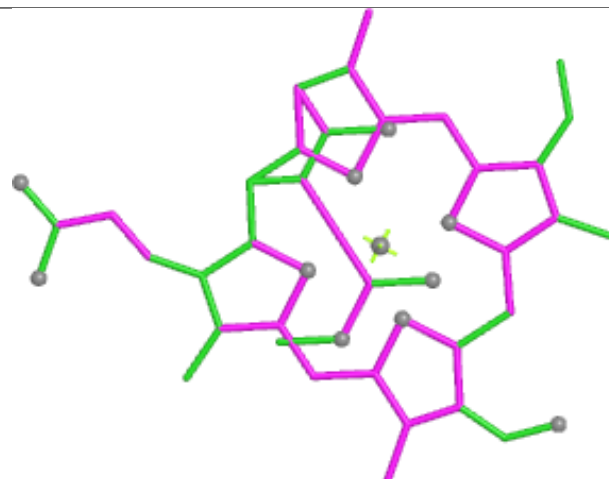




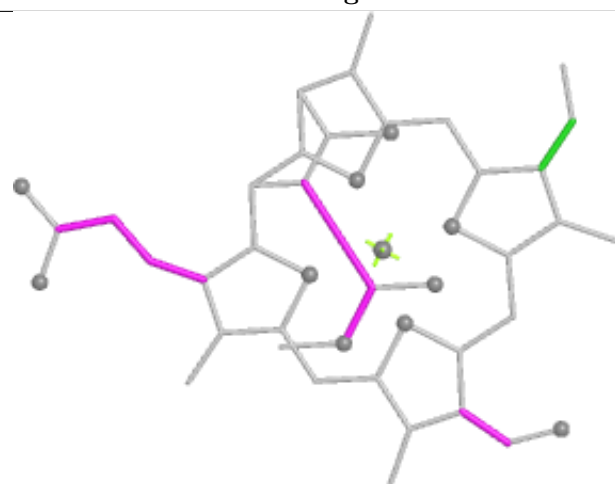
Ligand CL7 1 412



Bond lengths



Bond angles

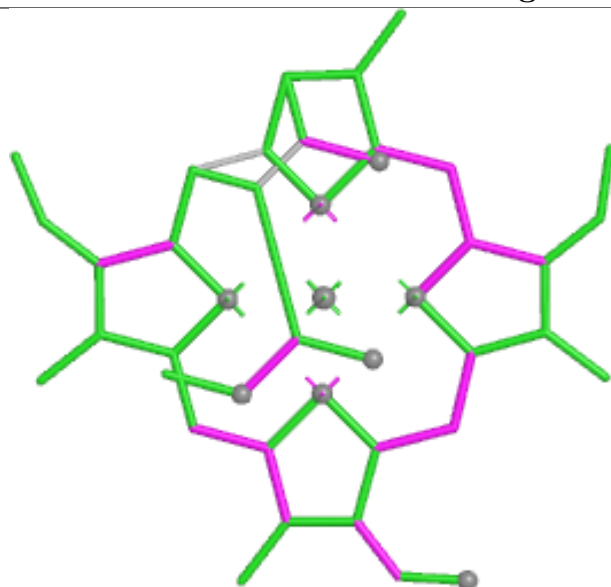


Torsions

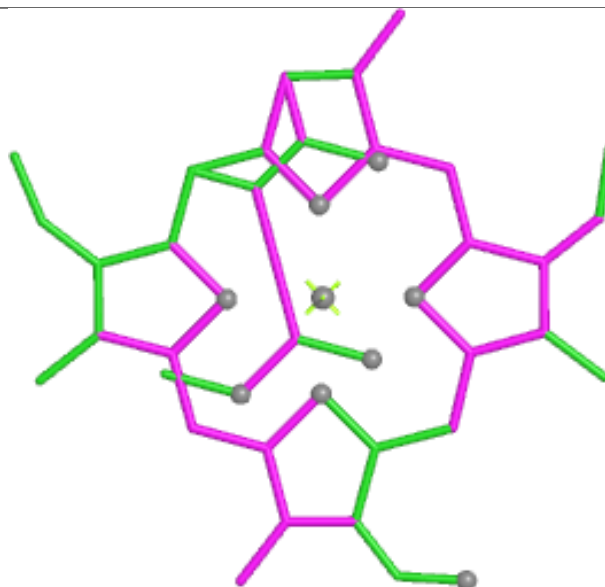


Rings

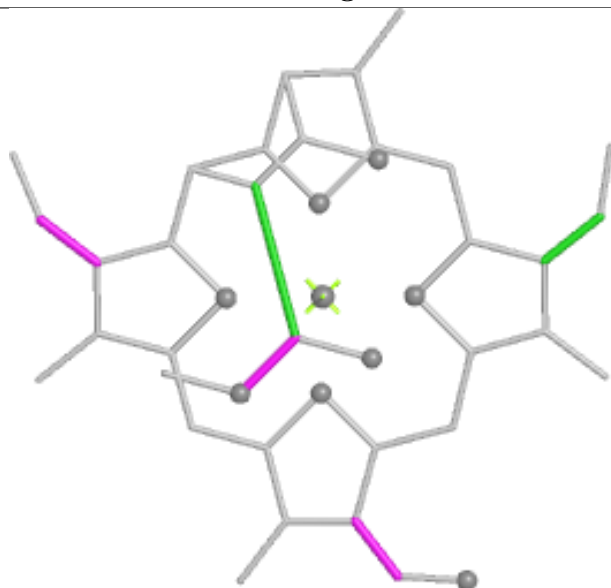
Ligand CL7 C 512



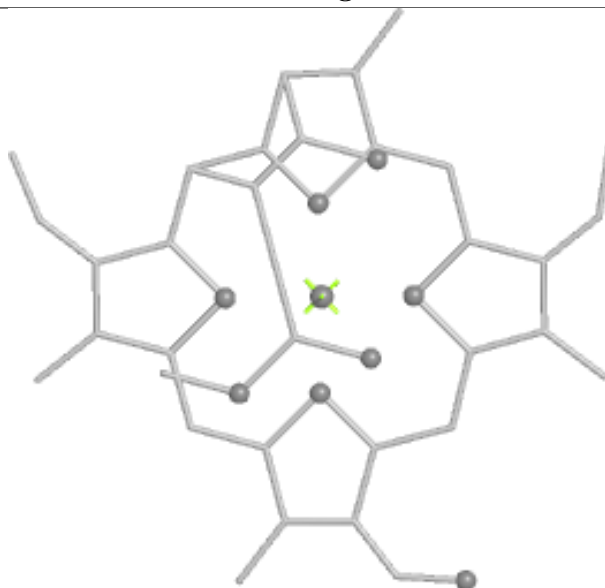
Bond lengths



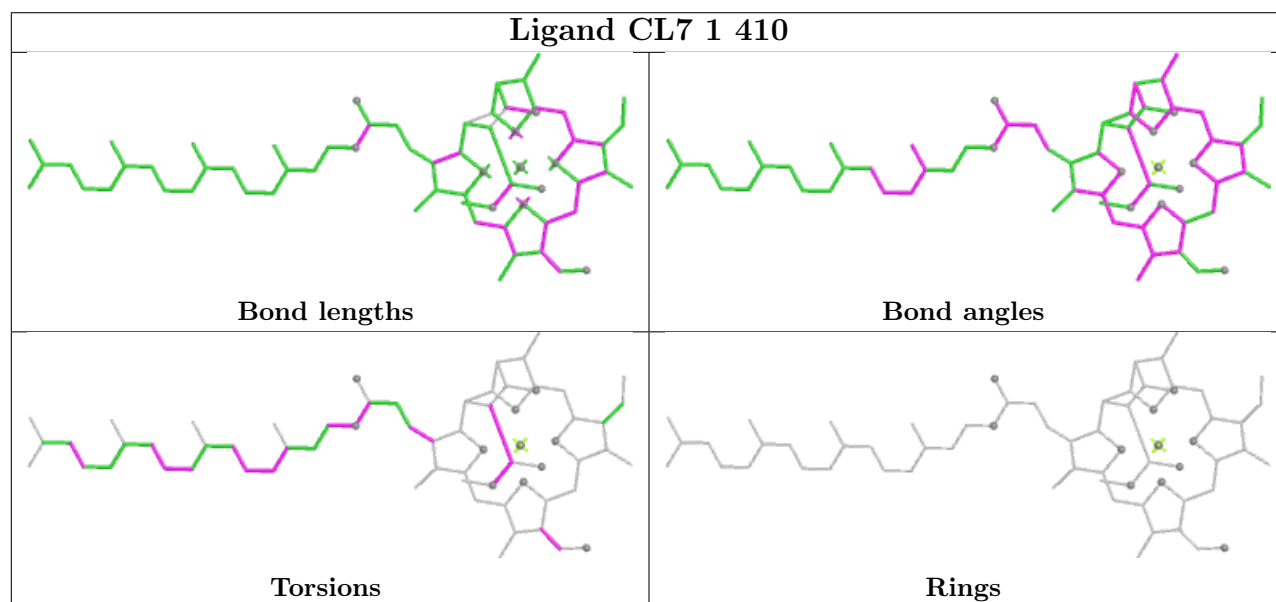
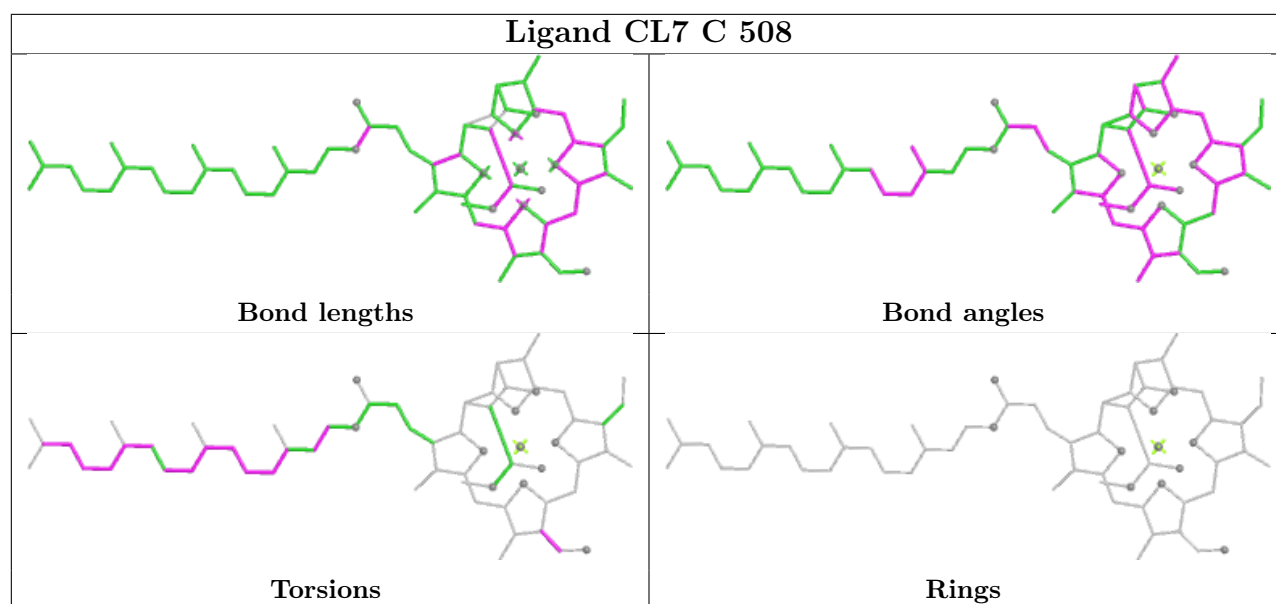
Bond angles

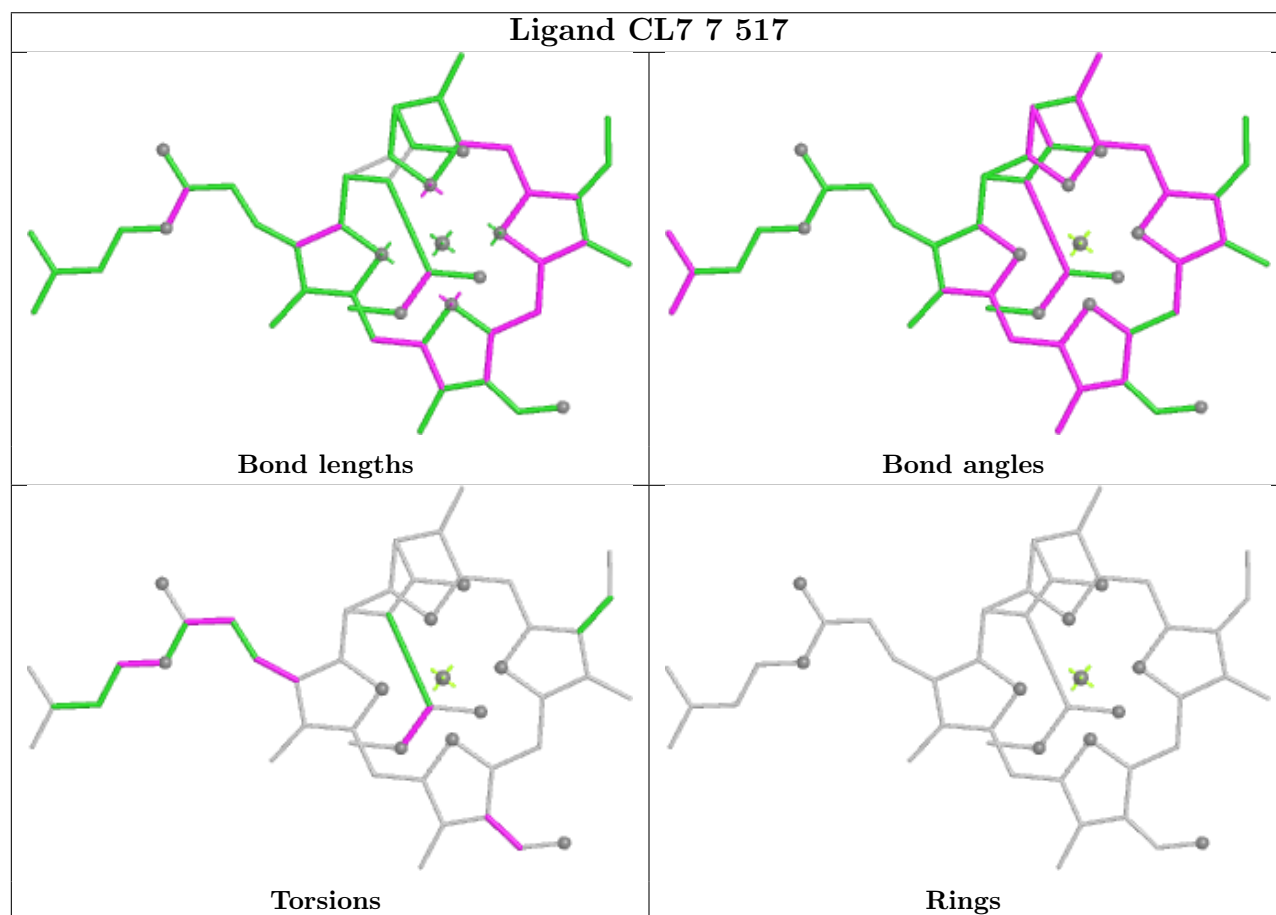
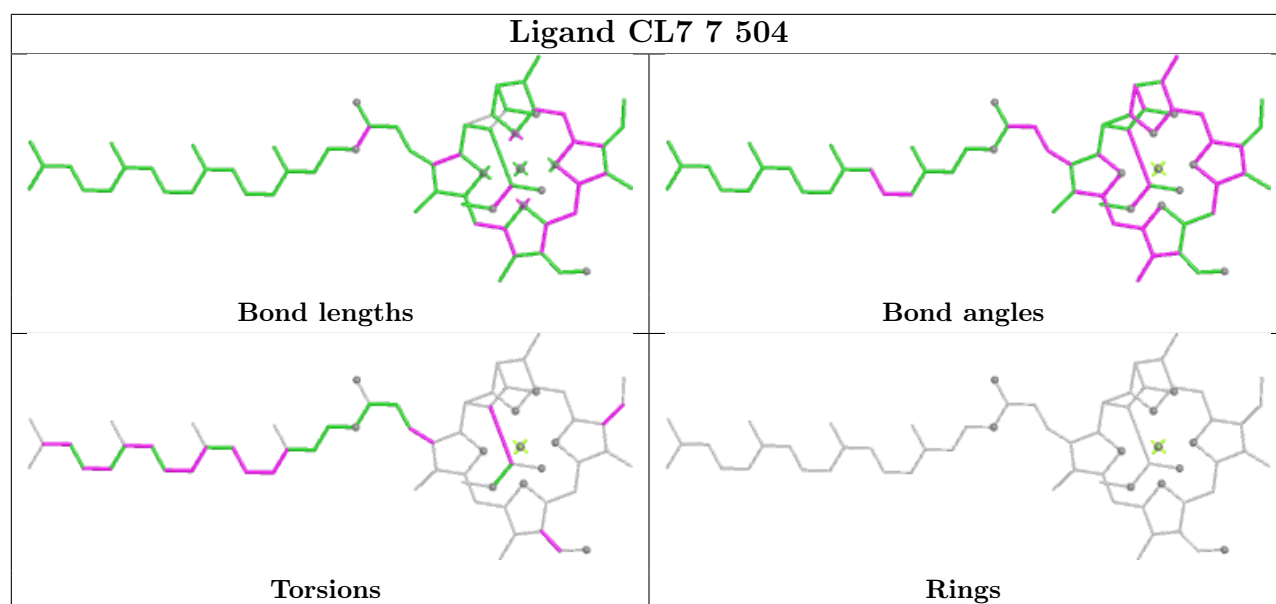


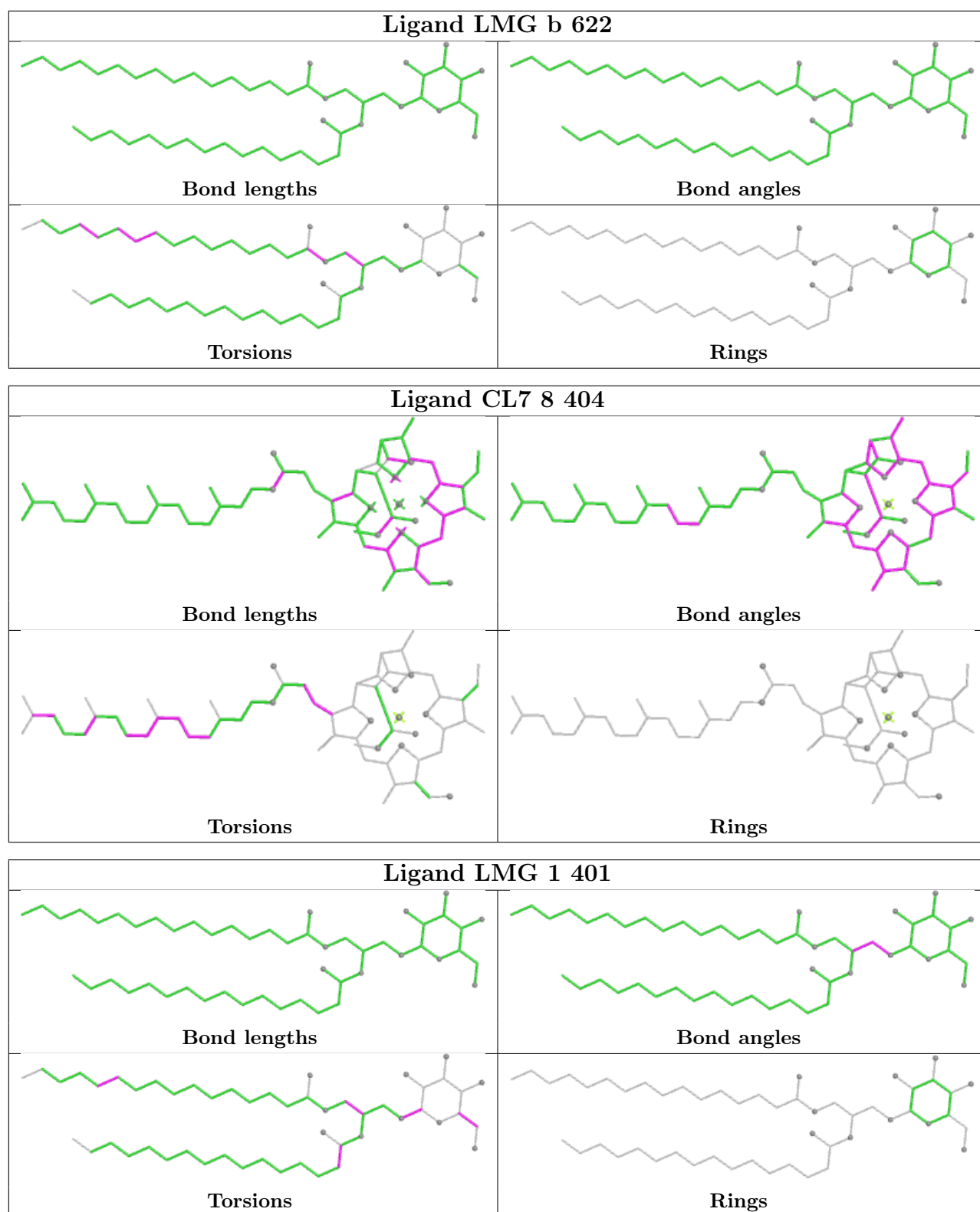
Torsions

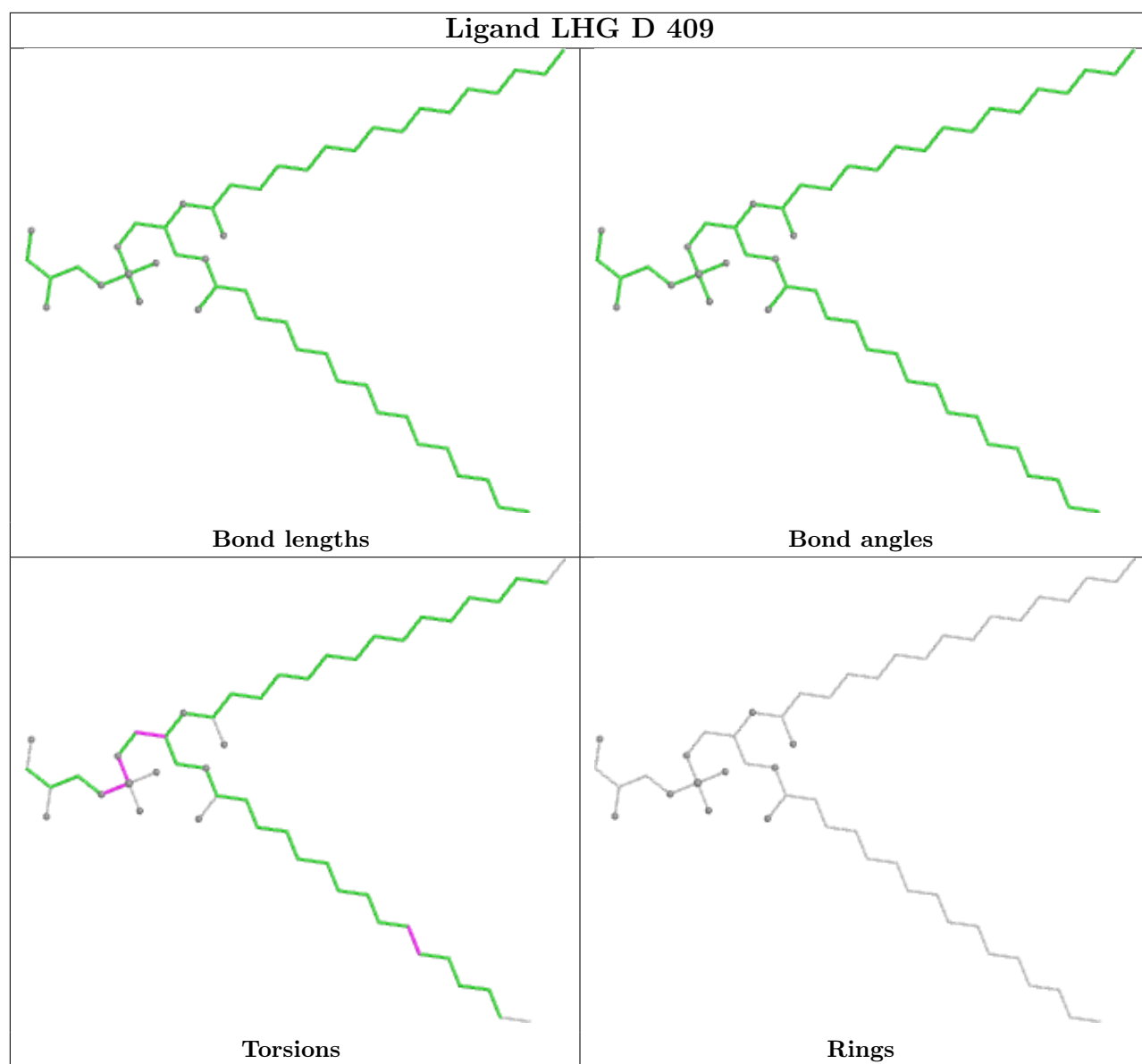


Rings

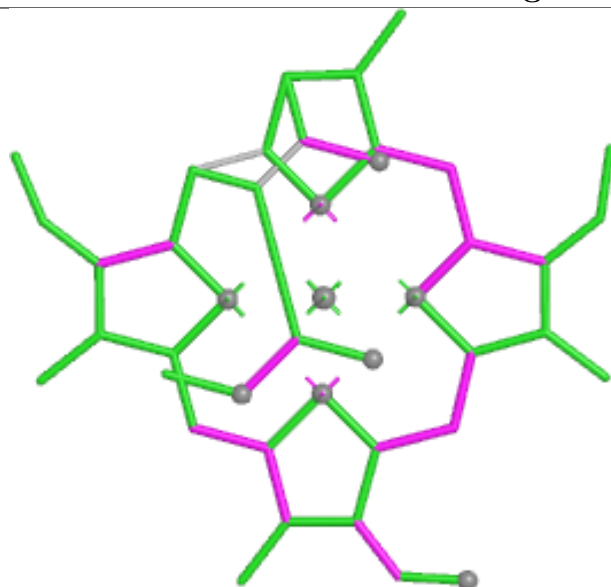




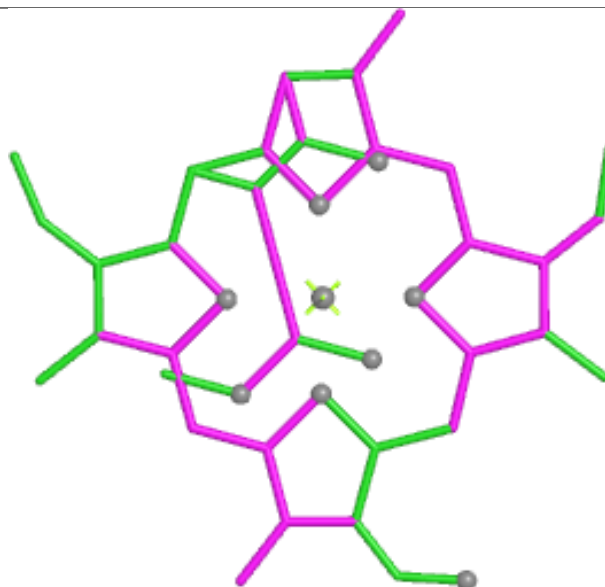




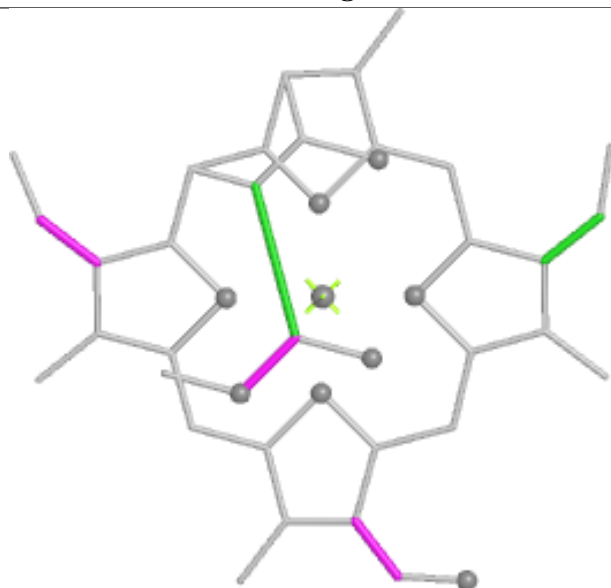
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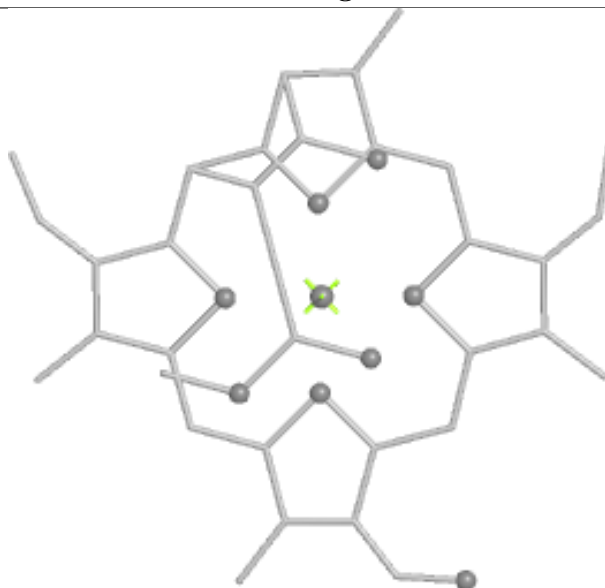
Bond lengths



Bond angles

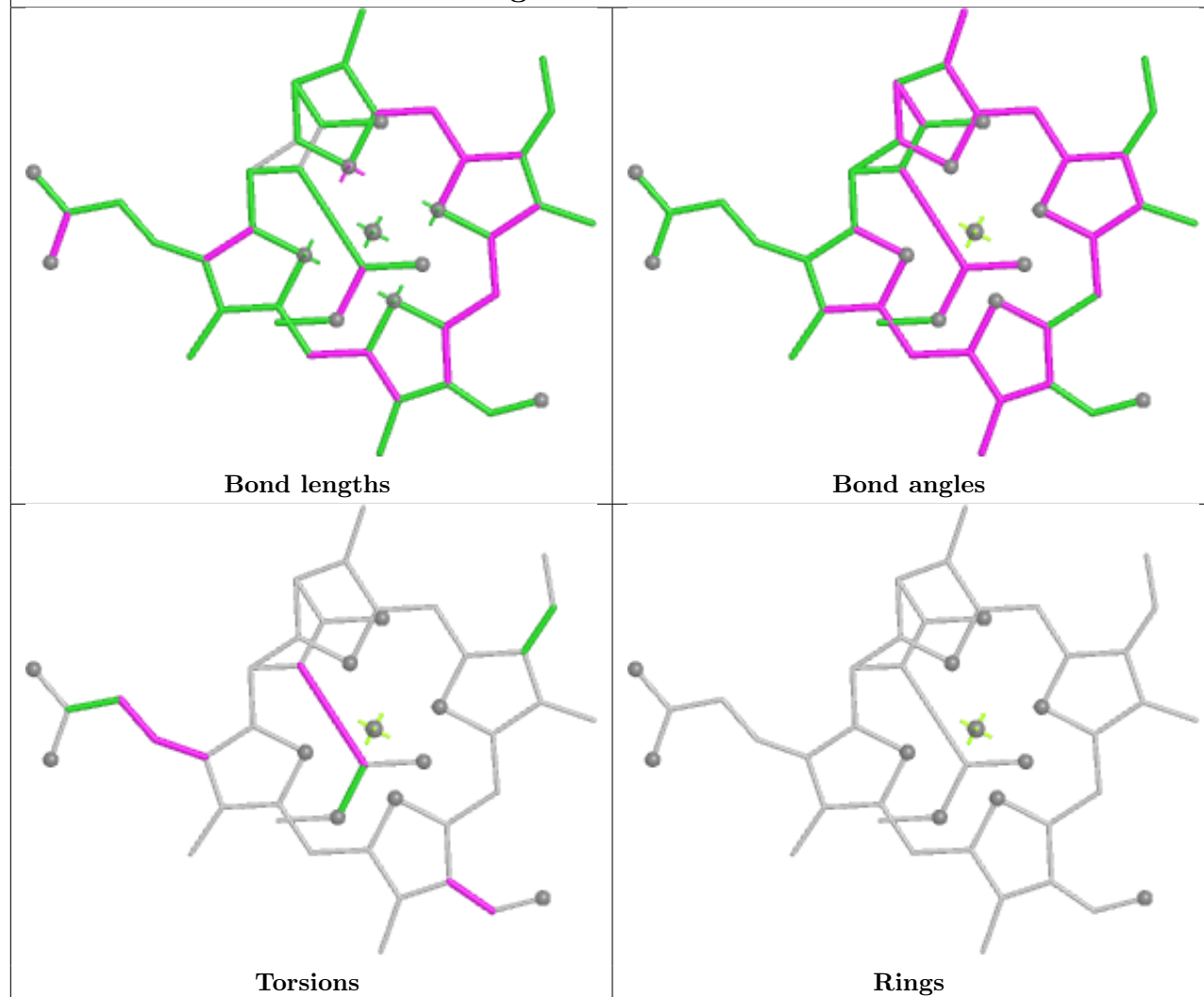


Torsions

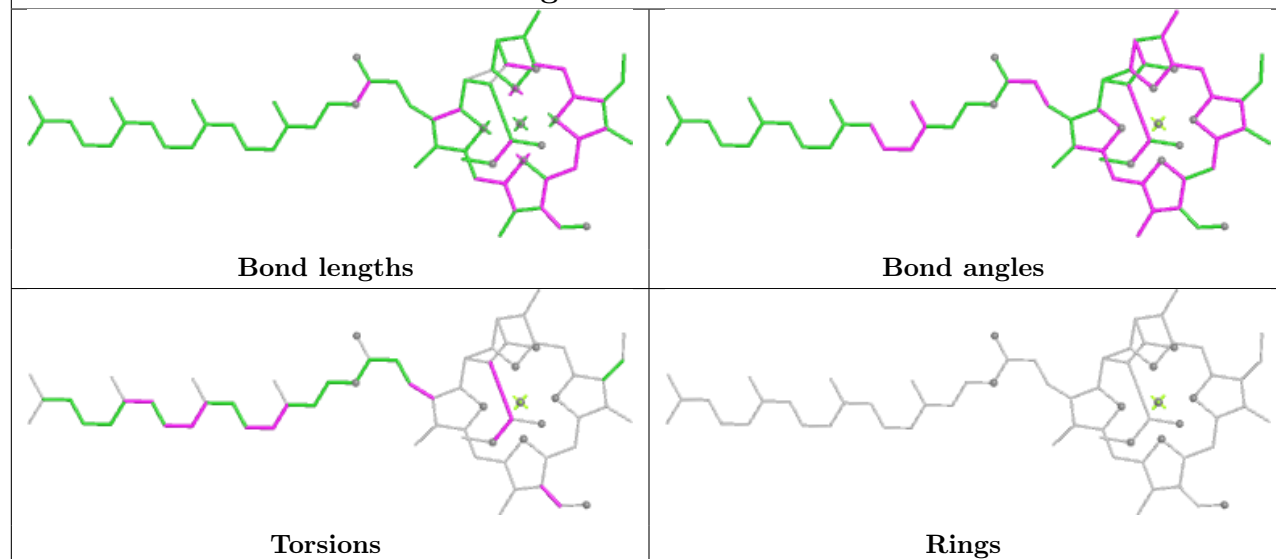


Rings

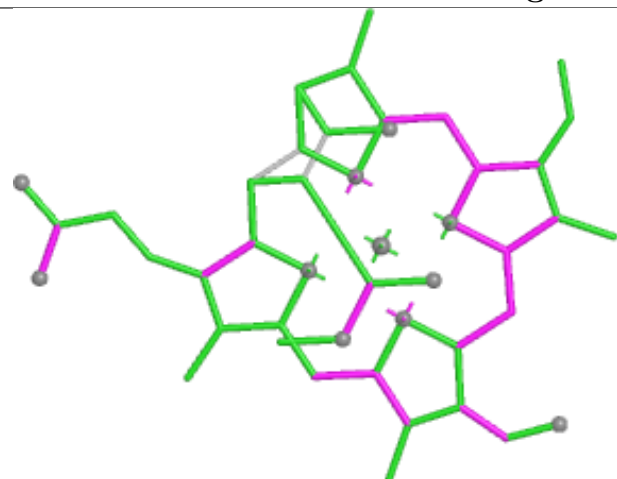
Ligand CL7 2 513



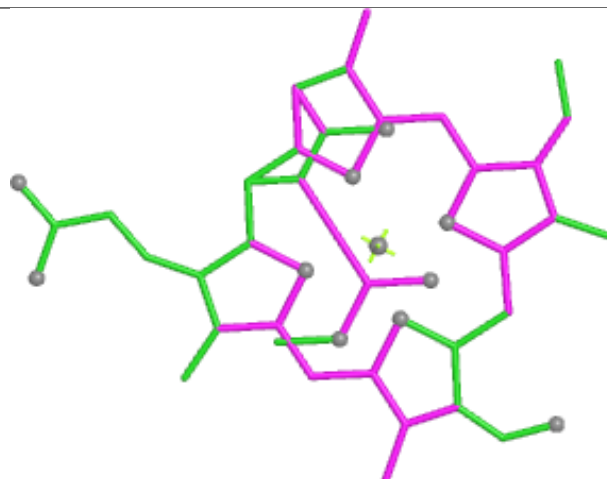
Ligand CL7 6 506



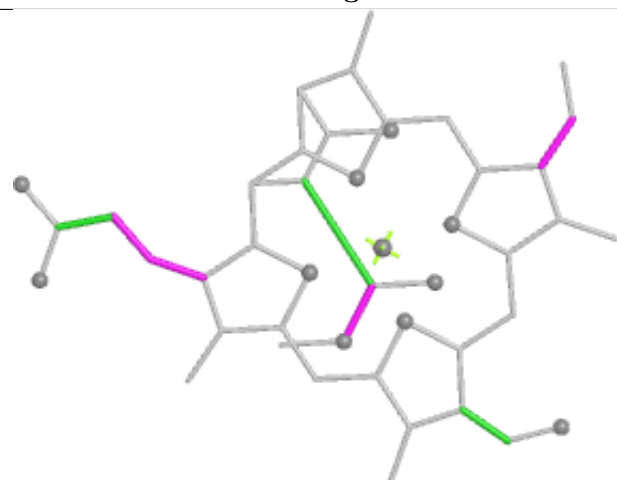
Ligand CL7 7 514



Bond lengths



Bond angles

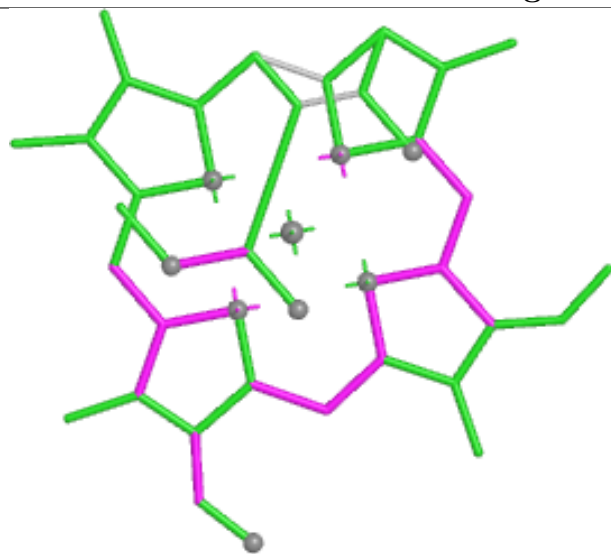


Torsions

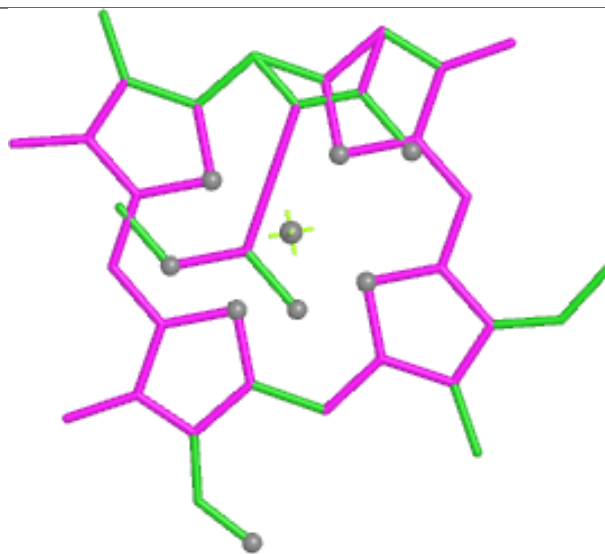


Rings

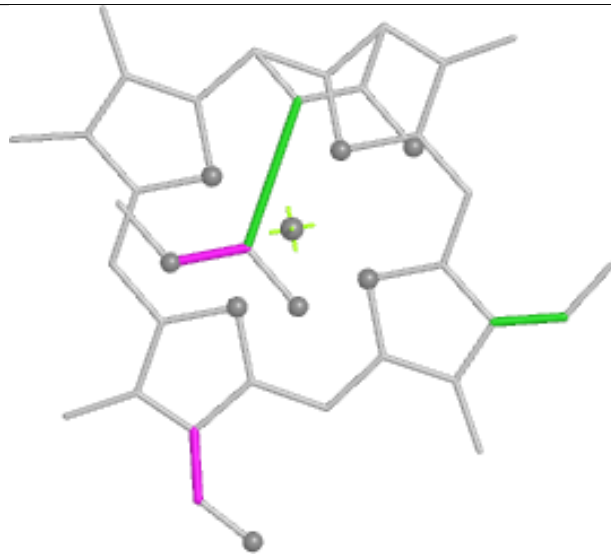
Ligand CL7 c 513



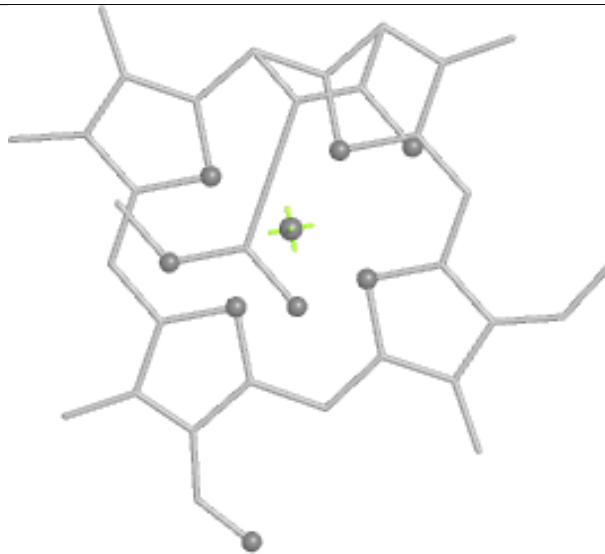
Bond lengths



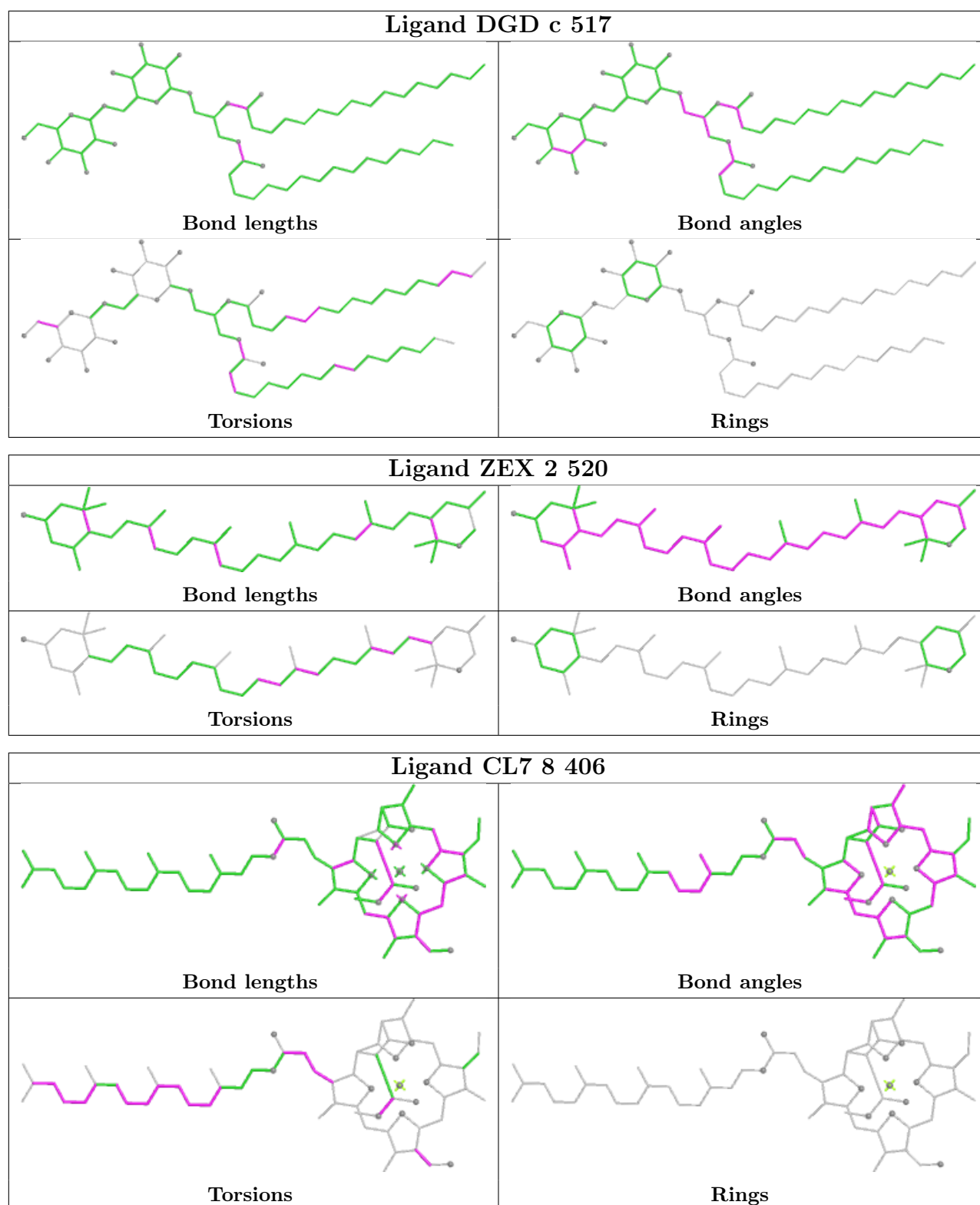
Bond angles

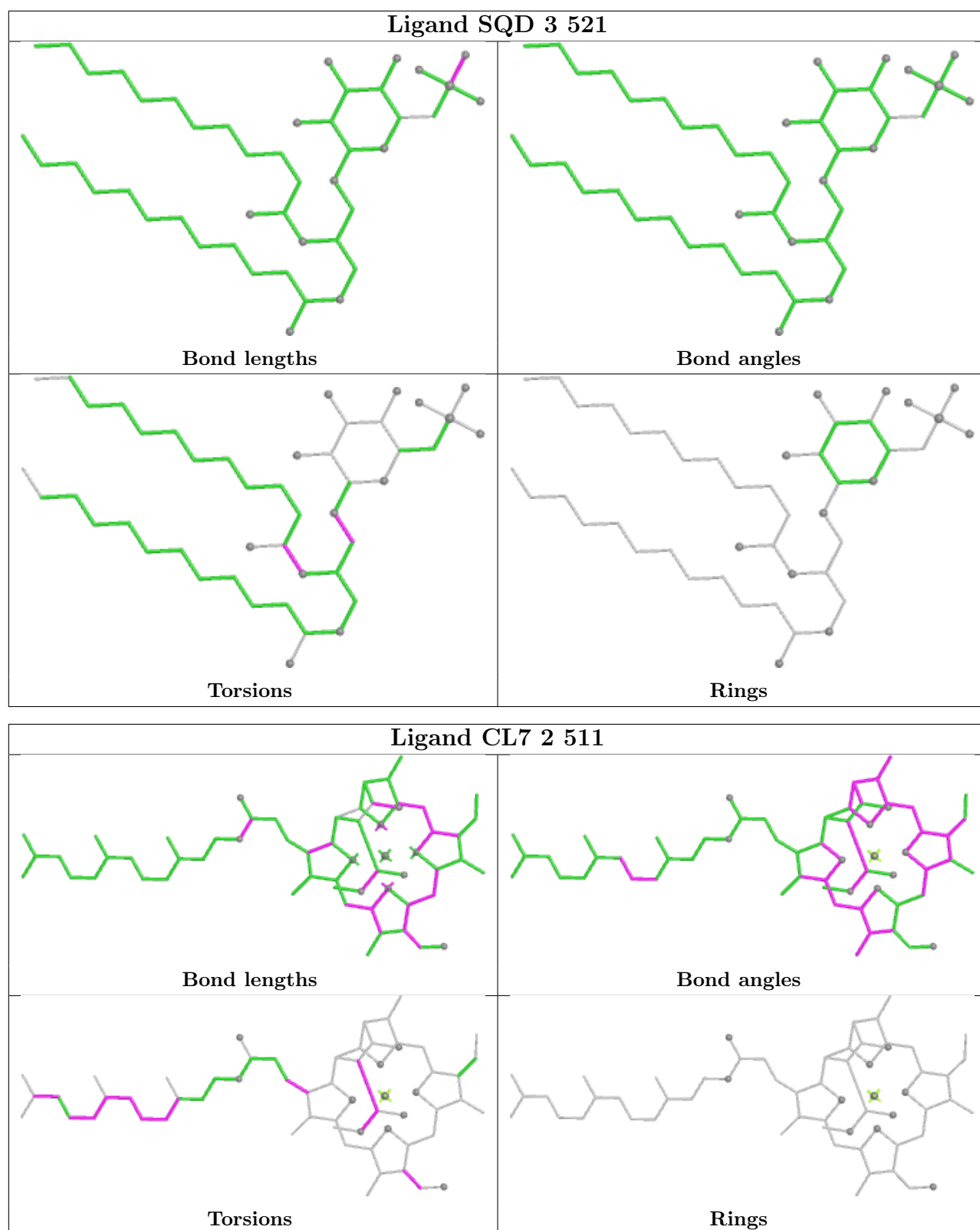


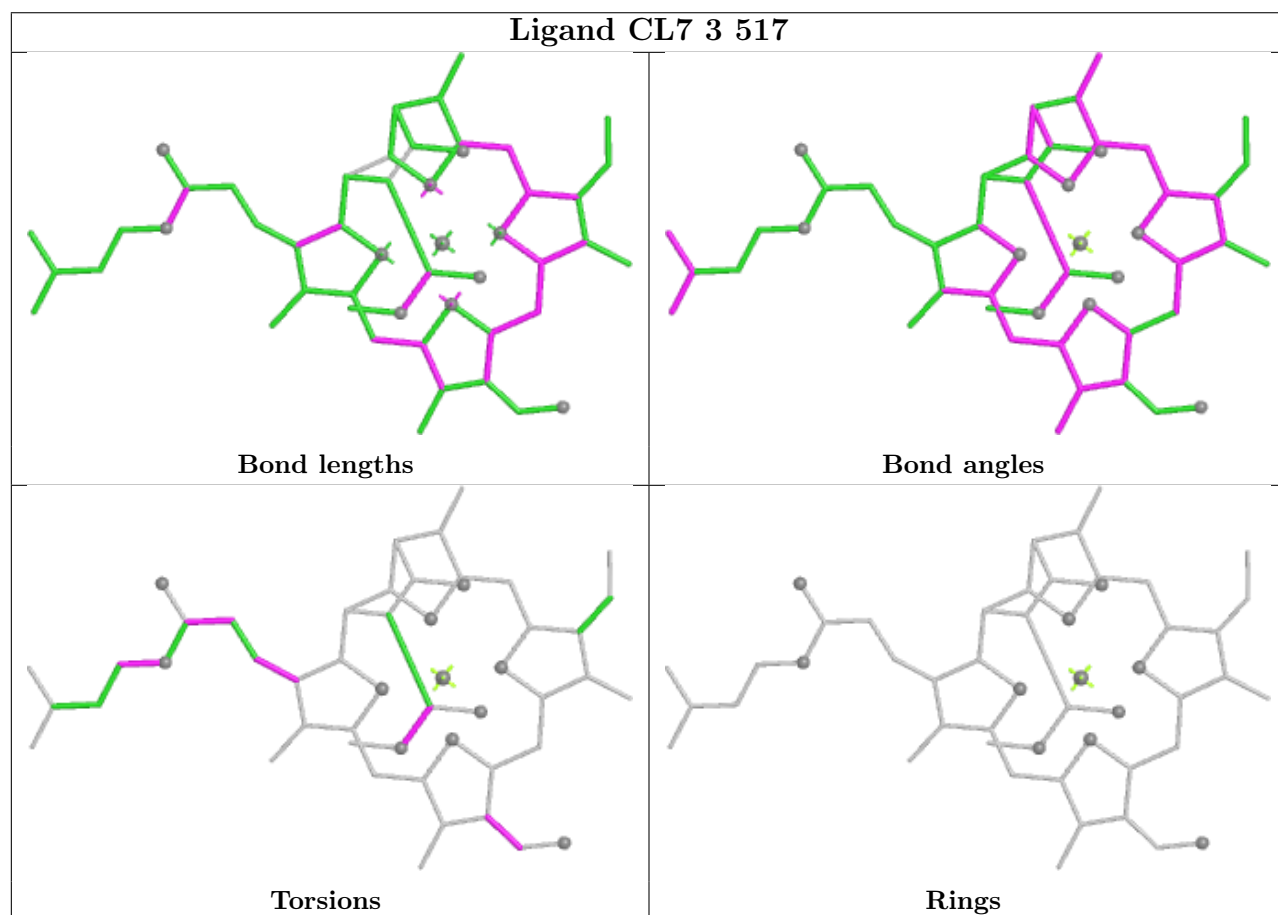
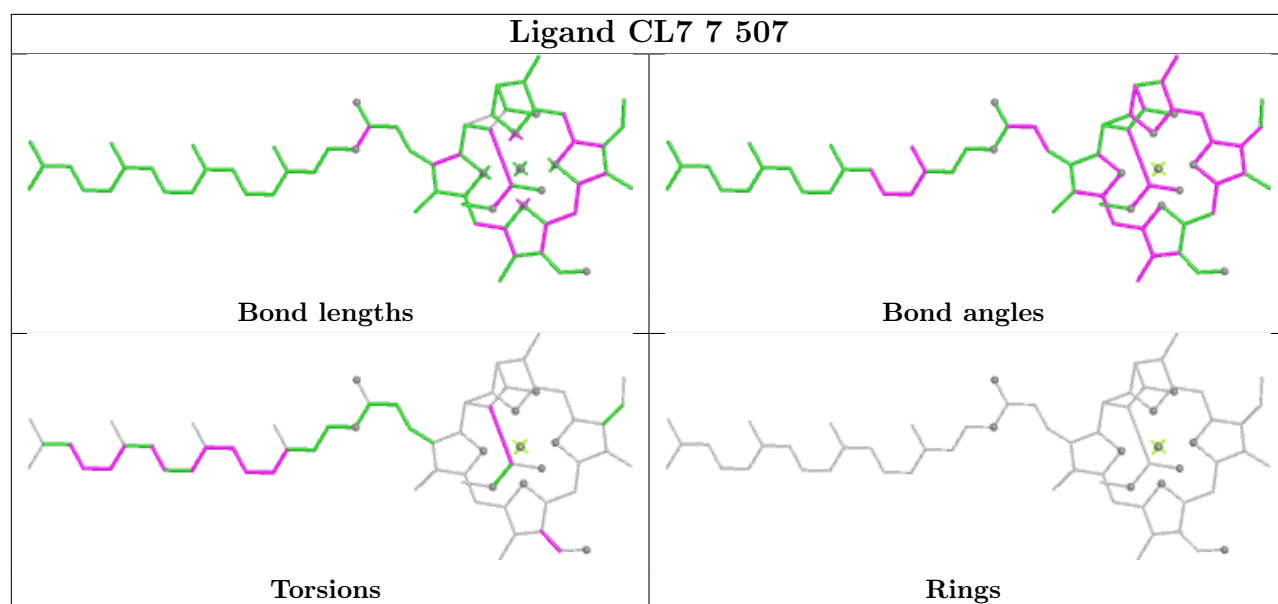
Torsions

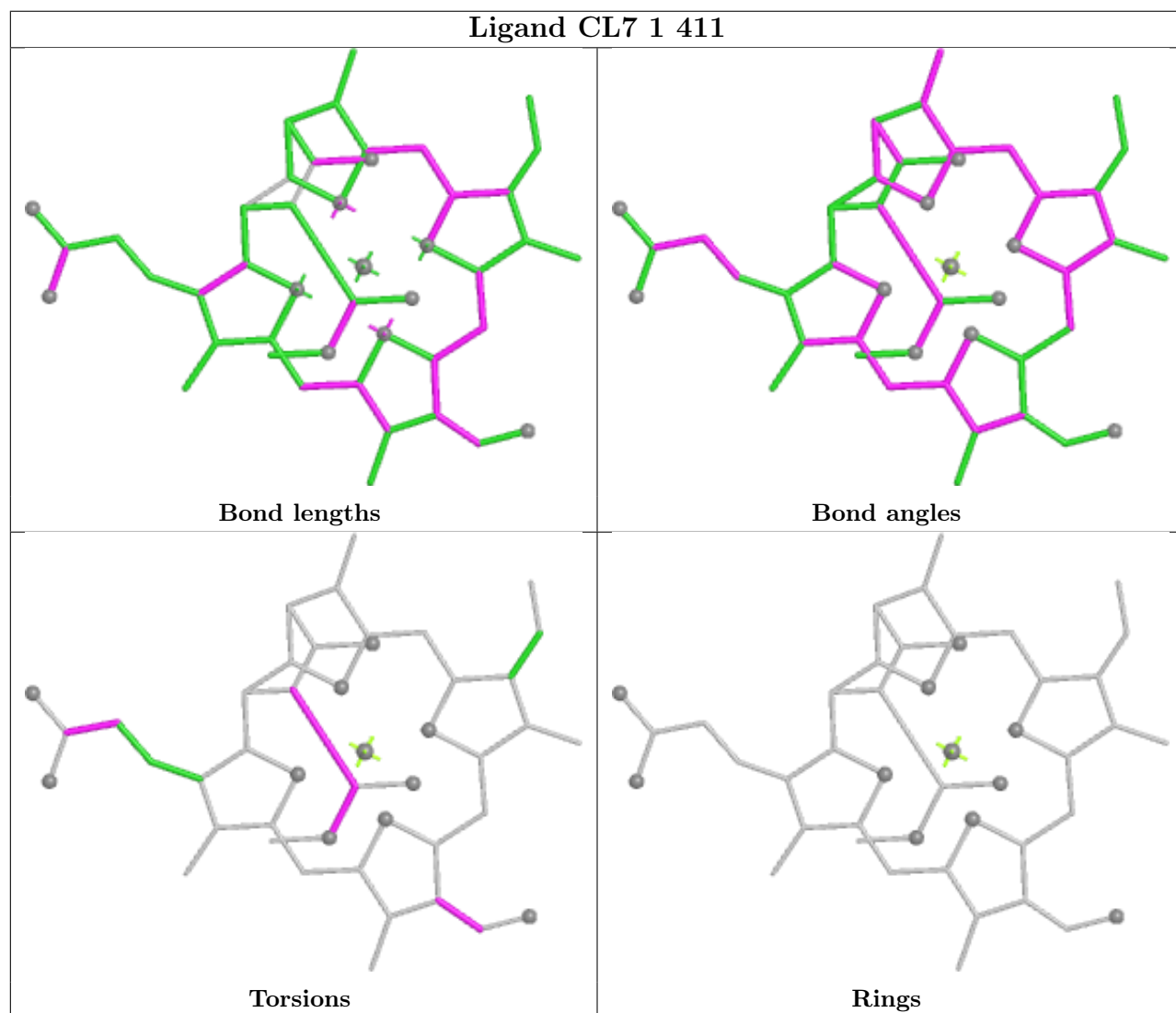
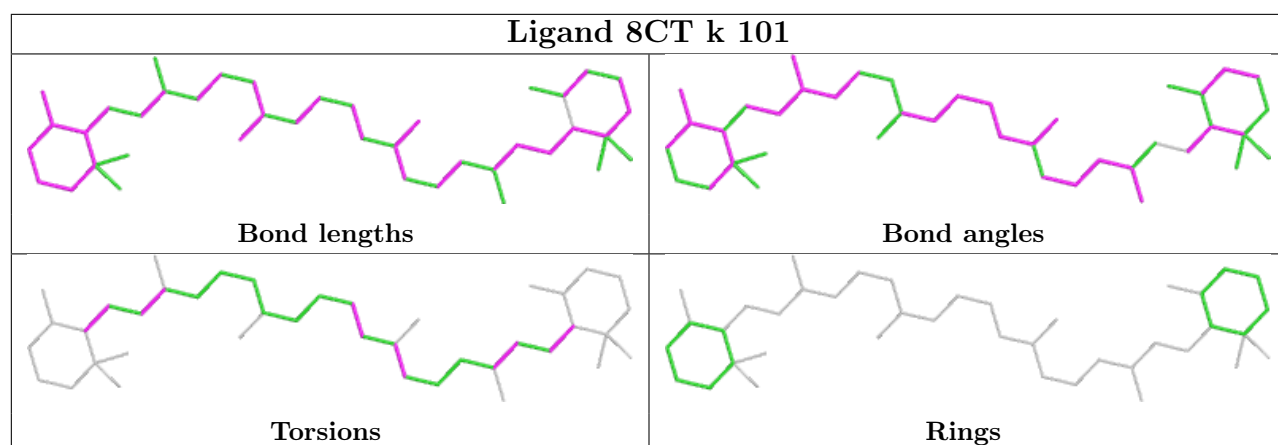


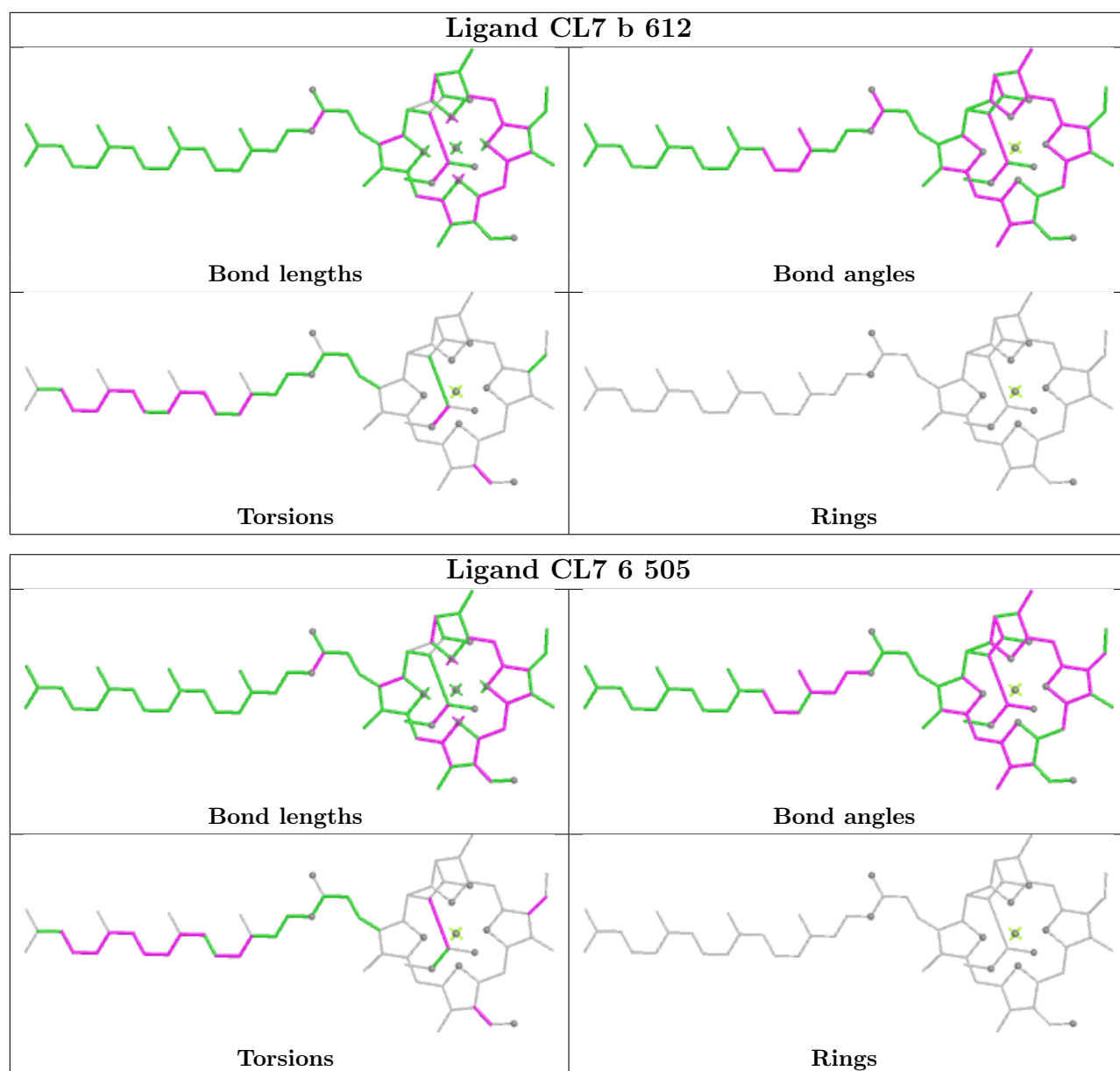
Rings

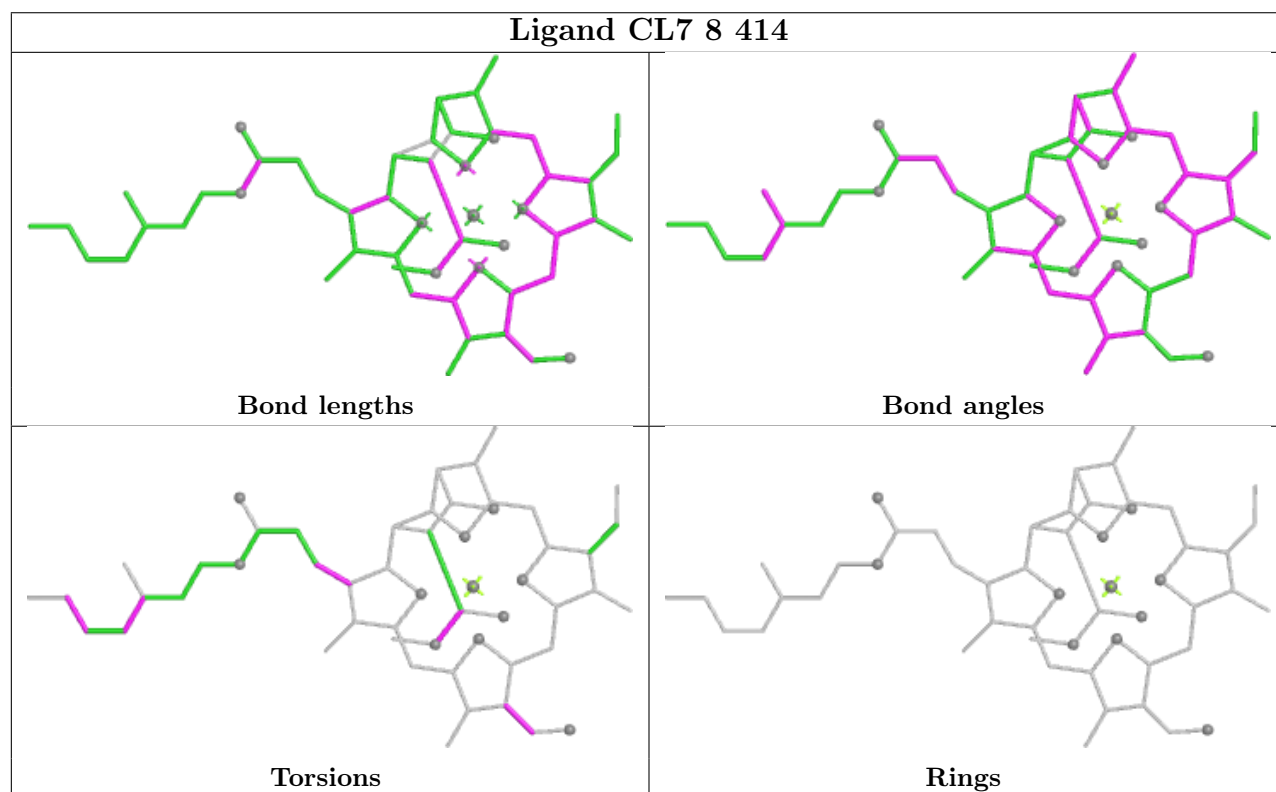
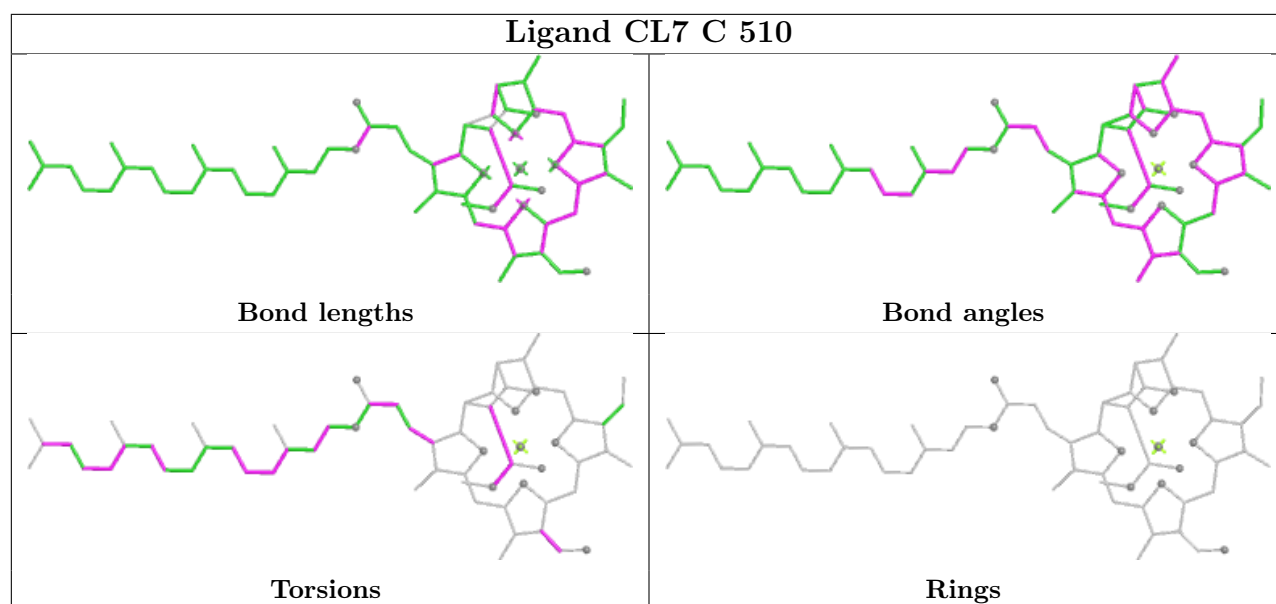


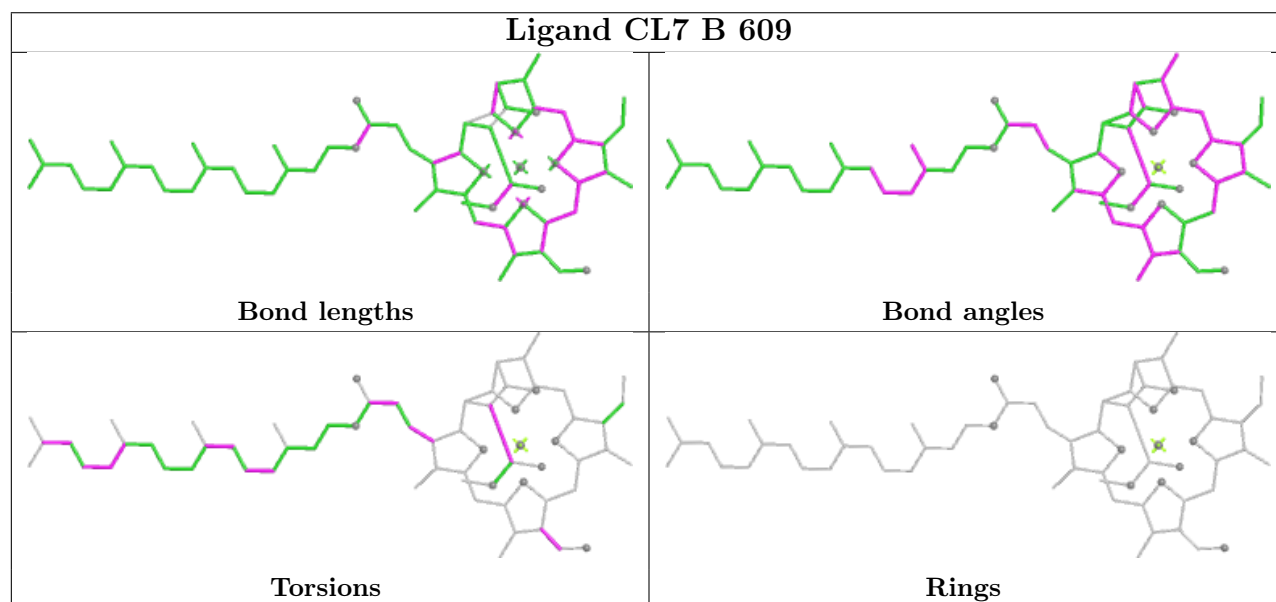
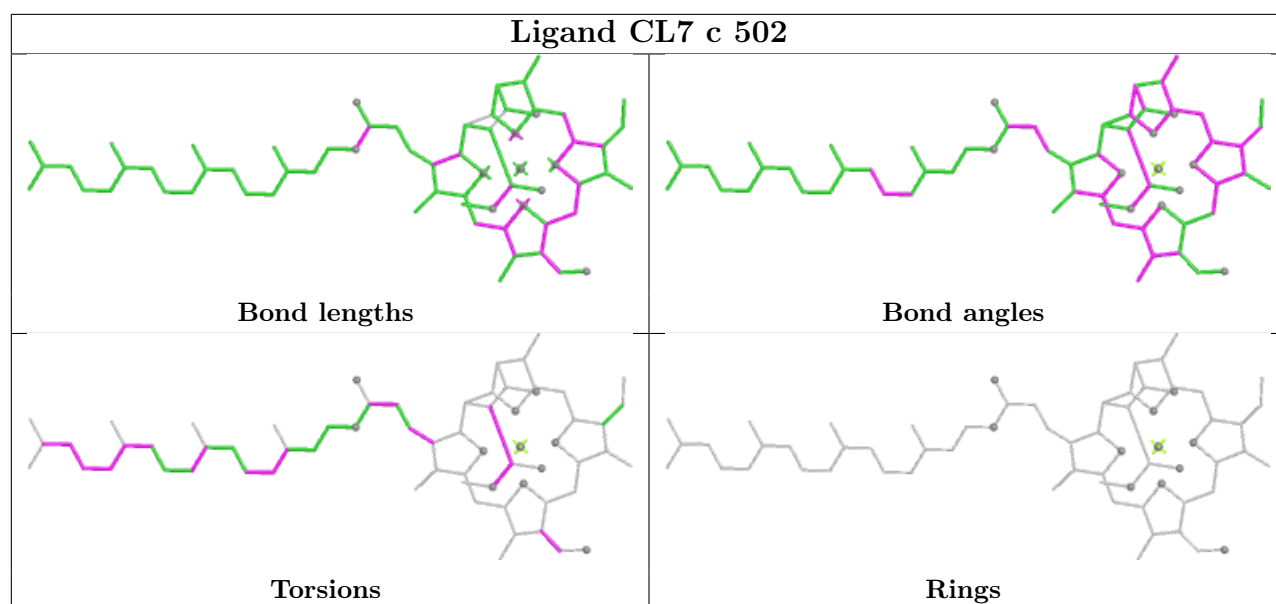


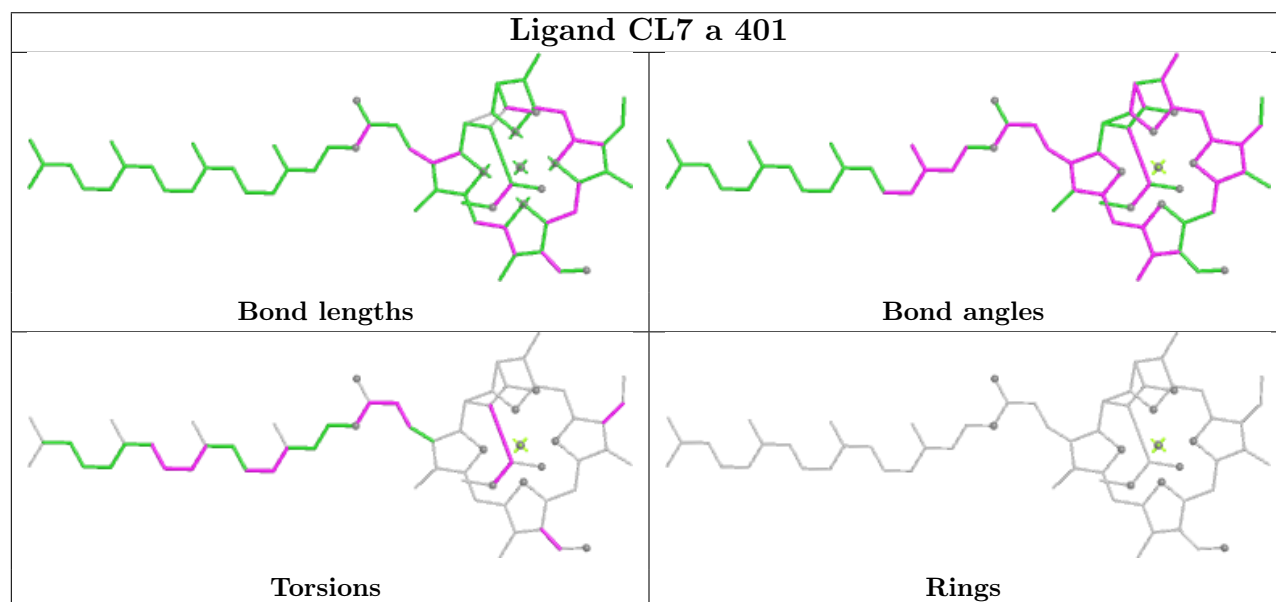
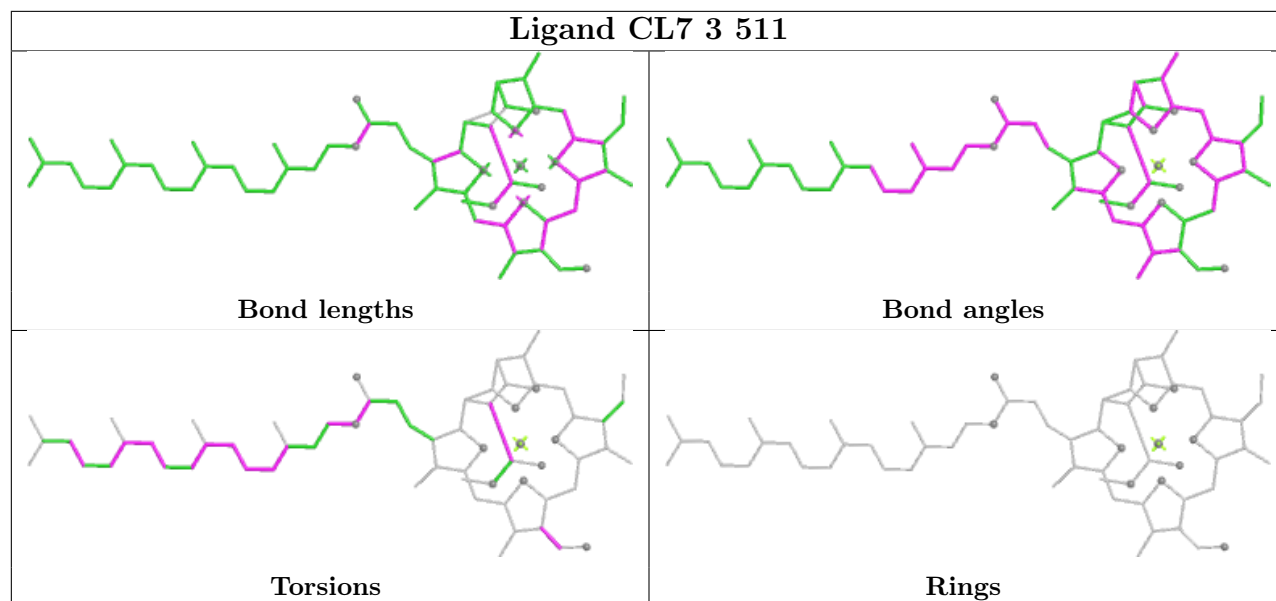


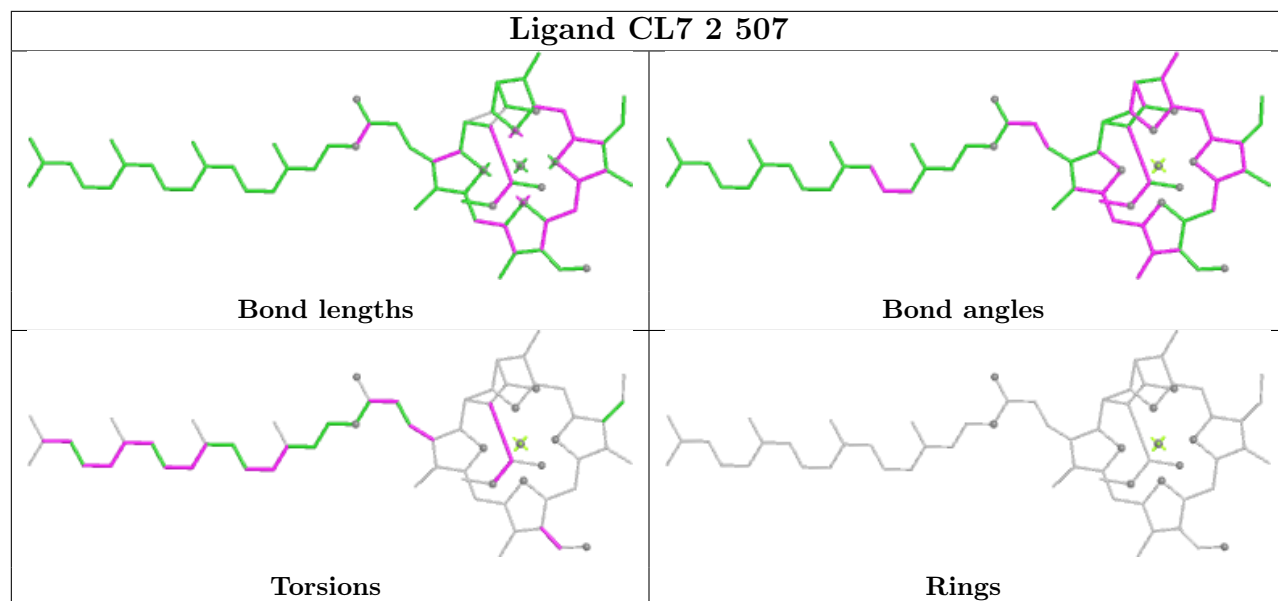


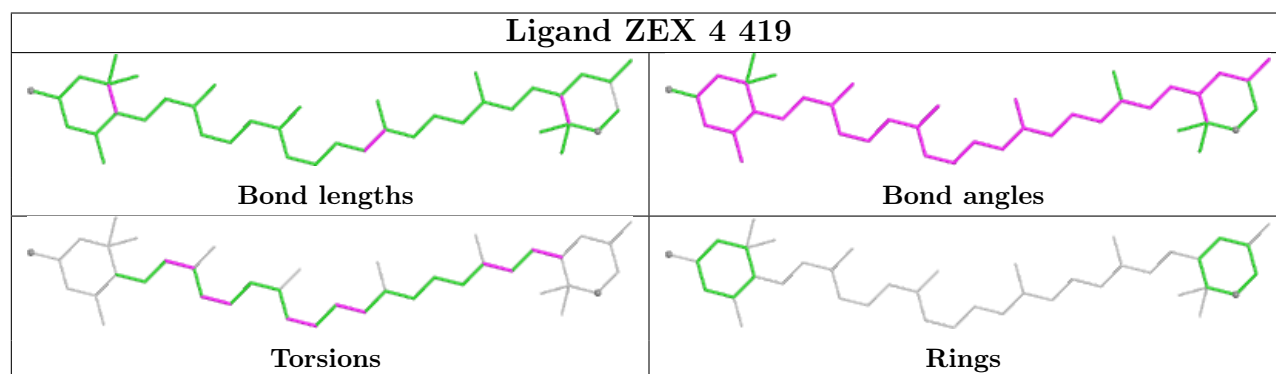
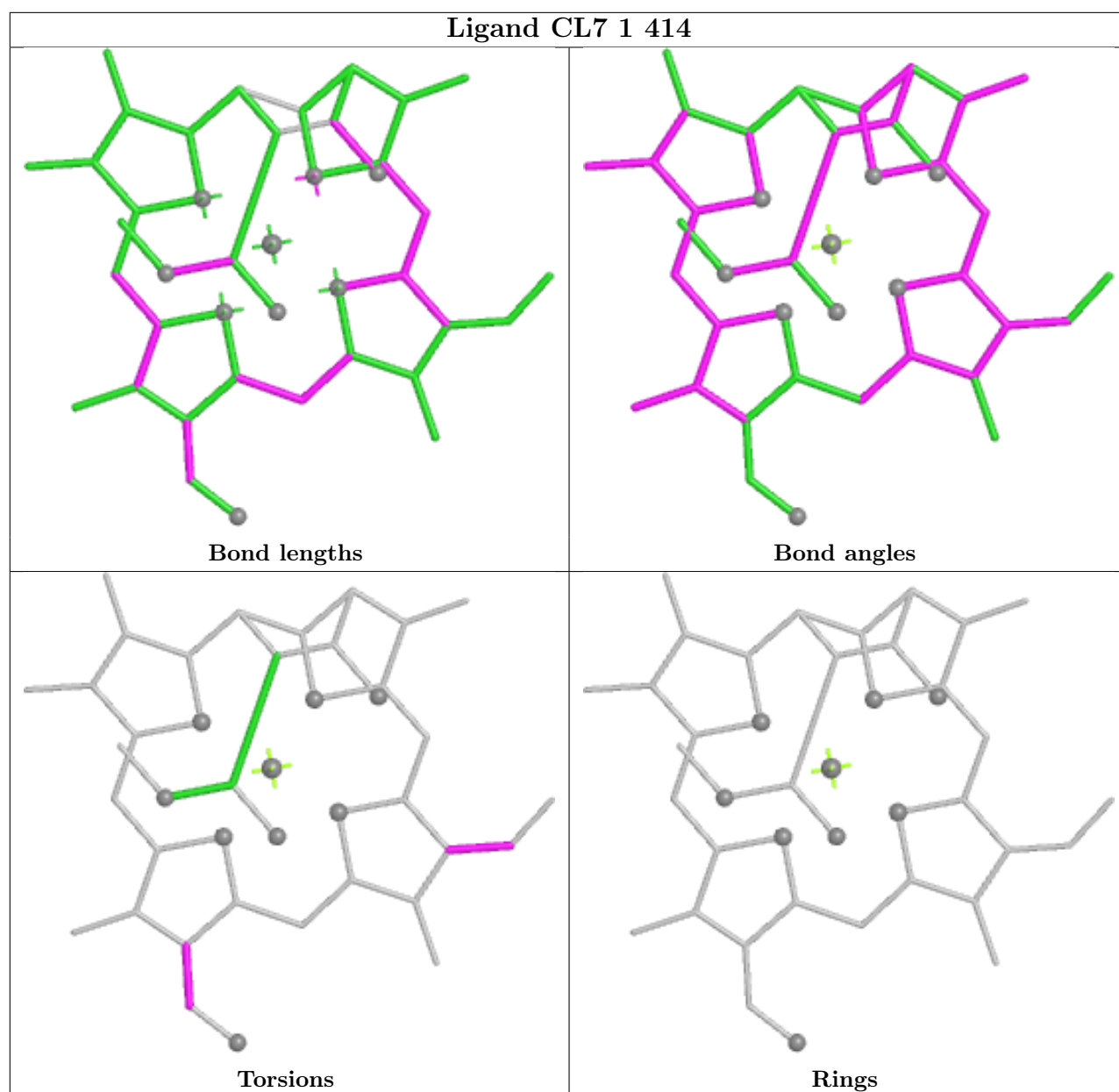


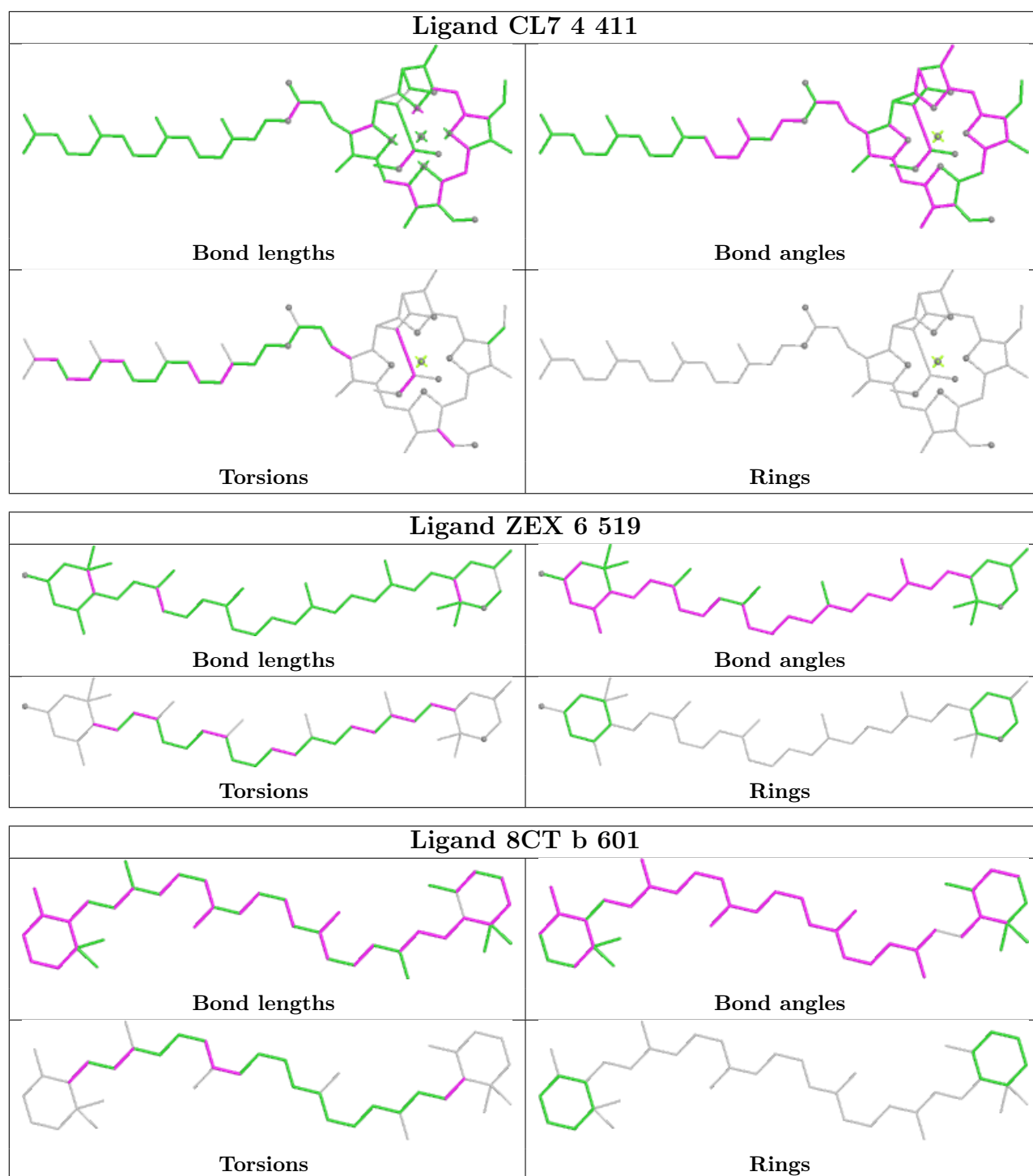


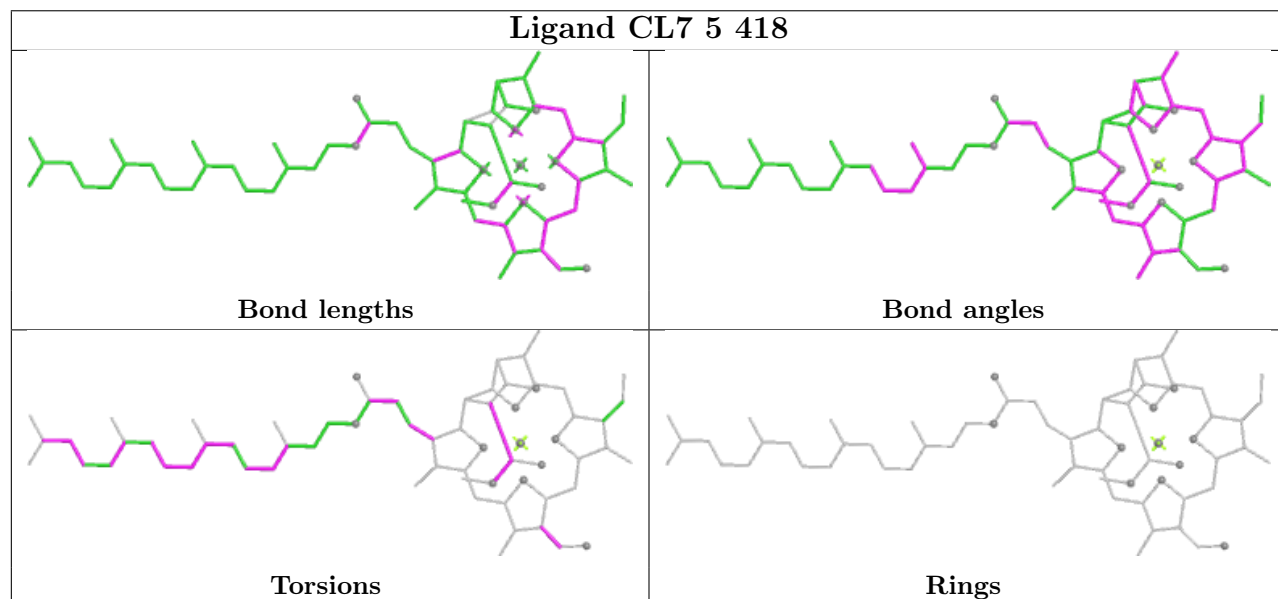
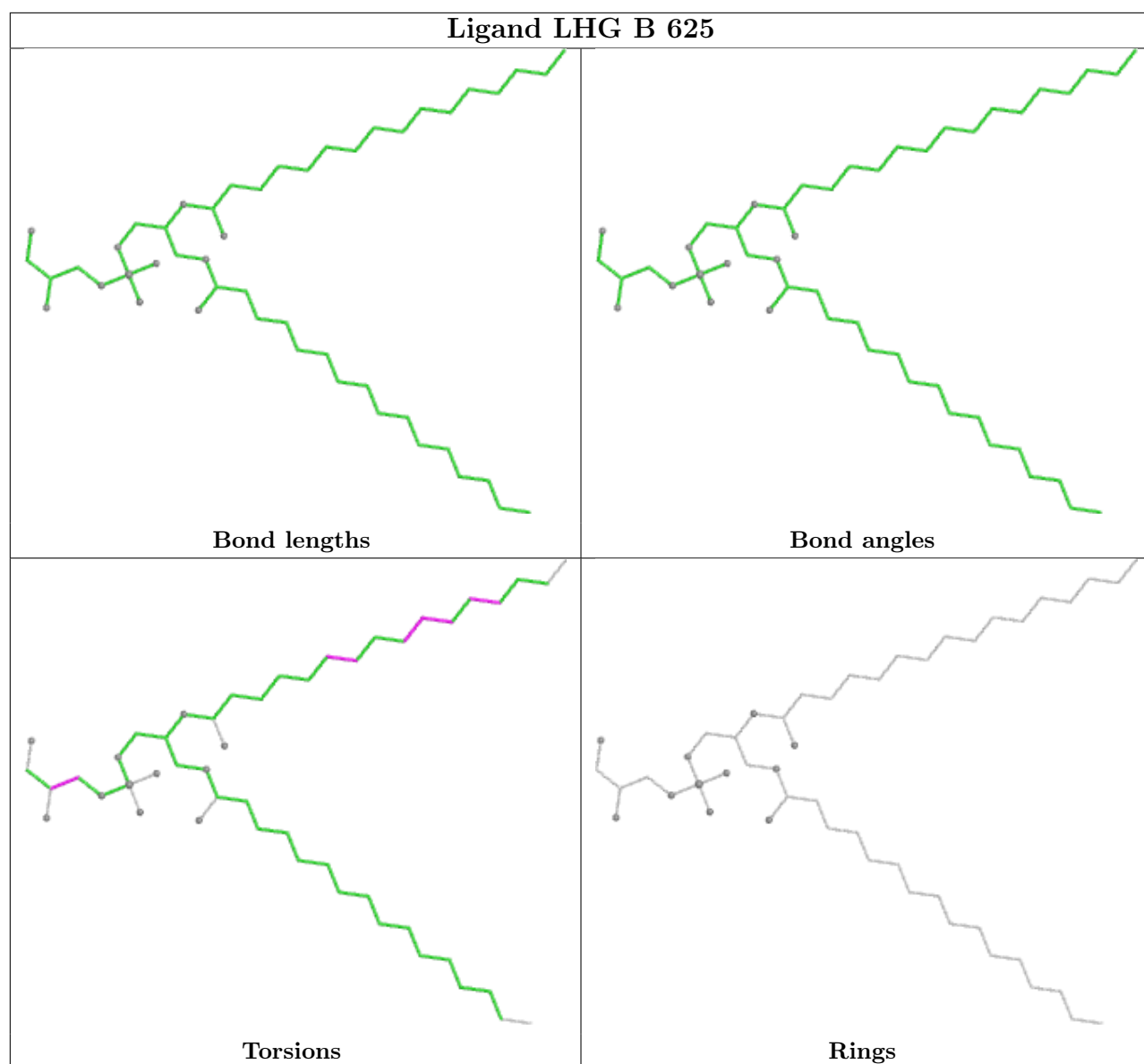




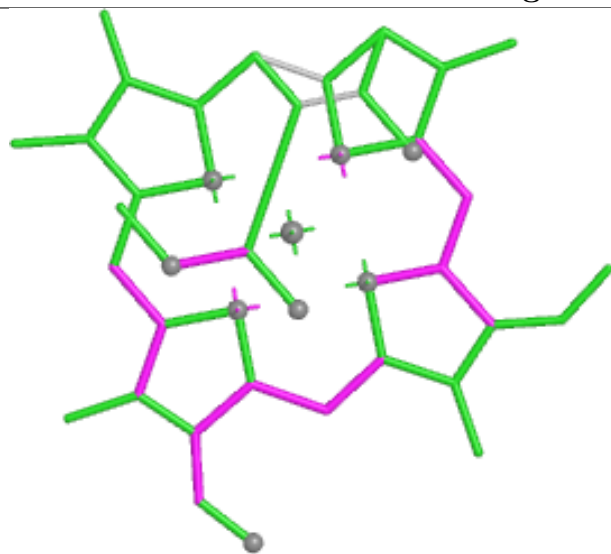




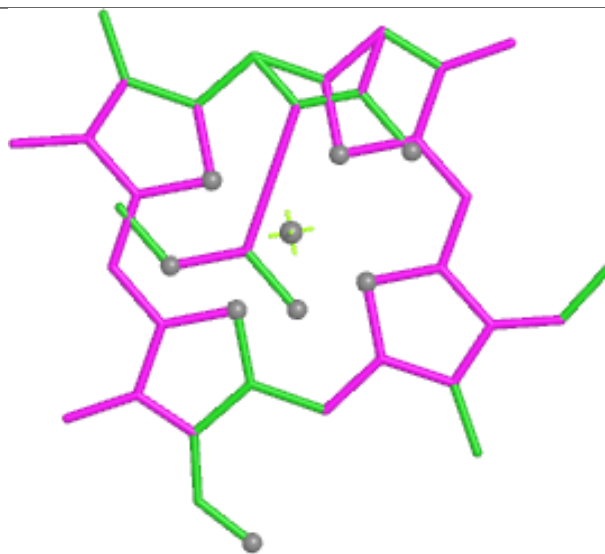




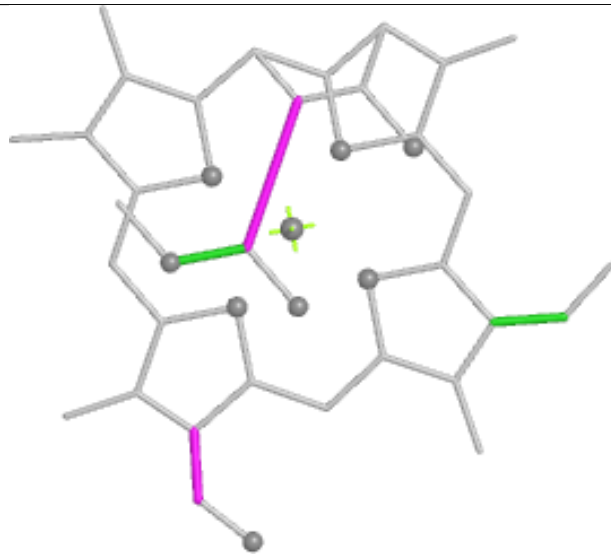
Ligand CL7 8 407



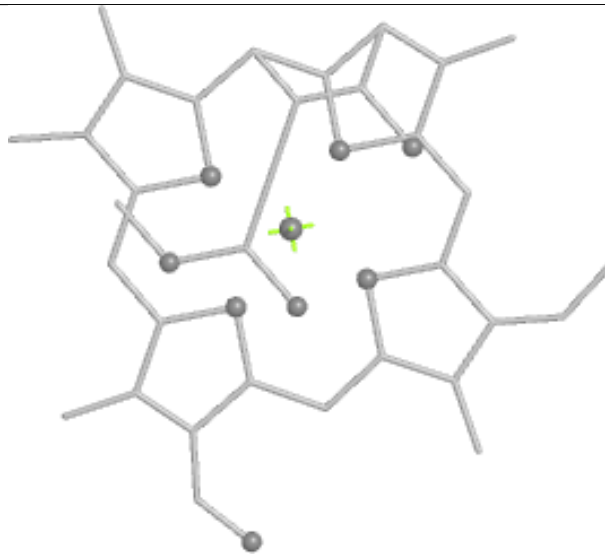
Bond lengths



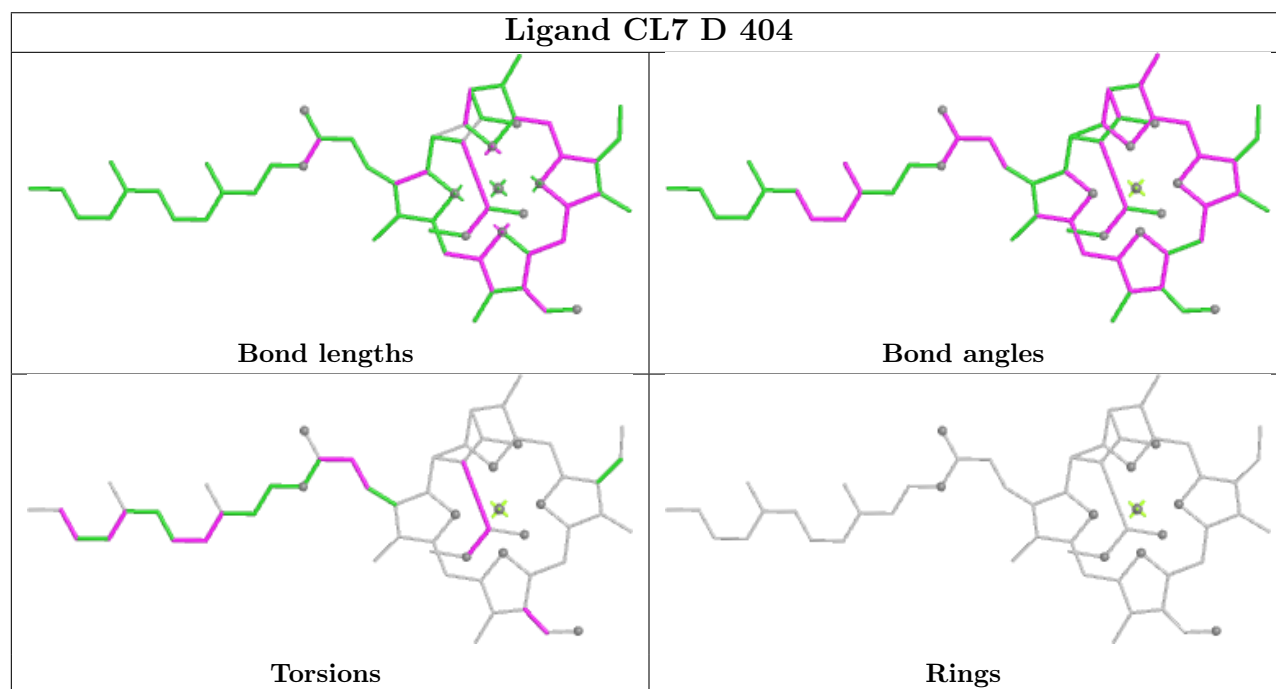
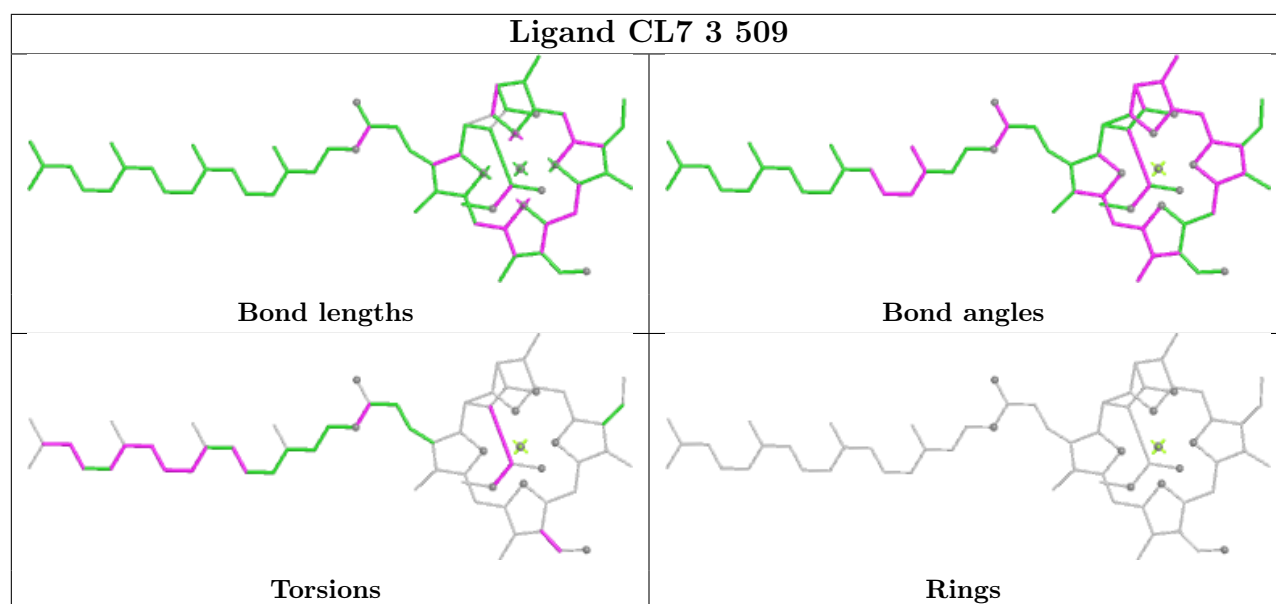
Bond angles

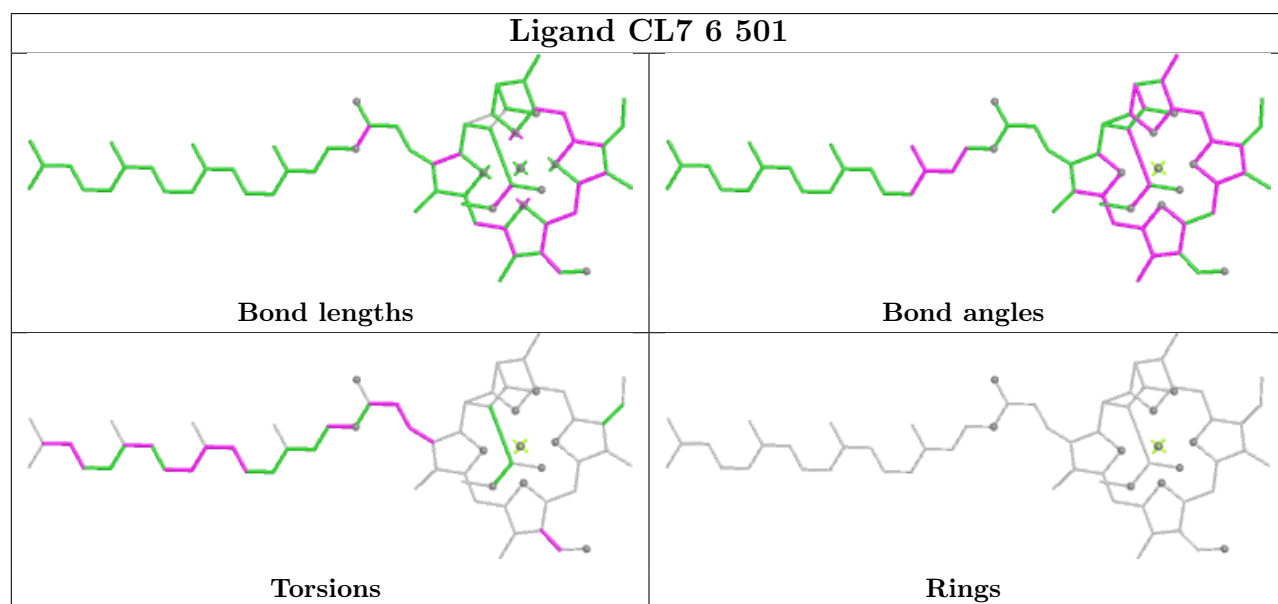
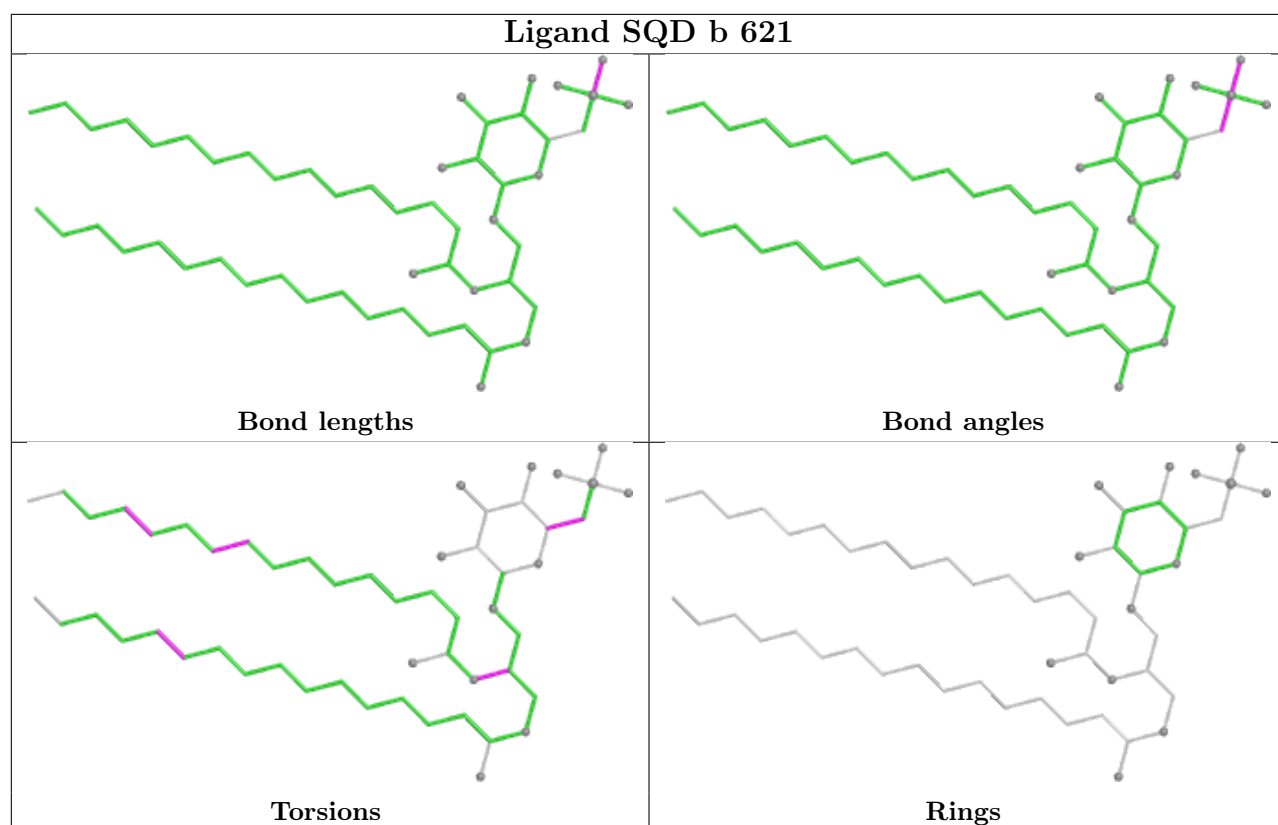


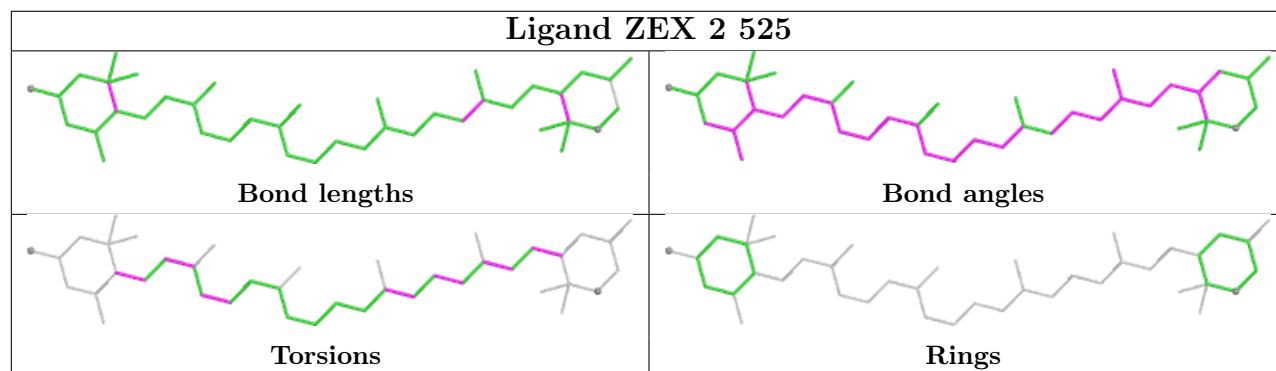
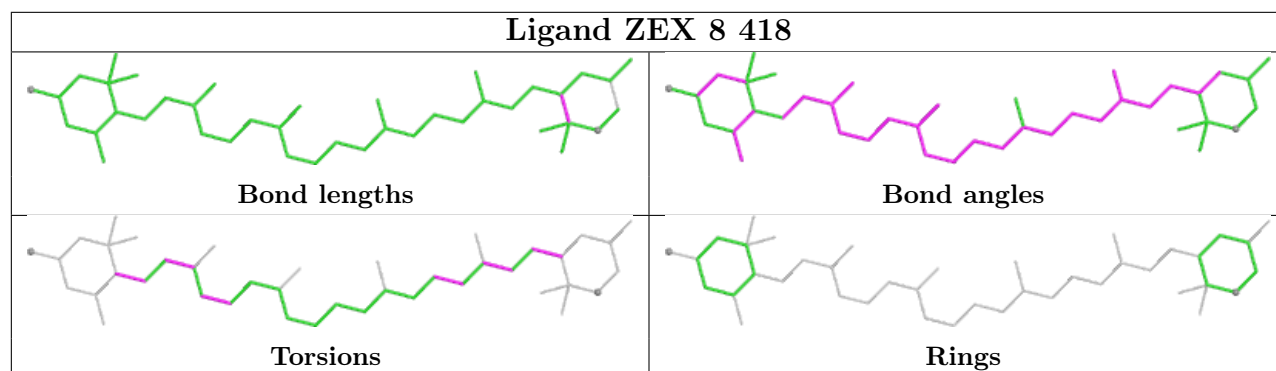
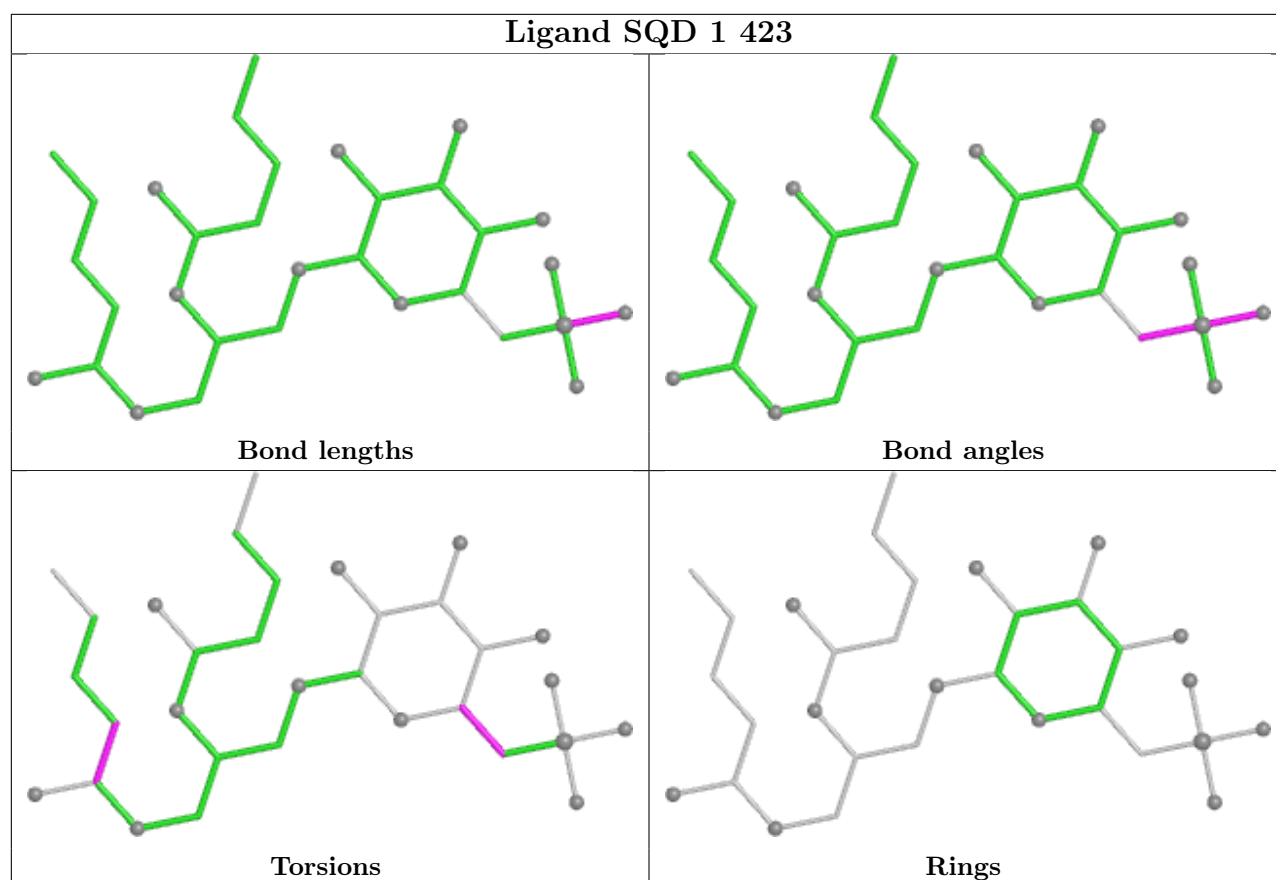
Torsions

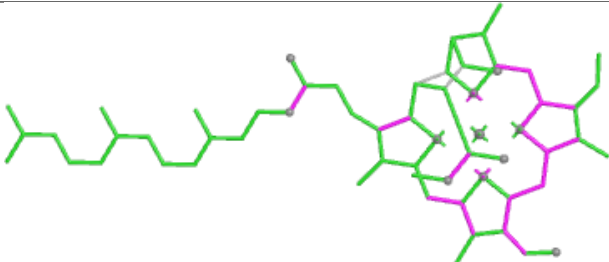
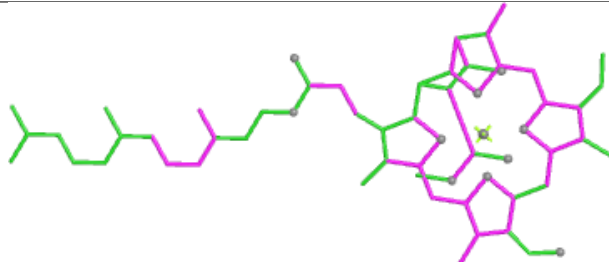
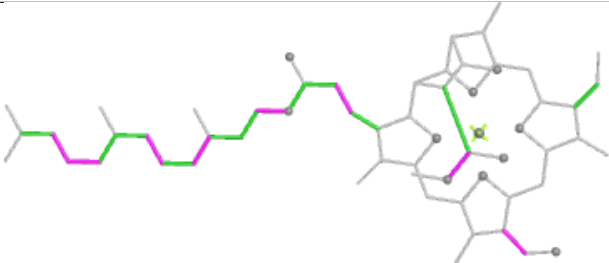
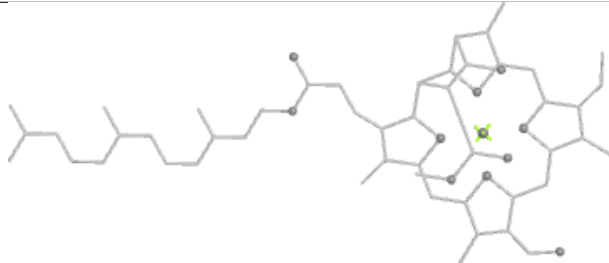


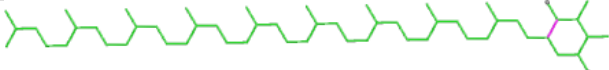
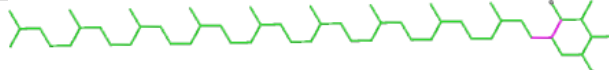
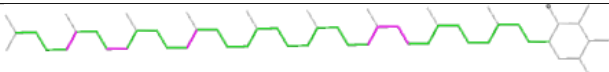
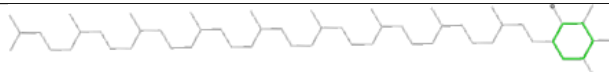
Rings

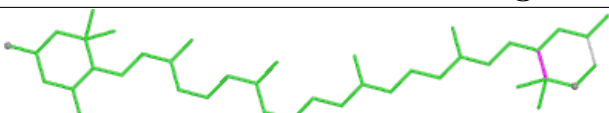
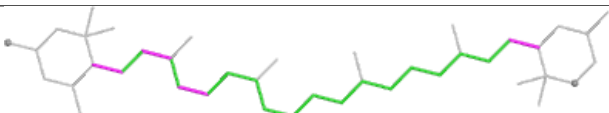




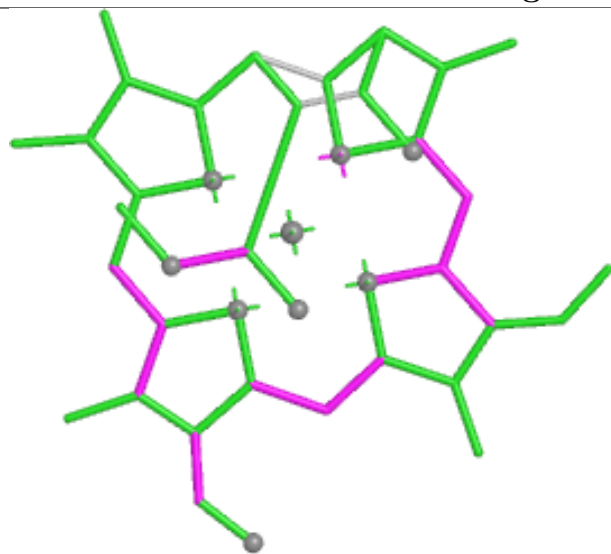


Ligand CL7 5 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

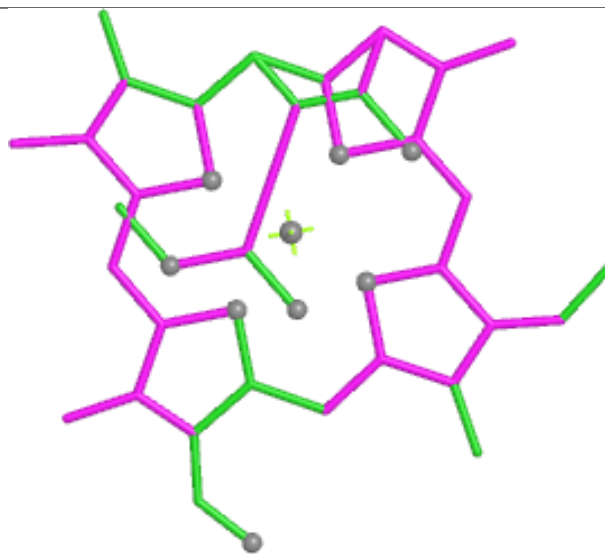
Ligand PL9 D 407	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ZEX 1 422	
	
Bond lengths	Bond angles
	
Torsions	Rings

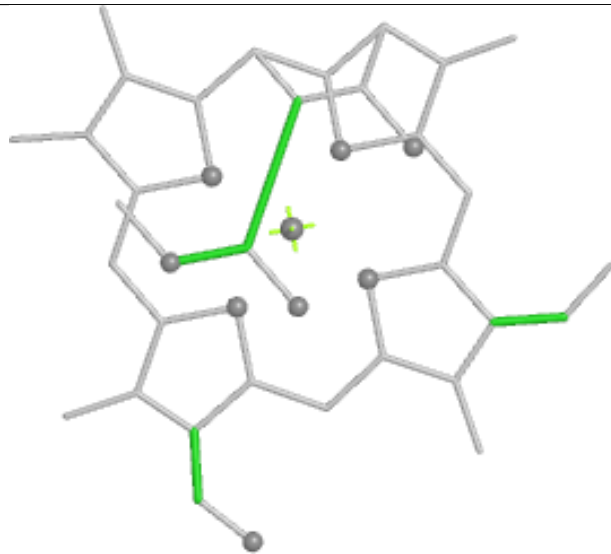
Ligand CL7 3 515



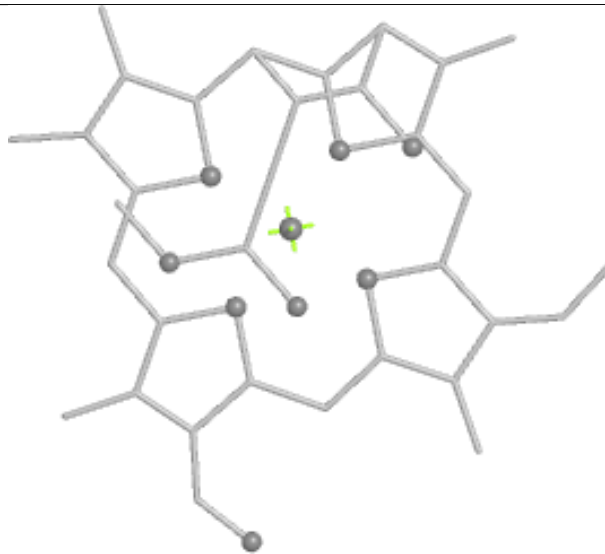
Bond lengths



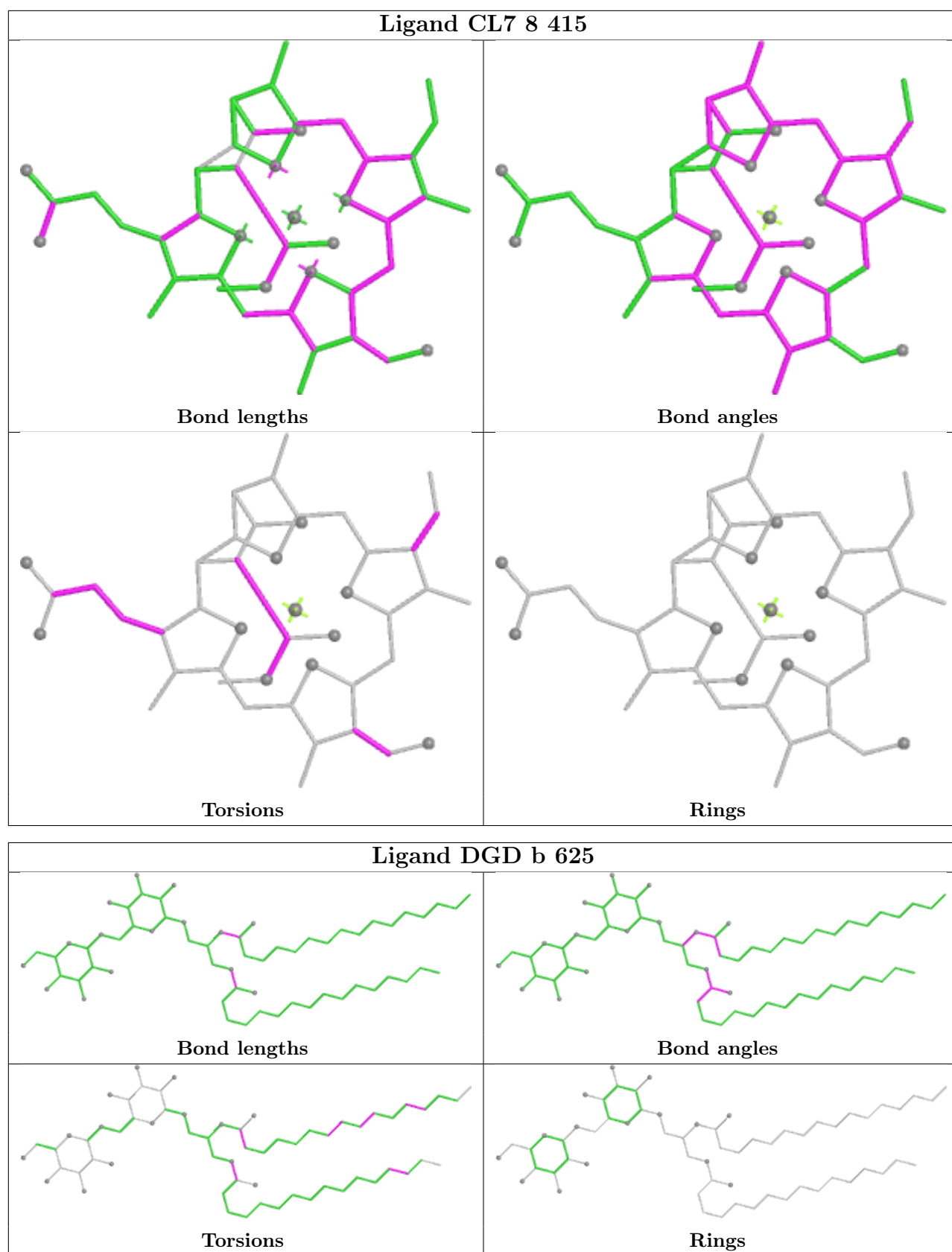
Bond angles

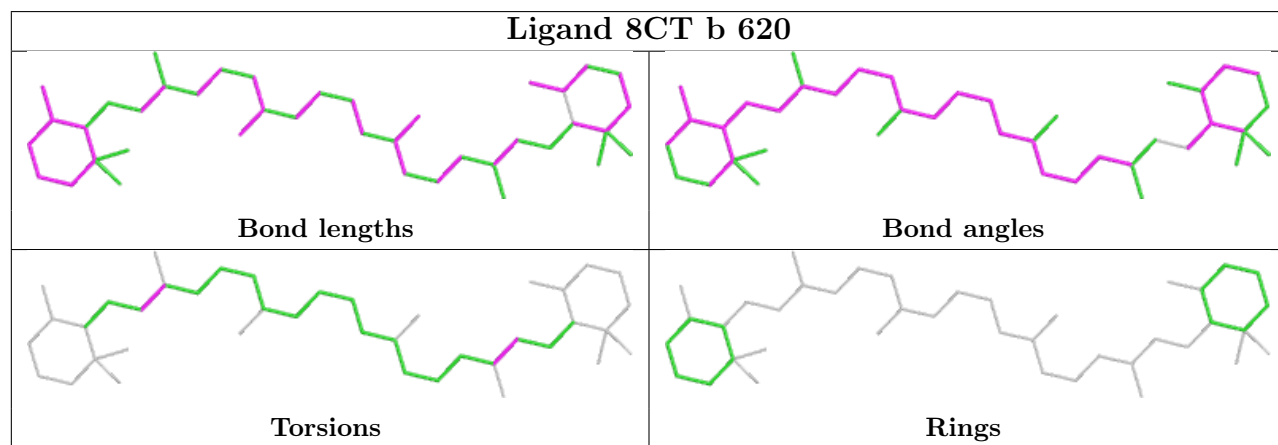
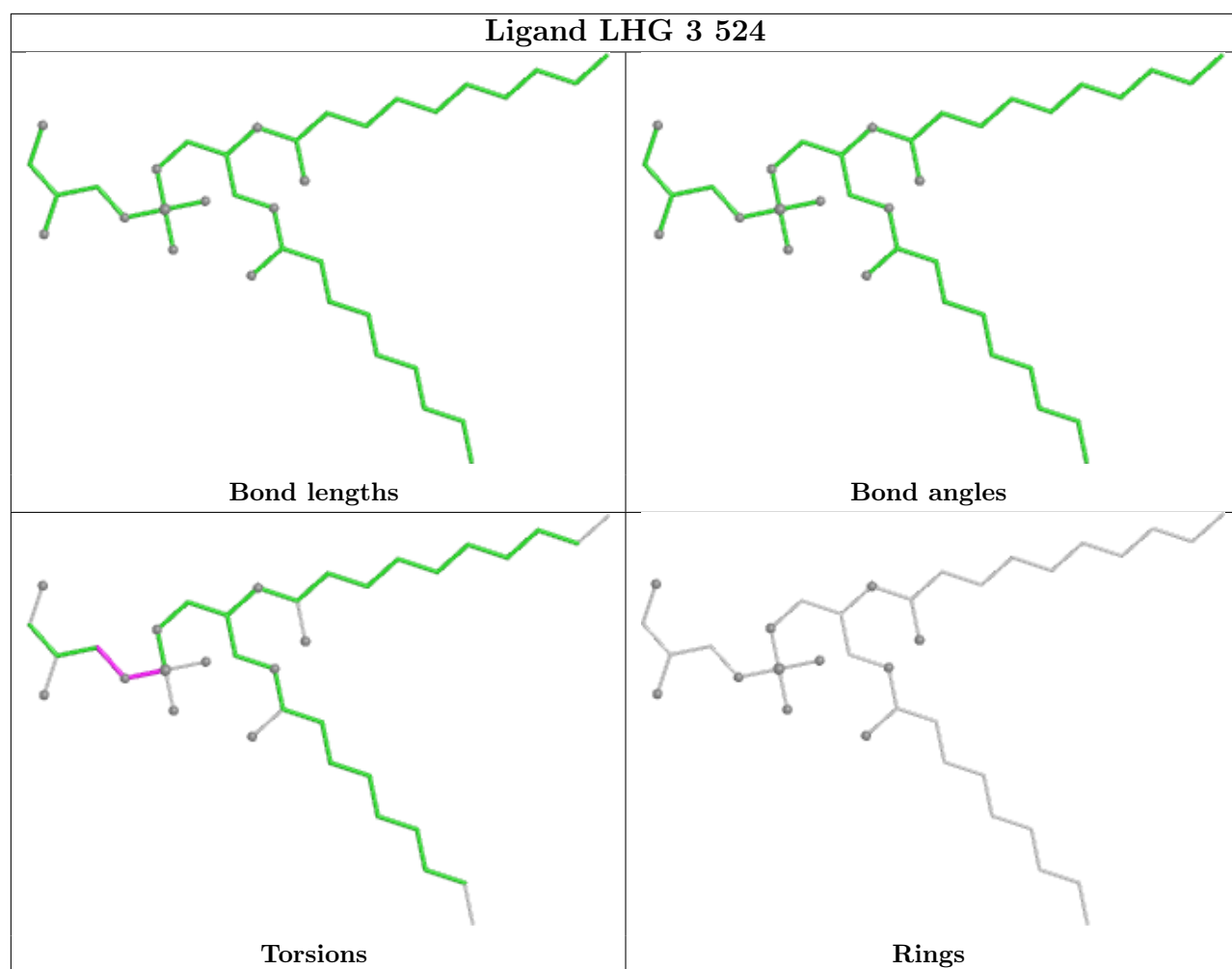


Torsions

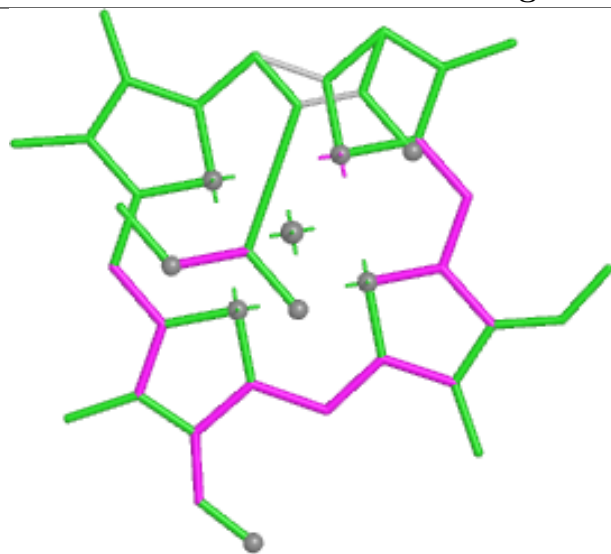


Rings

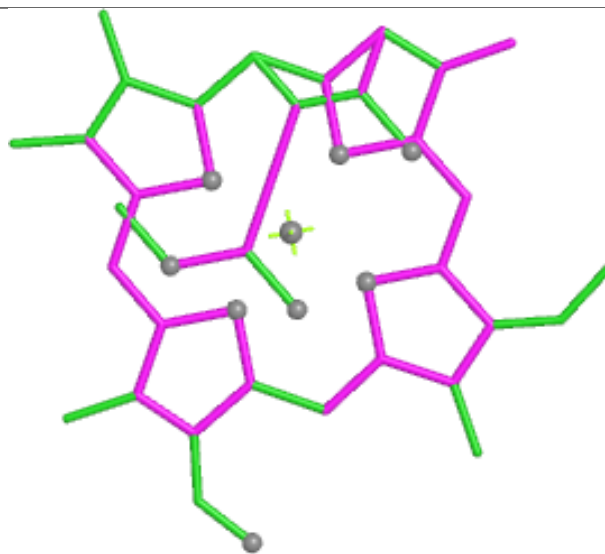




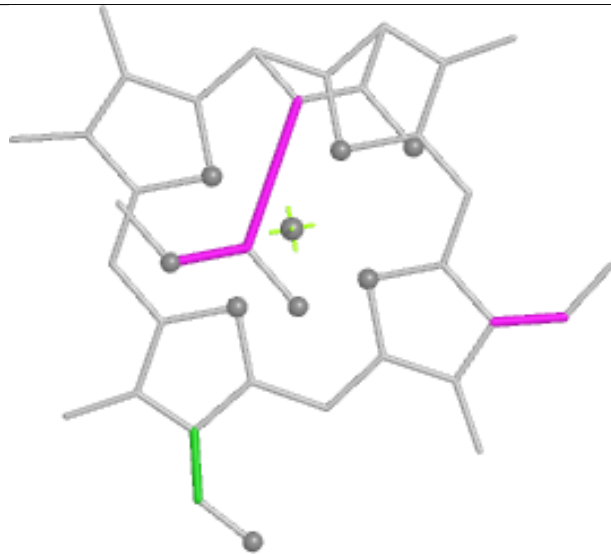
Ligand CL7 B 601



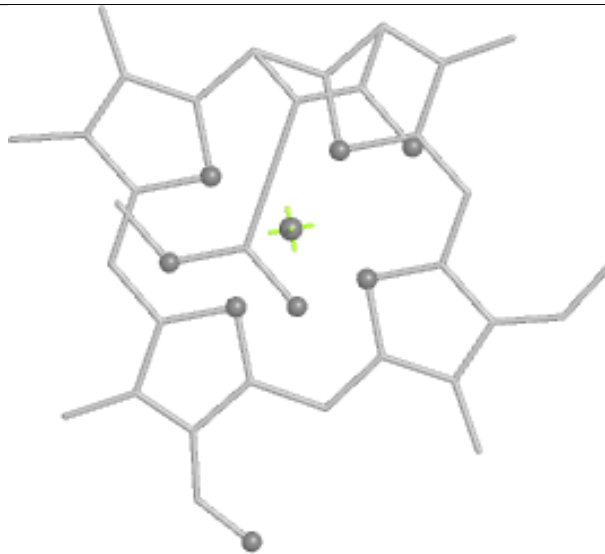
Bond lengths



Bond angles

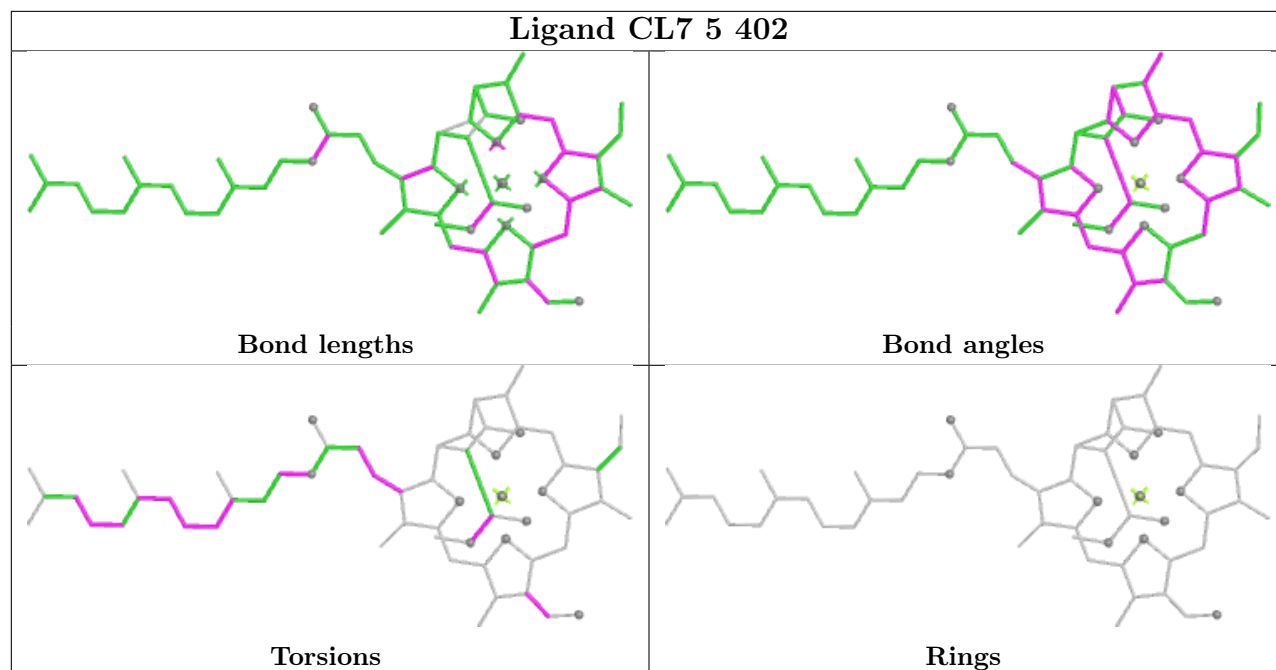


Torsions

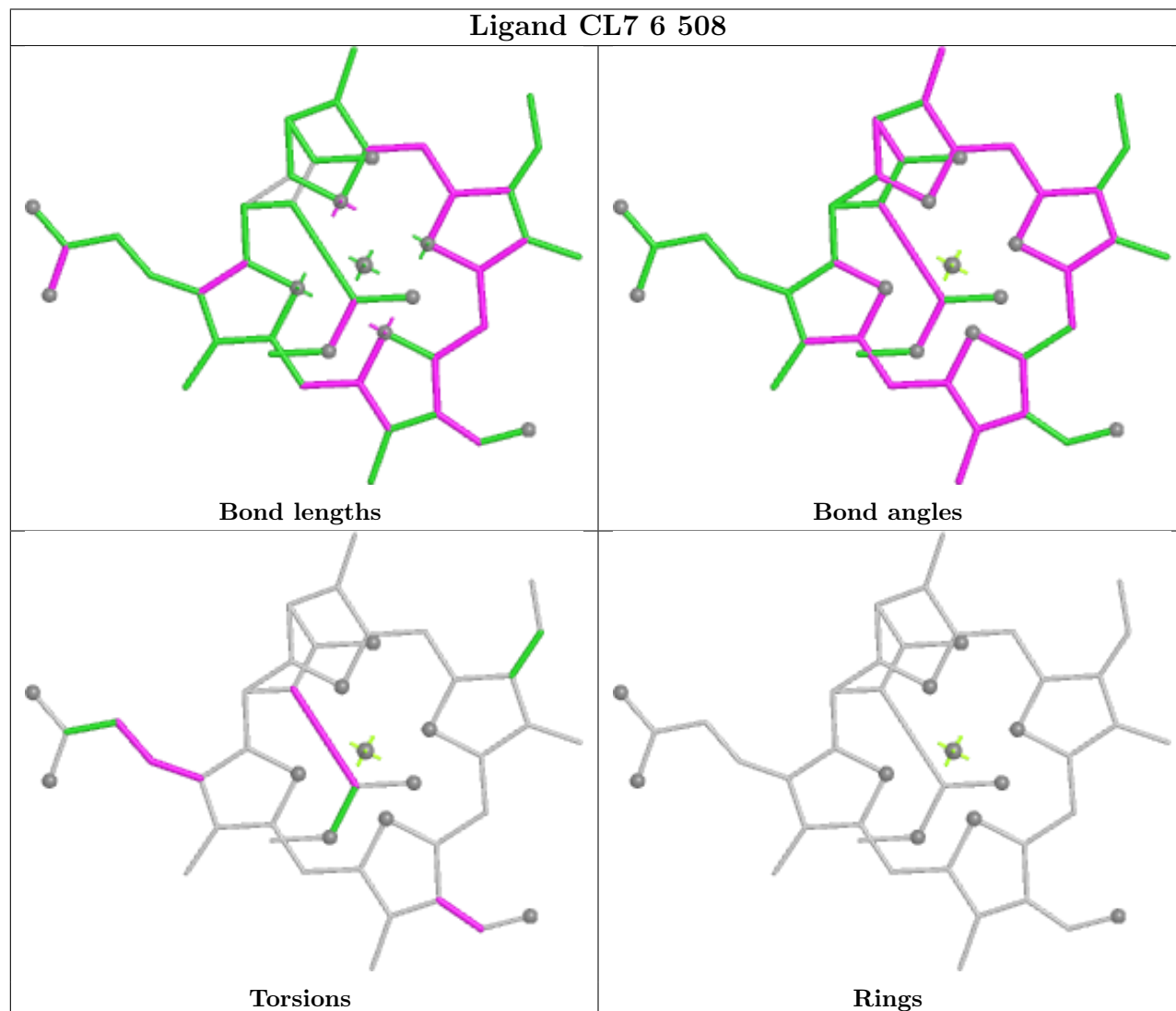


Rings

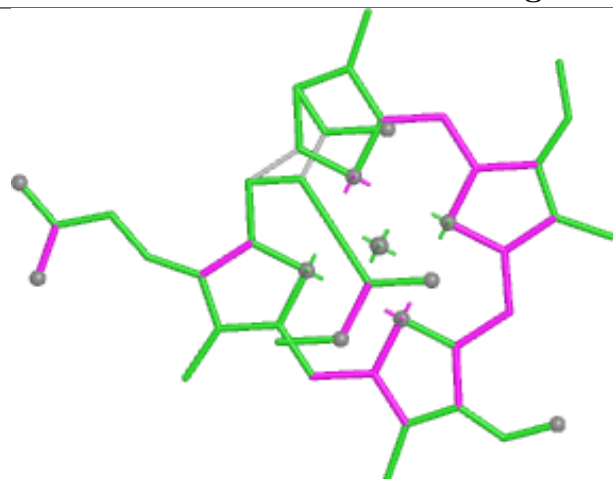
Ligand CL7 5 402



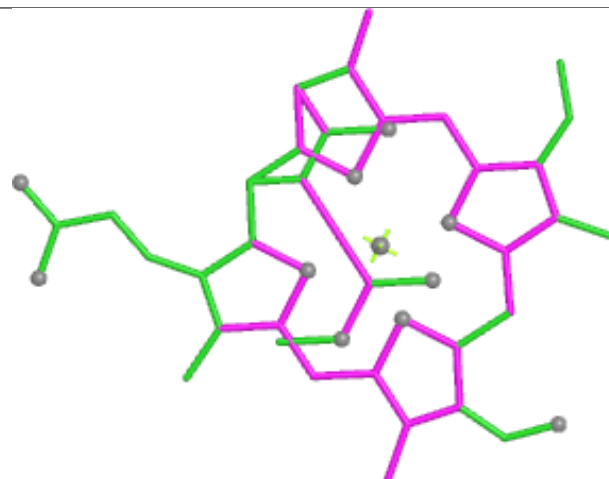
Ligand CL7 6 508



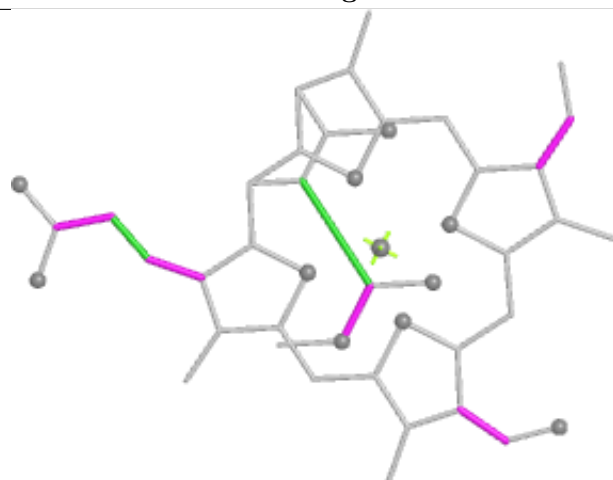
Ligand CL7 6 514



Bond lengths



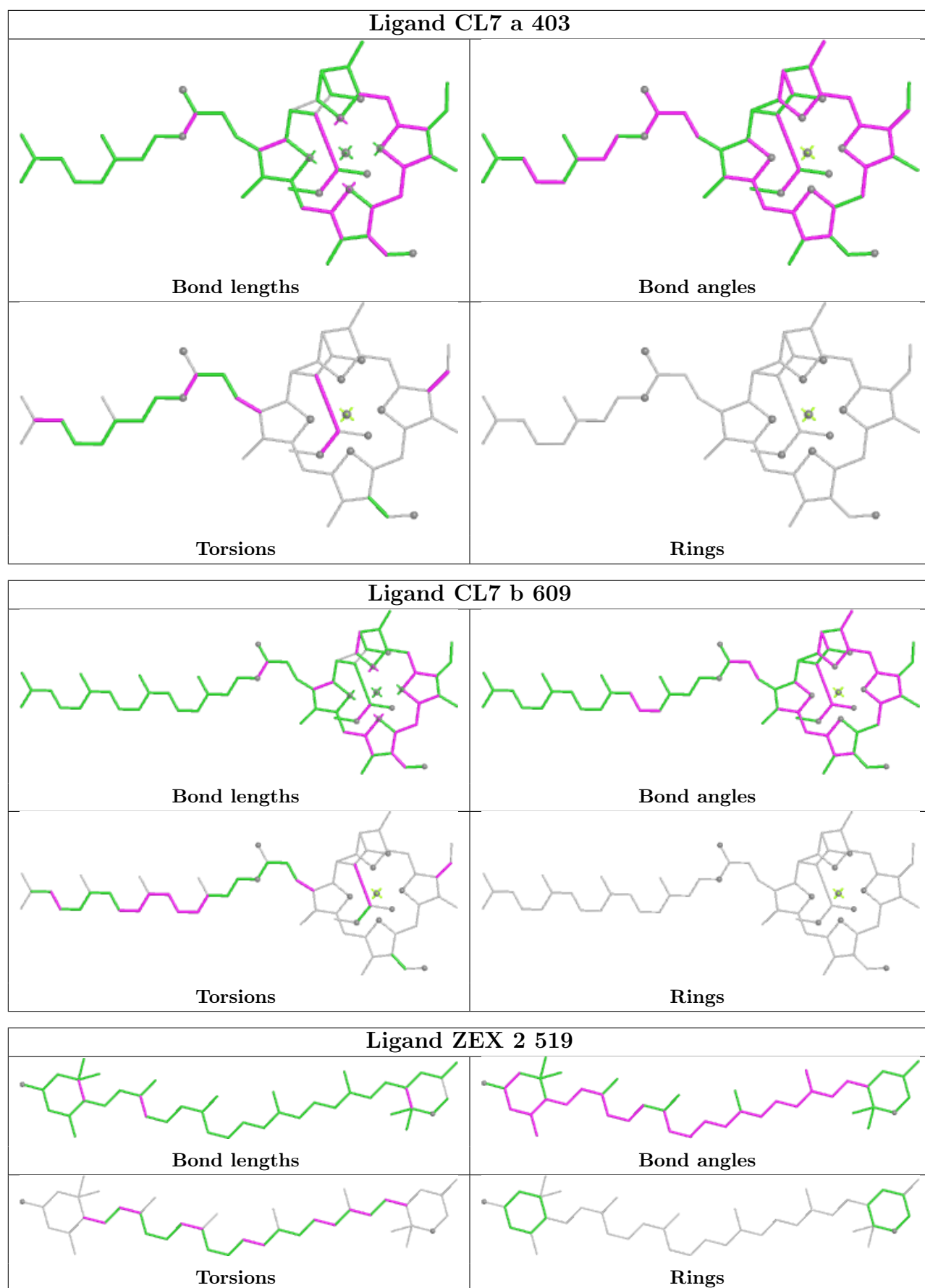
Bond angles

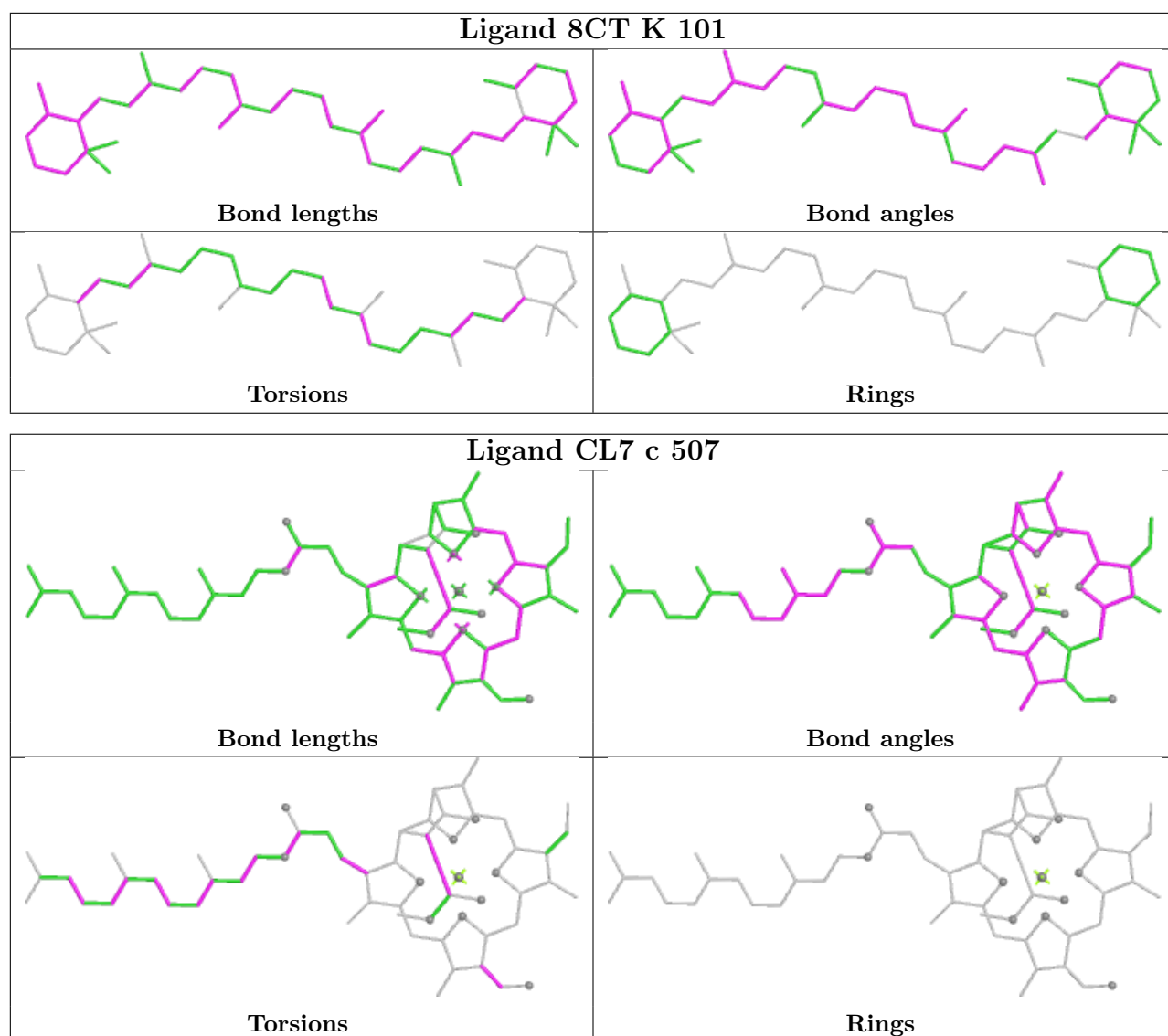


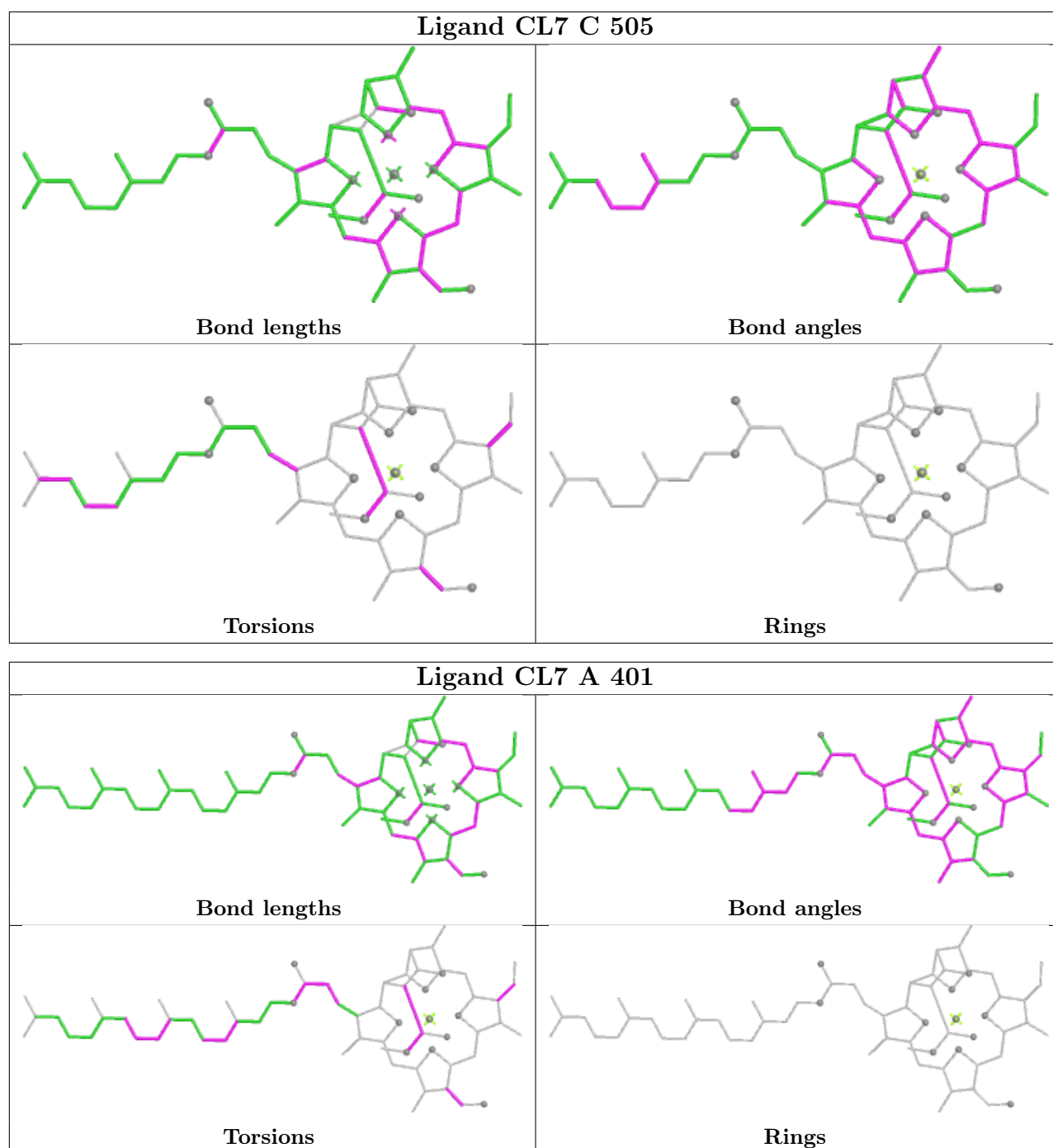
Torsions

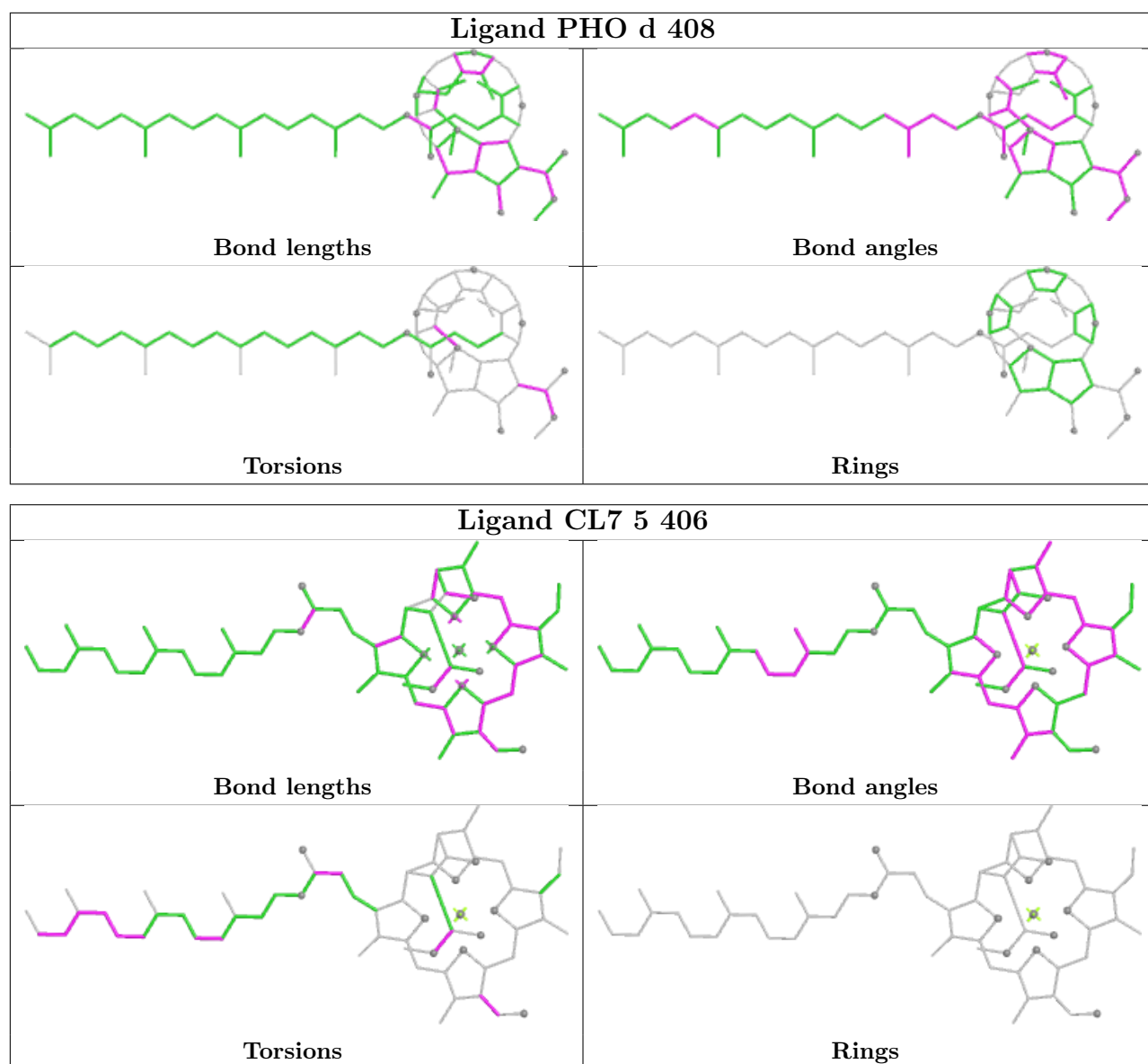


Rings

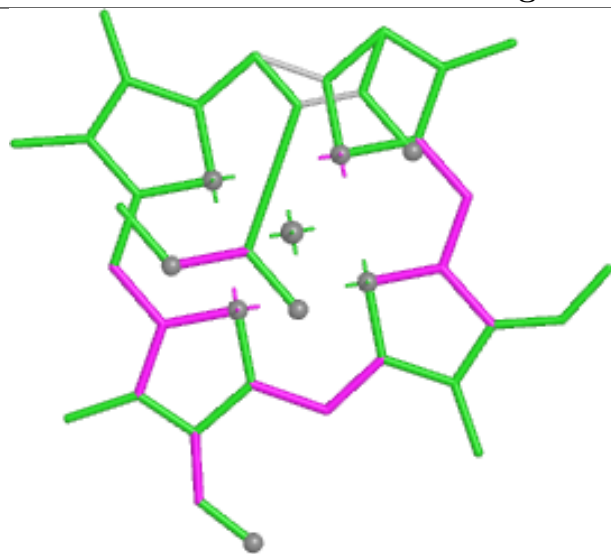




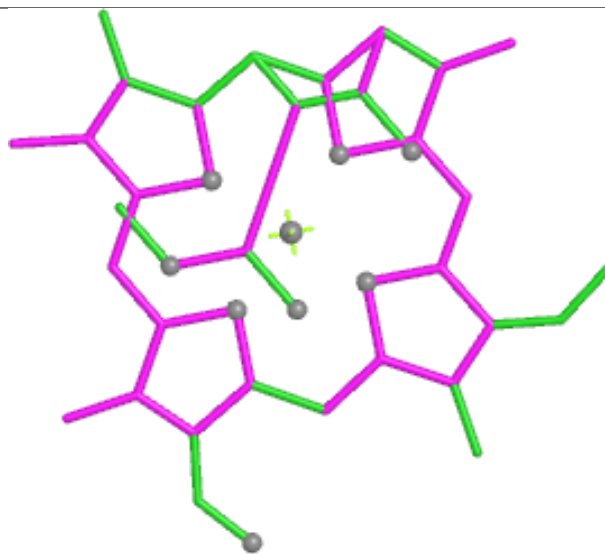




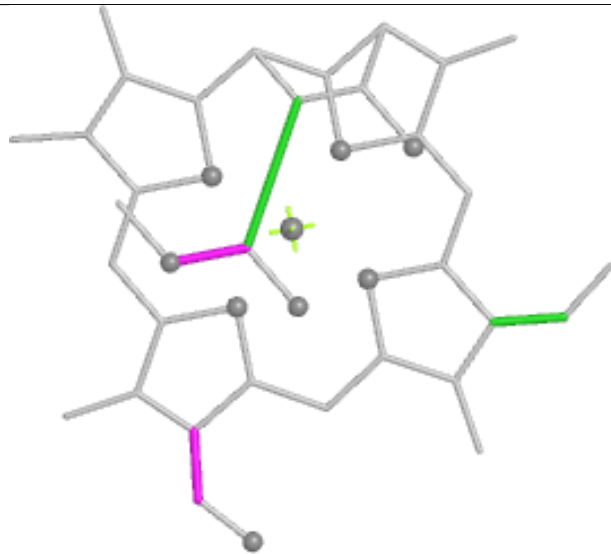
Ligand CL7 C 513



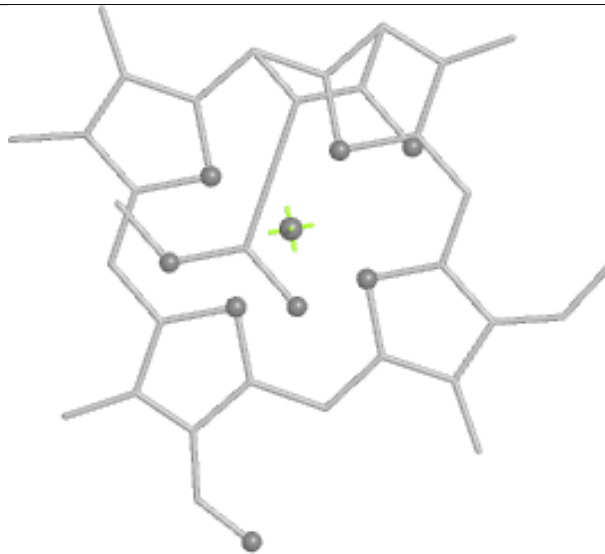
Bond lengths



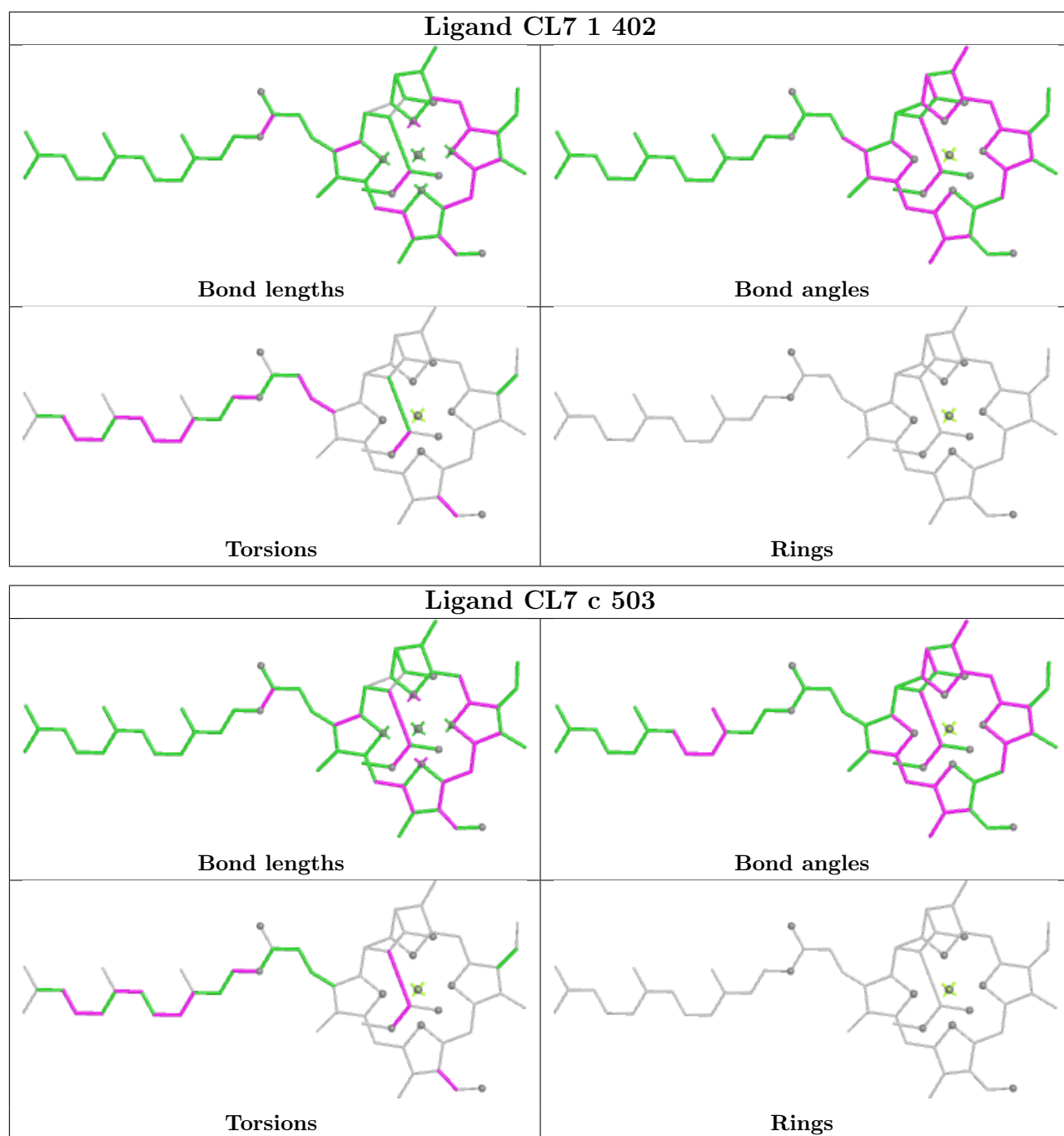
Bond angles

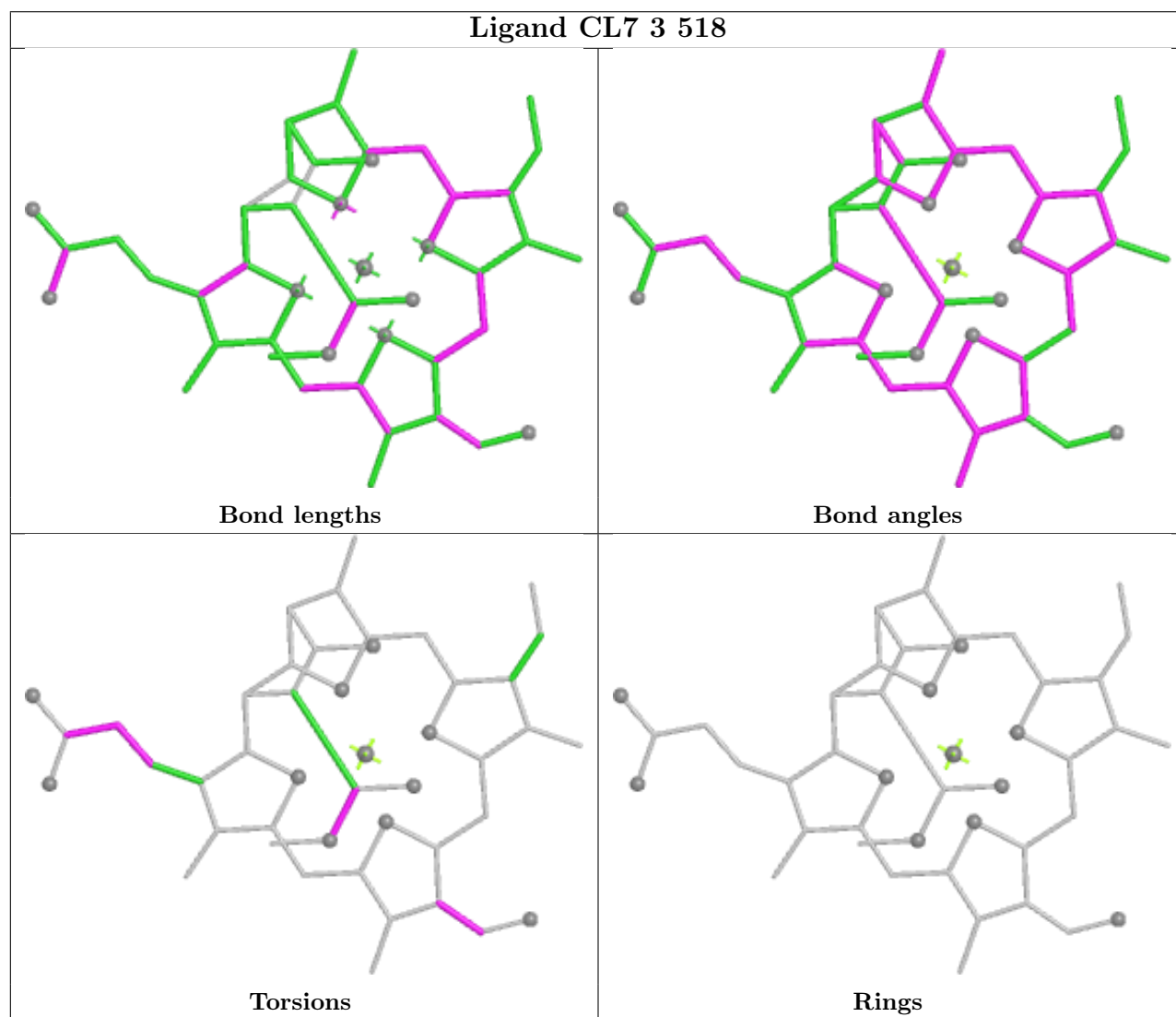
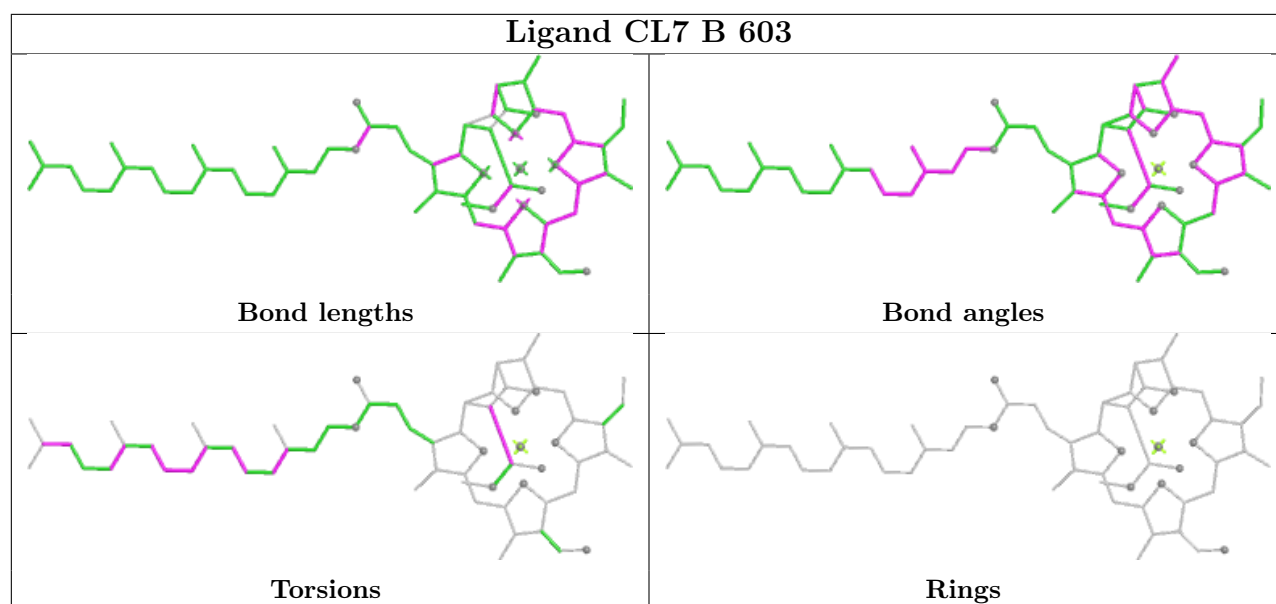


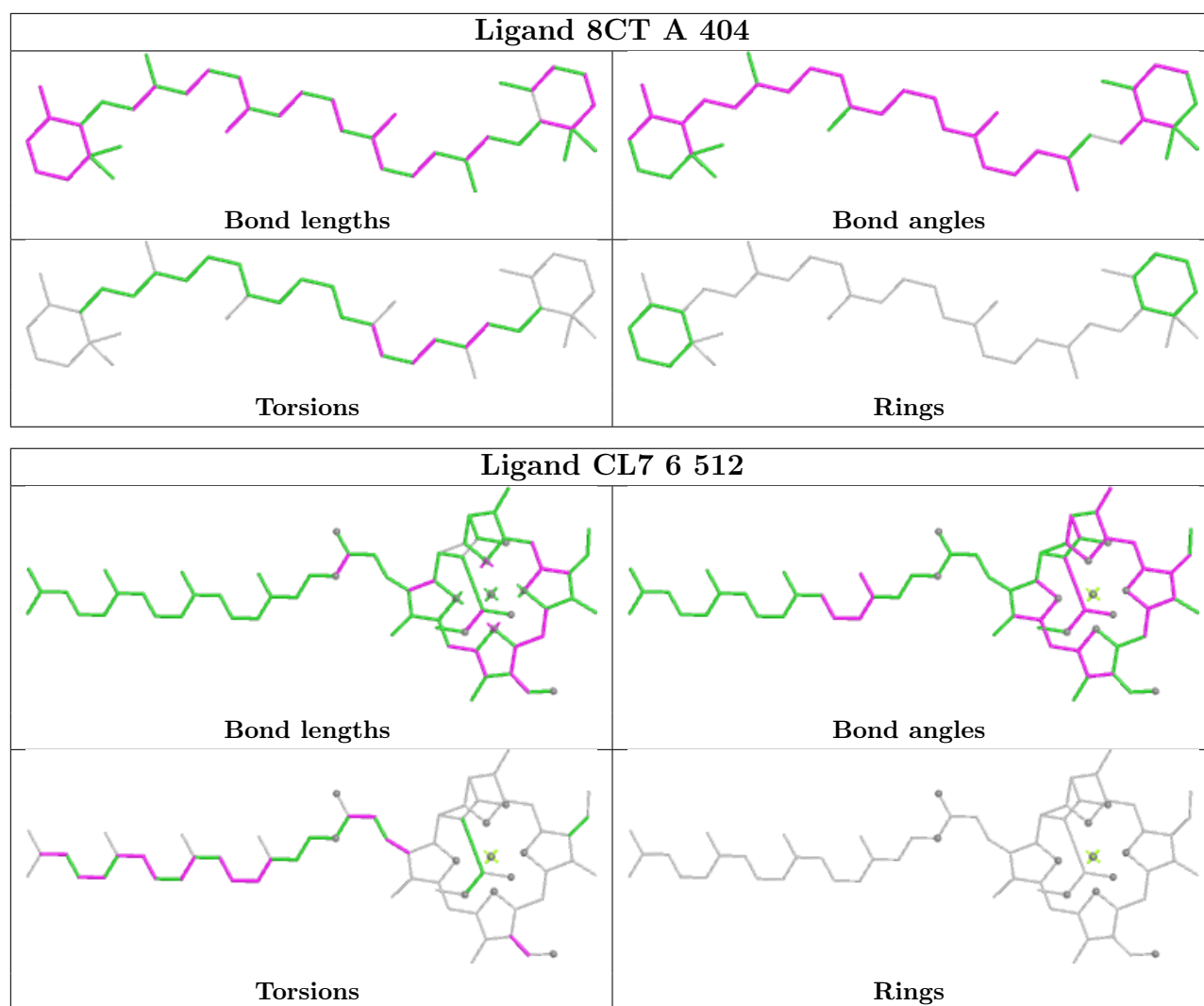
Torsions

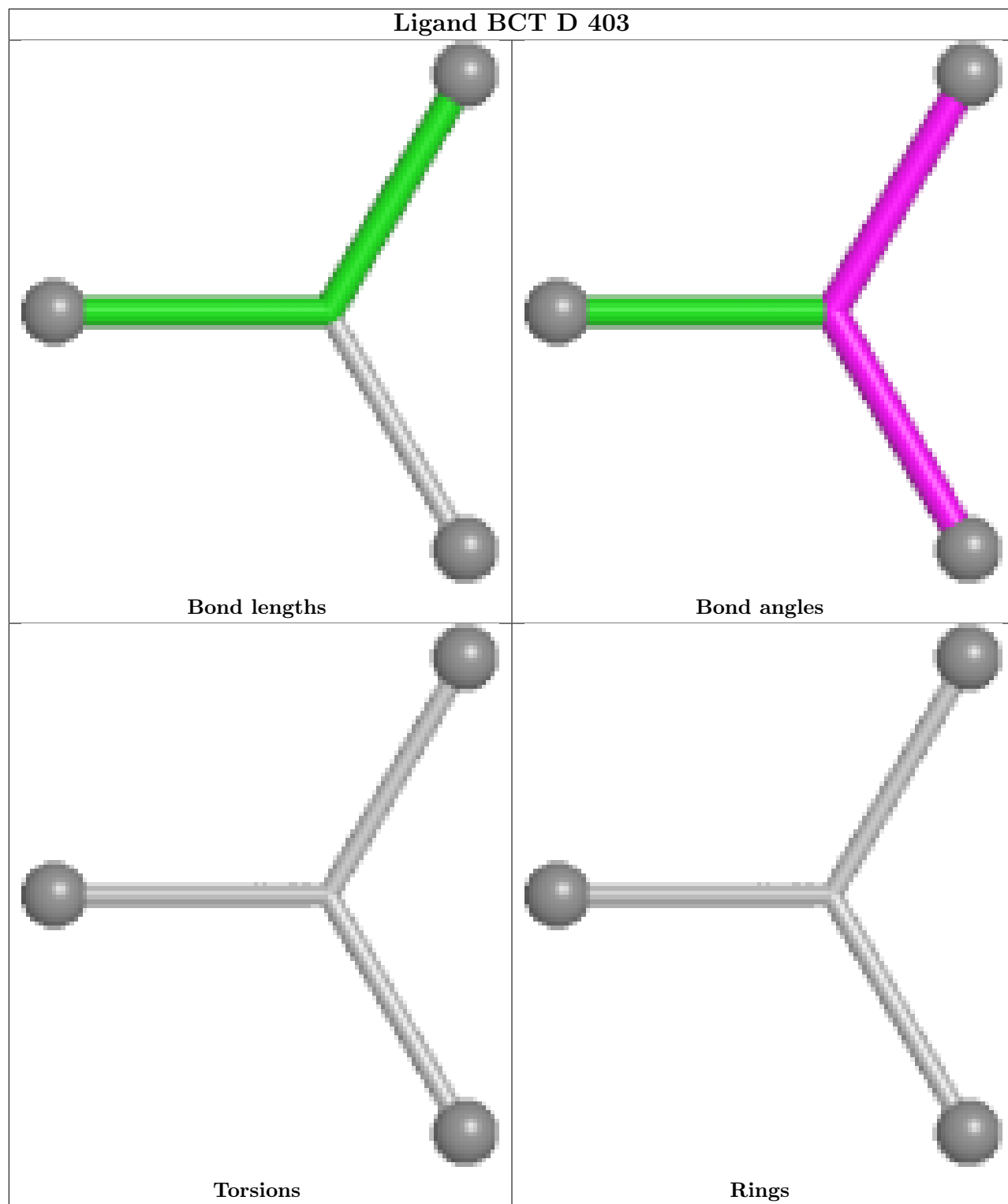


Rings

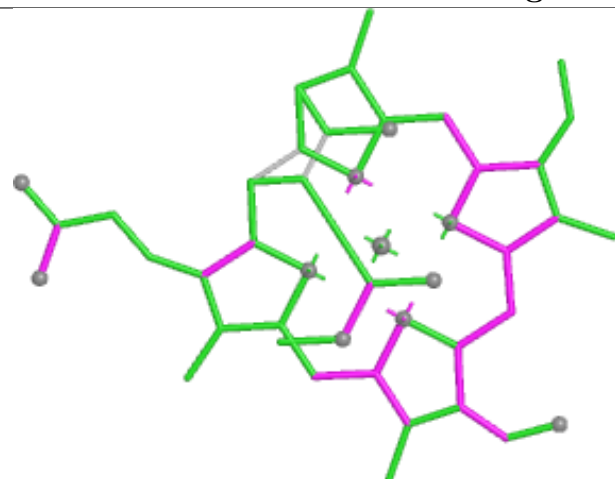








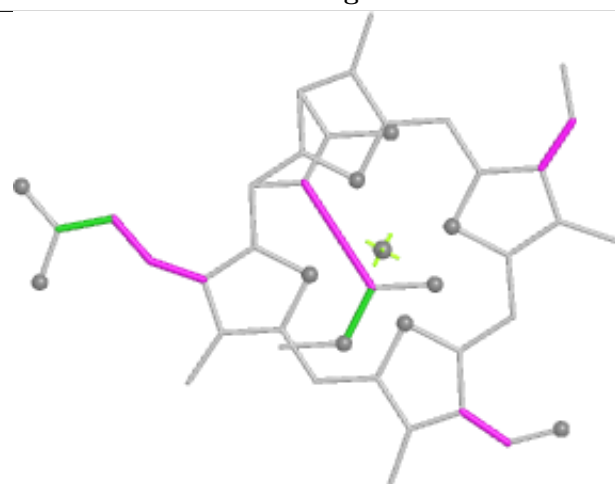
Ligand CL7 d 405



Bond lengths



Bond angles

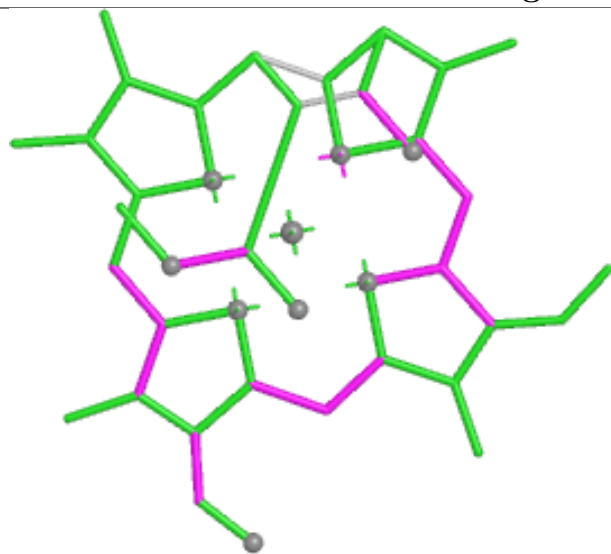


Torsions

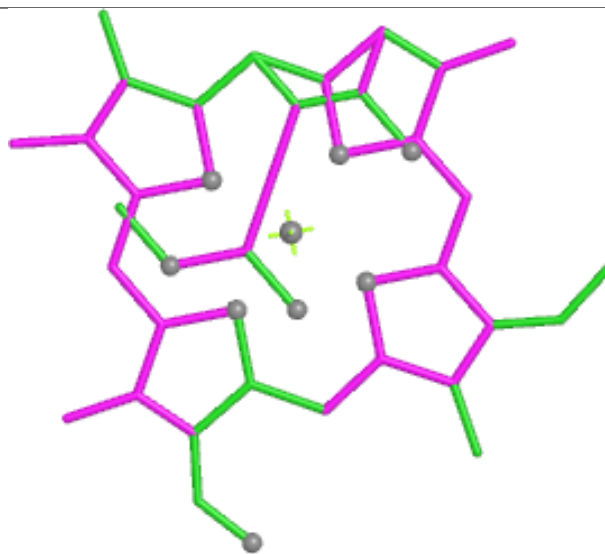


Rings

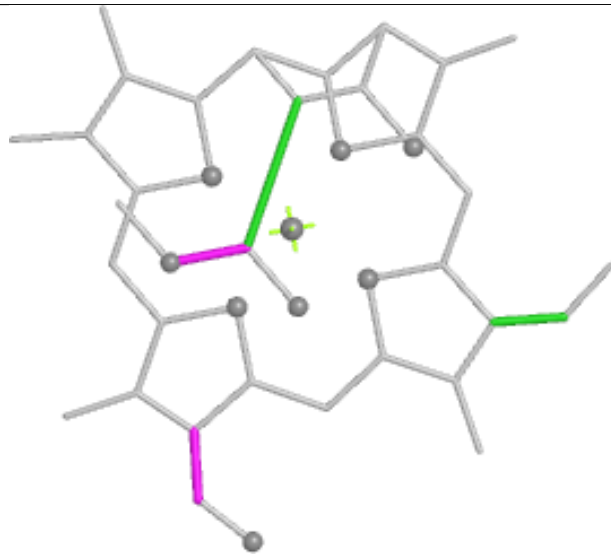
Ligand CL7 5 416



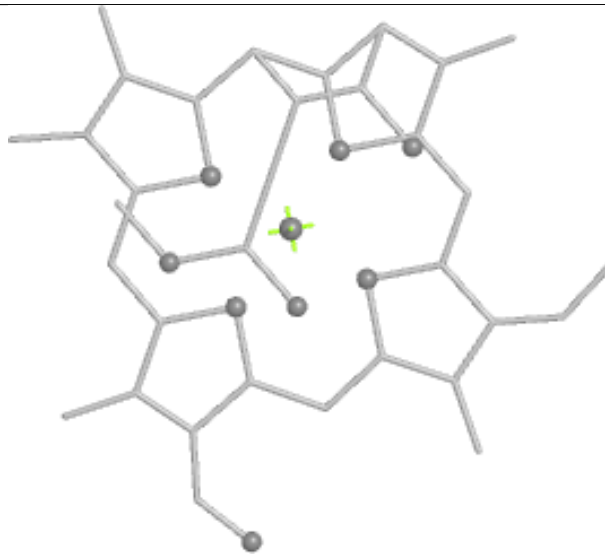
Bond lengths



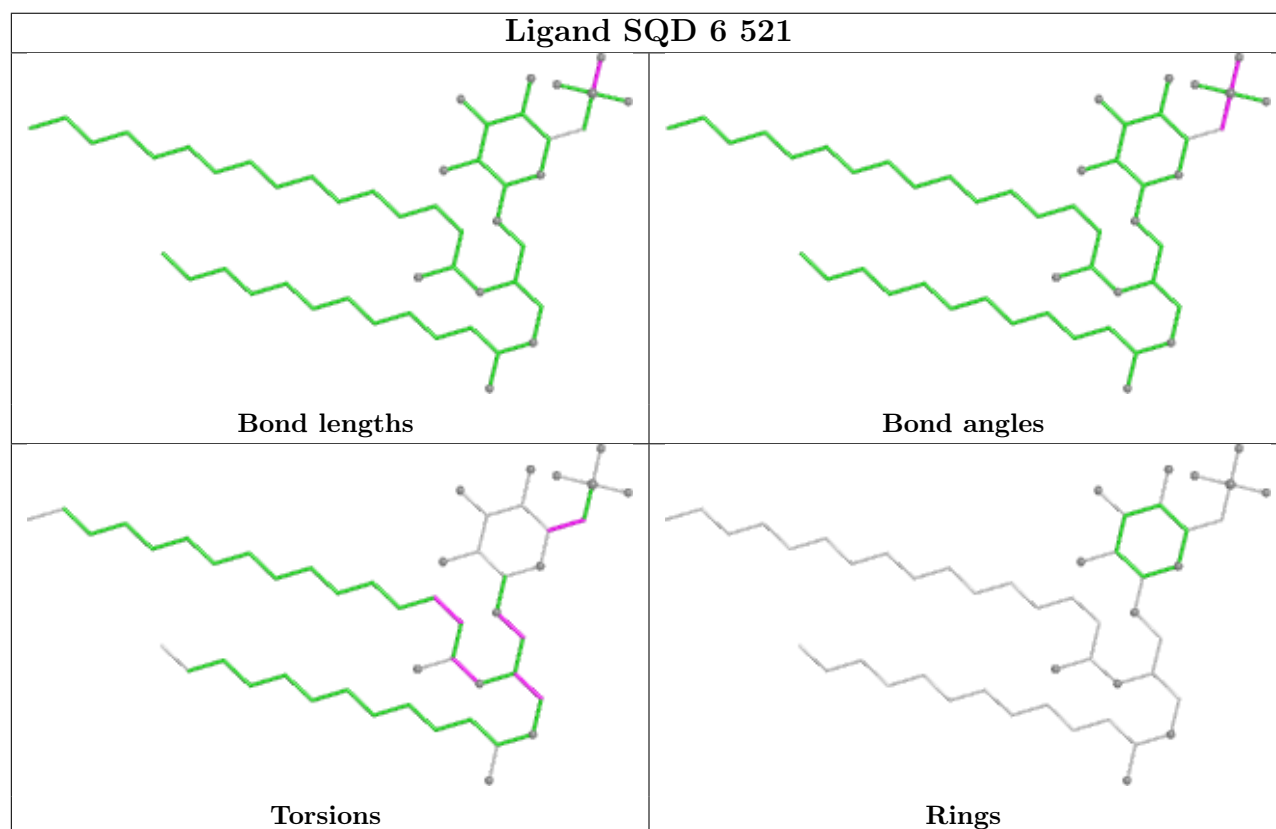
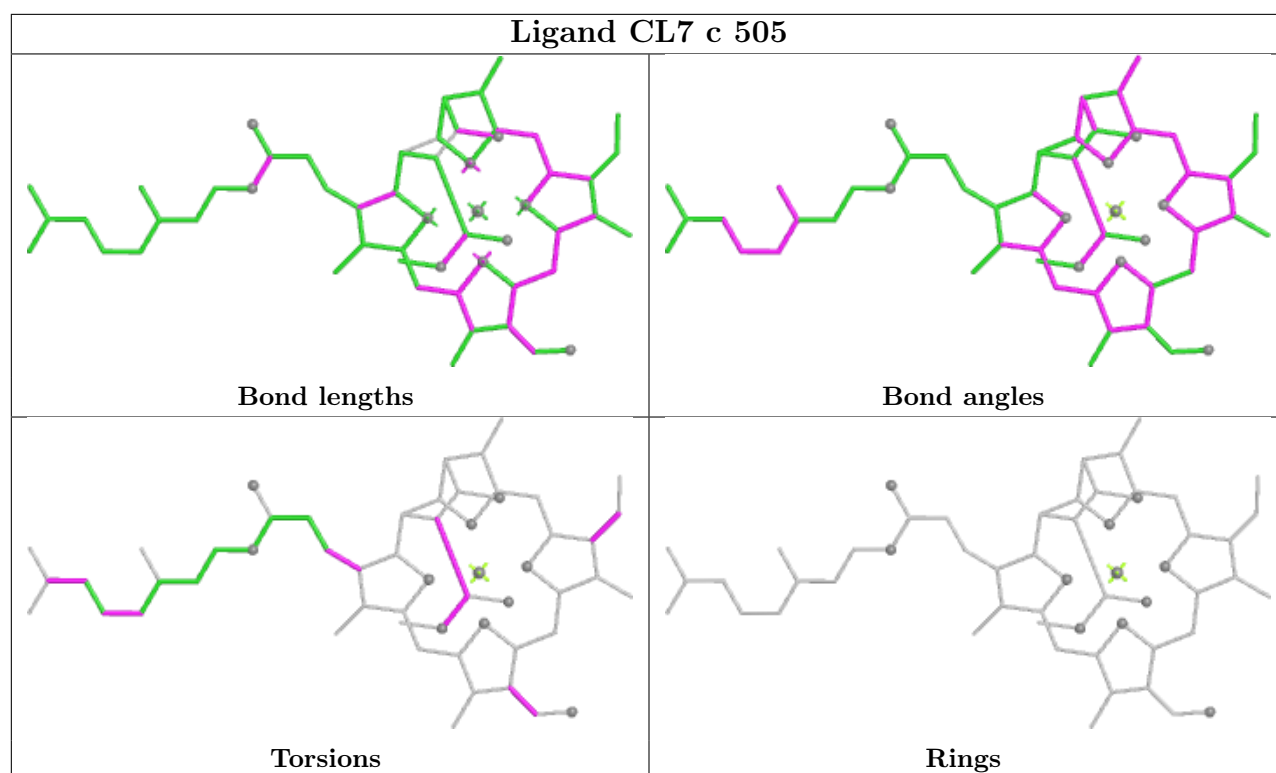
Bond angles



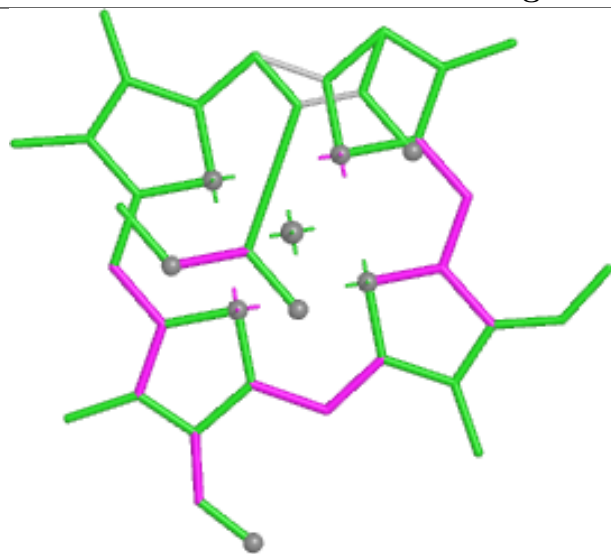
Torsions



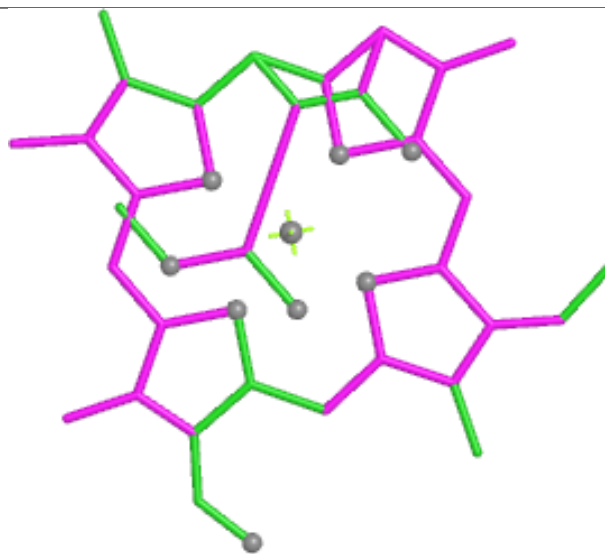
Rings



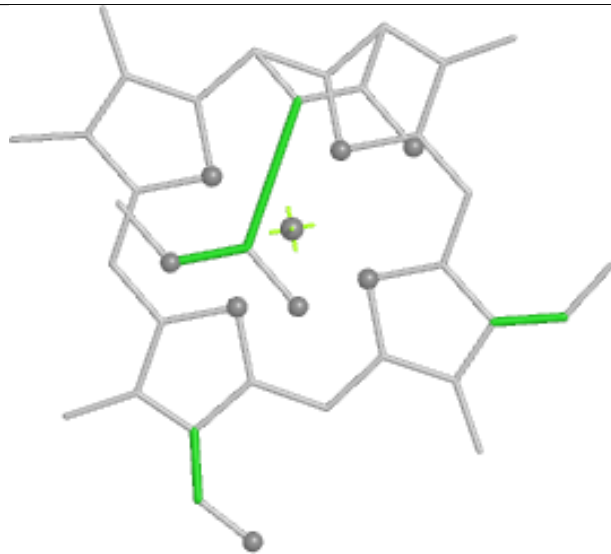
Ligand CL7 7 515



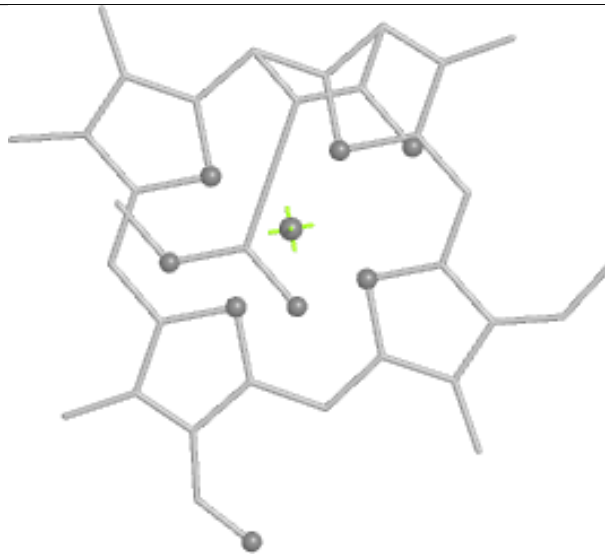
Bond lengths



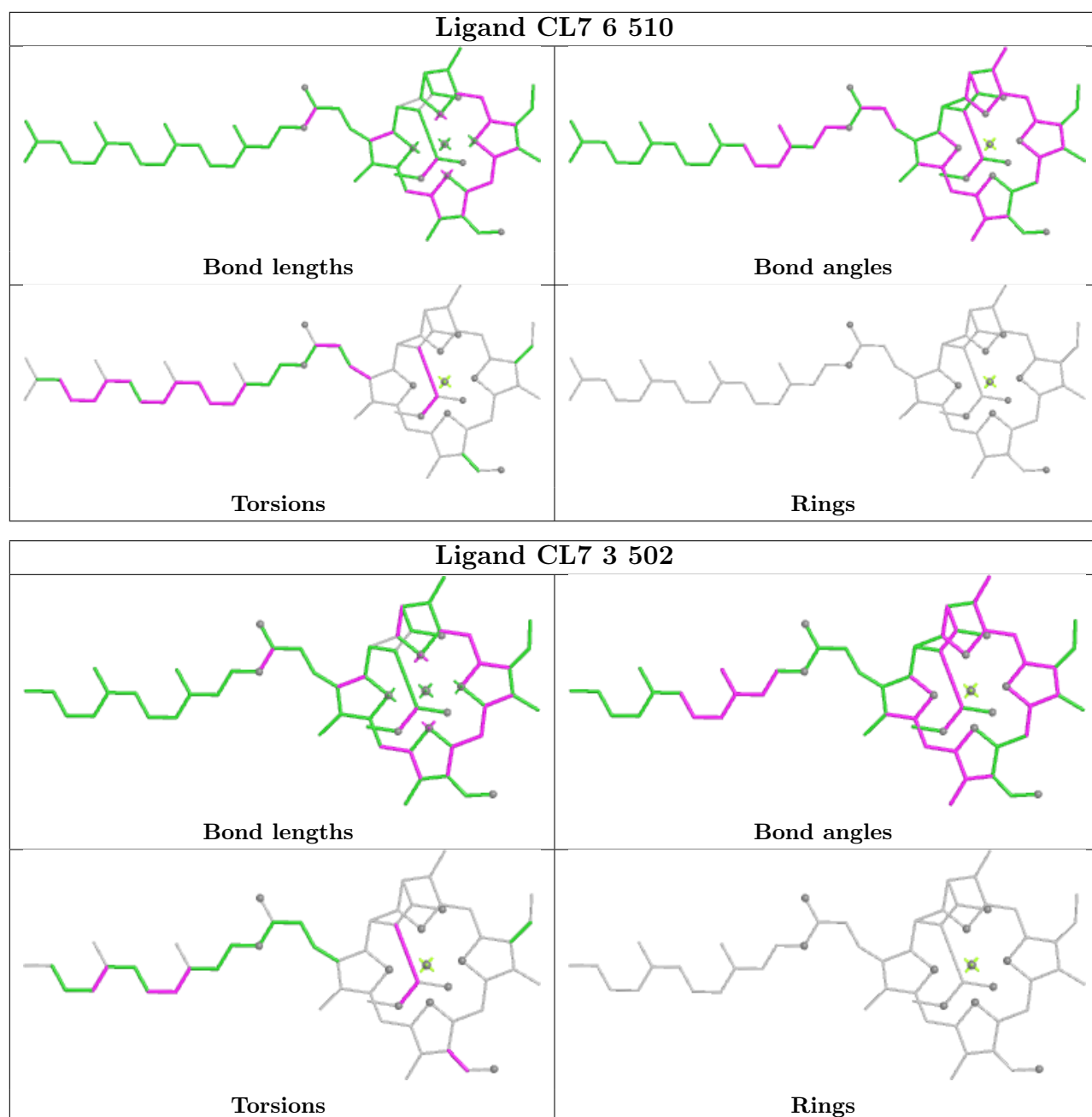
Bond angles

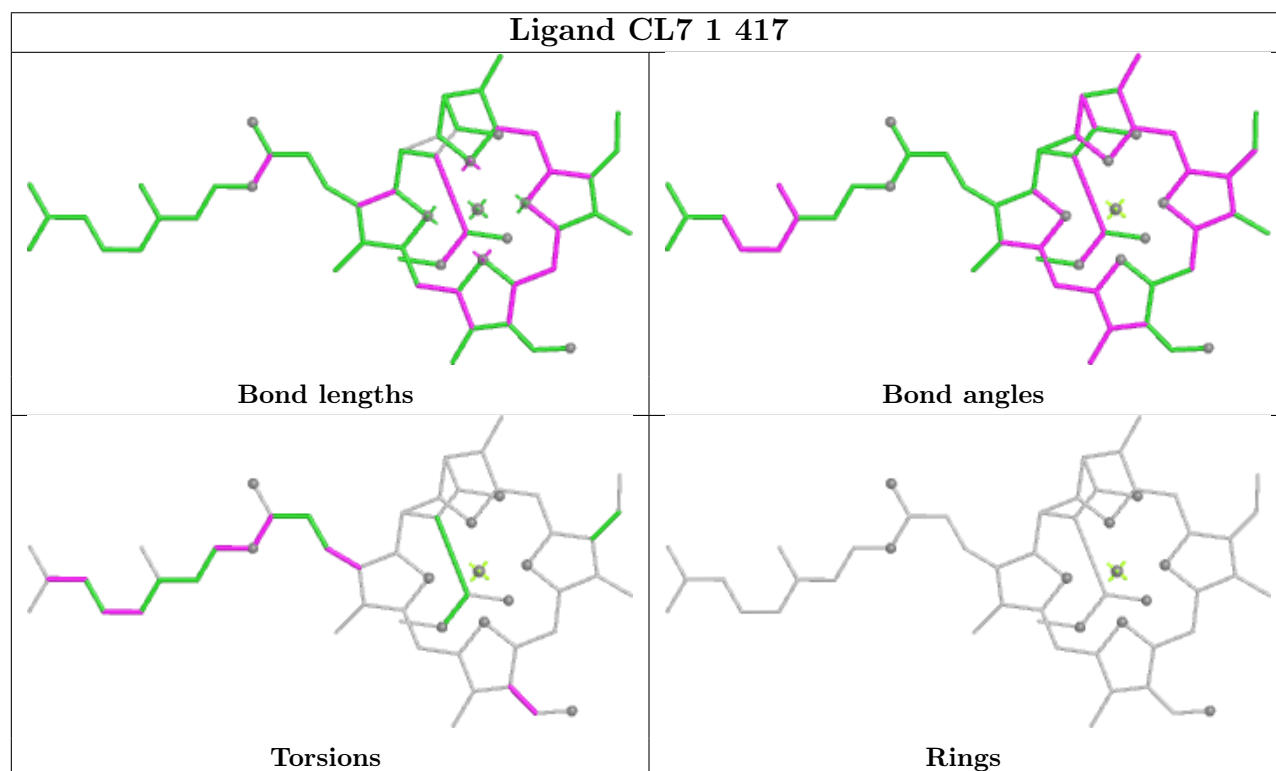
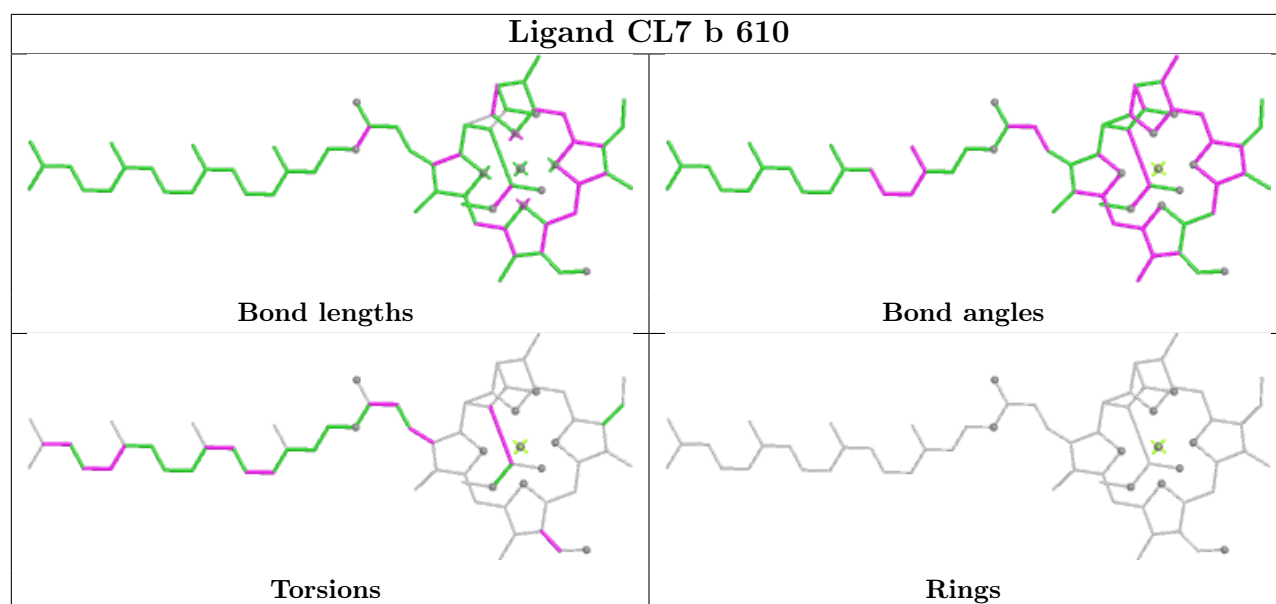


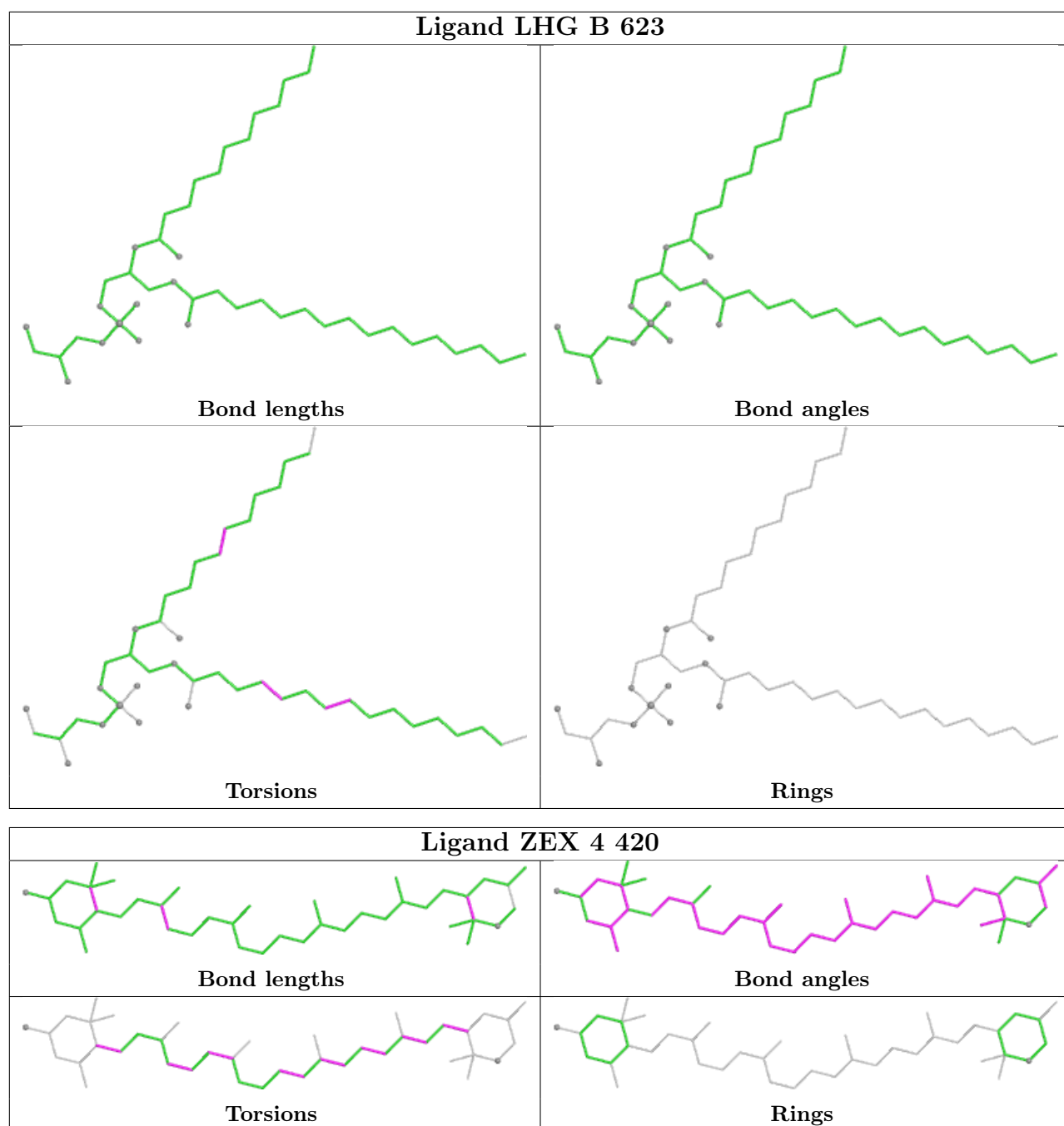
Torsions

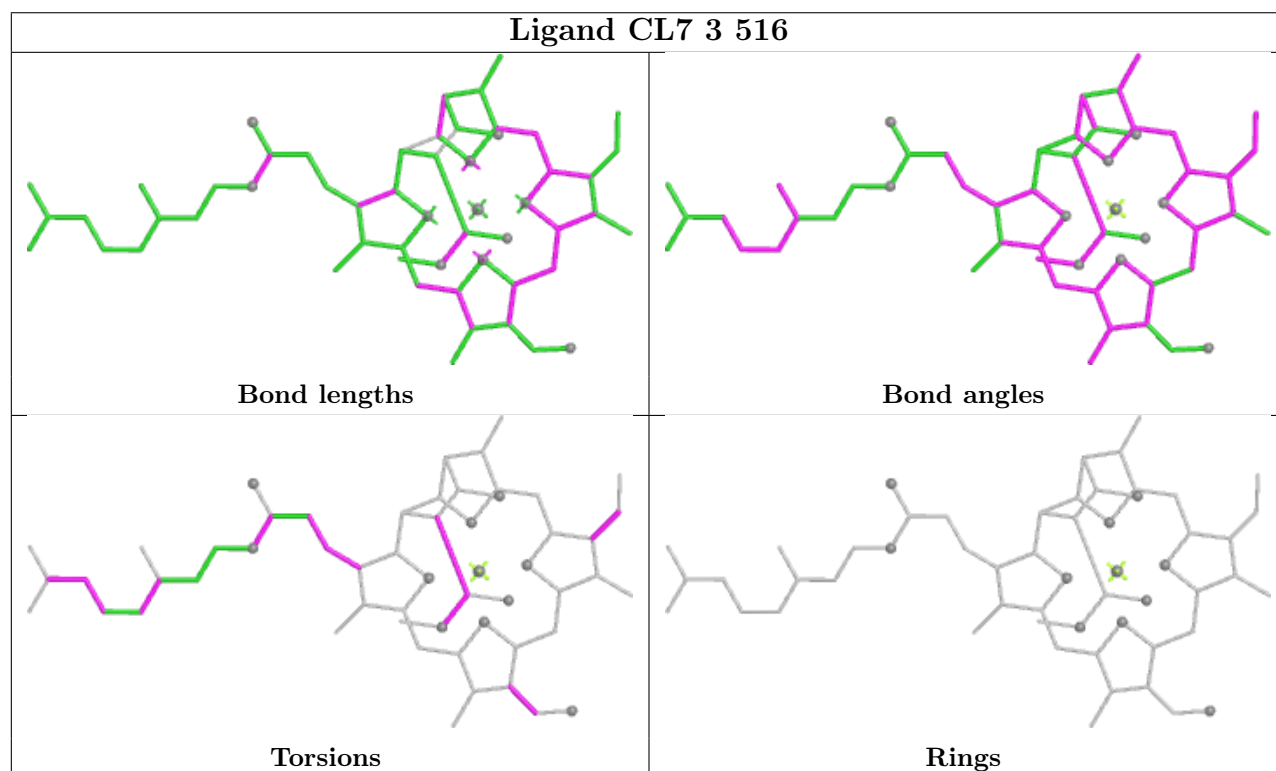
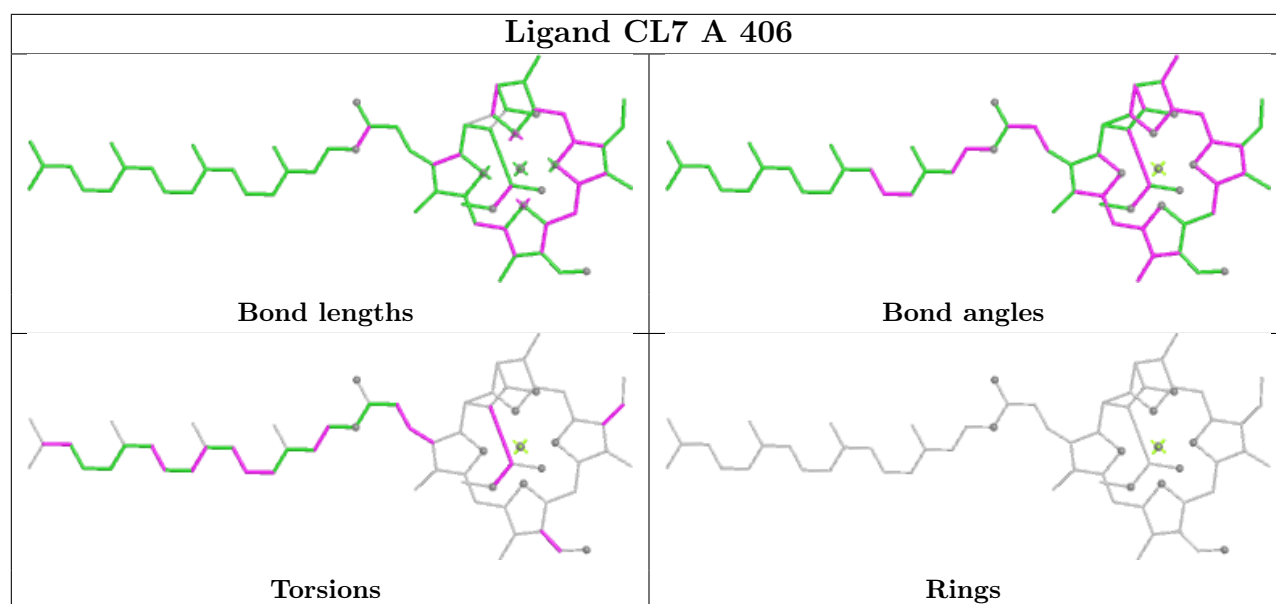


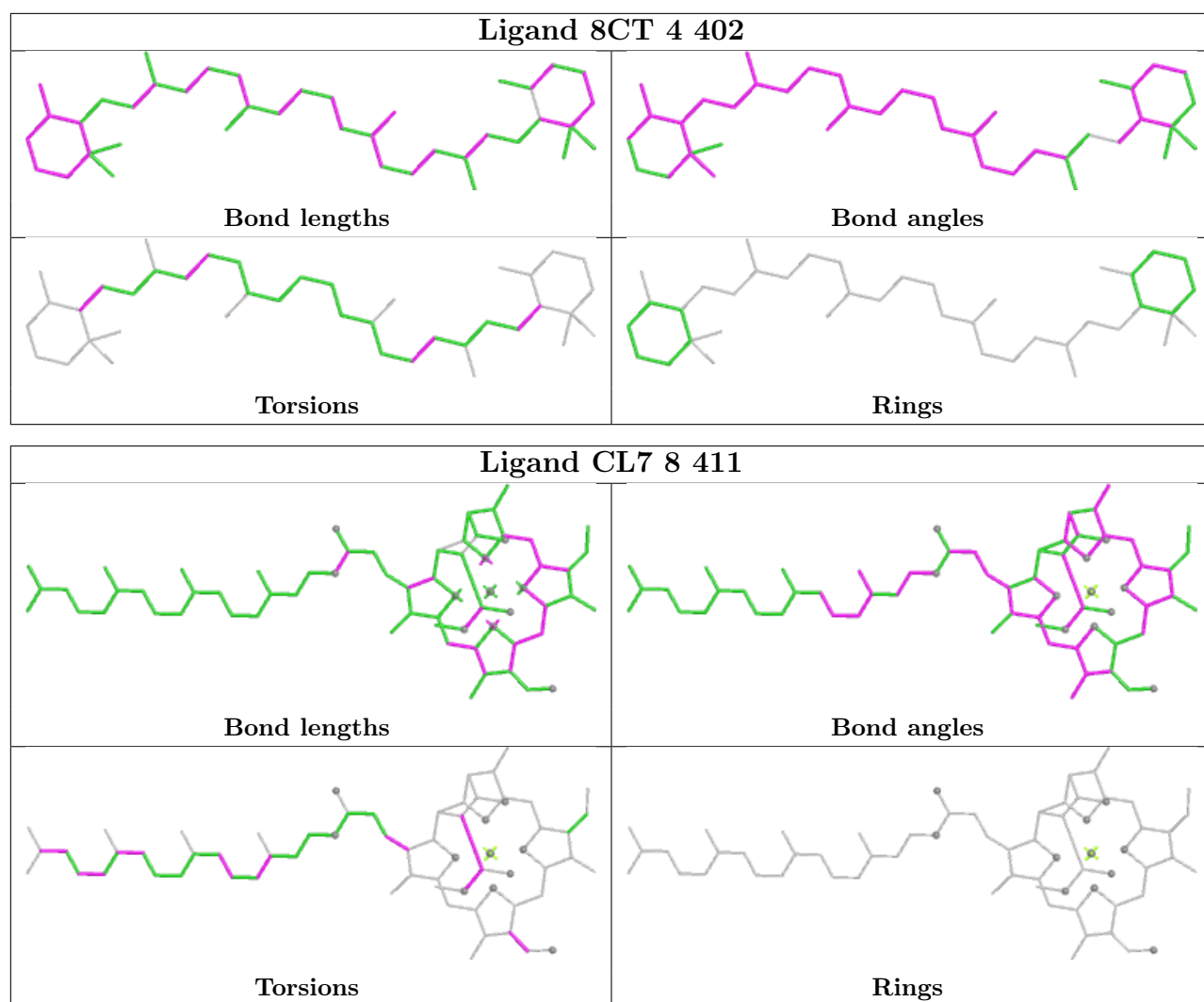
Rings



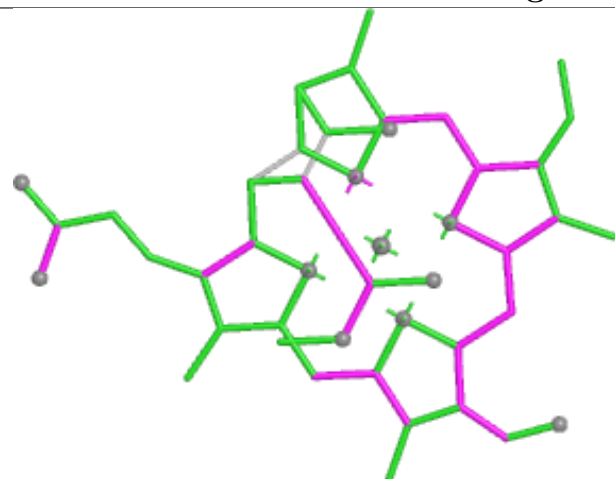








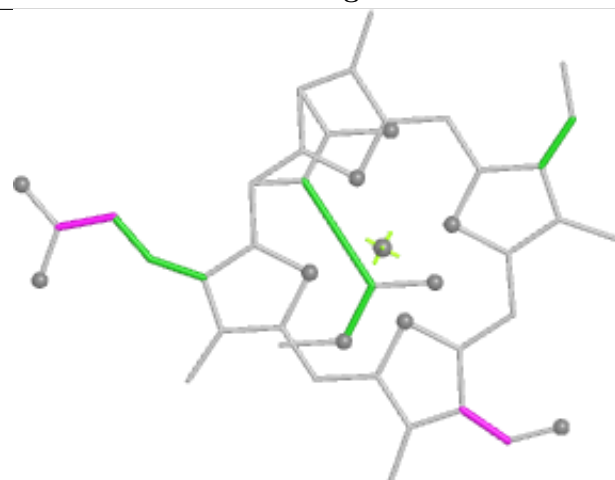
Ligand CL7 8 408



Bond lengths



Bond angles

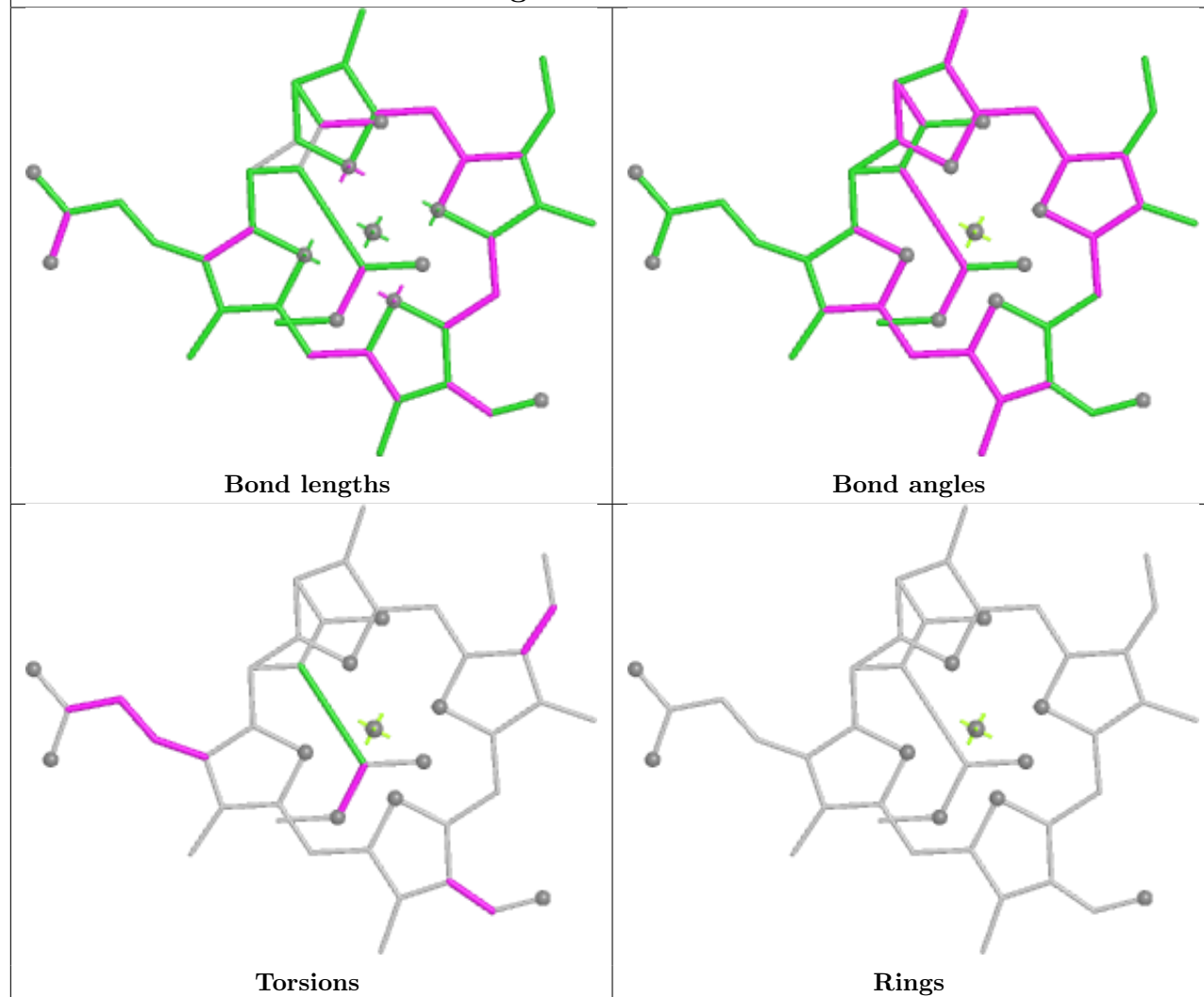


Torsions

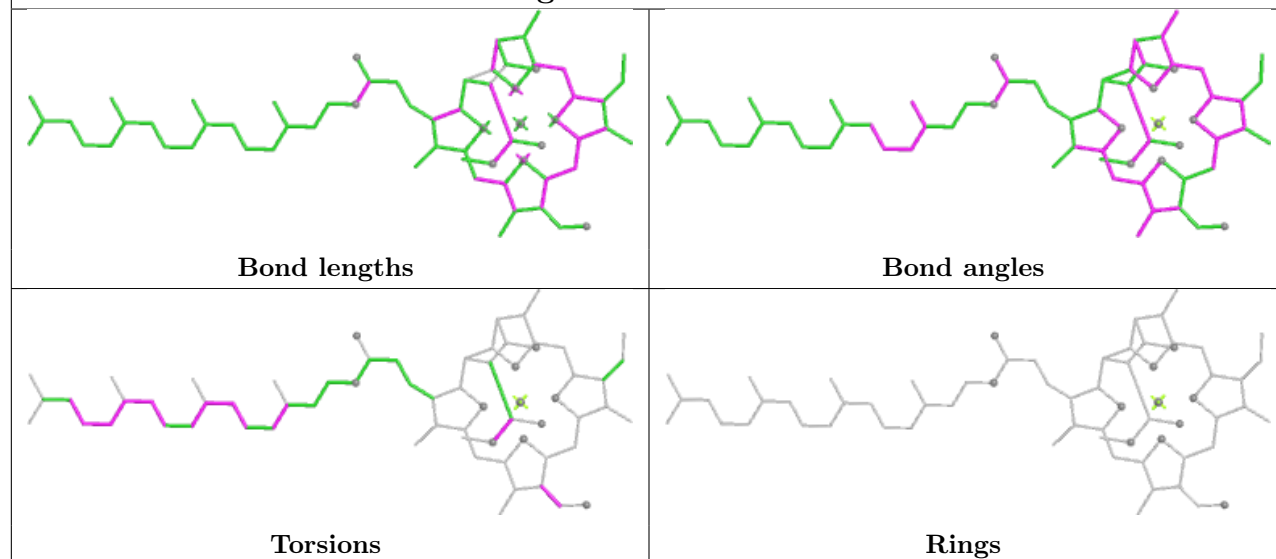


Rings

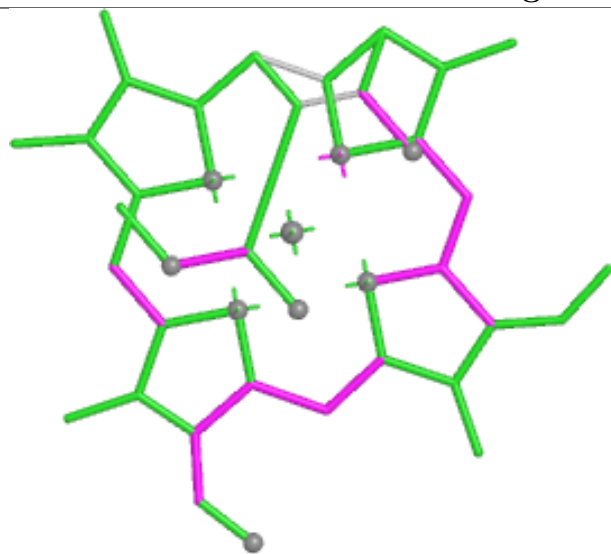
Ligand CL7 5 419



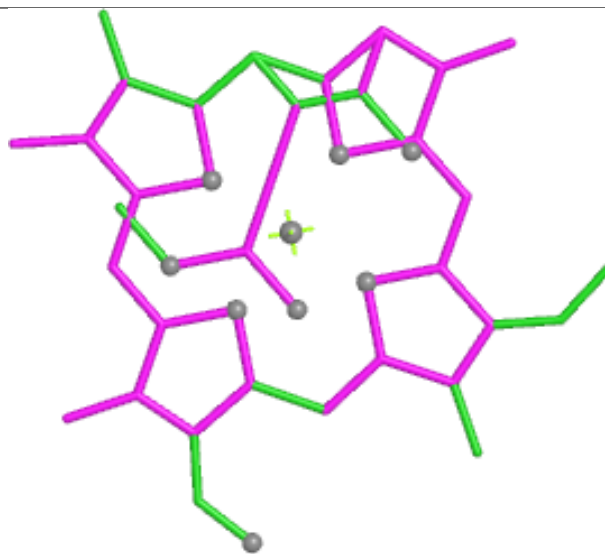
Ligand CL7 B 611



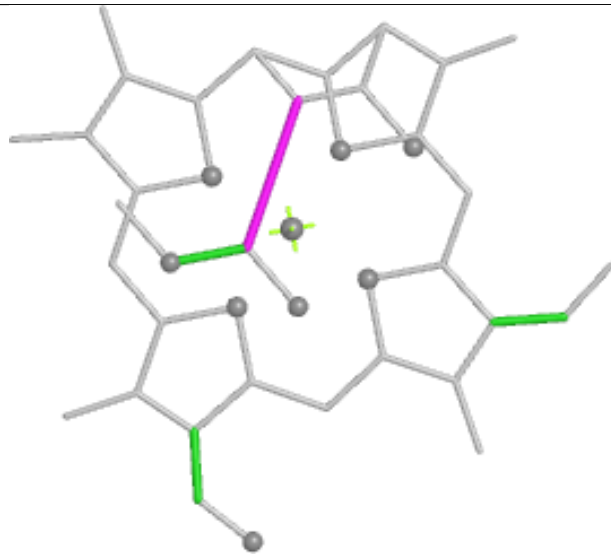
Ligand CL7 1 413



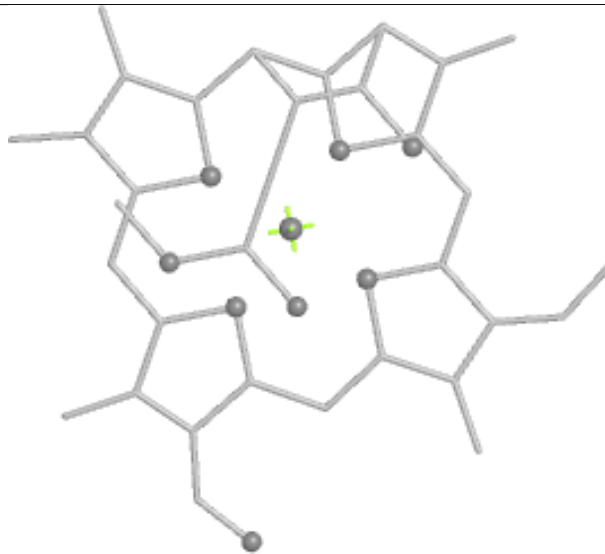
Bond lengths



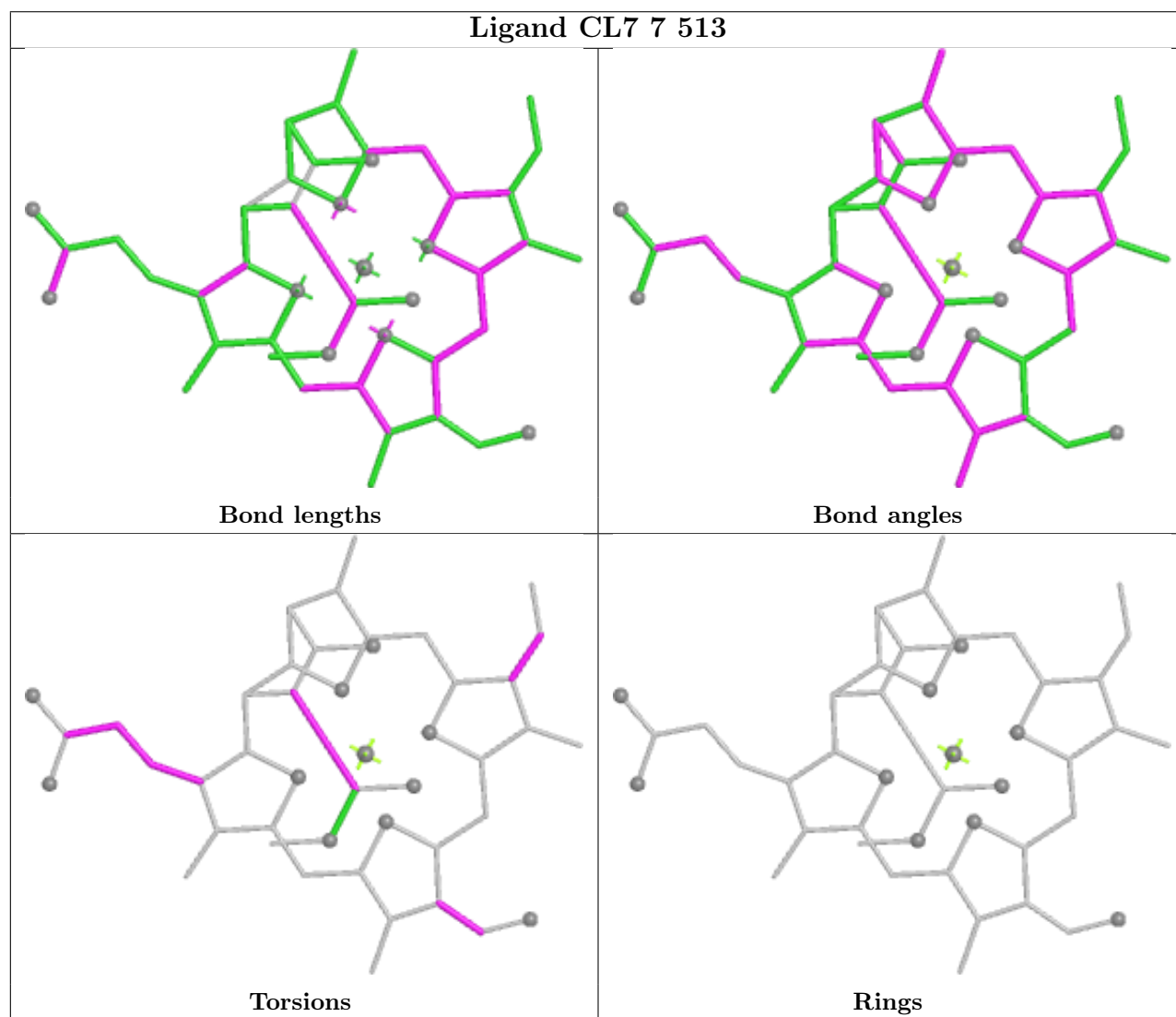
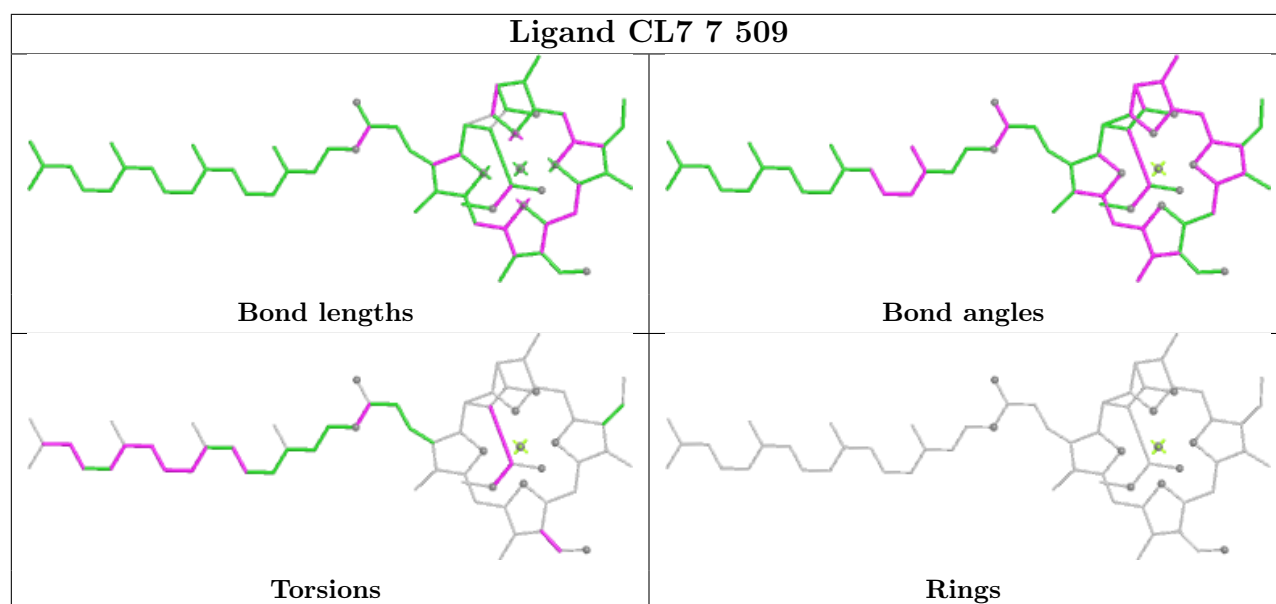
Bond angles



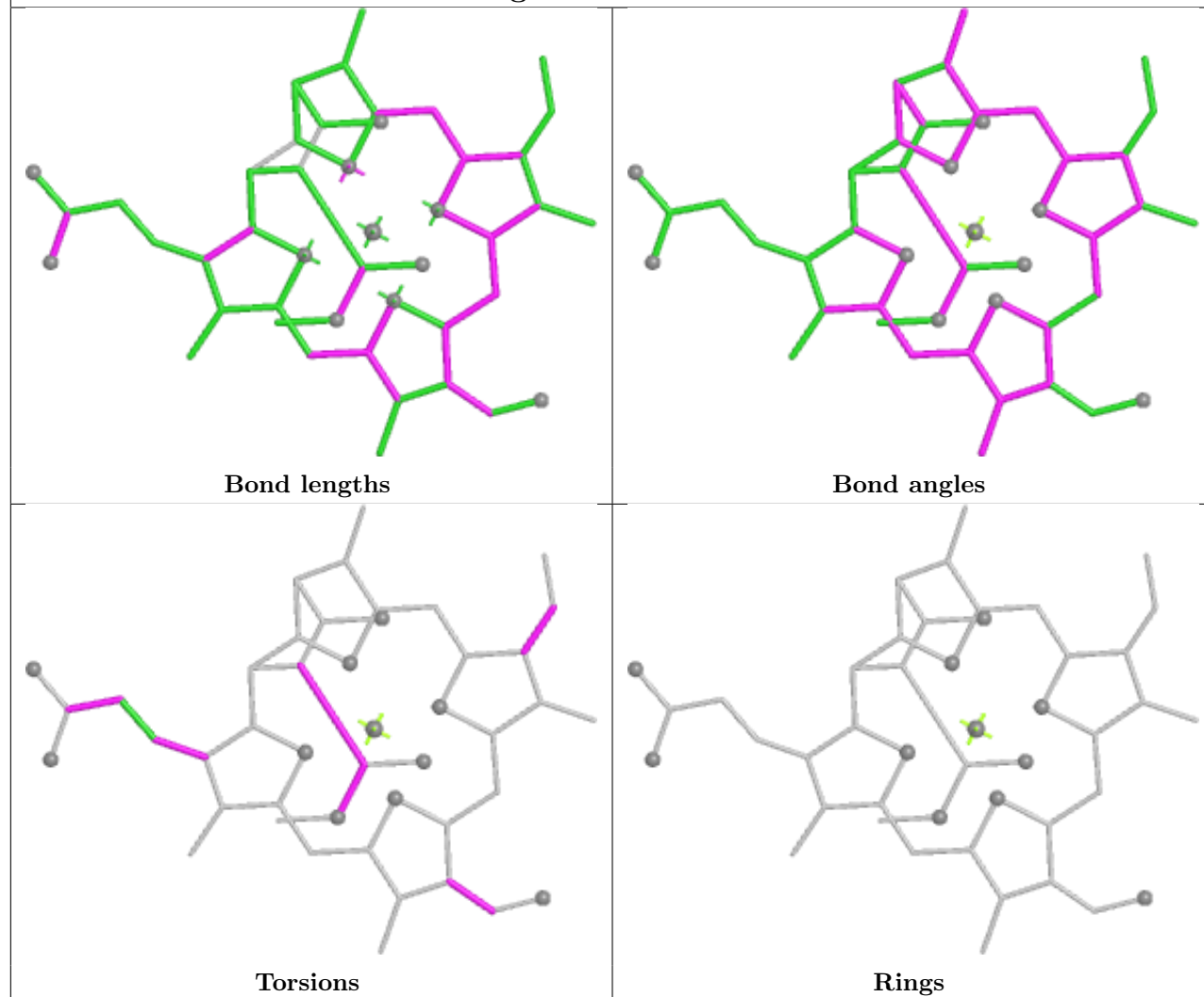
Torsions



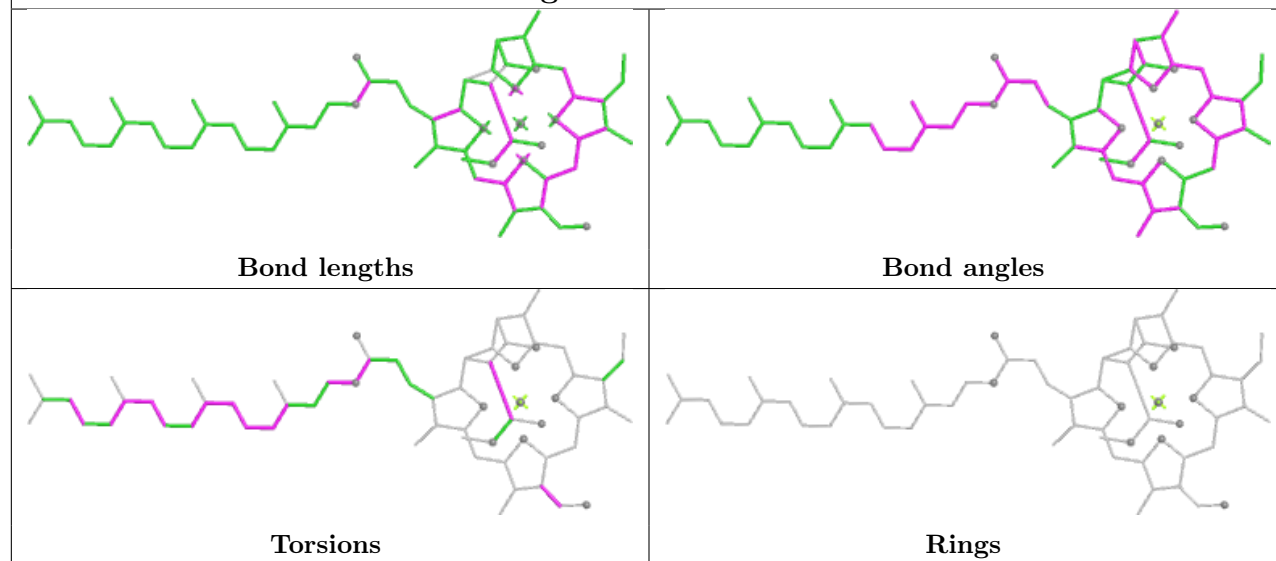
Rings

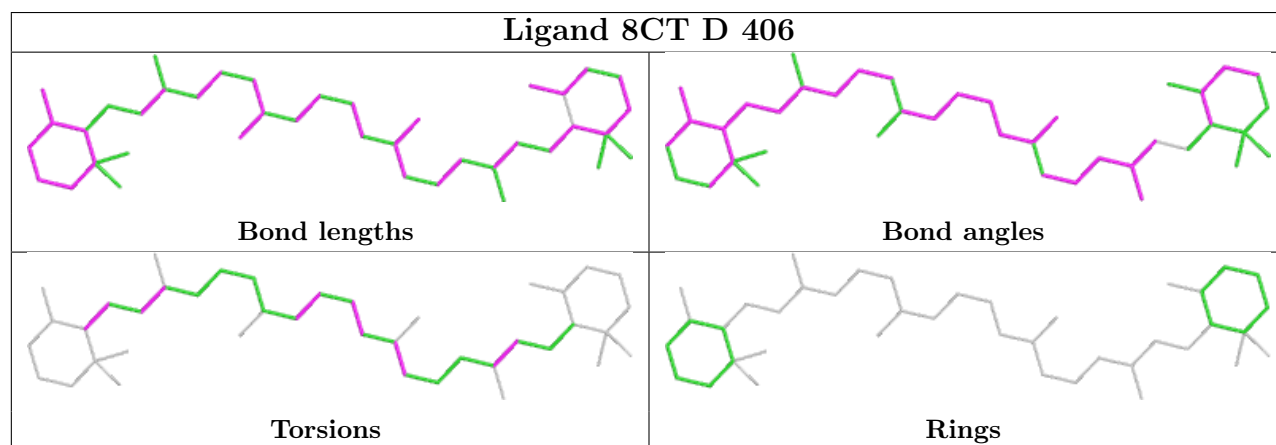
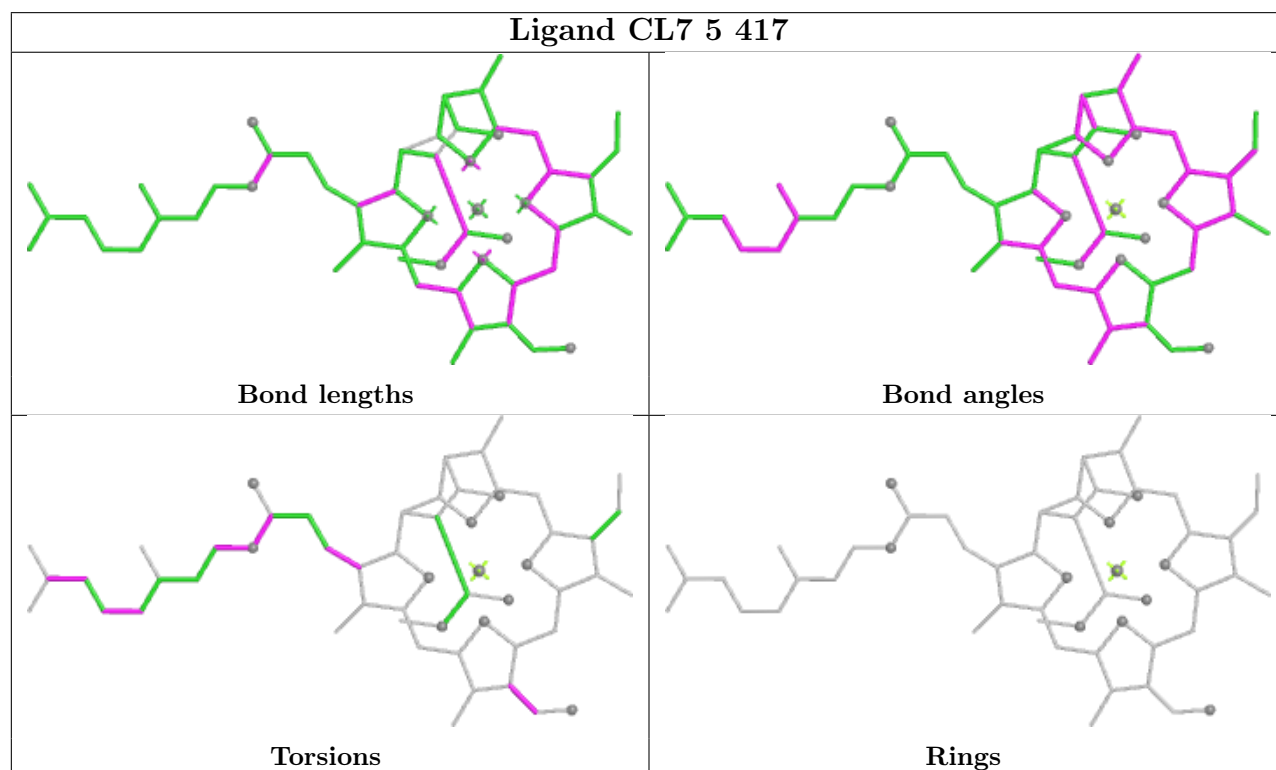
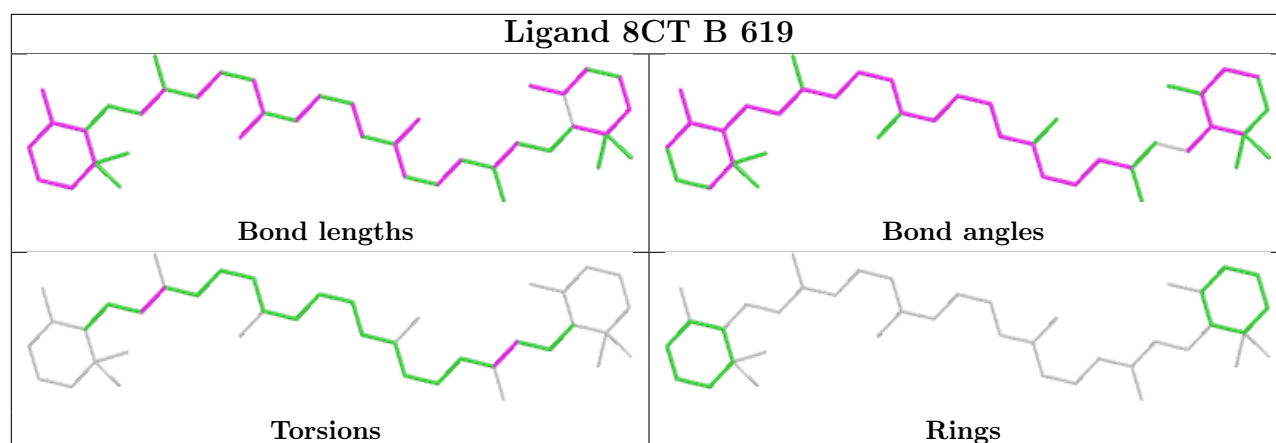


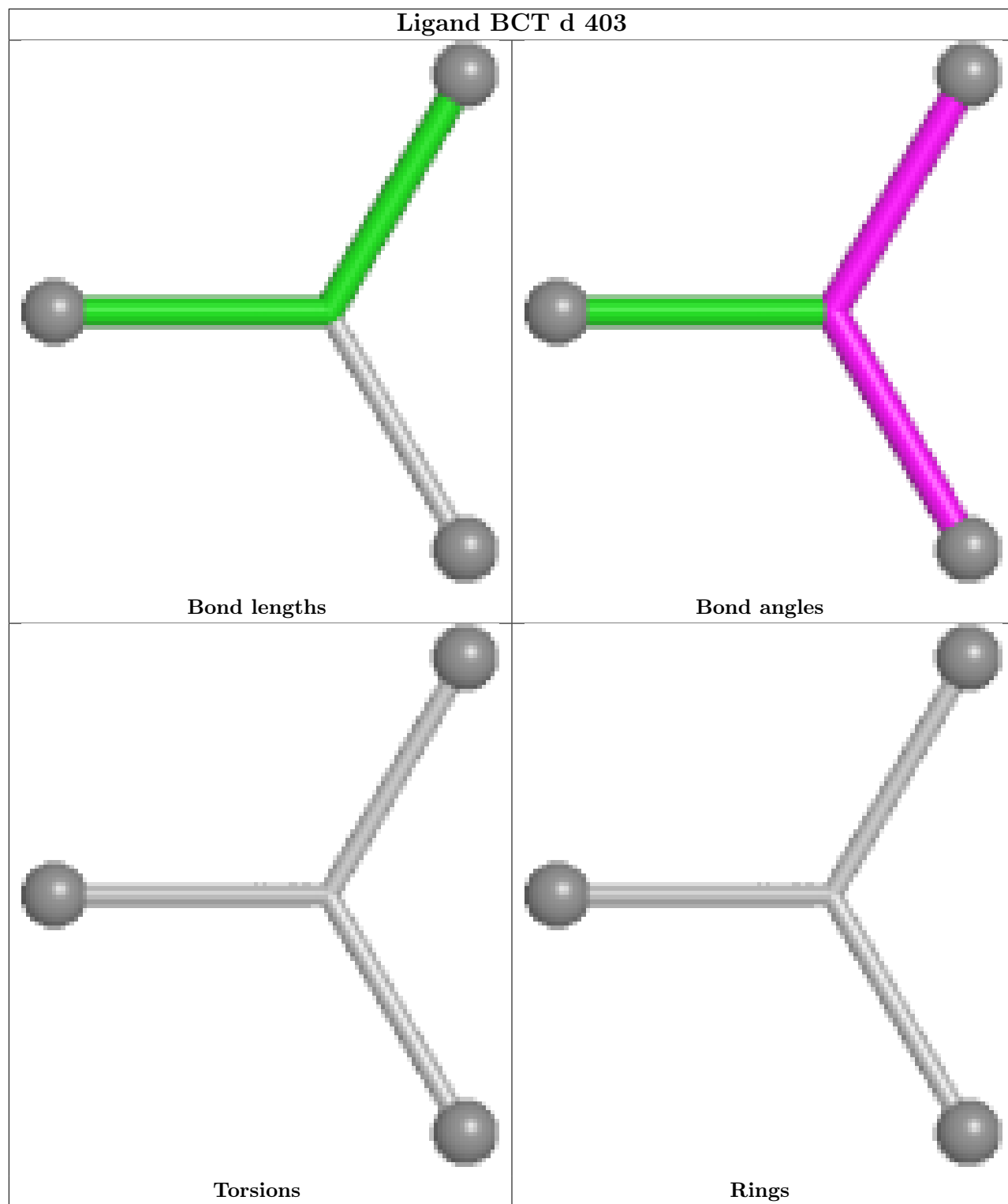
Ligand CL7 7 506

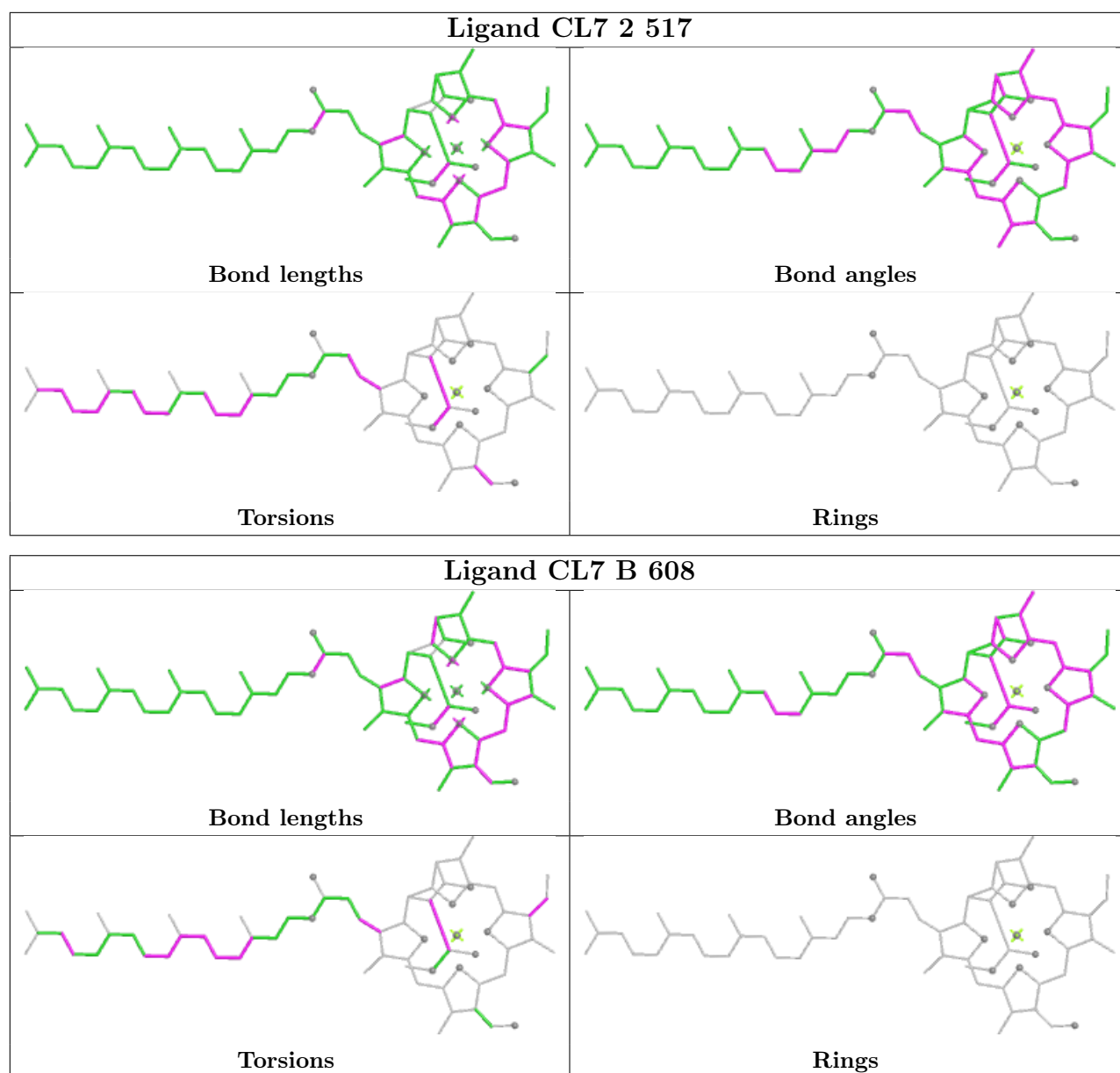


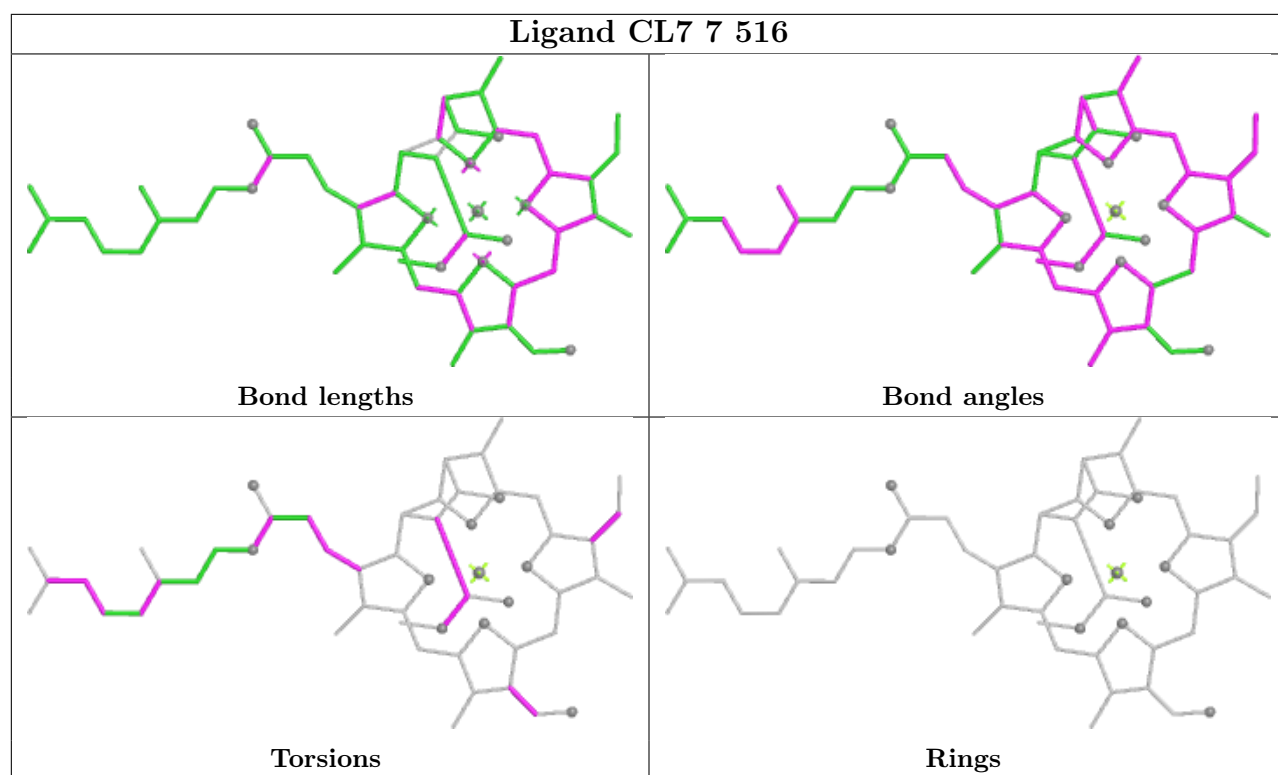
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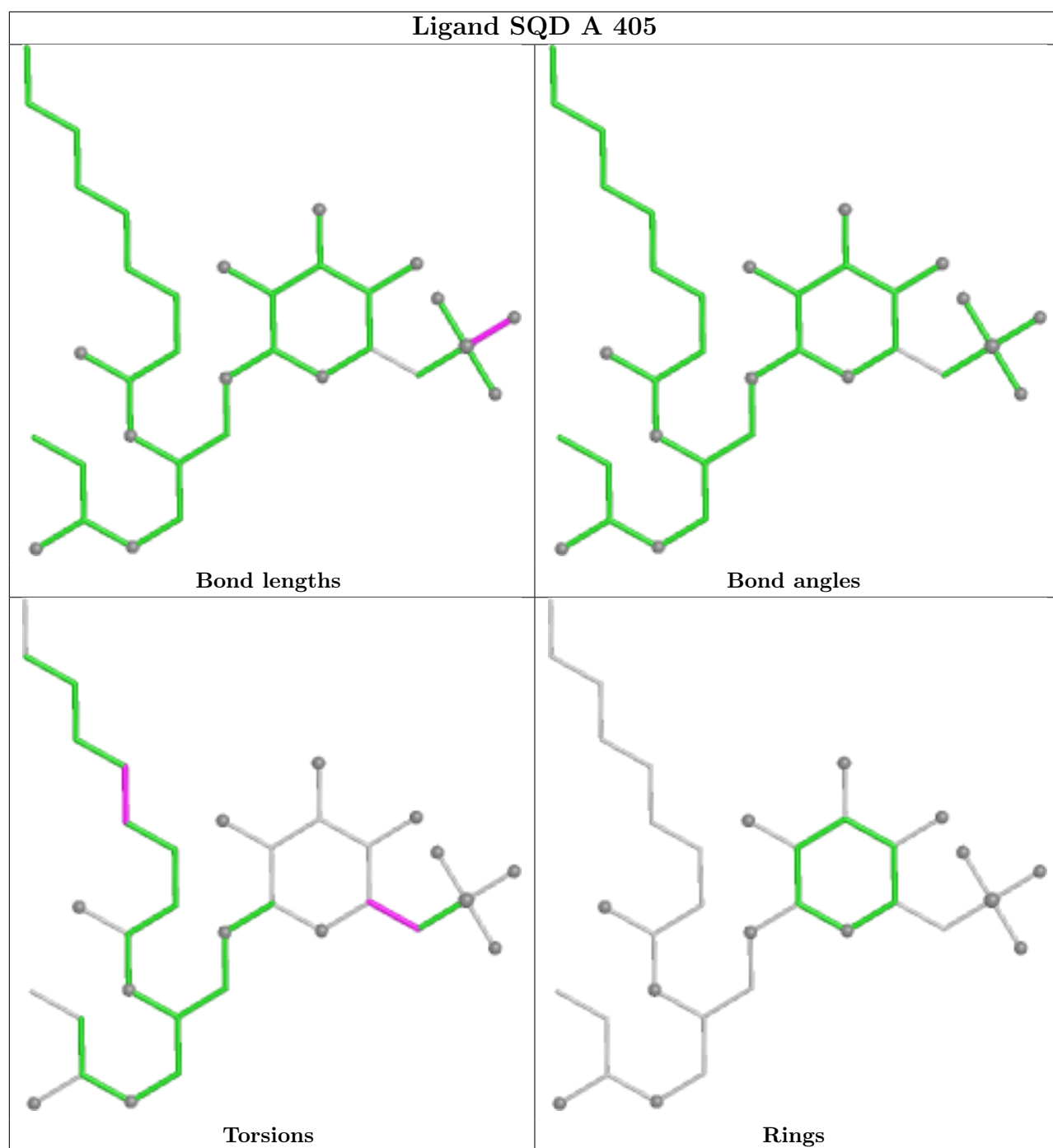


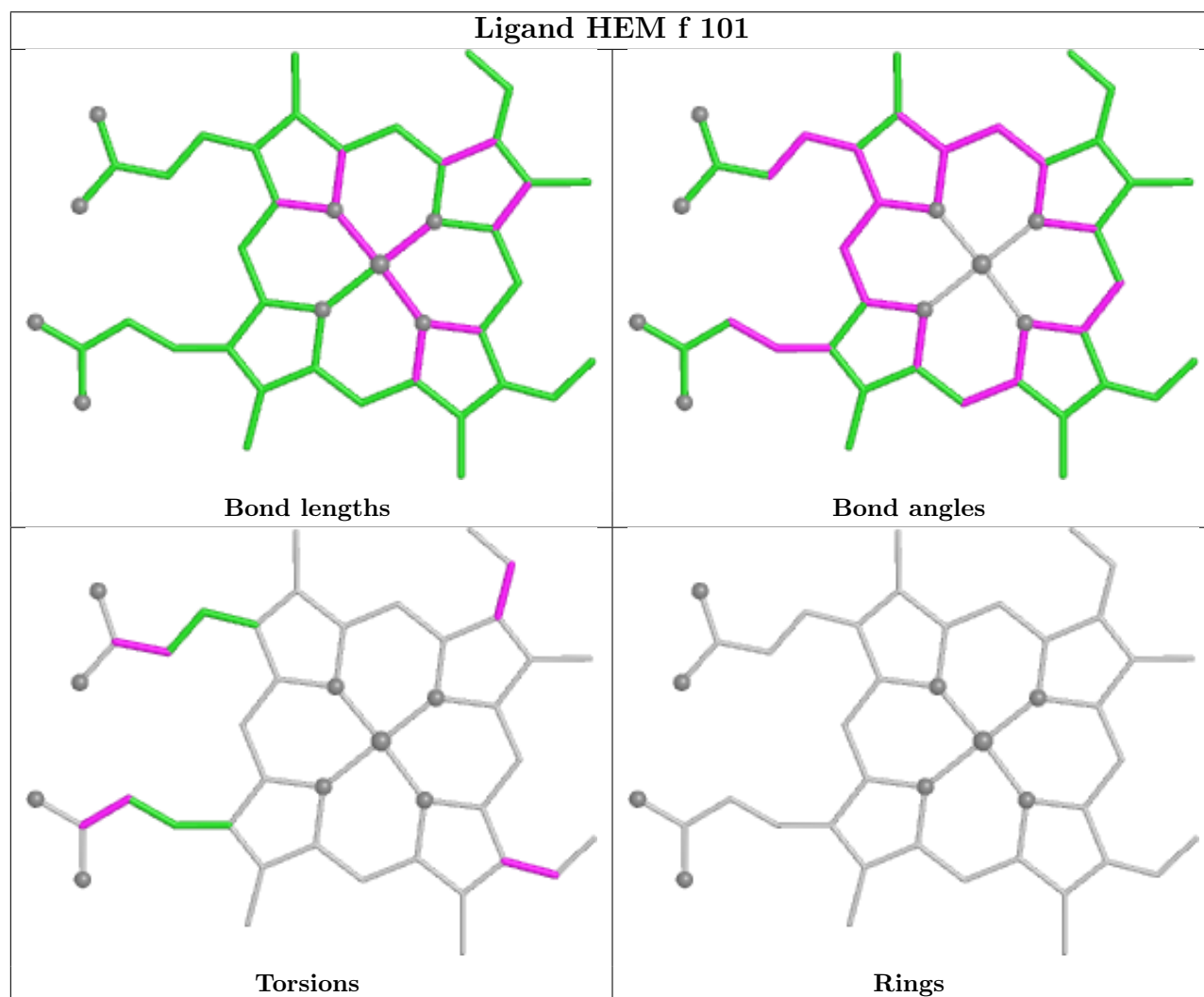
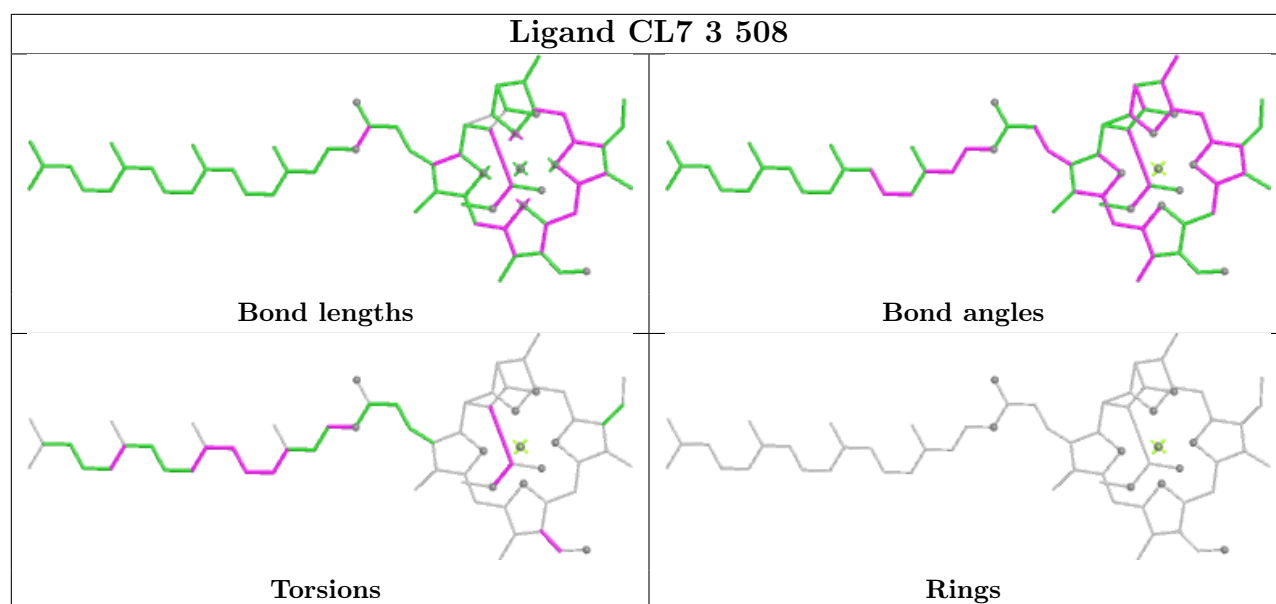


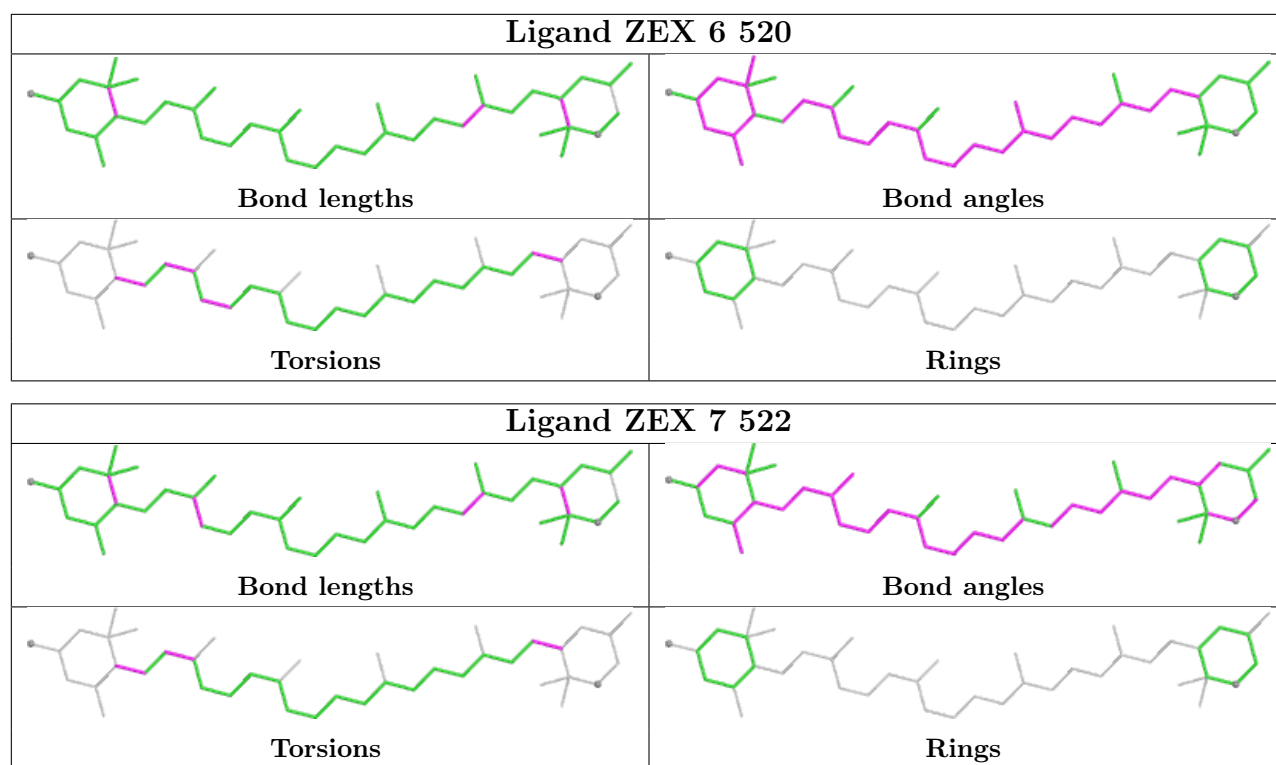




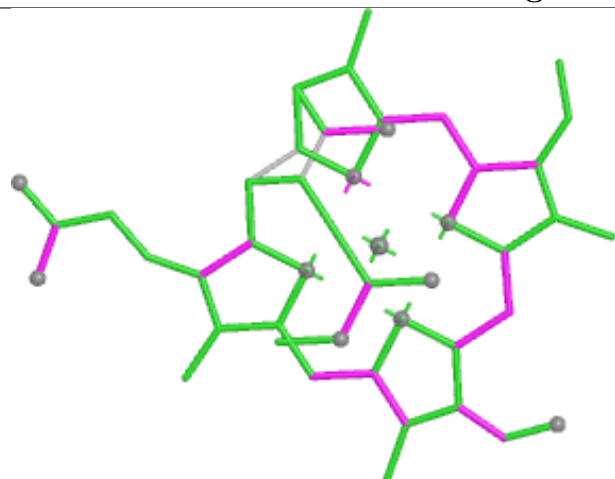




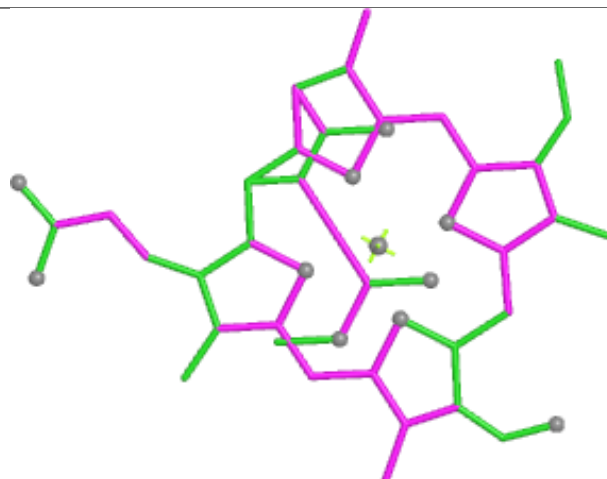




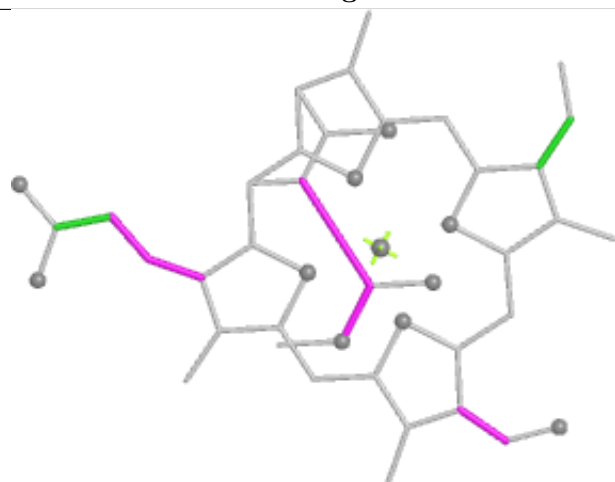
Ligand CL7 c 514



Bond lengths



Bond angles

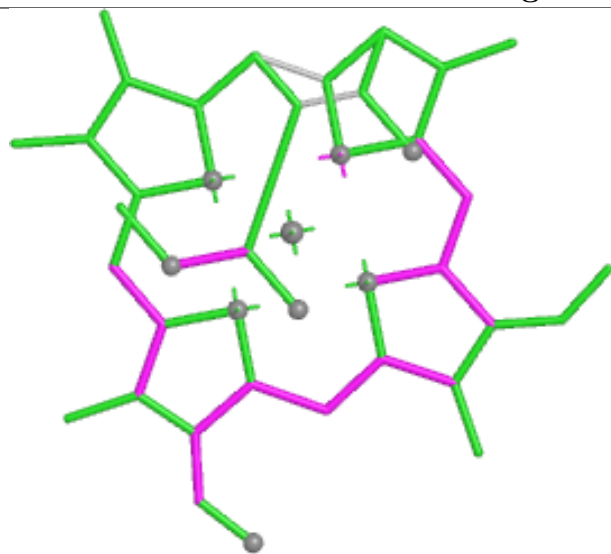


Torsions

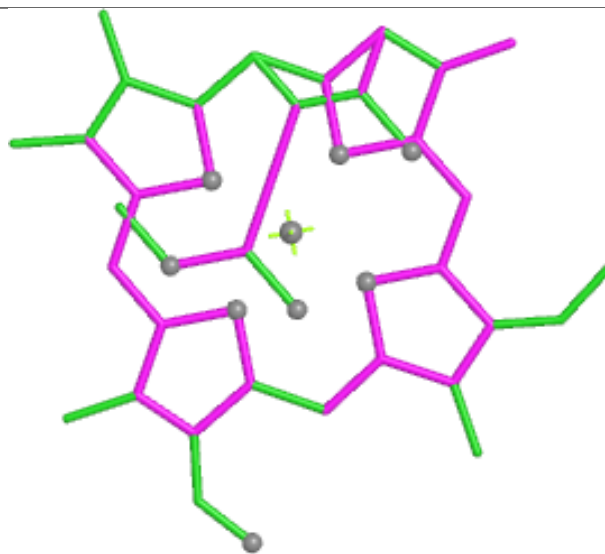


Rings

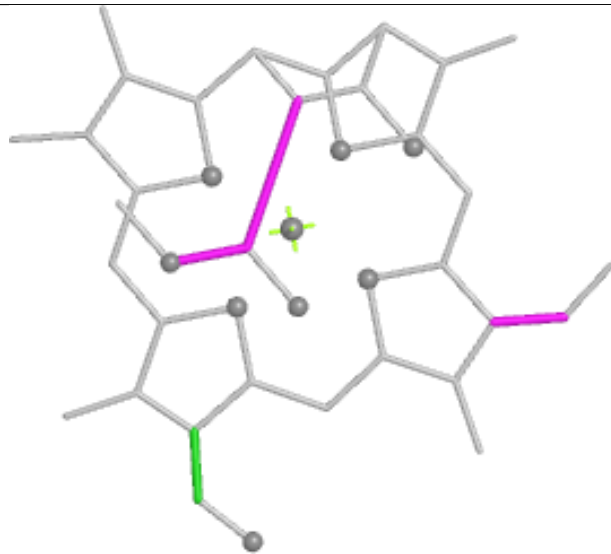
Ligand CL7 b 602



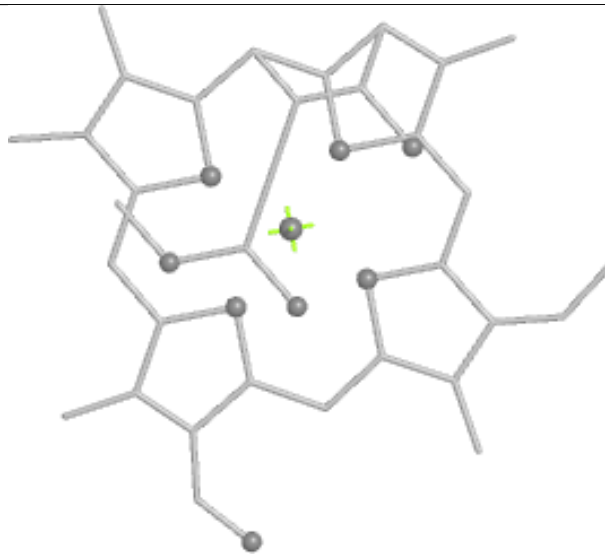
Bond lengths



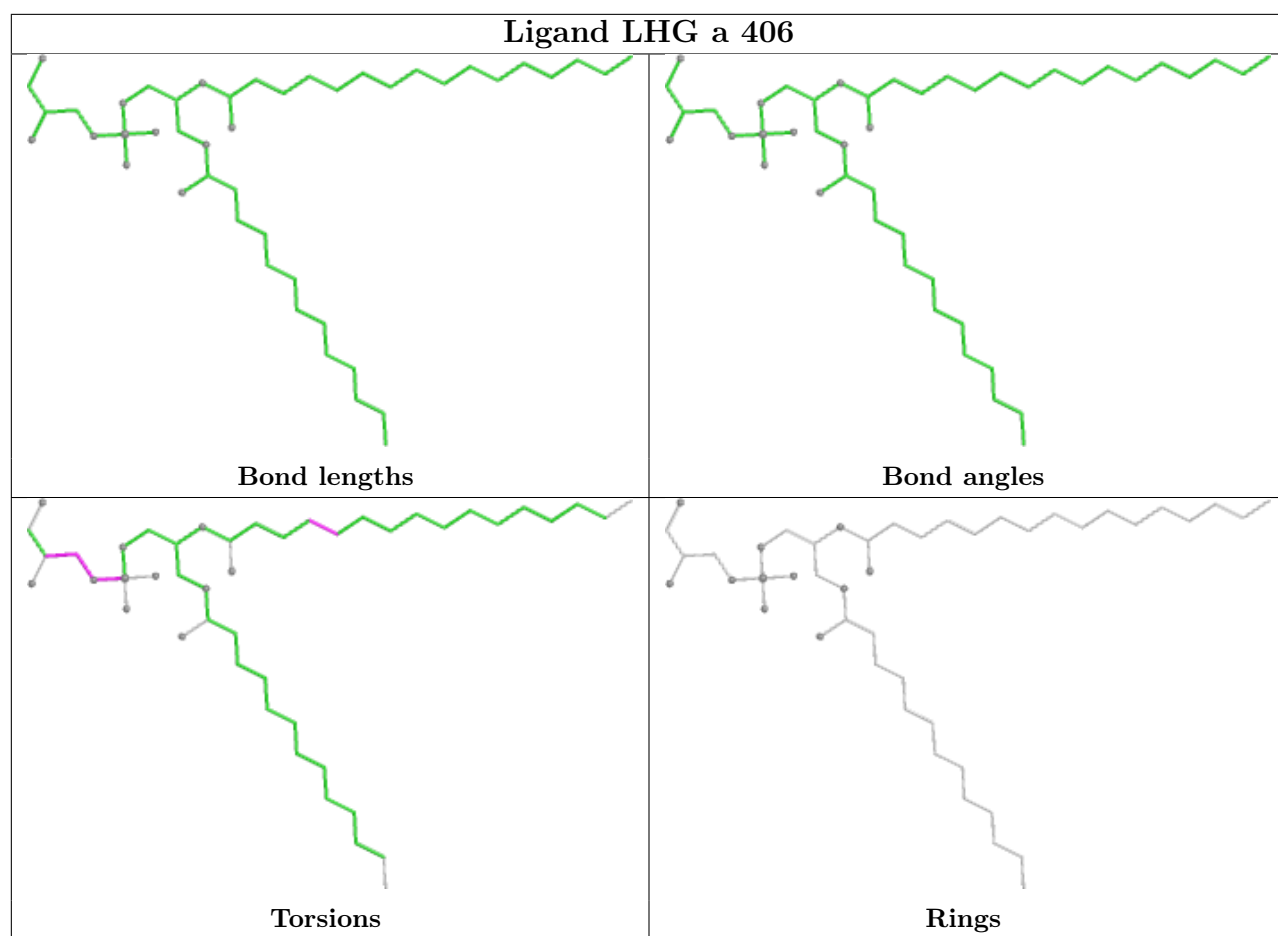
Bond angles



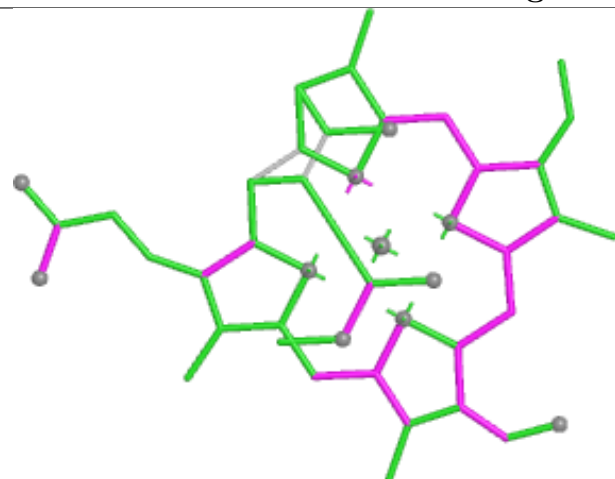
Torsions



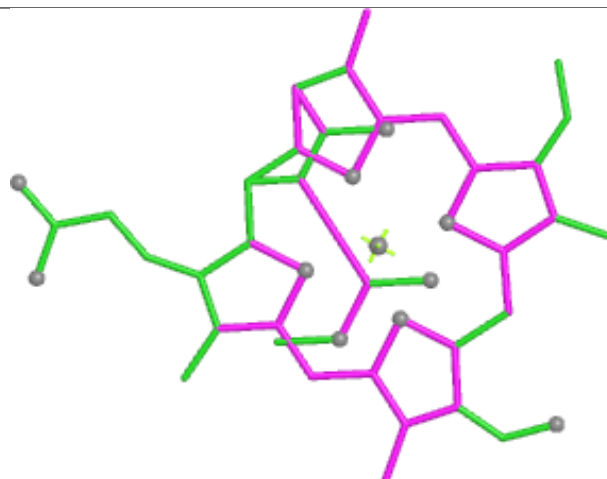
Rings



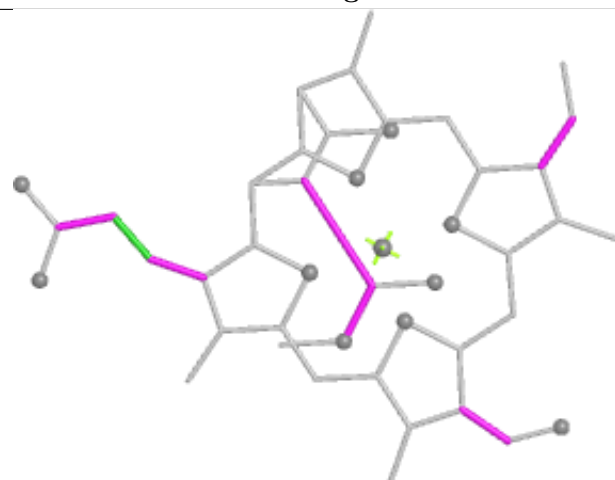
Ligand CL7 3 506



Bond lengths



Bond angles

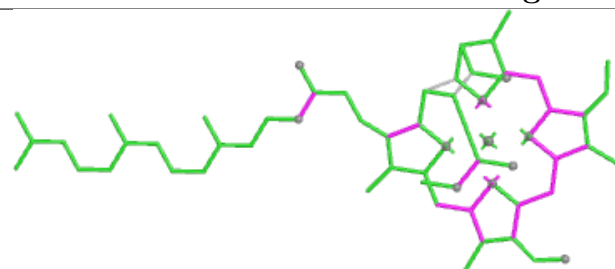


Torsions

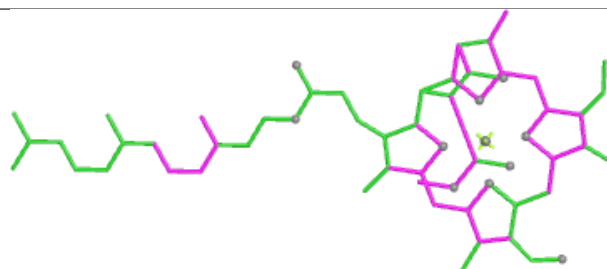


Rings

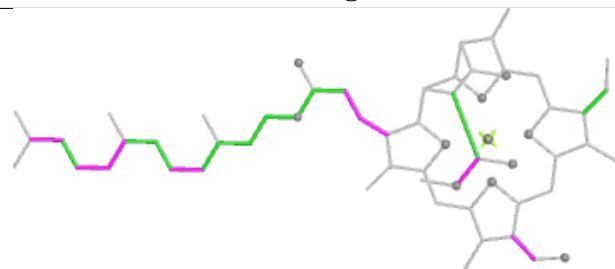
Ligand CL7 B 607



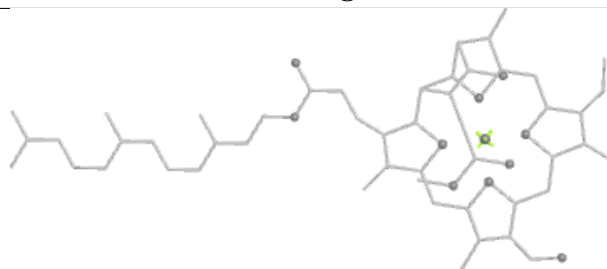
Bond lengths



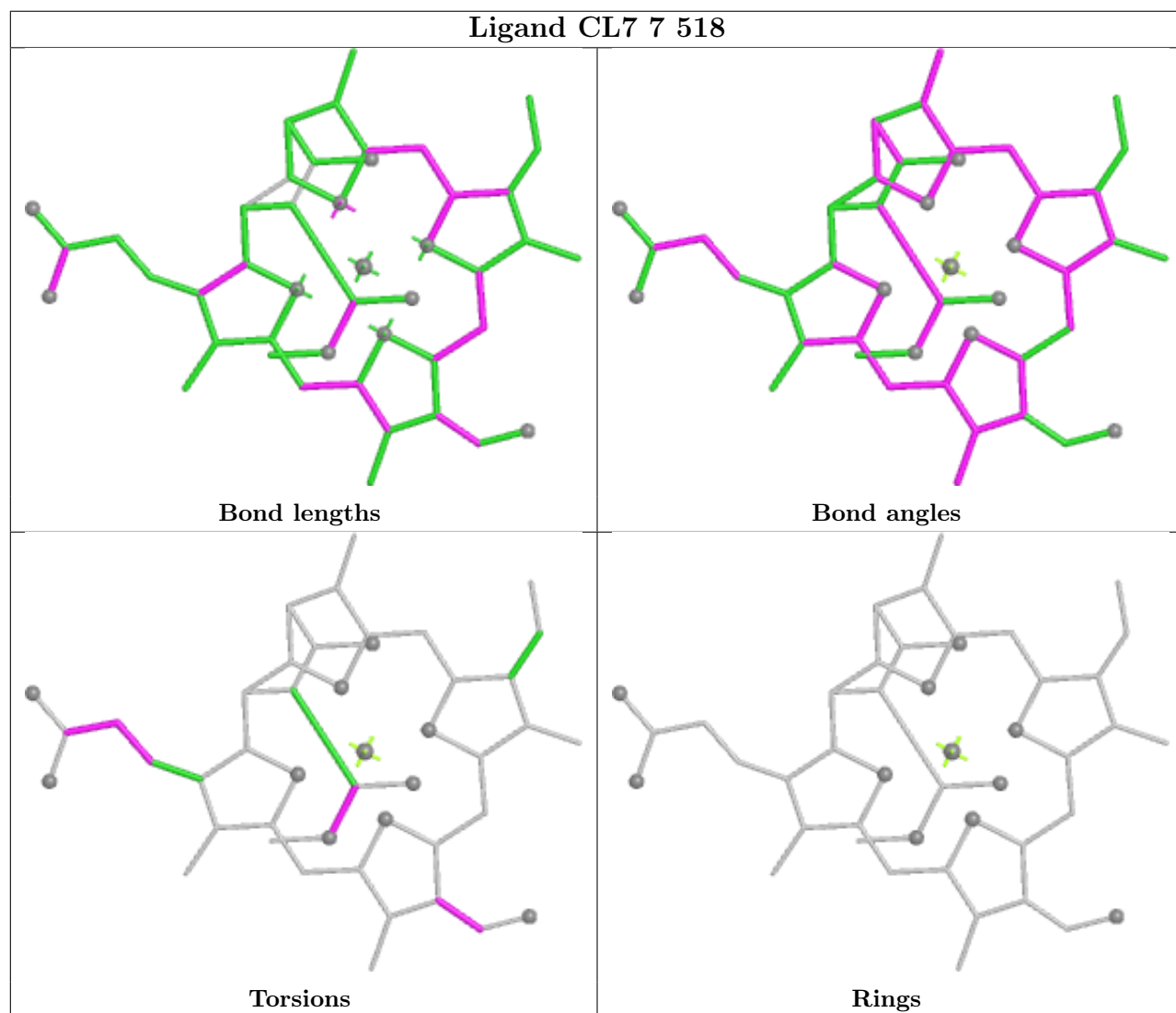
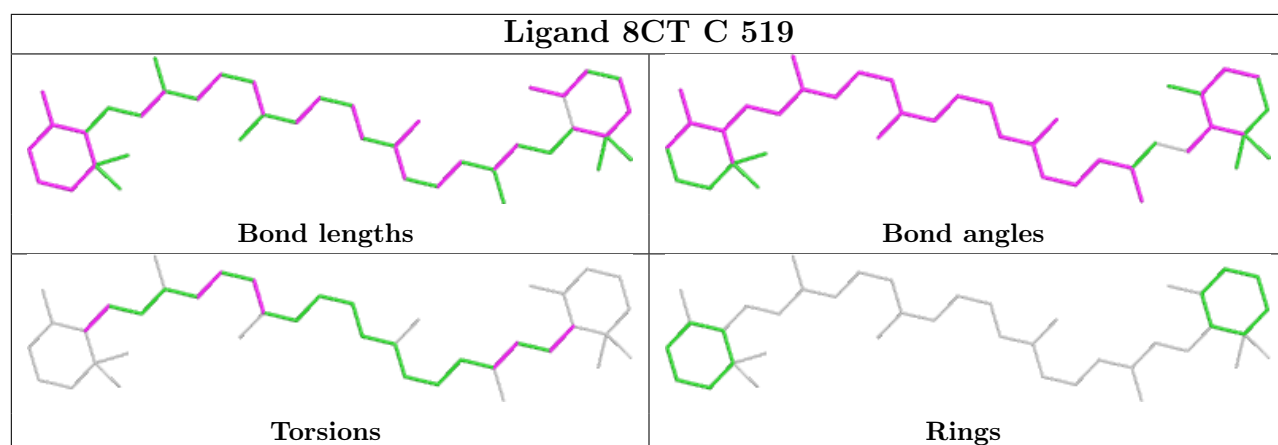
Bond angles

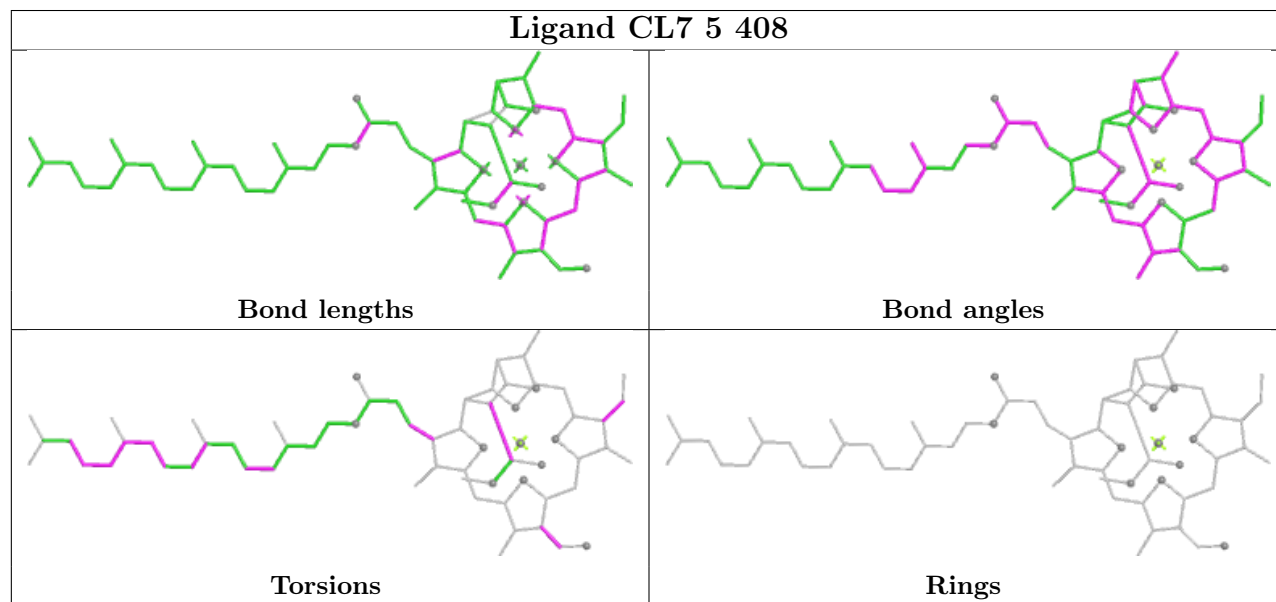
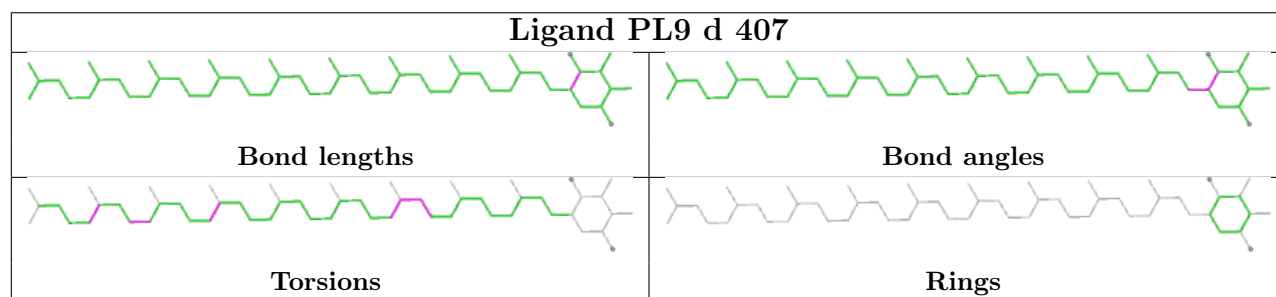
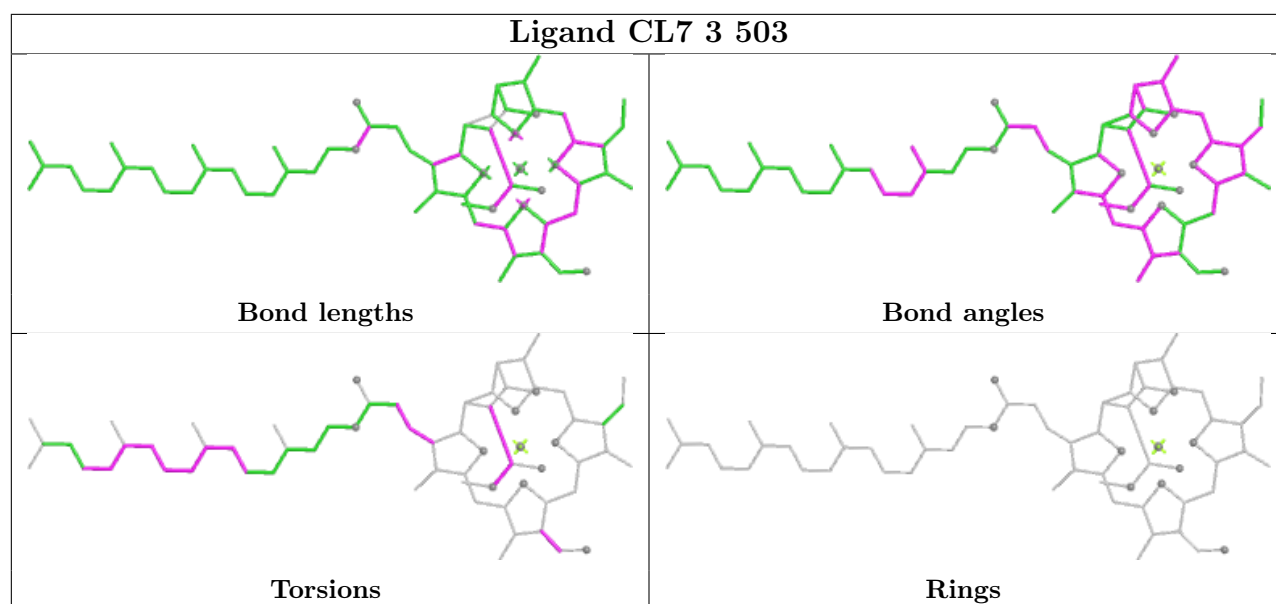


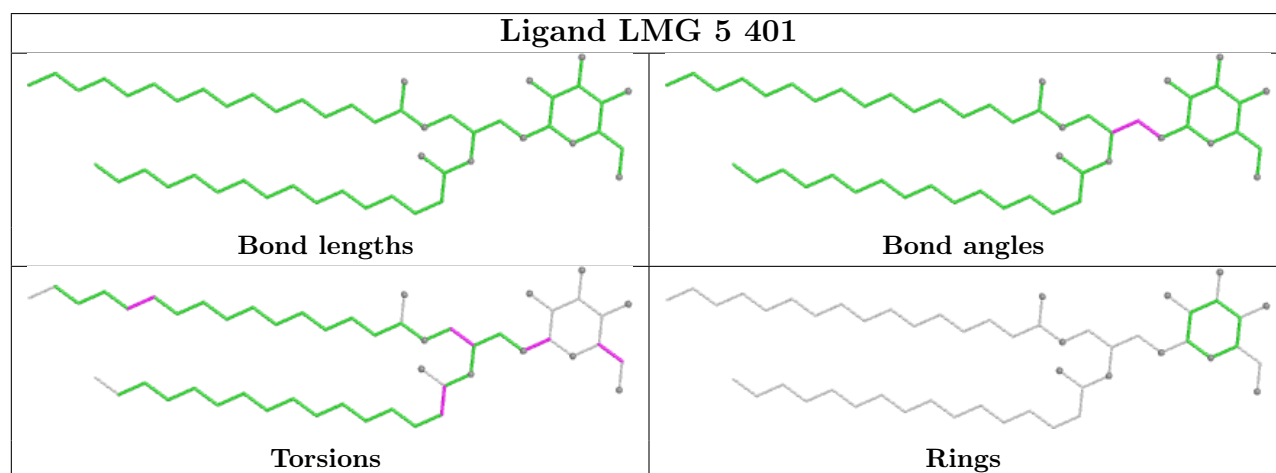
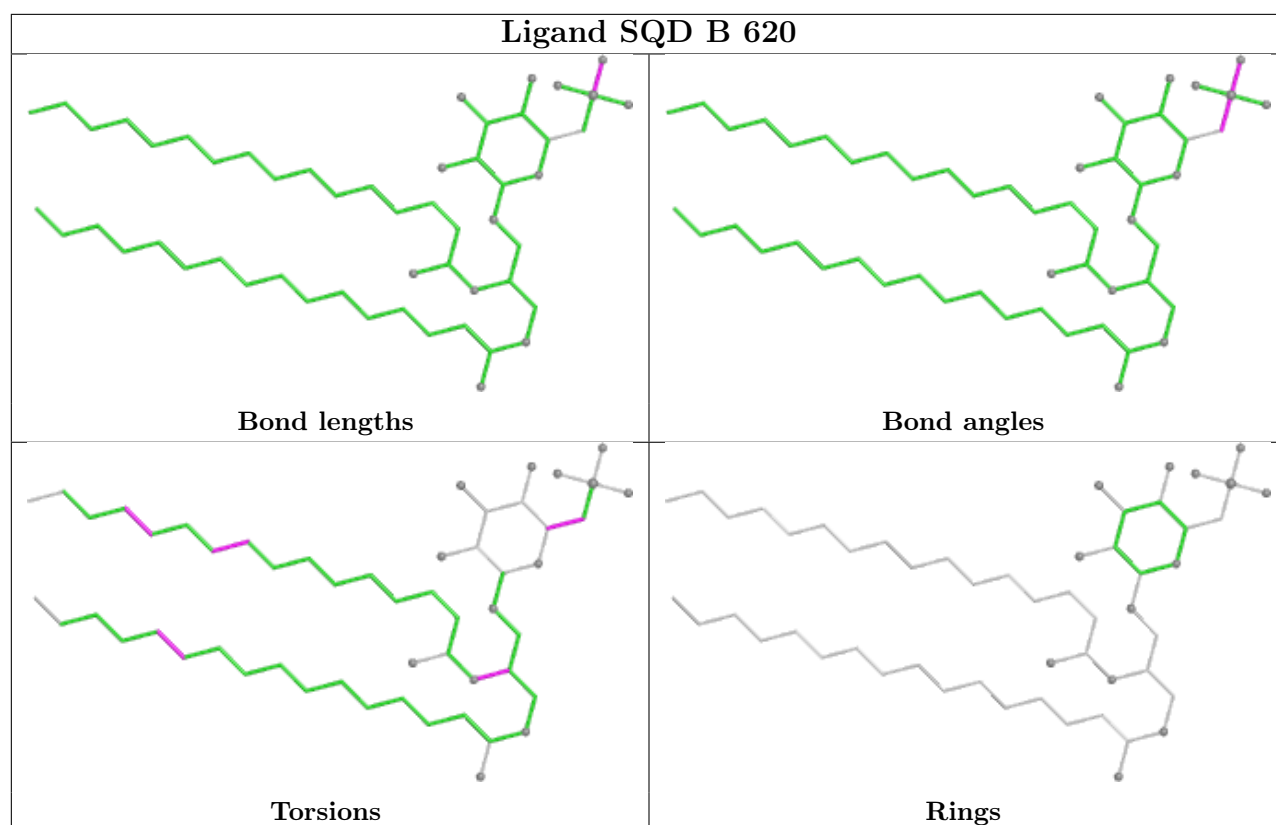
Torsions

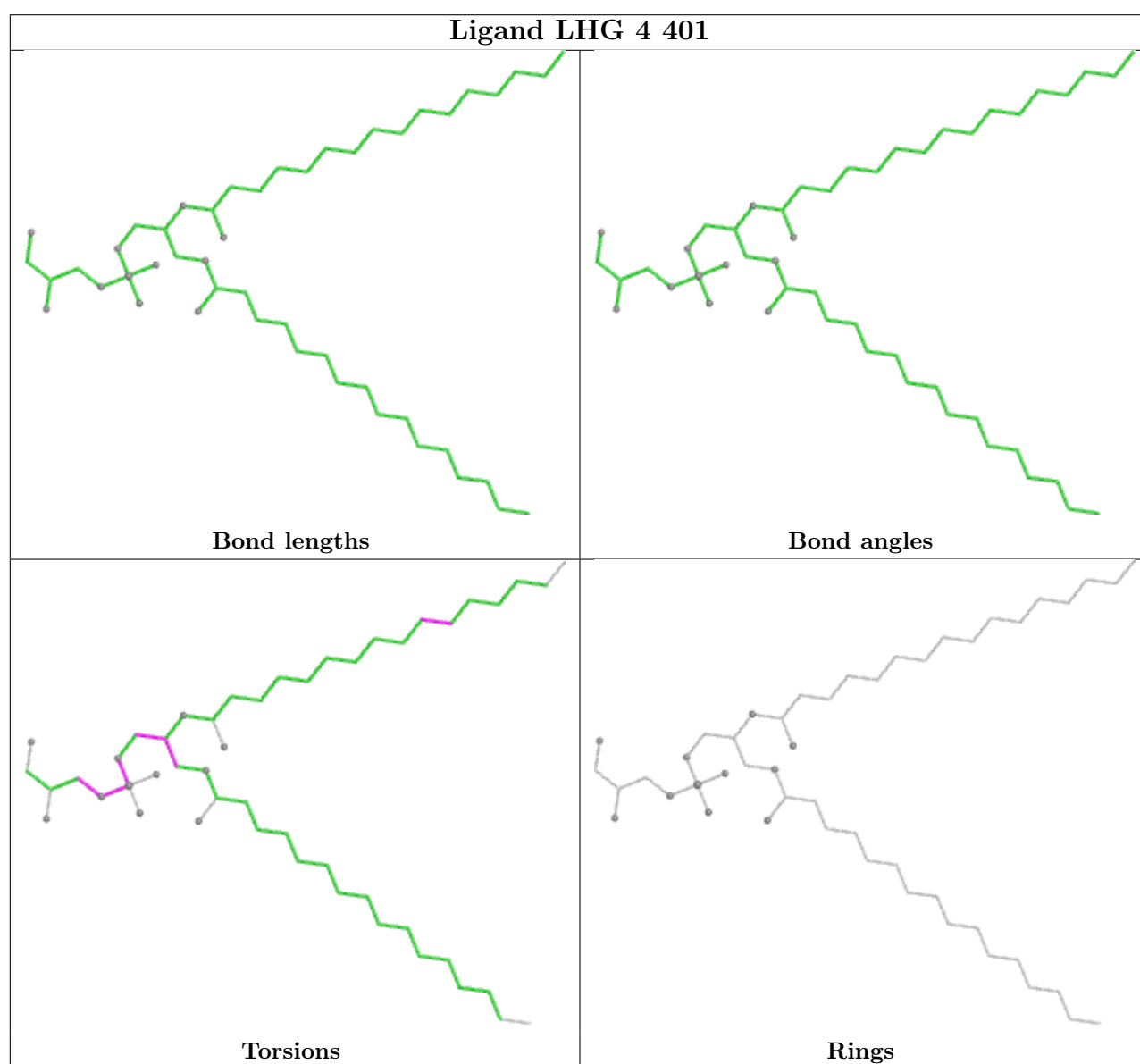
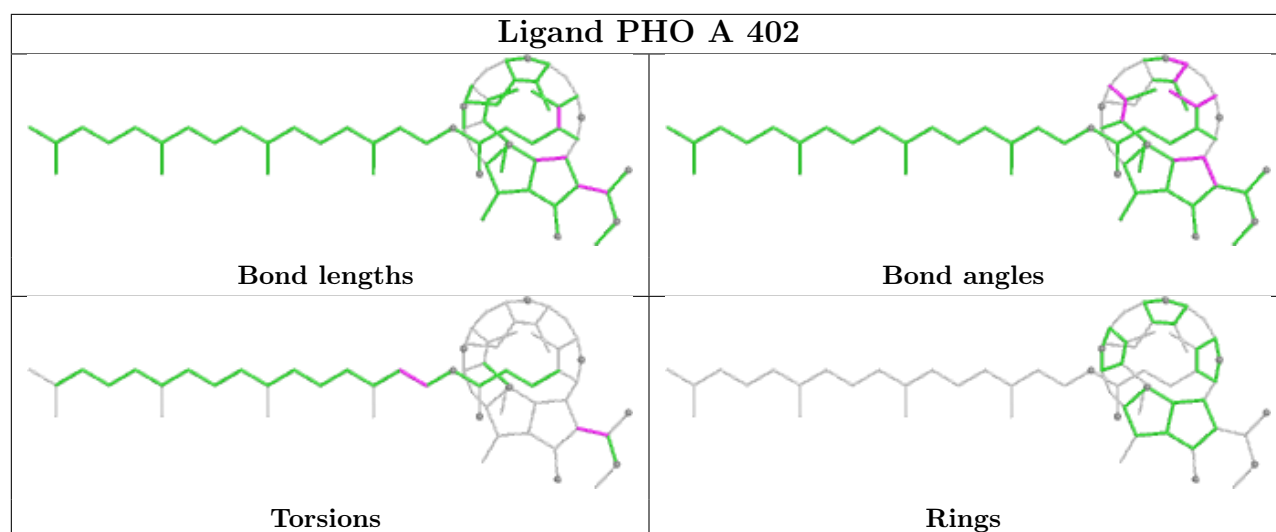


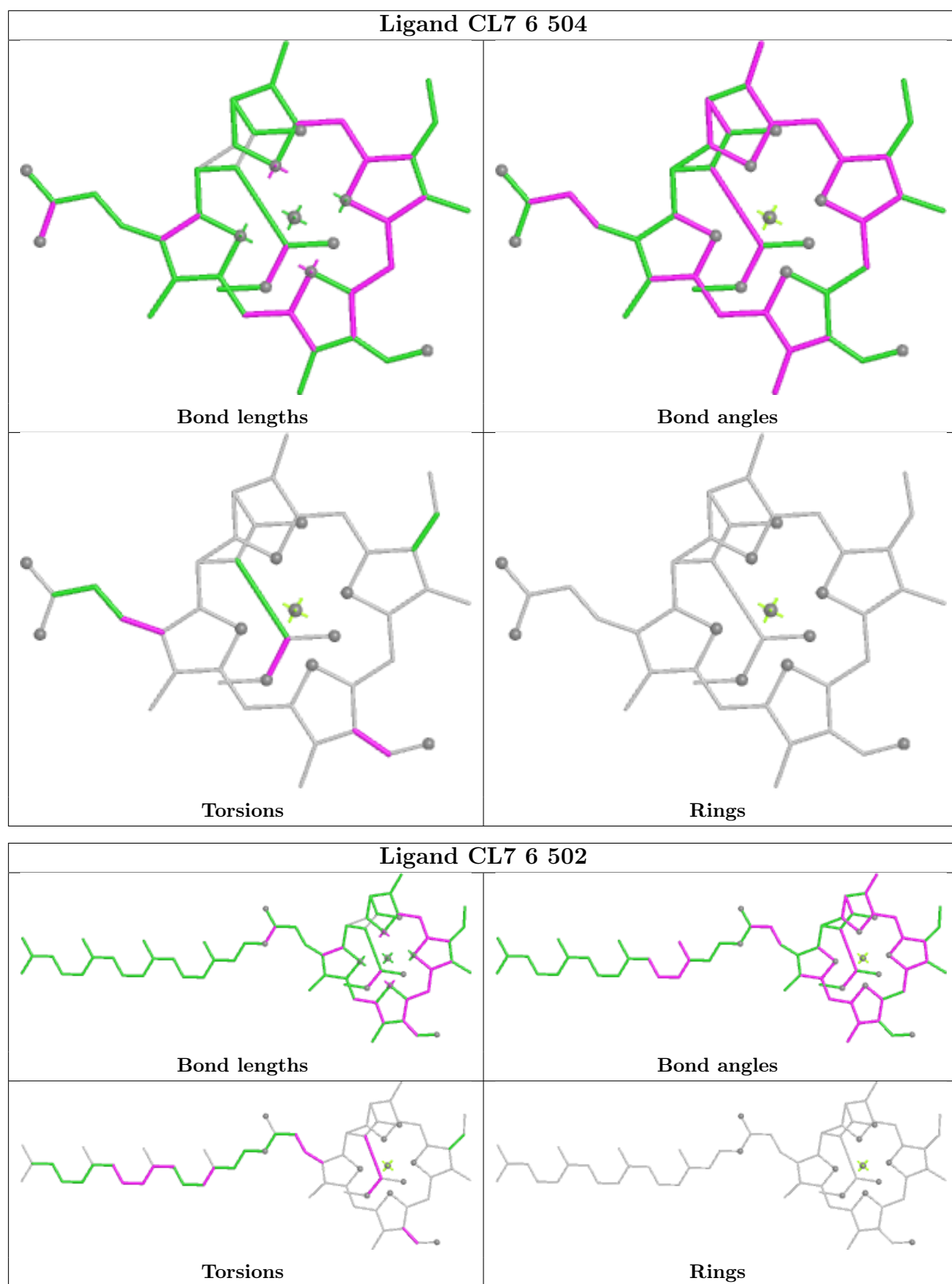
Rings

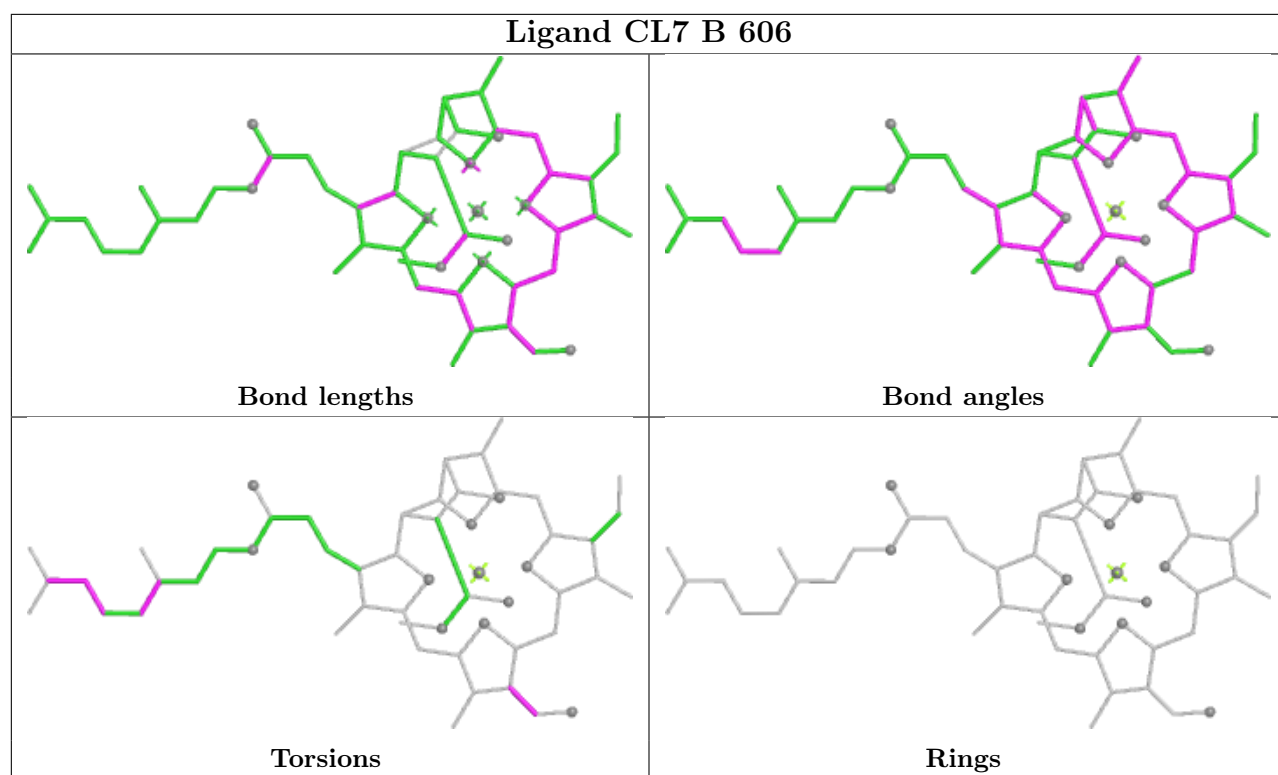




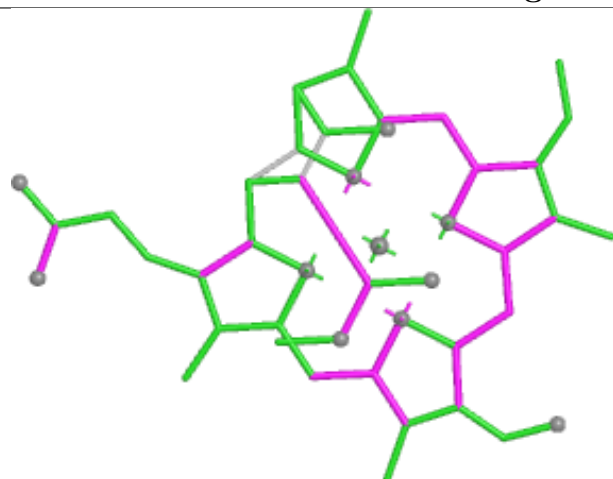




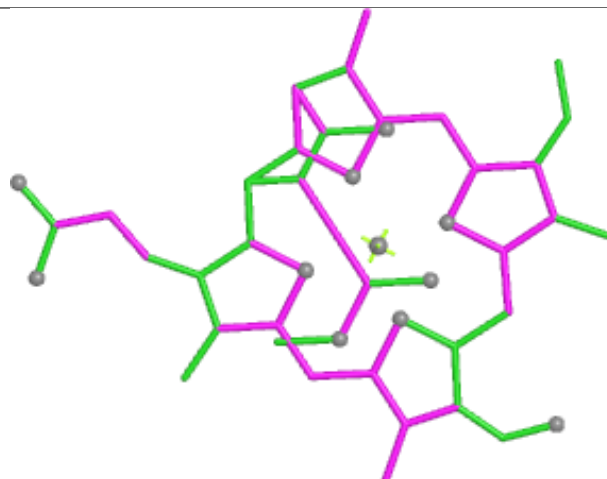




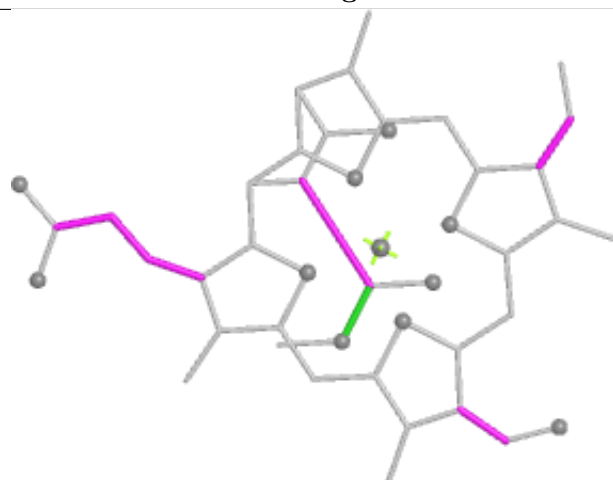
Ligand CL7 3 513



Bond lengths



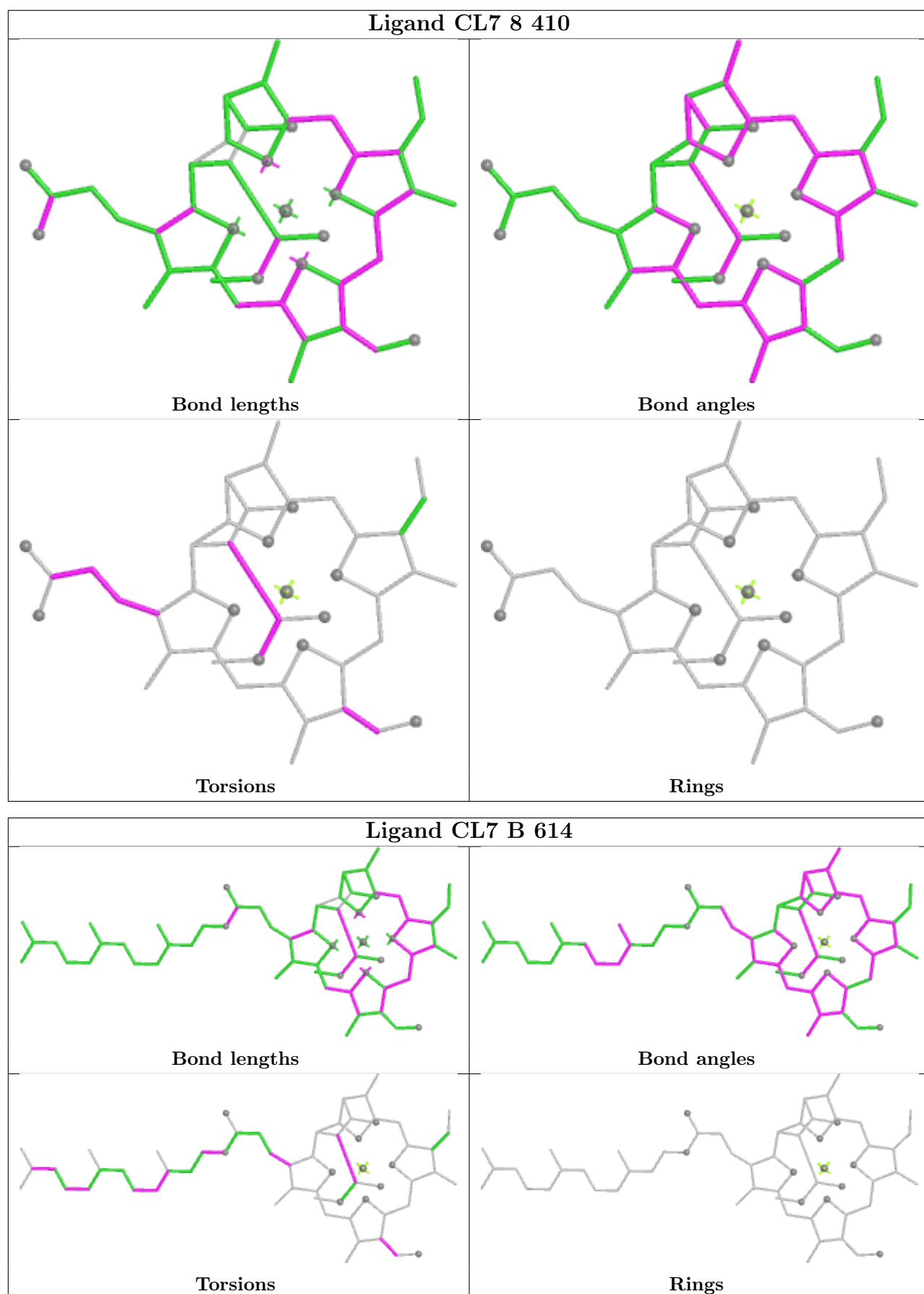
Bond angles

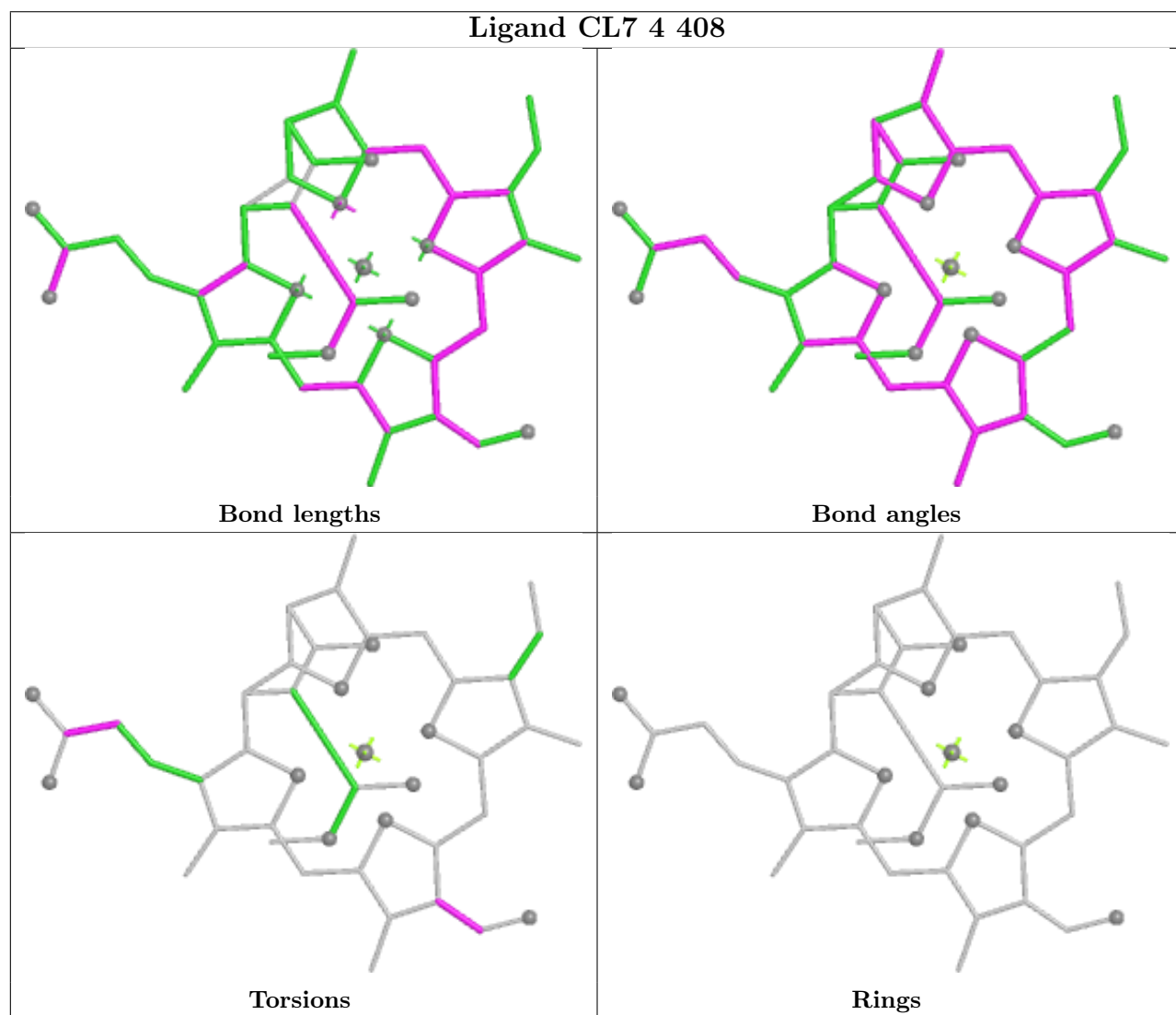
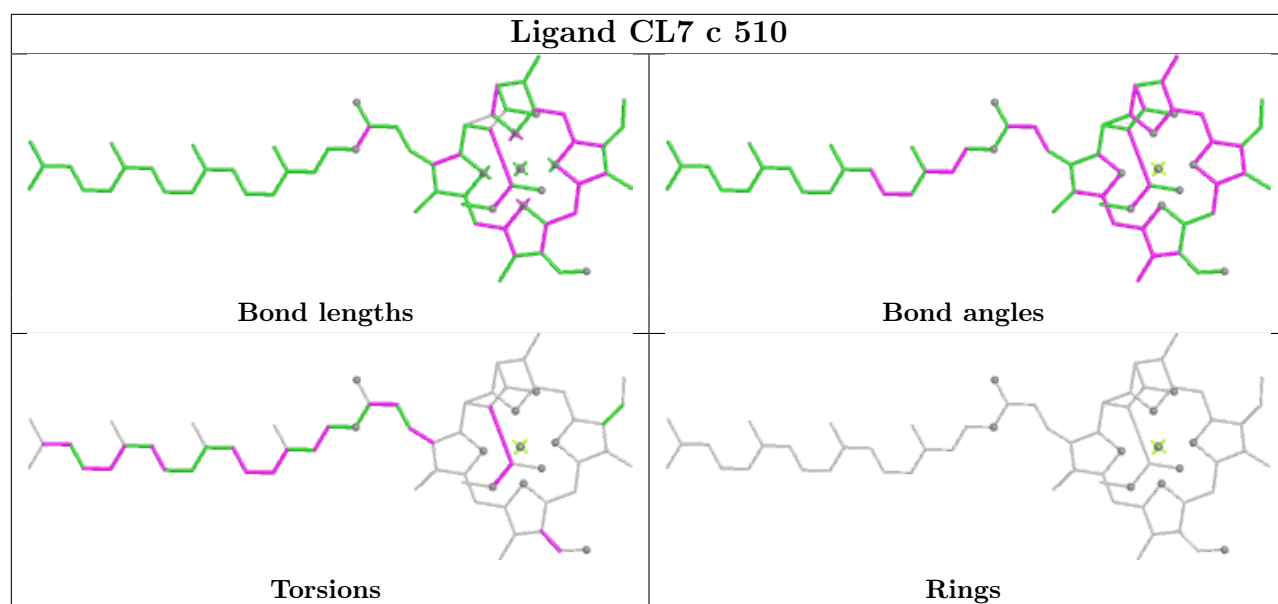


Torsions

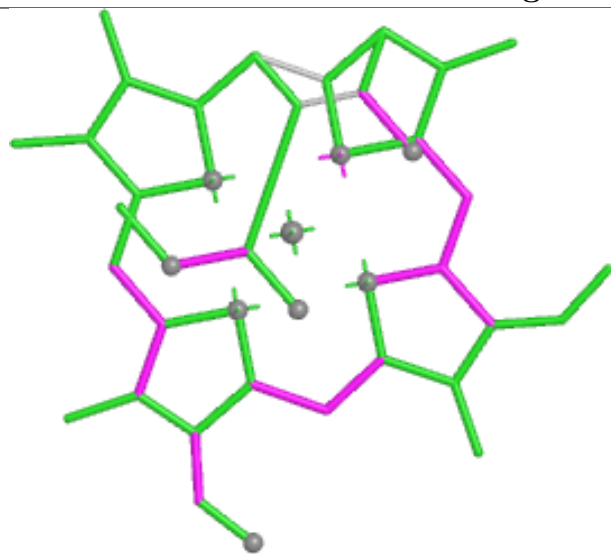


Rings

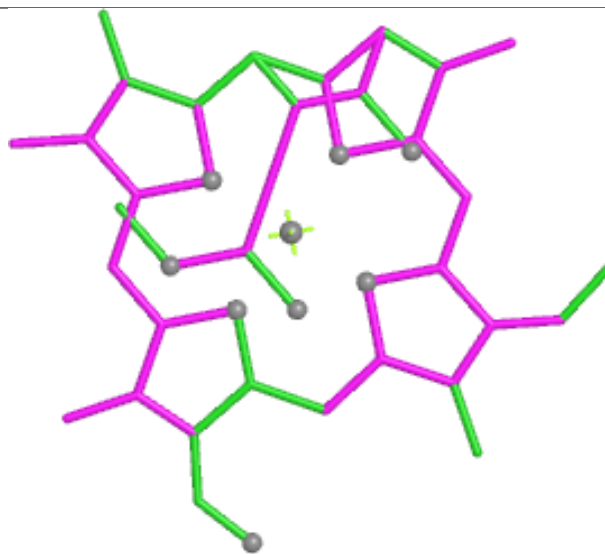




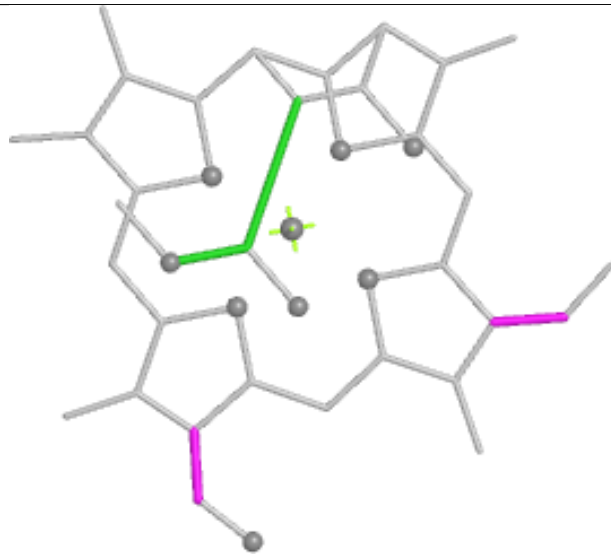
Ligand CL7 5 414



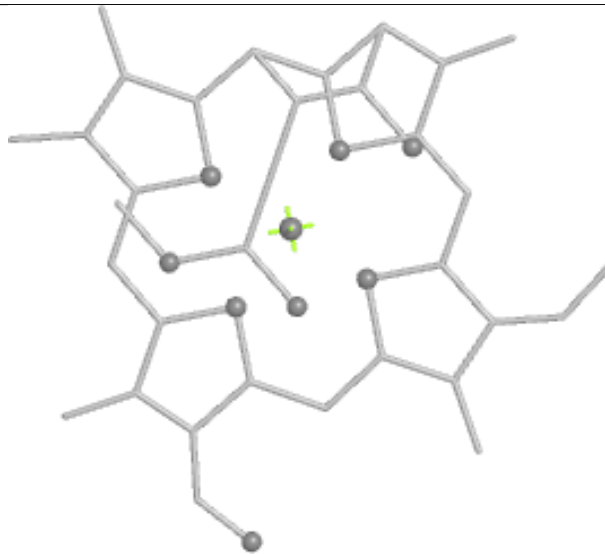
Bond lengths



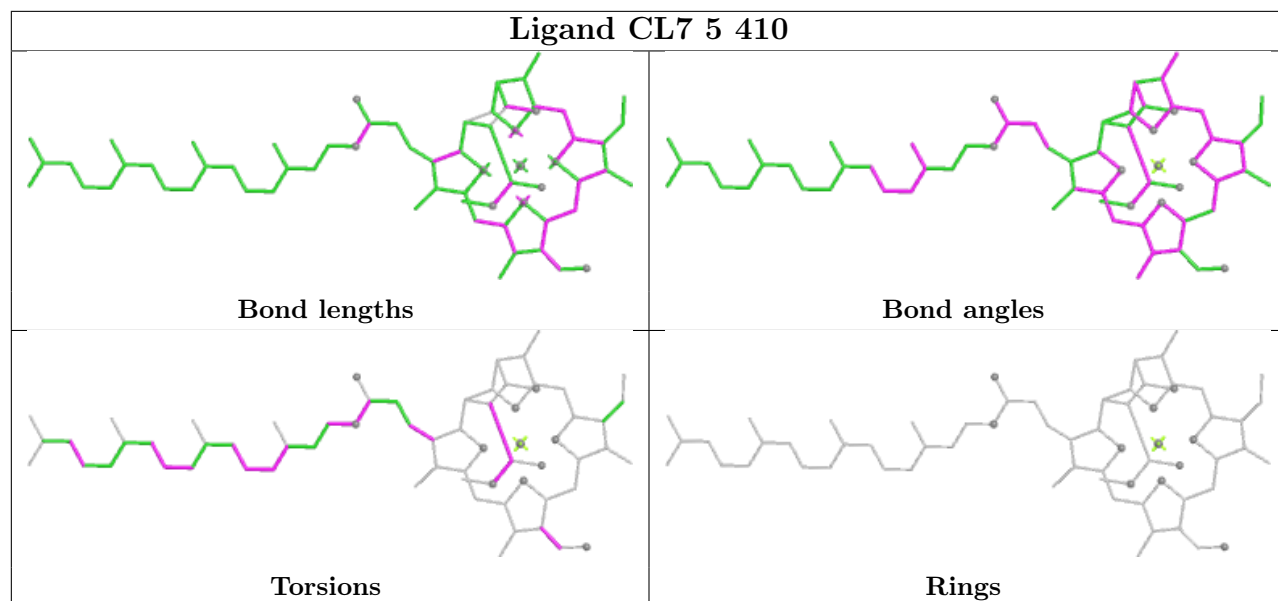
Bond angles



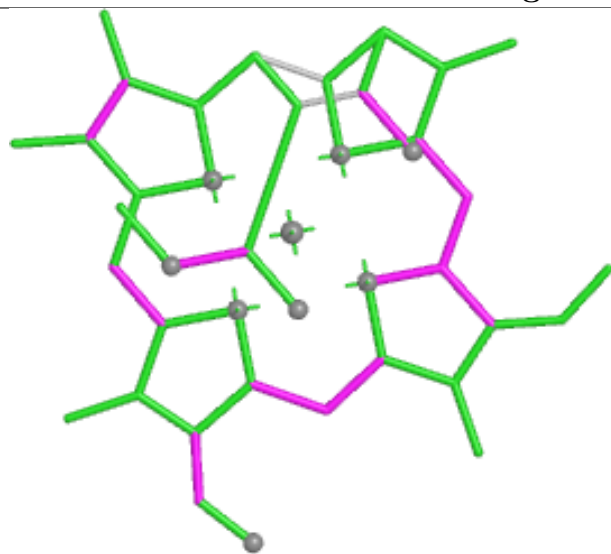
Torsions



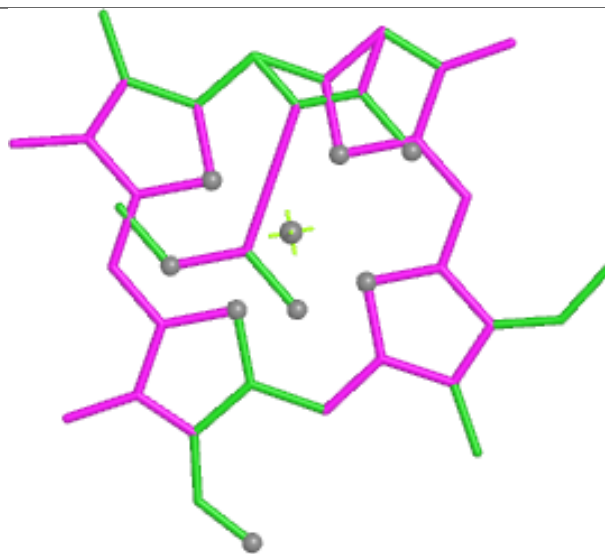
Rings



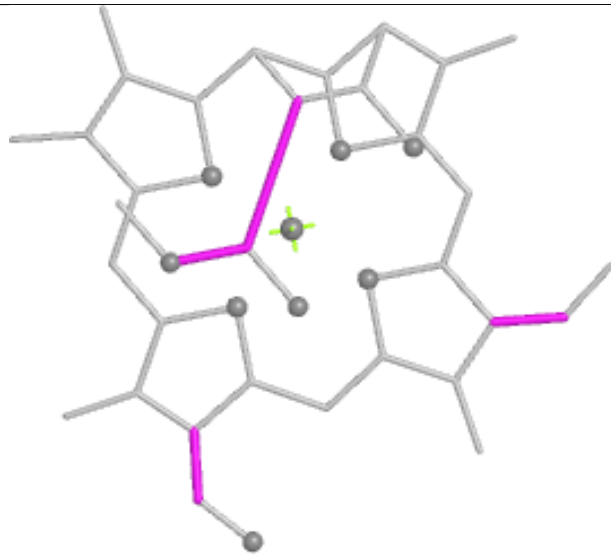
Ligand CL7 5 415



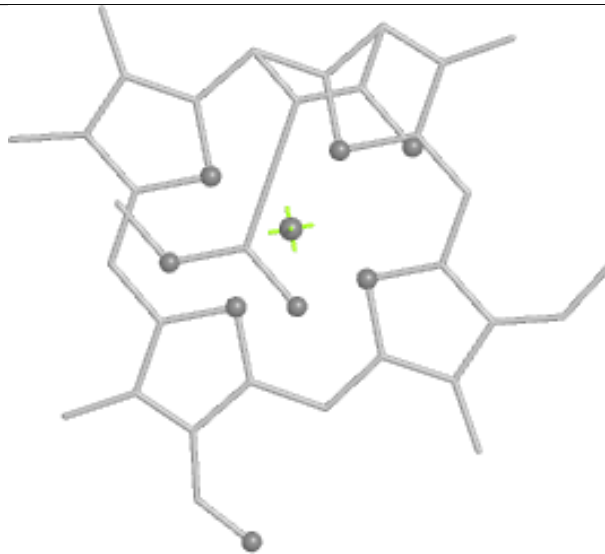
Bond lengths



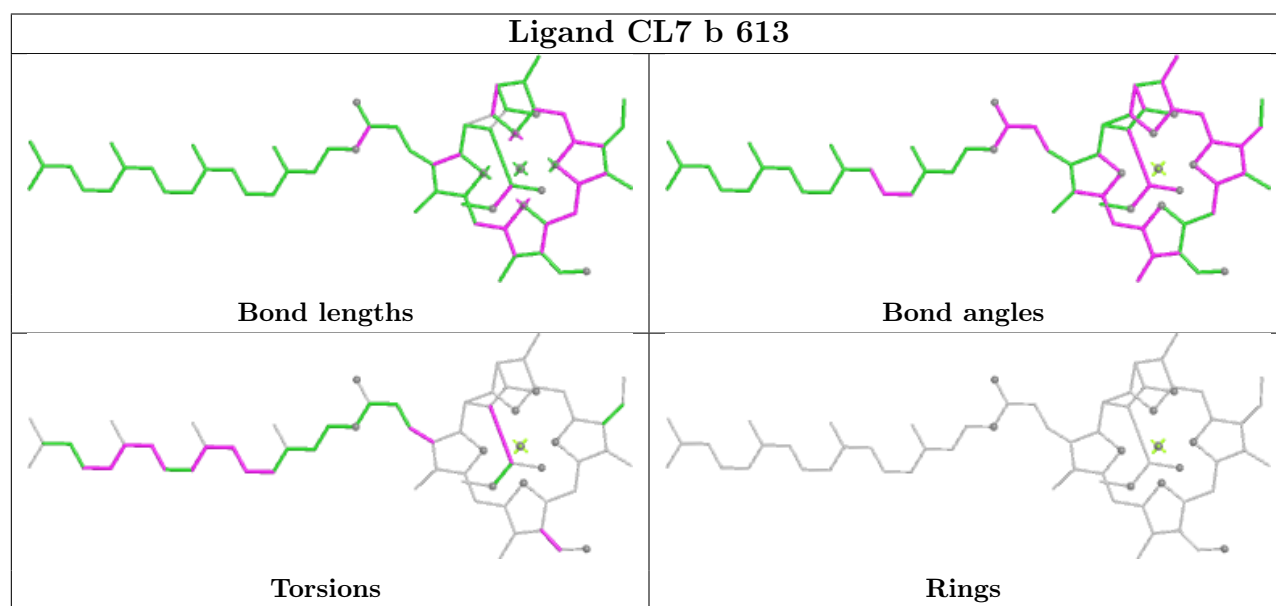
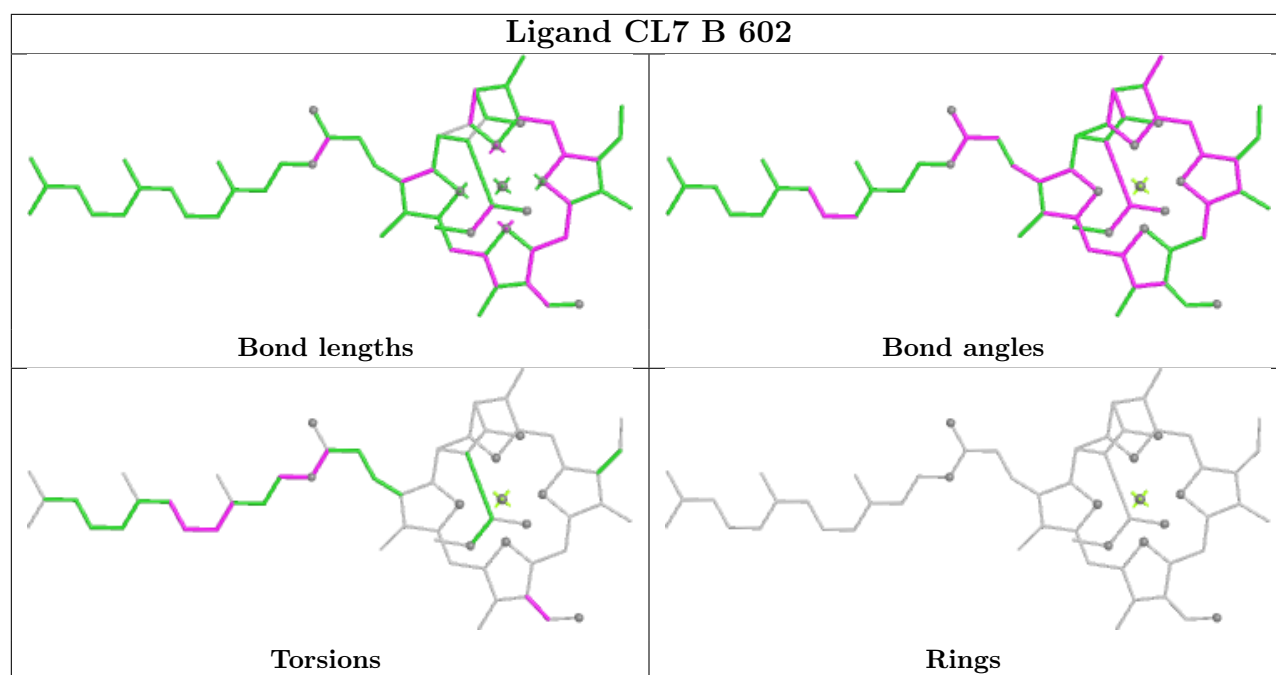
Bond angles



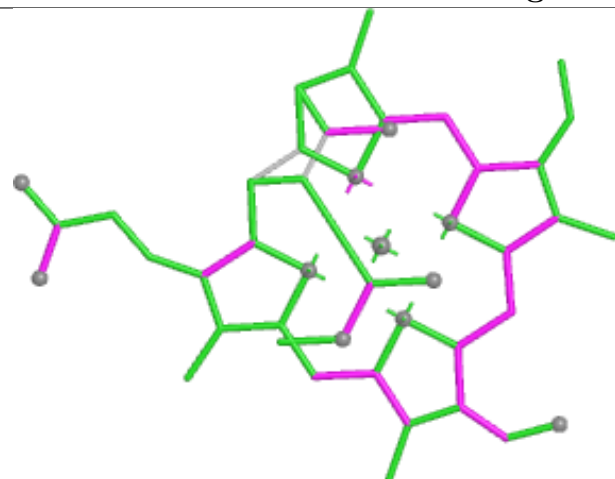
Torsions



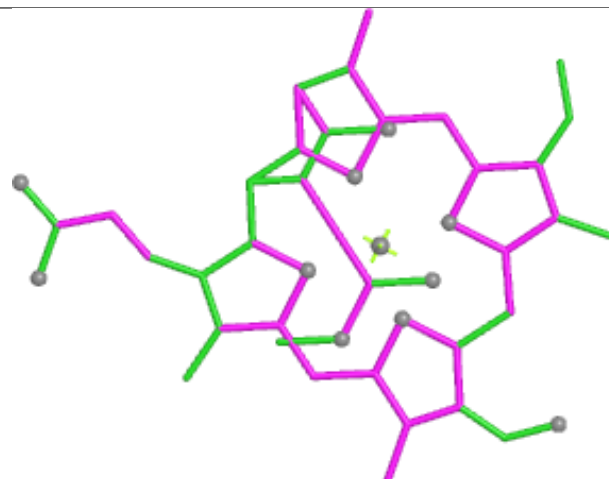
Rings



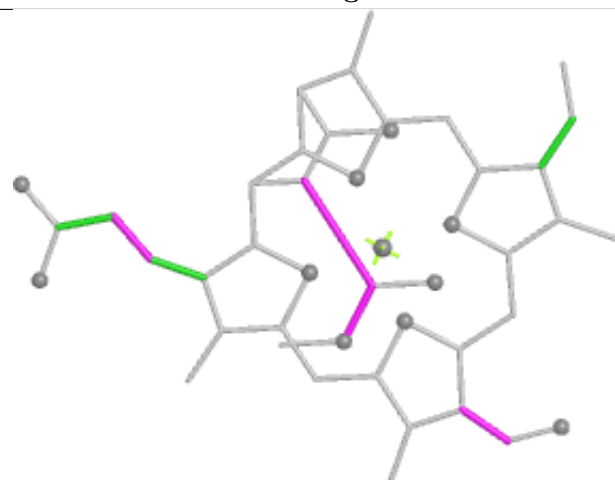
Ligand CL7 5 409



Bond lengths



Bond angles

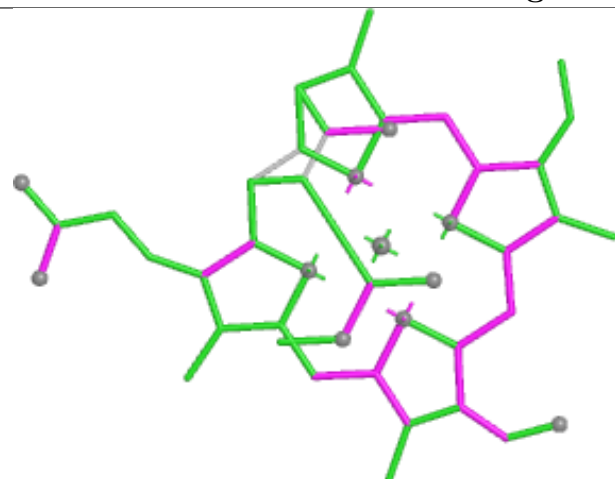


Torsions

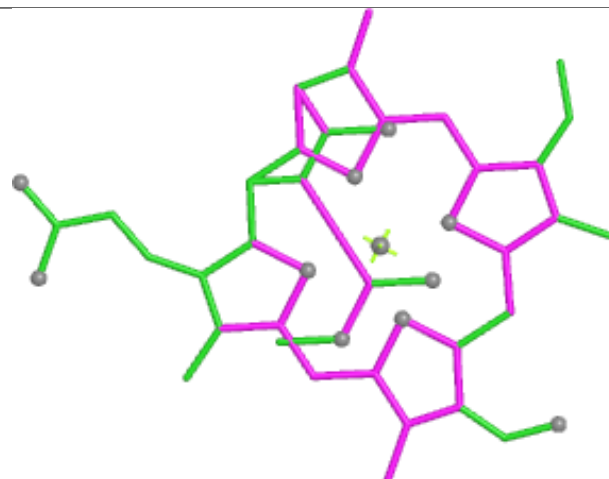


Rings

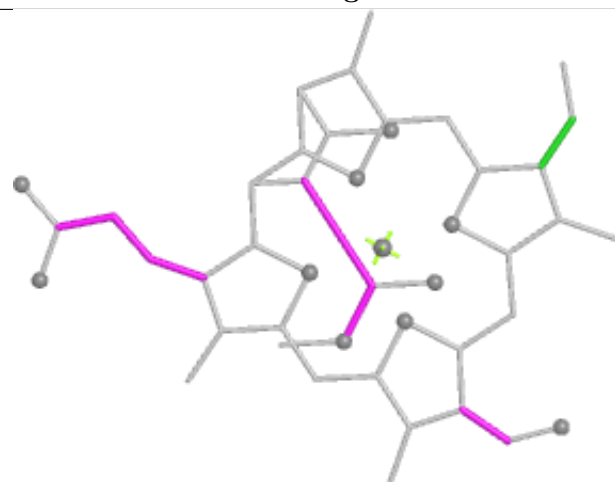
Ligand CL7 5 405



Bond lengths



Bond angles

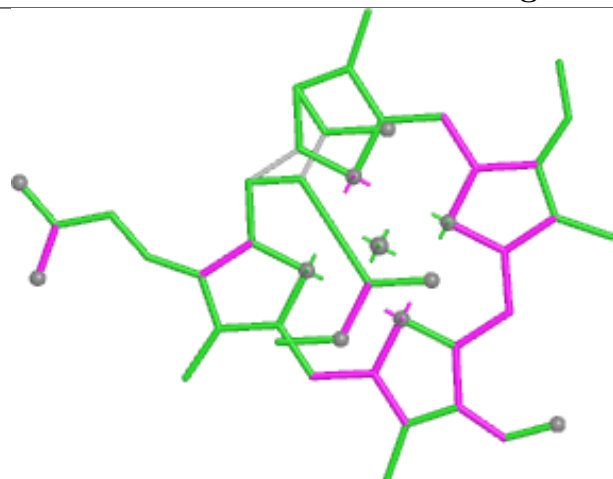


Torsions

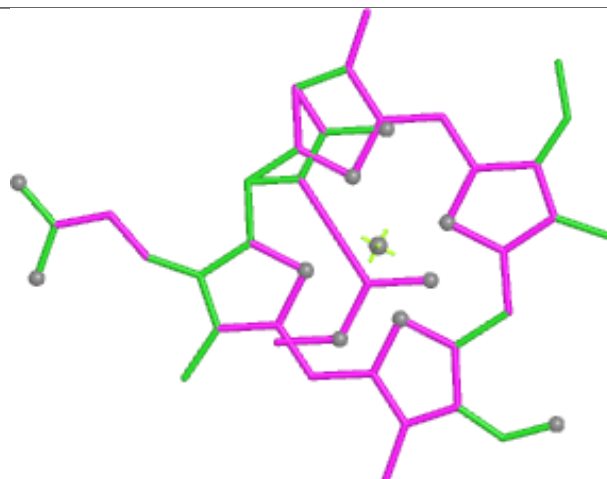


Rings

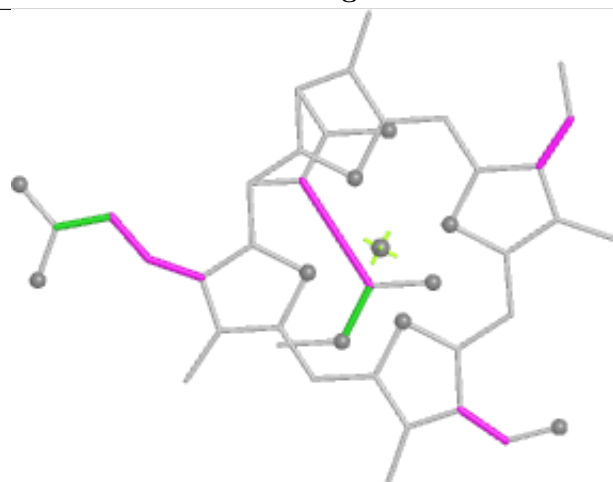
Ligand CL7 D 405



Bond lengths



Bond angles

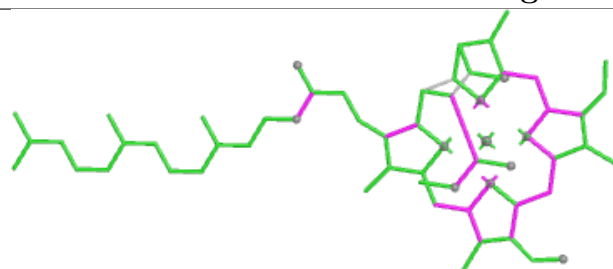


Torsions

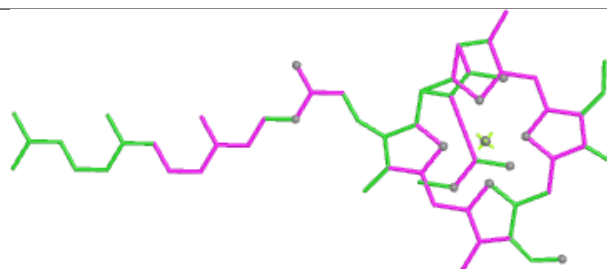


Rings

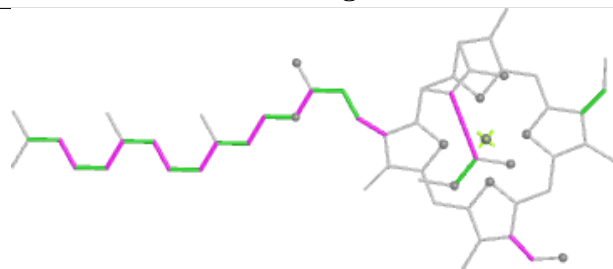
Ligand CL7 C 507



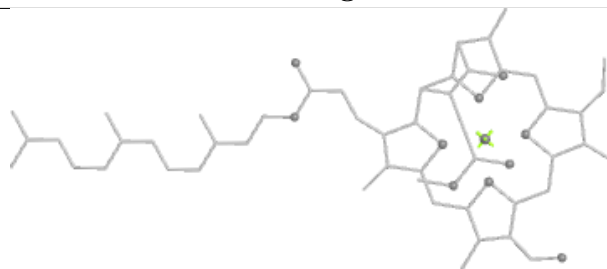
Bond lengths



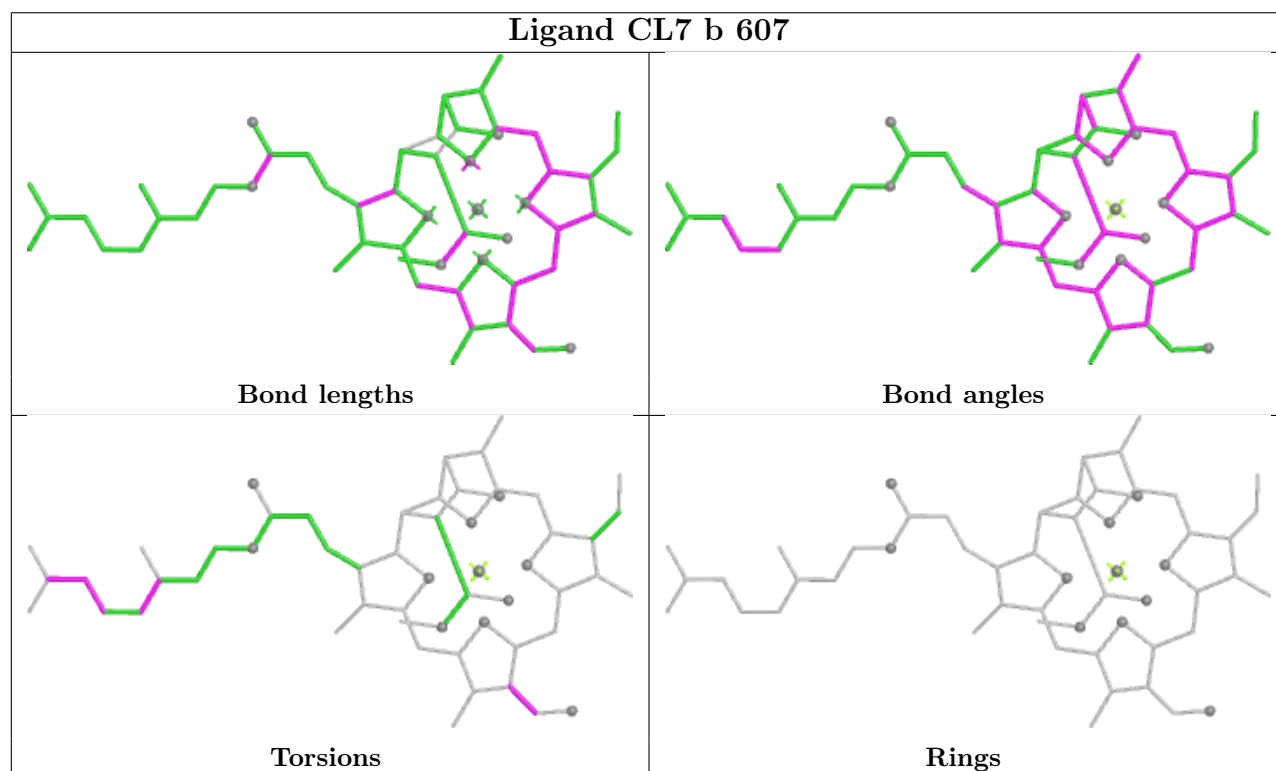
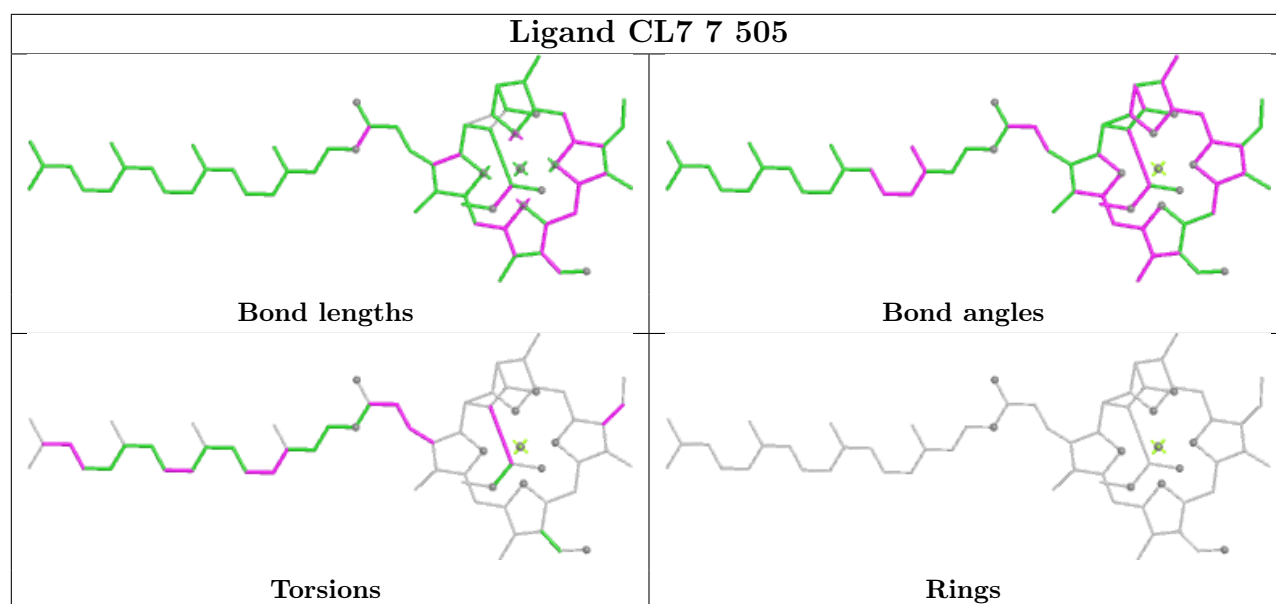
Bond angles

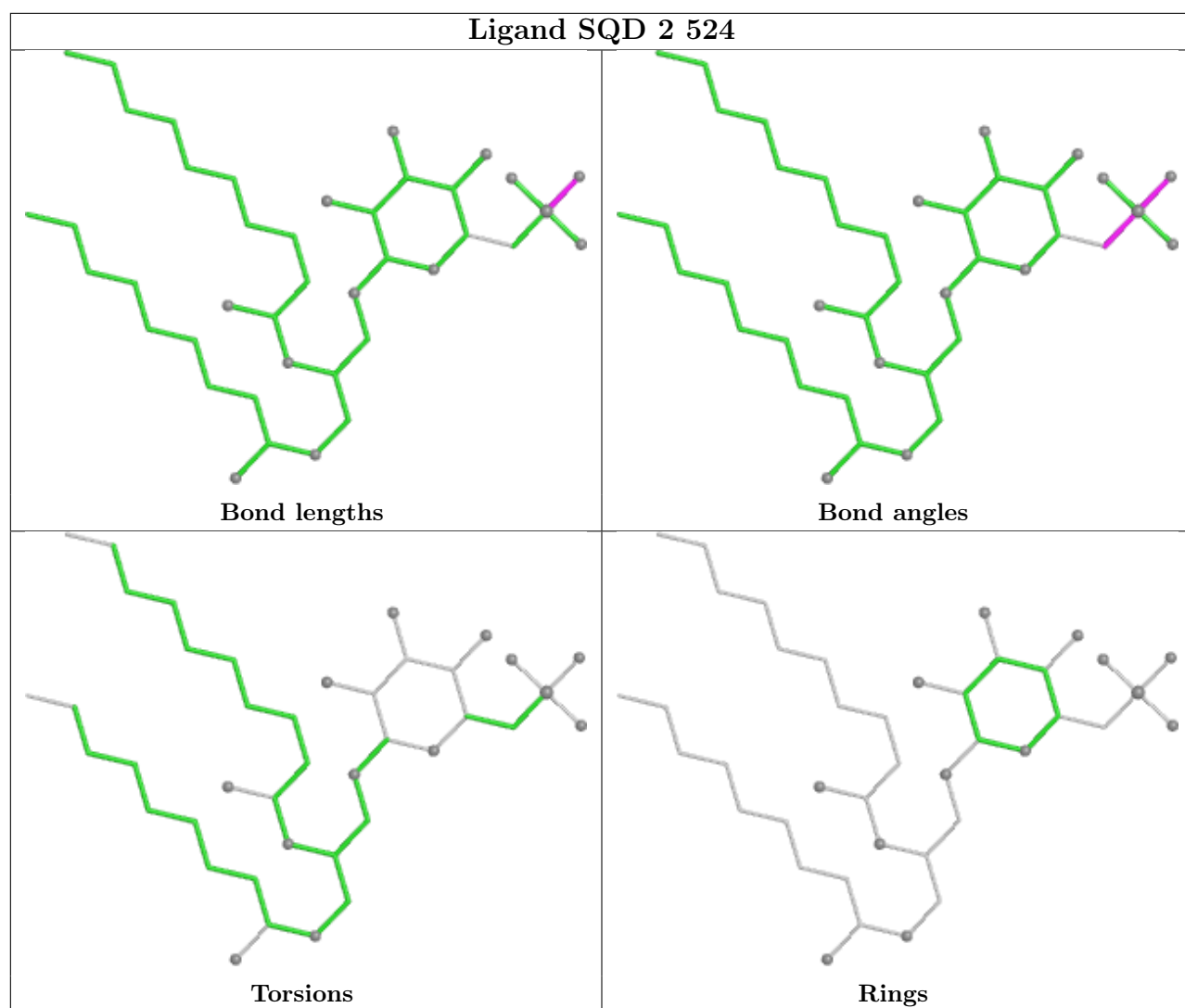


Torsions

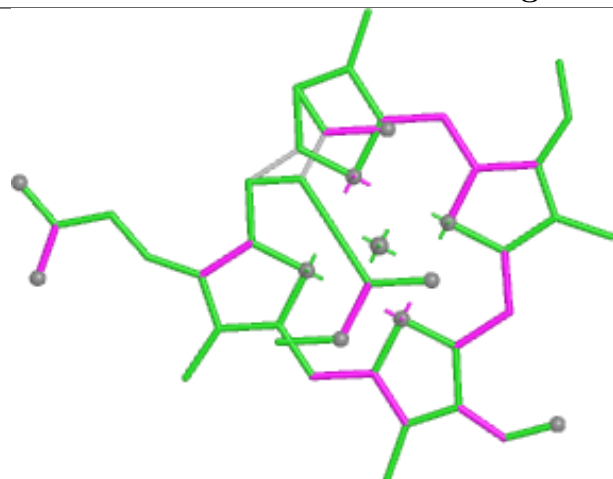


Rings

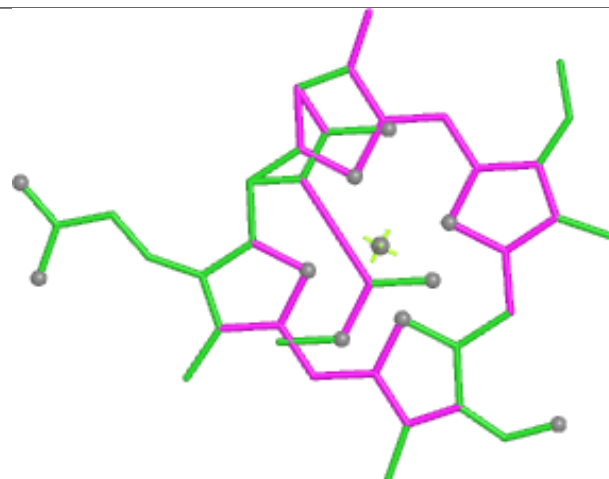




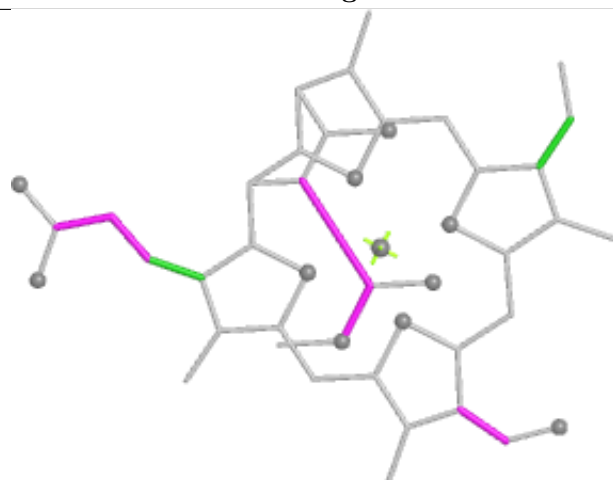
Ligand CL7 B 622



Bond lengths



Bond angles

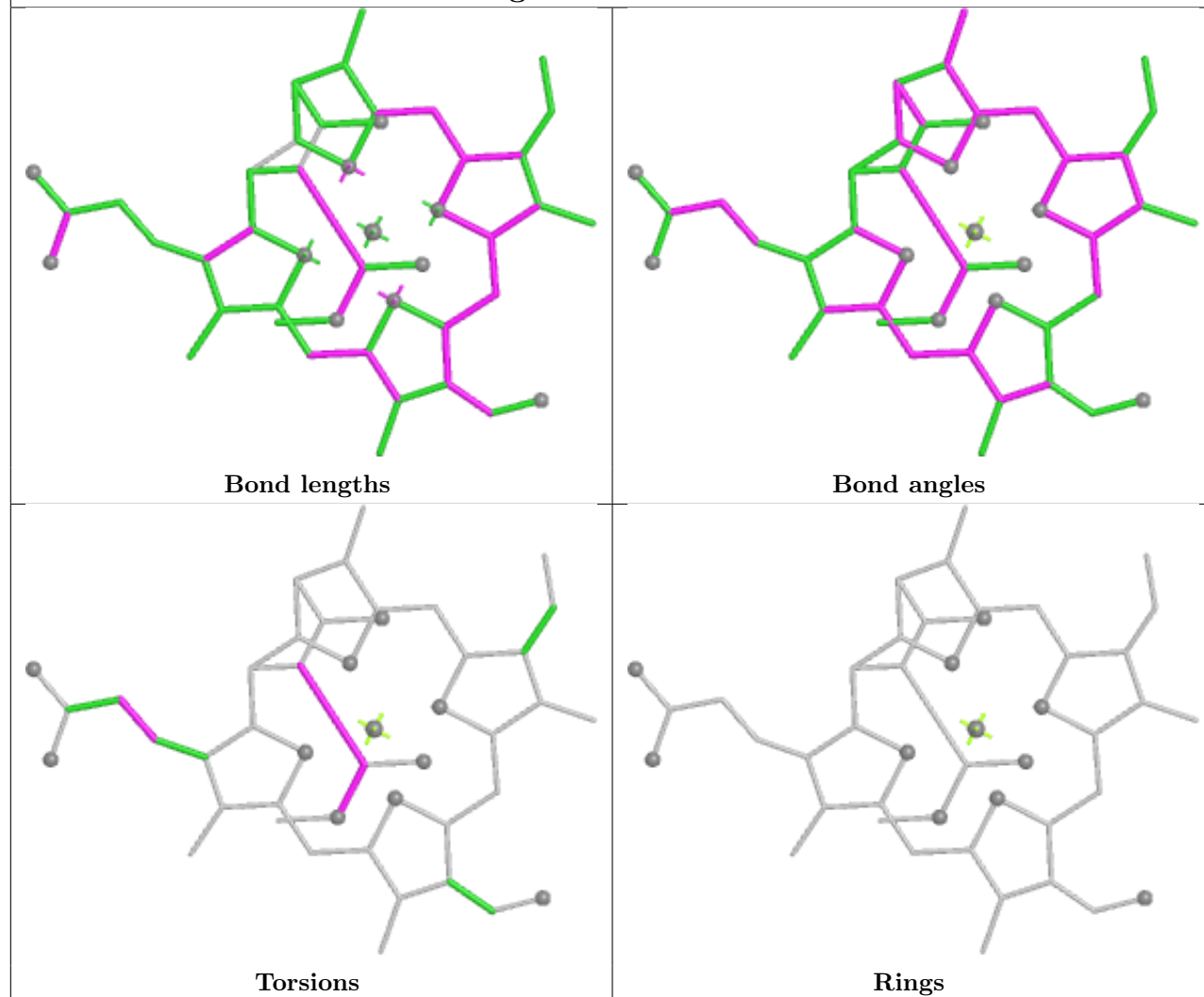


Torsions

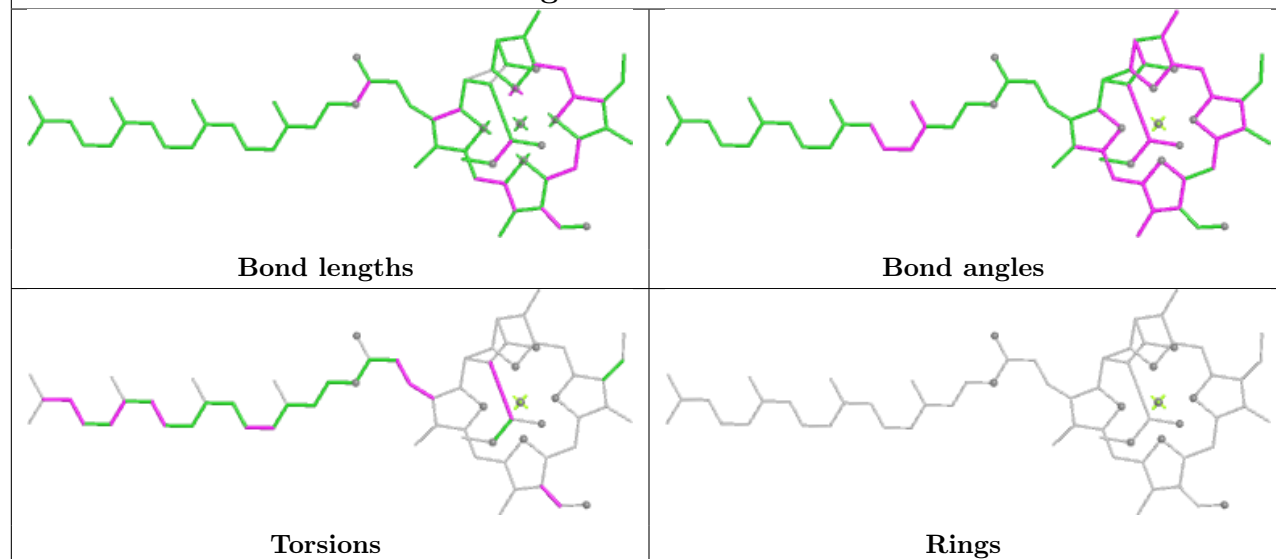


Rings

Ligand CL7 b 617



Ligand CL7 6 518



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.

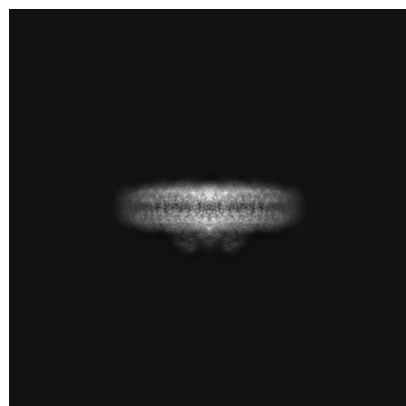
6 Map visualisation [i](#)

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.

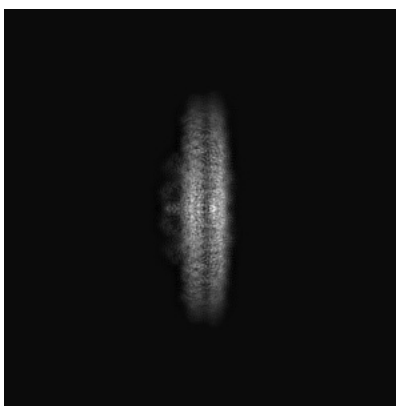
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

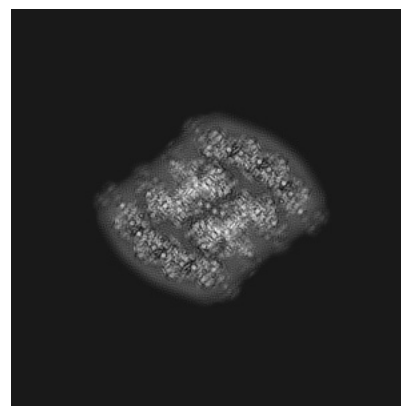
6.1.1 Primary map



X

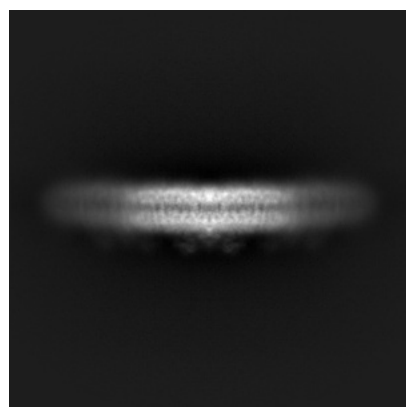


Y

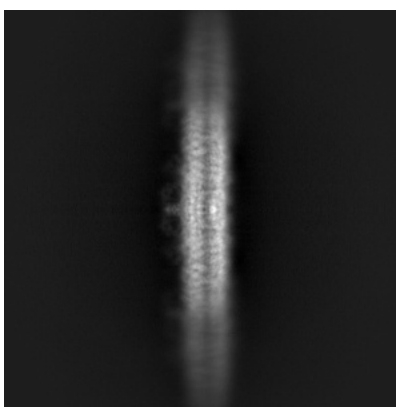


Z

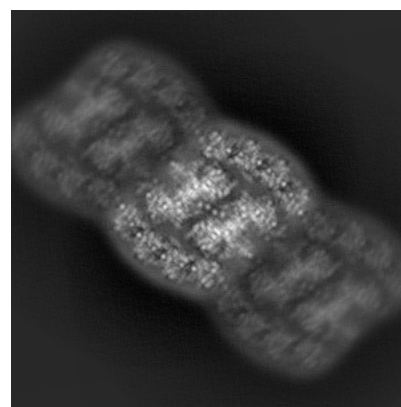
6.1.2 Raw map



X



Y

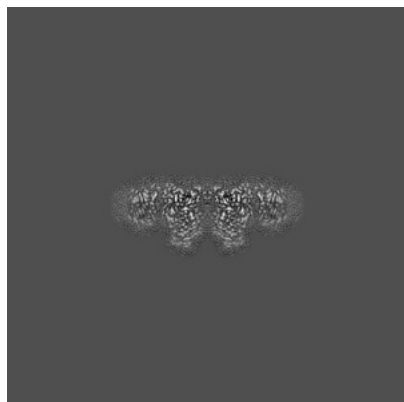


Z

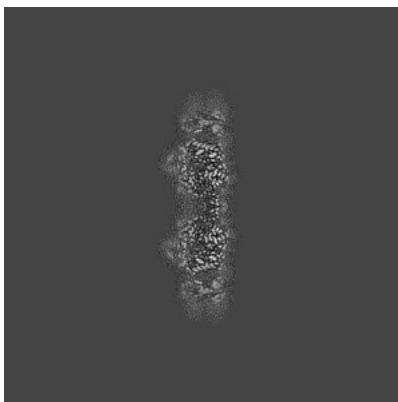
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

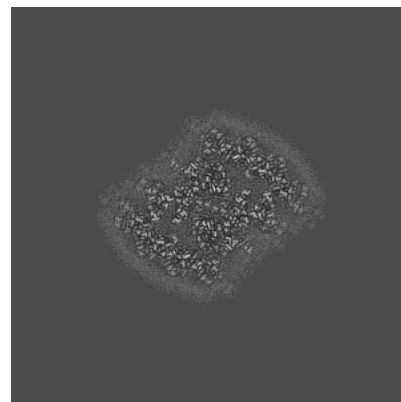
6.2.1 Primary map



X Index: 240

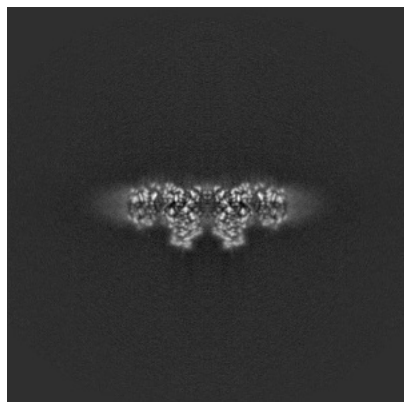


Y Index: 240

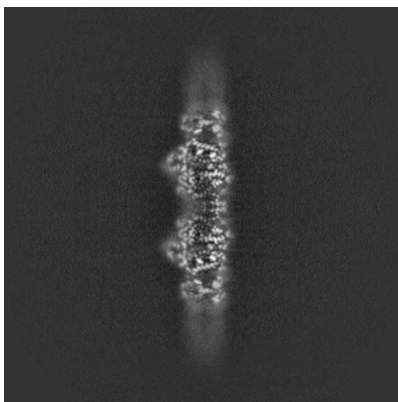


Z Index: 240

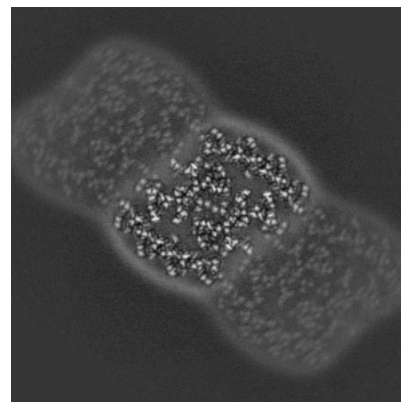
6.2.2 Raw map



X Index: 240



Y Index: 240



Z Index: 240

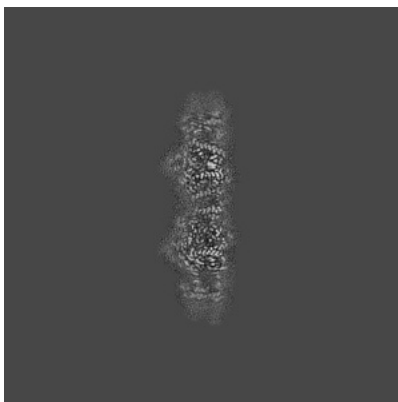
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

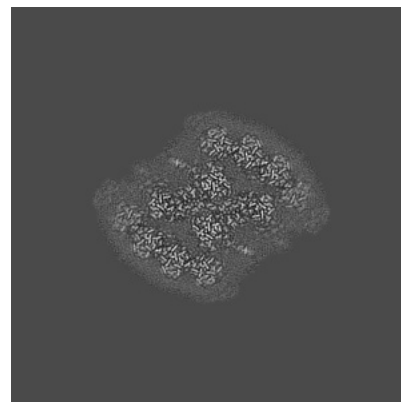
6.3.1 Primary map



X Index: 237



Y Index: 242

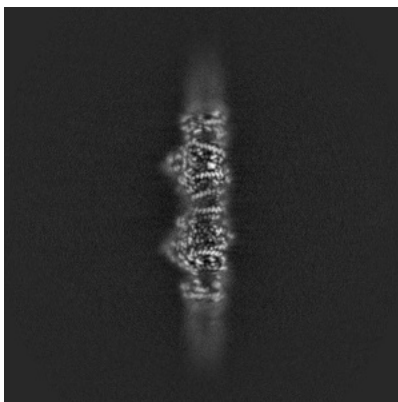


Z Index: 251

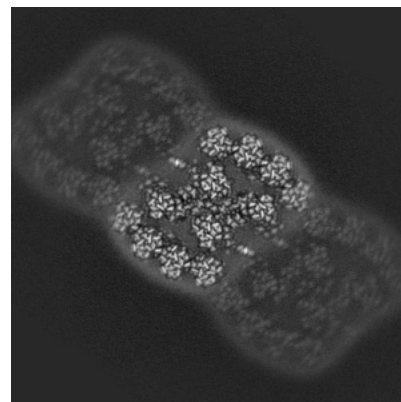
6.3.2 Raw map



X Index: 237



Y Index: 242

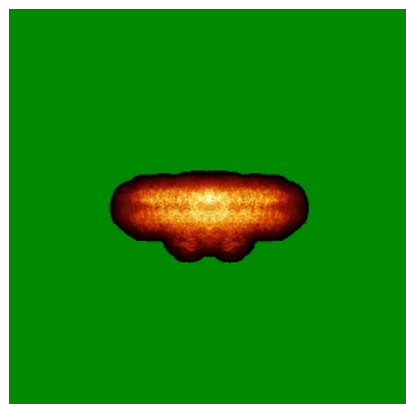


Z Index: 251

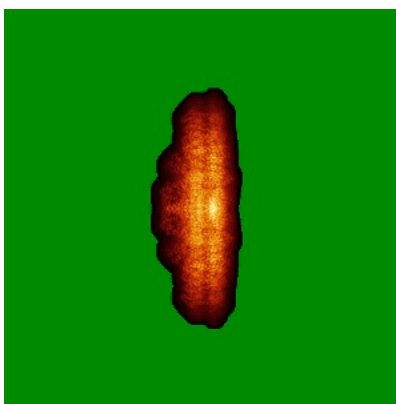
The images above show the largest variance slices of the map in three orthogonal directions.

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

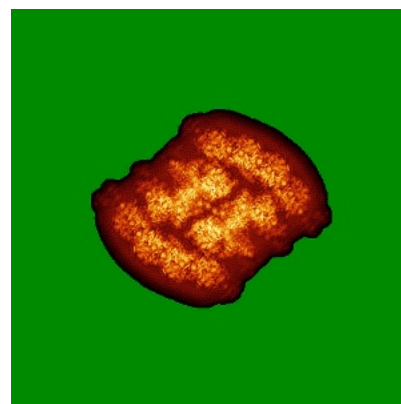
6.4.1 Primary map



X

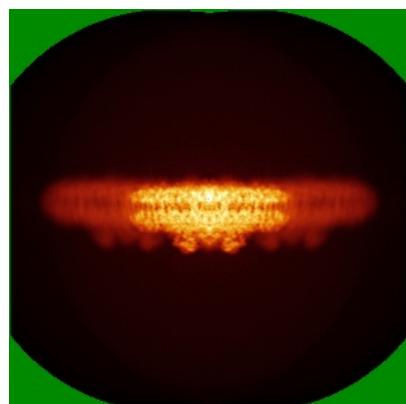


Y

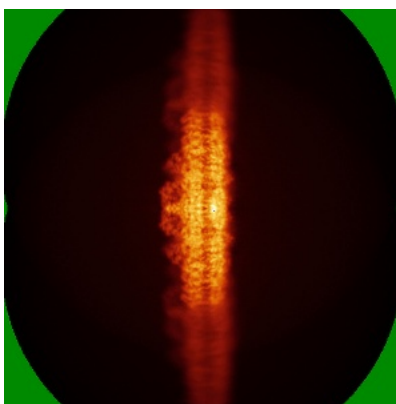


Z

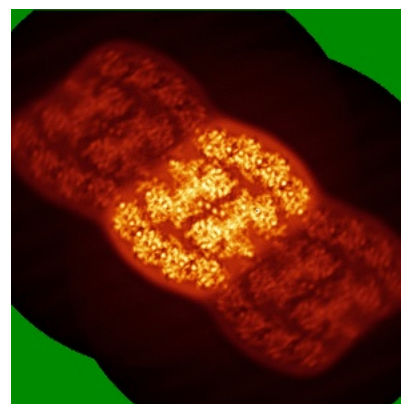
6.4.2 Raw map



X



Y

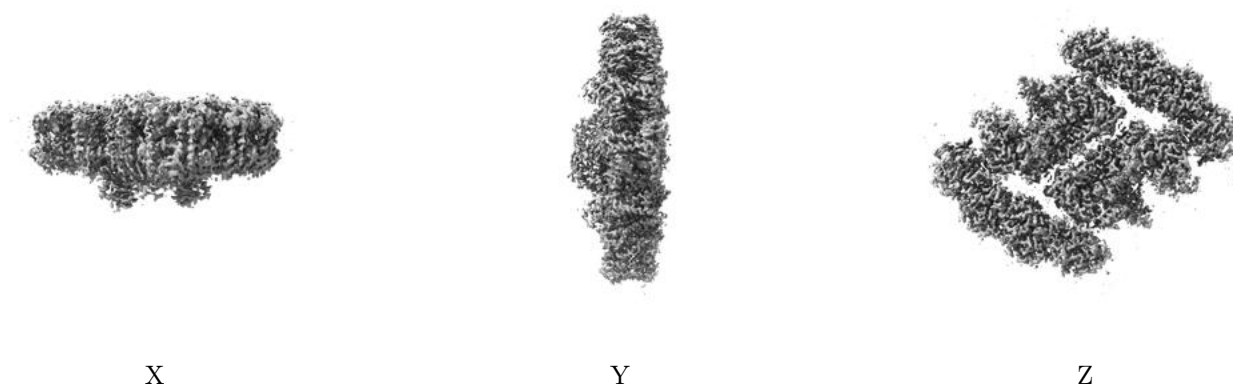


Z

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.

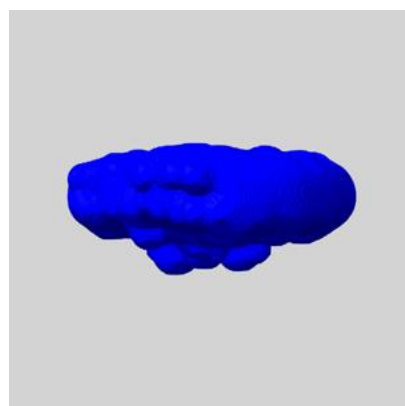
6.6 Mask visualisation [i](#)

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

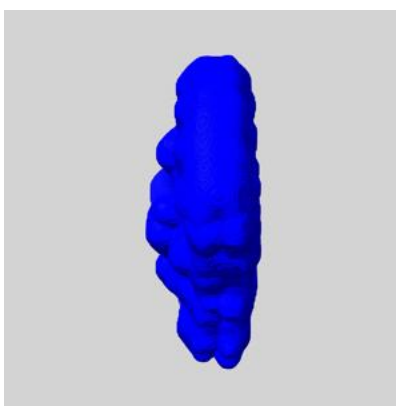
A mask typically either:

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

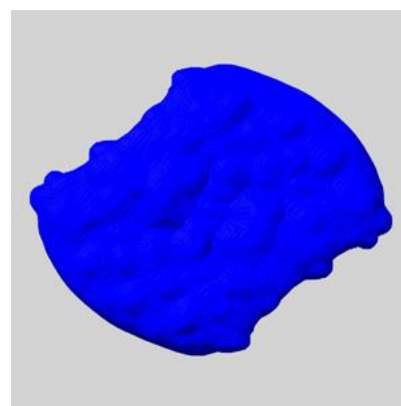
6.6.1 emd_33929_msk_1.map [i](#)



X



Y

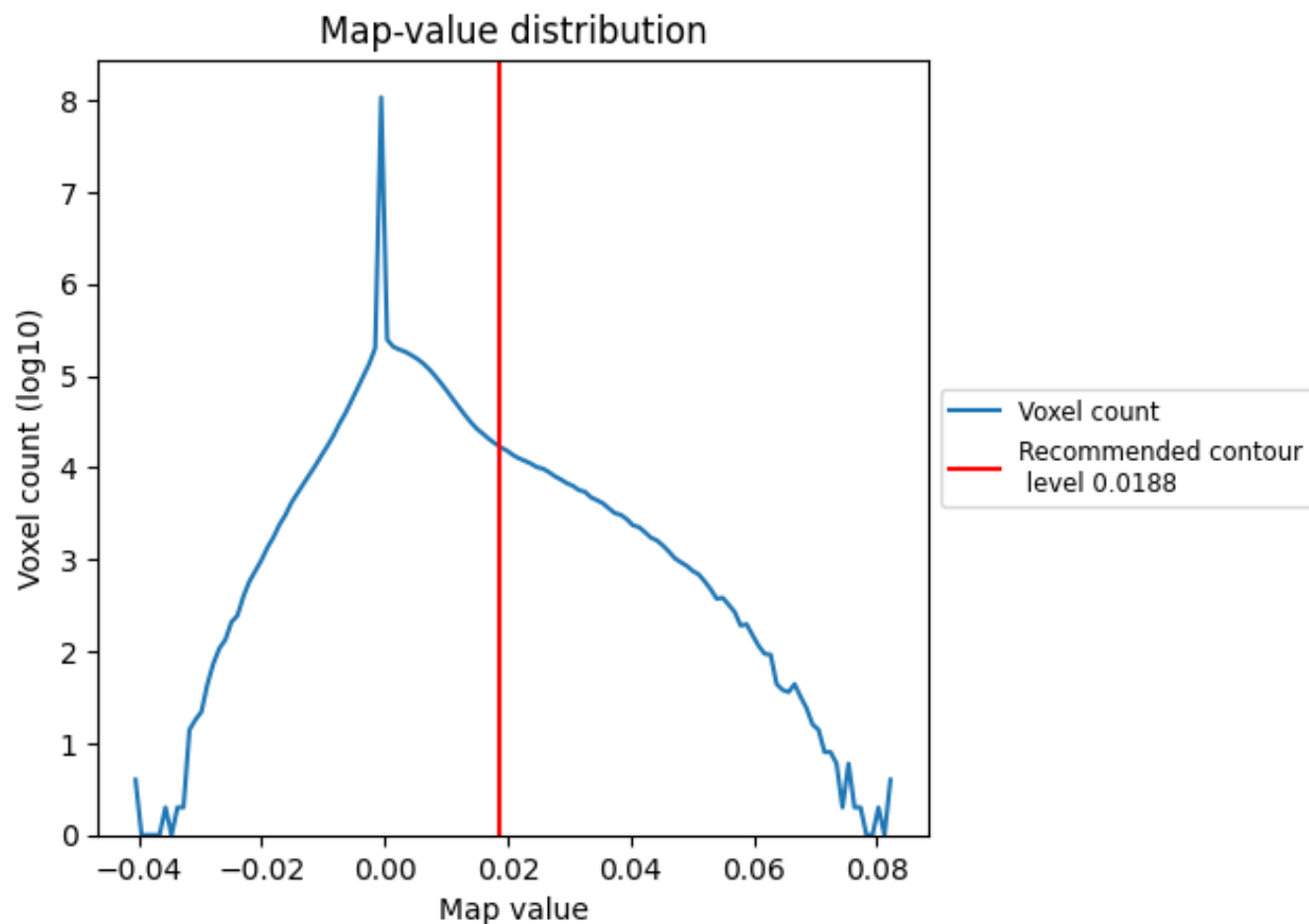


Z

7 Map analysis [i](#)

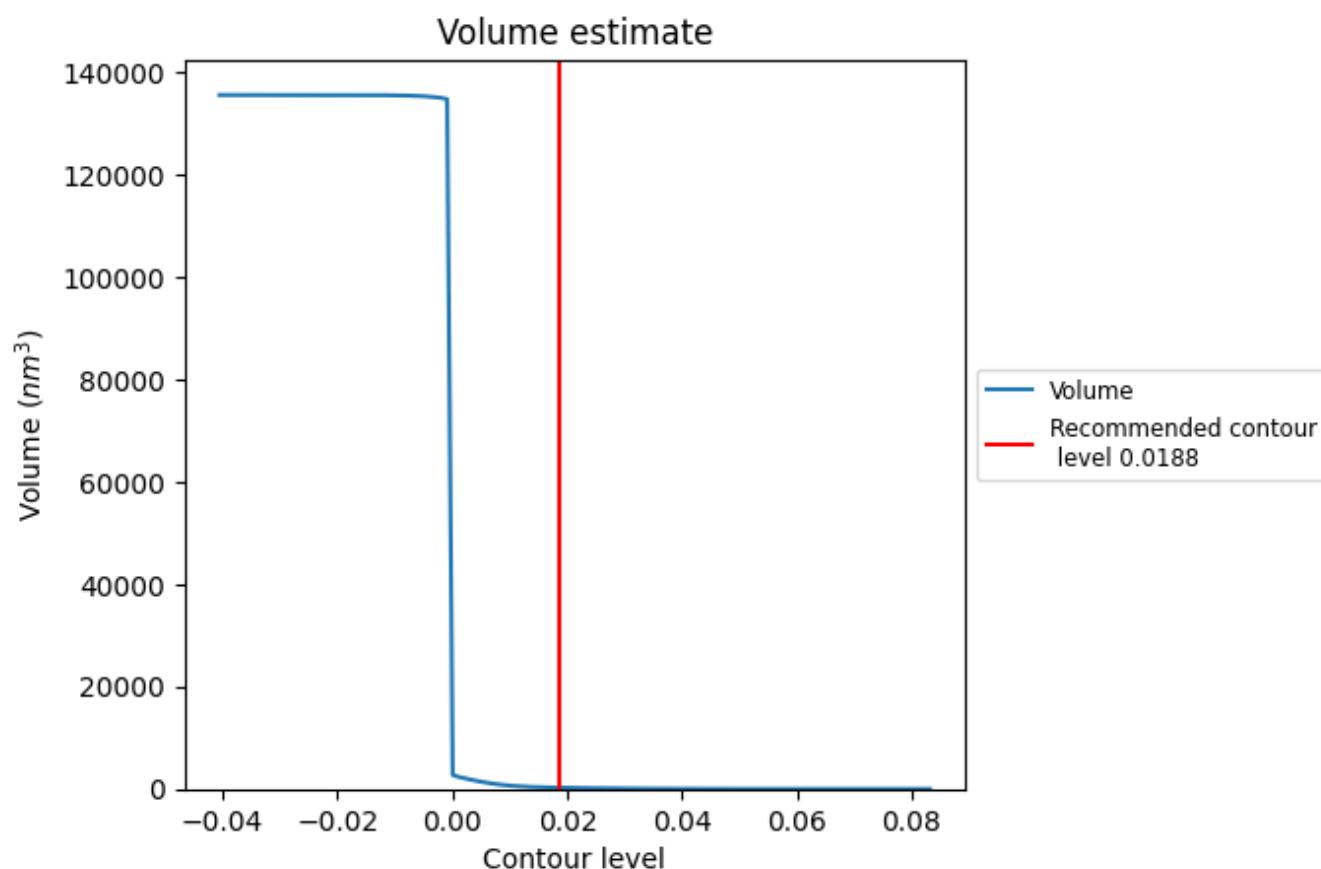
This section contains the results of statistical analysis of the map.

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.

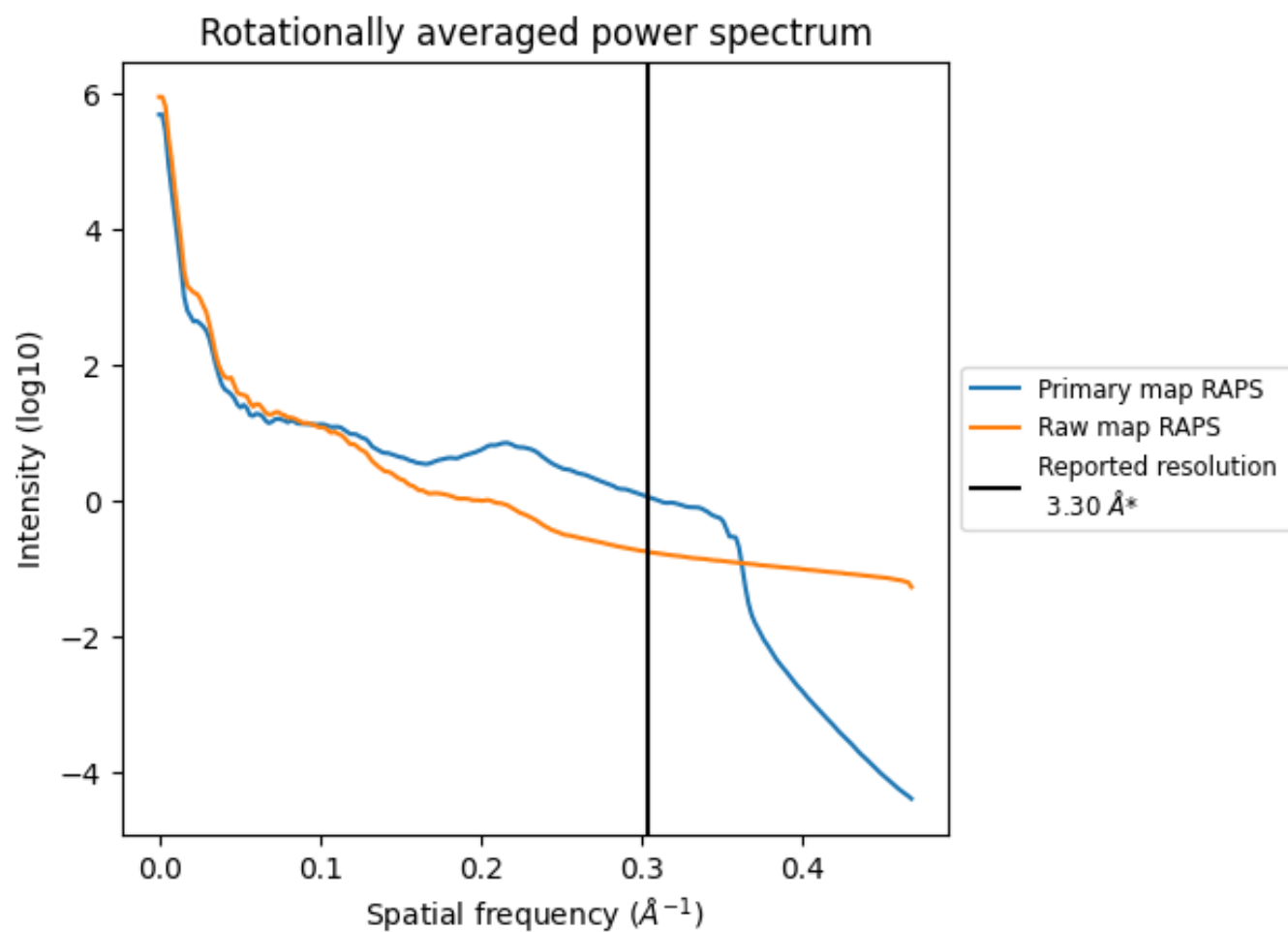
7.2 Volume estimate [i](#)



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 ⓘ

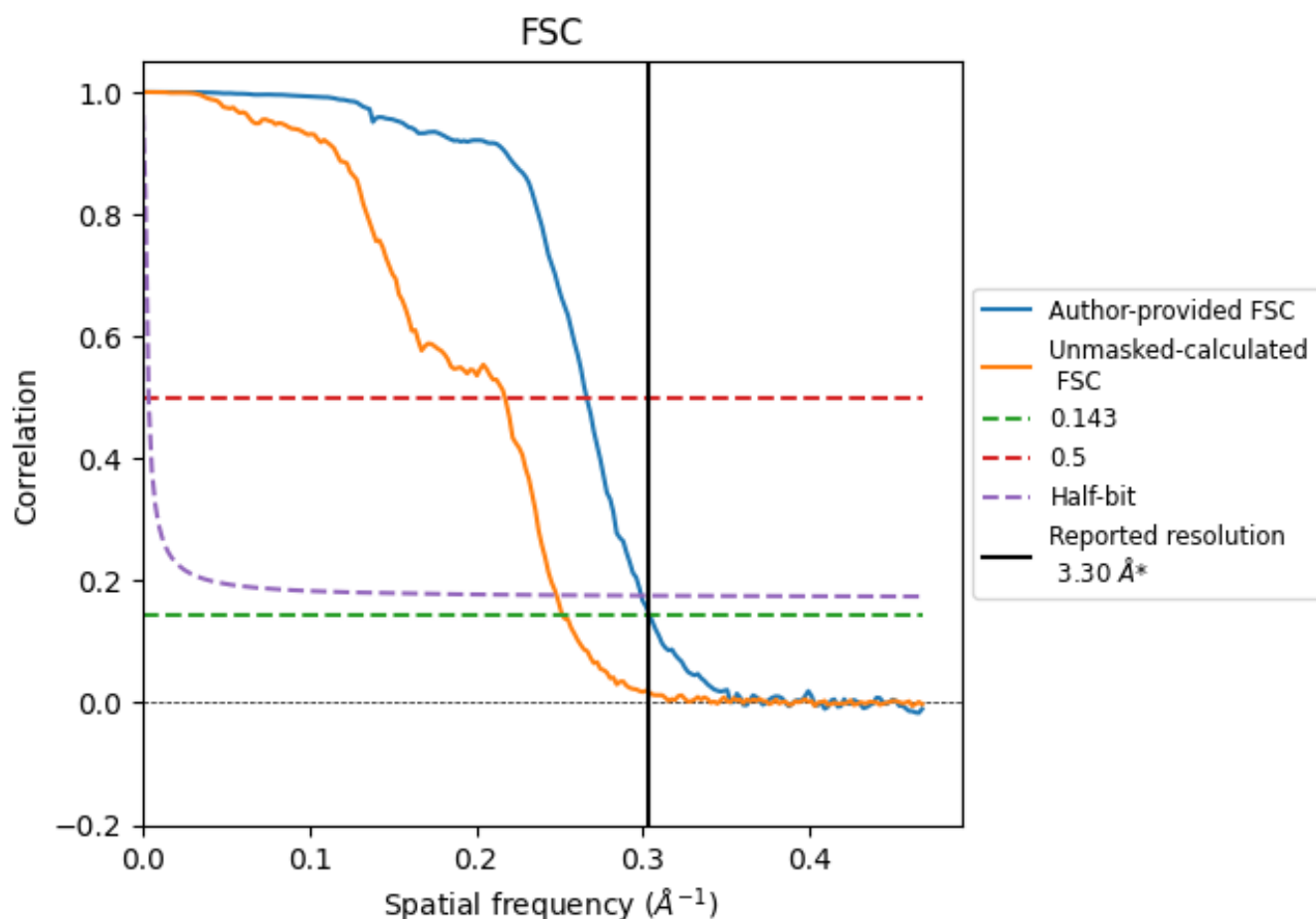


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

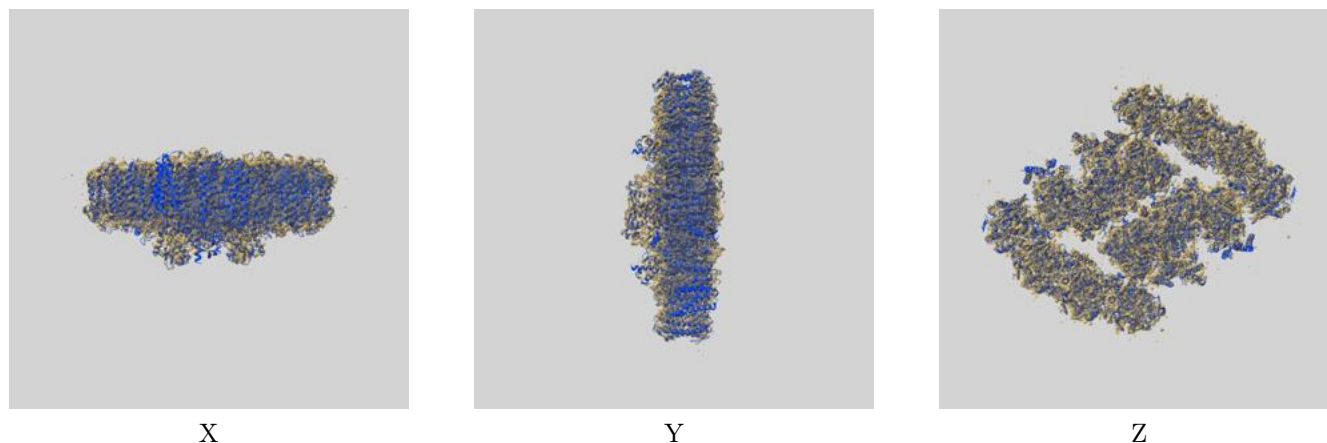
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.29	3.76	3.34
Unmasked-calculated*	3.97	4.60	4.03

*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](#)

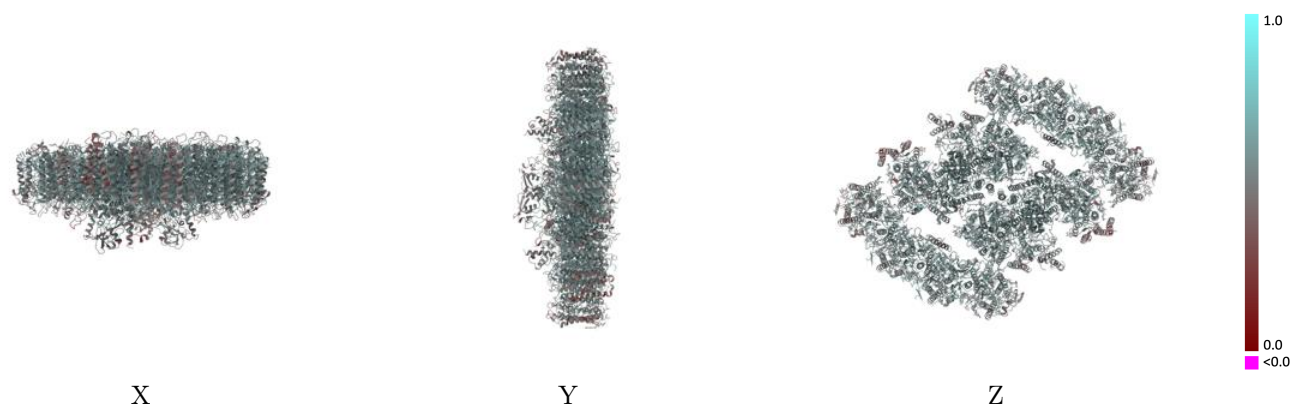
This section contains information regarding the fit between EMDB map EMD-33929 and PDB model 7YMI. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



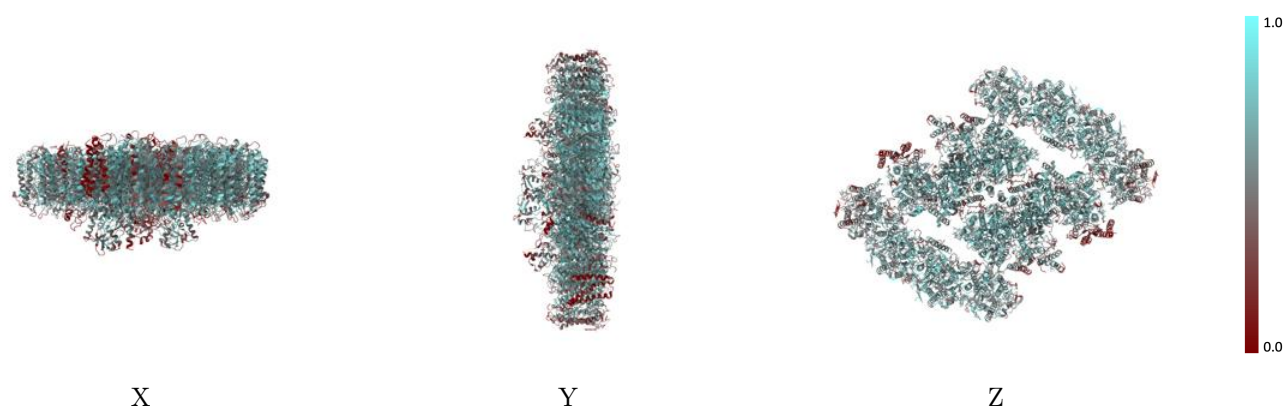
The images above show the 3D surface view of the map at the recommended contour level 0.0188 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



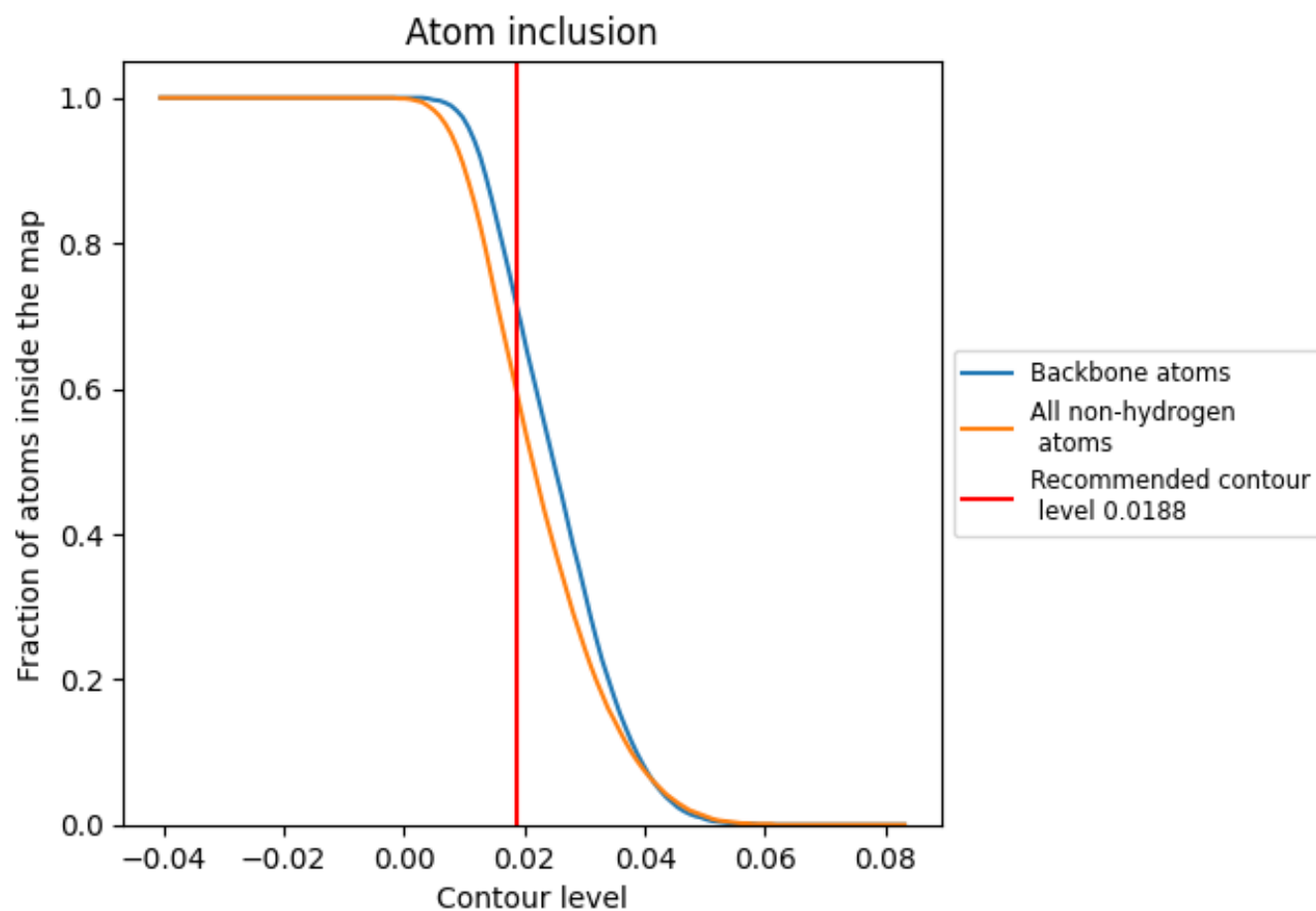
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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