



wwPDB EM Validation Summary Report ⓘ

Mar 31, 2025 – 06:54 PM JST

PDB ID : 6IGZ / pdb_00006igz
EMDB ID : EMD-9670
Title : Structure of PSI-LHCI
Authors : Xiong, P.; Xiaochun, Q.
Deposited on : 2018-09-27
Resolution : 3.49 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.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
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)	:	2.42

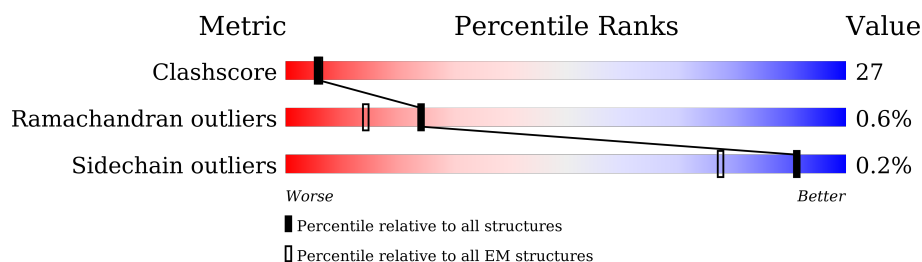
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 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	A	751	<div> <div>7%</div> <div>58%</div> <div>40%</div> <div>..</div> </div>
2	B	734	<div> <div>8%</div> <div>56%</div> <div>43%</div> </div>
3	C	81	<div> <div>11%</div> <div>51%</div> <div>47%</div> <div>..</div> </div>
4	D	198	<div> <div>16%</div> <div>44%</div> <div>27%</div> <div>..</div> <div>28%</div> </div>
5	E	91	<div> <div>18%</div> <div>46%</div> <div>21%</div> <div>33%</div> </div>
6	F	236	<div> <div>15%</div> <div>41%</div> <div>28%</div> <div>31%</div> </div>
7	G	167	<div> <div>54%</div> <div>30%</div> <div>25%</div> <div>45%</div> </div>
8	H	133	<div> <div>66%</div> <div>35%</div> <div>28%</div> <div>34%</div> </div>

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Mol	Chain	Length	Quality of chain
9	I	36	
10	J	41	
11	K	123	
12	L	204	
13	1	226	
13	5	226	
14	2	256	
15	3	281	
16	4	248	
16	8	248	
17	6	267	
18	7	264	
19	9	222	
20	0	245	
21	M	32	

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
22	CLA	0	302	X	-	-	-
22	CLA	0	303	X	-	-	-
22	CLA	0	304	X	-	-	-
22	CLA	0	305	X	-	-	-
22	CLA	0	307	X	-	-	-
22	CLA	0	308	X	-	-	-
22	CLA	0	309	X	-	-	-
22	CLA	0	310	X	-	-	-
22	CLA	0	311	X	-	-	-
22	CLA	0	312	X	-	-	-
22	CLA	1	301	X	-	-	-
22	CLA	1	302	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	303	X	-	-	-
22	CLA	1	304	X	-	-	-
22	CLA	1	306	X	-	-	-
22	CLA	1	307	X	-	-	-
22	CLA	1	308	X	-	-	-
22	CLA	1	309	X	-	-	-
22	CLA	1	310	X	-	-	-
22	CLA	1	311	X	-	-	-
22	CLA	1	312	X	-	-	-
22	CLA	1	313	X	-	-	-
22	CLA	2	302	X	-	-	-
22	CLA	2	303	X	-	-	-
22	CLA	2	304	X	-	-	-
22	CLA	2	308	X	-	-	-
22	CLA	2	309	X	-	-	-
22	CLA	2	310	X	-	-	-
22	CLA	2	311	X	-	-	-
22	CLA	2	312	X	-	-	-
22	CLA	2	313	X	-	-	-
22	CLA	2	314	X	-	-	-
22	CLA	2	319	X	-	-	-
22	CLA	3	301	X	-	-	-
22	CLA	3	302	X	-	-	-
22	CLA	3	303	X	-	-	-
22	CLA	3	304	X	-	-	-
22	CLA	3	305	X	-	-	-
22	CLA	3	307	X	-	-	-
22	CLA	3	308	X	-	-	-
22	CLA	3	309	X	-	-	-
22	CLA	3	310	X	-	-	-
22	CLA	3	311	X	-	-	-
22	CLA	3	312	X	-	-	-
22	CLA	3	313	X	-	-	-
22	CLA	3	319	X	-	-	-
22	CLA	4	302	X	-	-	-
22	CLA	4	303	X	-	-	-
22	CLA	4	304	X	-	-	-
22	CLA	4	308	X	-	-	-
22	CLA	4	309	X	-	-	-
22	CLA	4	310	X	-	-	-
22	CLA	4	311	X	-	-	-
22	CLA	4	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	4	313	X	-	-	-
22	CLA	4	314	X	-	-	-
22	CLA	5	302	X	-	-	-
22	CLA	5	304	X	-	-	-
22	CLA	5	305	X	-	-	-
22	CLA	5	307	X	-	-	-
22	CLA	5	308	X	-	-	-
22	CLA	5	309	X	-	-	-
22	CLA	5	310	X	-	-	-
22	CLA	5	311	X	-	-	-
22	CLA	5	312	X	-	-	-
22	CLA	5	313	X	-	-	-
22	CLA	5	314	X	-	-	-
22	CLA	6	301	X	-	-	-
22	CLA	6	303	X	-	-	-
22	CLA	6	304	X	-	-	-
22	CLA	6	305	X	-	-	-
22	CLA	6	309	X	-	-	-
22	CLA	6	310	X	-	-	-
22	CLA	6	311	X	-	-	-
22	CLA	6	312	X	-	-	-
22	CLA	6	313	X	-	-	-
22	CLA	6	314	X	-	-	-
22	CLA	6	315	X	-	-	-
22	CLA	6	317	X	-	-	-
22	CLA	6	318	X	-	-	-
22	CLA	6	323	X	-	-	-
22	CLA	7	302	X	-	-	-
22	CLA	7	303	X	-	-	-
22	CLA	7	304	X	-	-	-
22	CLA	7	305	X	-	-	-
22	CLA	7	306	X	-	-	-
22	CLA	7	307	X	-	-	-
22	CLA	7	309	X	-	-	-
22	CLA	7	310	X	-	-	-
22	CLA	7	311	X	-	-	-
22	CLA	7	312	X	-	-	-
22	CLA	7	313	X	-	-	-
22	CLA	7	314	X	-	-	-
22	CLA	7	315	X	-	-	-
22	CLA	7	316	X	-	-	-
22	CLA	7	317	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	7	318	X	-	-	-
22	CLA	8	302	X	-	-	-
22	CLA	8	303	X	-	-	-
22	CLA	8	304	X	-	-	-
22	CLA	8	308	X	-	-	-
22	CLA	8	309	X	-	-	-
22	CLA	8	310	X	-	-	-
22	CLA	8	312	X	-	-	-
22	CLA	8	313	X	-	-	-
22	CLA	8	315	X	-	-	-
22	CLA	9	301	X	-	-	-
22	CLA	9	303	X	-	-	-
22	CLA	9	304	X	-	-	-
22	CLA	9	305	X	-	-	-
22	CLA	9	306	X	-	-	-
22	CLA	9	308	X	-	-	-
22	CLA	9	309	X	-	-	-
22	CLA	9	310	X	-	-	-
22	CLA	9	311	X	-	-	-
22	CLA	9	312	X	-	-	-
22	CLA	9	313	X	-	-	-
22	CLA	A	801	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	852	X	-	-	-
22	CLA	A	853	X	-	-	-
22	CLA	B	801	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B	850	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	G	101	X	-	-	-
22	CLA	G	102	X	-	-	-
22	CLA	G	103	X	-	-	-
22	CLA	H	201	X	-	-	-
22	CLA	J	103	X	-	-	-
22	CLA	K	101	X	-	-	-
22	CLA	K	102	X	-	-	-
22	CLA	K	104	X	-	-	-
22	CLA	K	105	X	-	-	-
22	CLA	L	201	X	-	-	-
22	CLA	L	202	X	-	-	-
22	CLA	L	203	X	-	-	-
22	CLA	L	204	X	-	-	-
25	8CT	7	323	-	-	X	-
29	CHL	0	301	X	-	-	-
29	CHL	0	306	X	-	-	-
29	CHL	1	305	X	-	-	-
29	CHL	2	301	X	-	-	-
29	CHL	2	305	X	-	-	-
29	CHL	2	306	X	-	-	-
29	CHL	2	307	X	-	-	-
29	CHL	3	306	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CHL	4	301	X	-	-	-
29	CHL	4	305	X	-	-	-
29	CHL	4	306	X	-	-	-
29	CHL	4	307	X	-	-	-
29	CHL	5	301	X	-	-	-
29	CHL	5	306	X	-	-	-
29	CHL	6	302	X	-	-	-
29	CHL	6	306	X	-	-	-
29	CHL	6	307	X	-	-	-
29	CHL	6	308	X	-	-	-
29	CHL	6	316	X	-	-	-
29	CHL	7	308	X	-	-	-
29	CHL	8	305	X	-	-	-
29	CHL	8	306	X	-	-	-
29	CHL	8	307	X	-	-	-
29	CHL	8	314	X	-	-	-
29	CHL	9	302	X	-	-	-
29	CHL	9	307	X	-	-	-

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 51585 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 PsaA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5819	3803	988	1006	22		

- Molecule 2 is a protein called PsaB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5824	3824	979	1002	19		

- Molecule 3 is a protein called PsaC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			602	370	105	116	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	142	Total	C	N	O	S	0	0
			1109	709	193	202	5		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	61	Total	C	N	O	S	0	0
			488	308	87	92	1		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	163	Total	C	N	O	S	0	0
			1257	799	219	233	6		

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	92	Total	C	N	O	0	0
			714	462	118	134		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	88	Total	C	N	O	S	0	0
			677	426	119	131	1		

- Molecule 9 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	32	Total	C	N	O	S	0	0
			243	168	34	39	2		

- Molecule 10 is a protein called PsaJ.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	41	Total	C	N	O	S	0	0
			336	232	49	54	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	80	Total	C	N	O	S	0	0
			558	363	92	100	3		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	155	Total	C	N	O	S	0	0
			1139	736	187	212	4		

- Molecule 13 is a protein called Lhca-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1466	942	241	271	12		
13	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

- Molecule 14 is a protein called Lhca-c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	212	Total	C	N	O	S	0	0
			1641	1066	265	298	12		

- Molecule 15 is a protein called Lhca-d.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	226	Total	C	N	O	S	0	0
			1751	1132	283	326	10		

- Molecule 16 is a protein called Lhca-b.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	207	Total	C	N	O	S	0	0
			1589	1046	258	276	9		
16	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		

- Molecule 17 is a protein called Lhca-g.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

- Molecule 18 is a protein called Lhca-h.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 19 is a protein called Lhca-i.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	9	183	Total	C	N	O	S	0	0
			1416	913	235	259	9		

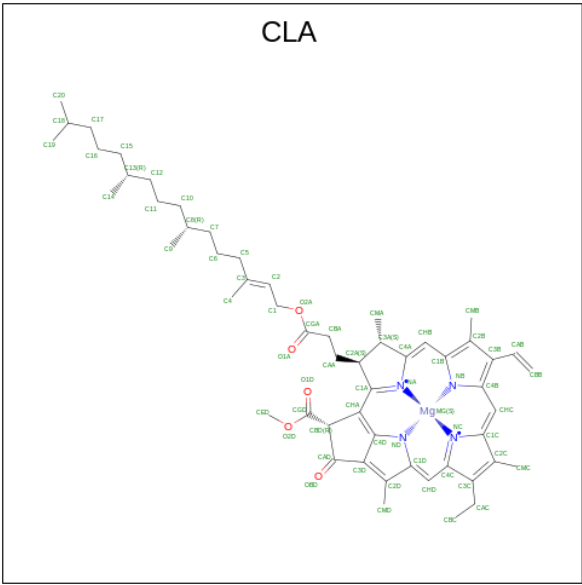
- Molecule 20 is a protein called Lhca-j.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	0	202	Total	C	N	O	S	0	0
			1560	1014	255	280	11		

- Molecule 21 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	M	31	Total	C	N	O	0	0
			238	158	37	43		

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	K	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	2	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	2	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	3	1	Total 37	C 31	Mg 1	N 4	O 1	0
22	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	4	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	4	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	6	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	5	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0

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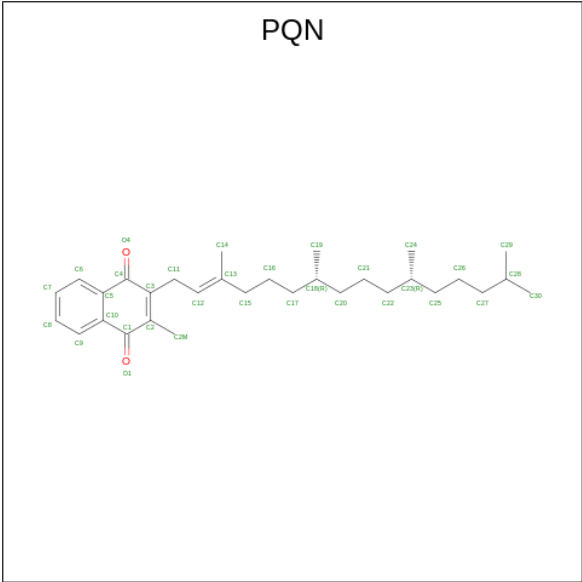
Mol	Chain	Residues	Atoms					AltConf
22	7	1	Total 37	C 31	Mg 1	N 4	O 1	0
22	7	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	9	1	Total 48	C 38	Mg 1	N 4	O 5	0

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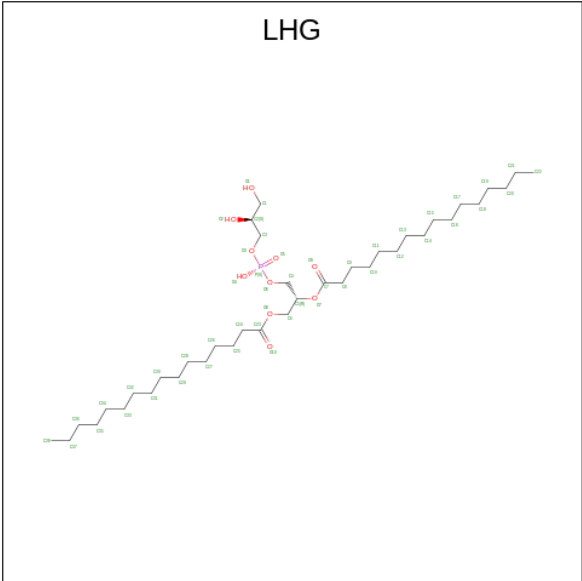
Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	0	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	M	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	31	2	
23	B	1	Total	C	O	0
			33	31	2	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



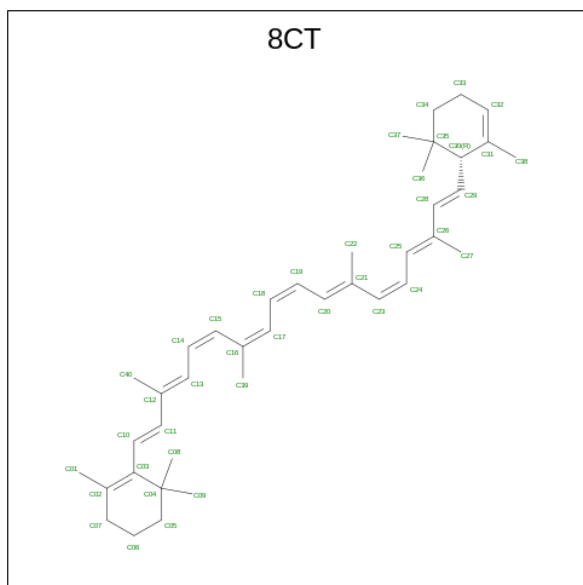
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			27	16	10	1	
24	B	1	Total	C	O	P	0
			23	12	10	1	
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			32	21	10	1	
24	3	1	Total	C	O	P	0
			20	10	9	1	
24	6	1	Total	C	O	P	0
			37	26	10	1	
24	5	1	Total	C	O	P	0
			49	38	10	1	
24	7	1	Total	C	O	P	0
			20	10	9	1	
24	9	1	Total	C	O	P	0
			49	38	10	1	
24	0	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
25	A	1	Total	C	0
			40	40	

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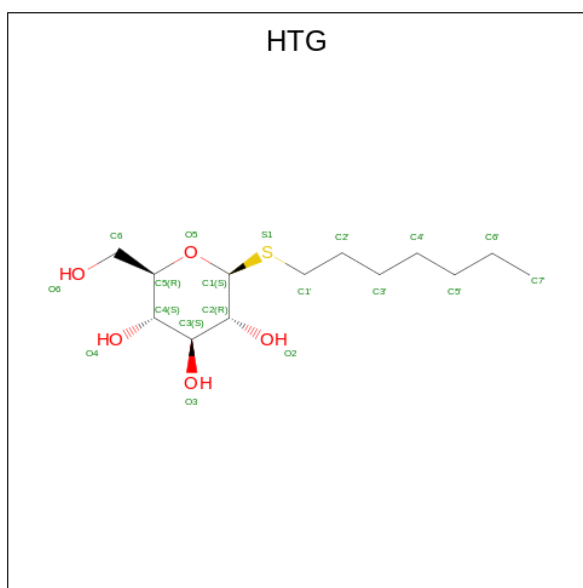
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	F	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0

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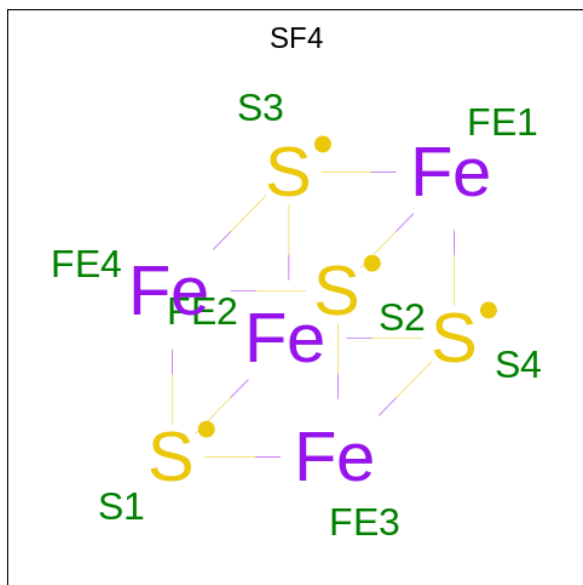
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	8	1	Total C 40 40	0

- Molecule 26 is heptyl 1-thio-beta-D-glucopyranoside (CCD ID: HTG) (formula: C₁₃H₂₆O₅S).



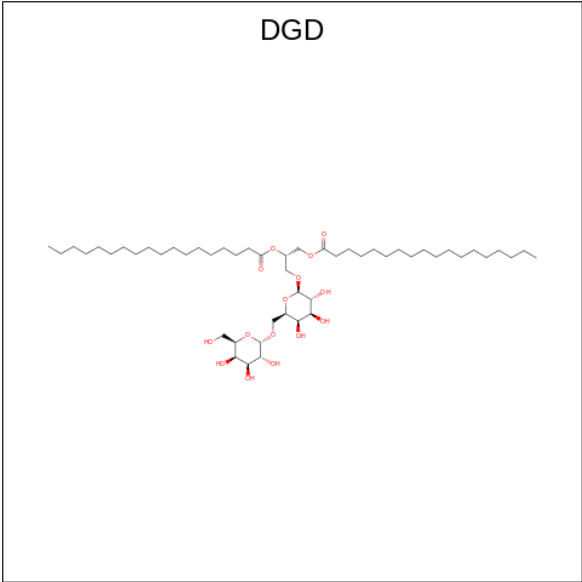
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			19	13	5	1	
26	J	1	Total	C	O	S	0
			19	13	5	1	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



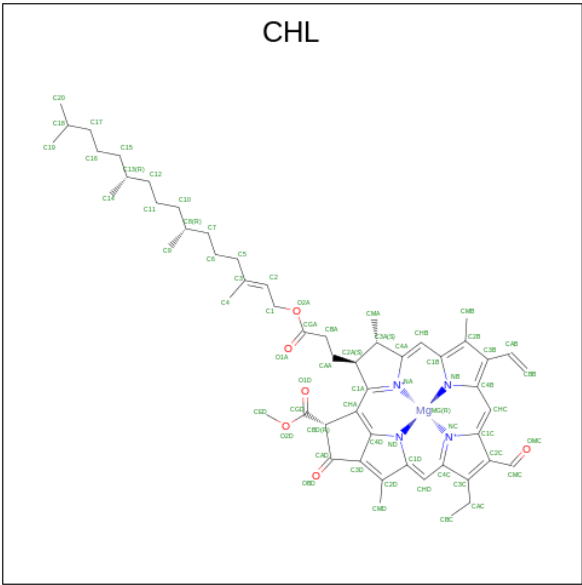
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			66	51	15	

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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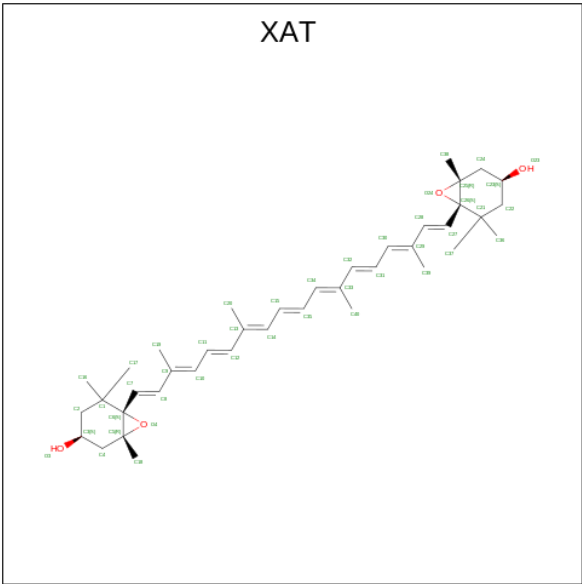
Mol	Chain	Residues	Atoms					AltConf
29	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
29	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
29	4	1	Total 61	C 50	Mg 1	N 4	O 6	0
29	4	1	Total 56	C 45	Mg 1	N 4	O 6	0
29	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	6	1	Total 61	C 50	Mg 1	N 4	O 6	0
29	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	5	1	Total 61	C 50	Mg 1	N 4	O 6	0
29	5	1	Total 48	C 37	Mg 1	N 4	O 6	0
29	7	1	Total 47	C 36	Mg 1	N 4	O 6	0
29	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
29	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	8	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	8	1	Total 43	C 34	Mg 1	N 4	O 4	0
29	9	1	Total 61	C 50	Mg 1	N 4	O 6	0
29	9	1	Total 48	C 37	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
29	0	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	0	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

- Molecule 30 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).



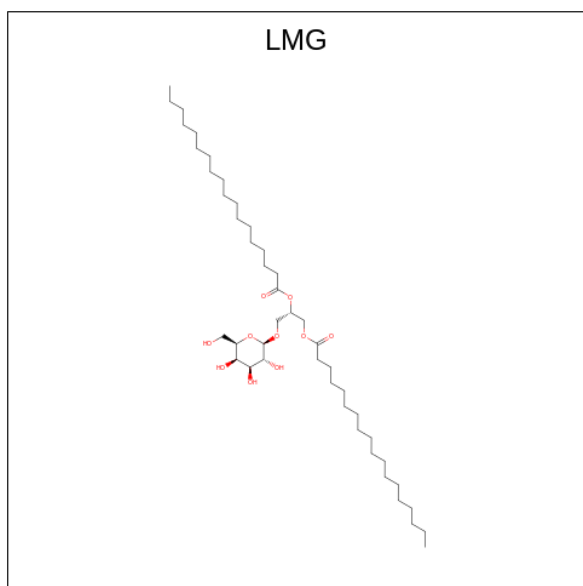
Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			44	40	4	
30	1	1	Total	C	O	0
			44	40	4	
30	2	1	Total	C	O	0
			44	40	4	
30	2	1	Total	C	O	0
			44	40	4	
30	3	1	Total	C	O	0
			44	40	4	
30	3	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	
30	6	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
30	6	1	Total	C	O	0
			44	40	4	
30	5	1	Total	C	O	0
			44	40	4	
30	5	1	Total	C	O	0
			44	40	4	
30	7	1	Total	C	O	0
			44	40	4	
30	7	1	Total	C	O	0
			44	40	4	
30	8	1	Total	C	O	0
			44	40	4	
30	8	1	Total	C	O	0
			44	40	4	
30	9	1	Total	C	O	0
			44	40	4	
30	9	1	Total	C	O	0
			44	40	4	
30	0	1	Total	C	O	0
			44	40	4	
30	0	1	Total	C	O	0
			44	40	4	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

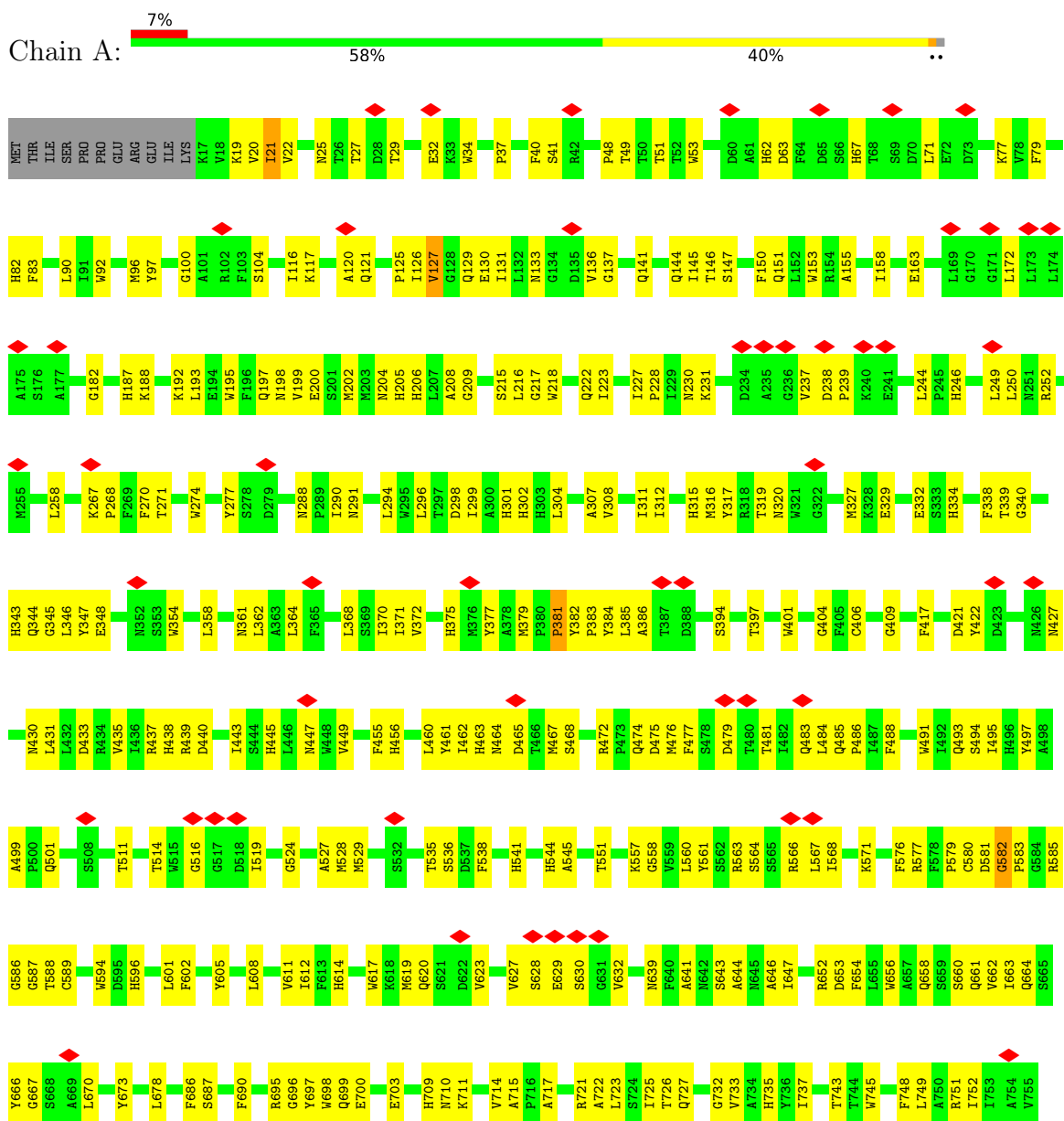


Mol	Chain	Residues	Atoms			AltConf
31	4	1	Total 44	C 34	O 10	0
31	5	1	Total 44	C 34	O 10	0
31	8	1	Total 44	C 34	O 10	0

3 Residue-property plots

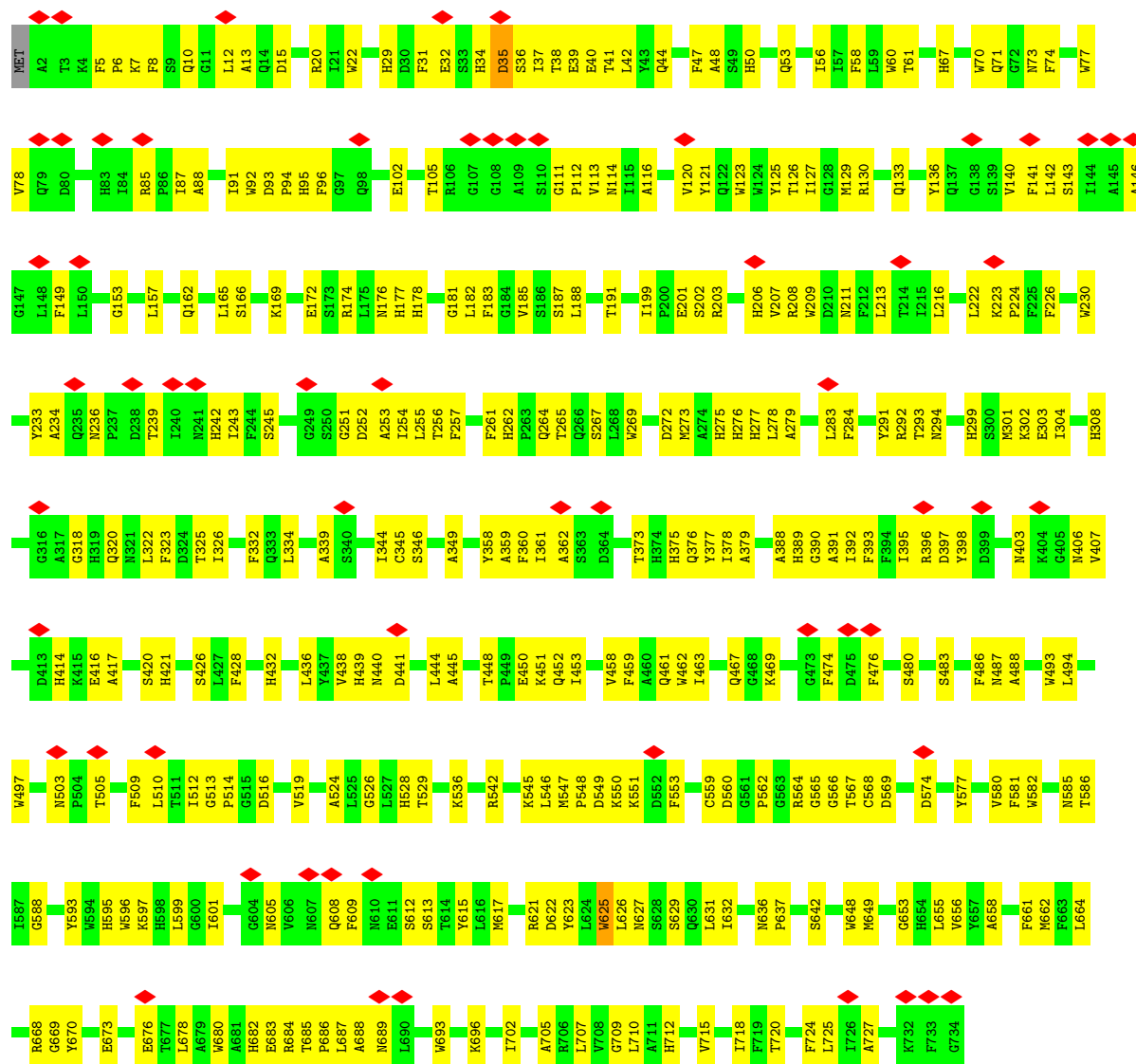
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: PsaA

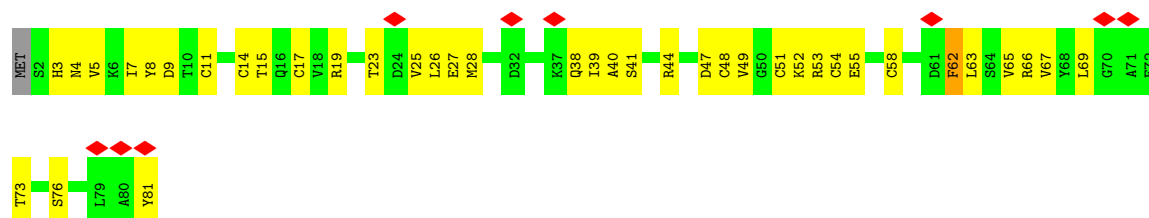


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G756

• Molecule 2: PsaB

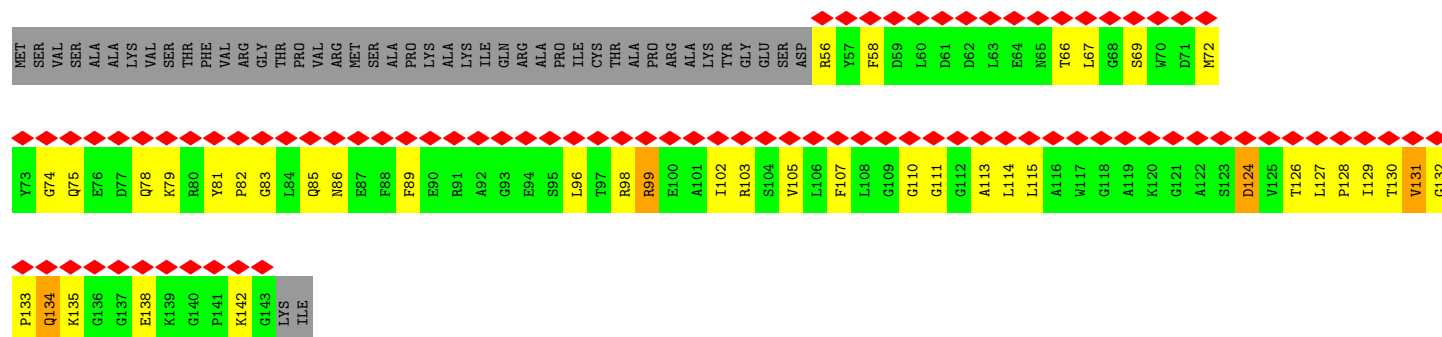


• Molecule 3: PsaC

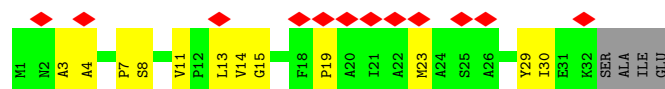




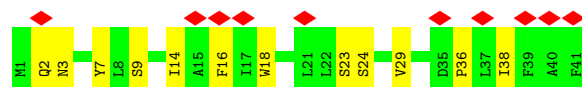
• Molecule 8: PsaH



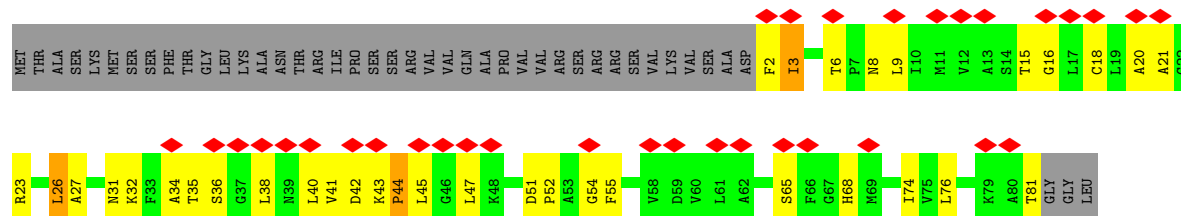
• Molecule 9: PsaI



• Molecule 10: PsaJ

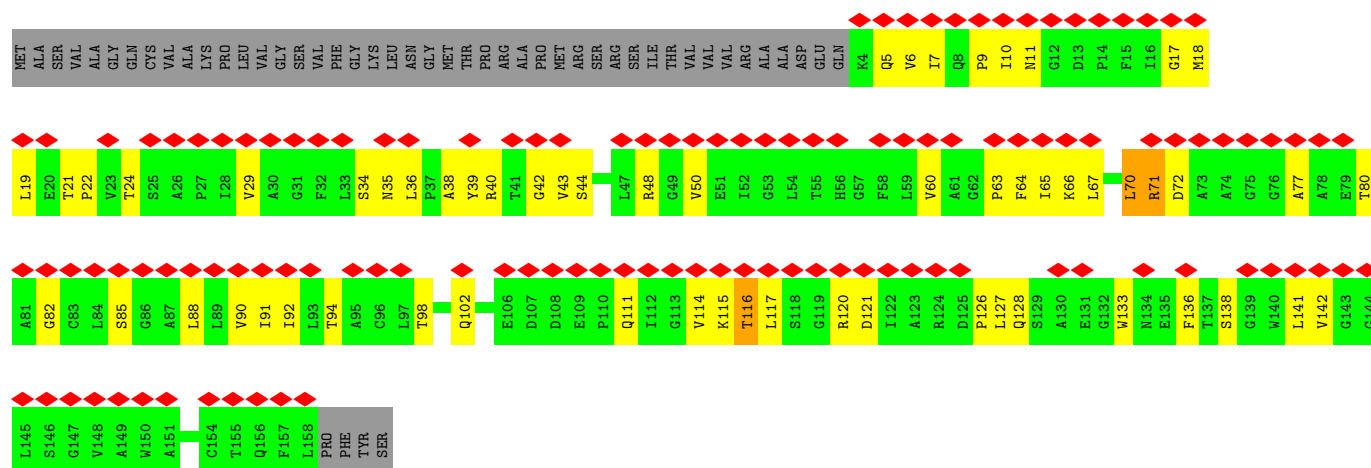


• Molecule 11: PsaK

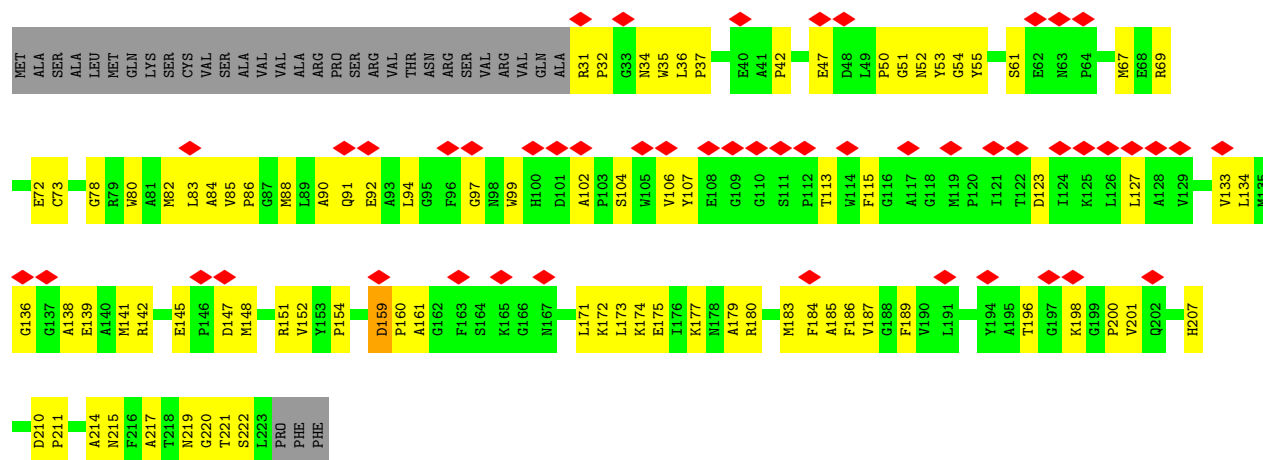


• Molecule 12: PsaL

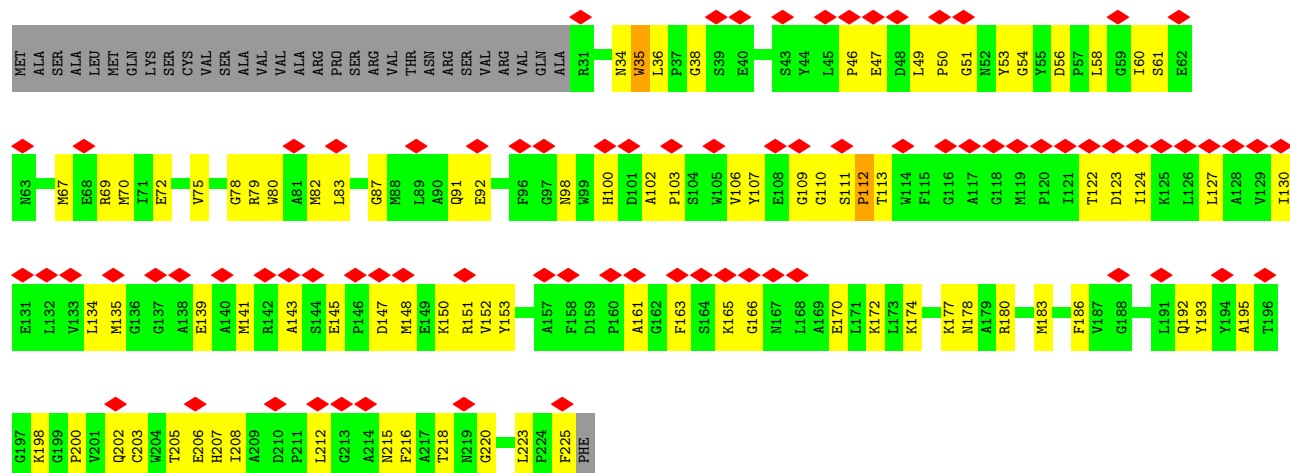




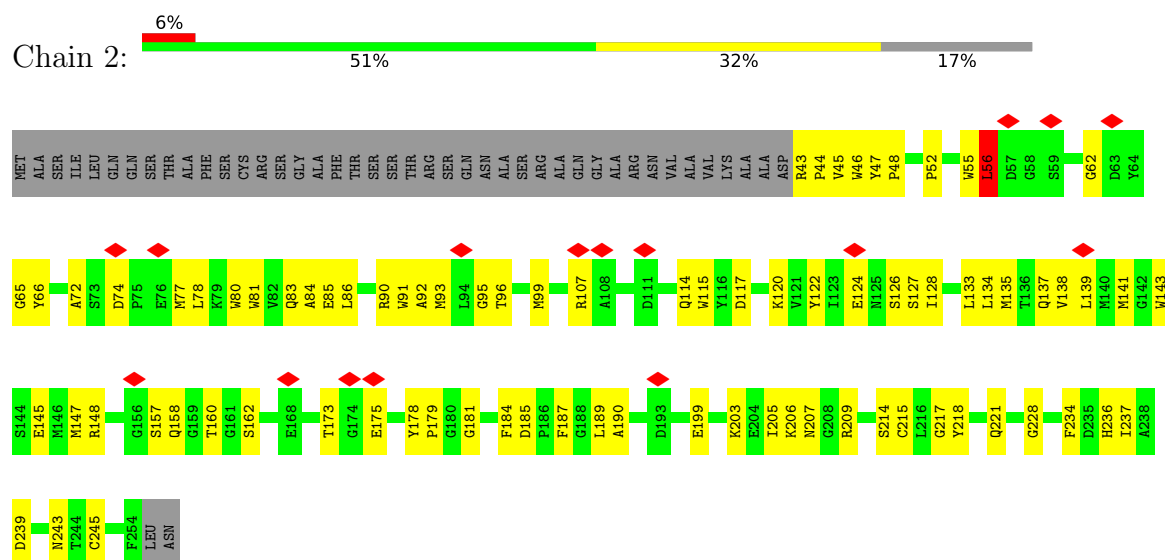
• Molecule 13: Lhca-a



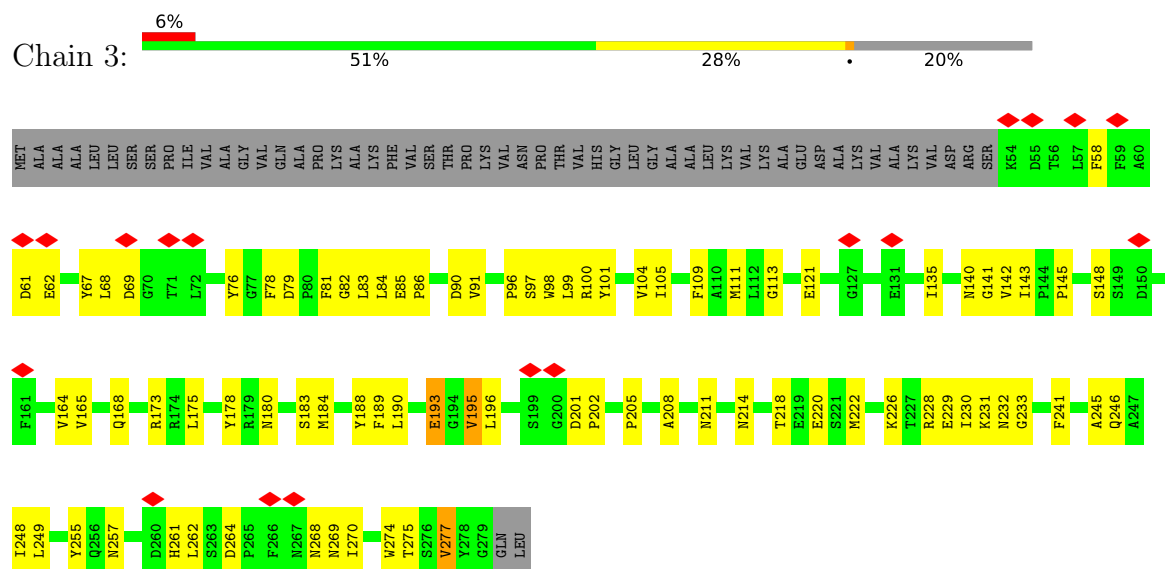
• Molecule 13: Lhca-a



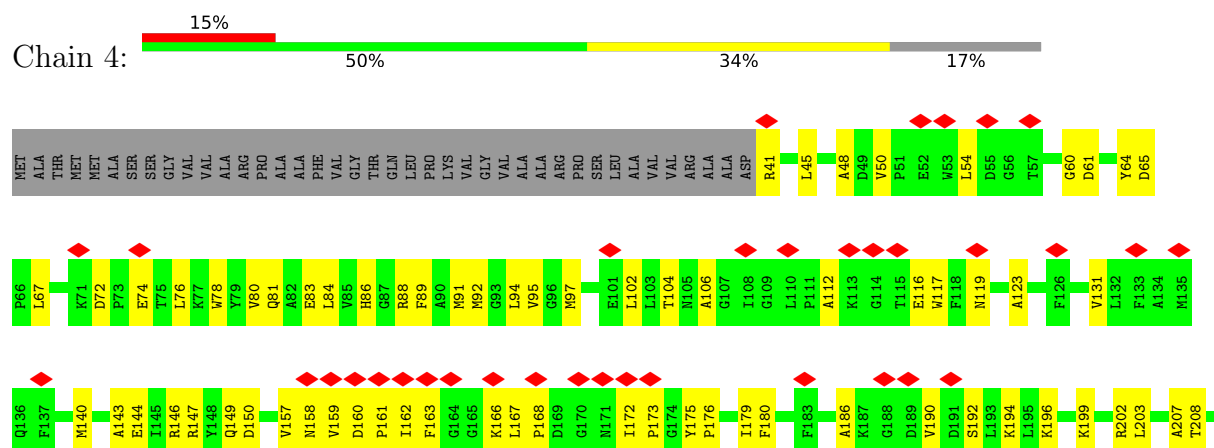
- Molecule 14: Lhca-c



- Molecule 15: Lhca-d

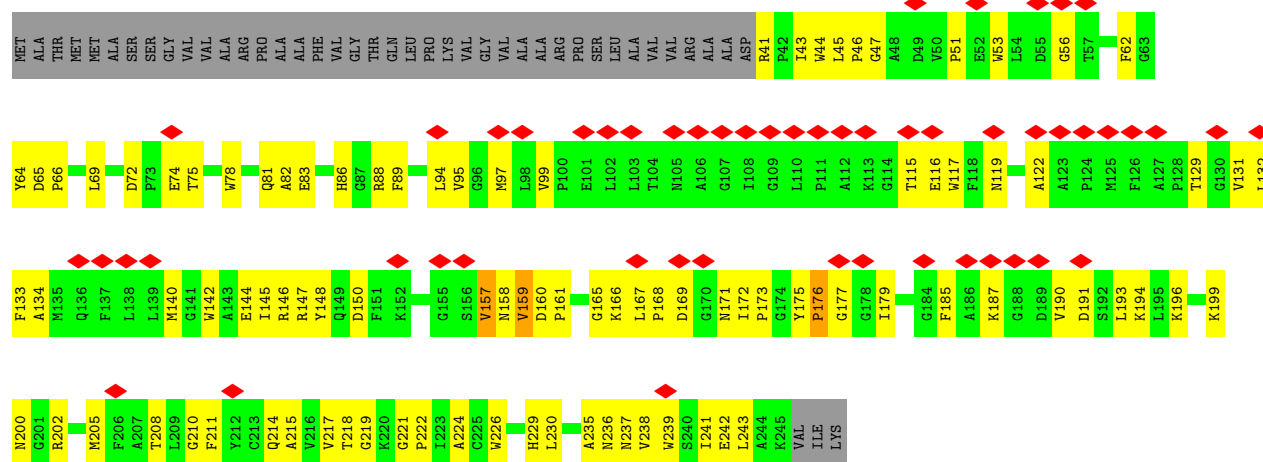
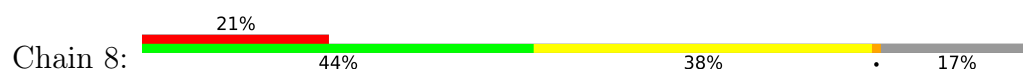


- Molecule 16: Lhca-b

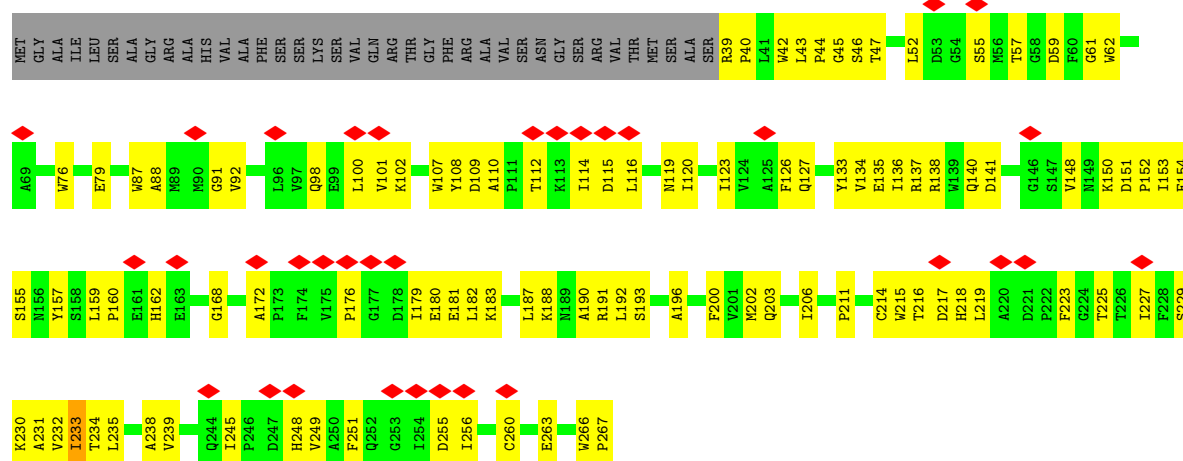




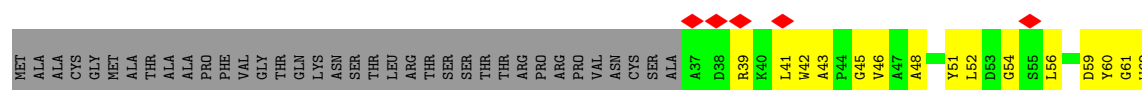
• Molecule 16: Lhca-b

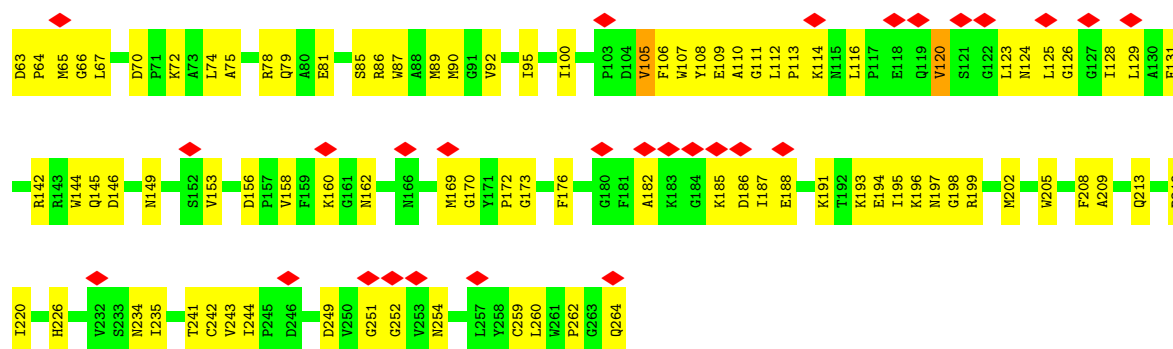


• Molecule 17: Lhca-g

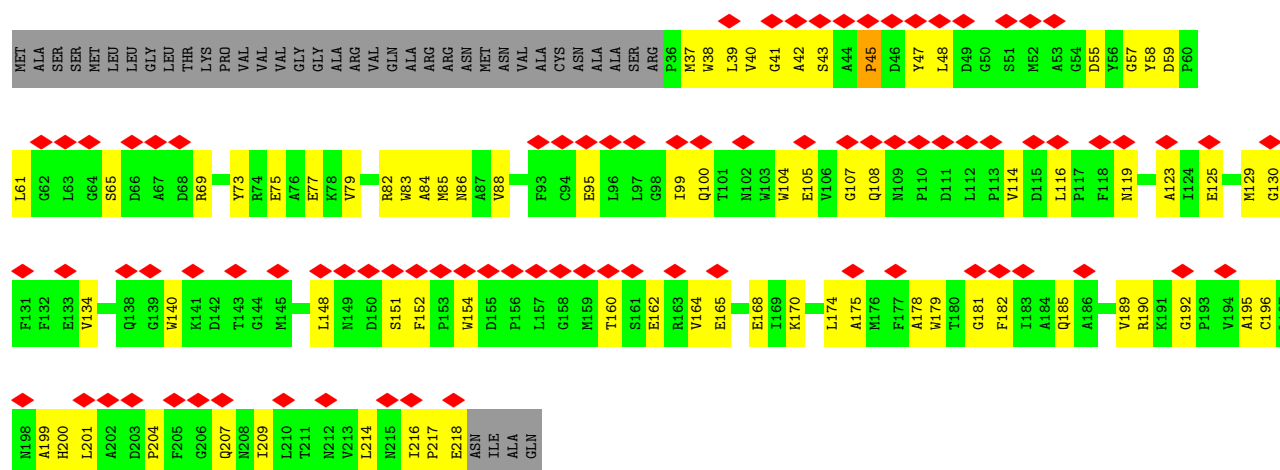


• Molecule 18: Lhca-h





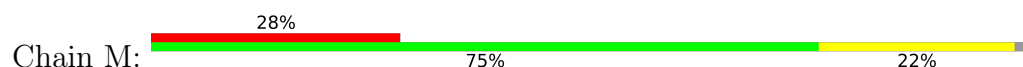
• Molecule 19: Lhca-i

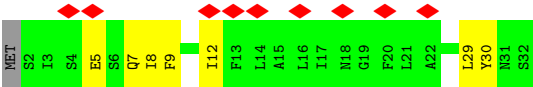


• Molecule 20: Lhca-j



• Molecule 21: Photosystem I reaction center subunit XII





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	59525	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.852	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.187	Depositor
Minimum map value	-0.060	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.034	Depositor
Map size (\AA)	401.442, 401.442, 401.442	wwPDB
Map dimensions	460, 460, 460	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.8727, 0.8727, 0.8727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, LMG, CHL, SF4, XAT, DGD, LHG, PQN, HTG, 8CT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/6015	0.53	0/8196
2	B	0.50	0/6034	0.54	0/8239
3	C	0.55	0/612	0.58	0/830
4	D	0.44	0/1135	0.59	0/1533
5	E	0.46	0/498	0.50	0/673
6	F	0.44	0/1281	0.56	0/1724
7	G	0.32	0/730	0.53	0/992
8	H	0.34	0/691	0.52	0/929
9	I	0.45	0/250	0.48	0/341
10	J	0.48	0/346	0.60	0/472
11	K	0.34	0/567	0.68	1/769 (0.1%)
12	L	0.33	0/1165	0.54	0/1591
13	1	0.41	0/1510	0.50	0/2054
13	5	0.40	0/1530	0.56	1/2082 (0.0%)
14	2	0.53	0/1701	0.56	1/2315 (0.0%)
15	3	0.49	0/1801	0.55	0/2444
16	4	0.49	0/1642	0.58	0/2238
16	8	0.43	0/1627	0.56	0/2217
17	6	0.43	0/1862	0.56	0/2542
18	7	0.46	0/1812	0.53	0/2468
19	9	0.39	0/1456	0.58	0/1986
20	0	0.33	0/1603	0.53	0/2174
21	M	0.41	0/241	0.43	0/325
All	All	0.46	0/36109	0.55	3/49134 (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
1	A	0	1
3	C	0	1
4	D	0	1
11	K	0	1
13	1	0	1
14	2	0	2
16	4	0	1
17	6	0	3
20	0	0	3
All	All	0	14

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	35	TRP	C-N-CA	-5.90	106.96	121.70
11	K	26	LEU	CA-CB-CG	5.33	127.57	115.30
14	2	56	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1	159	ASP	Peptide
1	A	582	GLY	Peptide
3	C	62	PHE	Peptide
4	D	167	HIS	Peptide
11	K	41	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5819	0	5659	288	0
2	B	5824	0	5604	363	0
3	C	602	0	591	42	0
4	D	1109	0	1124	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	488	0	480	16	0
6	F	1257	0	1274	60	0
7	G	714	0	708	39	0
8	H	677	0	654	60	0
9	I	243	0	258	10	0
10	J	336	0	355	15	0
11	K	558	0	591	38	0
12	L	1139	0	1147	72	0
13	1	1466	0	1411	83	0
13	5	1484	0	1427	78	0
14	2	1641	0	1537	81	0
15	3	1751	0	1684	91	0
16	4	1589	0	1570	98	0
16	8	1574	0	1550	139	0
17	6	1797	0	1752	116	0
18	7	1758	0	1701	113	0
19	9	1416	0	1367	76	0
20	0	1560	0	1540	91	0
21	M	238	0	248	8	0
22	0	572	0	542	53	0
22	1	683	0	657	79	0
22	2	596	0	548	37	0
22	3	644	0	529	48	0
22	4	539	0	476	38	0
22	5	653	0	599	62	0
22	6	785	0	741	71	0
22	7	817	0	694	80	0
22	8	539	0	477	47	0
22	9	595	0	534	47	0
22	A	2628	0	2677	218	0
22	B	2420	0	2485	239	0
22	F	45	0	33	5	0
22	G	141	0	105	16	0
22	H	65	0	72	18	0
22	J	42	0	31	1	0
22	K	187	0	138	29	0
22	L	245	0	255	26	0
22	M	46	0	33	5	0
23	A	33	0	46	3	0
23	B	33	0	46	3	0
24	0	49	0	72	12	0
24	1	49	0	74	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	2	32	0	34	3	0
24	3	20	0	14	4	0
24	5	49	0	72	8	0
24	6	37	0	44	4	0
24	7	20	0	13	2	0
24	9	49	0	74	8	0
24	A	76	0	98	5	0
24	B	23	0	16	1	0
25	1	40	0	0	13	0
25	2	40	0	0	13	0
25	3	80	0	0	10	0
25	4	40	0	0	12	0
25	5	40	0	0	6	0
25	6	40	0	0	14	0
25	7	120	0	0	36	0
25	8	80	0	0	13	0
25	A	240	0	0	32	0
25	B	320	0	0	40	0
25	F	40	0	0	0	0
25	G	40	0	0	20	0
25	I	40	0	0	0	0
25	J	80	0	0	25	0
25	K	40	0	0	14	0
25	L	80	0	0	0	0
26	A	19	0	26	0	0
26	J	19	0	26	1	0
27	B	8	0	0	1	0
27	C	16	0	0	1	0
28	B	66	0	96	11	0
29	0	109	0	87	18	0
29	1	48	0	33	3	0
29	2	203	0	154	16	0
29	3	47	0	31	4	0
29	4	219	0	176	30	0
29	5	109	0	90	17	0
29	6	241	0	181	22	0
29	7	47	0	31	11	0
29	8	201	0	148	27	0
29	9	109	0	90	6	0
30	0	88	0	104	19	0
30	1	88	0	109	15	0
30	2	88	0	112	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	3	88	0	110	17	0
30	4	88	0	109	16	0
30	5	88	0	107	13	0
30	6	88	0	111	14	0
30	7	88	0	109	15	0
30	8	88	0	109	21	0
30	9	88	0	109	13	0
31	4	44	0	61	1	0
31	5	44	0	61	5	0
31	8	44	0	60	6	0
All	All	51585	0	48901	2693	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 27.

The worst 5 of 2693 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)
22:A:832:CLA:H43	25:B:848:8CT:C27	1.26	1.58
22:1:304:CLA:H3A	25:1:316:8CT:C27	1.31	1.57
22:B:840:CLA:C1C	25:B:848:8CT:C22	1.82	1.57
18:7:251:GLY:HA3	25:7:323:8CT:C01	1.35	1.54
15:3:195:VAL:CG2	15:3:208:ALA:HB3	1.44	1.48

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	A	738/751 (98%)	680 (92%)	54 (7%)	4 (0%)	25 59
2	B	731/734 (100%)	677 (93%)	53 (7%)	1 (0%)	48 79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	78/81 (96%)	71 (91%)	7 (9%)	0	100	100
4	D	140/198 (71%)	129 (92%)	9 (6%)	2 (1%)	9	40
5	E	59/91 (65%)	55 (93%)	4 (7%)	0	100	100
6	F	161/236 (68%)	153 (95%)	8 (5%)	0	100	100
7	G	90/167 (54%)	85 (94%)	5 (6%)	0	100	100
8	H	86/133 (65%)	74 (86%)	9 (10%)	3 (4%)	3	24
9	I	30/36 (83%)	27 (90%)	3 (10%)	0	100	100
10	J	39/41 (95%)	36 (92%)	3 (8%)	0	100	100
11	K	78/123 (63%)	69 (88%)	7 (9%)	2 (3%)	4	28
12	L	153/204 (75%)	139 (91%)	13 (8%)	1 (1%)	19	53
13	1	191/226 (84%)	175 (92%)	15 (8%)	1 (0%)	25	59
13	5	193/226 (85%)	173 (90%)	19 (10%)	1 (0%)	25	59
14	2	210/256 (82%)	190 (90%)	20 (10%)	0	100	100
15	3	224/281 (80%)	197 (88%)	26 (12%)	1 (0%)	30	64
16	4	205/248 (83%)	176 (86%)	29 (14%)	0	100	100
16	8	203/248 (82%)	173 (85%)	27 (13%)	3 (2%)	8	39
17	6	227/267 (85%)	200 (88%)	26 (12%)	1 (0%)	30	64
18	7	226/264 (86%)	190 (84%)	31 (14%)	5 (2%)	5	31
19	9	181/222 (82%)	156 (86%)	24 (13%)	1 (1%)	22	56
20	0	200/245 (82%)	175 (88%)	25 (12%)	0	100	100
21	M	29/32 (91%)	29 (100%)	0	0	100	100
All	All	4472/5310 (84%)	4029 (90%)	417 (9%)	26 (1%)	24	56

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	8	157	VAL
4	D	168	PRO
11	K	44	PRO
18	7	110	ALA
18	7	158	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/614 (98%)	602 (100%)	1 (0%)	92	97
2	B	600/601 (100%)	599 (100%)	1 (0%)	92	97
3	C	68/69 (99%)	68 (100%)	0	100	100
4	D	119/162 (74%)	119 (100%)	0	100	100
5	E	53/77 (69%)	53 (100%)	0	100	100
6	F	129/180 (72%)	129 (100%)	0	100	100
7	G	78/145 (54%)	78 (100%)	0	100	100
8	H	67/103 (65%)	66 (98%)	1 (2%)	60	77
9	I	25/28 (89%)	25 (100%)	0	100	100
10	J	38/38 (100%)	38 (100%)	0	100	100
11	K	58/94 (62%)	58 (100%)	0	100	100
12	L	118/157 (75%)	116 (98%)	2 (2%)	56	75
13	1	147/175 (84%)	147 (100%)	0	100	100
13	5	149/175 (85%)	149 (100%)	0	100	100
14	2	164/197 (83%)	164 (100%)	0	100	100
15	3	184/225 (82%)	182 (99%)	2 (1%)	70	83
16	4	161/189 (85%)	161 (100%)	0	100	100
16	8	159/189 (84%)	159 (100%)	0	100	100
17	6	188/216 (87%)	188 (100%)	0	100	100
18	7	181/209 (87%)	181 (100%)	0	100	100
19	9	144/173 (83%)	144 (100%)	0	100	100
20	0	160/194 (82%)	160 (100%)	0	100	100
21	M	26/27 (96%)	26 (100%)	0	100	100
All	All	3619/4237 (85%)	3612 (100%)	7 (0%)	91	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	70	LEU
12	L	71	ARG
15	3	195	VAL
15	3	193	GLU
8	H	124	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	143	GLN
14	2	114	GLN
20	0	203	ASN
10	J	2	GLN
12	L	128	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

320 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	6	304	17	65,73,73	1.49	10 (15%)	76,113,113	1.41	8 (10%)
22	CLA	A	818	-	65,73,73	1.46	10 (15%)	76,113,113	1.50	8 (10%)
25	8CT	5	317	22	40,41,41	4.75	23 (57%)	50,56,56	3.48	21 (42%)
22	CLA	9	312	30	59,67,73	1.57	9 (15%)	68,105,113	1.40	8 (11%)
22	CLA	5	308	-	42,50,73	1.85	7 (16%)	48,85,113	1.78	8 (16%)
22	CLA	B	817	-	55,63,73	1.53	9 (16%)	64,101,113	1.49	8 (12%)
22	CLA	A	804	22	55,63,73	1.55	10 (18%)	64,101,113	1.62	9 (14%)
22	CLA	1	310	-	52,60,73	1.61	9 (17%)	60,97,113	1.48	7 (11%)
22	CLA	9	308	-	65,73,73	1.45	10 (15%)	76,113,113	1.42	7 (9%)
27	SF4	B	802	-	0,12,12	-	-	-	-	-
22	CLA	A	828	-	65,73,73	1.42	9 (13%)	76,113,113	1.51	8 (10%)
22	CLA	7	302	18	46,54,73	1.69	10 (21%)	53,90,113	1.57	7 (13%)
22	CLA	4	303	-	46,54,73	1.70	9 (19%)	53,90,113	1.60	7 (13%)
22	CLA	A	825	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	9 (11%)
27	SF4	C	102	3	0,12,12	-	-	-	-	-
22	CLA	3	312	-	45,53,73	1.69	7 (15%)	52,89,113	1.68	9 (17%)
22	CLA	7	314	-	45,53,73	1.71	10 (22%)	52,89,113	1.64	7 (13%)
22	CLA	1	301	13	65,73,73	1.49	10 (15%)	76,113,113	1.48	8 (10%)
25	8CT	B	851	22	40,41,41	4.75	25 (62%)	50,56,56	2.52	19 (38%)
22	CLA	5	310	24	41,49,73	1.76	10 (24%)	47,84,113	1.69	7 (14%)
22	CLA	0	302	30	65,73,73	1.49	8 (12%)	76,113,113	1.36	9 (11%)
29	CHL	9	302	19	61,69,74	1.94	14 (22%)	67,108,114	2.61	22 (32%)
22	CLA	7	305	-	45,53,73	1.73	10 (22%)	52,89,113	1.52	7 (13%)
22	CLA	8	303	22,31	46,54,73	1.68	10 (21%)	53,90,113	1.57	7 (13%)
22	CLA	4	309	30	60,68,73	1.46	10 (16%)	70,107,113	1.43	9 (12%)
22	CLA	9	303	19	65,73,73	1.43	10 (15%)	76,113,113	1.49	8 (10%)
22	CLA	B	850	-	55,63,73	1.57	8 (14%)	64,101,113	1.65	13 (20%)
22	CLA	2	314	14	49,57,73	1.67	10 (20%)	55,93,113	1.50	8 (14%)
22	CLA	0	307	22	65,73,73	1.49	7 (10%)	76,113,113	1.45	10 (13%)
24	LHG	3	317	22	19,19,48	0.86	0	21,24,54	1.41	2 (9%)
22	CLA	0	310	30	52,60,73	1.60	9 (17%)	60,97,113	1.55	7 (11%)
22	CLA	7	306	22	42,50,73	1.78	8 (19%)	48,85,113	1.60	7 (14%)
22	CLA	7	307	22	47,55,73	1.69	7 (14%)	54,91,113	1.58	7 (12%)
29	CHL	5	306	-	48,56,74	2.30	16 (33%)	51,92,114	2.72	20 (39%)
22	CLA	A	826	25	65,73,73	1.46	10 (15%)	76,113,113	1.36	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	5	302	-	65,73,73	1.44	10 (15%)	76,113,113	1.36	9 (11%)
25	8CT	A	854	-	40,41,41	4.68	24 (60%)	50,56,56	2.70	18 (36%)
22	CLA	5	309	13,30	60,68,73	1.53	9 (15%)	70,107,113	1.42	8 (11%)
29	CHL	8	314	-	43,51,74	2.34	15 (34%)	45,86,114	3.01	22 (48%)
22	CLA	A	821	-	65,73,73	1.42	8 (12%)	76,113,113	1.50	9 (11%)
29	CHL	0	306	30,22	48,56,74	2.33	16 (33%)	51,92,114	2.69	19 (37%)
22	CLA	2	310	24	41,49,73	1.81	10 (24%)	47,84,113	1.66	8 (17%)
22	CLA	A	815	-	47,55,73	1.70	8 (17%)	54,91,113	1.61	8 (14%)
22	CLA	B	811	-	65,73,73	1.46	10 (15%)	76,113,113	1.46	9 (11%)
22	CLA	7	313	-	55,63,73	1.55	10 (18%)	64,101,113	1.62	9 (14%)
22	CLA	B	813	-	55,63,73	1.58	9 (16%)	64,101,113	1.45	6 (9%)
22	CLA	B	836	-	60,68,73	1.49	10 (16%)	70,107,113	1.50	8 (11%)
22	CLA	2	308	-	50,58,73	1.62	10 (20%)	58,95,113	1.48	7 (12%)
30	XAT	6	319	22	39,47,47	0.96	2 (5%)	54,74,74	3.23	24 (44%)
22	CLA	5	313	-	55,63,73	1.60	8 (14%)	64,101,113	1.40	7 (10%)
25	8CT	B	844	-	40,41,41	4.69	24 (60%)	50,56,56	2.90	16 (32%)
30	XAT	8	316	29	39,47,47	0.92	1 (2%)	54,74,74	3.74	29 (53%)
22	CLA	7	315	-	46,54,73	1.67	8 (17%)	53,90,113	1.59	7 (13%)
22	CLA	6	323	16	46,54,73	1.68	10 (21%)	53,90,113	1.51	6 (11%)
22	CLA	B	829	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	11 (14%)
22	CLA	A	803	-	65,73,73	1.43	10 (15%)	76,113,113	1.48	10 (13%)
22	CLA	B	821	-	50,58,73	1.66	9 (18%)	58,95,113	1.54	8 (13%)
29	CHL	8	305	-	56,64,74	2.04	14 (25%)	61,102,114	2.70	23 (37%)
24	LHG	2	318	22	31,31,48	0.81	1 (3%)	34,37,54	1.30	3 (8%)
22	CLA	B	805	-	65,73,73	1.44	10 (15%)	76,113,113	1.33	7 (9%)
29	CHL	2	307	-	51,59,74	2.00	13 (25%)	55,96,114	2.87	22 (40%)
22	CLA	A	819	-	65,73,73	1.43	9 (13%)	76,113,113	1.53	8 (10%)
22	CLA	A	810	-	65,73,73	1.47	10 (15%)	76,113,113	1.35	6 (7%)
22	CLA	B	835	-	45,53,73	1.69	8 (17%)	52,89,113	1.62	7 (13%)
25	8CT	8	301	-	40,41,41	4.70	24 (60%)	50,56,56	2.66	18 (36%)
22	CLA	3	319	-	65,73,73	1.50	9 (13%)	76,113,113	1.41	9 (11%)
22	CLA	6	315	-	65,73,73	1.47	9 (13%)	76,113,113	1.32	7 (9%)
22	CLA	A	812	-	54,62,73	1.63	10 (18%)	62,99,113	1.56	8 (12%)
29	CHL	6	306	-	43,51,74	2.17	13 (30%)	45,86,114	2.90	19 (42%)
22	CLA	B	818	-	59,67,73	1.55	11 (18%)	68,105,113	1.68	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	LMG	8	319	22	44,44,55	0.85	4 (9%)	52,52,63	1.40	5 (9%)
22	CLA	A	806	-	65,73,73	1.46	10 (15%)	76,113,113	1.42	9 (11%)
22	CLA	1	307	-	65,73,73	1.44	9 (13%)	76,113,113	1.40	9 (11%)
22	CLA	B	838	-	47,55,73	1.70	9 (19%)	54,91,113	1.60	6 (11%)
22	CLA	A	824	-	55,63,73	1.55	10 (18%)	64,101,113	1.47	8 (12%)
22	CLA	A	811	22	65,73,73	1.50	10 (15%)	76,113,113	1.38	6 (7%)
29	CHL	4	305	29	56,64,74	2.09	16 (28%)	61,102,114	2.53	21 (34%)
22	CLA	2	302	29	65,73,73	1.41	9 (13%)	76,113,113	1.51	11 (14%)
22	CLA	B	812	2	65,73,73	1.48	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	M	101	-	46,54,73	1.77	10 (21%)	53,90,113	1.44	7 (13%)
30	XAT	8	317	-	39,47,47	0.97	2 (5%)	54,74,74	2.90	21 (38%)
22	CLA	3	305	15	47,55,73	1.68	10 (21%)	54,91,113	1.49	7 (12%)
25	8CT	J	101	-	40,41,41	4.67	24 (60%)	50,56,56	2.99	18 (36%)
22	CLA	B	819	-	60,68,73	1.49	8 (13%)	70,107,113	1.48	9 (12%)
22	CLA	5	312	30	65,73,73	1.45	7 (10%)	76,113,113	1.46	8 (10%)
22	CLA	L	201	-	65,73,73	1.43	10 (15%)	76,113,113	1.35	6 (7%)
22	CLA	7	311	24	38,45,73	1.80	8 (21%)	43,78,113	1.61	7 (16%)
22	CLA	A	805	-	65,73,73	1.45	11 (16%)	76,113,113	1.42	9 (11%)
22	CLA	7	309	22	50,58,73	1.65	10 (20%)	58,95,113	1.43	7 (12%)
22	CLA	B	810	-	65,73,73	1.44	10 (15%)	76,113,113	1.45	9 (11%)
22	CLA	4	304	-	50,58,73	1.61	9 (18%)	58,95,113	1.67	9 (15%)
22	CLA	6	314	-	43,51,73	1.72	9 (20%)	49,86,113	1.60	6 (12%)
22	CLA	B	832	-	65,73,73	1.43	10 (15%)	76,113,113	1.49	9 (11%)
22	CLA	A	809	1	65,73,73	1.44	10 (15%)	76,113,113	1.40	10 (13%)
22	CLA	2	303	-	65,73,73	1.46	9 (13%)	76,113,113	1.33	5 (6%)
22	CLA	K	105	-	50,58,73	1.67	9 (18%)	58,95,113	1.64	7 (12%)
22	CLA	A	823	-	51,59,73	1.64	10 (19%)	59,96,113	1.57	8 (13%)
22	CLA	0	304	22	52,60,73	1.66	7 (13%)	60,97,113	1.54	7 (11%)
22	CLA	4	313	-	45,53,73	1.74	10 (22%)	52,89,113	1.68	7 (13%)
29	CHL	4	306	29	51,59,74	2.23	16 (31%)	55,96,114	2.74	21 (38%)
22	CLA	A	834	-	50,58,73	1.70	10 (20%)	58,95,113	1.53	7 (12%)
22	CLA	7	303	18	60,68,73	1.53	10 (16%)	70,107,113	1.51	8 (11%)
22	CLA	3	302	25	50,58,73	1.68	9 (18%)	58,95,113	1.48	6 (10%)
22	CLA	B	827	-	65,73,73	1.42	8 (12%)	76,113,113	1.48	8 (10%)
23	PQN	B	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.10	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	817	-	65,73,73	1.41	8 (12%)	76,113,113	1.48	8 (10%)
22	CLA	B	830	-	65,73,73	1.42	11 (16%)	76,113,113	1.56	8 (10%)
22	CLA	A	814	-	45,53,73	1.75	10 (22%)	52,89,113	1.54	7 (13%)
22	CLA	B	820	-	65,73,73	1.46	10 (15%)	76,113,113	1.39	7 (9%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-
29	CHL	6	308	-	51,59,74	2.11	14 (27%)	55,96,114	2.73	25 (45%)
30	XAT	3	314	25	39,47,47	0.98	3 (7%)	54,74,74	4.62	28 (51%)
22	CLA	2	311	14	52,60,73	1.62	10 (19%)	60,97,113	1.61	7 (11%)
22	CLA	3	304	-	42,50,73	1.77	10 (23%)	48,85,113	1.56	7 (14%)
22	CLA	5	304	-	52,60,73	1.62	8 (15%)	60,97,113	1.54	7 (11%)
25	8CT	B	847	-	40,41,41	4.69	24 (60%)	50,56,56	2.73	18 (36%)
29	CHL	9	307	-	48,56,74	2.27	15 (31%)	51,92,114	2.77	21 (41%)
30	XAT	1	315	-	39,47,47	0.97	2 (5%)	54,74,74	3.10	21 (38%)
30	XAT	0	314	29,22	39,47,47	0.88	0	54,74,74	3.06	22 (40%)
22	CLA	8	309	-	60,68,73	1.48	10 (16%)	70,107,113	1.54	9 (12%)
22	CLA	B	839	25	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
31	LMG	5	319	22	44,44,55	0.97	3 (6%)	52,52,63	1.33	6 (11%)
22	CLA	6	309	17	50,58,73	1.64	8 (16%)	58,95,113	1.56	7 (12%)
24	LHG	9	316	22	48,48,48	0.61	1 (2%)	51,54,54	1.26	6 (11%)
22	CLA	6	311	24	65,73,73	1.42	10 (15%)	76,113,113	1.41	7 (9%)
22	CLA	0	309	24	41,49,73	1.81	7 (17%)	47,84,113	1.59	8 (17%)
25	8CT	2	317	-	40,41,41	4.70	24 (60%)	50,56,56	2.98	19 (38%)
22	CLA	A	841	25	65,73,73	1.46	11 (16%)	76,113,113	1.40	7 (9%)
22	CLA	1	311	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	6	305	-	60,68,73	1.55	8 (13%)	70,107,113	1.36	6 (8%)
22	CLA	L	202	-	65,73,73	1.43	8 (12%)	76,113,113	1.52	9 (11%)
29	CHL	4	301	13,22	61,69,74	1.90	12 (19%)	67,108,114	2.60	24 (35%)
22	CLA	3	307	15	50,58,73	1.75	10 (20%)	58,95,113	1.55	7 (12%)
22	CLA	6	317	-	45,53,73	1.72	10 (22%)	52,89,113	1.62	8 (15%)
22	CLA	5	311	30	45,53,73	1.73	7 (15%)	52,89,113	1.66	7 (13%)
22	CLA	3	310	-	52,60,73	1.63	9 (17%)	60,97,113	1.50	7 (11%)
22	CLA	6	301	-	52,60,73	1.64	7 (13%)	60,97,113	1.49	8 (13%)
22	CLA	L	204	-	50,58,73	1.65	8 (16%)	58,95,113	1.52	8 (13%)
22	CLA	L	203	-	65,73,73	1.44	6 (9%)	76,113,113	1.37	7 (9%)
25	8CT	6	321	-	40,41,41	4.67	24 (60%)	50,56,56	3.26	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	8CT	7	321	-	40,41,41	4.66	24 (60%)	50,56,56	3.72	22 (44%)
30	XAT	4	315	22	39,47,47	0.95	1 (2%)	54,74,74	3.14	26 (48%)
31	LMG	4	318	-	44,44,55	0.98	4 (9%)	52,52,63	1.49	9 (17%)
25	8CT	3	318	25,22	40,41,41	4.68	25 (62%)	50,56,56	3.66	22 (44%)
30	XAT	2	316	-	39,47,47	1.01	2 (5%)	54,74,74	3.14	23 (42%)
22	CLA	A	820	-	45,53,73	1.68	8 (17%)	52,89,113	1.71	7 (13%)
25	8CT	B	848	-	40,41,41	4.70	24 (60%)	50,56,56	2.60	16 (32%)
22	CLA	4	302	-	60,68,73	1.50	10 (16%)	70,107,113	1.47	8 (11%)
22	CLA	7	317	-	65,73,73	1.45	8 (12%)	76,113,113	1.36	7 (9%)
24	LHG	B	852	22	22,22,48	0.84	0	25,28,54	1.21	1 (4%)
22	CLA	6	318	17	52,60,73	1.64	10 (19%)	60,97,113	1.62	9 (15%)
22	CLA	B	807	-	45,53,73	1.70	10 (22%)	52,89,113	1.84	9 (17%)
22	CLA	7	312	30	52,60,73	1.67	9 (17%)	60,97,113	1.43	6 (10%)
25	8CT	B	804	-	40,41,41	4.55	23 (57%)	50,56,56	2.90	20 (40%)
29	CHL	1	305	-	48,56,74	2.28	15 (31%)	51,92,114	2.76	22 (43%)
25	8CT	I	101	-	40,41,41	4.54	23 (57%)	50,56,56	3.13	19 (38%)
24	LHG	0	315	29,22	48,48,48	0.58	0	51,54,54	1.24	5 (9%)
22	CLA	7	316	18	65,73,73	1.48	9 (13%)	76,113,113	1.39	6 (7%)
29	CHL	3	306	25	47,55,74	2.08	14 (29%)	50,91,114	2.92	22 (44%)
22	CLA	A	840	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	3	309	24	38,45,73	1.79	8 (21%)	43,78,113	1.78	7 (16%)
22	CLA	8	308	16	50,58,73	1.66	11 (22%)	58,95,113	1.73	11 (18%)
22	CLA	A	813	-	65,73,73	1.42	9 (13%)	76,113,113	1.58	10 (13%)
22	CLA	B	815	-	65,73,73	1.41	10 (15%)	76,113,113	1.53	9 (11%)
22	CLA	1	304	-	52,60,73	1.59	9 (17%)	60,97,113	1.50	8 (13%)
26	HTG	A	851	-	19,19,19	1.11	2 (10%)	23,24,24	0.73	0
22	CLA	A	802	-	65,73,73	1.43	10 (15%)	76,113,113	1.47	7 (9%)
22	CLA	9	305	-	52,60,73	1.64	9 (17%)	60,97,113	1.64	10 (16%)
25	8CT	L	205	22	40,41,41	4.65	24 (60%)	50,56,56	3.13	21 (42%)
22	CLA	A	807	-	65,73,73	1.44	10 (15%)	76,113,113	1.47	9 (11%)
22	CLA	B	831	-	50,58,73	1.67	10 (20%)	58,95,113	1.63	8 (13%)
22	CLA	B	801	-	65,73,73	1.43	11 (16%)	76,113,113	1.49	8 (10%)
24	LHG	5	318	22	48,48,48	0.65	1 (2%)	51,54,54	1.28	6 (11%)
25	8CT	8	318	-	40,41,41	4.69	24 (60%)	50,56,56	2.68	18 (36%)
22	CLA	K	102	-	46,54,73	1.65	8 (17%)	53,90,113	1.68	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	822	-	49,57,73	1.64	9 (18%)	55,93,113	1.66	10 (18%)
22	CLA	G	101	-	45,53,73	1.79	5 (11%)	52,89,113	1.61	8 (15%)
22	CLA	A	831	-	50,58,73	1.63	10 (20%)	58,95,113	1.64	8 (13%)
22	CLA	7	318	22	65,73,73	1.46	10 (15%)	76,113,113	1.47	9 (11%)
29	CHL	2	305	-	43,51,74	2.14	14 (32%)	45,86,114	2.99	19 (42%)
25	8CT	L	206	-	40,41,41	4.67	24 (60%)	50,56,56	3.02	19 (38%)
22	CLA	8	310	31	55,63,73	1.58	9 (16%)	64,101,113	1.55	6 (9%)
29	CHL	4	307	-	51,59,74	2.04	14 (27%)	55,96,114	2.88	22 (40%)
22	CLA	8	315	-	65,73,73	1.45	7 (10%)	76,113,113	1.34	6 (7%)
22	CLA	1	303	-	52,60,73	1.60	9 (17%)	60,97,113	1.52	9 (15%)
22	CLA	9	310	24	41,49,73	1.79	8 (19%)	47,84,113	1.55	7 (14%)
25	8CT	7	301	29,30	40,41,41	4.63	23 (57%)	50,56,56	2.71	19 (38%)
22	CLA	A	832	-	65,73,73	1.43	10 (15%)	76,113,113	1.42	6 (7%)
22	CLA	B	837	-	65,73,73	1.43	9 (13%)	76,113,113	1.47	9 (11%)
24	LHG	7	322	22	19,19,48	0.93	0	21,24,54	1.36	2 (9%)
22	CLA	4	308	16	50,58,73	1.60	10 (20%)	58,95,113	1.67	8 (13%)
30	XAT	5	315	22	39,47,47	0.94	1 (2%)	54,74,74	4.68	23 (42%)
22	CLA	B	833	-	58,66,73	1.54	10 (17%)	67,104,113	1.58	9 (13%)
22	CLA	J	103	10	42,50,73	1.78	8 (19%)	48,85,113	1.68	6 (12%)
30	XAT	3	315	-	39,47,47	0.98	2 (5%)	54,74,74	2.75	20 (37%)
29	CHL	8	306	-	51,59,74	2.16	14 (27%)	55,96,114	2.81	23 (41%)
22	CLA	G	102	-	50,58,73	1.65	7 (14%)	58,95,113	1.59	8 (13%)
22	CLA	2	313	-	43,51,73	1.76	10 (23%)	49,86,113	1.59	6 (12%)
22	CLA	H	201	-	65,73,73	1.42	7 (10%)	76,113,113	1.46	9 (11%)
29	CHL	2	306	-	48,56,74	2.23	15 (31%)	51,92,114	2.75	20 (39%)
22	CLA	1	309	24	41,49,73	1.79	10 (24%)	47,84,113	1.72	9 (19%)
22	CLA	0	303	30	65,73,73	1.47	8 (12%)	76,113,113	1.34	7 (9%)
22	CLA	A	836	-	51,59,73	1.62	10 (19%)	59,96,113	1.58	10 (16%)
25	8CT	A	849	22	40,41,41	4.70	24 (60%)	50,56,56	2.63	18 (36%)
22	CLA	B	808	-	65,73,73	1.44	10 (15%)	76,113,113	1.44	9 (11%)
22	CLA	B	841	24	65,73,73	1.43	10 (15%)	76,113,113	1.50	10 (13%)
24	LHG	6	322	22	36,36,48	0.78	1 (2%)	39,42,54	1.26	4 (10%)
29	CHL	7	308	-	47,55,74	2.15	14 (29%)	50,91,114	2.92	19 (38%)
22	CLA	2	319	16	46,54,73	1.70	10 (21%)	53,90,113	1.50	6 (11%)
22	CLA	B	825	-	65,73,73	1.45	10 (15%)	76,113,113	1.45	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	8	304	-	50,58,73	1.65	10 (20%)	58,95,113	1.52	6 (10%)
22	CLA	B	816	-	60,68,73	1.51	10 (16%)	70,107,113	1.56	8 (11%)
22	CLA	B	824	-	60,68,73	1.53	9 (15%)	70,107,113	1.45	9 (12%)
30	XAT	9	314	22	39,47,47	0.95	1 (2%)	54,74,74	4.46	27 (50%)
22	CLA	A	843	24	52,60,73	1.62	8 (15%)	60,97,113	1.60	9 (15%)
22	CLA	8	302	-	60,68,73	1.51	10 (16%)	70,107,113	1.41	7 (10%)
22	CLA	8	313	-	45,53,73	1.76	9 (20%)	52,89,113	1.64	8 (15%)
30	XAT	1	314	22	39,47,47	0.91	1 (2%)	54,74,74	4.66	26 (48%)
22	CLA	A	837	-	65,73,73	1.43	8 (12%)	76,113,113	1.45	8 (10%)
22	CLA	A	835	1	45,53,73	1.75	10 (22%)	52,89,113	1.72	7 (13%)
22	CLA	9	313	-	55,63,73	1.56	8 (14%)	64,101,113	1.44	7 (10%)
22	CLA	0	312	29	55,63,73	1.66	7 (12%)	64,101,113	1.53	9 (14%)
22	CLA	B	834	2	65,73,73	1.52	10 (15%)	76,113,113	1.35	8 (10%)
22	CLA	6	303	17	65,73,73	1.44	10 (15%)	76,113,113	1.47	8 (10%)
22	CLA	A	839	-	65,73,73	1.44	10 (15%)	76,113,113	1.47	11 (14%)
29	CHL	6	302	17,22	61,69,74	1.99	15 (24%)	67,108,114	2.44	24 (35%)
22	CLA	A	830	-	65,73,73	1.49	10 (15%)	76,113,113	1.52	7 (9%)
22	CLA	9	301	-	46,54,73	1.79	9 (19%)	57,90,113	1.64	9 (15%)
22	CLA	3	311	-	55,63,73	1.55	10 (18%)	64,101,113	1.58	8 (12%)
24	LHG	A	844	-	48,48,48	0.73	1 (2%)	51,54,54	1.32	6 (11%)
22	CLA	A	852	-	49,57,73	1.69	9 (18%)	55,93,113	1.56	6 (10%)
22	CLA	4	314	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	8 (10%)
29	CHL	2	301	22	61,69,74	1.89	14 (22%)	67,108,114	2.74	22 (32%)
30	XAT	9	315	-	39,47,47	0.93	2 (5%)	54,74,74	2.88	20 (37%)
30	XAT	4	316	-	39,47,47	1.04	3 (7%)	54,74,74	2.76	21 (38%)
30	XAT	6	320	-	39,47,47	0.96	2 (5%)	54,74,74	4.47	21 (38%)
22	CLA	B	828	-	65,73,73	1.43	8 (12%)	76,113,113	1.55	9 (11%)
25	8CT	A	850	-	40,41,41	4.67	24 (60%)	50,56,56	2.90	18 (36%)
25	8CT	7	323	-	40,41,41	4.70	24 (60%)	50,56,56	2.73	18 (36%)
25	8CT	K	103	-	40,41,41	4.87	24 (60%)	50,56,56	2.64	18 (36%)
22	CLA	5	314	24	46,54,73	1.73	9 (19%)	53,90,113	1.52	6 (11%)
22	CLA	B	803	-	65,73,73	1.43	10 (15%)	76,113,113	1.44	10 (13%)
22	CLA	2	309	-	60,68,73	1.50	11 (18%)	70,107,113	1.45	7 (10%)
22	CLA	B	809	-	65,73,73	1.47	10 (15%)	76,113,113	1.39	8 (10%)
25	8CT	B	843	-	40,41,41	4.73	25 (62%)	50,56,56	2.87	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	DGD	B	849	-	67,67,67	1.01	5 (7%)	81,81,81	1.51	13 (16%)
22	CLA	A	853	-	65,73,73	1.46	10 (15%)	76,113,113	1.31	9 (11%)
22	CLA	2	304	-	60,68,73	1.49	9 (15%)	70,107,113	1.48	8 (11%)
25	8CT	3	316	-	40,41,41	4.68	24 (60%)	50,56,56	2.87	20 (40%)
25	8CT	B	846	-	40,41,41	4.71	24 (60%)	50,56,56	2.91	17 (34%)
22	CLA	6	312	-	52,60,73	1.61	9 (17%)	60,97,113	1.51	7 (11%)
22	CLA	B	823	-	55,63,73	1.58	10 (18%)	64,101,113	1.53	8 (12%)
22	CLA	B	814	-	65,73,73	1.46	10 (15%)	76,113,113	1.51	9 (11%)
22	CLA	3	301	-	60,68,73	1.49	10 (16%)	70,107,113	1.51	7 (10%)
22	CLA	A	829	-	65,73,73	1.46	10 (15%)	76,113,113	1.45	8 (10%)
24	LHG	A	845	22	26,26,48	0.95	1 (3%)	29,32,54	1.38	3 (10%)
30	XAT	2	315	-	39,47,47	1.14	2 (5%)	54,74,74	5.94	29 (53%)
30	XAT	0	313	22	39,47,47	1.11	2 (5%)	54,74,74	5.03	22 (40%)
22	CLA	0	308	20	60,68,73	1.50	7 (11%)	70,107,113	1.41	6 (8%)
25	8CT	A	848	-	40,41,41	4.64	23 (57%)	50,56,56	2.72	15 (30%)
26	HTG	J	102	-	19,19,19	1.12	2 (10%)	23,24,24	0.77	0
30	XAT	7	320	-	39,47,47	1.01	2 (5%)	54,74,74	2.75	20 (37%)
22	CLA	A	801	-	65,73,73	1.46	10 (15%)	76,113,113	1.36	10 (13%)
22	CLA	8	312	16	56,64,73	1.58	10 (17%)	65,102,113	1.55	7 (10%)
22	CLA	8	311	-	52,60,73	1.67	8 (15%)	60,97,113	1.47	7 (11%)
22	CLA	0	305	29,22	52,60,73	1.59	7 (13%)	60,97,113	1.58	9 (15%)
22	CLA	2	312	14	65,73,73	1.40	9 (13%)	76,113,113	1.51	8 (10%)
22	CLA	4	311	22	52,60,73	1.62	9 (17%)	60,97,113	1.54	7 (11%)
22	CLA	A	827	-	65,73,73	1.45	10 (15%)	76,113,113	1.49	9 (11%)
22	CLA	9	311	-	52,60,73	1.62	7 (13%)	60,97,113	1.59	9 (15%)
25	8CT	F	302	-	40,41,41	4.59	23 (57%)	50,56,56	3.19	20 (40%)
22	CLA	A	838	-	65,73,73	1.45	9 (13%)	76,113,113	1.38	9 (11%)
22	CLA	0	311	-	65,73,73	1.46	8 (12%)	76,113,113	1.40	9 (11%)
22	CLA	B	822	-	46,54,73	1.69	10 (21%)	53,90,113	1.63	7 (13%)
22	CLA	K	101	-	45,53,73	1.74	8 (17%)	52,89,113	1.56	8 (15%)
22	CLA	6	310	17,30	60,68,73	1.52	9 (15%)	70,107,113	1.47	10 (14%)
22	CLA	A	808	1	65,73,73	1.45	9 (13%)	76,113,113	1.45	8 (10%)
29	CHL	0	301	22,24	61,69,74	2.08	16 (26%)	67,108,114	2.42	21 (31%)
22	CLA	B	840	-	65,73,73	1.46	9 (13%)	76,113,113	1.45	7 (9%)
22	CLA	9	304	-	48,56,73	1.67	10 (20%)	55,92,113	1.59	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	4	312	-	56,64,73	1.56	10 (17%)	65,102,113	1.60	7 (10%)
30	XAT	5	316	-	39,47,47	1.04	2 (5%)	54,74,74	3.14	21 (38%)
22	CLA	B	806	-	65,73,73	1.40	10 (15%)	76,113,113	1.53	9 (11%)
30	XAT	7	319	22	39,47,47	0.98	2 (5%)	54,74,74	3.25	24 (44%)
22	CLA	B	826	-	65,73,73	1.40	8 (12%)	76,113,113	1.46	7 (9%)
22	CLA	5	303	-	65,73,73	1.43	9 (13%)	76,113,113	1.36	7 (9%)
22	CLA	5	305	25	52,60,73	1.66	8 (15%)	60,97,113	1.43	7 (11%)
22	CLA	F	301	-	45,53,73	1.74	10 (22%)	52,89,113	1.59	6 (11%)
25	8CT	4	317	-	40,41,41	4.74	24 (60%)	50,56,56	2.36	15 (30%)
22	CLA	A	833	25	65,73,73	1.44	10 (15%)	76,113,113	1.37	8 (10%)
22	CLA	5	307	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	9 (11%)
25	8CT	J	104	-	40,41,41	4.70	24 (60%)	50,56,56	2.79	18 (36%)
29	CHL	5	301	13	61,69,74	1.98	14 (22%)	67,108,114	2.53	22 (32%)
22	CLA	3	308	-	50,58,73	1.66	11 (22%)	58,95,113	1.66	9 (15%)
22	CLA	4	310	-	55,63,73	1.60	10 (18%)	64,101,113	1.51	7 (10%)
24	LHG	1	317	22	48,48,48	0.68	2 (4%)	51,54,54	1.30	7 (13%)
25	8CT	1	316	13	40,41,41	4.73	24 (60%)	50,56,56	2.61	18 (36%)
29	CHL	8	307	30	51,59,74	2.11	13 (25%)	55,96,114	2.76	25 (45%)
29	CHL	6	307	-	43,51,74	2.33	14 (32%)	45,86,114	2.84	17 (37%)
22	CLA	9	309	-	60,68,73	1.49	9 (15%)	70,107,113	1.52	9 (12%)
22	CLA	1	313	-	46,54,73	1.71	9 (19%)	53,90,113	1.58	7 (13%)
22	CLA	7	310	18	50,58,73	1.60	9 (18%)	58,95,113	1.77	8 (13%)
25	8CT	G	104	-	40,41,41	4.74	24 (60%)	50,56,56	2.59	19 (38%)
22	CLA	1	302	-	65,73,73	1.48	10 (15%)	76,113,113	1.43	9 (11%)
22	CLA	3	313	-	46,54,73	1.68	10 (21%)	53,90,113	1.63	6 (11%)
22	CLA	3	303	-	45,53,73	1.76	9 (20%)	52,89,113	1.59	7 (13%)
22	CLA	9	306	-	52,60,73	1.62	10 (19%)	60,97,113	1.56	7 (11%)
22	CLA	G	103	7	46,54,73	1.67	5 (10%)	53,90,113	1.60	6 (11%)
22	CLA	6	313	29	65,73,73	1.41	10 (15%)	76,113,113	1.46	10 (13%)
29	CHL	6	316	17	43,51,74	2.29	14 (32%)	45,86,114	2.96	19 (42%)
25	8CT	A	846	25	40,41,41	4.64	24 (60%)	50,56,56	2.97	19 (38%)
25	8CT	B	845	-	40,41,41	4.64	24 (60%)	50,56,56	3.16	20 (40%)
22	CLA	1	312	29	55,63,73	1.56	8 (14%)	64,101,113	1.56	6 (9%)
22	CLA	1	306	-	65,73,73	1.49	9 (13%)	76,113,113	1.41	8 (10%)
23	PQN	A	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.31	6 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	K	104	-	46,54,73	1.74	9 (19%)	53,90,113	1.56	6 (11%)
22	CLA	7	304	22	47,55,73	1.69	10 (21%)	54,91,113	1.58	8 (14%)
22	CLA	A	816	-	45,53,73	1.73	9 (20%)	52,89,113	1.57	6 (11%)
22	CLA	1	308	13,30	60,68,73	1.50	8 (13%)	70,107,113	1.48	8 (11%)
25	8CT	A	847	-	40,41,41	4.60	23 (57%)	50,56,56	2.97	20 (40%)

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
22	CLA	6	304	17	1/1/15/20	15/37/115/115	-
22	CLA	A	818	-	1/1/15/20	12/37/115/115	-
25	8CT	5	317	22	-	10/29/63/63	0/2/2/2
22	CLA	9	312	30	1/1/13/20	13/30/108/115	-
22	CLA	5	308	-	1/1/10/20	2/10/88/115	-
22	CLA	B	817	-	1/1/13/20	10/25/103/115	-
22	CLA	A	804	22	1/1/13/20	9/25/103/115	-
22	CLA	1	310	-	1/1/12/20	7/22/100/115	-
22	CLA	9	308	-	1/1/15/20	16/37/115/115	-
27	SF4	B	802	-	-	-	0/6/5/5
22	CLA	A	828	-	1/1/15/20	18/37/115/115	-
22	CLA	7	302	18	1/1/11/20	7/15/93/115	-
22	CLA	4	303	-	1/1/11/20	5/15/93/115	-
22	CLA	A	825	-	-	15/37/115/115	-
27	SF4	C	102	3	-	-	0/6/5/5
22	CLA	3	312	-	1/1/11/20	7/13/91/115	-
22	CLA	7	314	-	1/1/11/20	4/13/91/115	-
22	CLA	1	301	13	1/1/15/20	10/37/115/115	-
25	8CT	B	851	22	-	15/29/63/63	0/2/2/2
22	CLA	5	310	24	1/1/10/20	3/8/86/115	-
22	CLA	0	302	30	1/1/15/20	16/37/115/115	-
29	CHL	9	302	19	4/4/19/26	11/33/131/137	-
22	CLA	7	305	-	1/1/11/20	8/13/91/115	-
22	CLA	8	303	22,31	1/1/11/20	3/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	309	30	1/1/14/20	14/31/109/115	-
22	CLA	9	303	19	1/1/15/20	12/37/115/115	-
22	CLA	B	850	-	1/1/13/20	11/25/103/115	-
22	CLA	2	314	14	1/1/11/20	7/18/96/115	-
22	CLA	0	307	22	1/1/15/20	26/37/115/115	-
24	LHG	3	317	22	-	12/23/23/53	-
22	CLA	0	310	30	1/1/12/20	2/22/100/115	-
22	CLA	7	306	22	1/1/10/20	4/10/88/115	-
22	CLA	7	307	22	1/1/11/20	3/16/94/115	-
29	CHL	5	306	-	3/3/16/26	7/18/116/137	-
22	CLA	A	826	25	1/1/15/20	13/37/115/115	-
22	CLA	5	302	-	1/1/15/20	9/37/115/115	-
25	8CT	A	854	-	-	12/29/63/63	0/2/2/2
22	CLA	5	309	13,30	1/1/14/20	8/31/109/115	-
29	CHL	8	314	-	3/3/15/26	3/12/110/137	-
22	CLA	A	821	-	1/1/15/20	9/37/115/115	-
29	CHL	0	306	30,22	3/3/16/26	5/18/116/137	-
22	CLA	2	310	24	1/1/10/20	4/8/86/115	-
22	CLA	A	815	-	1/1/11/20	3/16/94/115	-
22	CLA	B	811	-	1/1/15/20	11/37/115/115	-
22	CLA	7	313	-	1/1/13/20	13/25/103/115	-
22	CLA	B	813	-	1/1/13/20	7/25/103/115	-
22	CLA	B	836	-	1/1/14/20	13/31/109/115	-
22	CLA	2	308	-	1/1/12/20	5/19/97/115	-
30	XAT	6	319	22	-	3/31/93/93	0/4/4/4
22	CLA	5	313	-	1/1/13/20	7/25/103/115	-
25	8CT	B	844	-	-	15/29/63/63	0/2/2/2
30	XAT	8	316	29	-	7/31/93/93	0/4/4/4
22	CLA	7	315	-	1/1/11/20	4/15/93/115	-
22	CLA	6	323	16	1/1/11/20	11/15/93/115	-
22	CLA	B	829	-	1/1/15/20	11/37/115/115	-
22	CLA	A	803	-	1/1/15/20	17/37/115/115	-
22	CLA	B	821	-	1/1/12/20	8/19/97/115	-
29	CHL	8	305	-	4/4/18/26	9/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	2	318	22	-	19/36/36/53	-
22	CLA	B	805	-	1/1/15/20	16/37/115/115	-
29	CHL	2	307	-	3/3/17/26	9/21/119/137	-
22	CLA	A	819	-	1/1/15/20	14/37/115/115	-
22	CLA	A	810	-	1/1/15/20	11/37/115/115	-
22	CLA	B	835	-	1/1/11/20	3/13/91/115	-
25	8CT	8	301	-	-	13/29/63/63	0/2/2/2
22	CLA	3	319	-	1/1/15/20	21/37/115/115	-
22	CLA	6	315	-	1/1/15/20	14/37/115/115	-
22	CLA	A	812	-	1/1/12/20	1/24/102/115	-
29	CHL	6	306	-	3/3/15/26	2/12/110/137	-
22	CLA	B	818	-	1/1/13/20	12/30/108/115	-
31	LMG	8	319	22	-	17/39/59/70	0/1/1/1
22	CLA	A	806	-	1/1/15/20	20/37/115/115	-
22	CLA	1	307	-	1/1/15/20	16/37/115/115	-
22	CLA	B	838	-	1/1/11/20	4/16/94/115	-
22	CLA	A	824	-	1/1/13/20	8/25/103/115	-
22	CLA	A	811	22	1/1/15/20	18/37/115/115	-
29	CHL	4	305	29	4/4/18/26	12/27/125/137	-
22	CLA	2	302	29	1/1/15/20	17/37/115/115	-
22	CLA	B	812	2	1/1/15/20	13/37/115/115	-
22	CLA	M	101	-	-	8/15/93/115	-
30	XAT	8	317	-	-	0/31/93/93	0/4/4/4
22	CLA	3	305	15	1/1/11/20	8/16/94/115	-
25	8CT	J	101	-	-	9/29/63/63	0/2/2/2
22	CLA	B	819	-	1/1/14/20	19/31/109/115	-
22	CLA	5	312	30	1/1/15/20	12/37/115/115	-
22	CLA	L	201	-	1/1/15/20	17/37/115/115	-
22	CLA	7	311	24	1/1/8/20	0/2/76/115	-
22	CLA	A	805	-	1/1/15/20	14/37/115/115	-
22	CLA	7	309	22	1/1/12/20	4/19/97/115	-
22	CLA	B	810	-	1/1/15/20	6/37/115/115	-
22	CLA	4	304	-	1/1/12/20	4/19/97/115	-
22	CLA	6	314	-	1/1/10/20	6/11/89/115	-
22	CLA	B	832	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	809	1	1/1/15/20	13/37/115/115	-
22	CLA	2	303	-	1/1/15/20	11/37/115/115	-
22	CLA	K	105	-	1/1/12/20	9/19/97/115	-
22	CLA	A	823	-	1/1/12/20	6/21/99/115	-
22	CLA	0	304	22	1/1/12/20	11/22/100/115	-
22	CLA	4	313	-	1/1/11/20	6/13/91/115	-
29	CHL	4	306	29	3/3/17/26	7/21/119/137	-
22	CLA	A	834	-	1/1/12/20	1/19/97/115	-
22	CLA	7	303	18	1/1/14/20	17/31/109/115	-
22	CLA	3	302	25	1/1/12/20	2/19/97/115	-
22	CLA	B	827	-	1/1/15/20	18/37/115/115	-
23	PQN	B	842	-	-	5/23/43/43	0/2/2/2
22	CLA	A	817	-	1/1/15/20	19/37/115/115	-
22	CLA	B	830	-	1/1/15/20	9/37/115/115	-
22	CLA	A	814	-	1/1/11/20	10/13/91/115	-
22	CLA	B	820	-	1/1/15/20	9/37/115/115	-
27	SF4	C	101	-	-	-	0/6/5/5
29	CHL	6	308	-	3/3/17/26	6/21/119/137	-
30	XAT	3	314	25	-	4/31/93/93	0/4/4/4
22	CLA	2	311	14	1/1/12/20	7/22/100/115	-
22	CLA	3	304	-	1/1/10/20	3/10/88/115	-
22	CLA	5	304	-	1/1/12/20	8/22/100/115	-
25	8CT	B	847	-	-	10/29/63/63	0/2/2/2
29	CHL	9	307	-	3/3/16/26	10/18/116/137	-
30	XAT	1	315	-	-	1/31/93/93	0/4/4/4
30	XAT	0	314	29,22	-	8/31/93/93	0/4/4/4
22	CLA	8	309	-	1/1/14/20	8/31/109/115	-
22	CLA	B	839	25	1/1/15/20	13/37/115/115	-
31	LMG	5	319	22	-	18/39/59/70	0/1/1/1
22	CLA	6	309	17	1/1/12/20	10/19/97/115	-
24	LHG	9	316	22	-	22/53/53/53	-
22	CLA	6	311	24	1/1/15/20	20/37/115/115	-
22	CLA	0	309	24	1/1/10/20	2/8/86/115	-
25	8CT	2	317	-	-	10/29/63/63	0/2/2/2
22	CLA	A	841	25	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	311	-	1/1/15/20	15/37/115/115	-
22	CLA	6	305	-	1/1/14/20	13/31/109/115	-
22	CLA	L	202	-	1/1/15/20	15/37/115/115	-
29	CHL	4	301	13,22	4/4/19/26	11/33/131/137	-
22	CLA	3	307	15	1/1/12/20	8/19/97/115	-
22	CLA	6	317	-	1/1/11/20	5/13/91/115	-
22	CLA	5	311	30	1/1/11/20	1/13/91/115	-
22	CLA	3	310	-	1/1/12/20	2/22/100/115	-
22	CLA	6	301	-	1/1/12/20	11/22/100/115	-
22	CLA	L	204	-	1/1/12/20	9/19/97/115	-
22	CLA	L	203	-	1/1/15/20	14/37/115/115	-
25	8CT	6	321	-	-	9/29/63/63	0/2/2/2
25	8CT	7	321	-	-	10/29/63/63	0/2/2/2
30	XAT	4	315	22	-	8/31/93/93	0/4/4/4
31	LMG	4	318	-	-	19/39/59/70	0/1/1/1
25	8CT	3	318	25,22	-	6/29/63/63	0/2/2/2
30	XAT	2	316	-	-	3/31/93/93	0/4/4/4
22	CLA	A	820	-	1/1/11/20	4/13/91/115	-
25	8CT	B	848	-	-	10/29/63/63	0/2/2/2
22	CLA	4	302	-	1/1/14/20	8/31/109/115	-
22	CLA	7	317	-	1/1/15/20	19/37/115/115	-
24	LHG	B	852	22	-	10/26/26/53	-
22	CLA	6	318	17	1/1/12/20	6/22/100/115	-
22	CLA	B	807	-	1/1/11/20	5/13/91/115	-
22	CLA	7	312	30	1/1/12/20	3/22/100/115	-
25	8CT	B	804	-	-	15/29/63/63	0/2/2/2
29	CHL	1	305	-	3/3/16/26	7/18/116/137	-
25	8CT	I	101	-	-	10/29/63/63	0/2/2/2
24	LHG	0	315	29,22	-	27/53/53/53	-
22	CLA	7	316	18	1/1/15/20	18/37/115/115	-
29	CHL	3	306	25	3/3/16/26	3/17/115/137	-
22	CLA	A	840	-	1/1/15/20	14/37/115/115	-
22	CLA	3	309	24	1/1/8/20	0/2/76/115	-
22	CLA	8	308	16	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	813	-	1/1/15/20	16/37/115/115	-
22	CLA	B	815	-	1/1/15/20	11/37/115/115	-
22	CLA	1	304	-	1/1/12/20	6/22/100/115	-
26	HTG	A	851	-	-	4/10/30/30	0/1/1/1
22	CLA	A	802	-	1/1/15/20	8/37/115/115	-
22	CLA	9	305	-	1/1/12/20	7/22/100/115	-
25	8CT	L	205	22	-	13/29/63/63	0/2/2/2
22	CLA	A	807	-	1/1/15/20	14/37/115/115	-
22	CLA	B	831	-	1/1/12/20	8/19/97/115	-
22	CLA	B	801	-	1/1/15/20	10/37/115/115	-
24	LHG	5	318	22	-	29/53/53/53	-
25	8CT	8	318	-	-	13/29/63/63	0/2/2/2
22	CLA	K	102	-	1/1/11/20	9/15/93/115	-
22	CLA	A	822	-	1/1/11/20	10/18/96/115	-
22	CLA	G	101	-	1/1/11/20	5/13/91/115	-
22	CLA	A	831	-	1/1/12/20	1/19/97/115	-
22	CLA	7	318	22	1/1/15/20	18/37/115/115	-
29	CHL	2	305	-	3/3/15/26	3/12/110/137	-
29	CHL	4	307	-	3/3/17/26	5/21/119/137	-
22	CLA	8	310	31	1/1/13/20	8/25/103/115	-
25	8CT	L	206	-	-	15/29/63/63	0/2/2/2
22	CLA	8	315	-	1/1/15/20	25/37/115/115	-
22	CLA	1	303	-	1/1/12/20	8/22/100/115	-
22	CLA	9	310	24	1/1/10/20	4/8/86/115	-
25	8CT	7	301	29,30	-	11/29/63/63	0/2/2/2
22	CLA	A	832	-	1/1/15/20	16/37/115/115	-
22	CLA	B	837	-	1/1/15/20	17/37/115/115	-
24	LHG	7	322	22	-	16/23/23/53	-
22	CLA	4	308	16	1/1/12/20	1/19/97/115	-
30	XAT	5	315	22	-	6/31/93/93	0/4/4/4
22	CLA	B	833	-	1/1/13/20	13/29/107/115	-
22	CLA	J	103	10	1/1/10/20	8/10/88/115	-
30	XAT	3	315	-	-	0/31/93/93	0/4/4/4
29	CHL	8	306	-	3/3/17/26	9/21/119/137	-
22	CLA	G	102	-	1/1/12/20	5/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	313	-	1/1/10/20	2/11/89/115	-
22	CLA	H	201	-	1/1/15/20	16/37/115/115	-
29	CHL	2	306	-	3/3/16/26	8/18/116/137	-
22	CLA	1	309	24	1/1/10/20	2/8/86/115	-
22	CLA	0	303	30	1/1/15/20	14/37/115/115	-
22	CLA	A	836	-	1/1/12/20	11/21/99/115	-
25	8CT	A	849	22	-	11/29/63/63	0/2/2/2
22	CLA	B	808	-	1/1/15/20	16/37/115/115	-
22	CLA	B	841	24	1/1/15/20	13/37/115/115	-
24	LHG	6	322	22	-	22/41/41/53	-
29	CHL	7	308	-	3/3/16/26	8/17/115/137	-
22	CLA	2	319	16	1/1/11/20	9/15/93/115	-
22	CLA	B	825	-	1/1/15/20	17/37/115/115	-
22	CLA	8	304	-	1/1/12/20	10/19/97/115	-
22	CLA	B	816	-	1/1/14/20	13/31/109/115	-
22	CLA	B	824	-	1/1/14/20	13/31/109/115	-
30	XAT	9	314	22	-	4/31/93/93	0/4/4/4
22	CLA	A	843	24	1/1/12/20	11/22/100/115	-
22	CLA	8	302	-	1/1/14/20	7/31/109/115	-
22	CLA	8	313	-	1/1/11/20	3/13/91/115	-
30	XAT	1	314	22	-	11/31/93/93	0/4/4/4
22	CLA	A	837	-	1/1/15/20	19/37/115/115	-
22	CLA	A	835	1	1/1/11/20	5/13/91/115	-
22	CLA	9	313	-	1/1/13/20	13/25/103/115	-
22	CLA	0	312	29	1/1/13/20	10/25/103/115	-
22	CLA	B	834	2	1/1/15/20	16/37/115/115	-
22	CLA	6	303	17	1/1/15/20	16/37/115/115	-
22	CLA	A	839	-	1/1/15/20	17/37/115/115	-
29	CHL	6	302	17,22	4/4/19/26	14/33/131/137	-
22	CLA	A	830	-	1/1/15/20	11/37/115/115	-
22	CLA	9	301	-	1/1/11/20	6/16/92/115	-
22	CLA	3	311	-	1/1/13/20	11/25/103/115	-
24	LHG	A	844	-	-	25/53/53/53	-
22	CLA	A	852	-	1/1/11/20	7/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	314	-	1/1/15/20	18/37/115/115	-
29	CHL	2	301	22	4/4/19/26	13/33/131/137	-
30	XAT	9	315	-	-	0/31/93/93	0/4/4/4
30	XAT	4	316	-	-	3/31/93/93	0/4/4/4
30	XAT	6	320	-	-	4/31/93/93	0/4/4/4
22	CLA	B	828	-	1/1/15/20	16/37/115/115	-
25	8CT	A	850	-	-	11/29/63/63	0/2/2/2
25	8CT	7	323	-	-	14/29/63/63	0/2/2/2
25	8CT	K	103	-	-	12/29/63/63	0/2/2/2
22	CLA	5	314	24	1/1/11/20	9/15/93/115	-
22	CLA	B	803	-	1/1/15/20	19/37/115/115	-
22	CLA	2	309	-	1/1/14/20	10/31/109/115	-
22	CLA	B	809	-	1/1/15/20	20/37/115/115	-
25	8CT	B	843	-	-	16/29/63/63	0/2/2/2
28	DGD	B	849	-	-	31/55/95/95	0/2/2/2
22	CLA	A	853	-	1/1/15/20	15/37/115/115	-
22	CLA	2	304	-	1/1/14/20	16/31/109/115	-
25	8CT	3	316	-	-	12/29/63/63	0/2/2/2
25	8CT	B	846	-	-	13/29/63/63	0/2/2/2
22	CLA	6	312	-	1/1/12/20	9/22/100/115	-
22	CLA	B	823	-	-	11/25/103/115	-
22	CLA	B	814	-	1/1/15/20	21/37/115/115	-
22	CLA	3	301	-	1/1/14/20	11/31/109/115	-
22	CLA	A	829	-	1/1/15/20	10/37/115/115	-
24	LHG	A	845	22	-	16/31/31/53	-
30	XAT	2	315	-	-	2/31/93/93	0/4/4/4
30	XAT	0	313	22	-	16/31/93/93	0/4/4/4
22	CLA	0	308	20	1/1/14/20	16/31/109/115	-
25	8CT	A	848	-	-	6/29/63/63	0/2/2/2
26	HTG	J	102	-	-	3/10/30/30	0/1/1/1
30	XAT	7	320	-	-	0/31/93/93	0/4/4/4
22	CLA	A	801	-	1/1/15/20	8/37/115/115	-
22	CLA	8	312	16	1/1/13/20	5/27/105/115	-
22	CLA	8	311	-	-	5/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	0	305	29,22	1/1/12/20	8/22/100/115	-
22	CLA	2	312	14	1/1/15/20	15/37/115/115	-
22	CLA	4	311	22	1/1/12/20	8/22/100/115	-
22	CLA	A	827	-	1/1/15/20	15/37/115/115	-
22	CLA	9	311	-	1/1/12/20	4/22/100/115	-
25	8CT	F	302	-	-	9/29/63/63	0/2/2/2
22	CLA	A	838	-	1/1/15/20	16/37/115/115	-
22	CLA	0	311	-	1/1/15/20	14/37/115/115	-
22	CLA	B	822	-	1/1/11/20	6/15/93/115	-
22	CLA	K	101	-	1/1/11/20	7/13/91/115	-
22	CLA	6	310	17,30	1/1/14/20	10/31/109/115	-
22	CLA	A	808	1	1/1/15/20	20/37/115/115	-
29	CHL	0	301	22,24	4/4/19/26	17/33/131/137	-
22	CLA	B	840	-	1/1/15/20	14/37/115/115	-
22	CLA	9	304	-	1/1/11/20	8/17/95/115	-
22	CLA	4	312	-	1/1/13/20	6/27/105/115	-
30	XAT	5	316	-	-	2/31/93/93	0/4/4/4
22	CLA	B	806	-	1/1/15/20	17/37/115/115	-
30	XAT	7	319	22	-	7/31/93/93	0/4/4/4
22	CLA	B	826	-	1/1/15/20	13/37/115/115	-
22	CLA	5	303	-	-	23/37/115/115	-
22	CLA	5	305	25	1/1/12/20	6/22/100/115	-
22	CLA	F	301	-	1/1/11/20	8/13/91/115	-
25	8CT	4	317	-	-	8/29/63/63	0/2/2/2
22	CLA	A	833	25	1/1/15/20	14/37/115/115	-
22	CLA	5	307	-	1/1/15/20	16/37/115/115	-
25	8CT	J	104	-	-	7/29/63/63	0/2/2/2
29	CHL	5	301	13	4/4/19/26	14/33/131/137	-
22	CLA	3	308	-	1/1/12/20	3/19/97/115	-
22	CLA	4	310	-	1/1/13/20	7/25/103/115	-
24	LHG	1	317	22	-	25/53/53/53	-
25	8CT	1	316	13	-	11/29/63/63	0/2/2/2
29	CHL	8	307	30	3/3/17/26	7/21/119/137	-
29	CHL	6	307	-	3/3/15/26	6/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	9	309	-	1/1/14/20	15/31/109/115	-
22	CLA	1	313	-	1/1/11/20	7/15/93/115	-
22	CLA	7	310	18	1/1/12/20	7/19/97/115	-
25	8CT	G	104	-	-	13/29/63/63	0/2/2/2
22	CLA	1	302	-	1/1/15/20	21/37/115/115	-
22	CLA	3	313	-	1/1/11/20	7/15/93/115	-
22	CLA	3	303	-	1/1/11/20	5/13/91/115	-
22	CLA	9	306	-	1/1/12/20	8/22/100/115	-
22	CLA	G	103	7	1/1/11/20	9/15/93/115	-
22	CLA	6	313	29	1/1/15/20	10/37/115/115	-
29	CHL	6	316	17	3/3/15/26	8/12/110/137	-
25	8CT	A	846	25	-	13/29/63/63	0/2/2/2
25	8CT	B	845	-	-	12/29/63/63	0/2/2/2
22	CLA	1	312	29	1/1/13/20	10/25/103/115	-
22	CLA	1	306	-	1/1/15/20	12/37/115/115	-
23	PQN	A	842	-	-	7/23/43/43	0/2/2/2
22	CLA	K	104	-	1/1/11/20	5/15/93/115	-
22	CLA	7	304	22	1/1/11/20	6/16/94/115	-
22	CLA	A	816	-	1/1/11/20	4/13/91/115	-
22	CLA	1	308	13,30	1/1/14/20	11/31/109/115	-
25	8CT	A	847	-	-	9/29/63/63	0/2/2/2

The worst 5 of 3250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	318	8CT	C02-C03	14.68	1.59	1.34
25	5	317	8CT	C02-C03	14.38	1.59	1.34
25	K	103	8CT	C32-C31	14.37	1.61	1.32
25	7	301	8CT	C02-C03	14.33	1.59	1.34
25	1	316	8CT	C02-C03	14.33	1.59	1.34

The worst 5 of 3454 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	315	XAT	O4-C5-C4	-26.68	93.34	113.38
30	0	313	XAT	O24-C25-C24	-23.72	95.57	113.38
30	5	315	XAT	O24-C25-C38	-20.89	90.03	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	5	315	XAT	O24-C25-C24	-18.04	99.83	113.38
30	2	315	XAT	O4-C5-C18	-18.03	93.46	115.06

5 of 299 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	A	801	CLA	ND
22	A	802	CLA	ND
22	A	803	CLA	ND
22	A	804	CLA	ND
22	A	805	CLA	ND

5 of 3256 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	803	CLA	CAD-CBD-CGD-O1D
22	A	803	CLA	CAD-CBD-CGD-O2D
22	A	804	CLA	CHA-CBD-CGD-O1D
22	A	804	CLA	CHA-CBD-CGD-O2D
22	A	805	CLA	C14-C13-C15-C16

There are no ring outliers.

302 monomers are involved in 1491 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	304	CLA	5	0
22	A	818	CLA	4	0
25	5	317	8CT	6	0
22	9	312	CLA	9	0
22	5	308	CLA	6	0
22	B	817	CLA	6	0
22	A	804	CLA	4	0
22	1	310	CLA	6	0
22	9	308	CLA	5	0
27	B	802	SF4	1	0
22	A	828	CLA	11	0
22	7	302	CLA	1	0
22	4	303	CLA	2	0
22	A	825	CLA	9	0
22	3	312	CLA	2	0
22	7	314	CLA	2	0
22	1	301	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	851	8CT	1	0
22	5	310	CLA	2	0
22	0	302	CLA	15	0
29	9	302	CHL	2	0
22	7	305	CLA	3	0
22	8	303	CLA	1	0
22	4	309	CLA	8	0
22	9	303	CLA	7	0
22	B	850	CLA	17	0
22	2	314	CLA	1	0
22	0	307	CLA	7	0
24	3	317	LHG	4	0
22	0	310	CLA	2	0
22	7	306	CLA	6	0
22	7	307	CLA	13	0
29	5	306	CHL	5	0
22	A	826	CLA	12	0
22	5	302	CLA	8	0
25	A	854	8CT	3	0
22	5	309	CLA	10	0
29	8	314	CHL	11	0
22	A	821	CLA	4	0
29	0	306	CHL	2	0
22	A	815	CLA	3	0
22	B	811	CLA	4	0
22	7	313	CLA	7	0
22	B	813	CLA	10	0
22	B	836	CLA	2	0
22	2	308	CLA	7	0
30	6	319	XAT	7	0
22	5	313	CLA	6	0
30	8	316	XAT	12	0
22	7	315	CLA	2	0
22	6	323	CLA	5	0
22	B	829	CLA	8	0
22	A	803	CLA	5	0
29	8	305	CHL	6	0
24	2	318	LHG	3	0
22	B	805	CLA	7	0
29	2	307	CHL	4	0
22	A	819	CLA	6	0
22	A	810	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	835	CLA	1	0
25	8	301	8CT	11	0
22	3	319	CLA	8	0
22	6	315	CLA	5	0
22	A	812	CLA	4	0
29	6	306	CHL	2	0
22	B	818	CLA	6	0
31	8	319	LMG	6	0
22	A	806	CLA	4	0
22	1	307	CLA	6	0
22	B	838	CLA	1	0
22	A	824	CLA	3	0
22	A	811	CLA	5	0
29	4	305	CHL	9	0
22	2	302	CLA	8	0
22	B	812	CLA	4	0
22	M	101	CLA	5	0
30	8	317	XAT	9	0
25	J	101	8CT	10	0
22	B	819	CLA	4	0
22	5	312	CLA	6	0
22	L	201	CLA	5	0
22	A	805	CLA	8	0
22	7	309	CLA	5	0
22	B	810	CLA	8	0
22	4	304	CLA	1	0
22	6	314	CLA	4	0
22	B	832	CLA	8	0
22	A	809	CLA	14	0
22	2	303	CLA	3	0
22	K	105	CLA	14	0
22	A	823	CLA	1	0
22	0	304	CLA	4	0
22	4	313	CLA	5	0
29	4	306	CHL	2	0
22	A	834	CLA	1	0
22	7	303	CLA	10	0
22	3	302	CLA	3	0
22	B	827	CLA	8	0
23	B	842	PQN	3	0
22	A	817	CLA	7	0
22	B	830	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	814	CLA	4	0
22	B	820	CLA	5	0
27	C	101	SF4	1	0
29	6	308	CHL	4	0
30	3	314	XAT	8	0
22	2	311	CLA	1	0
22	3	304	CLA	1	0
22	5	304	CLA	8	0
25	B	847	8CT	13	0
29	9	307	CHL	4	0
30	1	315	XAT	5	0
30	0	314	XAT	11	0
22	8	309	CLA	11	0
22	B	839	CLA	4	0
31	5	319	LMG	5	0
22	6	309	CLA	5	0
24	9	316	LHG	8	0
22	6	311	CLA	5	0
22	0	309	CLA	2	0
25	2	317	8CT	13	0
22	A	841	CLA	6	0
22	1	311	CLA	12	0
22	6	305	CLA	11	0
22	L	202	CLA	12	0
29	4	301	CHL	9	0
22	3	307	CLA	9	0
22	6	317	CLA	6	0
22	5	311	CLA	6	0
22	3	310	CLA	1	0
22	6	301	CLA	4	0
22	L	204	CLA	5	0
22	L	203	CLA	5	0
25	6	321	8CT	14	0
25	7	321	8CT	14	0
30	4	315	XAT	9	0
31	4	318	LMG	1	0
30	2	316	XAT	7	0
22	A	820	CLA	4	0
25	B	848	8CT	12	0
22	4	302	CLA	4	0
22	7	317	CLA	12	0
24	B	852	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	318	CLA	8	0
22	B	807	CLA	5	0
22	7	312	CLA	3	0
29	1	305	CHL	3	0
24	0	315	LHG	12	0
22	7	316	CLA	7	0
29	3	306	CHL	4	0
22	A	840	CLA	7	0
22	3	309	CLA	1	0
22	8	308	CLA	9	0
22	A	813	CLA	14	0
22	B	815	CLA	6	0
22	1	304	CLA	15	0
22	A	802	CLA	4	0
22	A	807	CLA	4	0
22	B	831	CLA	2	0
22	B	801	CLA	4	0
24	5	318	LHG	8	0
25	8	318	8CT	2	0
22	K	102	CLA	6	0
22	A	822	CLA	4	0
22	G	101	CLA	1	0
22	A	831	CLA	3	0
22	7	318	CLA	4	0
29	2	305	CHL	8	0
22	8	310	CLA	9	0
29	4	307	CHL	11	0
22	8	315	CLA	3	0
22	1	303	CLA	11	0
22	9	310	CLA	2	0
22	A	832	CLA	5	0
22	B	837	CLA	6	0
24	7	322	LHG	2	0
22	4	308	CLA	4	0
30	5	315	XAT	8	0
22	B	833	CLA	10	0
22	J	103	CLA	1	0
30	3	315	XAT	9	0
29	8	306	CHL	4	0
22	G	102	CLA	8	0
22	2	313	CLA	1	0
22	H	201	CLA	18	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	2	306	CHL	2	0
22	1	309	CLA	3	0
22	0	303	CLA	4	0
22	A	836	CLA	4	0
25	A	849	8CT	8	0
22	B	808	CLA	10	0
22	B	841	CLA	7	0
24	6	322	LHG	4	0
29	7	308	CHL	11	0
22	2	319	CLA	1	0
22	B	825	CLA	4	0
22	8	304	CLA	2	0
22	B	816	CLA	5	0
22	B	824	CLA	8	0
30	9	314	XAT	5	0
22	A	843	CLA	2	0
22	8	302	CLA	4	0
22	8	313	CLA	4	0
30	1	314	XAT	10	0
22	A	837	CLA	6	0
22	A	835	CLA	2	0
22	9	313	CLA	3	0
22	0	312	CLA	6	0
22	B	834	CLA	5	0
22	6	303	CLA	6	0
22	A	839	CLA	9	0
29	6	302	CHL	7	0
22	A	830	CLA	3	0
22	9	301	CLA	5	0
22	3	311	CLA	10	0
24	A	844	LHG	3	0
22	A	852	CLA	1	0
22	4	314	CLA	5	0
29	2	301	CHL	3	0
30	9	315	XAT	8	0
30	4	316	XAT	7	0
30	6	320	XAT	7	0
22	B	828	CLA	7	0
25	A	850	8CT	20	0
25	7	323	8CT	22	0
25	K	103	8CT	14	0
22	5	314	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	803	CLA	18	0
22	2	309	CLA	6	0
22	B	809	CLA	8	0
25	B	843	8CT	3	0
28	B	849	DGD	11	0
22	A	853	CLA	5	0
22	2	304	CLA	5	0
25	3	316	8CT	10	0
25	B	846	8CT	11	0
22	6	312	CLA	2	0
22	B	823	CLA	3	0
22	B	814	CLA	9	0
22	3	301	CLA	5	0
22	A	829	CLA	6	0
24	A	845	LHG	2	0
30	2	315	XAT	7	0
30	0	313	XAT	8	0
22	0	308	CLA	4	0
26	J	102	HTG	1	0
30	7	320	XAT	8	0
22	A	801	CLA	7	0
22	8	312	CLA	5	0
22	8	311	CLA	8	0
22	0	305	CLA	4	0
22	2	312	CLA	5	0
22	4	311	CLA	5	0
22	A	827	CLA	9	0
22	9	311	CLA	3	0
22	A	838	CLA	3	0
22	0	311	CLA	7	0
22	K	101	CLA	3	0
22	6	310	CLA	9	0
22	A	808	CLA	10	0
29	0	301	CHL	16	0
22	B	840	CLA	14	0
22	9	304	CLA	6	0
22	4	312	CLA	6	0
30	5	316	XAT	5	0
22	B	806	CLA	10	0
30	7	319	XAT	7	0
22	B	826	CLA	9	0
22	5	303	CLA	11	0

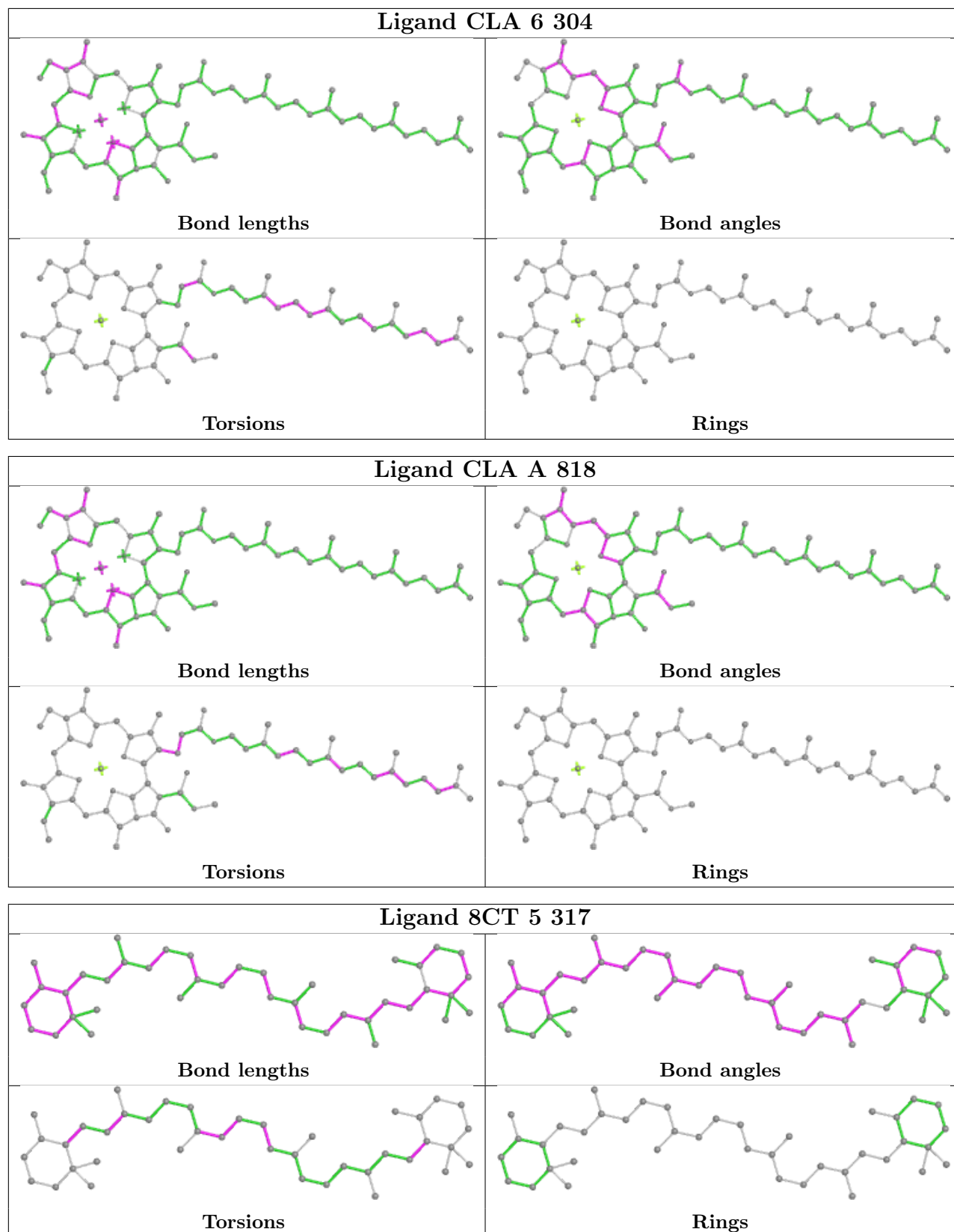
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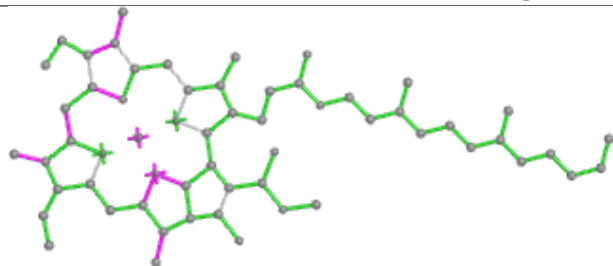
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22	F	301	CLA	5	0
25	4	317	8CT	12	0
22	A	833	CLA	6	0
22	5	307	CLA	3	0
25	J	104	8CT	16	0
29	5	301	CHL	12	0
22	3	308	CLA	6	0
22	4	310	CLA	1	0
24	1	317	LHG	3	0
25	1	316	8CT	13	0
29	8	307	CHL	6	0
29	6	307	CHL	8	0
22	9	309	CLA	8	0
22	1	313	CLA	1	0
22	7	310	CLA	9	0
25	G	104	8CT	20	0
22	1	302	CLA	6	0
22	3	313	CLA	5	0
22	3	303	CLA	2	0
22	9	306	CLA	5	0
22	G	103	CLA	7	0
22	6	313	CLA	5	0
29	6	316	CHL	3	0
25	A	846	8CT	1	0
22	1	312	CLA	8	0
22	1	306	CLA	5	0
23	A	842	PQN	3	0
22	K	104	CLA	6	0
22	7	304	CLA	4	0
22	A	816	CLA	3	0
22	1	308	CLA	6	0
25	A	847	8CT	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

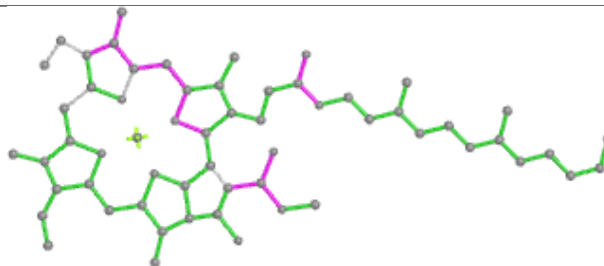
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



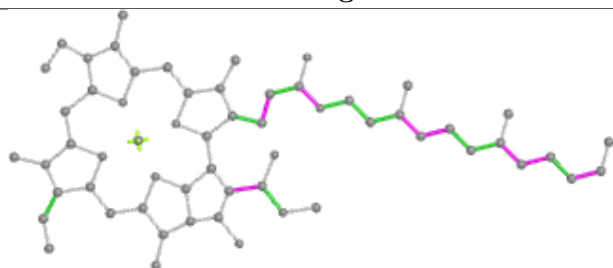
Ligand CLA 9 312



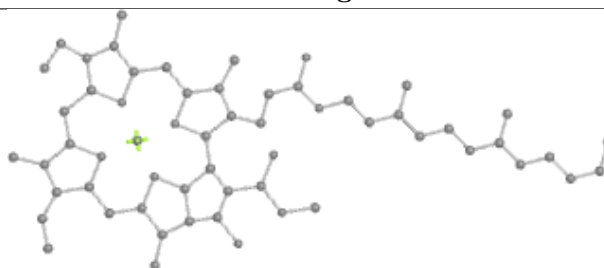
Bond lengths



Bond angles

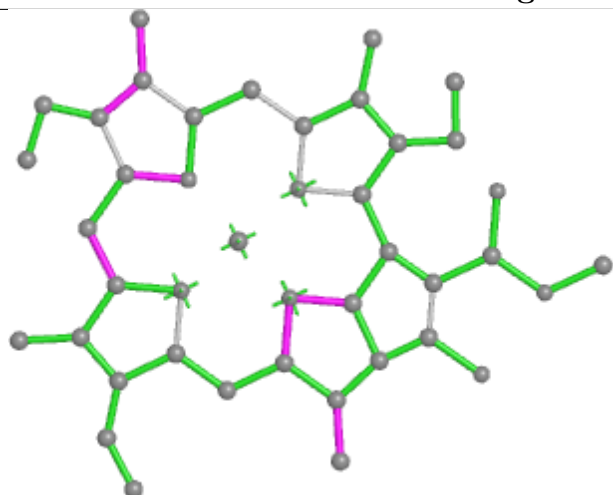


Torsions

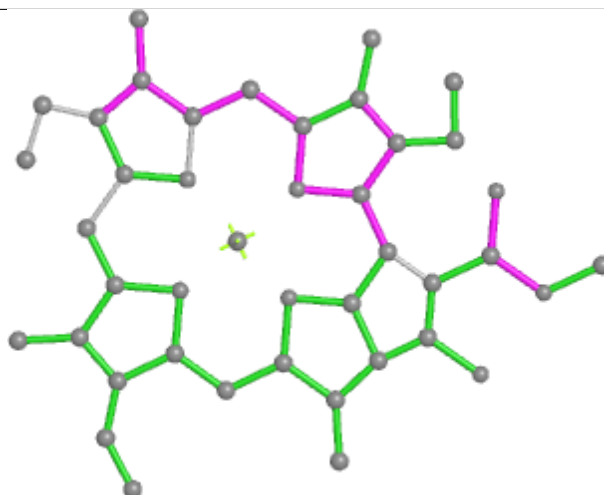


Rings

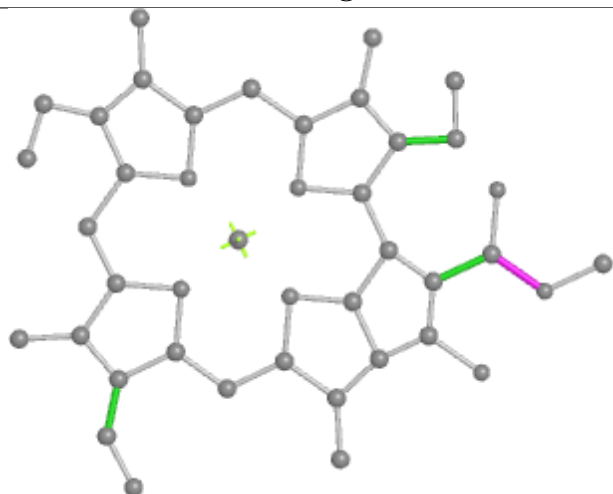
Ligand CLA 5 308



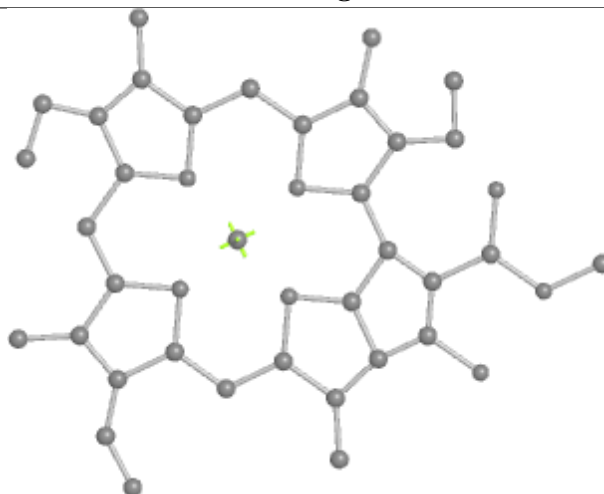
Bond lengths



Bond angles

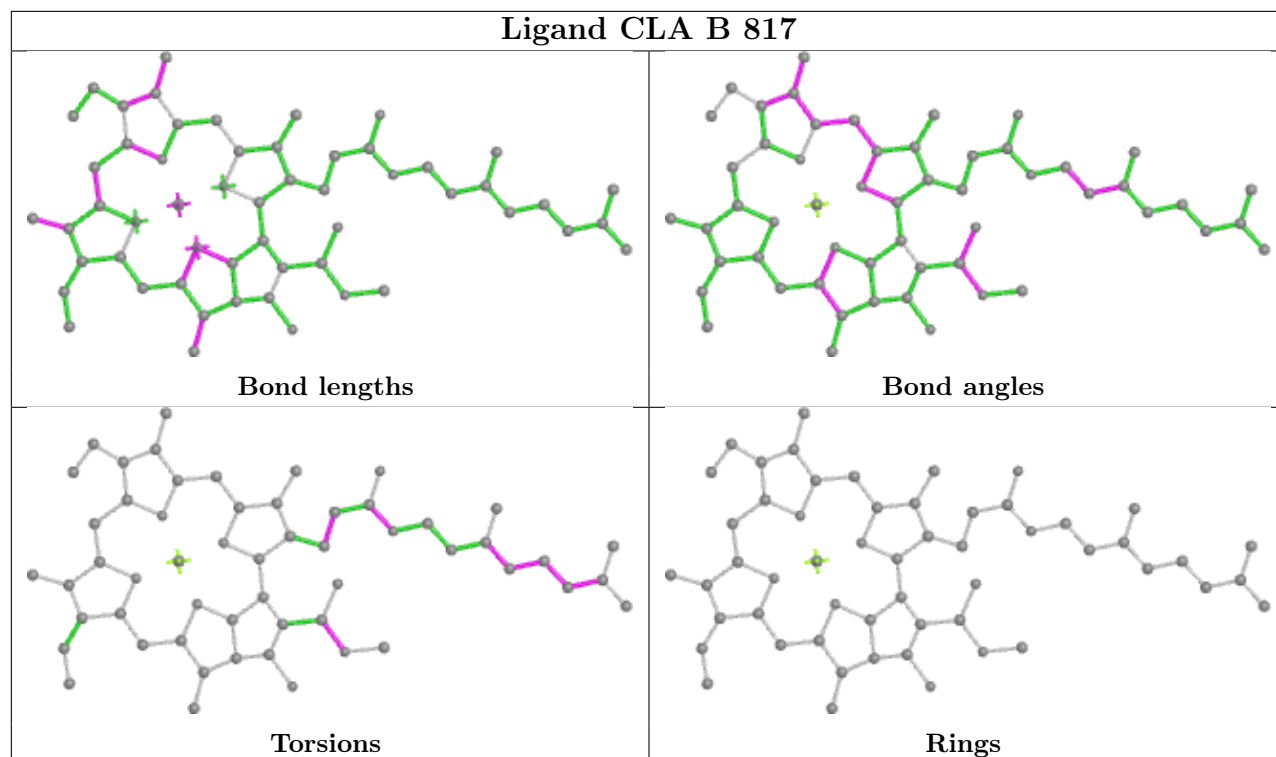


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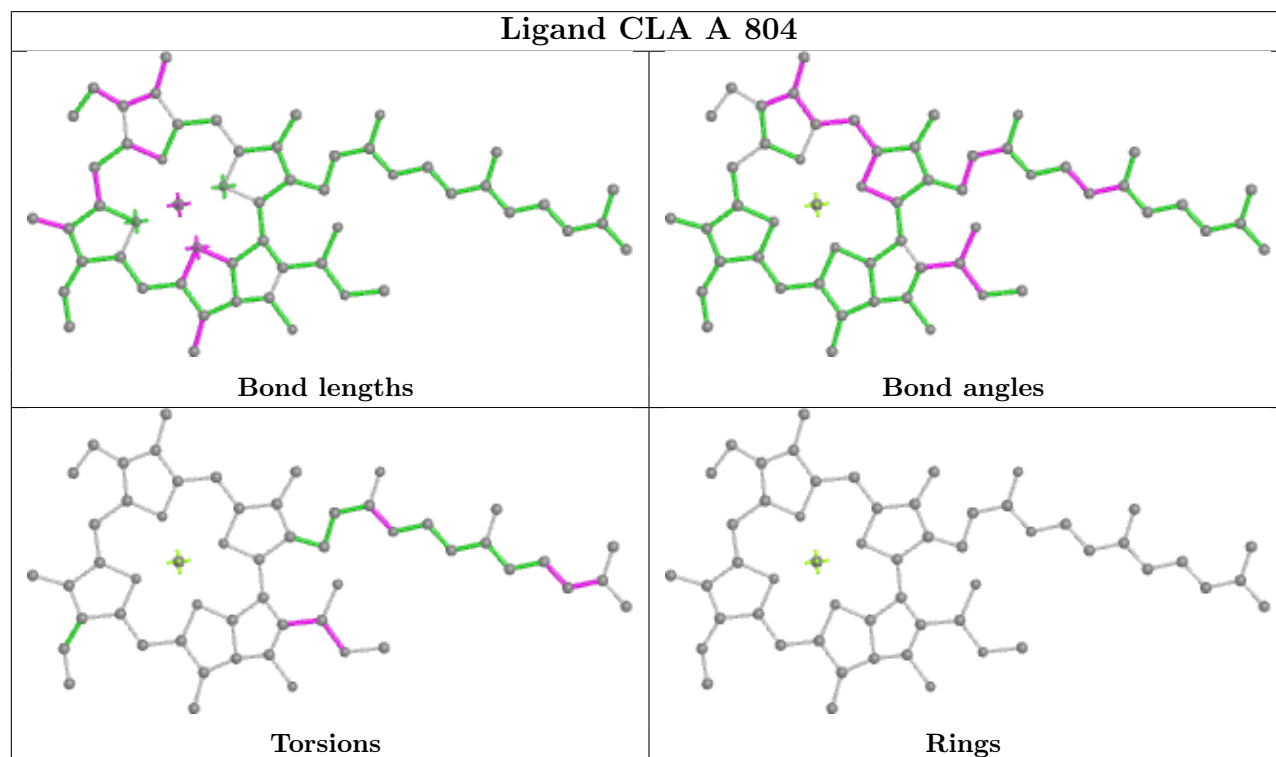


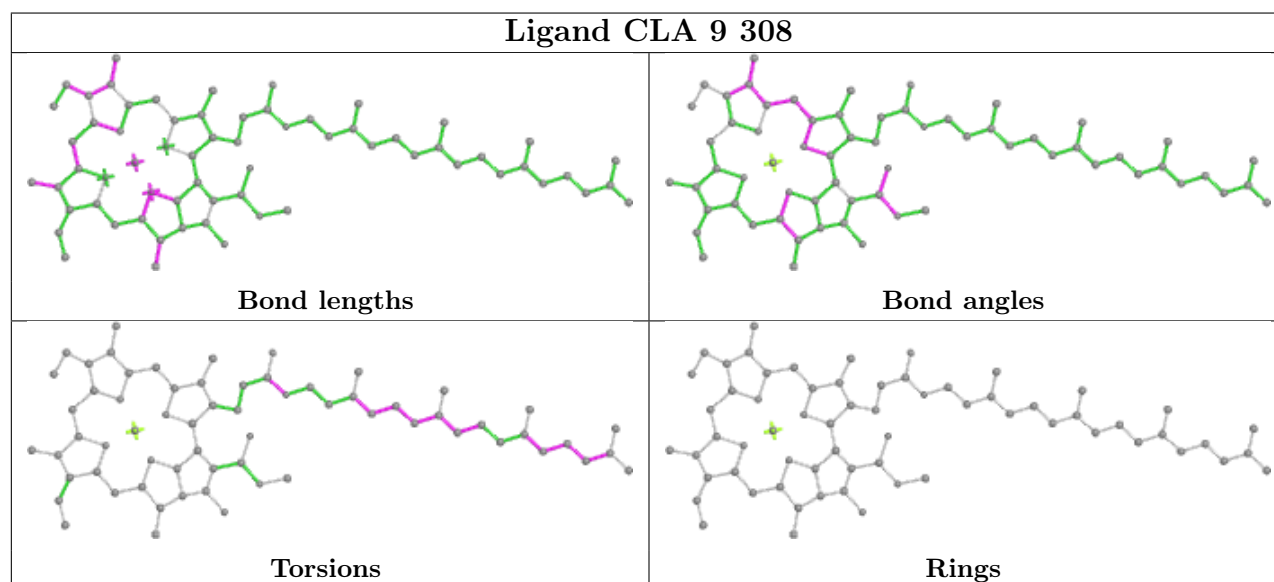
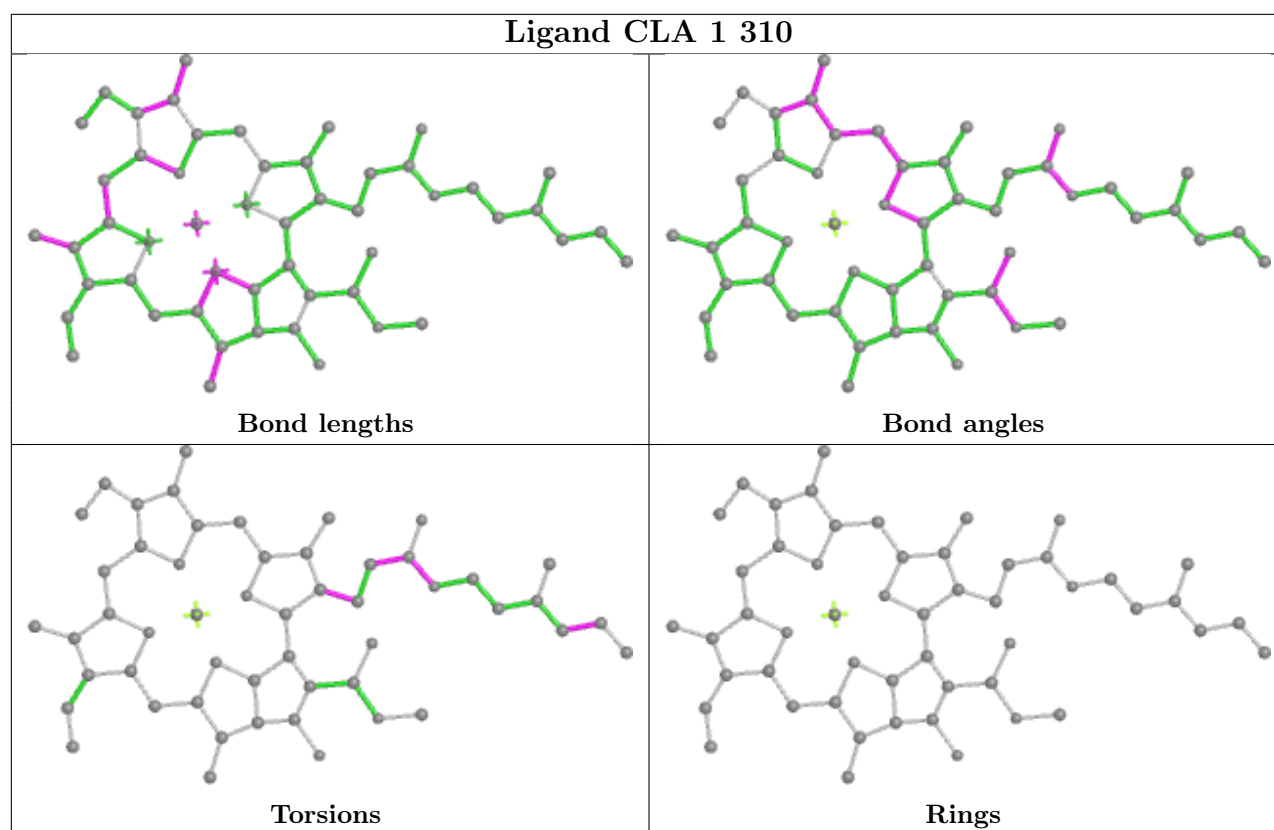
Rings

Ligand CLA B 817

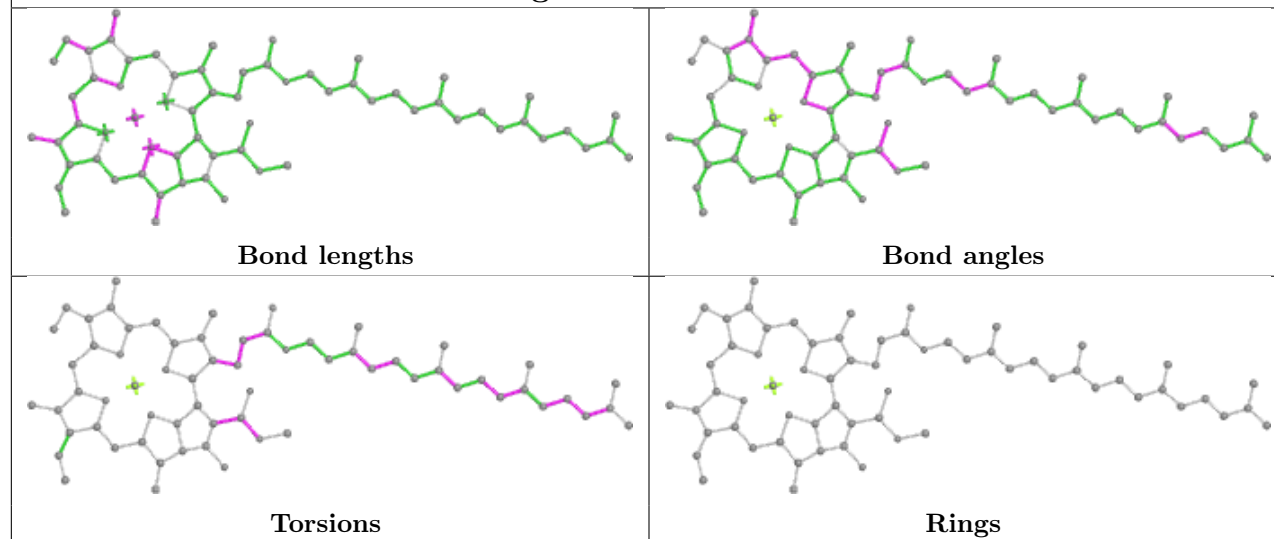


Ligand CLA A 804

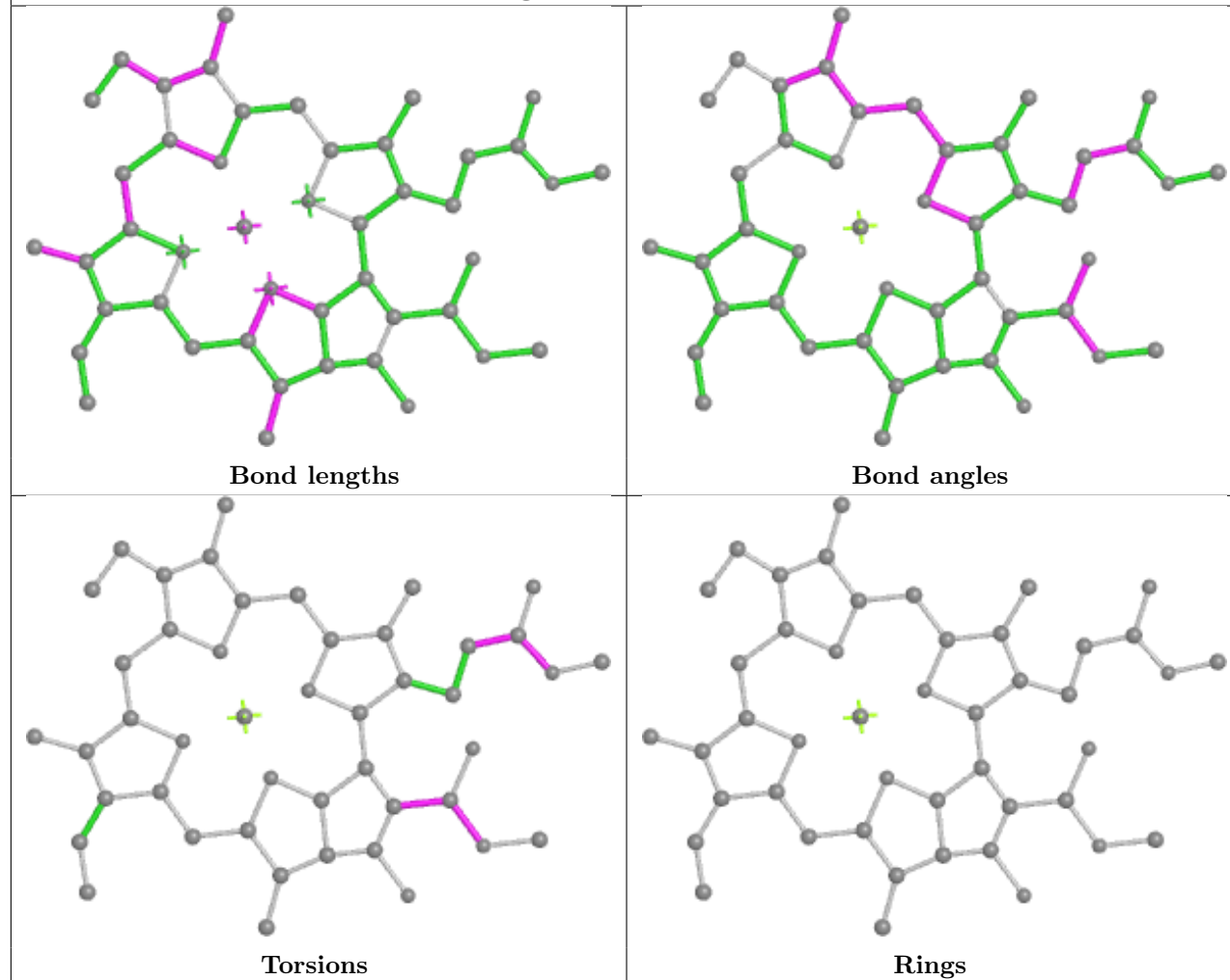




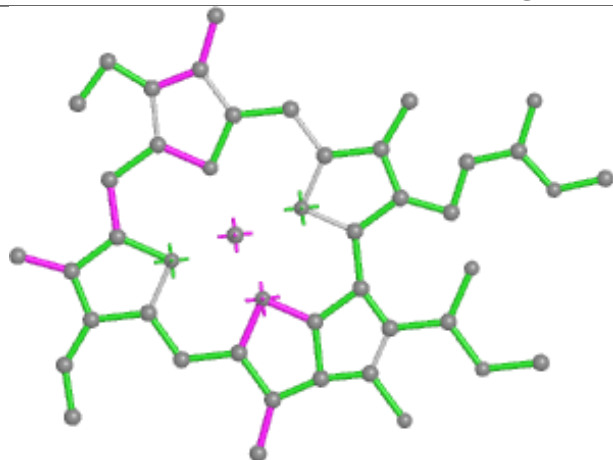
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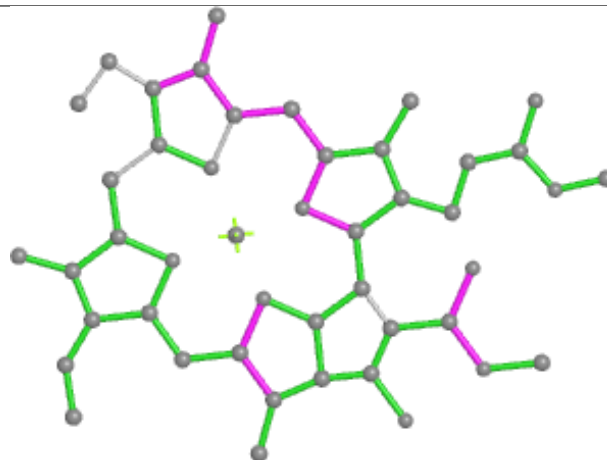
Ligand CLA 7 302



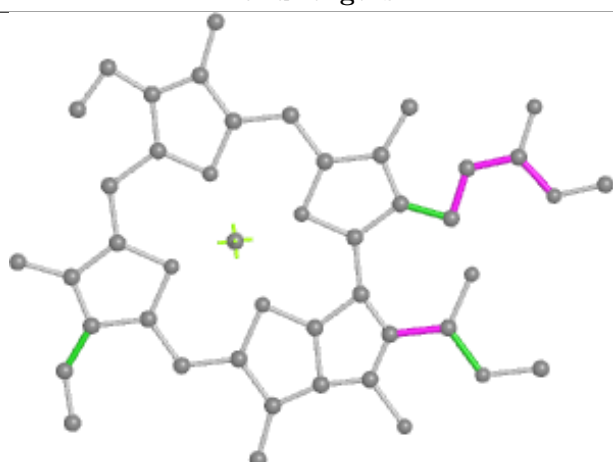
Ligand CLA 4 303



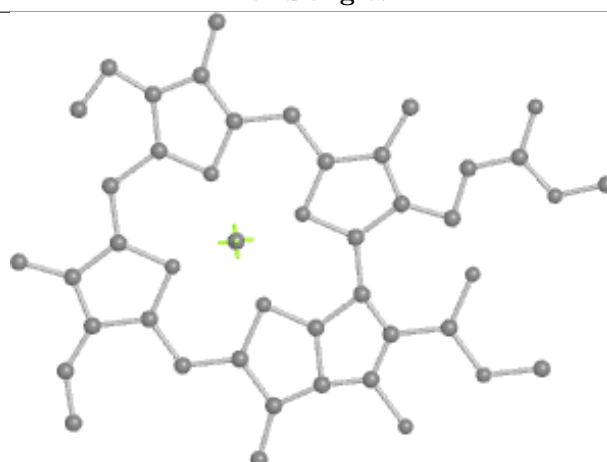
Bond lengths



Bond angles

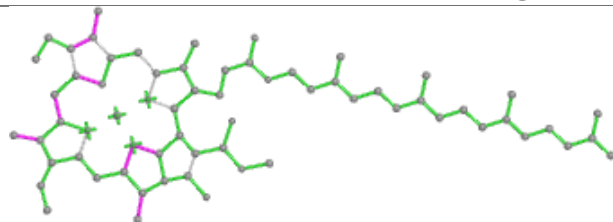


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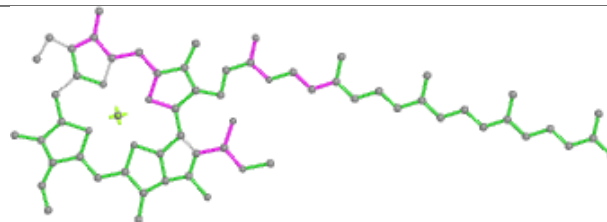


Rings

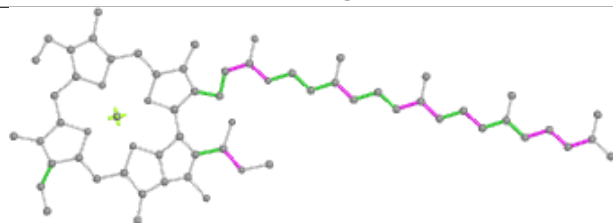
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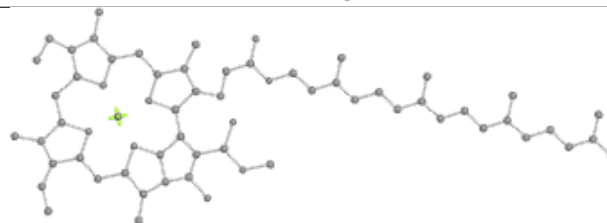
Bond lengths



Bond angles

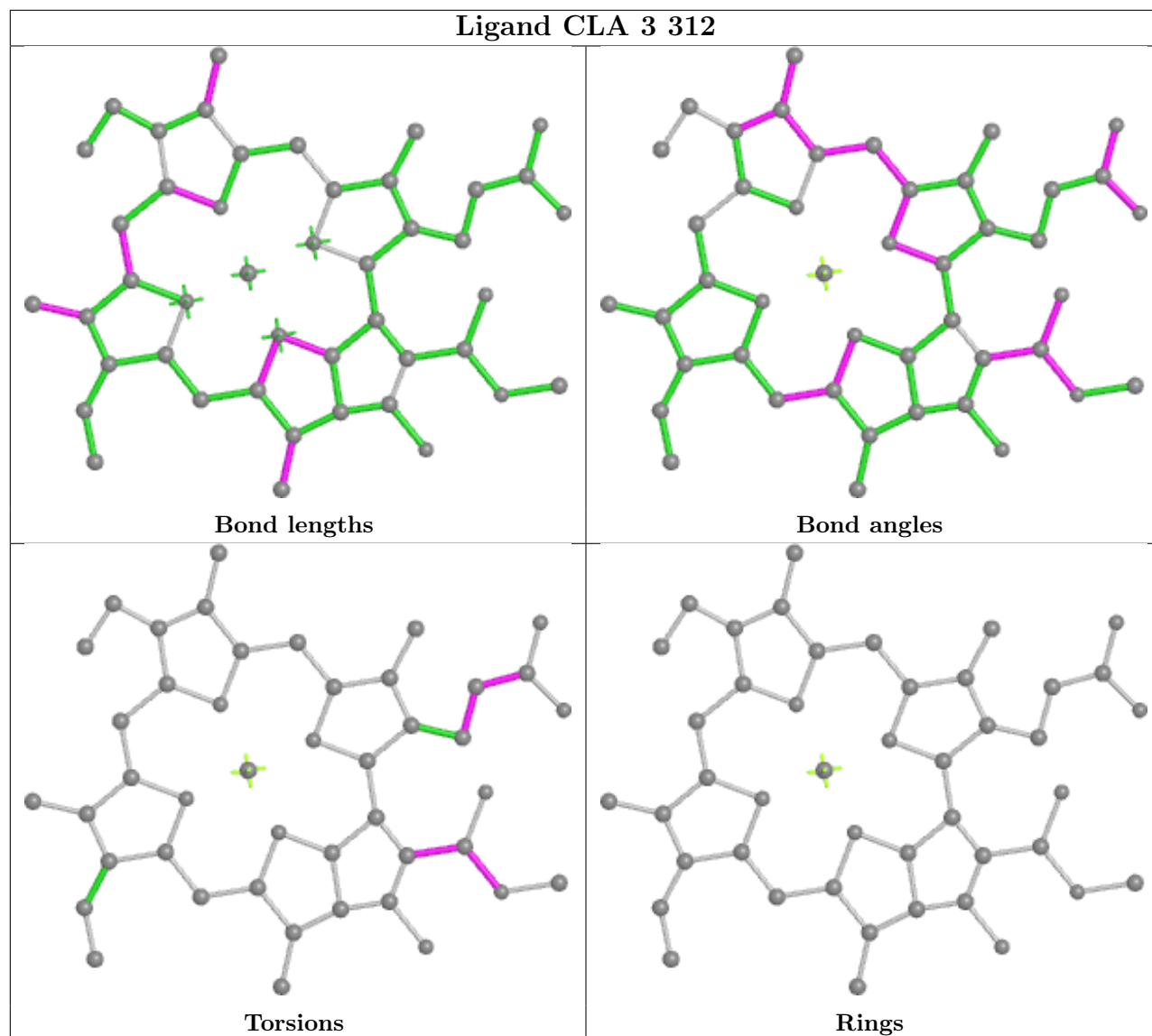


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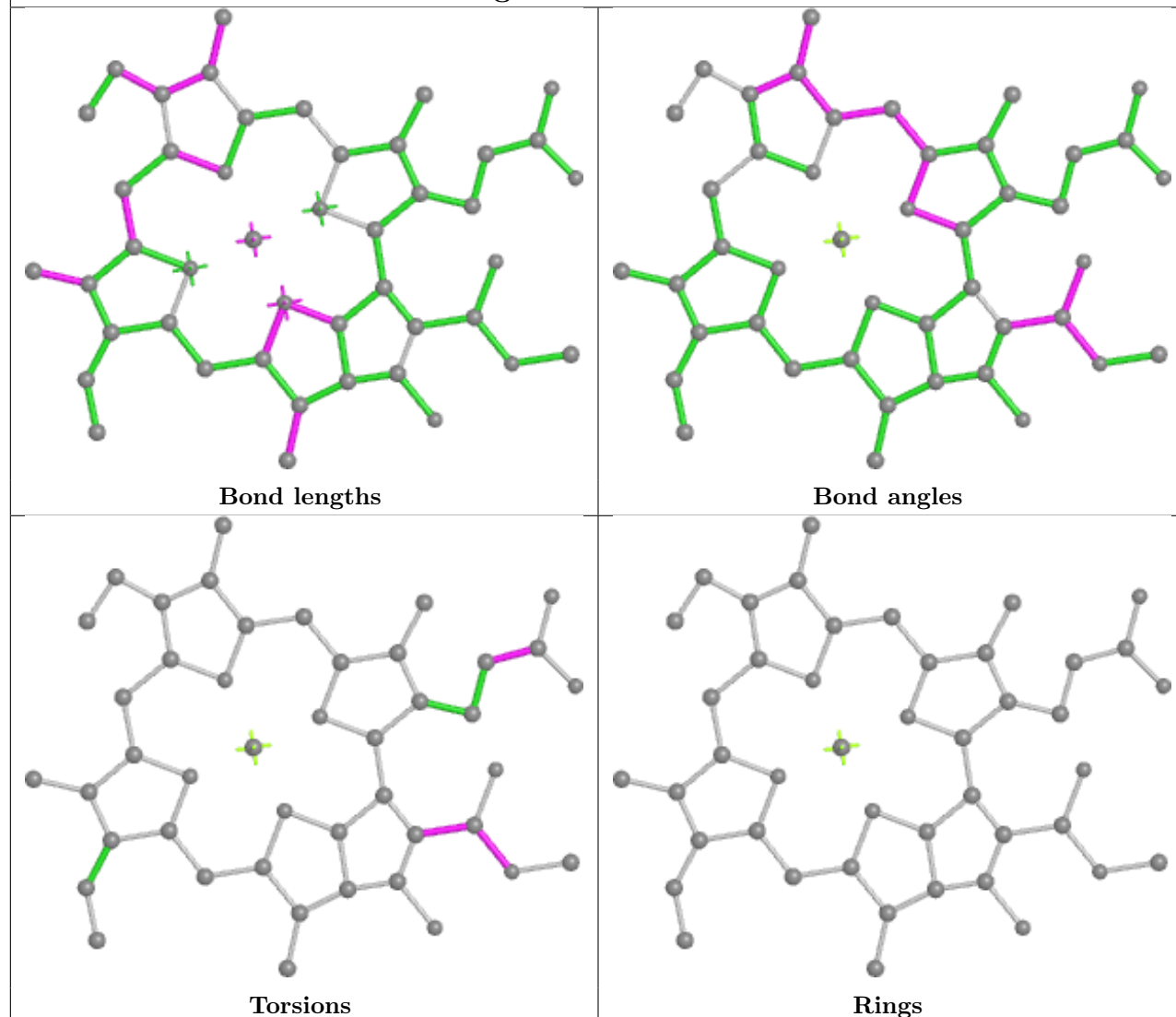


Rings

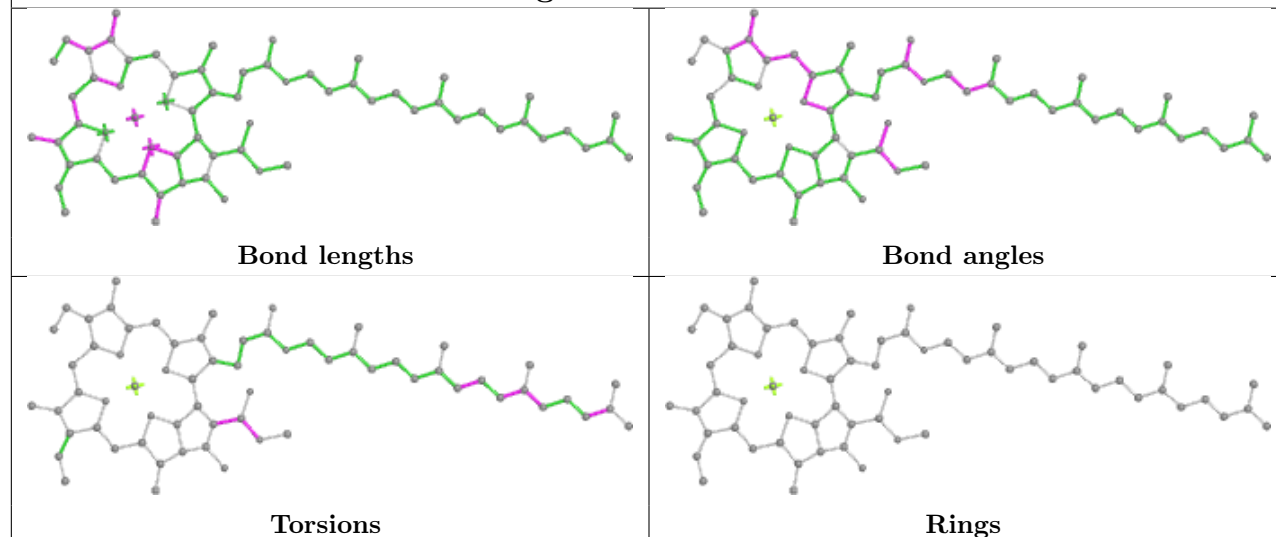
Ligand CLA 3 312



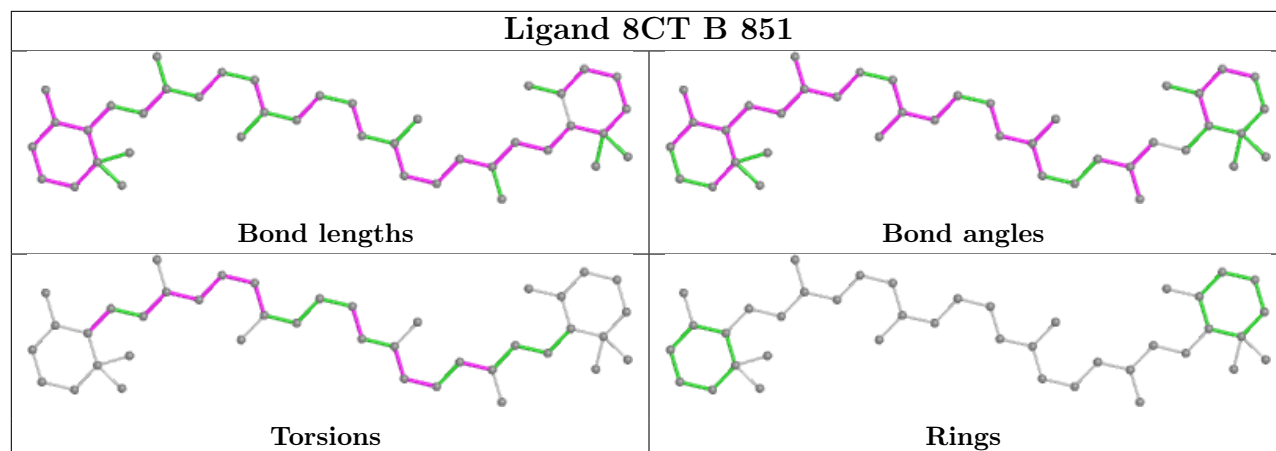
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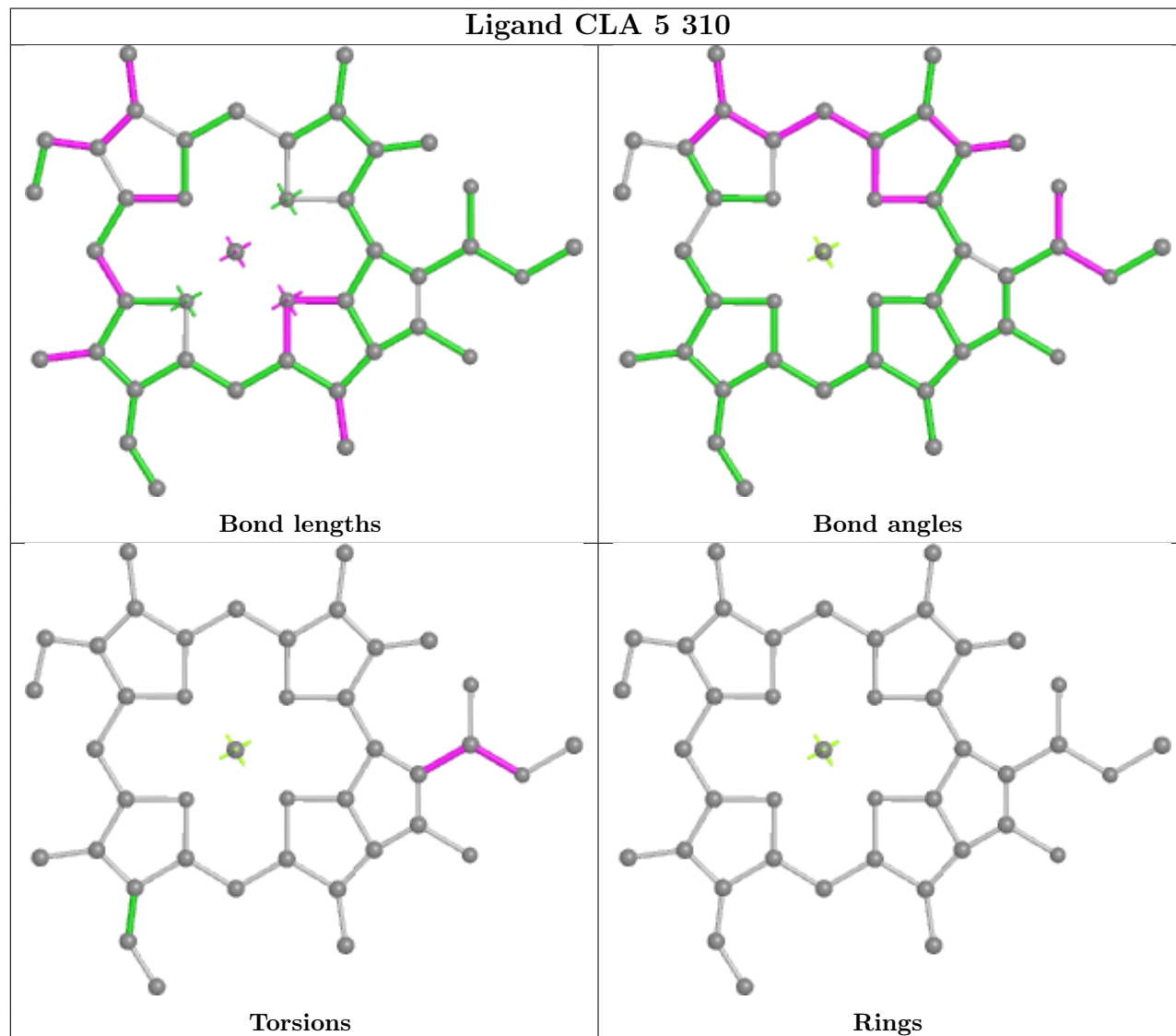
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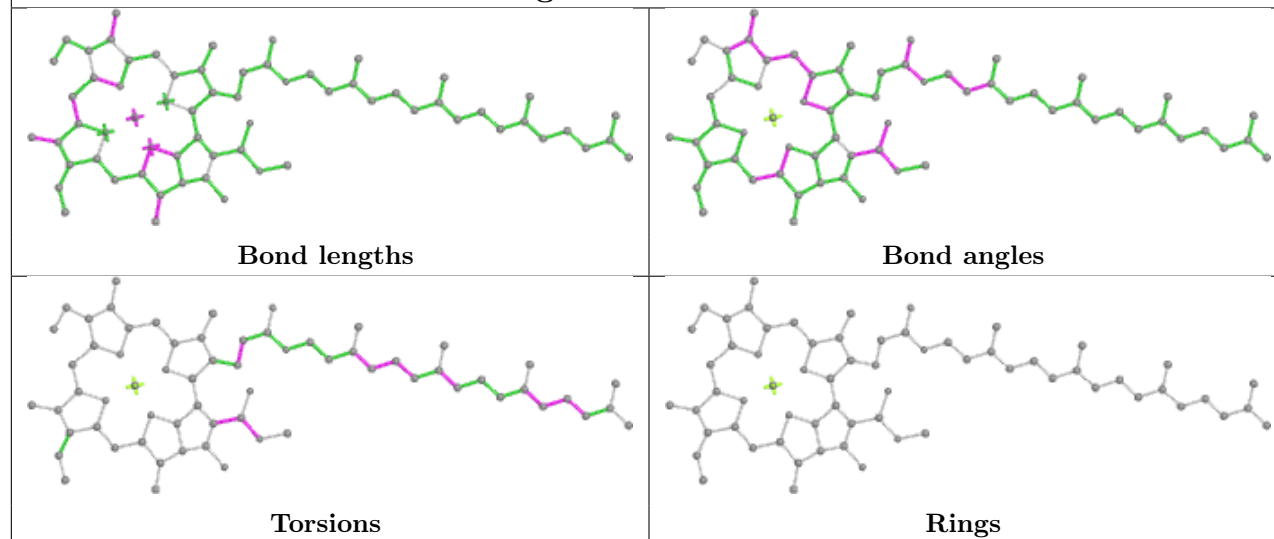
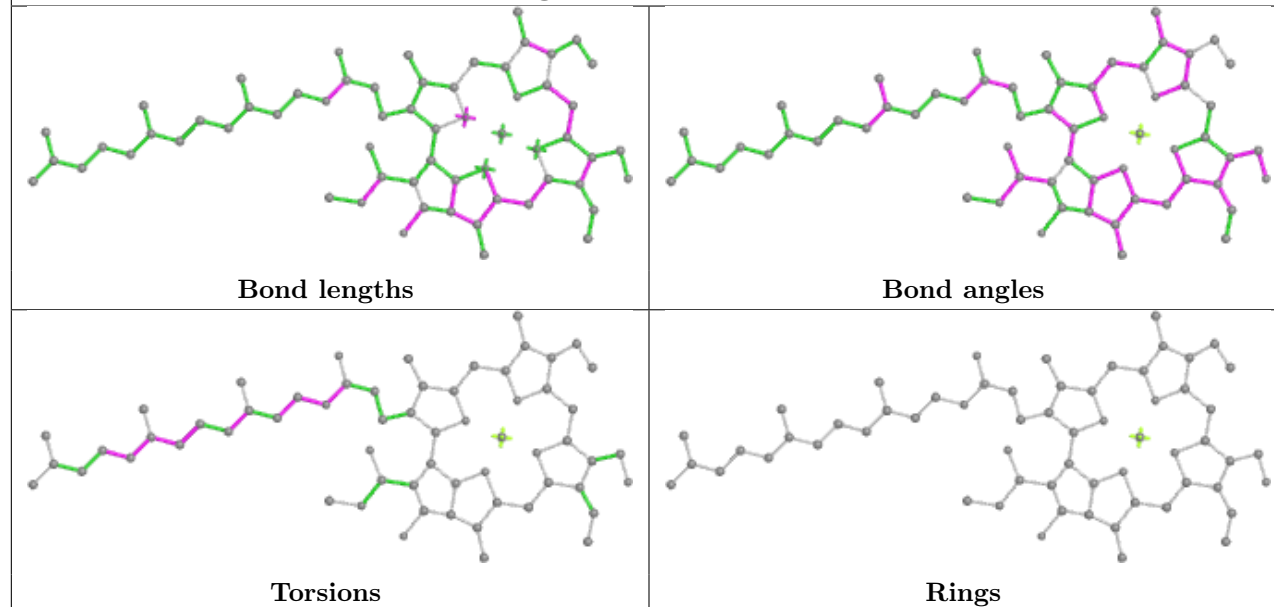


Ligand 8CT B 851

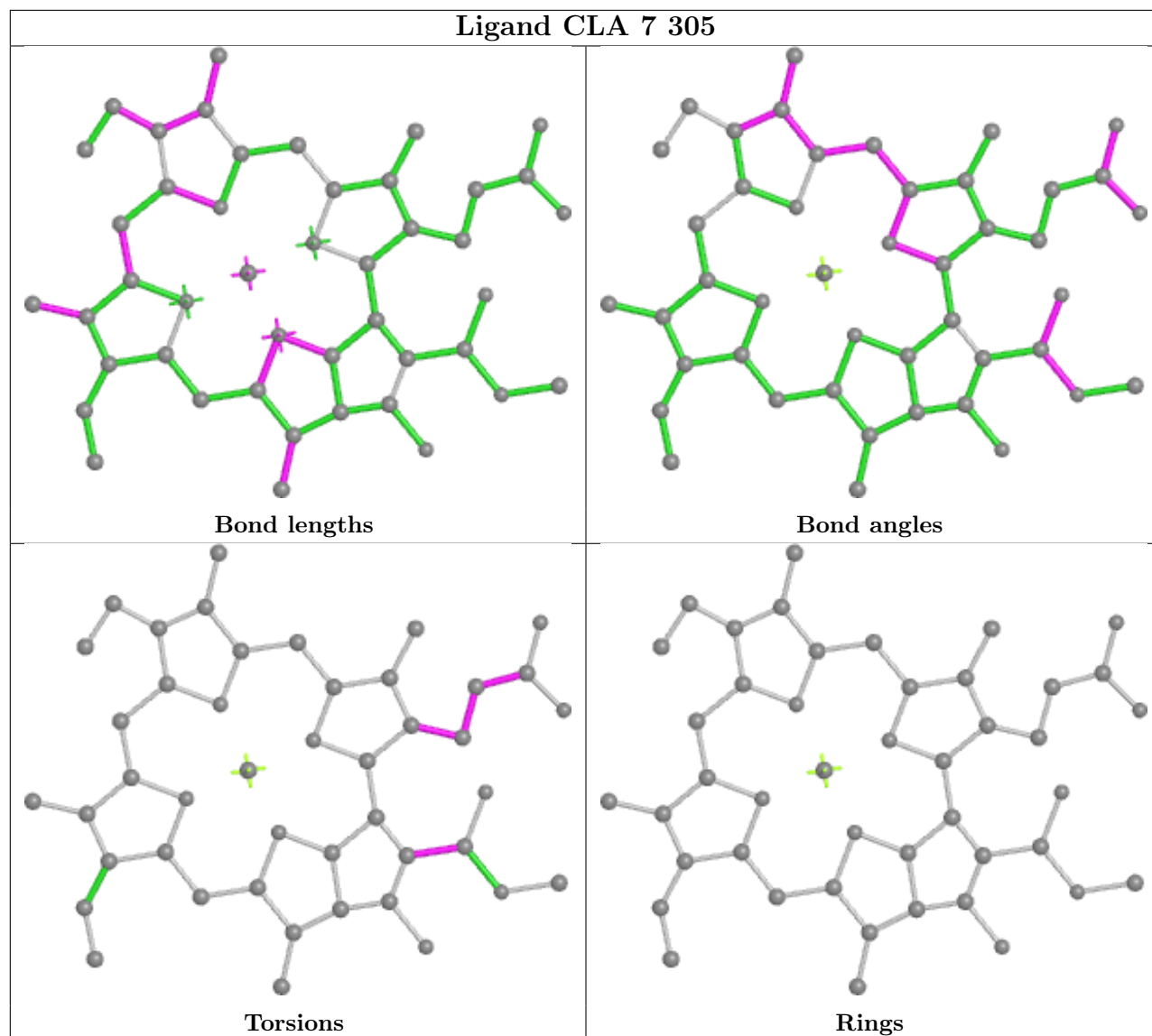


Ligand CLA 5 310

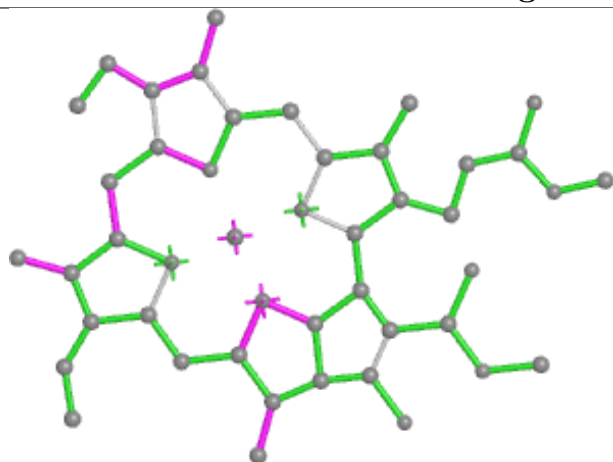


Ligand CLA 0 302**Ligand CHL 9 302**

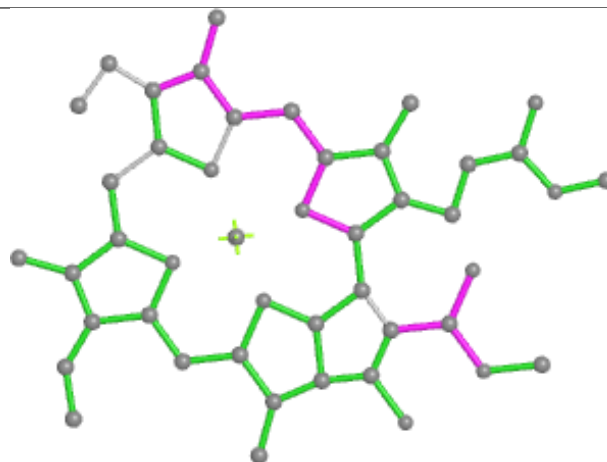
Ligand CLA 7 305



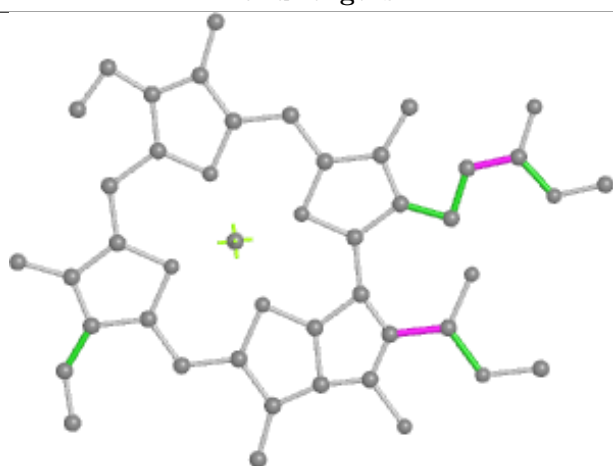
Ligand CLA 8 303



Bond lengths



Bond angles

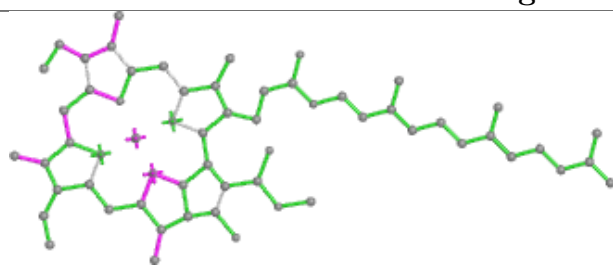


Torsions

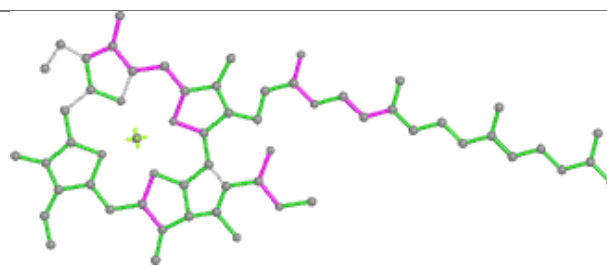


Rings

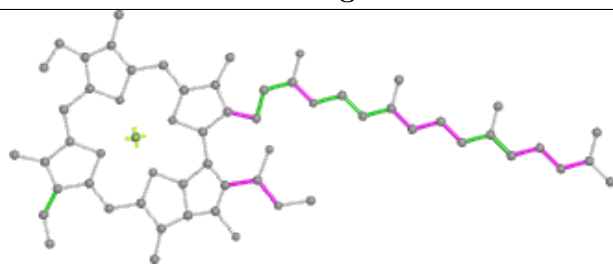
Ligand CLA 4 309



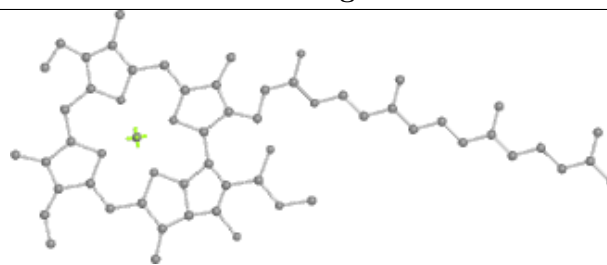
Bond lengths



Bond angles

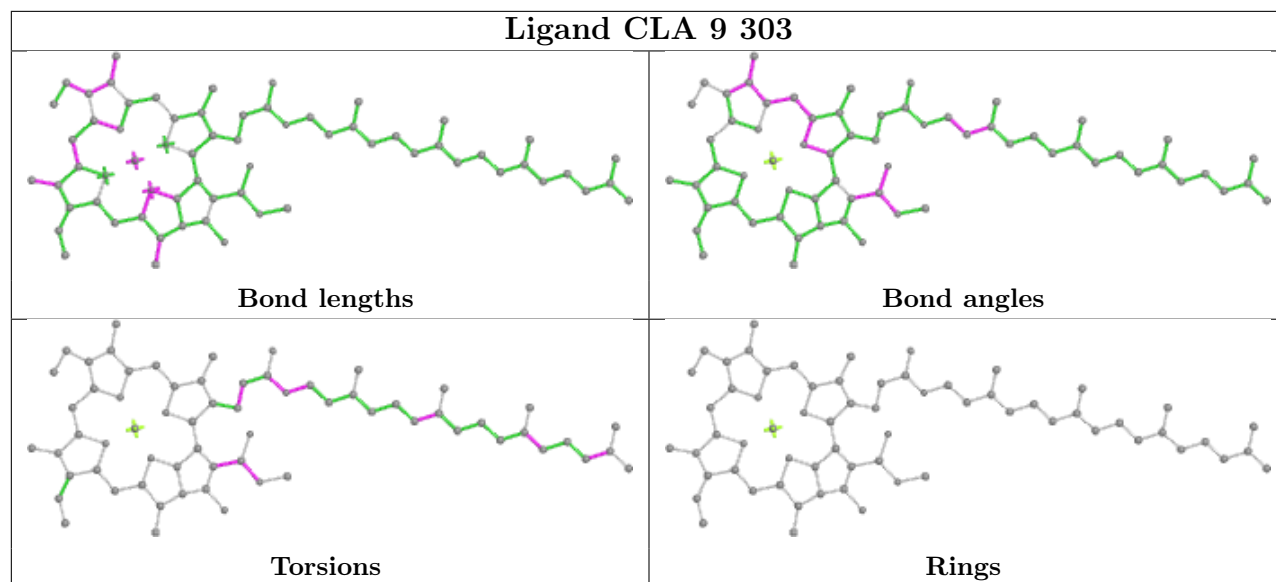


Torsions

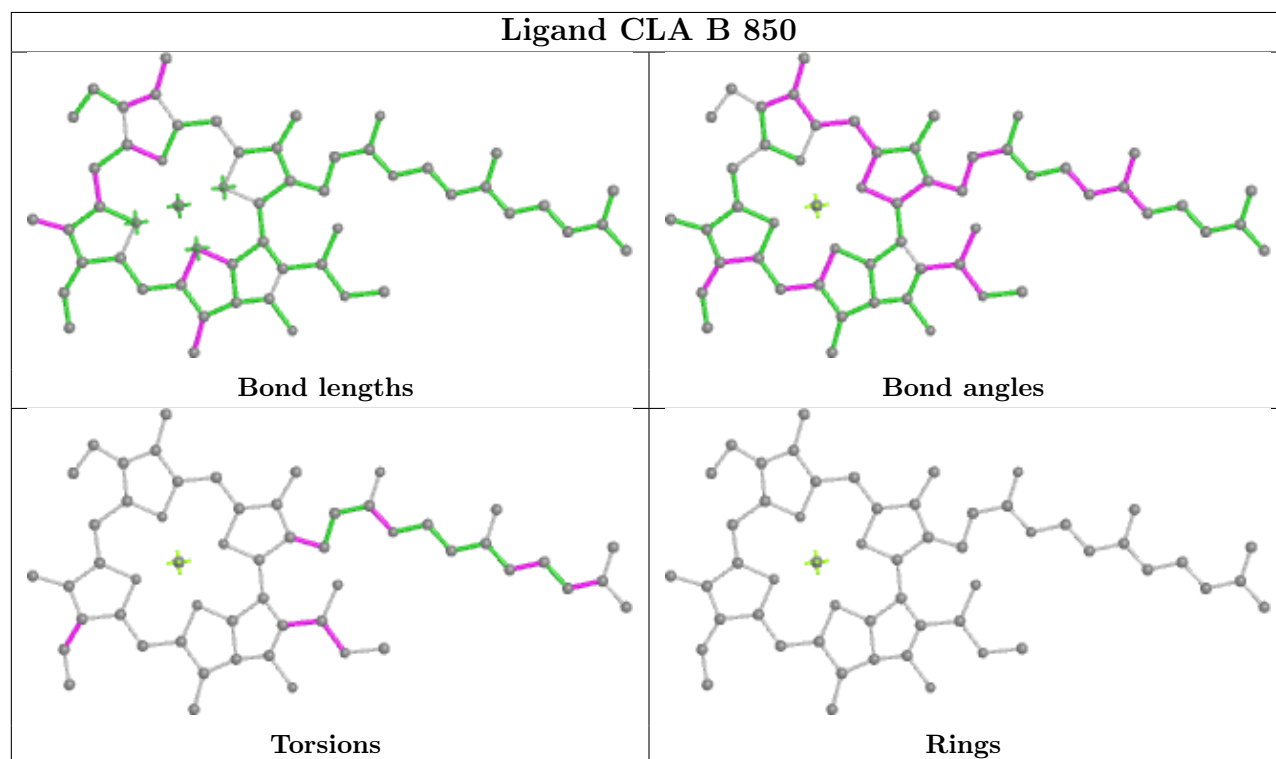


Rings

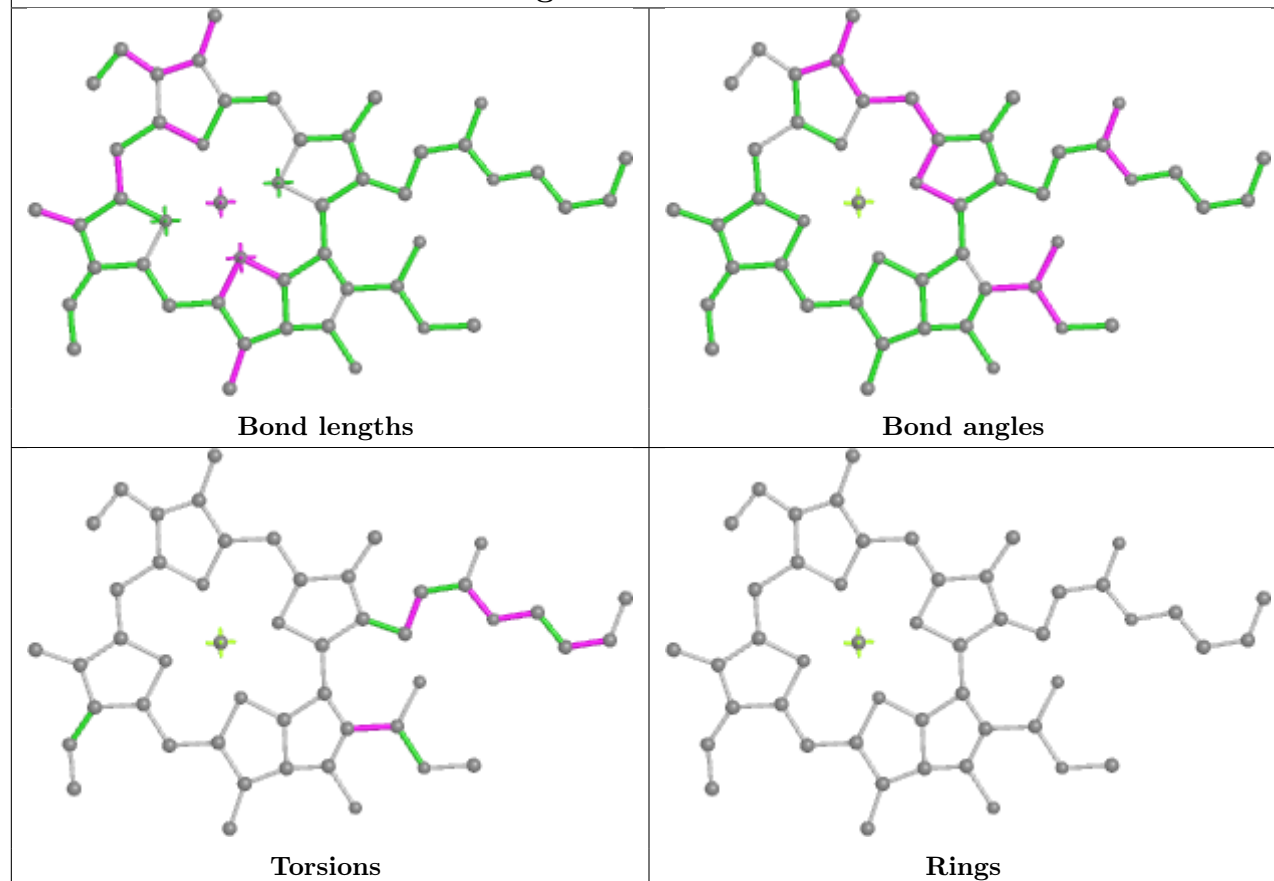
Ligand CLA 9 303



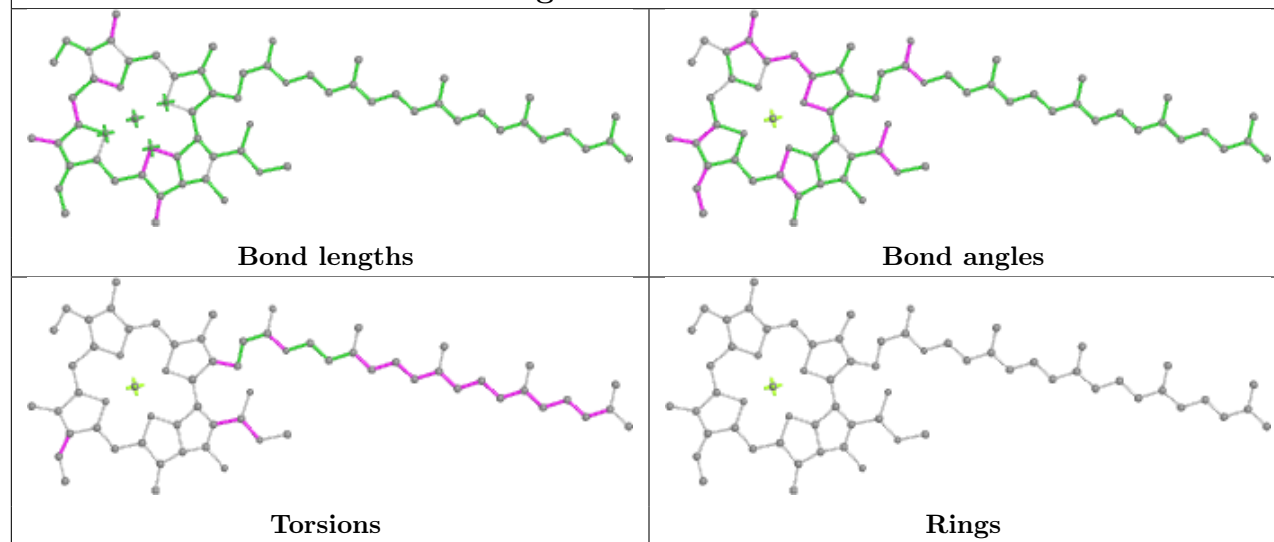
Ligand CLA B 850



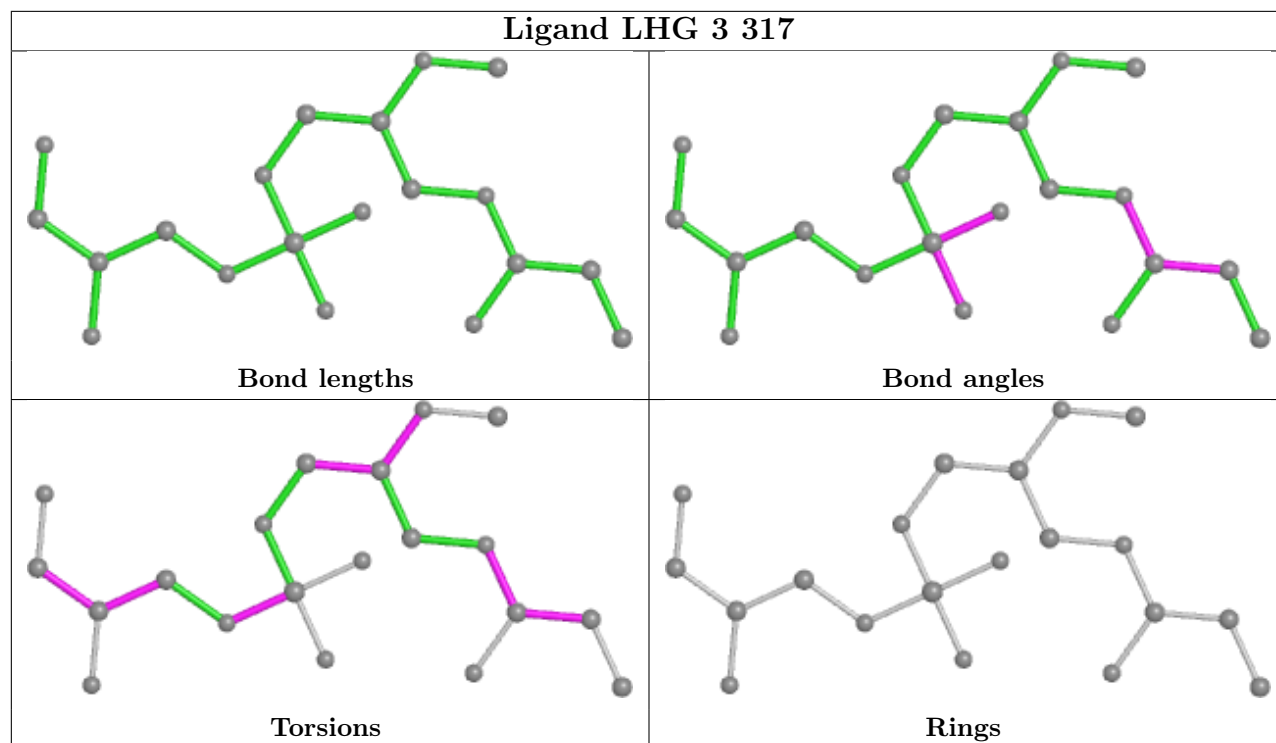
Ligand CLA 2 314



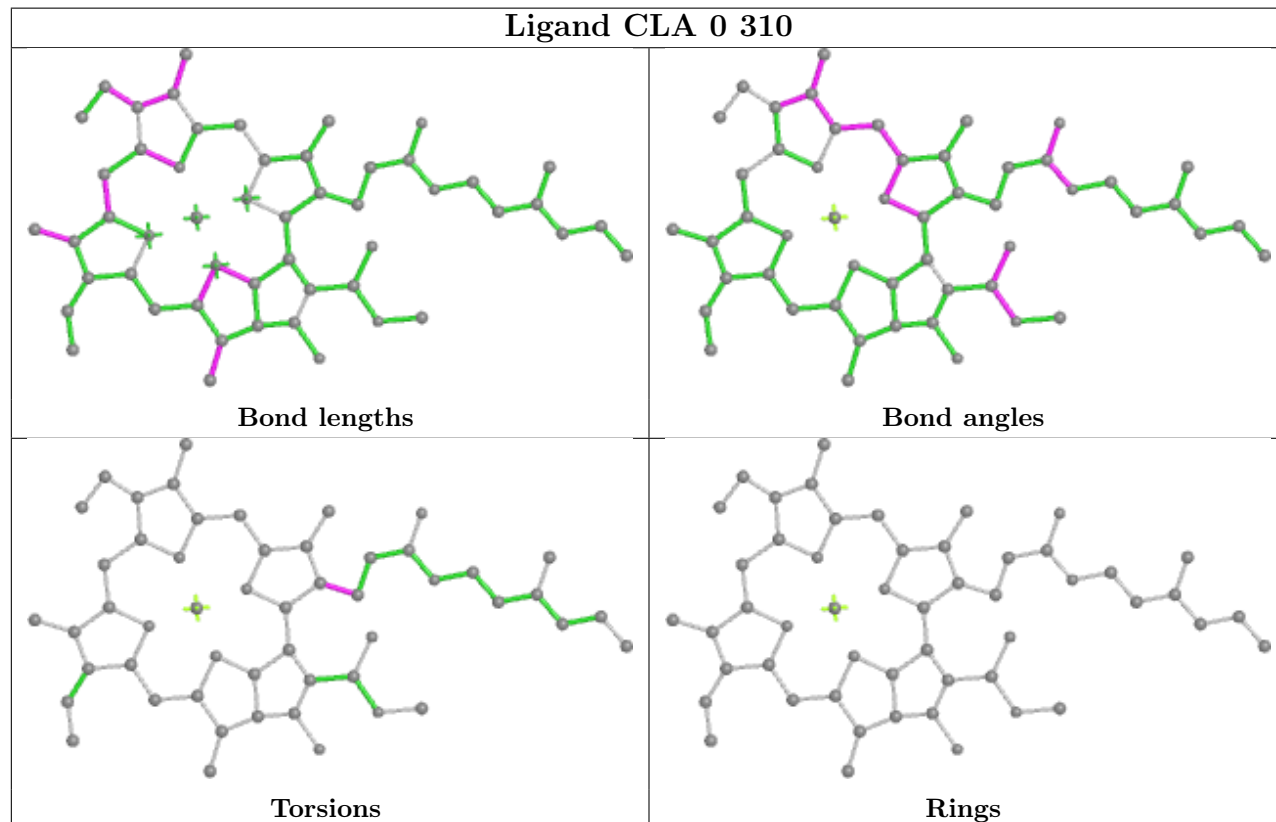
Ligand CLA 0 307



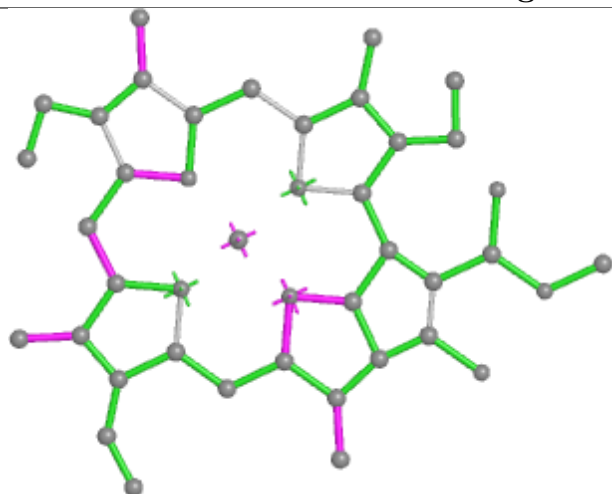
Ligand LHG 3 317



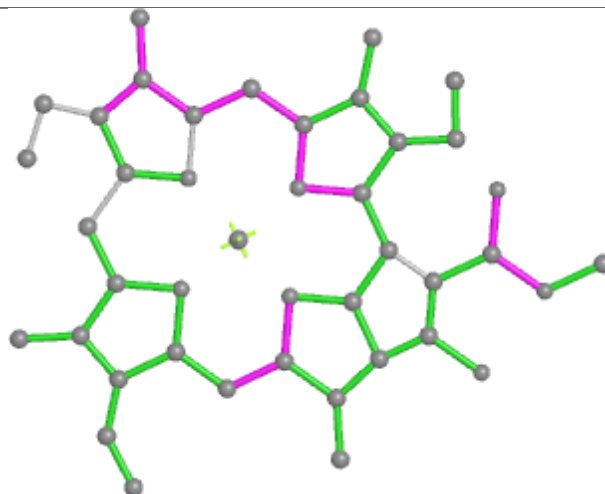
Ligand CLA 0 310



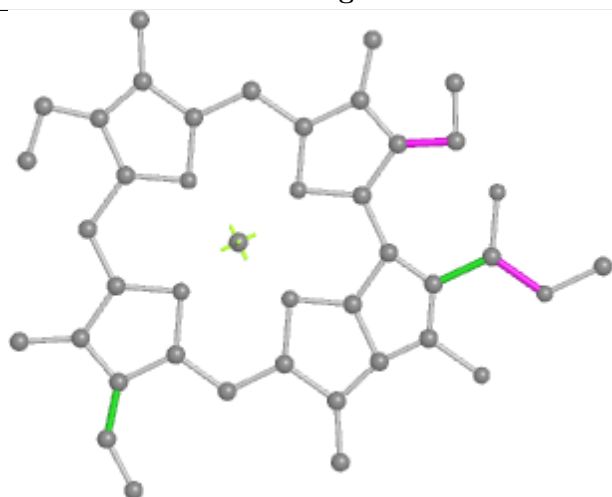
Ligand CLA 7 306



Bond lengths



Bond angles

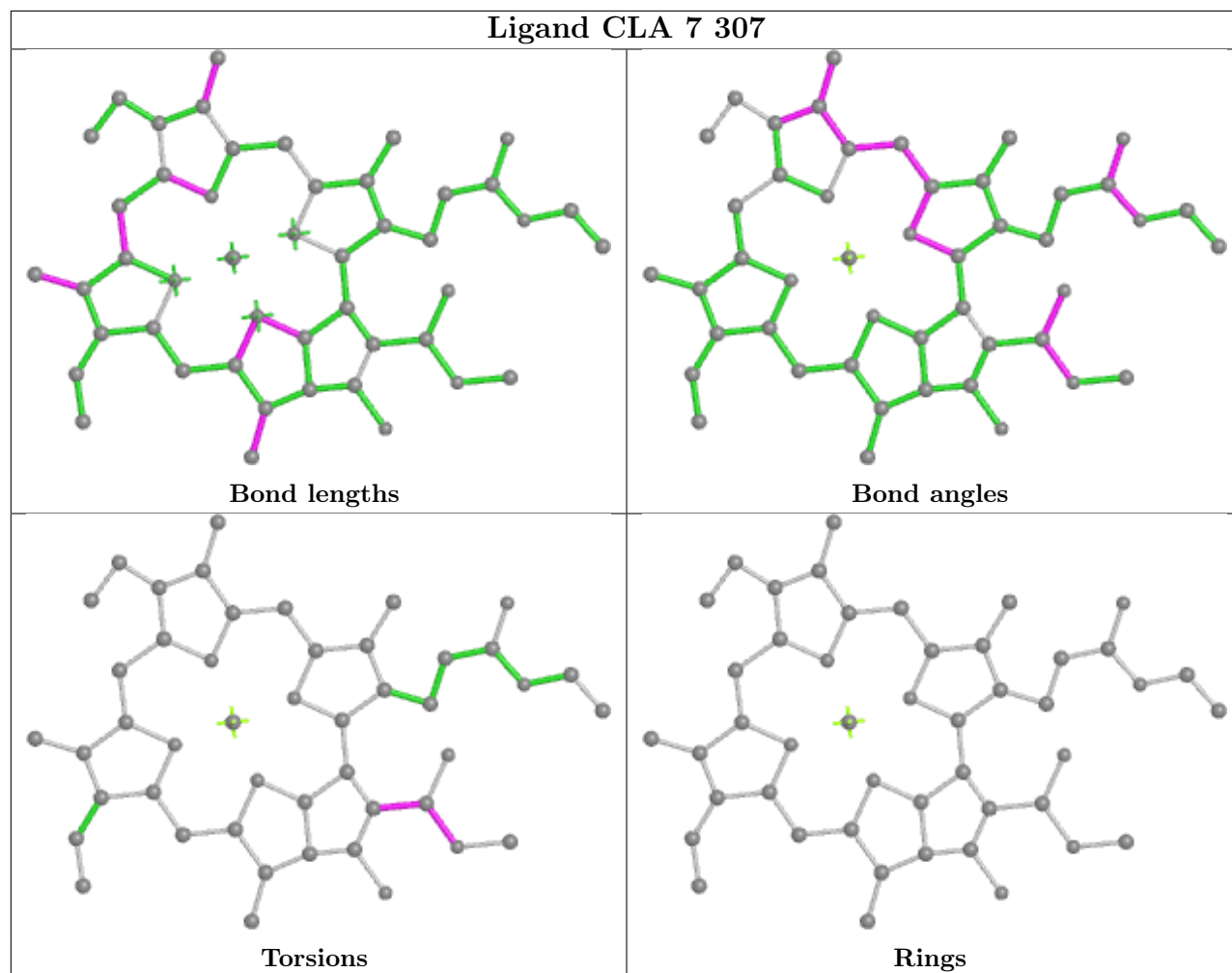


Torsions

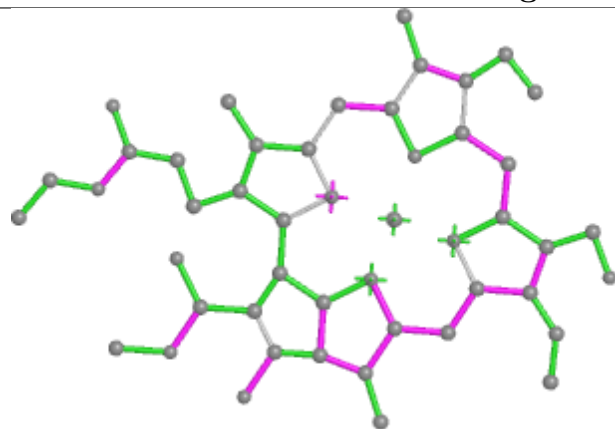


Rings

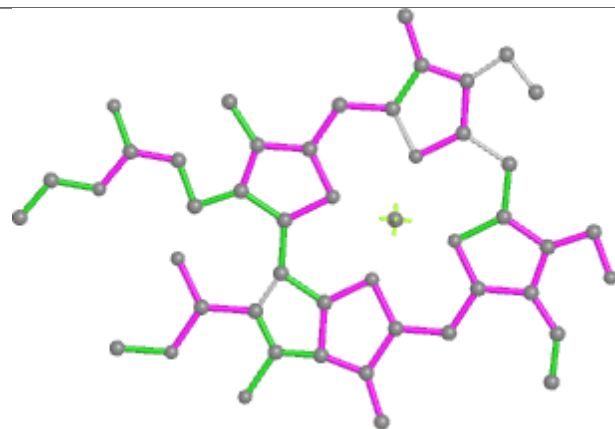
Ligand CLA 7 307



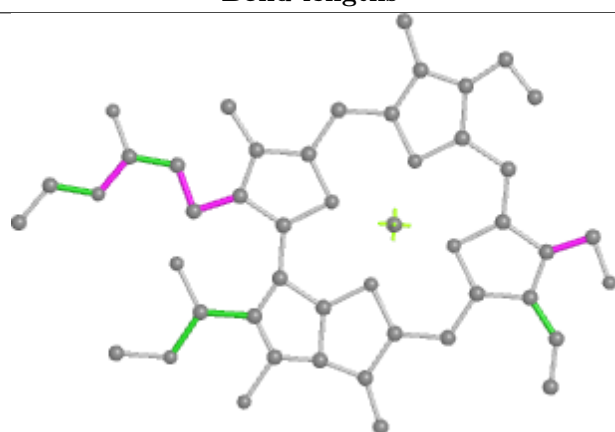
Ligand CHL 5 306



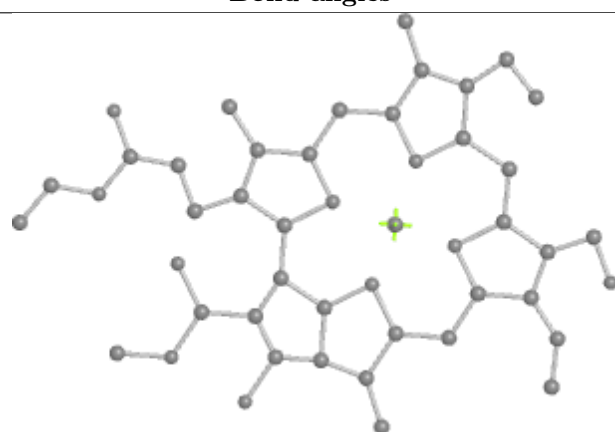
Bond lengths



Bond angles

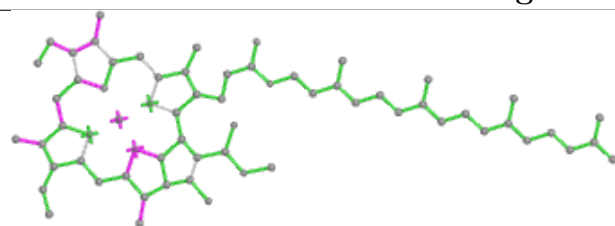


Torsions

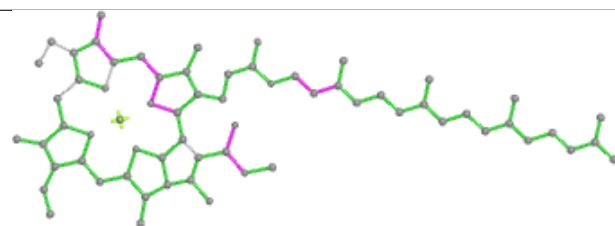


Rings

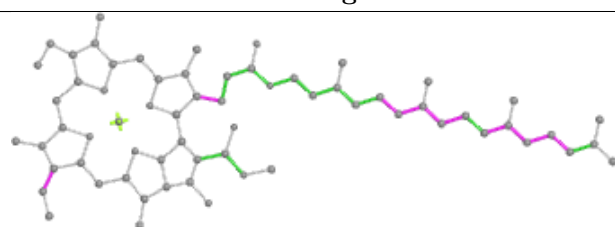
Ligand CLA A 826



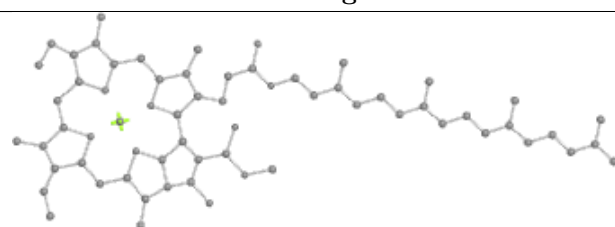
Bond lengths



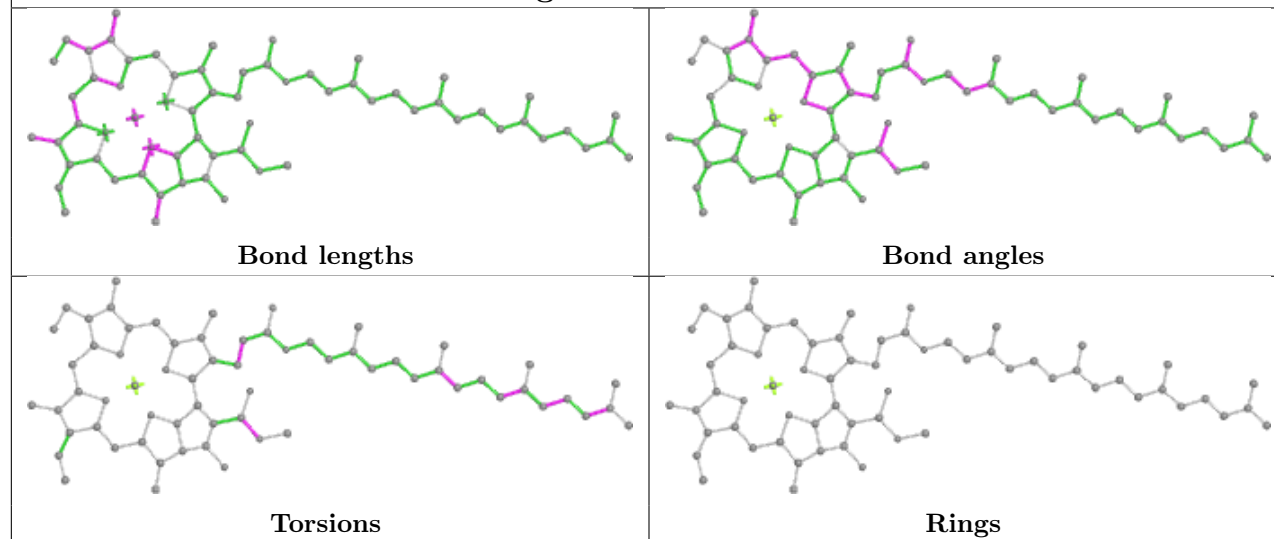
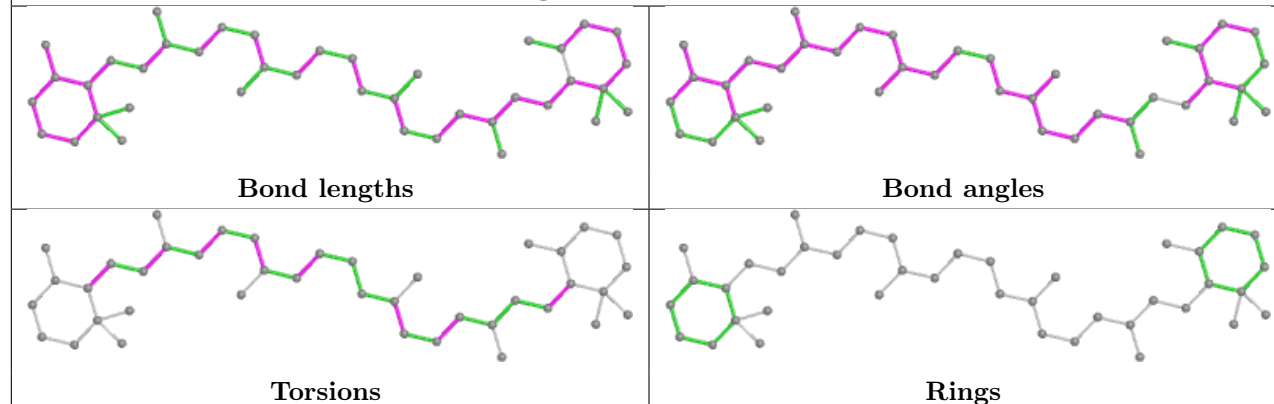
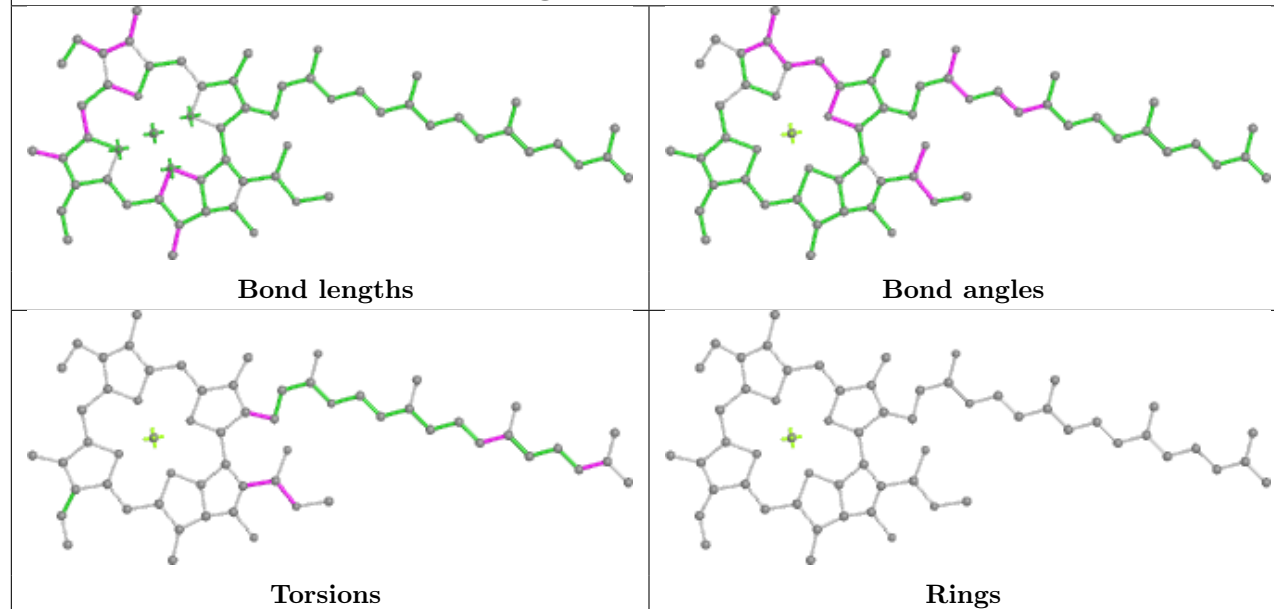
Bond angles



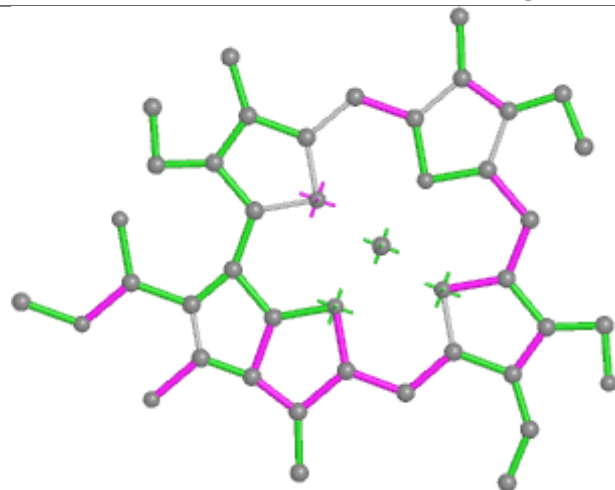
Torsions



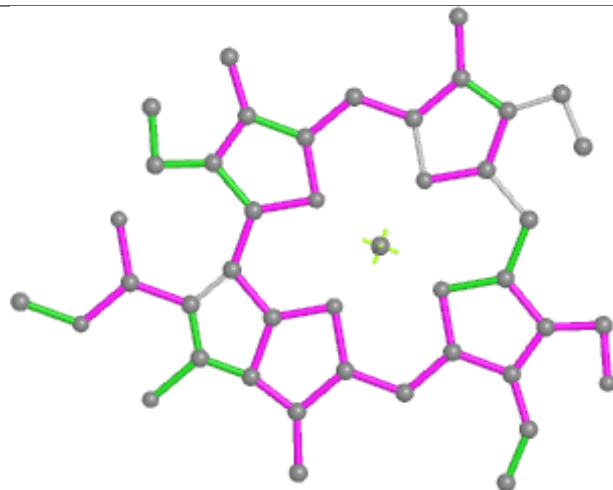
Rings

Ligand CLA 5 302**Ligand 8CT A 854****Ligand CLA 5 309**

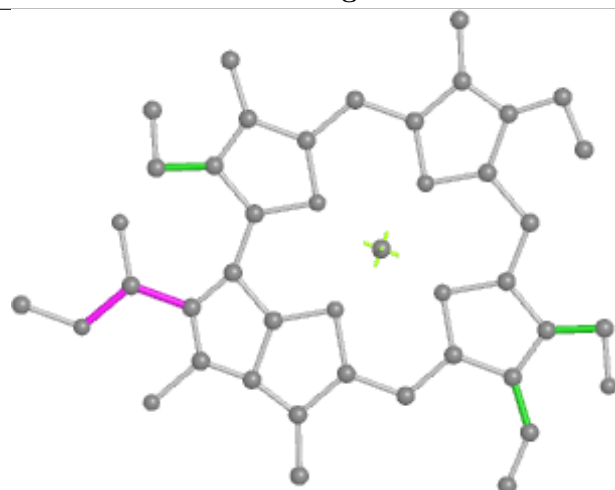
Ligand CHL 8 314



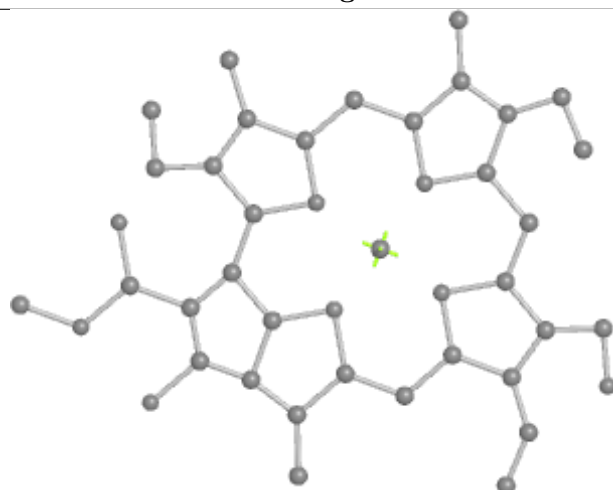
Bond lengths



Bond angles

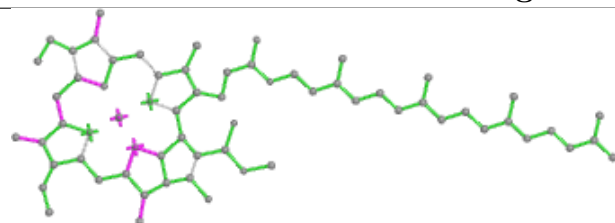


Torsions

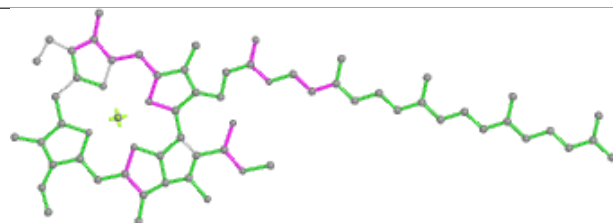


Rings

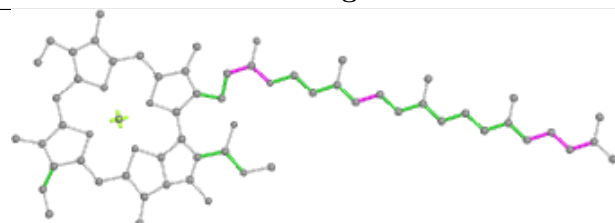
Ligand CLA A 821



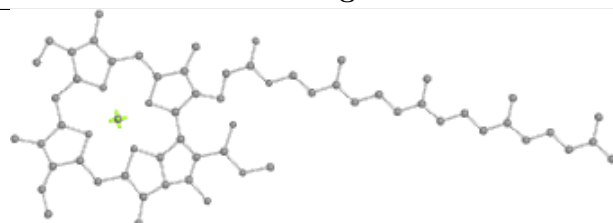
Bond lengths



Bond angles

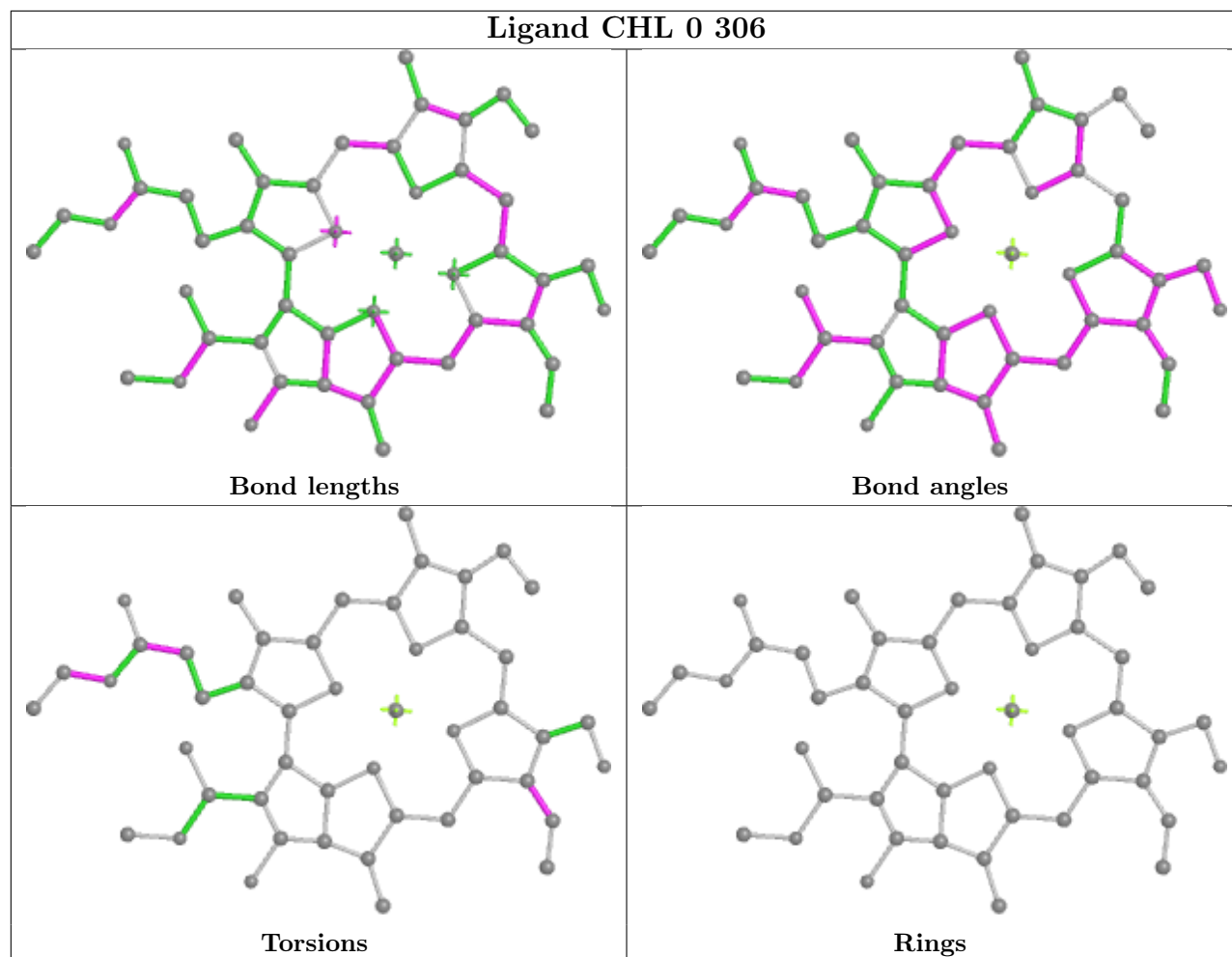


Torsions

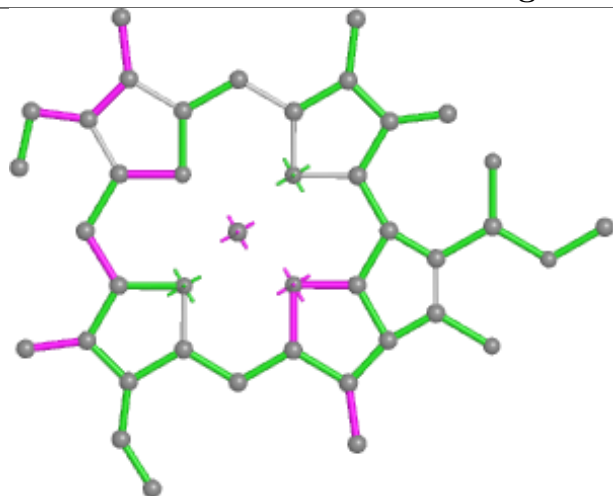


Rings

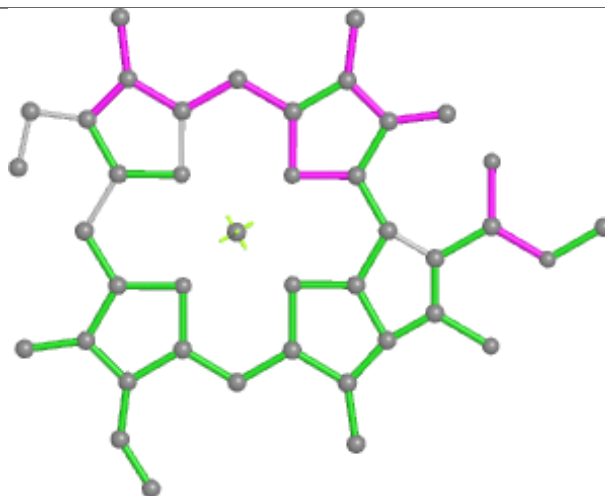
Ligand CHL 0 306



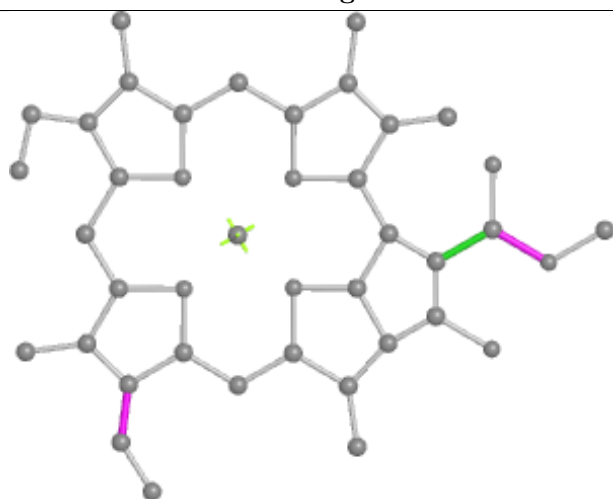
Ligand CLA 2 310



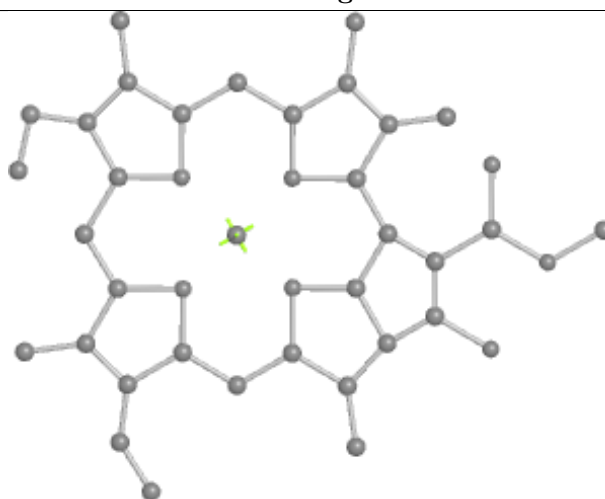
Bond lengths



Bond angles

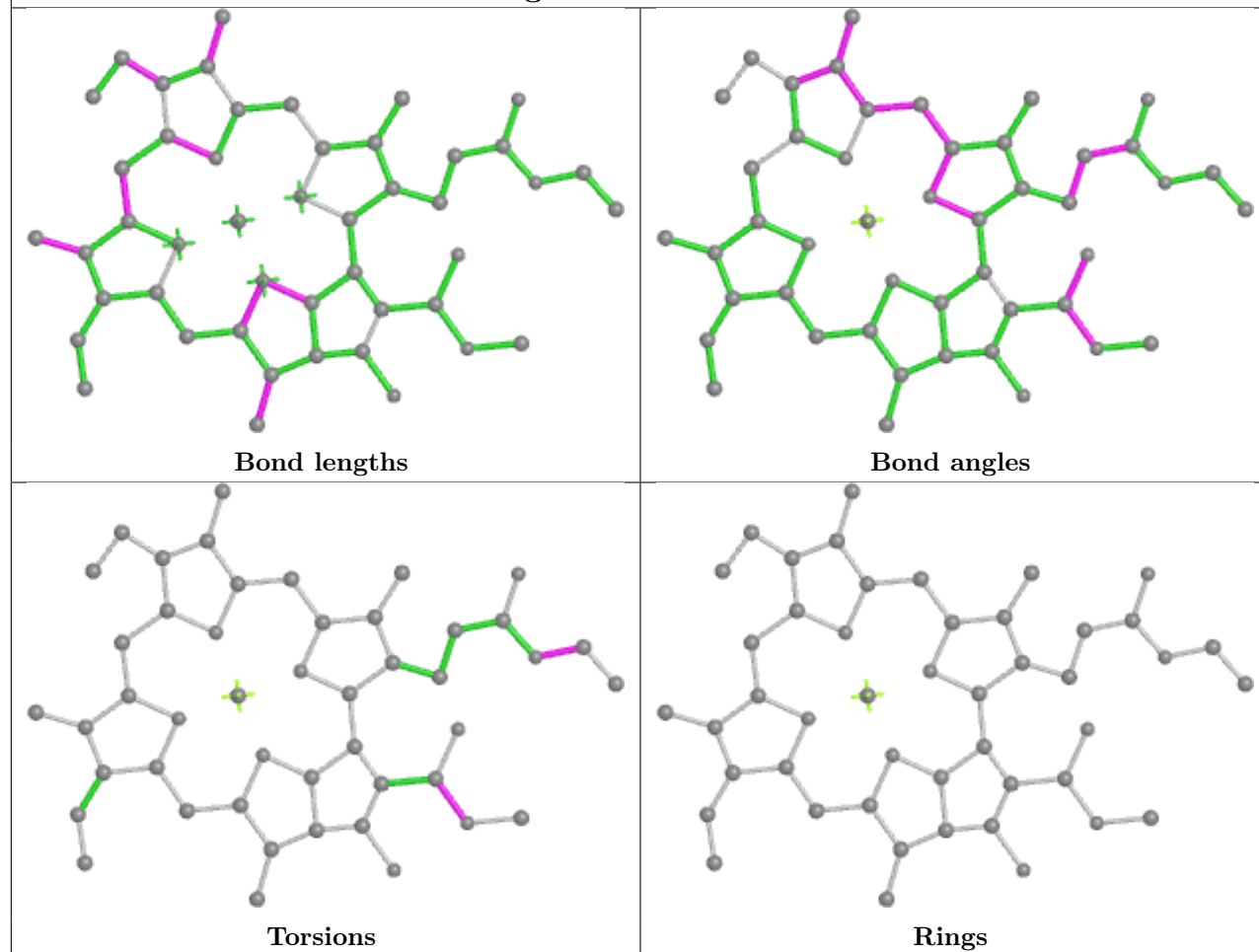


Torsions

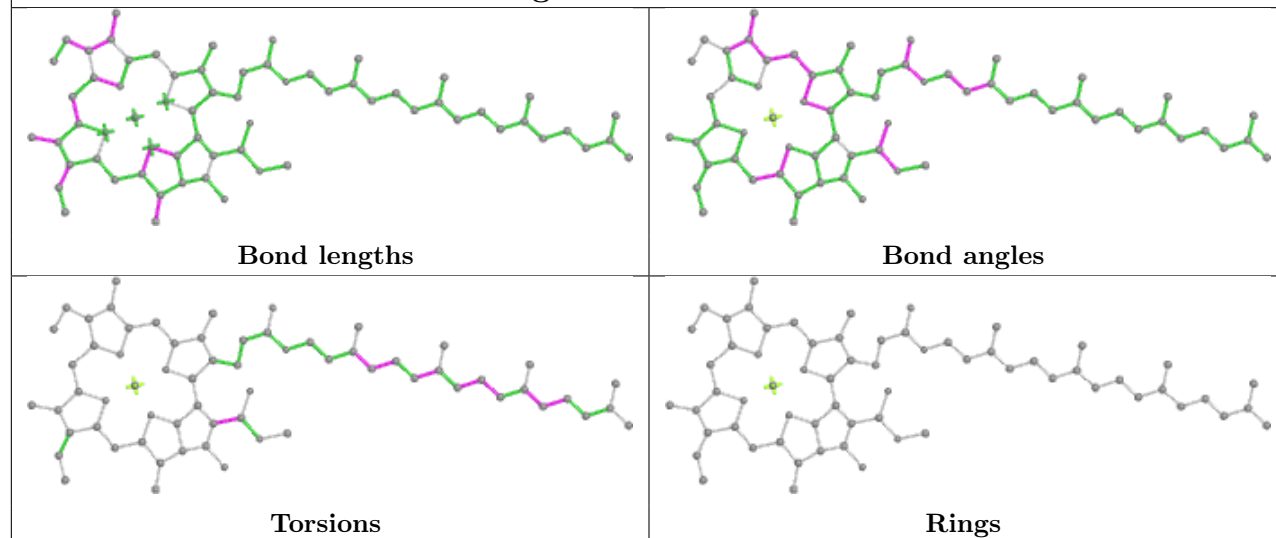


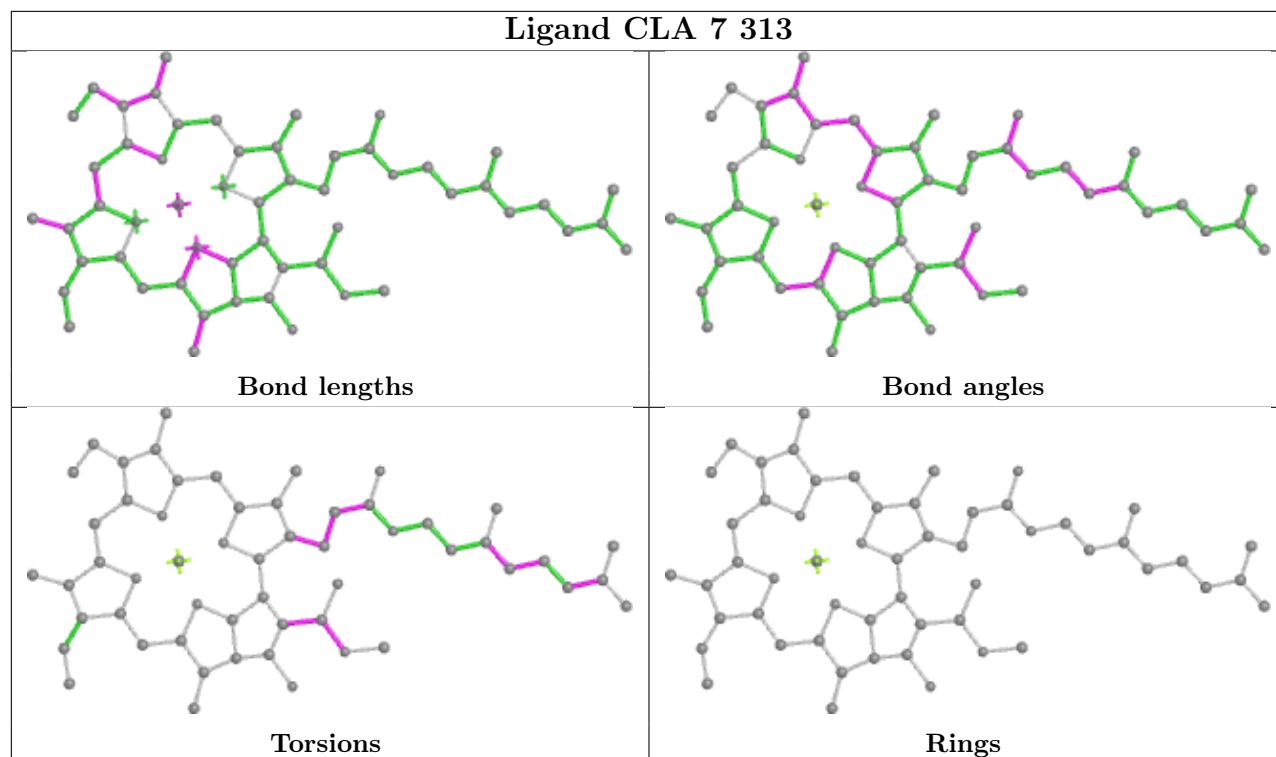
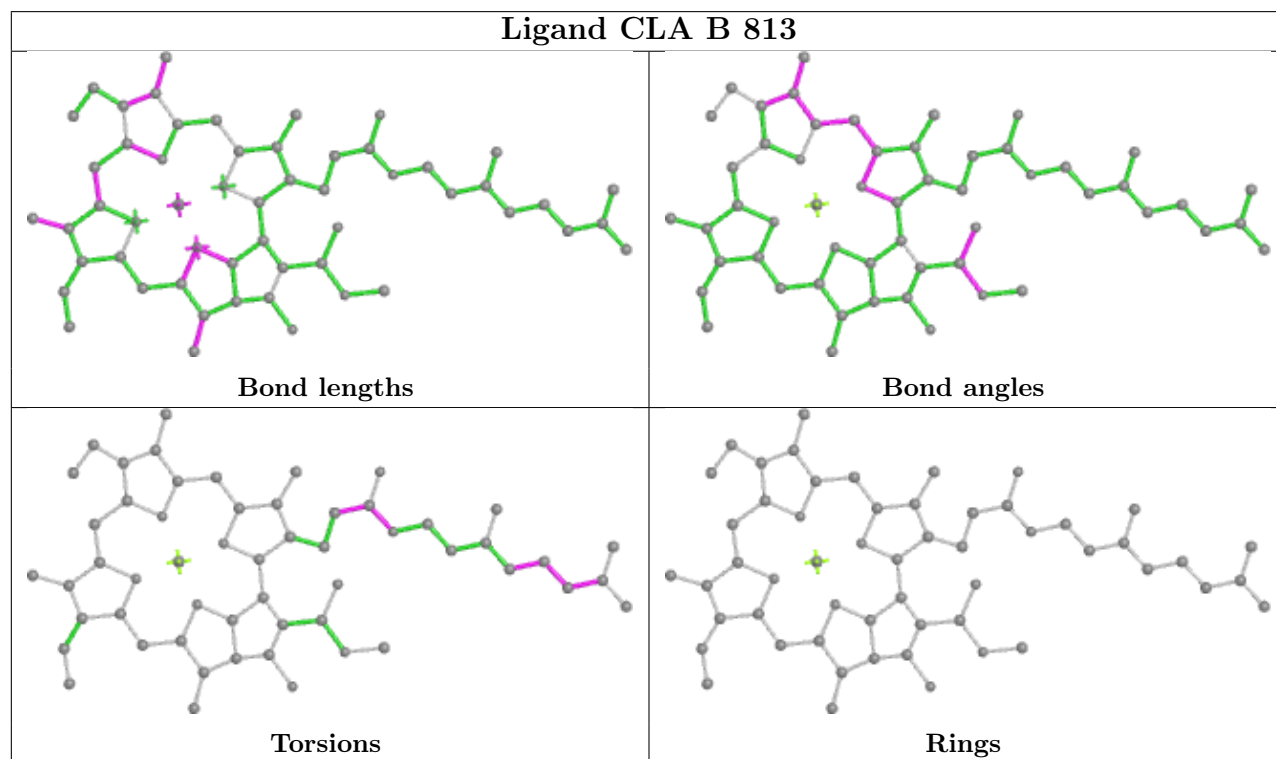
Rings

Ligand CLA A 815

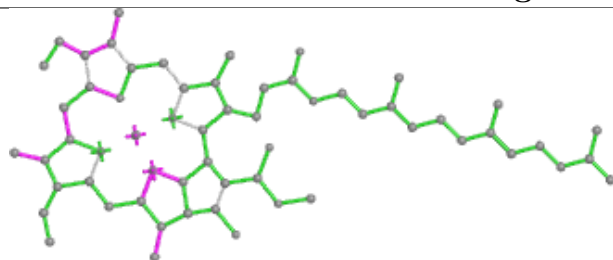


Ligand CLA B 811

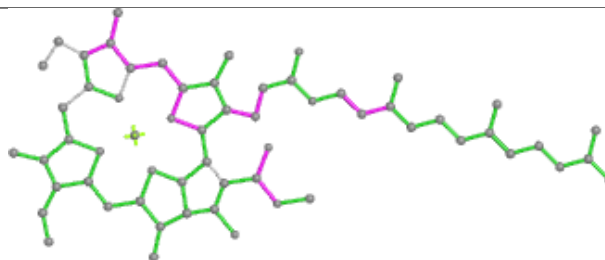


Ligand CLA 7 313**Ligand CLA B 813**

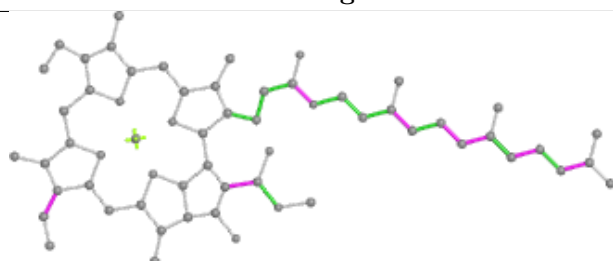
Ligand CLA B 836



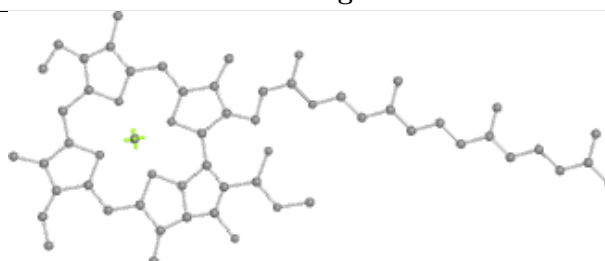
Bond lengths



Bond angles

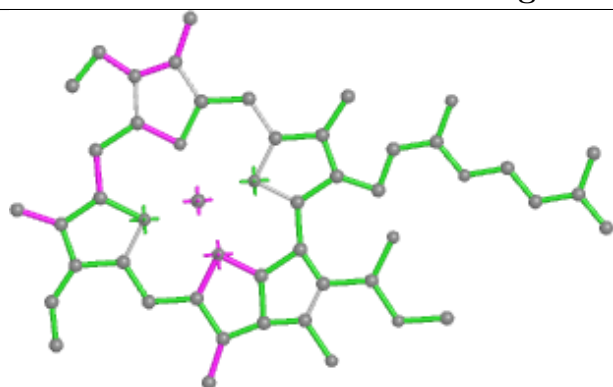


Torsions

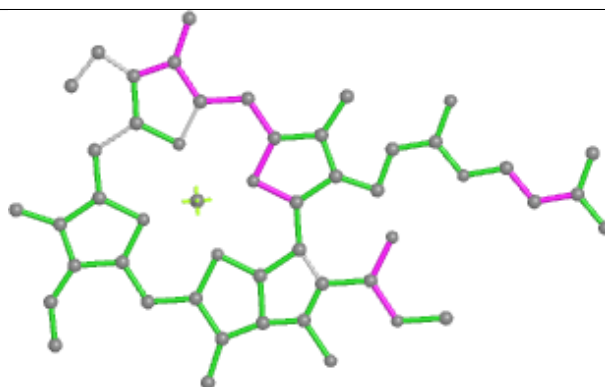


Rings

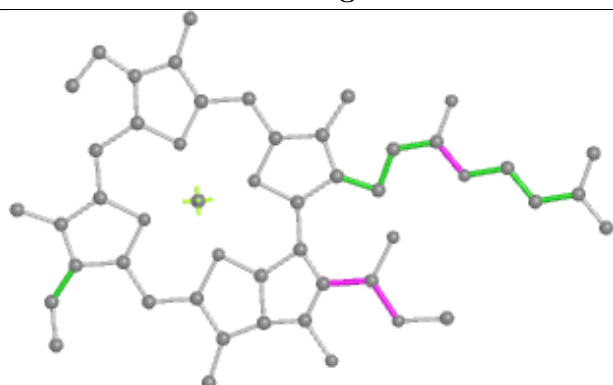
Ligand CLA 2 308



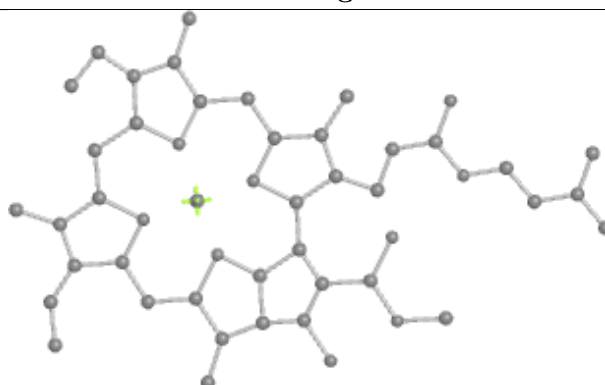
Bond lengths



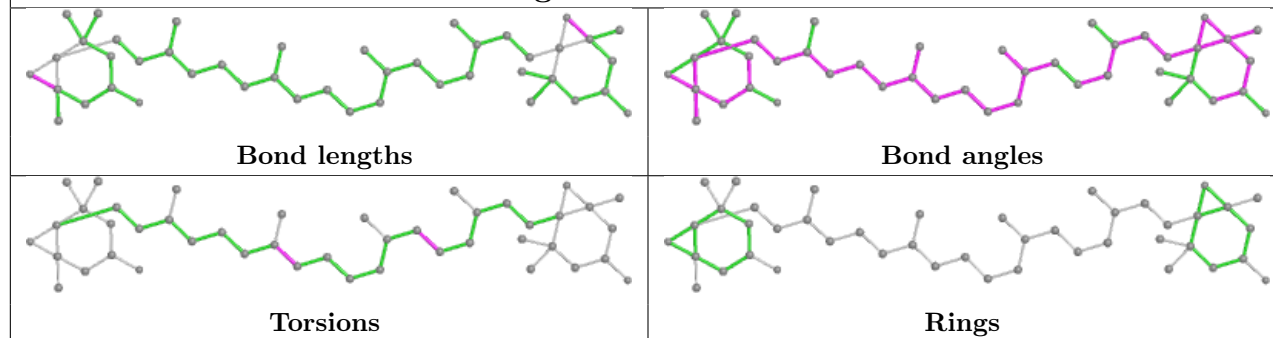
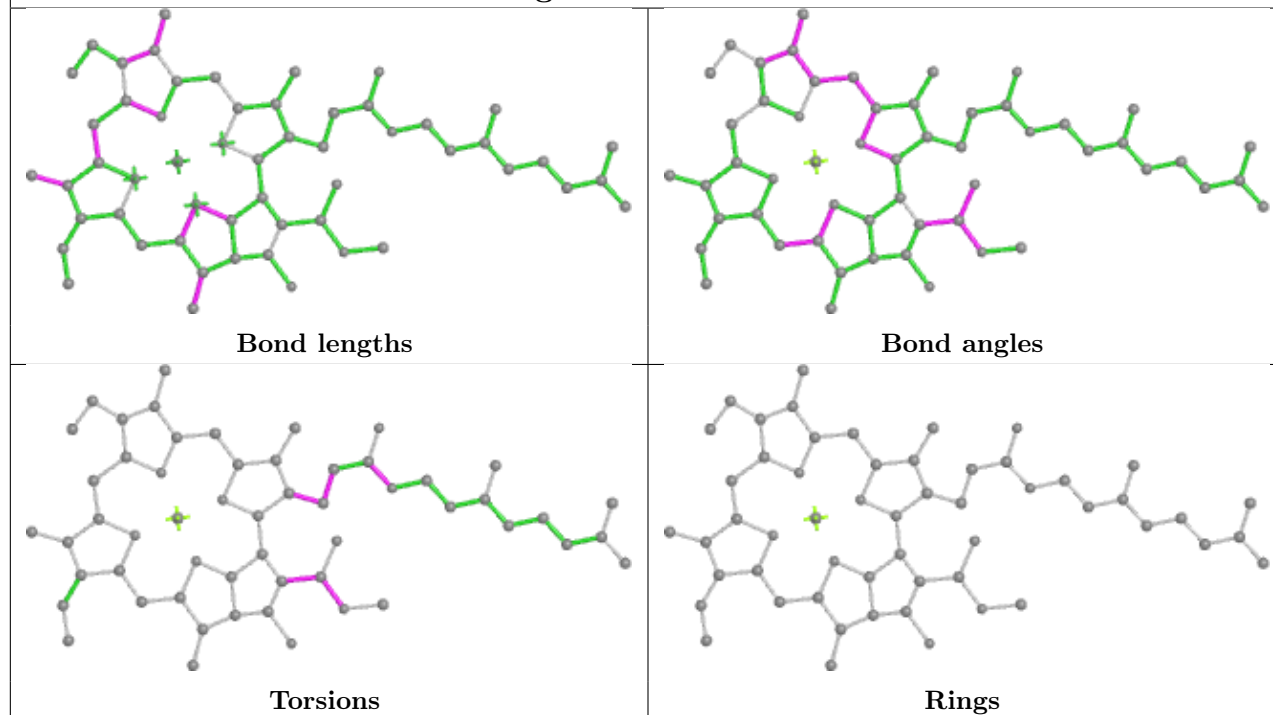
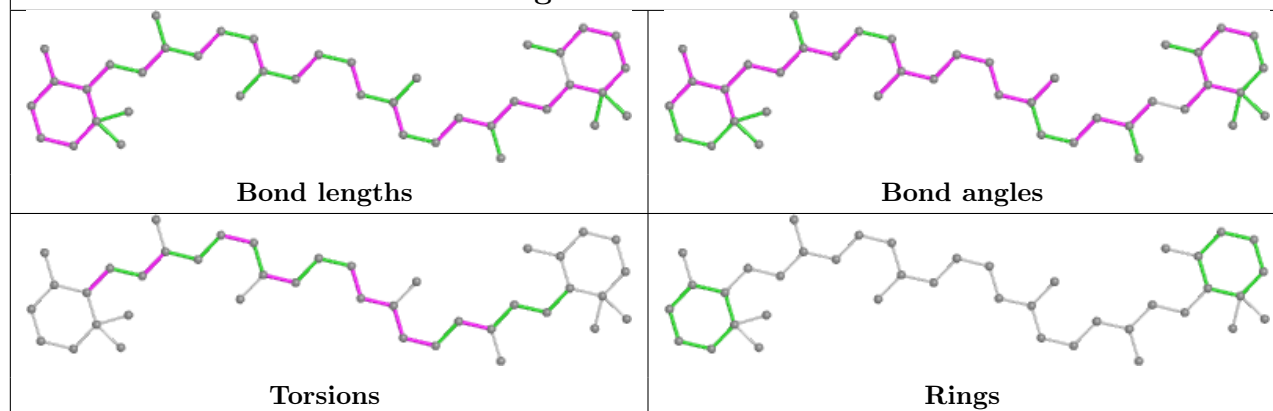
Bond angles

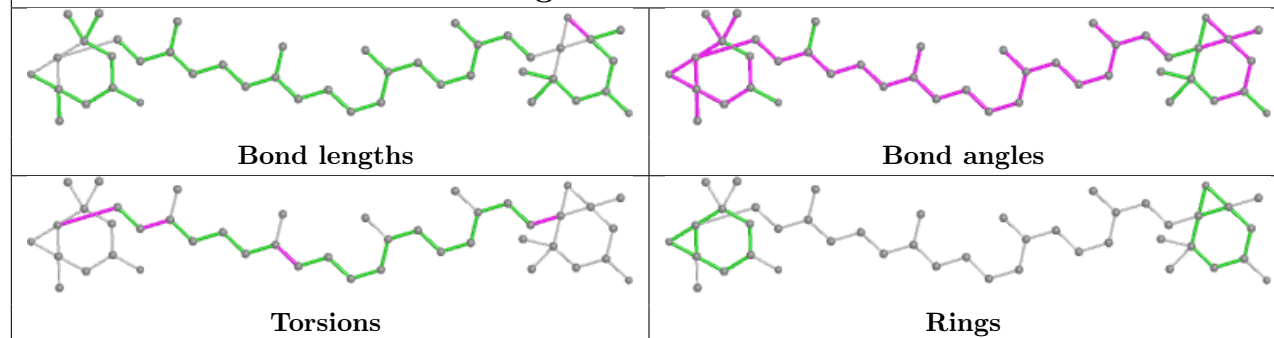
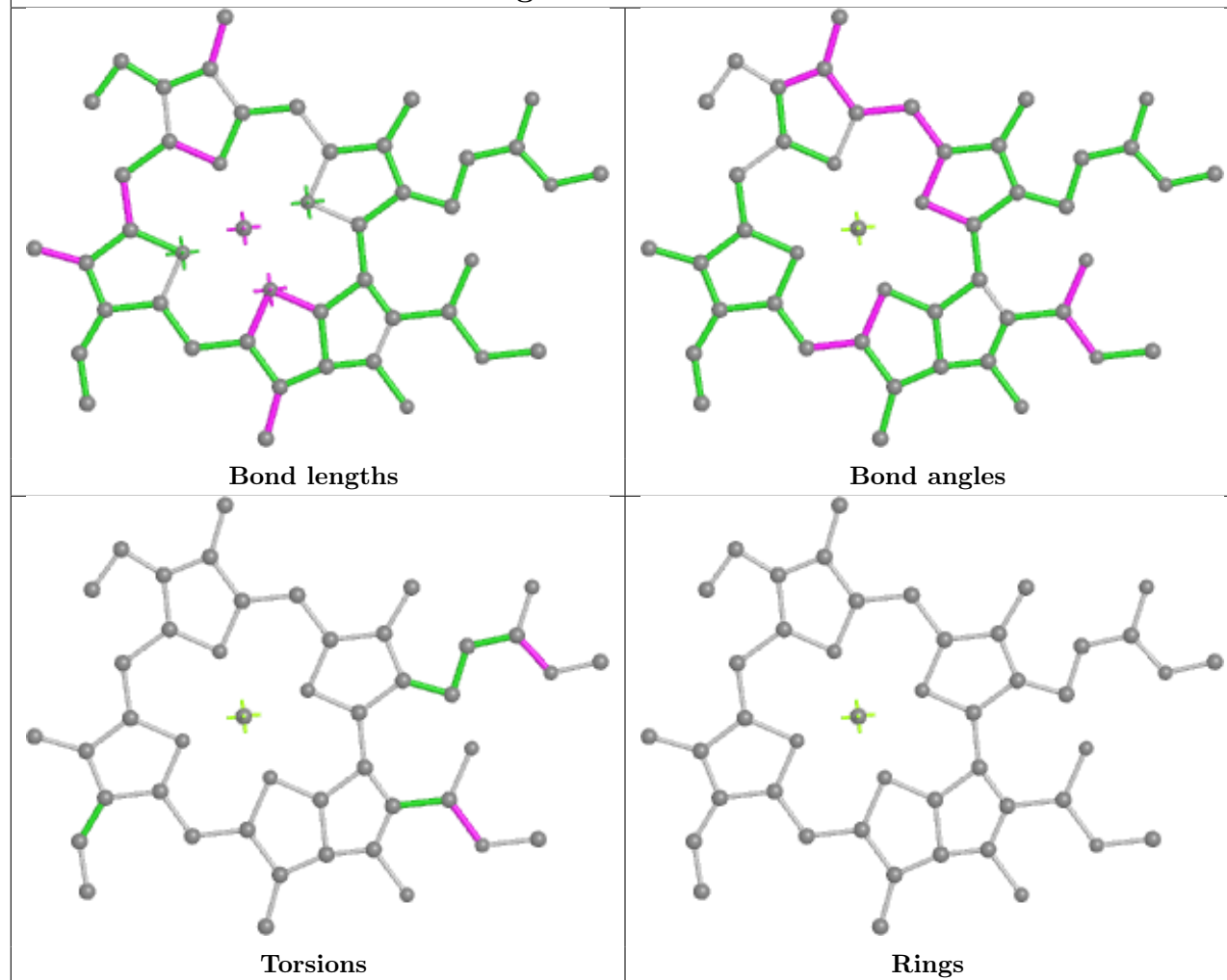


Torsions

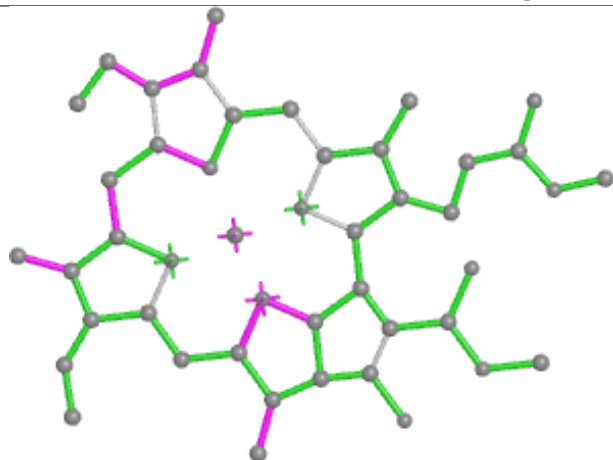


Rings

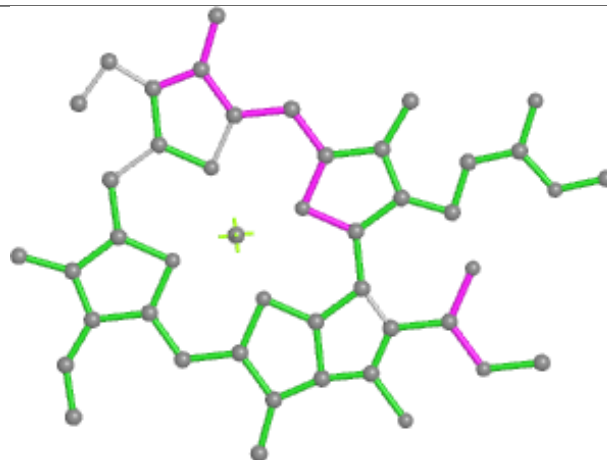
Ligand XAT 6 319**Ligand CLA 5 313****Ligand 8CT B 844**

Ligand XAT 8 316**Ligand CLA 7 315**

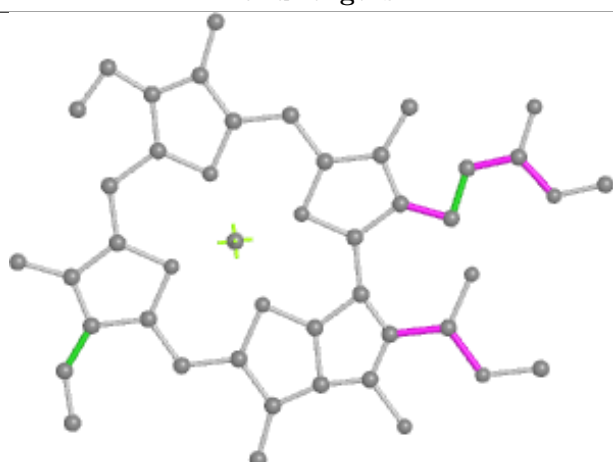
Ligand CLA 6 323



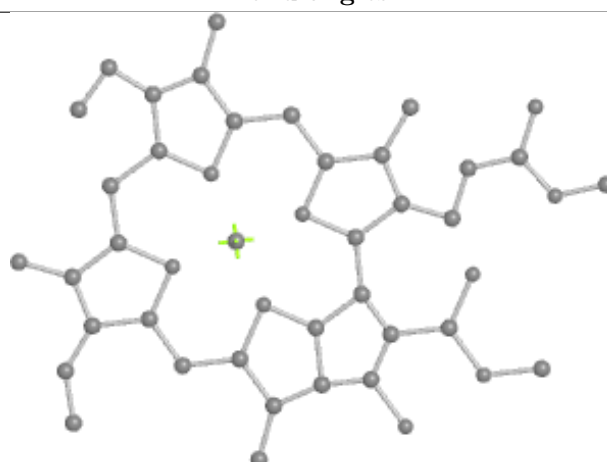
Bond lengths



Bond angles

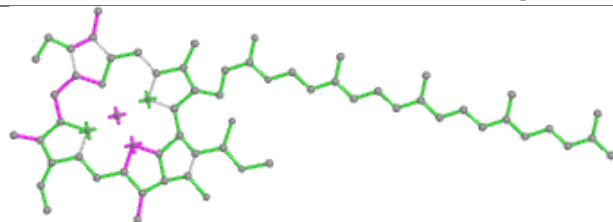


Torsions

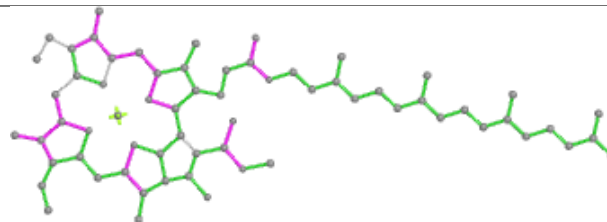


Rings

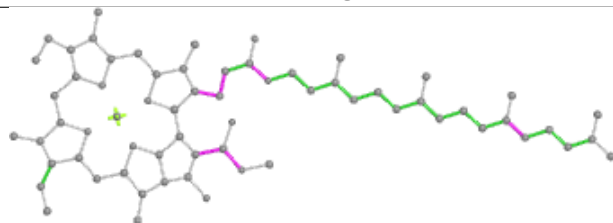
Ligand CLA B 829



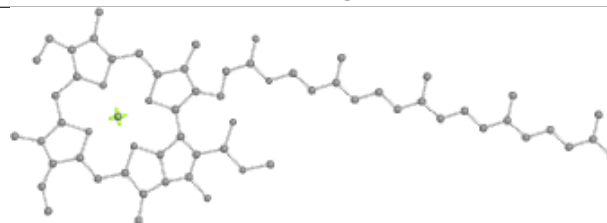
Bond lengths



Bond angles

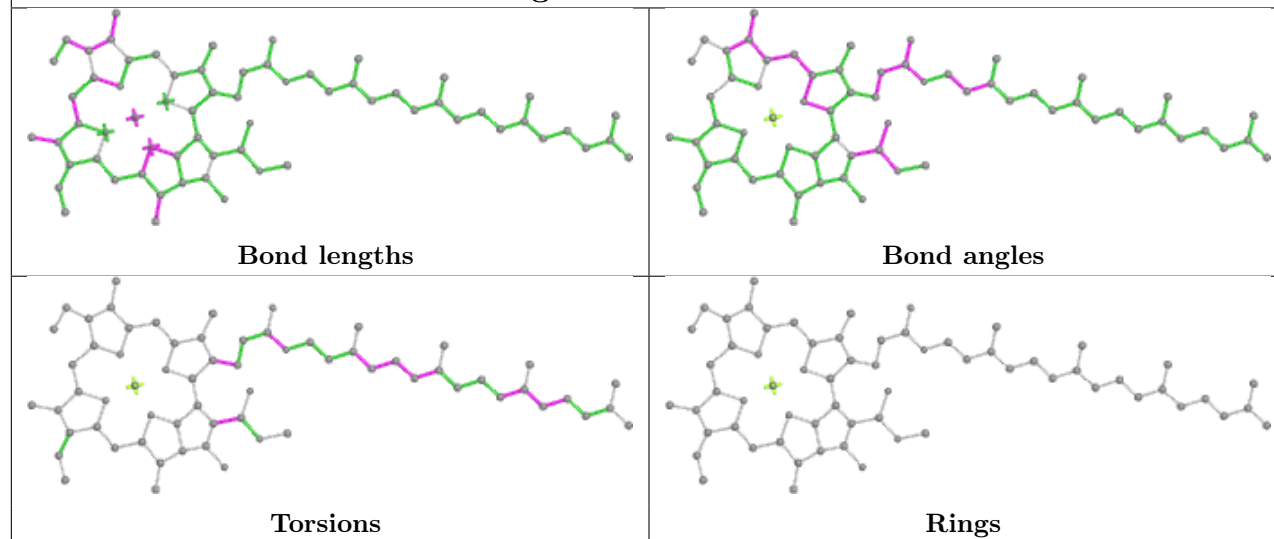


Torsions

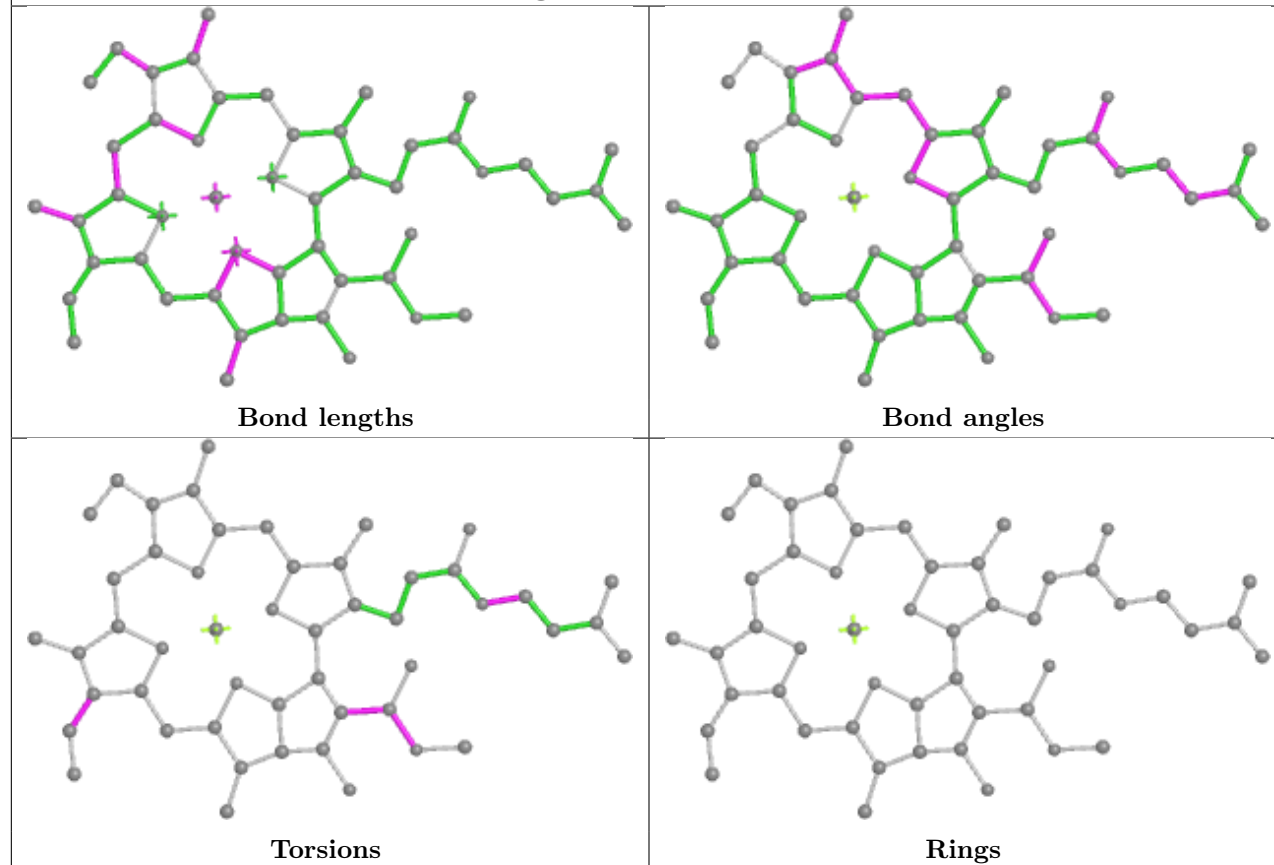


Rings

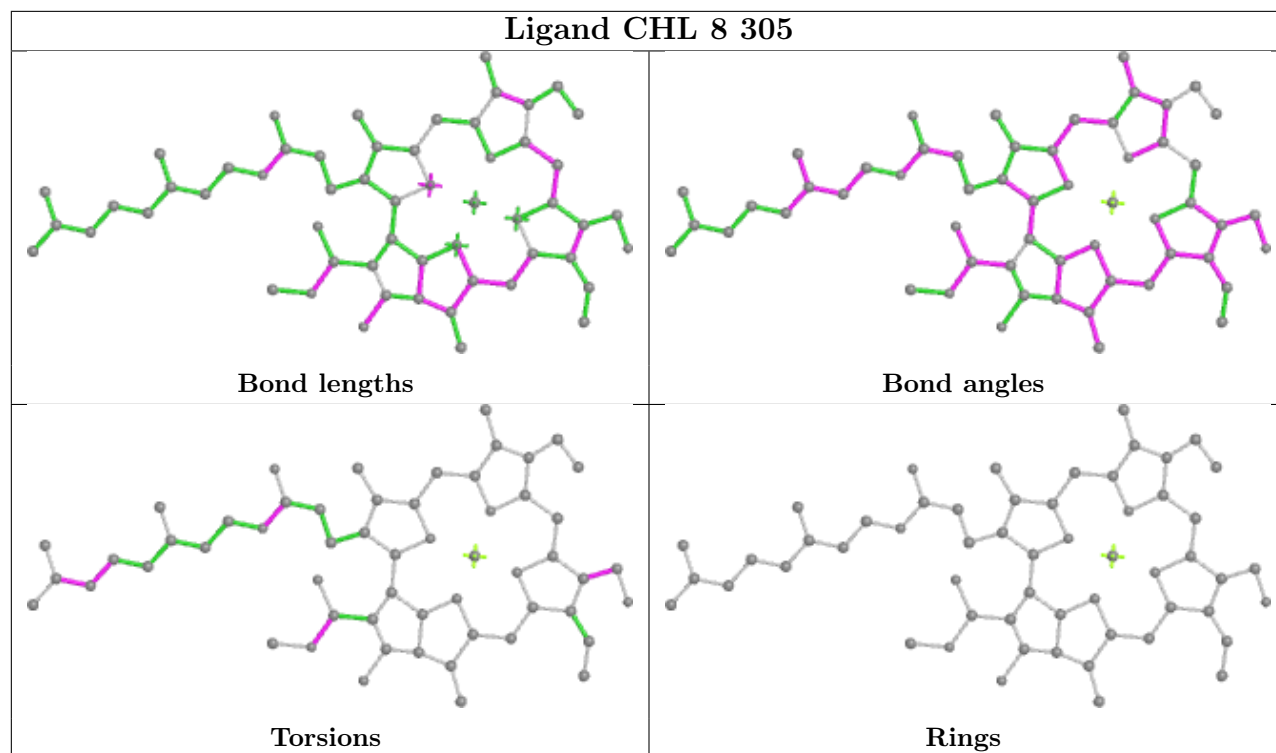
Ligand CLA A 803



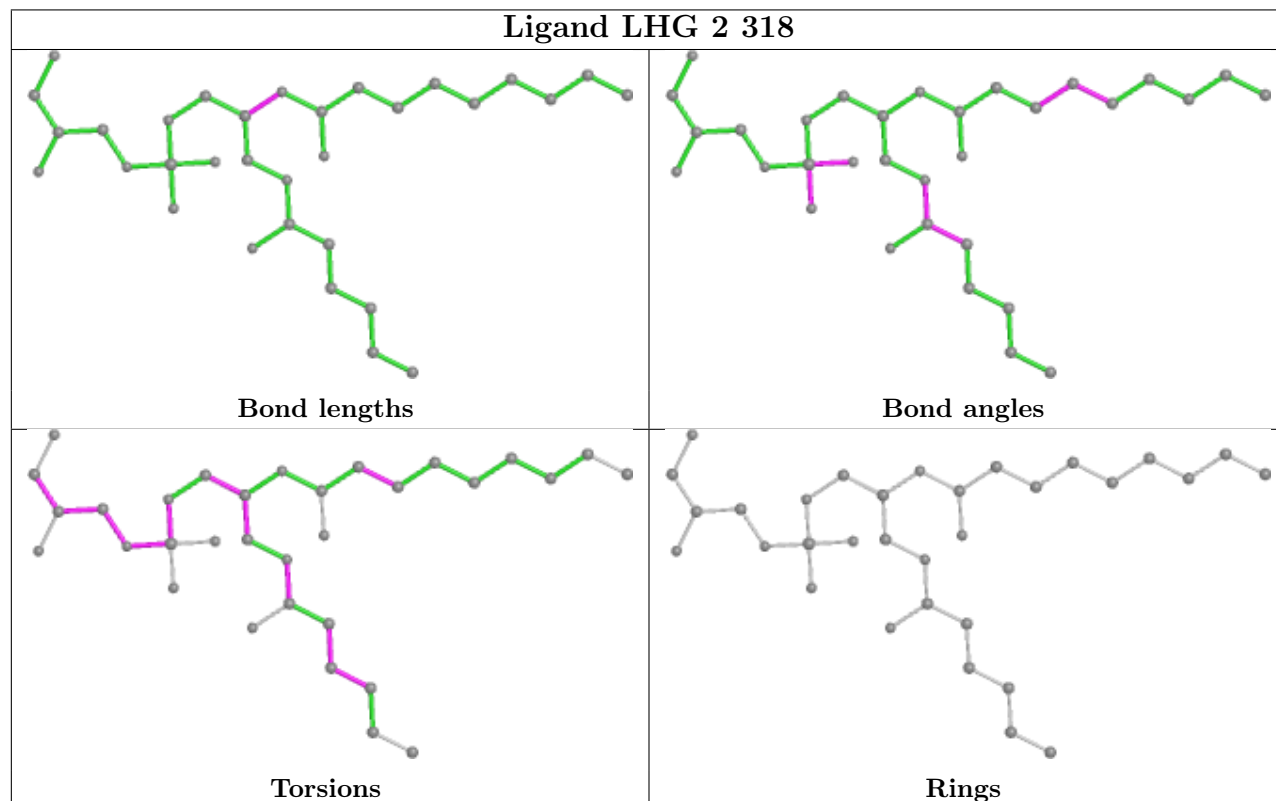
Ligand CLA B 821



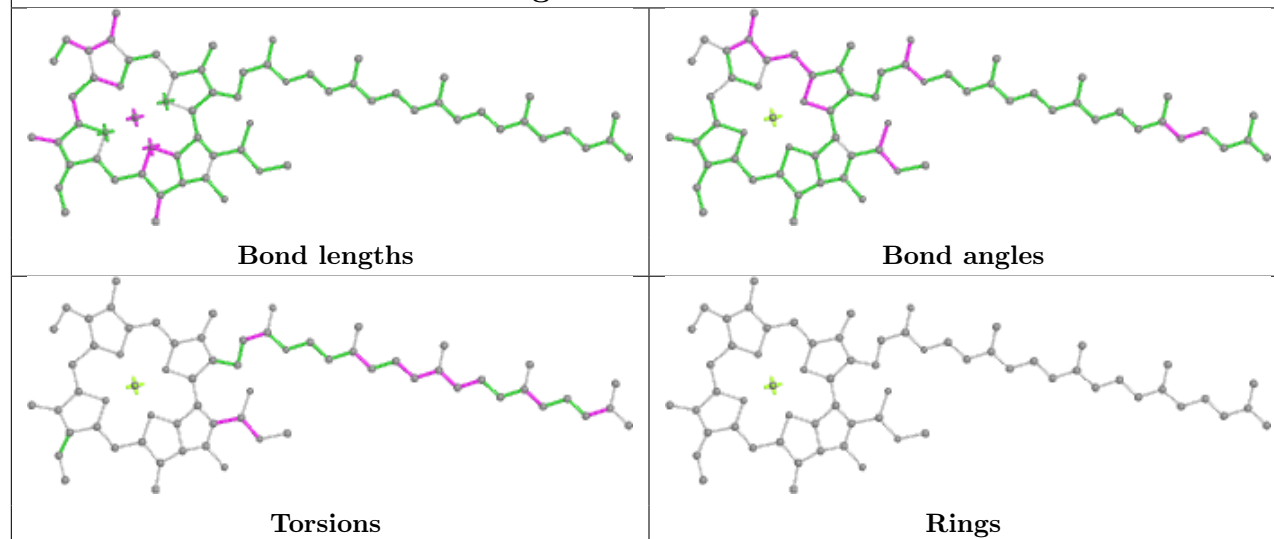
Ligand CHL 8 305



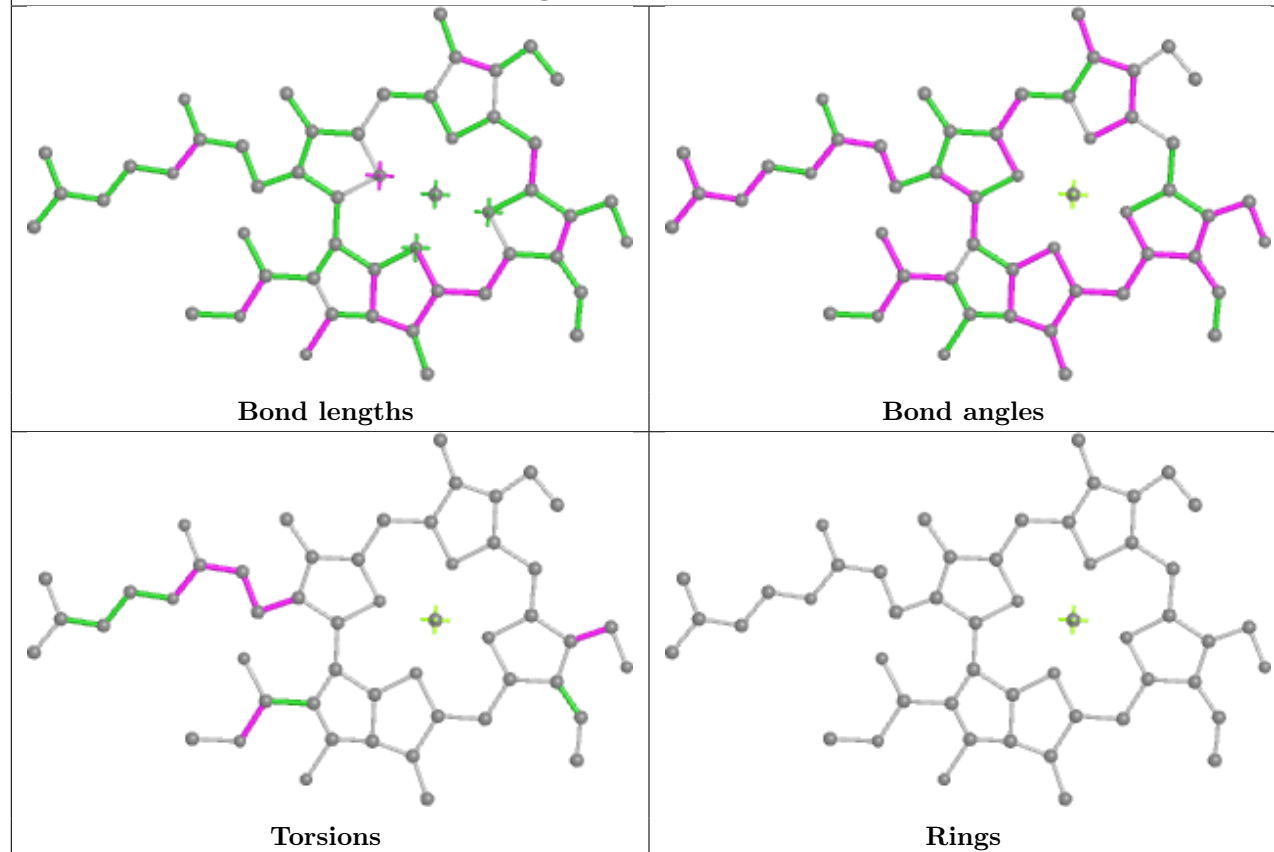
Ligand LHG 2 318

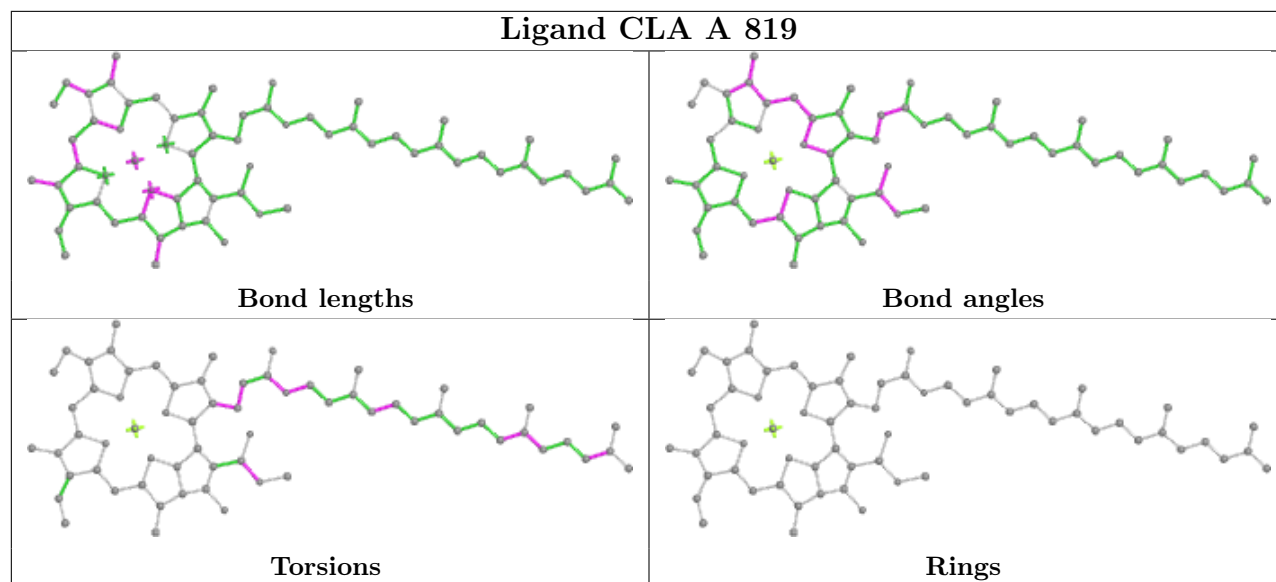
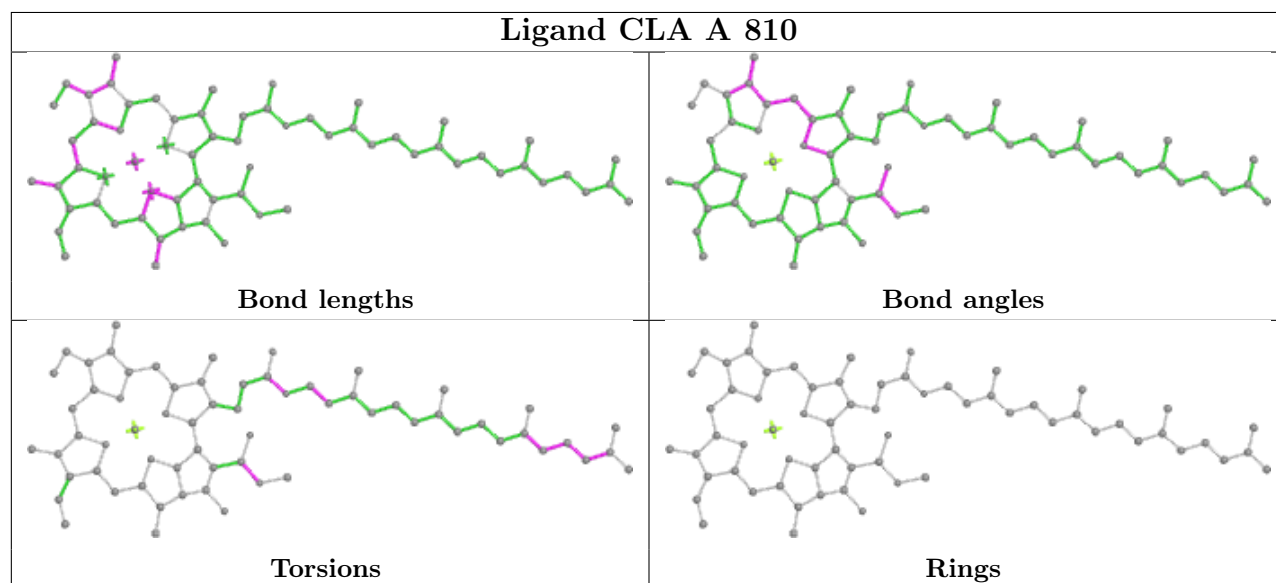


Ligand CLA B 805

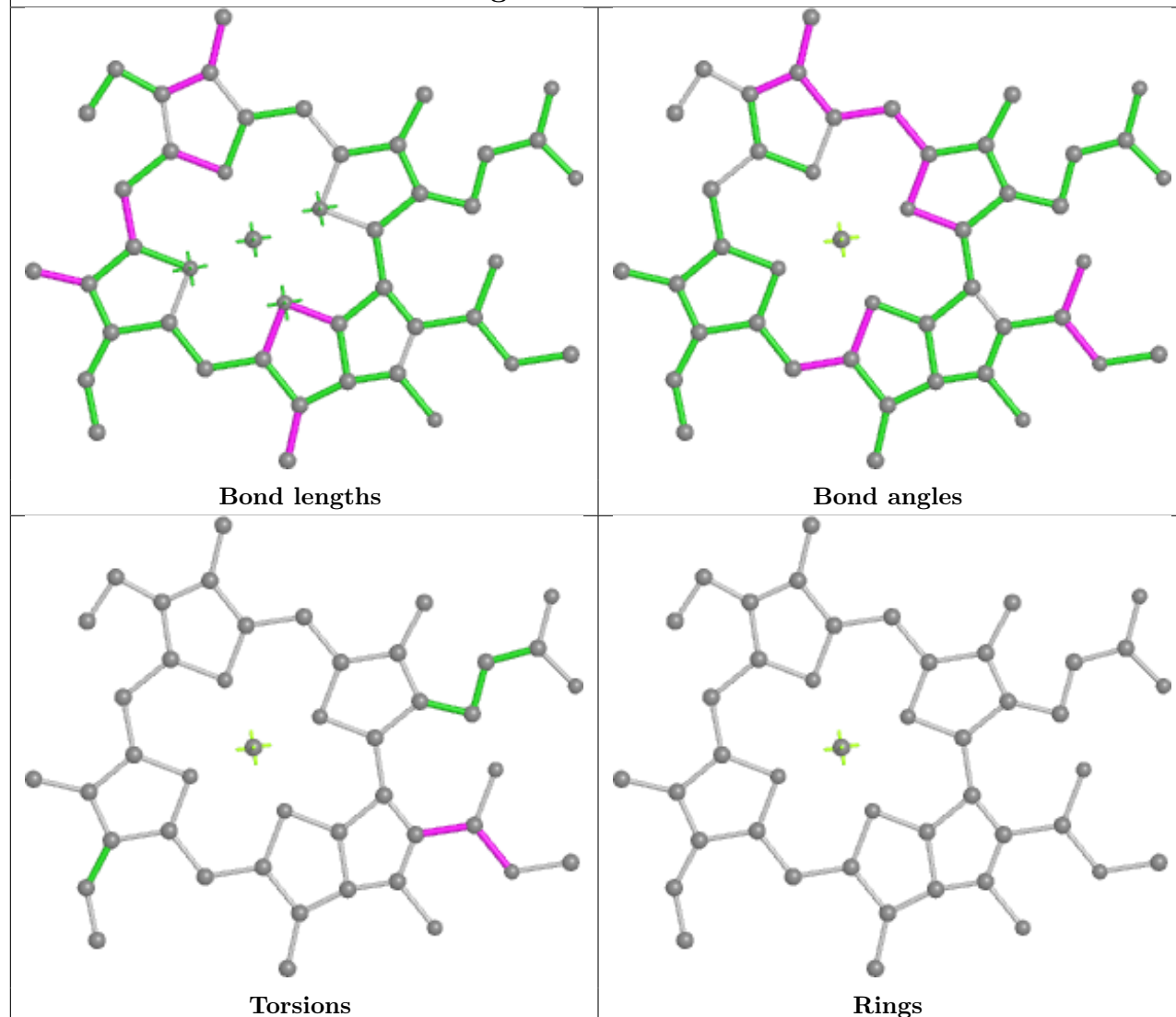


Ligand CHL 2 307

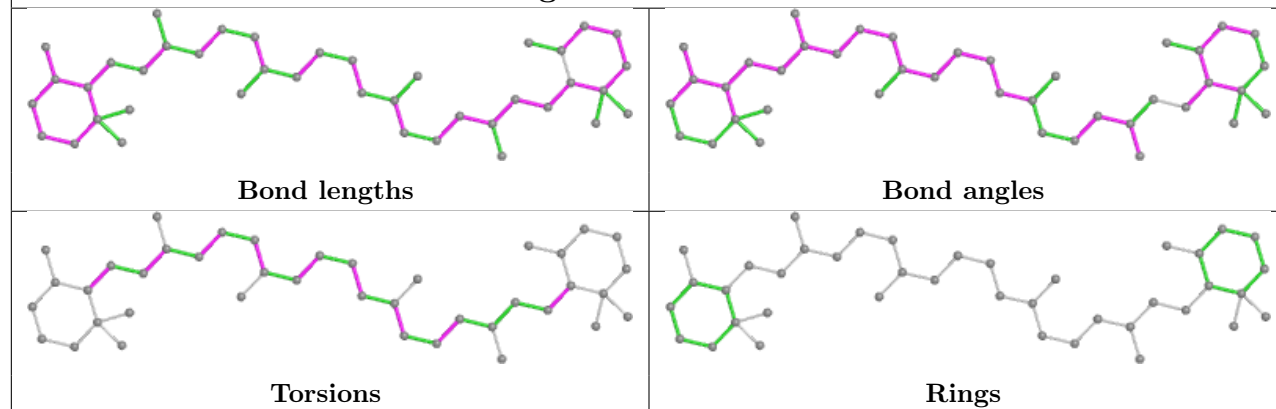


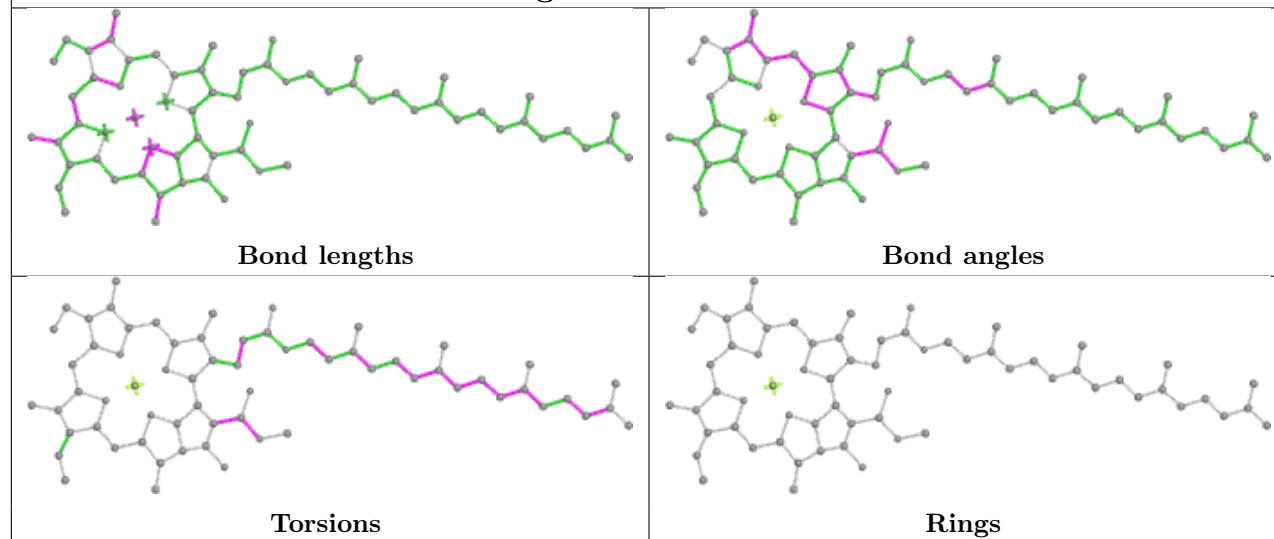
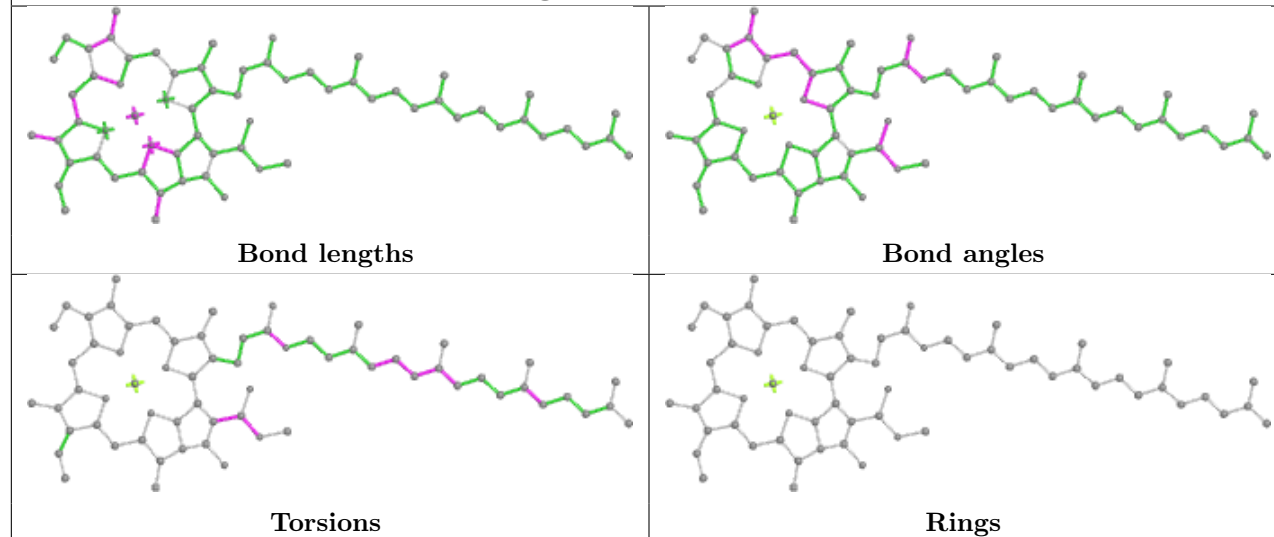
Ligand CLA A 819**Ligand CLA A 810**

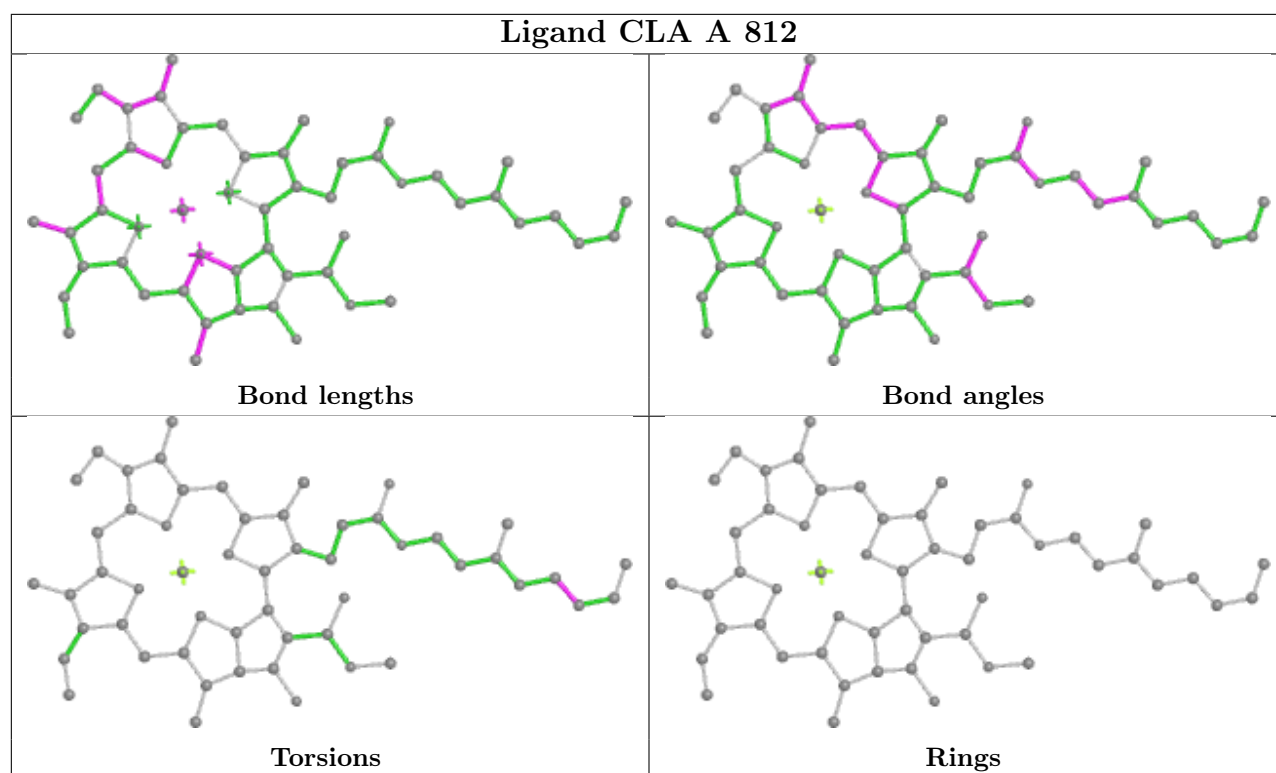
Ligand CLA B 835



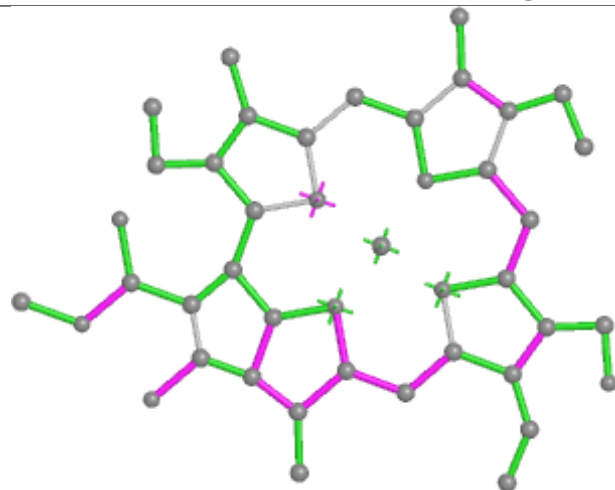
Ligand 8CT 8 301



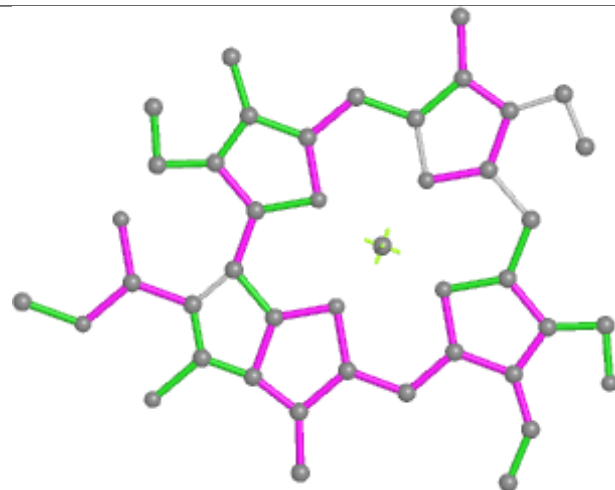
Ligand CLA 3 319**Ligand CLA 6 315**



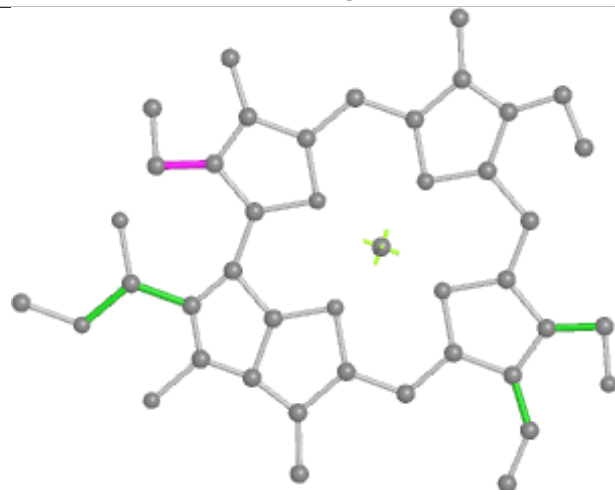
Ligand CHL 6 306



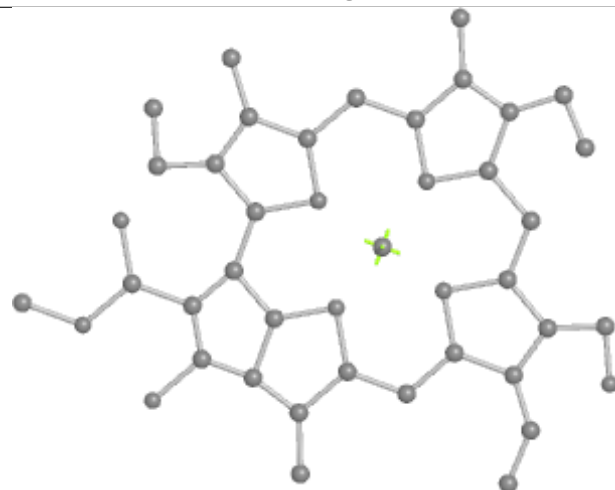
Bond lengths



Bond angles

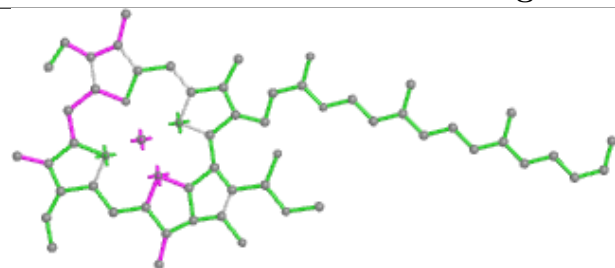


Torsions

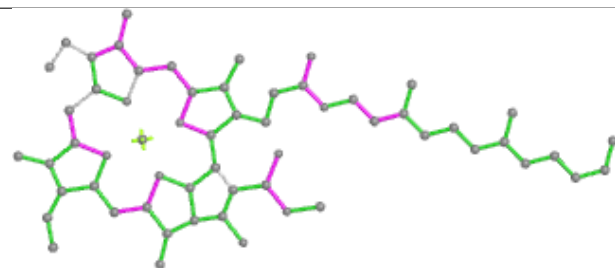


Rings

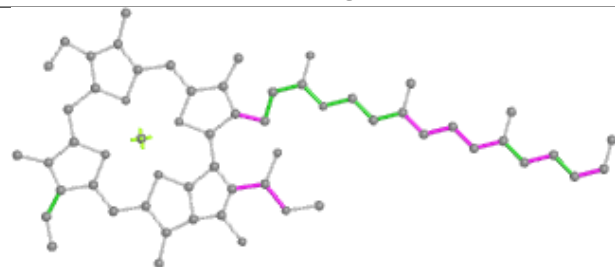
Ligand CLA B 818



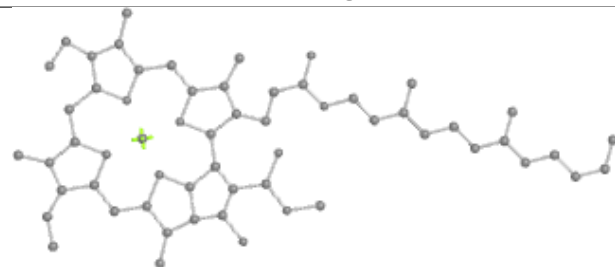
Bond lengths



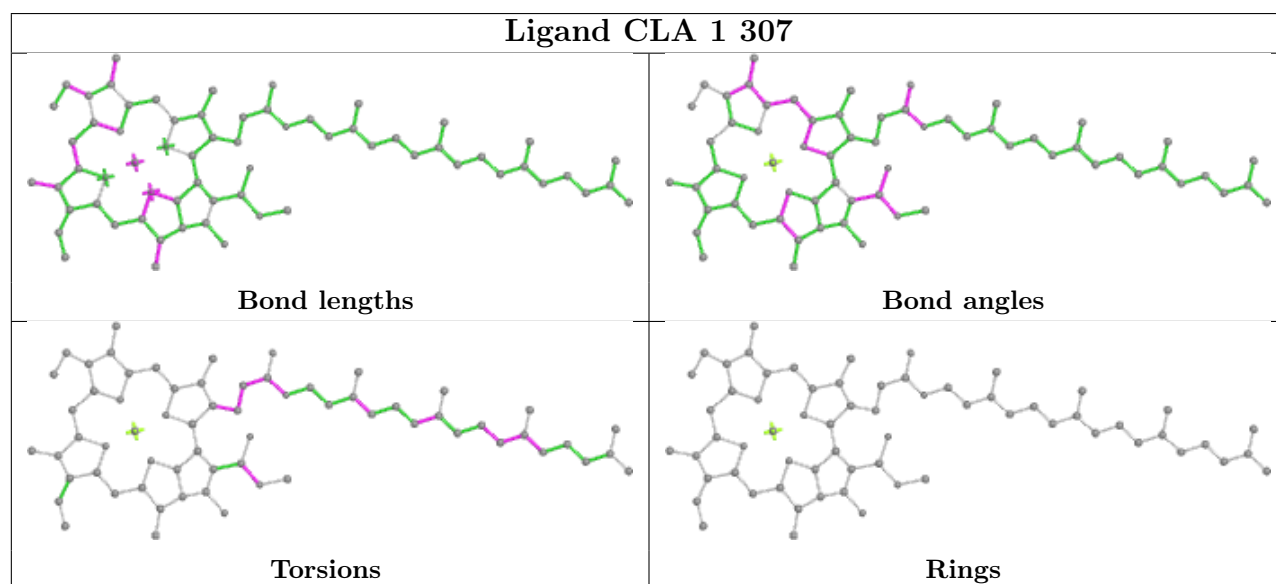
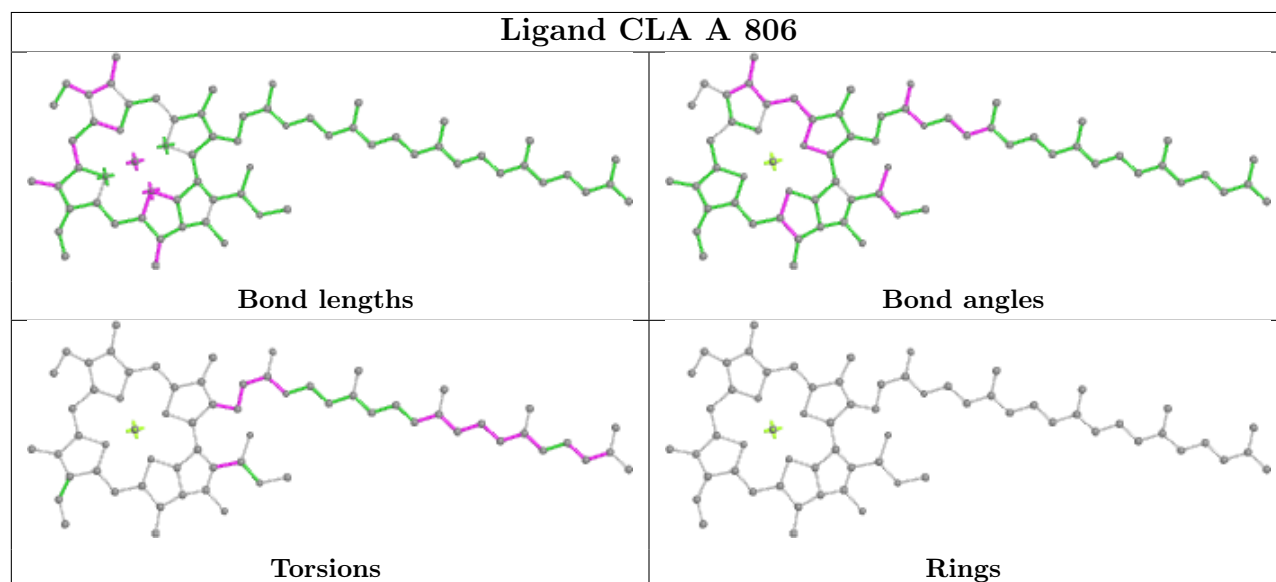
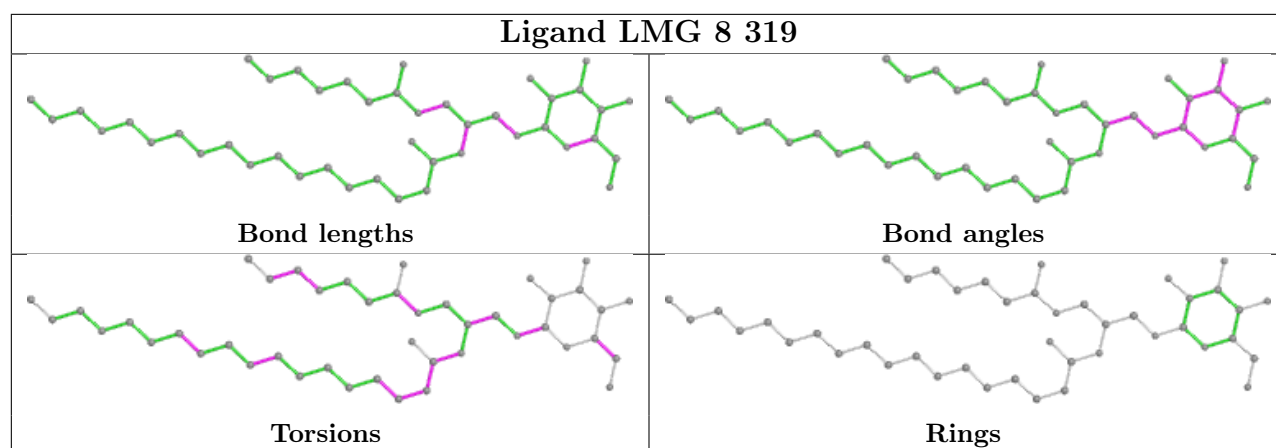
Bond angles



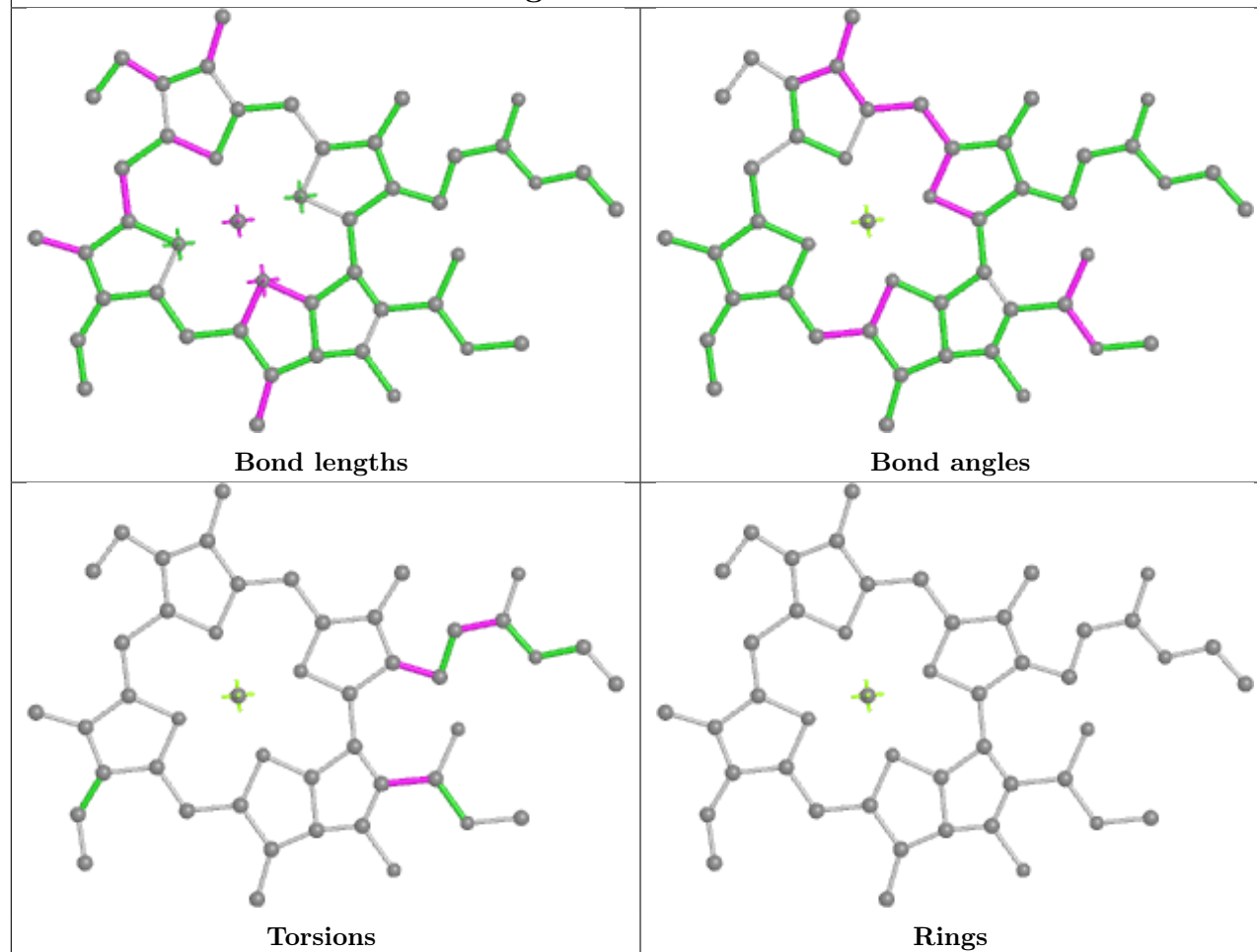
Torsions



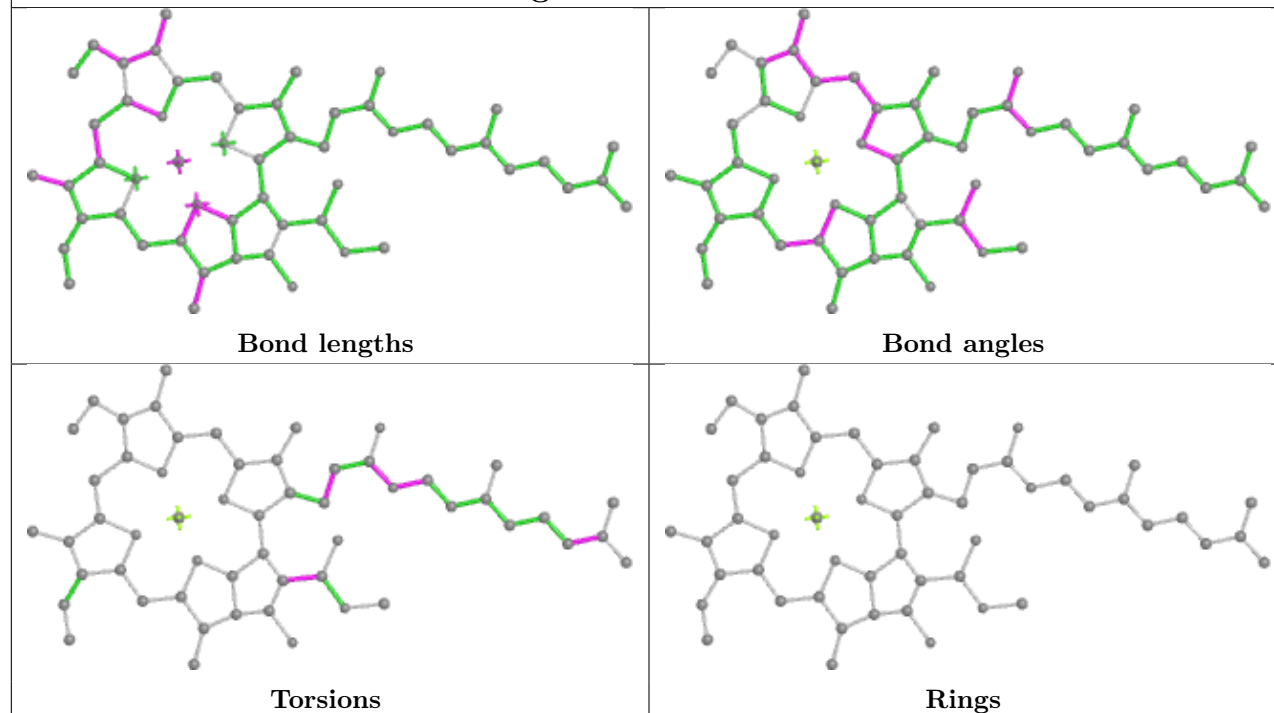
Rings



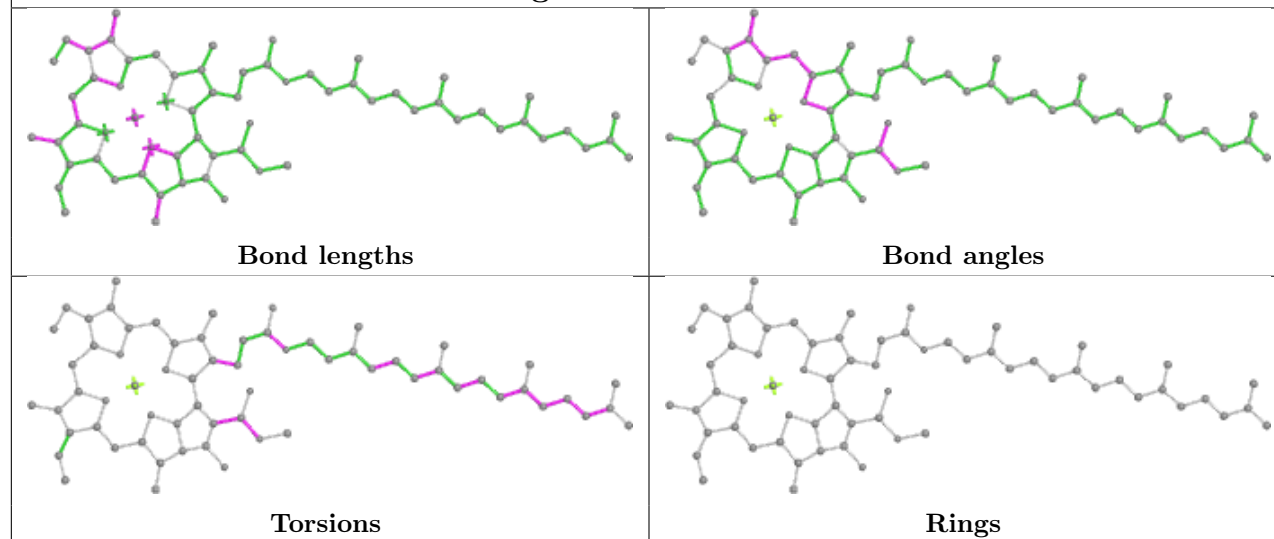
Ligand CLA B 838



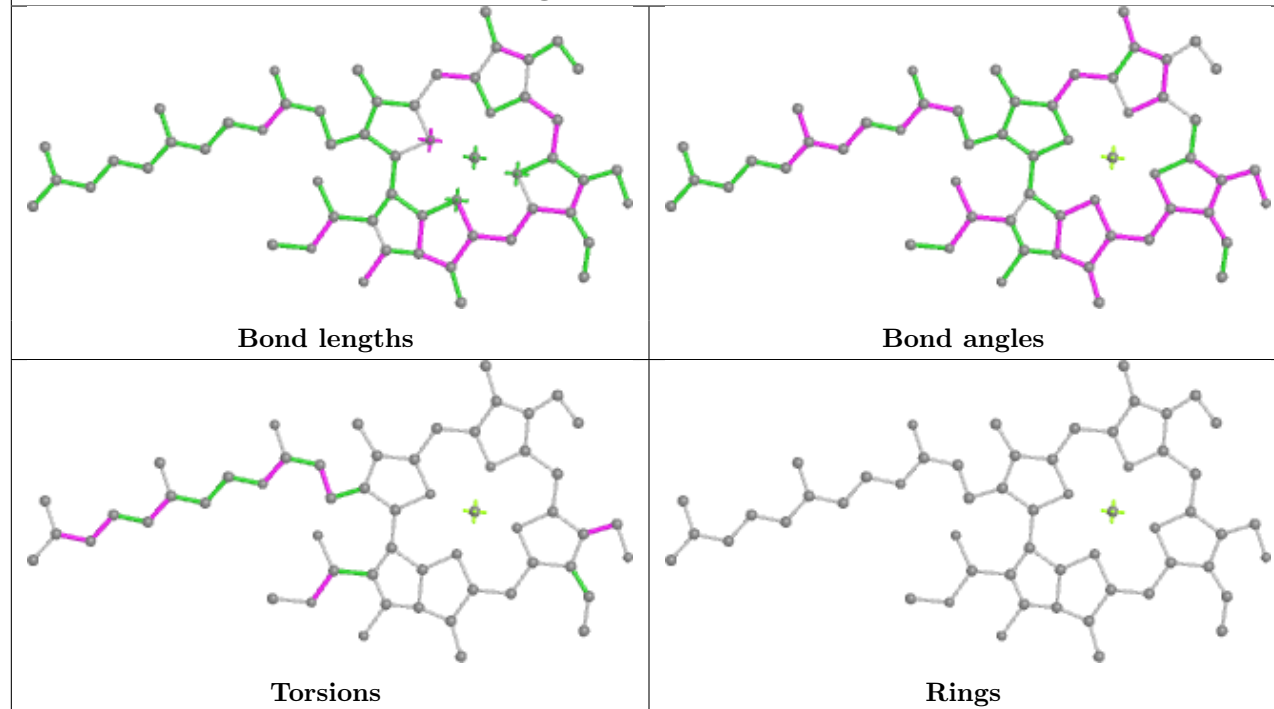
Ligand CLA A 824

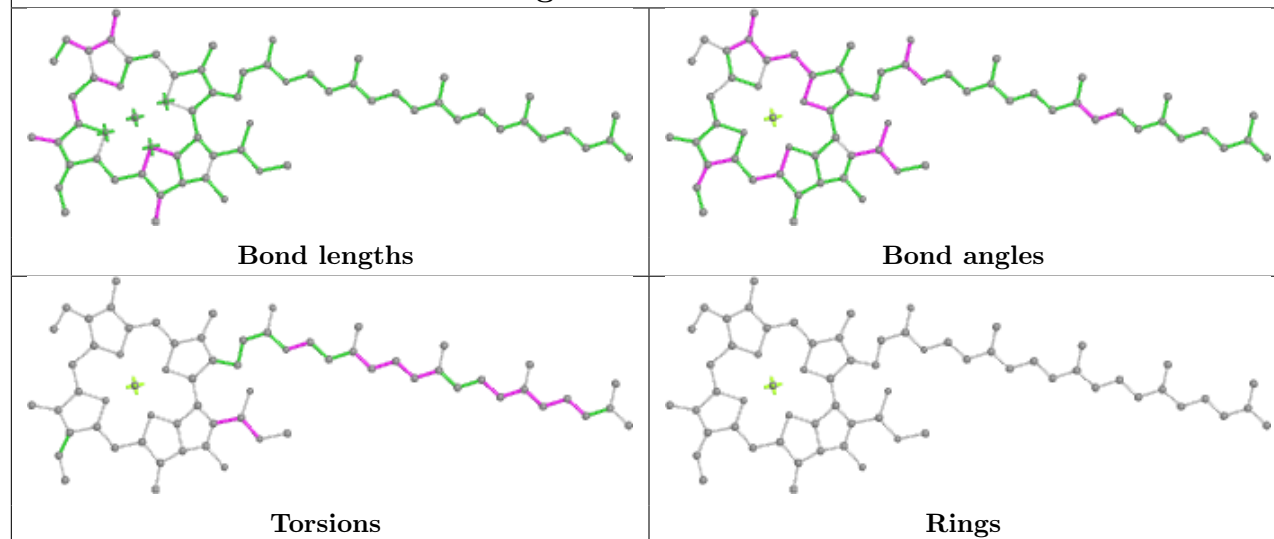
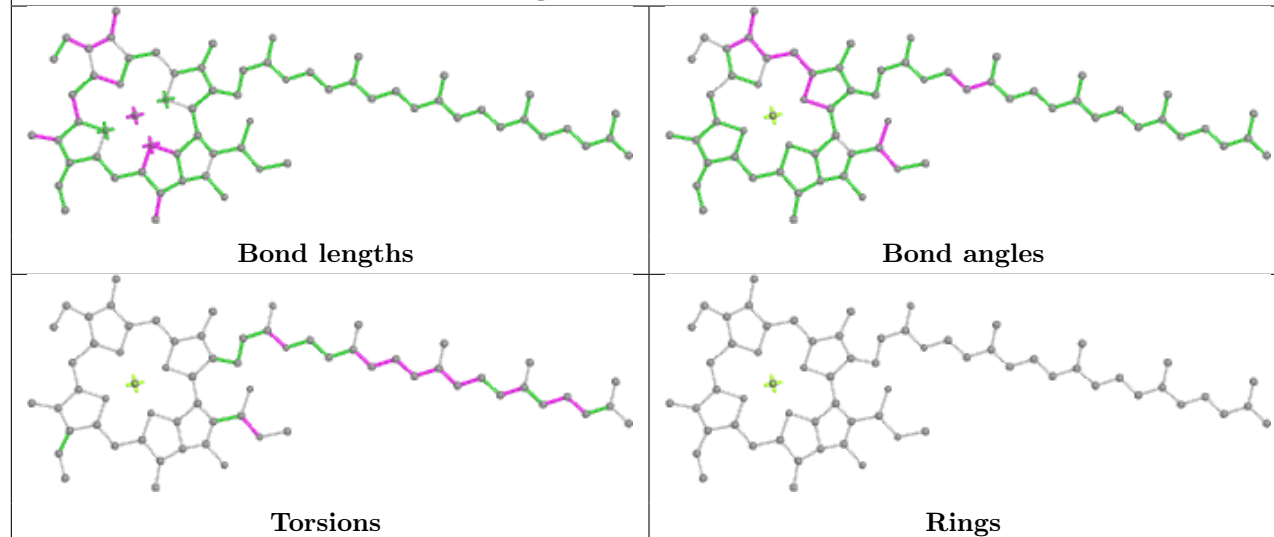


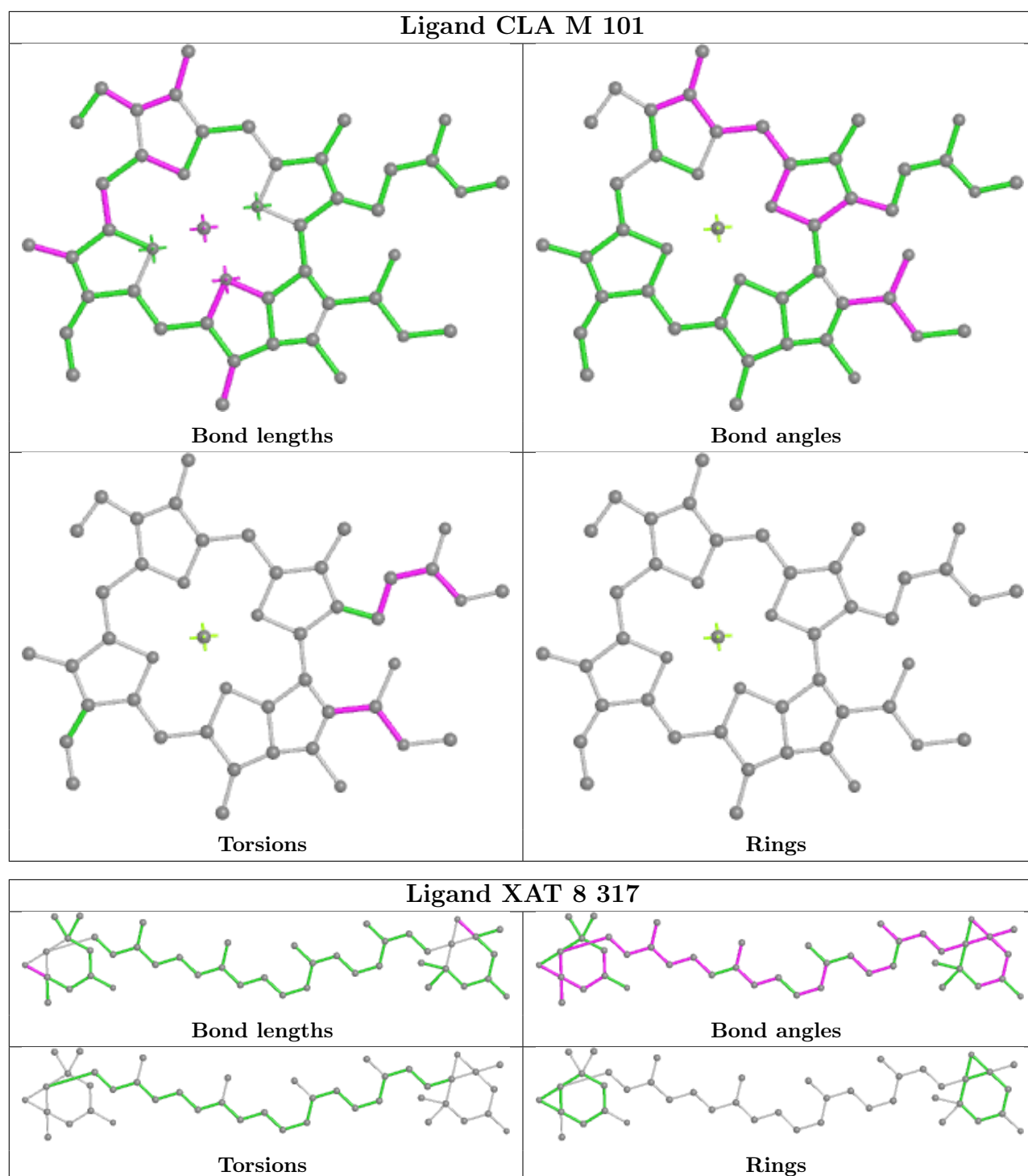
Ligand CLA A 811



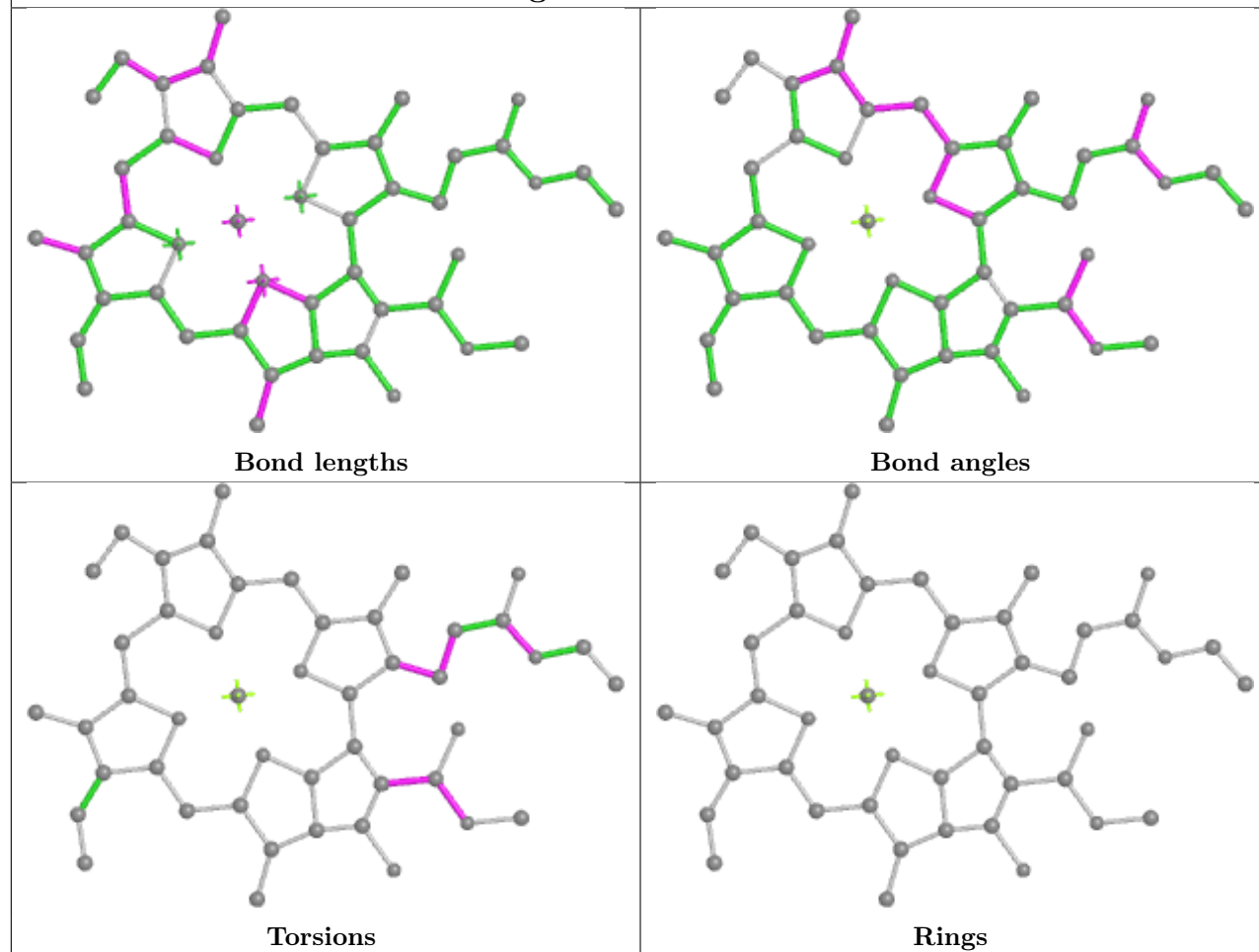
Ligand CHL 4 305



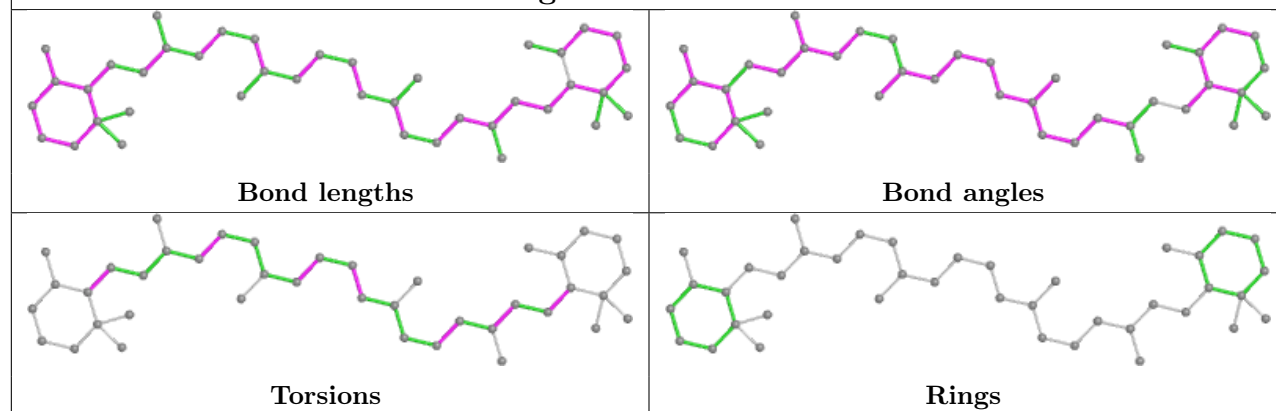
Ligand CLA 2 302**Ligand CLA B 812**

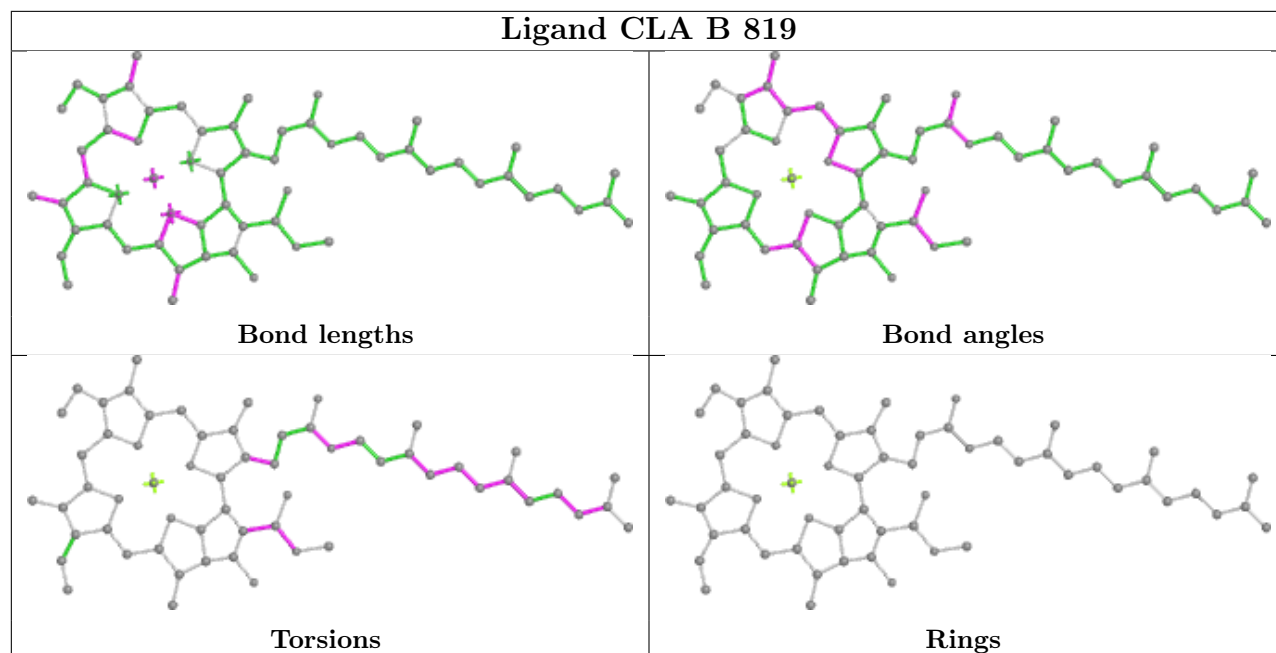
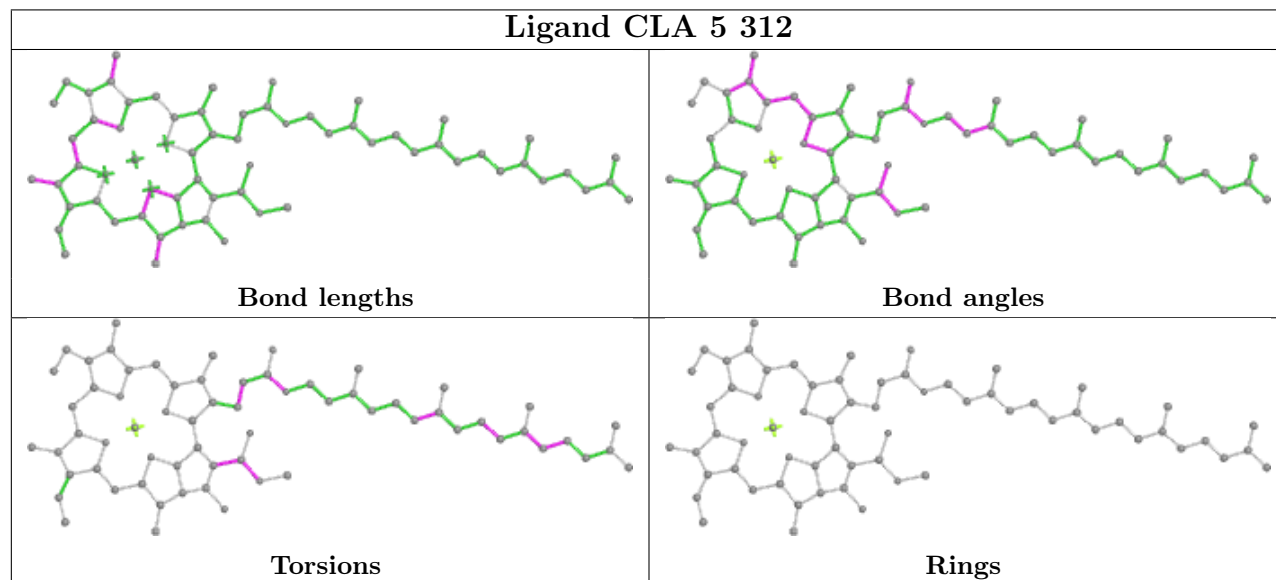


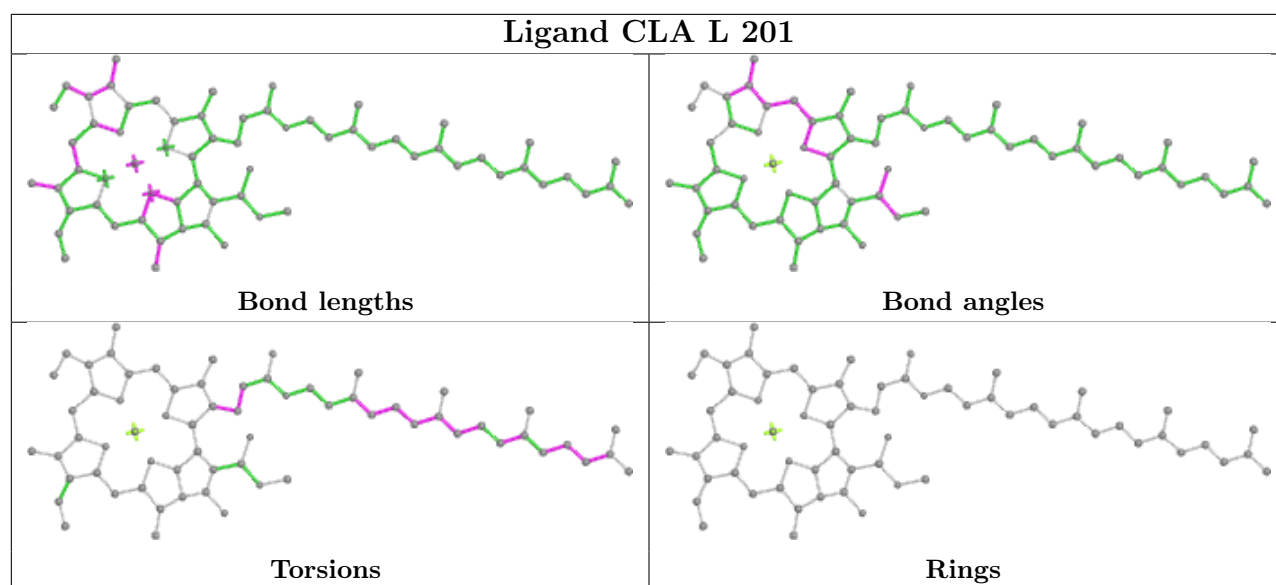
Ligand CLA 3 305



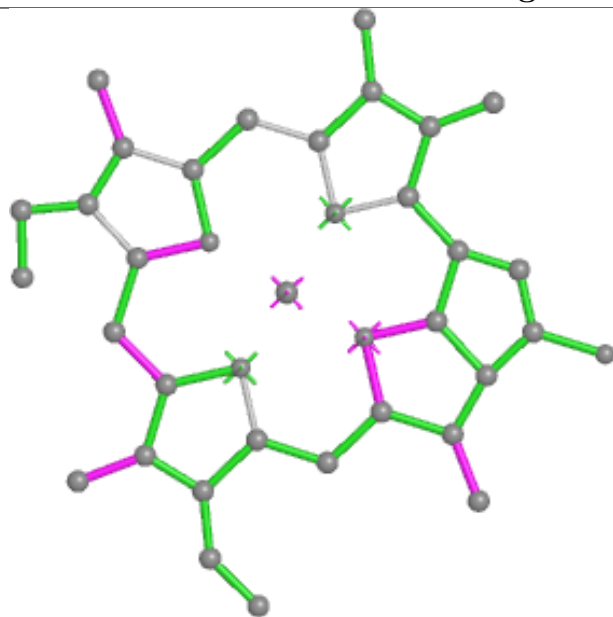
Ligand 8CT J 101



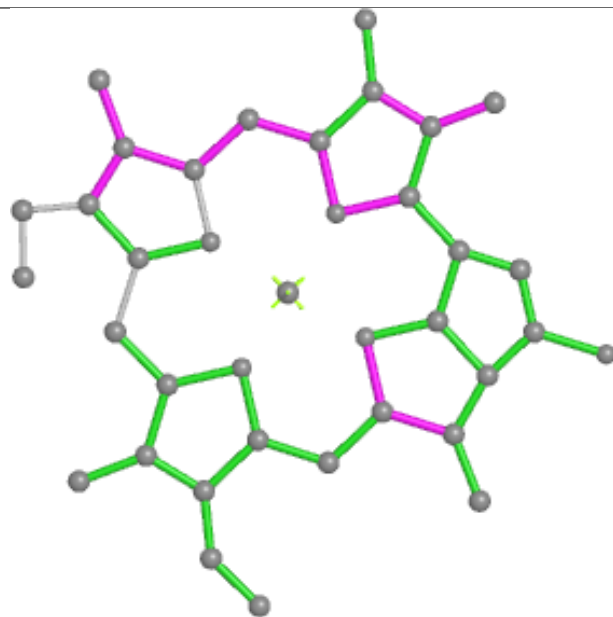
Ligand CLA B 819**Ligand CLA 5 312**



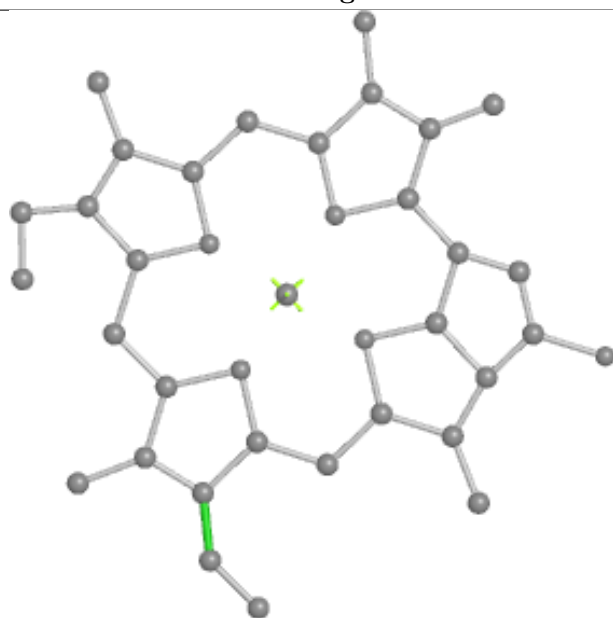
Ligand CLA 7 311



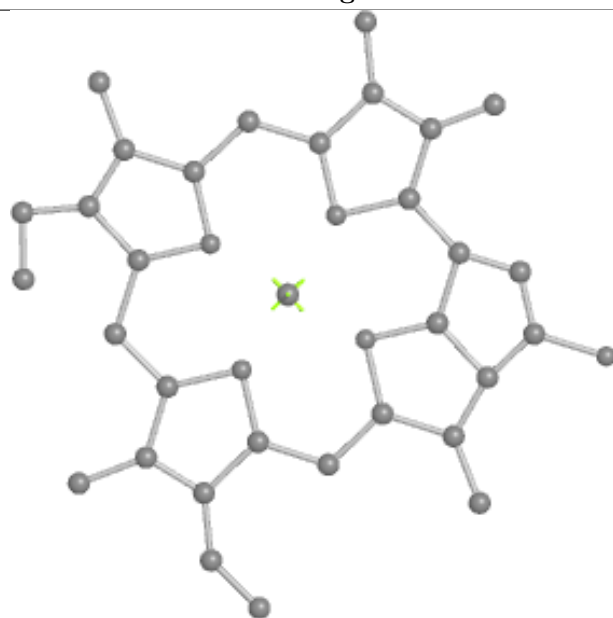
Bond lengths



Bond angles

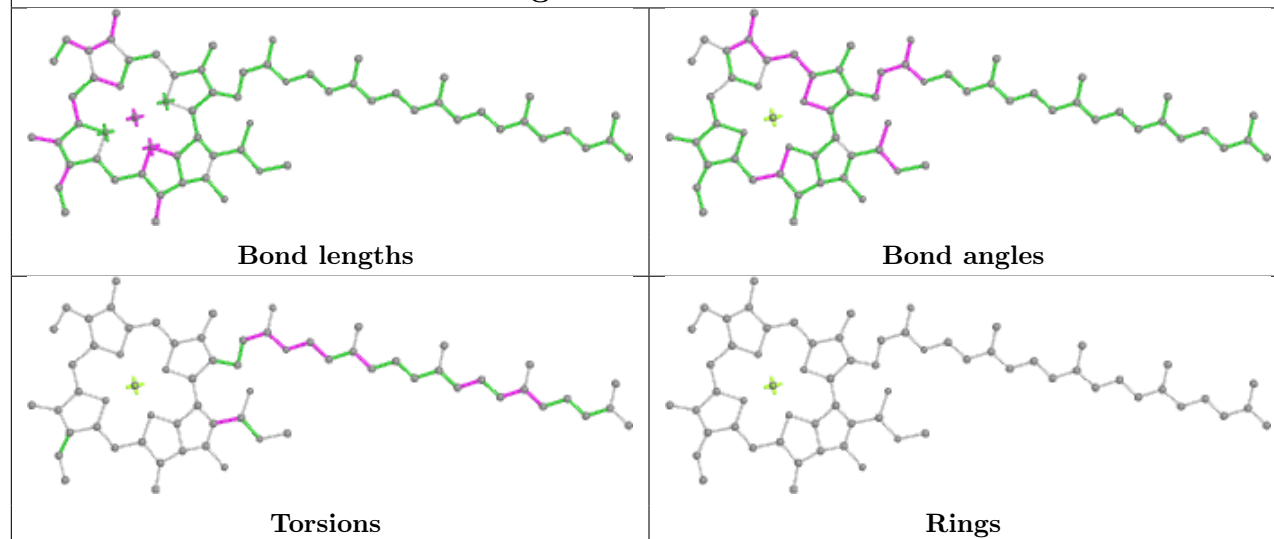


Torsions

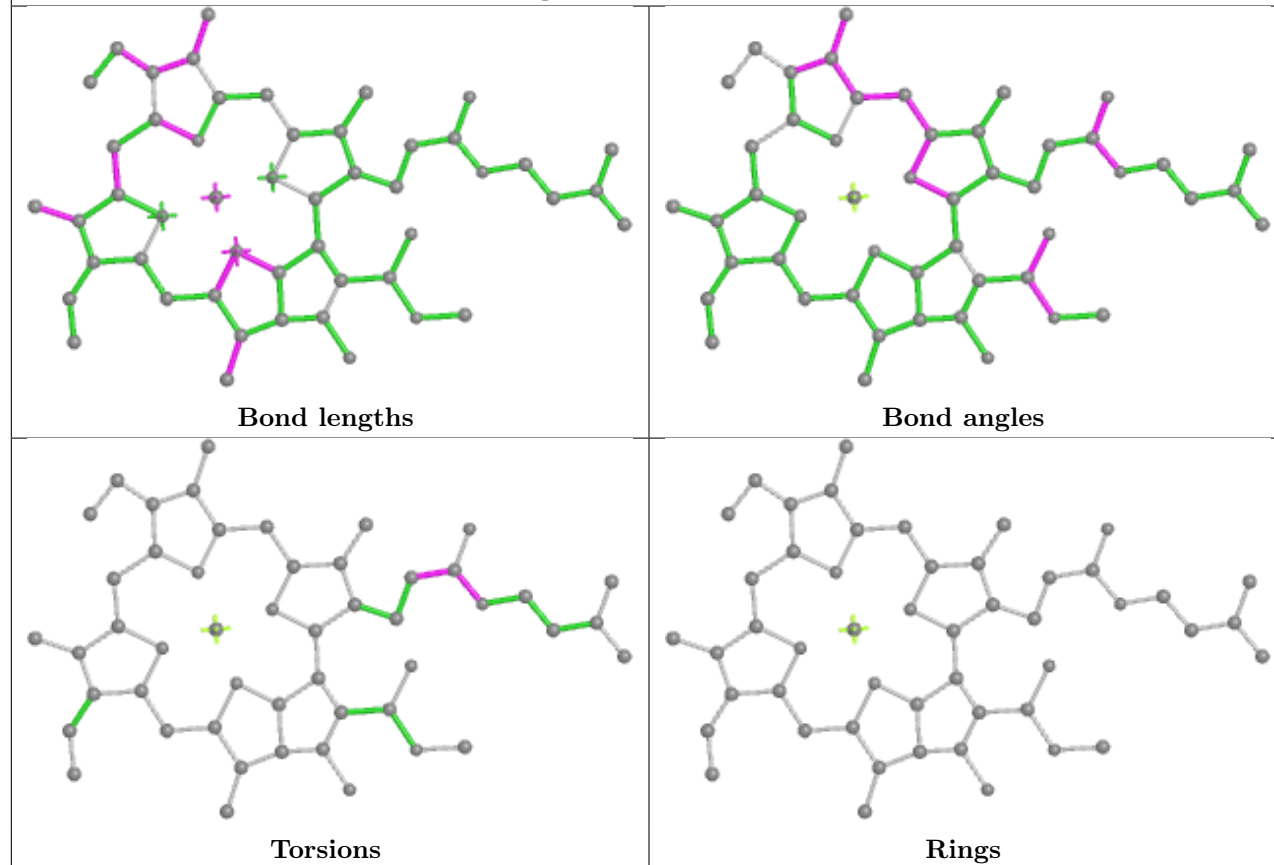


Rings

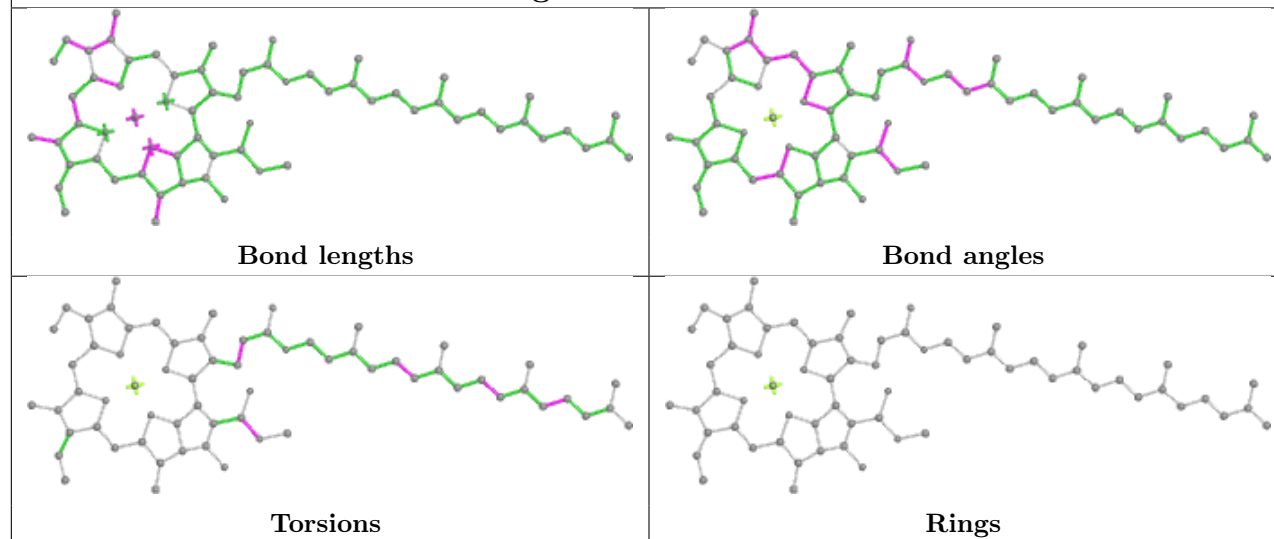
Ligand CLA A 805



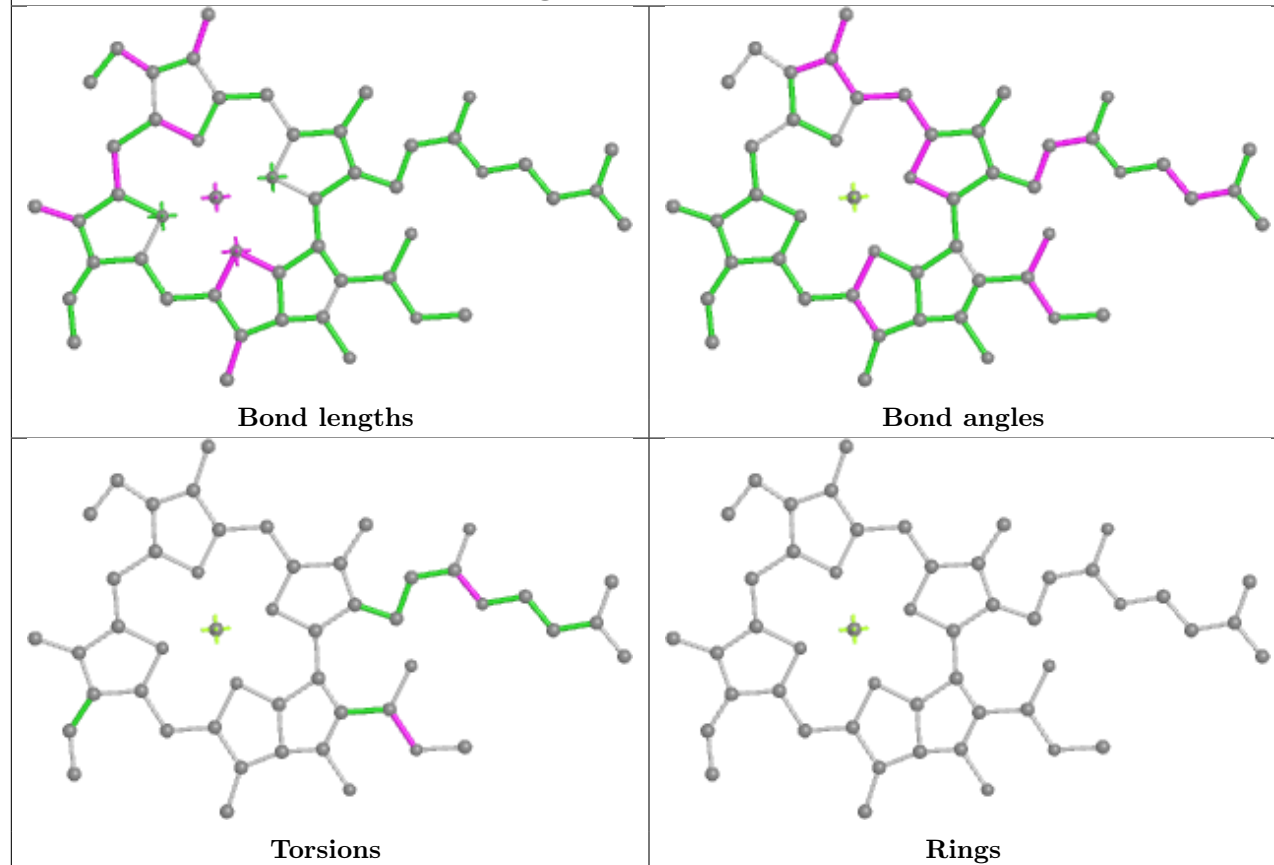
Ligand CLA 7 309



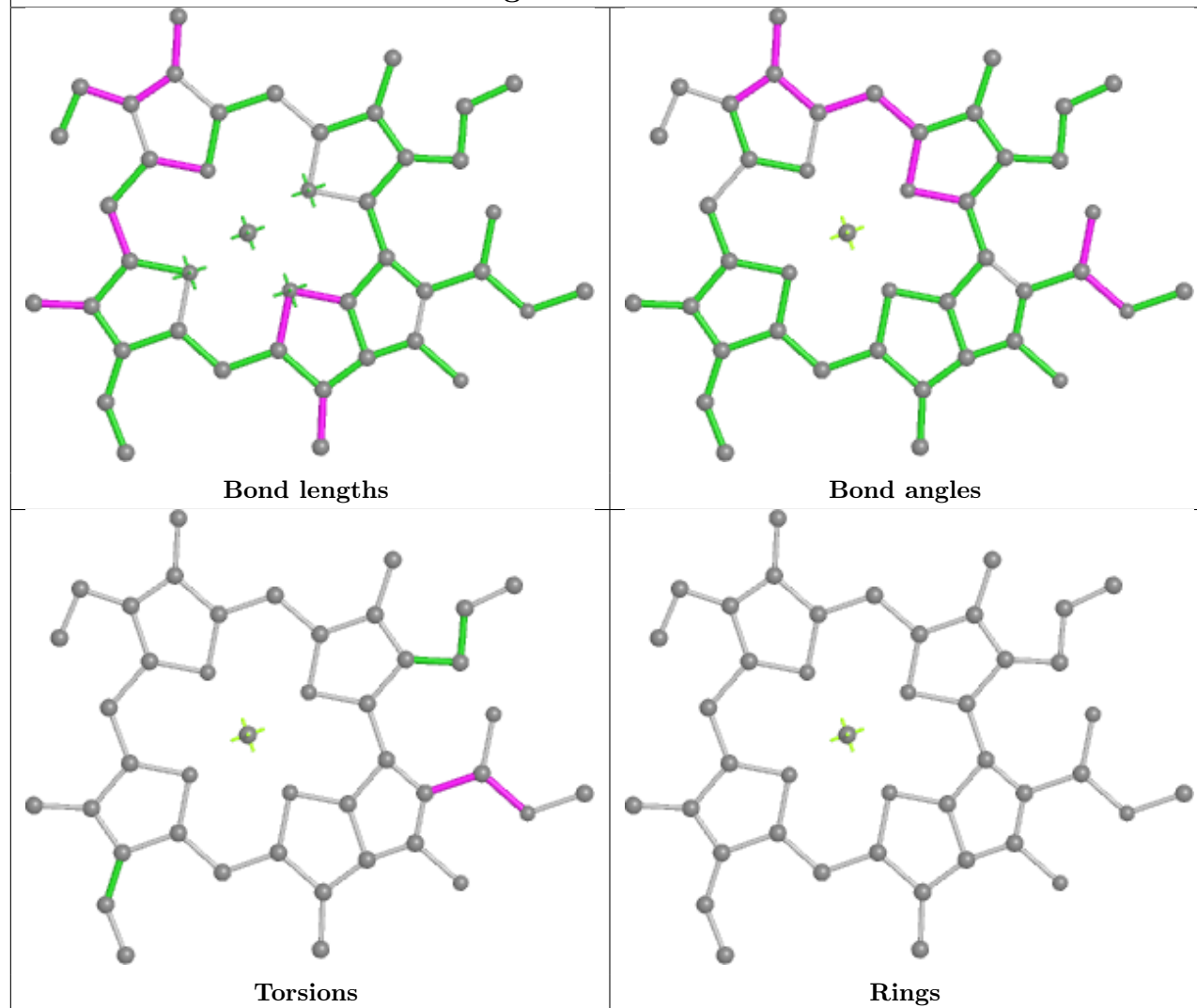
Ligand CLA B 810



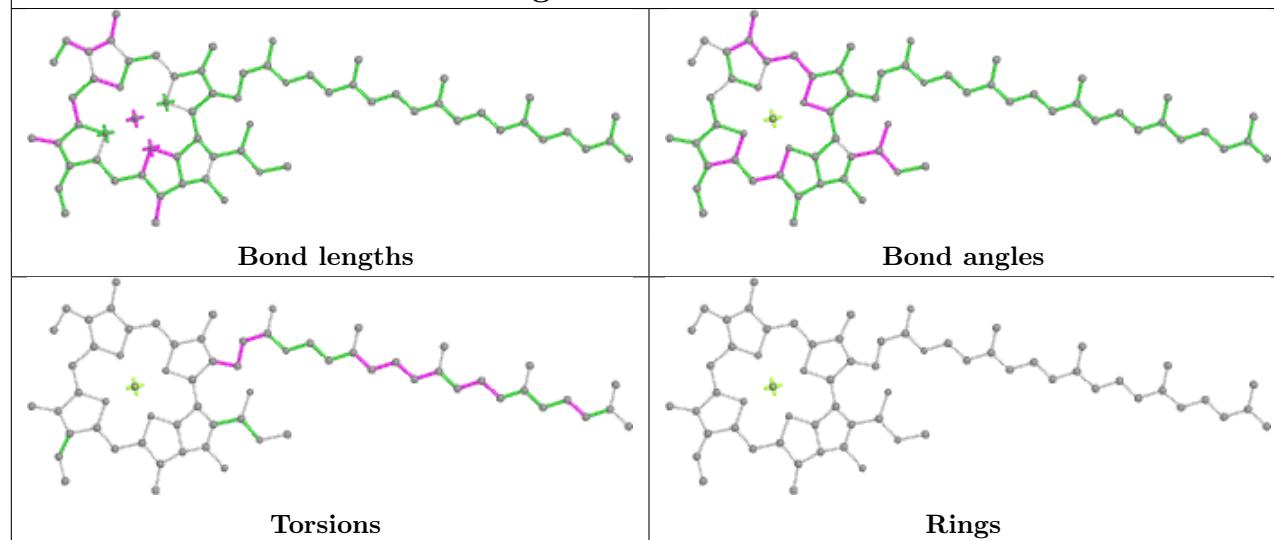
Ligand CLA 4 304



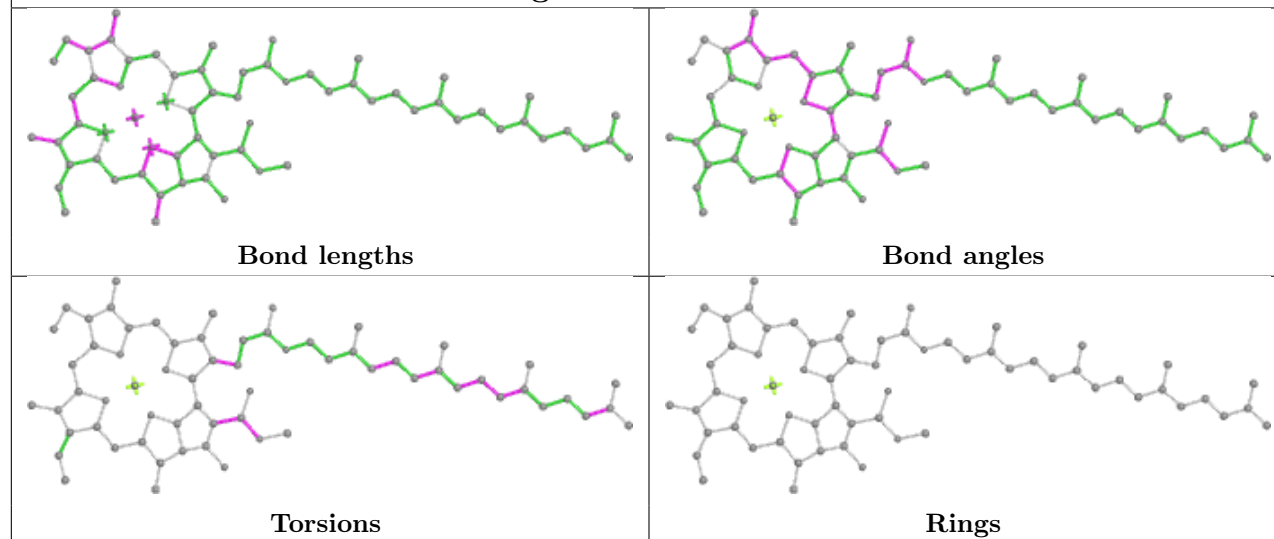
Ligand CLA 6 314



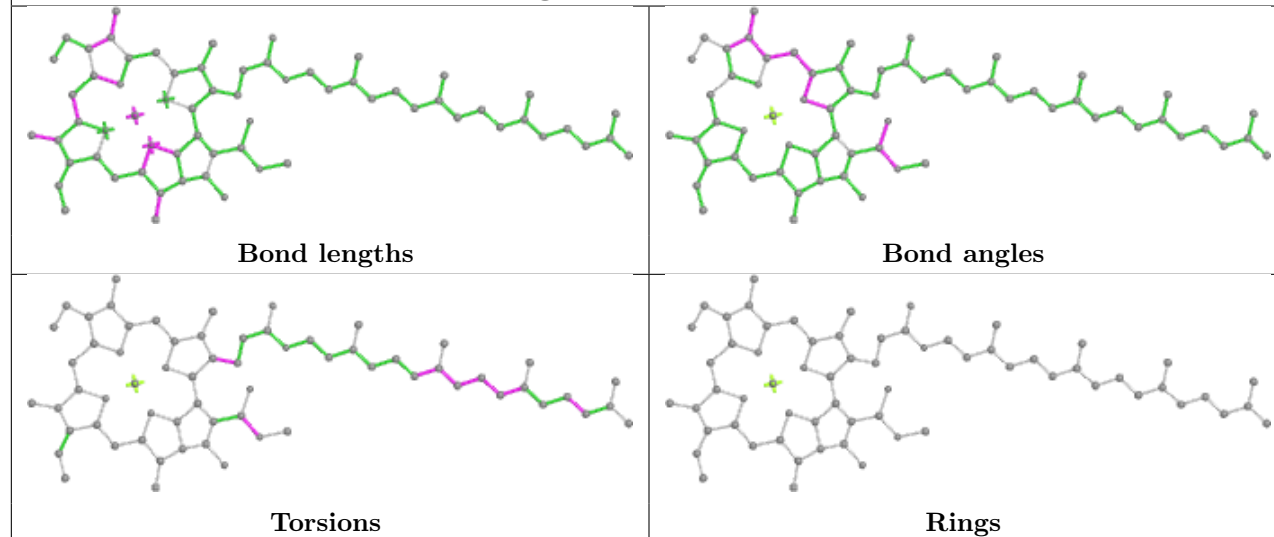
Ligand CLA B 832



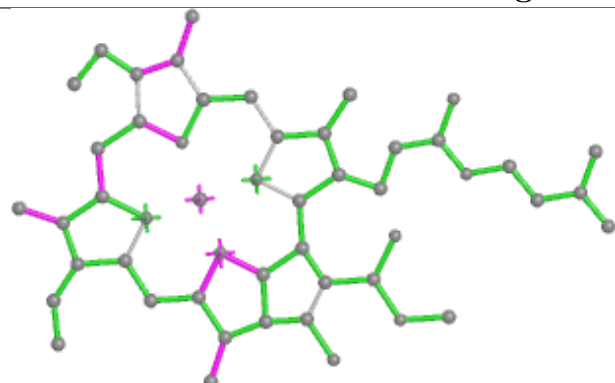
Ligand CLA A 809



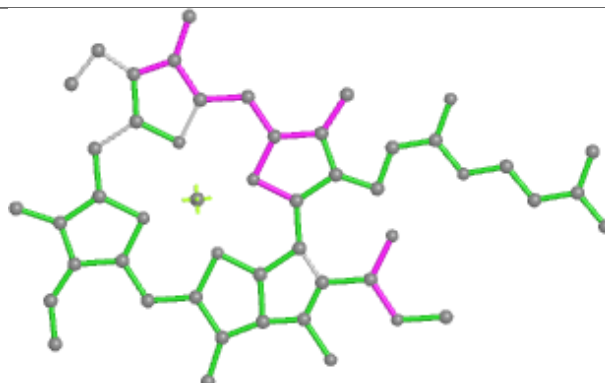
Ligand CLA 2 303



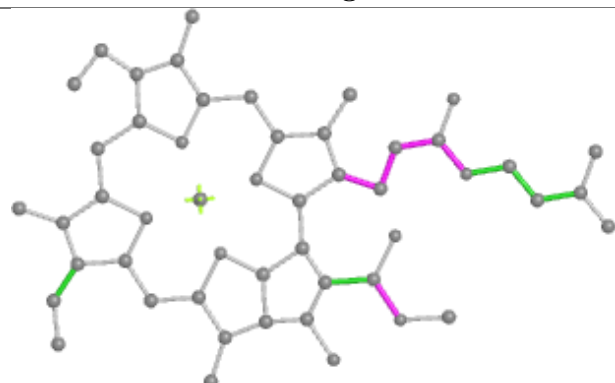
Ligand CLA K 105



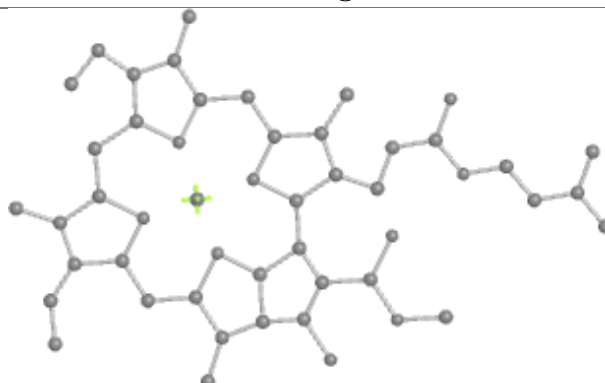
Bond lengths



Bond angles

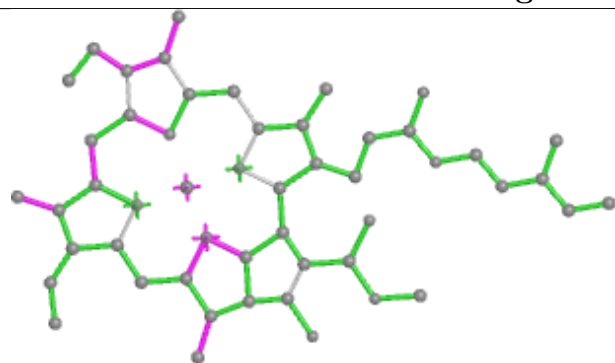


Torsions

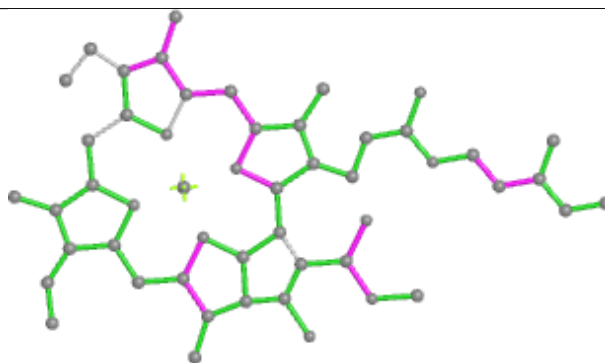


Rings

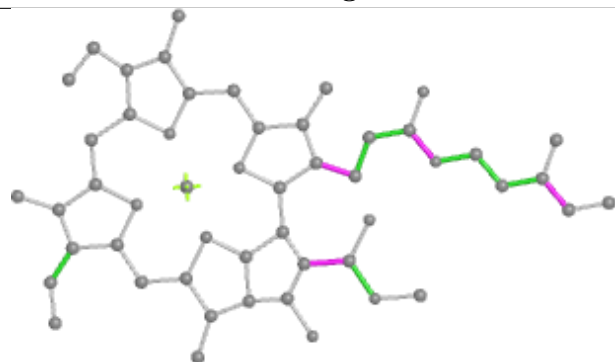
Ligand CLA A 823



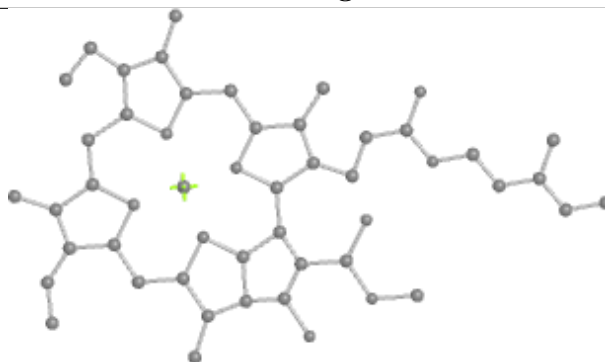
Bond lengths



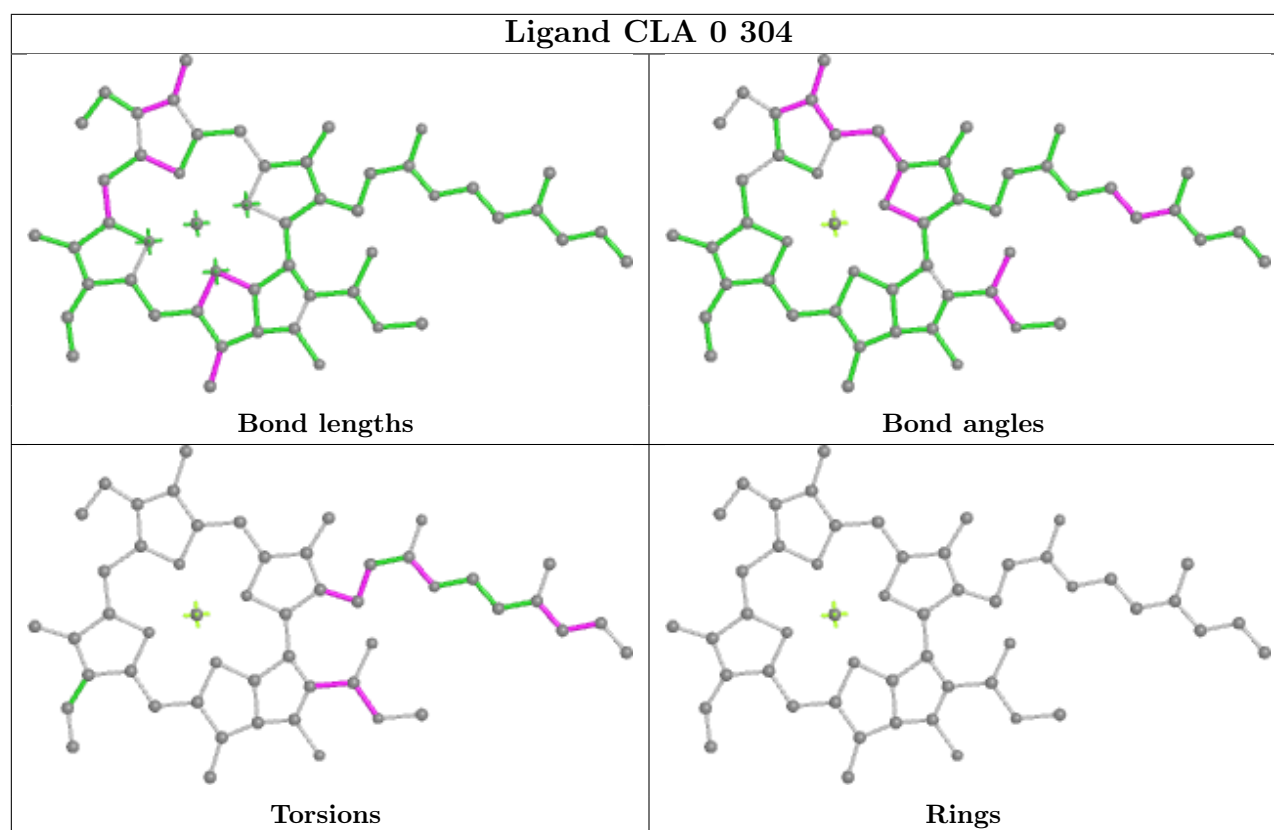
Bond angles



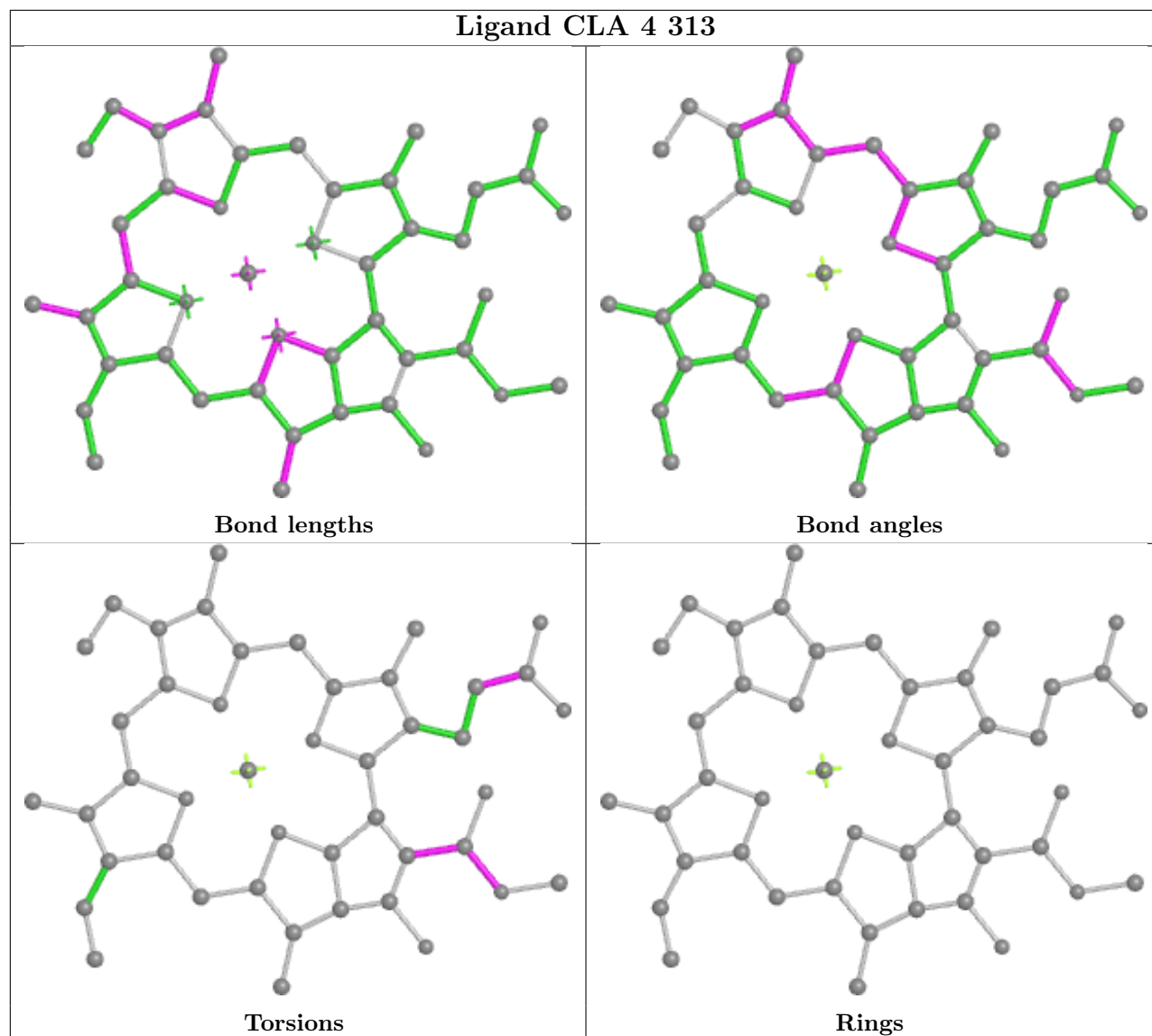
Torsions



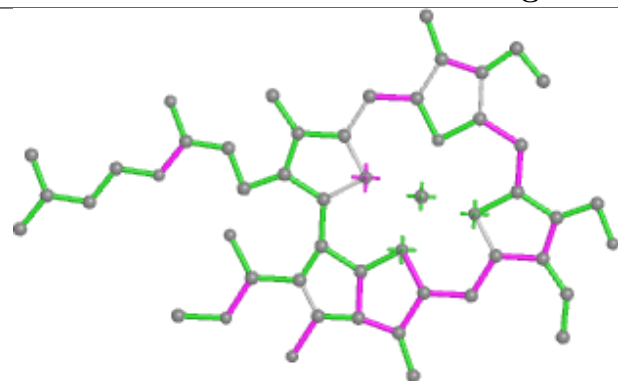
Rings



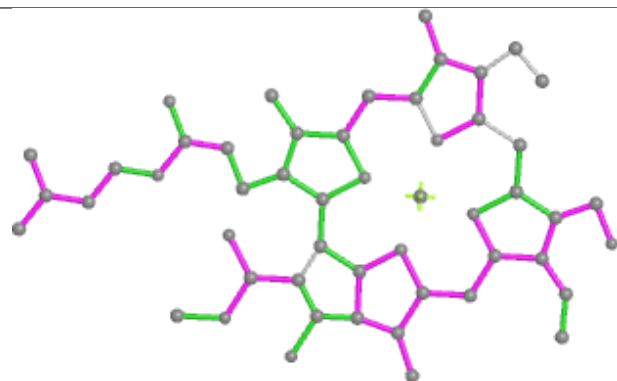
Ligand CLA 4 313



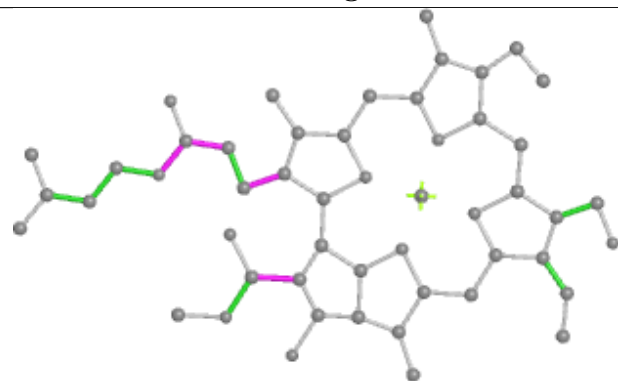
Ligand CHL 4 306



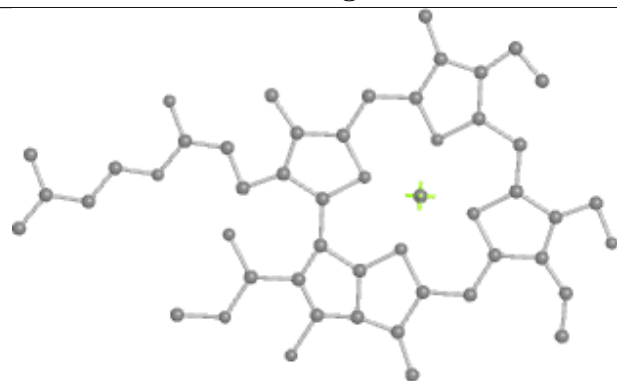
Bond lengths



Bond angles

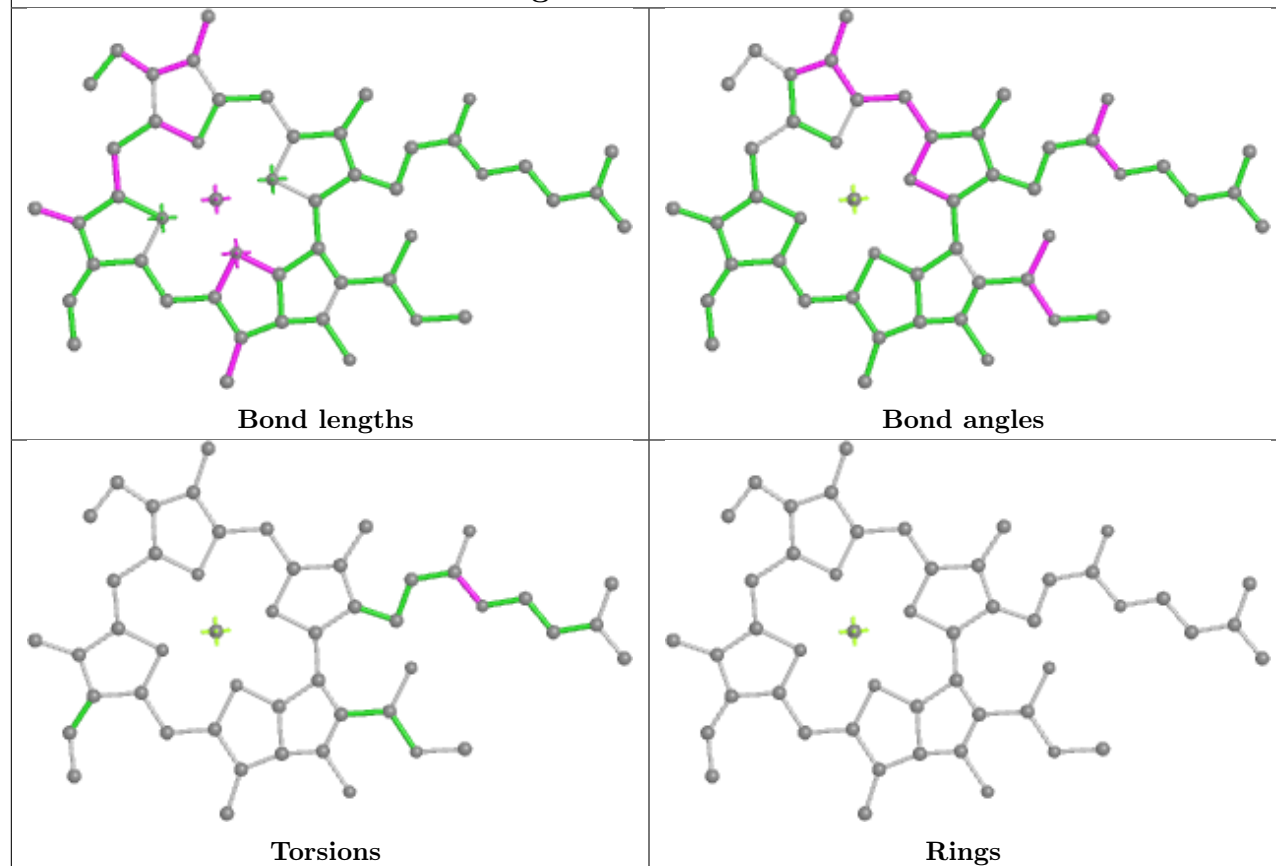


Torsions

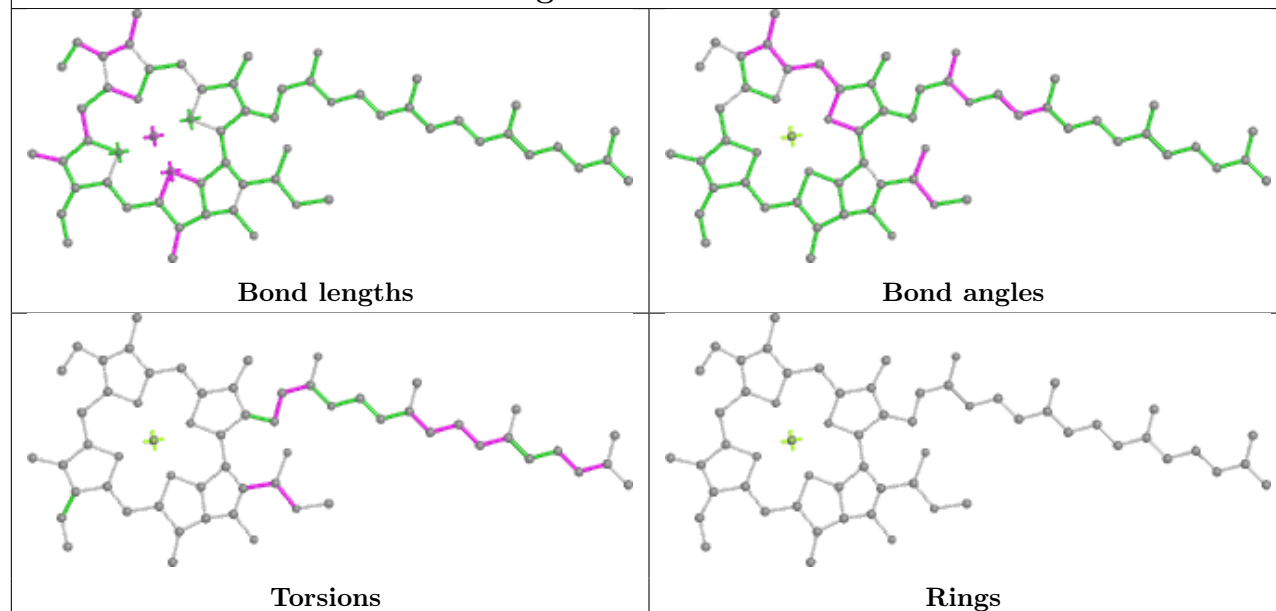


Rings

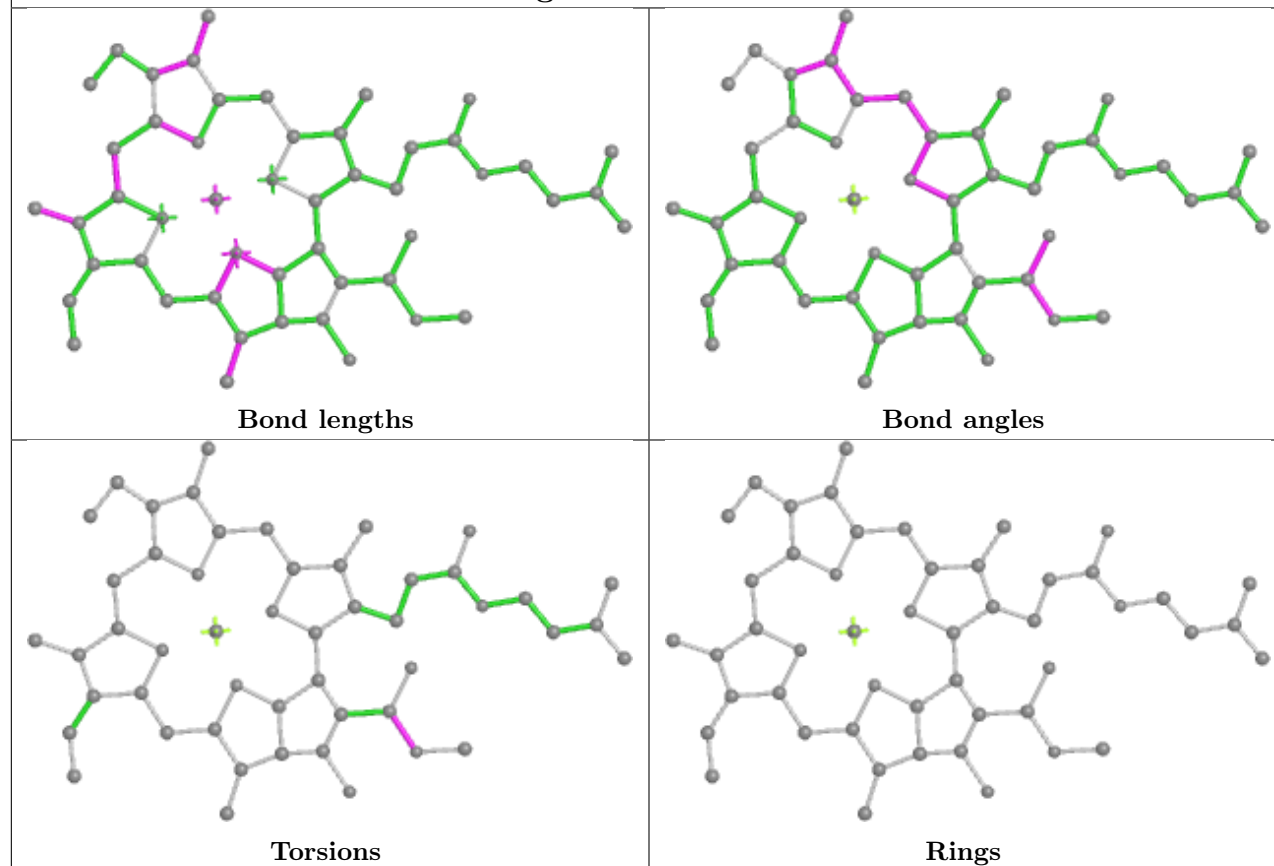
Ligand CLA A 834



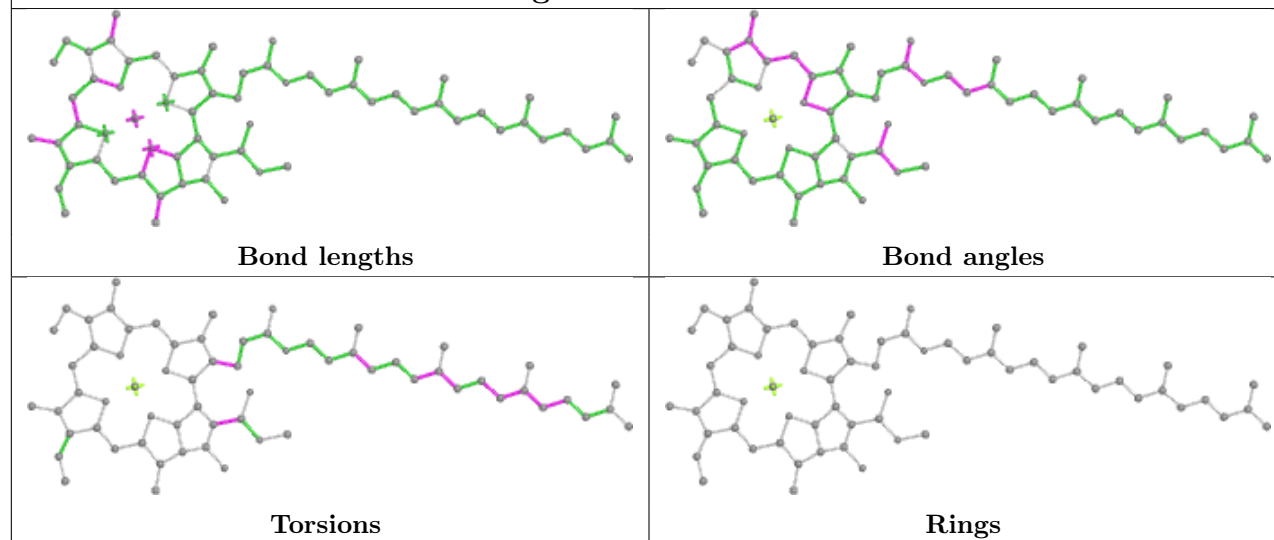
Ligand CLA 7 303

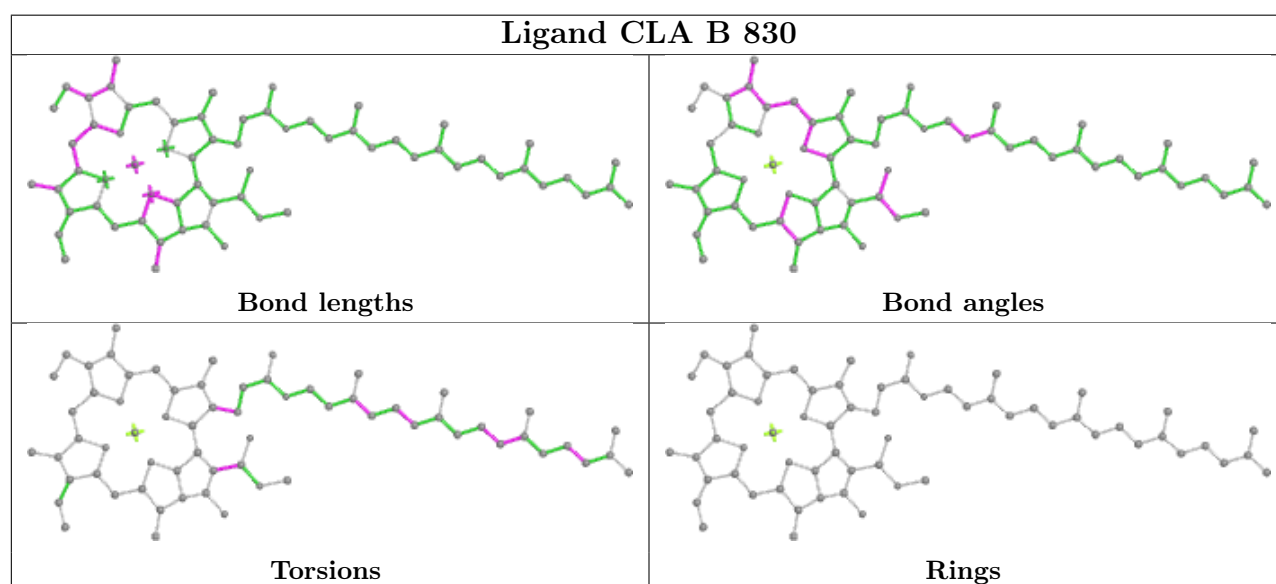
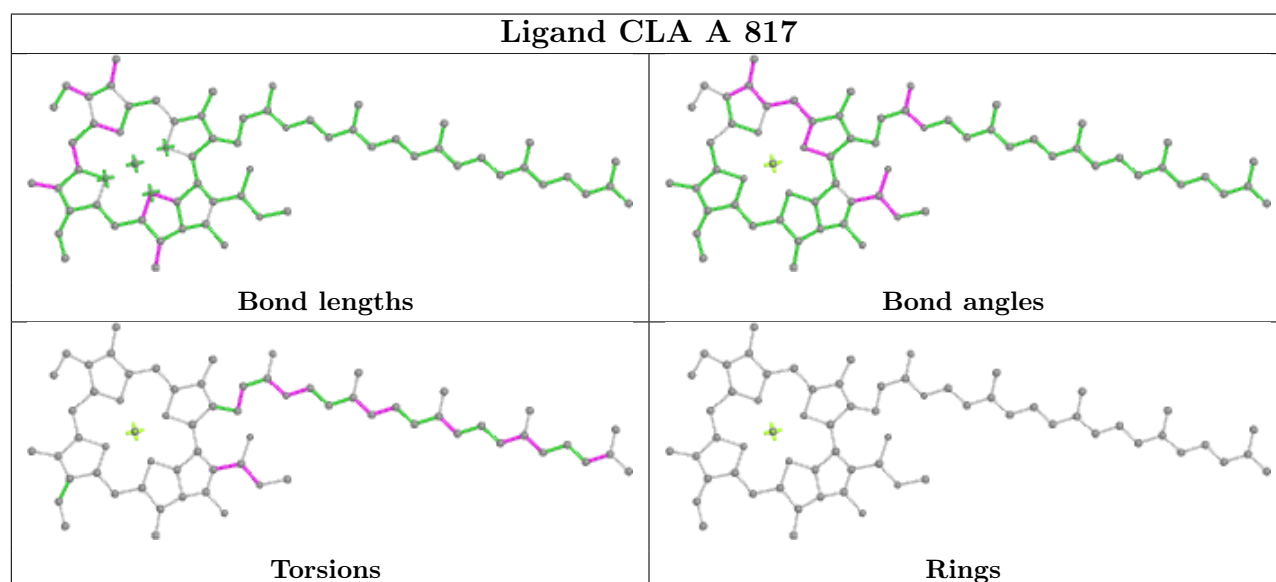
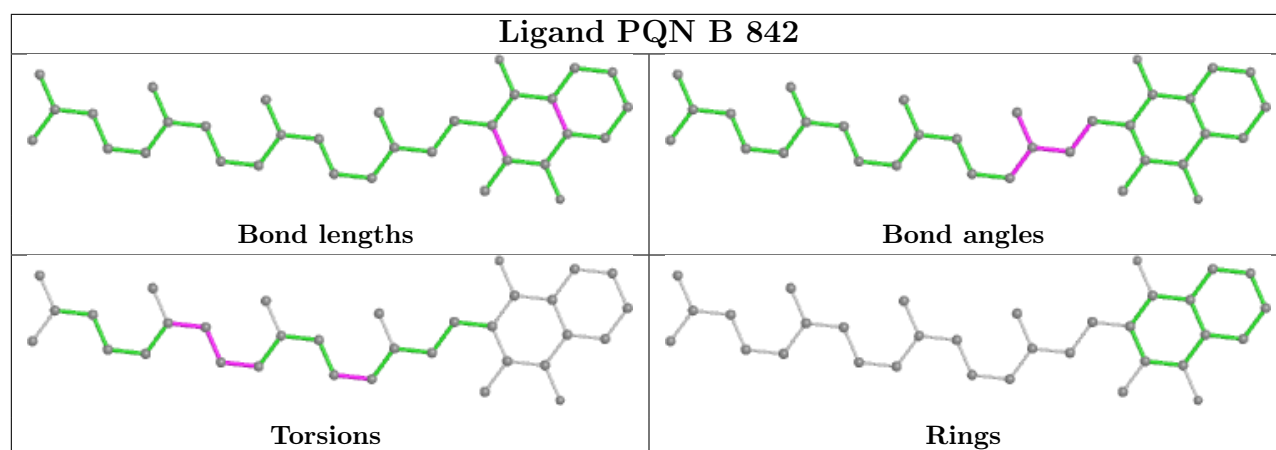


Ligand CLA 3 302

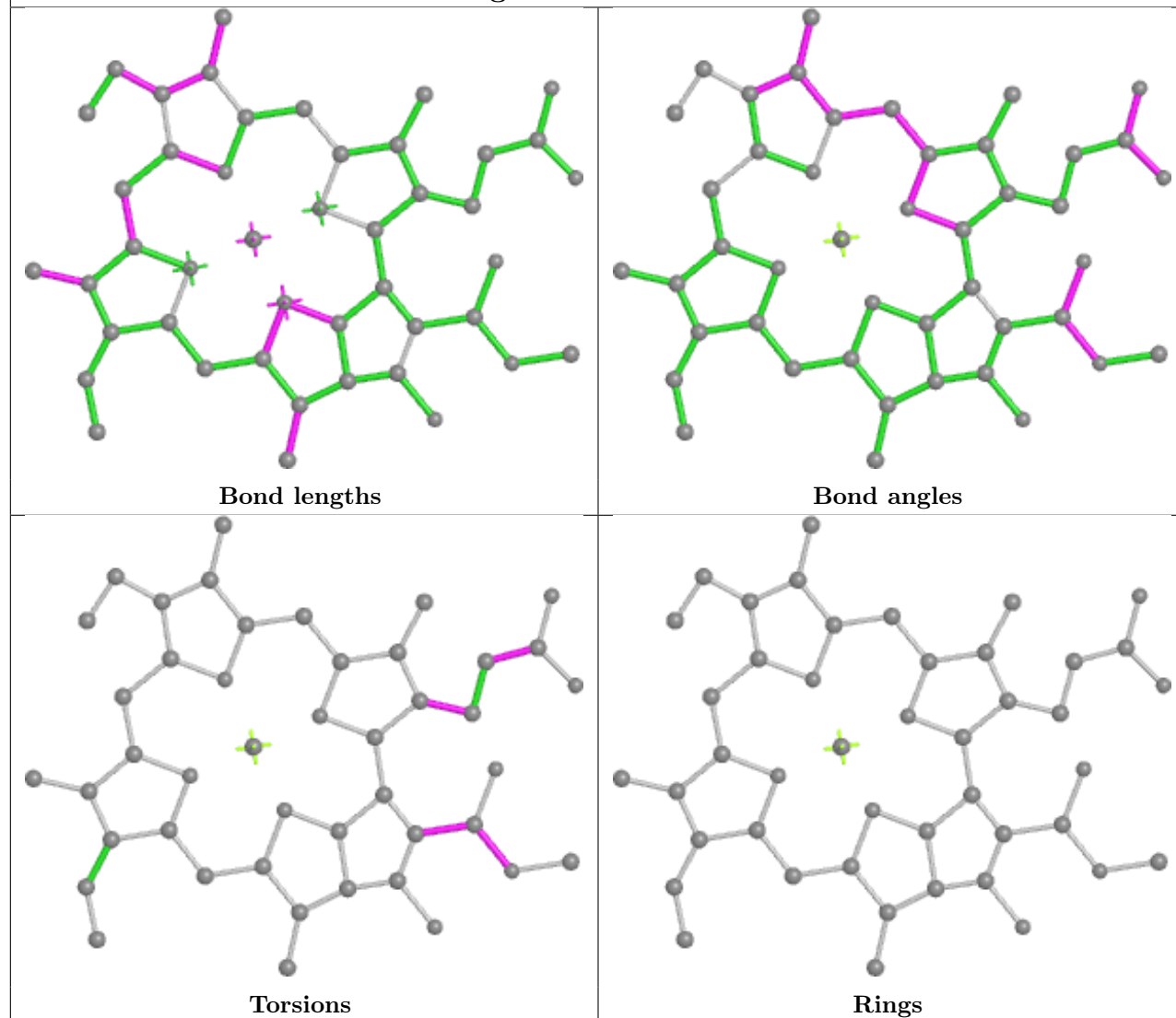


Ligand CLA B 827

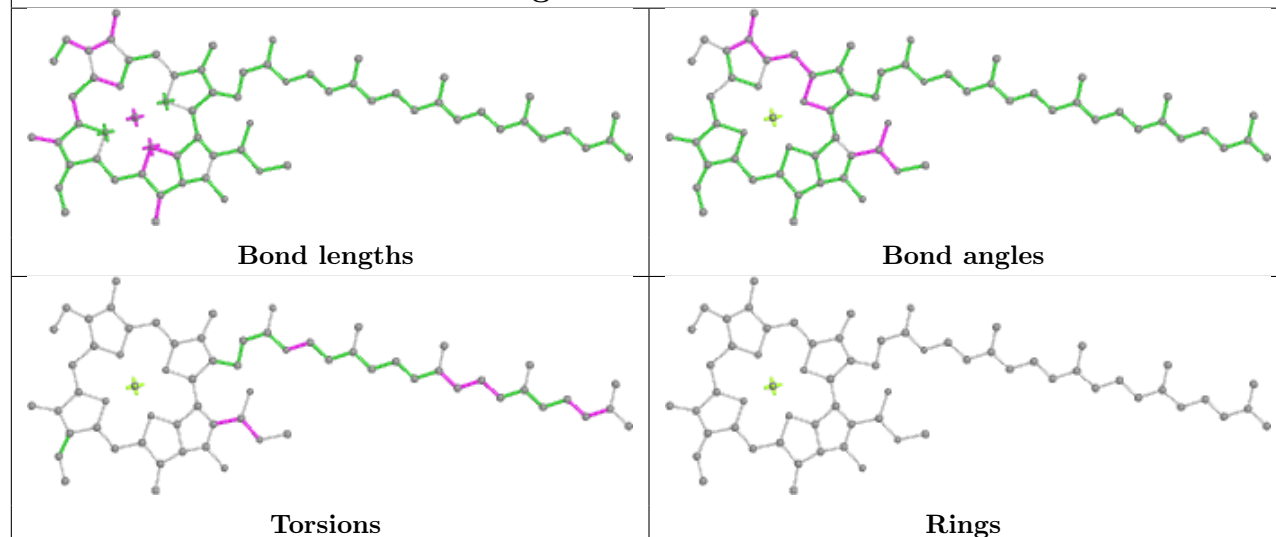




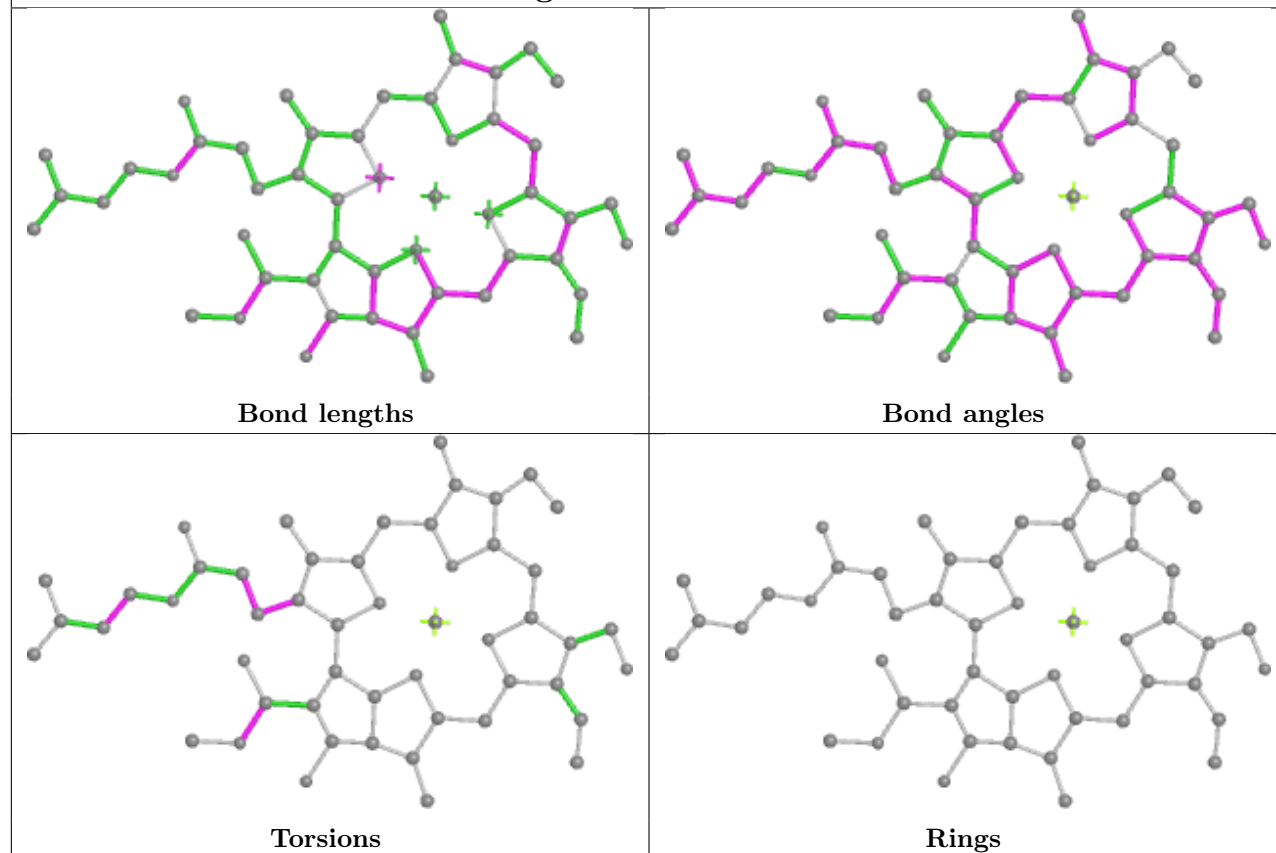
Ligand CLA A 814



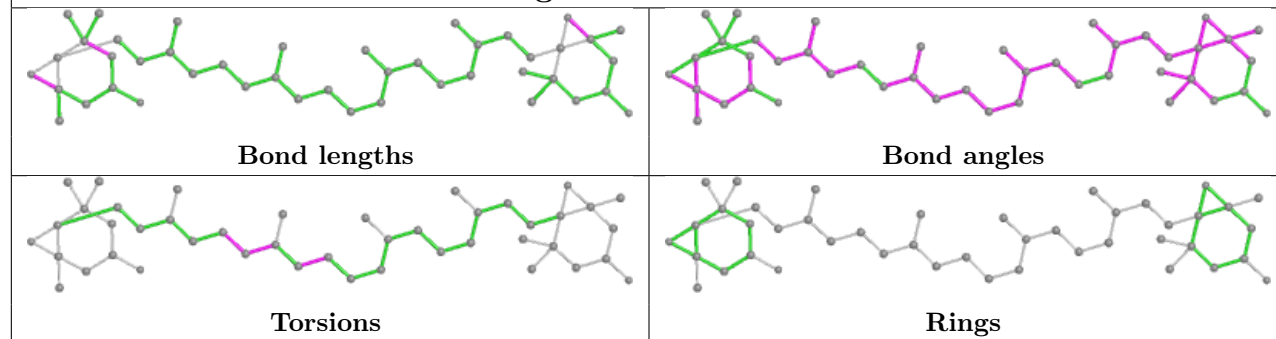
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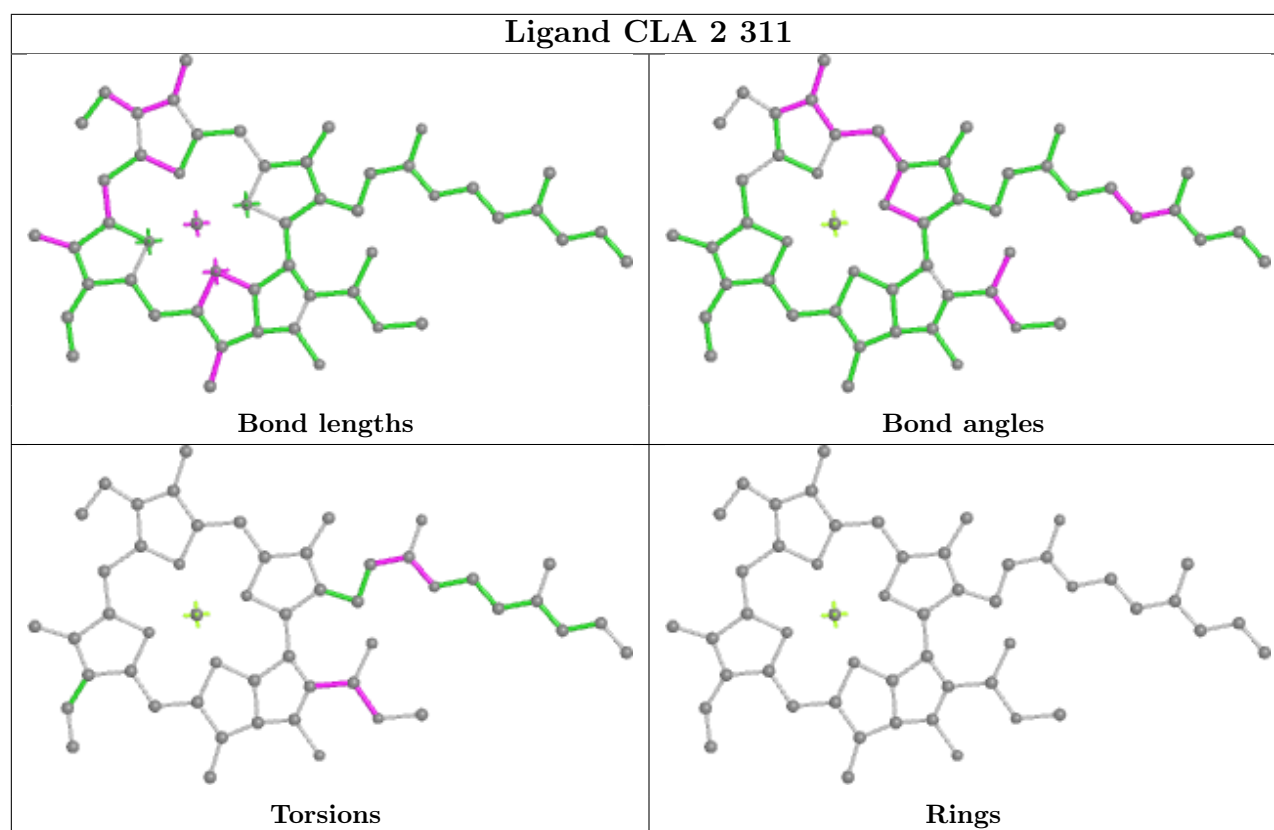


Ligand CHL 6 308

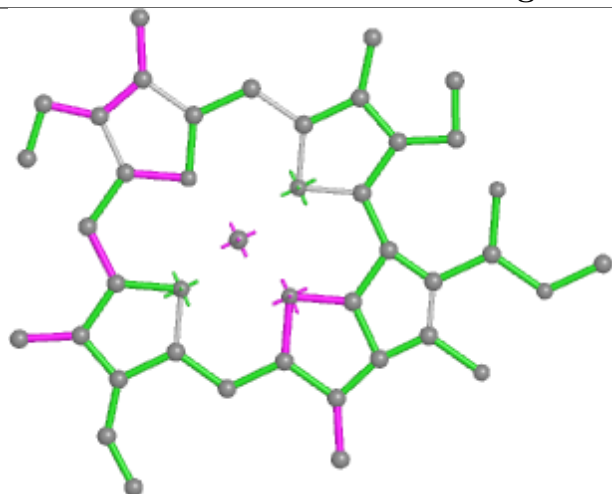


Ligand XAT 3 314

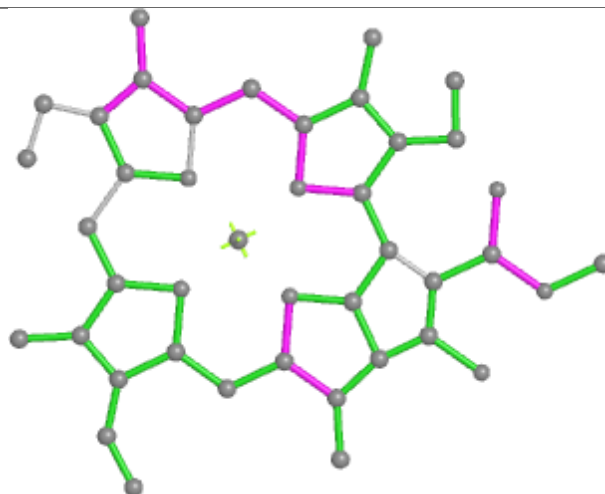




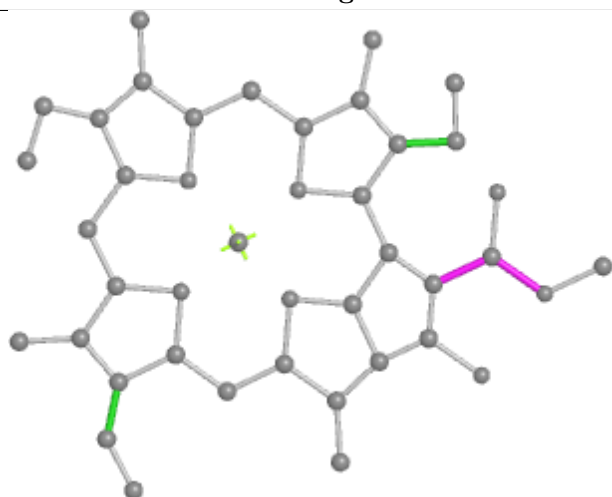
Ligand CLA 3 304



Bond lengths



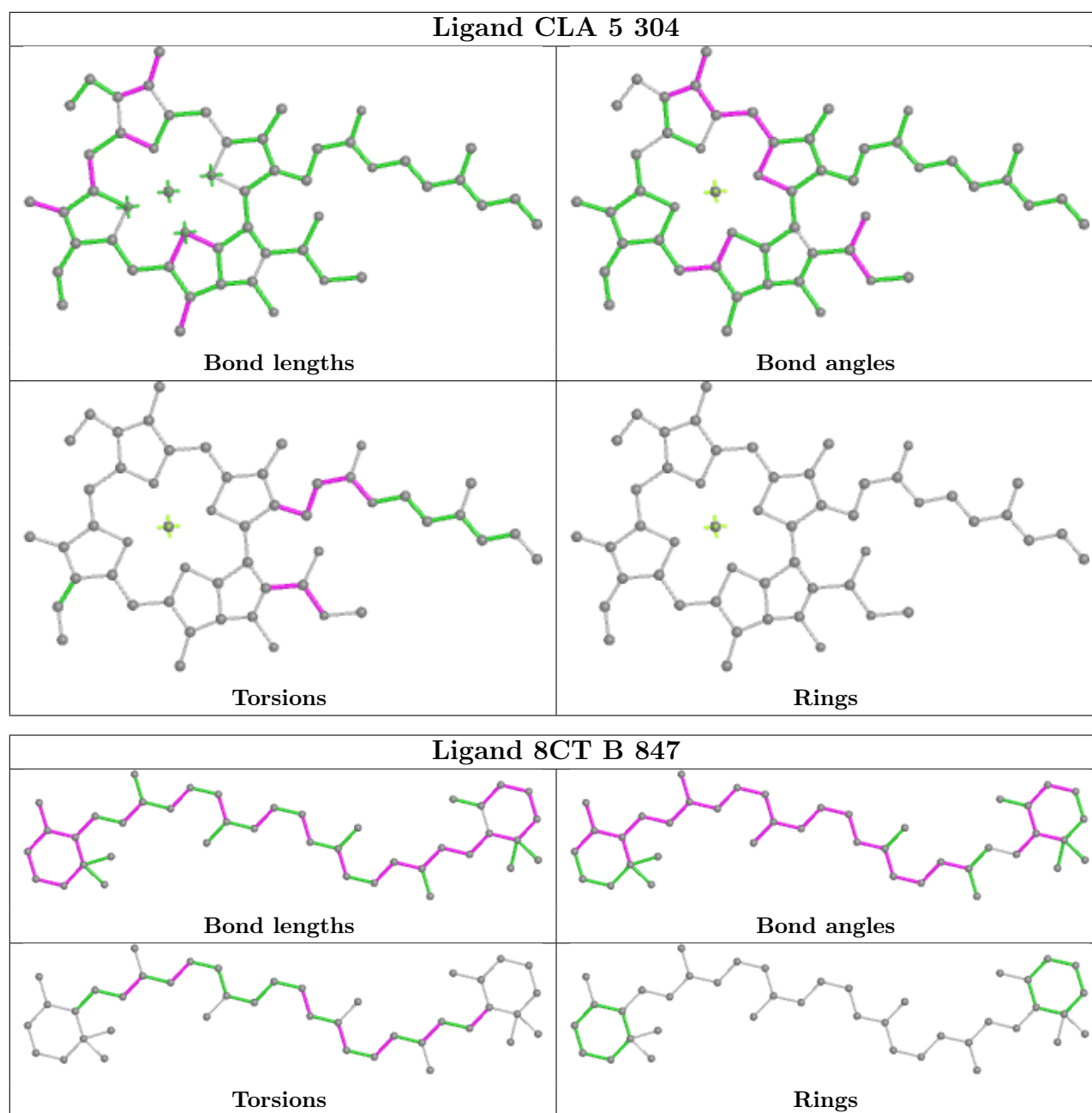
Bond angles

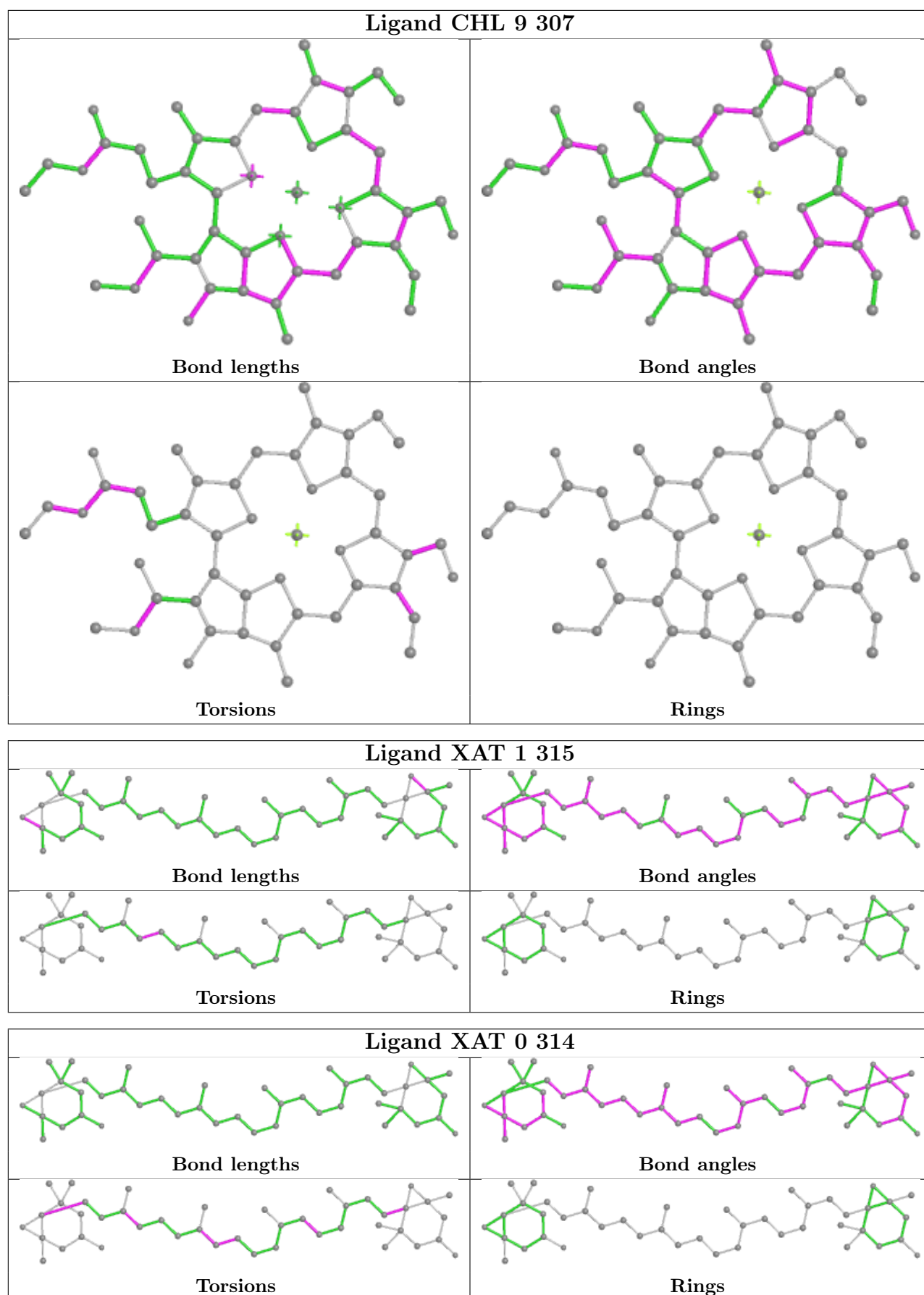


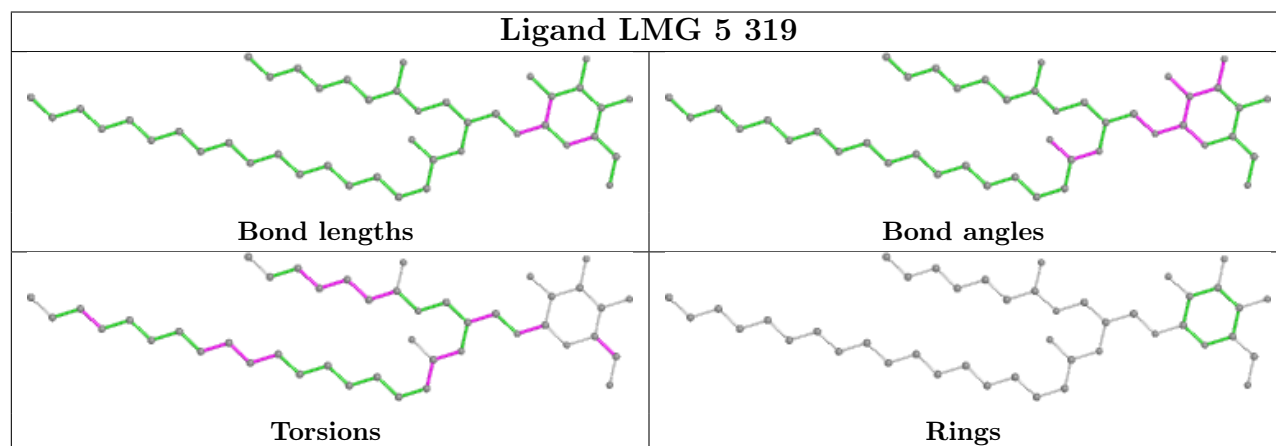
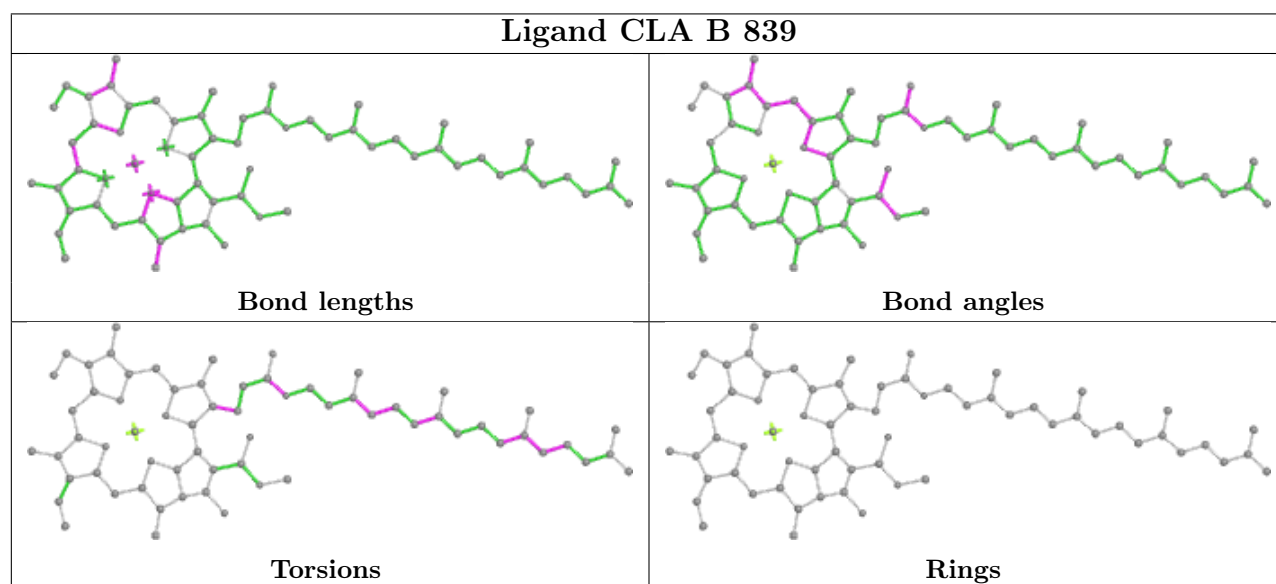
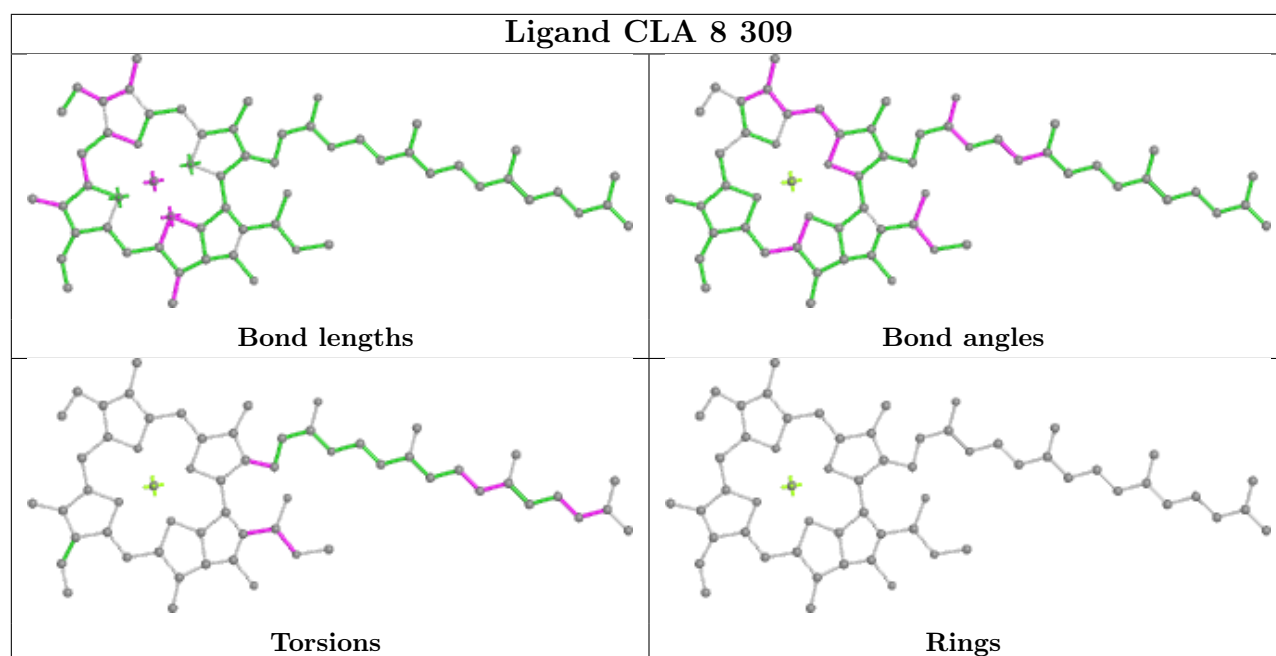
Torsions

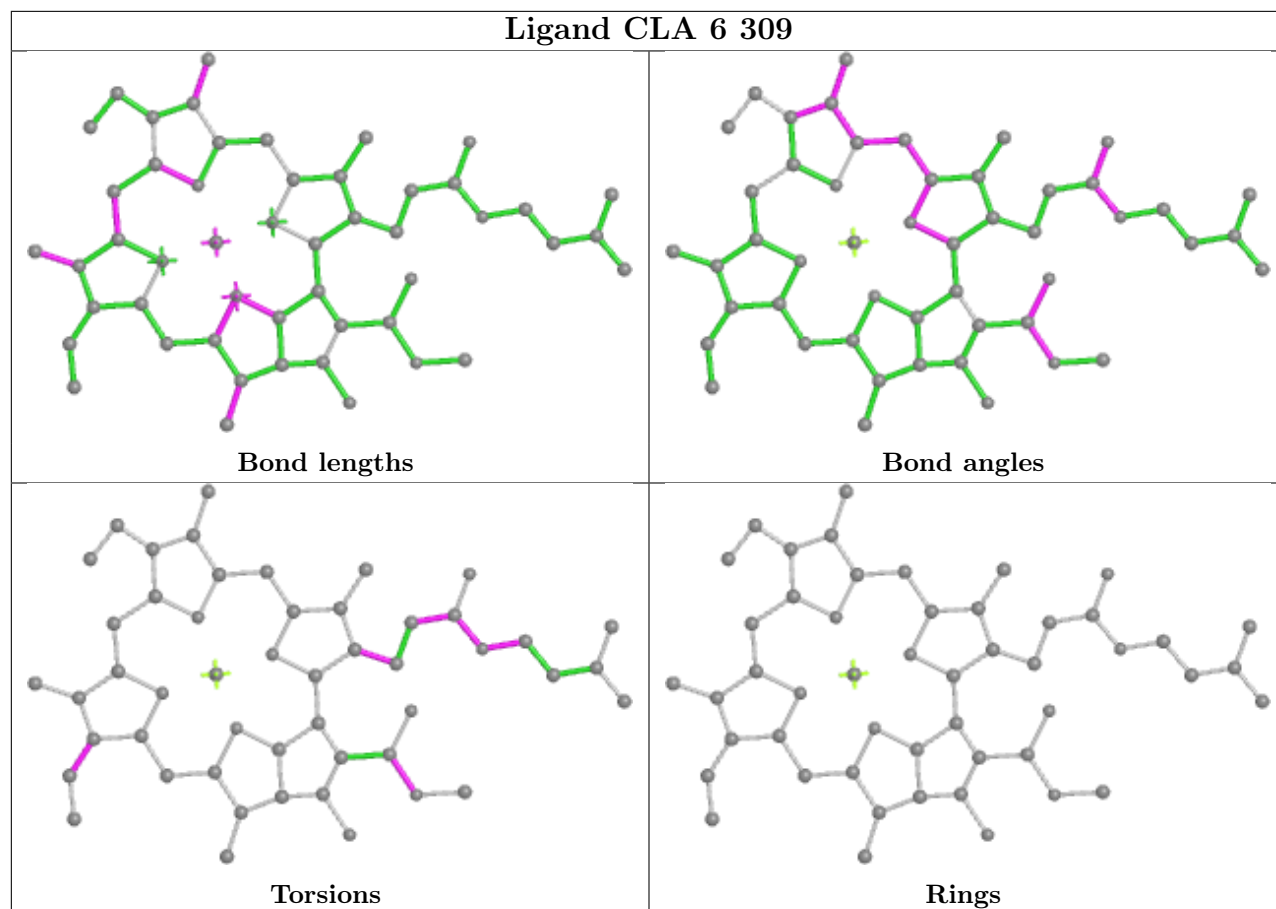


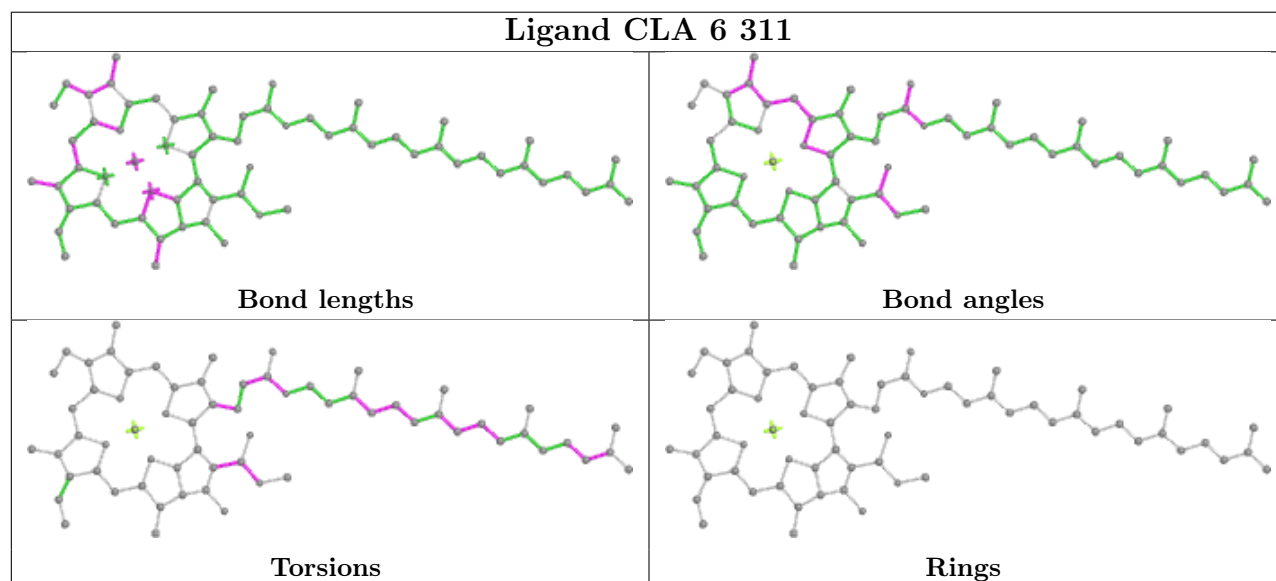
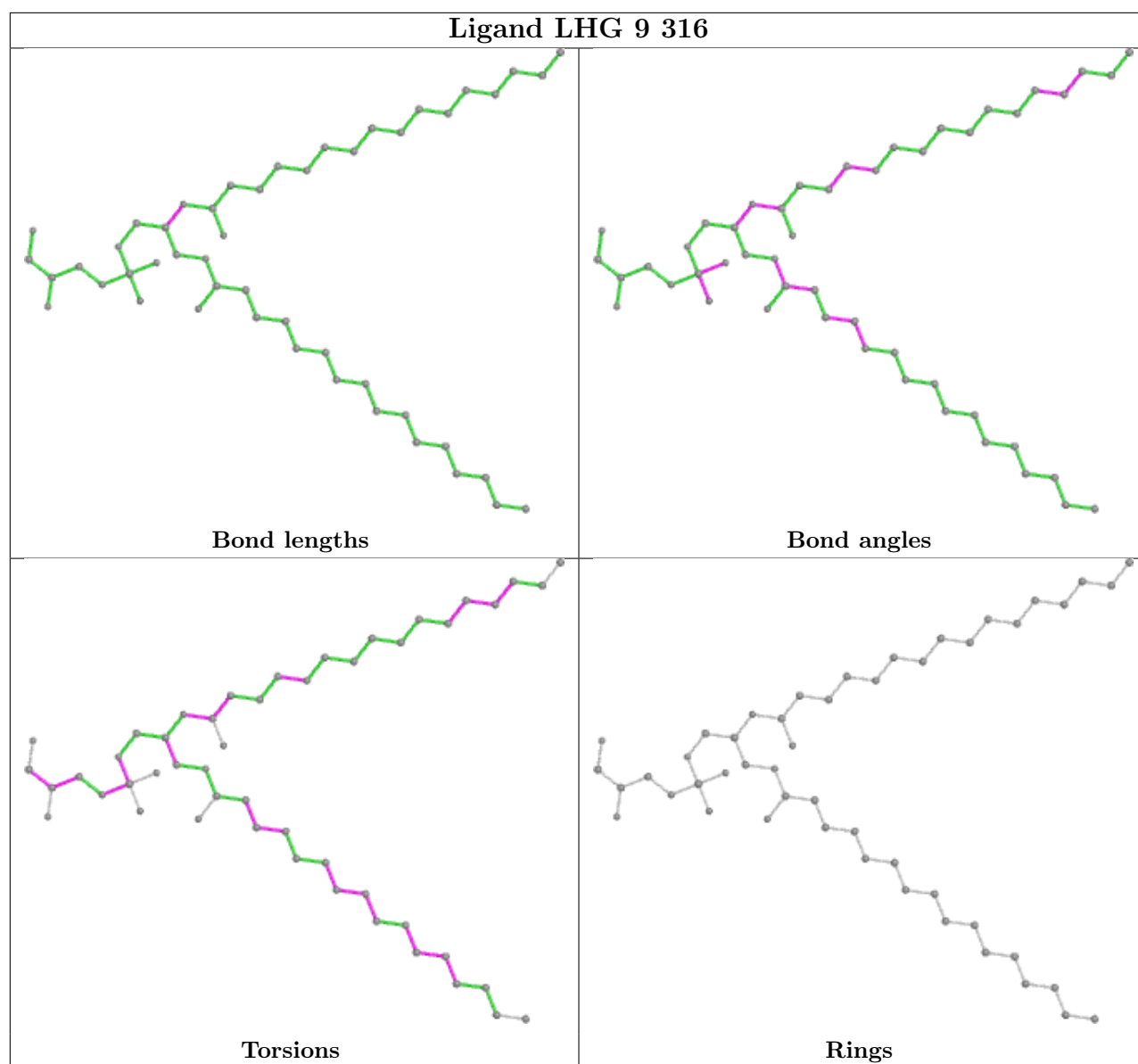
Rings



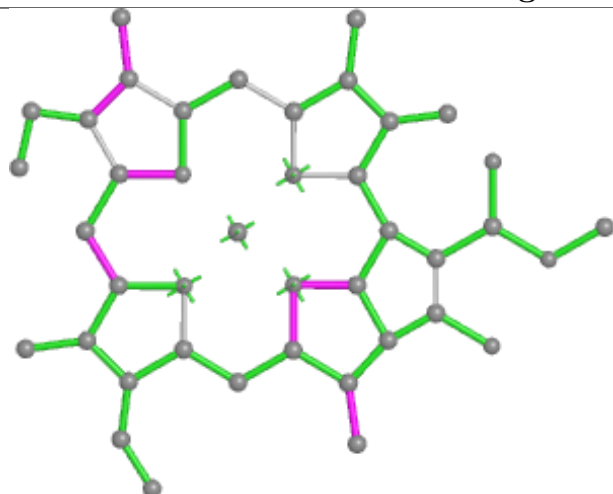




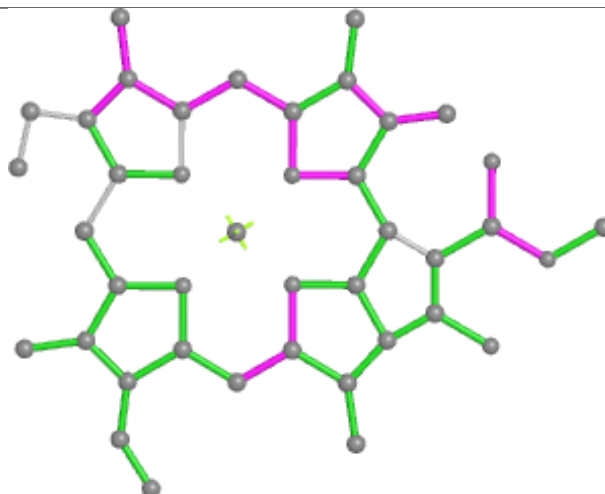




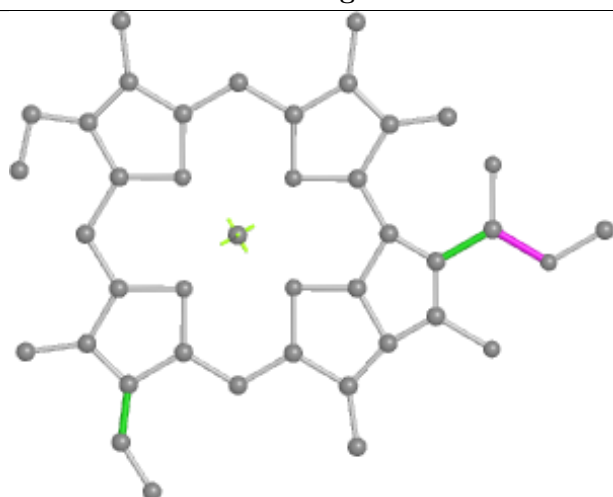
Ligand CLA 0 309



Bond lengths



Bond angles

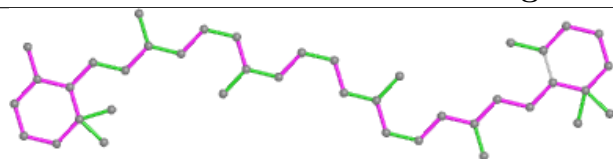


Torsions

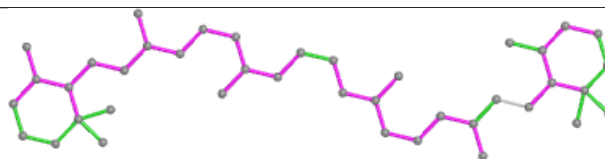


Rings

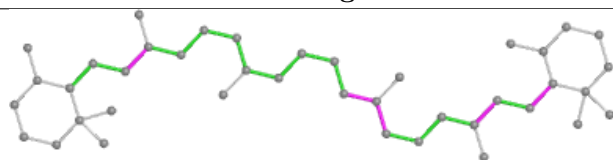
Ligand 8CT 2 317



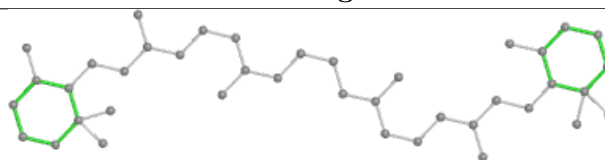
Bond lengths



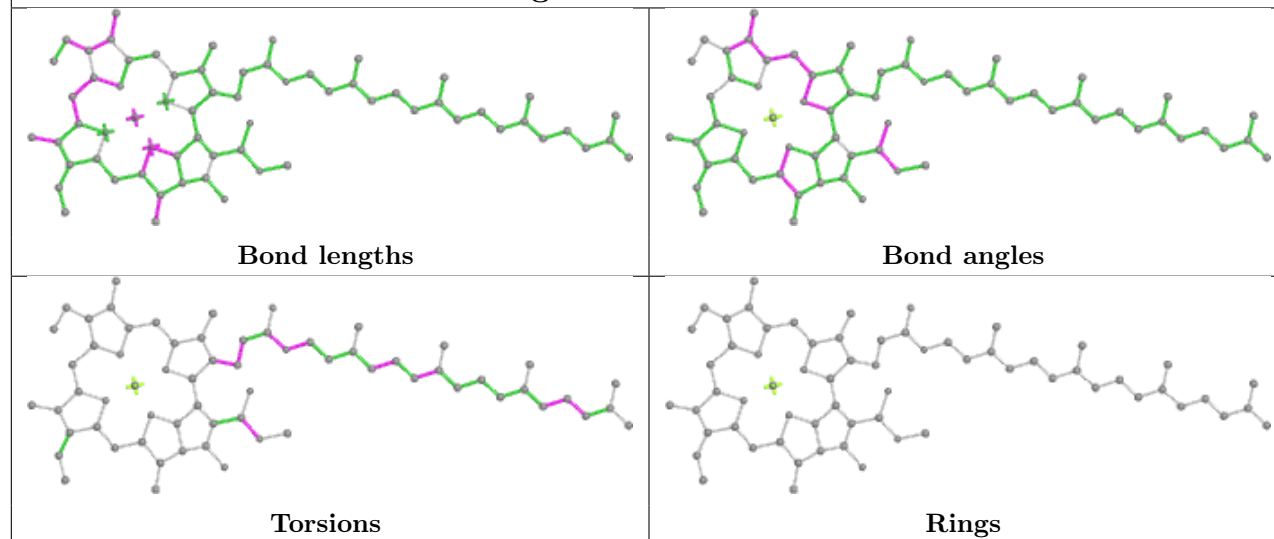
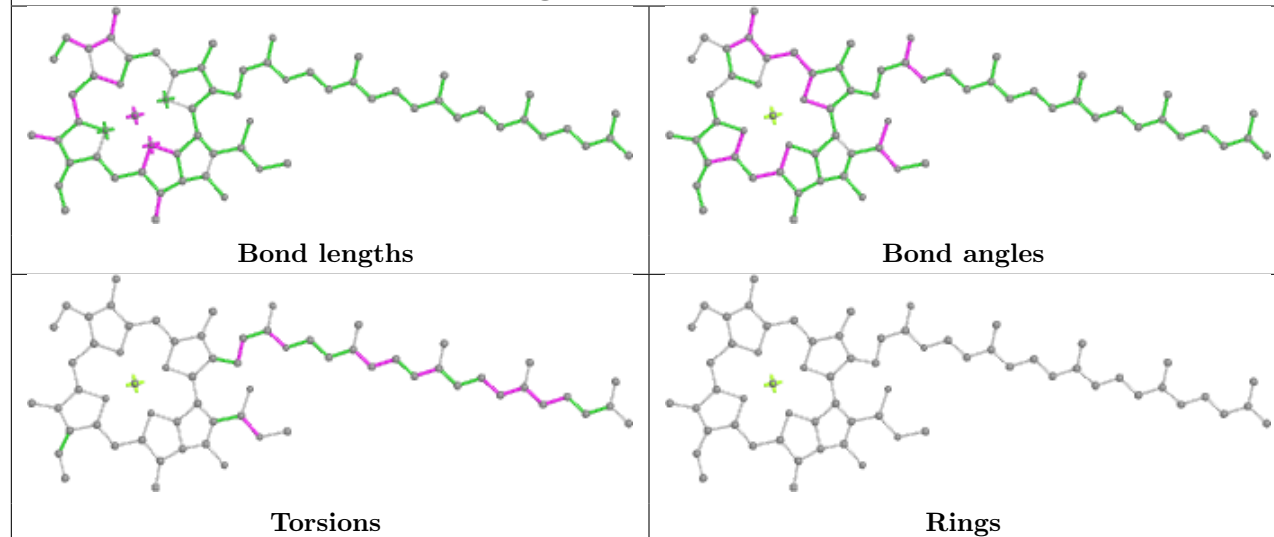
Bond angles

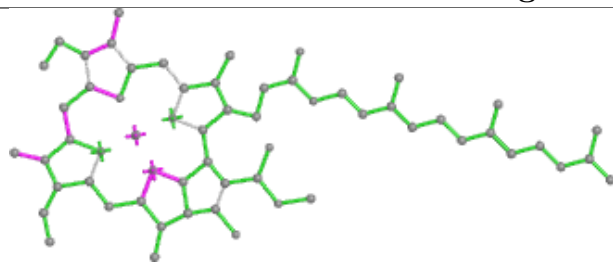


Torsions

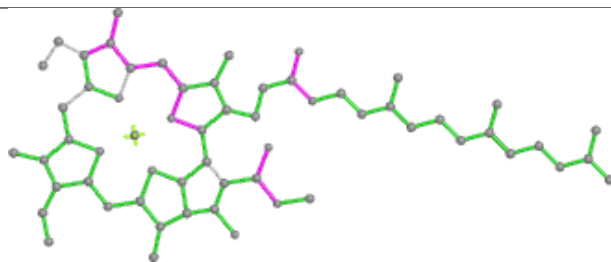


Rings

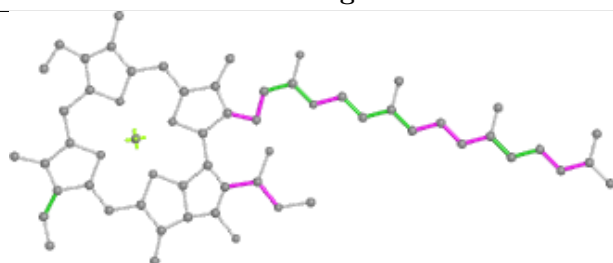
Ligand CLA A 841**Ligand CLA 1 311**

Ligand CLA 6 305

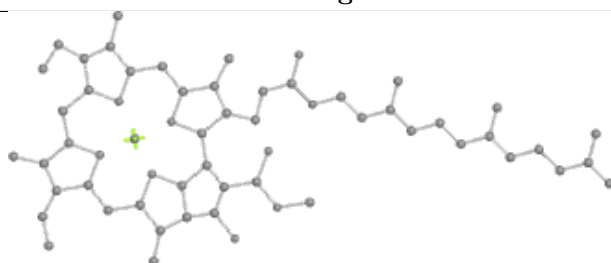
Bond lengths



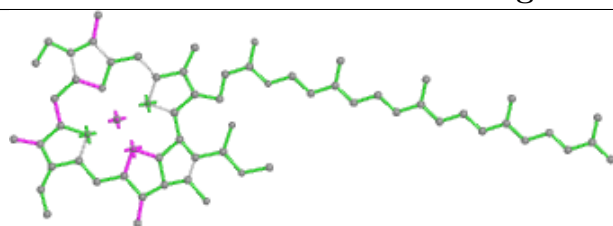
Bond angles



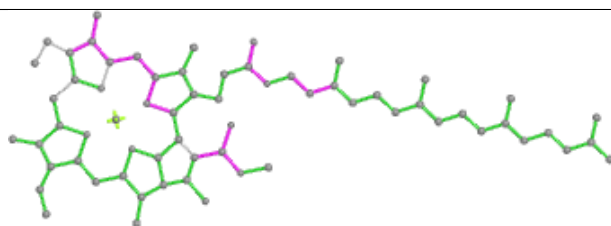
Torsions



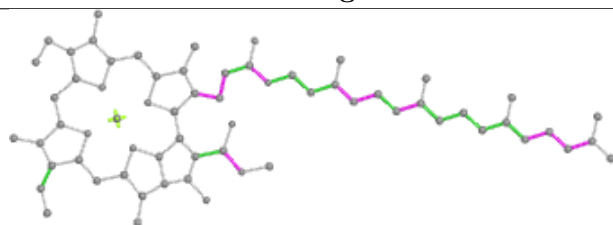
Rings

Ligand CLA L 202

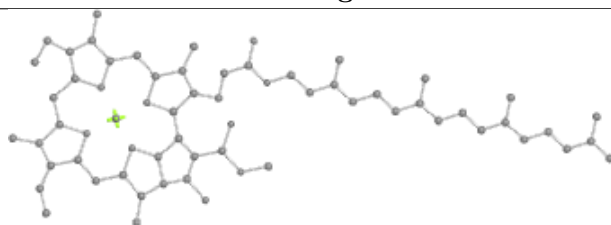
Bond lengths



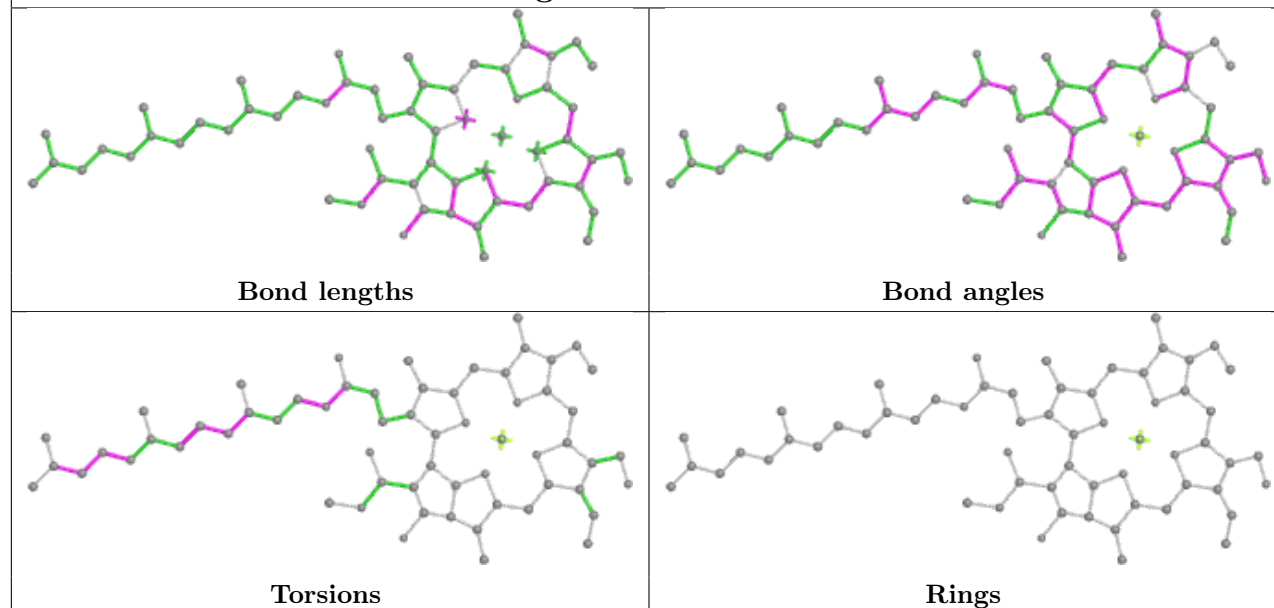
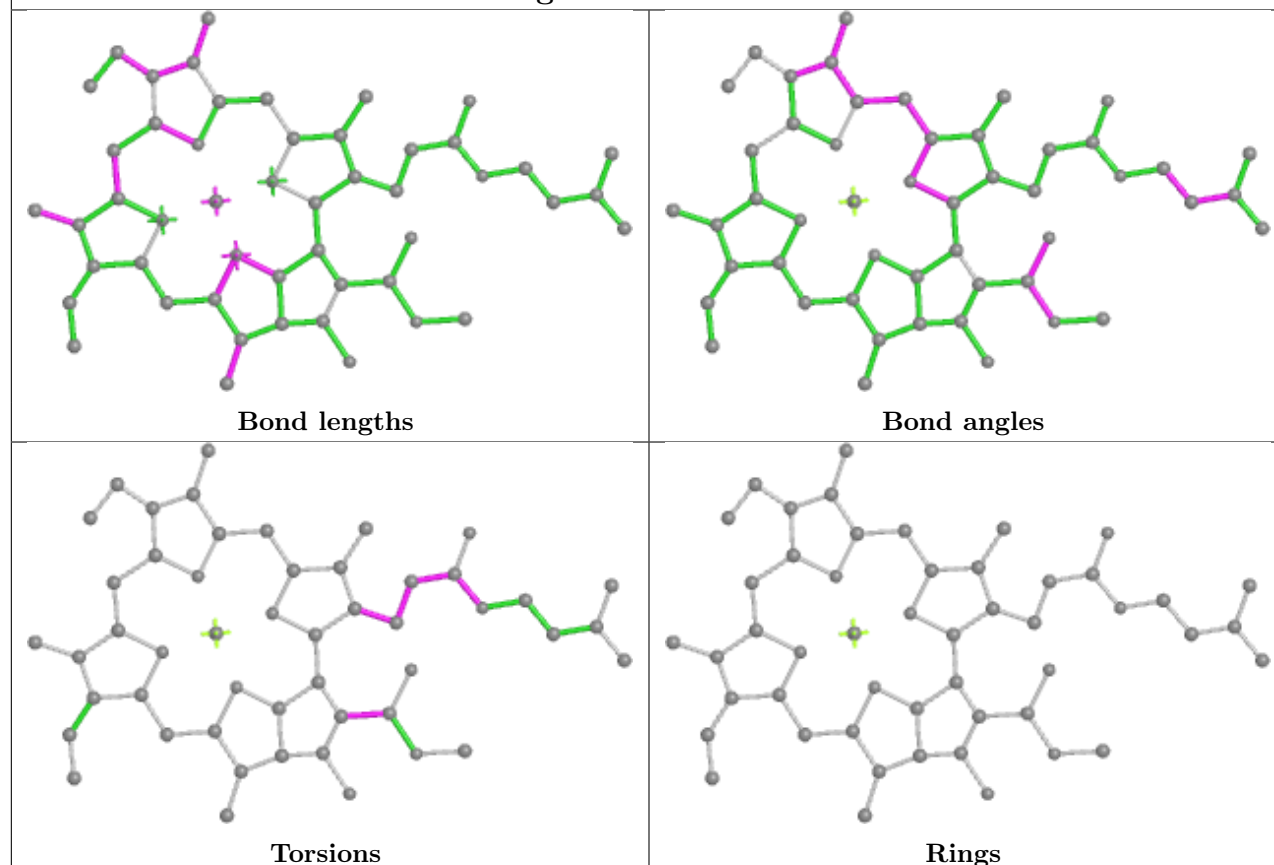
Bond angles



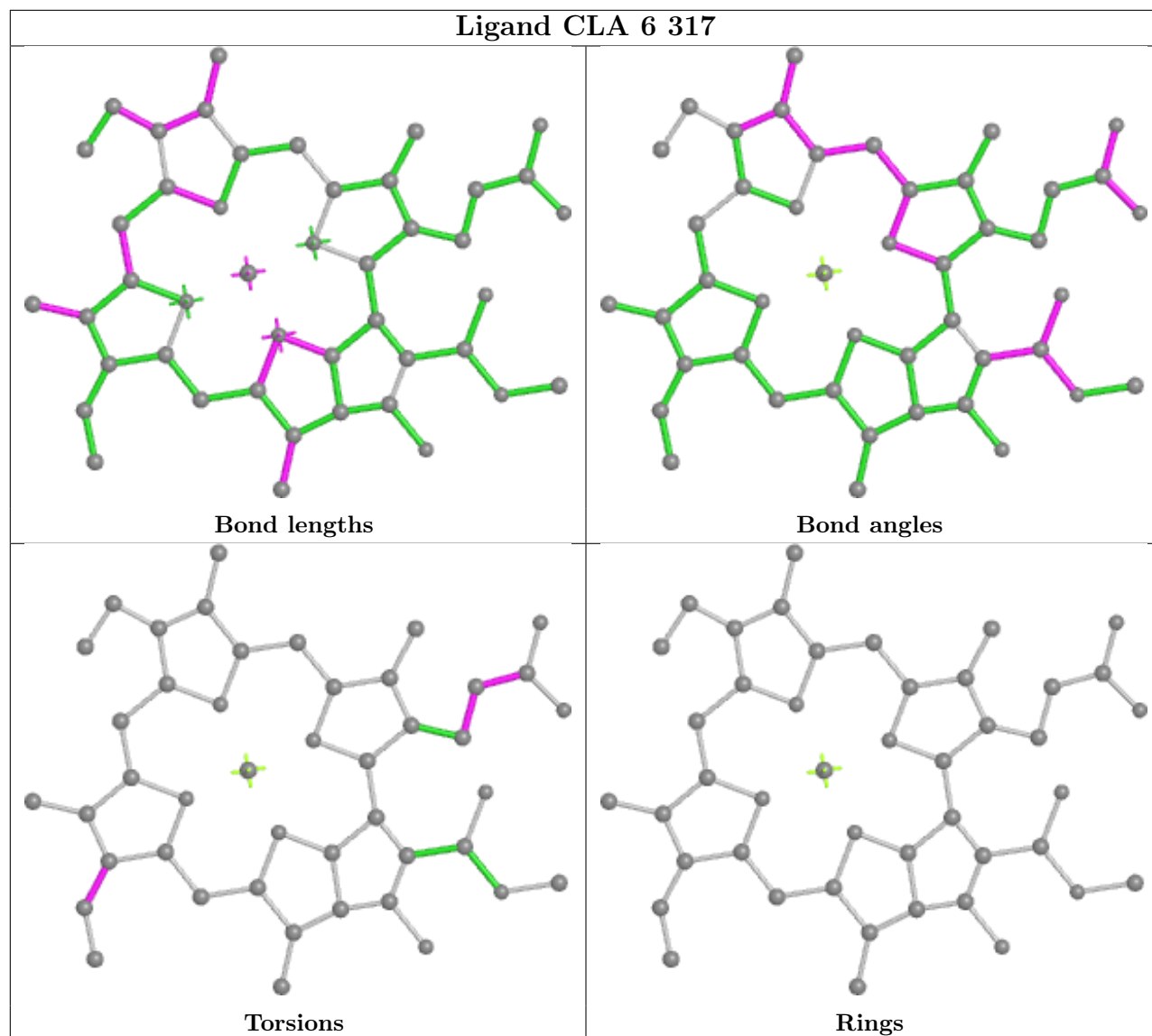
Torsions



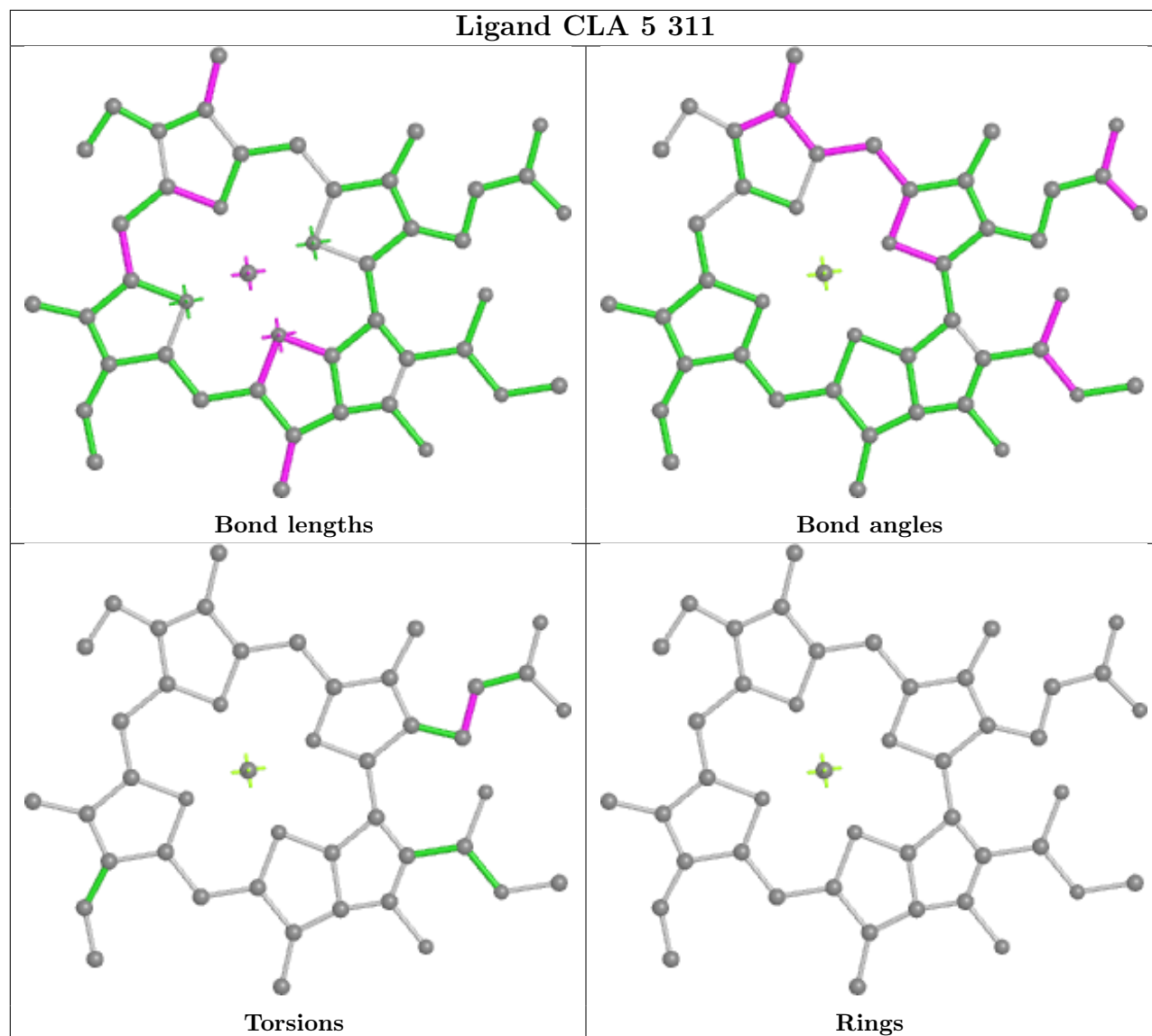
Rings

Ligand CHL 4 301**Ligand CLA 3 307**

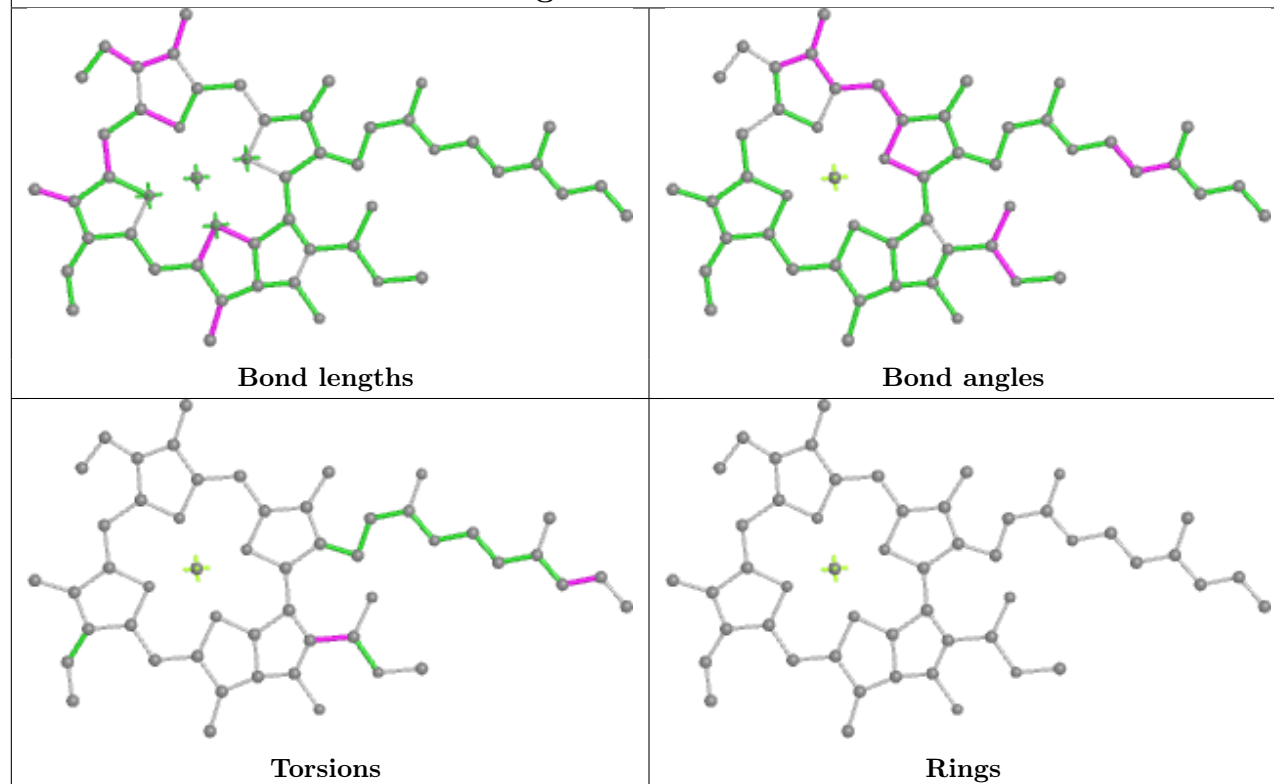
Ligand CLA 6 317



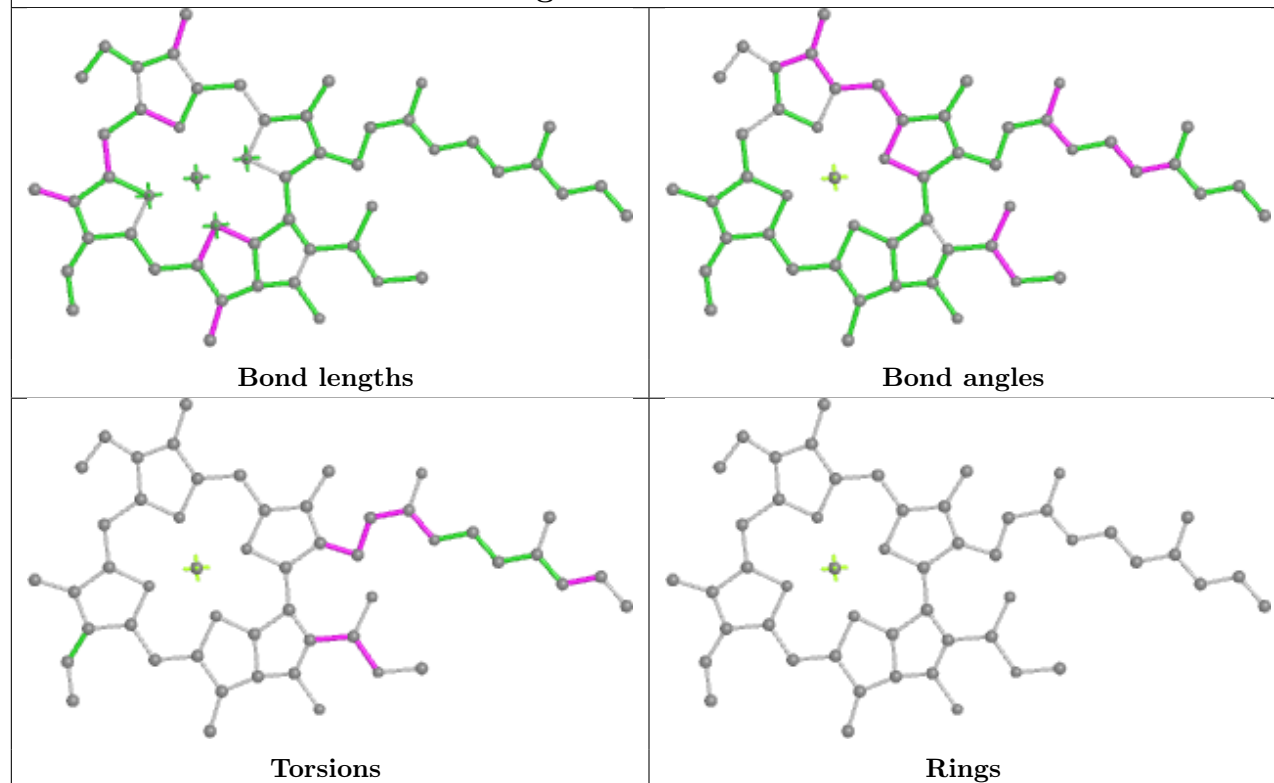
Ligand CLA 5 311



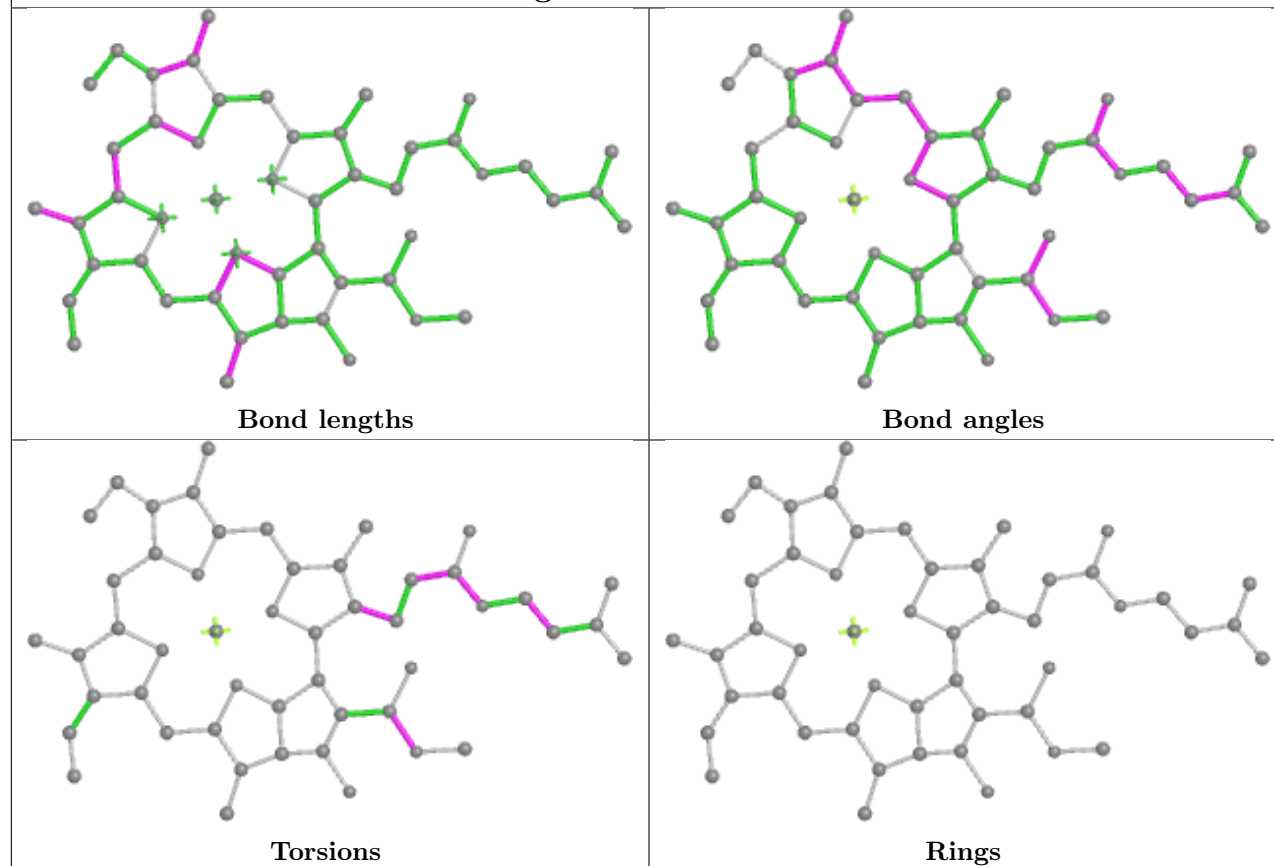
Ligand CLA 3 310



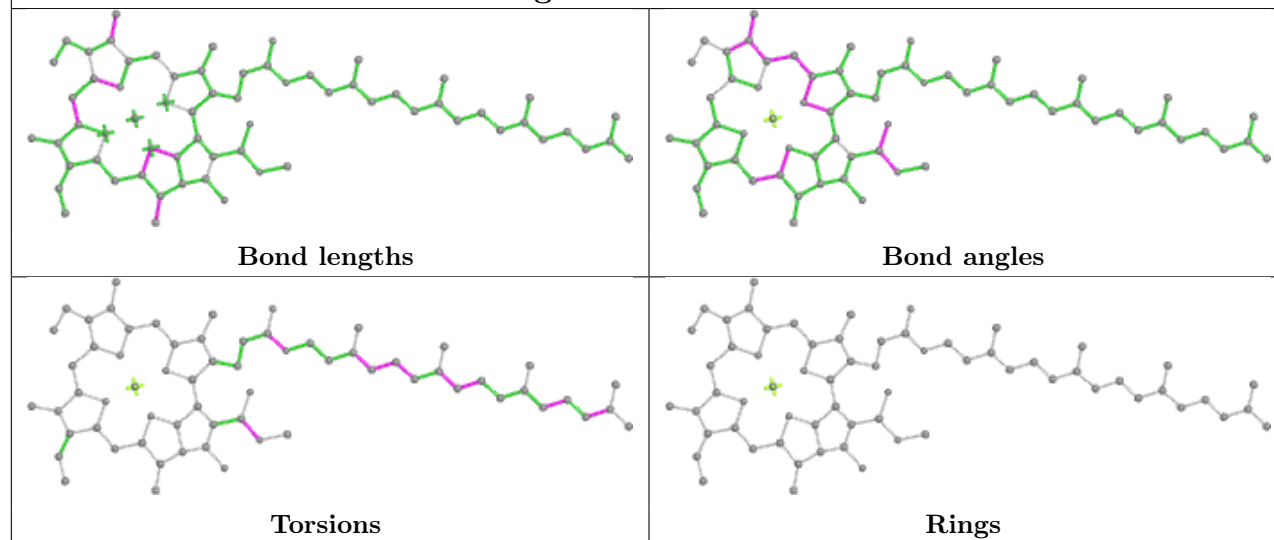
Ligand CLA 6 301

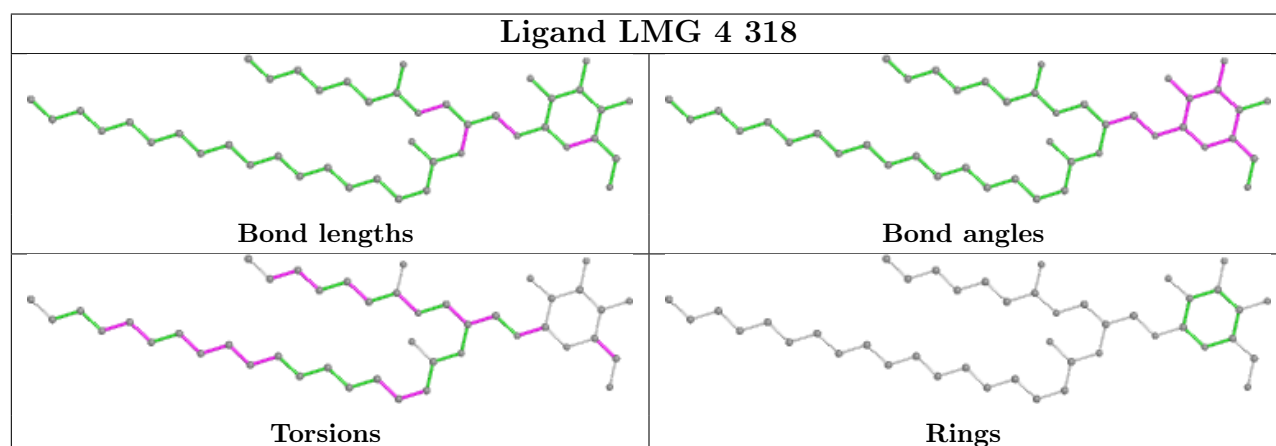
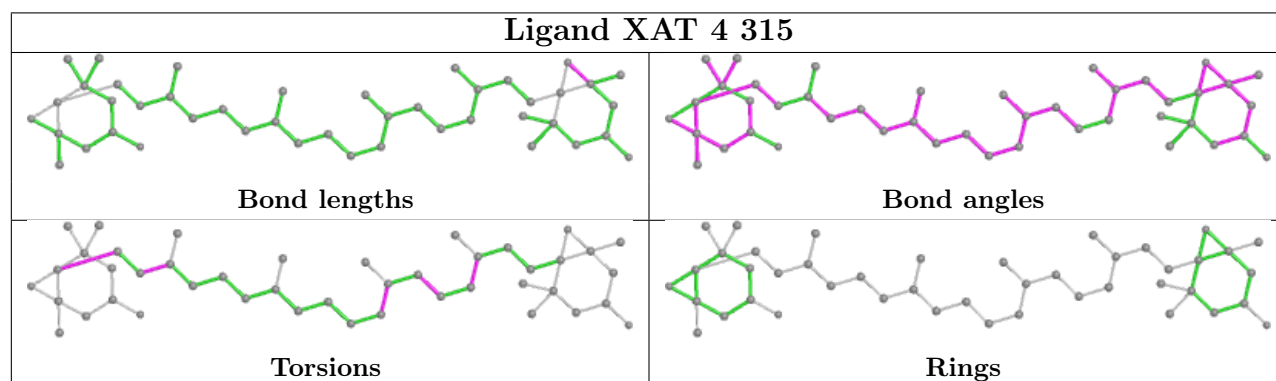
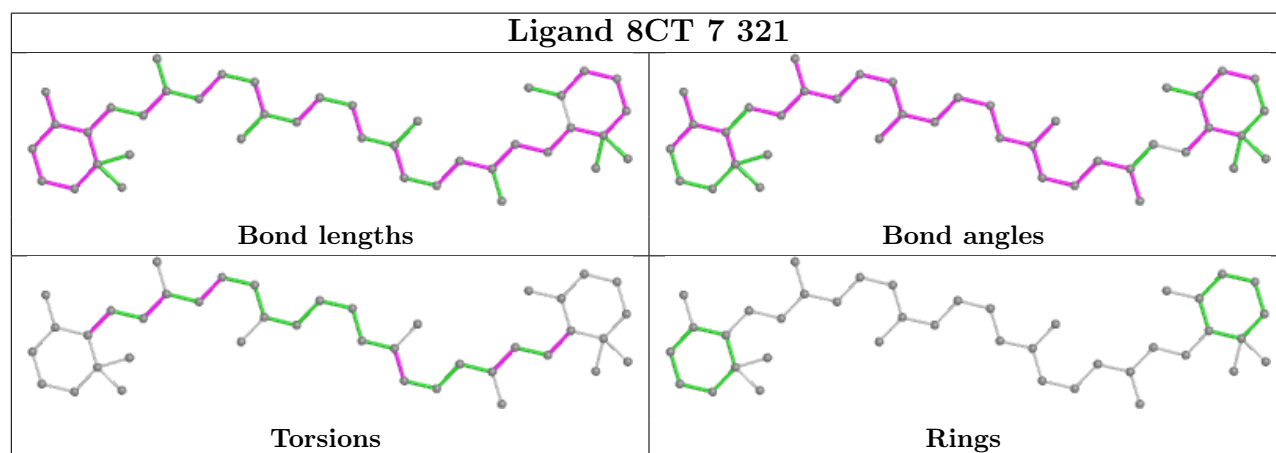
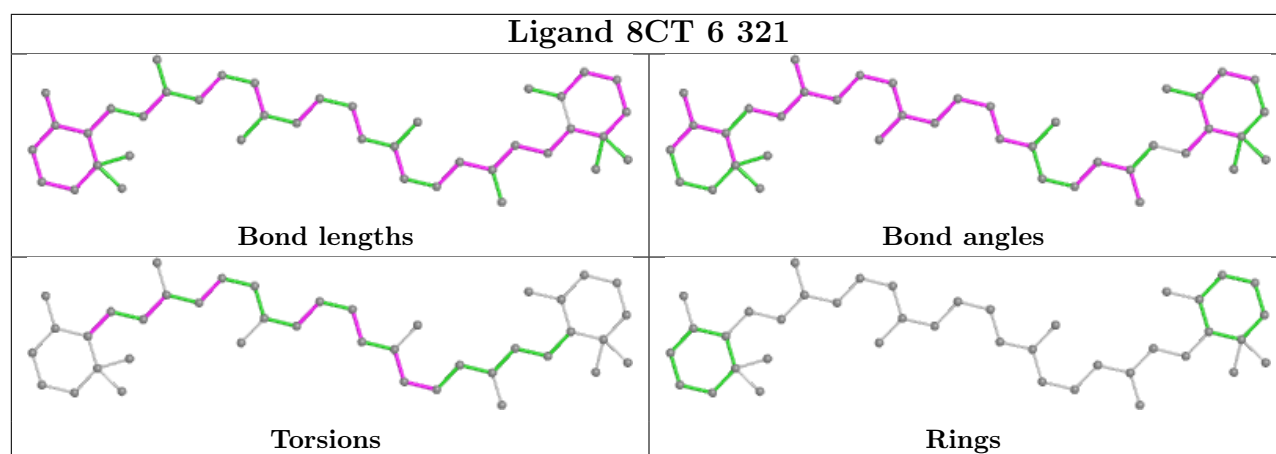


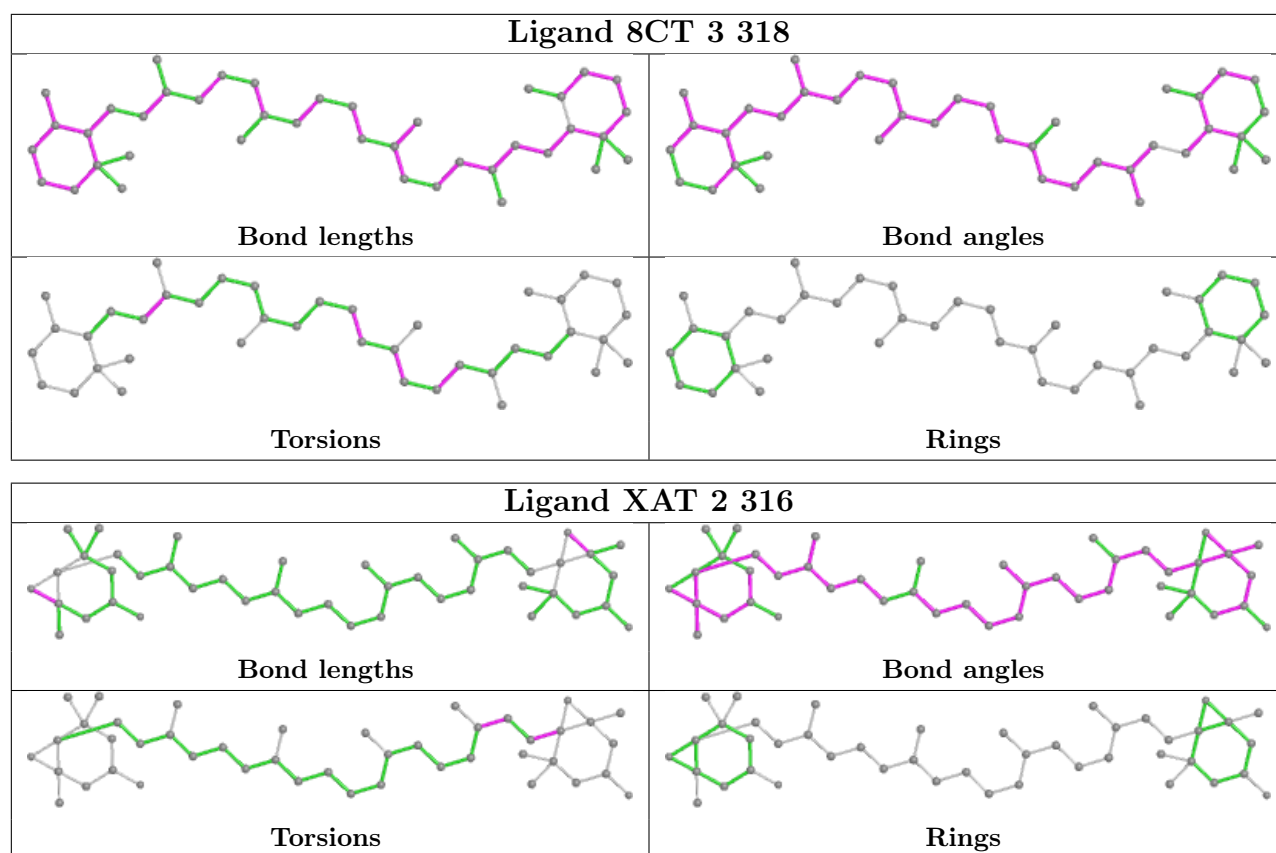
Ligand CLA L 204



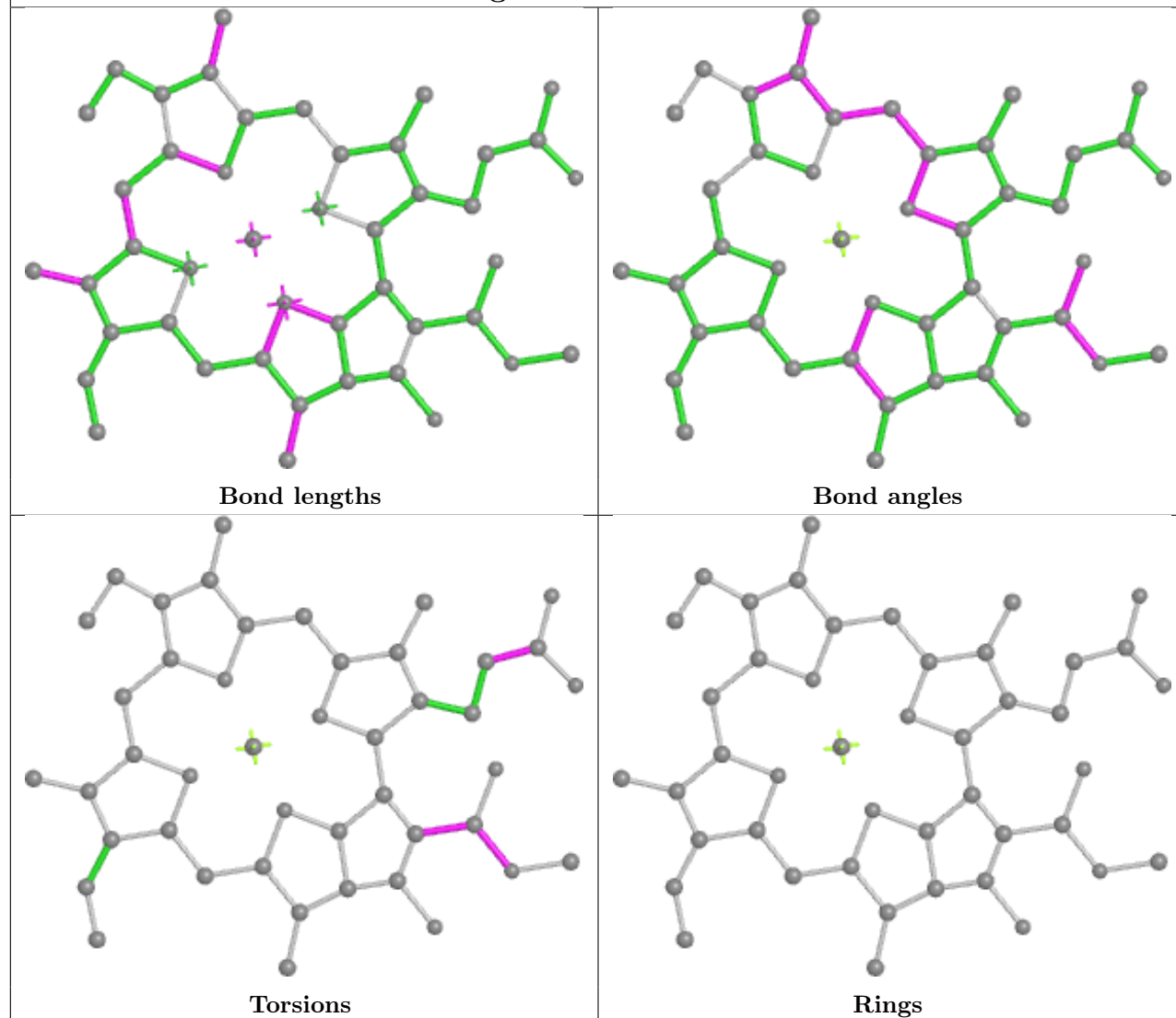
Ligand CLA L 203



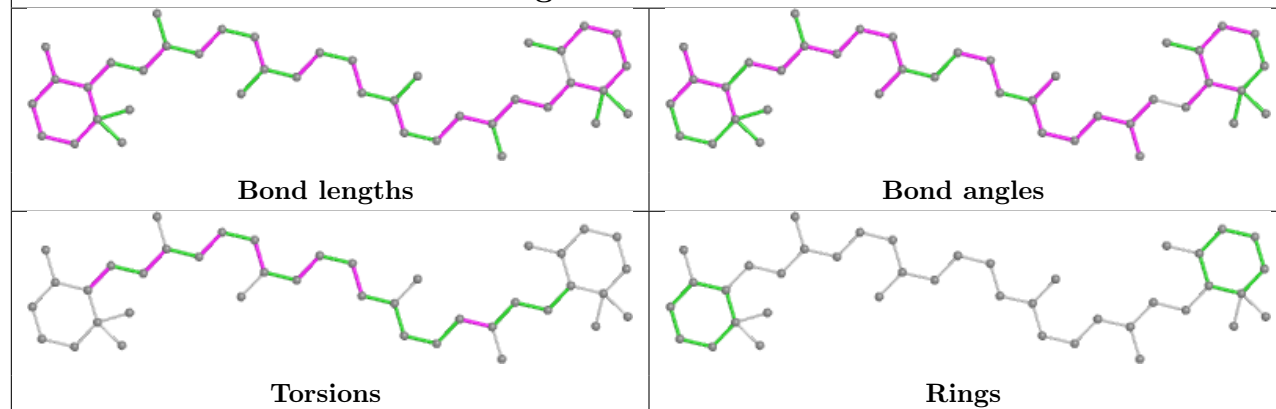


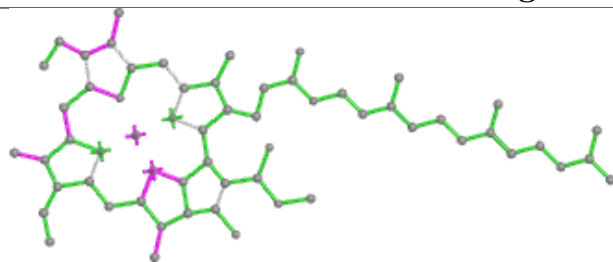


Ligand CLA A 820

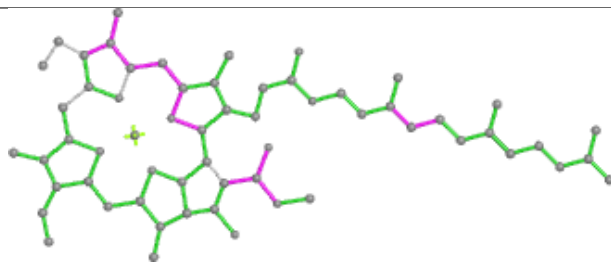


Ligand 8CT B 848

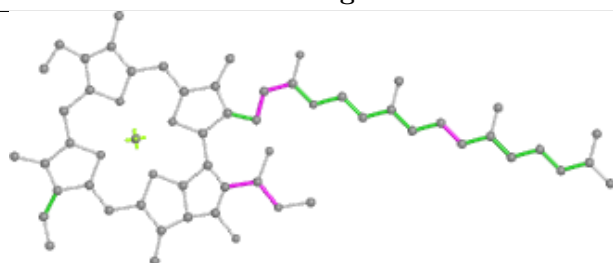


Ligand CLA 4 302

Bond lengths



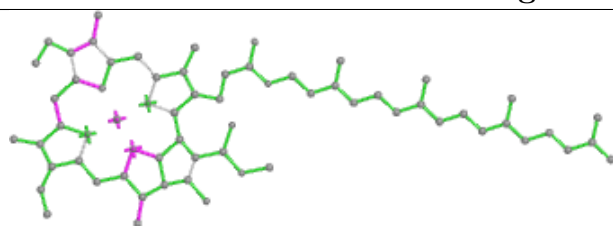
Bond angles



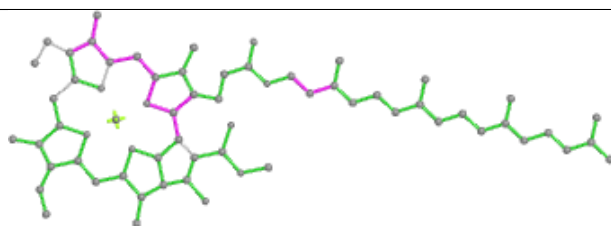
Torsions



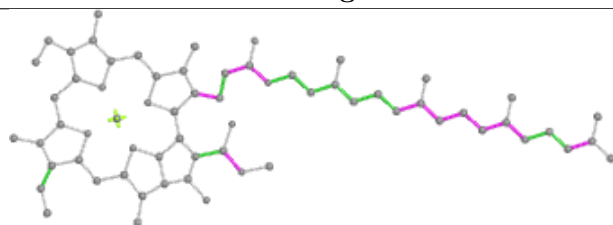
Rings

Ligand CLA 7 317

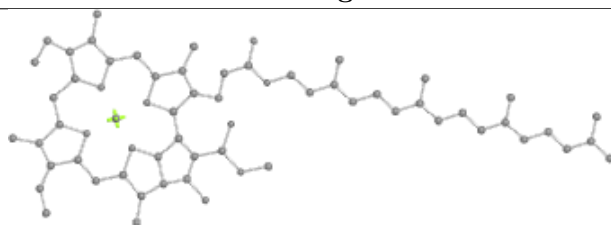
Bond lengths



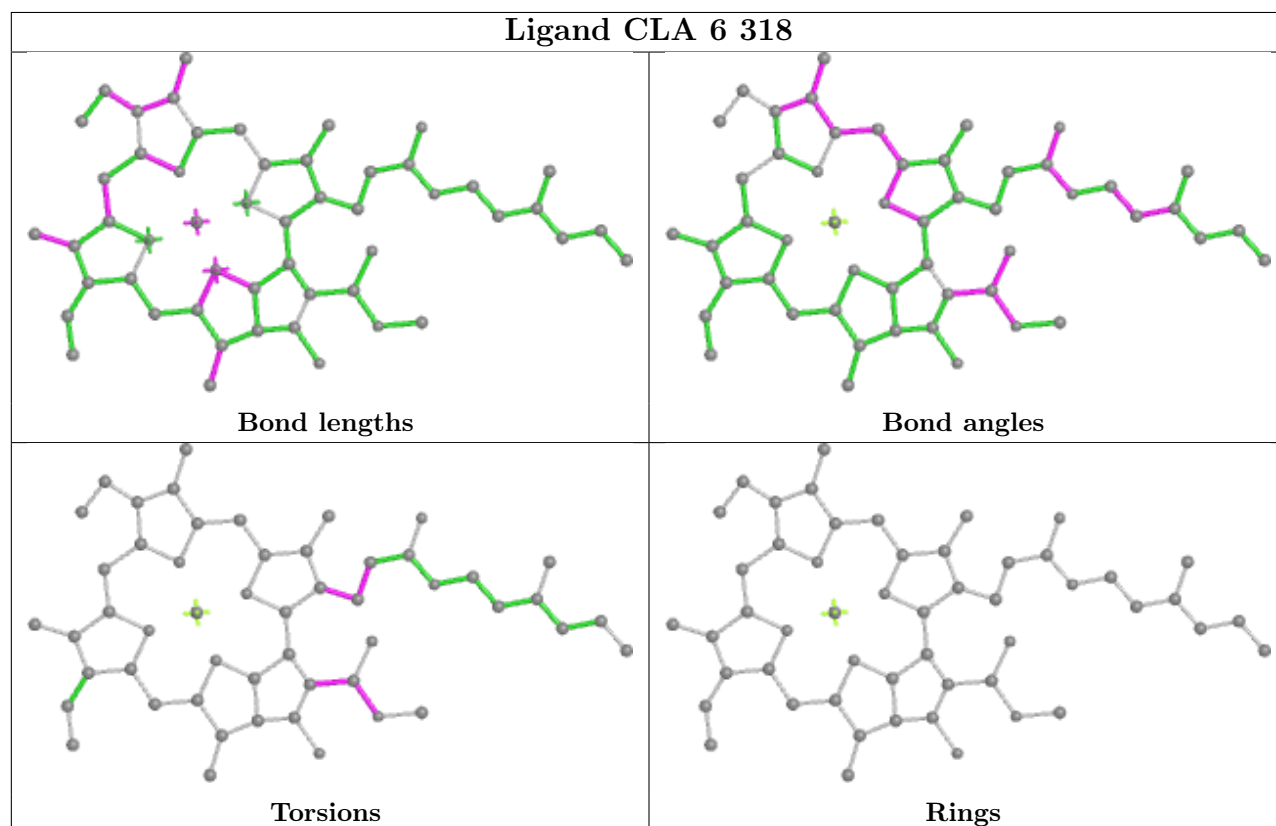
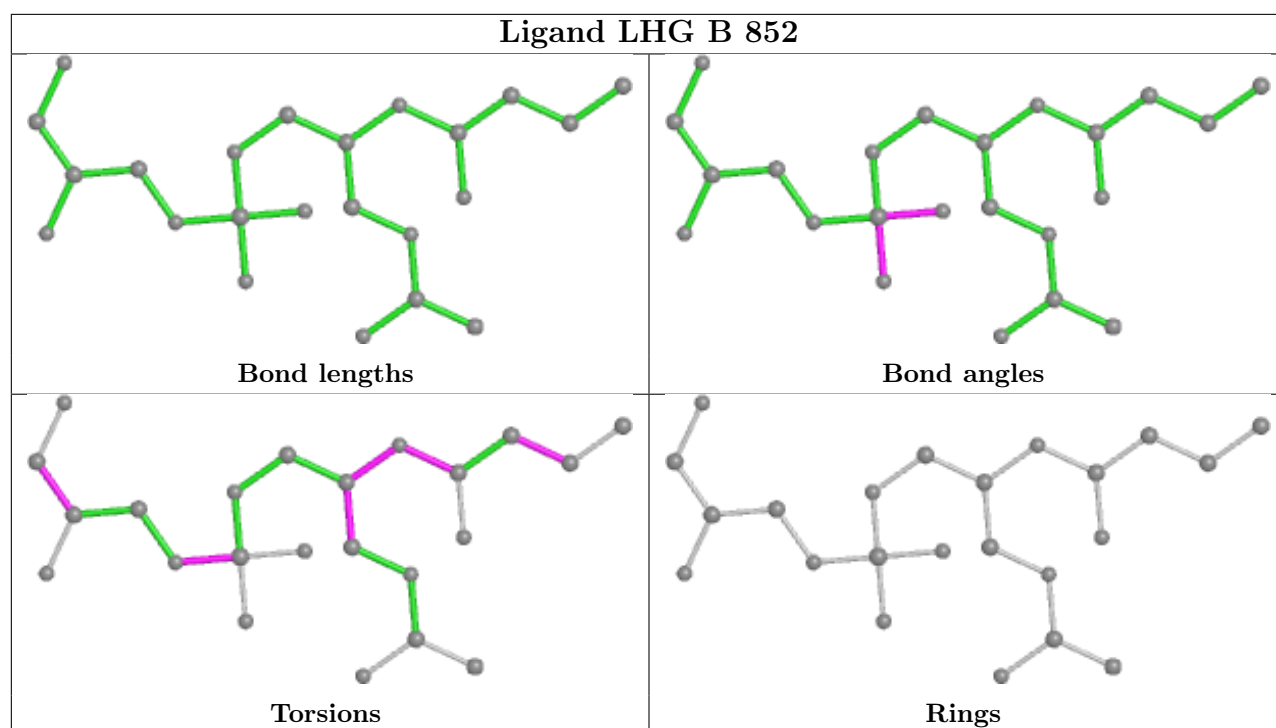
Bond angles



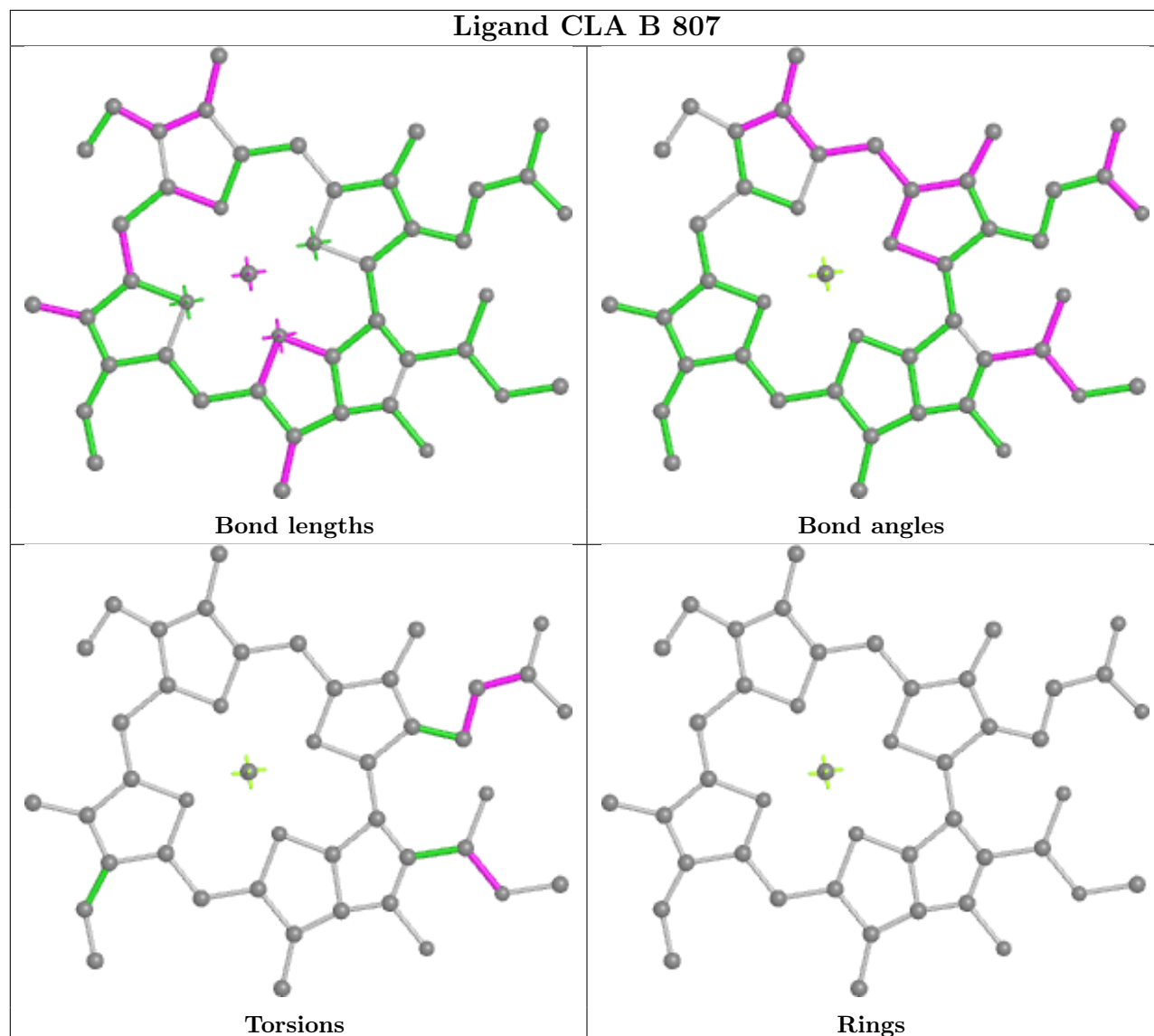
Torsions

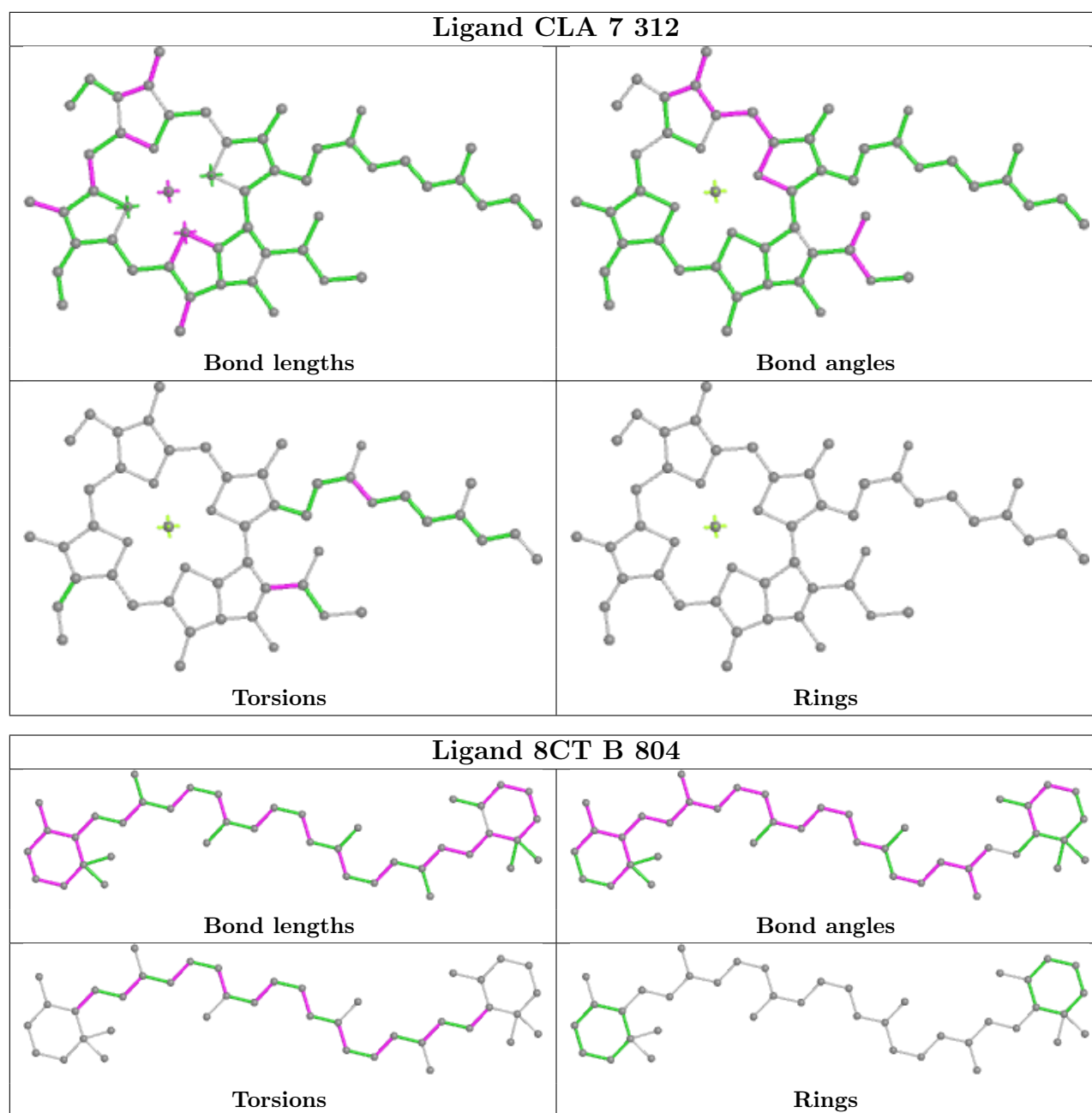


Rings

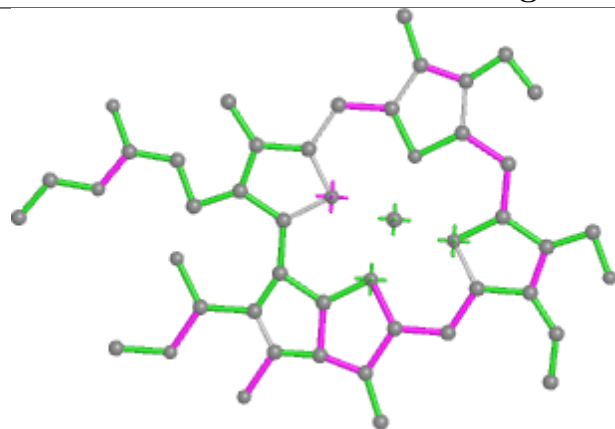


Ligand CLA B 807

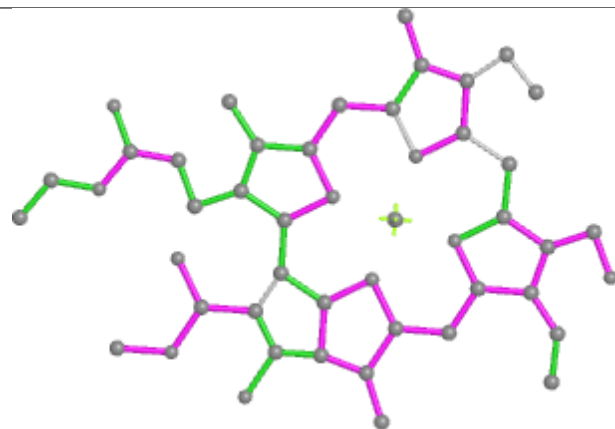




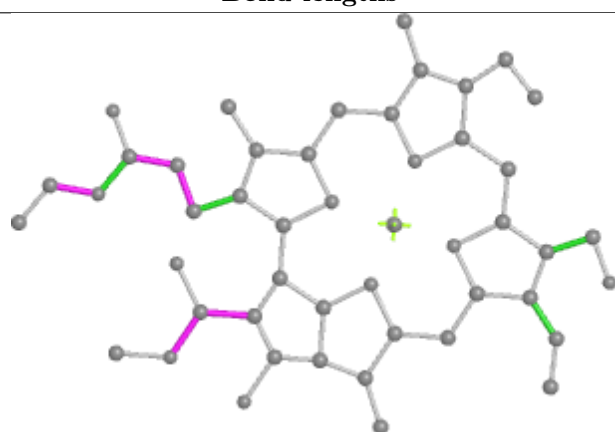
Ligand CHL 1 305



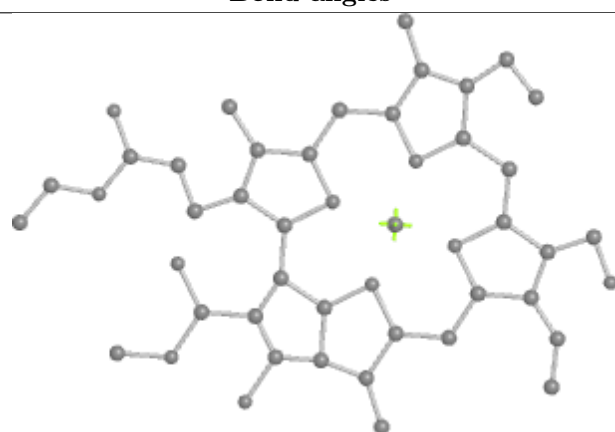
Bond lengths



Bond angles

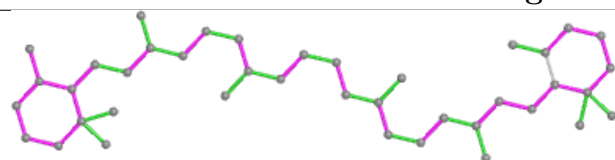


Torsions

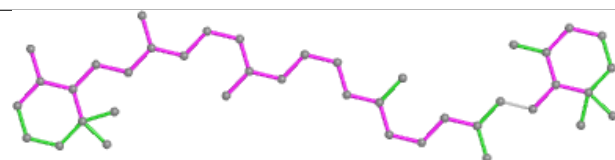


Rings

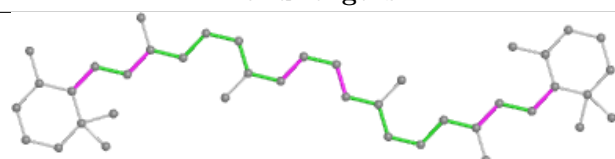
Ligand 8CT I 101



Bond lengths



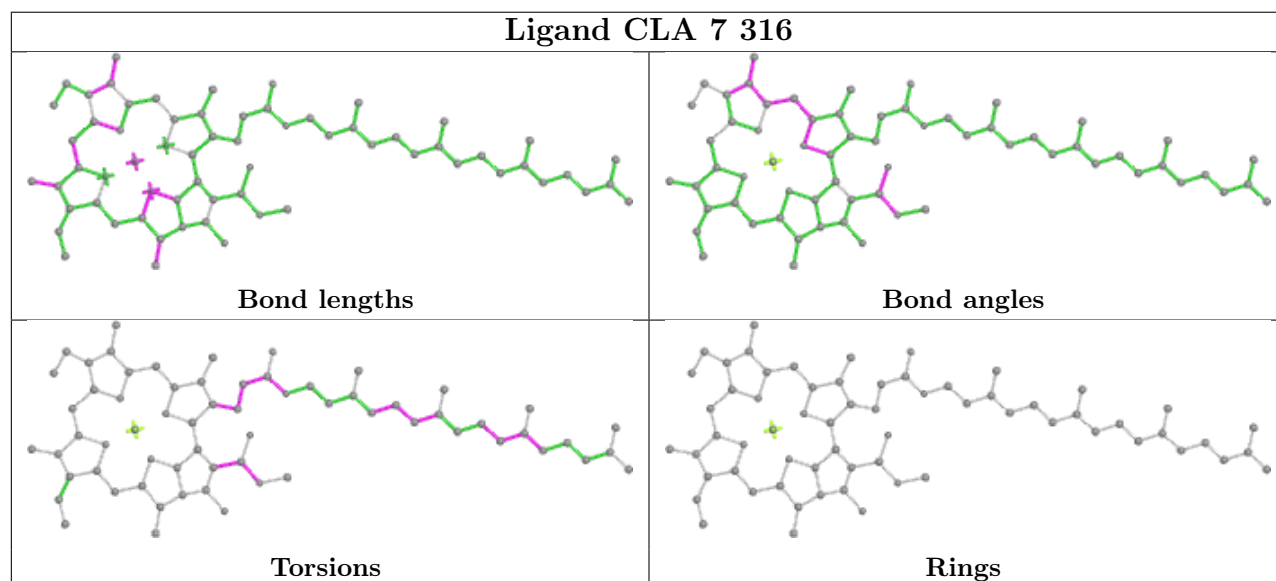
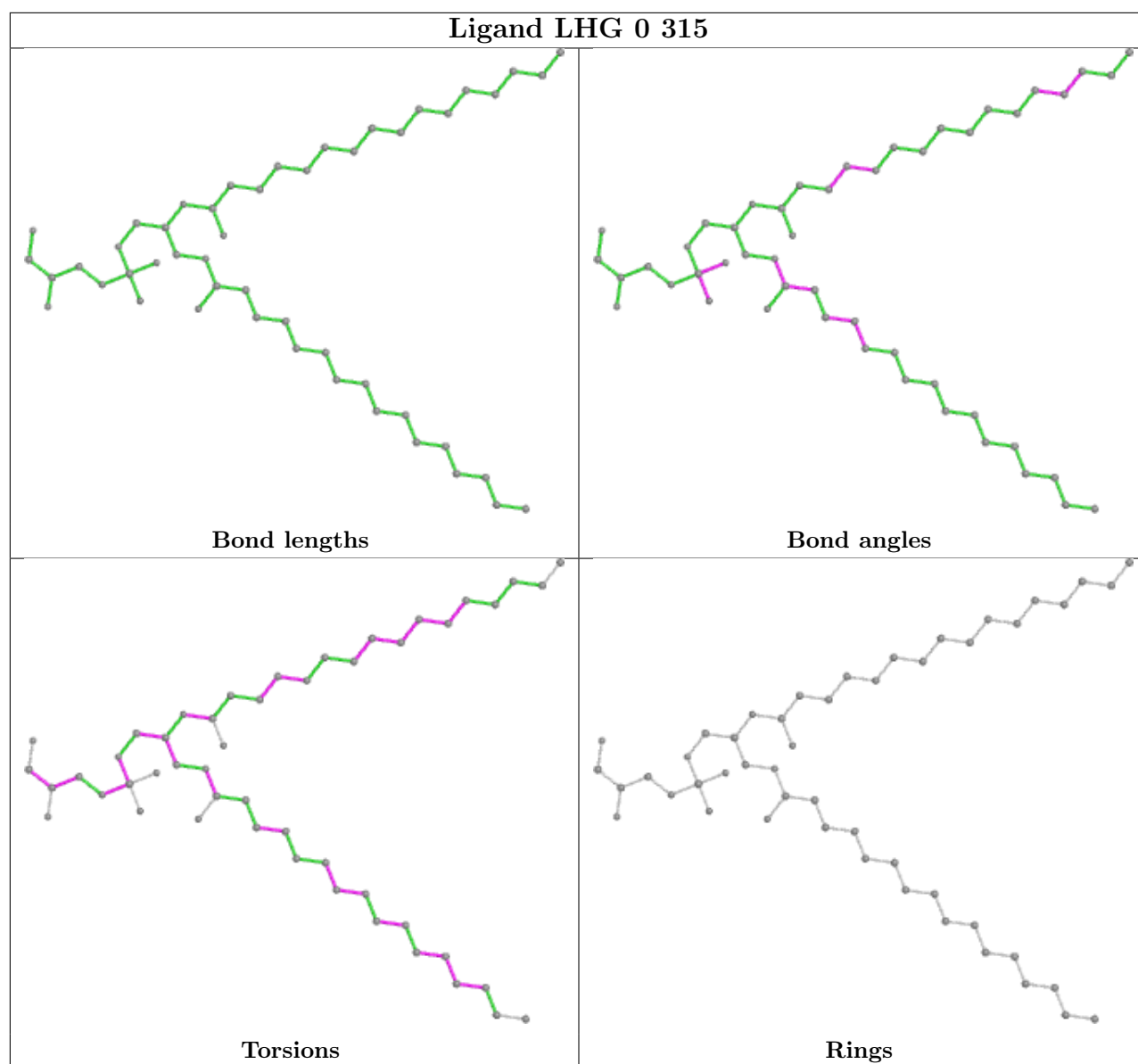
Bond angles



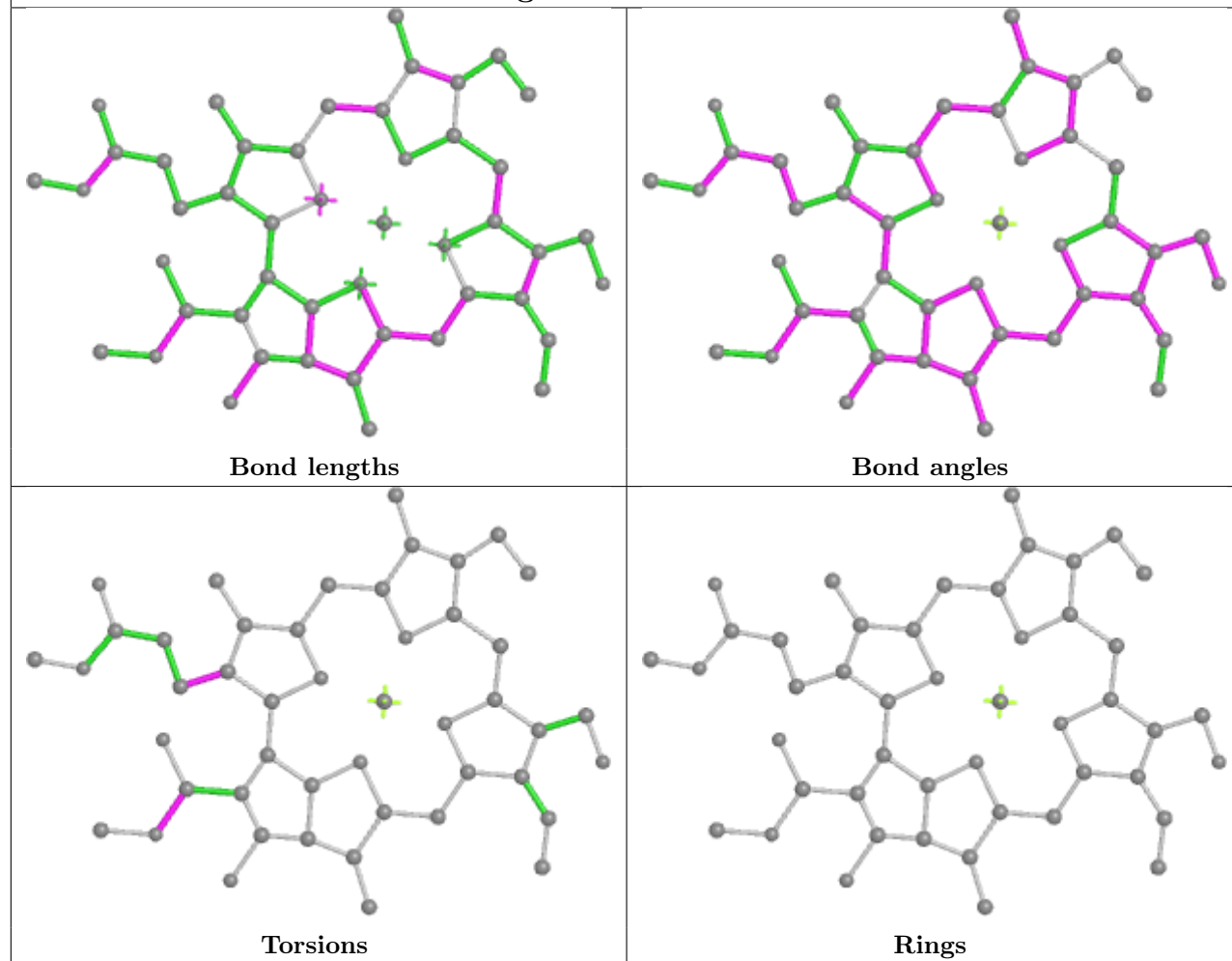
Torsions



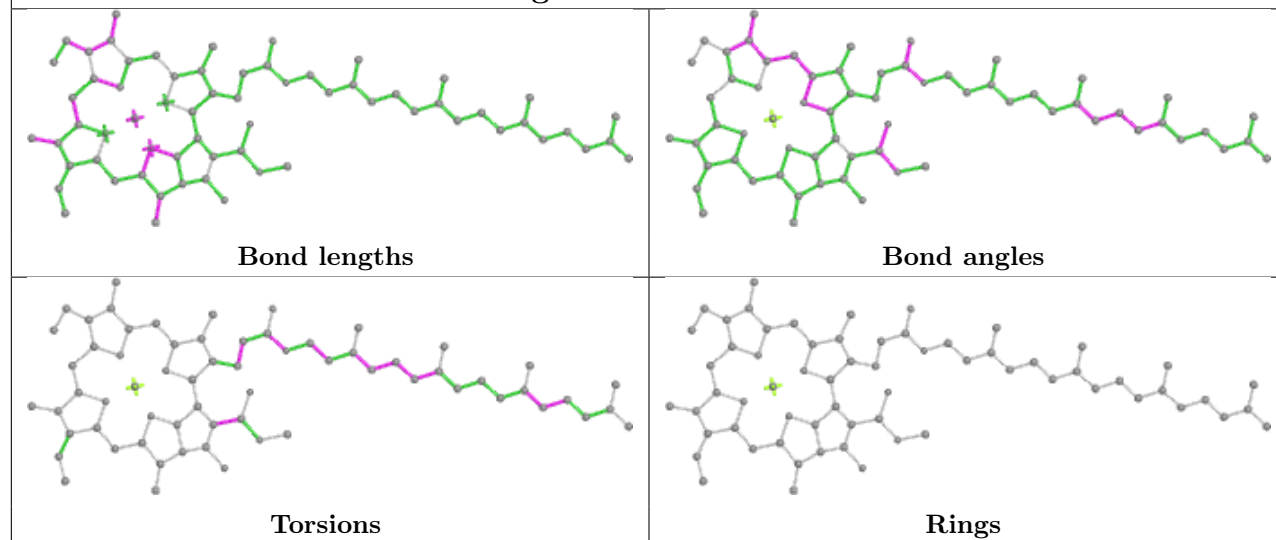
Rings



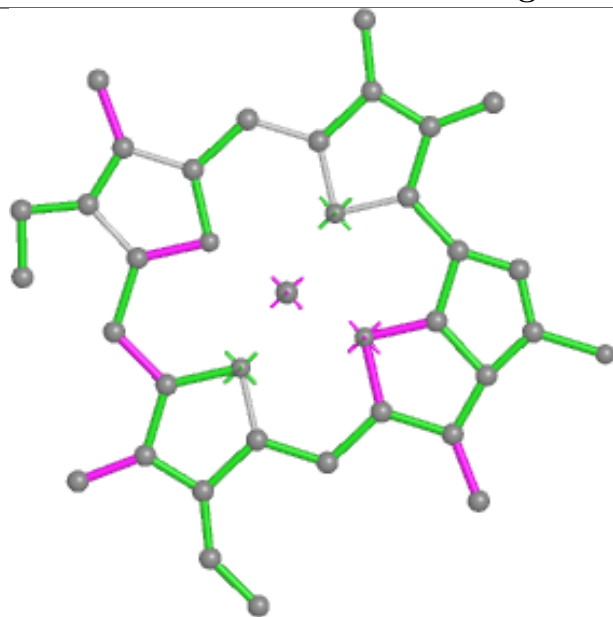
Ligand CHL 3 306



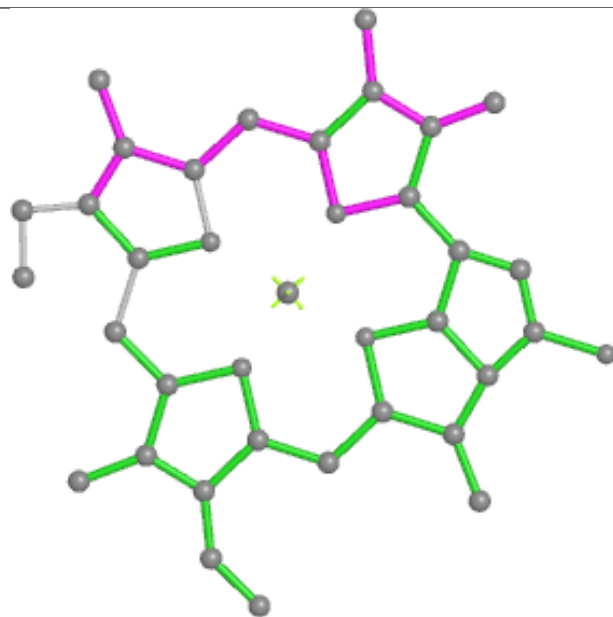
Ligand CLA A 840



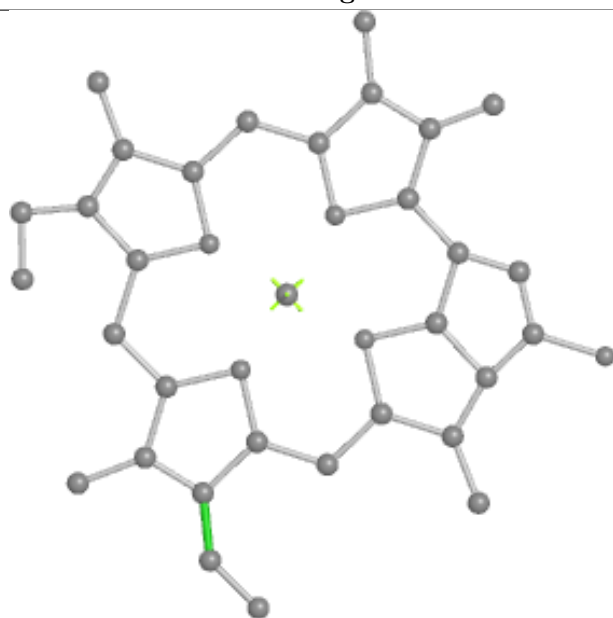
Ligand CLA 3 309



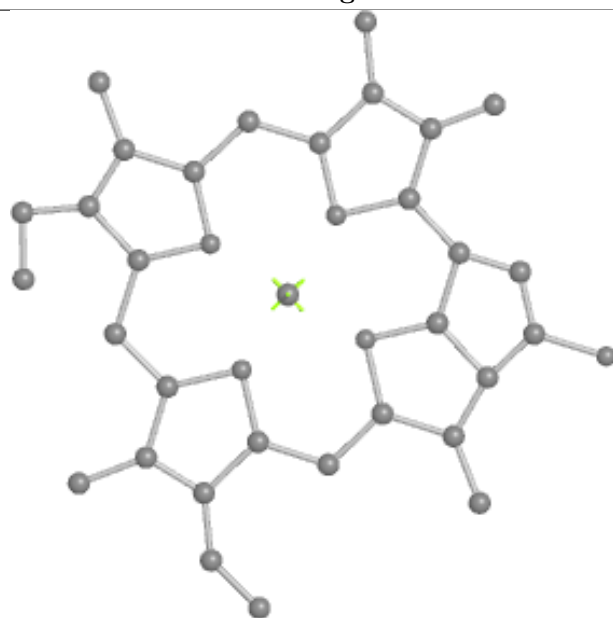
Bond lengths



Bond angles

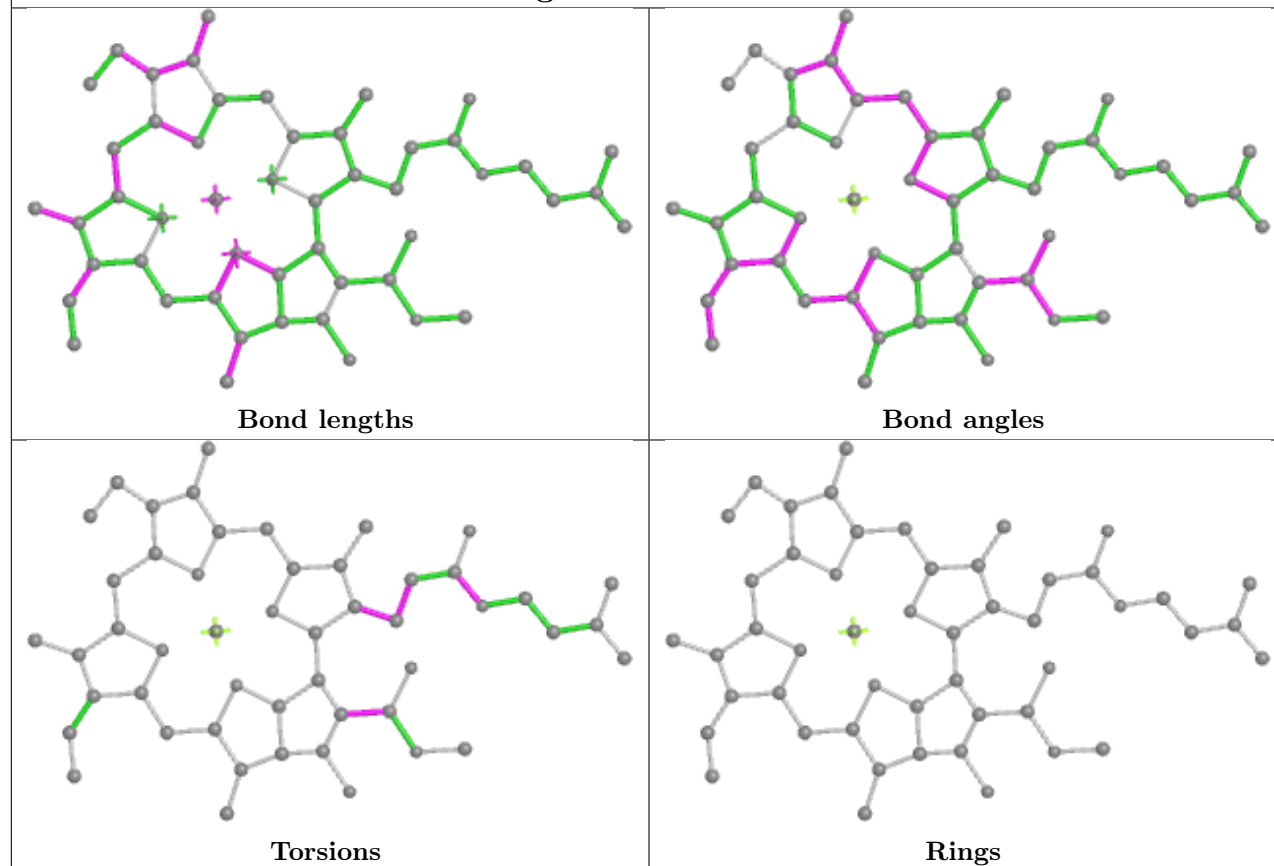


Torsions

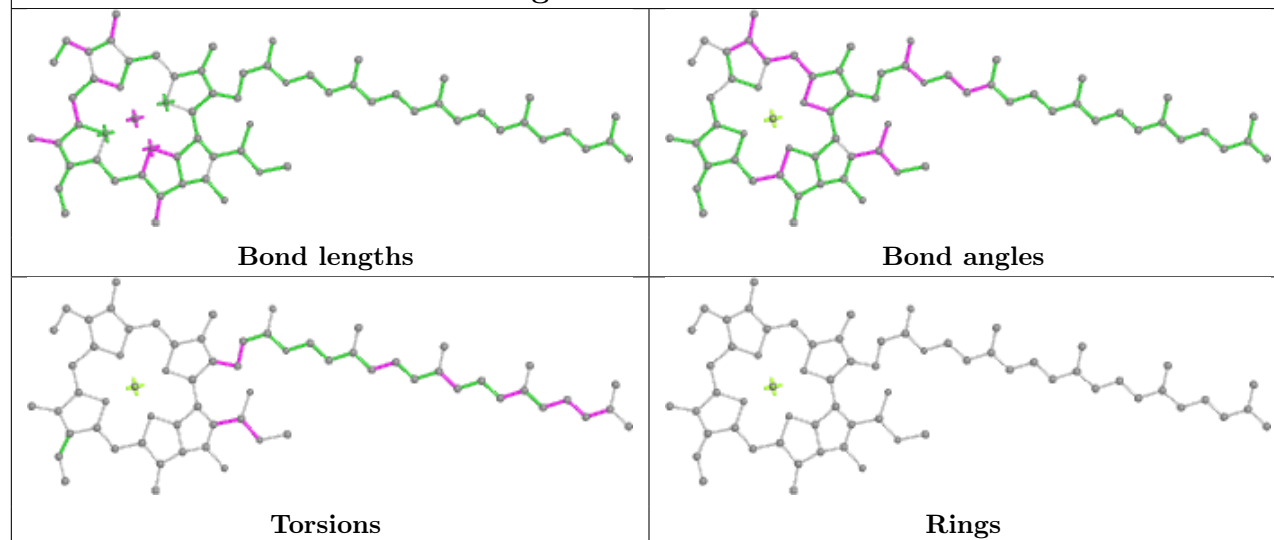


Rings

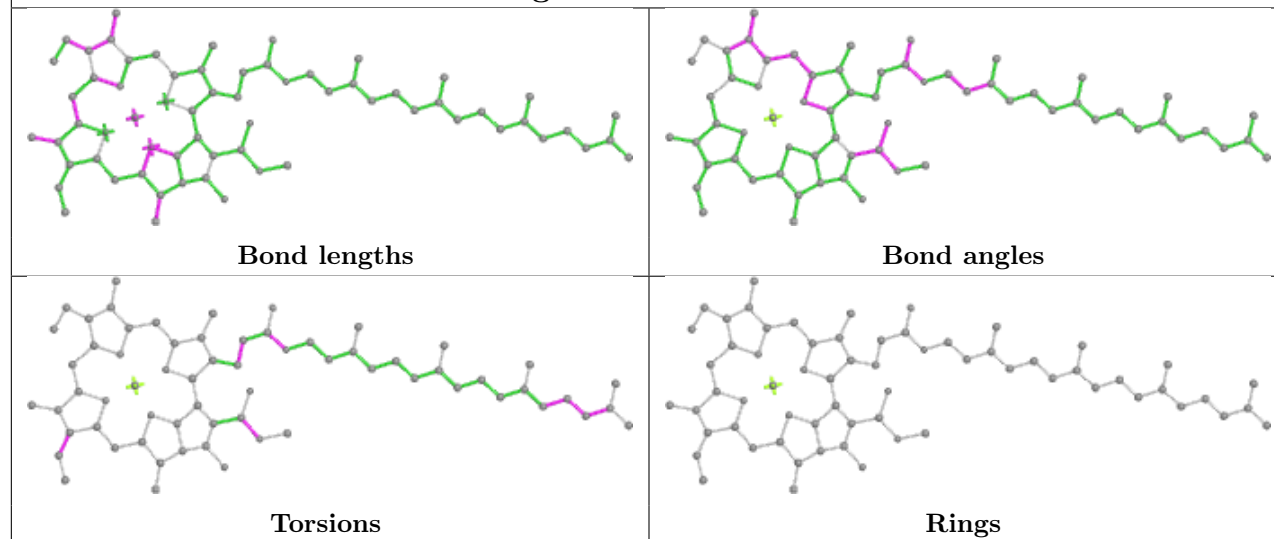
Ligand CLA 8 308



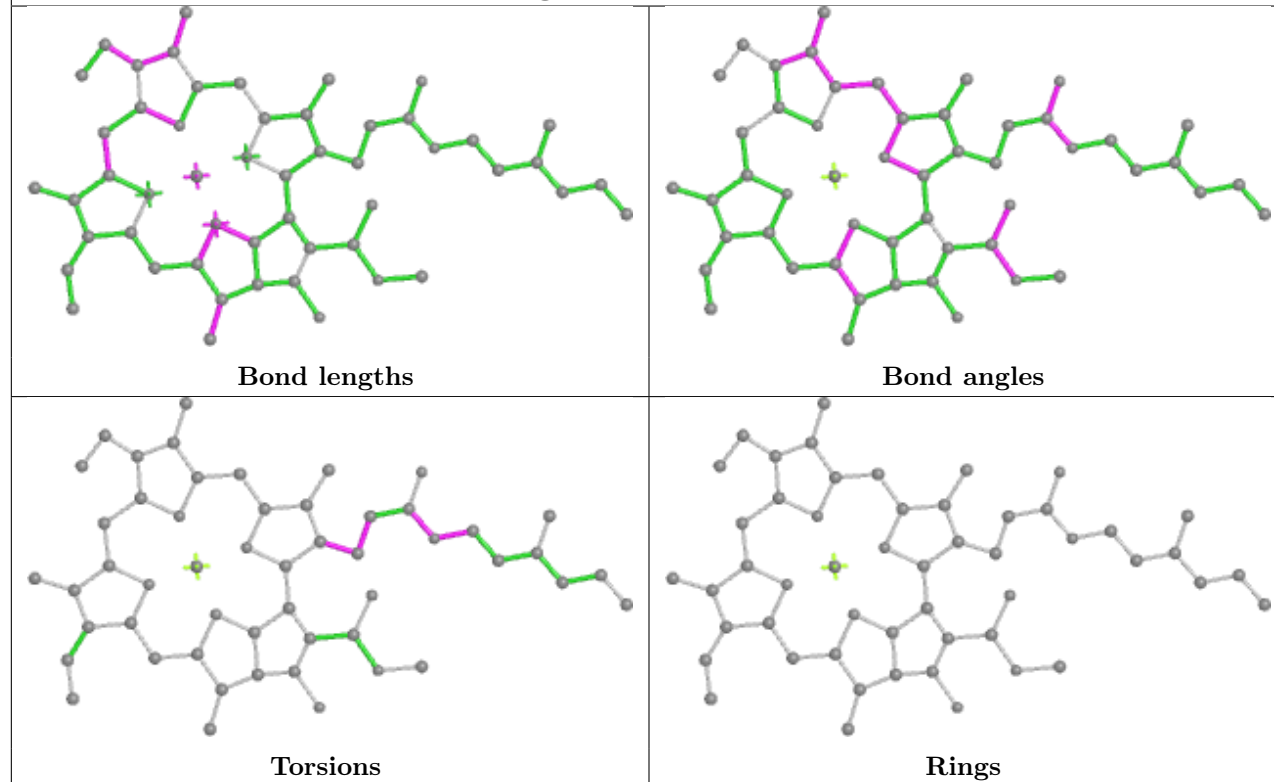
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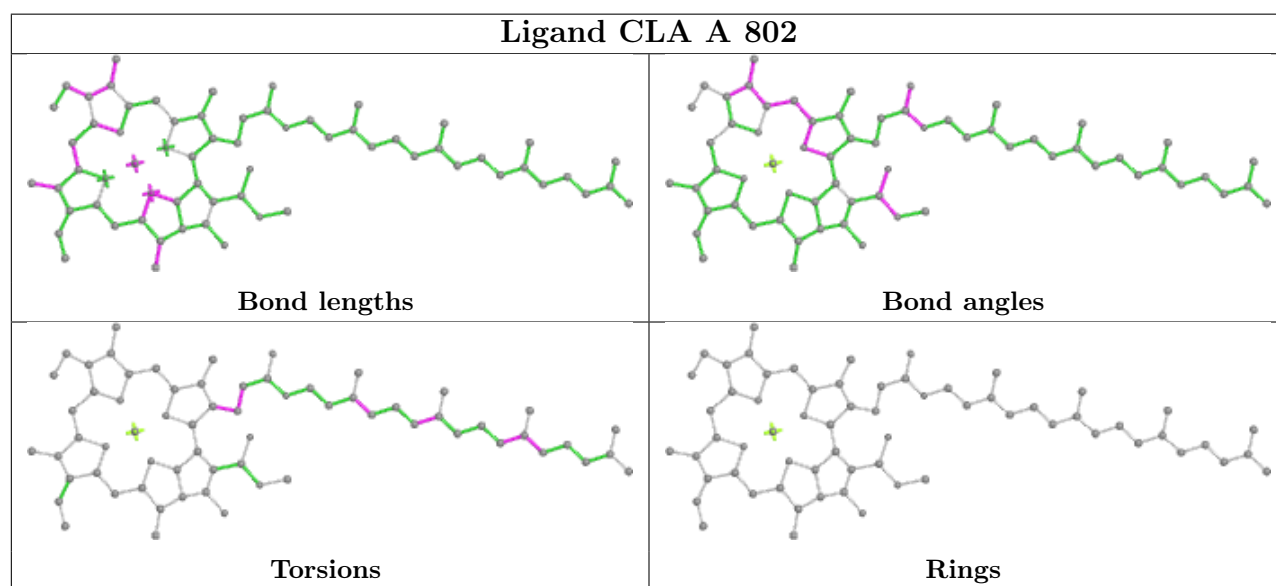
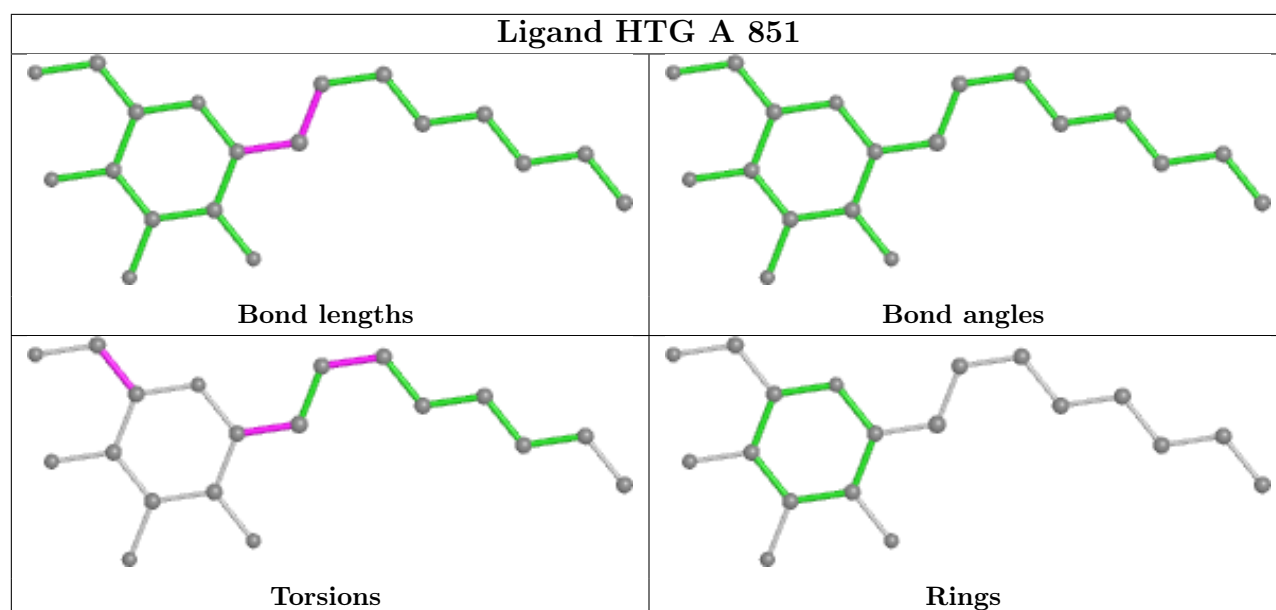


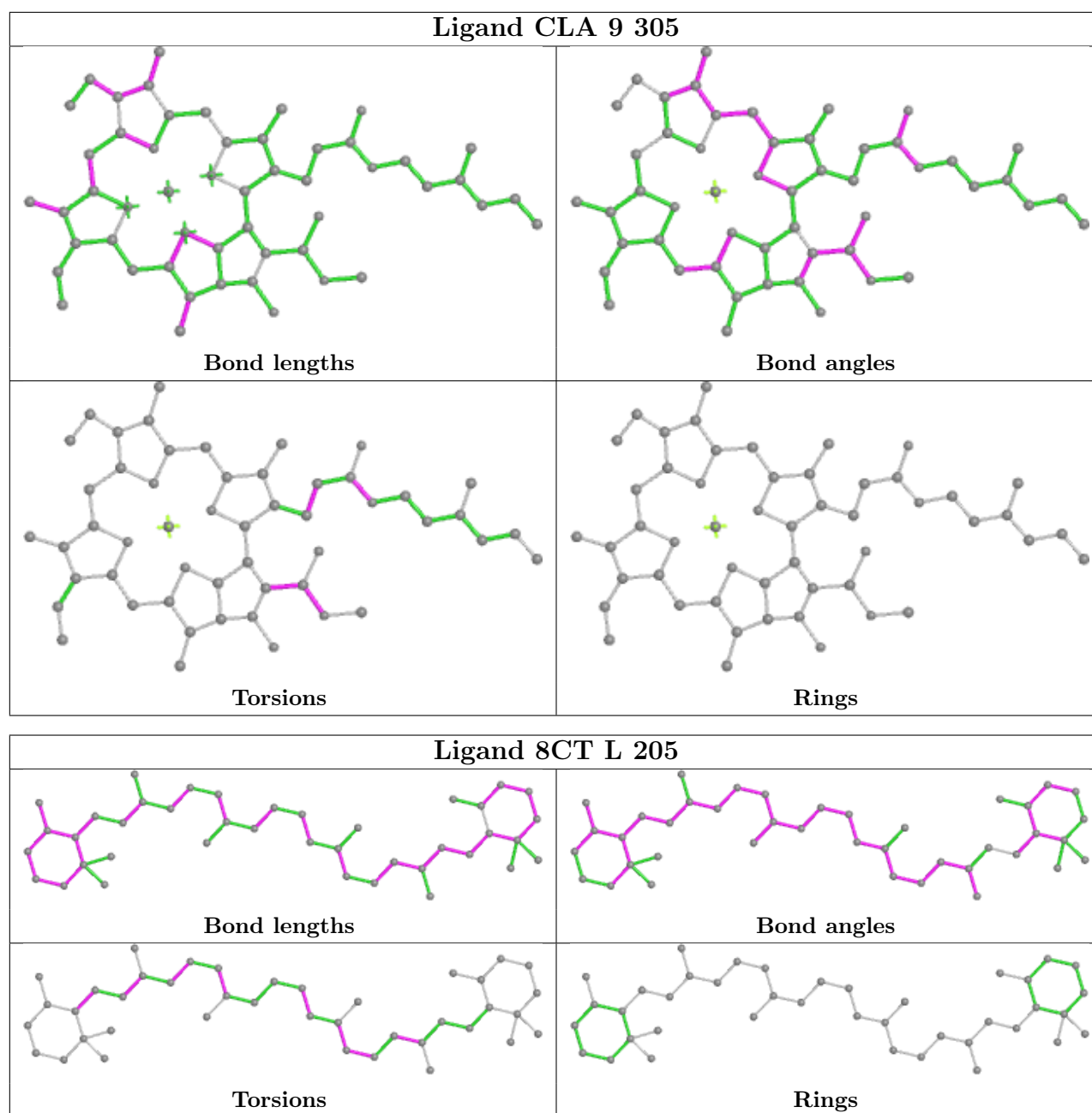
Ligand CLA B 815



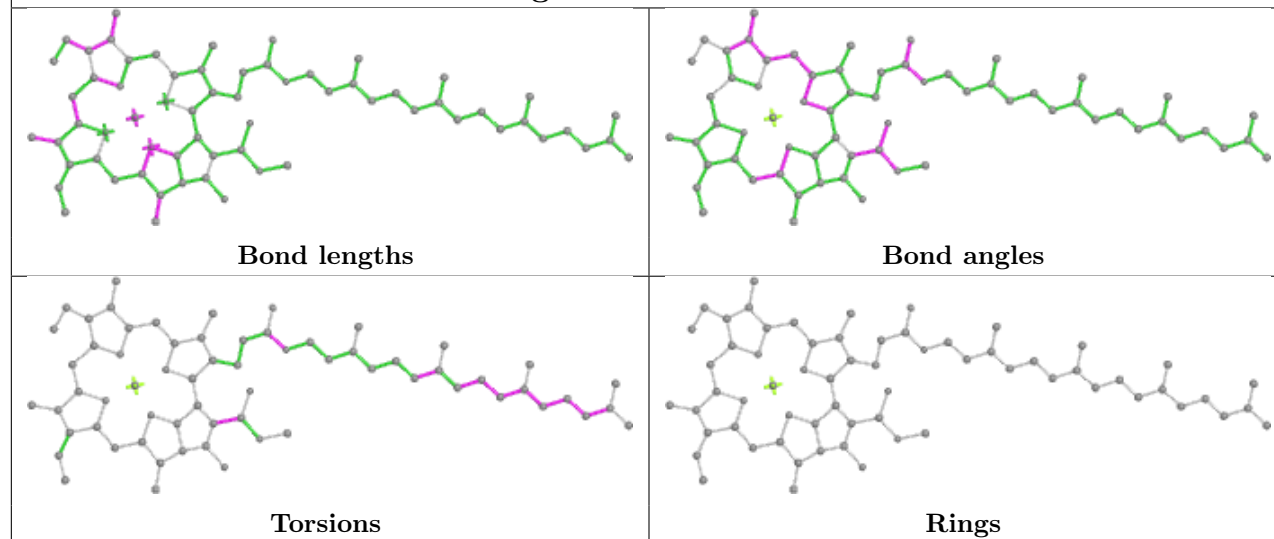
Ligand CLA 1 304



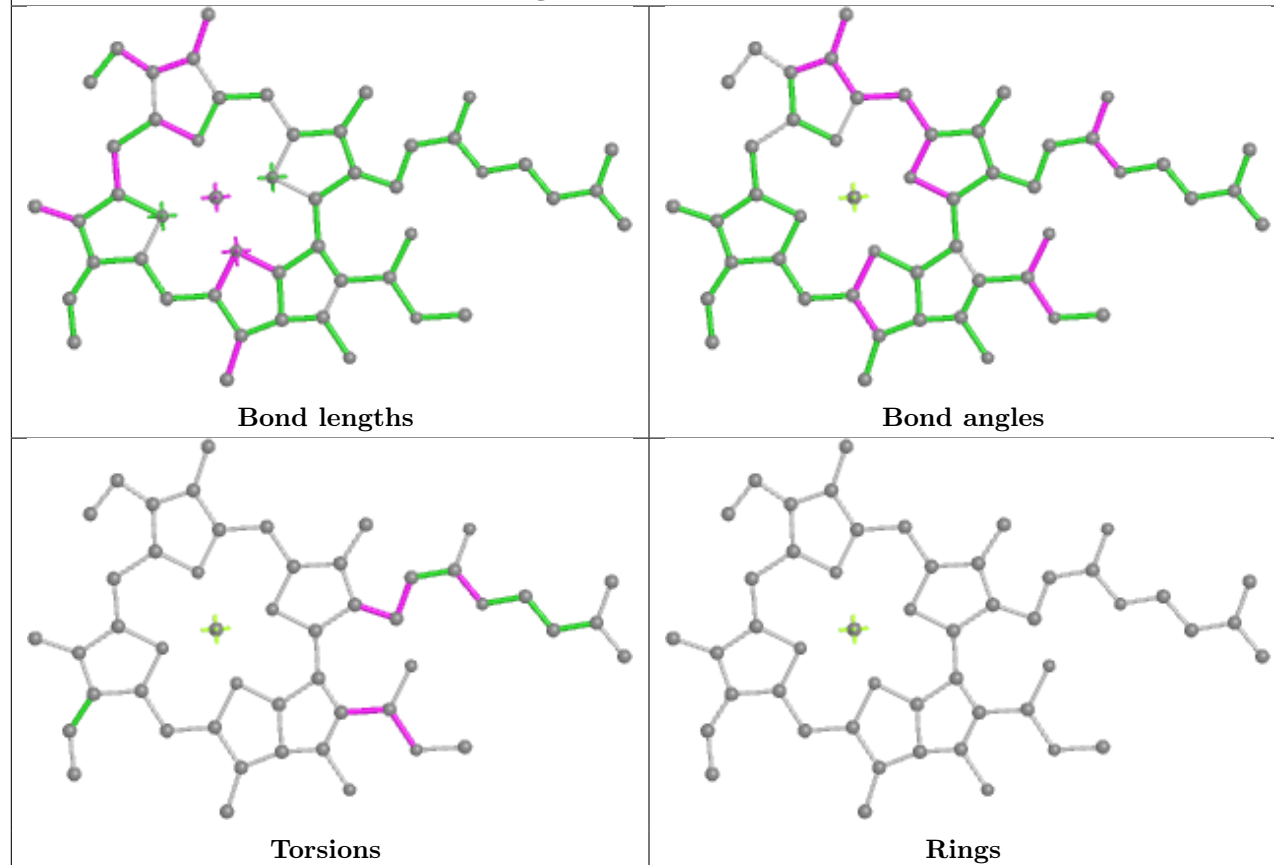


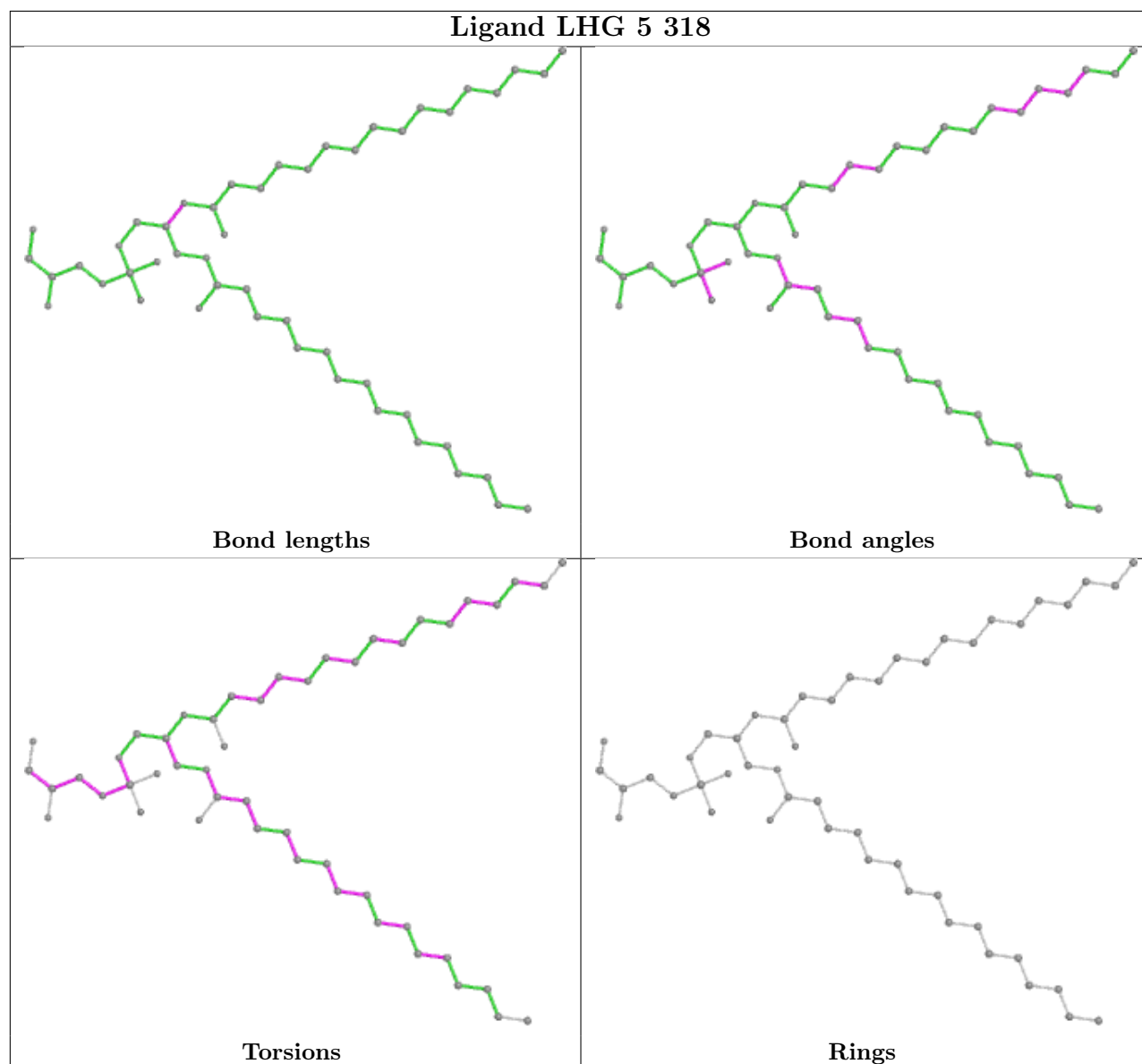
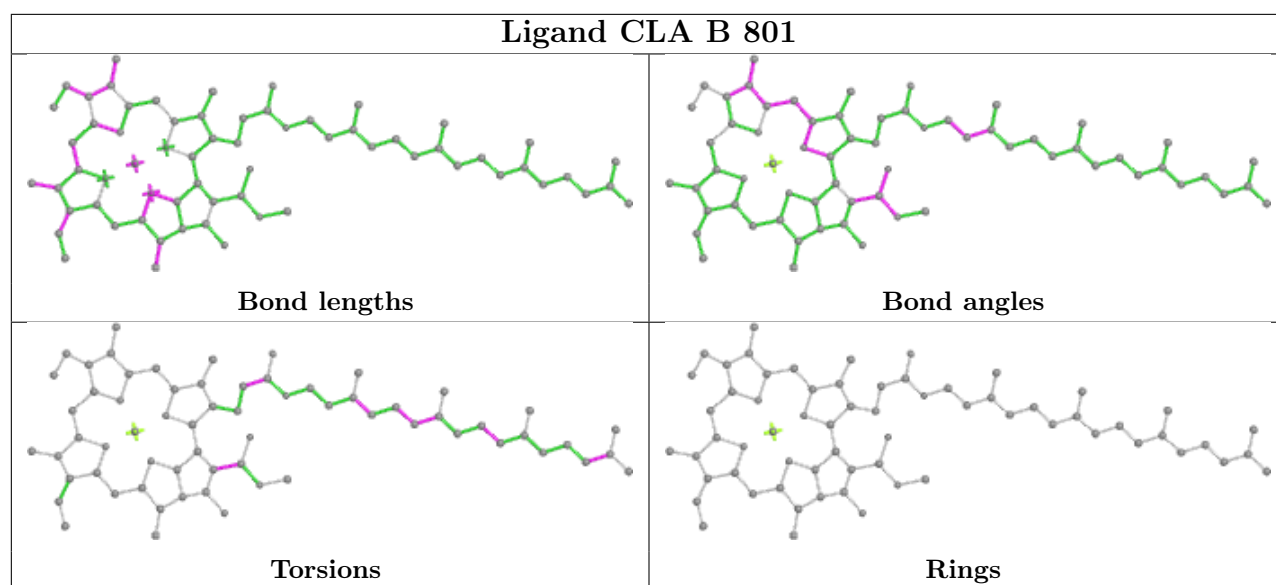


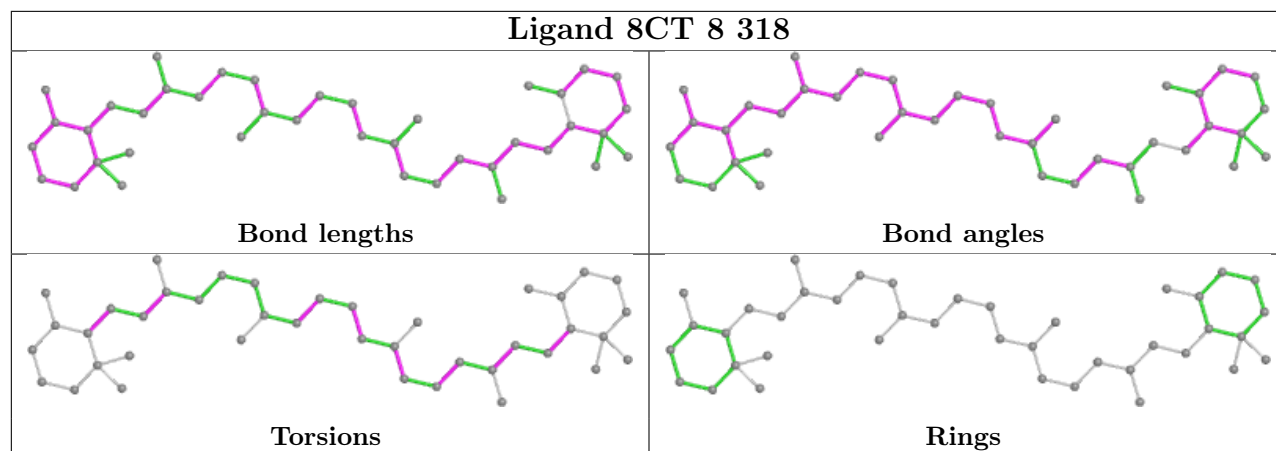
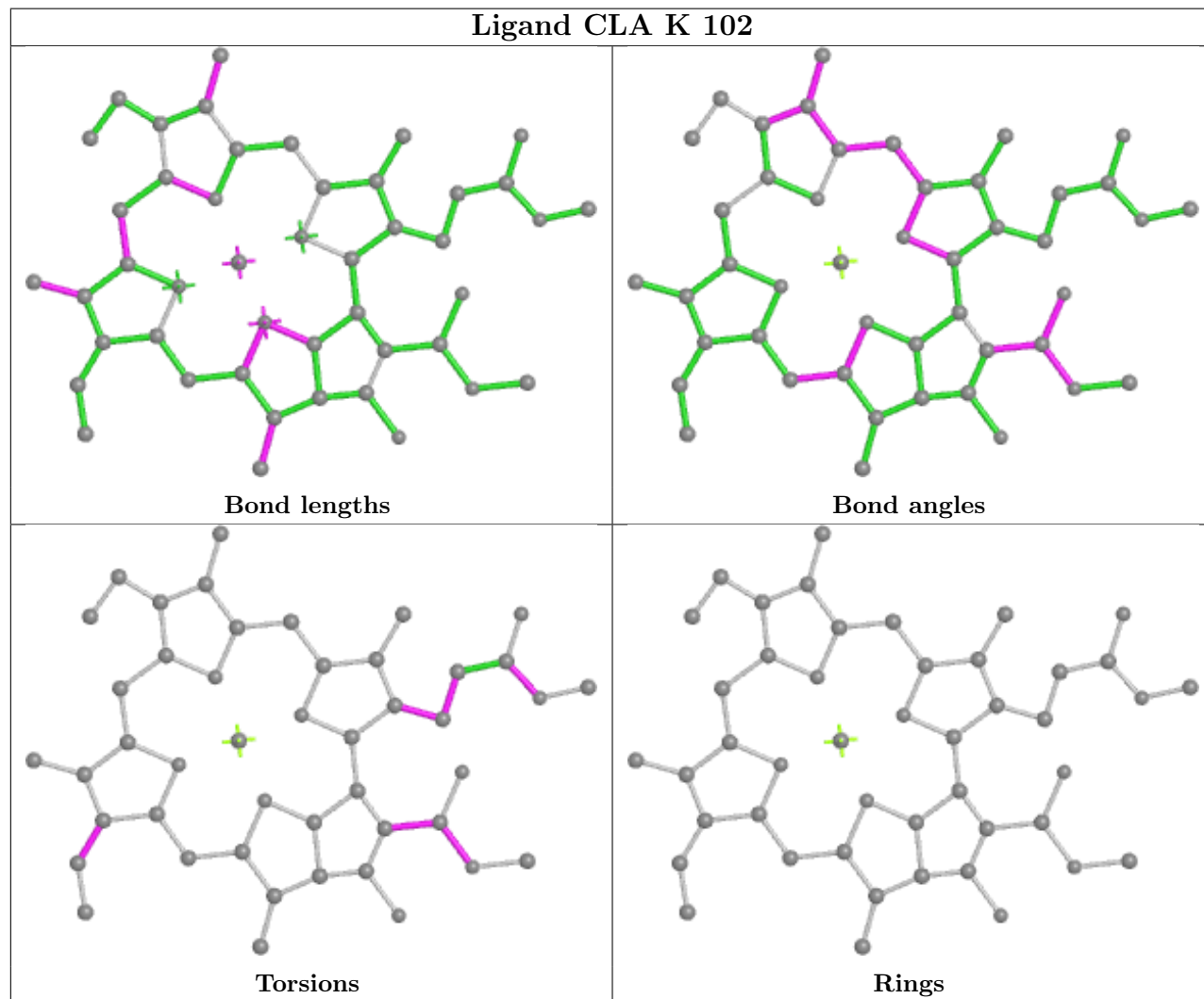
Ligand CLA A 807

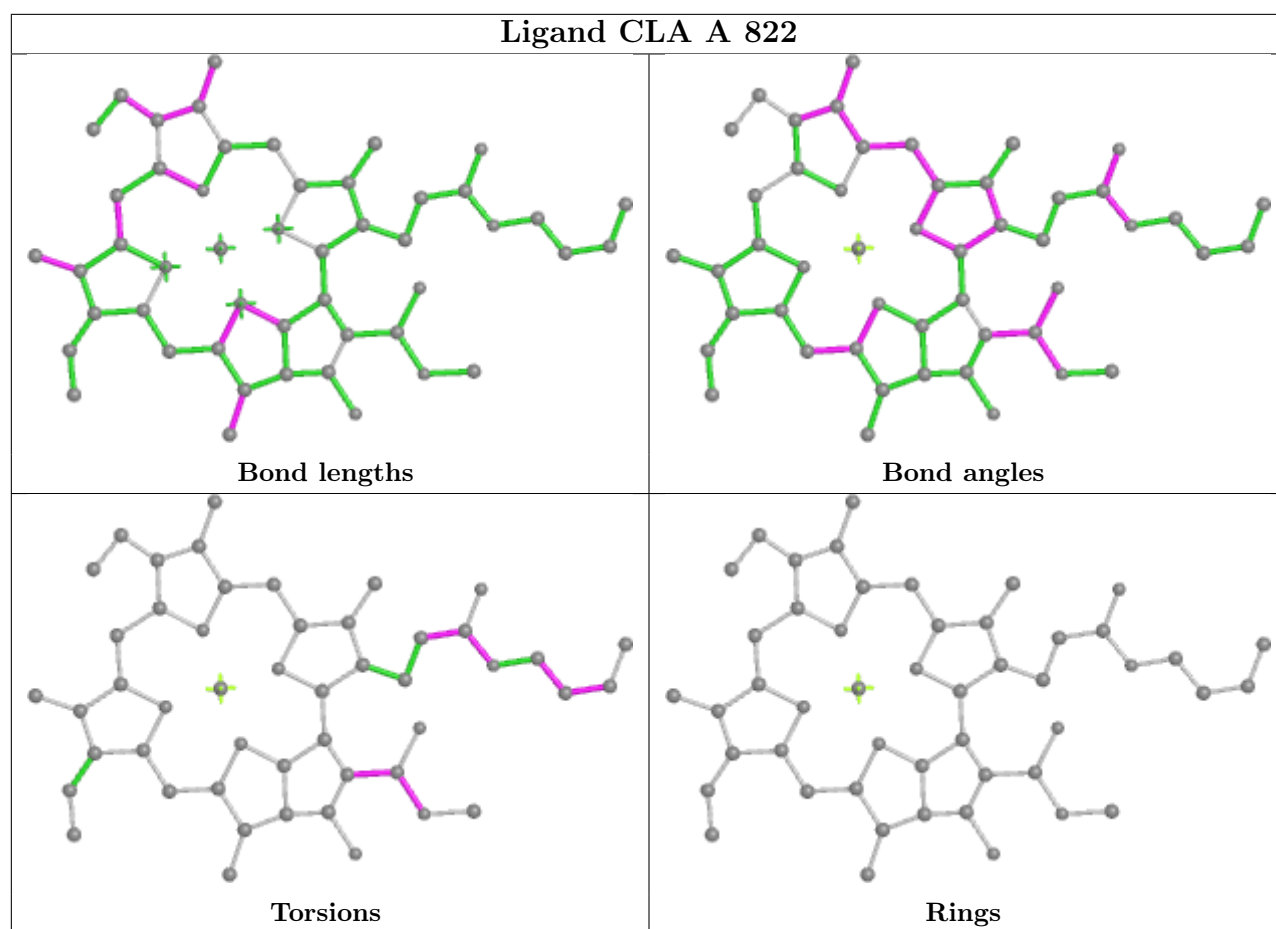


Ligand CLA B 831

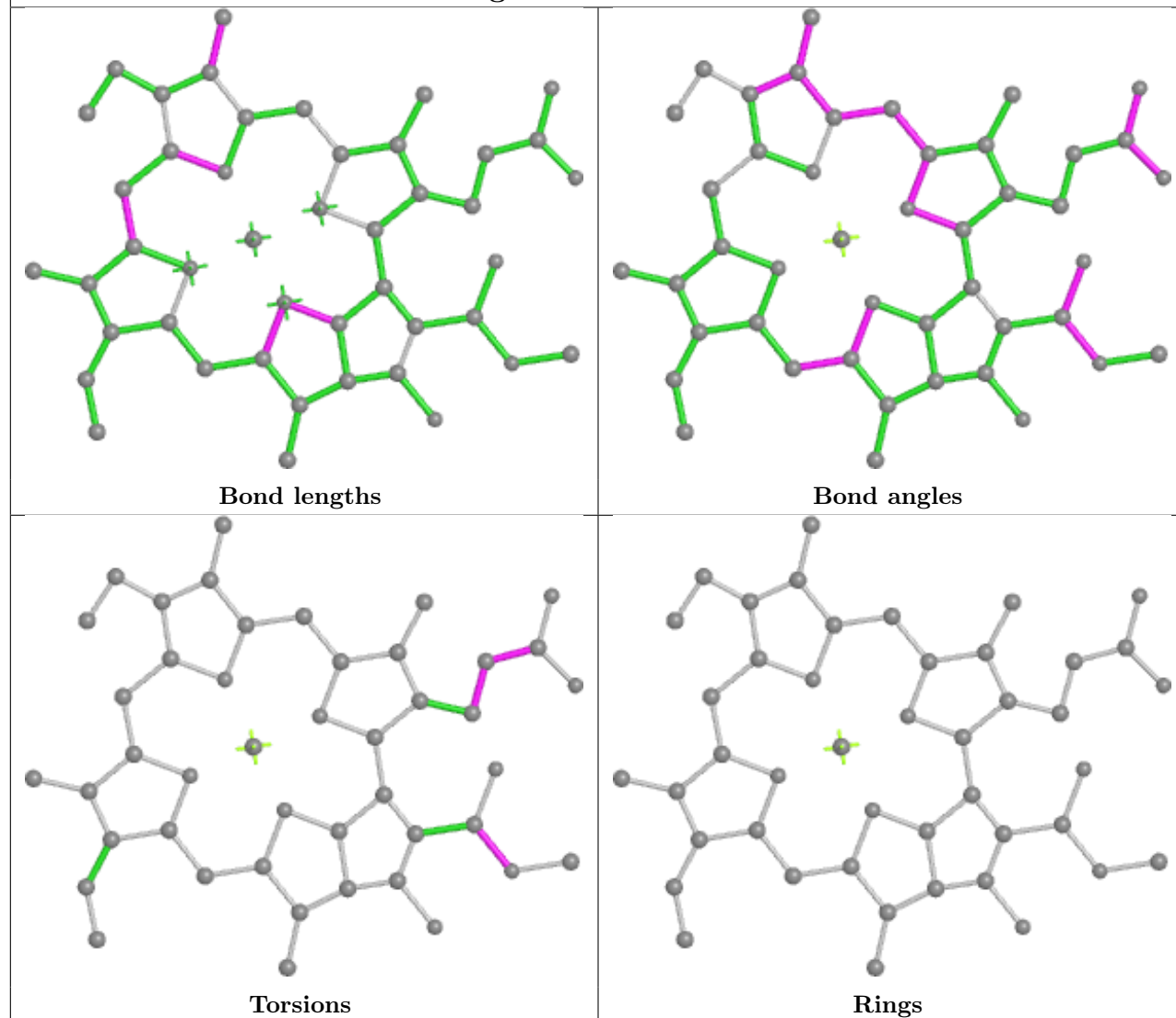




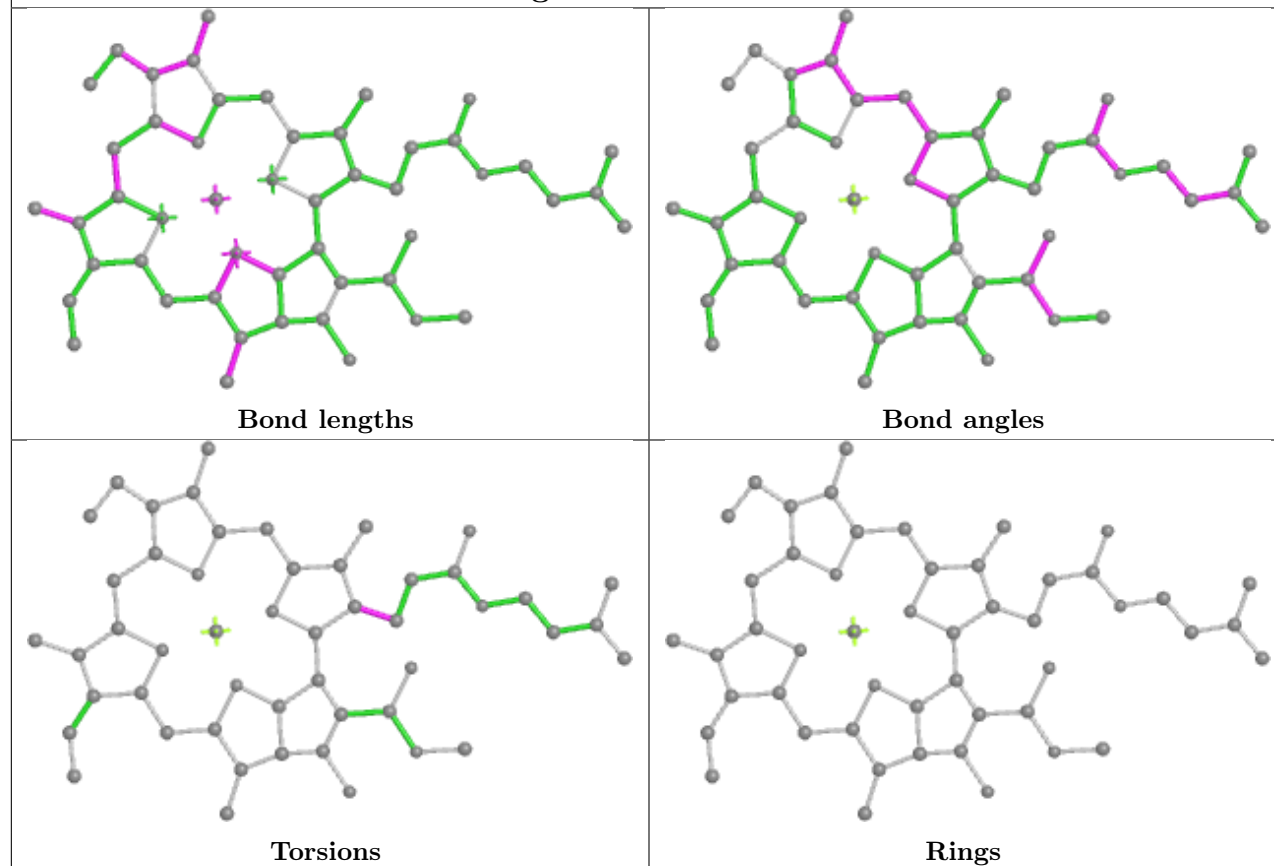
Ligand 8CT 8 318**Ligand CLA K 102**



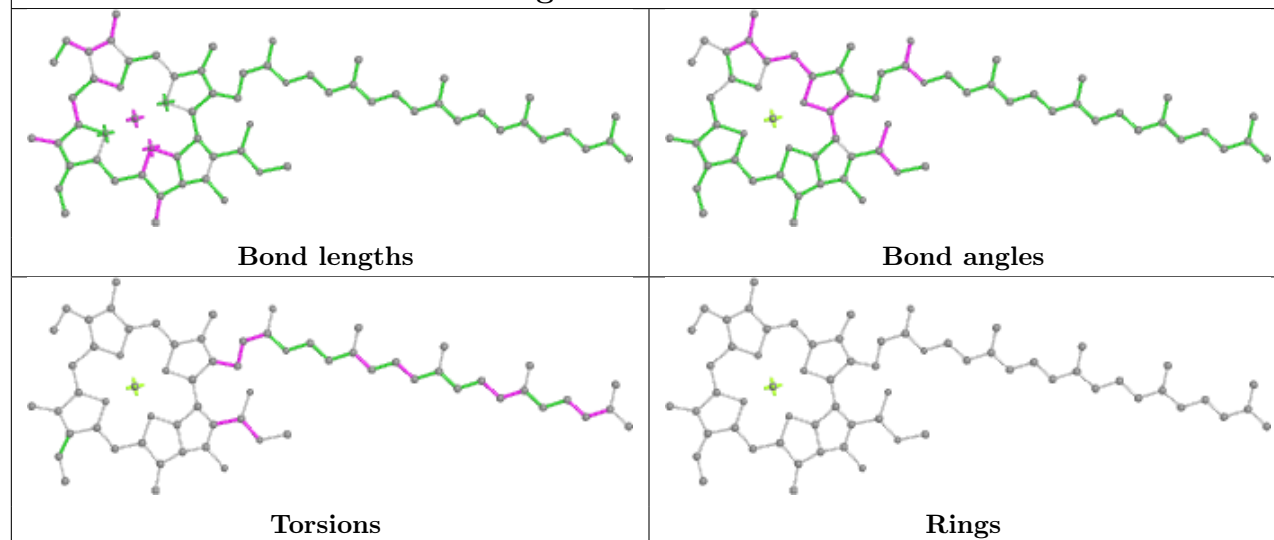
Ligand CLA G 101



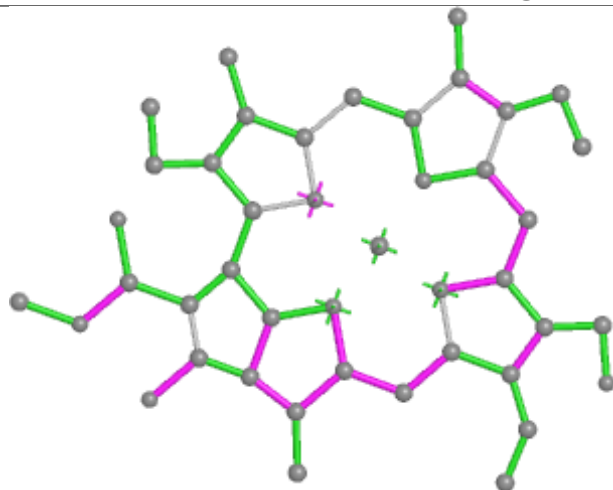
Ligand CLA A 831



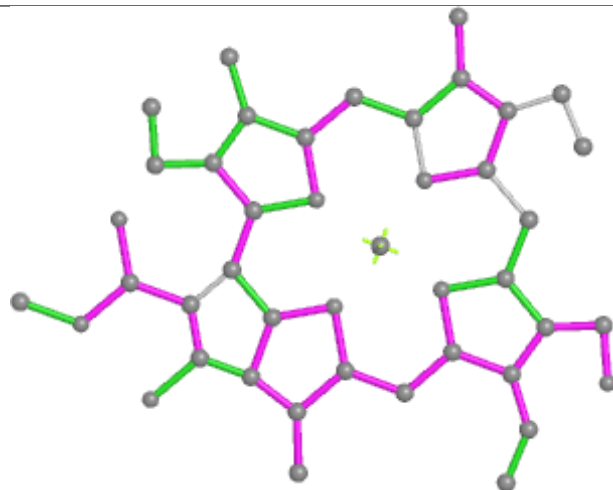
Ligand CLA 7 318



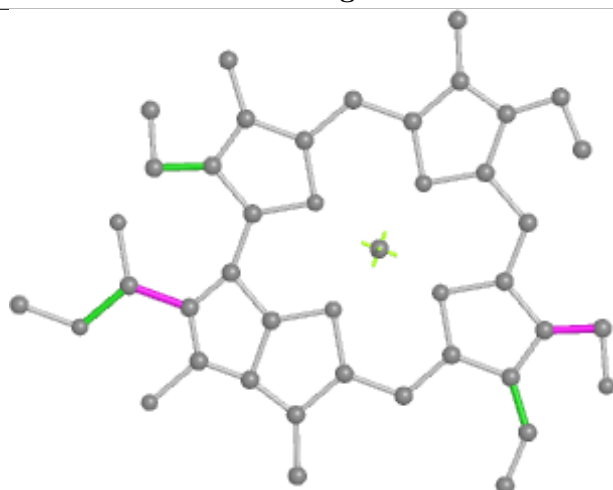
Ligand CHL 2 305



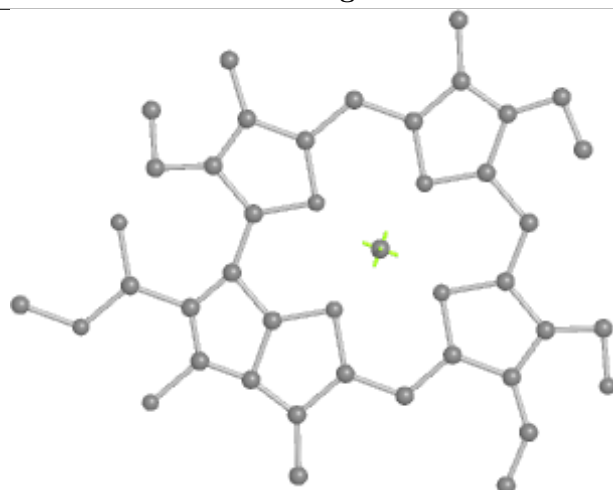
Bond lengths



Bond angles

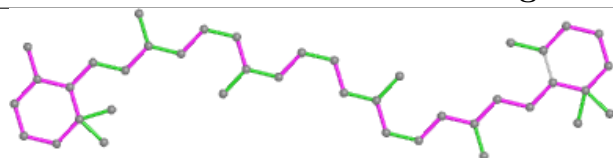


Torsions

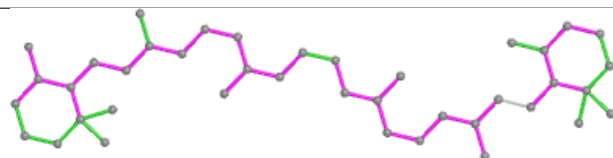


Rings

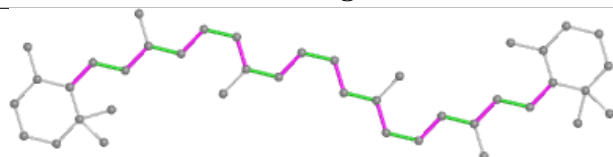
Ligand 8CT L 206



Bond lengths



Bond angles

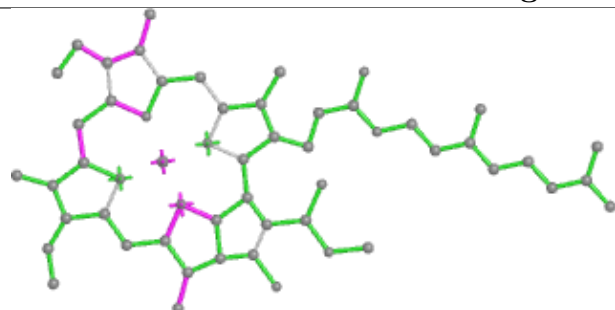


Torsions

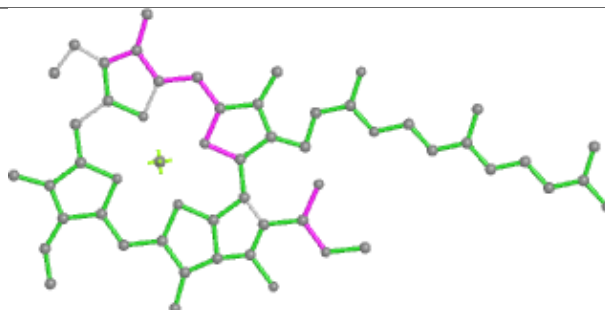


Rings

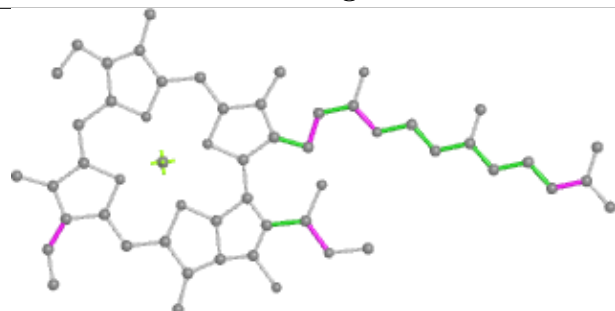
Ligand CLA 8 310



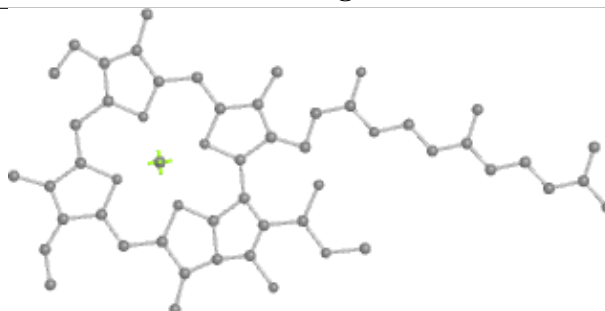
Bond lengths



Bond angles

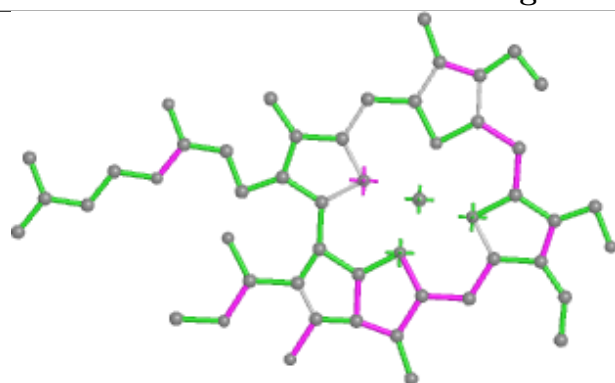


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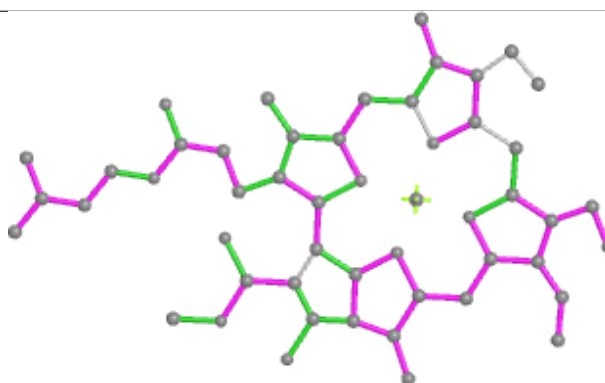


Rings

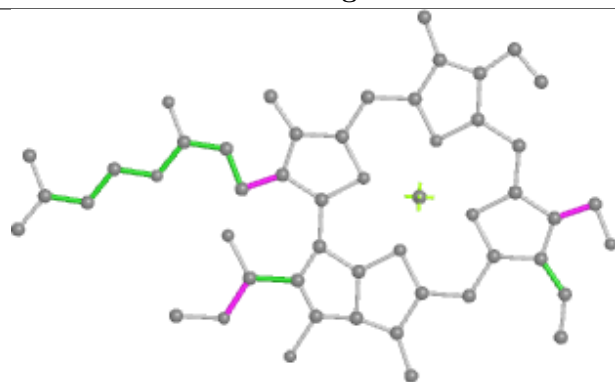
Ligand CHL 4 307



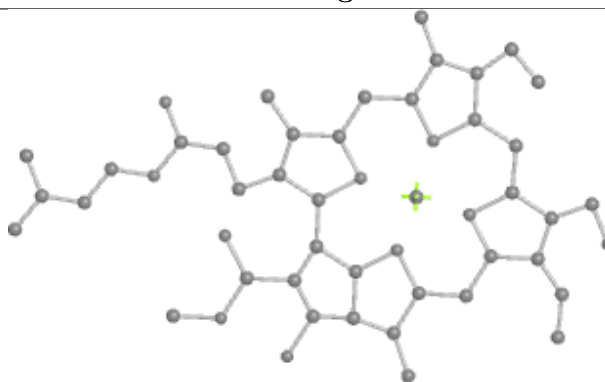
Bond lengths



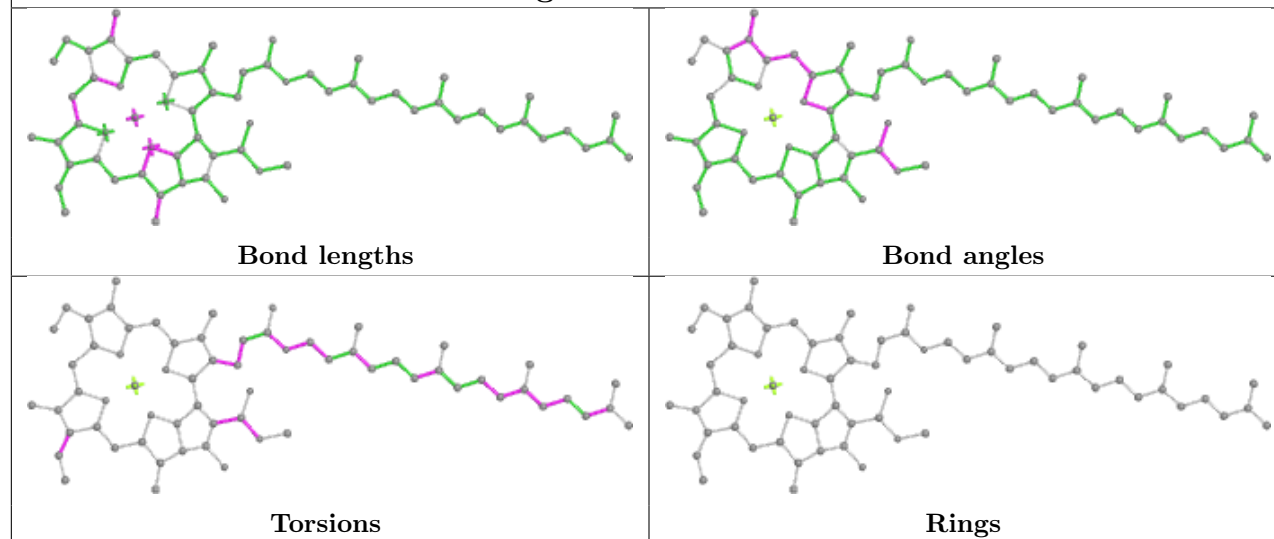
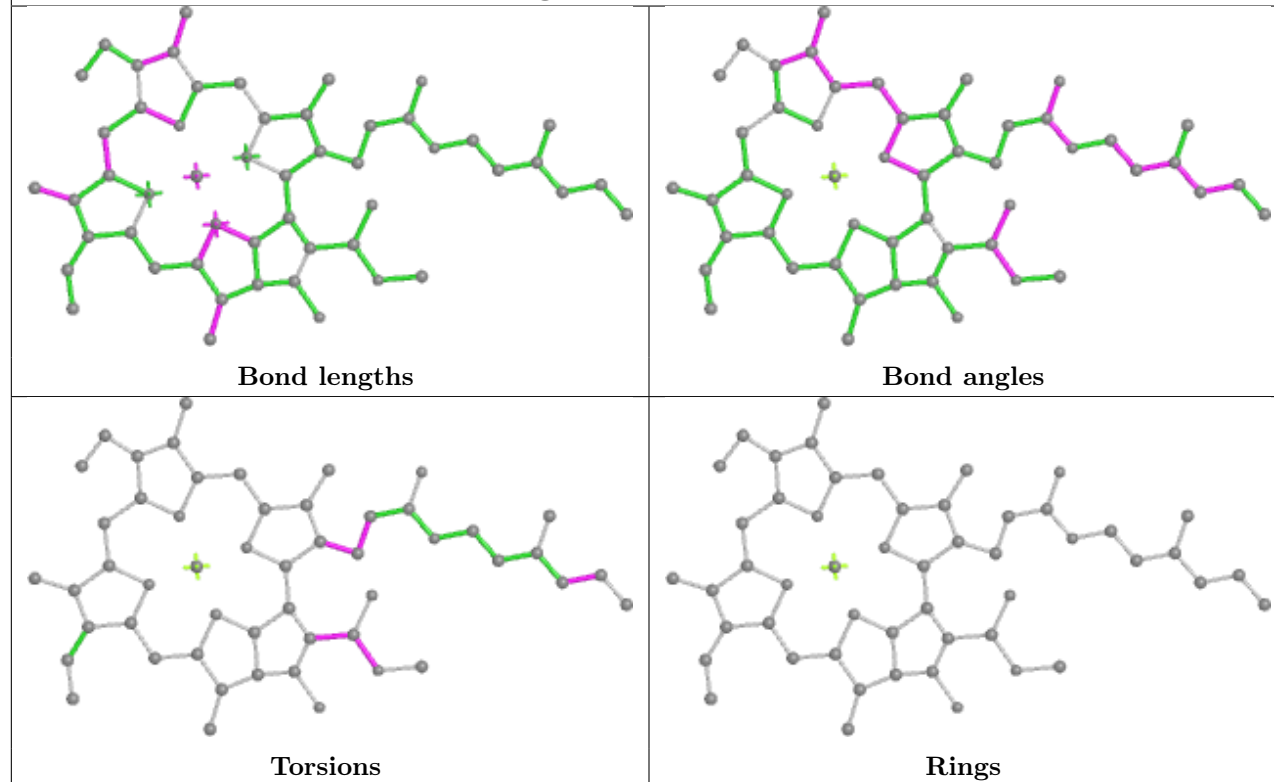
Bond angles



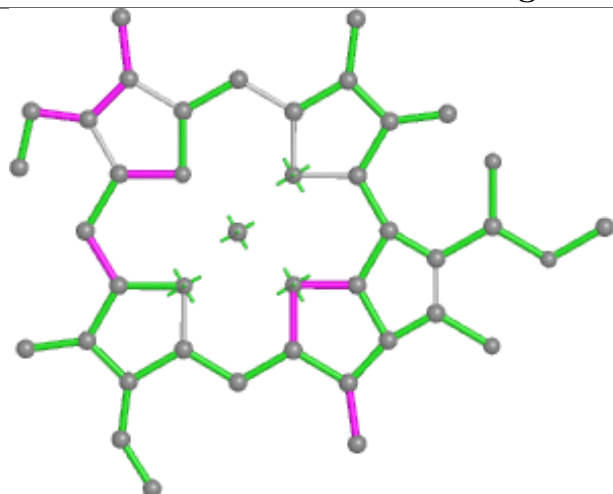
Torsions



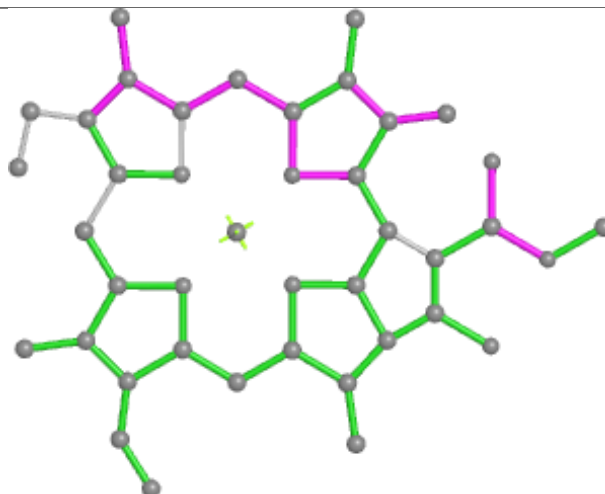
Rings

Ligand CLA 8 315**Ligand CLA 1 303**

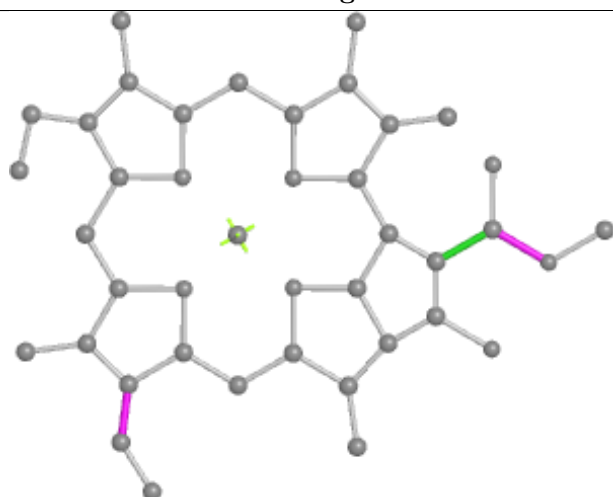
Ligand CLA 9 310



Bond lengths



Bond angles

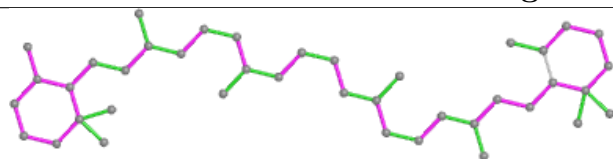


Torsions

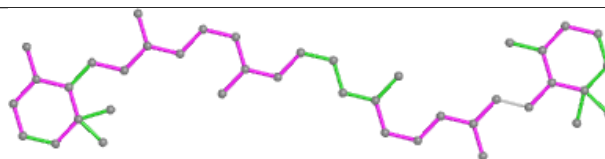


Rings

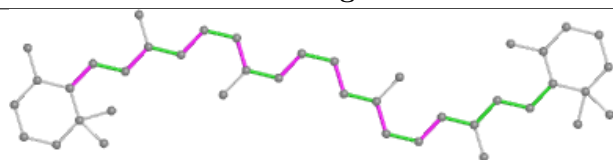
Ligand 8CT 7 301



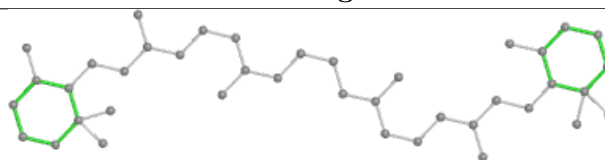
Bond lengths



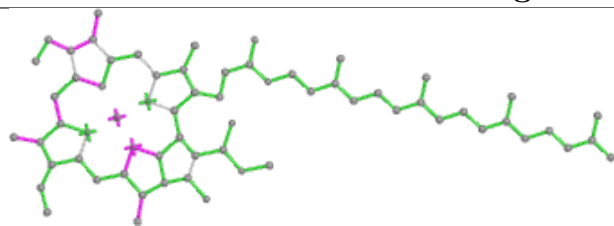
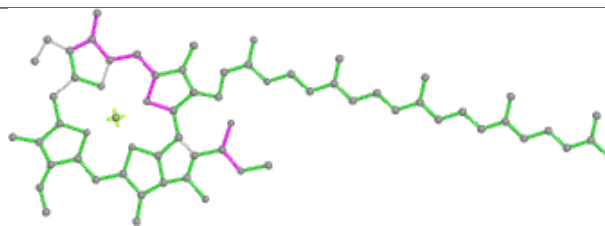
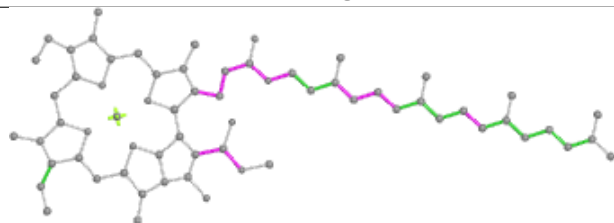
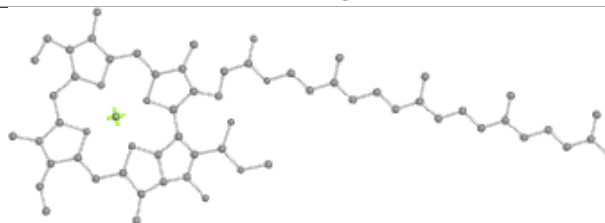
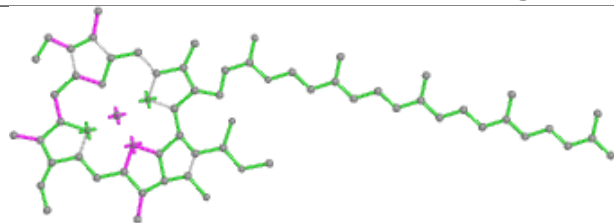
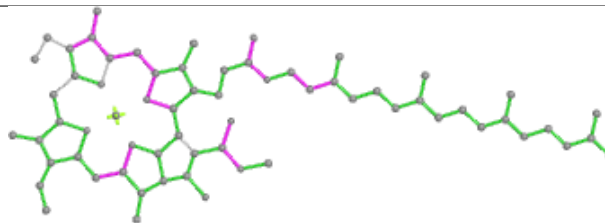
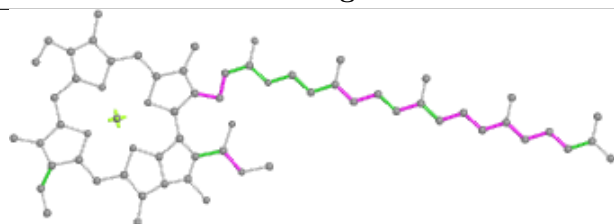
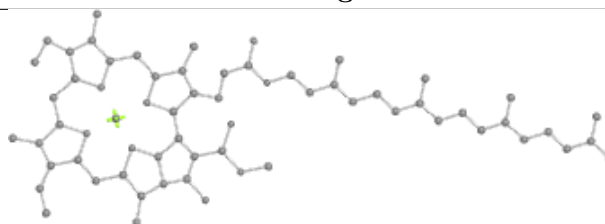
Bond angles



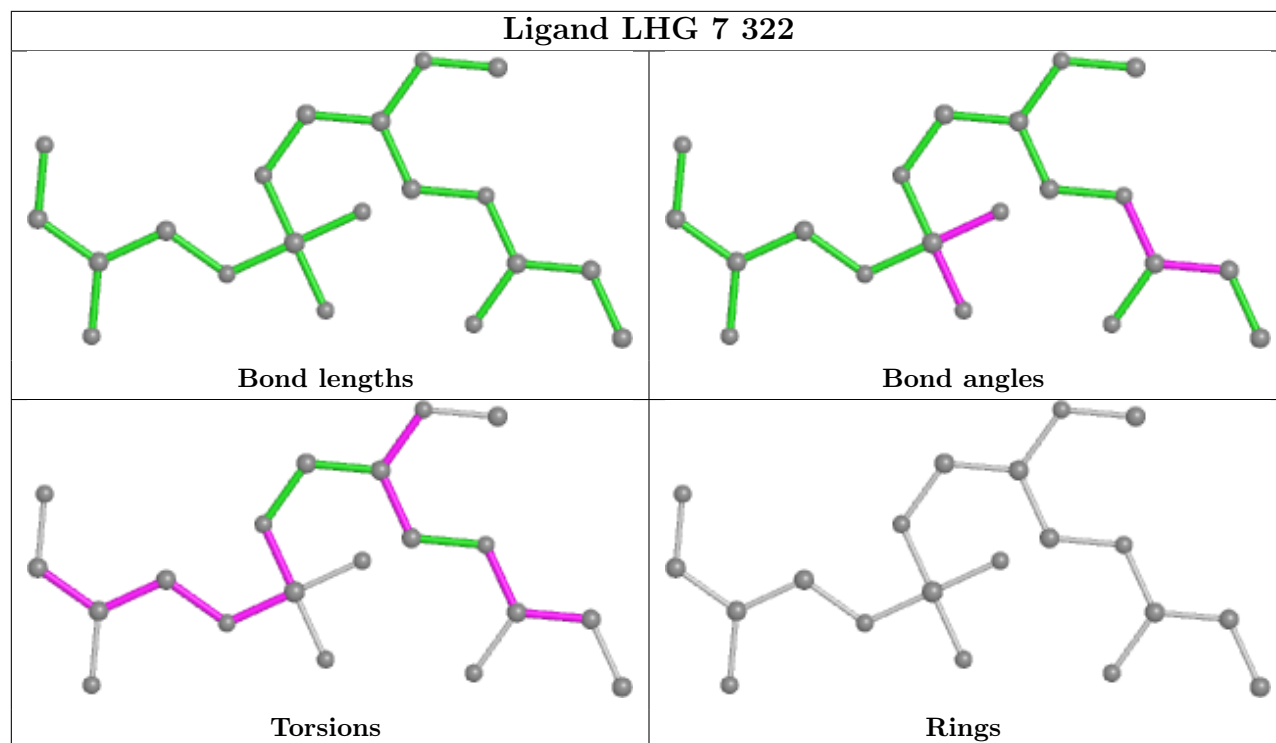
Torsions



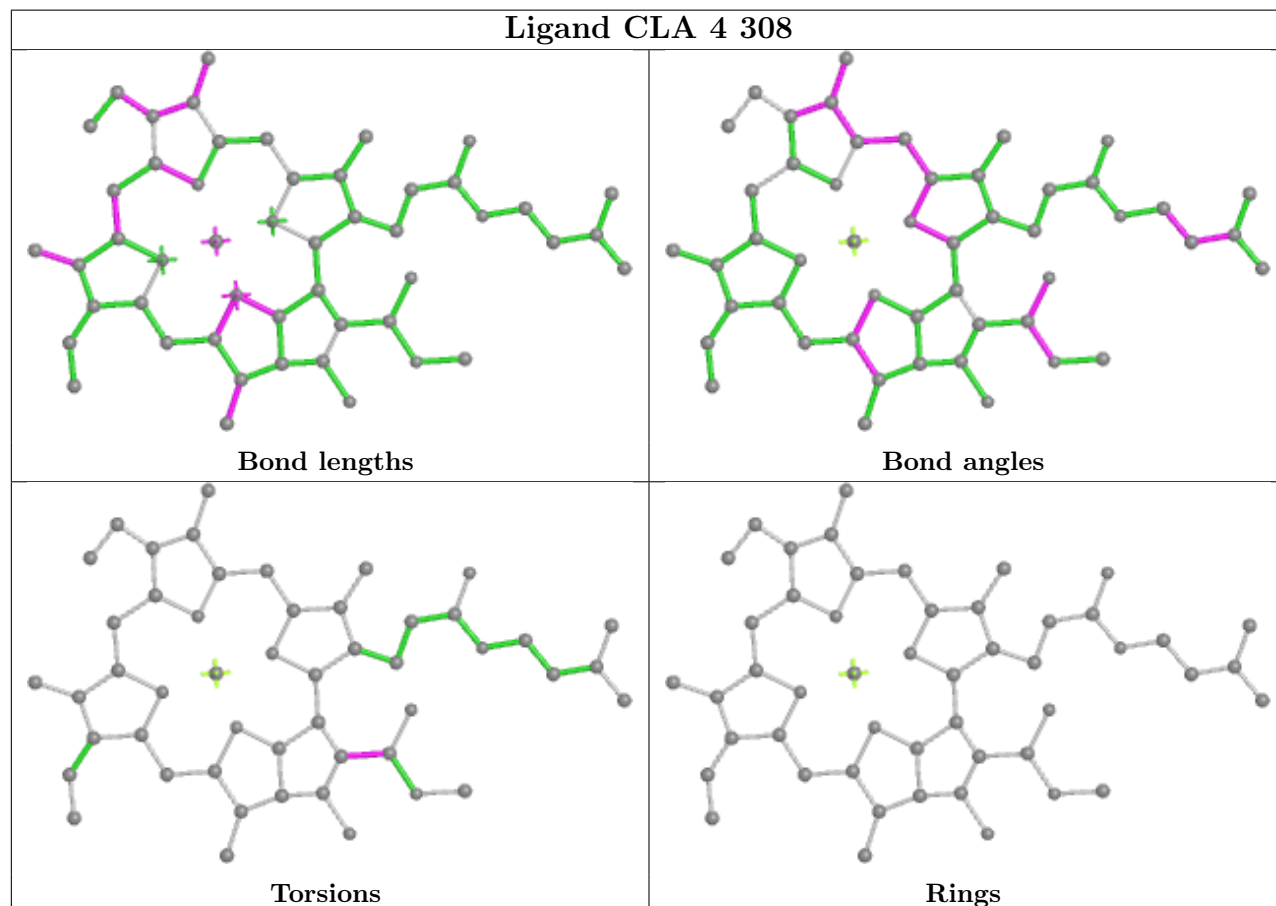
Rings

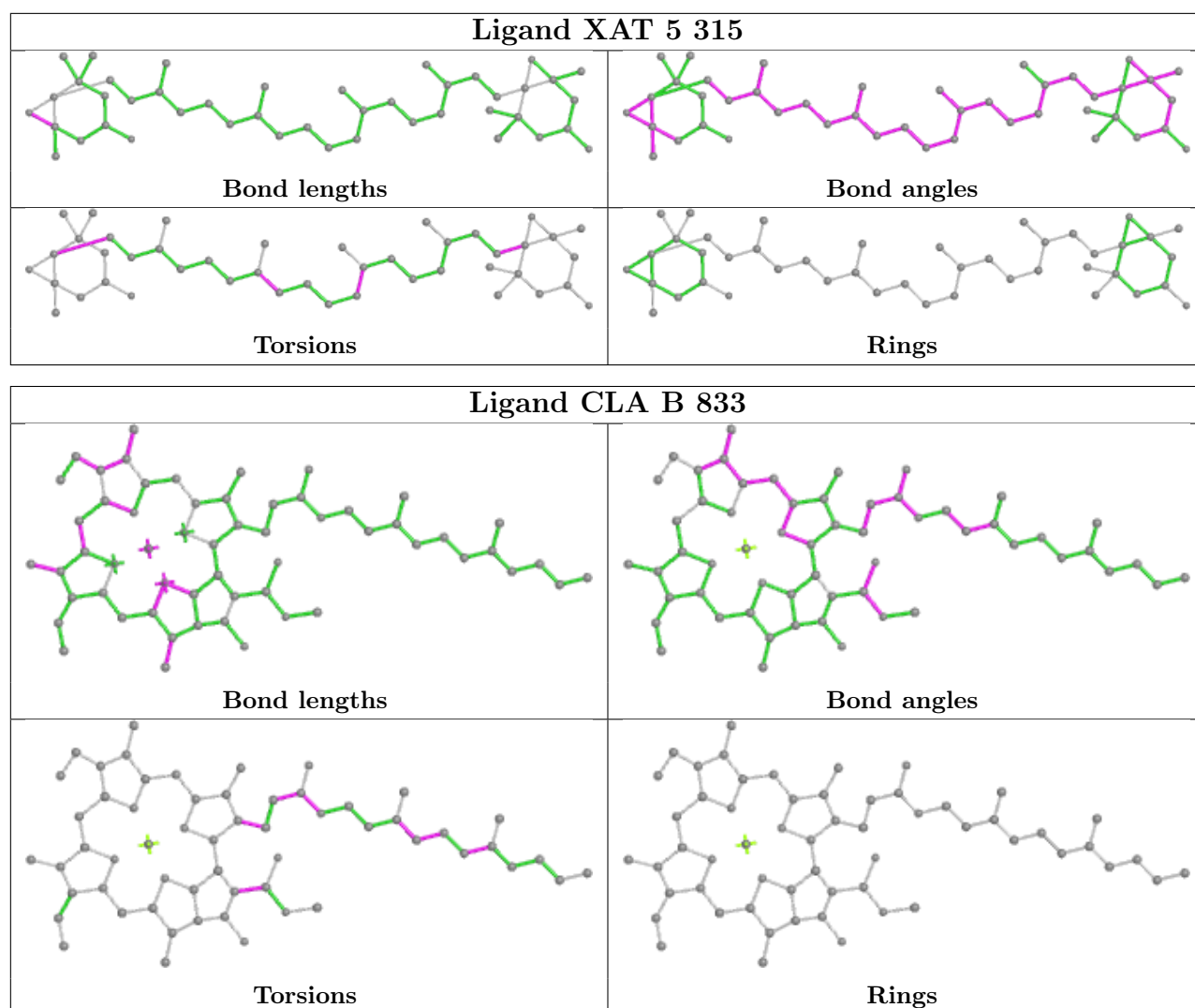
Ligand CLA A 832**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 837****Bond lengths****Bond angles****Torsions****Rings**

Ligand LHG 7 322

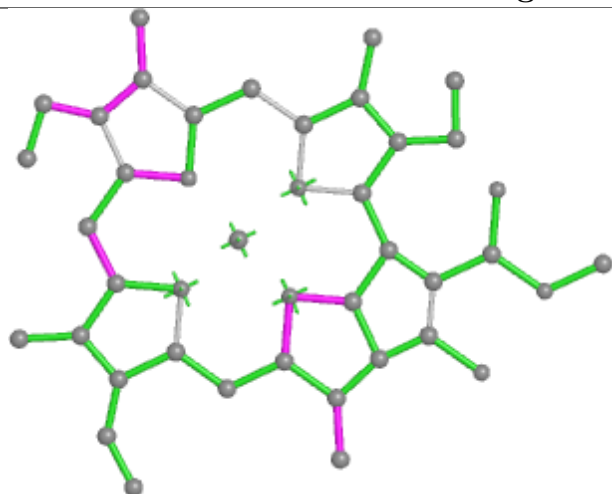


Ligand CLA 4 308

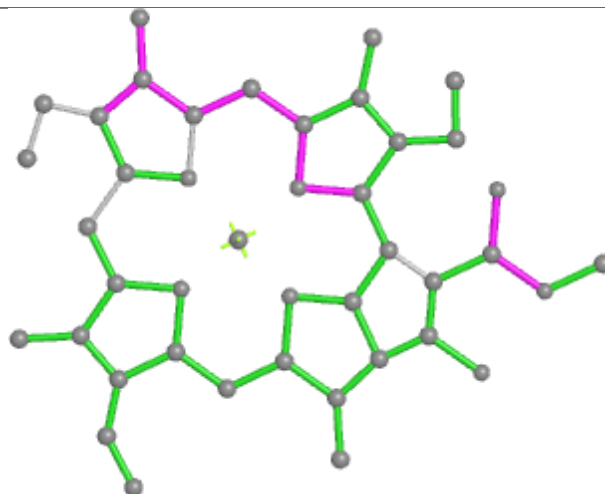




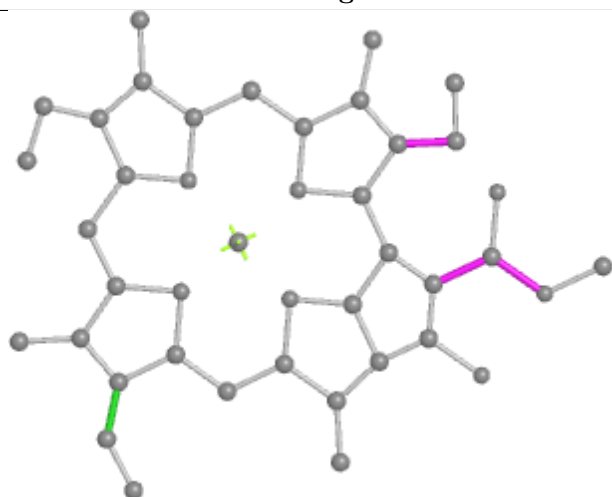
Ligand CLA J 103



Bond lengths



Bond angles

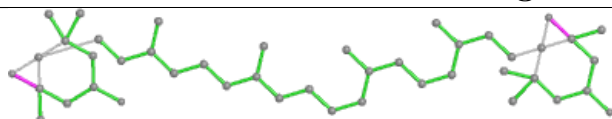


Torsions

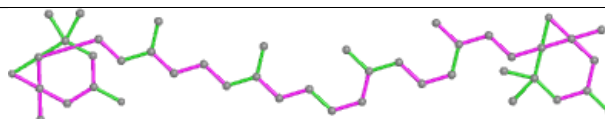


Rings

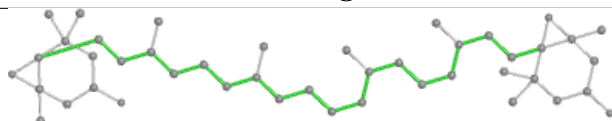
Ligand XAT 3 315



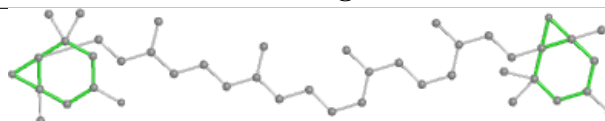
Bond lengths



Bond angles

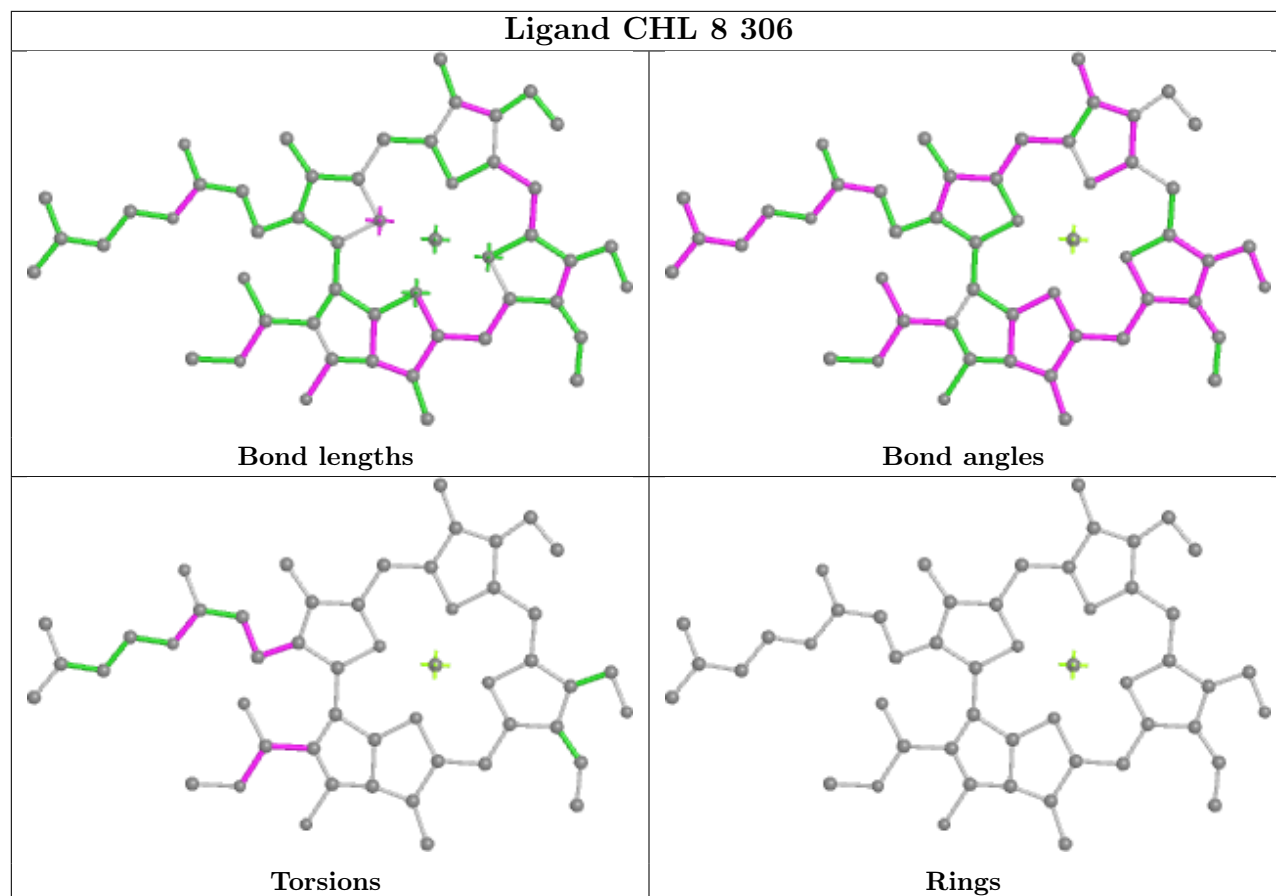


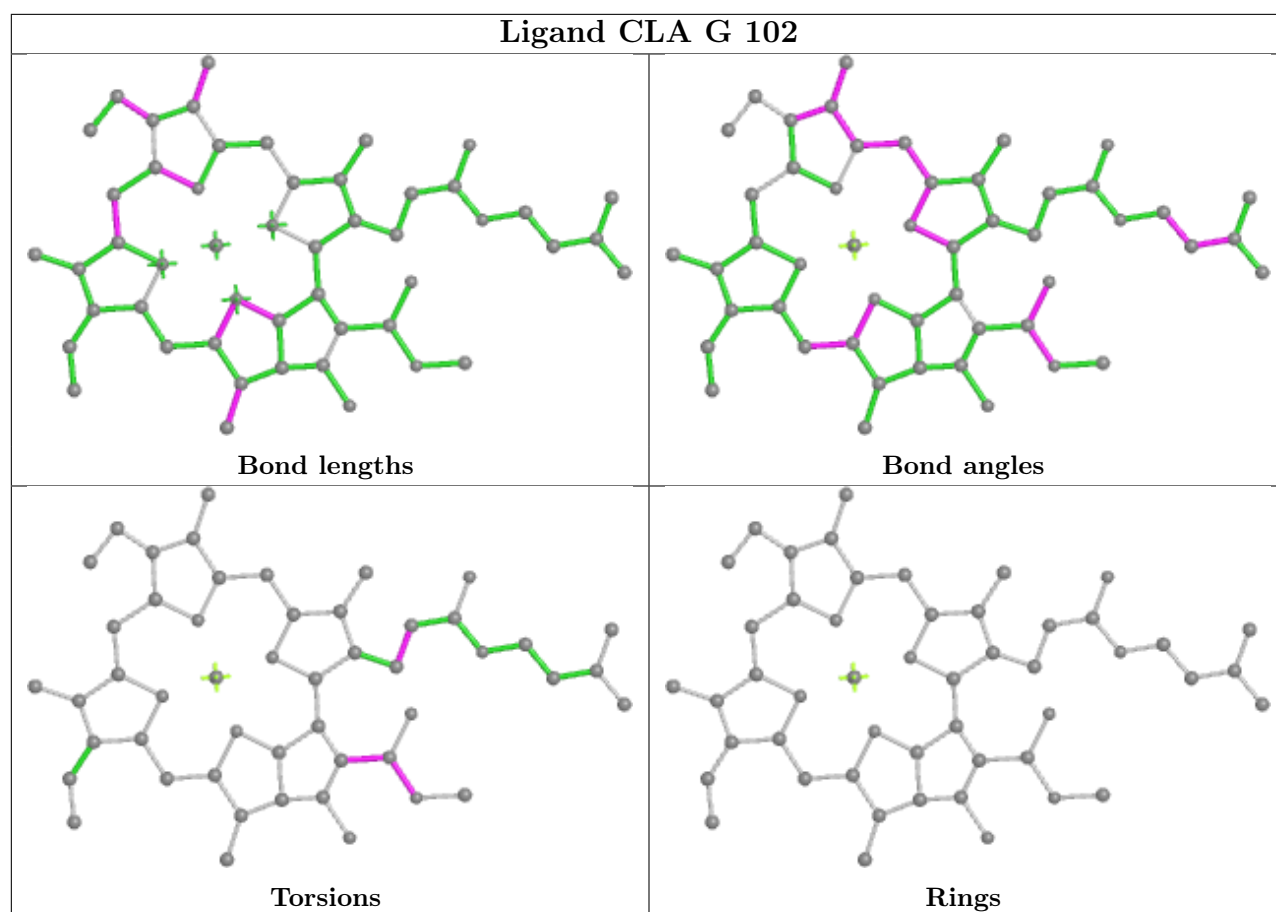
Torsions



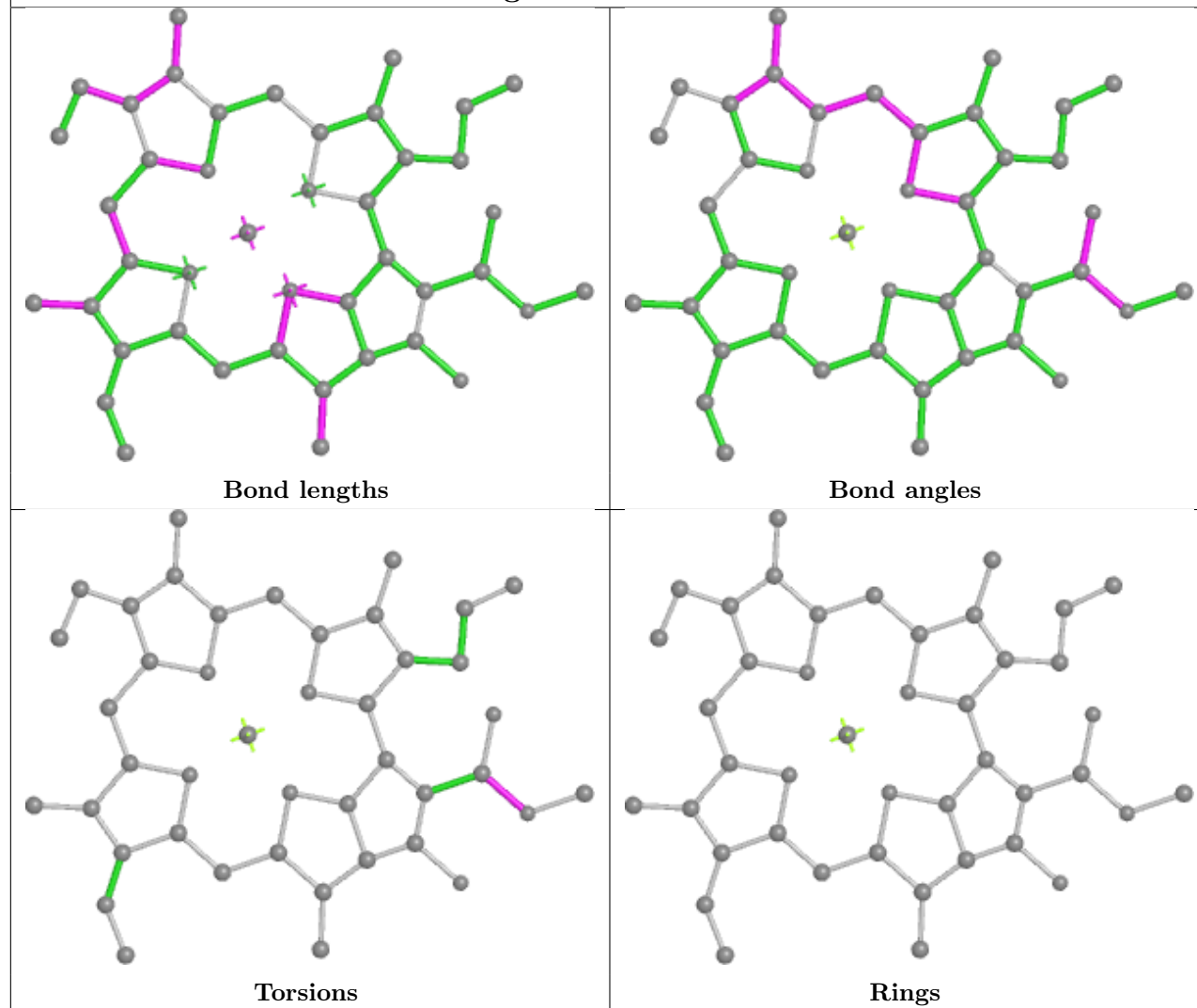
Rings

Ligand CHL 8 306

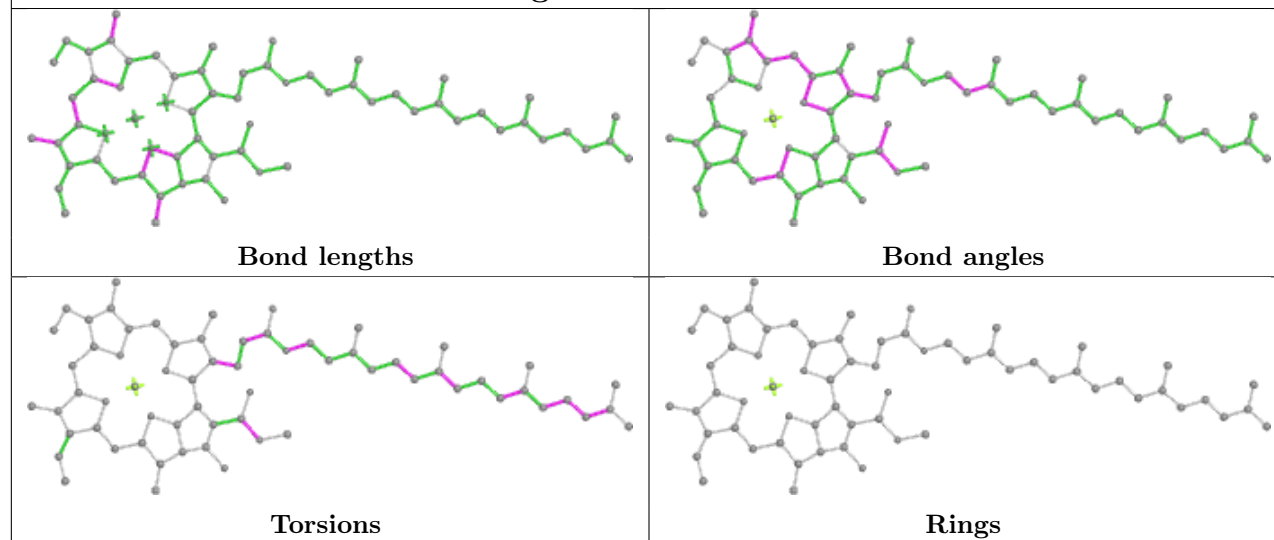




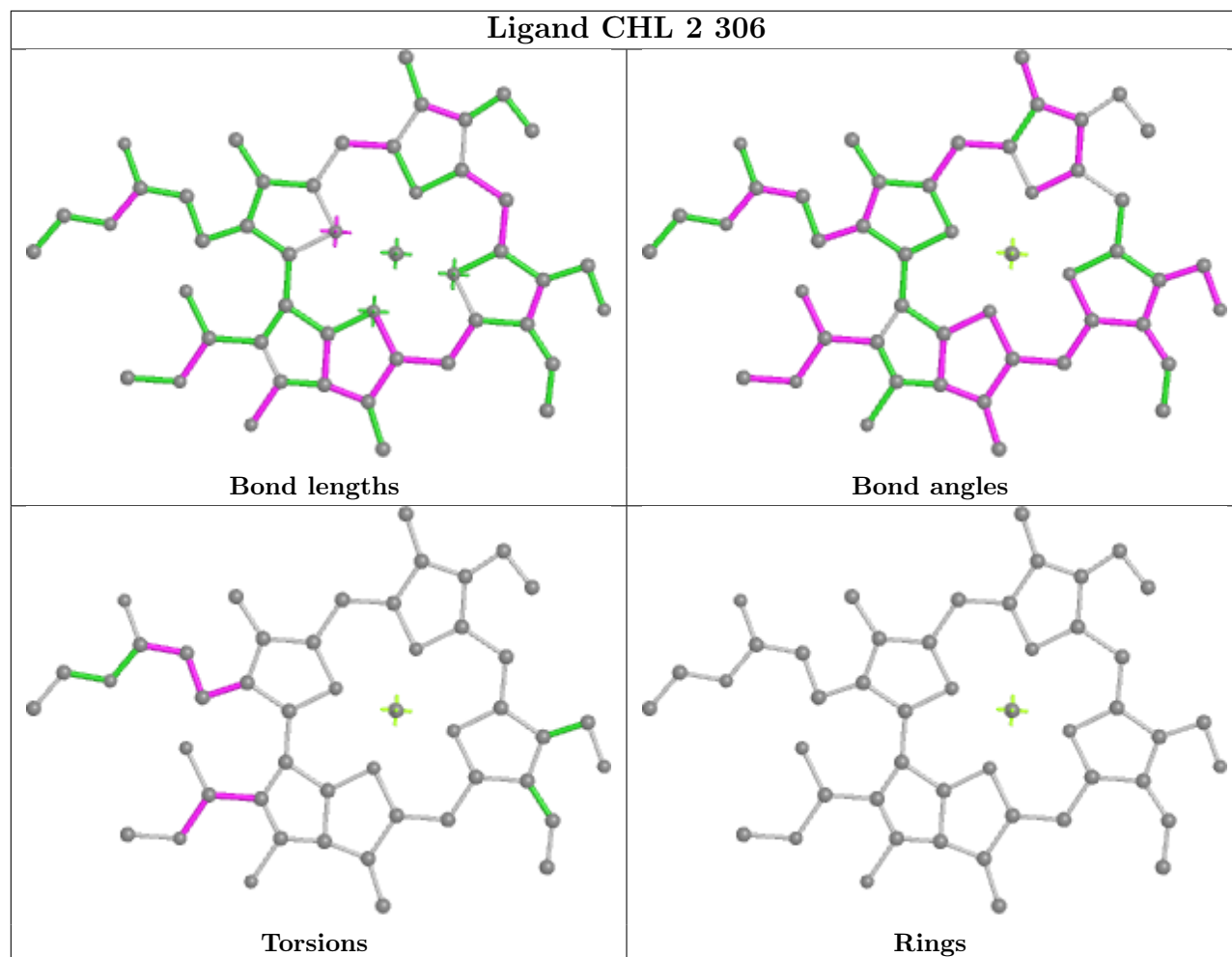
Ligand CLA 2 313



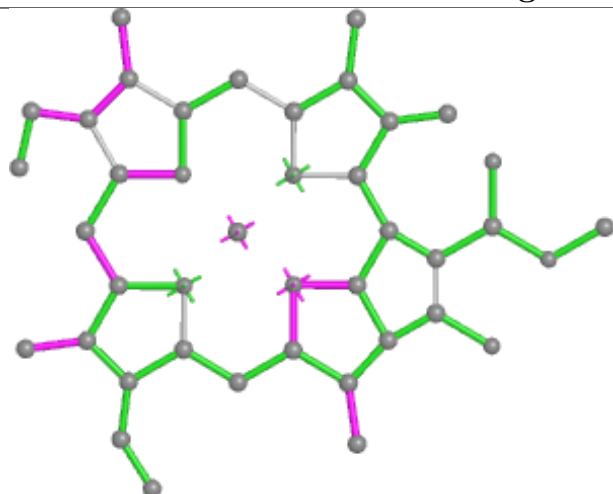
Ligand CLA H 201



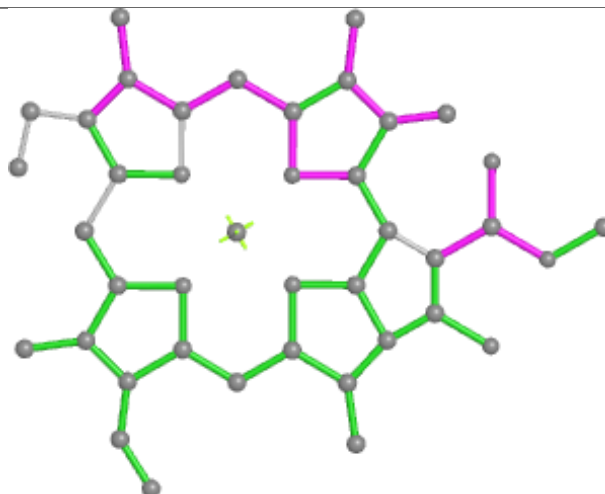
Ligand CHL 2 306



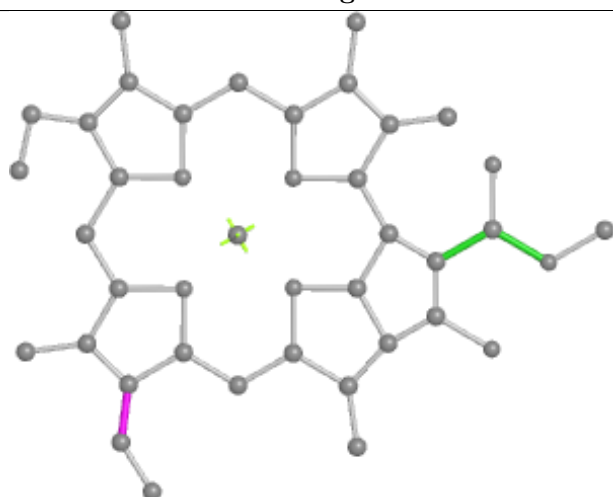
Ligand CLA 1 309



Bond lengths



Bond angles

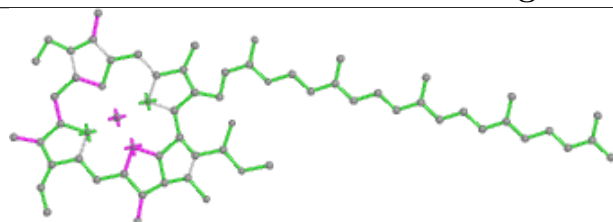


Torsions

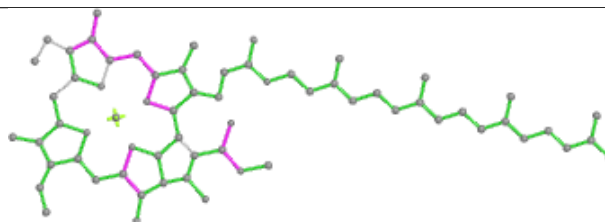


Rings

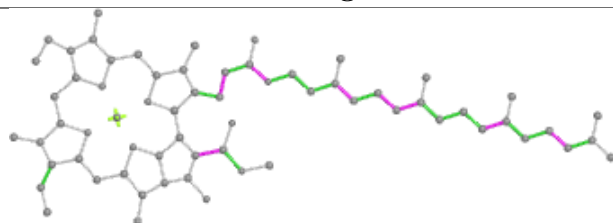
Ligand CLA 0 303



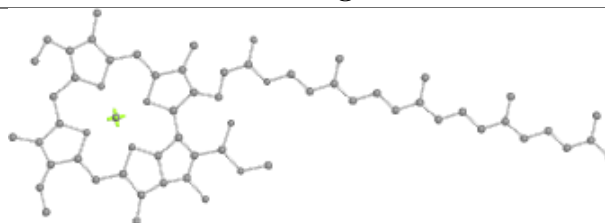
Bond lengths



Bond angles

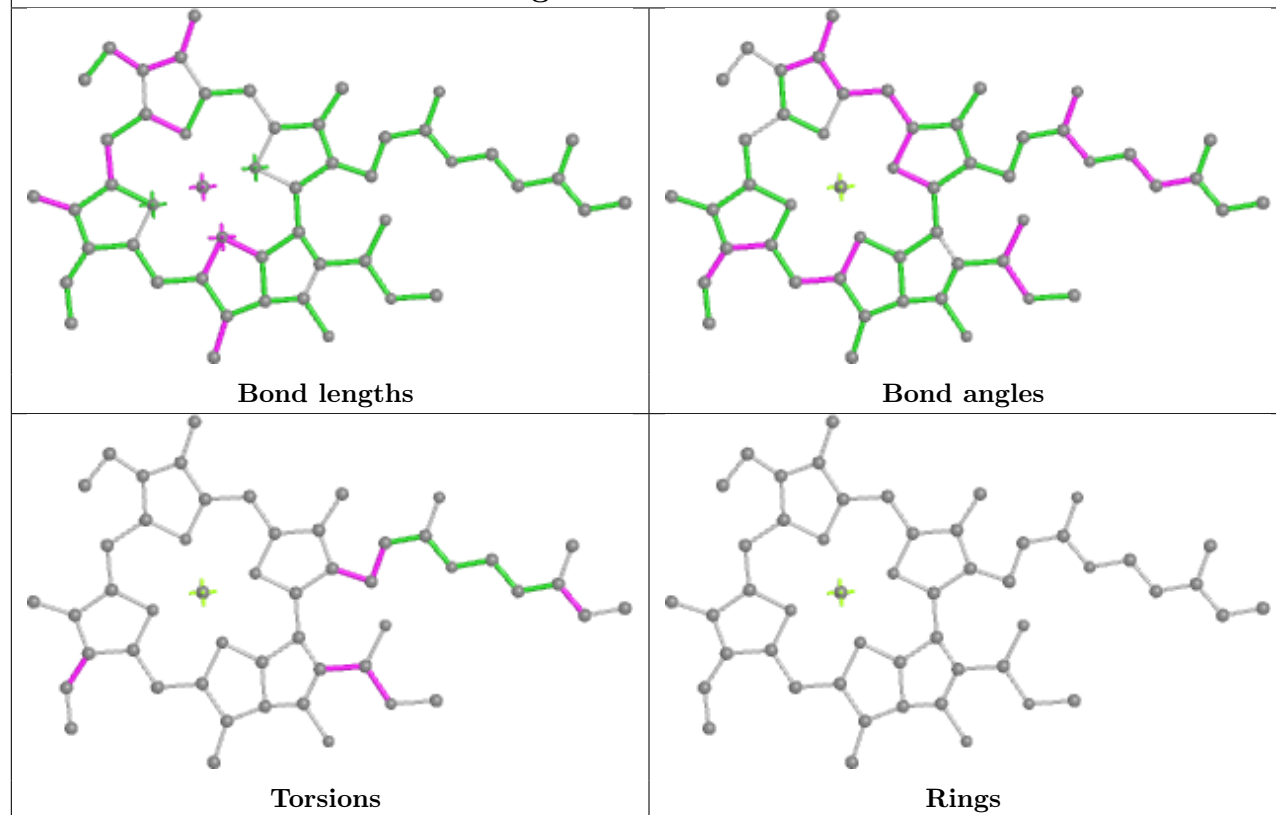


Torsions

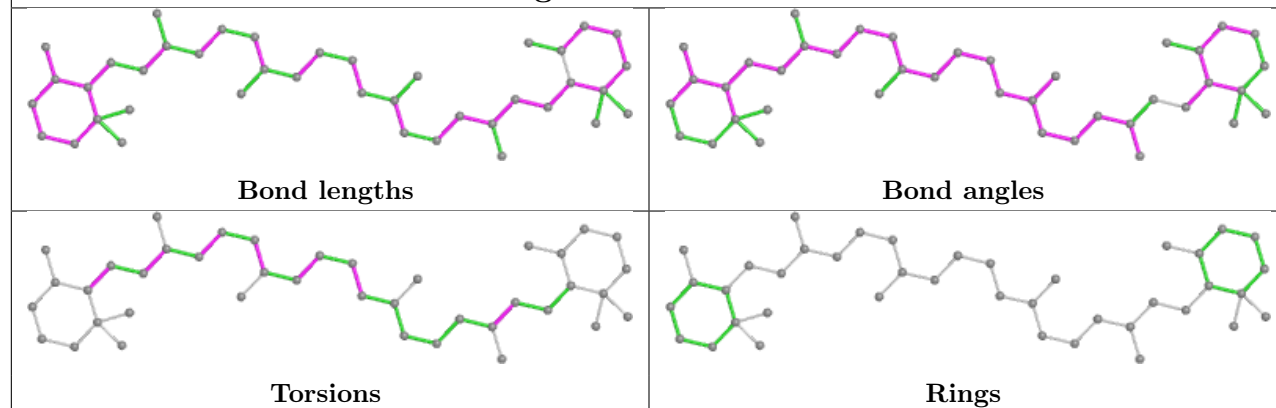


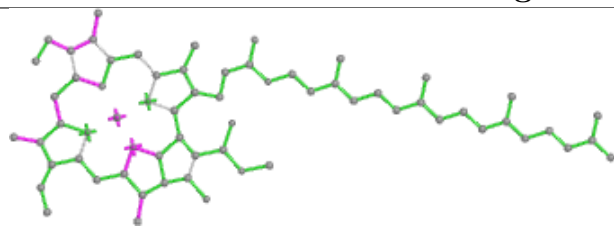
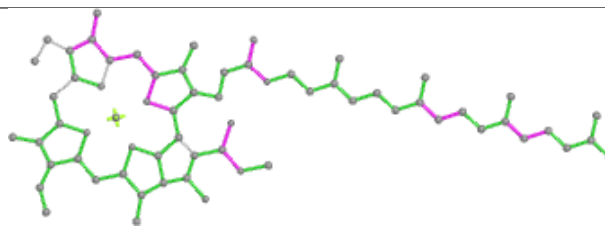
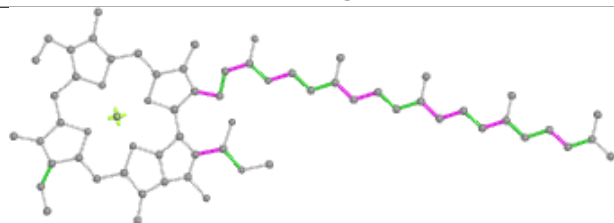
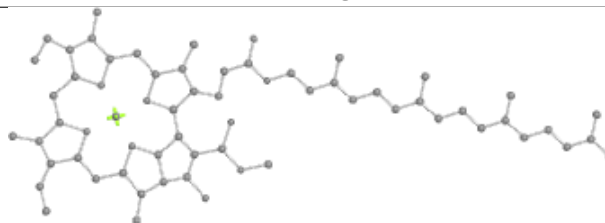
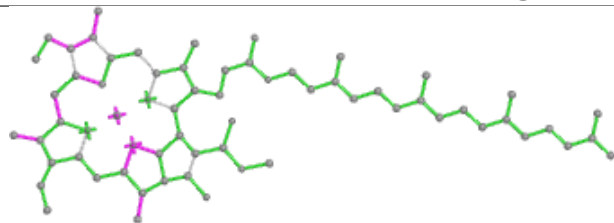
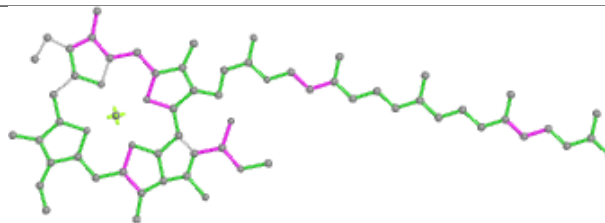
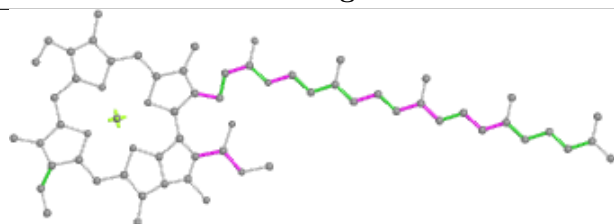
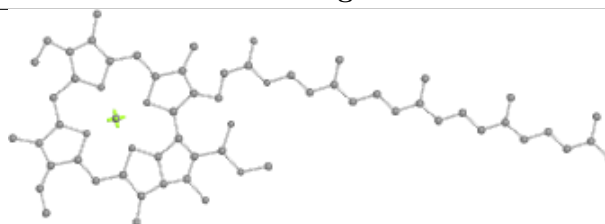
Rings

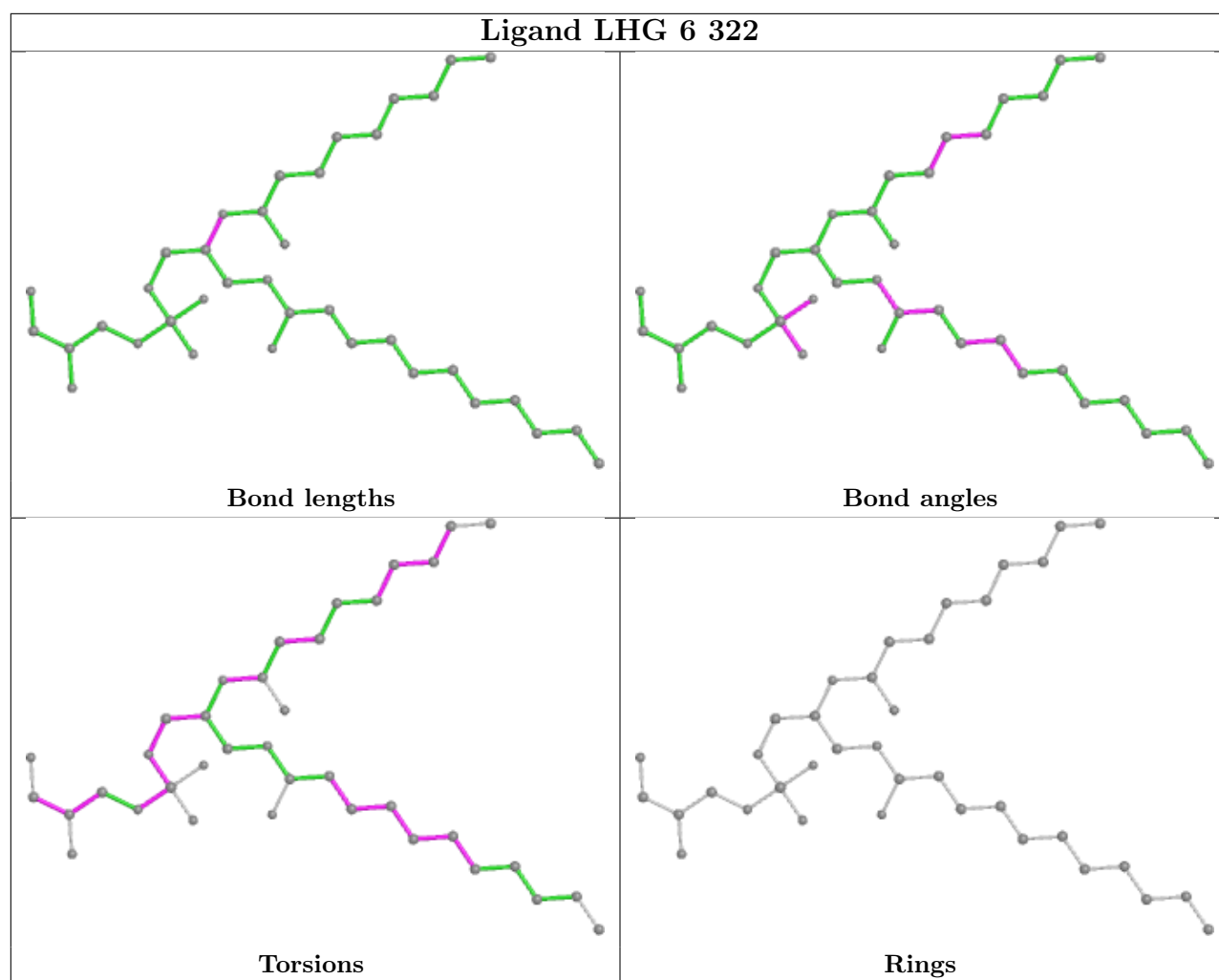
Ligand CLA A 836



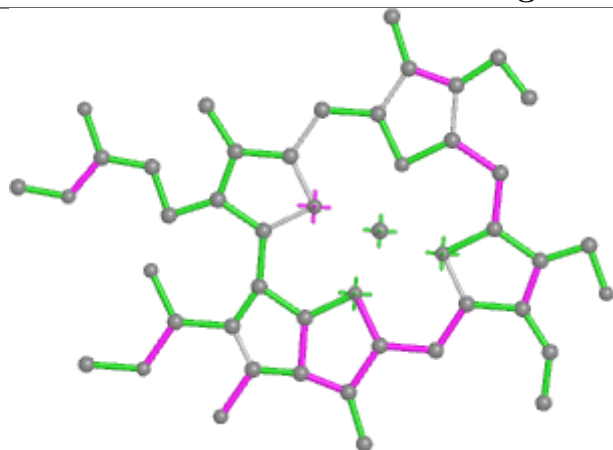
Ligand 8CT A 849



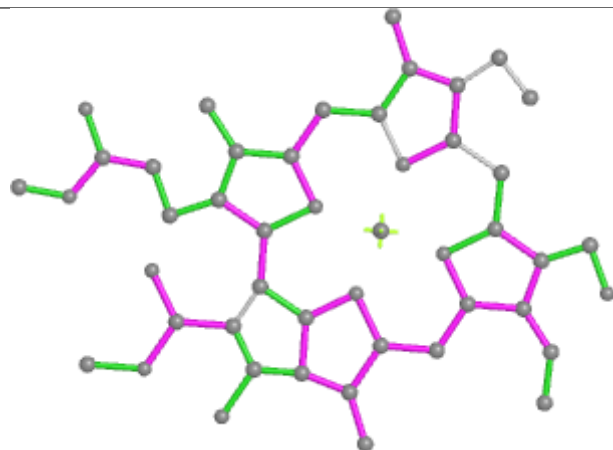
Ligand CLA B 808**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 841****Bond lengths****Bond angles****Torsions****Rings**



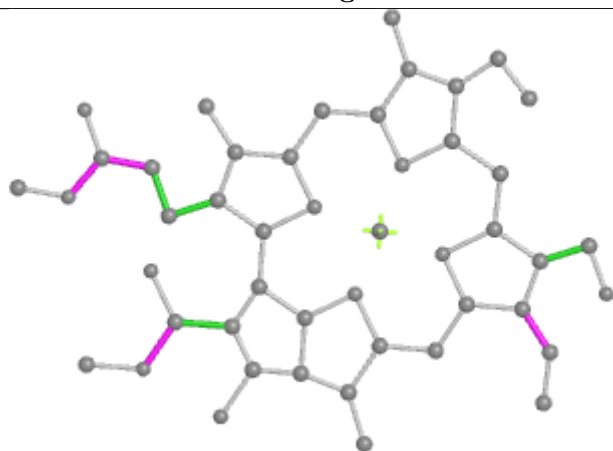
Ligand CHL 7 308



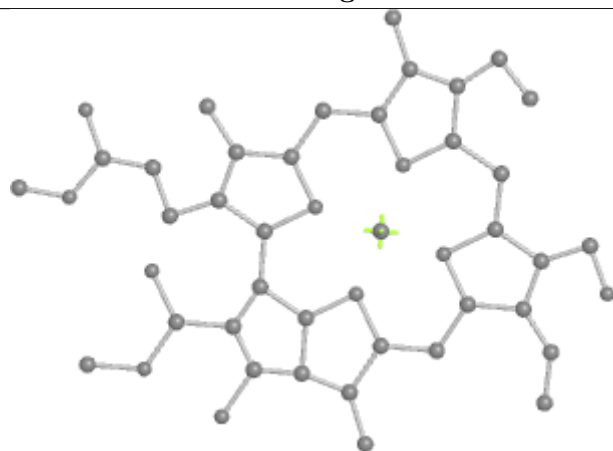
Bond lengths



Bond angles

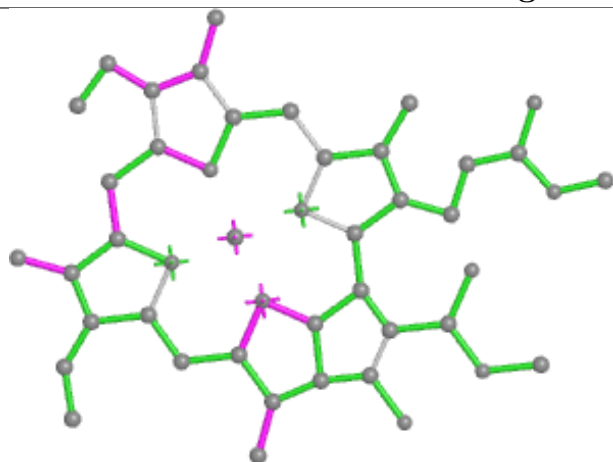


Torsions

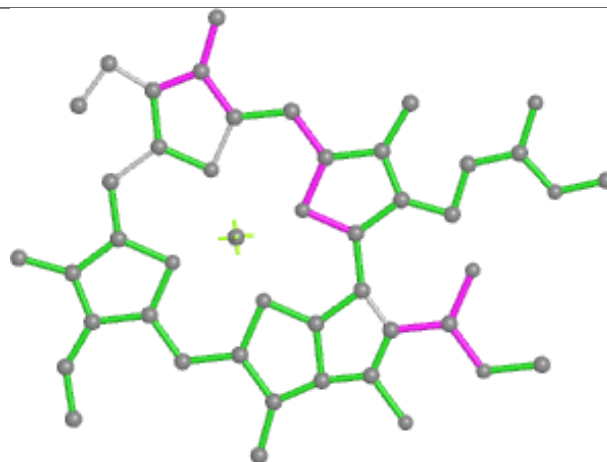


Rings

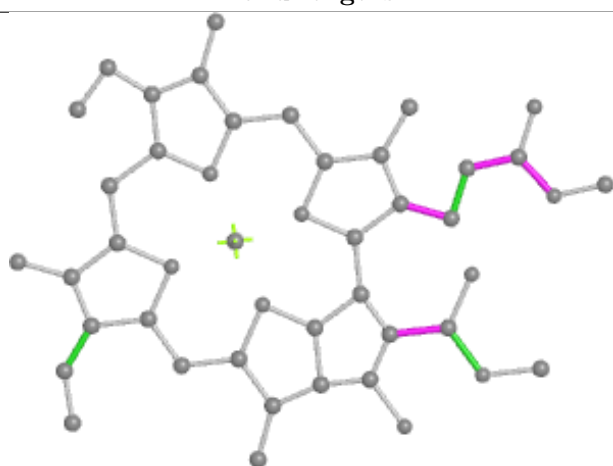
Ligand CLA 2 319



Bond lengths



Bond angles

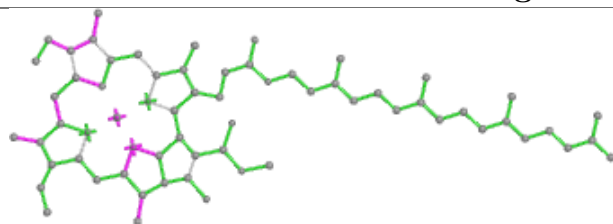


Torsions

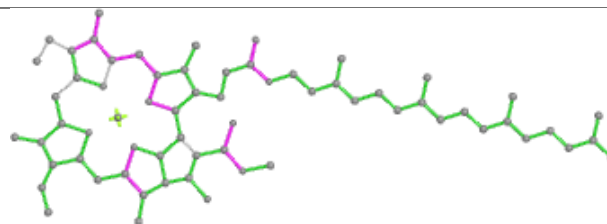


Rings

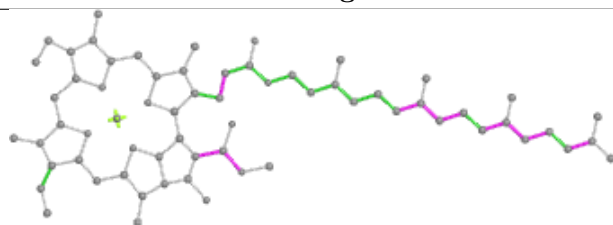
Ligand CLA B 825



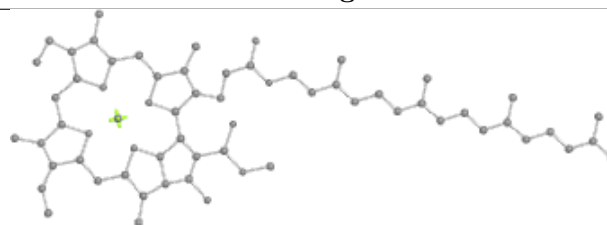
Bond lengths



Bond angles

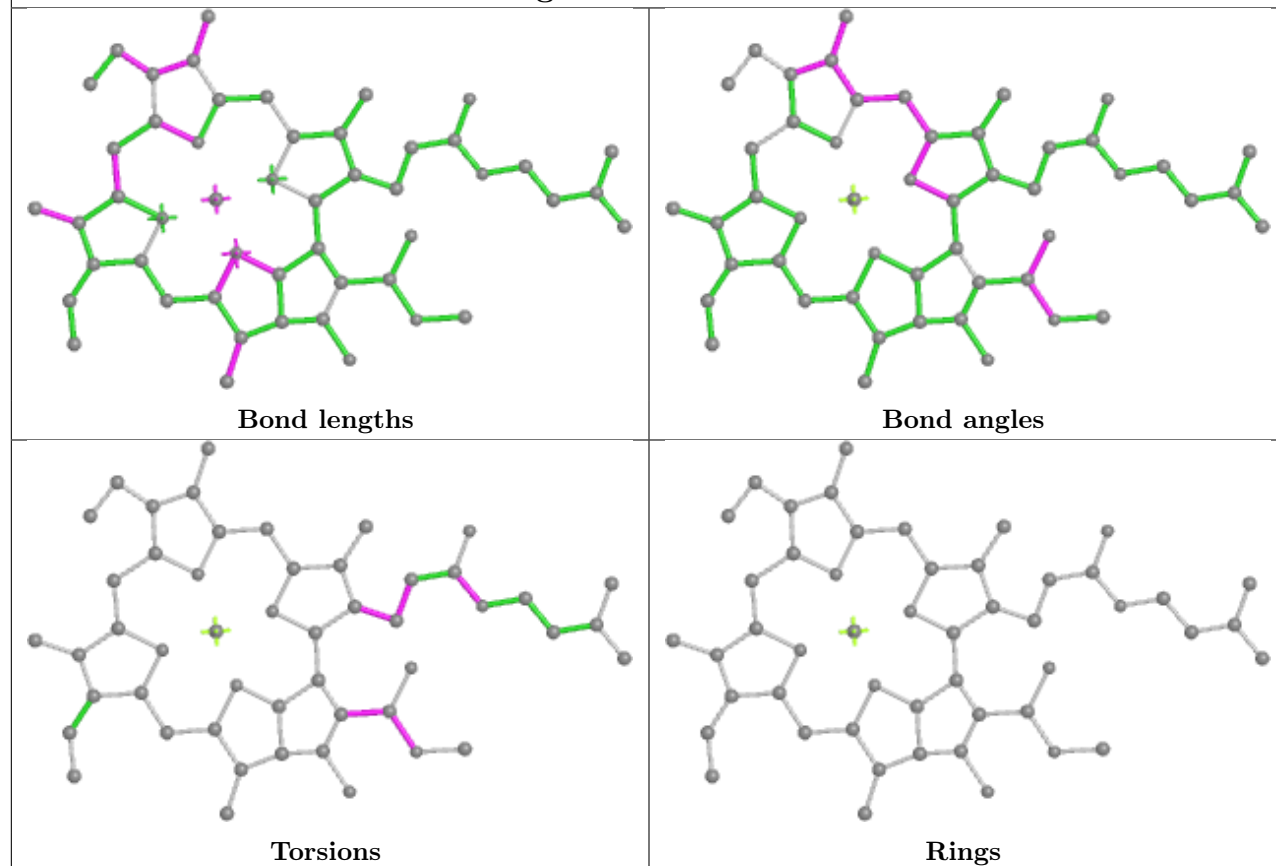


Torsions

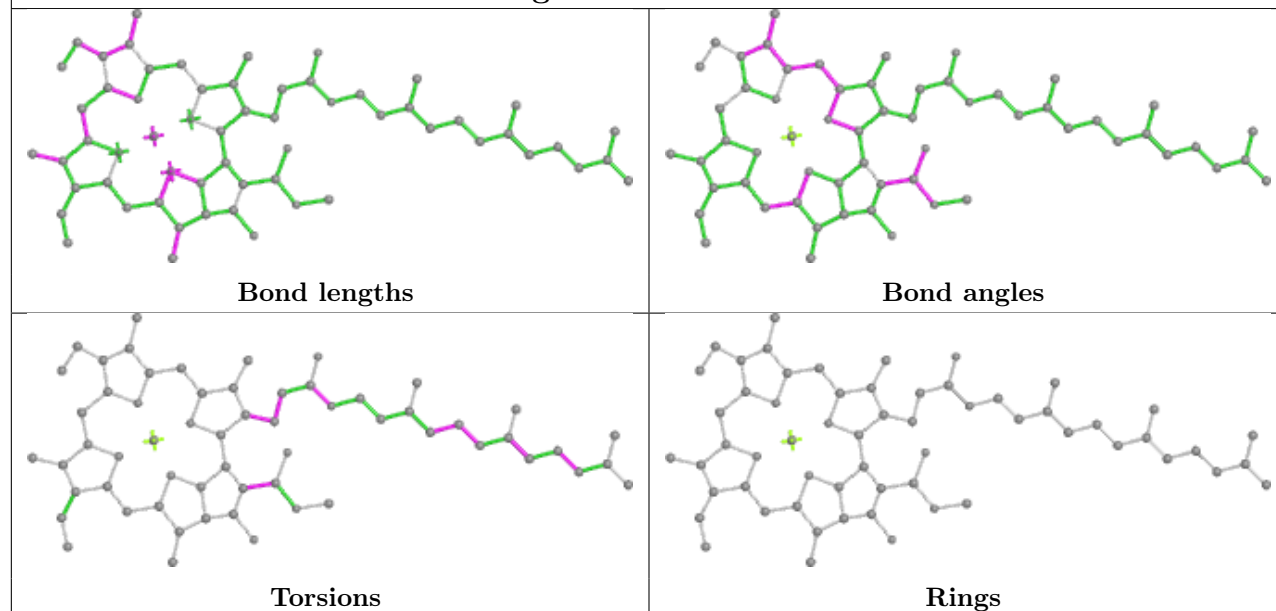


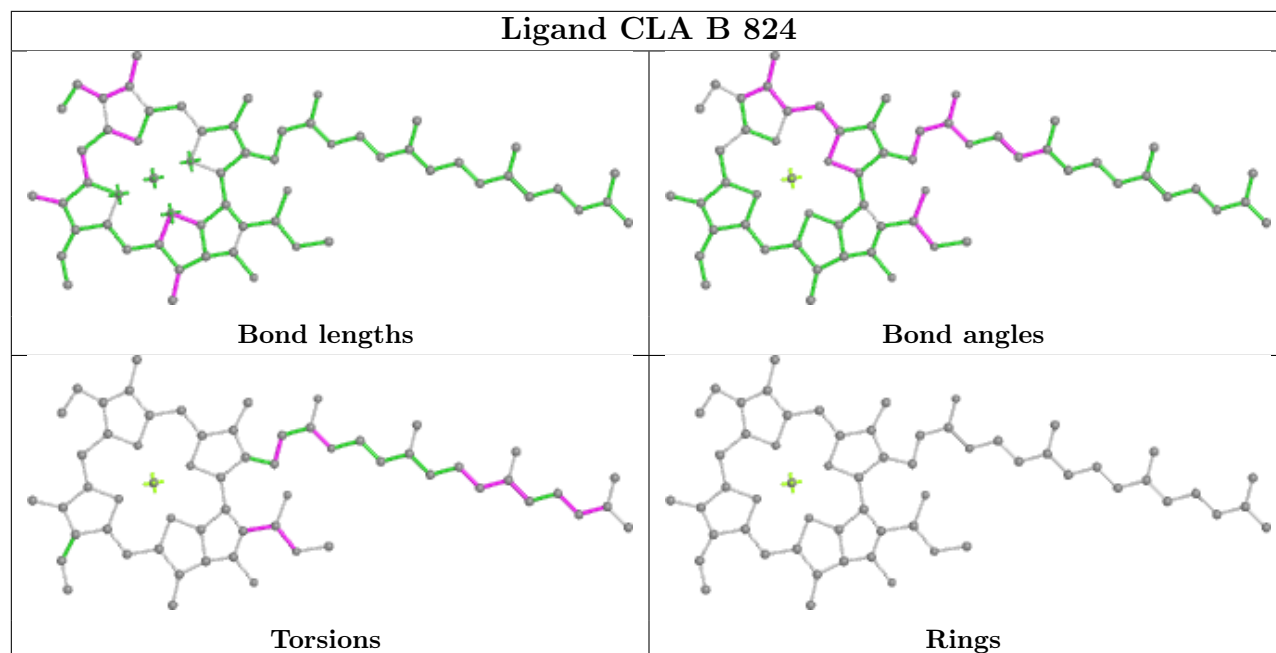
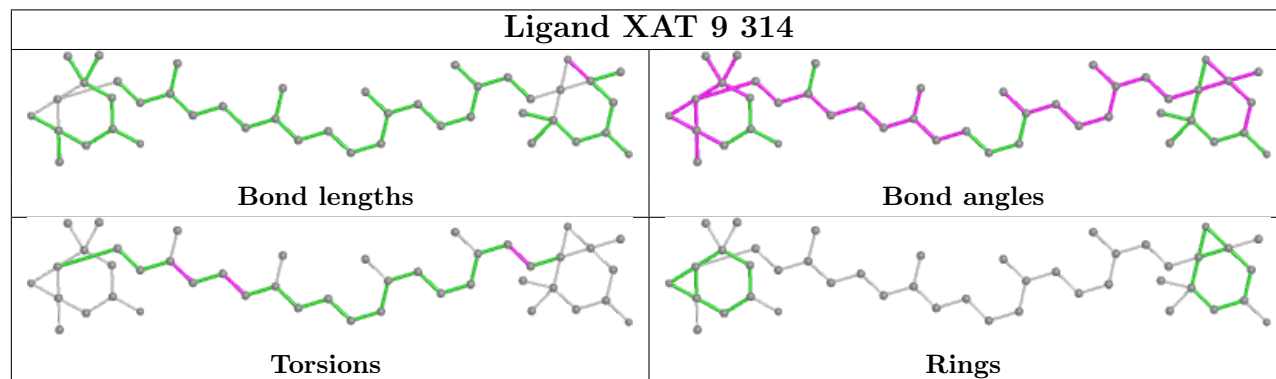
Rings

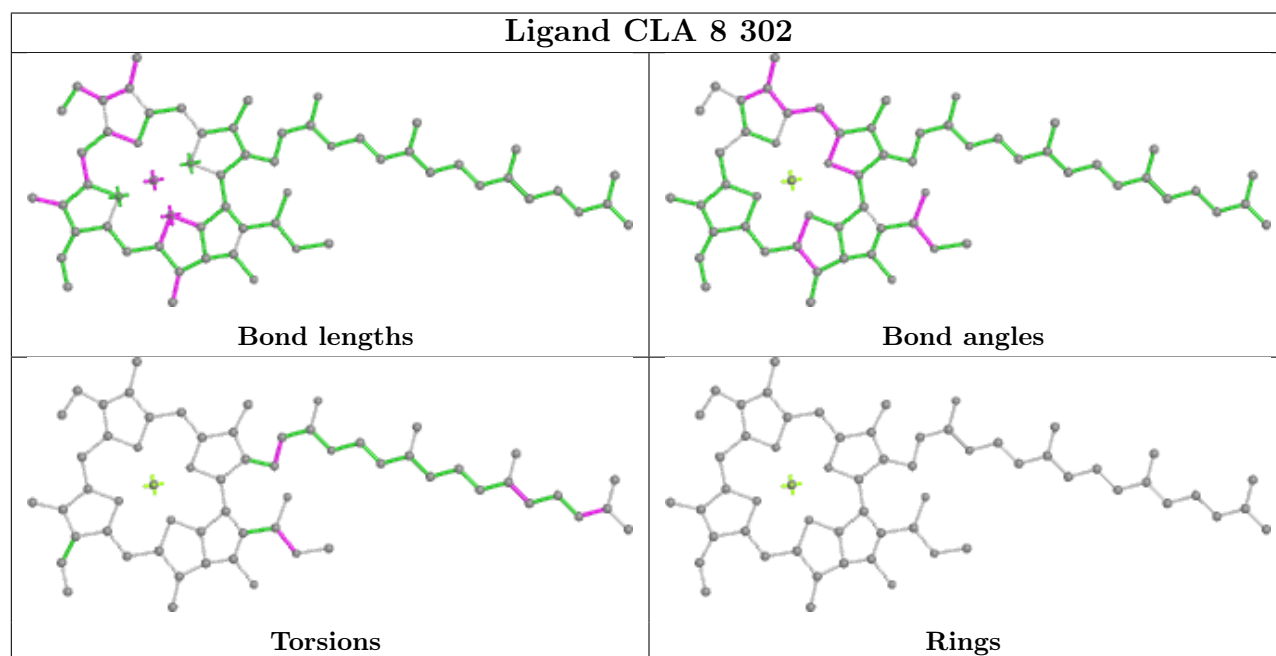
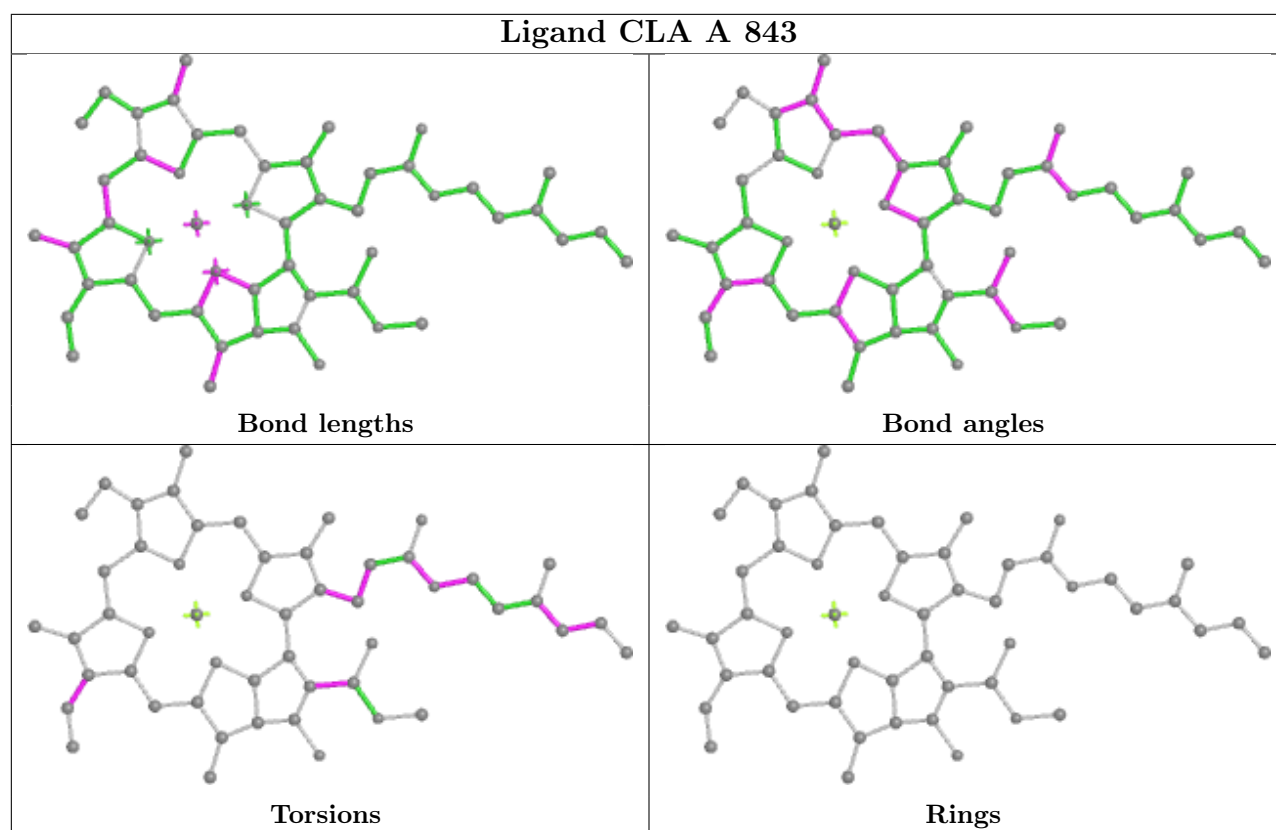
Ligand CLA 8 304



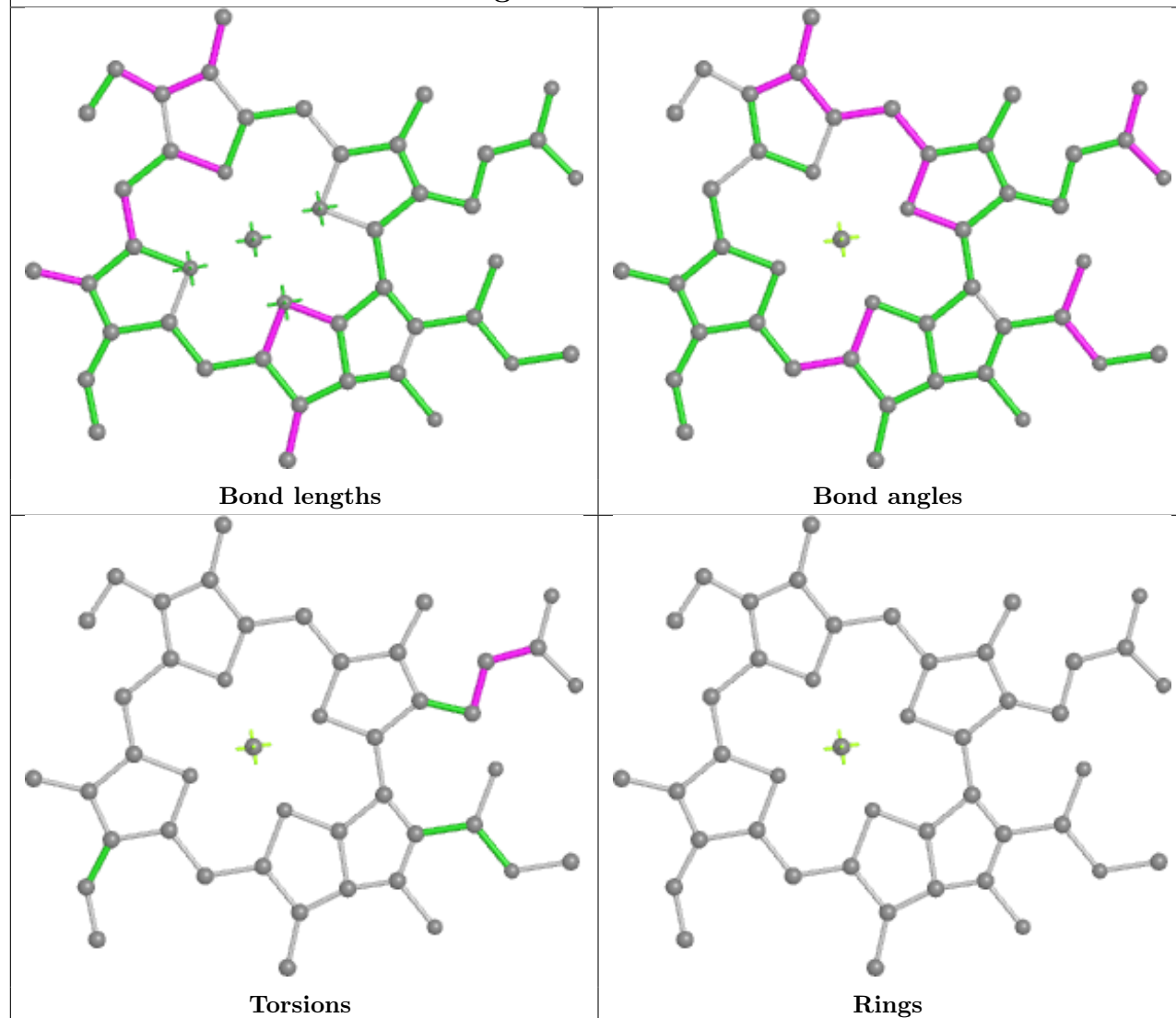
Ligand CLA B 816



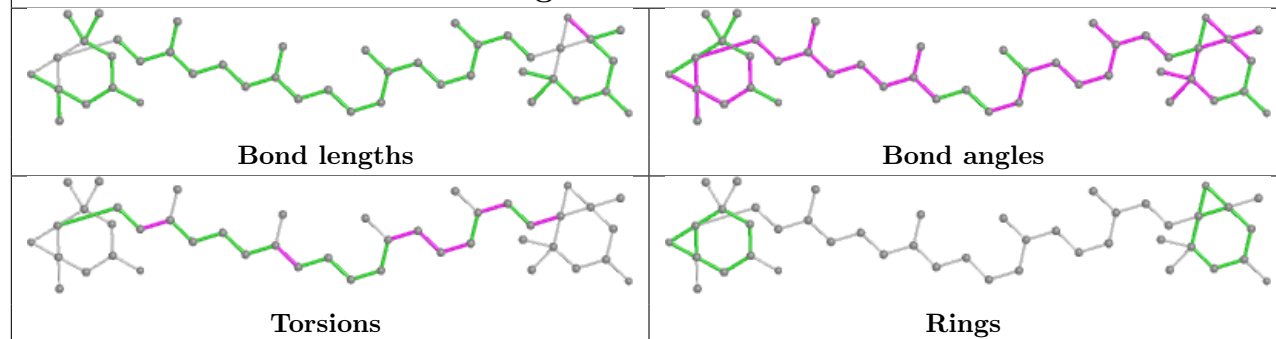
Ligand CLA B 824**Ligand XAT 9 314**



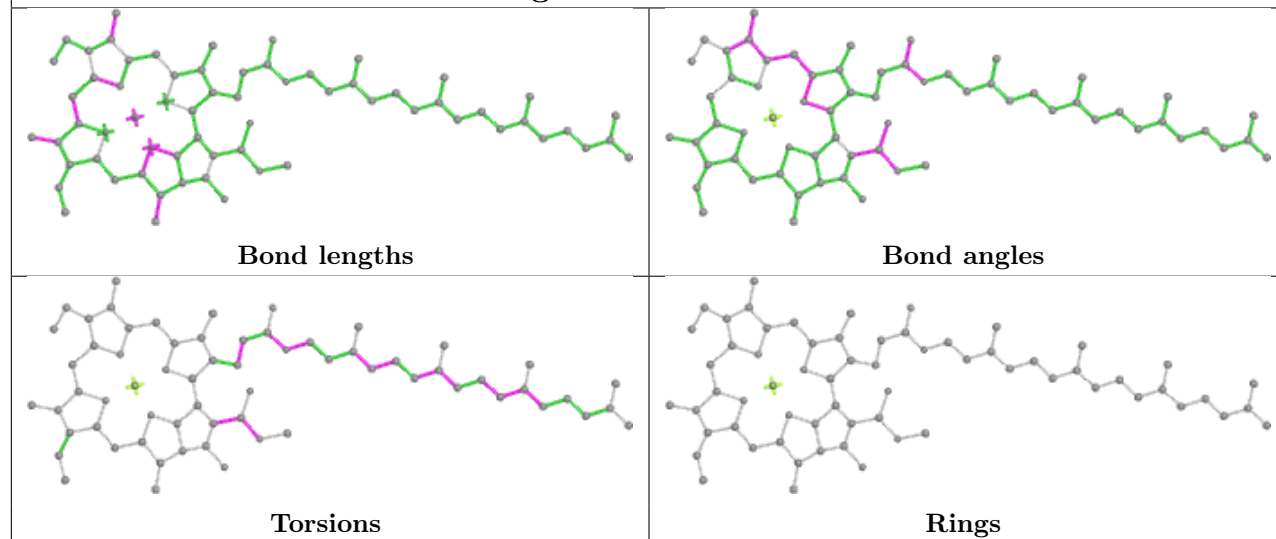
Ligand CLA 8 313



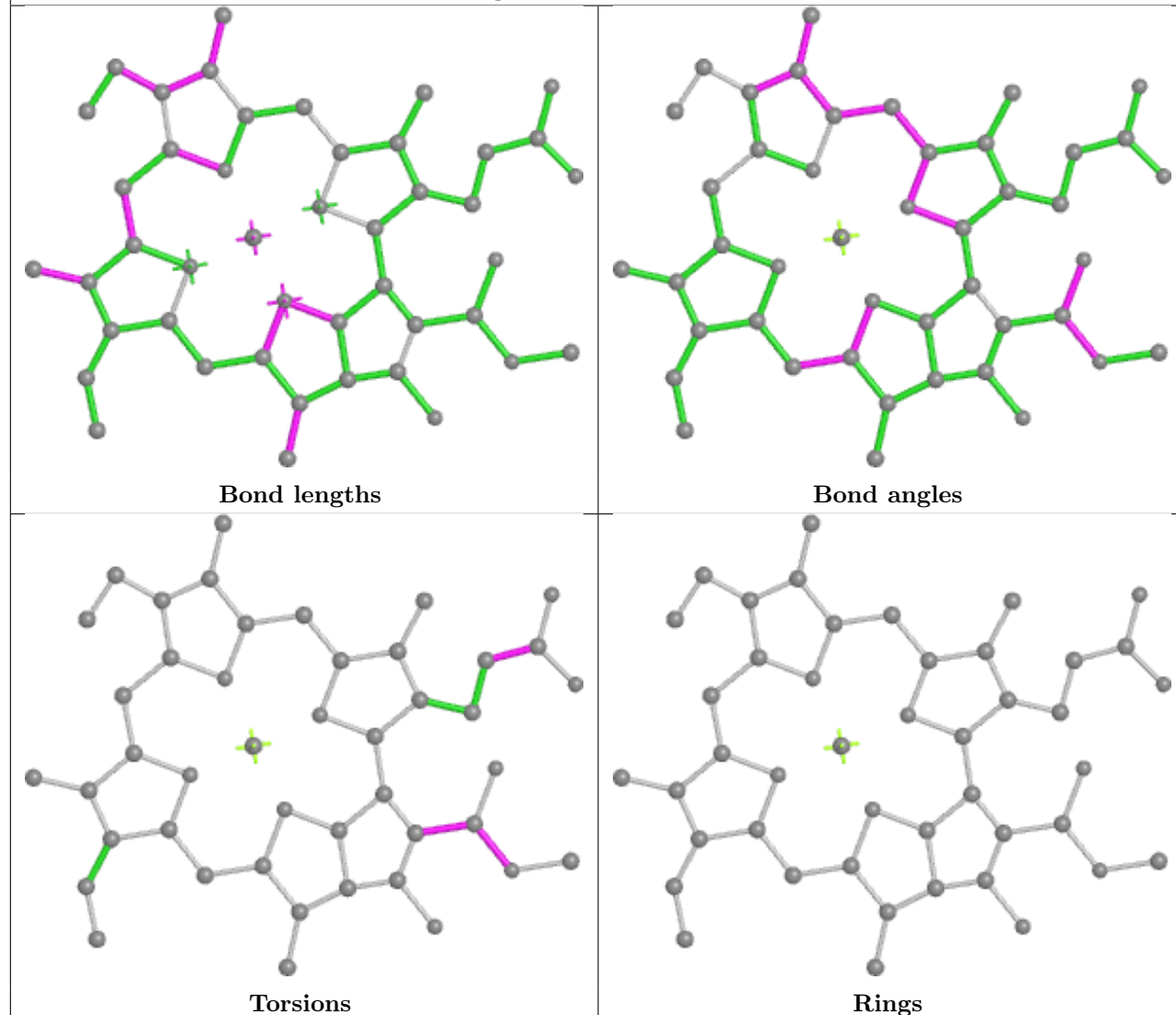
Ligand XAT 1 314

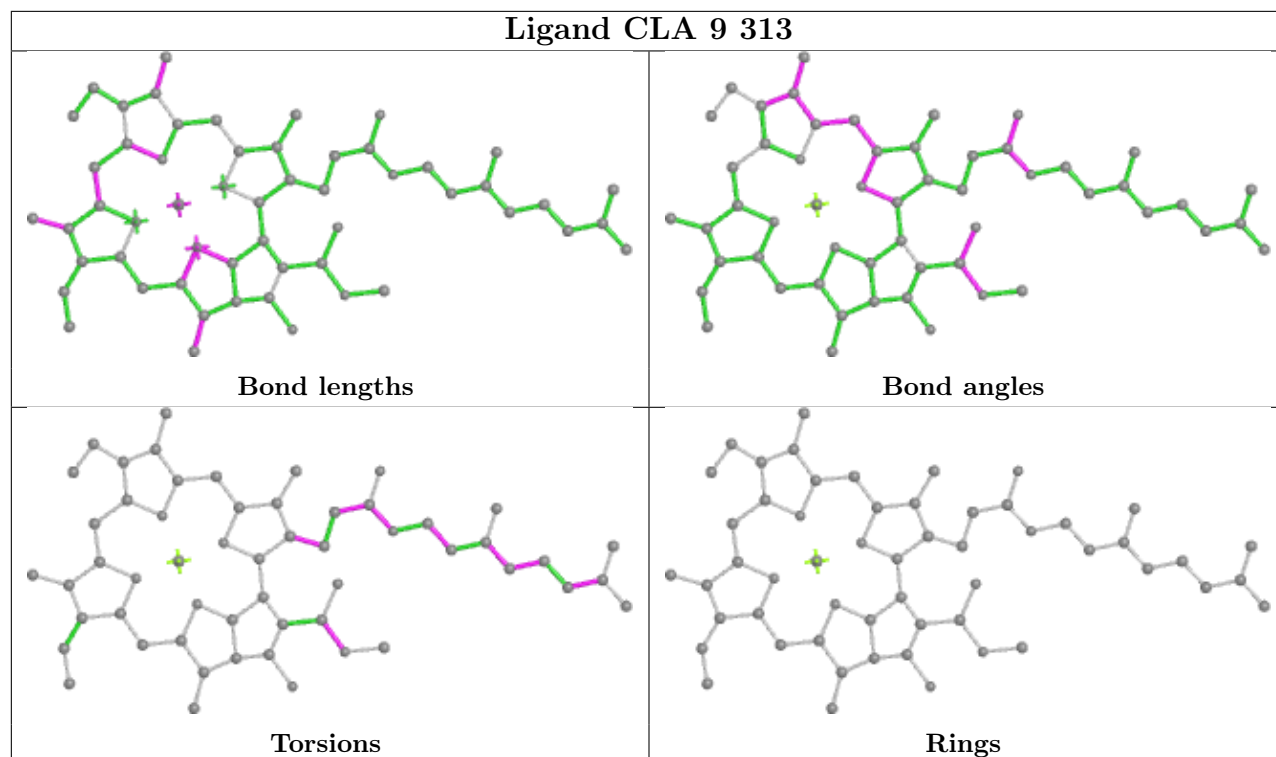
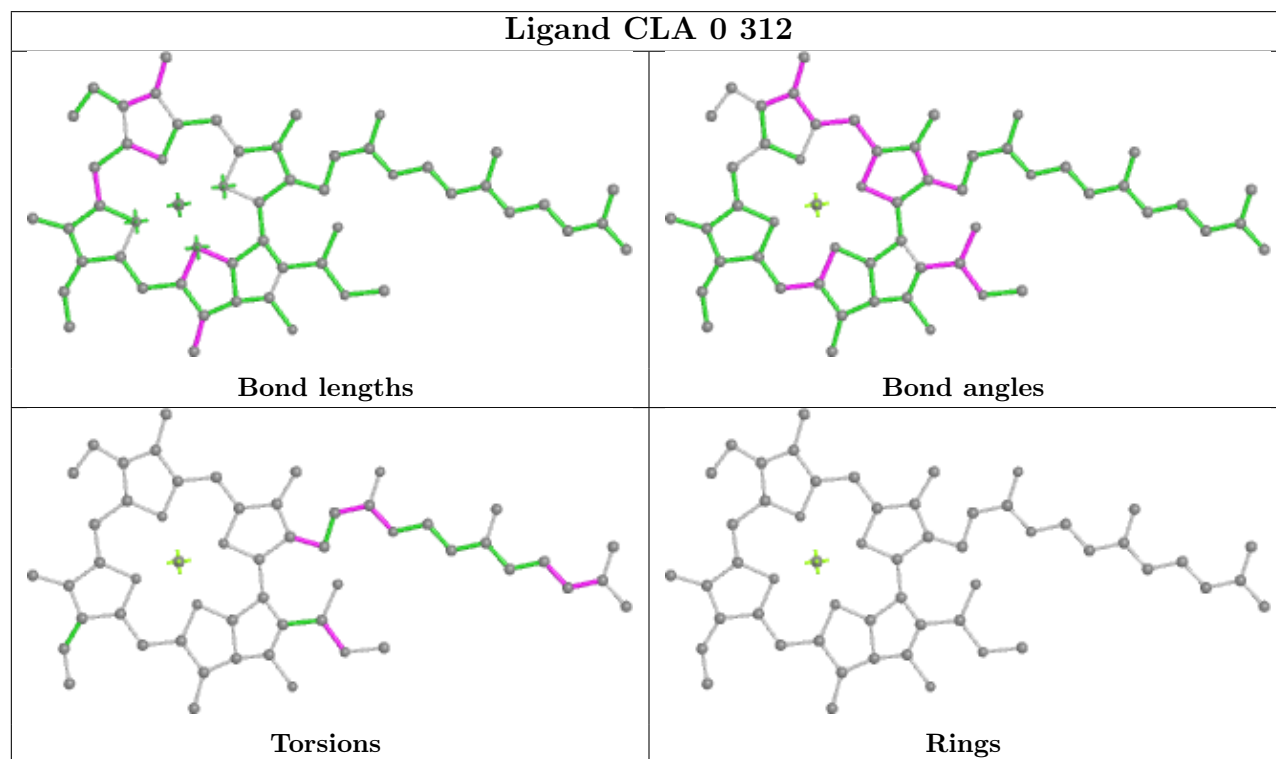


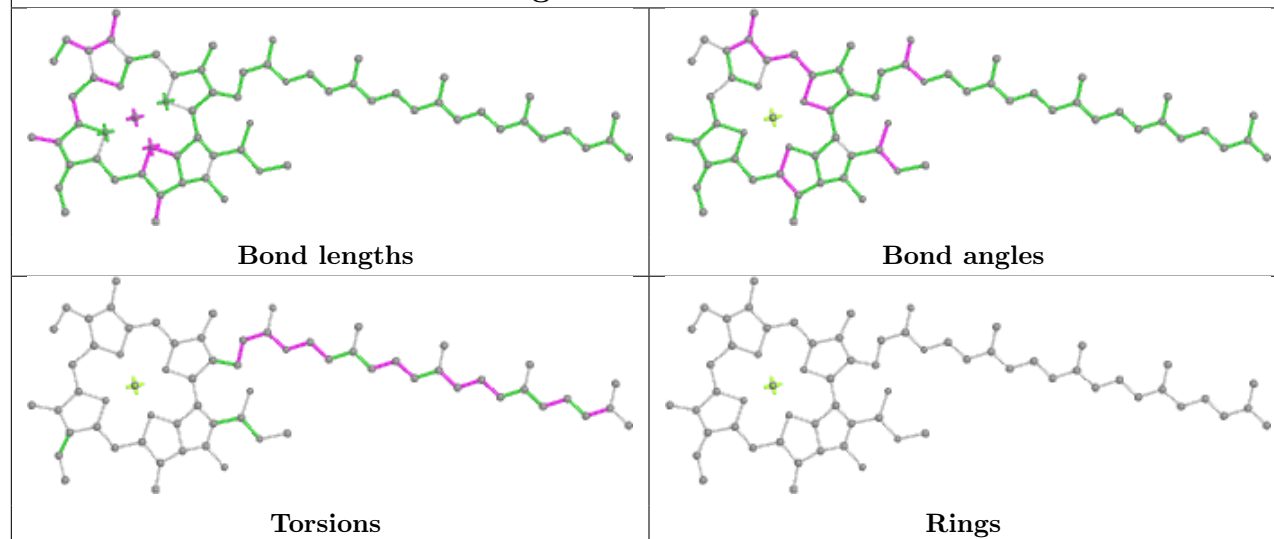
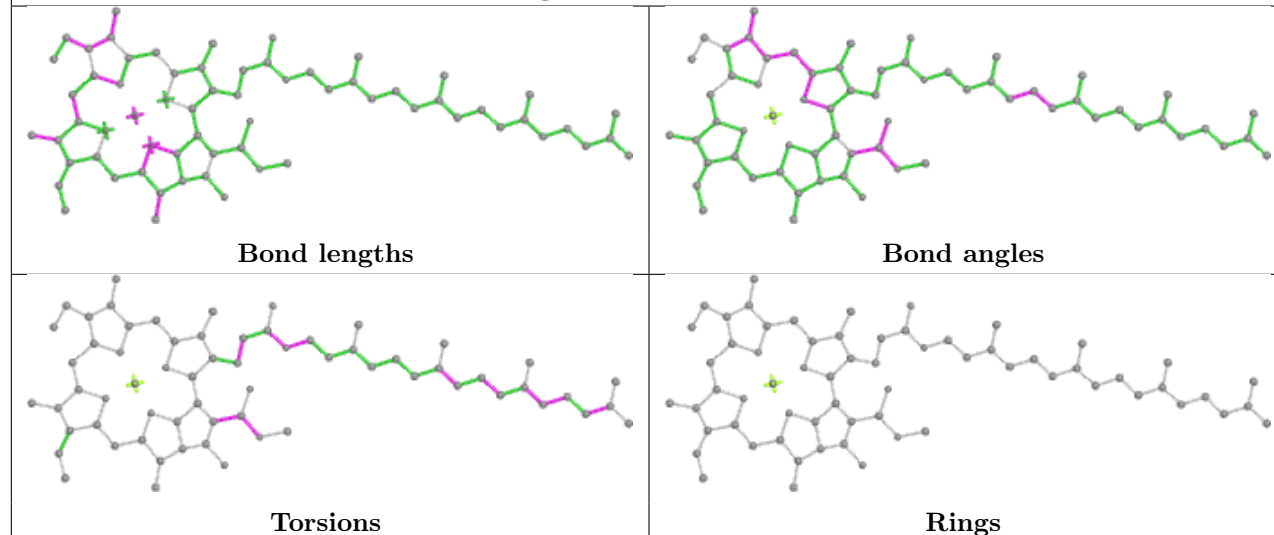
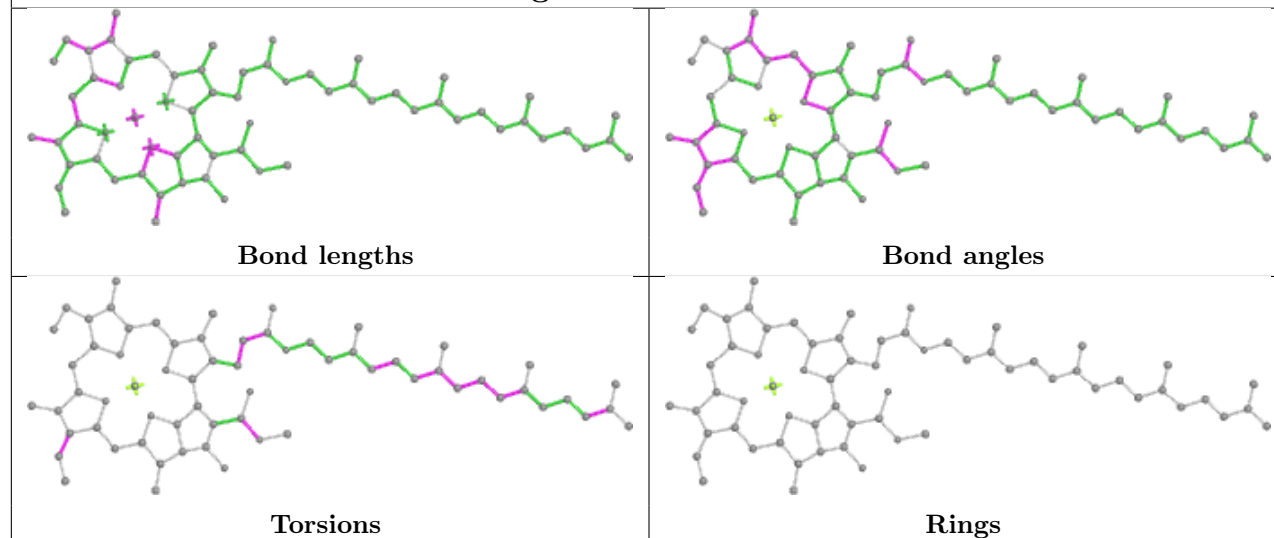
Ligand CLA A 837

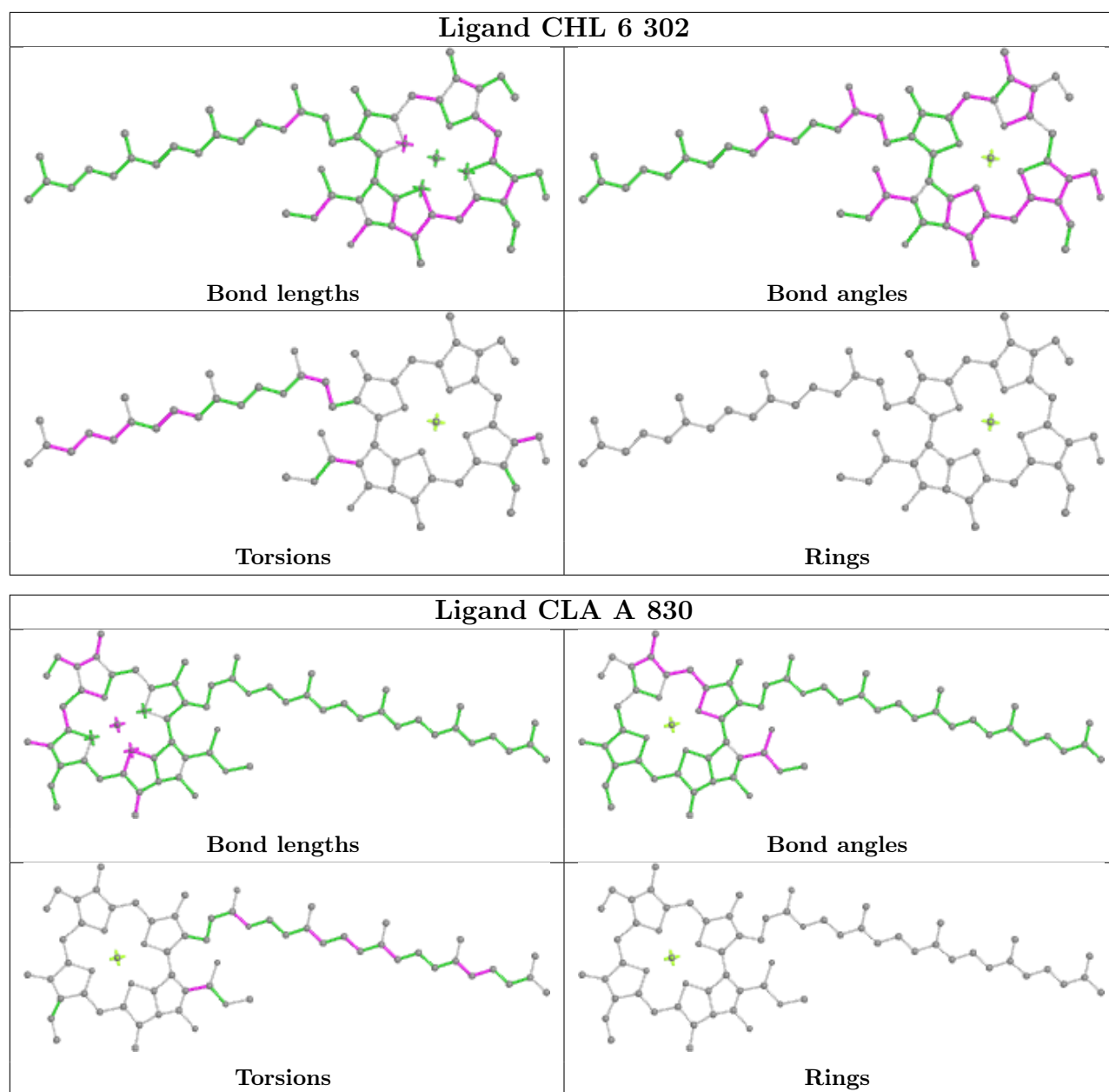


Ligand CLA A 835

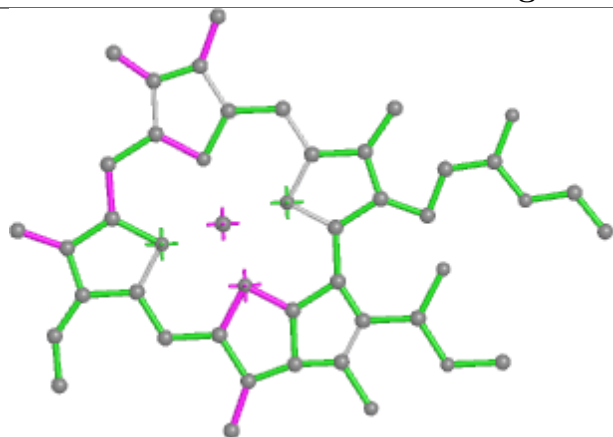


Ligand CLA 9 313**Ligand CLA 0 312**

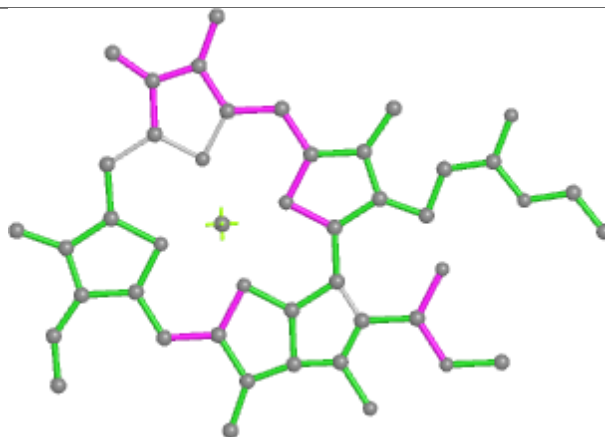
Ligand CLA B 834**Ligand CLA 6 303****Ligand CLA A 839**



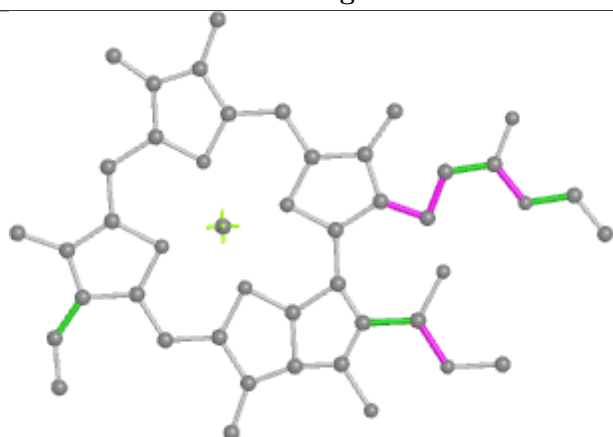
Ligand CLA 9 301



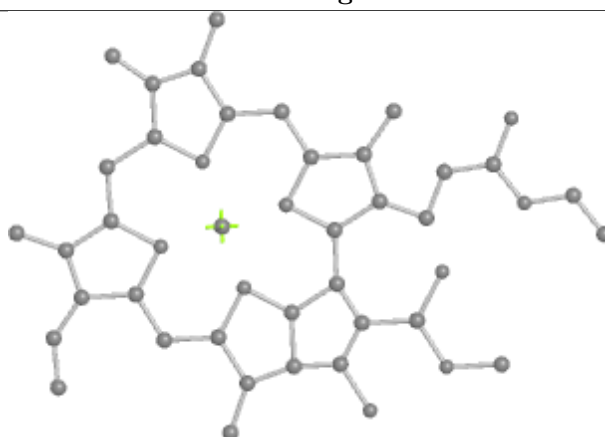
Bond lengths



Bond angles

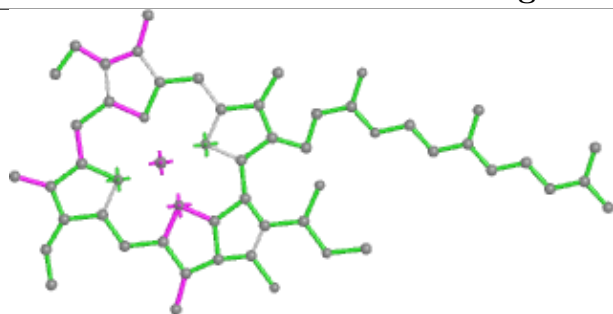


Torsions

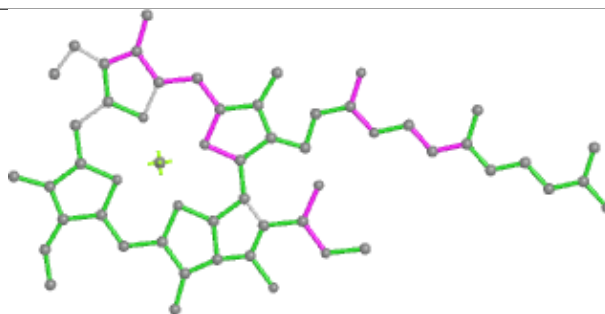


Rings

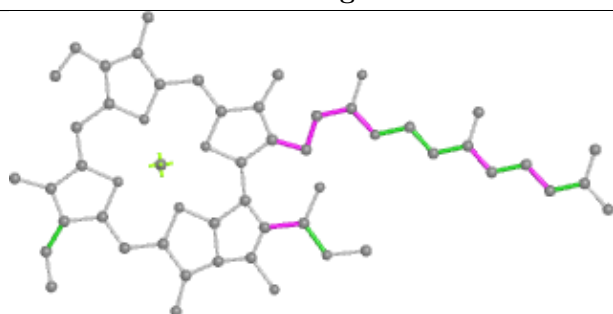
Ligand CLA 3 311



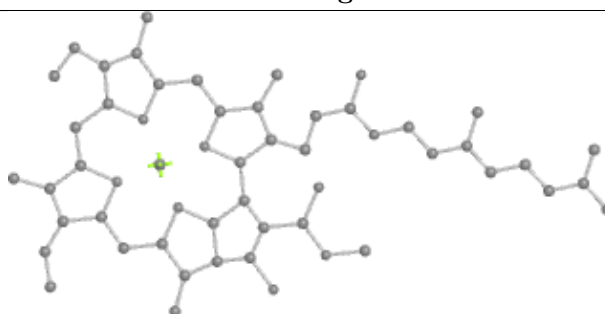
Bond lengths



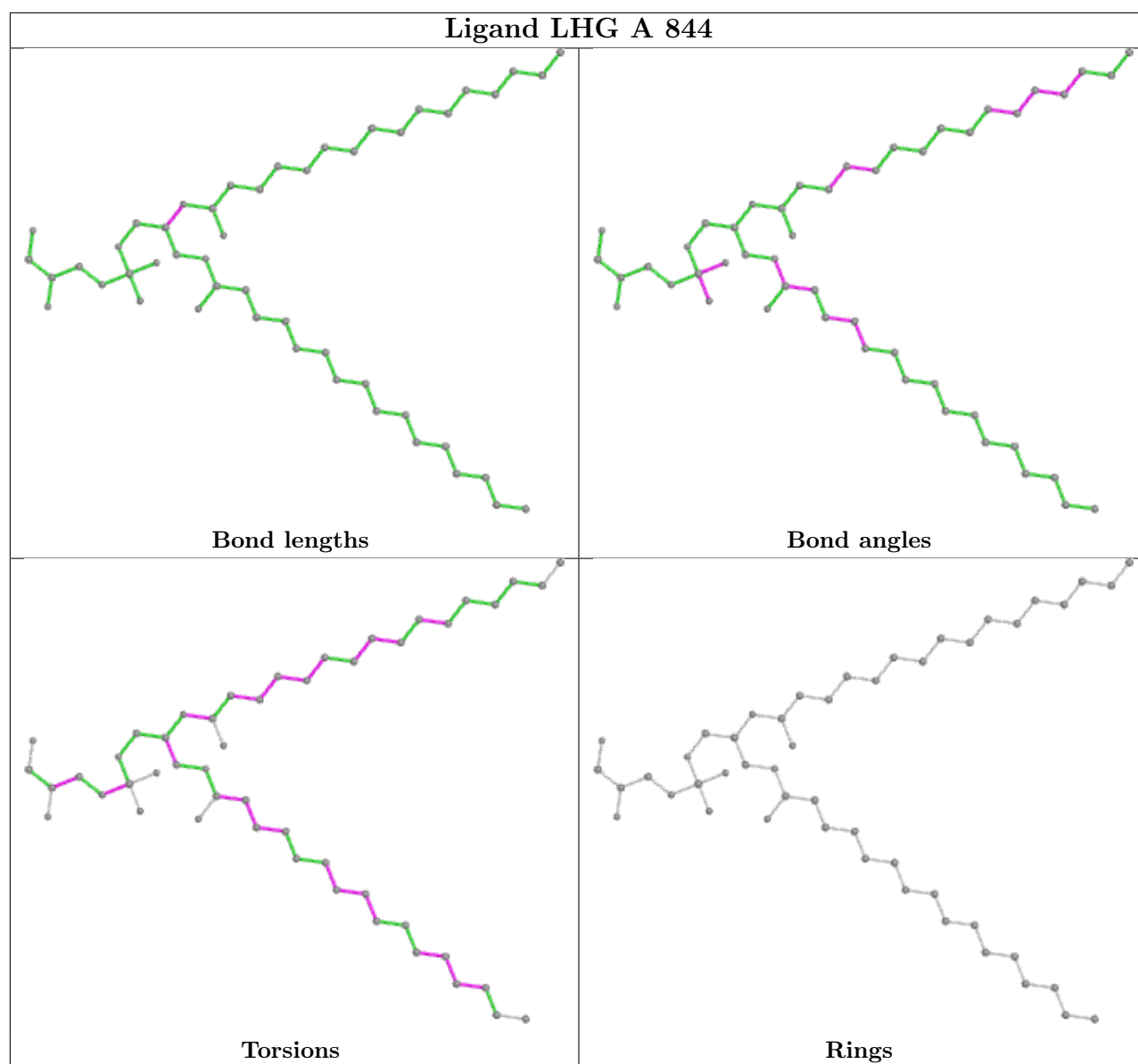
Bond angles



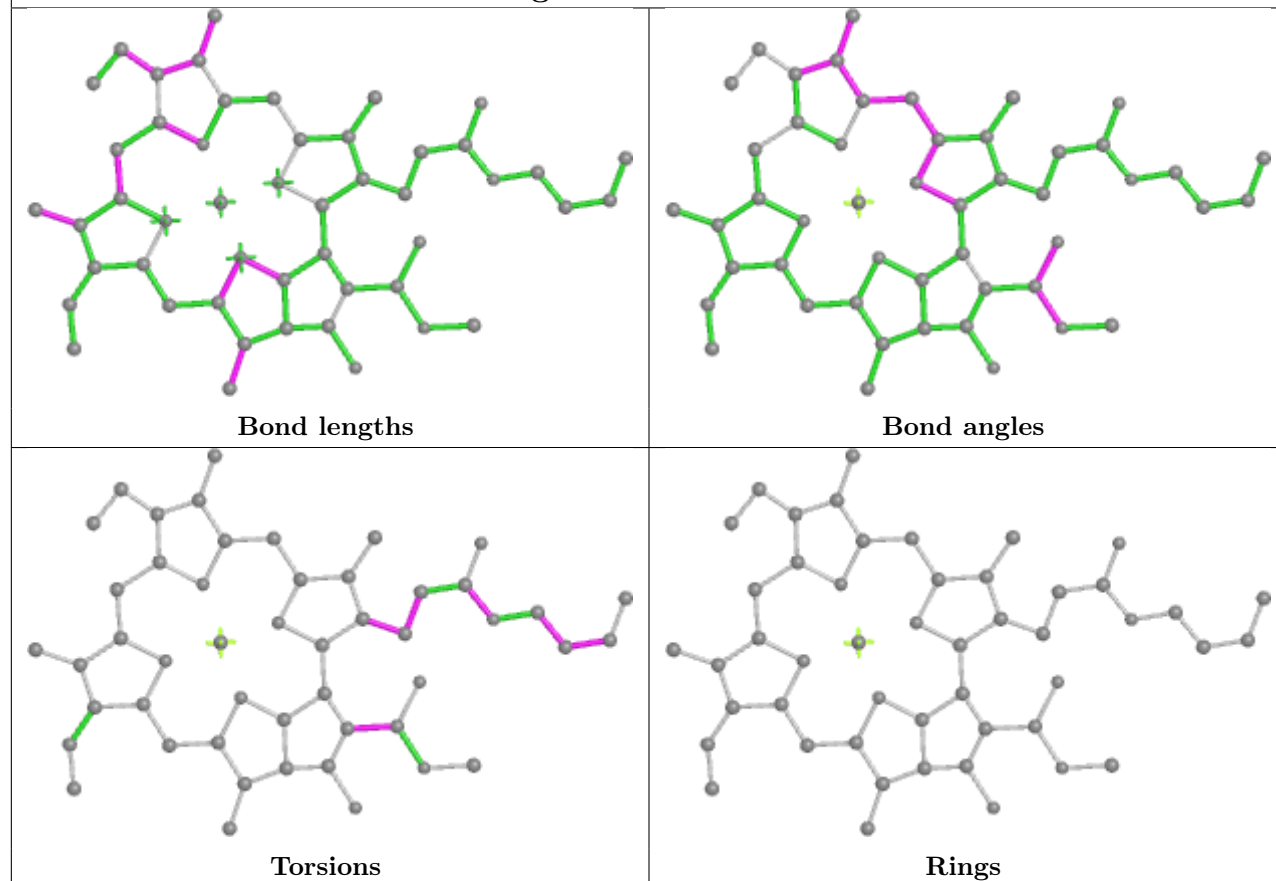
Torsions



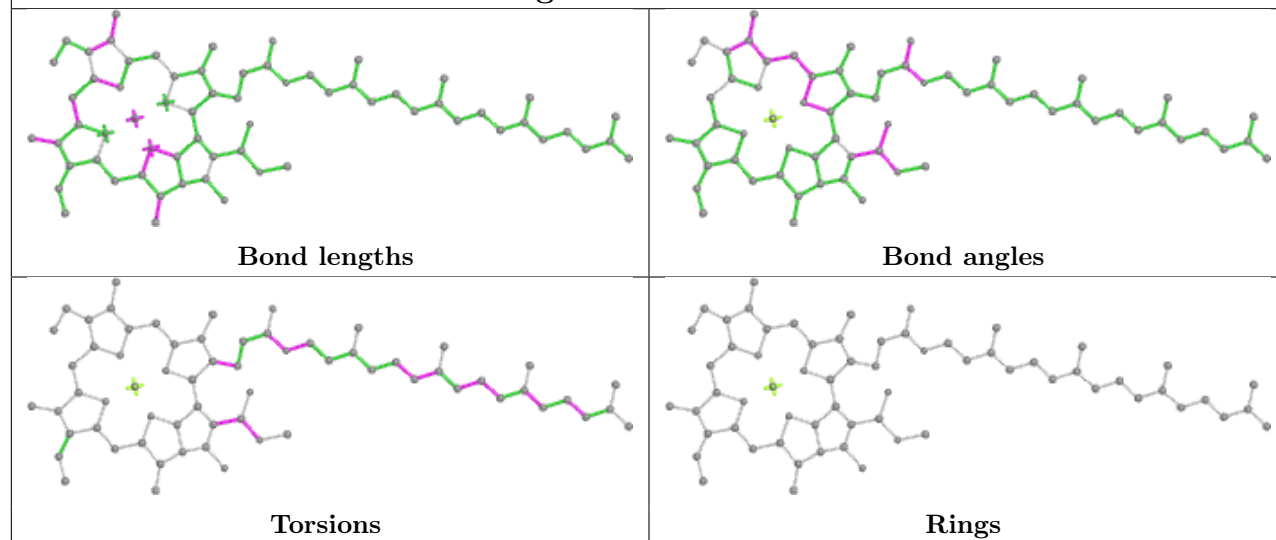
Rings

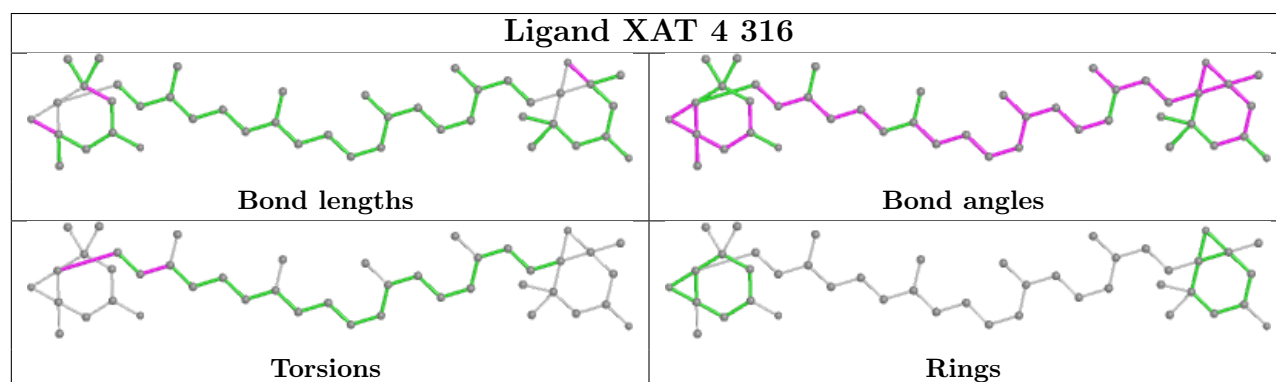
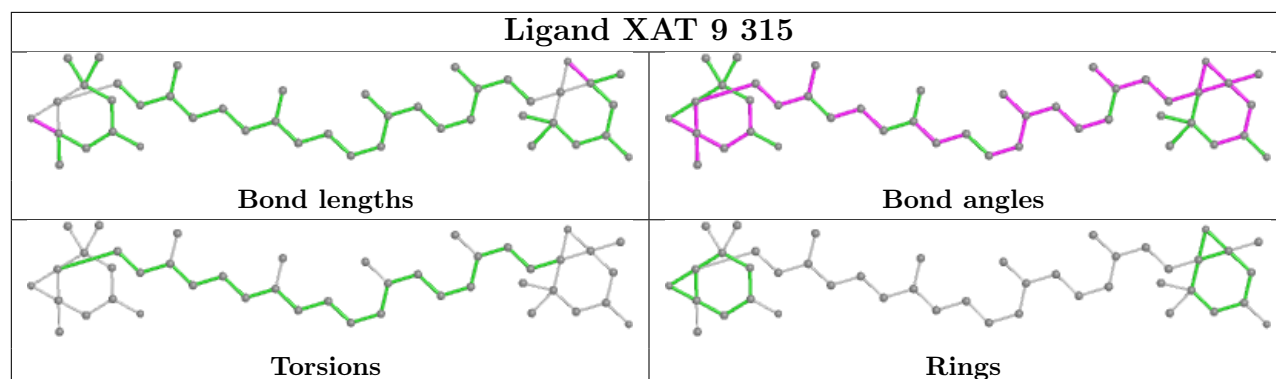
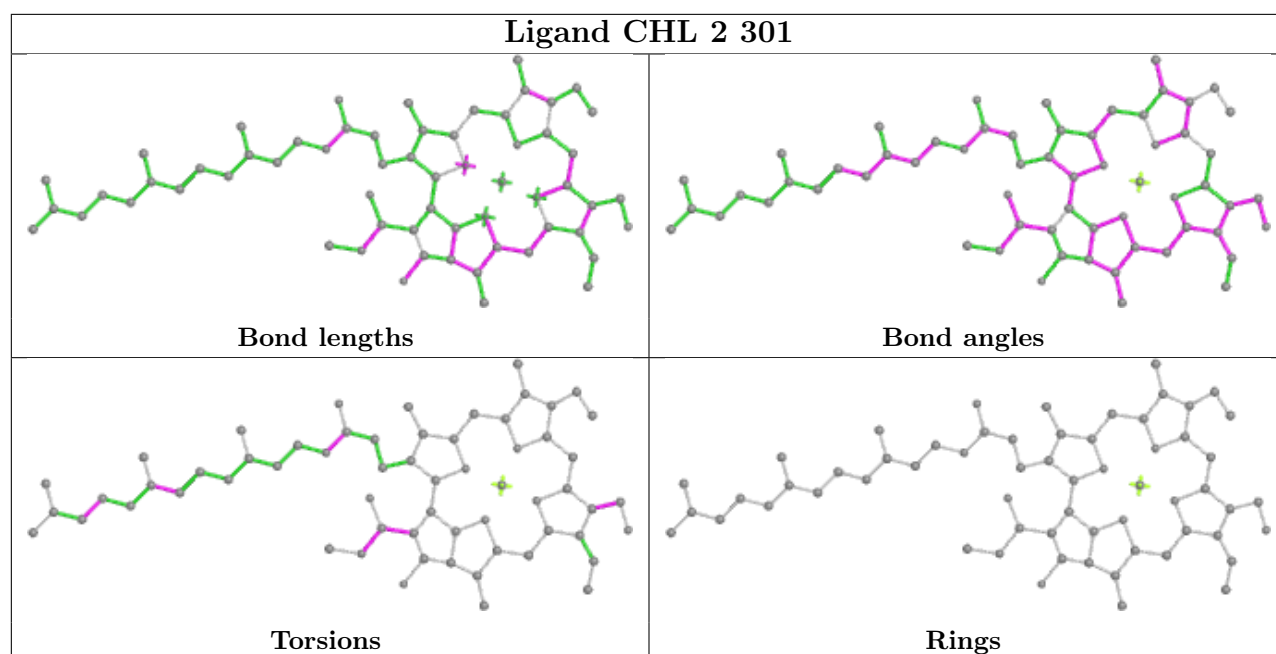


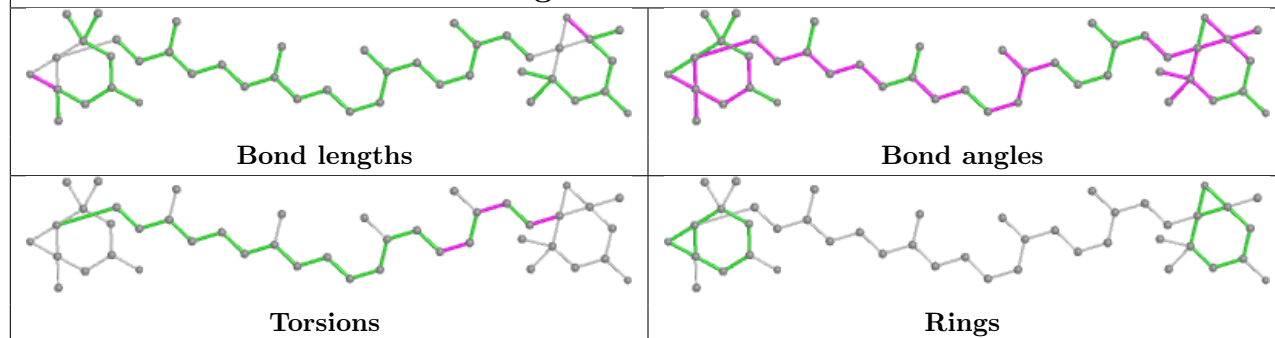
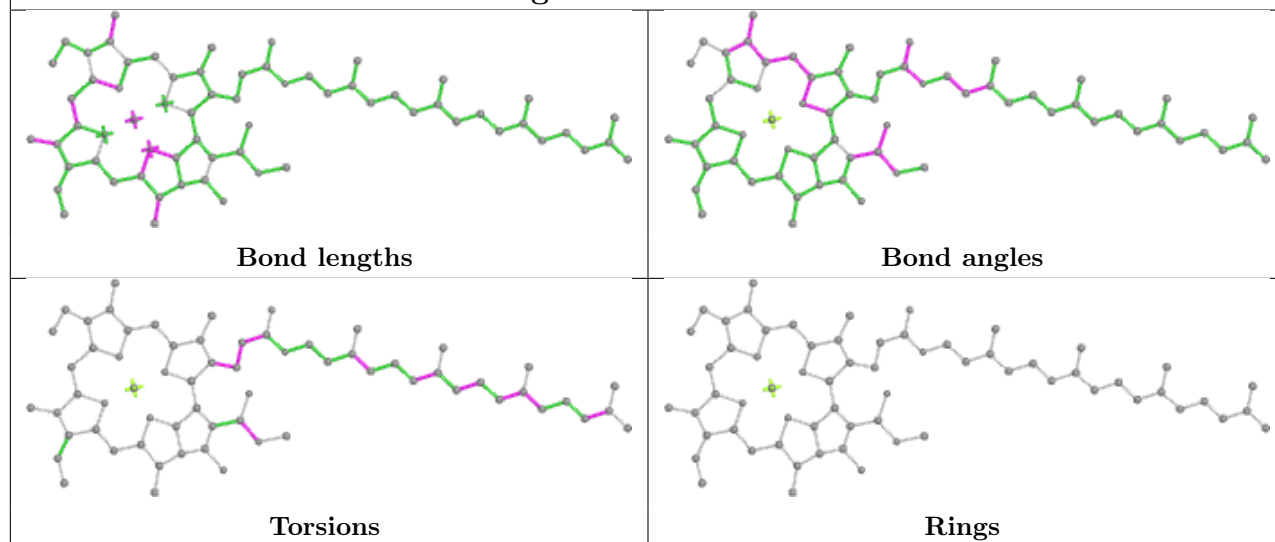
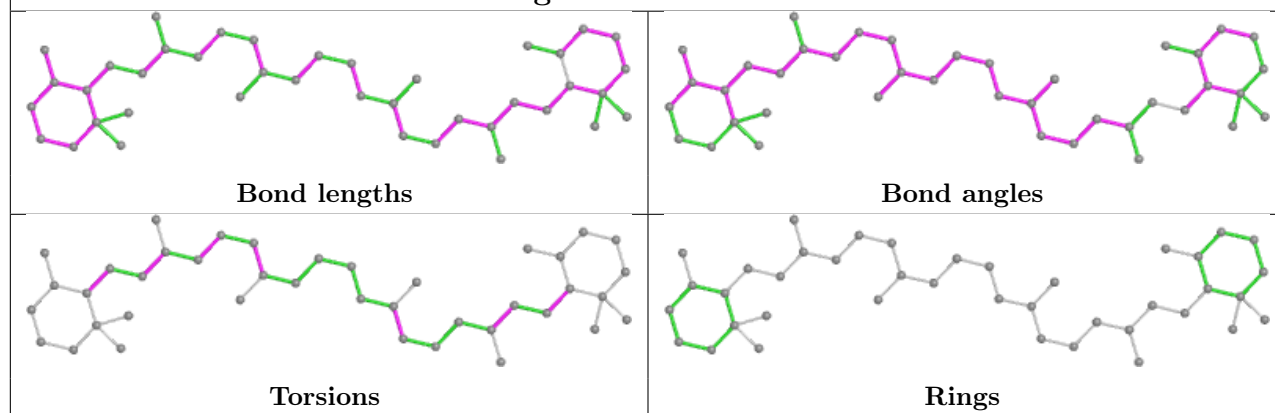
Ligand CLA A 852

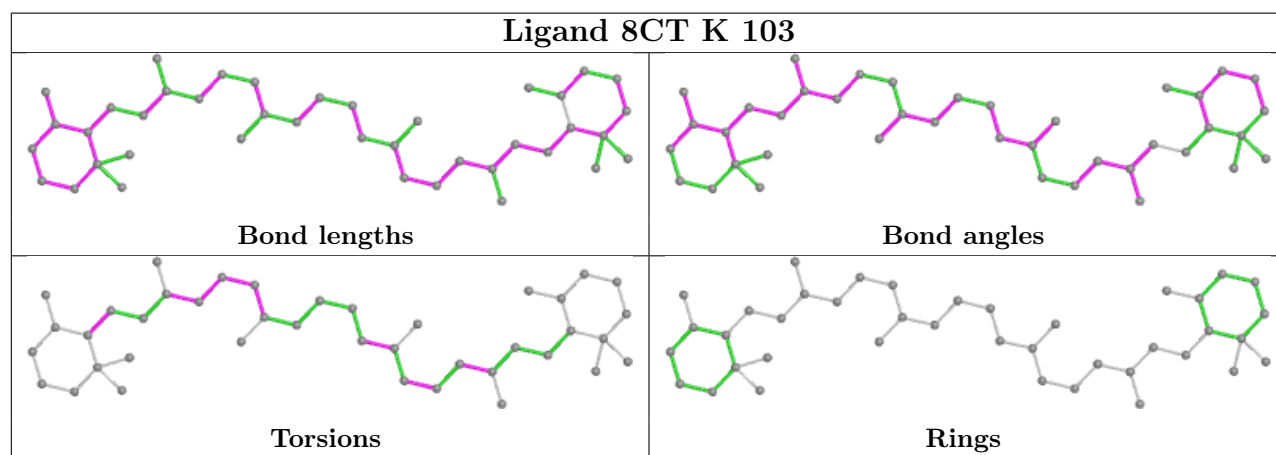
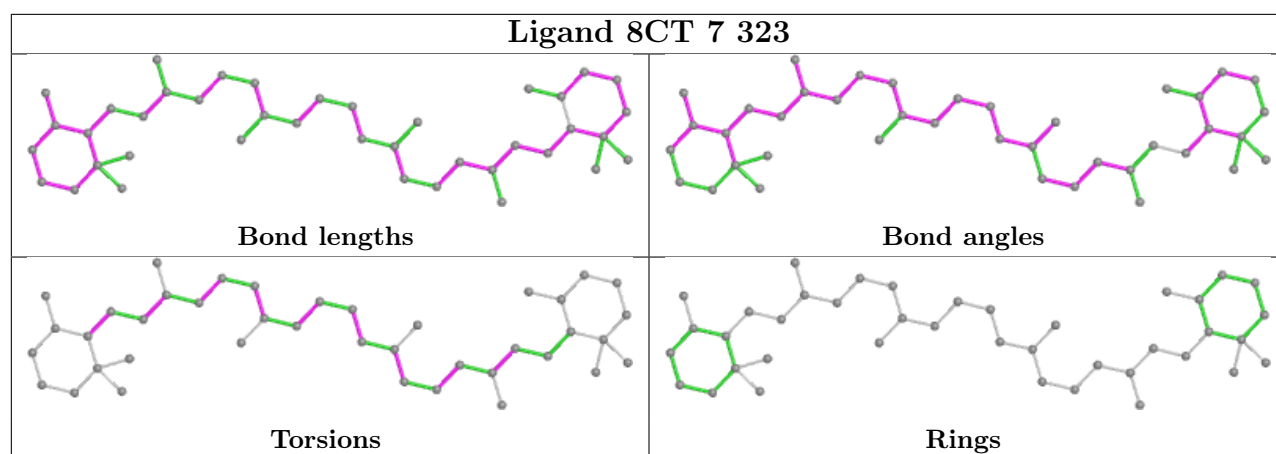


Ligand CLA 4 314

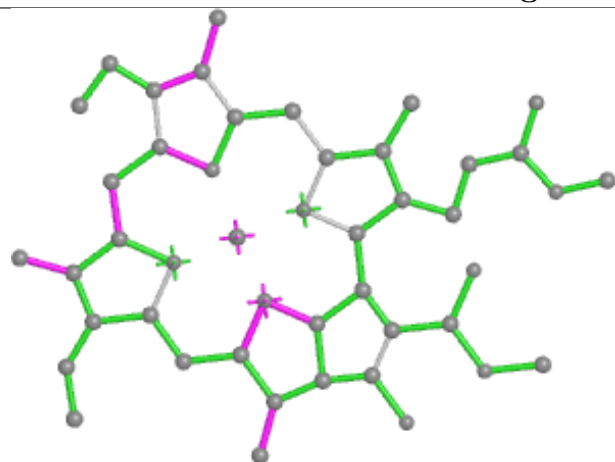




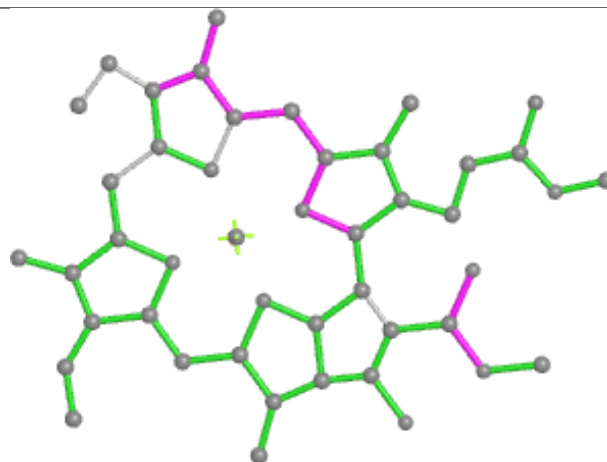
Ligand XAT 6 320**Ligand CLA B 828****Ligand 8CT A 850**



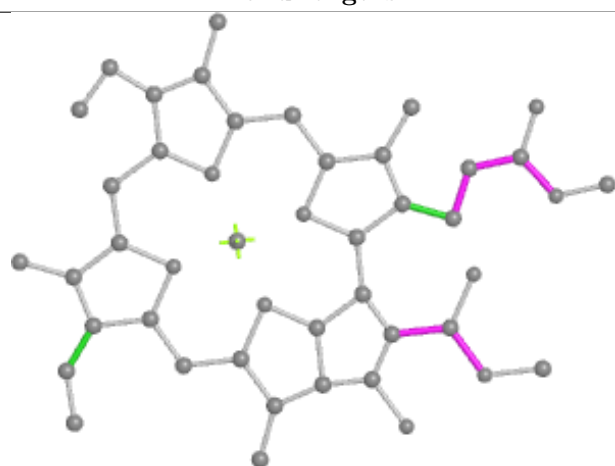
Ligand CLA 5 314



Bond lengths



Bond angles

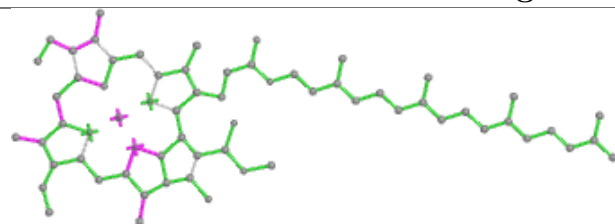


Torsions

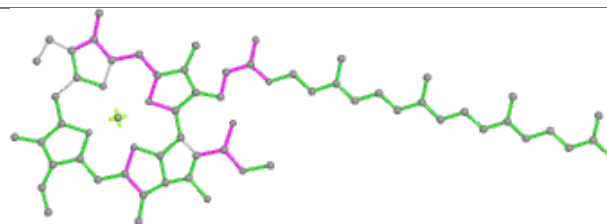


Rings

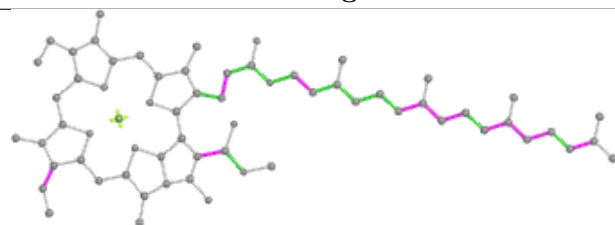
Ligand CLA B 803



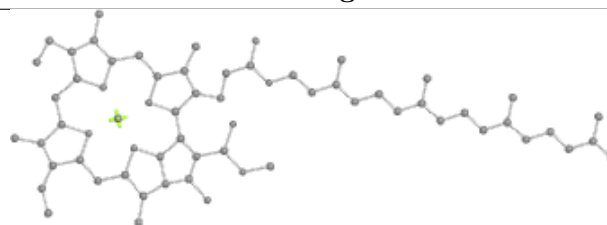
Bond lengths



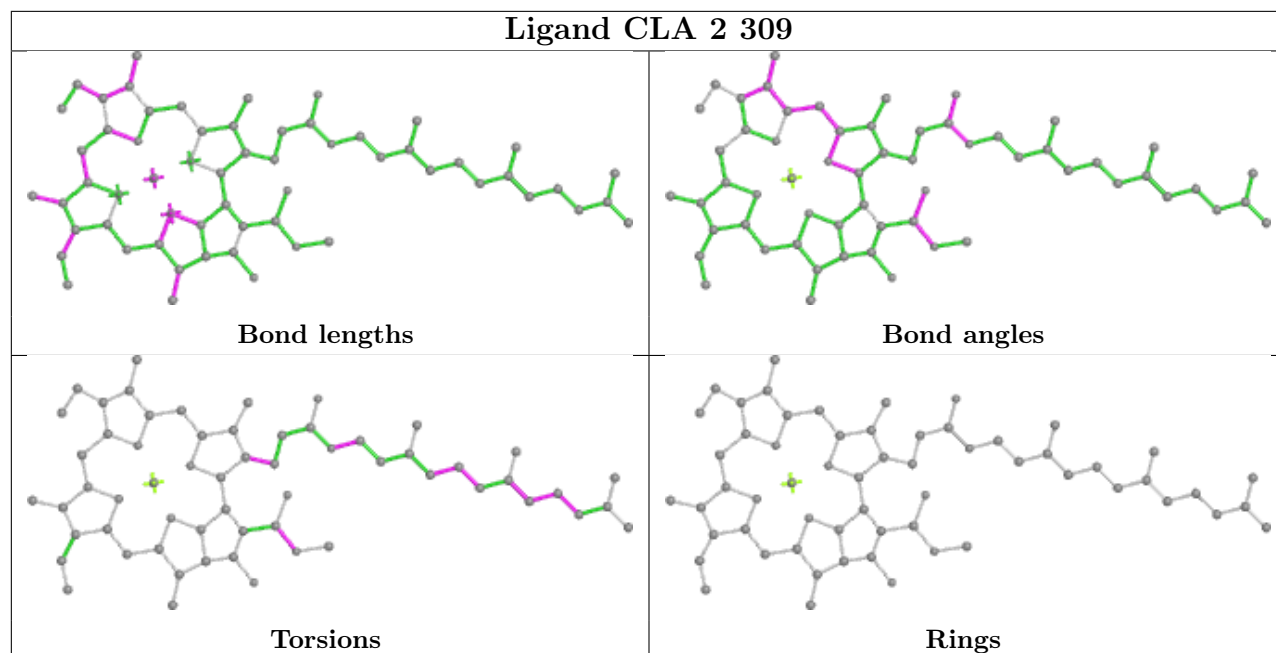
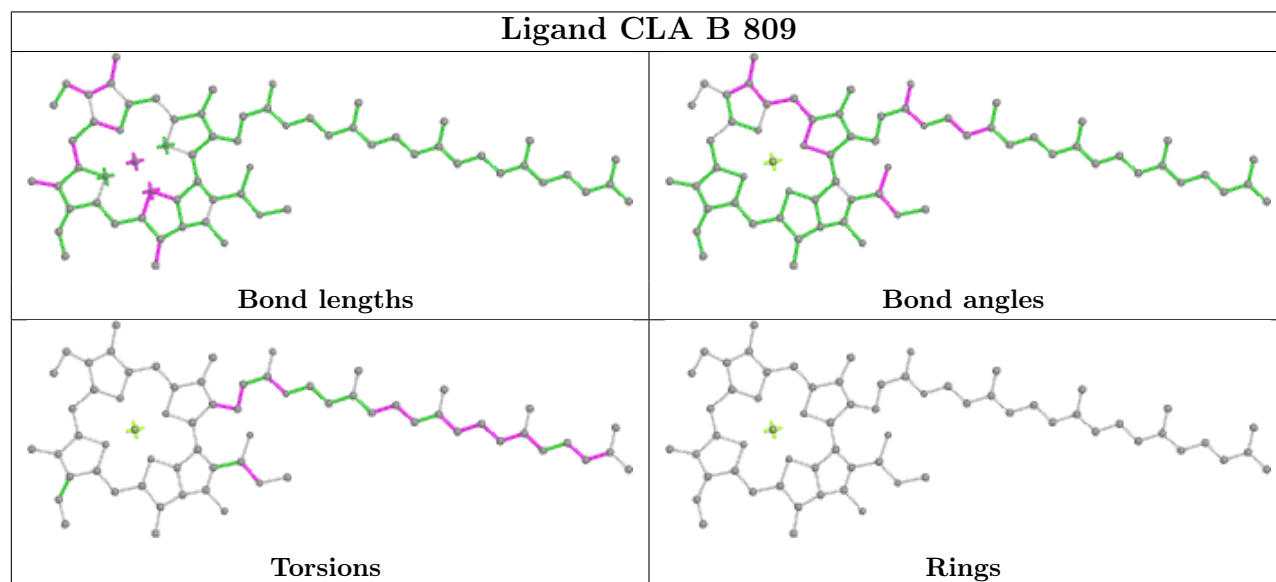
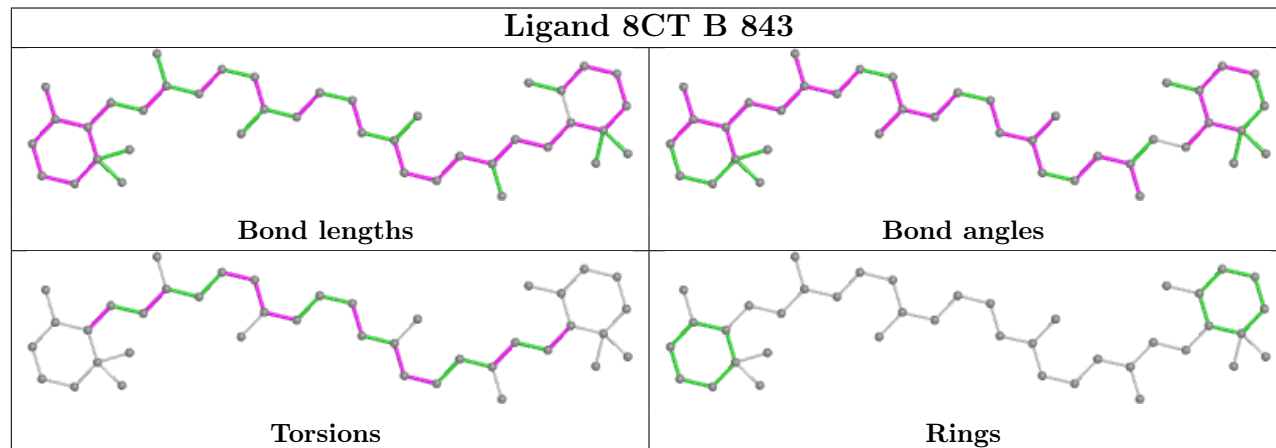
Bond angles

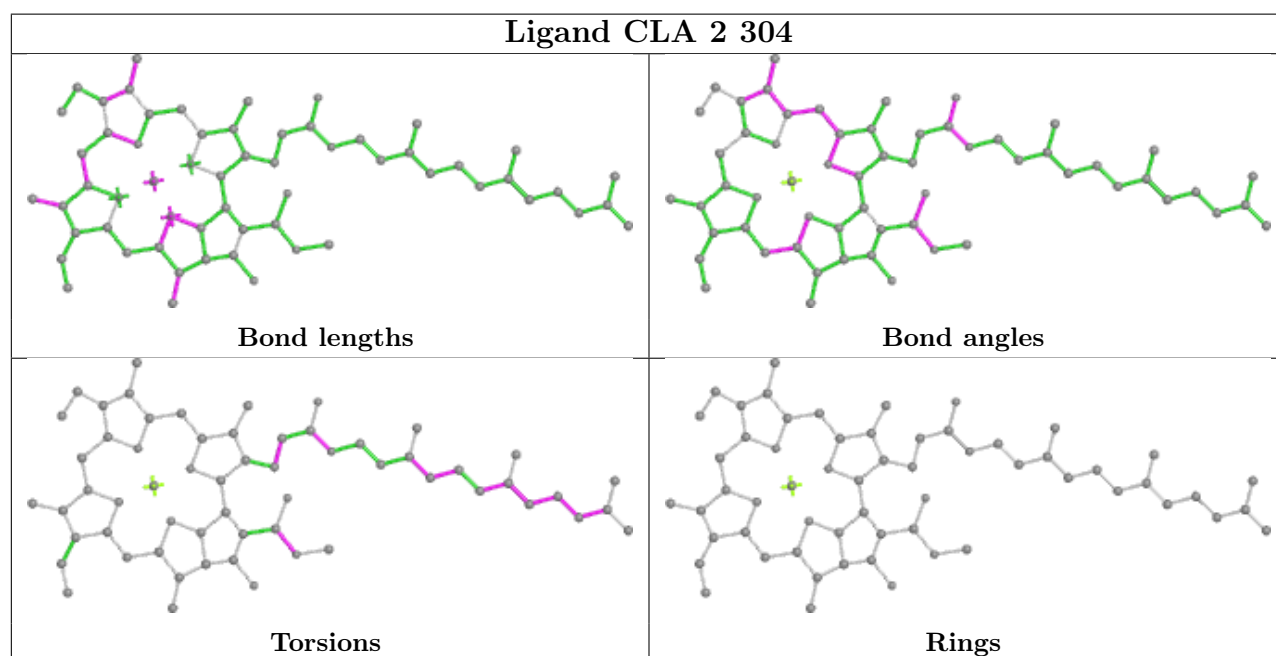
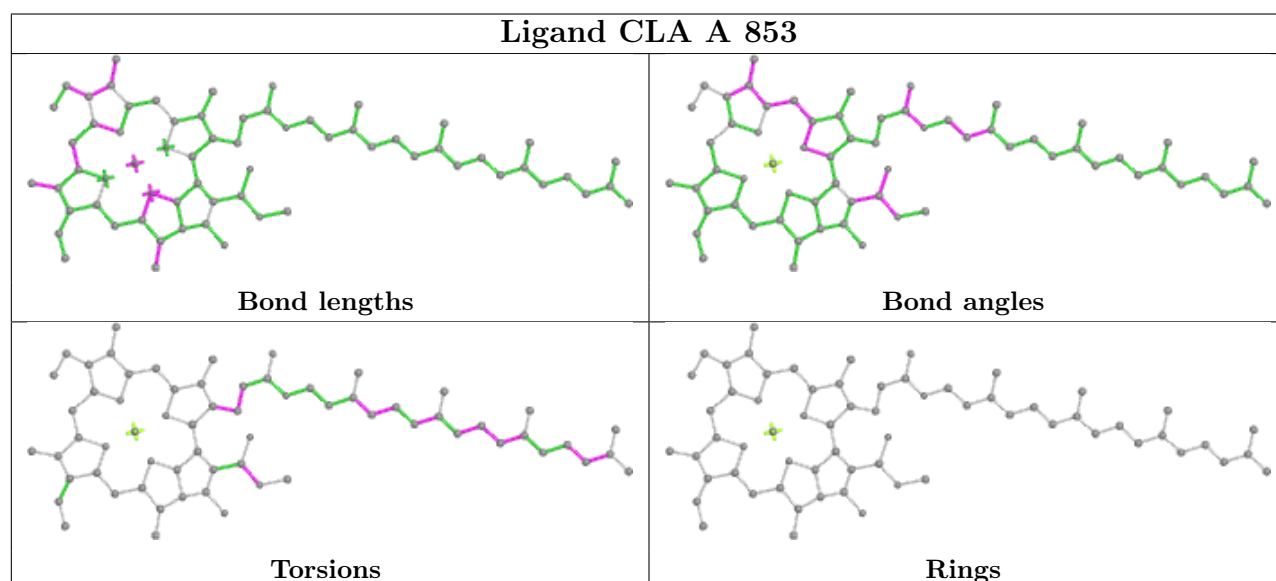
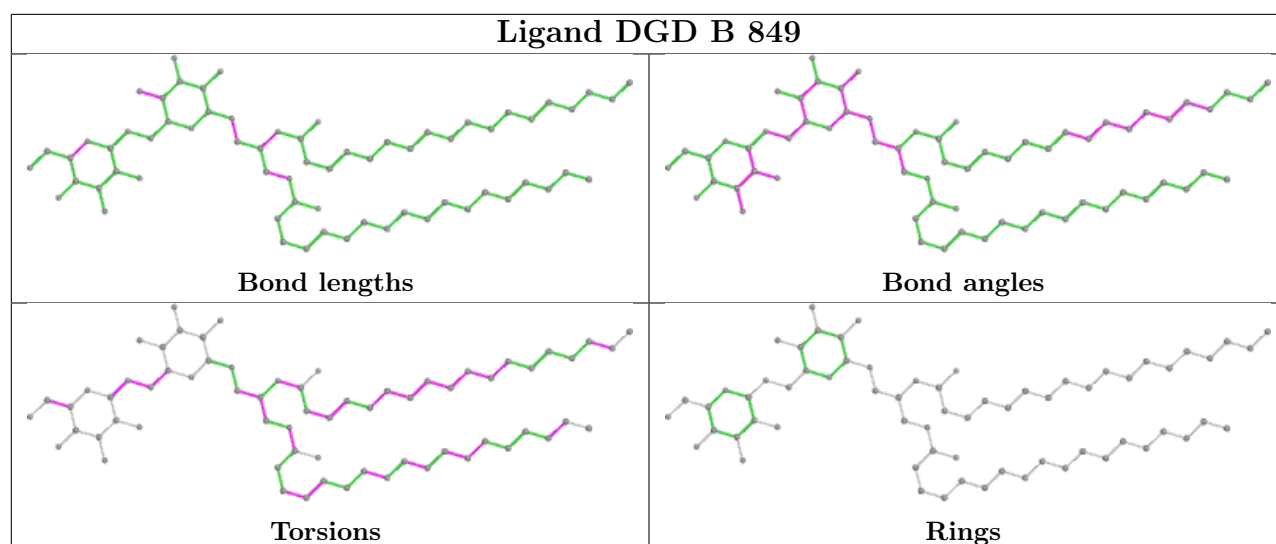


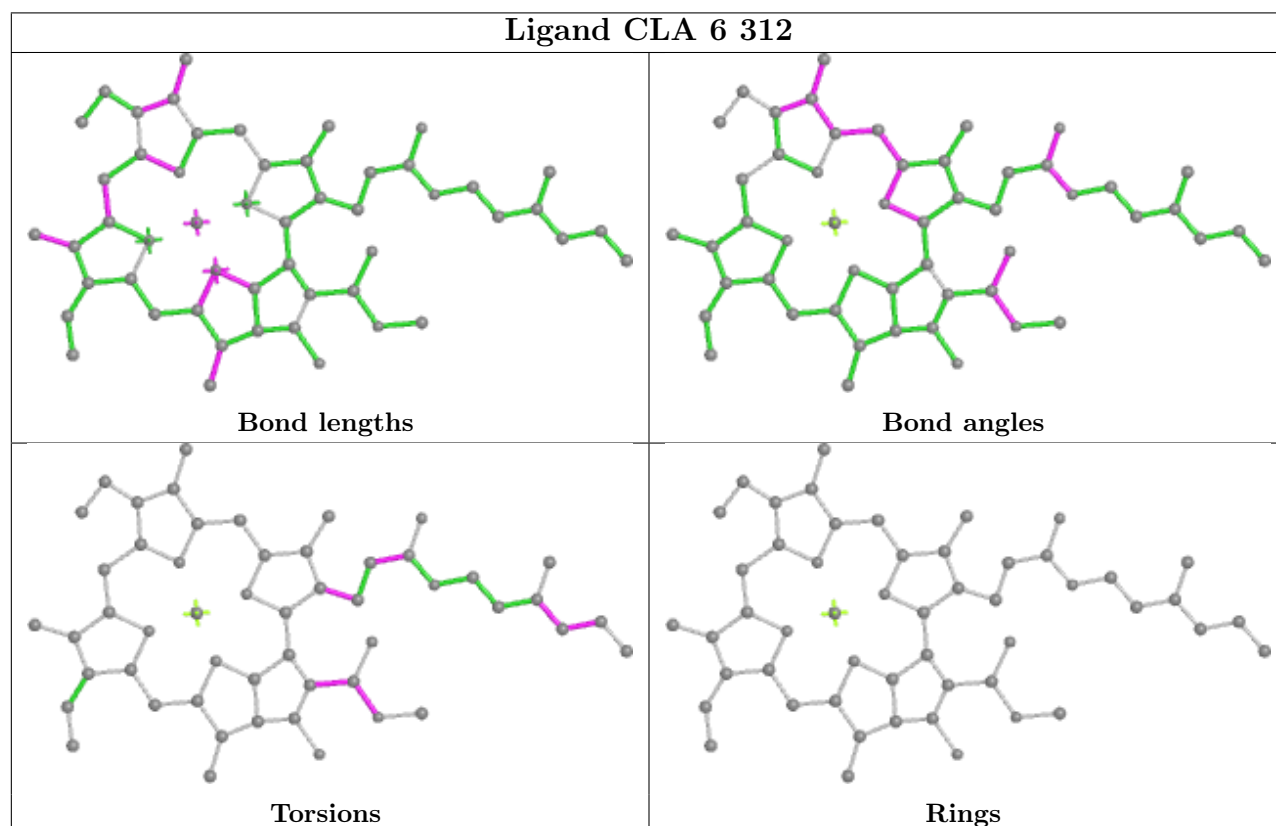
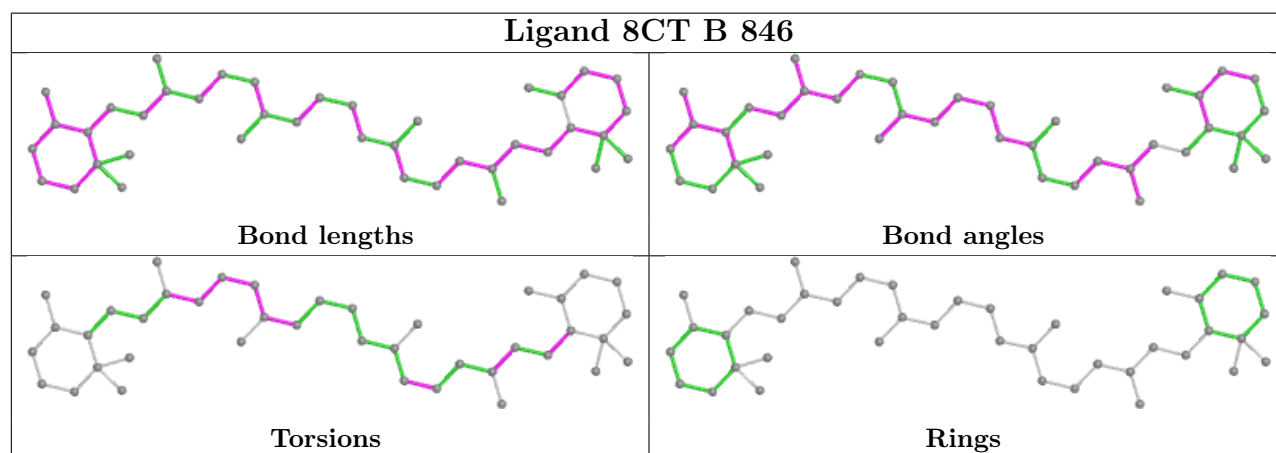
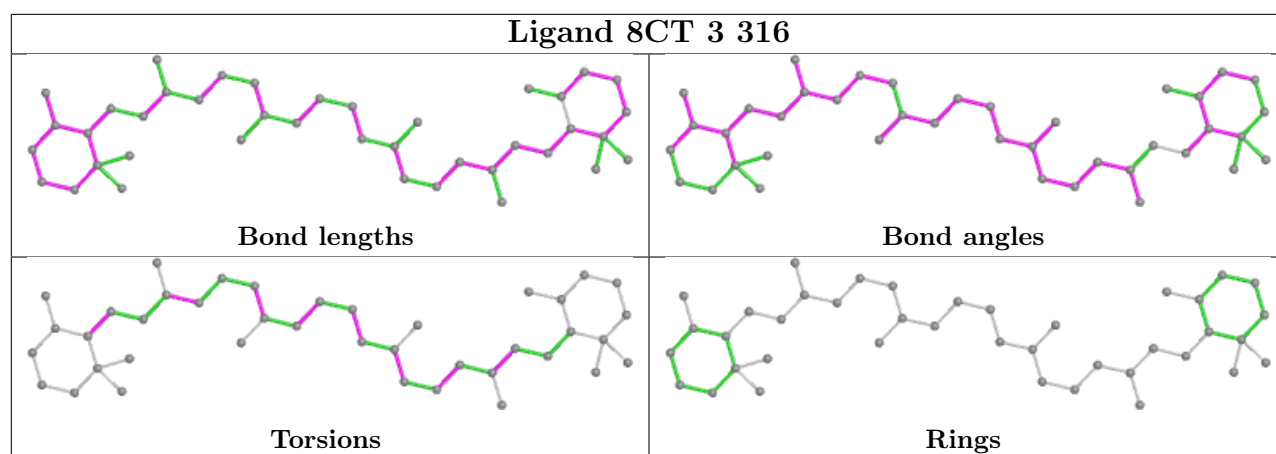
Torsions

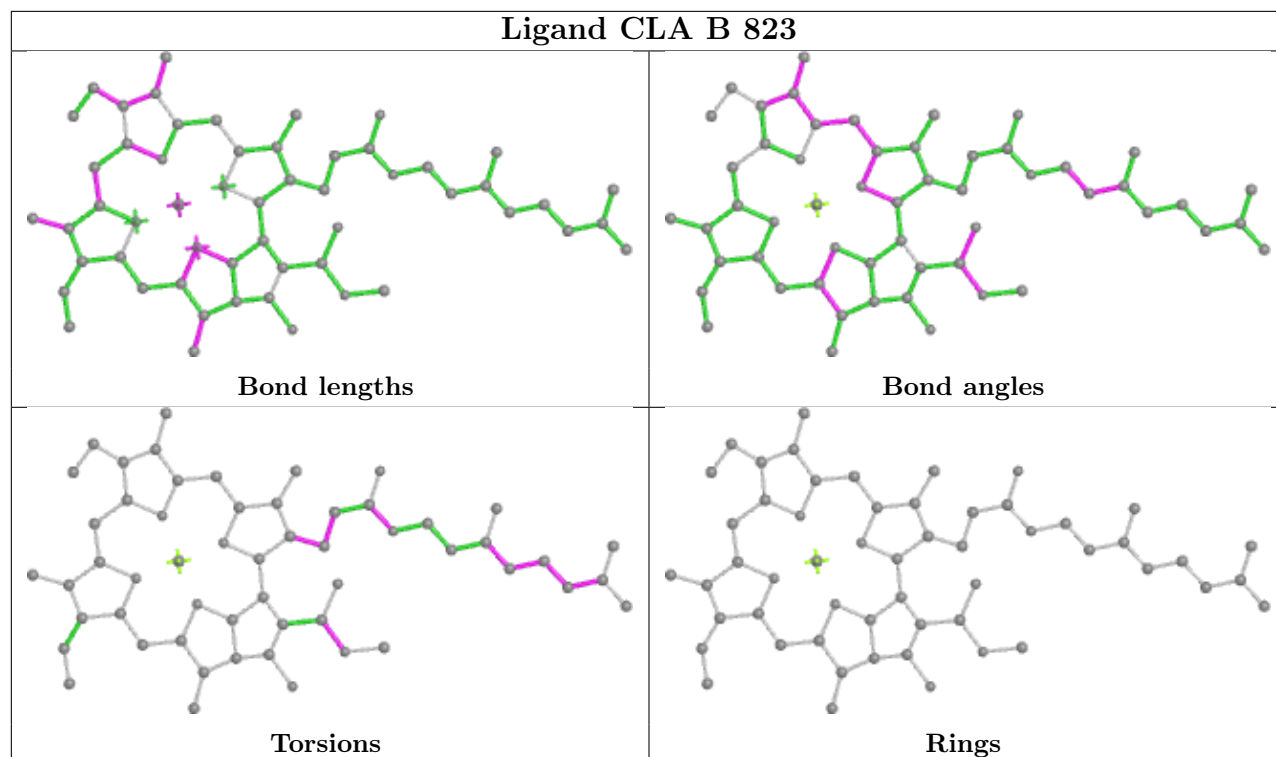
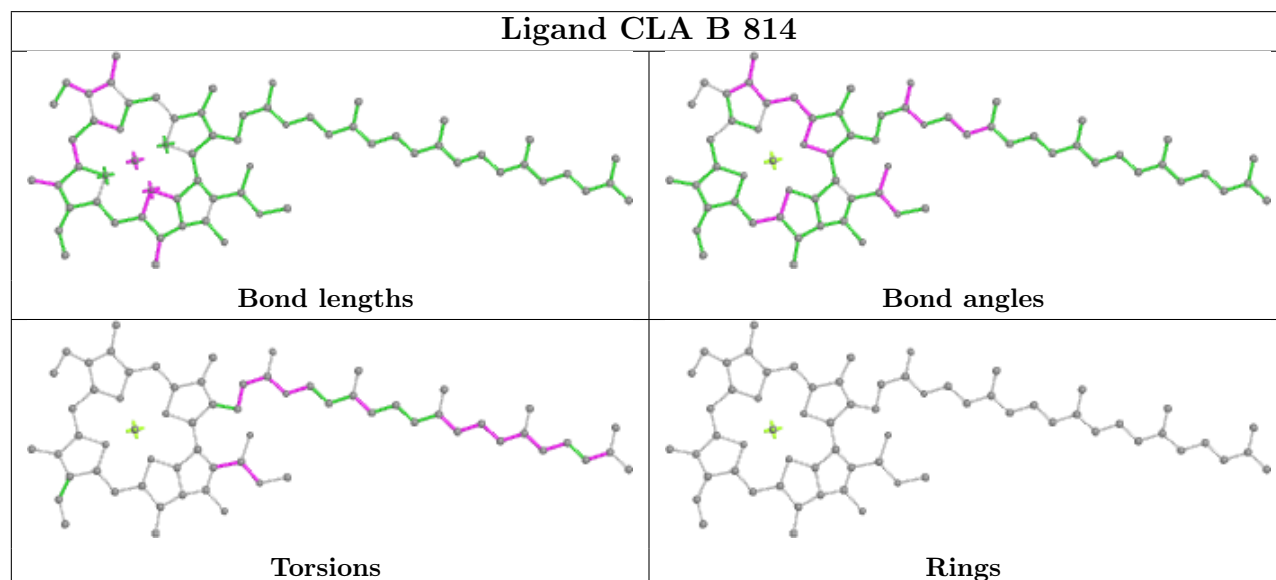


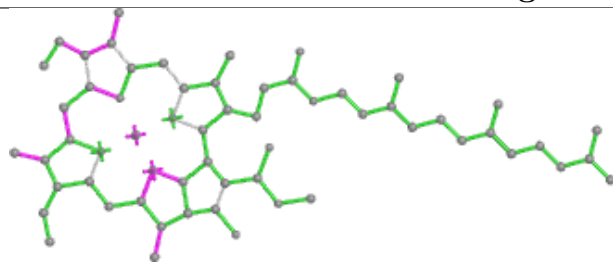
Rings

Ligand CLA 2 309**Ligand CLA B 809****Ligand 8CT B 843**

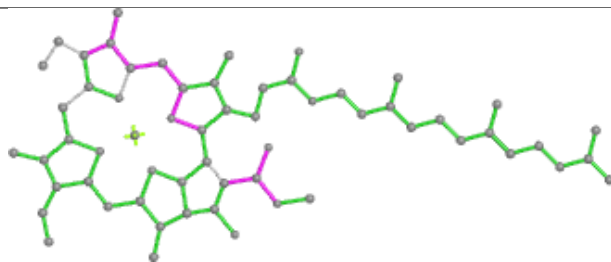




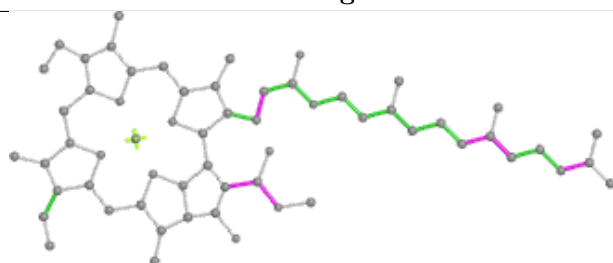
Ligand CLA B 823**Ligand CLA B 814**

Ligand CLA 3 301

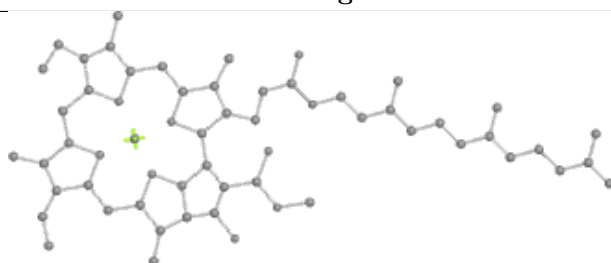
Bond lengths



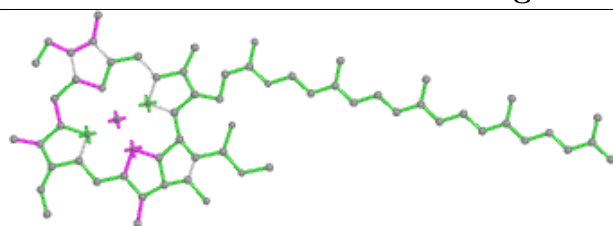
Bond angles



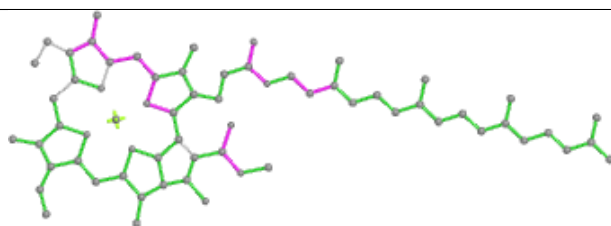
Torsions



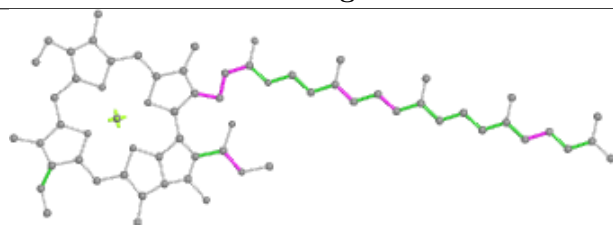
Rings

Ligand CLA A 829

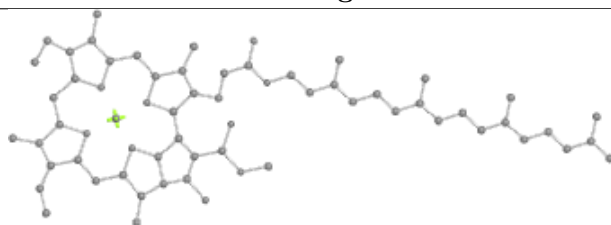
Bond lengths



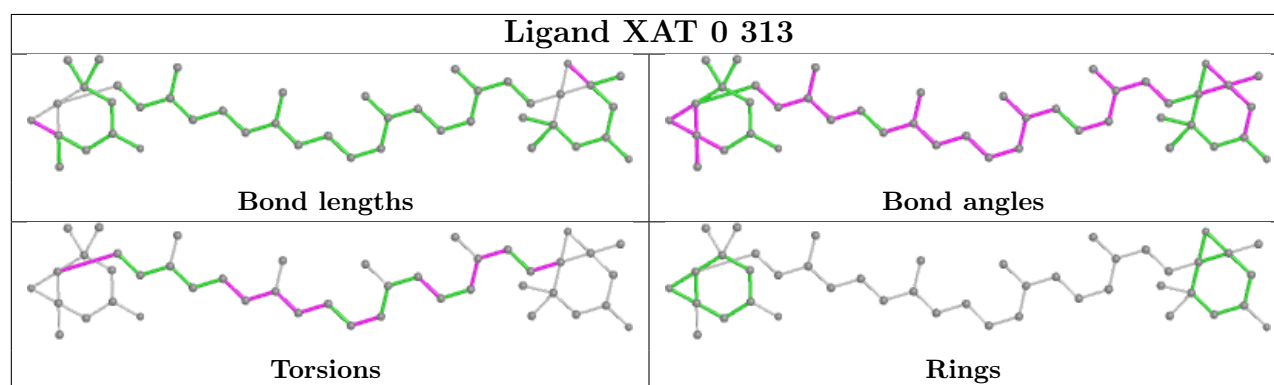
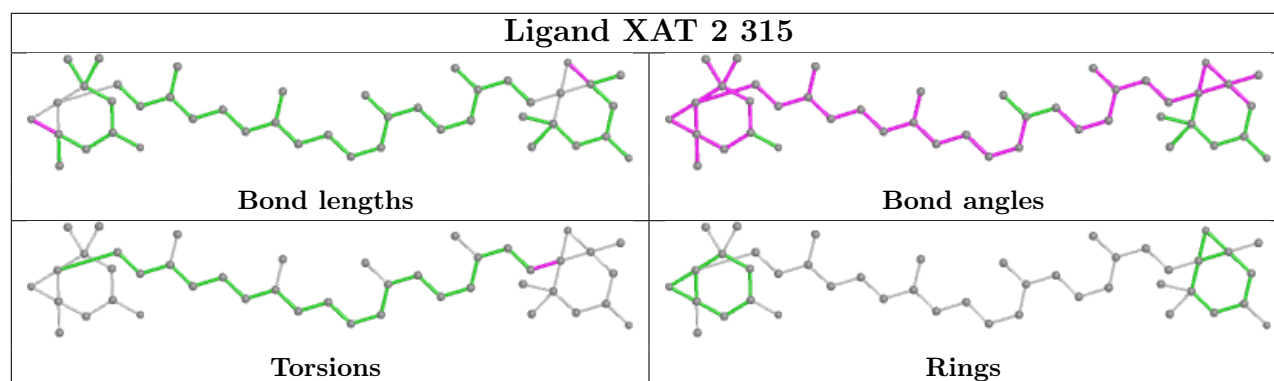
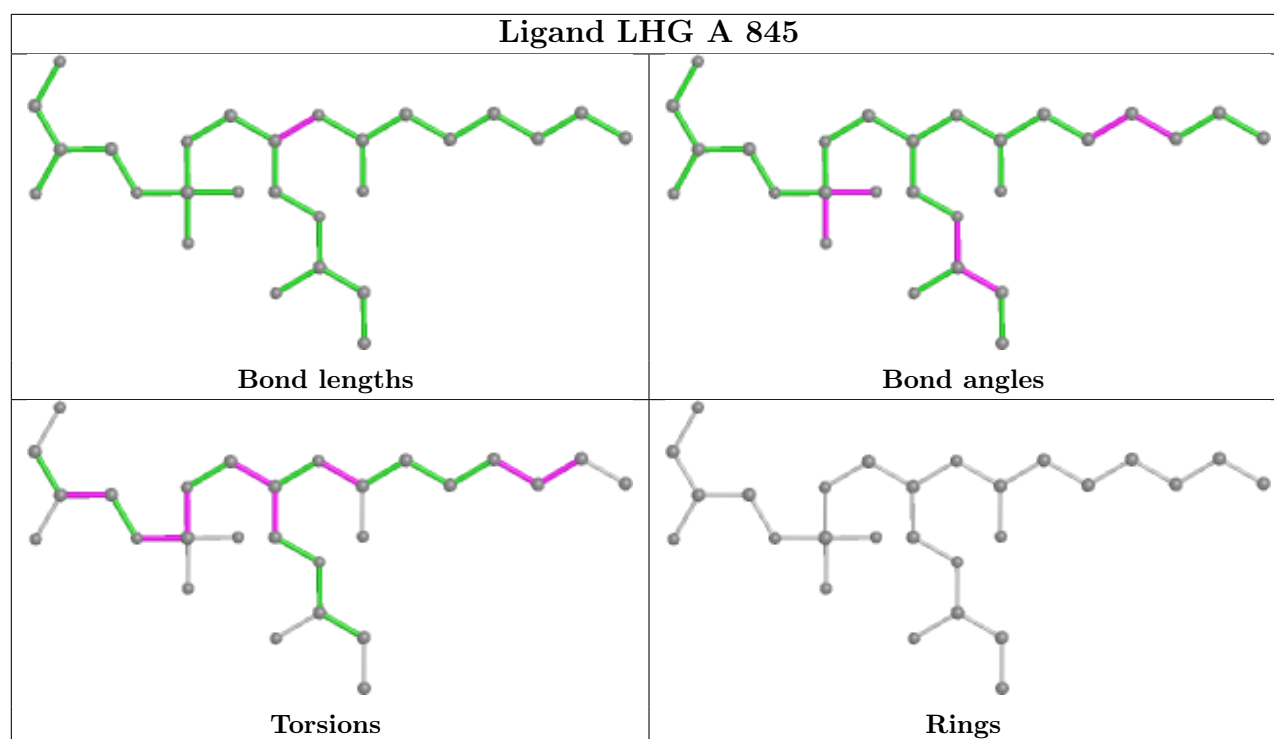
Bond angles



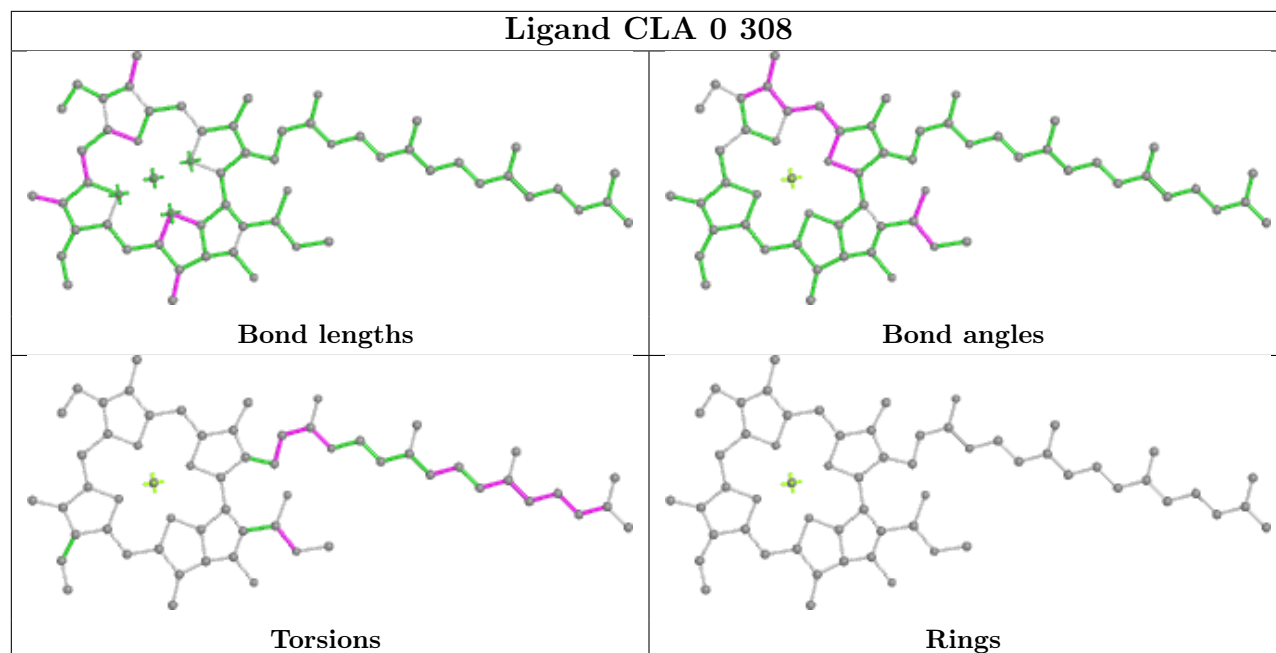
Torsions



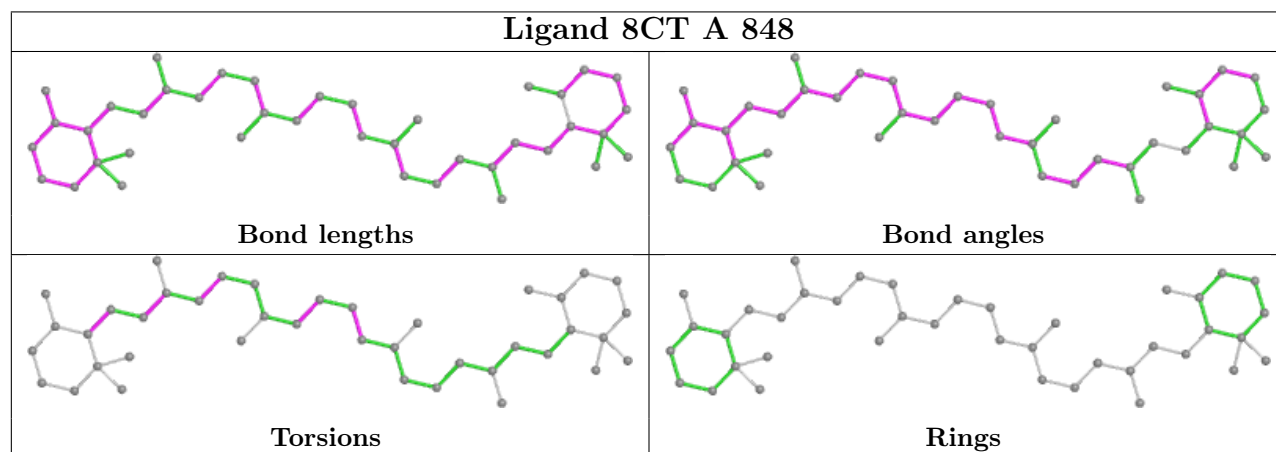
Rings



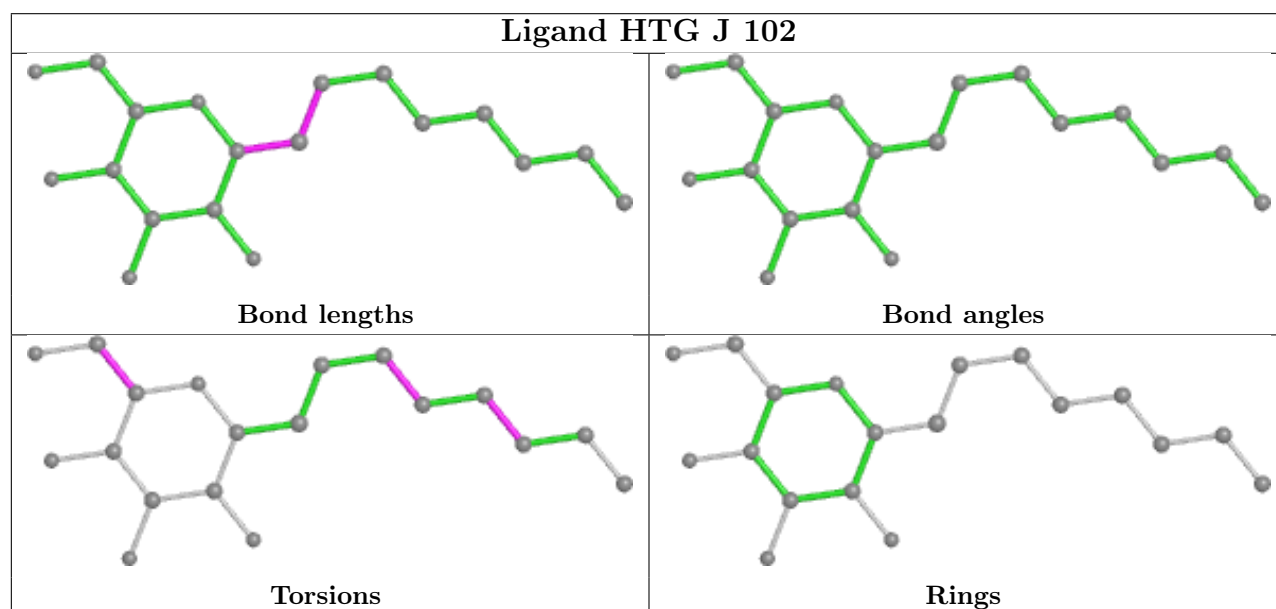
Ligand CLA 0 308

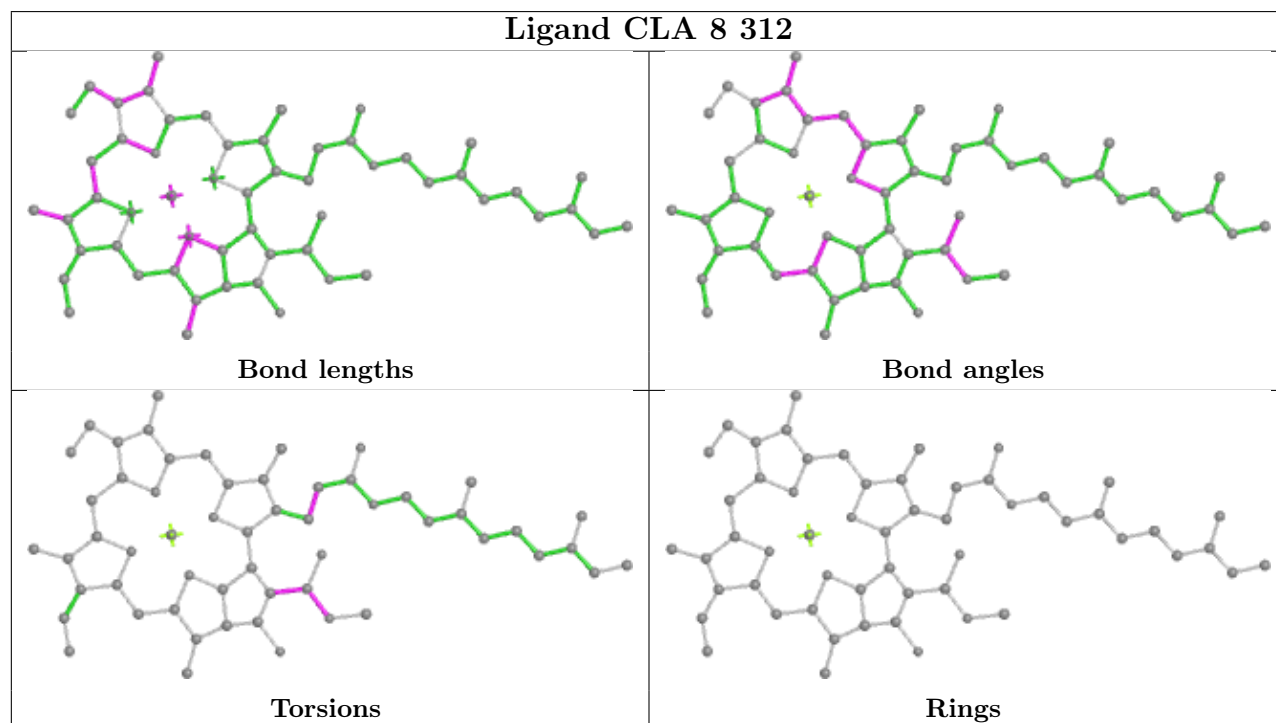
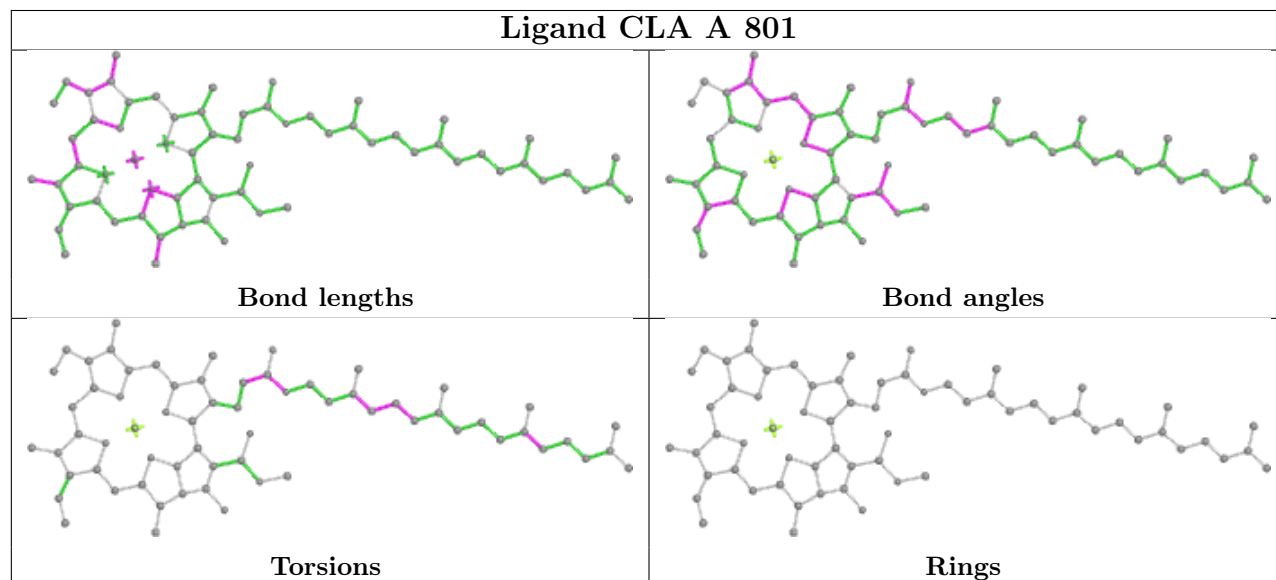
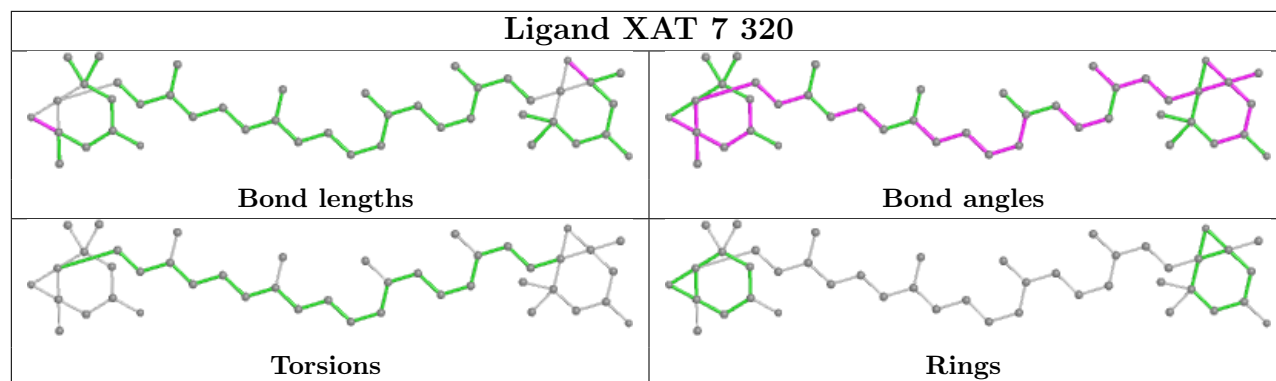


Ligand 8CT A 848

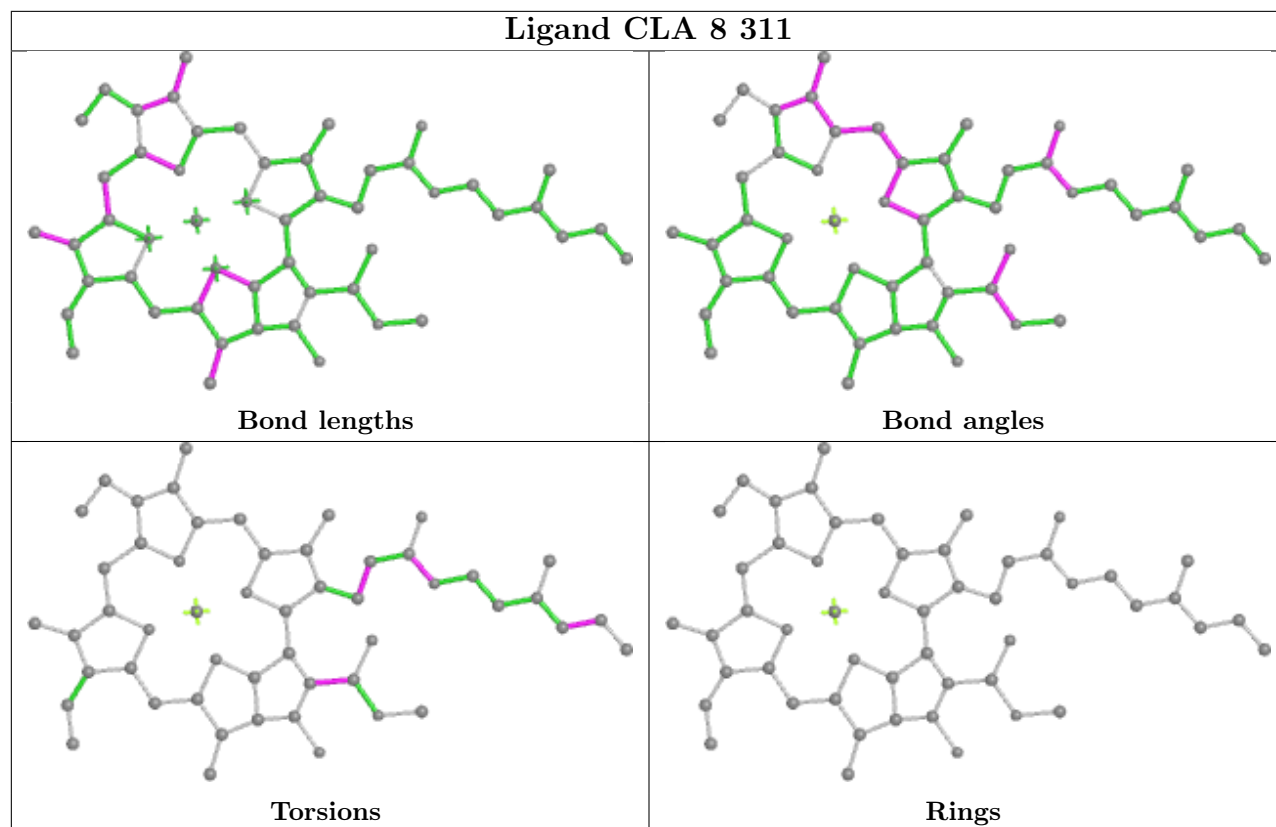


Ligand HTG J 102

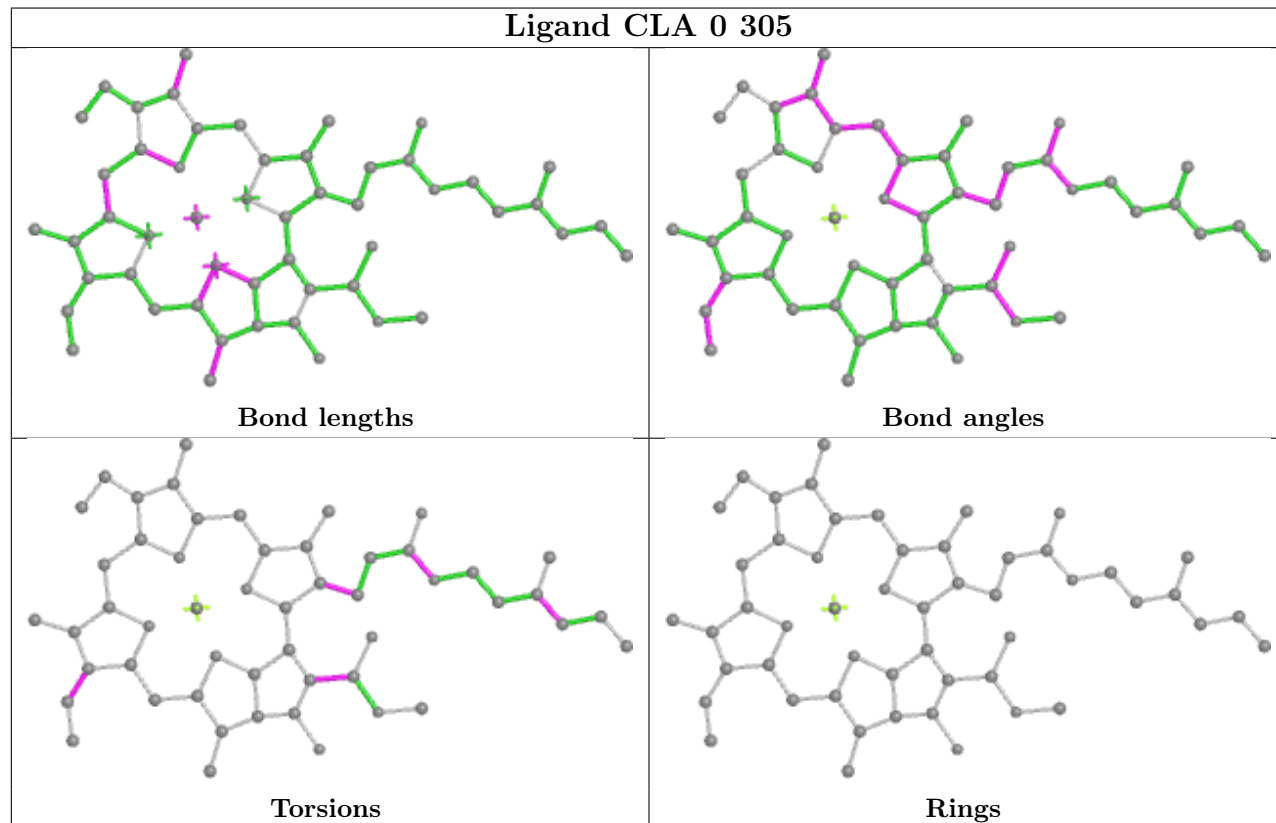




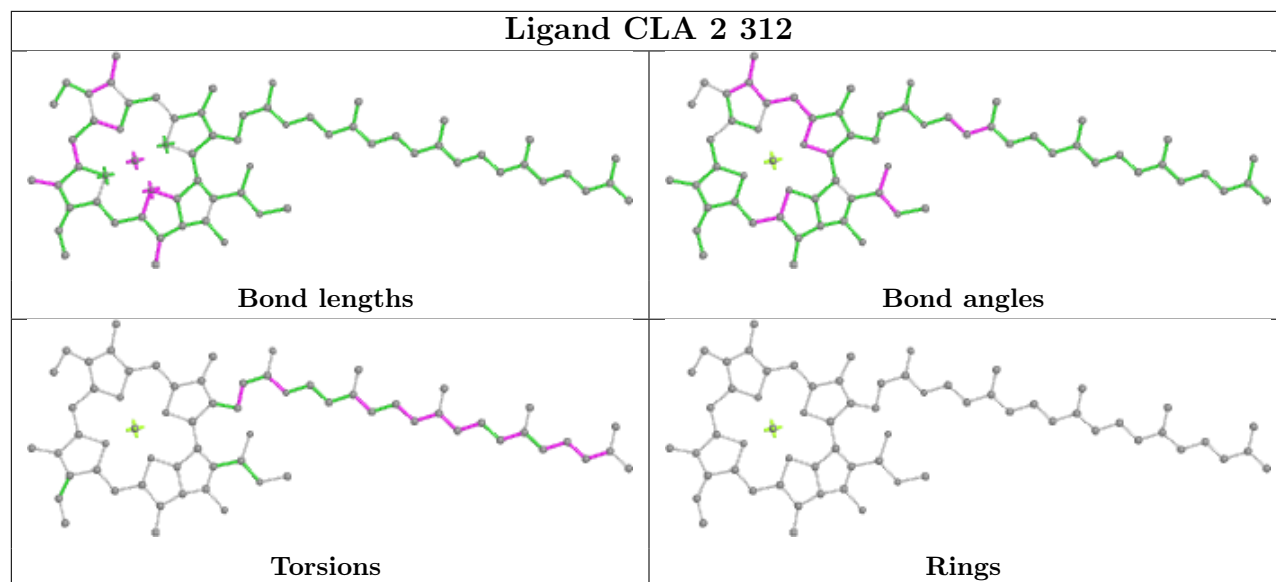
Ligand CLA 8 311



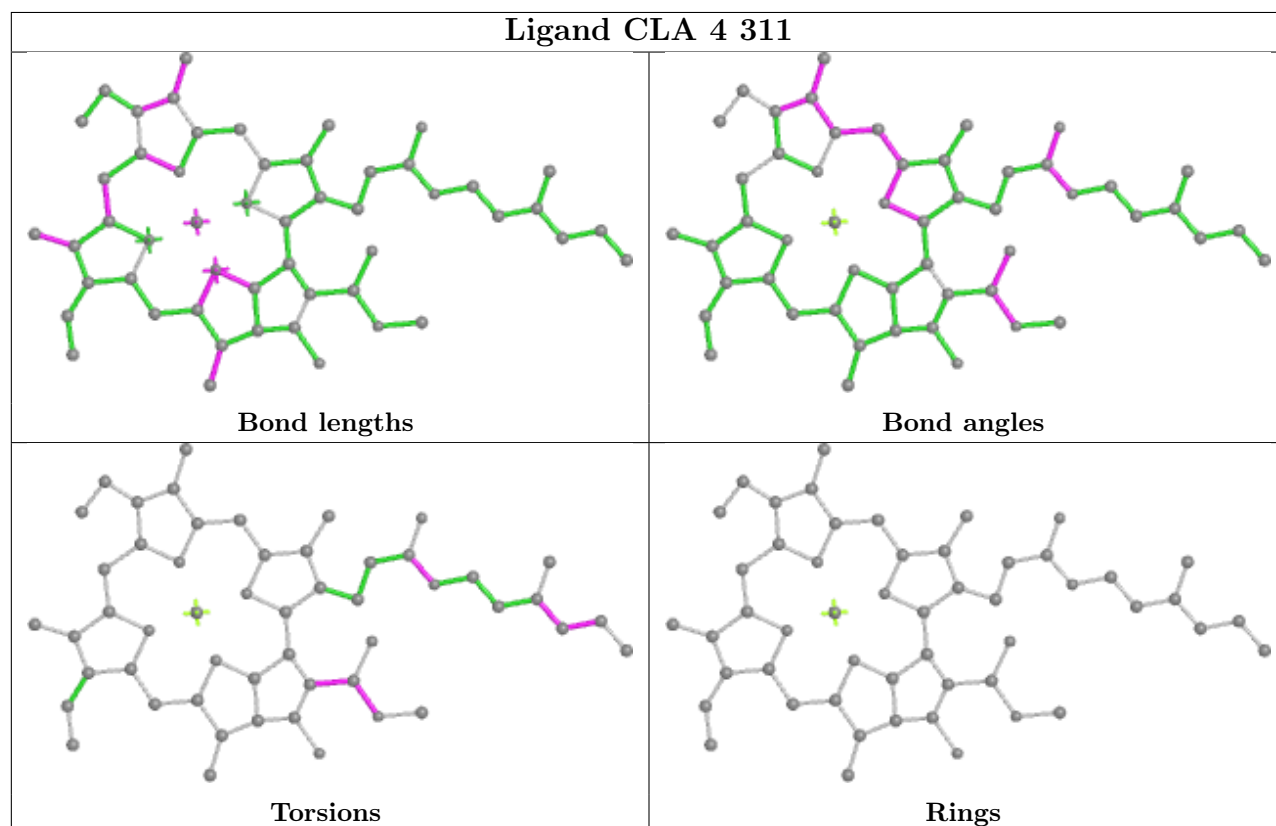
Ligand CLA 0 305



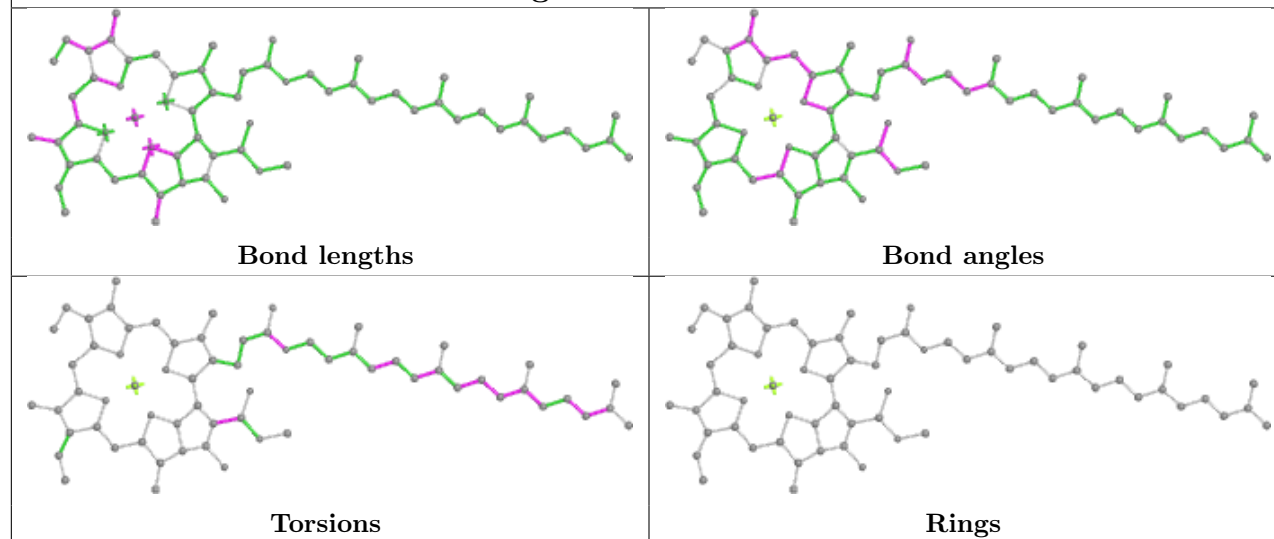
Ligand CLA 2 312



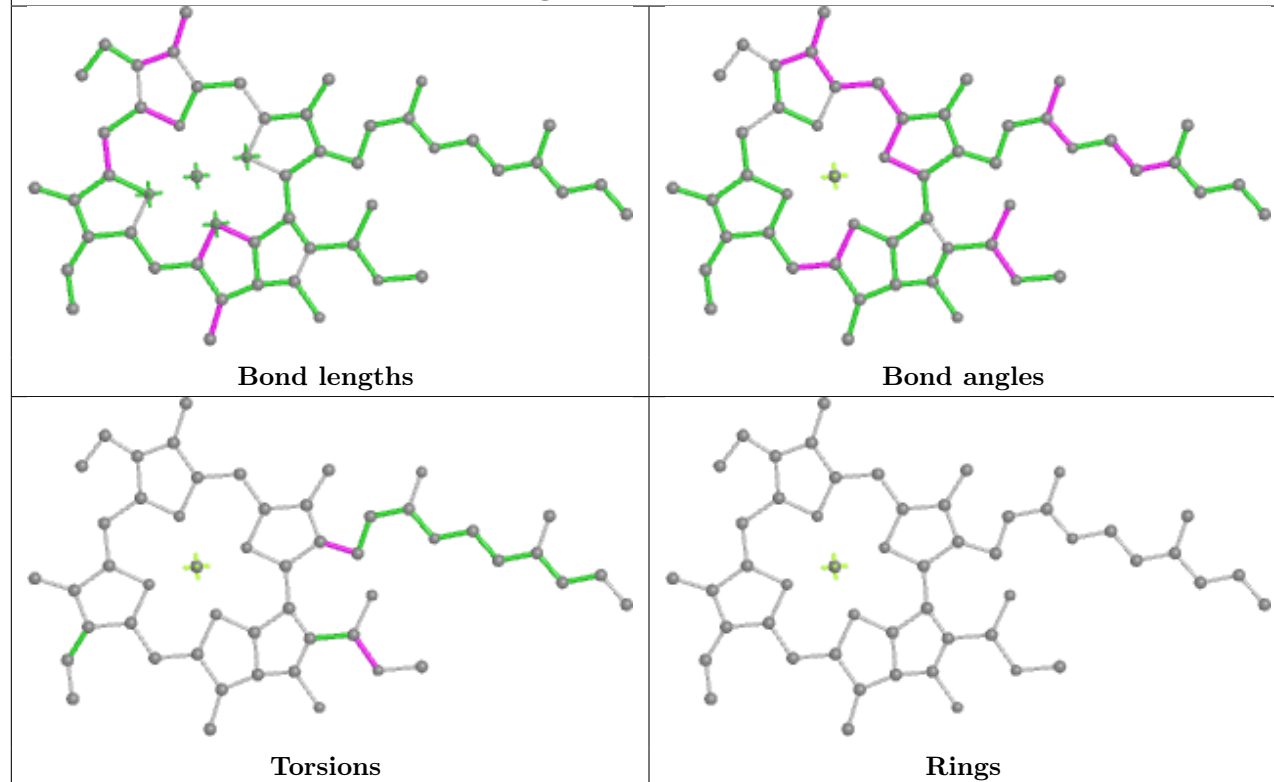
Ligand CLA 4 311

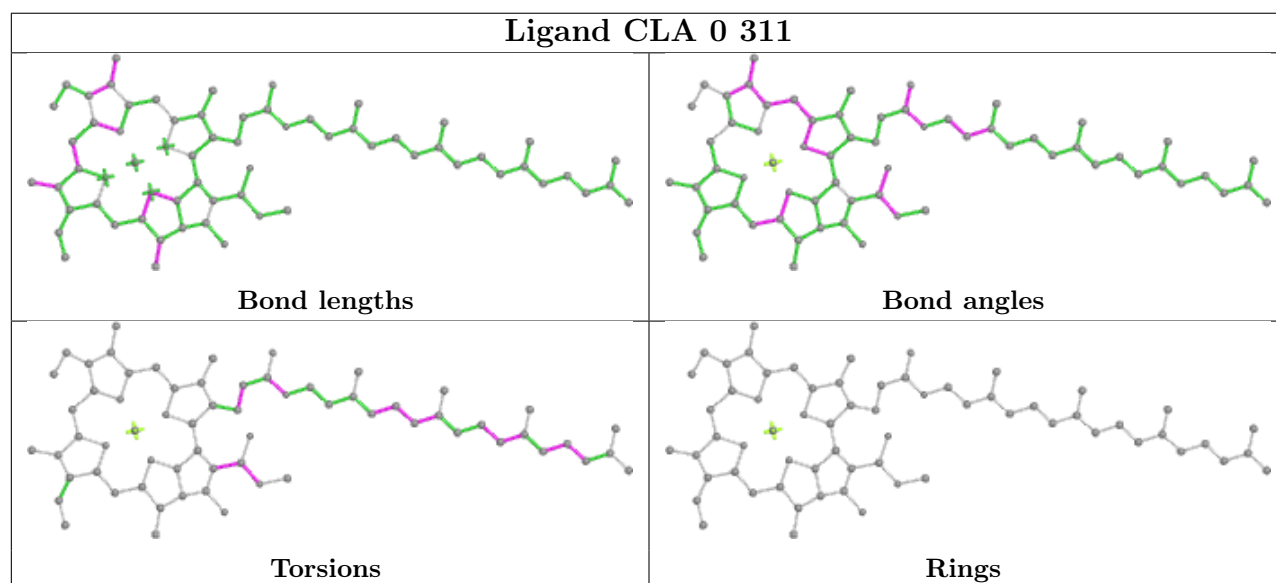
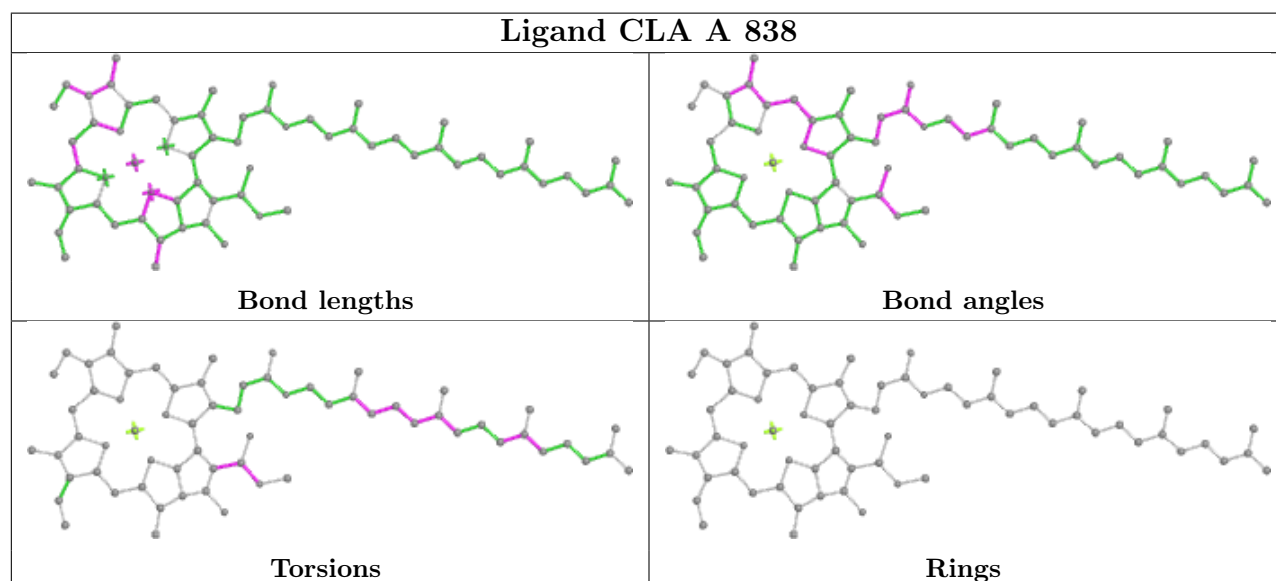
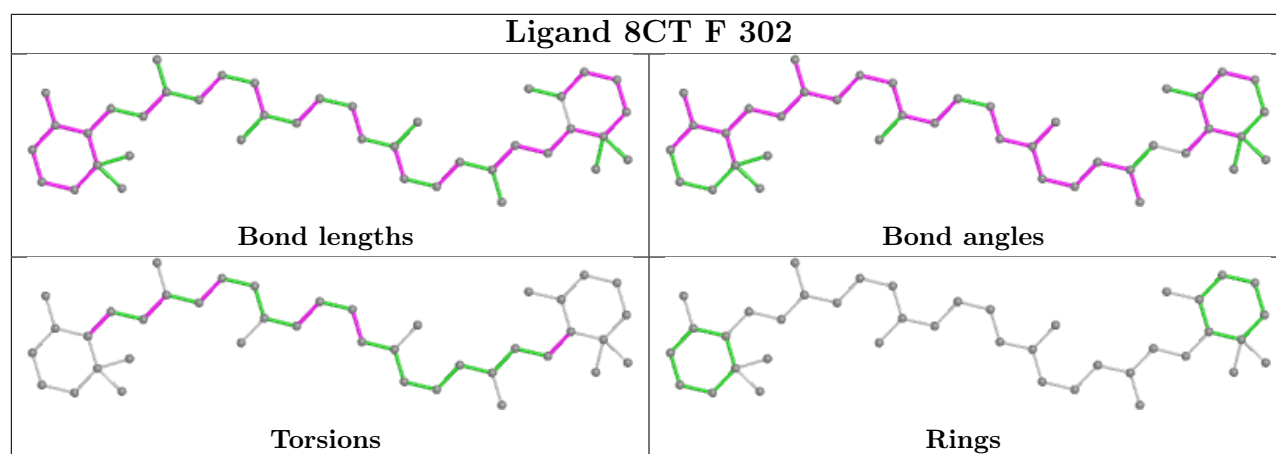


Ligand CLA A 827

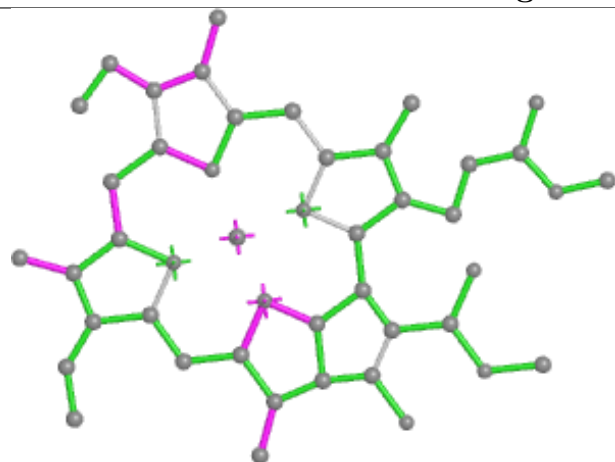


Ligand CLA 9 311

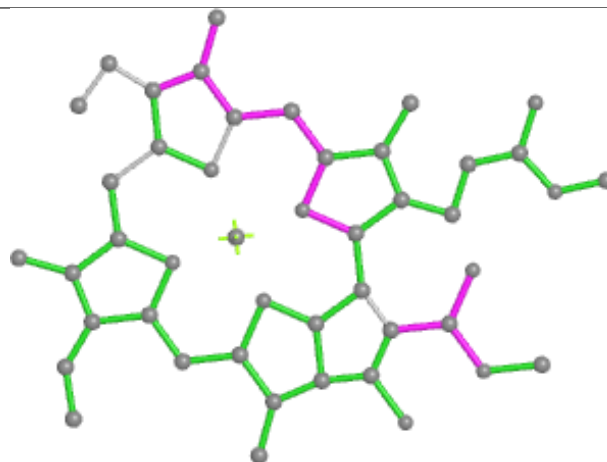




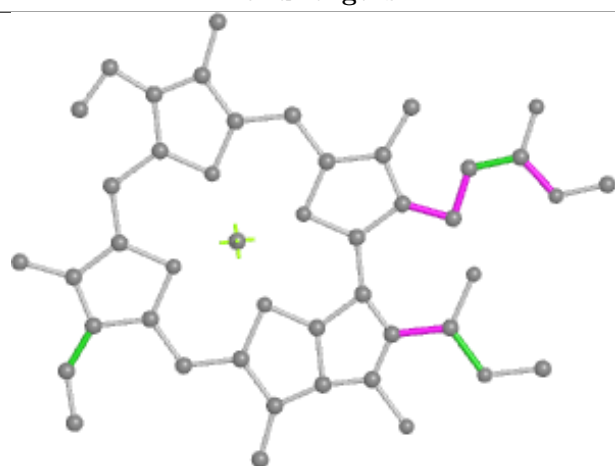
Ligand CLA B 822



Bond lengths



Bond angles

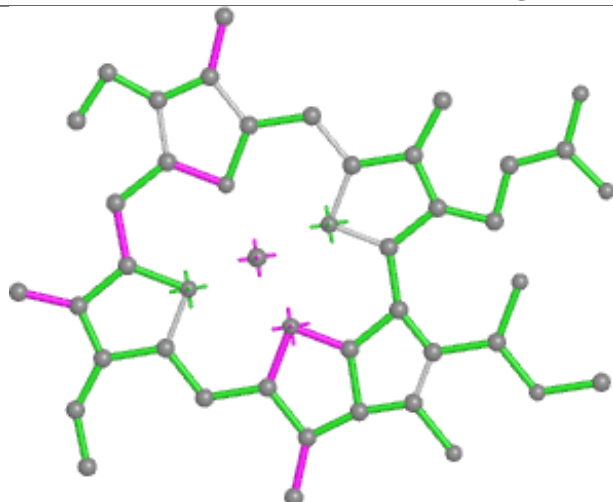


Torsions

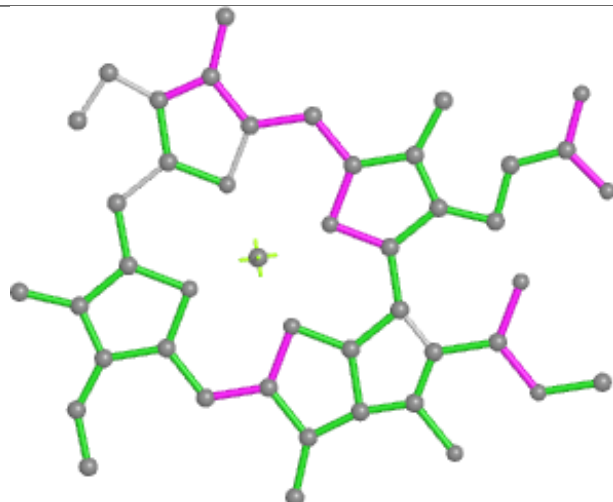


Rings

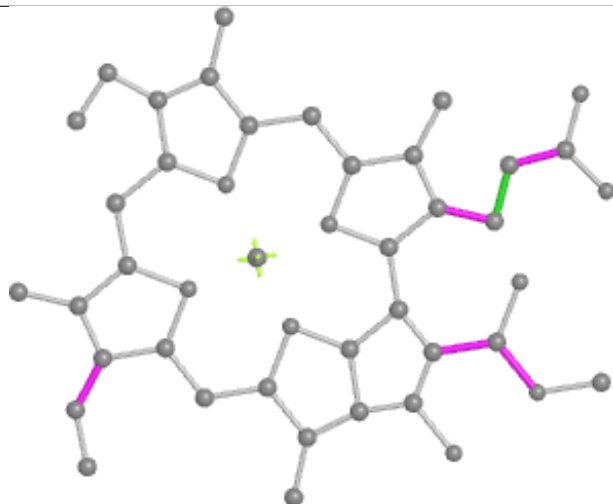
Ligand CLA K 101



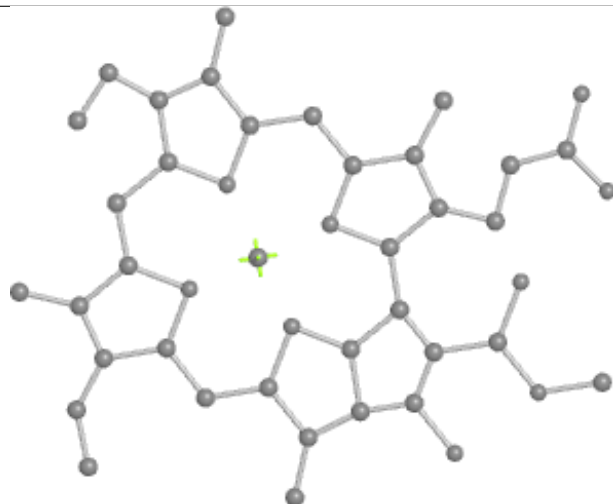
Bond lengths



Bond angles

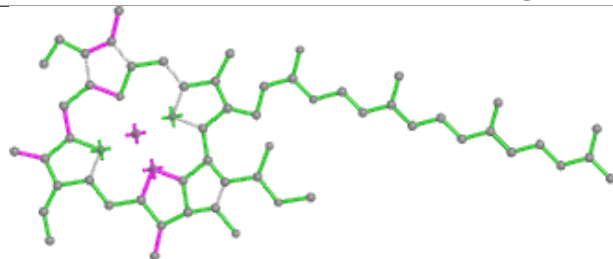


Torsions

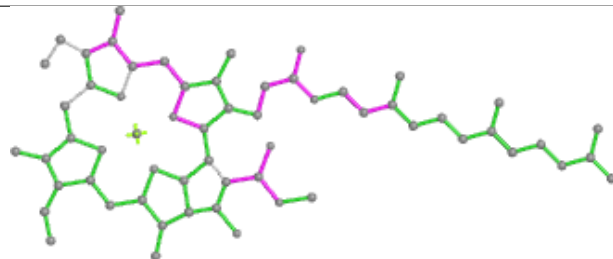


Rings

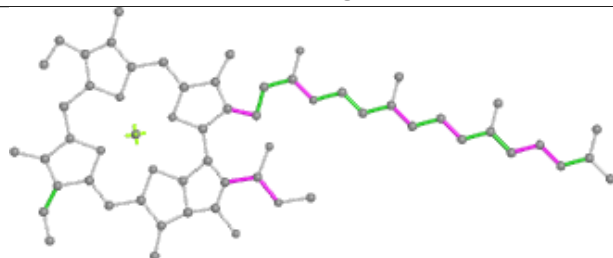
Ligand CLA 6 310



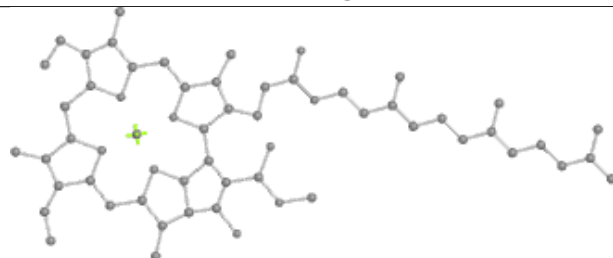
Bond lengths



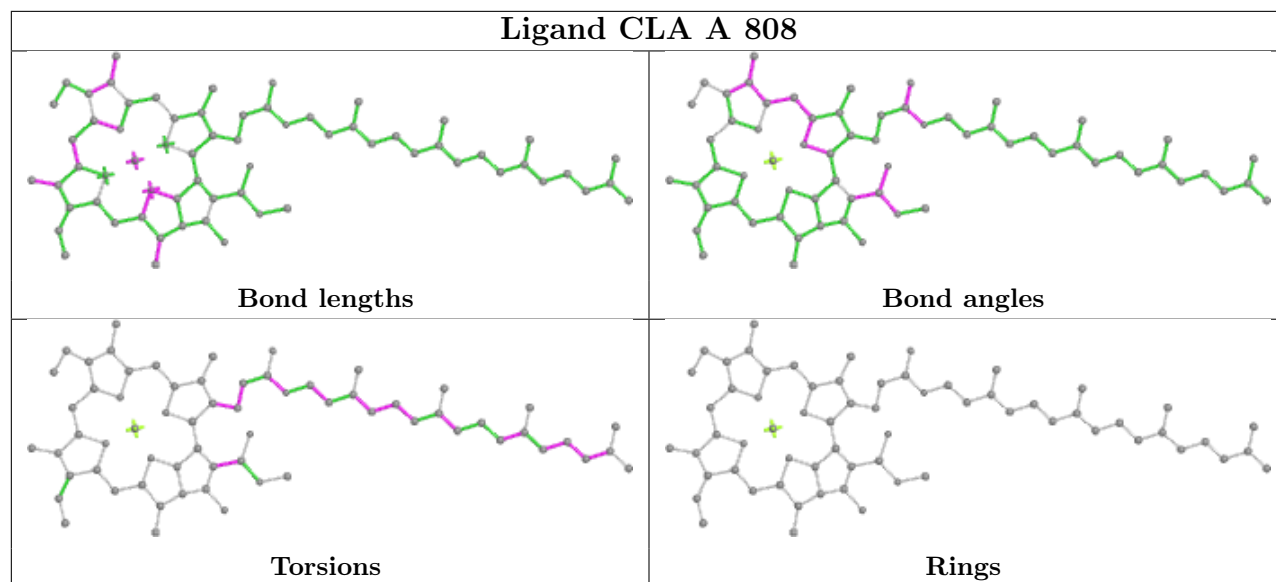
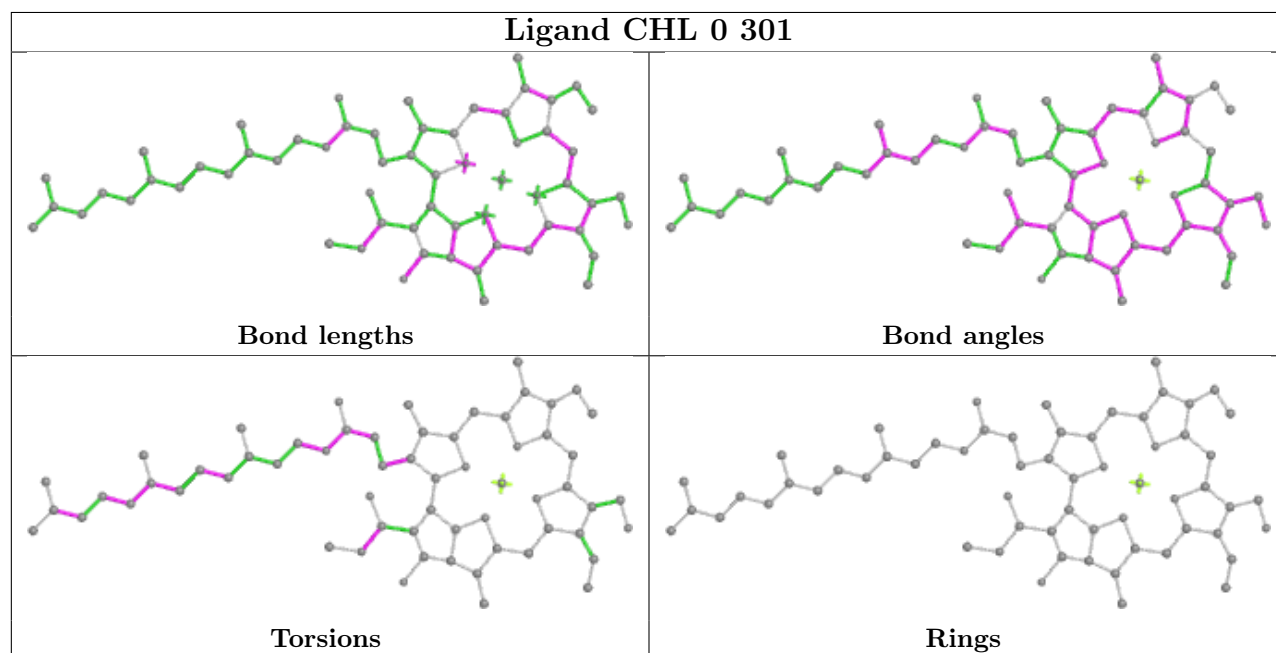
Bond angles



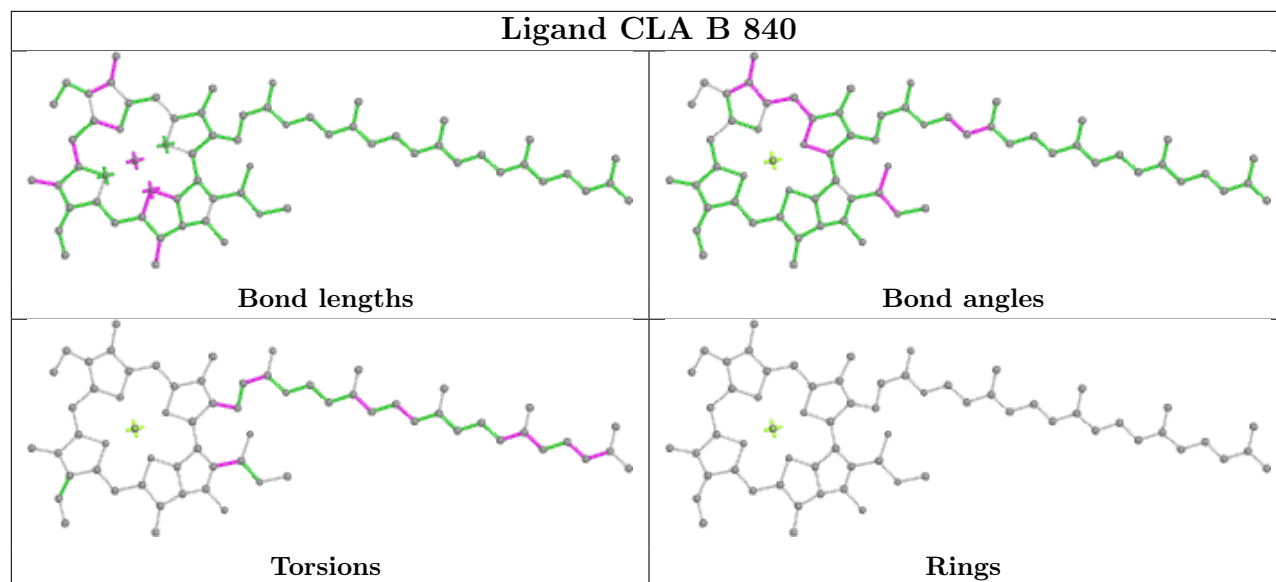
Torsions



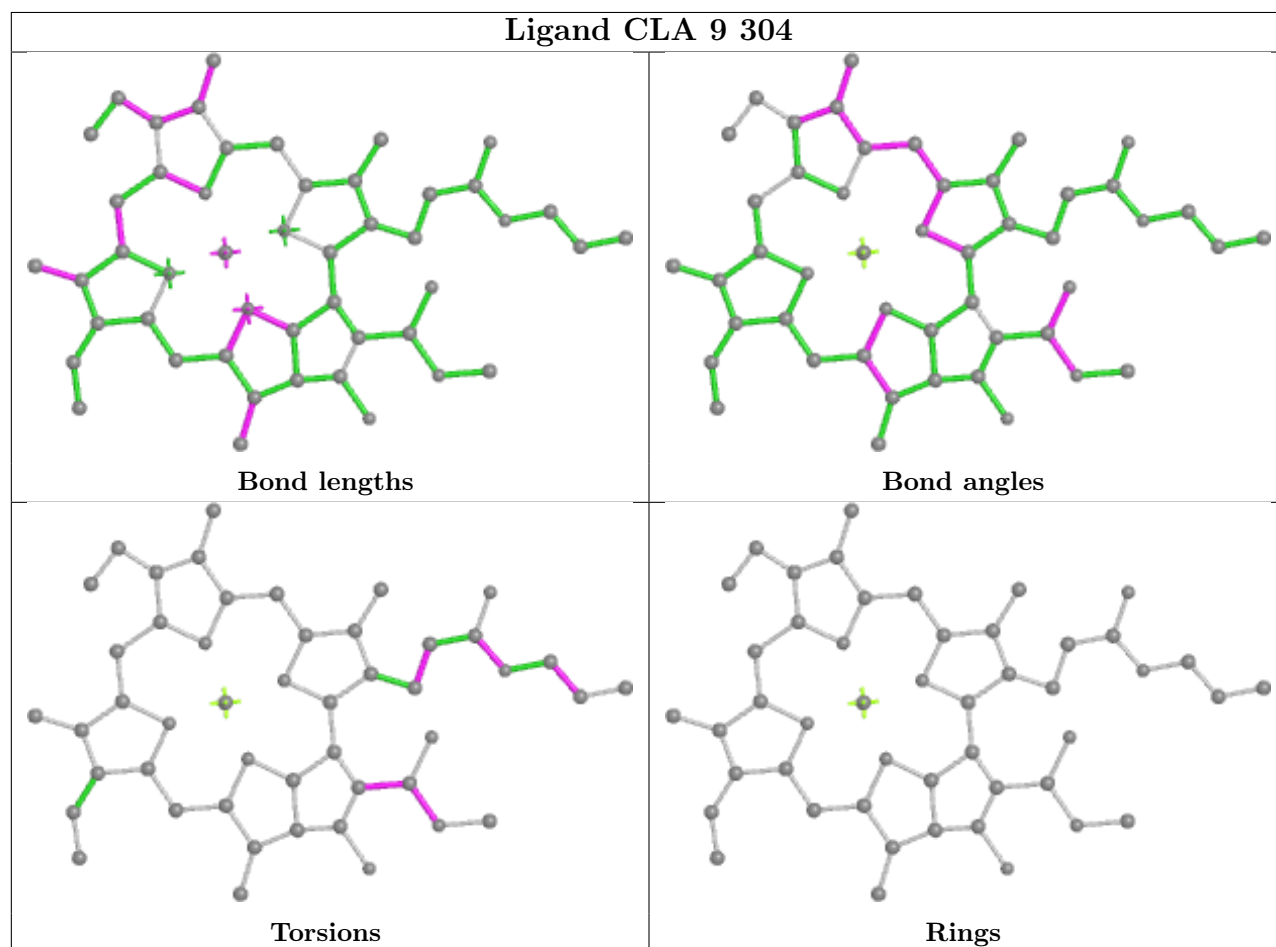
Rings

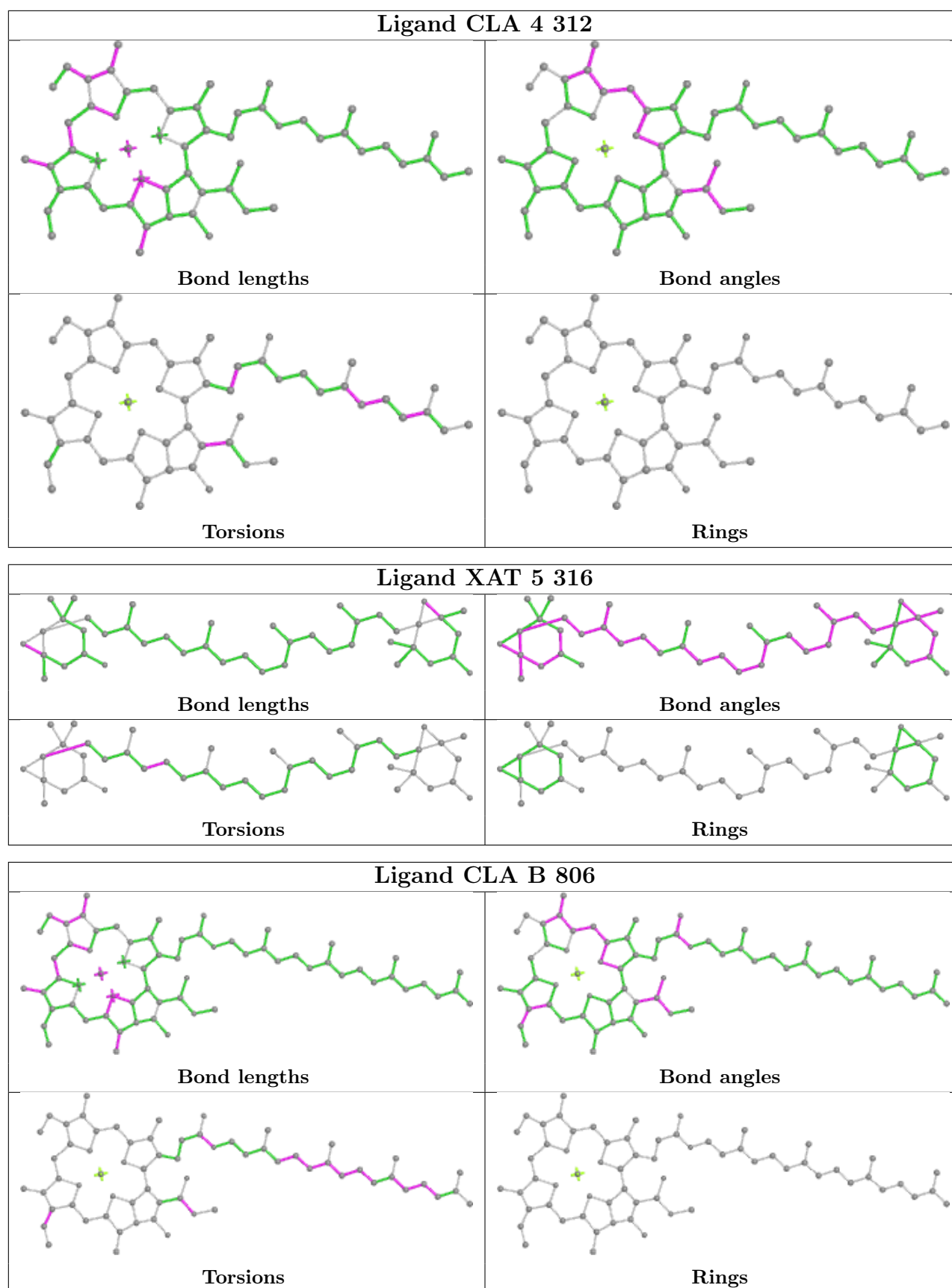
Ligand CLA A 808**Ligand CHL 0 301**

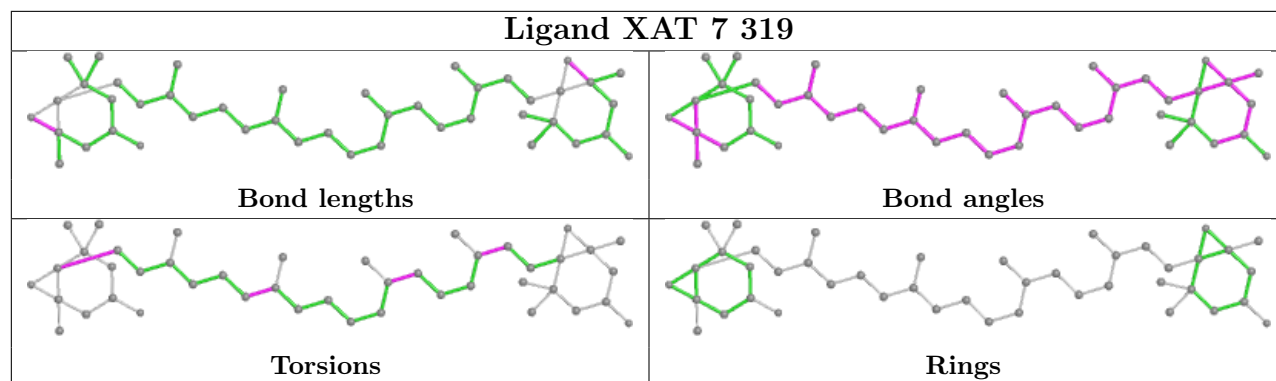
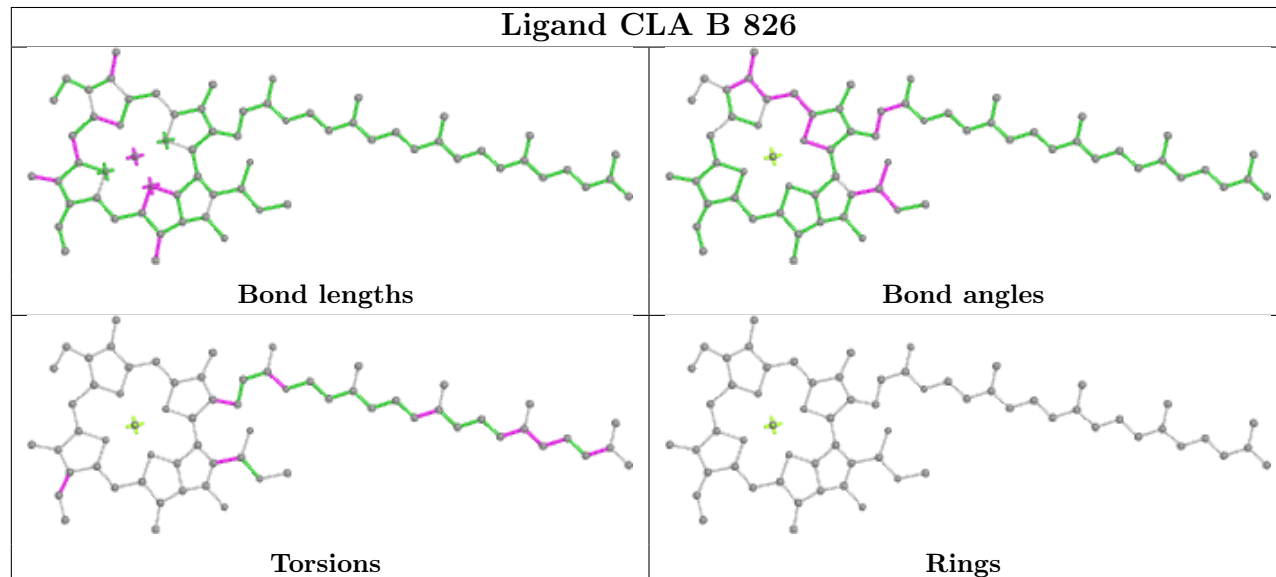
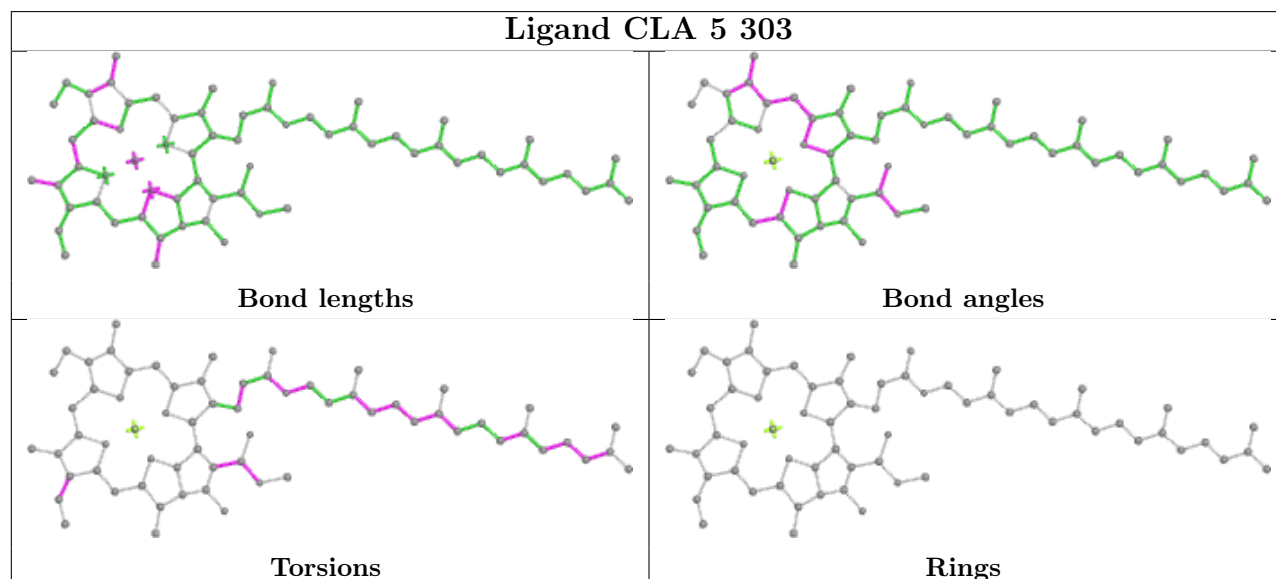
Ligand CLA B 840

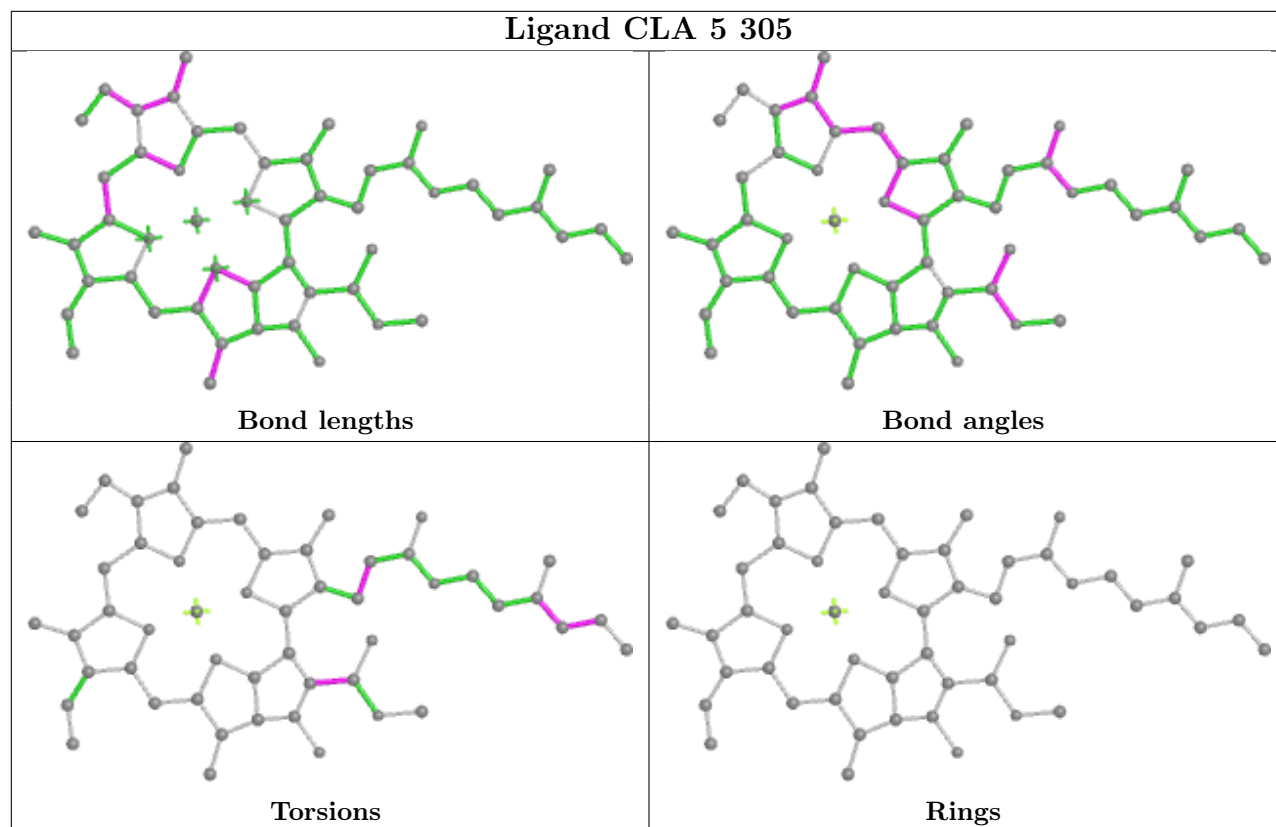


Ligand CLA 9 304

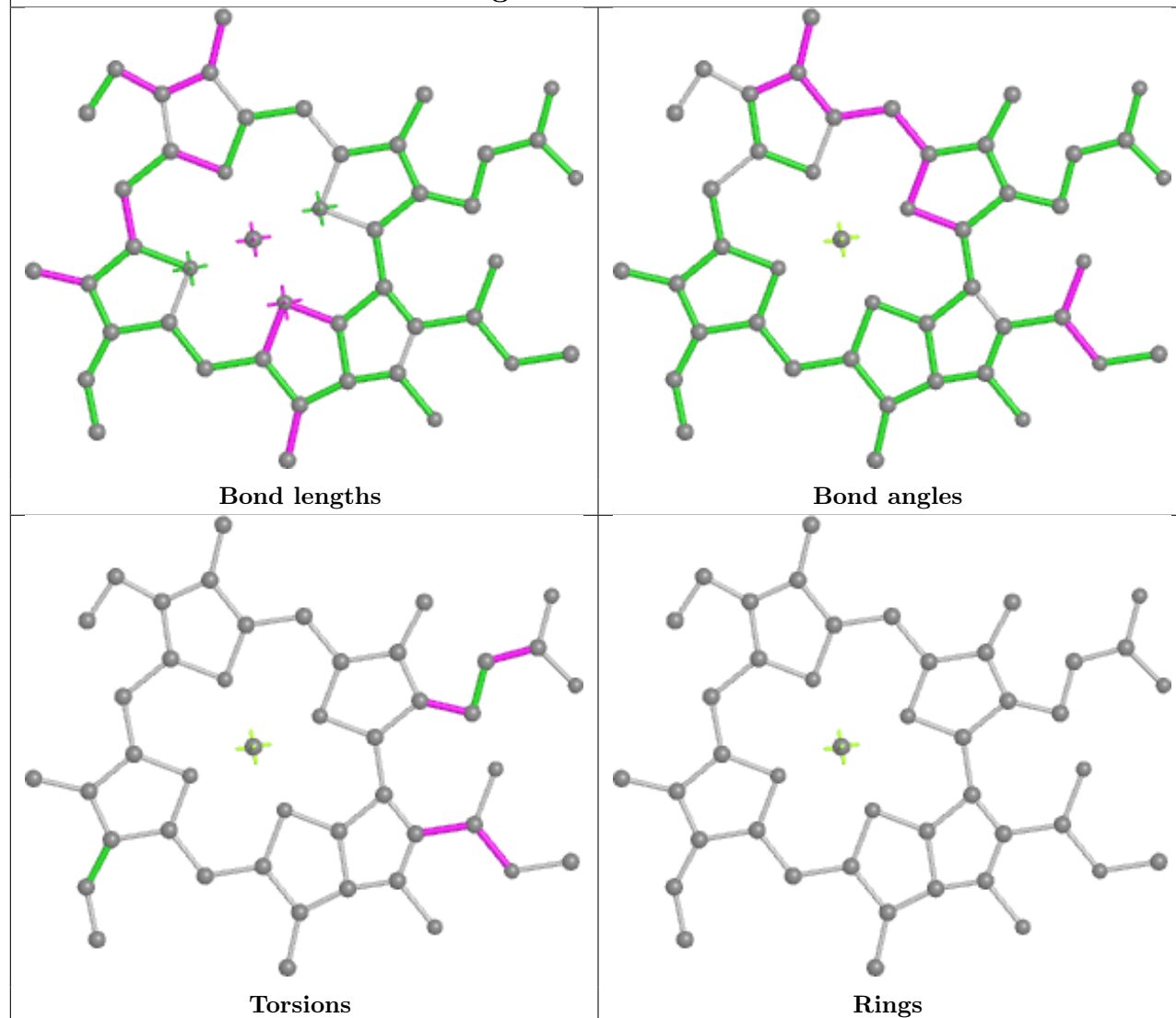




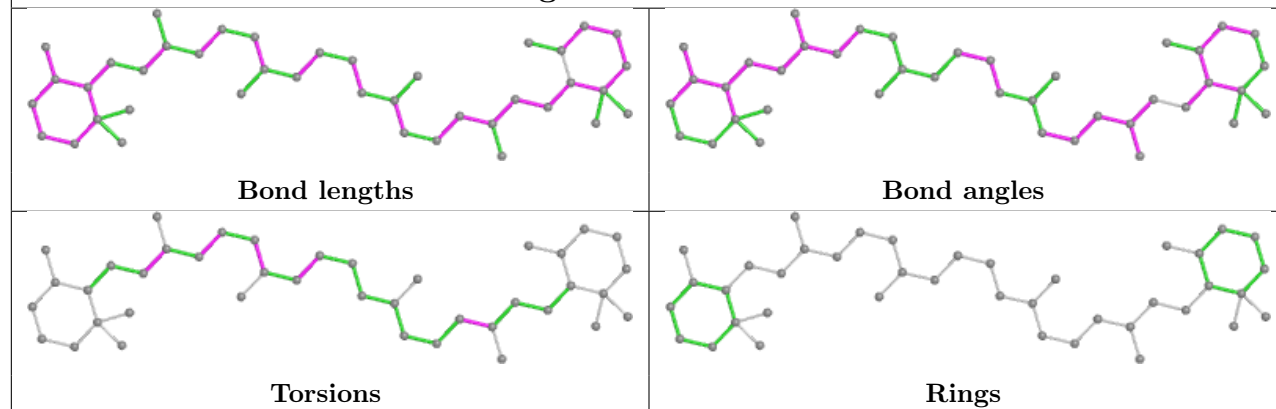
Ligand XAT 7 319**Ligand CLA B 826****Ligand CLA 5 303**

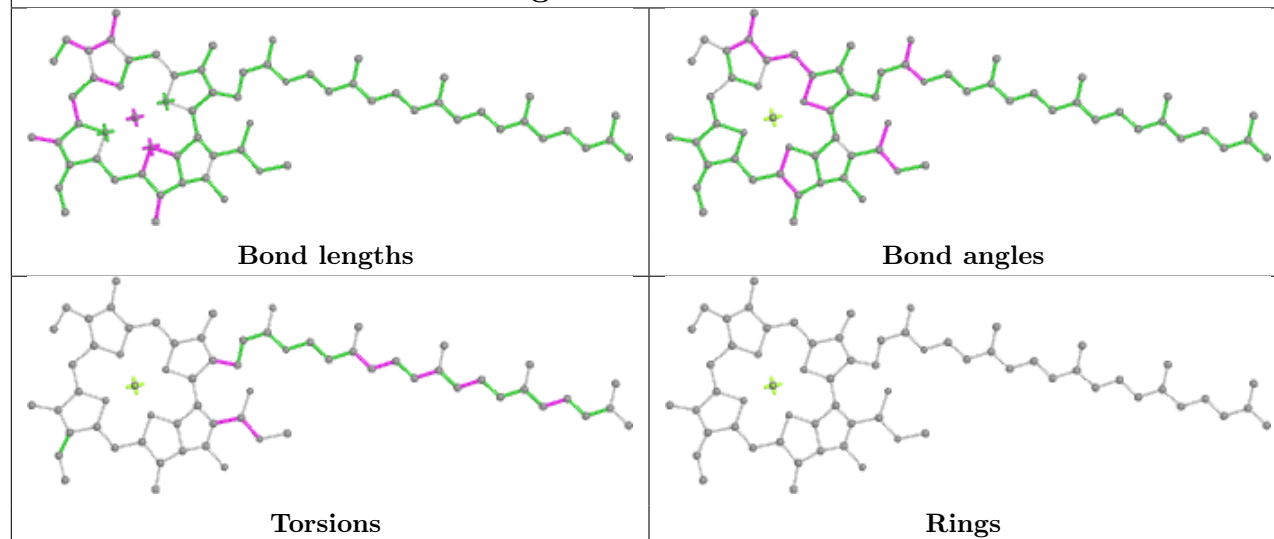
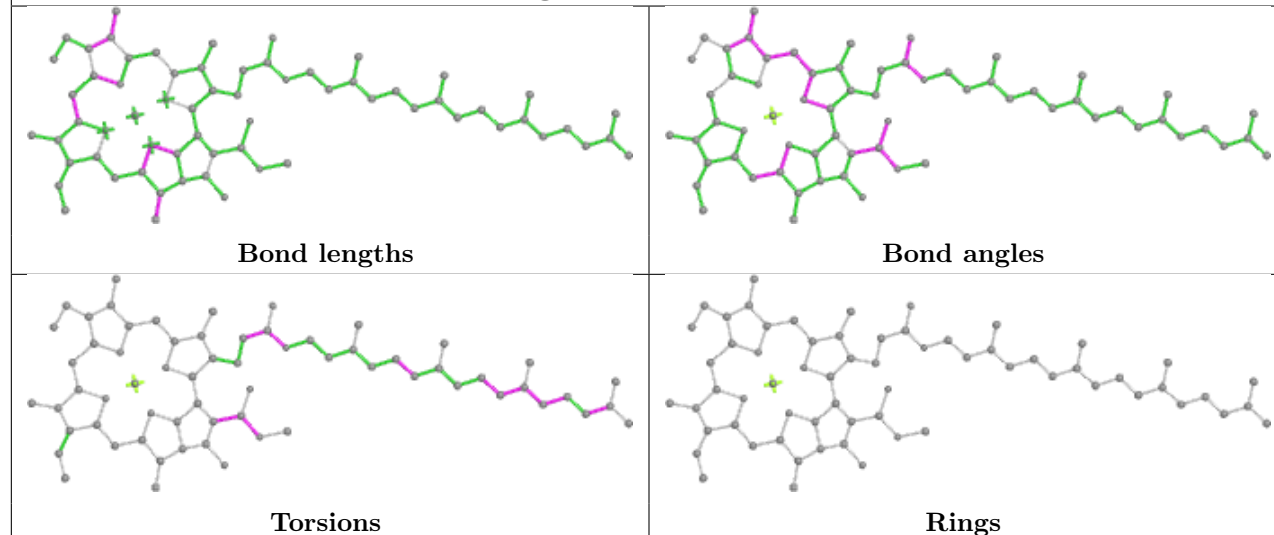
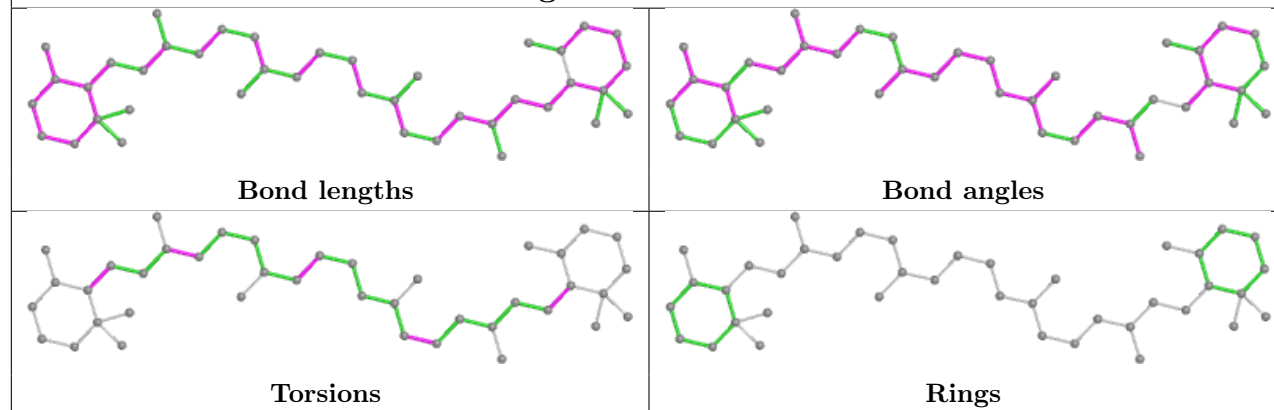


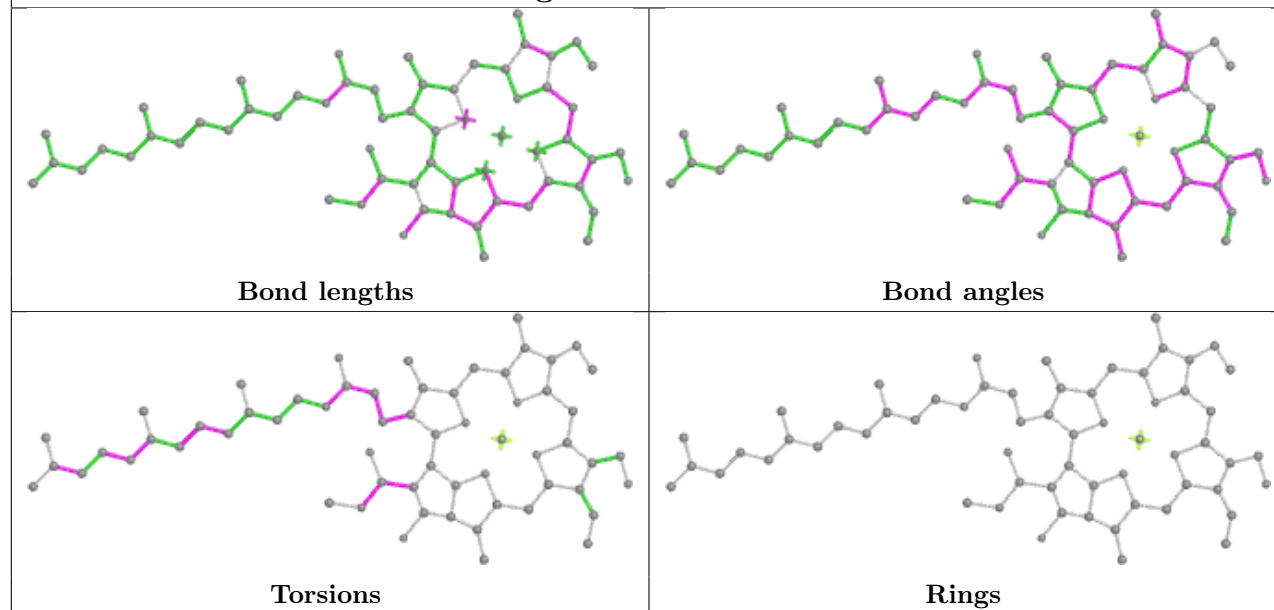
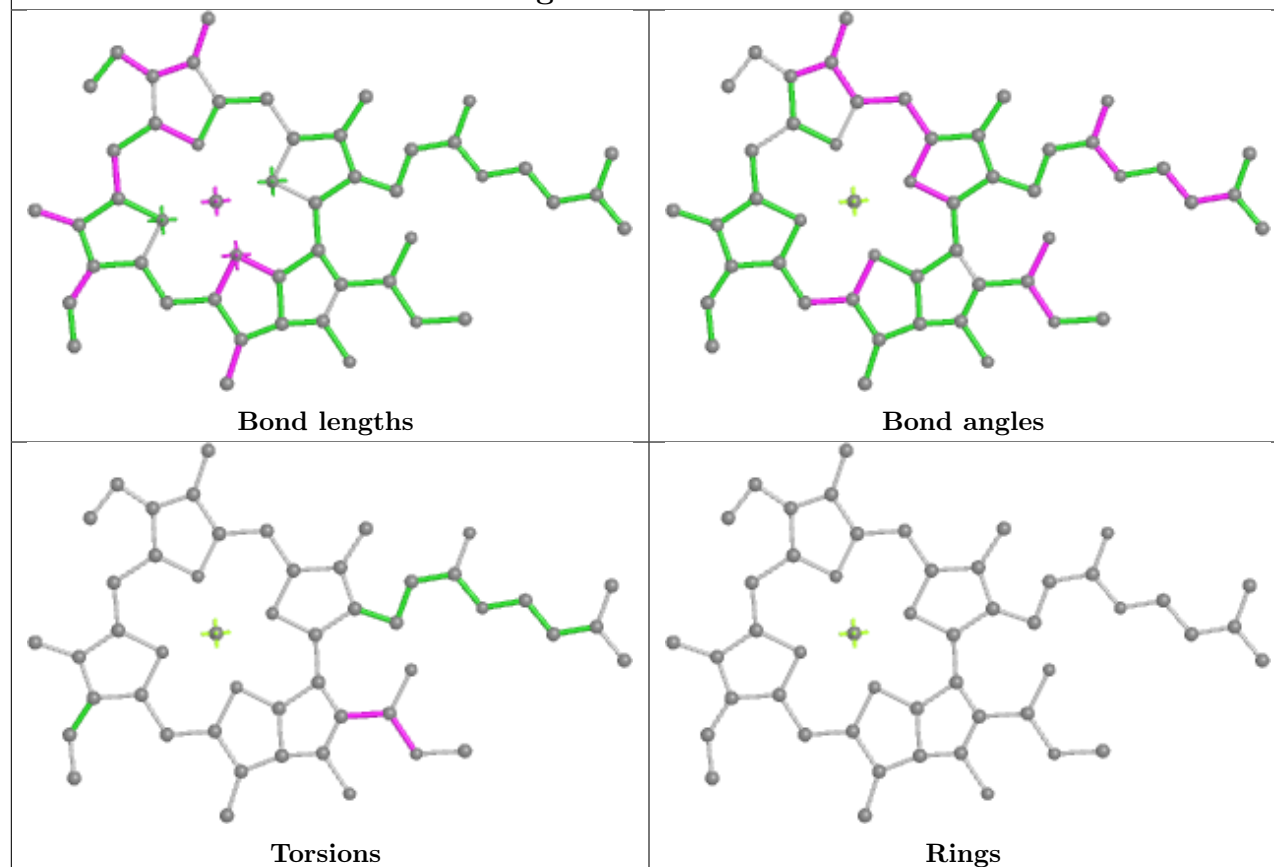
Ligand CLA F 301

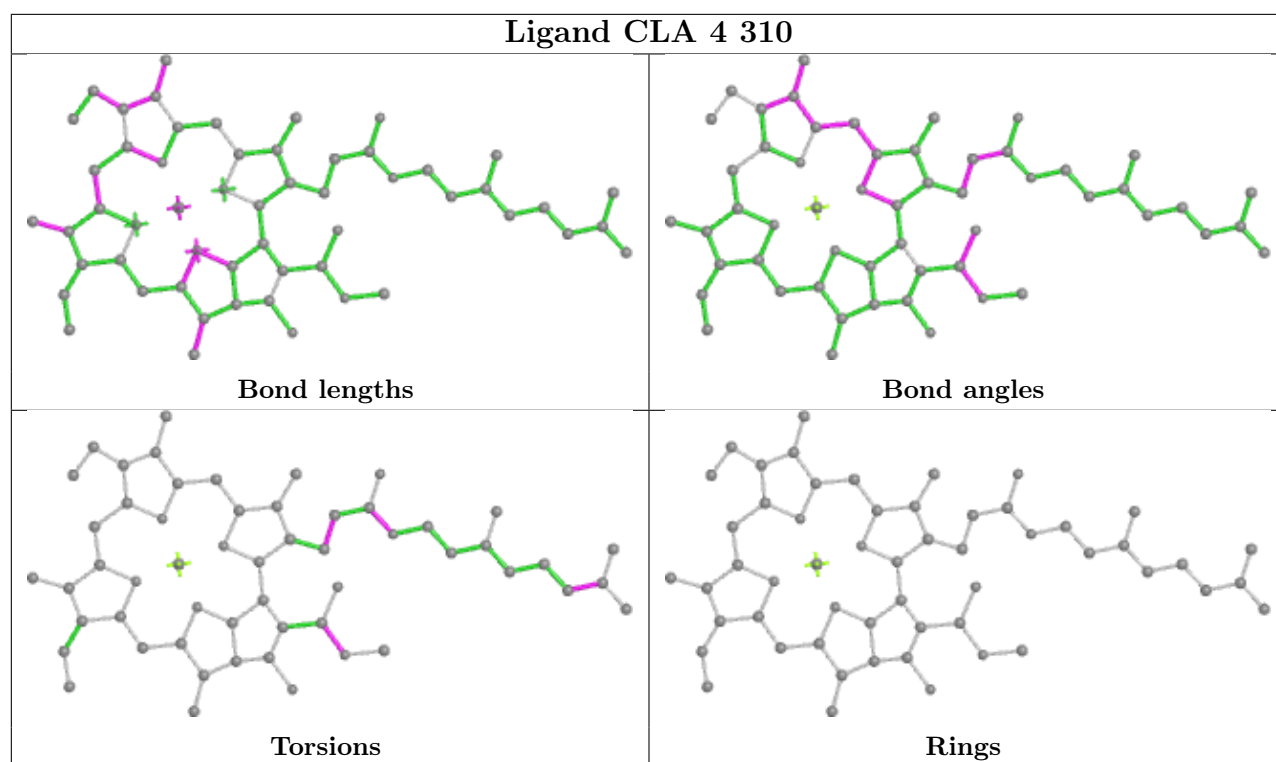


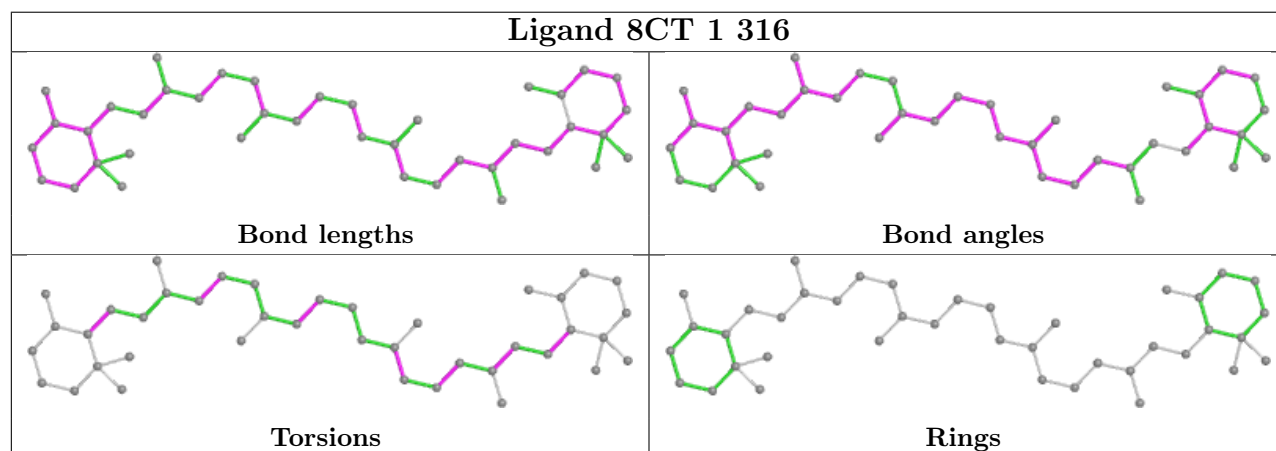
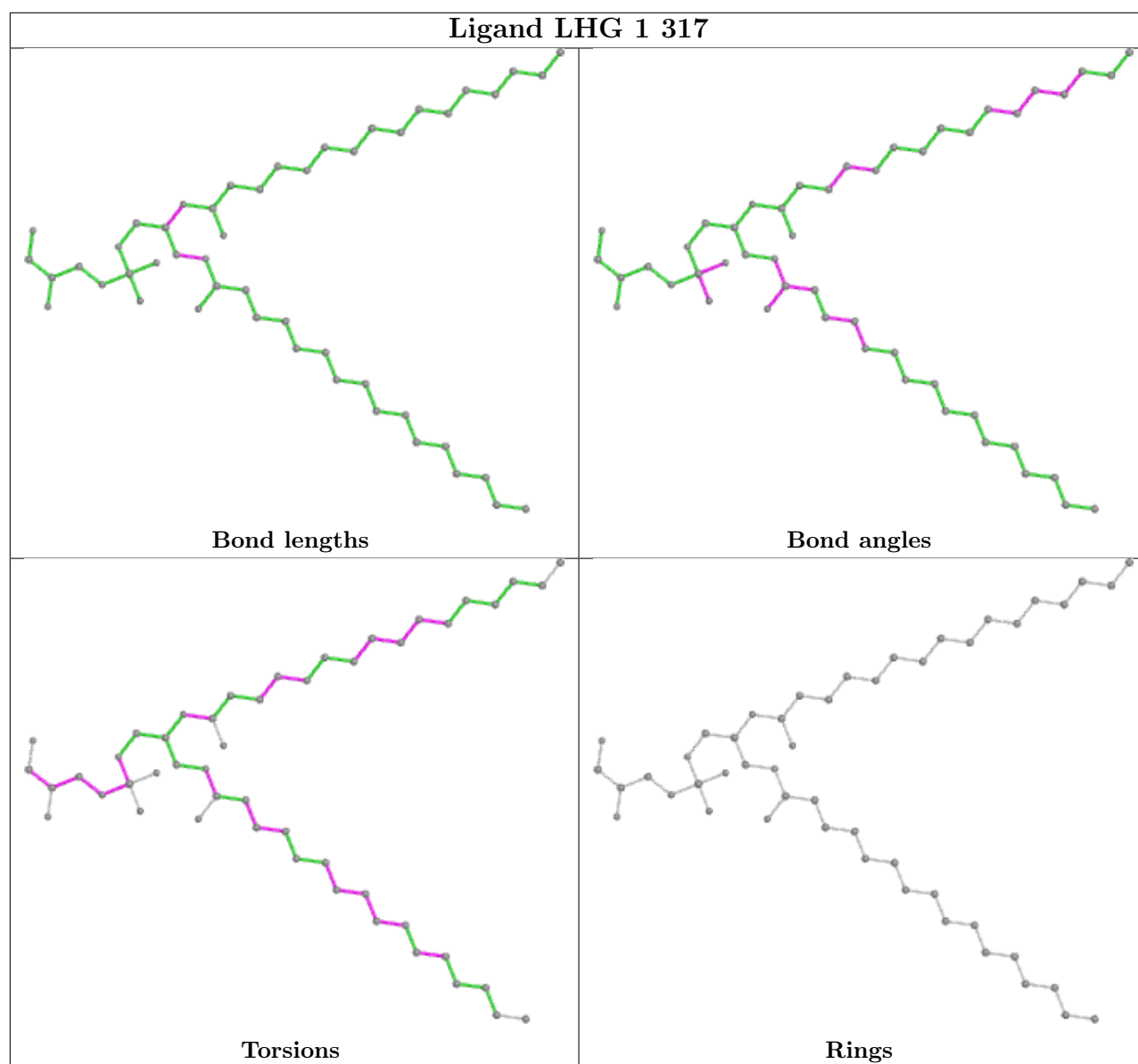
Ligand 8CT 4 317



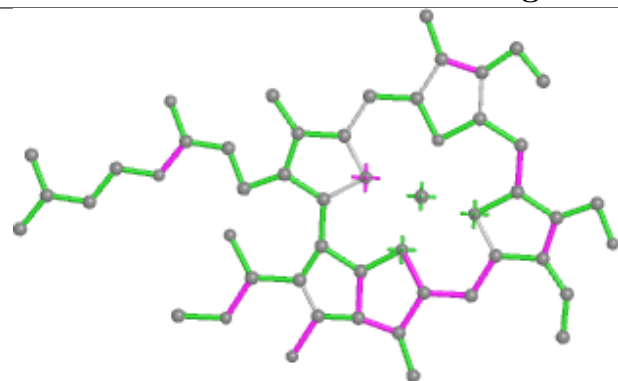
Ligand CLA A 833**Ligand CLA 5 307****Ligand 8CT J 104**

Ligand CHL 5 301**Ligand CLA 3 308**

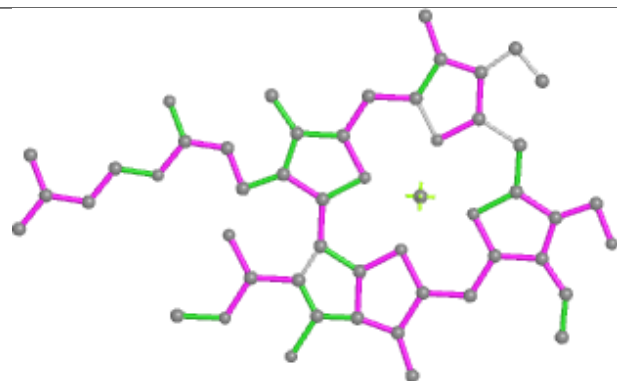




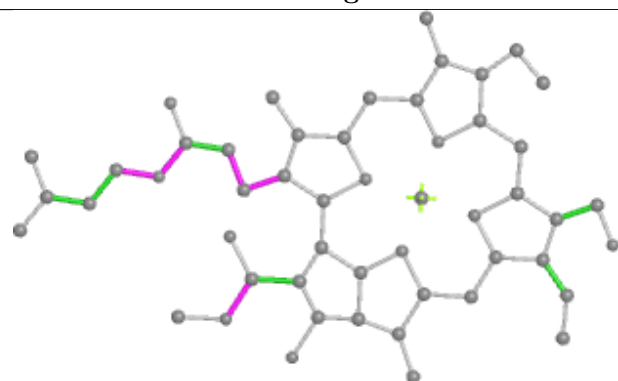
Ligand CHL 8 307



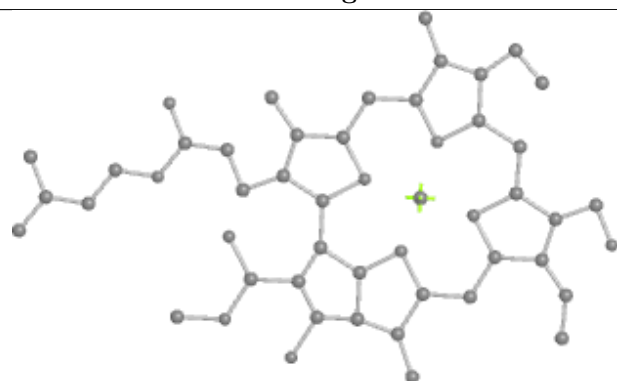
Bond lengths



Bond angles

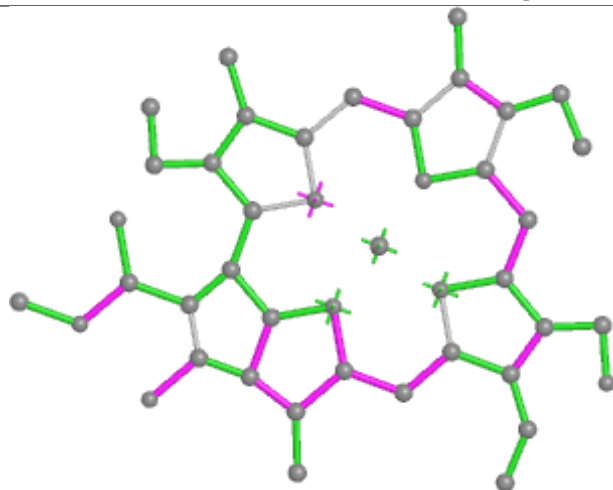


Torsions

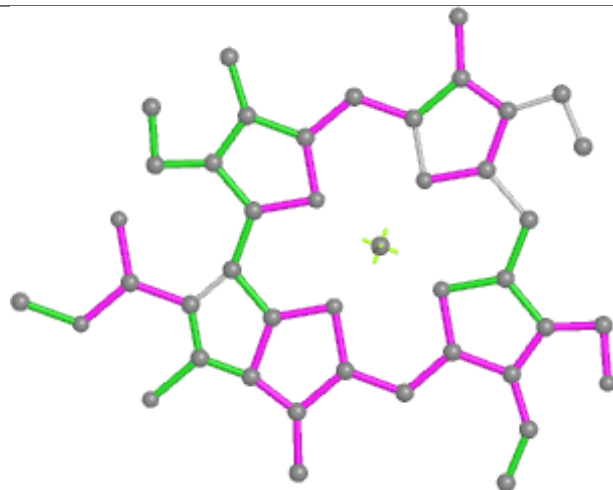


Rings

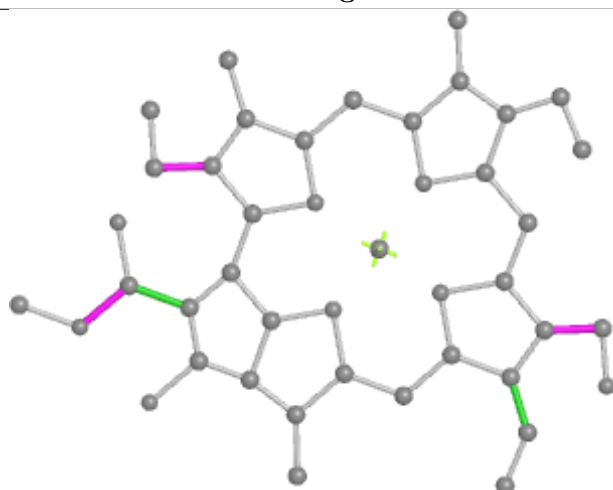
Ligand CHL 6 307



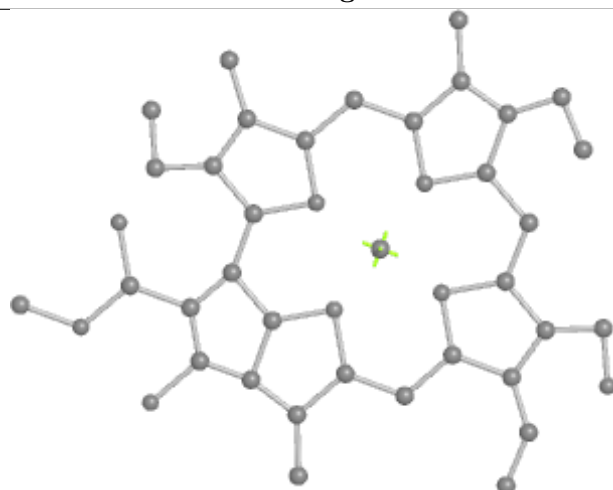
Bond lengths



Bond angles

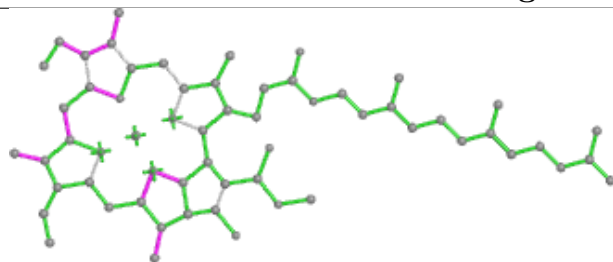


Torsions

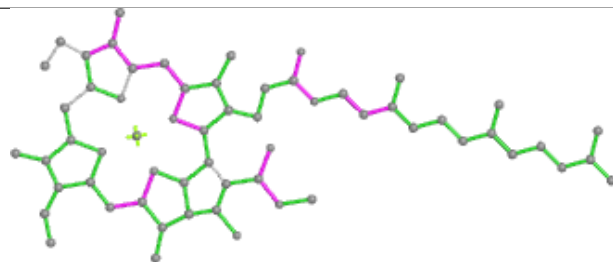


Rings

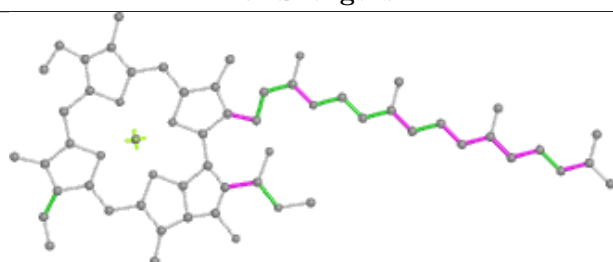
Ligand CLA 9 309



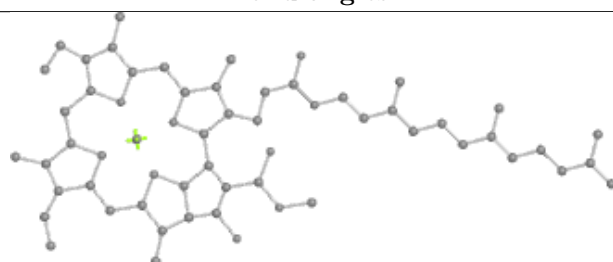
Bond lengths



Bond angles

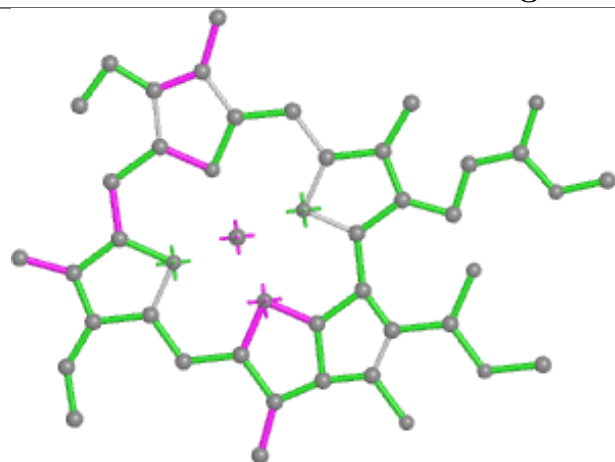


Torsions

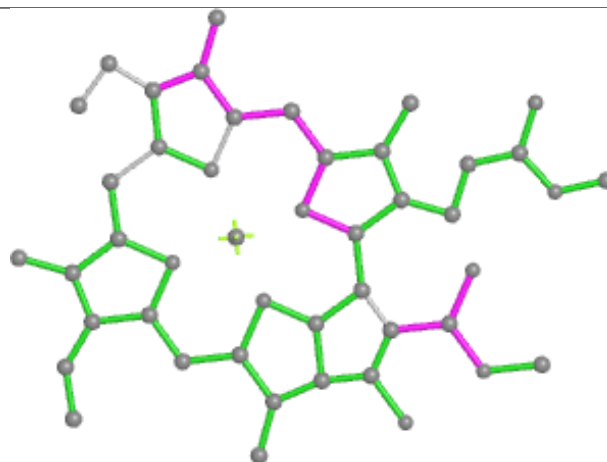


Rings

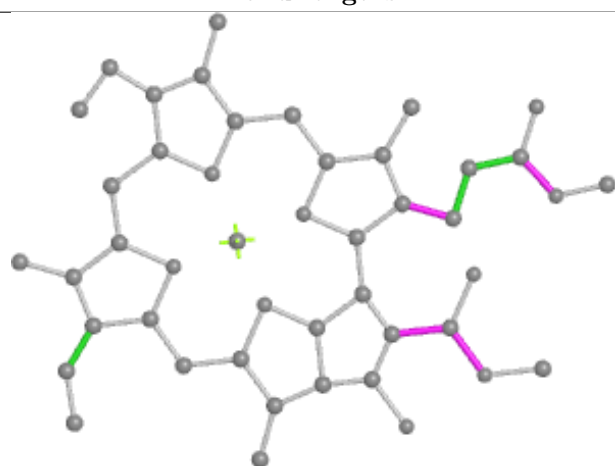
Ligand CLA 1 313



Bond lengths



Bond angles

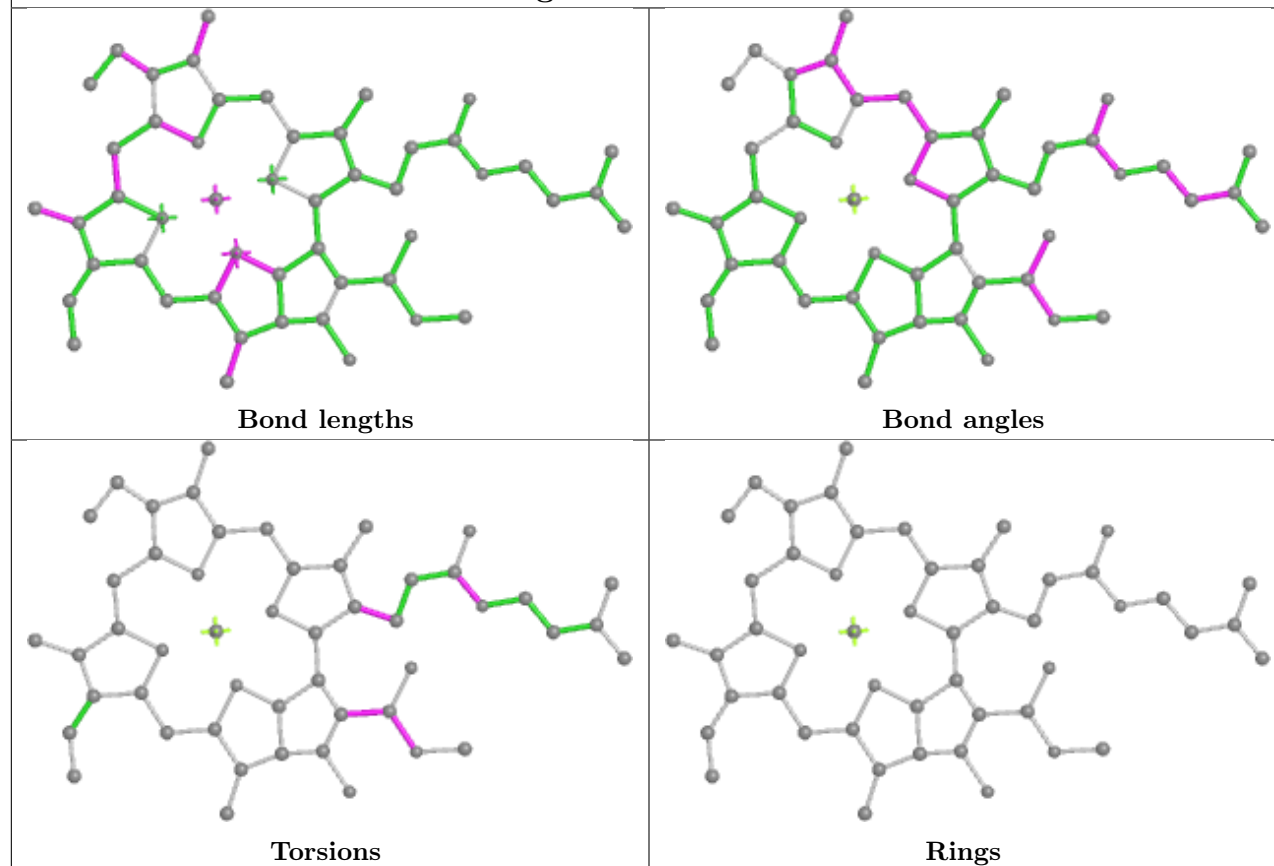


Torsions

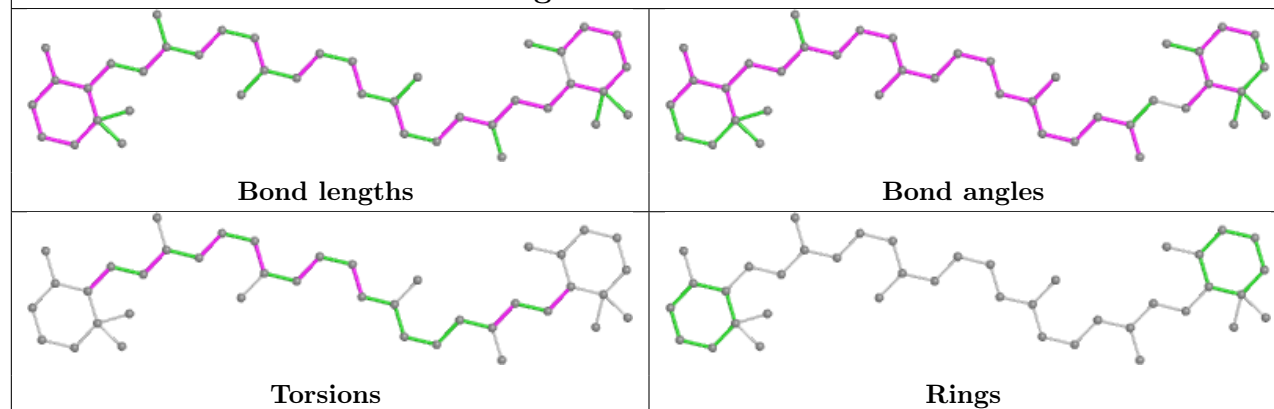


Rings

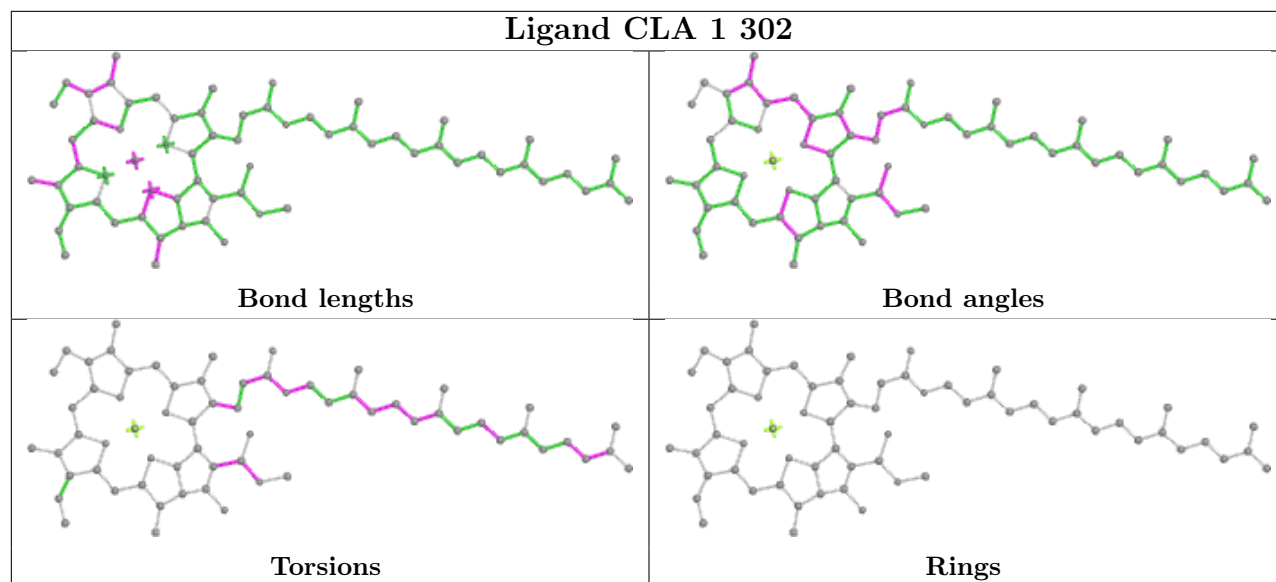
Ligand CLA 7 310



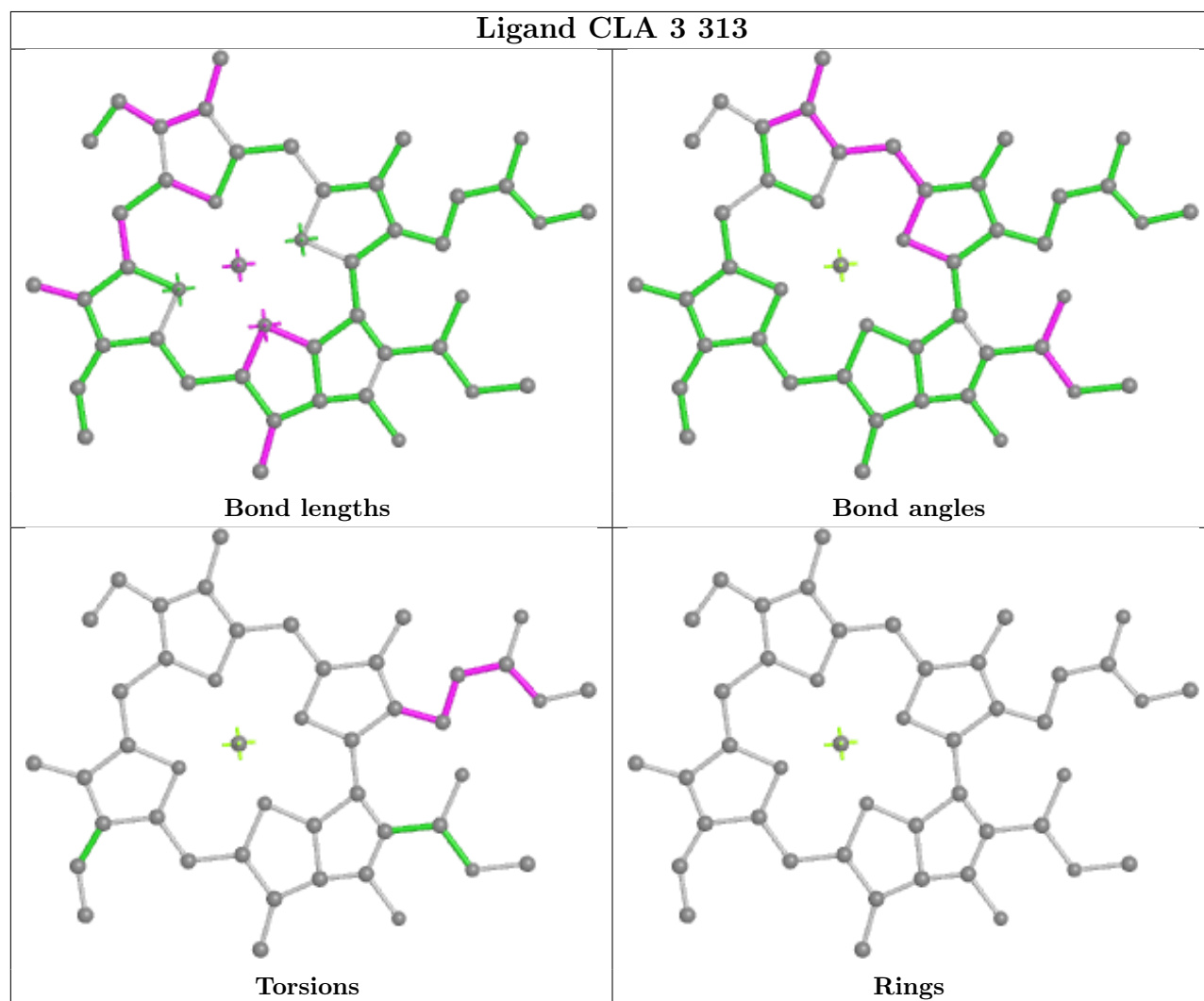
Ligand 8CT G 104



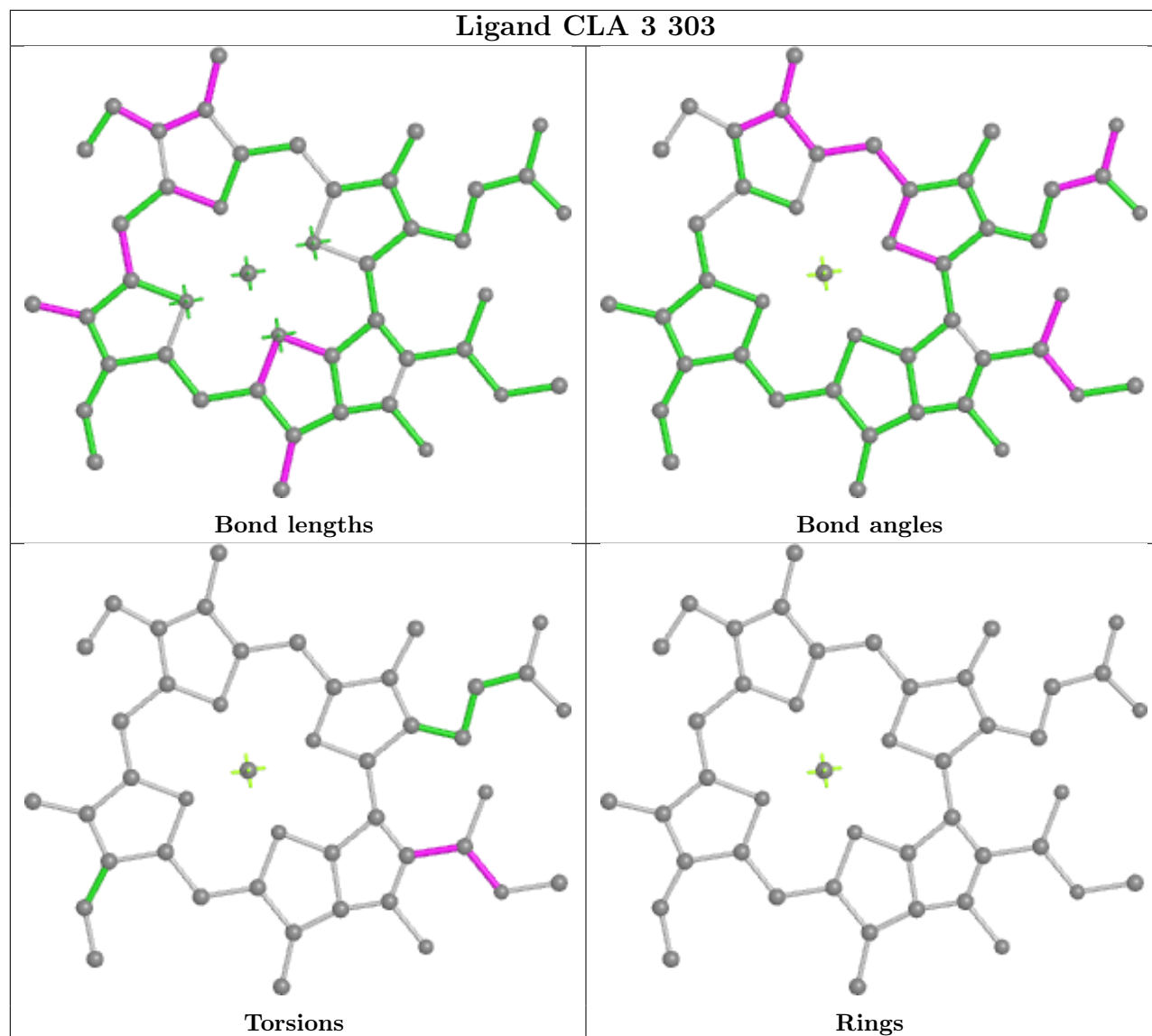
Ligand CLA 1 302

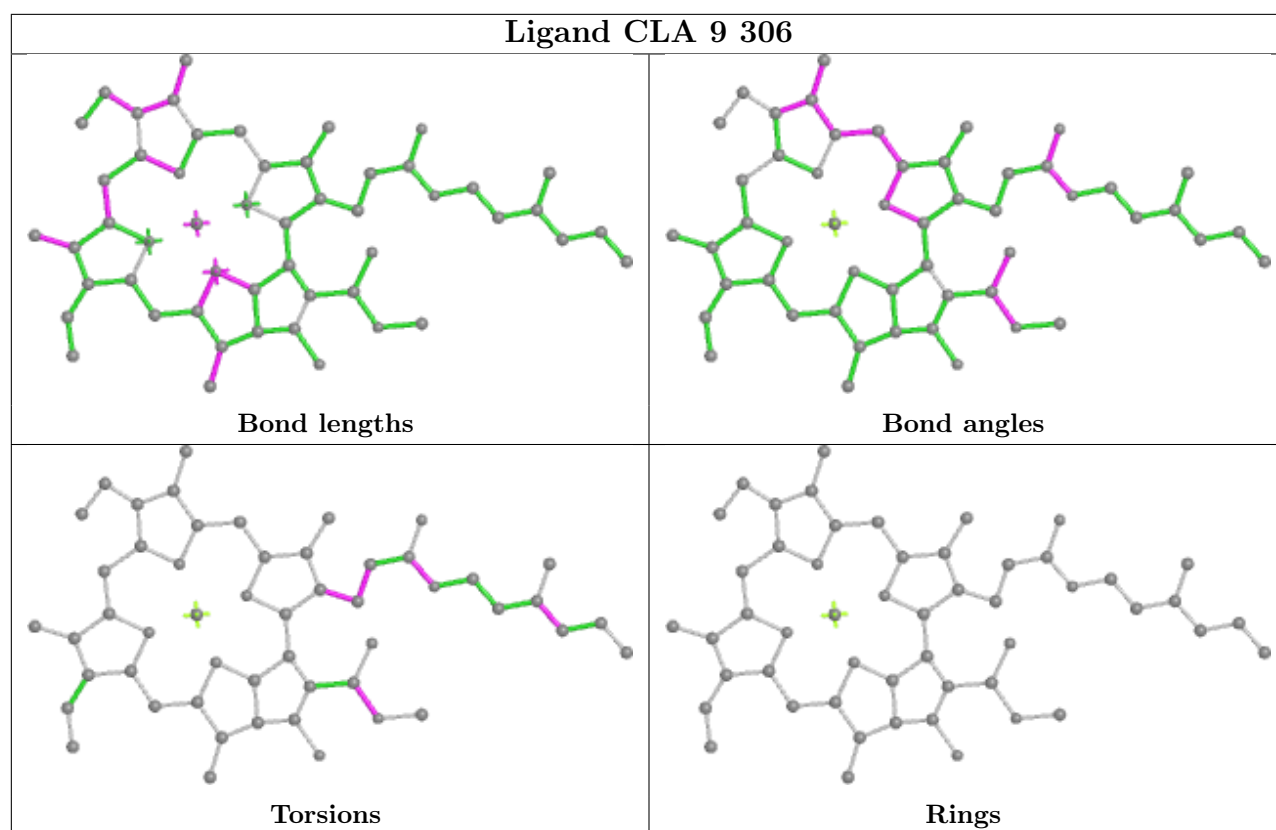


Ligand CLA 3 313

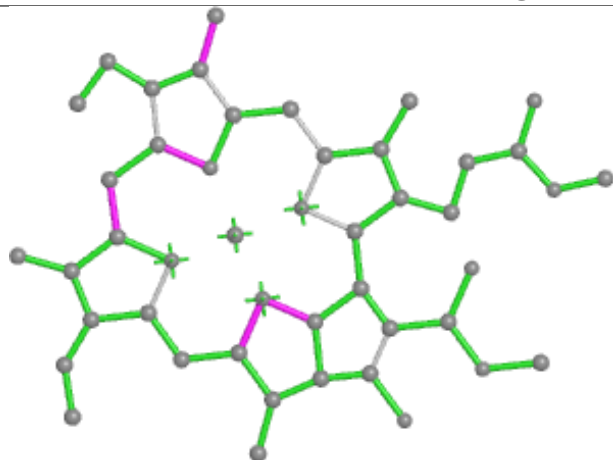


Ligand CLA 3 303

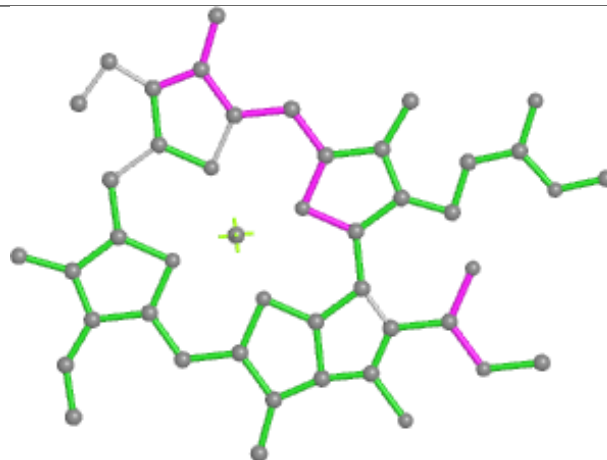




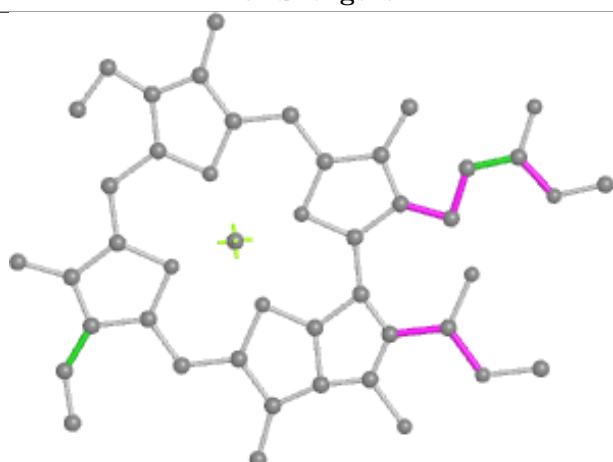
Ligand CLA G 103



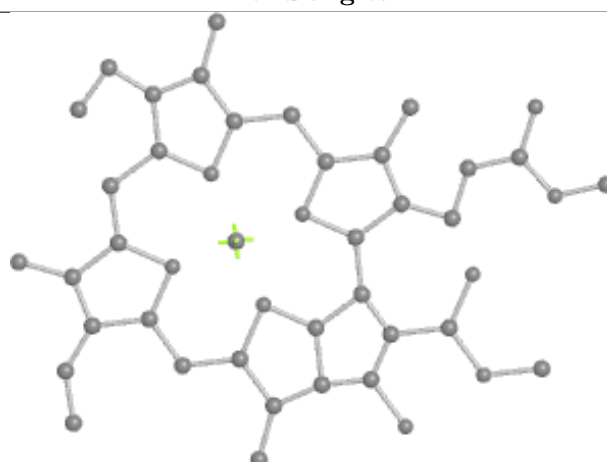
Bond lengths



Bond angles

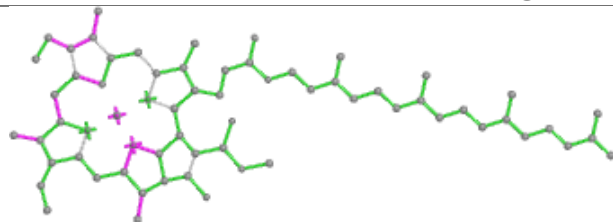


Torsions

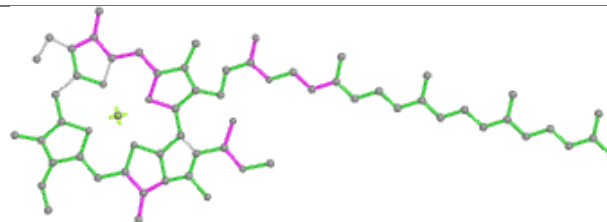


Rings

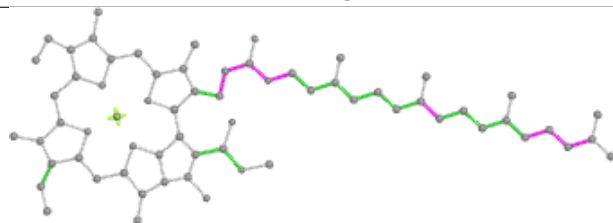
Ligand CLA 6 313



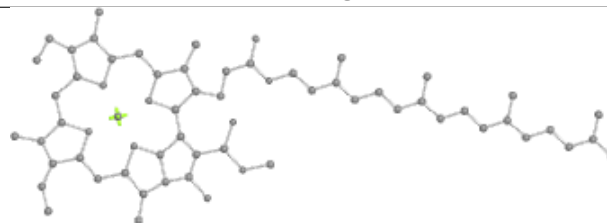
Bond lengths



Bond angles

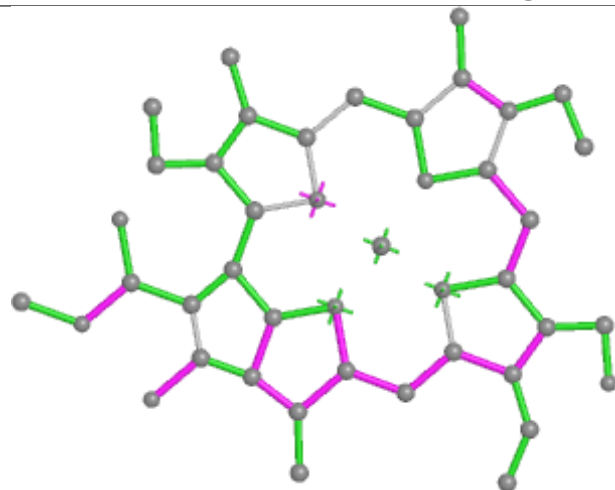


Torsions

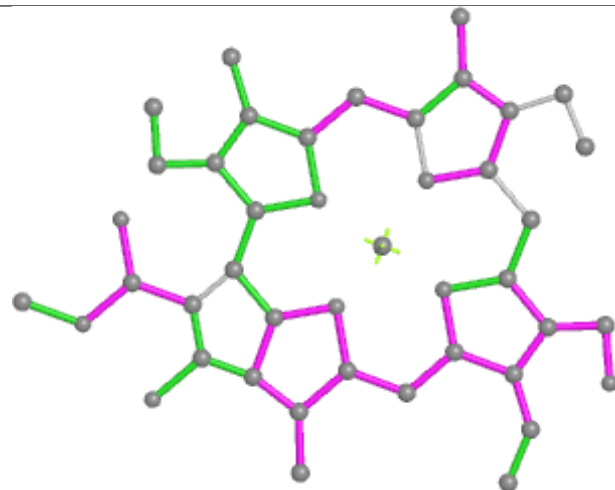


Rings

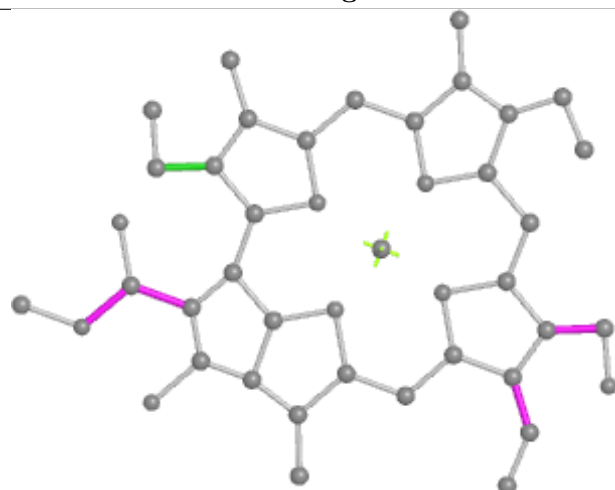
Ligand CHL 6 316



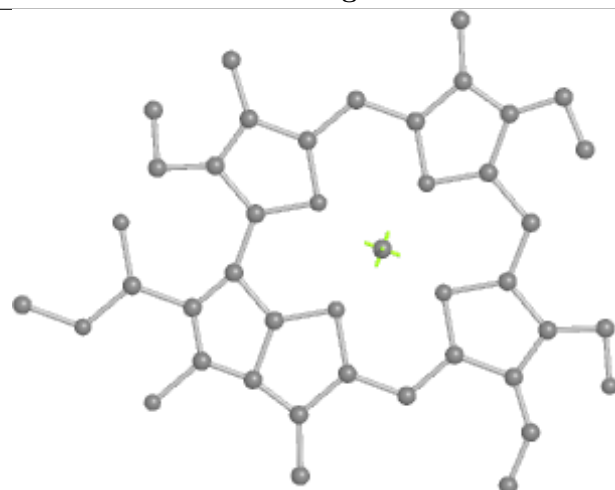
Bond lengths



Bond angles

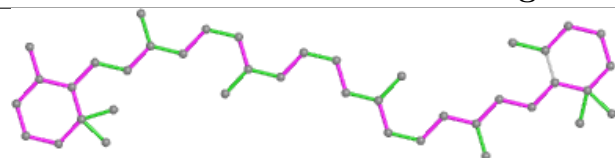


Torsions

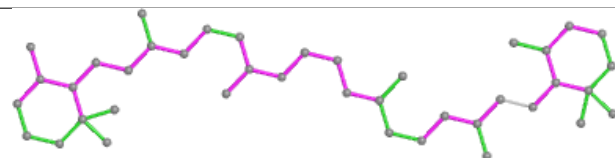


Rings

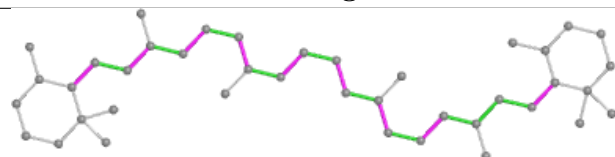
Ligand 8CT A 846



Bond lengths



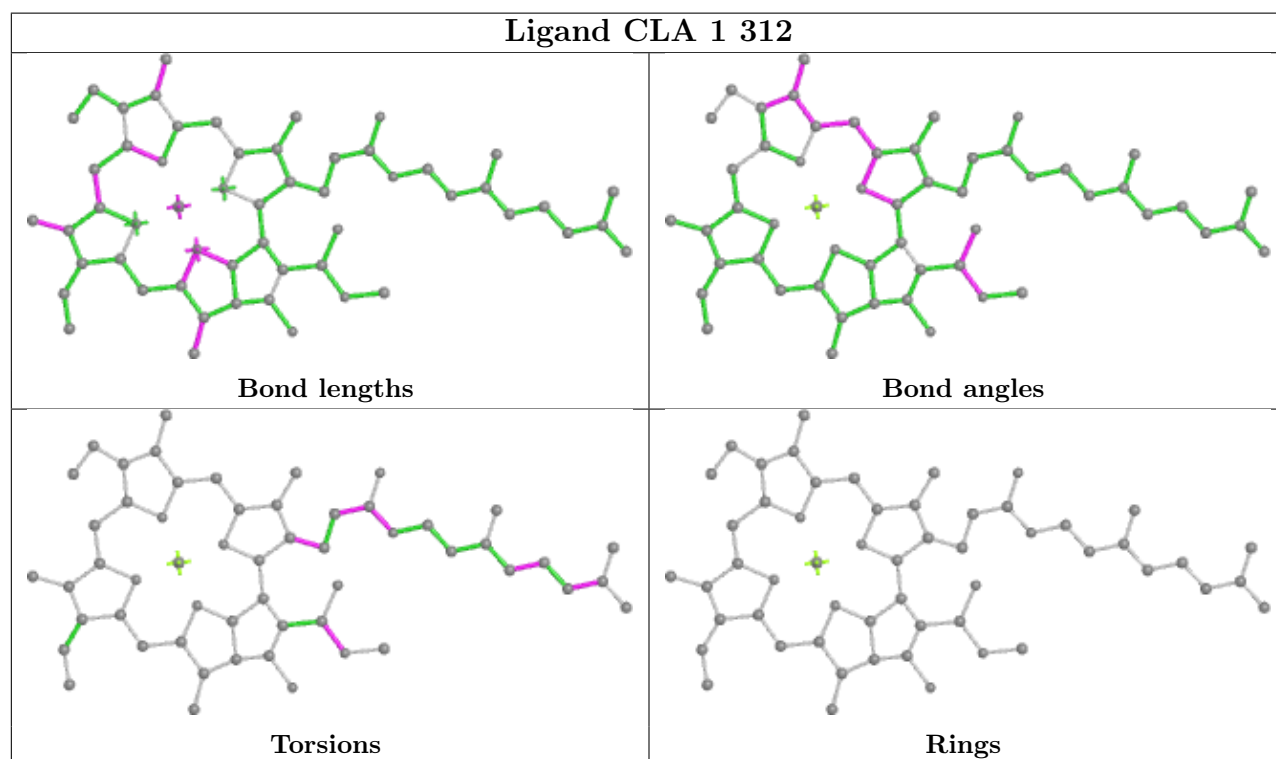
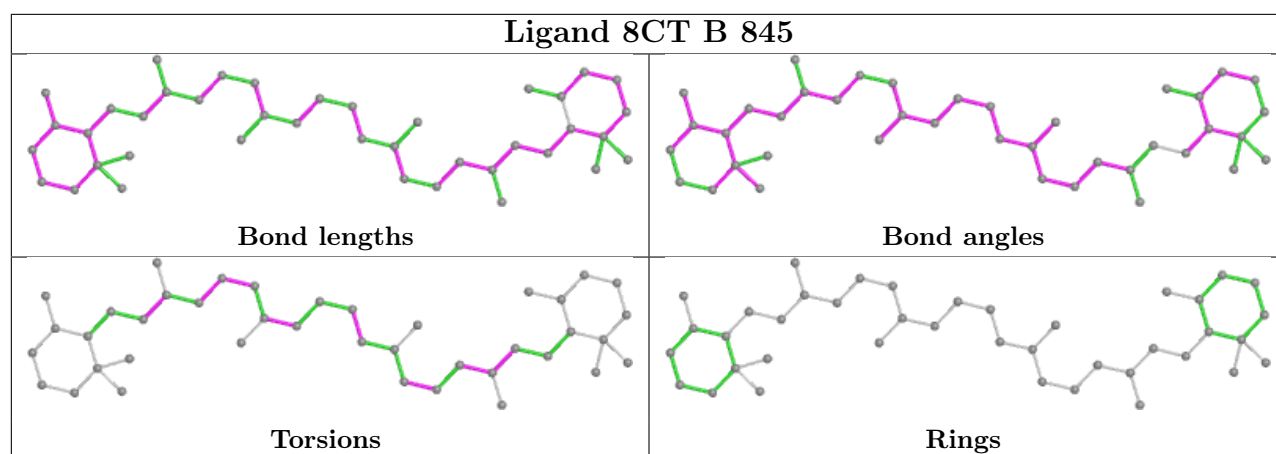
Bond angles

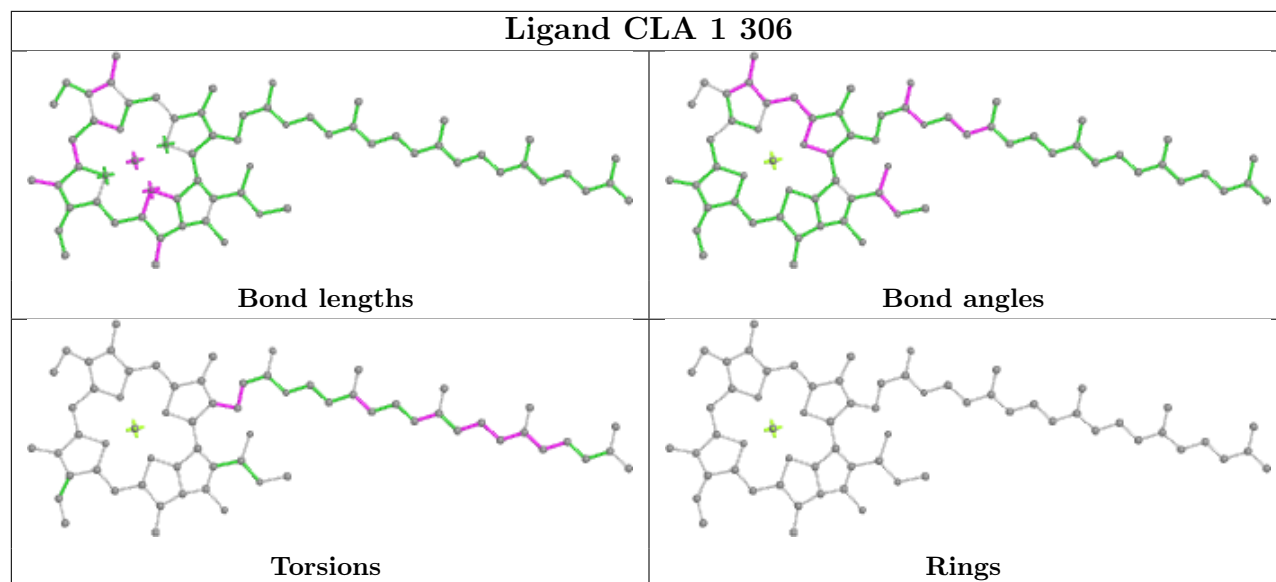
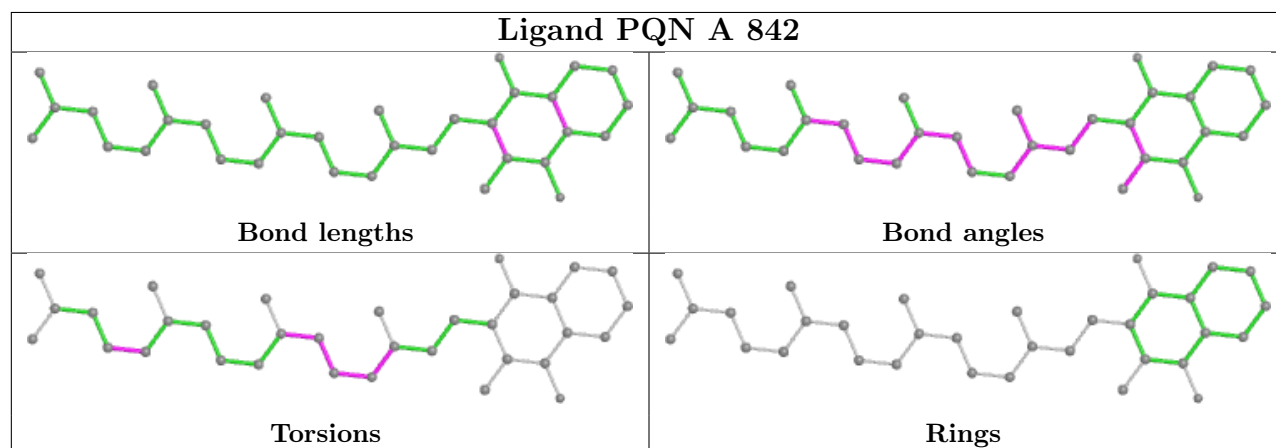


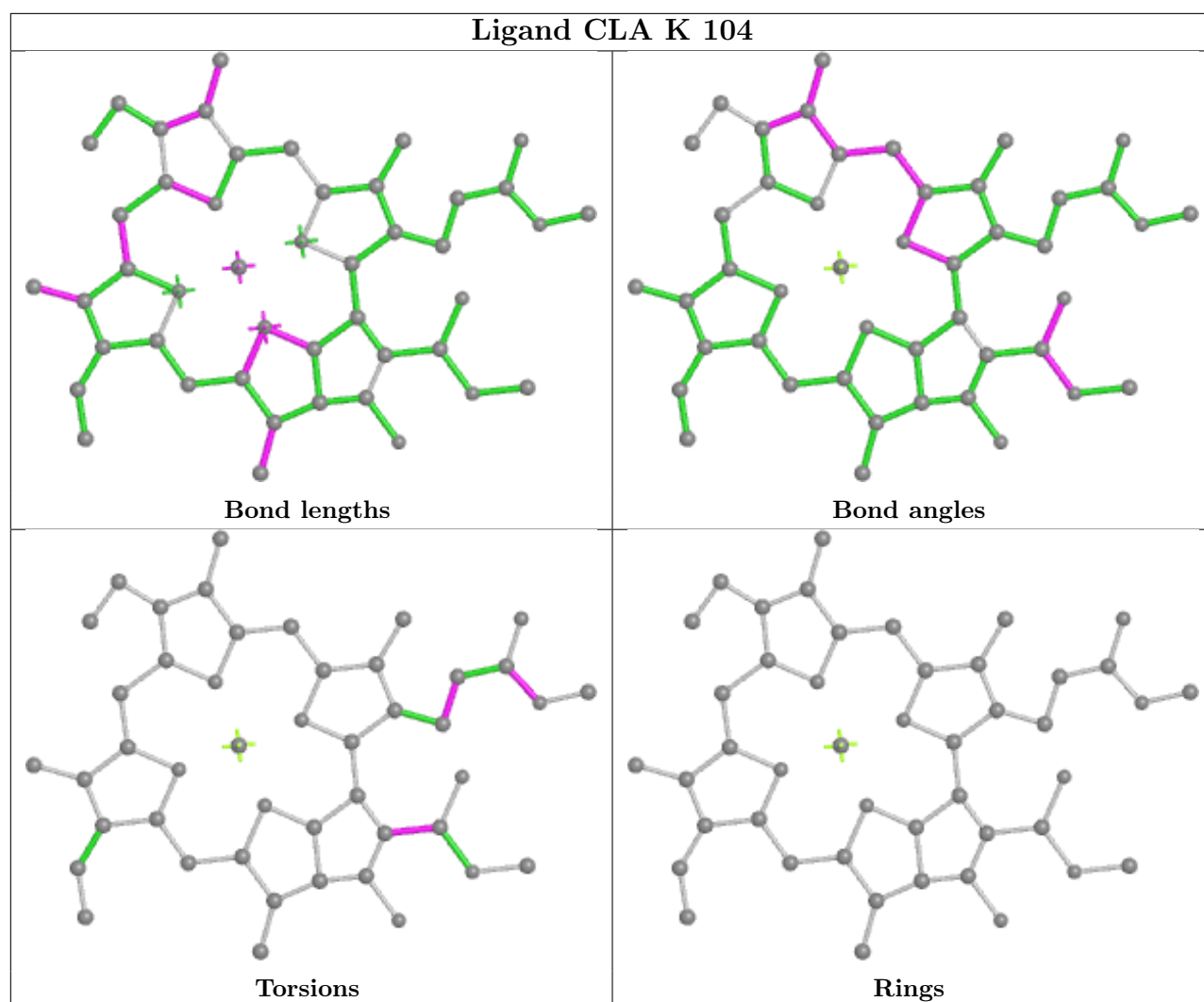
Torsions



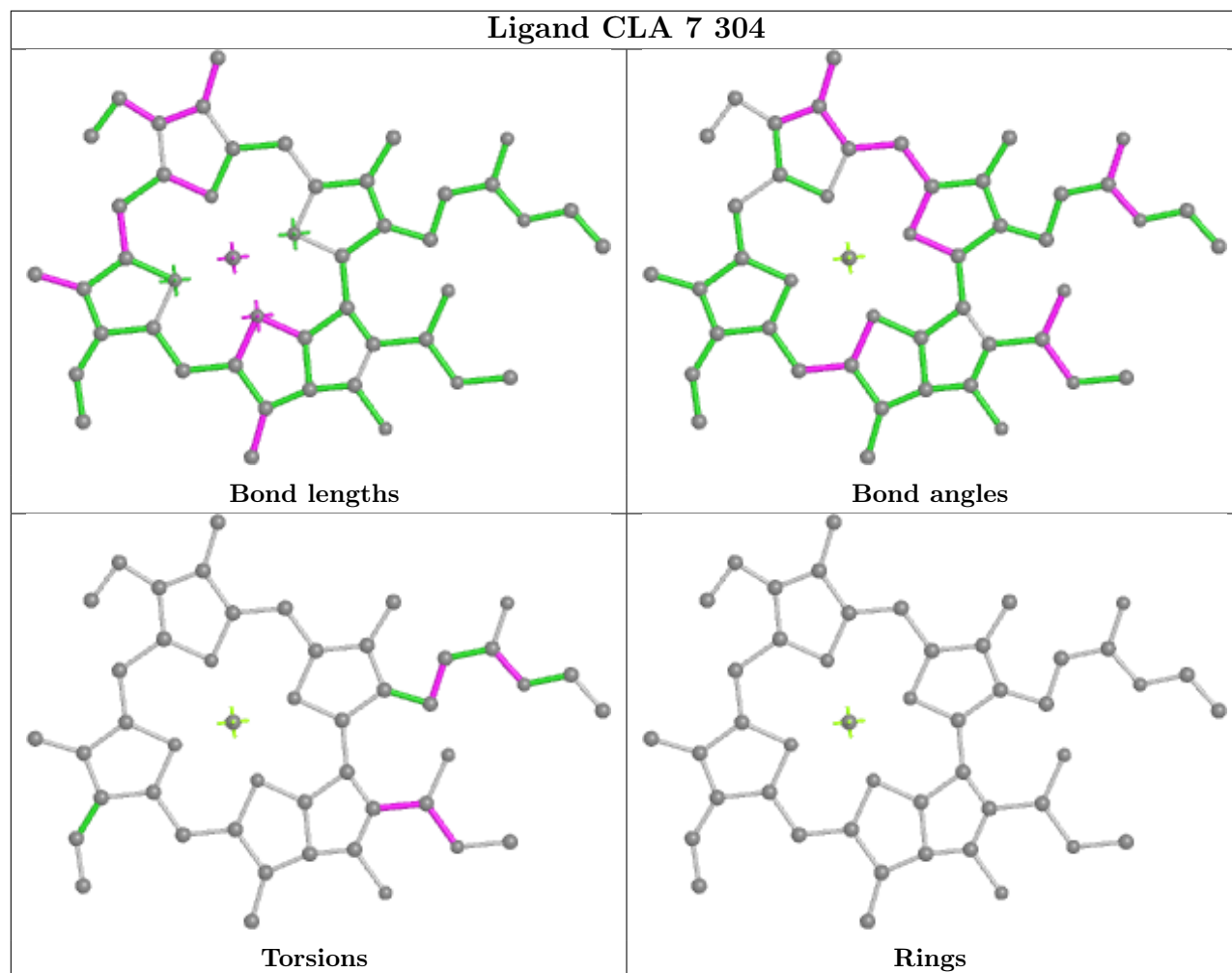
Rings



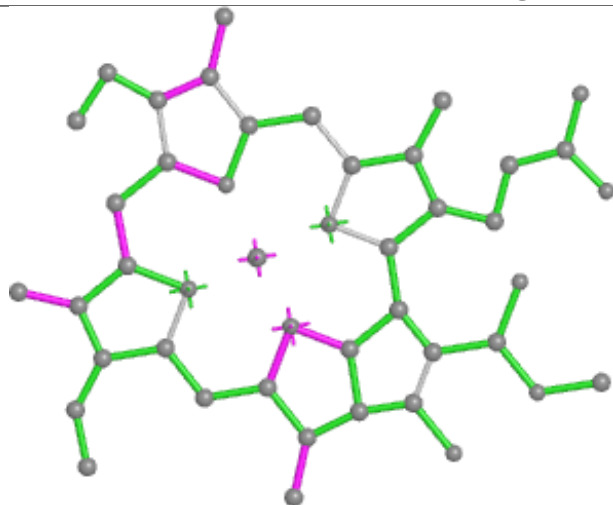
Ligand CLA 1 306**Ligand PQN A 842**



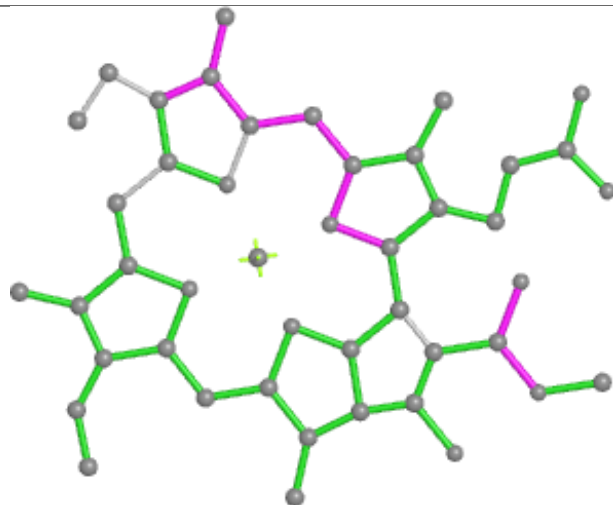
Ligand CLA 7 304



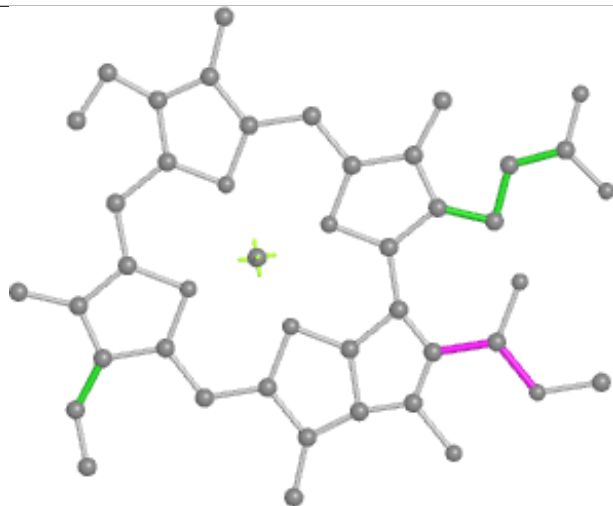
Ligand CLA A 816



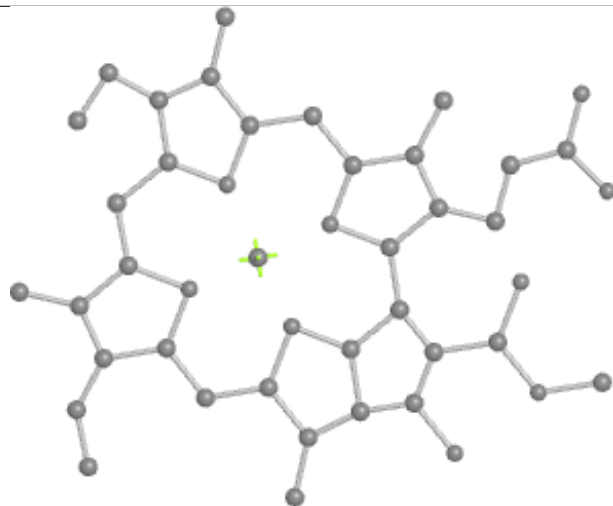
Bond lengths



Bond angles

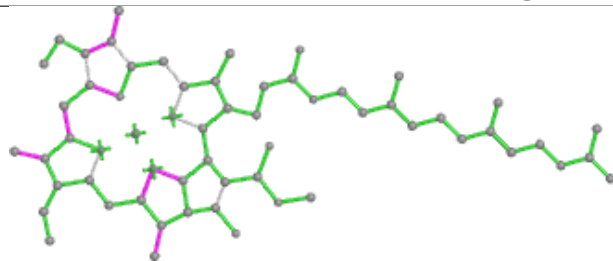


Torsions

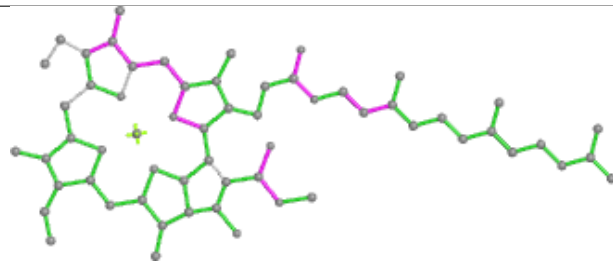


Rings

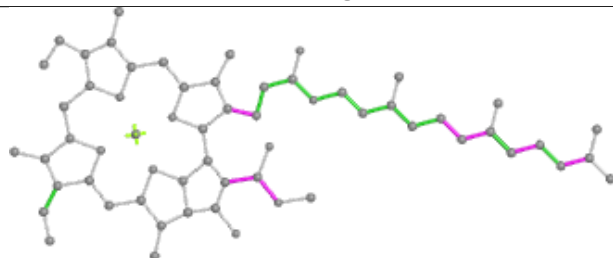
Ligand CLA 1 308



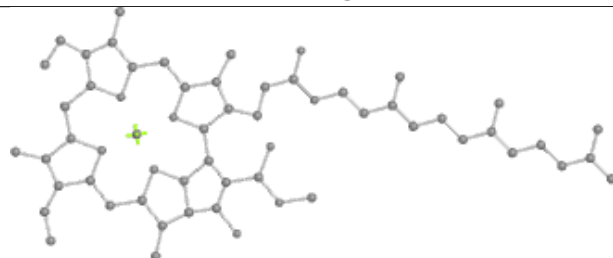
Bond lengths



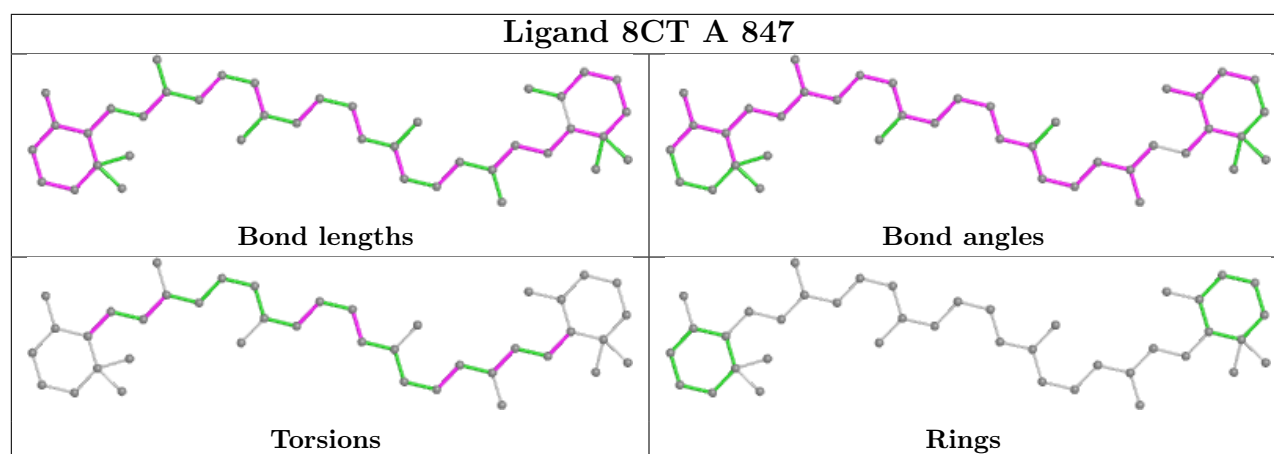
Bond angles



Torsions



Rings



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.

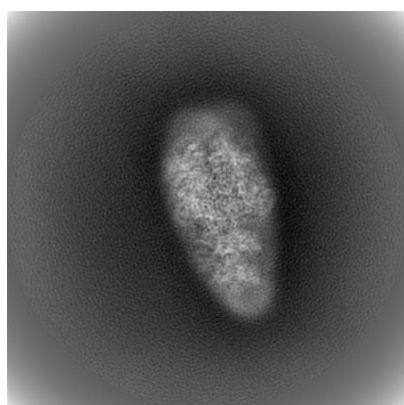
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9670. These allow visual inspection of the internal detail of the map and identification of artifacts.

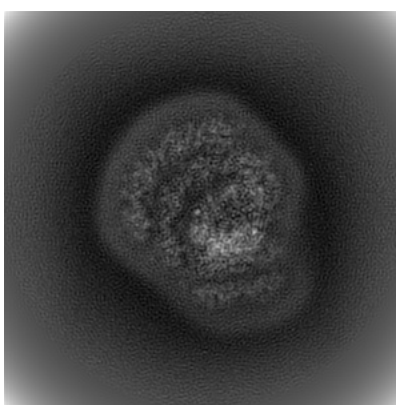
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

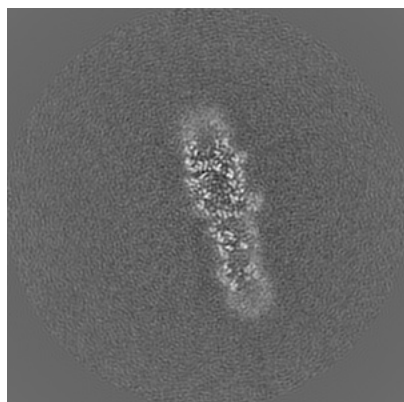


Z

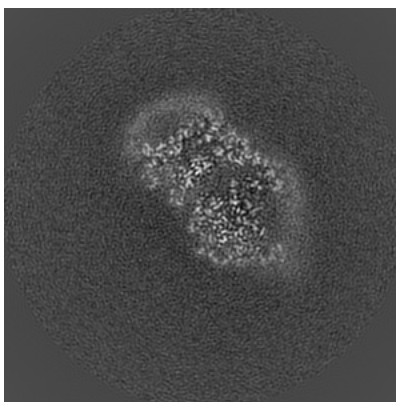
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

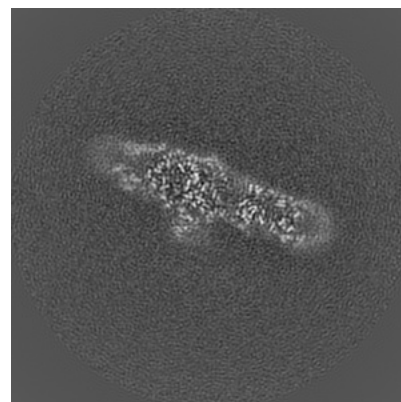
6.2.1 Primary map



X Index: 230



Y Index: 230

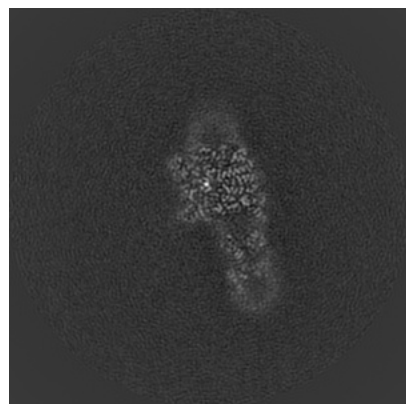


Z Index: 230

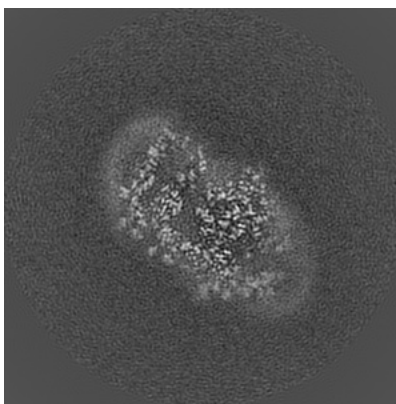
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

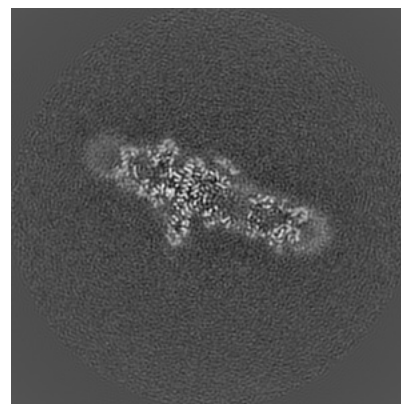
6.3.1 Primary map



X Index: 202



Y Index: 254

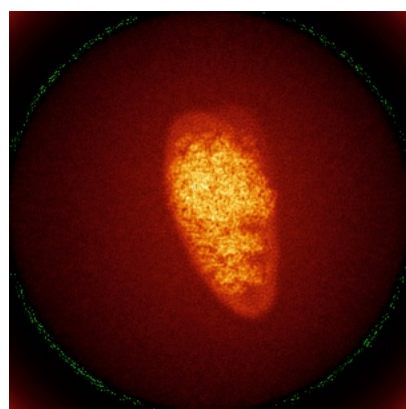


Z Index: 250

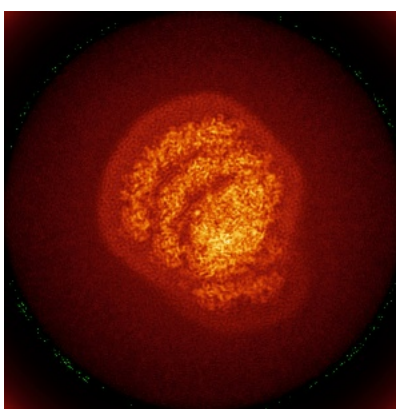
The images above show the largest variance slices of the map in three orthogonal directions.

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

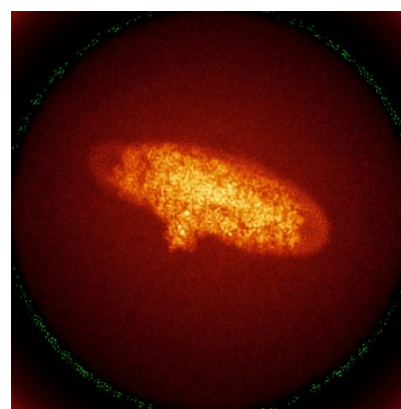
6.4.1 Primary map



X



Y

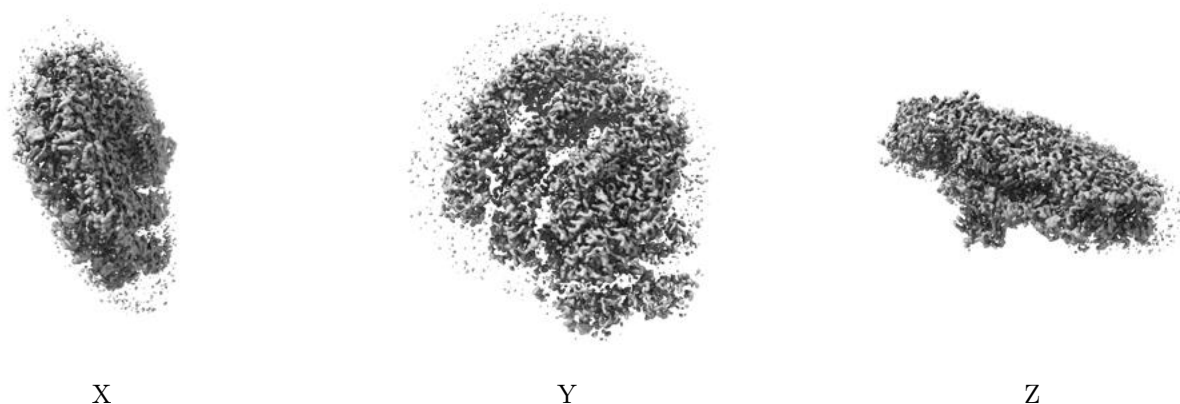


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

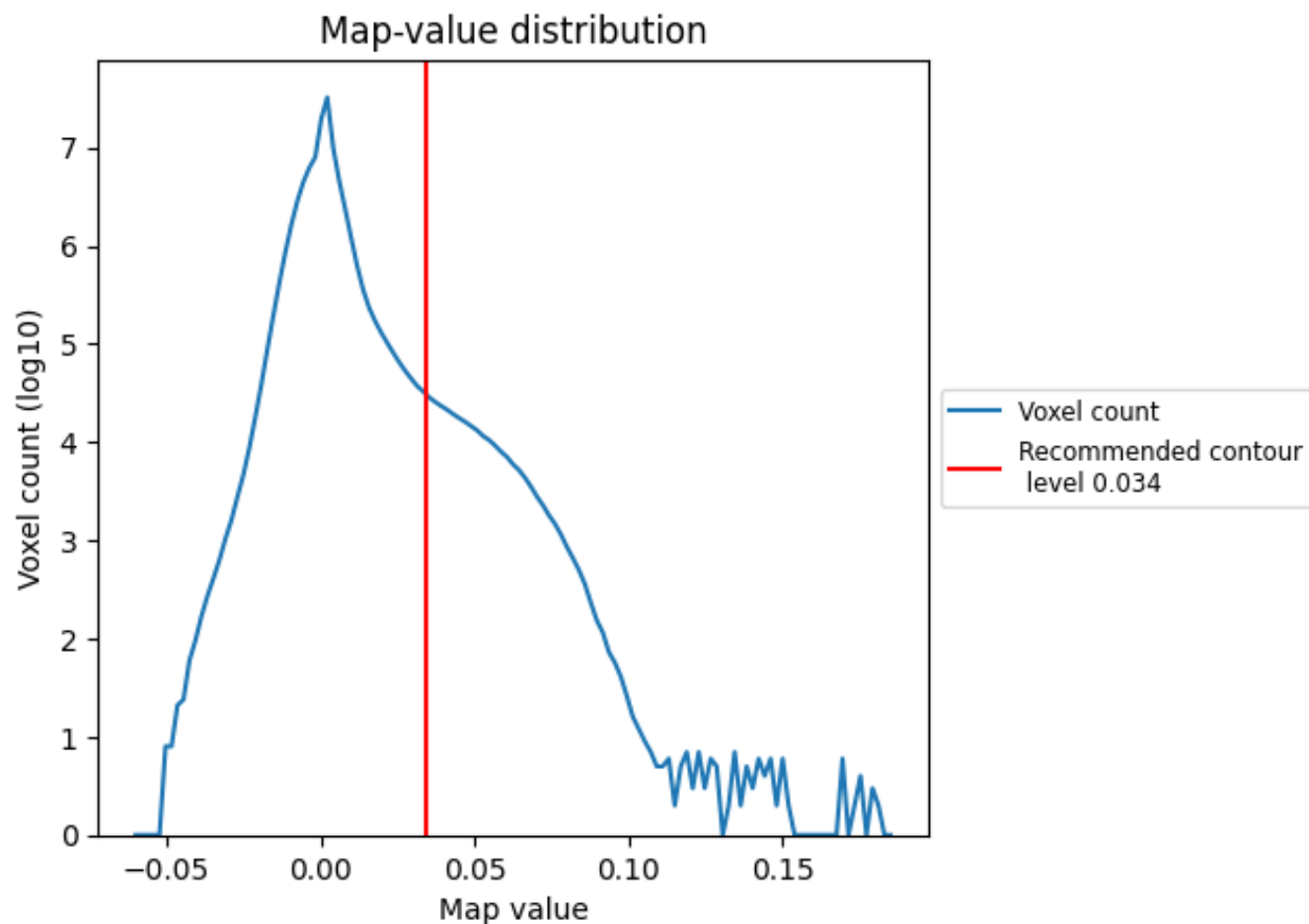
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

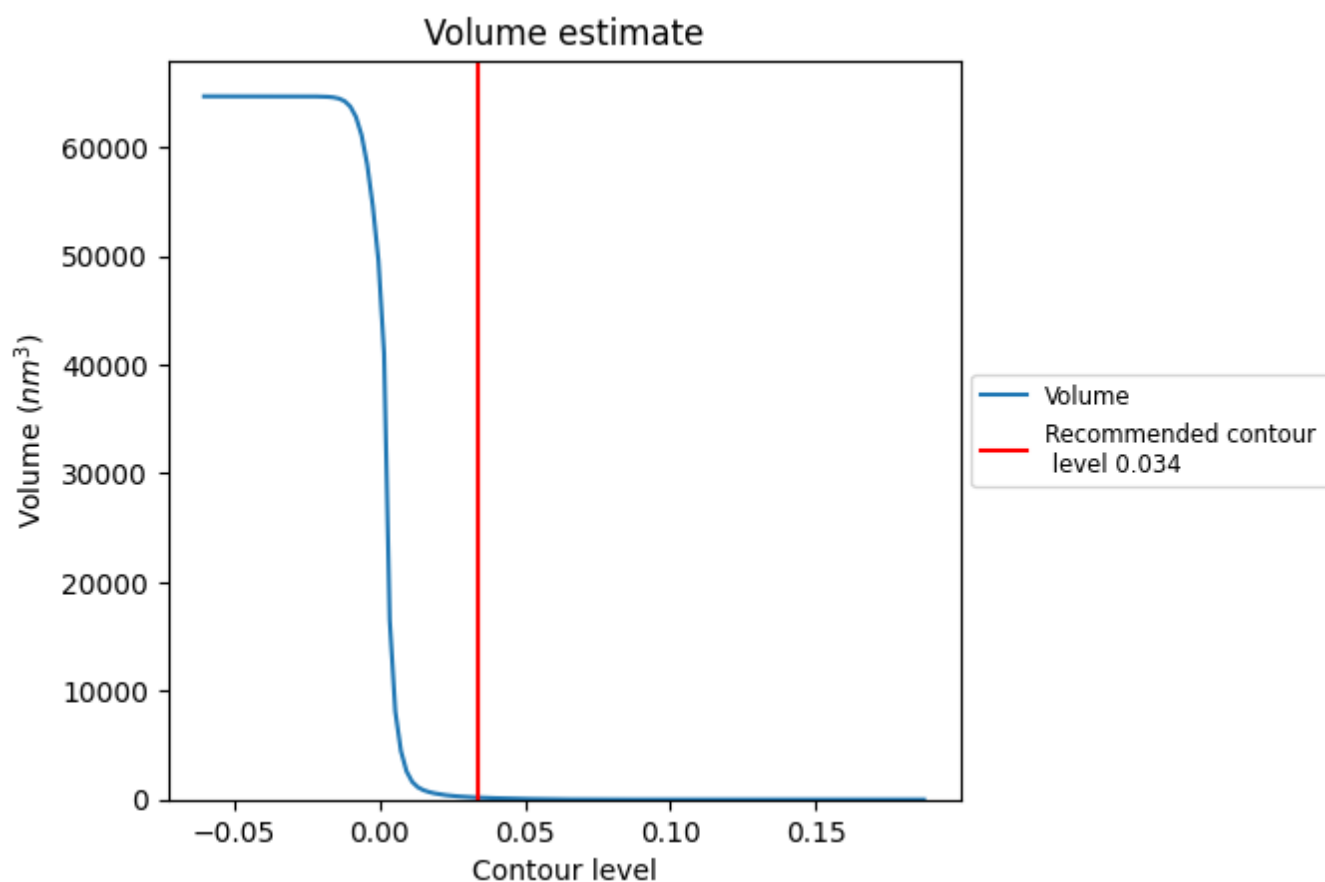
This section contains the results of statistical analysis of the map.

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.

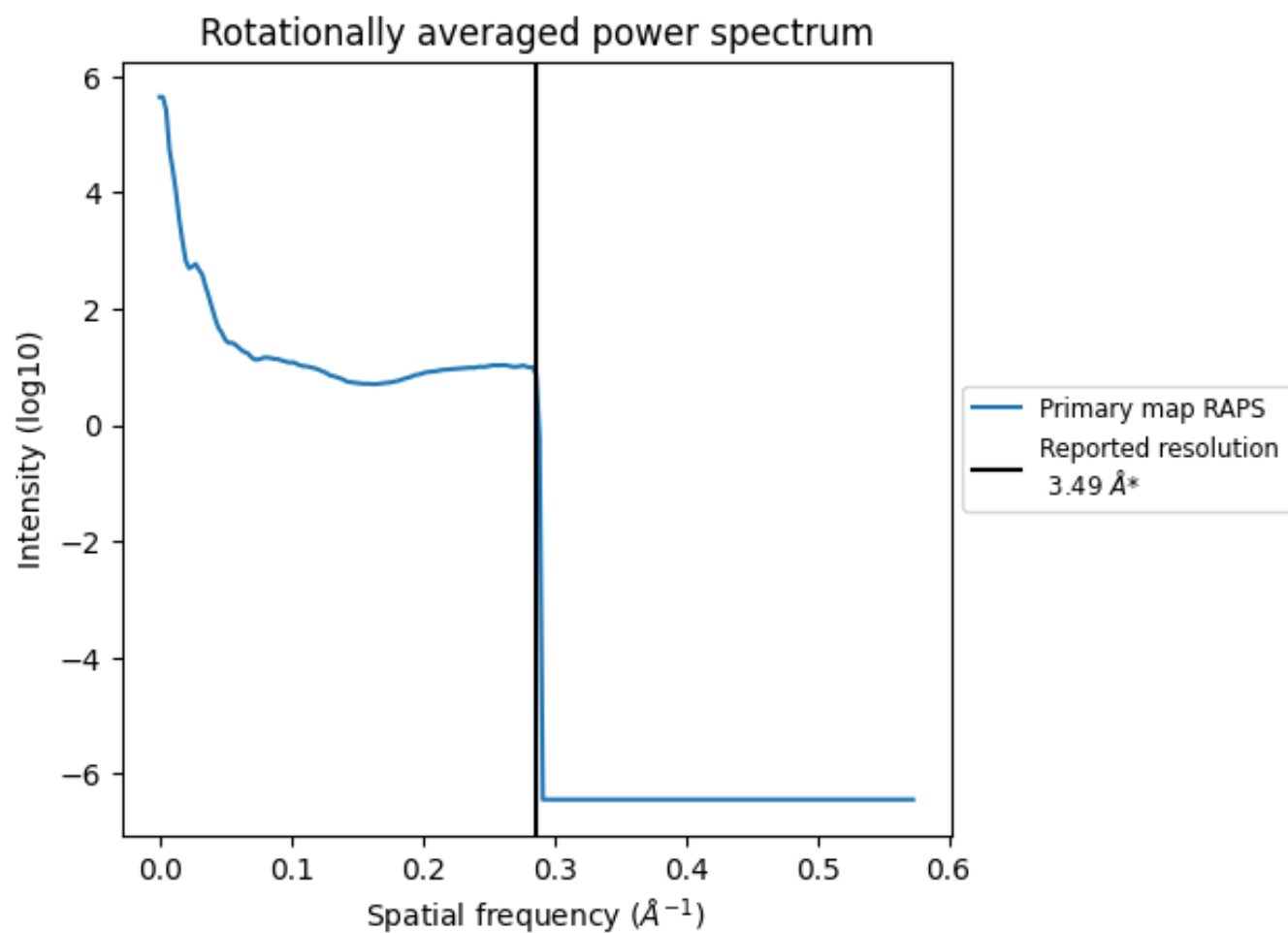
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 186 nm³; this corresponds to an approximate mass of 168 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 0.287 Å⁻¹

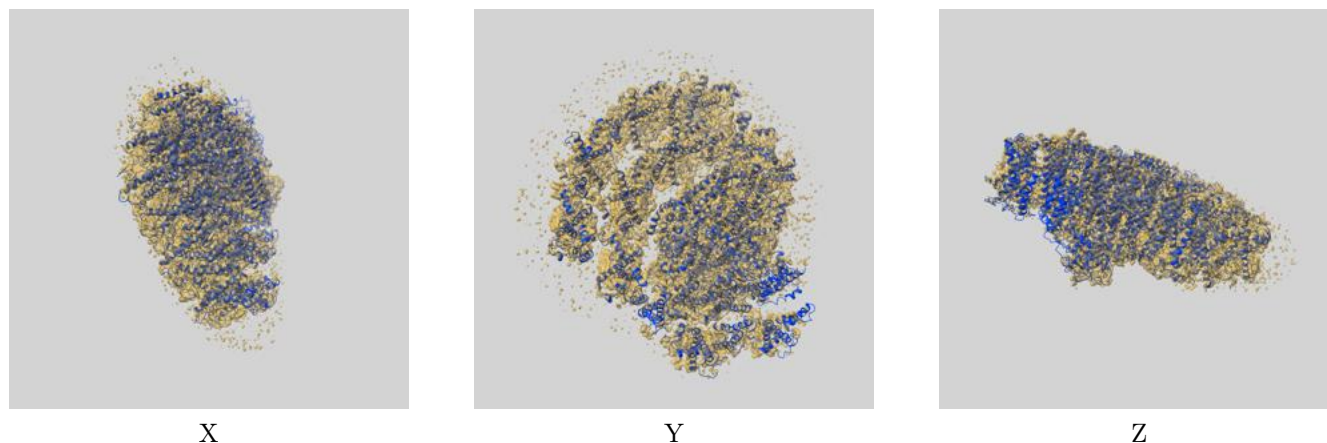
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

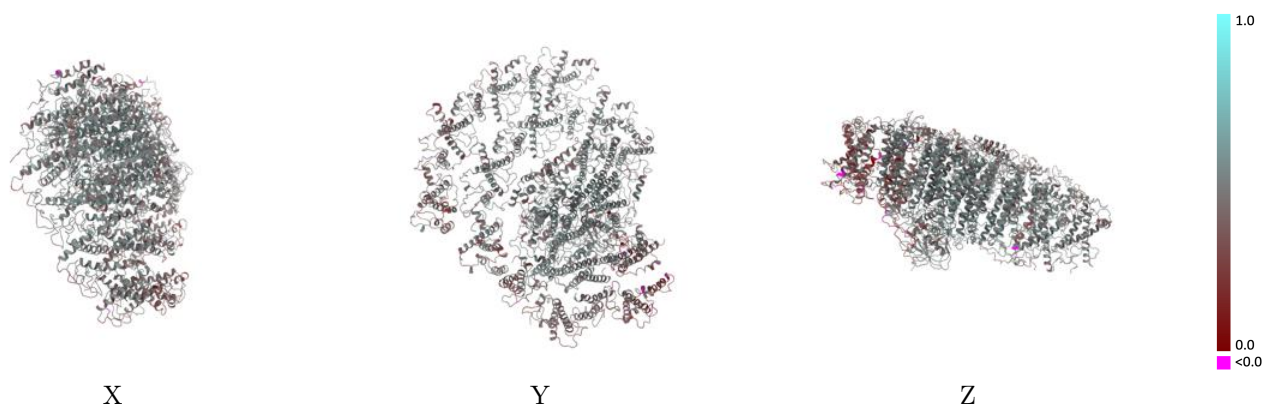
This section contains information regarding the fit between EMDB map EMD-9670 and PDB model 6IGZ. Per-residue inclusion information can be found in section [3](#) on page [34](#).

9.1 Map-model overlay [i](#)



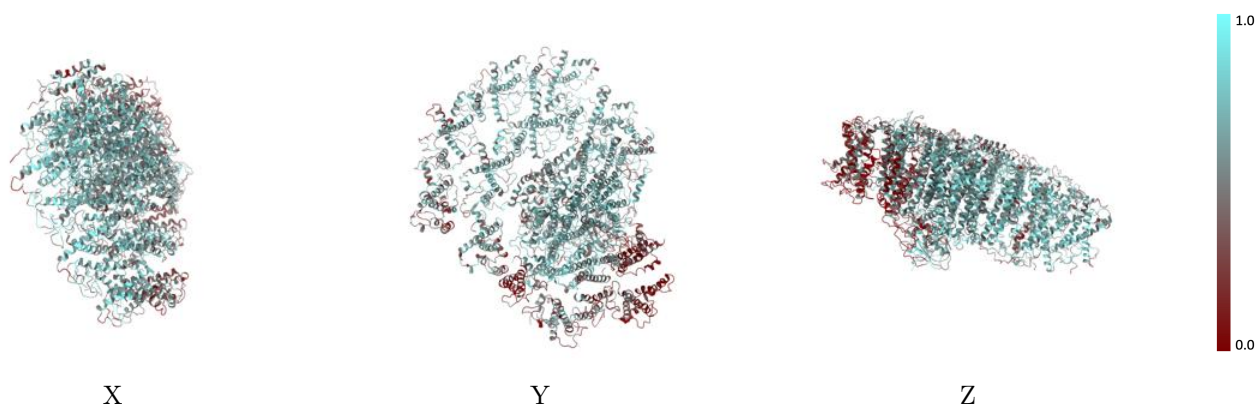
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



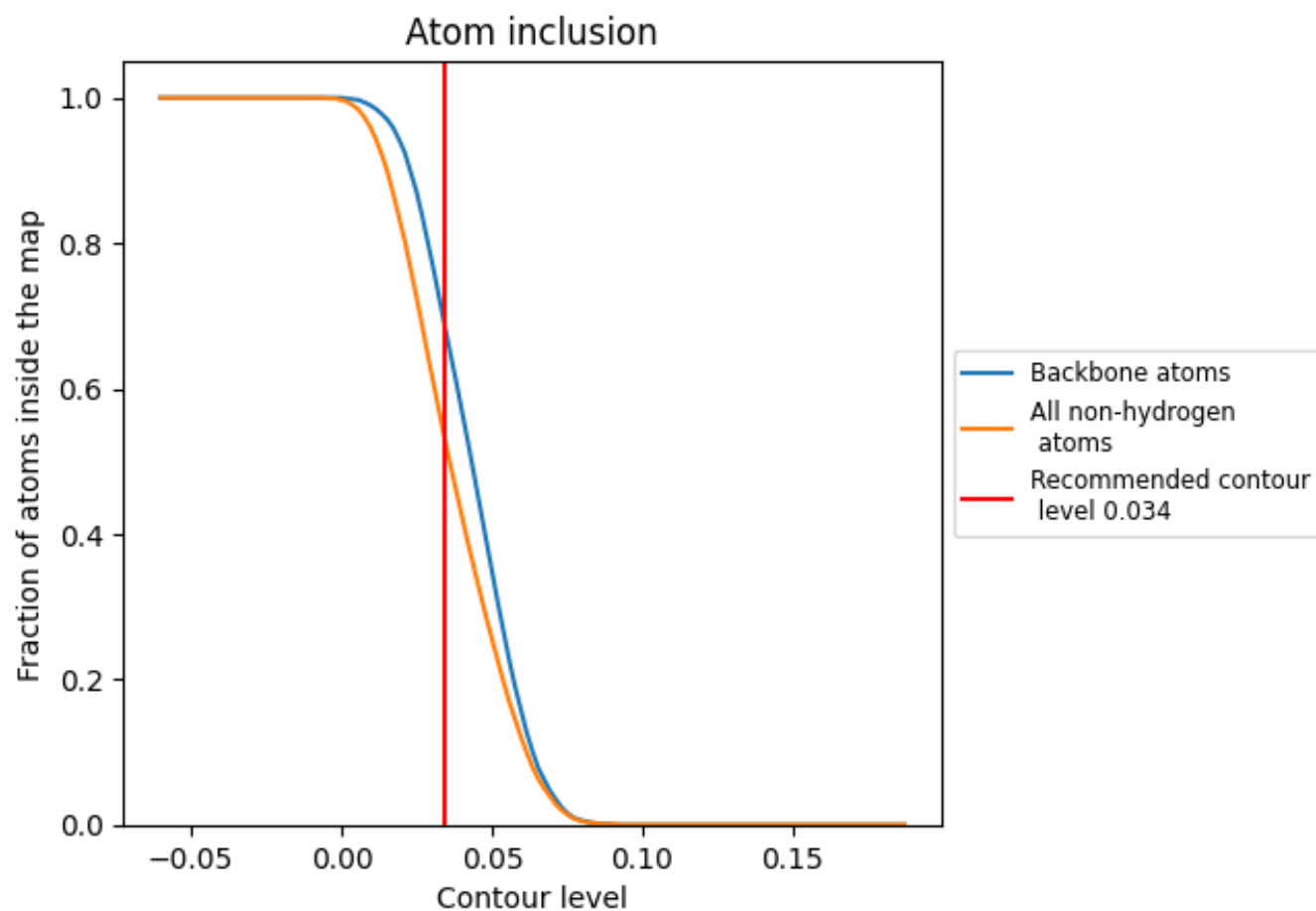
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.034).

9.4 Atom inclusion ⓘ



At the recommended contour level, 69% of all backbone atoms, 54% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5360	<div></div> 0.4750
0	<div></div> 0.2070	<div></div> 0.3440
1	<div></div> 0.5270	<div></div> 0.4620
2	<div></div> 0.6430	<div></div> 0.5160
3	<div></div> 0.6390	<div></div> 0.5010
4	<div></div> 0.5880	<div></div> 0.4810
5	<div></div> 0.4560	<div></div> 0.4250
6	<div></div> 0.5840	<div></div> 0.4770
7	<div></div> 0.5990	<div></div> 0.4760
8	<div></div> 0.5460	<div></div> 0.4490
9	<div></div> 0.4150	<div></div> 0.4280
A	<div></div> 0.6220	<div></div> 0.5250
B	<div></div> 0.6010	<div></div> 0.5160
C	<div></div> 0.7150	<div></div> 0.4740
D	<div></div> 0.5960	<div></div> 0.4680
E	<div></div> 0.5750	<div></div> 0.4740
F	<div></div> 0.5360	<div></div> 0.4700
G	<div></div> 0.1210	<div></div> 0.3640
H	<div></div> 0.0650	<div></div> 0.2890
I	<div></div> 0.4310	<div></div> 0.4880
J	<div></div> 0.4920	<div></div> 0.4980
K	<div></div> 0.4900	<div></div> 0.4400
L	<div></div> 0.2280	<div></div> 0.4030
M	<div></div> 0.5130	<div></div> 0.4760

