



wwPDB EM Validation Summary Report ⓘ

May 11, 2025 – 08:35 AM JST

PDB ID : 9IS4 / pdb_00009is4
EMDB ID : EMD-60830
Title : Cryo-EM structure of a TEF30-associated intermediate C2S-type PSII-LHCII supercomplex from *Chlamydomonas reinhardtii*
Authors : Wang, Y.; Wang, C.; Li, A.; Liu, Z.
Deposited on : 2024-07-16
Resolution : 2.90 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

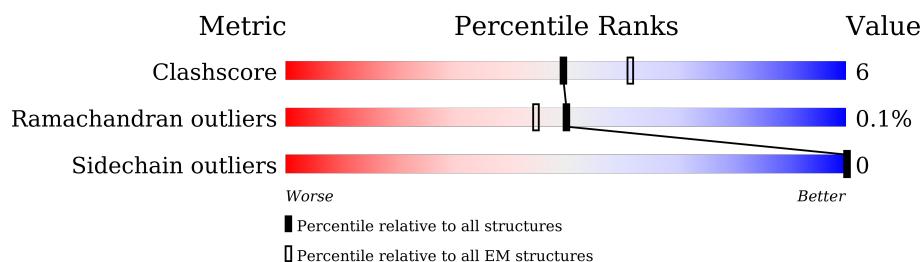
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1	159	
2	A	335	
2	a	335	
3	B	481	
3	b	481	
4	C	449	
4	c	449	
5	D	351	

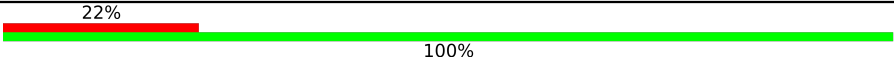
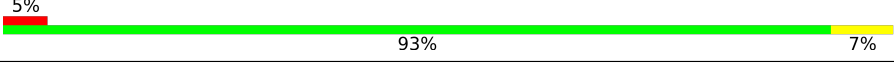
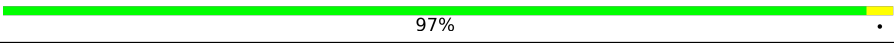
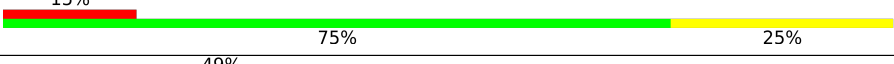
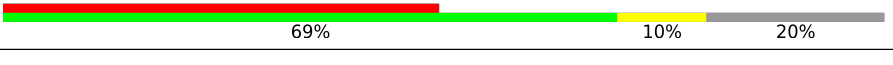
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Mol	Chain	Length	Quality of chain
5	d	351	
6	E	75	
6	e	75	
7	F	31	
7	f	31	
8	G	219	
9	H	69	
9	h	69	
10	I	35	
10	i	35	
11	K	37	
11	k	37	
12	L	37	
12	l	37	
13	M	31	
13	m	31	
14	N	219	
15	O	240	
16	S	250	
17	T	30	
17	t	30	
18	V	32	
18	v	32	
19	W	56	
20	X	32	

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Mol	Chain	Length	Quality of chain
20	x	32	
21	Y	220	
22	Z	61	
22	z	61	
23	r	201	

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
25	CLA	A	402	X	-	-	-
25	CLA	A	403	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	B	501	X	-	-	-
25	CLA	B	502	X	-	-	-
25	CLA	B	503	X	-	-	-
25	CLA	B	504	X	-	-	-
25	CLA	B	505	X	-	-	-
25	CLA	B	506	X	-	-	-
25	CLA	B	507	X	-	-	-
25	CLA	B	508	X	-	-	-
25	CLA	B	509	X	-	-	-
25	CLA	B	510	X	-	-	-
25	CLA	B	511	X	-	-	-
25	CLA	B	512	X	-	-	-
25	CLA	B	513	X	-	-	-
25	CLA	B	514	X	-	-	-
25	CLA	B	515	X	-	-	-
25	CLA	B	516	X	-	-	-
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	510	X	-	-	-
25	CLA	C	511	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	401	X	-	-	-
25	CLA	D	404	X	-	-	-
25	CLA	D	405	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	604	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	613	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	303	X	-	-	-
25	CLA	N	304	X	-	-	-
25	CLA	N	305	X	-	-	-
25	CLA	N	311	X	-	-	-
25	CLA	N	312	X	-	-	-
25	CLA	N	313	X	-	-	-
25	CLA	N	314	X	-	-	-
25	CLA	N	315	X	-	-	-
25	CLA	S	602	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	605	X	-	-	-
25	CLA	S	609	X	-	-	-
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	613	X	-	-	-
25	CLA	S	614	X	-	-	-
25	CLA	Y	304	X	-	-	-
25	CLA	Y	305	X	-	-	-
25	CLA	Y	306	X	-	-	-
25	CLA	Y	311	X	-	-	-
25	CLA	Y	312	X	-	-	-
25	CLA	Y	313	X	-	-	-
25	CLA	Y	314	X	-	-	-
25	CLA	Y	315	X	-	-	-
25	CLA	a	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	a	403	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	b	501	X	-	-	-
25	CLA	b	502	X	-	-	-
25	CLA	b	503	X	-	-	-
25	CLA	b	504	X	-	-	-
25	CLA	b	505	X	-	-	-
25	CLA	b	506	X	-	-	-
25	CLA	b	507	X	-	-	-
25	CLA	b	508	X	-	-	-
25	CLA	b	509	X	-	-	-
25	CLA	b	510	X	-	-	-
25	CLA	b	511	X	-	-	-
25	CLA	b	512	X	-	-	-
25	CLA	b	513	X	-	-	-
25	CLA	b	514	X	-	-	-
25	CLA	b	515	X	-	-	-
25	CLA	b	516	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	511	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	401	X	-	-	-
25	CLA	d	403	X	-	-	-
25	CLA	d	404	X	-	-	-
25	CLA	r	301	X	-	-	-
25	CLA	r	302	X	-	-	-
25	CLA	r	303	X	-	-	-
25	CLA	r	307	X	-	-	-
25	CLA	r	308	X	-	-	-
33	BCT	a	409	-	-	X	-
36	CHL	G	601	X	-	-	-
36	CHL	G	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	CHL	G	606	X	-	-	-
36	CHL	G	607	X	-	-	-
36	CHL	G	608	X	-	-	-
36	CHL	G	609	X	-	-	-
36	CHL	G	619	X	-	-	-
36	CHL	N	302	X	-	-	-
36	CHL	N	306	X	-	-	-
36	CHL	N	307	X	-	-	-
36	CHL	N	308	X	-	-	-
36	CHL	N	309	X	-	-	-
36	CHL	N	310	X	-	-	-
36	CHL	S	601	X	-	-	-
36	CHL	S	606	X	-	-	-
36	CHL	S	607	X	-	-	-
36	CHL	S	608	X	-	-	-
36	CHL	Y	303	X	-	-	-
36	CHL	Y	307	X	-	-	-
36	CHL	Y	308	X	-	-	-
36	CHL	Y	309	X	-	-	-
36	CHL	Y	310	X	-	-	-
36	CHL	r	304	X	-	-	-
36	CHL	r	305	X	-	-	-
36	CHL	r	306	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 55146 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 PDZ domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	159	Total	C	N	O	S	0	0
			1285	803	231	245	6		

- Molecule 2 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	315	Total	C	N	O	S	0	0
			2465	1620	407	423	15		
2	a	304	Total	C	N	O	S	0	0
			2375	1561	392	407	15		

- Molecule 3 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	480	Total	C	N	O	S	0	0
			3755	2462	630	651	12		
3	b	481	Total	C	N	O	S	0	0
			3763	2468	631	652	12		

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total	C	N	O	S	0	0
			3498	2288	584	609	17		
4	c	438	Total	C	N	O	S	0	0
			3431	2249	571	594	17		

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total	C	N	O	S	0	0
			2771	1828	456	475	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	d	337	Total	C	N	O	S	0	0
			2686	1777	439	458	12		

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	75	Total	C	N	O		0	0
			610	399	101	110			
6	e	71	Total	C	N	O		0	0
			575	376	94	105			

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total	C	N	O	S	0	0
			251	171	42	37	1		
7	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

- Molecule 8 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	68	Total	C	N	O	S	0	0
			519	347	77	93	2		
9	h	68	Total	C	N	O	S	0	0
			519	346	77	94	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	35	Total	C	N	O	S	0	0
			283	193	43	45	2		
10	i	34	Total	C	N	O	S	0	0
			275	189	41	43	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	209	43	45		
11	k	37	Total	C	N	O	0	0
			296	209	43	44		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	L	36	Total	C	N	O	0	0
			301	202	49	50		
12	l	37	Total	C	N	O	0	0
			306	205	50	51		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	30	Total	C	N	O	0	0
			230	158	32	40		
13	m	30	Total	C	N	O	0	0
			232	158	33	41		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		

- Molecule 15 is a protein called Oxygen-evolving enhancer protein 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	207	Total	C	N	O	S	0	0
			1565	1001	246	314	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S	250	Total	C	N	O	S	0	0
			1894	1225	310	355	4		

- Molecule 17 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		
17	t	27	Total	C	N	O	S	0	0
			220	154	30	35	1		

- Molecule 18 is a protein called Photosystem II reaction center protein Psb30.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	V	32	Total	C	N	O		0	0
			224	147	37	40			
18	v	32	Total	C	N	O		0	0
			224	147	37	40			

- Molecule 19 is a protein called Photosystem II reaction center W protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	56	Total	C	N	O	S	0	0
			434	281	70	81	2		

- Molecule 20 is a protein called Chloroplast photosystem II subunit X.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	X	32	Total	C	N	O		0	0
			214	140	35	39			
20	x	32	Total	C	N	O		0	0
			214	140	35	39			

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Y	220	Total	C	N	O	S	0	0
			1686	1100	271	310	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
22	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

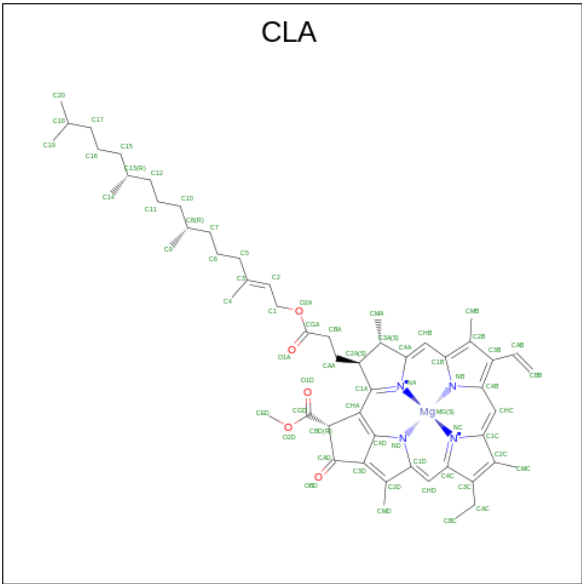
- Molecule 23 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	r	160	Total	C	N	O	S	0	0
			1235	795	208	227	5		

- Molecule 24 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 25 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	C	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	D	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	G	1	Total 43	C 35	Mg 1	N 4	O 3	0
25	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	G	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	N	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 42	C 34	Mg 1	N 4	O 3	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 50	C 40	Mg 1	N 4	O 5	0
25	S	1	Total 41	C 33	Mg 1	N 4	O 3	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	S	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	S	1	Total 48	C 38	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 58	C 48	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	Y	1	Total 54	C 44	Mg 1	N 4	O 5	0

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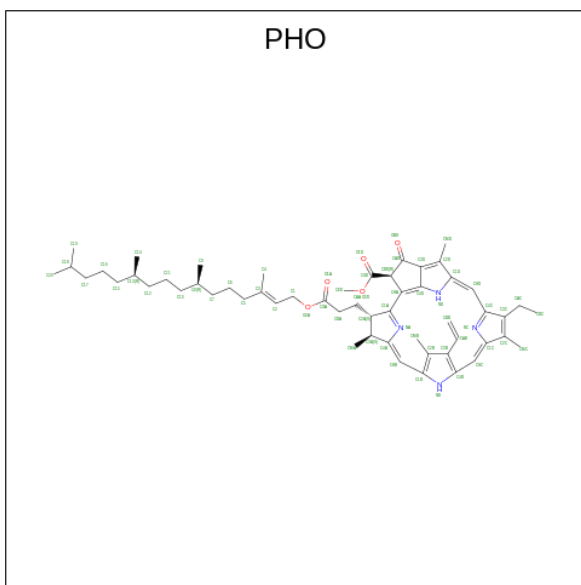
Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
25	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
25	c	1	Total 65	C 55	Mg 1	N 4	O 5	0

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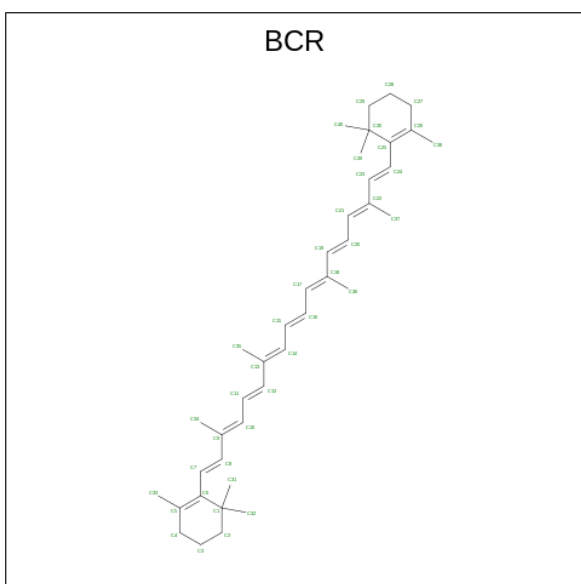
Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
25	c	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
25	d	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
25	r	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
25	r	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

- Molecule 26 is PHEOPHYTIN A (CCD ID: PHO) (formula: C₅₅H₇₄N₄O₅) (labeled as "Lig- and of Interest" by depositor).



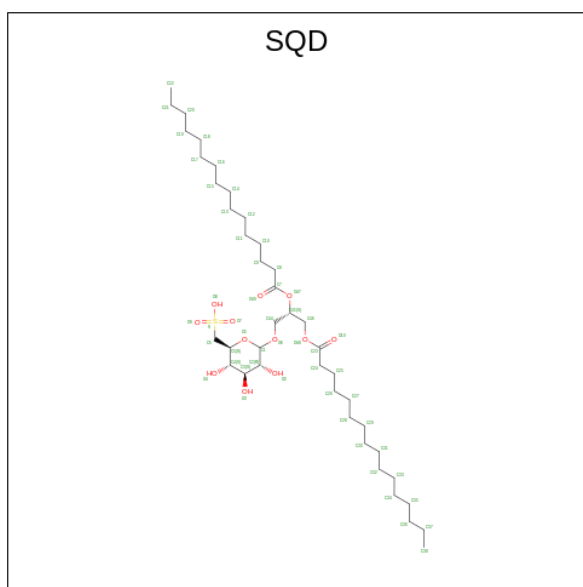
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	N	O	0
			64	55	4	5	
26	D	1	Total	C	N	O	0
			64	55	4	5	
26	a	1	Total	C	N	O	0
			64	55	4	5	
26	d	1	Total	C	N	O	0
			64	55	4	5	

- Molecule 27 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



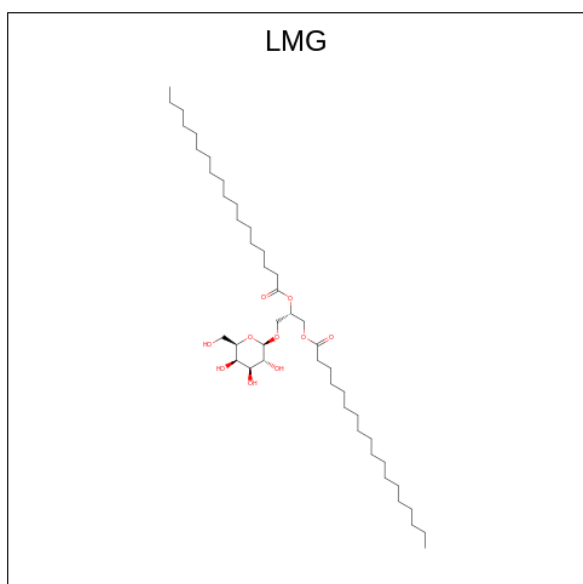
Mol	Chain	Residues	Atoms	AltConf
27	A	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	B	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	C	1	Total C 40 40	0
27	D	1	Total C 40 40	0
27	H	1	Total C 40 40	0
27	V	1	Total C 40 40	0
27	a	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	b	1	Total C 40 40	0
27	c	1	Total C 40 40	0
27	d	1	Total C 40 40	0
27	h	1	Total C 40 40	0
27	k	1	Total C 40 40	0
27	t	1	Total C 40 40	0
27	v	1	Total C 40 40	0
27	z	1	Total C 40 40	0

- Molecule 28 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).



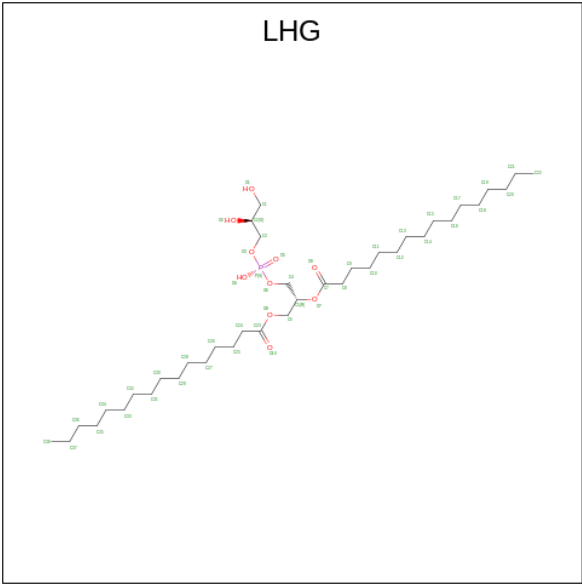
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	O	S	0
			51	38	12	1	
28	a	1	Total	C	O	S	0
			51	38	12	1	
28	t	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 29 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
29	B	1	Total	C	O	0
			51	41	10	
29	C	1	Total	C	O	0
			51	41	10	
29	D	1	Total	C	O	0
			46	36	10	
29	H	1	Total	C	O	0
			48	38	10	
29	W	1	Total	C	O	0
			48	38	10	
29	a	1	Total	C	O	0
			46	36	10	
29	b	1	Total	C	O	0
			42	32	10	
29	c	1	Total	C	O	0
			40	30	10	
29	d	1	Total	C	O	0
			41	31	10	
29	d	1	Total	C	O	0
			48	38	10	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



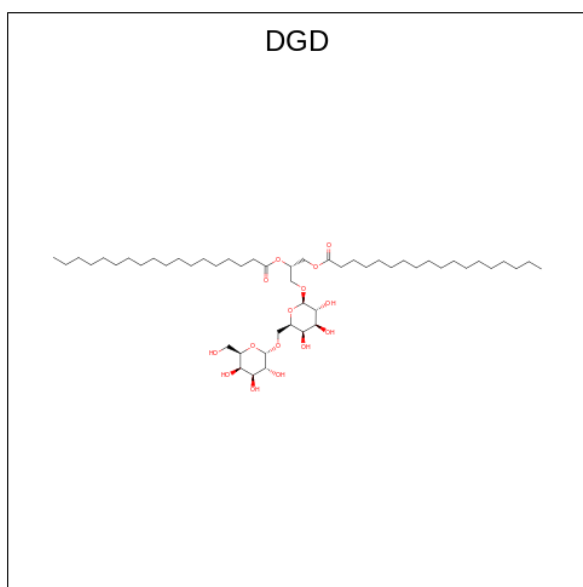
Mol	Chain	Residues	Atoms				AltConf
30	B	1	Total	C	O	P	0
			44	33	10	1	

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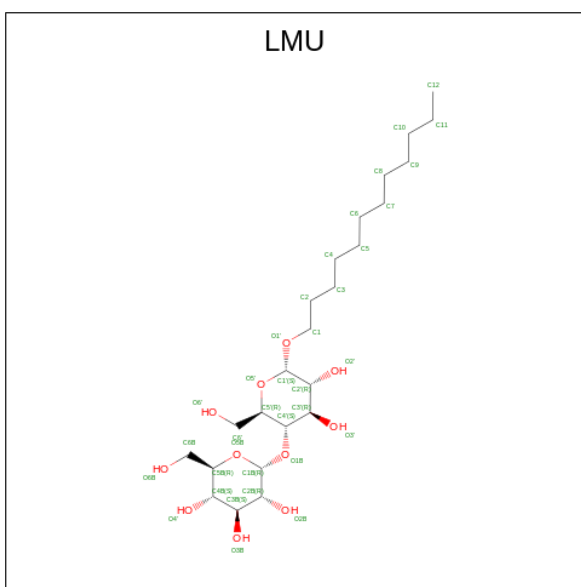
Mol	Chain	Residues	Atoms				AltConf
30	C	1	Total 47	C 36	O 10	P 1	0
30	D	1	Total 49	C 38	O 10	P 1	0
30	D	1	Total 39	C 28	O 10	P 1	0
30	G	1	Total 49	C 38	O 10	P 1	0
30	L	1	Total 49	C 38	O 10	P 1	0
30	N	1	Total 49	C 38	O 10	P 1	0
30	S	1	Total 45	C 34	O 10	P 1	0
30	Y	1	Total 49	C 38	O 10	P 1	0
30	a	1	Total 43	C 32	O 10	P 1	0
30	a	1	Total 44	C 33	O 10	P 1	0
30	b	1	Total 49	C 38	O 10	P 1	0
30	d	1	Total 44	C 33	O 10	P 1	0
30	d	1	Total 49	C 38	O 10	P 1	0
30	l	1	Total 49	C 38	O 10	P 1	0

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



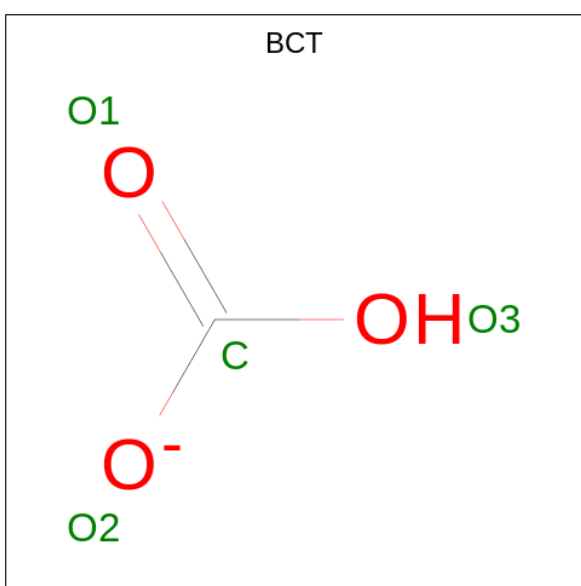
Mol	Chain	Residues	Atoms			AltConf
31	C	1	Total	C	O	0
			55	40	15	
31	C	1	Total	C	O	0
			62	47	15	
31	C	1	Total	C	O	0
			59	44	15	
31	W	1	Total	C	O	0
			66	51	15	
31	Y	1	Total	C	O	0
			66	51	15	
31	c	1	Total	C	O	0
			53	38	15	
31	c	1	Total	C	O	0
			49	34	15	
31	c	1	Total	C	O	0
			59	44	15	

- Molecule 32 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



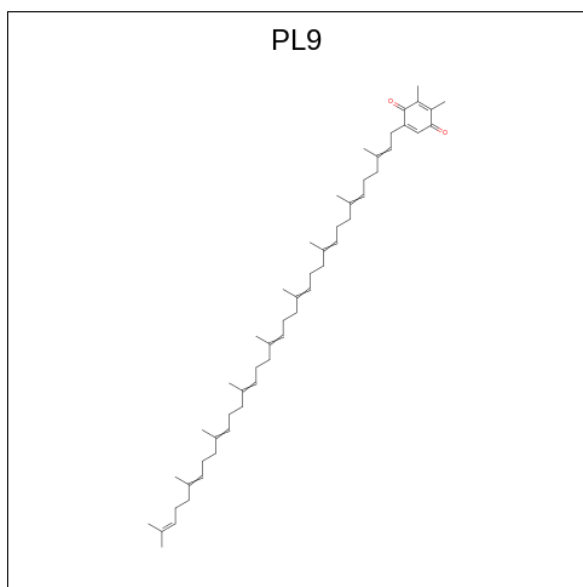
Mol	Chain	Residues	Atoms			AltConf
32	C	1	Total 35	C 24	O 11	0
32	C	1	Total 35	C 24	O 11	0
32	S	1	Total 35	C 24	O 11	0
32	c	1	Total 35	C 24	O 11	0

- Molecule 33 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3) (labeled as "Ligand of Interest" by depositor).



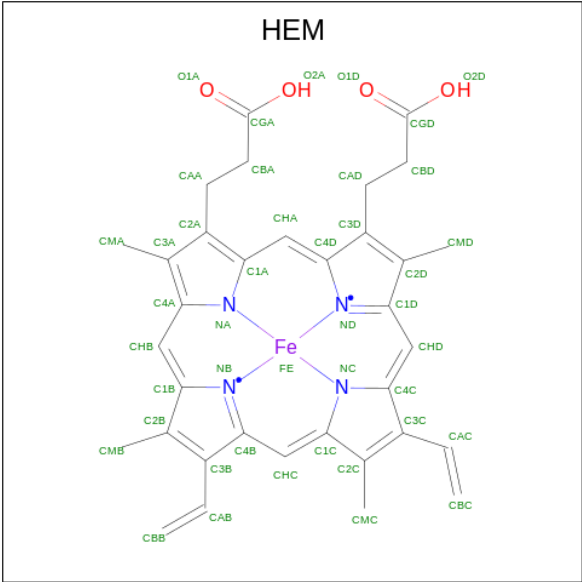
Mol	Chain	Residues	Atoms			AltConf
33	D	1	Total	C	O	0
			4	1	3	
33	a	1	Total	C	O	0
			4	1	3	

- Molecule 34 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: $C_{53}H_{80}O_2$) (labeled as "Ligand of Interest" by depositor).



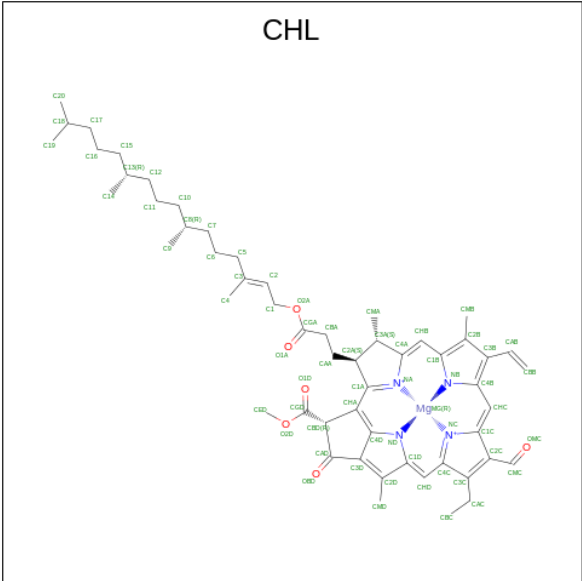
Mol	Chain	Residues	Atoms			AltConf
34	D	1	Total	C	O	0
			55	53	2	
34	d	1	Total	C	O	0
			55	53	2	

- Molecule 35 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
35	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
35	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 36 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



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

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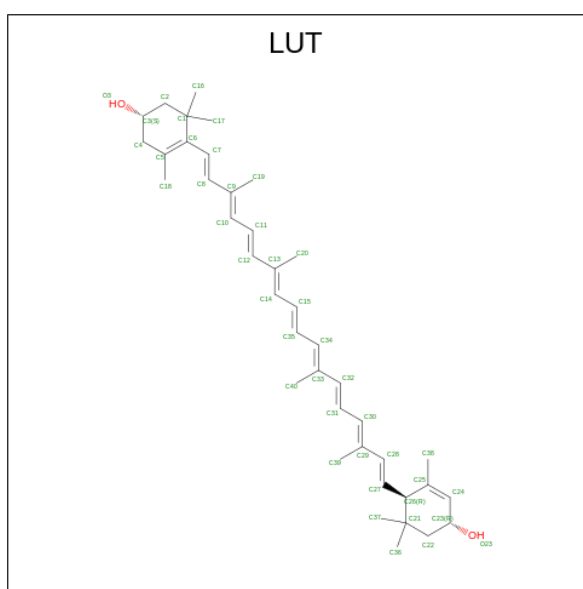
Mol	Chain	Residues	Atoms					AltConf
36	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
36	G	1	Total 43	C 34	Mg 1	N 4	O 4	0
36	G	1	Total 50	C 39	Mg 1	N 4	O 6	0
36	G	1	Total 44	C 35	Mg 1	N 4	O 4	0
36	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	G	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	N	1	Total 46	C 35	Mg 1	N 4	O 6	0
36	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	N	1	Total 50	C 39	Mg 1	N 4	O 6	0
36	N	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	S	1	Total 46	C 35	Mg 1	N 4	O 6	0
36	S	1	Total 44	C 35	Mg 1	N 4	O 4	0
36	S	1	Total 43	C 34	Mg 1	N 4	O 4	0
36	S	1	Total 49	C 38	Mg 1	N 4	O 6	0
36	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0
36	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
36	Y	1	Total 46	C 35	Mg 1	N 4	O 6	0
36	Y	1	Total 50	C 39	Mg 1	N 4	O 6	0
36	Y	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
36	r	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
36	r	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
36	r	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 37 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



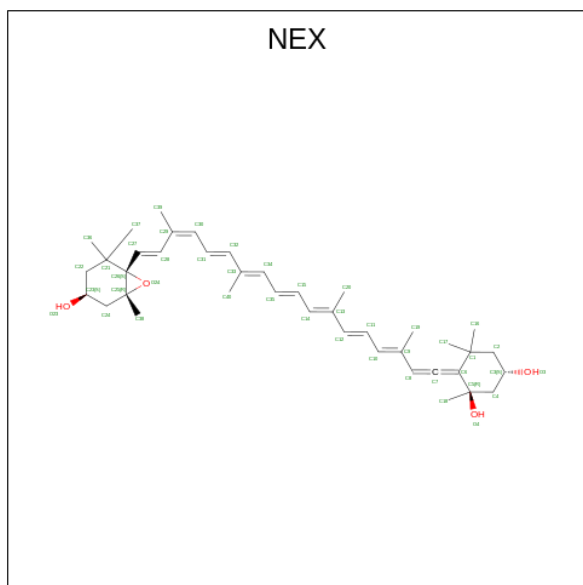
Mol	Chain	Residues	Atoms					AltConf
37	G	1	Total	C	O			0
			42	40	2			
37	G	1	Total	C	O			0
			42	40	2			
37	N	1	Total	C	O			0
			42	40	2			
37	N	1	Total	C	O			0
			42	40	2			
37	S	1	Total	C	O			0
			42	40	2			
37	S	1	Total	C	O			0
			42	40	2			
37	Y	1	Total	C	O			0
			42	40	2			

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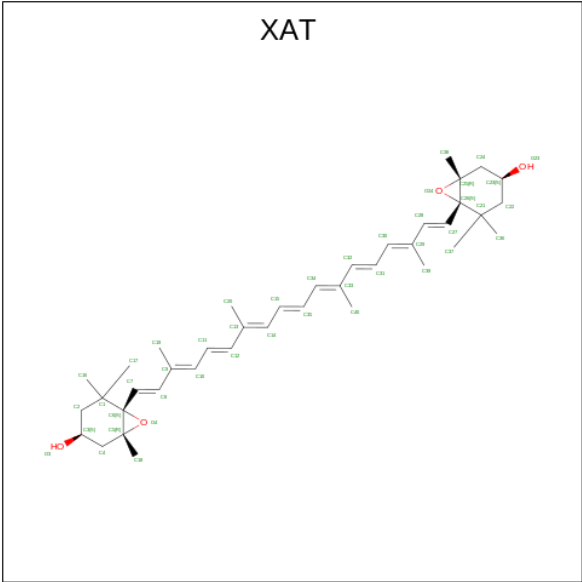
Mol	Chain	Residues	Atoms			AltConf
37	Y	1	Total	C	O	0
			42	40	2	

- Molecule 38 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
38	G	1	Total	C	O	0
			44	40	4	
38	N	1	Total	C	O	0
			44	40	4	
38	S	1	Total	C	O	0
			44	40	4	
38	Y	1	Total	C	O	0
			44	40	4	
38	r	1	Total	C	O	0
			44	40	4	

- Molecule 39 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA, BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).

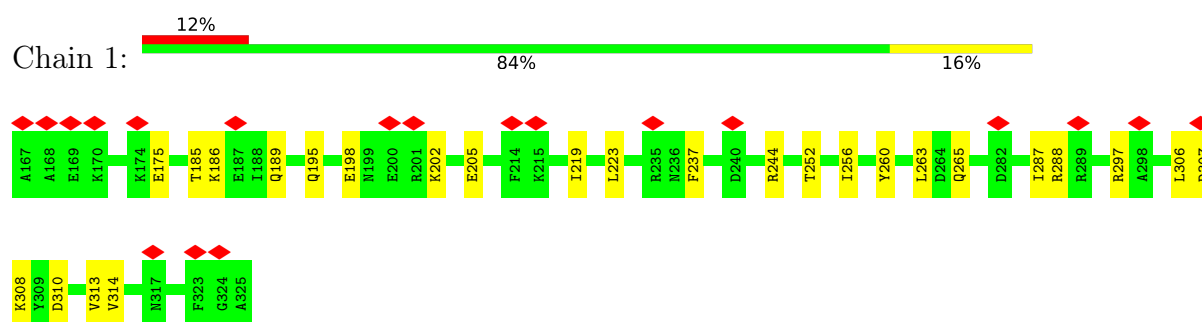


Mol	Chain	Residues	Atoms			AltConf
39	G	1	Total	C	O	0
			44	40	4	
39	N	1	Total	C	O	0
			44	40	4	
39	Y	1	Total	C	O	0
			44	40	4	
39	r	1	Total	C	O	0
			44	40	4	

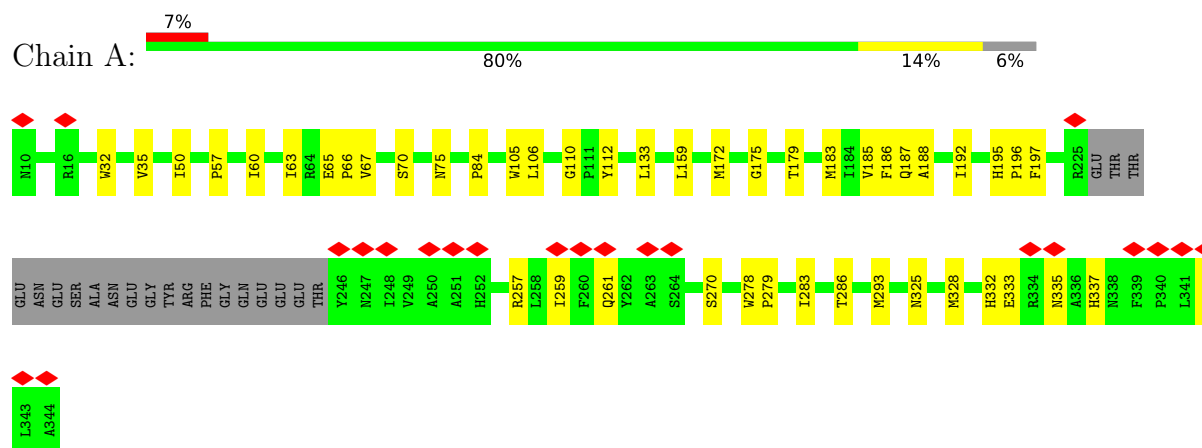
3 Residue-property plots [i](#)

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

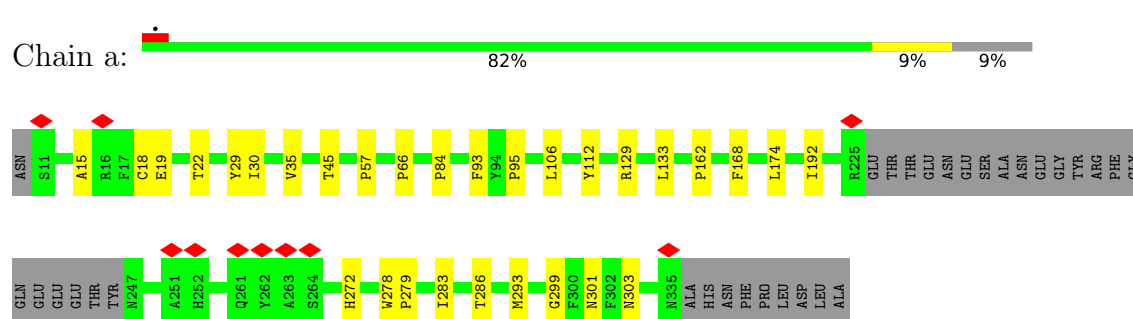
- Molecule 1: PDZ domain-containing protein



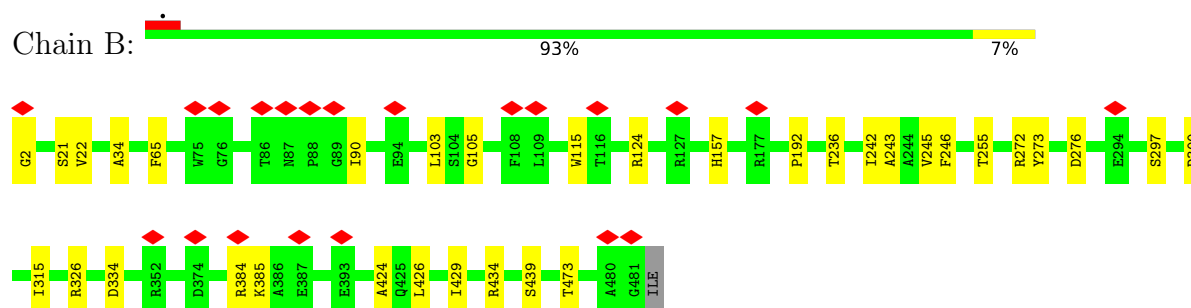
- Molecule 2: Photosystem II protein D1



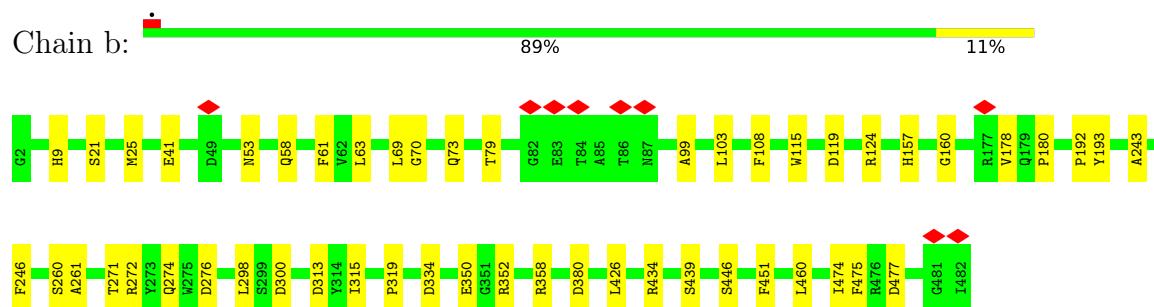
- Molecule 2: Photosystem II protein D1



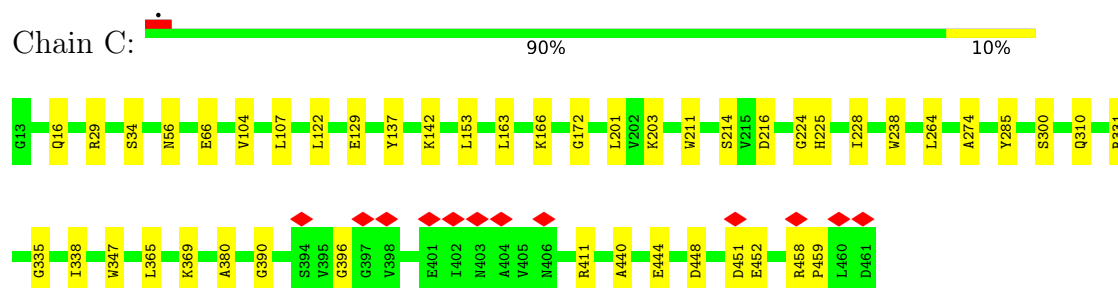
- Molecule 3: Photosystem II CP47 reaction center protein



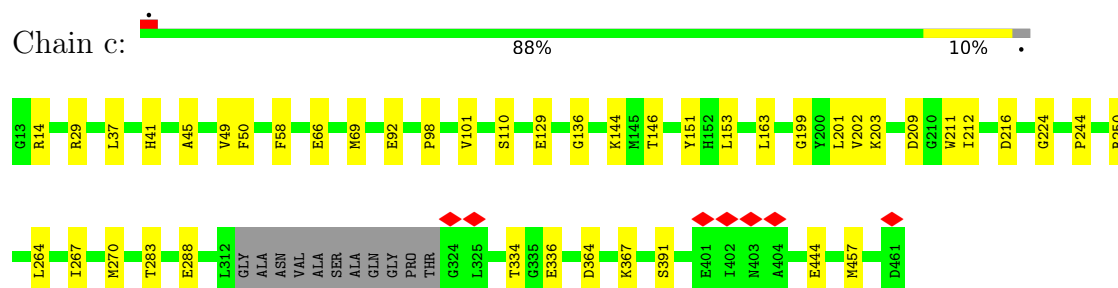
- Molecule 3: Photosystem II CP47 reaction center protein



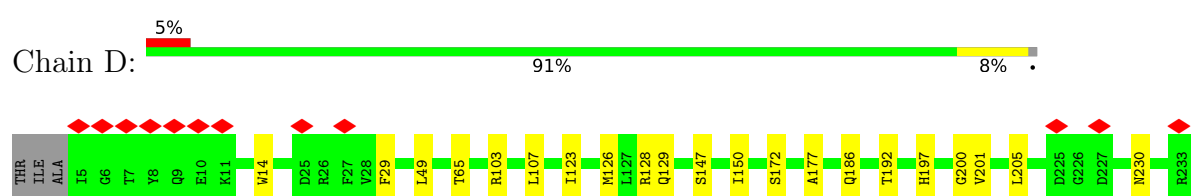
- Molecule 4: Photosystem II CP43 reaction center protein

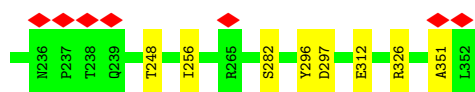


- Molecule 4: Photosystem II CP43 reaction center protein



- Molecule 5: Photosystem II D2 protein





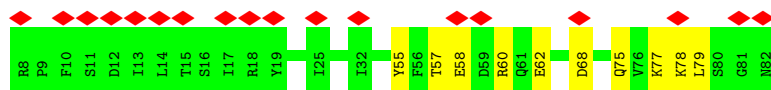
- Molecule 5: Photosystem II D2 protein

Chain d: 91% 5%



- Molecule 6: Cytochrome b559 subunit alpha

Chain E: 24% 87% 13%



- Molecule 6: Cytochrome b559 subunit alpha

Chain e: 88% 7% 5%



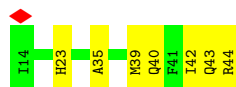
- Molecule 7: Cytochrome b559 subunit beta

Chain F: 6% 77% 23%



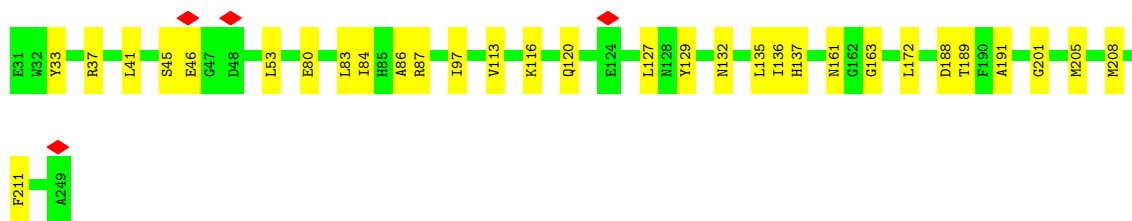
- Molecule 7: Cytochrome b559 subunit beta

Chain f: 77% 23%

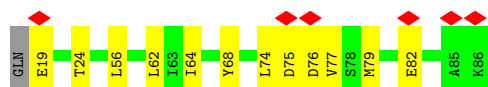
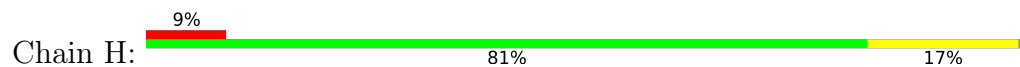


- Molecule 8: Chlorophyll a-b binding protein, chloroplastic

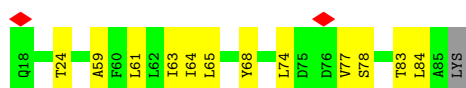
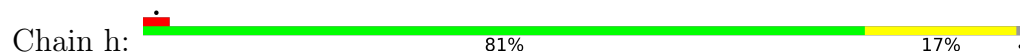
Chain G: 86% 14%



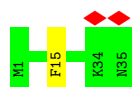
- Molecule 9: Photosystem II reaction center protein H



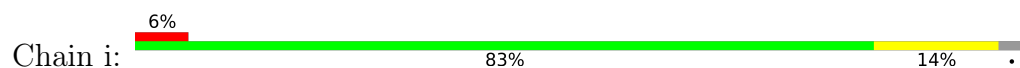
- Molecule 9: Photosystem II reaction center protein H



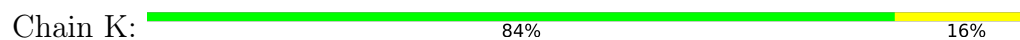
- Molecule 10: Photosystem II reaction center protein I



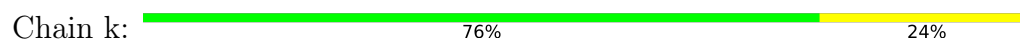
- Molecule 10: Photosystem II reaction center protein I

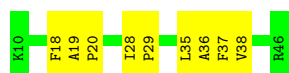


- Molecule 11: Photosystem II reaction center protein K

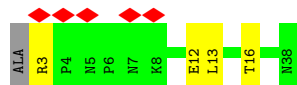
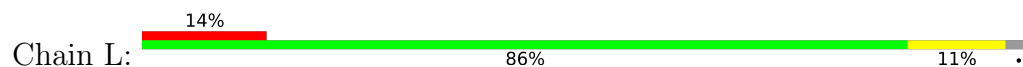


- Molecule 11: Photosystem II reaction center protein K

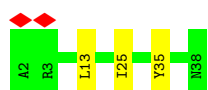




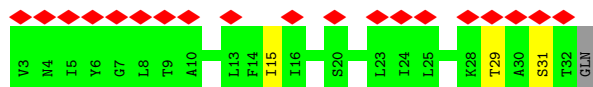
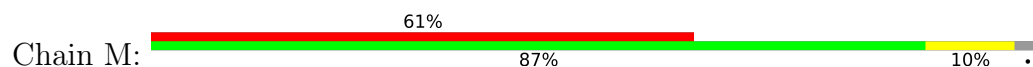
- Molecule 12: Photosystem II reaction center protein L



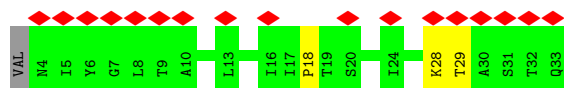
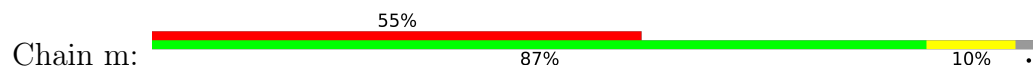
- Molecule 12: Photosystem II reaction center protein L



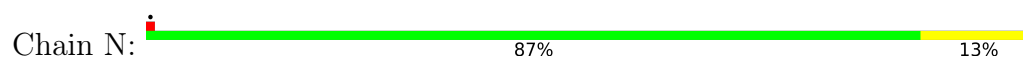
- Molecule 13: Photosystem II reaction center protein M



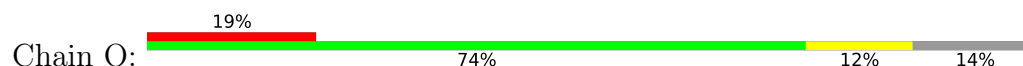
- Molecule 13: Photosystem II reaction center protein M

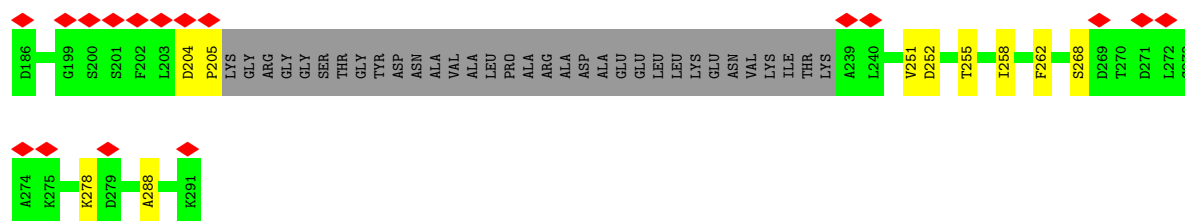


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



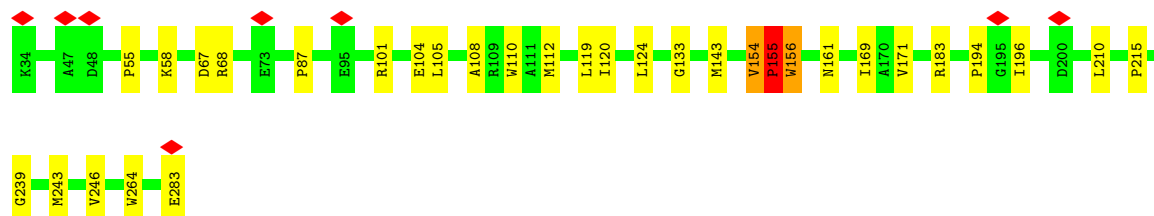
- Molecule 15: Oxygen-evolving enhancer protein 1, chloroplastic





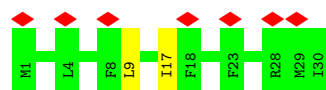
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain S: 87% 12%



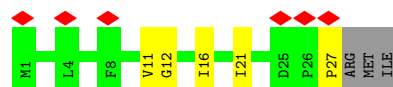
- Molecule 17: Photosystem II reaction center protein T

Chain T: 23% 93% 7%



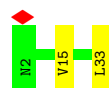
- Molecule 17: Photosystem II reaction center protein T

Chain t: 20% 73% 17% 10%



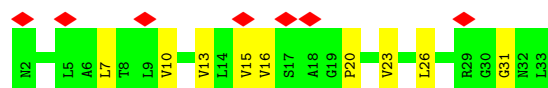
- Molecule 18: Photosystem II reaction center protein Psb30

Chain V: 94% 6%

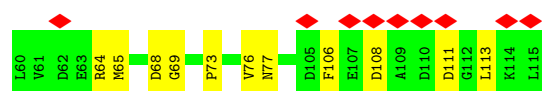
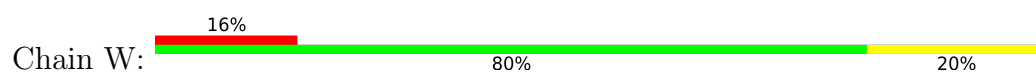


- Molecule 18: Photosystem II reaction center protein Psb30

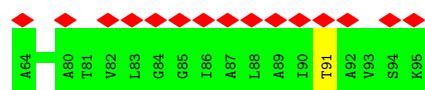
Chain v: 22% 72% 28%



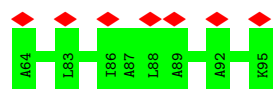
- Molecule 19: Photosystem II reaction center W protein, chloroplastic



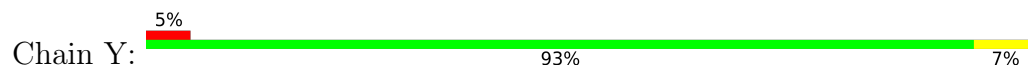
- Molecule 20: Chloroplast photosystem II subunit X



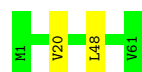
- Molecule 20: Chloroplast photosystem II subunit X



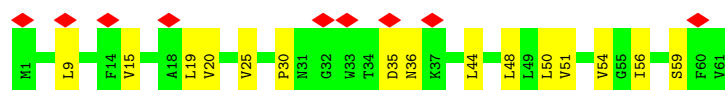
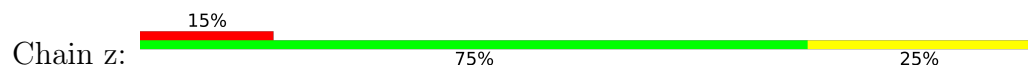
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



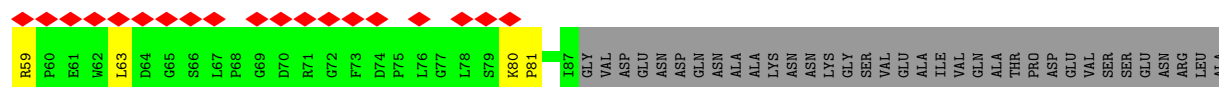
- Molecule 22: Photosystem II reaction center protein Z



- Molecule 22: Photosystem II reaction center protein Z



- Molecule 23: Chlorophyll a-b binding protein CP29



PRO	TYR	SER	GLU	VAL	PHE	G129	L130	A131	R132	F133	R134	E137	L138	G141	R142	W143	A144	M145	L146	G150	A151	L152	E155	A156	T157	T158	G159	W162	V163	E164	K167	V168	E169	L170	D171	G172	A173	G177	L178	P181	F182	S183	I184	T185	Q186	L187	I188	W189	I193	L194							
V195	G196	G197	A198	E199	F200	Y201	R202	N203	S204	E205	T206	N207	P208	E209	K210	R211	C212	Y213	P214	G215	G216	V217	F218	D219	P220	L221	K222	L223	A224	S225	E226	D227	E228	E229	R230	A231	F232	R233	L234	K235	T236	A237	E238	A242	R243	L244	F249	F250	G251	Y252	G253	V254	Q255	A256	L257	S258	T259

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97962	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	39.154	Depositor
Minimum map value	-20.689	Depositor
Average map value	0.008	Depositor
Map value standard deviation	1.163	Depositor
Recommended contour level	6.8	Depositor
Map size (\AA)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	1	0.11	0/1307	0.29	0/1755
2	A	0.16	0/2544	0.28	0/3470
2	a	0.18	0/2450	0.29	0/3340
3	B	0.14	0/3883	0.27	0/5286
3	b	0.17	0/3891	0.29	0/5297
4	C	0.15	0/3619	0.27	0/4931
4	c	0.15	0/3550	0.31	0/4834
5	D	0.16	0/2866	0.29	0/3909
5	d	0.17	0/2777	0.28	0/3787
6	E	0.12	0/628	0.29	0/857
6	e	0.13	0/591	0.29	0/807
7	F	0.12	0/258	0.27	0/349
7	f	0.15	0/258	0.26	0/349
8	G	0.14	0/1717	0.29	0/2337
9	H	0.13	0/530	0.28	0/725
9	h	0.31	0/530	0.46	0/726
10	I	0.14	0/291	0.23	0/394
10	i	0.15	0/283	0.32	0/383
11	K	0.17	0/309	0.32	0/425
11	k	0.17	0/308	0.41	0/425
12	L	0.12	0/309	0.21	0/420
12	l	0.15	0/314	0.25	0/427
13	M	0.13	0/234	0.25	0/321
13	m	0.14	0/236	0.30	0/323
14	N	0.14	0/1720	0.28	0/2341
15	O	0.11	0/1593	0.29	0/2150
16	S	0.16	0/1948	0.42	3/2653 (0.1%)
17	T	0.10	0/254	0.22	0/343
17	t	0.13	0/227	0.24	0/308
18	V	0.10	0/224	0.22	0/307
18	v	0.13	0/224	0.34	0/307
19	W	0.12	0/445	0.27	0/603

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	X	0.11	0/215	0.22	0/292
20	x	0.13	0/215	0.24	0/292
21	Y	0.14	0/1739	0.26	0/2364
22	Z	0.13	0/469	0.26	0/644
22	z	0.13	0/469	0.34	0/644
23	r	0.16	0/1264	0.39	2/1711 (0.1%)
All	All	0.15	0/44689	0.30	5/60836 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
16	S	0	1
23	r	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	S	155	PRO	CA-N-CD	-6.95	102.27	112.00
16	S	155	PRO	CA-C-N	5.51	132.07	121.54
16	S	155	PRO	C-N-CA	5.51	132.07	121.54
23	r	225	SER	CB-CA-C	-5.21	110.55	116.54
23	r	199	GLU	CA-CB-CG	5.17	124.45	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	S	154	VAL	Peptide
23	r	199	GLU	Sidechain

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	l	1285	0	1254	16	0
2	A	2465	0	2396	34	0
2	a	2375	0	2316	20	0
3	B	3755	0	3642	29	0
3	b	3763	0	3653	35	0
4	C	3498	0	3372	36	0
4	c	3431	0	3308	34	0
5	D	2771	0	2655	28	0
5	d	2686	0	2585	15	0
6	E	610	0	599	8	0
6	e	575	0	565	4	0
7	F	251	0	263	5	0
7	f	251	0	263	7	0
8	G	1667	0	1606	22	0
9	H	519	0	549	13	0
9	h	519	0	544	9	0
10	I	283	0	293	1	0
10	i	275	0	287	4	0
11	K	297	0	308	5	0
11	k	296	0	308	8	0
12	L	301	0	310	4	0
12	l	306	0	315	3	0
13	M	230	0	252	3	0
13	m	232	0	251	3	0
14	N	1672	0	1611	18	0
15	O	1565	0	1562	20	0
16	S	1894	0	1838	30	0
17	T	247	0	260	2	0
17	t	220	0	227	4	0
18	V	224	0	256	3	0
18	v	224	0	256	7	0
19	W	434	0	411	9	0
20	X	214	0	240	1	0
20	x	214	0	240	0	0
21	Y	1686	0	1623	11	0
22	Z	458	0	490	2	0
22	z	458	0	490	11	0
23	r	1235	0	1221	17	0
24	A	1	0	0	0	0
24	a	1	0	0	0	0
25	A	174	0	170	1	0
25	B	1040	0	1152	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	C	845	0	936	12	0
25	D	195	0	216	4	0
25	G	432	0	416	2	0
25	N	461	0	463	5	0
25	S	471	0	363	9	0
25	Y	502	0	535	0	0
25	a	174	0	170	2	0
25	b	1000	0	1074	19	0
25	c	808	0	861	14	0
25	d	172	0	175	4	0
25	r	241	0	193	3	0
26	A	64	0	74	2	0
26	D	64	0	74	1	0
26	a	64	0	74	2	0
26	d	64	0	74	1	0
27	A	40	0	56	5	0
27	B	80	0	112	6	0
27	C	120	0	168	12	0
27	D	40	0	56	3	0
27	H	40	0	56	5	0
27	V	40	0	56	4	0
27	a	40	0	56	2	0
27	b	120	0	168	4	0
27	c	40	0	56	4	0
27	d	40	0	56	2	0
27	h	40	0	56	5	0
27	k	40	0	56	4	0
27	t	40	0	56	3	0
27	v	40	0	56	8	0
27	z	40	0	56	3	0
28	A	51	0	69	2	0
28	a	51	0	69	0	0
28	t	54	0	78	0	0
29	B	51	0	72	2	0
29	C	51	0	72	0	0
29	D	46	0	62	0	0
29	H	48	0	66	2	0
29	W	48	0	66	1	0
29	a	46	0	62	0	0
29	b	42	0	54	0	0
29	c	40	0	46	0	0
29	d	89	0	118	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	B	44	0	61	1	0
30	C	47	0	67	0	0
30	D	88	0	122	2	0
30	G	49	0	74	0	0
30	L	49	0	74	1	0
30	N	49	0	74	1	0
30	S	45	0	63	2	0
30	Y	49	0	74	2	0
30	a	87	0	117	1	0
30	b	49	0	74	1	0
30	d	93	0	135	4	0
30	l	49	0	74	4	0
31	C	176	0	226	1	0
31	W	66	0	96	0	0
31	Y	66	0	96	1	0
31	c	161	0	196	3	0
32	C	70	0	92	3	0
32	S	35	0	46	0	0
32	c	35	0	46	0	0
33	D	4	0	0	0	0
33	a	4	0	0	2	0
34	D	55	0	80	0	0
34	d	55	0	80	1	0
35	F	43	0	30	5	0
35	f	43	0	30	4	0
36	G	378	0	336	9	0
36	N	360	0	348	13	0
36	S	182	0	125	10	0
36	Y	274	0	239	8	0
36	r	133	0	91	4	0
37	G	84	0	112	4	0
37	N	84	0	112	4	0
37	S	84	0	112	8	0
37	Y	84	0	112	6	0
38	G	44	0	56	3	0
38	N	44	0	56	1	0
38	S	44	0	56	1	0
38	Y	44	0	56	4	0
38	r	44	0	56	3	0
39	G	44	0	56	2	0
39	N	44	0	56	3	0
39	Y	44	0	56	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	r	44	0	56	3	0
All	All	55146	0	55711	611	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 6.

The worst 5 of 611 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)
8:G:208:MET:HE2	37:G:616:LUT:H10	1.55	0.89
2:A:185:VAL:HG13	2:A:332:HIS:HE1	1.37	0.89
35:f:101:HEM:HHC	35:f:101:HEM:HBB2	1.66	0.77
4:c:264:LEU:HD21	25:c:508:CLA:HAB	1.66	0.77
36:G:606:CHL:HHC	36:G:606:CHL:HBB1	1.66	0.76

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	157/159 (99%)	151 (96%)	6 (4%)	0	100	100
2	A	311/335 (93%)	304 (98%)	7 (2%)	0	100	100
2	a	300/335 (90%)	295 (98%)	5 (2%)	0	100	100
3	B	478/481 (99%)	472 (99%)	6 (1%)	0	100	100
3	b	479/481 (100%)	468 (98%)	11 (2%)	0	100	100
4	C	447/449 (100%)	440 (98%)	7 (2%)	0	100	100
4	c	434/449 (97%)	418 (96%)	16 (4%)	0	100	100
5	D	346/351 (99%)	341 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	d	333/351 (95%)	325 (98%)	8 (2%)	0	100	100
6	E	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
6	e	69/75 (92%)	67 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	f	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
8	G	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
9	H	66/69 (96%)	66 (100%)	0	0	100	100
9	h	66/69 (96%)	63 (96%)	3 (4%)	0	100	100
10	I	33/35 (94%)	33 (100%)	0	0	100	100
10	i	32/35 (91%)	31 (97%)	1 (3%)	0	100	100
11	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	35 (100%)	0	0	100	100
12	L	34/37 (92%)	34 (100%)	0	0	100	100
12	l	35/37 (95%)	35 (100%)	0	0	100	100
13	M	28/31 (90%)	28 (100%)	0	0	100	100
13	m	28/31 (90%)	28 (100%)	0	0	100	100
14	N	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	25	56
15	O	203/240 (85%)	197 (97%)	6 (3%)	0	100	100
16	S	248/250 (99%)	235 (95%)	11 (4%)	2 (1%)	16	45
17	T	28/30 (93%)	28 (100%)	0	0	100	100
17	t	25/30 (83%)	25 (100%)	0	0	100	100
18	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
18	v	30/32 (94%)	30 (100%)	0	0	100	100
19	W	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
20	X	30/32 (94%)	30 (100%)	0	0	100	100
20	x	30/32 (94%)	30 (100%)	0	0	100	100
21	Y	218/220 (99%)	213 (98%)	5 (2%)	0	100	100
22	Z	59/61 (97%)	59 (100%)	0	0	100	100
22	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
23	r	156/201 (78%)	148 (95%)	8 (5%)	0	100	100
All	All	5481/5736 (96%)	5351 (98%)	127 (2%)	3 (0%)	50	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	S	155	PRO
16	S	156	TRP
14	N	144	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	132/132 (100%)	132 (100%)	0	100	100
2	A	256/273 (94%)	256 (100%)	0	100	100
2	a	247/273 (90%)	247 (100%)	0	100	100
3	B	382/383 (100%)	382 (100%)	0	100	100
3	b	383/383 (100%)	383 (100%)	0	100	100
4	C	352/352 (100%)	352 (100%)	0	100	100
4	c	346/352 (98%)	346 (100%)	0	100	100
5	D	278/280 (99%)	278 (100%)	0	100	100
5	d	270/280 (96%)	270 (100%)	0	100	100
6	E	66/66 (100%)	66 (100%)	0	100	100
6	e	62/66 (94%)	62 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	f	25/25 (100%)	25 (100%)	0	100	100
8	G	164/164 (100%)	164 (100%)	0	100	100
9	H	58/59 (98%)	58 (100%)	0	100	100
9	h	58/59 (98%)	58 (100%)	0	100	100
10	I	32/32 (100%)	32 (100%)	0	100	100
10	i	31/32 (97%)	31 (100%)	0	100	100
11	K	31/31 (100%)	31 (100%)	0	100	100
11	k	31/31 (100%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	34/34 (100%)	34 (100%)	0	100	100
12	l	34/34 (100%)	34 (100%)	0	100	100
13	M	26/27 (96%)	26 (100%)	0	100	100
13	m	26/27 (96%)	26 (100%)	0	100	100
14	N	169/169 (100%)	169 (100%)	0	100	100
15	O	171/195 (88%)	171 (100%)	0	100	100
16	S	188/188 (100%)	188 (100%)	0	100	100
17	T	27/27 (100%)	27 (100%)	0	100	100
17	t	24/27 (89%)	24 (100%)	0	100	100
18	V	26/26 (100%)	26 (100%)	0	100	100
18	v	26/26 (100%)	26 (100%)	0	100	100
19	W	44/44 (100%)	44 (100%)	0	100	100
20	X	22/22 (100%)	22 (100%)	0	100	100
20	x	22/22 (100%)	22 (100%)	0	100	100
21	Y	169/169 (100%)	169 (100%)	0	100	100
22	Z	51/51 (100%)	51 (100%)	0	100	100
22	z	51/51 (100%)	51 (100%)	0	100	100
23	r	127/161 (79%)	127 (100%)	0	100	100
All	All	4466/4598 (97%)	4466 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
5	d	164	GLN
4	c	370	ASN
14	N	148	ASN
3	b	179	GLN
8	G	105	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 223 ligands modelled in this entry, 2 are monoatomic - leaving 221 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$
25	CLA	B	514	-	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
38	NEX	N	318	-	38,46,46	0.98	2 (5%)	50,70,70	2.26	12 (24%)
30	LHG	Y	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.05	3 (5%)
39	XAT	r	309	-	39,47,47	0.89	0	54,74,74	2.74	19 (35%)
25	CLA	C	511	4	65,73,73	1.51	6 (9%)	76,113,113	1.32	7 (9%)
25	CLA	B	509	-	65,73,73	1.51	5 (7%)	76,113,113	1.28	8 (10%)
25	CLA	a	403	-	49,57,73	1.72	7 (14%)	55,93,113	1.45	8 (14%)
25	CLA	b	502	-	65,73,73	1.49	6 (9%)	76,113,113	1.29	9 (11%)
27	BCR	h	101	-	41,41,41	0.72	0	56,56,56	2.03	13 (23%)
25	CLA	c	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.20	7 (9%)
25	CLA	S	613	16	49,57,73	1.77	7 (14%)	55,93,113	1.38	8 (14%)
36	CHL	N	308	-	66,74,74	1.89	15 (22%)	73,114,114	2.75	22 (30%)
30	LHG	l	101	-	48,48,48	0.92	2 (4%)	51,54,54	1.06	4 (7%)
37	LUT	N	316	-	42,43,43	0.77	0	51,60,60	1.63	12 (23%)
34	PL9	D	407	-	55,55,55	1.26	4 (7%)	68,69,69	1.54	13 (19%)
25	CLA	B	512	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
25	CLA	D	405	-	65,73,73	1.51	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	S	611	30	49,57,73	1.70	6 (12%)	55,93,113	1.44	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	Y	315	-	54,62,73	1.64	6 (11%)	62,99,113	1.34	7 (11%)
25	CLA	S	604	-	49,57,73	1.73	6 (12%)	55,93,113	1.43	8 (14%)
25	CLA	Y	304	21	65,73,73	1.48	6 (9%)	76,113,113	1.27	7 (9%)
27	BCR	H	101	-	41,41,41	0.73	0	56,56,56	2.01	14 (25%)
27	BCR	C	516	-	41,41,41	0.75	0	56,56,56	2.04	19 (33%)
27	BCR	d	405	-	41,41,41	0.76	1 (2%)	56,56,56	2.14	18 (32%)
27	BCR	v	101	-	41,41,41	0.75	0	56,56,56	2.52	19 (33%)
25	CLA	D	404	-	65,73,73	1.51	7 (10%)	76,113,113	1.29	9 (11%)
25	CLA	S	602	16	49,57,73	1.74	7 (14%)	55,93,113	1.38	9 (16%)
25	CLA	a	405	-	60,68,73	1.54	6 (10%)	70,107,113	1.35	7 (10%)
36	CHL	S	601	16	46,54,74	2.27	14 (30%)	49,90,114	3.29	20 (40%)
25	CLA	r	307	23	45,53,73	1.92	7 (15%)	52,89,113	1.40	7 (13%)
31	DGD	Y	301	-	67,67,67	0.84	2 (2%)	81,81,81	0.90	3 (3%)
25	CLA	b	514	-	45,53,73	1.80	6 (13%)	52,89,113	1.44	7 (13%)
30	LHG	S	618	25	44,44,48	0.95	2 (4%)	47,50,54	1.12	3 (6%)
29	LMG	D	410	-	46,46,55	0.97	2 (4%)	54,54,63	1.02	3 (5%)
32	LMU	c	519	-	36,36,36	1.16	2 (5%)	47,47,47	0.93	1 (2%)
36	CHL	Y	308	-	46,54,74	2.29	16 (34%)	49,90,114	3.24	18 (36%)
25	CLA	c	503	-	65,73,73	1.51	6 (9%)	76,113,113	1.32	8 (10%)
25	CLA	Y	305	-	65,73,73	1.50	6 (9%)	76,113,113	1.31	6 (7%)
28	SQD	A	407	-	50,51,54	1.20	4 (8%)	59,62,65	1.19	4 (6%)
27	BCR	V	101	-	41,41,41	0.79	1 (2%)	56,56,56	1.89	17 (30%)
25	CLA	B	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	7 (9%)
25	CLA	r	301	23	60,68,73	1.60	6 (10%)	70,107,113	1.30	7 (10%)
27	BCR	C	515	-	41,41,41	0.79	1 (2%)	56,56,56	1.94	16 (28%)
38	NEX	Y	318	-	38,46,46	0.96	1 (2%)	50,70,70	2.34	12 (24%)
34	PL9	d	406	-	55,55,55	1.27	5 (9%)	68,69,69	1.55	13 (19%)
26	PHO	D	402	-	51,69,69	1.00	4 (7%)	47,99,99	1.17	5 (10%)
29	LMG	d	410	-	48,48,55	0.94	2 (4%)	56,56,63	1.05	4 (7%)
25	CLA	Y	314	21	65,73,73	1.52	6 (9%)	76,113,113	1.29	7 (9%)
36	CHL	G	608	-	44,52,74	2.24	14 (31%)	46,87,114	3.25	18 (39%)
25	CLA	C	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.22	7 (9%)
25	CLA	c	501	-	65,73,73	1.53	7 (10%)	76,113,113	1.26	9 (11%)
25	CLA	b	501	-	65,73,73	1.53	7 (10%)	76,113,113	1.25	7 (9%)
28	SQD	a	407	-	50,51,54	1.20	4 (8%)	59,62,65	1.13	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LMG	C	520	-	51,51,55	0.93	2 (3%)	59,59,63	0.97	3 (5%)
25	CLA	S	610	16	49,57,73	1.72	7 (14%)	55,93,113	1.36	8 (14%)
25	CLA	C	507	-	65,73,73	1.48	6 (9%)	76,113,113	1.34	7 (9%)
29	LMG	H	102	-	48,48,55	0.97	2 (4%)	56,56,63	1.04	3 (5%)
36	CHL	r	304	-	44,52,74	2.25	14 (31%)	46,87,114	3.29	18 (39%)
25	CLA	A	402	-	65,73,73	1.51	7 (10%)	76,113,113	1.28	6 (7%)
25	CLA	C	504	-	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
36	CHL	N	310	14	66,74,74	1.93	15 (22%)	73,114,114	2.75	21 (28%)
25	CLA	B	501	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	7 (9%)
37	LUT	Y	317	-	42,43,43	0.80	0	51,60,60	1.68	11 (21%)
27	BCR	B	517	-	41,41,41	0.72	0	56,56,56	2.64	19 (33%)
30	LHG	L	101	-	48,48,48	0.93	2 (4%)	51,54,54	1.08	3 (5%)
25	CLA	G	613	8	65,73,73	1.51	5 (7%)	76,113,113	1.29	7 (9%)
25	CLA	d	404	-	42,50,73	1.86	6 (14%)	48,85,113	1.51	7 (14%)
37	LUT	S	616	-	42,43,43	0.82	0	51,60,60	1.74	17 (33%)
31	DGD	c	516	-	50,50,67	0.96	2 (4%)	64,64,81	1.04	3 (4%)
25	CLA	C	513	-	65,73,73	1.48	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	D	401	-	65,73,73	1.50	7 (10%)	76,113,113	1.35	10 (13%)
25	CLA	b	507	-	65,73,73	1.50	6 (9%)	76,113,113	1.27	8 (10%)
25	CLA	N	315	-	42,50,73	1.87	6 (14%)	48,85,113	1.36	7 (14%)
32	LMU	C	523	-	36,36,36	1.16	2 (5%)	47,47,47	0.98	2 (4%)
25	CLA	c	502	-	65,73,73	1.50	6 (9%)	76,113,113	1.34	9 (11%)
30	LHG	D	409	-	38,38,48	1.03	2 (5%)	41,44,54	1.09	2 (4%)
36	CHL	S	607	-	43,51,74	2.28	15 (34%)	45,86,114	3.33	18 (40%)
25	CLA	b	509	-	65,73,73	1.50	6 (9%)	76,113,113	1.30	8 (10%)
25	CLA	c	506	-	65,73,73	1.51	6 (9%)	76,113,113	1.27	8 (10%)
37	LUT	G	616	-	42,43,43	0.80	0	51,60,60	1.64	12 (23%)
25	CLA	C	502	-	65,73,73	1.50	8 (12%)	76,113,113	1.30	7 (9%)
25	CLA	B	508	-	65,73,73	1.51	6 (9%)	76,113,113	1.26	8 (10%)
25	CLA	c	512	-	56,64,73	1.63	7 (12%)	65,102,113	1.38	7 (10%)
30	LHG	b	521	-	48,48,48	0.93	2 (4%)	51,54,54	0.95	2 (3%)
25	CLA	G	614	-	42,50,73	1.85	6 (14%)	48,85,113	1.42	7 (14%)
31	DGD	c	517	-	60,60,67	0.88	2 (3%)	74,74,81	1.00	3 (4%)
32	LMU	S	619	-	36,36,36	1.15	2 (5%)	47,47,47	0.92	1 (2%)
25	CLA	S	612	16	45,53,73	1.79	6 (13%)	52,89,113	1.45	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	CHL	N	307	-	46,54,74	2.30	16 (34%)	49,90,114	3.21	18 (36%)
30	LHG	a	411	-	43,43,48	0.99	2 (4%)	46,49,54	1.02	3 (6%)
39	XAT	N	301	-	39,47,47	0.92	1 (2%)	54,74,74	2.73	20 (37%)
33	BCT	D	403	24	2,3,3	1.26	0	2,3,3	4.14	2 (100%)
36	CHL	G	619	-	66,74,74	1.90	15 (22%)	73,114,114	2.76	22 (30%)
31	DGD	C	519	-	60,60,67	0.89	2 (3%)	74,74,81	0.89	3 (4%)
27	BCR	b	517	-	41,41,41	0.75	1 (2%)	56,56,56	1.93	16 (28%)
25	CLA	c	507	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
29	LMG	W	201	-	48,48,55	0.95	2 (4%)	56,56,63	1.07	4 (7%)
25	CLA	Y	306	-	58,66,73	1.58	5 (8%)	67,104,113	1.38	9 (13%)
25	CLA	C	509	-	65,73,73	1.49	5 (7%)	76,113,113	1.33	6 (7%)
25	CLA	S	605	16	50,58,73	1.72	7 (14%)	58,95,113	1.43	8 (13%)
30	LHG	d	408	-	48,48,48	0.91	2 (4%)	51,54,54	1.07	3 (5%)
39	XAT	Y	302	-	39,47,47	0.92	1 (2%)	54,74,74	2.76	19 (35%)
25	CLA	S	609	16	41,49,73	1.89	7 (17%)	47,84,113	1.45	7 (14%)
27	BCR	k	101	-	41,41,41	0.74	1 (2%)	56,56,56	2.08	16 (28%)
25	CLA	G	603	-	65,73,73	1.52	7 (10%)	76,113,113	1.29	7 (9%)
28	SQD	t	102	-	53,54,54	1.18	4 (7%)	62,65,65	1.05	5 (8%)
38	NEX	r	310	-	38,46,46	0.99	1 (2%)	50,70,70	2.36	14 (28%)
25	CLA	N	313	14	45,53,73	1.83	7 (15%)	52,89,113	1.42	6 (11%)
26	PHO	a	404	-	51,69,69	1.02	4 (7%)	47,99,99	1.19	6 (12%)
36	CHL	G	606	-	43,51,74	2.24	15 (34%)	45,86,114	3.33	19 (42%)
27	BCR	b	519	-	41,41,41	0.75	0	56,56,56	2.01	15 (26%)
25	CLA	b	512	-	65,73,73	1.48	7 (10%)	76,113,113	1.39	7 (9%)
30	LHG	N	319	25	48,48,48	0.92	2 (4%)	51,54,54	1.06	3 (5%)
25	CLA	N	311	14	65,73,73	1.49	6 (9%)	76,113,113	1.22	7 (9%)
25	CLA	G	602	8	65,73,73	1.49	6 (9%)	76,113,113	1.27	7 (9%)
25	CLA	B	503	-	65,73,73	1.51	6 (9%)	76,113,113	1.26	7 (9%)
25	CLA	B	507	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	6 (7%)
25	CLA	G	612	8	43,51,73	1.83	7 (16%)	49,86,113	1.41	6 (12%)
25	CLA	C	512	-	65,73,73	1.53	7 (10%)	76,113,113	1.25	6 (7%)
25	CLA	a	402	-	65,73,73	1.50	7 (10%)	76,113,113	1.28	8 (10%)
36	CHL	Y	303	21	66,74,74	1.90	14 (21%)	73,114,114	2.73	22 (30%)
37	LUT	Y	316	-	42,43,43	0.77	0	51,60,60	1.67	13 (25%)
27	BCR	B	518	-	41,41,41	0.76	0	56,56,56	1.93	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	G	611	30	45,53,73	1.79	6 (13%)	52,89,113	1.47	6 (11%)
25	CLA	r	308	23	41,49,73	1.95	7 (17%)	47,84,113	1.48	6 (12%)
27	BCR	c	514	-	41,41,41	0.76	1 (2%)	56,56,56	1.97	14 (25%)
25	CLA	r	302	-	46,54,73	1.80	6 (13%)	53,90,113	1.47	7 (13%)
36	CHL	S	608	-	49,57,74	2.20	15 (30%)	52,93,114	3.13	20 (38%)
36	CHL	S	606	-	44,52,74	2.22	15 (34%)	46,87,114	3.32	19 (41%)
31	DGD	W	202	-	67,67,67	0.84	2 (2%)	81,81,81	0.96	5 (6%)
39	XAT	G	620	-	39,47,47	0.91	1 (2%)	54,74,74	4.21	23 (42%)
35	HEM	f	101	7,6	41,50,50	1.48	3 (7%)	45,82,82	1.44	6 (13%)
38	NEX	G	617	-	38,46,46	0.97	1 (2%)	50,70,70	2.40	15 (30%)
25	CLA	S	614	-	48,56,73	1.77	7 (14%)	55,92,113	1.36	8 (14%)
25	CLA	B	515	-	65,73,73	1.50	5 (7%)	76,113,113	1.25	6 (7%)
36	CHL	Y	310	21	66,74,74	1.95	15 (22%)	73,114,114	2.68	22 (30%)
25	CLA	b	506	-	65,73,73	1.50	6 (9%)	76,113,113	1.28	7 (9%)
25	CLA	b	515	-	65,73,73	1.50	7 (10%)	76,113,113	1.28	6 (7%)
35	HEM	F	101	7,6	41,50,50	1.55	6 (14%)	45,82,82	1.12	3 (6%)
25	CLA	G	610	8	65,73,73	1.51	5 (7%)	76,113,113	1.26	7 (9%)
25	CLA	Y	312	30	65,73,73	1.51	6 (9%)	76,113,113	1.28	8 (10%)
25	CLA	C	503	-	65,73,73	1.50	5 (7%)	76,113,113	1.28	8 (10%)
25	CLA	B	502	-	65,73,73	1.50	6 (9%)	76,113,113	1.29	8 (10%)
25	CLA	d	403	-	65,73,73	1.51	7 (10%)	76,113,113	1.34	9 (11%)
31	DGD	c	515	-	54,54,67	0.92	2 (3%)	68,68,81	1.03	4 (5%)
25	CLA	b	513	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
25	CLA	B	506	-	65,73,73	1.51	7 (10%)	76,113,113	1.26	8 (10%)
27	BCR	C	514	-	41,41,41	0.79	1 (2%)	56,56,56	1.89	14 (25%)
36	CHL	N	306	14	66,74,74	1.90	15 (22%)	73,114,114	2.74	21 (28%)
25	CLA	C	506	-	65,73,73	1.51	6 (9%)	76,113,113	1.29	9 (11%)
29	LMG	d	409	-	41,41,55	1.03	2 (4%)	49,49,63	1.08	3 (6%)
30	LHG	a	410	-	42,42,48	0.99	2 (4%)	45,48,54	1.12	2 (4%)
36	CHL	G	607	-	50,58,74	2.19	15 (30%)	52,94,114	3.17	20 (38%)
29	LMG	B	519	-	51,51,55	0.92	2 (3%)	59,59,63	1.00	3 (5%)
25	CLA	A	403	-	49,57,73	1.73	7 (14%)	55,93,113	1.45	8 (14%)
27	BCR	A	406	-	41,41,41	0.76	0	56,56,56	1.92	12 (21%)
36	CHL	N	302	14	66,74,74	1.91	15 (22%)	73,114,114	2.76	22 (30%)
29	LMG	b	520	-	42,42,55	1.00	2 (4%)	50,50,63	1.03	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	b	505	-	65,73,73	1.50	6 (9%)	76,113,113	1.25	7 (9%)
25	CLA	d	401	-	65,73,73	1.54	7 (10%)	76,113,113	1.33	10 (13%)
25	CLA	N	312	30	49,57,73	1.74	6 (12%)	55,93,113	1.39	6 (10%)
27	BCR	z	101	-	41,41,41	0.72	0	56,56,56	2.09	17 (30%)
30	LHG	G	618	25	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
25	CLA	b	516	-	45,53,73	1.78	7 (15%)	52,89,113	1.54	6 (11%)
25	CLA	B	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.32	6 (7%)
25	CLA	B	511	-	65,73,73	1.51	7 (10%)	76,113,113	1.29	9 (11%)
27	BCR	a	406	-	41,41,41	0.78	1 (2%)	56,56,56	1.91	17 (30%)
25	CLA	Y	311	21	65,73,73	1.51	6 (9%)	76,113,113	1.25	7 (9%)
29	LMG	a	408	-	46,46,55	0.98	2 (4%)	54,54,63	1.06	3 (5%)
29	LMG	c	518	-	39,39,55	1.05	2 (5%)	46,46,63	1.05	3 (6%)
36	CHL	r	306	-	46,54,74	2.29	15 (32%)	49,90,114	3.19	18 (36%)
37	LUT	G	615	-	42,43,43	0.77	0	51,60,60	1.67	13 (25%)
25	CLA	C	510	-	65,73,73	1.50	6 (9%)	76,113,113	1.35	8 (10%)
25	CLA	A	405	-	60,68,73	1.54	6 (10%)	70,107,113	1.37	9 (12%)
38	NEX	S	617	-	38,46,46	0.96	1 (2%)	50,70,70	2.31	13 (26%)
25	CLA	C	508	-	65,73,73	1.51	7 (10%)	76,113,113	1.27	7 (9%)
25	CLA	c	504	-	60,68,73	1.59	7 (11%)	70,107,113	1.29	8 (11%)
25	CLA	S	603	-	42,50,73	1.85	6 (14%)	48,85,113	1.52	8 (16%)
30	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	1.02	3 (5%)
25	CLA	N	304	-	65,73,73	1.51	7 (10%)	76,113,113	1.28	7 (9%)
25	CLA	b	504	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
37	LUT	N	317	-	42,43,43	0.82	0	51,60,60	1.72	13 (25%)
25	CLA	G	604	-	42,50,73	1.85	6 (14%)	48,85,113	1.46	7 (14%)
30	LHG	B	520	-	43,43,48	0.98	2 (4%)	46,49,54	1.06	3 (6%)
30	LHG	C	521	-	46,46,48	0.96	2 (4%)	49,52,54	1.01	3 (6%)
36	CHL	N	309	-	50,58,74	2.18	15 (30%)	52,94,114	3.16	19 (36%)
25	CLA	N	303	14	65,73,73	1.50	6 (9%)	76,113,113	1.30	9 (11%)
36	CHL	Y	307	21	46,54,74	2.29	15 (32%)	49,90,114	3.24	18 (36%)
25	CLA	c	510	-	65,73,73	1.52	6 (9%)	76,113,113	1.31	7 (9%)
25	CLA	b	510	-	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
33	BCT	a	409	24	2,3,3	1.27	0	2,3,3	4.16	1 (50%)
25	CLA	B	504	-	65,73,73	1.50	6 (9%)	76,113,113	1.36	10 (13%)
25	CLA	c	511	4	65,73,73	1.51	6 (9%)	76,113,113	1.34	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LUT	S	615	-	42,43,43	0.80	0	51,60,60	1.66	12 (23%)
25	CLA	b	511	-	65,73,73	1.50	8 (12%)	76,113,113	1.30	8 (10%)
36	CHL	G	601	8	66,74,74	1.90	15 (22%)	73,114,114	2.74	21 (28%)
36	CHL	r	305	-	43,51,74	2.30	14 (32%)	45,86,114	3.31	18 (40%)
30	LHG	d	407	-	43,43,48	0.96	2 (4%)	46,49,54	1.08	4 (8%)
25	CLA	N	314	14	65,73,73	1.52	6 (9%)	76,113,113	1.29	7 (9%)
25	CLA	b	503	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	6 (7%)
25	CLA	c	509	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
25	CLA	B	516	-	65,73,73	1.51	6 (9%)	76,113,113	1.30	6 (7%)
26	PHO	A	404	-	51,69,69	1.02	4 (7%)	47,99,99	1.12	5 (10%)
32	LMU	C	522	-	36,36,36	1.15	2 (5%)	47,47,47	0.96	1 (2%)
25	CLA	B	513	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	6 (7%)
25	CLA	c	513	-	42,50,73	1.83	5 (11%)	48,85,113	1.43	7 (14%)
31	DGD	C	518	-	63,63,67	0.88	2 (3%)	77,77,81	0.99	4 (5%)
36	CHL	G	605	8	43,51,74	2.27	14 (32%)	45,86,114	3.41	18 (40%)
36	CHL	Y	309	-	50,58,74	2.21	15 (30%)	52,94,114	3.09	19 (36%)
25	CLA	C	501	-	65,73,73	1.52	7 (10%)	76,113,113	1.26	7 (9%)
27	BCR	b	518	-	41,41,41	0.73	0	56,56,56	1.93	16 (28%)
36	CHL	G	609	8	66,74,74	1.92	15 (22%)	73,114,114	2.75	21 (28%)
27	BCR	t	101	-	41,41,41	0.72	1 (2%)	56,56,56	2.00	16 (28%)
31	DGD	C	517	-	56,56,67	0.90	2 (3%)	70,70,81	1.04	4 (5%)
25	CLA	N	305	-	65,73,73	1.51	6 (9%)	76,113,113	1.29	8 (10%)
27	BCR	D	406	-	41,41,41	0.74	0	56,56,56	2.06	20 (35%)
25	CLA	r	303	-	49,57,73	1.75	6 (12%)	55,93,113	1.43	8 (14%)
25	CLA	c	508	-	65,73,73	1.51	7 (10%)	76,113,113	1.25	7 (9%)
25	CLA	Y	313	21	65,73,73	1.50	6 (9%)	76,113,113	1.29	6 (7%)
25	CLA	b	508	-	65,73,73	1.52	7 (10%)	76,113,113	1.29	8 (10%)
26	PHO	d	402	-	51,69,69	1.01	4 (7%)	47,99,99	1.21	5 (10%)

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
25	CLA	B	514	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	NEX	N	318	-	-	2/27/83/83	0/3/3/3
30	LHG	Y	319	25	-	13/53/53/53	-
39	XAT	r	309	-	-	0/31/93/93	0/4/4/4
25	CLA	C	511	4	1/1/15/20	8/37/115/115	-
25	CLA	B	509	-	1/1/15/20	13/37/115/115	-
25	CLA	a	403	-	1/1/11/20	7/18/96/115	-
25	CLA	b	502	-	1/1/15/20	13/37/115/115	-
27	BCR	h	101	-	-	2/29/63/63	0/2/2/2
25	CLA	c	505	-	1/1/15/20	16/37/115/115	-
25	CLA	S	613	16	1/1/11/20	6/18/96/115	-
36	CHL	N	308	-	3/3/20/26	24/39/137/137	-
30	LHG	l	101	-	-	7/53/53/53	-
37	LUT	N	316	-	-	0/29/67/67	0/2/2/2
34	PL9	D	407	-	-	3/53/73/73	0/1/1/1
25	CLA	B	512	-	1/1/15/20	11/37/115/115	-
25	CLA	D	405	-	1/1/15/20	18/37/115/115	-
25	CLA	S	611	30	1/1/11/20	4/18/96/115	-
25	CLA	Y	315	-	1/1/12/20	5/24/102/115	-
25	CLA	S	604	-	1/1/11/20	6/18/96/115	-
25	CLA	Y	304	21	1/1/15/20	9/37/115/115	-
27	BCR	H	101	-	-	2/29/63/63	0/2/2/2
27	BCR	C	516	-	-	1/29/63/63	0/2/2/2
27	BCR	d	405	-	-	4/29/63/63	0/2/2/2
27	BCR	v	101	-	-	5/29/63/63	0/2/2/2
25	CLA	D	404	-	1/1/15/20	8/37/115/115	-
25	CLA	S	602	16	1/1/11/20	7/18/96/115	-
25	CLA	a	405	-	1/1/14/20	5/31/109/115	-
36	CHL	S	601	16	3/3/16/26	6/15/113/137	-
25	CLA	r	307	23	1/1/11/20	6/13/91/115	-
31	DGD	Y	301	-	-	9/55/95/95	0/2/2/2
25	CLA	b	514	-	1/1/11/20	4/13/91/115	-
30	LHG	S	618	25	-	8/49/49/53	-
29	LMG	D	410	-	-	6/41/61/70	0/1/1/1
32	LMU	c	519	-	-	6/21/61/61	0/2/2/2
36	CHL	Y	308	-	3/3/16/26	5/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	503	-	1/1/15/20	14/37/115/115	-
25	CLA	Y	305	-	1/1/15/20	17/37/115/115	-
28	SQD	A	407	-	-	7/46/66/69	0/1/1/1
27	BCR	V	101	-	-	4/29/63/63	0/2/2/2
25	CLA	B	505	-	1/1/15/20	8/37/115/115	-
25	CLA	r	301	23	1/1/14/20	7/31/109/115	-
27	BCR	C	515	-	-	6/29/63/63	0/2/2/2
38	NEX	Y	318	-	-	3/27/83/83	0/3/3/3
34	PL9	d	406	-	-	4/53/73/73	0/1/1/1
26	PHO	D	402	-	-	10/37/103/103	0/5/6/6
29	LMG	d	410	-	-	12/43/63/70	0/1/1/1
25	CLA	Y	314	21	1/1/15/20	13/37/115/115	-
36	CHL	G	608	-	3/3/15/26	3/13/111/137	-
25	CLA	C	505	-	1/1/15/20	9/37/115/115	-
25	CLA	c	501	-	1/1/15/20	15/37/115/115	-
25	CLA	b	501	-	1/1/15/20	17/37/115/115	-
28	SQD	a	407	-	-	5/46/66/69	0/1/1/1
29	LMG	C	520	-	-	5/46/66/70	0/1/1/1
25	CLA	S	610	16	1/1/11/20	5/18/96/115	-
25	CLA	C	507	-	1/1/15/20	5/37/115/115	-
29	LMG	H	102	-	-	8/43/63/70	0/1/1/1
36	CHL	r	304	-	3/3/15/26	3/13/111/137	-
25	CLA	A	402	-	1/1/15/20	12/37/115/115	-
25	CLA	C	504	-	1/1/15/20	9/37/115/115	-
36	CHL	N	310	14	3/3/20/26	14/39/137/137	-
25	CLA	B	501	-	1/1/15/20	11/37/115/115	-
37	LUT	Y	317	-	-	0/29/67/67	0/2/2/2
27	BCR	B	517	-	-	8/29/63/63	0/2/2/2
30	LHG	L	101	-	-	8/53/53/53	-
25	CLA	G	613	8	1/1/15/20	13/37/115/115	-
25	CLA	d	404	-	1/1/10/20	6/10/88/115	-
37	LUT	S	616	-	-	0/29/67/67	0/2/2/2
31	DGD	c	516	-	-	5/38/78/95	0/2/2/2
25	CLA	C	513	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	D	401	-	1/1/15/20	7/37/115/115	-
25	CLA	b	507	-	1/1/15/20	14/37/115/115	-
25	CLA	N	315	-	1/1/10/20	4/10/88/115	-
36	CHL	S	607	-	3/3/15/26	2/12/110/137	-
25	CLA	c	502	-	1/1/15/20	17/37/115/115	-
30	LHG	D	409	-	-	7/43/43/53	-
32	LMU	C	523	-	-	8/21/61/61	0/2/2/2
25	CLA	b	509	-	1/1/15/20	16/37/115/115	-
25	CLA	c	506	-	1/1/15/20	19/37/115/115	-
37	LUT	G	616	-	-	0/29/67/67	0/2/2/2
25	CLA	C	502	-	1/1/15/20	11/37/115/115	-
25	CLA	B	508	-	1/1/15/20	16/37/115/115	-
25	CLA	c	512	-	1/1/13/20	4/27/105/115	-
30	LHG	b	521	-	-	9/53/53/53	-
25	CLA	G	614	-	1/1/10/20	1/10/88/115	-
31	DGD	c	517	-	-	9/48/88/95	0/2/2/2
32	LMU	S	619	-	-	7/21/61/61	0/2/2/2
25	CLA	S	612	16	1/1/11/20	2/13/91/115	-
36	CHL	N	307	-	3/3/16/26	7/15/113/137	-
30	LHG	a	411	-	-	8/48/48/53	-
39	XAT	N	301	-	-	0/31/93/93	0/4/4/4
36	CHL	G	619	-	3/3/20/26	19/39/137/137	-
31	DGD	C	519	-	-	3/48/88/95	0/2/2/2
27	BCR	b	517	-	-	4/29/63/63	0/2/2/2
25	CLA	c	507	-	1/1/15/20	13/37/115/115	-
29	LMG	W	201	-	-	9/43/63/70	0/1/1/1
25	CLA	Y	306	-	1/1/13/20	6/29/107/115	-
25	CLA	C	509	-	1/1/15/20	9/37/115/115	-
25	CLA	S	605	16	1/1/12/20	6/19/97/115	-
30	LHG	d	408	-	-	7/53/53/53	-
39	XAT	Y	302	-	-	0/31/93/93	0/4/4/4
25	CLA	S	609	16	1/1/10/20	5/8/86/115	-
27	BCR	k	101	-	-	1/29/63/63	0/2/2/2
25	CLA	G	603	-	1/1/15/20	17/37/115/115	-
28	SQD	t	102	-	-	5/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	NEX	r	310	-	-	3/27/83/83	0/3/3/3
25	CLA	N	313	14	1/1/11/20	3/13/91/115	-
36	CHL	G	606	-	3/3/15/26	1/12/110/137	-
26	PHO	a	404	-	-	9/37/103/103	0/5/6/6
27	BCR	b	519	-	-	4/29/63/63	0/2/2/2
25	CLA	b	512	-	1/1/15/20	14/37/115/115	-
30	LHG	N	319	25	-	10/53/53/53	-
25	CLA	N	311	14	1/1/15/20	7/37/115/115	-
25	CLA	G	602	8	1/1/15/20	12/37/115/115	-
25	CLA	B	503	-	1/1/15/20	6/37/115/115	-
25	CLA	B	507	-	1/1/15/20	8/37/115/115	-
25	CLA	G	612	8	1/1/10/20	2/11/89/115	-
25	CLA	C	512	-	1/1/15/20	6/37/115/115	-
25	CLA	a	402	-	1/1/15/20	9/37/115/115	-
36	CHL	Y	303	21	3/3/20/26	18/39/137/137	-
37	LUT	Y	316	-	-	0/29/67/67	0/2/2/2
27	BCR	B	518	-	-	2/29/63/63	0/2/2/2
25	CLA	G	611	30	1/1/11/20	5/13/91/115	-
25	CLA	r	308	23	1/1/10/20	3/8/86/115	-
27	BCR	c	514	-	-	5/29/63/63	0/2/2/2
25	CLA	r	302	-	1/1/11/20	3/15/93/115	-
36	CHL	S	608	-	3/3/16/26	10/19/117/137	-
36	CHL	S	606	-	3/3/15/26	6/13/111/137	-
31	DGD	W	202	-	-	7/55/95/95	0/2/2/2
39	XAT	G	620	-	-	0/31/93/93	0/4/4/4
35	HEM	f	101	7,6	-	1/12/54/54	-
38	NEX	G	617	-	-	2/27/83/83	0/3/3/3
25	CLA	S	614	-	1/1/11/20	5/17/95/115	-
25	CLA	B	515	-	1/1/15/20	3/37/115/115	-
36	CHL	Y	310	21	3/3/20/26	19/39/137/137	-
25	CLA	b	506	-	1/1/15/20	17/37/115/115	-
25	CLA	b	515	-	1/1/15/20	14/37/115/115	-
35	HEM	F	101	7,6	-	0/12/54/54	-
25	CLA	G	610	8	1/1/15/20	8/37/115/115	-
25	CLA	Y	312	30	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	503	-	1/1/15/20	8/37/115/115	-
25	CLA	B	502	-	1/1/15/20	5/37/115/115	-
25	CLA	d	403	-	1/1/15/20	12/37/115/115	-
31	DGD	c	515	-	-	3/42/82/95	0/2/2/2
25	CLA	b	513	-	1/1/15/20	6/37/115/115	-
25	CLA	B	506	-	1/1/15/20	7/37/115/115	-
27	BCR	C	514	-	-	6/29/63/63	0/2/2/2
36	CHL	N	306	14	3/3/20/26	19/39/137/137	-
25	CLA	C	506	-	1/1/15/20	9/37/115/115	-
29	LMG	d	409	-	-	6/36/56/70	0/1/1/1
30	LHG	a	410	-	-	8/47/47/53	-
36	CHL	G	607	-	3/3/16/26	8/20/118/137	-
29	LMG	B	519	-	-	2/46/66/70	0/1/1/1
25	CLA	A	403	-	1/1/11/20	5/18/96/115	-
27	BCR	A	406	-	-	0/29/63/63	0/2/2/2
36	CHL	N	302	14	3/3/20/26	15/39/137/137	-
29	LMG	b	520	-	-	5/37/57/70	0/1/1/1
25	CLA	b	505	-	1/1/15/20	18/37/115/115	-
25	CLA	d	401	-	1/1/15/20	14/37/115/115	-
25	CLA	N	312	30	1/1/11/20	9/18/96/115	-
27	BCR	z	101	-	-	6/29/63/63	0/2/2/2
30	LHG	G	618	25	-	9/53/53/53	-
25	CLA	b	516	-	1/1/11/20	4/13/91/115	-
25	CLA	B	510	-	1/1/15/20	12/37/115/115	-
25	CLA	B	511	-	1/1/15/20	7/37/115/115	-
27	BCR	a	406	-	-	2/29/63/63	0/2/2/2
25	CLA	Y	311	21	1/1/15/20	7/37/115/115	-
29	LMG	a	408	-	-	5/41/61/70	0/1/1/1
29	LMG	c	518	-	-	5/32/52/70	0/1/1/1
36	CHL	r	306	-	3/3/16/26	5/15/113/137	-
37	LUT	G	615	-	-	0/29/67/67	0/2/2/2
25	CLA	C	510	-	1/1/15/20	14/37/115/115	-
25	CLA	A	405	-	1/1/14/20	4/31/109/115	-
38	NEX	S	617	-	-	3/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	C	508	-	1/1/15/20	10/37/115/115	-
25	CLA	c	504	-	1/1/14/20	8/31/109/115	-
25	CLA	S	603	-	1/1/10/20	2/10/88/115	-
30	LHG	D	408	-	-	10/53/53/53	-
25	CLA	N	304	-	1/1/15/20	10/37/115/115	-
25	CLA	b	504	-	1/1/15/20	17/37/115/115	-
37	LUT	N	317	-	-	0/29/67/67	0/2/2/2
25	CLA	G	604	-	1/1/10/20	2/10/88/115	-
36	CHL	Y	307	21	3/3/16/26	3/15/113/137	-
36	CHL	N	309	-	3/3/16/26	5/20/118/137	-
30	LHG	B	520	-	-	12/48/48/53	-
25	CLA	N	303	14	1/1/15/20	10/37/115/115	-
30	LHG	C	521	-	-	11/51/51/53	-
25	CLA	c	510	-	1/1/15/20	10/37/115/115	-
25	CLA	b	510	-	1/1/15/20	14/37/115/115	-
37	LUT	S	615	-	-	0/29/67/67	0/2/2/2
25	CLA	B	504	-	1/1/15/20	18/37/115/115	-
25	CLA	c	511	4	1/1/15/20	14/37/115/115	-
25	CLA	b	511	-	1/1/15/20	20/37/115/115	-
36	CHL	G	601	8	3/3/20/26	15/39/137/137	-
36	CHL	r	305	-	3/3/15/26	3/12/110/137	-
30	LHG	d	407	-	-	7/48/48/53	-
25	CLA	N	314	14	1/1/15/20	11/37/115/115	-
25	CLA	b	503	-	1/1/15/20	12/37/115/115	-
25	CLA	c	509	-	1/1/15/20	15/37/115/115	-
25	CLA	B	516	-	1/1/15/20	11/37/115/115	-
26	PHO	A	404	-	-	7/37/103/103	0/5/6/6
32	LMU	C	522	-	-	9/21/61/61	0/2/2/2
25	CLA	B	513	-	1/1/15/20	5/37/115/115	-
25	CLA	c	513	-	1/1/10/20	5/10/88/115	-
36	CHL	Y	309	-	3/3/16/26	7/20/118/137	-
36	CHL	G	605	8	3/3/15/26	2/12/110/137	-
31	DGD	C	518	-	-	10/51/91/95	0/2/2/2
25	CLA	C	501	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	CHL	G	609	8	3/3/20/26	19/39/137/137	-
27	BCR	b	518	-	-	2/29/63/63	0/2/2/2
27	BCR	t	101	-	-	6/29/63/63	0/2/2/2
31	DGD	C	517	-	-	6/44/84/95	0/2/2/2
25	CLA	N	305	-	1/1/15/20	13/37/115/115	-
27	BCR	D	406	-	-	2/29/63/63	0/2/2/2
25	CLA	r	303	-	1/1/11/20	9/18/96/115	-
25	CLA	c	508	-	1/1/15/20	13/37/115/115	-
25	CLA	Y	313	21	1/1/15/20	9/37/115/115	-
25	CLA	b	508	-	1/1/15/20	10/37/115/115	-
26	PHO	d	402	-	-	8/37/103/103	0/5/6/6

The worst 5 of 1194 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	308	CLA	C4B-NB	8.30	1.42	1.35
25	r	307	CLA	C4B-NB	8.16	1.42	1.35
25	r	301	CLA	C4B-NB	8.01	1.42	1.35
25	r	303	CLA	C4B-NB	7.89	1.42	1.35
25	d	401	CLA	C4B-NB	7.86	1.42	1.35

The worst 5 of 2053 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	G	620	XAT	C37-C21-C36	-16.15	83.54	107.37
39	G	620	XAT	C37-C21-C22	-13.76	85.08	108.98
27	B	517	BCR	C16-C17-C18	-9.63	113.57	127.31
36	G	605	CHL	C1D-ND-C4D	-9.02	99.93	106.33
36	S	601	CHL	C1D-ND-C4D	-8.88	100.03	106.33

5 of 184 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
25	A	402	CLA	ND
25	A	403	CLA	ND
25	A	405	CLA	ND
25	B	501	CLA	ND
25	B	502	CLA	ND

5 of 1697 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	B	501	CLA	CHA-CBD-CGD-O1D
25	B	501	CLA	CHA-CBD-CGD-O2D
25	B	501	CLA	CAD-CBD-CGD-O1D
25	B	504	CLA	C1A-C2A-CAA-CBA
25	B	504	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

152 monomers are involved in 298 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	514	CLA	2	0
38	N	318	NEX	1	0
30	Y	319	LHG	2	0
39	r	309	XAT	3	0
25	C	511	CLA	2	0
25	B	509	CLA	1	0
25	b	502	CLA	3	0
27	h	101	BCR	5	0
36	N	308	CHL	2	0
30	l	101	LHG	4	0
37	N	316	LUT	1	0
25	B	512	CLA	1	0
25	D	405	CLA	2	0
25	S	604	CLA	1	0
27	H	101	BCR	5	0
27	C	516	BCR	3	0
27	d	405	BCR	2	0
27	v	101	BCR	8	0
25	D	404	CLA	2	0
25	S	602	CLA	2	0
25	a	405	CLA	1	0
36	S	601	CHL	2	0
25	r	307	CLA	2	0
31	Y	301	DGD	1	0
30	S	618	LHG	2	0
36	Y	308	CHL	1	0
28	A	407	SQD	2	0
27	V	101	BCR	4	0
25	B	505	CLA	1	0
27	C	515	BCR	5	0
38	Y	318	NEX	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	d	406	PL9	1	0
26	D	402	PHO	1	0
29	d	410	LMG	2	0
36	G	608	CHL	3	0
25	c	501	CLA	2	0
25	b	501	CLA	1	0
25	S	610	CLA	1	0
29	H	102	LMG	2	0
36	r	304	CHL	1	0
25	A	402	CLA	1	0
25	C	504	CLA	2	0
36	N	310	CHL	2	0
25	B	501	CLA	2	0
37	Y	317	LUT	4	0
27	B	517	BCR	4	0
30	L	101	LHG	1	0
37	S	616	LUT	4	0
25	C	513	CLA	1	0
25	b	507	CLA	1	0
25	c	502	CLA	1	0
36	S	607	CHL	2	0
25	c	506	CLA	4	0
37	G	616	LUT	3	0
25	C	502	CLA	3	0
25	B	508	CLA	1	0
25	c	512	CLA	1	0
30	b	521	LHG	1	0
31	c	517	DGD	1	0
36	N	307	CHL	1	0
39	N	301	XAT	3	0
27	b	517	BCR	1	0
29	W	201	LMG	1	0
25	C	509	CLA	1	0
25	S	605	CLA	3	0
30	d	408	LHG	1	0
39	Y	302	XAT	6	0
25	S	609	CLA	2	0
27	k	101	BCR	4	0
38	r	310	NEX	3	0
25	N	313	CLA	1	0
26	a	404	PHO	2	0
36	G	606	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	b	519	BCR	2	0
25	b	512	CLA	2	0
30	N	319	LHG	1	0
25	G	602	CLA	1	0
25	B	503	CLA	1	0
25	C	512	CLA	1	0
25	a	402	CLA	1	0
36	Y	303	CHL	2	0
37	Y	316	LUT	2	0
27	B	518	BCR	2	0
25	G	611	CLA	1	0
25	r	308	CLA	1	0
27	c	514	BCR	4	0
36	S	608	CHL	2	0
36	S	606	CHL	4	0
39	G	620	XAT	2	0
35	f	101	HEM	4	0
38	G	617	NEX	3	0
25	B	515	CLA	1	0
36	Y	310	CHL	3	0
25	b	506	CLA	4	0
35	F	101	HEM	5	0
25	B	502	CLA	3	0
25	d	403	CLA	2	0
31	c	515	DGD	2	0
25	B	506	CLA	4	0
27	C	514	BCR	4	0
36	N	306	CHL	4	0
25	C	506	CLA	1	0
29	d	409	LMG	2	0
30	a	410	LHG	1	0
36	G	607	CHL	1	0
29	B	519	LMG	2	0
27	A	406	BCR	5	0
36	N	302	CHL	2	0
25	b	505	CLA	2	0
25	d	401	CLA	2	0
25	N	312	CLA	1	0
27	z	101	BCR	3	0
25	b	516	CLA	1	0
27	a	406	BCR	2	0
36	r	306	CHL	2	0

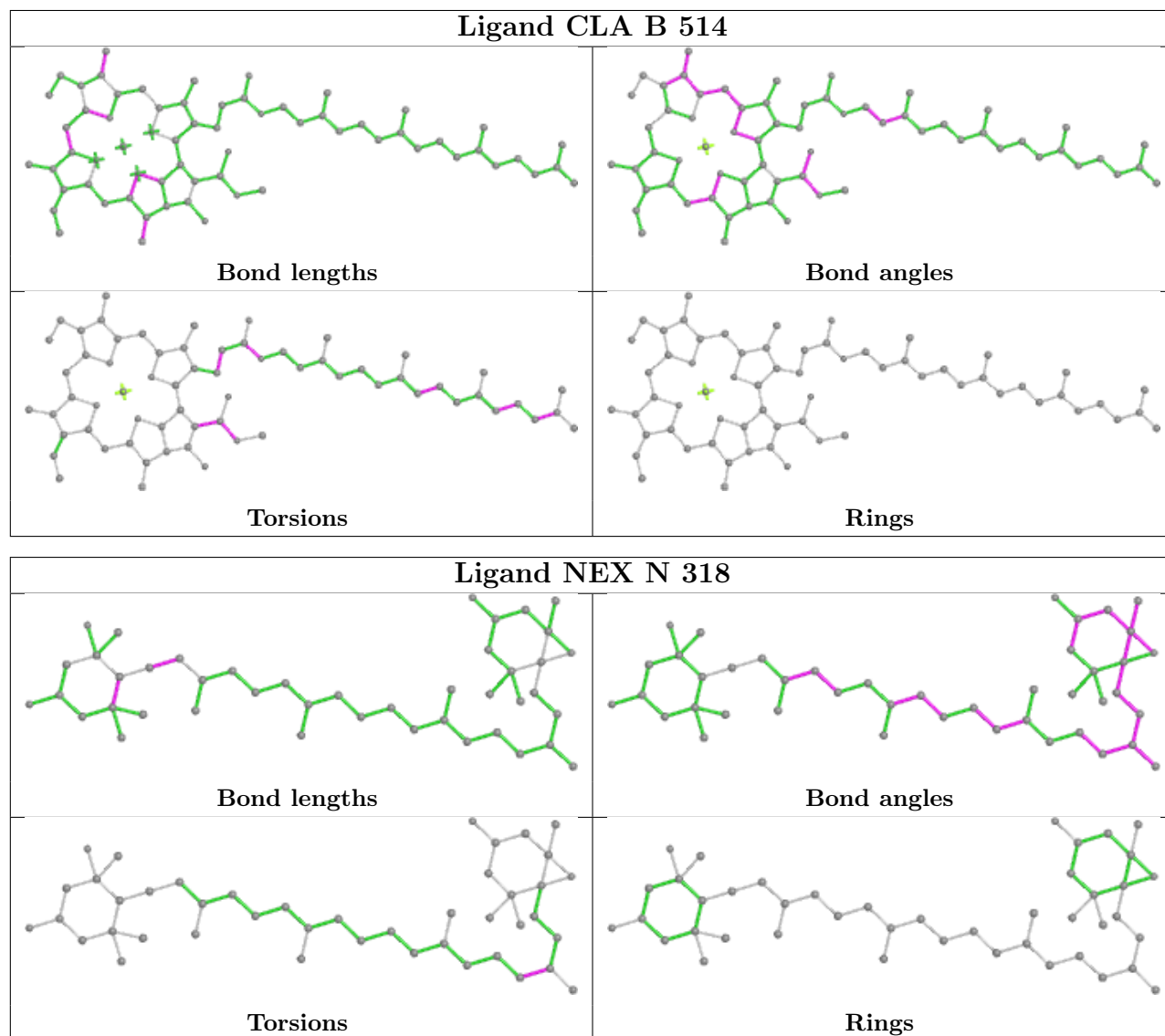
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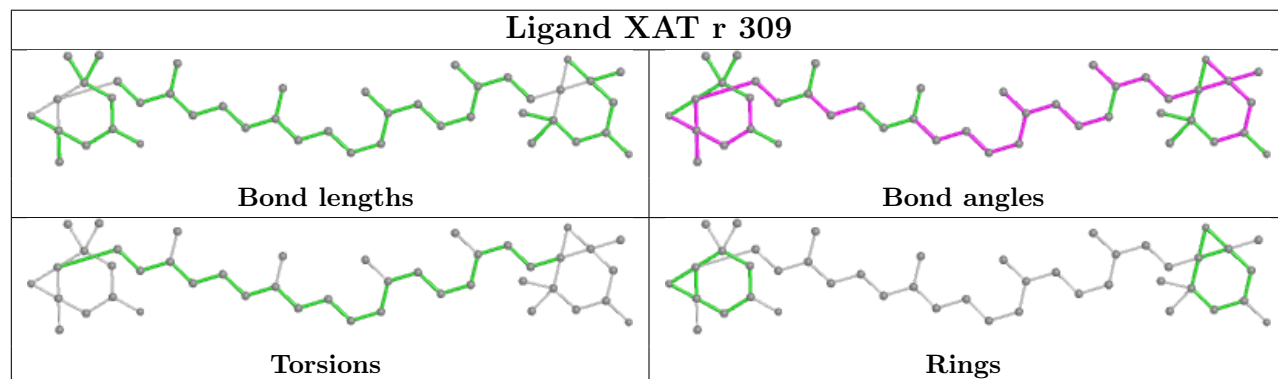
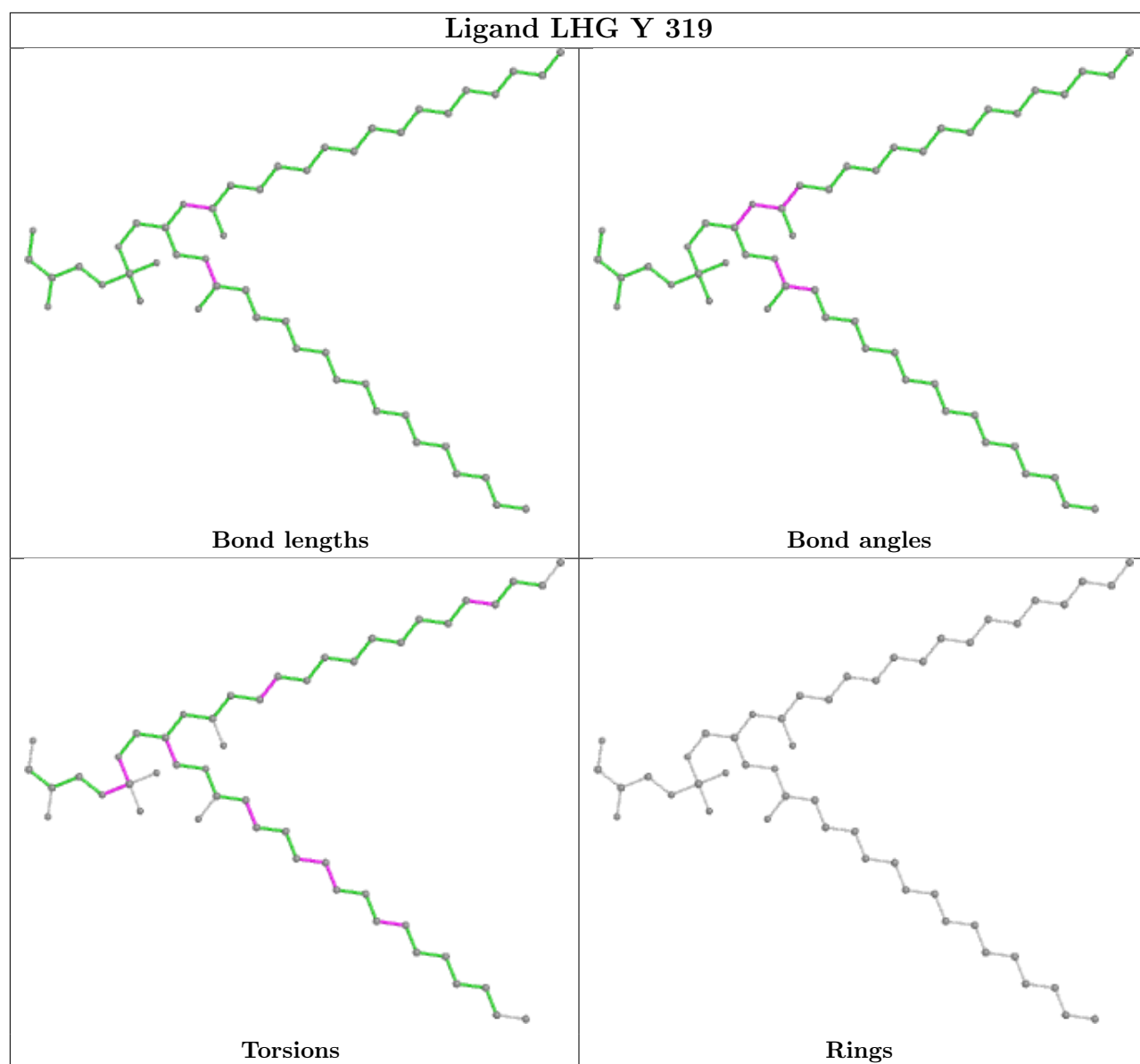
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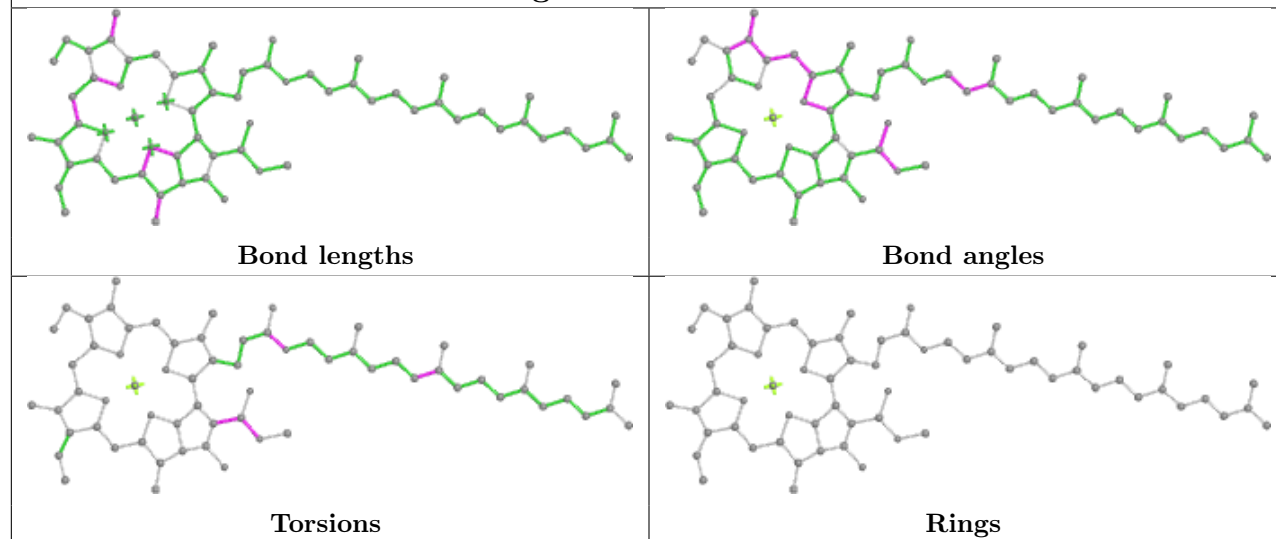
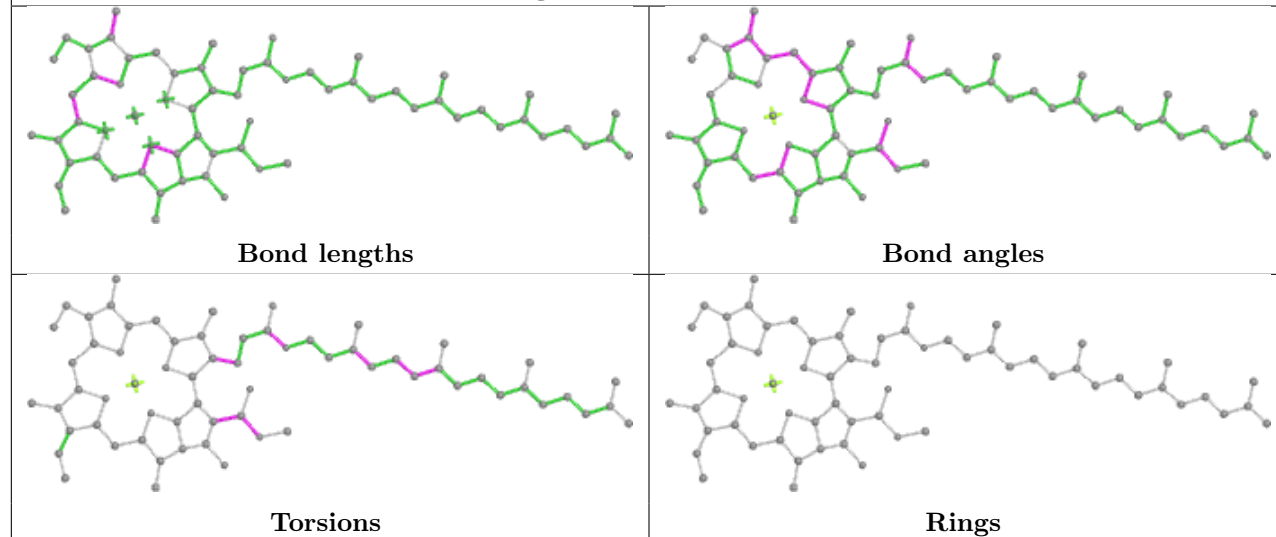
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	G	615	LUT	1	0
38	S	617	NEX	1	0
25	C	508	CLA	1	0
25	c	504	CLA	1	0
30	D	408	LHG	2	0
25	b	504	CLA	2	0
37	N	317	LUT	3	0
30	B	520	LHG	1	0
36	N	309	CHL	2	0
25	N	303	CLA	1	0
25	c	510	CLA	1	0
25	b	510	CLA	2	0
33	a	409	BCT	2	0
25	B	504	CLA	2	0
25	c	511	CLA	2	0
37	S	615	LUT	4	0
25	b	511	CLA	2	0
36	G	601	CHL	1	0
36	r	305	CHL	1	0
30	d	407	LHG	3	0
25	b	503	CLA	1	0
25	c	509	CLA	1	0
25	B	516	CLA	2	0
26	A	404	PHO	2	0
32	C	522	LMU	3	0
25	B	513	CLA	1	0
36	G	605	CHL	1	0
36	Y	309	CHL	2	0
25	C	501	CLA	1	0
27	b	518	BCR	1	0
36	G	609	CHL	1	0
27	t	101	BCR	3	0
31	C	517	DGD	1	0
25	N	305	CLA	3	0
27	D	406	BCR	3	0
25	c	508	CLA	2	0
26	d	402	PHO	1	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.

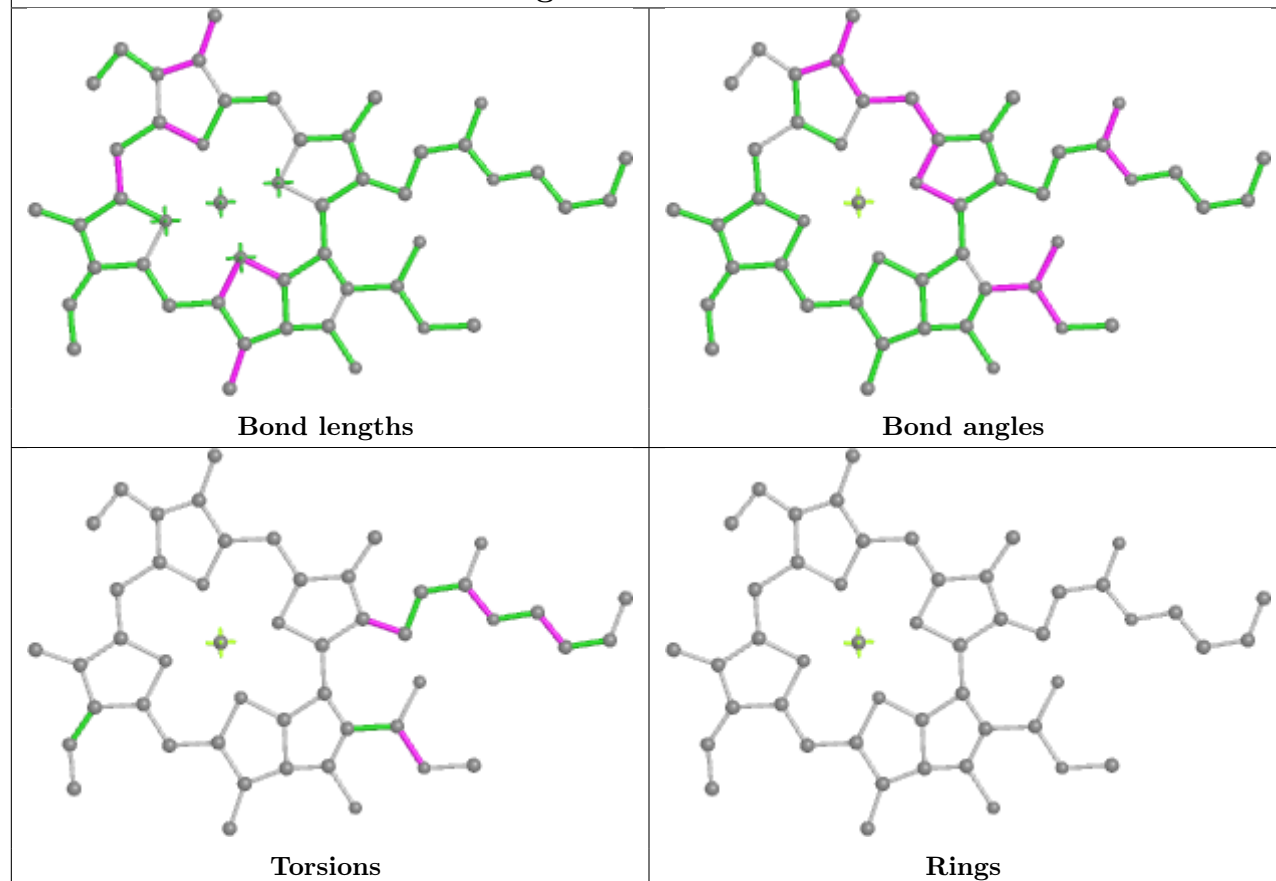
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



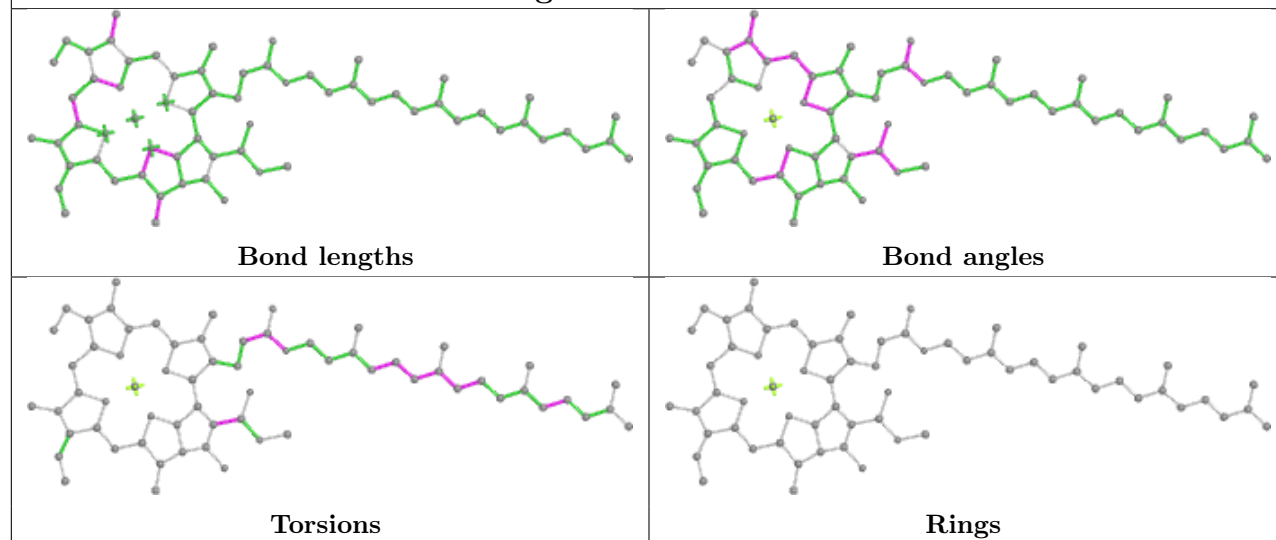


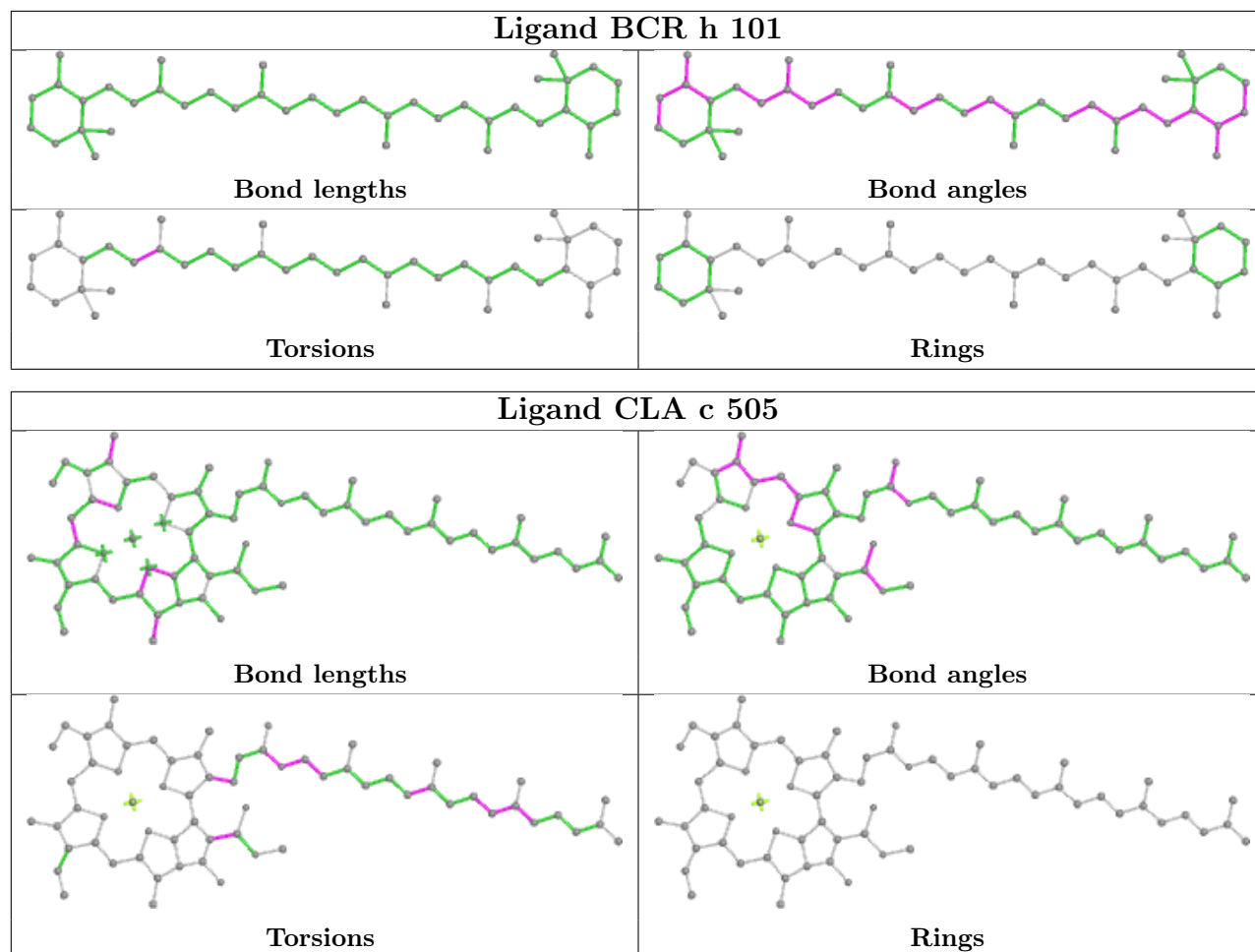
Ligand CLA C 511**Ligand CLA B 509**

Ligand CLA a 403

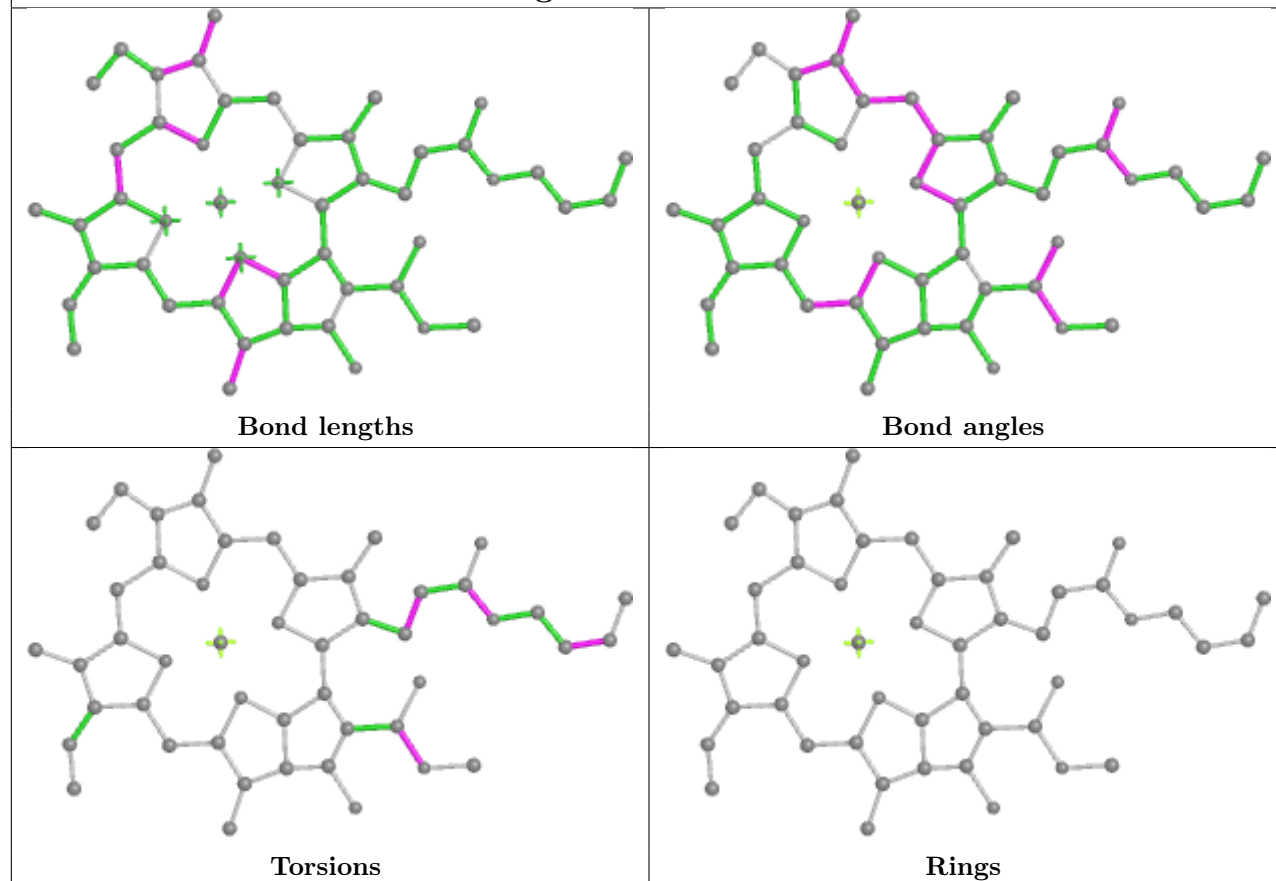


Ligand CLA b 502

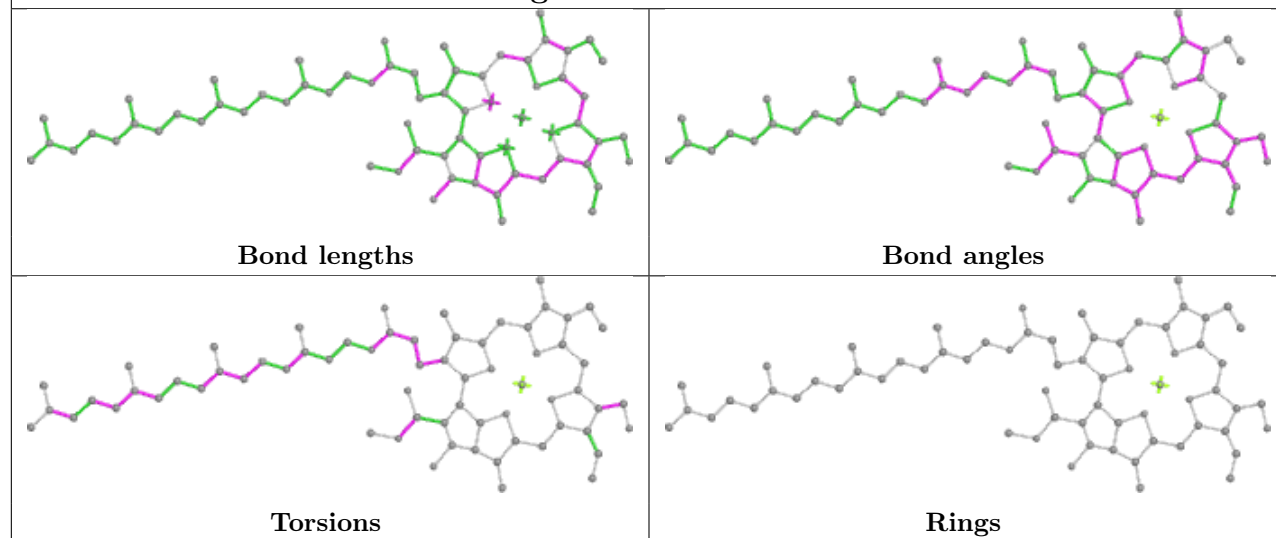


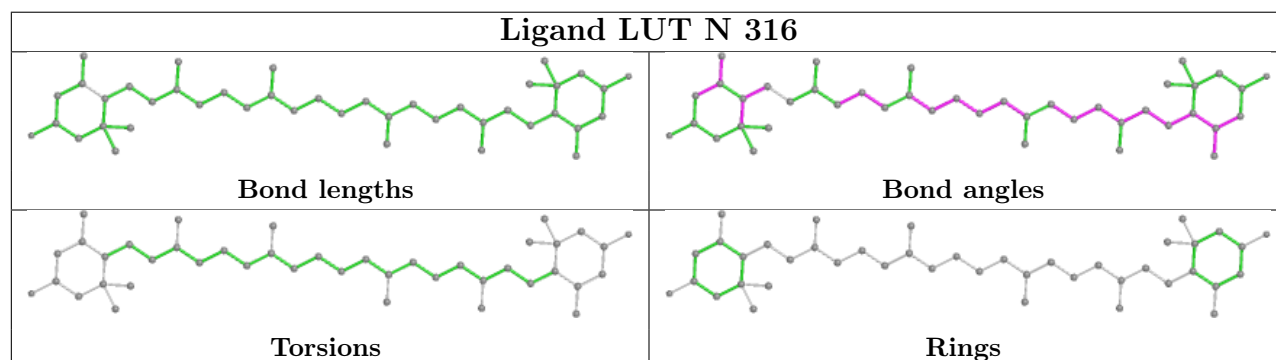
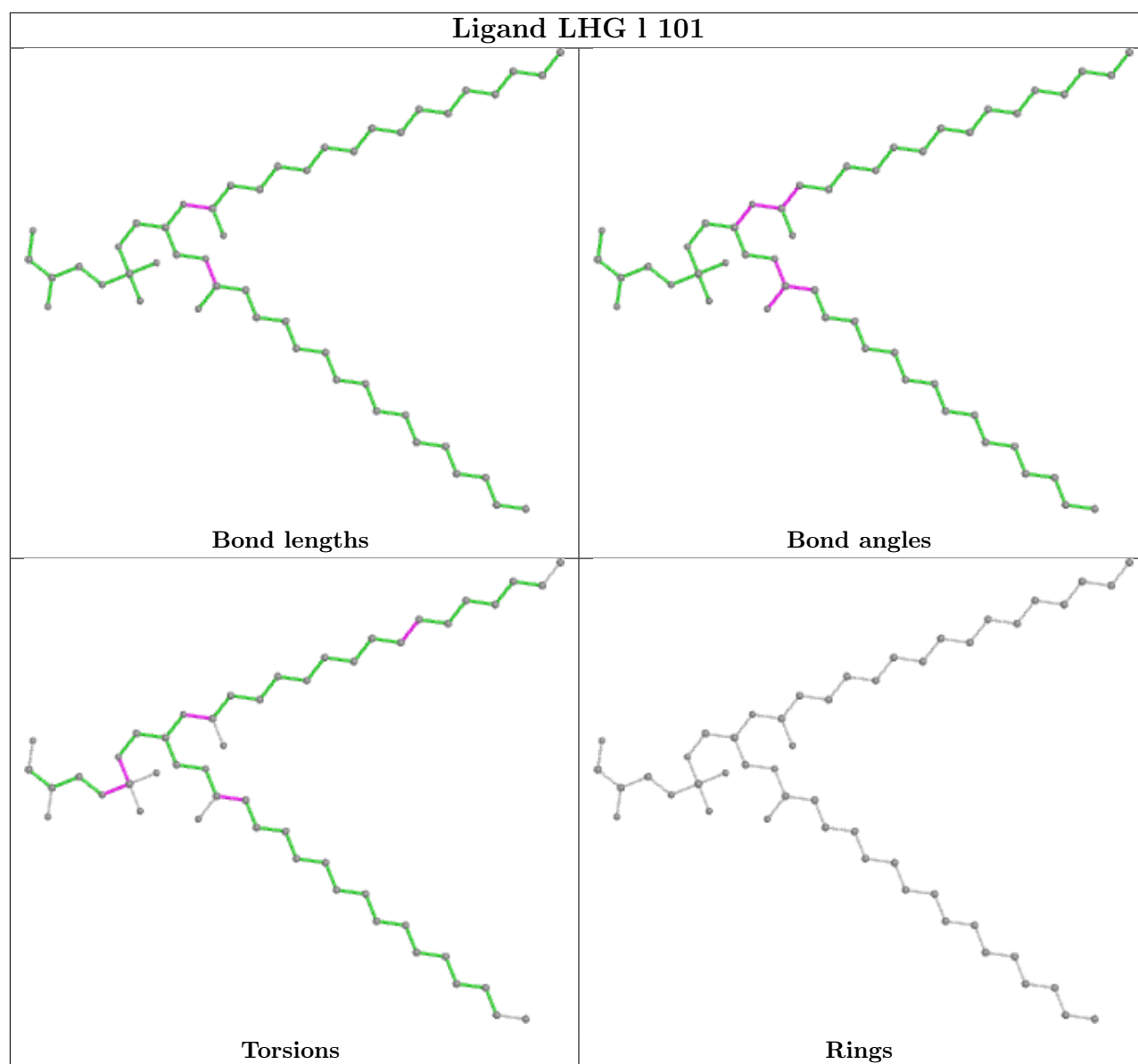


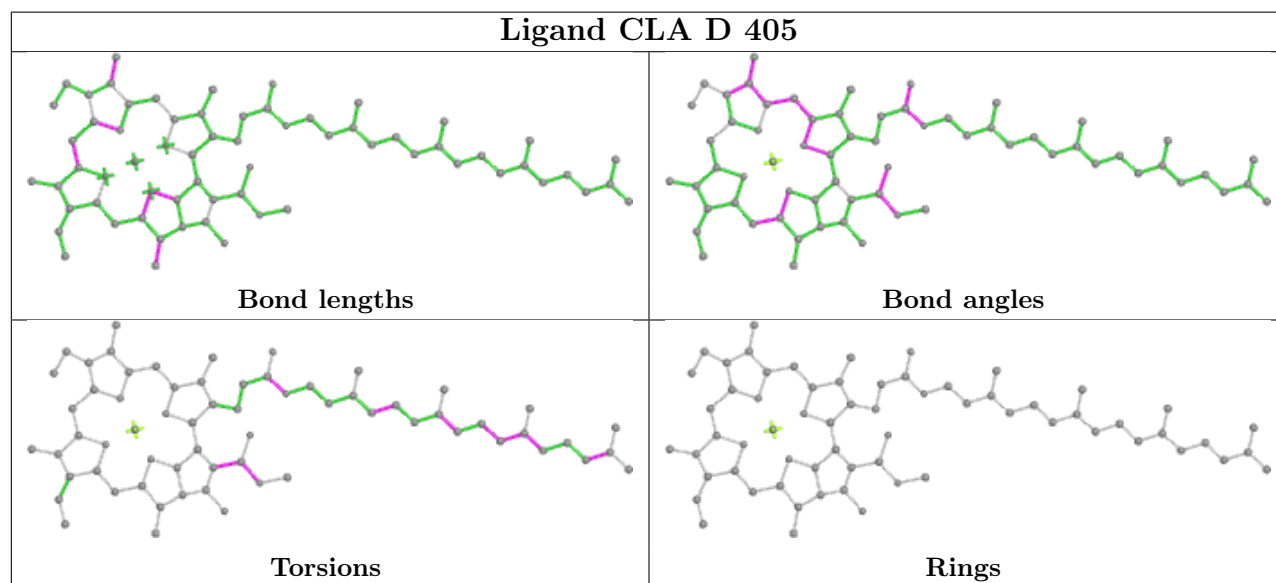
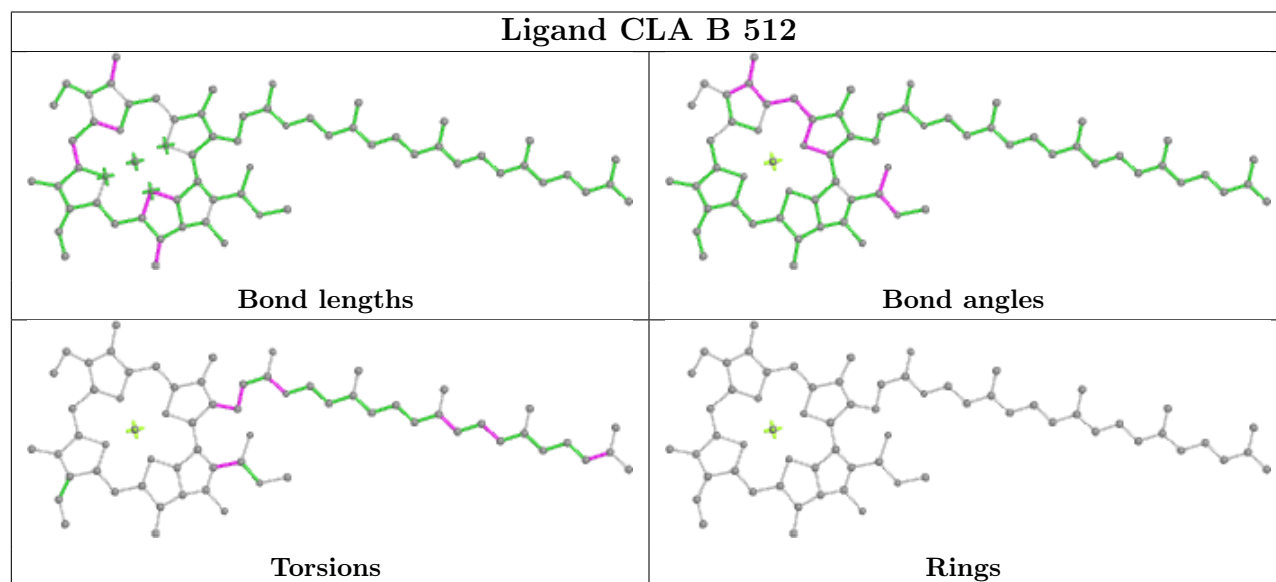
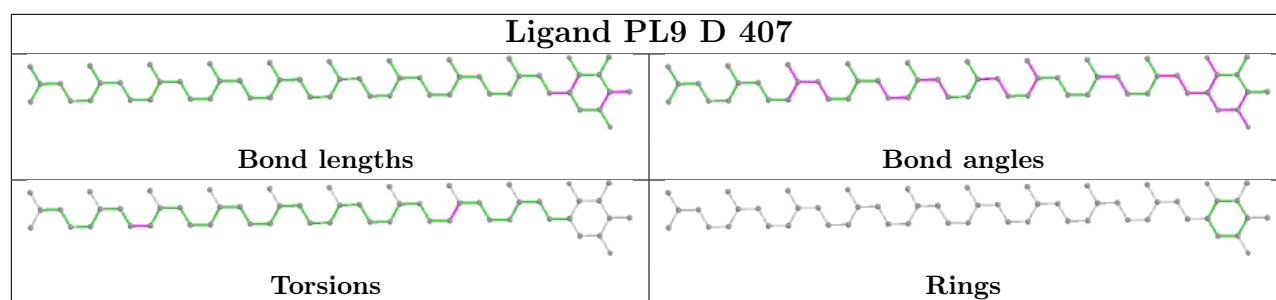
Ligand CLA S 613



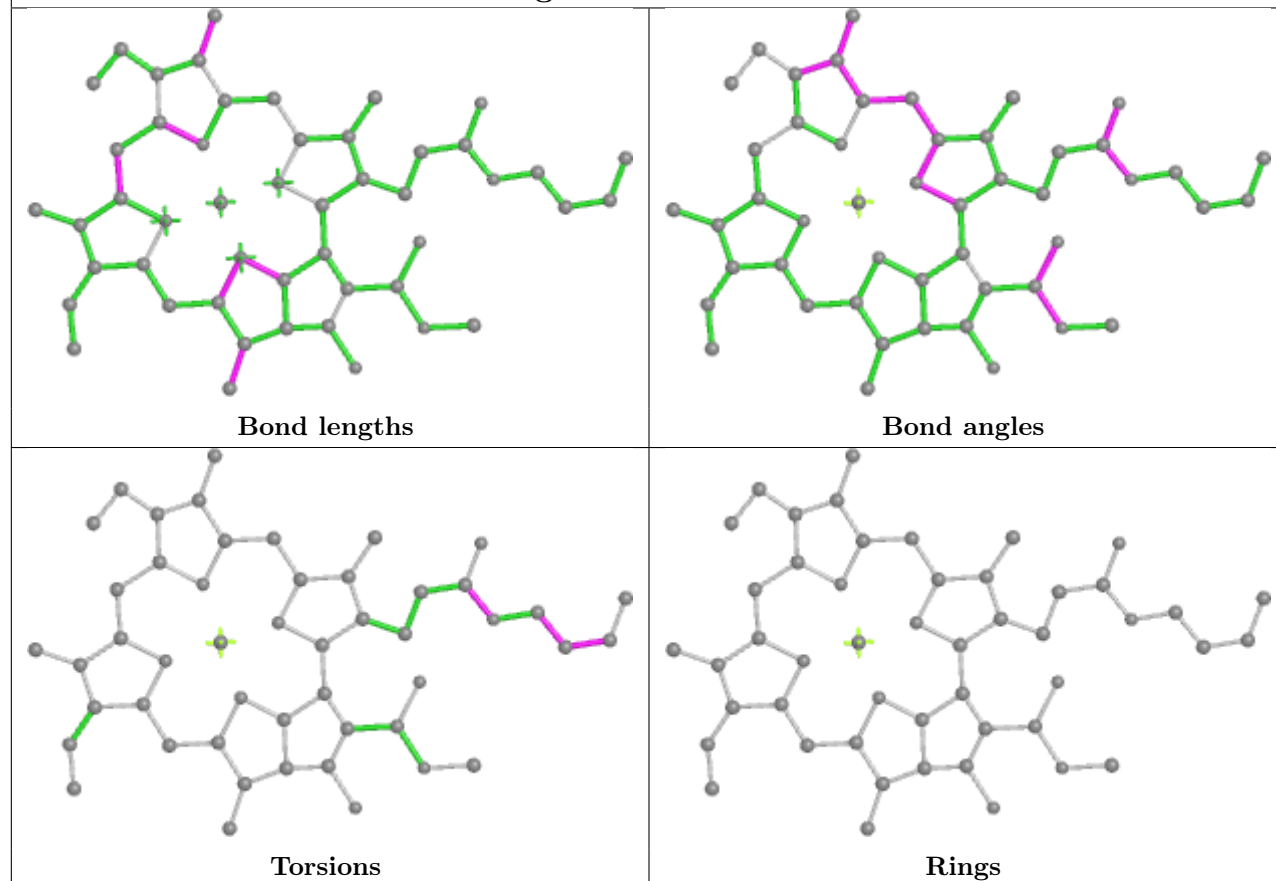
Ligand CHL N 308



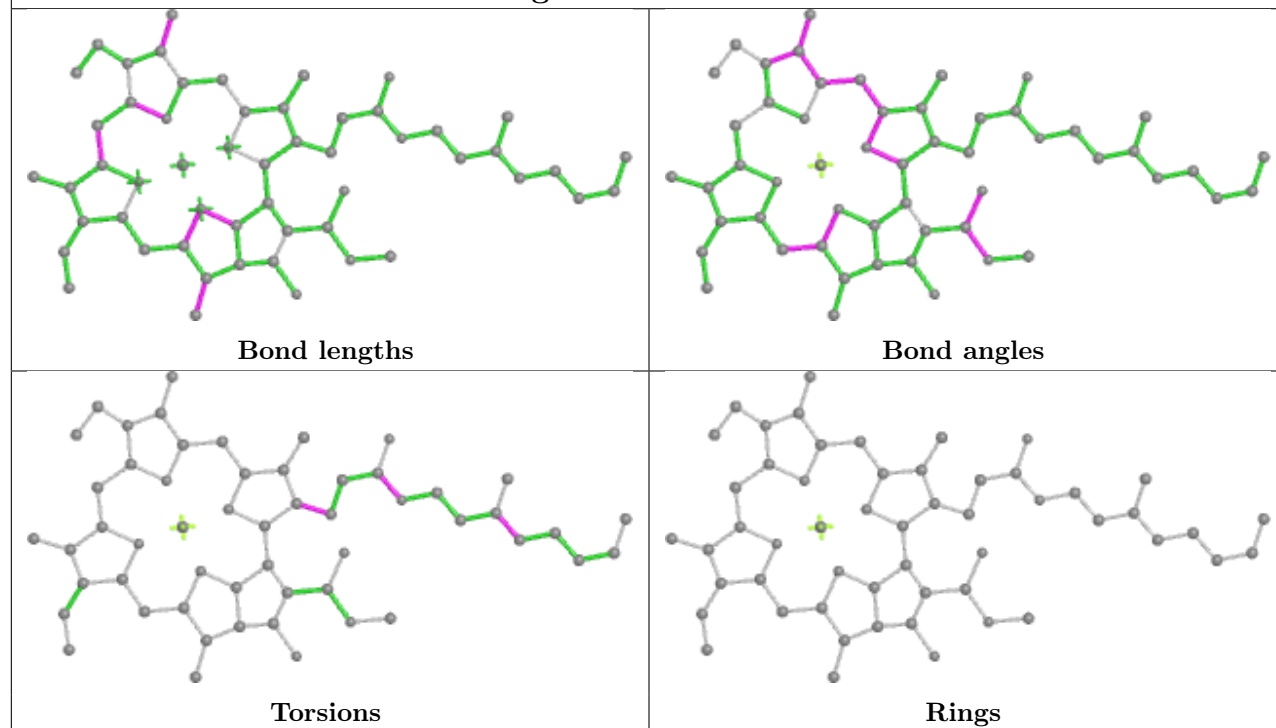




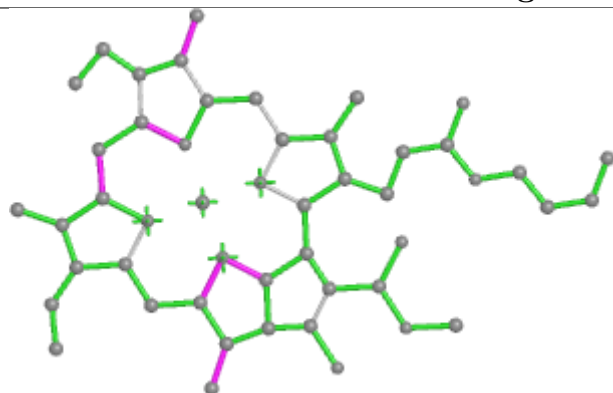
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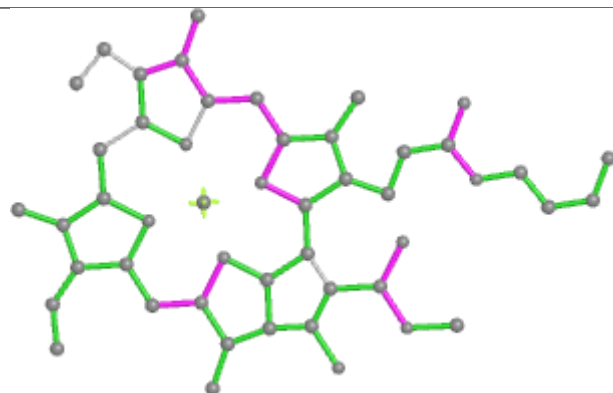
Ligand CLA Y 315



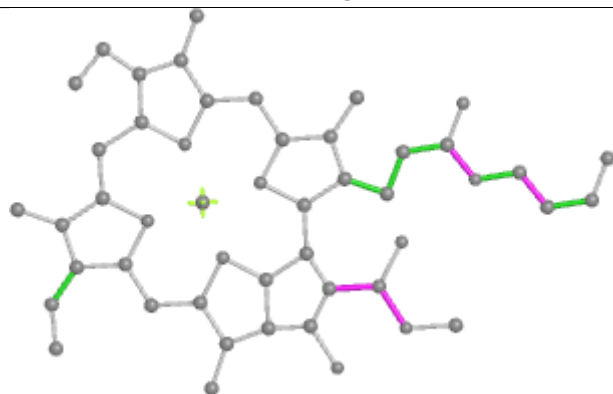
Ligand CLA S 604



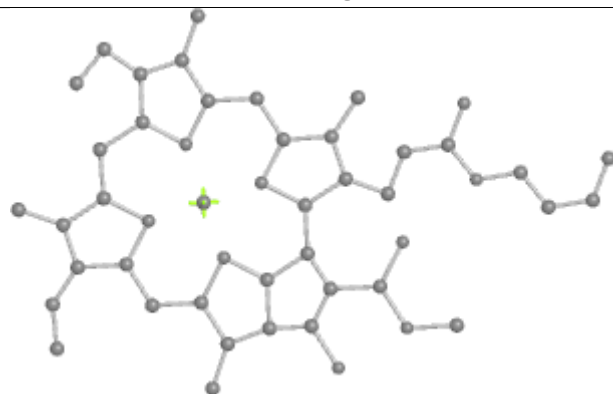
Bond lengths



Bond angles

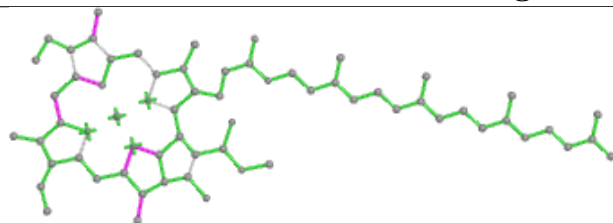


Torsions

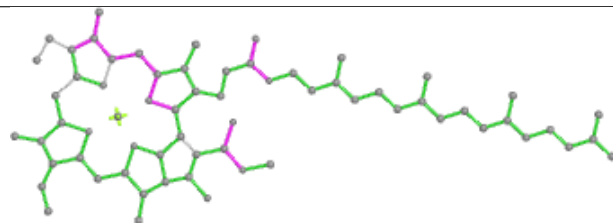


Rings

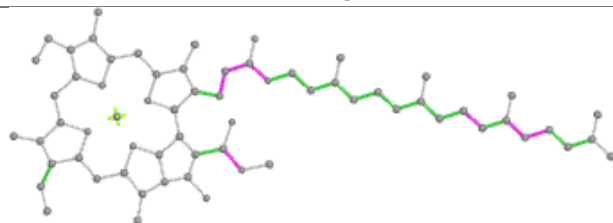
Ligand CLA Y 304



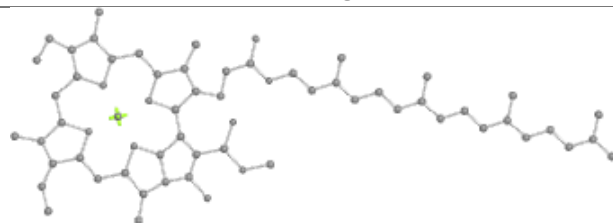
Bond lengths



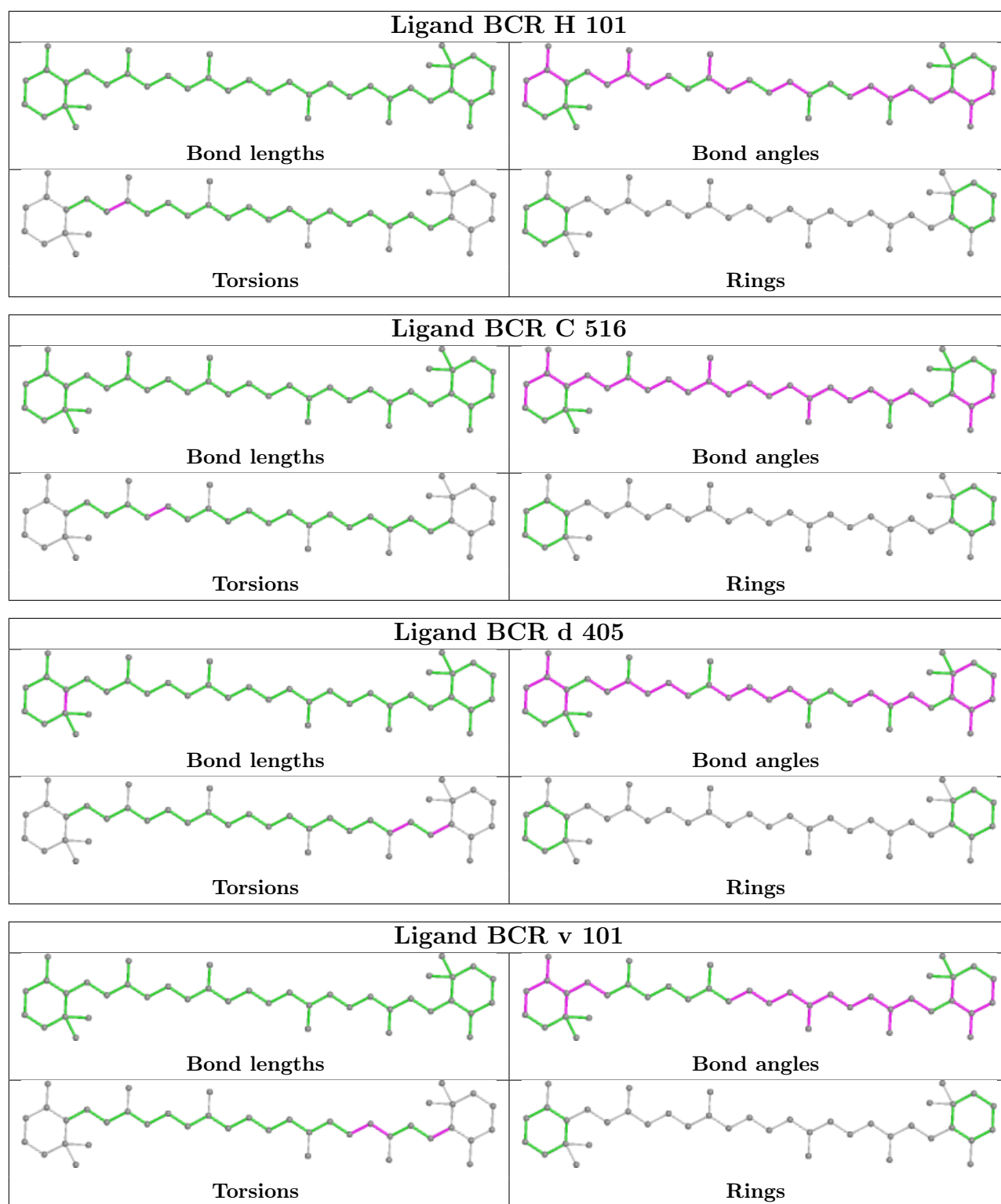
Bond angles



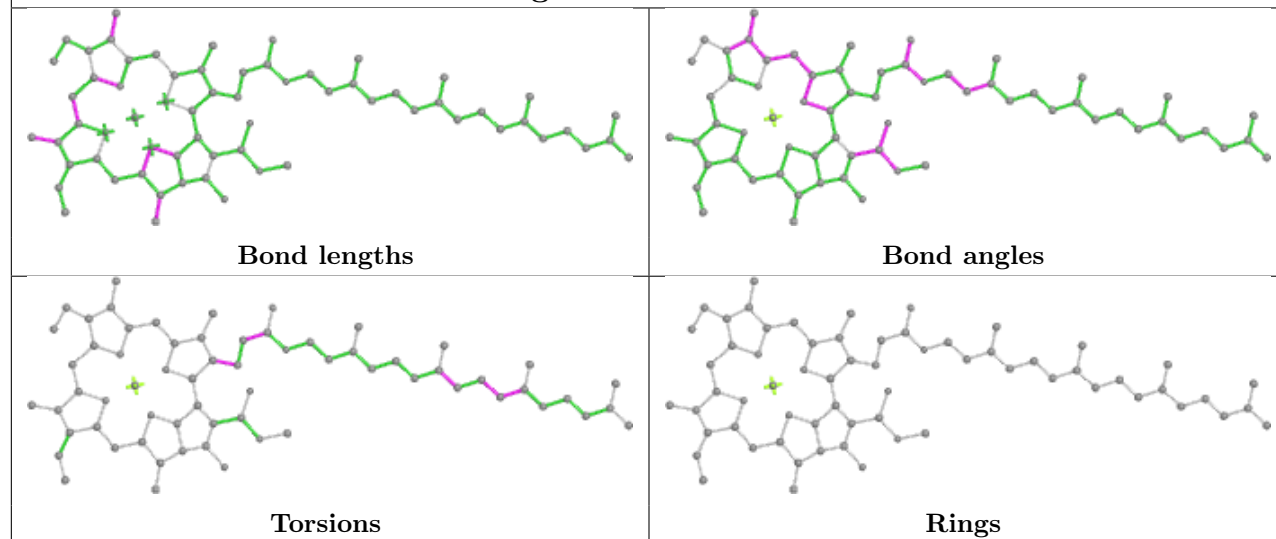
Torsions



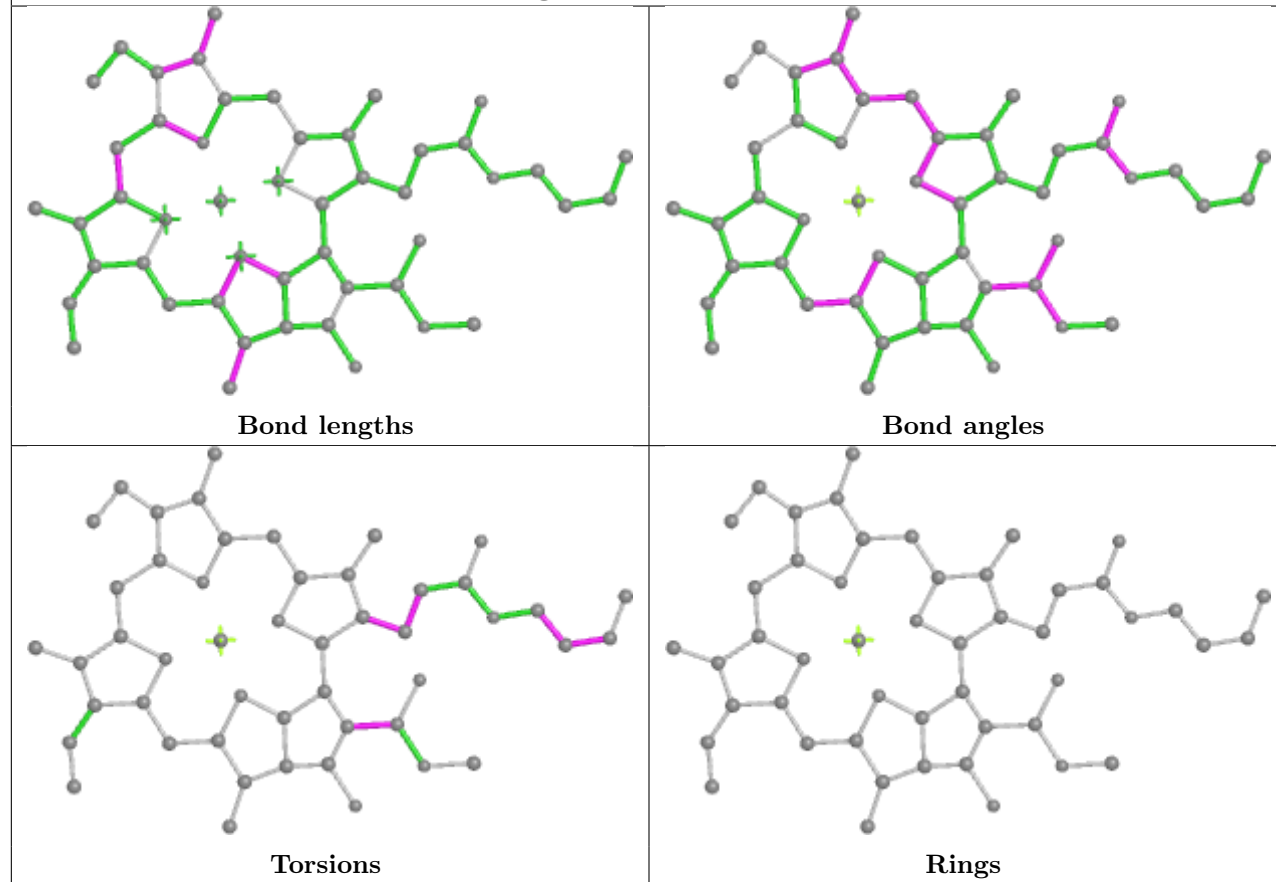
Rings



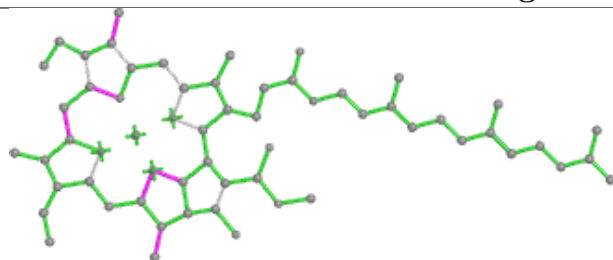
Ligand CLA D 404



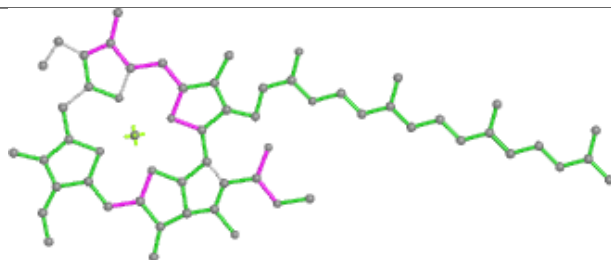
Ligand CLA S 602



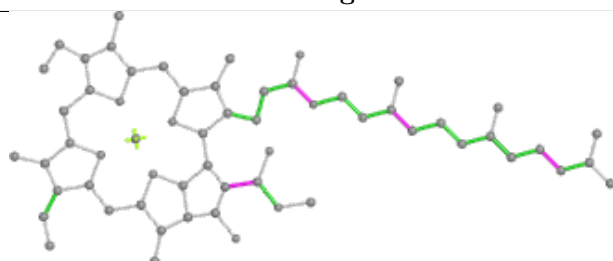
Ligand CLA a 405



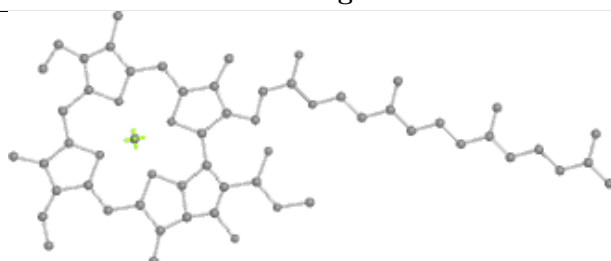
Bond lengths



Bond angles

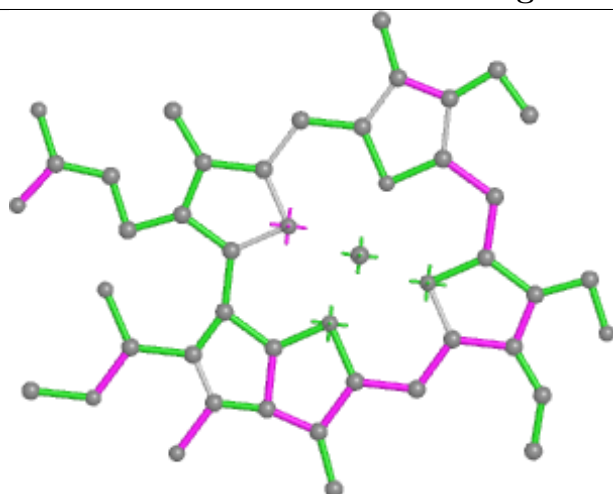


Torsions

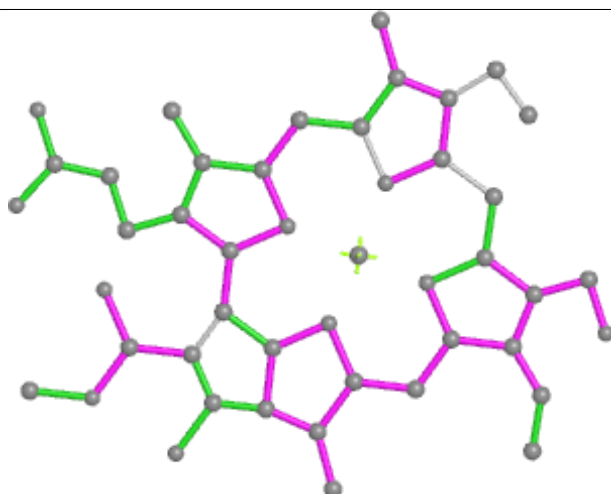


Rings

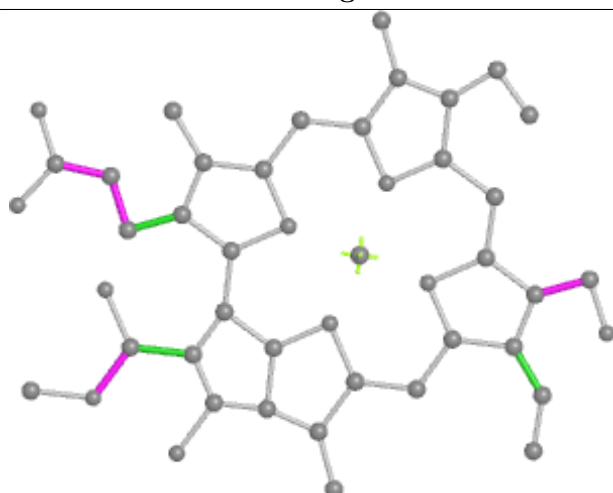
Ligand CHL S 601



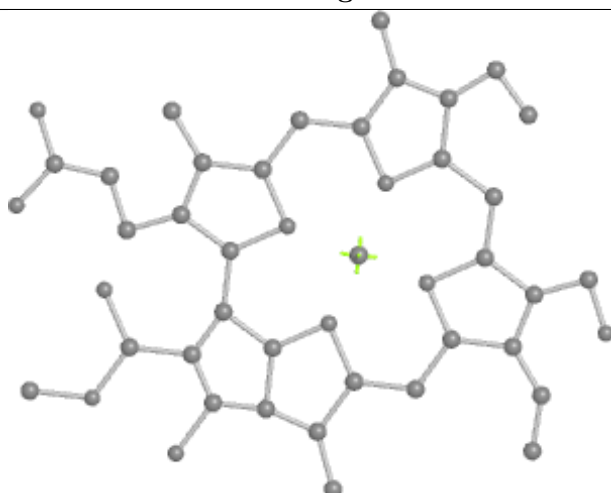
Bond lengths



Bond angles

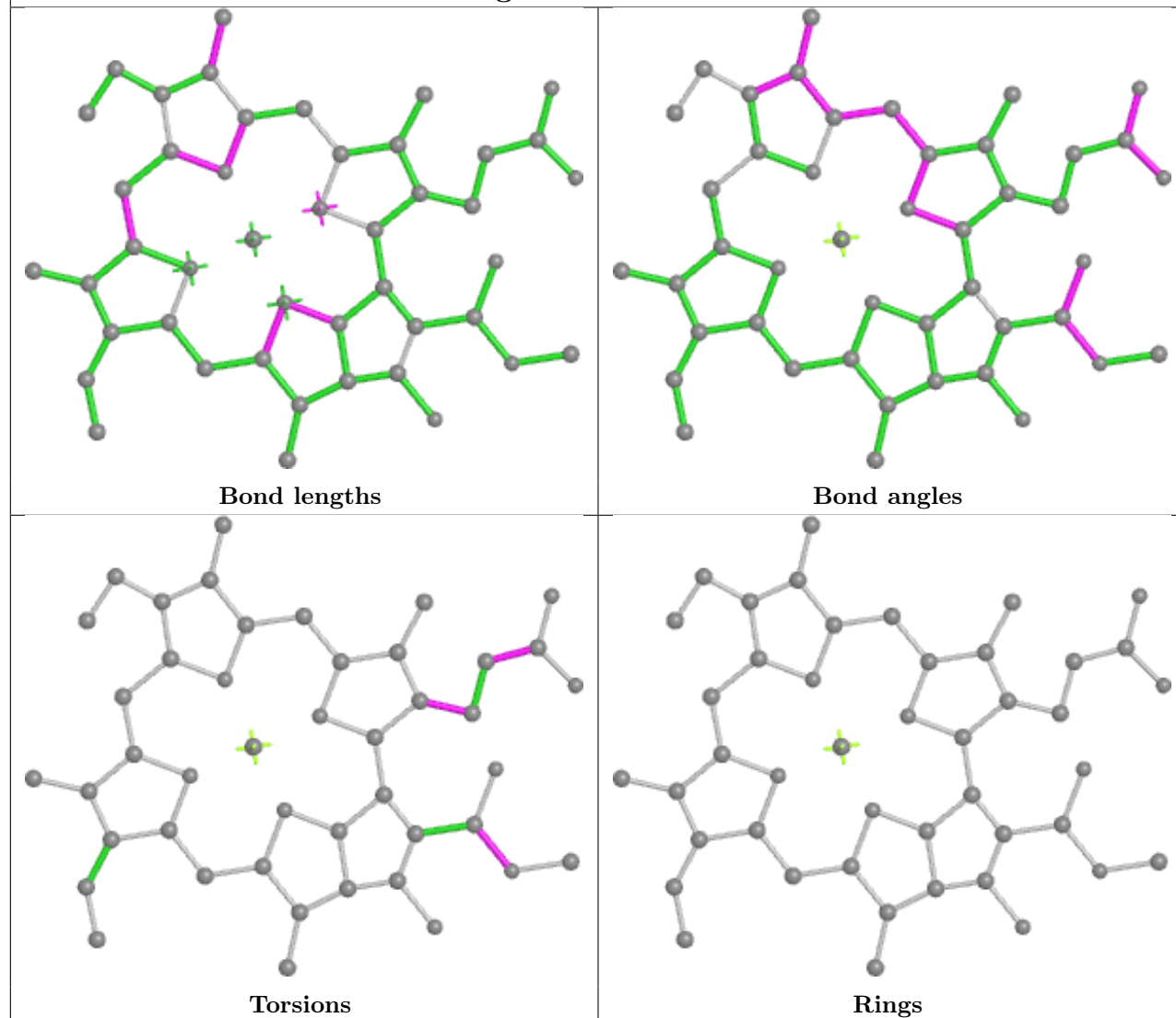


Torsions

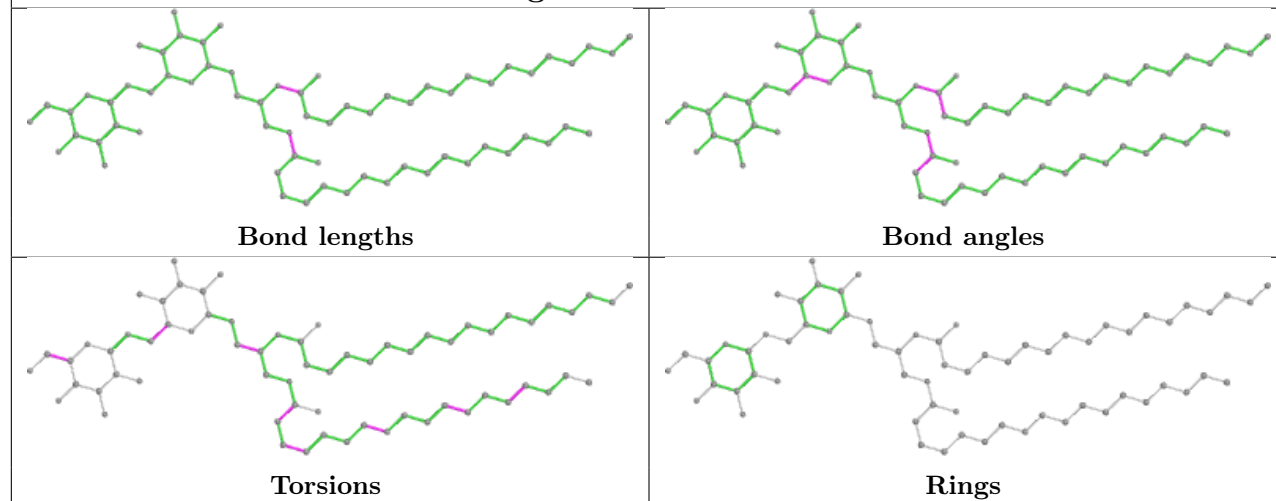


Rings

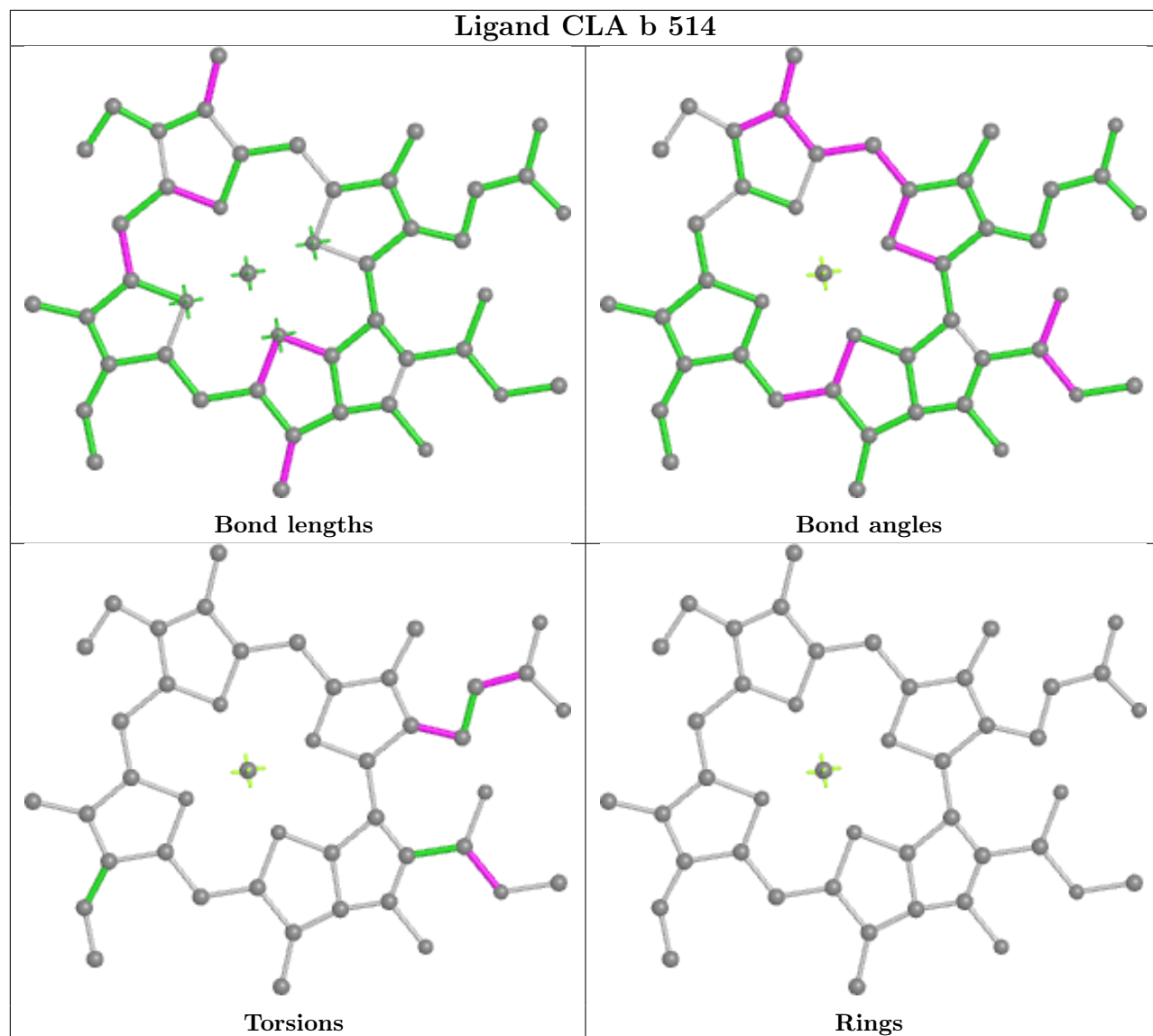
Ligand CLA r 307



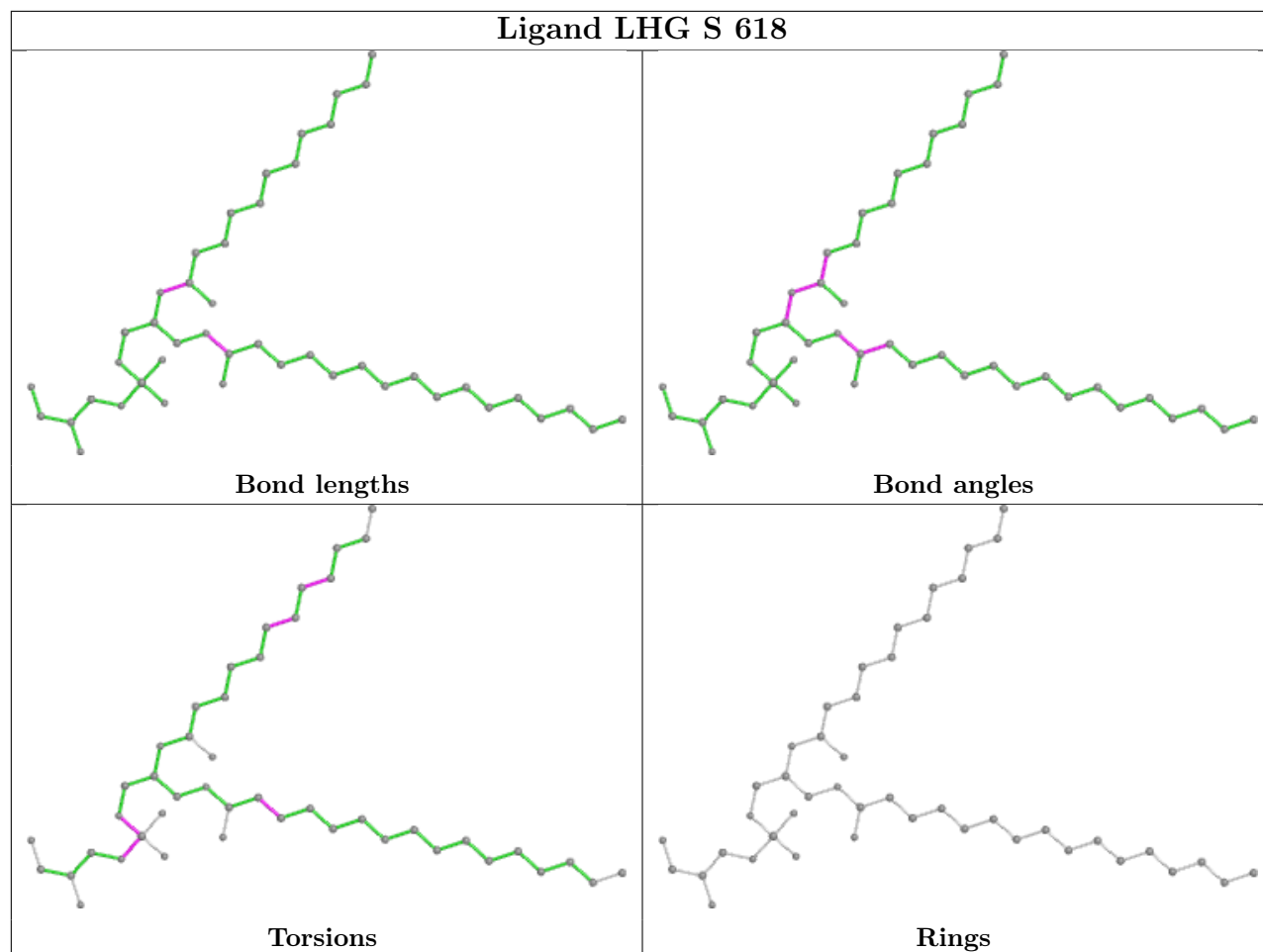
Ligand DGD Y 301



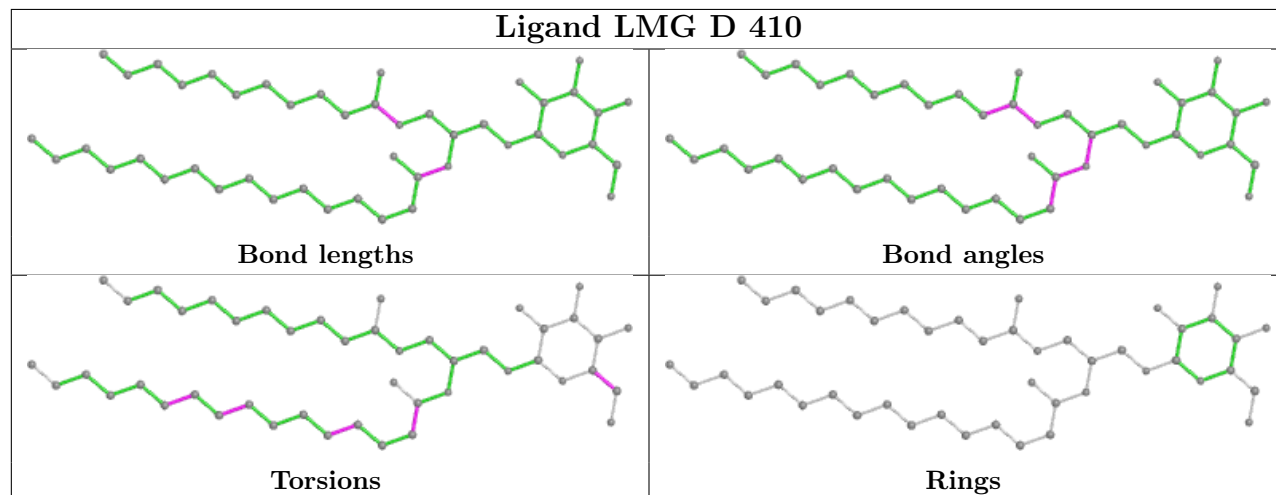
Ligand CLA b 514

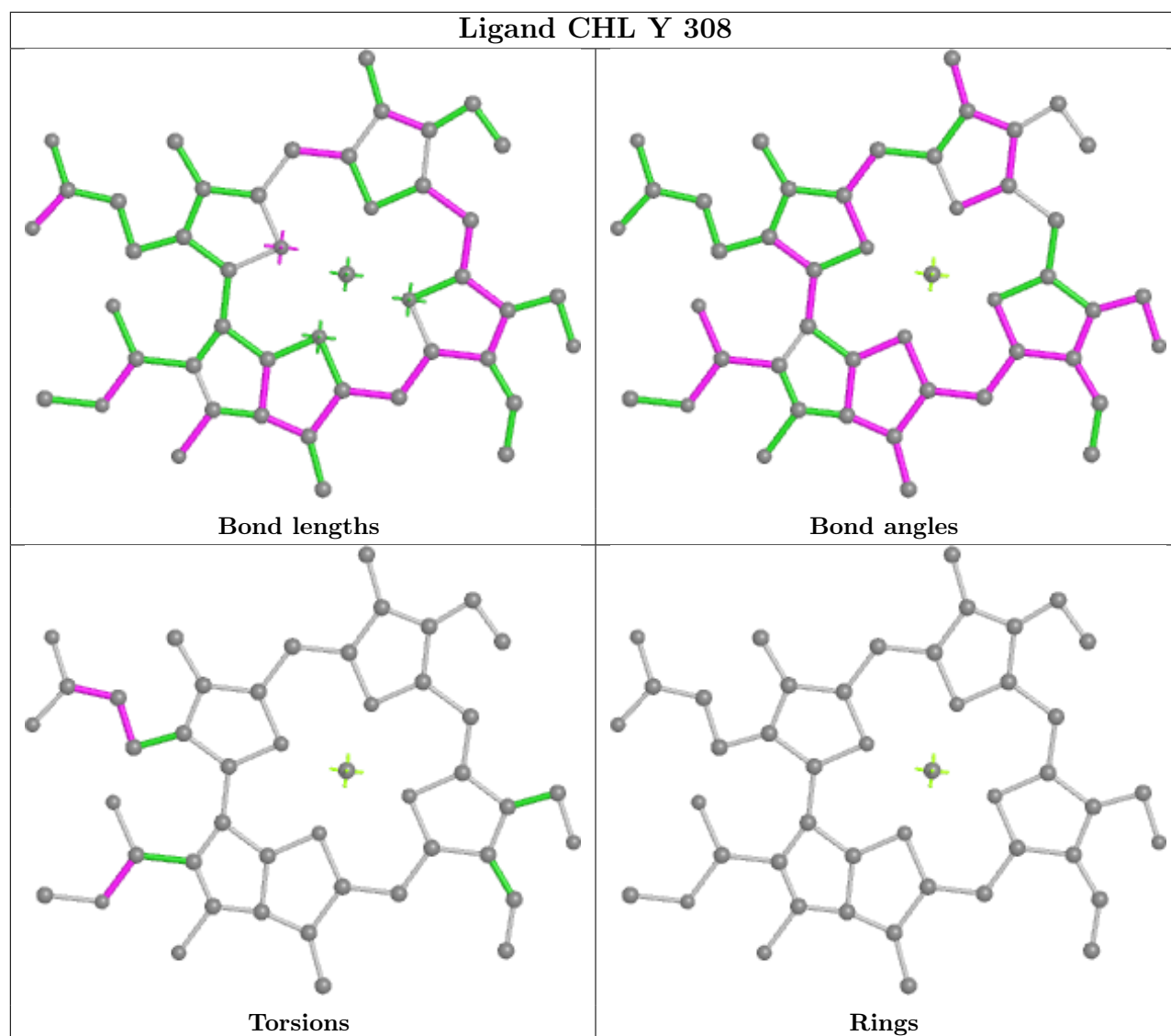
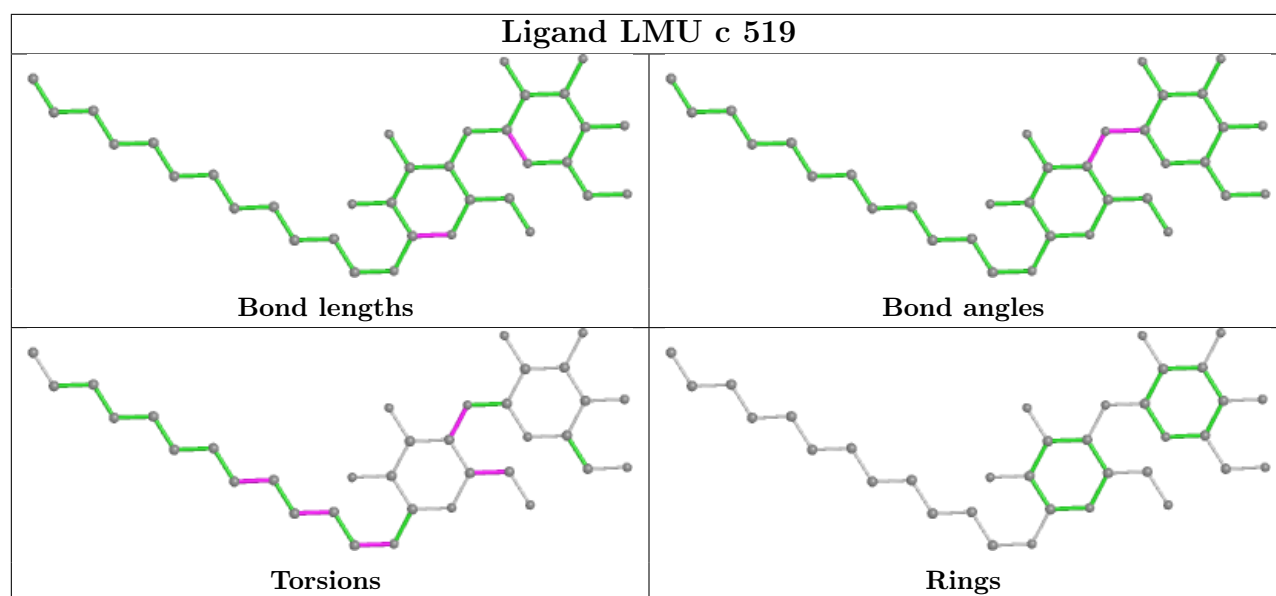


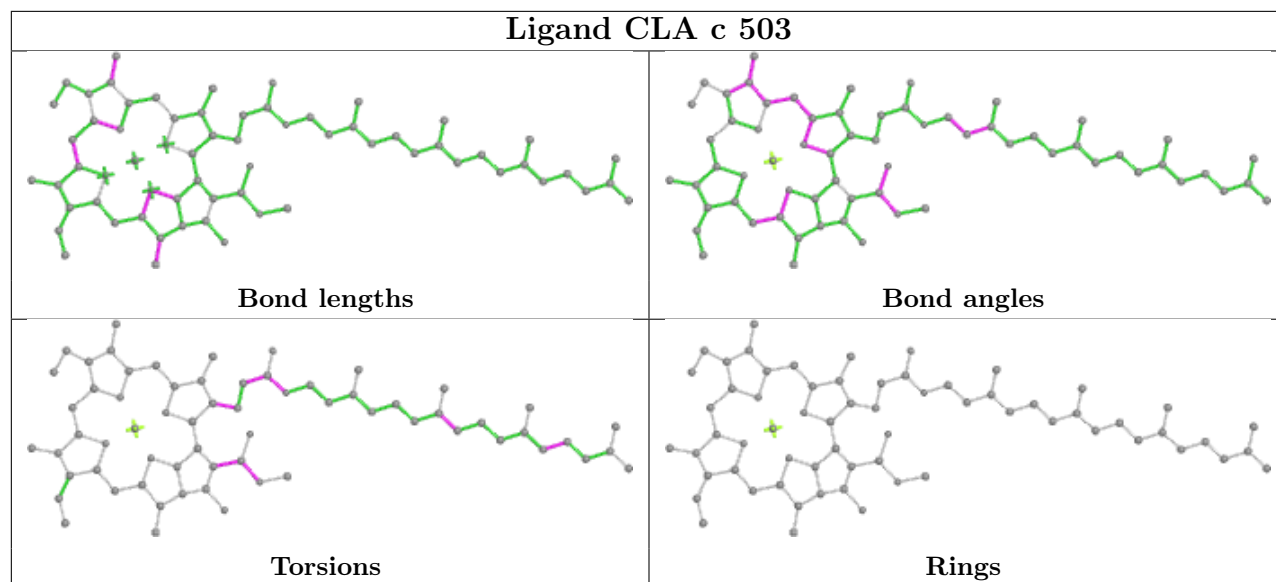
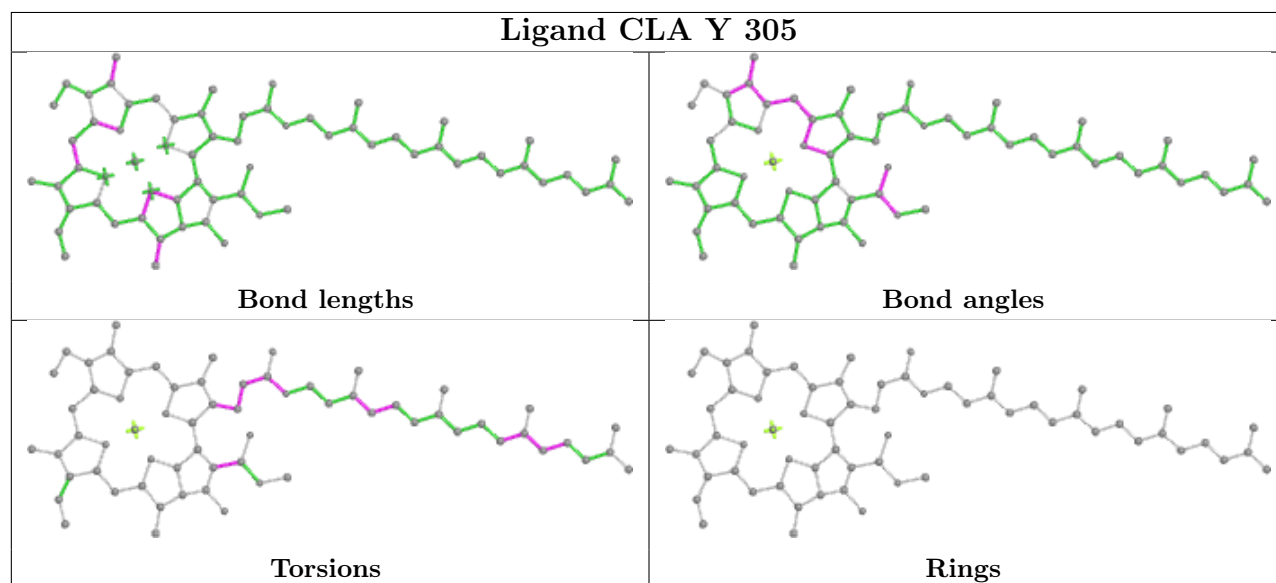
Ligand LHG S 618

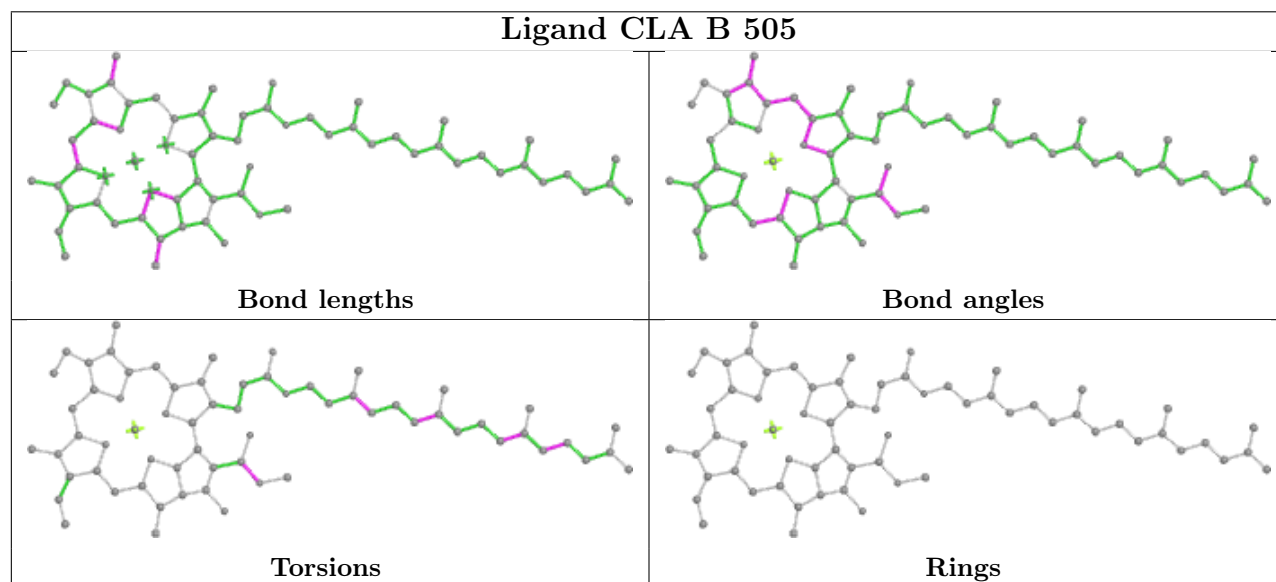
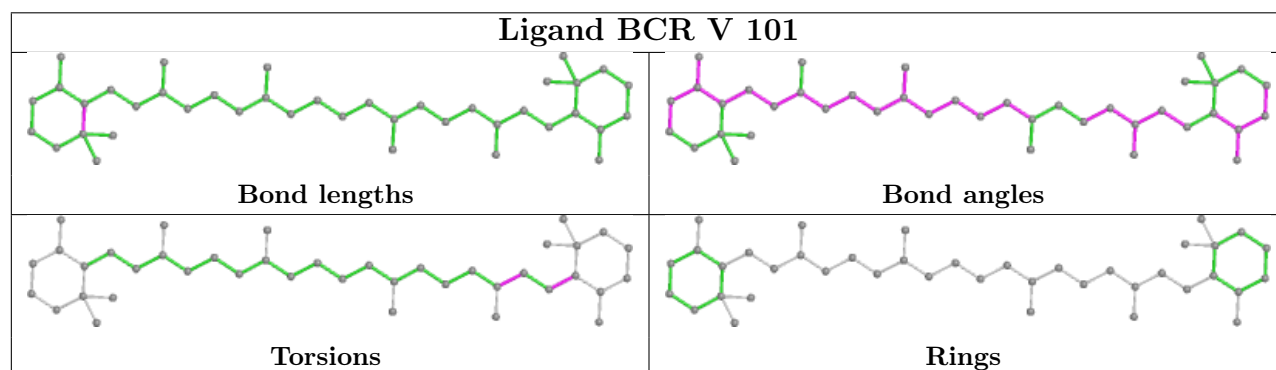
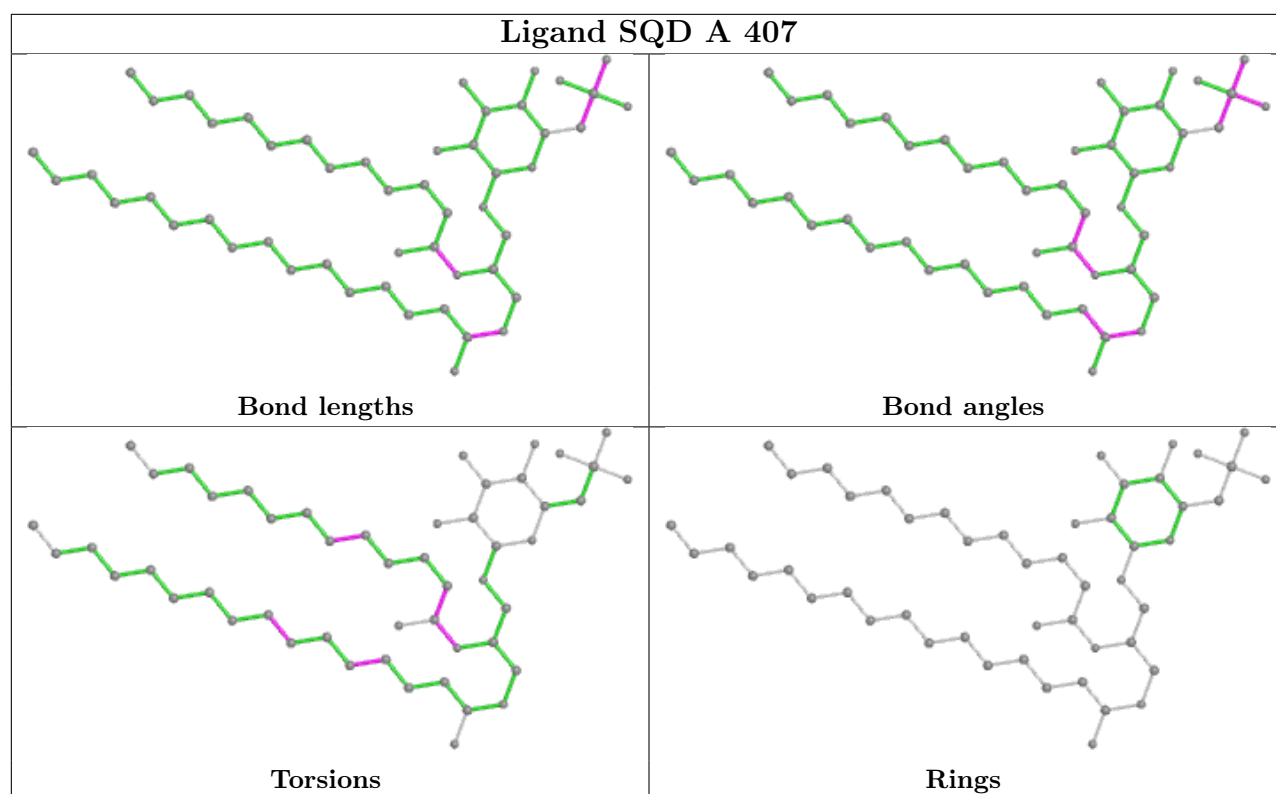


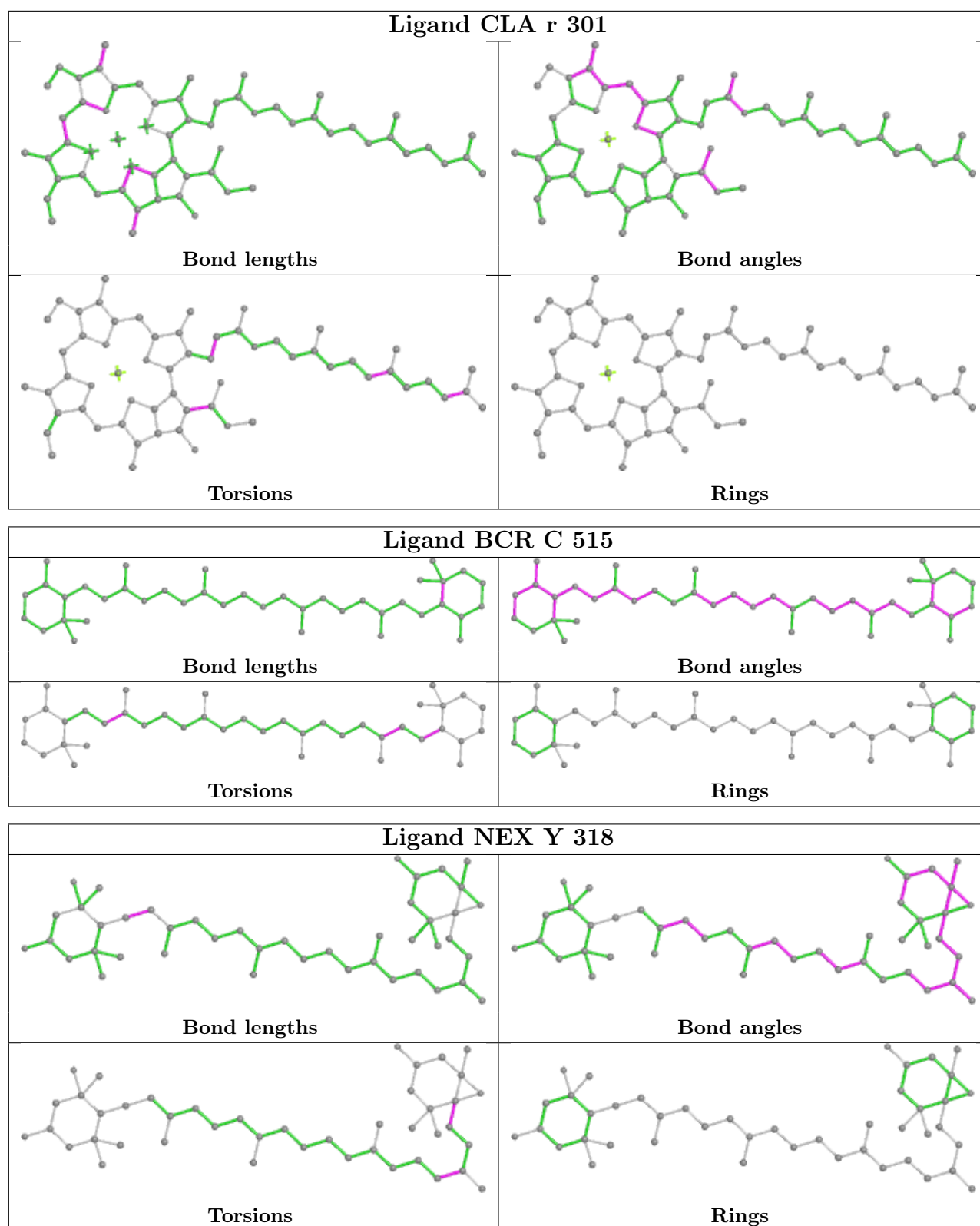
Ligand LMG D 410

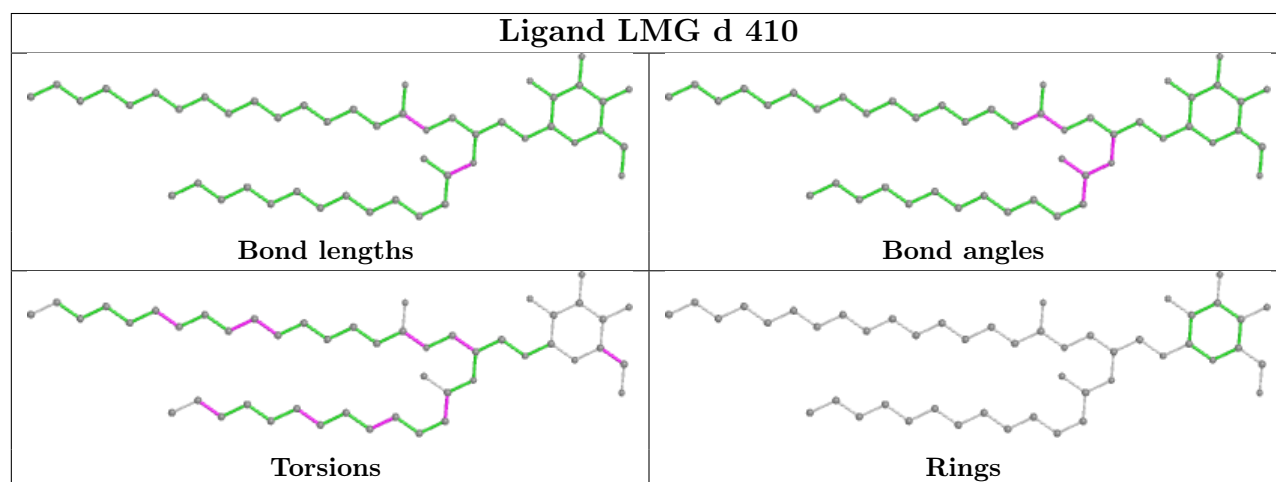
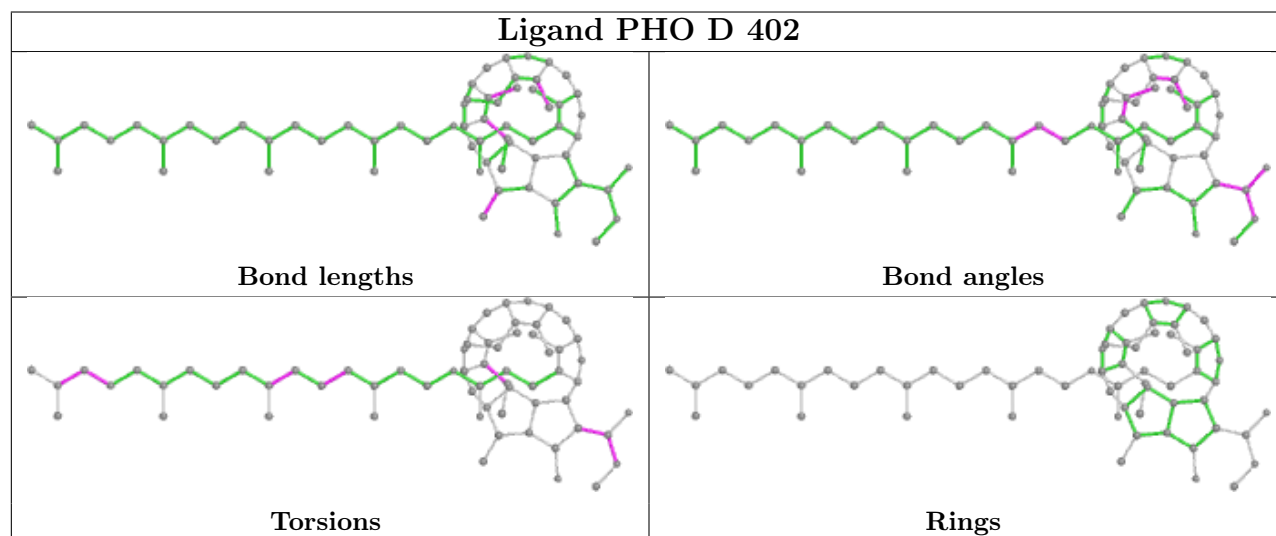
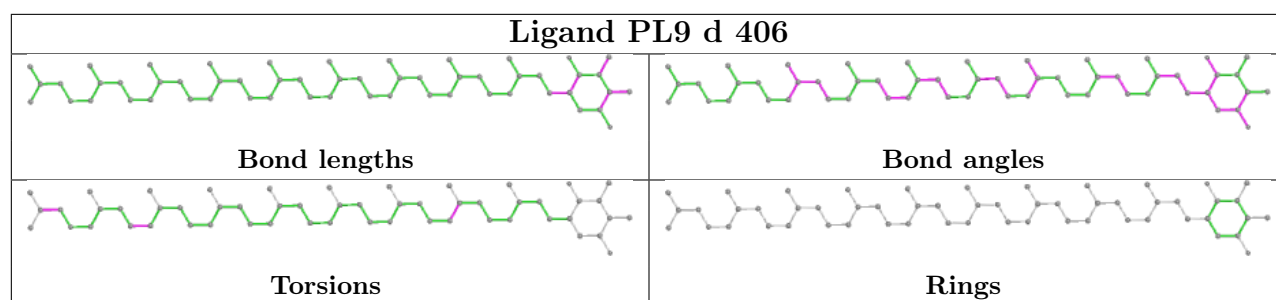




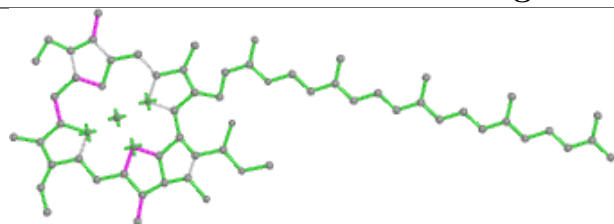
Ligand CLA c 503**Ligand CLA Y 305**



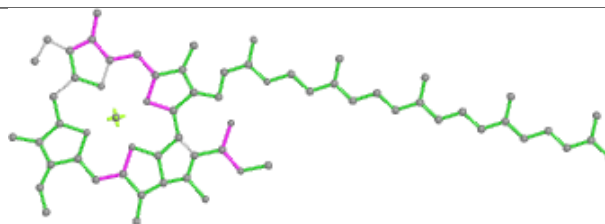




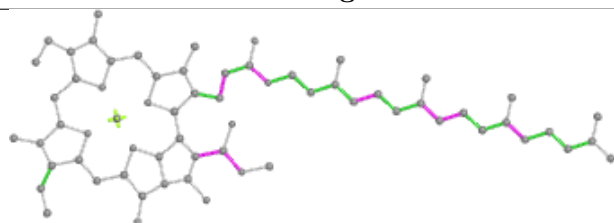
Ligand CLA Y 314



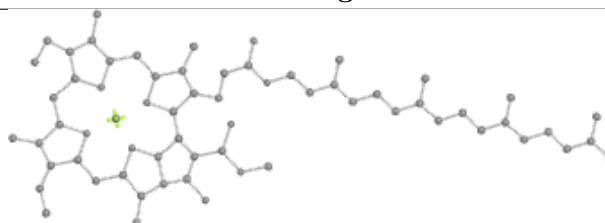
Bond lengths



Bond angles

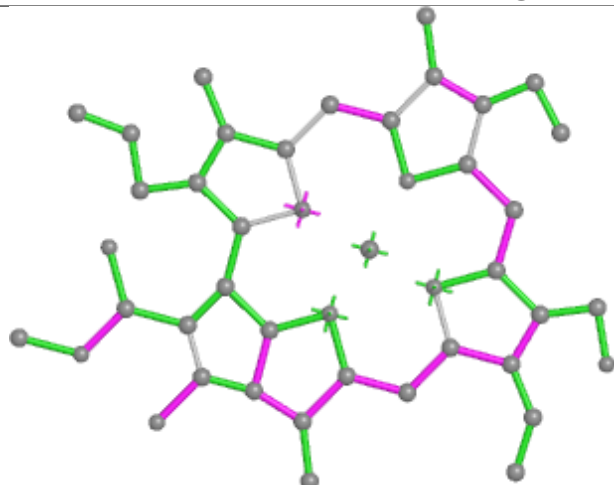


Torsions

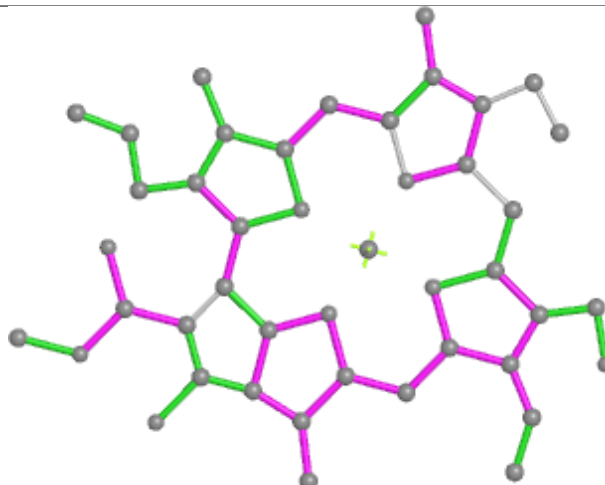


Rings

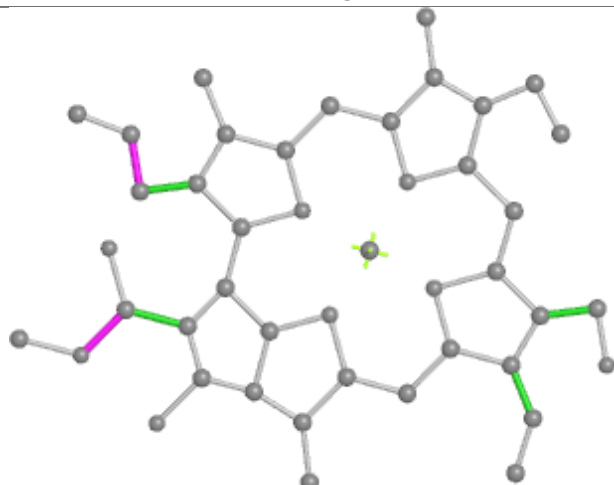
Ligand CHL G 608



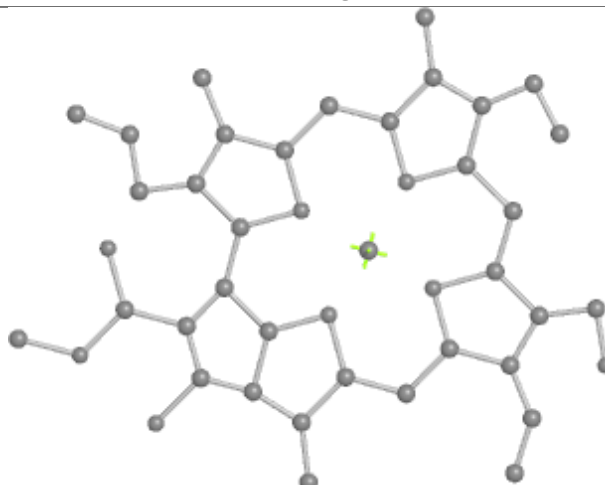
Bond lengths



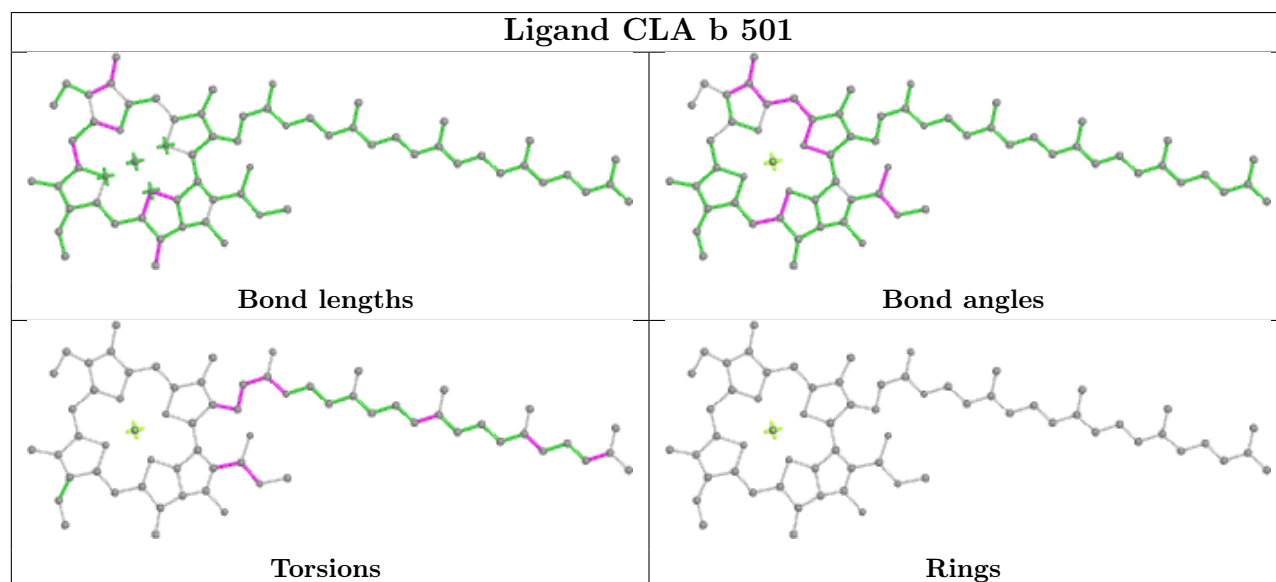
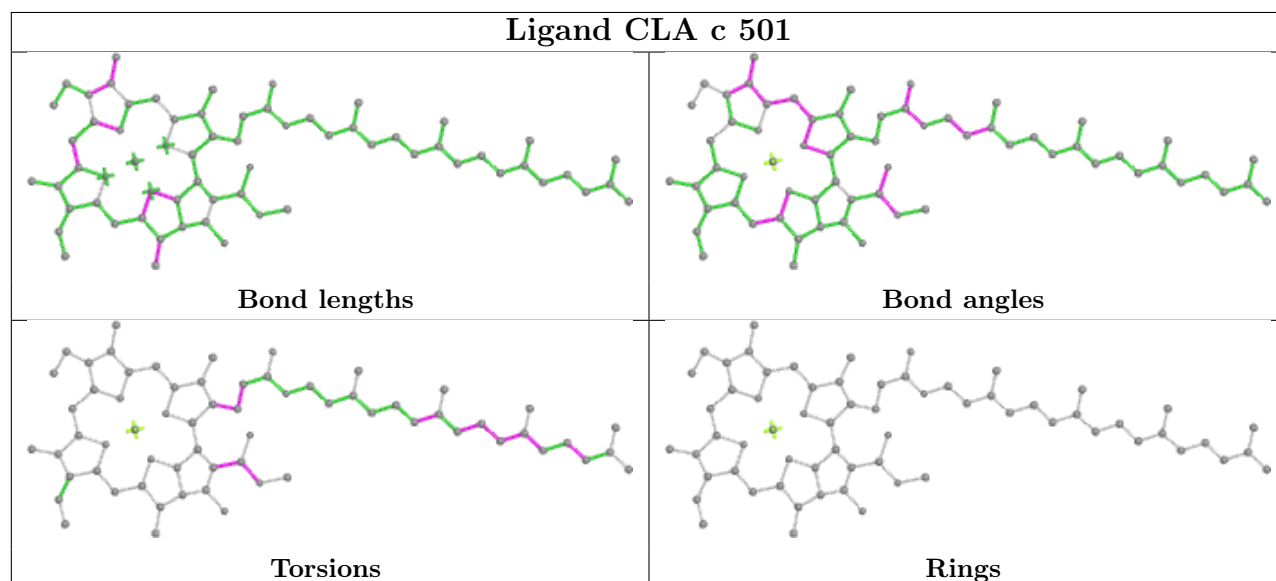
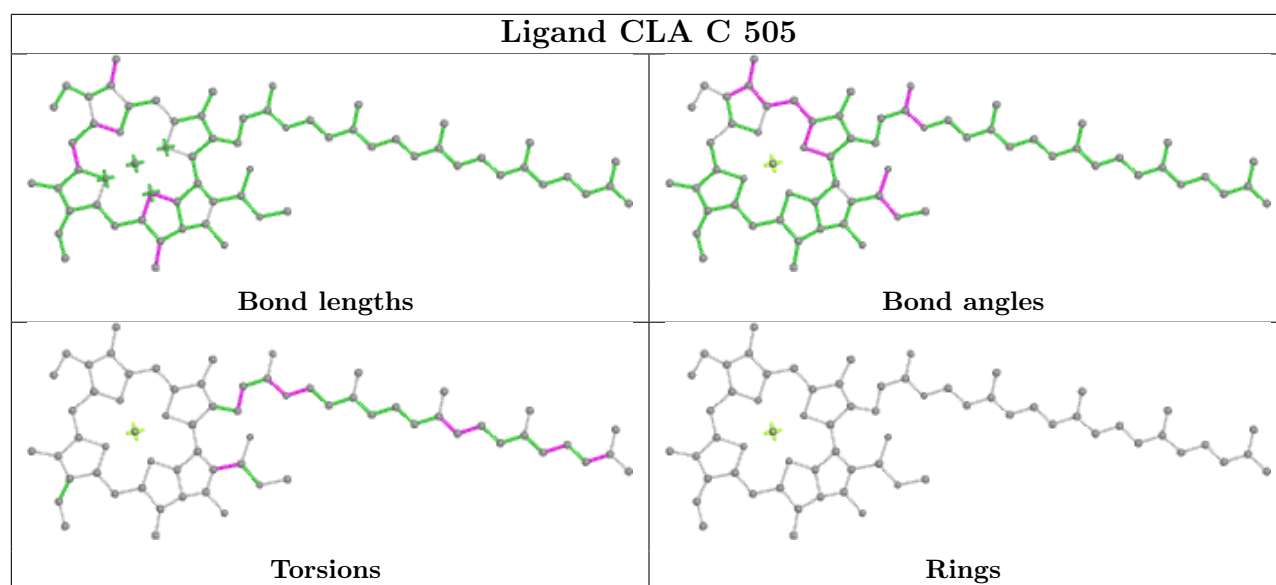
Bond angles

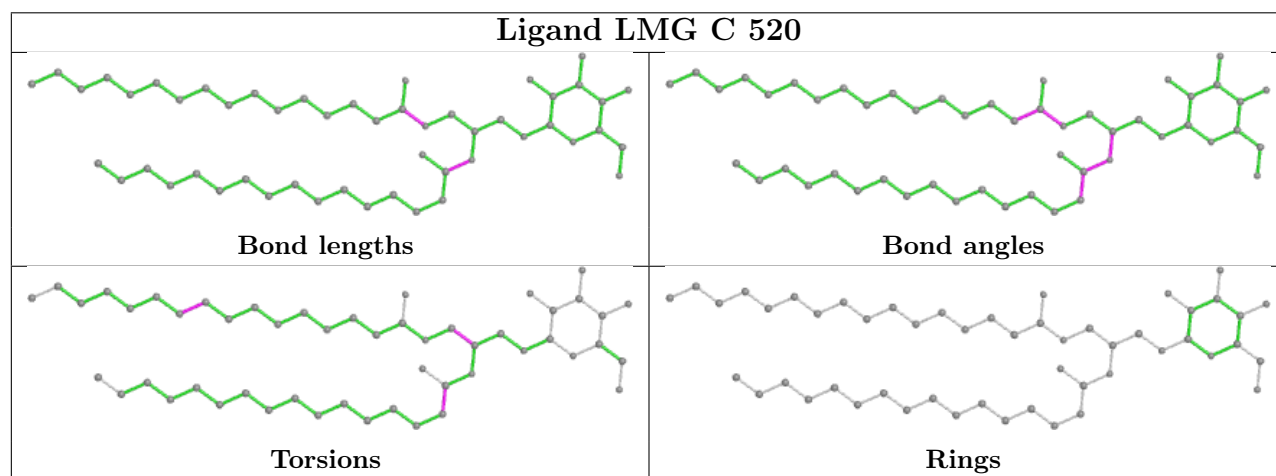
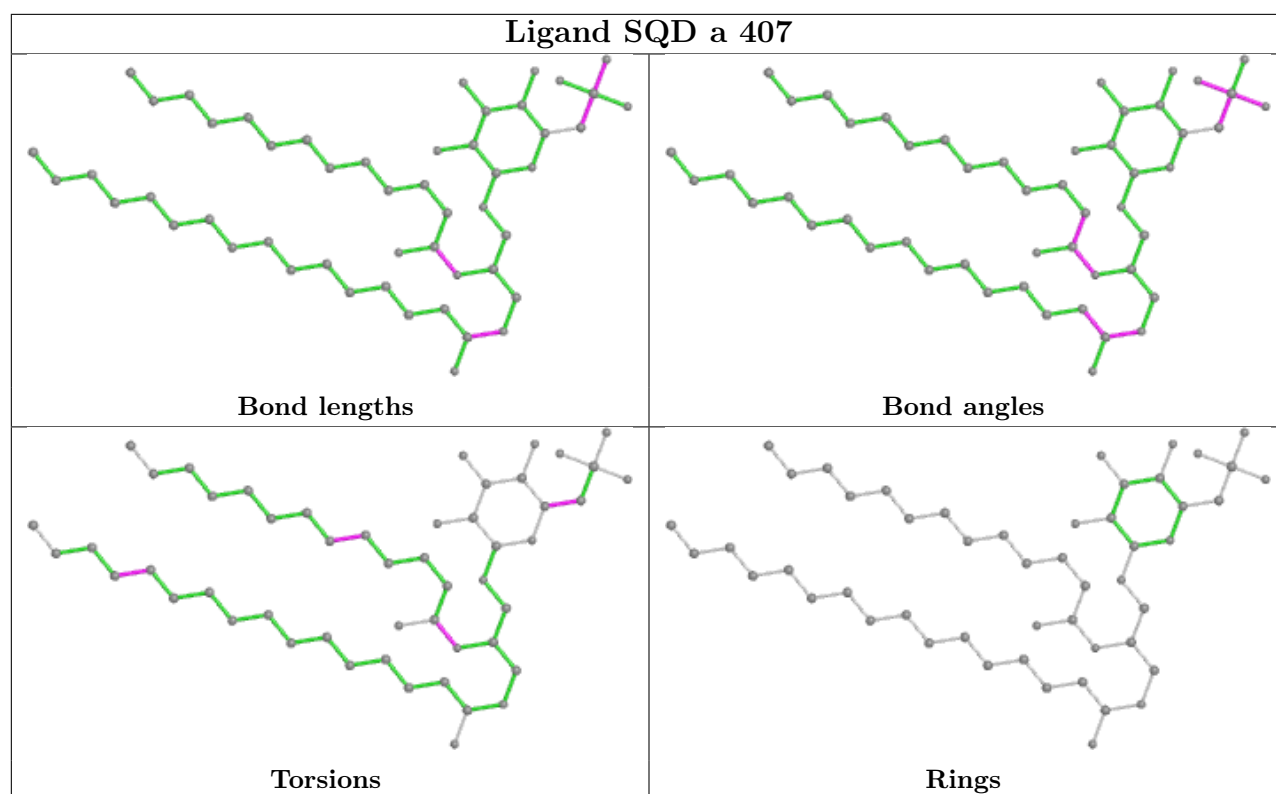


Torsions

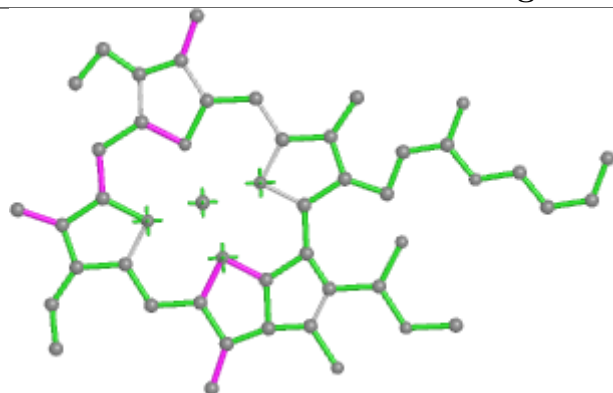


Rings

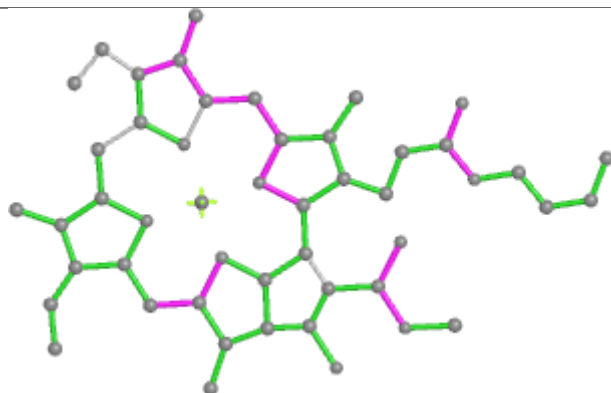




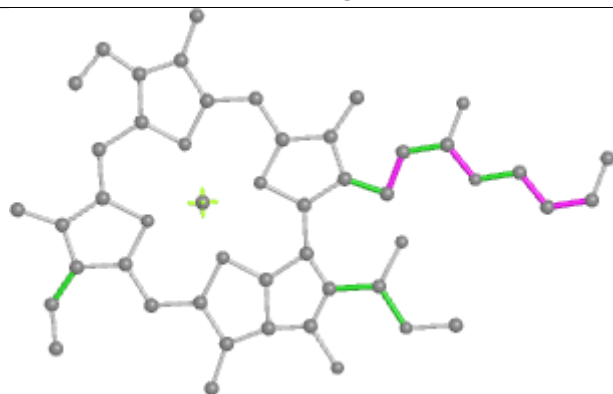
Ligand CLA S 610



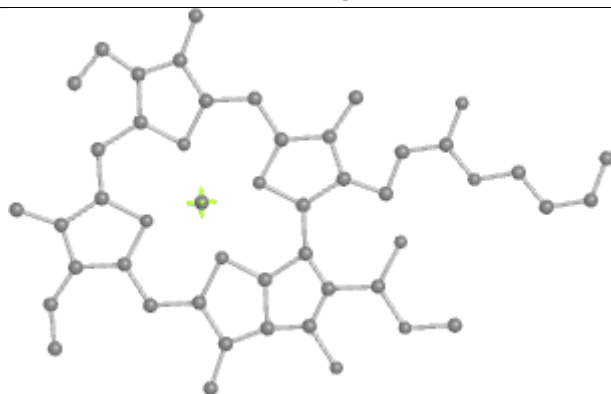
Bond lengths



Bond angles

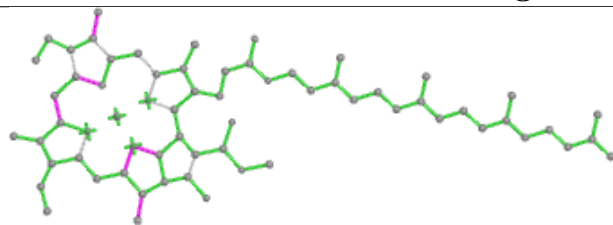


Torsions

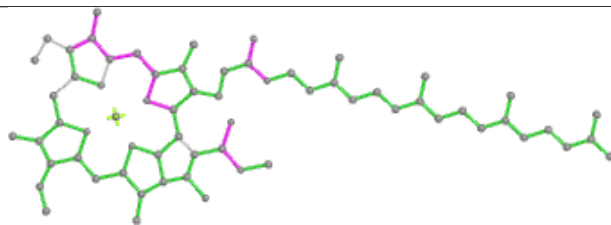


Rings

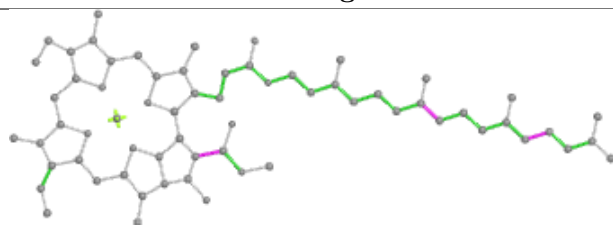
Ligand CLA C 507



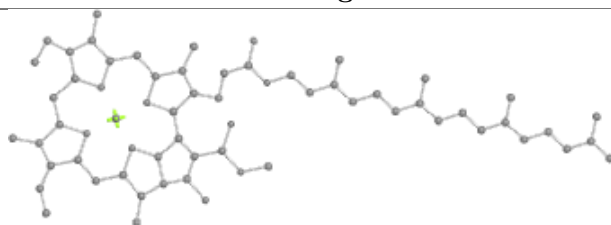
Bond lengths



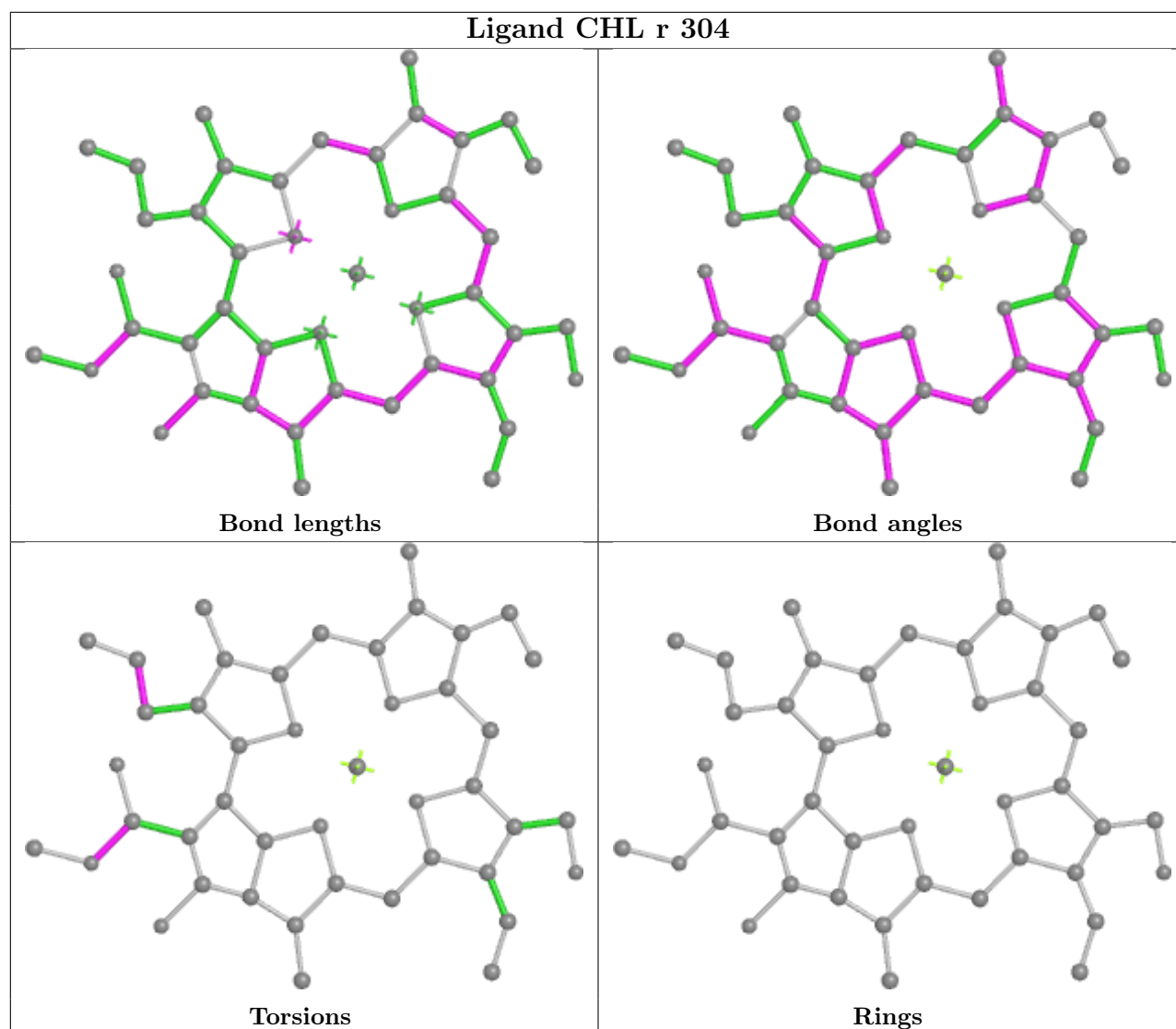
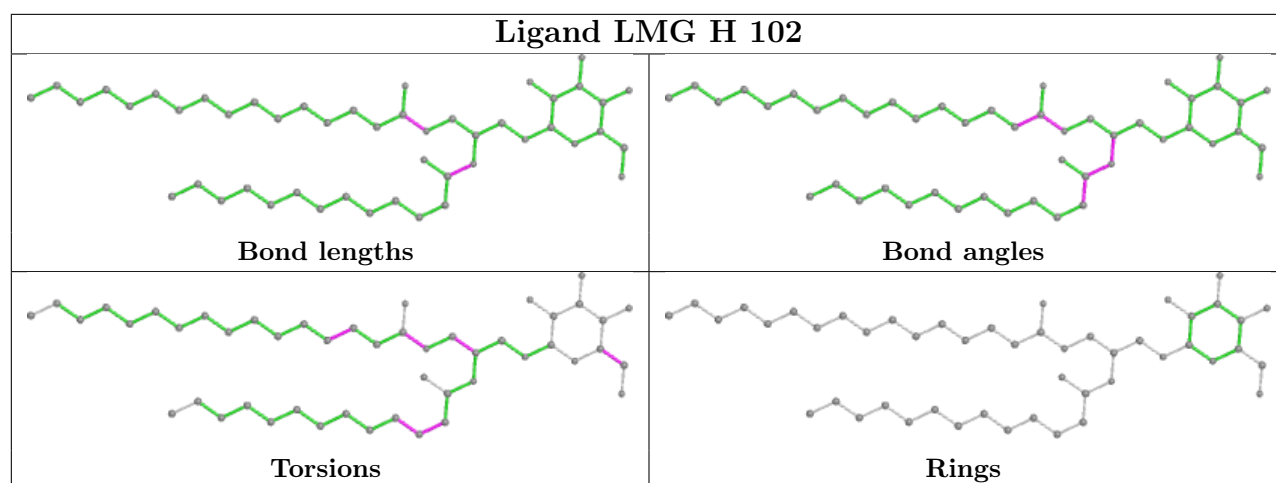
Bond angles

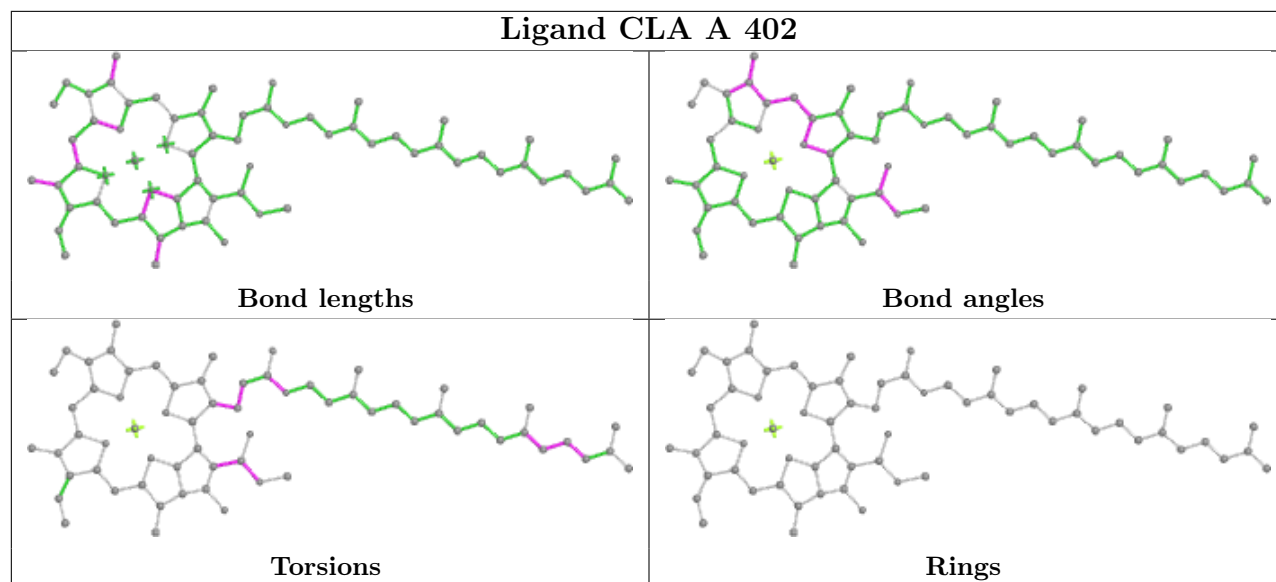
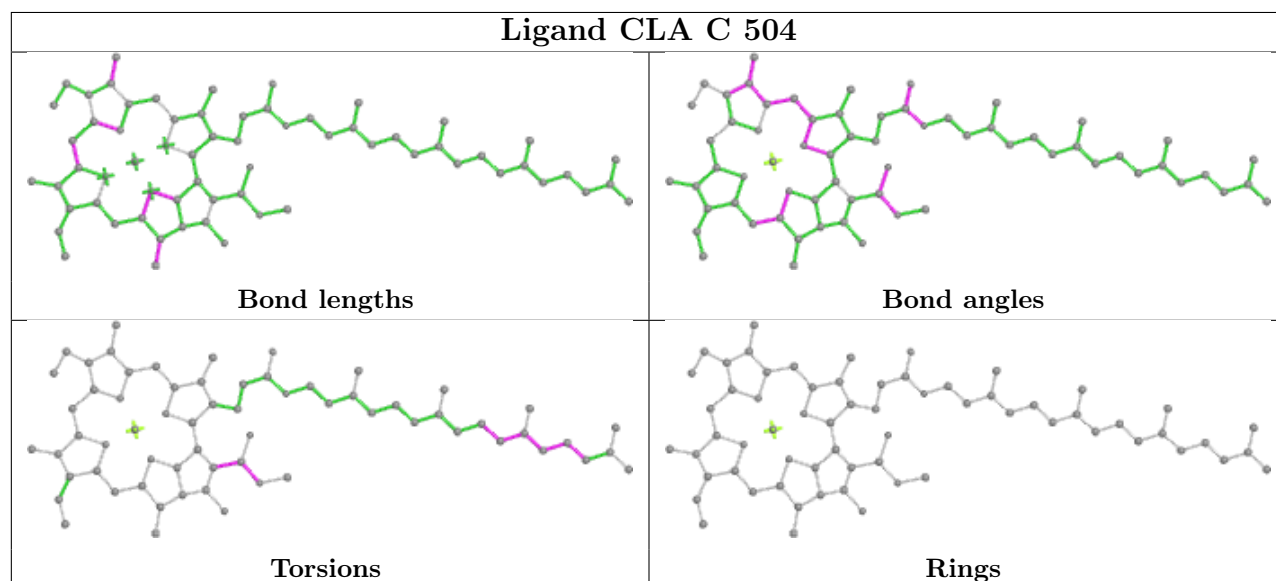
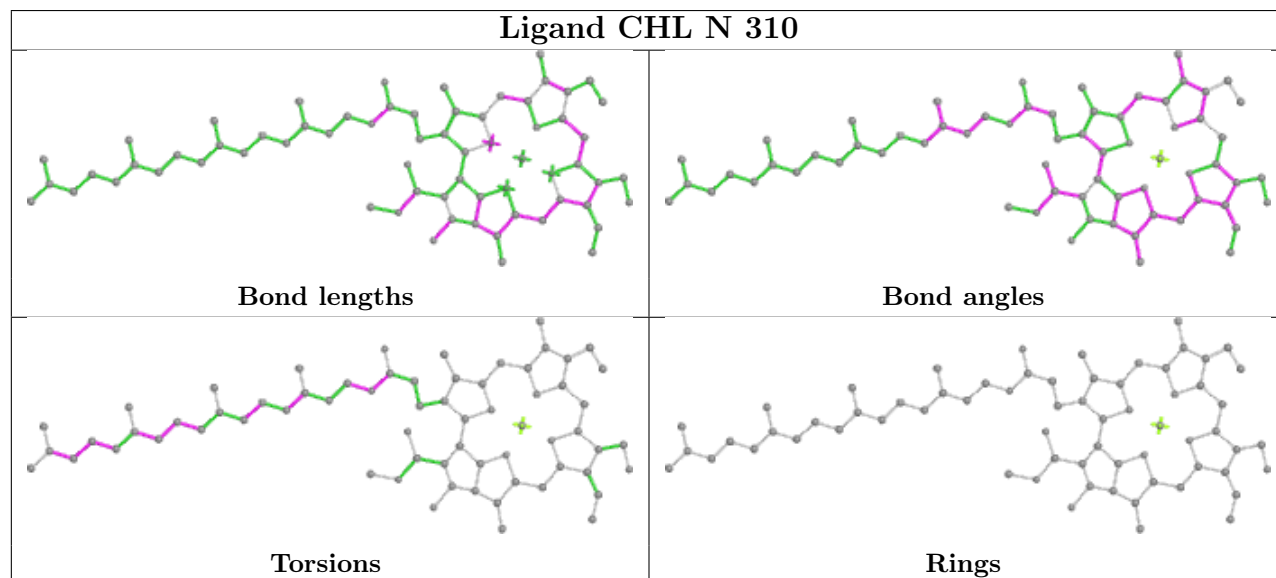


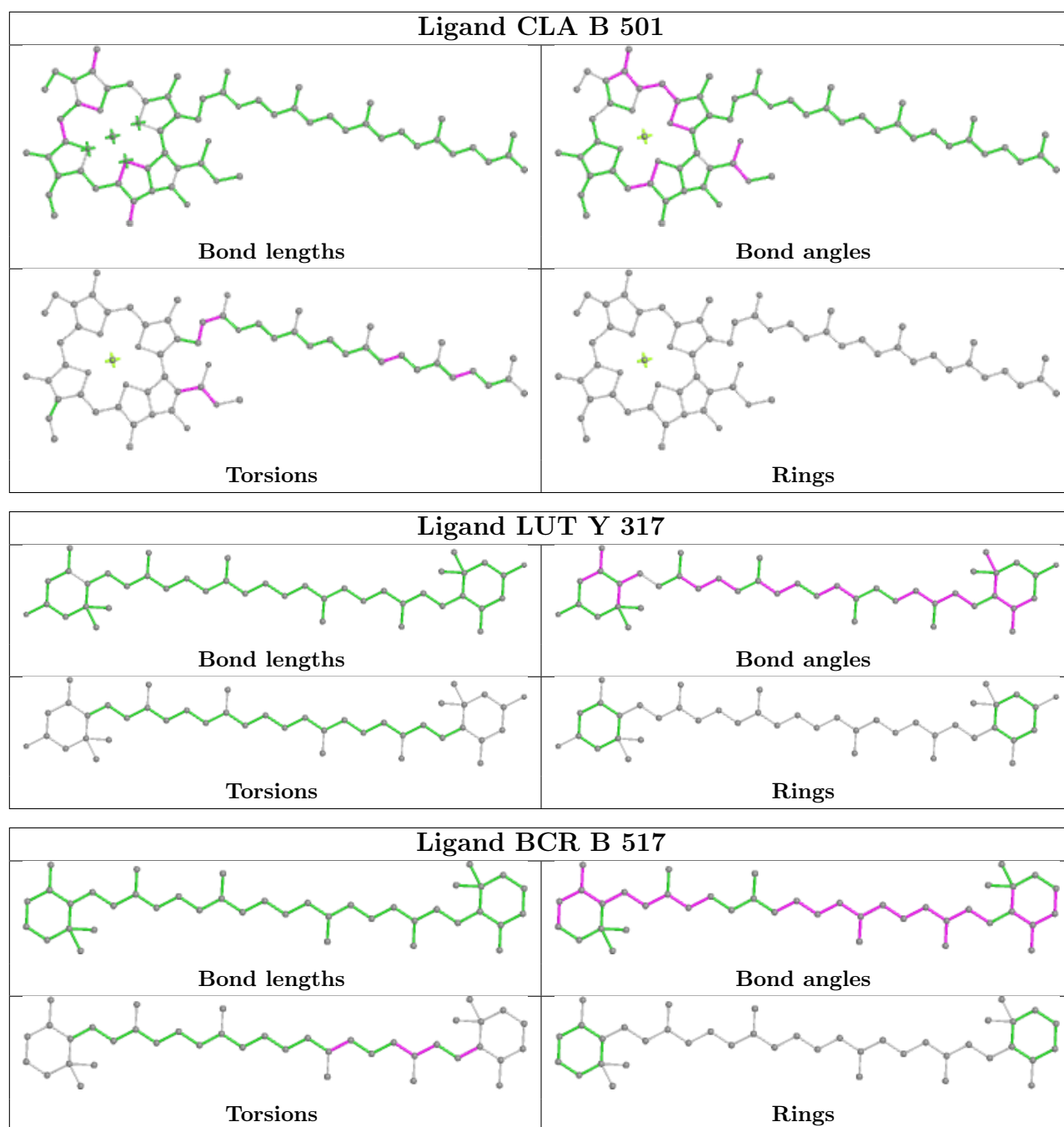
Torsions

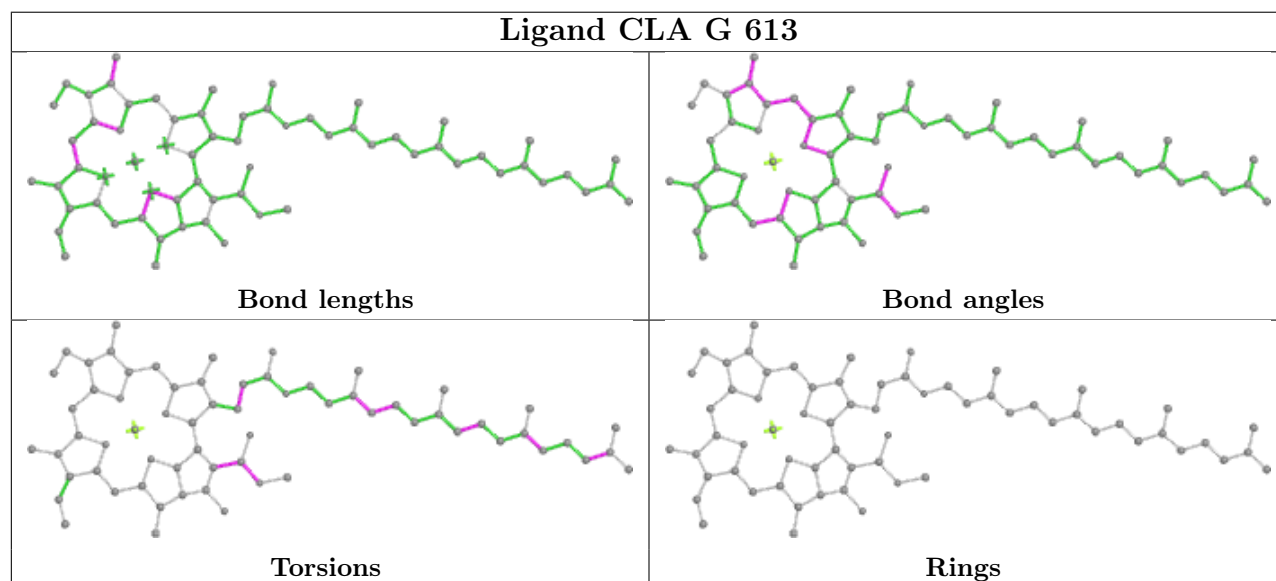
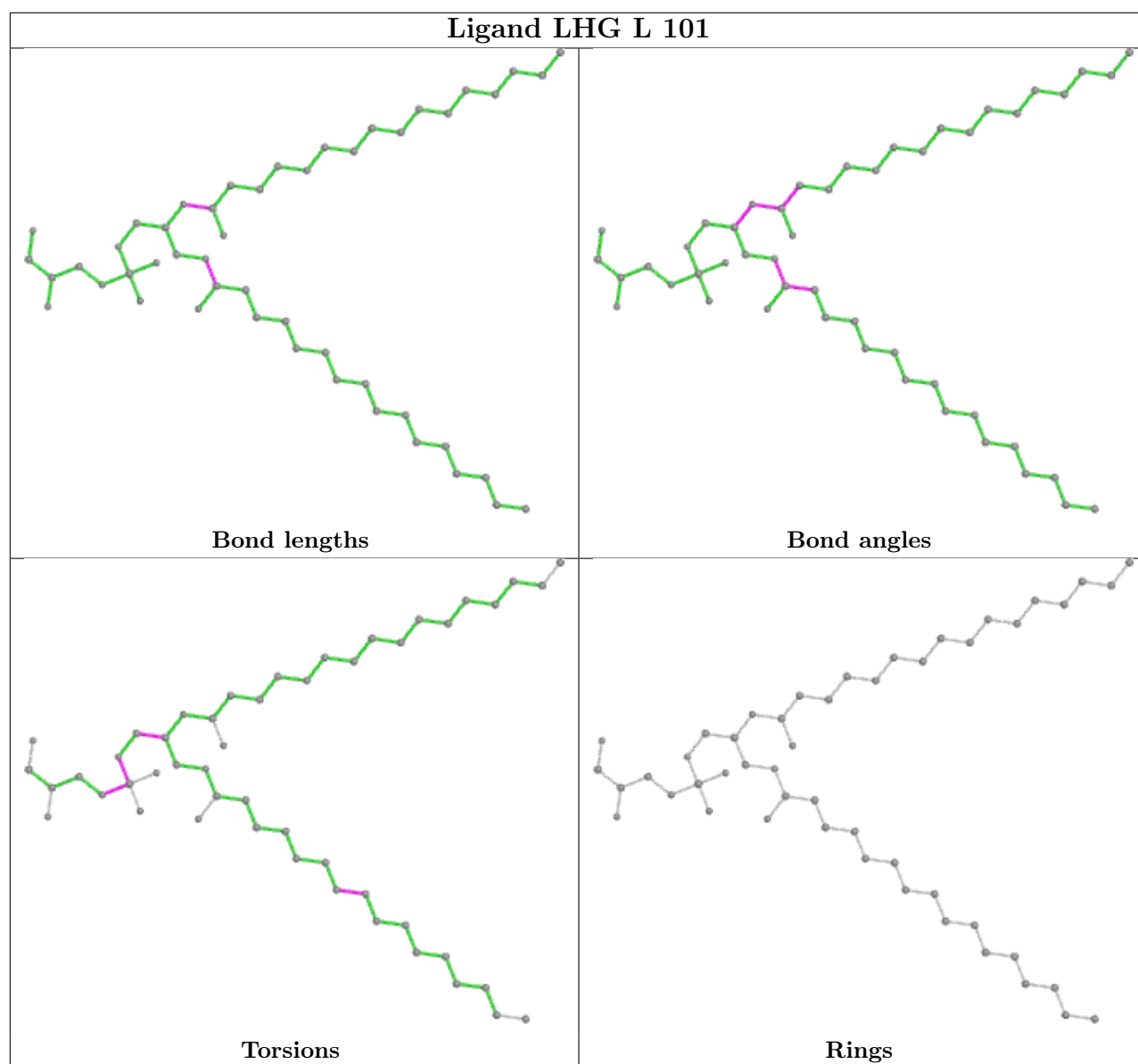


Rings

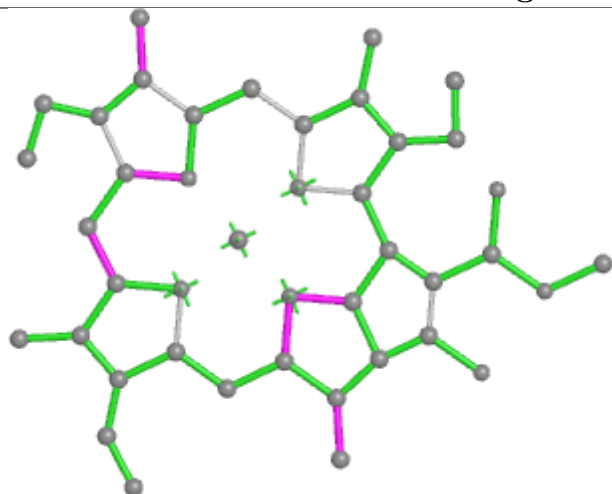


Ligand CLA A 402**Ligand CLA C 504****Ligand CHL N 310**

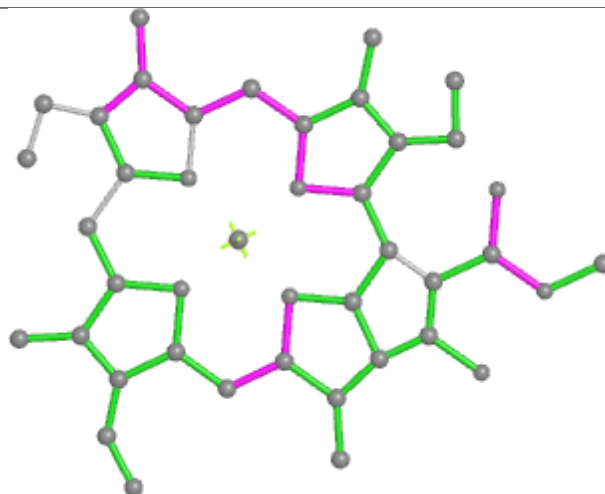




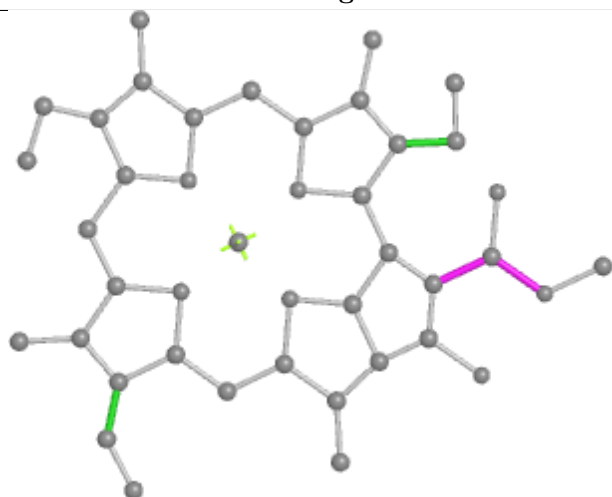
Ligand CLA d 404



Bond lengths



Bond angles

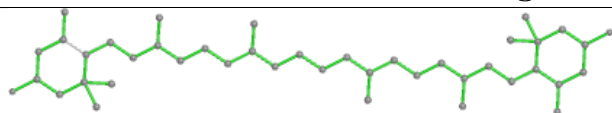


Torsions

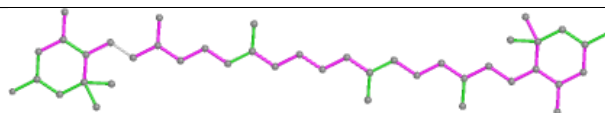


Rings

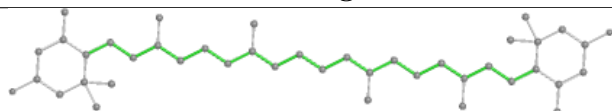
Ligand LUT S 616



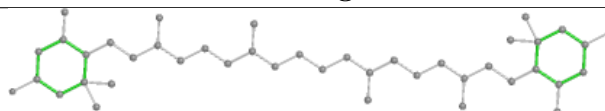
Bond lengths



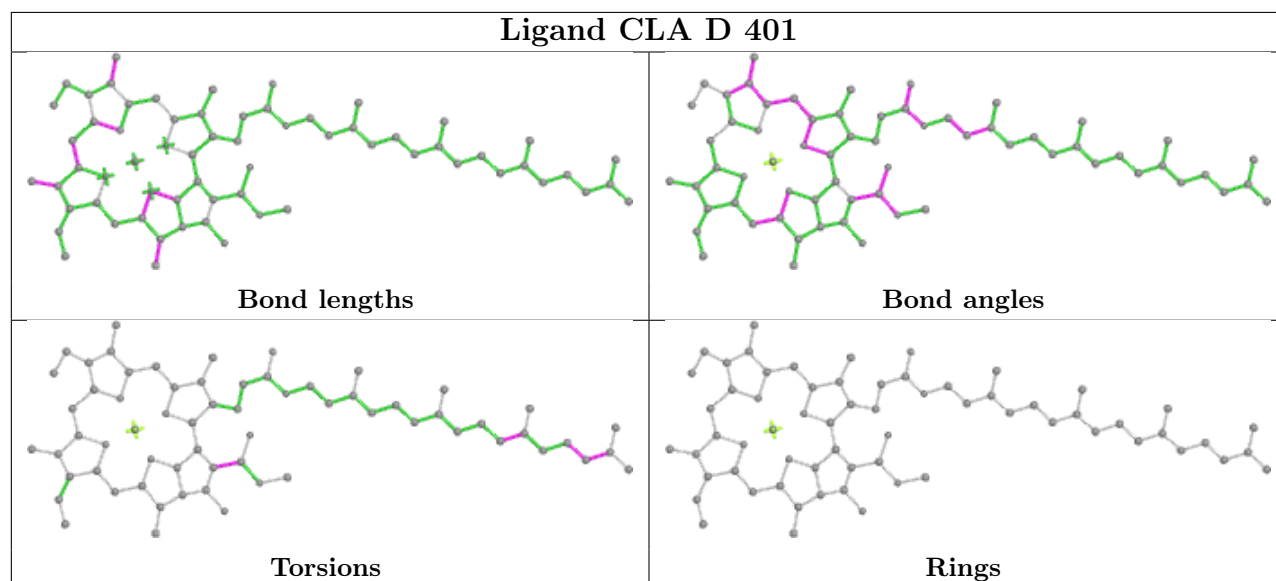
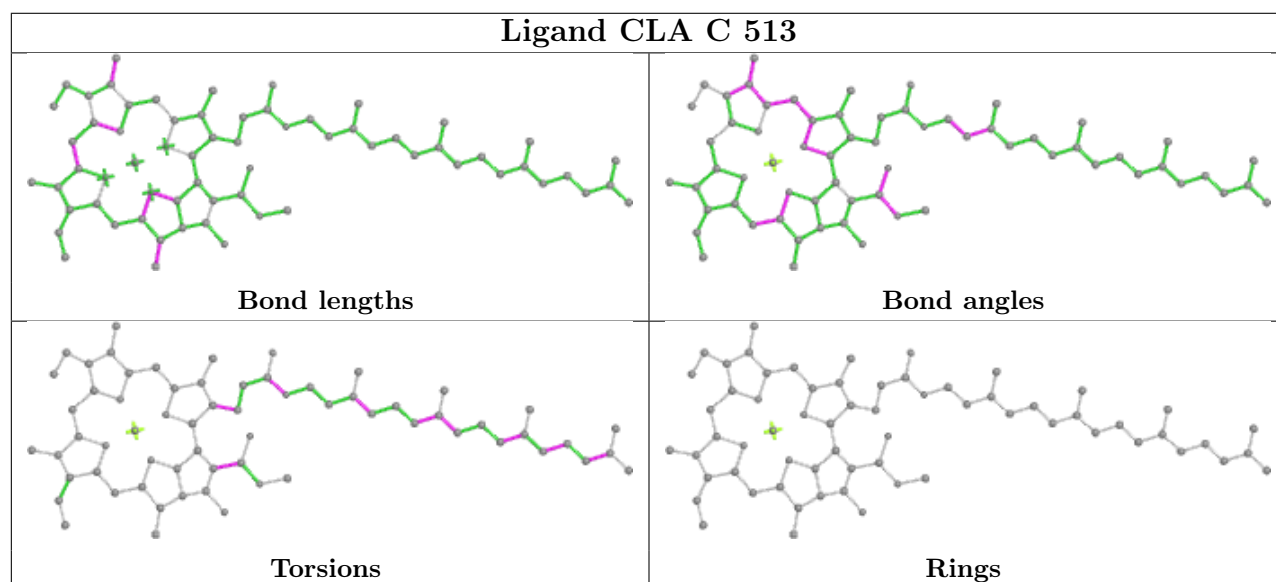
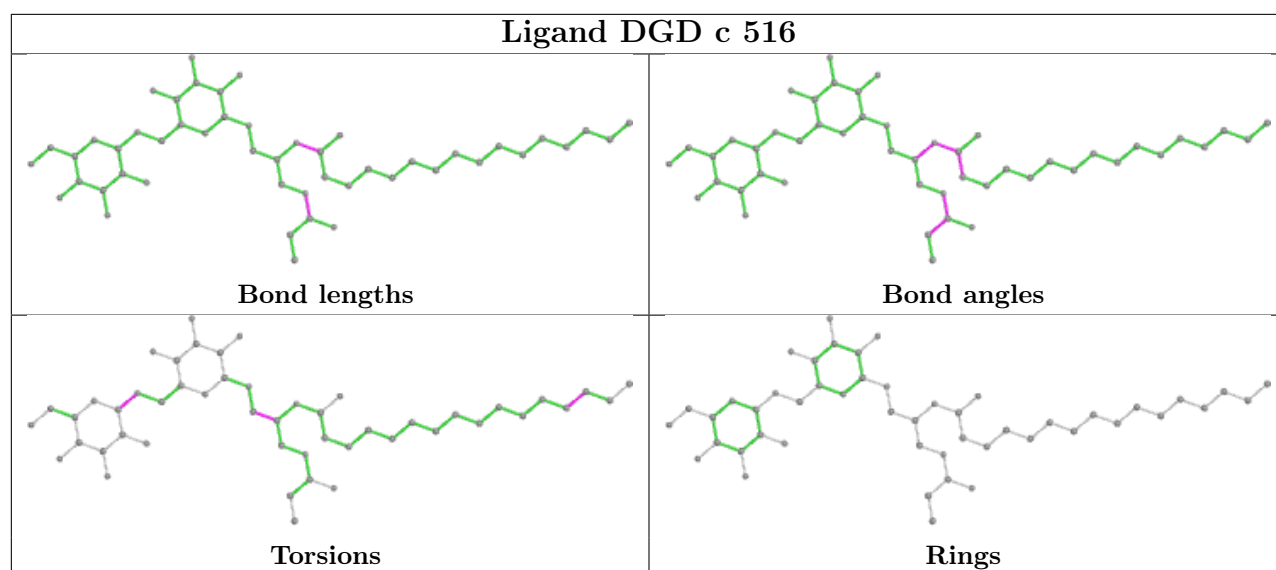
Bond angles



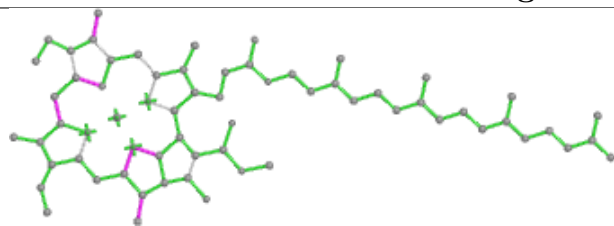
Torsions



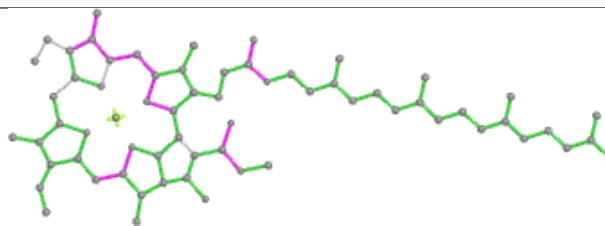
Rings



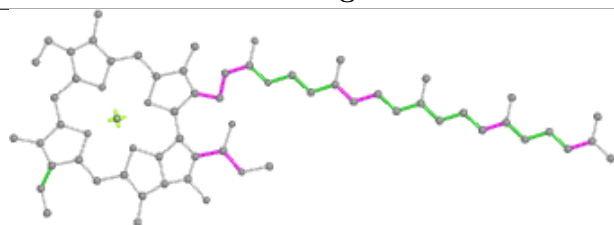
Ligand CLA b 507



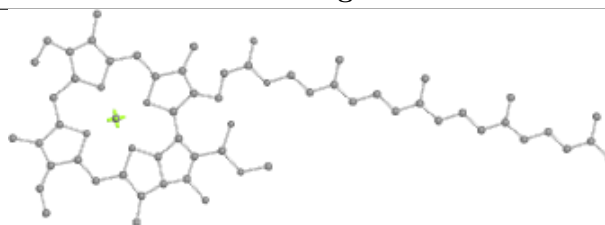
Bond lengths



Bond angles

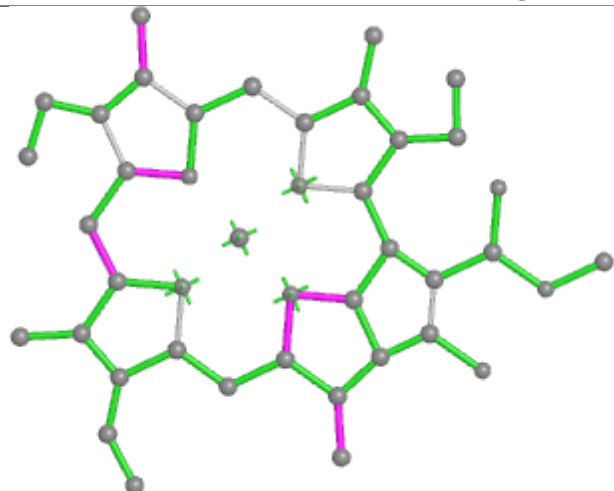


Torsions

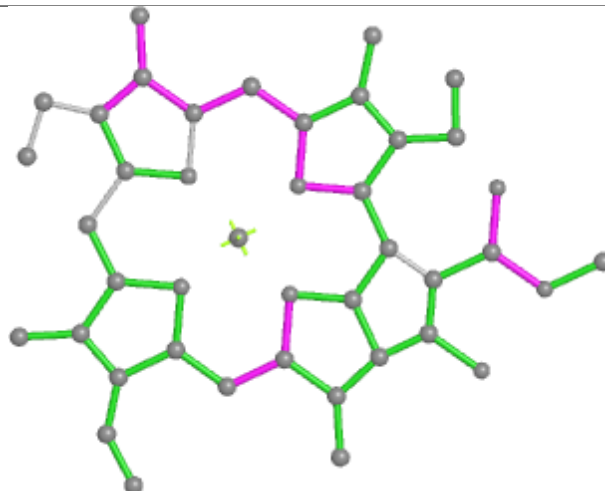


Rings

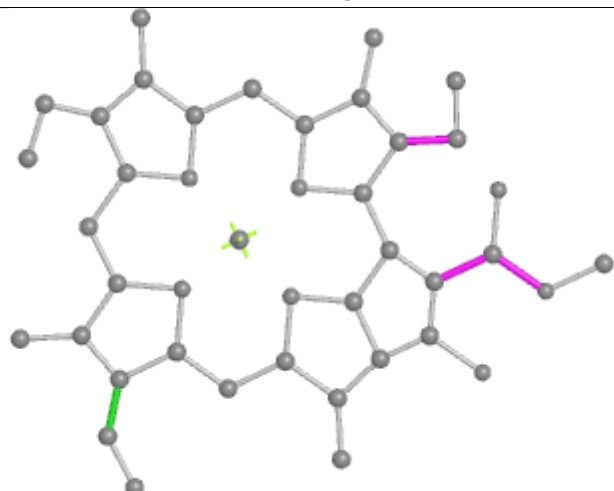
Ligand CLA N 315



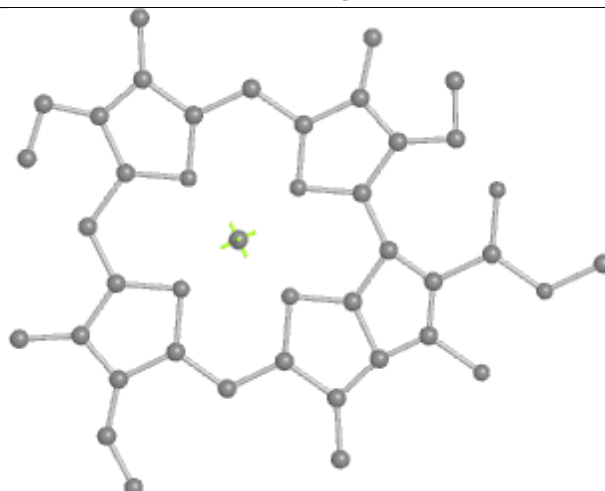
Bond lengths



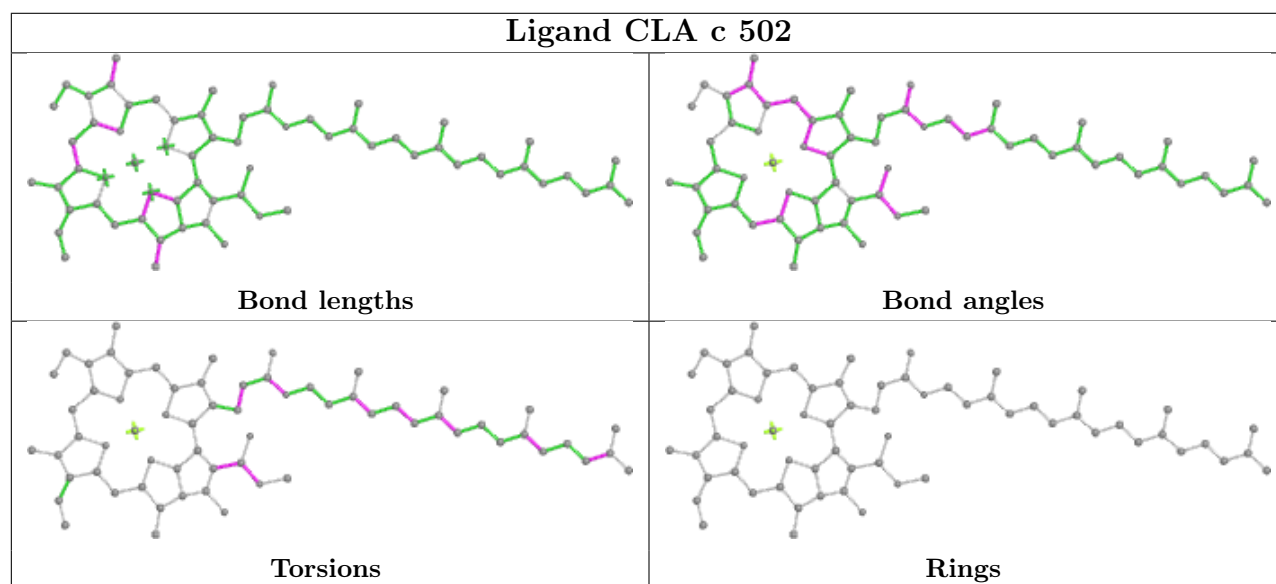
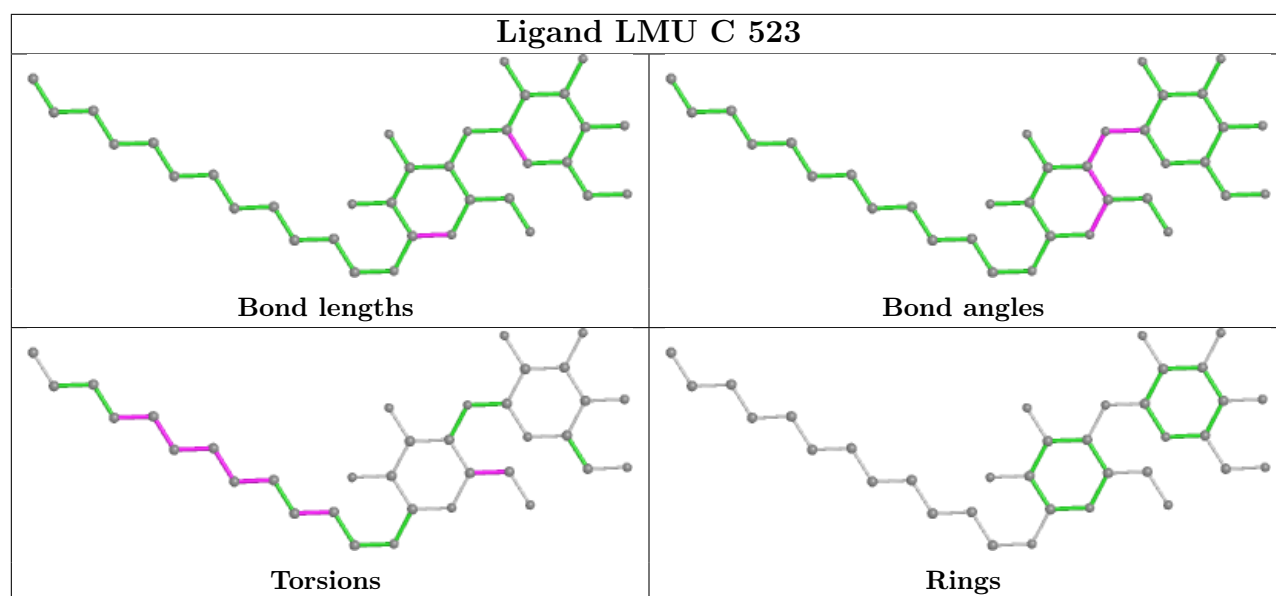
Bond angles

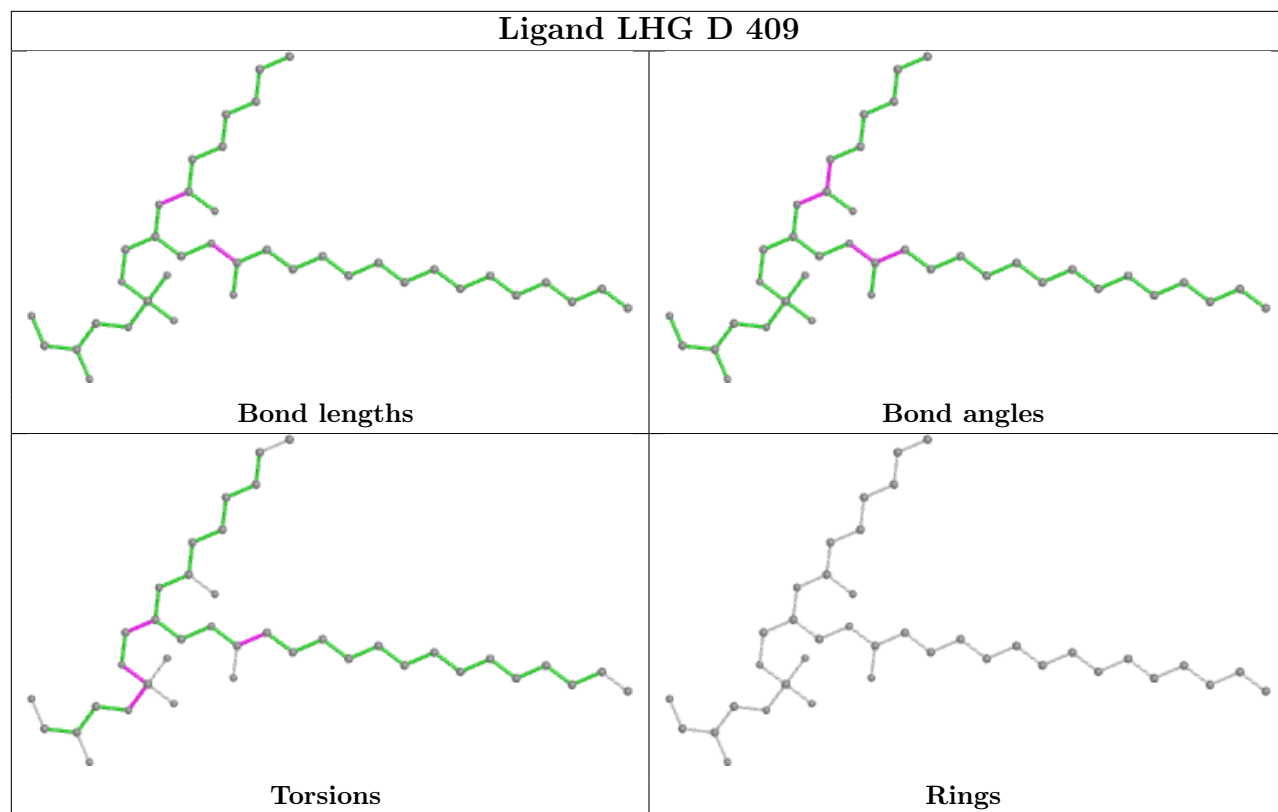


Torsions

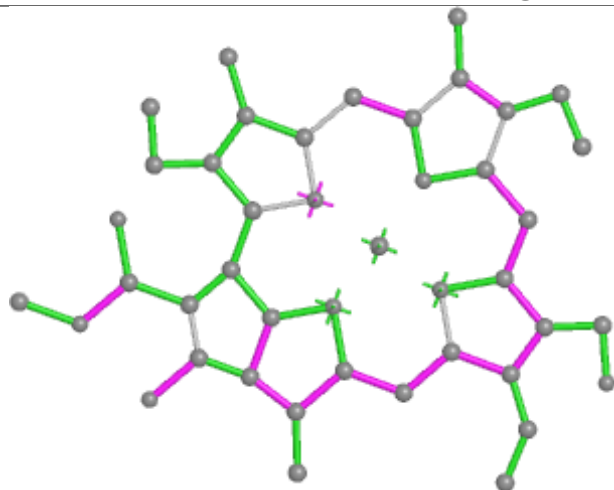


Rings

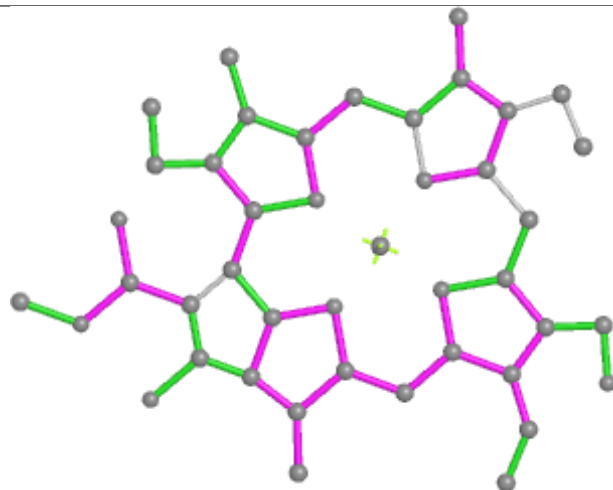




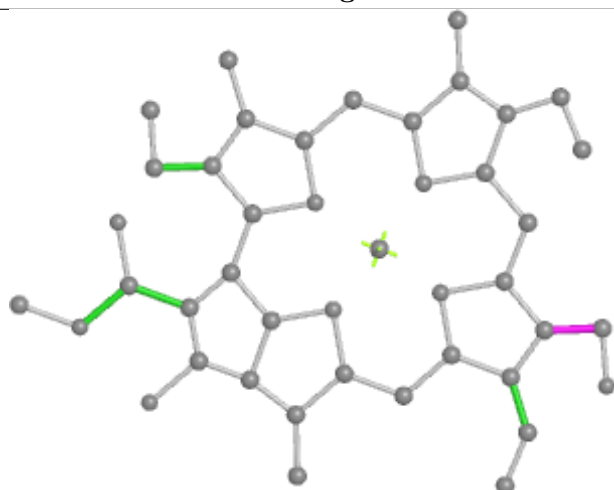
Ligand CHL S 607



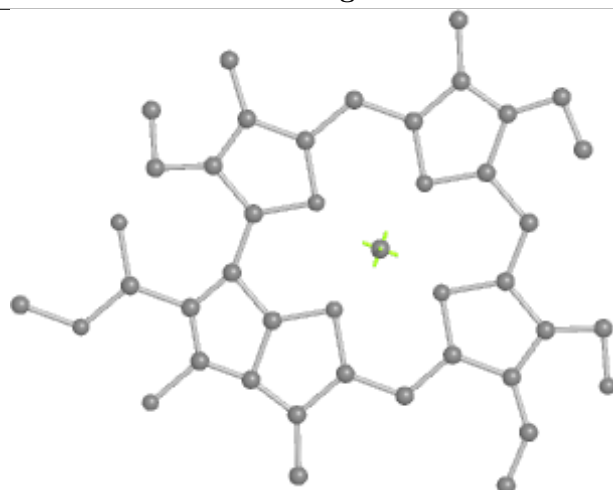
Bond lengths



Bond angles

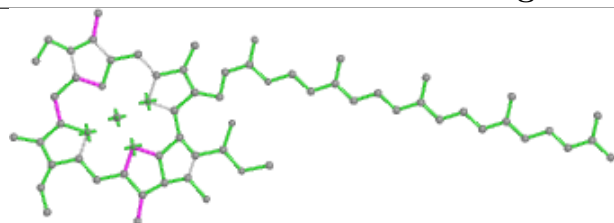


Torsions

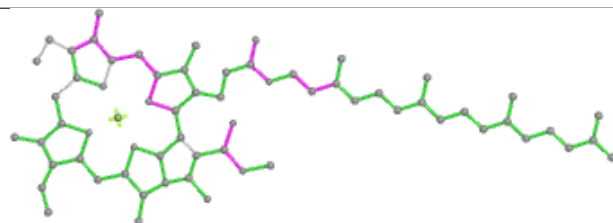


Rings

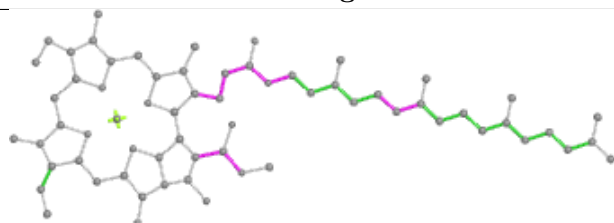
Ligand CLA b 509



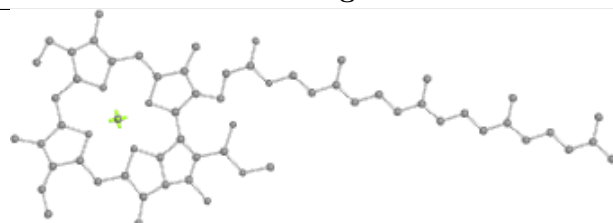
Bond lengths



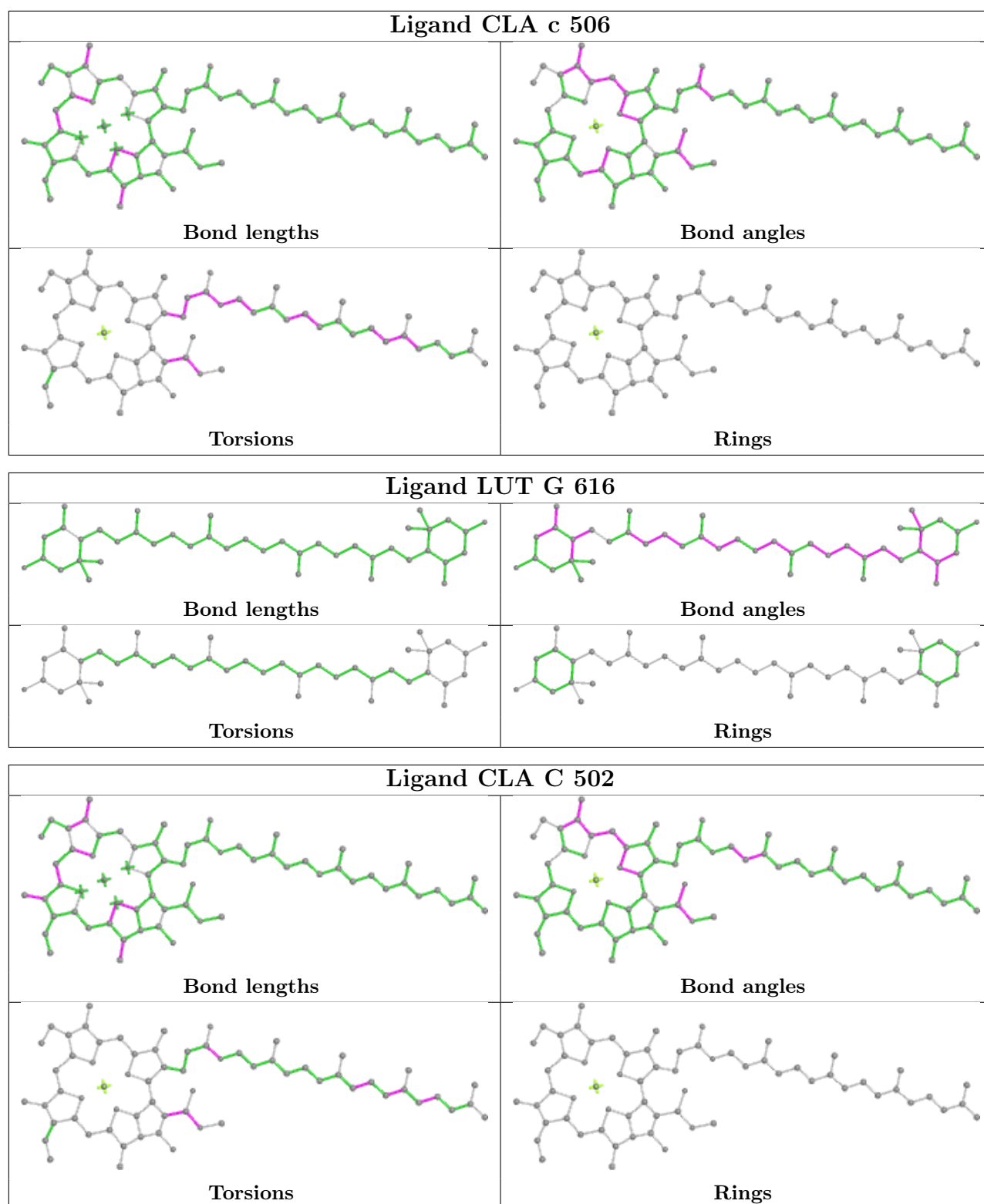
Bond angles

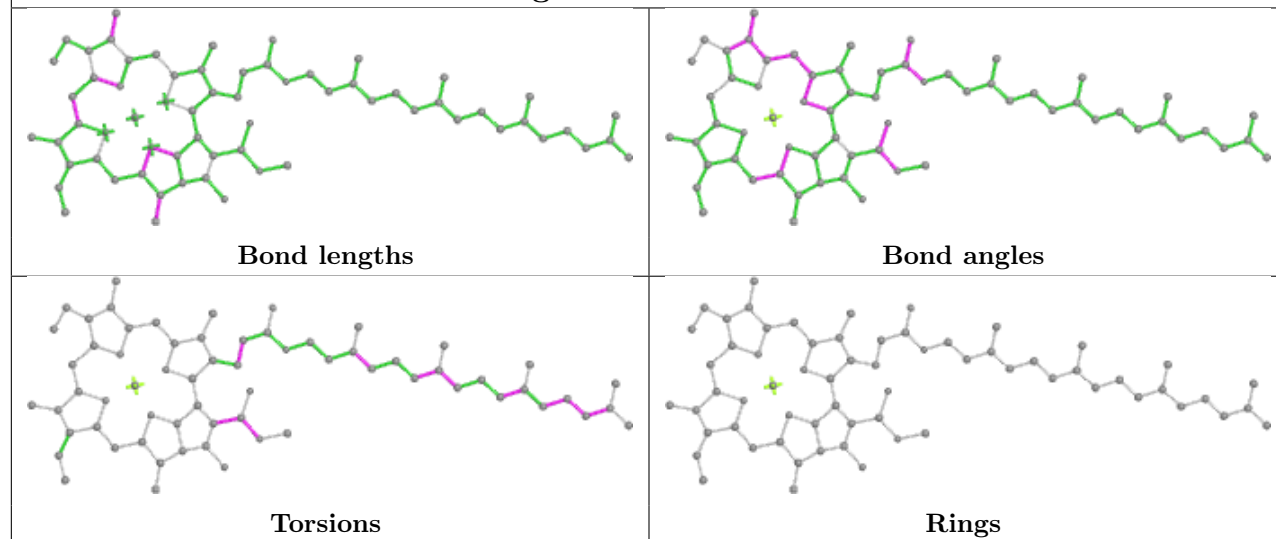
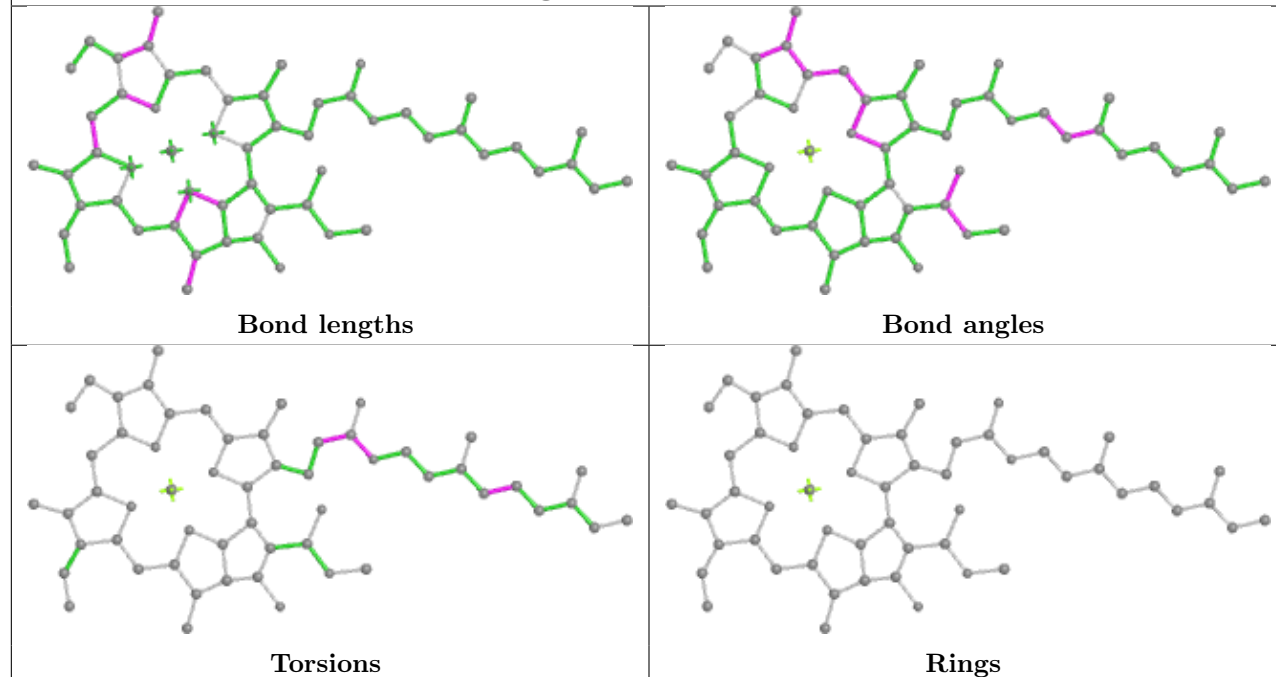


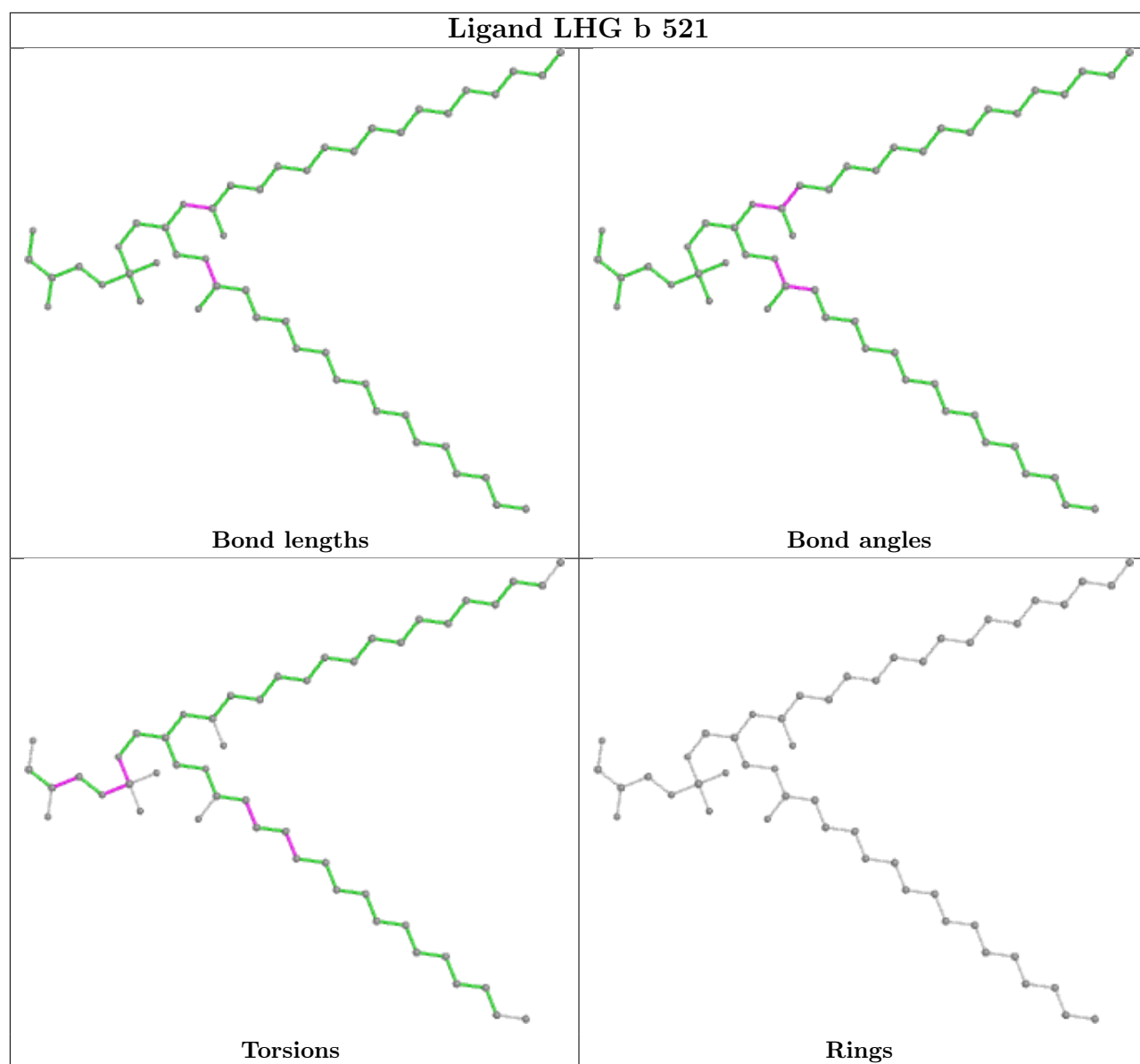
Torsions



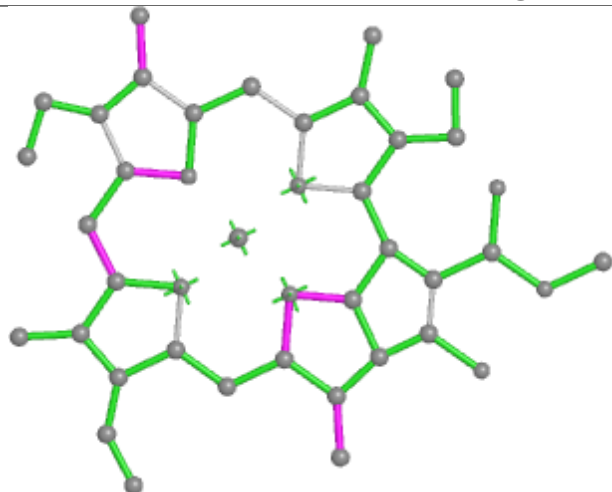
Rings



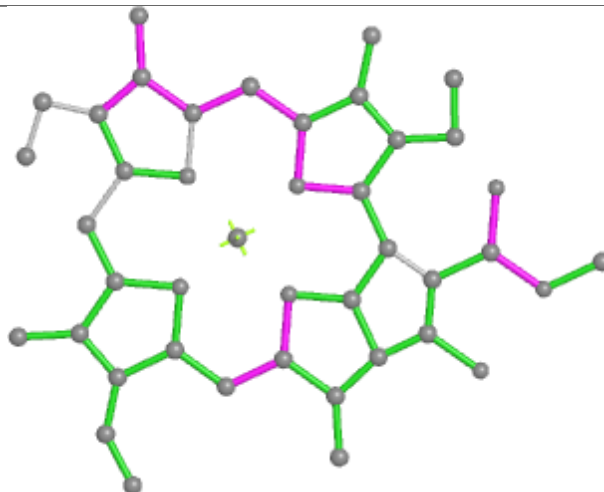
Ligand CLA B 508**Ligand CLA c 512**



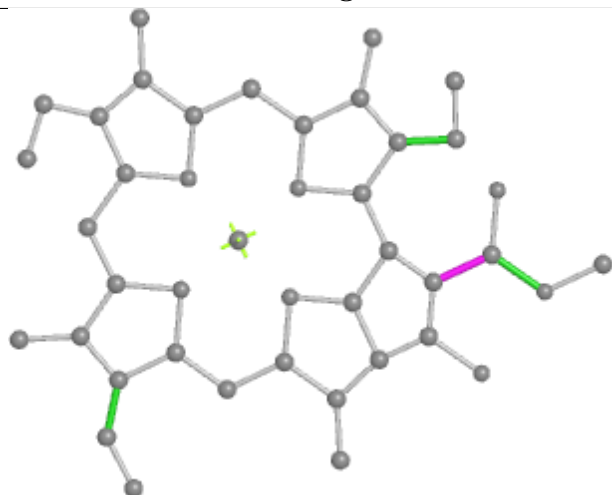
Ligand CLA G 614



Bond lengths



Bond angles

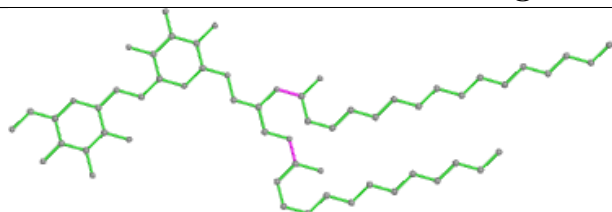


Torsions

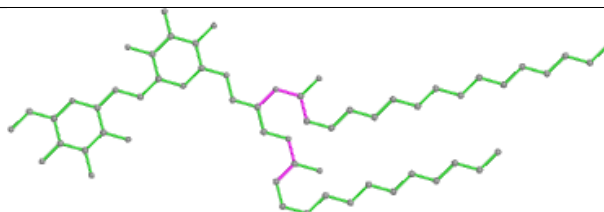


Rings

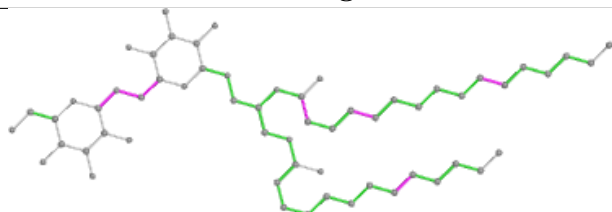
Ligand DGD c 517



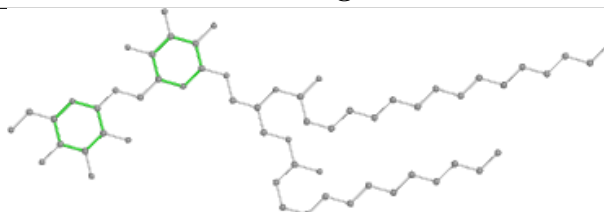
Bond lengths



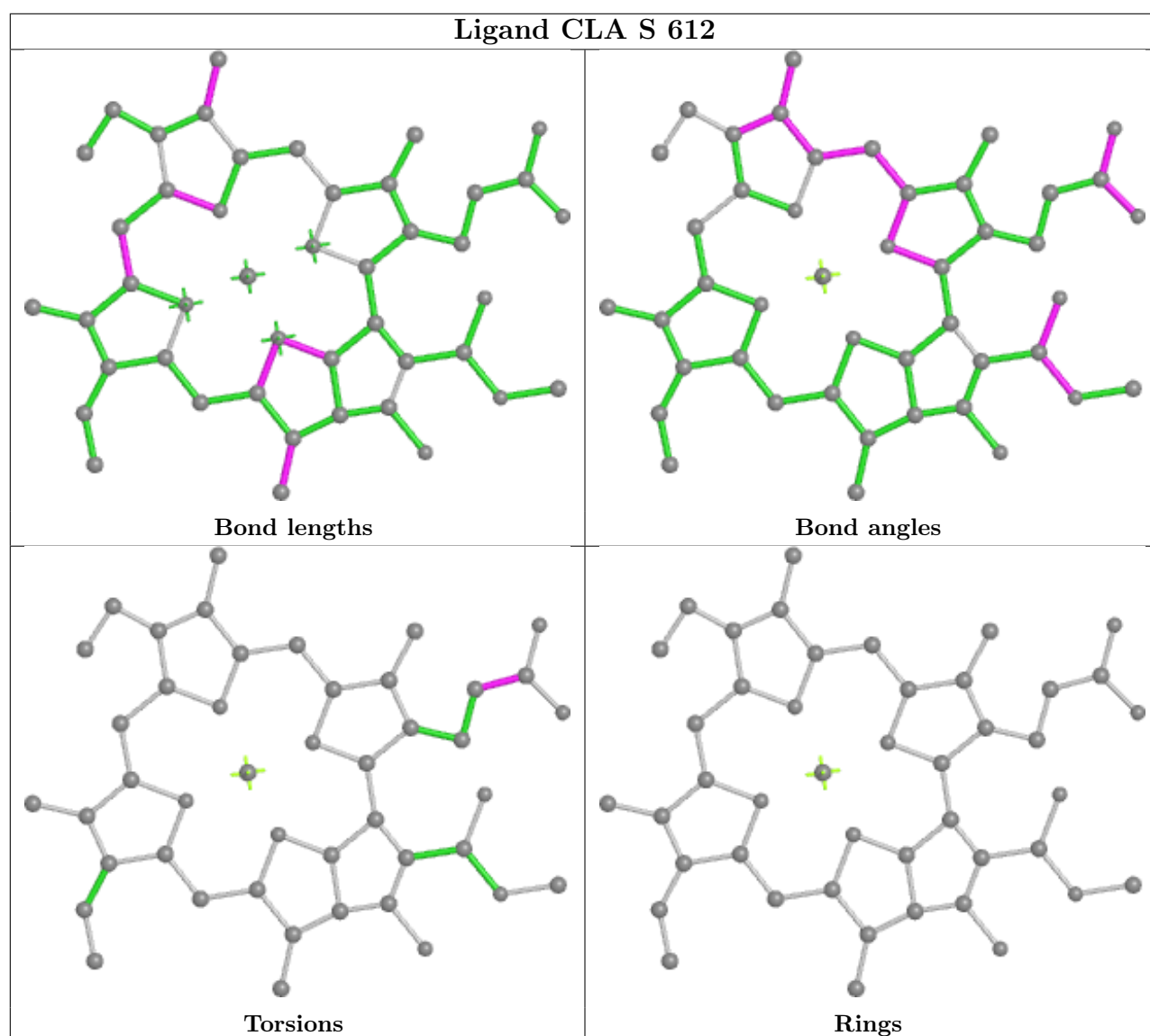
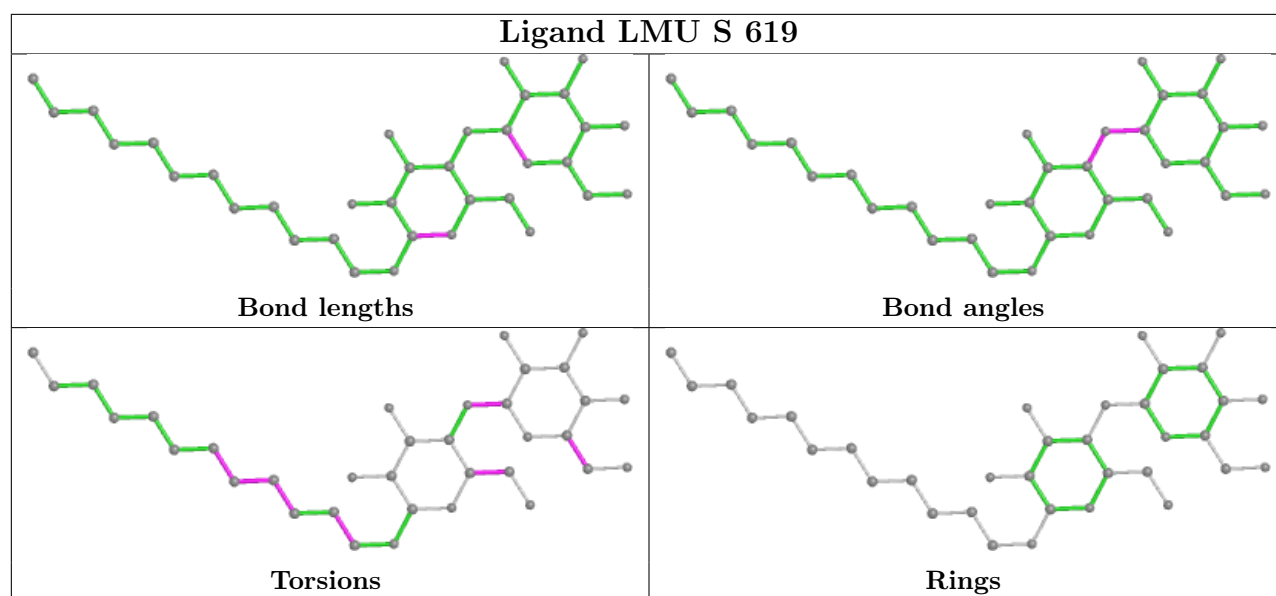
Bond angles



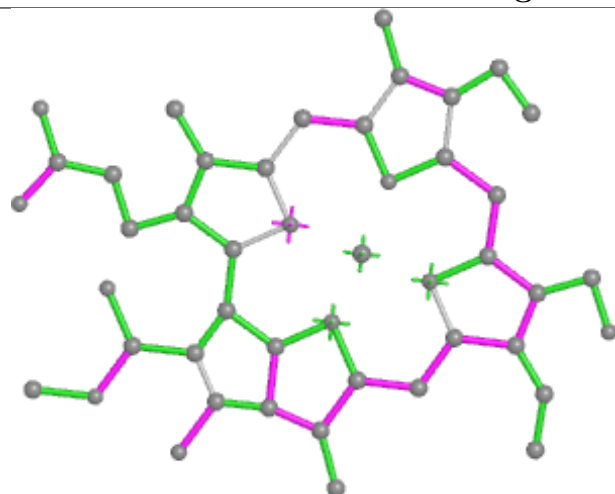
Torsions



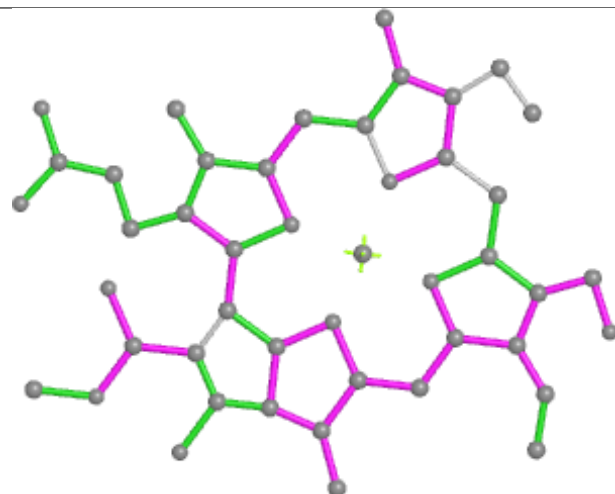
Rings



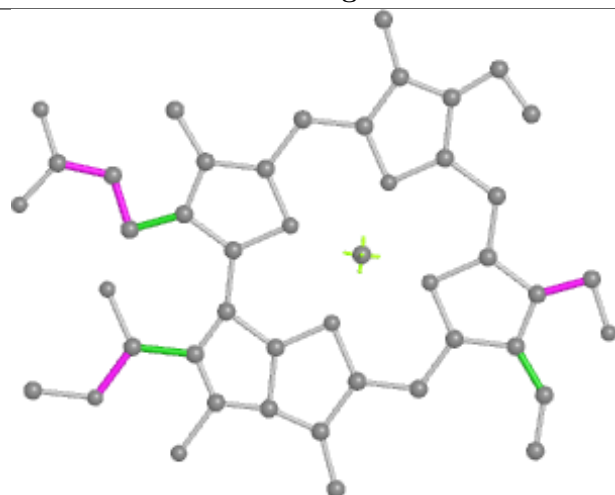
Ligand CHL N 307



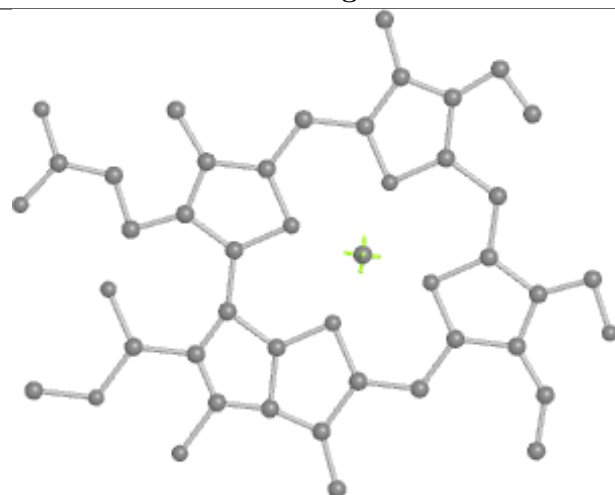
Bond lengths



Bond angles

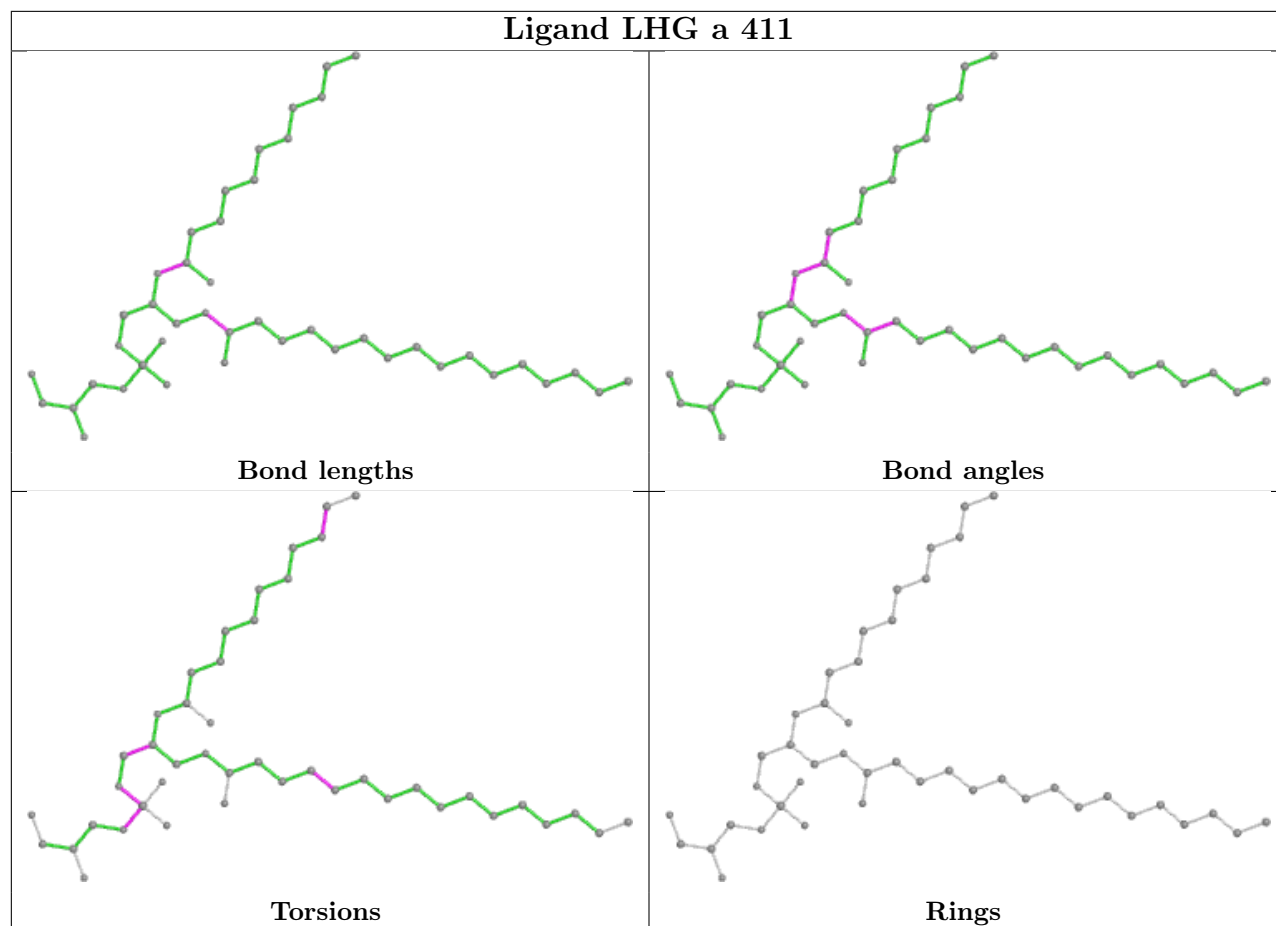


Torsions

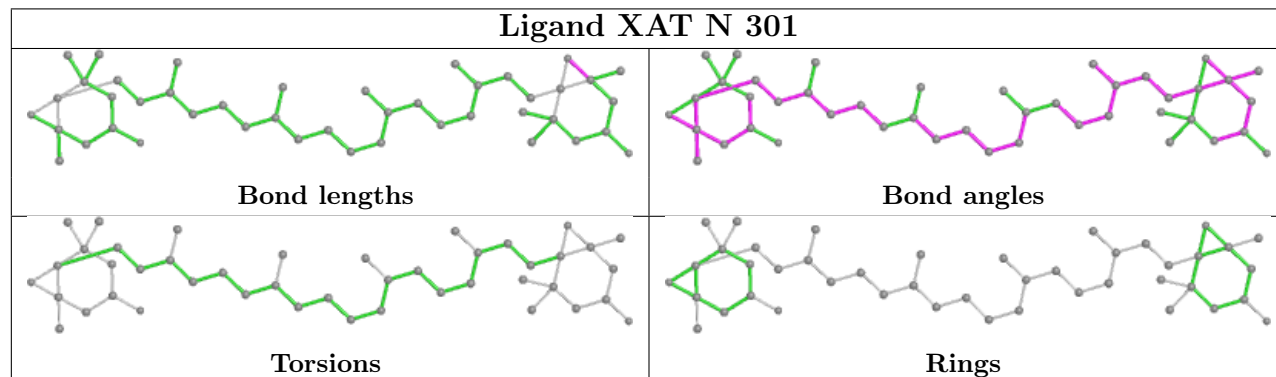


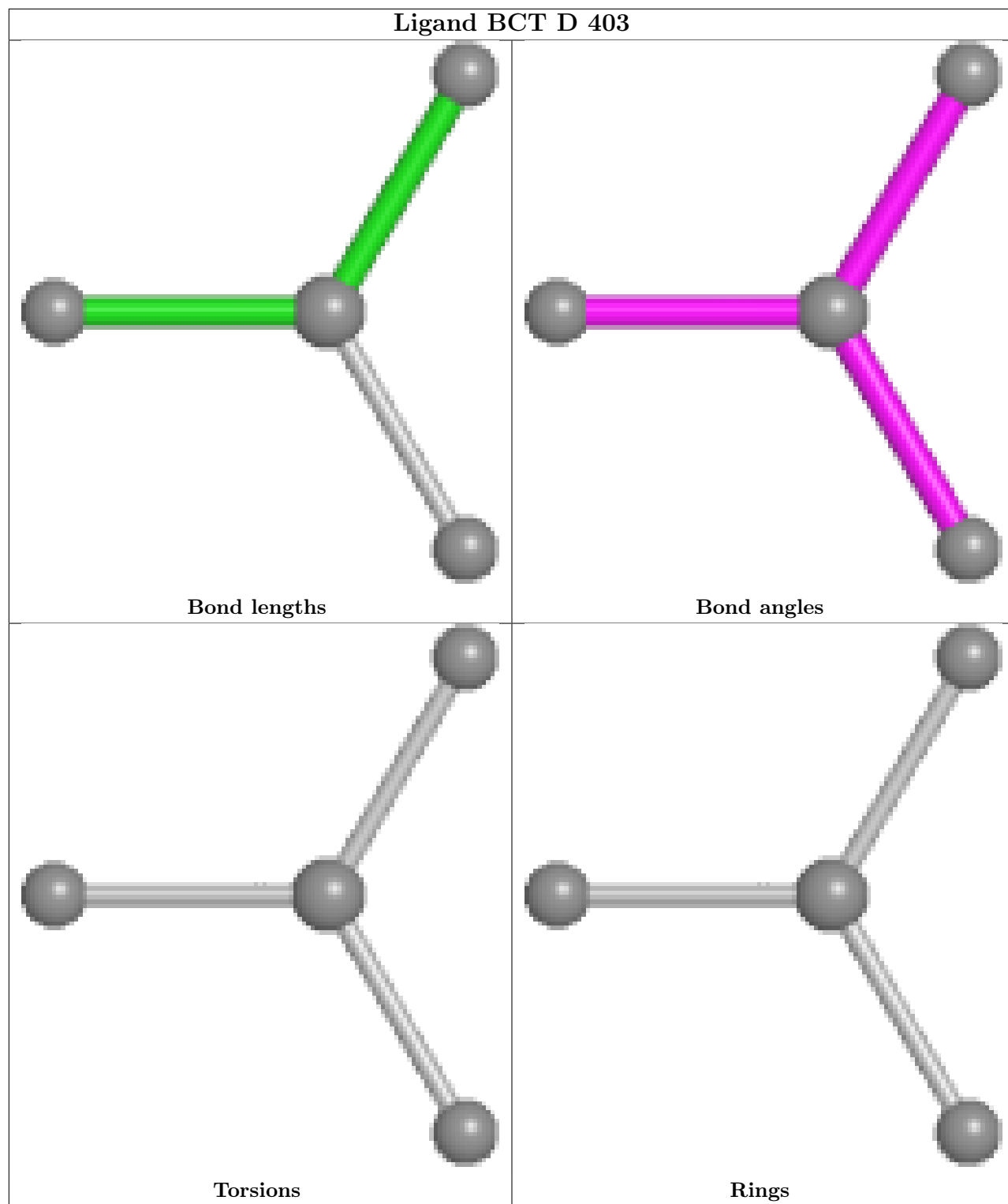
Rings

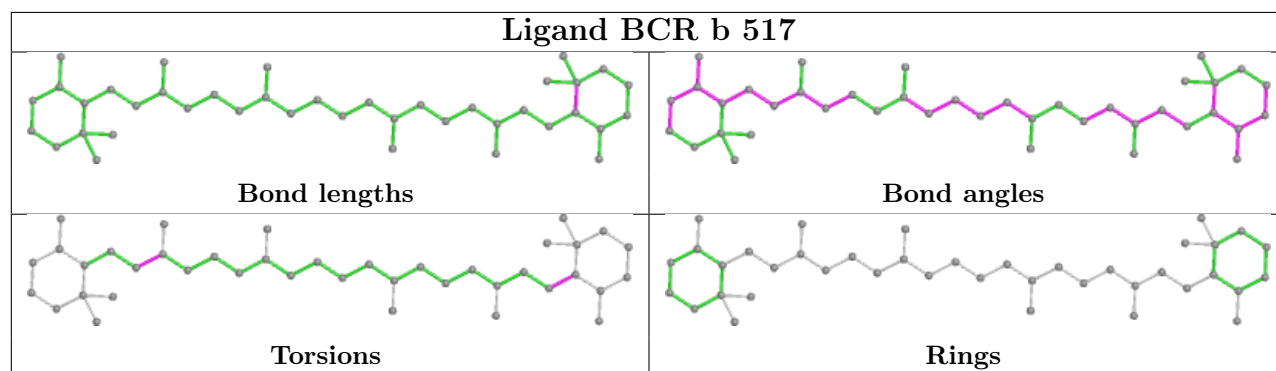
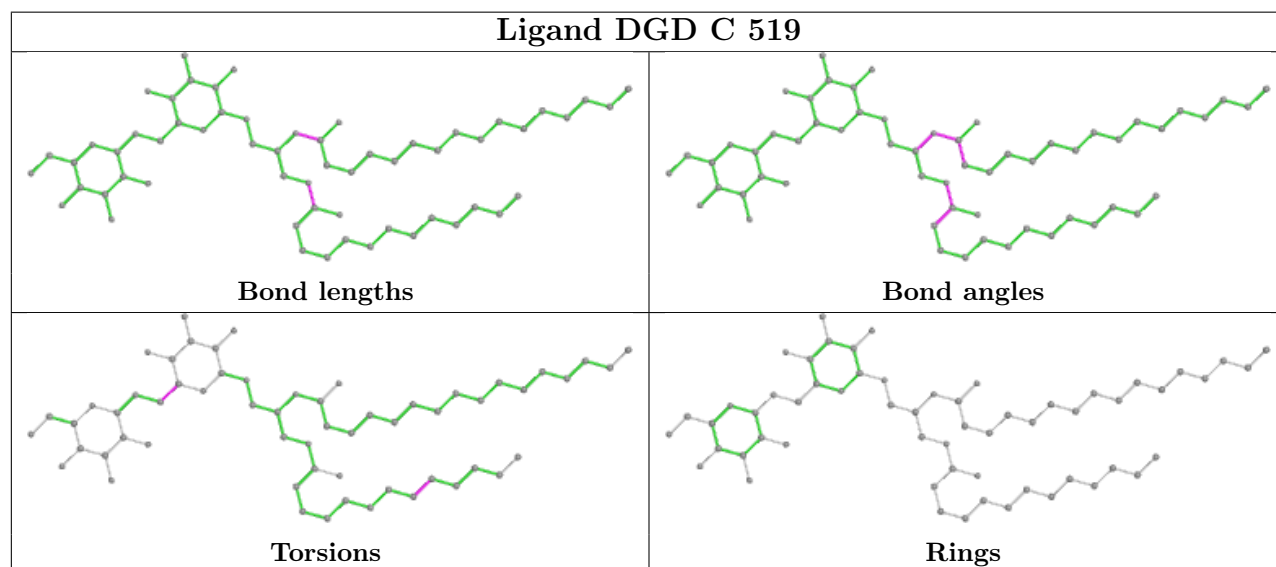
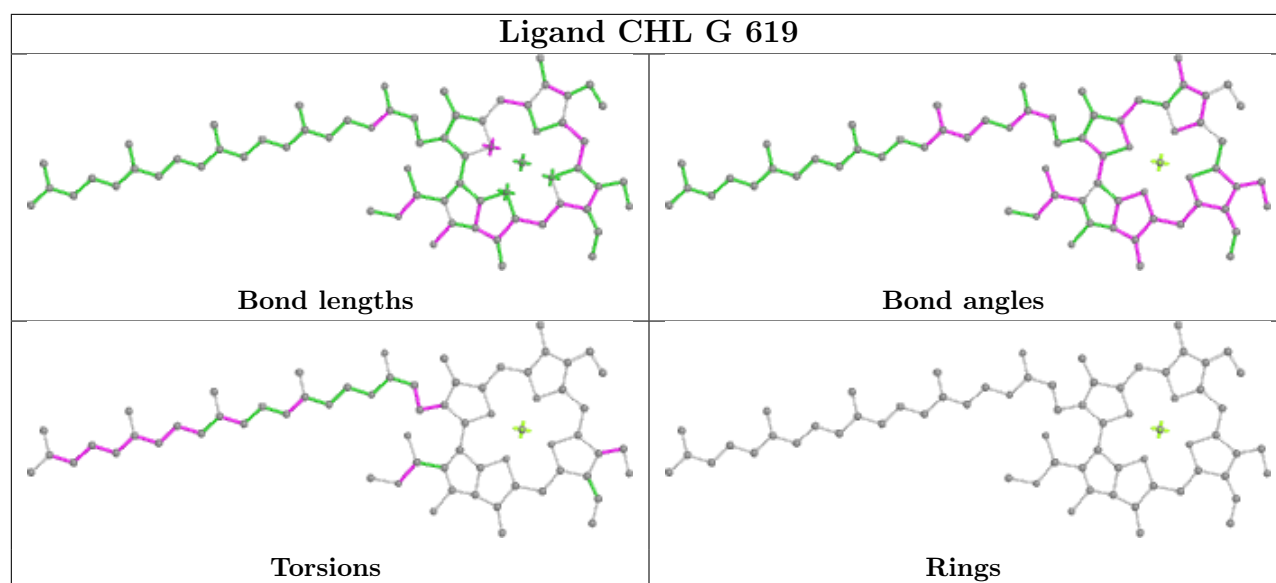
Ligand LHG a 411



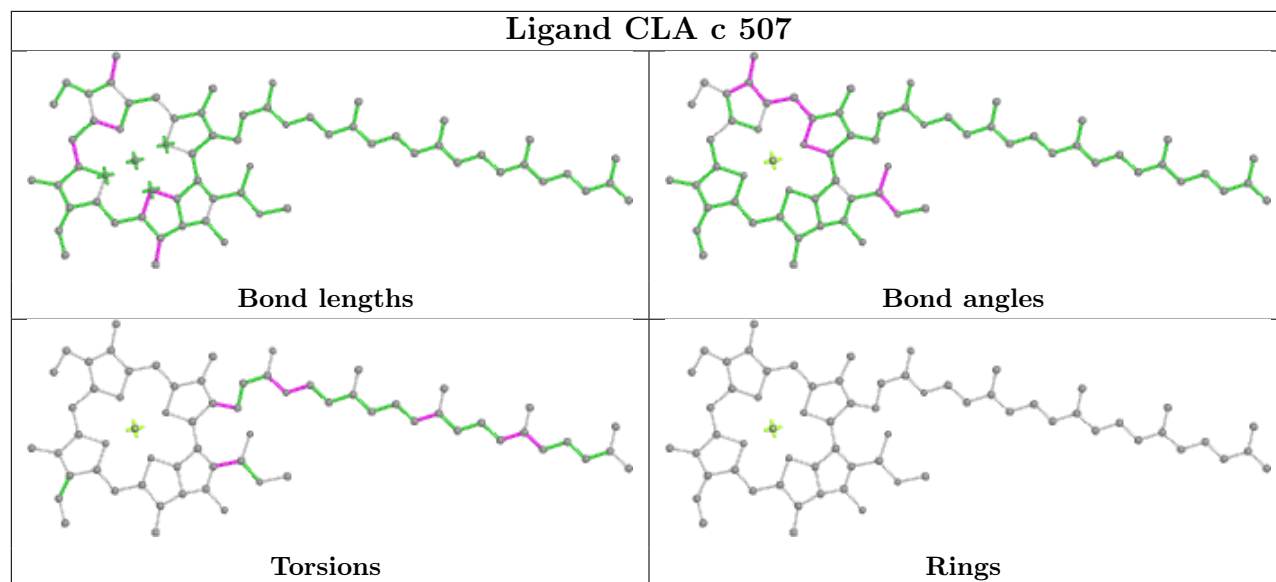
Ligand XAT N 301



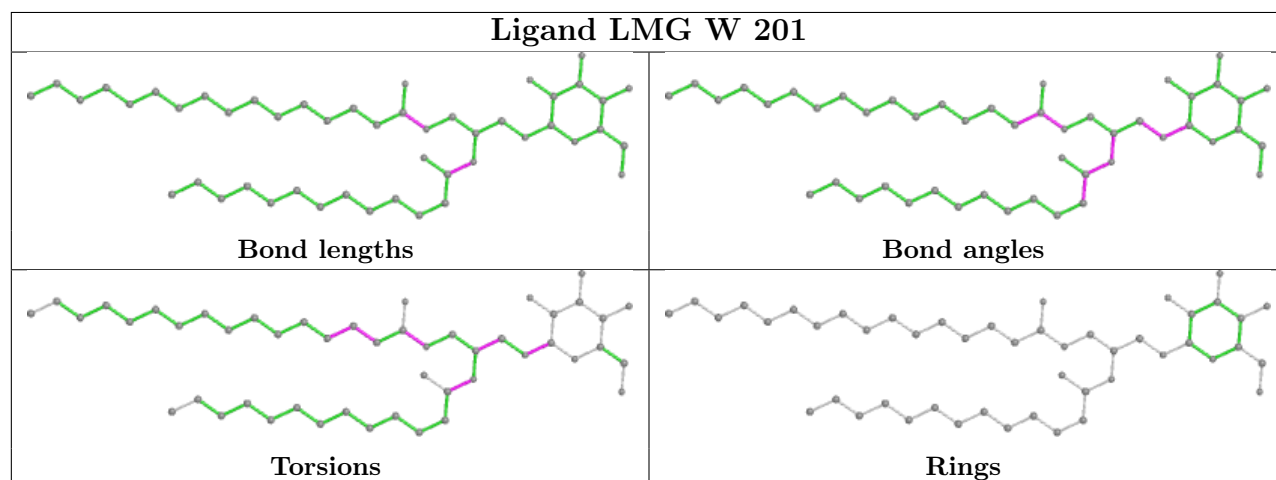




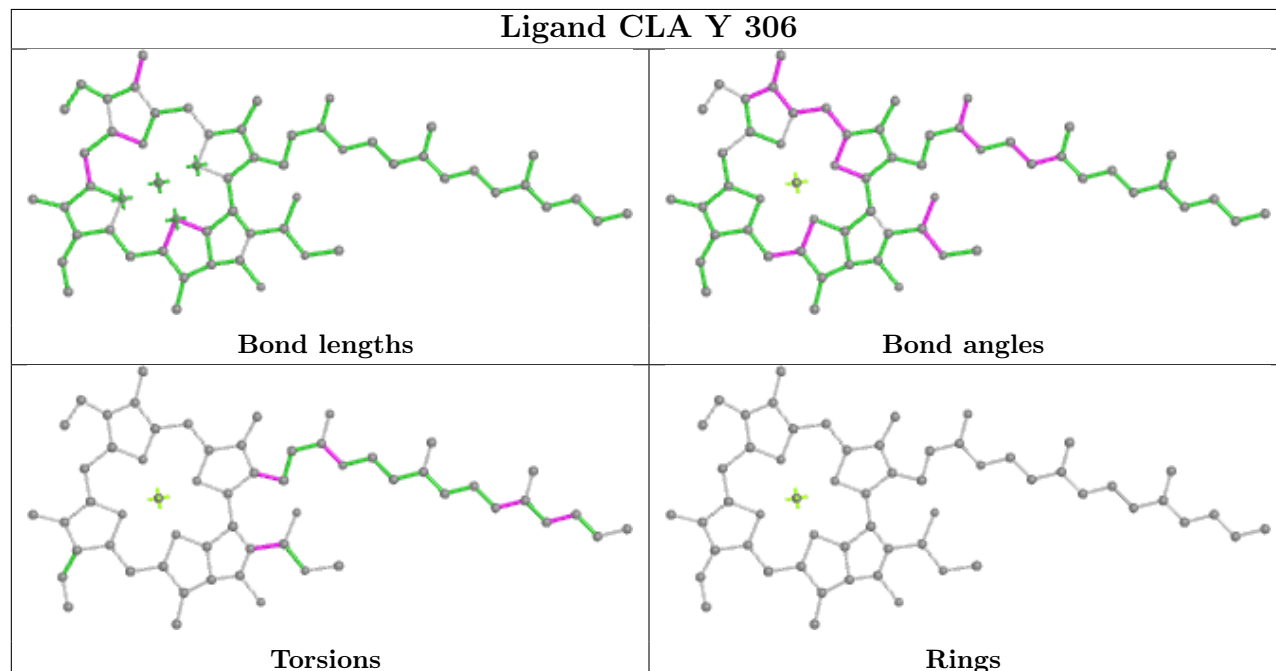
Ligand CLA c 507



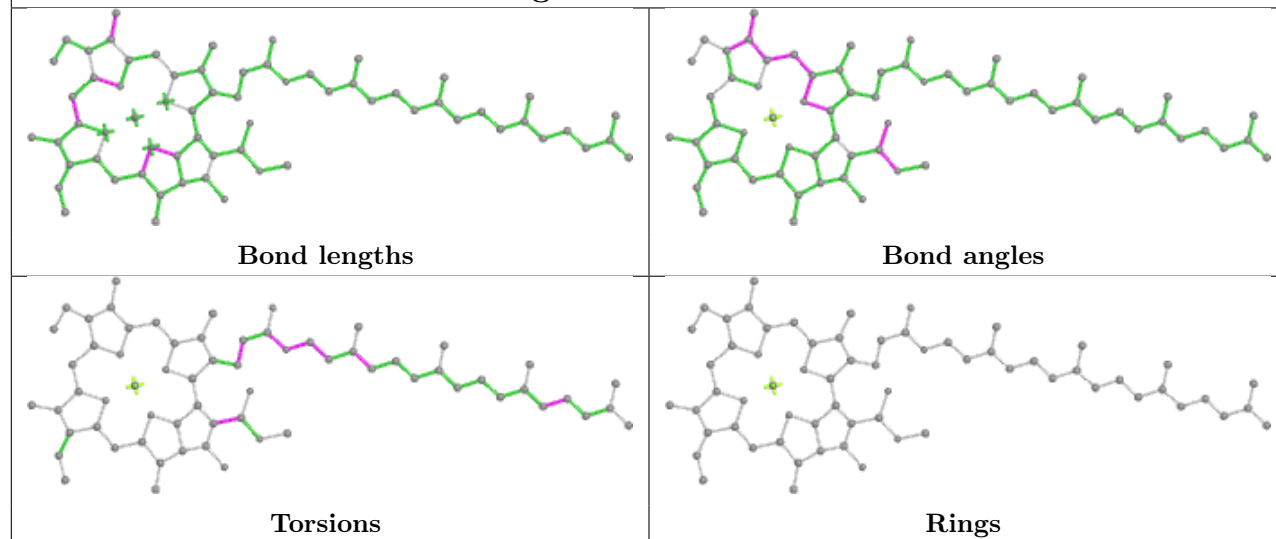
Ligand LMG W 201



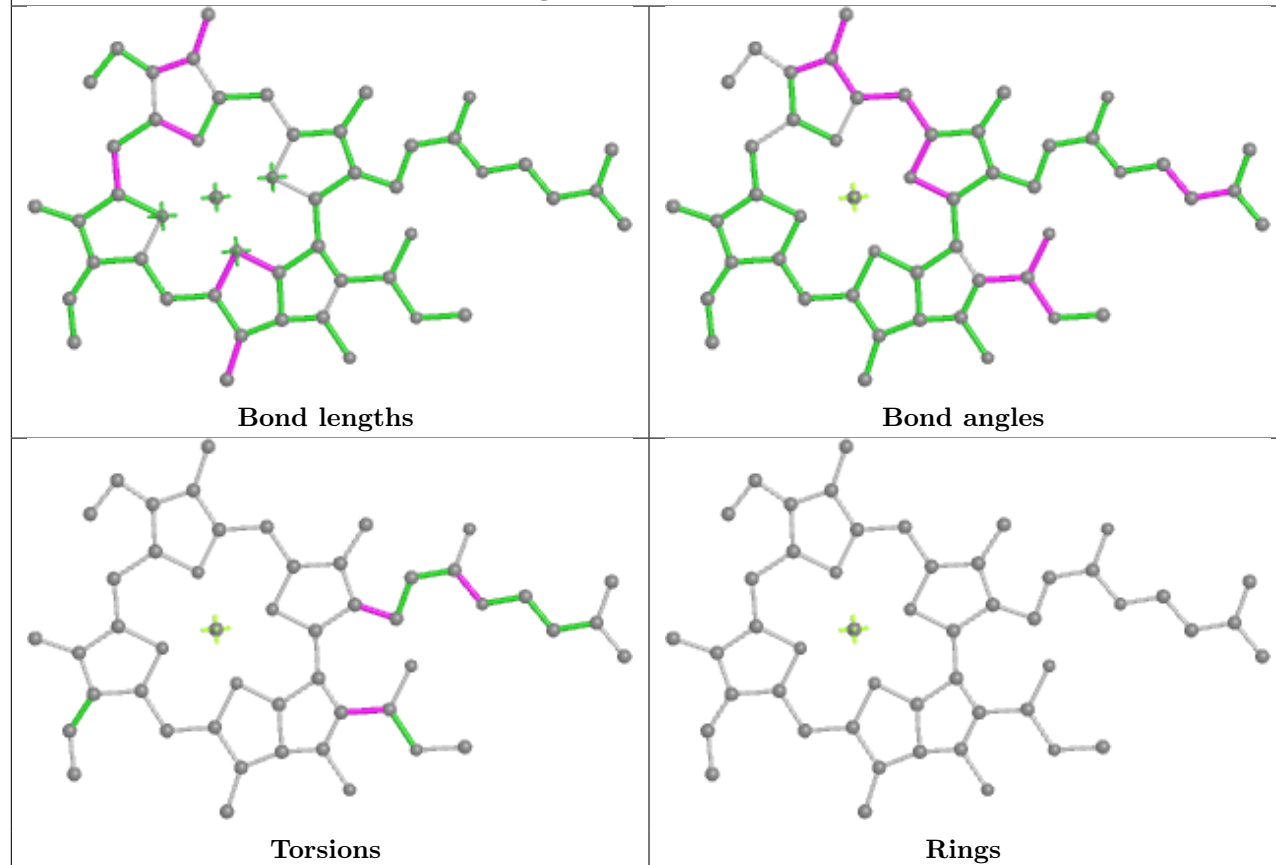
Ligand CLA Y 306



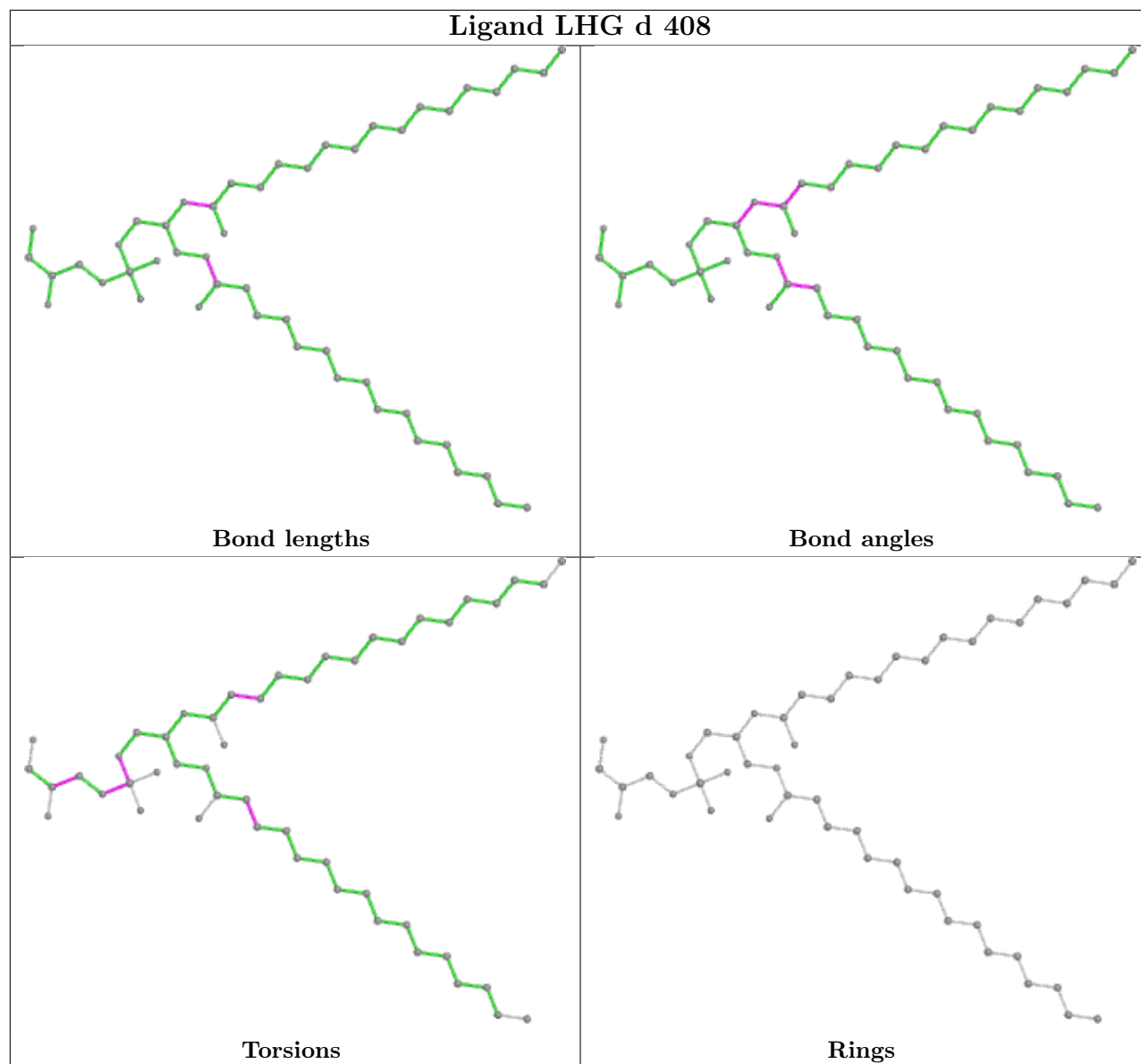
Ligand CLA C 509



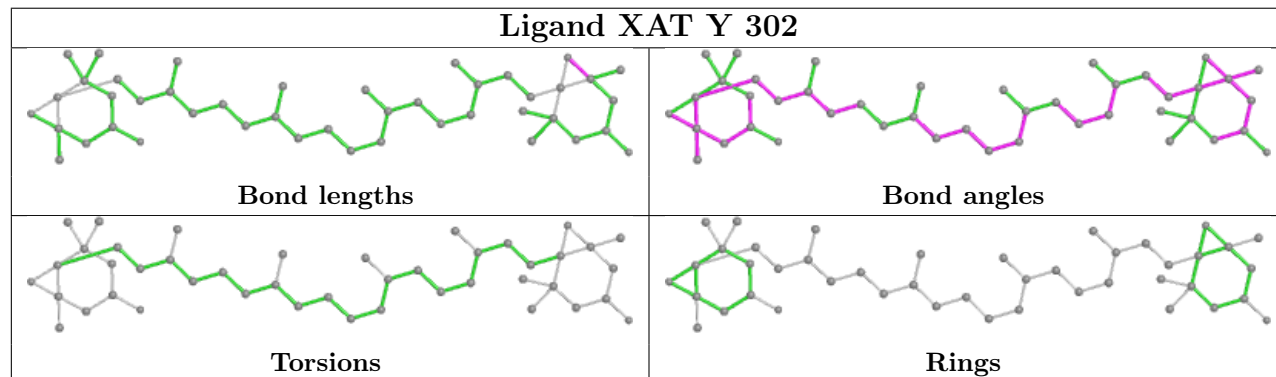
Ligand CLA S 605



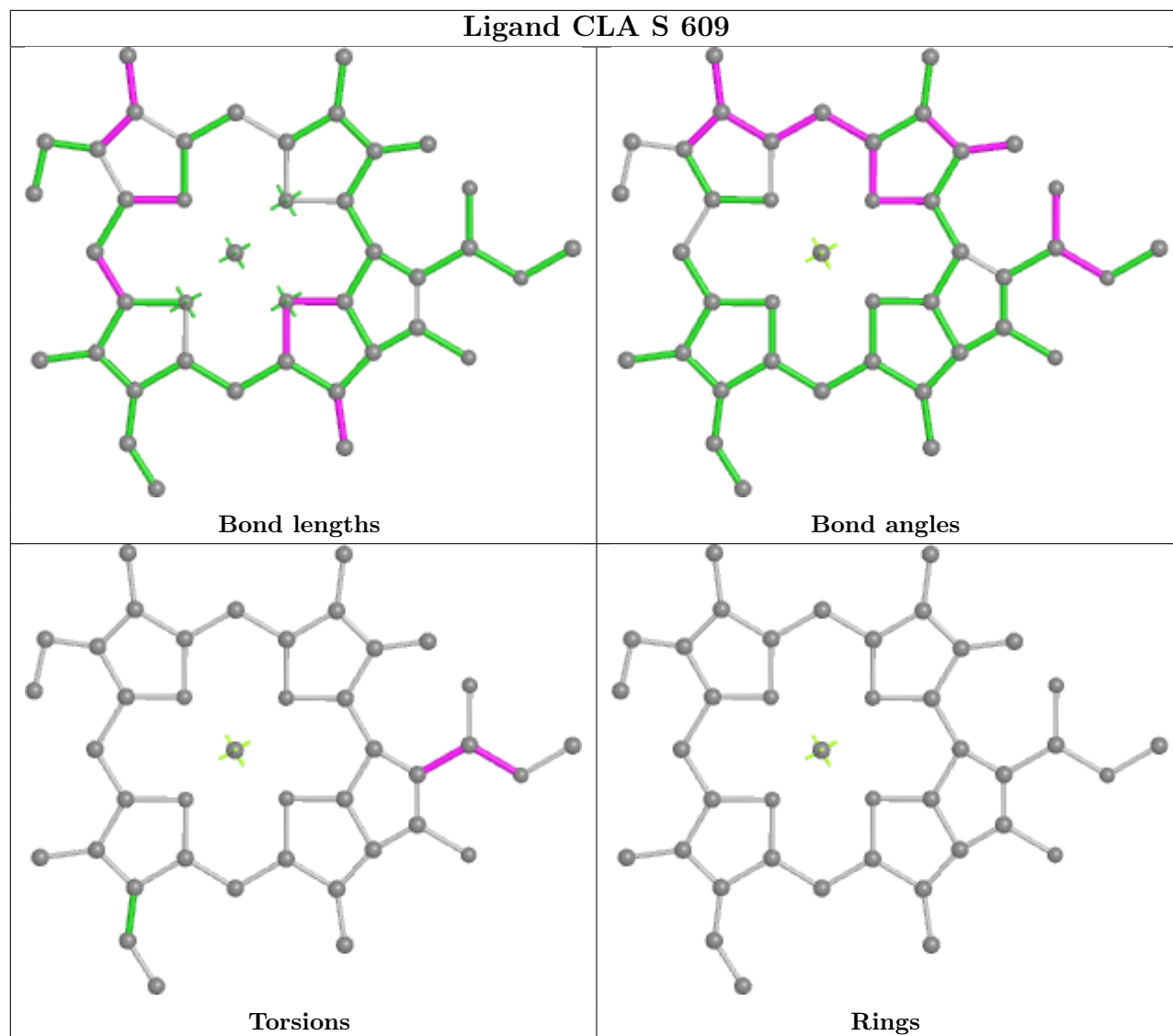
Ligand LHG d 408



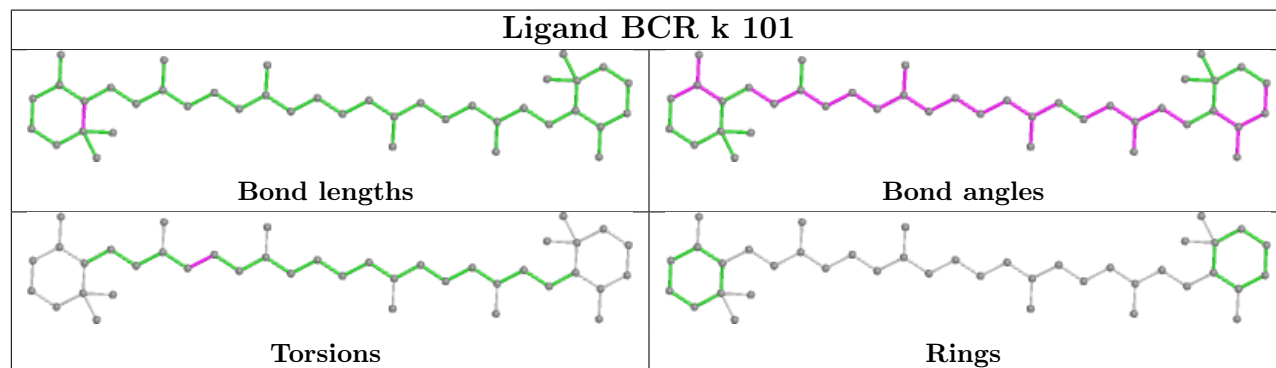
Ligand XAT Y 302

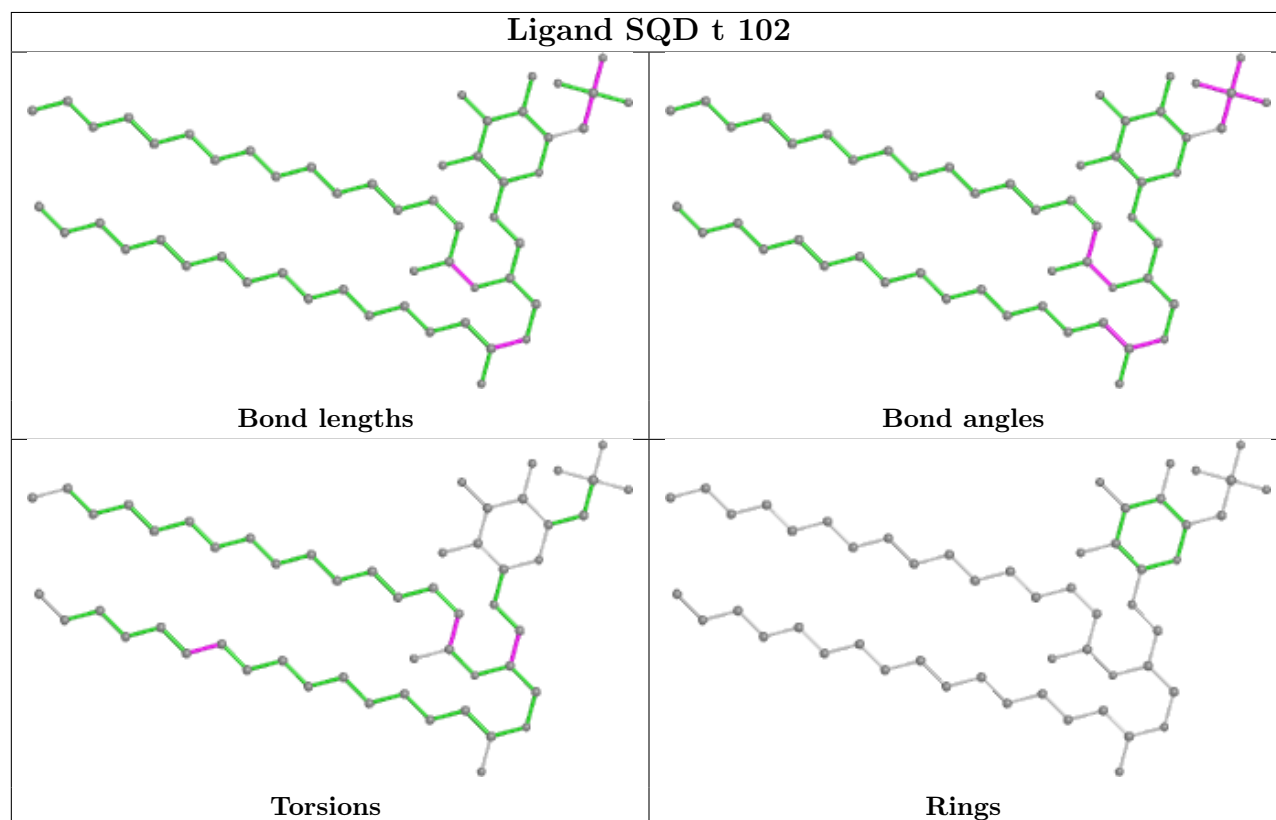
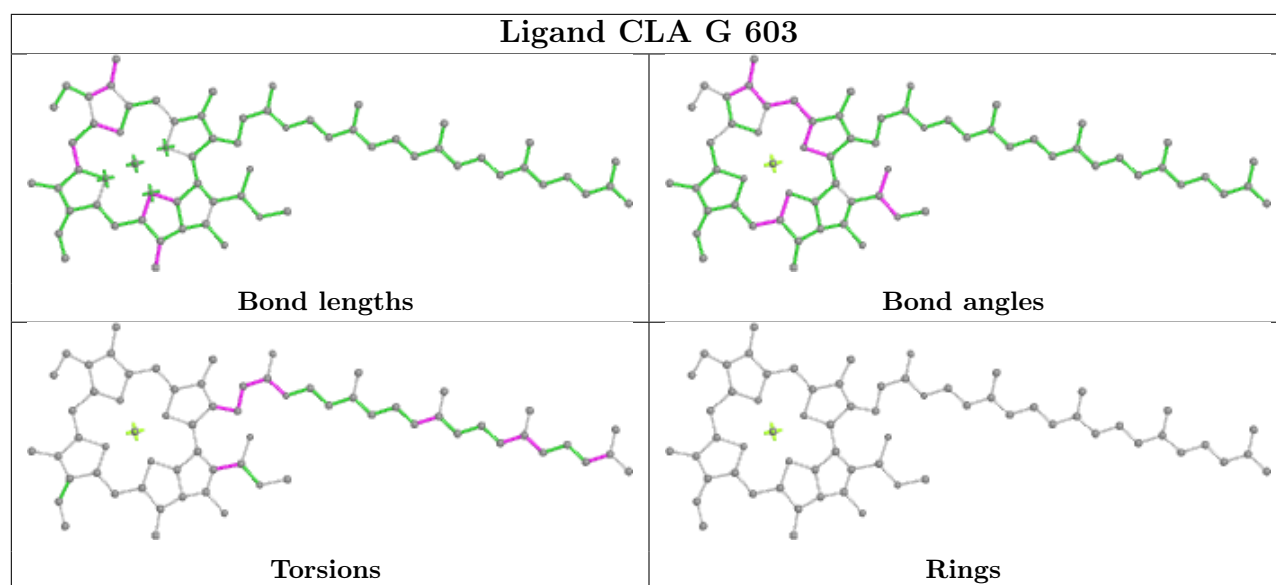


Ligand CLA S 609

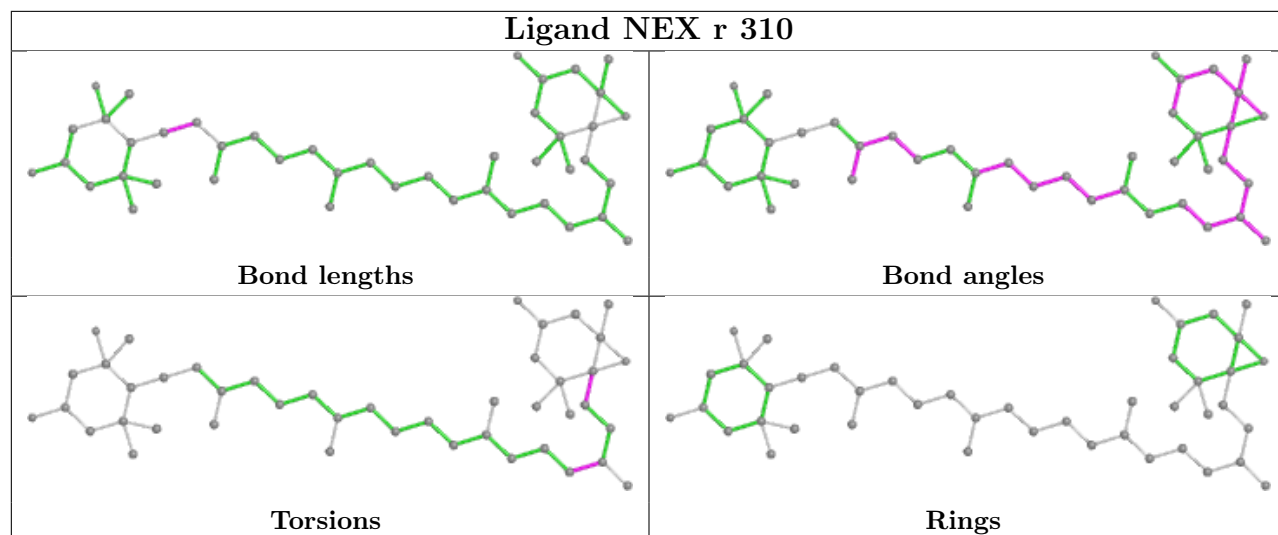


Ligand BCR k 101

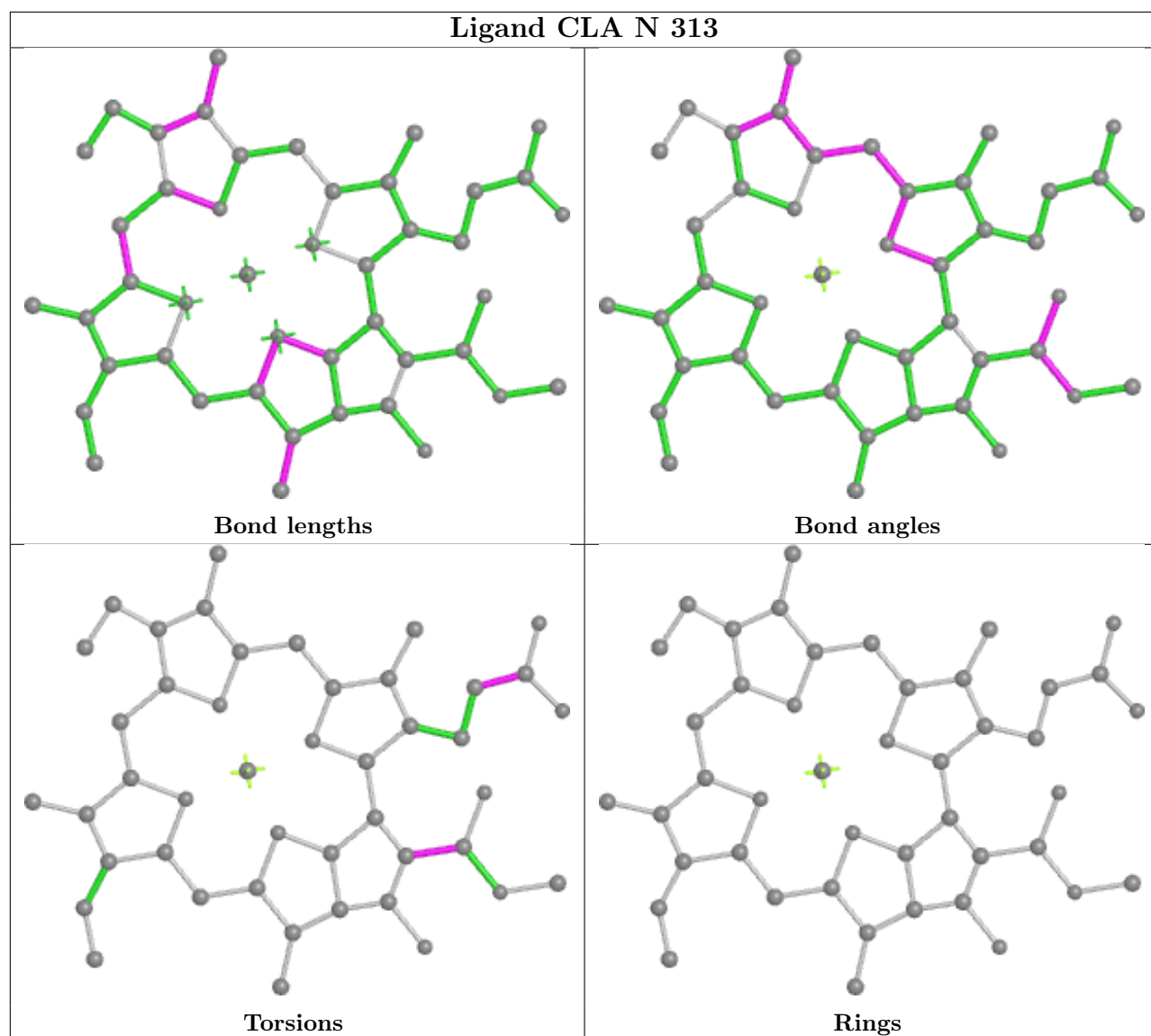


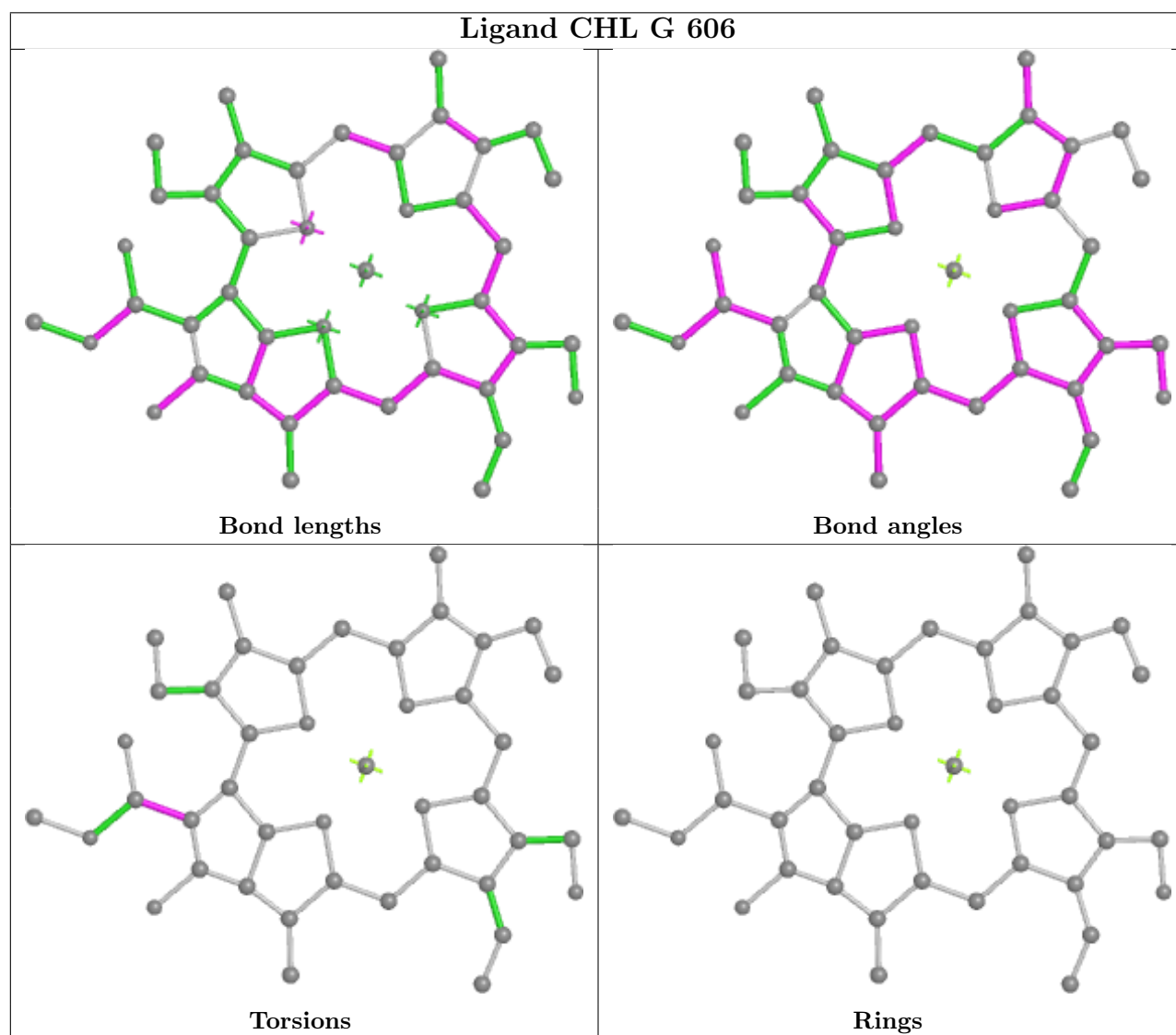
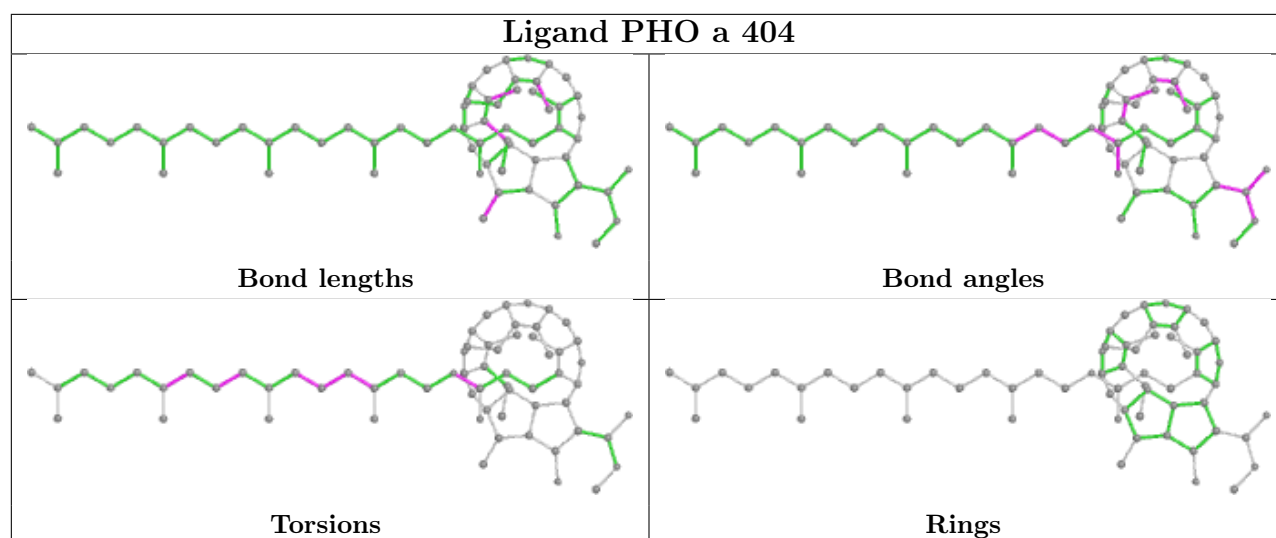


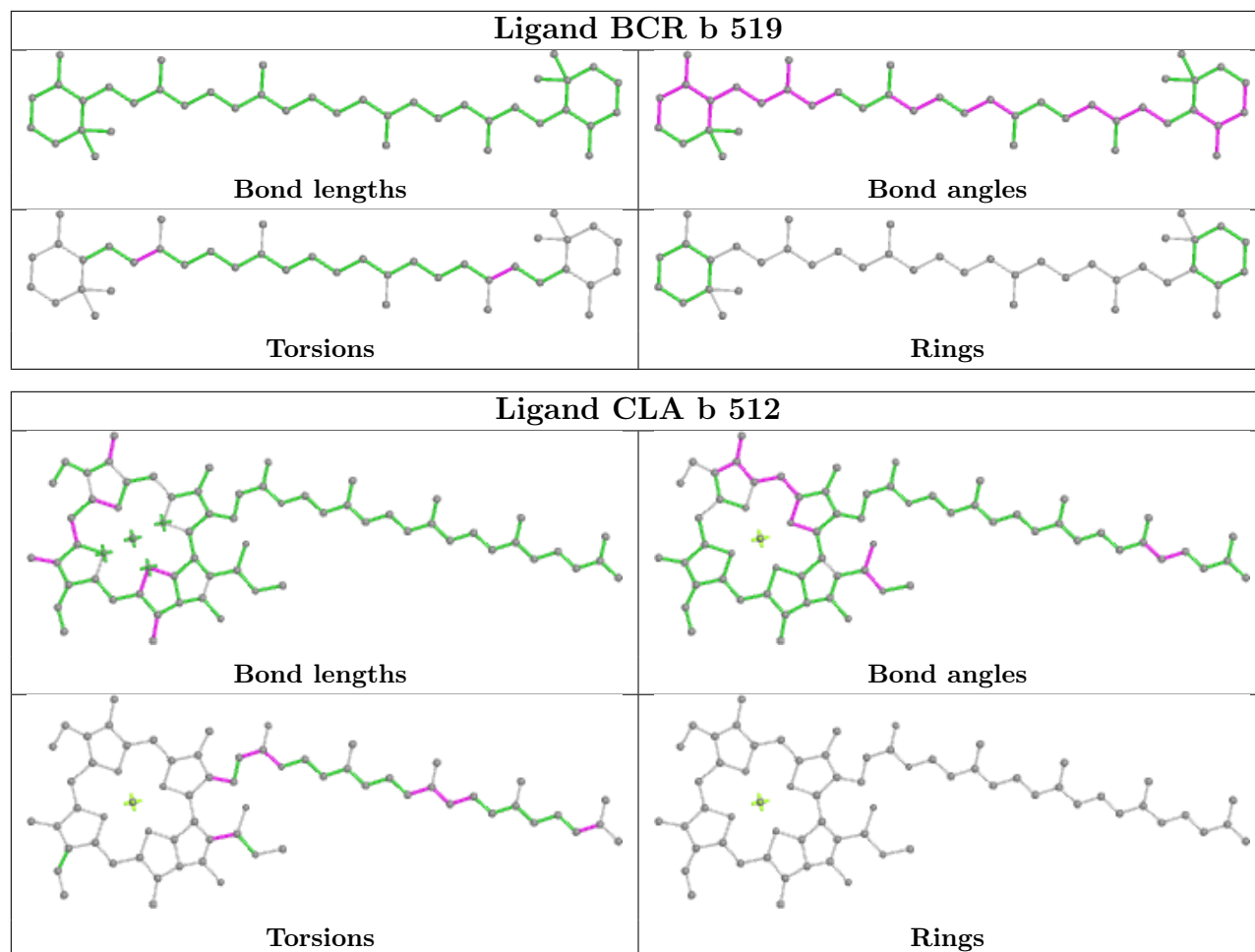
Ligand NEX r 310

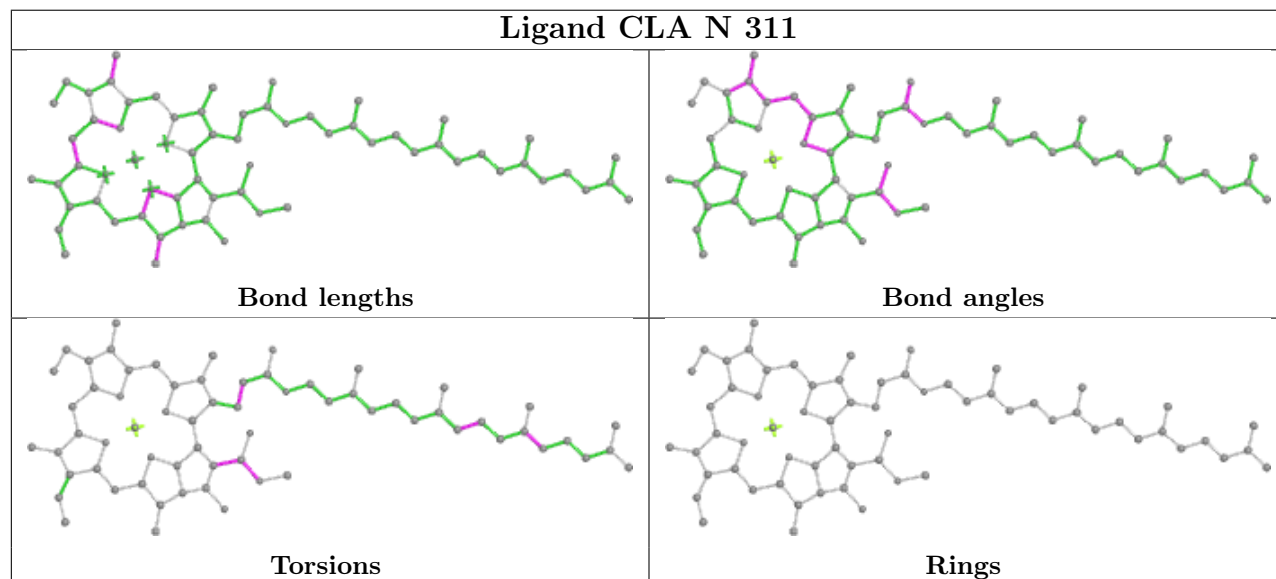
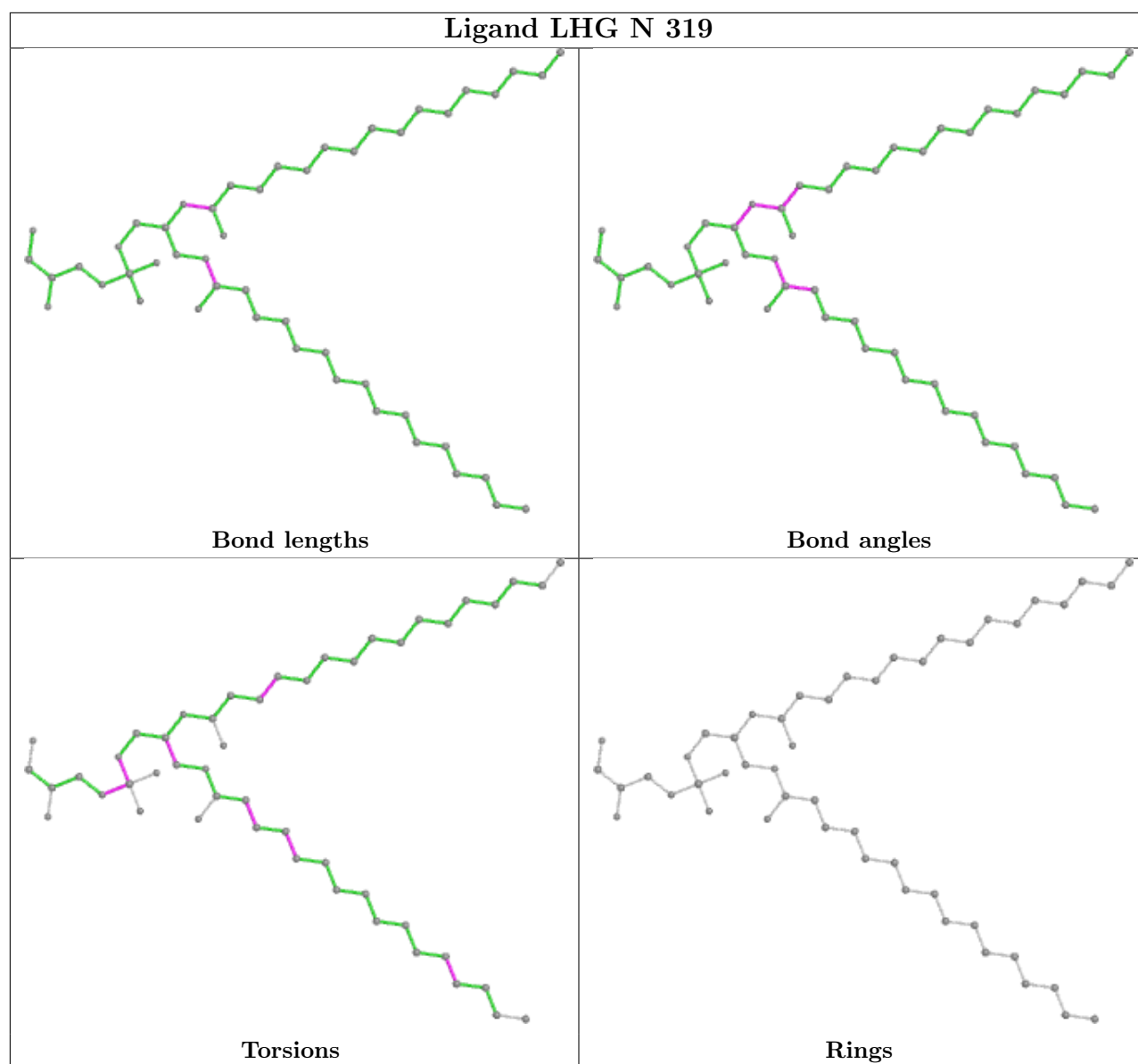


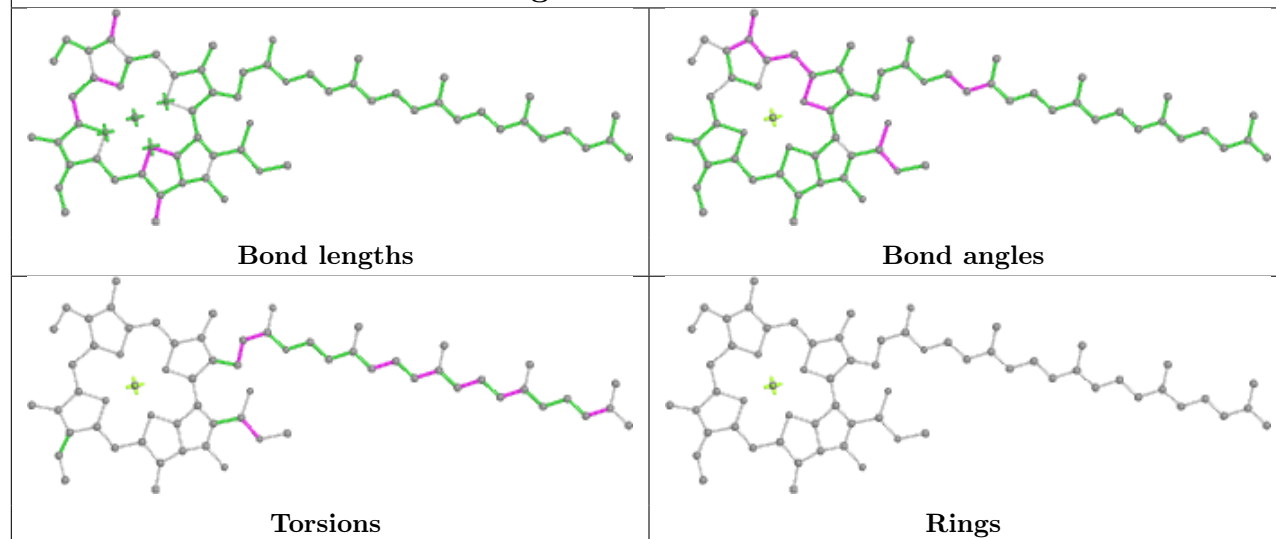
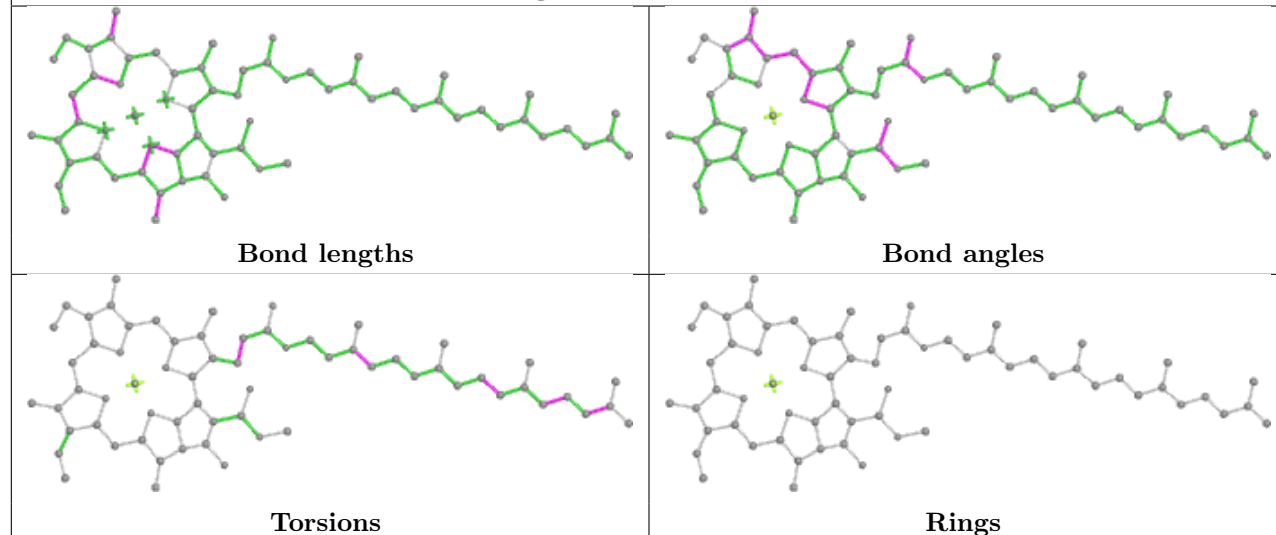
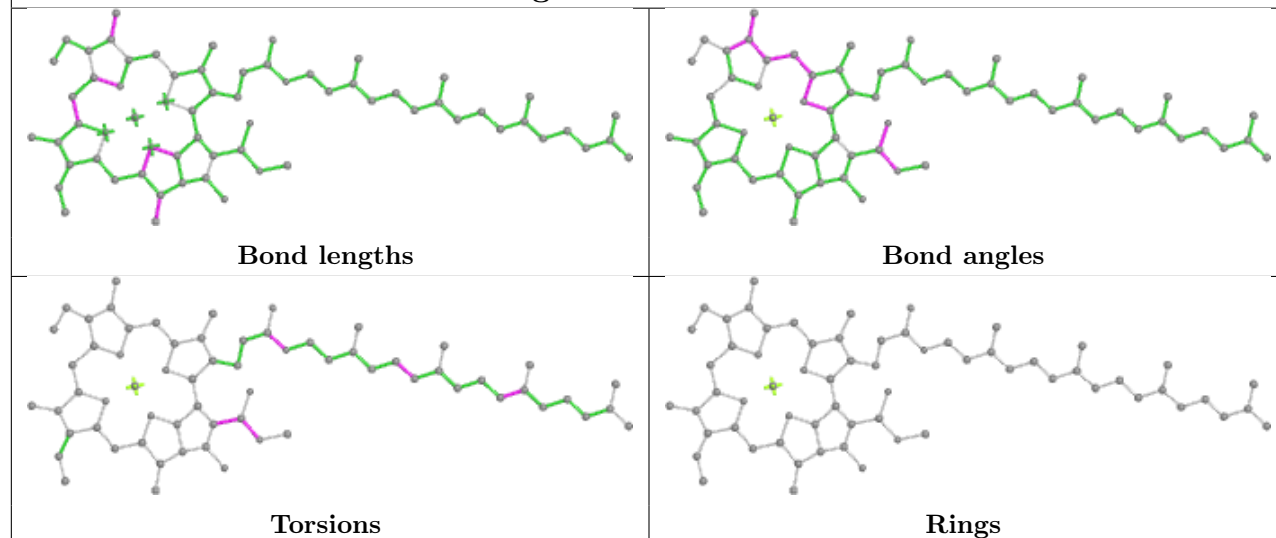
Ligand CLA N 313



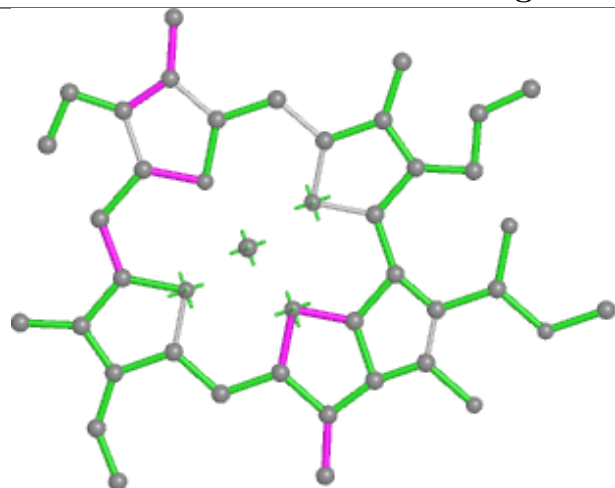




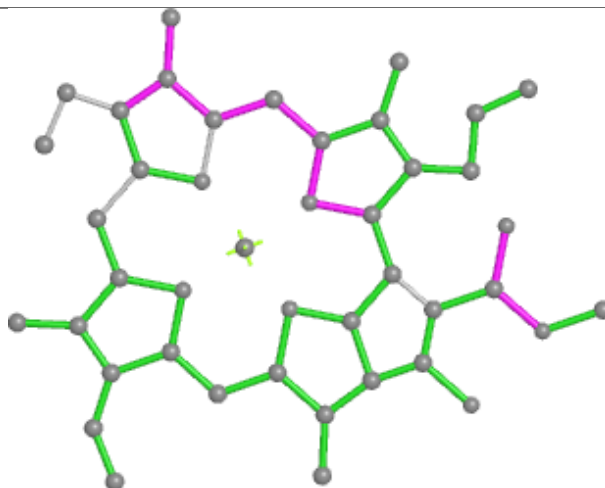


Ligand CLA G 602**Ligand CLA B 503****Ligand CLA B 507**

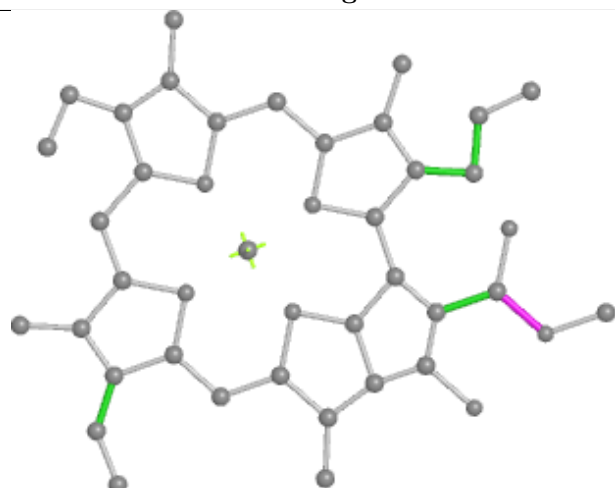
Ligand CLA G 612



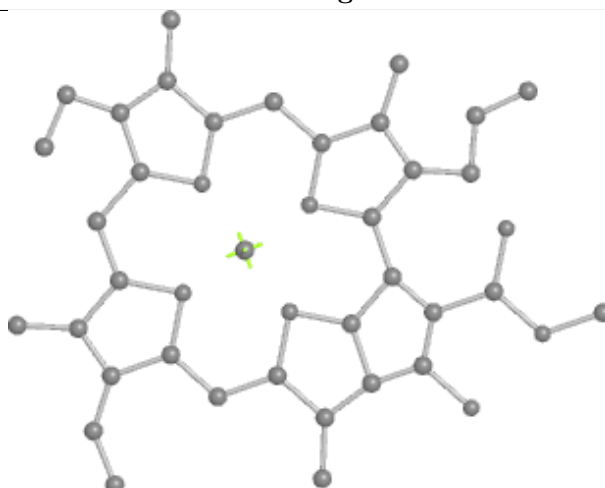
Bond lengths



Bond angles

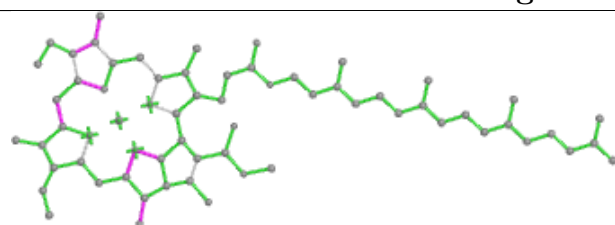


Torsions

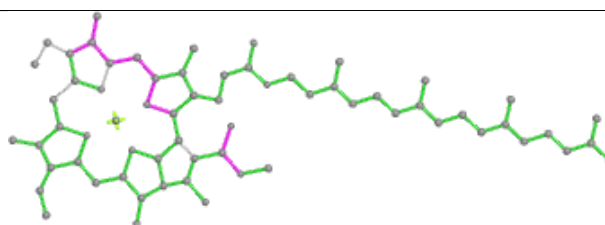


Rings

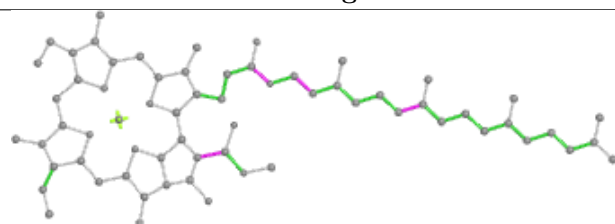
Ligand CLA C 512



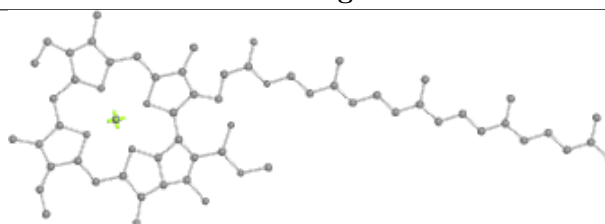
Bond lengths



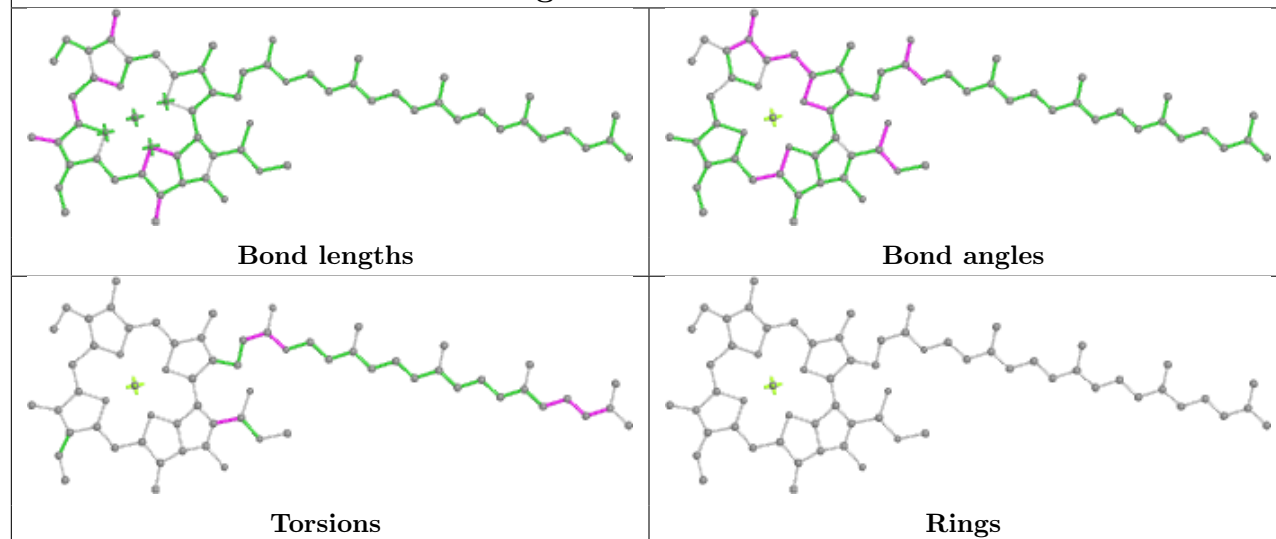
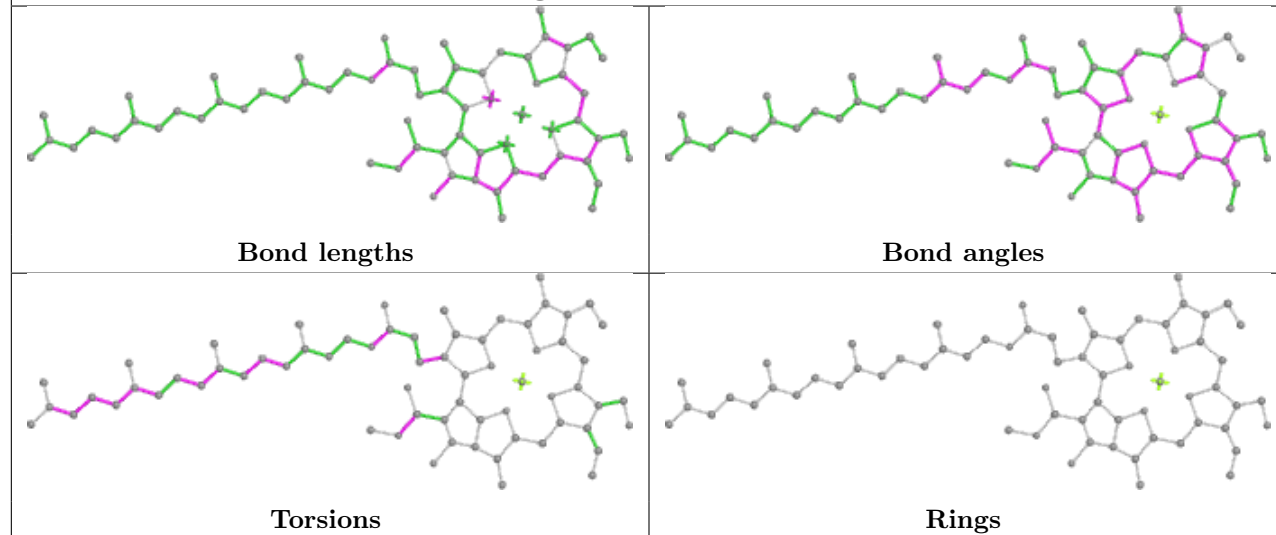
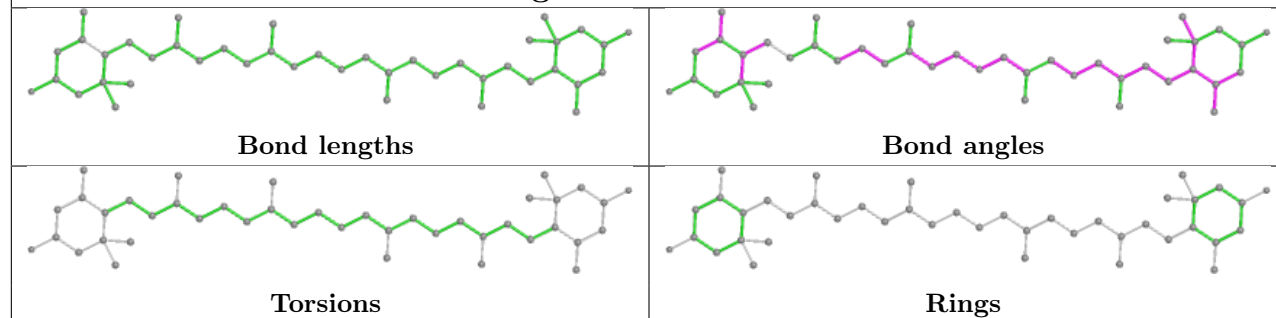
Bond angles

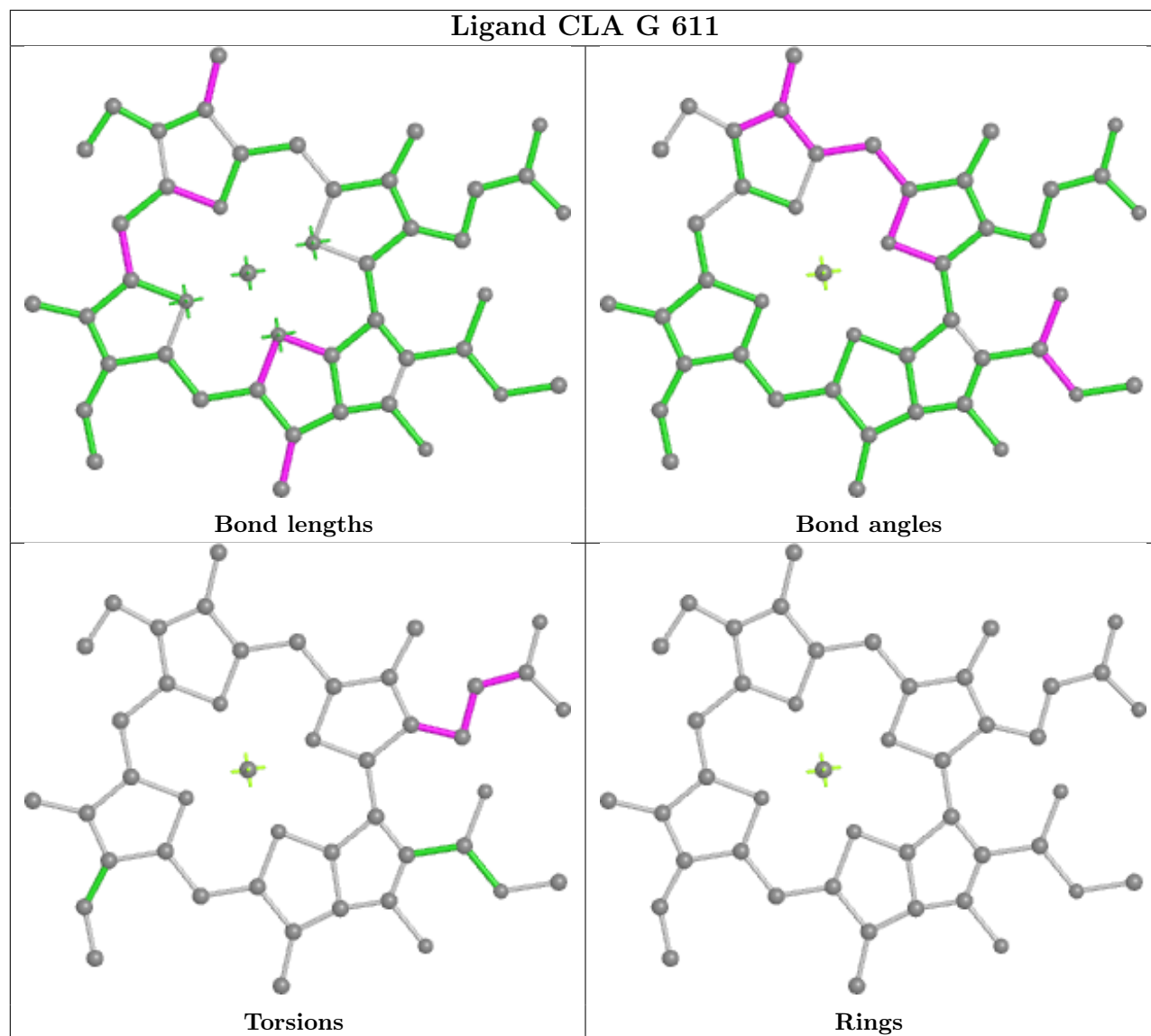
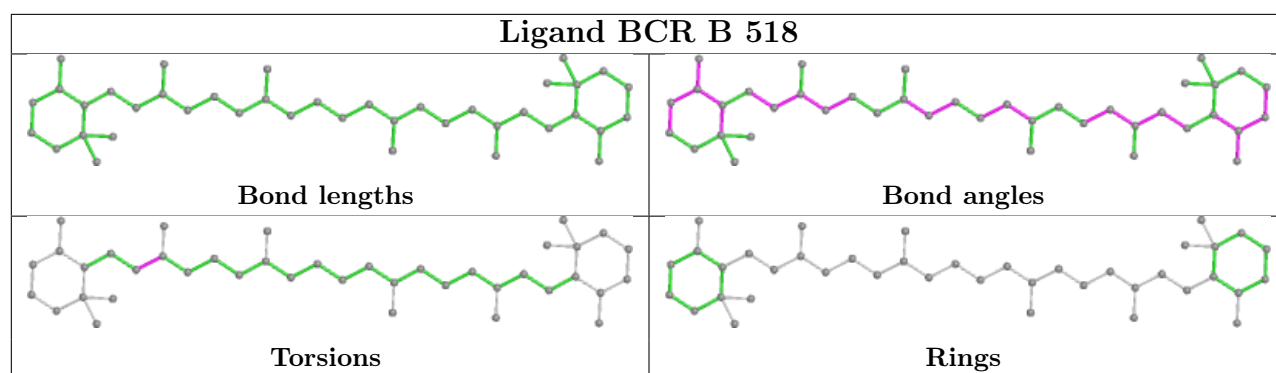


Torsions

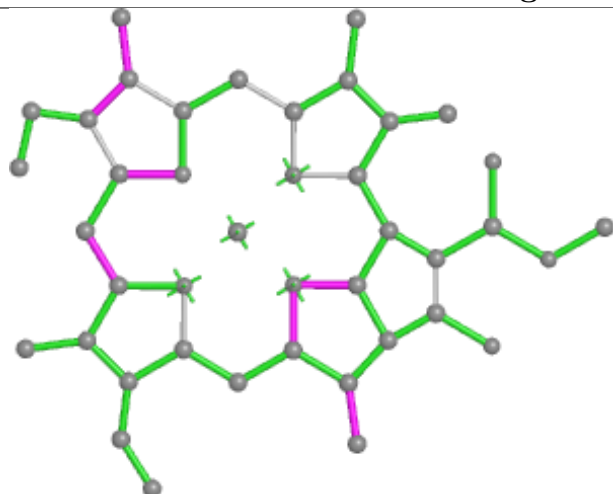


Rings

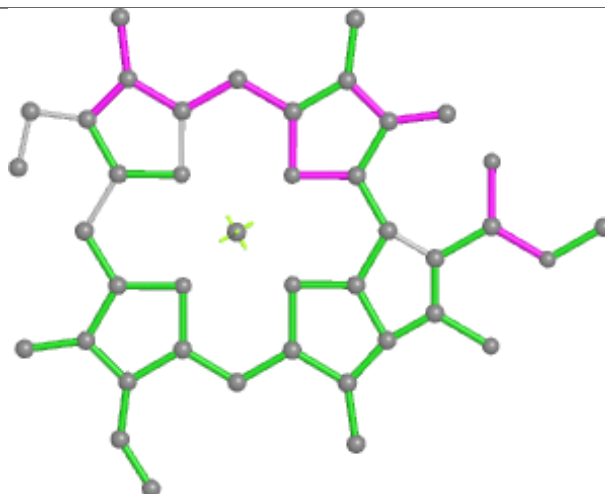
Ligand CLA a 402**Ligand CHL Y 303****Ligand LUT Y 316**



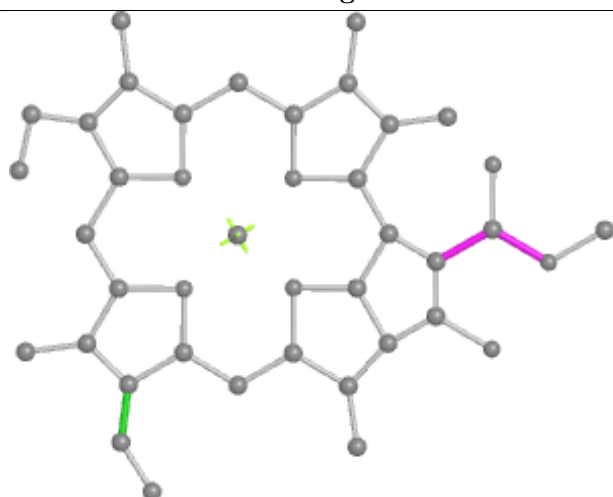
Ligand CLA r 308



Bond lengths



Bond angles

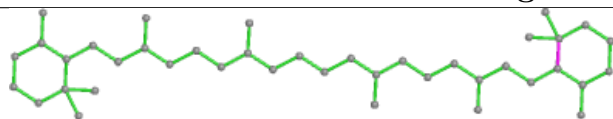


Torsions

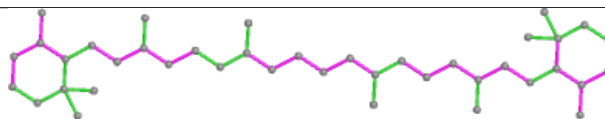


Rings

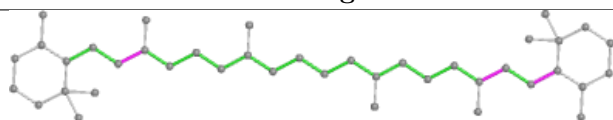
Ligand BCR c 514



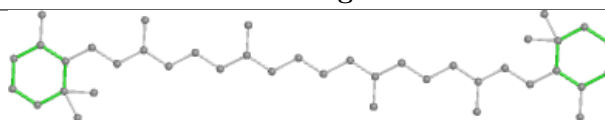
Bond lengths



Bond angles

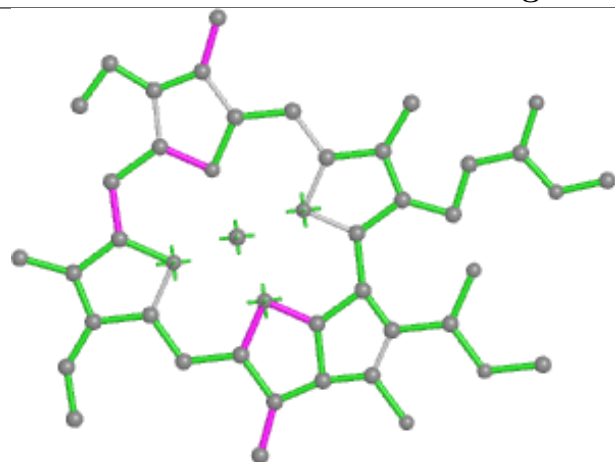


Torsions

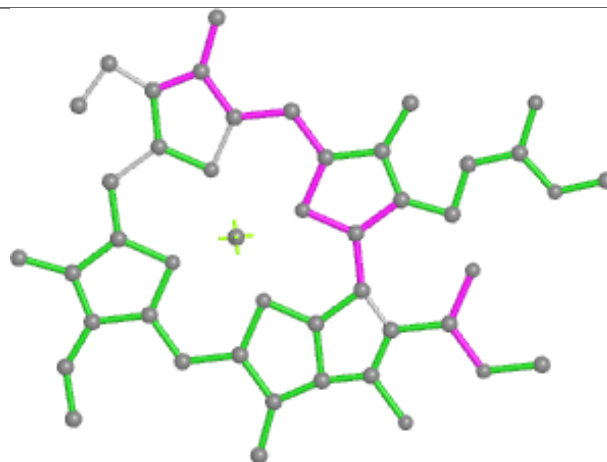


Rings

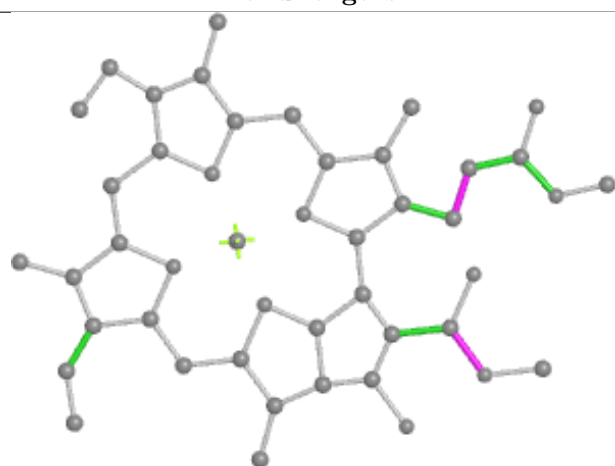
Ligand CLA r 302



Bond lengths



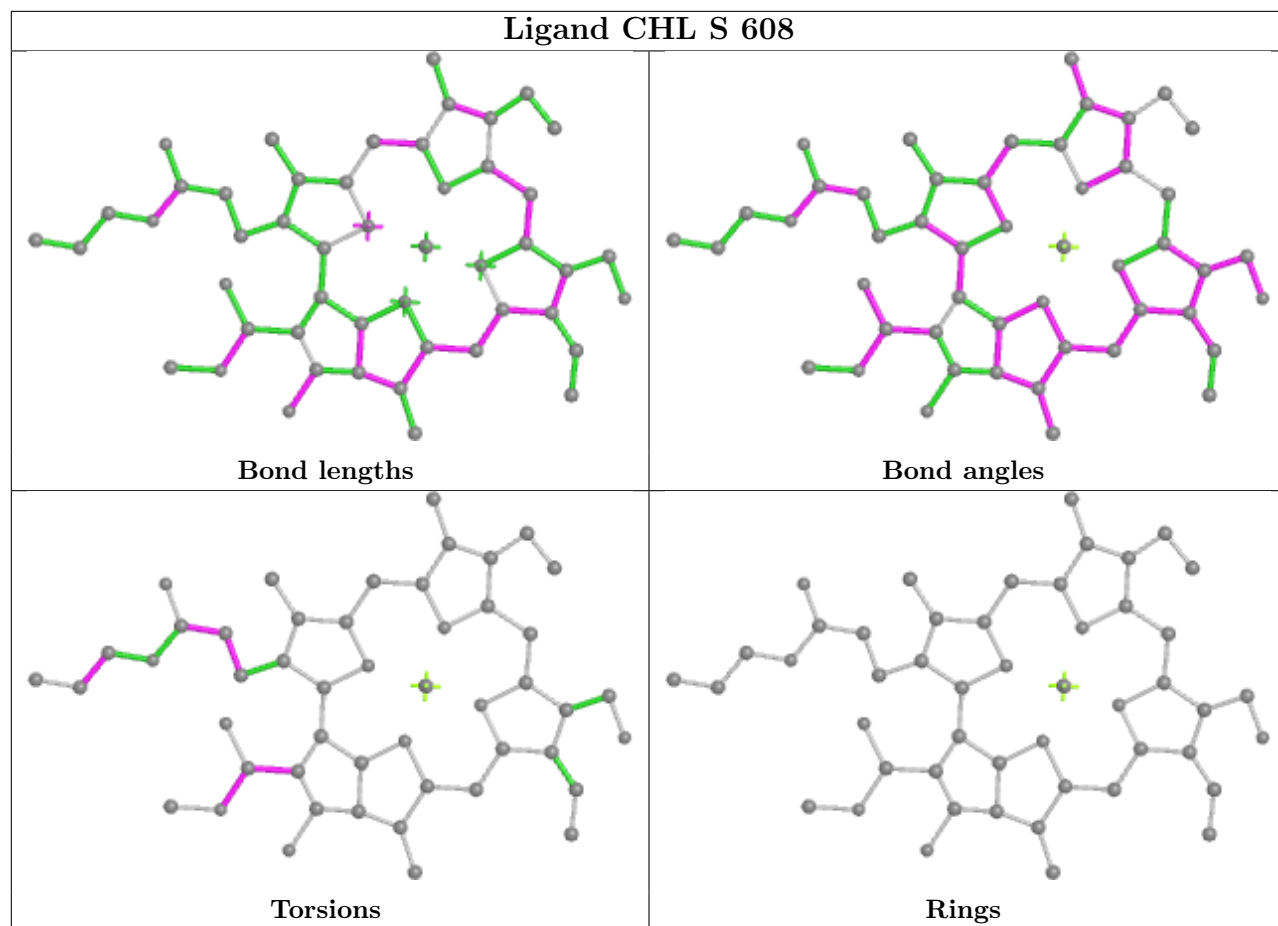
Bond angles



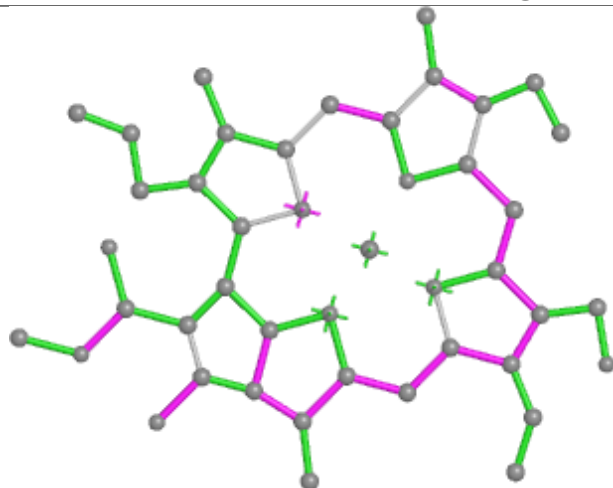
Torsions



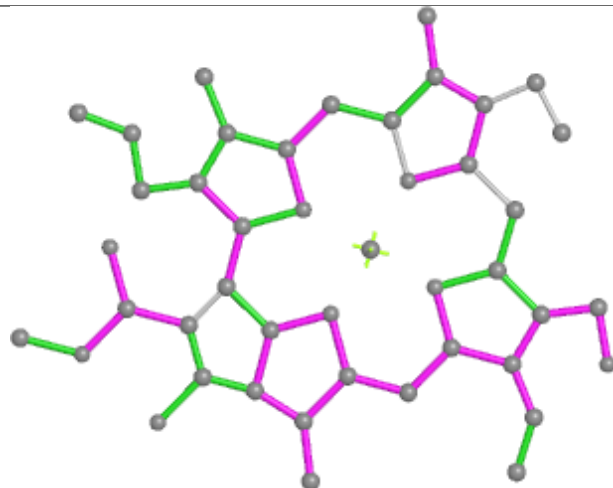
Rings



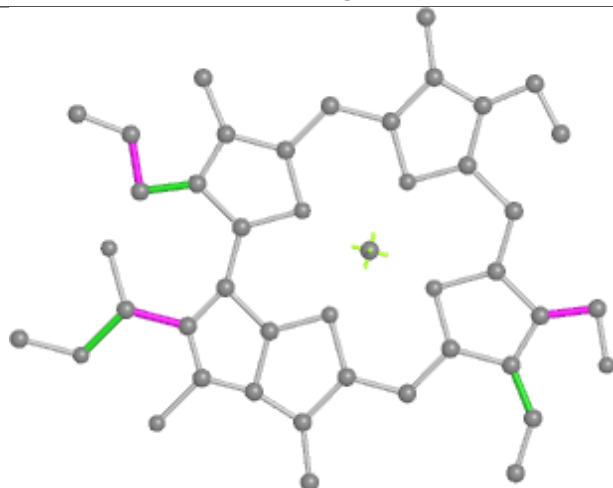
Ligand CHL S 606



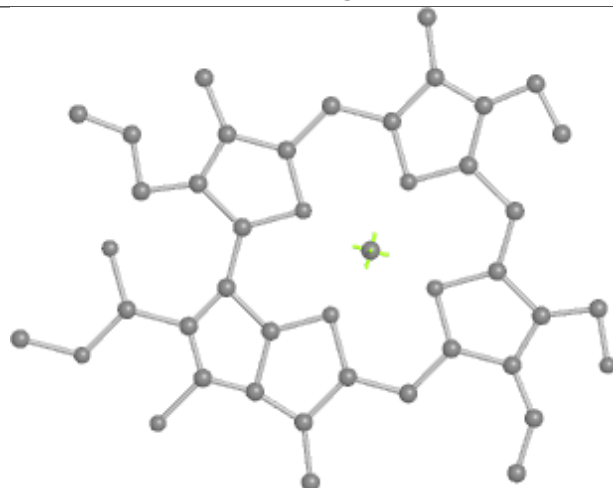
Bond lengths



Bond angles

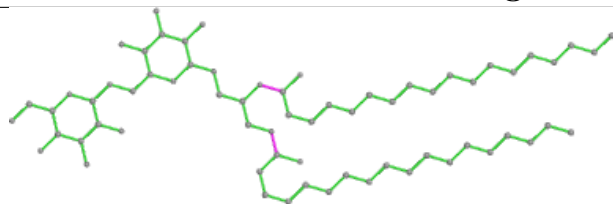


Torsions

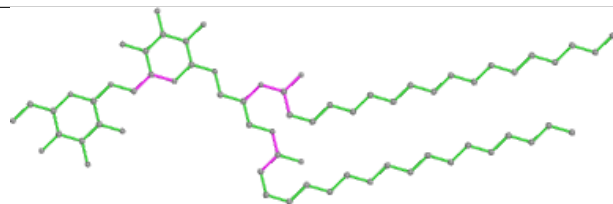


Rings

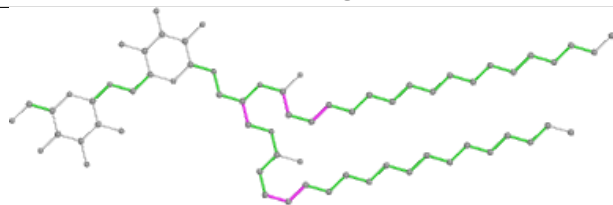
Ligand DGD W 202



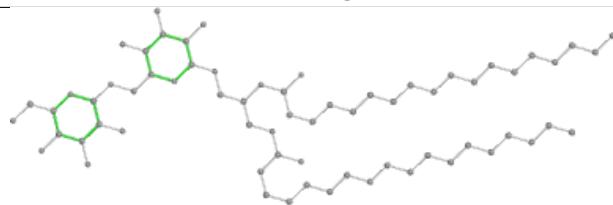
Bond lengths



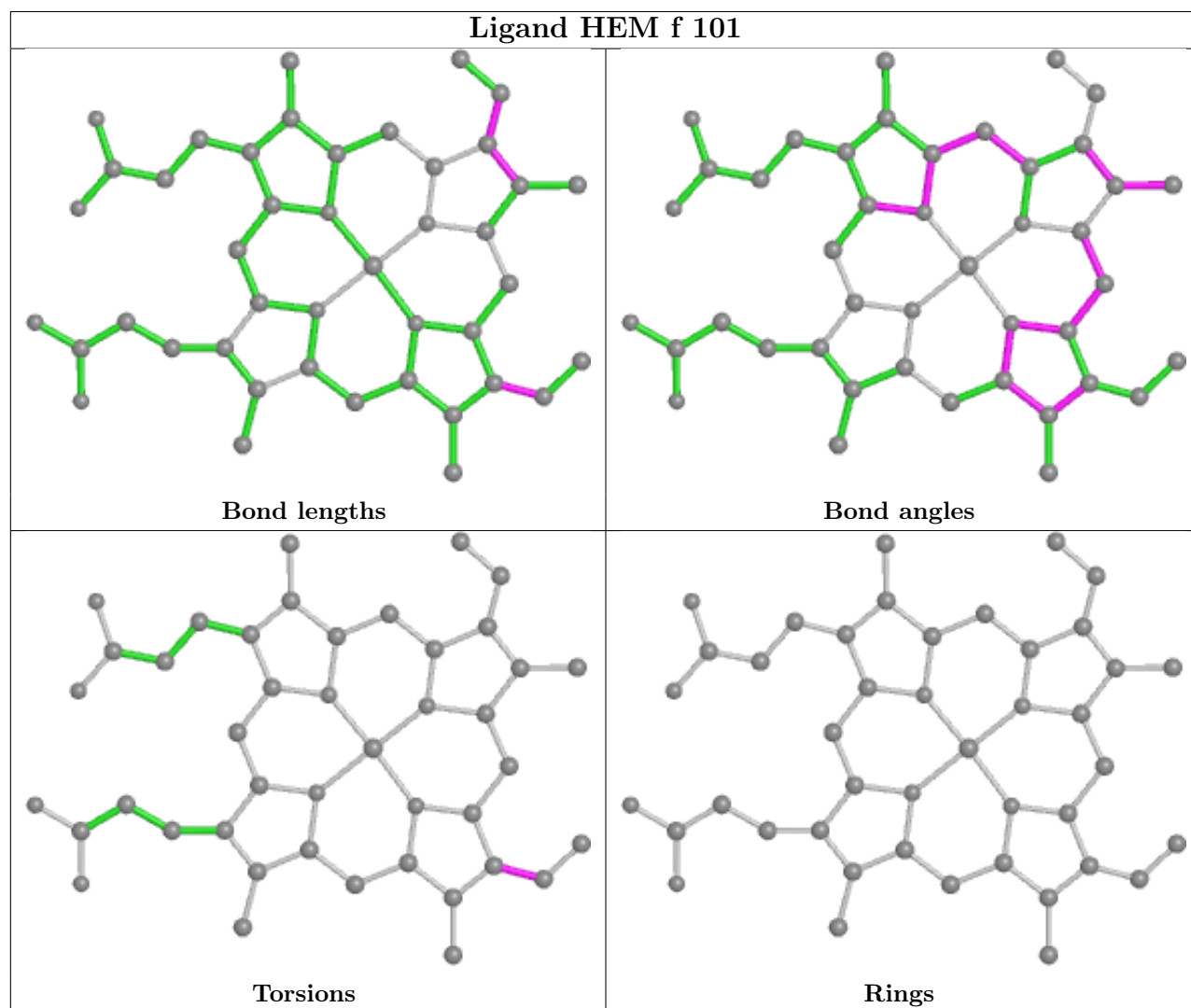
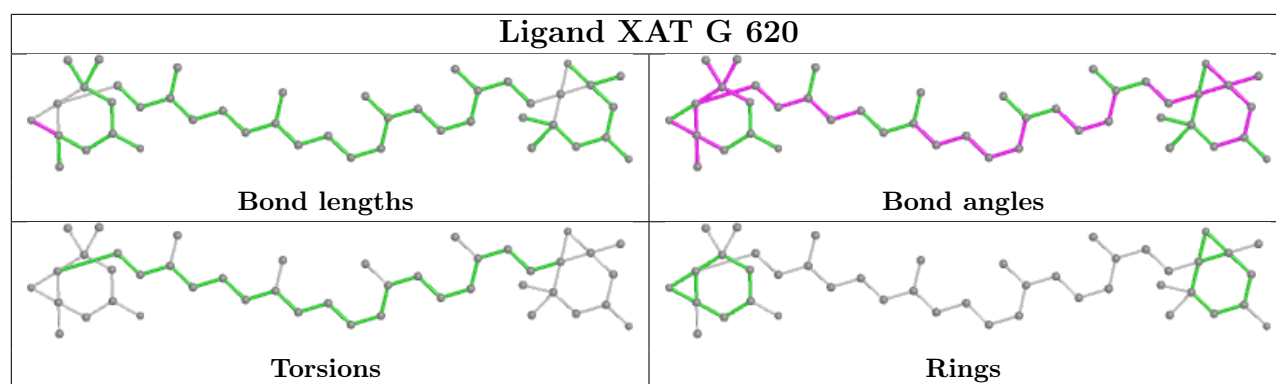
Bond angles

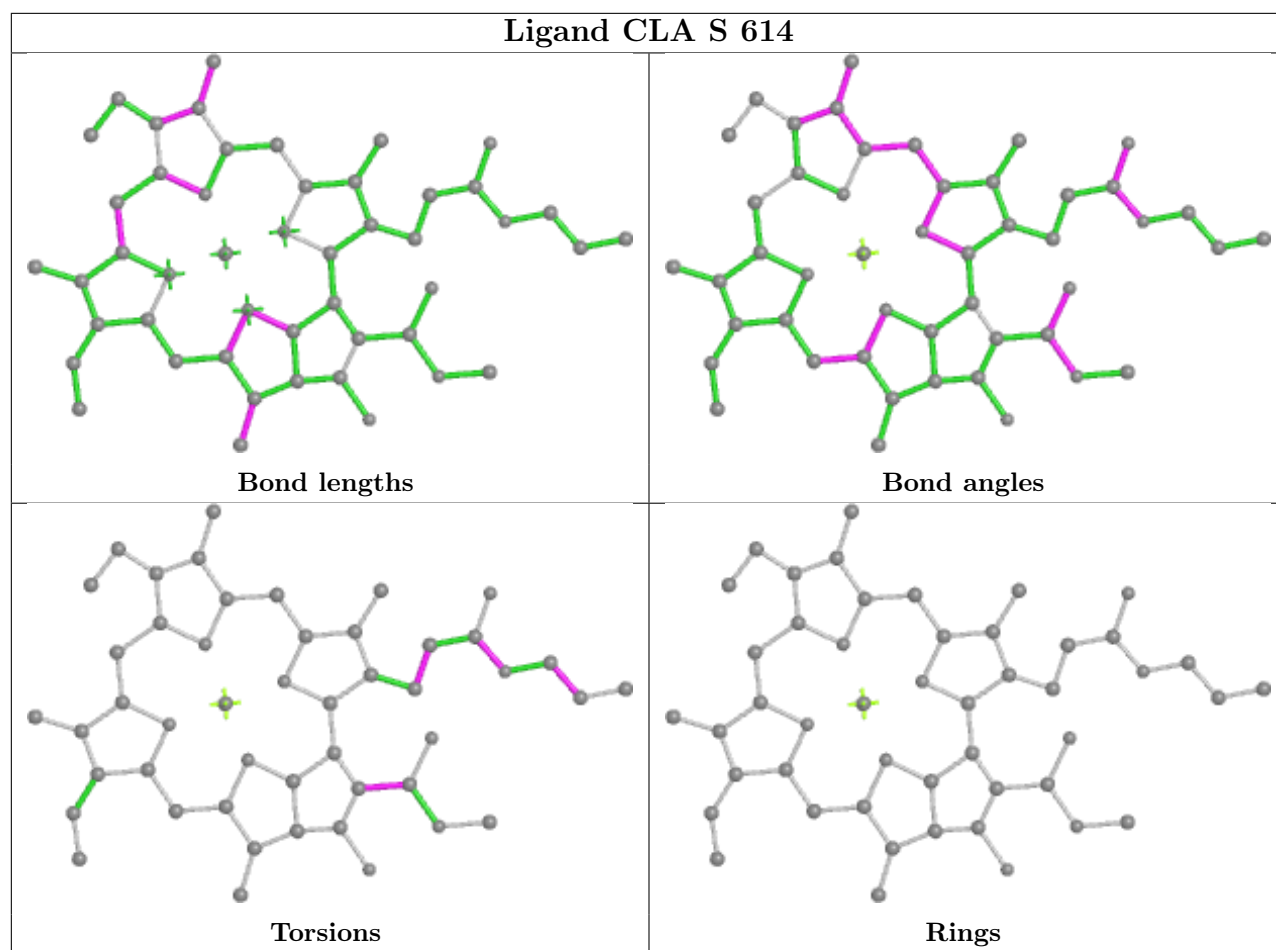
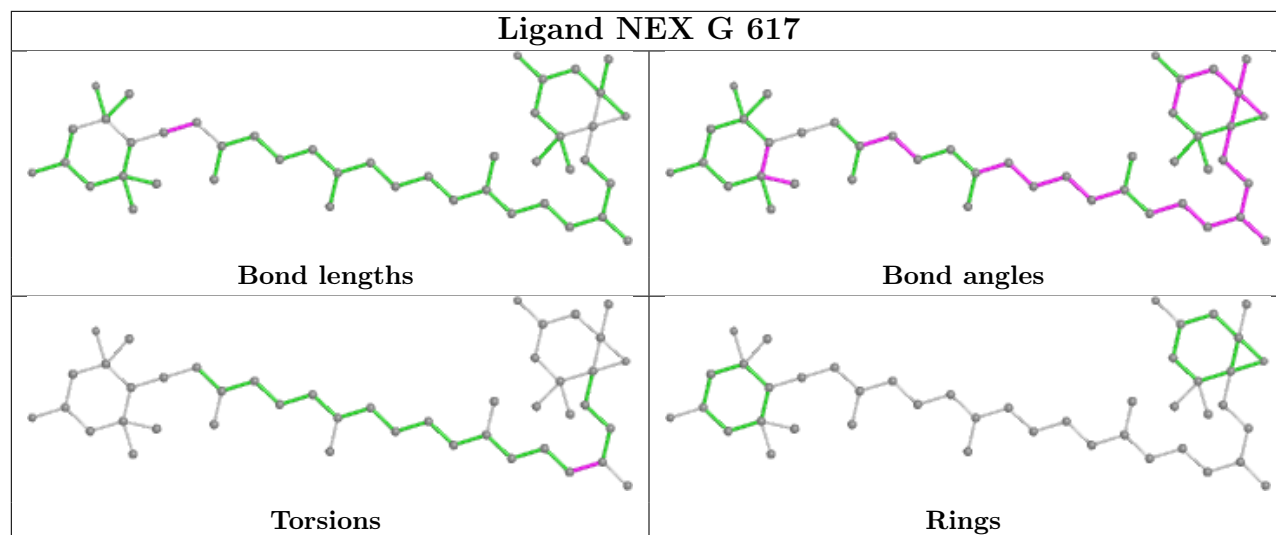


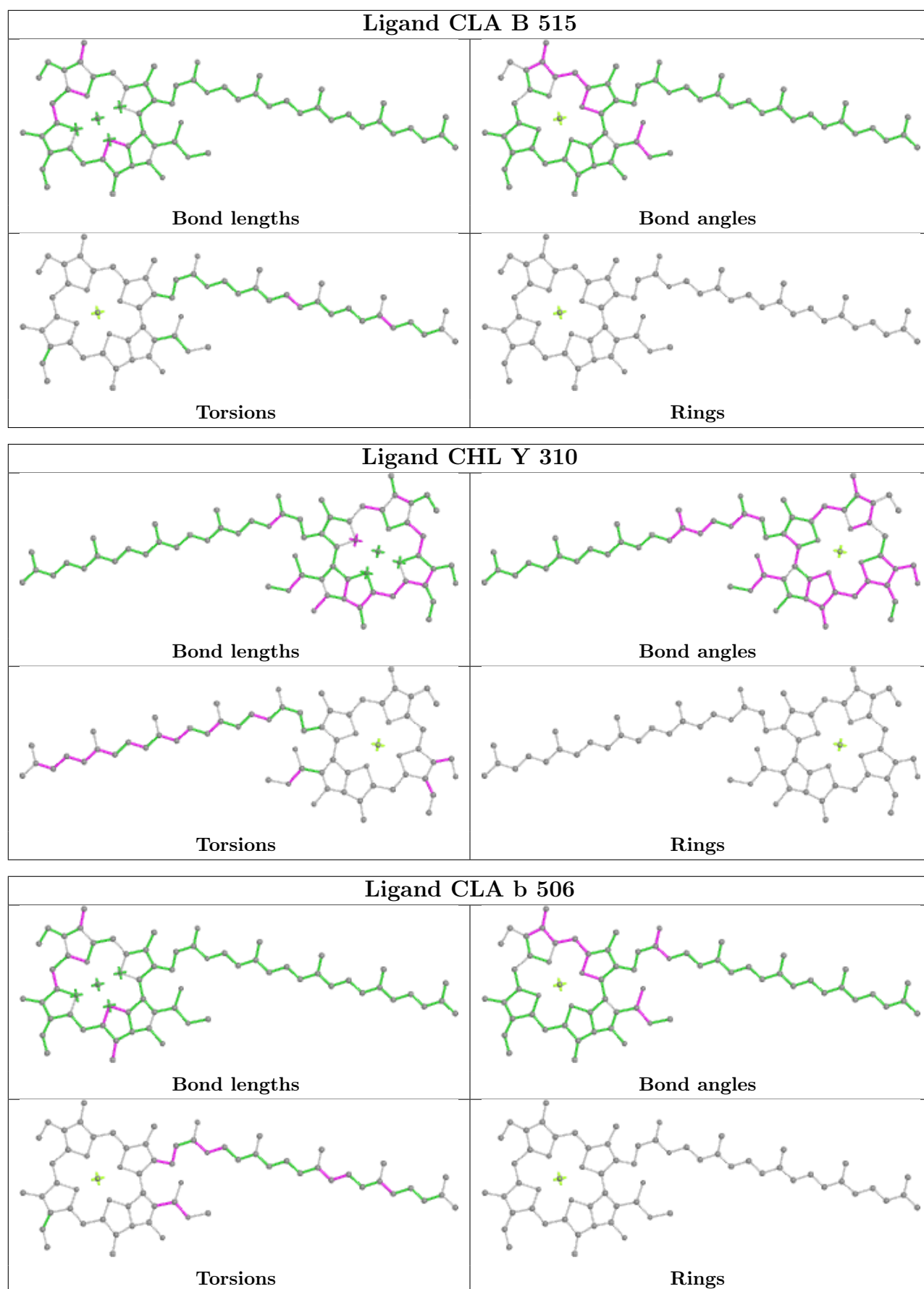
Torsions



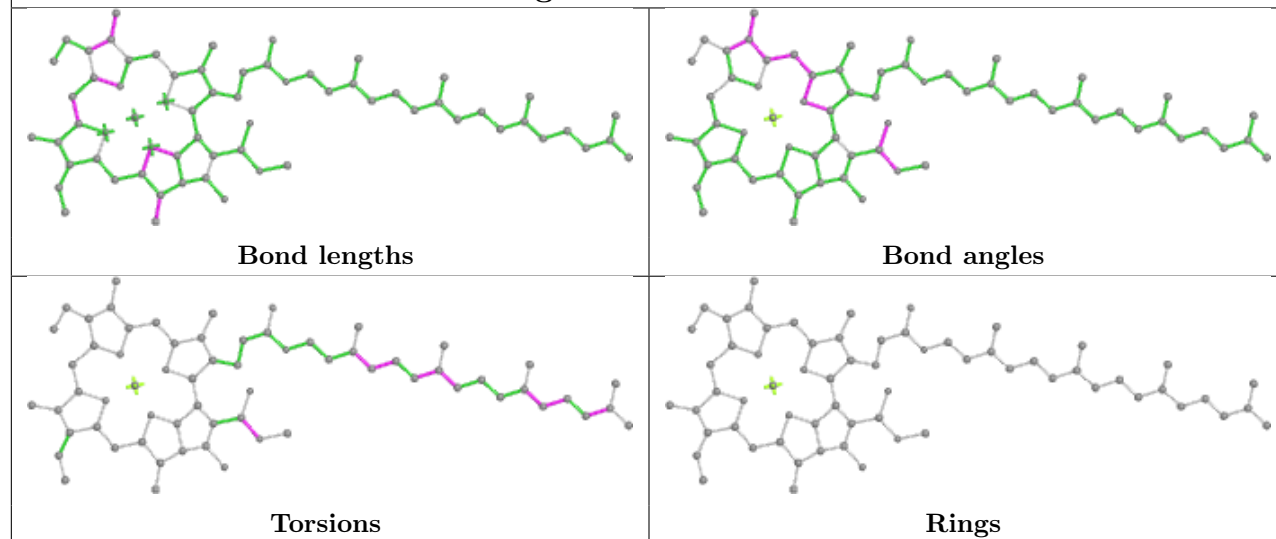
Rings



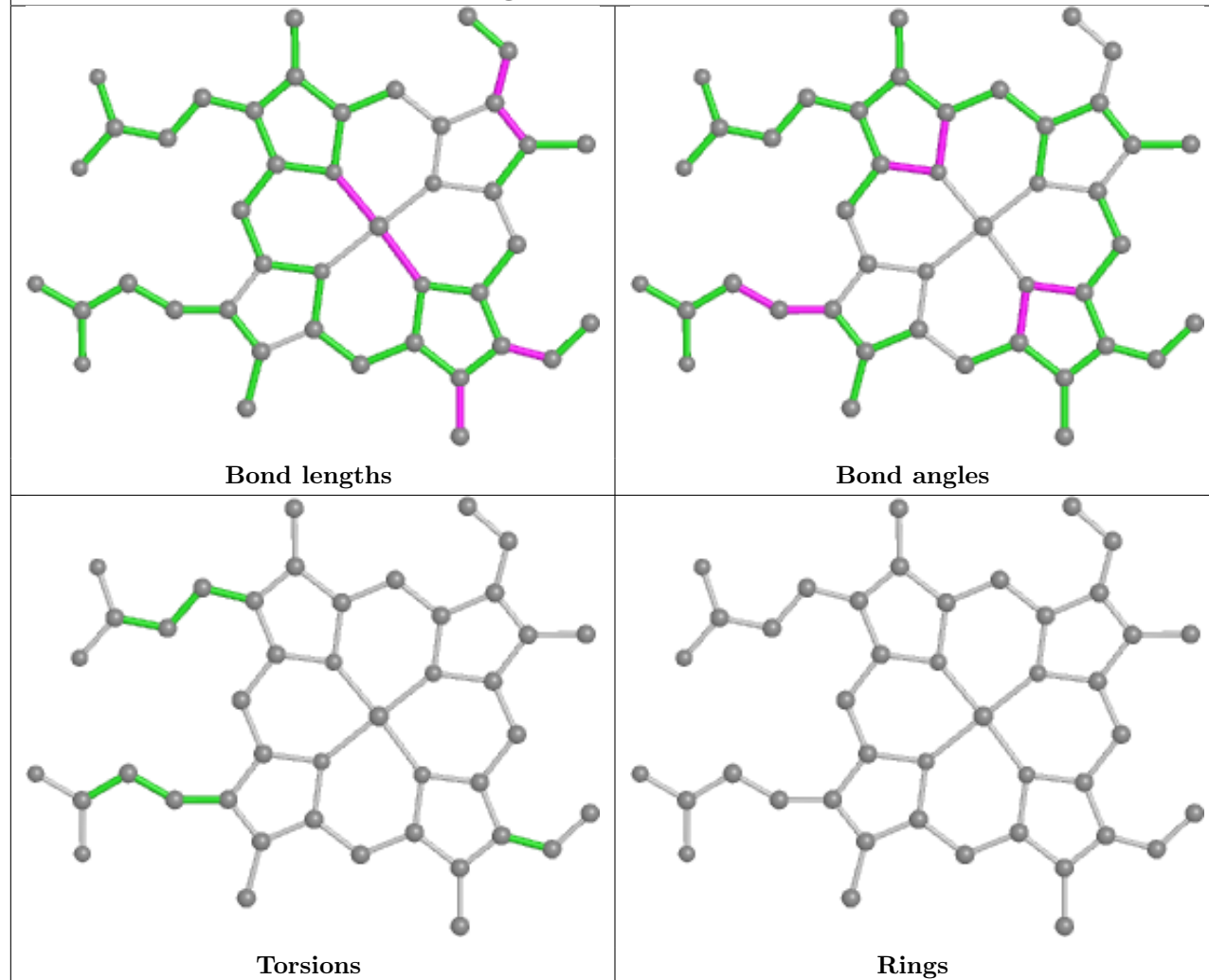




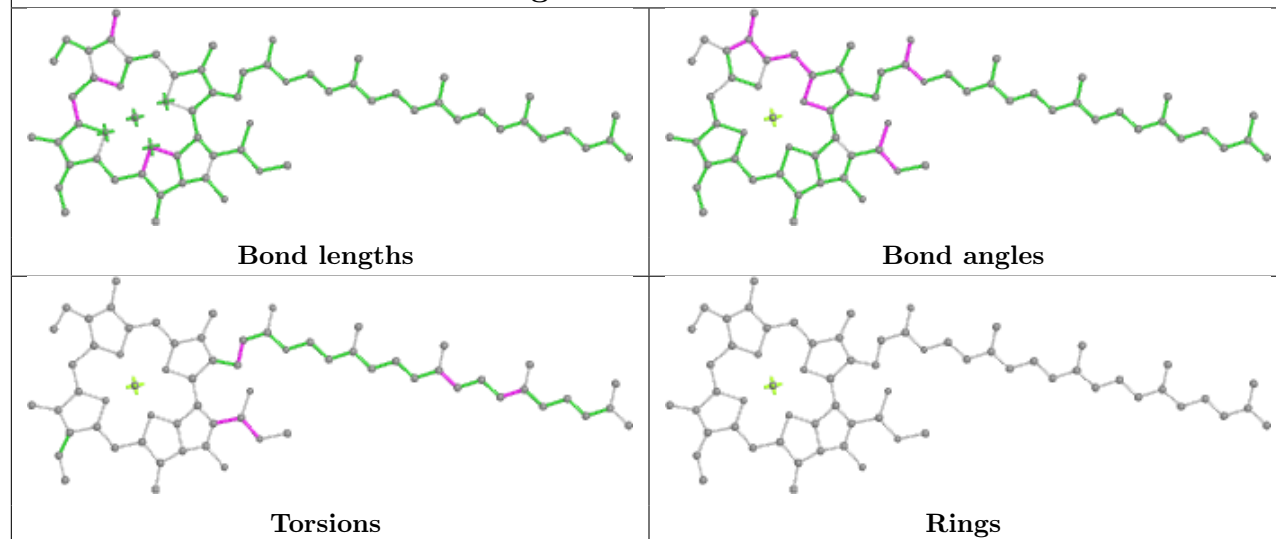
Ligand CLA b 515



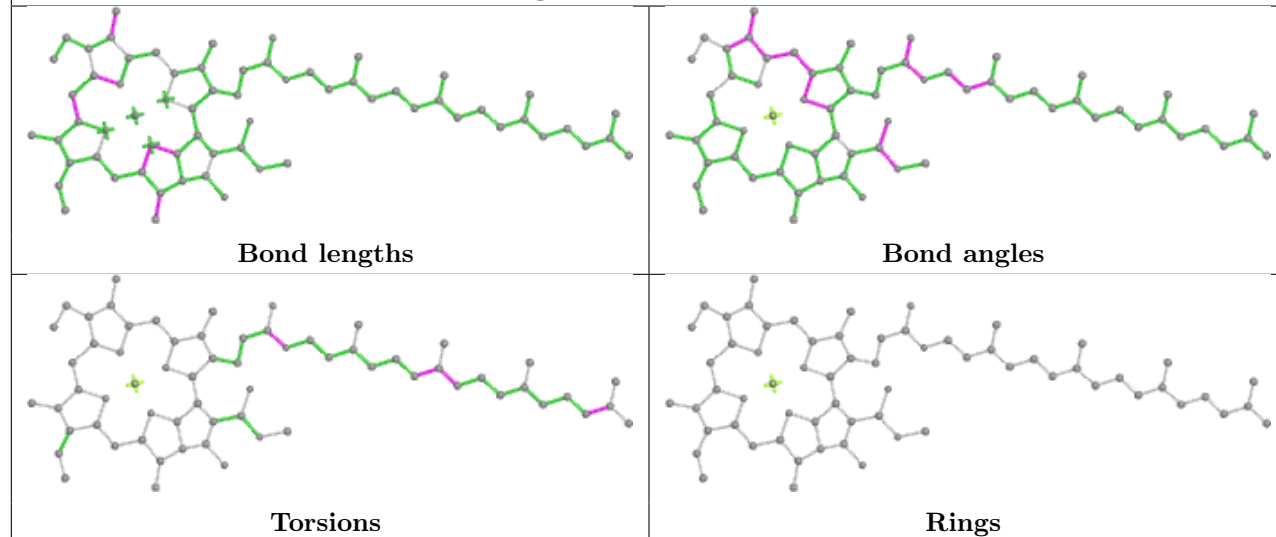
Ligand HEM F 101



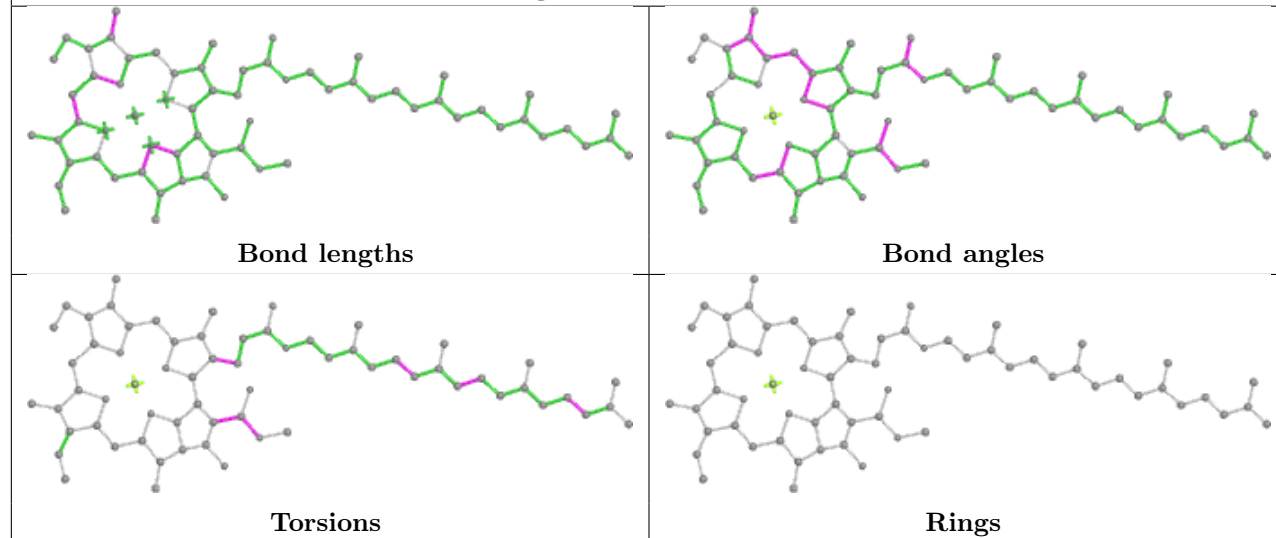
Ligand CLA G 610

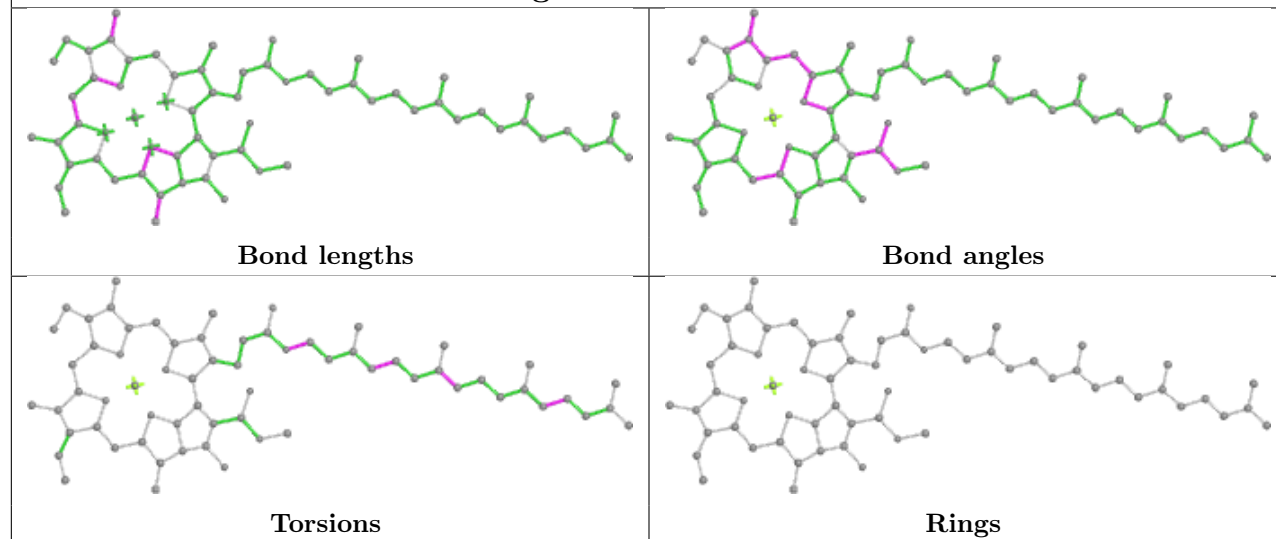
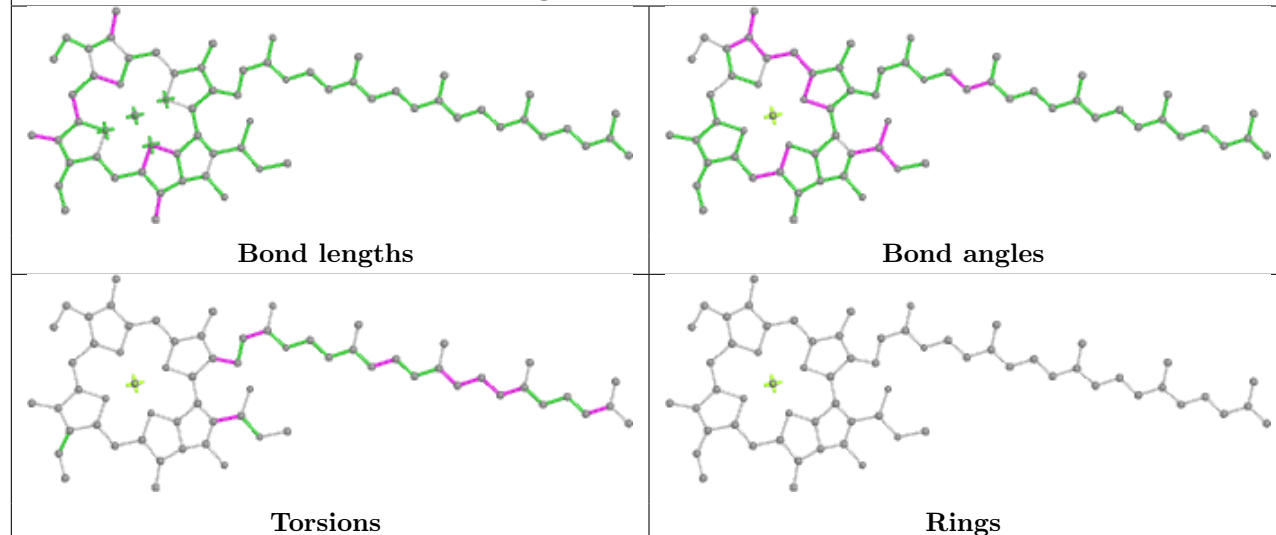
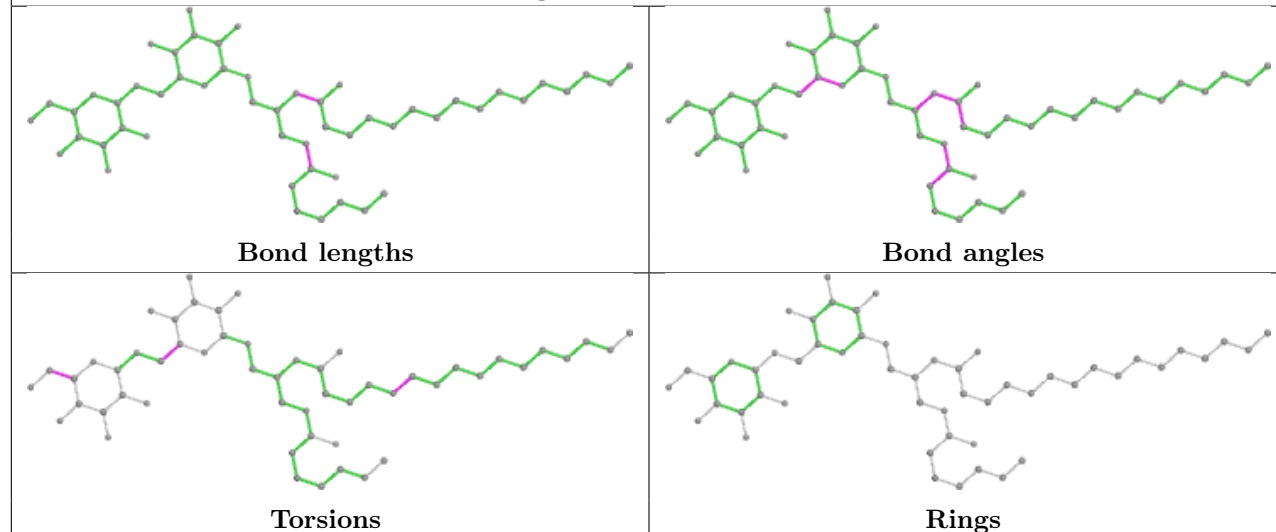


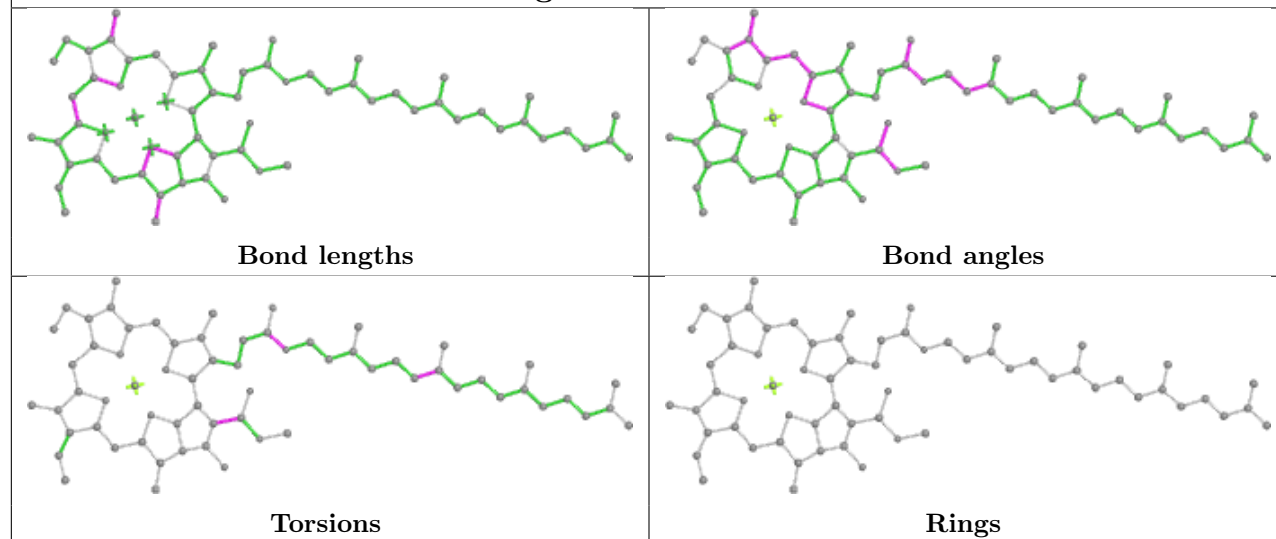
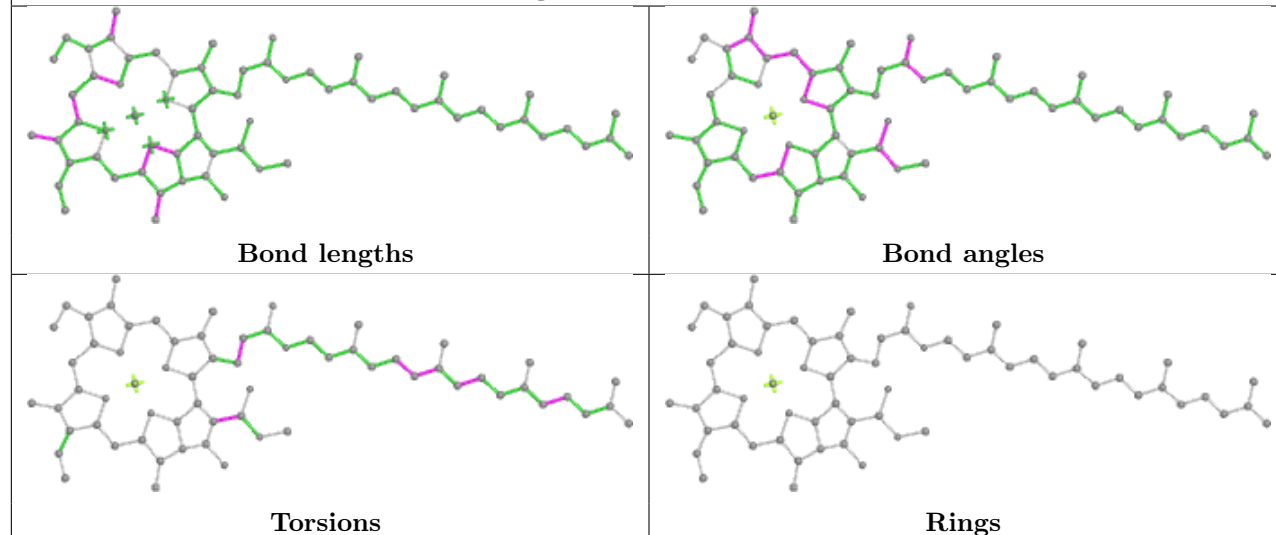
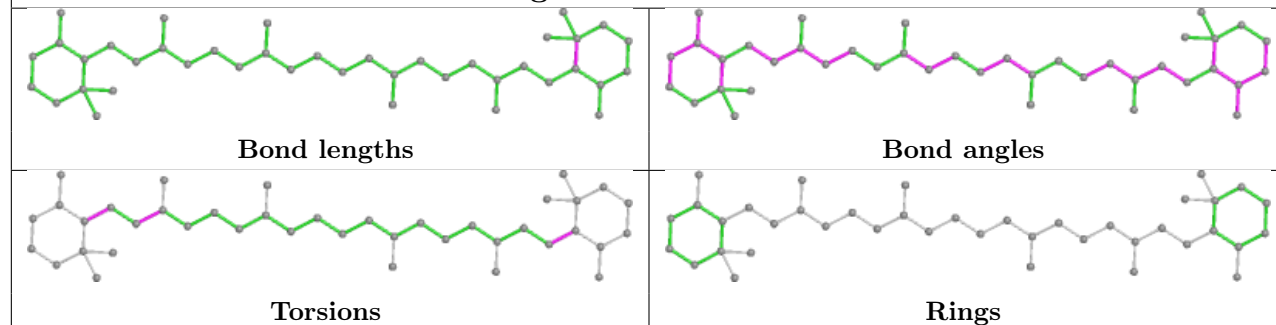
Ligand CLA Y 312

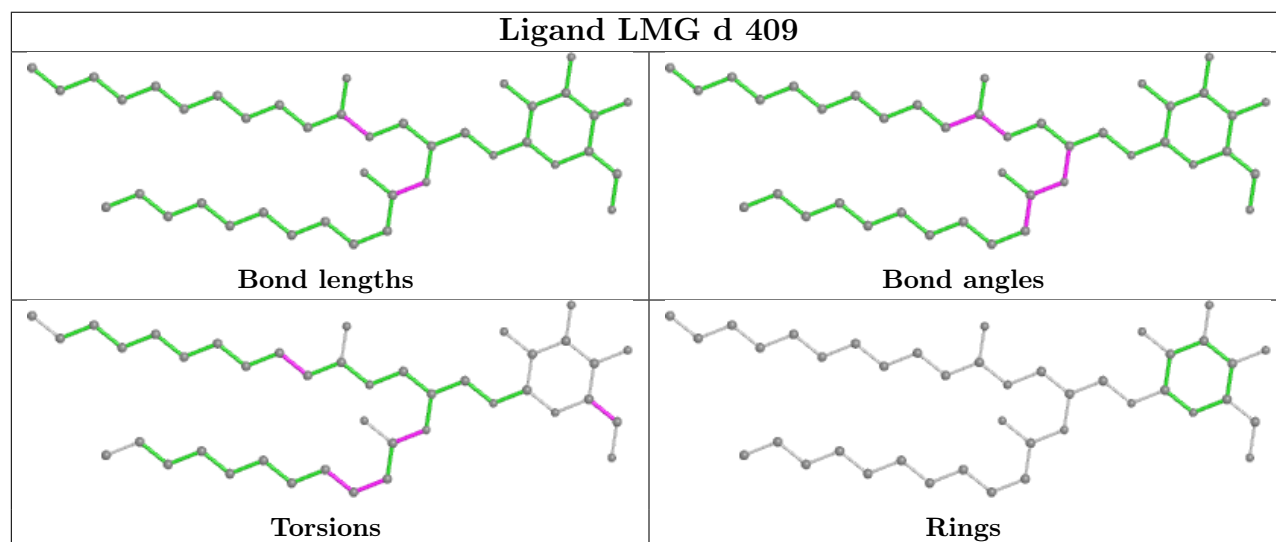
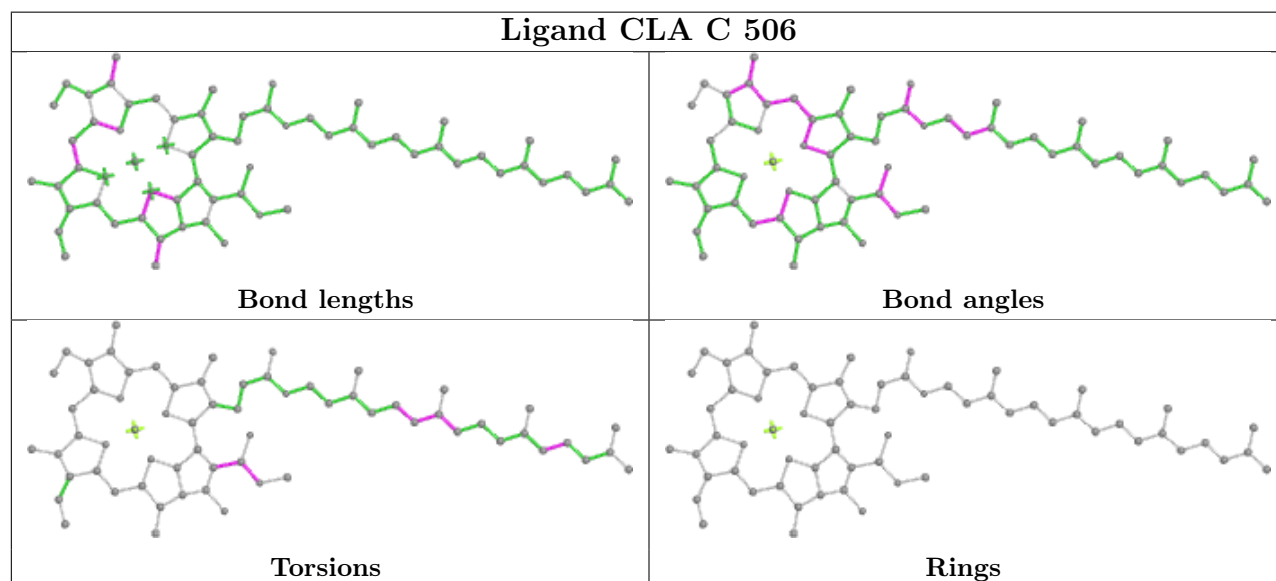
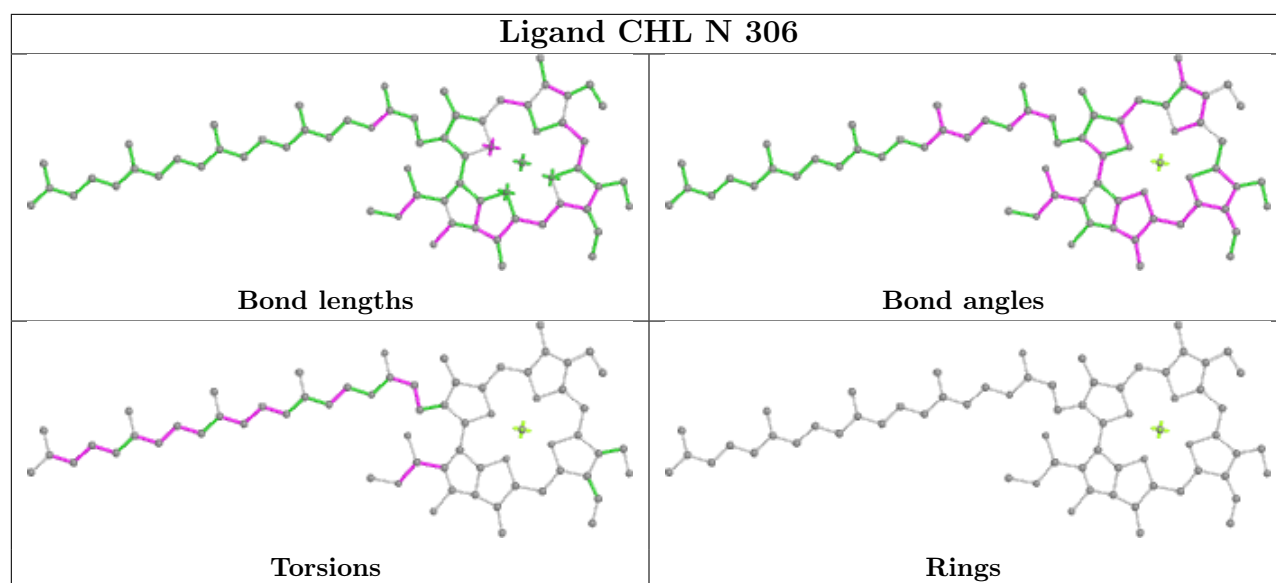


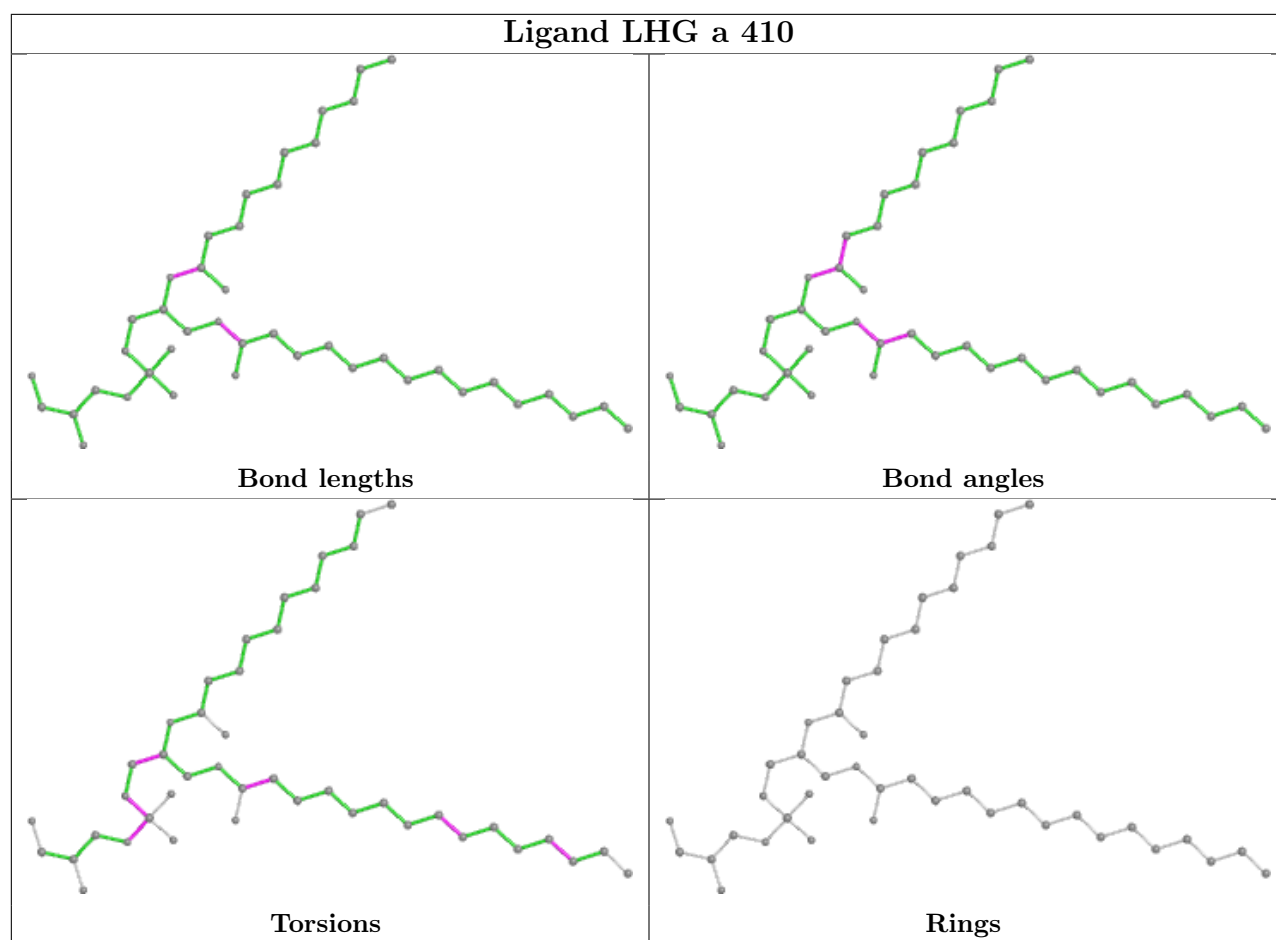
Ligand CLA C 503

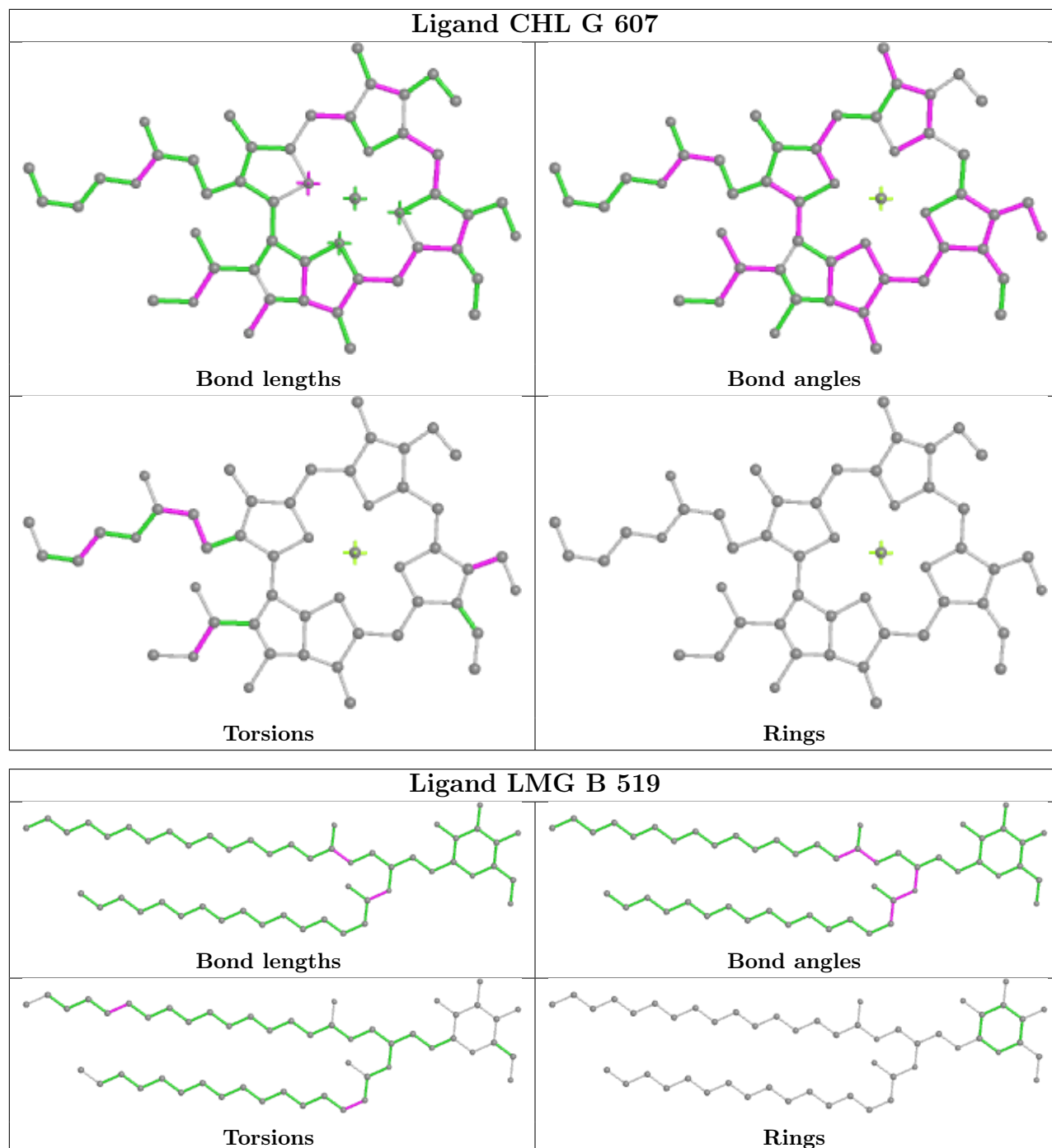


Ligand CLA B 502**Ligand CLA d 403****Ligand DGD c 515**

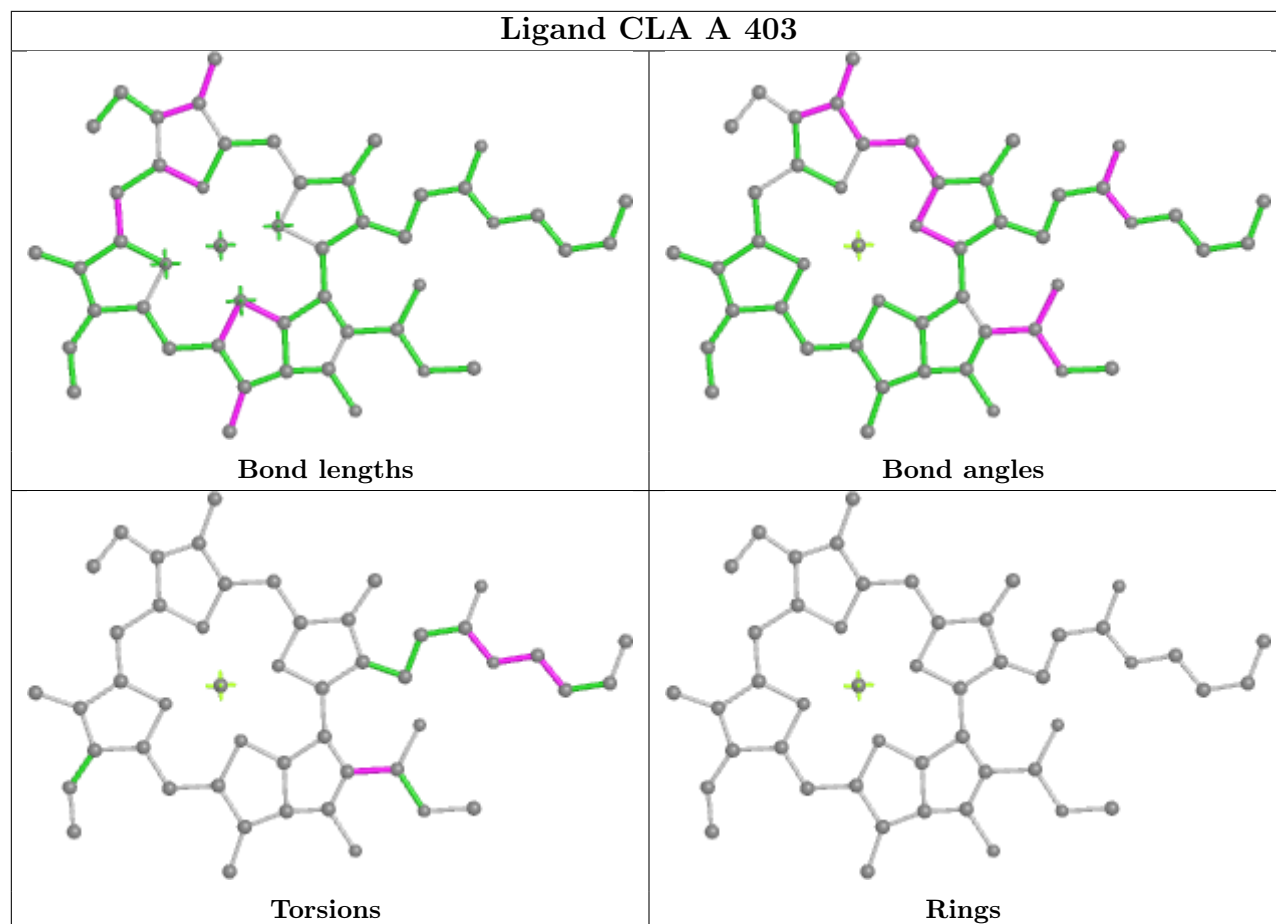
Ligand CLA b 513**Ligand CLA B 506****Ligand BCR C 514**



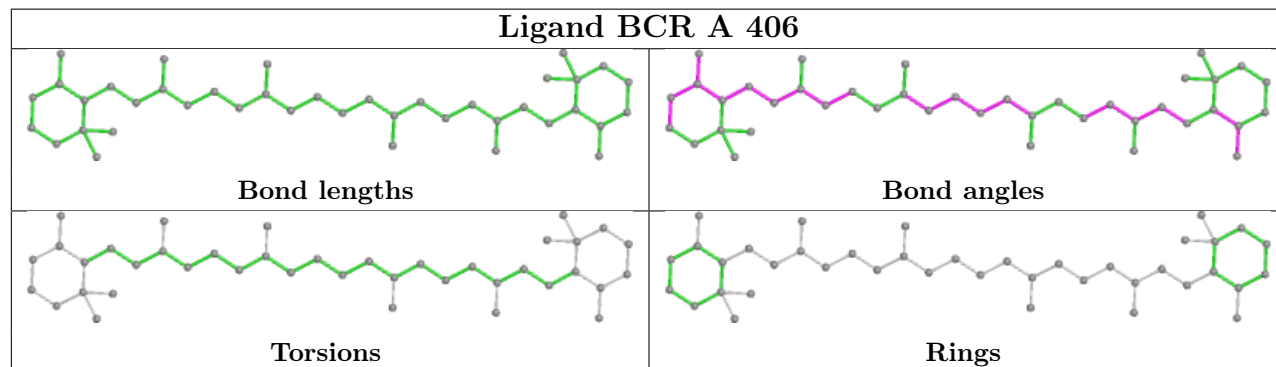


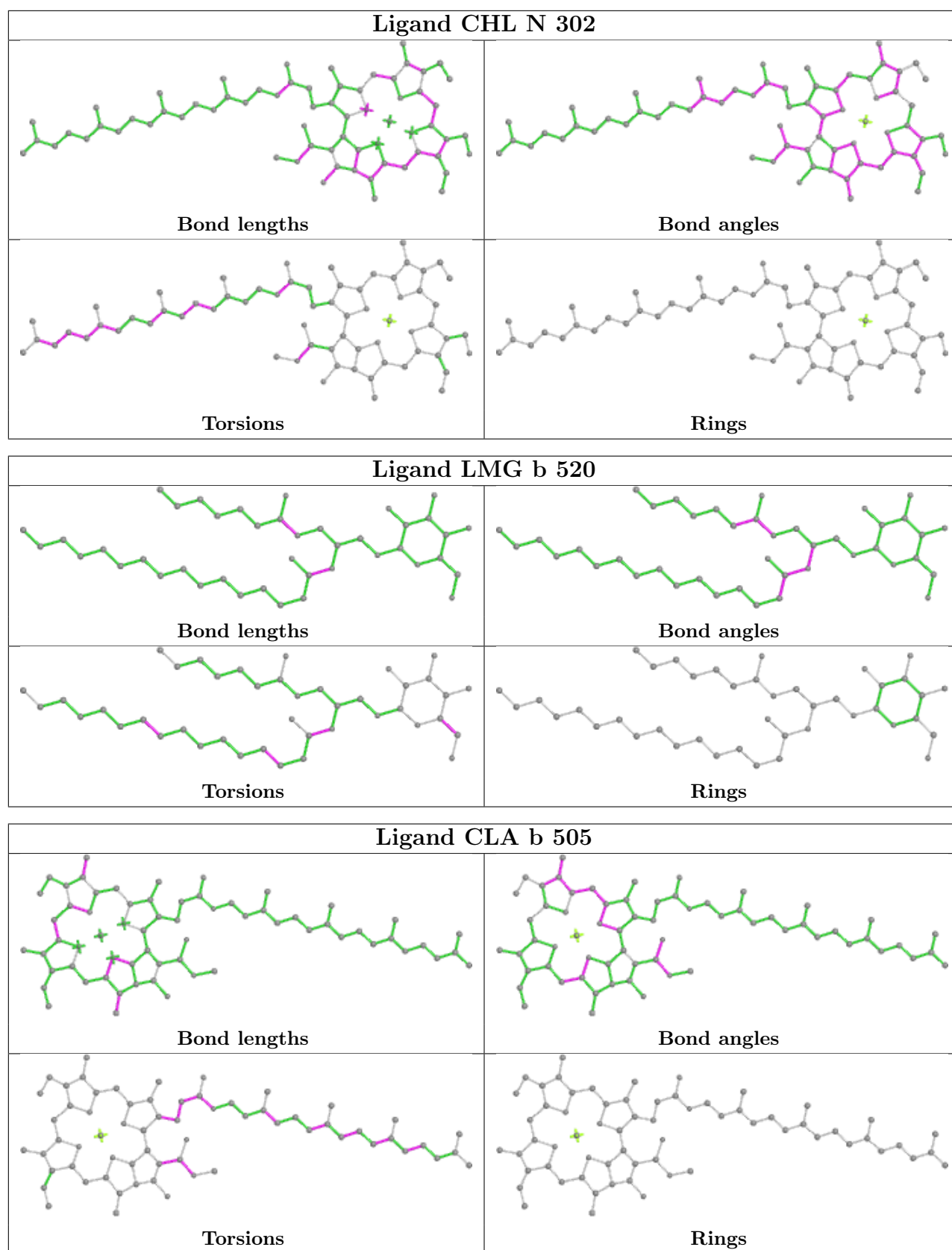


Ligand CLA A 403

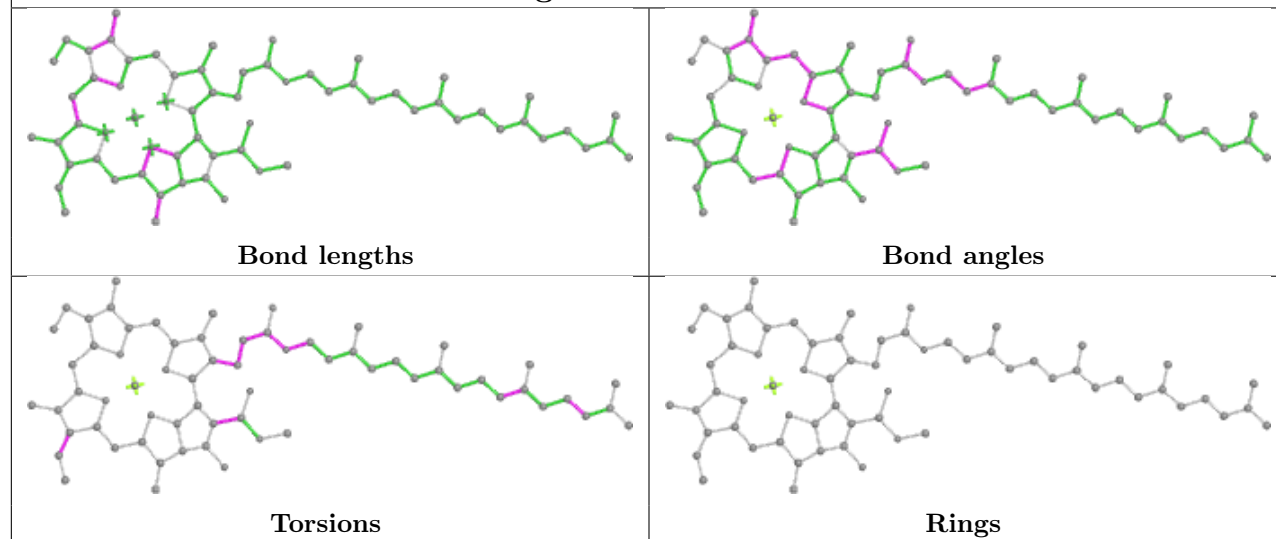


Ligand BCR A 406

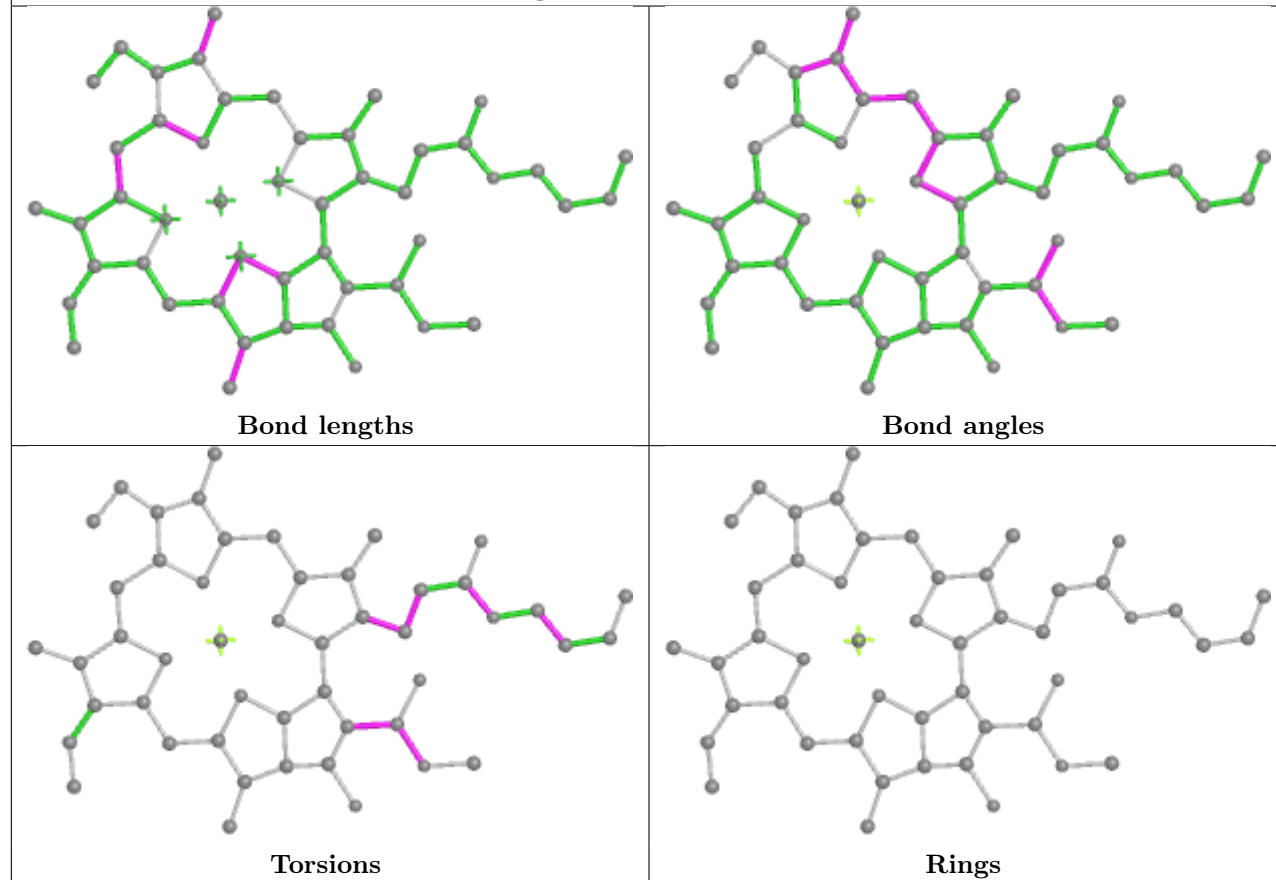


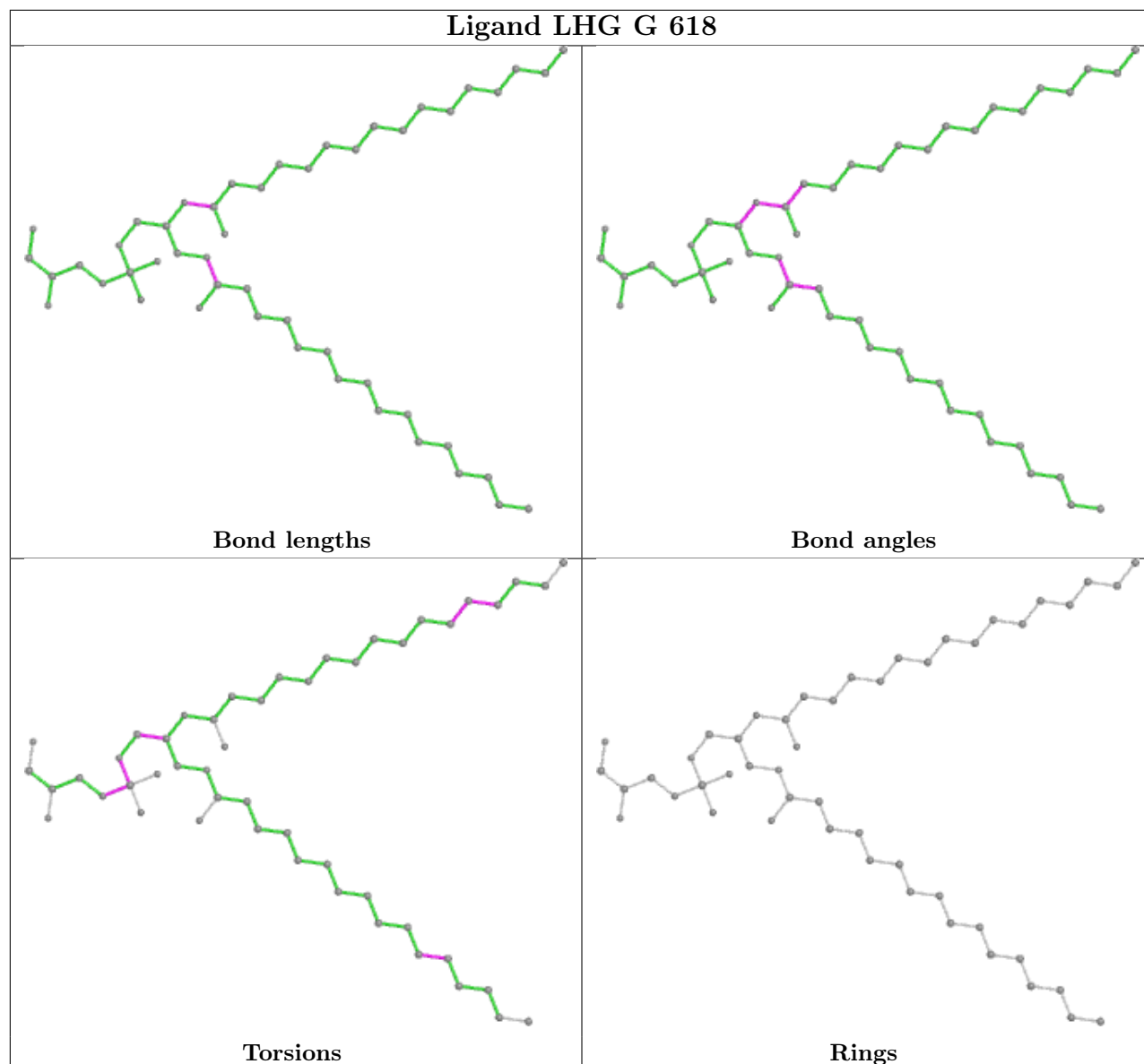
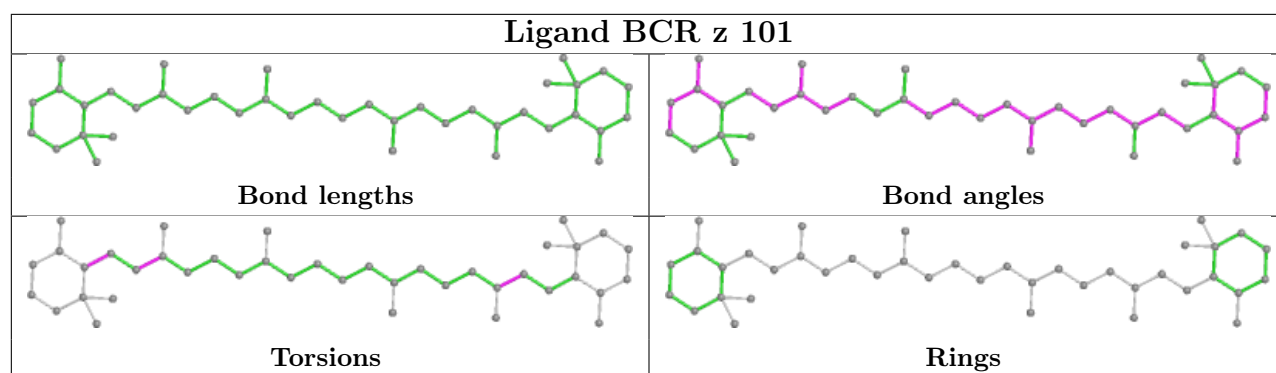


Ligand CLA d 401

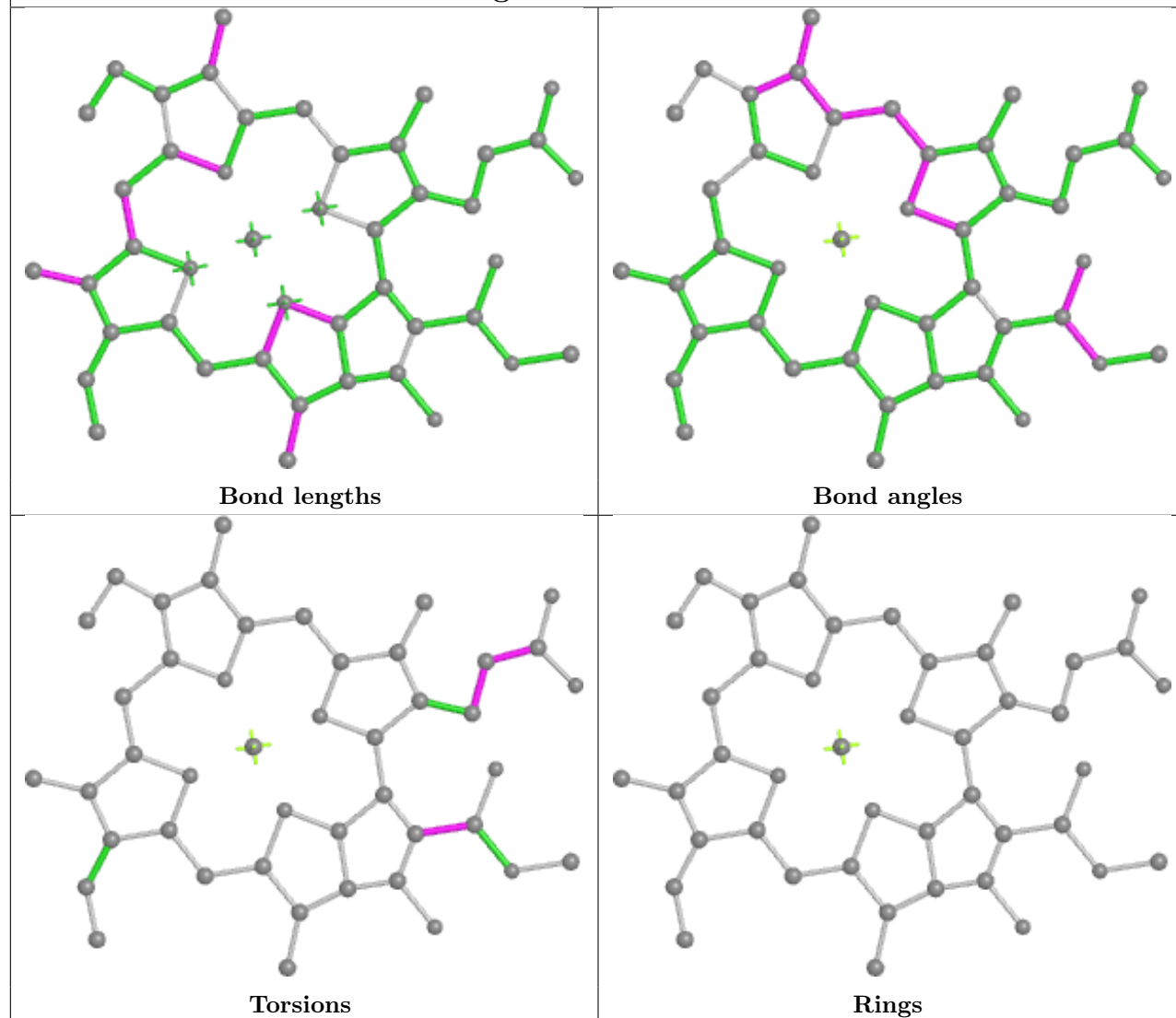


Ligand CLA N 312

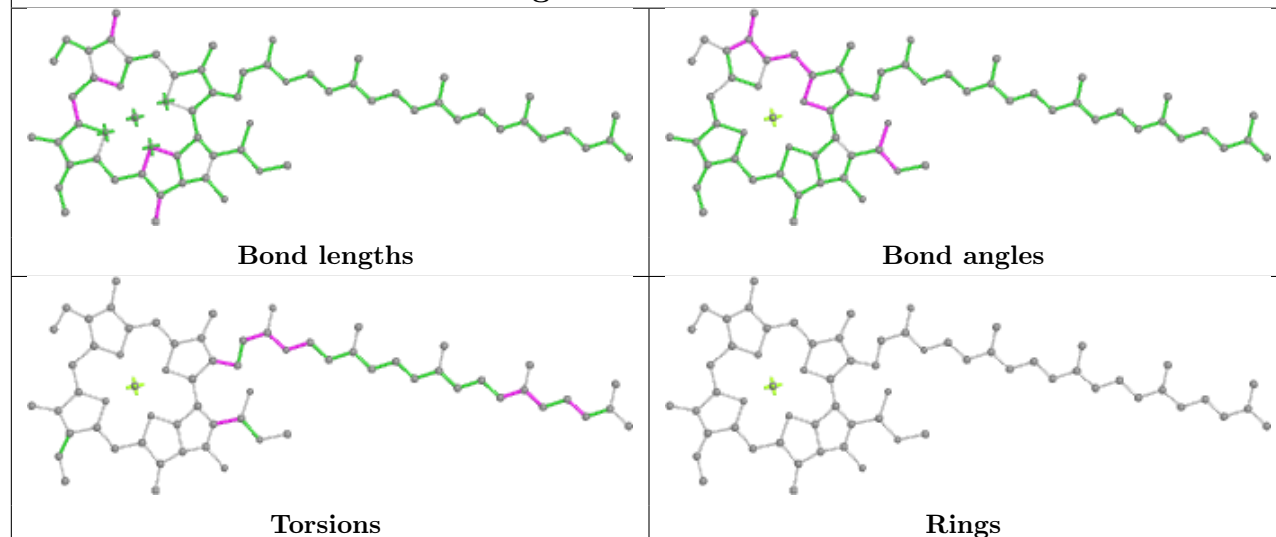


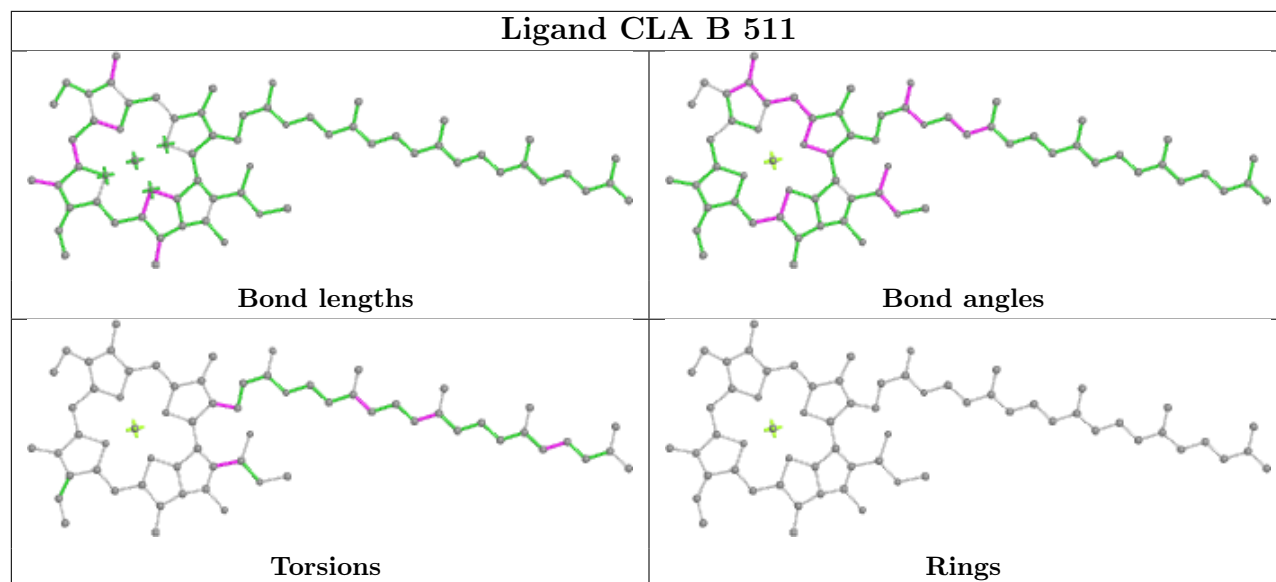
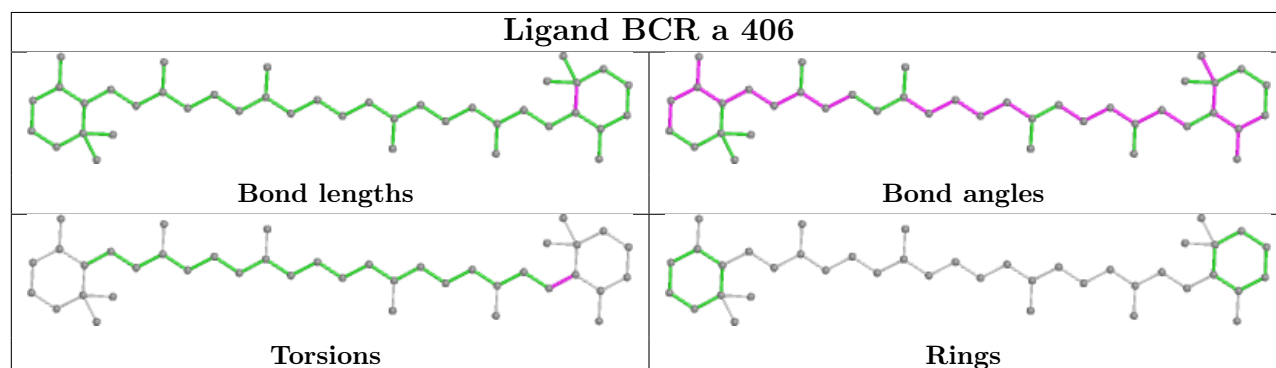
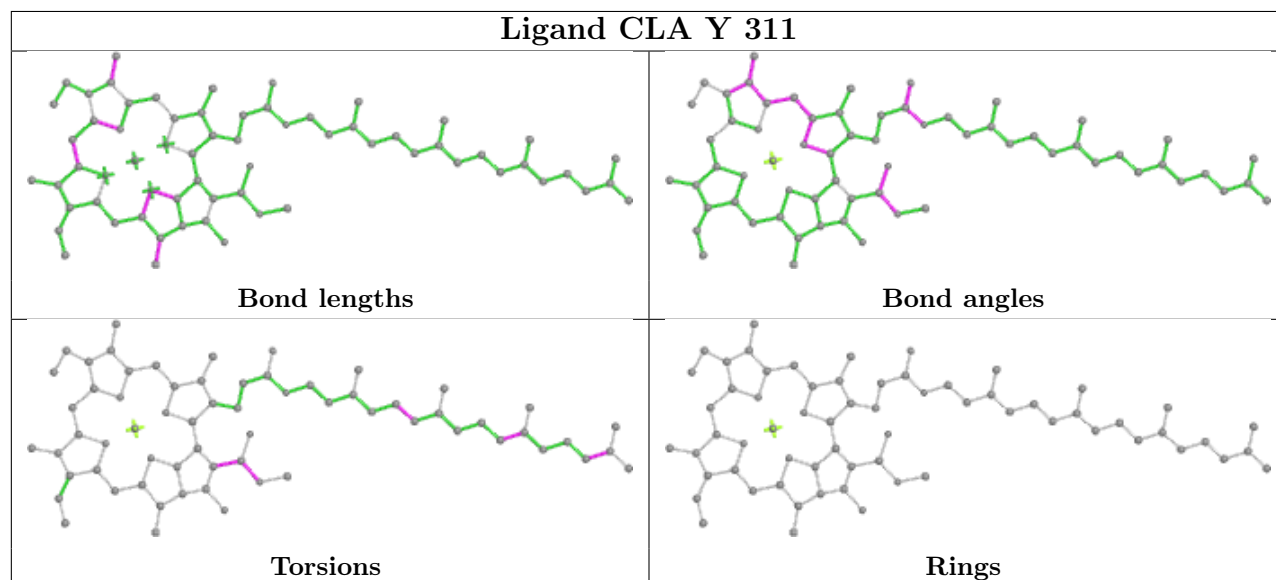


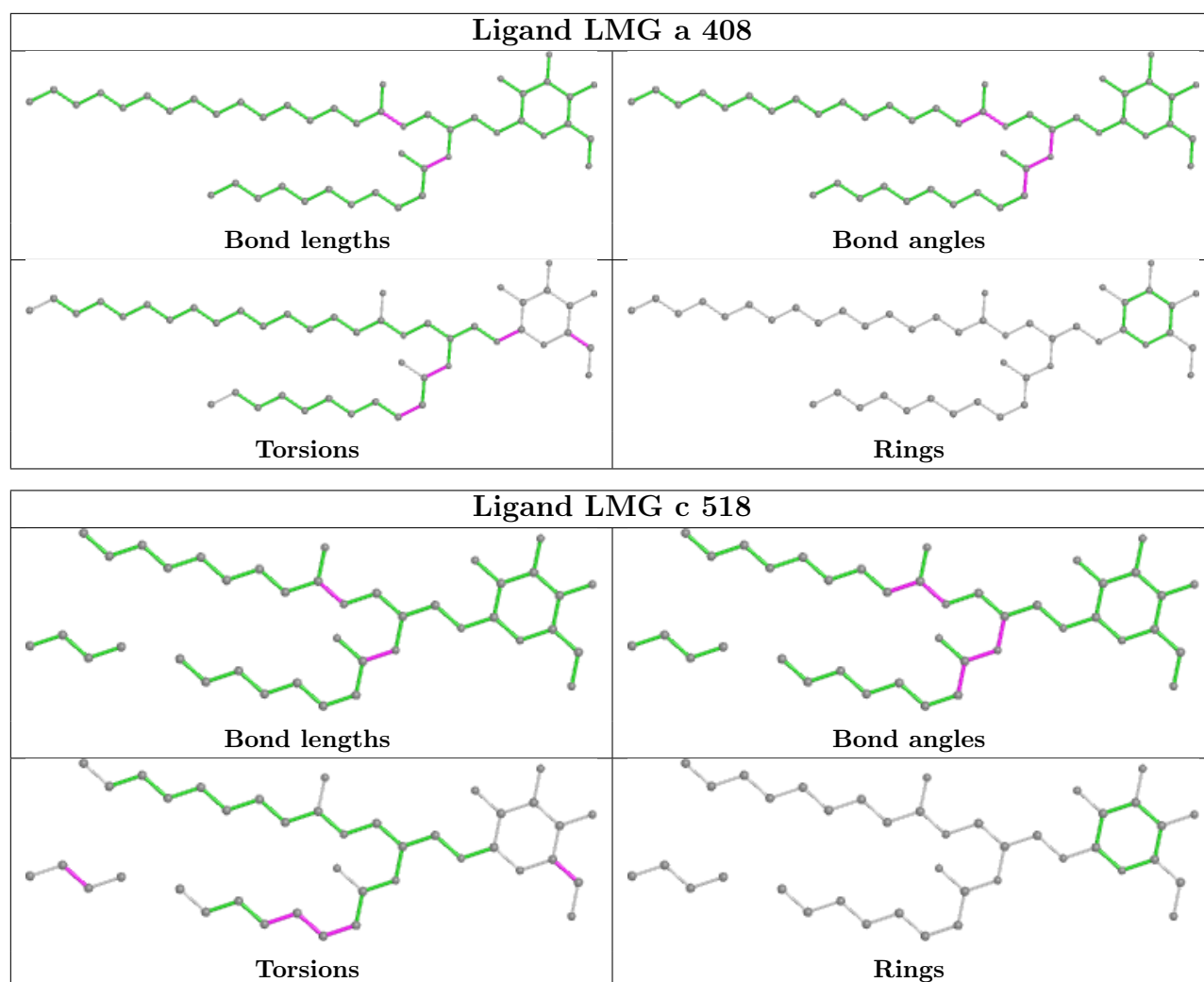
Ligand CLA b 516



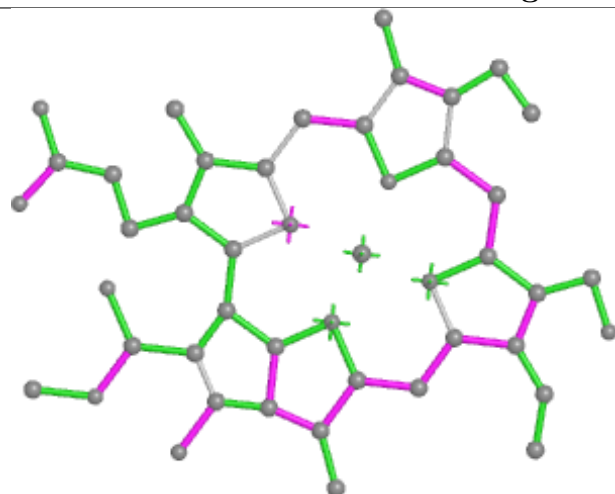
Ligand CLA B 510



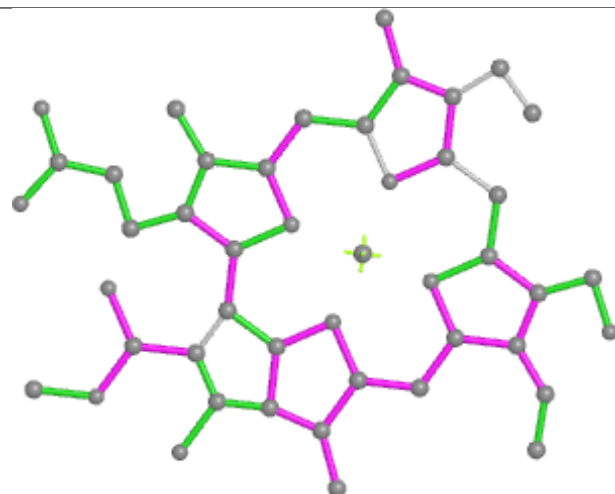
Ligand CLA B 511**Ligand BCR a 406****Ligand CLA Y 311**



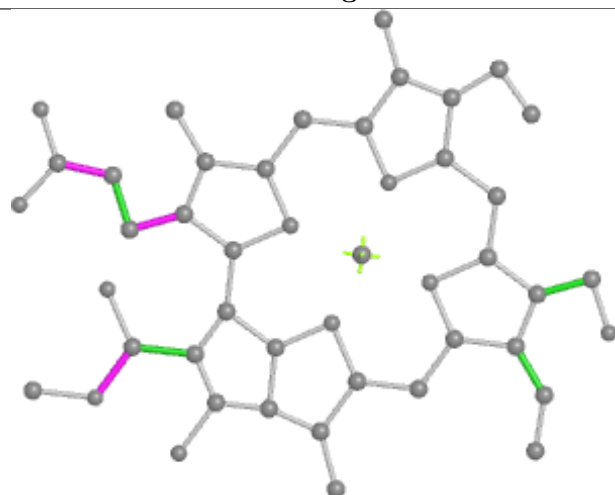
Ligand CHL r 306



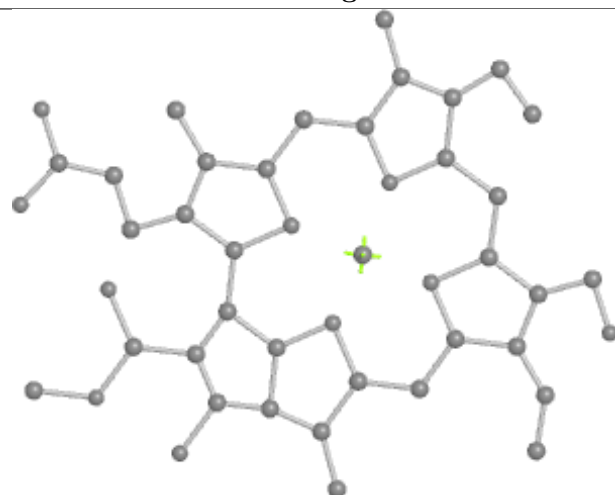
Bond lengths



Bond angles

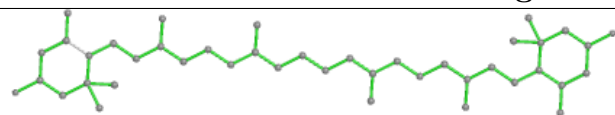


Torsions

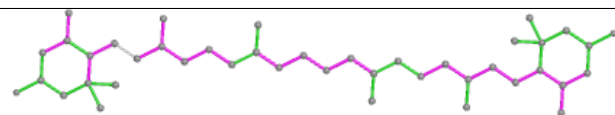


Rings

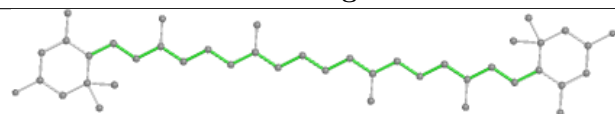
Ligand LUT G 615



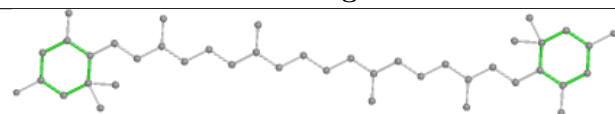
Bond lengths



Bond angles

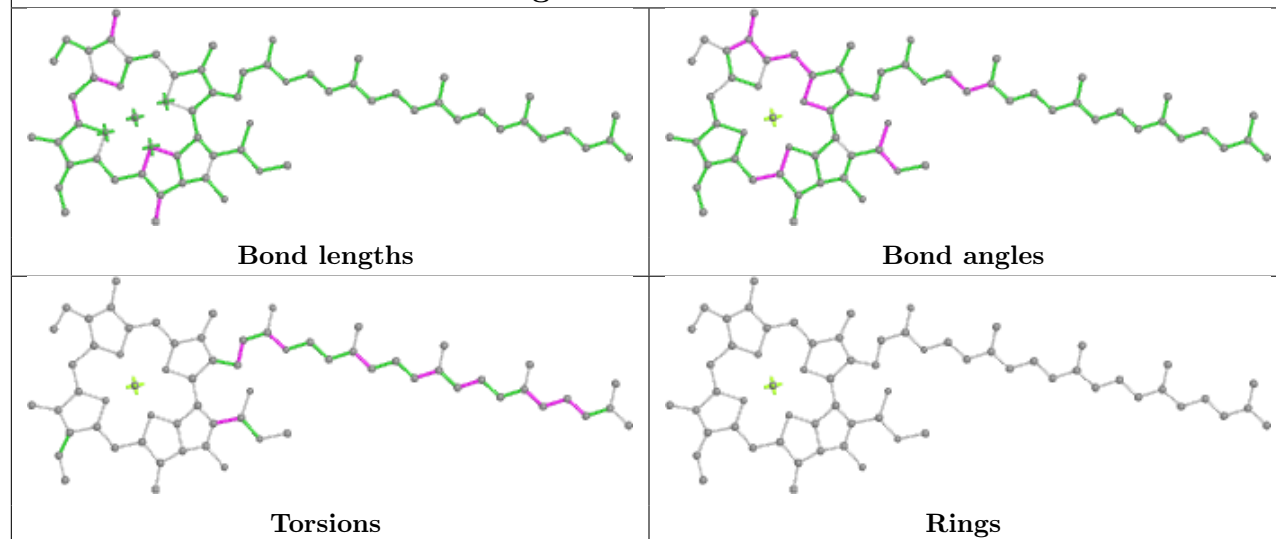


Torsions

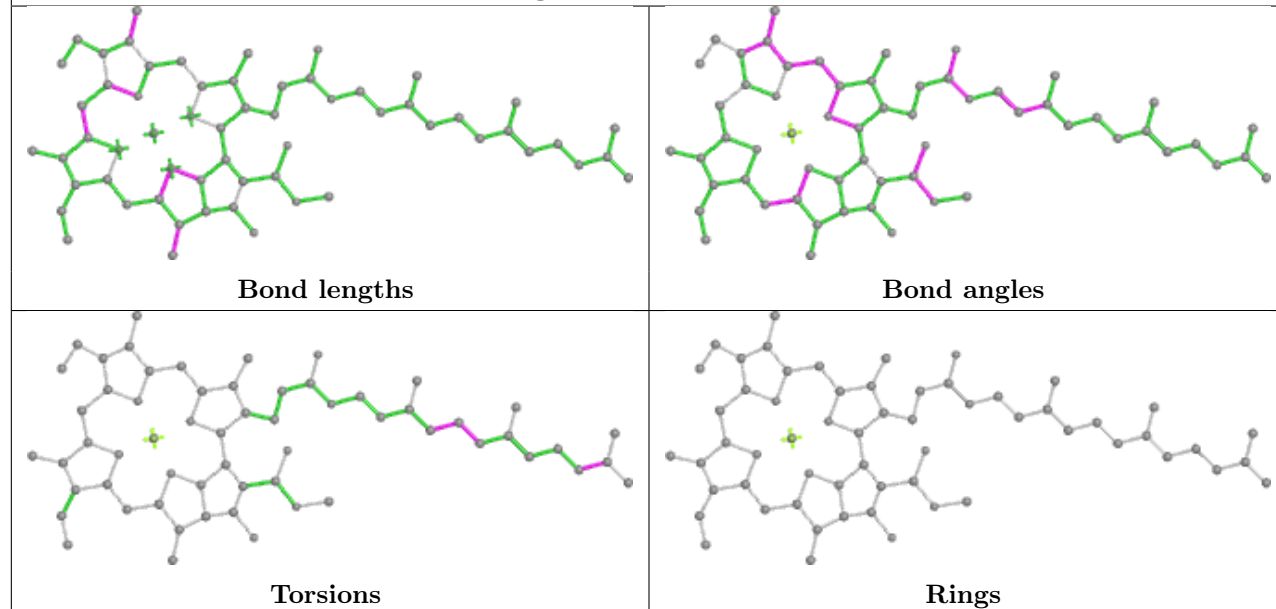


Rings

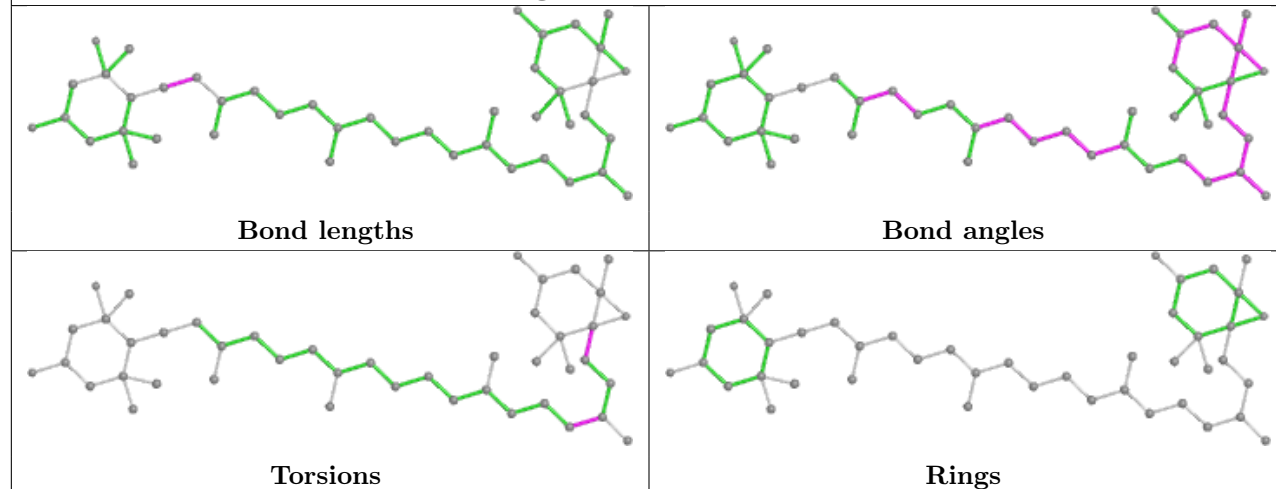
Ligand CLA C 510



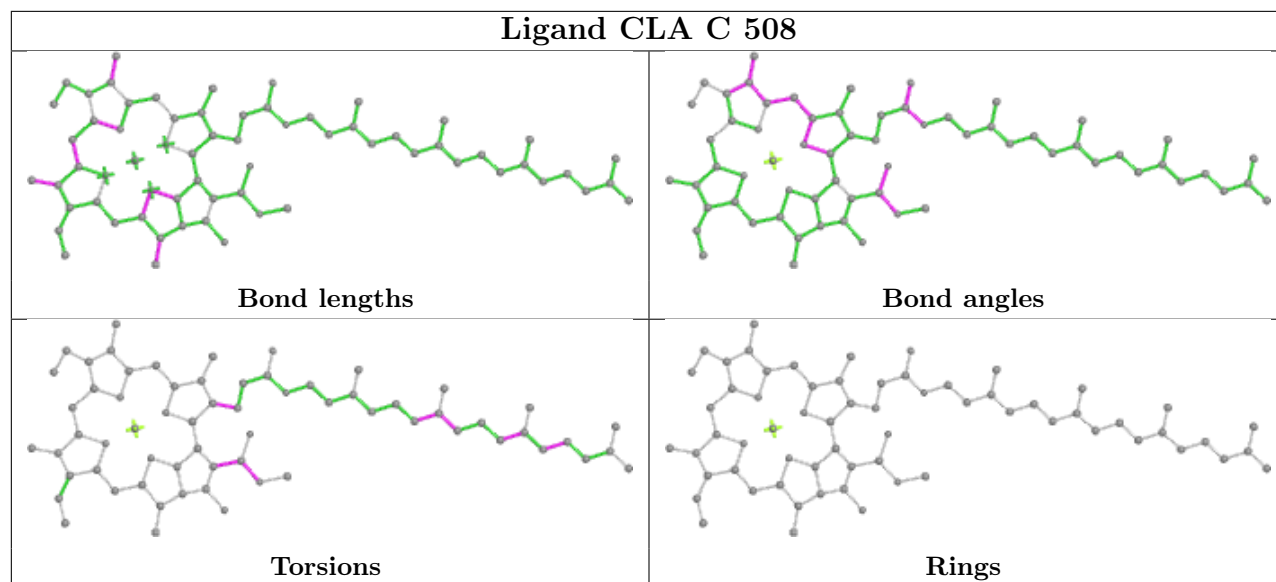
Ligand CLA A 405



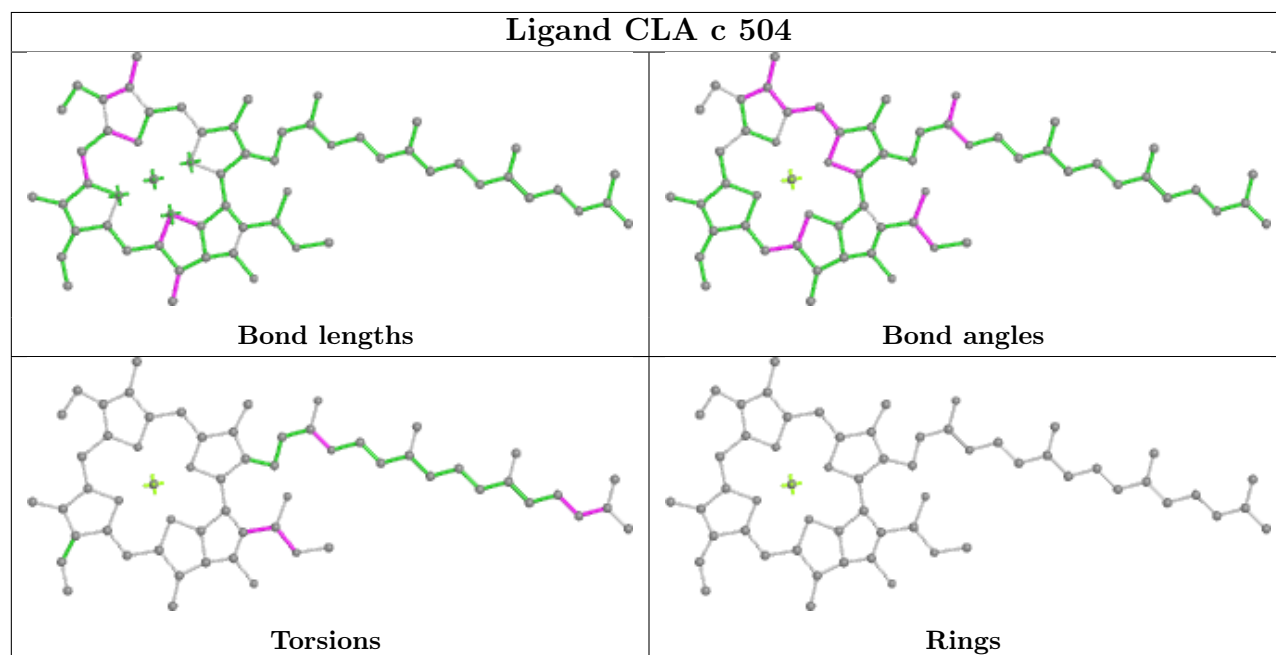
Ligand NEX S 617



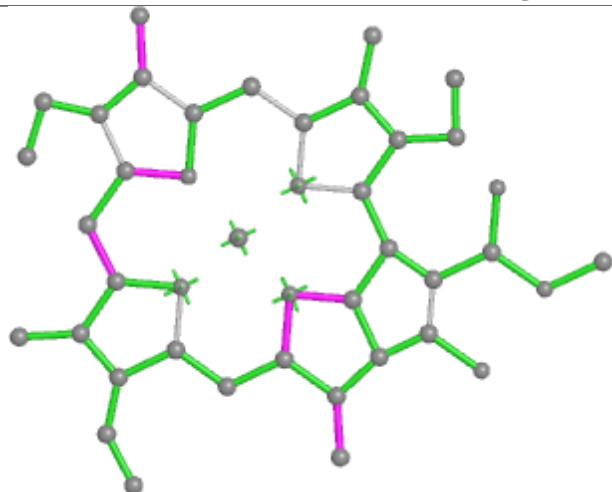
Ligand CLA C 508



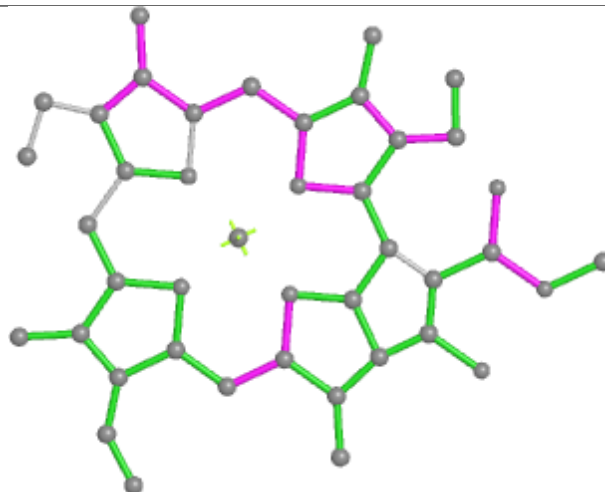
Ligand CLA c 504



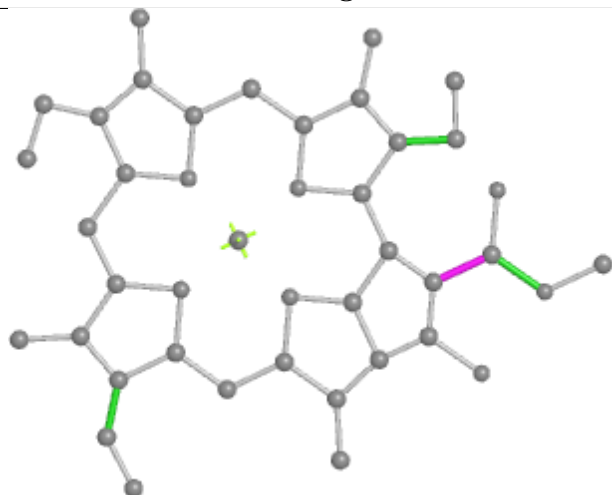
Ligand CLA S 603



Bond lengths



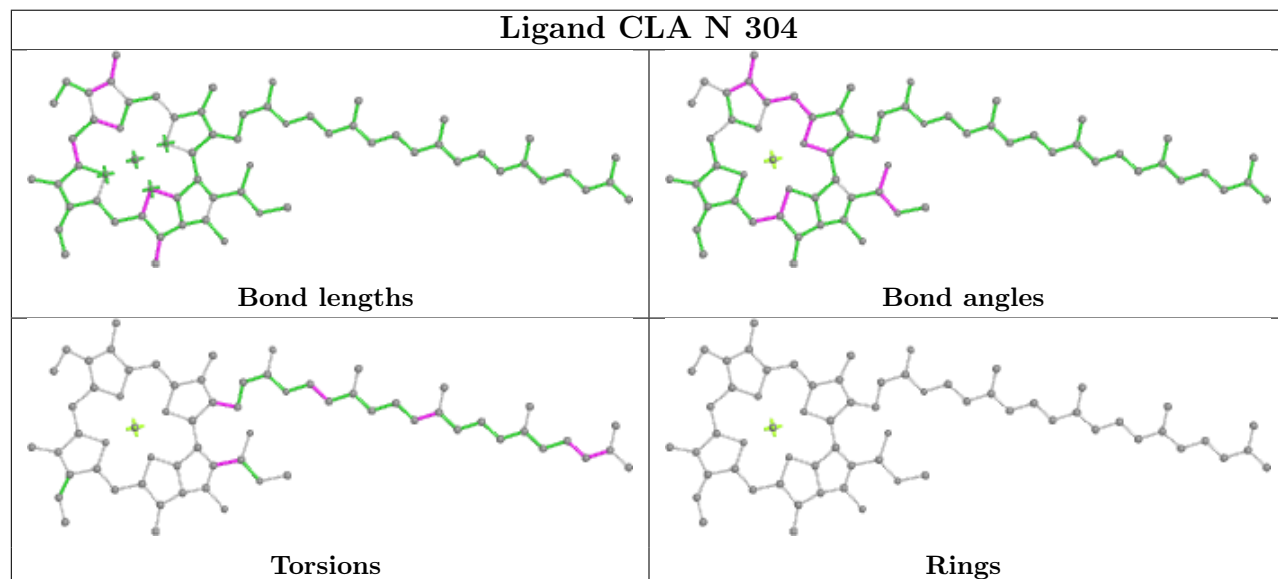
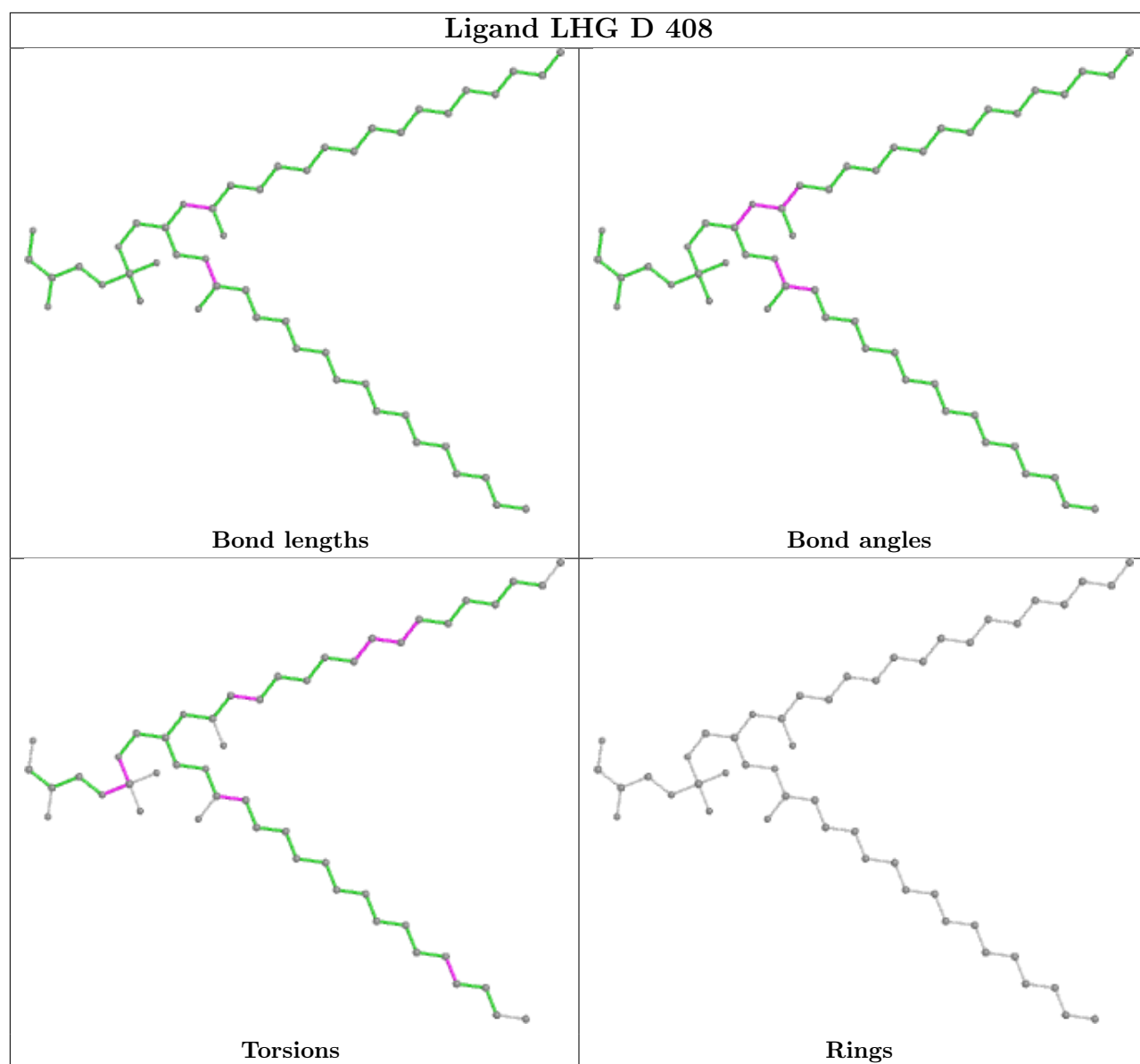
Bond angles

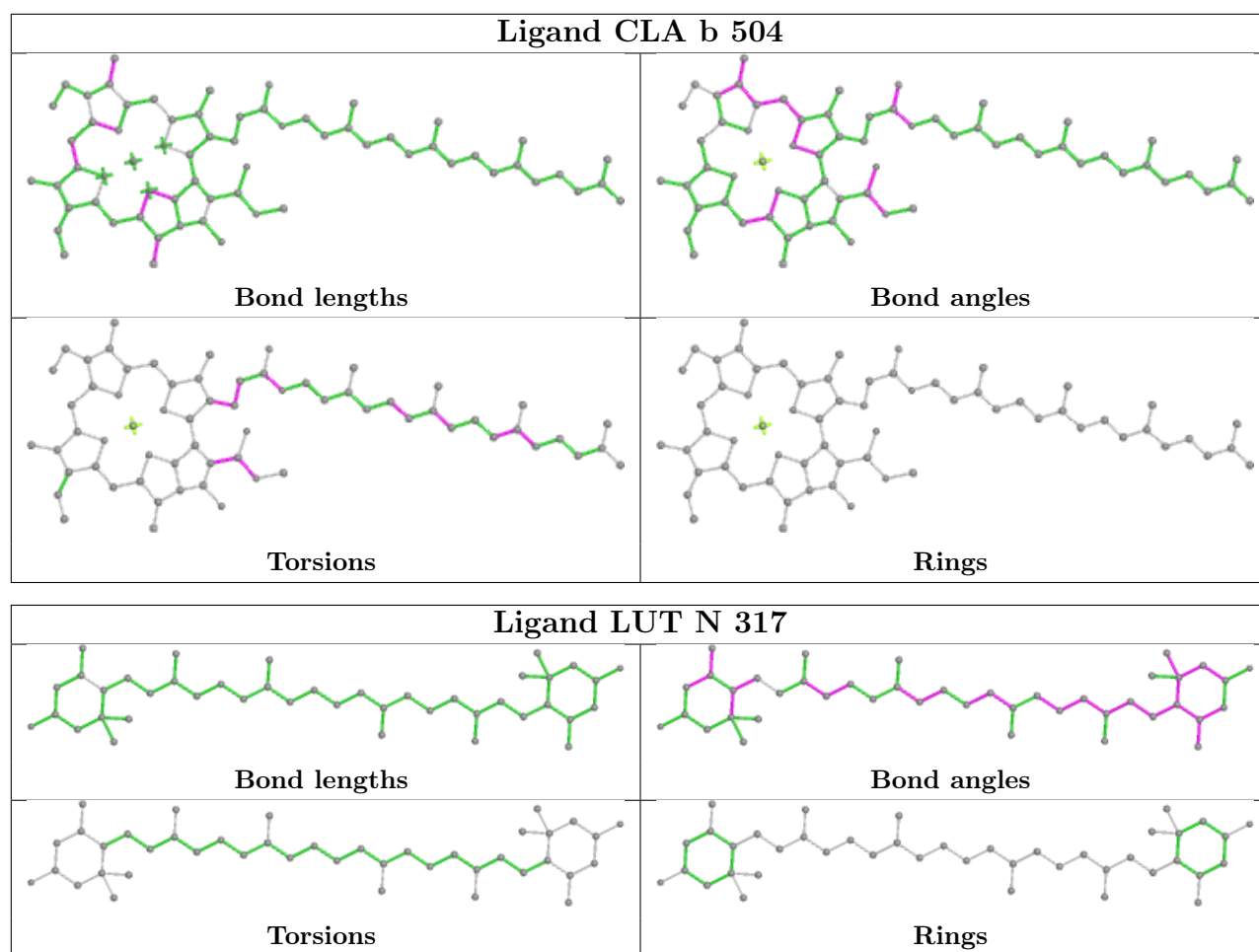


Torsions

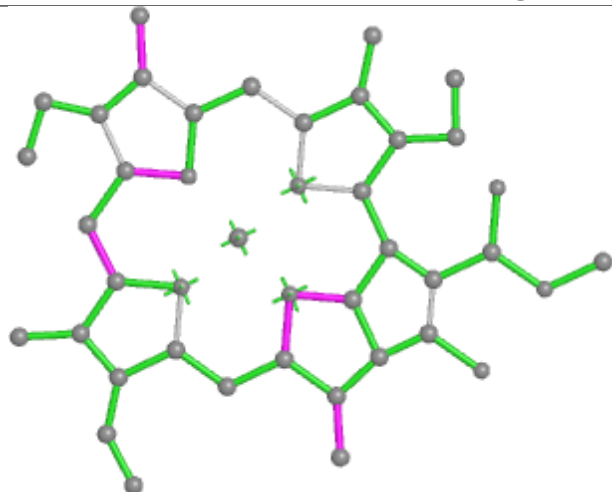


Rings

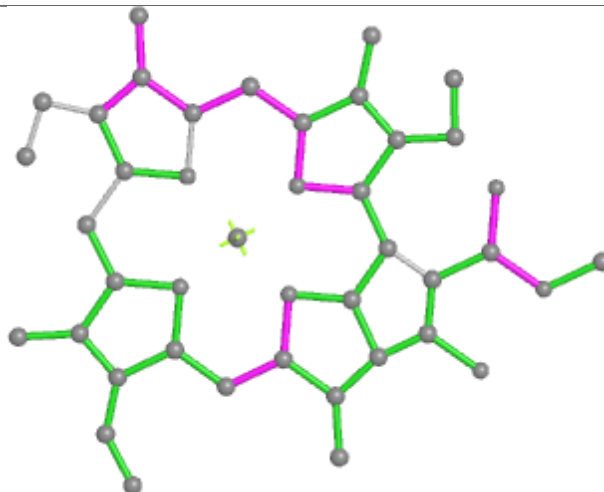




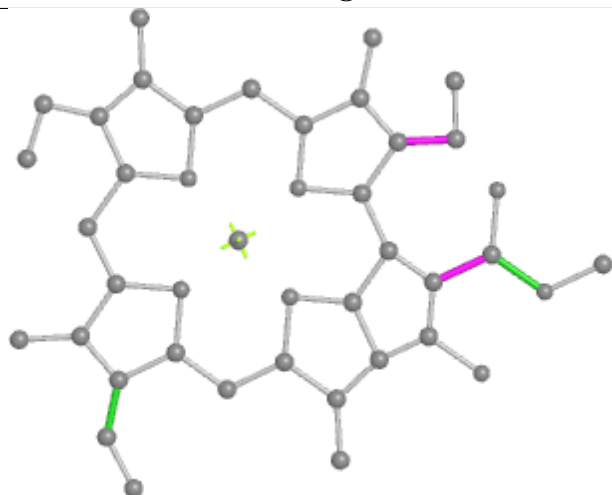
Ligand CLA G 604



Bond lengths



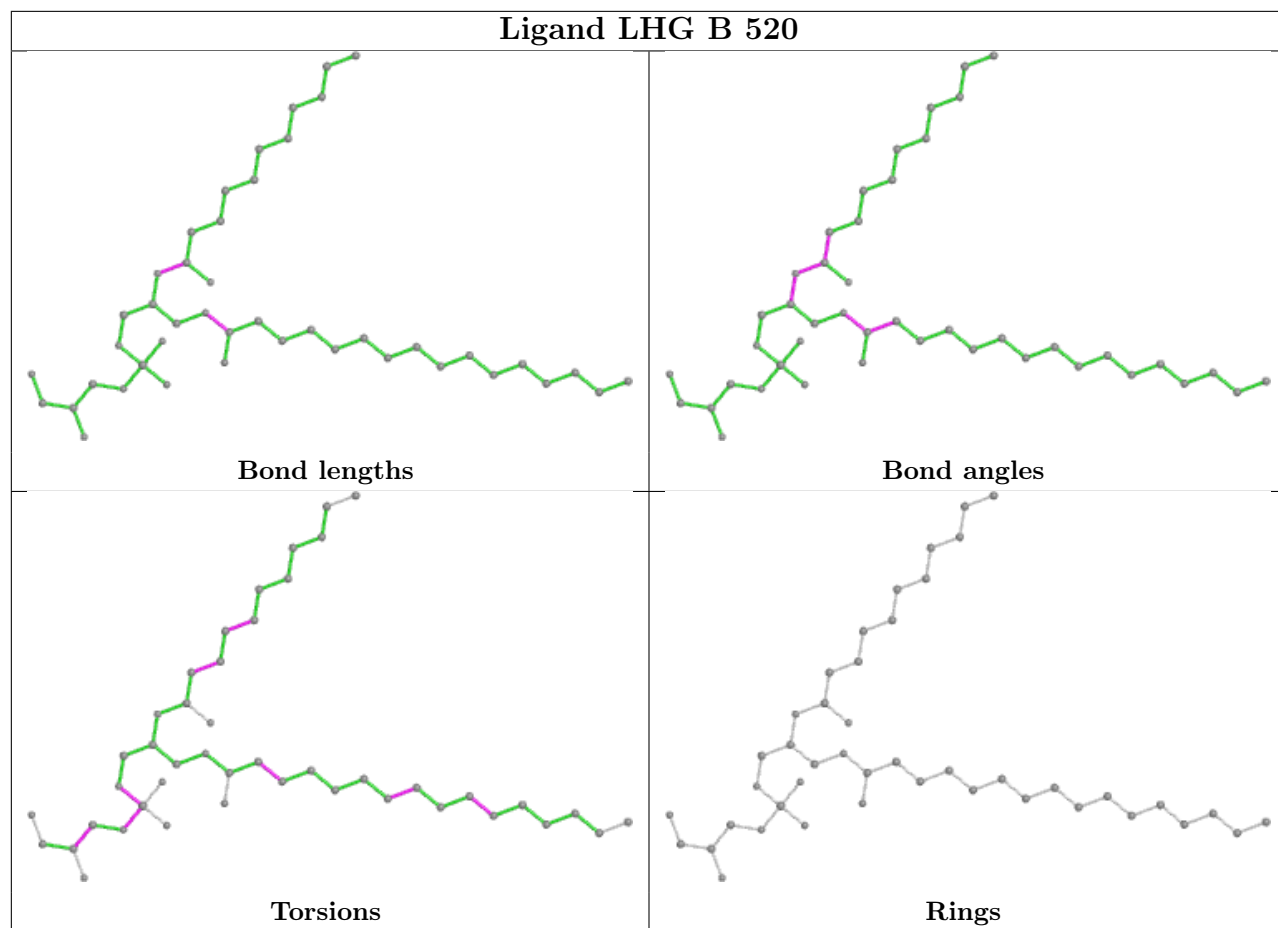
Bond angles

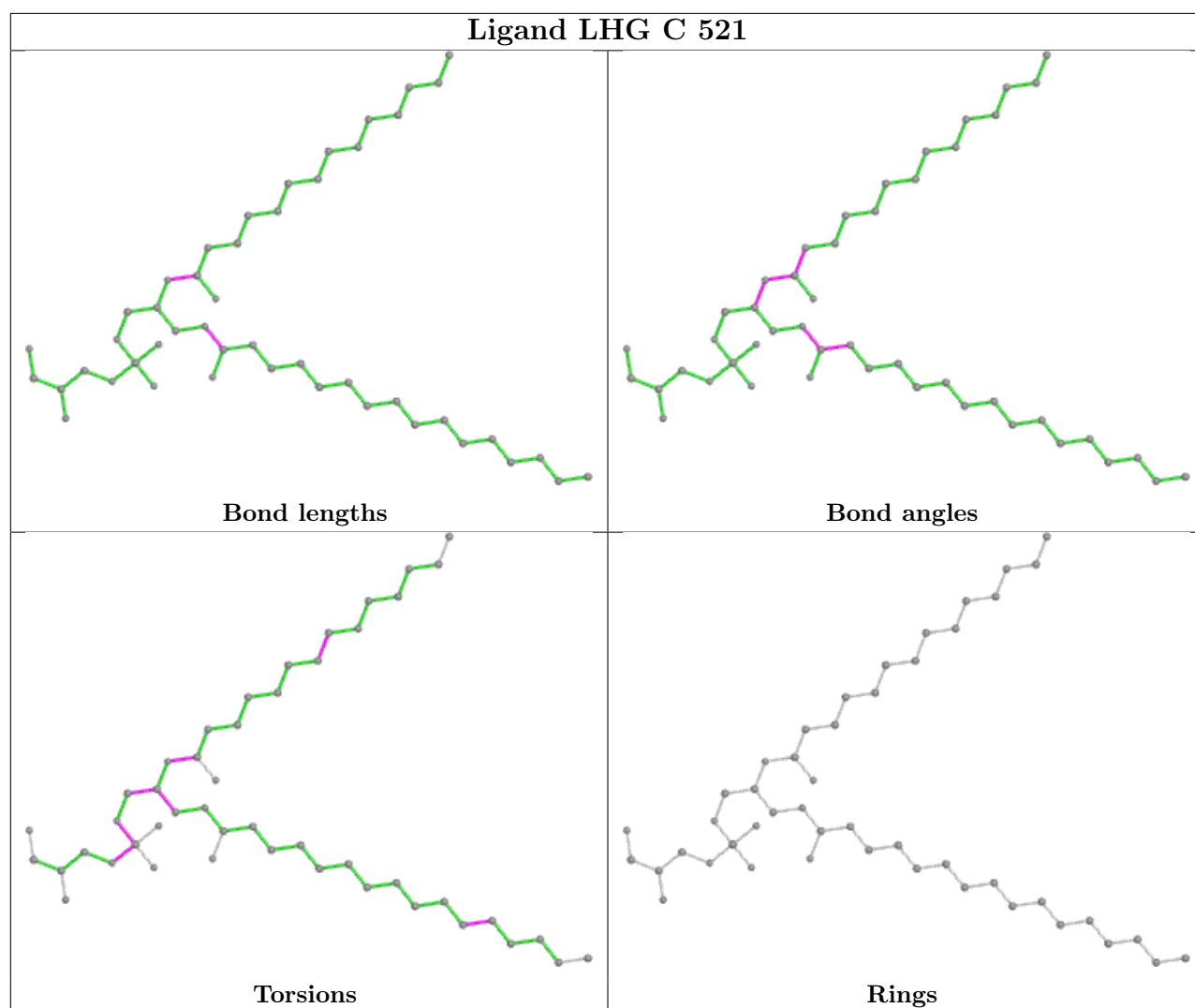


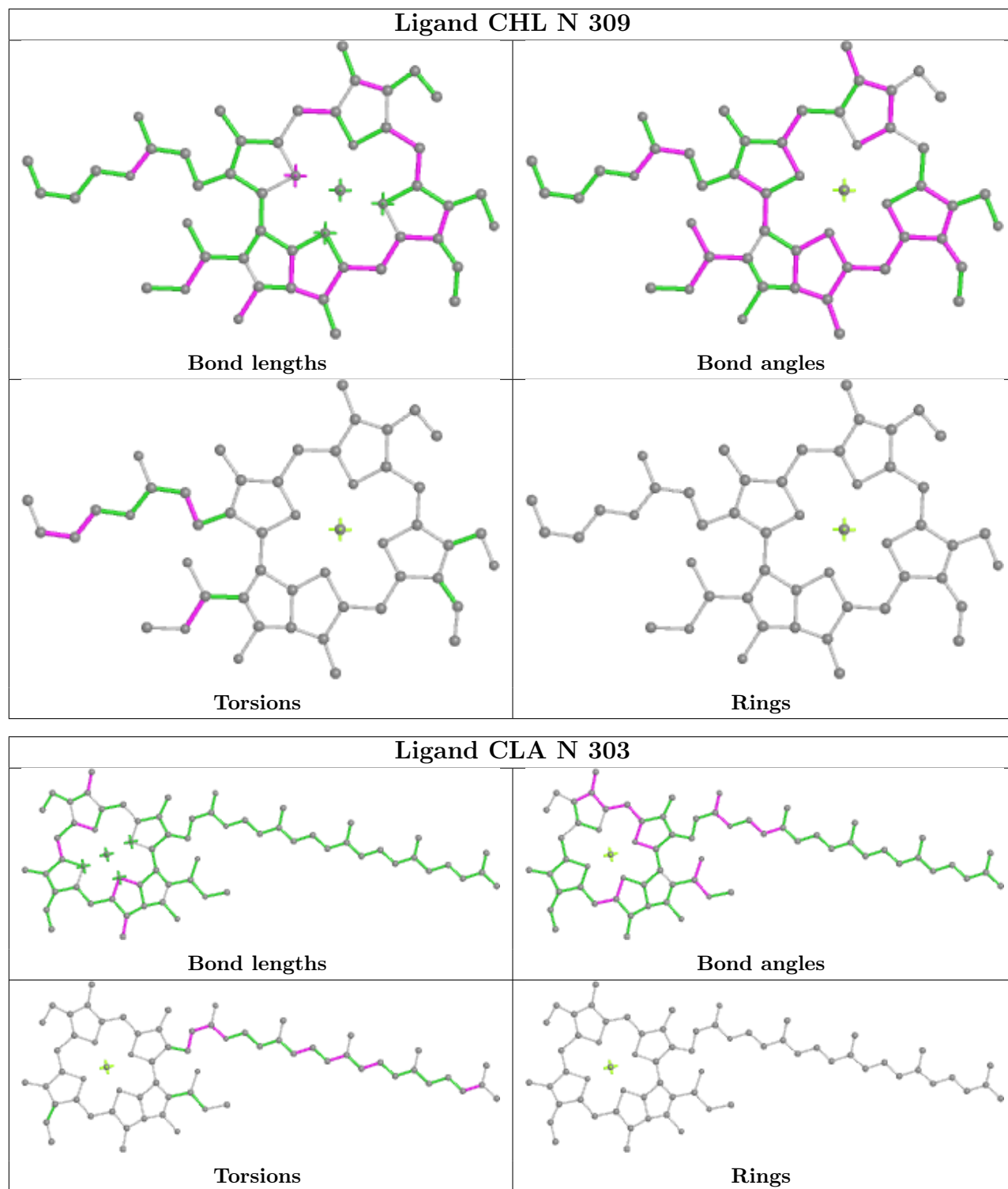
Torsions



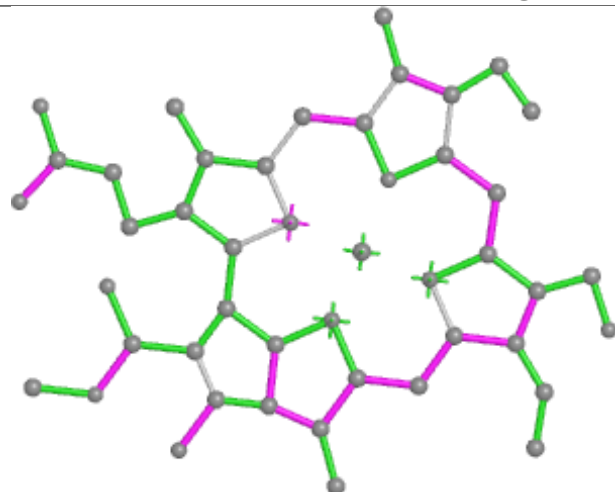
Rings



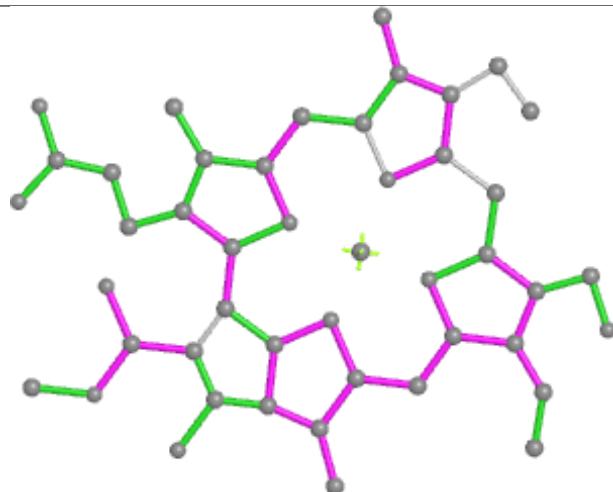




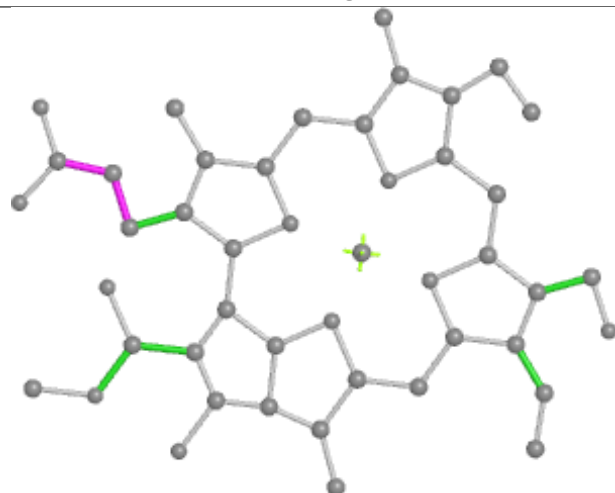
Ligand CHL Y 307



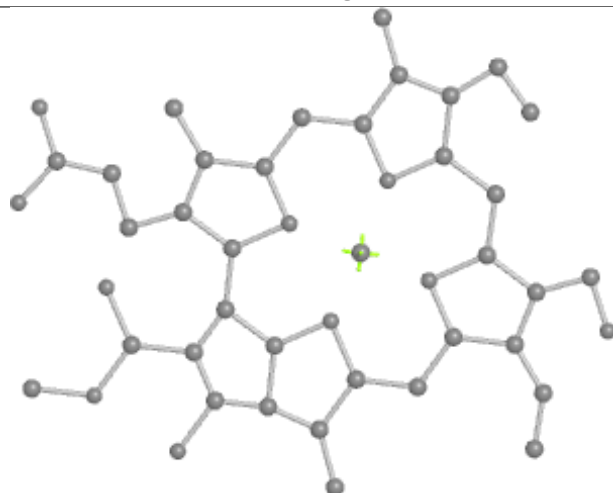
Bond lengths



Bond angles

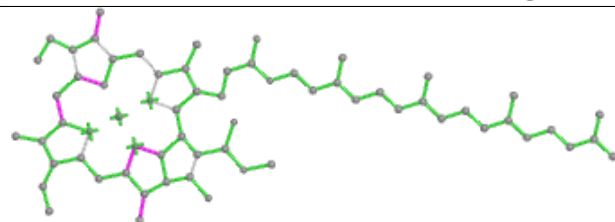


Torsions

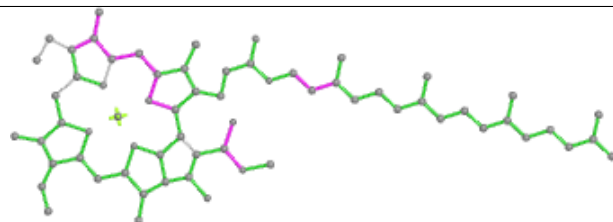


Rings

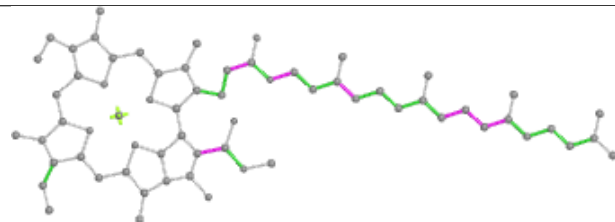
Ligand CLA c 510



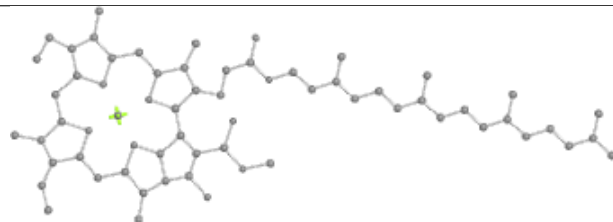
Bond lengths



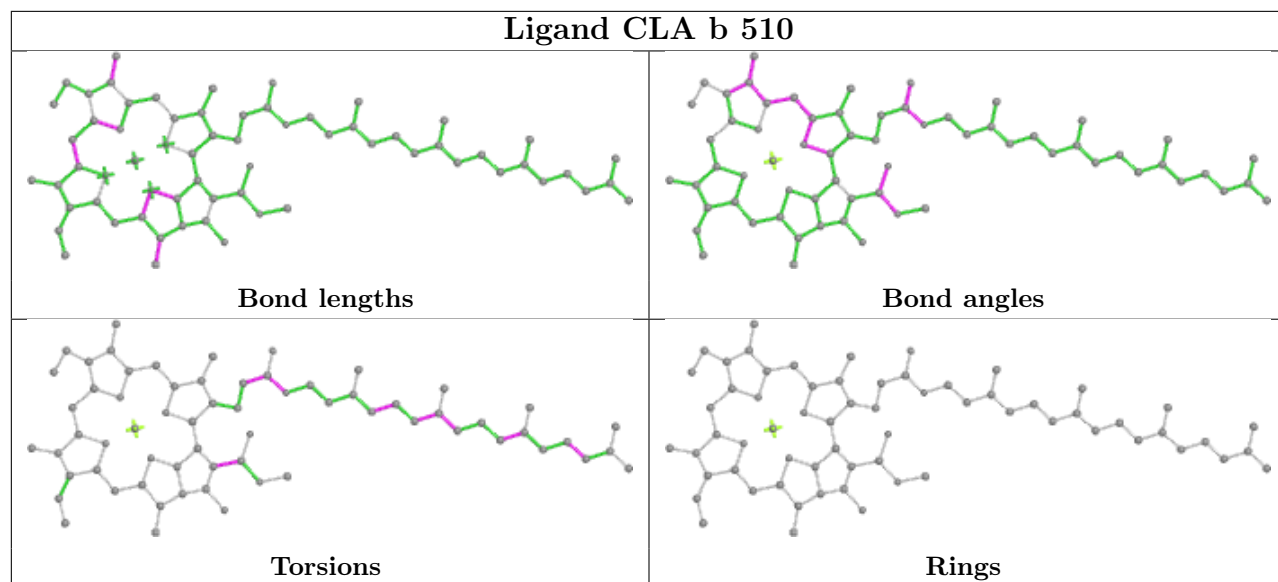
Bond angles

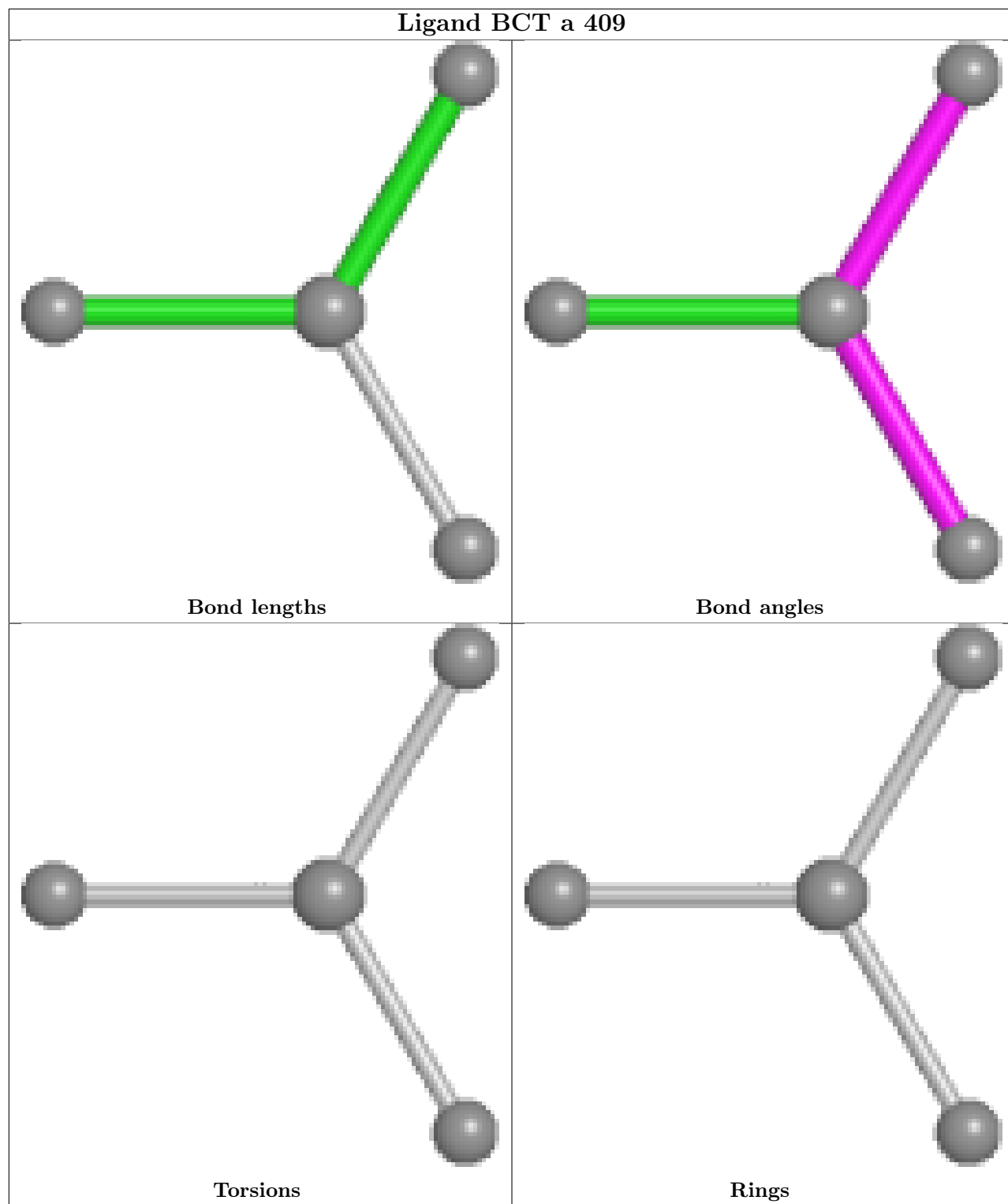


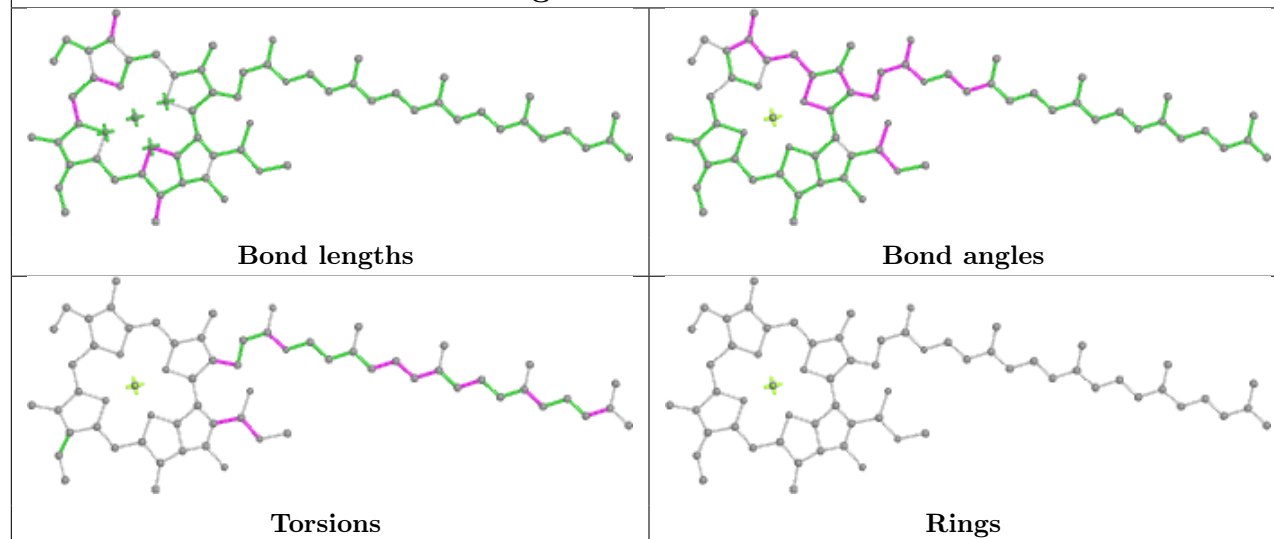
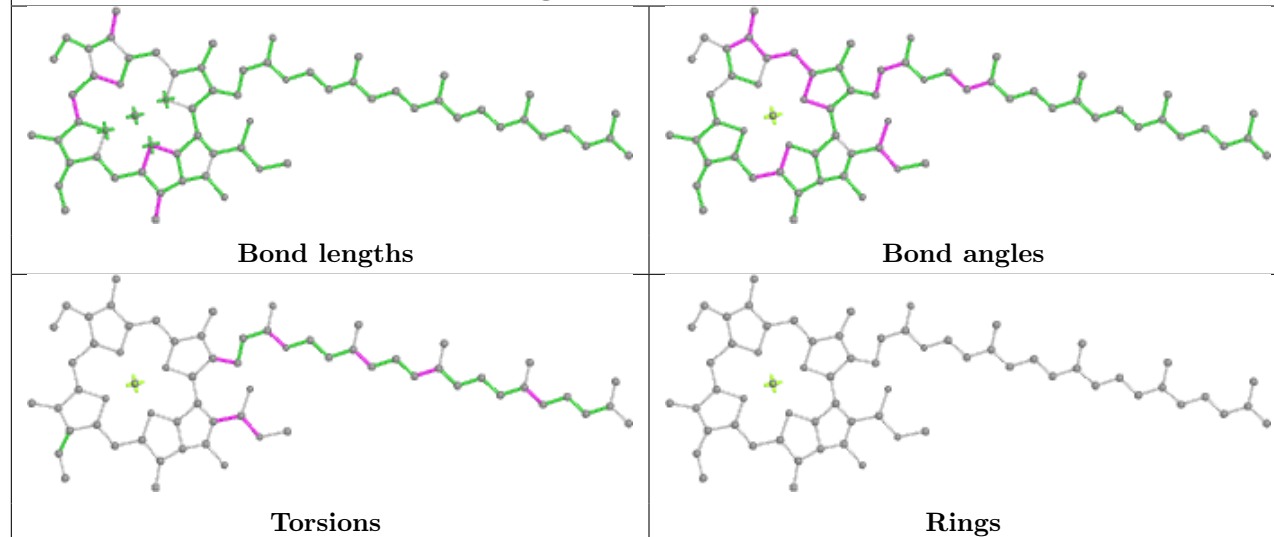
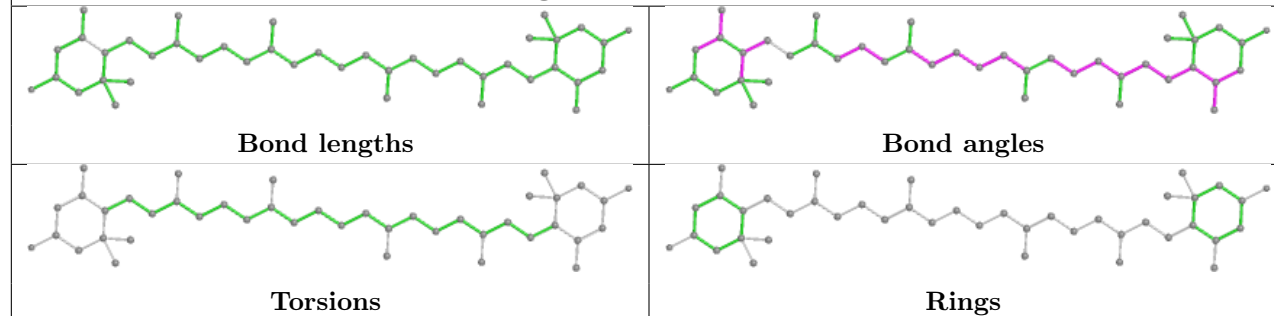
Torsions

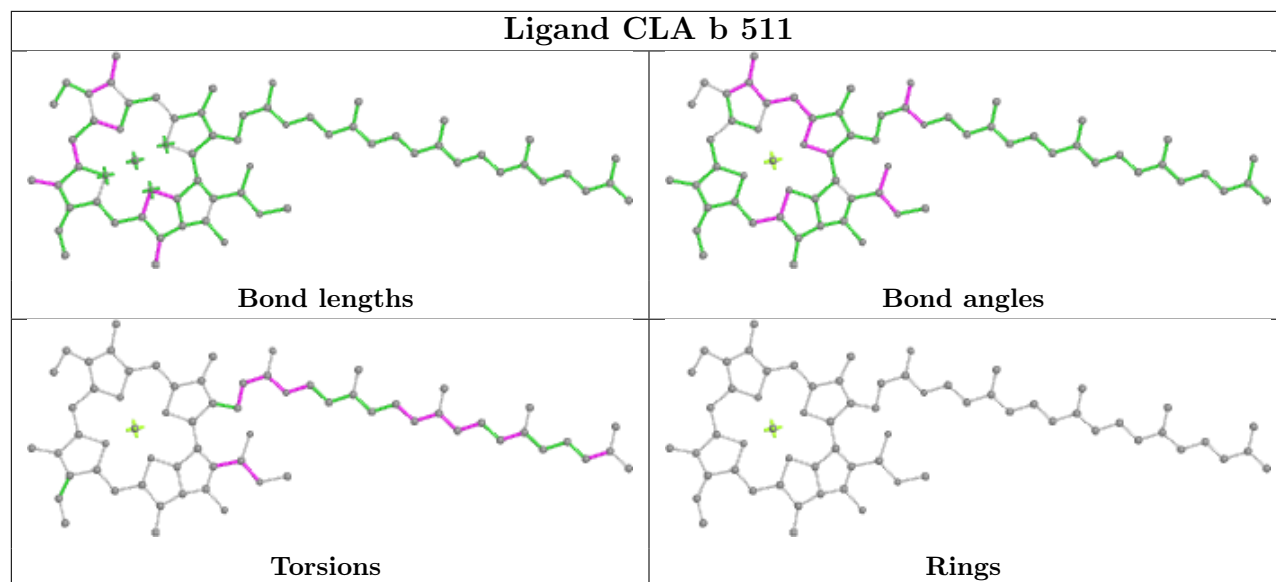
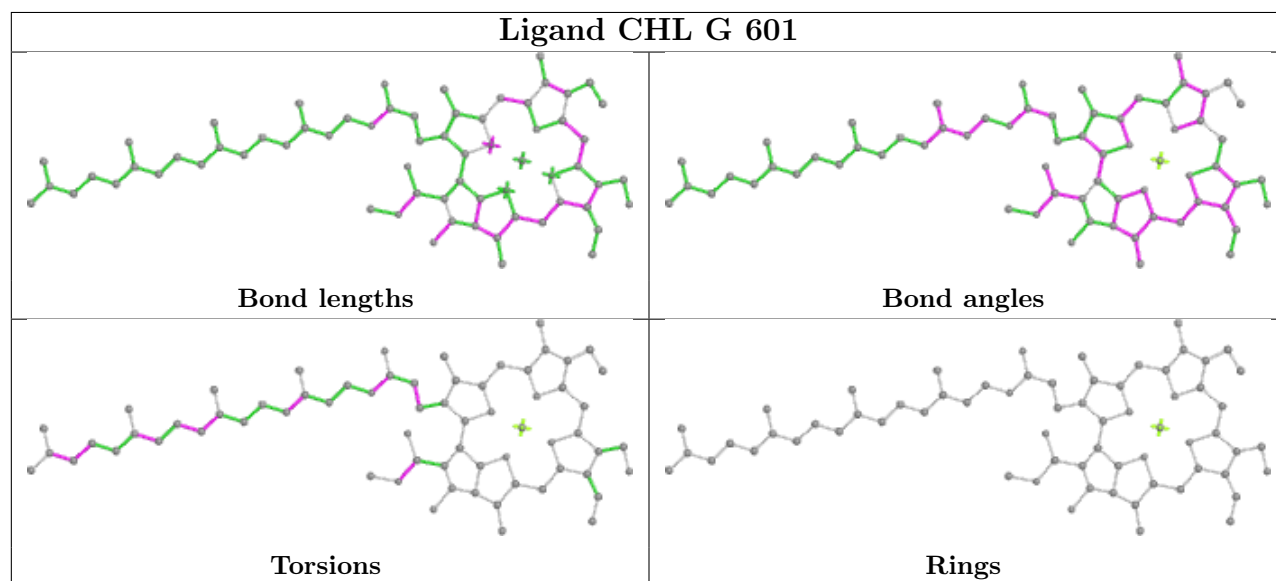


Rings

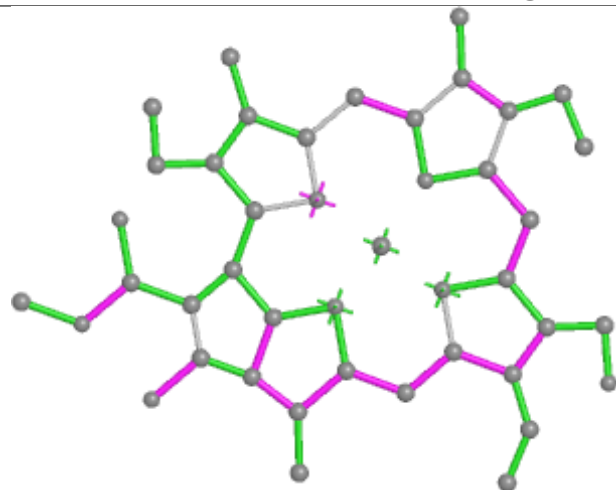




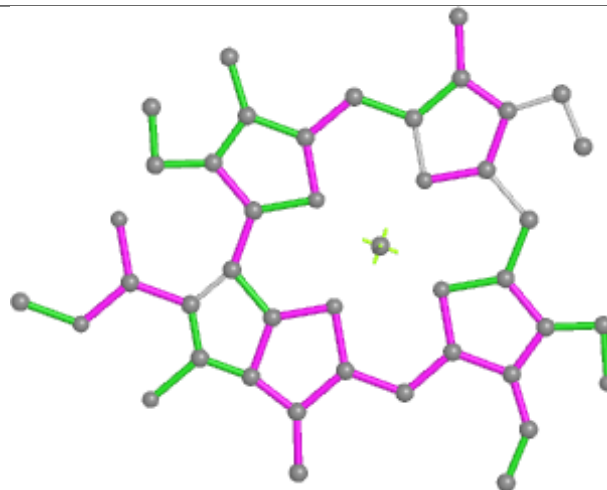
Ligand CLA B 504**Ligand CLA c 511****Ligand LUT S 615**

Ligand CLA b 511**Ligand CHL G 601**

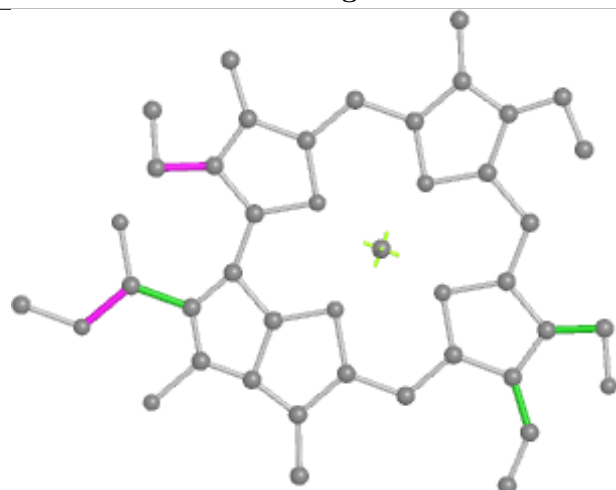
Ligand CHL r 305



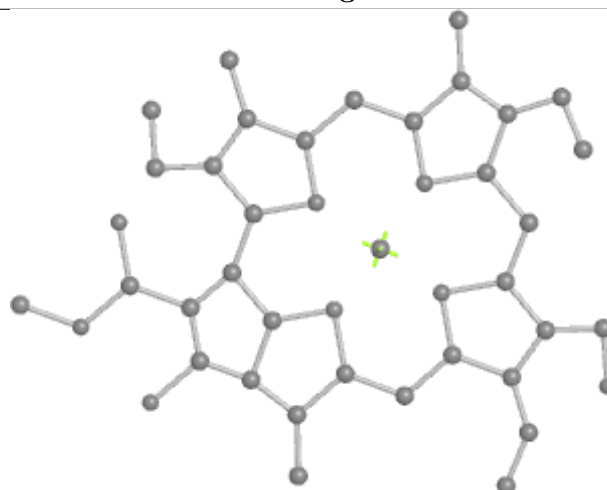
Bond lengths



Bond angles

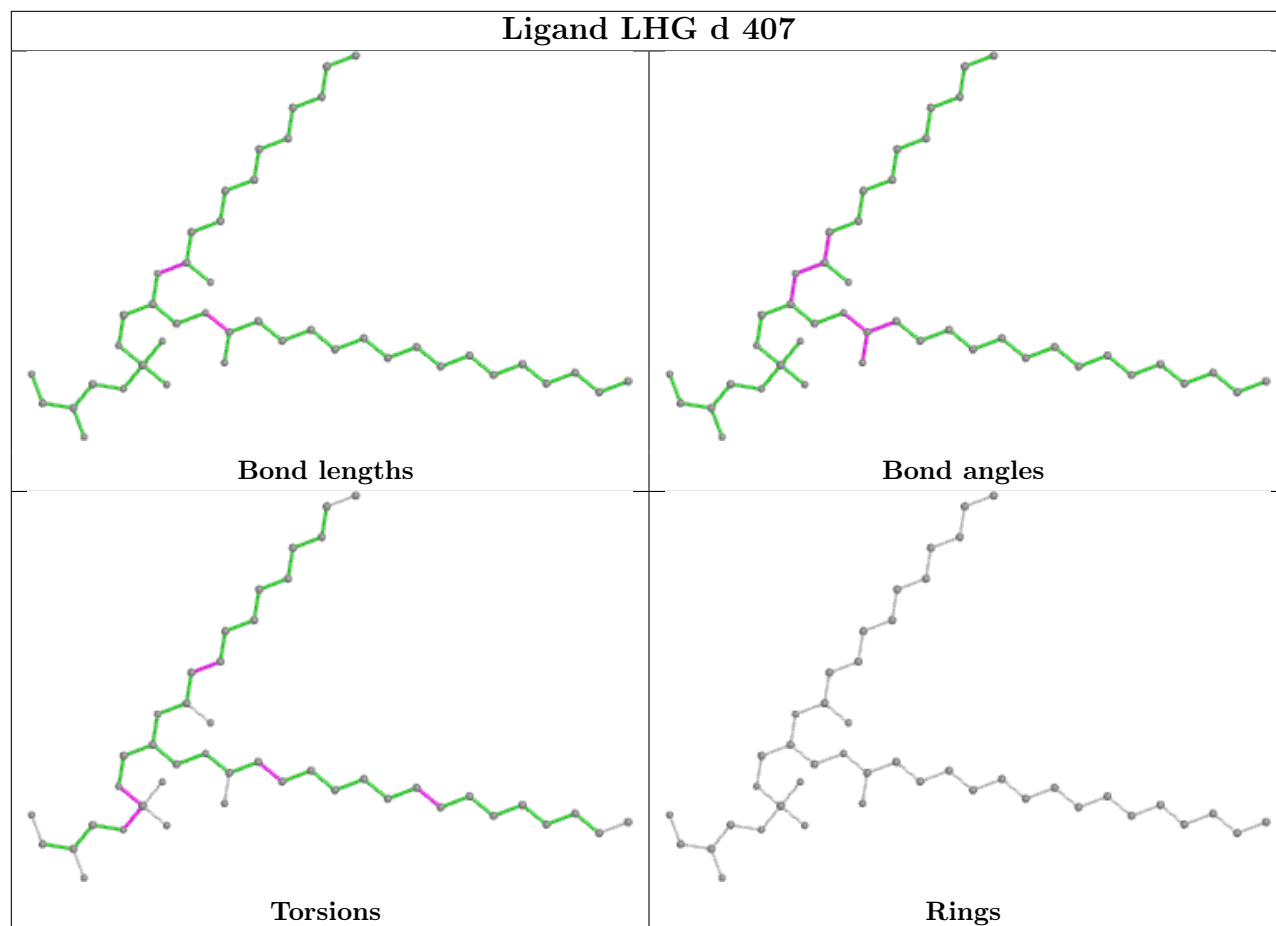


Torsions

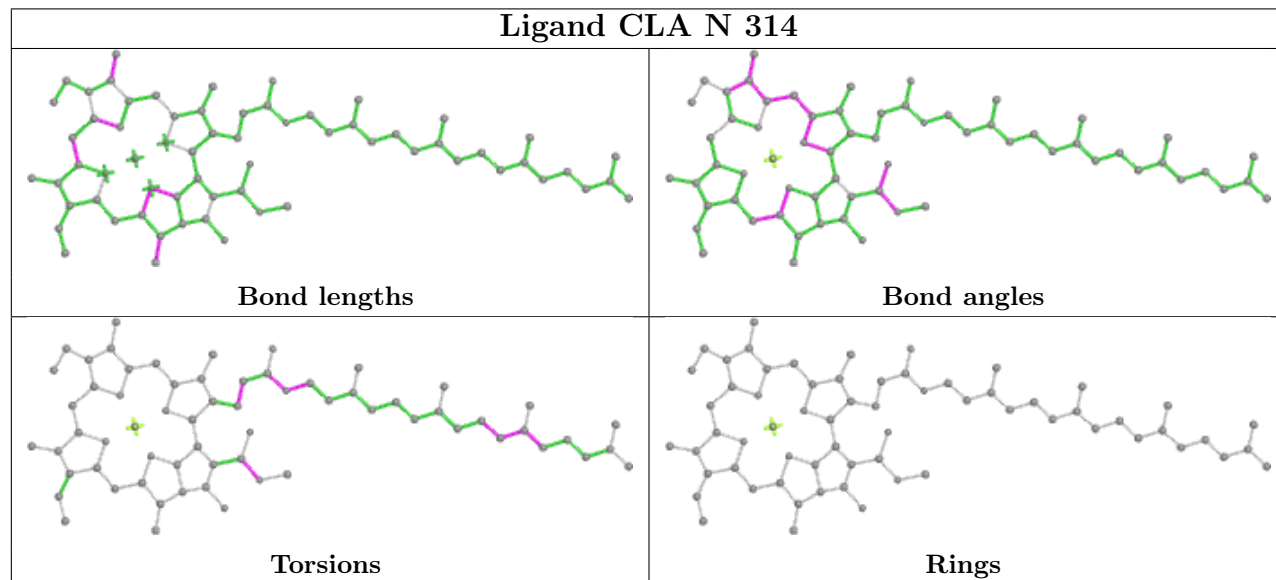


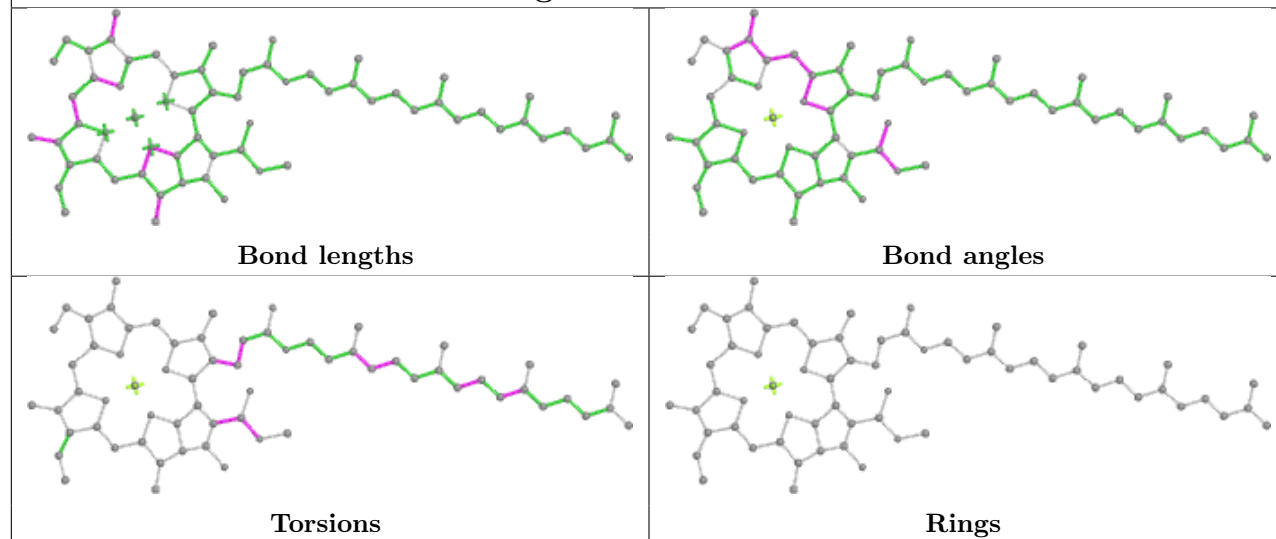
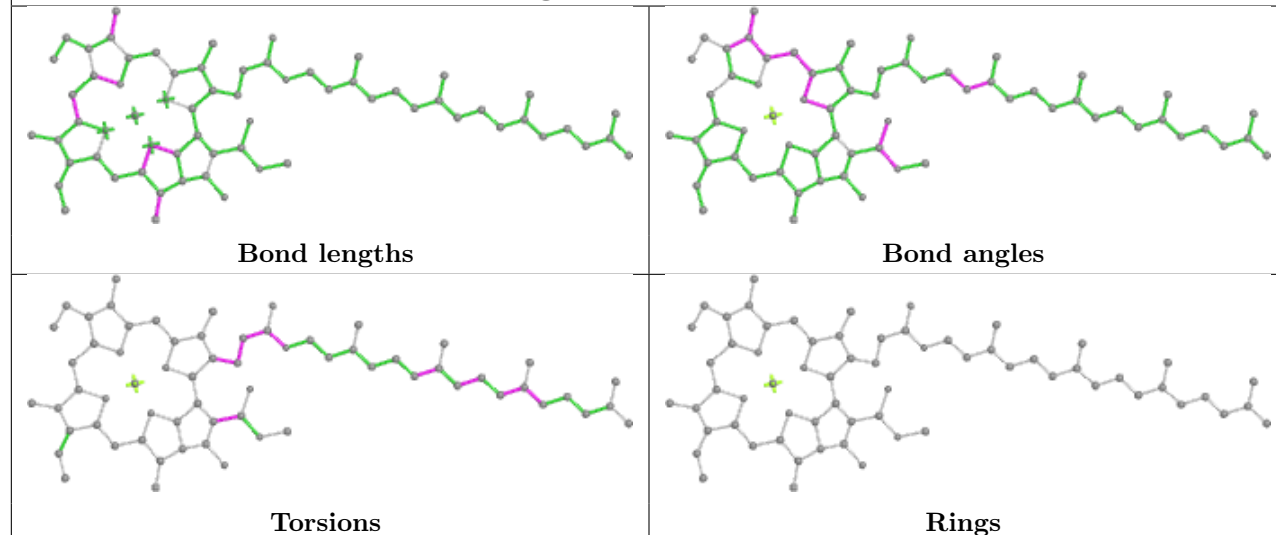
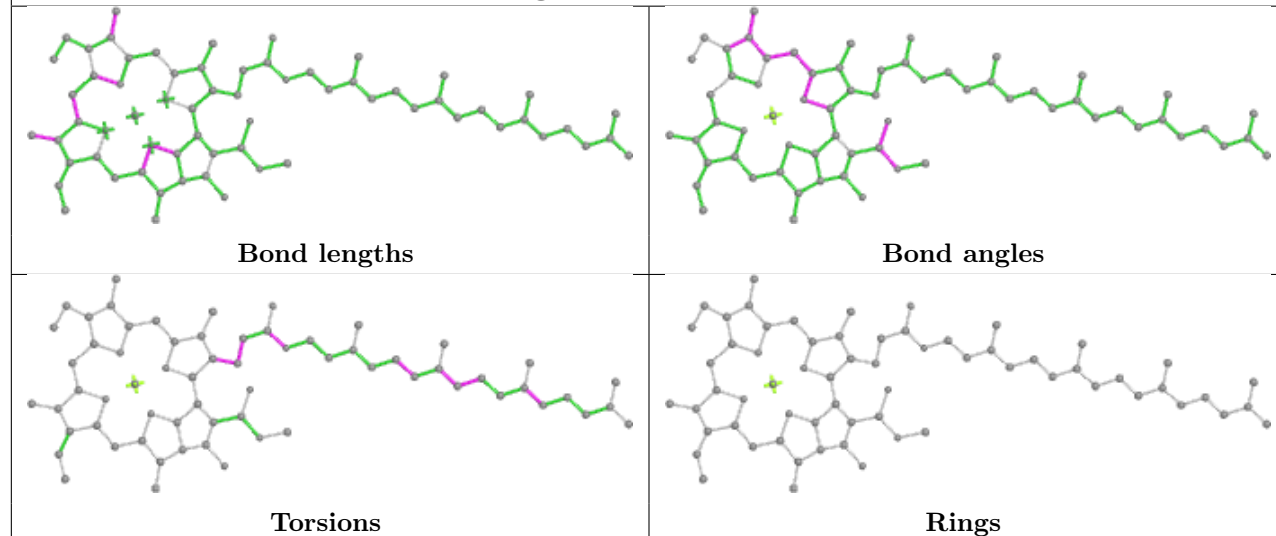
Rings

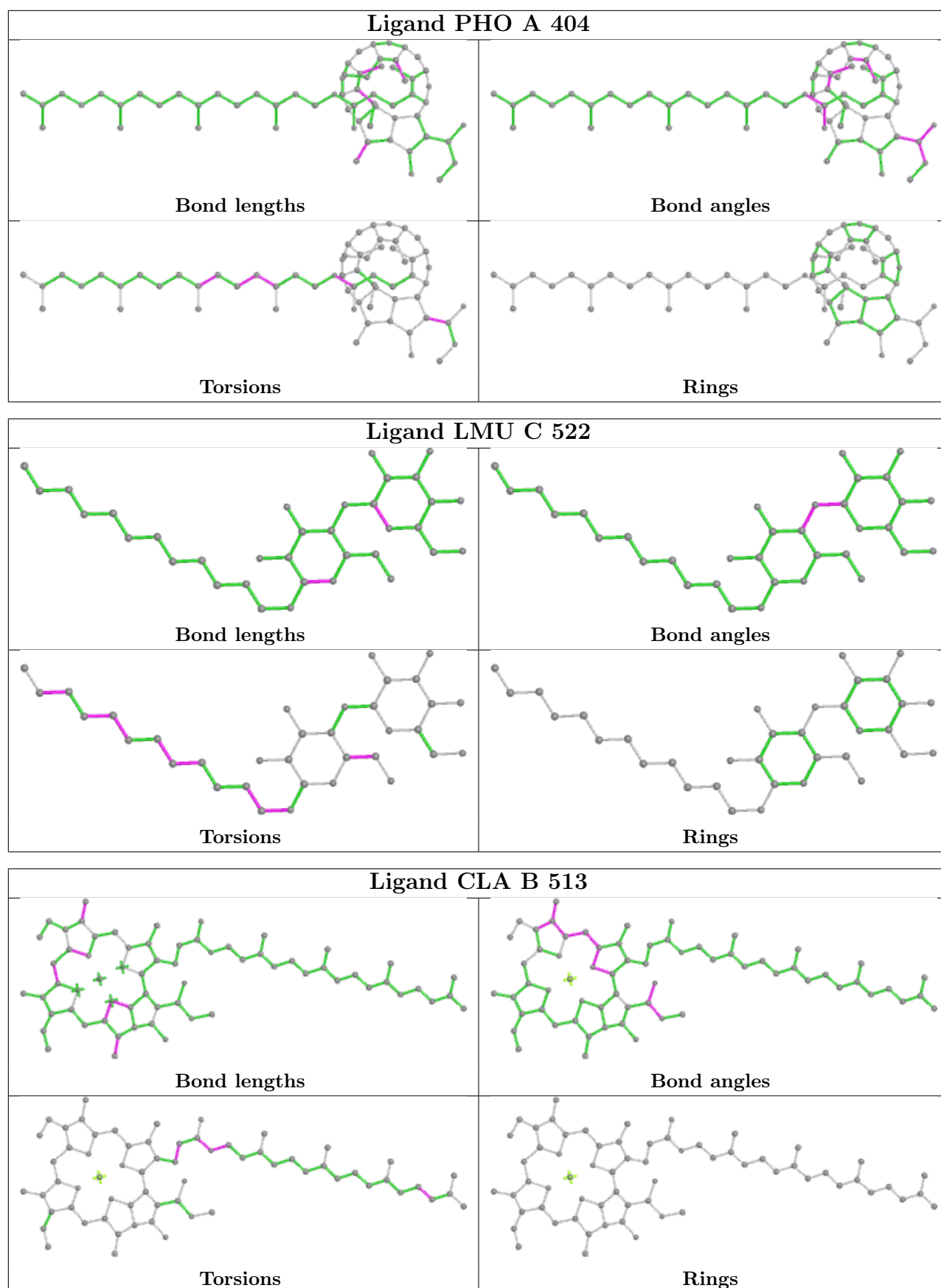
Ligand LHG d 407



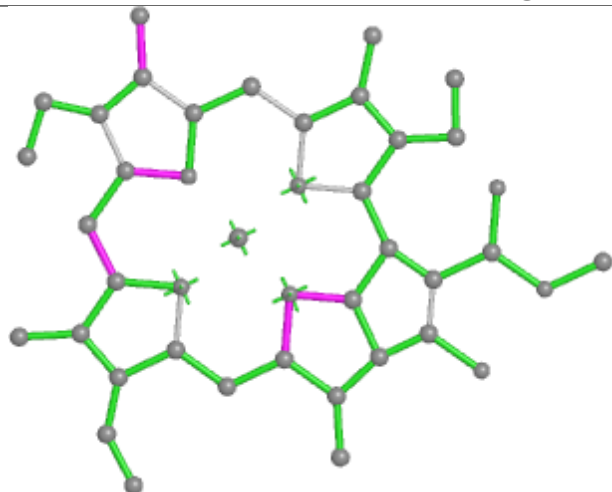
Ligand CLA N 314



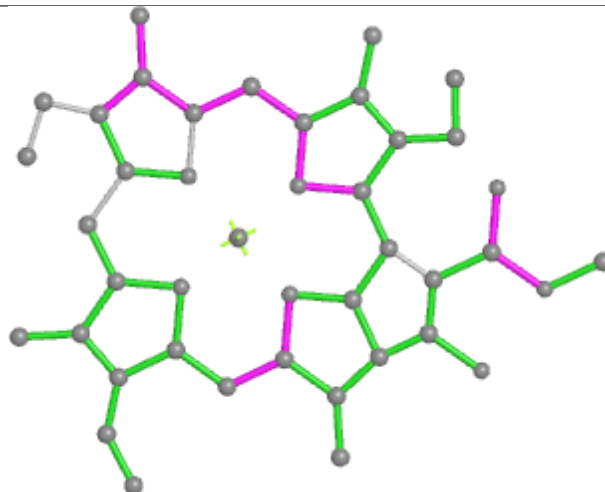
Ligand CLA b 503**Ligand CLA c 509****Ligand CLA B 516**



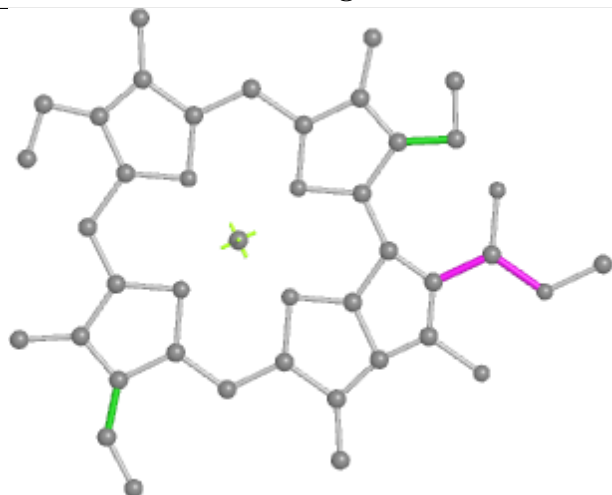
Ligand CLA c 513



Bond lengths



Bond angles

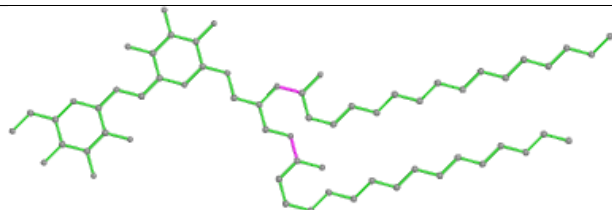


Torsions

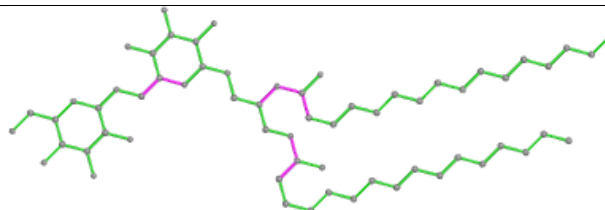


Rings

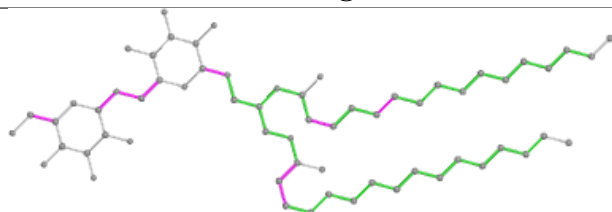
Ligand DGD C 518



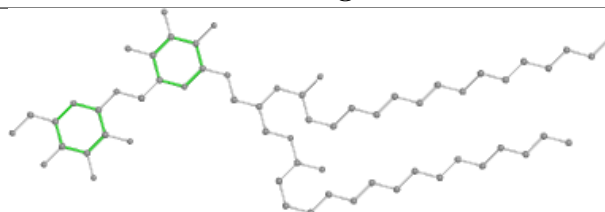
Bond lengths



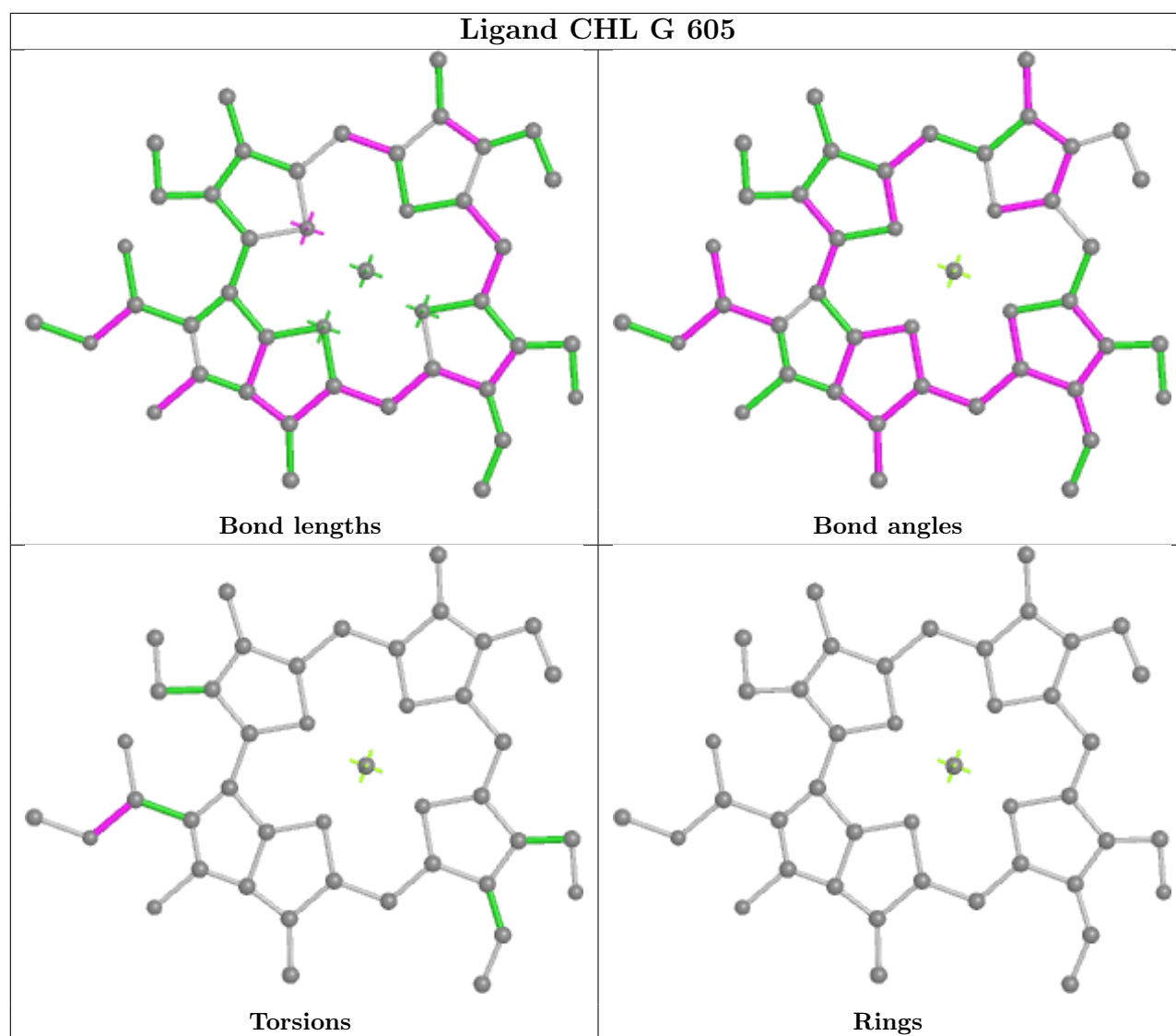
Bond angles



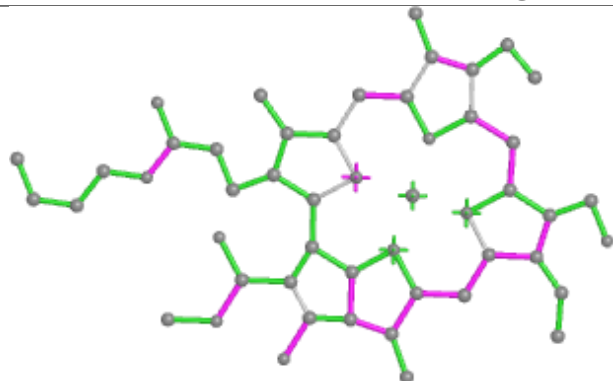
Torsions



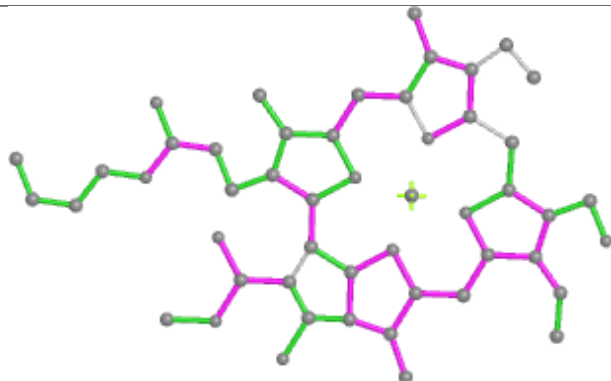
Rings



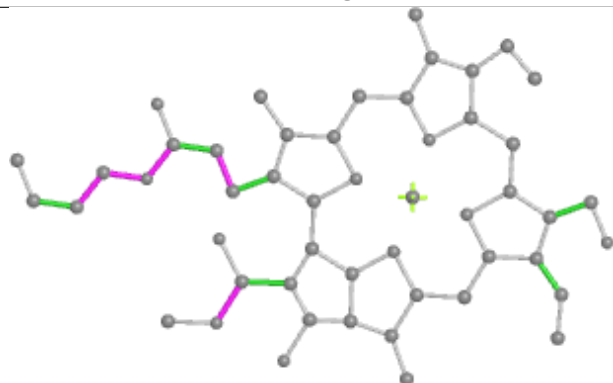
Ligand CHL Y 309



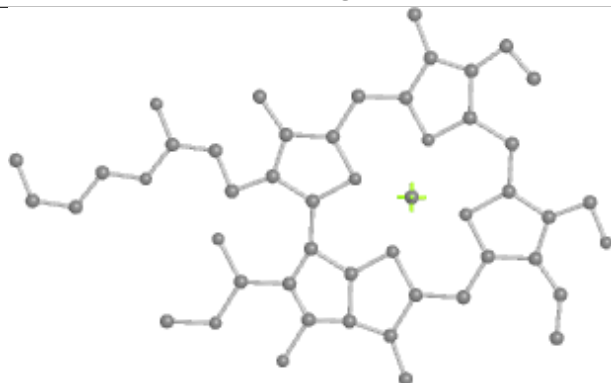
Bond lengths



Bond angles

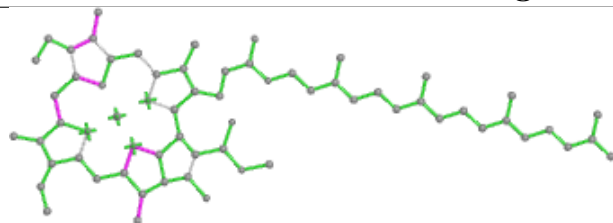


Torsions

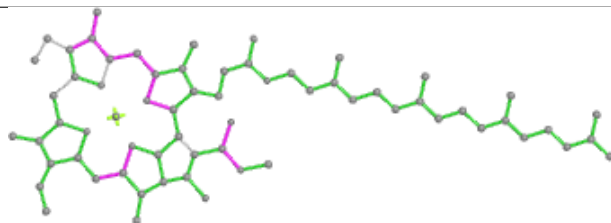


Rings

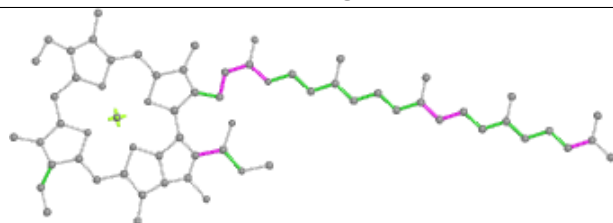
Ligand CLA C 501



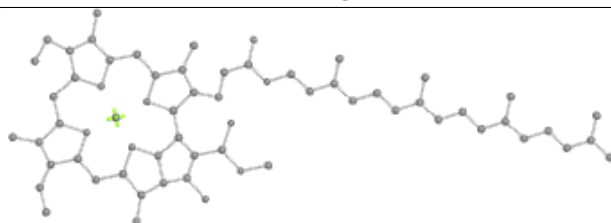
Bond lengths



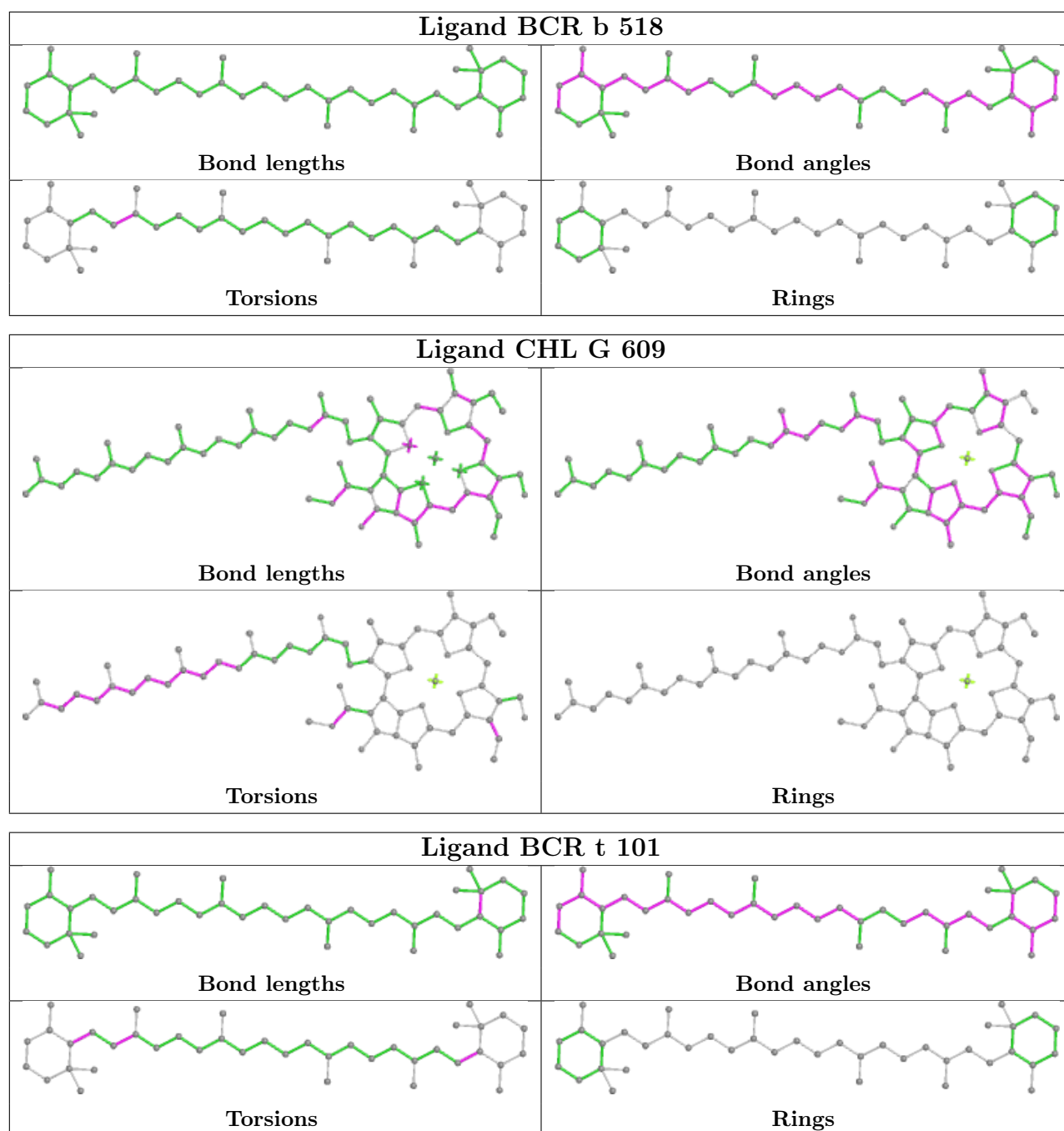
Bond angles

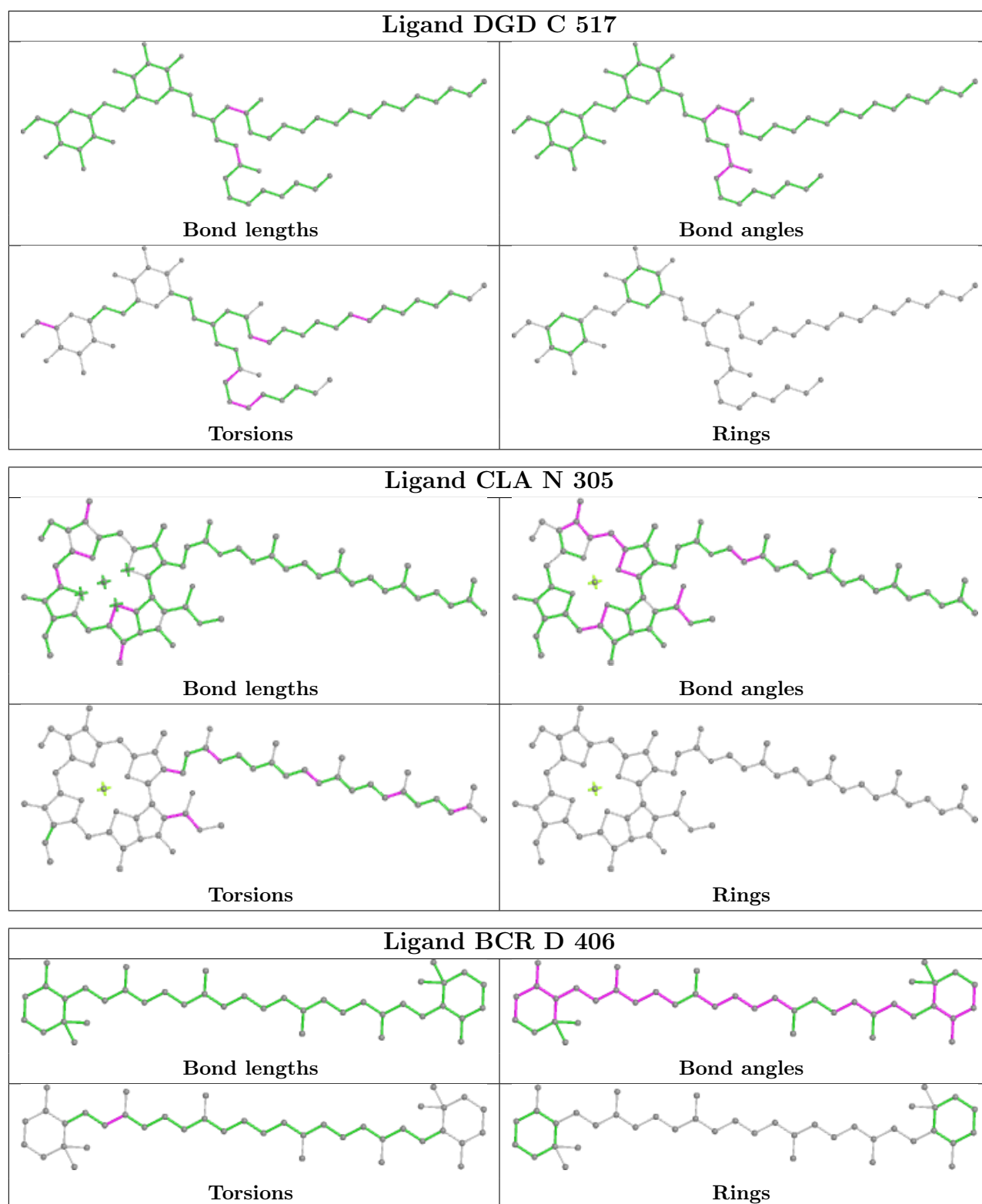


Torsions

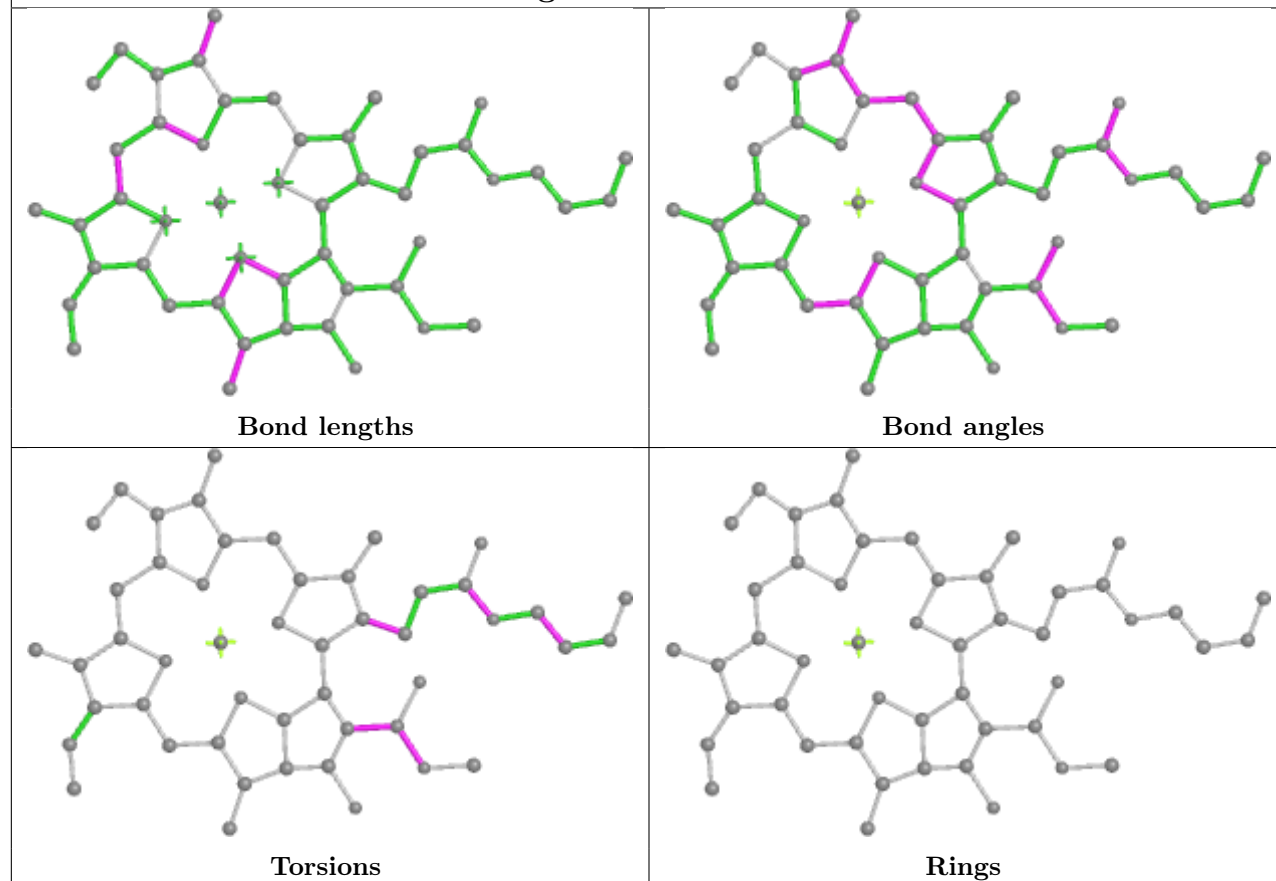


Rings

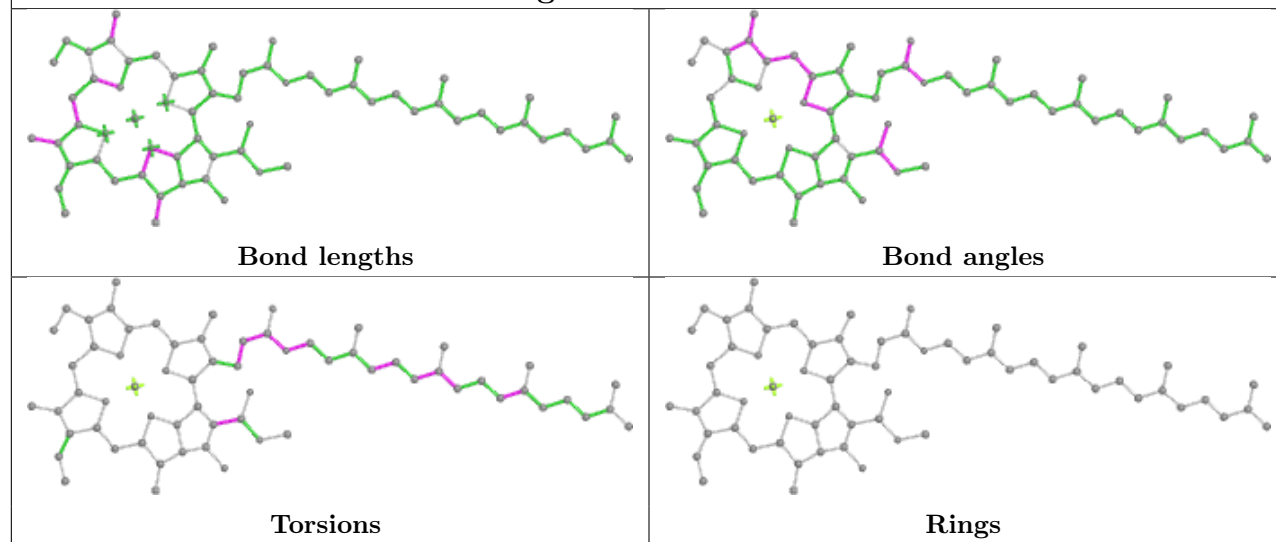


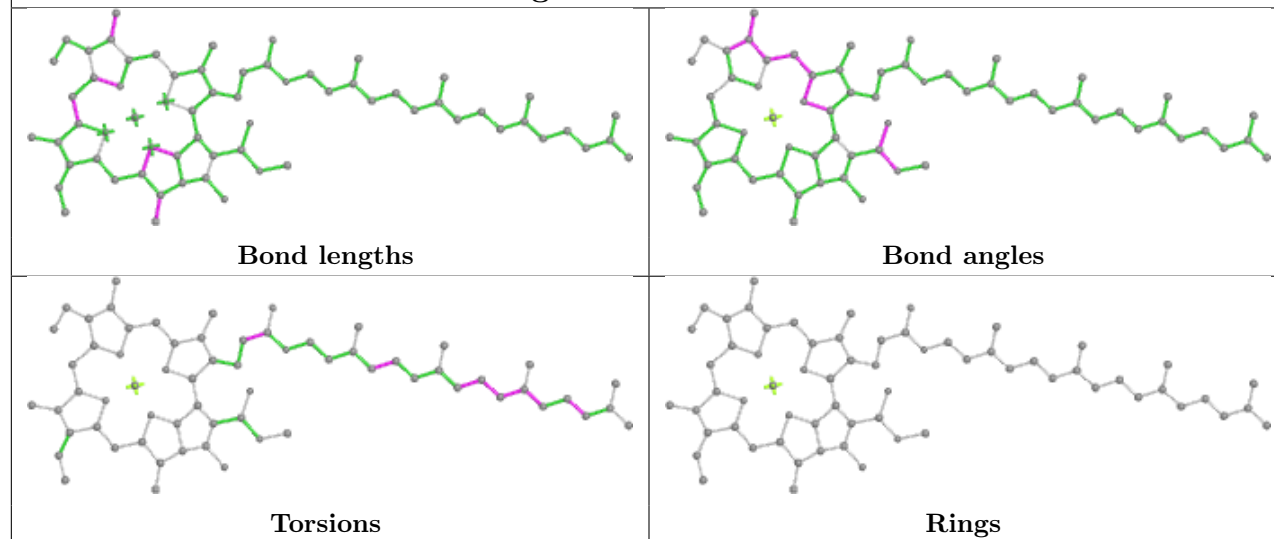
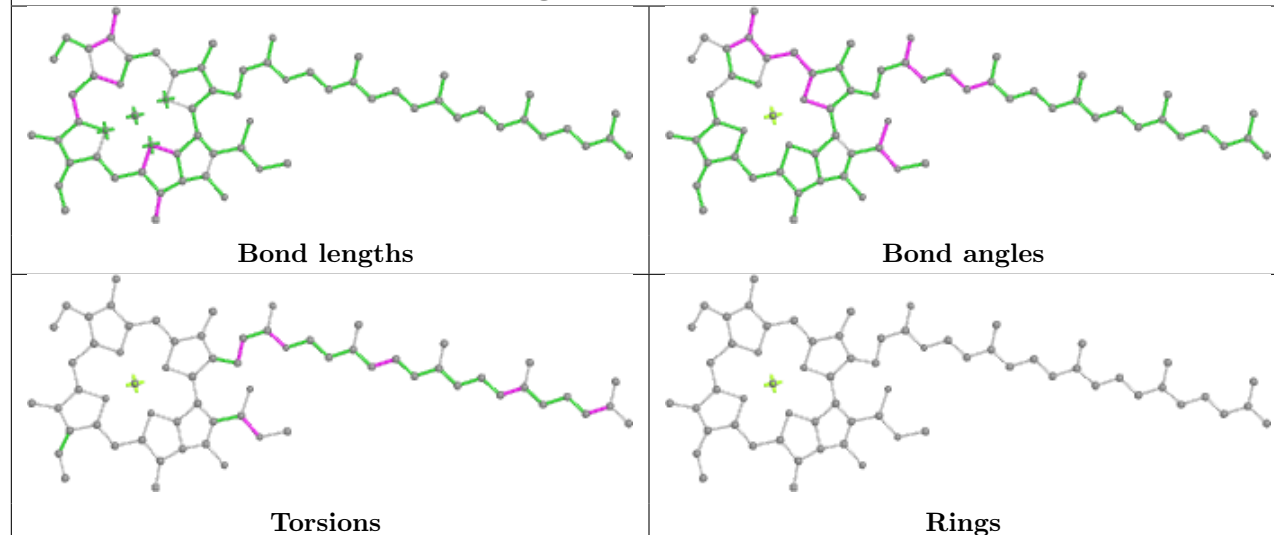
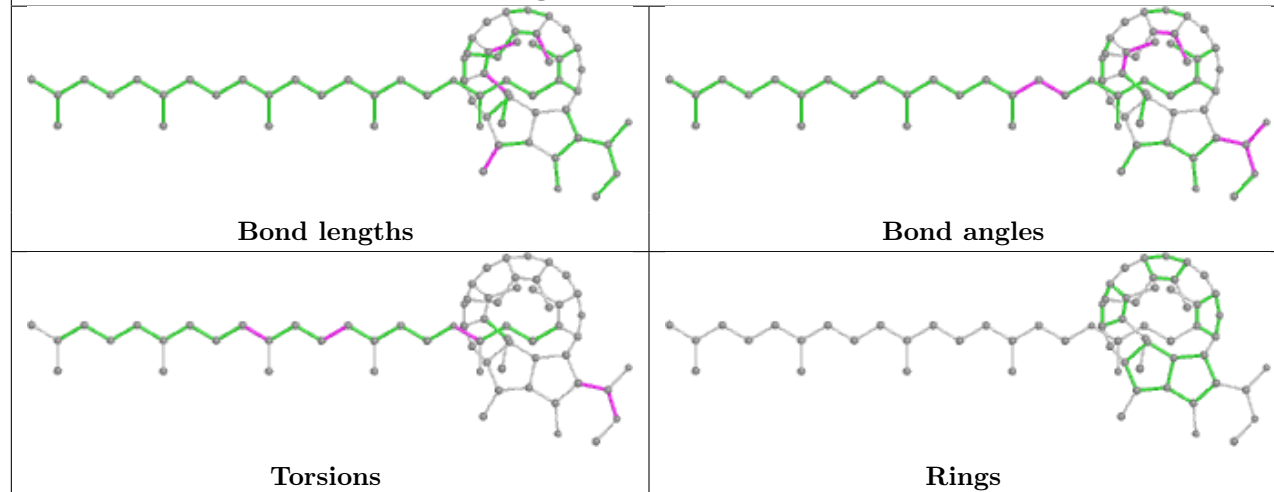


Ligand CLA r 303



Ligand CLA c 508



Ligand CLA Y 313**Ligand CLA b 508****Ligand PHO d 402**

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.

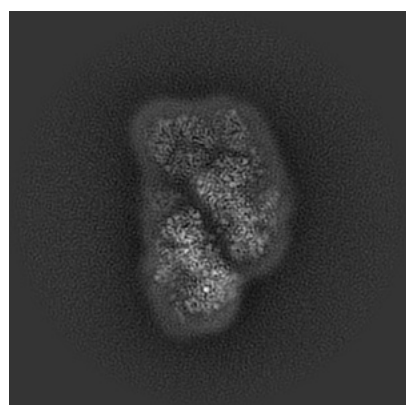
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-60830. These allow visual inspection of the internal detail of the map and identification of artifacts.

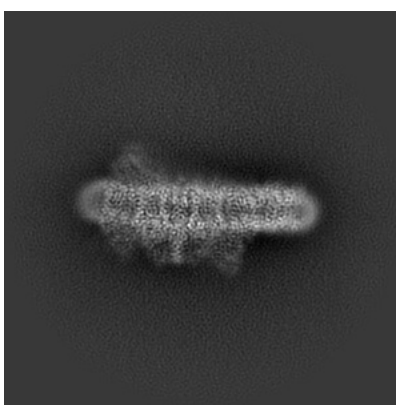
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

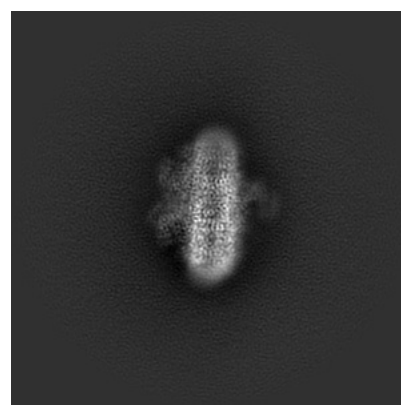
6.1.1 Primary map



X



Y

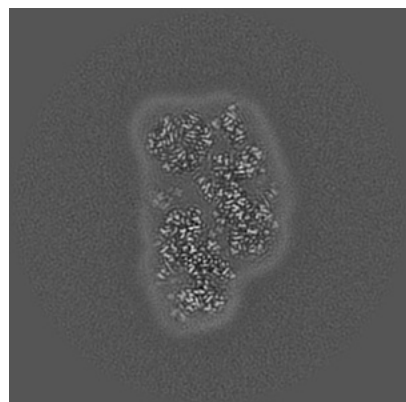


Z

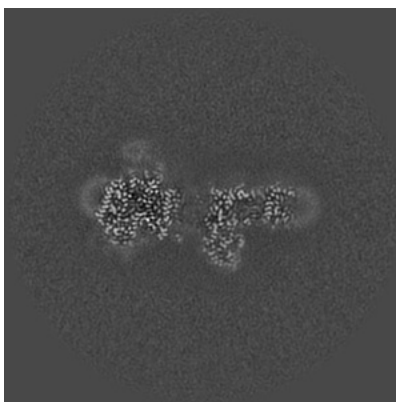
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

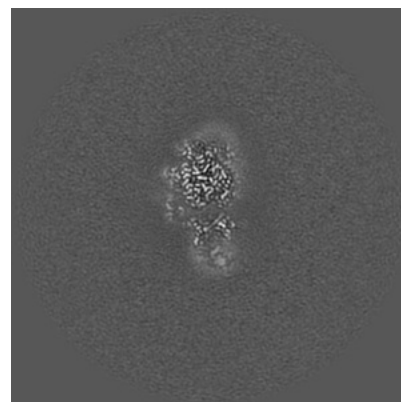
6.2.1 Primary map



X Index: 200



Y Index: 200

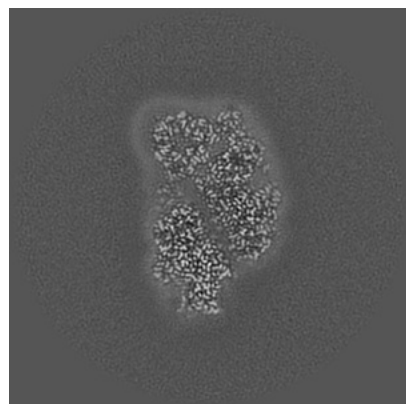


Z Index: 200

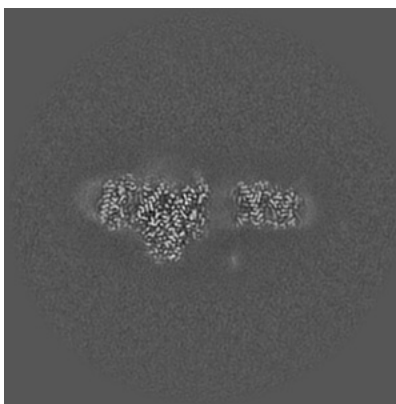
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

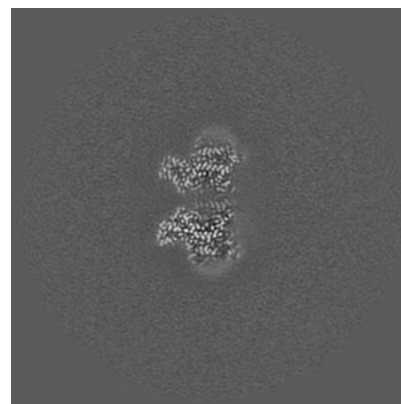
6.3.1 Primary map



X Index: 188



Y Index: 181

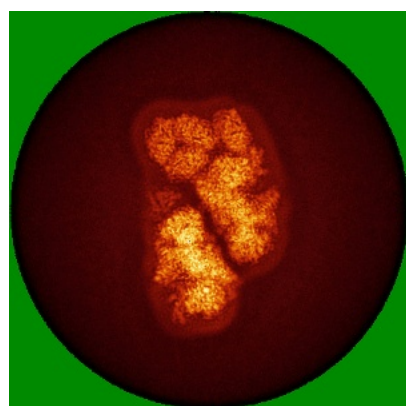


Z Index: 174

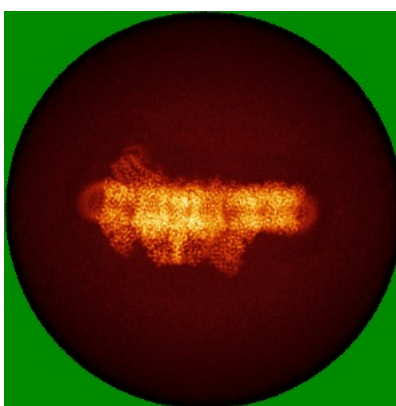
The images above show the largest variance slices of the map in three orthogonal directions.

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

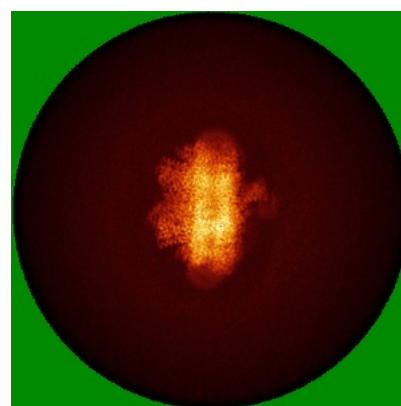
6.4.1 Primary map



X



Y

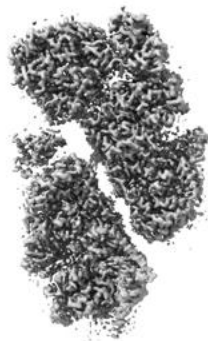


Z

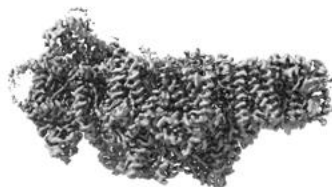
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

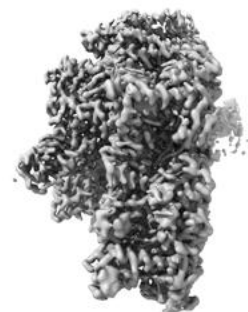
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

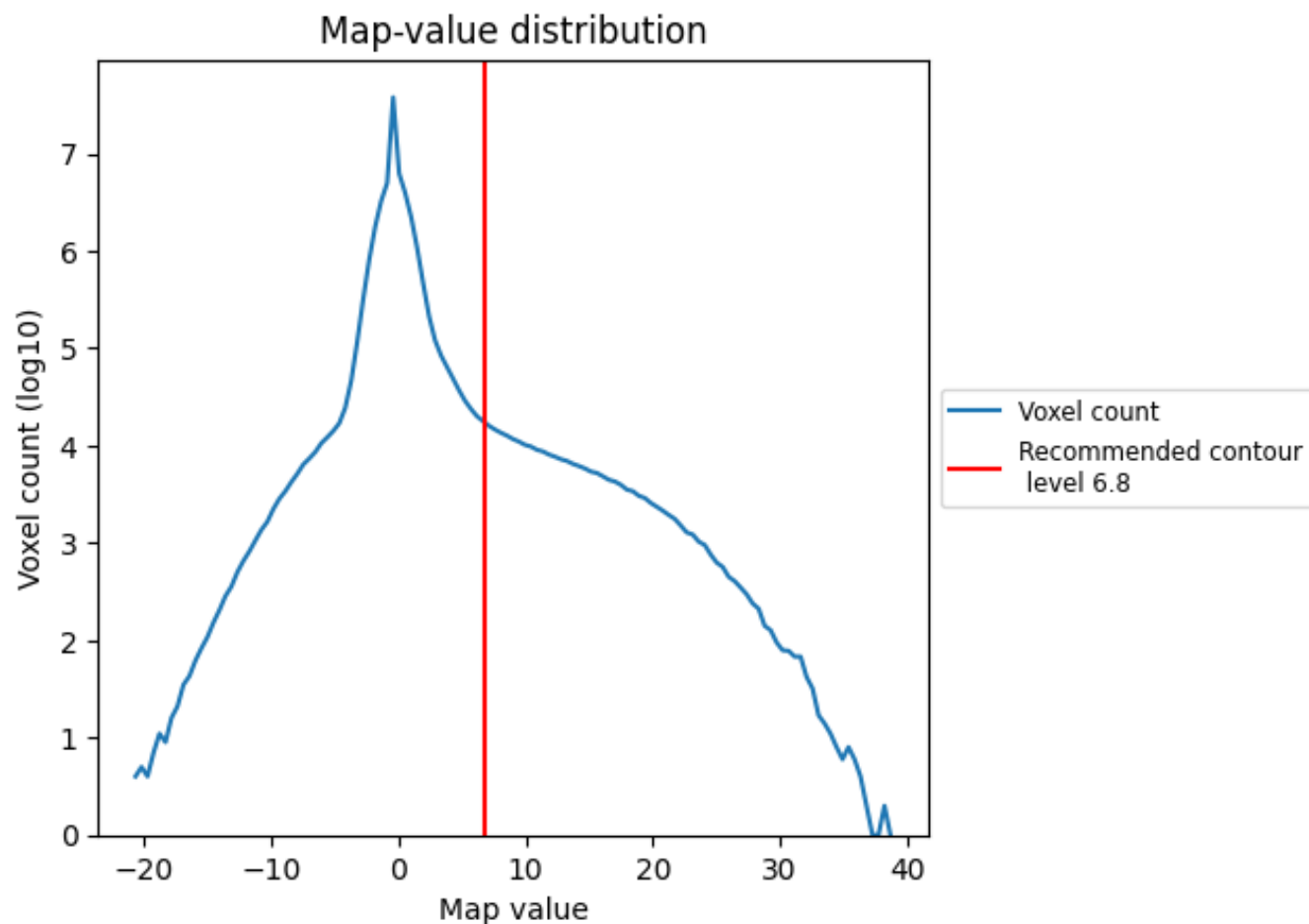
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

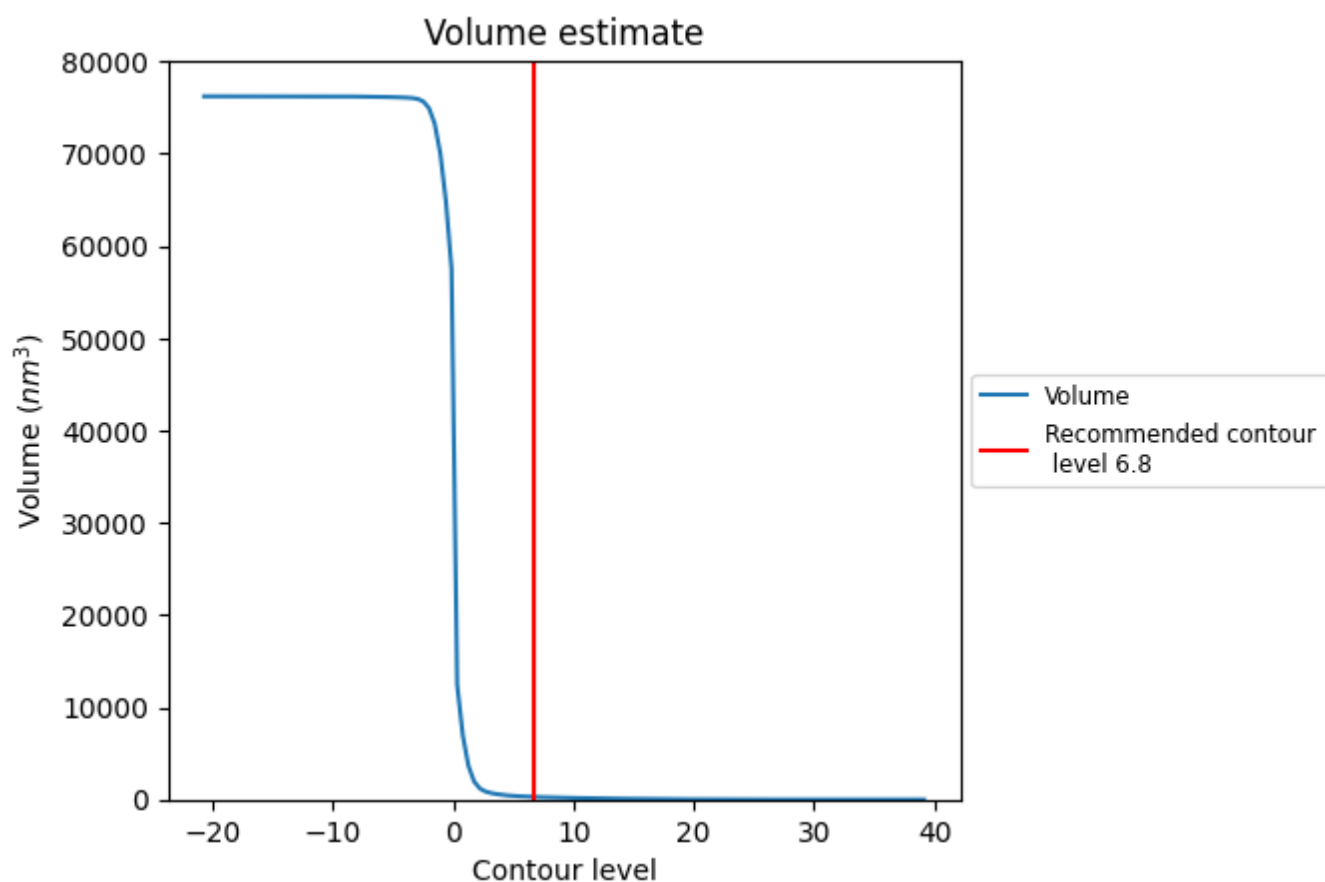
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

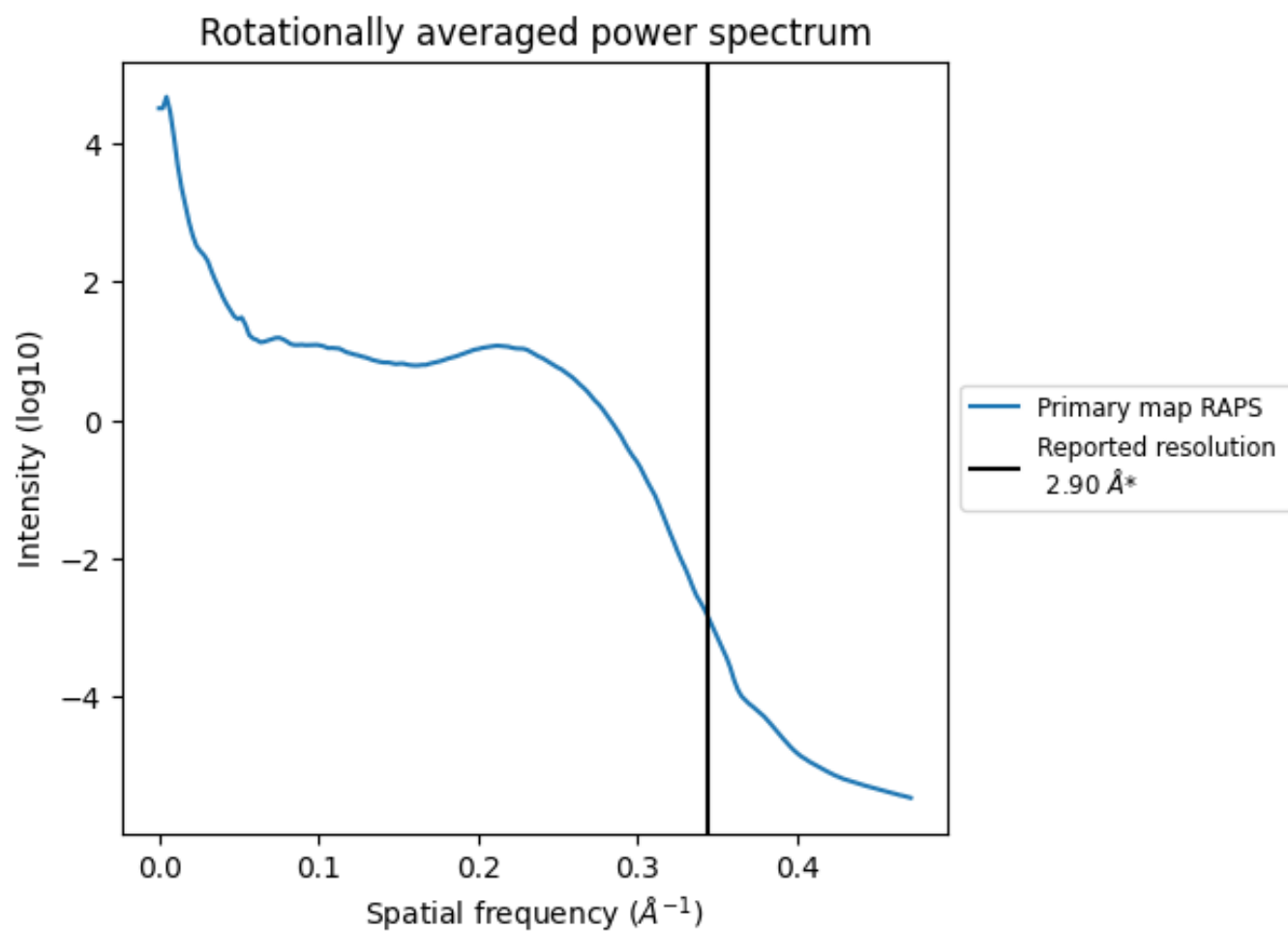
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 285 nm³; this corresponds to an approximate mass of 258 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 0.345 Å⁻¹

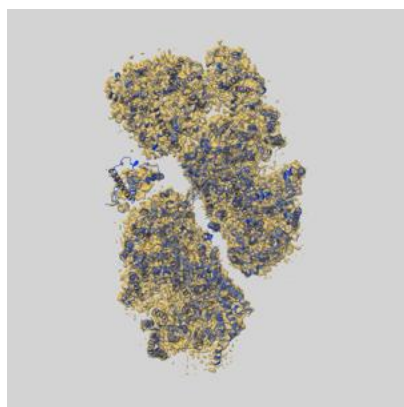
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

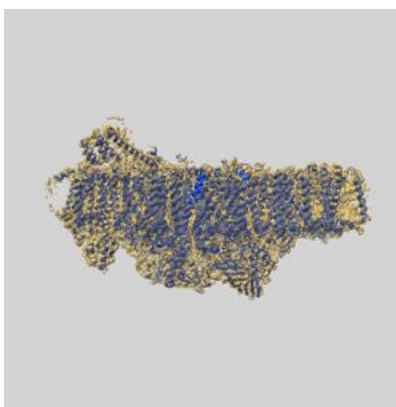
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-60830 and PDB model 9IS4. Per-residue inclusion information can be found in section [3](#) on page [31](#).

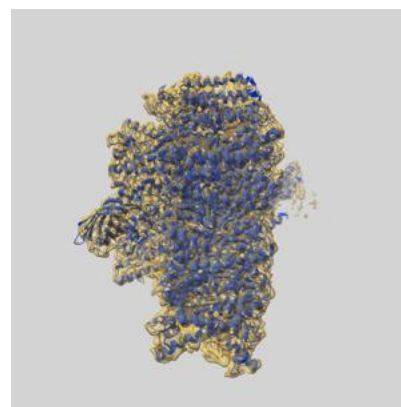
9.1 Map-model overlay [i](#)



X



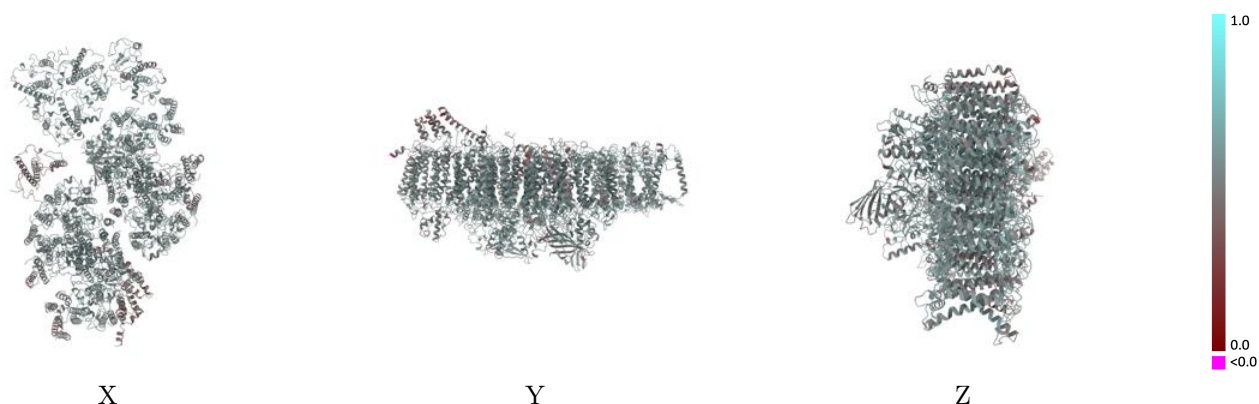
Y



Z

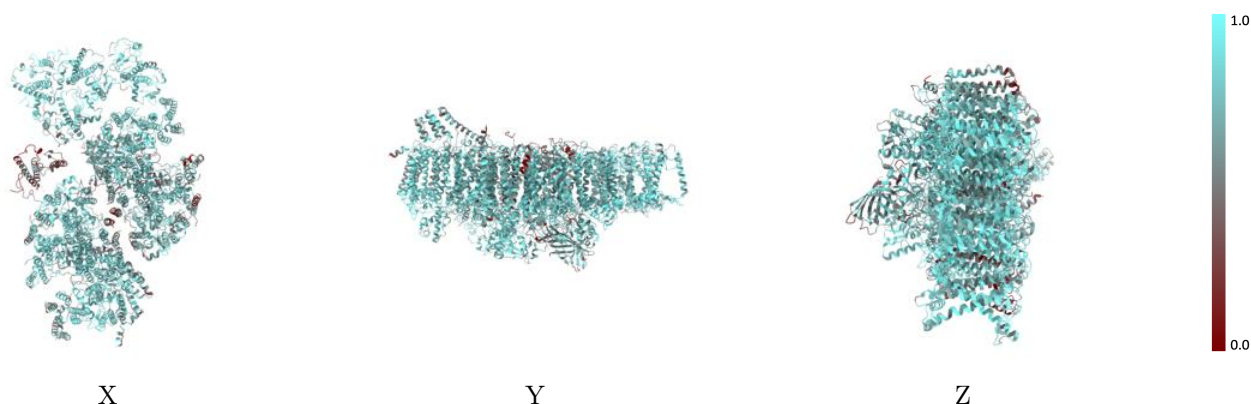
The images above show the 3D surface view of the map at the recommended contour level 6.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



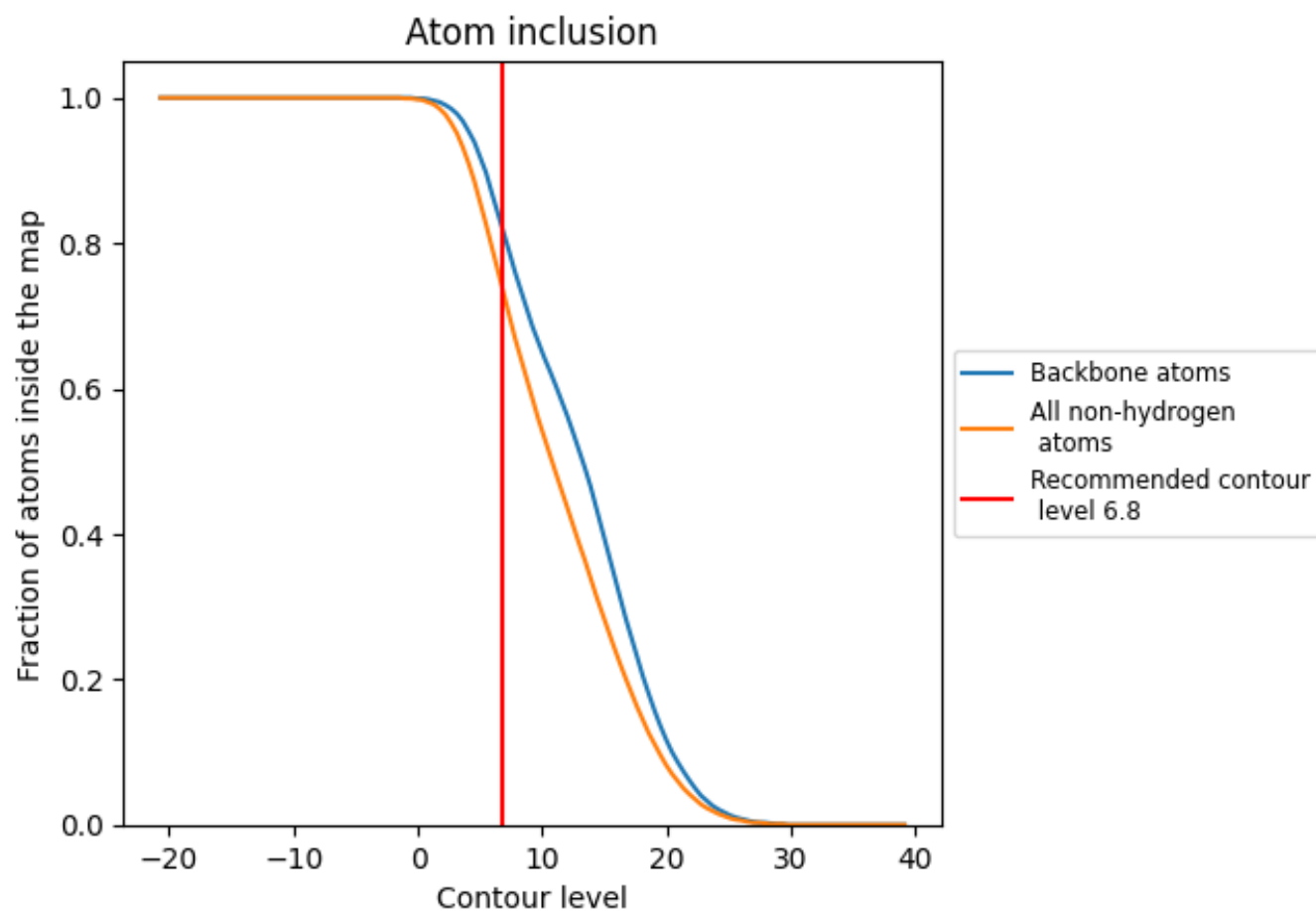
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (6.8).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 74% 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 (6.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7390	 0.5410
1	 0.6550	 0.4420
A	 0.7560	 0.5570
B	 0.7390	 0.5550
C	 0.7710	 0.5630
D	 0.7740	 0.5590
E	 0.5850	 0.4840
F	 0.6420	 0.4700
G	 0.7610	 0.5440
H	 0.6610	 0.5350
I	 0.7790	 0.5600
K	 0.7990	 0.5520
L	 0.6360	 0.5600
M	 0.3420	 0.4950
N	 0.7790	 0.5590
O	 0.5660	 0.5080
S	 0.7790	 0.5390
T	 0.5450	 0.5260
V	 0.5990	 0.4990
W	 0.6120	 0.5410
X	 0.3970	 0.4580
Y	 0.7480	 0.5640
Z	 0.7150	 0.5180
a	 0.7870	 0.5550
b	 0.8230	 0.5630
c	 0.8060	 0.5390
d	 0.8450	 0.5650
e	 0.7830	 0.4830
f	 0.7330	 0.4730
h	 0.7960	 0.5390
i	 0.7130	 0.5000
k	 0.7500	 0.5230
l	 0.7300	 0.5610
m	 0.3480	 0.5110
r	 0.3650	 0.4400



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Chain	Atom inclusion	Q-score
t	 0.4210	 0.5210
v	 0.5080	 0.4330
x	 0.6220	 0.4900
z	 0.5690	 0.4530