



wwPDB EM Validation Summary Report ⓘ

Mar 12, 2026 – 04:42 PM UTC

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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

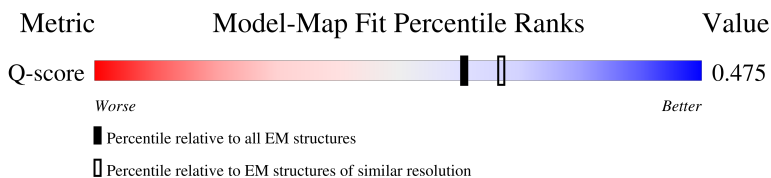
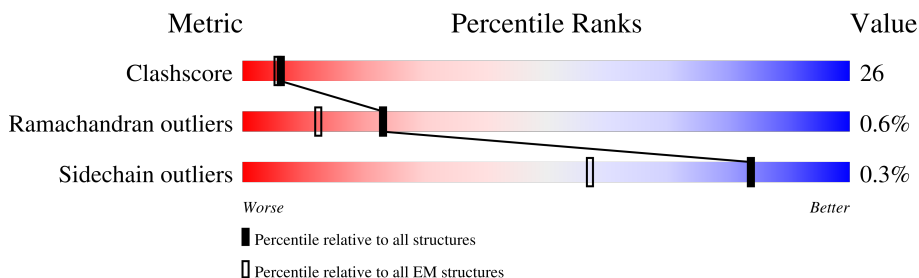
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13600 (2.99 - 3.99)

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	
2	B	734	
3	C	81	
4	D	198	

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Mol	Chain	Length	Quality of chain
5	E	91	
6	F	236	
7	G	167	
8	H	133	
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	-	-	-

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

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

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

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

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

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

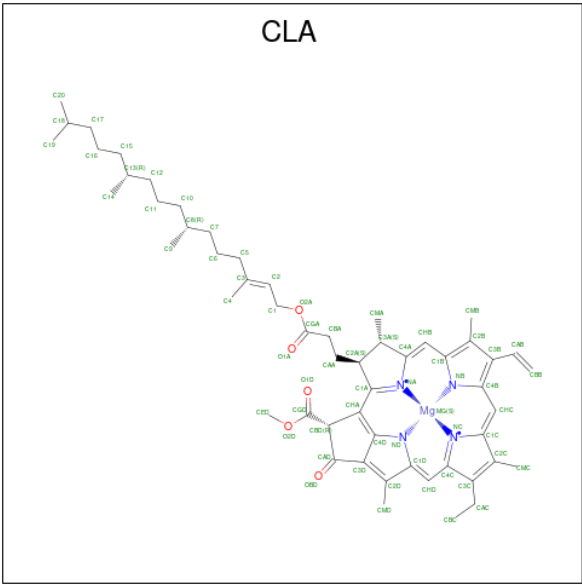
- Molecule 20 is a protein called Lhca-j.

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

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

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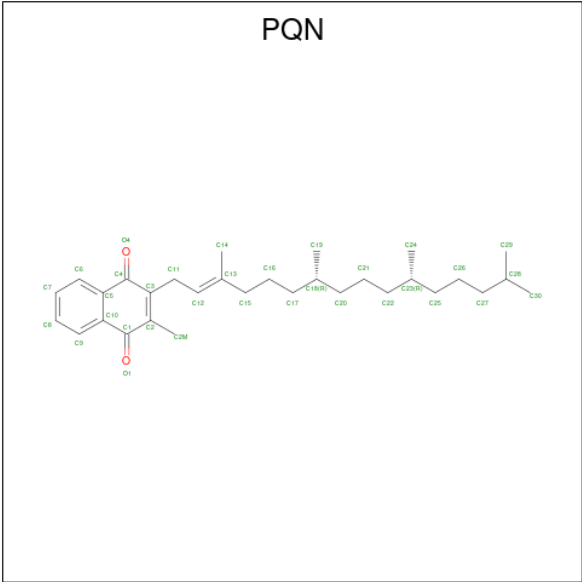
Mol	Chain	Residues	Atoms					AltConf
22	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
22	7	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	7	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	7	1	Total	C	Mg	N	O	0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

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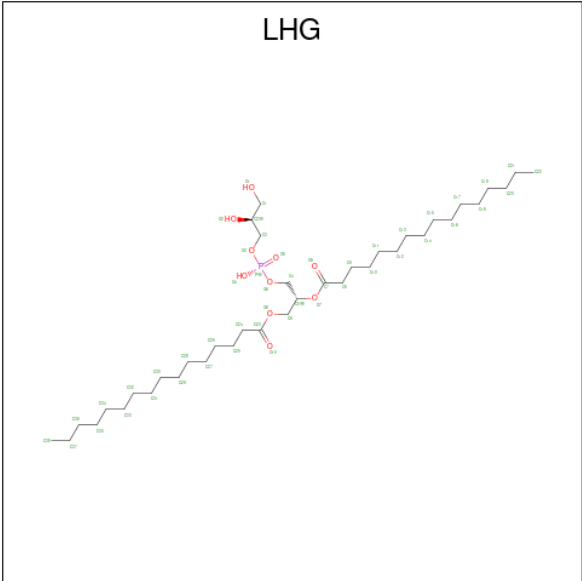
Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
22	9	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			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: $C_{31}H_{46}O_2$).



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).



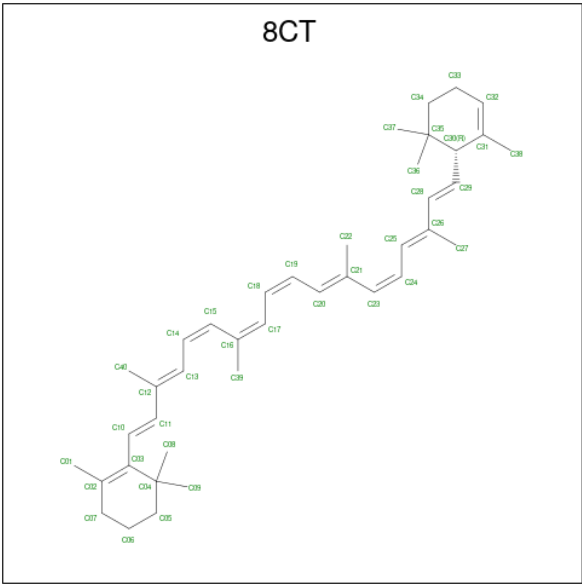
Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			49	38	10	1	

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

- 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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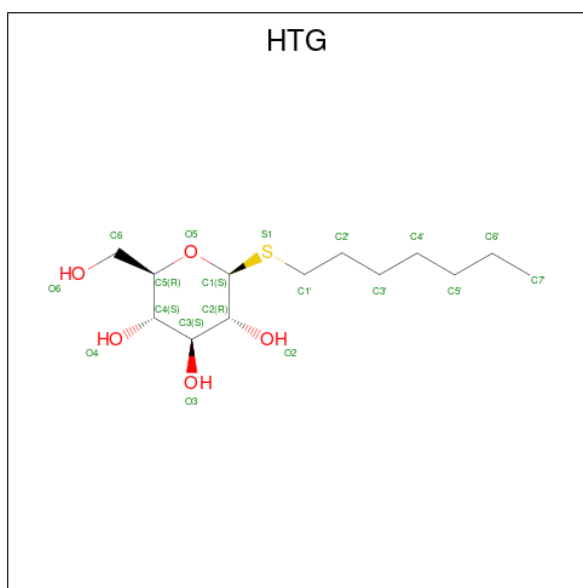
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 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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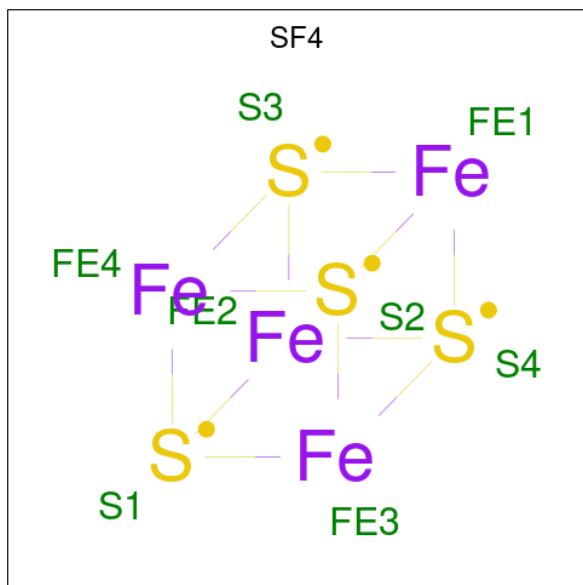
Mol	Chain	Residues	Atoms	AltConf
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	4	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	5	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 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).



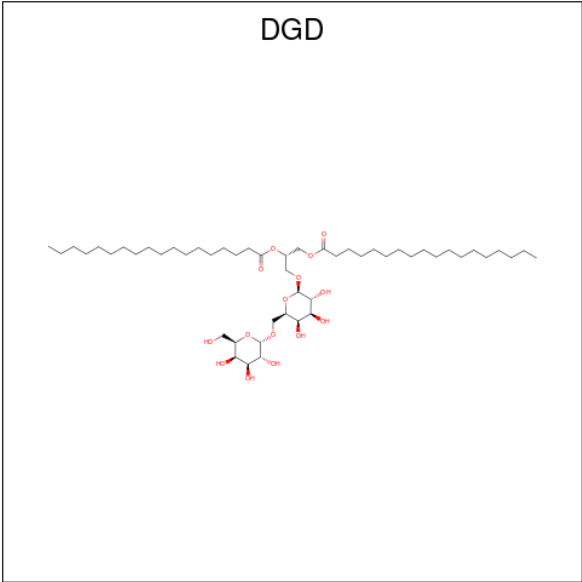
Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			19	13	5	1	
26	J	1	Total	C	O	S	0
			19	13	5	1	

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



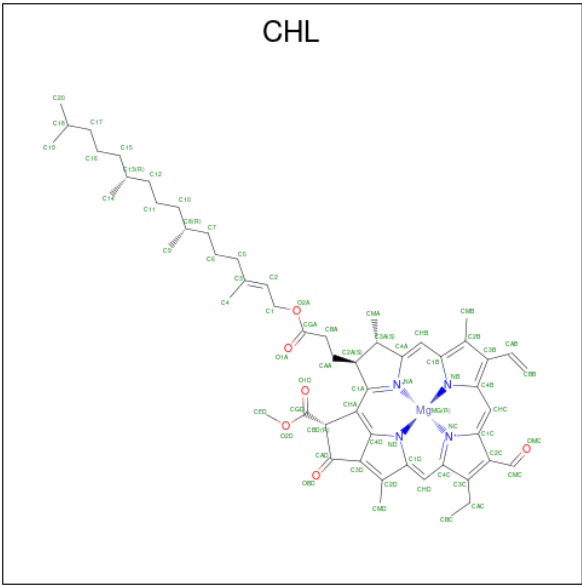
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	

- 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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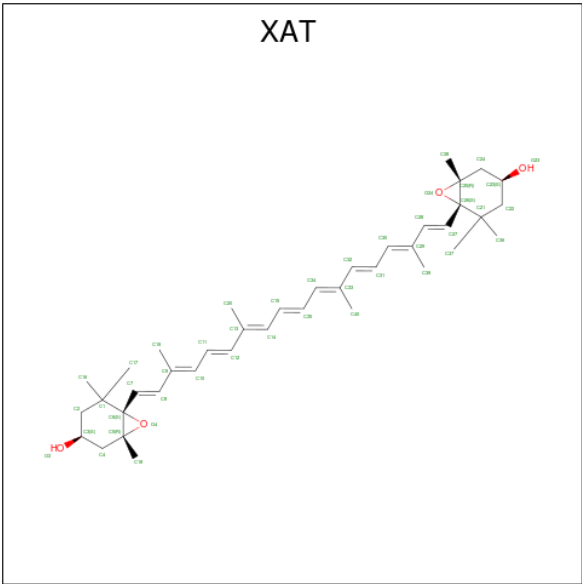
Mol	Chain	Residues	Atoms					AltConf
29	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
29	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
29	4	1	Total 61	C 50	Mg 1	N 4	O 6	0
29	4	1	Total 56	C 45	Mg 1	N 4	O 6	0
29	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
29	6	1	Total 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).



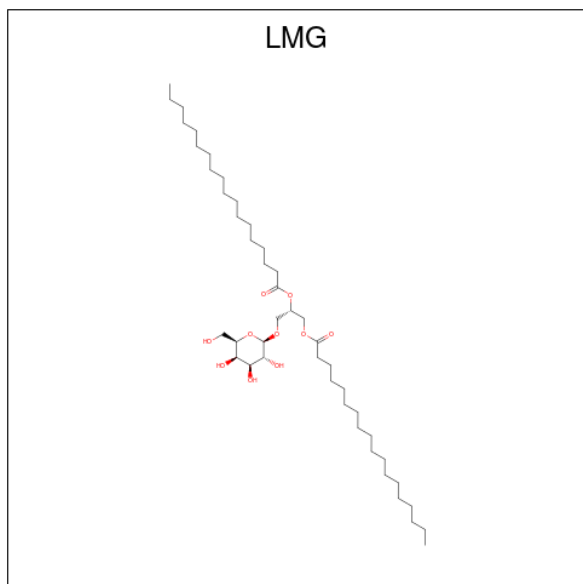
Mol	Chain	Residues	Atoms			AltConf
30	1	1	Total	C	O	0
			44	40	4	
30	1	1	Total	C	O	0
			44	40	4	
30	2	1	Total	C	O	0
			44	40	4	
30	2	1	Total	C	O	0
			44	40	4	
30	3	1	Total	C	O	0
			44	40	4	
30	3	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	
30	6	1	Total	C	O	0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

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

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

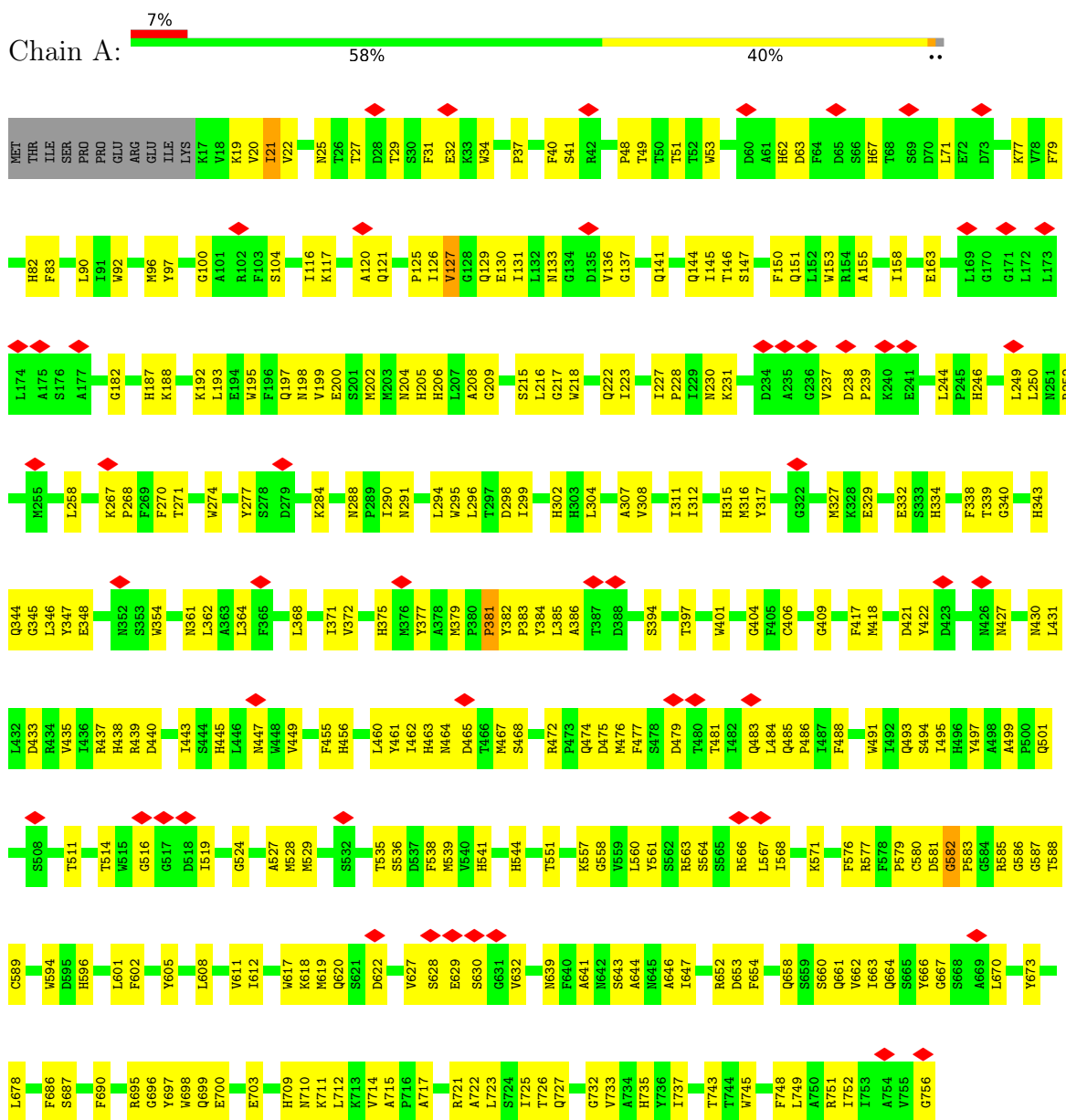


Mol	Chain	Residues	Atoms			AltConf
31	4	1	Total 44	C 34	O 10	0
31	5	1	Total 44	C 34	O 10	0
31	8	1	Total 44	C 34	O 10	0

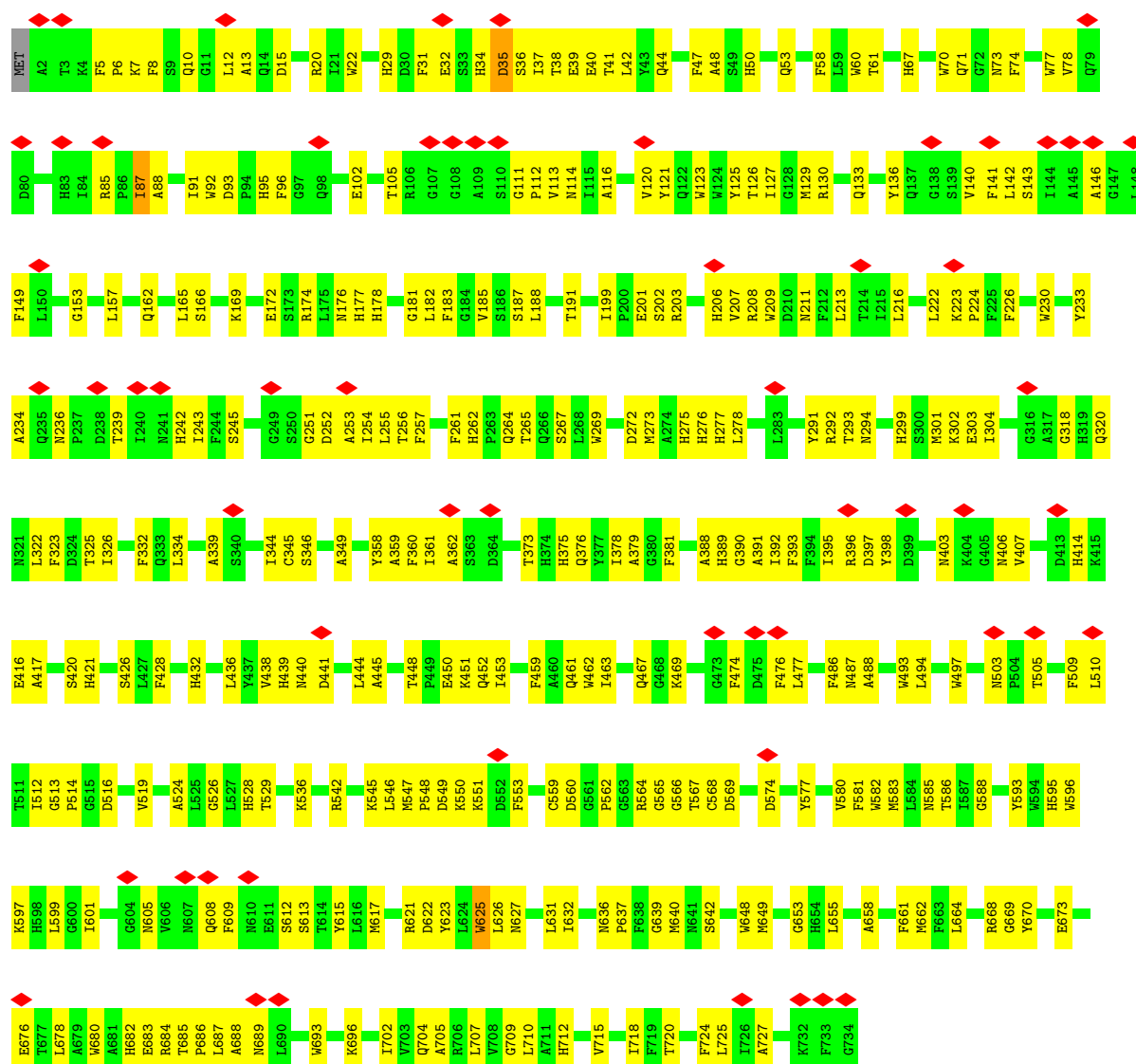
3 Residue-property plots

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.

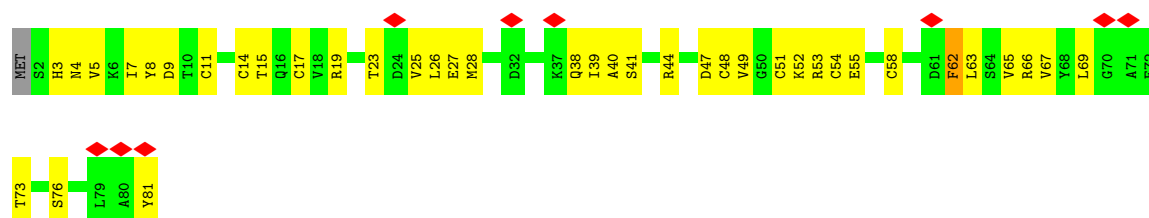
• Molecule 1: PsaA



• Molecule 2: PsaB

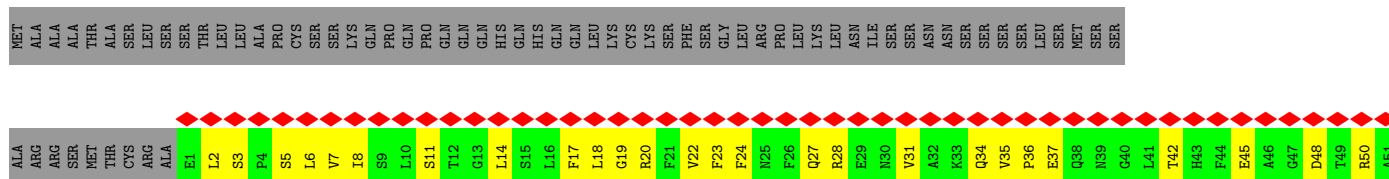


• Molecule 3: PsaC



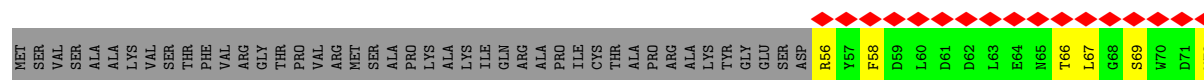
• Molecule 4: PsaD

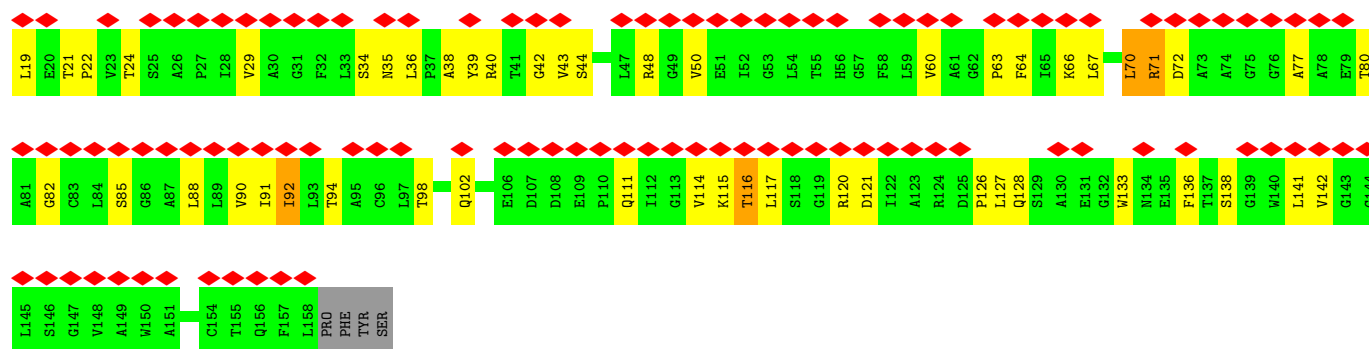




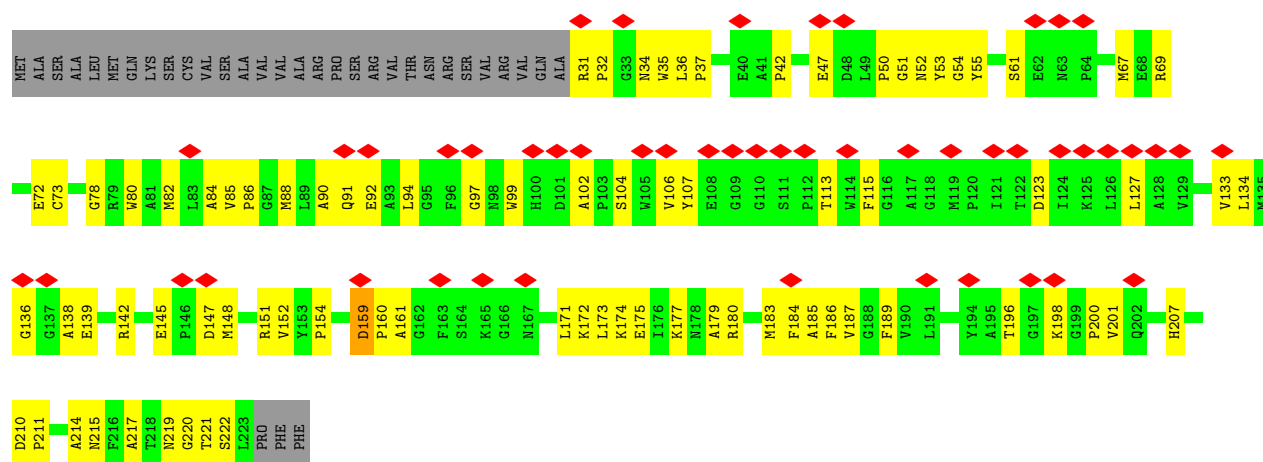


• Molecule 8: PsaH

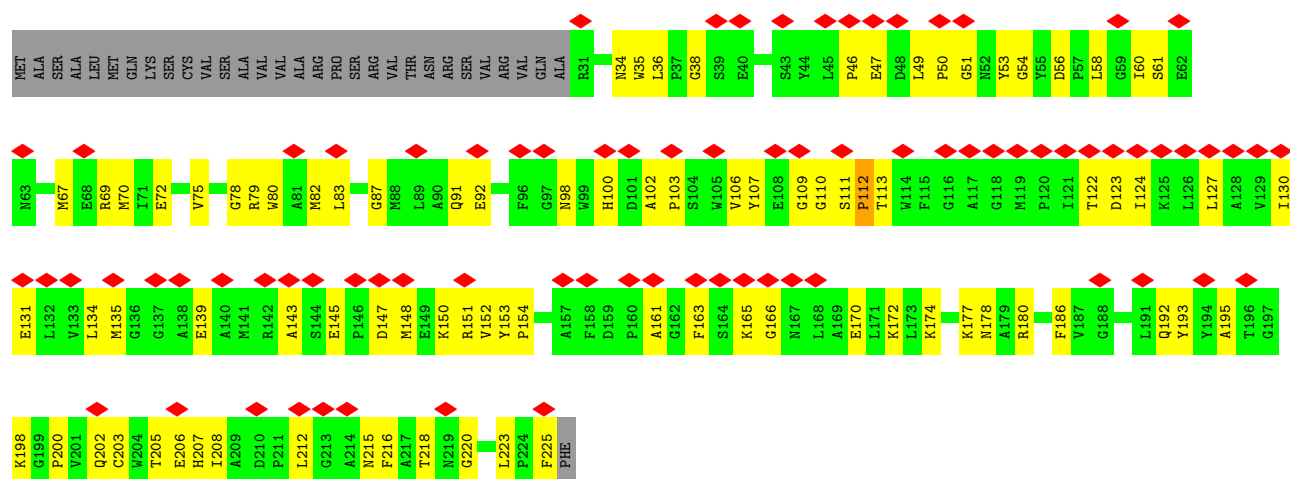




• Molecule 13: Lhca-a

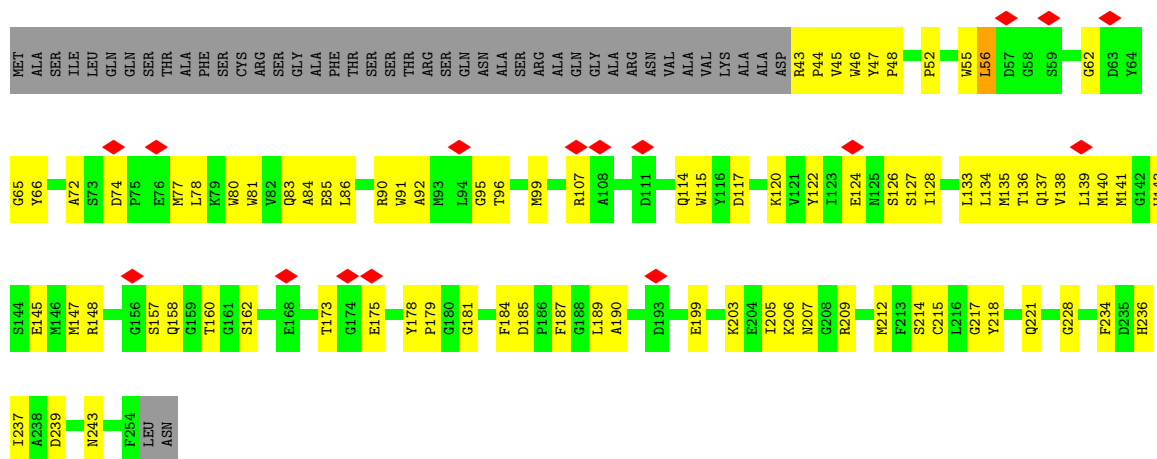


• Molecule 13: Lhca-a

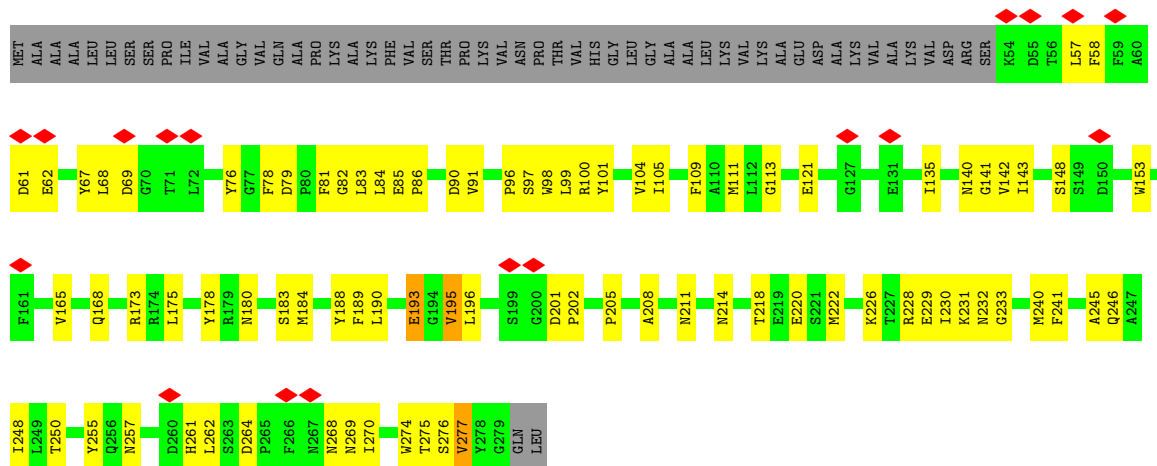


• Molecule 14: Lhca-c

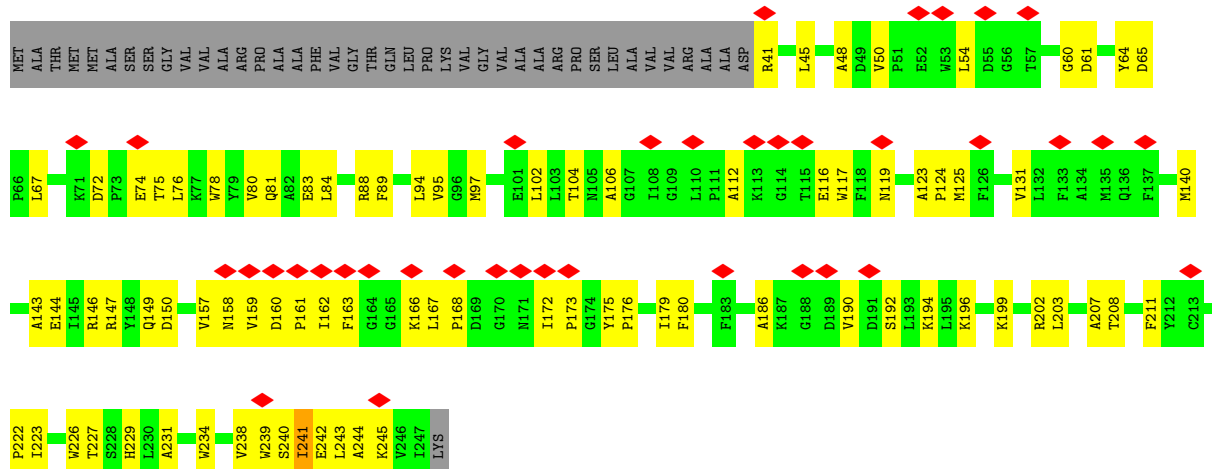




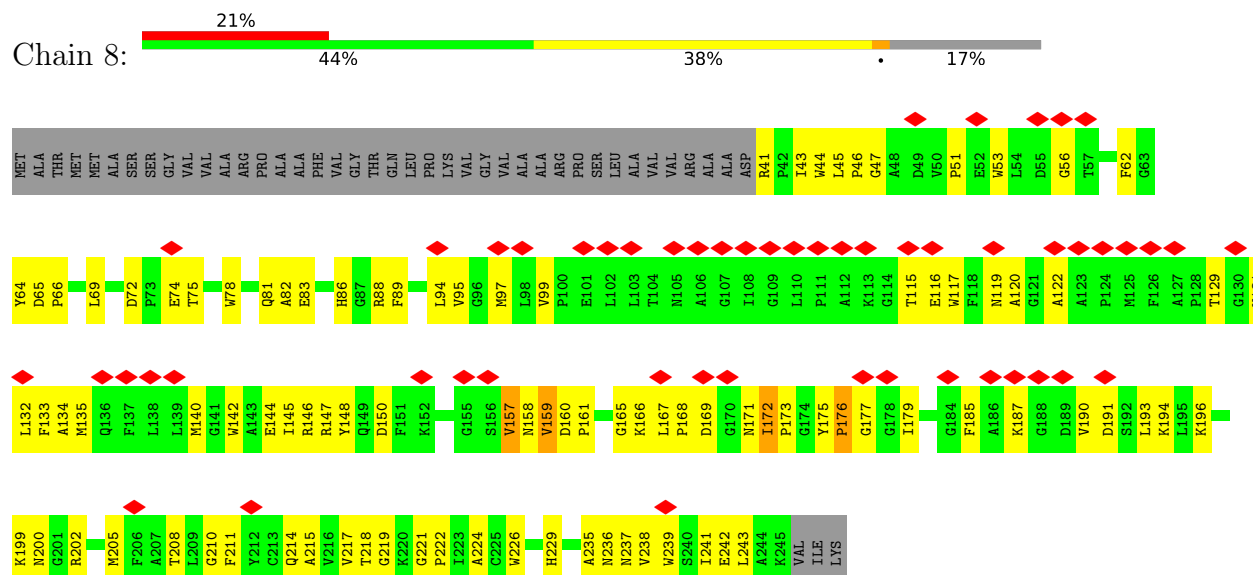
• Molecule 15: Lhca-d



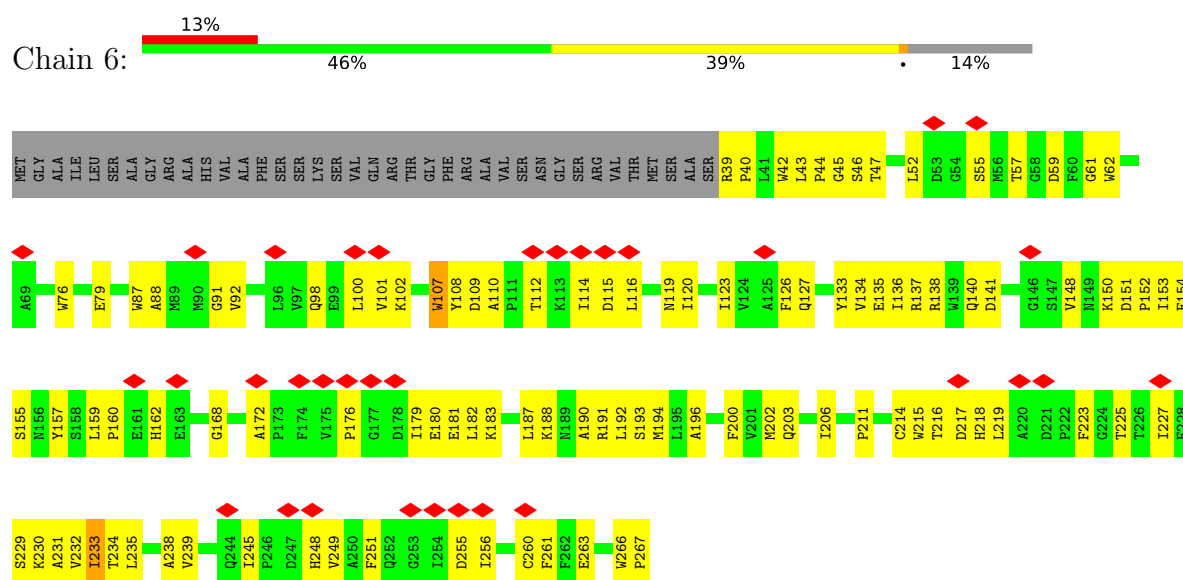
• Molecule 16: Lhca-b



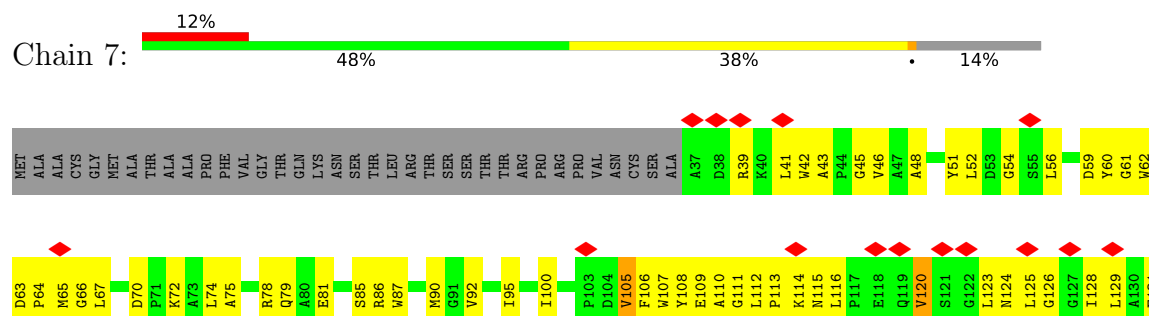
- Molecule 16: Lhca-b

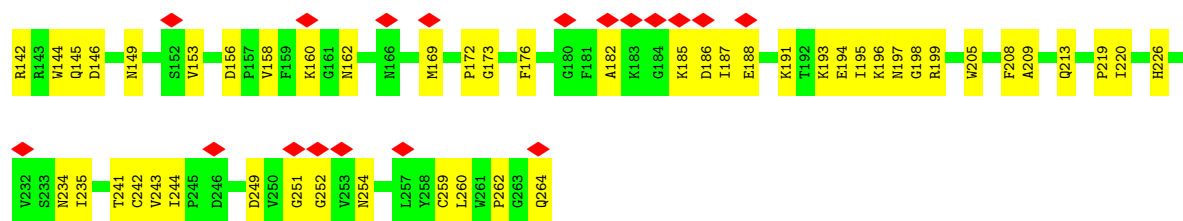


- Molecule 17: Lhca-g

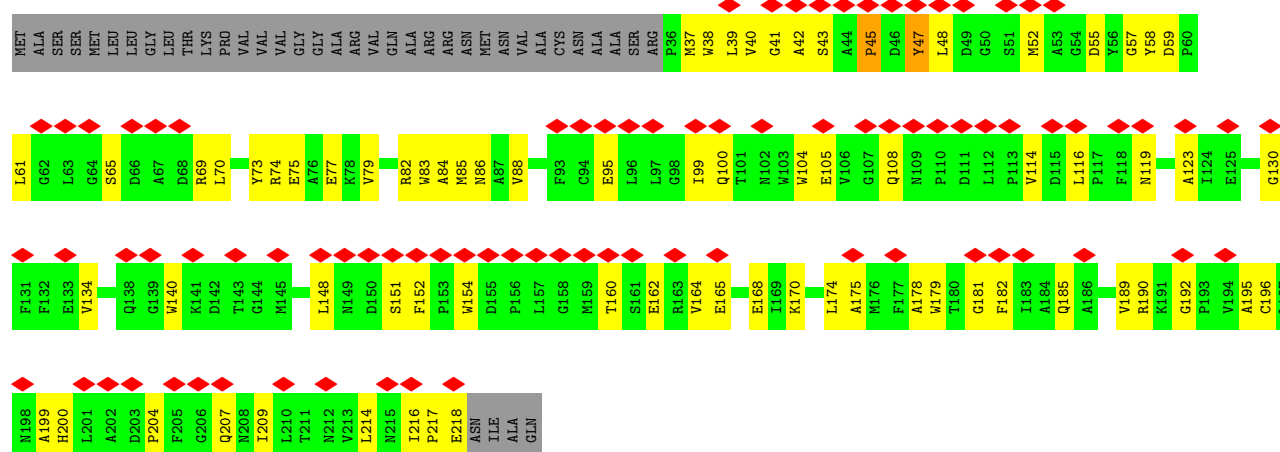


- Molecule 18: Lhca-h





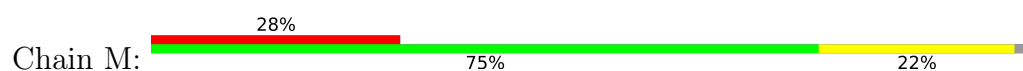
• Molecule 19: Lhca-i



• 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 ($\text{\AA}$)	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 ($\text{\AA}$)	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: PQN, HTG, DGD, LHG, CHL, 8CT, SF4, LMG, XAT, CLA

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	0.46	0/6015	0.50	0/8196
2	B	0.46	0/6034	0.54	0/8239
3	C	0.46	0/612	0.61	0/830
4	D	0.36	0/1135	0.58	0/1533
5	E	0.32	0/498	0.45	0/673
6	F	0.35	0/1281	0.54	0/1724
7	G	0.22	0/730	0.49	0/992
8	H	0.30	0/691	0.55	0/929
9	I	0.32	0/250	0.48	0/341
10	J	0.40	0/346	0.54	0/472
11	K	0.31	0/567	0.72	1/769 (0.1%)
12	L	0.28	0/1165	0.64	0/1591
13	1	0.33	0/1510	0.48	0/2054
13	5	0.31	0/1530	0.53	0/2082
14	2	0.43	0/1701	0.55	0/2315
15	3	0.46	0/1801	0.60	0/2444
16	4	0.40	0/1642	0.55	0/2238
16	8	0.41	0/1627	0.61	0/2217
17	6	0.37	0/1862	0.57	0/2542
18	7	0.38	0/1812	0.54	0/2468
19	9	0.34	0/1456	0.64	2/1986 (0.1%)
20	0	0.24	0/1603	0.53	0/2174
21	M	0.36	0/241	0.36	0/325
All	All	0.40	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(°)
19	9	47	TYR	CA-C-N	-5.66	115.19	123.00
19	9	47	TYR	C-N-CA	-5.66	115.19	123.00
11	K	25	GLY	N-CA-C	5.17	122.24	115.47

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	289	0
2	B	5824	0	5604	353	0
3	C	602	0	591	42	0
4	D	1109	0	1124	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	488	0	480	15	0
6	F	1257	0	1274	63	0
7	G	714	0	708	39	0
8	H	677	0	654	59	0
9	I	243	0	258	11	0
10	J	336	0	355	16	0
11	K	558	0	591	40	0
12	L	1139	0	1147	73	0
13	1	1466	0	1411	77	0
13	5	1484	0	1427	80	0
14	2	1641	0	1537	83	0
15	3	1751	0	1684	87	0
16	4	1589	0	1570	97	0
16	8	1574	0	1550	139	0
17	6	1797	0	1752	117	0
18	7	1758	0	1701	112	0
19	9	1416	0	1367	75	0
20	0	1560	0	1540	89	0
21	M	238	0	248	8	0
22	0	572	0	542	44	0
22	1	683	0	657	69	0
22	2	596	0	548	28	0
22	3	644	0	529	37	0
22	4	539	0	476	29	0
22	5	653	0	599	55	0
22	6	785	0	741	63	0
22	7	817	0	694	71	0
22	8	539	0	477	40	0
22	9	595	0	534	38	0
22	A	2628	0	2677	187	0
22	B	2420	0	2485	213	0
22	F	45	0	33	5	0
22	G	141	0	105	15	0
22	H	65	0	72	16	0
22	J	42	0	31	1	0
22	K	187	0	138	28	0
22	L	245	0	255	22	0
22	M	46	0	33	4	0
23	A	33	0	46	3	0
23	B	33	0	46	3	0
24	0	49	0	72	11	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	4	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	11	0
25	4	40	0	0	12	0
25	5	40	0	0	5	0
25	6	40	0	0	14	0
25	7	120	0	0	35	0
25	8	80	0	0	13	0
25	A	240	0	0	30	0
25	B	320	0	0	41	0
25	F	40	0	0	0	0
25	G	40	0	0	19	0
25	I	40	0	0	0	0
25	J	80	0	0	25	0
25	K	40	0	0	13	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	17	0
29	1	48	0	33	3	0
29	2	203	0	154	18	0
29	3	47	0	31	4	0
29	4	219	0	176	28	0
29	5	109	0	90	16	0
29	6	241	0	181	23	0
29	7	47	0	31	8	0
29	8	201	0	148	28	0
29	9	109	0	90	3	0
30	0	88	0	104	16	0
30	1	88	0	109	14	0
30	2	88	0	112	12	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	14	0
30	5	88	0	107	13	0
30	6	88	0	111	14	0
30	7	88	0	109	14	0
30	8	88	0	109	20	0
30	9	88	0	109	12	0
31	4	44	0	61	1	0
31	5	44	0	61	6	0
31	8	44	0	60	6	0
All	All	51585	0	48901	2587	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 26.

The worst 5 of 2587 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%)	24 57
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	38
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	23
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	27
12	L	153/204 (75%)	139 (91%)	13 (8%)	1 (1%)	18	51
13	1	191/226 (84%)	175 (92%)	15 (8%)	1 (0%)	24	57
13	5	193/226 (85%)	173 (90%)	19 (10%)	1 (0%)	24	57
14	2	210/256 (82%)	190 (90%)	20 (10%)	0	100	100
15	3	224/281 (80%)	197 (88%)	26 (12%)	1 (0%)	30	62
16	4	205/248 (83%)	176 (86%)	29 (14%)	0	100	100
16	8	203/248 (82%)	173 (85%)	27 (13%)	3 (2%)	8	37
17	6	227/267 (85%)	200 (88%)	26 (12%)	1 (0%)	30	62
18	7	226/264 (86%)	190 (84%)	31 (14%)	5 (2%)	5	30
19	9	181/222 (82%)	156 (86%)	24 (13%)	1 (1%)	21	54
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%)	23	54

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%)	87	85
2	B	600/601 (100%)	598 (100%)	2 (0%)	86	83
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%)	57	71
9	I	25/28 (89%)	25 (100%)	0	100	100
10	J	38/38 (100%)	37 (97%)	1 (3%)	40	62
11	K	58/94 (62%)	58 (100%)	0	100	100
12	L	118/157 (75%)	115 (98%)	3 (2%)	42	63
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%)	65	74
16	4	161/189 (85%)	160 (99%)	1 (1%)	78	79
16	8	159/189 (84%)	158 (99%)	1 (1%)	78	79
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%)	3607 (100%)	12 (0%)	84	83

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	92	ILE
15	3	193	GLU
16	8	172	ILE
15	3	195	VAL
8	H	124	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	595	HIS
13	1	98	ASN
16	8	237	ASN
2	B	607	ASN
6	F	235	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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
25	8CT	K	103	-	40,41,41	4.98	24 (60%)	51,56,56	2.66	18 (35%)
22	CLA	B	808	-	69,73,73	1.16	10 (14%)	82,113,113	1.35	6 (7%)
22	CLA	A	817	-	69,73,73	1.15	7 (10%)	82,113,113	1.34	8 (9%)
30	XAT	0	314	29,22	41,47,47	0.90	2 (4%)	54,74,74	2.92	22 (40%)
22	CLA	1	302	-	69,73,73	1.19	10 (14%)	82,113,113	1.33	6 (7%)
29	CHL	7	308	-	41,55,74	3.79	20 (48%)	35,91,114	2.71	13 (37%)
22	CLA	5	310	24	45,49,73	1.37	9 (20%)	54,84,113	1.53	6 (11%)
22	CLA	B	832	-	69,73,73	1.18	10 (14%)	82,113,113	1.37	6 (7%)
25	8CT	B	844	-	40,41,41	4.82	23 (57%)	51,56,56	2.97	17 (33%)
22	CLA	9	311	-	56,60,73	1.26	9 (16%)	65,97,113	1.46	6 (9%)
22	CLA	0	307	22	69,73,73	1.19	9 (13%)	82,113,113	1.33	7 (8%)
22	CLA	1	307	-	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
22	CLA	A	816	-	49,53,73	1.37	9 (18%)	58,89,113	1.44	4 (6%)
22	CLA	6	311	24	69,73,73	1.15	10 (14%)	82,113,113	1.30	5 (6%)
22	CLA	8	302	-	64,68,73	1.22	10 (15%)	76,107,113	1.27	5 (6%)
22	CLA	G	101	-	49,53,73	1.36	6 (12%)	58,89,113	1.39	5 (8%)
23	PQN	B	842	-	34,34,34	1.50	2 (5%)	43,45,45	1.15	3 (6%)
22	CLA	1	301	13	69,73,73	1.17	10 (14%)	82,113,113	1.38	8 (9%)
22	CLA	0	308	20	64,68,73	1.19	9 (14%)	76,107,113	1.28	5 (6%)
22	CLA	G	103	7	50,54,73	1.31	6 (12%)	59,90,113	1.44	5 (8%)
22	CLA	2	313	14	47,51,73	1.36	9 (19%)	55,86,113	1.48	4 (7%)
25	8CT	J	104	-	40,41,41	4.83	23 (57%)	51,56,56	2.85	19 (37%)
28	DGD	B	849	-	67,67,67	1.02	4 (5%)	81,81,81	1.51	13 (16%)
22	CLA	0	305	29,22	56,60,73	1.29	7 (12%)	65,97,113	1.46	8 (12%)
22	CLA	A	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.39	9 (10%)
22	CLA	5	305	-	56,60,73	1.30	7 (12%)	65,97,113	1.33	5 (7%)
22	CLA	A	843	24	56,60,73	1.28	9 (16%)	65,97,113	1.46	7 (10%)
22	CLA	A	841	-	69,73,73	1.19	8 (11%)	82,113,113	1.31	5 (6%)
22	CLA	5	312	30,13	69,73,73	1.15	8 (11%)	82,113,113	1.34	6 (7%)
22	CLA	A	820	-	49,53,73	1.37	9 (18%)	58,89,113	1.52	4 (6%)
22	CLA	A	818	1	69,73,73	1.18	10 (14%)	82,113,113	1.37	8 (9%)
22	CLA	9	309	-	64,68,73	1.18	9 (14%)	76,107,113	1.38	6 (7%)
22	CLA	A	815	1	51,55,73	1.32	9 (17%)	60,91,113	1.47	5 (8%)
29	CHL	0	301	22,24	55,69,74	3.50	19 (34%)	52,108,114	1.94	12 (23%)
22	CLA	A	822	-	53,57,73	1.30	8 (15%)	61,93,113	1.53	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	834	-	54,58,73	1.32	10 (18%)	64,95,113	1.41	6 (9%)
29	CHL	8	306	-	45,59,74	3.78	20 (44%)	40,96,114	2.55	14 (35%)
22	CLA	6	323	16	50,54,73	1.33	9 (18%)	59,90,113	1.38	4 (6%)
22	CLA	A	821	-	69,73,73	1.15	9 (13%)	82,113,113	1.38	9 (10%)
22	CLA	J	103	10	46,50,73	1.37	9 (19%)	53,85,113	1.50	4 (7%)
22	CLA	A	808	1	69,73,73	1.16	10 (14%)	82,113,113	1.35	7 (8%)
29	CHL	4	307	-	45,59,74	3.66	19 (42%)	40,96,114	2.67	13 (32%)
25	8CT	F	302	-	40,41,41	4.74	23 (57%)	51,56,56	3.24	21 (41%)
22	CLA	9	306	-	56,60,73	1.28	8 (14%)	65,97,113	1.41	6 (9%)
22	CLA	A	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	8 (9%)
22	CLA	B	828	-	69,73,73	1.16	11 (15%)	82,113,113	1.40	9 (10%)
27	SF4	C	102	3	0,12,12	-	-	-	-	-
22	CLA	9	310	24	45,49,73	1.38	9 (20%)	54,84,113	1.39	5 (9%)
25	8CT	4	317	-	40,41,41	4.88	23 (57%)	51,56,56	2.44	18 (35%)
29	CHL	2	306	-	42,56,74	3.93	20 (47%)	36,92,114	2.51	13 (36%)
22	CLA	8	315	-	69,73,73	1.15	9 (13%)	82,113,113	1.25	4 (4%)
22	CLA	7	317	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
25	8CT	7	321	-	40,41,41	4.80	23 (57%)	51,56,56	3.78	25 (49%)
22	CLA	9	305	-	56,60,73	1.27	9 (16%)	65,97,113	1.53	8 (12%)
22	CLA	4	309	30	64,68,73	1.18	9 (14%)	76,107,113	1.29	6 (7%)
22	CLA	K	105	-	54,58,73	1.30	9 (16%)	64,95,113	1.48	5 (7%)
22	CLA	B	811	2	69,73,73	1.18	10 (14%)	82,113,113	1.37	7 (8%)
29	CHL	4	305	29	50,64,74	3.60	19 (38%)	46,102,114	2.09	14 (30%)
30	XAT	6	320	-	41,47,47	0.99	3 (7%)	54,74,74	4.38	22 (40%)
25	8CT	1	316	-	40,41,41	4.87	23 (57%)	51,56,56	2.66	18 (35%)
25	8CT	J	101	-	40,41,41	4.81	23 (57%)	51,56,56	3.03	18 (35%)
22	CLA	4	310	-	59,63,73	1.24	10 (16%)	70,101,113	1.39	6 (8%)
22	CLA	3	311	-	59,63,73	1.24	8 (13%)	70,101,113	1.45	6 (8%)
22	CLA	8	304	-	54,58,73	1.30	9 (16%)	64,95,113	1.40	4 (6%)
22	CLA	B	837	-	69,73,73	1.13	9 (13%)	82,113,113	1.33	8 (9%)
22	CLA	3	308	-	54,58,73	1.31	11 (20%)	64,95,113	1.51	8 (12%)
22	CLA	A	852	-	53,57,73	1.31	9 (16%)	61,93,113	1.43	4 (6%)
22	CLA	B	813	-	59,63,73	1.25	10 (16%)	70,101,113	1.34	4 (5%)
22	CLA	7	311	24	41,45,73	1.38	8 (19%)	50,78,113	1.41	5 (10%)
25	8CT	I	101	-	40,41,41	4.68	22 (55%)	51,56,56	3.23	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	K	101	-	49,53,73	1.36	10 (20%)	58,89,113	1.40	5 (8%)
22	CLA	H	201	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	8 (9%)
22	CLA	7	318	22	69,73,73	1.16	9 (13%)	82,113,113	1.34	7 (8%)
22	CLA	B	823	-	59,63,73	1.26	10 (16%)	70,101,113	1.40	6 (8%)
22	CLA	4	312	16	60,64,73	1.24	8 (13%)	71,102,113	1.47	6 (8%)
22	CLA	A	835	1	49,53,73	1.38	10 (20%)	58,89,113	1.50	7 (12%)
27	SF4	B	802	-	0,12,12	-	-	-	-	-
22	CLA	7	314	18	49,53,73	1.36	9 (18%)	58,89,113	1.46	5 (8%)
25	8CT	2	317	-	40,41,41	4.83	23 (57%)	51,56,56	2.99	18 (35%)
22	CLA	7	305	-	49,53,73	1.35	8 (16%)	58,89,113	1.38	4 (6%)
25	8CT	3	316	-	40,41,41	4.82	23 (57%)	51,56,56	2.92	20 (39%)
30	XAT	1	315	-	41,47,47	0.92	2 (4%)	54,74,74	2.94	21 (38%)
22	CLA	5	314	24	50,54,73	1.34	9 (18%)	59,90,113	1.39	4 (6%)
22	CLA	B	833	-	62,66,73	1.23	8 (12%)	73,104,113	1.47	7 (9%)
22	CLA	M	101	-	50,54,73	1.34	9 (18%)	59,90,113	1.30	6 (10%)
30	XAT	6	319	22	41,47,47	0.96	2 (4%)	54,74,74	3.17	26 (48%)
22	CLA	A	833	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
22	CLA	8	311	-	56,60,73	1.31	9 (16%)	65,97,113	1.34	5 (7%)
22	CLA	1	306	-	69,73,73	1.17	10 (14%)	82,113,113	1.30	8 (9%)
22	CLA	2	309	-	64,68,73	1.21	12 (18%)	76,107,113	1.29	7 (9%)
30	XAT	3	315	-	41,47,47	0.98	2 (4%)	54,74,74	2.68	19 (35%)
22	CLA	B	836	2	64,68,73	1.20	11 (17%)	76,107,113	1.39	8 (10%)
22	CLA	A	819	-	69,73,73	1.17	10 (14%)	82,113,113	1.38	9 (10%)
22	CLA	5	313	-	59,63,73	1.24	9 (15%)	70,101,113	1.24	5 (7%)
25	8CT	B	848	-	40,41,41	4.84	23 (57%)	51,56,56	2.70	17 (33%)
22	CLA	K	104	-	50,54,73	1.35	9 (18%)	59,90,113	1.45	4 (6%)
30	XAT	4	316	-	41,47,47	1.03	3 (7%)	54,74,74	2.66	21 (38%)
22	CLA	2	308	-	54,58,73	1.29	10 (18%)	64,95,113	1.37	5 (7%)
22	CLA	B	839	-	69,73,73	1.16	10 (14%)	82,113,113	1.25	6 (7%)
22	CLA	A	828	-	69,73,73	1.15	10 (14%)	82,113,113	1.38	9 (10%)
22	CLA	A	837	1	69,73,73	1.15	10 (14%)	82,113,113	1.32	9 (10%)
22	CLA	6	303	17	69,73,73	1.17	8 (11%)	82,113,113	1.36	7 (8%)
22	CLA	3	319	-	69,73,73	1.18	10 (14%)	82,113,113	1.33	7 (8%)
22	CLA	2	319	16	50,54,73	1.35	10 (20%)	59,90,113	1.41	5 (8%)
22	CLA	5	309	30,13	64,68,73	1.21	9 (14%)	76,107,113	1.33	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	809	2	69,73,73	1.17	10 (14%)	82,113,113	1.31	6 (7%)
22	CLA	A	809	1	69,73,73	1.17	9 (13%)	82,113,113	1.32	7 (8%)
22	CLA	2	314	14	53,57,73	1.31	9 (16%)	61,93,113	1.39	6 (9%)
22	CLA	A	807	1	69,73,73	1.14	9 (13%)	82,113,113	1.36	6 (7%)
22	CLA	6	317	-	49,53,73	1.36	8 (16%)	58,89,113	1.48	6 (10%)
29	CHL	6	316	17	37,51,74	4.13	18 (48%)	30,86,114	2.67	11 (36%)
22	CLA	F	301	-	49,53,73	1.37	8 (16%)	58,89,113	1.46	6 (10%)
22	CLA	B	826	-	69,73,73	1.14	9 (13%)	82,113,113	1.33	7 (8%)
29	CHL	8	314	-	37,51,74	4.24	17 (45%)	30,86,114	2.58	11 (36%)
22	CLA	A	826	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	5 (6%)
22	CLA	3	310	-	56,60,73	1.28	8 (14%)	65,97,113	1.40	5 (7%)
22	CLA	1	311	13	69,73,73	1.18	9 (13%)	82,113,113	1.33	6 (7%)
22	CLA	6	318	17	56,60,73	1.29	8 (14%)	65,97,113	1.51	7 (10%)
22	CLA	7	306	-	46,50,73	1.40	10 (21%)	53,85,113	1.39	6 (11%)
22	CLA	3	302	15	54,58,73	1.31	8 (14%)	64,95,113	1.37	5 (7%)
29	CHL	8	305	-	50,64,74	3.60	20 (40%)	46,102,114	2.40	12 (26%)
22	CLA	A	831	1	54,58,73	1.30	9 (16%)	64,95,113	1.49	7 (10%)
30	XAT	9	314	22	41,47,47	0.96	2 (4%)	54,74,74	4.38	26 (48%)
22	CLA	B	815	2	69,73,73	1.15	10 (14%)	82,113,113	1.44	7 (8%)
22	CLA	5	307	-	69,73,73	1.14	8 (11%)	82,113,113	1.26	7 (8%)
22	CLA	1	309	24	45,49,73	1.38	9 (20%)	54,84,113	1.56	7 (12%)
22	CLA	B	822	2	50,54,73	1.32	8 (16%)	59,90,113	1.50	5 (8%)
22	CLA	4	308	16	54,58,73	1.31	8 (14%)	64,95,113	1.51	7 (10%)
29	CHL	2	307	-	45,59,74	3.53	19 (42%)	40,96,114	2.75	16 (40%)
22	CLA	7	310	18	54,58,73	1.27	8 (14%)	64,95,113	1.60	8 (12%)
22	CLA	7	302	18	50,54,73	1.33	9 (18%)	59,90,113	1.43	5 (8%)
22	CLA	4	302	-	64,68,73	1.23	10 (15%)	76,107,113	1.37	7 (9%)
22	CLA	B	821	-	54,58,73	1.31	9 (16%)	64,95,113	1.42	7 (10%)
22	CLA	B	810	2	69,73,73	1.15	8 (11%)	82,113,113	1.35	7 (8%)
22	CLA	L	202	-	69,73,73	1.14	9 (13%)	82,113,113	1.39	9 (10%)
29	CHL	6	307	-	37,51,74	4.18	18 (48%)	30,86,114	2.42	9 (30%)
22	CLA	6	305	-	64,68,73	1.20	8 (12%)	76,107,113	1.22	4 (5%)
25	8CT	B	847	-	40,41,41	4.83	23 (57%)	51,56,56	2.81	18 (35%)
22	CLA	2	303	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	4 (4%)
25	8CT	L	206	-	40,41,41	4.80	23 (57%)	51,56,56	3.11	19 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	8CT	A	848	-	40,41,41	4.78	23 (57%)	51,56,56	2.83	16 (31%)
22	CLA	9	303	19	69,73,73	1.16	9 (13%)	82,113,113	1.39	6 (7%)
31	LMG	5	319	22	44,44,55	0.97	3 (6%)	52,52,63	1.32	7 (13%)
22	CLA	8	308	16	54,58,73	1.31	10 (18%)	64,95,113	1.56	8 (12%)
29	CHL	3	306	-	41,55,74	3.74	19 (46%)	35,91,114	2.62	13 (37%)
22	CLA	A	805	-	69,73,73	1.17	8 (11%)	82,113,113	1.32	7 (8%)
22	CLA	B	840	-	69,73,73	1.17	9 (13%)	82,113,113	1.36	5 (6%)
22	CLA	4	303	16	50,54,73	1.34	9 (18%)	59,90,113	1.43	4 (6%)
22	CLA	6	315	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	5 (6%)
22	CLA	4	313	16	49,53,73	1.36	10 (20%)	58,89,113	1.49	5 (8%)
22	CLA	A	806	1	69,73,73	1.20	11 (15%)	82,113,113	1.34	8 (9%)
31	LMG	4	318	-	44,44,55	0.99	4 (9%)	52,52,63	1.49	10 (19%)
22	CLA	0	304	22	56,60,73	1.29	9 (16%)	65,97,113	1.40	5 (7%)
24	LHG	1	317	22	48,48,48	0.70	2 (4%)	51,54,54	1.32	7 (13%)
22	CLA	A	830	1	69,73,73	1.17	9 (13%)	82,113,113	1.39	8 (9%)
25	8CT	8	301	-	40,41,41	4.84	23 (57%)	51,56,56	2.73	19 (37%)
29	CHL	1	305	-	42,56,74	3.92	19 (45%)	36,92,114	2.28	11 (30%)
22	CLA	A	825	-	69,73,73	1.17	7 (10%)	82,113,113	1.33	7 (8%)
22	CLA	9	312	30	63,67,73	1.22	10 (15%)	74,105,113	1.29	6 (8%)
22	CLA	4	304	-	54,58,73	1.29	10 (18%)	64,95,113	1.50	8 (12%)
22	CLA	1	310	-	56,60,73	1.29	9 (16%)	65,97,113	1.38	5 (7%)
23	PQN	A	842	-	34,34,34	1.50	2 (5%)	43,45,45	1.34	7 (16%)
22	CLA	A	814	-	49,53,73	1.37	10 (20%)	58,89,113	1.41	5 (8%)
22	CLA	A	836	-	55,59,73	1.29	9 (16%)	64,96,113	1.46	7 (10%)
22	CLA	0	312	29,20	59,63,73	1.27	9 (15%)	70,101,113	1.41	7 (10%)
22	CLA	6	312	-	56,60,73	1.29	10 (17%)	65,97,113	1.40	5 (7%)
22	CLA	B	824	-	64,68,73	1.20	9 (14%)	76,107,113	1.38	7 (9%)
29	CHL	9	307	-	42,56,74	4.03	20 (47%)	36,92,114	2.47	11 (30%)
29	CHL	8	307	30	45,59,74	3.73	19 (42%)	40,96,114	2.65	15 (37%)
29	CHL	5	301	13	55,69,74	3.46	20 (36%)	52,108,114	2.05	14 (26%)
22	CLA	A	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	5 (6%)
22	CLA	G	102	-	54,58,73	1.30	9 (16%)	64,95,113	1.46	6 (9%)
29	CHL	2	305	-	37,51,74	4.03	19 (51%)	30,86,114	2.64	12 (40%)
22	CLA	3	305	15	51,55,73	1.31	9 (17%)	60,91,113	1.39	5 (8%)
22	CLA	2	310	24	45,49,73	1.39	10 (22%)	54,84,113	1.51	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	L	204	-	54,58,73	1.31	9 (16%)	64,95,113	1.40	6 (9%)
22	CLA	3	303	-	49,53,73	1.36	10 (20%)	58,89,113	1.45	6 (10%)
22	CLA	A	813	-	69,73,73	1.15	9 (13%)	82,113,113	1.46	10 (12%)
22	CLA	A	823	-	55,59,73	1.30	9 (16%)	64,96,113	1.44	5 (7%)
22	CLA	7	307	-	51,55,73	1.33	8 (15%)	60,91,113	1.42	5 (8%)
22	CLA	A	804	22	59,63,73	1.25	9 (15%)	70,101,113	1.49	7 (10%)
22	CLA	7	316	18	69,73,73	1.15	9 (13%)	82,113,113	1.25	4 (4%)
22	CLA	B	814	-	69,73,73	1.16	10 (14%)	82,113,113	1.39	9 (10%)
25	8CT	B	804	-	40,41,41	4.70	23 (57%)	51,56,56	2.98	20 (39%)
22	CLA	3	309	24	41,45,73	1.40	9 (21%)	50,78,113	1.52	7 (14%)
22	CLA	7	303	18	64,68,73	1.22	8 (12%)	76,107,113	1.40	8 (10%)
30	XAT	4	315	22	41,47,47	0.99	1 (2%)	54,74,74	3.04	27 (50%)
22	CLA	4	314	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	6 (7%)
24	LHG	B	852	22	22,22,48	0.85	0	25,28,54	1.25	1 (4%)
22	CLA	7	309	22	54,58,73	1.31	10 (18%)	64,95,113	1.32	5 (7%)
22	CLA	L	201	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	4 (4%)
30	XAT	0	313	22	41,47,47	1.16	3 (7%)	54,74,74	4.82	22 (40%)
22	CLA	B	827	-	69,73,73	1.15	10 (14%)	82,113,113	1.36	9 (10%)
22	CLA	B	838	-	51,55,73	1.32	8 (15%)	60,91,113	1.38	5 (8%)
22	CLA	B	807	-	49,53,73	1.35	10 (20%)	58,89,113	1.65	8 (13%)
22	CLA	A	838	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	7 (8%)
22	CLA	B	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	8 (9%)
26	HTG	A	851	-	19,19,19	1.01	2 (10%)	23,24,24	0.73	0
22	CLA	8	303	22,16,31	50,54,73	1.33	9 (18%)	59,90,113	1.42	5 (8%)
22	CLA	A	839	-	69,73,73	1.17	9 (13%)	82,113,113	1.37	8 (9%)
22	CLA	8	313	16	49,53,73	1.37	9 (18%)	58,89,113	1.46	5 (8%)
22	CLA	B	831	-	54,58,73	1.32	9 (16%)	64,95,113	1.46	8 (12%)
22	CLA	L	203	-	69,73,73	1.13	8 (11%)	82,113,113	1.26	5 (6%)
22	CLA	9	308	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	5 (6%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-
30	XAT	5	316	-	41,47,47	0.99	4 (9%)	54,74,74	3.02	22 (40%)
22	CLA	B	830	2	69,73,73	1.17	9 (13%)	82,113,113	1.40	10 (12%)
25	8CT	5	317	-	40,41,41	4.88	22 (55%)	51,56,56	3.52	22 (43%)
22	CLA	4	311	22	56,60,73	1.29	8 (14%)	65,97,113	1.43	6 (9%)
22	CLA	K	102	-	50,54,73	1.33	10 (20%)	59,90,113	1.49	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	4	301	22,13	55,69,74	3.31	20 (36%)	52,108,114	2.56	13 (25%)
30	XAT	8	317	-	41,47,47	0.95	2 (4%)	54,74,74	2.78	19 (35%)
22	CLA	A	811	22,1	69,73,73	1.18	8 (11%)	82,113,113	1.30	4 (4%)
22	CLA	B	850	-	59,63,73	1.23	9 (15%)	70,101,113	1.48	10 (14%)
22	CLA	1	313	-	50,54,73	1.33	9 (18%)	59,90,113	1.44	5 (8%)
25	8CT	7	323	-	40,41,41	4.83	23 (57%)	51,56,56	2.81	19 (37%)
22	CLA	B	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	6 (7%)
22	CLA	5	308	-	46,50,73	1.42	8 (17%)	53,85,113	1.58	6 (11%)
22	CLA	3	304	-	46,50,73	1.36	8 (17%)	53,85,113	1.40	4 (7%)
22	CLA	1	308	30,13	64,68,73	1.20	9 (14%)	76,107,113	1.34	7 (9%)
30	XAT	3	314	-	41,47,47	0.98	3 (7%)	54,74,74	4.54	29 (53%)
22	CLA	B	801	-	69,73,73	1.16	11 (15%)	82,113,113	1.40	6 (7%)
22	CLA	7	313	18	59,63,73	1.25	9 (15%)	70,101,113	1.50	7 (10%)
22	CLA	2	304	-	64,68,73	1.19	9 (14%)	76,107,113	1.33	6 (7%)
22	CLA	B	818	2	63,67,73	1.23	8 (12%)	74,105,113	1.53	8 (10%)
22	CLA	5	302	-	69,73,73	1.16	10 (14%)	82,113,113	1.27	7 (8%)
22	CLA	8	310	31	59,63,73	1.25	8 (13%)	70,101,113	1.44	4 (5%)
22	CLA	3	301	-	64,68,73	1.20	10 (15%)	76,107,113	1.36	8 (10%)
22	CLA	0	309	24	45,49,73	1.39	8 (17%)	54,84,113	1.38	5 (9%)
30	XAT	1	314	22	41,47,47	0.97	3 (7%)	54,74,74	4.66	27 (50%)
22	CLA	1	303	-	56,60,73	1.26	10 (17%)	65,97,113	1.41	6 (9%)
22	CLA	6	309	17	54,58,73	1.30	8 (14%)	64,95,113	1.42	5 (7%)
22	CLA	0	302	30	69,73,73	1.16	10 (14%)	82,113,113	1.27	6 (7%)
22	CLA	3	307	15	54,58,73	1.34	8 (14%)	64,95,113	1.45	5 (7%)
24	LHG	6	322	22	36,36,48	0.79	1 (2%)	39,42,54	1.29	5 (12%)
25	8CT	B	846	-	40,41,41	4.84	23 (57%)	51,56,56	2.94	18 (35%)
25	8CT	A	854	-	40,41,41	4.82	23 (57%)	51,56,56	2.76	17 (33%)
22	CLA	5	311	30	49,53,73	1.37	9 (18%)	58,89,113	1.46	7 (12%)
24	LHG	5	318	22	48,48,48	0.67	1 (2%)	51,54,54	1.30	6 (11%)
25	8CT	7	301	-	40,41,41	4.77	24 (60%)	51,56,56	2.81	19 (37%)
24	LHG	2	318	22	31,31,48	0.82	1 (3%)	34,37,54	1.34	4 (11%)
22	CLA	0	311	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
22	CLA	A	840	-	69,73,73	1.14	8 (11%)	82,113,113	1.36	7 (8%)
22	CLA	6	313	29,17	69,73,73	1.15	9 (13%)	82,113,113	1.38	8 (9%)
22	CLA	B	806	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	XAT	7	320	-	41,47,47	0.97	2 (4%)	54,74,74	2.62	20 (37%)
22	CLA	8	312	16	60,64,73	1.24	9 (15%)	71,102,113	1.41	5 (7%)
29	CHL	6	306	-	37,51,74	4.00	18 (48%)	30,86,114	2.99	12 (40%)
22	CLA	3	312	15	49,53,73	1.34	9 (18%)	58,89,113	1.49	6 (10%)
25	8CT	G	104	-	40,41,41	4.87	23 (57%)	51,56,56	2.64	18 (35%)
22	CLA	2	302	29	69,73,73	1.15	10 (14%)	82,113,113	1.40	11 (13%)
22	CLA	2	312	14	69,73,73	1.13	8 (11%)	82,113,113	1.38	6 (7%)
30	XAT	9	315	-	41,47,47	0.93	2 (4%)	54,74,74	2.76	21 (38%)
22	CLA	9	304	-	52,56,73	1.33	9 (17%)	61,92,113	1.43	5 (8%)
29	CHL	9	302	19	55,69,74	3.36	20 (36%)	52,108,114	2.42	16 (30%)
22	CLA	6	304	17	69,73,73	1.18	11 (15%)	82,113,113	1.32	7 (8%)
29	CHL	6	302	22,17	55,69,74	3.45	20 (36%)	52,108,114	2.06	15 (28%)
22	CLA	7	312	30	56,60,73	1.30	11 (19%)	65,97,113	1.32	6 (9%)
29	CHL	5	306	-	42,56,74	4.04	19 (45%)	36,92,114	2.27	10 (27%)
29	CHL	6	308	-	45,59,74	3.75	20 (44%)	40,96,114	2.54	16 (40%)
22	CLA	B	835	-	49,53,73	1.35	8 (16%)	58,89,113	1.47	4 (6%)
22	CLA	6	310	17,30	64,68,73	1.22	10 (15%)	76,107,113	1.36	8 (10%)
22	CLA	B	817	-	59,63,73	1.23	9 (15%)	70,101,113	1.38	5 (7%)
30	XAT	7	319	22	41,47,47	0.99	3 (7%)	54,74,74	3.08	21 (38%)
24	LHG	0	315	29,22	48,48,48	0.59	0	51,54,54	1.26	5 (9%)
31	LMG	8	319	22	44,44,55	0.87	4 (9%)	52,52,63	1.40	4 (7%)
25	8CT	A	849	-	40,41,41	4.84	23 (57%)	51,56,56	2.69	18 (35%)
22	CLA	9	313	19	59,63,73	1.24	9 (15%)	70,101,113	1.31	5 (7%)
29	CHL	0	306	22,30	42,56,74	4.05	20 (47%)	36,92,114	2.23	9 (25%)
22	CLA	5	304	-	56,60,73	1.27	8 (14%)	65,97,113	1.40	4 (6%)
25	8CT	3	318	-	40,41,41	4.82	24 (60%)	51,56,56	3.74	21 (41%)
22	CLA	7	315	18	50,54,73	1.31	10 (20%)	59,90,113	1.43	5 (8%)
24	LHG	7	322	22	19,19,48	0.94	0	21,24,54	1.35	2 (9%)
22	CLA	A	801	-	69,73,73	1.20	9 (13%)	82,113,113	1.28	8 (9%)
22	CLA	0	310	30	56,60,73	1.28	8 (14%)	65,97,113	1.44	5 (7%)
22	CLA	1	312	29,13	59,63,73	1.27	9 (15%)	70,101,113	1.41	7 (10%)
22	CLA	A	853	-	69,73,73	1.17	10 (14%)	82,113,113	1.23	7 (8%)
26	HTG	J	102	-	19,19,19	1.02	2 (10%)	23,24,24	0.75	0
22	CLA	A	824	-	59,63,73	1.24	11 (18%)	70,101,113	1.36	6 (8%)
22	CLA	7	304	22	51,55,73	1.33	9 (17%)	60,91,113	1.46	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	9	301	2	50,54,73	1.46	10 (20%)	61,90,113	1.46	7 (11%)
22	CLA	6	314	-	47,51,73	1.34	8 (17%)	55,86,113	1.45	4 (7%)
22	CLA	6	301	-	56,60,73	1.30	9 (16%)	65,97,113	1.37	6 (9%)
24	LHG	3	317	22	19,19,48	0.86	0	21,24,54	1.41	2 (9%)
22	CLA	B	819	-	64,68,73	1.20	11 (17%)	76,107,113	1.31	7 (9%)
25	8CT	8	318	-	40,41,41	4.83	23 (57%)	51,56,56	2.74	17 (33%)
22	CLA	B	820	-	69,73,73	1.16	10 (14%)	82,113,113	1.32	5 (6%)
25	8CT	A	847	-	40,41,41	4.75	23 (57%)	51,56,56	3.01	19 (37%)
22	CLA	5	303	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
22	CLA	A	827	-	69,73,73	1.18	11 (15%)	82,113,113	1.37	9 (10%)
29	CHL	2	301	22	55,69,74	3.32	19 (34%)	52,108,114	2.59	17 (32%)
22	CLA	B	834	2	69,73,73	1.19	10 (14%)	82,113,113	1.27	5 (6%)
22	CLA	A	810	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
25	8CT	L	205	-	40,41,41	4.79	23 (57%)	51,56,56	3.18	22 (43%)
22	CLA	8	309	-	64,68,73	1.18	9 (14%)	76,107,113	1.43	7 (9%)
22	CLA	B	816	2	64,68,73	1.19	10 (15%)	76,107,113	1.45	5 (6%)
22	CLA	B	812	2	69,73,73	1.18	9 (13%)	82,113,113	1.32	7 (8%)
22	CLA	B	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	6 (7%)
25	8CT	B	851	-	40,41,41	4.88	24 (60%)	51,56,56	2.55	19 (37%)
22	CLA	A	812	-	58,62,73	1.27	9 (15%)	68,99,113	1.45	6 (8%)
22	CLA	0	303	30	69,73,73	1.17	10 (14%)	82,113,113	1.25	5 (6%)
22	CLA	2	311	14	56,60,73	1.30	10 (17%)	65,97,113	1.48	7 (10%)
25	8CT	A	846	-	40,41,41	4.78	23 (57%)	51,56,56	3.12	21 (41%)
30	XAT	2	316	-	41,47,47	0.98	3 (7%)	54,74,74	3.07	21 (38%)
25	8CT	B	843	-	40,41,41	4.87	23 (57%)	51,56,56	2.89	19 (37%)
24	LHG	9	316	22	48,48,48	0.62	1 (2%)	51,54,54	1.29	6 (11%)
30	XAT	2	315	-	41,47,47	1.10	2 (4%)	54,74,74	5.74	30 (55%)
30	XAT	8	316	29	41,47,47	0.94	2 (4%)	54,74,74	3.68	28 (51%)
30	XAT	5	315	22	41,47,47	1.02	2 (4%)	54,74,74	4.62	24 (44%)
22	CLA	B	841	24	69,73,73	1.16	9 (13%)	82,113,113	1.38	9 (10%)
24	LHG	A	844	-	48,48,48	0.76	1 (2%)	51,54,54	1.34	6 (11%)
29	CHL	4	306	29	45,59,74	3.87	19 (42%)	40,96,114	2.47	14 (35%)
22	CLA	1	304	-	56,60,73	1.28	9 (16%)	65,97,113	1.40	6 (9%)
24	LHG	A	845	22	26,26,48	0.97	1 (3%)	29,32,54	1.38	3 (10%)
22	CLA	B	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	8CT	6	321	-	40,41,41	4.81	23 (57%)	51,56,56	3.32	21 (41%)
25	8CT	B	845	-	40,41,41	4.78	23 (57%)	51,56,56	3.27	21 (41%)
25	8CT	A	850	-	40,41,41	4.81	23 (57%)	51,56,56	2.96	20 (39%)
22	CLA	A	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.33	7 (8%)
22	CLA	3	313	15	50,54,73	1.34	9 (18%)	59,90,113	1.48	4 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	K	103	-	-	13/29/63/63	0/2/2/2
22	CLA	B	808	-	1/1/15/20	17/39/115/115	-
22	CLA	A	817	-	1/1/15/20	17/39/115/115	-
30	XAT	0	314	29,22	-	8/31/93/93	0/4/4/4
22	CLA	1	302	-	1/1/15/20	23/39/115/115	-
29	CHL	7	308	-	3/3/16/26	9/17/115/137	-
22	CLA	5	310	24	1/1/10/20	4/10/86/115	-
22	CLA	B	832	-	1/1/15/20	14/39/115/115	-
25	8CT	B	844	-	-	15/29/63/63	0/2/2/2
22	CLA	9	311	-	1/1/12/20	6/24/100/115	-
22	CLA	0	307	22	1/1/15/20	27/39/115/115	-
22	CLA	1	307	-	1/1/15/20	18/39/115/115	-
22	CLA	A	816	-	1/1/11/20	4/15/91/115	-
22	CLA	6	311	24	1/1/15/20	20/39/115/115	-
22	CLA	8	302	-	1/1/14/20	5/33/109/115	-
22	CLA	G	101	-	1/1/11/20	7/15/91/115	-
23	PQN	B	842	-	-	3/23/43/43	0/2/2/2
22	CLA	1	301	13	1/1/15/20	12/39/115/115	-
22	CLA	0	308	20	1/1/14/20	16/33/109/115	-
22	CLA	G	103	7	1/1/11/20	7/17/93/115	-
22	CLA	2	313	14	1/1/10/20	4/13/89/115	-
25	8CT	J	104	-	-	7/29/63/63	0/2/2/2
28	DGD	B	849	-	-	31/55/95/95	0/2/2/2
22	CLA	0	305	29,22	1/1/12/20	10/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	803	-	1/1/15/20	17/39/115/115	-
22	CLA	5	305	-	1/1/12/20	6/24/100/115	-
22	CLA	A	843	24	1/1/12/20	12/24/100/115	-
22	CLA	A	841	-	1/1/15/20	15/39/115/115	-
22	CLA	5	312	30,13	1/1/15/20	11/39/115/115	-
22	CLA	A	820	-	1/1/11/20	3/15/91/115	-
22	CLA	A	818	1	1/1/15/20	13/39/115/115	-
22	CLA	9	309	-	1/1/14/20	15/33/109/115	-
22	CLA	A	815	1	1/1/11/20	3/18/94/115	-
29	CHL	0	301	22,24	4/4/19/26	18/33/131/137	-
22	CLA	A	822	-	1/1/11/20	12/20/96/115	-
22	CLA	A	834	-	1/1/12/20	3/21/97/115	-
29	CHL	8	306	-	3/3/17/26	6/21/119/137	-
22	CLA	6	323	16	1/1/11/20	11/17/93/115	-
22	CLA	A	821	-	1/1/15/20	9/39/115/115	-
22	CLA	J	103	10	1/1/10/20	6/12/88/115	-
22	CLA	A	808	1	1/1/15/20	18/39/115/115	-
29	CHL	4	307	-	3/3/17/26	5/21/119/137	-
25	8CT	F	302	-	-	8/29/63/63	0/2/2/2
22	CLA	9	306	-	1/1/12/20	9/24/100/115	-
22	CLA	A	802	-	1/1/15/20	6/39/115/115	-
22	CLA	B	828	-	1/1/15/20	15/39/115/115	-
27	SF4	C	102	3	-	-	0/6/5/5
22	CLA	9	310	24	1/1/10/20	6/10/86/115	-
29	CHL	2	306	-	3/3/16/26	6/18/116/137	-
25	8CT	4	317	-	-	8/29/63/63	0/2/2/2
22	CLA	8	315	-	1/1/15/20	23/39/115/115	-
22	CLA	7	317	-	1/1/15/20	20/39/115/115	-
25	8CT	7	321	-	-	10/29/63/63	0/2/2/2
22	CLA	9	305	-	1/1/12/20	6/24/100/115	-
22	CLA	4	309	30	1/1/14/20	13/33/109/115	-
22	CLA	K	105	-	1/1/12/20	11/21/97/115	-
22	CLA	B	811	2	1/1/15/20	10/39/115/115	-
29	CHL	4	305	29	4/4/18/26	12/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	XAT	6	320	-	-	4/31/93/93	0/4/4/4
25	8CT	1	316	-	-	11/29/63/63	0/2/2/2
25	8CT	J	101	-	-	9/29/63/63	0/2/2/2
22	CLA	4	310	-	1/1/13/20	9/27/103/115	-
22	CLA	3	311	-	1/1/13/20	12/27/103/115	-
22	CLA	8	304	-	1/1/12/20	11/21/97/115	-
22	CLA	B	837	-	1/1/15/20	17/39/115/115	-
22	CLA	3	308	-	1/1/12/20	2/21/97/115	-
22	CLA	A	852	-	1/1/11/20	5/20/96/115	-
22	CLA	B	813	-	1/1/13/20	6/27/103/115	-
22	CLA	7	311	24	1/1/8/20	2/4/76/115	-
25	8CT	I	101	-	-	10/29/63/63	0/2/2/2
22	CLA	K	101	-	1/1/11/20	8/15/91/115	-
22	CLA	H	201	-	1/1/15/20	16/39/115/115	-
22	CLA	7	318	22	1/1/15/20	18/39/115/115	-
22	CLA	B	823	-	-	11/27/103/115	-
22	CLA	4	312	16	1/1/13/20	7/29/105/115	-
22	CLA	A	835	1	1/1/11/20	4/15/91/115	-
27	SF4	B	802	-	-	-	0/6/5/5
22	CLA	7	314	18	1/1/11/20	6/15/91/115	-
25	8CT	2	317	-	-	11/29/63/63	0/2/2/2
22	CLA	7	305	-	1/1/11/20	9/15/91/115	-
25	8CT	3	316	-	-	12/29/63/63	0/2/2/2
30	XAT	1	315	-	-	1/31/93/93	0/4/4/4
22	CLA	5	314	24	1/1/11/20	9/17/93/115	-
22	CLA	B	833	-	1/1/13/20	15/31/107/115	-
22	CLA	M	101	-	-	6/17/93/115	-
30	XAT	6	319	22	-	3/31/93/93	0/4/4/4
22	CLA	A	833	-	1/1/15/20	14/39/115/115	-
22	CLA	8	311	-	-	8/24/100/115	-
22	CLA	1	306	-	1/1/15/20	14/39/115/115	-
22	CLA	2	309	-	1/1/14/20	10/33/109/115	-
30	XAT	3	315	-	-	0/31/93/93	0/4/4/4
22	CLA	B	836	2	1/1/14/20	12/33/109/115	-
22	CLA	A	819	-	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	313	-	1/1/13/20	8/27/103/115	-
25	8CT	B	848	-	-	10/29/63/63	0/2/2/2
22	CLA	K	104	-	1/1/11/20	7/17/93/115	-
30	XAT	4	316	-	-	3/31/93/93	0/4/4/4
22	CLA	2	308	-	1/1/12/20	4/21/97/115	-
22	CLA	B	839	-	1/1/15/20	15/39/115/115	-
22	CLA	A	828	-	1/1/15/20	17/39/115/115	-
22	CLA	A	837	1	1/1/15/20	19/39/115/115	-
22	CLA	6	303	17	1/1/15/20	16/39/115/115	-
22	CLA	3	319	-	1/1/15/20	21/39/115/115	-
22	CLA	2	319	16	1/1/11/20	10/17/93/115	-
22	CLA	5	309	30,13	1/1/14/20	9/33/109/115	-
22	CLA	B	809	2	1/1/15/20	20/39/115/115	-
22	CLA	A	809	1	1/1/15/20	13/39/115/115	-
22	CLA	2	314	14	1/1/11/20	7/20/96/115	-
22	CLA	A	807	1	1/1/15/20	13/39/115/115	-
22	CLA	6	317	-	1/1/11/20	7/15/91/115	-
29	CHL	6	316	17	3/3/15/26	6/12/110/137	-
22	CLA	F	301	-	1/1/11/20	8/15/91/115	-
22	CLA	B	826	-	1/1/15/20	11/39/115/115	-
29	CHL	8	314	-	3/3/15/26	4/12/110/137	-
22	CLA	A	826	-	1/1/15/20	15/39/115/115	-
22	CLA	3	310	-	1/1/12/20	3/24/100/115	-
22	CLA	1	311	13	1/1/15/20	14/39/115/115	-
22	CLA	6	318	17	1/1/12/20	6/24/100/115	-
22	CLA	7	306	-	1/1/10/20	4/12/88/115	-
22	CLA	3	302	15	1/1/12/20	2/21/97/115	-
29	CHL	8	305	-	4/4/18/26	9/27/125/137	-
22	CLA	A	831	1	1/1/12/20	1/21/97/115	-
30	XAT	9	314	22	-	4/31/93/93	0/4/4/4
22	CLA	B	815	2	1/1/15/20	11/39/115/115	-
22	CLA	5	307	-	1/1/15/20	18/39/115/115	-
22	CLA	1	309	24	1/1/10/20	4/10/86/115	-
22	CLA	B	822	2	1/1/11/20	6/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	4	308	16	1/1/12/20	1/21/97/115	-
29	CHL	2	307	-	3/3/17/26	10/21/119/137	-
22	CLA	7	310	18	1/1/12/20	5/21/97/115	-
22	CLA	7	302	18	1/1/11/20	9/17/93/115	-
22	CLA	4	302	-	1/1/14/20	9/33/109/115	-
22	CLA	B	821	-	1/1/12/20	7/21/97/115	-
22	CLA	B	810	2	1/1/15/20	8/39/115/115	-
22	CLA	L	202	-	1/1/15/20	15/39/115/115	-
29	CHL	6	307	-	3/3/15/26	6/12/110/137	-
22	CLA	6	305	-	1/1/14/20	14/33/109/115	-
25	8CT	B	847	-	-	11/29/63/63	0/2/2/2
22	CLA	2	303	-	1/1/15/20	11/39/115/115	-
25	8CT	L	206	-	-	15/29/63/63	0/2/2/2
25	8CT	A	848	-	-	6/29/63/63	0/2/2/2
22	CLA	9	303	19	1/1/15/20	13/39/115/115	-
31	LMG	5	319	22	-	18/39/59/70	0/1/1/1
22	CLA	8	308	16	1/1/12/20	5/21/97/115	-
29	CHL	3	306	-	3/3/16/26	3/17/115/137	-
22	CLA	A	805	-	1/1/15/20	14/39/115/115	-
22	CLA	B	840	-	1/1/15/20	13/39/115/115	-
22	CLA	4	303	16	1/1/11/20	5/17/93/115	-
22	CLA	6	315	-	1/1/15/20	14/39/115/115	-
22	CLA	4	313	16	1/1/11/20	8/15/91/115	-
22	CLA	A	806	1	1/1/15/20	19/39/115/115	-
31	LMG	4	318	-	-	20/39/59/70	0/1/1/1
22	CLA	0	304	22	1/1/12/20	11/24/100/115	-
24	LHG	1	317	22	-	23/53/53/53	-
22	CLA	A	830	1	1/1/15/20	11/39/115/115	-
25	8CT	8	301	-	-	13/29/63/63	0/2/2/2
29	CHL	1	305	-	3/3/16/26	6/18/116/137	-
22	CLA	A	825	-	-	15/39/115/115	-
22	CLA	9	312	30	1/1/13/20	11/32/108/115	-
22	CLA	4	304	-	1/1/12/20	4/21/97/115	-
22	CLA	1	310	-	1/1/12/20	9/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PQN	A	842	-	-	7/23/43/43	0/2/2/2
22	CLA	A	814	-	1/1/11/20	8/15/91/115	-
22	CLA	A	836	-	1/1/12/20	12/23/99/115	-
22	CLA	0	312	29,20	1/1/13/20	10/27/103/115	-
22	CLA	6	312	-	1/1/12/20	9/24/100/115	-
22	CLA	B	824	-	1/1/14/20	14/33/109/115	-
29	CHL	9	307	-	3/3/16/26	11/18/116/137	-
29	CHL	8	307	30	3/3/17/26	7/21/119/137	-
29	CHL	5	301	13	4/4/19/26	12/33/131/137	-
22	CLA	A	832	-	1/1/15/20	17/39/115/115	-
22	CLA	G	102	-	1/1/12/20	5/21/97/115	-
29	CHL	2	305	-	3/3/15/26	4/12/110/137	-
22	CLA	3	305	15	1/1/11/20	9/18/94/115	-
22	CLA	2	310	24	1/1/10/20	5/10/86/115	-
22	CLA	L	204	-	1/1/12/20	9/21/97/115	-
22	CLA	3	303	-	1/1/11/20	6/15/91/115	-
22	CLA	A	813	-	1/1/15/20	12/39/115/115	-
22	CLA	A	823	-	1/1/12/20	7/23/99/115	-
22	CLA	7	307	-	1/1/11/20	4/18/94/115	-
22	CLA	A	804	22	1/1/13/20	9/27/103/115	-
22	CLA	7	316	18	1/1/15/20	19/39/115/115	-
22	CLA	B	814	-	1/1/15/20	20/39/115/115	-
25	8CT	B	804	-	-	15/29/63/63	0/2/2/2
22	CLA	3	309	24	1/1/8/20	0/4/76/115	-
22	CLA	7	303	18	1/1/14/20	15/33/109/115	-
30	XAT	4	315	22	-	8/31/93/93	0/4/4/4
22	CLA	4	314	-	1/1/15/20	17/39/115/115	-
24	LHG	B	852	22	-	9/26/26/53	-
22	CLA	7	309	22	1/1/12/20	4/21/97/115	-
22	CLA	L	201	-	1/1/15/20	19/39/115/115	-
30	XAT	0	313	22	-	16/31/93/93	0/4/4/4
22	CLA	B	827	-	1/1/15/20	14/39/115/115	-
22	CLA	B	838	-	1/1/11/20	3/18/94/115	-
22	CLA	B	807	-	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	838	-	1/1/15/20	14/39/115/115	-
22	CLA	B	829	-	1/1/15/20	9/39/115/115	-
26	HTG	A	851	-	-	4/10/30/30	0/1/1/1
22	CLA	8	303	22,16,31	1/1/11/20	3/17/93/115	-
22	CLA	A	839	-	1/1/15/20	18/39/115/115	-
22	CLA	8	313	16	1/1/11/20	3/15/91/115	-
22	CLA	B	831	-	1/1/12/20	7/21/97/115	-
22	CLA	L	203	-	1/1/15/20	16/39/115/115	-
22	CLA	9	308	-	1/1/15/20	15/39/115/115	-
27	SF4	C	101	-	-	-	0/6/5/5
30	XAT	5	316	-	-	2/31/93/93	0/4/4/4
22	CLA	B	830	2	1/1/15/20	8/39/115/115	-
25	8CT	5	317	-	-	10/29/63/63	0/2/2/2
22	CLA	4	311	22	1/1/12/20	9/24/100/115	-
22	CLA	K	102	-	1/1/11/20	9/17/93/115	-
29	CHL	4	301	22,13	4/4/19/26	11/33/131/137	-
30	XAT	8	317	-	-	0/31/93/93	0/4/4/4
22	CLA	A	811	22,1	1/1/15/20	17/39/115/115	-
22	CLA	B	850	-	1/1/13/20	9/27/103/115	-
22	CLA	1	313	-	1/1/11/20	8/17/93/115	-
25	8CT	7	323	-	-	13/29/63/63	0/2/2/2
22	CLA	B	805	-	1/1/15/20	17/39/115/115	-
22	CLA	5	308	-	1/1/10/20	4/12/88/115	-
22	CLA	3	304	-	1/1/10/20	4/12/88/115	-
22	CLA	1	308	30,13	1/1/14/20	9/33/109/115	-
30	XAT	3	314	-	-	4/31/93/93	0/4/4/4
22	CLA	B	801	-	1/1/15/20	7/39/115/115	-
22	CLA	7	313	18	1/1/13/20	13/27/103/115	-
22	CLA	2	304	-	1/1/14/20	14/33/109/115	-
22	CLA	B	818	2	1/1/13/20	12/32/108/115	-
22	CLA	5	302	-	1/1/15/20	9/39/115/115	-
22	CLA	8	310	31	1/1/13/20	8/27/103/115	-
22	CLA	3	301	-	1/1/14/20	11/33/109/115	-
22	CLA	0	309	24	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	XAT	1	314	22	-	11/31/93/93	0/4/4/4
22	CLA	1	303	-	1/1/12/20	8/24/100/115	-
22	CLA	6	309	17	1/1/12/20	9/21/97/115	-
22	CLA	0	302	30	1/1/15/20	17/39/115/115	-
22	CLA	3	307	15	1/1/12/20	9/21/97/115	-
24	LHG	6	322	22	-	22/41/41/53	-
25	8CT	B	846	-	-	13/29/63/63	0/2/2/2
25	8CT	A	854	-	-	12/29/63/63	0/2/2/2
22	CLA	5	311	30	1/1/11/20	1/15/91/115	-
24	LHG	5	318	22	-	28/53/53/53	-
25	8CT	7	301	-	-	11/29/63/63	0/2/2/2
24	LHG	2	318	22	-	19/36/36/53	-
22	CLA	0	311	-	1/1/15/20	14/39/115/115	-
22	CLA	A	840	-	1/1/15/20	14/39/115/115	-
22	CLA	6	313	29,17	1/1/15/20	10/39/115/115	-
22	CLA	B	806	-	1/1/15/20	17/39/115/115	-
30	XAT	7	320	-	-	0/31/93/93	0/4/4/4
22	CLA	8	312	16	1/1/13/20	6/29/105/115	-
29	CHL	6	306	-	3/3/15/26	2/12/110/137	-
22	CLA	3	312	15	1/1/11/20	5/15/91/115	-
25	8CT	G	104	-	-	13/29/63/63	0/2/2/2
22	CLA	2	302	29	1/1/15/20	16/39/115/115	-
22	CLA	2	312	14	1/1/15/20	15/39/115/115	-
30	XAT	9	315	-	-	0/31/93/93	0/4/4/4
22	CLA	9	304	-	1/1/11/20	6/19/95/115	-
29	CHL	9	302	19	4/4/19/26	11/33/131/137	-
22	CLA	6	304	17	1/1/15/20	17/39/115/115	-
29	CHL	6	302	22,17	4/4/19/26	11/33/131/137	-
22	CLA	7	312	30	1/1/12/20	4/24/100/115	-
29	CHL	5	306	-	3/3/16/26	8/18/116/137	-
29	CHL	6	308	-	3/3/17/26	5/21/119/137	-
22	CLA	B	835	-	1/1/11/20	4/15/91/115	-
22	CLA	6	310	17,30	1/1/14/20	9/33/109/115	-
22	CLA	B	817	-	1/1/13/20	12/27/103/115	-
30	XAT	7	319	22	-	7/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	0	315	29,22	-	28/53/53/53	-
31	LMG	8	319	22	-	17/39/59/70	0/1/1/1
25	8CT	A	849	-	-	11/29/63/63	0/2/2/2
22	CLA	9	313	19	1/1/13/20	14/27/103/115	-
22	CLA	5	304	-	1/1/12/20	10/24/100/115	-
29	CHL	0	306	22,30	3/3/16/26	6/18/116/137	-
25	8CT	3	318	-	-	6/29/63/63	0/2/2/2
22	CLA	7	315	18	1/1/11/20	4/17/93/115	-
24	LHG	7	322	22	-	16/23/23/53	-
22	CLA	A	801	-	1/1/15/20	10/39/115/115	-
22	CLA	0	310	30	1/1/12/20	4/24/100/115	-
22	CLA	1	312	29,13	1/1/13/20	10/27/103/115	-
22	CLA	A	853	-	1/1/15/20	16/39/115/115	-
26	HTG	J	102	-	-	3/10/30/30	0/1/1/1
22	CLA	A	824	-	1/1/13/20	8/27/103/115	-
22	CLA	7	304	22	1/1/11/20	7/18/94/115	-
22	CLA	9	301	2	1/1/11/20	6/16/92/115	-
22	CLA	6	314	-	1/1/10/20	6/13/89/115	-
22	CLA	6	301	-	1/1/12/20	13/24/100/115	-
24	LHG	3	317	22	-	11/23/23/53	-
22	CLA	B	819	-	1/1/14/20	18/33/109/115	-
25	8CT	8	318	-	-	13/29/63/63	0/2/2/2
22	CLA	B	820	-	1/1/15/20	10/39/115/115	-
25	8CT	A	847	-	-	9/29/63/63	0/2/2/2
22	CLA	5	303	-	-	25/39/115/115	-
22	CLA	A	827	-	1/1/15/20	12/39/115/115	-
29	CHL	2	301	22	4/4/19/26	10/33/131/137	-
22	CLA	B	834	2	1/1/15/20	17/39/115/115	-
22	CLA	A	810	1	1/1/15/20	10/39/115/115	-
25	8CT	L	205	-	-	13/29/63/63	0/2/2/2
22	CLA	8	309	-	1/1/14/20	7/33/109/115	-
22	CLA	B	816	2	1/1/14/20	13/33/109/115	-
22	CLA	B	812	2	1/1/15/20	13/39/115/115	-
22	CLA	B	825	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	B	851	-	-	15/29/63/63	0/2/2/2
22	CLA	A	812	-	1/1/12/20	3/26/102/115	-
22	CLA	0	303	30	1/1/15/20	14/39/115/115	-
22	CLA	2	311	14	1/1/12/20	6/24/100/115	-
25	8CT	A	846	-	-	13/29/63/63	0/2/2/2
30	XAT	2	316	-	-	3/31/93/93	0/4/4/4
25	8CT	B	843	-	-	16/29/63/63	0/2/2/2
24	LHG	9	316	22	-	21/53/53/53	-
30	XAT	2	315	-	-	2/31/93/93	0/4/4/4
30	XAT	8	316	29	-	7/31/93/93	0/4/4/4
30	XAT	5	315	22	-	6/31/93/93	0/4/4/4
22	CLA	B	841	24	1/1/15/20	14/39/115/115	-
24	LHG	A	844	-	-	25/53/53/53	-
29	CHL	4	306	29	3/3/17/26	6/21/119/137	-
22	CLA	1	304	-	1/1/12/20	7/24/100/115	-
24	LHG	A	845	22	-	16/31/31/53	-
22	CLA	B	803	-	1/1/15/20	16/39/115/115	-
25	8CT	6	321	-	-	10/29/63/63	0/2/2/2
25	8CT	B	845	-	-	12/29/63/63	0/2/2/2
25	8CT	A	850	-	-	10/29/63/63	0/2/2/2
22	CLA	A	829	-	1/1/15/20	10/39/115/115	-
22	CLA	3	313	15	1/1/11/20	9/17/93/115	-

The worst 5 of 3344 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	318	8CT	C02-C03	15.13	1.59	1.34
25	K	103	8CT	C32-C31	14.87	1.61	1.32
25	5	317	8CT	C02-C03	14.81	1.59	1.34
25	7	301	8CT	C02-C03	14.77	1.59	1.34
25	1	316	8CT	C02-C03	14.76	1.59	1.34

The worst 5 of 2896 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	5	315	XAT	O24-C25-C38	-22.39	90.03	115.05
30	2	315	XAT	O4-C5-C4	-21.50	93.34	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	2	315	XAT	O4-C5-C18	-19.32	93.46	115.05
30	0	313	XAT	O24-C25-C38	-19.21	93.58	115.05
30	0	313	XAT	O24-C25-C24	-19.13	95.57	113.49

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 3276 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.

295 monomers are involved in 1342 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	K	103	8CT	13	0
22	B	808	CLA	7	0
22	A	817	CLA	6	0
30	0	314	XAT	8	0
22	1	302	CLA	4	0
29	7	308	CHL	8	0
22	5	310	CLA	1	0
22	B	832	CLA	8	0
22	9	311	CLA	2	0
22	0	307	CLA	5	0
22	1	307	CLA	4	0
22	A	816	CLA	2	0
22	6	311	CLA	3	0
22	8	302	CLA	2	0
22	G	101	CLA	1	0
23	B	842	PQN	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	301	CLA	6	0
22	0	308	CLA	3	0
22	G	103	CLA	7	0
25	J	104	8CT	16	0
28	B	849	DGD	11	0
22	0	305	CLA	4	0
22	A	803	CLA	5	0
22	5	305	CLA	2	0
22	A	843	CLA	1	0
22	A	841	CLA	4	0
22	5	312	CLA	5	0
22	A	820	CLA	4	0
22	A	818	CLA	2	0
22	9	309	CLA	9	0
22	A	815	CLA	2	0
29	0	301	CHL	15	0
22	A	822	CLA	4	0
22	A	834	CLA	1	0
29	8	306	CHL	4	0
22	6	323	CLA	4	0
22	A	821	CLA	2	0
22	J	103	CLA	1	0
22	A	808	CLA	9	0
29	4	307	CHL	10	0
22	9	306	CLA	2	0
22	A	802	CLA	4	0
22	B	828	CLA	5	0
22	9	310	CLA	2	0
25	4	317	8CT	12	0
29	2	306	CHL	2	0
22	8	315	CLA	3	0
22	7	317	CLA	11	0
25	7	321	8CT	13	0
22	4	309	CLA	6	0
22	K	105	CLA	15	0
22	B	811	CLA	3	0
29	4	305	CHL	9	0
30	6	320	XAT	7	0
25	1	316	8CT	13	0
25	J	101	8CT	10	0
22	4	310	CLA	1	0
22	3	311	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	304	CLA	3	0
22	B	837	CLA	5	0
22	3	308	CLA	4	0
22	B	813	CLA	9	0
22	K	101	CLA	2	0
22	H	201	CLA	16	0
22	7	318	CLA	4	0
22	B	823	CLA	3	0
22	4	312	CLA	5	0
22	A	835	CLA	1	0
27	B	802	SF4	1	0
22	7	314	CLA	2	0
25	2	317	8CT	13	0
22	7	305	CLA	3	0
25	3	316	8CT	11	0
30	1	315	XAT	5	0
22	5	314	CLA	1	0
22	B	833	CLA	8	0
22	M	101	CLA	4	0
30	6	319	XAT	7	0
22	A	833	CLA	5	0
22	8	311	CLA	6	0
22	1	306	CLA	4	0
22	2	309	CLA	4	0
30	3	315	XAT	9	0
22	B	836	CLA	2	0
22	A	819	CLA	5	0
22	5	313	CLA	6	0
25	B	848	8CT	13	0
22	K	104	CLA	6	0
30	4	316	XAT	6	0
22	2	308	CLA	6	0
22	B	839	CLA	2	0
22	A	828	CLA	9	0
22	A	837	CLA	5	0
22	6	303	CLA	4	0
22	3	319	CLA	8	0
22	2	319	CLA	1	0
22	5	309	CLA	9	0
22	B	809	CLA	6	0
22	A	809	CLA	11	0
22	A	807	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	317	CLA	3	0
29	6	316	CHL	3	0
22	F	301	CLA	5	0
22	B	826	CLA	9	0
29	8	314	CHL	11	0
22	A	826	CLA	9	0
22	3	310	CLA	1	0
22	1	311	CLA	12	0
22	6	318	CLA	6	0
22	7	306	CLA	5	0
22	3	302	CLA	1	0
29	8	305	CHL	7	0
22	A	831	CLA	4	0
30	9	314	XAT	5	0
22	B	815	CLA	6	0
22	5	307	CLA	2	0
22	1	309	CLA	2	0
22	4	308	CLA	2	0
29	2	307	CHL	3	0
22	7	310	CLA	5	0
22	7	302	CLA	1	0
22	4	302	CLA	3	0
22	B	810	CLA	7	0
22	L	202	CLA	10	0
29	6	307	CHL	9	0
22	6	305	CLA	11	0
25	B	847	8CT	13	0
22	2	303	CLA	2	0
22	9	303	CLA	5	0
31	5	319	LMG	6	0
22	8	308	CLA	9	0
29	3	306	CHL	4	0
22	A	805	CLA	7	0
22	B	840	CLA	14	0
22	4	303	CLA	1	0
22	6	315	CLA	4	0
22	4	313	CLA	4	0
22	A	806	CLA	4	0
31	4	318	LMG	1	0
22	0	304	CLA	3	0
24	1	317	LHG	3	0
22	A	830	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	8	301	8CT	11	0
29	1	305	CHL	3	0
22	A	825	CLA	9	0
22	9	312	CLA	9	0
22	1	310	CLA	4	0
23	A	842	PQN	3	0
22	A	814	CLA	5	0
22	A	836	CLA	3	0
22	0	312	CLA	5	0
22	6	312	CLA	1	0
22	B	824	CLA	7	0
29	9	307	CHL	1	0
29	8	307	CHL	6	0
29	5	301	CHL	12	0
22	A	832	CLA	4	0
22	G	102	CLA	7	0
29	2	305	CHL	9	0
22	L	204	CLA	4	0
22	3	303	CLA	1	0
22	A	813	CLA	12	0
22	A	823	CLA	1	0
22	7	307	CLA	12	0
22	A	804	CLA	3	0
22	7	316	CLA	6	0
22	B	814	CLA	8	0
22	3	309	CLA	1	0
22	7	303	CLA	9	0
30	4	315	XAT	8	0
22	4	314	CLA	4	0
24	B	852	LHG	1	0
22	7	309	CLA	4	0
22	L	201	CLA	4	0
30	0	313	XAT	8	0
22	B	827	CLA	8	0
22	B	807	CLA	5	0
22	A	838	CLA	2	0
22	B	829	CLA	9	0
22	A	839	CLA	8	0
22	8	313	CLA	1	0
22	B	831	CLA	1	0
22	L	203	CLA	5	0
22	9	308	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	C	101	SF4	1	0
30	5	316	XAT	6	0
22	B	830	CLA	6	0
25	5	317	8CT	5	0
22	4	311	CLA	4	0
22	K	102	CLA	5	0
29	4	301	CHL	8	0
30	8	317	XAT	9	0
22	A	811	CLA	4	0
22	B	850	CLA	16	0
22	1	313	CLA	1	0
25	7	323	8CT	22	0
22	B	805	CLA	7	0
22	5	308	CLA	6	0
22	1	308	CLA	6	0
30	3	314	XAT	8	0
22	B	801	CLA	3	0
22	7	313	CLA	7	0
22	2	304	CLA	4	0
22	B	818	CLA	4	0
22	5	302	CLA	7	0
22	8	310	CLA	8	0
22	3	301	CLA	4	0
22	0	309	CLA	2	0
30	1	314	XAT	9	0
22	1	303	CLA	11	0
22	6	309	CLA	5	0
22	0	302	CLA	12	0
22	3	307	CLA	5	0
24	6	322	LHG	4	0
25	B	846	8CT	11	0
25	A	854	8CT	3	0
22	5	311	CLA	4	0
24	5	318	LHG	8	0
24	2	318	LHG	3	0
22	0	311	CLA	7	0
22	A	840	CLA	7	0
22	6	313	CLA	5	0
22	B	806	CLA	10	0
30	7	320	XAT	8	0
22	8	312	CLA	2	0
29	6	306	CHL	2	0

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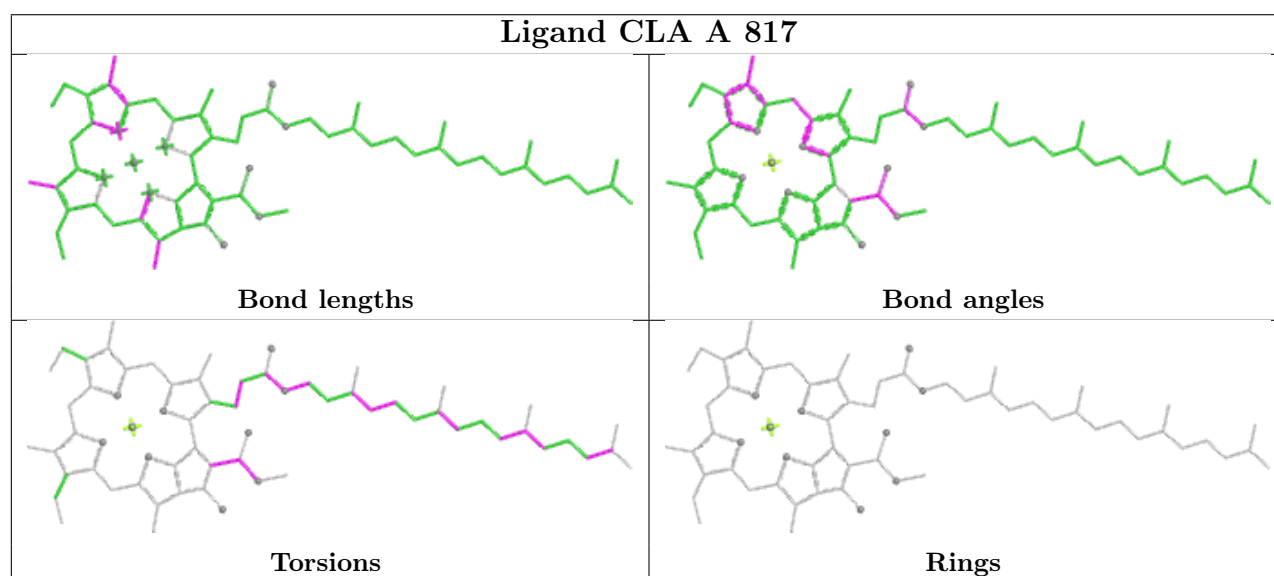
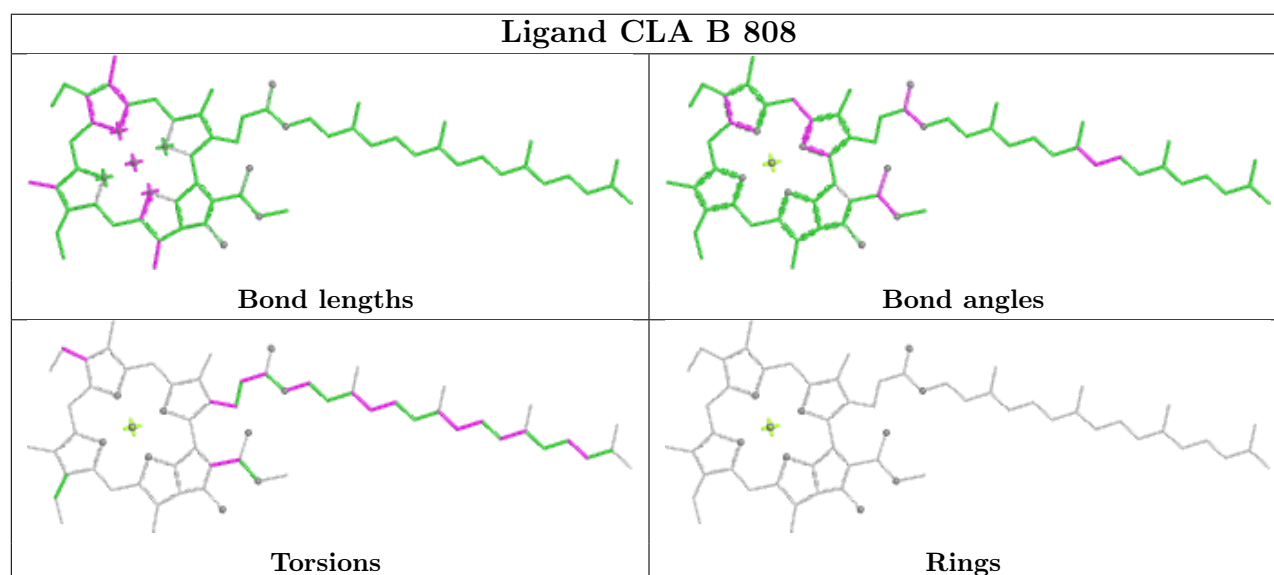
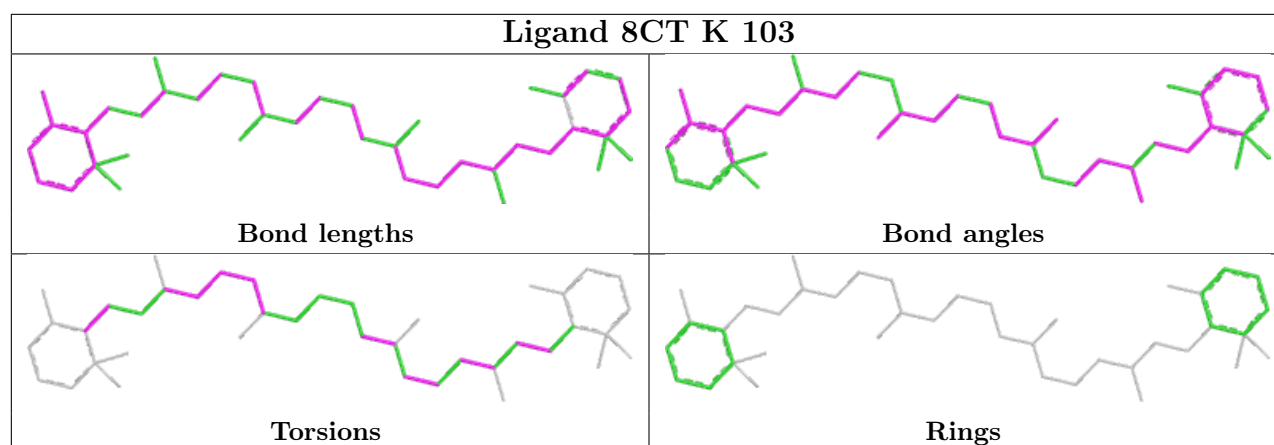
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30	9	315	XAT	7	0
22	9	304	CLA	2	0
29	9	302	CHL	2	0
22	6	304	CLA	4	0
29	6	302	CHL	7	0
22	7	312	CLA	3	0
29	5	306	CHL	4	0
29	6	308	CHL	4	0
22	B	835	CLA	1	0
22	6	310	CLA	9	0
22	B	817	CLA	5	0
30	7	319	XAT	6	0
24	0	315	LHG	11	0
31	8	319	LMG	6	0
25	A	849	8CT	7	0
22	9	313	CLA	2	0
29	0	306	CHL	2	0
22	5	304	CLA	8	0
22	7	315	CLA	1	0
24	7	322	LHG	2	0
22	A	801	CLA	6	0
22	0	310	CLA	2	0
22	1	312	CLA	8	0
22	A	853	CLA	5	0
26	J	102	HTG	1	0
22	A	824	CLA	2	0
22	7	304	CLA	3	0
22	9	301	CLA	5	0
22	6	314	CLA	5	0
22	6	301	CLA	4	0
24	3	317	LHG	4	0
22	B	819	CLA	3	0
25	8	318	8CT	2	0
22	B	820	CLA	3	0
25	A	847	8CT	1	0
22	5	303	CLA	11	0
22	A	827	CLA	8	0
29	2	301	CHL	5	0

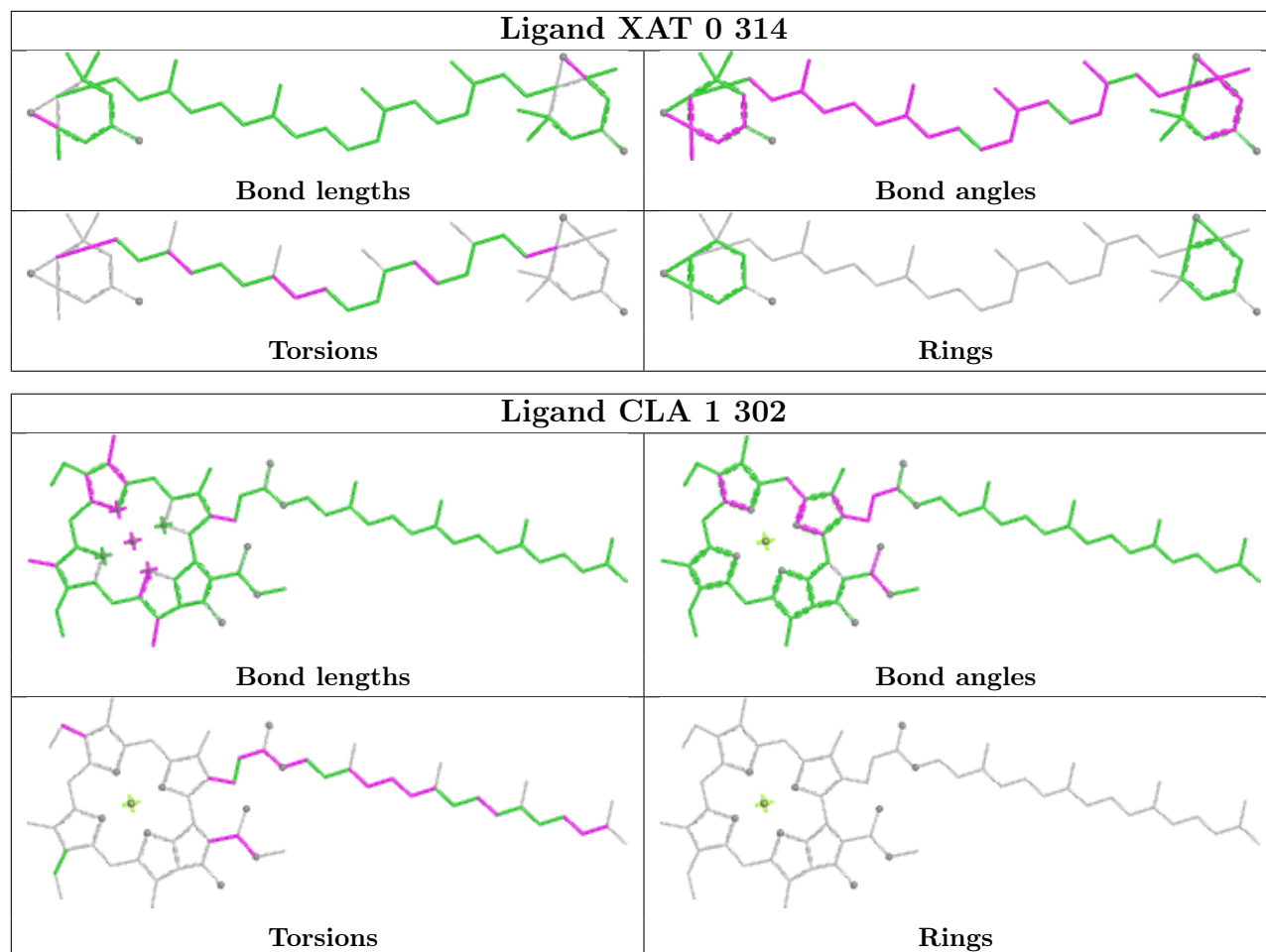
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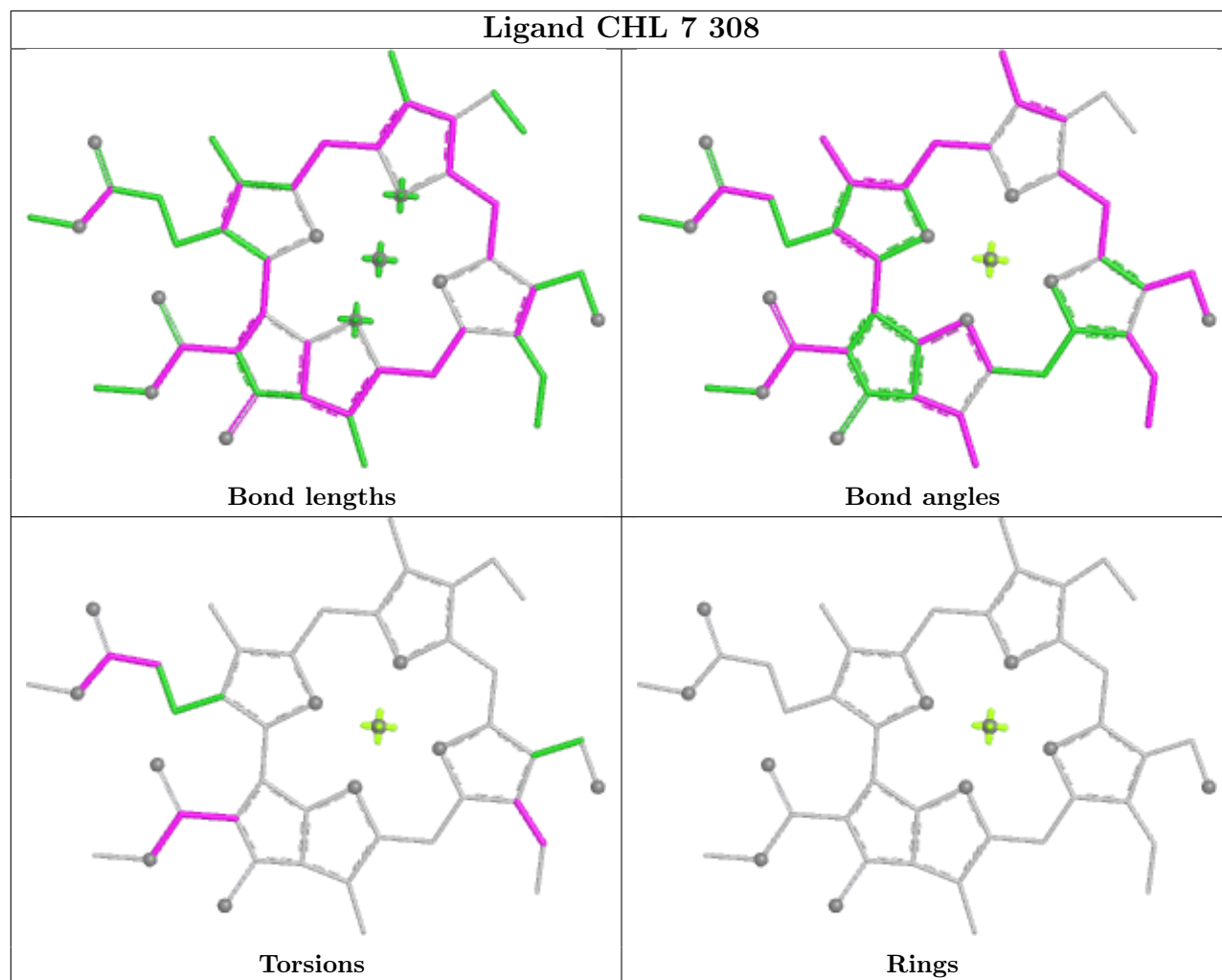
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22	A	810	CLA	4	0
22	8	309	CLA	11	0
22	B	816	CLA	5	0
22	B	812	CLA	3	0
22	B	825	CLA	4	0
25	B	851	8CT	1	0
22	A	812	CLA	3	0
22	0	303	CLA	1	0
22	2	311	CLA	1	0
25	A	846	8CT	1	0
30	2	316	XAT	6	0
25	B	843	8CT	3	0
24	9	316	LHG	8	0
30	2	315	XAT	6	0
30	8	316	XAT	11	0
30	5	315	XAT	7	0
22	B	841	CLA	5	0
24	A	844	LHG	3	0
29	4	306	CHL	2	0
22	1	304	CLA	13	0
24	A	845	LHG	1	0
22	B	803	CLA	16	0
25	6	321	8CT	14	0
25	A	850	8CT	19	0
22	A	829	CLA	4	0
22	3	313	CLA	4	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.

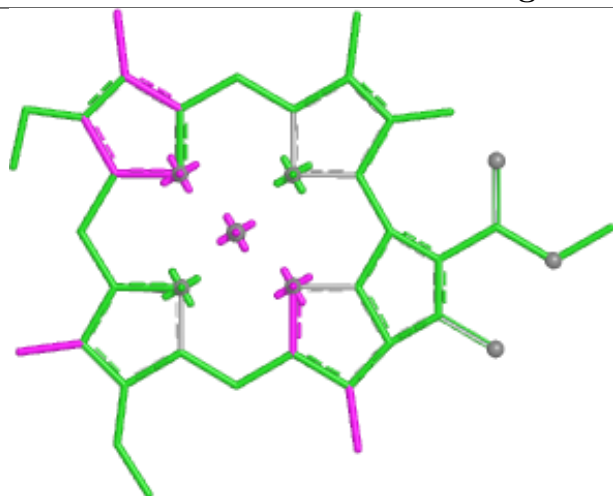




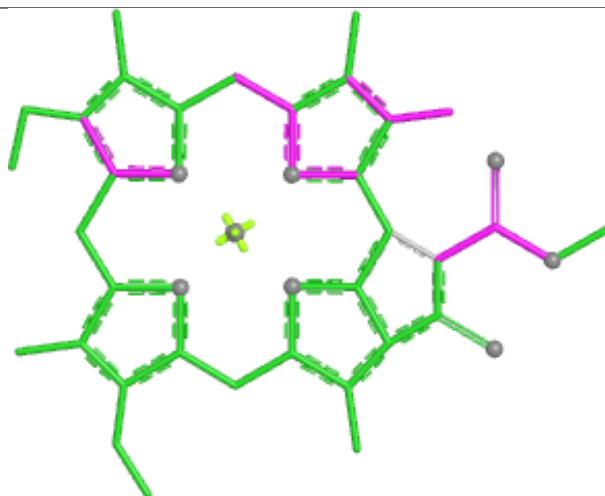
Ligand CHL 7 308



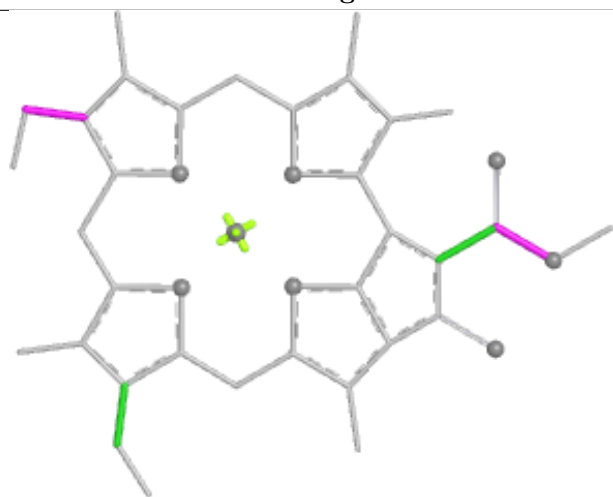
Ligand CLA 5 310



Bond lengths



Bond angles

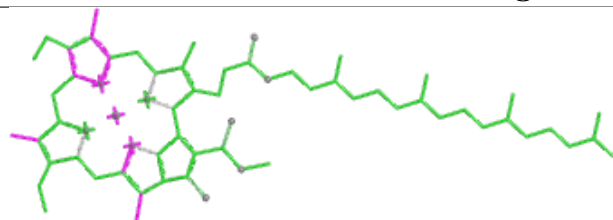


Torsions

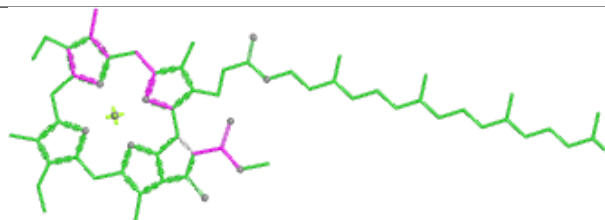


Rings

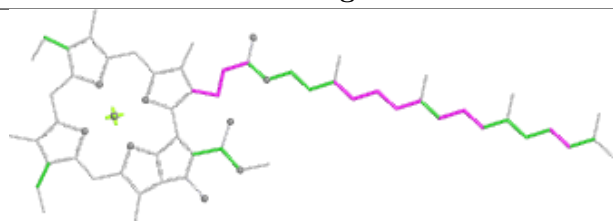
Ligand CLA B 832



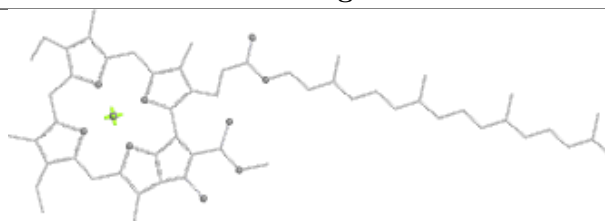
Bond lengths



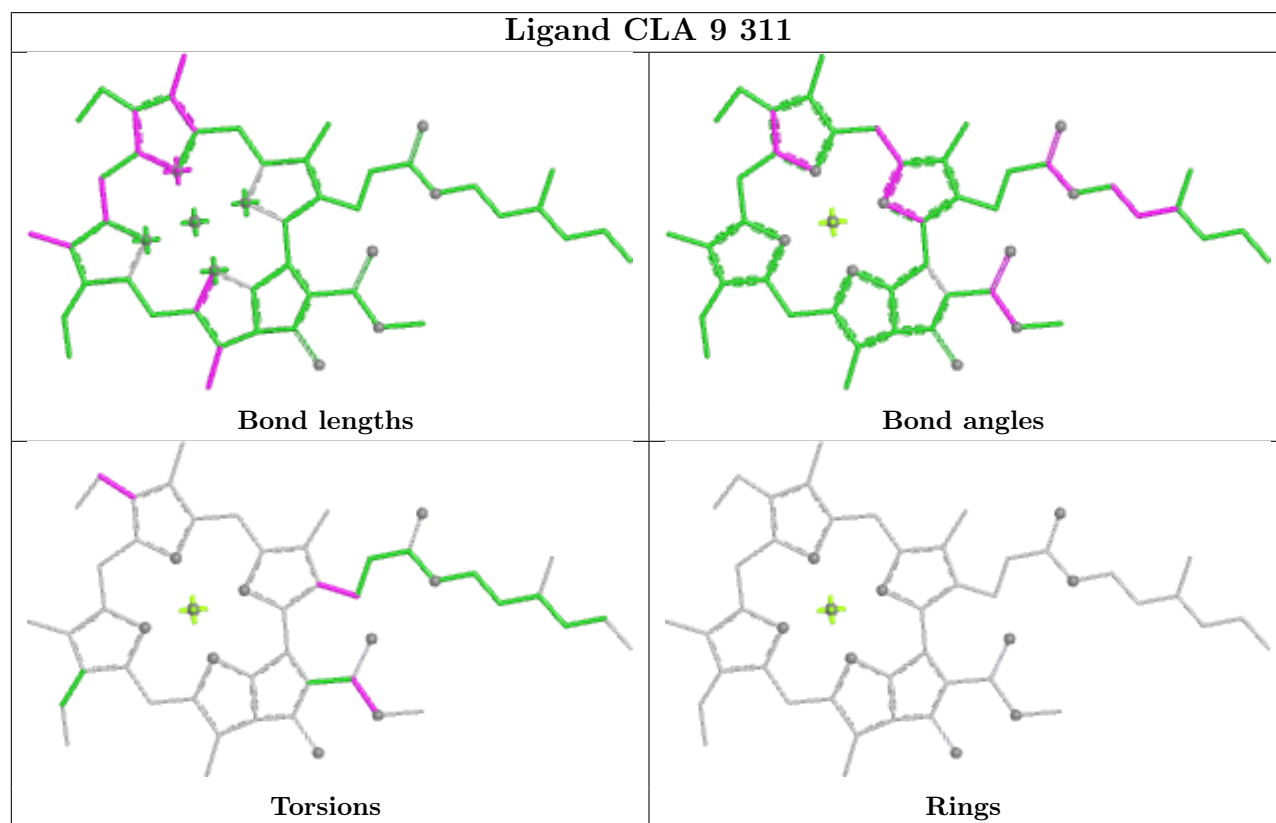
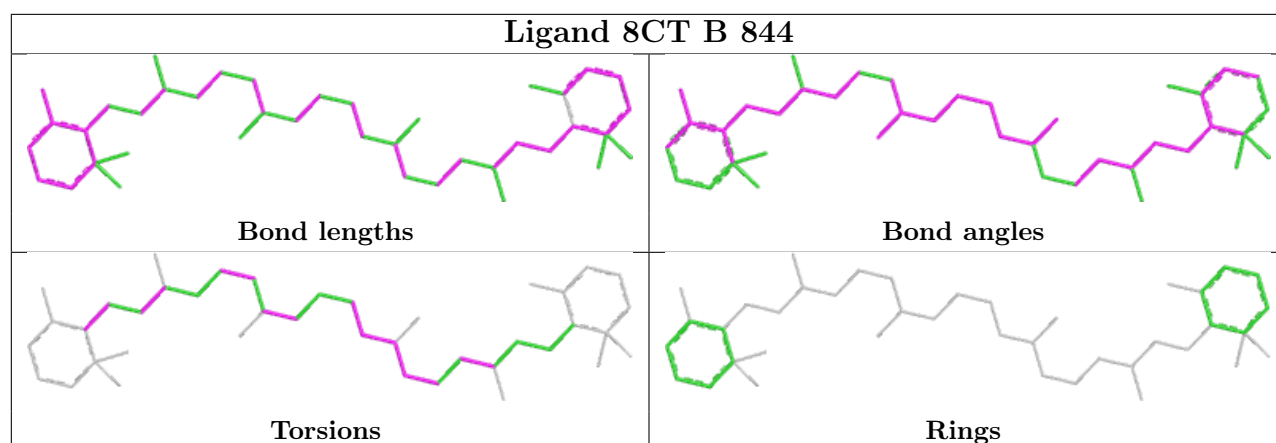
Bond angles

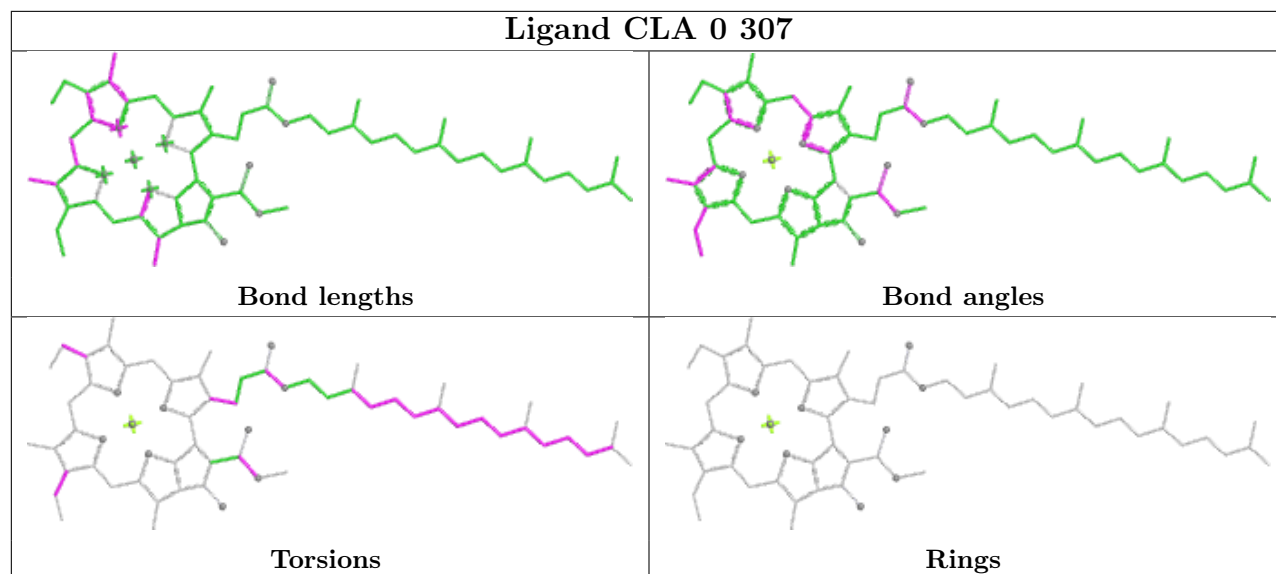
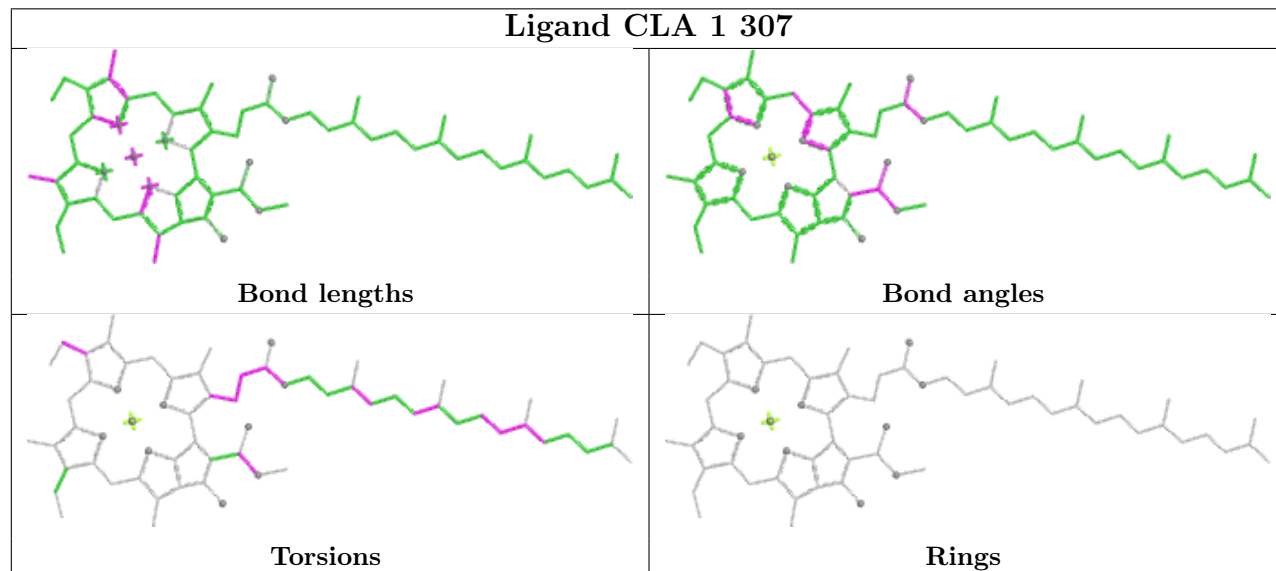


Torsions

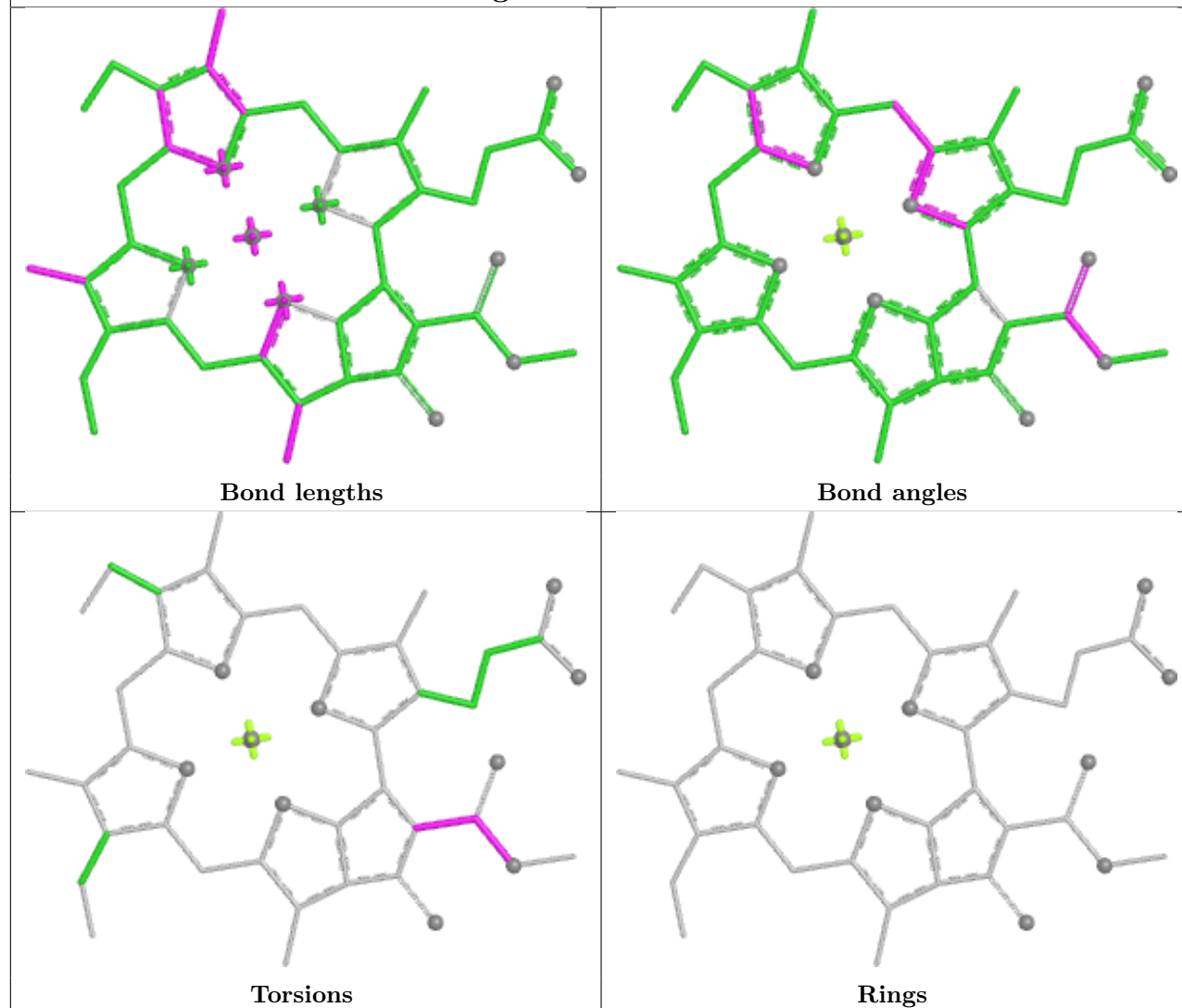


Rings

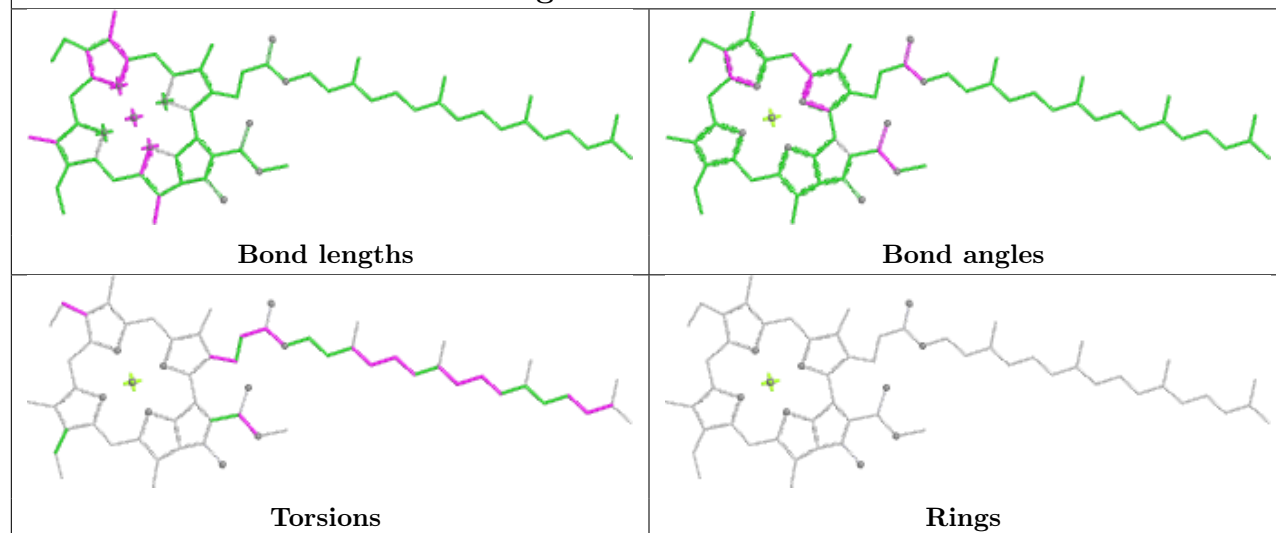


Ligand CLA 0 307**Ligand CLA 1 307**

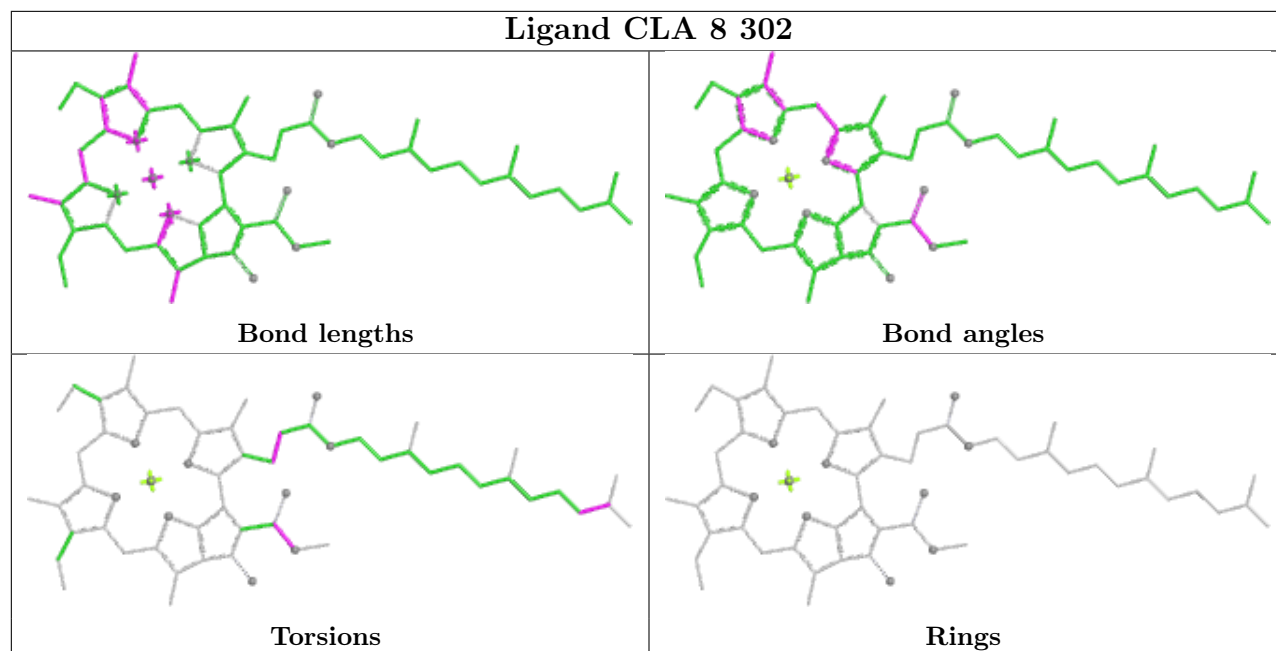
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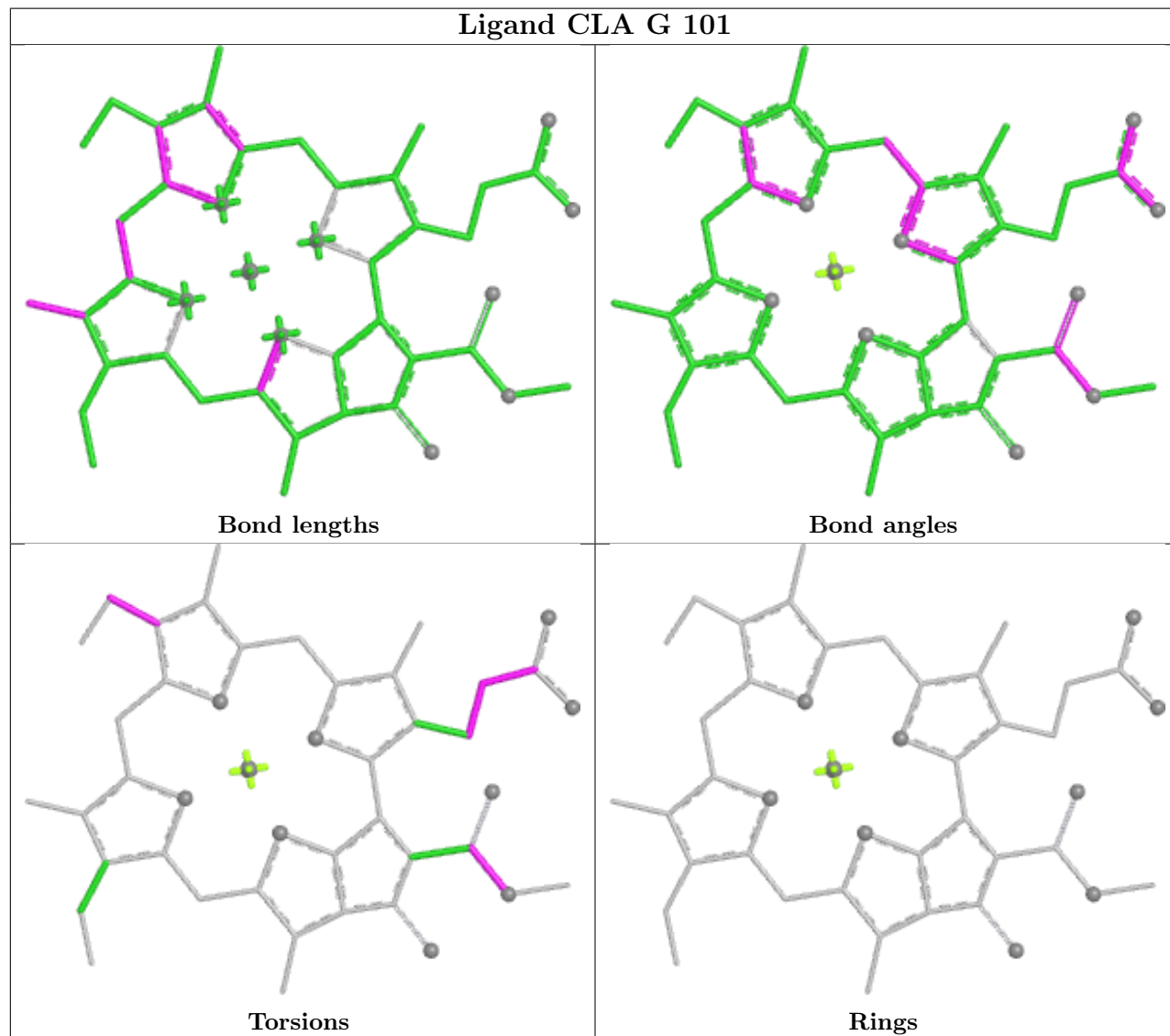
Ligand CLA 6 311

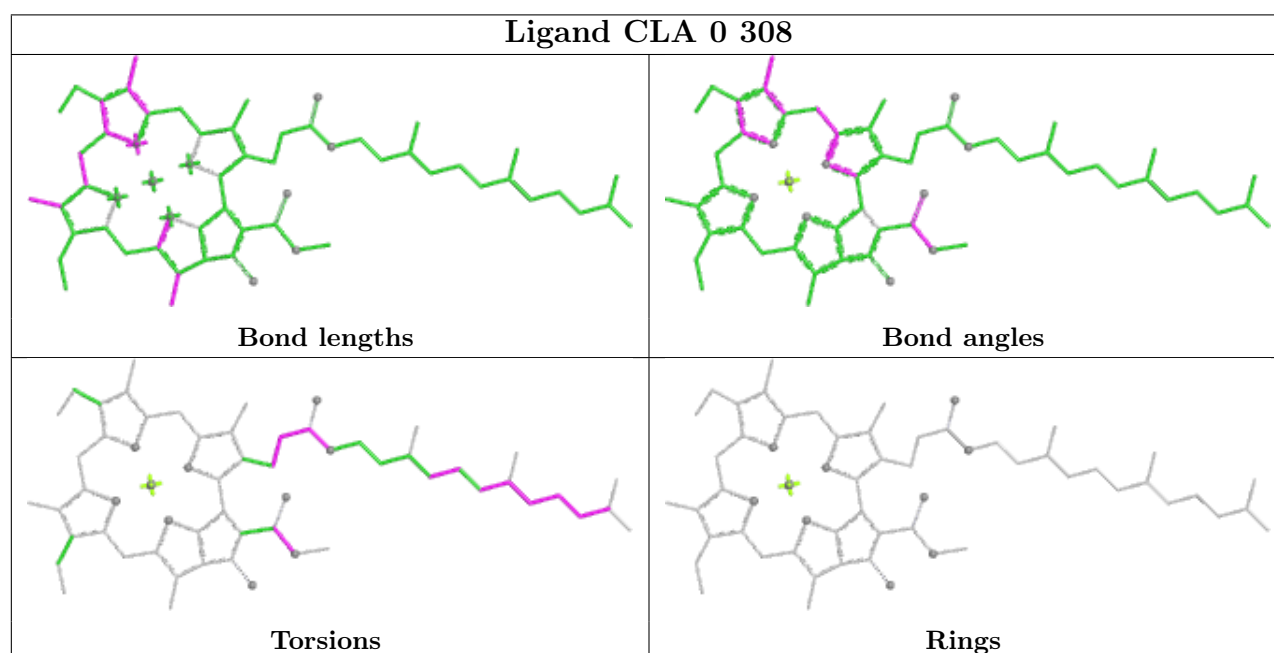
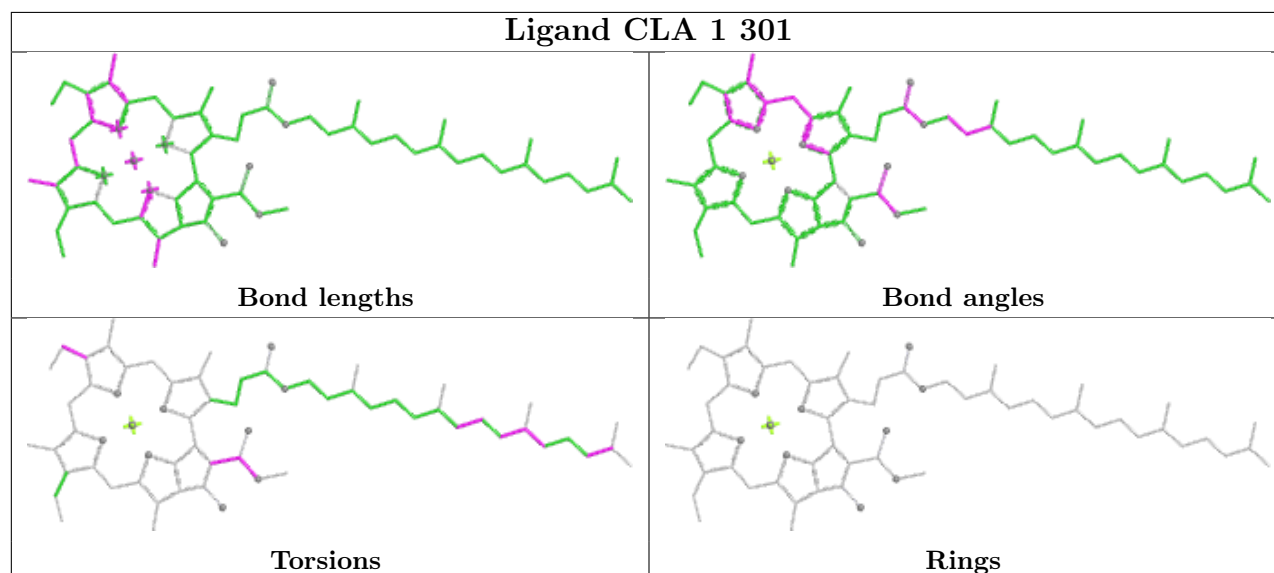
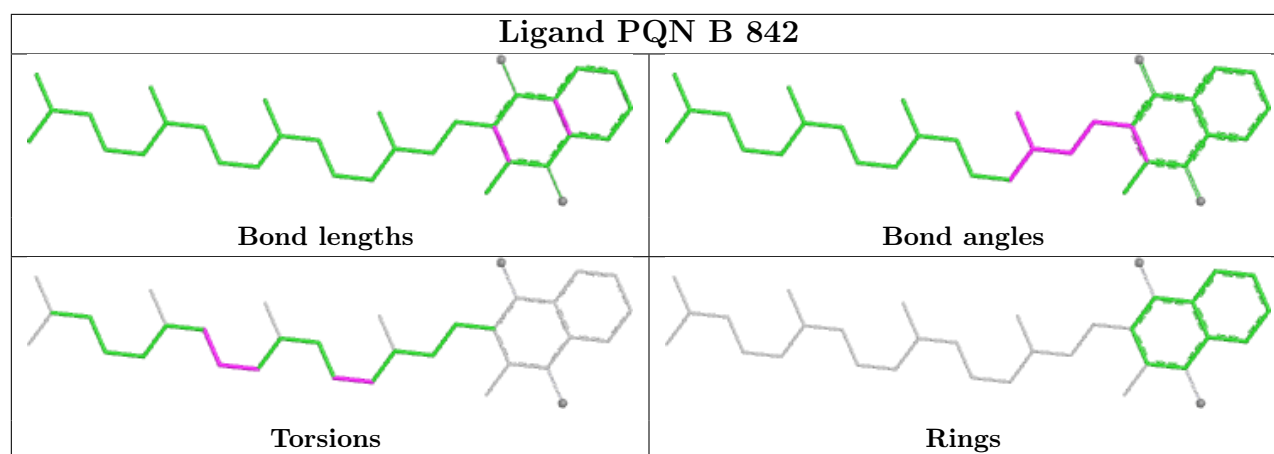


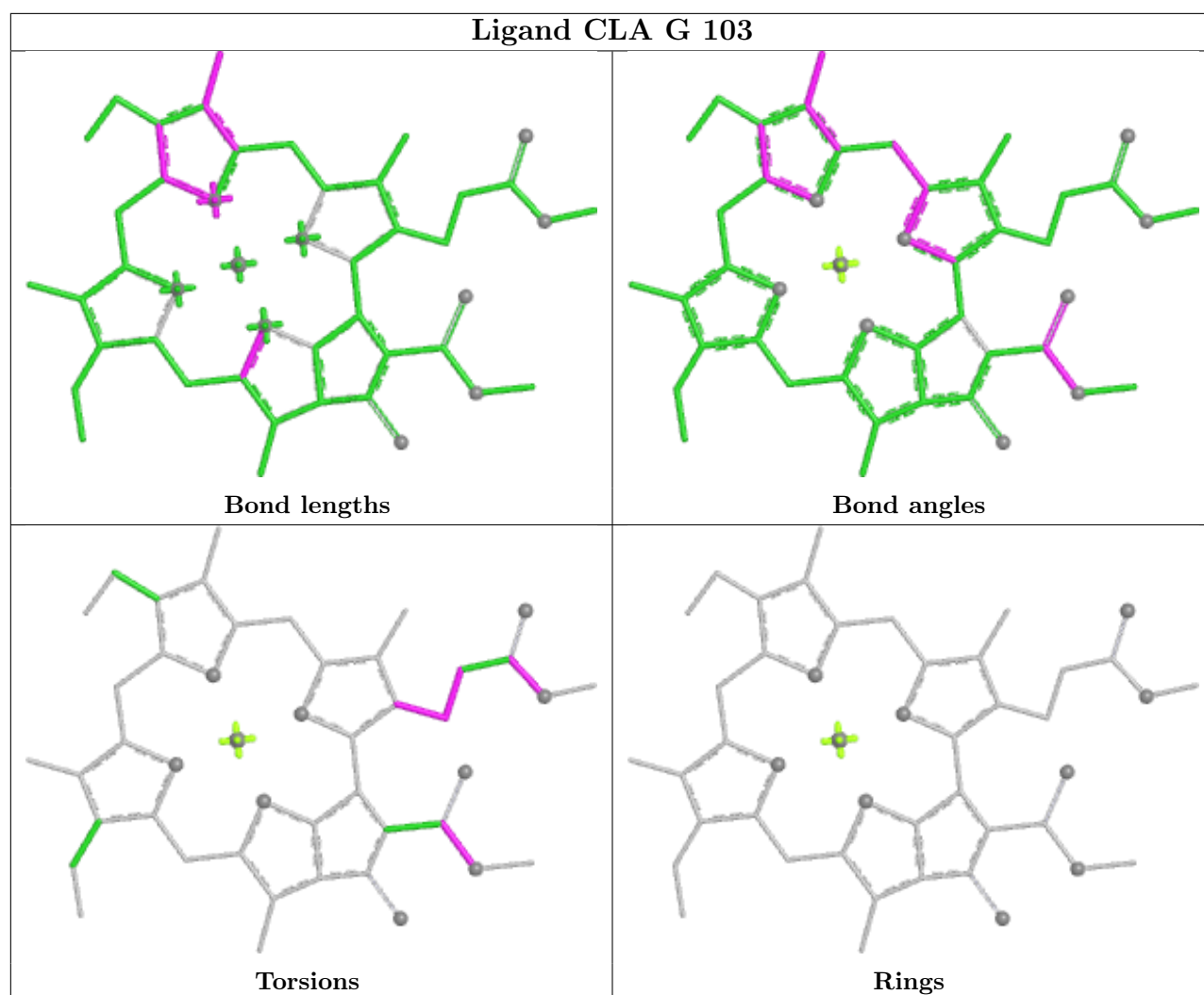
Ligand CLA 8 302



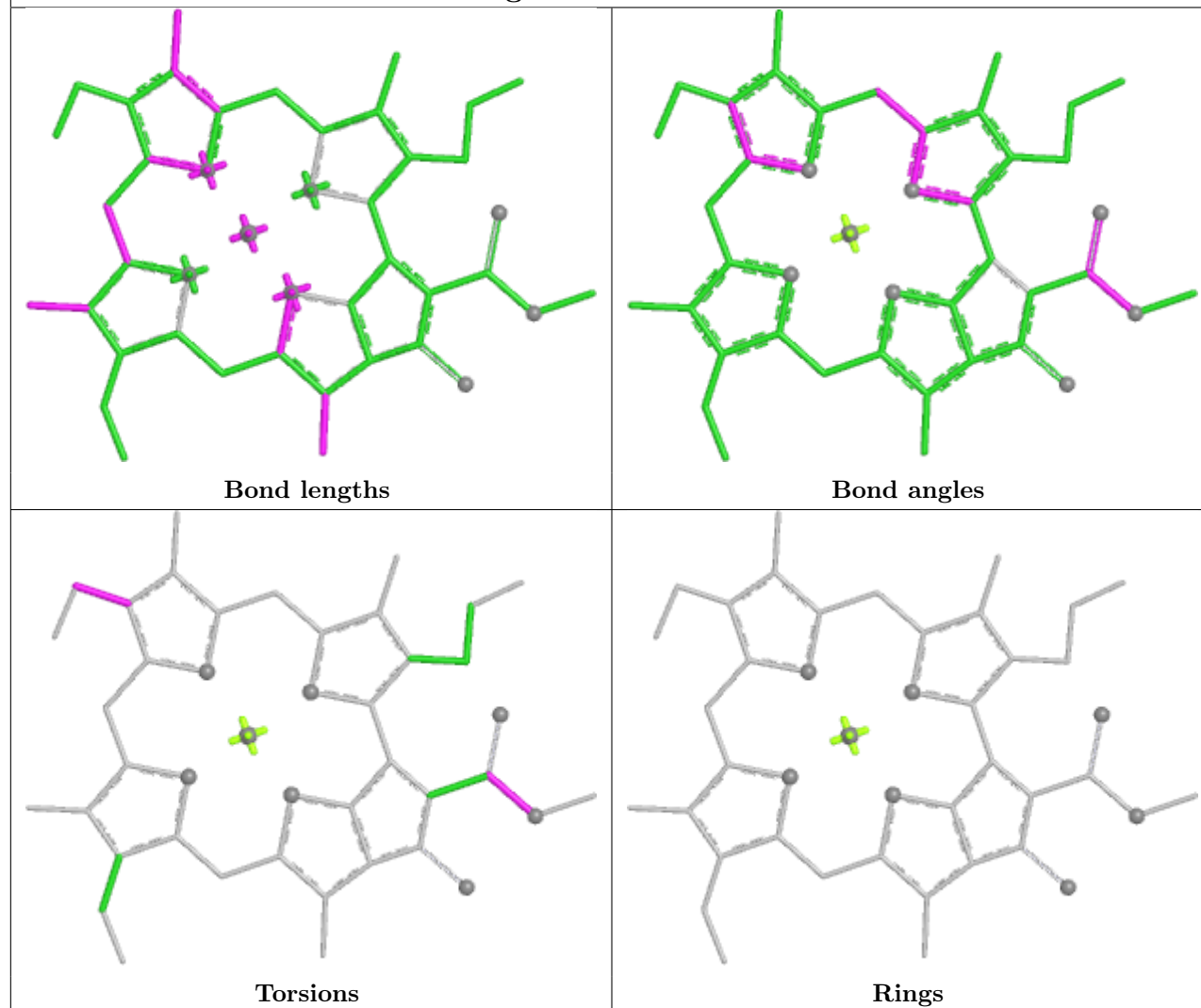
Ligand CLA G 101



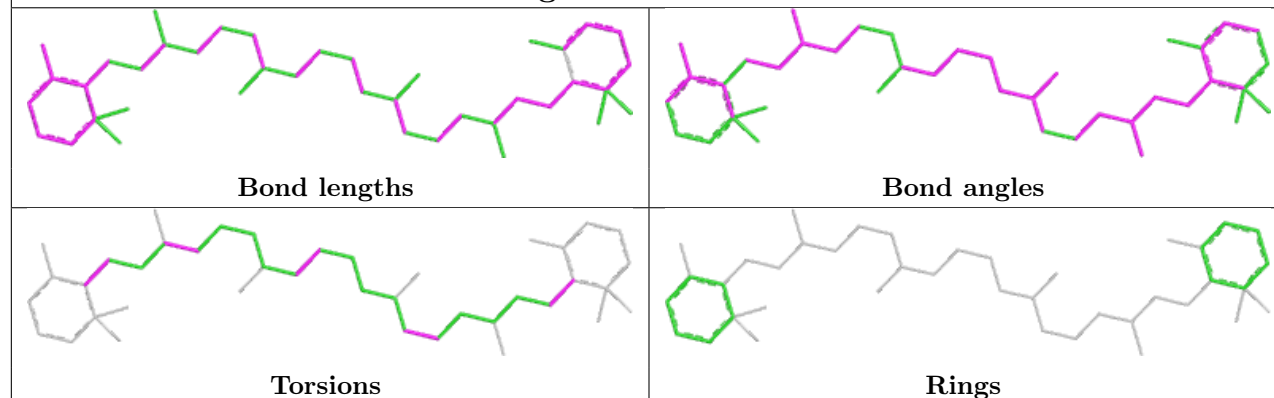


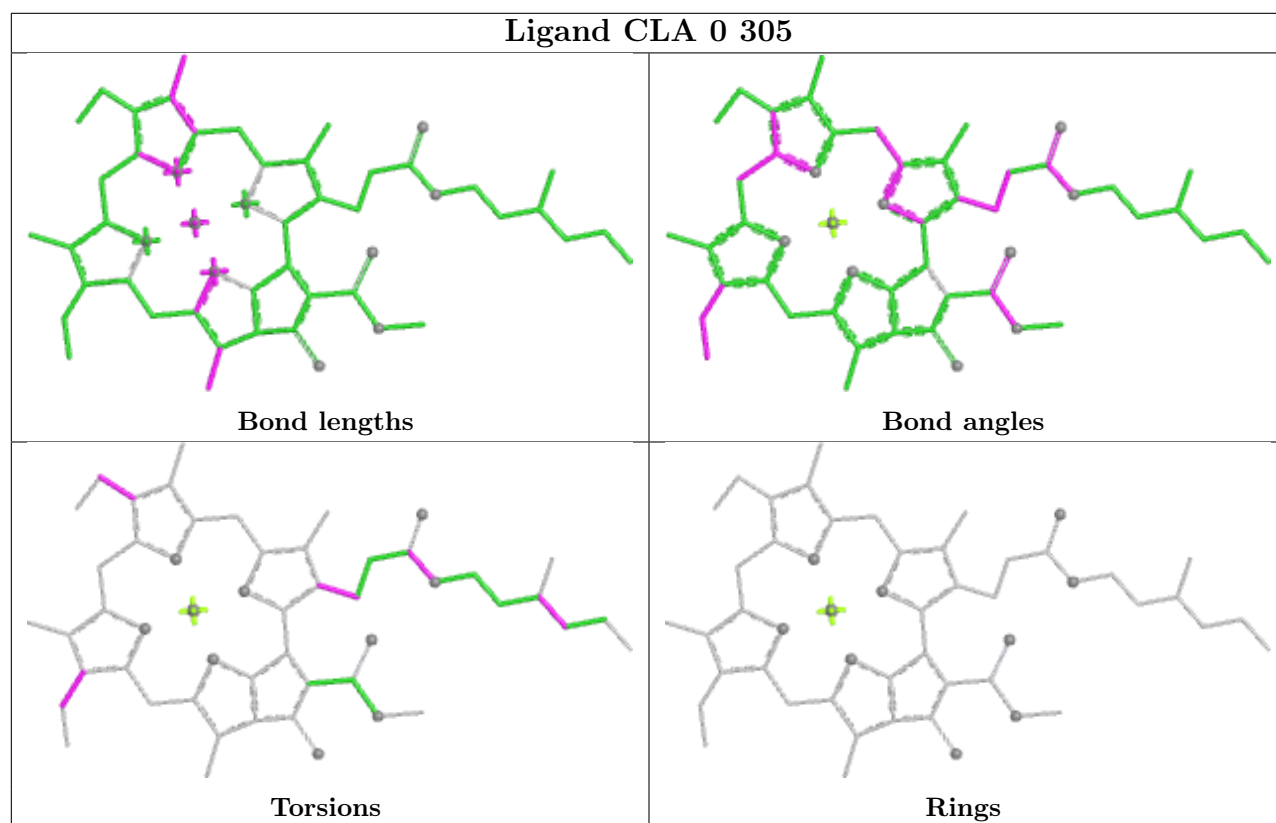
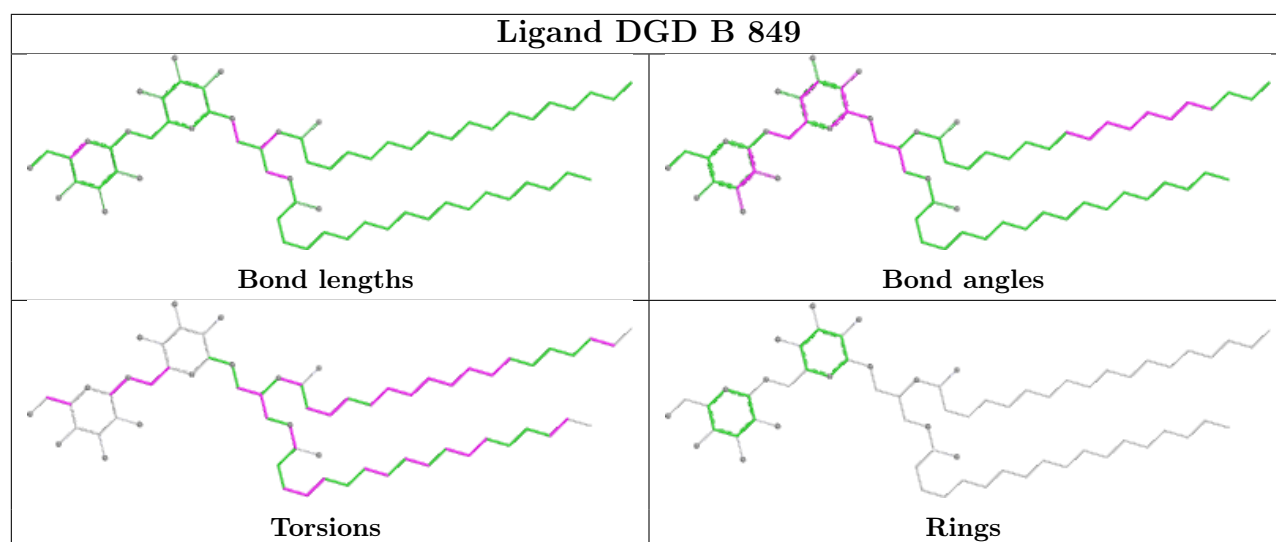


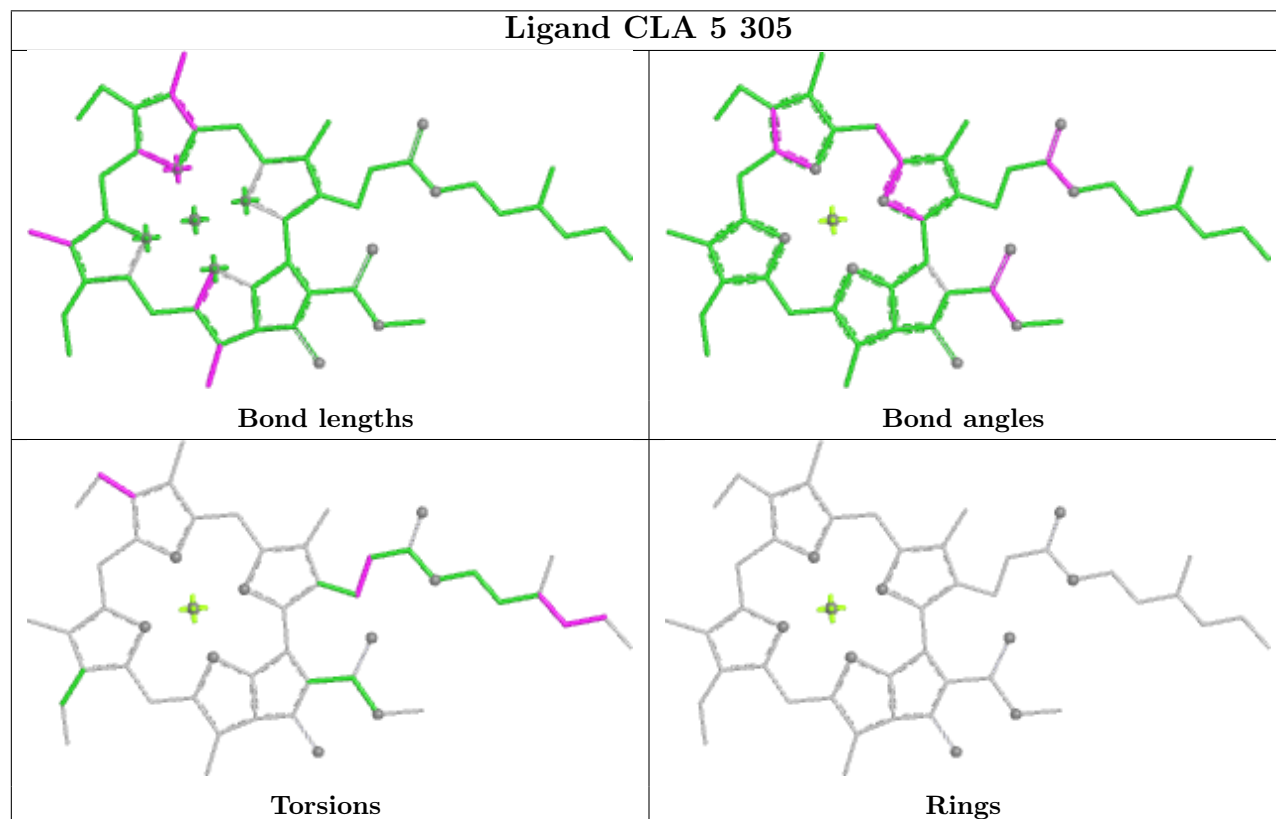
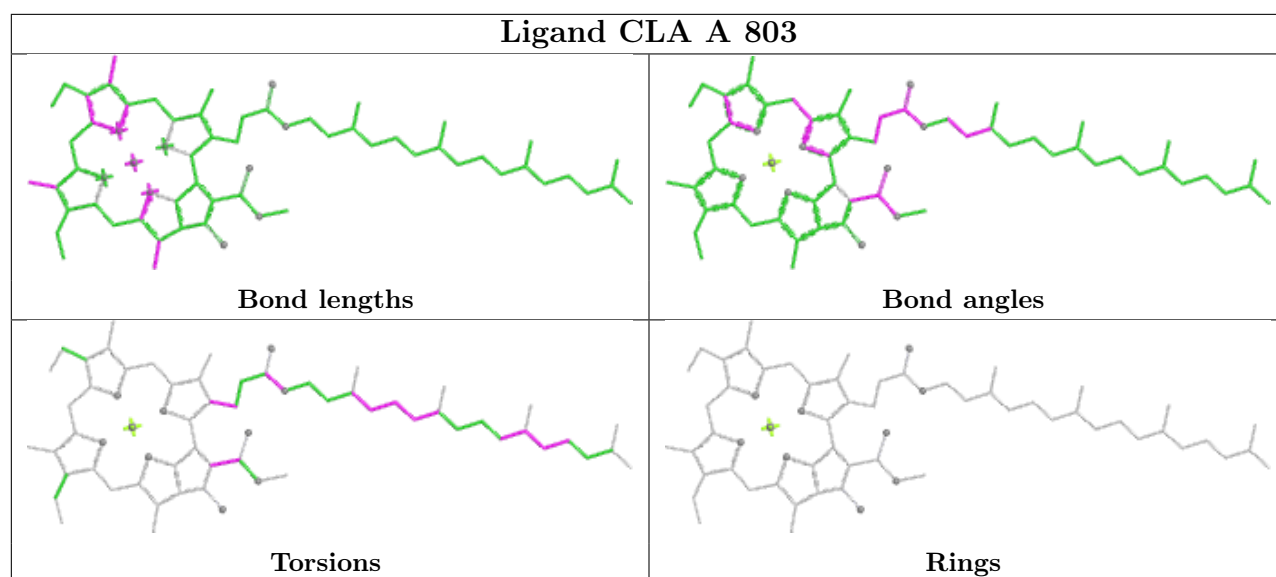
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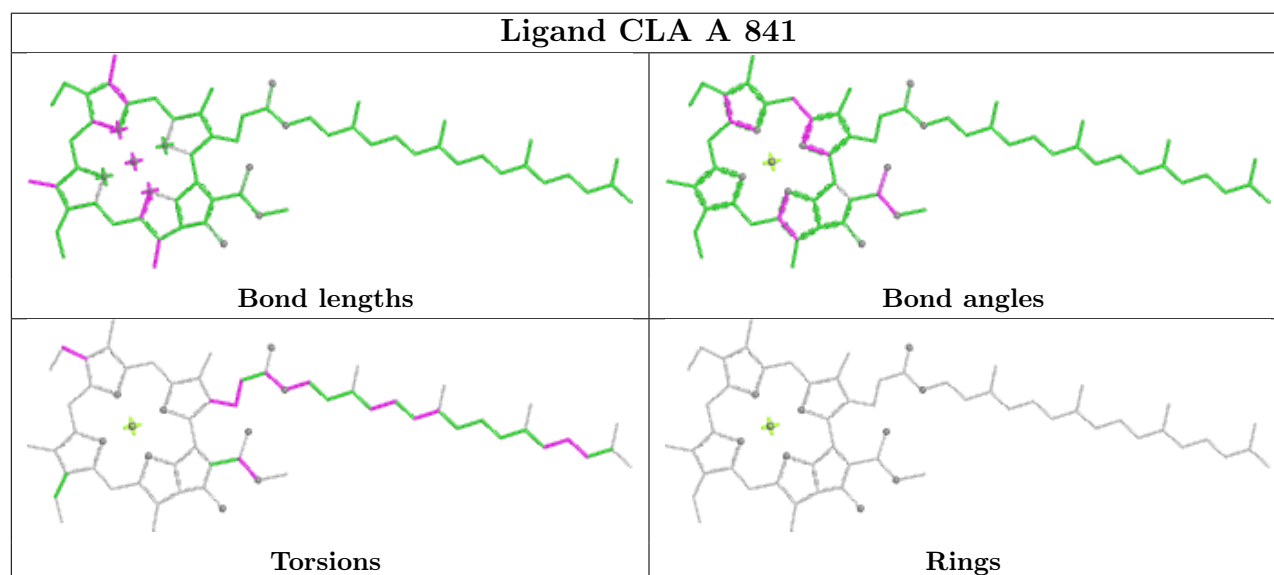
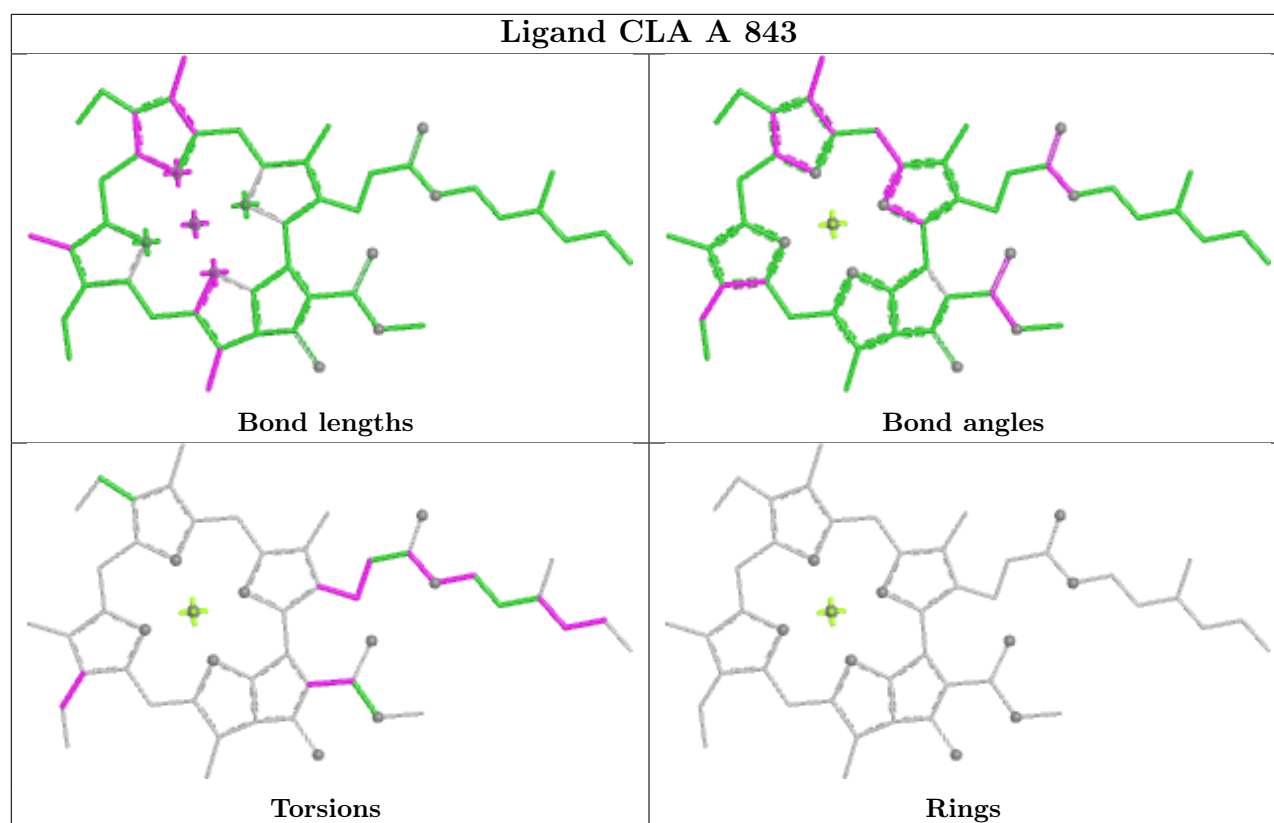


Ligand 8CT J 104

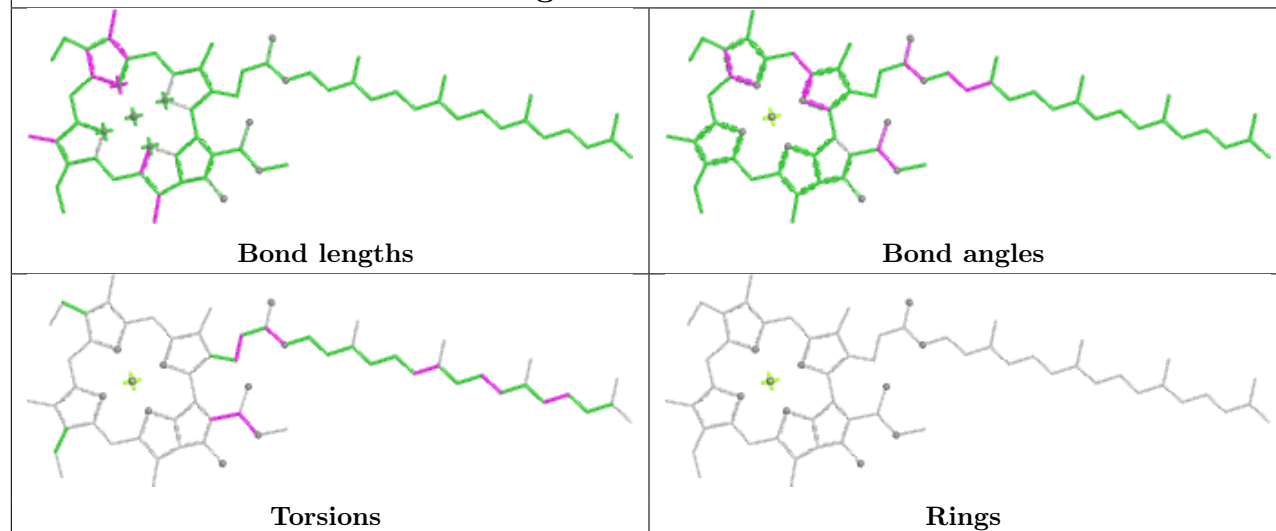




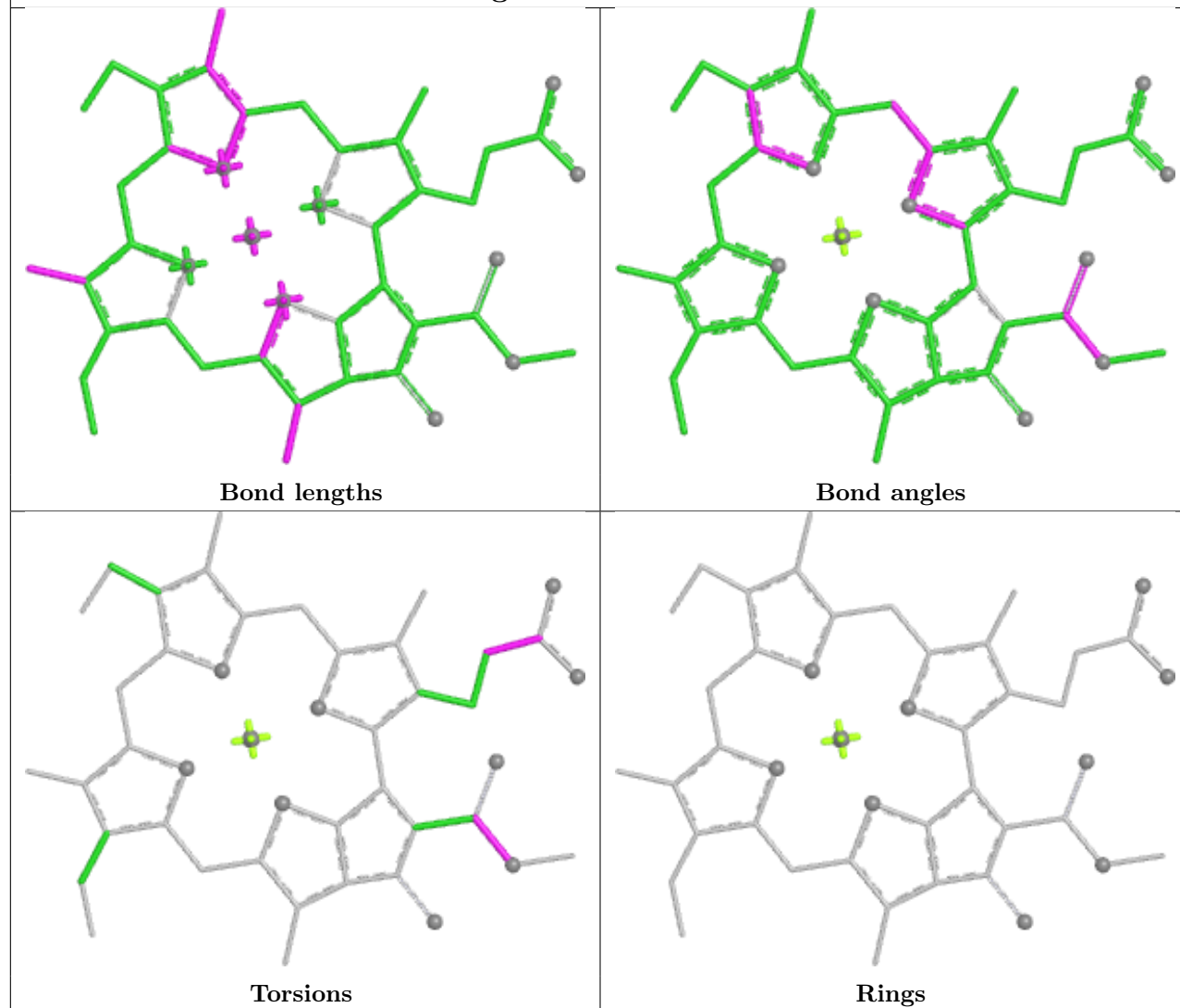


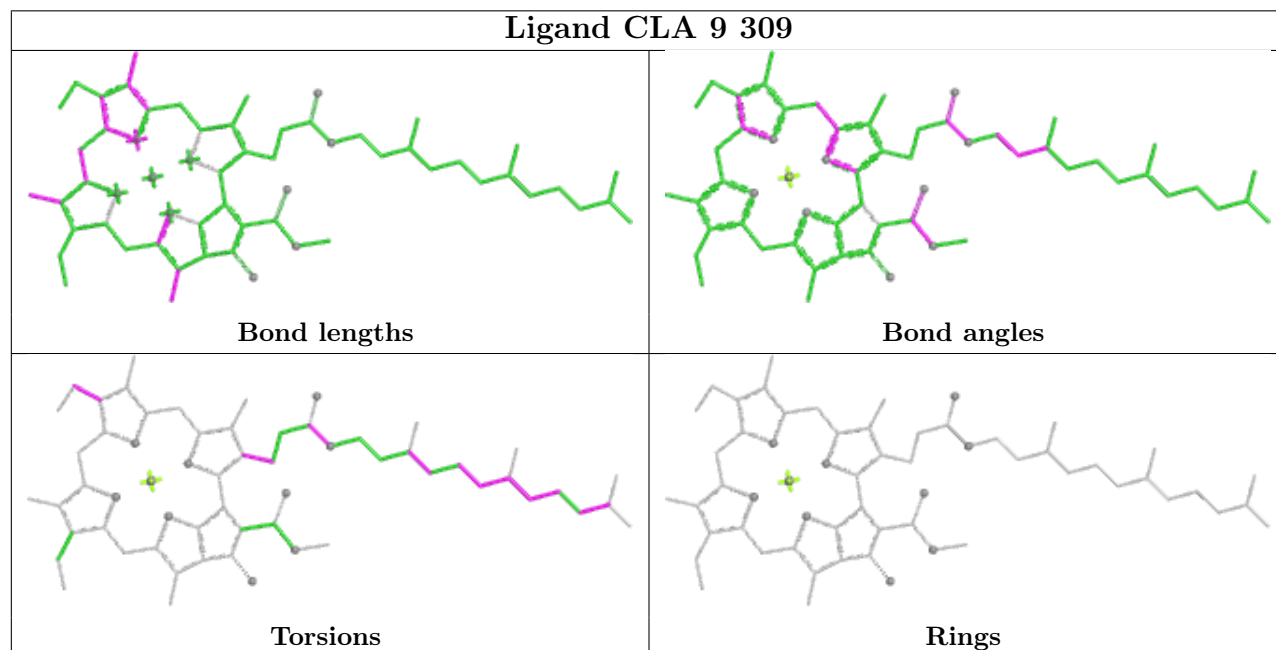
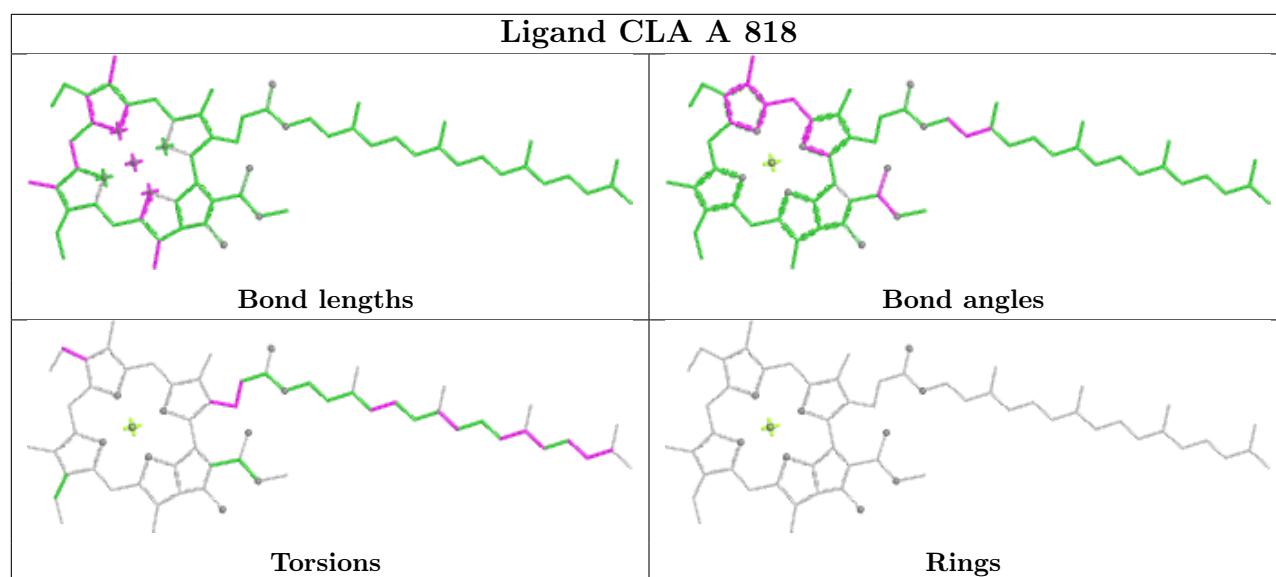


Ligand CLA 5 312

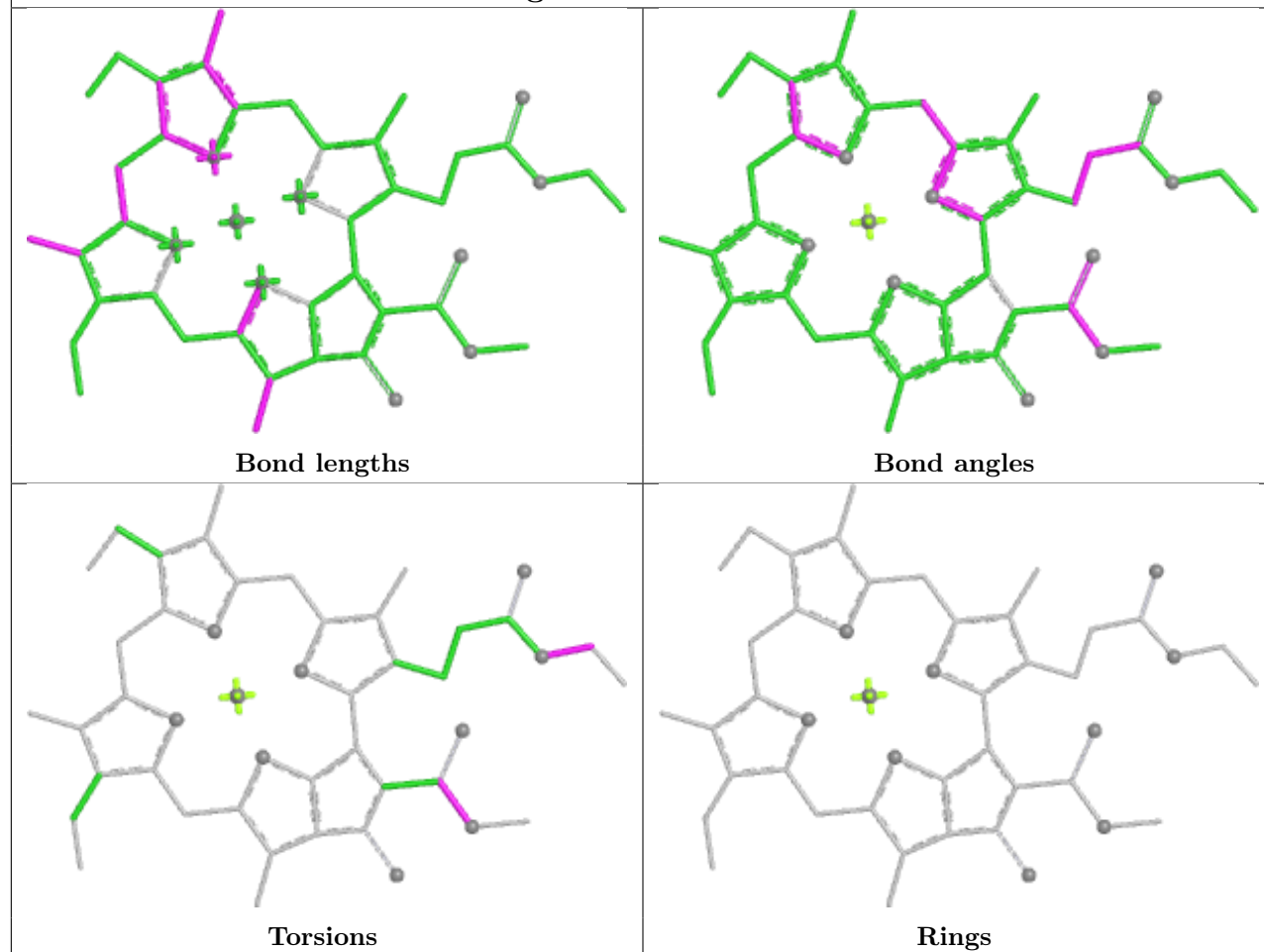


Ligand CLA A 820

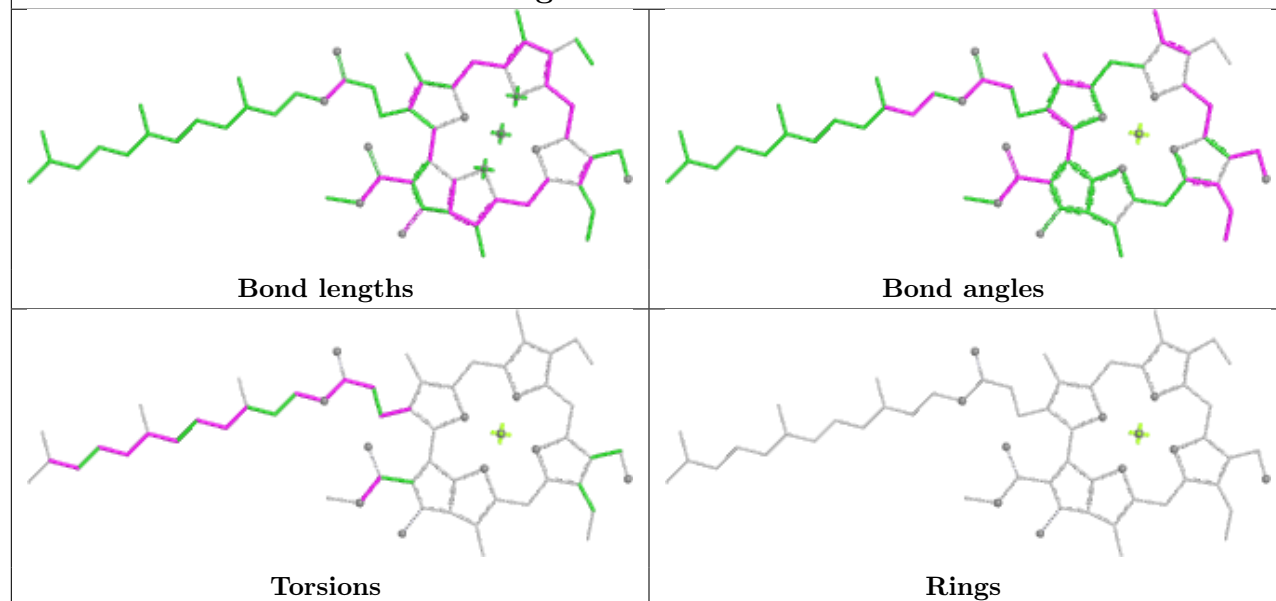


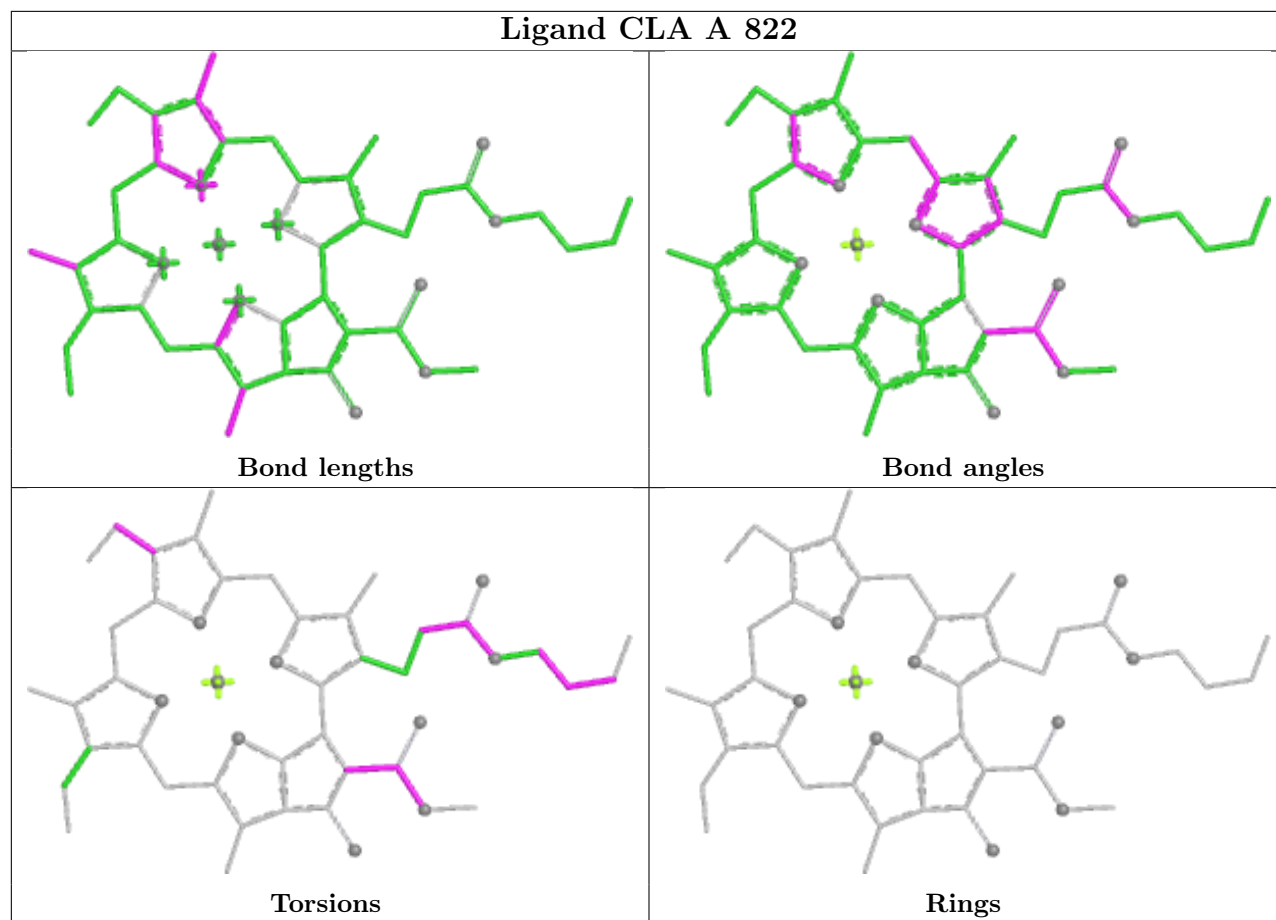


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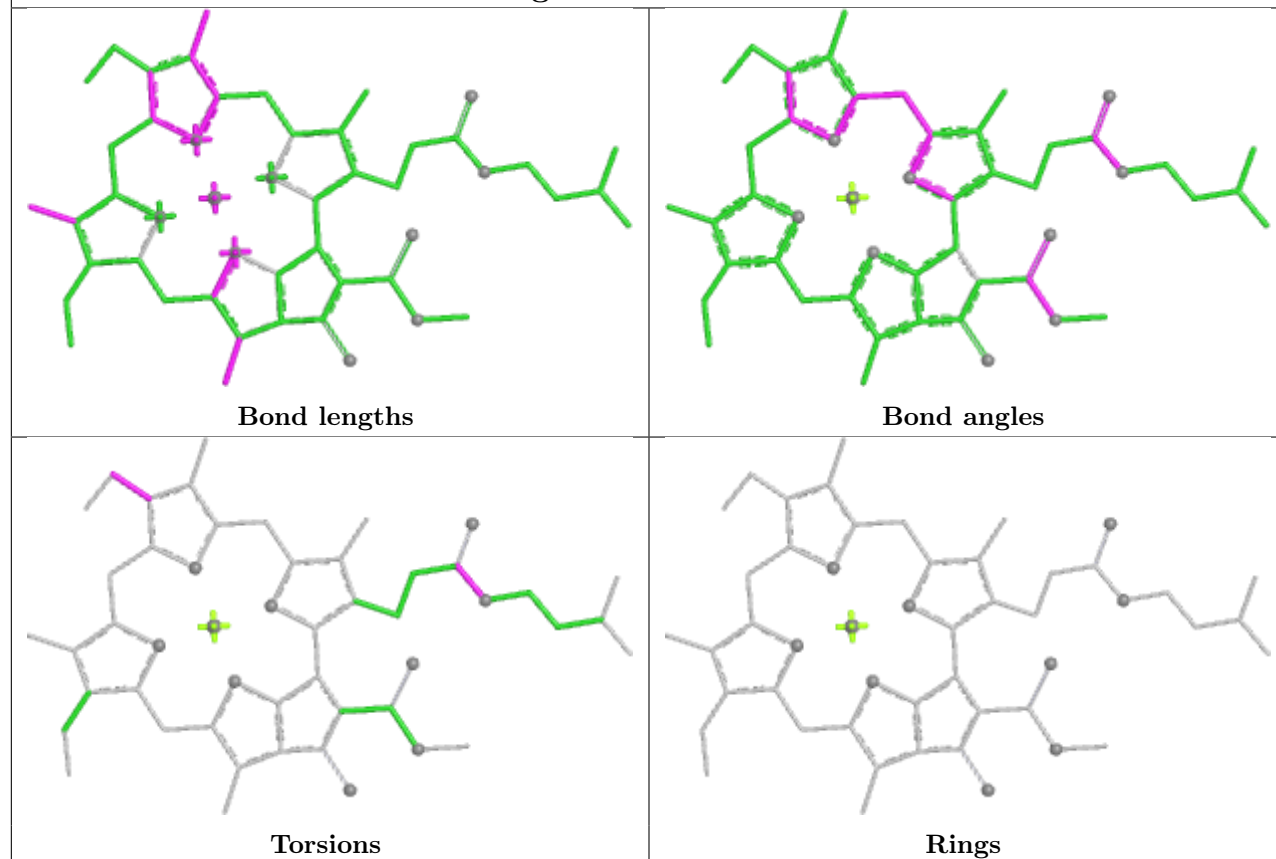


Ligand CHL 0 301

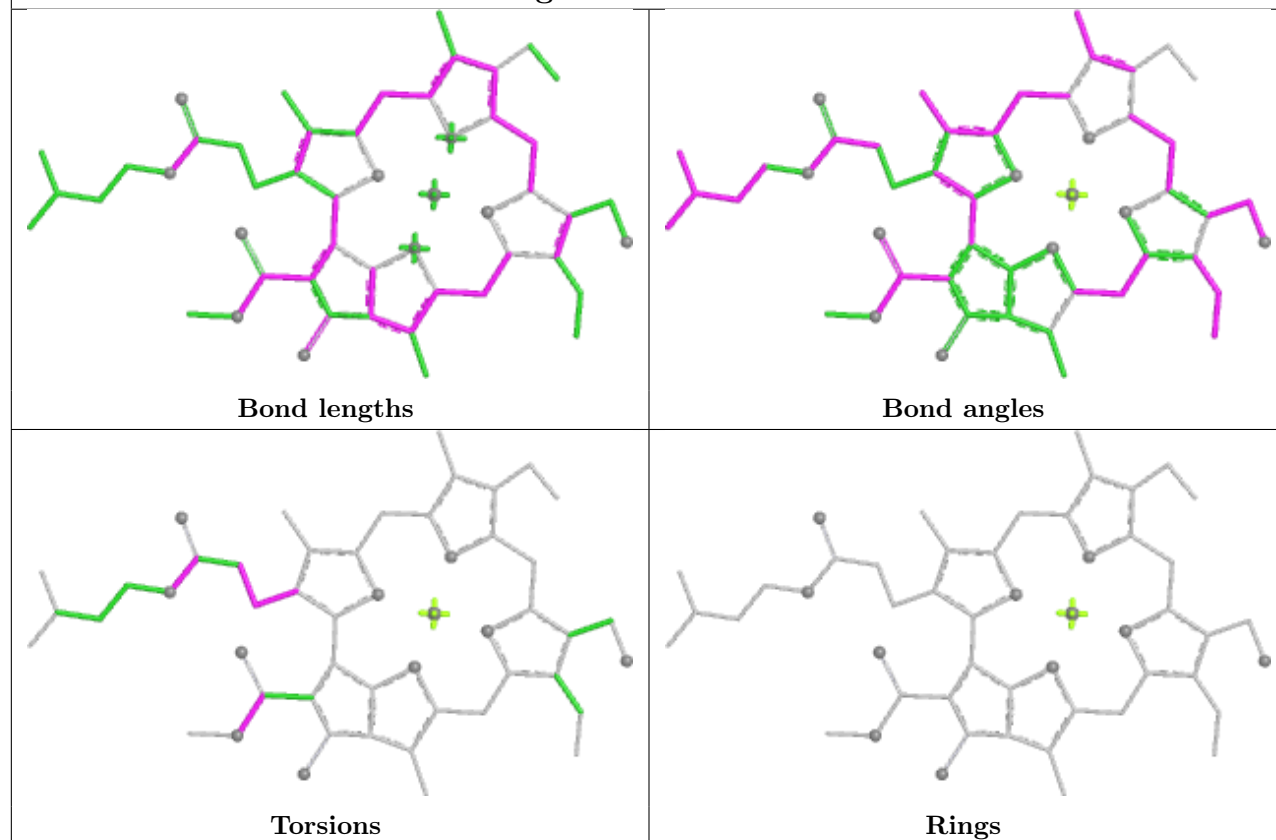




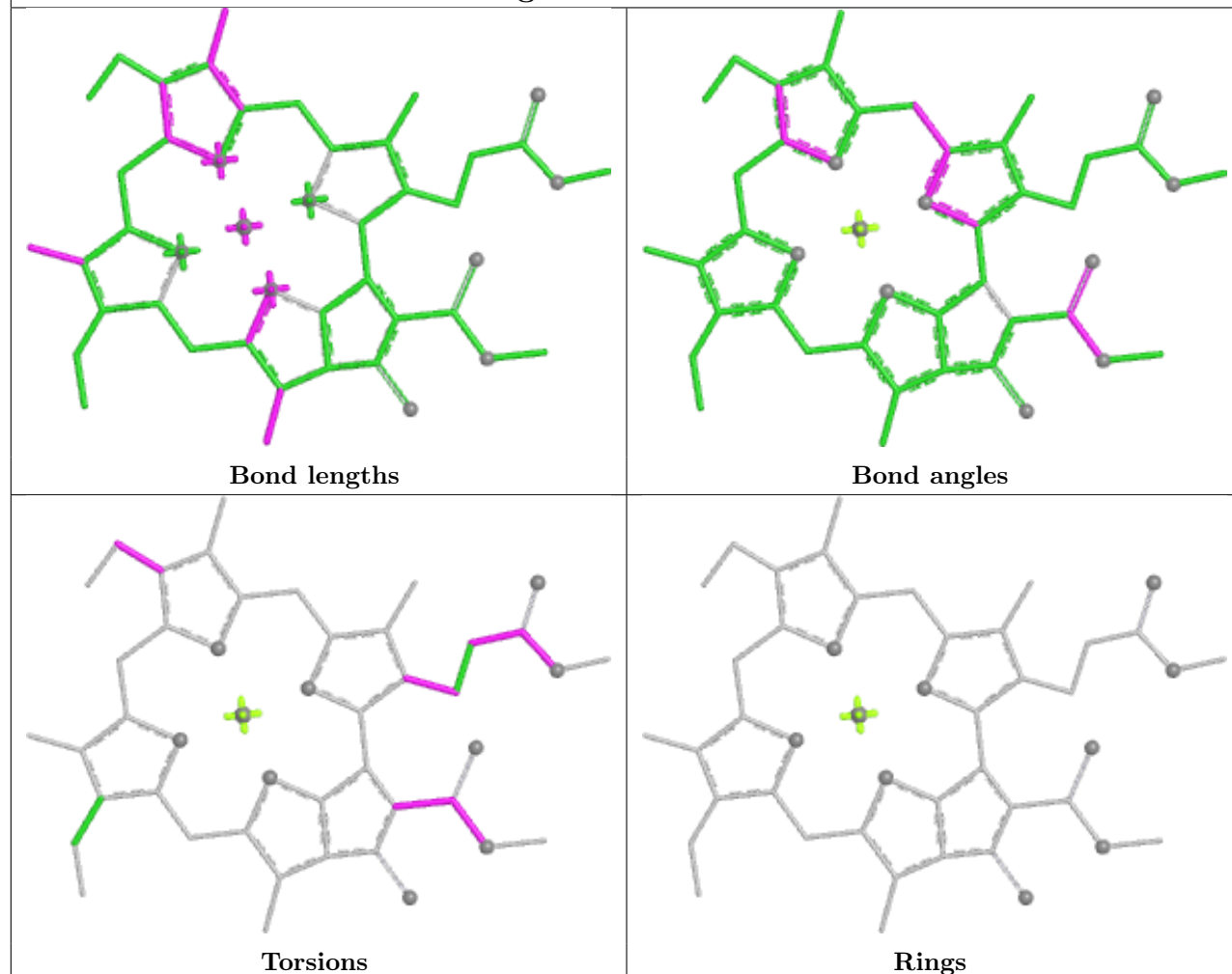
Ligand CLA A 834



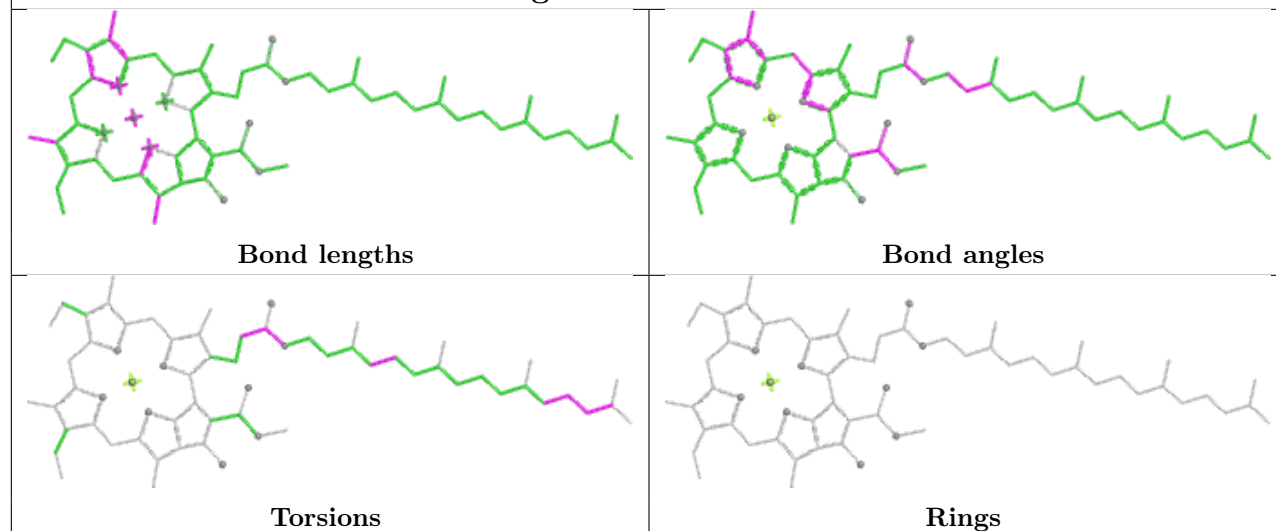
Ligand CHL 8 306



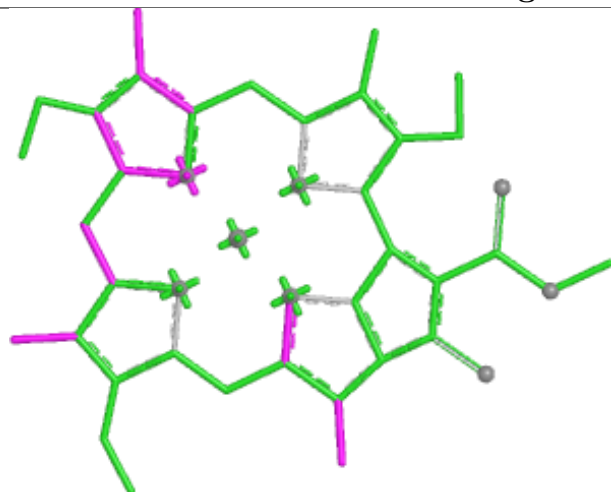
Ligand CLA 6 323



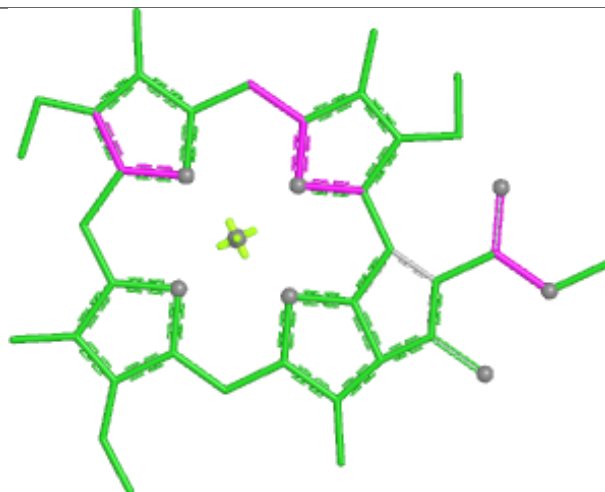
Ligand CLA A 821



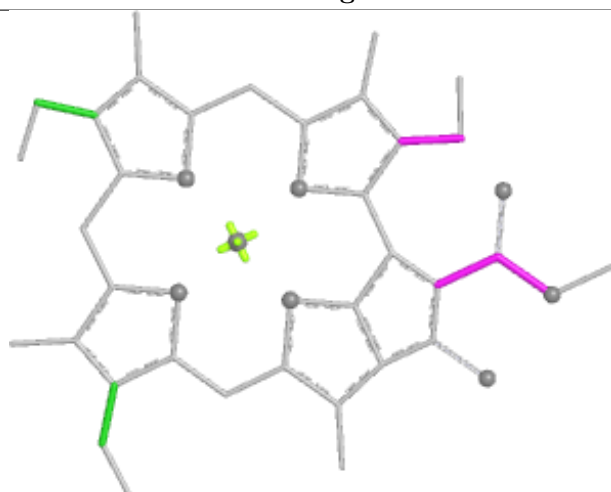
Ligand CLA J 103



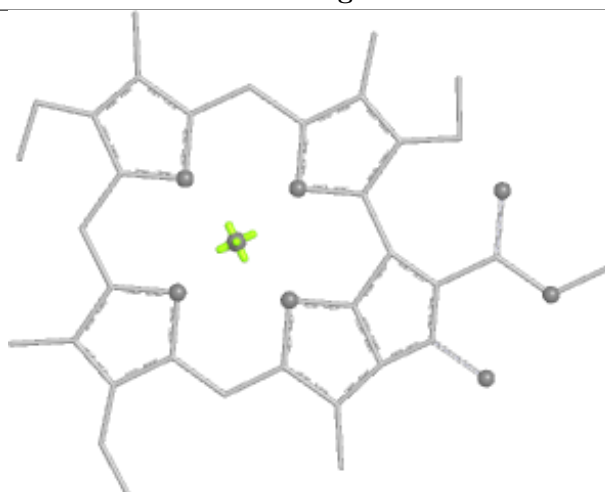
Bond lengths



Bond angles

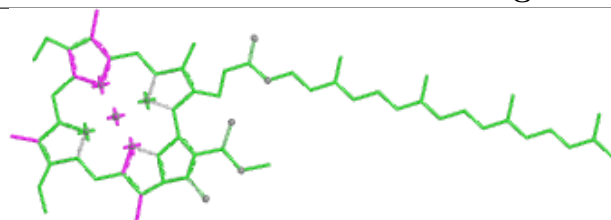


Torsions

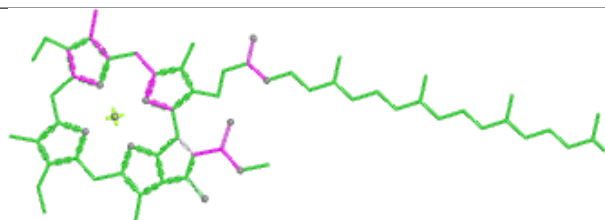


Rings

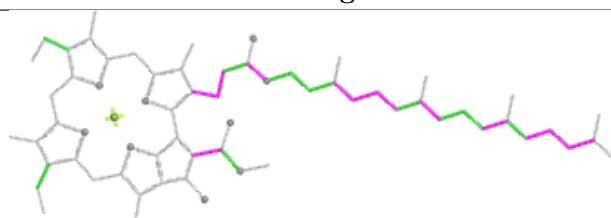
Ligand CLA A 808



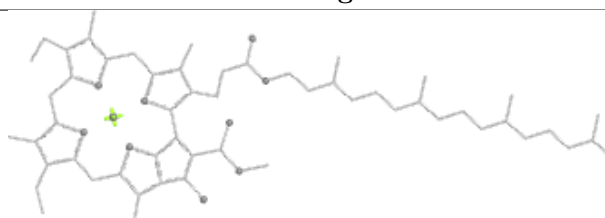
Bond lengths



Bond angles

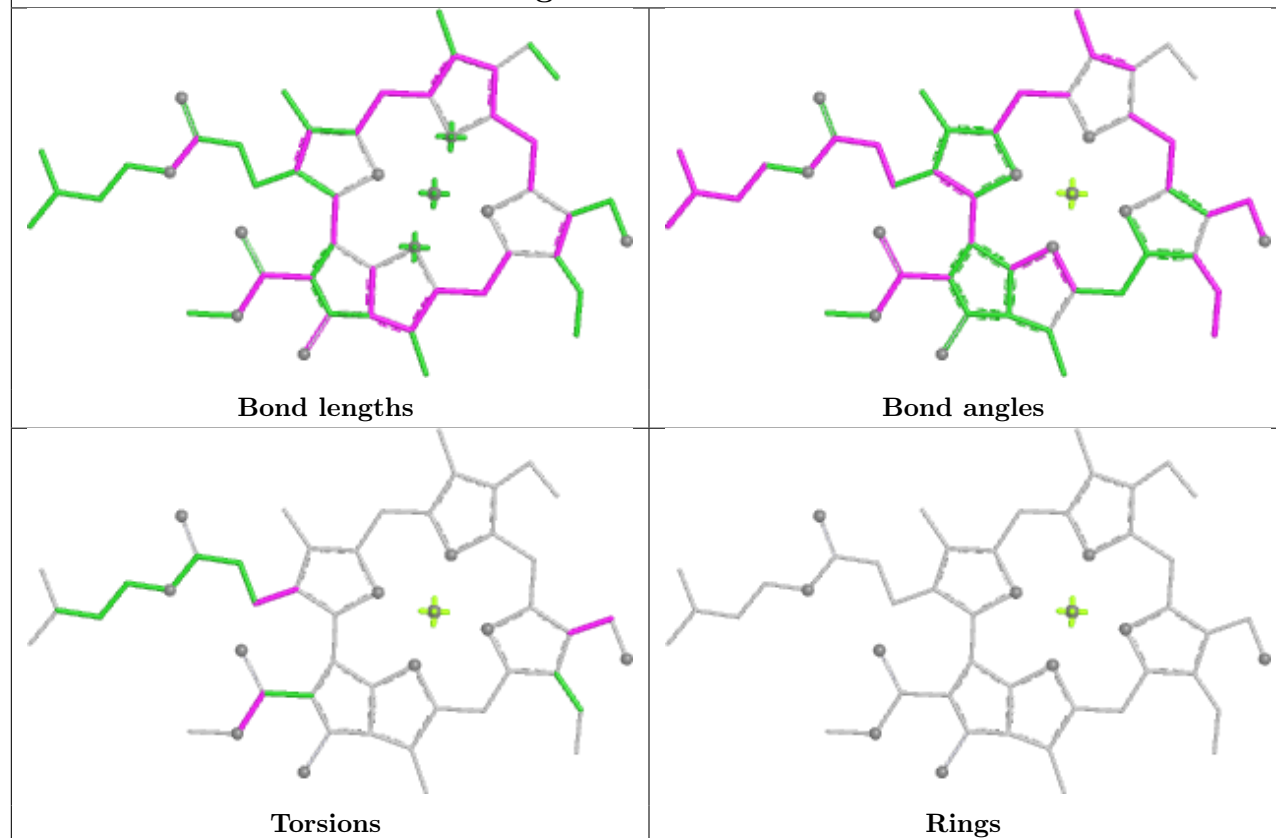


Torsions

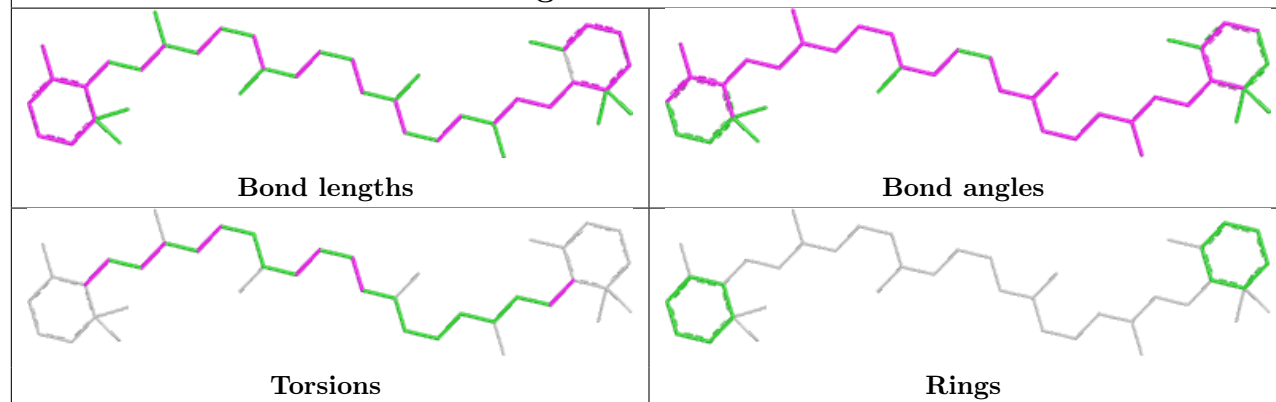


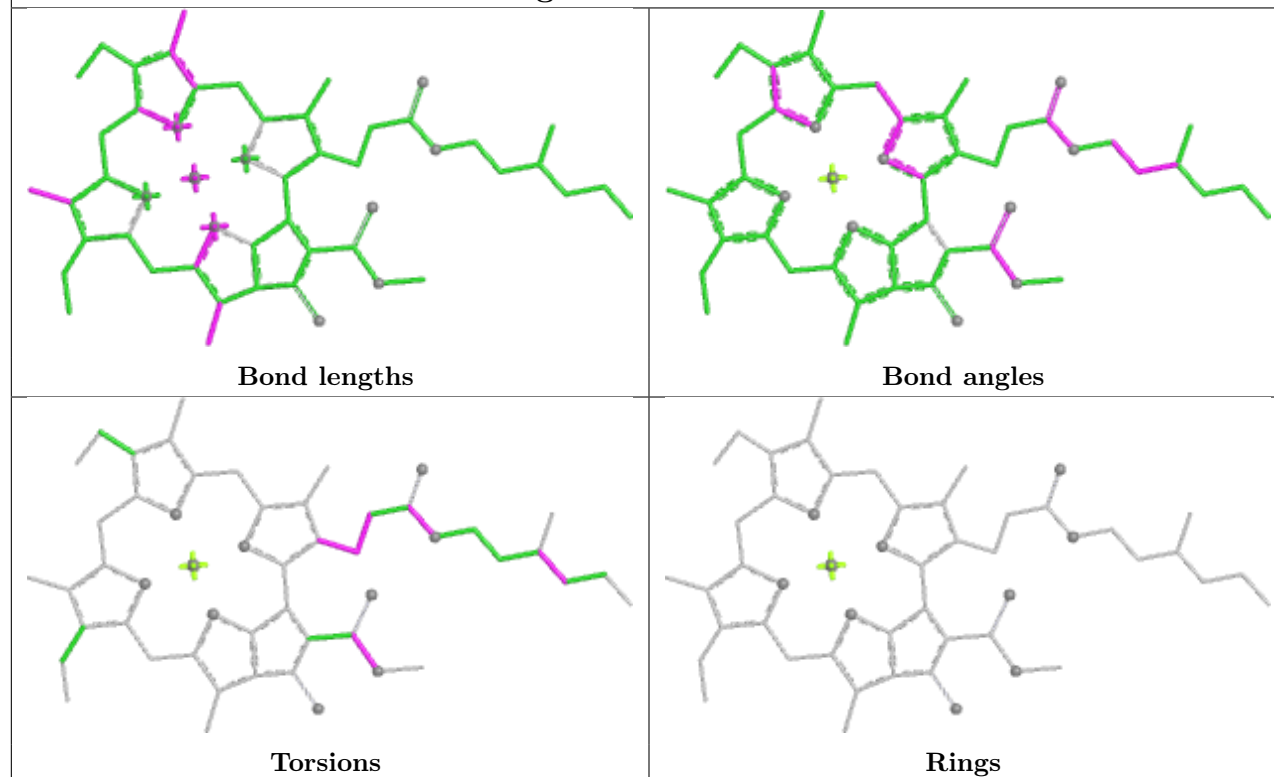
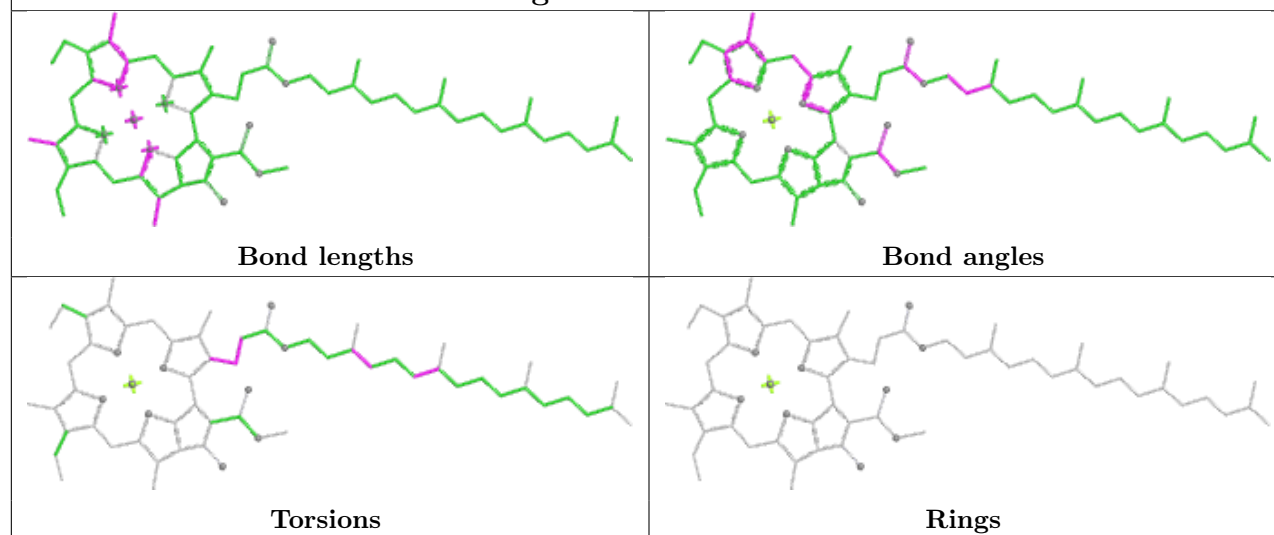
Rings

Ligand CHL 4 307

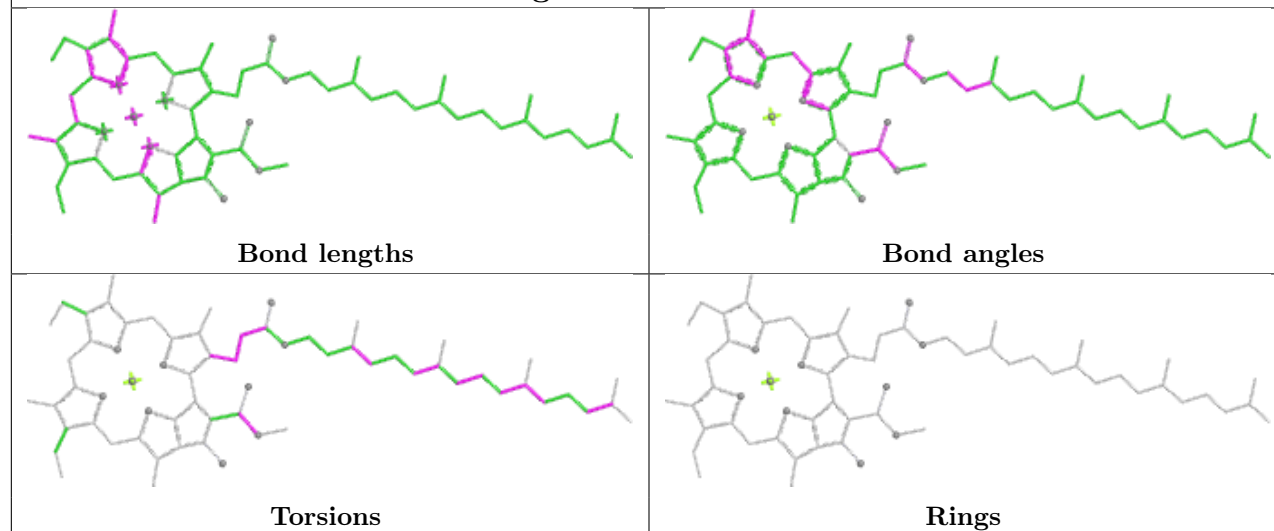


Ligand 8CT F 302

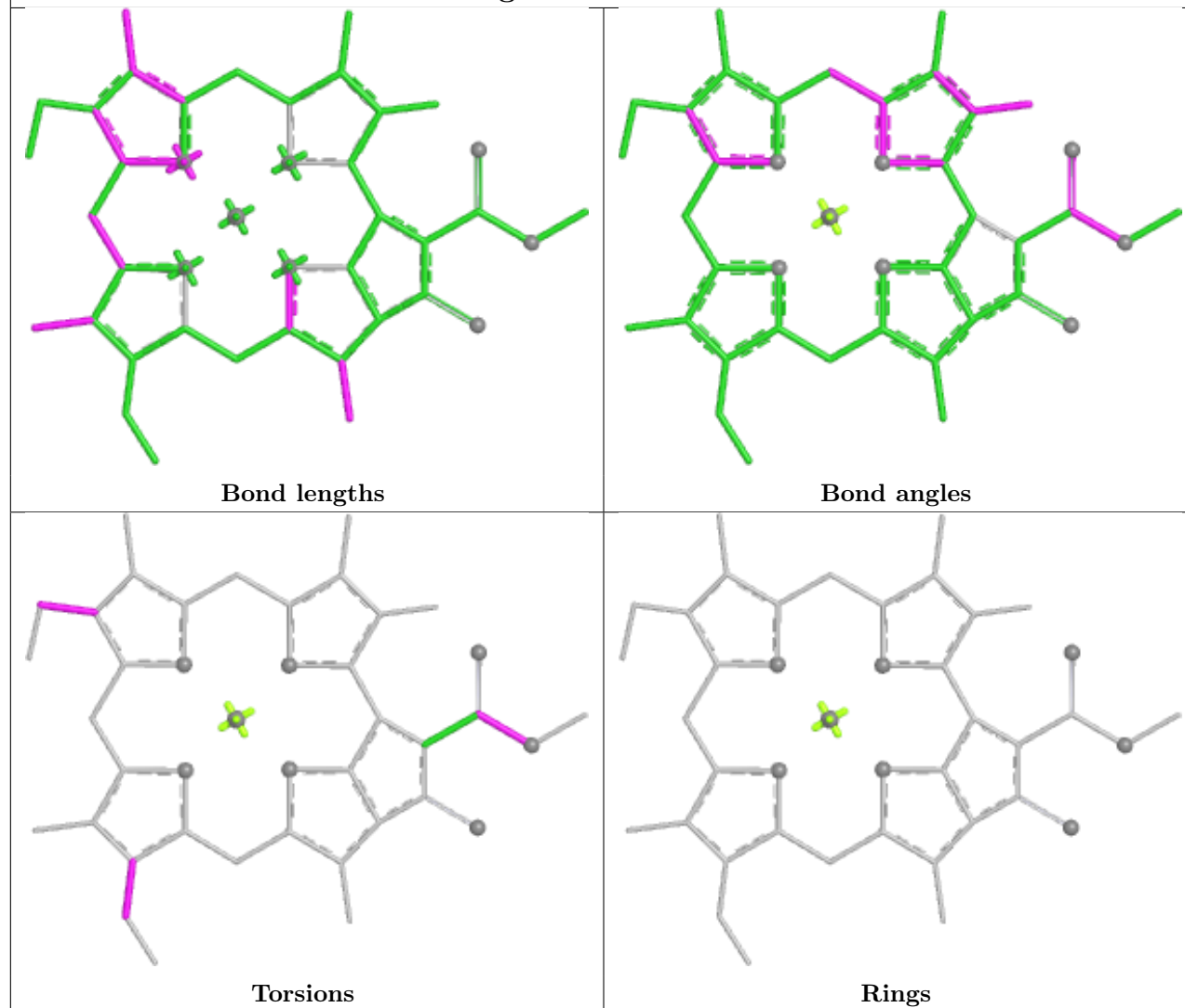


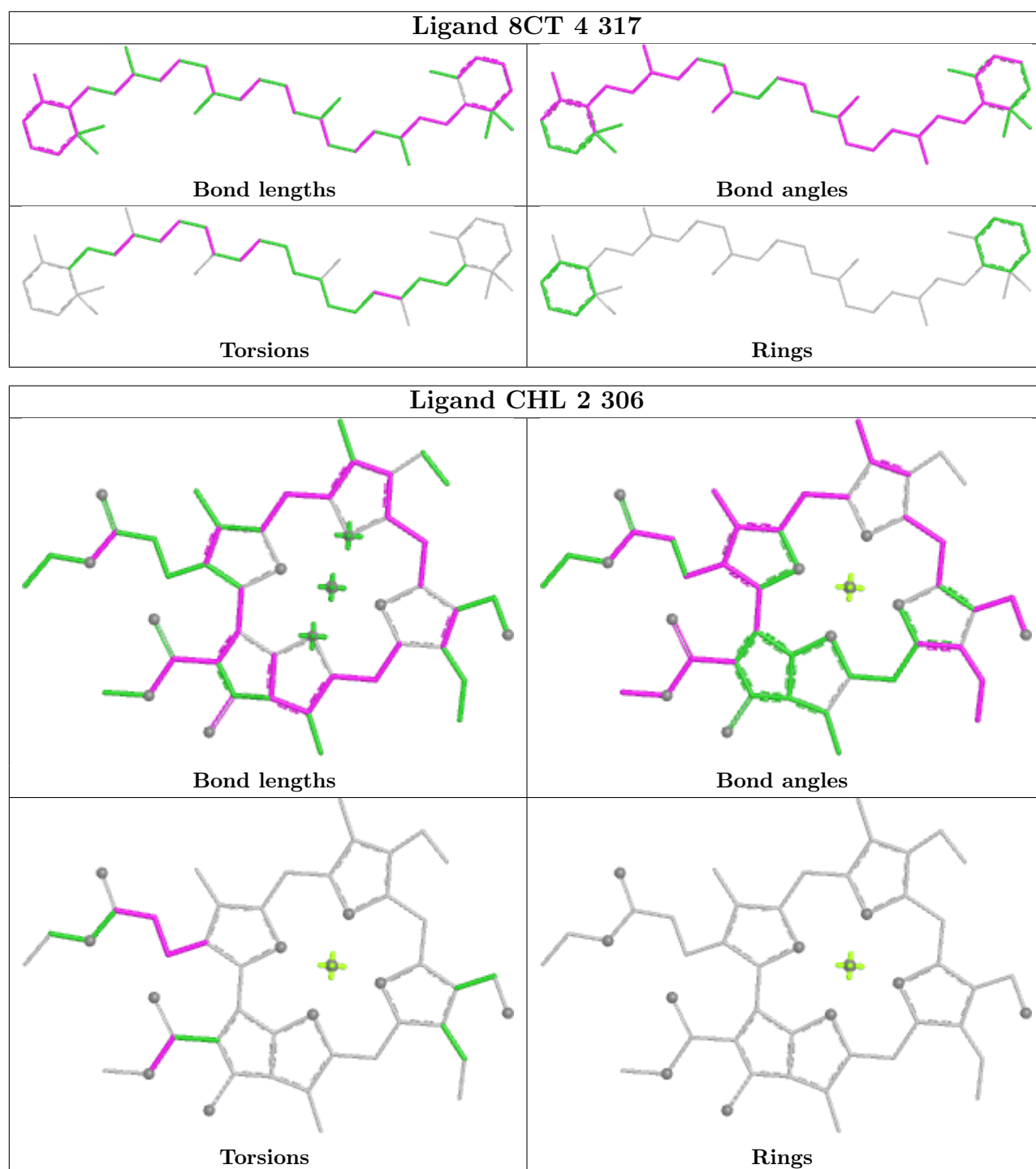
Ligand CLA 9 306**Ligand CLA A 802**

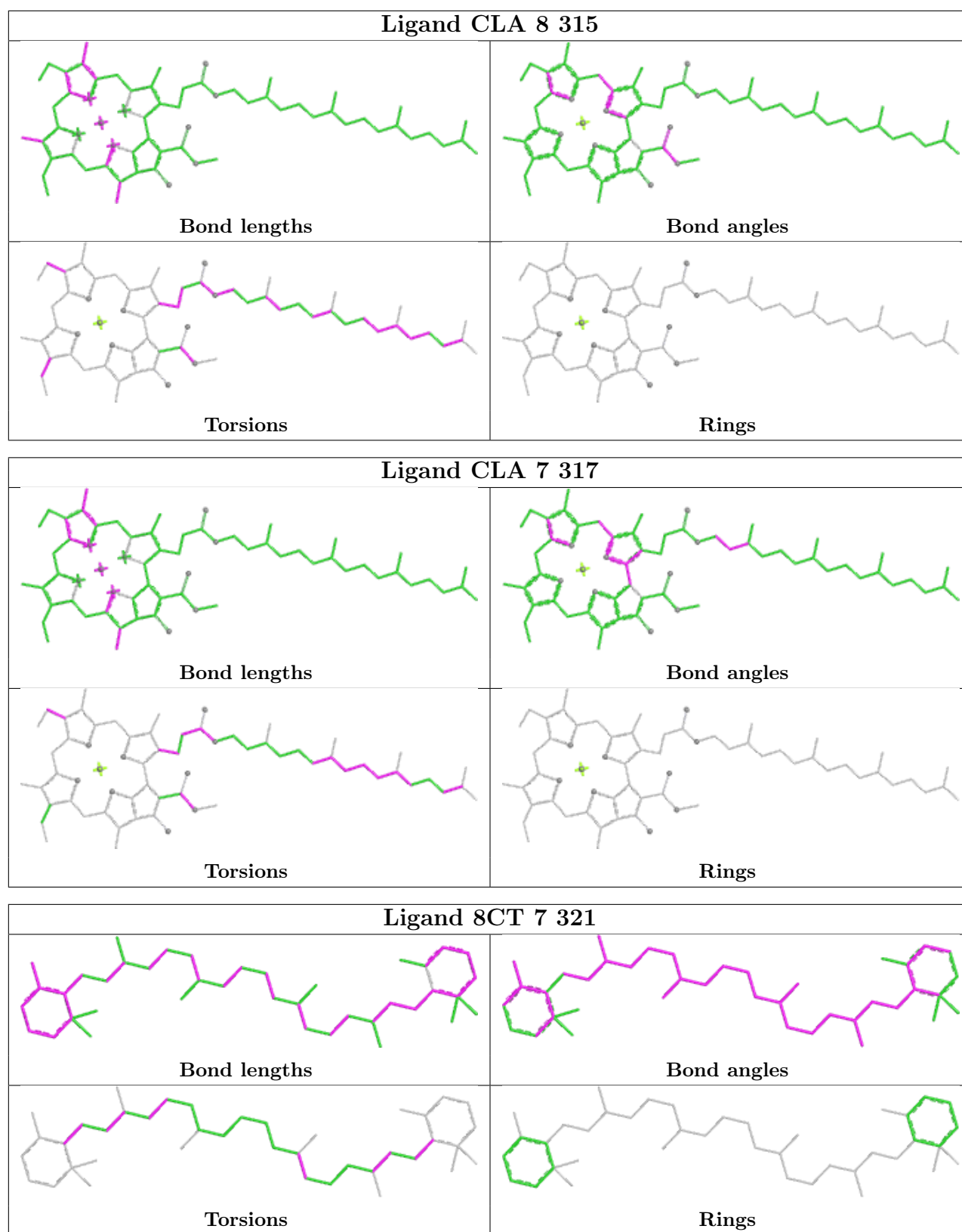
Ligand CLA B 828



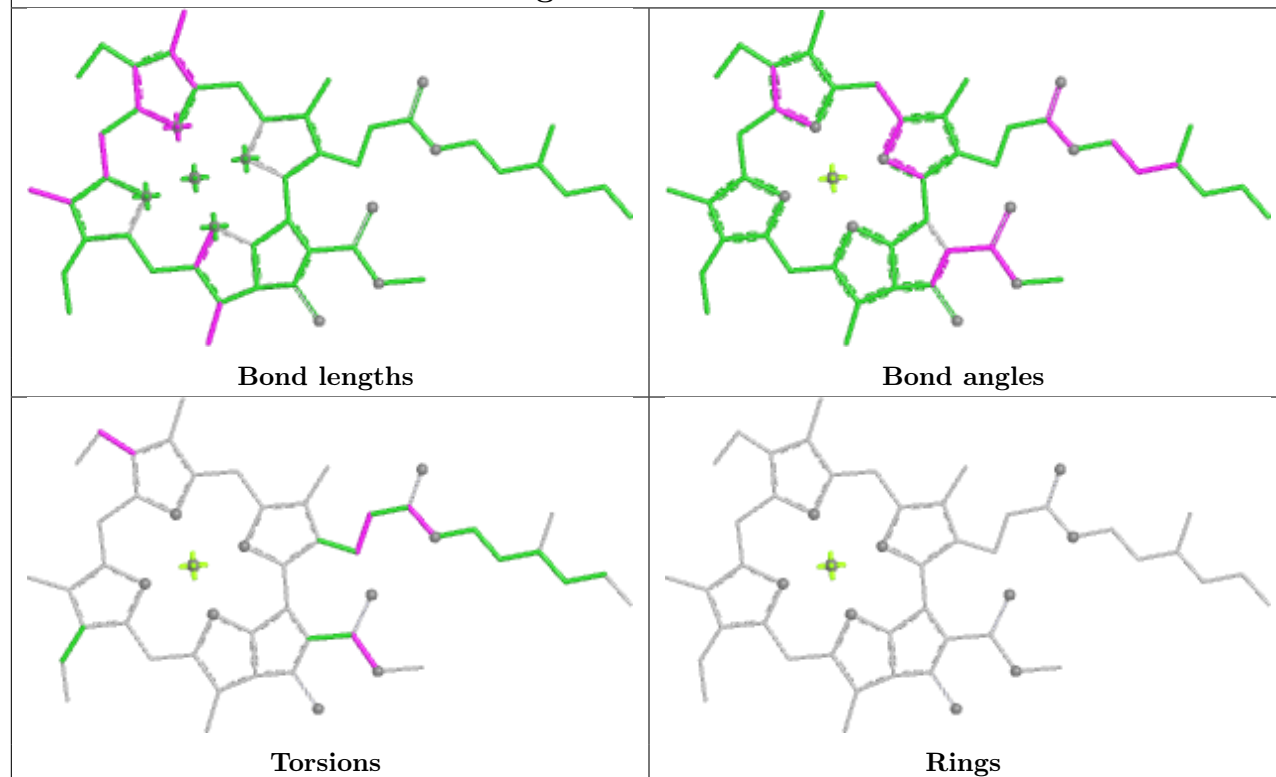
Ligand CLA 9 310



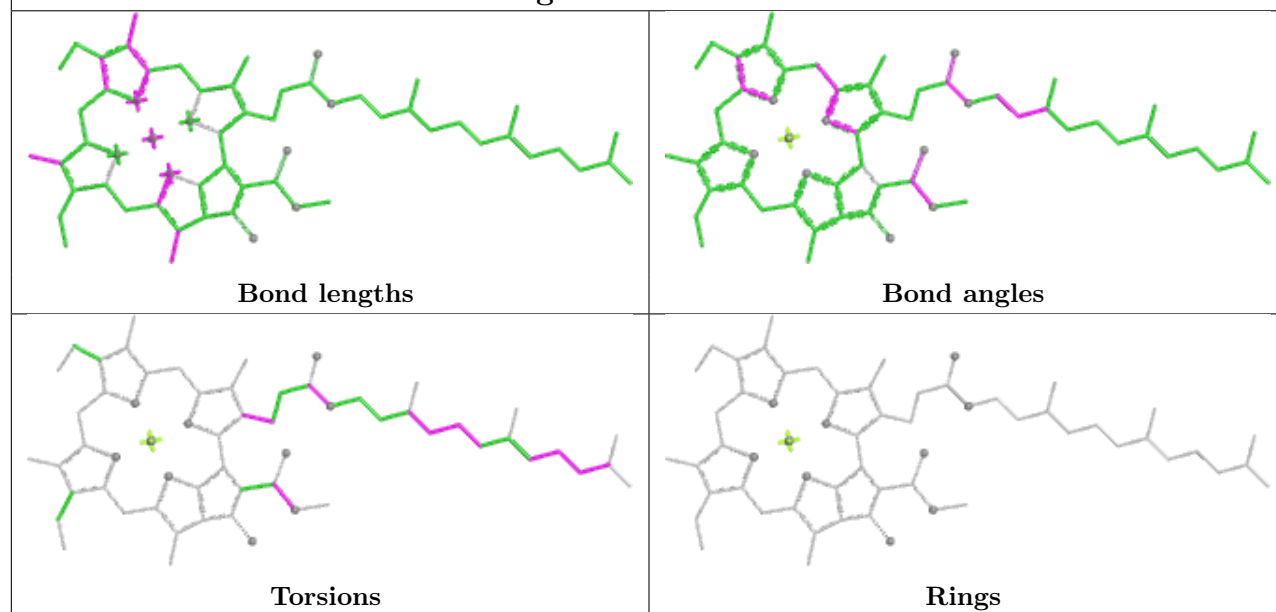




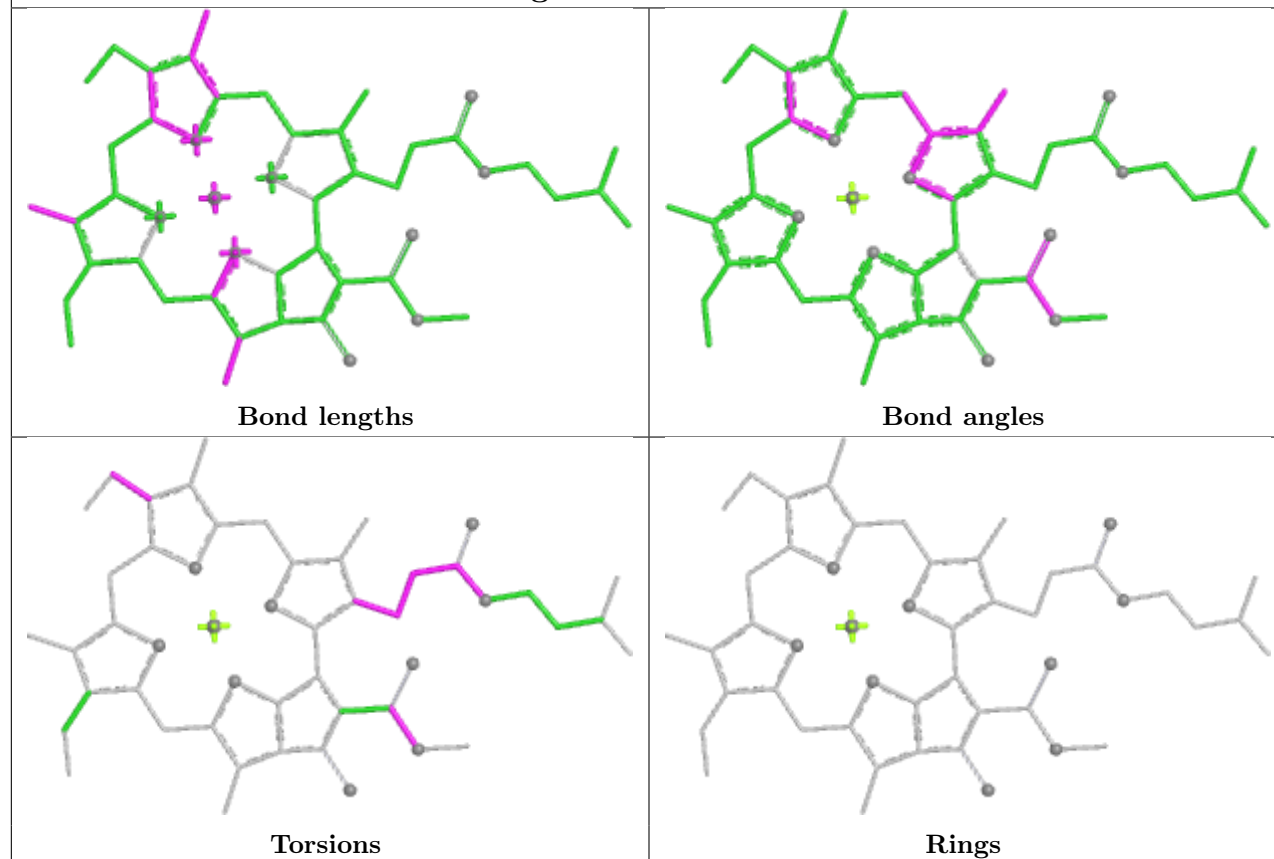
Ligand CLA 9 305



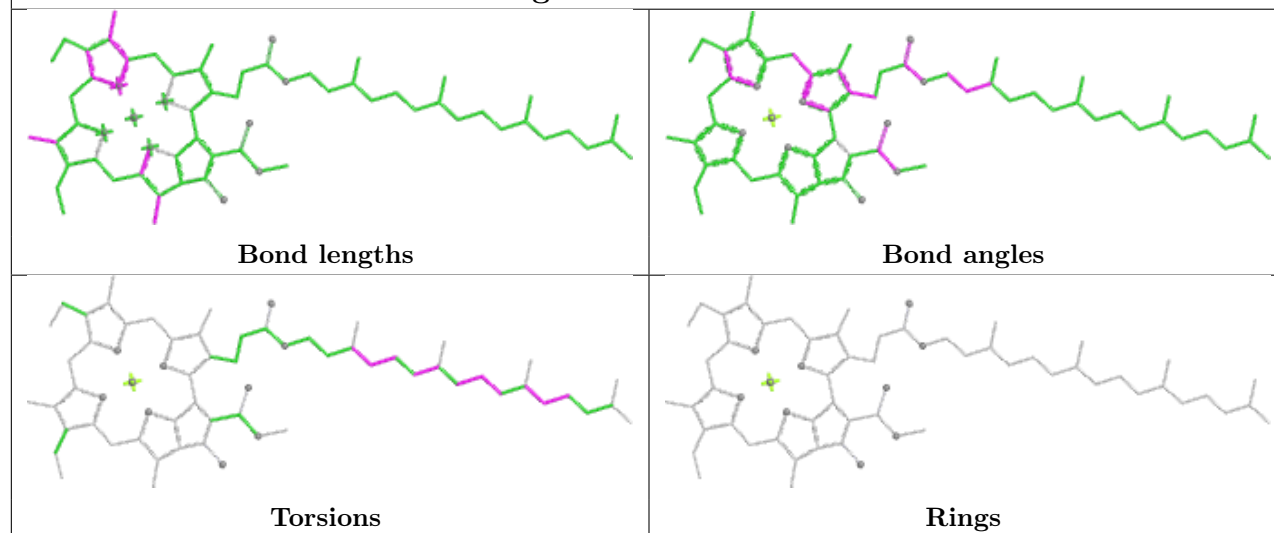
Ligand CLA 4 309

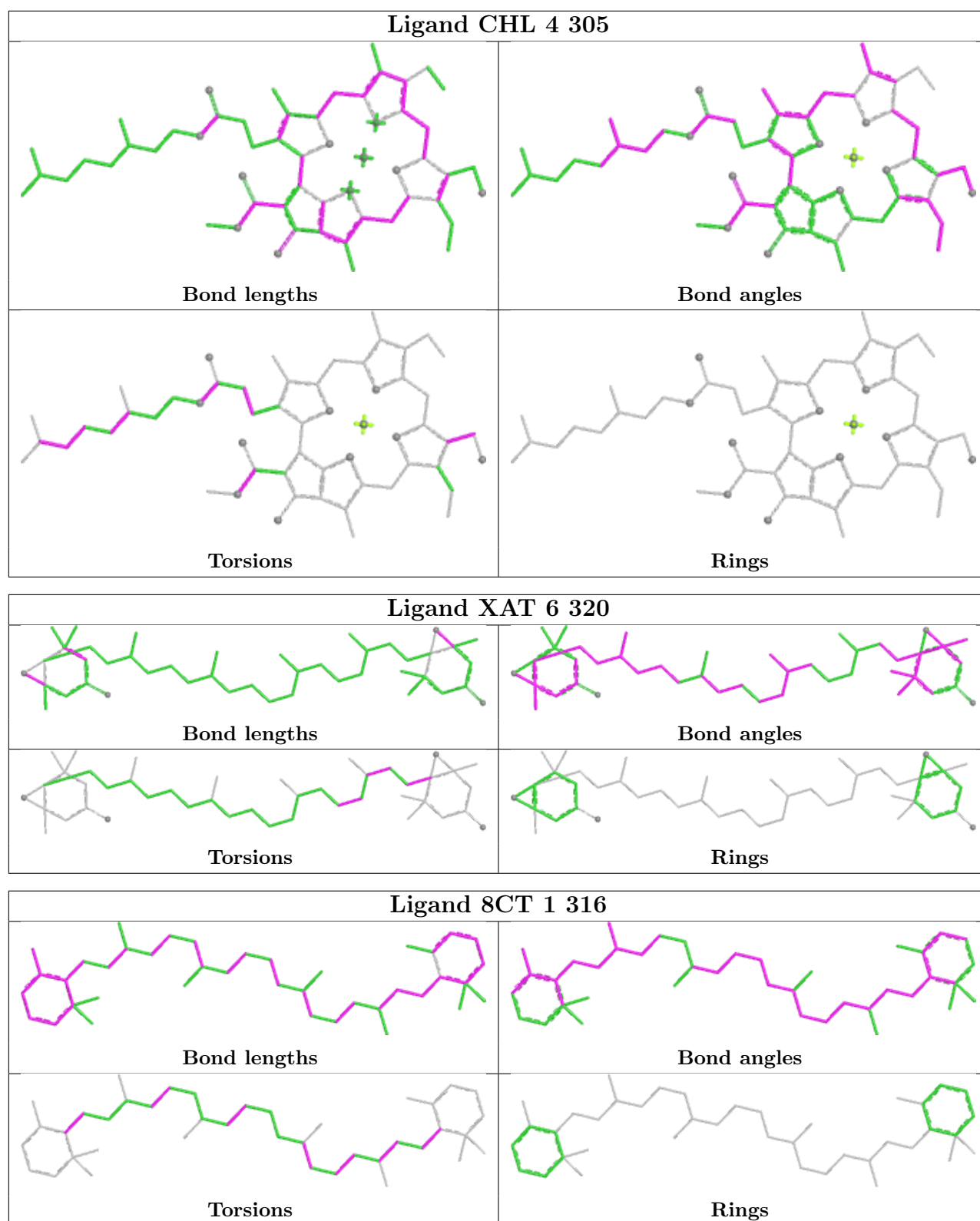


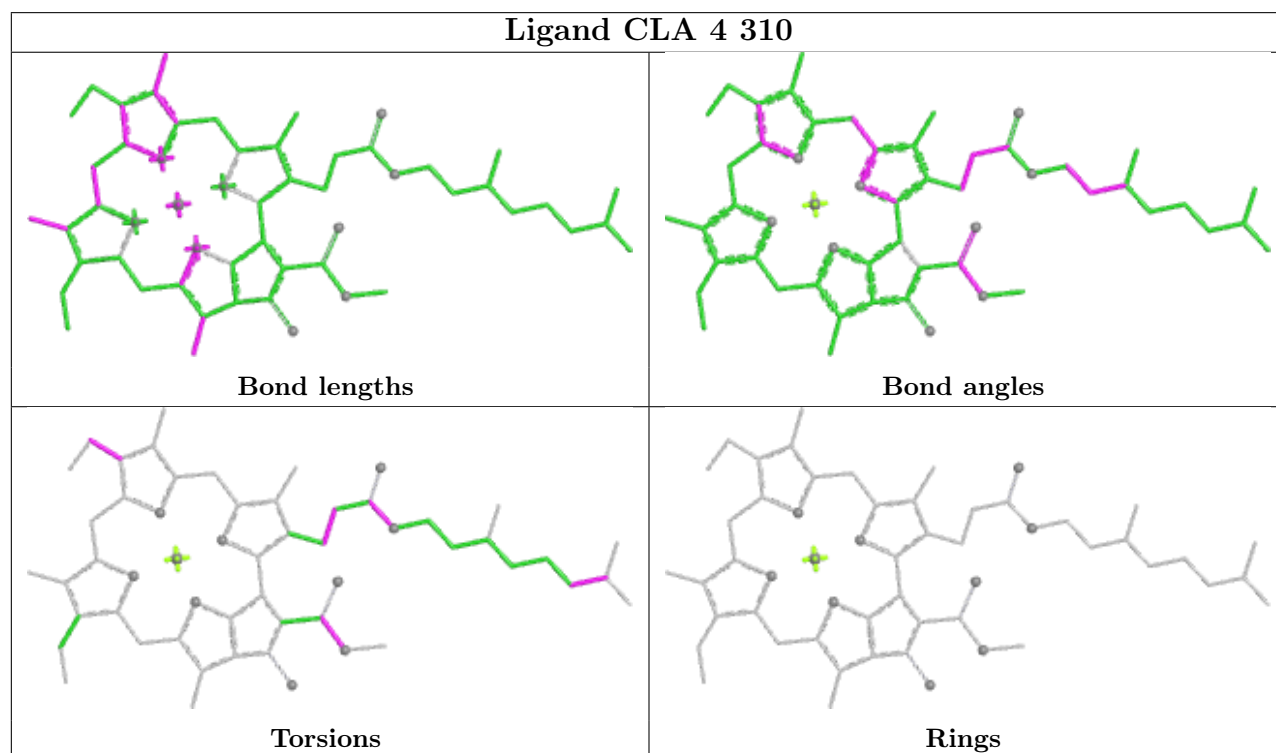
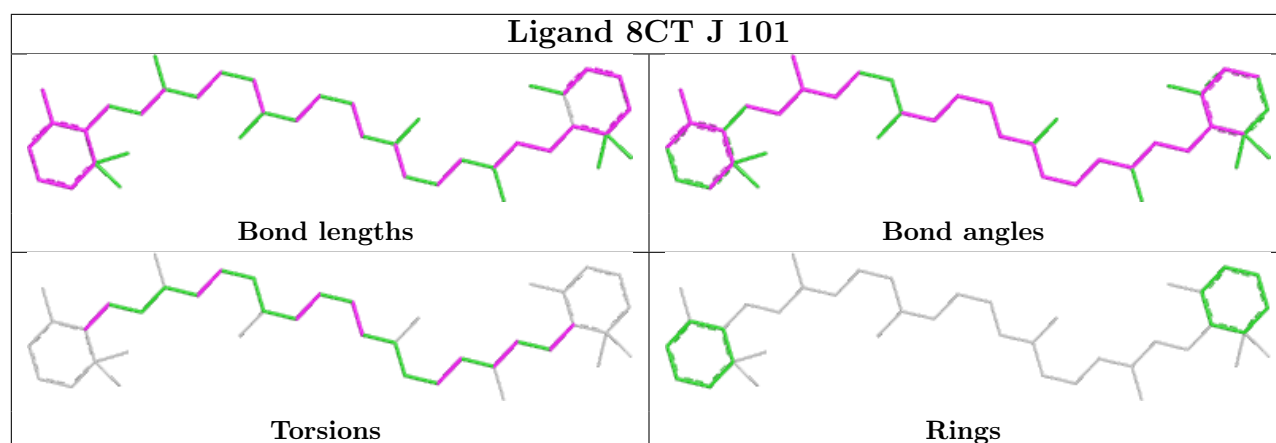
Ligand CLA K 105



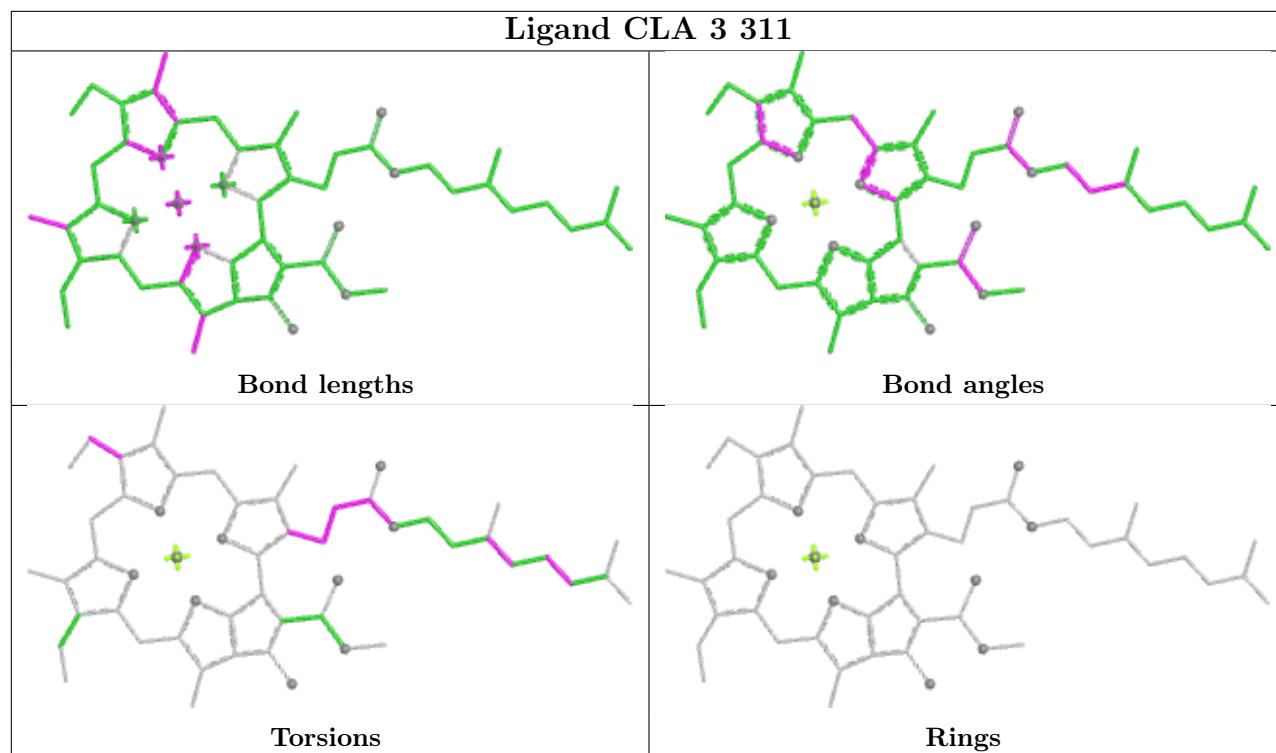
Ligand CLA B 811



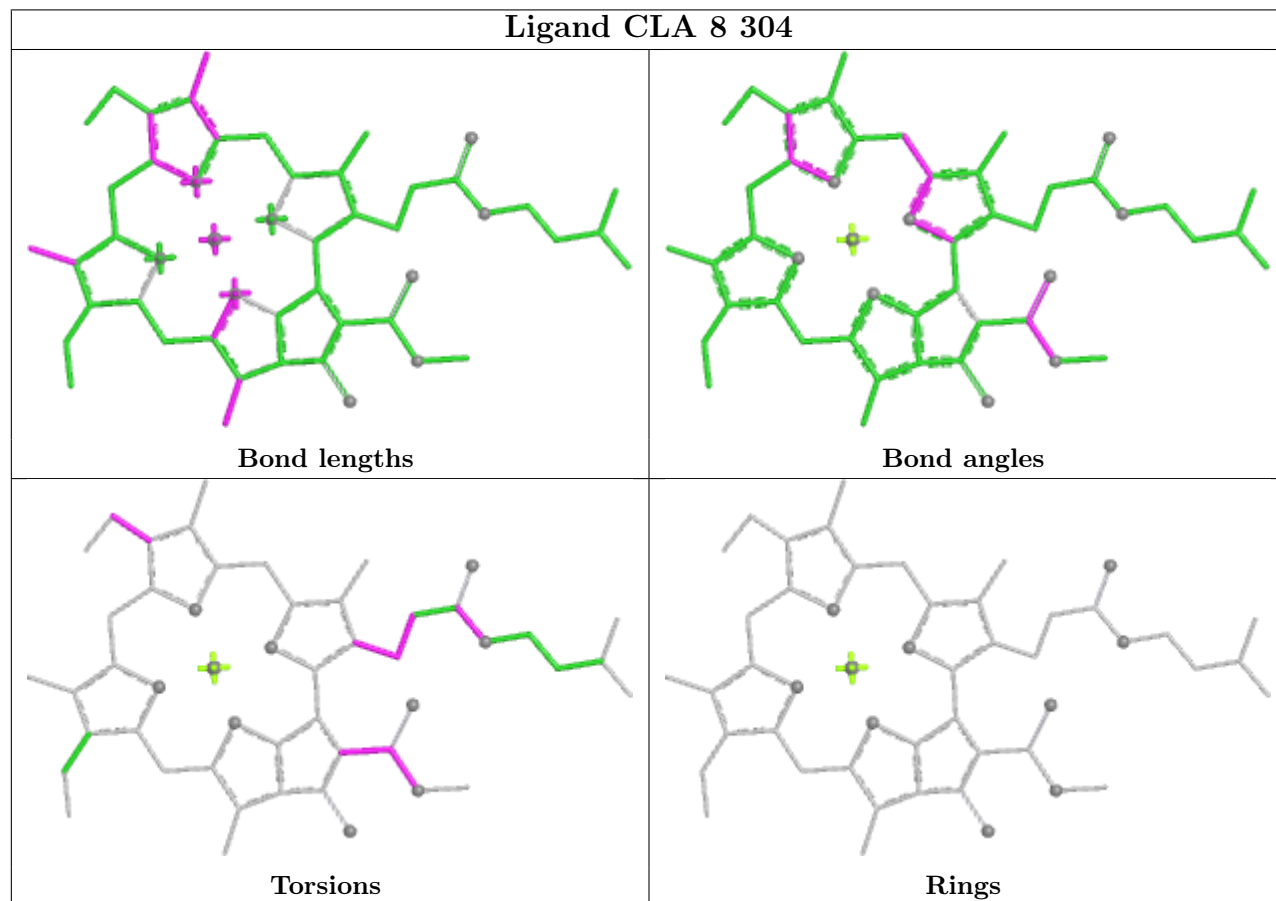




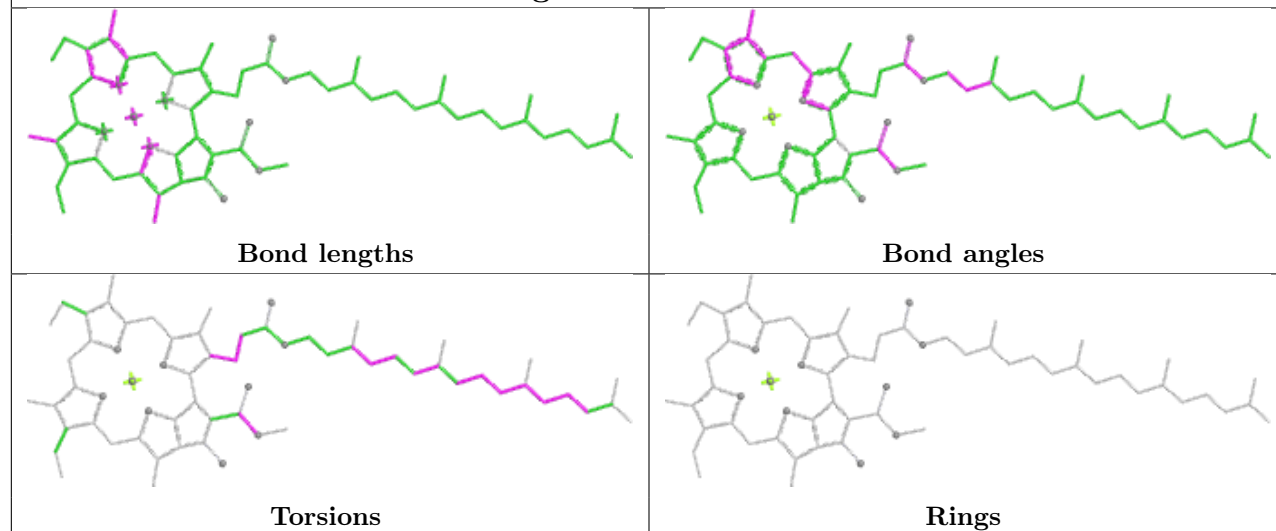
Ligand CLA 3 311



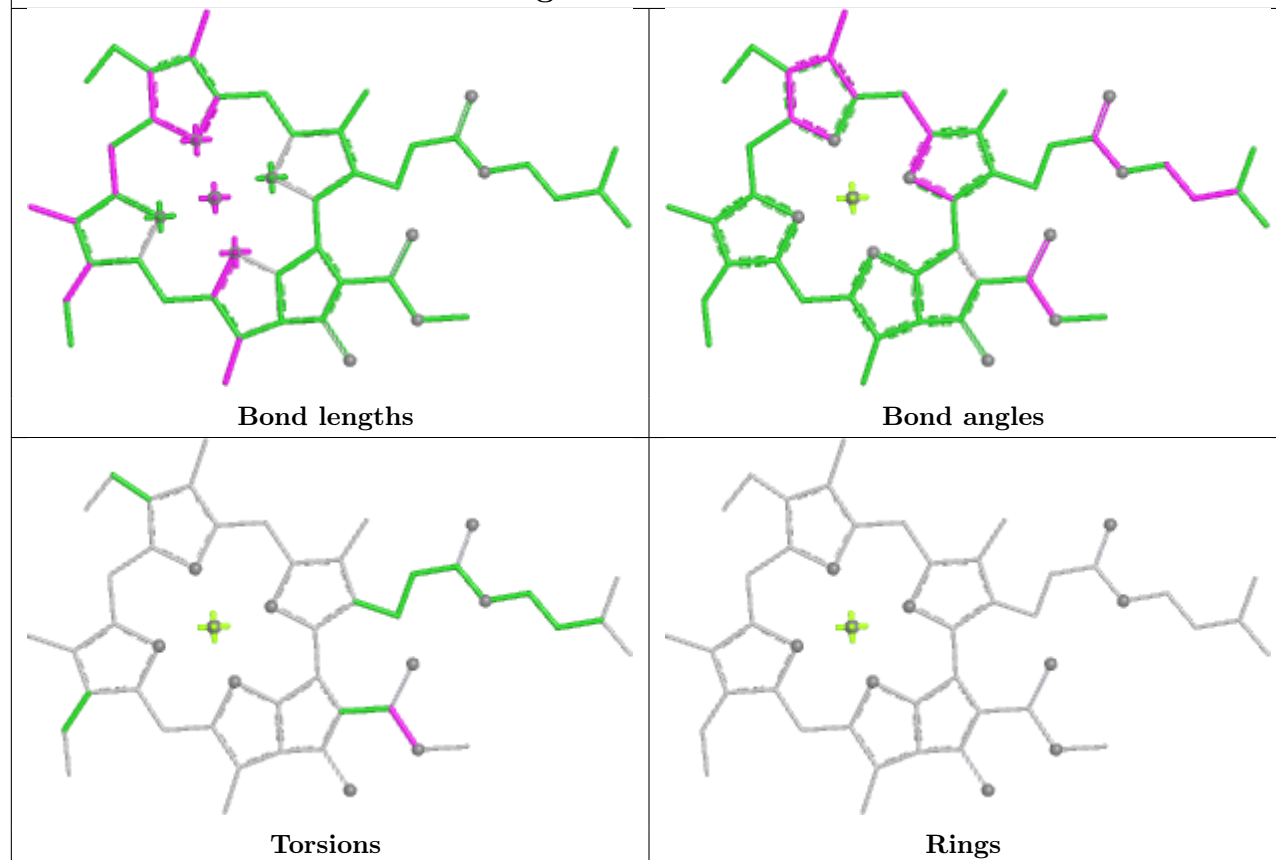
Ligand CLA 8 304



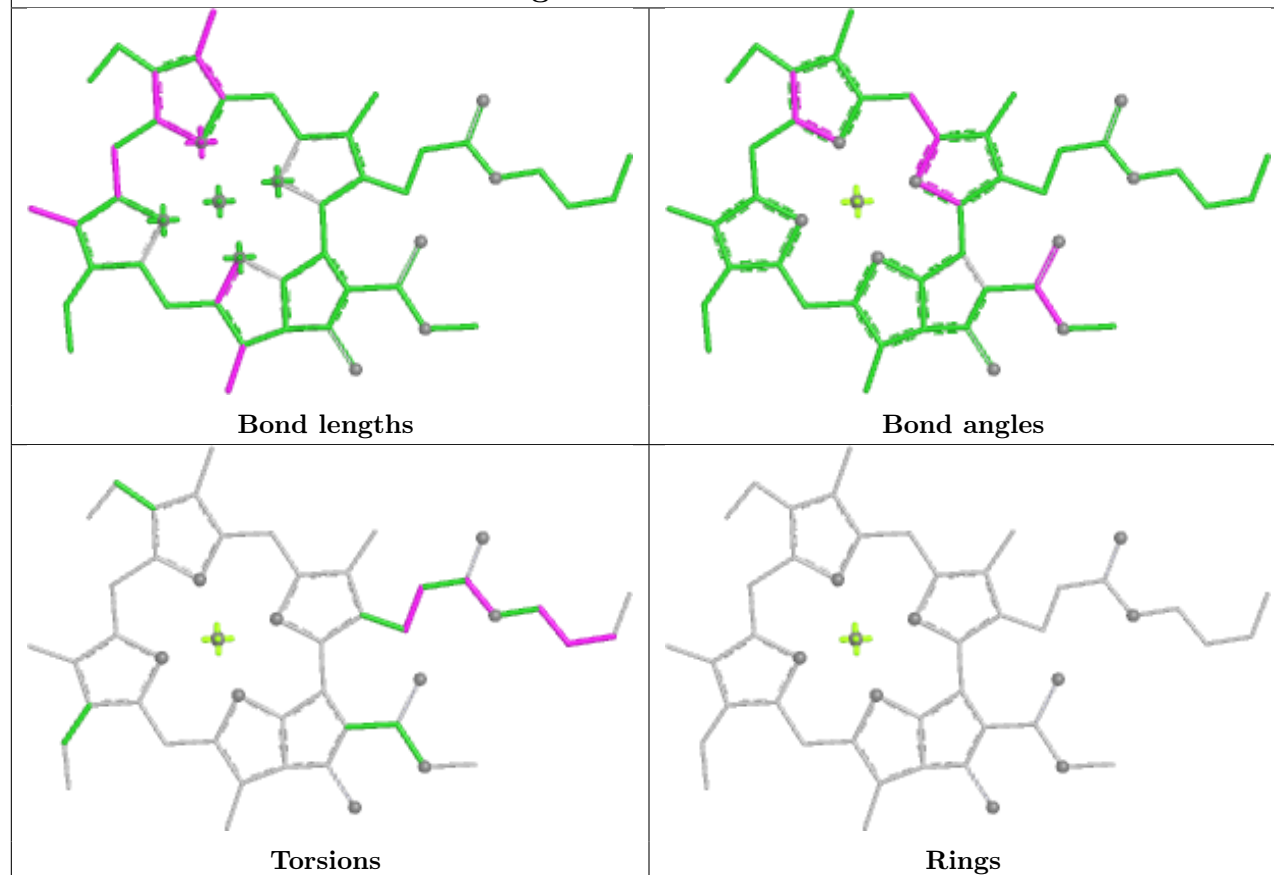
Ligand CLA B 837



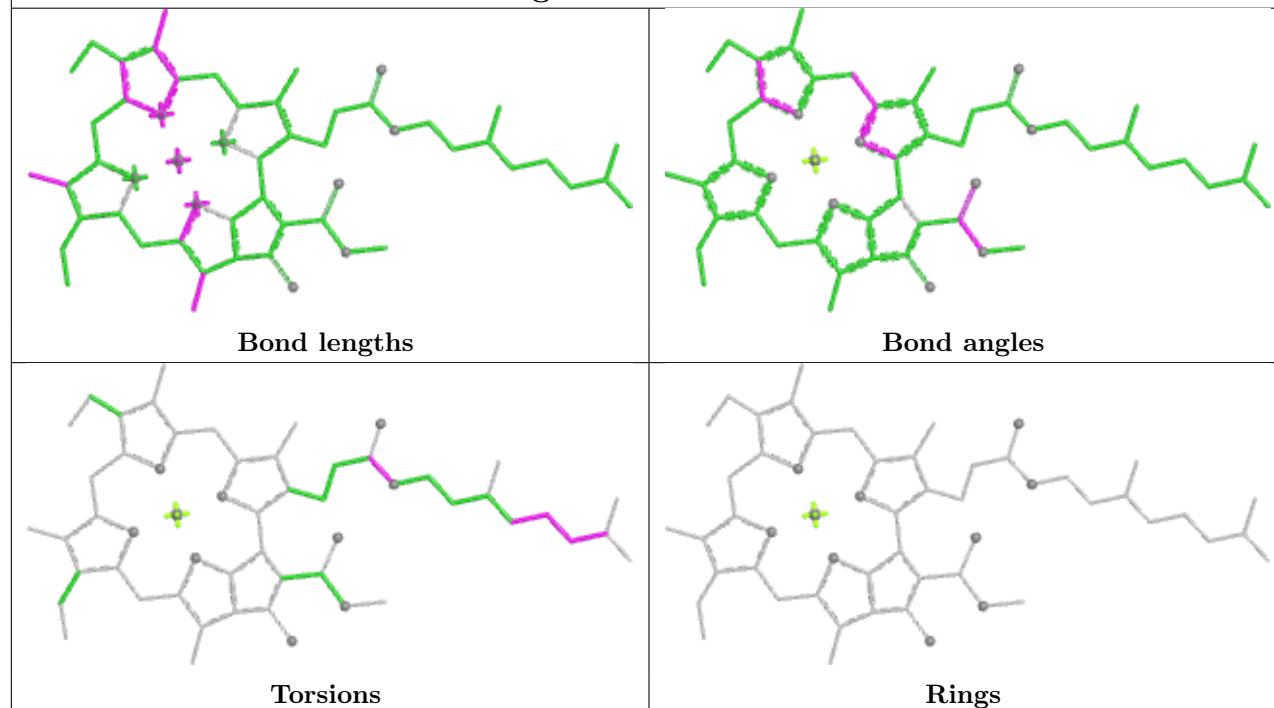
Ligand CLA 3 308



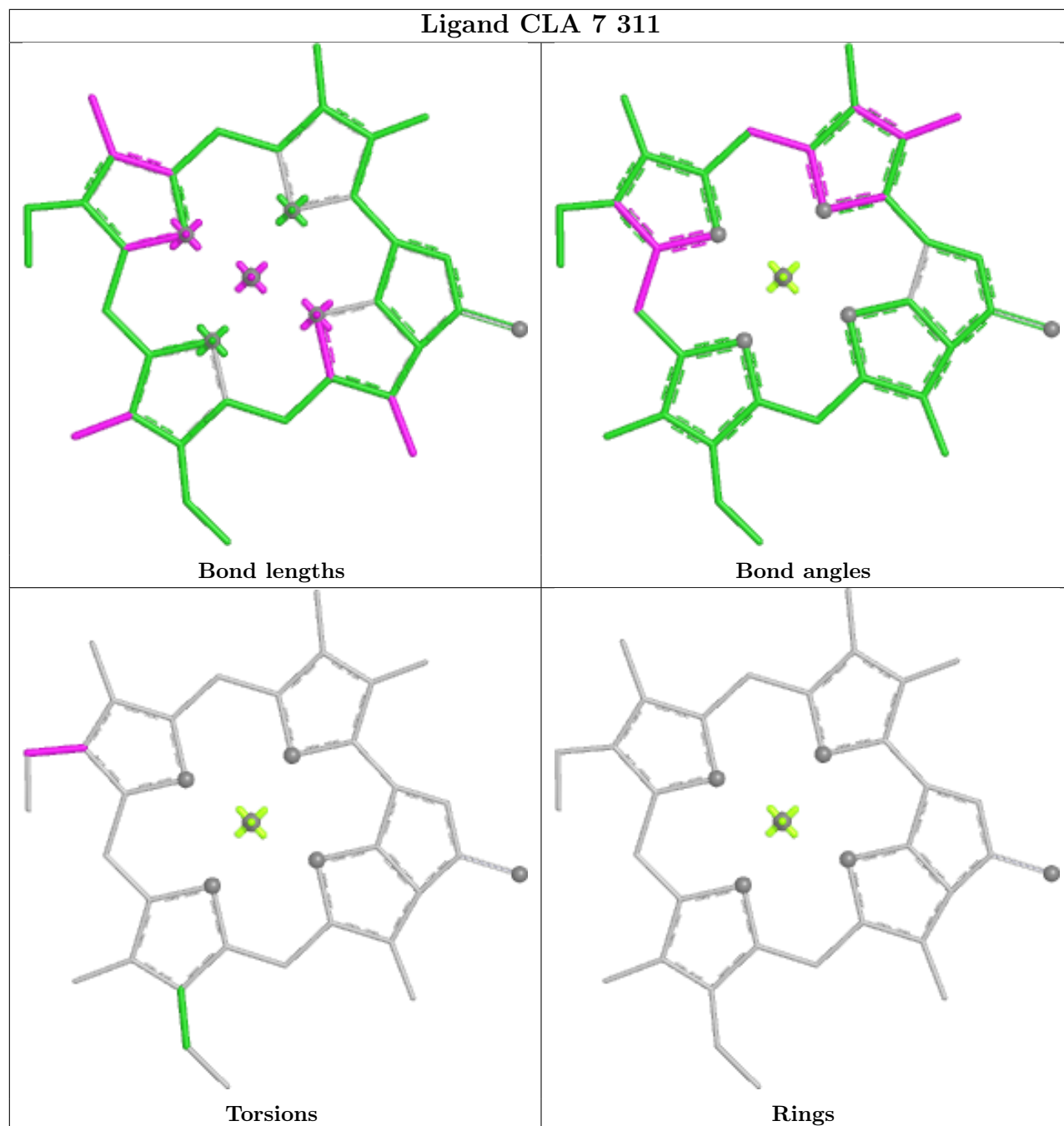
Ligand CLA A 852



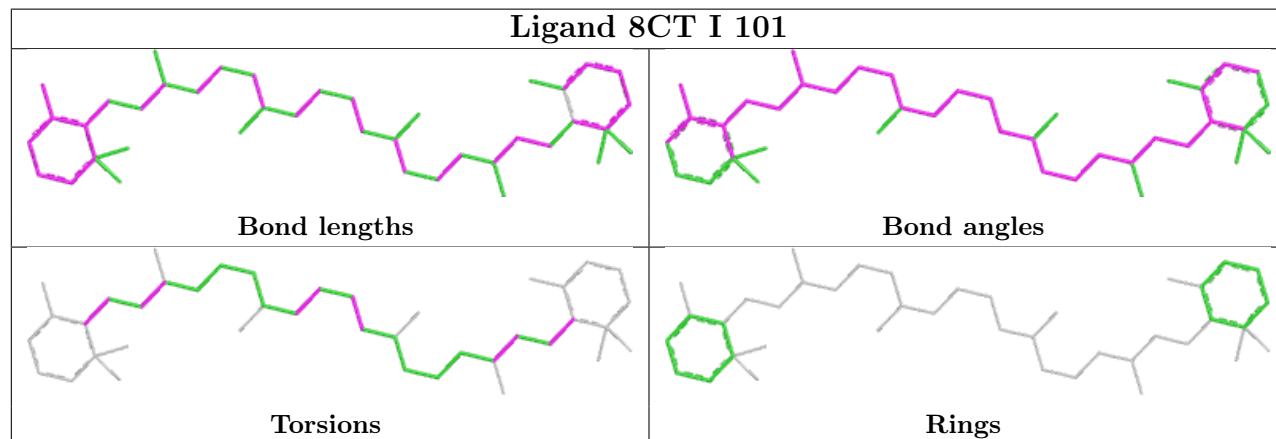
Ligand CLA B 813



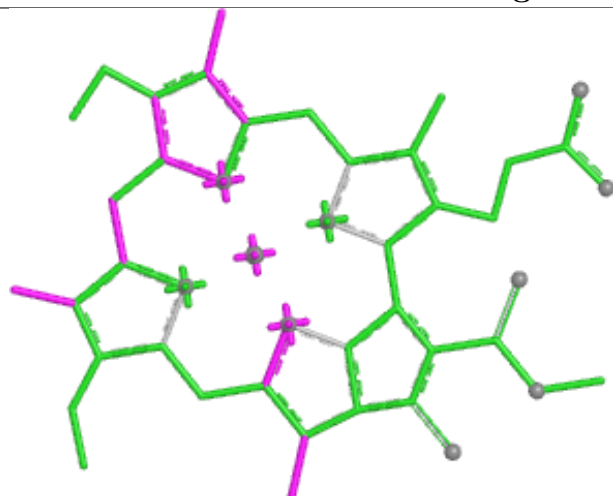
Ligand CLA 7 311



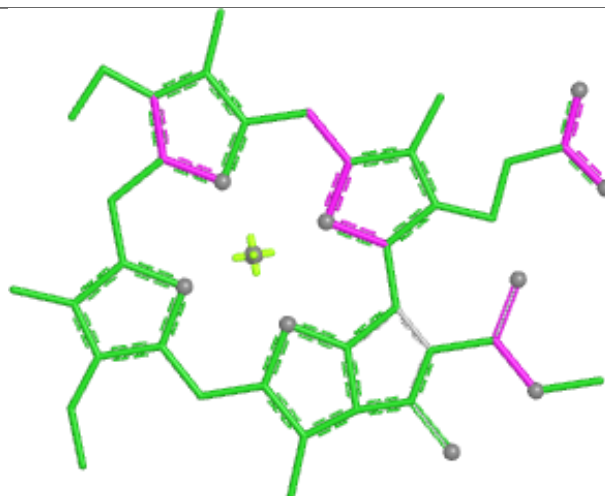
Ligand 8CT I 101



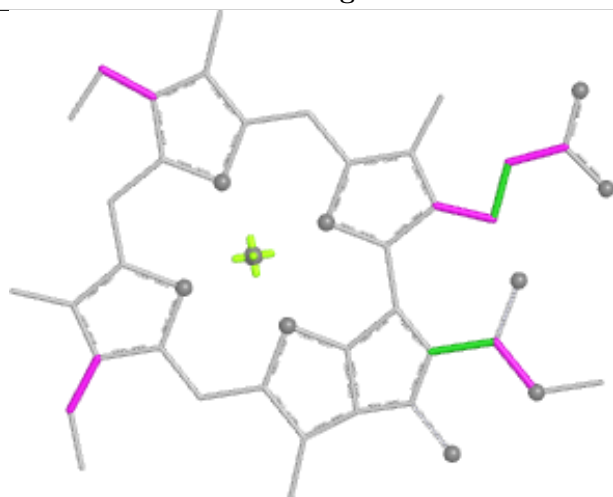
Ligand CLA K 101



Bond lengths



Bond angles

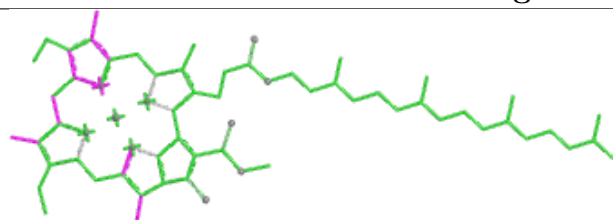


Torsions

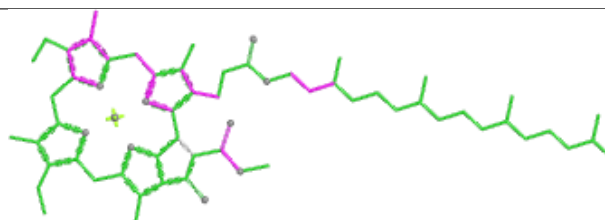


Rings

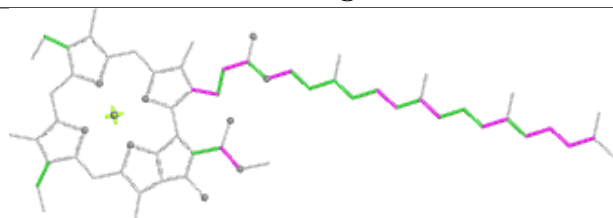
Ligand CLA H 201



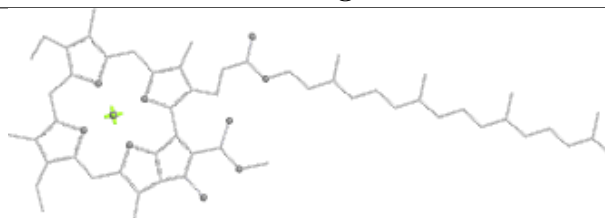
Bond lengths



Bond angles

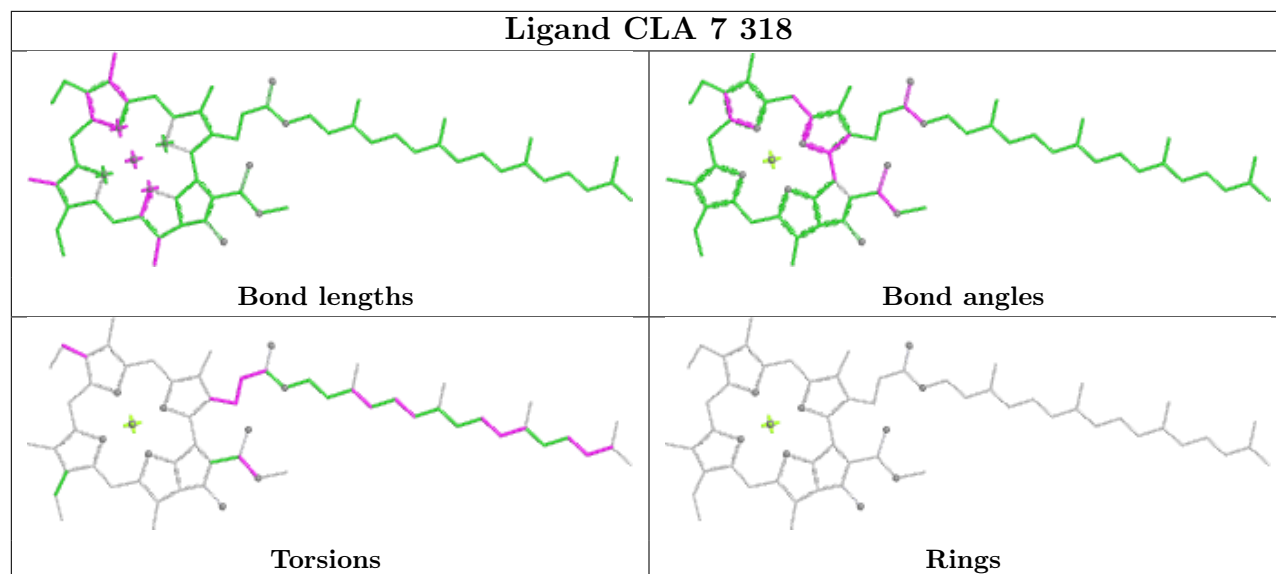


Torsions

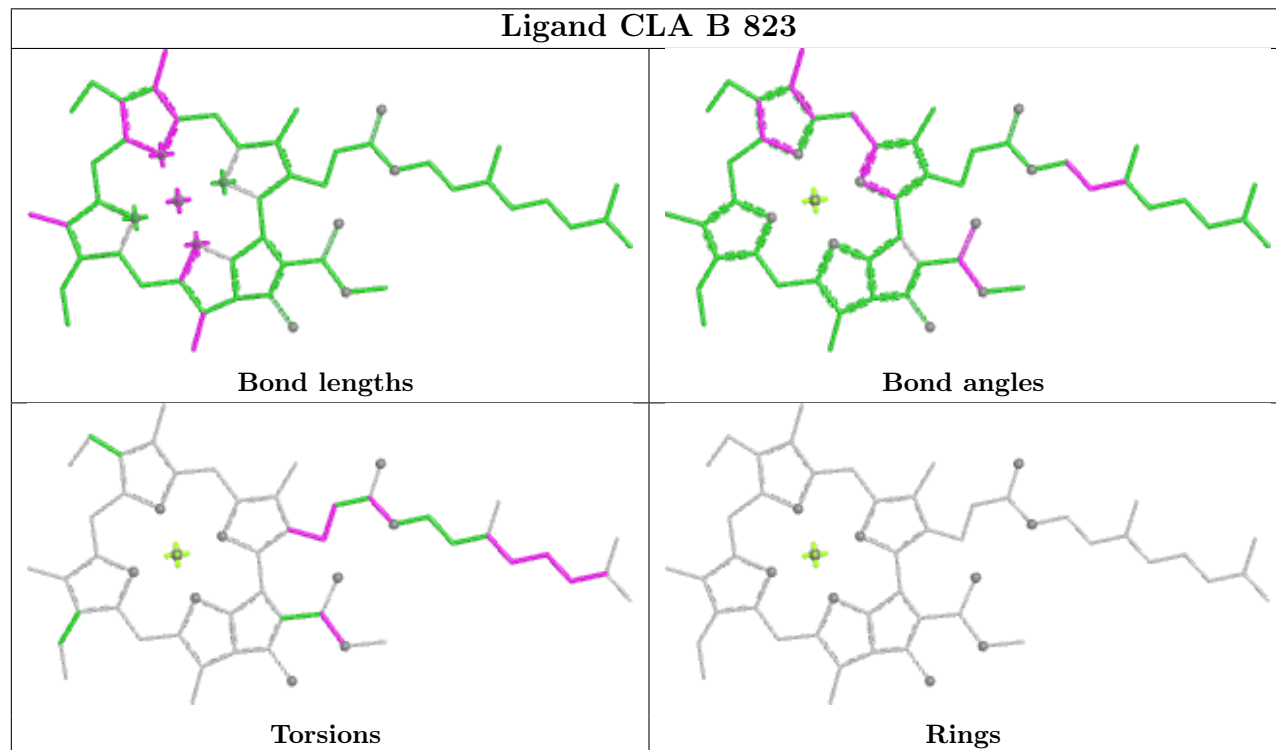


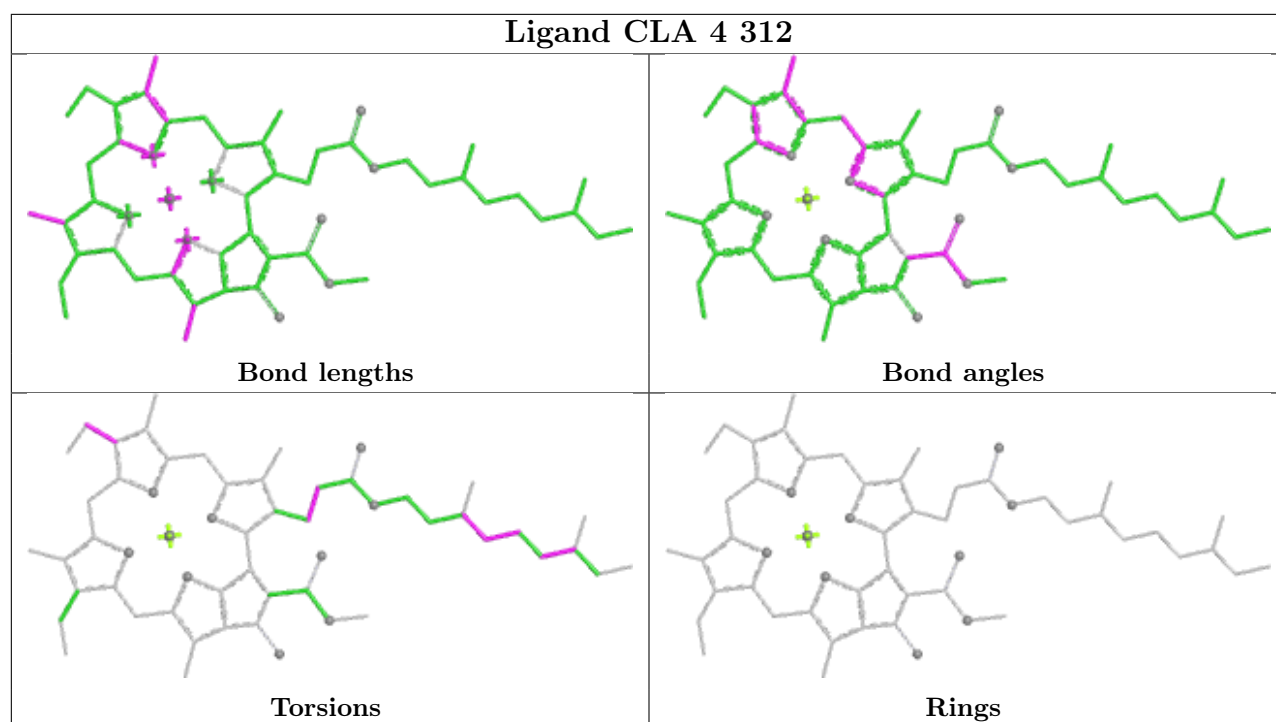
Rings

Ligand CLA 7 318

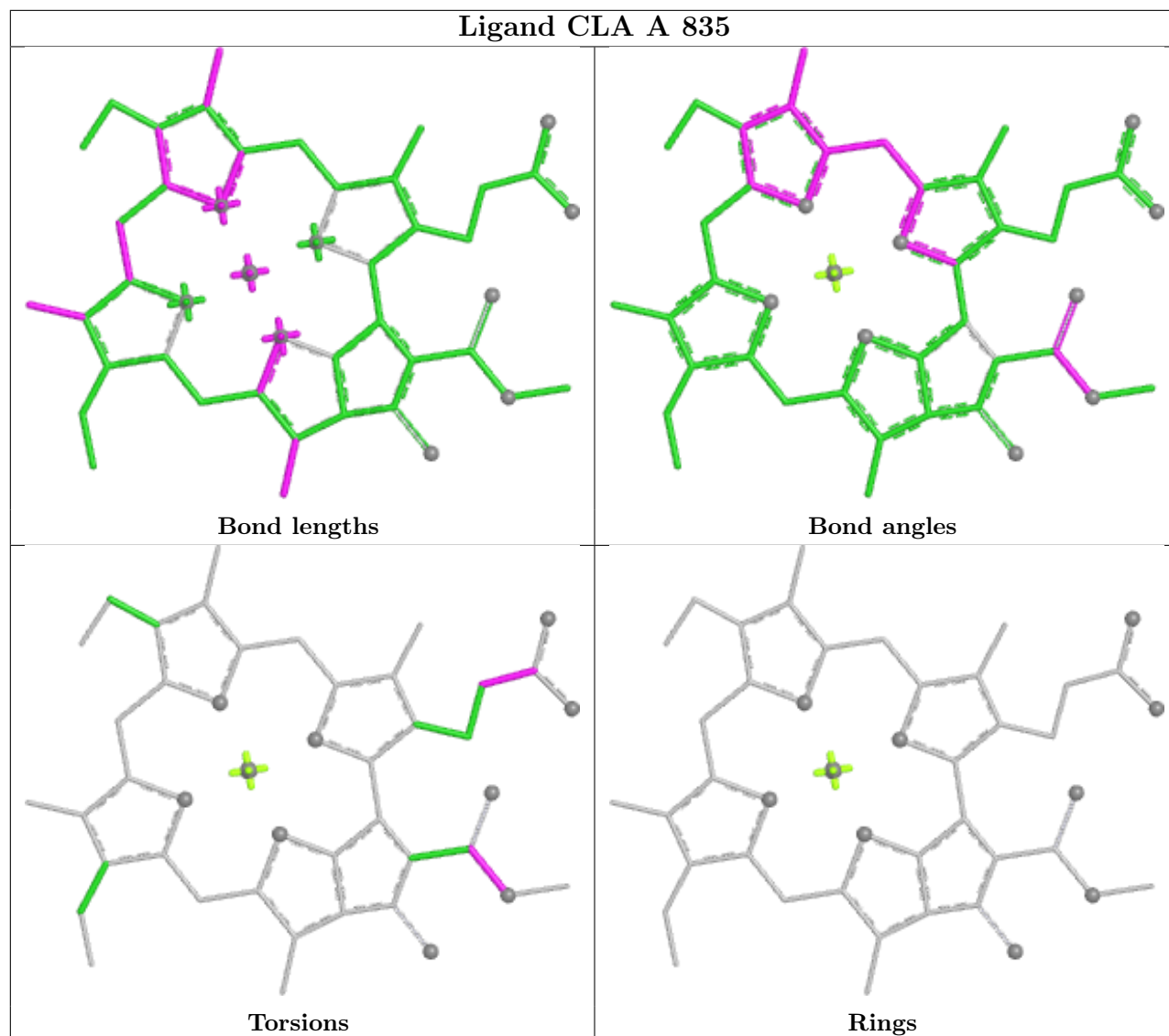


Ligand CLA B 823

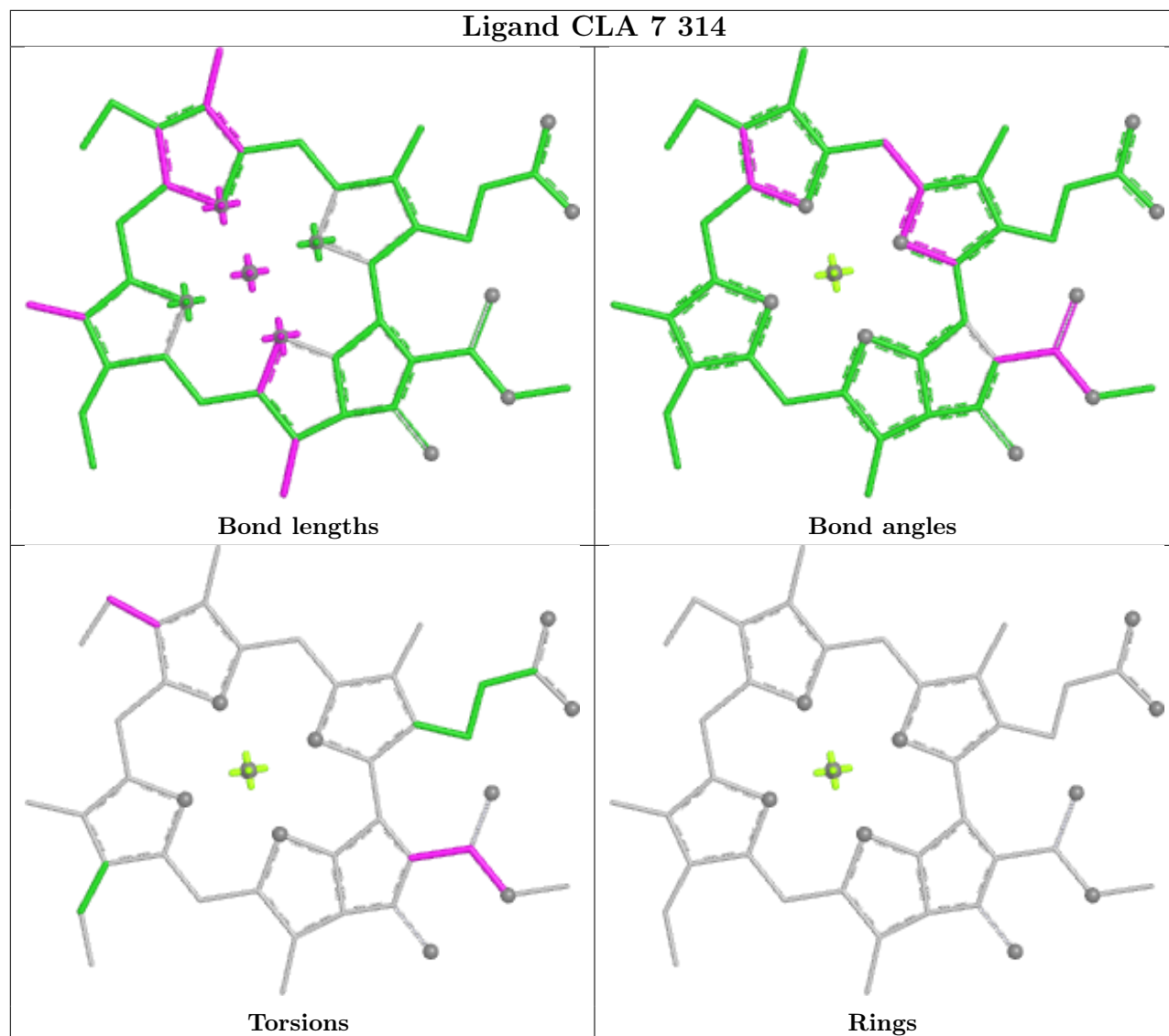




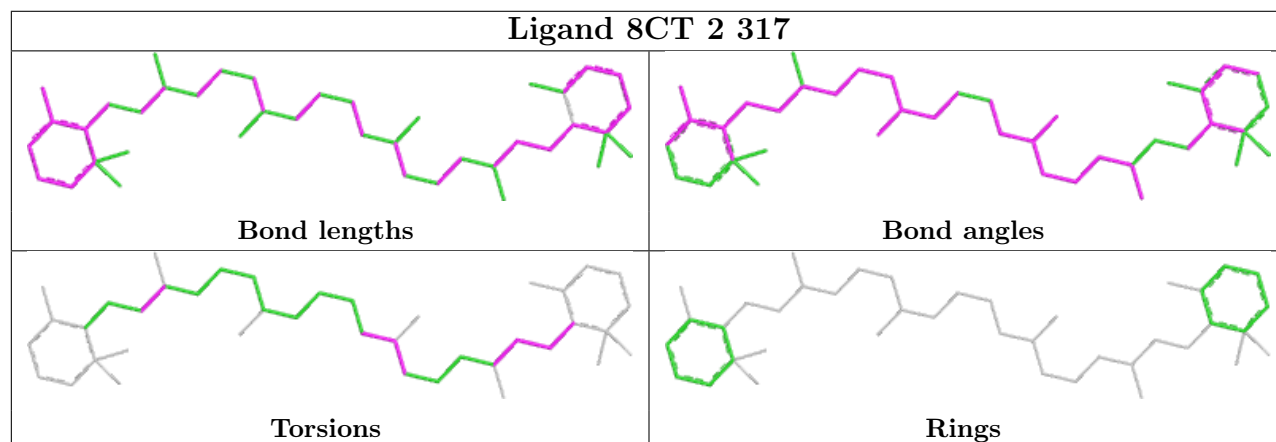
Ligand CLA A 835



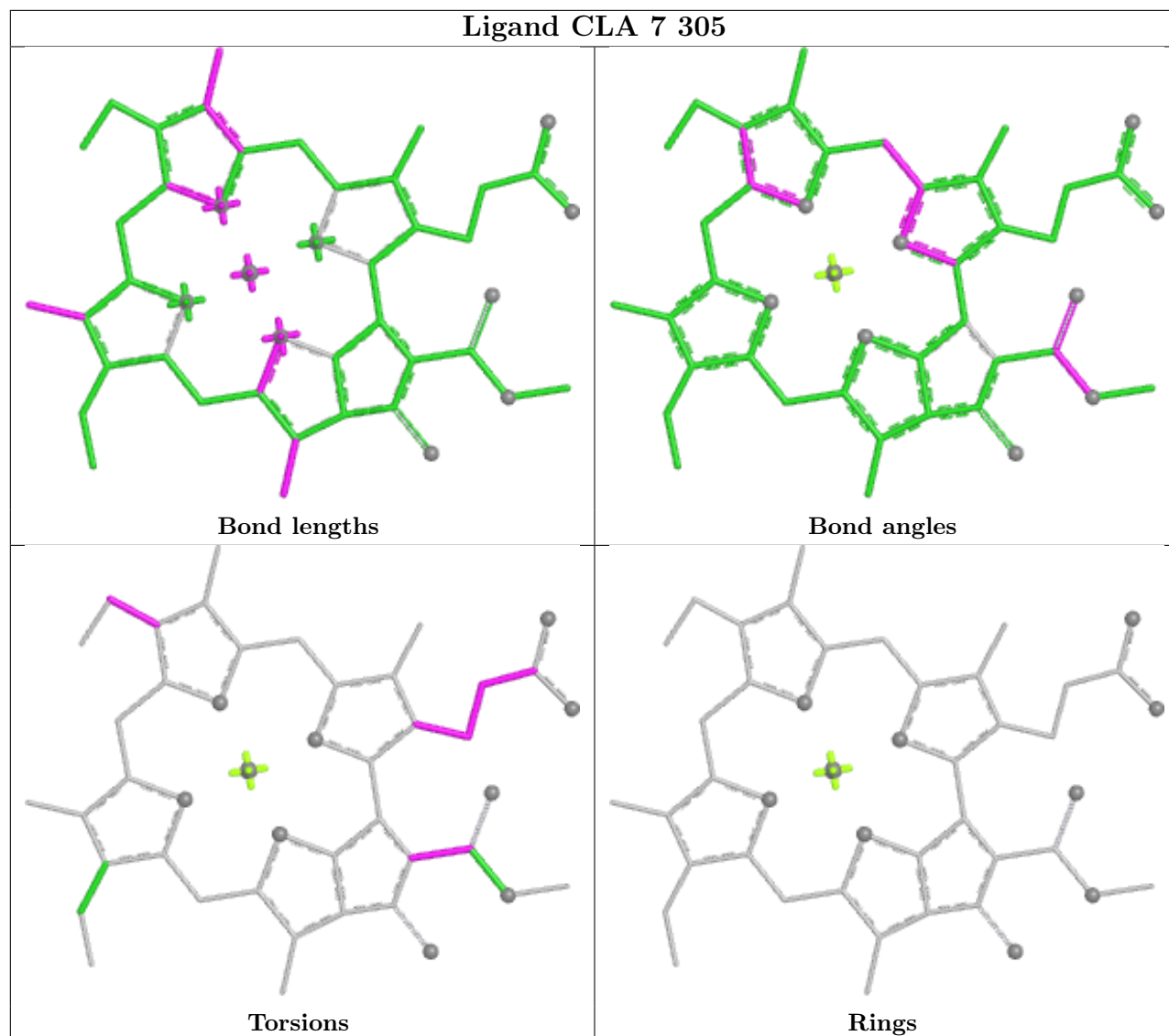
Ligand CLA 7 314



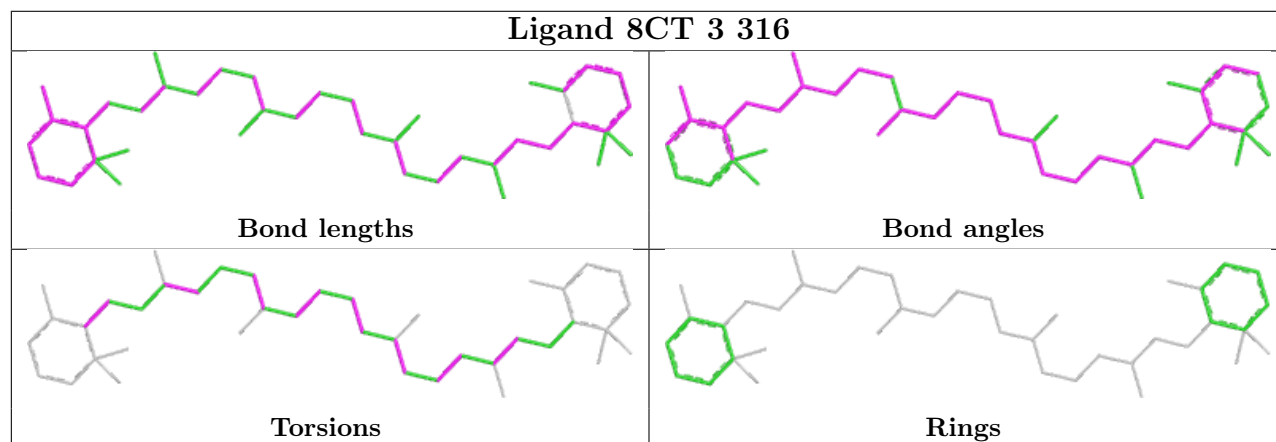
Ligand 8CT 2 317

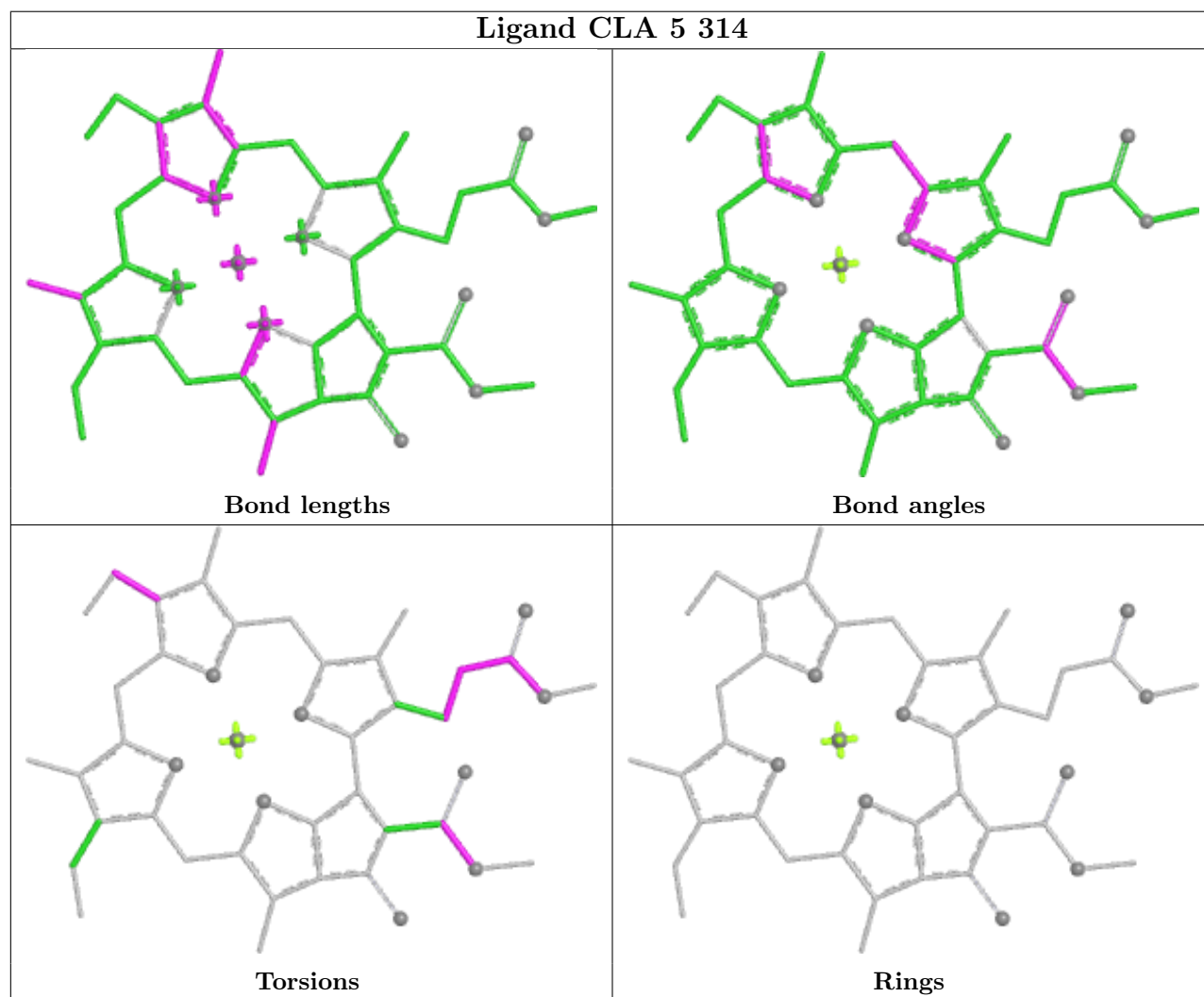
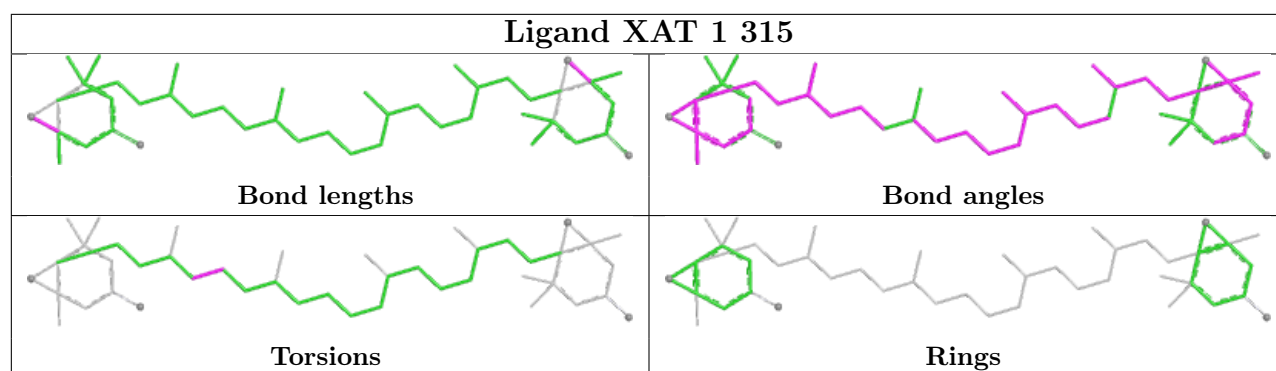


Ligand CLA 7 305

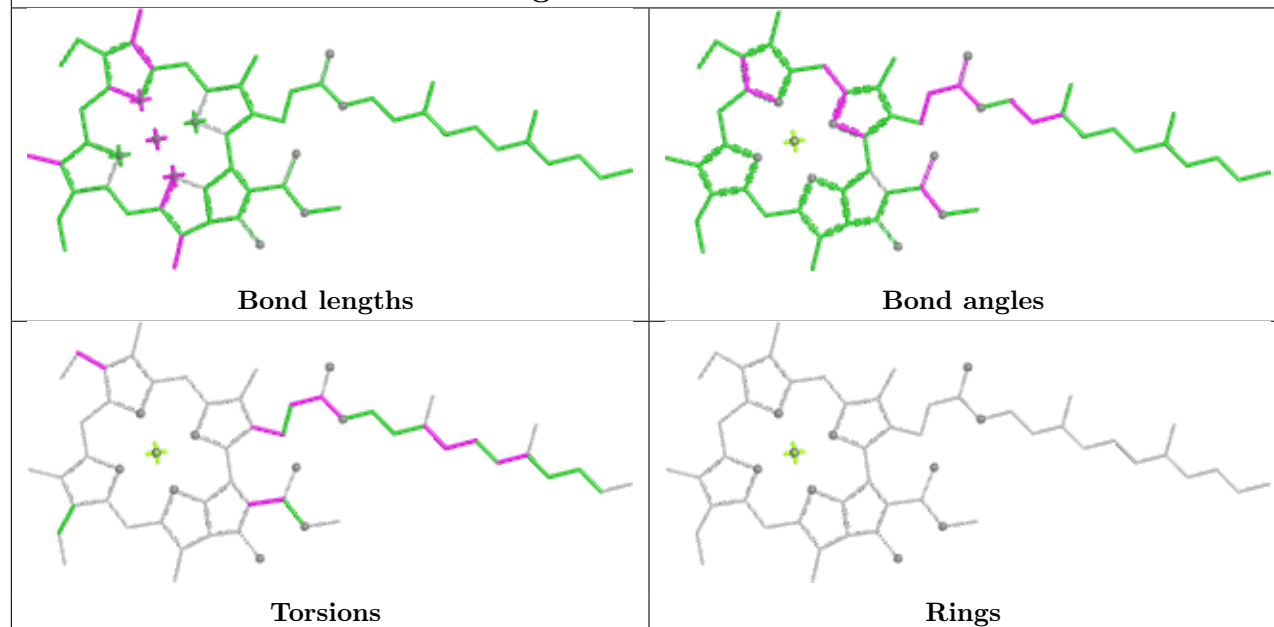


Ligand 8CT 3 316

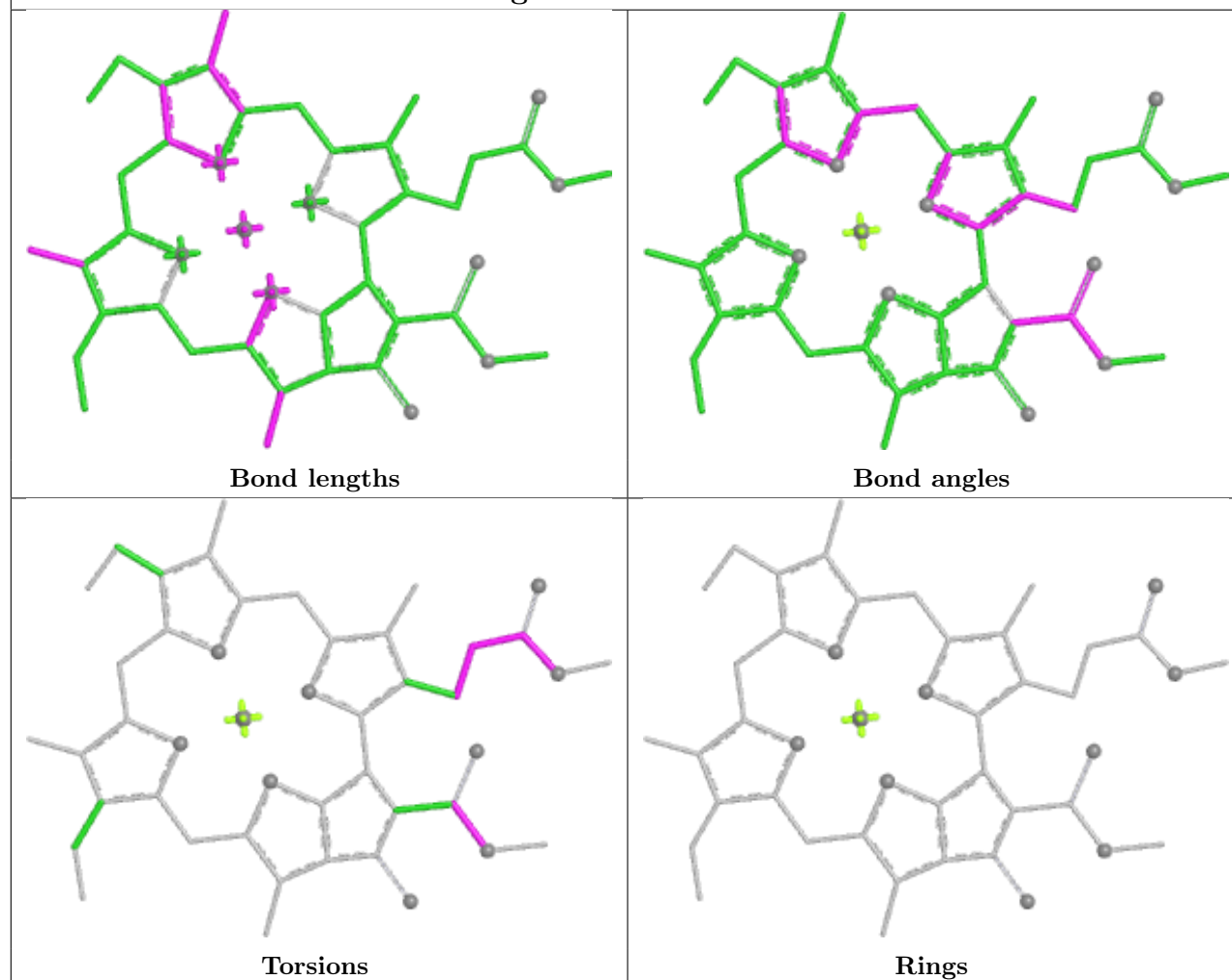


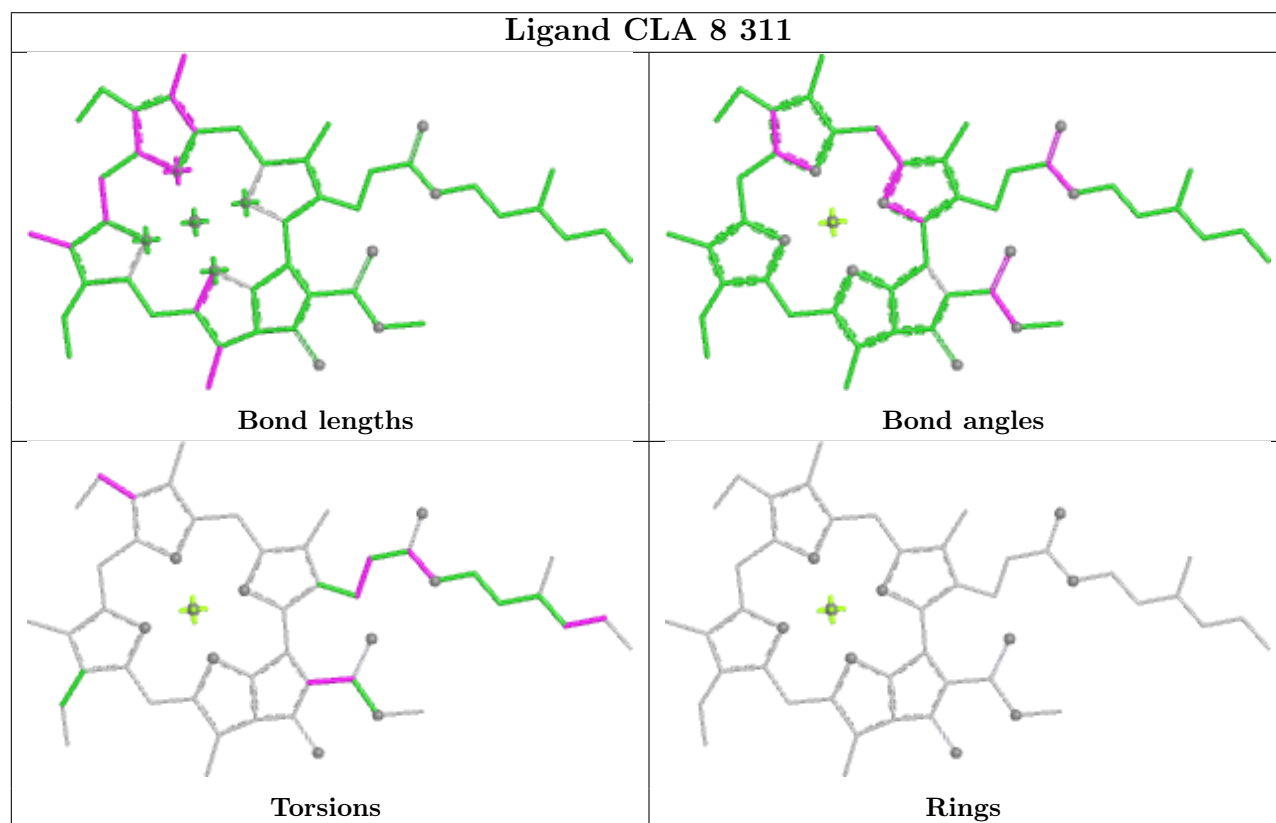
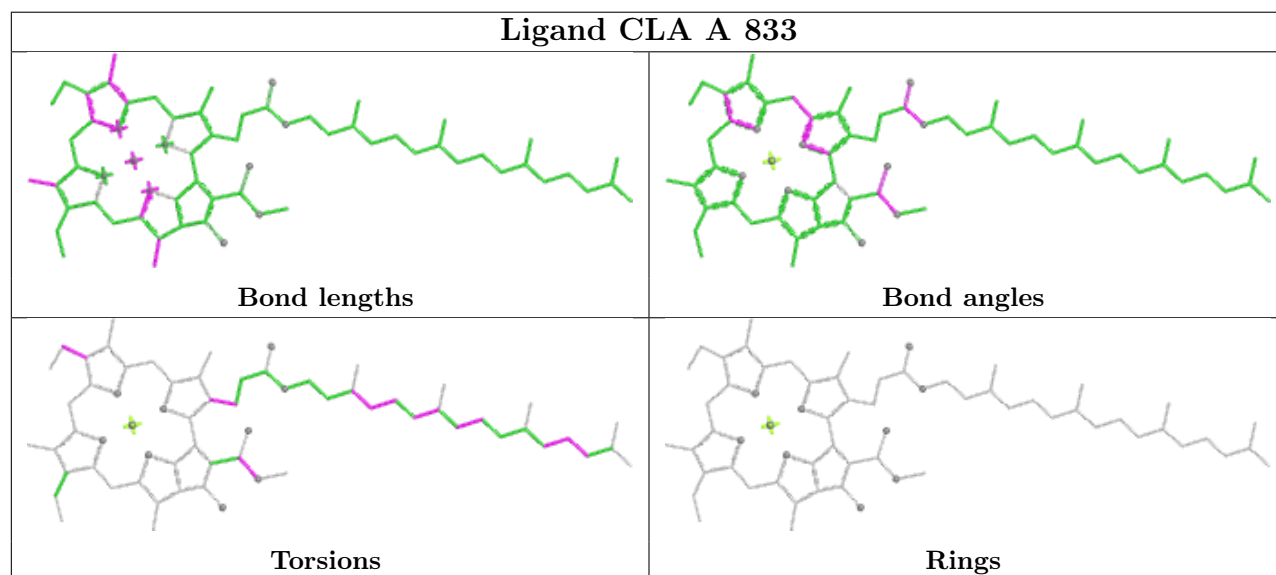
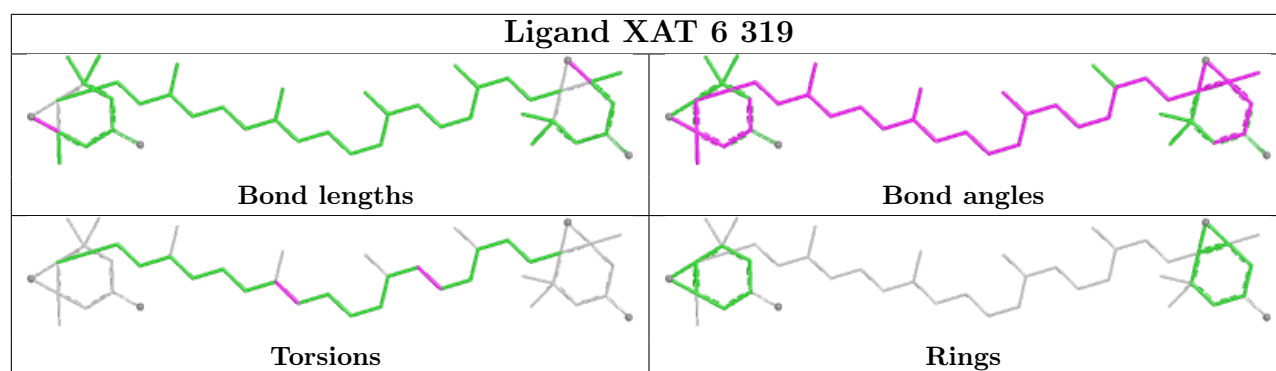


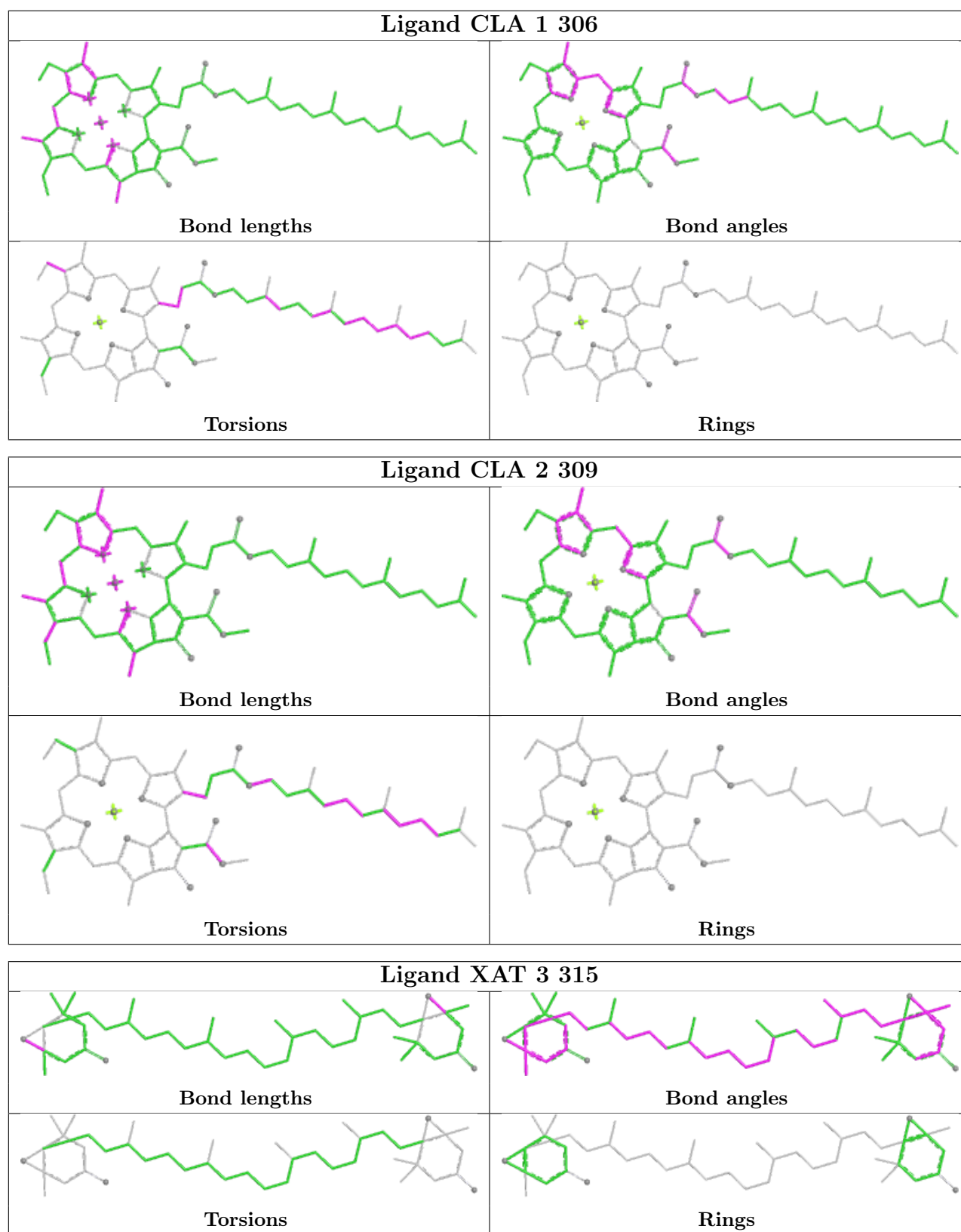
Ligand CLA B 833

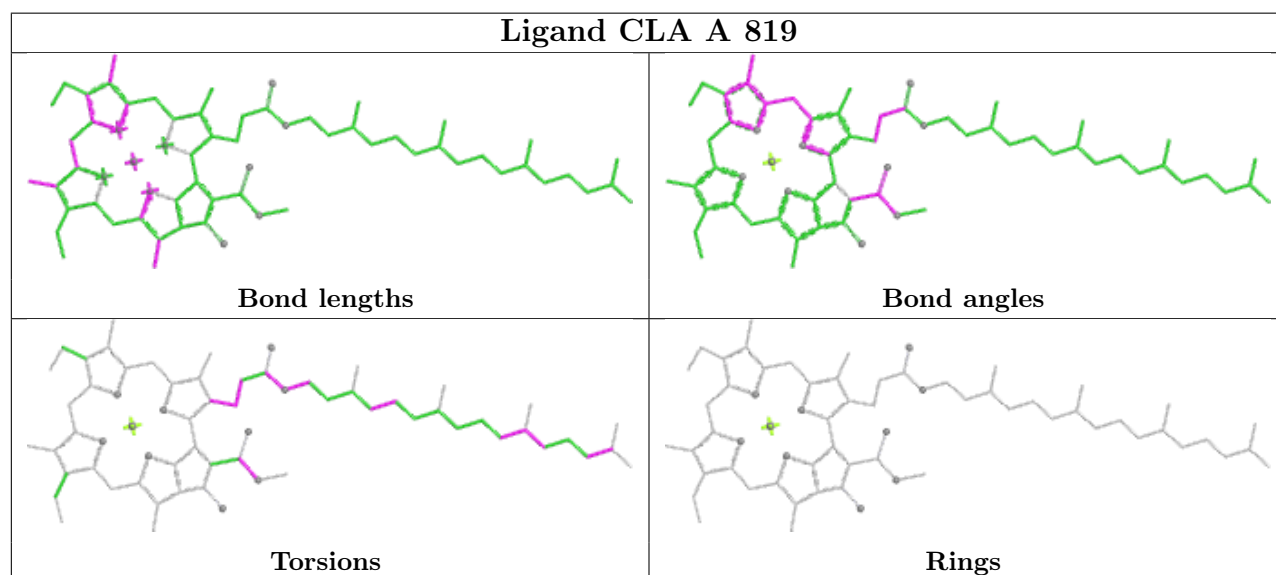
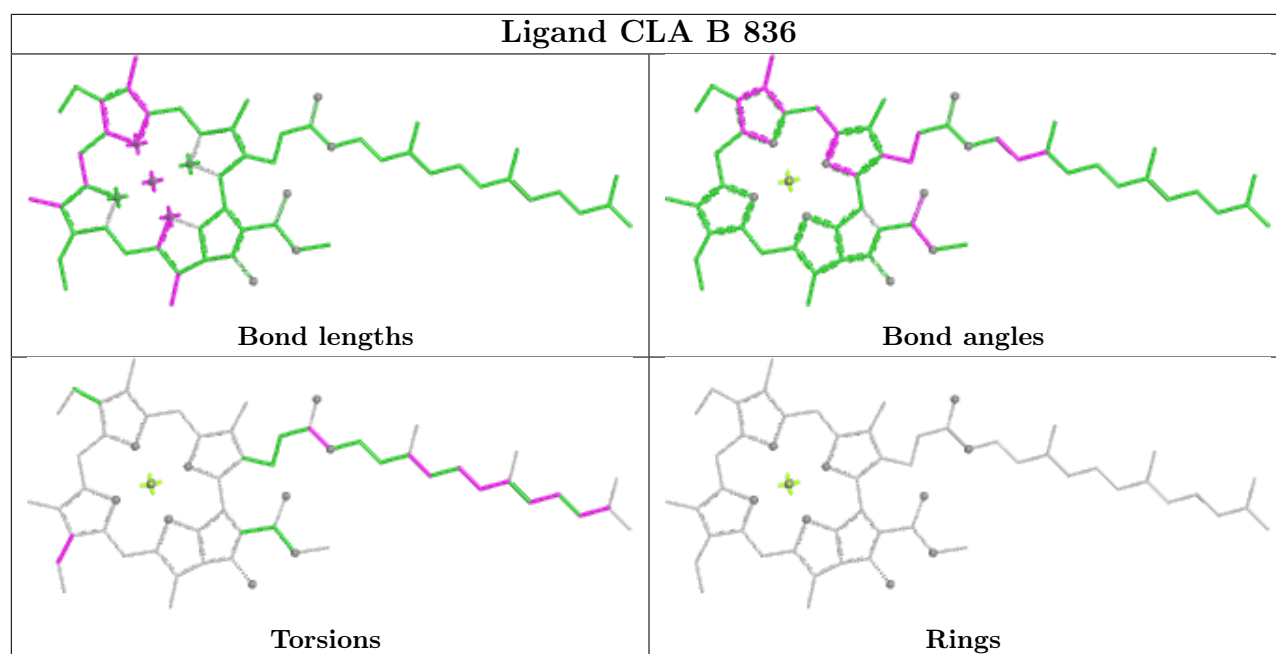


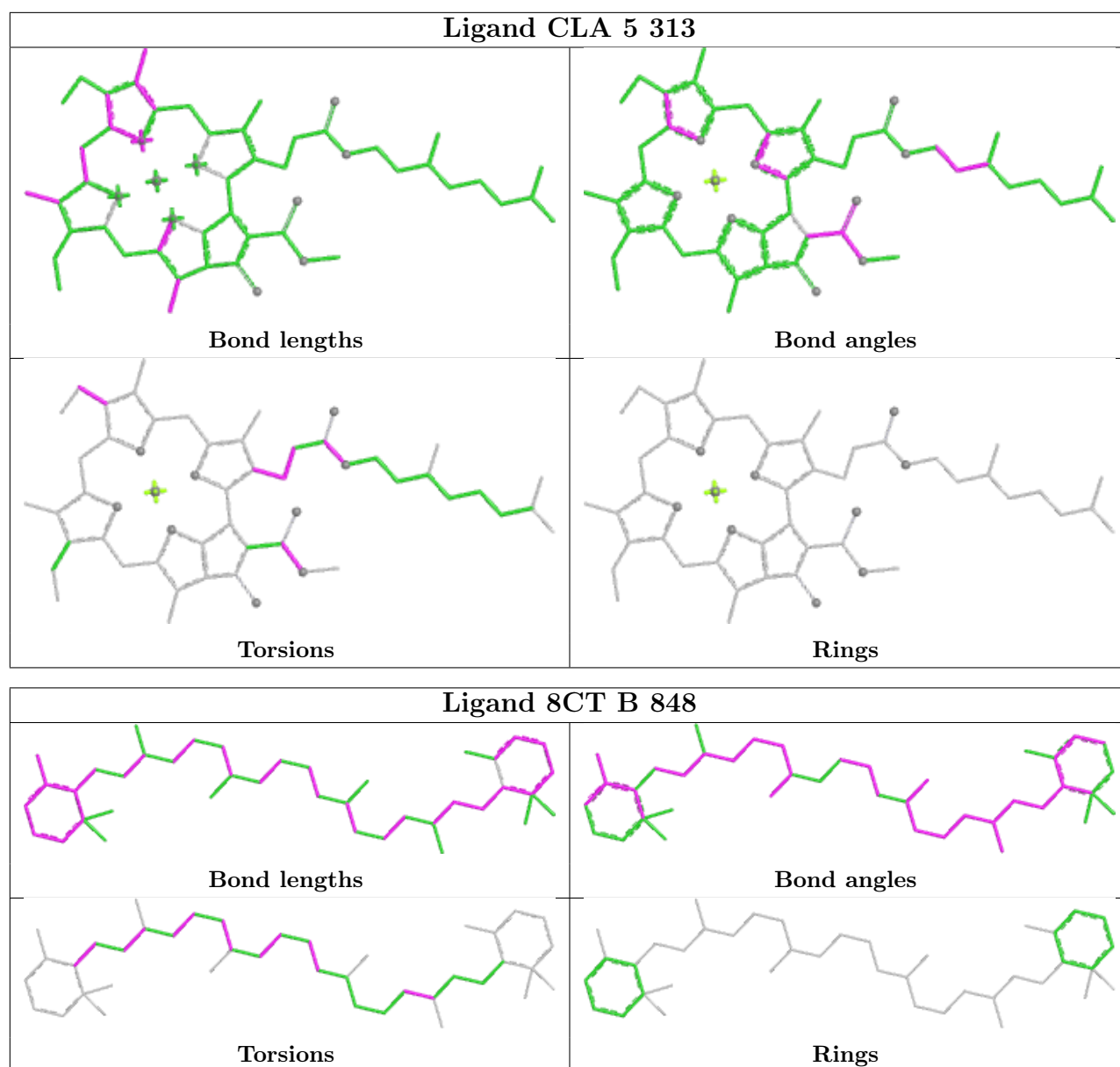
Ligand CLA M 101

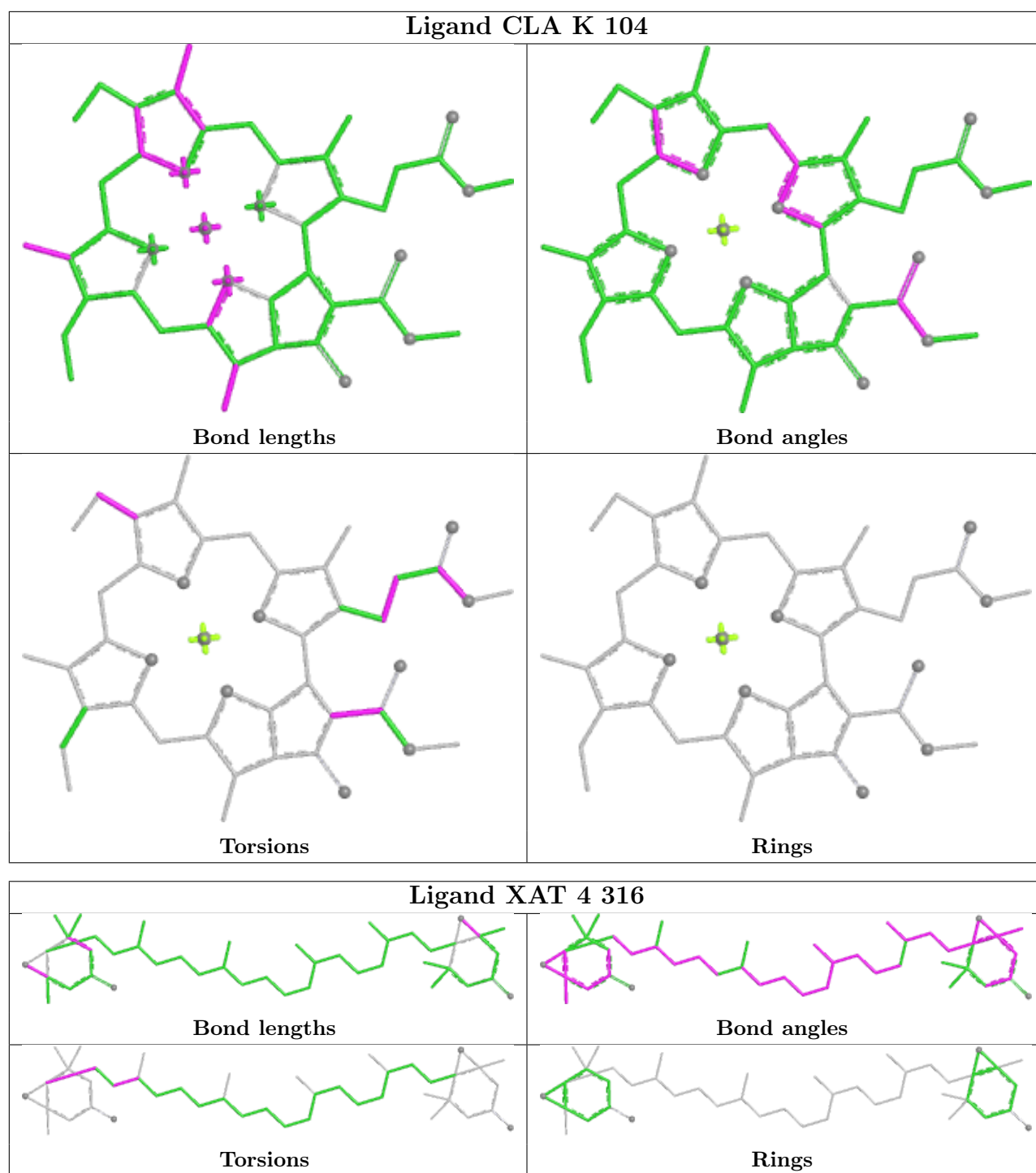




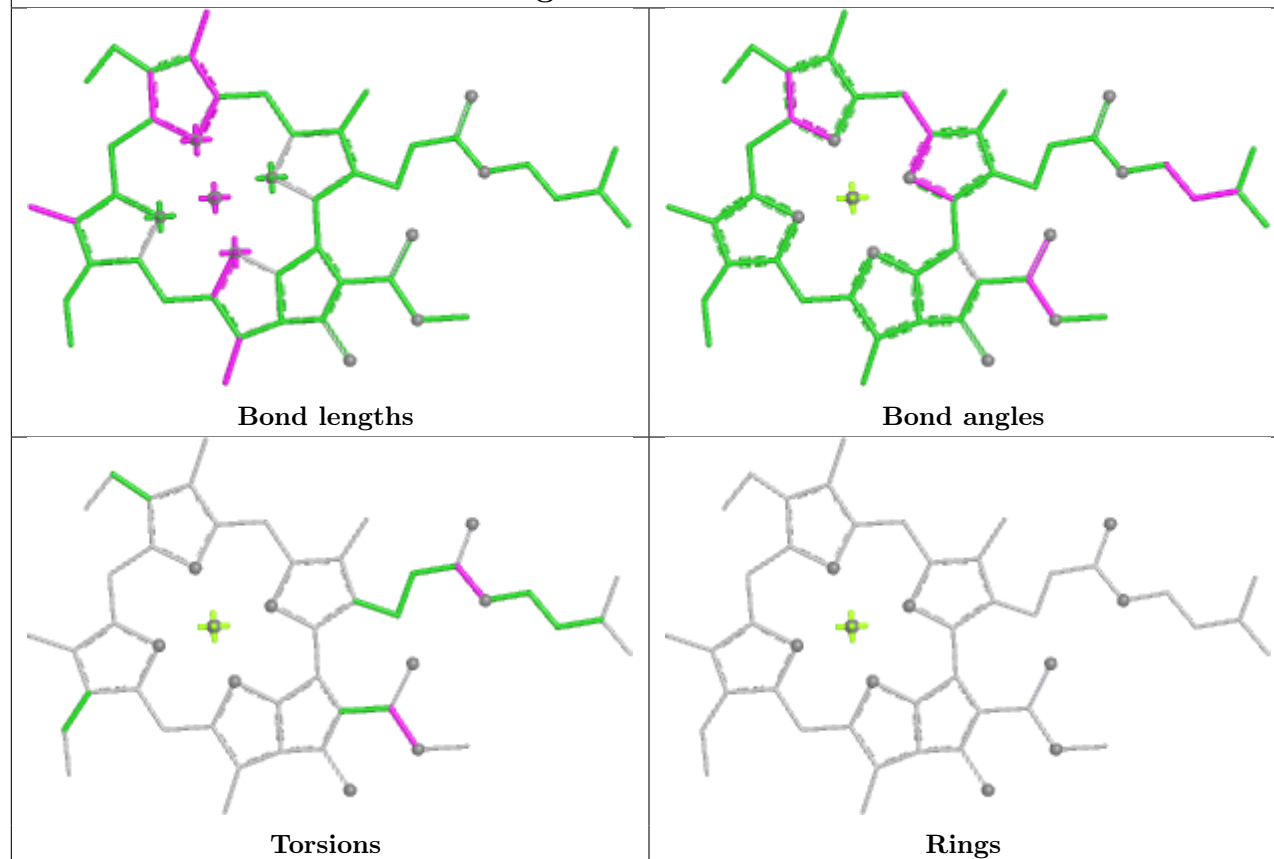




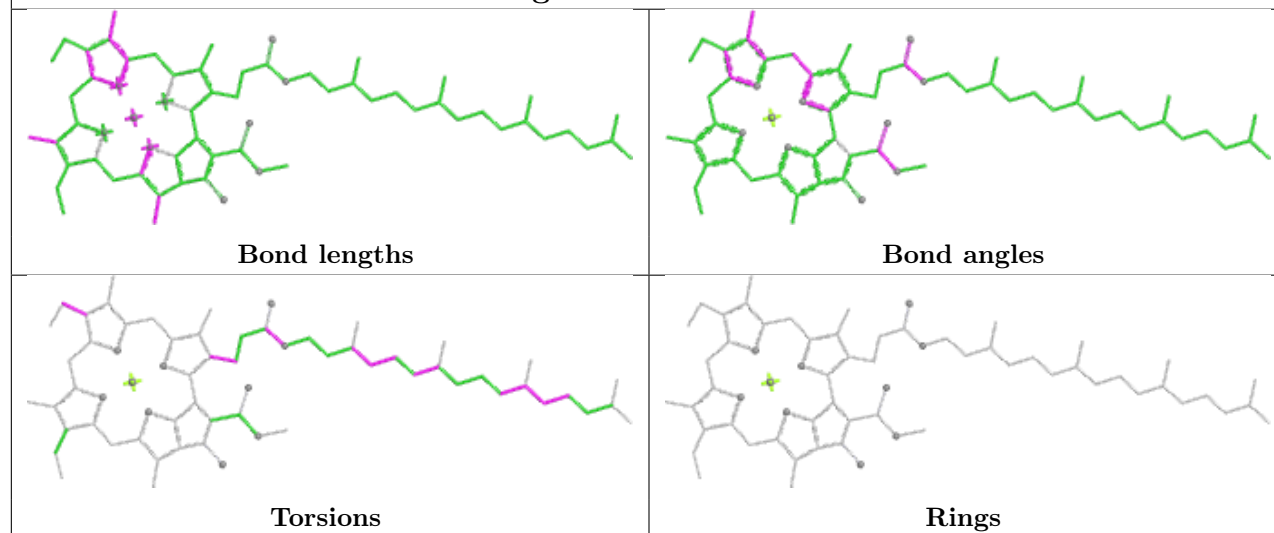


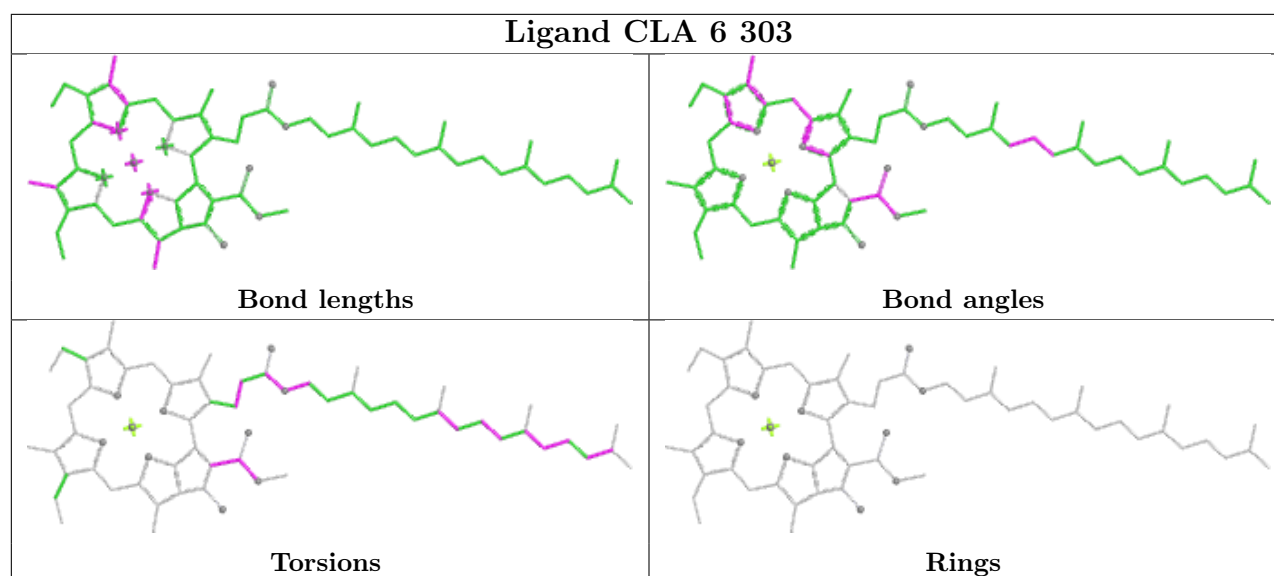
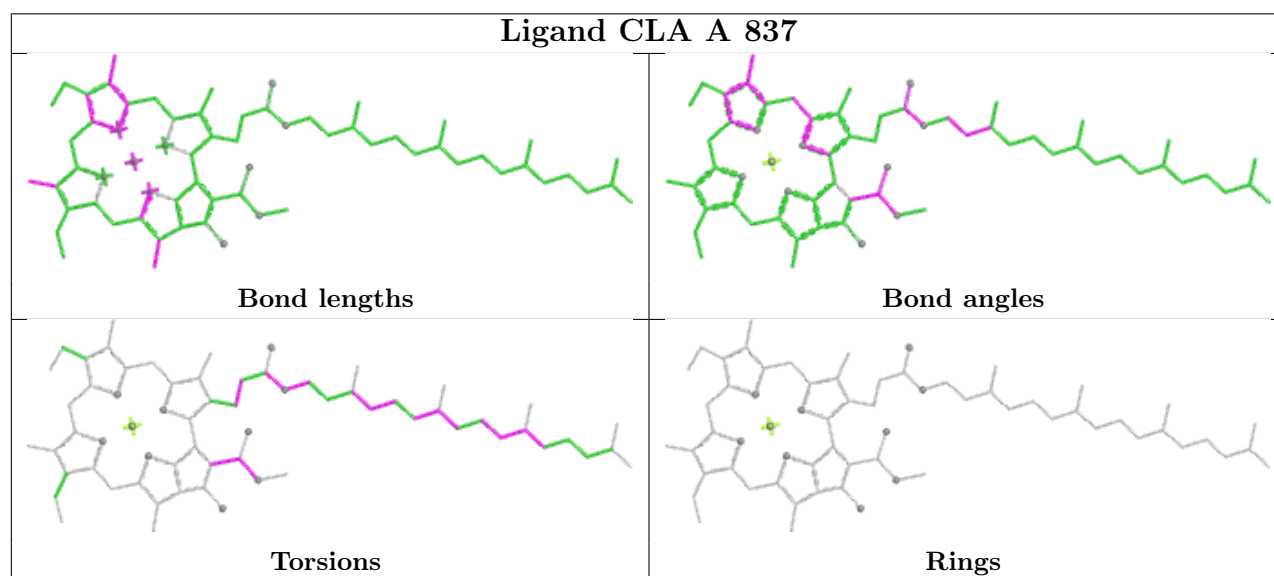
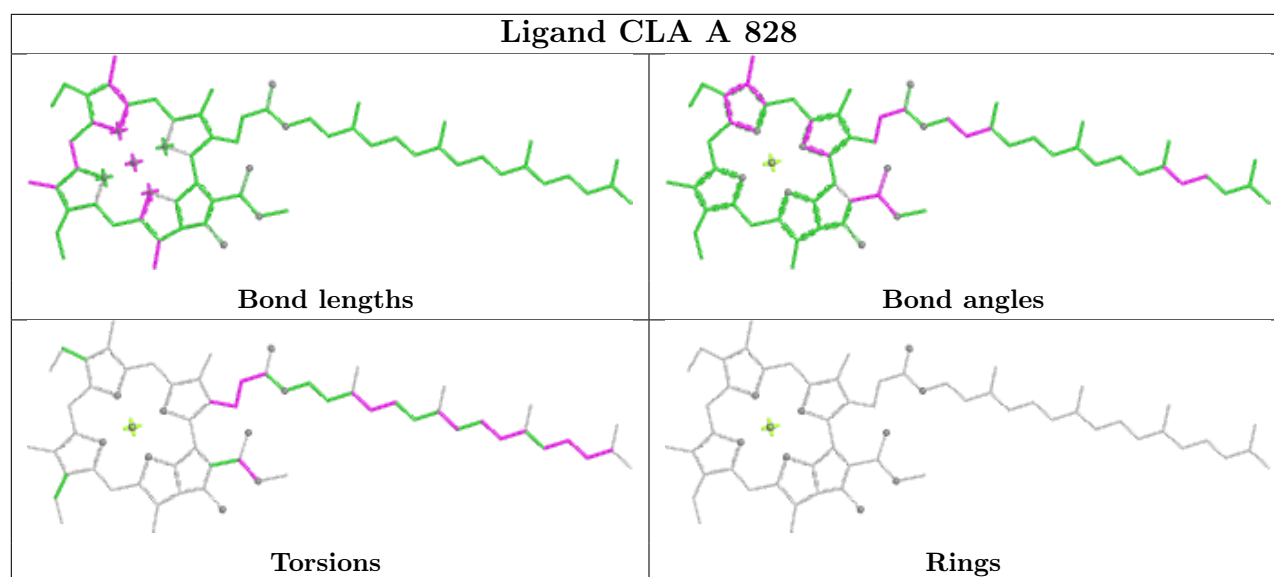


Ligand CLA 2 308

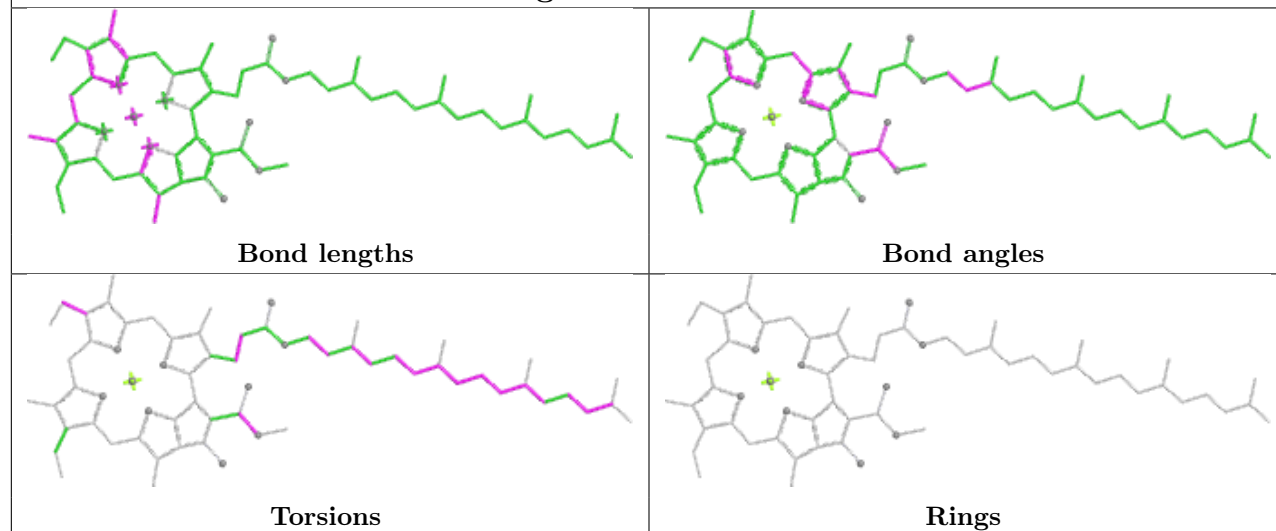


Ligand CLA B 839

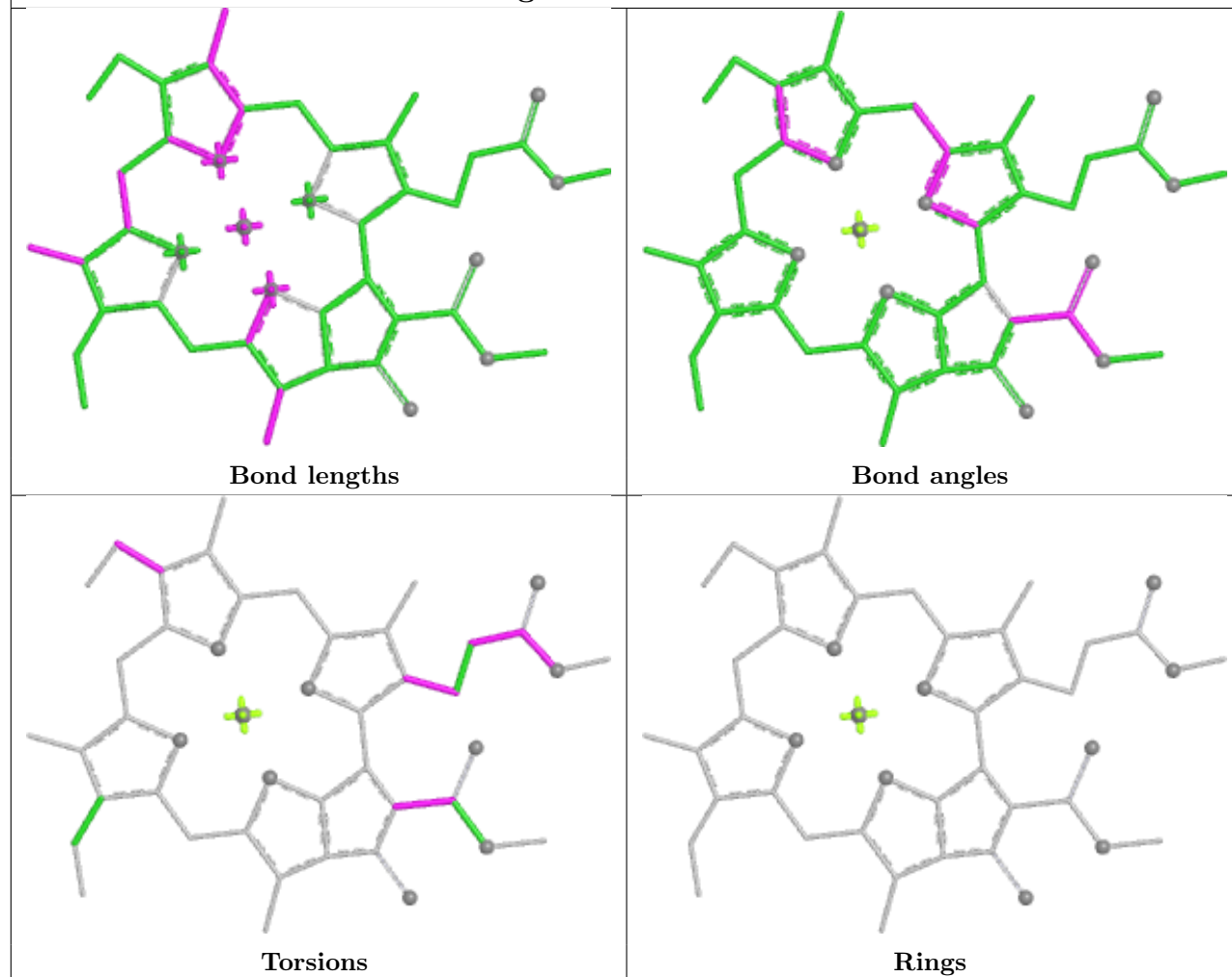


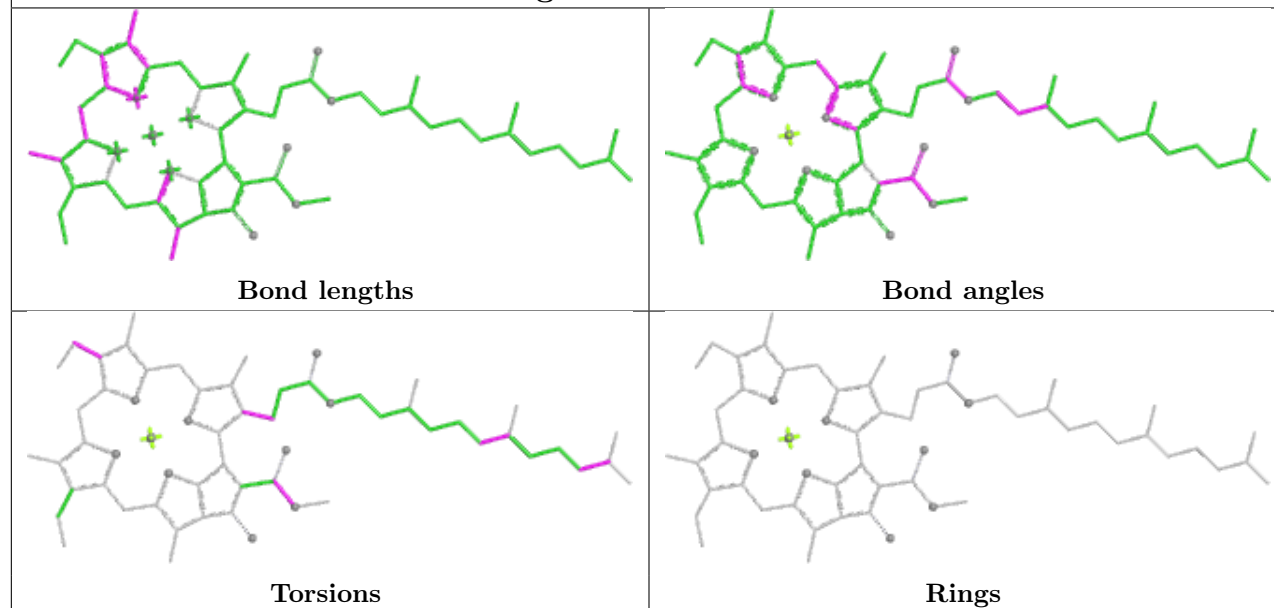
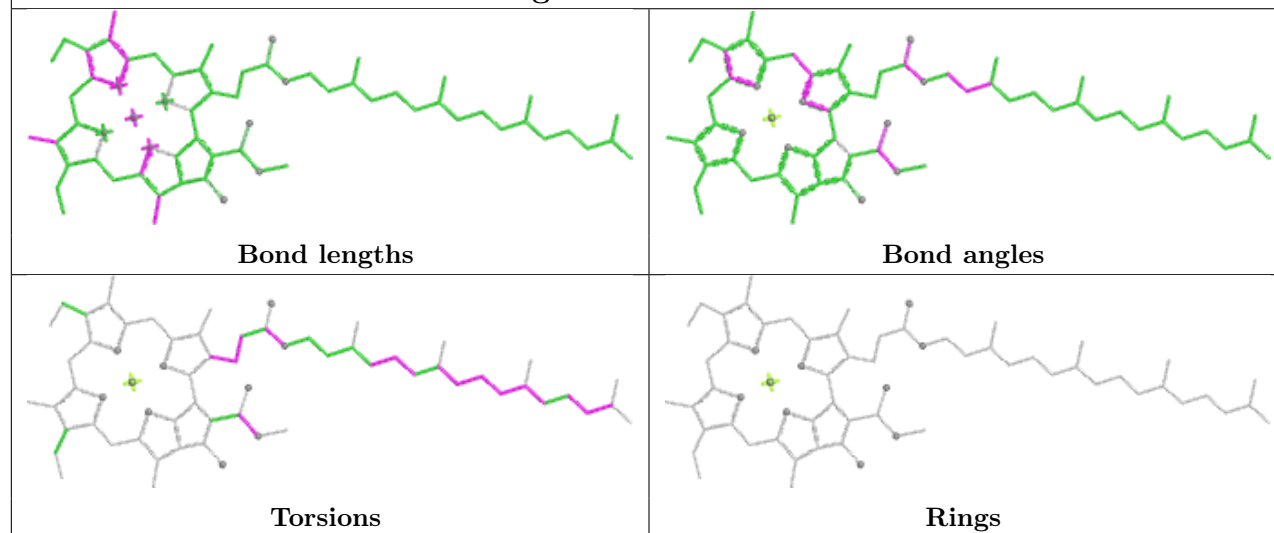


Ligand CLA 3 319

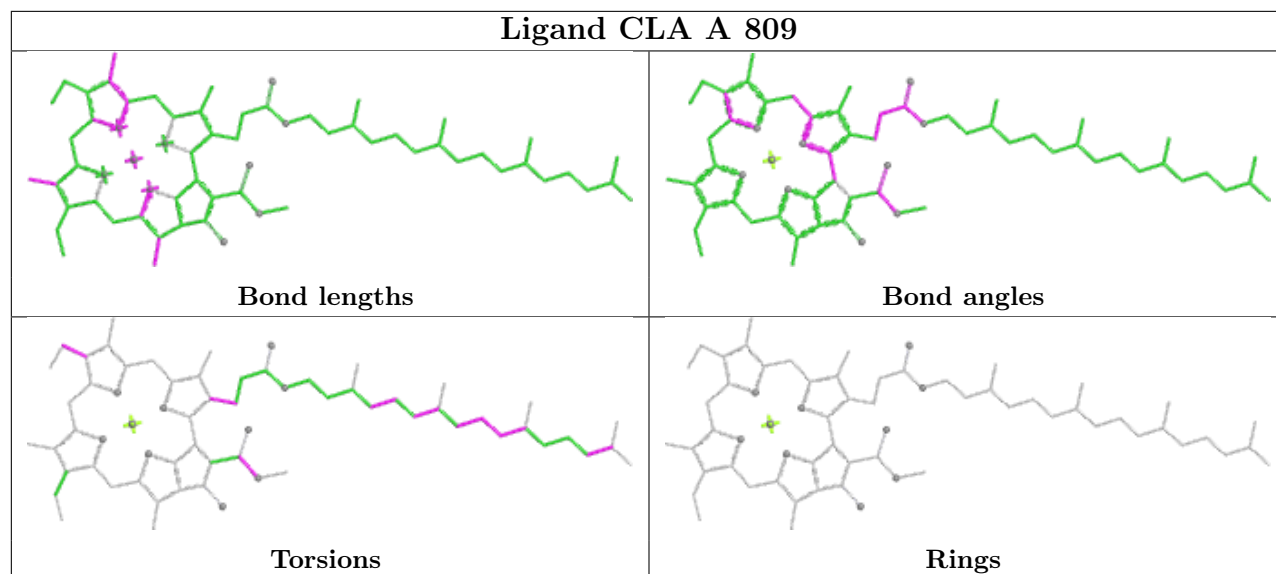


Ligand CLA 2 319

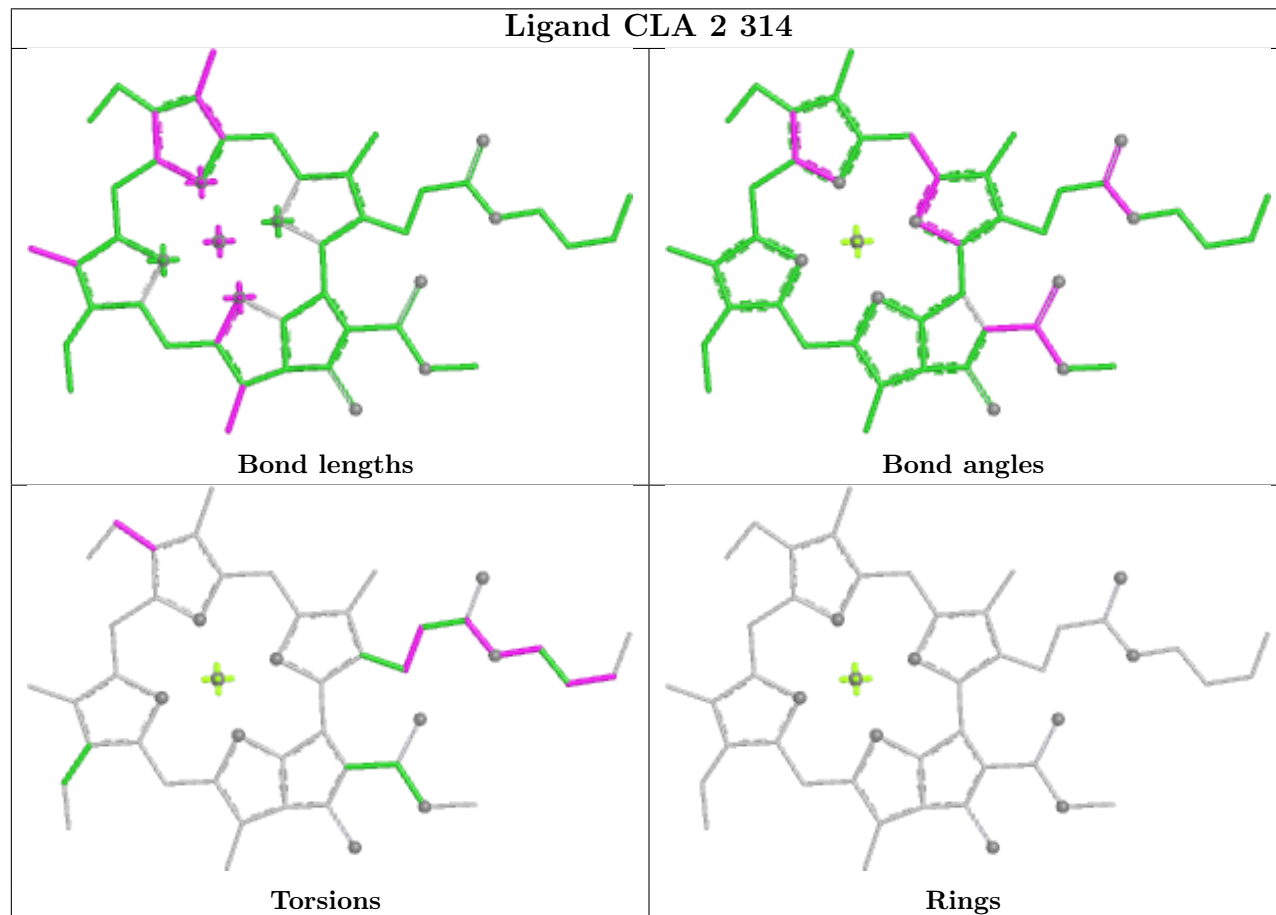


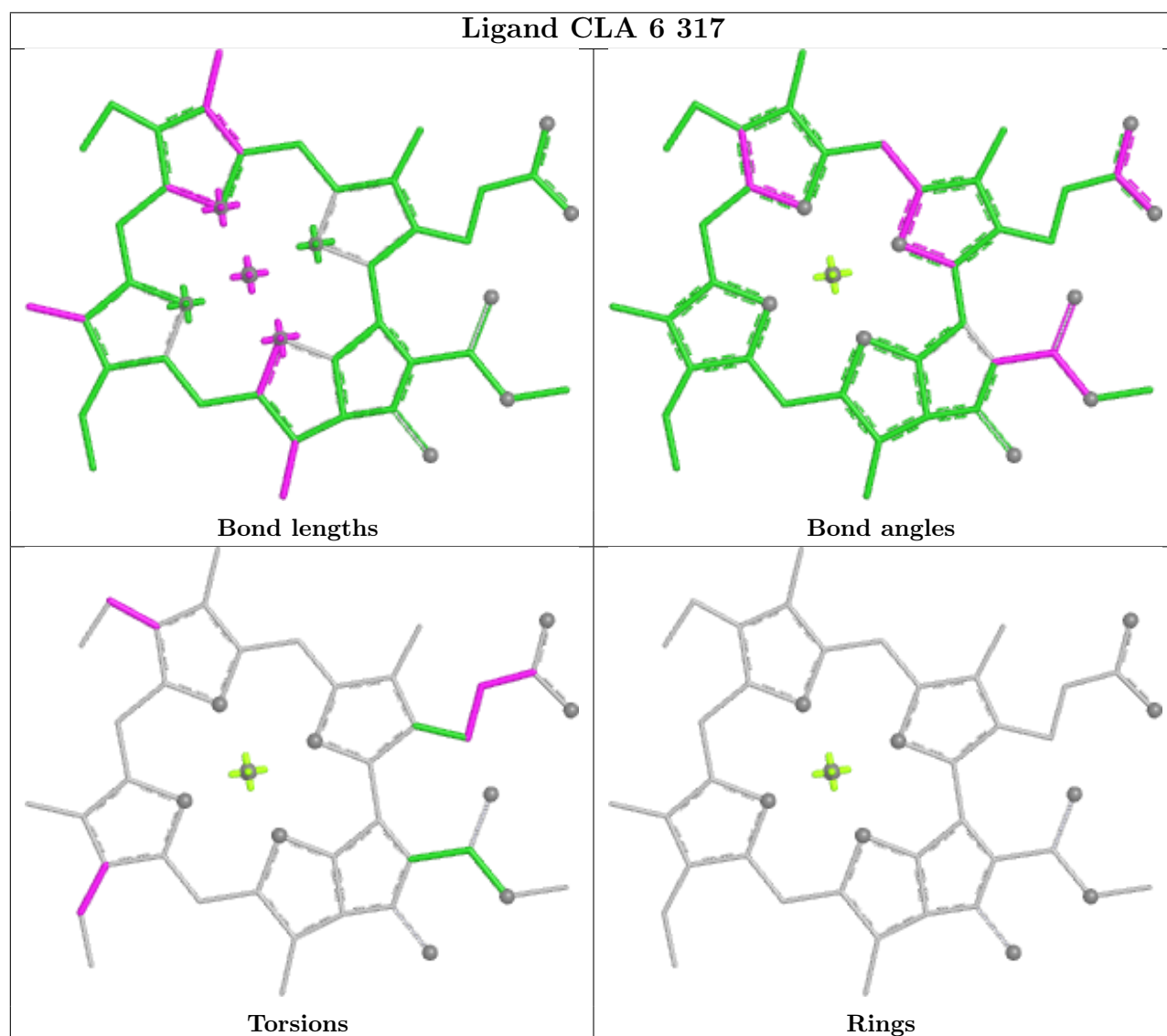
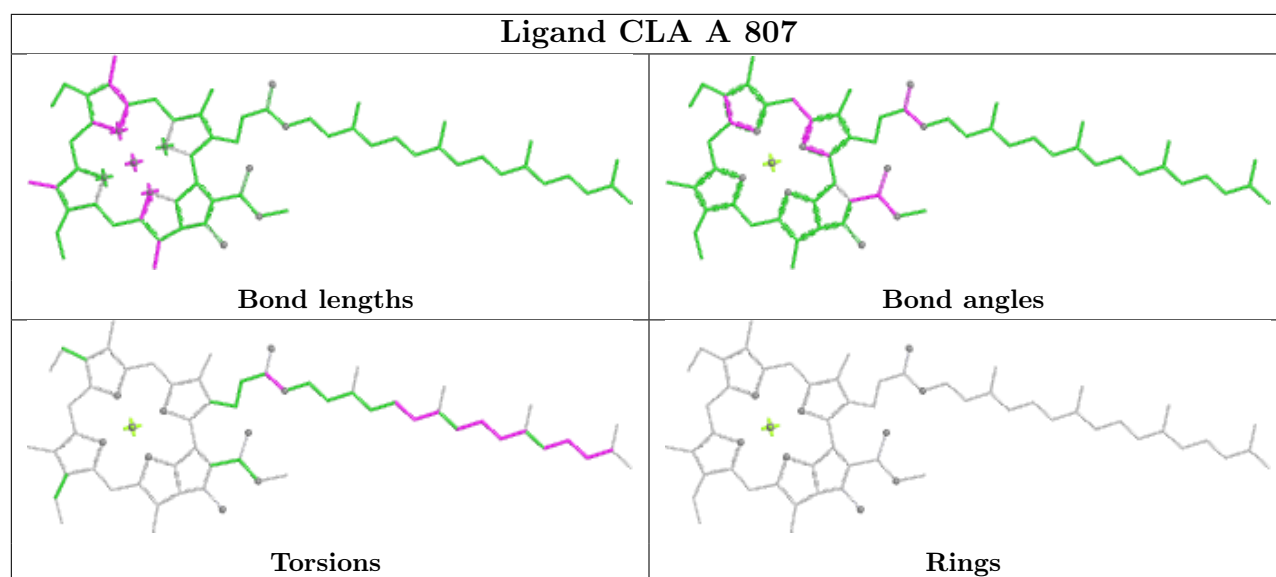
Ligand CLA 5 309**Ligand CLA B 809**

Ligand CLA A 809

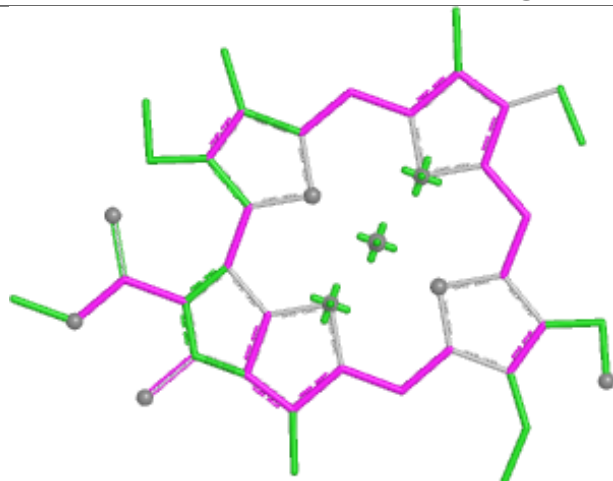


Ligand CLA 2 314

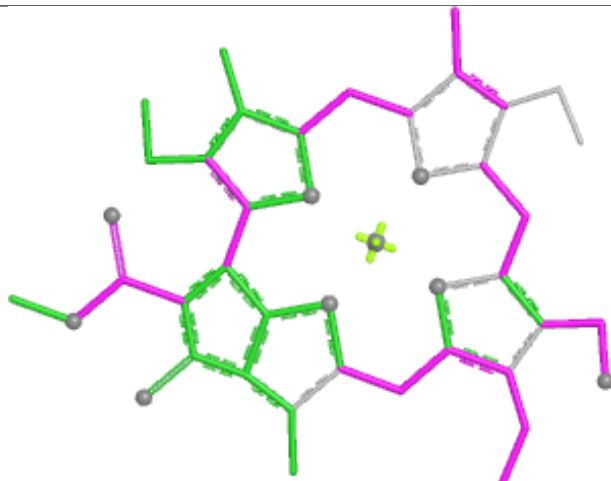




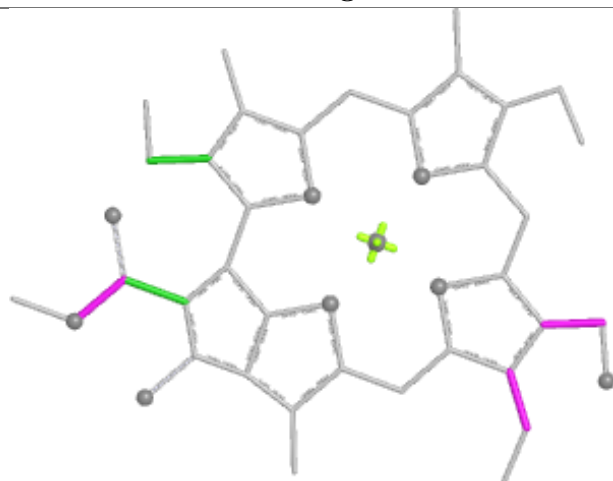
Ligand CHL 6 316



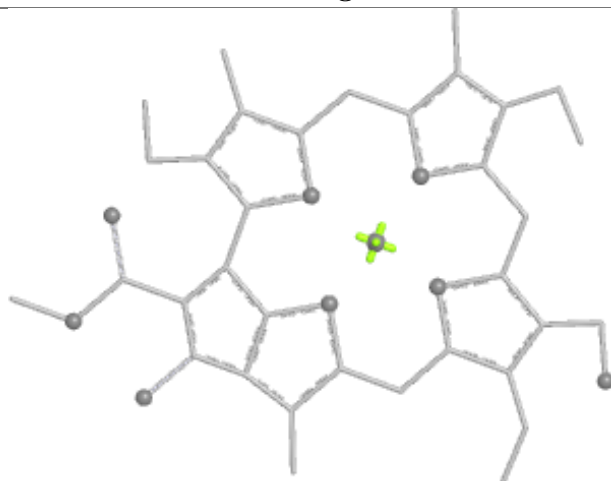
Bond lengths



Bond angles

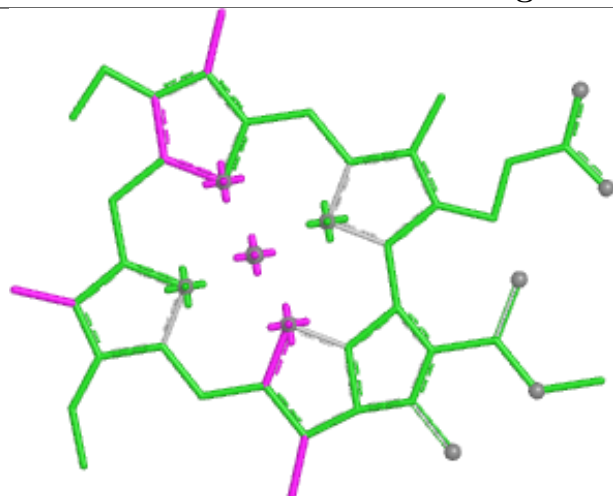


Torsions

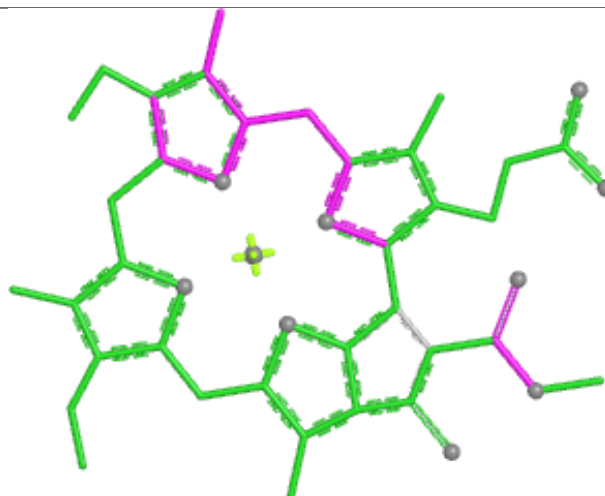


Rings

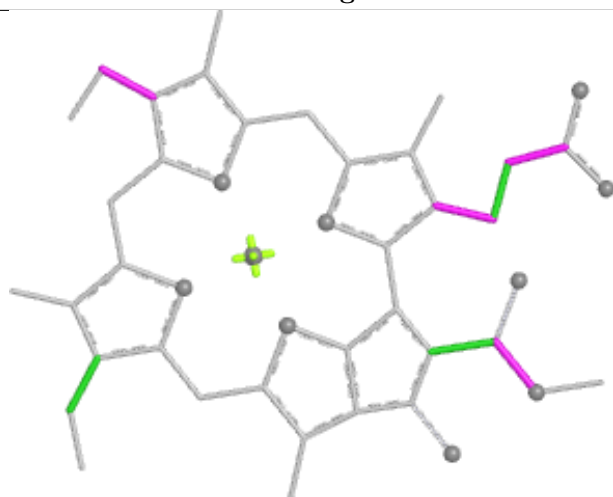
Ligand CLA F 301



Bond lengths



Bond angles

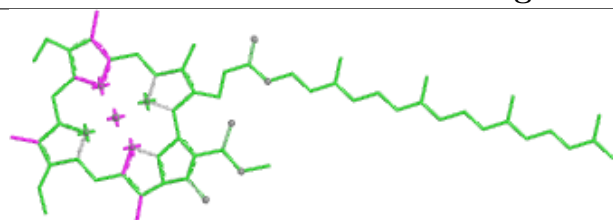


Torsions

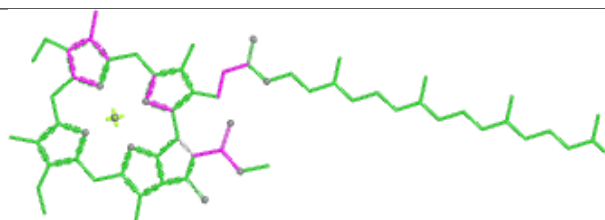


Rings

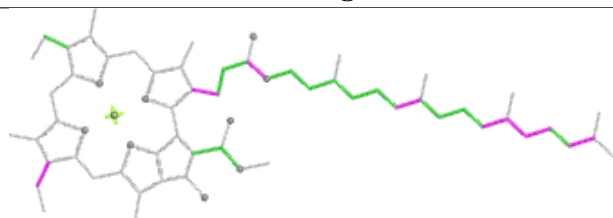
Ligand CLA B 826



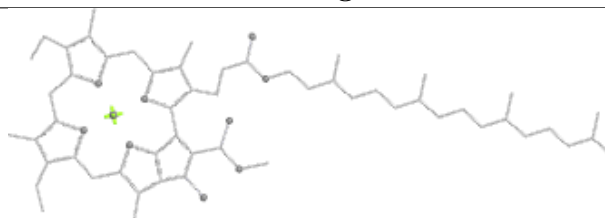
Bond lengths



Bond angles

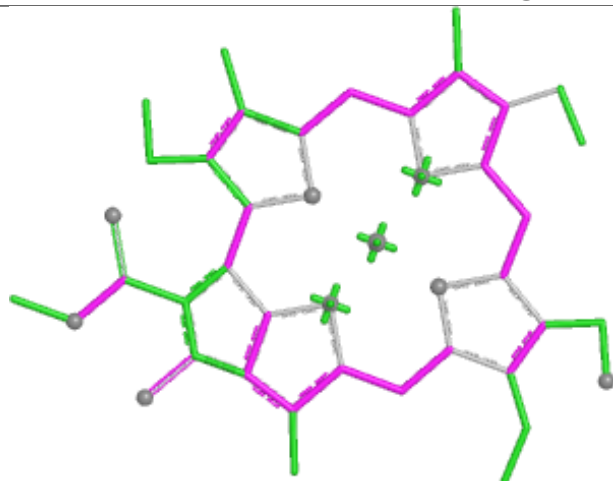


Torsions

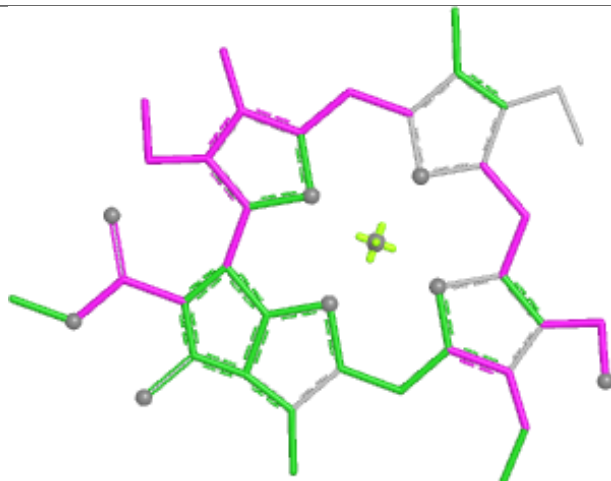


Rings

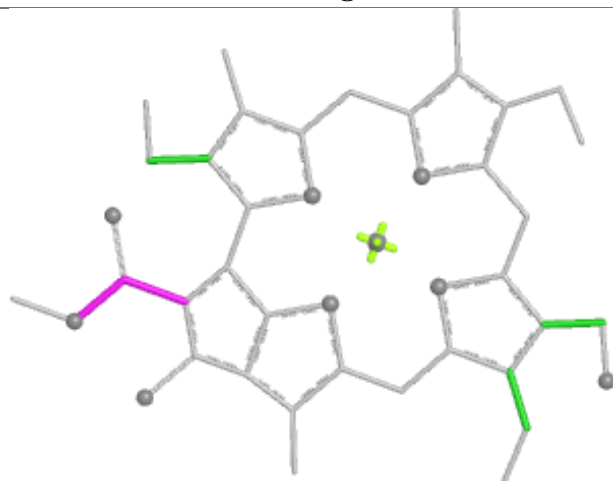
Ligand CHL 8 314



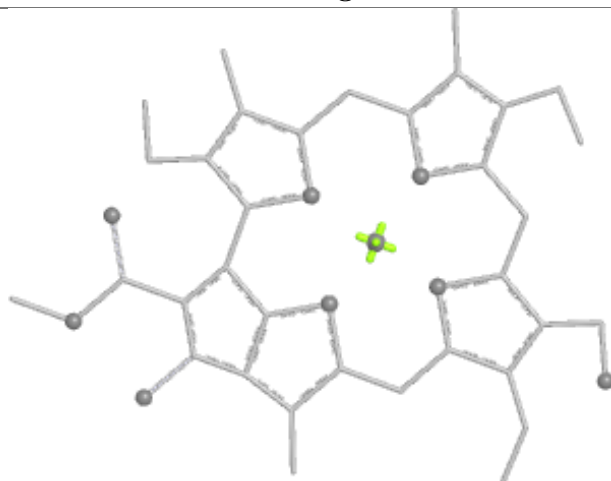
Bond lengths



Bond angles

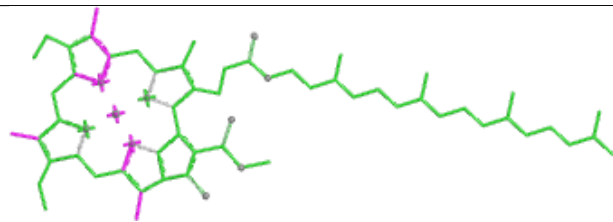


Torsions

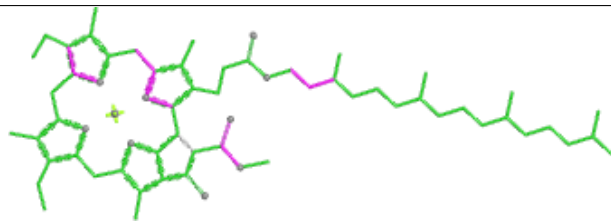


Rings

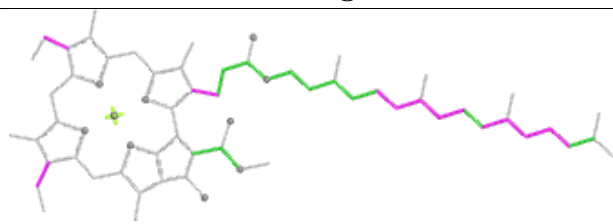
Ligand CLA A 826



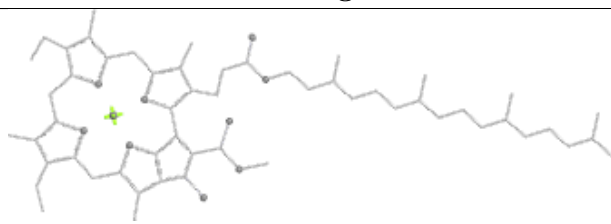
Bond lengths



Bond angles

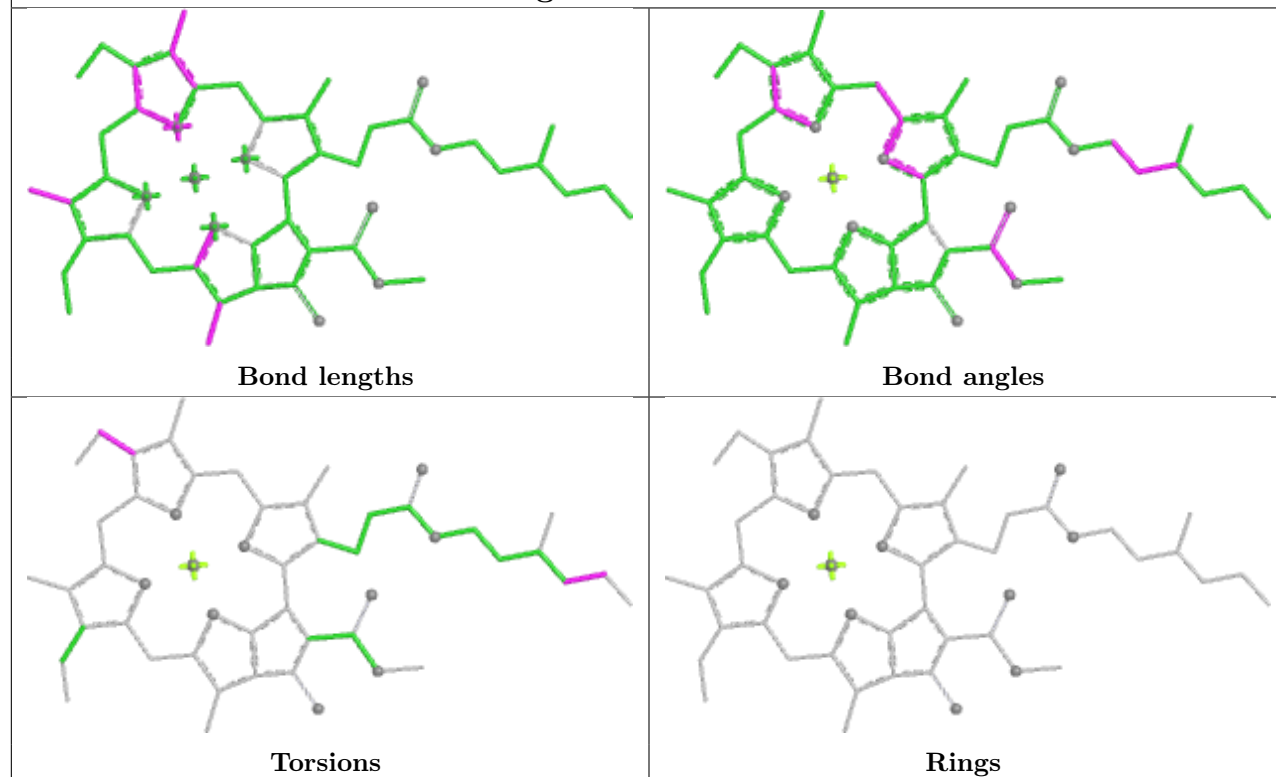


Torsions

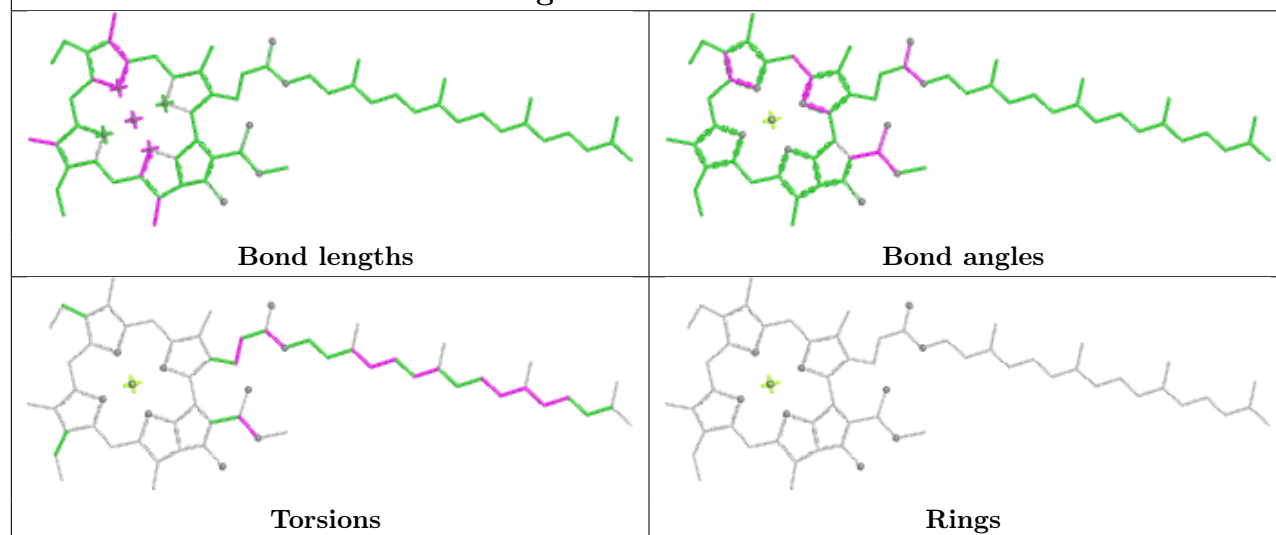


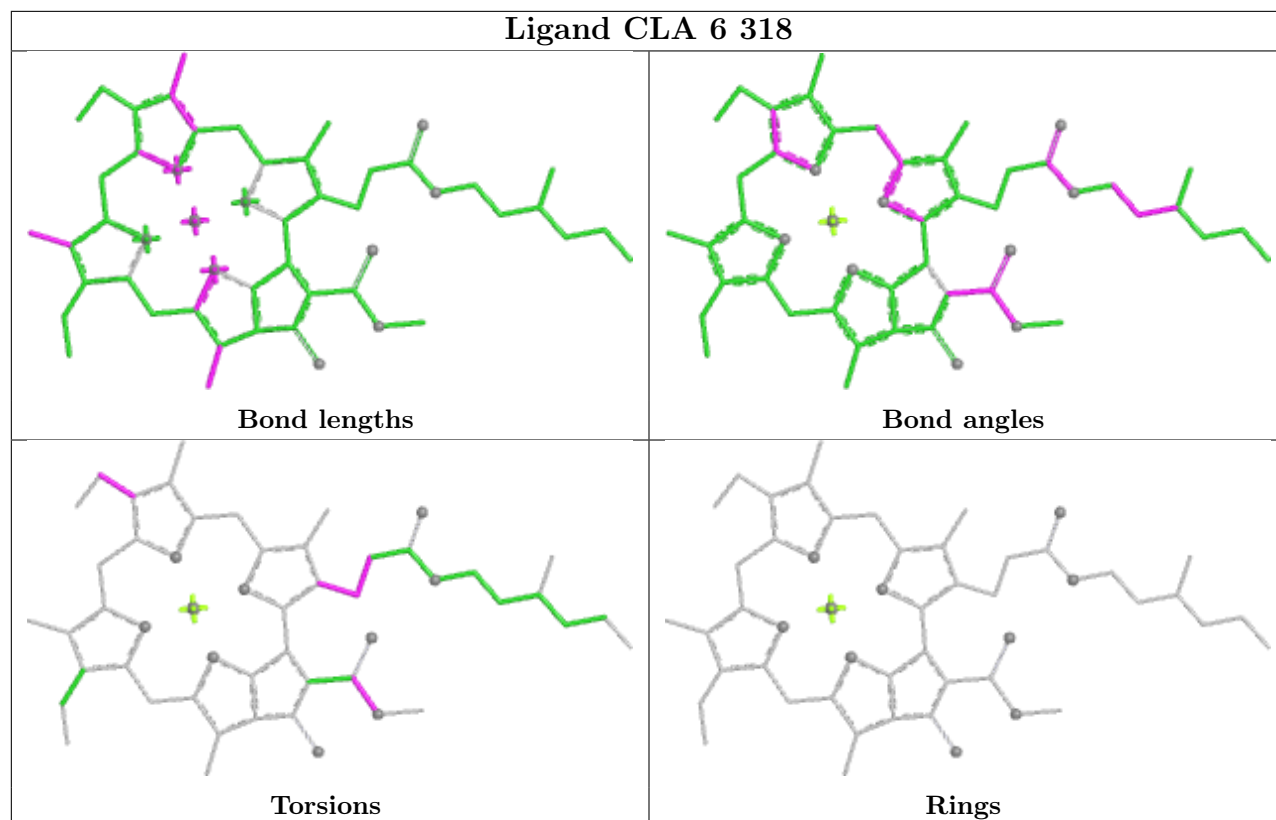
Rings

Ligand CLA 3 310

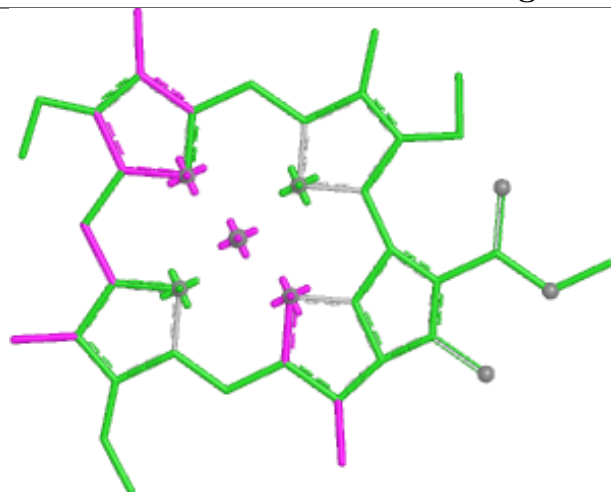


Ligand CLA 1 311





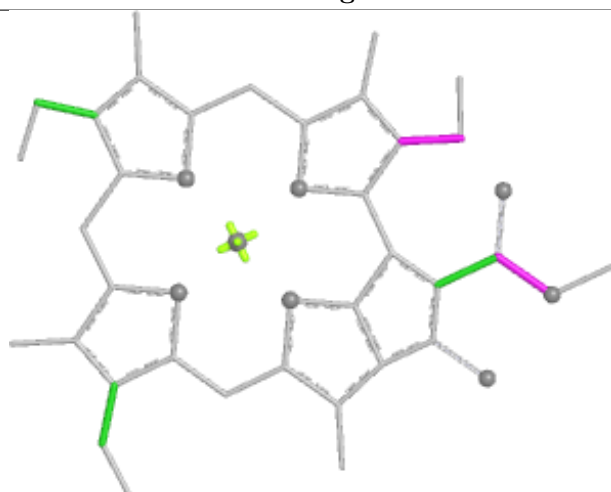
Ligand CLA 7 306



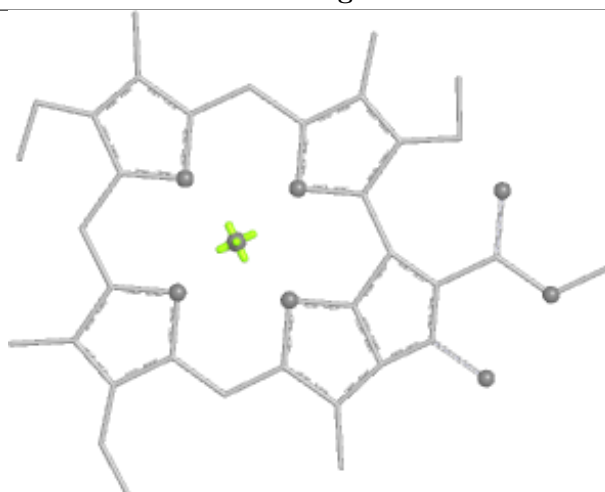
Bond lengths



Bond angles

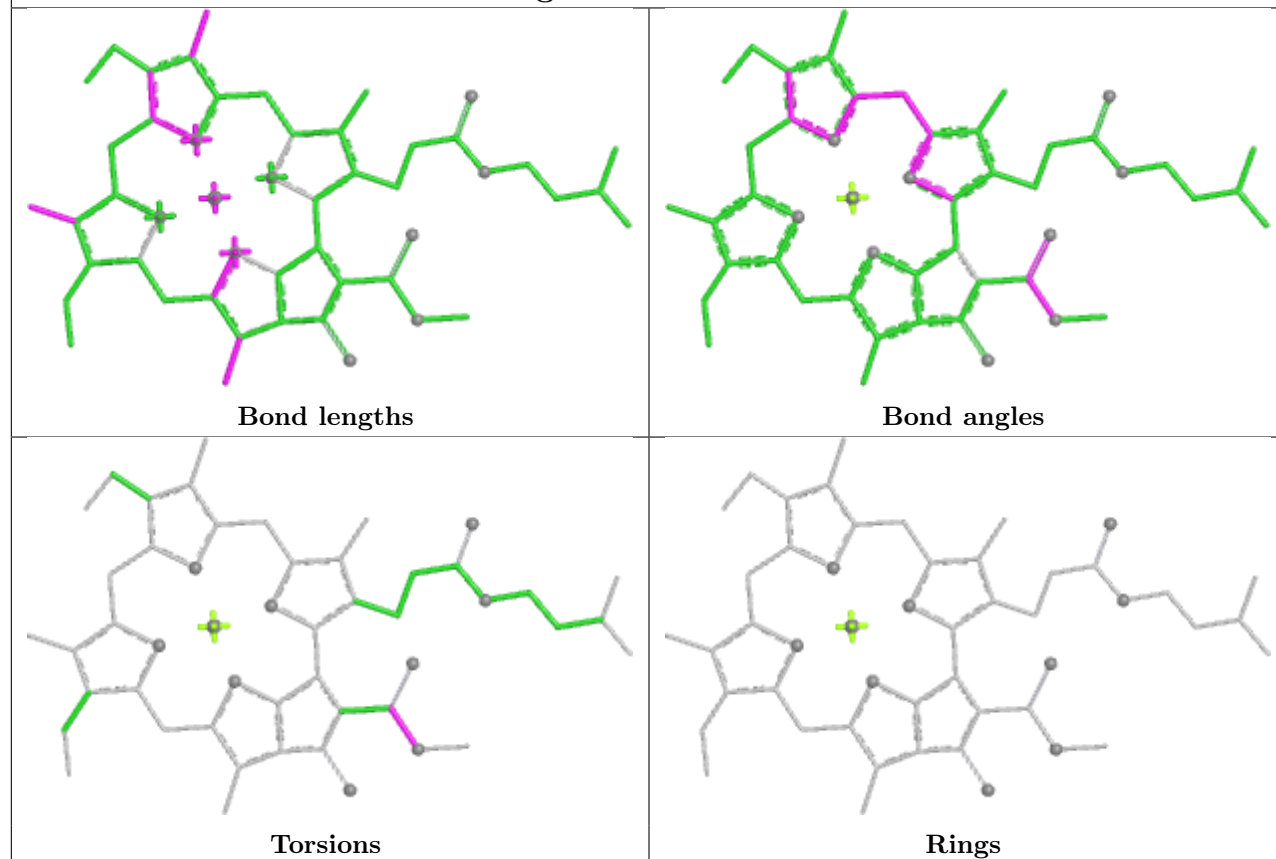


Torsions

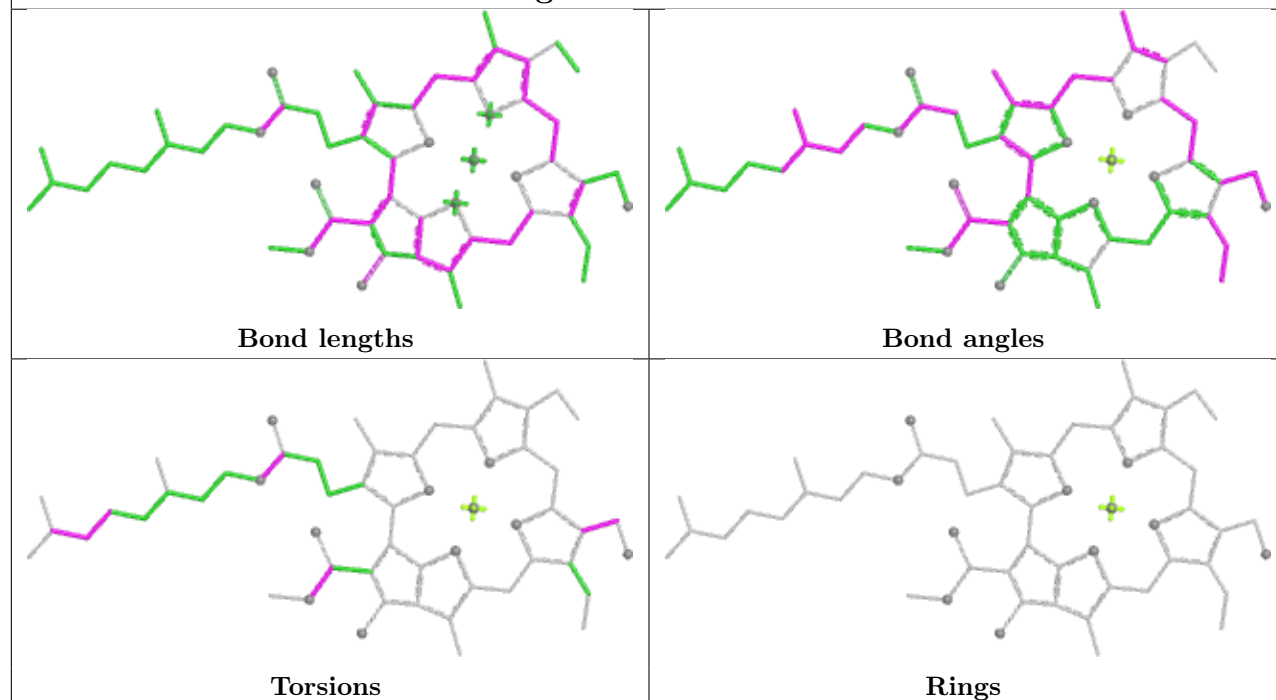


Rings

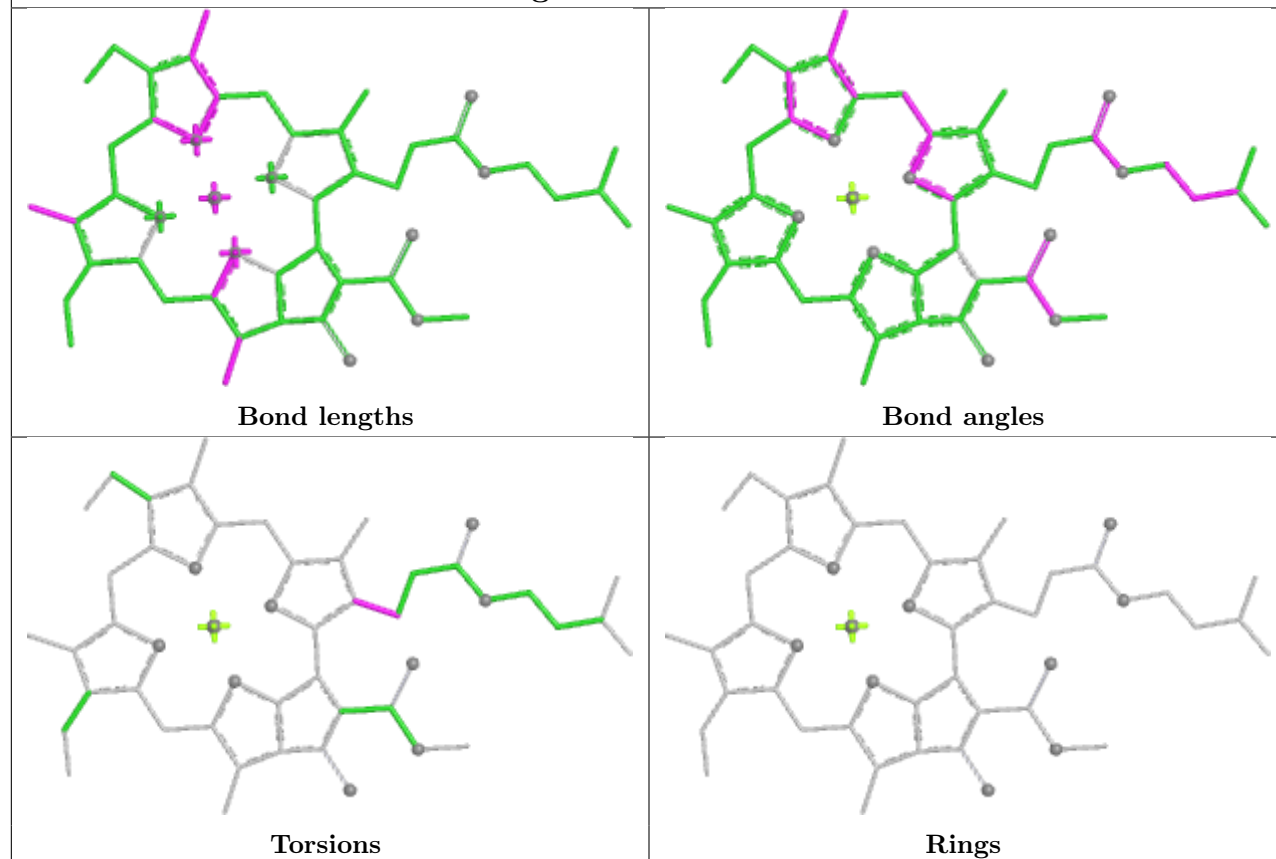
Ligand CLA 3 302



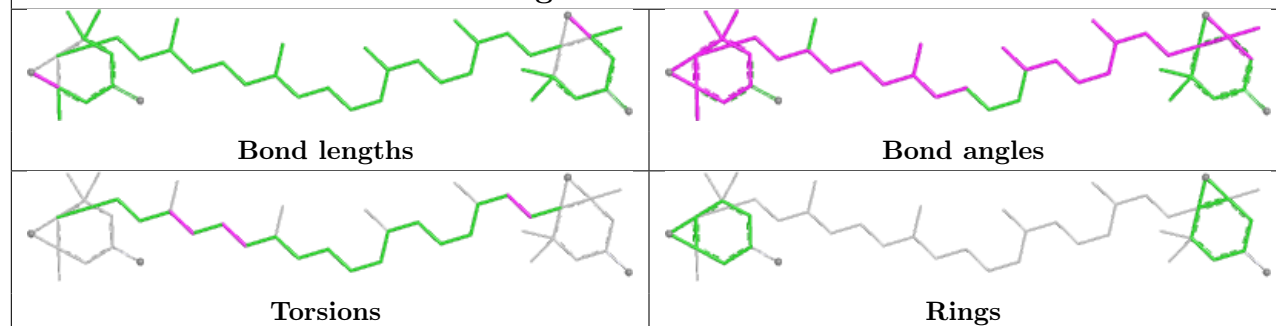
Ligand CHL 8 305

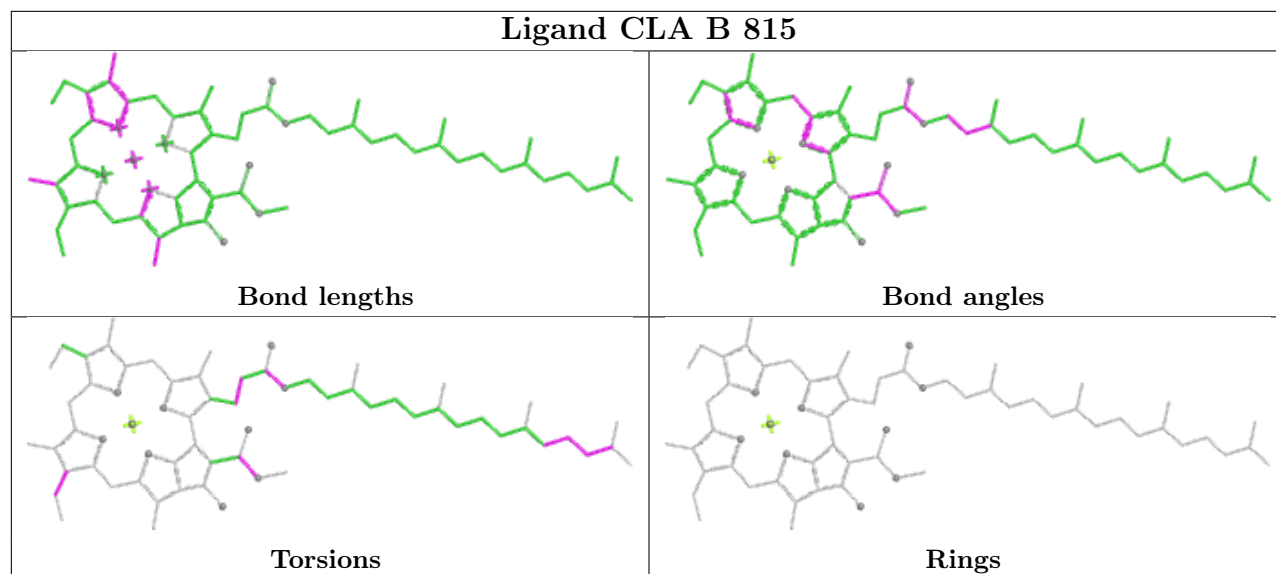
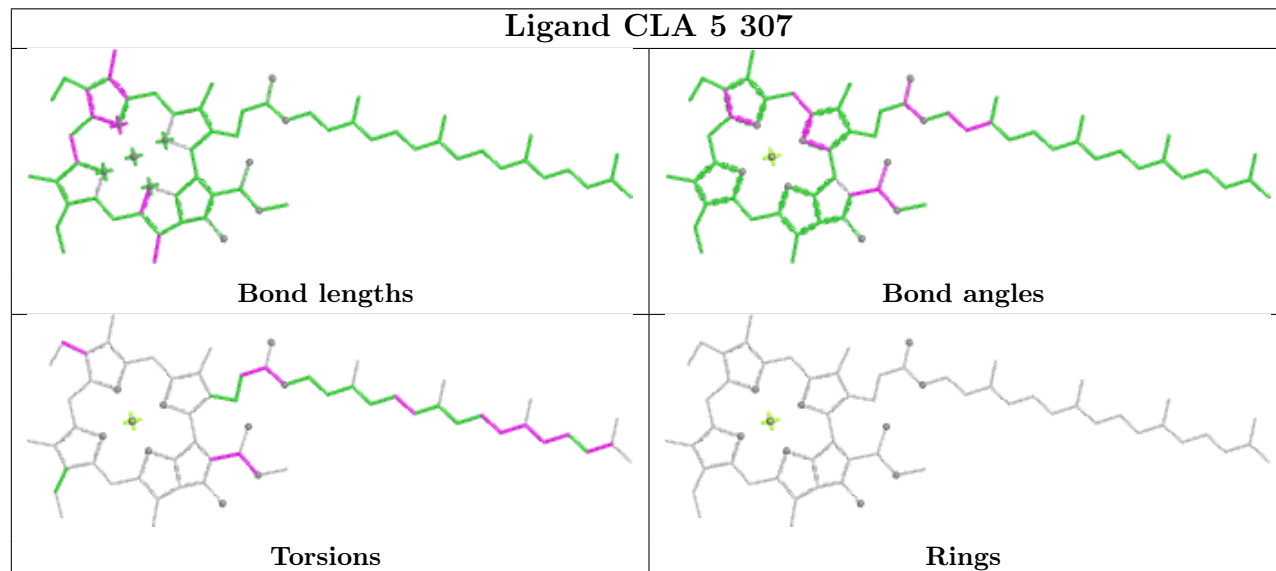


Ligand CLA A 831

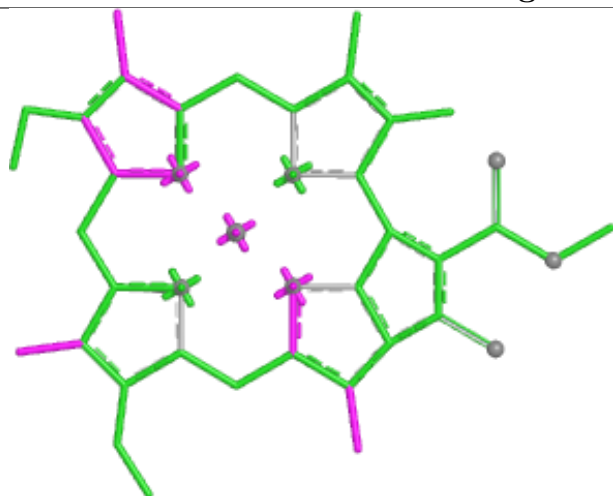


Ligand XAT 9 314

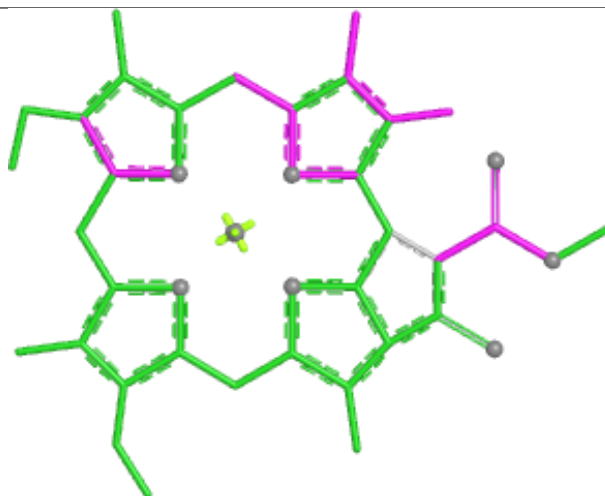


Ligand CLA B 815**Ligand CLA 5 307**

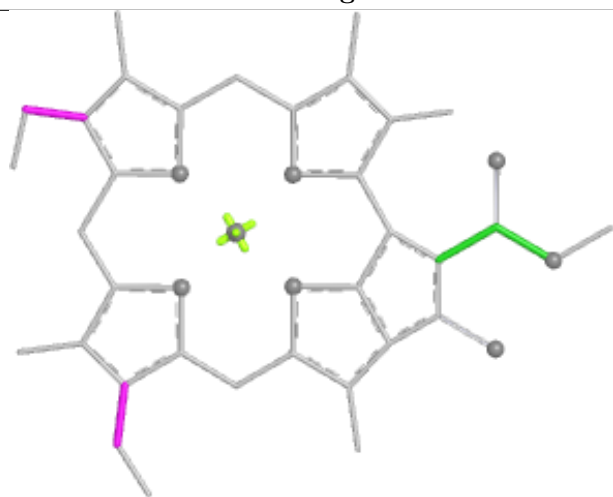
Ligand CLA 1 309



Bond lengths



Bond angles

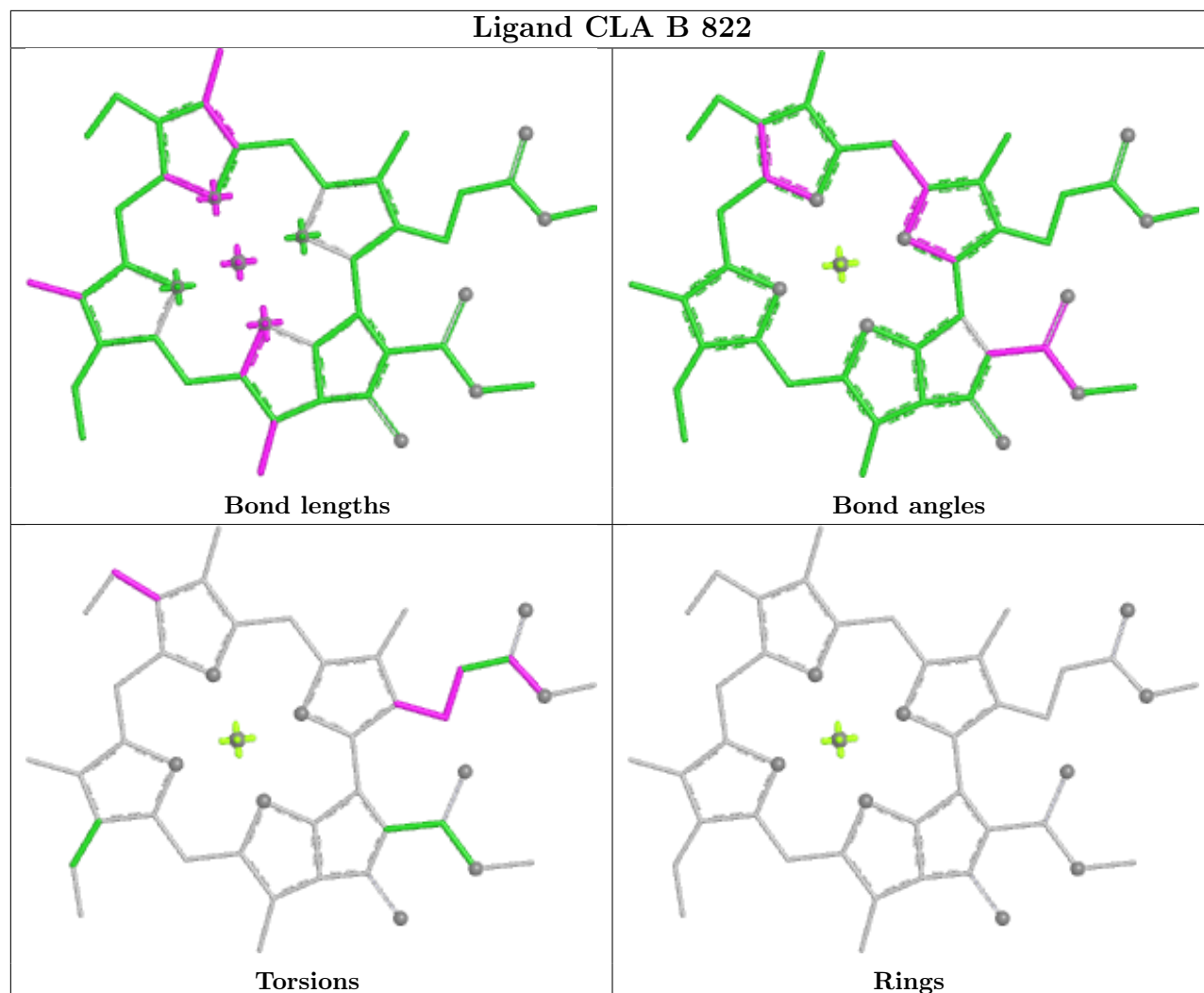


Torsions

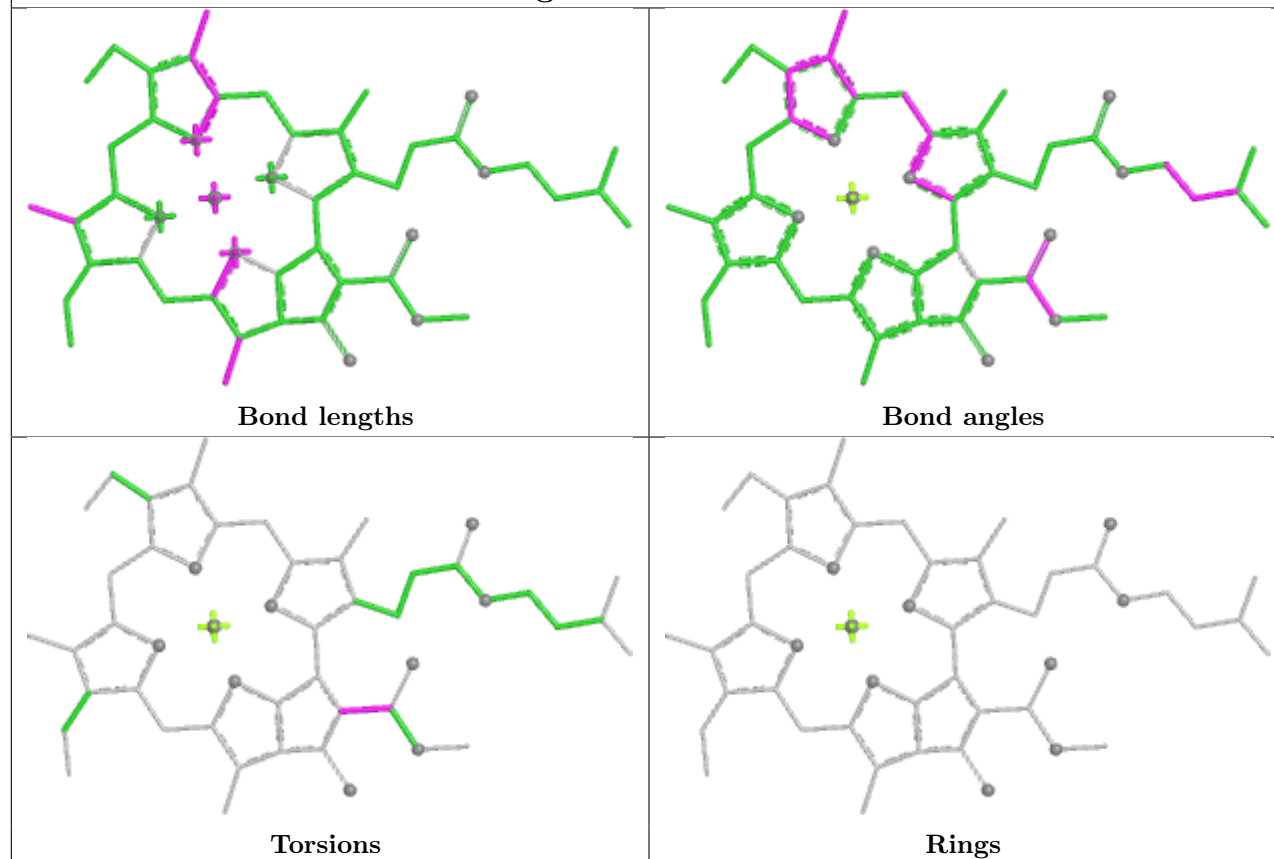


Rings

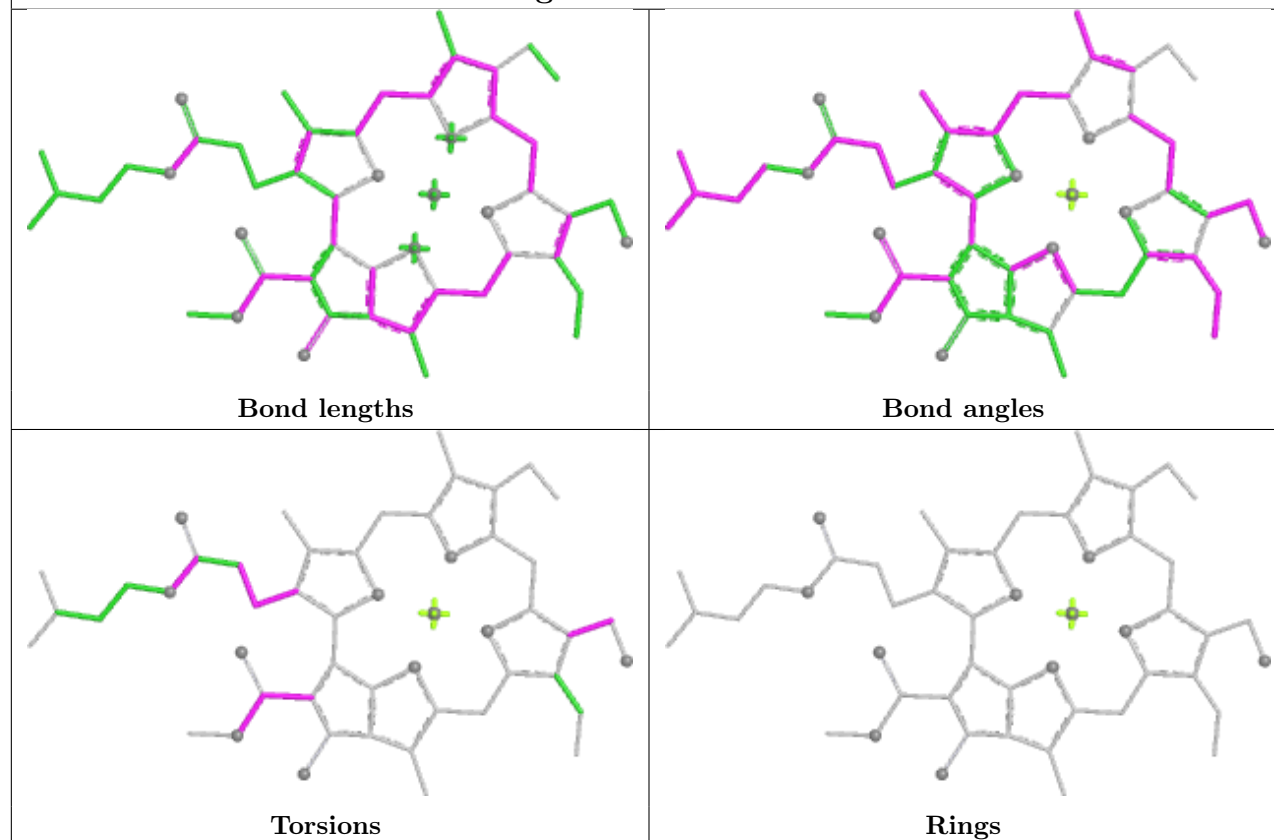
Ligand CLA B 822



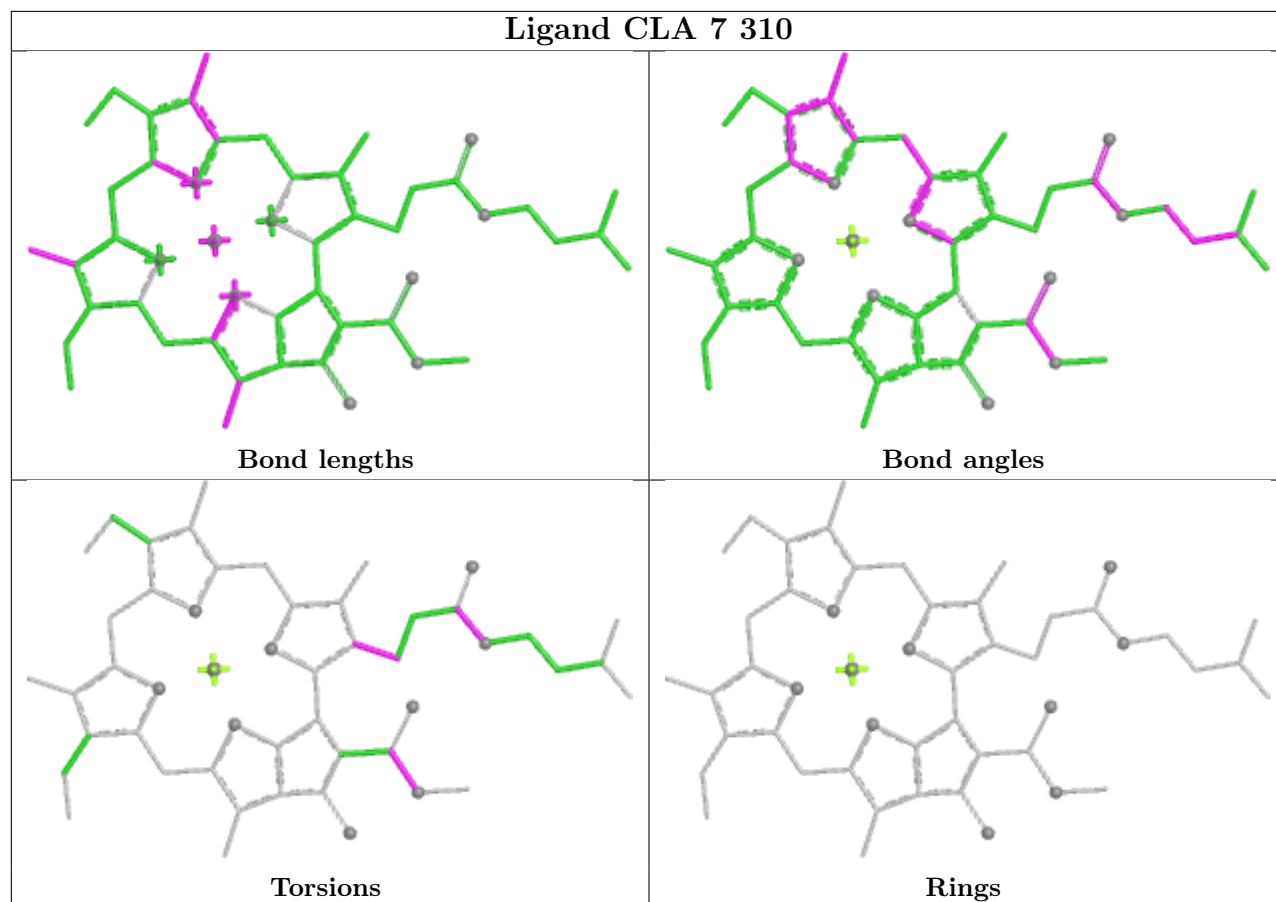
Ligand CLA 4 308



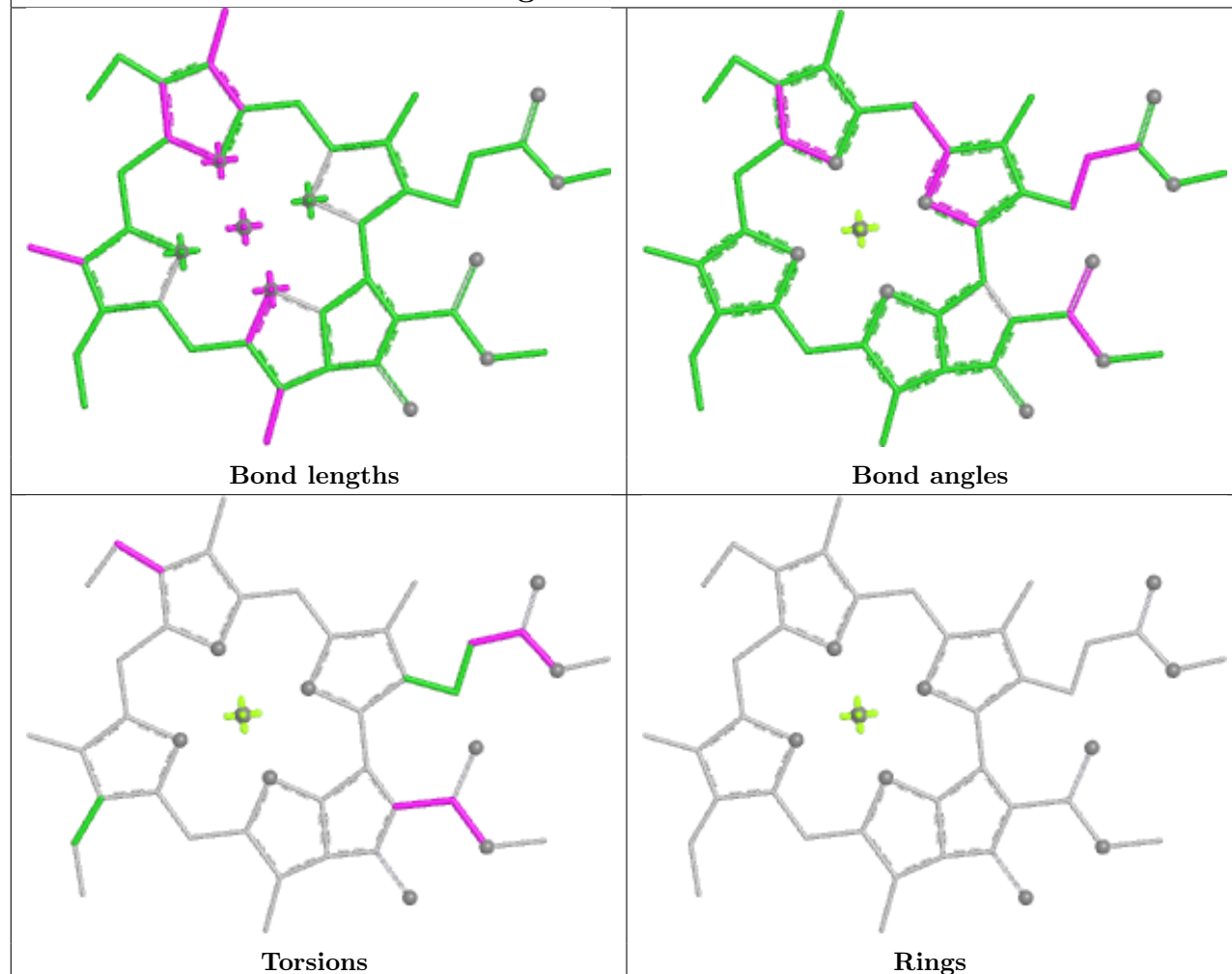
Ligand CHL 2 307



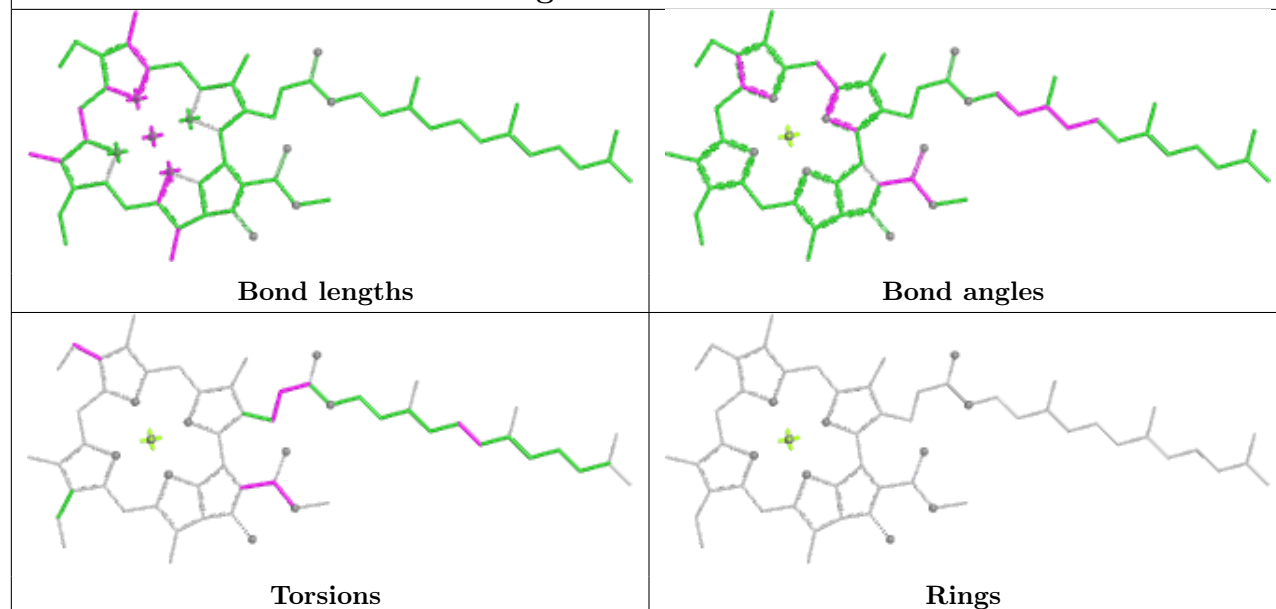
Ligand CLA 7 310



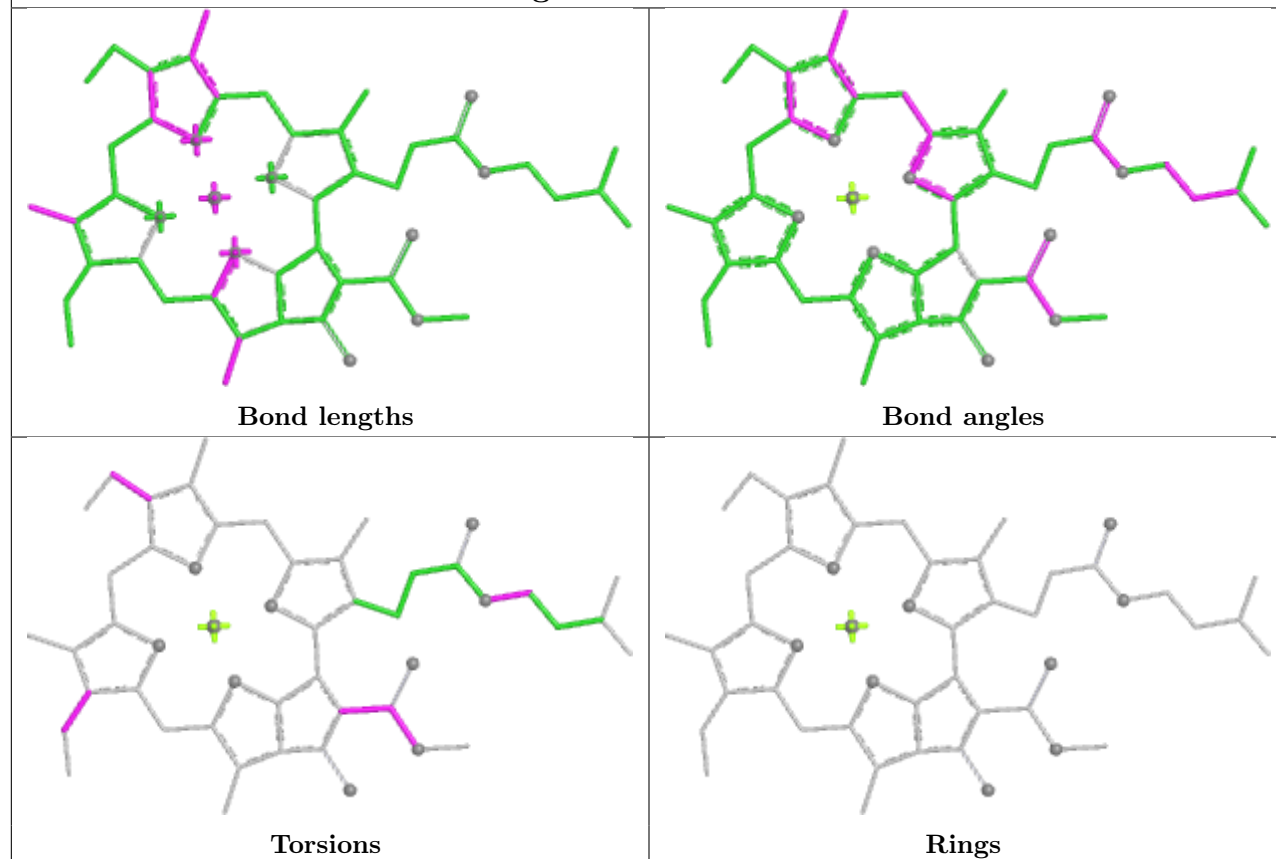
Ligand CLA 7 302



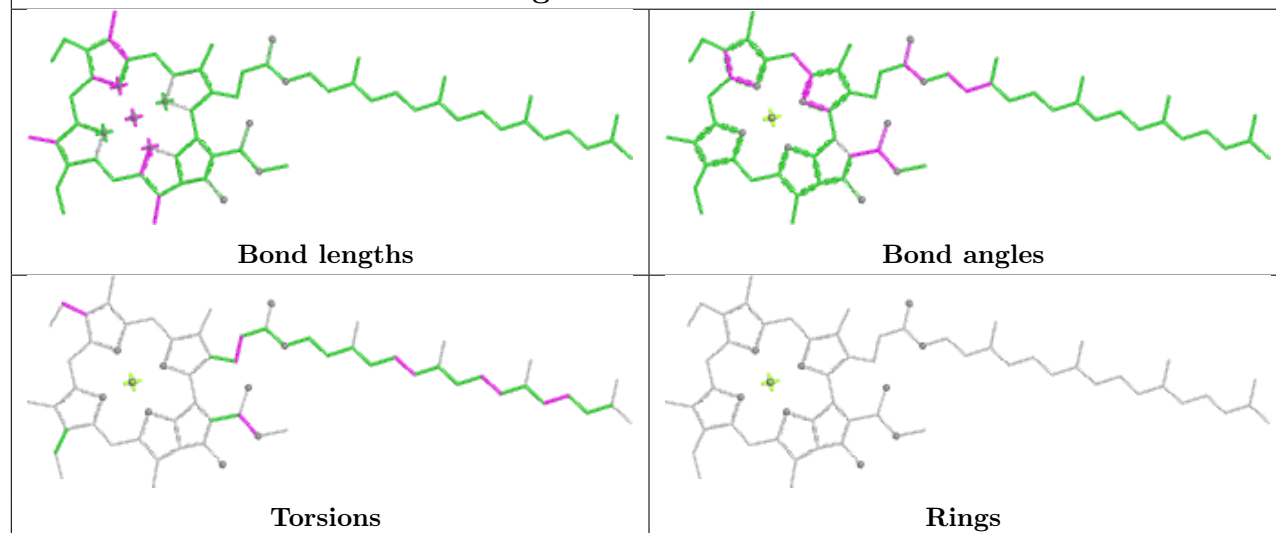
Ligand CLA 4 302



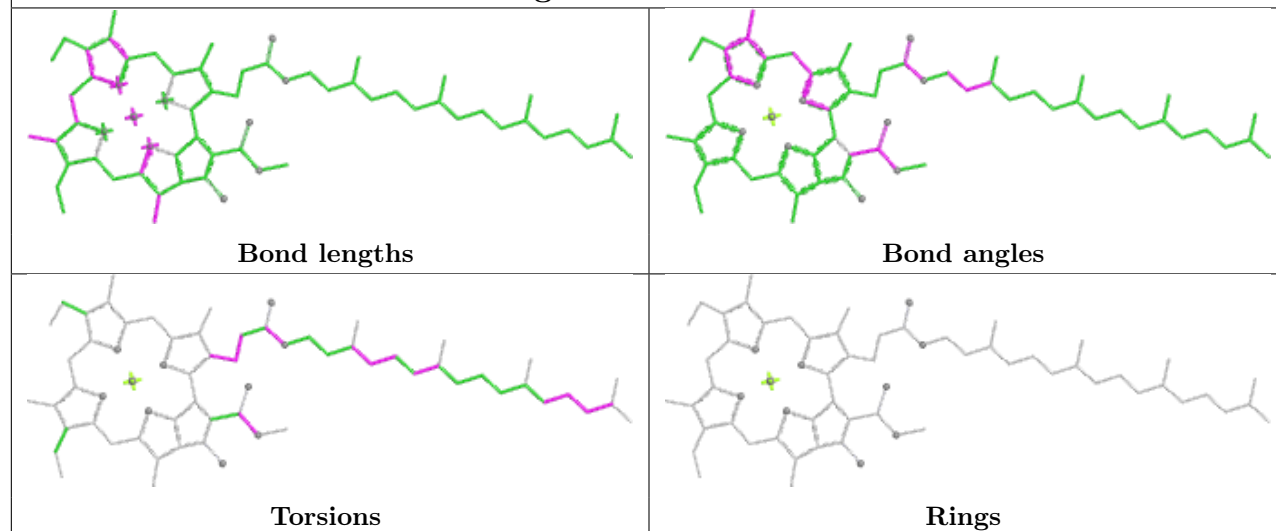
Ligand CLA B 821



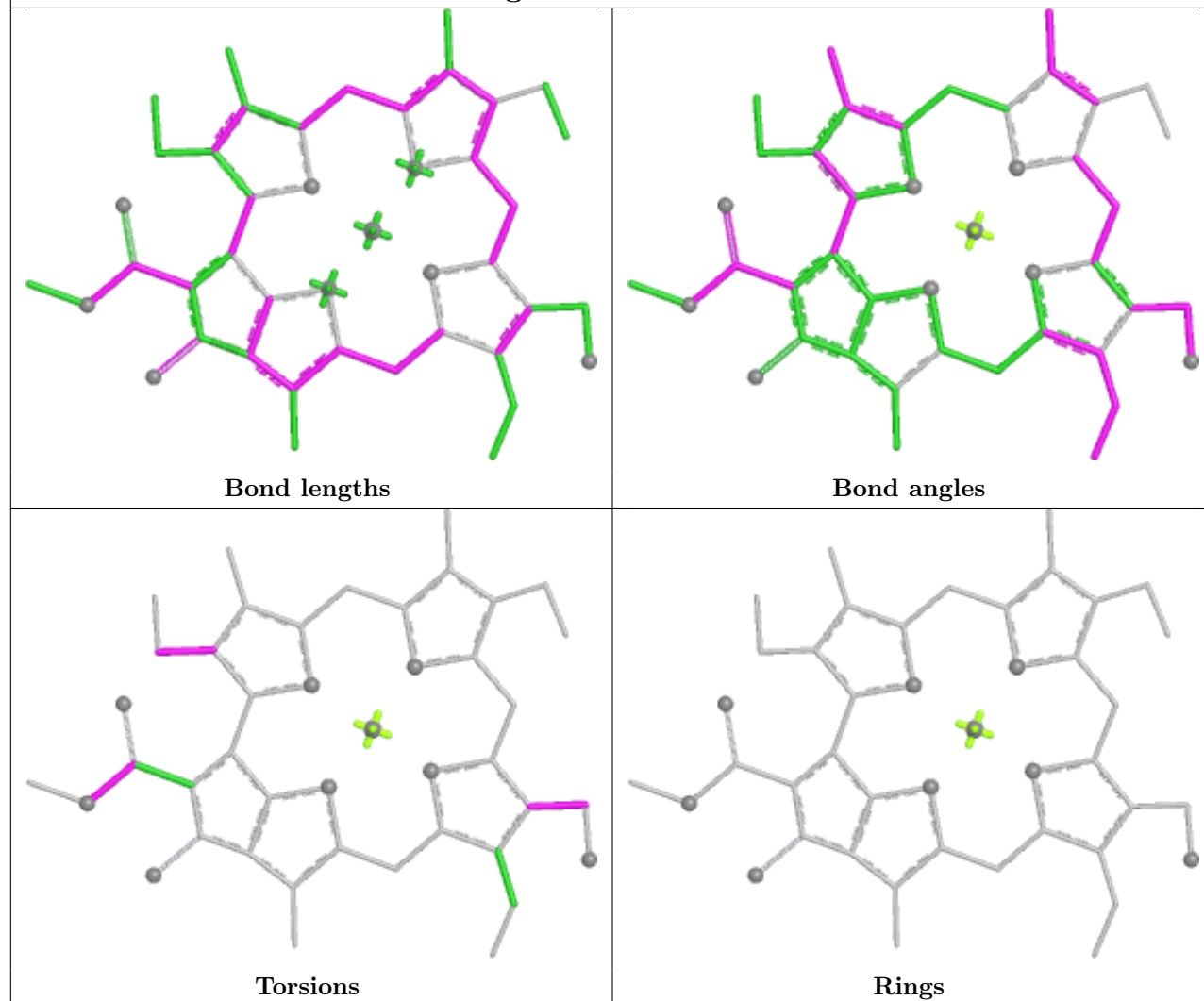
Ligand CLA B 810

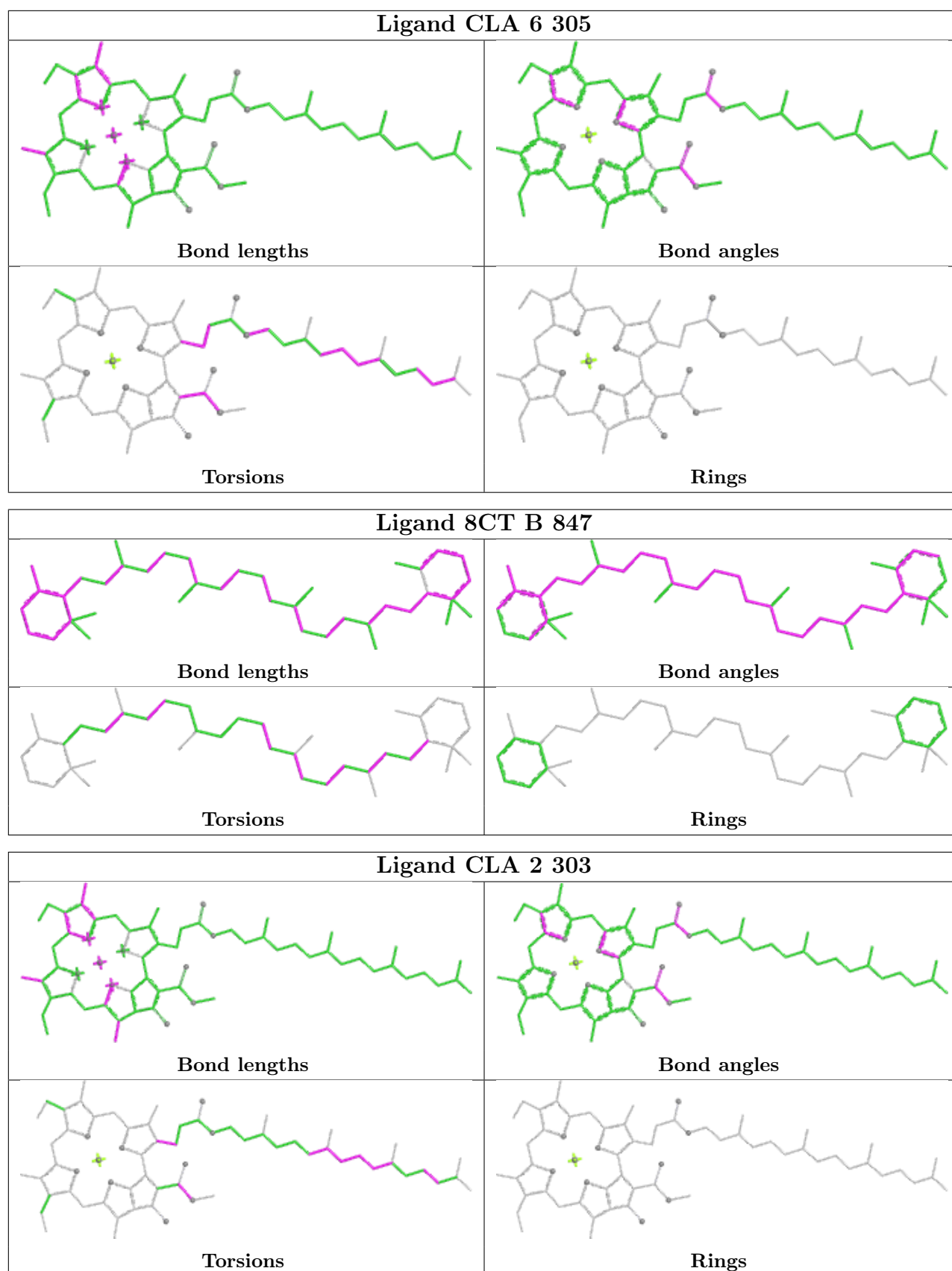


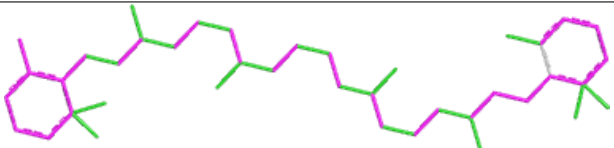
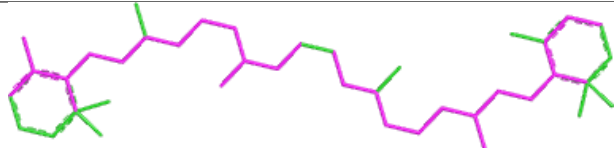
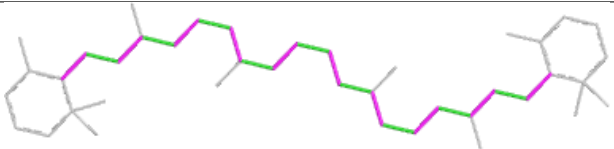
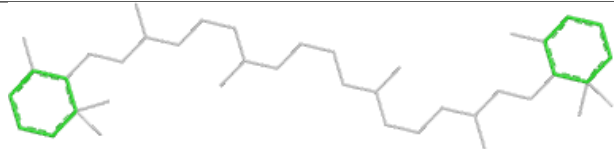
Ligand CLA L 202

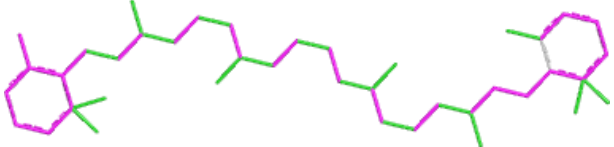
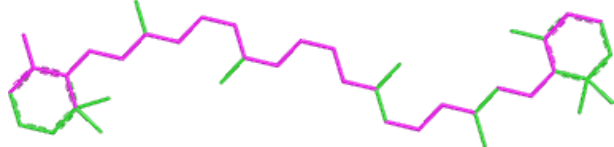
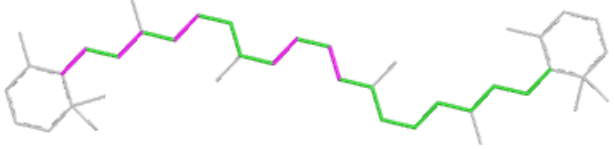
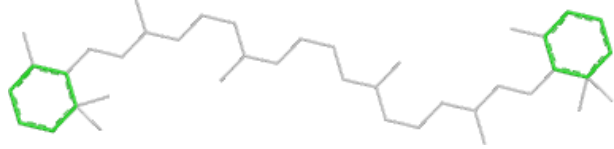


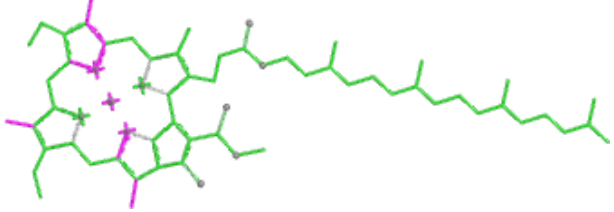
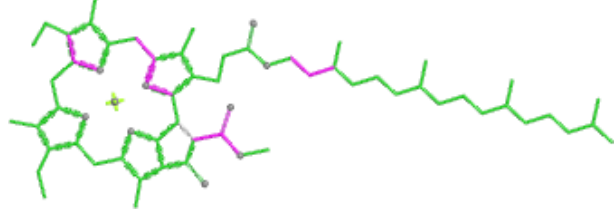
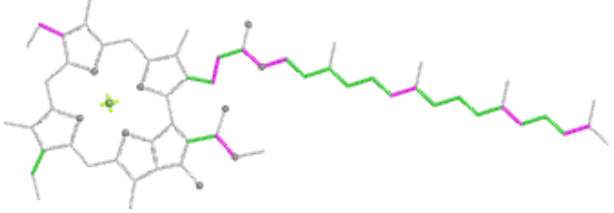
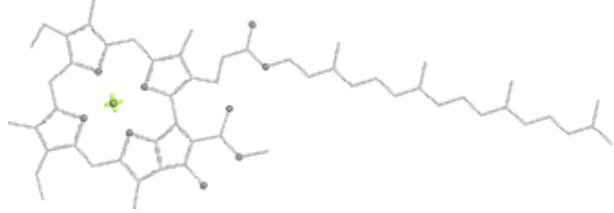
Ligand CHL 6 307

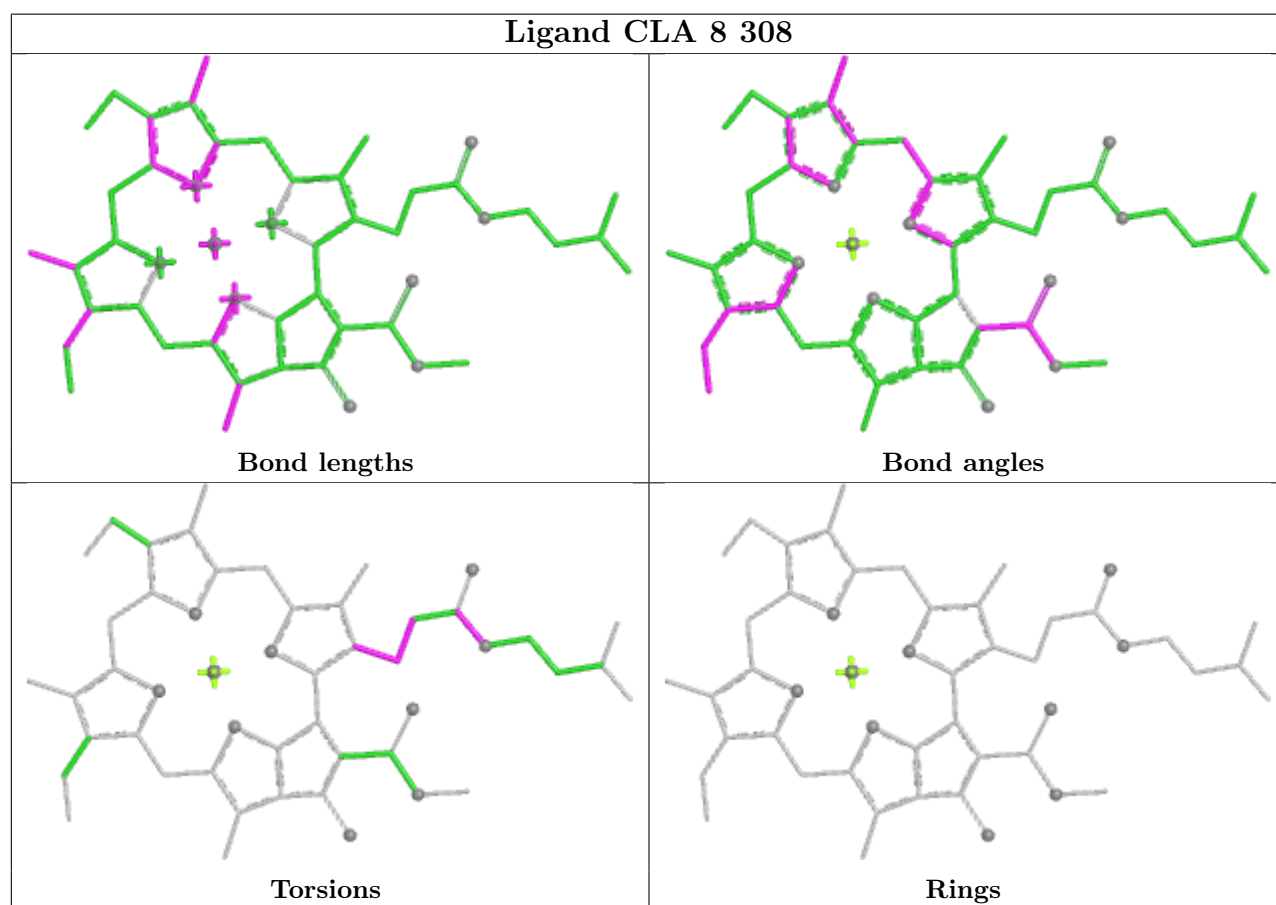
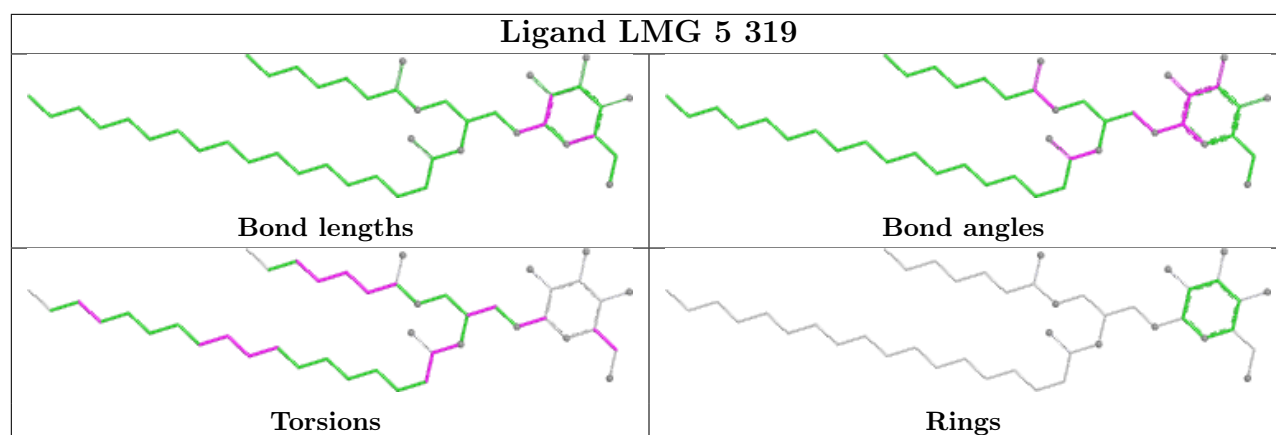




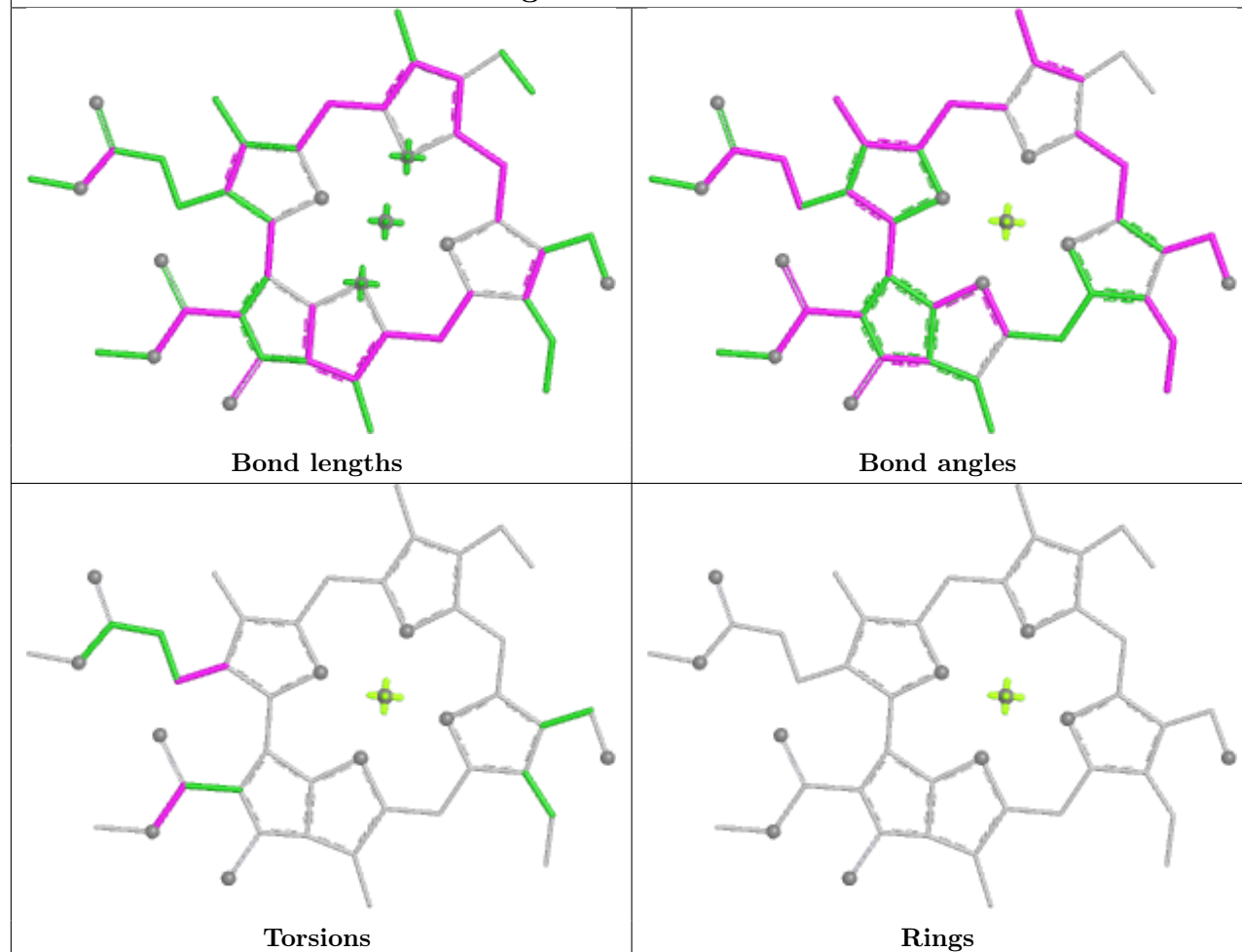
Ligand 8CT L 206	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand 8CT A 848	
	Bond lengths
	Bond angles
	Torsions
	Rings

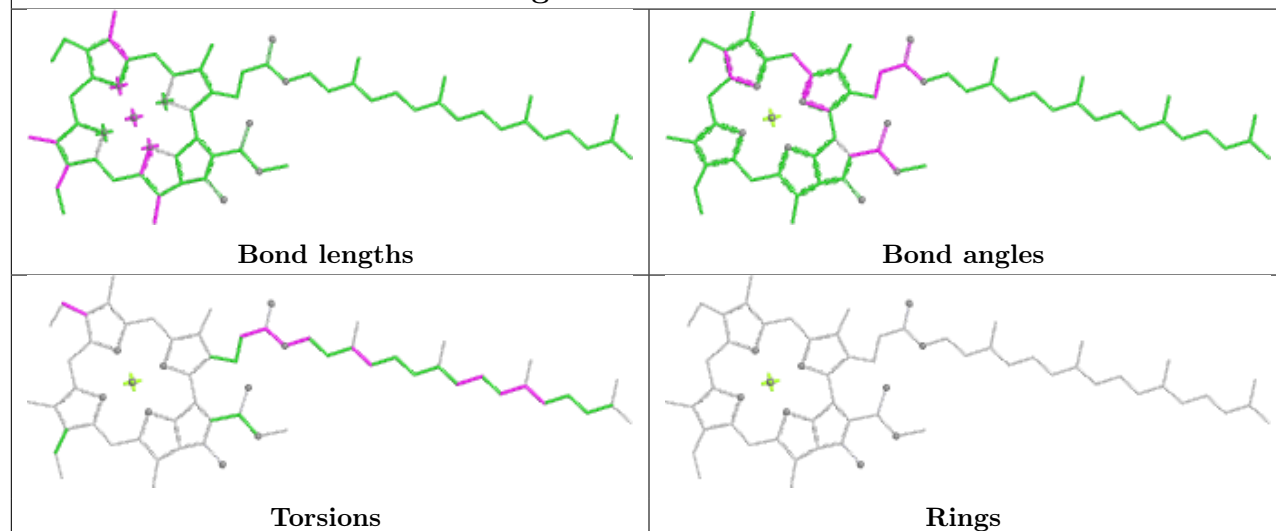
Ligand CLA 9 303	
	Bond lengths
	Bond angles
	Torsions
	Rings



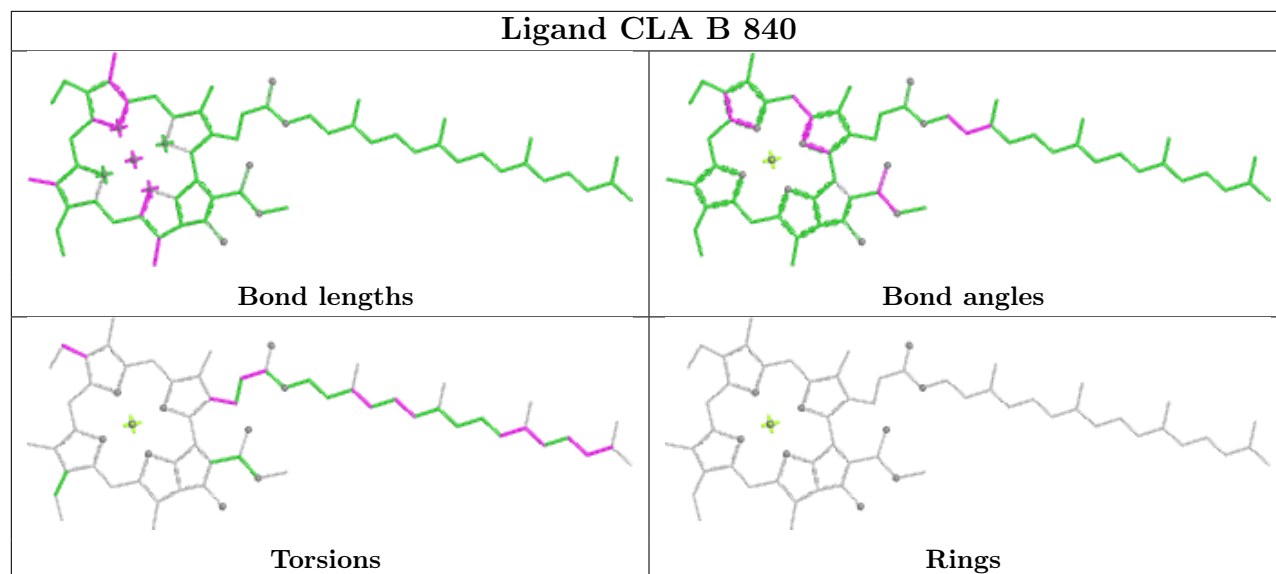
Ligand CHL 3 306



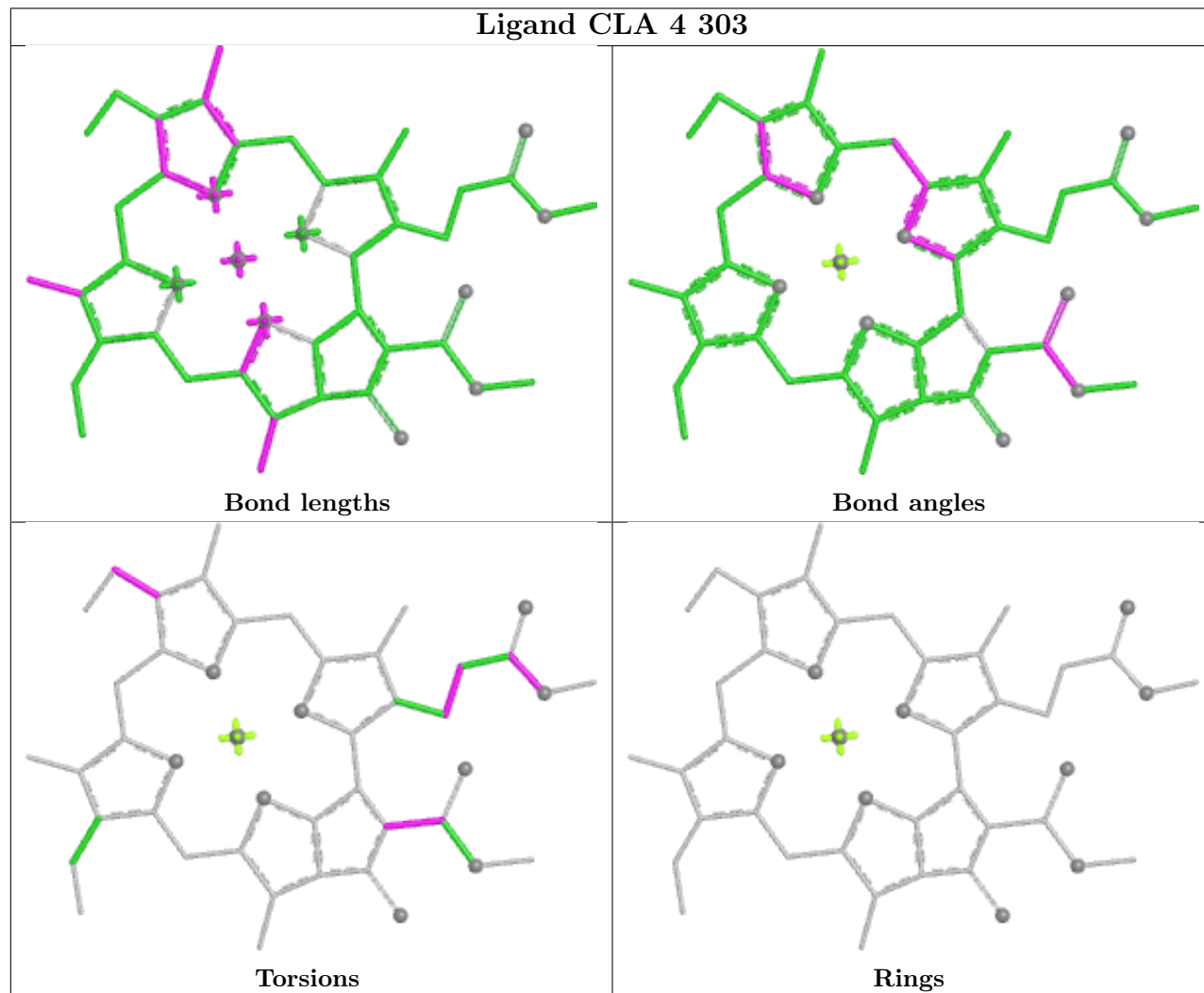
Ligand CLA A 805



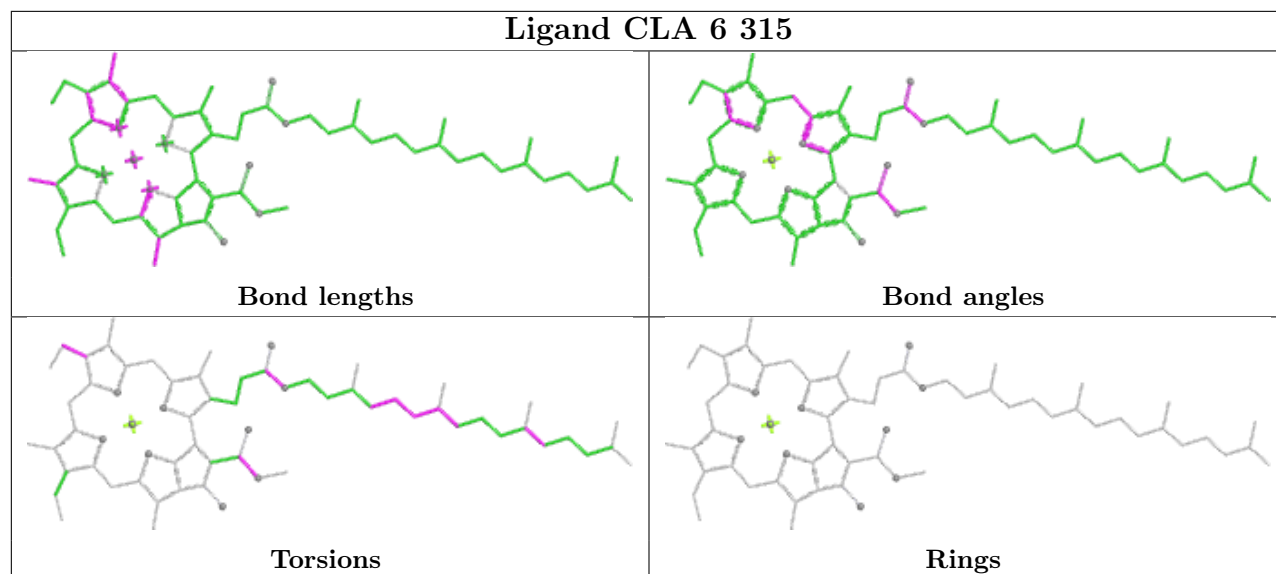
Ligand CLA B 840



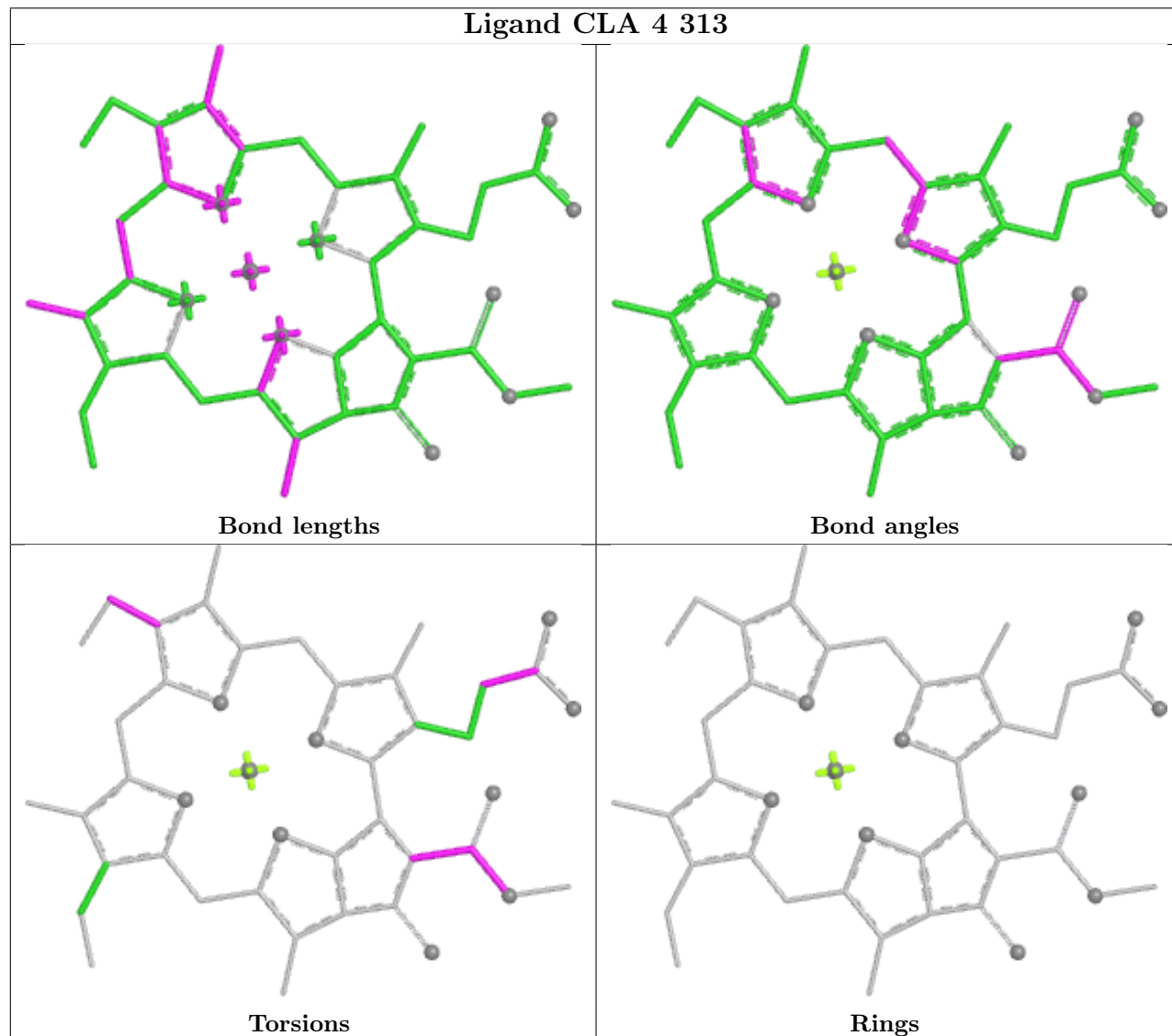
Ligand CLA 4 303

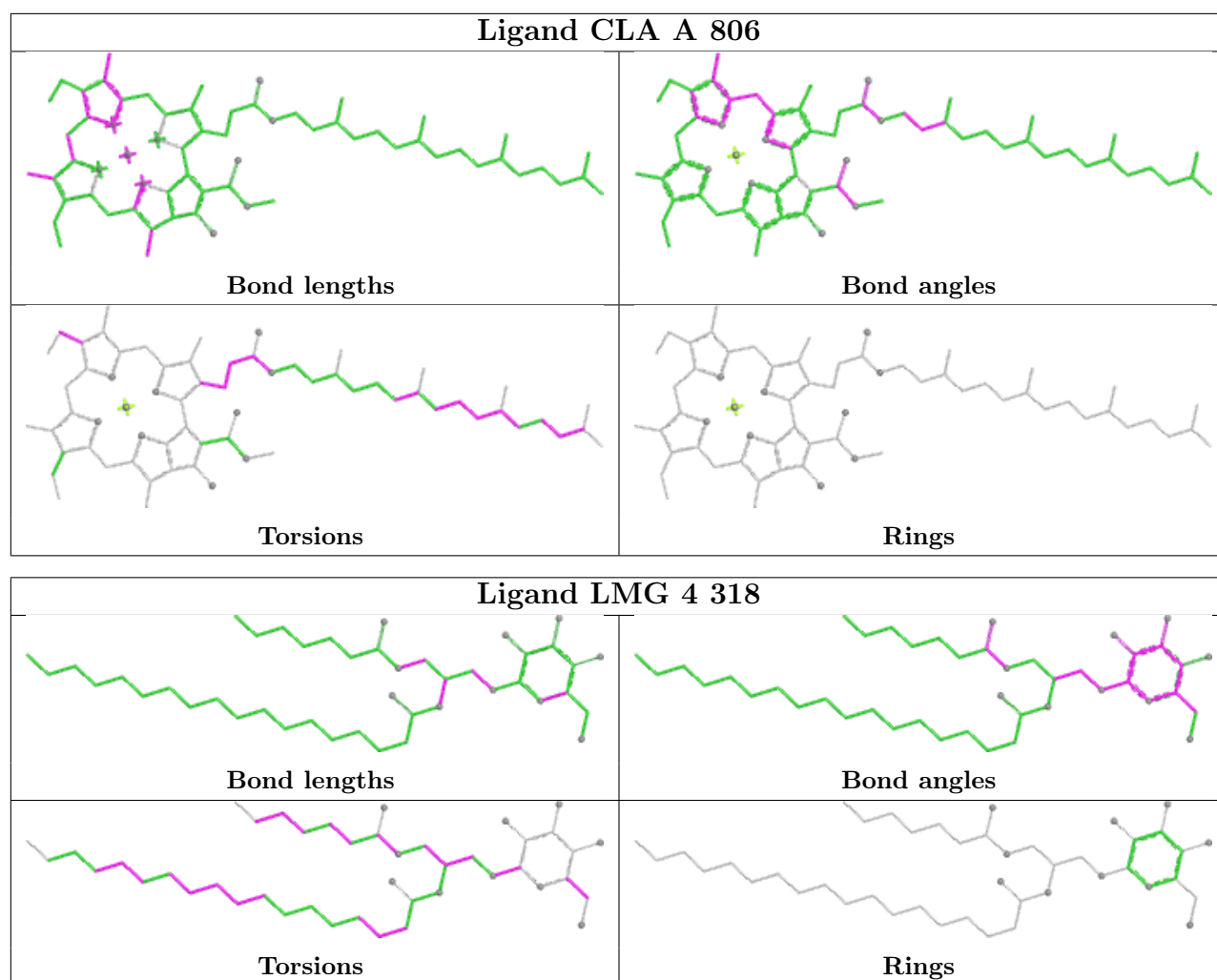


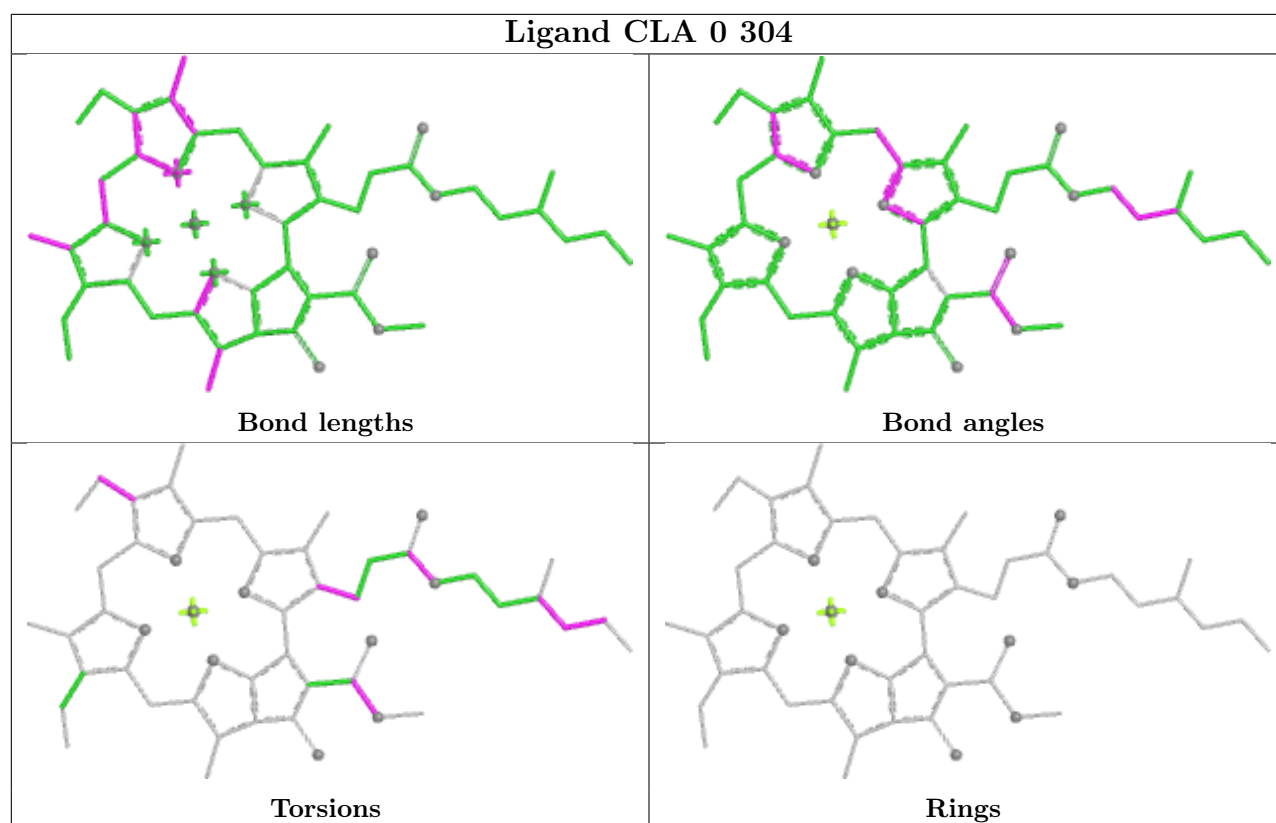
Ligand CLA 6 315

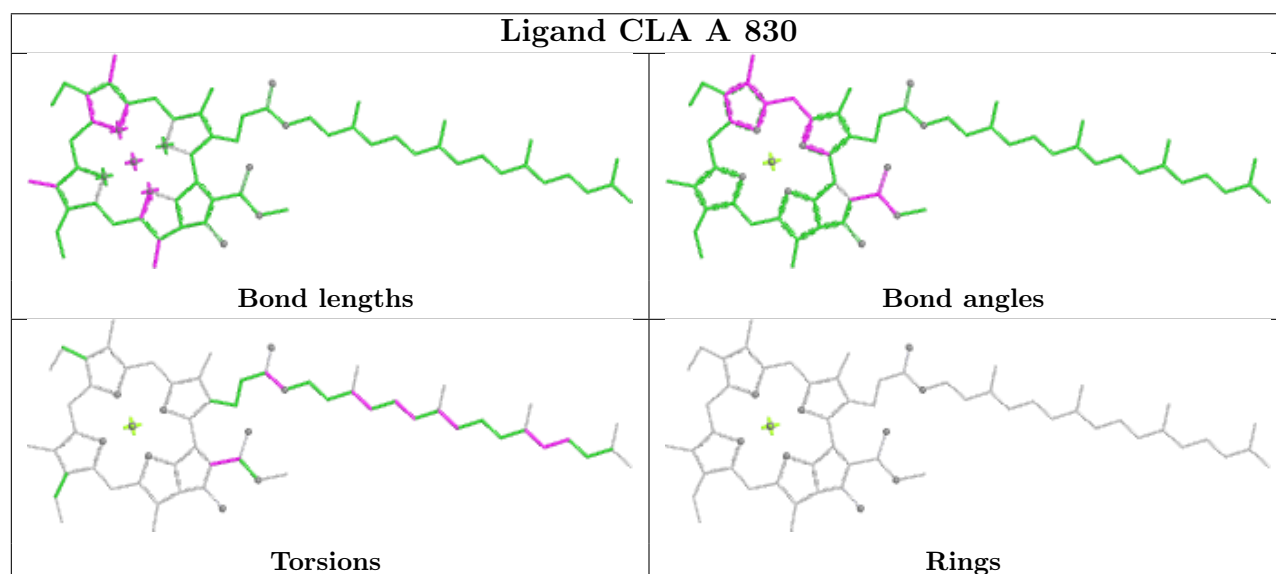
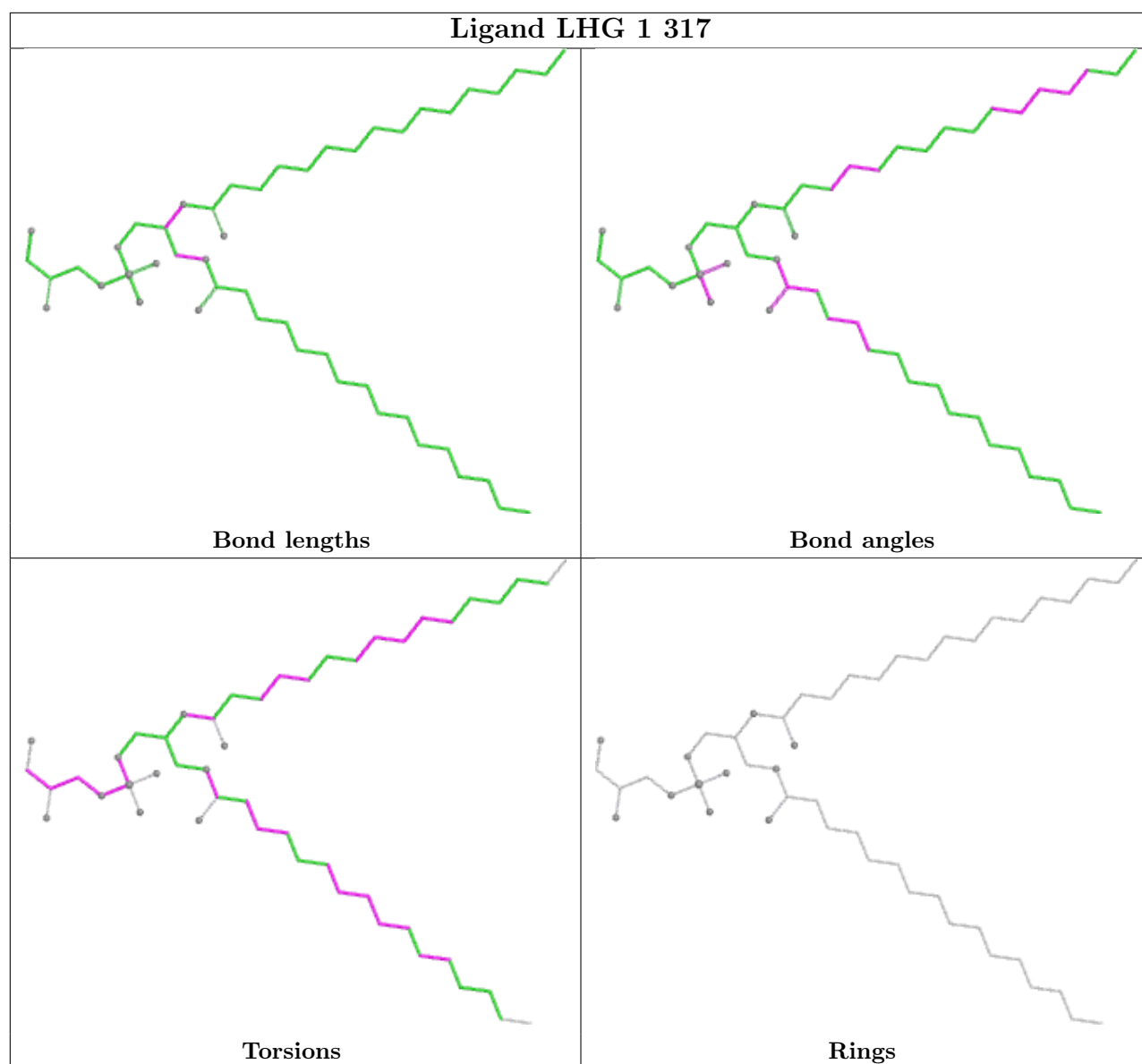


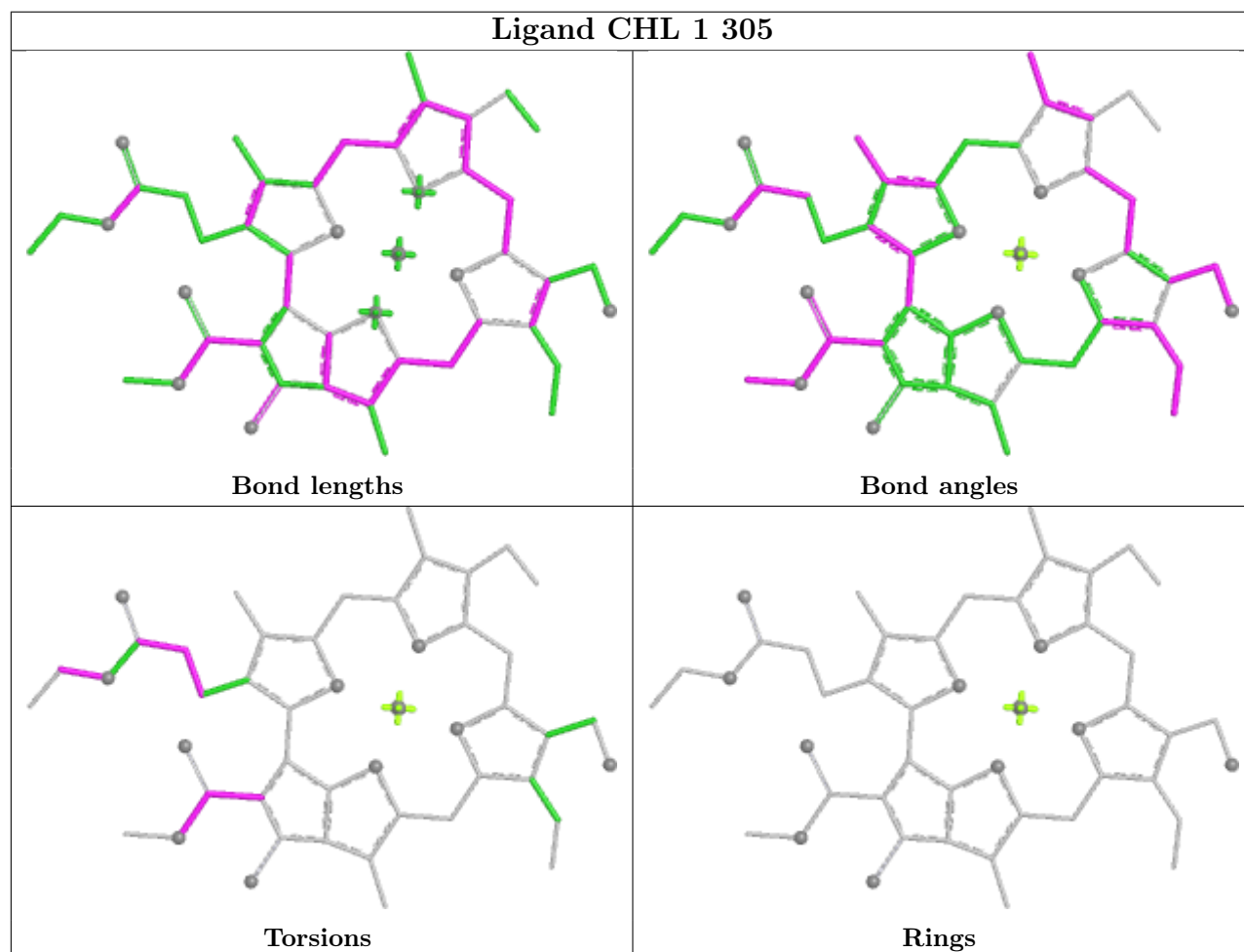
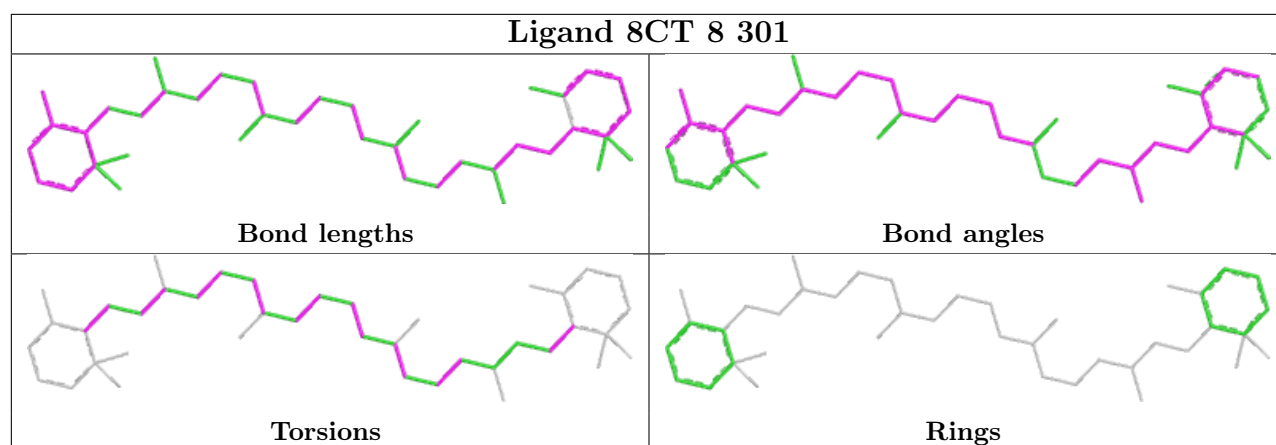
Ligand CLA 4 313

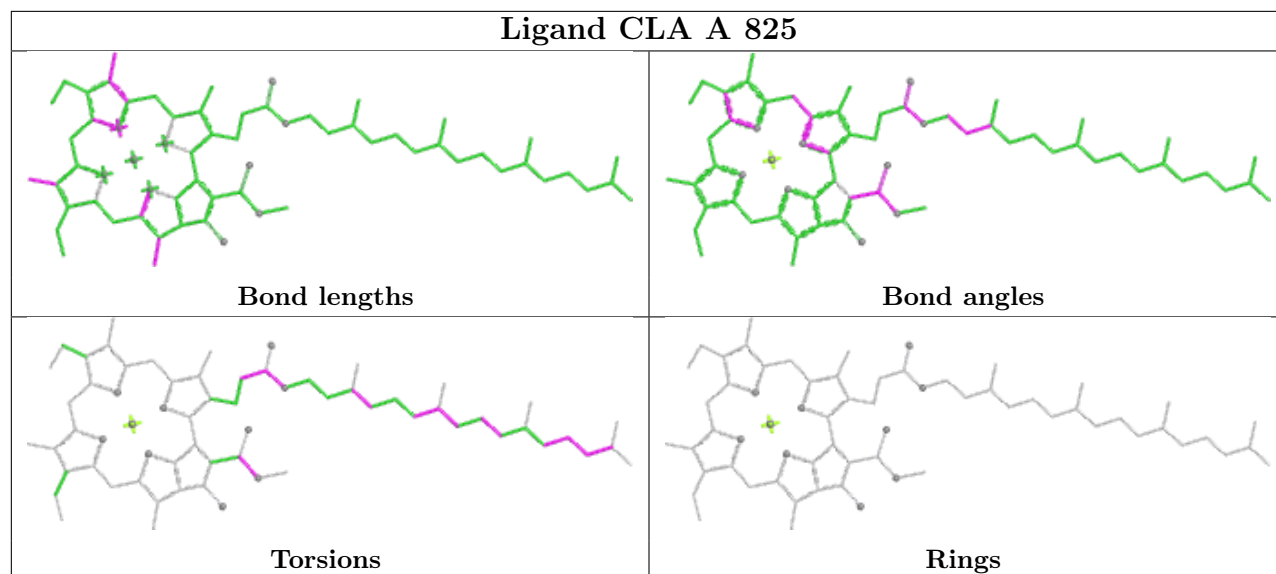
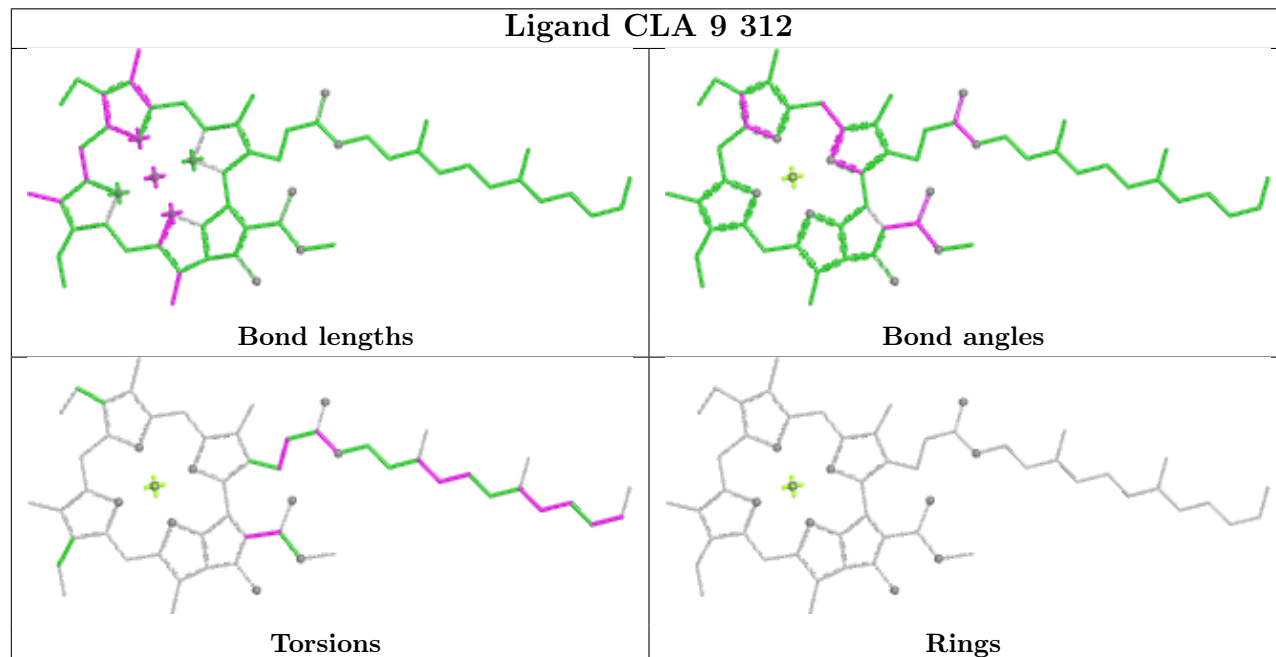




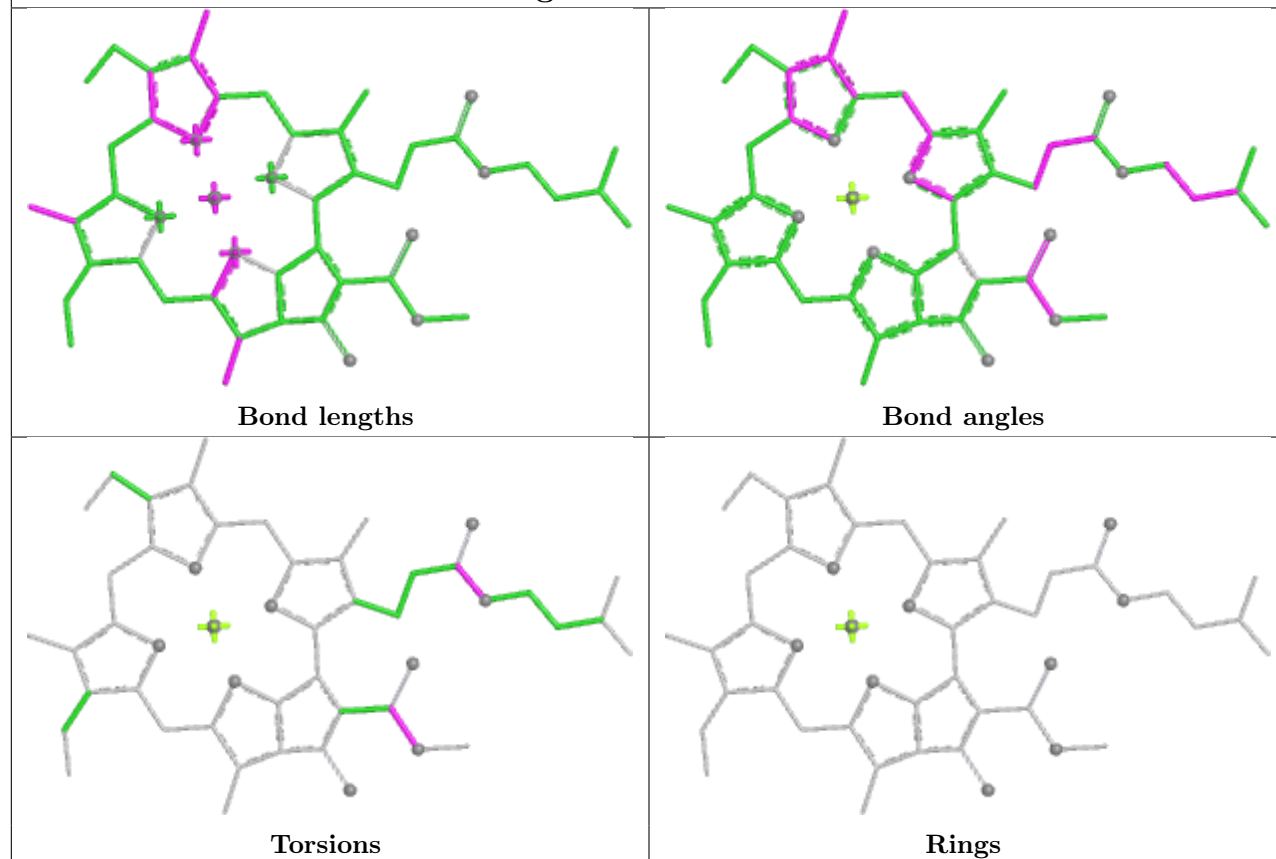




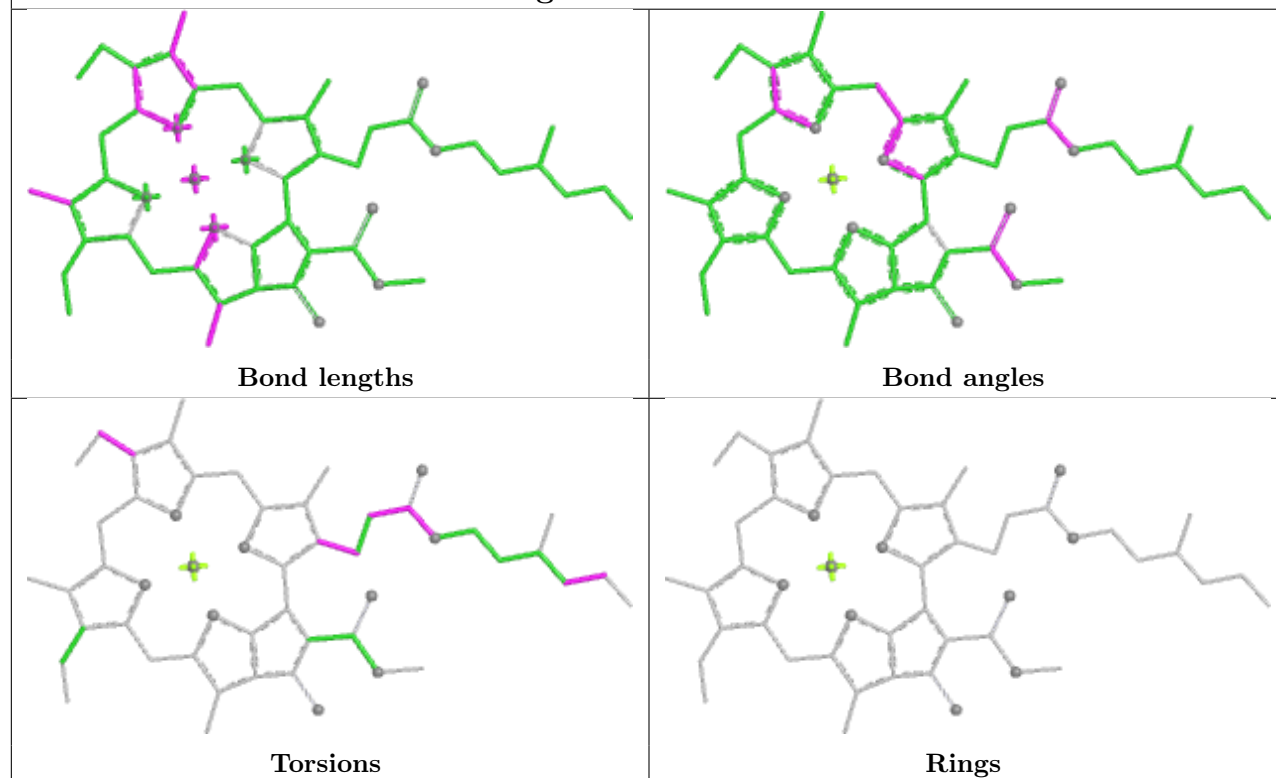


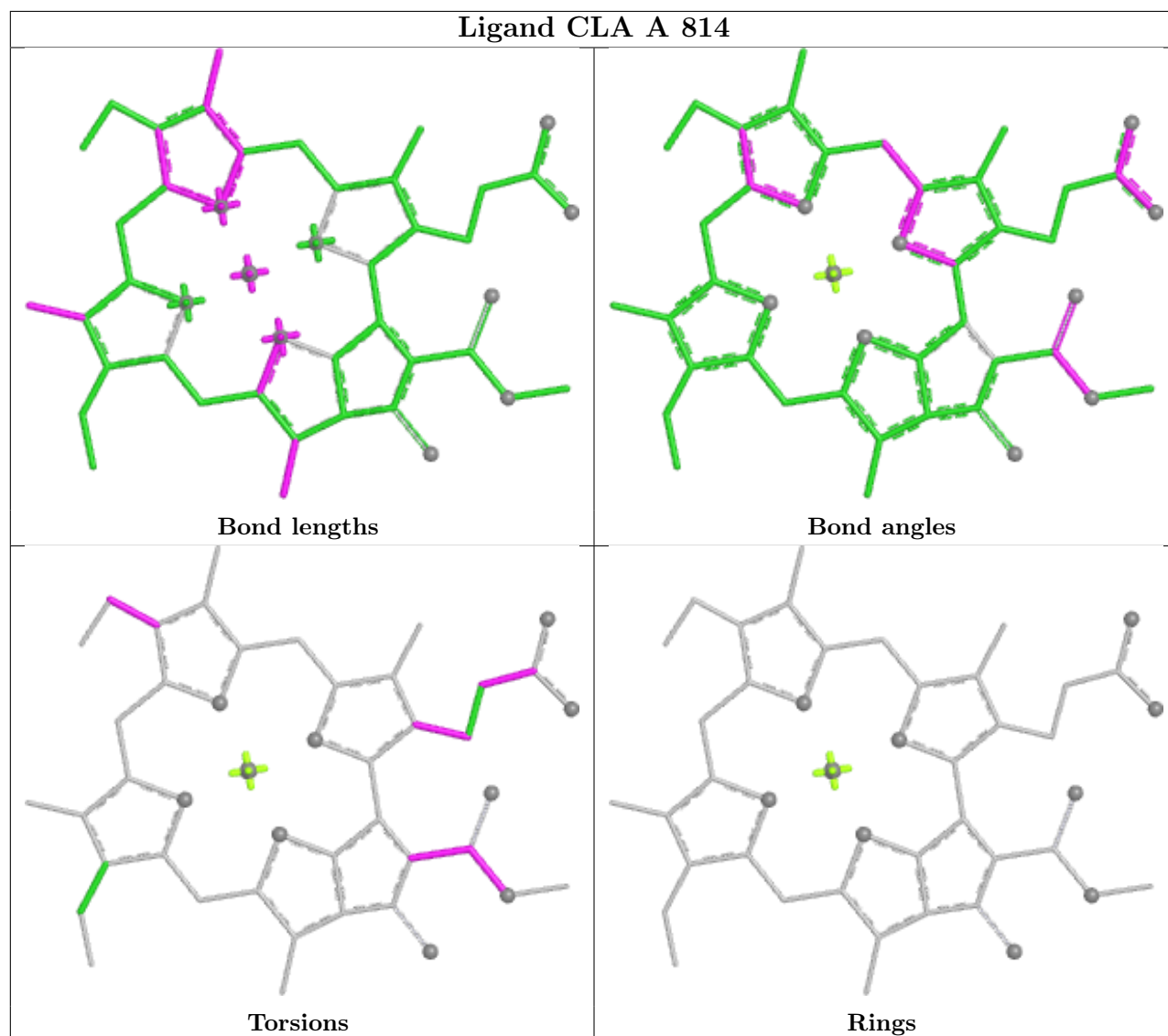
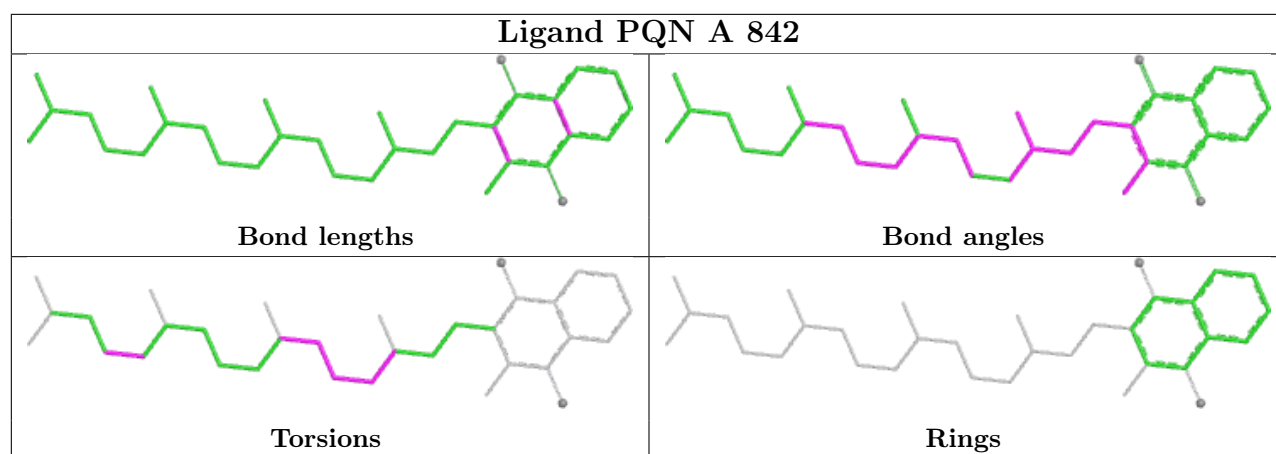
Ligand CLA A 825**Ligand CLA 9 312**

Ligand CLA 4 304

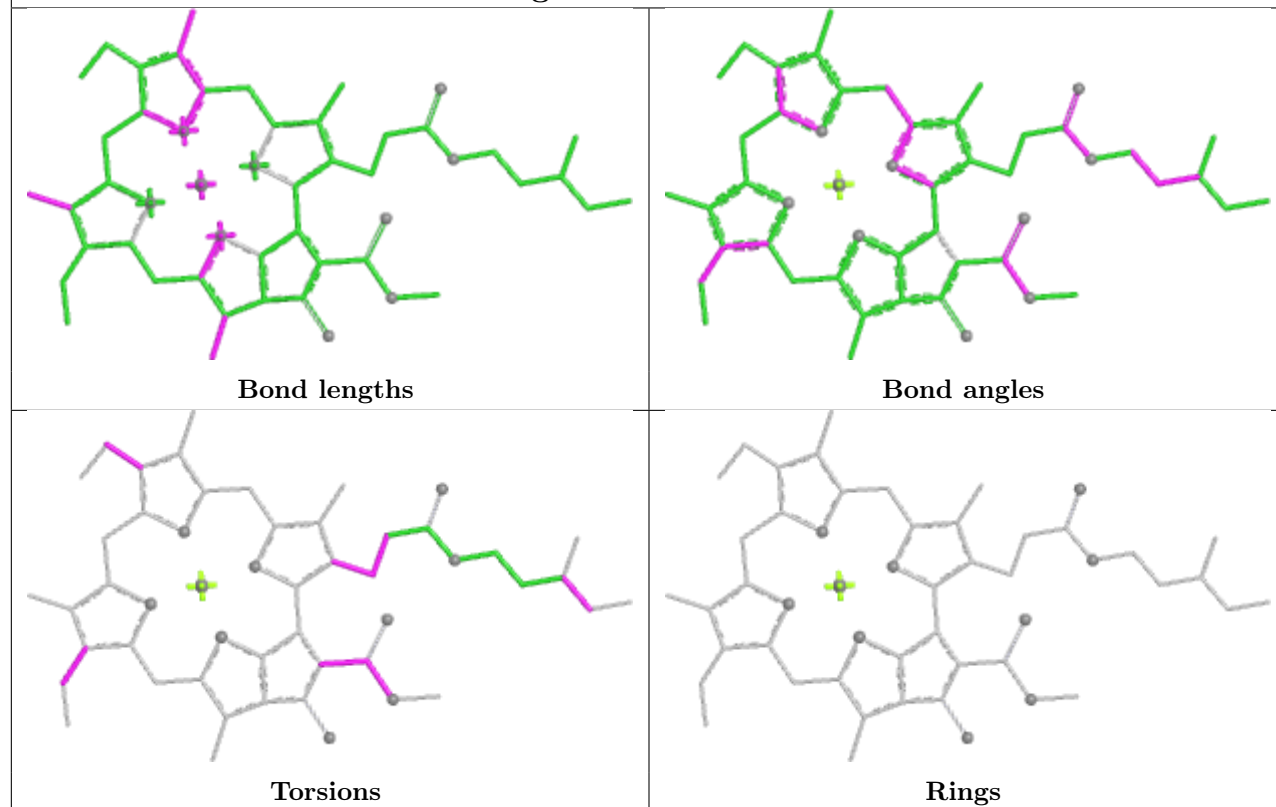


Ligand CLA 1 310

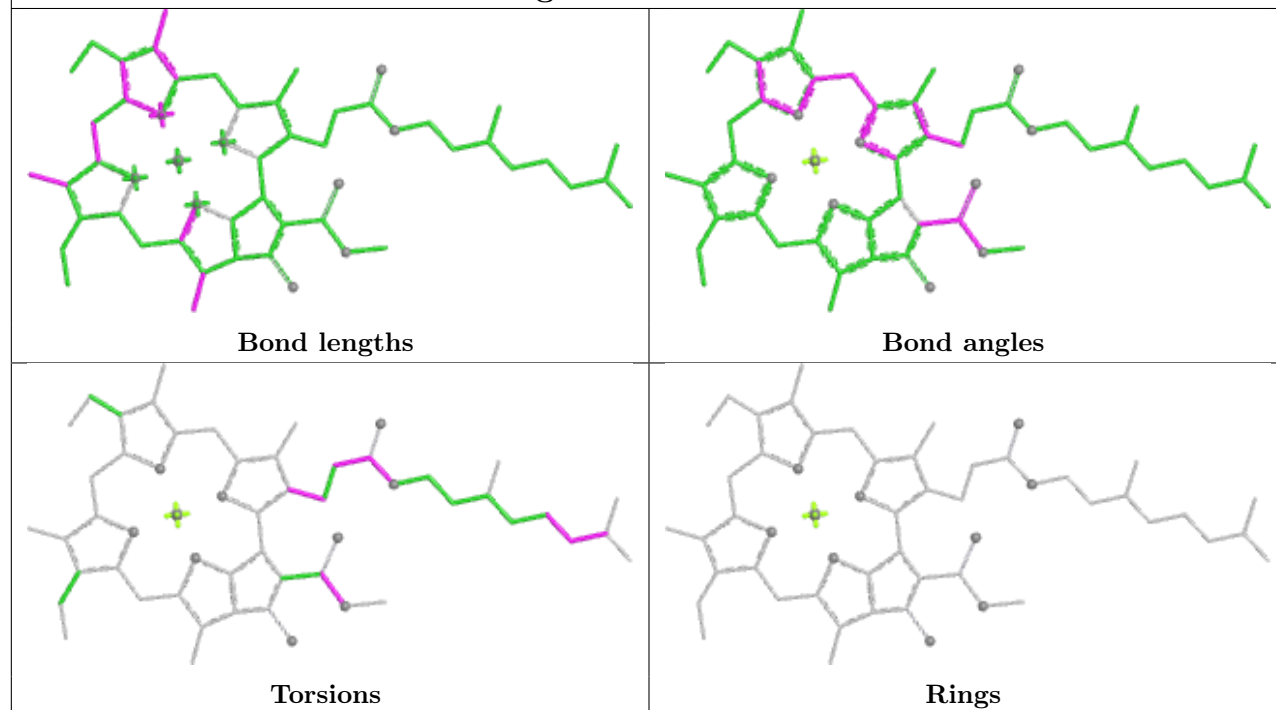




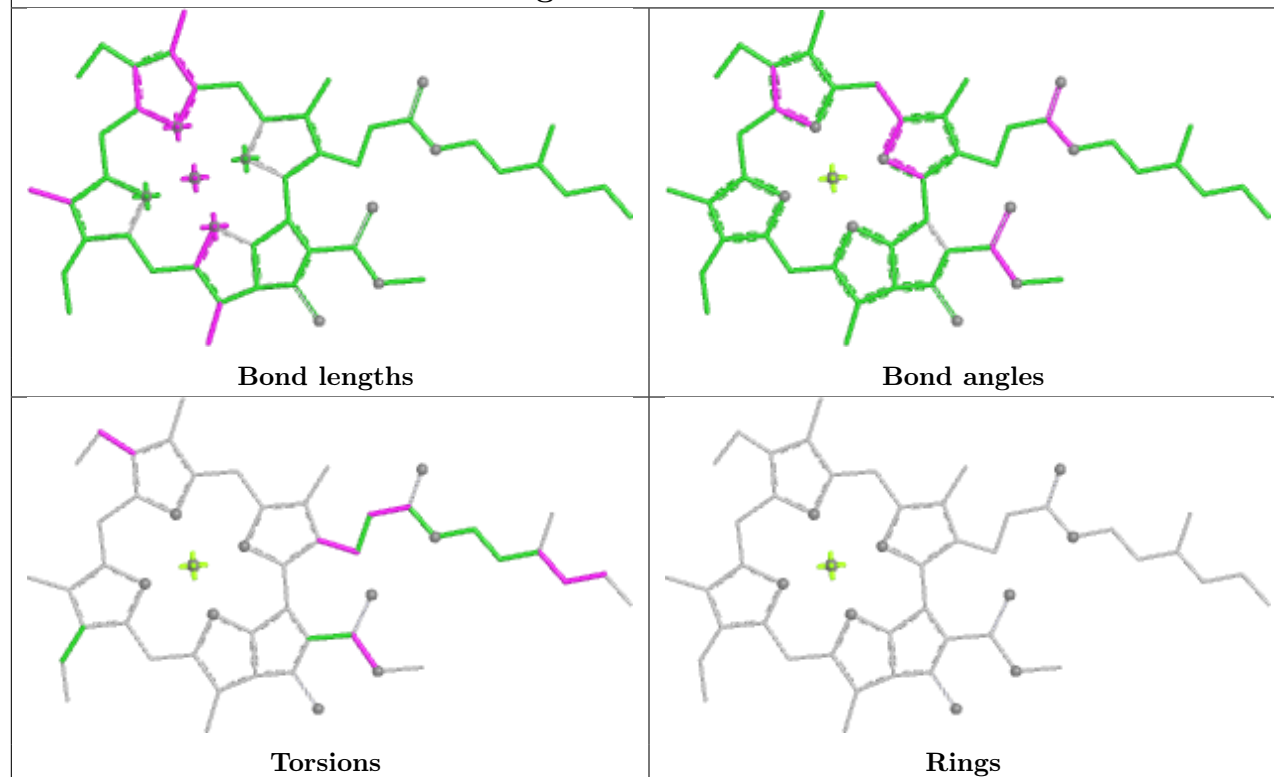
Ligand CLA A 836



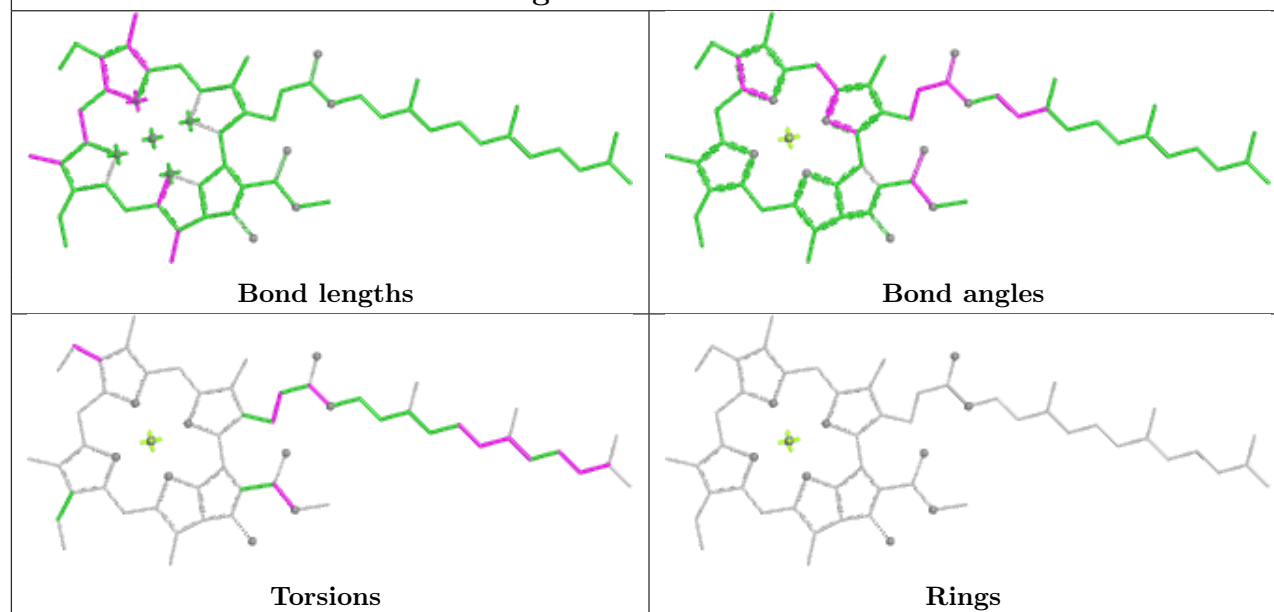
Ligand CLA 0 312

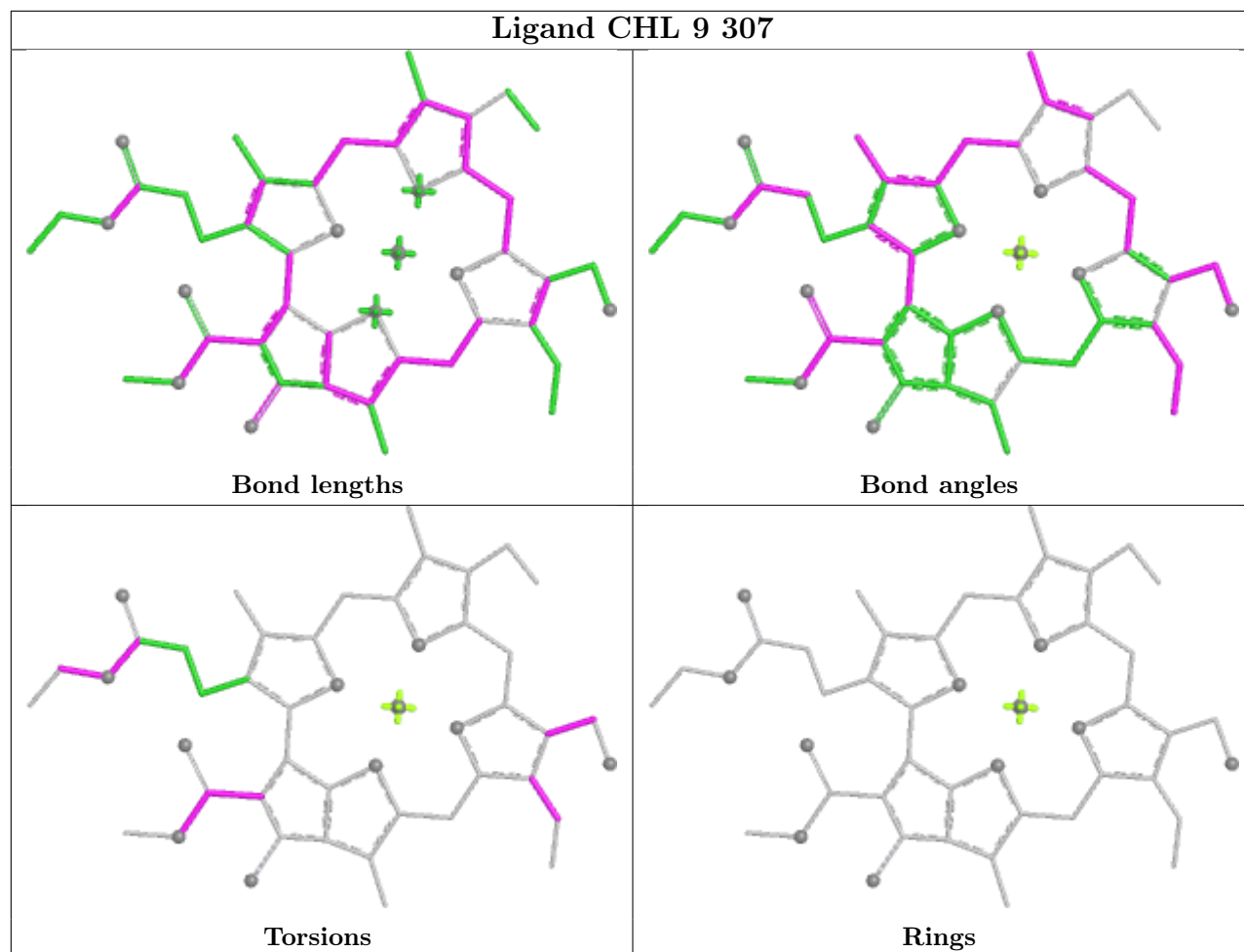


Ligand CLA 6 312

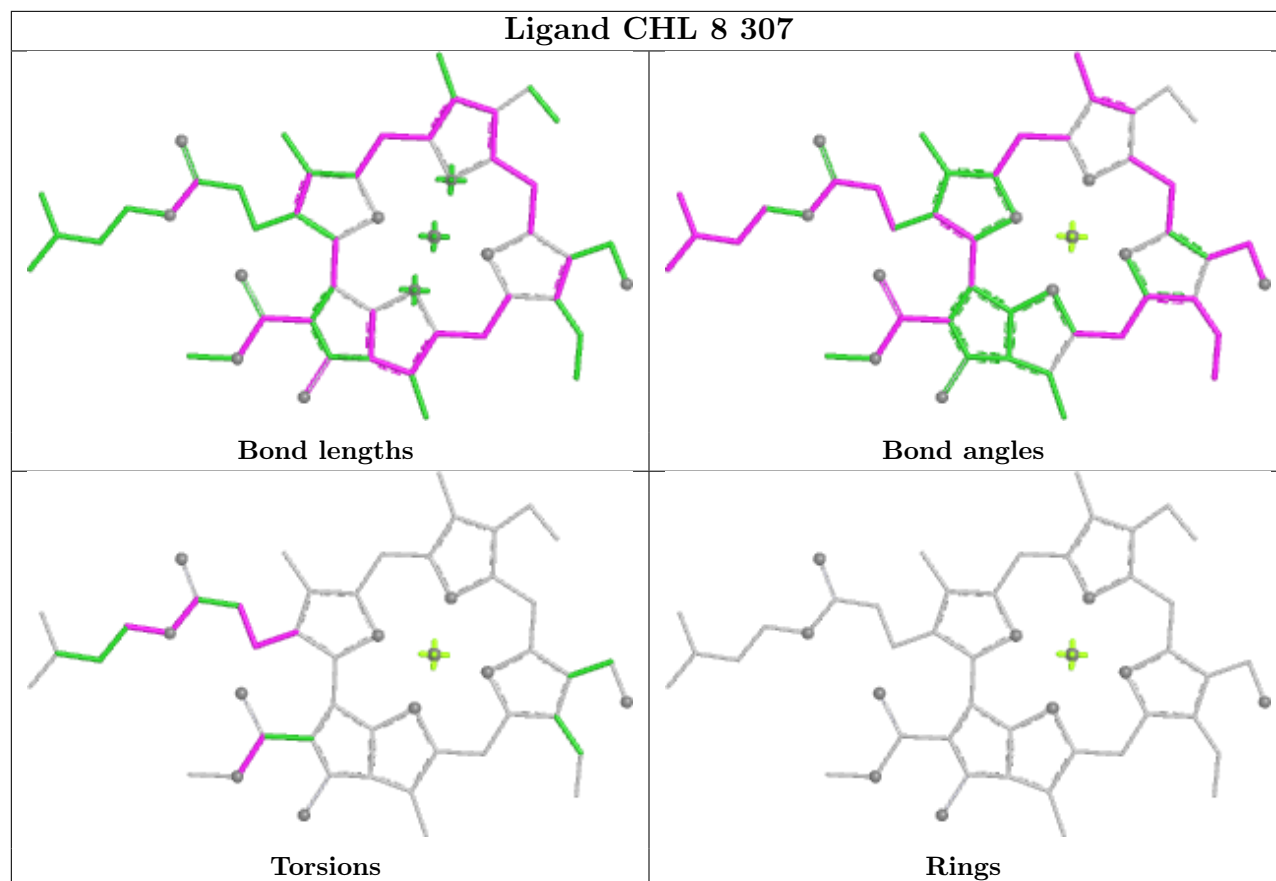


Ligand CLA B 824

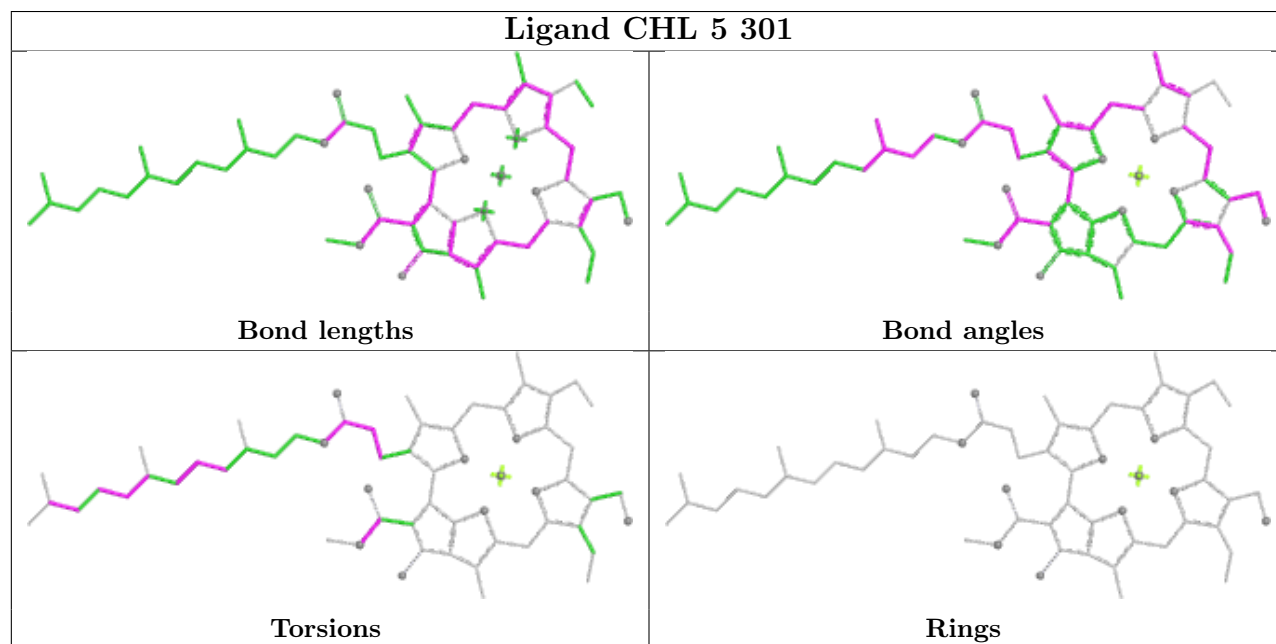




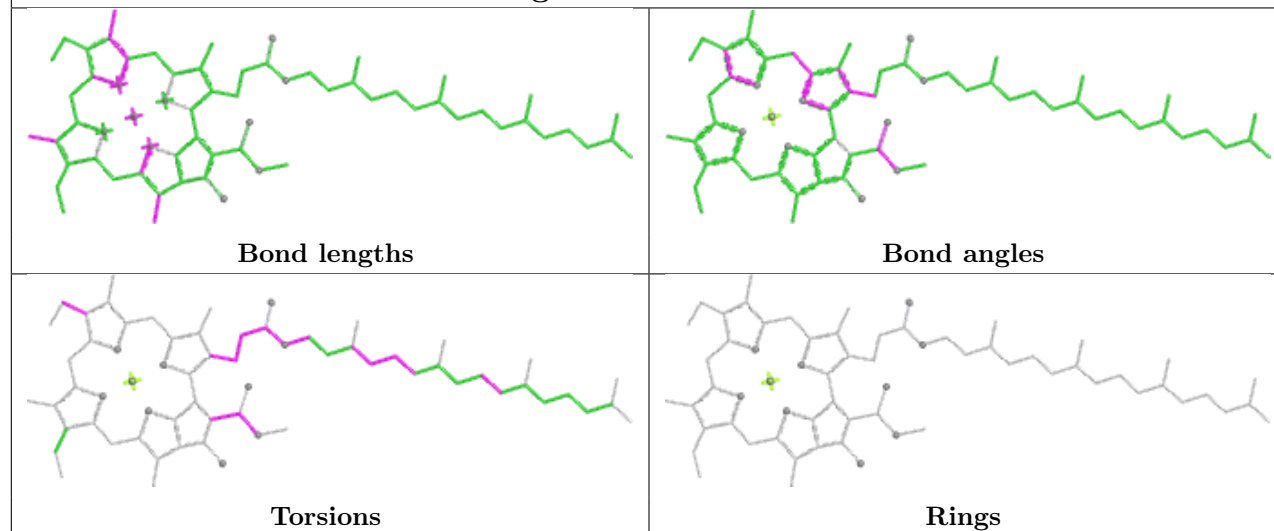
Ligand CHL 8 307



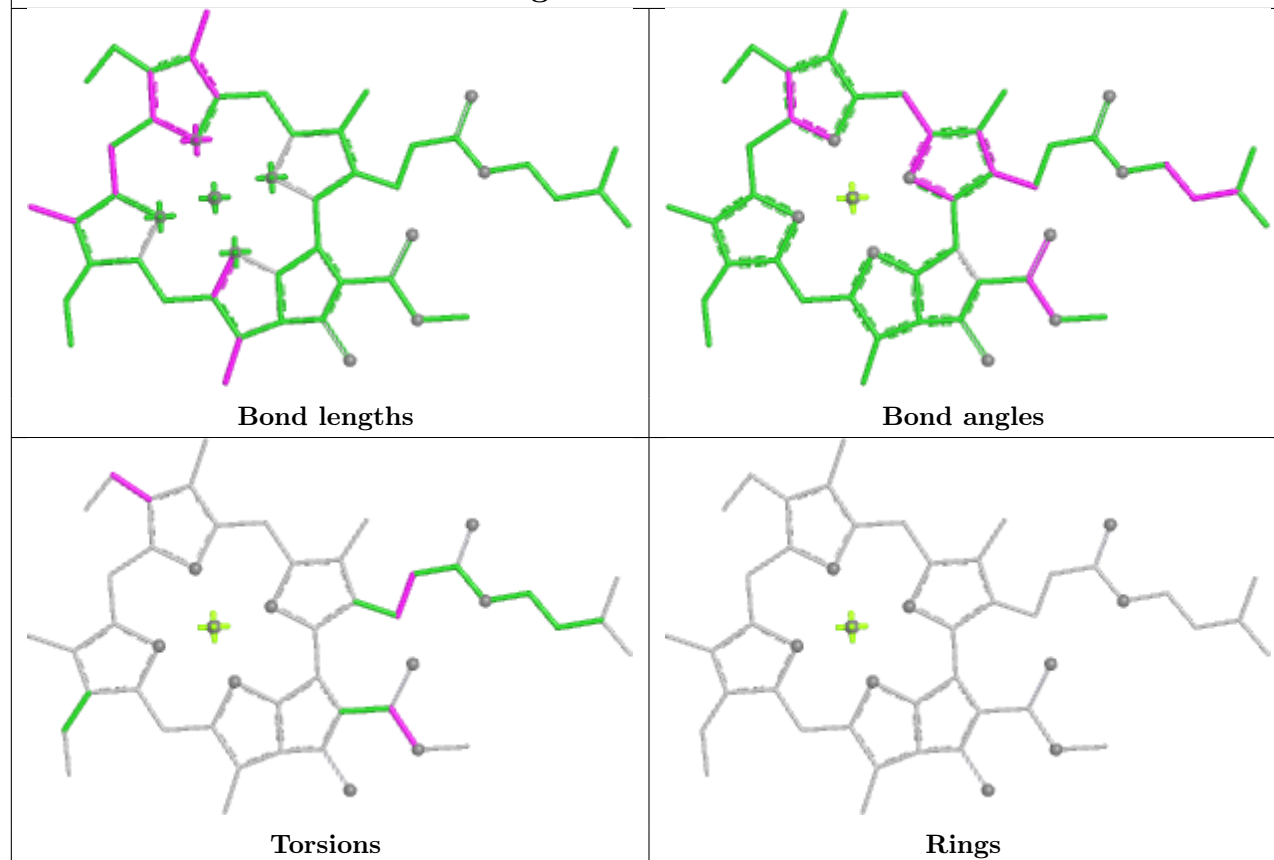
Ligand CHL 5 301



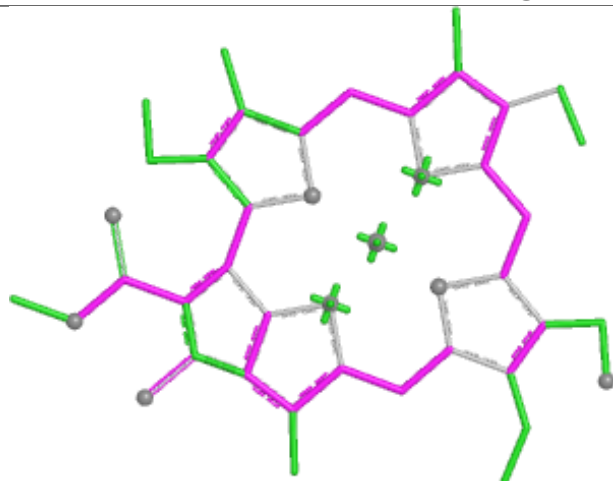
Ligand CLA A 832



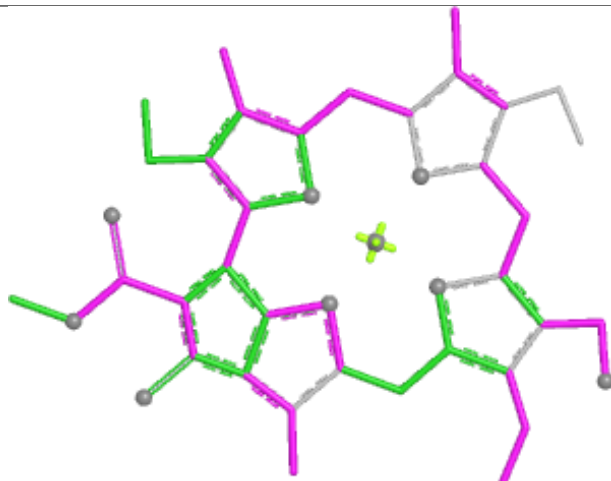
Ligand CLA G 102



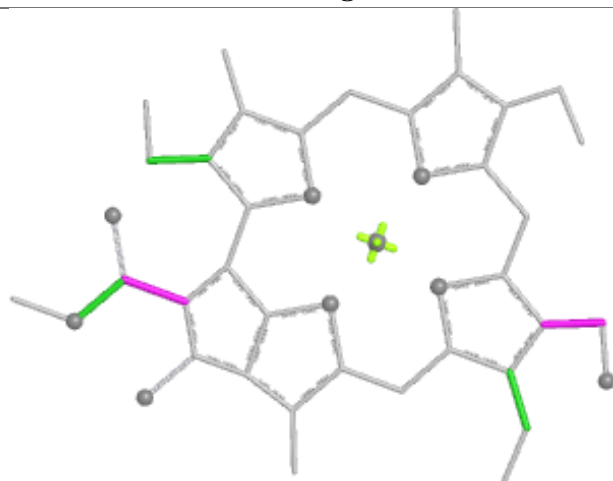
Ligand CHL 2 305



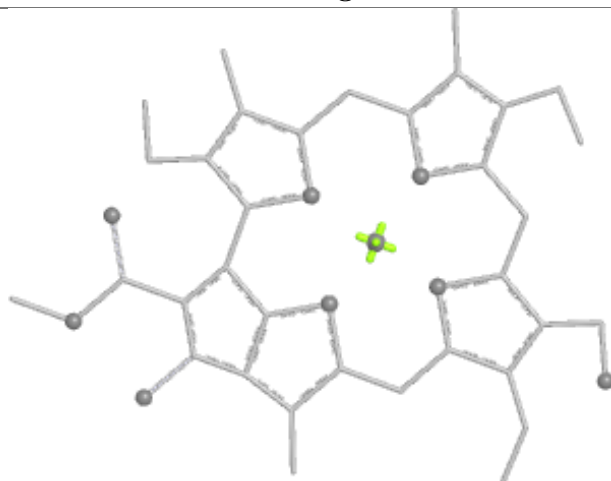
Bond lengths



Bond angles

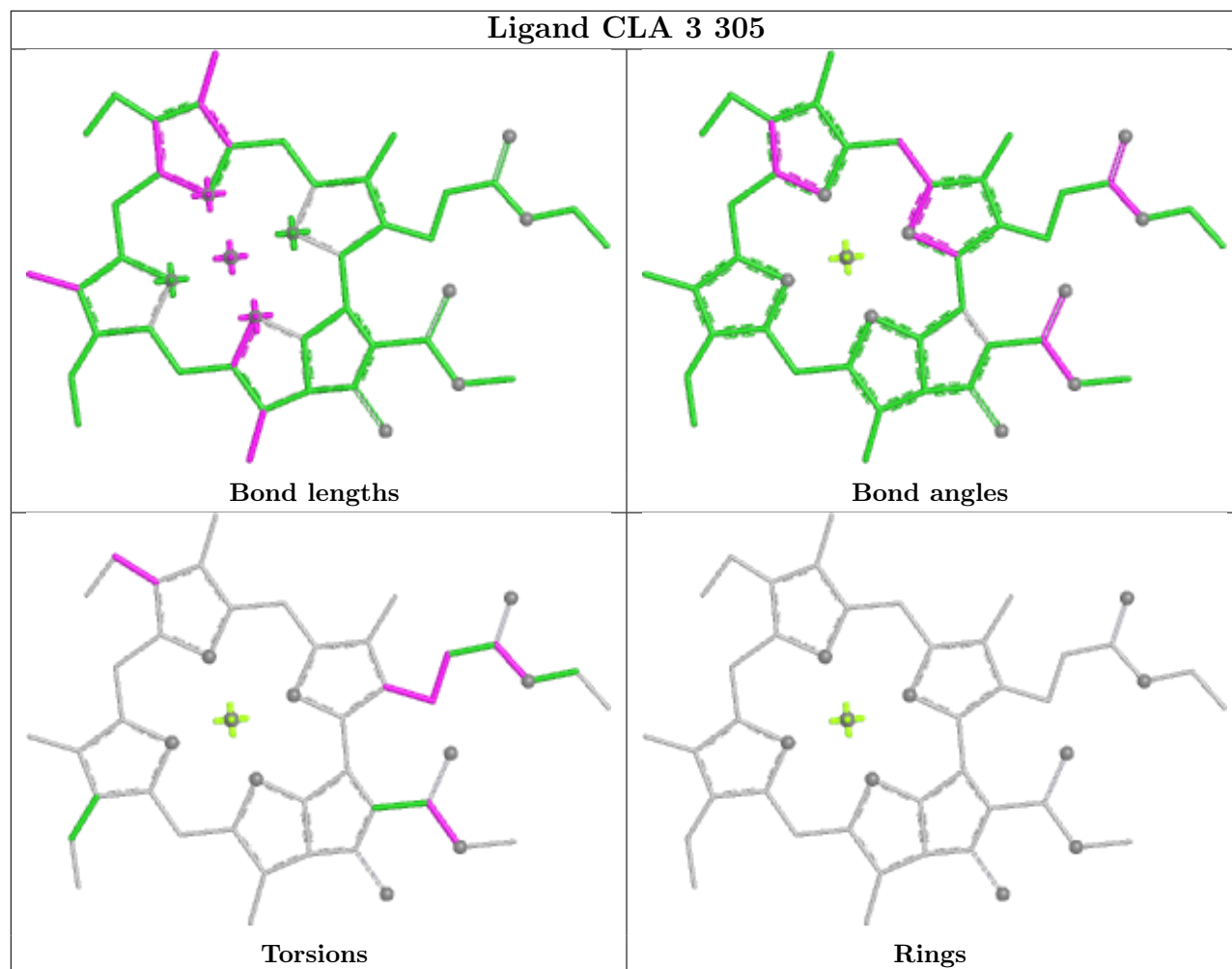


Torsions

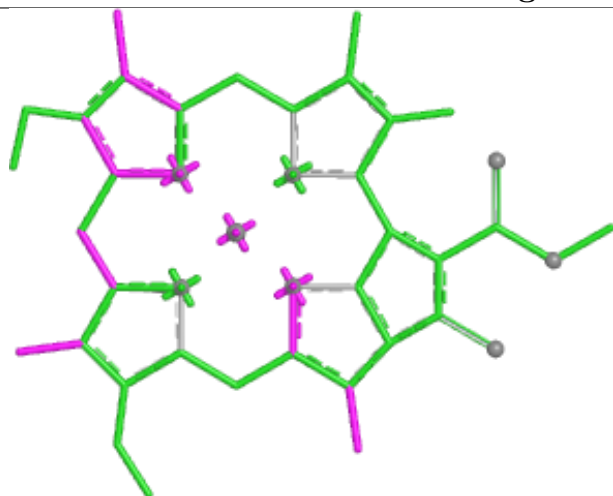


Rings

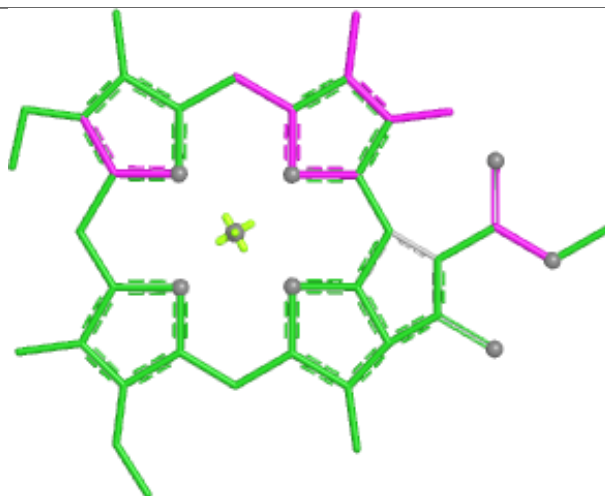
Ligand CLA 3 305



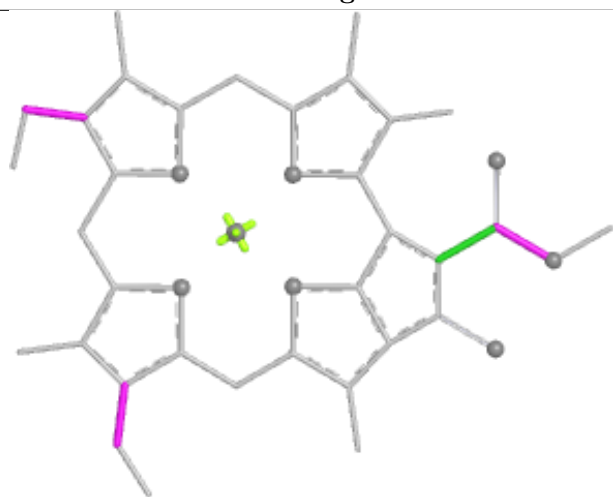
Ligand CLA 2 310



Bond lengths



Bond angles

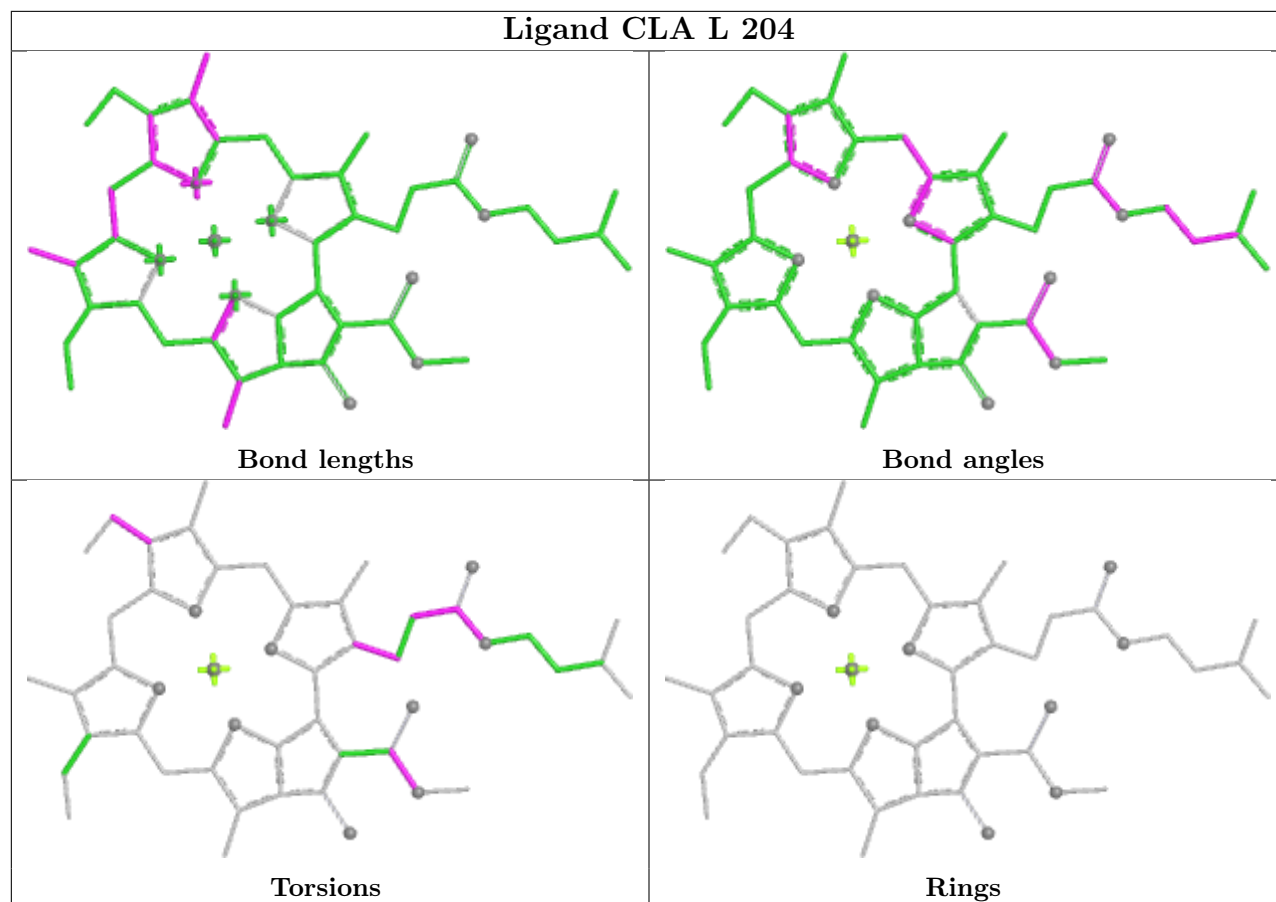


Torsions

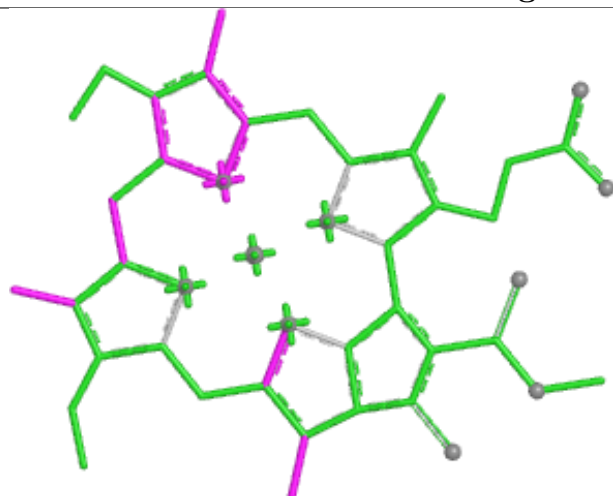


Rings

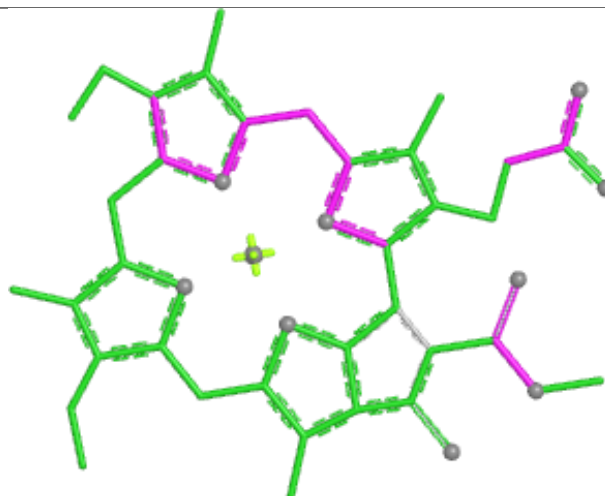
Ligand CLA L 204



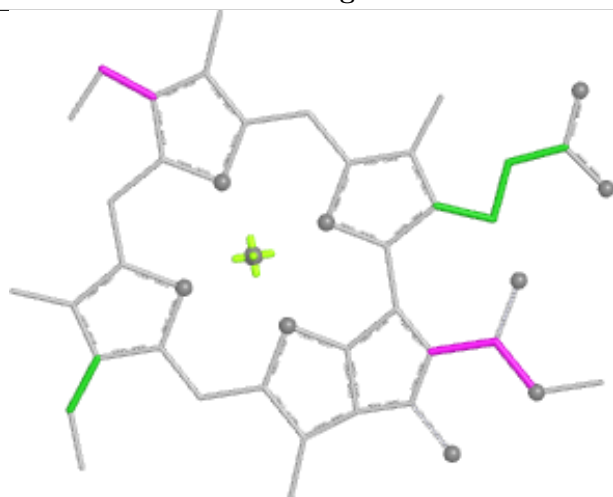
Ligand CLA 3 303



Bond lengths



Bond angles

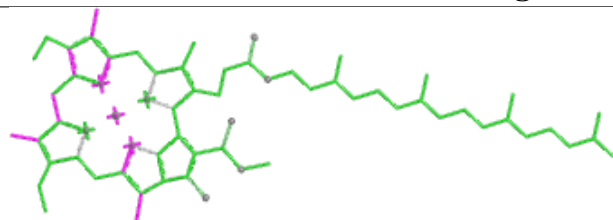


Torsions

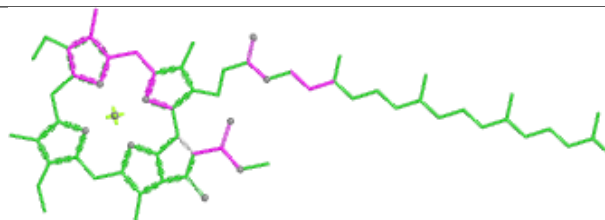


Rings

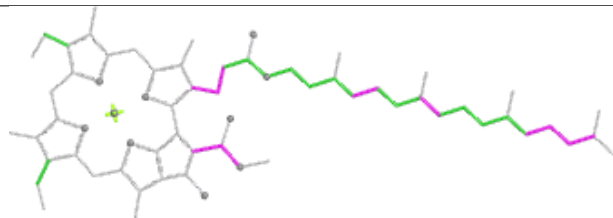
Ligand CLA A 813



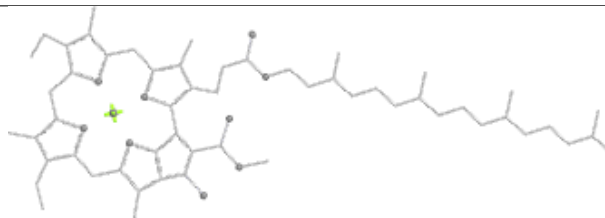
Bond lengths



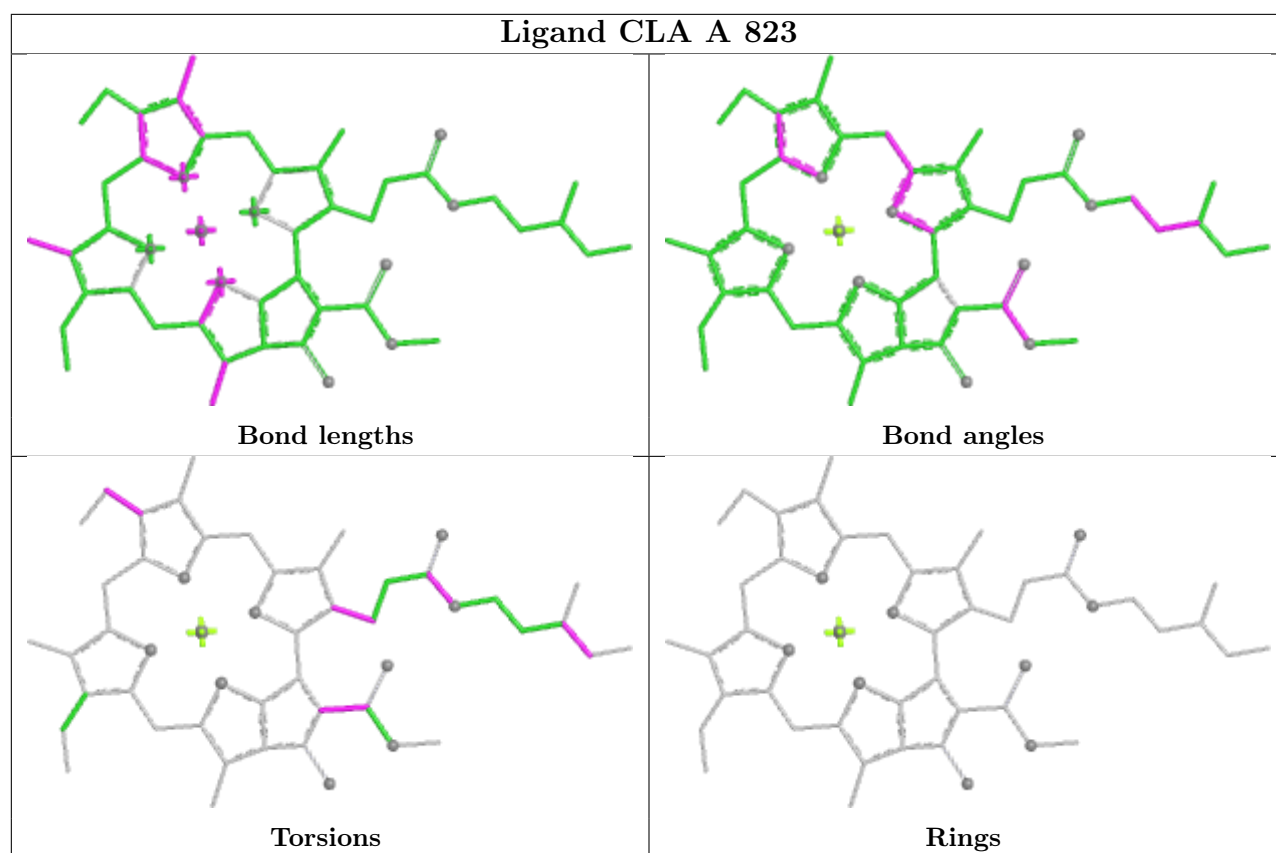
Bond angles



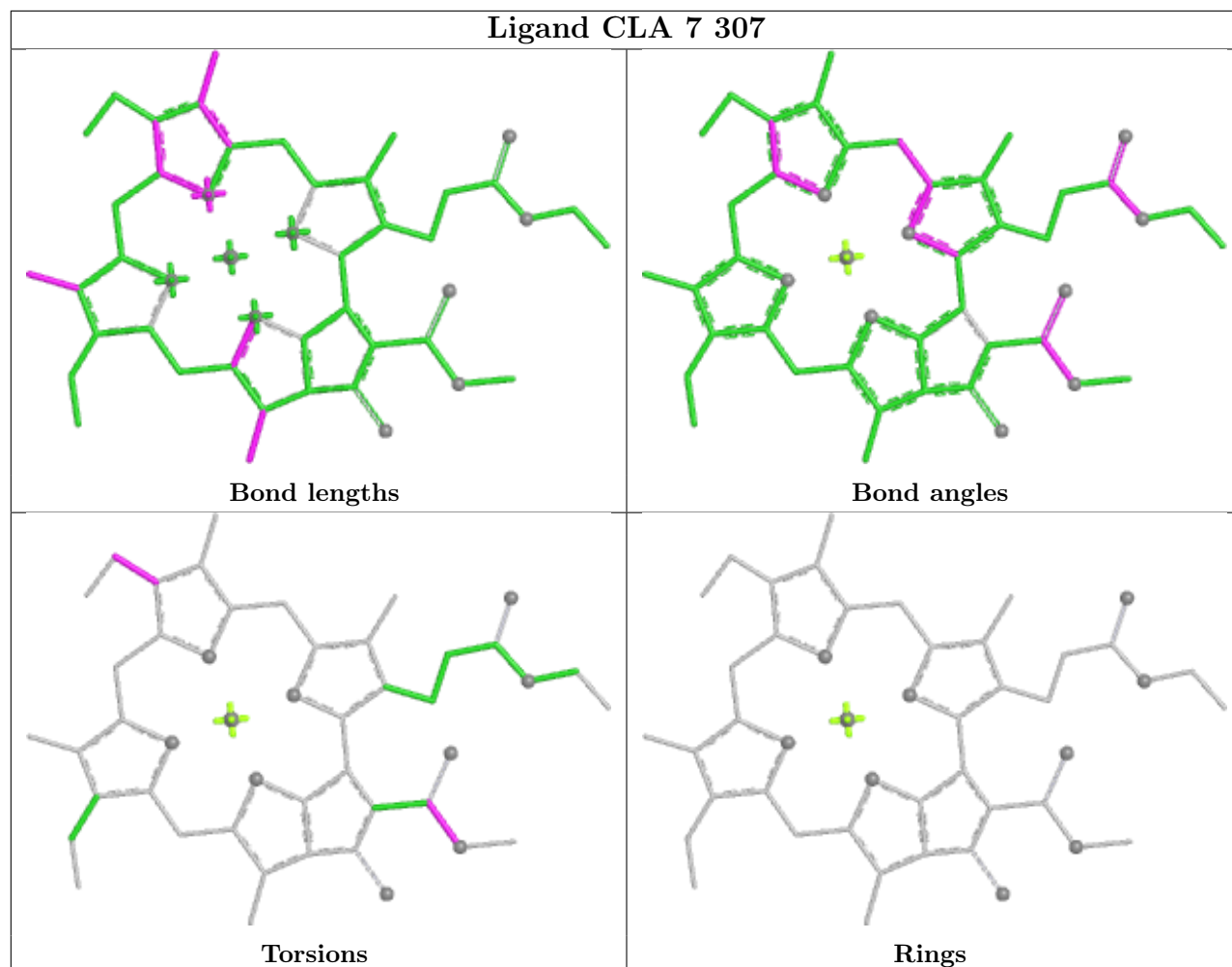
Torsions



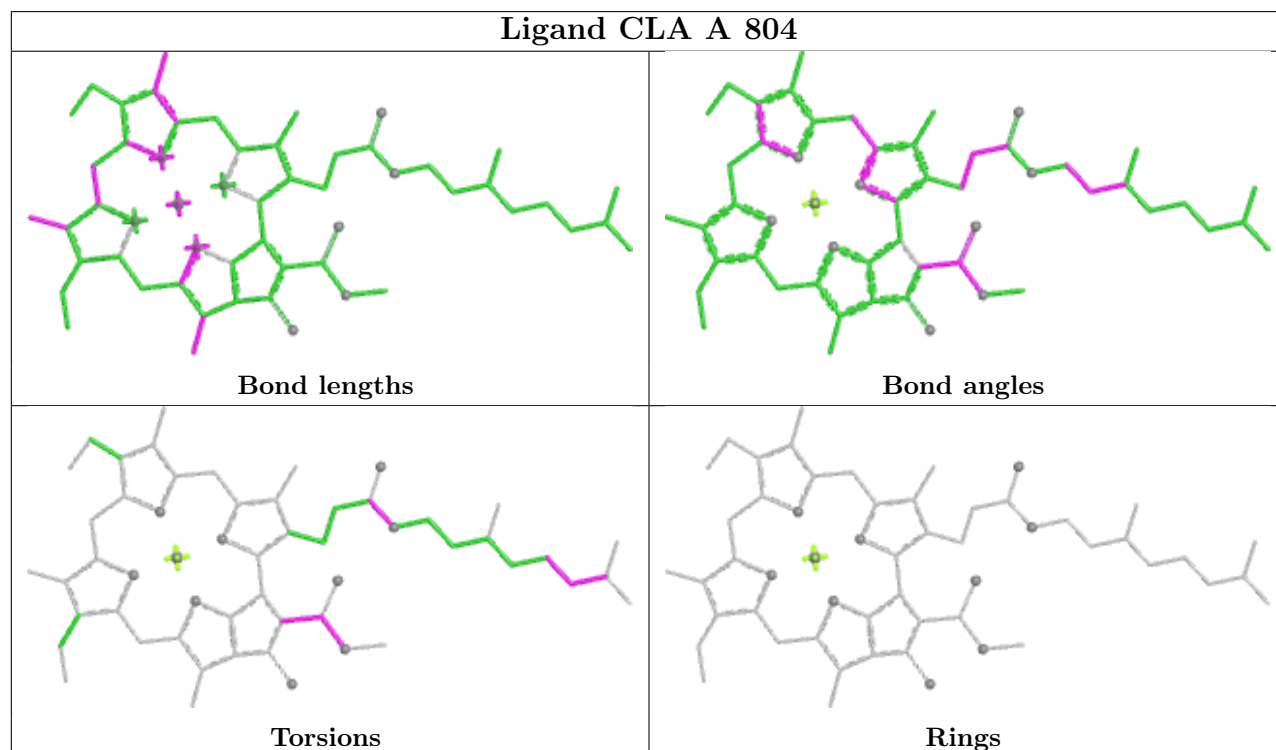
Rings

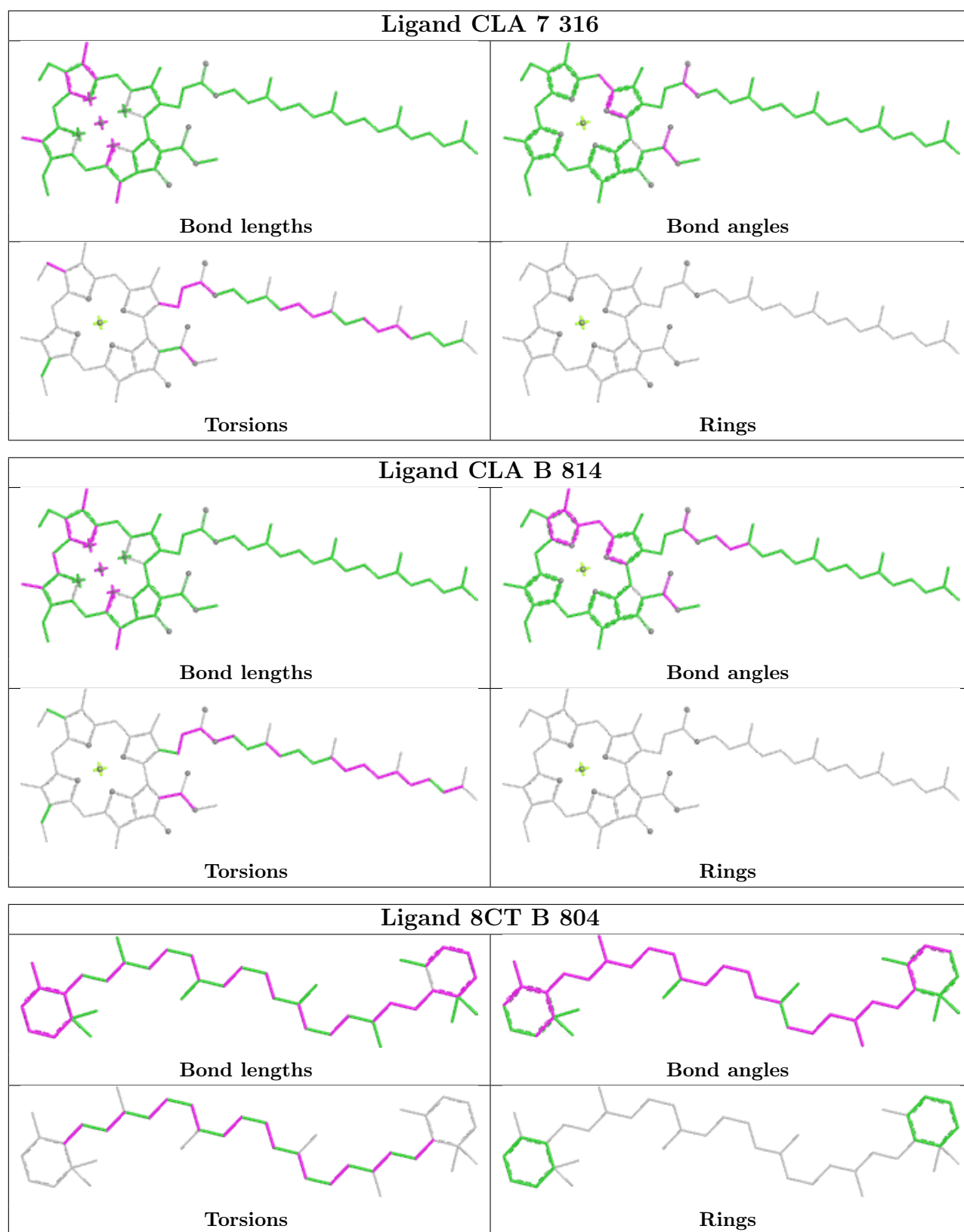


Ligand CLA 7 307

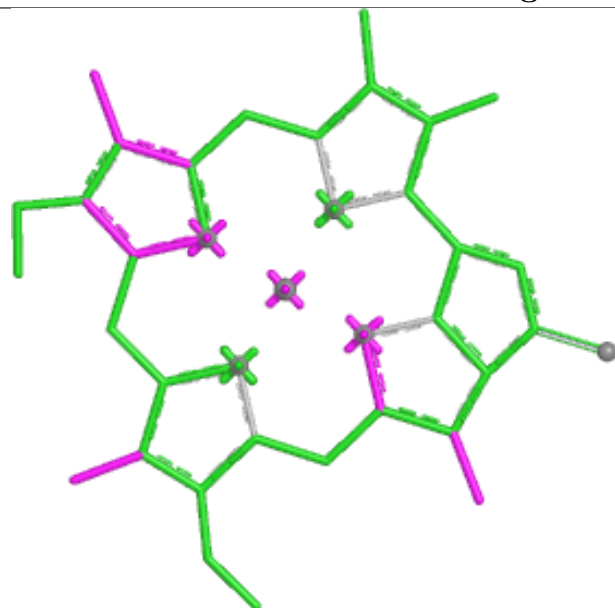


Ligand CLA A 804

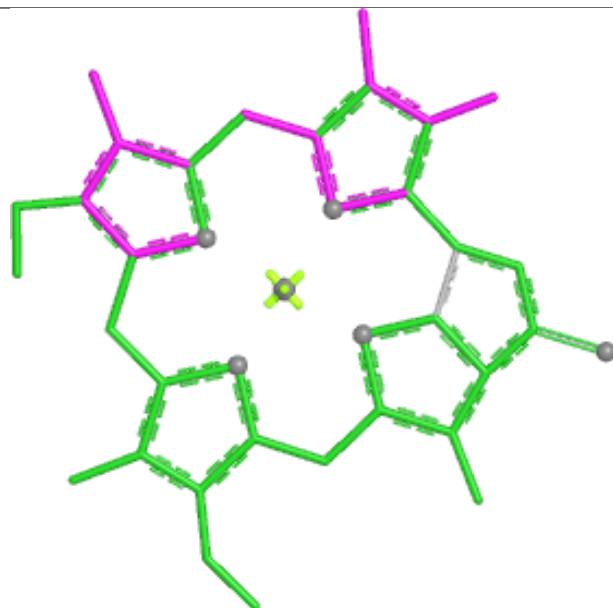




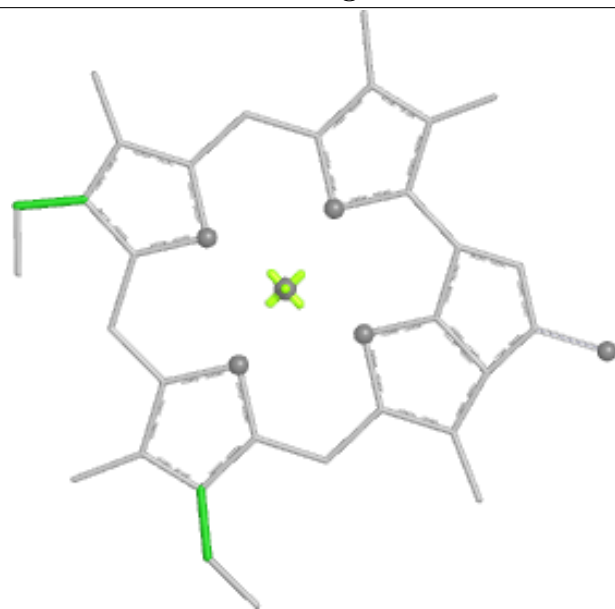
Ligand CLA 3 309



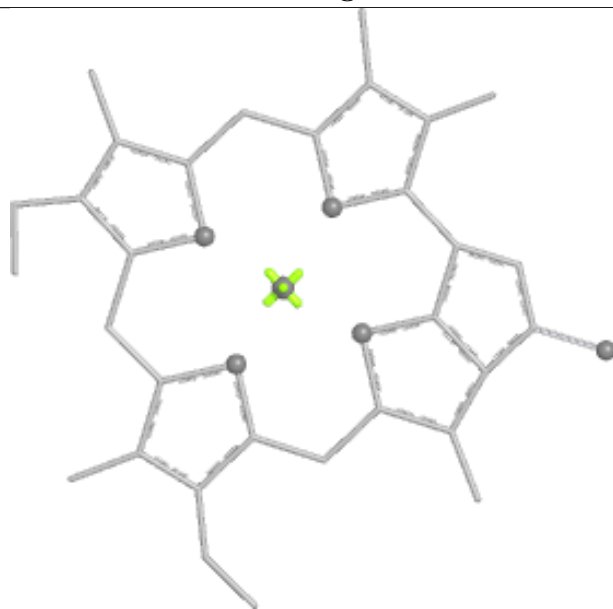
Bond lengths



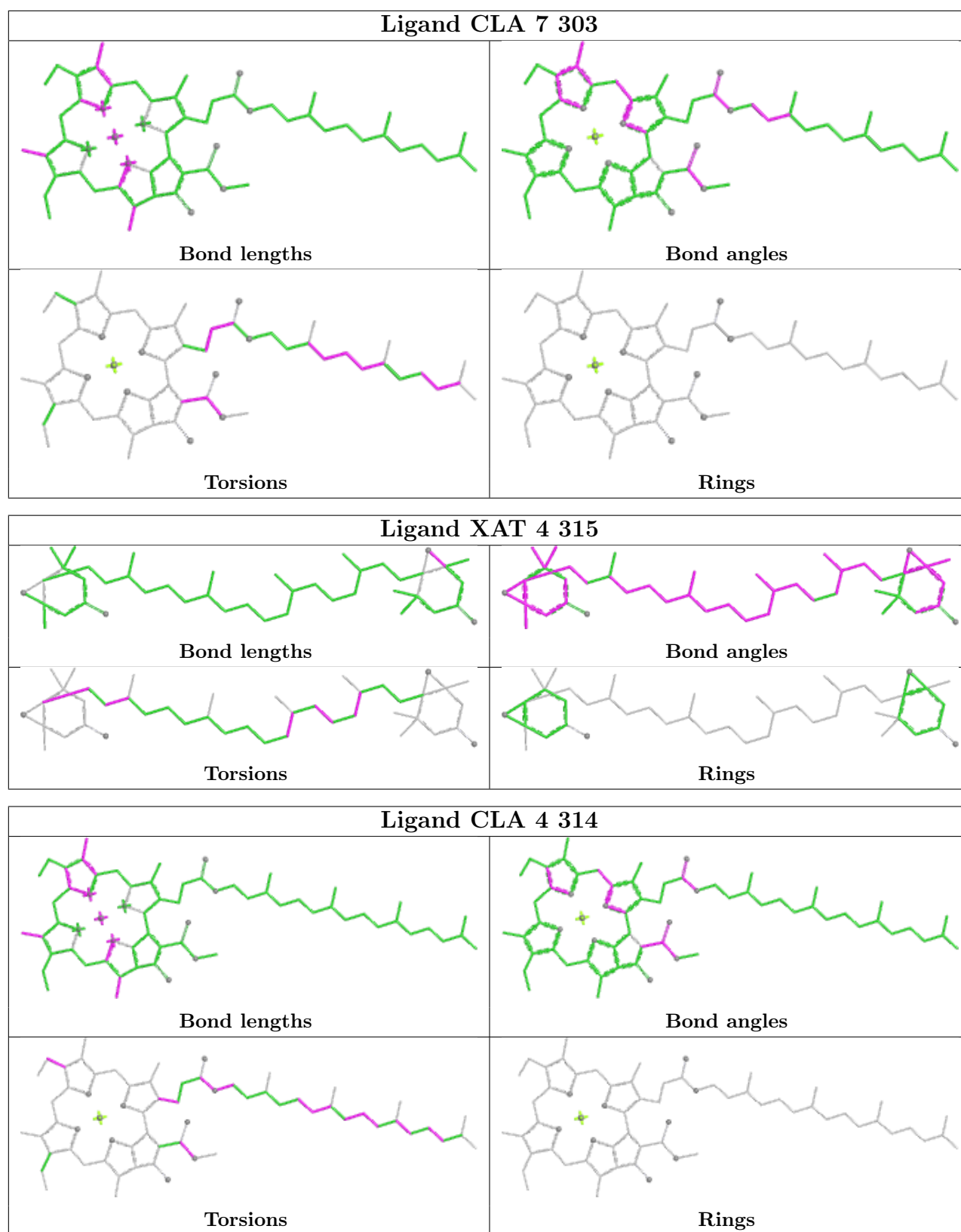
Bond angles

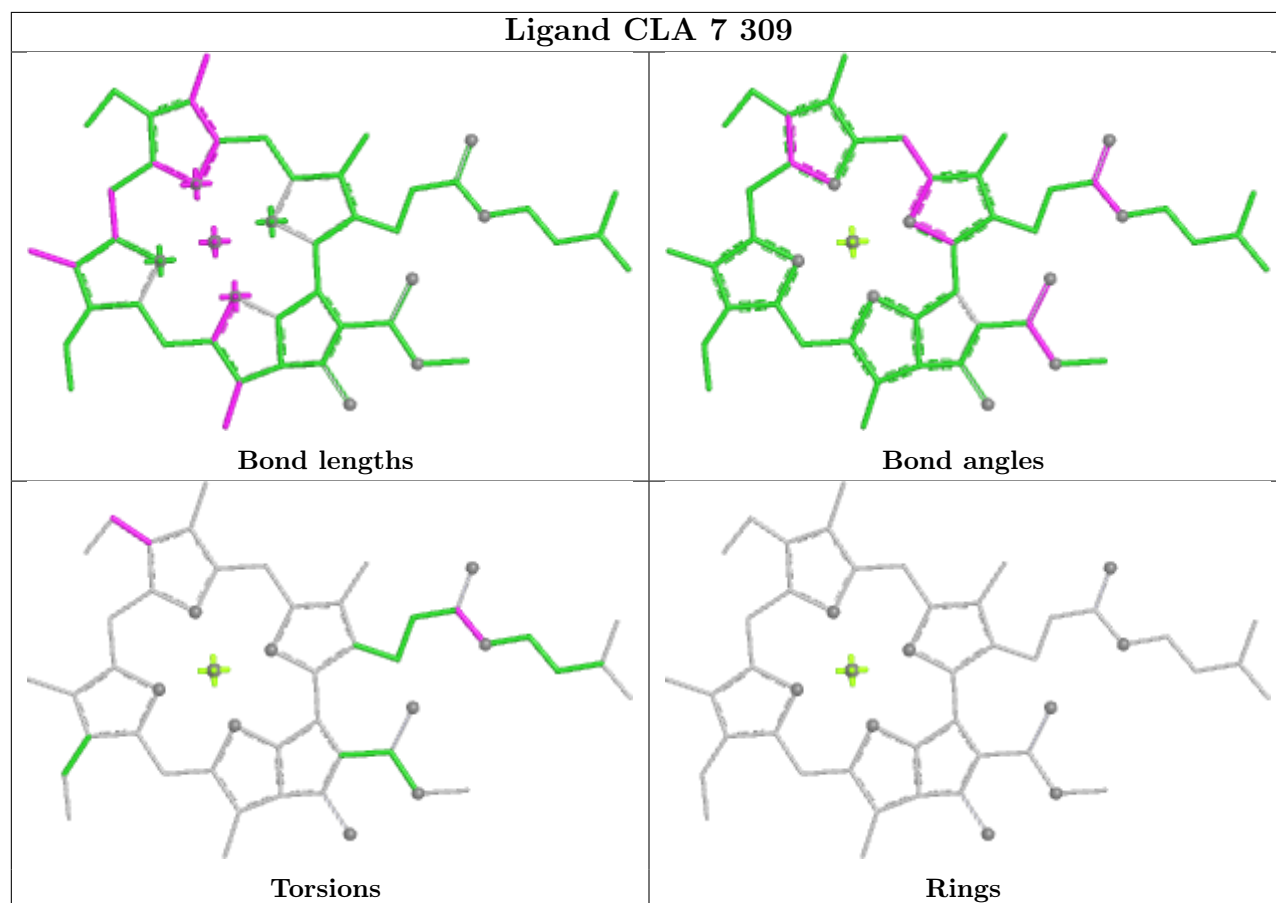
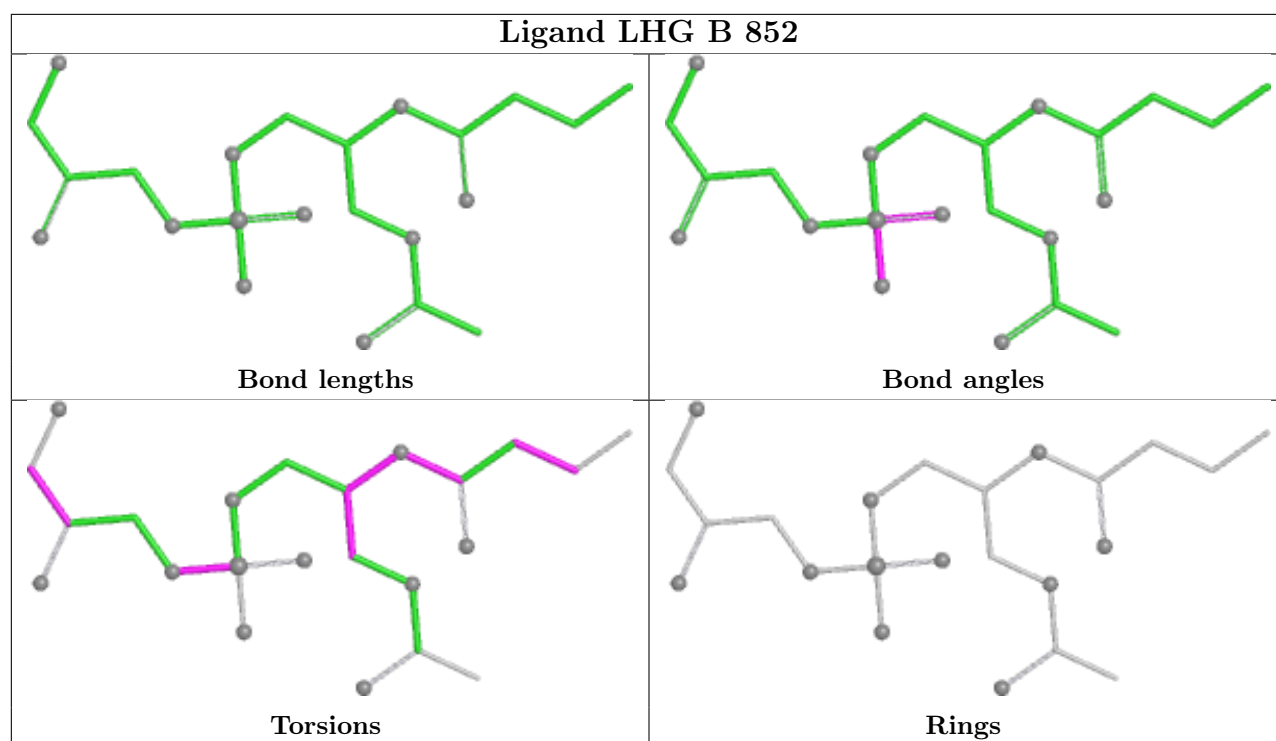


Torsions

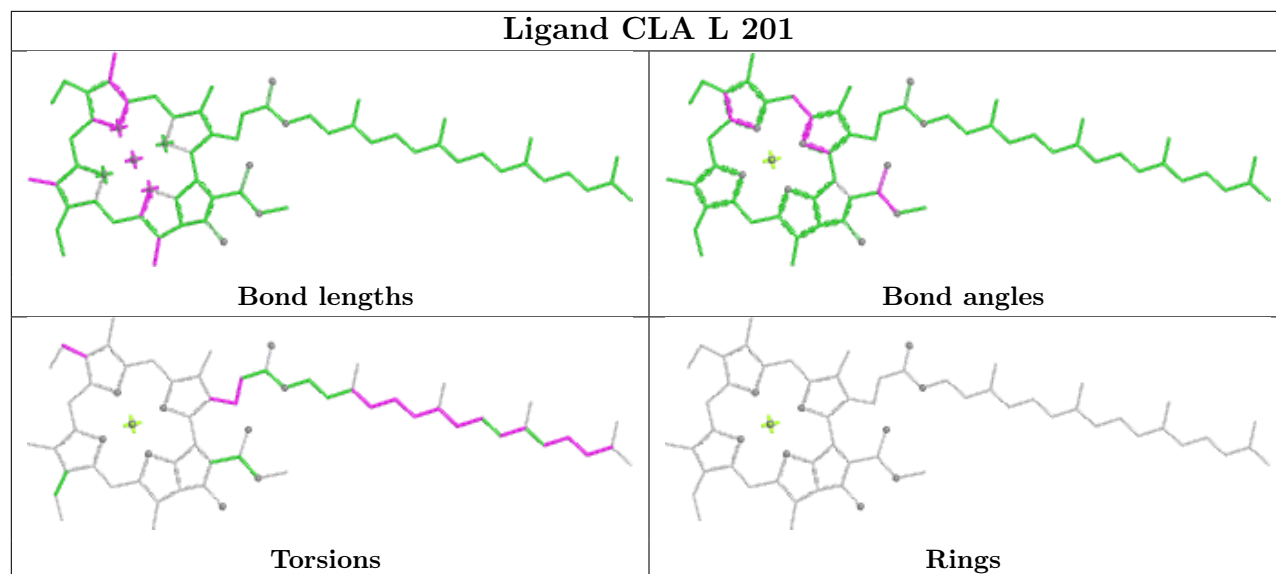


Rings

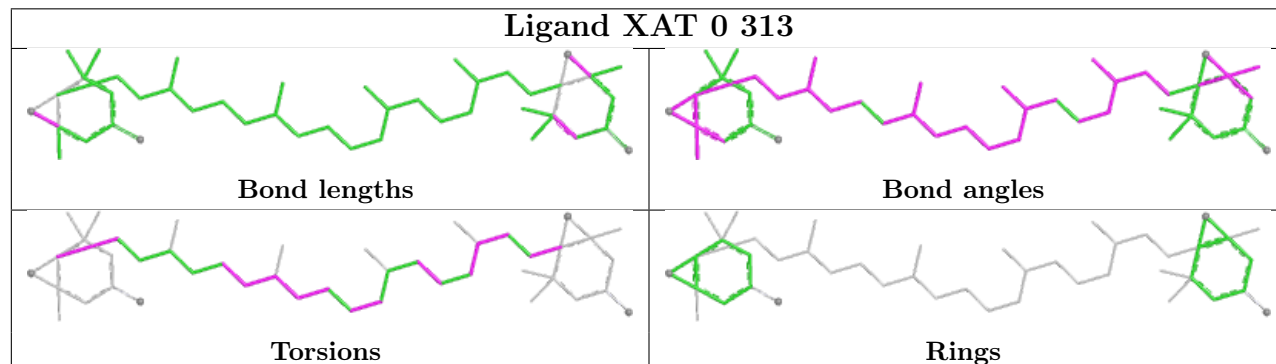




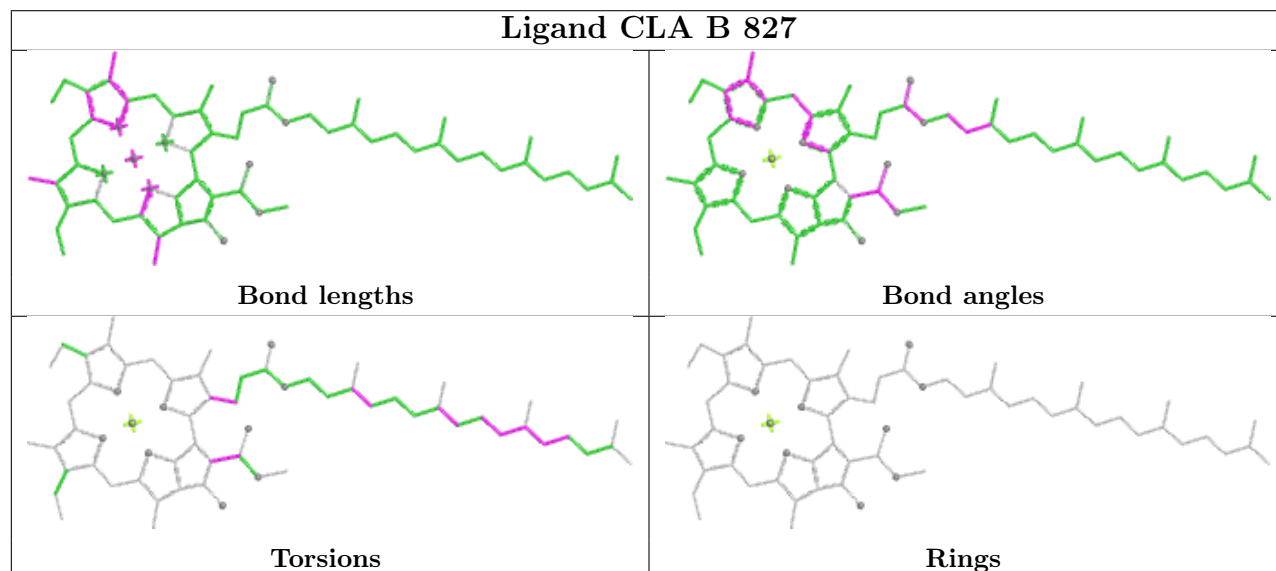
Ligand CLA L 201



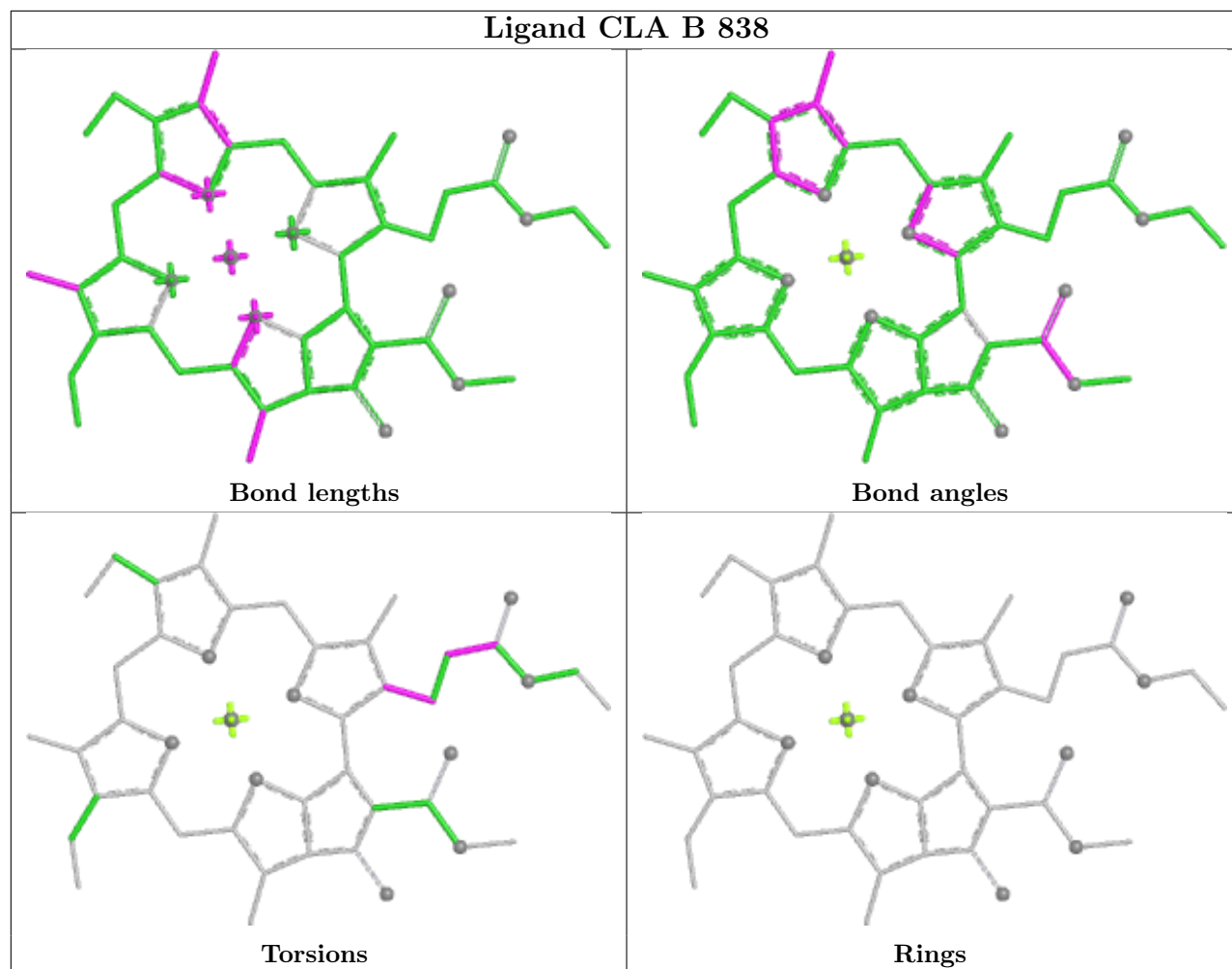
Ligand XAT 0 313



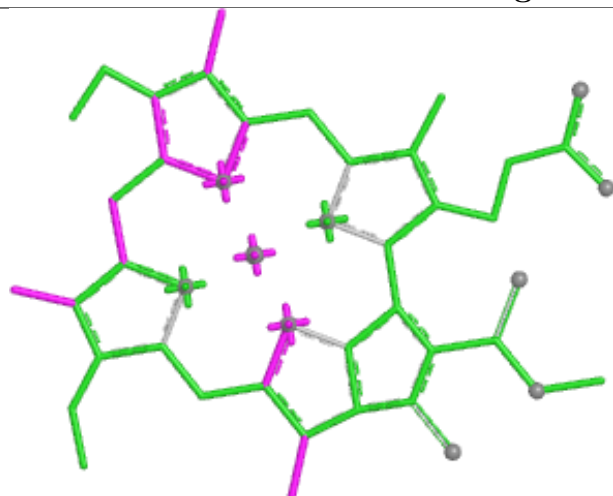
Ligand CLA B 827



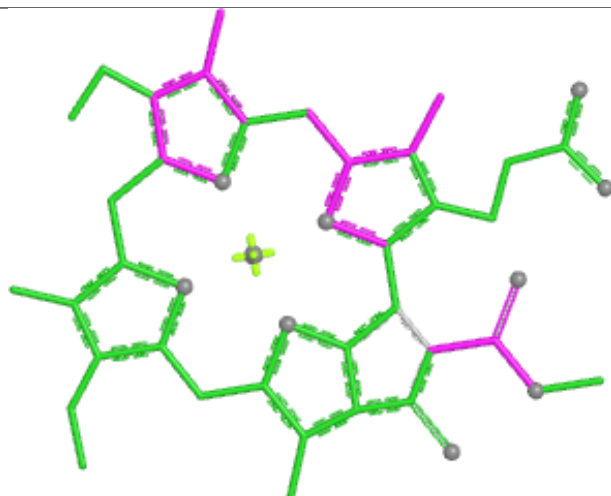
Ligand CLA B 838



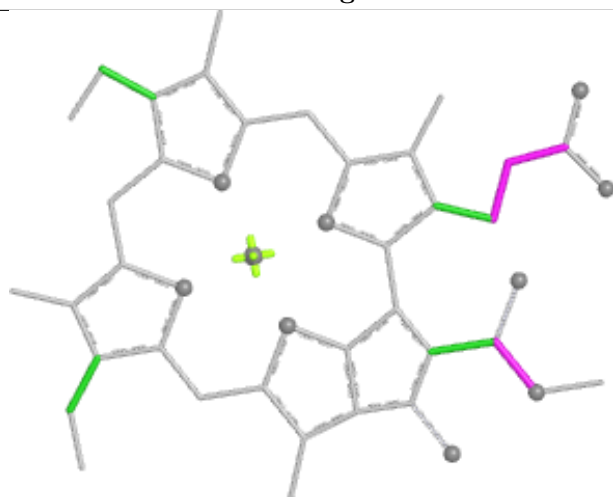
Ligand CLA B 807



Bond lengths



Bond angles

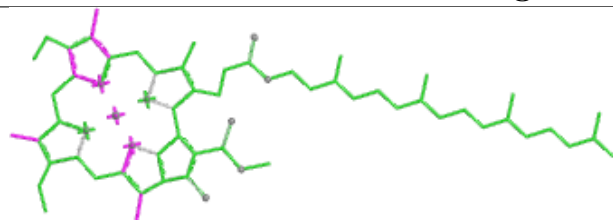


Torsions

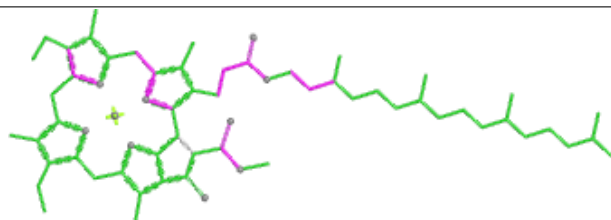


Rings

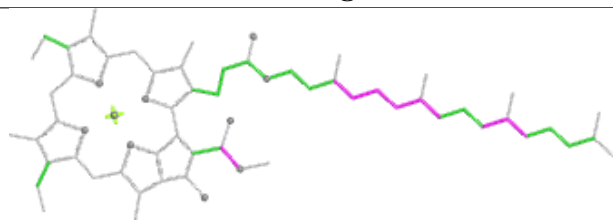
Ligand CLA A 838



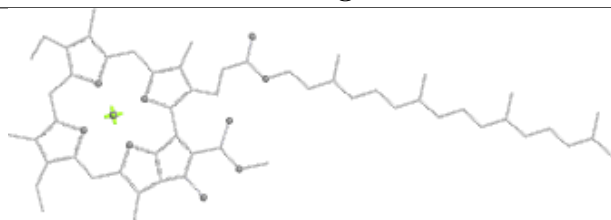
Bond lengths



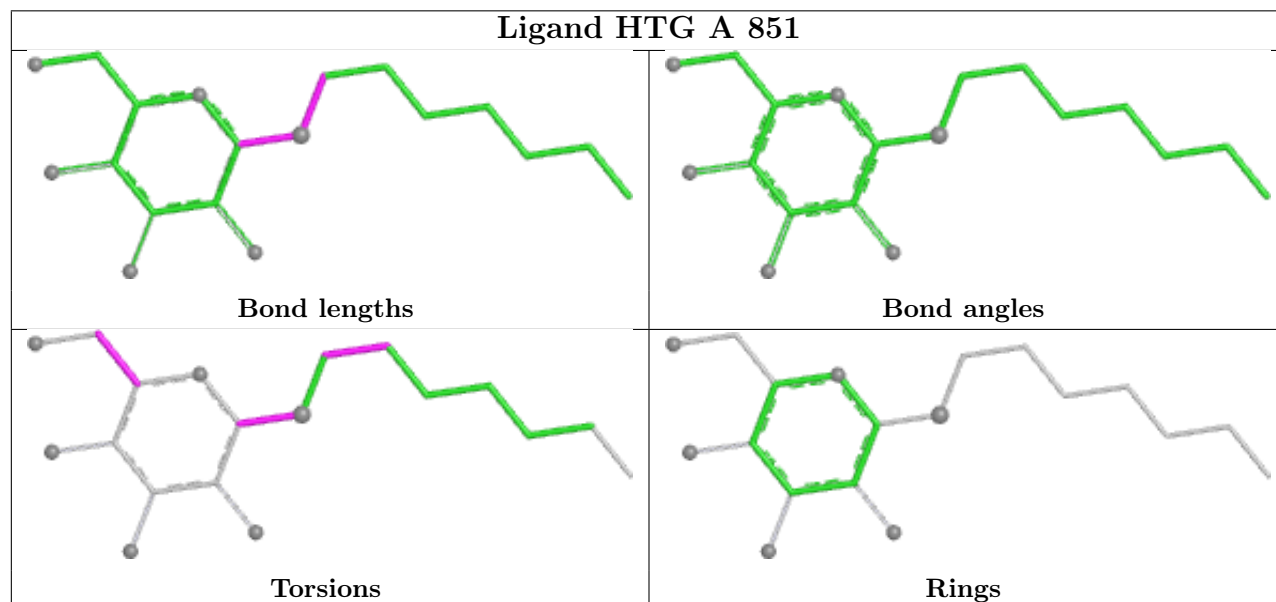
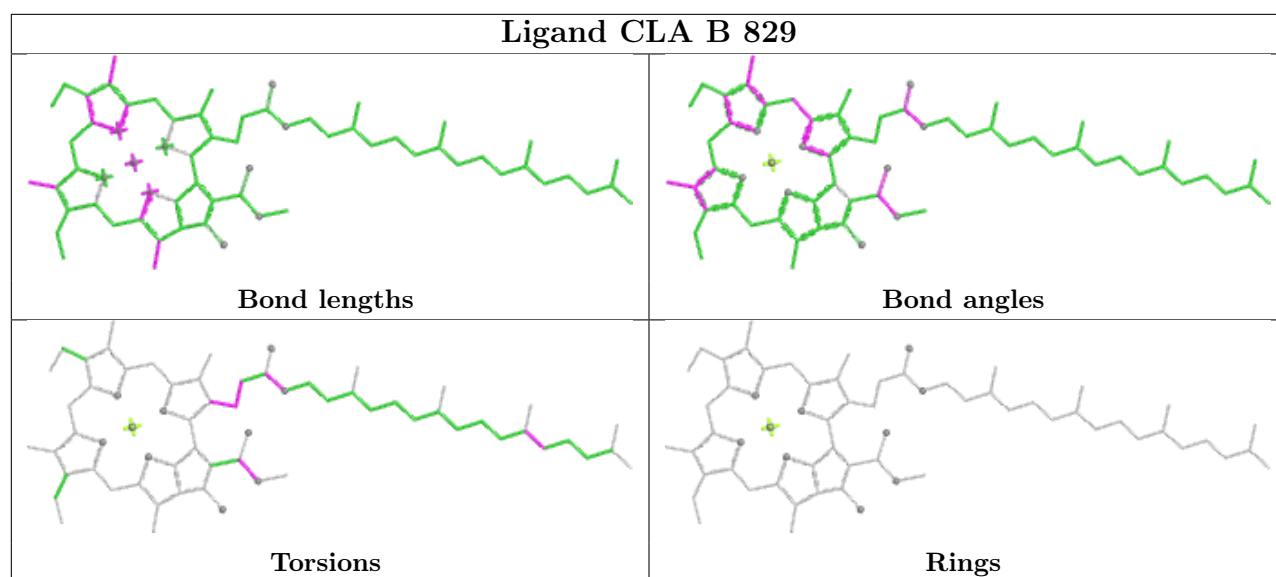
Bond angles



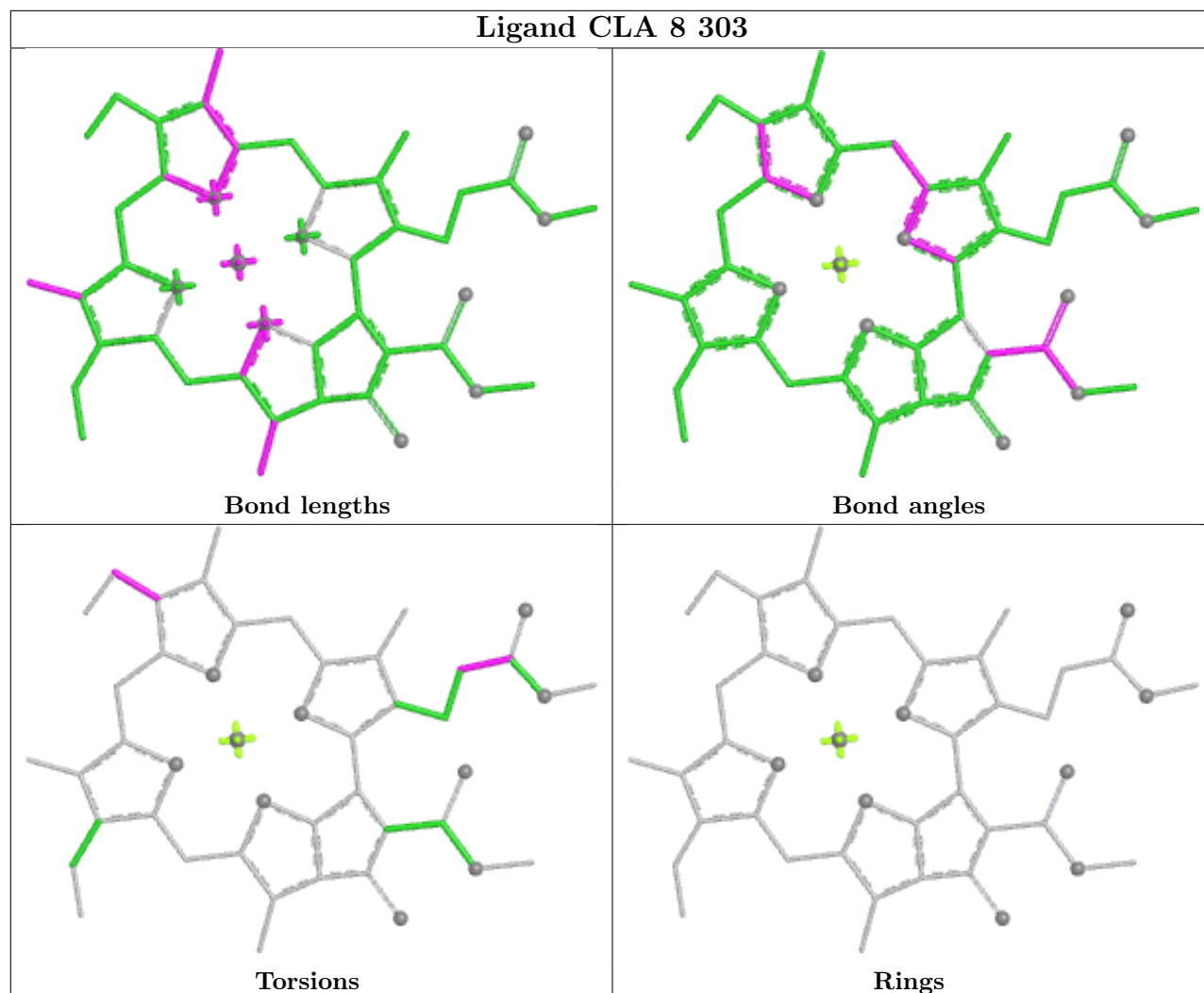
Torsions



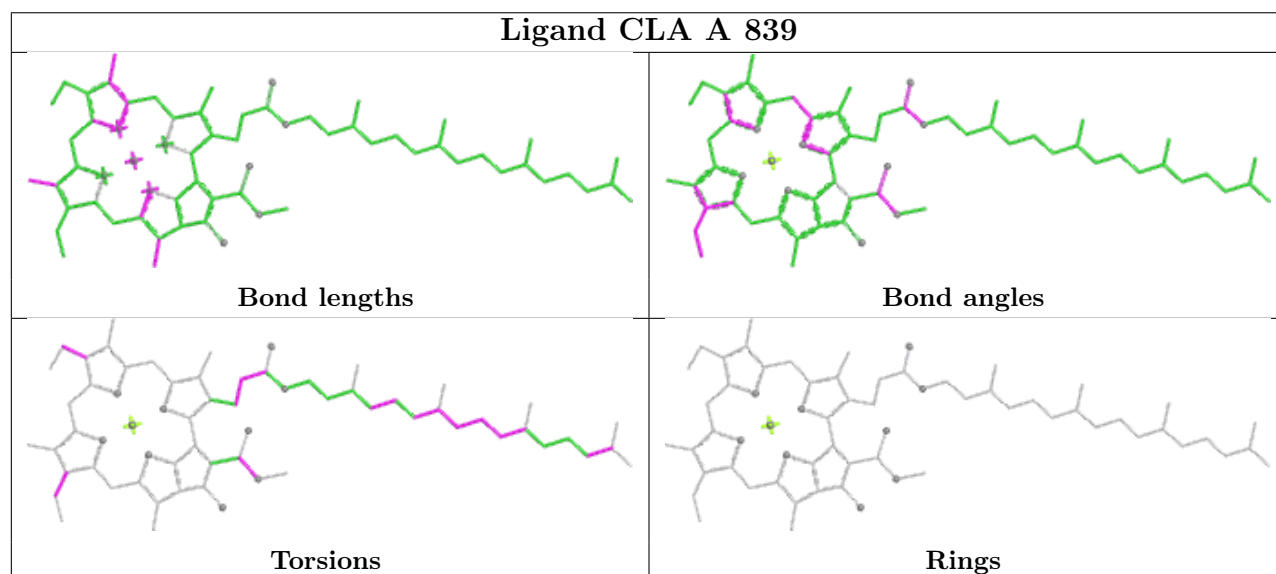
Rings



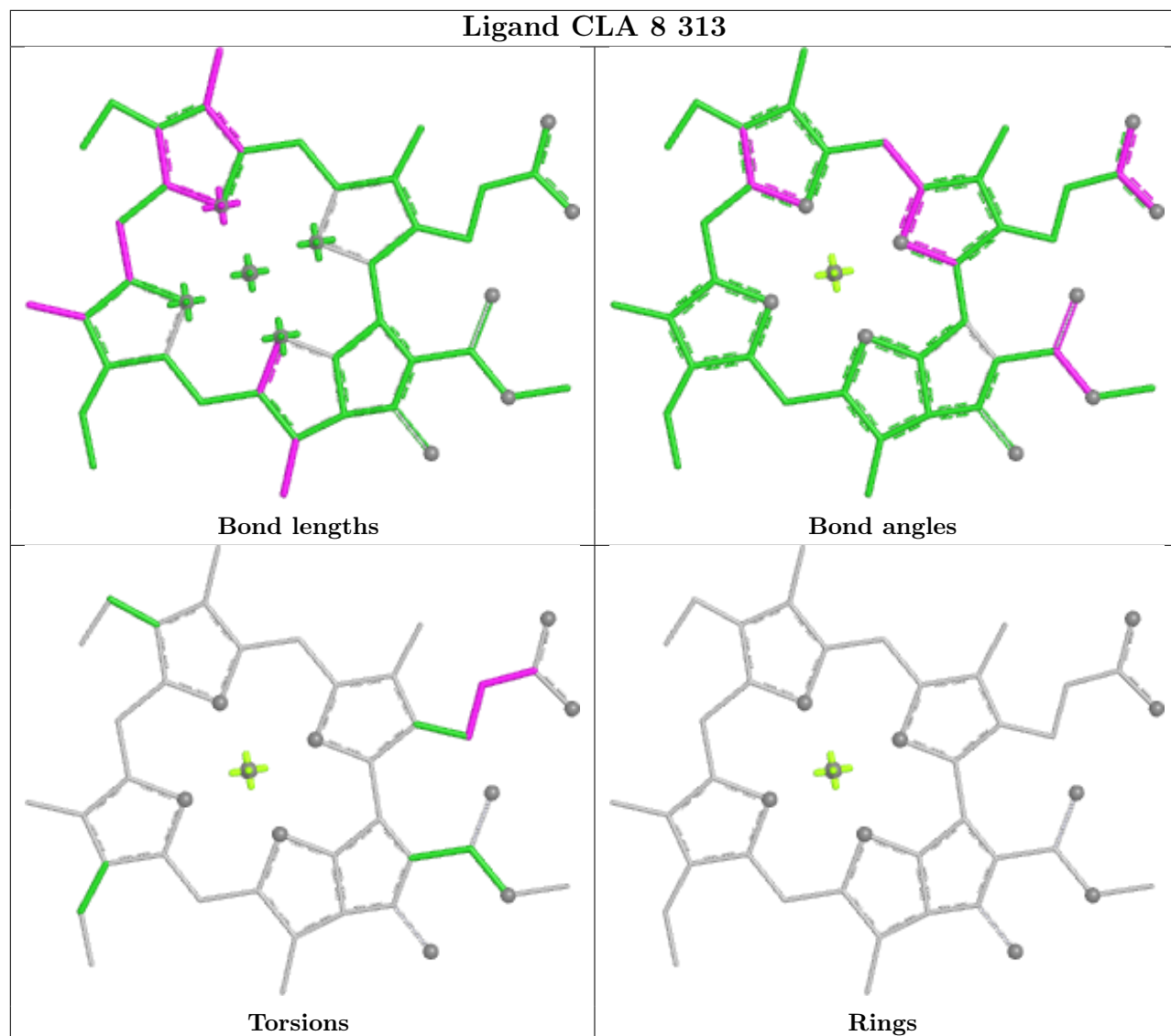
Ligand CLA 8 303



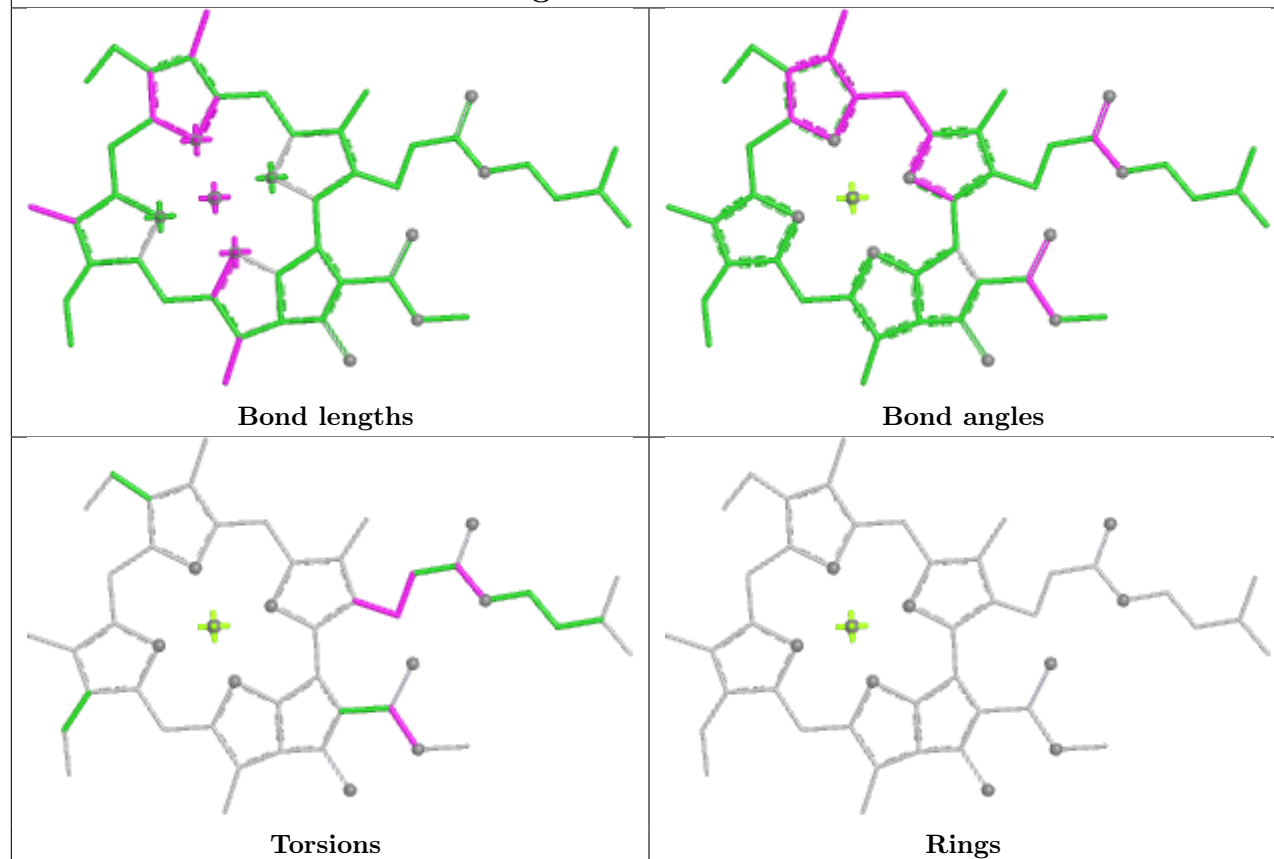
Ligand CLA A 839



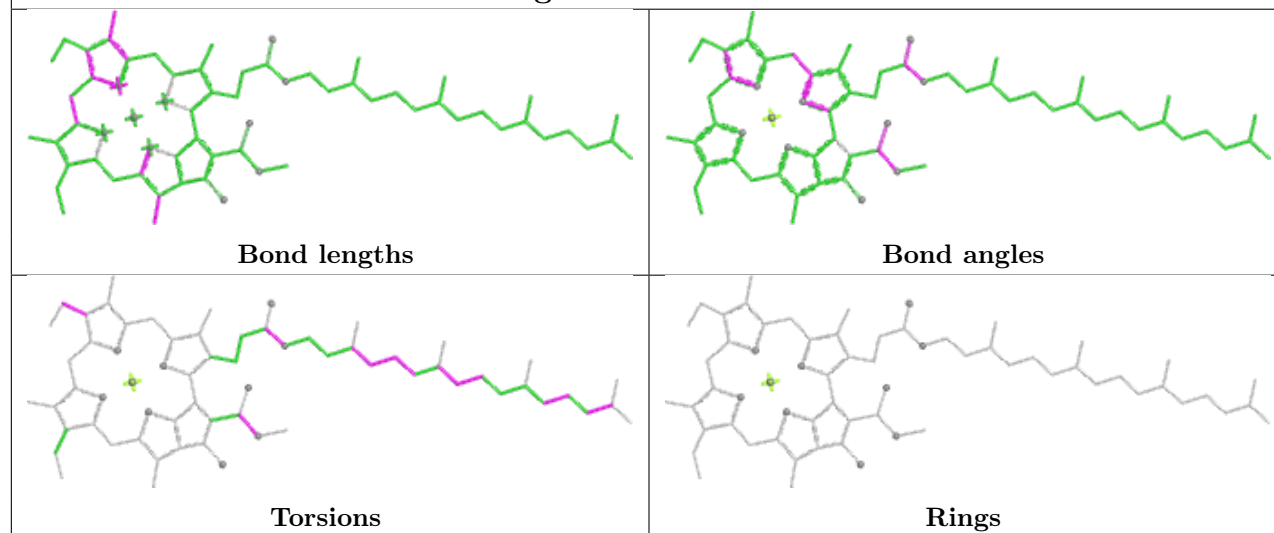
Ligand CLA 8 313

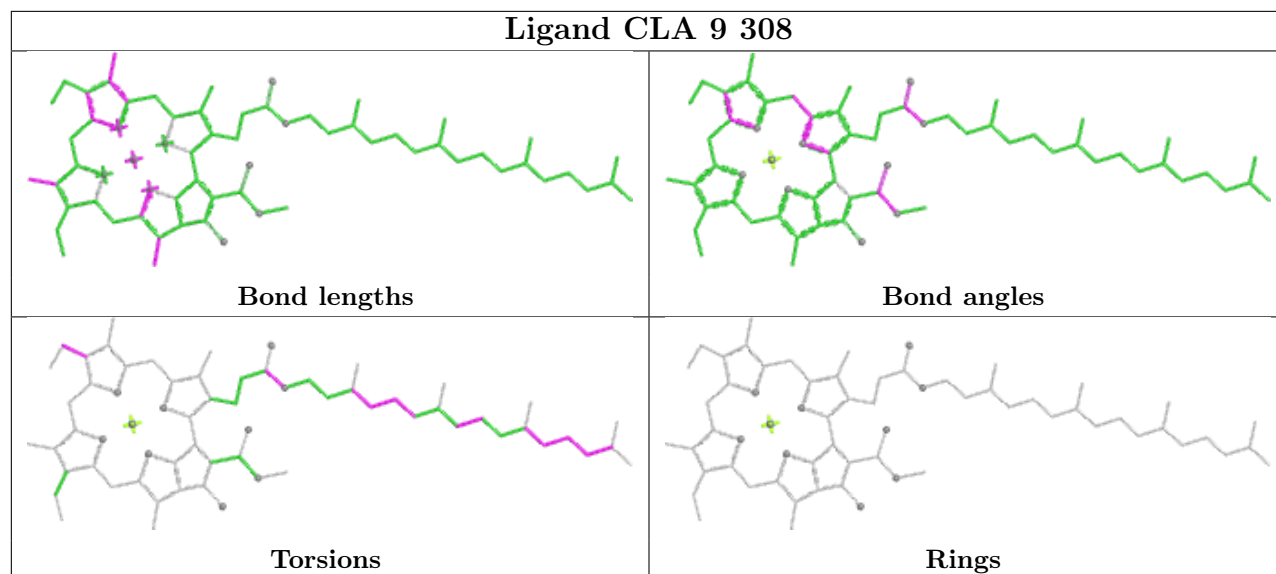
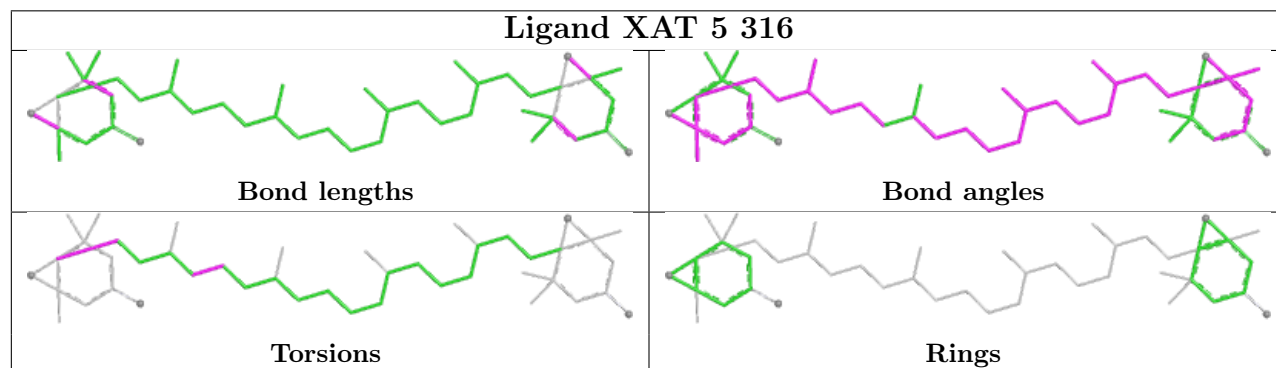
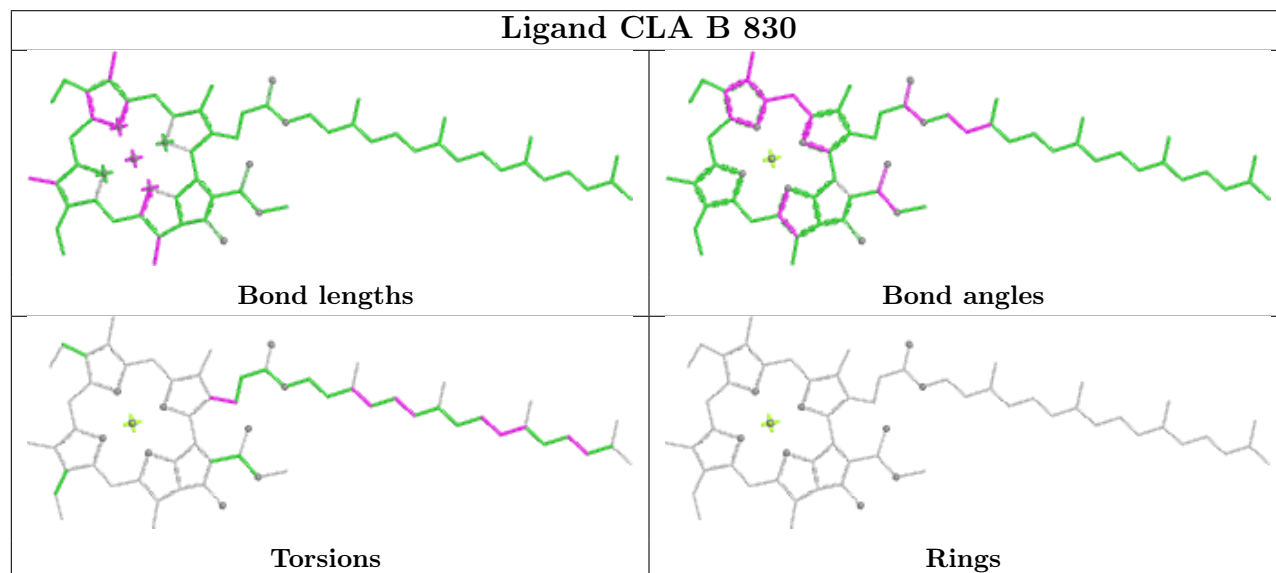


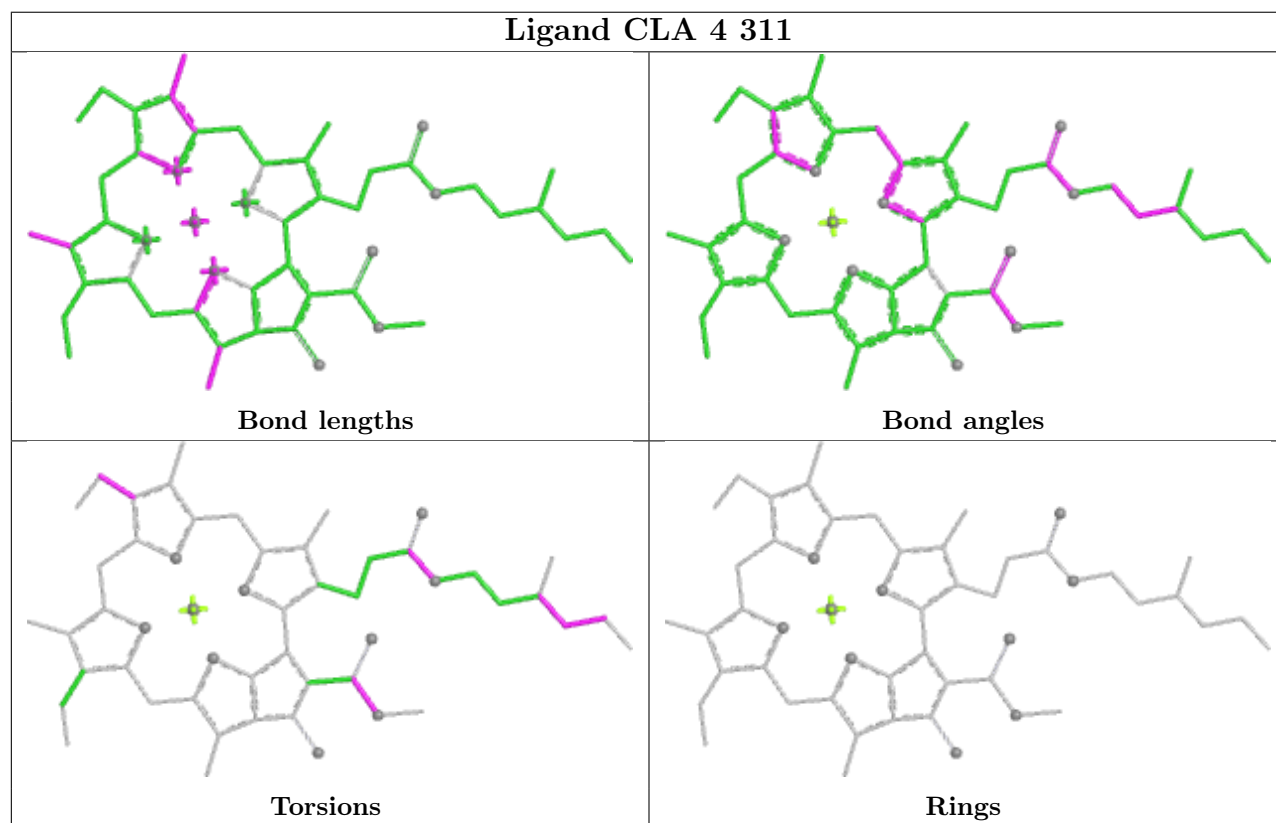
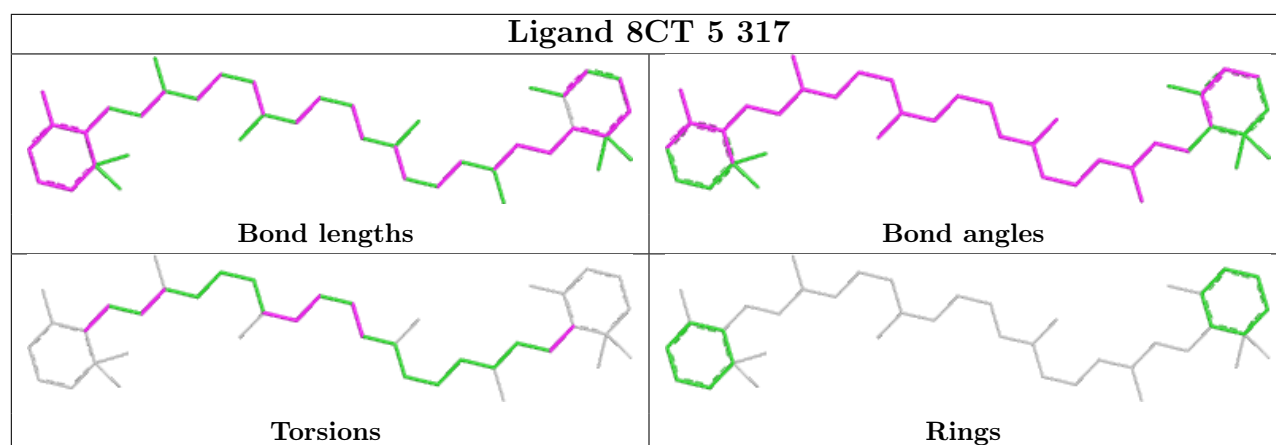
Ligand CLA B 831



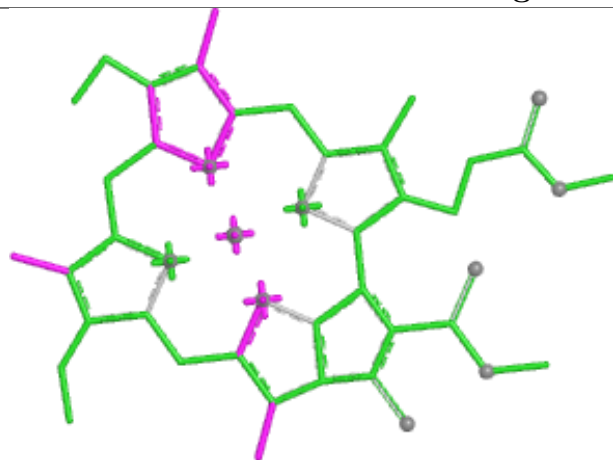
Ligand CLA L 203



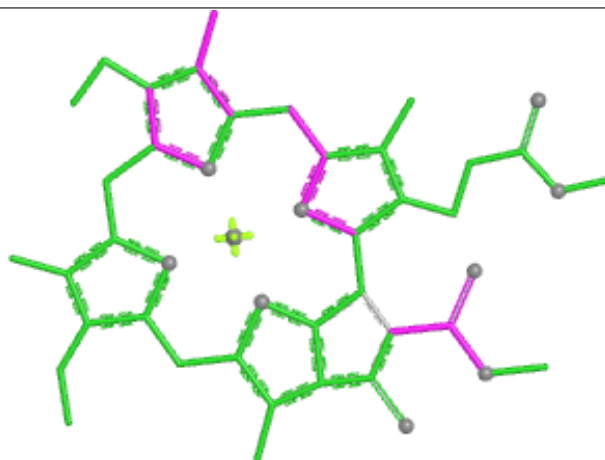
Ligand CLA 9 308**Ligand XAT 5 316****Ligand CLA B 830**



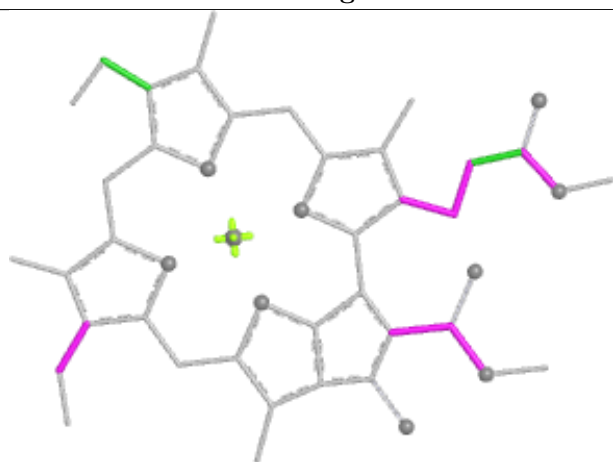
Ligand CLA K 102



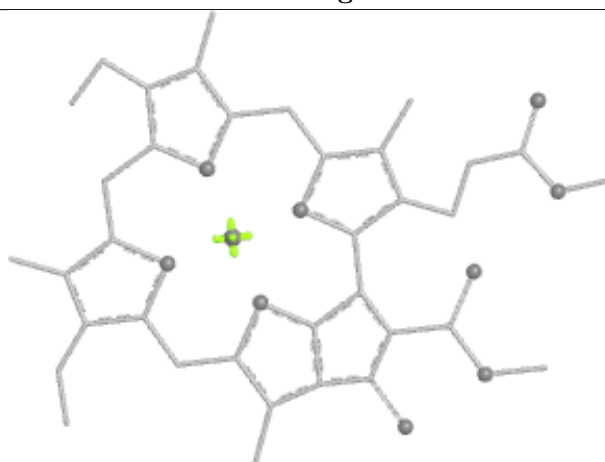
Bond lengths



Bond angles

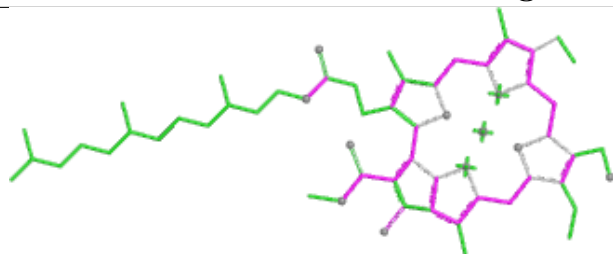


Torsions

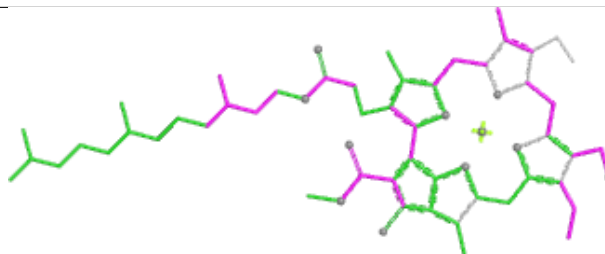


Rings

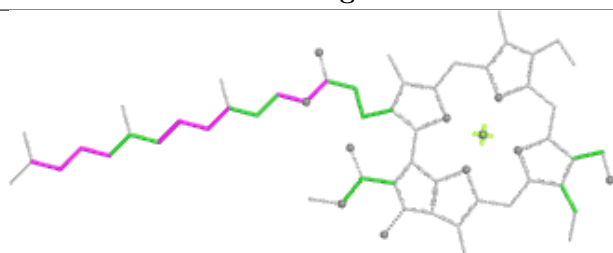
Ligand CHL 4 301



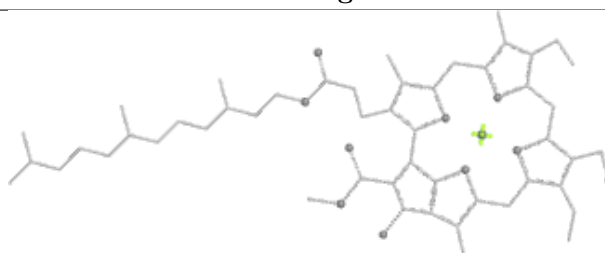
Bond lengths



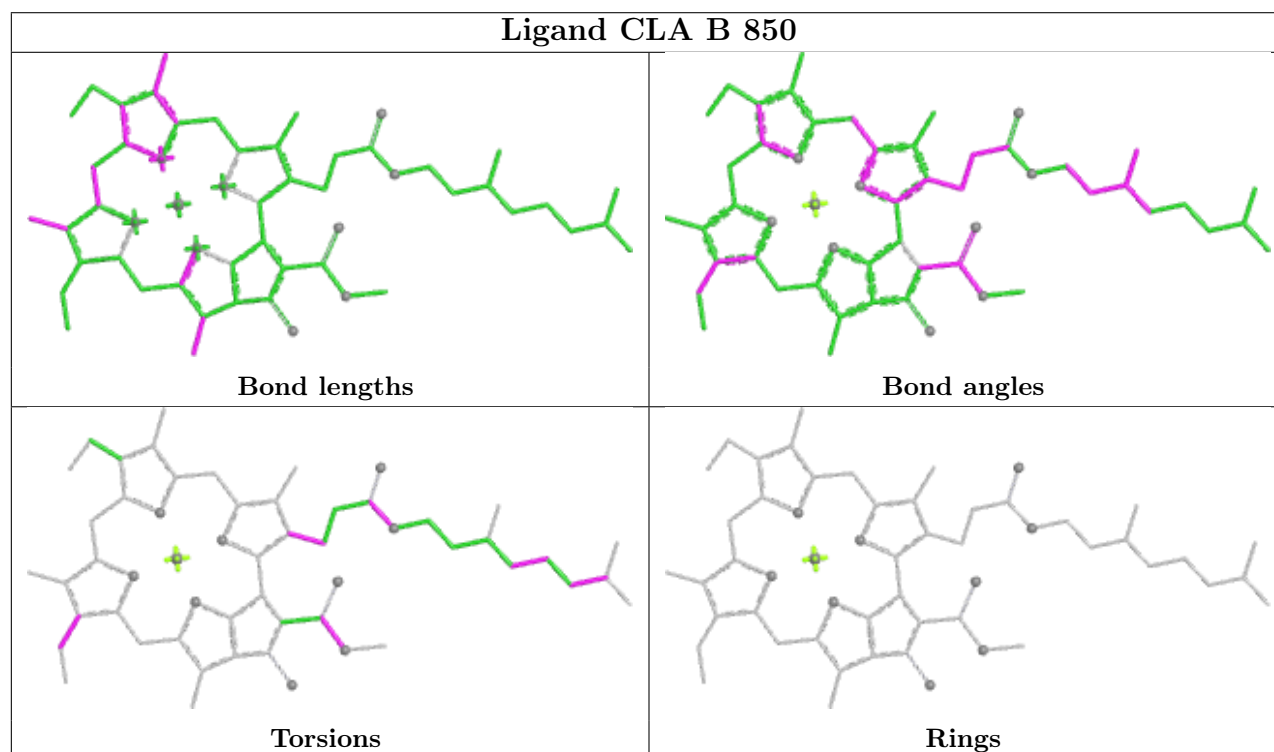
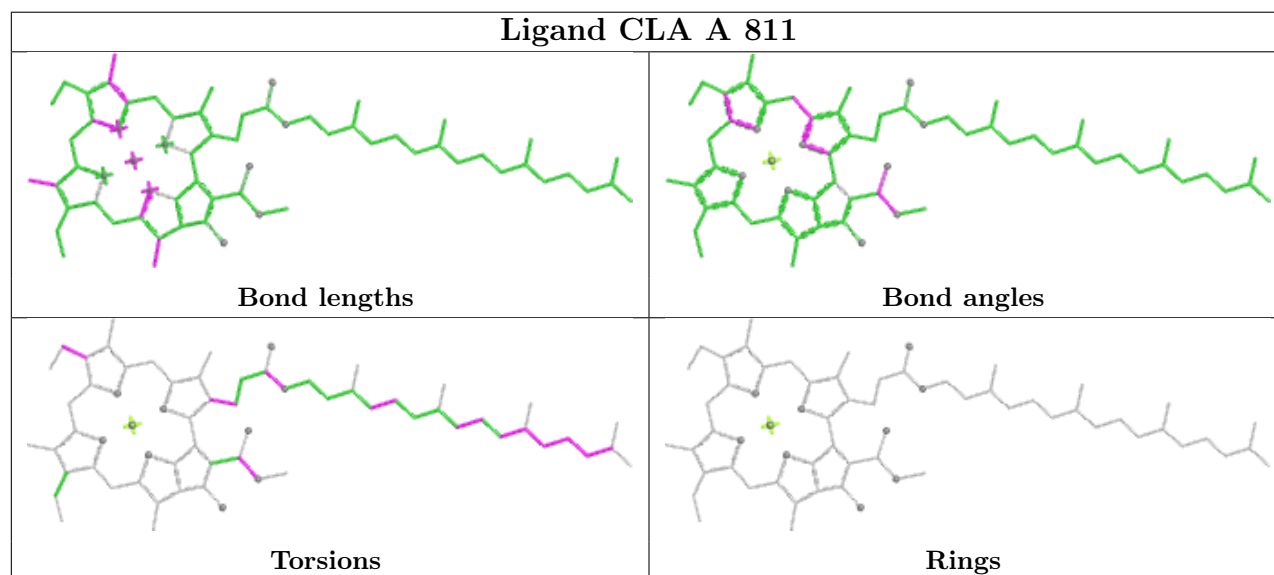
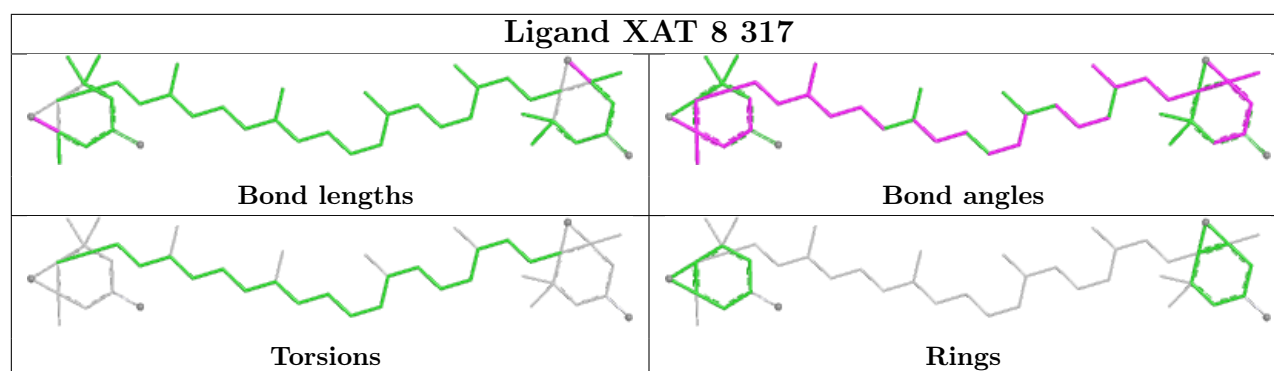
Bond angles



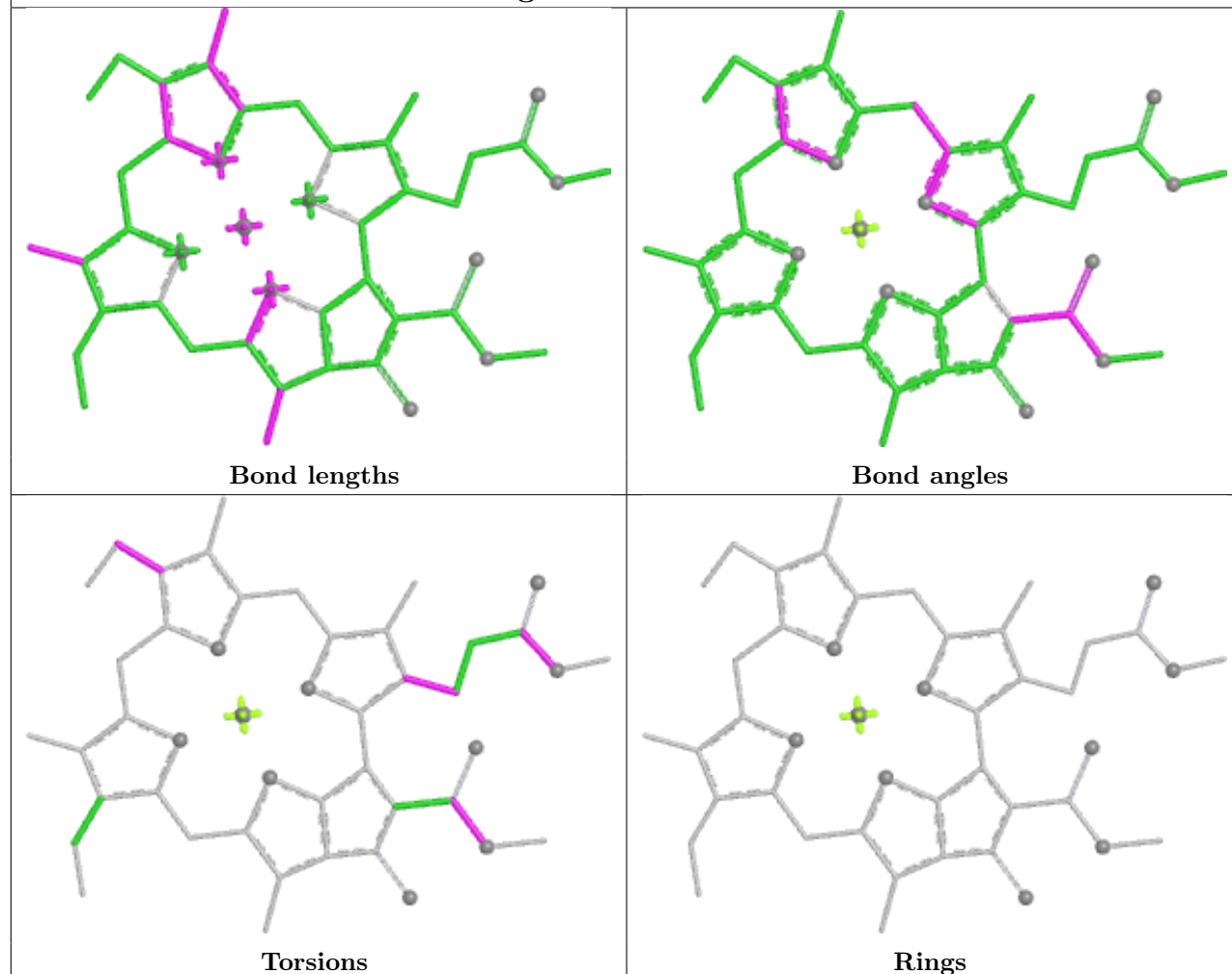
Torsions



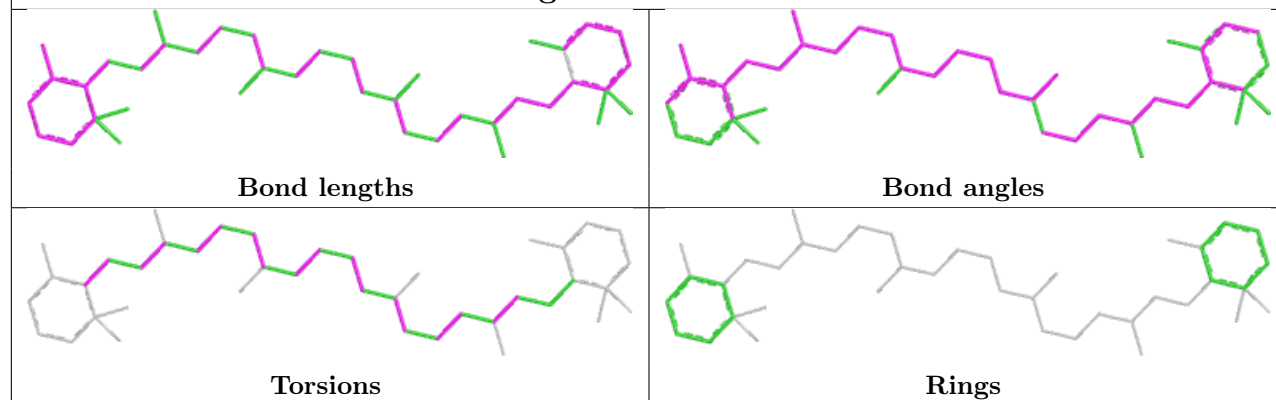
Rings



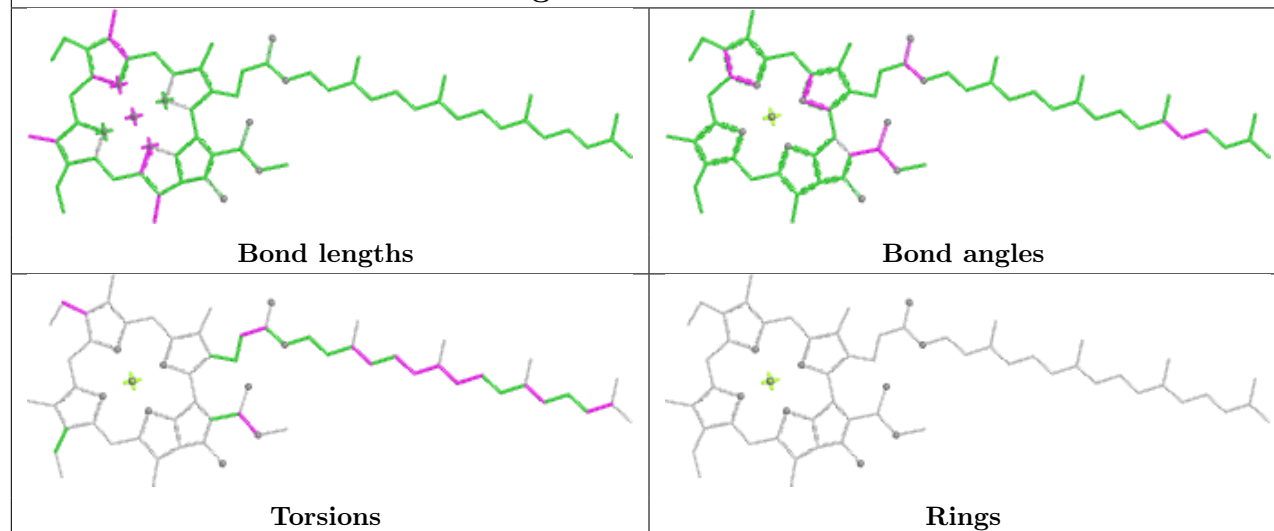
Ligand CLA 1 313



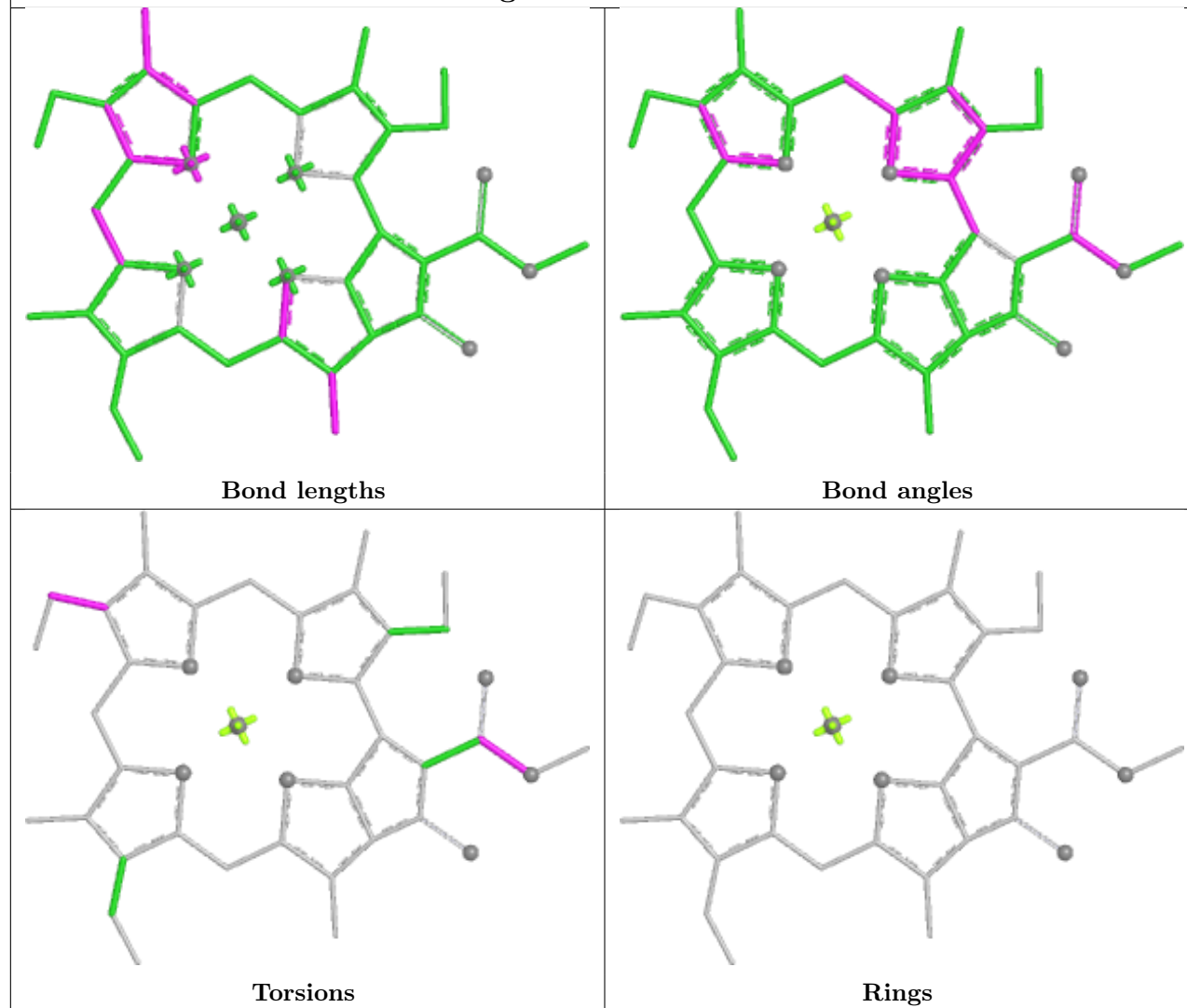
Ligand 8CT 7 323



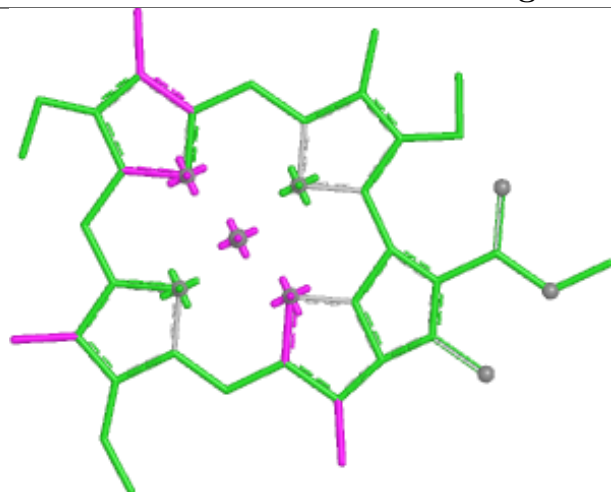
Ligand CLA B 805



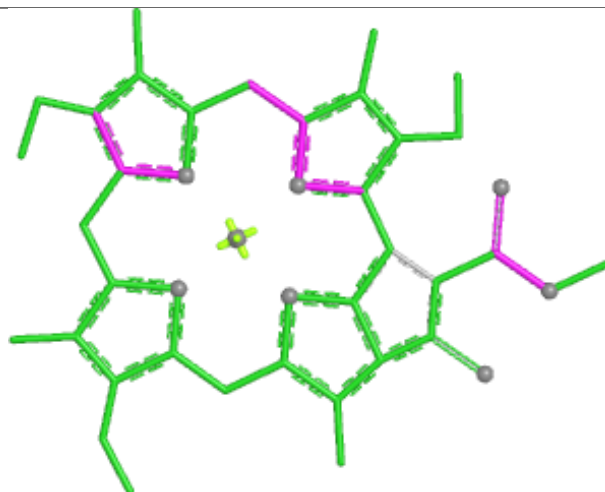
Ligand CLA 5 308



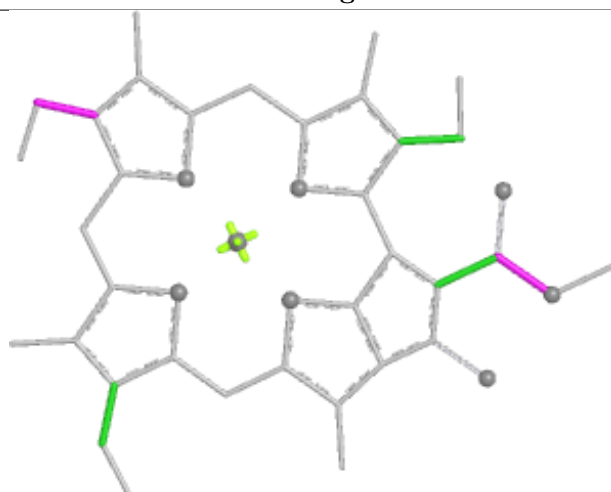
Ligand CLA 3 304



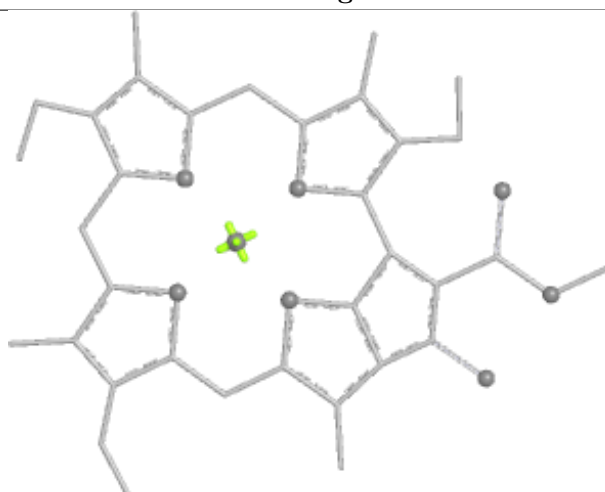
Bond lengths



Bond angles

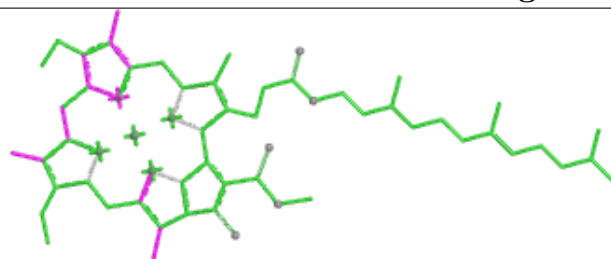


Torsions

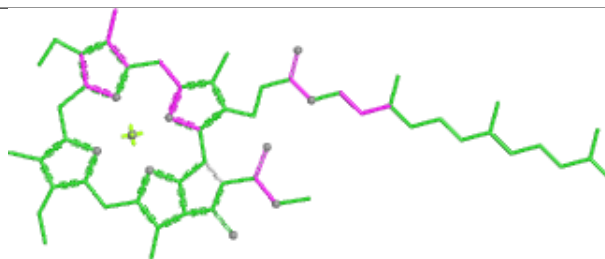


Rings

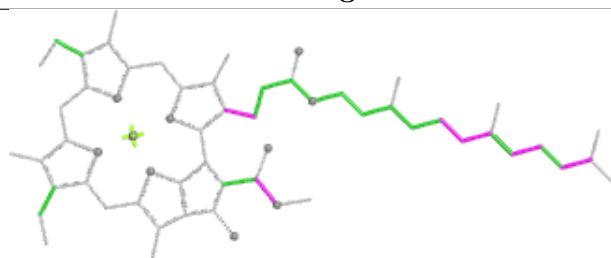
Ligand CLA 1 308



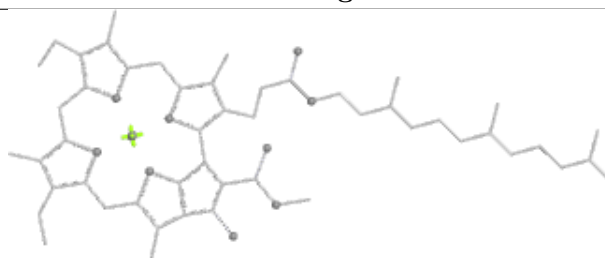
Bond lengths



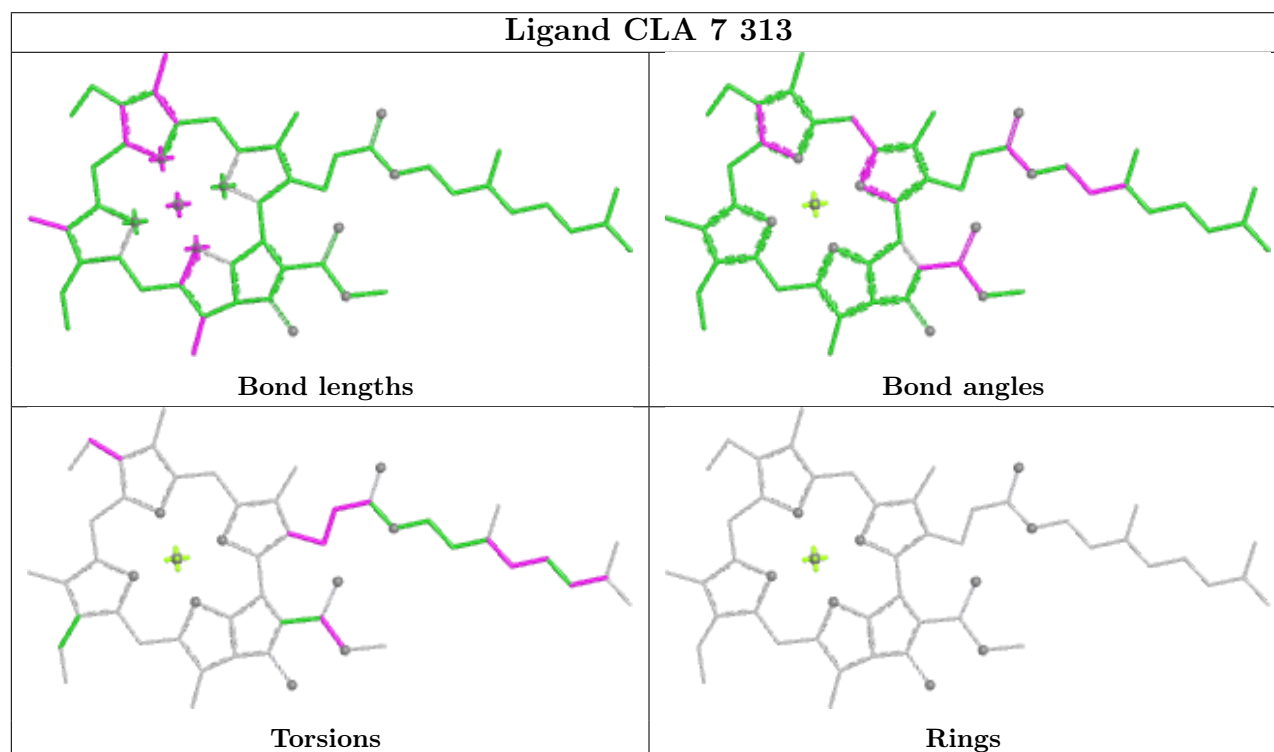
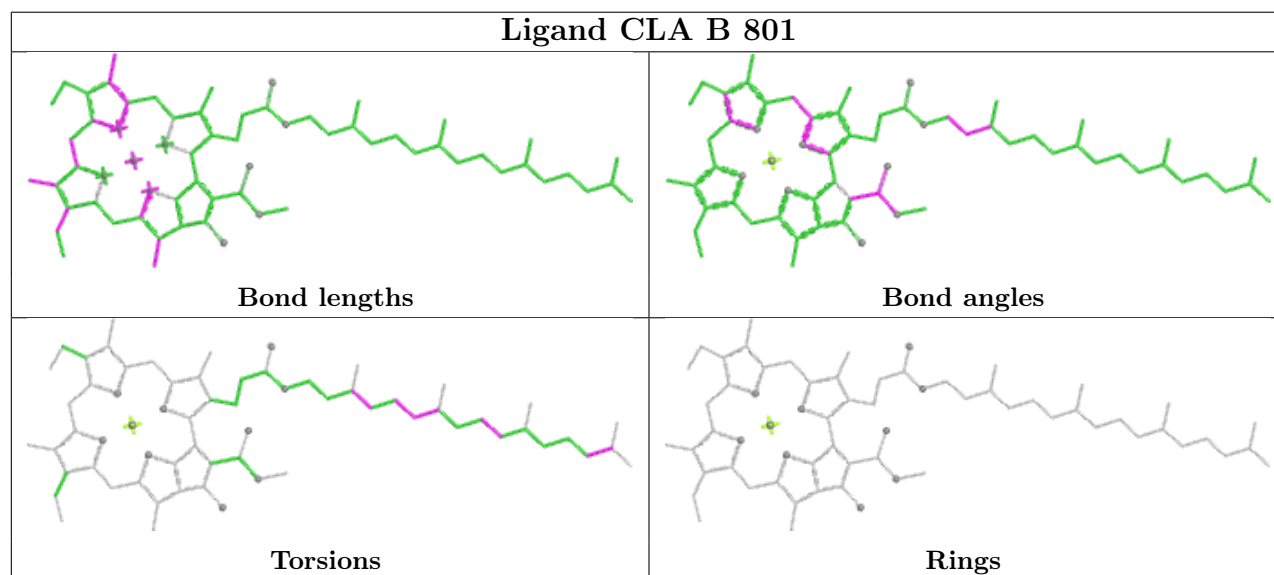
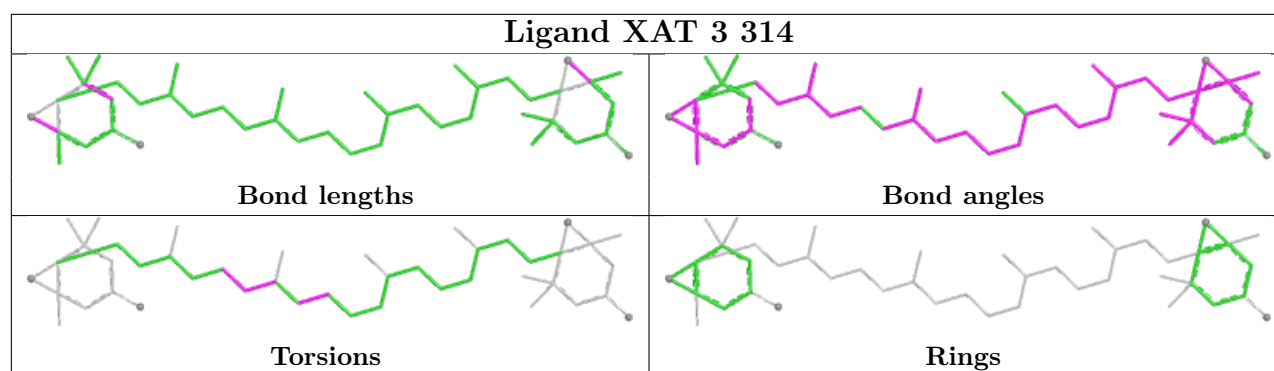
Bond angles

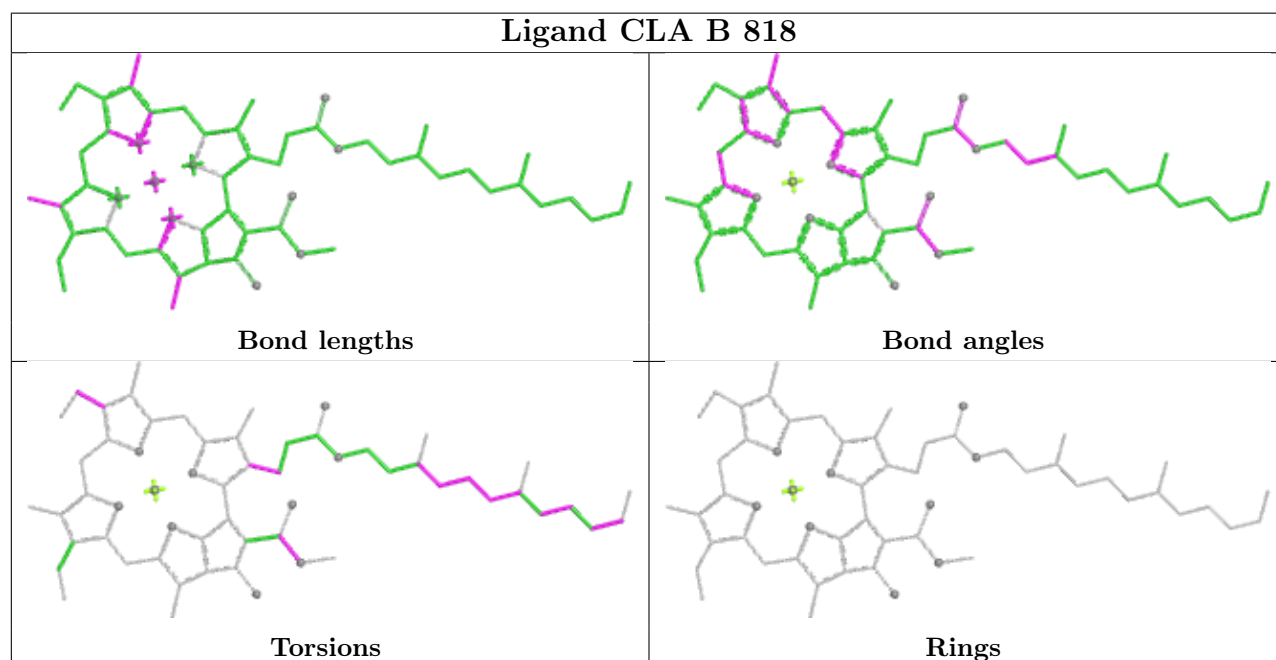
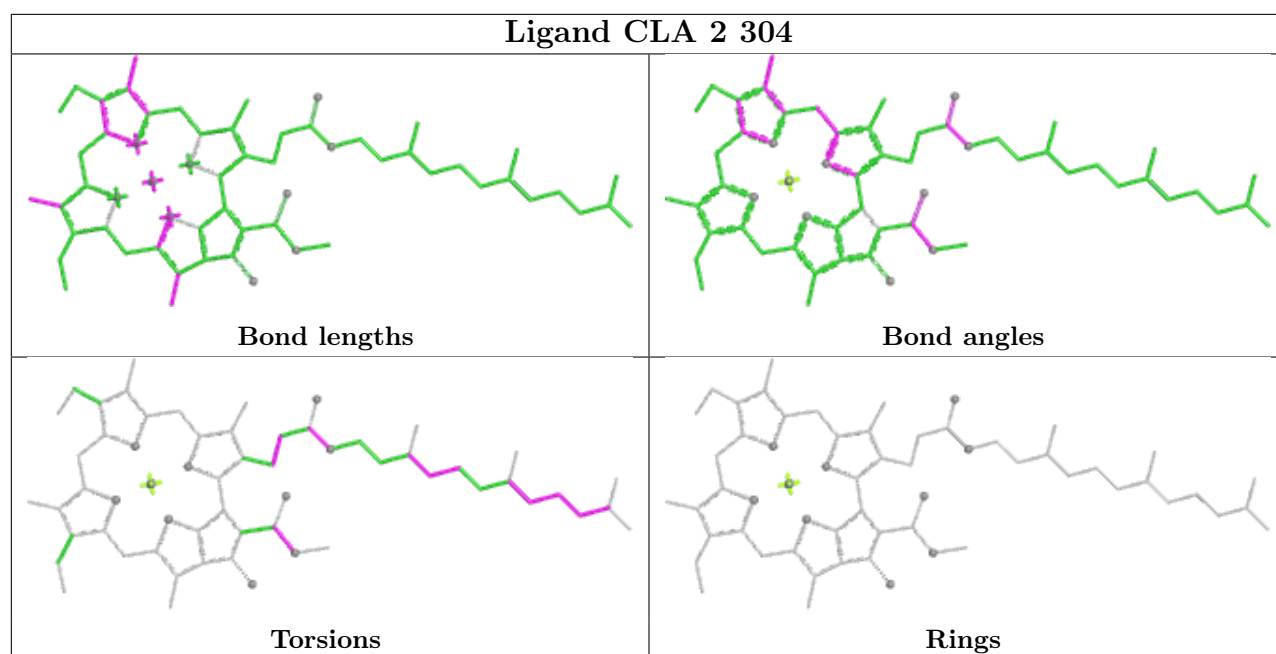


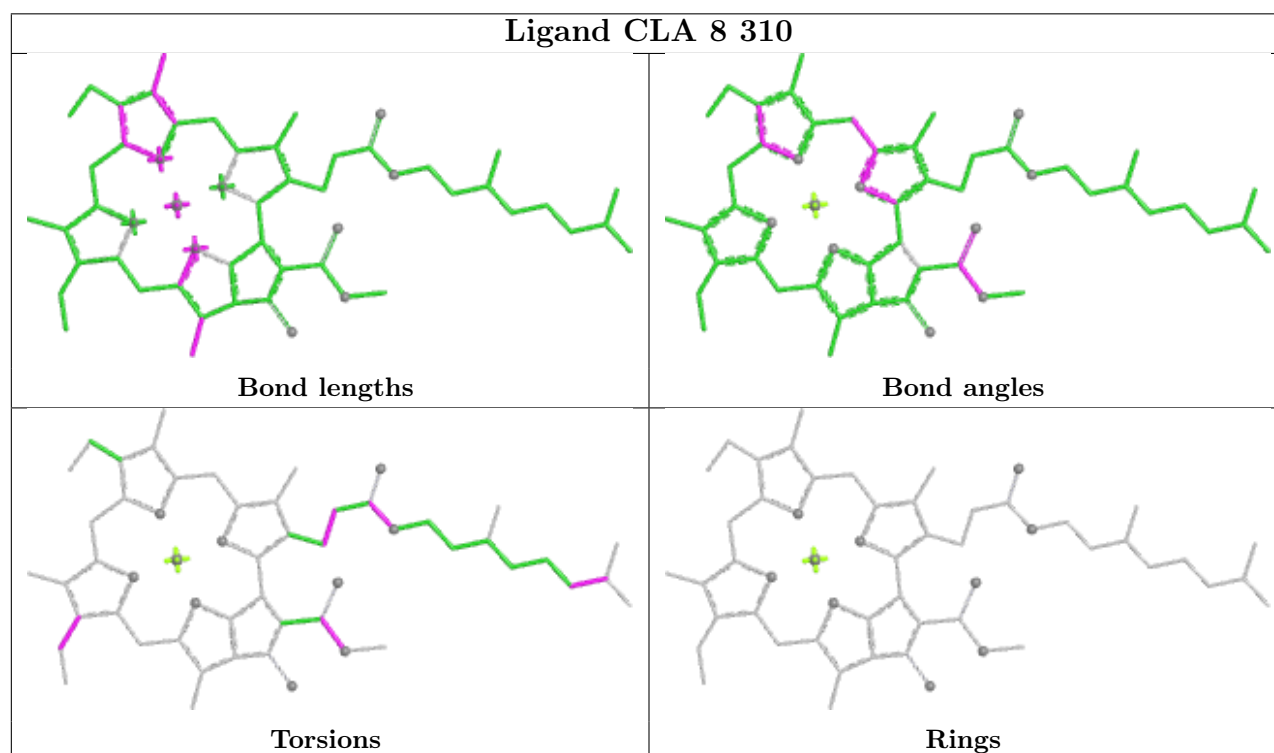
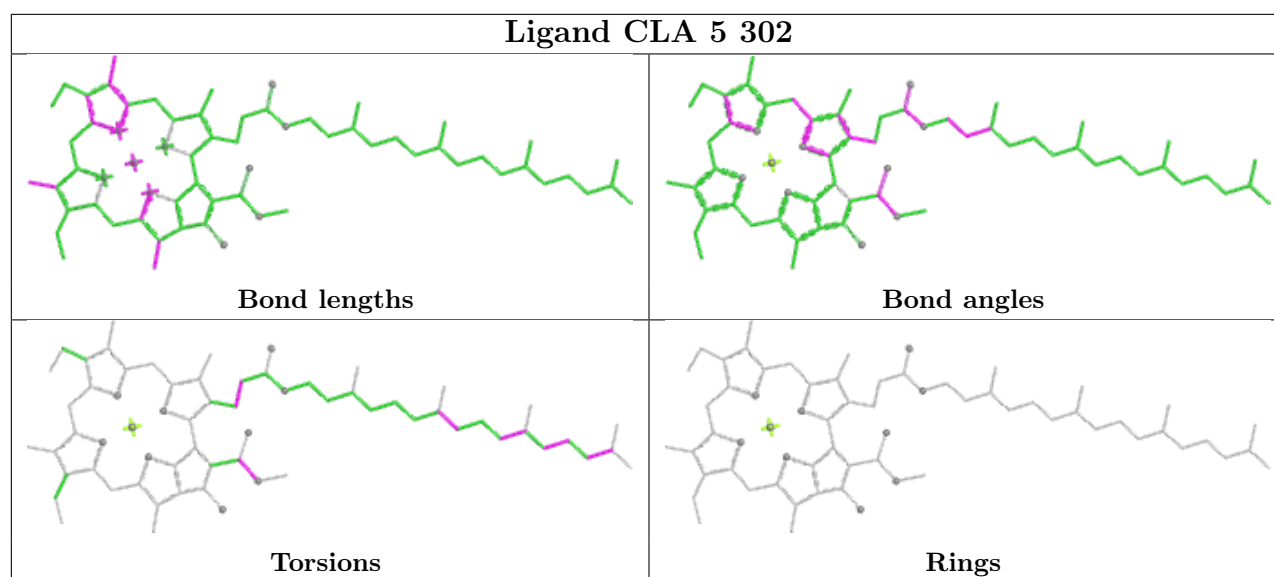
Torsions



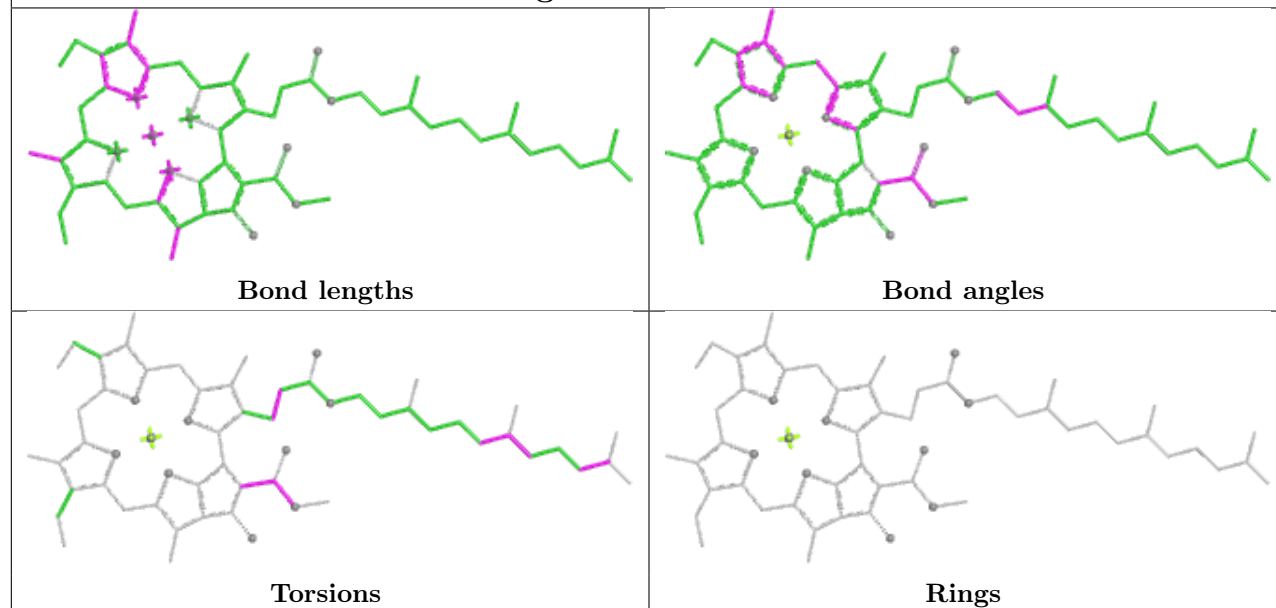
Rings



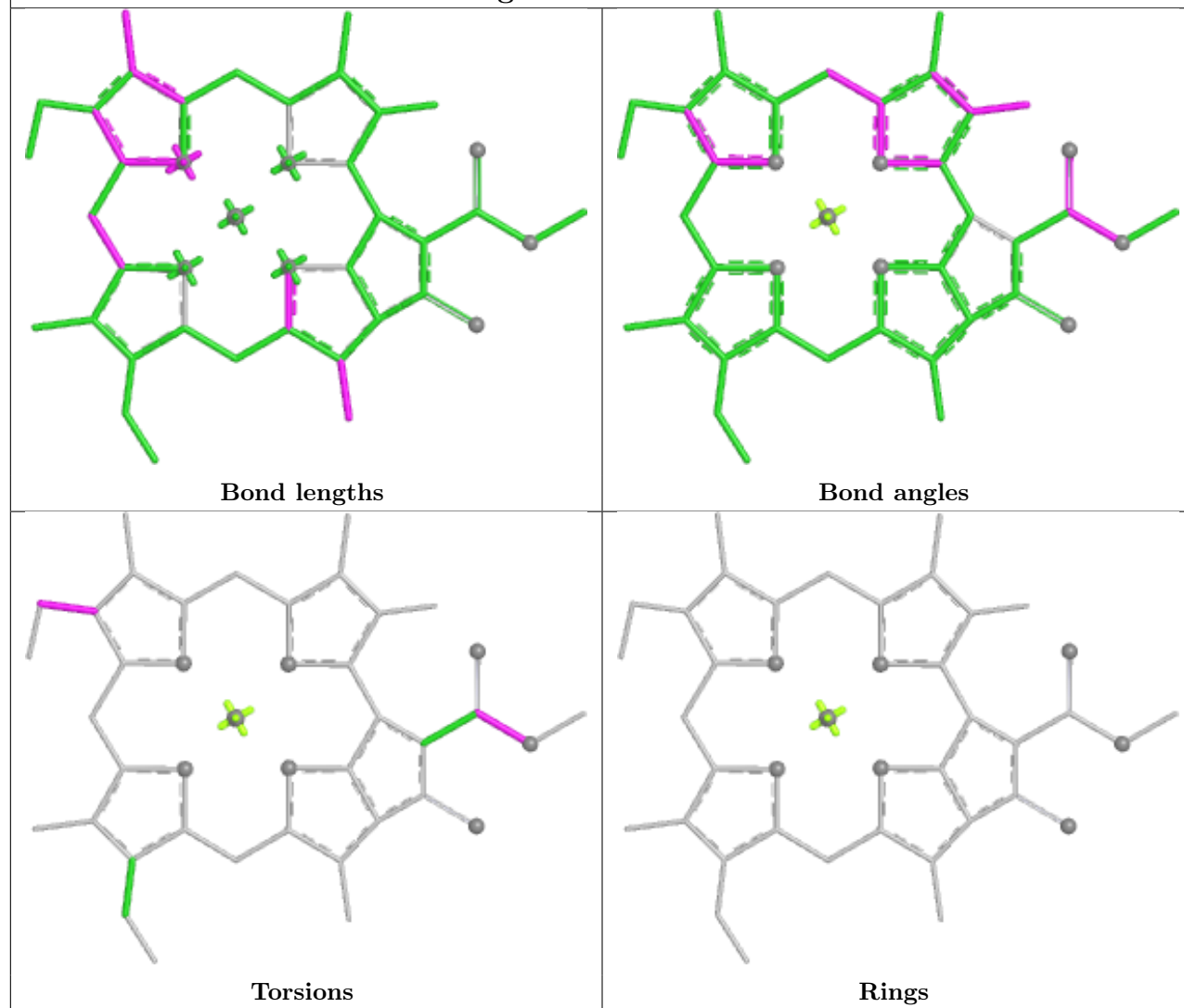


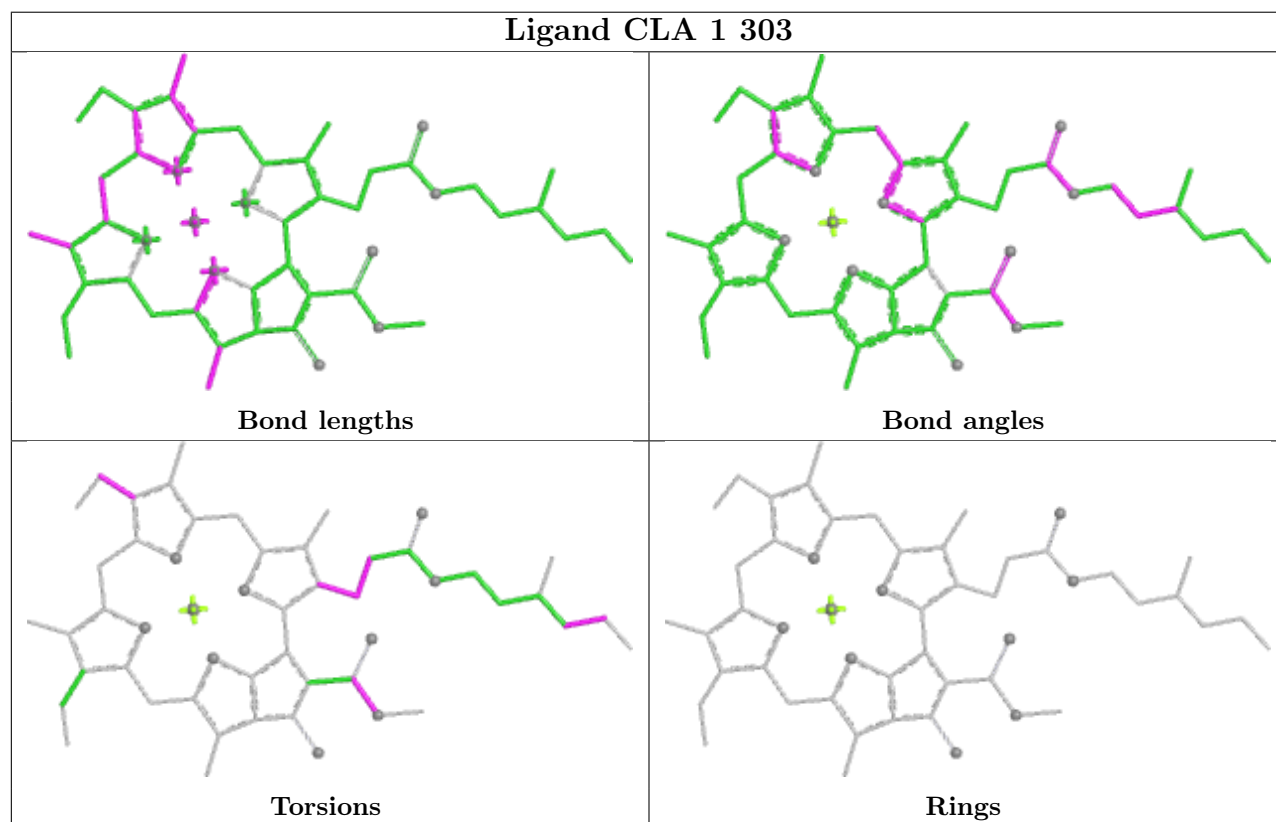
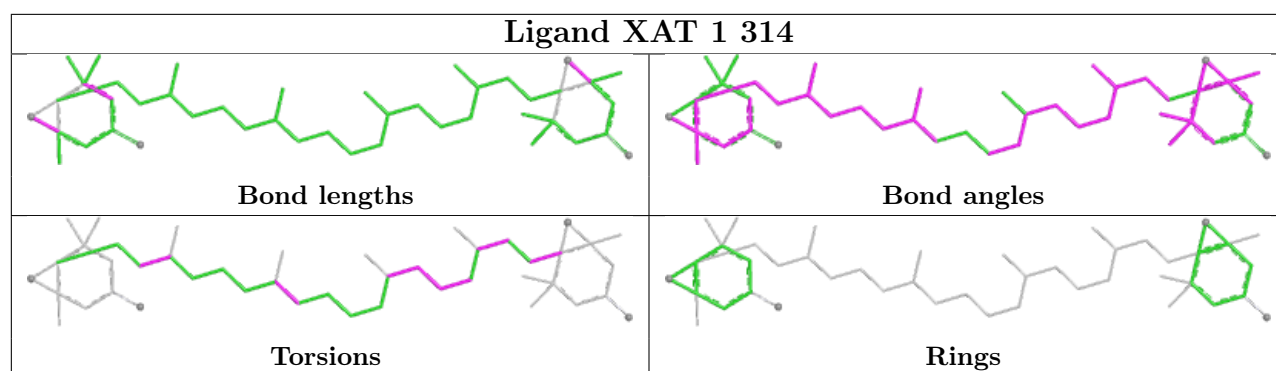


Ligand CLA 3 301

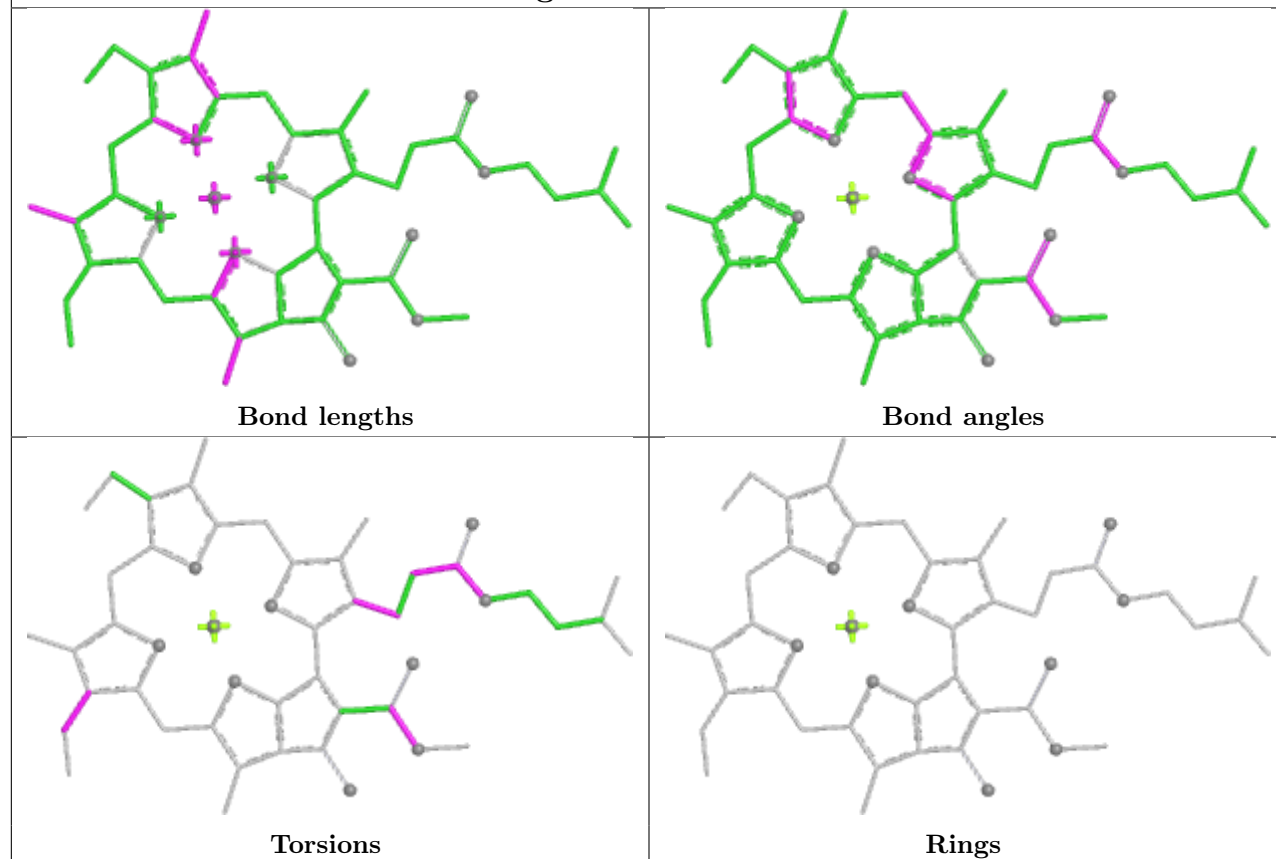


Ligand CLA 0 309

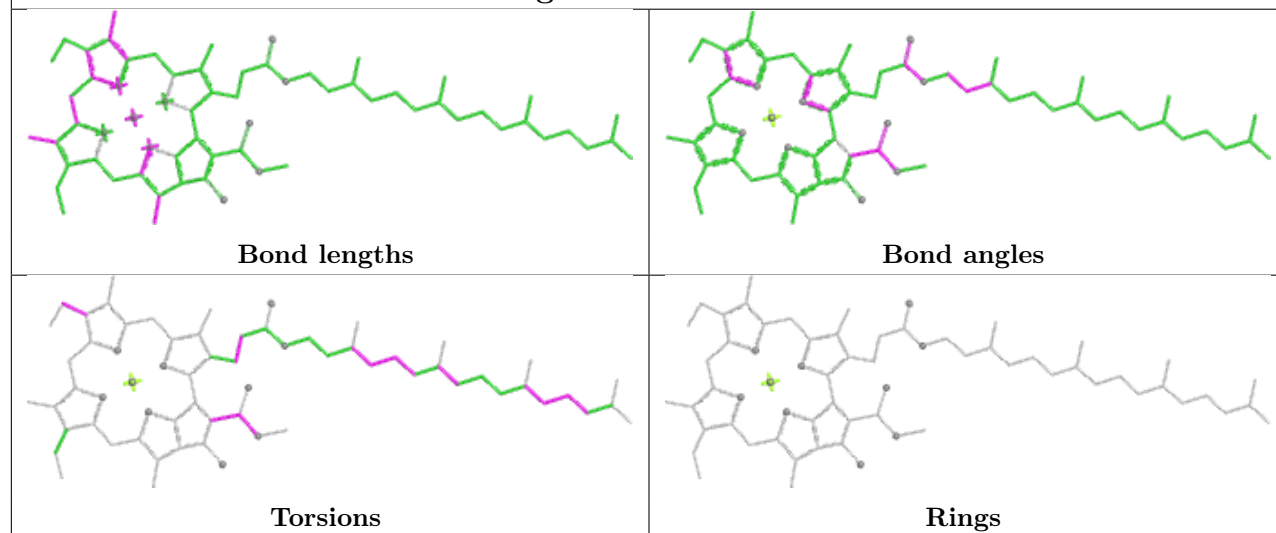


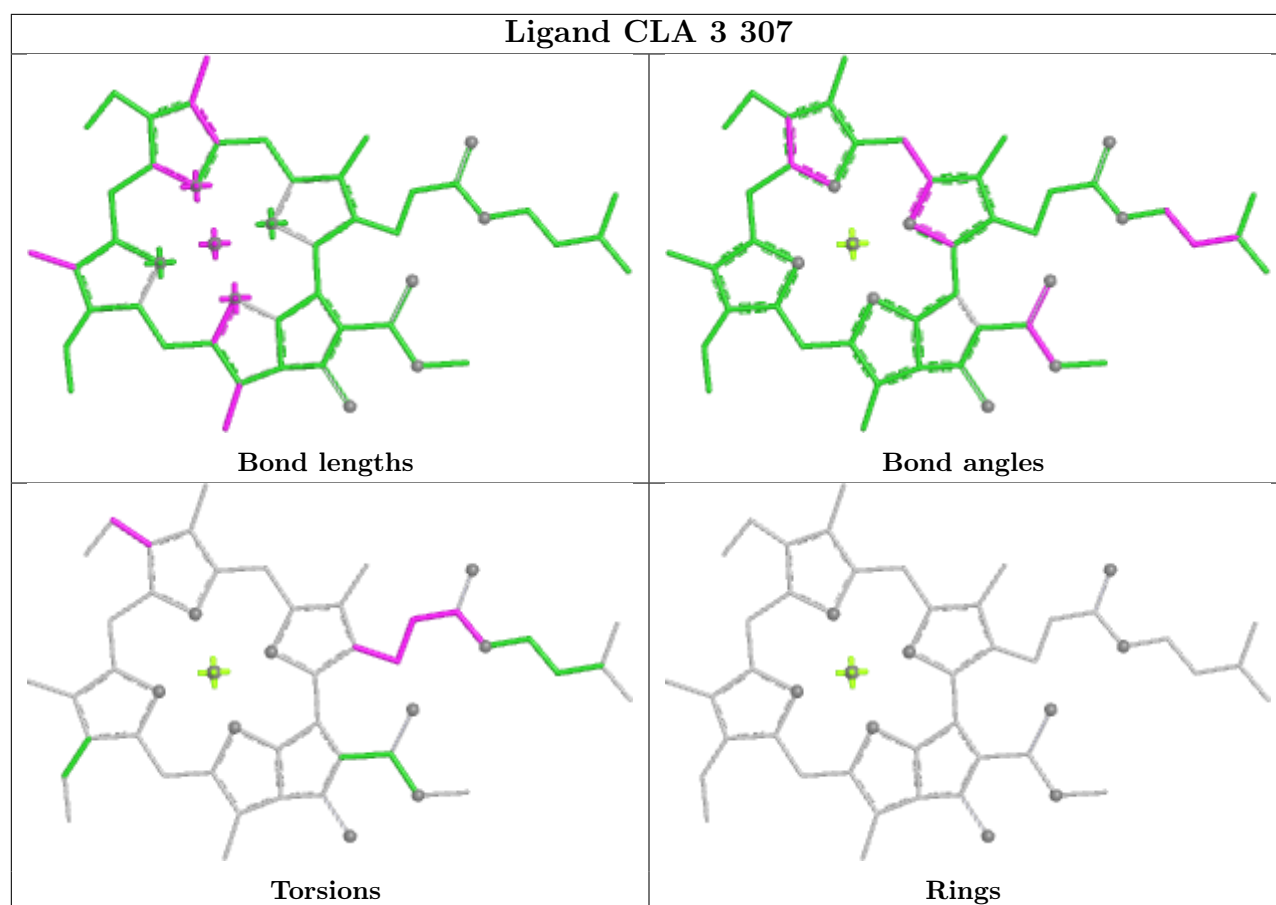


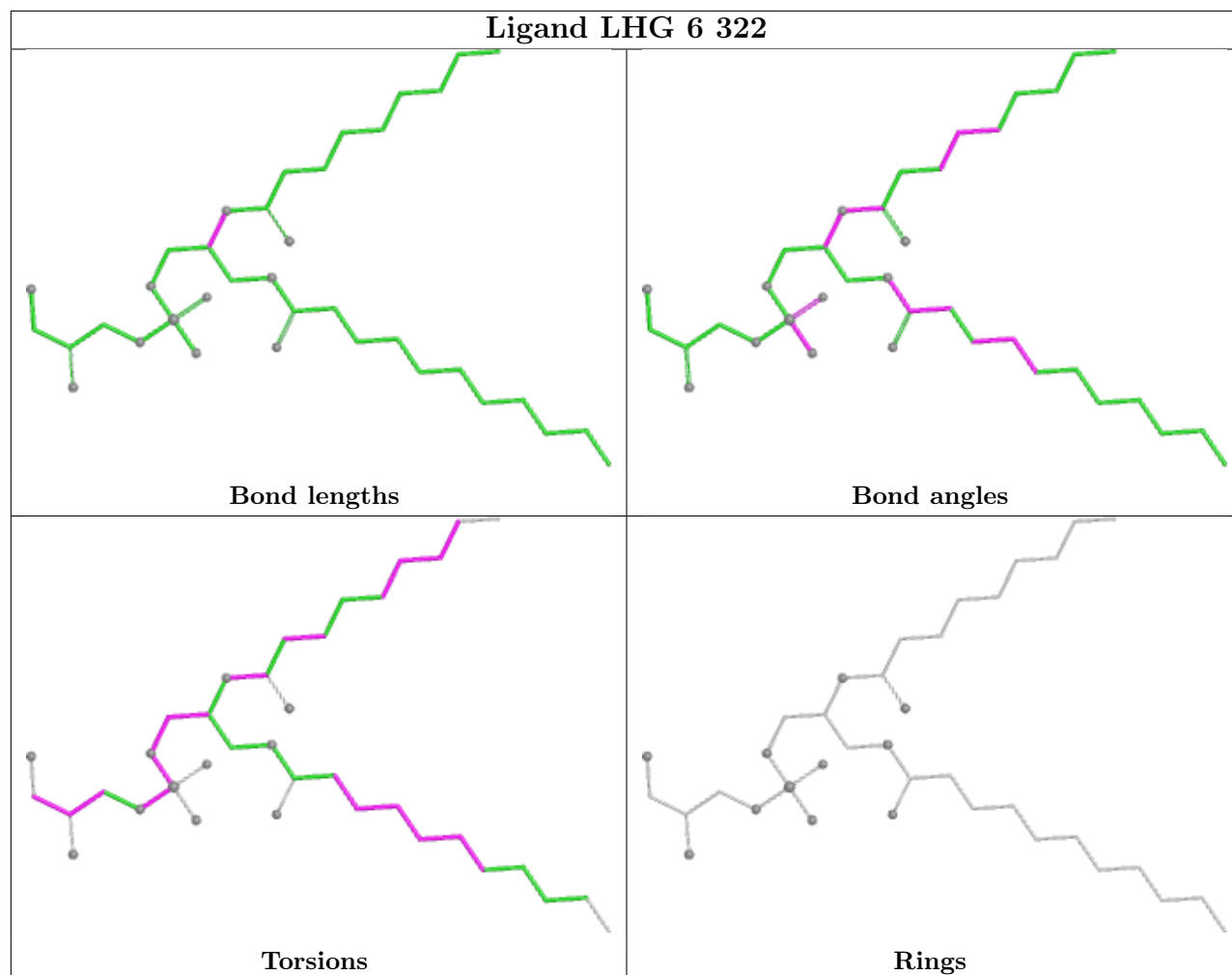
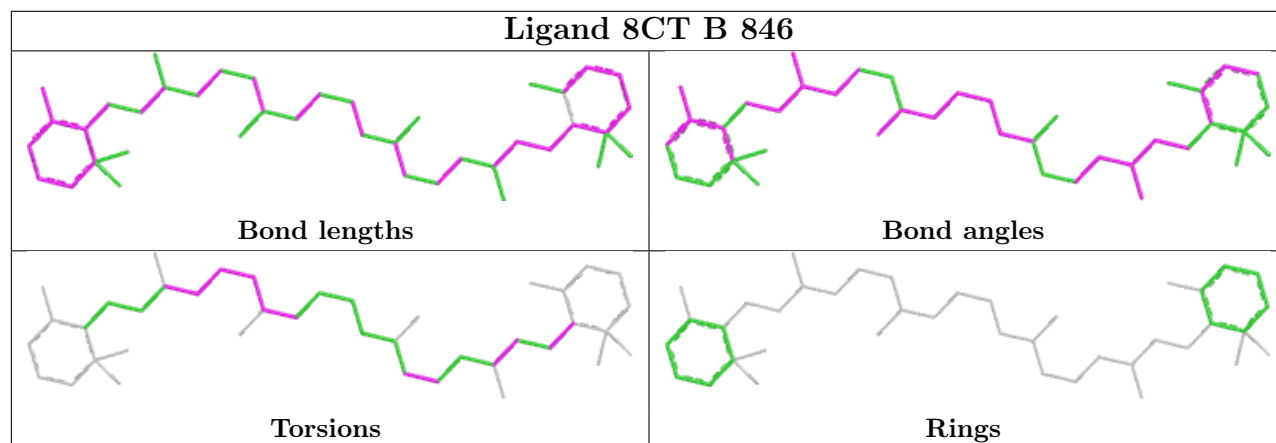
Ligand CLA 6 309

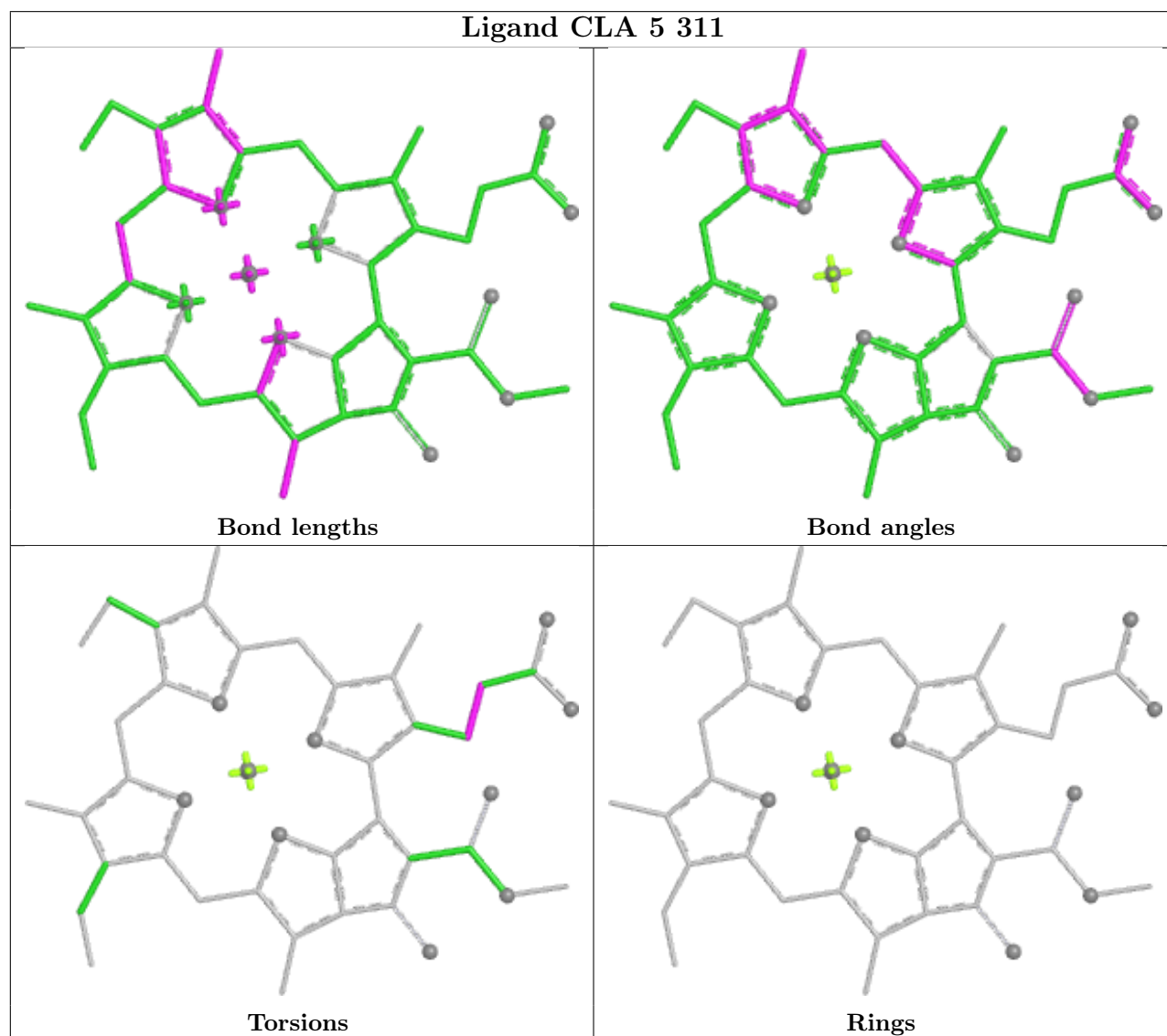
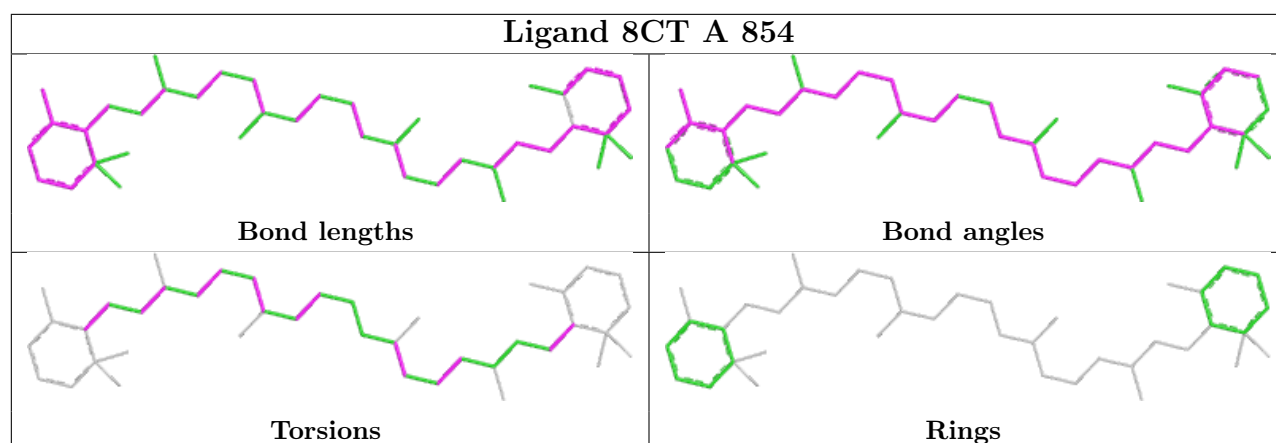


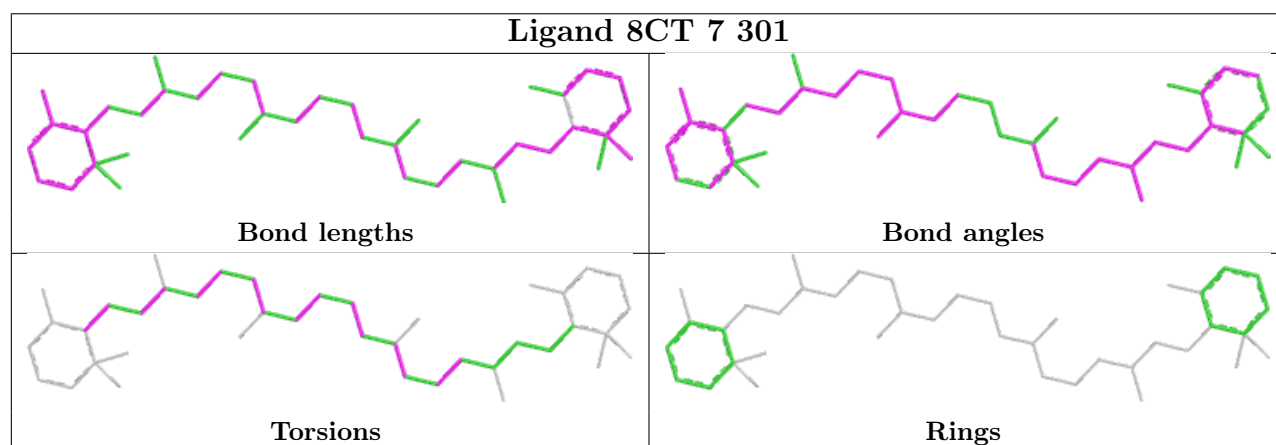
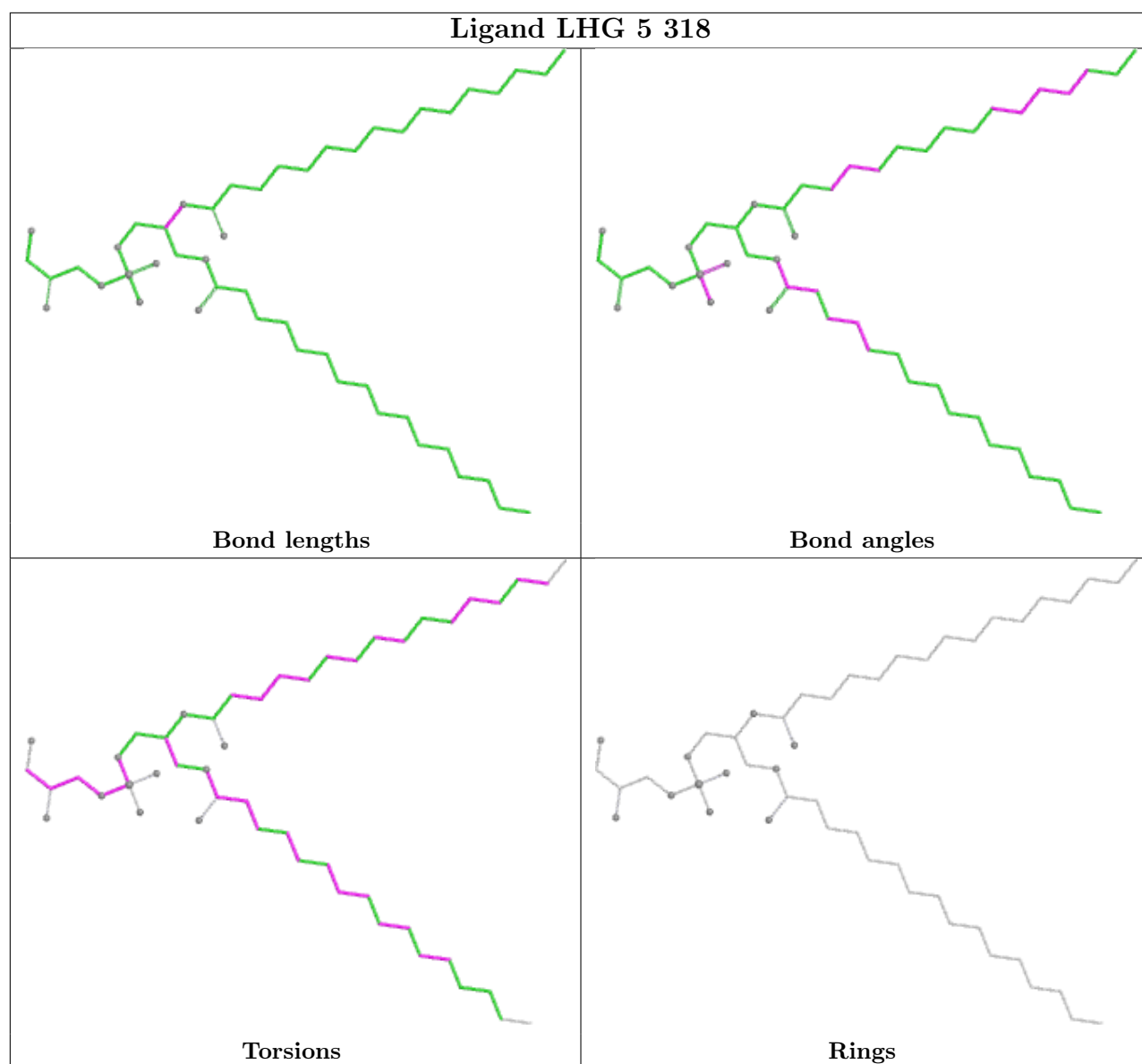
Ligand CLA 0 302

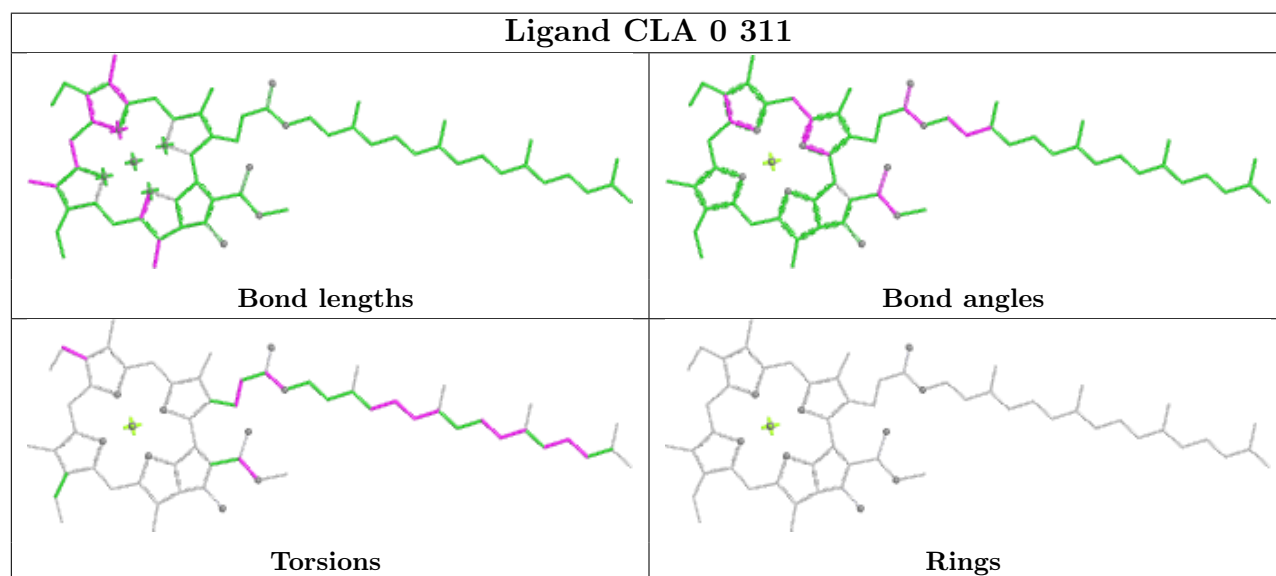
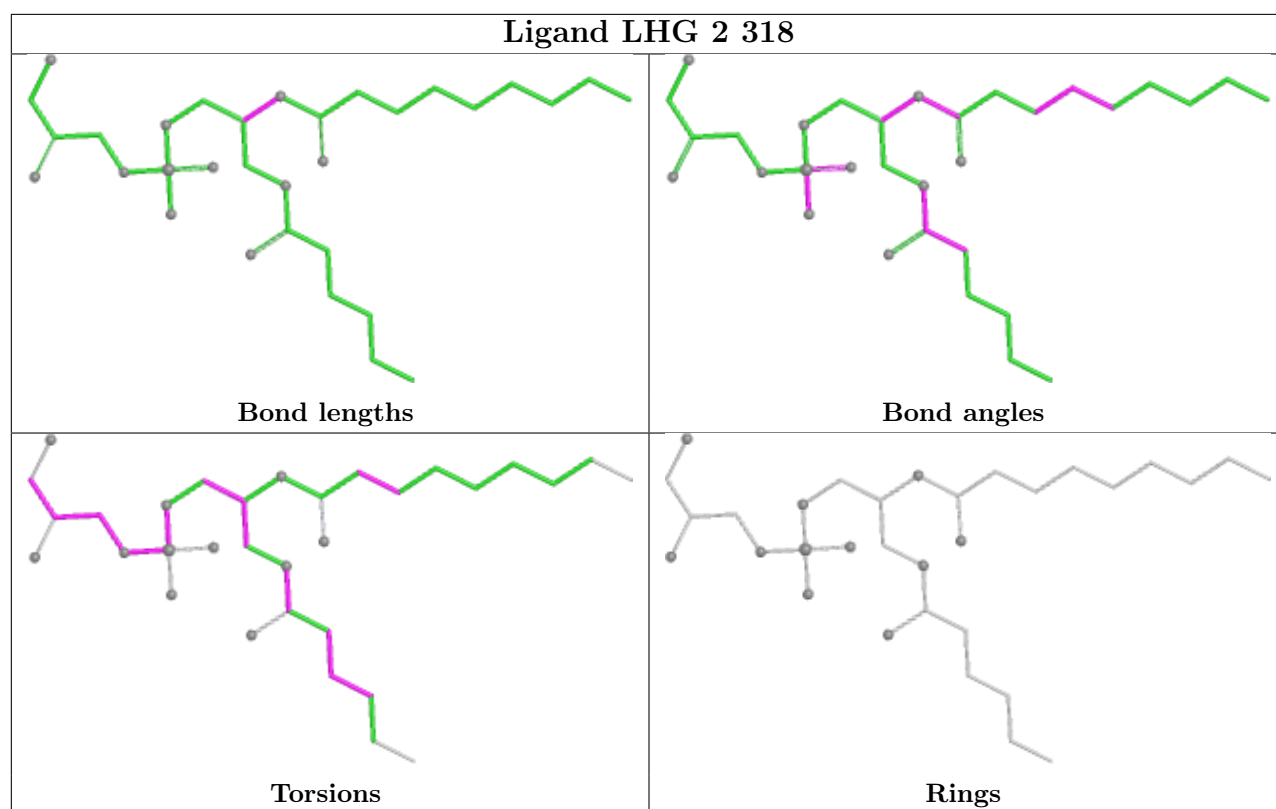


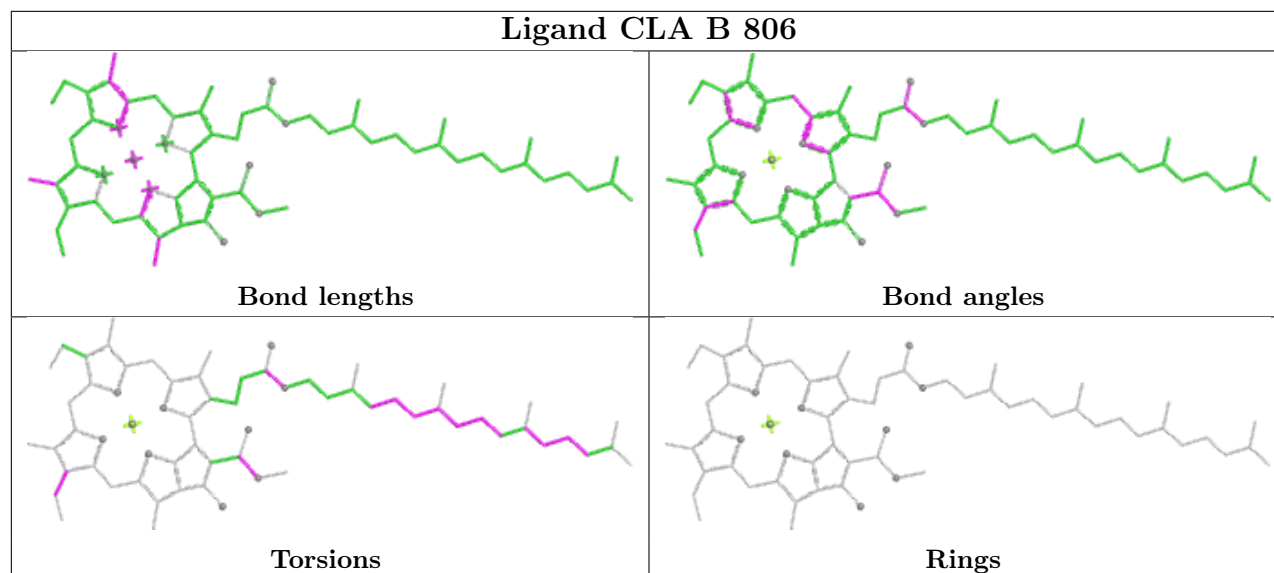
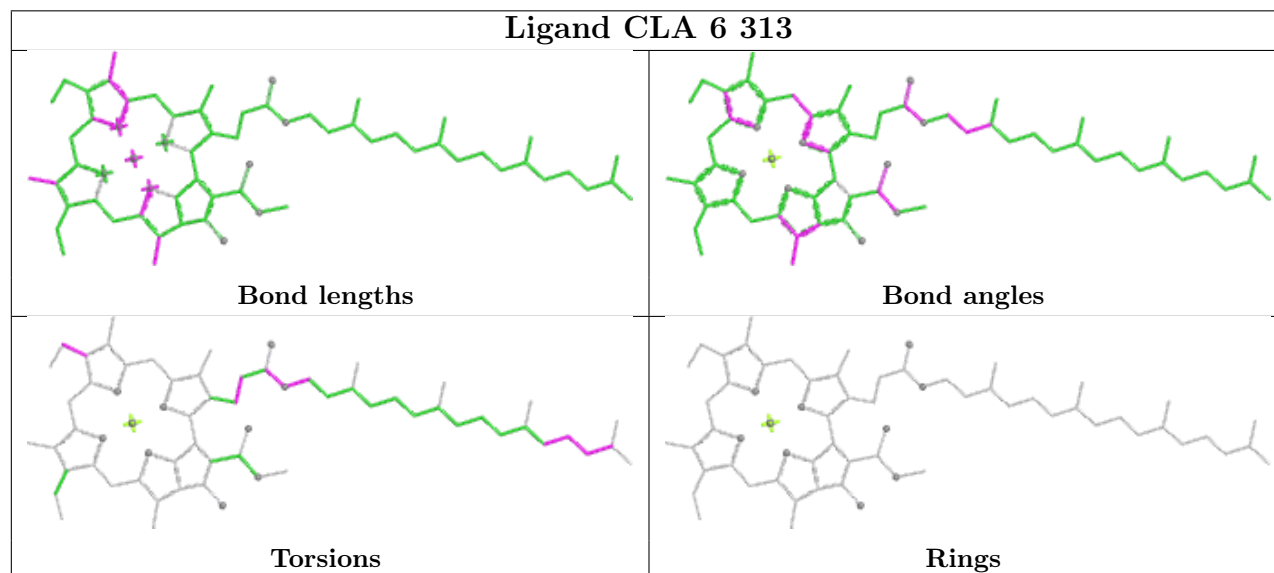
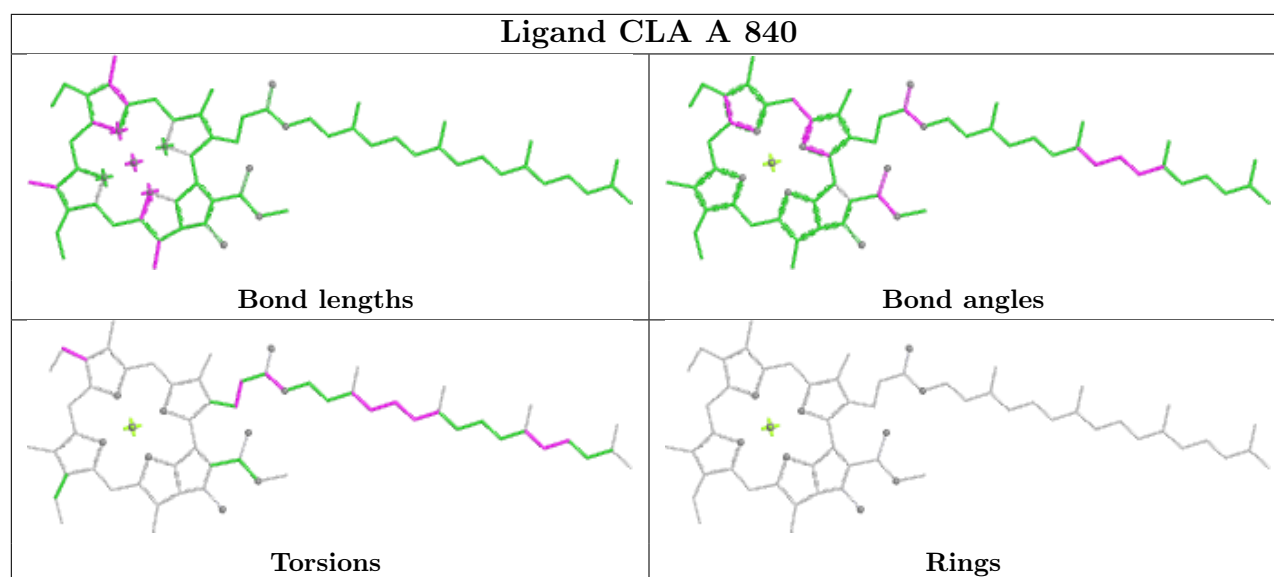


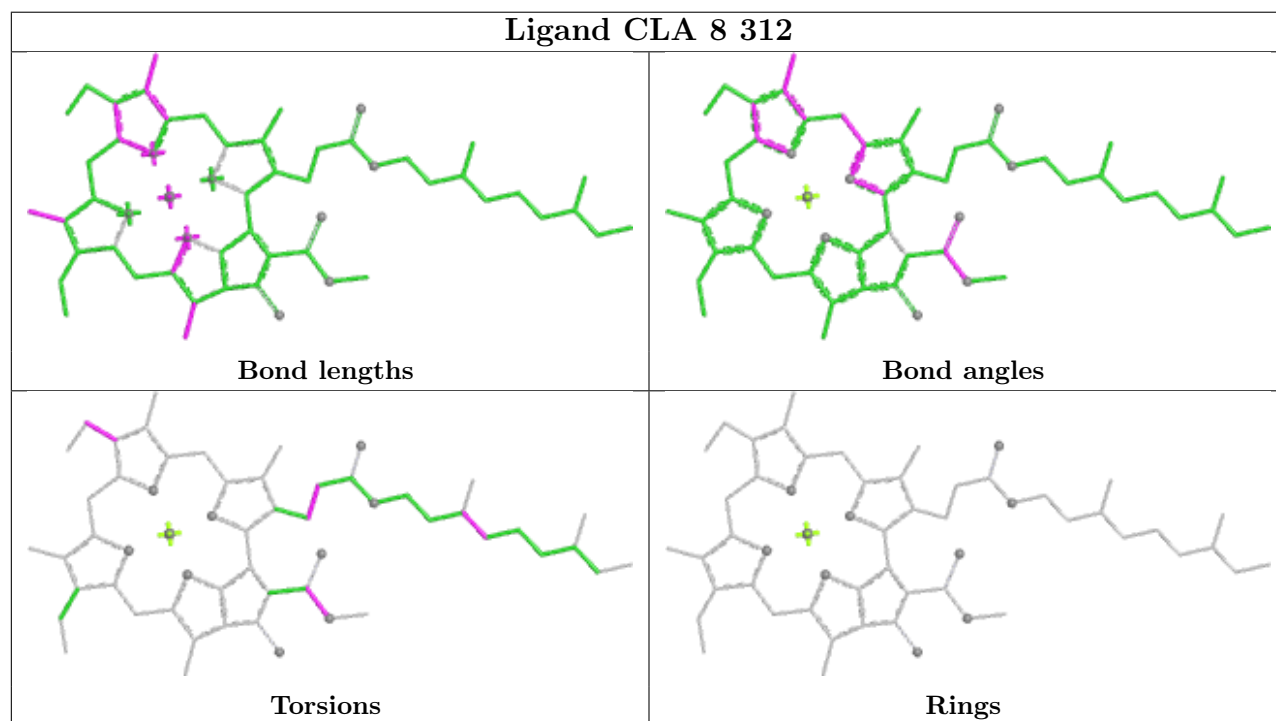
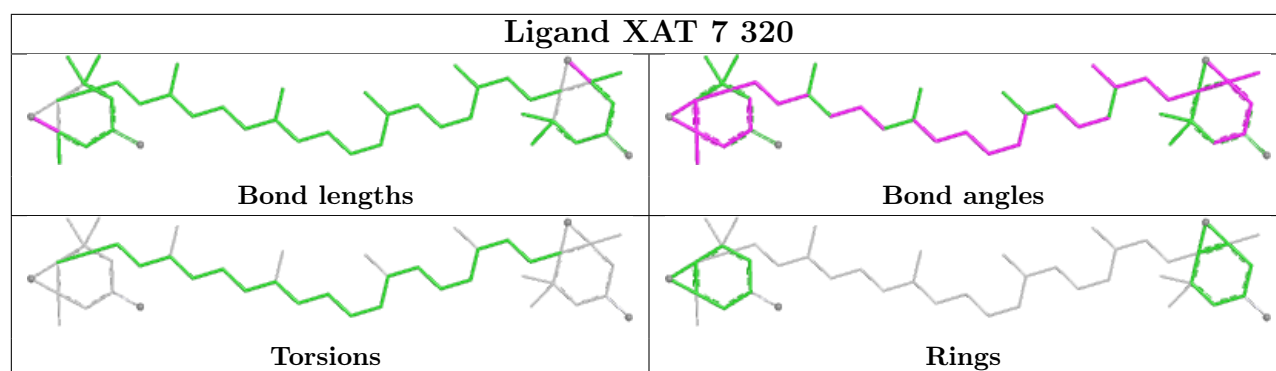
Ligand LHG 6 322**Ligand 8CT B 846**



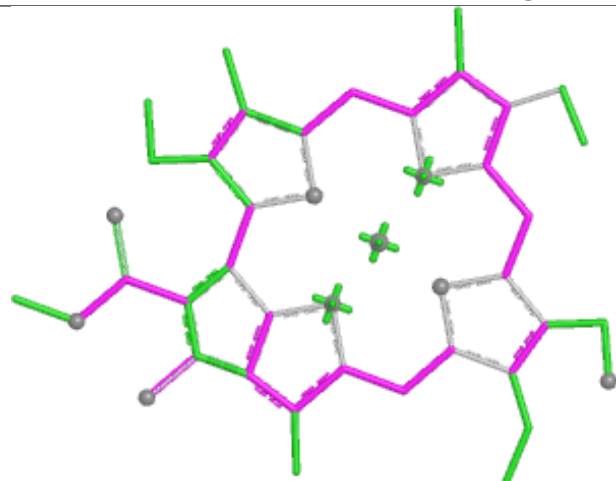




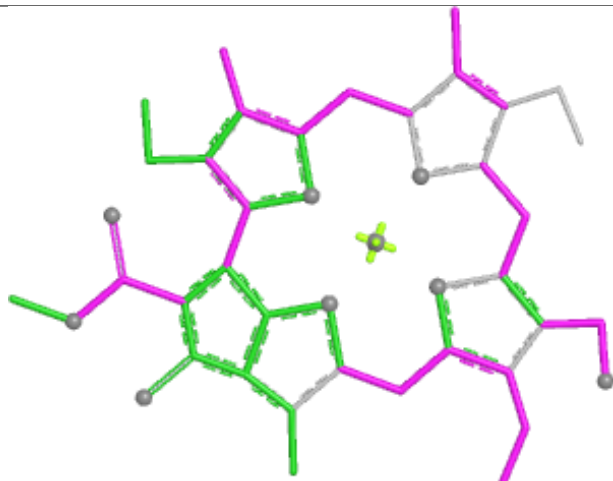




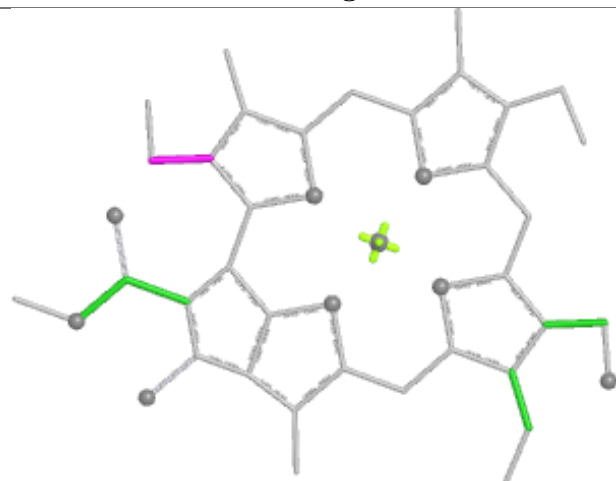
Ligand CHL 6 306



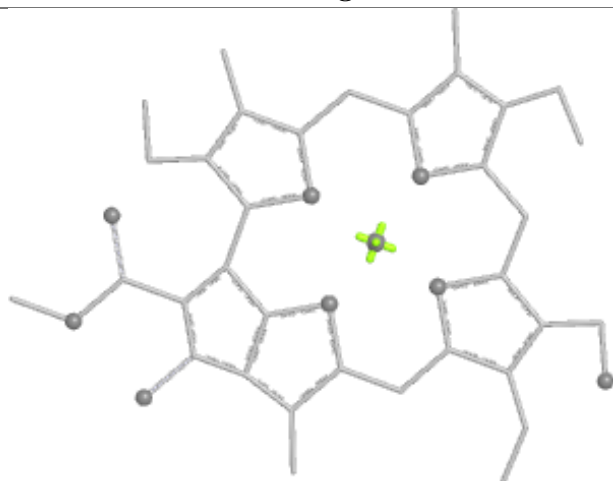
Bond lengths



Bond angles

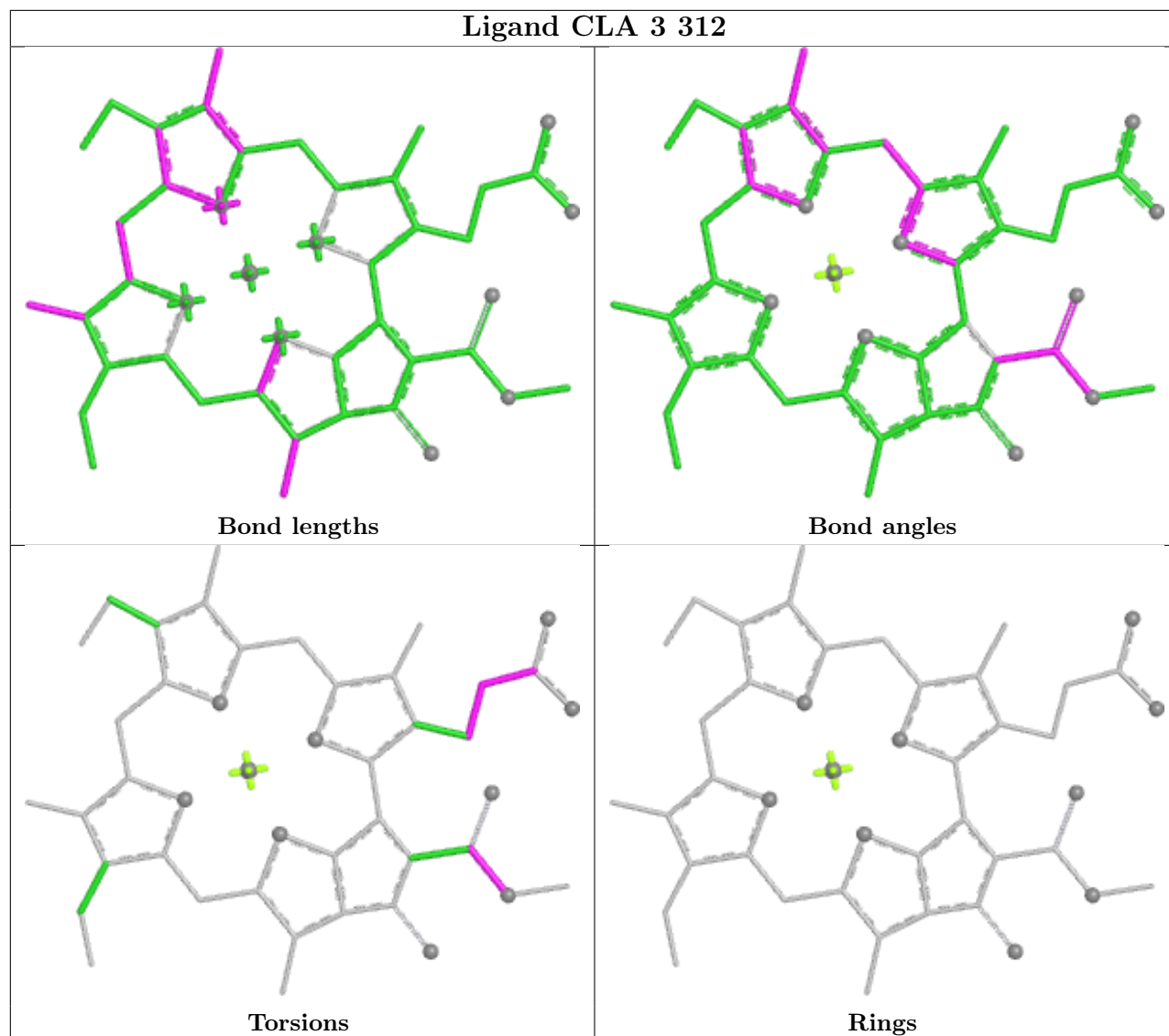


Torsions

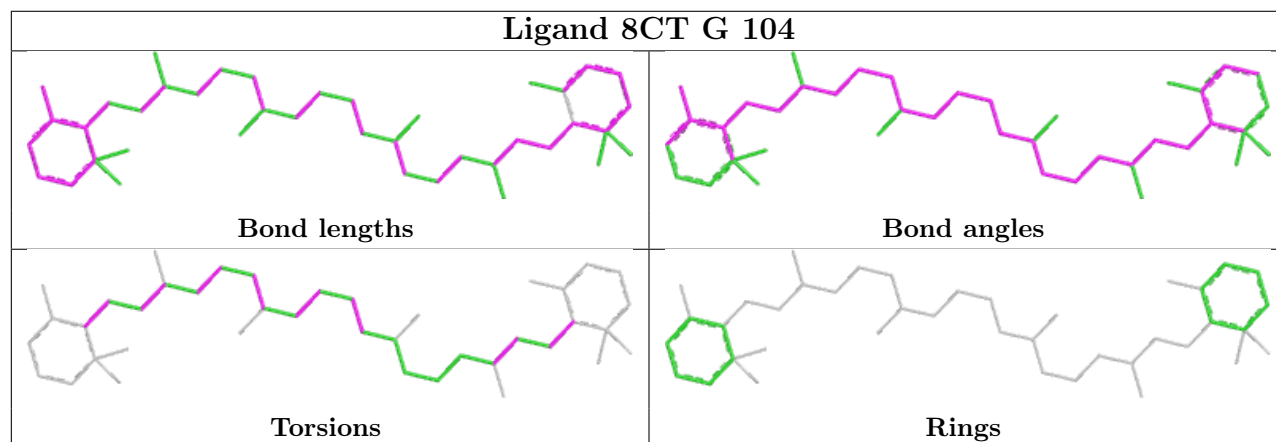


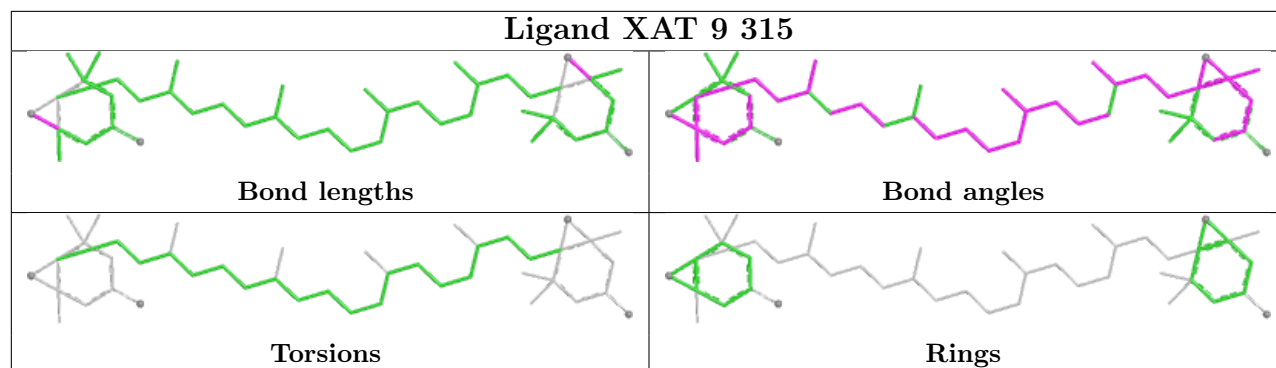
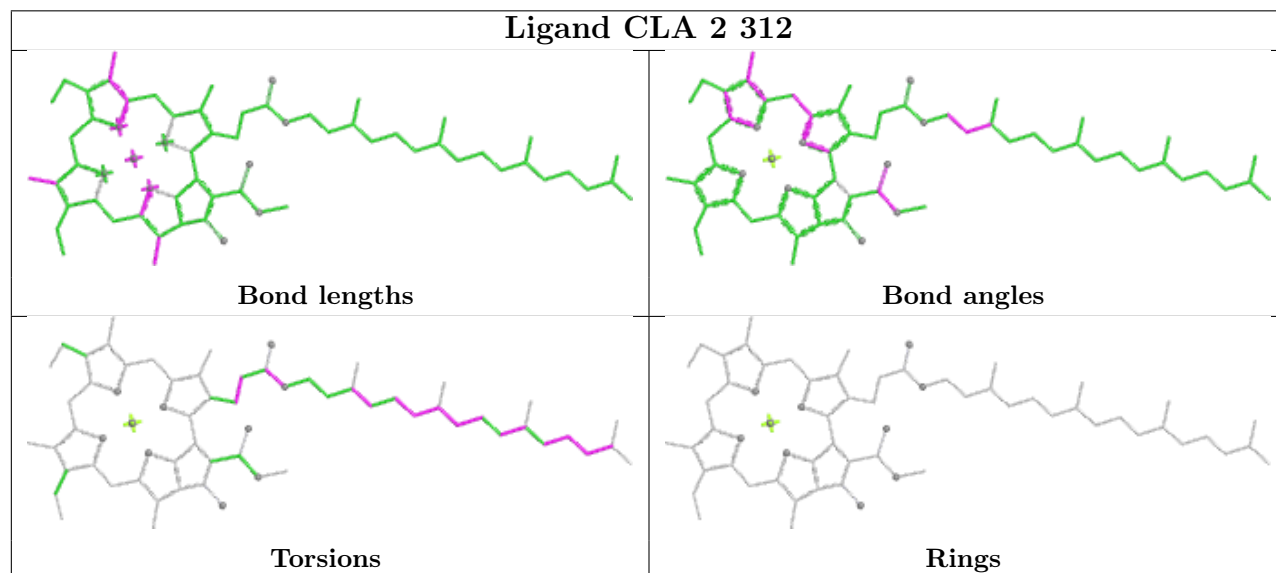
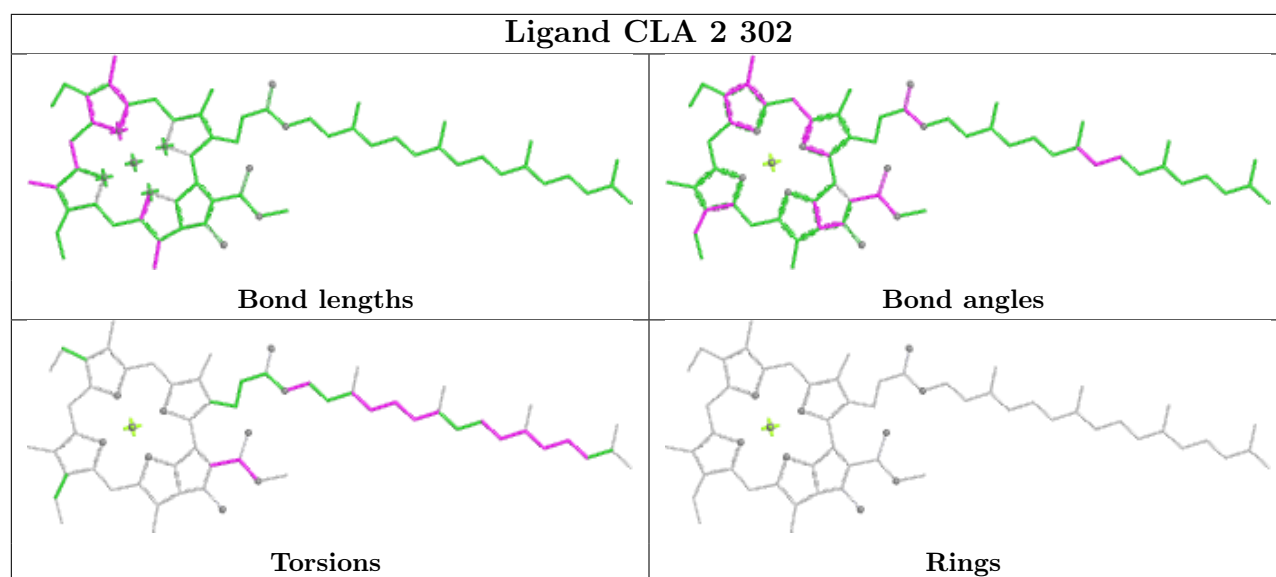
Rings

Ligand CLA 3 312

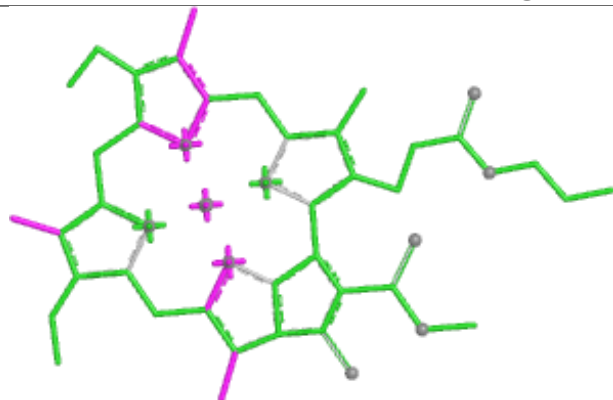


Ligand 8CT G 104

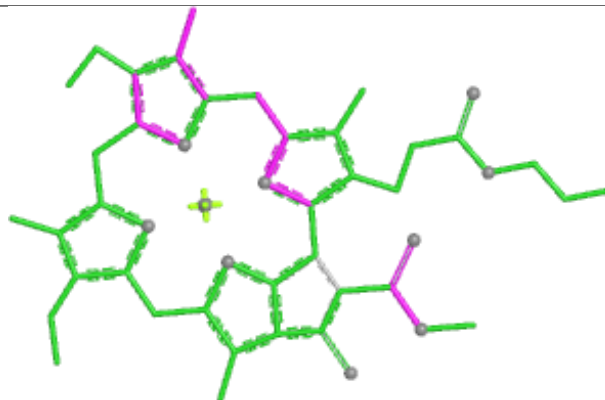




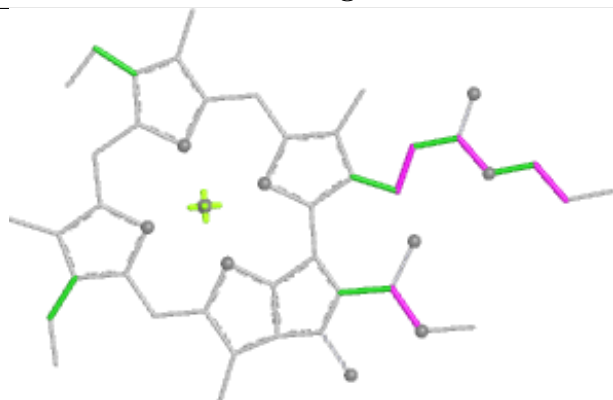
Ligand CLA 9 304



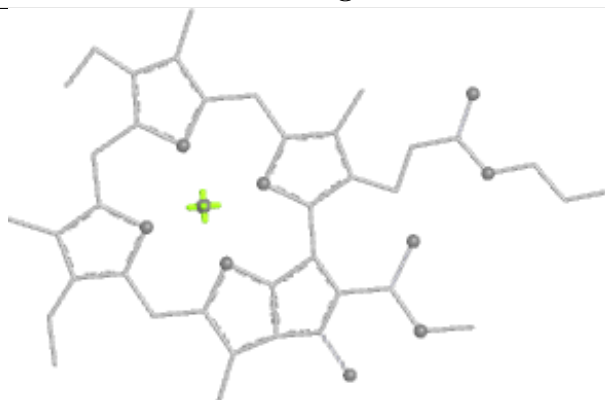
Bond lengths



Bond angles

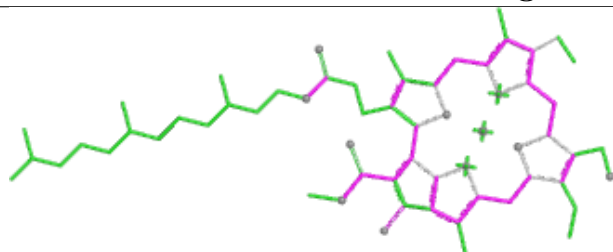


Torsions

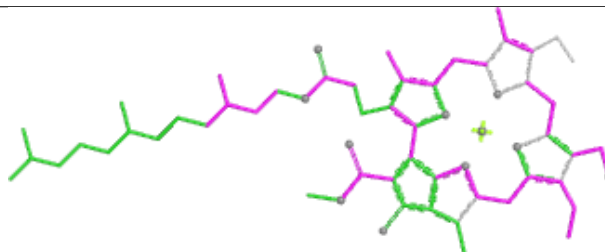


Rings

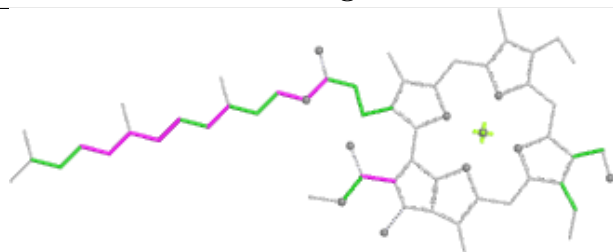
Ligand CHL 9 302



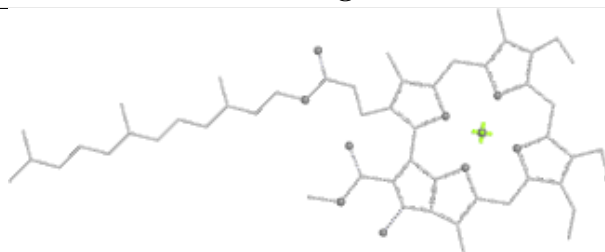
Bond lengths



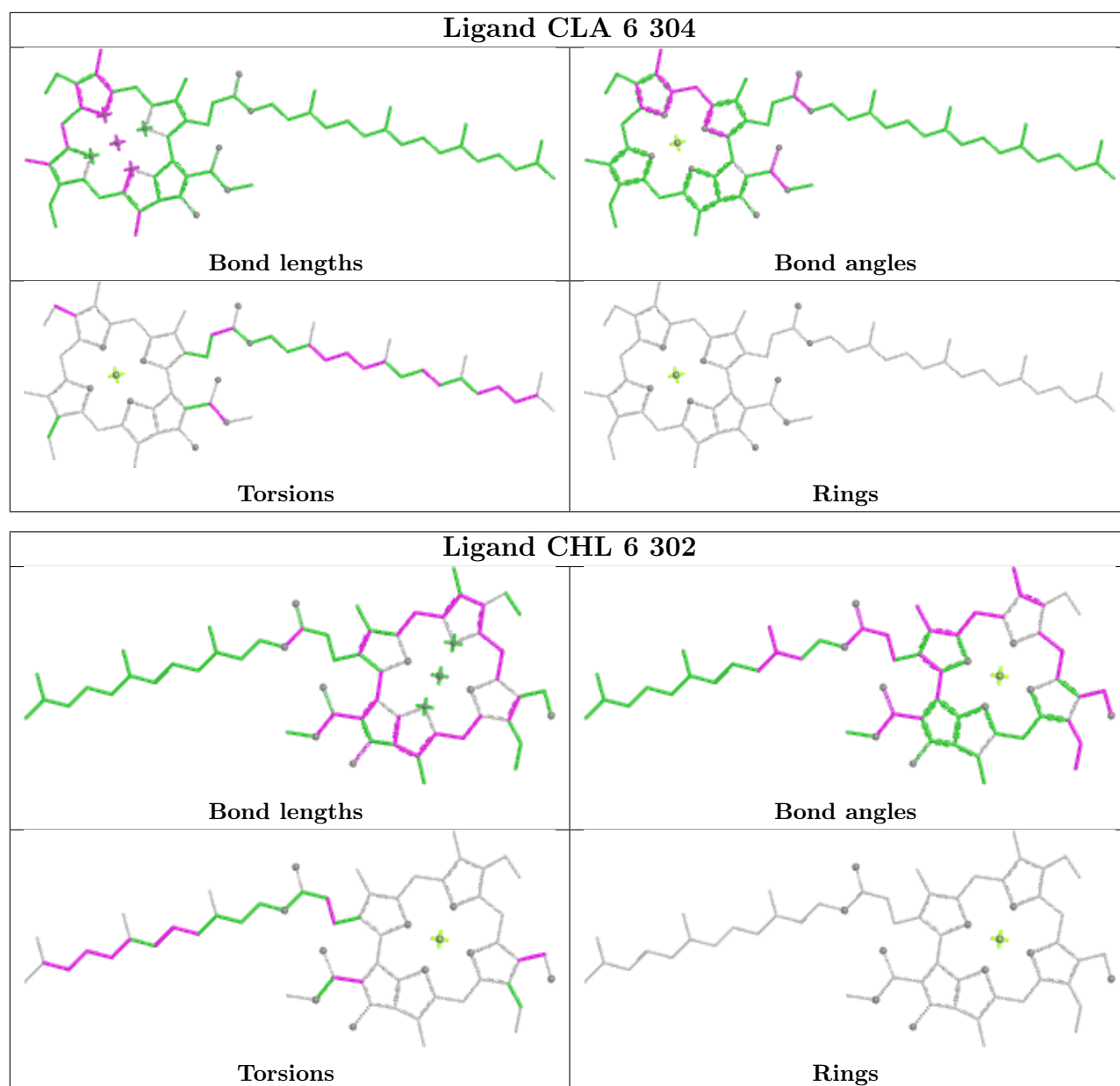
Bond angles



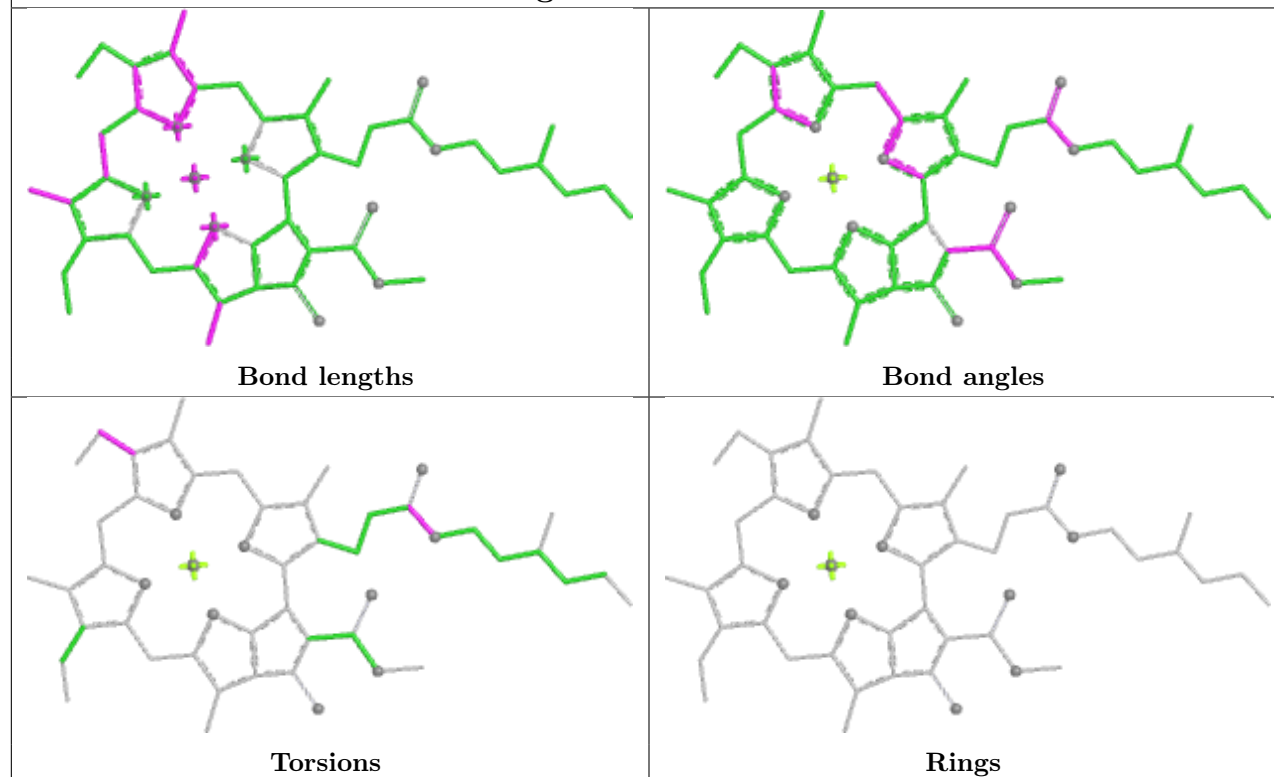
Torsions



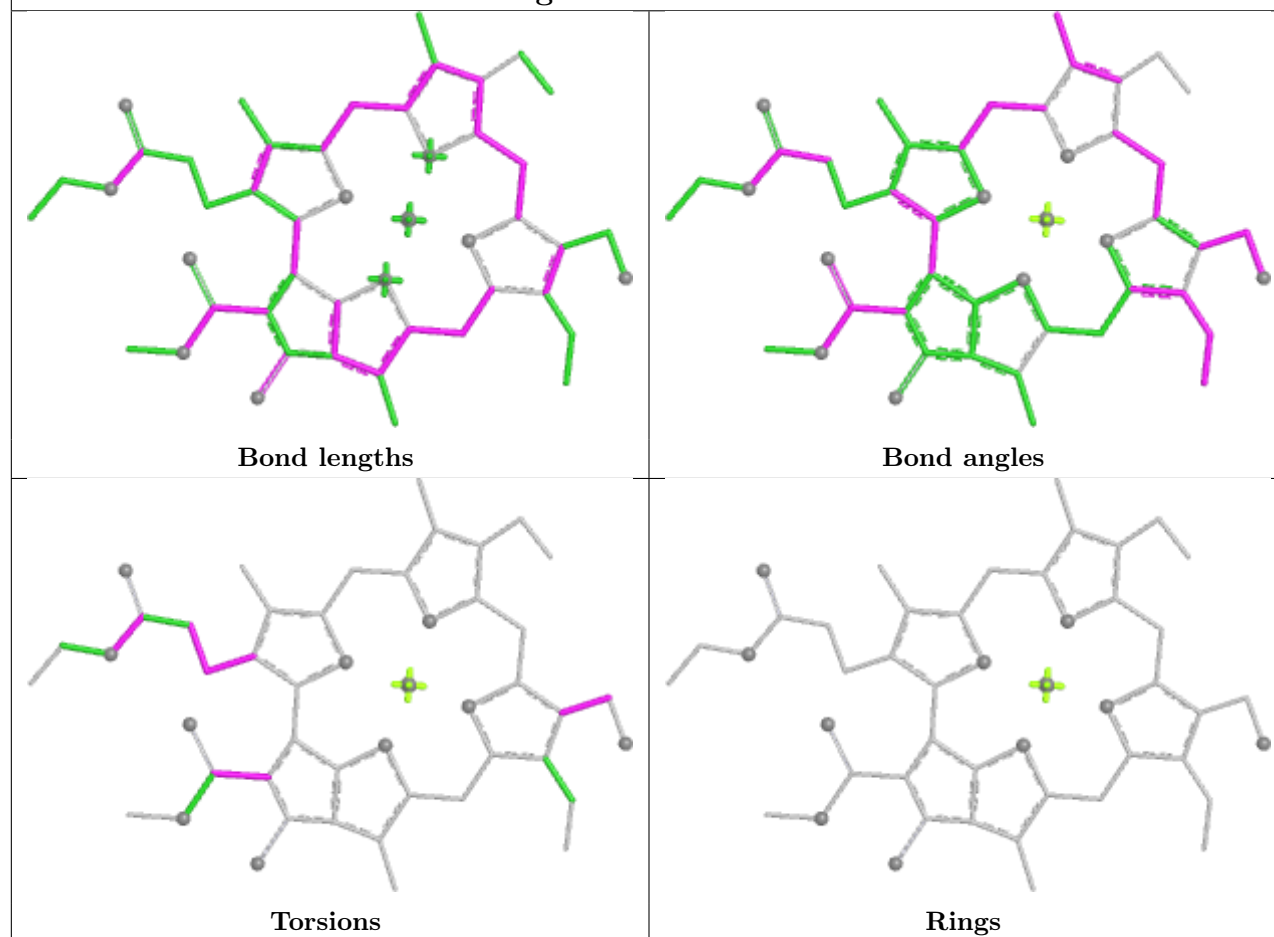
Rings

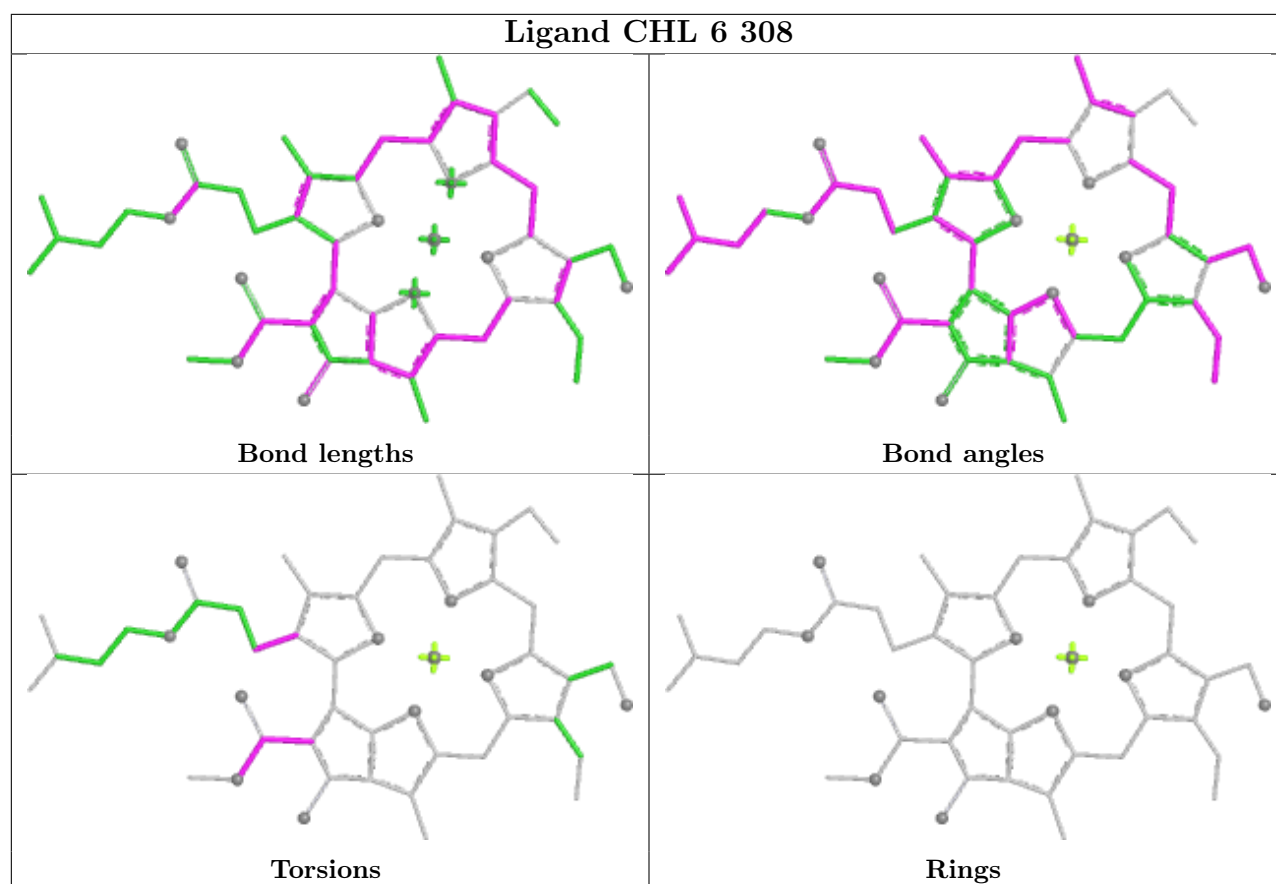


Ligand CLA 7 312

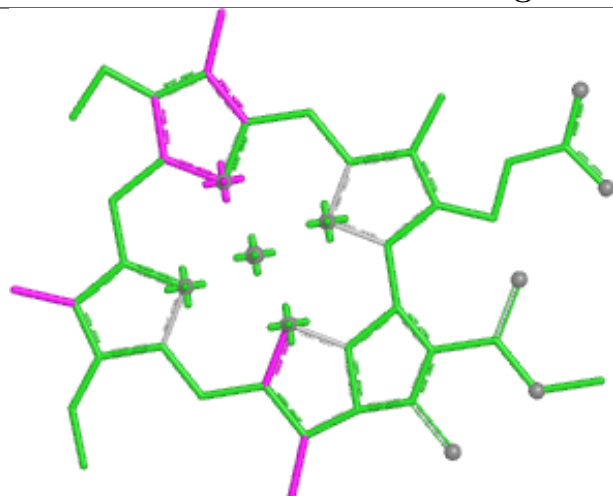


Ligand CHL 5 306

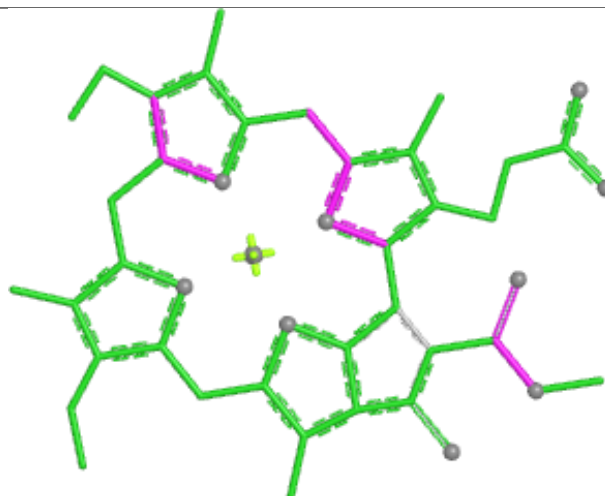




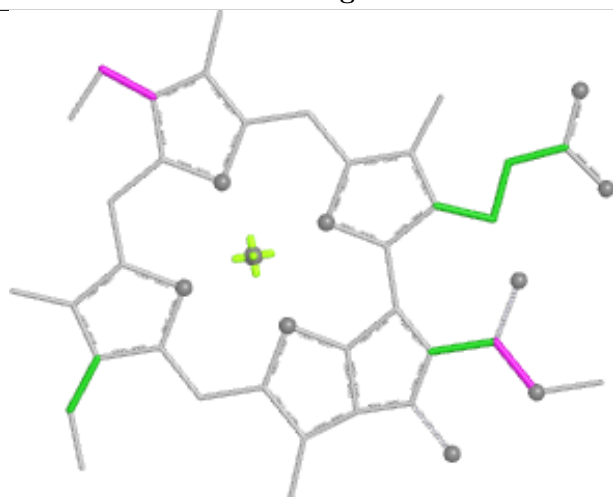
Ligand CLA B 835



Bond lengths



Bond angles

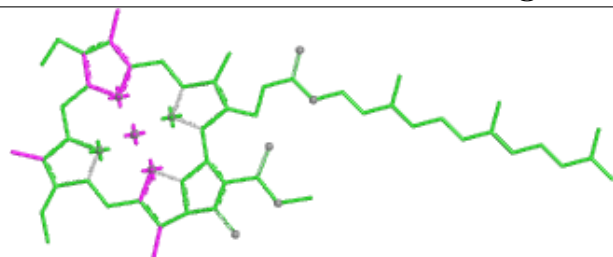


Torsions

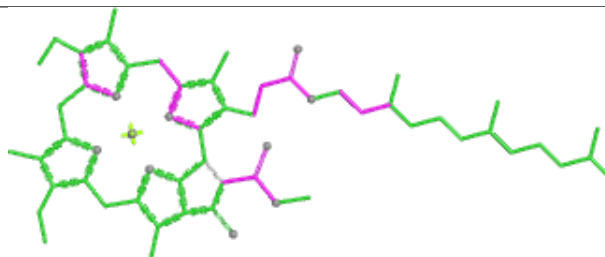


Rings

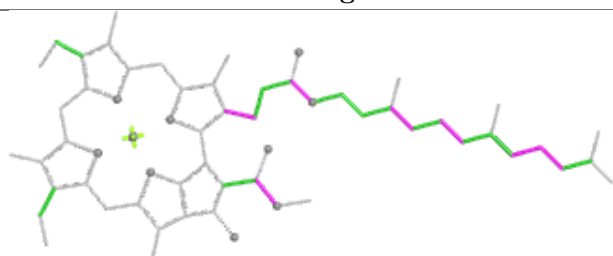
Ligand CLA 6 310



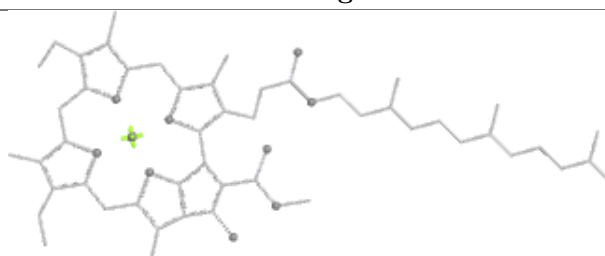
Bond lengths



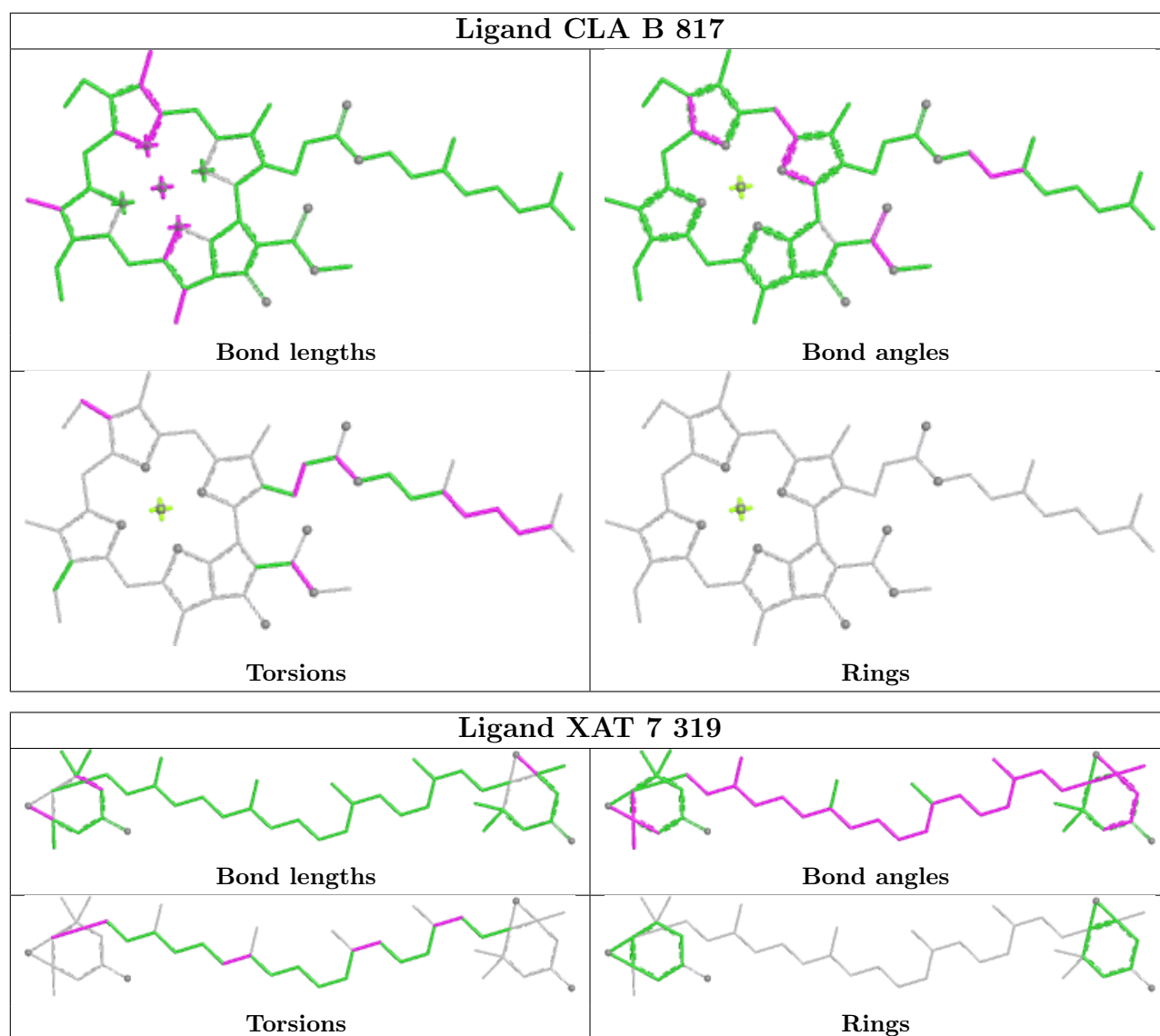
Bond angles

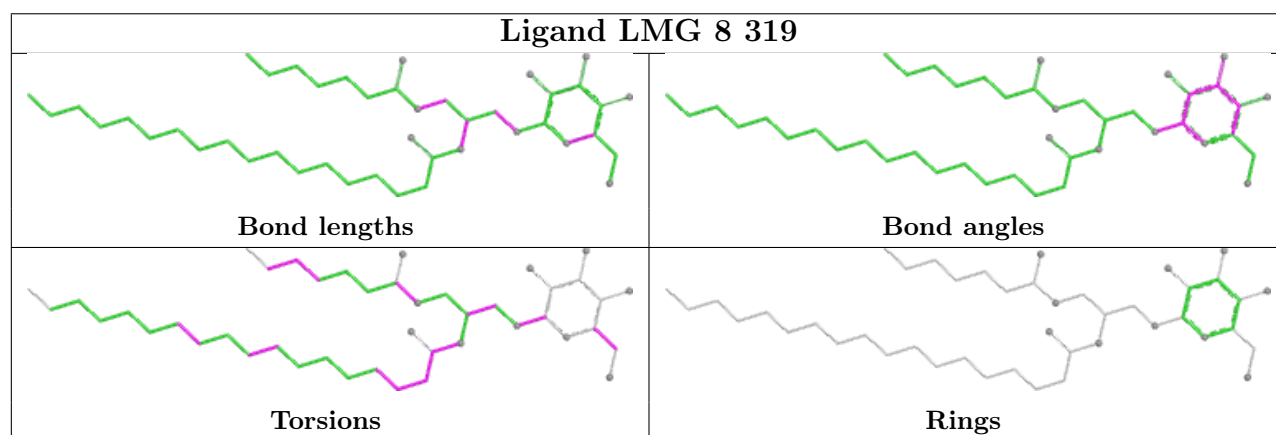
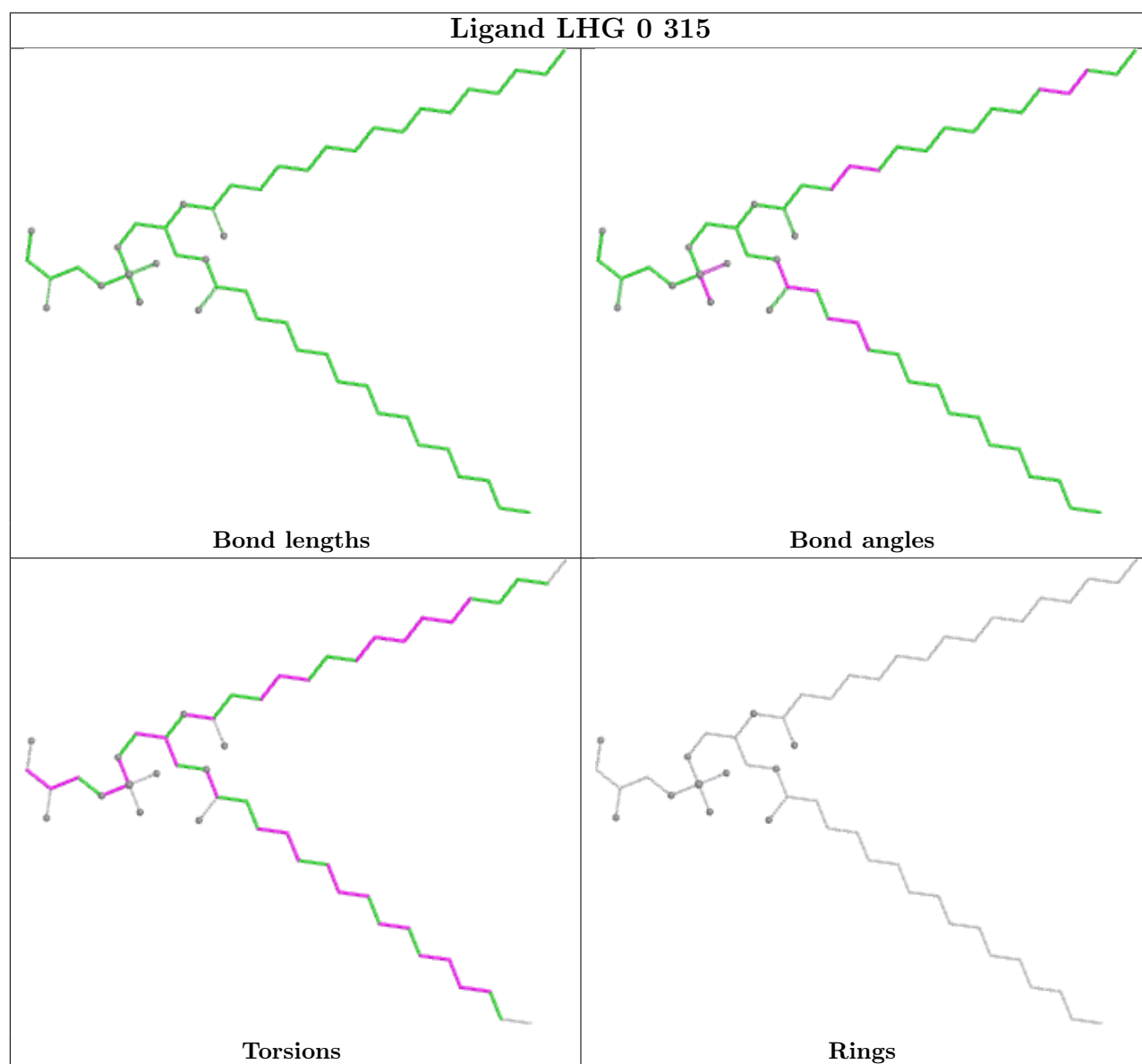


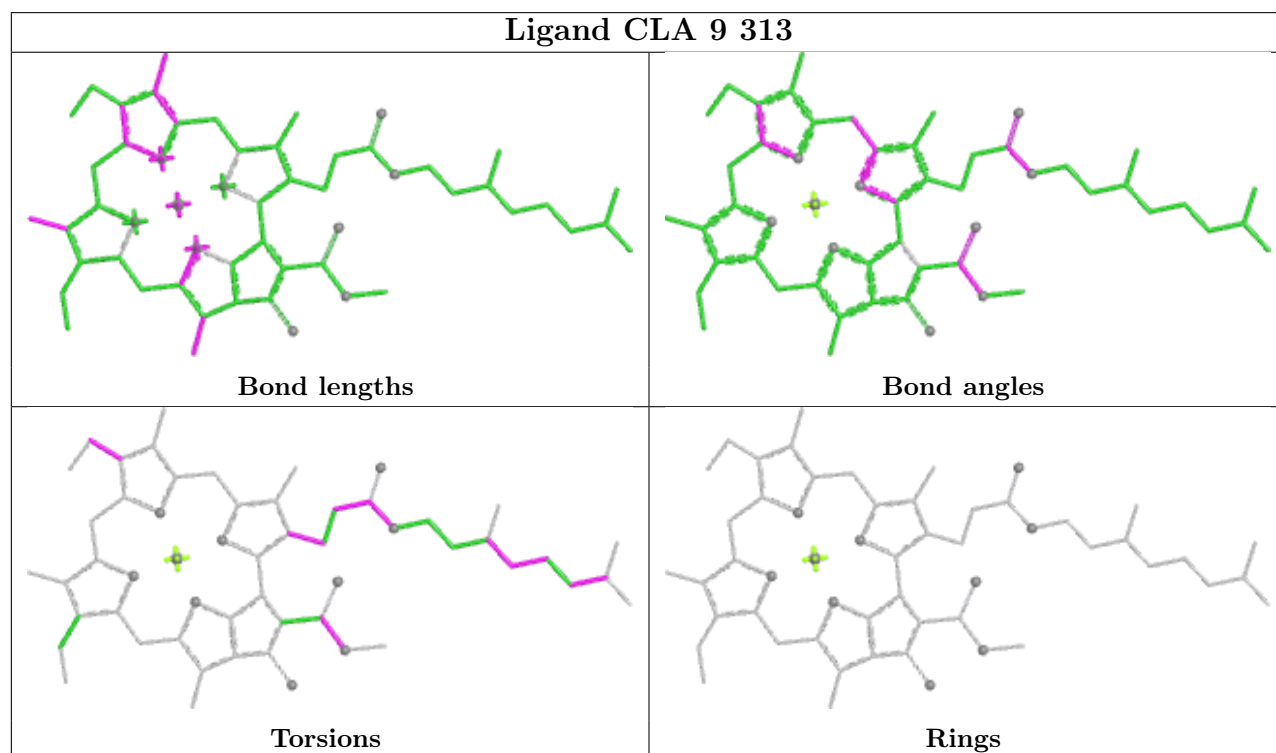
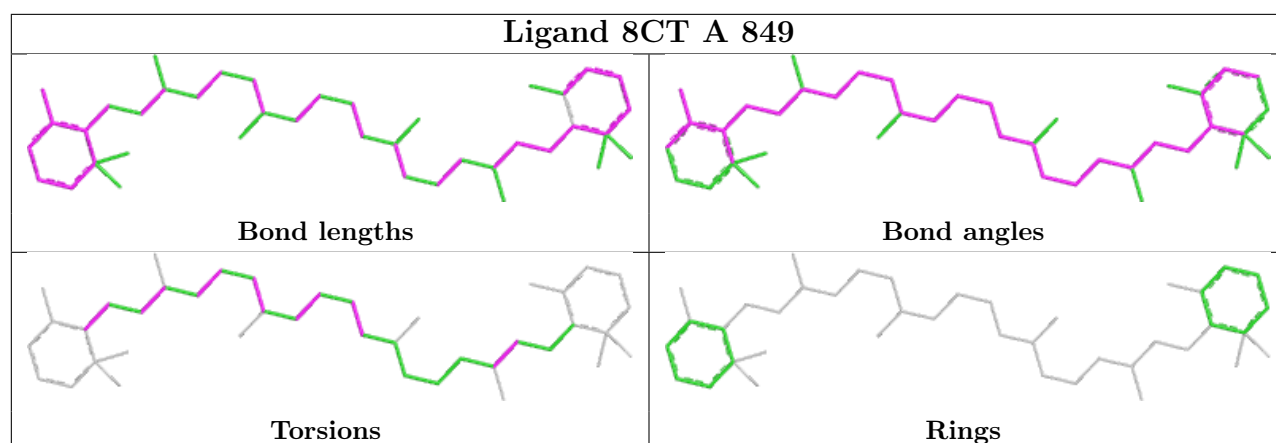
Torsions



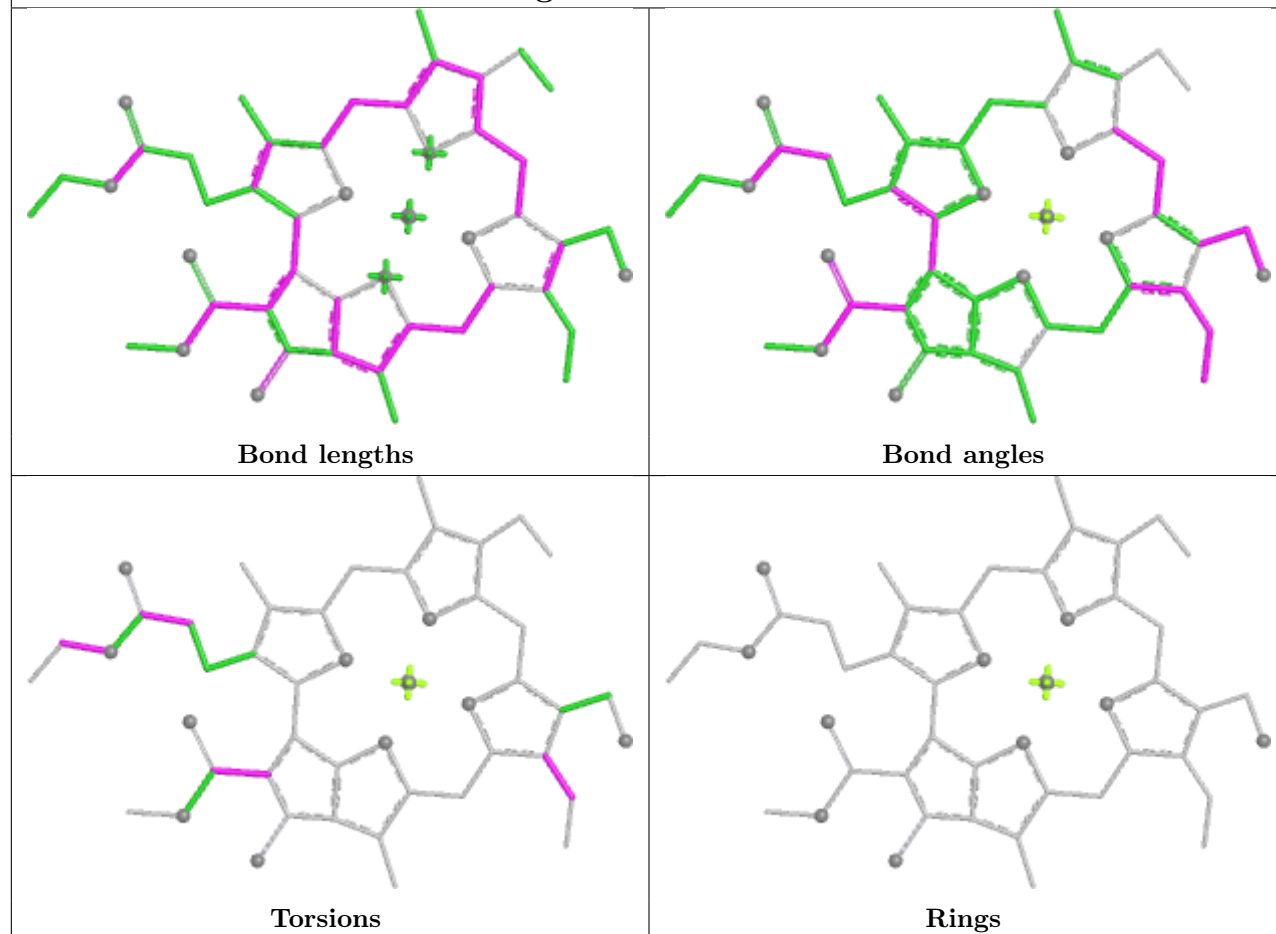
Rings



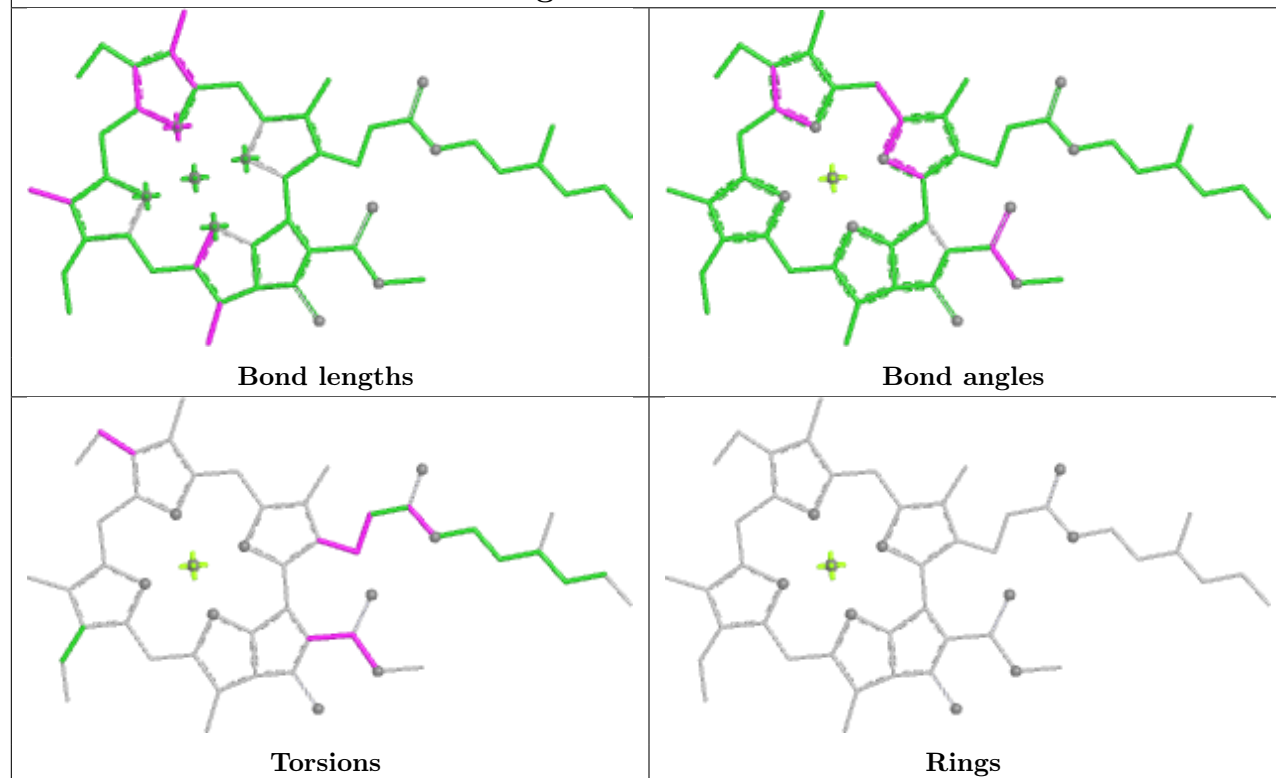


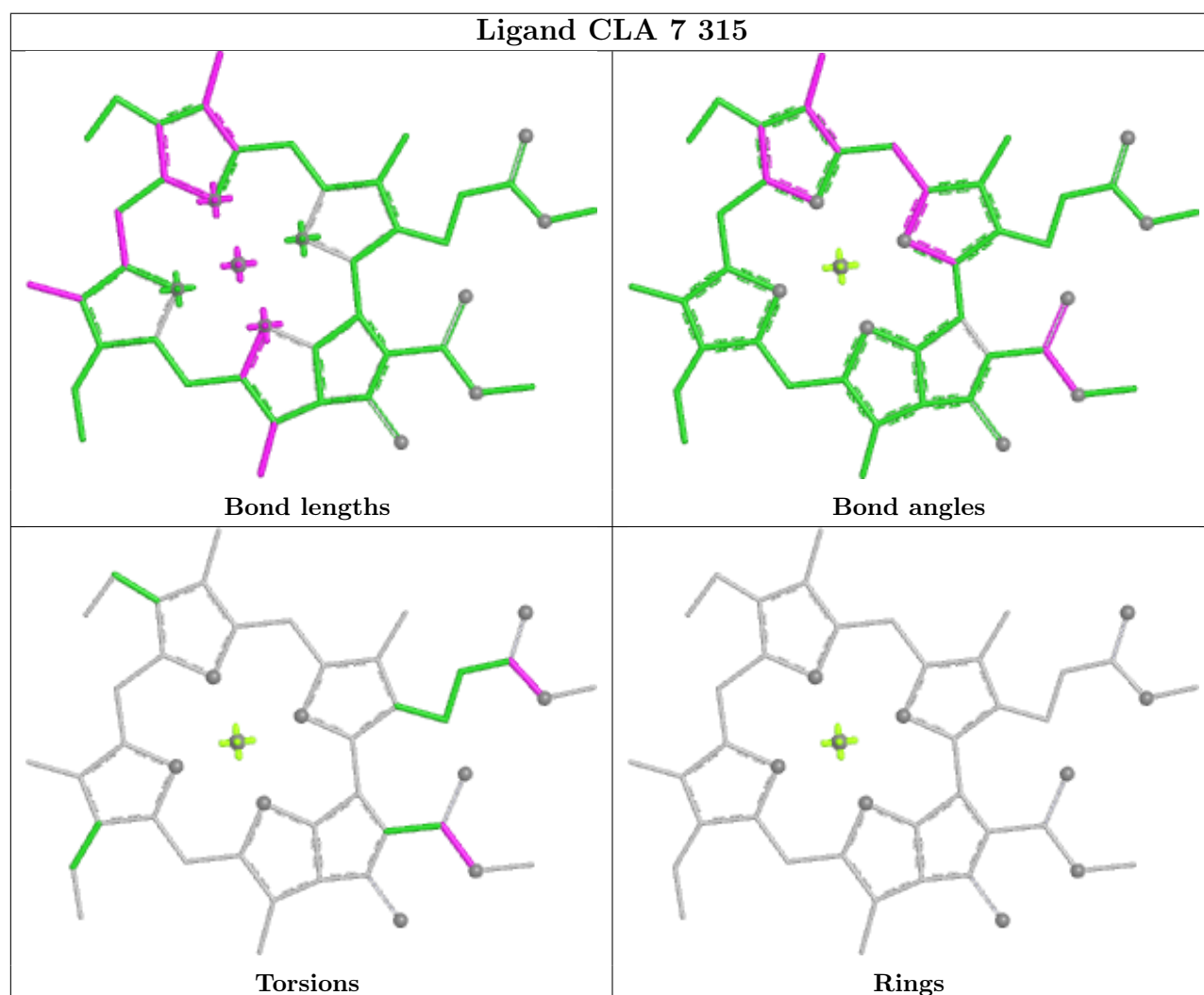
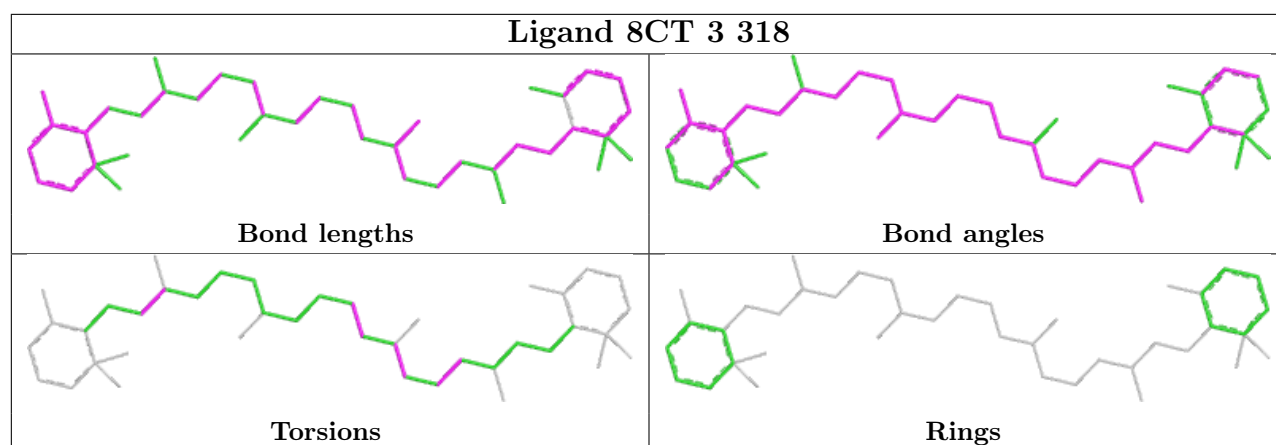


Ligand CHL 0 306

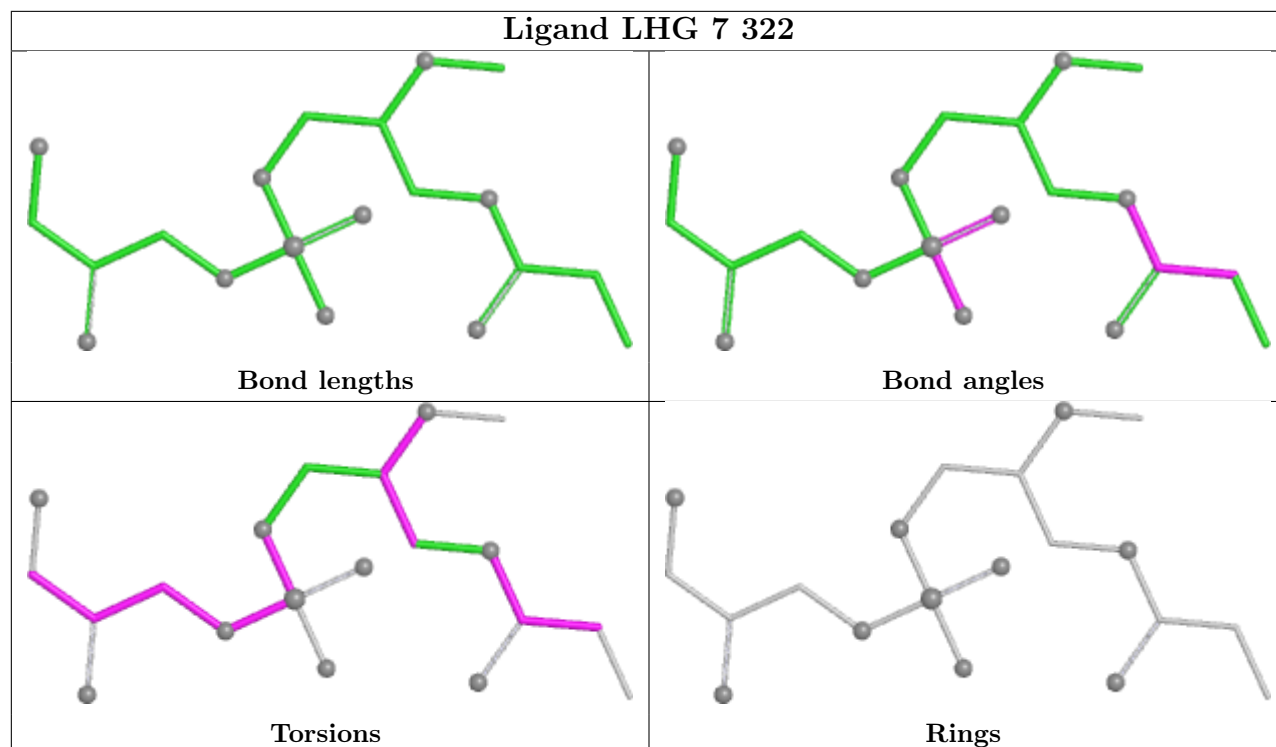


Ligand CLA 5 304

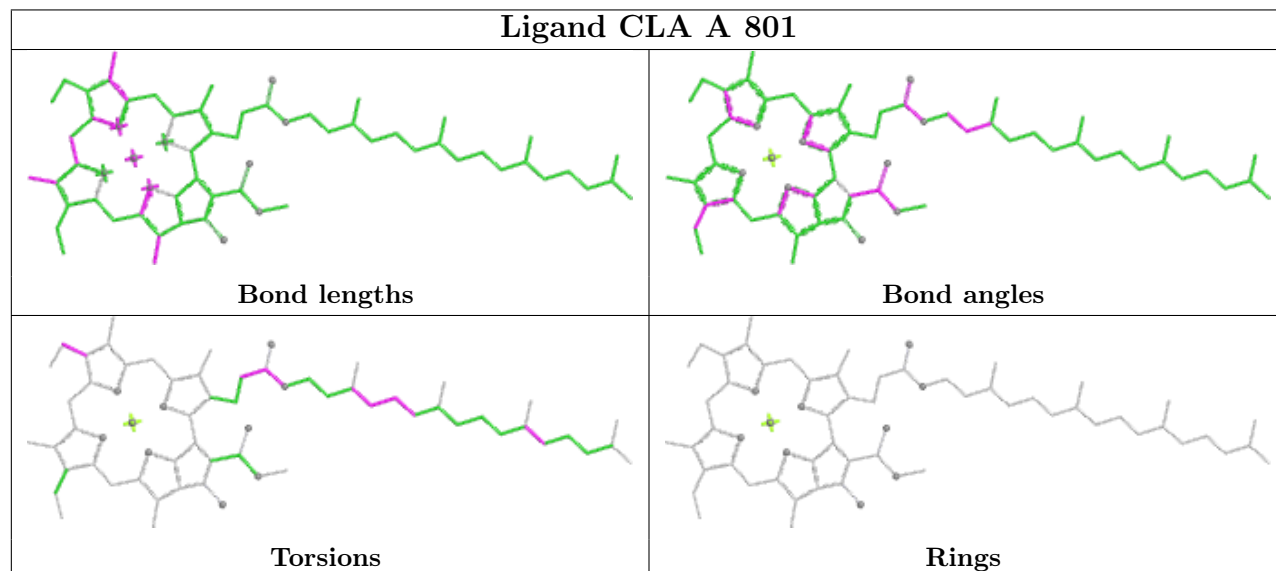




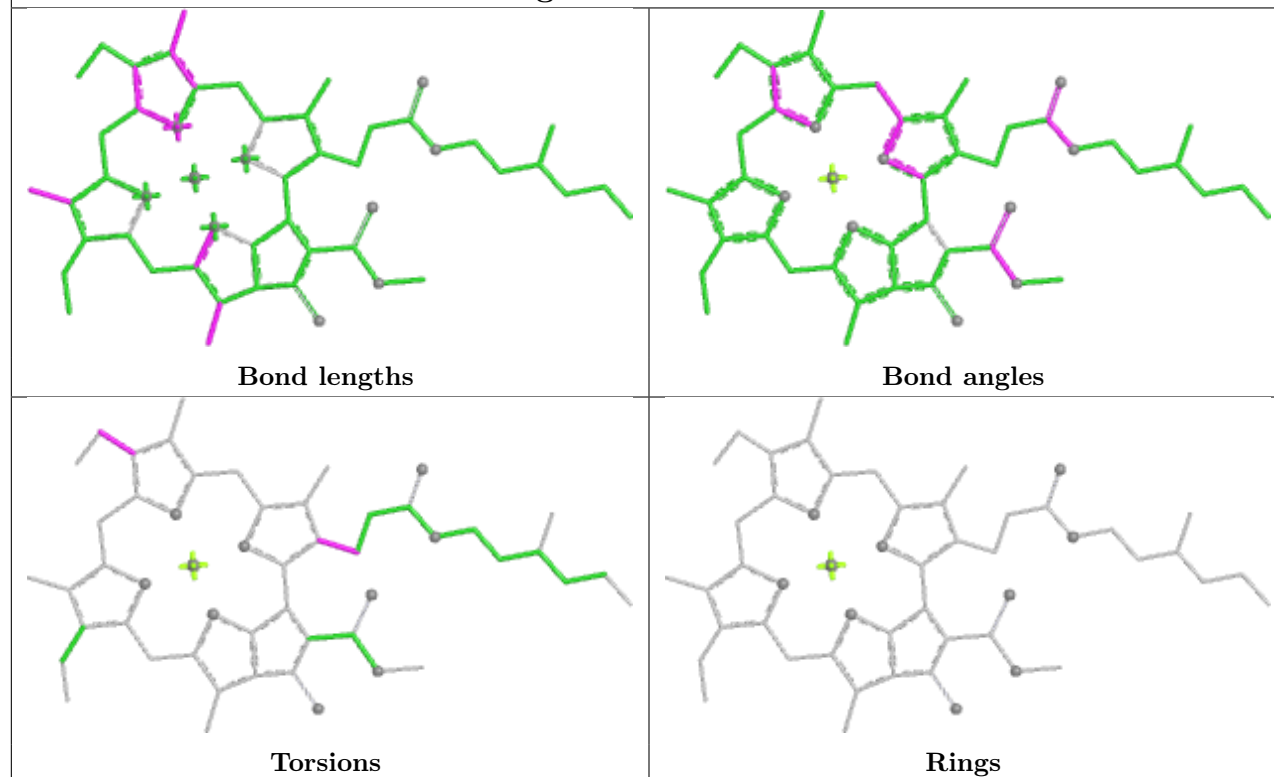
Ligand LHG 7 322



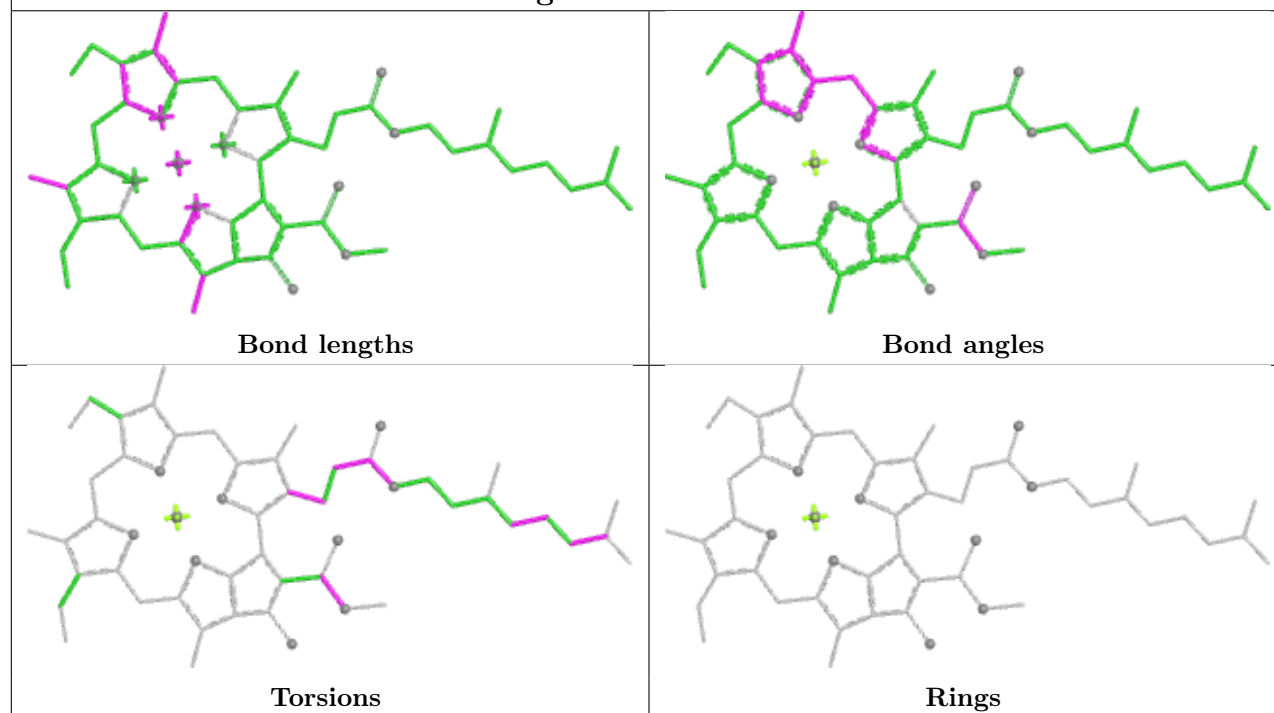
Ligand CLA A 801

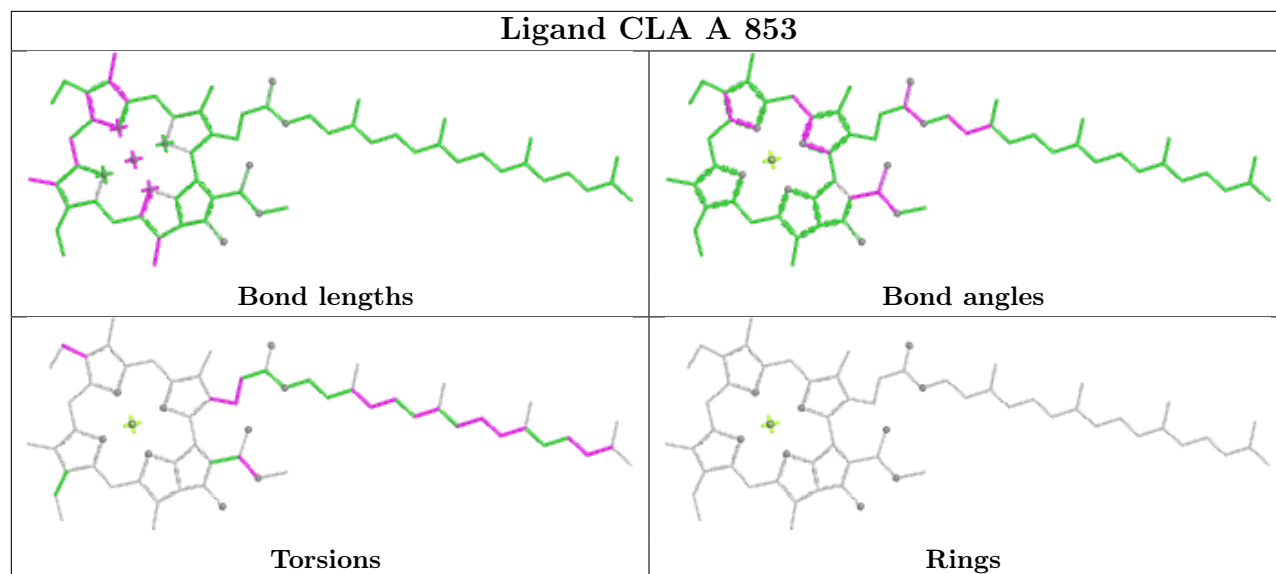
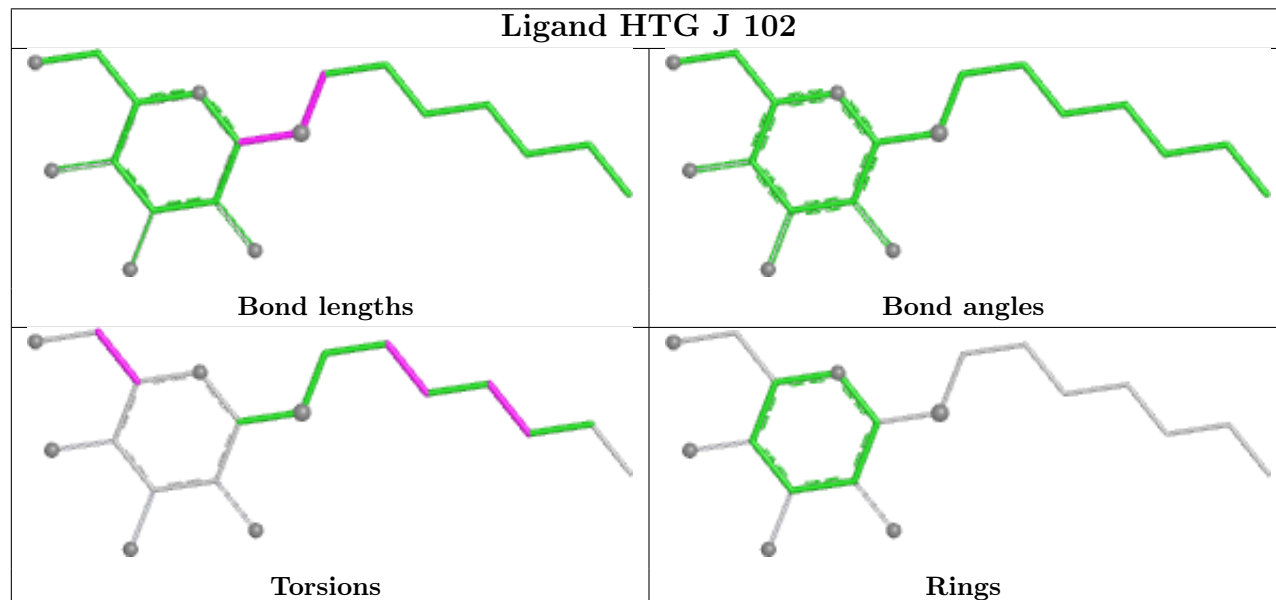


Ligand CLA 0 310

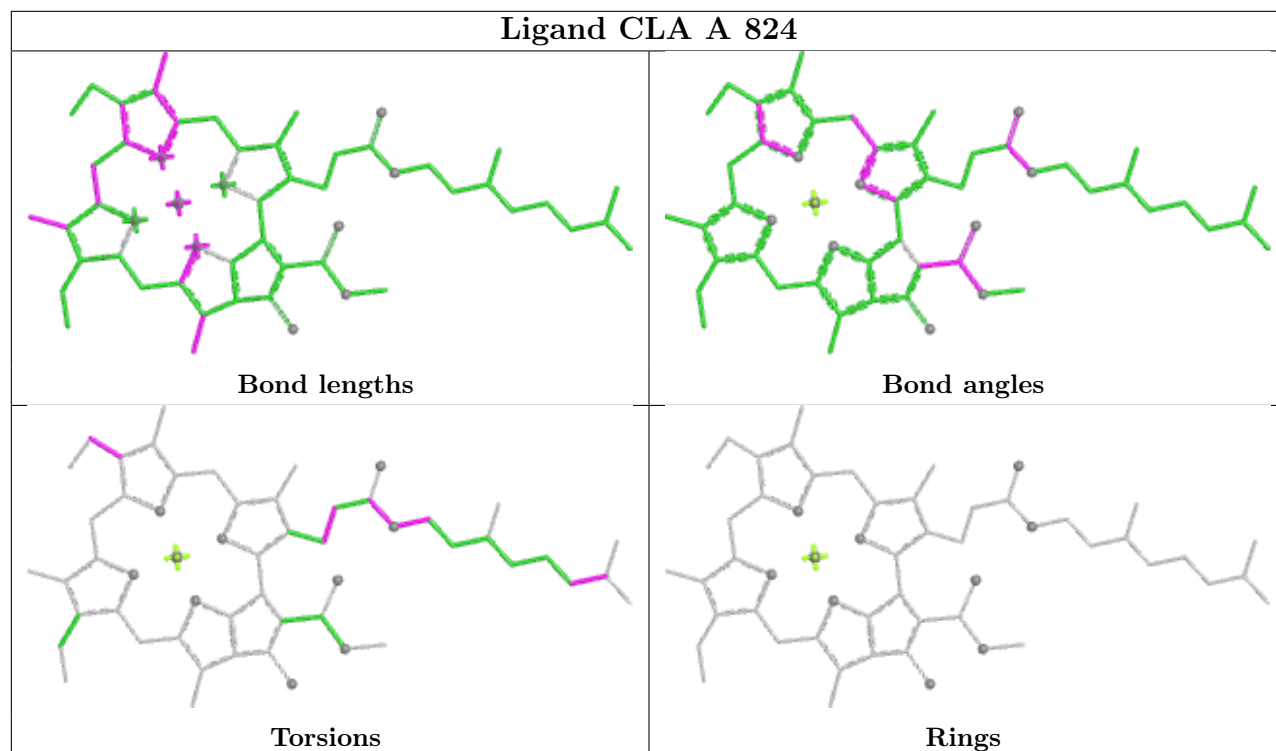


Ligand CLA 1 312

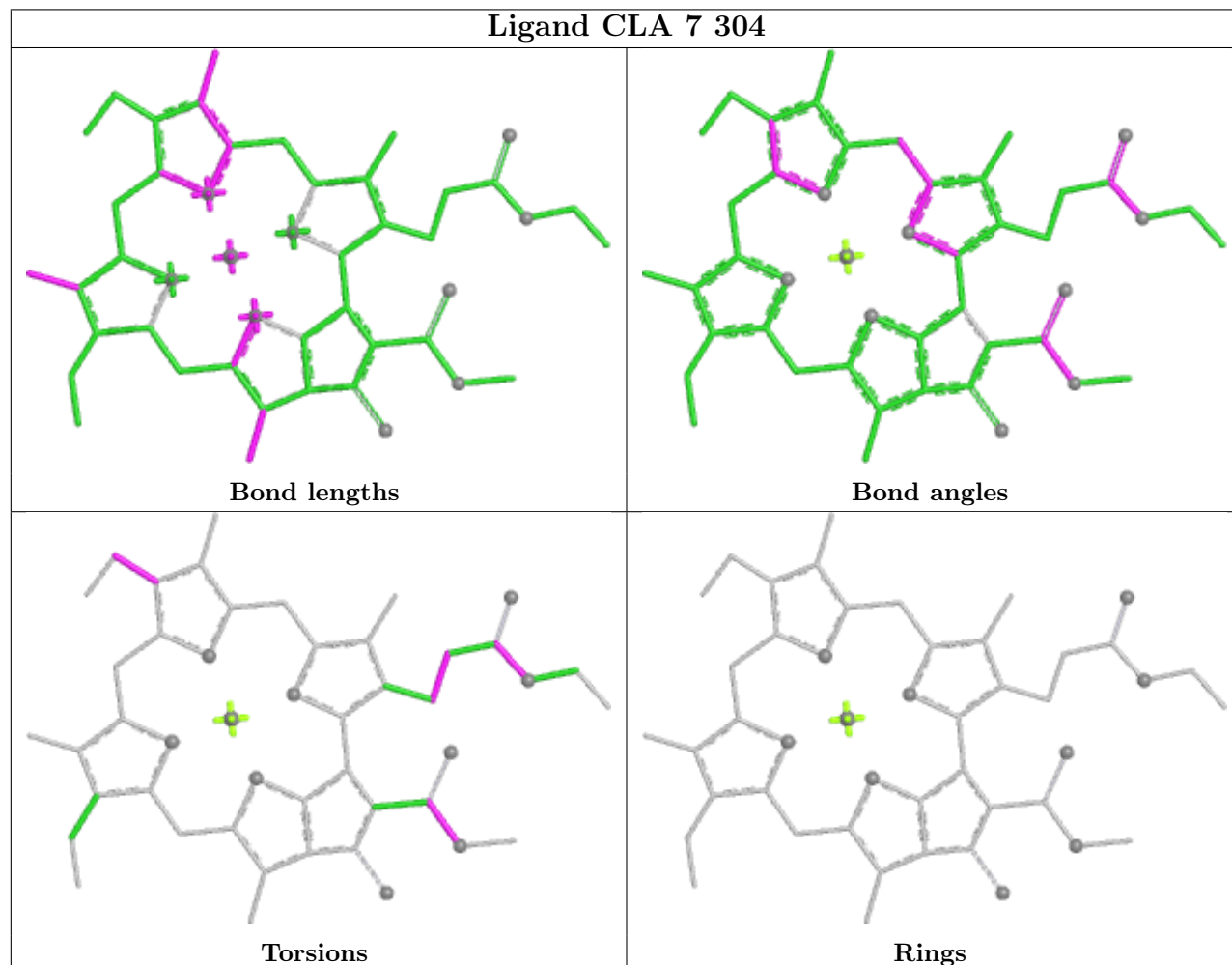


Ligand CLA A 853**Ligand HTG J 102**

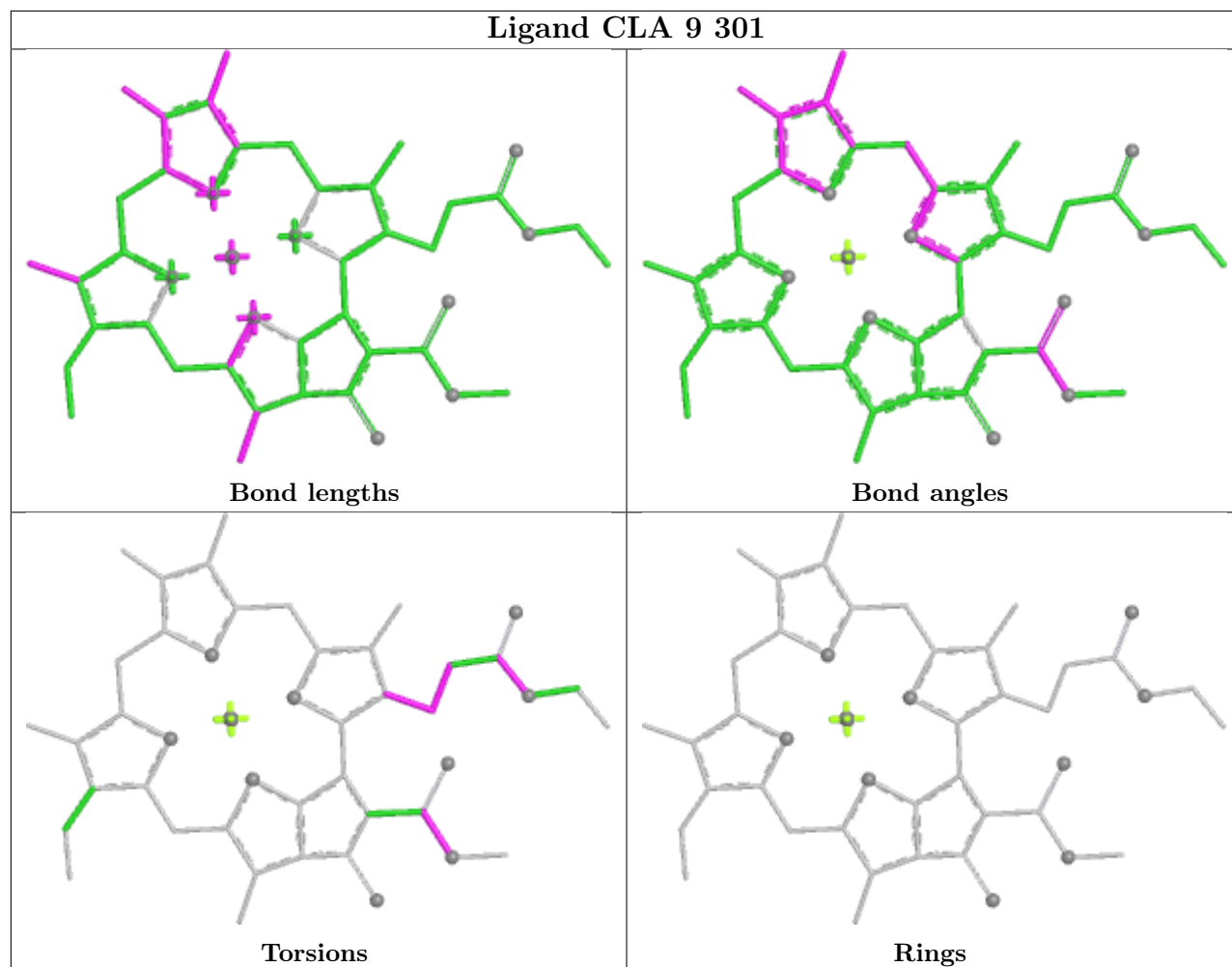
Ligand CLA A 824



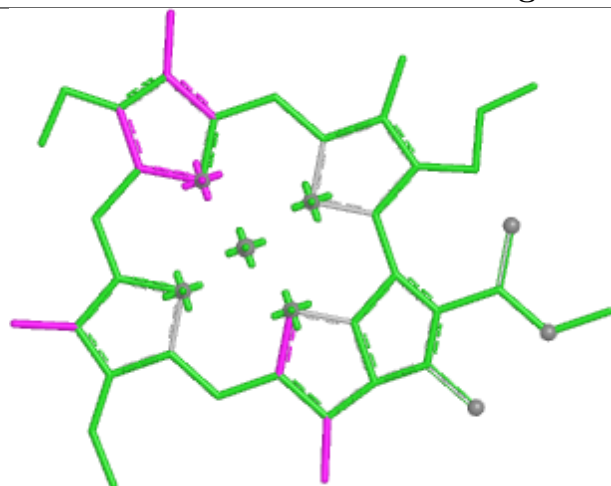
Ligand CLA 7 304



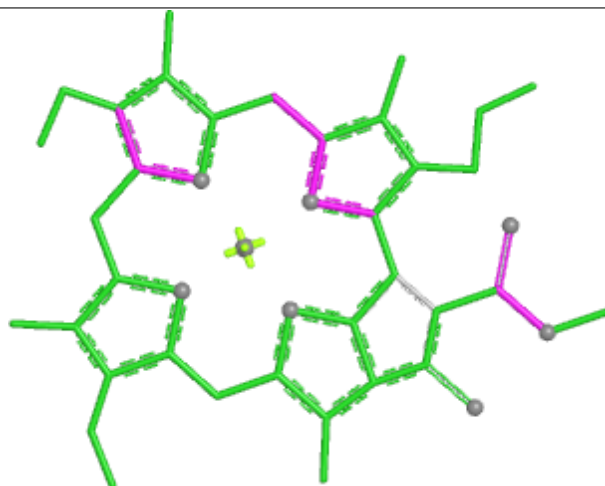
Ligand CLA 9 301



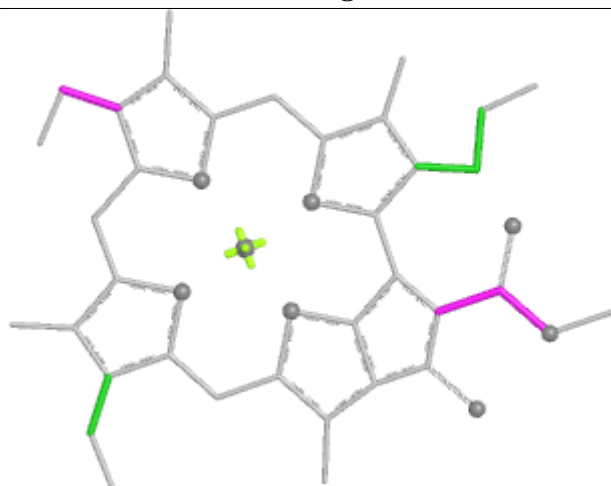
Ligand CLA 6 314



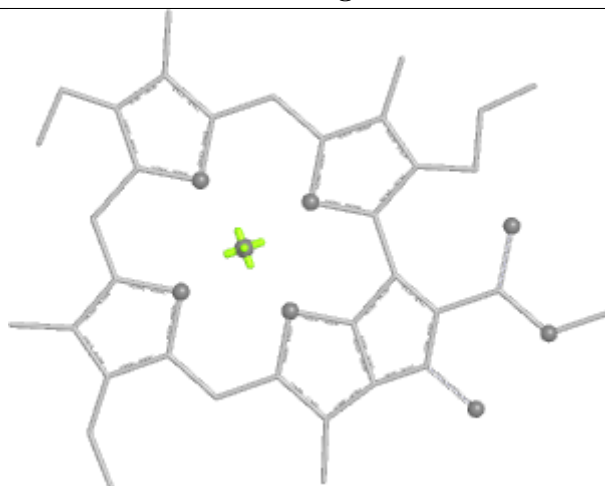
Bond lengths



Bond angles

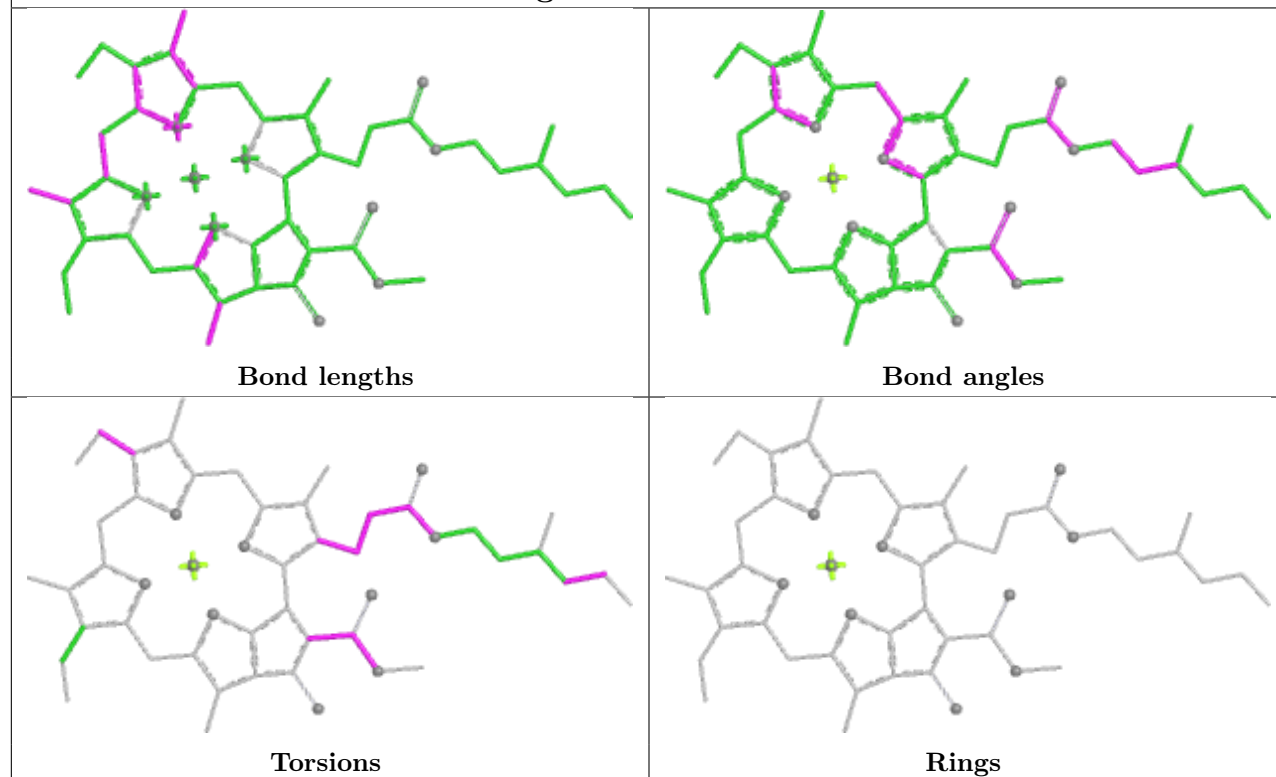


Torsions

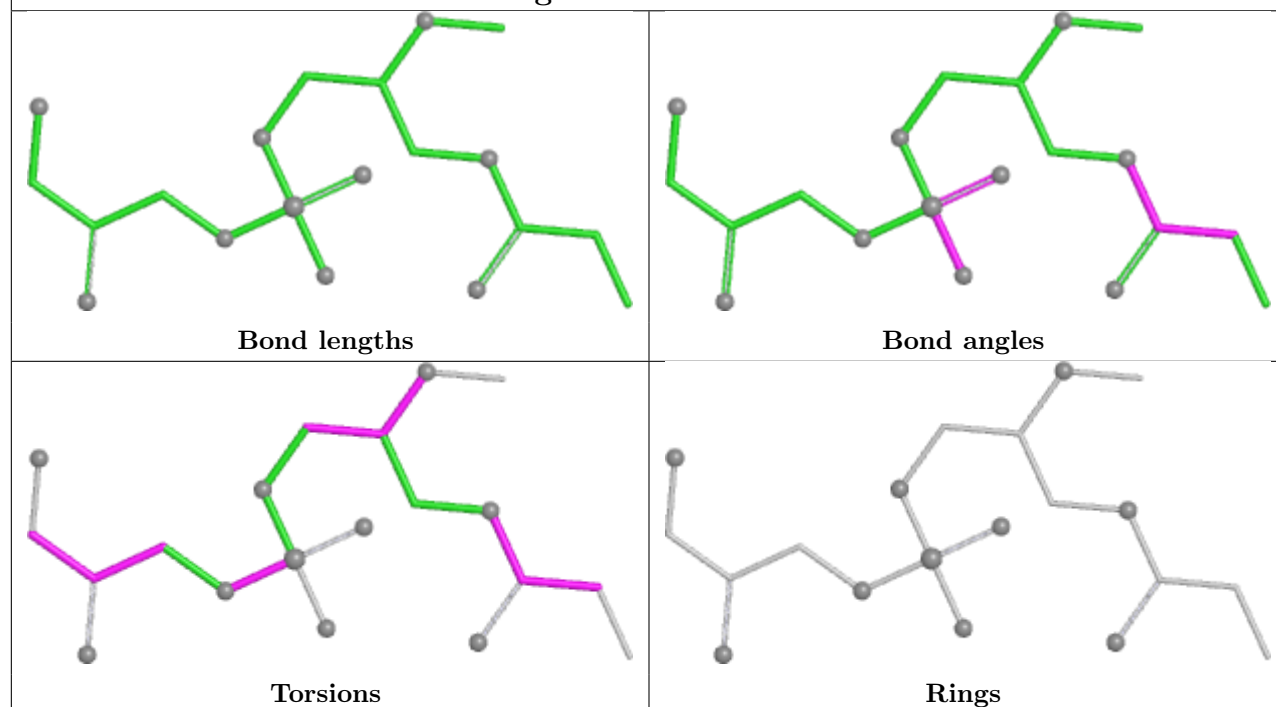


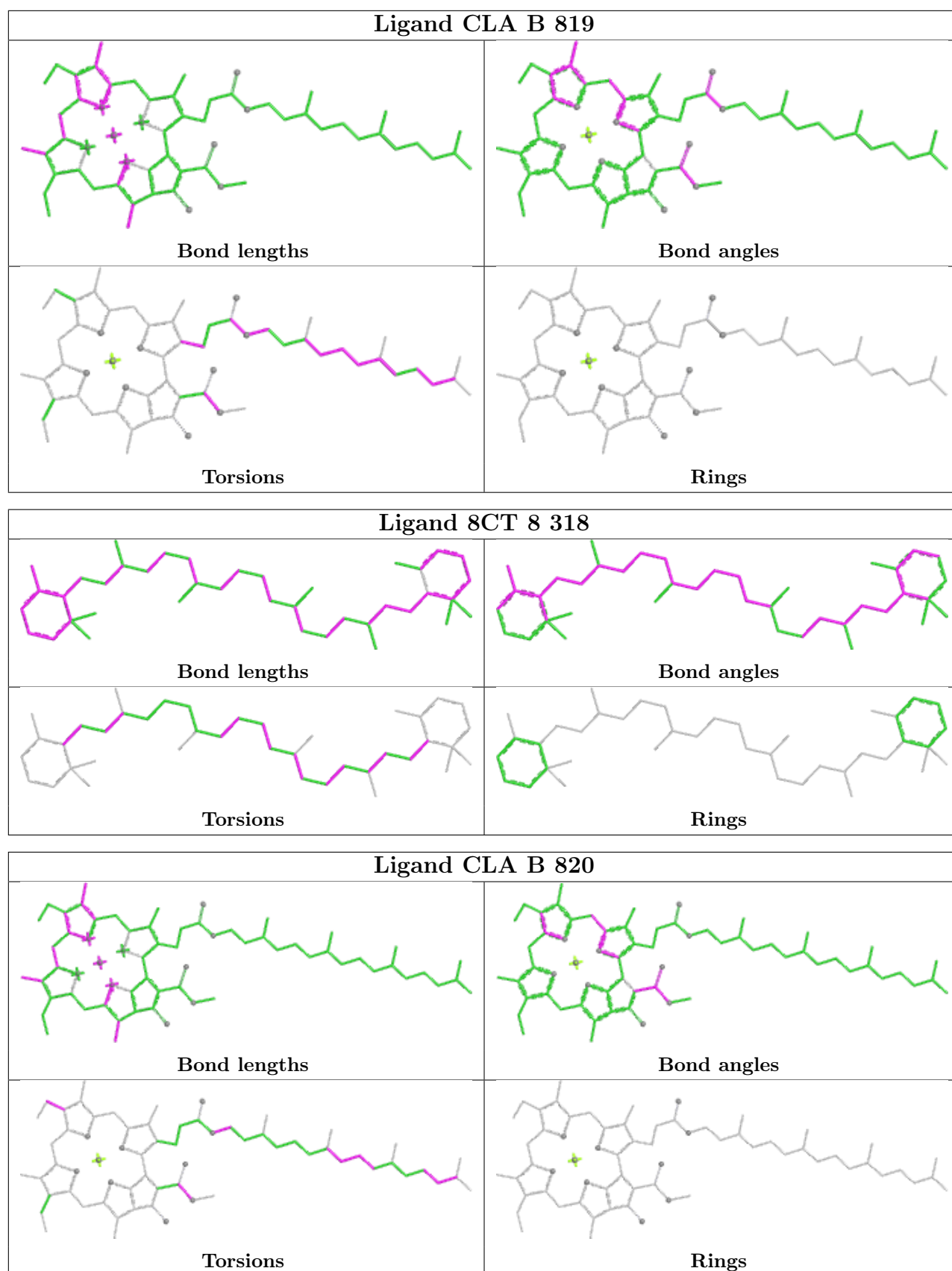
Rings

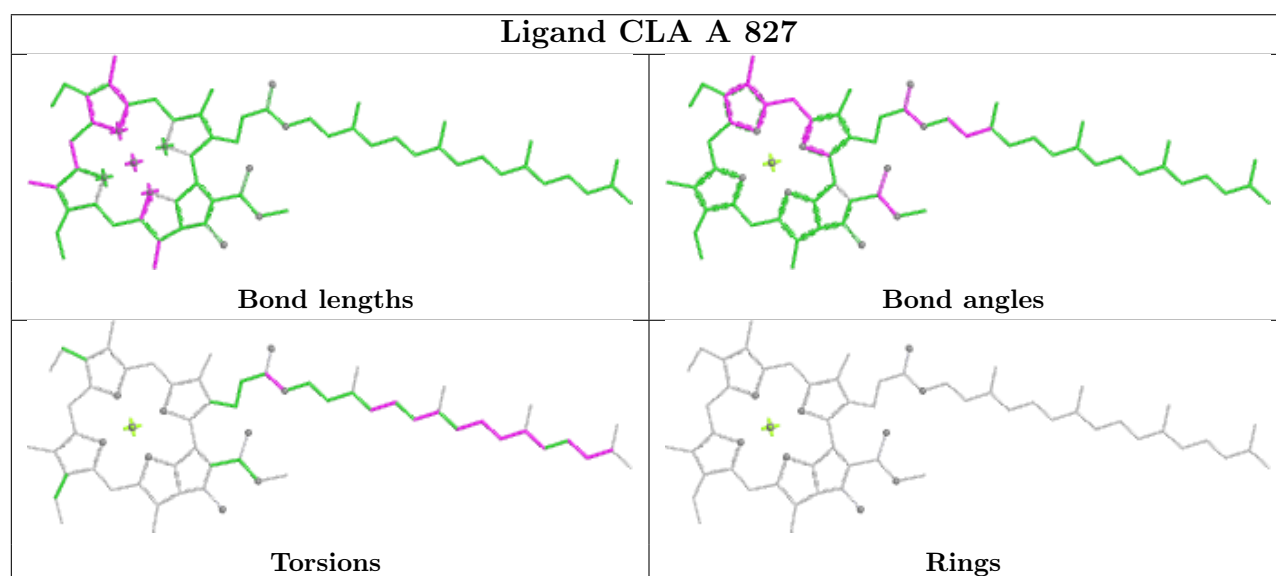
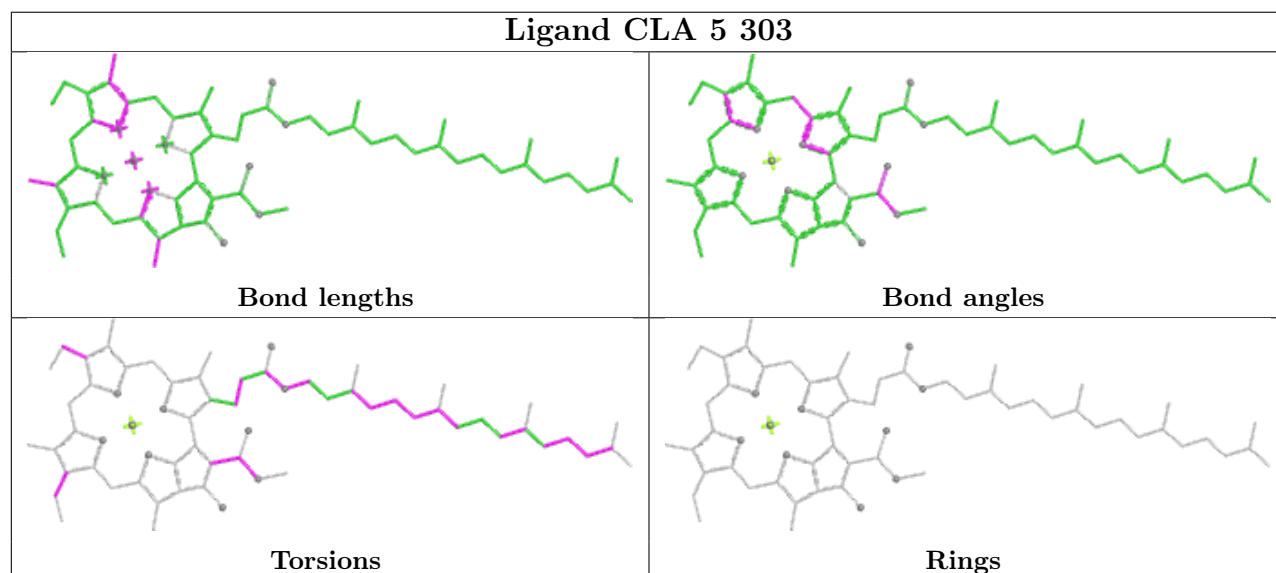
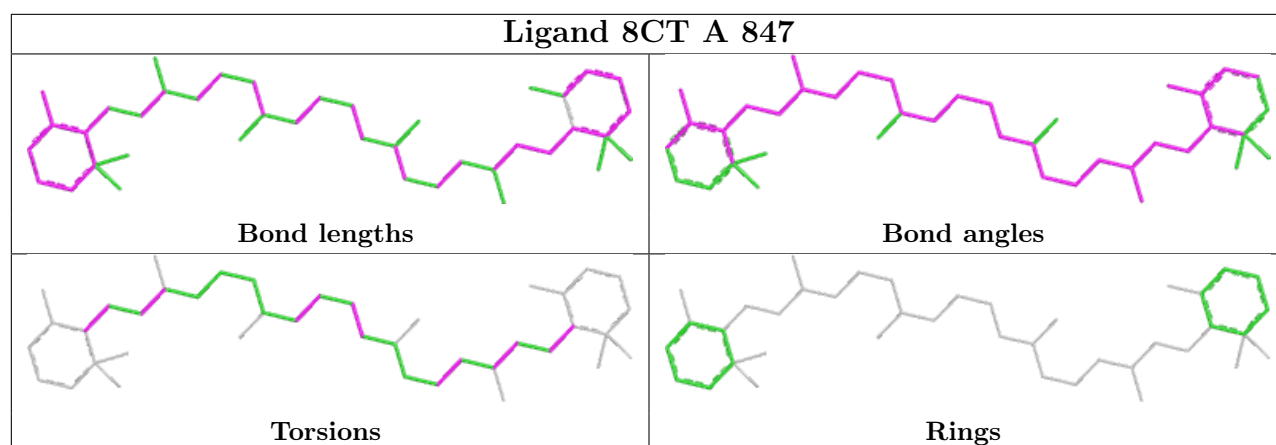
Ligand CLA 6 301

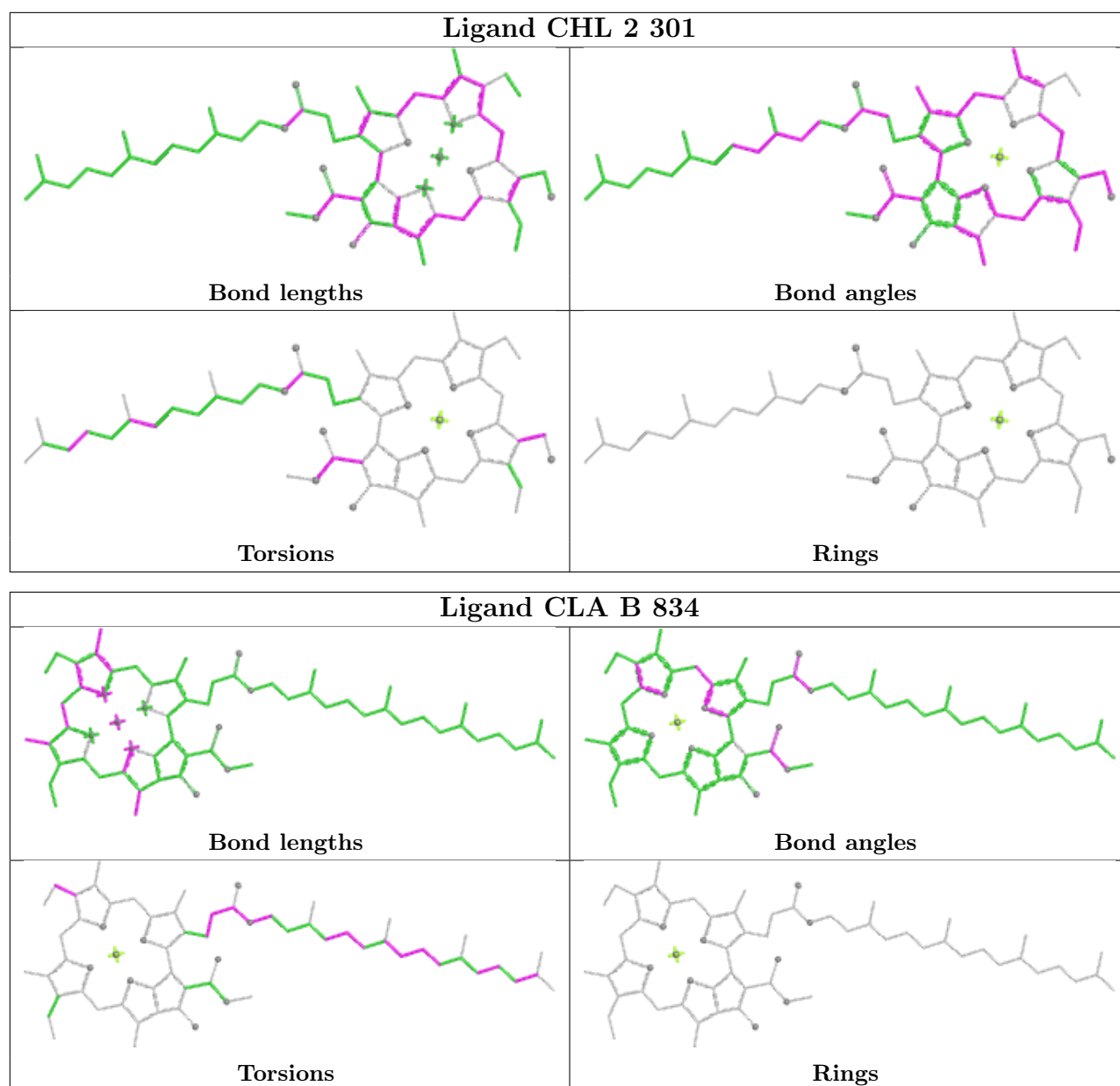


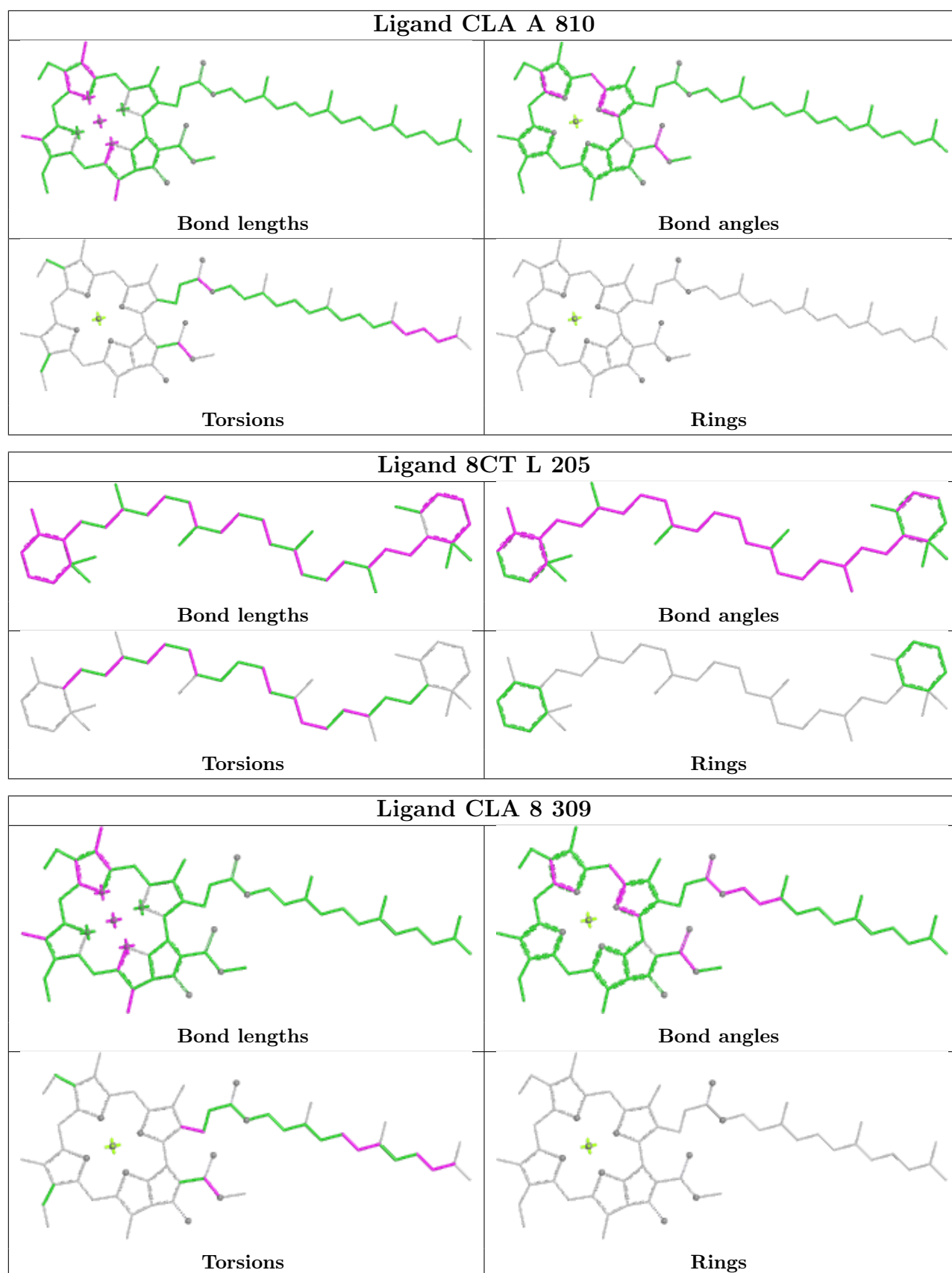
Ligand LHG 3 317

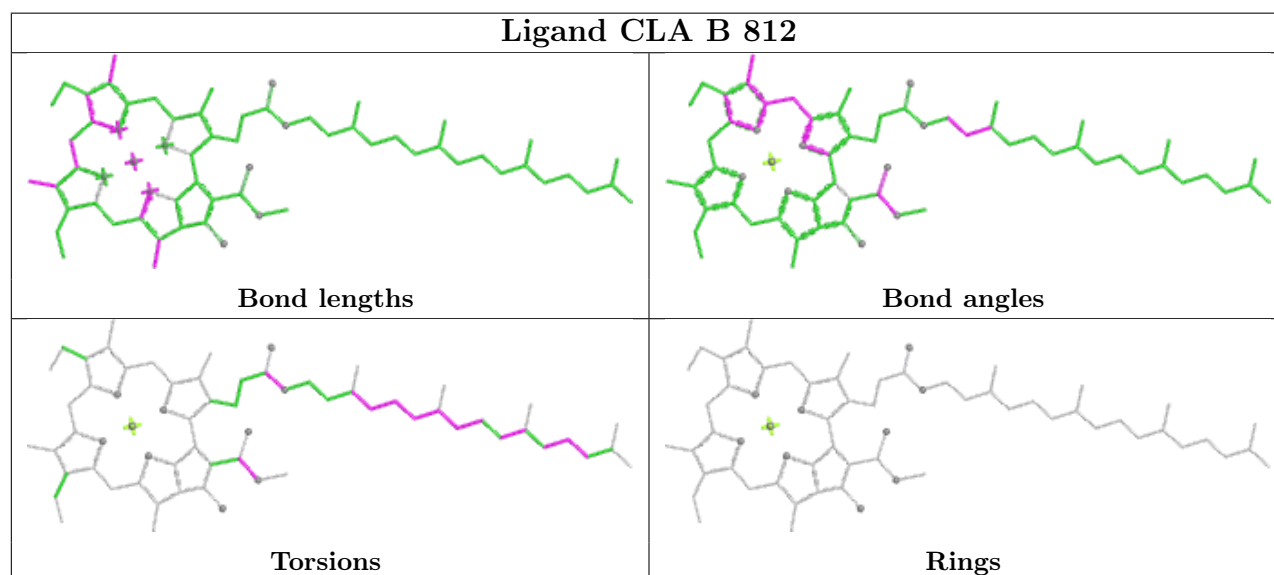
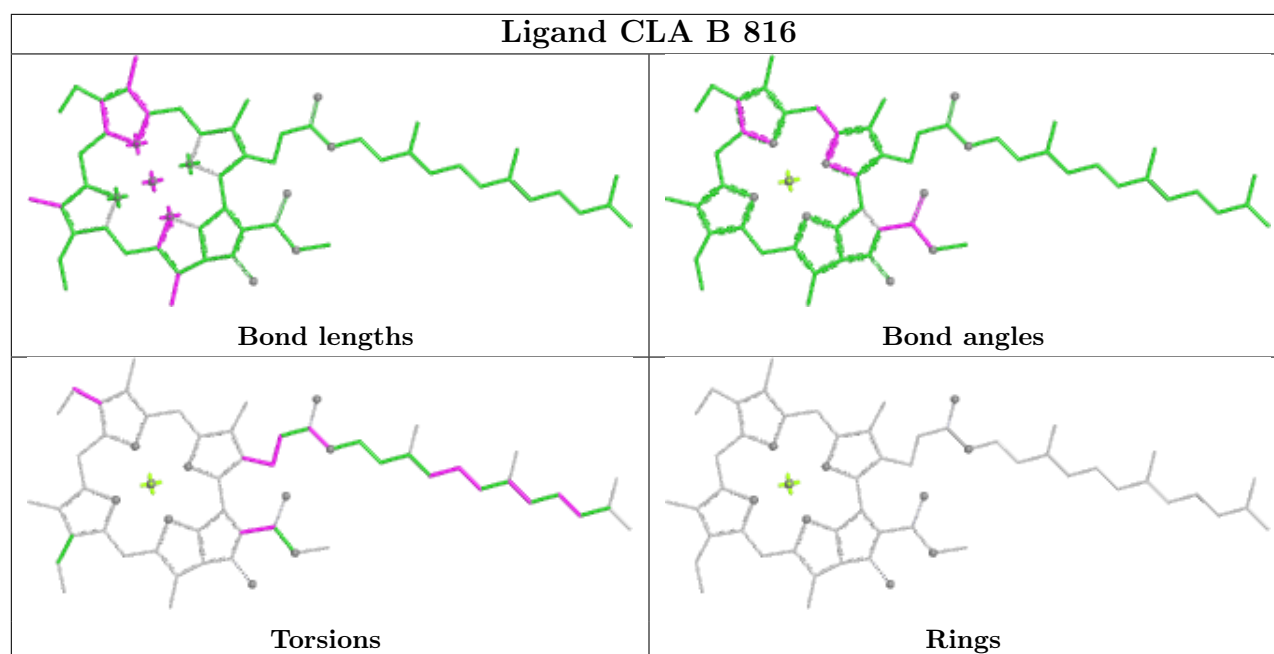


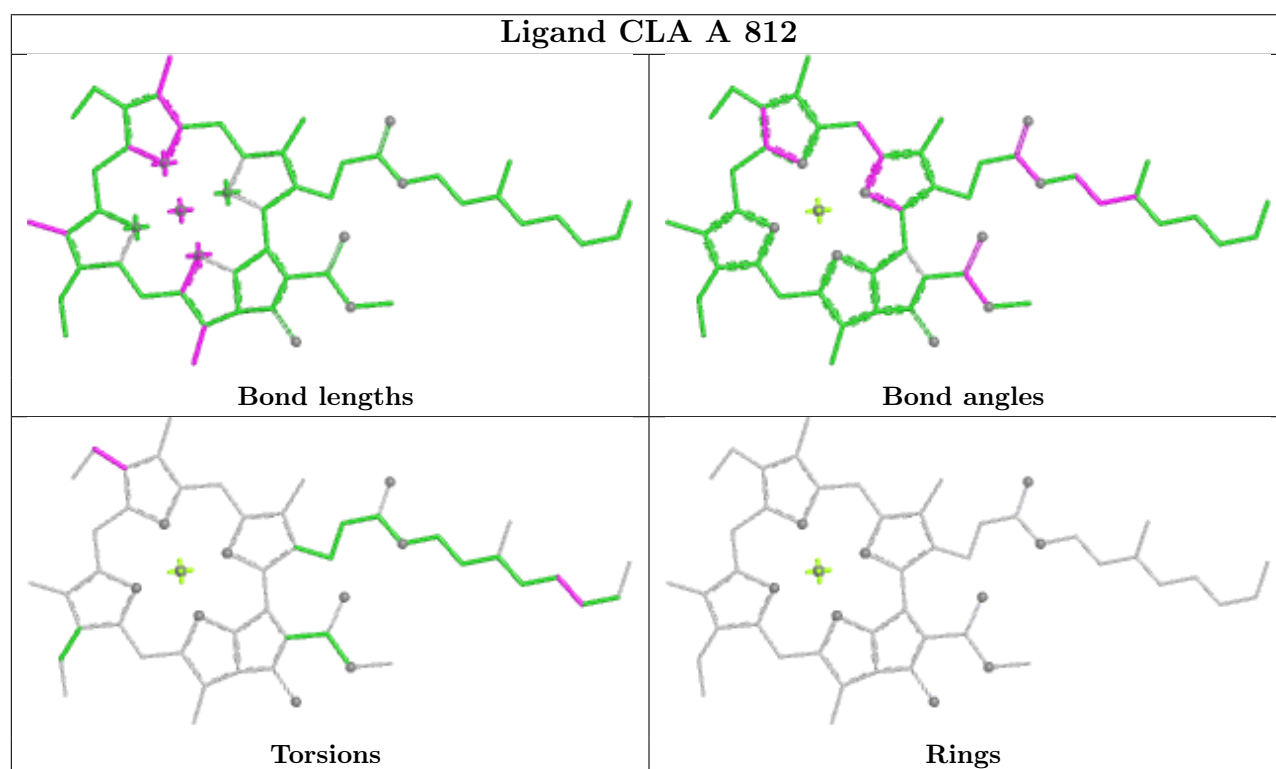
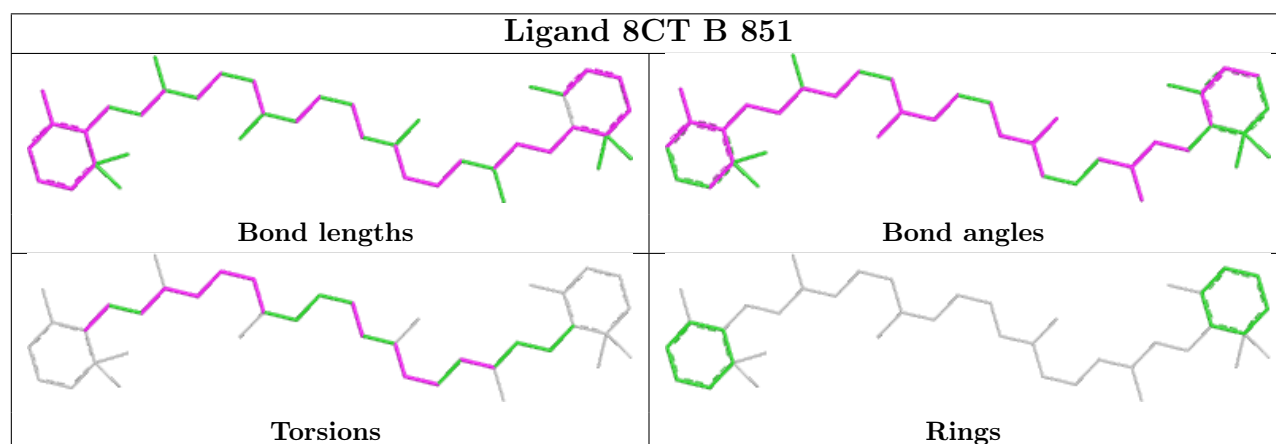
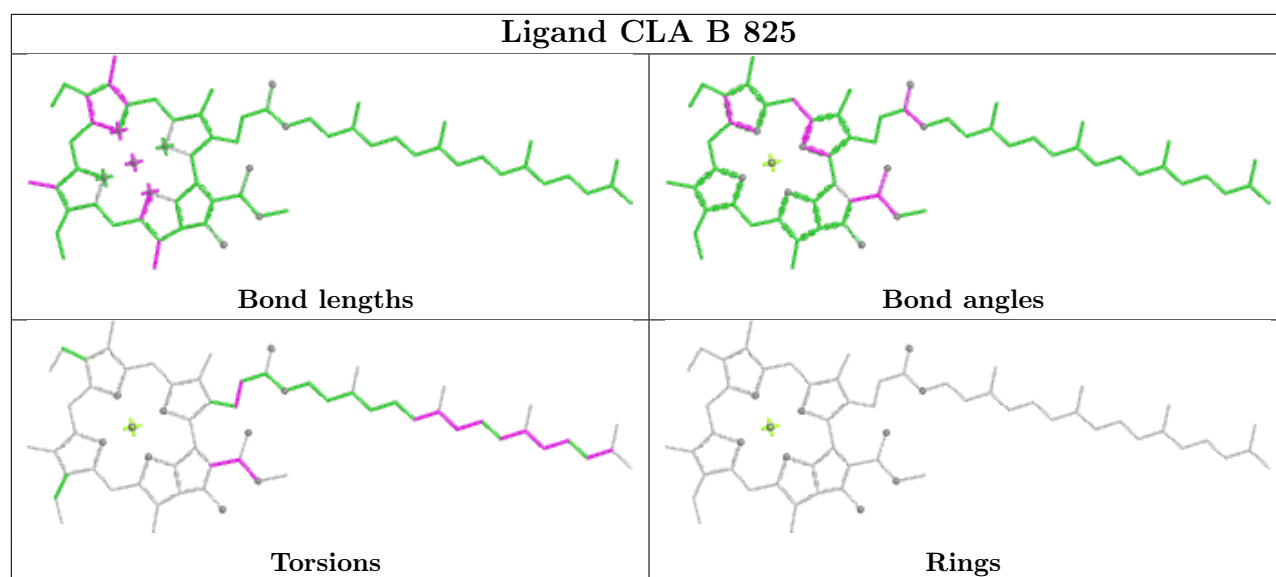




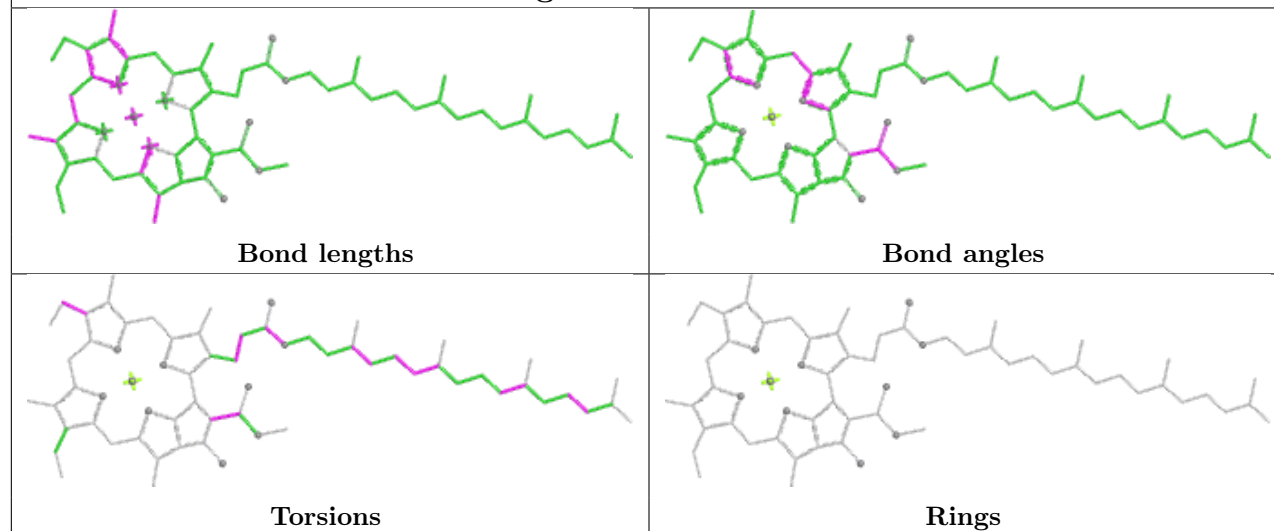




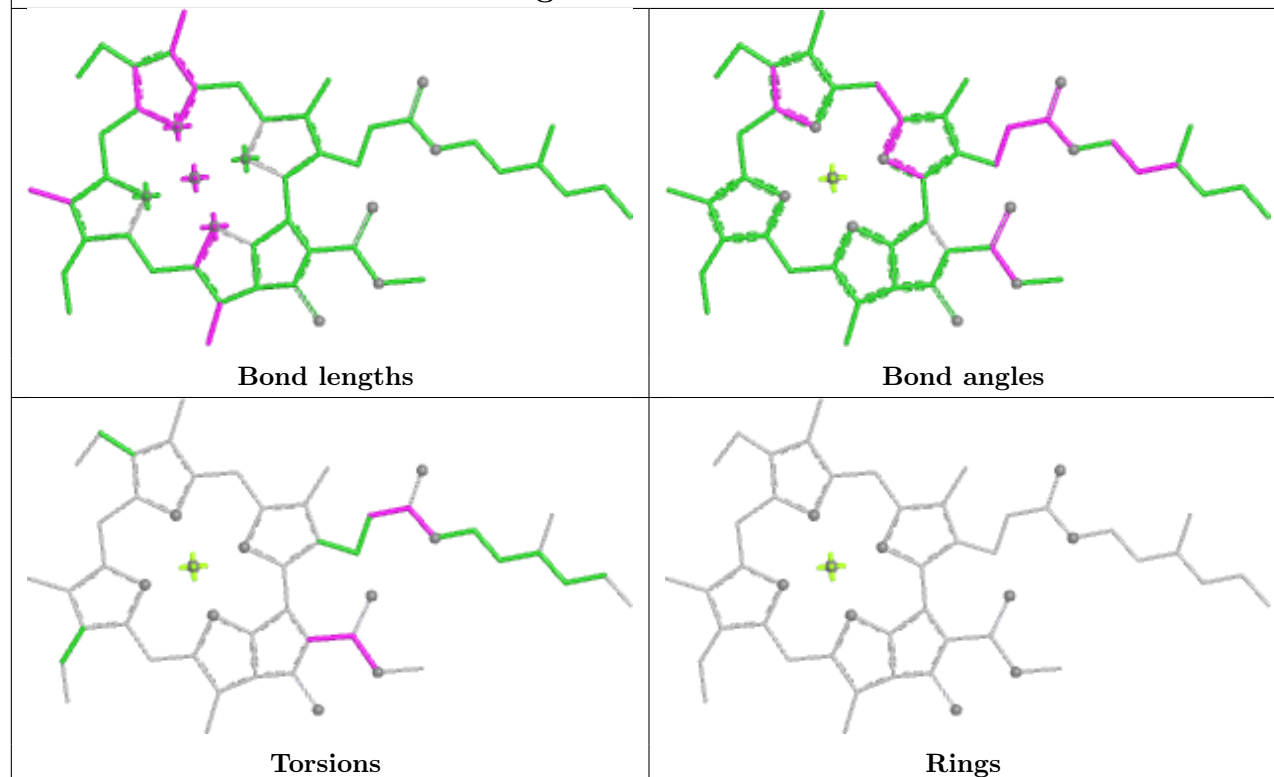


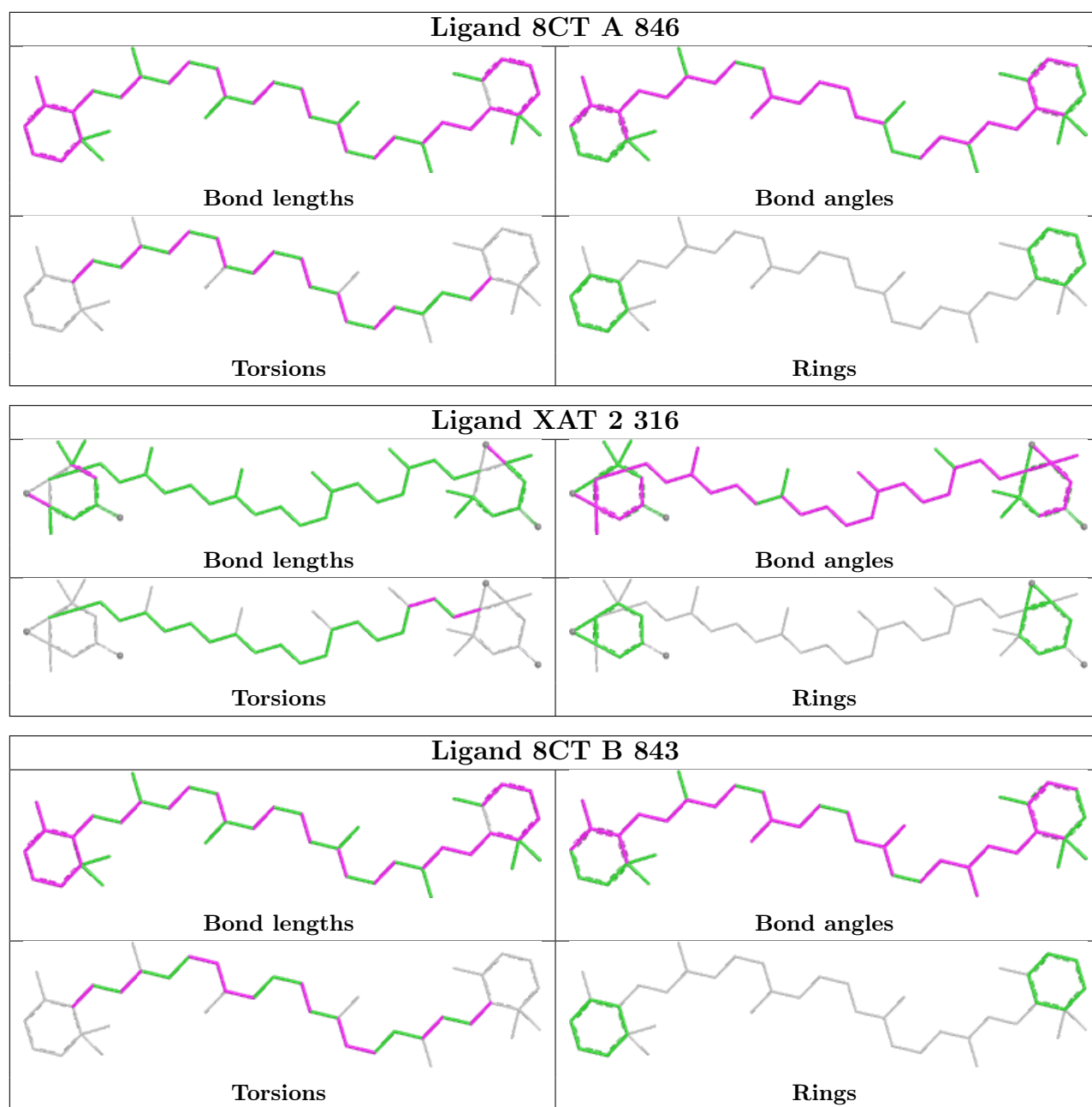


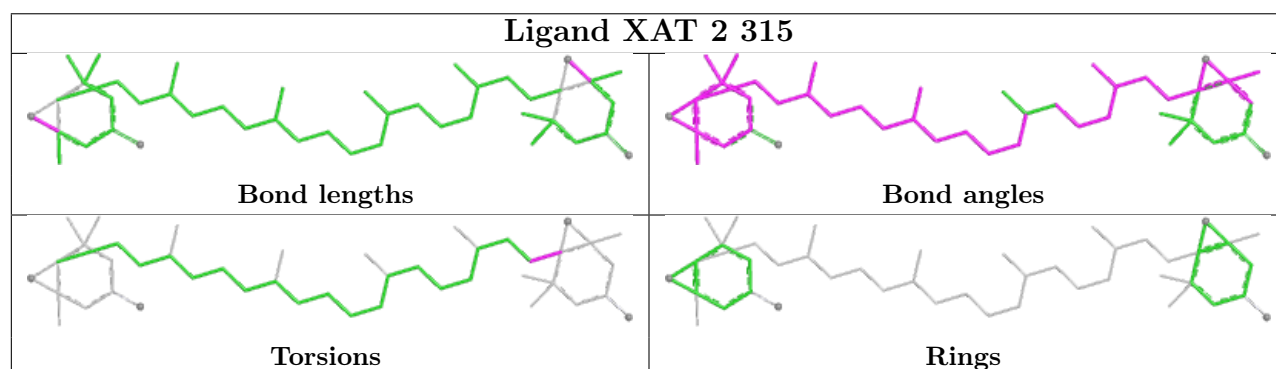
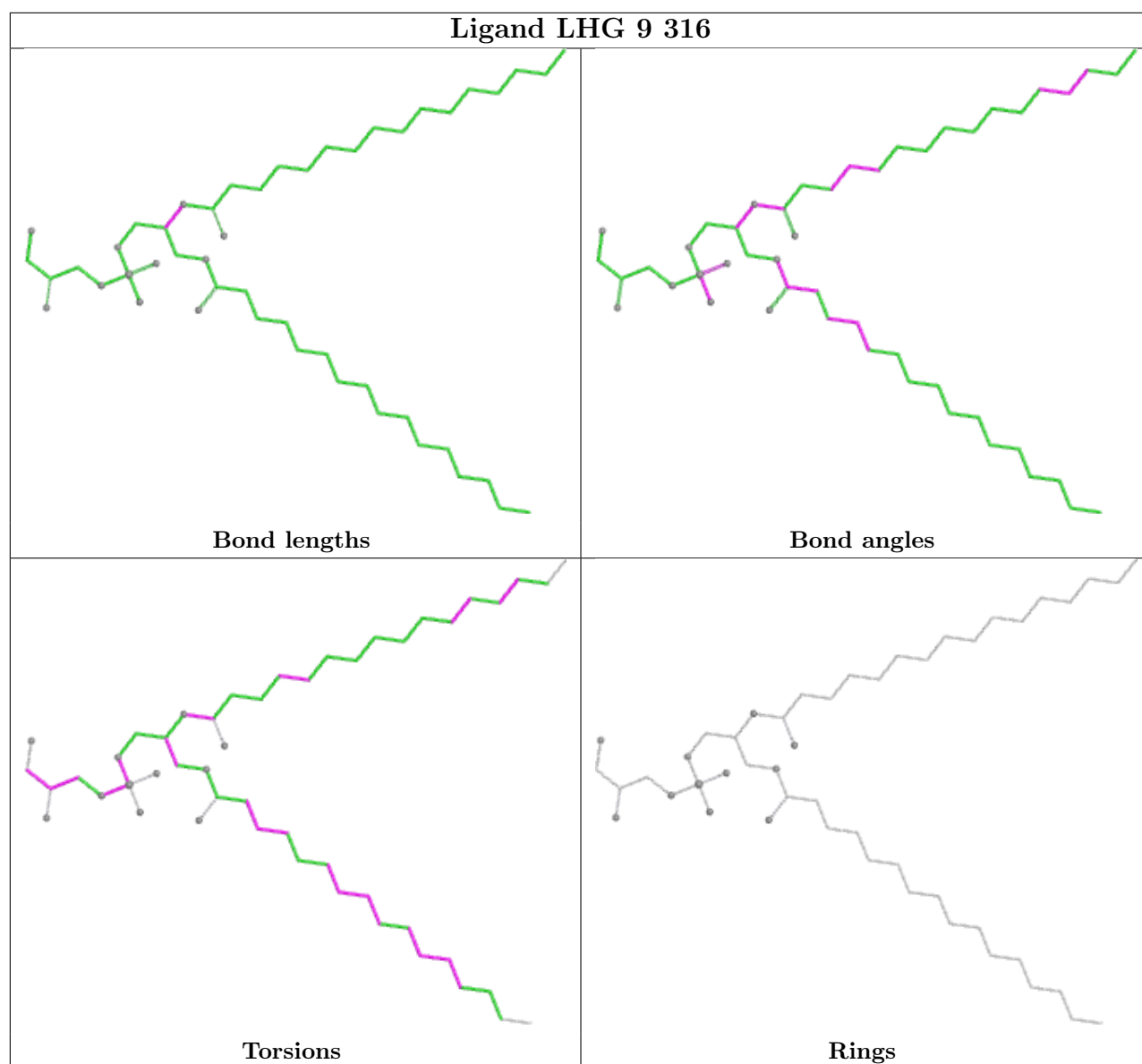
Ligand CLA 0 303

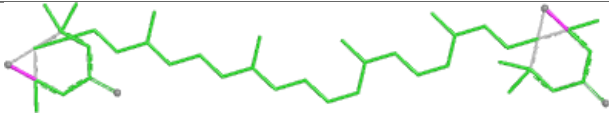
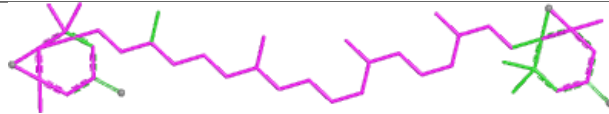
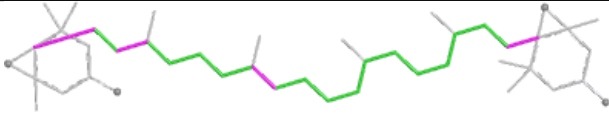
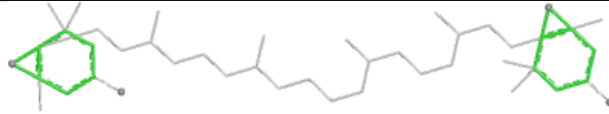


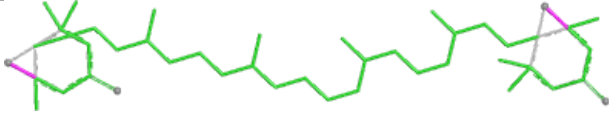
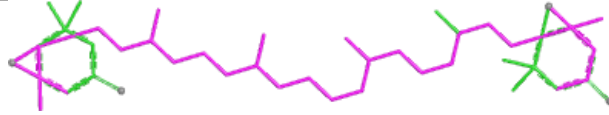
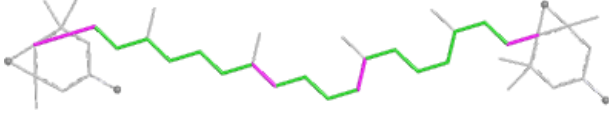
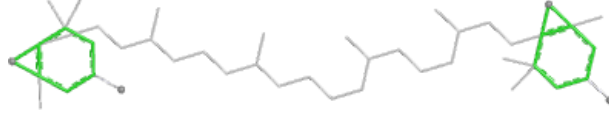
Ligand CLA 2 311

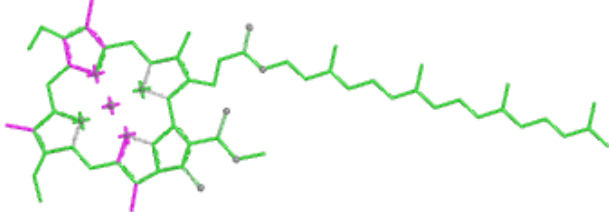
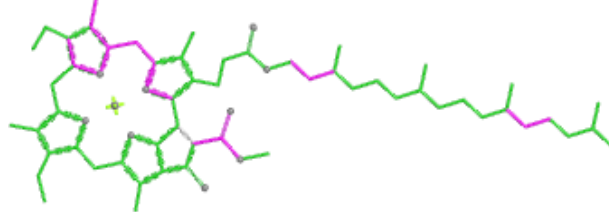
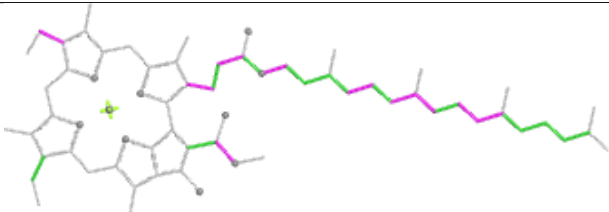
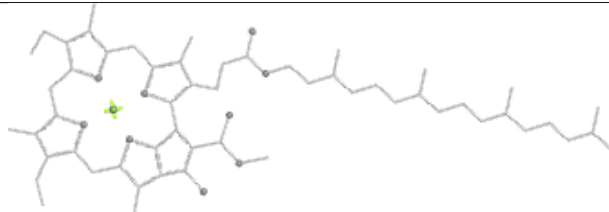


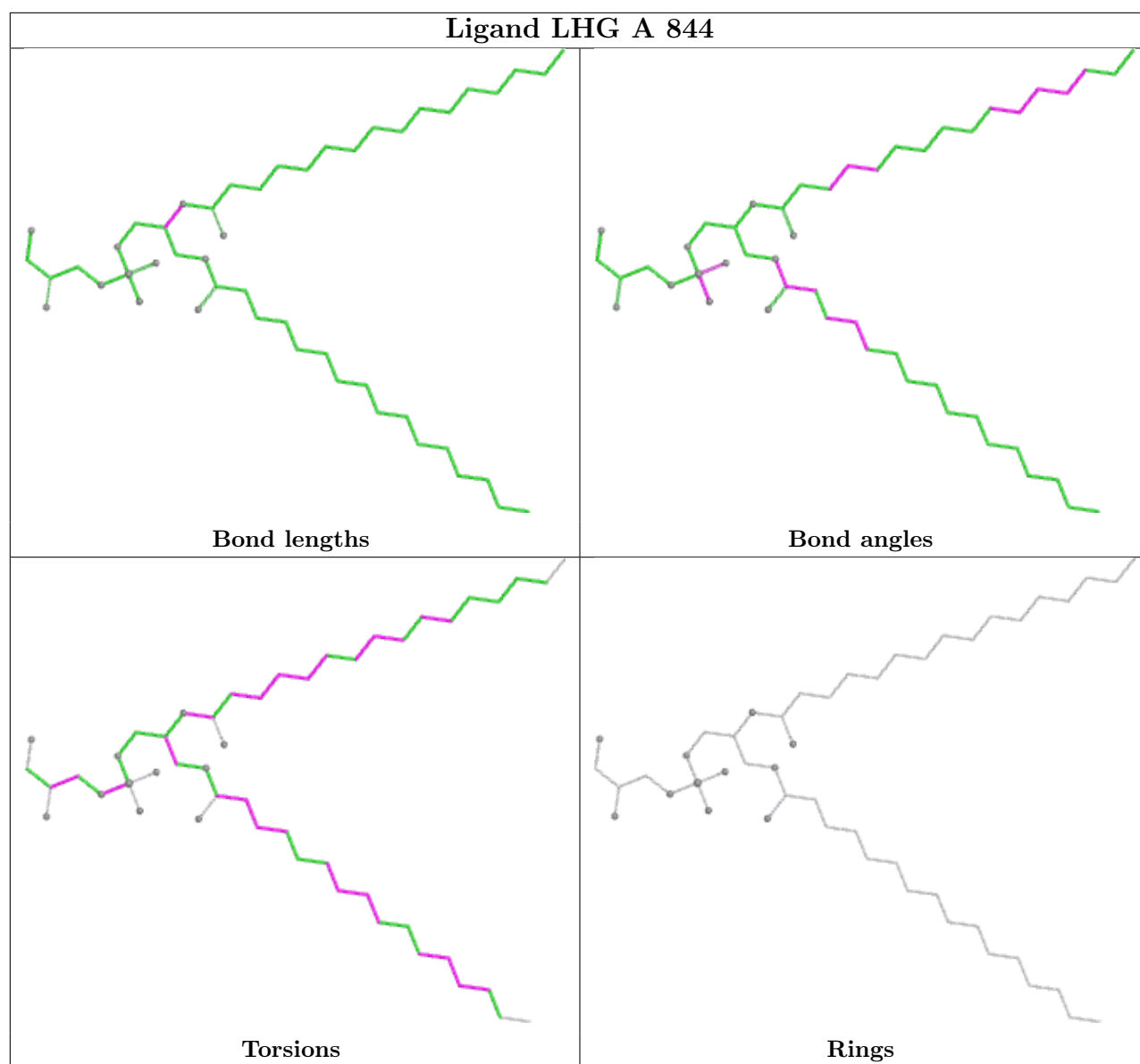




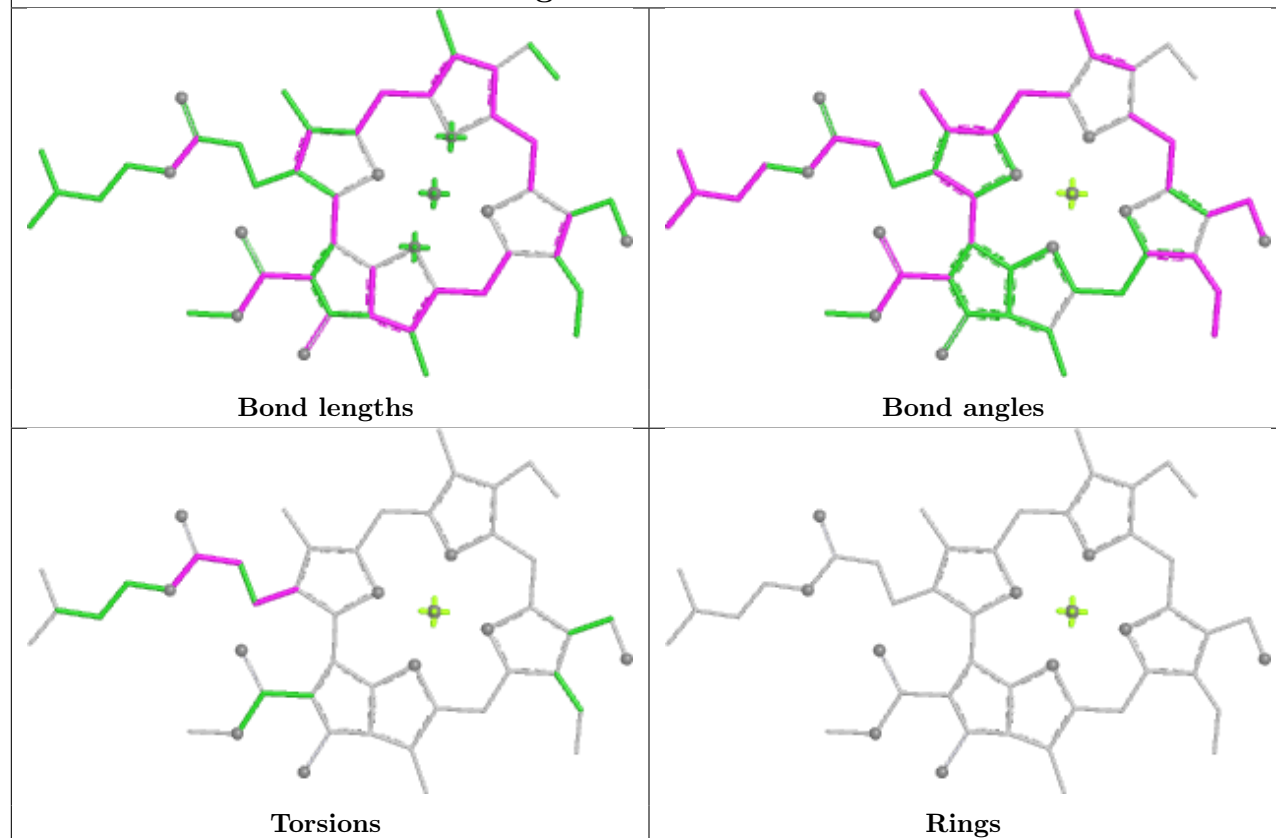
Ligand XAT 8 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 5 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

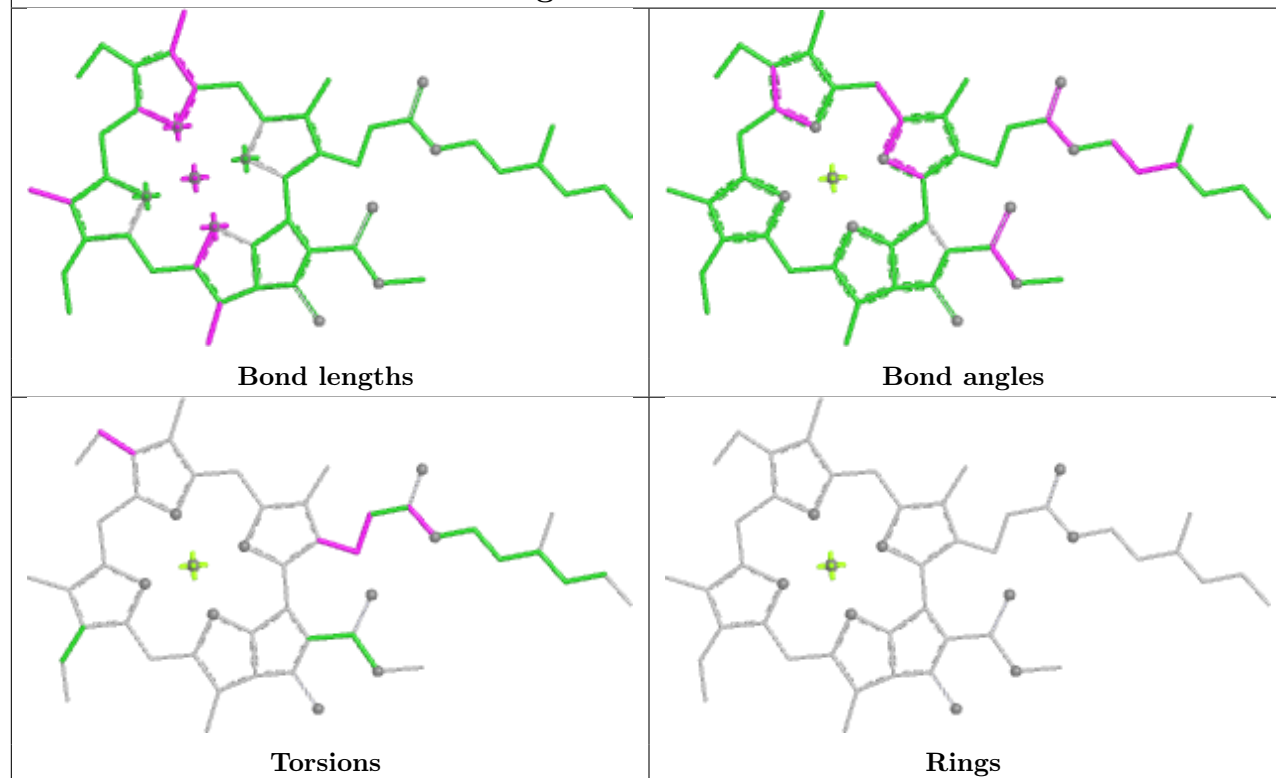
Ligand CLA B 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

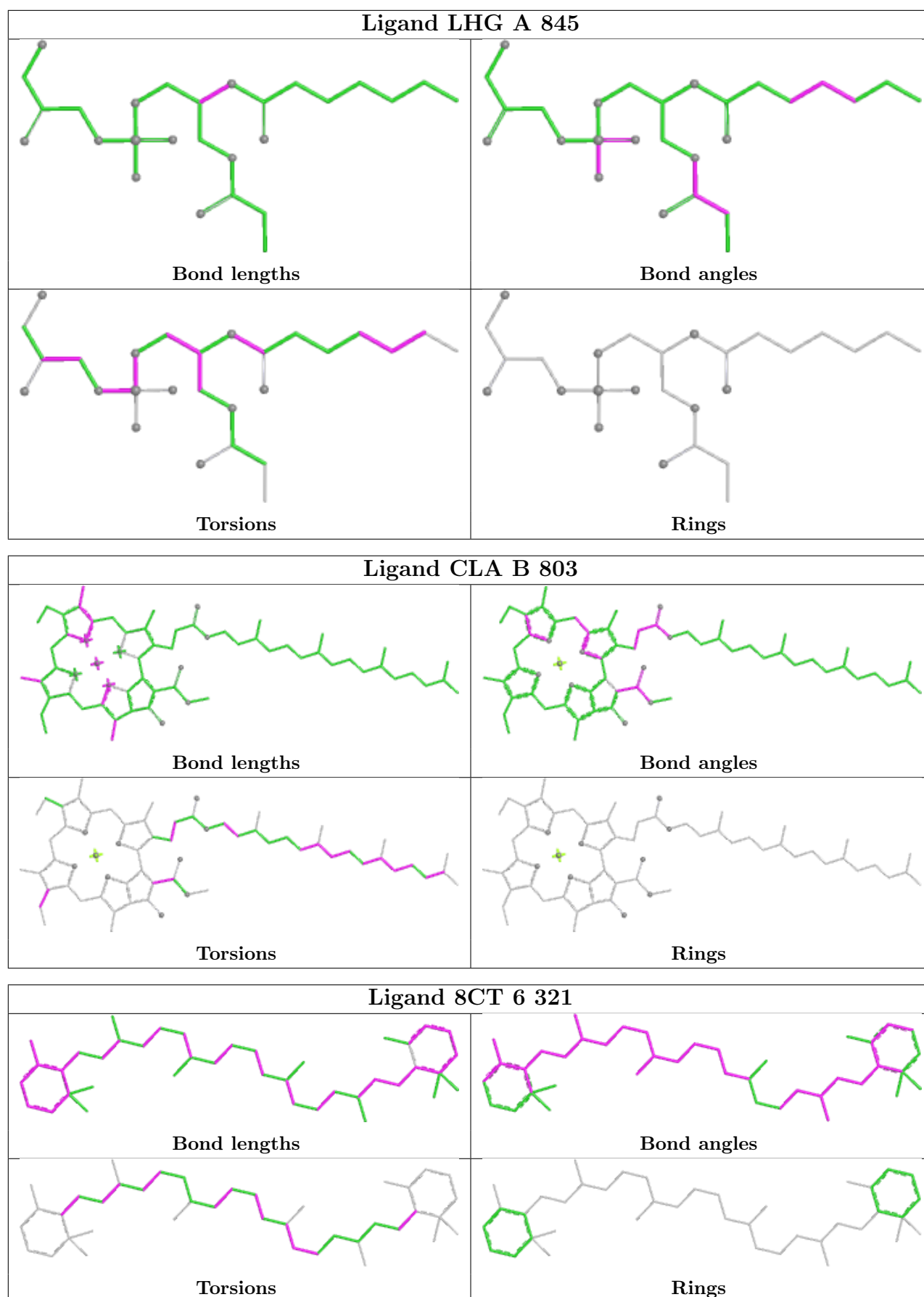


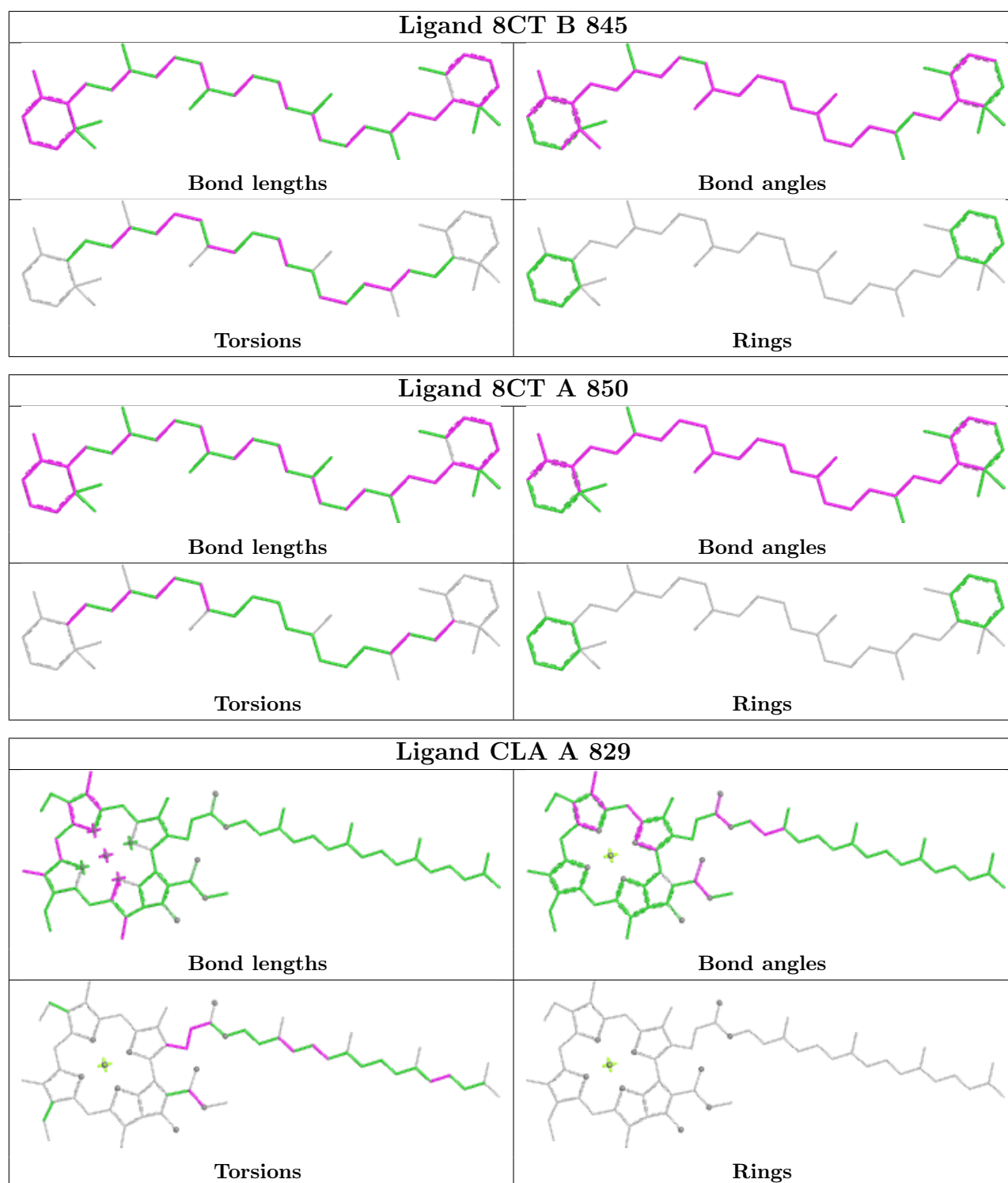
Ligand CHL 4 306

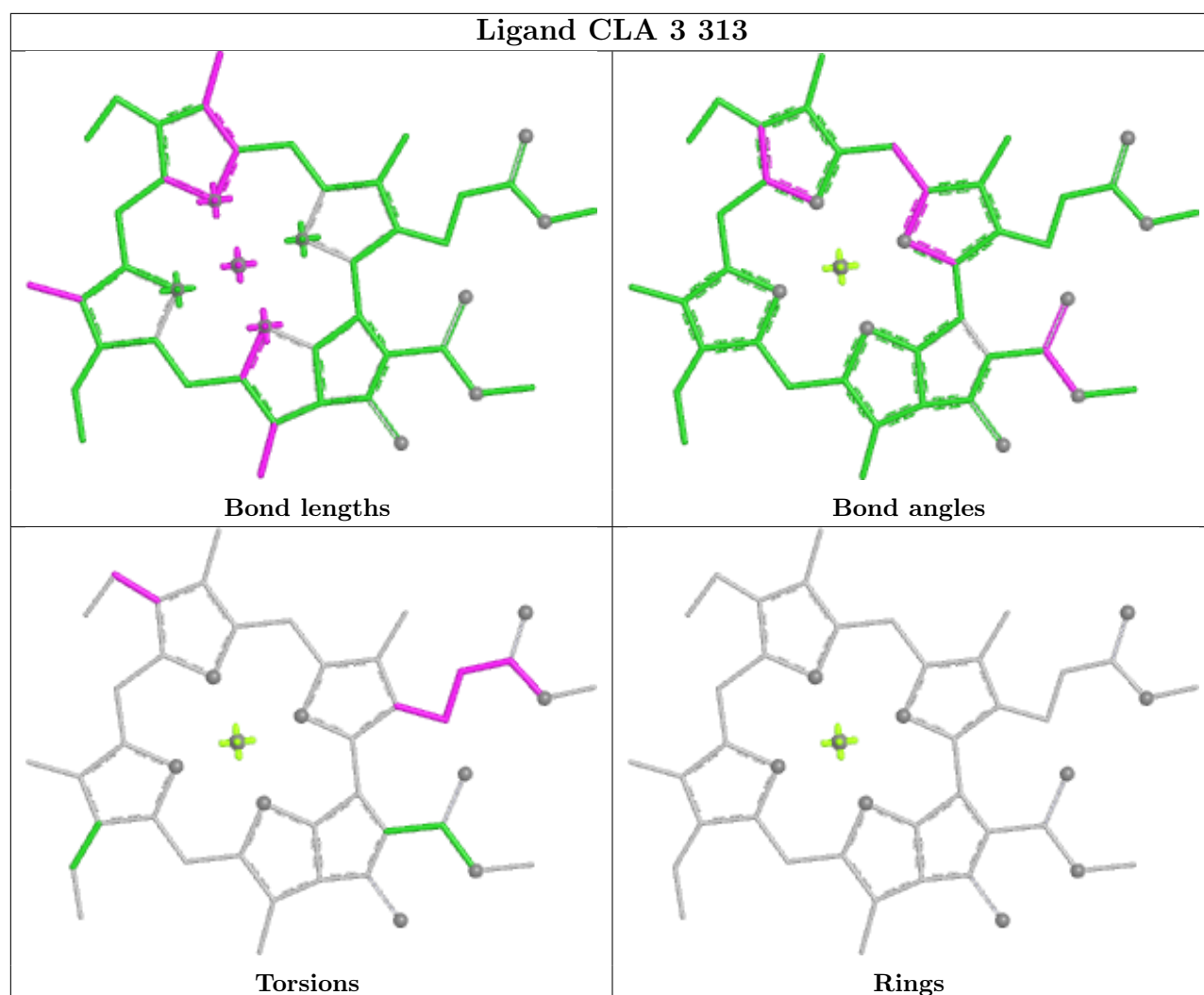


Ligand CLA 1 304









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.

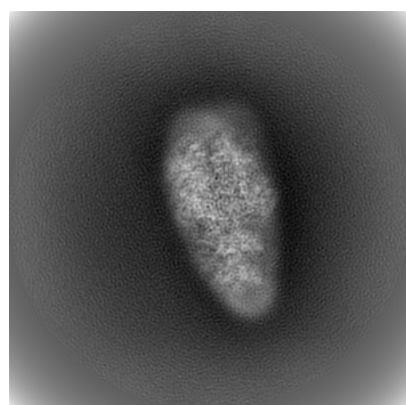
6 Map visualisation [i](#)

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.

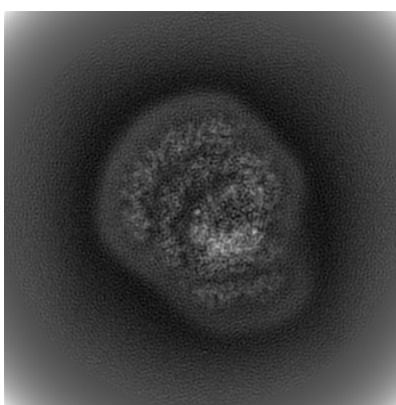
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

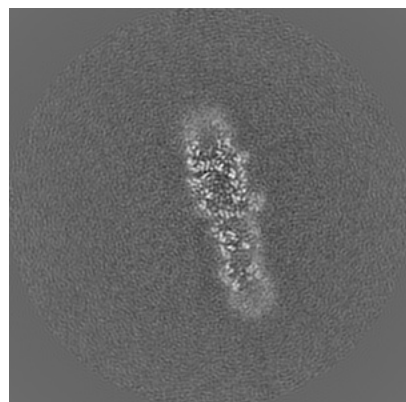


Z

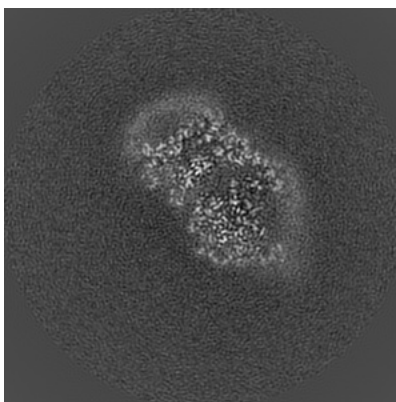
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

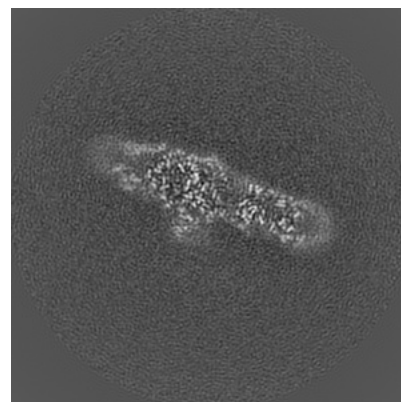
6.2.1 Primary map



X Index: 230



Y Index: 230

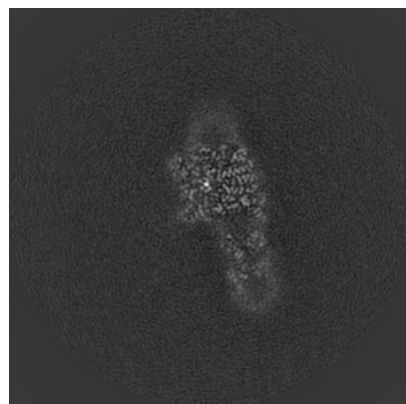


Z Index: 230

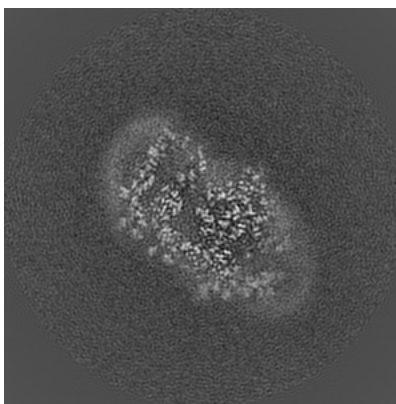
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

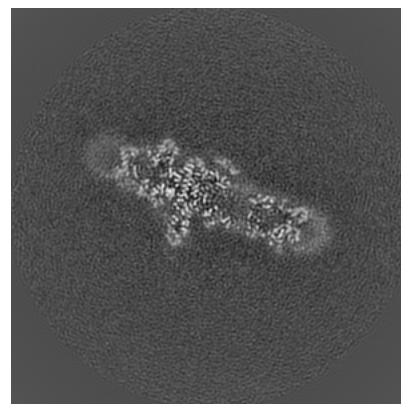
6.3.1 Primary map



X Index: 202



Y Index: 254

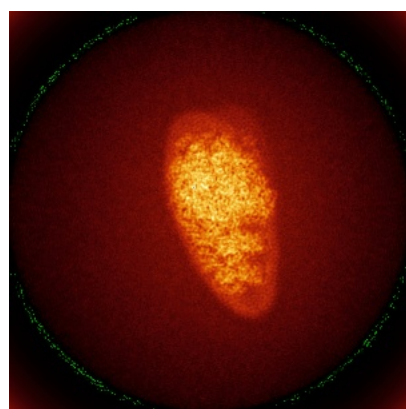


Z Index: 250

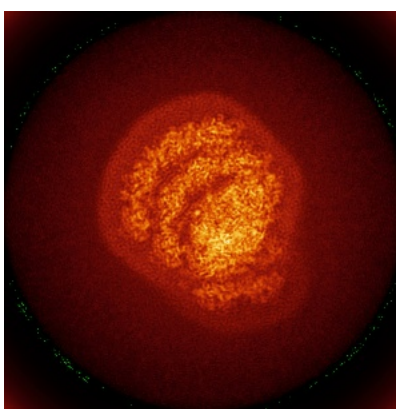
The images above show the largest variance slices of the map in three orthogonal directions.

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

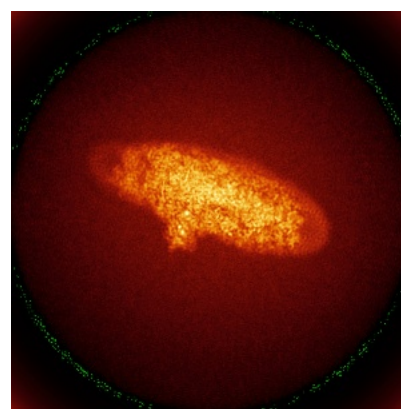
6.4.1 Primary map



X



Y

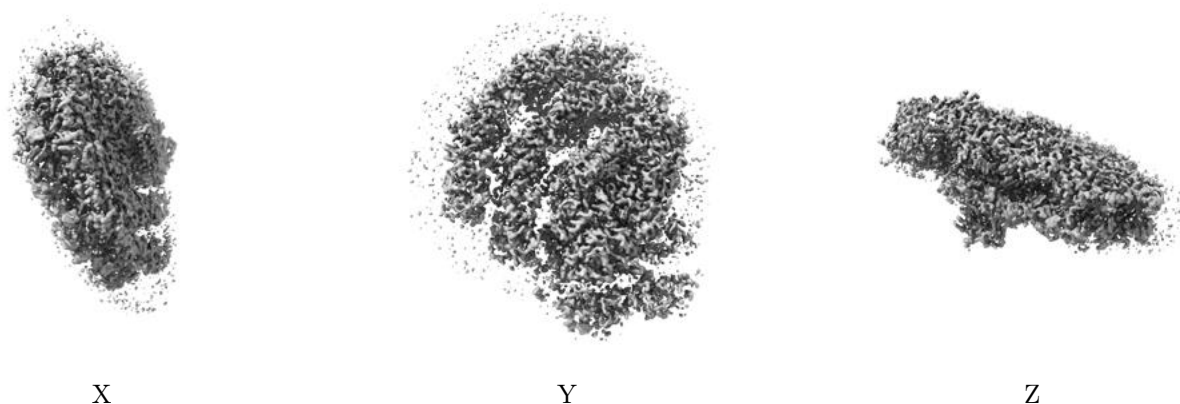


Z

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.

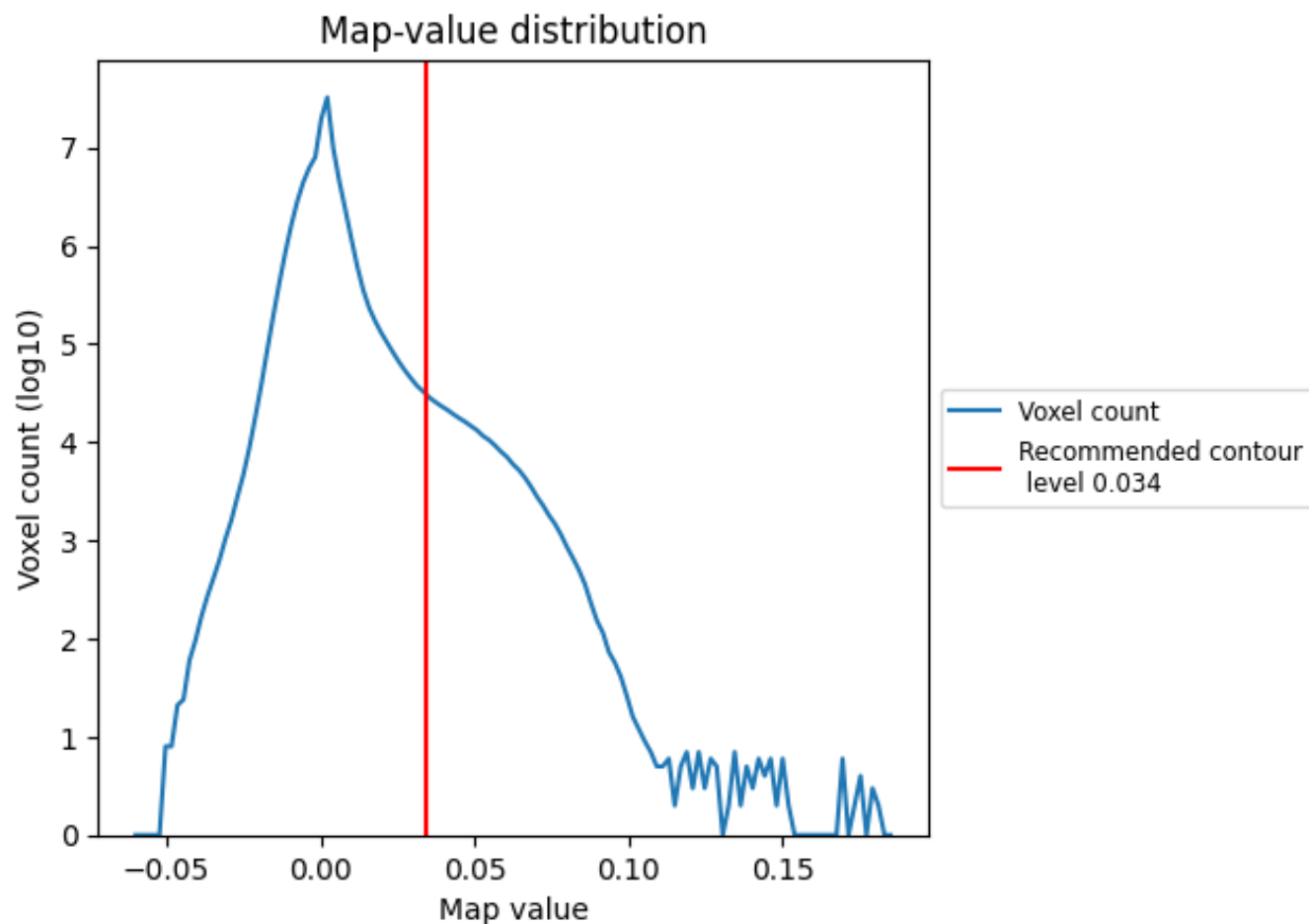
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

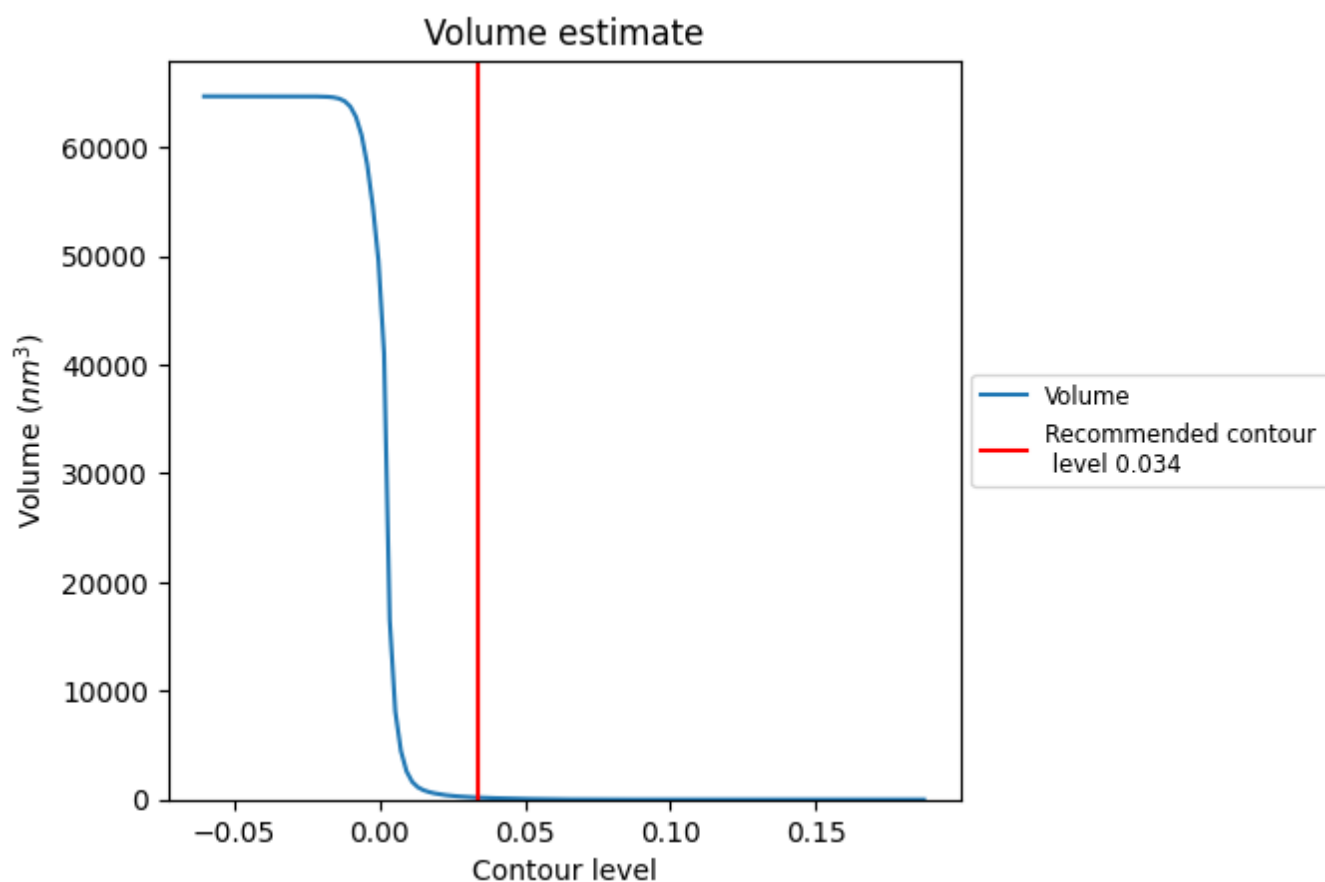
This section contains the results of statistical analysis of the map.

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.

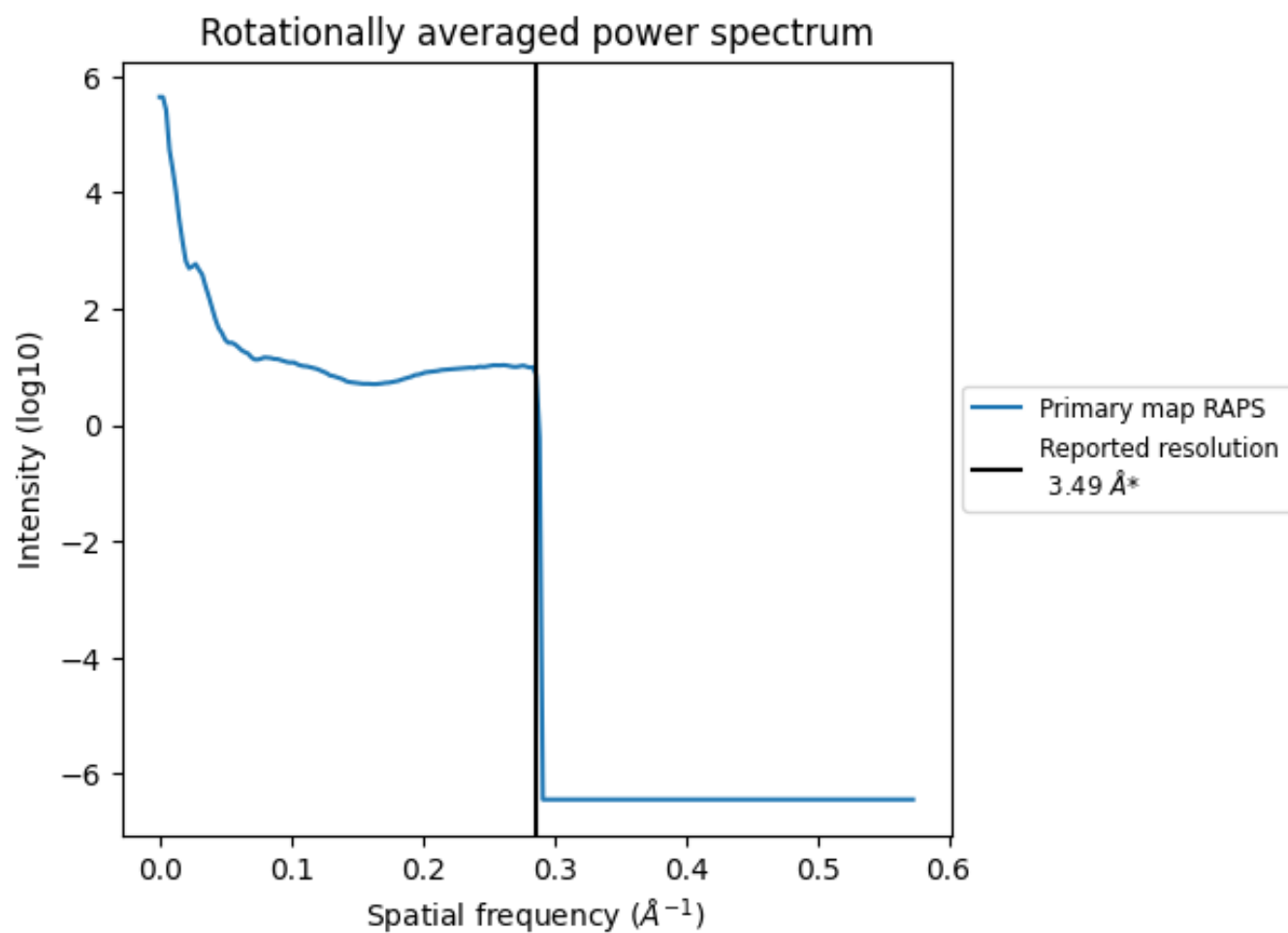
7.2 Volume estimate [i](#)



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

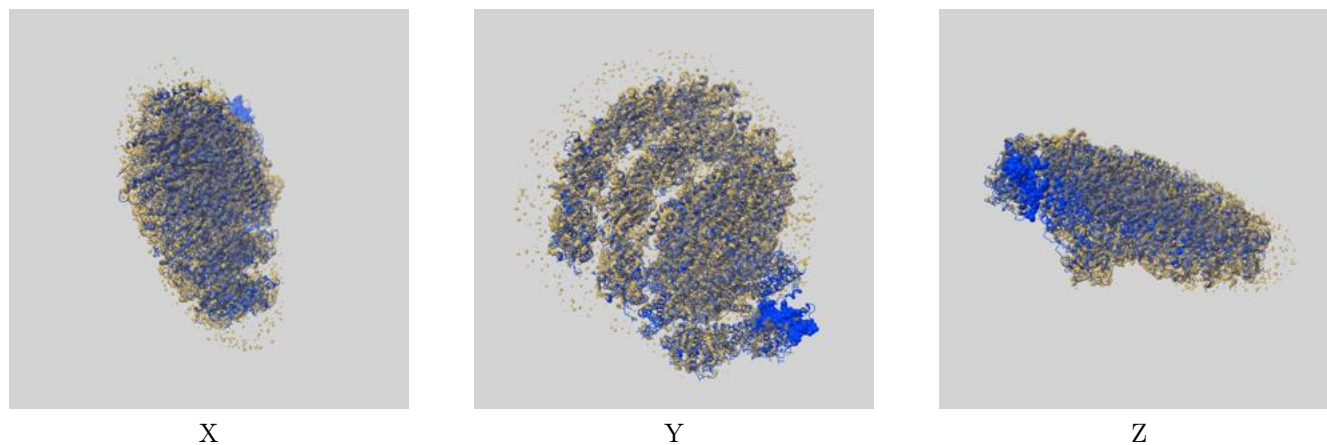
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

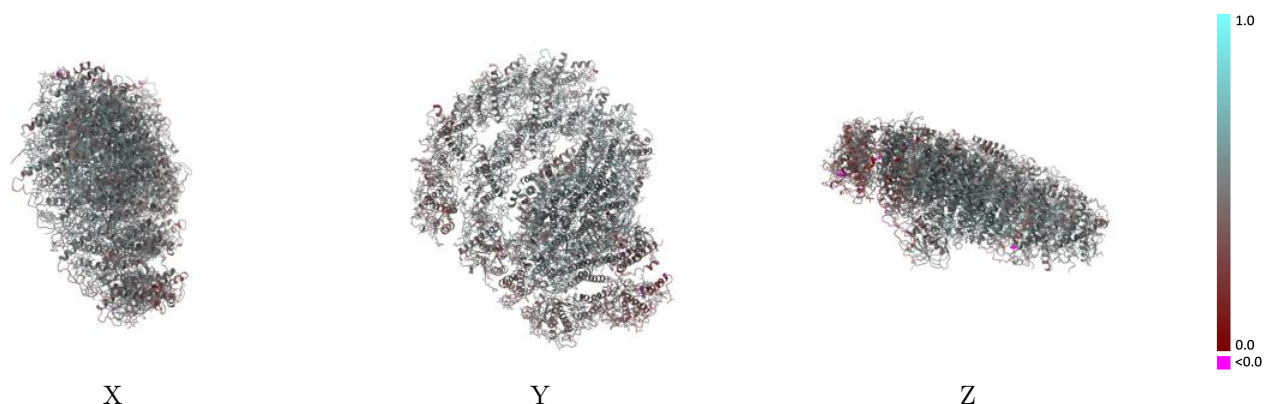
This section contains information regarding the fit between EMDB map EMD-9670 and PDB model 6IGZ. Per-residue inclusion information can be found in section [3](#) on page [34](#).

9.1 Map-model overlay [i](#)



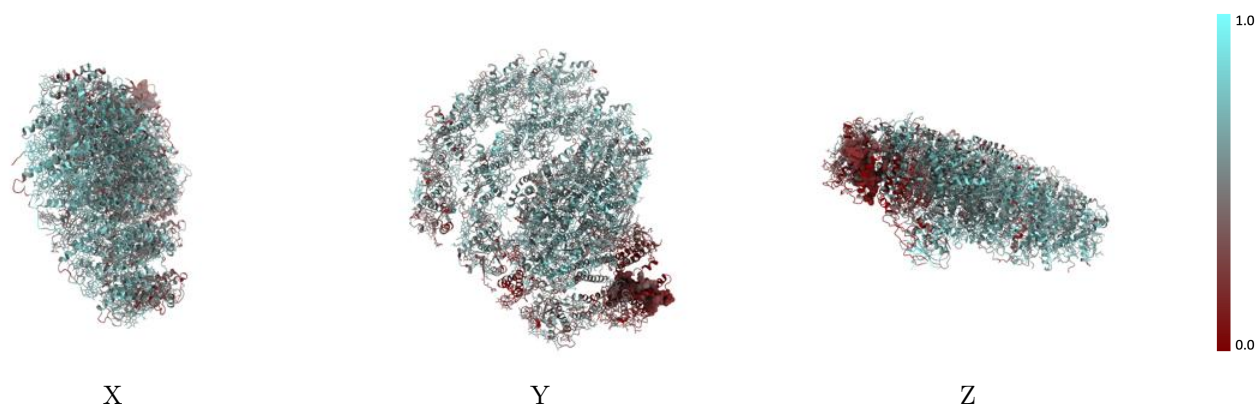
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



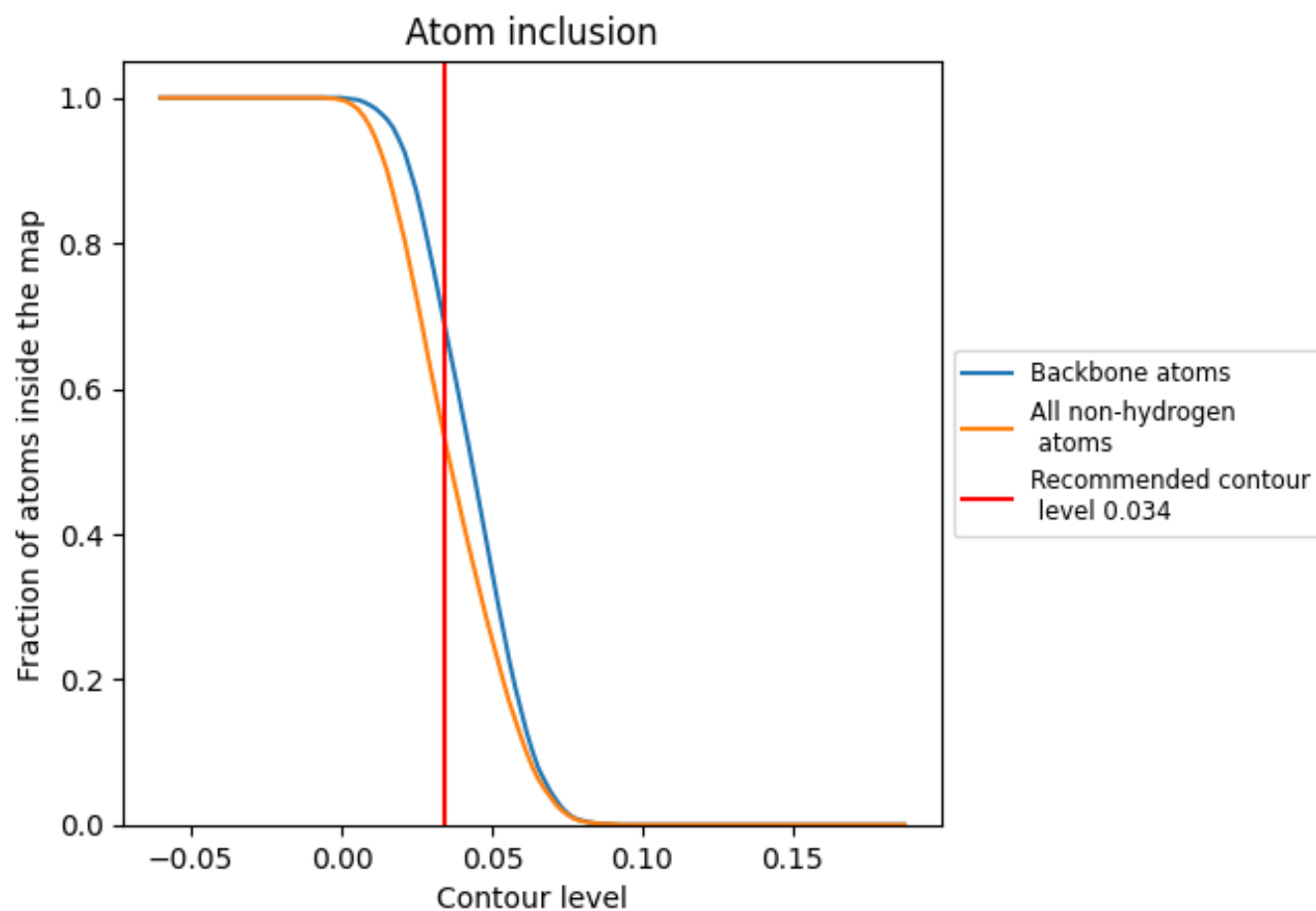
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

