



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 06:54 PM JST

PDB ID : 9K1E / pdb_00009k1e
EMDB ID : EMD-61973
Title : Structural insights into photosystem I complex of Bryopsis corticulans
Authors : Liu, X.Y.; Wang, W.D.
Deposited on : 2024-10-16
Resolution : 2.68 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

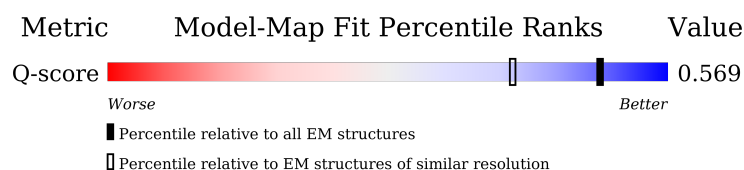
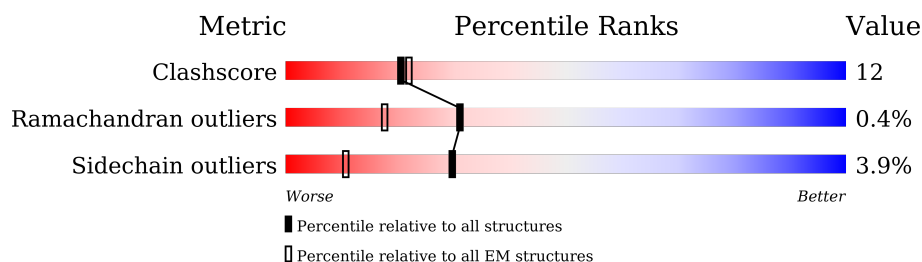
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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.



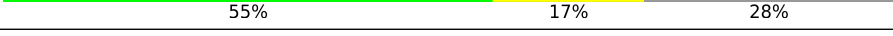
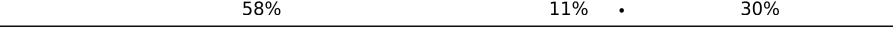
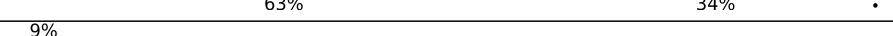
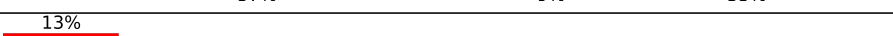
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9255 (2.18 - 3.18)

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	0	245	
2	1	226	
2	5	226	
3	2	256	

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Mol	Chain	Length	Quality of chain
4	3	281	
5	6	267	
6	7	264	
7	4	248	
7	8	248	
8	9	222	
9	A	751	
10	B	734	
11	D	198	
12	E	91	
13	F	236	
14	G	167	
15	I	36	
16	J	41	
17	L	204	
18	C	81	
19	K	123	
20	M	32	
21	O	137	
22	H	133	

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 54077 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	213	Total	C	N	O	S	0	0
			1640	1063	270	296	11		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	195	Total	C	N	O	S	0	0
			1478	950	243	273	12		
2	5	195	Total	C	N	O	S	0	0
			1484	956	243	273	12		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	216	Total	C	N	O	S	0	0
			1667	1082	269	304	12		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	228	Total	C	N	O	S	0	0
			1768	1141	288	329	10		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	229	Total	C	N	O	S	0	0
			1797	1182	292	313	10		

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	228	Total	C	N	O	S	0	0
			1758	1137	291	319	11		

- Molecule 7 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	205	Total	C	N	O	S	0	0
			1574	1035	256	274	9		
7	4	207	Total	C	N	O	S	0	0
			1569	1030	257	273	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	9	189	Total	C	N	O	S	0	0
			1453	932	245	267	9		

- Molecule 9 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	746	Total	C	N	O	S	0	0
			5872	3836	998	1016	22		

- Molecule 10 is a protein called photosystem I.

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

- Molecule 11 is a protein called Photosystem I reaction center subunit II, chloroplastic.

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

- Molecule 12 is a protein called PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	64	Total	C	N	O	S	0	0
			509	323	90	95	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	165	Total	C	N	O	S	0	0
			1273	810	224	235	4		

- Molecule 14 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	93	Total	C	N	O	S	0	0
			726	471	119	136			

- Molecule 15 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I	35	Total	C	N	O	S	0	0
			262	180	37	43	2		

- Molecule 16 is a protein called Photosystem I reaction center subunit IX.

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

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	162	Total	C	N	O	S	0	0
			1195	773	192	226	4		

- Molecule 18 is a protein called Photosystem I iron-sulfur center.

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

- Molecule 19 is a protein called PsaK.

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

- Molecule 20 is a protein called Photosystem I reaction center subunit XII.

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

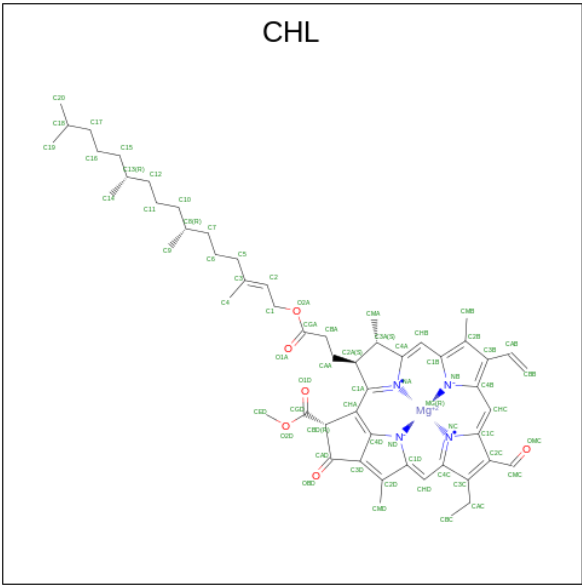
- Molecule 21 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	92	Total	C	N	O	S	0	0
			728	488	116	120	4		

- Molecule 22 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	94	Total	C	N	O	S	0	0
			717	451	126	139	1		

- Molecule 23 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
23	0	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	0	1	Total	C	Mg	N	O	0
			48	37	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
23	1	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	1	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			62	51	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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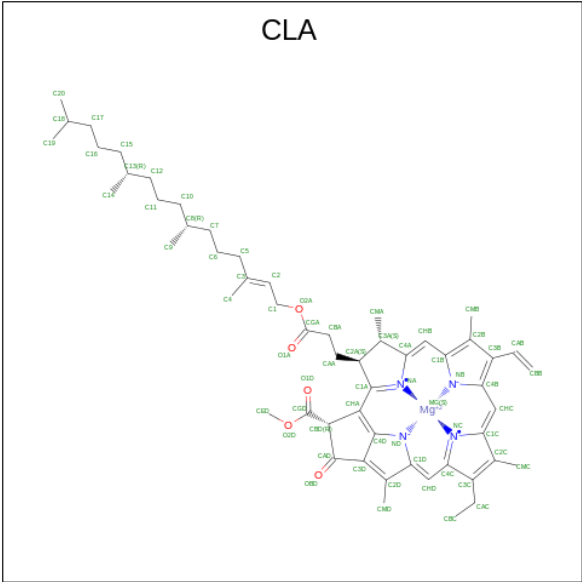
Mol	Chain	Residues	Atoms					AltConf
23	6	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			60	49	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	6	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			63	52	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			64	53	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	8	1	Total	C	Mg	N	O	0
			56	45	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
23	8	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
23	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
23	4	1	Total	C	Mg	N	O	0
			54	43	1	4	6	

- Molecule 24 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	0	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
24	0	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total 63	C 53	Mg 1	N 4	O 5	0
24	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	2	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	3	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	3	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
24	6	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	7	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
24	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	7	1	Total 59	C 49	Mg 1	N 4	O 5	0
24	7	1	Total 37	C 31	Mg 1	N 4	O 1	0
24	7	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	7	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	9	1	Total 48	C 38	Mg 1	N 4	O 5	0
24	9	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	9	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	9	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	9	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
24	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
24	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
24	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
24	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
24	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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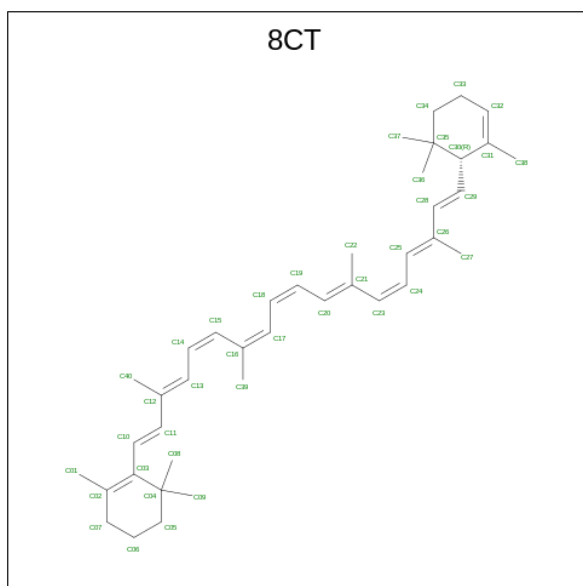
Mol	Chain	Residues	Atoms					AltConf
24	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
24	F	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
24	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
24	L	1	Total 58	C 48	Mg 1	N 4	O 5	0
24	L	1	Total 63	C 53	Mg 1	N 4	O 5	0
24	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	L	1	Total 47	C 37	Mg 1	N 4	O 5	0
24	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
24	K	1	Total 53	C 43	Mg 1	N 4	O 5	0
24	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
24	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
24	O	1	Total 52	C 42	Mg 1	N 4	O 5	0
24	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
24	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
24	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
24	O	1	Total 51	C 41	Mg 1	N 4	O 5	0
24	H	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
24	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
24	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
24	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 25 is (6'R,11cis,11'cis,13cis,15cis)-4',5'-didehydro-5',6'-dihydro-beta,beta-carotene (CCD ID: 8CT) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



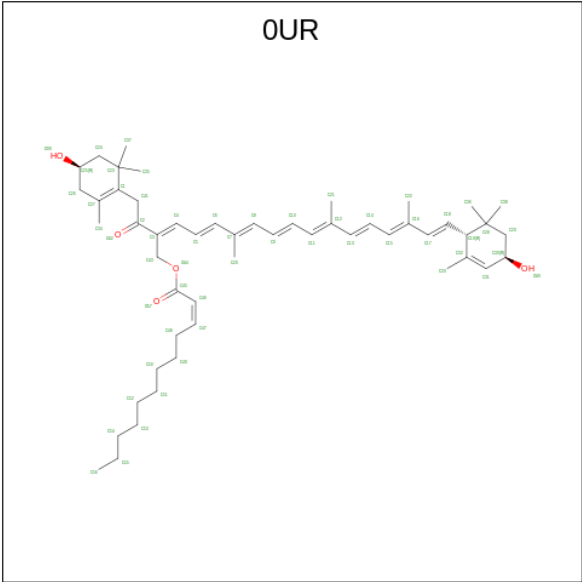
Mol	Chain	Residues	Atoms	AltConf
25	0	1	Total C 40 40	0
25	1	1	Total C 40 40	0
25	2	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	6	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	7	1	Total C 40 40	0
25	8	1	Total C 40 40	0
25	9	1	Total C 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	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

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Mol	Chain	Residues	Atoms	AltConf
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	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	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	M	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	O	1	Total C 40 40	0
25	4	1	Total C 40 40	0

- Molecule 26 is Siphonein (CCD ID: 0UR) (formula: C₅₂H₇₆O₅) (labeled as "Ligand of Interest" by depositor).



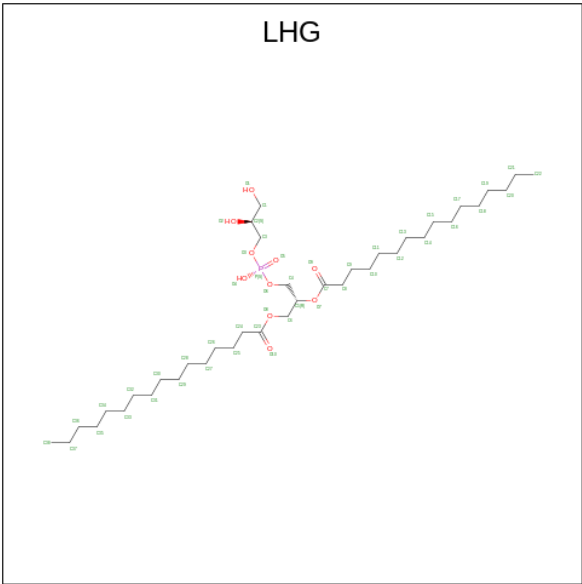
Mol	Chain	Residues	Atoms			AltConf
26	0	1	Total	C	O	0
			52	47	5	
26	0	1	Total	C	O	0
			52	47	5	
26	1	1	Total	C	O	0
			52	47	5	
26	1	1	Total	C	O	0
			52	47	5	
26	2	1	Total	C	O	0
			51	46	5	
26	2	1	Total	C	O	0
			50	45	5	
26	3	1	Total	C	O	0
			51	46	5	
26	5	1	Total	C	O	0
			51	46	5	
26	5	1	Total	C	O	0
			52	47	5	
26	6	1	Total	C	O	0
			51	46	5	
26	6	1	Total	C	O	0
			52	47	5	
26	7	1	Total	C	O	0
			51	46	5	
26	8	1	Total	C	O	0
			51	46	5	
26	8	1	Total	C	O	0
			52	47	5	

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Mol	Chain	Residues	Atoms			AltConf
26	9	1	Total	C	O	0
			52	47	5	
26	9	1	Total	C	O	0
			52	47	5	
26	O	1	Total	C	O	0
			52	47	5	
26	4	1	Total	C	O	0
			51	46	5	
26	4	1	Total	C	O	0
			50	45	5	

- Molecule 27 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



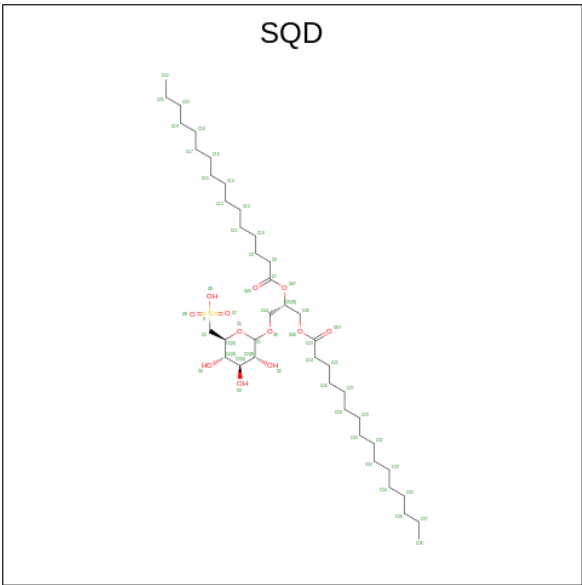
Mol	Chain	Residues	Atoms				AltConf
27	0	1	Total	C	O	P	0
			49	38	10	1	
27	1	1	Total	C	O	P	0
			49	38	10	1	
27	1	1	Total	C	O	P	0
			43	32	10	1	
27	2	1	Total	C	O	P	0
			32	21	10	1	
27	2	1	Total	C	O	P	0
			32	21	10	1	
27	3	1	Total	C	O	P	0
			36	25	10	1	

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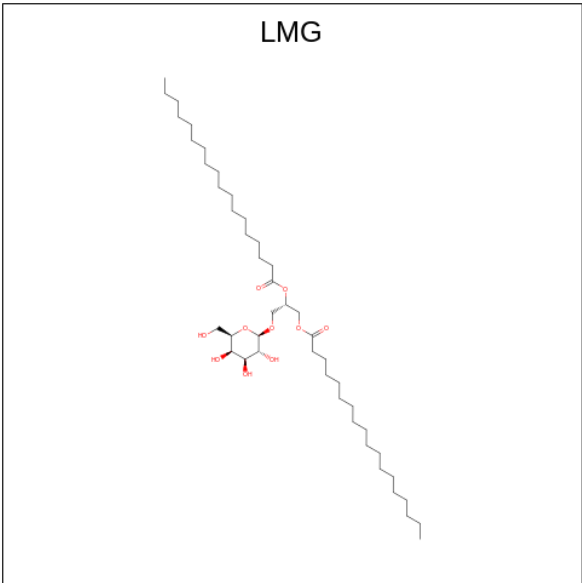
Mol	Chain	Residues	Atoms				AltConf
27	3	1	Total	C	O	P	0
			37	26	10	1	
27	3	1	Total	C	O	P	0
			43	34	8	1	
27	5	1	Total	C	O	P	0
			37	26	10	1	
27	6	1	Total	C	O	P	0
			37	26	10	1	
27	7	1	Total	C	O	P	0
			30	19	10	1	
27	7	1	Total	C	O	P	0
			38	27	10	1	
27	7	1	Total	C	O	P	0
			39	28	10	1	
27	8	1	Total	C	O	P	0
			31	20	10	1	
27	8	1	Total	C	O	P	0
			44	33	10	1	
27	9	1	Total	C	O	P	0
			47	36	10	1	
27	A	1	Total	C	O	P	0
			49	38	10	1	
27	A	1	Total	C	O	P	0
			27	16	10	1	
27	A	1	Total	C	O	P	0
			42	31	10	1	
27	B	1	Total	C	O	P	0
			23	12	10	1	
27	B	1	Total	C	O	P	0
			38	27	10	1	
27	I	1	Total	C	O	P	0
			46	35	10	1	
27	L	1	Total	C	O	P	0
			31	20	10	1	

- Molecule 28 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
28	0	1	36	26	9	1	0

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



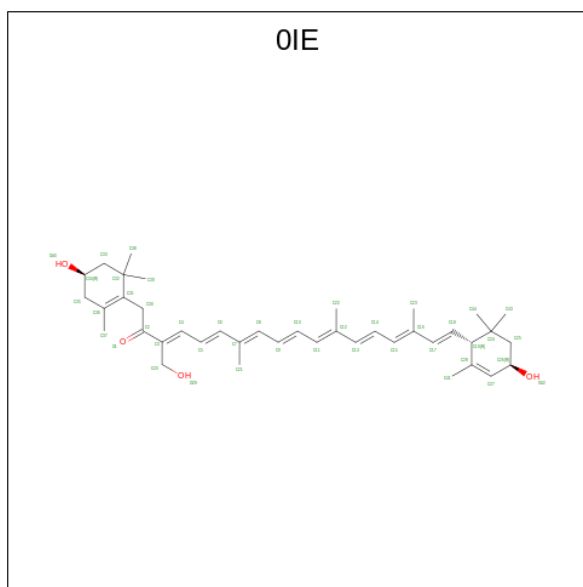
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	2	1	36	26	10	0
29	3	1	36	26	10	0

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Mol	Chain	Residues	Atoms			AltConf
29	9	1	Total	C	O	0
			55	45	10	
29	A	1	Total	C	O	0
			36	26	10	
29	A	1	Total	C	O	0
			37	27	10	
29	J	1	Total	C	O	0
			29	19	10	
29	J	1	Total	C	O	0
			46	36	10	
29	M	1	Total	C	O	0
			42	32	10	
29	O	1	Total	C	O	0
			31	21	10	
29	O	1	Total	C	O	0
			39	29	10	

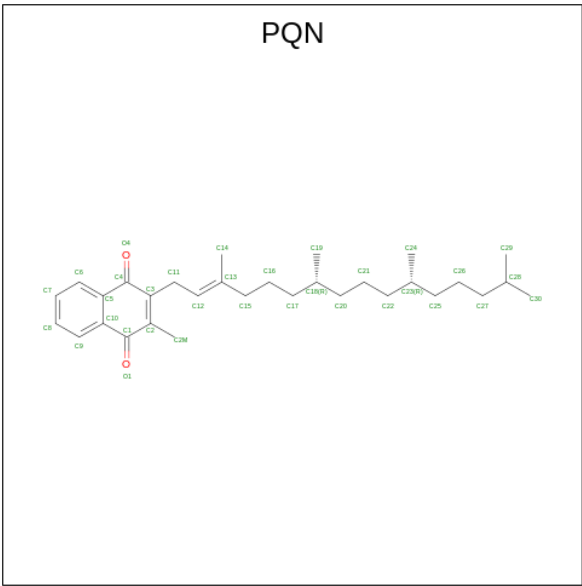
- Molecule 30 is Siphonaxanthin (CCD ID: 0IE) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	3	1	Total	C	O	0
			44	40	4	
30	7	1	Total	C	O	0
			44	40	4	

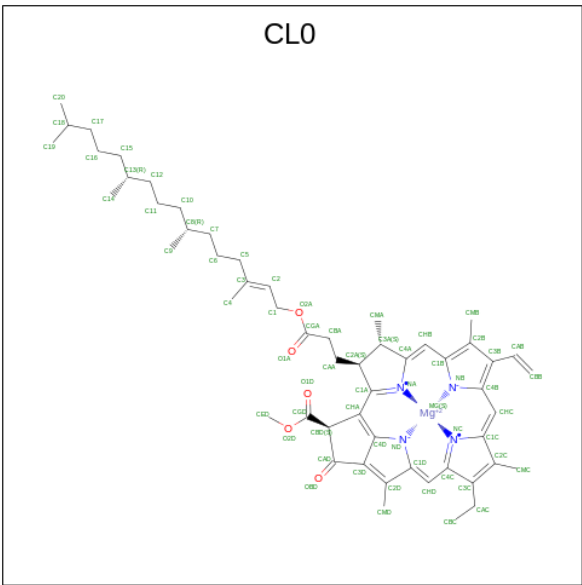
- Molecule 31 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Lig-

and of Interest" by depositor).



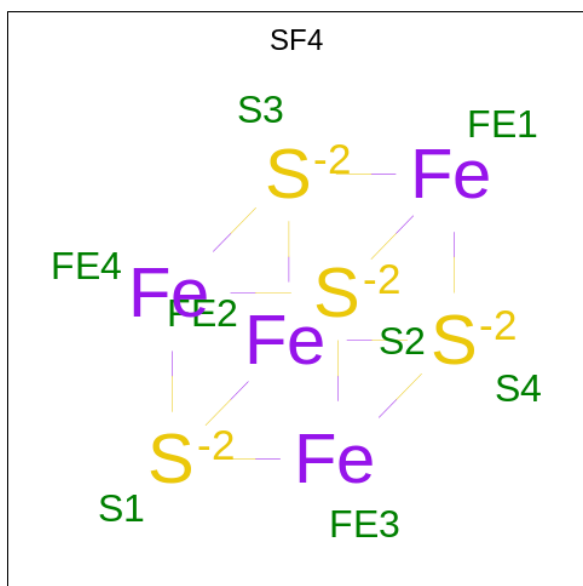
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			33	31	2	
31	B	1	Total	C	O	0
			33	31	2	

- Molecule 32 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



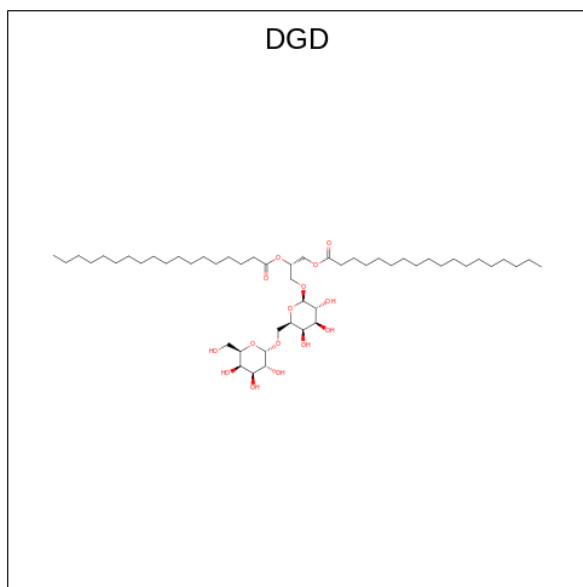
Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 33 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).

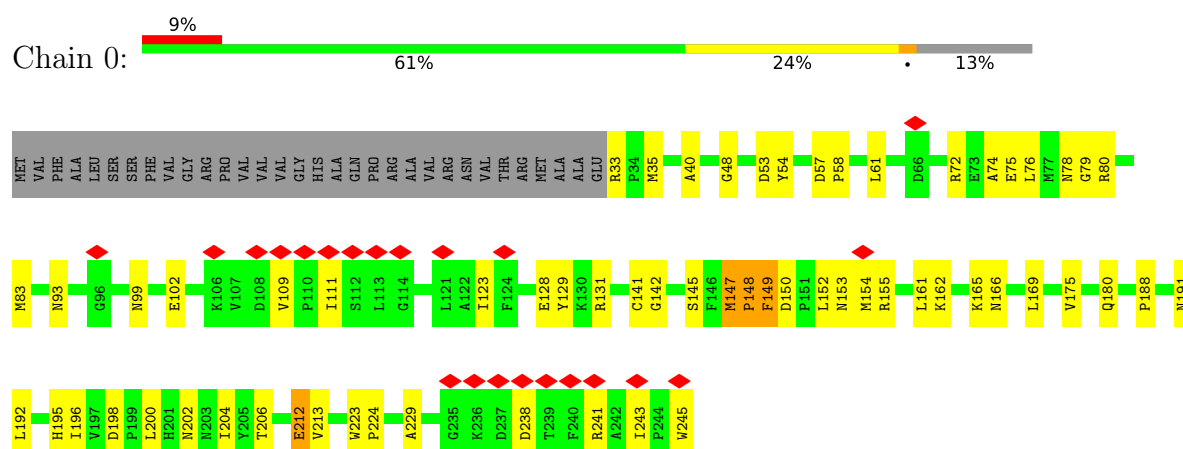


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
34	B	1	56	41	15	0

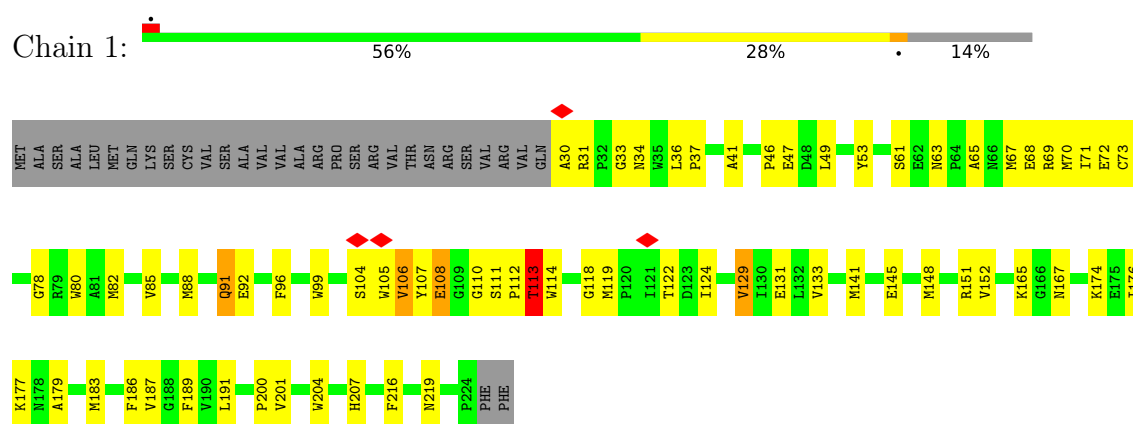
3 Residue-property plots

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.

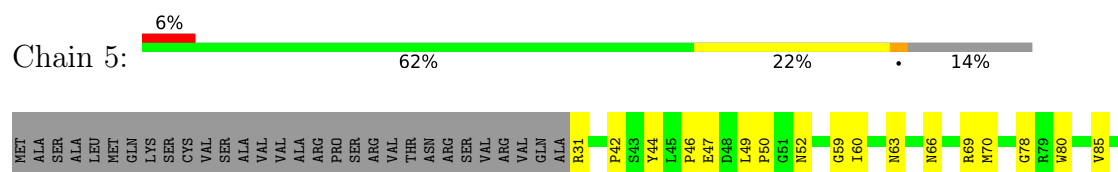
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

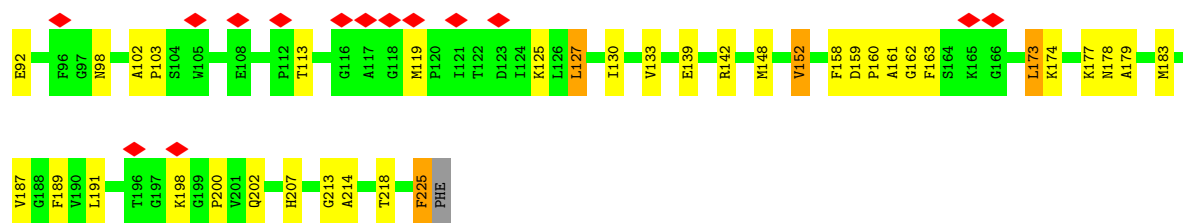


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



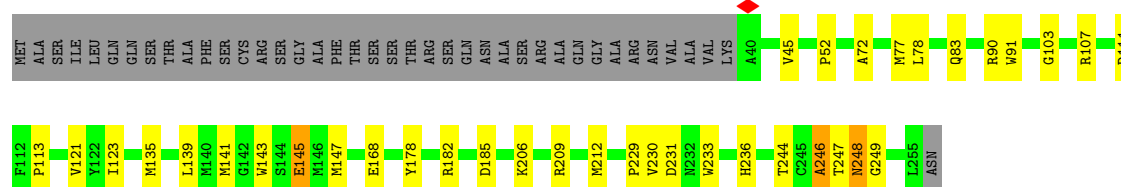
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic





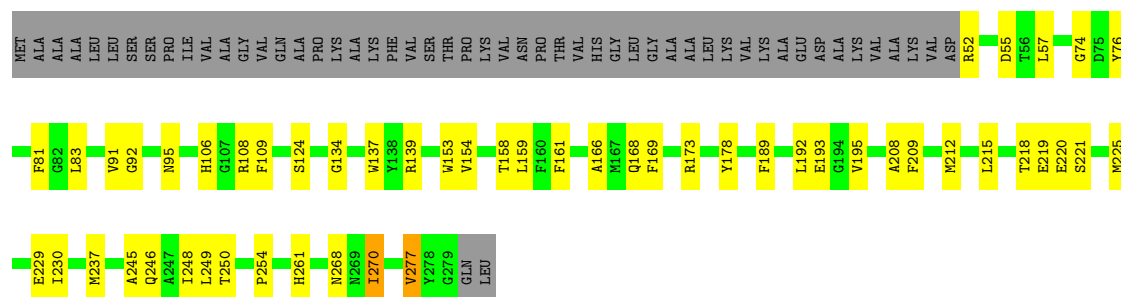
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 2: 70% 13% 16%



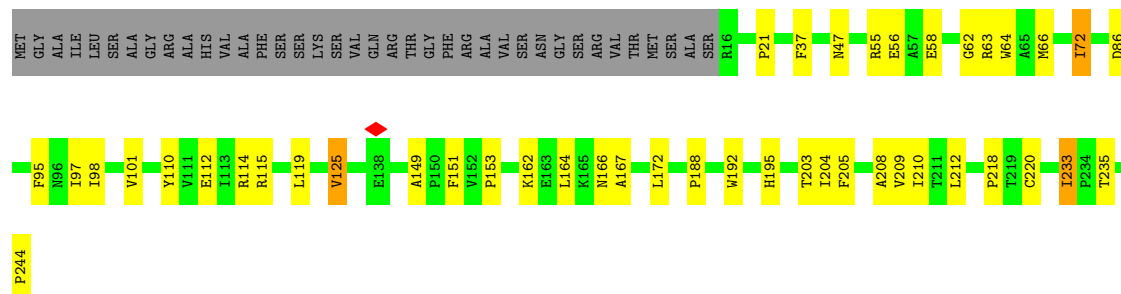
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic

Chain 3: 62% 18% 19%



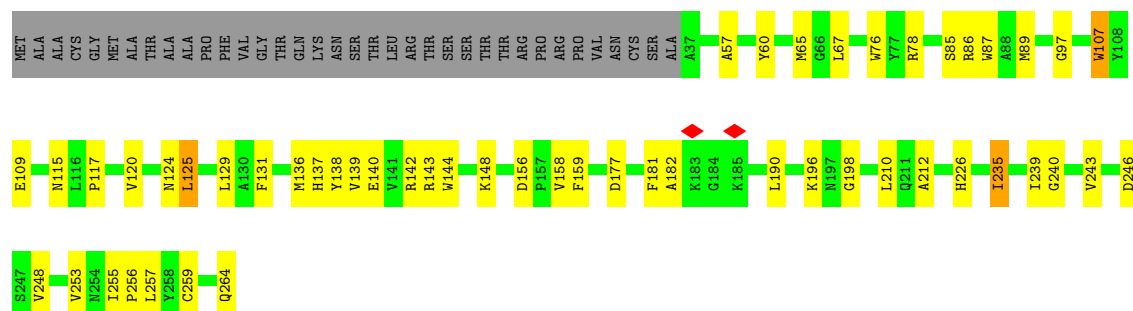
- Molecule 5: Chlorophyll a-b binding protein, chloroplastic

Chain 6: 69% 16% 14%

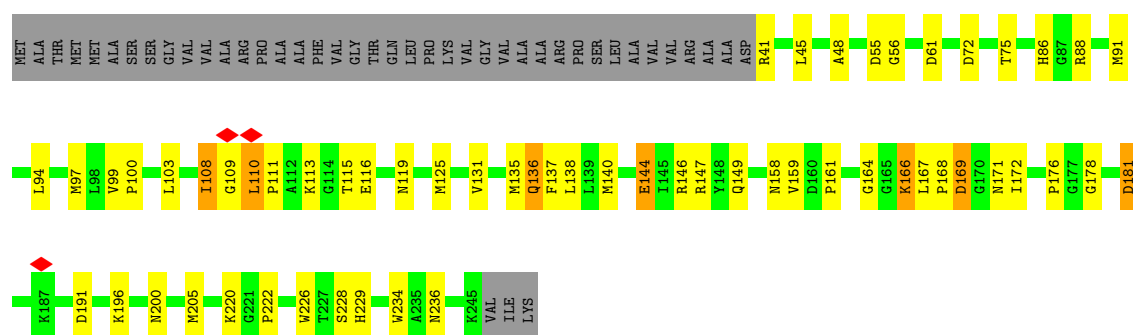


- Molecule 6: Chlorophyll a-b binding protein, chloroplastic

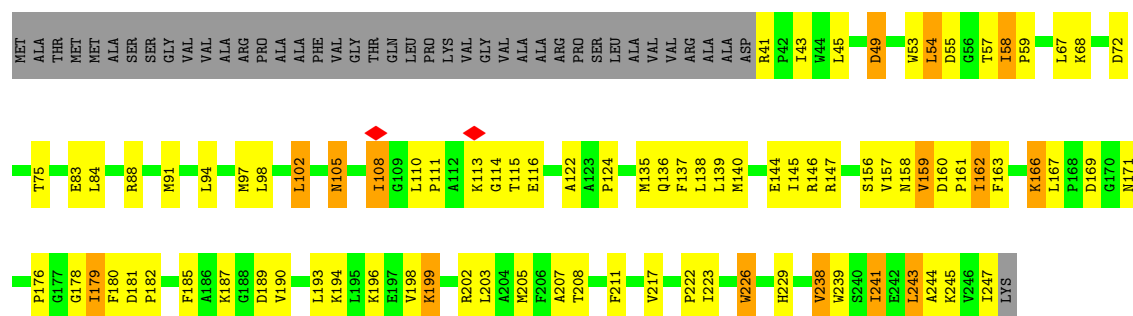
Chain 7: 66% 19% 14%



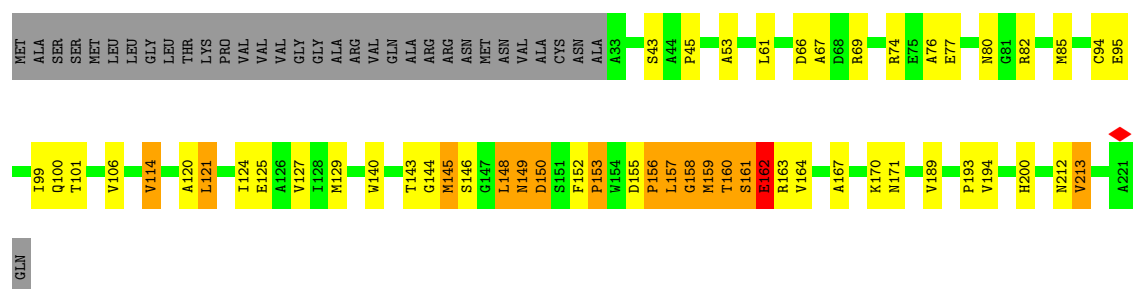
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



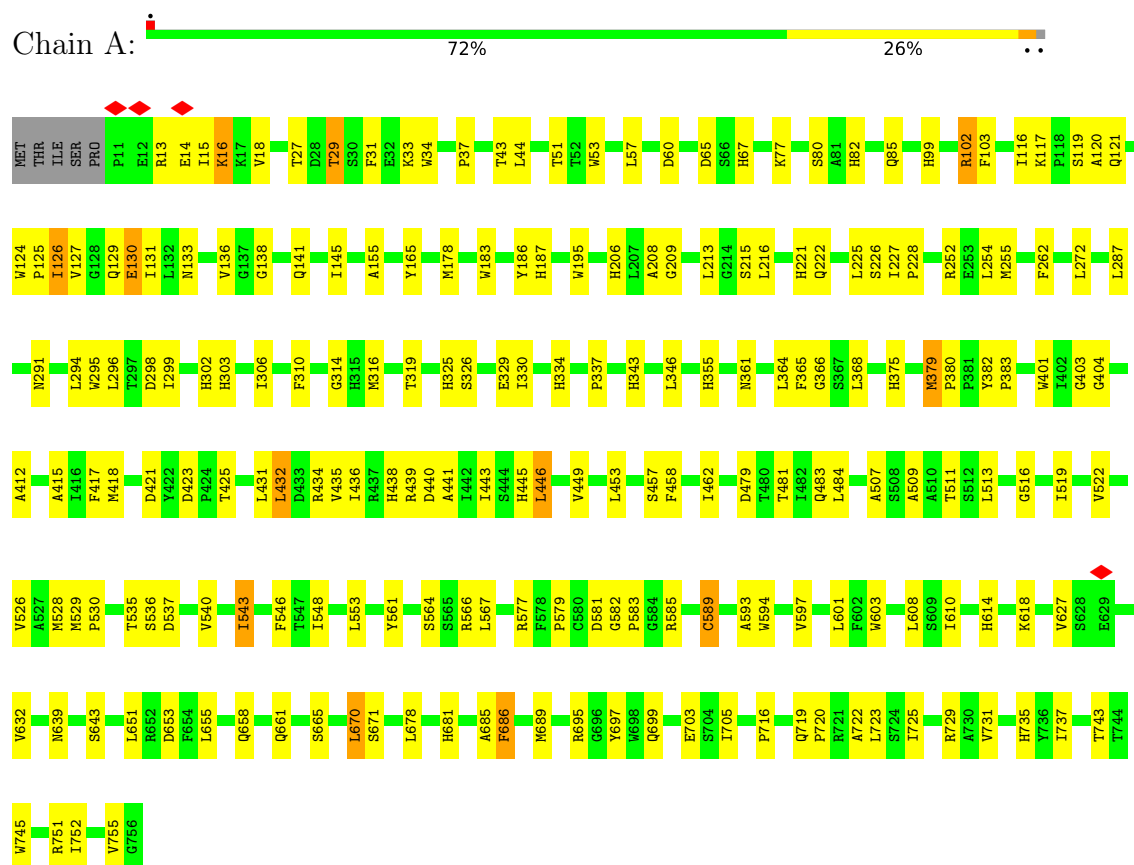
- Molecule 7: Chlorophyll a-b binding protein, chloroplastic



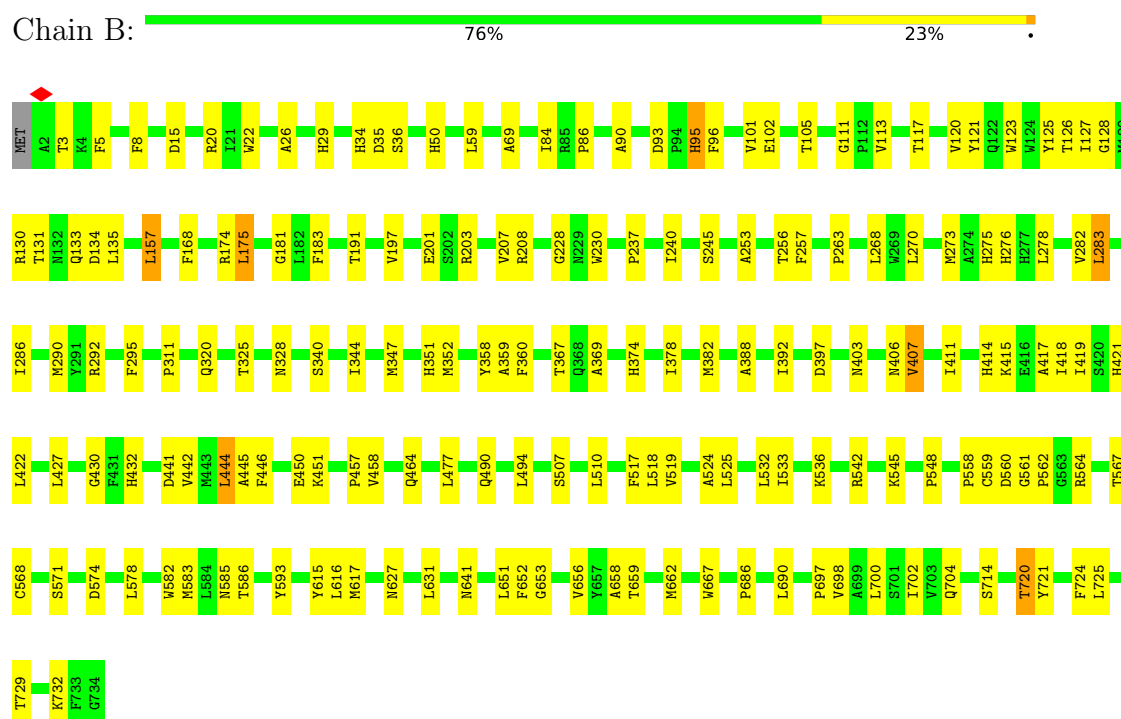
- Molecule 8: Chlorophyll a-b binding protein, chloroplastic



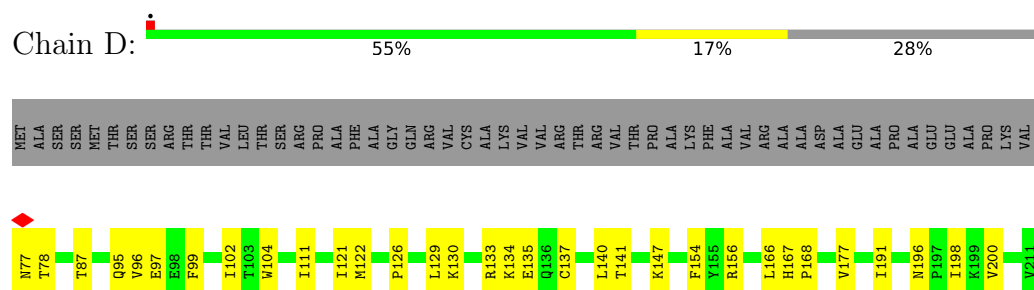
• Molecule 9: Photosystem I P700 chlorophyll a apoprotein A1



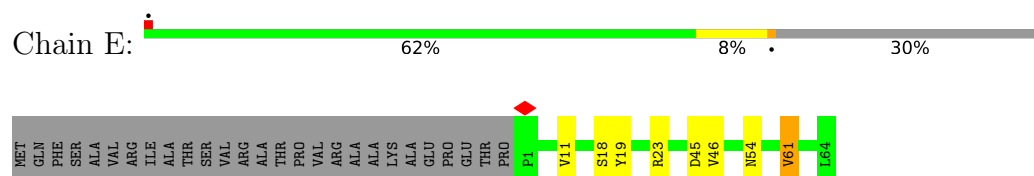
• Molecule 10: photosystem I



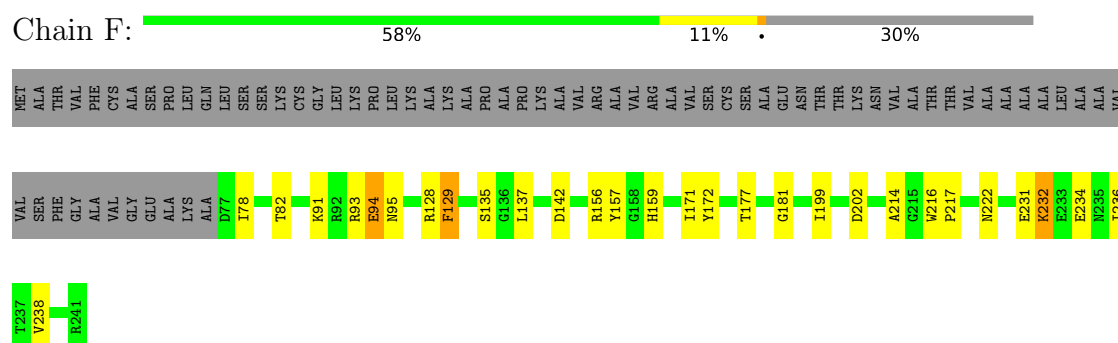
- Molecule 11: Photosystem I reaction center subunit II, chloroplastic



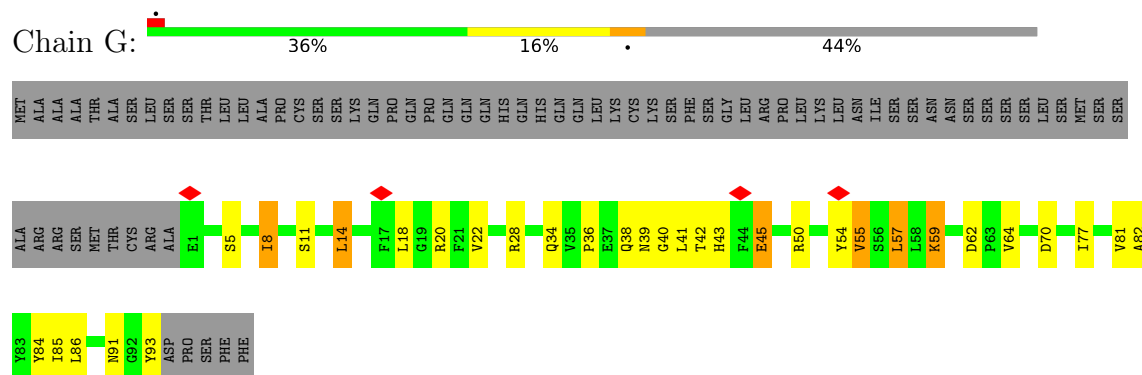
- Molecule 12: PsaE



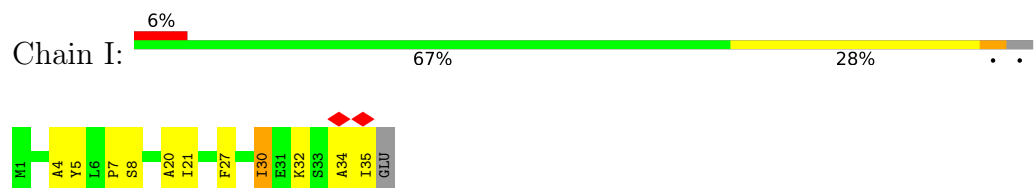
- Molecule 13: Photosystem I reaction center subunit III



- Molecule 14: PsaG



- Molecule 15: Photosystem I reaction center subunit VIII



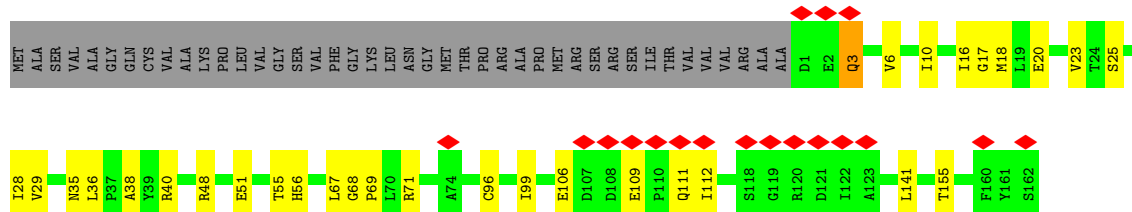
- Molecule 16: Photosystem I reaction center subunit IX

Chain J:  63% 34% .



- Molecule 17: PSI subunit V

Chain L:  9% 64% 15% 21% .



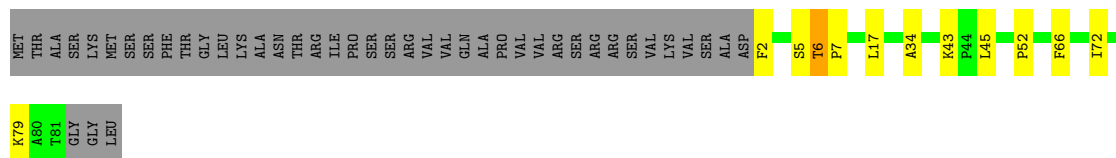
- Molecule 18: Photosystem I iron-sulfur center

Chain C:  77% 22% .



- Molecule 19: PsaK

Chain K:  55% 9% 35% .



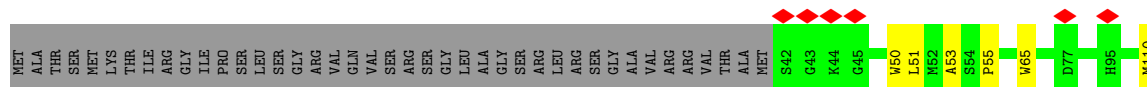
- Molecule 20: Photosystem I reaction center subunit XII

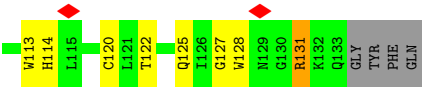
Chain M:  84% 12% .



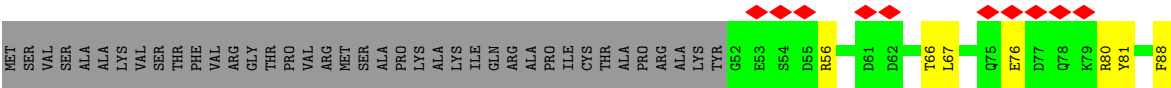
- Molecule 21: PsaO

Chain O:  6% 57% 9% 33% .





• Molecule 22: PsaH



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	287144	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.536	Depositor
Minimum map value	-0.386	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.203	Depositor
Map size (Å)	532.48, 532.48, 532.48	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 8CT, 0UR, DGD, 0IE, CLA, SF4, LMG, CHL, SQD, LHG, PQN, CL0

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	0	0.27	0/1685	0.38	0/2285
2	1	0.41	1/1523 (0.1%)	0.45	1/2073 (0.0%)
2	5	0.21	0/1530	0.41	0/2082
3	2	0.47	2/1727 (0.1%)	0.42	2/2351 (0.1%)
4	3	0.25	0/1818	0.32	0/2466
5	6	0.22	0/1862	0.30	0/2542
6	7	0.22	0/1812	0.31	0/2468
7	4	0.34	0/1619	0.62	1/2206 (0.0%)
7	8	0.20	0/1627	0.41	2/2217 (0.1%)
8	9	0.53	0/1492	0.48	1/2036 (0.0%)
9	A	0.42	1/6069 (0.0%)	0.35	1/8267 (0.0%)
10	B	0.37	0/6034	0.35	0/8239
11	D	0.21	0/1135	0.34	0/1533
12	E	0.20	0/521	0.26	0/706
13	F	0.21	0/1298	0.31	0/1748
14	G	0.25	0/743	0.41	0/1010
15	I	0.60	0/269	0.45	0/367
16	J	0.25	0/346	0.37	0/472
17	L	0.22	0/1224	0.34	0/1673
18	C	0.25	0/612	0.37	0/830
19	K	0.20	0/567	0.27	0/769
20	M	0.66	0/241	0.34	0/325
21	O	0.22	0/760	0.32	0/1042
22	H	0.18	0/729	0.34	0/979
All	All	0.34	4/37243 (0.0%)	0.38	8/50686 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	246	ALA	CA-C	-5.28	1.46	1.52
9	A	689	MET	CA-C	-5.25	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	113	THR	CA-C	-5.14	1.46	1.53
3	2	247	THR	N-CA	-5.12	1.39	1.46

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	4	180	PHE	N-CA-C	-13.95	96.82	112.72
8	9	163	ARG	N-CA-C	-8.43	102.05	111.07
7	8	109	GLY	CA-C-N	6.63	129.47	123.10
7	8	109	GLY	C-N-CA	6.63	129.47	123.10
2	1	108	GLU	N-CA-C	-6.22	104.39	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	1640	0	1609	47	0
2	1	1478	0	1423	55	0
2	5	1484	0	1427	40	0
3	2	1667	0	1562	26	0
4	3	1768	0	1702	45	0
5	6	1797	0	1752	37	0
6	7	1758	0	1701	46	0
7	4	1569	0	1551	67	0
7	8	1574	0	1550	48	0
8	9	1453	0	1404	45	0
9	A	5872	0	5715	162	0
10	B	5824	0	5603	147	0
11	D	1109	0	1124	27	0
12	E	509	0	506	8	0
13	F	1273	0	1290	24	0
14	G	726	0	717	33	0
15	I	262	0	279	10	0
16	J	336	0	355	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1195	0	1187	25	0
18	C	602	0	591	20	0
19	K	558	0	591	9	0
20	M	238	0	248	4	0
21	O	728	0	699	16	0
22	H	717	0	684	18	0
23	0	215	0	172	14	0
23	1	291	0	262	16	0
23	2	304	0	230	15	0
23	3	240	0	223	10	0
23	4	408	0	308	28	0
23	5	252	0	189	13	0
23	6	486	0	404	28	0
23	7	334	0	280	20	0
23	8	411	0	314	23	0
23	9	193	0	132	5	0
24	0	524	0	459	22	0
24	1	434	0	386	17	0
24	2	389	0	356	8	0
24	3	603	0	554	18	0
24	4	371	0	324	12	0
24	5	409	0	340	13	0
24	6	527	0	456	15	0
24	7	569	0	496	27	0
24	8	364	0	314	10	0
24	9	438	0	403	18	0
24	A	2547	0	2613	127	0
24	B	2368	0	2356	147	0
24	F	92	0	68	4	0
24	G	141	0	105	2	0
24	H	246	0	193	6	0
24	J	42	0	31	2	0
24	K	209	0	176	6	0
24	L	214	0	188	9	0
24	O	220	0	151	10	0
25	0	40	0	0	0	0
25	1	40	0	0	0	0
25	2	40	0	0	0	0
25	3	120	0	0	2	0
25	4	40	0	0	1	0
25	6	80	0	0	0	0
25	7	80	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	8	40	0	0	1	0
25	9	40	0	0	0	0
25	A	200	0	0	1	0
25	B	280	0	0	1	0
25	F	80	0	0	1	0
25	G	40	0	0	0	0
25	I	40	0	0	0	0
25	J	80	0	0	1	0
25	K	40	0	0	0	0
25	L	120	0	0	1	0
25	M	40	0	0	0	0
25	O	80	0	0	0	0
26	0	104	0	0	1	0
26	1	104	0	0	1	0
26	2	101	0	0	3	0
26	3	51	0	0	1	0
26	4	101	0	0	3	0
26	5	103	0	0	4	0
26	6	103	0	0	1	0
26	7	51	0	0	2	0
26	8	103	0	0	2	0
26	9	104	0	0	3	0
26	O	52	0	0	2	0
27	0	49	0	74	2	0
27	1	92	0	133	7	0
27	2	64	0	68	2	0
27	3	116	0	144	7	0
27	5	37	0	44	1	0
27	6	37	0	44	5	0
27	7	107	0	127	5	0
27	8	75	0	90	0	0
27	9	47	0	63	5	0
27	A	118	0	152	11	0
27	B	61	0	62	2	0
27	I	46	0	65	4	0
27	L	31	0	32	0	0
28	0	36	0	41	2	0
29	2	36	0	42	0	0
29	3	36	0	42	2	0
29	9	55	0	86	4	0
29	A	73	0	86	7	0
29	J	75	0	93	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	M	42	0	54	1	0
29	O	70	0	80	1	0
30	3	44	0	0	0	0
30	7	44	0	0	0	0
31	A	33	0	46	4	0
31	B	33	0	46	1	0
32	A	65	0	72	8	0
33	B	8	0	0	1	0
33	C	16	0	0	0	0
34	B	56	0	70	3	0
All	All	54077	0	49609	1253	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 12.

The worst 5 of 1253 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)
2:5:160:PRO:HD2	26:5:314:0UR:C30	1.90	1.01
1:0:147:MET:HB3	1:0:148:PRO:HD2	1.42	1.01
24:A:804:CLA:H11	24:A:805:CLA:HBB1	1.51	0.91
32:A:852:CL0:H15	24:B:804:CLA:HED1	1.52	0.89
9:A:29:THR:HG21	9:A:183:TRP:HE1	1.39	0.88

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	0	211/245 (86%)	192 (91%)	17 (8%)	2 (1%)	14	31
2	1	193/226 (85%)	186 (96%)	6 (3%)	1 (0%)	24	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	5	193/226 (85%)	177 (92%)	15 (8%)	1 (0%)	24	45
3	2	214/256 (84%)	205 (96%)	9 (4%)	0	100	100
4	3	226/281 (80%)	219 (97%)	7 (3%)	0	100	100
5	6	227/267 (85%)	222 (98%)	5 (2%)	0	100	100
6	7	226/264 (86%)	212 (94%)	12 (5%)	2 (1%)	14	31
7	4	205/248 (83%)	176 (86%)	28 (14%)	1 (0%)	24	45
7	8	203/248 (82%)	187 (92%)	14 (7%)	2 (1%)	12	28
8	9	187/222 (84%)	168 (90%)	12 (6%)	7 (4%)	2	5
9	A	744/751 (99%)	711 (96%)	32 (4%)	1 (0%)	48	71
10	B	731/734 (100%)	707 (97%)	24 (3%)	0	100	100
11	D	140/198 (71%)	134 (96%)	6 (4%)	0	100	100
12	E	62/91 (68%)	60 (97%)	2 (3%)	0	100	100
13	F	163/236 (69%)	155 (95%)	8 (5%)	0	100	100
14	G	91/167 (54%)	85 (93%)	6 (7%)	0	100	100
15	I	33/36 (92%)	30 (91%)	3 (9%)	0	100	100
16	J	39/41 (95%)	39 (100%)	0	0	100	100
17	L	160/204 (78%)	157 (98%)	3 (2%)	0	100	100
18	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
19	K	78/123 (63%)	78 (100%)	0	0	100	100
20	M	29/32 (91%)	29 (100%)	0	0	100	100
21	O	90/137 (66%)	85 (94%)	5 (6%)	0	100	100
22	H	92/133 (69%)	82 (89%)	10 (11%)	0	100	100
All	All	4615/5447 (85%)	4371 (95%)	227 (5%)	17 (0%)	31	51

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	148	PRO
6	7	125	LEU
7	8	108	ILE
8	9	153	PRO
1	0	149	PHE

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	0	167/194 (86%)	162 (97%)	5 (3%)	36	63
2	1	148/175 (85%)	139 (94%)	9 (6%)	17	37
2	5	149/175 (85%)	144 (97%)	5 (3%)	32	59
3	2	166/197 (84%)	163 (98%)	3 (2%)	51	76
4	3	186/225 (83%)	183 (98%)	3 (2%)	55	78
5	6	188/216 (87%)	181 (96%)	7 (4%)	30	56
6	7	181/209 (87%)	176 (97%)	5 (3%)	38	65
7	4	158/189 (84%)	133 (84%)	25 (16%)	2	6
7	8	159/189 (84%)	150 (94%)	9 (6%)	18	40
8	9	147/173 (85%)	136 (92%)	11 (8%)	12	28
9	A	609/614 (99%)	591 (97%)	18 (3%)	36	63
10	B	600/601 (100%)	586 (98%)	14 (2%)	44	71
11	D	119/162 (74%)	117 (98%)	2 (2%)	53	77
12	E	56/77 (73%)	54 (96%)	2 (4%)	31	57
13	F	129/180 (72%)	123 (95%)	6 (5%)	23	47
14	G	79/145 (54%)	71 (90%)	8 (10%)	7	16
15	I	27/28 (96%)	26 (96%)	1 (4%)	30	56
16	J	38/38 (100%)	36 (95%)	2 (5%)	20	43
17	L	124/157 (79%)	119 (96%)	5 (4%)	28	53
18	C	68/69 (99%)	66 (97%)	2 (3%)	37	64
19	K	58/94 (62%)	55 (95%)	3 (5%)	21	43
20	M	26/27 (96%)	26 (100%)	0	100	100
21	O	76/111 (68%)	75 (99%)	1 (1%)	61	81
22	H	69/103 (67%)	69 (100%)	0	100	100
All	All	3727/4348 (86%)	3581 (96%)	146 (4%)	30	54

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	C	11	CYS
7	4	238	VAL
19	K	45	LEU
7	4	113	LYS
8	9	145	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
17	L	35	ASN
18	C	3	HIS
21	O	129	ASN
8	9	215	ASN
8	9	86	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](#)

352 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
24	CLA	A	822	9	55,59,73	1.42	10 (18%)	66,96,113	1.40	5 (7%)
24	CLA	0	303	1	66,70,73	1.28	9 (13%)	79,109,113	1.28	5 (6%)
23	CHL	5	304	-	50,54,74	2.24	19 (38%)	56,90,114	3.28	25 (44%)
24	CLA	A	824	-	69,73,73	1.24	10 (14%)	83,113,113	1.32	9 (10%)
24	CLA	2	302	3	60,64,73	1.35	9 (15%)	72,102,113	1.38	6 (8%)
29	LMG	9	317	-	55,55,55	0.70	1 (1%)	63,63,63	1.39	9 (14%)
23	CHL	7	305	-	52,56,74	2.12	19 (36%)	58,92,114	3.27	26 (44%)
25	8CT	J	104	-	40,41,41	4.66	23 (57%)	50,56,56	3.42	22 (44%)
24	CLA	3	315	-	56,60,73	1.37	9 (16%)	67,97,113	1.49	7 (10%)
24	CLA	B	824	10	64,68,73	1.30	10 (15%)	77,107,113	1.30	6 (7%)
25	8CT	6	324	-	40,41,41	4.70	24 (60%)	50,56,56	2.49	18 (36%)
25	8CT	G	104	-	40,41,41	4.67	24 (60%)	50,56,56	3.08	19 (38%)
24	CLA	6	310	27	64,68,73	1.30	9 (14%)	77,107,113	1.32	5 (6%)
29	LMG	A	854	-	37,37,55	0.88	1 (2%)	45,45,63	1.26	4 (8%)
23	CHL	7	301	6	67,71,74	1.91	18 (26%)	76,110,114	2.89	28 (36%)
23	CHL	8	306	-	51,55,74	2.16	18 (35%)	57,91,114	3.25	26 (45%)
25	8CT	B	848	-	40,41,41	4.67	24 (60%)	50,56,56	2.54	19 (38%)
27	LHG	3	324	-	42,42,48	1.14	6 (14%)	45,47,54	1.05	3 (6%)
24	CLA	0	310	-	51,55,73	1.43	10 (19%)	61,91,113	1.48	6 (9%)
24	CLA	A	837	9	60,64,73	1.33	10 (16%)	72,102,113	1.33	7 (9%)
27	LHG	L	208	-	30,30,48	1.32	6 (20%)	33,36,54	1.14	3 (9%)
24	CLA	1	308	2	59,63,73	1.34	10 (16%)	71,101,113	1.33	6 (8%)
24	CLA	G	101	14	54,58,73	1.41	9 (16%)	65,95,113	1.43	6 (9%)
24	CLA	A	809	9	69,73,73	1.26	10 (14%)	83,113,113	1.31	7 (8%)
24	CLA	L	202	17	67,71,73	1.26	10 (14%)	80,110,113	1.34	7 (8%)
24	CLA	7	303	6	49,53,73	1.49	10 (20%)	59,89,113	1.45	5 (8%)
23	CHL	0	302	1	68,72,74	1.86	19 (27%)	77,111,114	2.91	28 (36%)
25	8CT	O	208	-	40,41,41	4.65	23 (57%)	50,56,56	2.55	17 (34%)
24	CLA	A	801	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	4 (4%)
24	CLA	B	814	10	69,73,73	1.25	10 (14%)	83,113,113	1.31	7 (8%)
24	CLA	1	313	-	50,54,73	1.44	9 (18%)	60,90,113	1.43	6 (10%)
24	CLA	B	826	-	53,56,73	1.45	11 (20%)	61,89,113	2.07	11 (18%)
24	CLA	A	816	9	65,69,73	1.26	10 (15%)	78,108,113	1.37	7 (8%)
24	CLA	B	804	-	69,73,73	1.23	9 (13%)	83,113,113	1.26	6 (7%)
24	CLA	4	312	7	57,61,73	1.36	9 (15%)	68,98,113	1.38	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	6	303	5	56,60,73	1.39	9 (16%)	67,97,113	1.40	7 (10%)
24	CLA	A	832	9	69,73,73	1.23	9 (13%)	83,113,113	1.31	6 (7%)
23	CHL	3	305	-	55,59,74	2.08	18 (32%)	62,96,114	3.22	29 (46%)
30	OIE	3	319	-	42,45,45	1.41	6 (14%)	49,63,63	1.53	10 (20%)
24	CLA	0	319	-	50,54,73	1.44	9 (18%)	60,90,113	1.41	4 (6%)
27	LHG	1	317	24	48,48,48	1.09	5 (10%)	51,54,54	0.97	2 (3%)
24	CLA	3	306	4	51,55,73	1.43	9 (17%)	61,91,113	1.42	6 (9%)
23	CHL	3	301	-	65,69,74	1.91	18 (27%)	74,108,114	2.93	28 (37%)
24	CLA	B	825	-	69,73,73	1.24	10 (14%)	83,113,113	1.33	5 (6%)
27	LHG	7	324	-	38,38,48	1.22	6 (15%)	41,44,54	0.99	2 (4%)
24	CLA	4	314	7	49,53,73	1.46	9 (18%)	59,89,113	1.44	8 (13%)
34	DGD	B	849	-	57,57,67	0.88	2 (3%)	71,71,81	1.17	5 (7%)
24	CLA	4	309	-	64,68,73	1.30	8 (12%)	77,107,113	1.25	8 (10%)
27	LHG	0	317	-	48,48,48	1.09	5 (10%)	51,54,54	0.93	2 (3%)
24	CLA	9	311	8	60,64,73	1.32	9 (15%)	72,102,113	1.35	7 (9%)
23	CHL	8	307	-	55,59,74	2.10	19 (34%)	62,96,114	3.19	28 (45%)
23	CHL	0	305	-	55,59,74	2.14	18 (32%)	62,96,114	3.13	29 (46%)
23	CHL	7	302	6	68,72,74	1.84	18 (26%)	77,111,114	2.92	30 (38%)
24	CLA	4	310	27	64,68,73	1.30	10 (15%)	77,107,113	1.31	6 (7%)
23	CHL	4	308	-	51,55,74	2.17	19 (37%)	57,91,114	3.17	25 (43%)
23	CHL	4	313	7	55,59,74	2.05	18 (32%)	62,96,114	3.22	31 (50%)
25	8CT	A	846	-	40,41,41	4.57	23 (57%)	50,56,56	3.04	20 (40%)
24	CLA	A	802	9	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
23	CHL	2	305	-	52,56,74	2.15	19 (36%)	58,92,114	3.26	26 (44%)
24	CLA	A	810	9	69,73,73	1.23	9 (13%)	83,113,113	1.29	5 (6%)
23	CHL	2	307	-	51,55,74	2.14	19 (37%)	57,91,114	3.19	23 (40%)
24	CLA	1	307	-	49,53,73	1.47	9 (18%)	59,89,113	1.46	6 (10%)
24	CLA	5	313	2	50,54,73	1.46	8 (16%)	60,90,113	1.37	4 (6%)
24	CLA	B	833	10	59,63,73	1.36	10 (16%)	71,101,113	1.38	9 (12%)
23	CHL	9	312	8	51,55,74	2.17	17 (33%)	57,91,114	3.27	28 (49%)
24	CLA	5	310	-	49,53,73	1.48	9 (18%)	59,89,113	1.48	7 (11%)
24	CLA	5	311	2	60,64,73	1.33	10 (16%)	72,102,113	1.36	5 (6%)
24	CLA	G	102	14	49,53,73	1.46	8 (16%)	59,89,113	1.47	4 (6%)
23	CHL	8	303	7	68,72,74	1.85	19 (27%)	77,111,114	2.92	30 (38%)
23	CHL	8	316	-	47,51,74	2.26	18 (38%)	52,86,114	3.30	24 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	SF4	C	102	18	0,12,12	-	-	-		
24	CLA	7	317	6	64,68,73	1.28	9 (14%)	77,107,113	1.34	6 (7%)
25	8CT	8	317	-	40,41,41	4.67	23 (57%)	50,56,56	2.66	19 (38%)
24	CLA	H	205	-	55,59,73	1.40	9 (16%)	66,96,113	1.39	7 (10%)
24	CLA	B	835	-	49,53,73	1.47	10 (20%)	59,89,113	1.48	5 (8%)
29	LMG	O	203	-	31,31,55	0.92	0	39,39,63	1.25	5 (12%)
23	CHL	5	312	2	51,55,74	2.29	18 (35%)	57,91,114	3.20	26 (45%)
23	CHL	8	309	-	51,55,74	2.17	18 (35%)	57,91,114	3.19	24 (42%)
24	CLA	9	304	-	55,59,73	1.40	9 (16%)	66,96,113	1.38	5 (7%)
24	CLA	A	827	9	69,73,73	1.22	9 (13%)	83,113,113	1.30	7 (8%)
27	LHG	A	850	-	41,41,48	1.19	6 (14%)	44,47,54	1.03	3 (6%)
24	CLA	A	848	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	7 (8%)
24	CLA	0	312	1	50,54,73	1.45	9 (18%)	60,90,113	1.38	4 (6%)
24	CLA	2	313	3	49,53,73	1.48	10 (20%)	59,89,113	1.44	5 (8%)
24	CLA	6	304	-	50,54,73	1.46	10 (20%)	60,90,113	1.43	5 (8%)
27	LHG	I	102	-	45,45,48	1.12	5 (11%)	48,51,54	0.97	3 (6%)
27	LHG	6	322	24	36,36,48	1.24	5 (13%)	39,42,54	1.05	2 (5%)
24	CLA	7	310	27	42,45,73	1.54	9 (21%)	50,78,113	1.44	5 (10%)
24	CLA	A	811	9	58,62,73	1.37	10 (17%)	69,99,113	1.34	7 (10%)
24	CLA	A	828	9	69,73,73	1.24	10 (14%)	83,113,113	1.31	6 (7%)
23	CHL	4	305	-	47,51,74	2.14	18 (38%)	52,86,114	3.39	25 (48%)
25	8CT	9	313	-	40,41,41	4.66	23 (57%)	50,56,56	2.71	17 (34%)
27	LHG	9	316	24	45,45,48	1.13	5 (11%)	47,50,54	0.96	2 (4%)
24	CLA	0	311	1	69,73,73	1.24	9 (13%)	83,113,113	1.29	7 (8%)
24	CLA	A	812	9	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)
25	8CT	B	847	-	40,41,41	4.61	23 (57%)	50,56,56	3.09	22 (44%)
23	CHL	1	312	2	66,70,74	1.91	18 (27%)	75,109,114	2.92	27 (36%)
25	8CT	B	846	-	40,41,41	4.76	24 (60%)	50,56,56	3.25	20 (40%)
27	LHG	8	320	24	43,43,48	1.16	5 (11%)	46,49,54	0.92	2 (4%)
23	CHL	6	315	5	47,51,74	2.21	17 (36%)	52,86,114	3.32	23 (44%)
24	CLA	7	314	6	51,55,73	1.44	10 (19%)	61,91,113	1.44	5 (8%)
24	CLA	3	314	4	50,54,73	1.44	10 (20%)	60,90,113	1.43	6 (10%)
23	CHL	6	306	-	55,59,74	2.06	18 (32%)	62,96,114	3.22	28 (45%)
24	CLA	1	309	27	67,71,73	1.26	10 (14%)	80,110,113	1.30	4 (5%)
27	LHG	1	318	-	42,42,48	1.17	6 (14%)	45,48,54	0.97	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LHG	5	316	24	36,36,48	1.24	5 (13%)	39,42,54	1.08	3 (7%)
24	CLA	B	802	10	69,73,73	1.24	10 (14%)	83,113,113	1.29	8 (9%)
26	OUR	6	320	-	49,52,58	0.99	1 (2%)	57,71,77	1.92	18 (31%)
25	8CT	0	314	-	40,41,41	4.66	24 (60%)	50,56,56	2.78	18 (36%)
23	CHL	4	306	-	52,56,74	2.15	19 (36%)	58,92,114	3.24	27 (46%)
24	CLA	3	310	-	66,70,73	1.28	9 (13%)	79,109,113	1.30	6 (7%)
23	CHL	7	313	6	51,55,74	2.19	19 (37%)	57,91,114	3.22	24 (42%)
26	OUR	3	318	-	49,52,58	1.01	1 (2%)	57,71,77	2.10	17 (29%)
24	CLA	B	810	10	66,70,73	1.25	10 (15%)	79,109,113	1.34	7 (8%)
24	CLA	8	311	27	50,54,73	1.44	10 (20%)	60,90,113	1.37	5 (8%)
29	LMG	J	102	-	29,29,55	0.98	1 (3%)	37,37,63	1.27	4 (10%)
23	CHL	6	323	7	65,69,74	1.95	19 (29%)	74,108,114	2.99	29 (39%)
25	8CT	M	102	-	40,41,41	4.62	23 (57%)	50,56,56	2.83	18 (36%)
25	8CT	K	105	-	40,41,41	4.61	23 (57%)	50,56,56	3.28	24 (48%)
26	OUR	5	314	-	49,52,58	0.95	1 (2%)	57,71,77	1.74	12 (21%)
23	CHL	6	307	-	55,59,74	2.06	18 (32%)	62,96,114	3.24	31 (50%)
25	8CT	3	323	-	40,41,41	4.62	24 (60%)	50,56,56	3.57	23 (46%)
24	CLA	9	310	8	56,60,73	1.39	10 (17%)	67,97,113	1.38	7 (10%)
24	CLA	A	806	9	57,61,73	1.36	10 (17%)	66,97,113	1.44	10 (15%)
24	CLA	A	839	9	69,73,73	1.24	10 (14%)	83,113,113	1.35	8 (9%)
24	CLA	A	819	9	59,63,73	1.33	10 (16%)	71,101,113	1.38	6 (8%)
24	CLA	9	307	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	6 (7%)
24	CLA	A	814	9	69,73,73	1.24	9 (13%)	83,113,113	1.35	8 (9%)
24	CLA	A	829	9	69,73,73	1.25	11 (15%)	83,113,113	1.44	8 (9%)
27	LHG	B	851	24	22,22,48	1.30	2 (9%)	25,28,54	1.07	1 (4%)
24	CLA	L	201	9	62,66,73	1.30	10 (16%)	74,104,113	1.39	7 (9%)
24	CLA	0	309	-	45,49,73	1.50	9 (20%)	54,84,113	1.50	7 (12%)
24	CLA	O	205	21	40,46,73	1.60	9 (22%)	48,80,113	1.51	7 (14%)
24	CLA	A	831	9	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
24	CLA	J	103	16	46,50,73	1.49	10 (21%)	55,85,113	1.46	5 (9%)
25	8CT	A	849	-	40,41,41	4.63	23 (57%)	50,56,56	2.90	20 (40%)
24	CLA	L	203	-	50,54,73	1.45	10 (20%)	60,90,113	1.40	5 (8%)
26	OUR	9	315	-	50,53,58	0.98	1 (2%)	58,72,77	1.69	16 (27%)
24	CLA	9	302	-	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
24	CLA	3	312	4	59,63,73	1.34	10 (16%)	71,101,113	1.35	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	0	313	1	49,53,73	1.49	9 (18%)	59,89,113	1.48	5 (8%)
27	LHG	B	852	-	37,37,48	1.24	6 (16%)	40,43,54	1.15	4 (10%)
25	8CT	J	101	-	40,41,41	4.61	23 (57%)	50,56,56	2.81	17 (34%)
29	LMG	2	318	-	36,36,55	0.89	1 (2%)	44,44,63	1.24	5 (11%)
24	CLA	2	309	27	64,68,73	1.29	10 (15%)	77,107,113	1.30	6 (7%)
32	CL0	A	852	9	69,73,73	1.32	8 (11%)	83,113,113	1.39	11 (13%)
26	0UR	8	318	-	49,52,58	0.96	1 (2%)	57,71,77	1.74	17 (29%)
24	CLA	L	206	-	51,55,73	1.45	9 (17%)	61,91,113	1.39	6 (9%)
24	CLA	1	311	2	69,73,73	1.24	10 (14%)	83,113,113	1.33	8 (9%)
24	CLA	5	309	27	49,53,73	1.47	9 (18%)	59,89,113	1.43	4 (6%)
24	CLA	B	838	10	51,55,73	1.40	10 (19%)	61,91,113	1.42	6 (9%)
24	CLA	B	830	10	60,64,73	1.37	10 (16%)	72,102,113	1.48	10 (13%)
24	CLA	B	829	-	69,73,73	1.25	10 (14%)	83,113,113	1.23	5 (6%)
24	CLA	7	311	6	56,60,73	1.38	10 (17%)	67,97,113	1.39	5 (7%)
23	CHL	8	314	7	60,64,74	1.98	18 (30%)	68,102,114	3.07	31 (45%)
24	CLA	A	838	9	69,73,73	1.23	10 (14%)	83,113,113	1.33	7 (8%)
23	CHL	3	307	-	70,74,74	1.78	18 (25%)	80,114,114	2.85	31 (38%)
26	0UR	4	317	-	49,52,58	0.98	1 (2%)	57,71,77	2.10	19 (33%)
24	CLA	7	312	6	59,63,73	1.35	9 (15%)	71,101,113	1.35	6 (8%)
25	8CT	B	844	-	40,41,41	4.72	25 (62%)	50,56,56	2.70	19 (38%)
24	CLA	4	304	-	64,68,73	1.28	9 (14%)	77,107,113	1.29	5 (6%)
29	LMG	J	105	-	46,46,55	0.87	2 (4%)	54,54,63	1.35	8 (14%)
24	CLA	7	309	-	63,67,73	1.29	10 (15%)	75,105,113	1.35	7 (9%)
24	CLA	K	101	-	64,68,73	1.30	9 (14%)	77,107,113	1.31	7 (9%)
23	CHL	6	301	5	65,69,74	1.92	18 (27%)	74,108,114	2.91	30 (40%)
24	CLA	3	309	4	69,73,73	1.24	10 (14%)	83,113,113	1.31	8 (9%)
24	CLA	A	813	9	61,65,73	1.31	9 (14%)	73,103,113	1.35	5 (6%)
27	LHG	7	322	24	29,29,48	1.35	5 (17%)	32,35,54	1.10	2 (6%)
28	SQD	0	318	-	36,36,54	1.21	5 (13%)	44,44,65	1.48	6 (13%)
24	CLA	B	813	10	59,63,73	1.35	10 (16%)	71,101,113	1.35	7 (9%)
24	CLA	B	820	-	60,64,73	1.33	9 (15%)	72,102,113	1.38	7 (9%)
24	CLA	3	311	4	50,54,73	1.45	10 (20%)	60,90,113	1.49	6 (10%)
24	CLA	7	308	-	69,73,73	1.24	10 (14%)	83,113,113	1.27	6 (7%)
23	CHL	9	305	-	55,59,74	2.07	19 (34%)	62,96,114	3.20	28 (45%)
26	0UR	9	314	-	50,53,58	0.95	1 (2%)	58,72,77	1.69	16 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CHL	4	315	2	58,62,74	2.02	19 (32%)	65,99,114	3.12	30 (46%)
24	CLA	B	837	-	69,73,73	1.24	9 (13%)	83,113,113	1.33	8 (9%)
24	CLA	O	206	-	41,46,73	1.67	9 (21%)	52,81,113	1.59	8 (15%)
23	CHL	9	301	8	51,55,74	2.14	19 (37%)	57,91,114	3.24	26 (45%)
25	8CT	O	202	-	40,41,41	4.58	23 (57%)	50,56,56	2.69	22 (44%)
24	CLA	O	204	-	45,49,73	1.51	9 (20%)	54,84,113	1.54	6 (11%)
24	CLA	K	104	19	54,58,73	1.40	9 (16%)	65,95,113	1.41	7 (10%)
25	8CT	F	304	-	40,41,41	4.63	23 (57%)	50,56,56	2.71	19 (38%)
24	CLA	B	836	10	64,68,73	1.29	10 (15%)	77,107,113	1.35	10 (12%)
24	CLA	9	303	8	52,56,73	1.42	9 (17%)	62,92,113	1.44	6 (9%)
24	CLA	K	103	19	50,54,73	1.45	10 (20%)	60,90,113	1.45	5 (8%)
24	CLA	A	820	-	69,73,73	1.24	10 (14%)	83,113,113	1.29	7 (8%)
24	CLA	A	826	9	69,73,73	1.25	10 (14%)	83,113,113	1.34	9 (10%)
25	8CT	B	845	-	40,41,41	4.62	23 (57%)	50,56,56	3.23	22 (44%)
27	LHG	A	843	24	26,26,48	1.27	4 (15%)	29,32,54	1.22	2 (6%)
25	8CT	L	205	-	40,41,41	4.65	23 (57%)	50,56,56	2.78	19 (38%)
24	CLA	6	311	5	52,56,73	1.44	10 (19%)	62,92,113	1.39	6 (9%)
26	OUR	1	316	-	50,53,58	0.99	2 (4%)	58,72,77	1.90	15 (25%)
24	CLA	3	308	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
23	CHL	4	307	-	55,59,74	2.06	18 (32%)	62,96,114	3.22	30 (48%)
24	CLA	B	827	-	69,73,73	1.25	9 (13%)	83,113,113	1.35	7 (8%)
24	CLA	3	313	4	49,53,73	1.48	9 (18%)	59,89,113	1.46	6 (10%)
24	CLA	B	805	10	69,73,73	1.23	10 (14%)	83,113,113	1.27	7 (8%)
25	8CT	4	316	-	40,41,41	4.64	24 (60%)	50,56,56	3.01	20 (40%)
23	CHL	6	313	5	56,60,74	2.06	17 (30%)	63,97,114	3.22	30 (47%)
24	CLA	6	318	-	55,59,73	1.39	9 (16%)	66,96,113	1.33	5 (7%)
24	CLA	5	308	-	64,68,73	1.30	9 (14%)	77,107,113	1.31	9 (11%)
23	CHL	5	306	-	51,55,74	2.23	18 (35%)	57,91,114	3.21	26 (45%)
25	8CT	A	847	-	40,41,41	4.55	23 (57%)	50,56,56	3.10	21 (42%)
24	CLA	0	308	-	64,68,73	1.29	9 (14%)	77,107,113	1.34	7 (9%)
24	CLA	B	801	10	62,66,73	1.29	9 (14%)	74,104,113	1.39	7 (9%)
24	CLA	8	310	-	64,68,73	1.29	10 (15%)	77,107,113	1.33	8 (10%)
24	CLA	K	102	19	57,61,73	1.35	9 (15%)	68,98,113	1.41	7 (10%)
24	CLA	A	807	9	69,73,73	1.22	9 (13%)	83,113,113	1.31	6 (7%)
24	CLA	B	823	-	56,60,73	1.38	10 (17%)	67,97,113	3.52	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	B	828	-	64,68,73	1.28	10 (15%)	77,107,113	1.29	6 (7%)
24	CLA	B	811	10	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)
24	CLA	B	821	10	54,58,73	1.38	7 (12%)	65,95,113	1.47	7 (10%)
23	CHL	0	306	-	52,56,74	2.19	19 (36%)	58,92,114	3.28	25 (43%)
26	OUR	6	321	-	50,53,58	1.00	2 (4%)	58,72,77	1.81	15 (25%)
24	CLA	B	818	10	63,67,73	1.30	10 (15%)	75,105,113	1.38	6 (8%)
24	CLA	A	830	9	54,58,73	1.39	10 (18%)	65,95,113	1.46	7 (10%)
24	CLA	F	303	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
24	CLA	B	841	27	69,73,73	1.25	9 (13%)	83,113,113	1.33	7 (8%)
25	8CT	B	850	-	40,41,41	4.61	23 (57%)	50,56,56	2.48	14 (28%)
24	CLA	6	316	5	69,73,73	1.24	10 (14%)	83,113,113	1.34	9 (10%)
23	CHL	1	306	-	70,74,74	1.87	19 (27%)	80,114,114	2.84	28 (35%)
23	CHL	2	306	-	55,59,74	2.02	18 (32%)	62,96,114	3.24	31 (50%)
25	8CT	A	845	-	40,41,41	4.59	23 (57%)	50,56,56	2.97	18 (36%)
24	CLA	5	307	-	50,54,73	1.46	8 (16%)	60,90,113	1.38	4 (6%)
24	CLA	A	821	-	53,57,73	1.40	10 (18%)	62,93,113	1.41	6 (9%)
23	CHL	8	308	-	55,59,74	2.06	18 (32%)	62,96,114	3.17	28 (45%)
24	CLA	H	201	17	50,54,73	1.44	9 (18%)	60,90,113	1.45	5 (8%)
24	CLA	8	312	7	50,54,73	1.46	10 (20%)	60,90,113	1.41	5 (8%)
25	8CT	2	314	-	40,41,41	4.66	24 (60%)	50,56,56	3.05	20 (40%)
31	PQN	A	841	-	34,34,34	1.50	2 (5%)	42,45,45	1.26	5 (11%)
30	OIE	7	321	-	42,45,45	1.41	6 (14%)	49,63,63	1.53	10 (20%)
24	CLA	1	310	2	56,60,73	1.38	10 (17%)	67,97,113	1.41	5 (7%)
24	CLA	O	209	-	55,59,73	1.40	9 (16%)	66,96,113	1.34	6 (9%)
25	8CT	3	317	-	40,41,41	4.65	23 (57%)	50,56,56	2.55	16 (32%)
24	CLA	B	812	10	56,60,73	1.37	9 (16%)	67,97,113	1.43	7 (10%)
23	CHL	7	307	-	55,59,74	2.09	19 (34%)	62,96,114	3.14	26 (41%)
29	LMG	3	321	-	36,36,55	0.87	0	44,44,63	1.26	4 (9%)
24	CLA	H	204	-	51,55,73	1.43	10 (19%)	61,91,113	1.45	5 (8%)
25	8CT	A	844	-	40,41,41	4.62	23 (57%)	50,56,56	2.80	20 (40%)
24	CLA	A	823	9	59,63,73	1.34	10 (16%)	71,101,113	1.34	7 (9%)
24	CLA	5	302	2	63,67,73	1.31	9 (14%)	75,105,113	1.38	6 (8%)
23	CHL	0	301	1	56,60,74	2.05	19 (33%)	63,97,114	3.17	28 (44%)
26	OUR	2	316	-	48,51,58	0.98	1 (2%)	56,70,77	1.95	14 (25%)
24	CLA	A	835	-	55,59,73	1.38	9 (16%)	66,96,113	1.43	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	8CT	I	101	-	40,41,41	4.58	23 (57%)	50,56,56	2.77	15 (30%)
24	CLA	O	201	27	56,60,73	1.37	10 (17%)	67,97,113	1.42	8 (11%)
24	CLA	6	317	-	50,54,73	1.45	9 (18%)	60,90,113	1.42	6 (10%)
24	CLA	1	303	-	56,60,73	1.38	9 (16%)	67,97,113	1.35	7 (10%)
24	CLA	B	815	10	59,63,73	1.33	9 (15%)	71,101,113	1.38	9 (12%)
27	LHG	2	317	24	31,31,48	1.32	5 (16%)	34,37,54	1.12	3 (8%)
24	CLA	H	202	10	59,63,73	1.34	9 (15%)	71,101,113	1.37	6 (8%)
24	CLA	B	839	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	7 (8%)
26	OUR	0	315	-	50,53,58	0.94	1 (2%)	58,72,77	1.67	12 (20%)
24	CLA	A	815	-	49,53,73	1.49	10 (20%)	59,89,113	1.48	5 (8%)
27	LHG	3	320	-	35,35,48	1.27	6 (17%)	38,41,54	1.12	2 (5%)
27	LHG	7	323	-	37,37,48	1.18	6 (16%)	40,43,54	1.04	2 (5%)
24	CLA	A	803	9	59,63,73	1.31	10 (16%)	71,101,113	1.40	7 (9%)
25	8CT	F	301	-	40,41,41	4.63	23 (57%)	50,56,56	2.57	19 (38%)
23	CHL	6	302	5	68,72,74	1.84	18 (26%)	77,111,114	2.93	30 (38%)
29	LMG	M	101	-	42,42,55	0.80	0	50,50,63	1.30	6 (12%)
25	8CT	L	207	-	40,41,41	4.66	23 (57%)	50,56,56	2.54	18 (36%)
24	CLA	B	817	10	64,68,73	1.26	10 (15%)	77,107,113	1.46	9 (11%)
24	CLA	B	822	10	64,68,73	1.30	9 (14%)	77,107,113	1.35	6 (7%)
24	CLA	A	825	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	9 (10%)
24	CLA	H	203	22	51,55,73	1.43	10 (19%)	61,91,113	1.40	5 (8%)
24	CLA	B	832	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	8 (9%)
23	CHL	5	305	-	52,56,74	2.28	19 (36%)	58,92,114	3.12	25 (43%)
25	8CT	6	319	-	40,41,41	4.66	24 (60%)	50,56,56	3.43	21 (42%)
25	8CT	3	316	-	40,41,41	4.64	23 (57%)	50,56,56	3.05	16 (32%)
24	CLA	0	307	-	64,68,73	1.30	9 (14%)	77,107,113	1.30	7 (9%)
29	LMG	A	851	-	36,36,55	0.91	0	44,44,63	1.30	5 (11%)
25	8CT	B	843	-	40,41,41	4.75	24 (60%)	50,56,56	2.76	18 (36%)
26	OUR	1	315	-	50,53,58	0.96	1 (2%)	58,72,77	1.71	16 (27%)
24	CLA	B	840	10	69,73,73	1.25	8 (11%)	83,113,113	1.32	6 (7%)
24	CLA	B	831	10	54,58,73	1.39	10 (18%)	65,95,113	1.42	6 (9%)
24	CLA	2	311	3	64,68,73	1.27	9 (14%)	77,107,113	1.36	7 (9%)
24	CLA	5	303	-	56,60,73	1.38	8 (14%)	67,97,113	1.36	4 (5%)
24	CLA	6	314	-	49,53,73	1.45	9 (18%)	59,89,113	1.47	5 (8%)
24	CLA	A	805	-	69,73,73	1.25	10 (14%)	83,113,113	1.32	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	840	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
24	CLA	B	809	10	69,73,73	1.25	10 (14%)	83,113,113	1.30	8 (9%)
26	OUR	O	207	-	50,53,58	0.99	1 (2%)	58,72,77	1.92	16 (27%)
24	CLA	3	303	-	59,63,73	1.33	10 (16%)	71,101,113	1.37	7 (9%)
24	CLA	6	309	5	62,66,73	1.31	10 (16%)	74,104,113	1.34	9 (12%)
24	CLA	B	816	10	64,68,73	1.28	10 (15%)	77,107,113	1.37	8 (10%)
24	CLA	2	310	3	52,56,73	1.41	9 (17%)	62,92,113	1.47	6 (9%)
23	CHL	8	301	2	56,60,74	2.15	19 (33%)	63,97,114	3.08	29 (46%)
24	CLA	F	302	13	51,55,73	1.44	10 (19%)	61,91,113	1.41	4 (6%)
25	8CT	1	314	-	40,41,41	4.69	24 (60%)	50,56,56	2.73	20 (40%)
23	CHL	2	312	3	55,59,74	2.07	18 (32%)	62,96,114	3.22	28 (45%)
23	CHL	7	306	-	65,69,74	1.95	19 (29%)	73,107,114	2.91	30 (41%)
24	CLA	B	808	10	69,73,73	1.23	10 (14%)	83,113,113	1.35	8 (9%)
27	LHG	3	322	-	35,35,48	1.26	6 (17%)	38,41,54	1.05	2 (5%)
25	8CT	7	318	-	40,41,41	4.58	23 (57%)	50,56,56	2.60	17 (34%)
24	CLA	9	309	27	45,49,73	1.51	10 (22%)	54,84,113	1.48	6 (11%)
24	CLA	A	818	9	69,73,73	1.24	10 (14%)	83,113,113	1.33	11 (13%)
24	CLA	6	312	5	60,64,73	1.32	10 (16%)	72,102,113	1.35	7 (9%)
23	CHL	1	301	-	68,72,74	1.85	18 (26%)	77,111,114	2.92	30 (38%)
23	CHL	3	302	4	66,70,74	1.89	19 (28%)	75,109,114	2.95	30 (40%)
23	CHL	2	304	-	47,51,74	2.13	18 (38%)	52,86,114	3.48	26 (50%)
26	OUR	7	320	-	49,52,58	0.99	1 (2%)	57,71,77	2.07	16 (28%)
31	PQN	B	842	-	34,34,34	1.54	2 (5%)	42,45,45	1.10	2 (4%)
24	CLA	2	308	3	64,68,73	1.29	10 (15%)	77,107,113	1.32	10 (12%)
24	CLA	2	303	-	64,68,73	1.29	9 (14%)	77,107,113	1.31	6 (7%)
27	LHG	A	842	-	48,48,48	1.07	5 (10%)	51,54,54	0.99	3 (5%)
24	CLA	B	806	-	69,73,73	1.24	11 (15%)	83,113,113	1.36	8 (9%)
26	OUR	4	318	-	48,51,58	0.97	1 (2%)	56,70,77	1.68	14 (25%)
23	CHL	1	304	-	55,59,74	2.07	19 (34%)	62,96,114	3.24	30 (48%)
24	CLA	A	804	9	69,73,73	1.27	10 (14%)	83,113,113	1.31	7 (8%)
23	CHL	4	301	7	65,69,74	1.91	18 (27%)	74,108,114	2.93	31 (41%)
24	CLA	A	808	9	69,73,73	1.22	10 (14%)	83,113,113	1.34	9 (10%)
24	CLA	1	302	2	60,64,73	1.34	10 (16%)	72,102,113	1.41	6 (8%)
24	CLA	8	315	-	49,53,73	1.47	9 (18%)	59,89,113	1.45	6 (10%)
23	CHL	6	308	5	64,68,74	1.95	18 (28%)	72,106,114	2.90	28 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	853	-	69,73,73	1.23	9 (13%)	83,113,113	1.37	8 (9%)
24	CLA	7	315	6	52,56,73	1.40	10 (19%)	62,92,113	1.43	6 (9%)
33	SF4	C	101	-	0,12,12	-	-	-	-	-
24	CLA	8	313	7	60,64,73	1.34	10 (16%)	72,102,113	1.35	6 (8%)
26	OUR	8	319	-	50,53,58	0.96	1 (2%)	58,72,77	1.87	15 (25%)
27	LHG	2	319	24	31,31,48	1.31	5 (16%)	34,37,54	1.15	3 (8%)
24	CLA	0	304	-	56,60,73	1.39	10 (17%)	67,97,113	1.39	7 (10%)
25	8CT	L	204	-	40,41,41	4.62	23 (57%)	50,56,56	2.96	19 (38%)
24	CLA	4	311	-	52,56,73	1.42	10 (19%)	62,92,113	1.43	5 (8%)
23	CHL	5	301	2	68,72,74	1.84	18 (26%)	77,111,114	2.91	31 (40%)
26	OUR	2	315	-	49,52,58	1.00	1 (2%)	57,71,77	2.13	17 (29%)
26	OUR	0	316	-	50,53,58	0.97	1 (2%)	58,72,77	1.89	16 (27%)
24	CLA	9	308	-	64,68,73	1.29	9 (14%)	77,107,113	1.34	9 (11%)
26	OUR	5	315	-	50,53,58	0.96	1 (2%)	58,72,77	2.05	15 (25%)
24	CLA	G	103	14	50,54,73	1.45	9 (18%)	60,90,113	1.41	6 (10%)
24	CLA	8	305	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	6 (7%)
27	LHG	8	302	-	30,30,48	1.33	6 (20%)	33,36,54	1.11	3 (9%)
24	CLA	A	833	9	50,54,73	1.42	9 (18%)	60,90,113	1.45	5 (8%)
24	CLA	B	819	10	64,68,73	1.28	8 (12%)	77,107,113	1.34	10 (12%)
24	CLA	B	807	10	49,53,73	1.46	10 (20%)	59,89,113	1.53	9 (15%)
24	CLA	7	304	-	59,63,73	1.35	9 (15%)	71,101,113	1.38	7 (9%)
23	CHL	9	306	-	52,56,74	2.15	18 (34%)	58,92,114	3.24	25 (43%)
24	CLA	A	834	9	61,65,73	1.32	9 (14%)	73,103,113	1.39	7 (9%)
24	CLA	8	304	7	50,54,73	1.46	10 (20%)	60,90,113	1.40	5 (8%)
24	CLA	A	836	9	65,69,73	1.28	10 (15%)	78,108,113	1.37	7 (8%)
25	8CT	7	319	-	40,41,41	4.59	23 (57%)	50,56,56	2.69	19 (38%)
23	CHL	4	302	7	57,61,74	2.02	18 (31%)	64,98,114	3.20	33 (51%)
24	CLA	B	834	10	65,69,73	1.29	10 (15%)	78,108,113	1.29	6 (7%)
23	CHL	2	301	3	68,72,74	1.84	18 (26%)	77,111,114	2.94	33 (42%)
23	CHL	6	305	-	47,51,74	2.15	18 (38%)	52,86,114	3.39	25 (48%)
24	CLA	7	316	-	49,53,73	1.48	8 (16%)	59,89,113	1.49	5 (8%)
24	CLA	4	303	7	49,53,73	1.47	10 (20%)	59,89,113	1.45	5 (8%)
29	LMG	O	210	-	39,39,55	0.81	1 (2%)	47,47,63	1.26	4 (8%)
33	SF4	B	803	-	0,12,12	-	-	-	-	-
24	CLA	3	304	-	69,73,73	1.24	9 (13%)	83,113,113	1.36	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CLA	A	817	9	69,73,73	1.23	9 (13%)	83,113,113	1.34	9 (10%)
23	CHL	1	305	-	52,56,74	2.18	18 (34%)	58,92,114	3.21	25 (43%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	A	822	9	-	4/23/99/115	-
24	CLA	0	303	1	-	11/36/112/115	-
23	CHL	5	304	-	-	7/17/93/117	-
24	CLA	A	824	-	-	8/39/115/115	-
24	CLA	2	302	3	-	10/29/105/115	-
29	LMG	9	317	-	-	31/50/70/70	0/1/1/1
23	CHL	7	305	-	-	9/20/96/117	-
25	8CT	J	104	-	-	9/29/63/63	0/2/2/2
24	CLA	3	315	-	-	7/24/100/115	-
24	CLA	B	824	10	-	10/33/109/115	-
25	8CT	6	324	-	-	12/29/63/63	0/2/2/2
25	8CT	G	104	-	-	13/29/63/63	0/2/2/2
24	CLA	6	310	27	-	11/33/109/115	-
29	LMG	A	854	-	-	15/32/52/70	0/1/1/1
23	CHL	7	301	6	-	14/38/114/117	-
23	CHL	8	306	-	-	8/19/95/117	-
25	8CT	B	848	-	-	9/29/63/63	0/2/2/2
27	LHG	3	324	-	-	23/46/46/53	-
24	CLA	0	310	-	-	10/18/94/115	-
24	CLA	A	837	9	-	5/29/105/115	-
27	LHG	L	208	-	-	13/35/35/53	-
24	CLA	1	308	2	-	6/27/103/115	-
24	CLA	G	101	14	-	7/21/97/115	-
24	CLA	A	809	9	-	3/39/115/115	-
24	CLA	L	202	17	-	21/37/113/115	-
24	CLA	7	303	6	-	7/15/91/115	-
23	CHL	0	302	1	-	14/39/115/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	O	208	-	-	6/29/63/63	0/2/2/2
24	CLA	A	801	-	-	5/39/115/115	-
24	CLA	B	814	10	-	16/39/115/115	-
24	CLA	1	313	-	-	5/17/93/115	-
24	CLA	B	826	-	-	2/23/87/115	-
24	CLA	A	816	9	-	16/35/111/115	-
24	CLA	B	804	-	-	15/39/115/115	-
24	CLA	4	312	7	-	9/25/101/115	-
24	CLA	6	303	5	-	7/24/100/115	-
24	CLA	A	832	9	-	12/39/115/115	-
23	CHL	3	305	-	-	8/23/99/117	-
30	0IE	3	319	-	-	2/33/72/72	0/2/2/2
24	CLA	0	319	-	-	3/17/93/115	-
27	LHG	1	317	24	-	21/53/53/53	-
24	CLA	3	306	4	-	5/18/94/115	-
23	CHL	3	301	-	-	10/35/111/117	-
24	CLA	B	825	-	-	5/39/115/115	-
27	LHG	7	324	-	-	21/43/43/53	-
24	CLA	4	314	7	-	5/15/91/115	-
34	DGD	B	849	-	-	28/45/85/95	0/2/2/2
24	CLA	4	309	-	-	6/33/109/115	-
27	LHG	0	317	-	-	33/53/53/53	-
24	CLA	9	311	8	-	6/29/105/115	-
23	CHL	8	307	-	-	16/23/99/117	-
23	CHL	0	305	-	-	7/23/99/117	-
23	CHL	7	302	6	-	18/39/115/117	-
24	CLA	4	310	27	-	13/33/109/115	-
23	CHL	4	308	-	-	5/19/95/117	-
23	CHL	4	313	7	-	5/23/99/117	-
25	8CT	A	846	-	-	8/29/63/63	0/2/2/2
24	CLA	A	802	9	-	10/39/115/115	-
23	CHL	2	305	-	-	5/20/96/117	-
24	CLA	A	810	9	-	13/39/115/115	-
23	CHL	2	307	-	-	4/19/95/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	1	307	-	-	7/15/91/115	-
24	CLA	5	313	2	-	11/17/93/115	-
24	CLA	B	833	10	-	9/27/103/115	-
23	CHL	9	312	8	-	9/19/95/117	-
24	CLA	5	310	-	-	9/15/91/115	-
24	CLA	5	311	2	-	11/29/105/115	-
24	CLA	G	102	14	-	4/15/91/115	-
23	CHL	8	303	7	-	19/39/115/117	-
23	CHL	8	316	-	-	4/14/90/117	-
33	SF4	C	102	18	-	-	0/6/5/5
24	CLA	7	317	6	-	9/33/109/115	-
25	8CT	8	317	-	-	10/29/63/63	0/2/2/2
24	CLA	H	205	-	-	9/23/99/115	-
24	CLA	B	835	-	-	0/15/91/115	-
29	LMG	O	203	-	-	12/26/46/70	0/1/1/1
23	CHL	5	312	2	-	8/19/95/117	-
23	CHL	8	309	-	-	2/19/95/117	-
24	CLA	9	304	-	-	0/23/99/115	-
24	CLA	A	827	9	-	19/39/115/115	-
27	LHG	A	850	-	-	27/46/46/53	-
24	CLA	A	848	-	-	15/39/115/115	-
24	CLA	0	312	1	-	11/17/93/115	-
24	CLA	2	313	3	-	5/15/91/115	-
24	CLA	6	304	-	-	5/17/93/115	-
27	LHG	I	102	-	-	19/50/50/53	-
27	LHG	6	322	24	-	17/41/41/53	-
24	CLA	7	310	27	-	2/4/76/115	-
24	CLA	A	811	9	-	3/26/102/115	-
24	CLA	A	828	9	-	13/39/115/115	-
23	CHL	4	305	-	-	0/14/90/117	-
25	8CT	9	313	-	-	11/29/63/63	0/2/2/2
27	LHG	9	316	24	-	19/48/48/53	-
24	CLA	0	311	1	-	14/39/115/115	-
24	CLA	A	812	9	-	8/39/115/115	-
25	8CT	B	847	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	1	312	2	-	19/37/113/117	-
25	8CT	B	846	-	-	12/29/63/63	0/2/2/2
27	LHG	8	320	24	-	30/48/48/53	-
23	CHL	6	315	5	-	5/14/90/117	-
24	CLA	7	314	6	-	9/18/94/115	-
24	CLA	3	314	4	-	0/17/93/115	-
23	CHL	6	306	-	-	6/23/99/117	-
24	CLA	1	309	27	-	12/37/113/115	-
27	LHG	1	318	-	-	17/47/47/53	-
27	LHG	5	316	24	-	13/41/41/53	-
24	CLA	B	802	10	-	13/39/115/115	-
26	0UR	6	320	-	-	11/41/80/86	0/2/2/2
25	8CT	0	314	-	-	5/29/63/63	0/2/2/2
23	CHL	4	306	-	-	6/20/96/117	-
24	CLA	3	310	-	-	15/36/112/115	-
23	CHL	7	313	6	-	7/19/95/117	-
26	0UR	3	318	-	-	9/41/80/86	0/2/2/2
24	CLA	B	810	10	-	8/36/112/115	-
24	CLA	8	311	27	-	4/17/93/115	-
29	LMG	J	102	-	-	12/24/44/70	0/1/1/1
23	CHL	6	323	7	-	6/35/111/117	-
25	8CT	M	102	-	-	7/29/63/63	0/2/2/2
25	8CT	K	105	-	-	12/29/63/63	0/2/2/2
26	0UR	5	314	-	-	11/41/80/86	0/2/2/2
23	CHL	6	307	-	-	12/23/99/117	-
25	8CT	3	323	-	-	7/29/63/63	0/2/2/2
24	CLA	9	310	8	-	6/24/100/115	-
24	CLA	A	806	9	-	5/23/99/115	-
24	CLA	A	839	9	-	17/39/115/115	-
24	CLA	A	819	9	-	9/27/103/115	-
24	CLA	9	307	-	-	13/39/115/115	-
24	CLA	A	814	9	-	11/39/115/115	-
24	CLA	A	829	9	-	14/39/115/115	-
27	LHG	B	851	24	-	17/26/26/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	L	201	9	-	8/31/107/115	-
24	CLA	O	309	-	-	3/10/86/115	-
24	CLA	O	205	21	-	1/6/78/115	-
24	CLA	A	831	9	-	14/39/115/115	-
24	CLA	J	103	16	-	2/12/88/115	-
25	8CT	A	849	-	-	10/29/63/63	0/2/2/2
24	CLA	L	203	-	-	7/17/93/115	-
26	0UR	9	315	-	-	8/42/81/86	0/2/2/2
24	CLA	9	302	-	-	15/39/115/115	-
24	CLA	3	312	4	-	8/27/103/115	-
24	CLA	O	313	1	-	11/15/91/115	-
27	LHG	B	852	-	-	27/42/42/53	-
25	8CT	J	101	-	-	11/29/63/63	0/2/2/2
29	LMG	2	318	-	-	13/31/51/70	0/1/1/1
24	CLA	2	309	27	-	12/33/109/115	-
32	CL0	A	852	9	-	10/39/115/115	-
26	0UR	8	318	-	-	7/41/80/86	0/2/2/2
24	CLA	L	206	-	-	7/18/94/115	-
24	CLA	1	311	2	-	14/39/115/115	-
24	CLA	5	309	27	-	6/15/91/115	-
24	CLA	B	838	10	-	3/18/94/115	-
24	CLA	B	830	10	-	8/29/105/115	-
24	CLA	B	829	-	-	9/39/115/115	-
24	CLA	7	311	6	-	8/24/100/115	-
23	CHL	8	314	7	-	9/29/105/117	-
24	CLA	A	838	9	-	13/39/115/115	-
23	CHL	3	307	-	-	27/41/117/117	-
26	0UR	4	317	-	-	9/41/80/86	0/2/2/2
24	CLA	7	312	6	-	13/27/103/115	-
25	8CT	B	844	-	-	11/29/63/63	0/2/2/2
24	CLA	4	304	-	-	8/33/109/115	-
29	LMG	J	105	-	-	15/41/61/70	0/1/1/1
24	CLA	7	309	-	-	11/32/108/115	-
24	CLA	K	101	-	-	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	6	301	5	-	15/35/111/117	-
24	CLA	3	309	4	-	12/39/115/115	-
24	CLA	A	813	9	-	10/30/106/115	-
27	LHG	7	322	24	-	10/34/34/53	-
28	SQD	0	318	-	-	17/31/51/69	0/1/1/1
24	CLA	B	813	10	-	9/27/103/115	-
24	CLA	B	820	-	-	10/29/105/115	-
24	CLA	3	311	4	-	3/17/93/115	-
24	CLA	7	308	-	-	16/39/115/115	-
23	CHL	9	305	-	-	8/23/99/117	-
26	OUR	9	314	-	-	3/42/81/86	0/2/2/2
23	CHL	4	315	2	-	9/27/103/117	-
24	CLA	B	837	-	-	4/39/115/115	-
24	CLA	O	206	-	-	0/4/80/115	-
23	CHL	9	301	8	-	6/19/95/117	-
25	8CT	O	202	-	-	7/29/63/63	0/2/2/2
24	CLA	O	204	-	-	7/10/86/115	-
24	CLA	K	104	19	-	12/21/97/115	-
25	8CT	F	304	-	-	9/29/63/63	0/2/2/2
24	CLA	B	836	10	-	11/33/109/115	-
24	CLA	9	303	8	-	4/19/95/115	-
24	CLA	K	103	19	-	6/17/93/115	-
24	CLA	A	820	-	-	10/39/115/115	-
24	CLA	A	826	9	-	4/39/115/115	-
25	8CT	B	845	-	-	10/29/63/63	0/2/2/2
27	LHG	A	843	24	-	17/31/31/53	-
25	8CT	L	205	-	-	8/29/63/63	0/2/2/2
24	CLA	6	311	5	-	4/19/95/115	-
26	OUR	1	316	-	-	10/42/81/86	0/2/2/2
24	CLA	3	308	-	-	19/39/115/115	-
23	CHL	4	307	-	-	8/23/99/117	-
24	CLA	B	827	-	-	12/39/115/115	-
24	CLA	3	313	4	-	7/15/91/115	-
24	CLA	B	805	10	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	8CT	4	316	-	-	8/29/63/63	0/2/2/2
23	CHL	6	313	5	-	7/25/101/117	-
24	CLA	6	318	-	-	11/23/99/115	-
24	CLA	5	308	-	-	9/33/109/115	-
23	CHL	5	306	-	-	8/19/95/117	-
25	8CT	A	847	-	-	10/29/63/63	0/2/2/2
24	CLA	0	308	-	-	11/33/109/115	-
24	CLA	B	801	10	-	13/31/107/115	-
24	CLA	8	310	-	-	7/33/109/115	-
24	CLA	K	102	19	-	13/25/101/115	-
24	CLA	A	807	9	-	20/39/115/115	-
24	CLA	B	823	-	-	10/24/100/115	-
24	CLA	B	828	-	-	8/33/109/115	-
24	CLA	B	811	10	-	10/39/115/115	-
24	CLA	B	821	10	-	2/21/97/115	-
23	CHL	0	306	-	-	10/20/96/117	-
26	0UR	6	321	-	-	11/42/81/86	0/2/2/2
24	CLA	B	818	10	-	9/32/108/115	-
24	CLA	A	830	9	-	4/21/97/115	-
24	CLA	F	303	-	-	8/15/91/115	-
24	CLA	B	841	27	-	8/39/115/115	-
25	8CT	B	850	-	-	13/29/63/63	0/2/2/2
24	CLA	6	316	5	-	17/39/115/115	-
23	CHL	1	306	-	-	23/41/117/117	-
23	CHL	2	306	-	-	5/23/99/117	-
25	8CT	A	845	-	-	10/29/63/63	0/2/2/2
24	CLA	5	307	-	-	7/17/93/115	-
24	CLA	A	821	-	-	5/20/96/115	-
23	CHL	8	308	-	-	11/23/99/117	-
24	CLA	H	201	17	-	6/17/93/115	-
24	CLA	8	312	7	-	8/17/93/115	-
25	8CT	2	314	-	-	12/29/63/63	0/2/2/2
31	PQN	A	841	-	-	7/23/43/43	0/2/2/2
30	0IE	7	321	-	-	2/33/72/72	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	1	310	2	-	6/24/100/115	-
24	CLA	O	209	-	-	11/23/99/115	-
25	8CT	3	317	-	-	9/29/63/63	0/2/2/2
24	CLA	B	812	10	-	6/24/100/115	-
23	CHL	7	307	-	-	6/23/99/117	-
29	LMG	3	321	-	-	16/31/51/70	0/1/1/1
24	CLA	H	204	-	-	3/18/94/115	-
25	8CT	A	844	-	-	4/29/63/63	0/2/2/2
24	CLA	A	823	9	-	10/27/103/115	-
24	CLA	5	302	2	-	11/32/108/115	-
23	CHL	0	301	1	-	11/25/101/117	-
26	0UR	2	316	-	-	11/40/79/86	0/2/2/2
24	CLA	A	835	-	-	9/23/99/115	-
25	8CT	I	101	-	-	9/29/63/63	0/2/2/2
24	CLA	O	201	27	-	8/24/100/115	-
24	CLA	6	317	-	-	14/17/93/115	-
24	CLA	1	303	-	-	4/24/100/115	-
24	CLA	B	815	10	-	3/27/103/115	-
27	LHG	2	317	24	-	18/36/36/53	-
24	CLA	H	202	10	-	8/27/103/115	-
24	CLA	B	839	-	-	12/39/115/115	-
26	0UR	0	315	-	-	3/42/81/86	0/2/2/2
24	CLA	A	815	-	-	5/15/91/115	-
27	LHG	3	320	-	-	16/40/40/53	-
27	LHG	7	323	-	-	21/42/42/53	-
24	CLA	A	803	9	-	8/27/103/115	-
25	8CT	F	301	-	-	14/29/63/63	0/2/2/2
23	CHL	6	302	5	-	20/39/115/117	-
29	LMG	M	101	-	-	22/37/57/70	0/1/1/1
25	8CT	L	207	-	-	9/29/63/63	0/2/2/2
24	CLA	B	817	10	-	21/33/109/115	-
24	CLA	B	822	10	-	13/33/109/115	-
24	CLA	A	825	-	-	11/39/115/115	-
24	CLA	H	203	22	-	8/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	832	-	-	9/39/115/115	-
23	CHL	5	305	-	-	9/20/96/117	-
25	8CT	6	319	-	-	8/29/63/63	0/2/2/2
25	8CT	3	316	-	-	9/29/63/63	0/2/2/2
24	CLA	0	307	-	-	12/33/109/115	-
29	LMG	A	851	-	-	13/31/51/70	0/1/1/1
25	8CT	B	843	-	-	14/29/63/63	0/2/2/2
26	0UR	1	315	-	-	3/42/81/86	0/2/2/2
24	CLA	B	840	10	-	11/39/115/115	-
24	CLA	B	831	10	-	11/21/97/115	-
24	CLA	2	311	3	-	12/33/109/115	-
24	CLA	5	303	-	-	12/24/100/115	-
24	CLA	6	314	-	-	3/15/91/115	-
24	CLA	A	805	-	-	19/39/115/115	-
24	CLA	A	840	-	-	11/39/115/115	-
24	CLA	B	809	10	-	12/39/115/115	-
26	0UR	O	207	-	-	5/42/81/86	0/2/2/2
24	CLA	3	303	-	-	8/27/103/115	-
24	CLA	6	309	5	-	2/31/107/115	-
24	CLA	B	816	10	-	9/33/109/115	-
24	CLA	2	310	3	-	5/19/95/115	-
23	CHL	8	301	2	-	12/25/101/117	-
24	CLA	F	302	13	-	5/18/94/115	-
25	8CT	1	314	-	-	8/29/63/63	0/2/2/2
23	CHL	2	312	3	-	5/23/99/117	-
23	CHL	7	306	-	-	17/35/111/117	-
24	CLA	B	808	10	-	11/39/115/115	-
27	LHG	3	322	-	-	18/40/40/53	-
25	8CT	7	318	-	-	15/29/63/63	0/2/2/2
24	CLA	9	309	27	-	5/10/86/115	-
24	CLA	A	818	9	-	18/39/115/115	-
24	CLA	6	312	5	-	10/29/105/115	-
23	CHL	1	301	-	-	16/39/115/117	-
23	CHL	3	302	4	-	22/37/113/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CHL	2	304	-	-	0/14/90/117	-
26	OUR	7	320	-	-	9/41/80/86	0/2/2/2
31	PQN	B	842	-	-	6/23/43/43	0/2/2/2
24	CLA	2	308	3	-	3/33/109/115	-
24	CLA	2	303	-	-	11/33/109/115	-
27	LHG	A	842	-	-	20/53/53/53	-
24	CLA	B	806	-	-	11/39/115/115	-
26	OUR	4	318	-	-	14/40/79/86	0/2/2/2
23	CHL	1	304	-	-	9/23/99/117	-
24	CLA	A	804	9	-	14/39/115/115	-
23	CHL	4	301	7	-	18/35/111/117	-
24	CLA	A	808	9	-	11/39/115/115	-
24	CLA	1	302	2	-	14/29/105/115	-
24	CLA	8	315	-	-	10/15/91/115	-
23	CHL	6	308	5	-	10/34/110/117	-
24	CLA	A	853	-	-	11/39/115/115	-
24	CLA	7	315	6	-	3/15/91/115	-
33	SF4	C	101	-	-	-	0/6/5/5
24	CLA	8	313	7	-	10/29/105/115	-
26	OUR	8	319	-	-	8/42/81/86	0/2/2/2
27	LHG	2	319	24	-	12/36/36/53	-
24	CLA	0	304	-	-	5/24/100/115	-
25	8CT	L	204	-	-	6/29/63/63	0/2/2/2
24	CLA	4	311	-	-	6/19/95/115	-
23	CHL	5	301	2	-	21/39/115/117	-
26	OUR	2	315	-	-	7/41/80/86	0/2/2/2
26	OUR	0	316	-	-	12/42/81/86	0/2/2/2
24	CLA	9	308	-	-	7/33/109/115	-
26	OUR	5	315	-	-	10/42/81/86	0/2/2/2
24	CLA	G	103	14	-	5/17/93/115	-
24	CLA	8	305	-	-	11/39/115/115	-
27	LHG	8	302	-	-	13/35/35/53	-
24	CLA	A	833	9	-	2/17/93/115	-
24	CLA	B	819	10	-	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CLA	B	807	10	-	5/15/91/115	-
24	CLA	7	304	-	-	7/27/103/115	-
23	CHL	9	306	-	-	6/20/96/117	-
24	CLA	A	834	9	-	14/30/106/115	-
24	CLA	8	304	7	-	7/17/93/115	-
24	CLA	A	836	9	-	12/35/111/115	-
25	8CT	7	319	-	-	10/29/63/63	0/2/2/2
23	CHL	4	302	7	-	15/26/102/117	-
24	CLA	B	834	10	-	16/35/111/115	-
23	CHL	2	301	3	-	29/39/115/117	-
23	CHL	6	305	-	-	0/14/90/117	-
24	CLA	7	316	-	-	13/15/91/115	-
24	CLA	4	303	7	-	4/15/91/115	-
29	LMG	O	210	-	-	10/34/54/70	0/1/1/1
33	SF4	B	803	-	-	-	0/6/5/5
24	CLA	3	304	-	-	6/39/115/115	-
24	CLA	A	817	9	-	12/39/115/115	-
23	CHL	1	305	-	-	7/20/96/117	-

The worst 5 of 3981 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	J	104	8CT	C02-C03	14.46	1.59	1.34
25	B	844	8CT	C02-C03	14.43	1.59	1.34
25	6	324	8CT	C02-C03	14.42	1.59	1.34
25	A	844	8CT	C02-C03	14.35	1.59	1.34
25	G	104	8CT	C02-C03	14.34	1.59	1.34

The worst 5 of 4098 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	823	CLA	O2A-CGA-O1A	-19.76	73.72	123.59
24	B	823	CLA	O2A-CGA-CBA	14.56	157.60	111.91
25	K	105	8CT	C33-C32-C31	-11.83	113.51	124.85
25	G	104	8CT	C33-C32-C31	-11.75	113.58	124.85
24	B	826	CLA	CHA-C4D-ND	11.22	135.06	125.21

There are no chirality outliers.

5 of 3534 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	0	301	CHL	C1A-C2A-CAA-CBA
23	0	301	CHL	C3A-C2A-CAA-CBA
23	0	301	CHL	C1C-C2C-CMC-OMC
23	0	301	CHL	C3C-C2C-CMC-OMC
23	0	301	CHL	C2-C3-C5-C6

There are no ring outliers.

268 monomers are involved in 685 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	0	303	CLA	4	0
23	5	304	CHL	4	0
24	A	824	CLA	5	0
29	9	317	LMG	4	0
23	7	305	CHL	4	0
25	J	104	8CT	1	0
24	3	315	CLA	1	0
24	B	824	CLA	5	0
24	6	310	CLA	3	0
29	A	854	LMG	3	0
23	7	301	CHL	3	0
23	8	306	CHL	3	0
27	3	324	LHG	3	0
24	0	310	CLA	2	0
24	A	837	CLA	3	0
24	1	308	CLA	2	0
24	A	809	CLA	4	0
24	L	202	CLA	5	0
23	0	302	CHL	3	0
24	A	801	CLA	2	0
24	B	814	CLA	7	0
24	B	826	CLA	3	0
24	A	816	CLA	2	0
24	B	804	CLA	9	0
24	4	312	CLA	2	0
24	6	303	CLA	1	0
23	3	305	CHL	1	0
27	1	317	LHG	5	0
24	3	306	CLA	2	0
23	3	301	CHL	1	0
24	B	825	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	4	314	CLA	1	0
34	B	849	DGD	3	0
24	4	309	CLA	5	0
27	0	317	LHG	2	0
24	9	311	CLA	2	0
23	8	307	CHL	1	0
23	0	305	CHL	5	0
23	7	302	CHL	3	0
24	4	310	CLA	2	0
23	4	308	CHL	2	0
23	4	313	CHL	3	0
24	A	802	CLA	3	0
23	2	305	CHL	2	0
24	A	810	CLA	6	0
23	2	307	CHL	1	0
24	1	307	CLA	2	0
24	5	313	CLA	1	0
24	B	833	CLA	6	0
23	9	312	CHL	1	0
24	5	310	CLA	2	0
24	5	311	CLA	3	0
24	G	102	CLA	1	0
23	8	303	CHL	1	0
23	8	316	CHL	3	0
24	7	317	CLA	1	0
25	8	317	8CT	1	0
24	B	835	CLA	1	0
23	5	312	CHL	1	0
23	8	309	CHL	2	0
24	A	827	CLA	7	0
27	A	850	LHG	3	0
24	A	848	CLA	4	0
24	0	312	CLA	2	0
24	2	313	CLA	1	0
24	6	304	CLA	2	0
27	I	102	LHG	4	0
27	6	322	LHG	5	0
24	A	811	CLA	2	0
24	A	828	CLA	4	0
23	4	305	CHL	3	0
27	9	316	LHG	5	0
24	0	311	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A	812	CLA	7	0
25	B	847	8CT	1	0
23	1	312	CHL	3	0
23	6	315	CHL	1	0
24	7	314	CLA	1	0
24	3	314	CLA	3	0
23	6	306	CHL	2	0
27	1	318	LHG	2	0
27	5	316	LHG	1	0
24	B	802	CLA	5	0
23	4	306	CHL	2	0
26	3	318	0UR	1	0
24	B	810	CLA	4	0
29	J	102	LMG	1	0
23	6	323	CHL	4	0
26	5	314	0UR	4	0
23	6	307	CHL	3	0
25	3	323	8CT	1	0
24	9	310	CLA	2	0
24	A	806	CLA	2	0
24	A	839	CLA	5	0
24	9	307	CLA	6	0
24	A	814	CLA	2	0
24	A	829	CLA	5	0
27	B	851	LHG	1	0
24	L	201	CLA	3	0
24	0	309	CLA	2	0
24	A	831	CLA	4	0
24	J	103	CLA	2	0
24	L	203	CLA	2	0
26	9	315	0UR	1	0
24	9	302	CLA	4	0
24	3	312	CLA	2	0
24	0	313	CLA	4	0
27	B	852	LHG	1	0
24	2	309	CLA	3	0
32	A	852	CL0	8	0
26	8	318	0UR	2	0
24	1	311	CLA	8	0
24	B	838	CLA	4	0
24	B	830	CLA	6	0
24	B	829	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	8	314	CHL	3	0
24	A	838	CLA	6	0
23	3	307	CHL	5	0
26	4	317	OUR	3	0
24	7	312	CLA	5	0
24	4	304	CLA	1	0
29	J	105	LMG	2	0
24	7	309	CLA	3	0
23	6	301	CHL	9	0
24	3	309	CLA	4	0
24	A	813	CLA	4	0
27	7	322	LHG	2	0
28	0	318	SQD	2	0
24	B	813	CLA	4	0
24	B	820	CLA	4	0
24	7	308	CLA	8	0
23	9	305	CHL	1	0
26	9	314	OUR	2	0
23	4	315	CHL	7	0
24	B	837	CLA	3	0
24	O	206	CLA	4	0
23	9	301	CHL	1	0
24	O	204	CLA	1	0
24	K	104	CLA	2	0
24	B	836	CLA	3	0
24	9	303	CLA	1	0
24	K	103	CLA	1	0
24	A	820	CLA	6	0
24	A	826	CLA	3	0
27	A	843	LHG	3	0
24	6	311	CLA	1	0
24	3	308	CLA	1	0
23	4	307	CHL	3	0
24	B	827	CLA	4	0
24	3	313	CLA	1	0
24	B	805	CLA	4	0
25	4	316	8CT	1	0
23	6	313	CHL	2	0
24	5	308	CLA	3	0
23	5	306	CHL	2	0
25	A	847	8CT	1	0
24	0	308	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	801	CLA	1	0
24	8	310	CLA	1	0
24	K	102	CLA	3	0
24	A	807	CLA	7	0
24	B	823	CLA	4	0
24	B	828	CLA	3	0
24	B	811	CLA	8	0
23	0	306	CHL	5	0
26	6	321	0UR	1	0
24	B	818	CLA	11	0
24	A	830	CLA	3	0
24	F	303	CLA	3	0
24	B	841	CLA	4	0
24	6	316	CLA	4	0
23	1	306	CHL	4	0
23	2	306	CHL	3	0
24	5	307	CLA	2	0
24	A	821	CLA	2	0
23	8	308	CHL	4	0
24	H	201	CLA	2	0
24	8	312	CLA	2	0
31	A	841	PQN	4	0
24	1	310	CLA	2	0
24	O	209	CLA	1	0
24	B	812	CLA	1	0
23	7	307	CHL	6	0
29	3	321	LMG	2	0
24	H	204	CLA	1	0
24	A	823	CLA	1	0
24	5	302	CLA	3	0
23	0	301	CHL	6	0
24	A	835	CLA	1	0
24	O	201	CLA	4	0
24	1	303	CLA	1	0
27	2	317	LHG	2	0
24	H	202	CLA	3	0
24	B	839	CLA	5	0
26	0	315	0UR	1	0
24	A	815	CLA	1	0
27	3	320	LHG	1	0
27	7	323	LHG	3	0
24	A	803	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	F	301	8CT	1	0
23	6	302	CHL	2	0
29	M	101	LMG	1	0
24	B	817	CLA	8	0
24	B	822	CLA	4	0
24	A	825	CLA	2	0
24	B	832	CLA	3	0
23	5	305	CHL	1	0
25	3	316	8CT	1	0
24	0	307	CLA	1	0
29	A	851	LMG	4	0
26	1	315	0UR	1	0
24	B	840	CLA	1	0
24	B	831	CLA	3	0
24	2	311	CLA	2	0
24	5	303	CLA	2	0
24	A	805	CLA	5	0
24	A	840	CLA	4	0
24	B	809	CLA	10	0
26	O	207	0UR	2	0
24	3	303	CLA	3	0
24	6	309	CLA	1	0
24	B	816	CLA	2	0
23	8	301	CHL	6	0
24	F	302	CLA	1	0
23	2	312	CHL	6	0
23	7	306	CHL	4	0
24	B	808	CLA	6	0
27	3	322	LHG	3	0
24	A	818	CLA	4	0
24	6	312	CLA	3	0
23	1	301	CHL	4	0
23	3	302	CHL	3	0
26	7	320	0UR	2	0
31	B	842	PQN	1	0
24	2	308	CLA	2	0
27	A	842	LHG	5	0
24	B	806	CLA	6	0
23	1	304	CHL	3	0
24	A	804	CLA	2	0
23	4	301	CHL	7	0
24	A	808	CLA	7	0

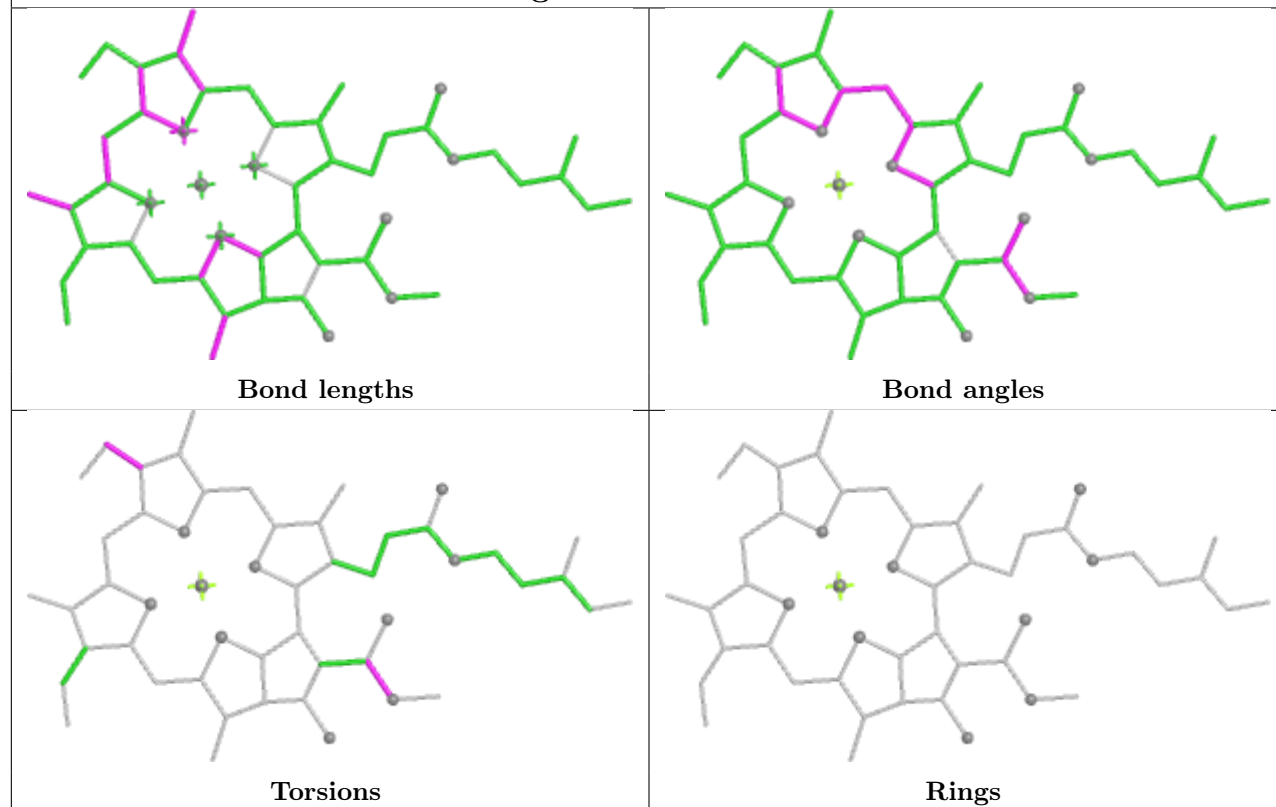
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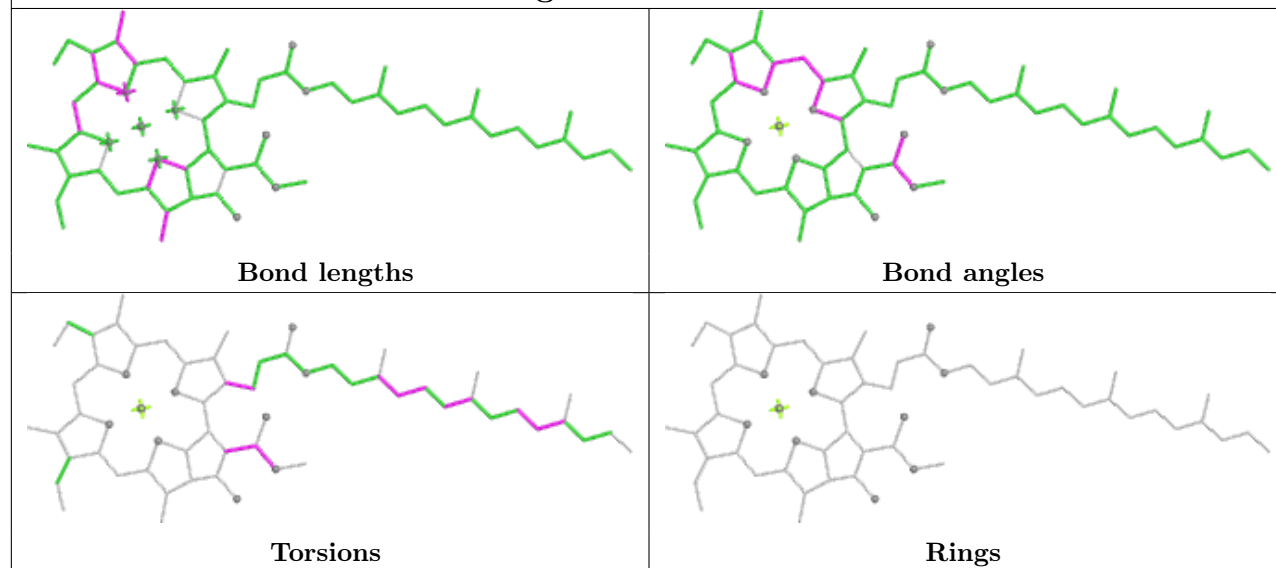
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	1	302	CLA	2	0
24	8	315	CLA	2	0
23	6	308	CHL	3	0
24	A	853	CLA	8	0
24	8	313	CLA	3	0
25	L	204	8CT	1	0
24	4	311	CLA	4	0
23	5	301	CHL	5	0
26	2	315	0UR	3	0
24	9	308	CLA	4	0
24	G	103	CLA	1	0
24	8	305	CLA	3	0
24	B	819	CLA	4	0
24	B	807	CLA	1	0
24	7	304	CLA	5	0
23	9	306	CHL	2	0
24	A	836	CLA	3	0
23	4	302	CHL	2	0
24	B	834	CLA	7	0
23	2	301	CHL	3	0
23	6	305	CHL	2	0
24	7	316	CLA	6	0
29	O	210	LMG	1	0
33	B	803	SF4	1	0
24	3	304	CLA	1	0
24	A	817	CLA	8	0
23	1	305	CHL	2	0

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

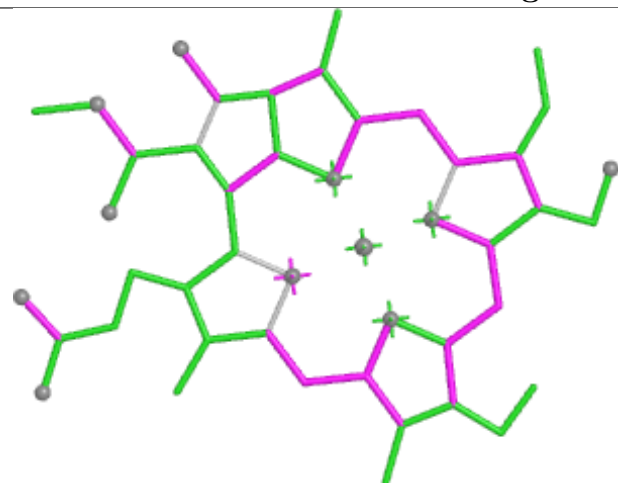
Ligand CLA A 822



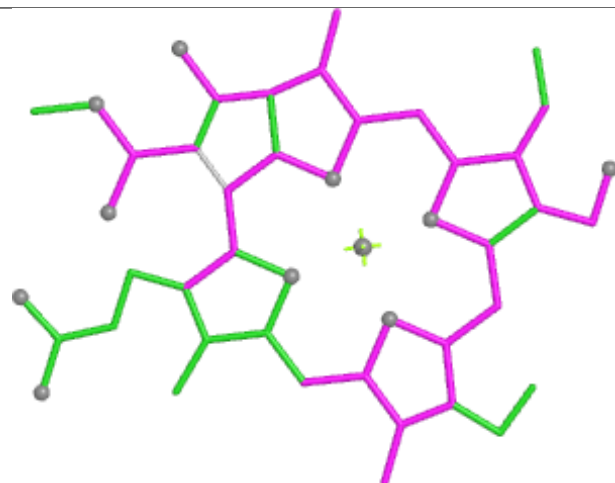
Ligand CLA 0 303



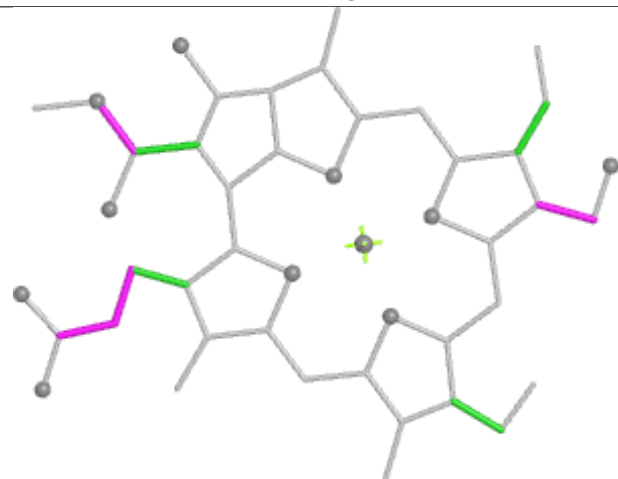
Ligand CHL 5 304



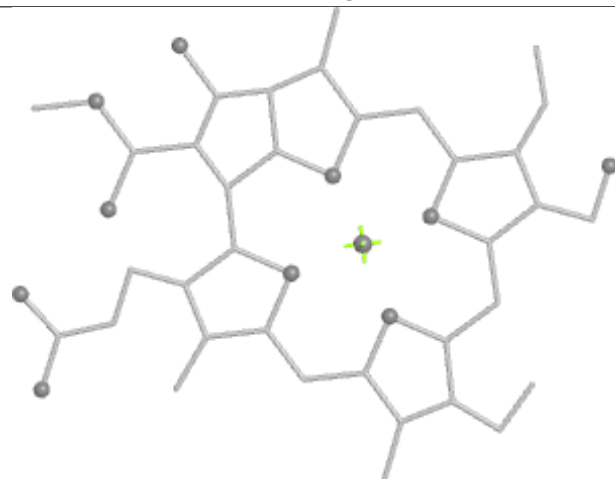
Bond lengths



Bond angles

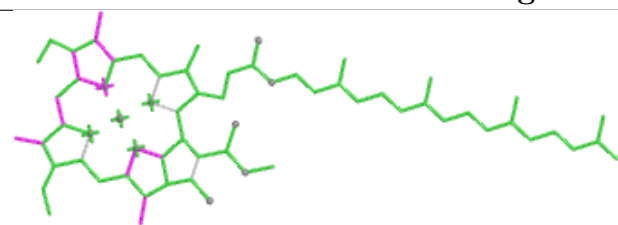


Torsions

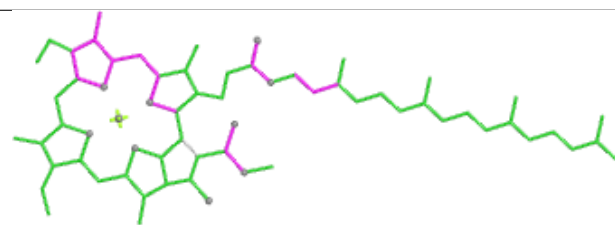


Rings

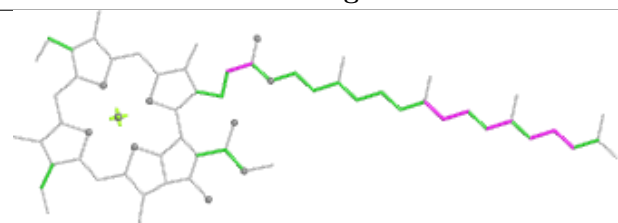
Ligand CLA A 824



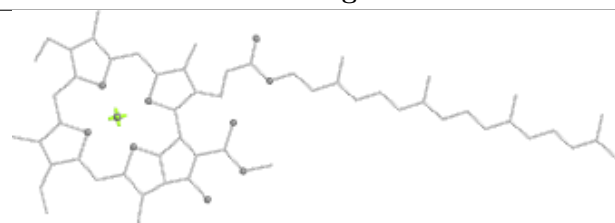
Bond lengths



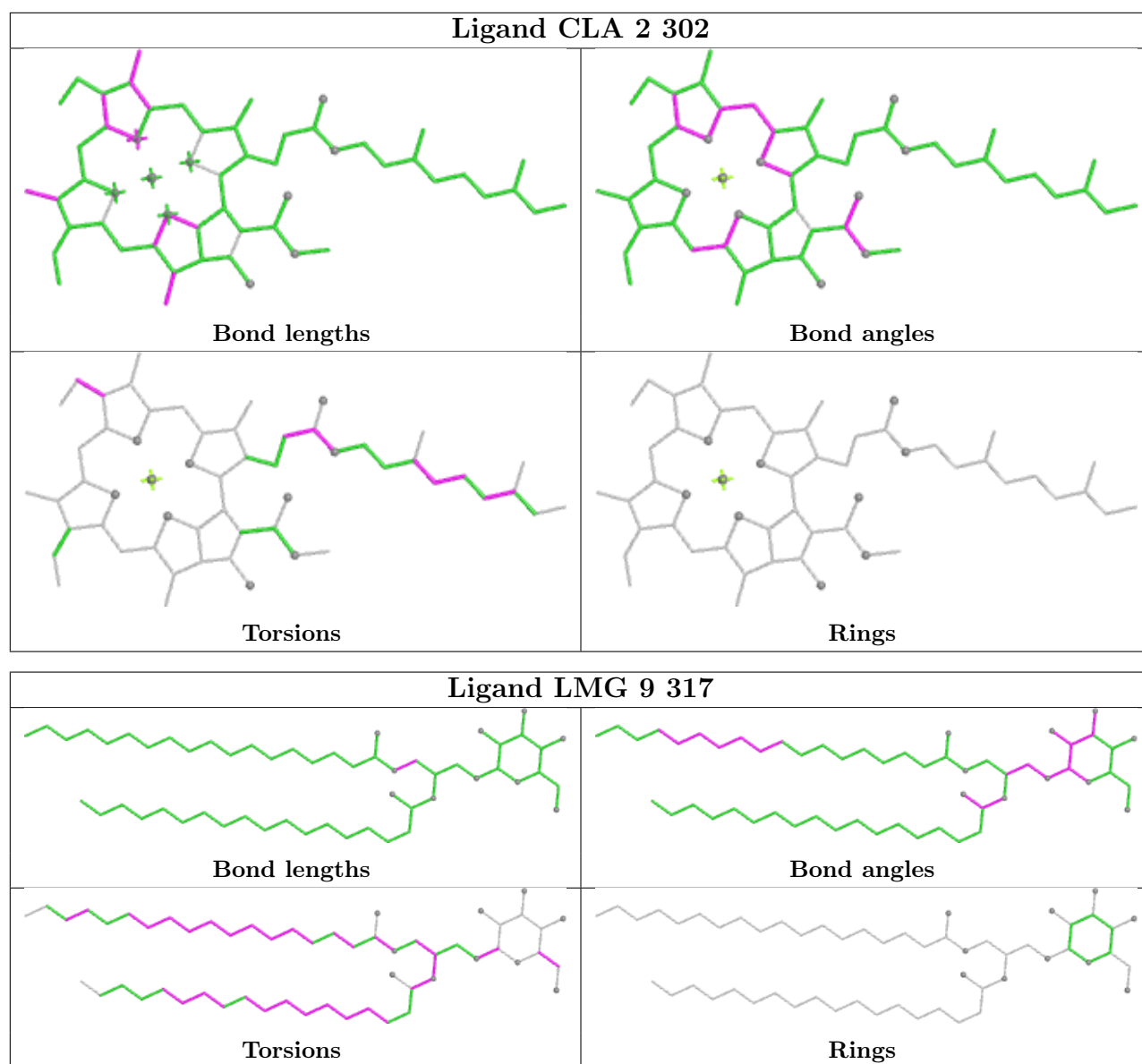
Bond angles



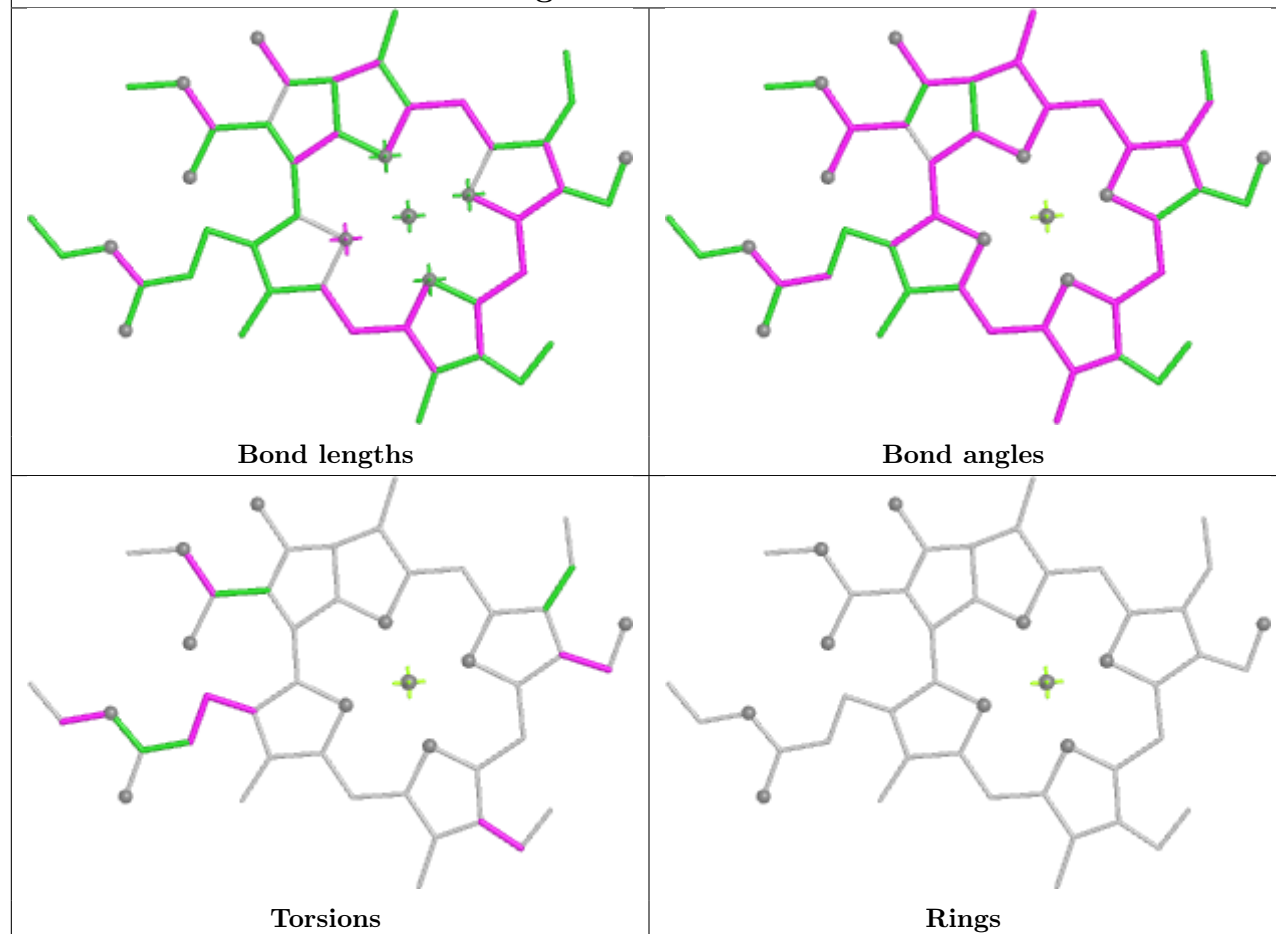
Torsions



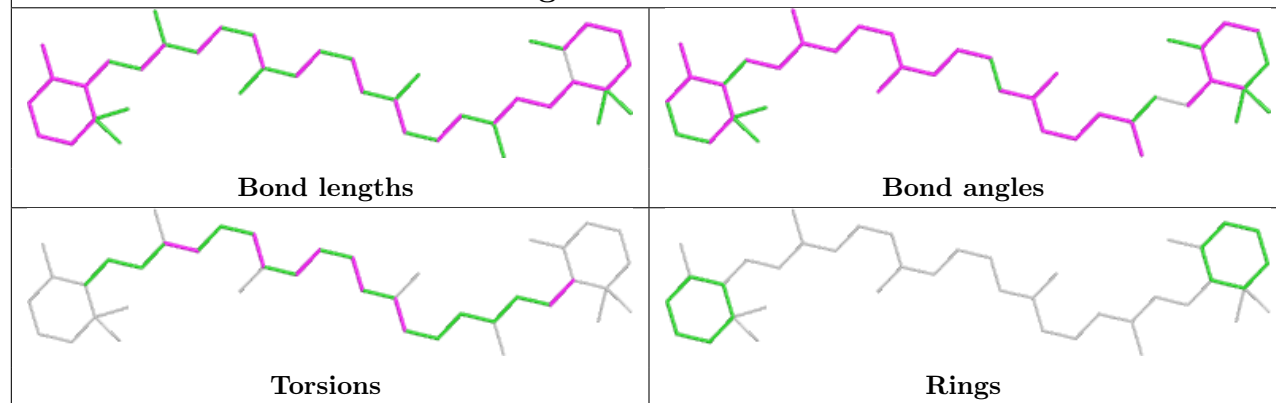
Rings



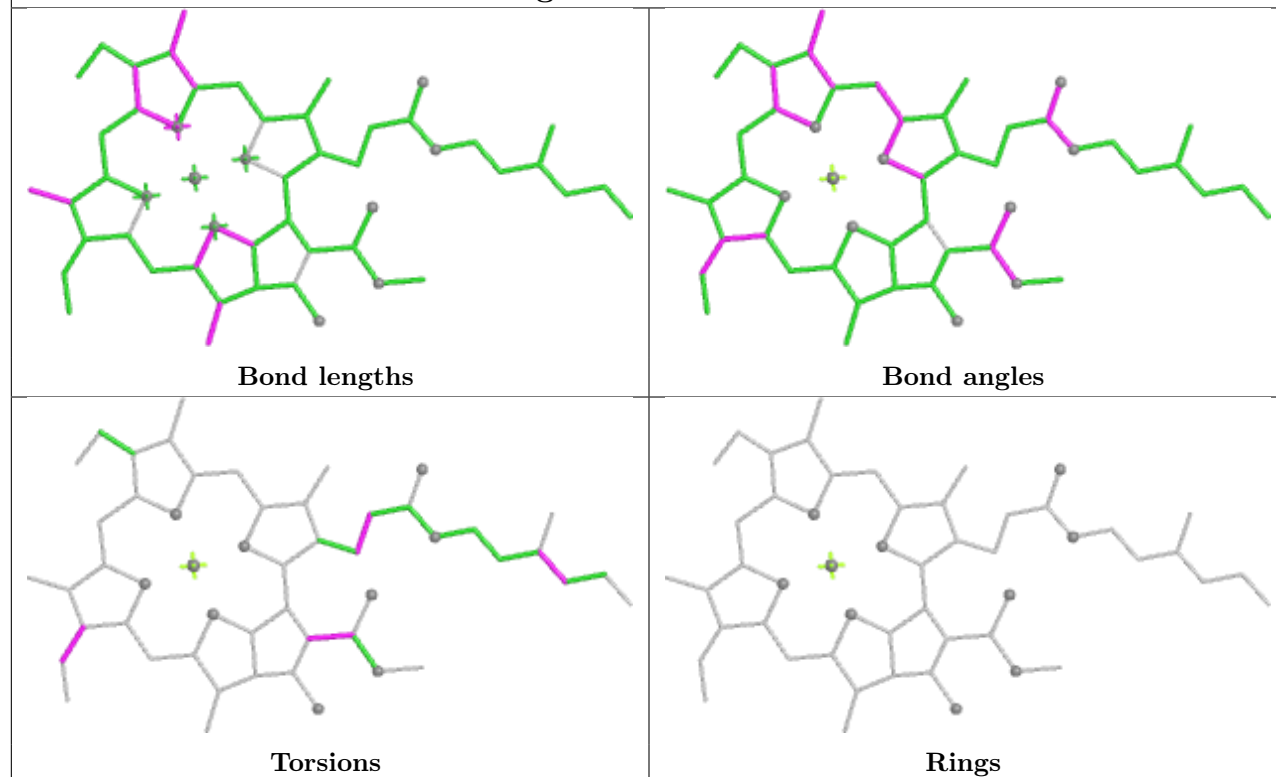
Ligand CHL 7 305



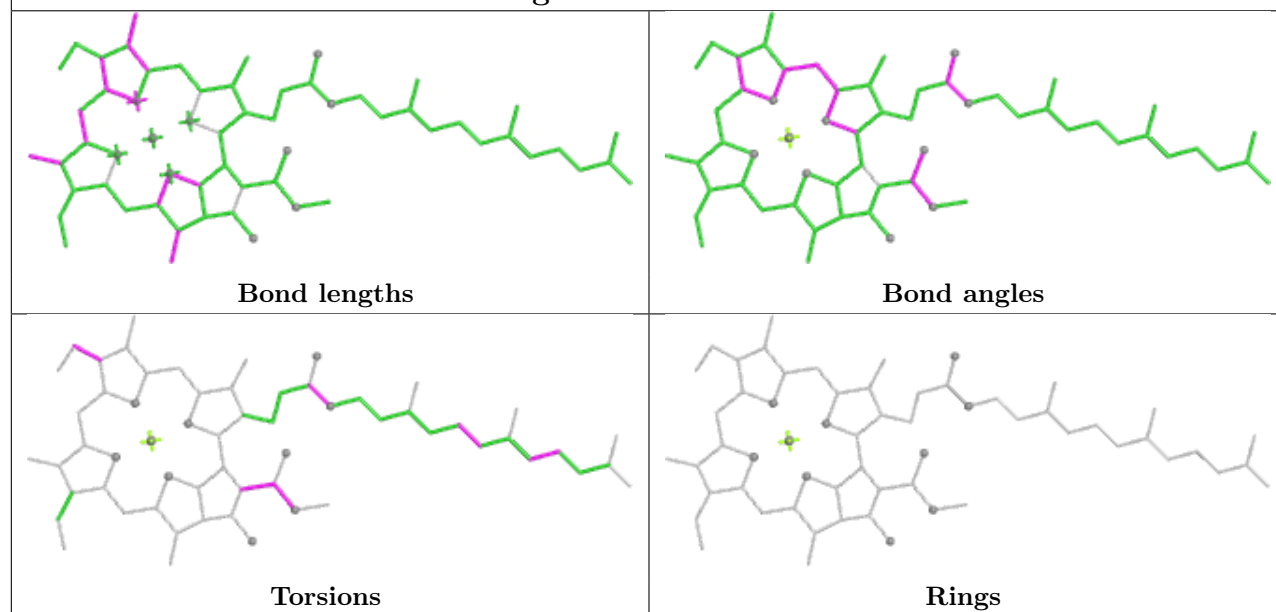
Ligand 8CT J 104

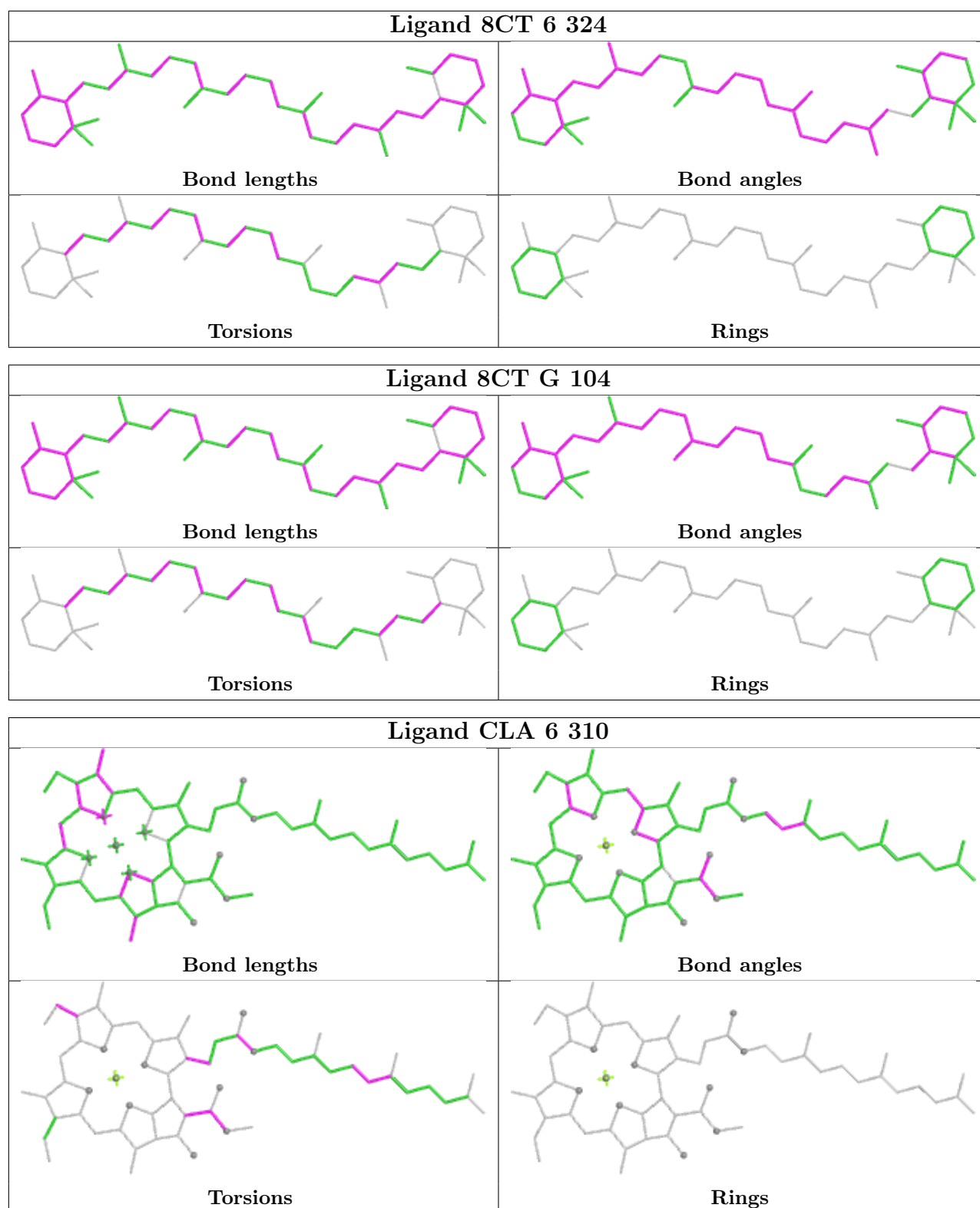


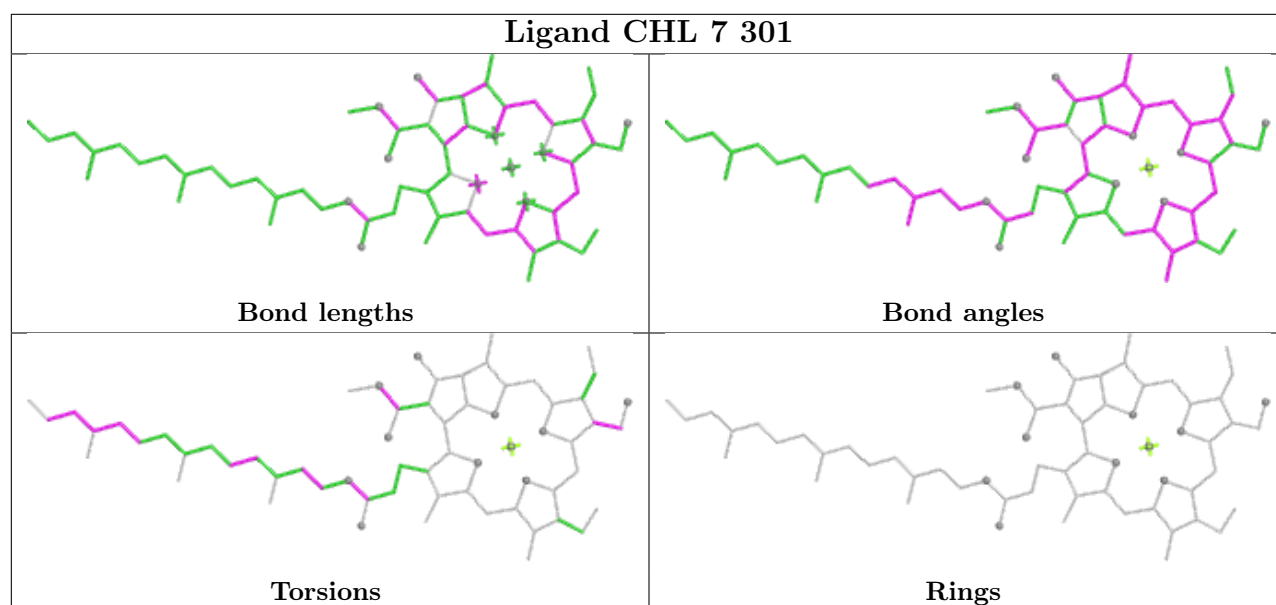
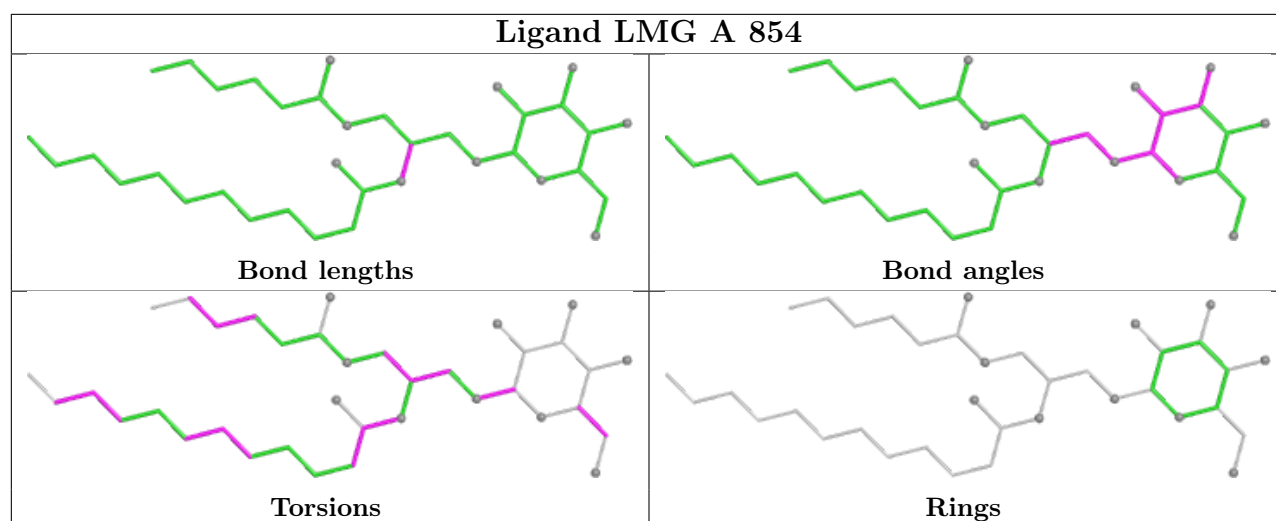
Ligand CLA 3 315



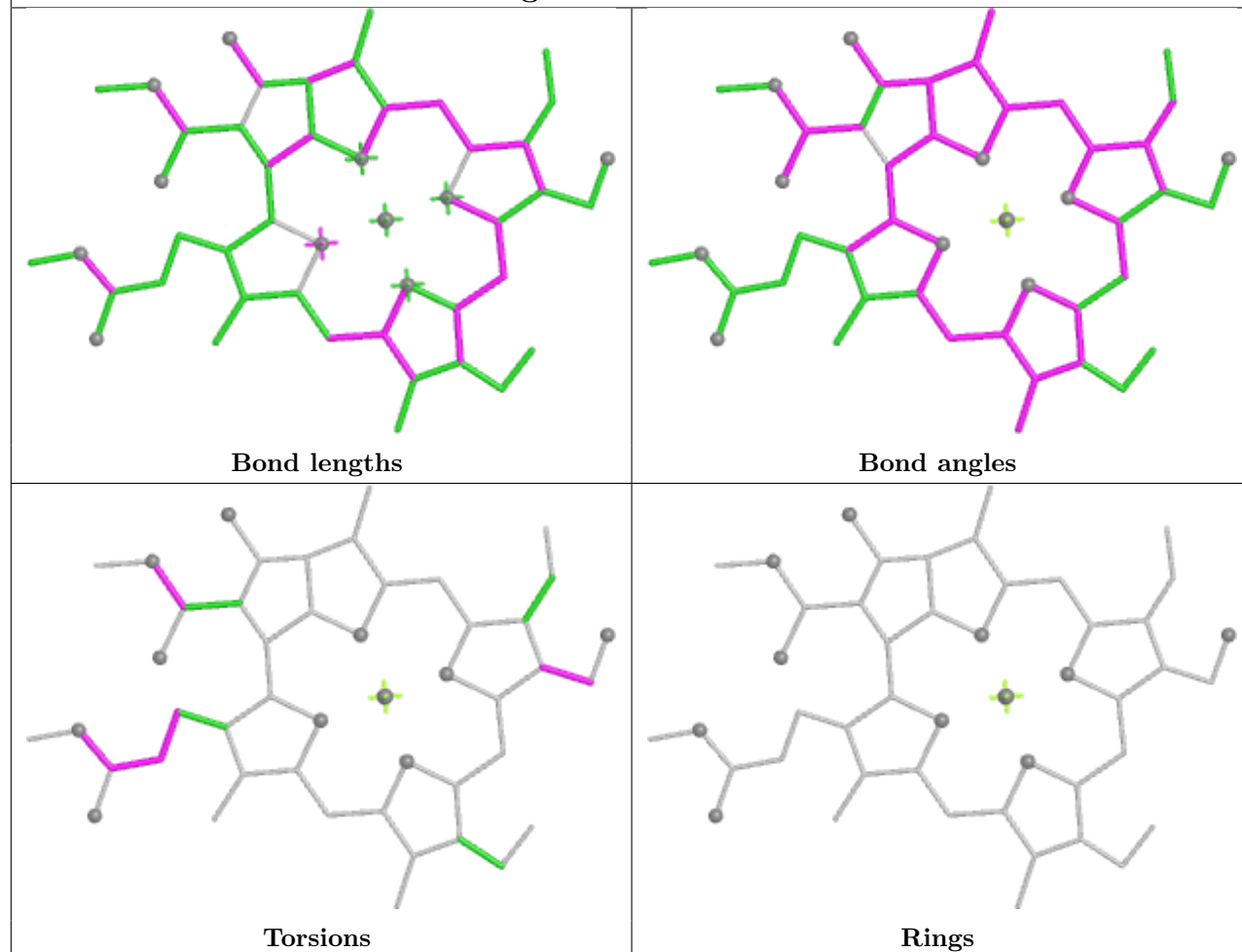
Ligand CLA B 824



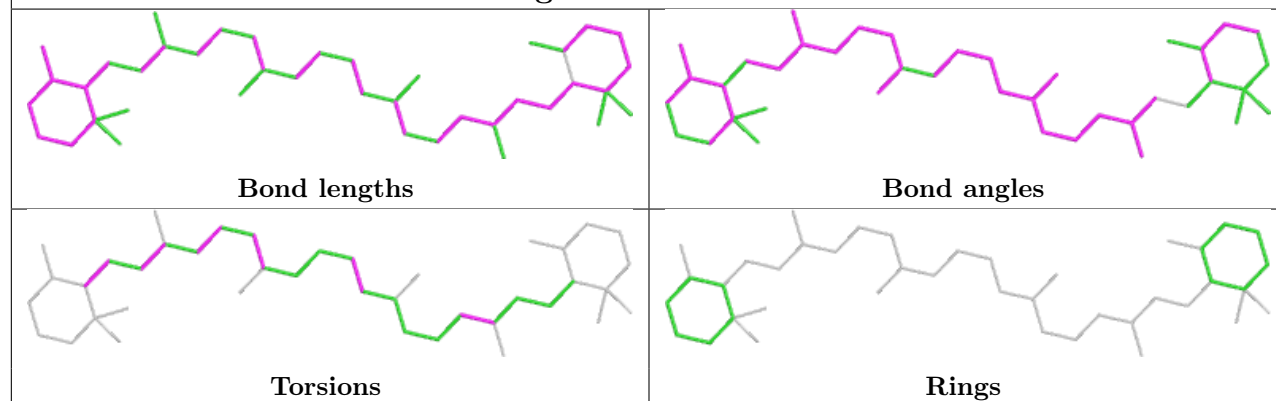




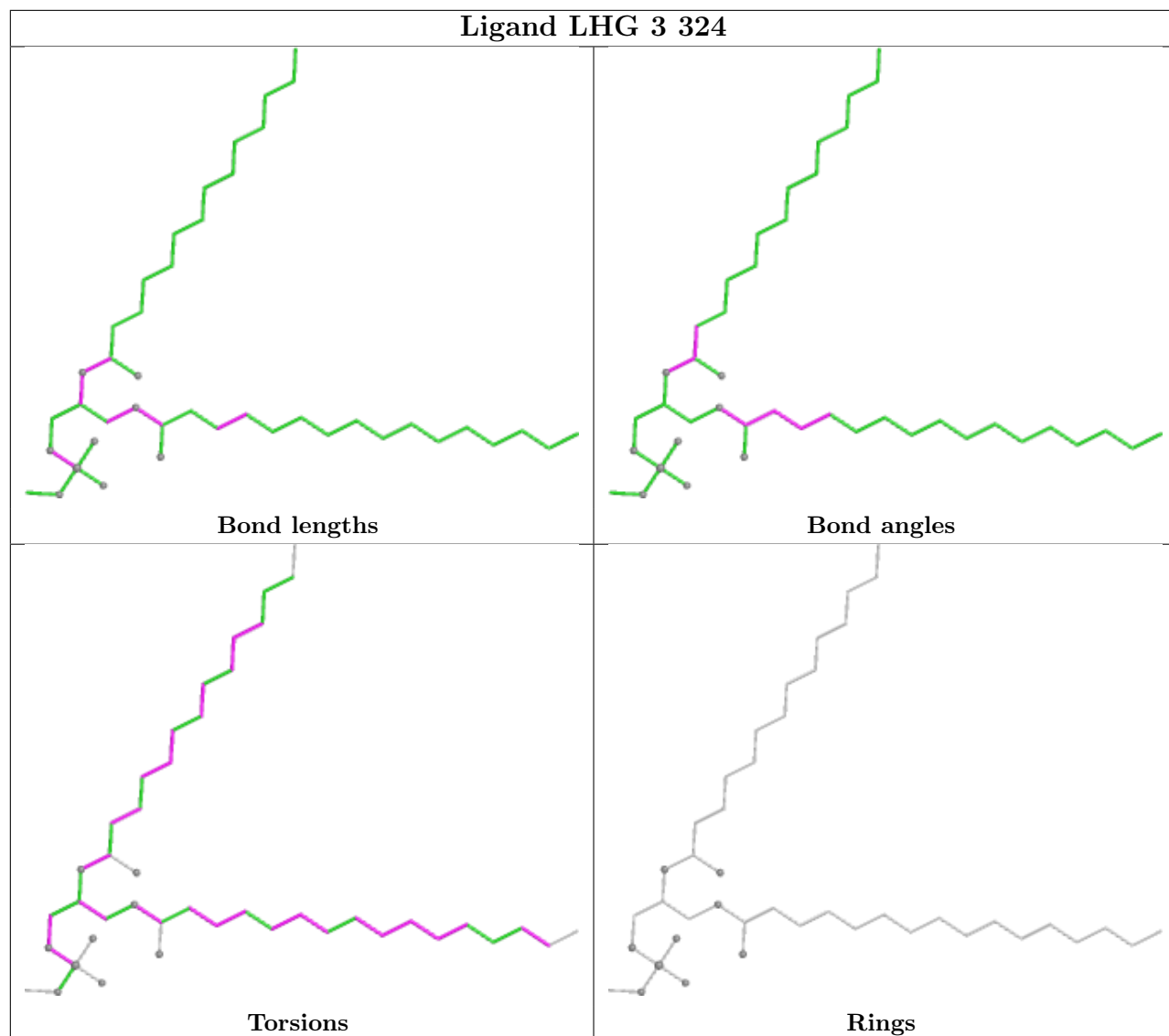
Ligand CHL 8 306



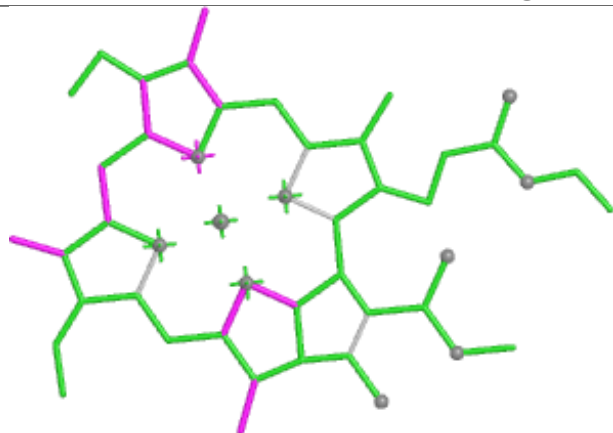
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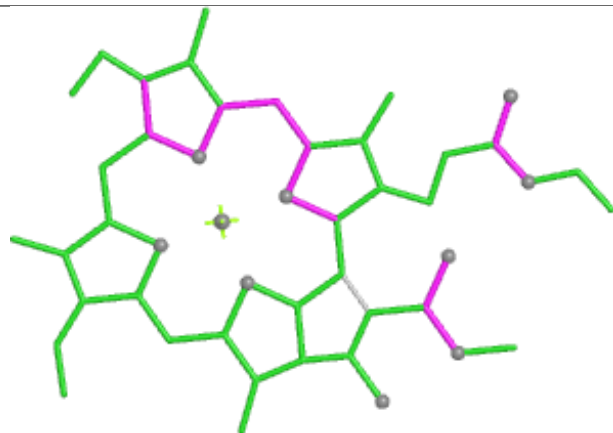
Ligand LHG 3 324



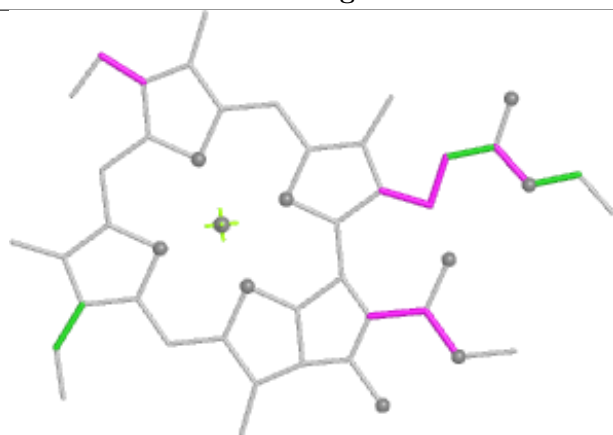
Ligand CLA 0 310



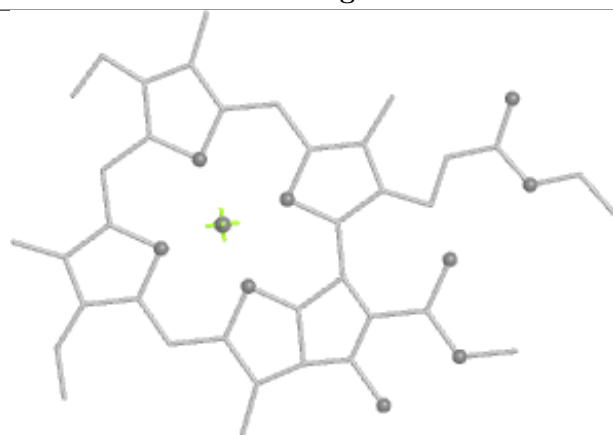
Bond lengths



Bond angles

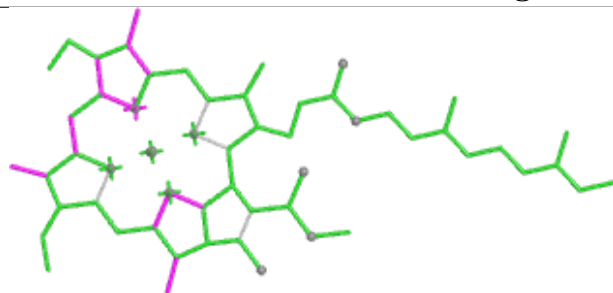


Torsions

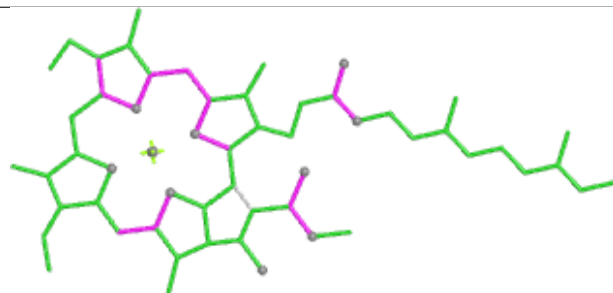


Rings

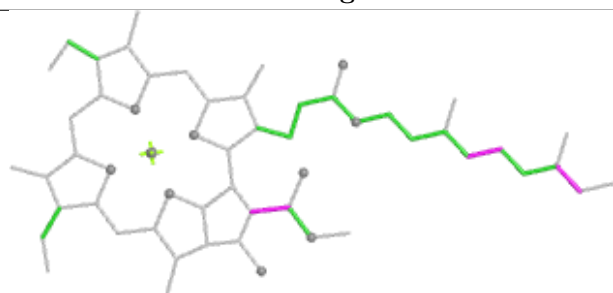
Ligand CLA A 837



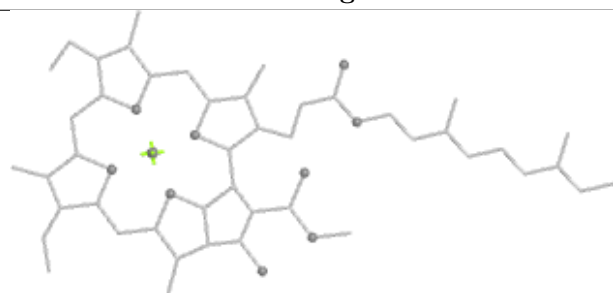
Bond lengths



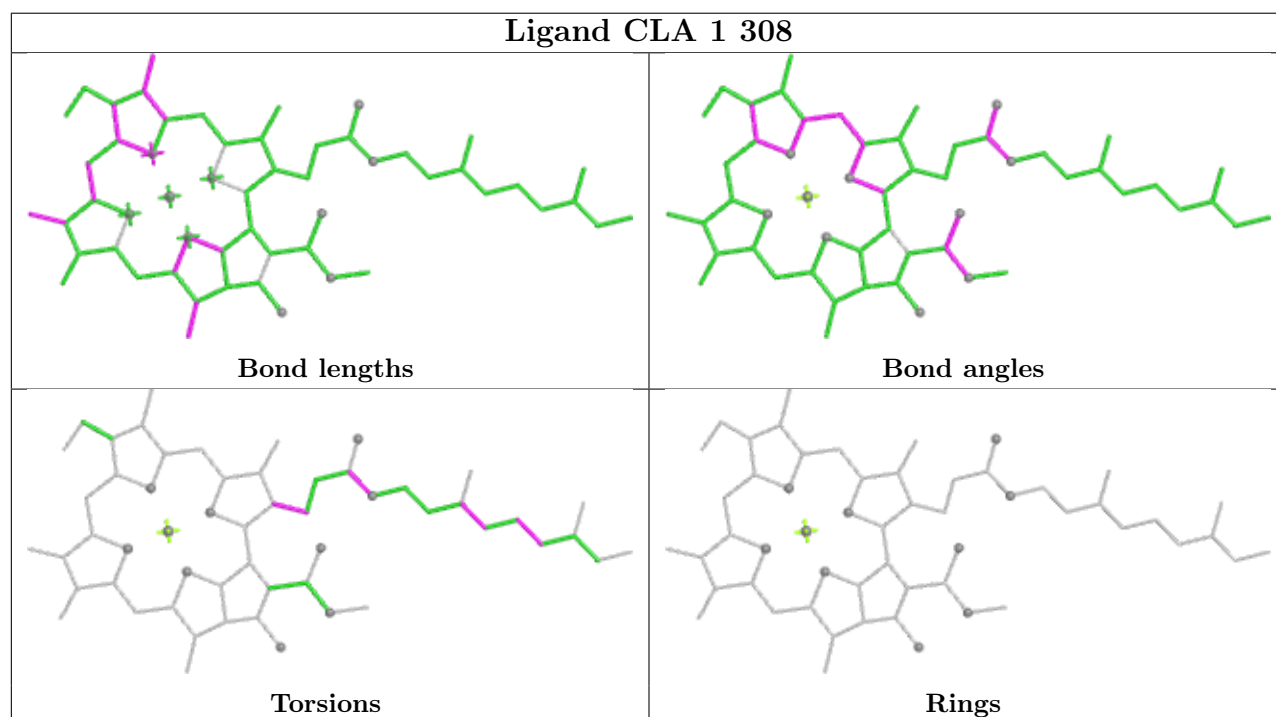
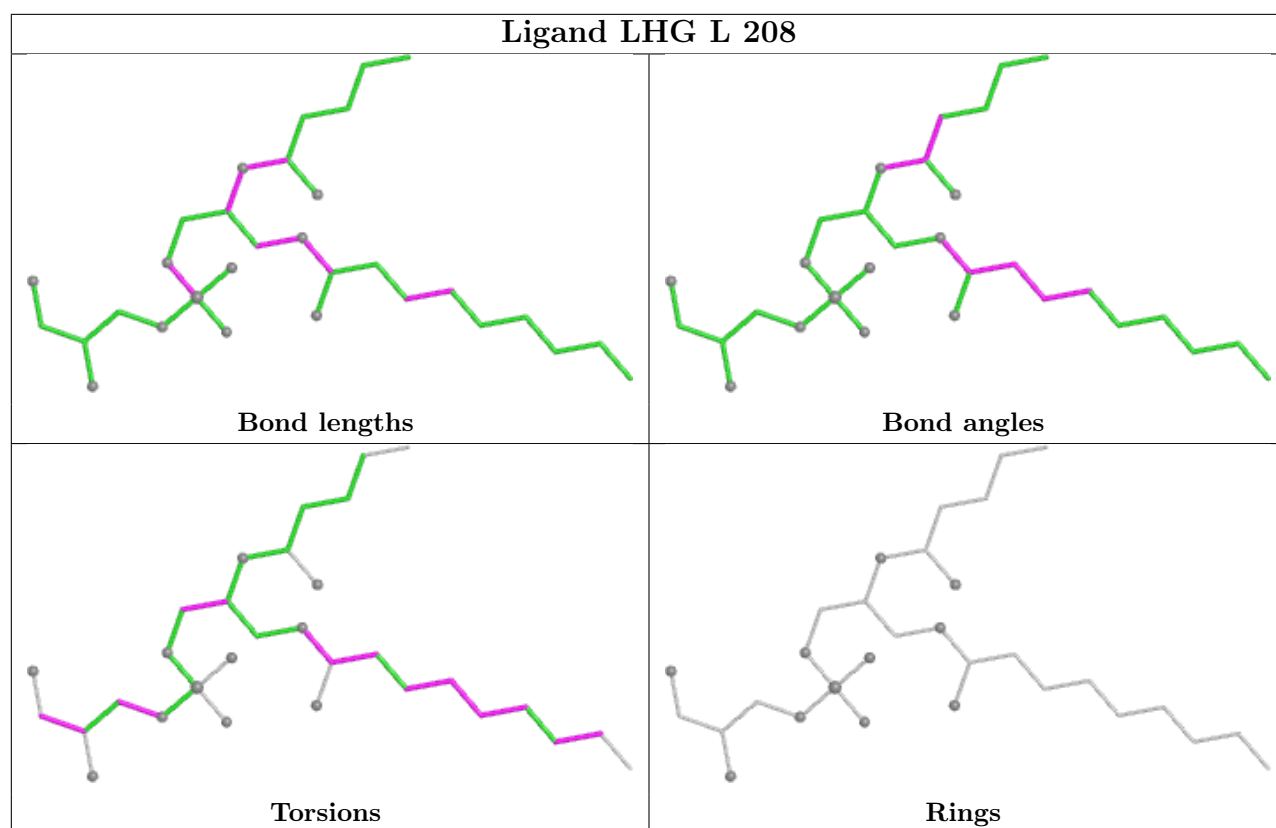
Bond angles



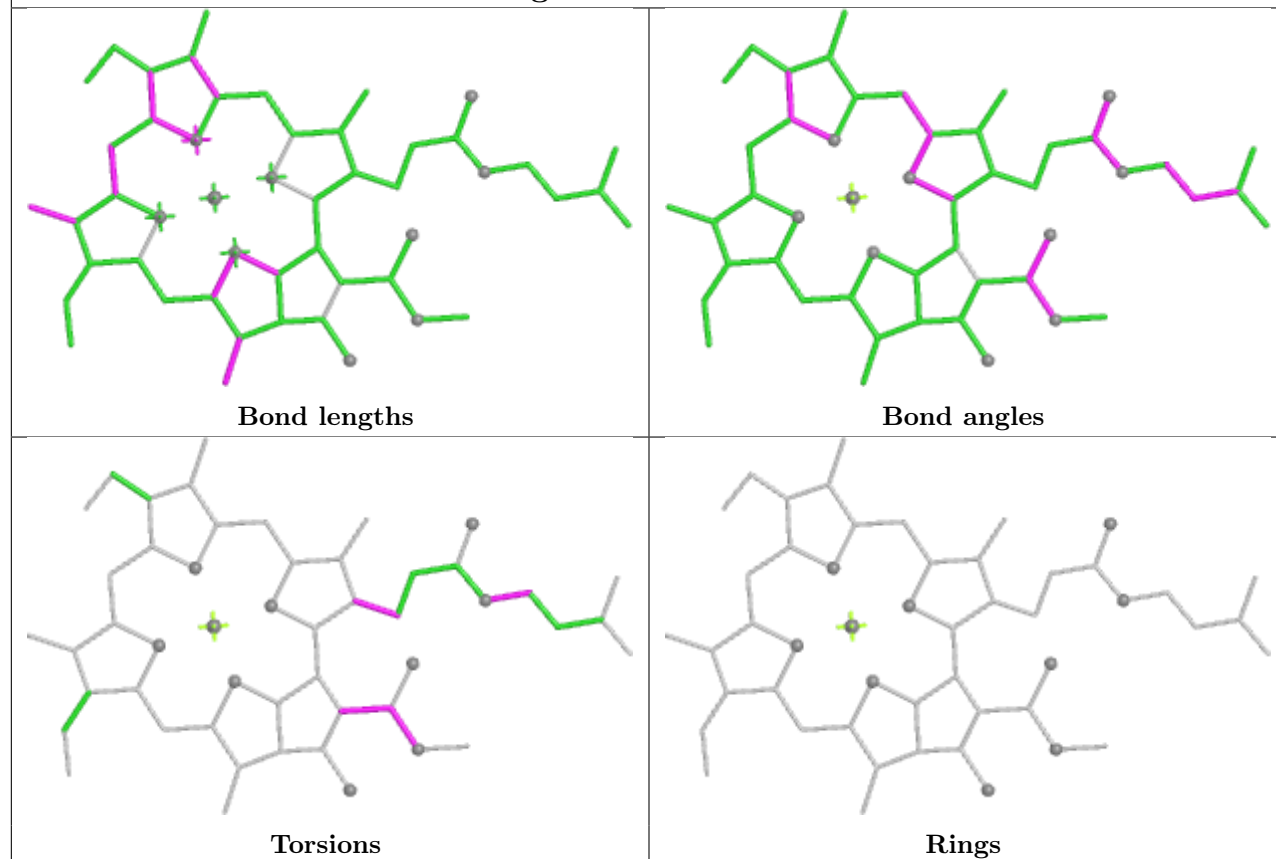
Torsions



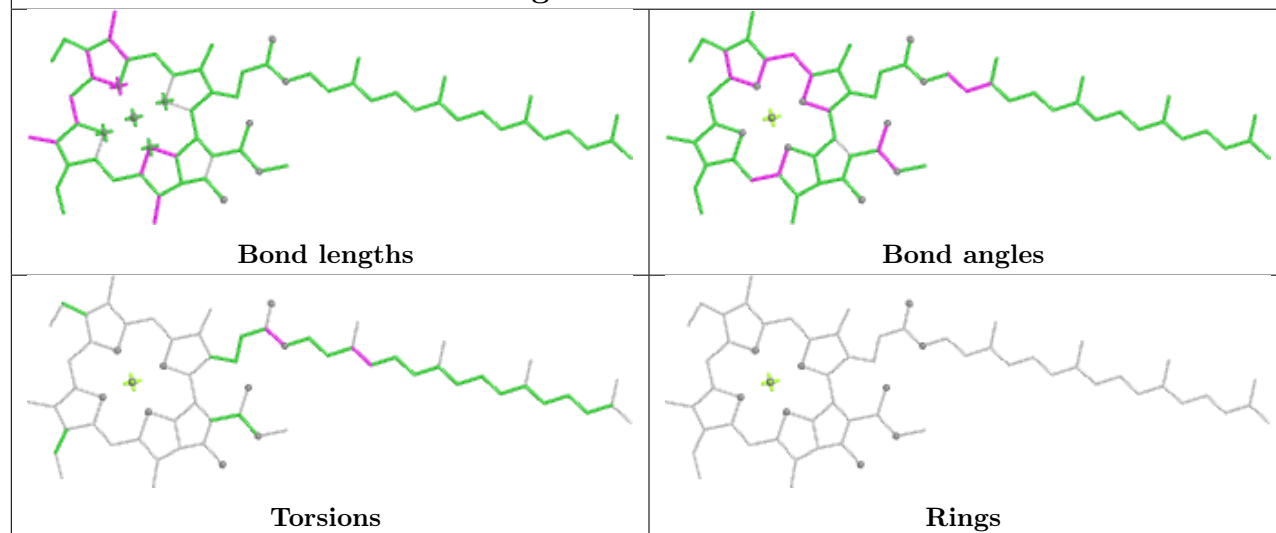
Rings



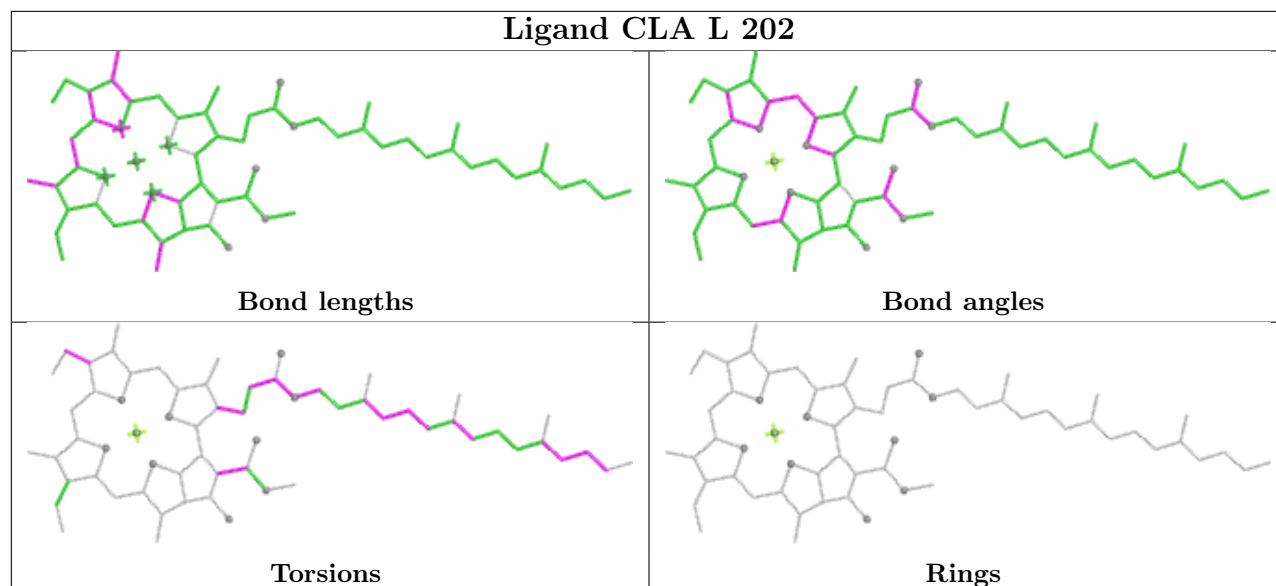
Ligand CLA G 101



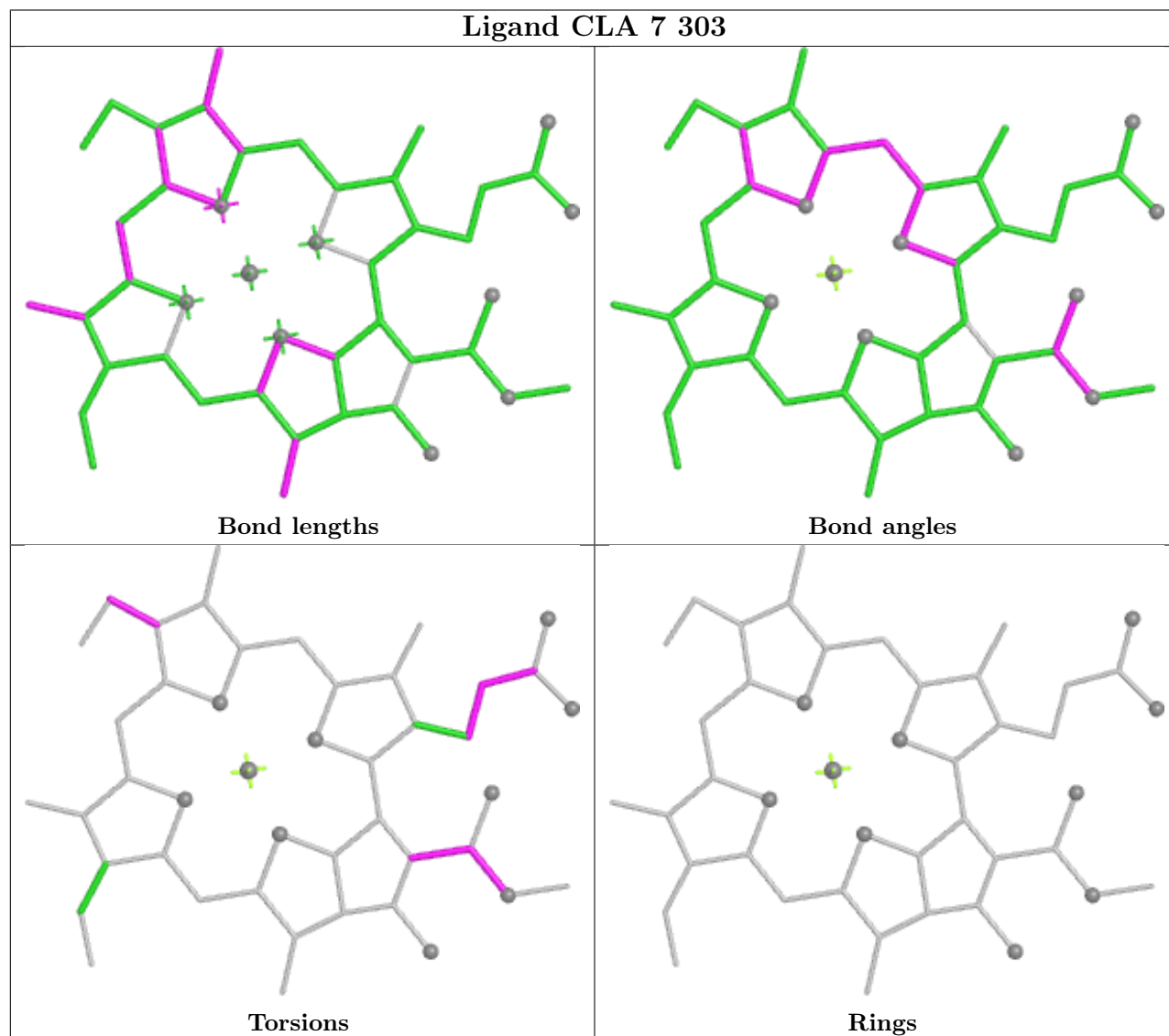
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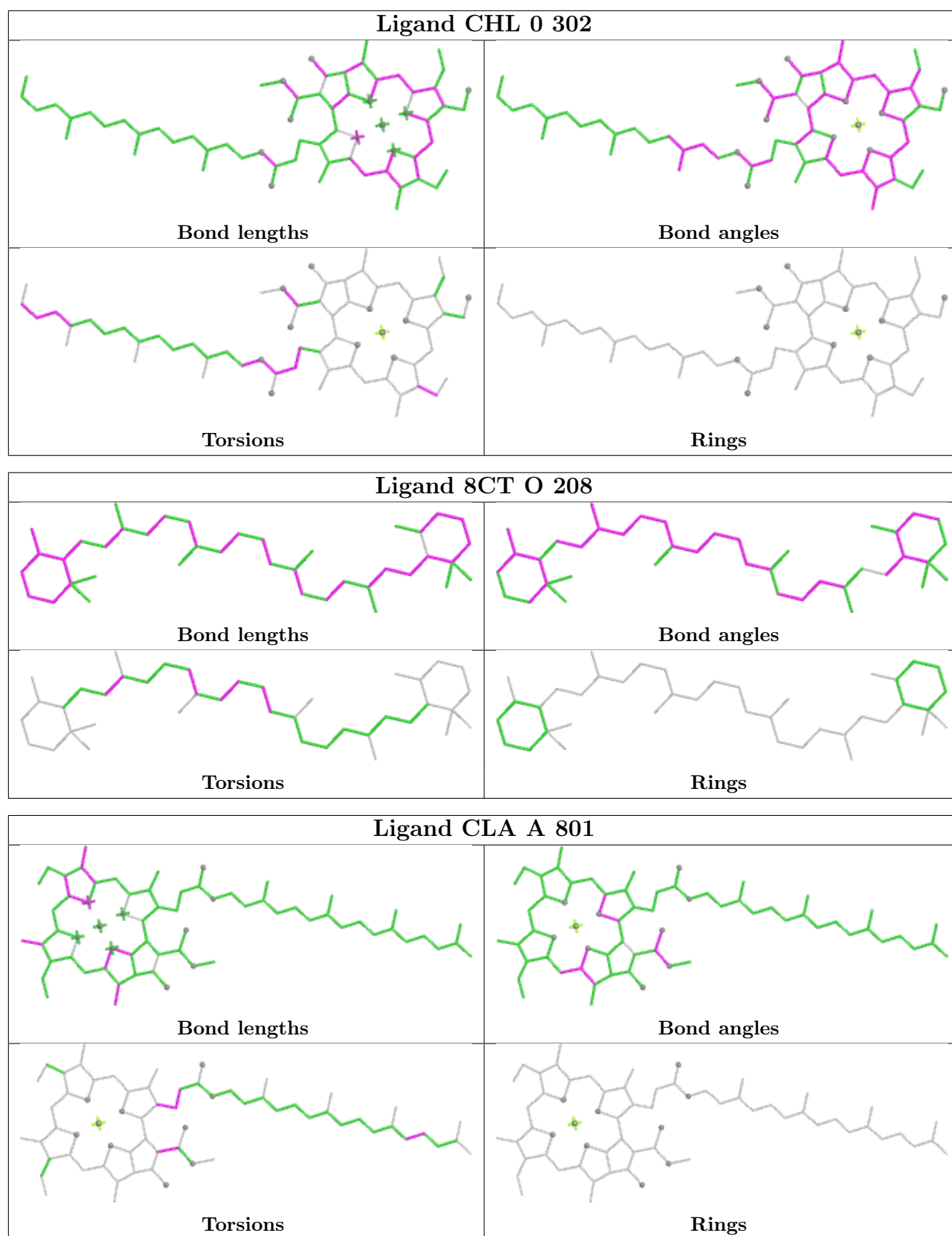


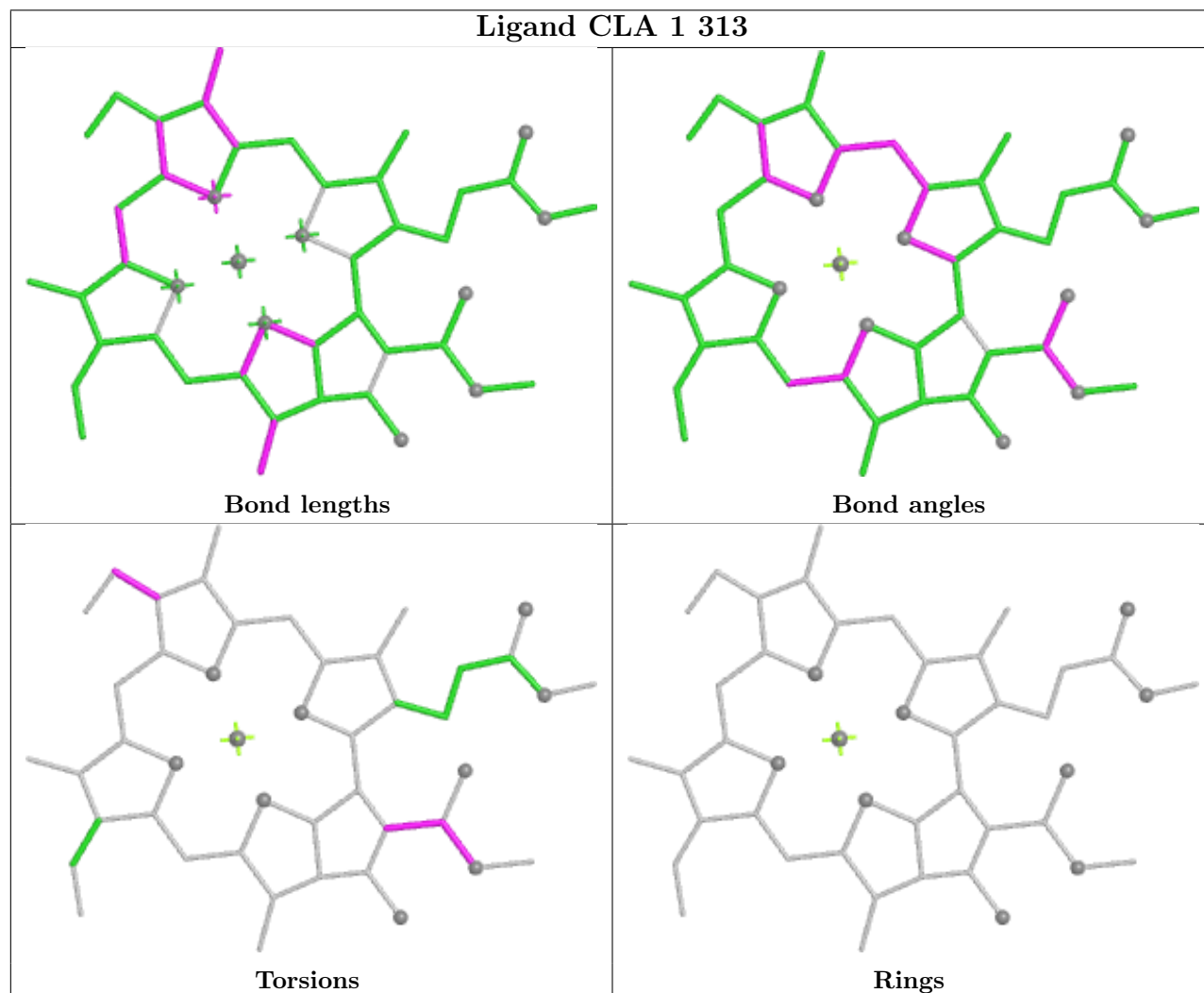
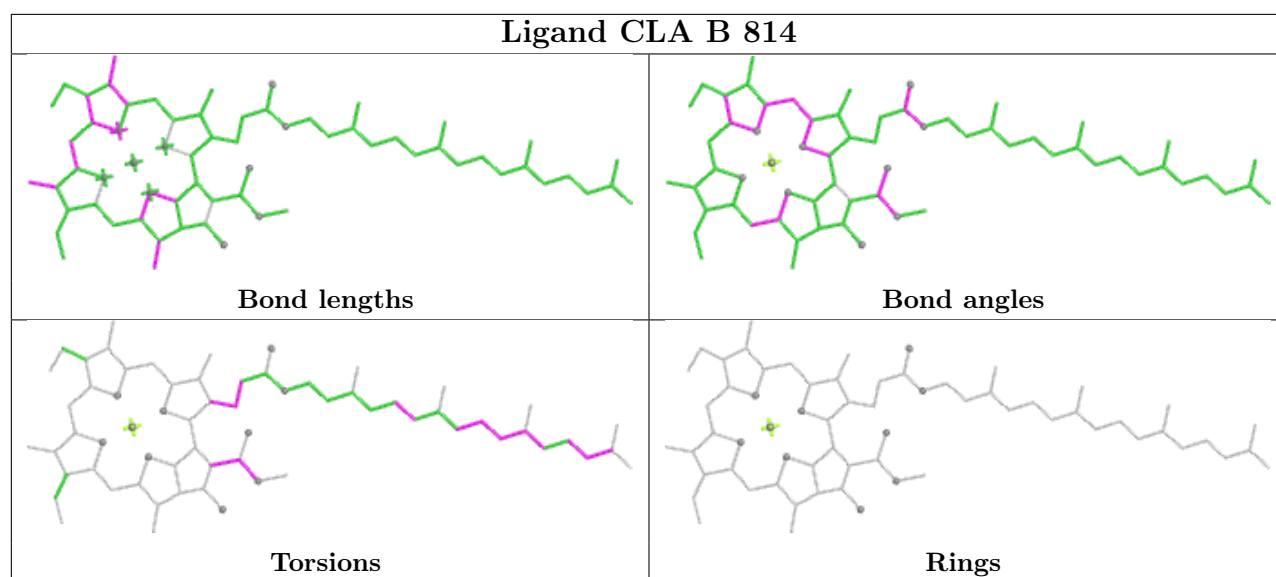
Ligand CLA L 202



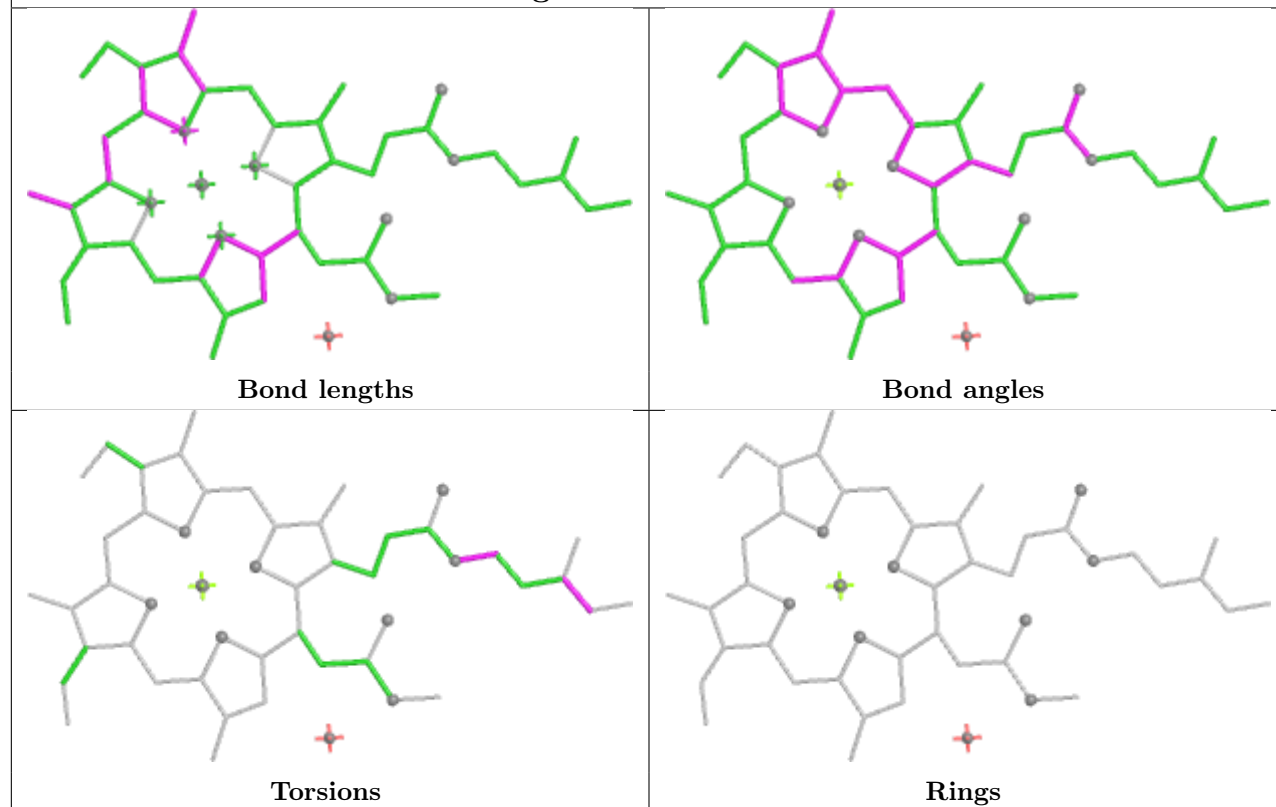
Ligand CLA 7 303



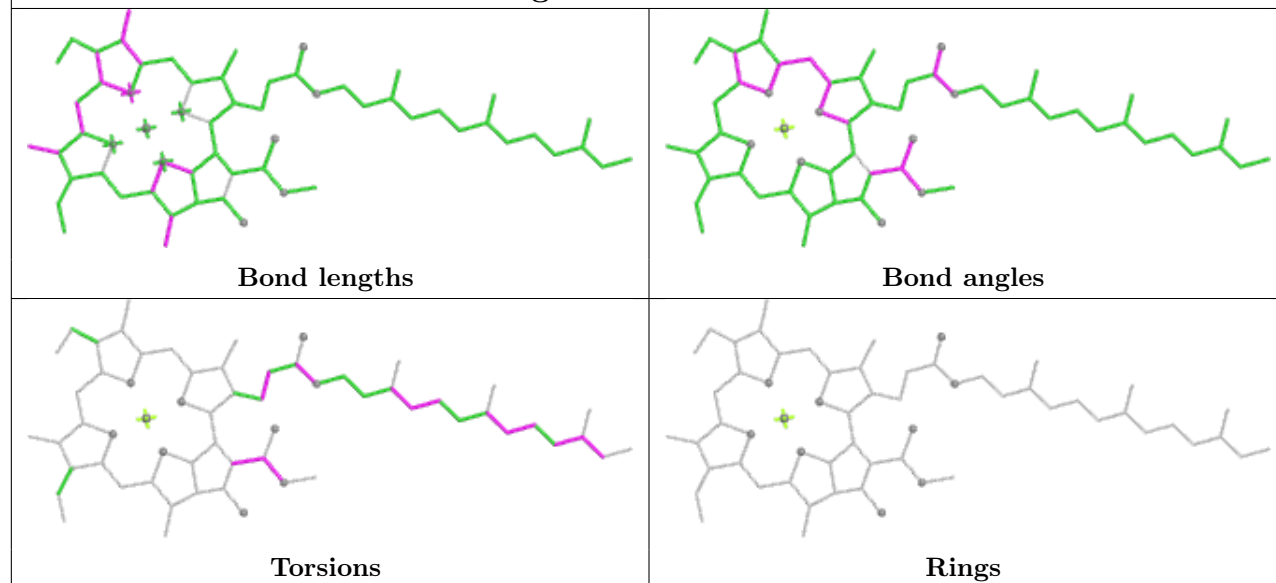


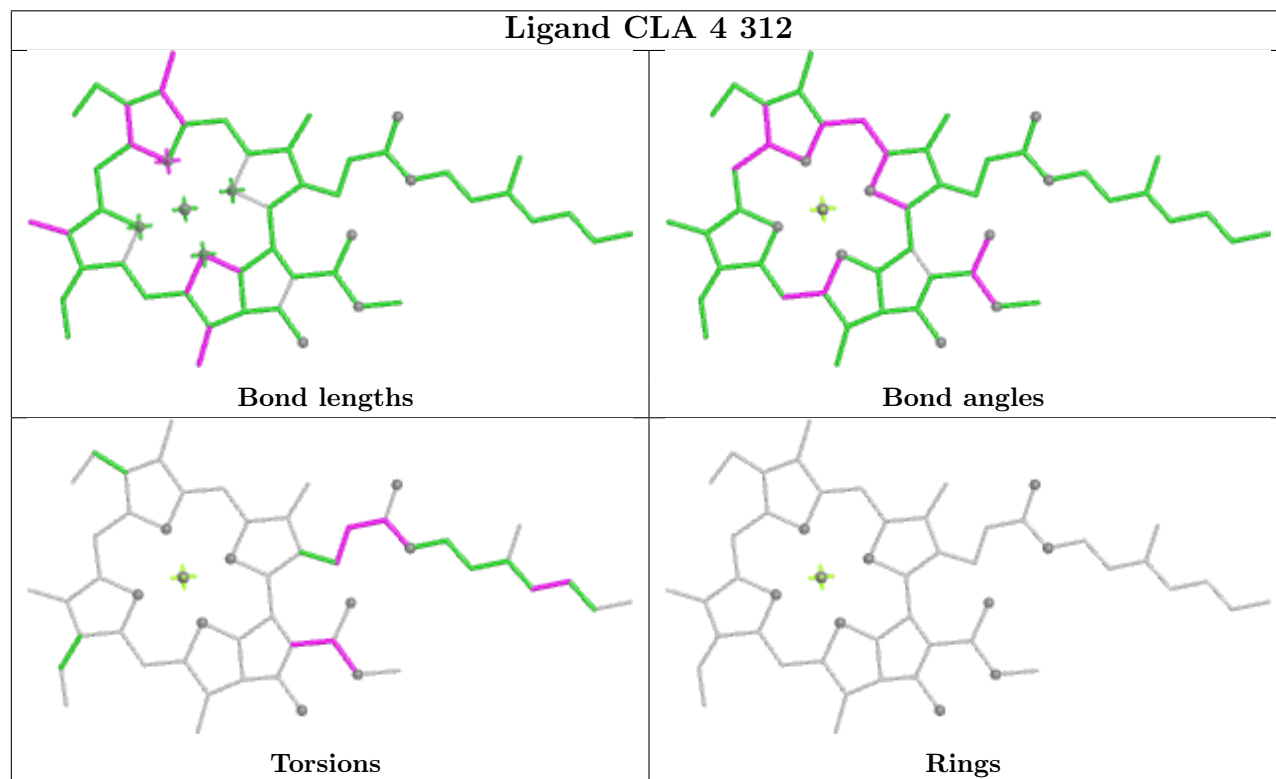
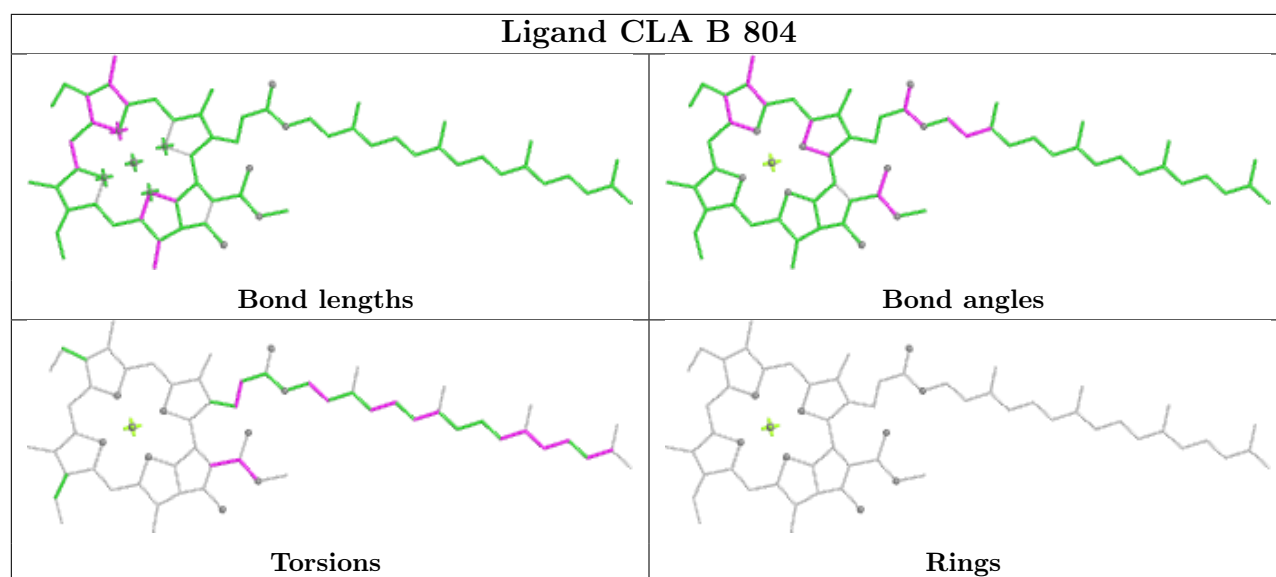


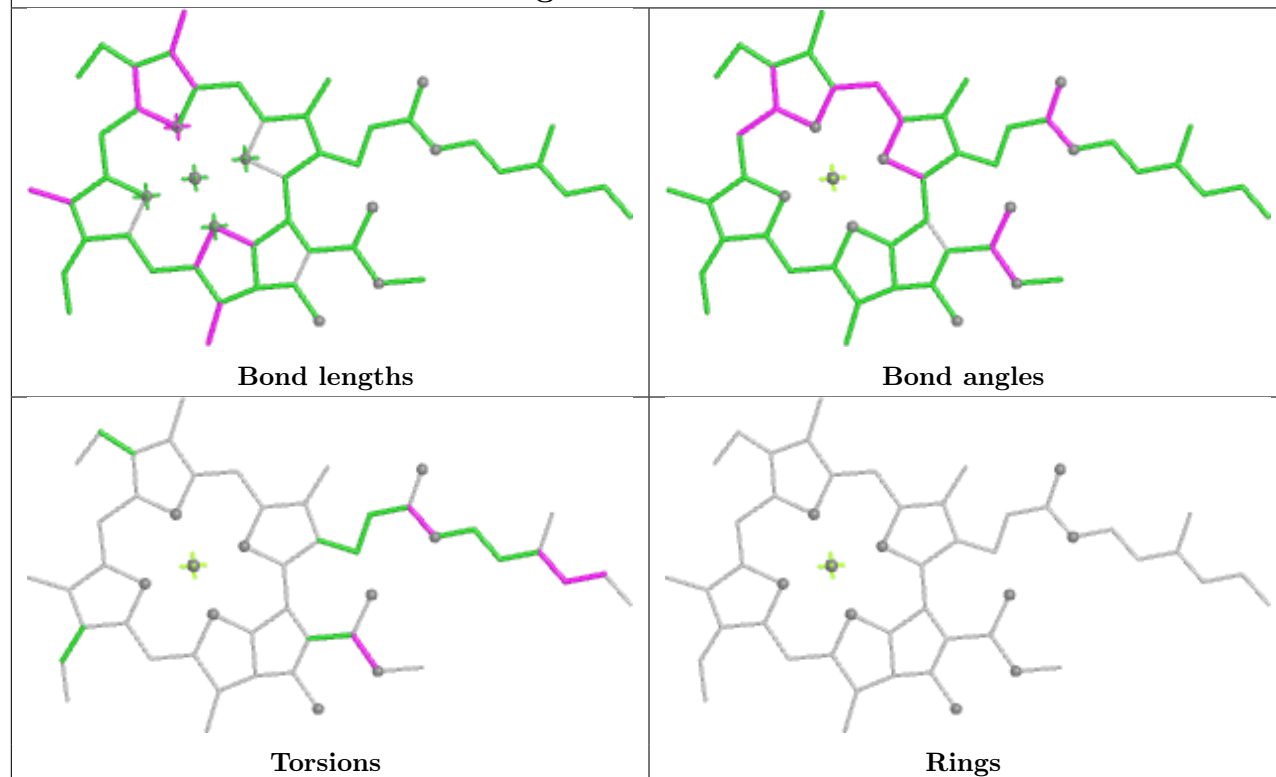
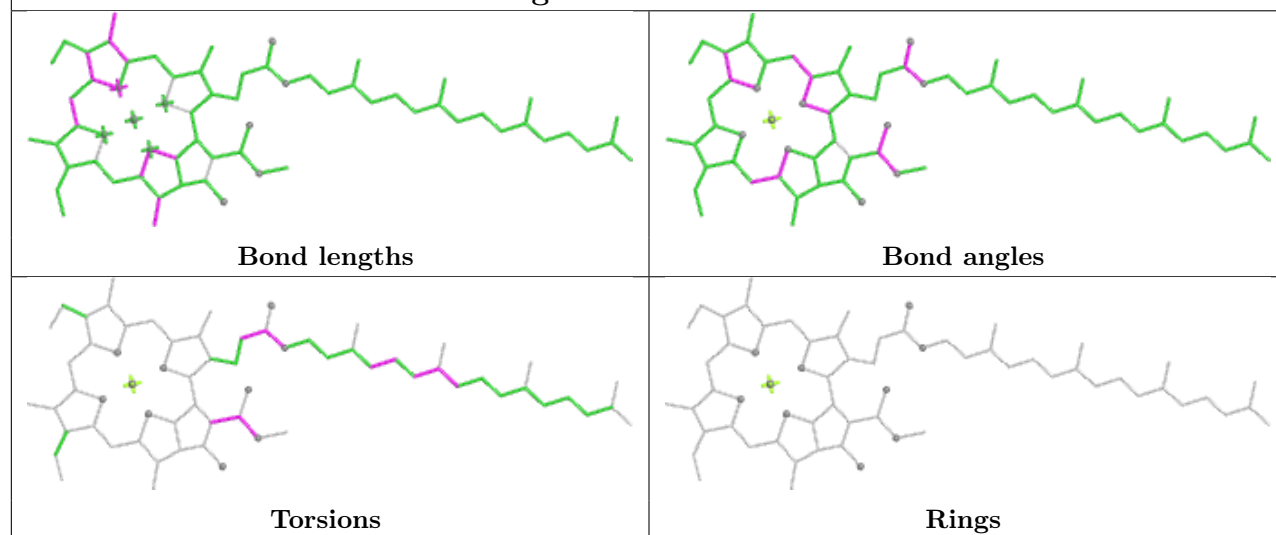
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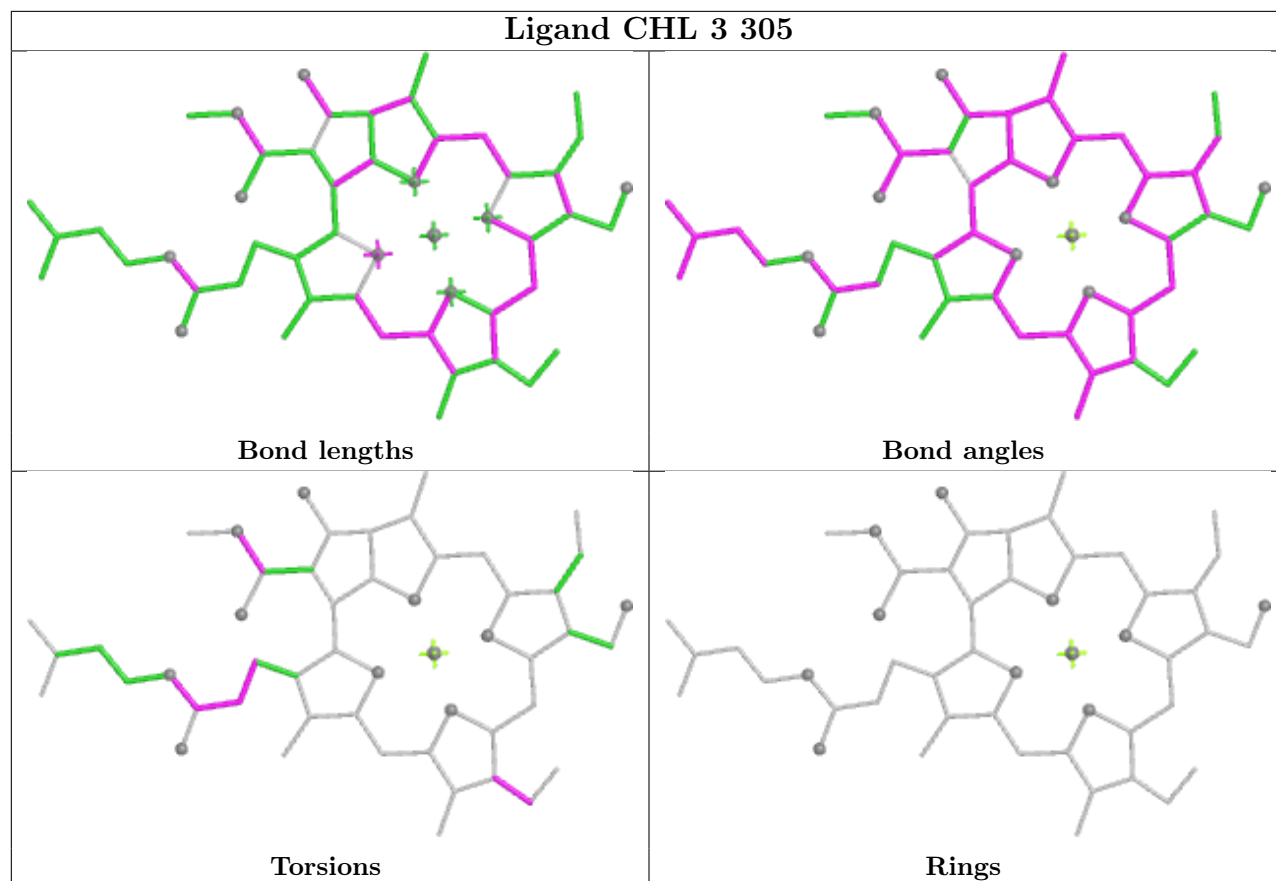
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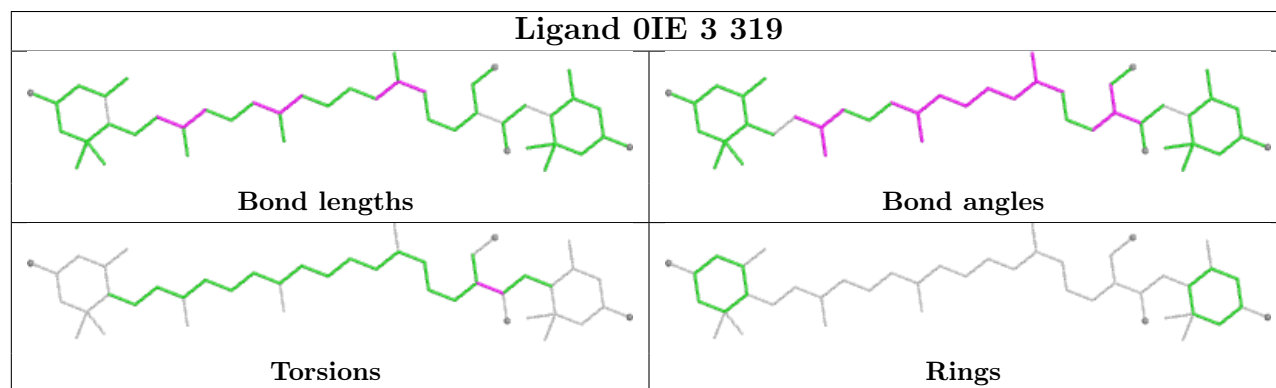


Ligand CLA 6 303**Ligand CLA A 832**

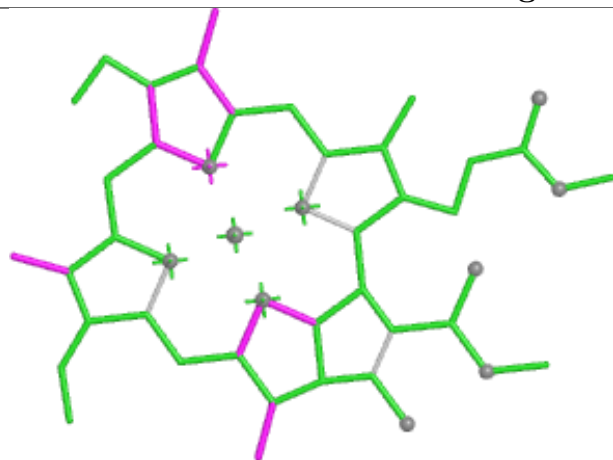
Ligand CHL 3 305



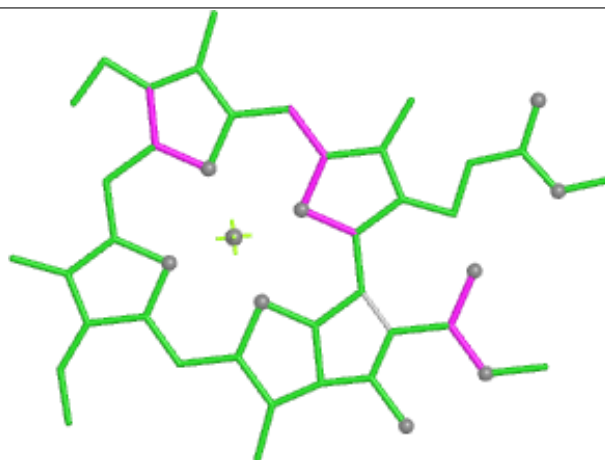
Ligand OIE 3 319



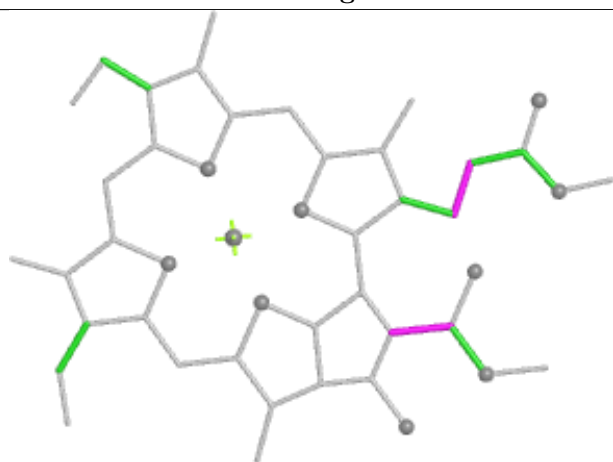
Ligand CLA 0 319



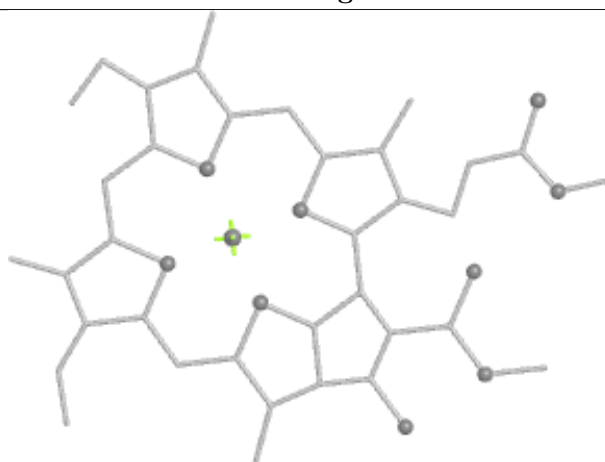
Bond lengths



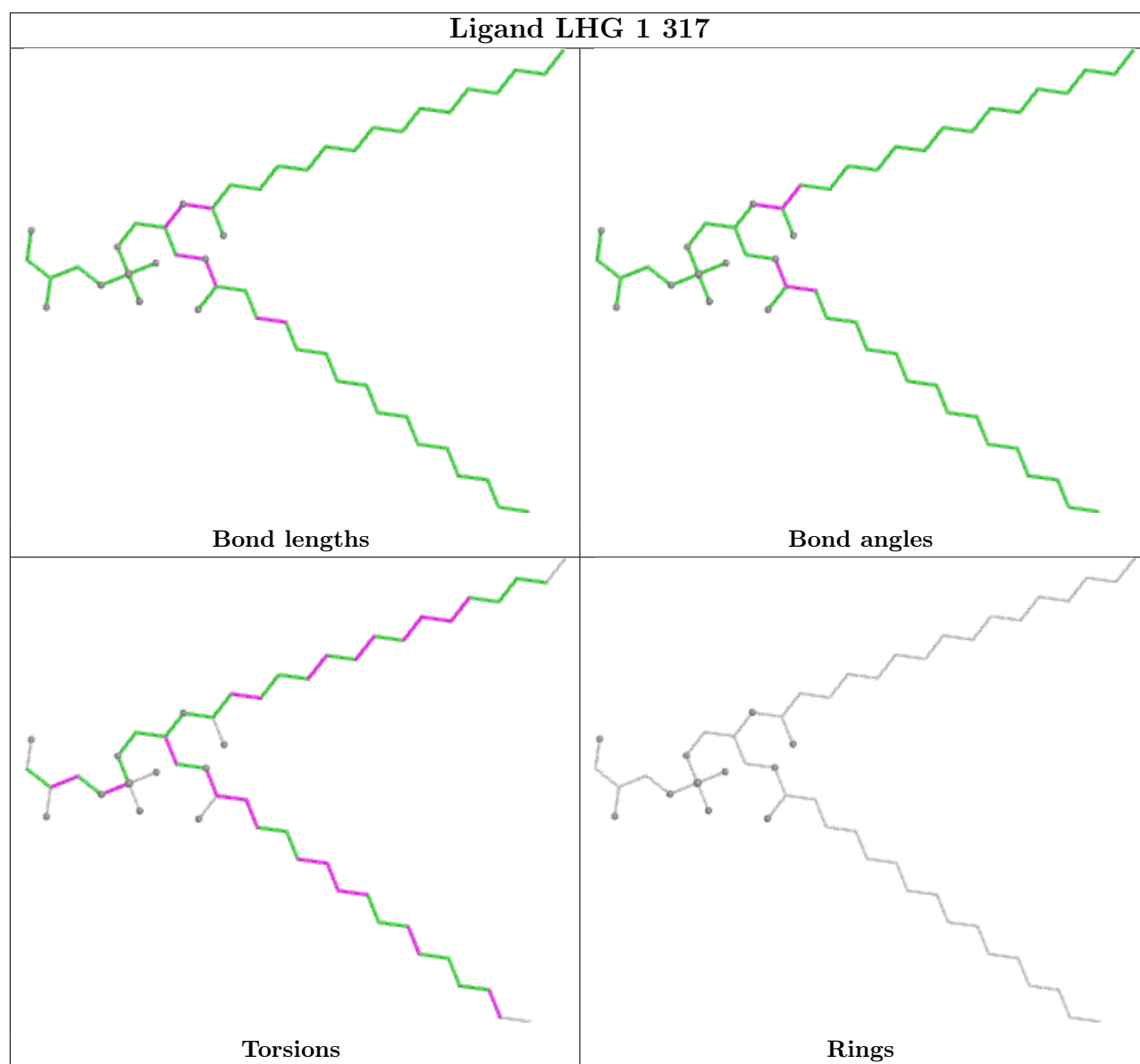
Bond angles



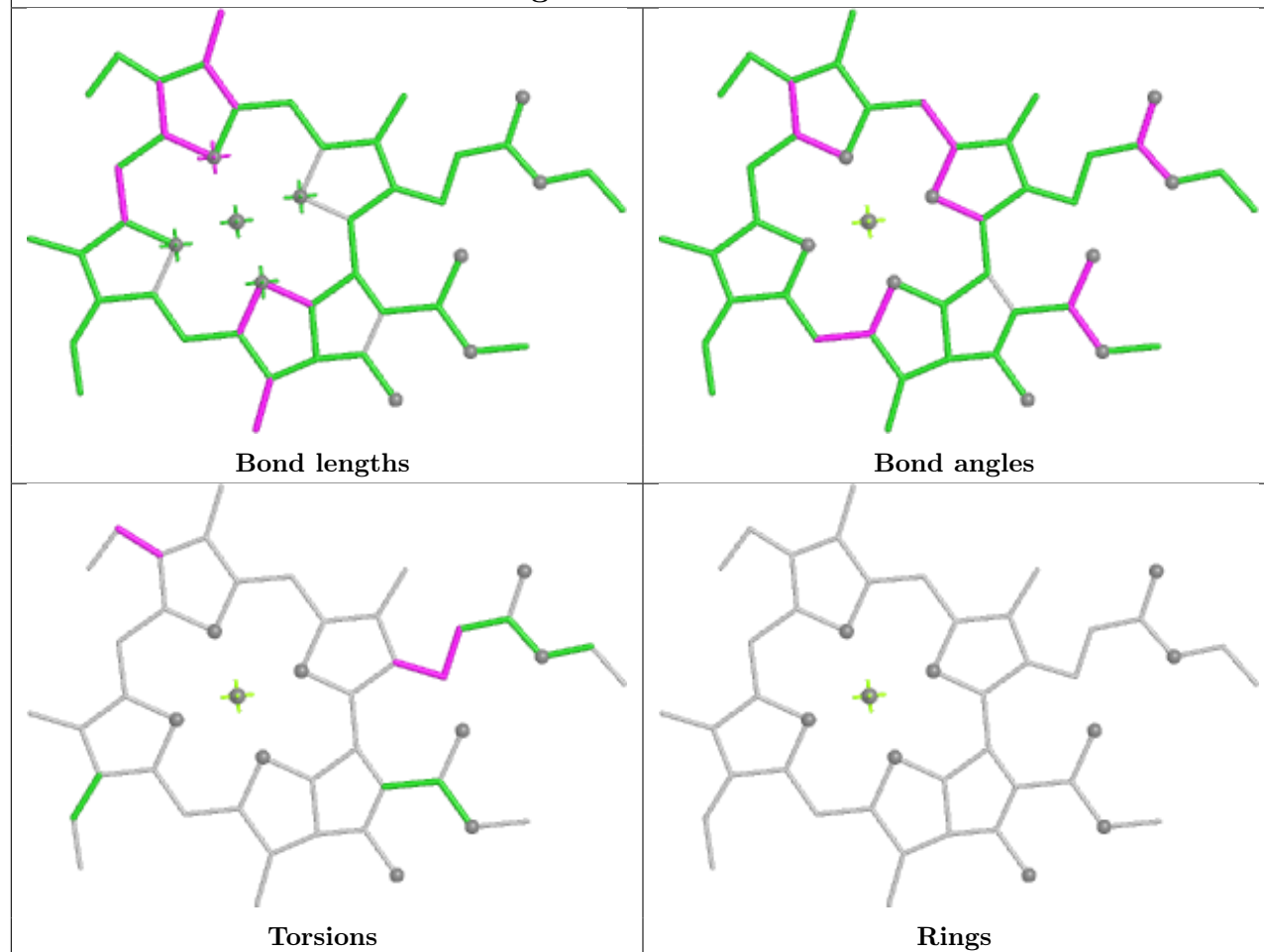
Torsions



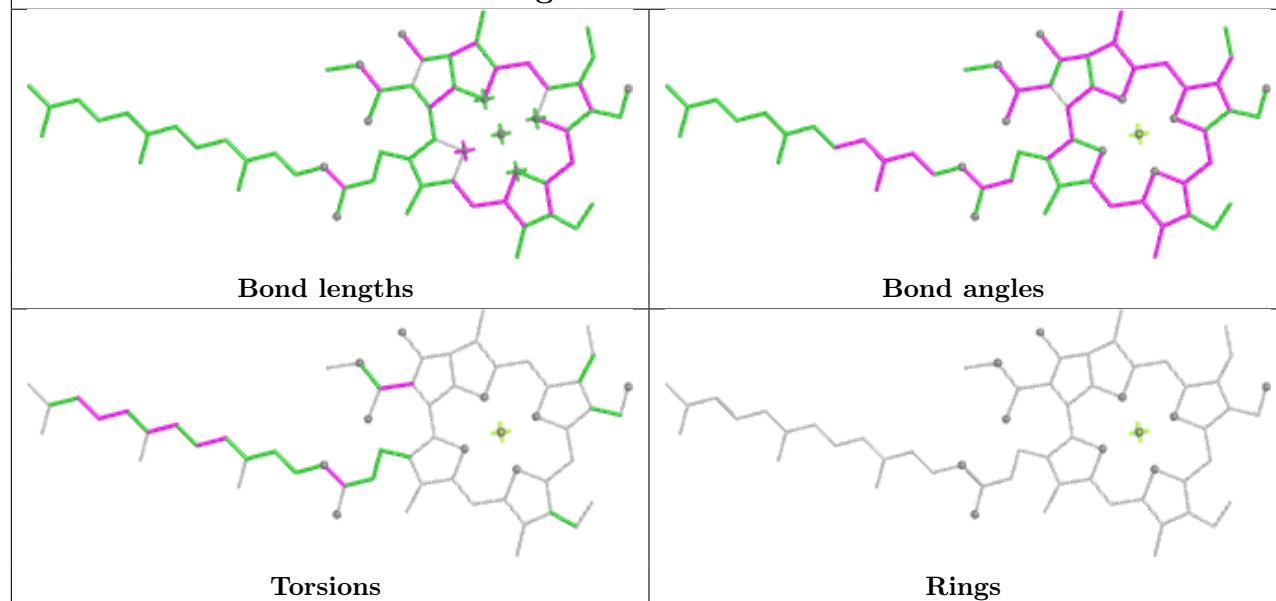
Rings

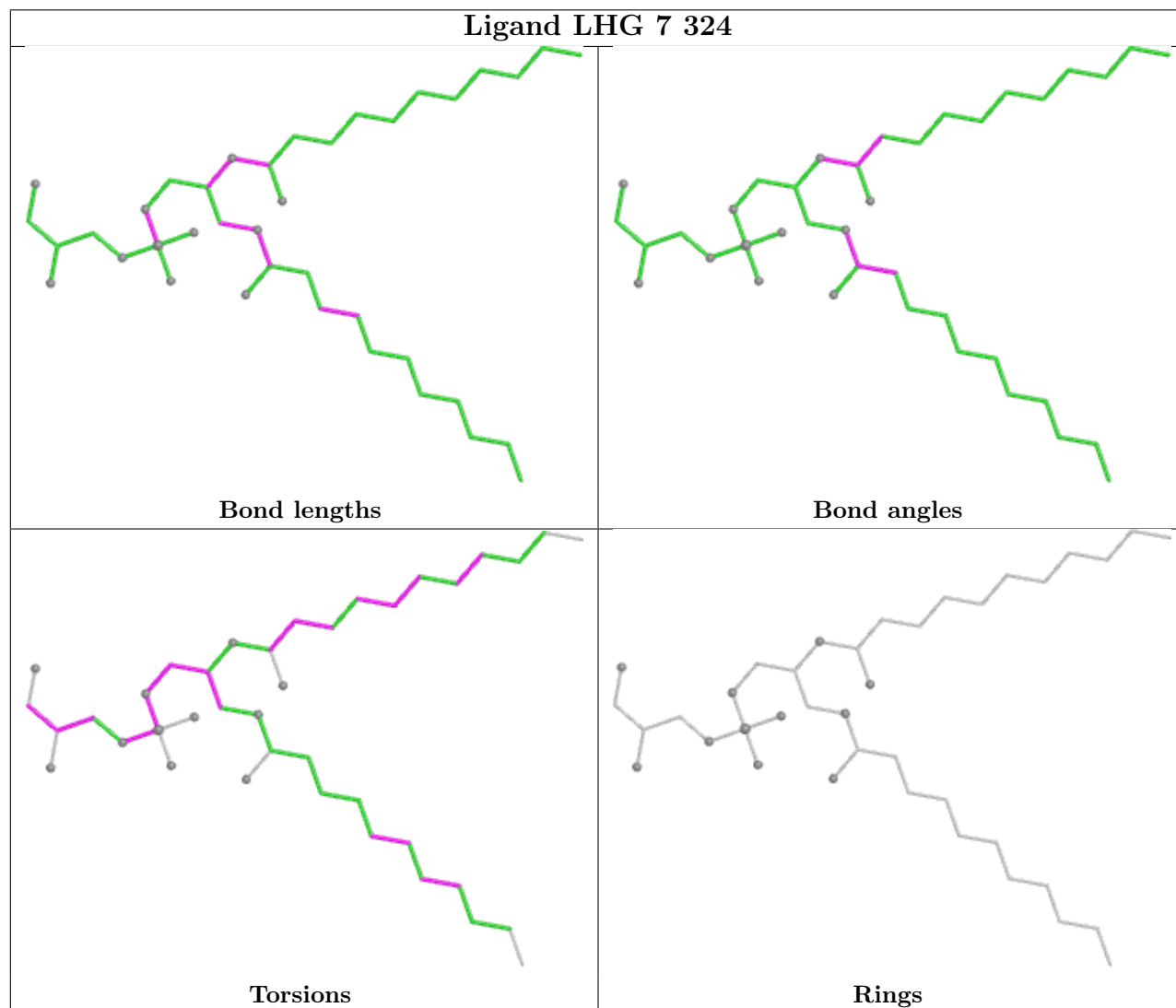
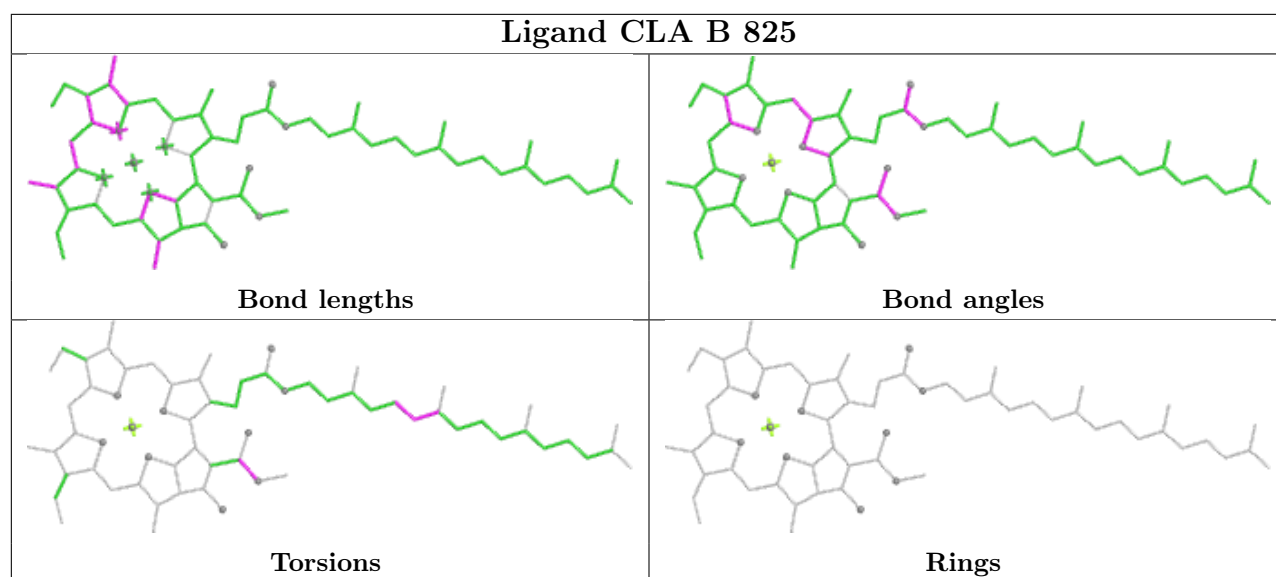


Ligand CLA 3 306

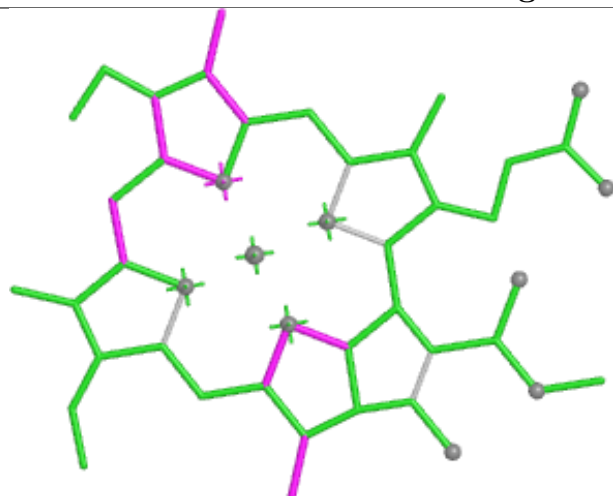


Ligand CHL 3 301

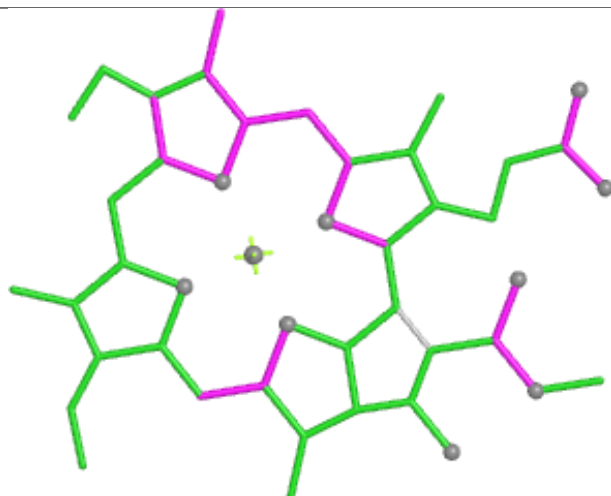




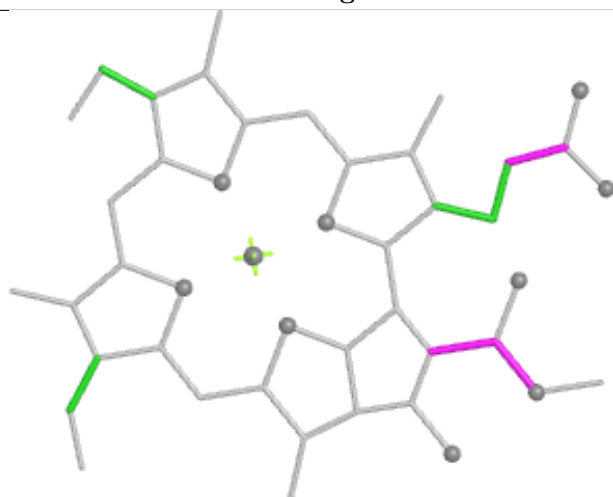
Ligand CLA 4 314



Bond lengths



Bond angles

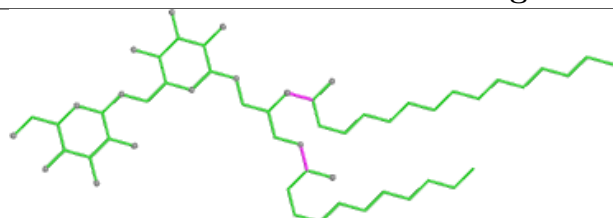


Torsions

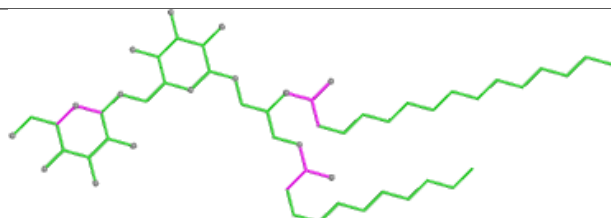


Rings

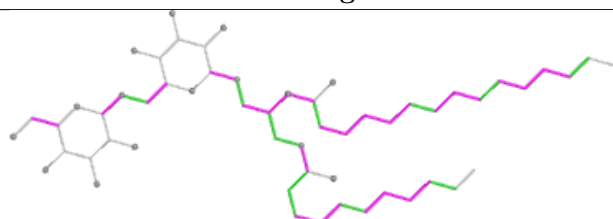
Ligand DGD B 849



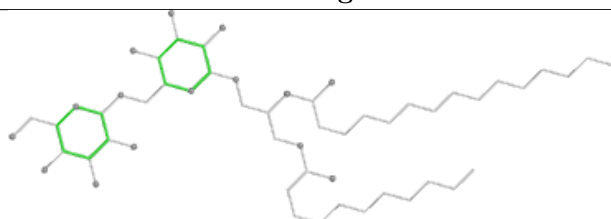
Bond lengths



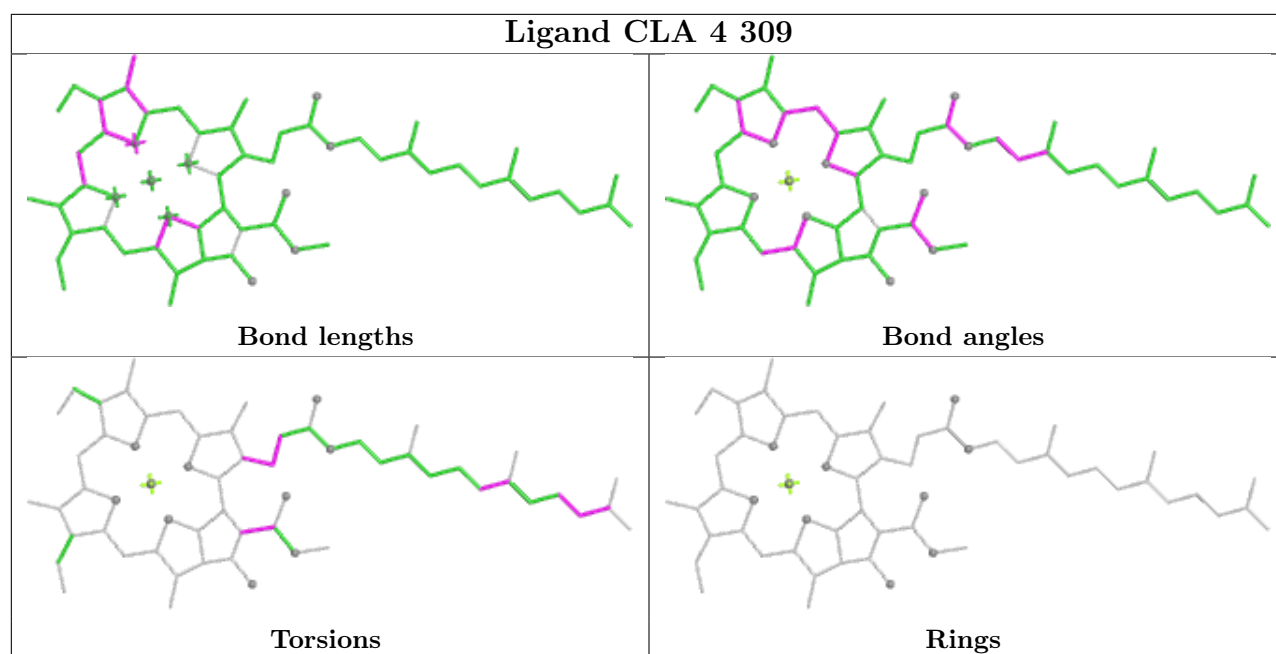
Bond angles

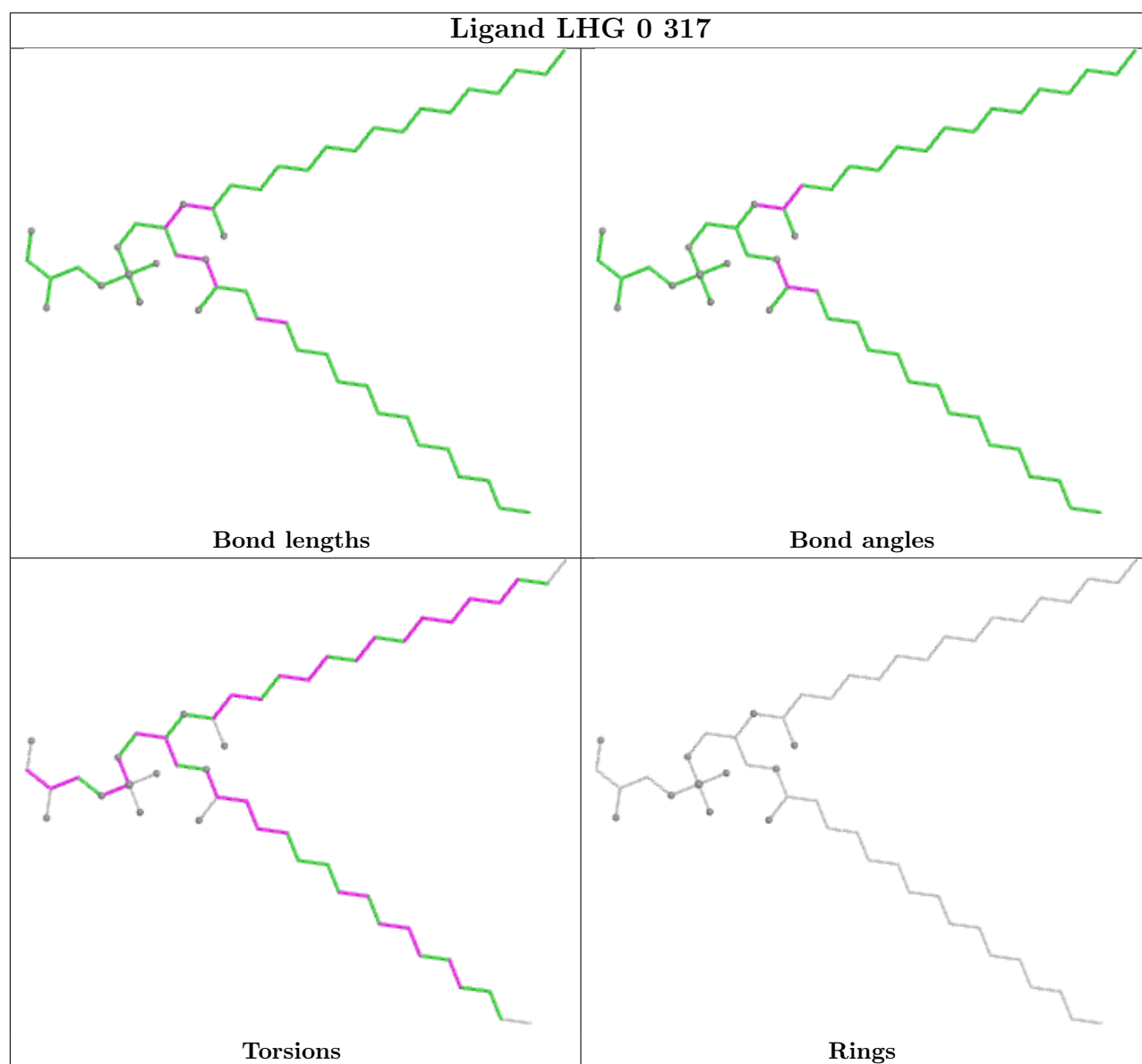


Torsions

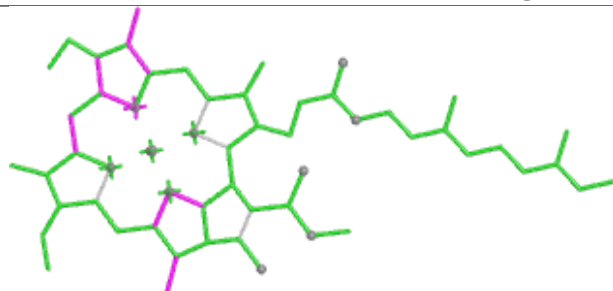


Rings

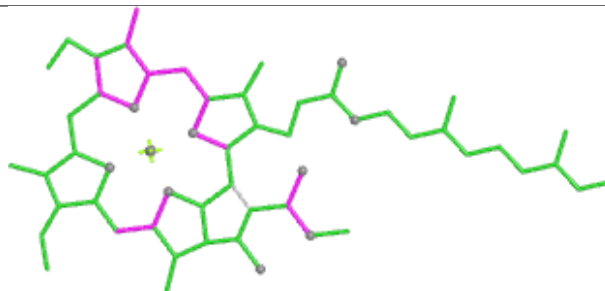




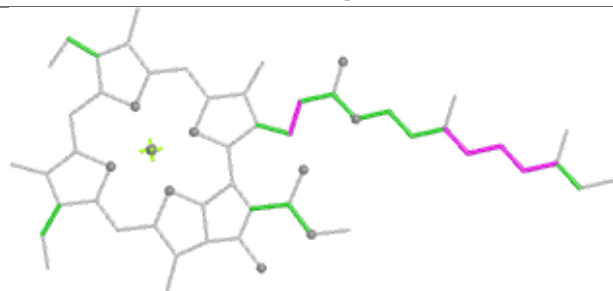
Ligand CLA 9 311



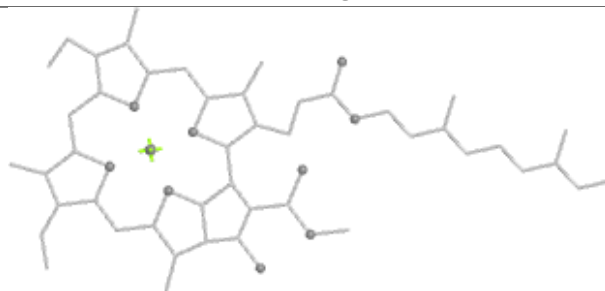
Bond lengths



Bond angles

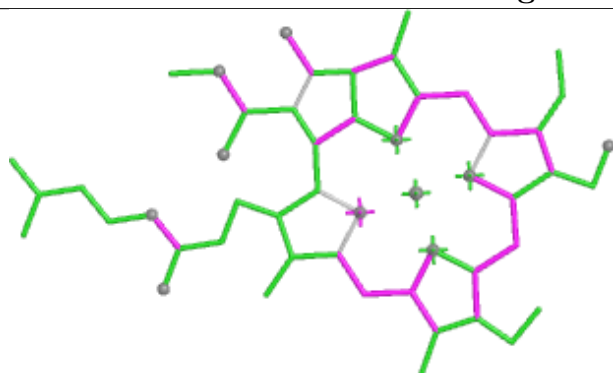


Torsions

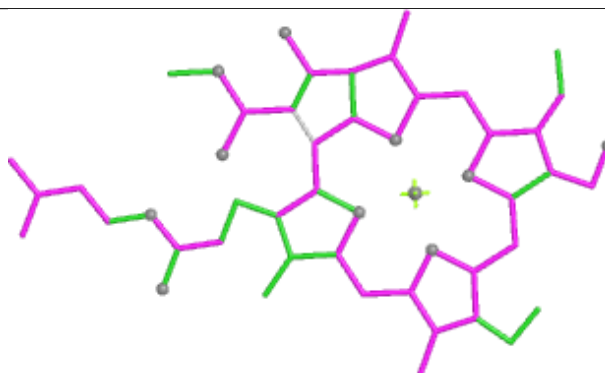


Rings

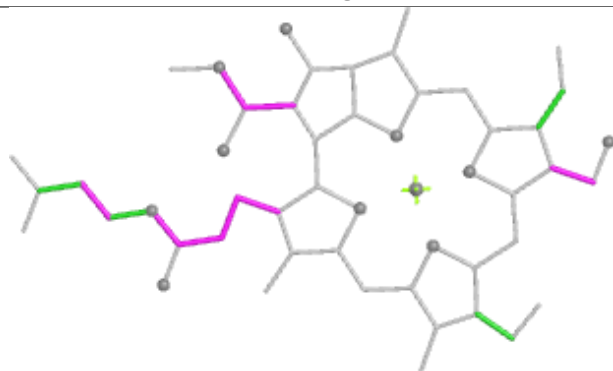
Ligand CHL 8 307



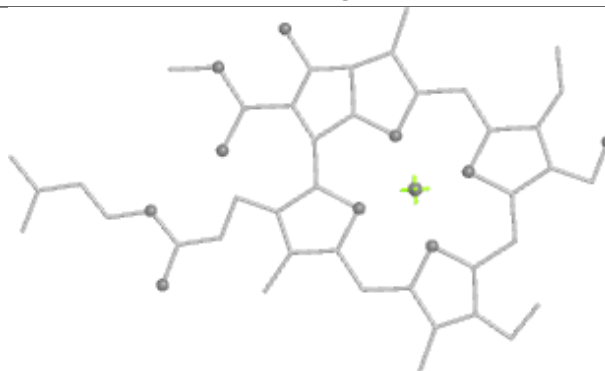
Bond lengths



Bond angles

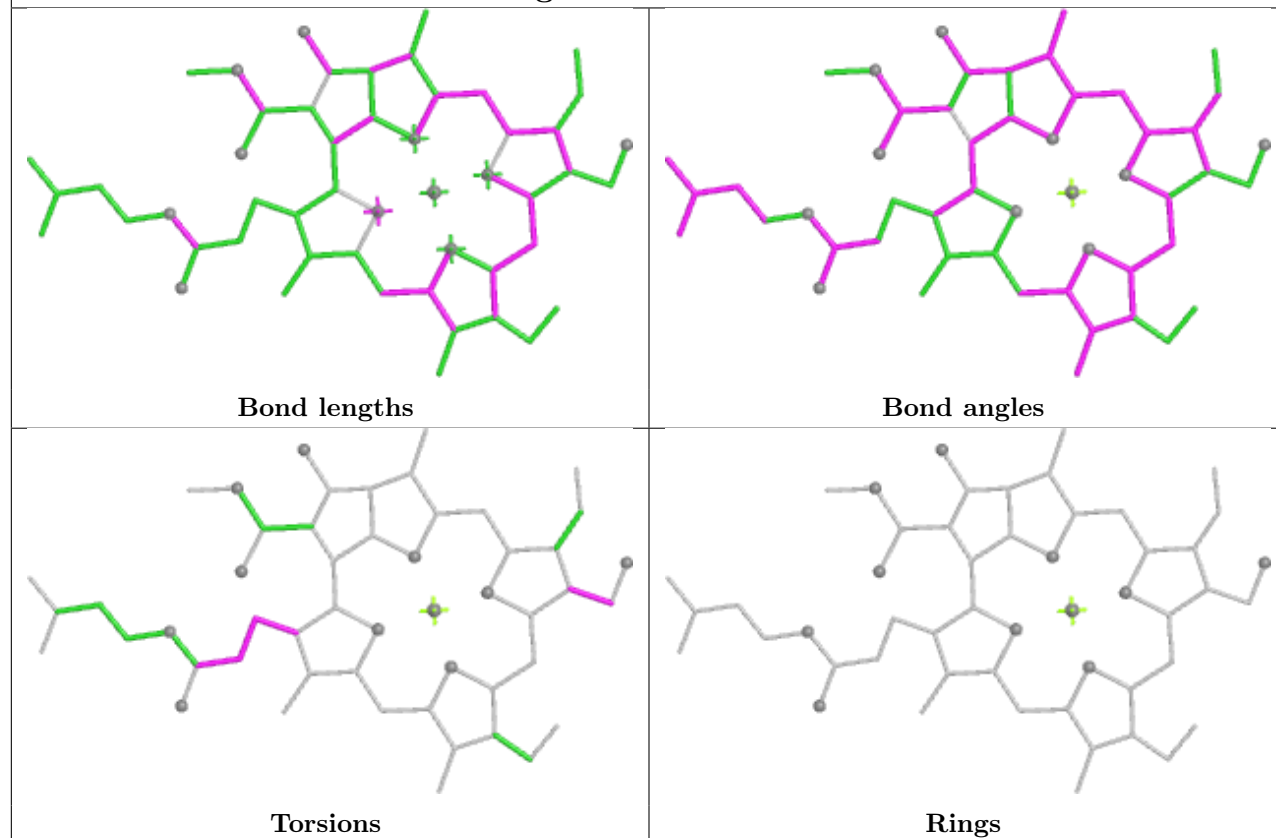


Torsions

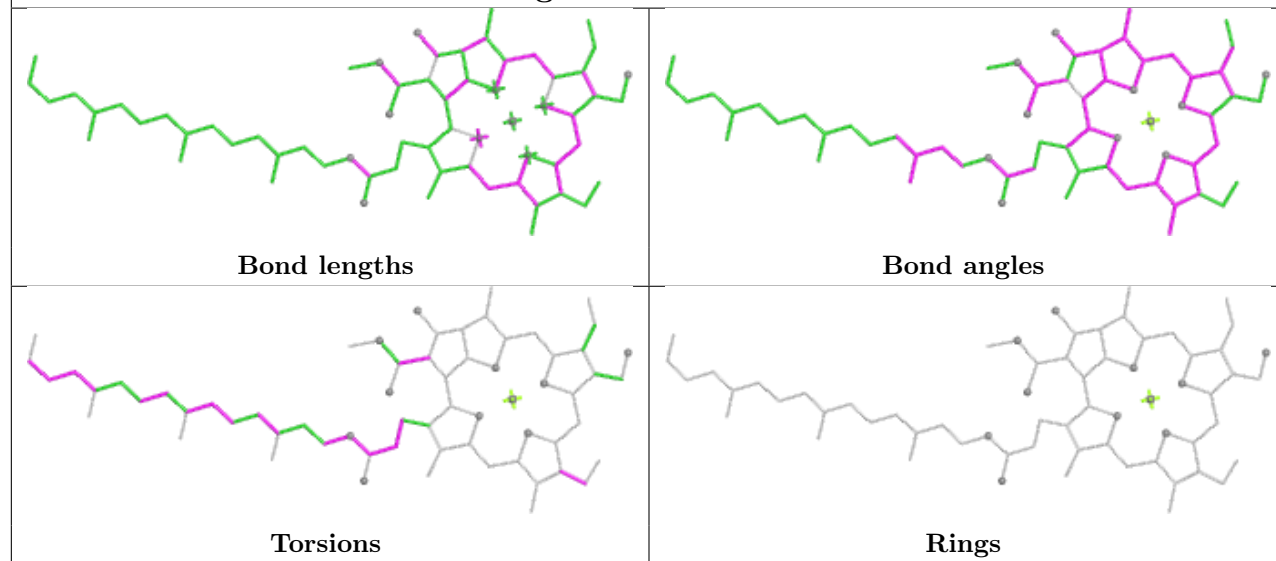


Rings

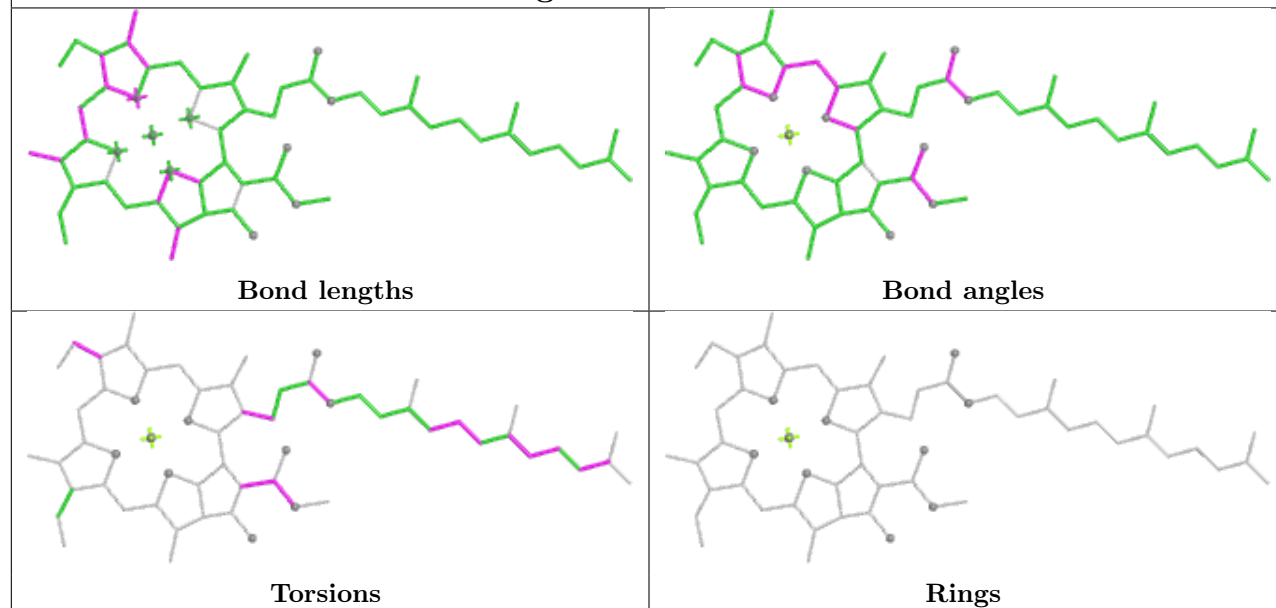
Ligand CHL 0 305



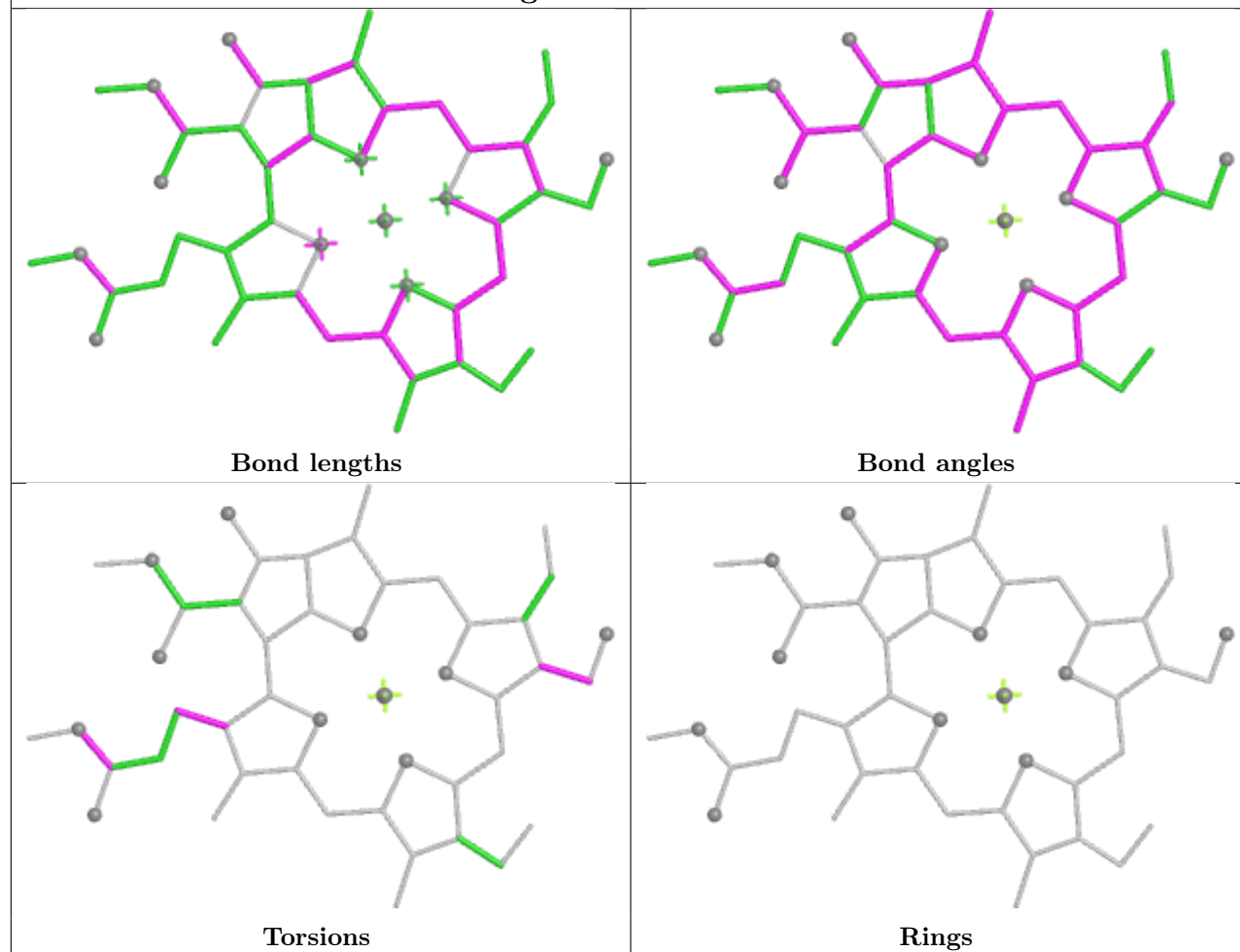
Ligand CHL 7 302



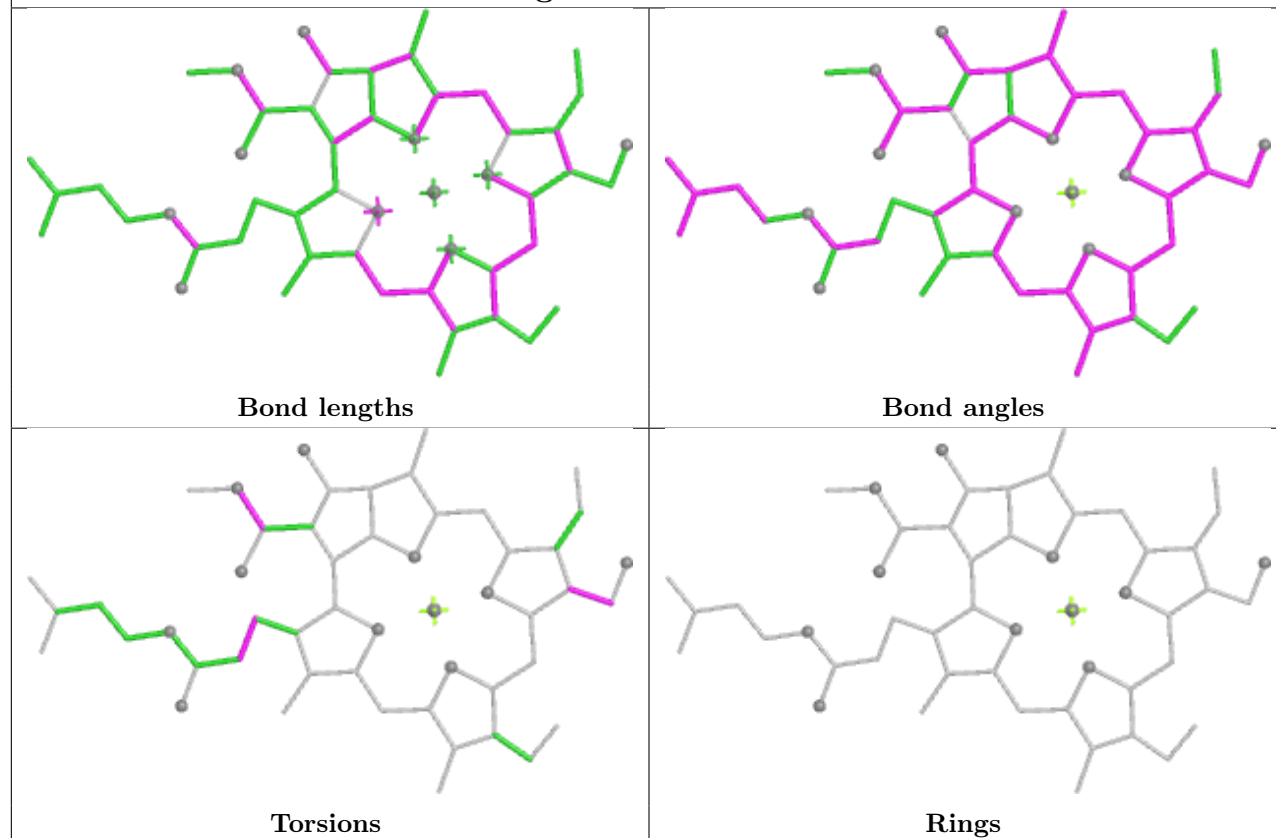
Ligand CLA 4 310



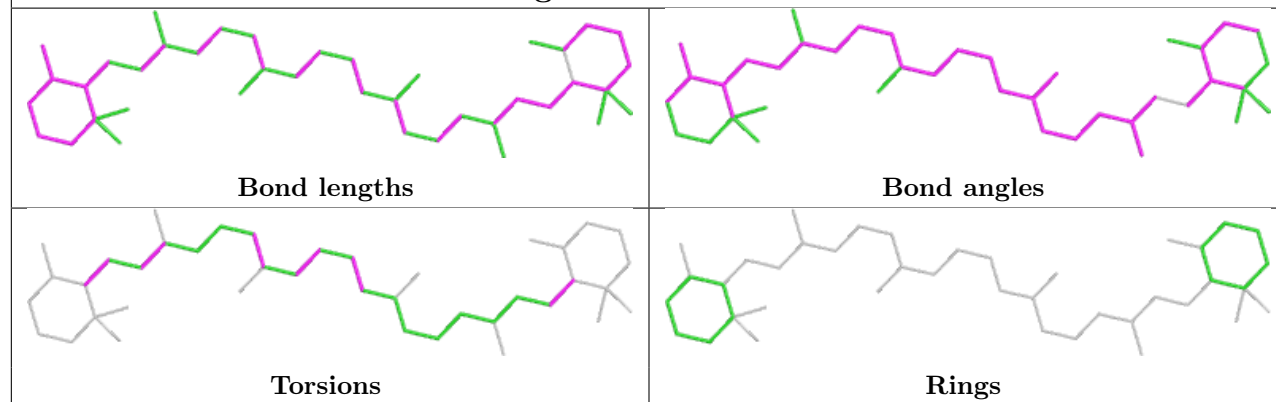
Ligand CHL 4 308

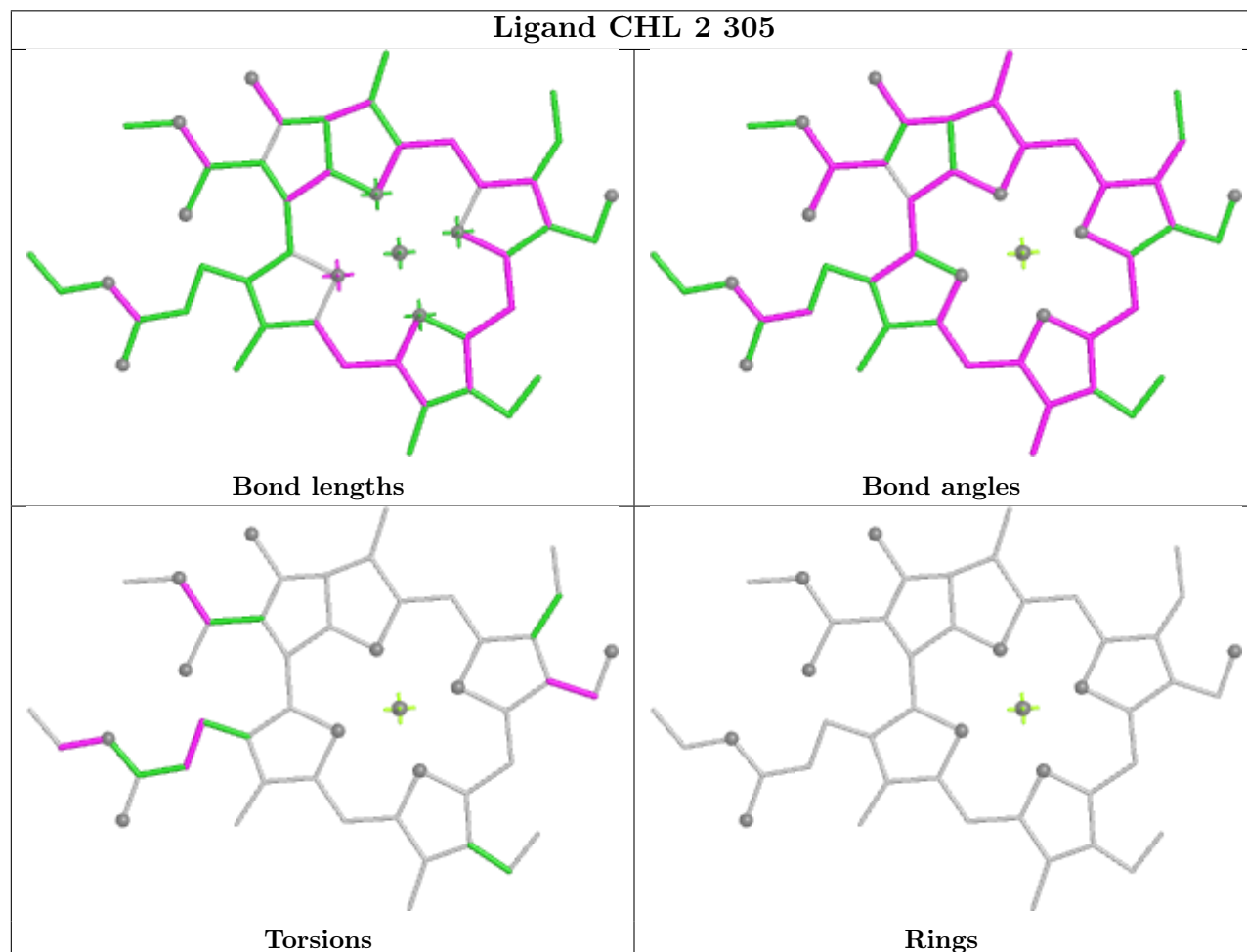
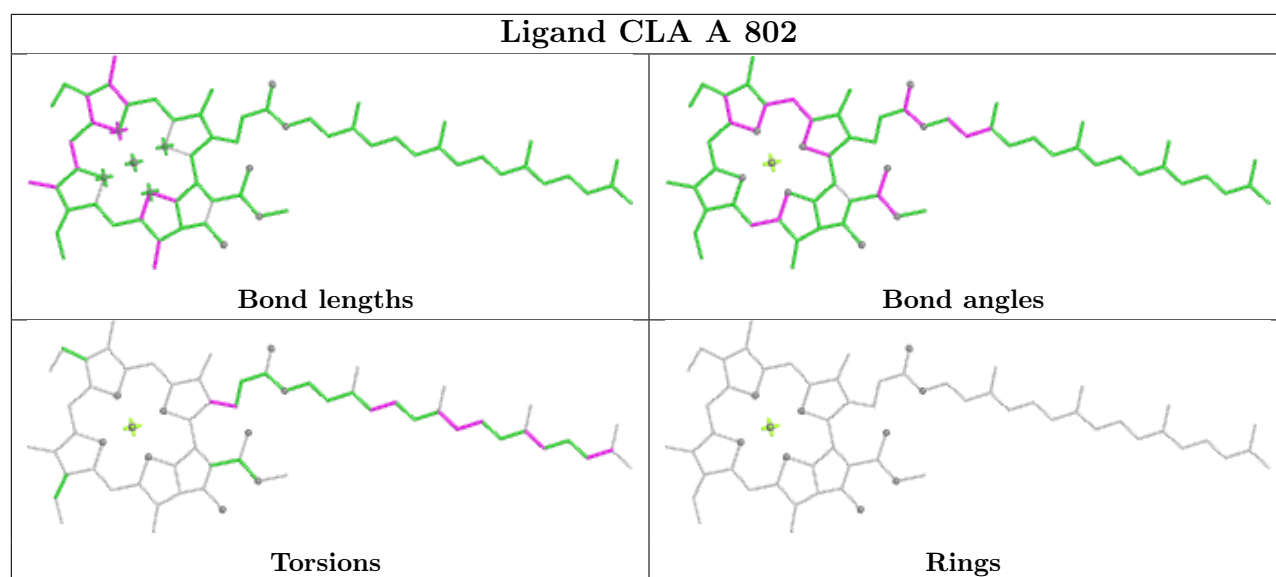


Ligand CHL 4 313

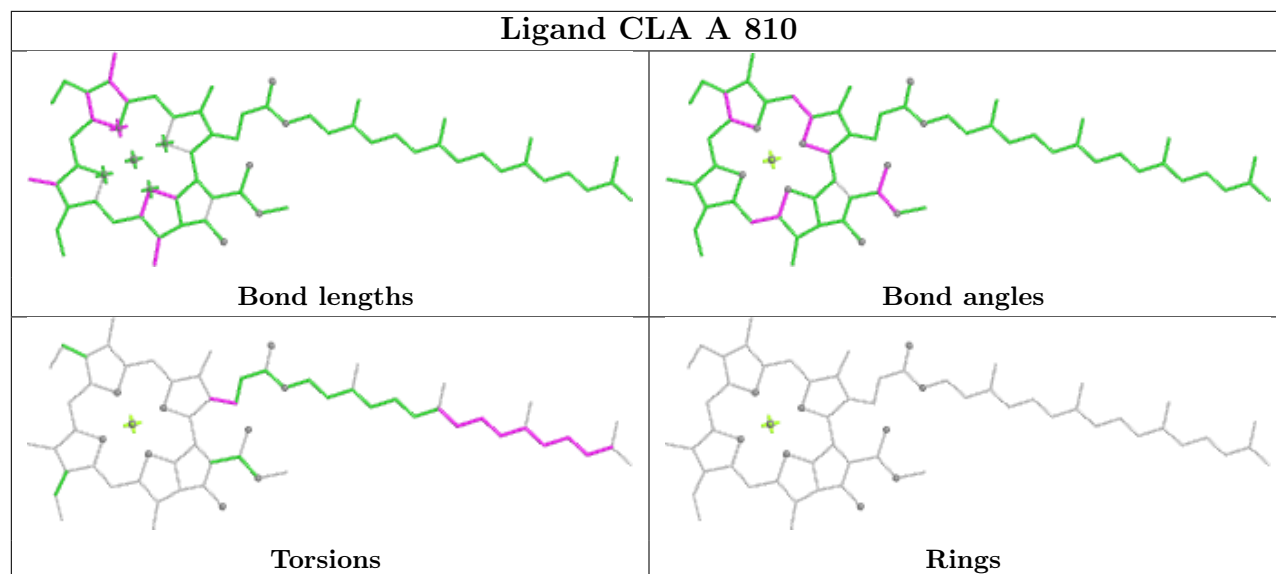


Ligand 8CT A 846

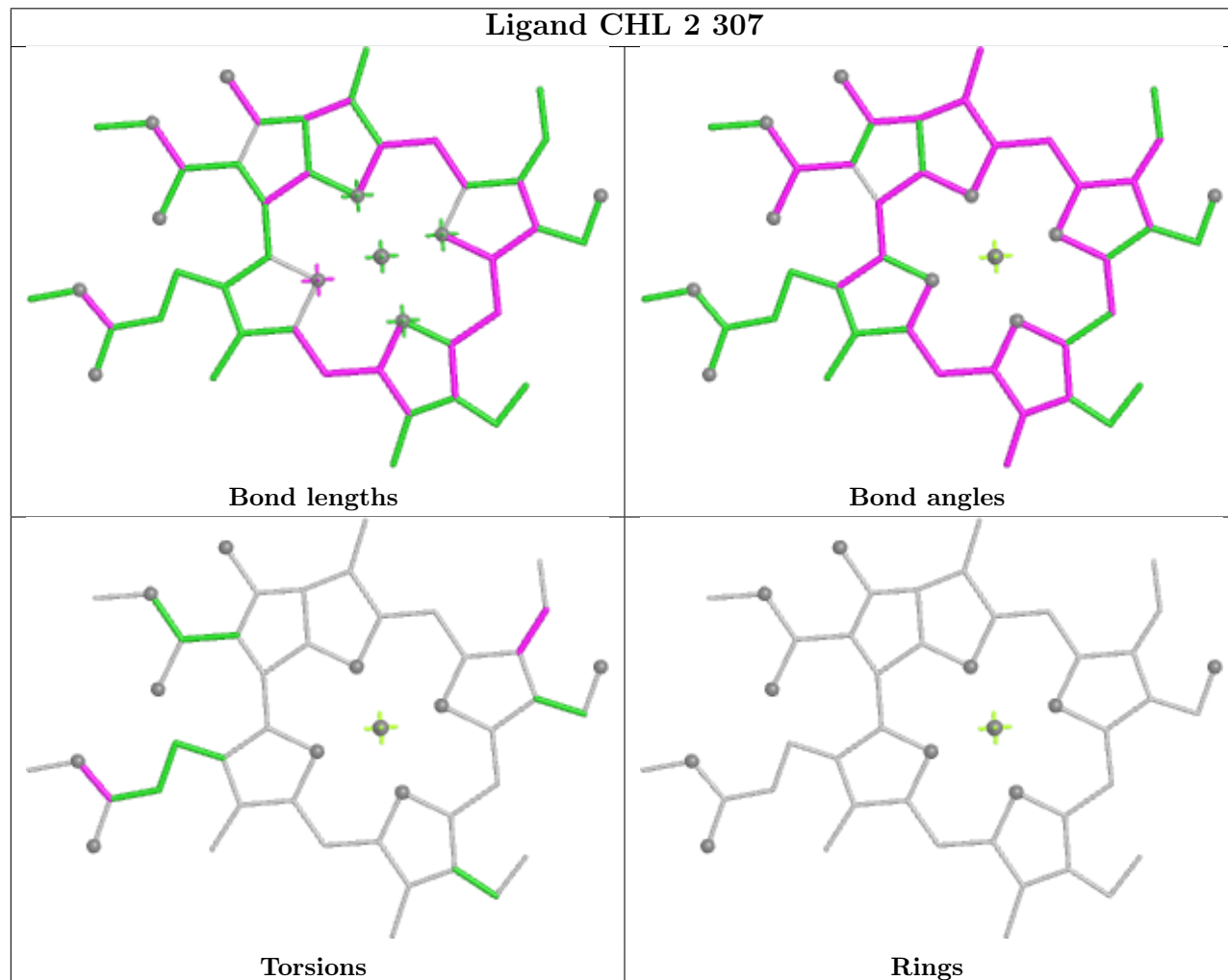




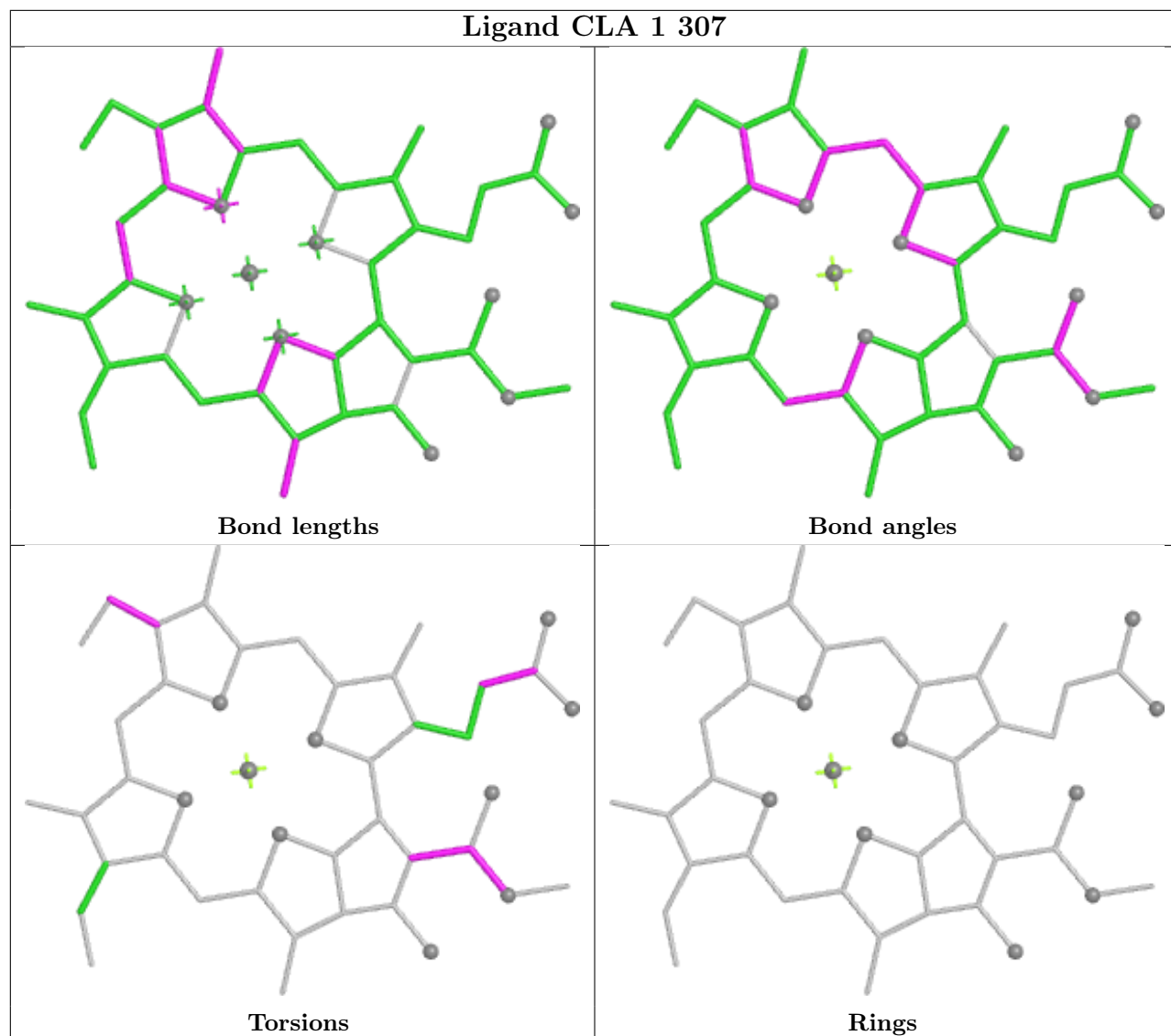
Ligand CLA A 810



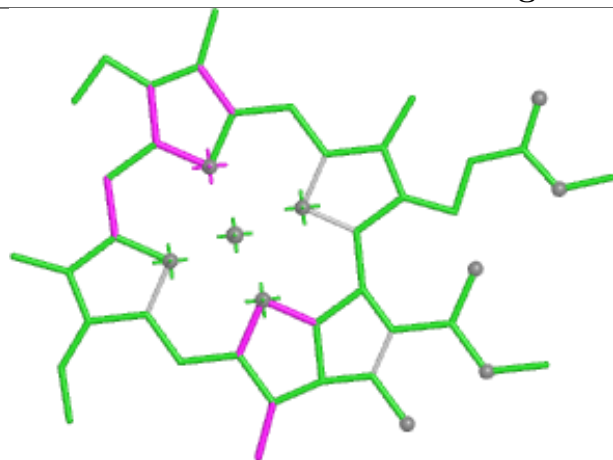
Ligand CHL 2 307



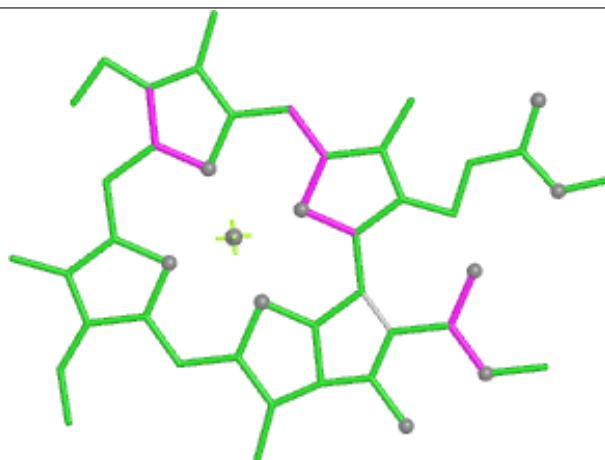
Ligand CLA 1 307



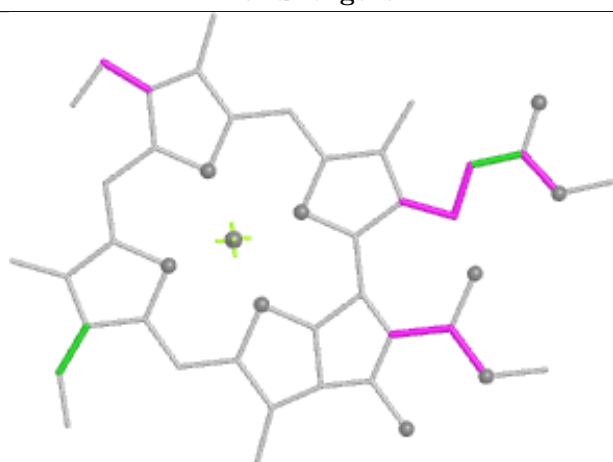
Ligand CLA 5 313



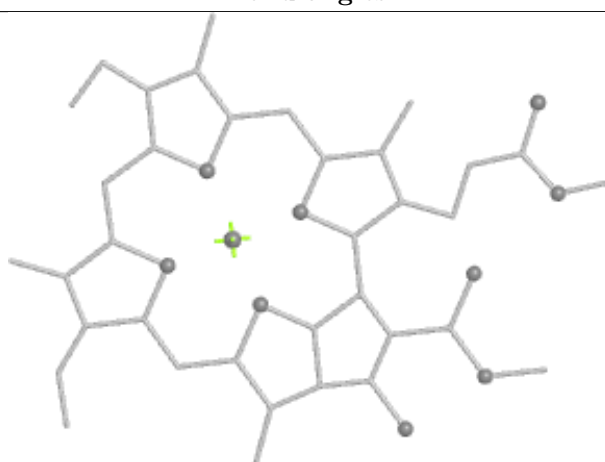
Bond lengths



Bond angles

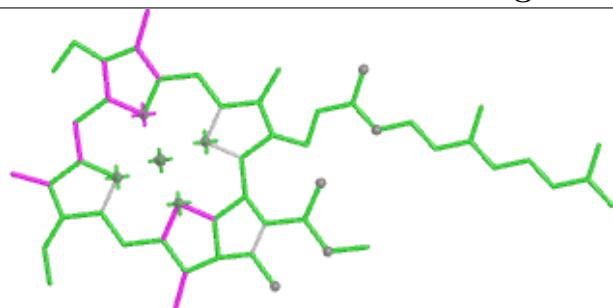


Torsions

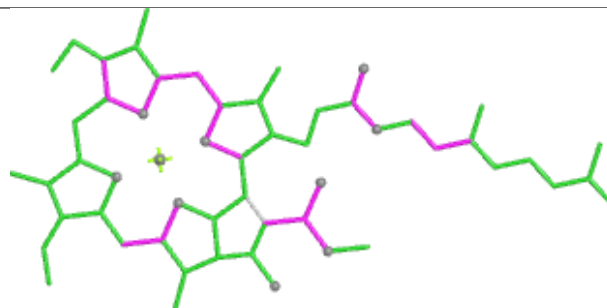


Rings

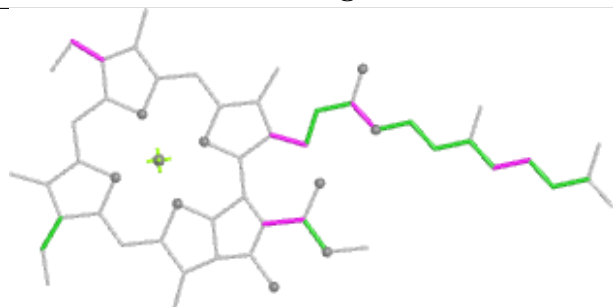
Ligand CLA B 833



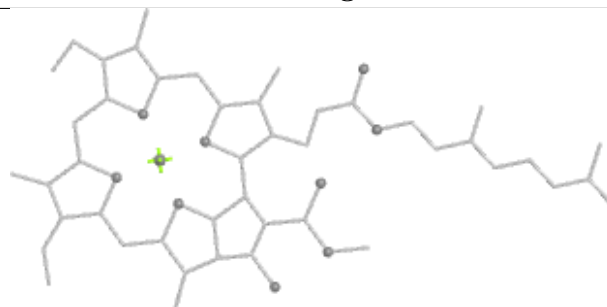
Bond lengths



Bond angles

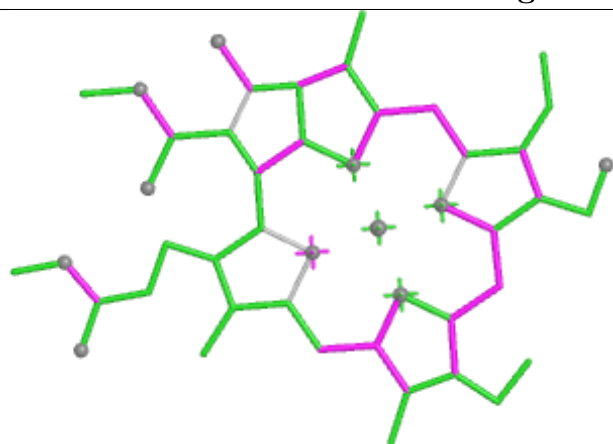


Torsions

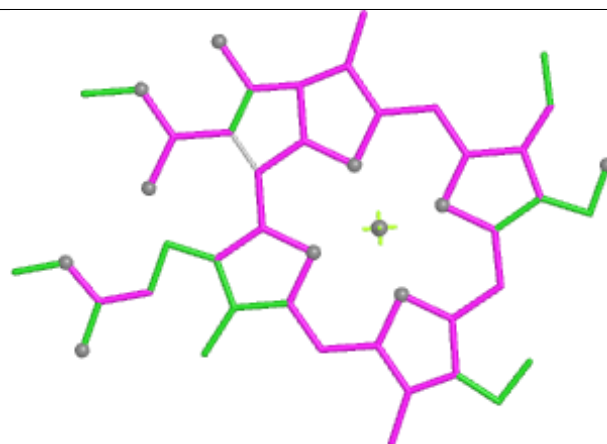


Rings

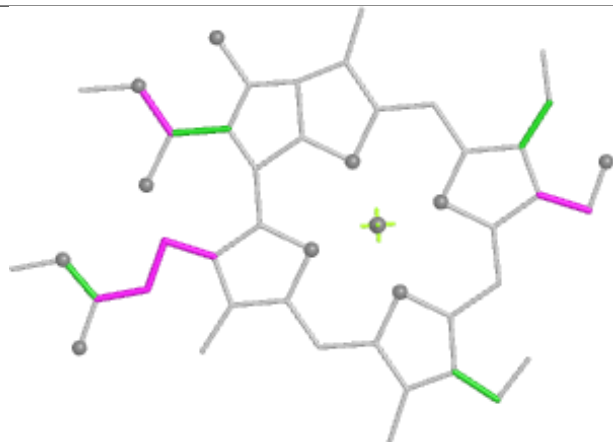
Ligand CHL 9 312



Bond lengths



Bond angles

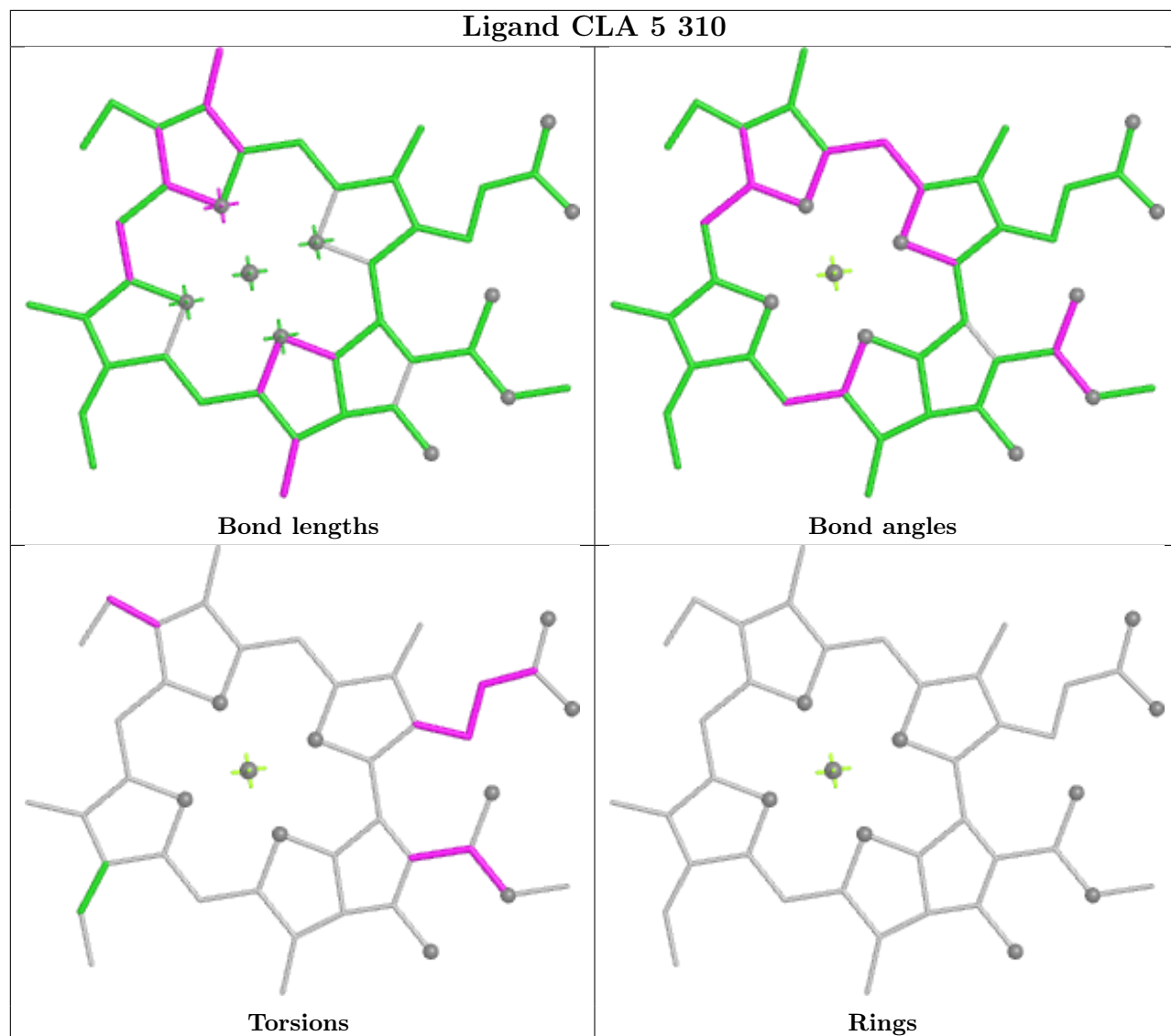


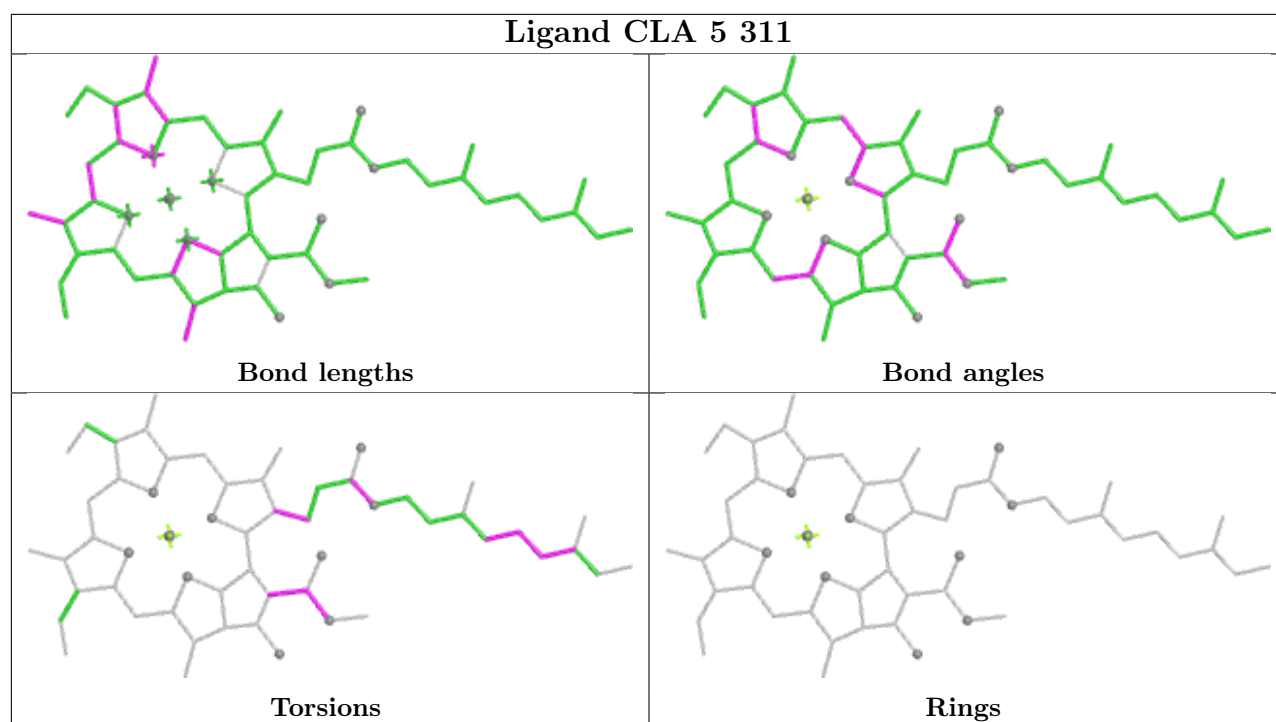
Torsions

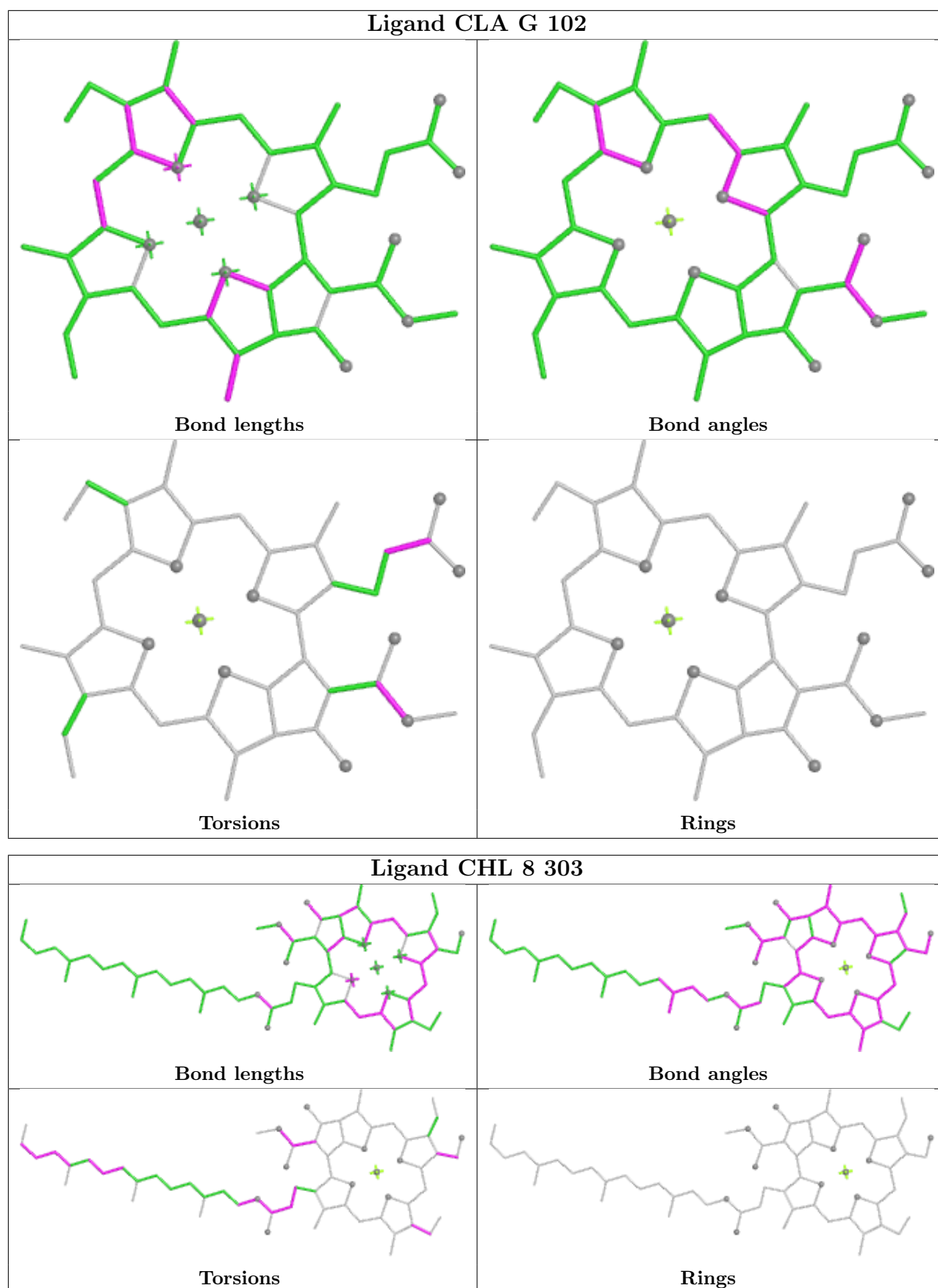


Rings

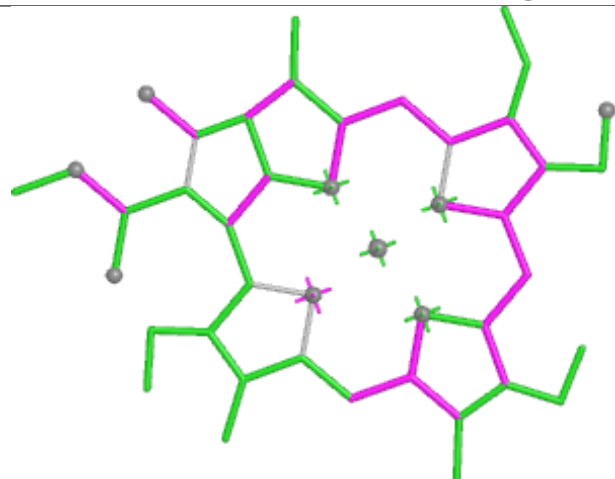
Ligand CLA 5 310



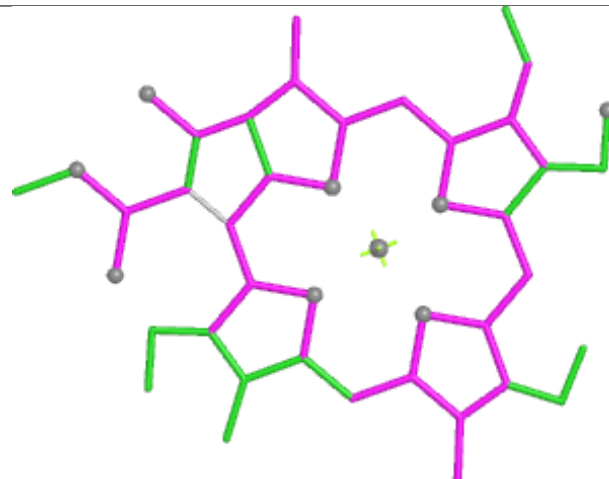




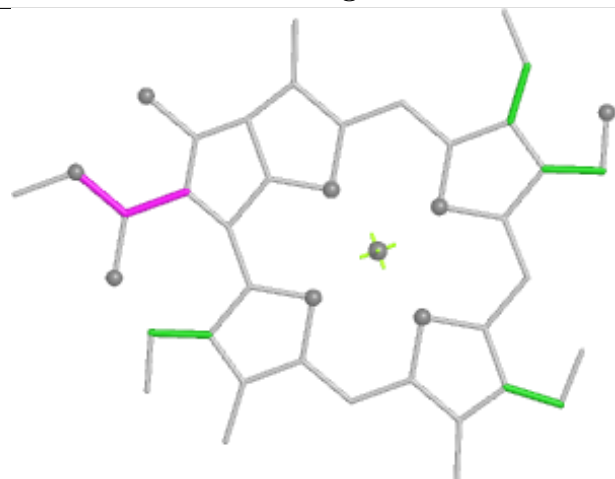
Ligand CHL 8 316



Bond lengths



Bond angles

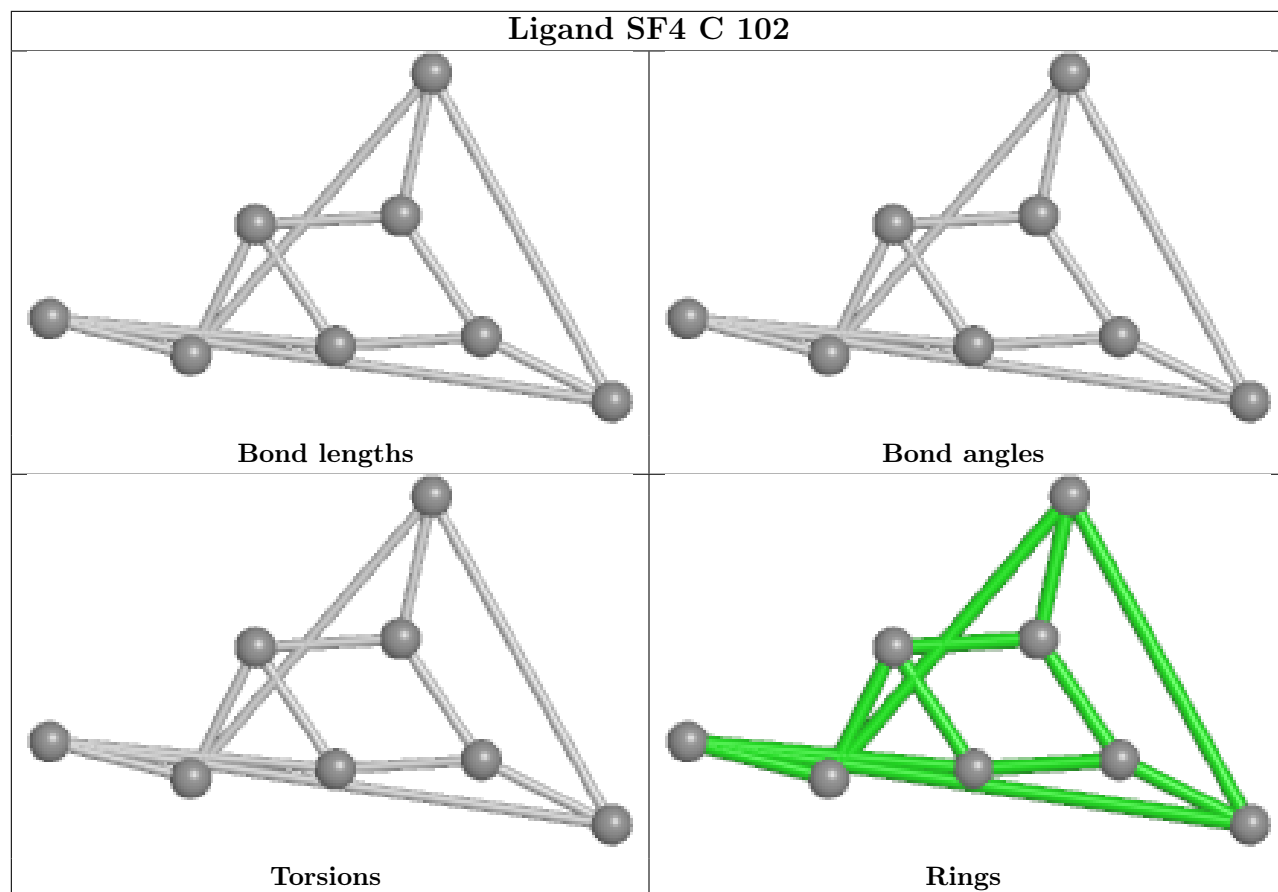


Torsions

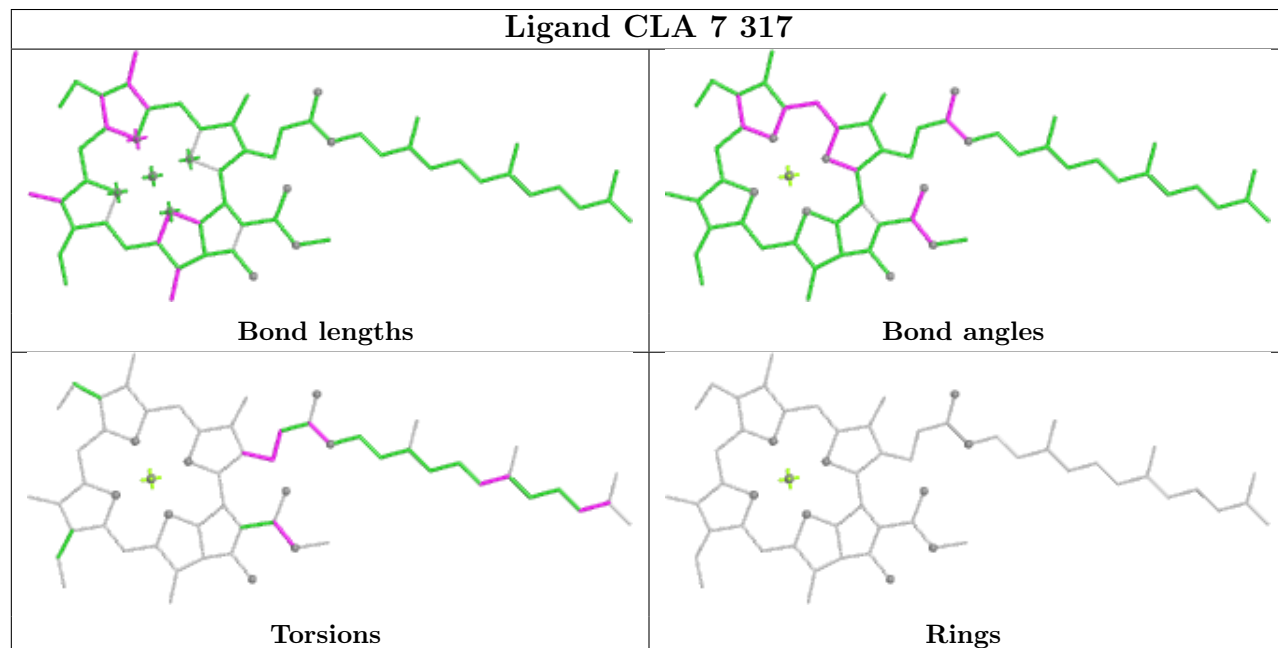


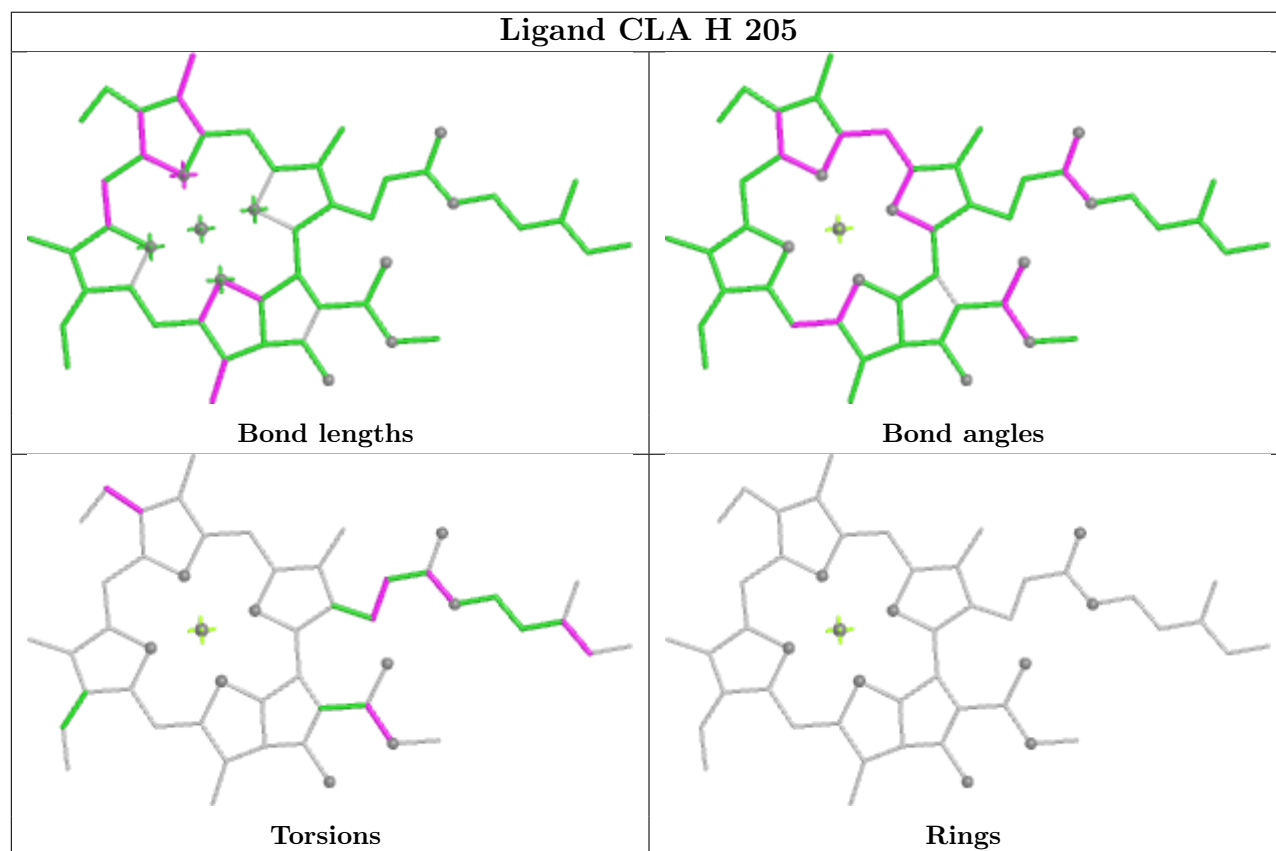
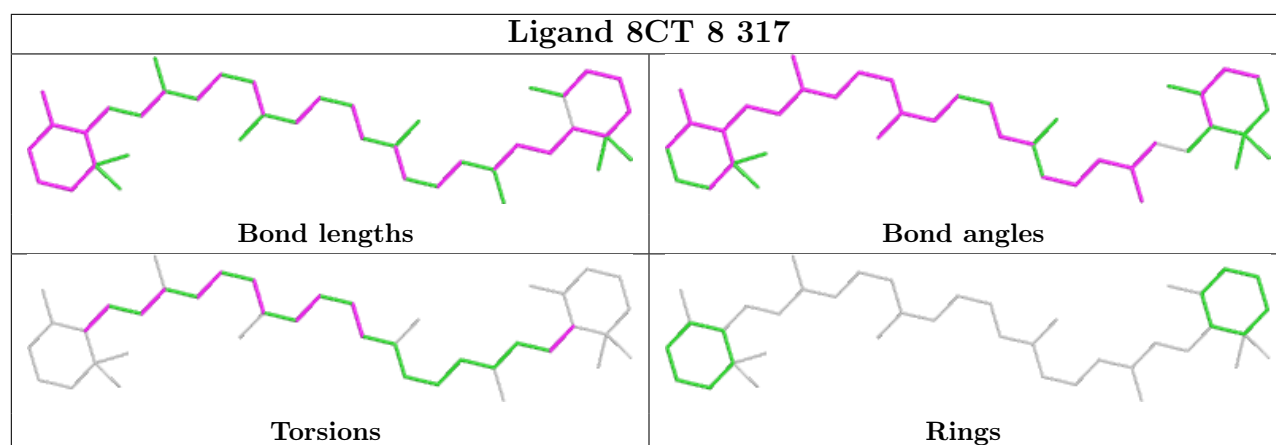
Rings

Ligand SF4 C 102

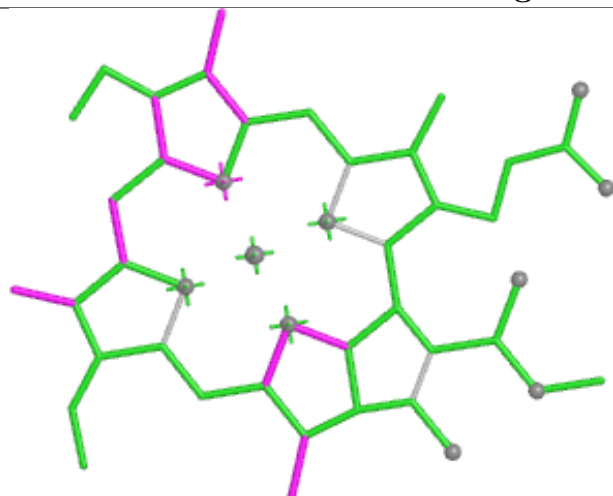


Ligand CLA 7 317

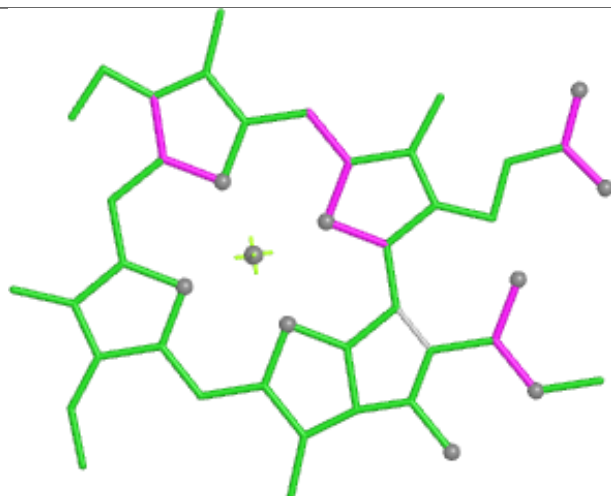




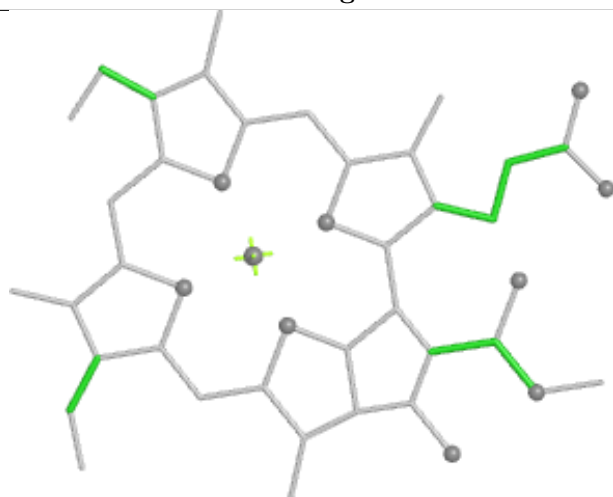
Ligand CLA B 835



Bond lengths



Bond angles

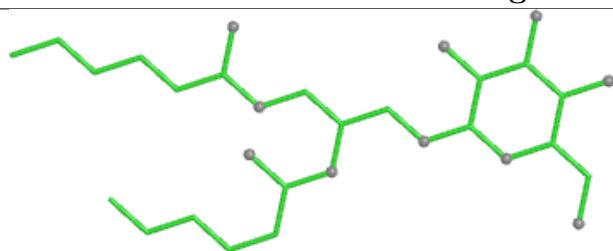


Torsions

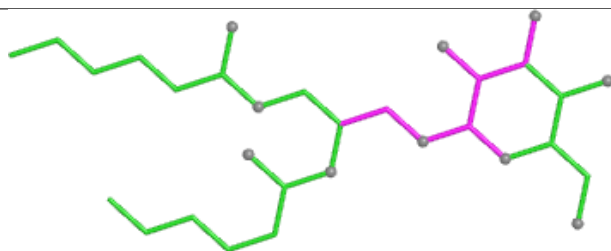


Rings

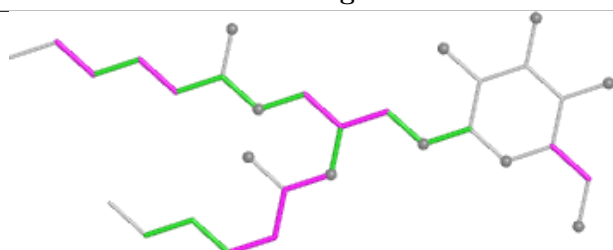
Ligand LMG O 203



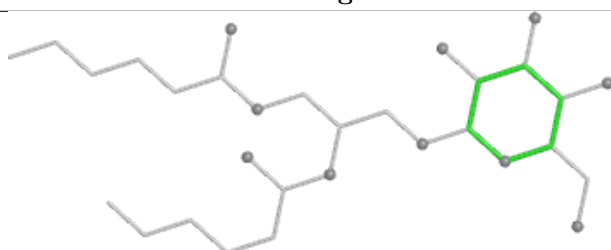
Bond lengths



Bond angles

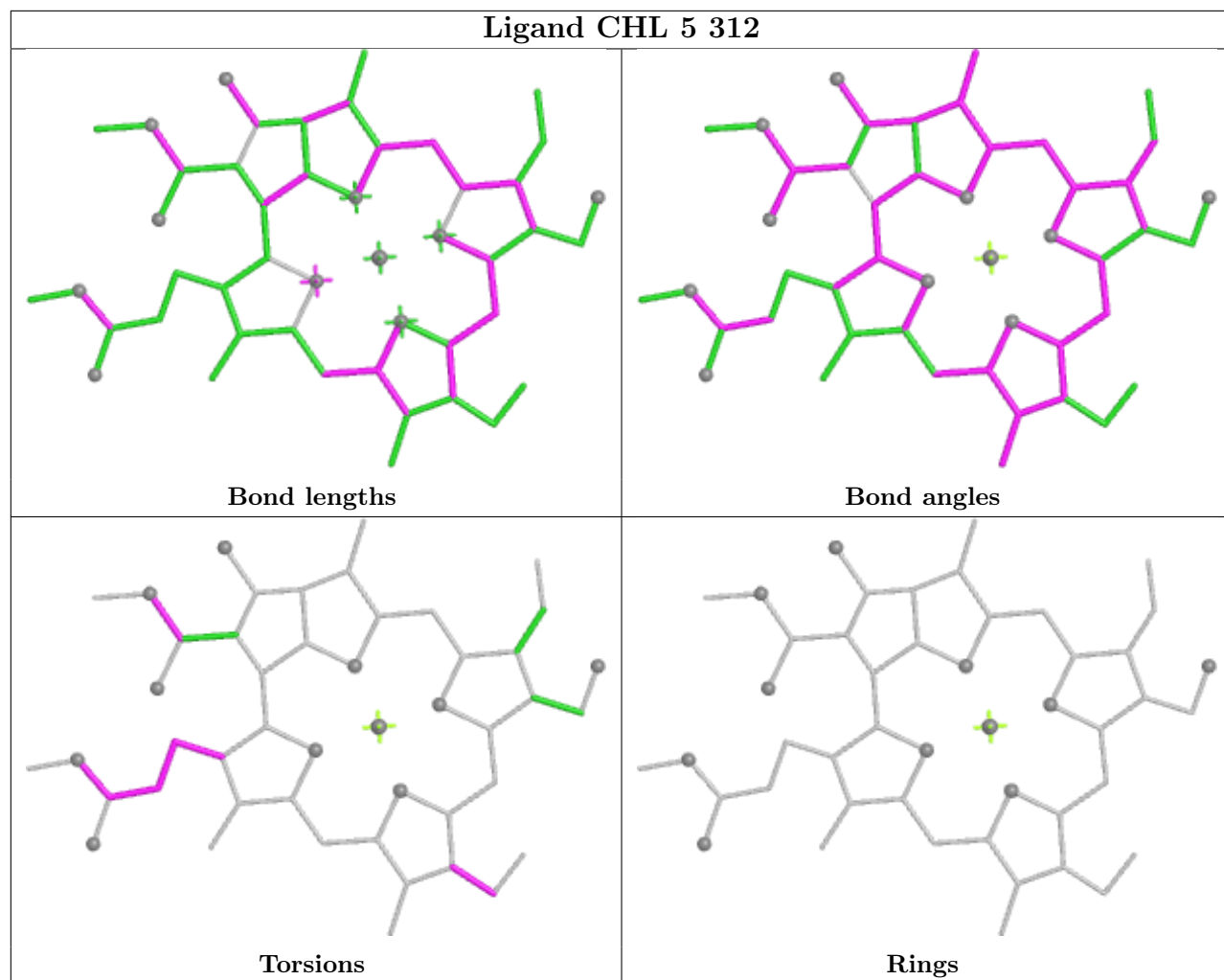


Torsions

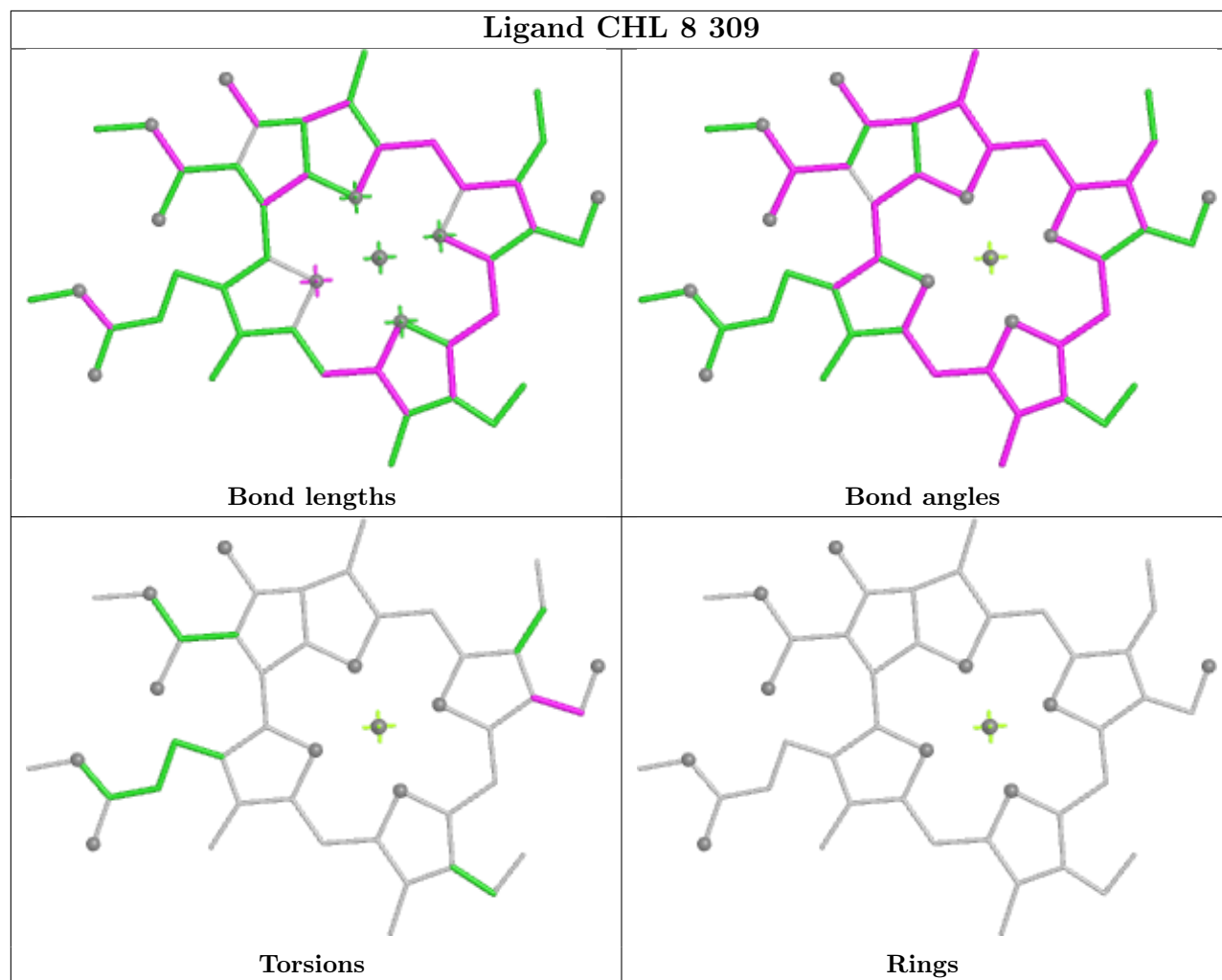


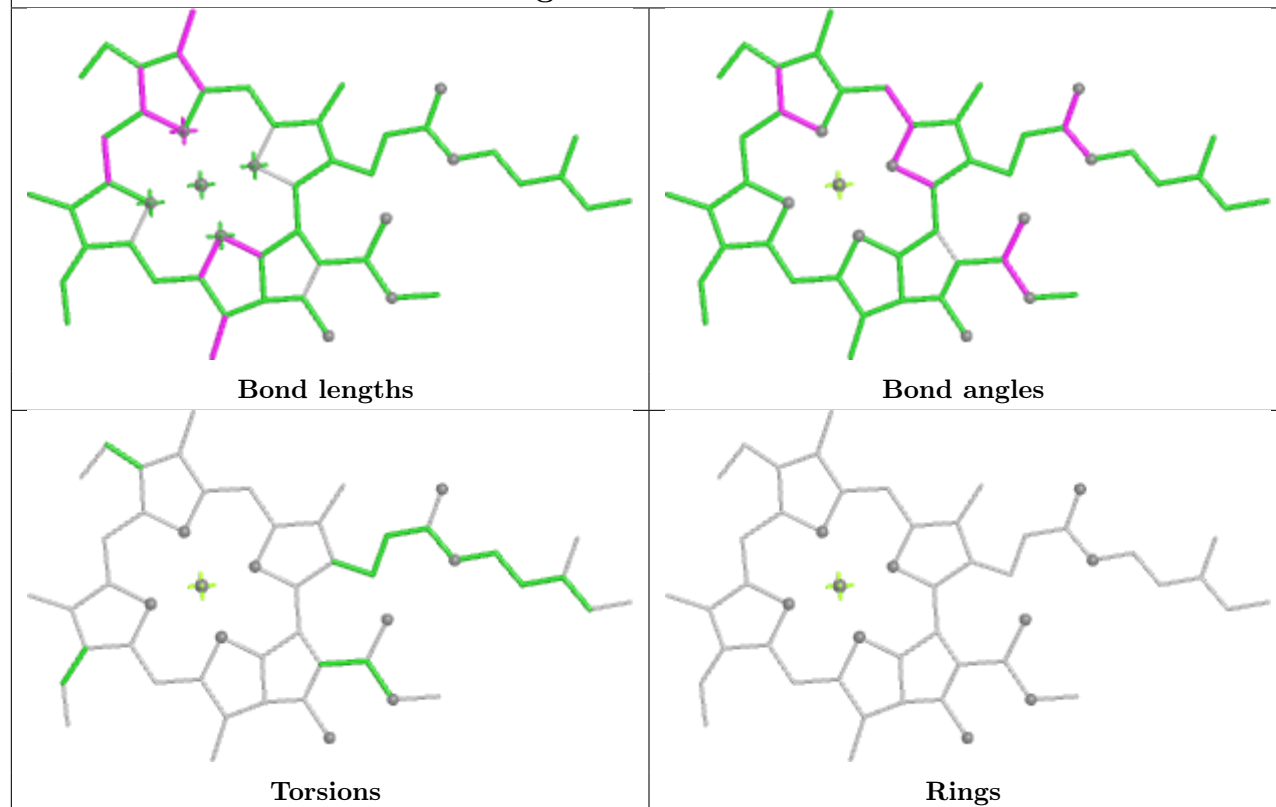
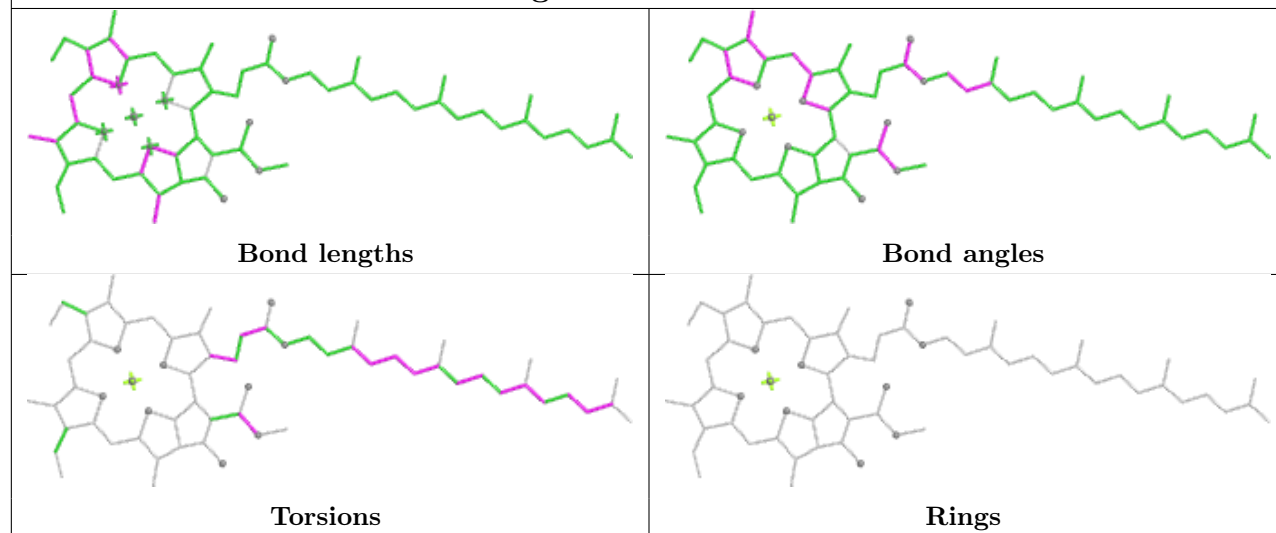
Rings

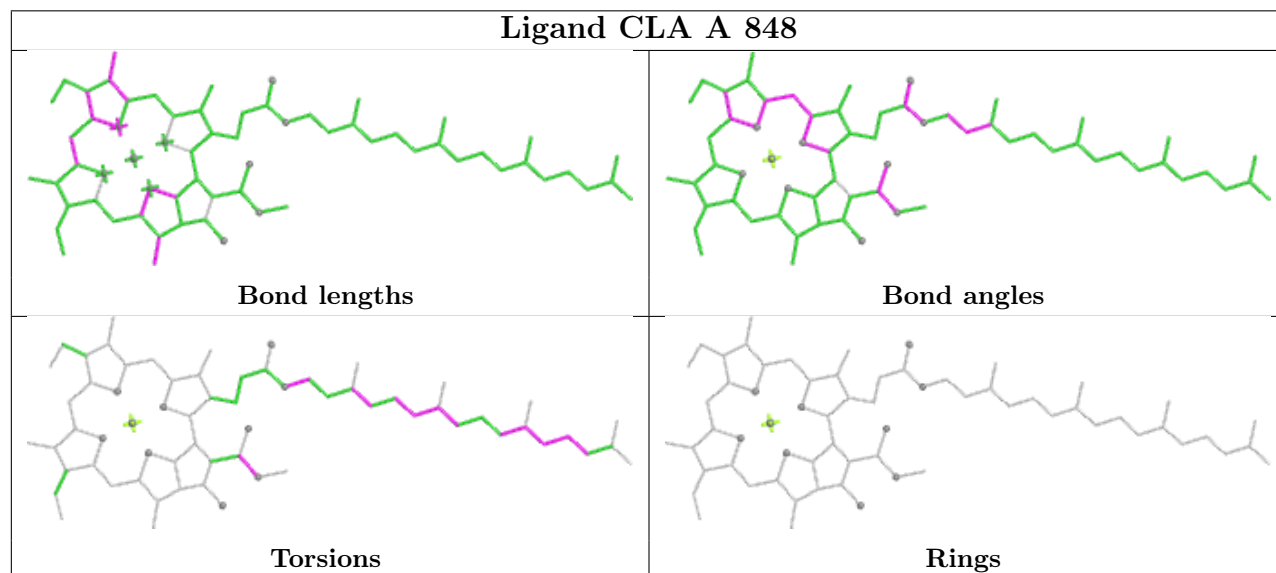
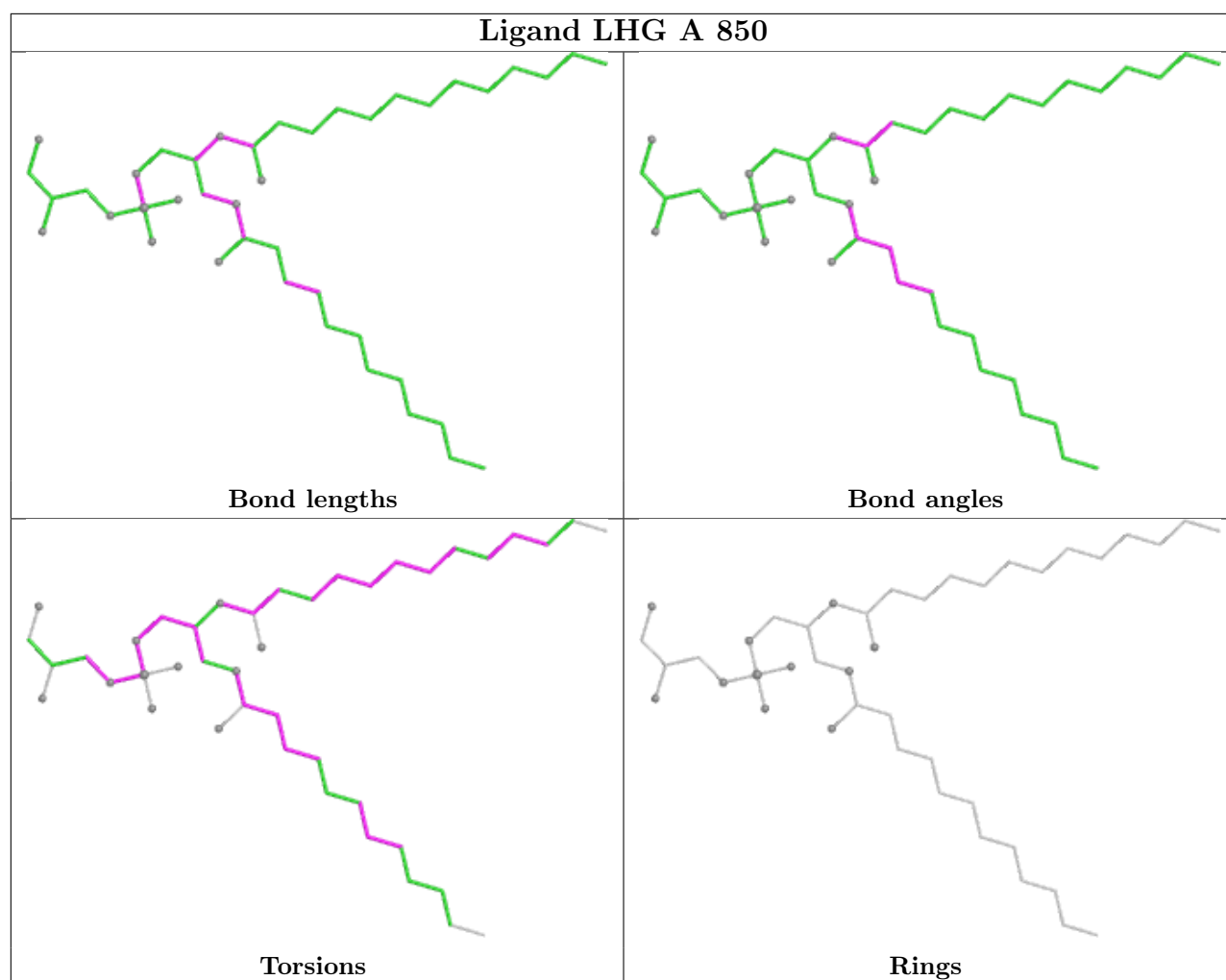
Ligand CHL 5 312



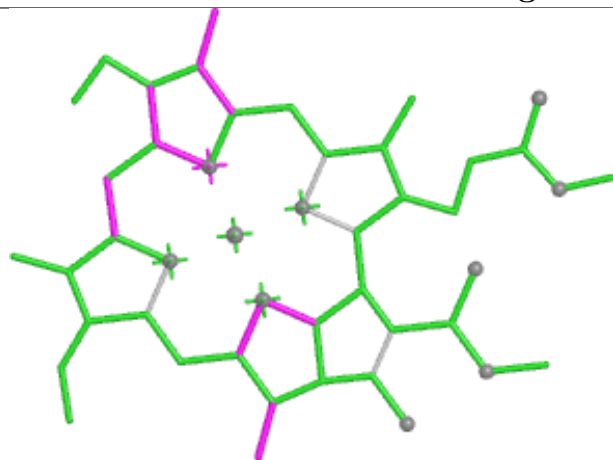
Ligand CHL 8 309



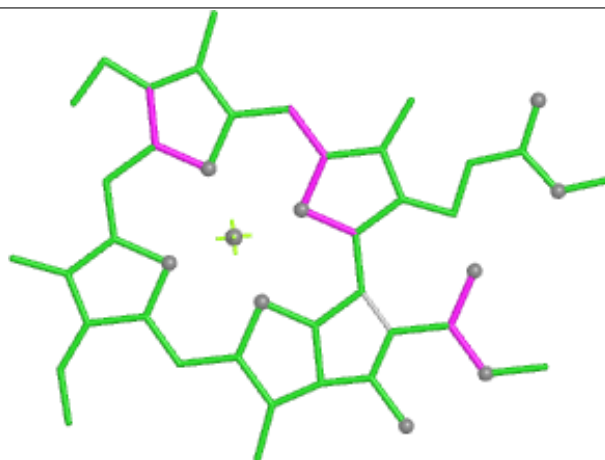
Ligand CLA 9 304**Ligand CLA A 827**



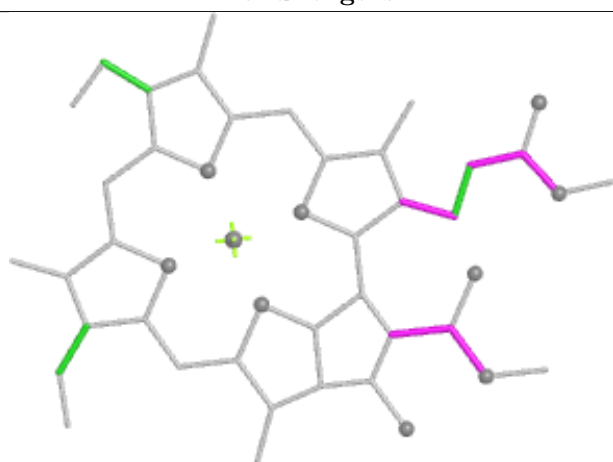
Ligand CLA 0 312



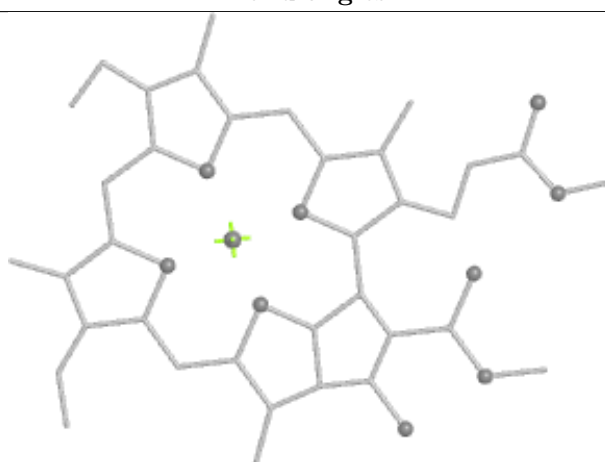
Bond lengths



Bond angles

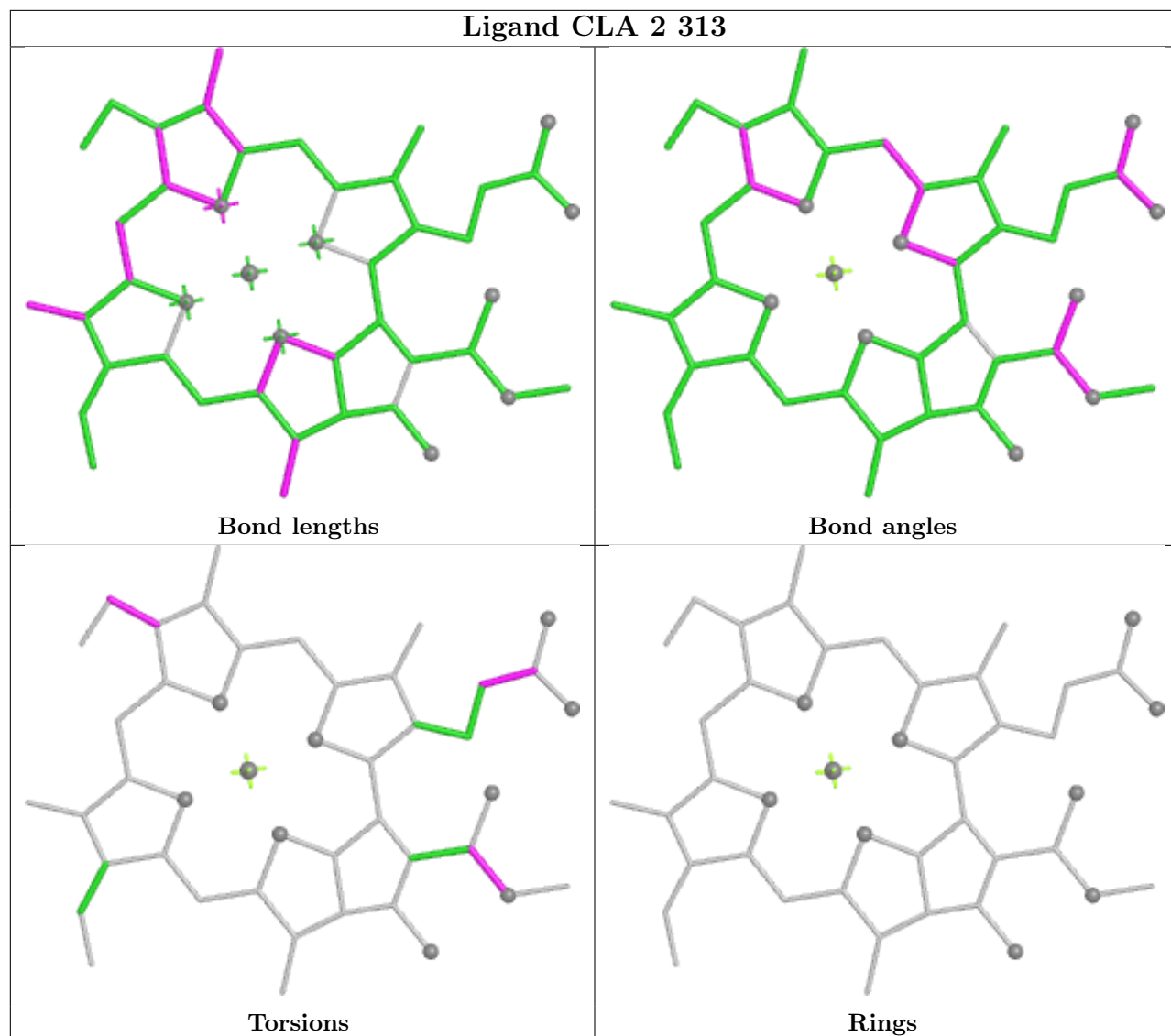


Torsions

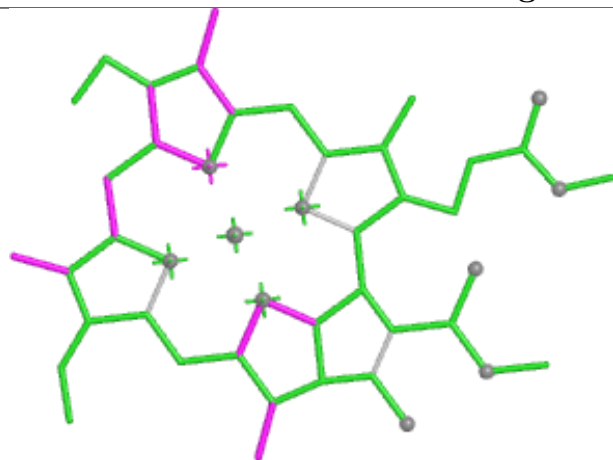


Rings

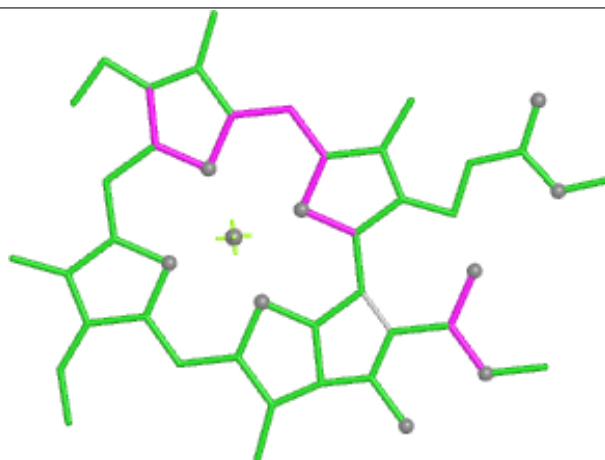
Ligand CLA 2 313



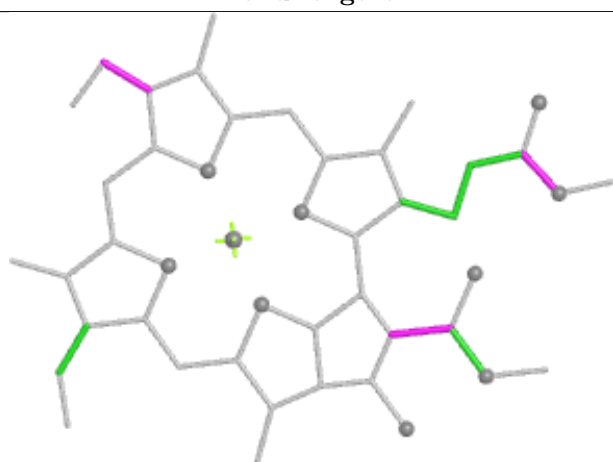
Ligand CLA 6 304



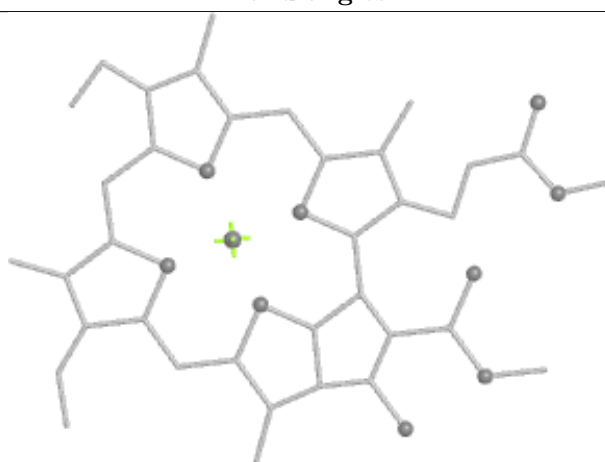
Bond lengths



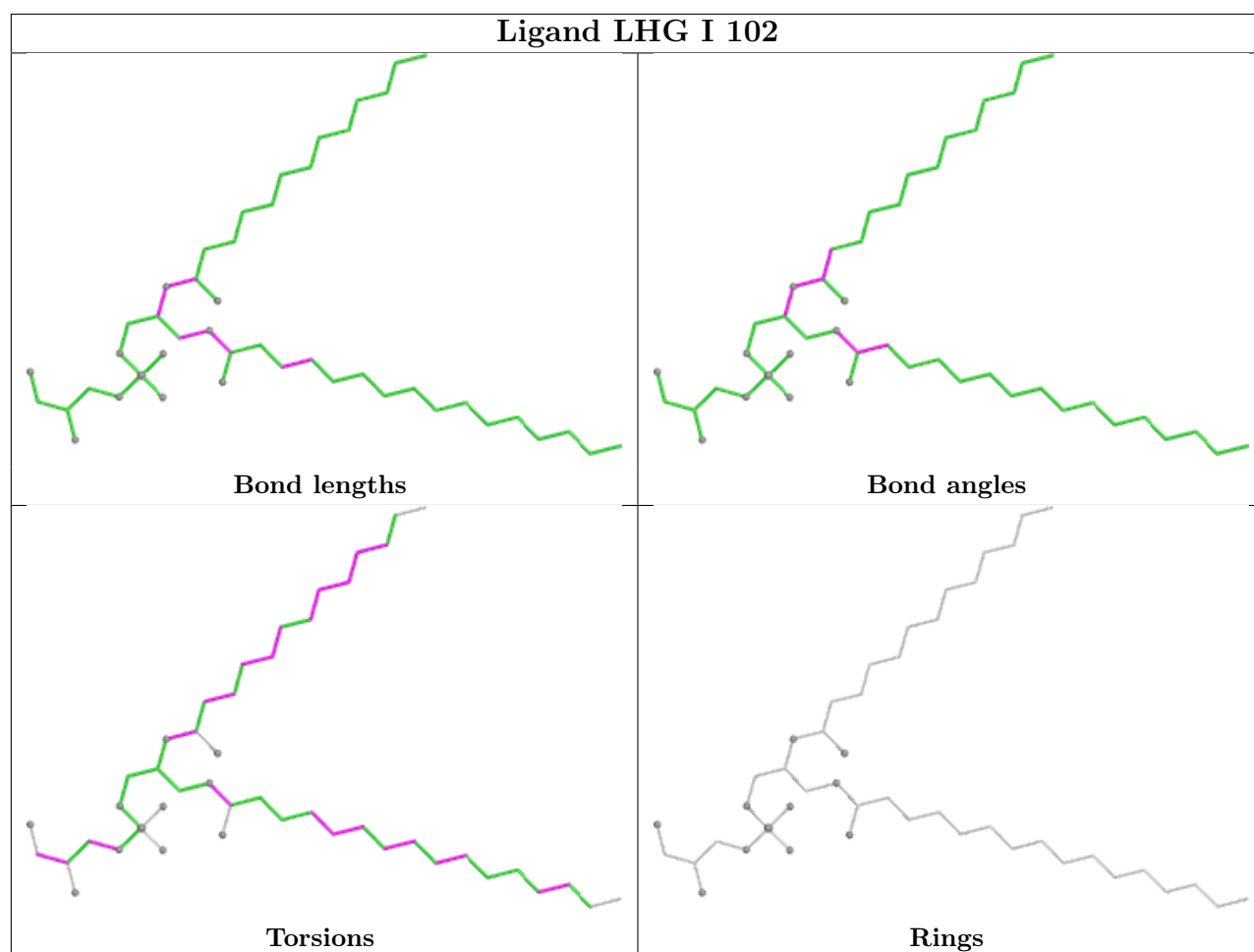
Bond angles

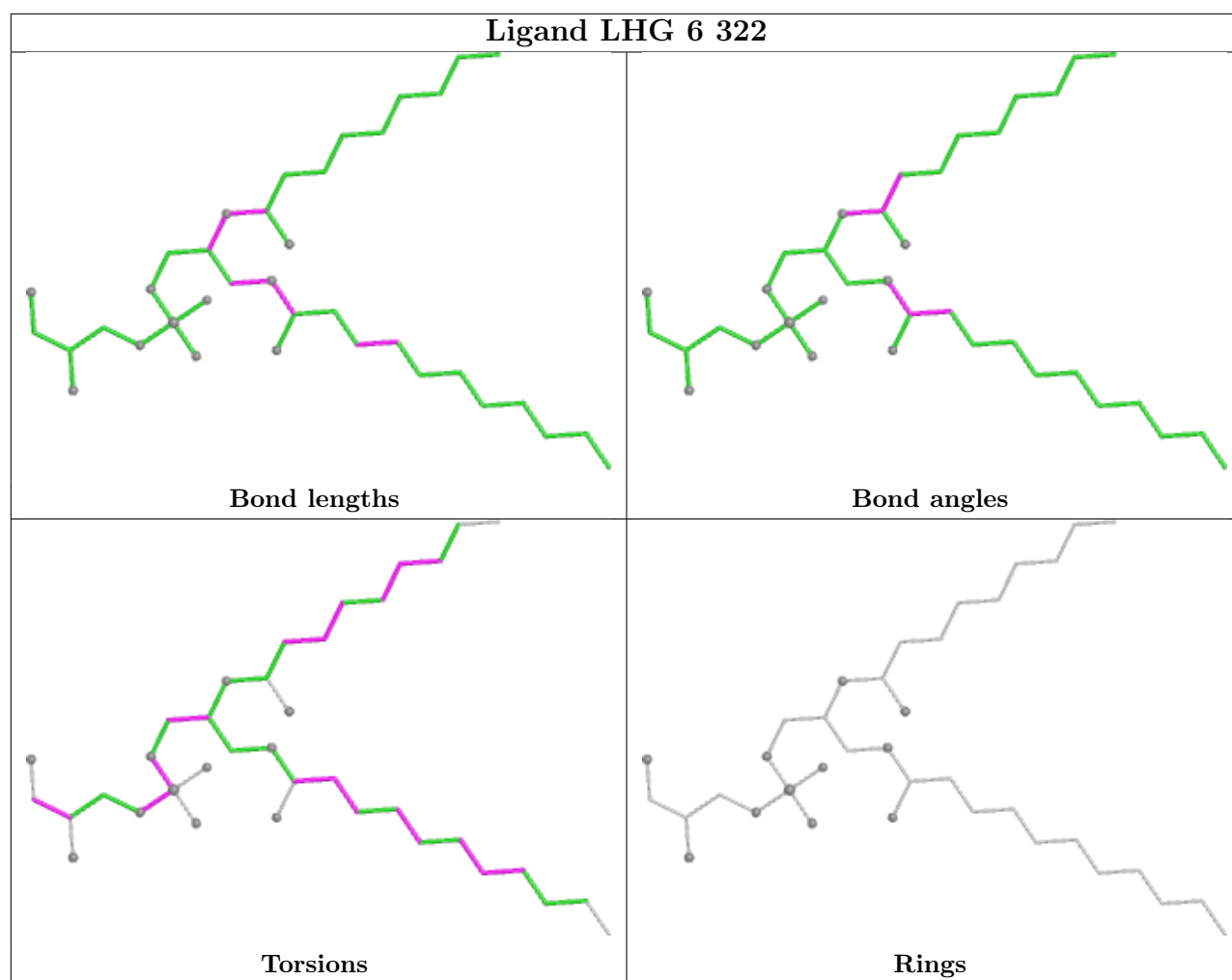


Torsions

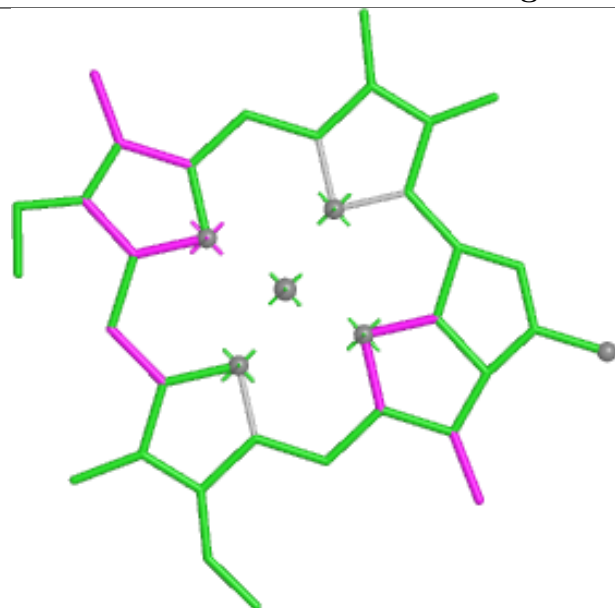


Rings

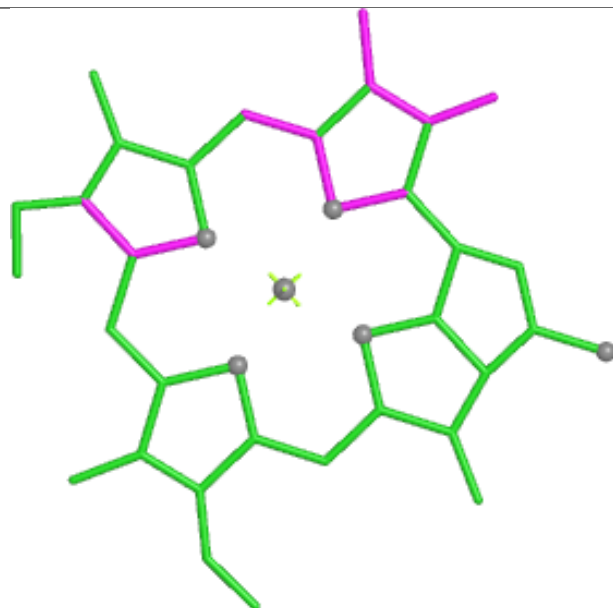




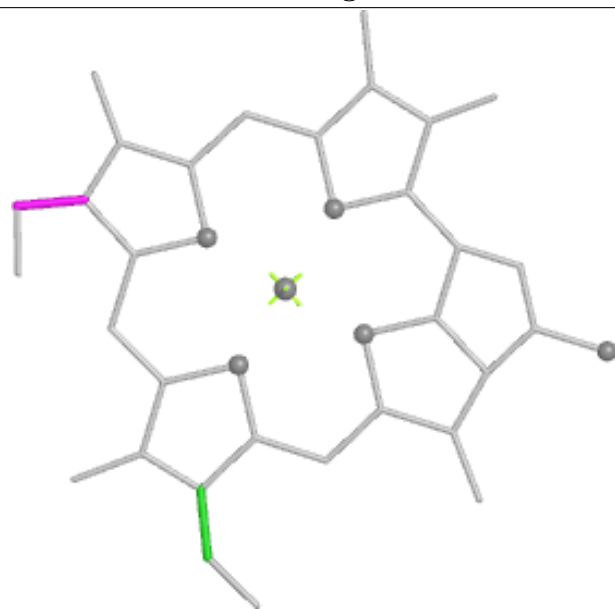
Ligand CLA 7 310



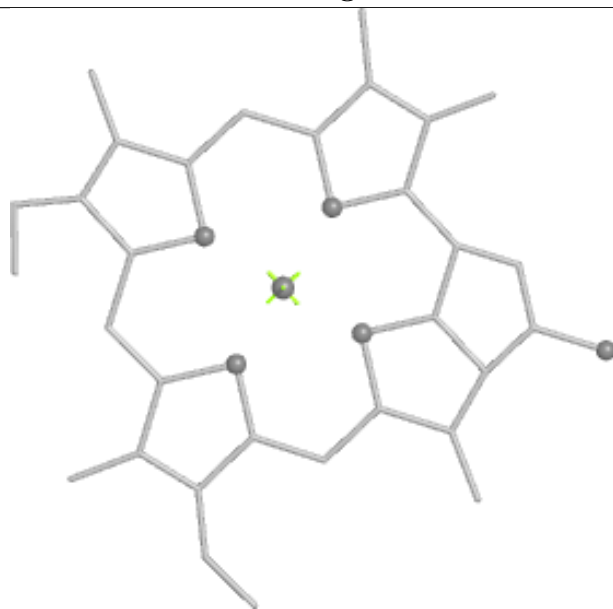
Bond lengths



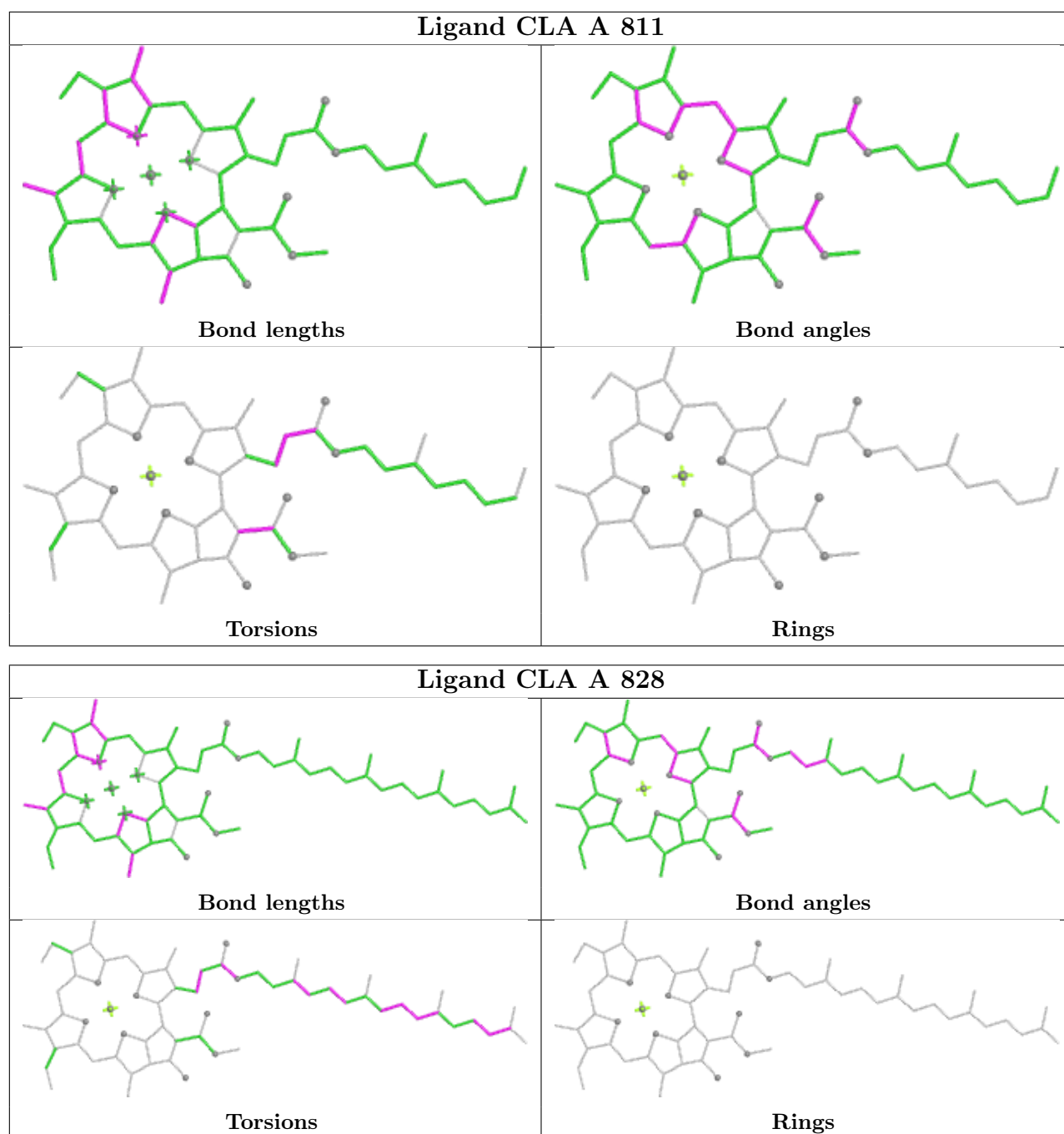
Bond angles



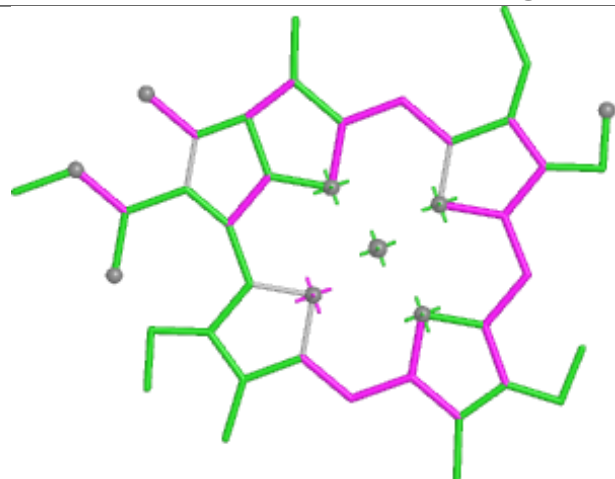
Torsions



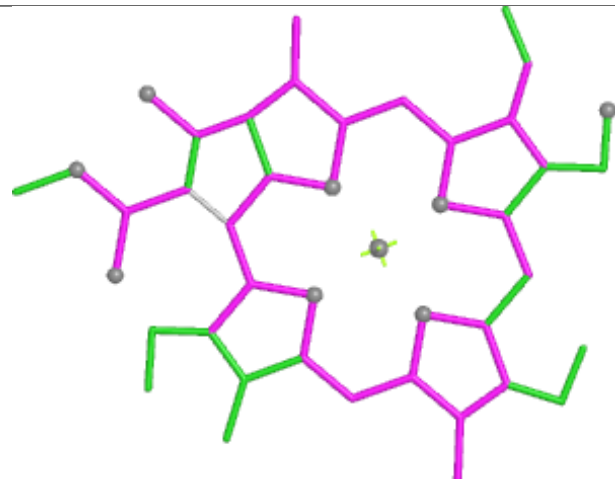
Rings



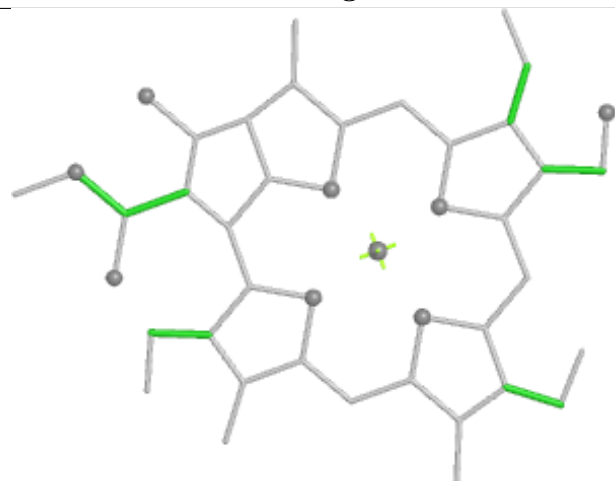
Ligand CHL 4 305



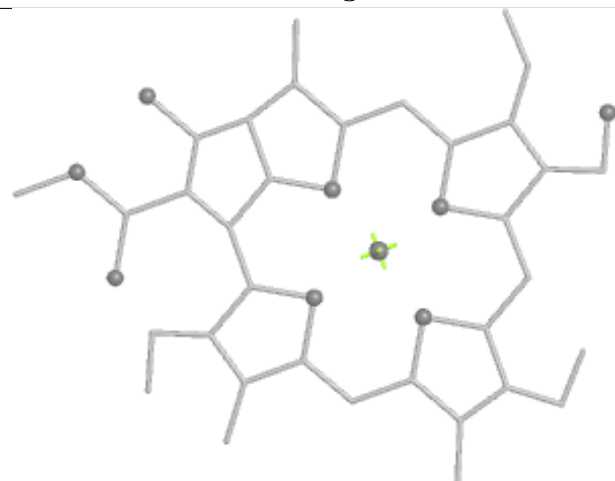
Bond lengths



Bond angles

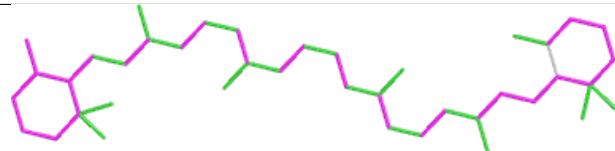


Torsions

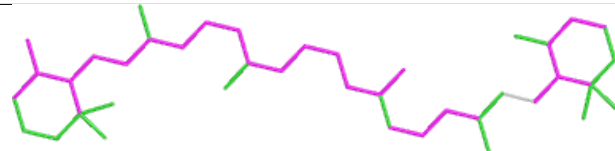


Rings

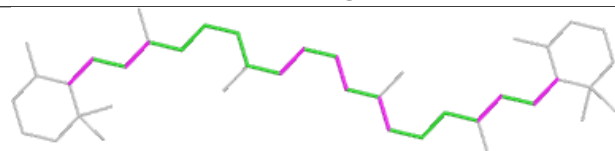
Ligand 8CT 9 313



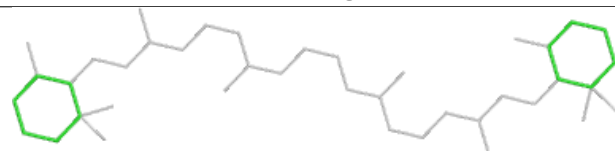
Bond lengths



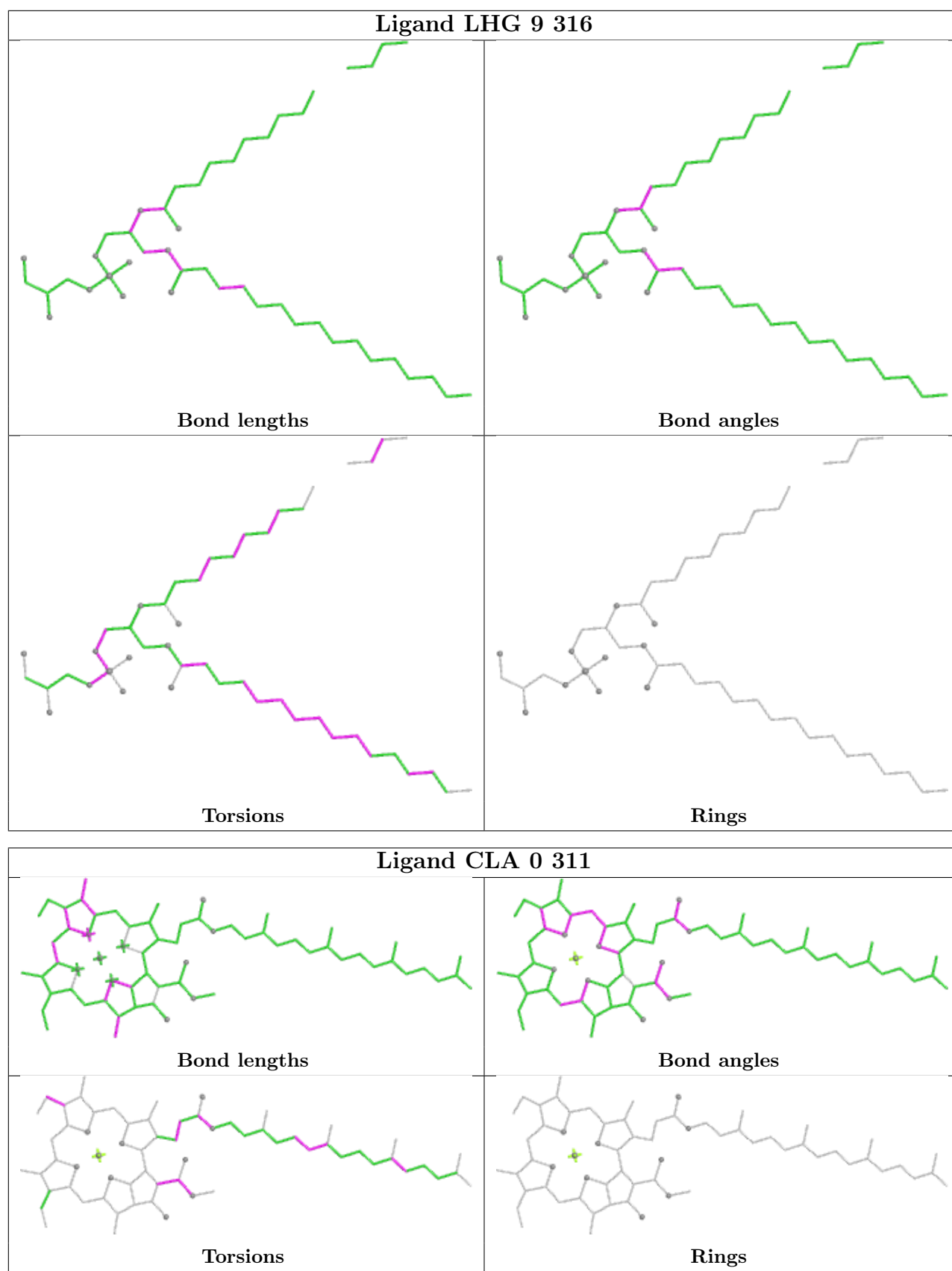
Bond angles

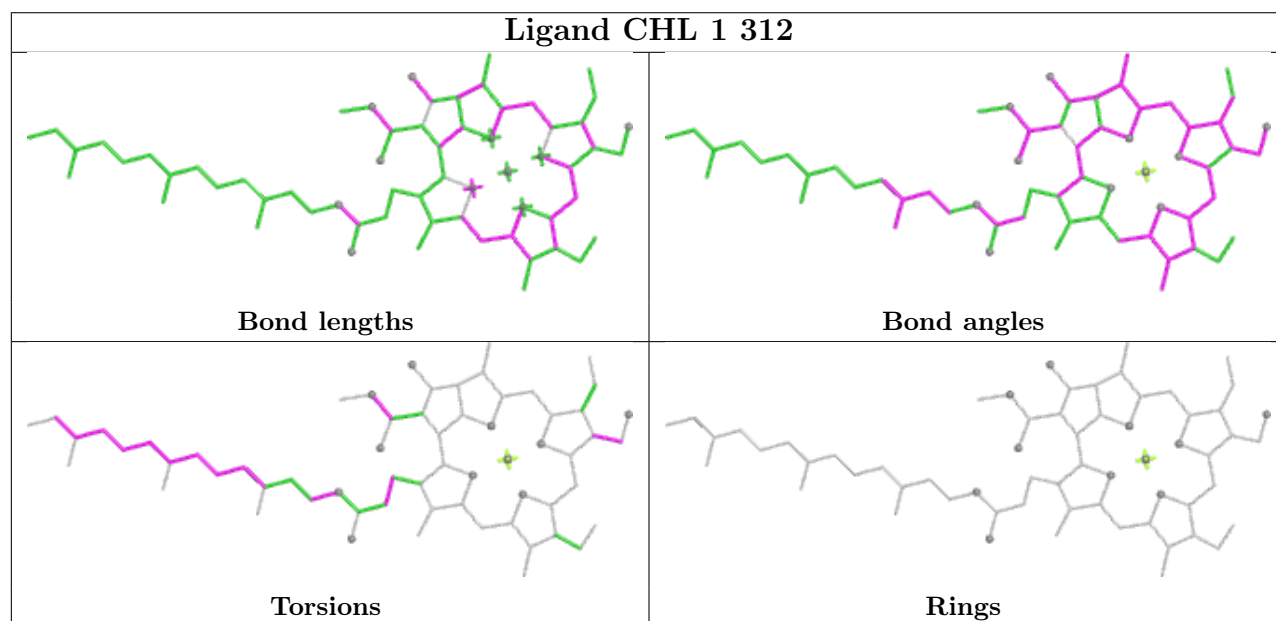
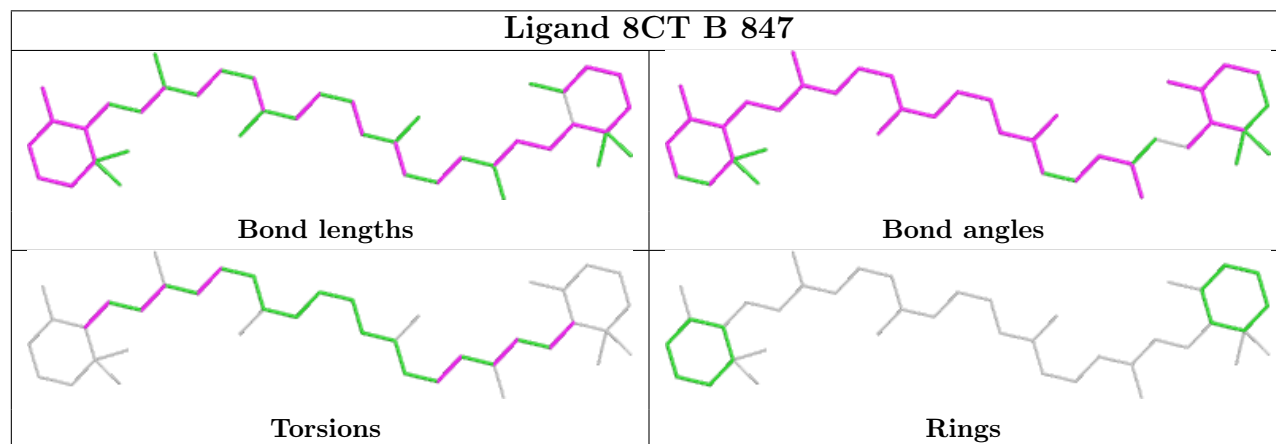
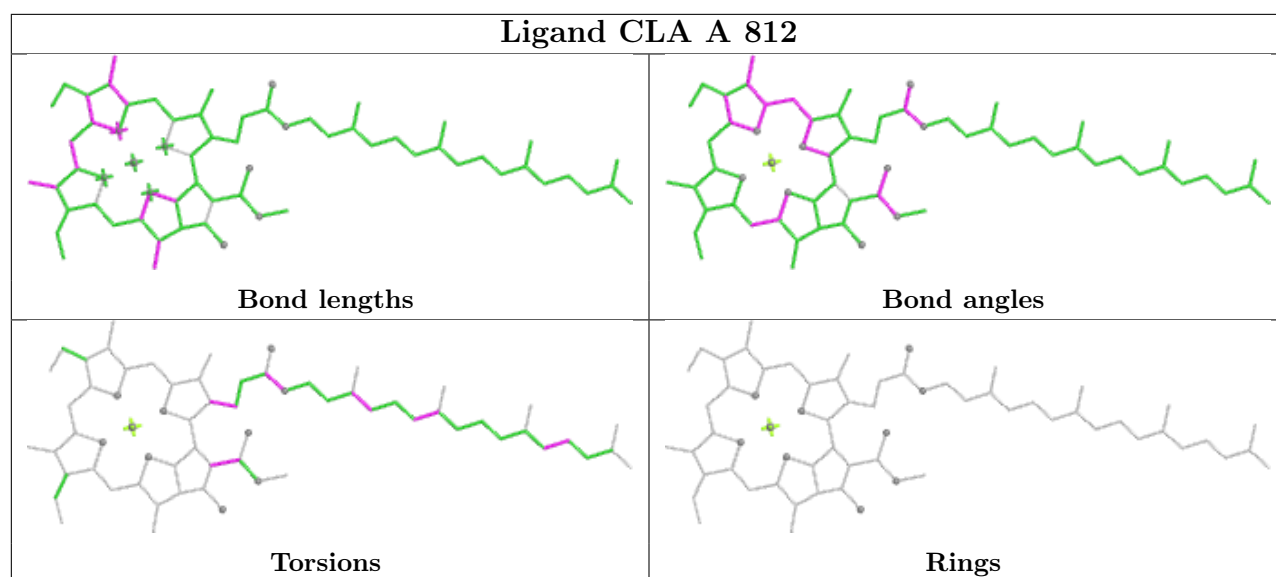


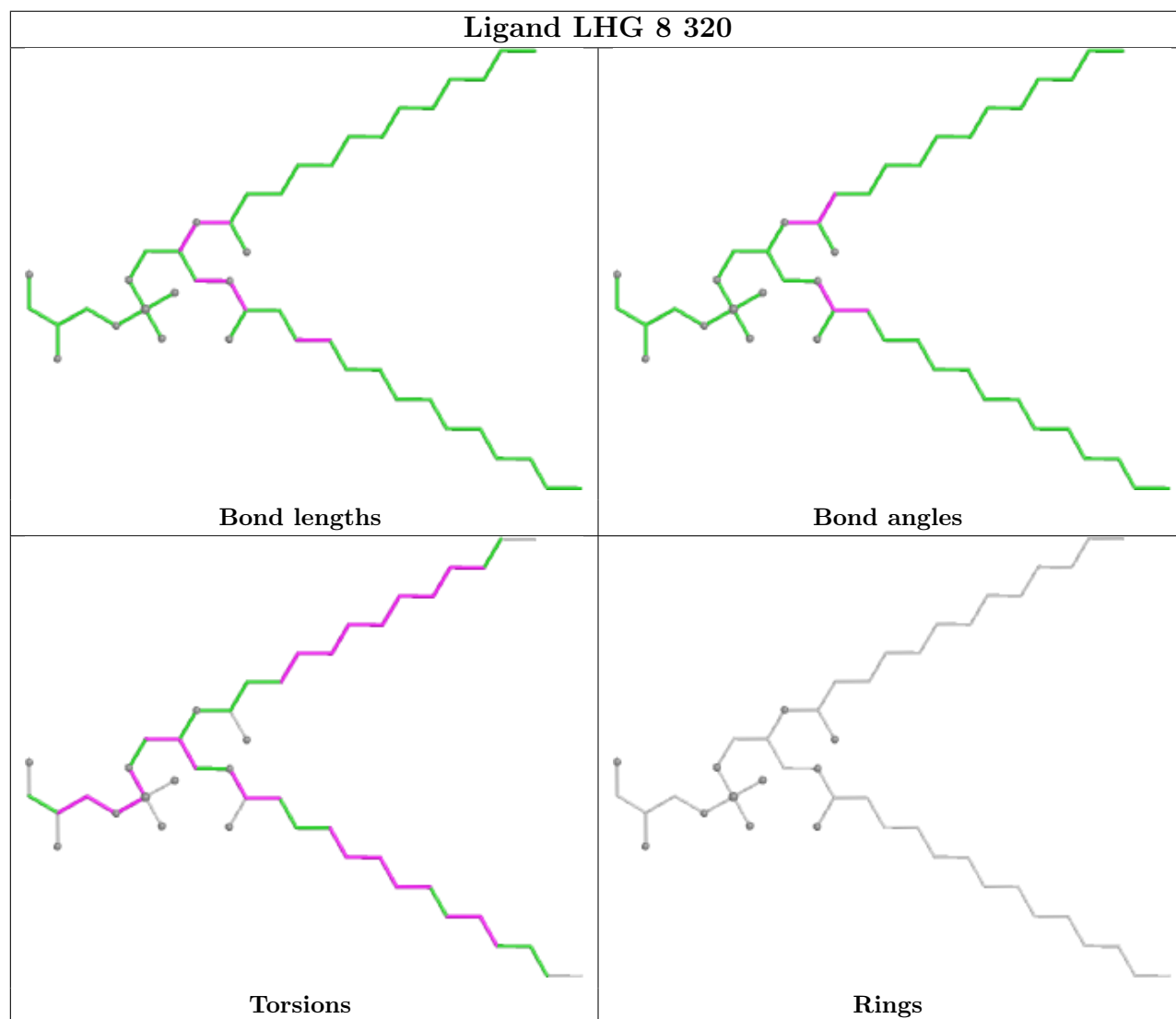
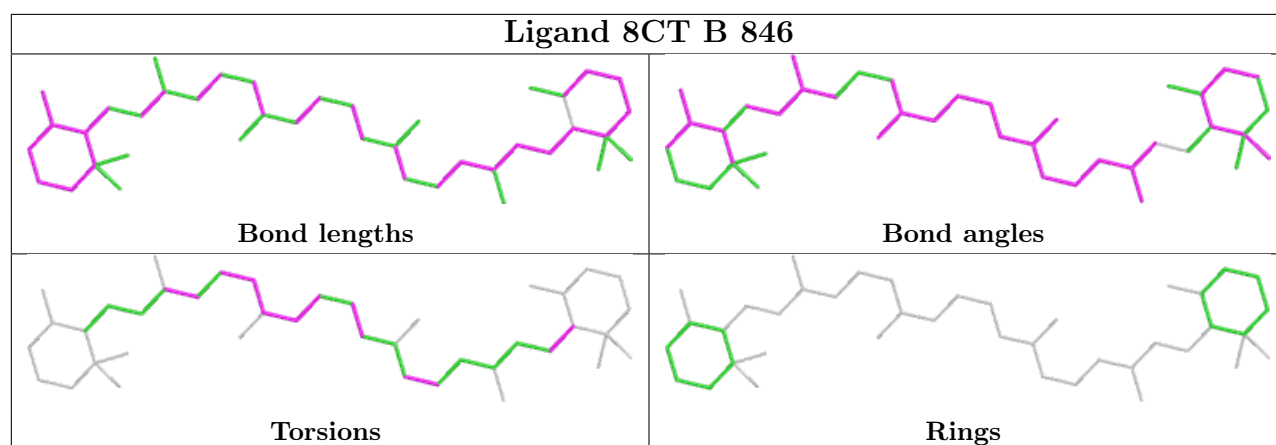
Torsions



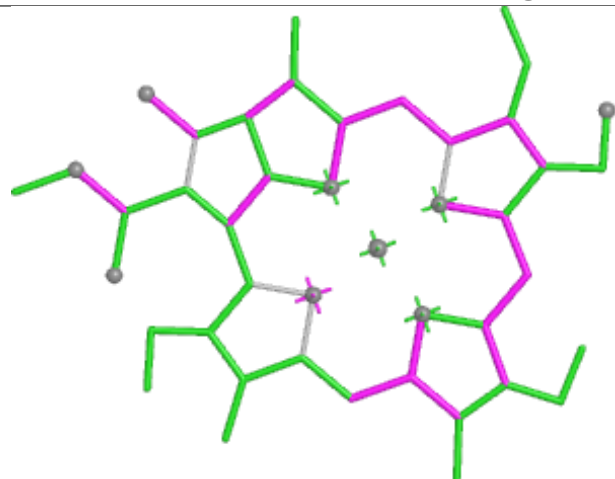
Rings



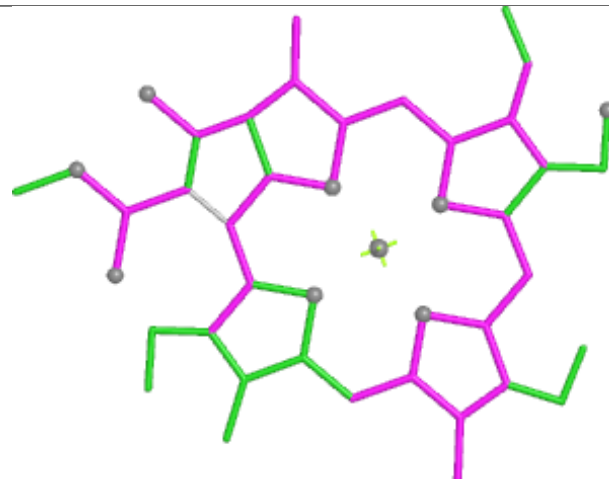




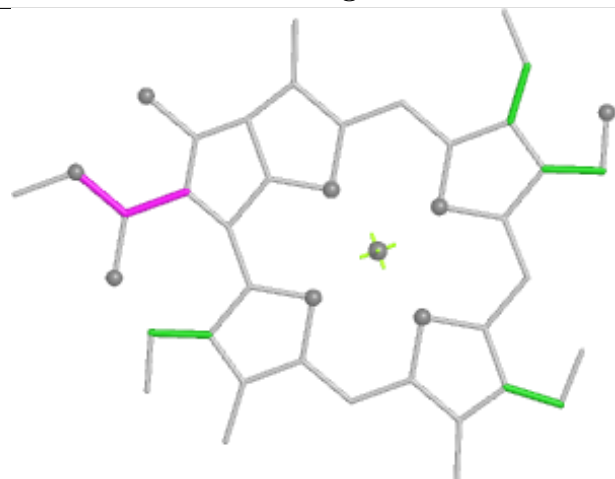
Ligand CHL 6 315



Bond lengths



Bond angles

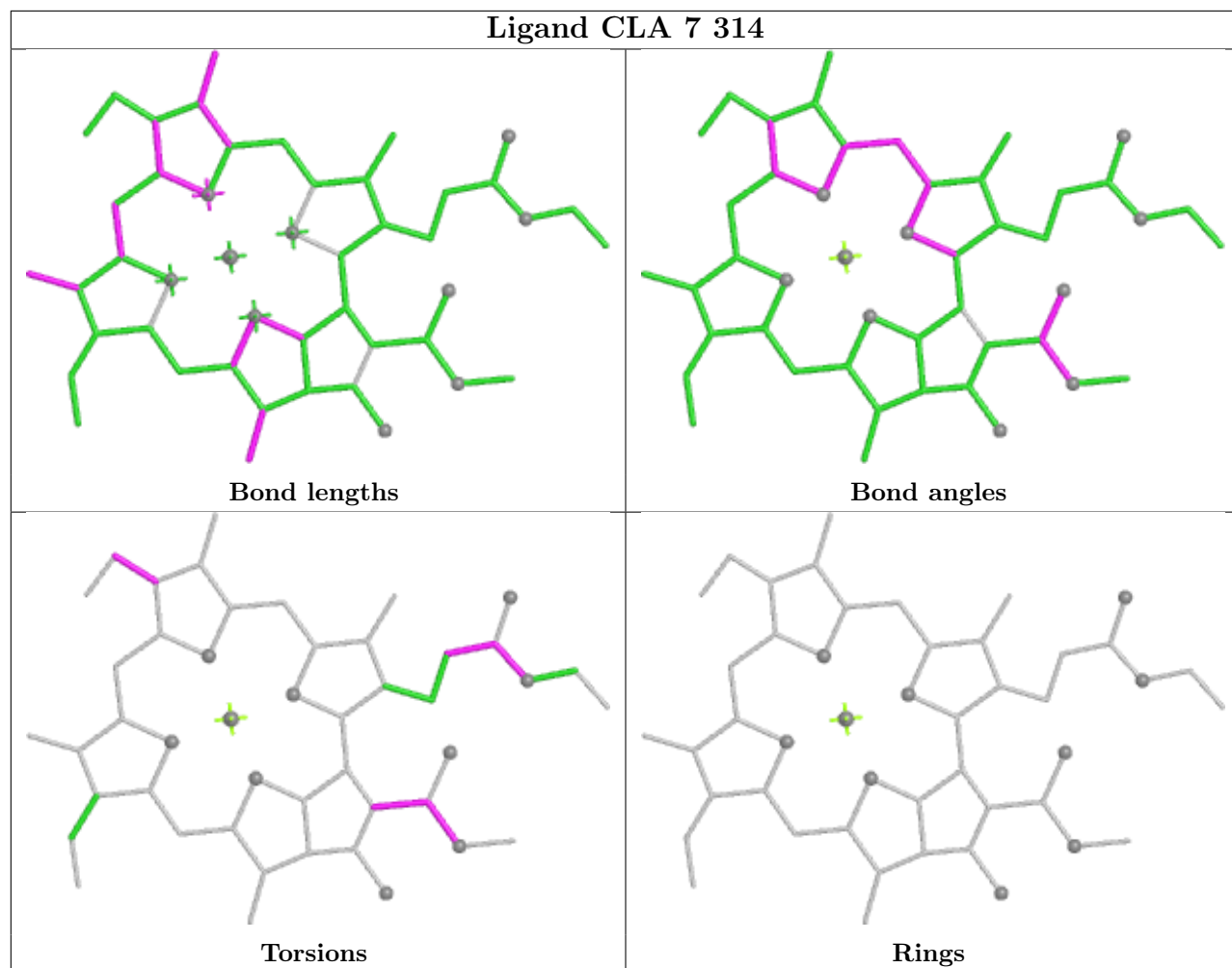


Torsions

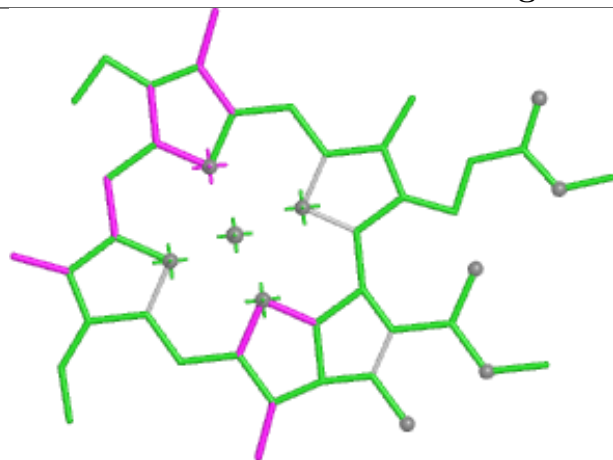


Rings

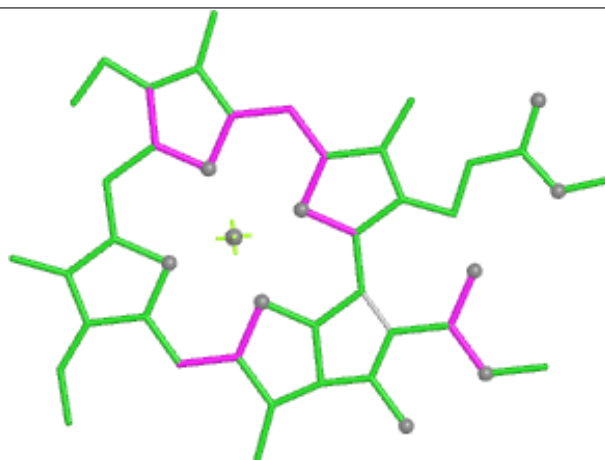
Ligand CLA 7 314



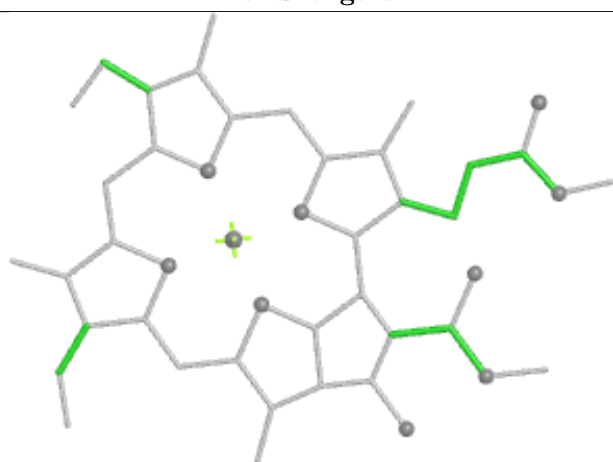
Ligand CLA 3 314



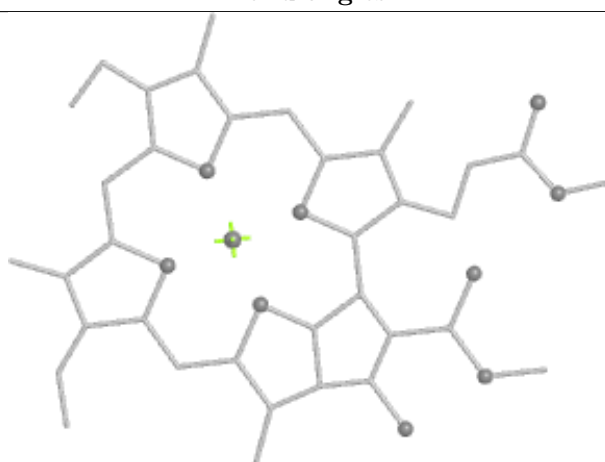
Bond lengths



Bond angles

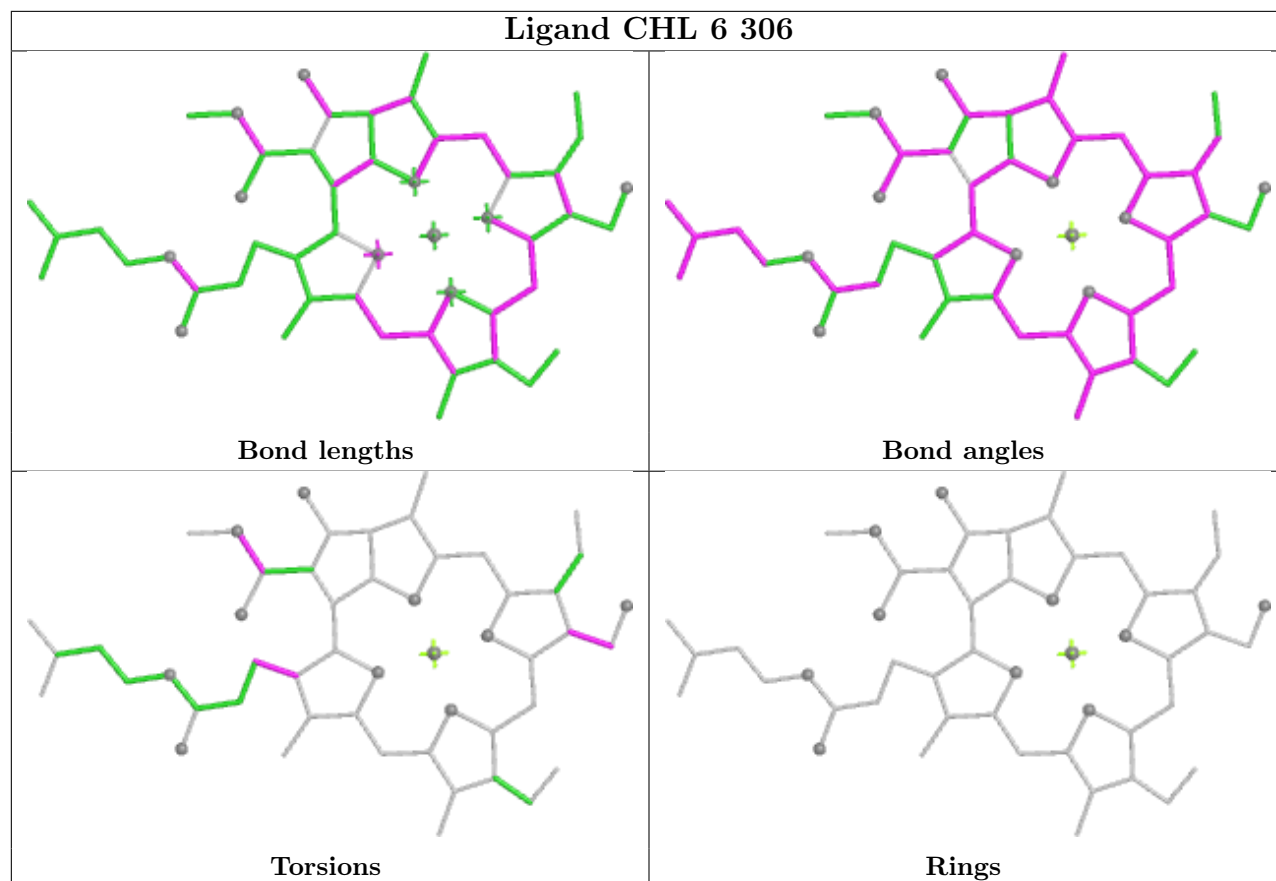


Torsions

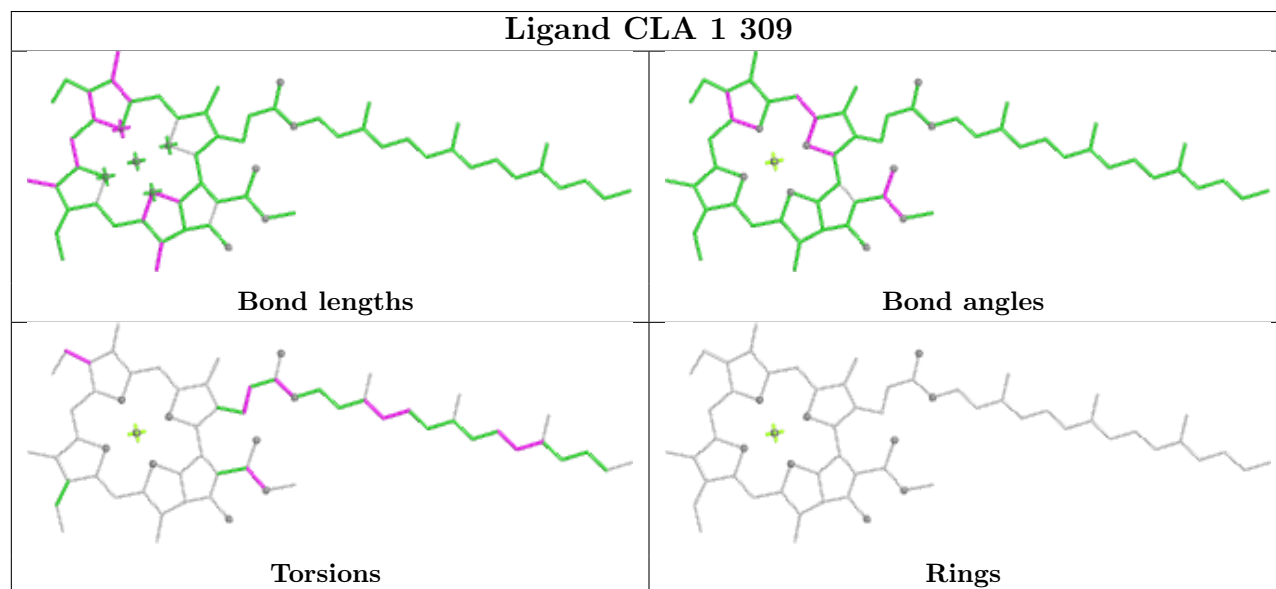


Rings

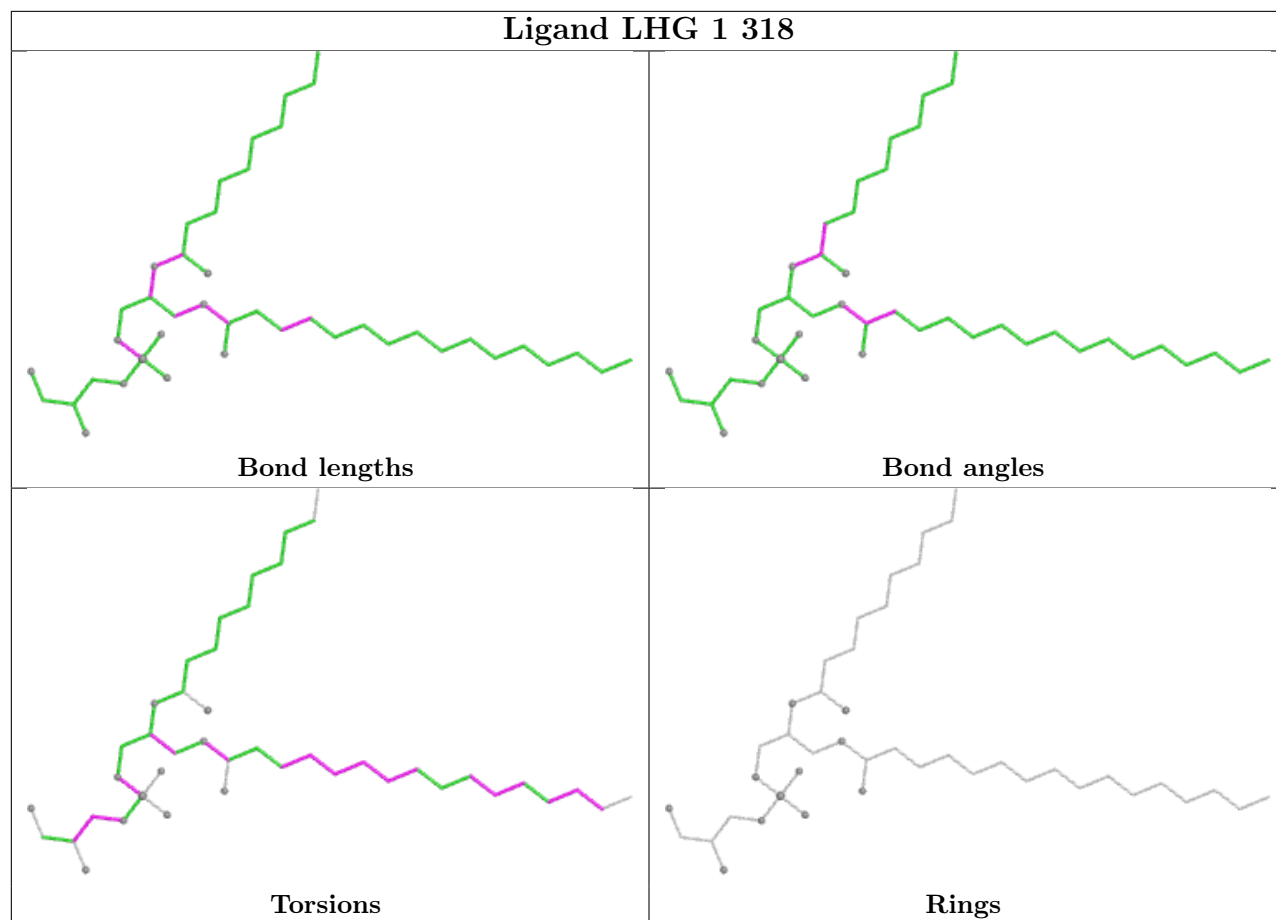
Ligand CHL 6 306



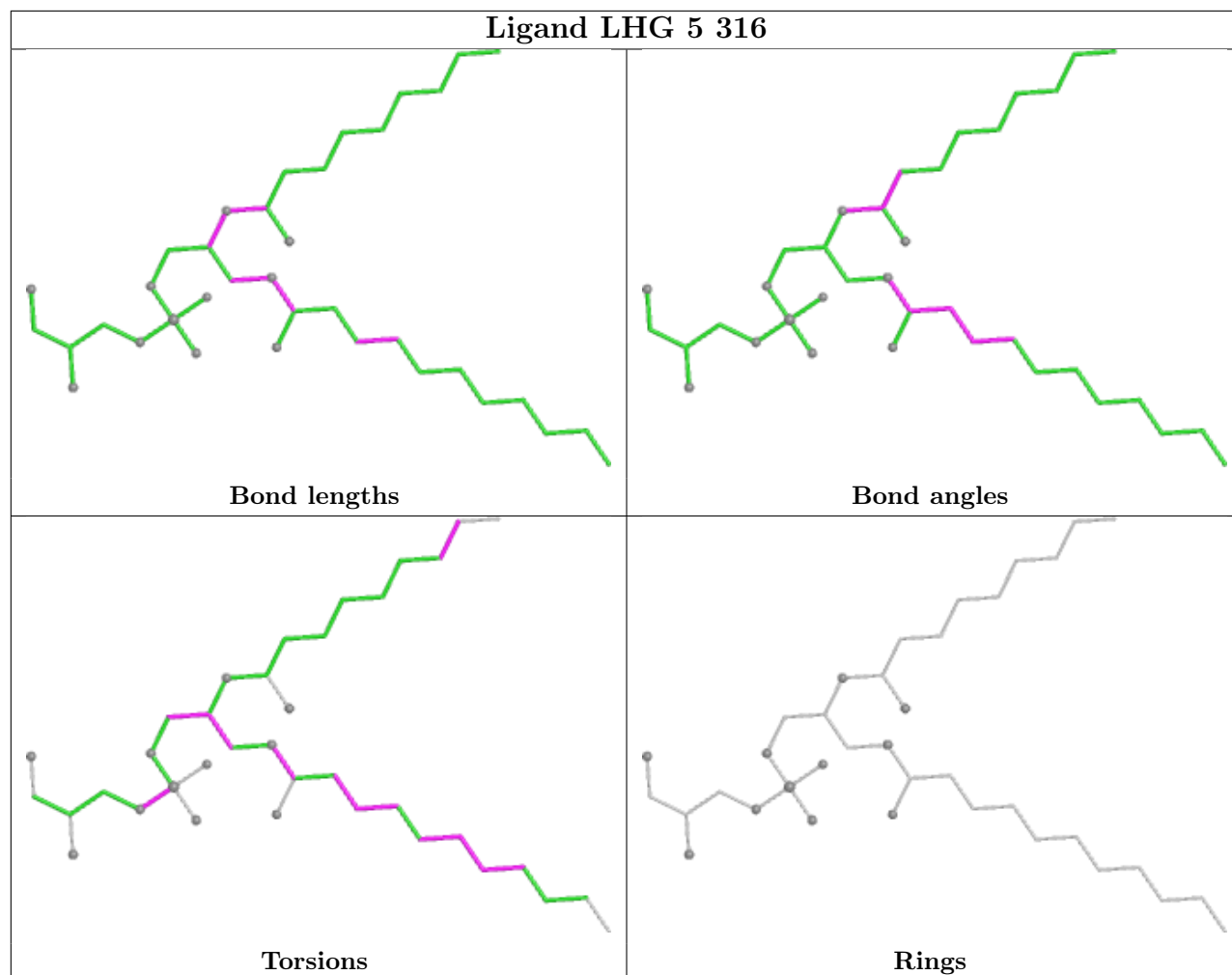
Ligand CLA 1 309



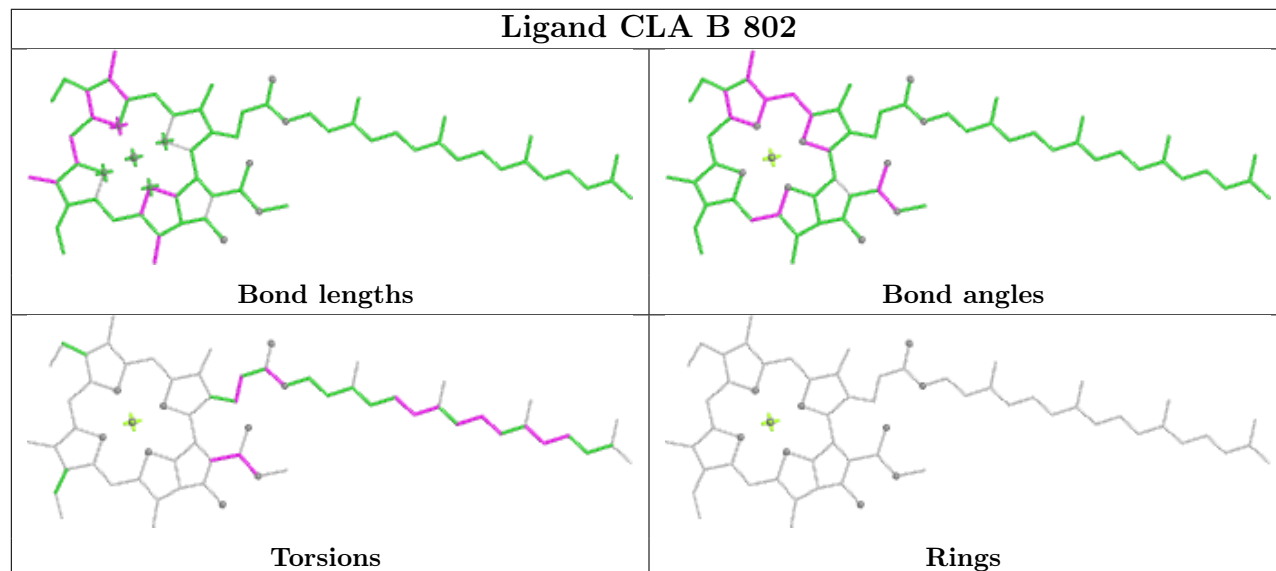
Ligand LHG 1 318

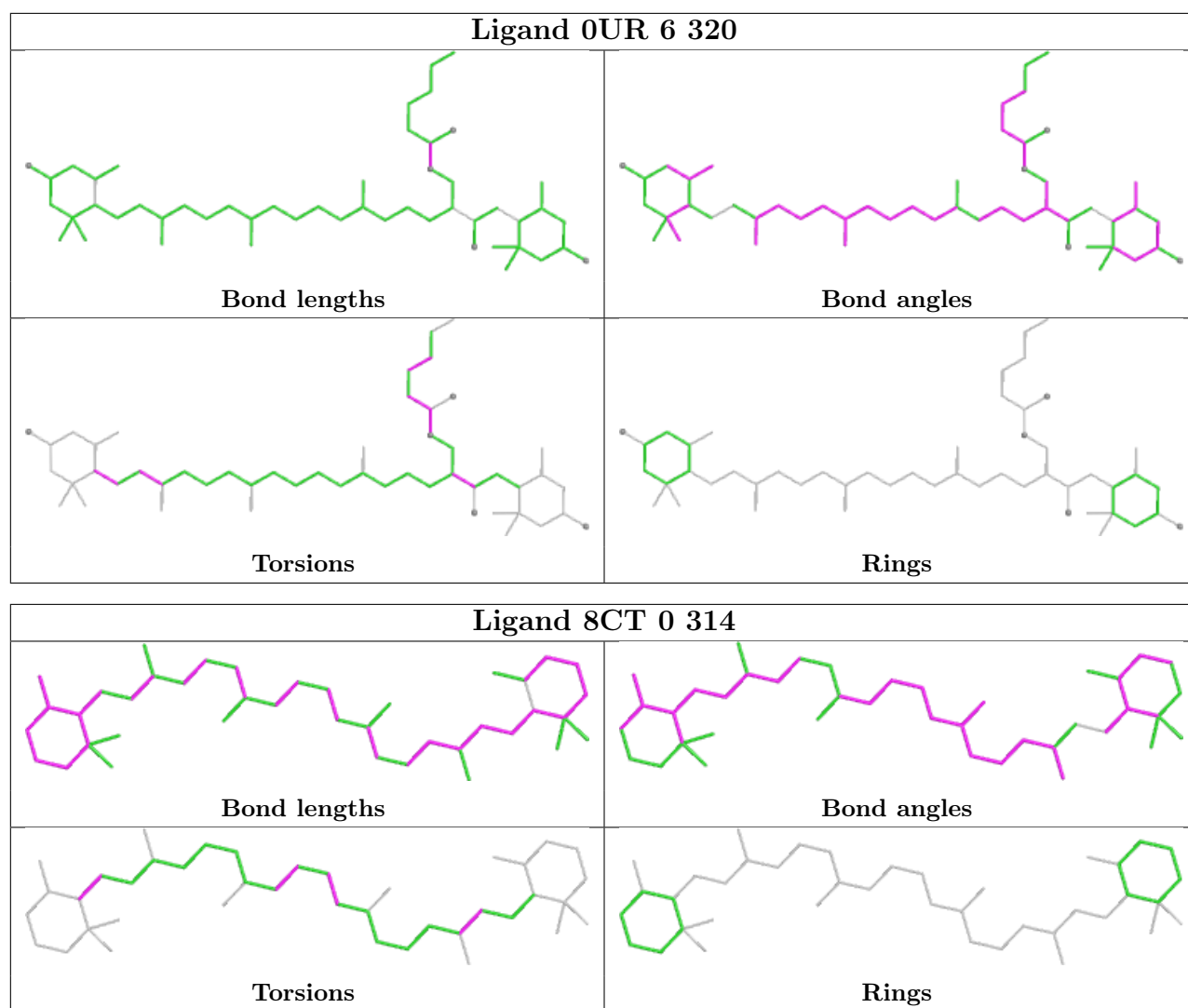


Ligand LHG 5 316

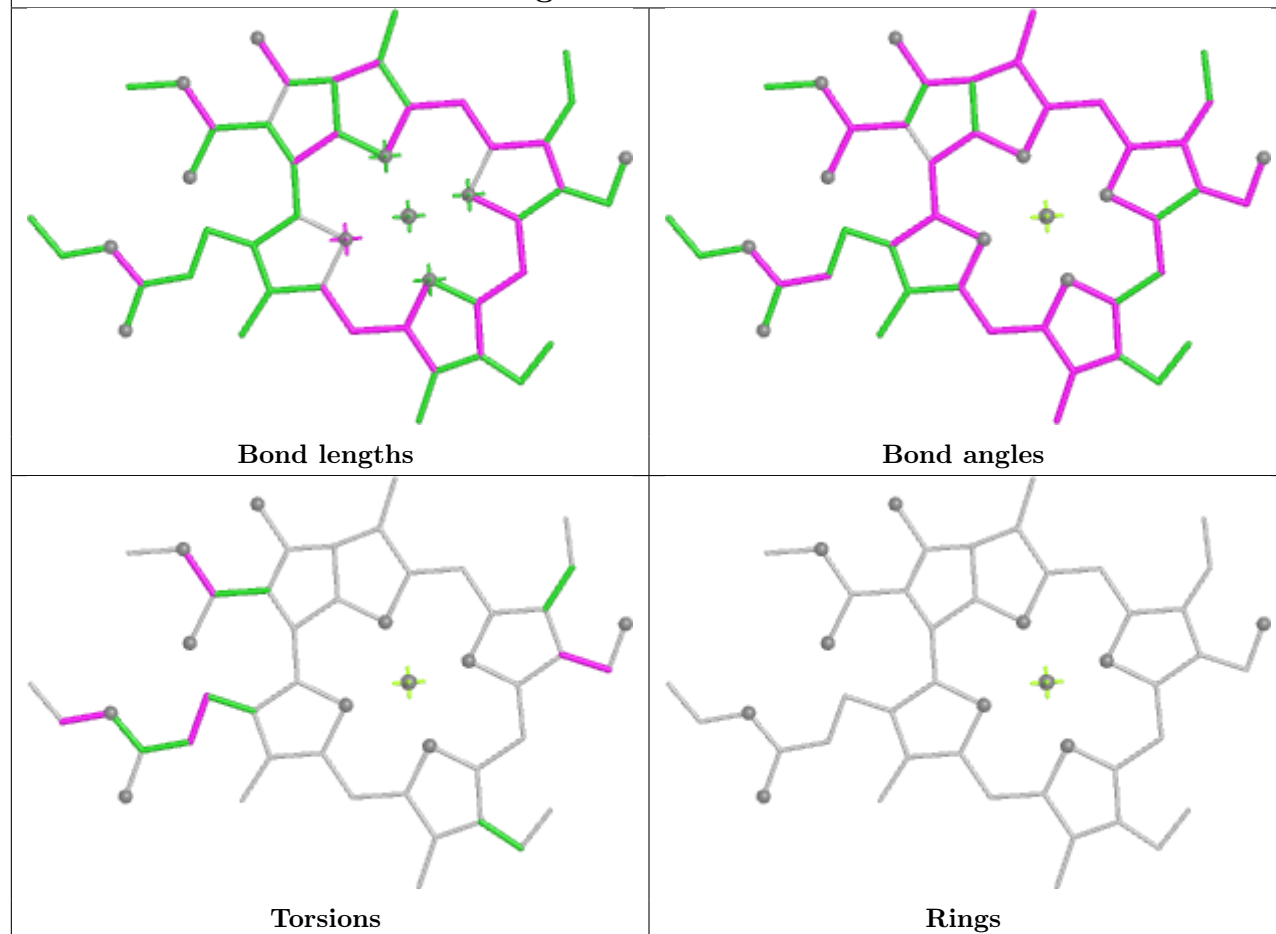


Ligand CLA B 802

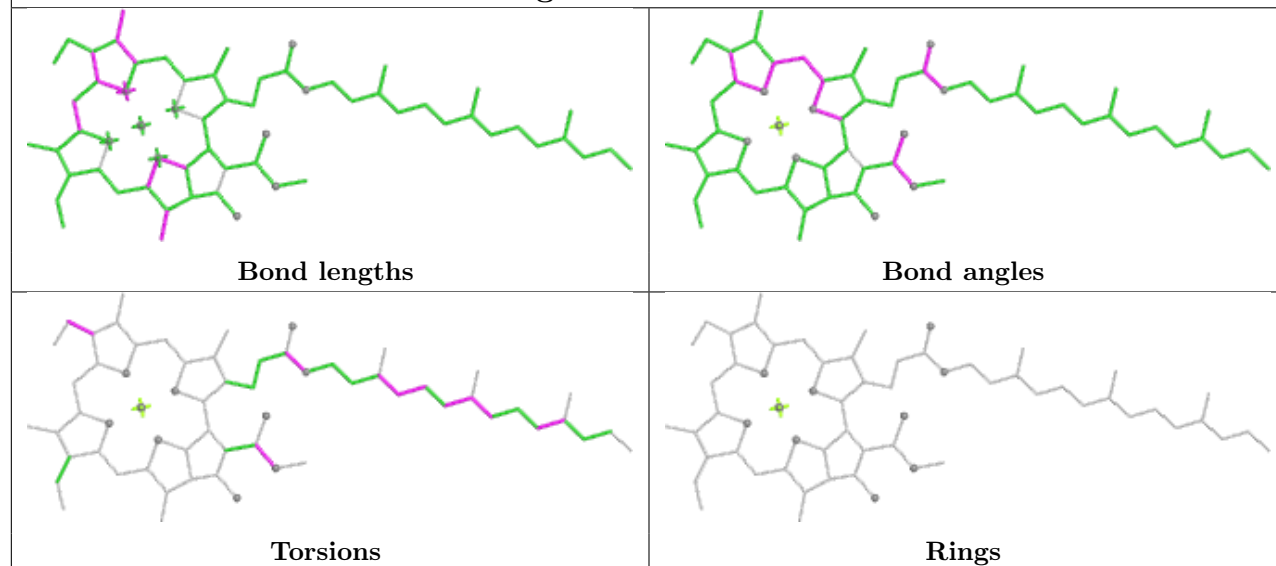




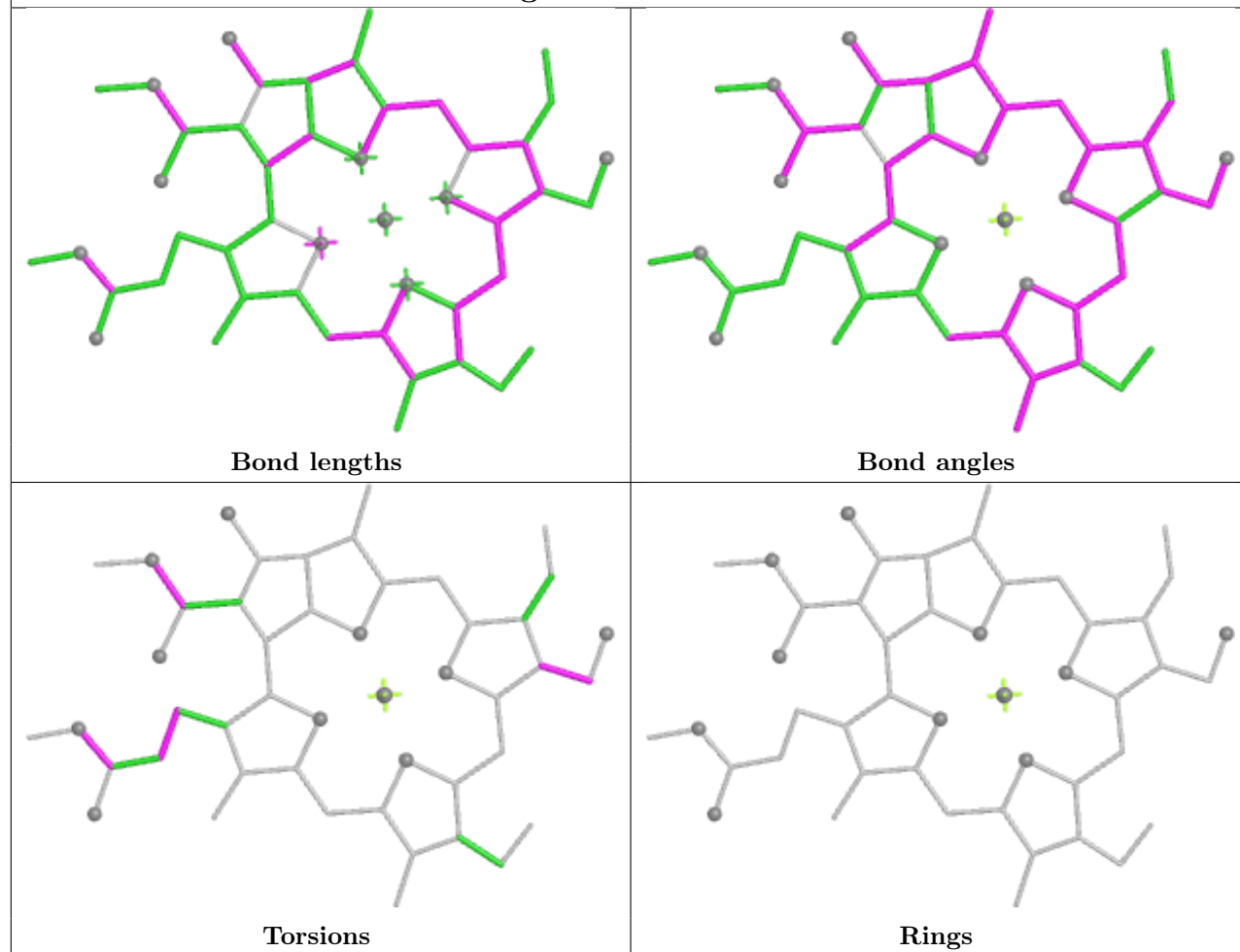
Ligand CHL 4 306



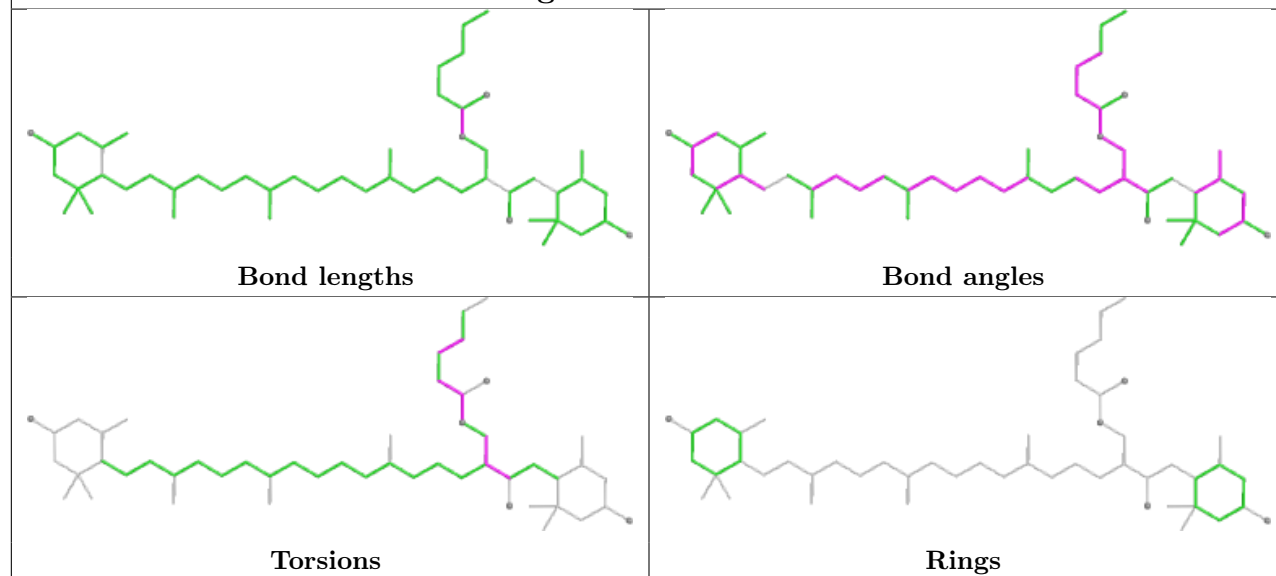
Ligand CLA 3 310



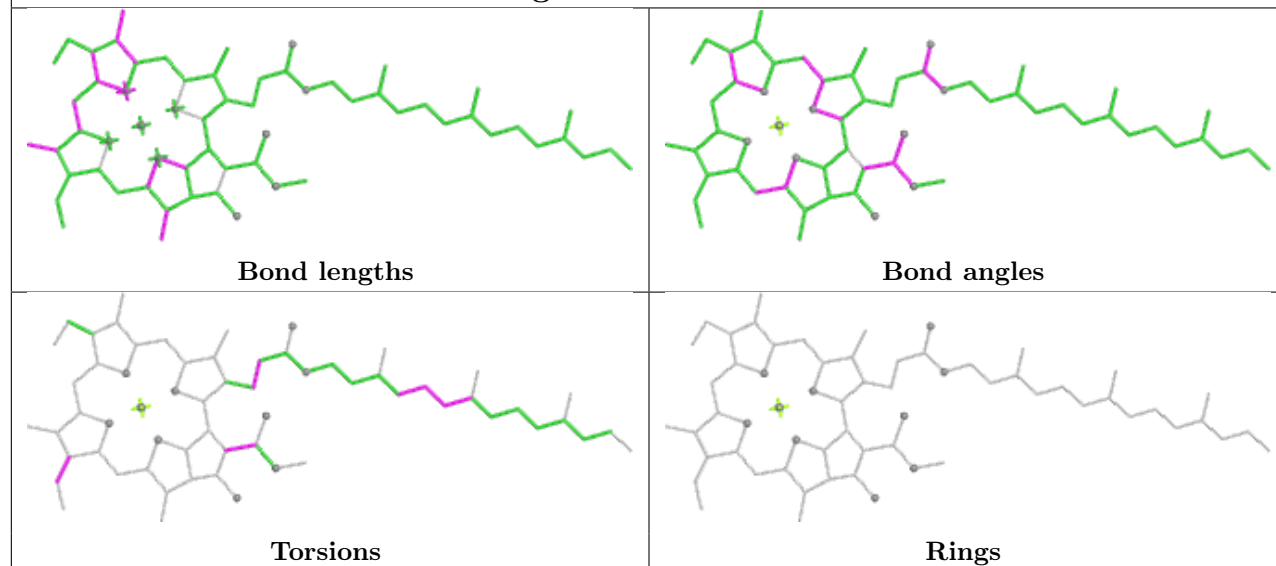
Ligand CHL 7 313



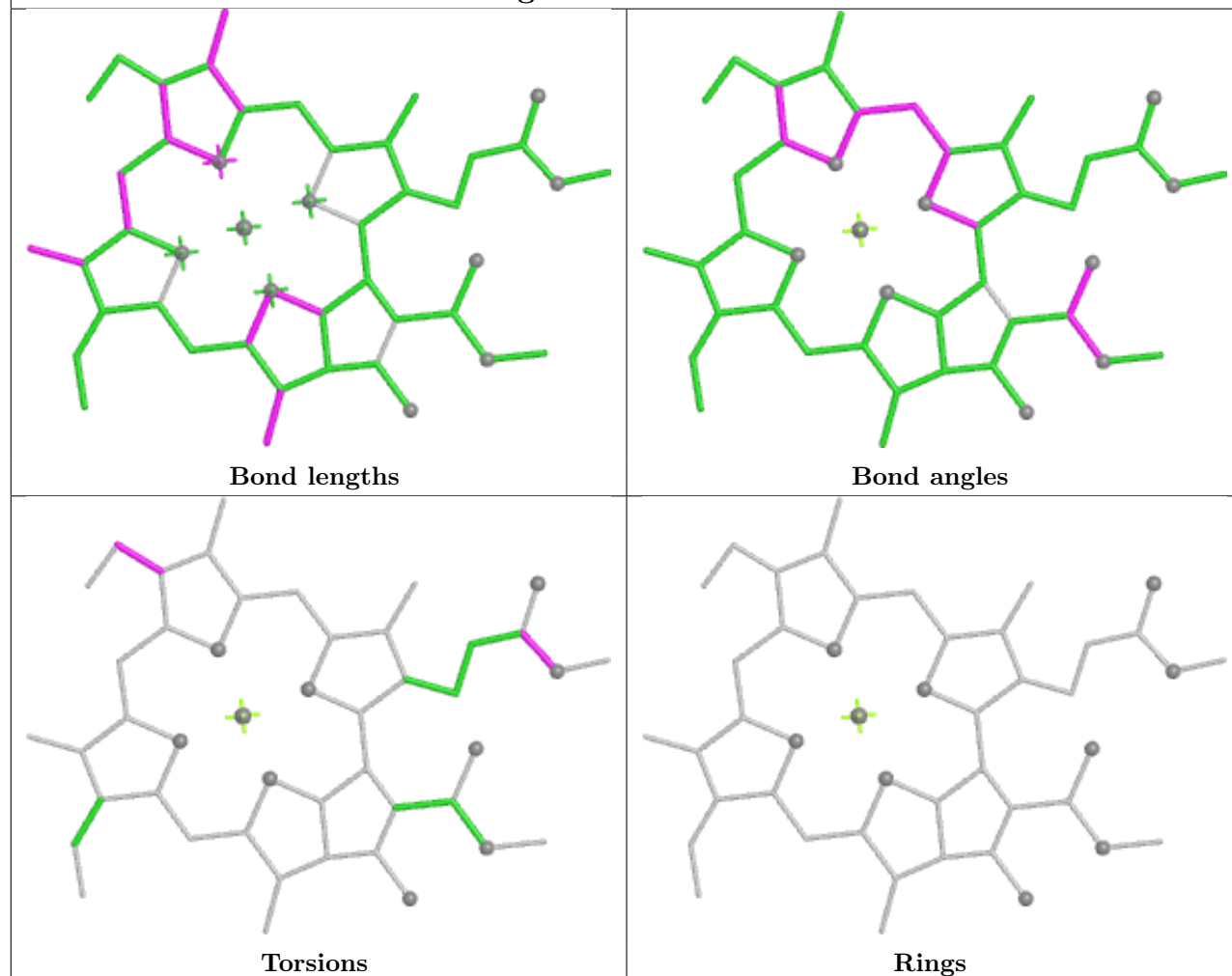
Ligand OUR 3 318

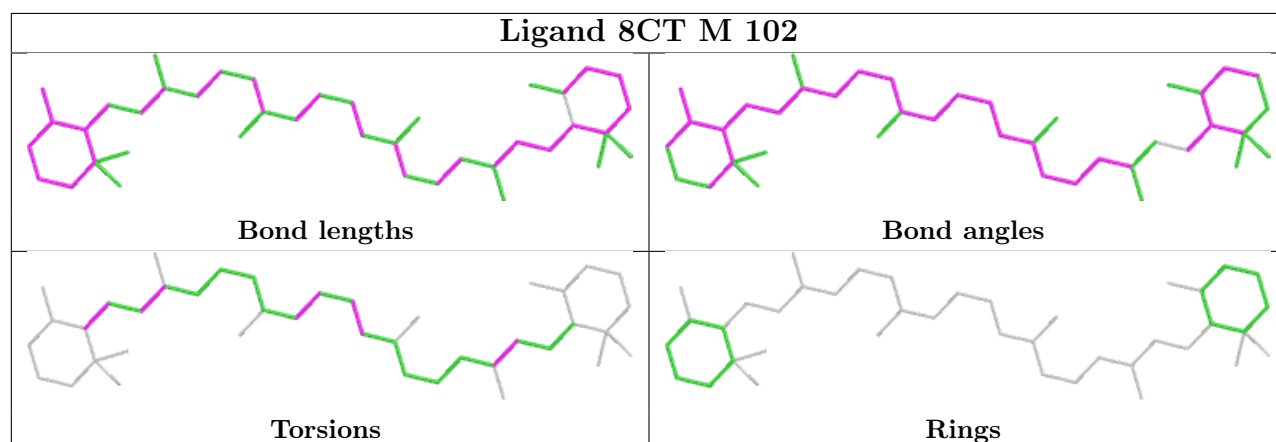
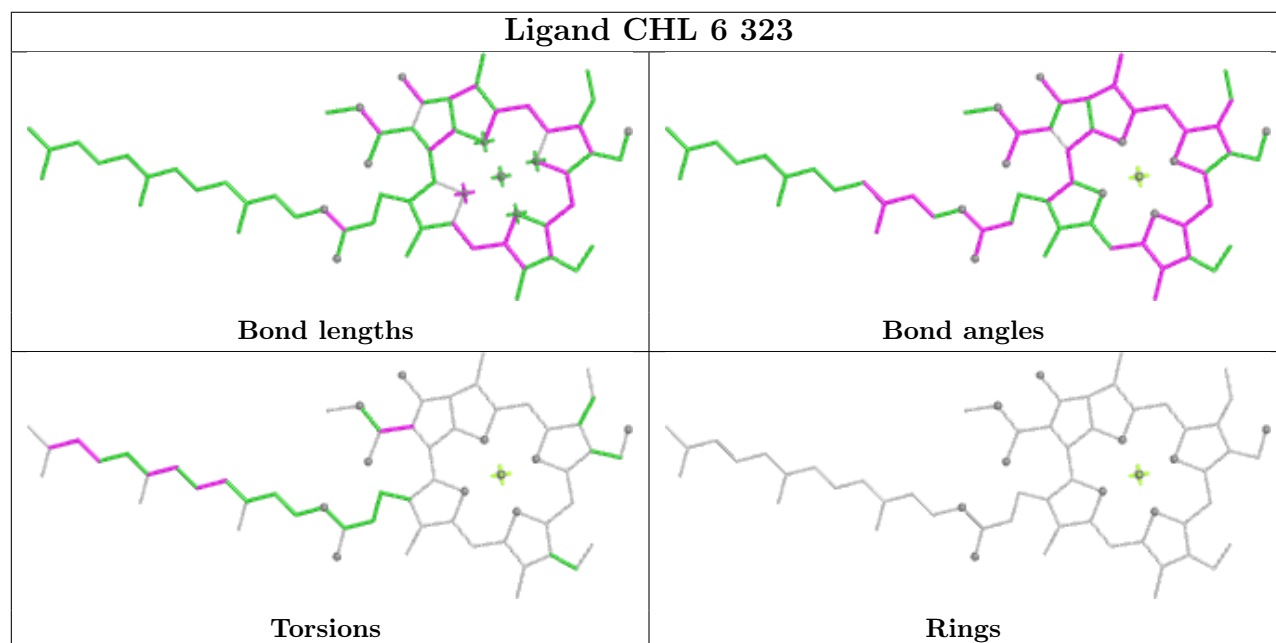
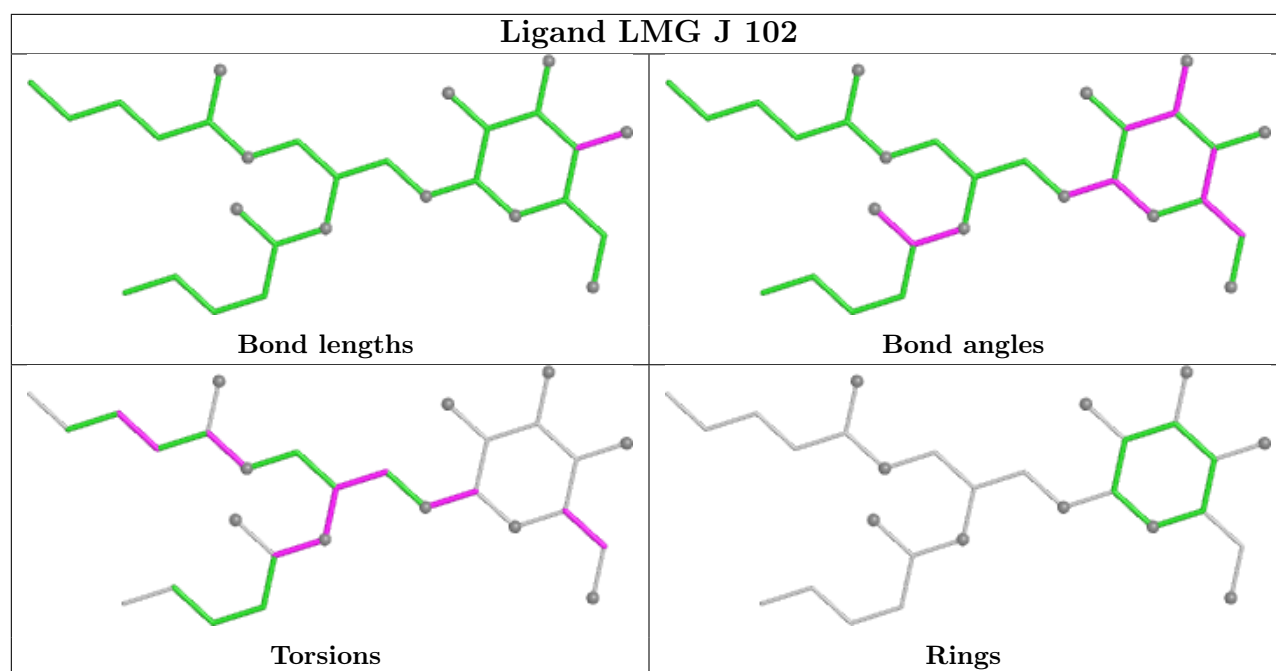


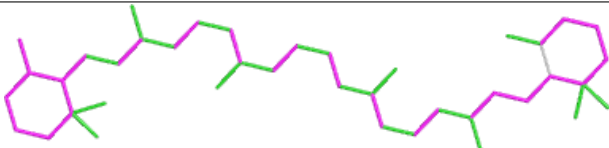
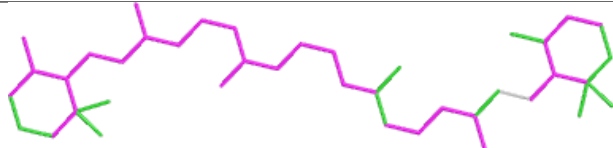
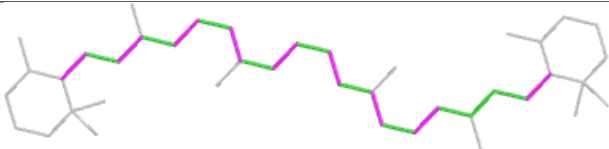
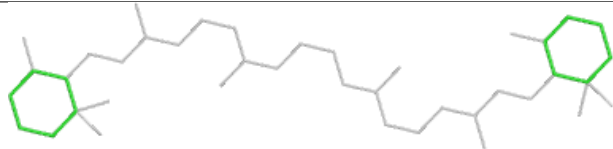
Ligand CLA B 810

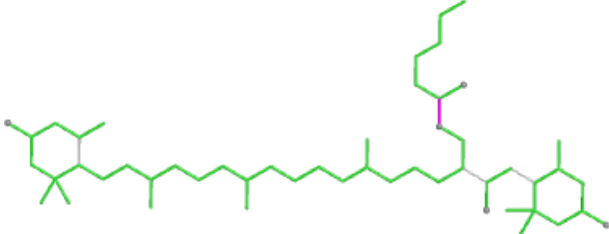
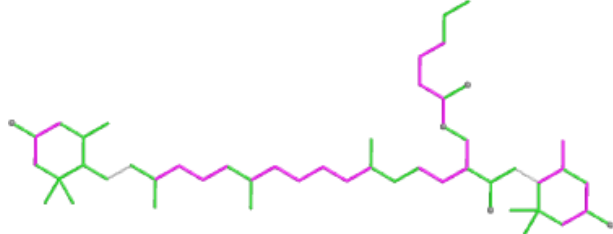
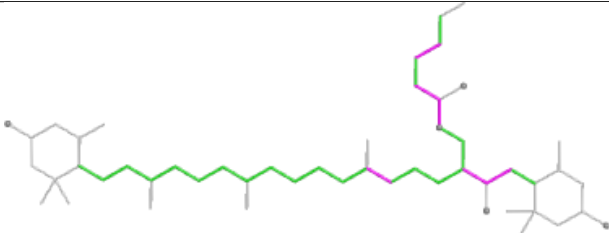
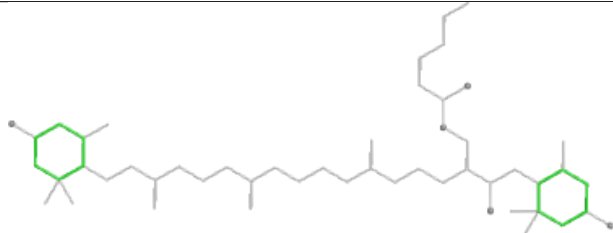


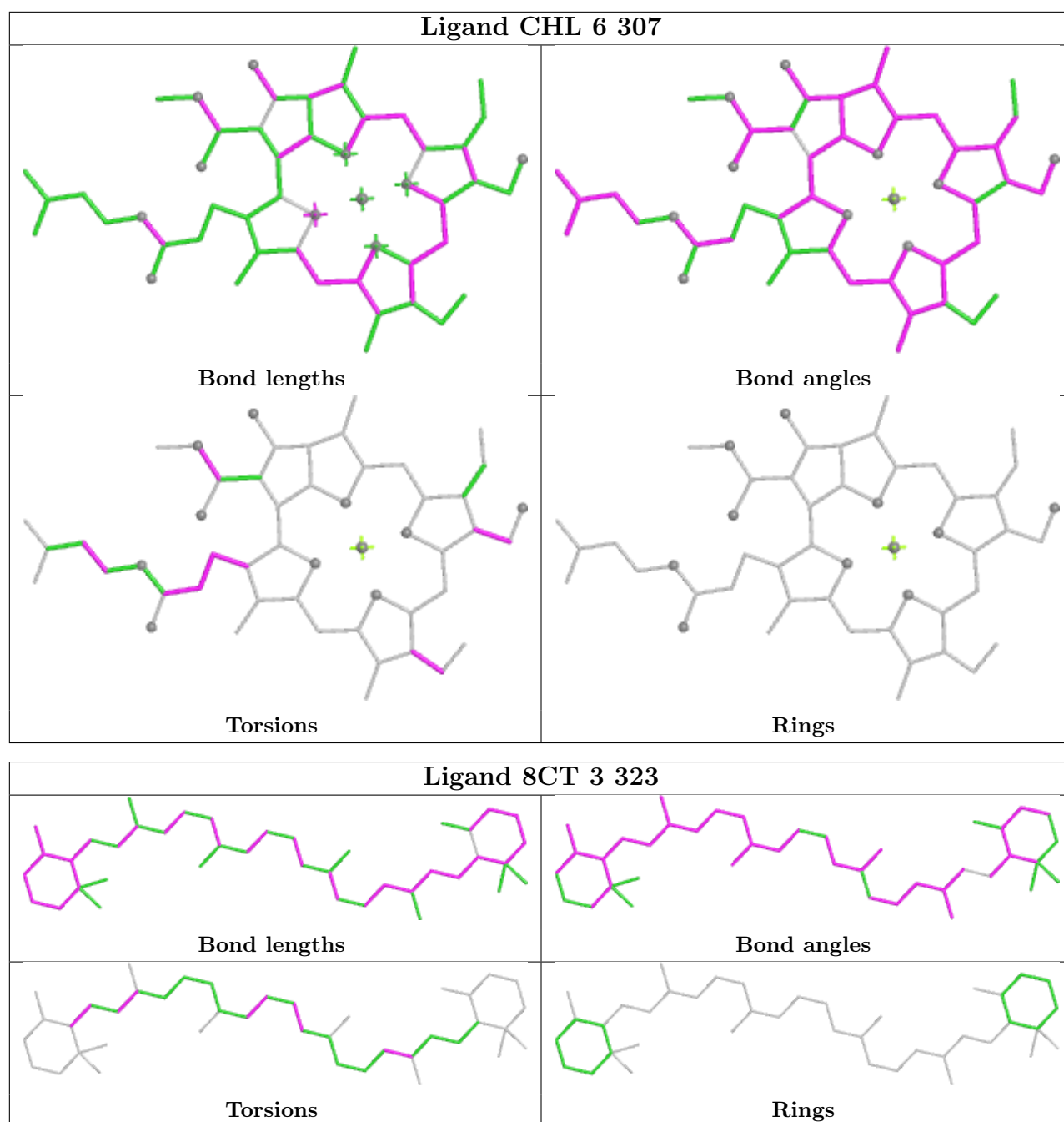
Ligand CLA 8 311

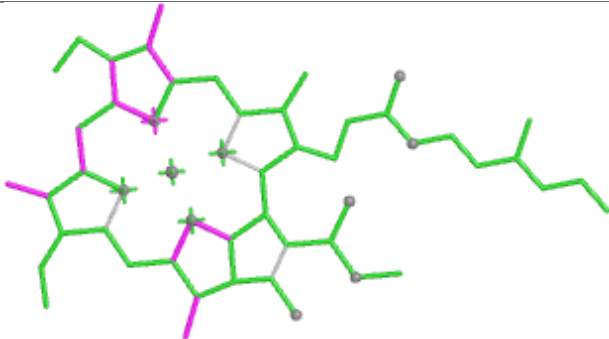
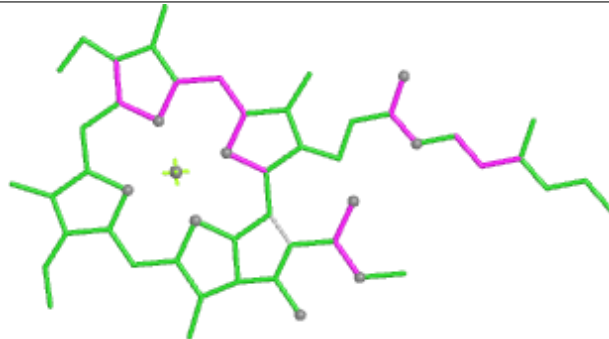
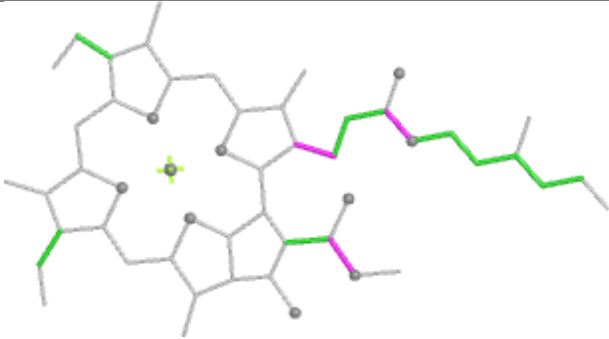
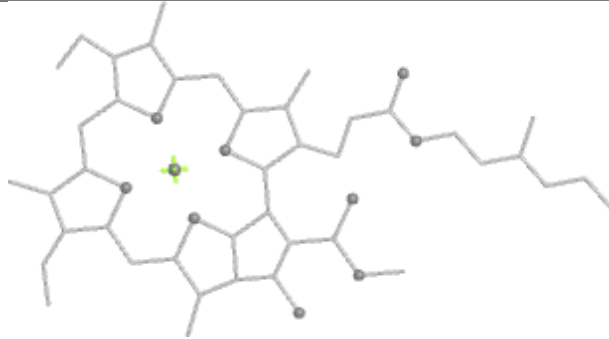


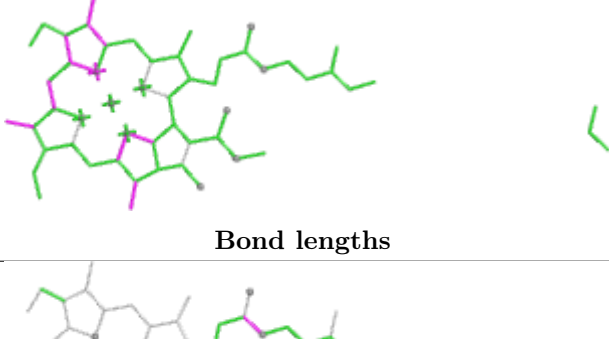
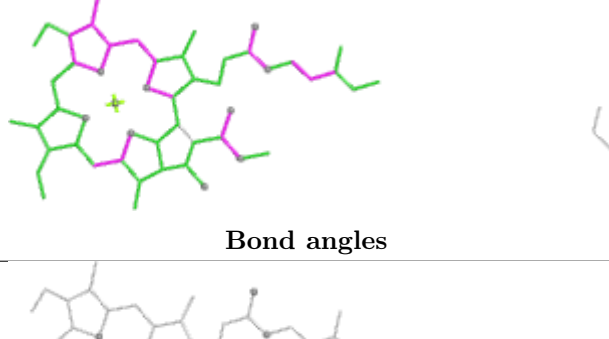
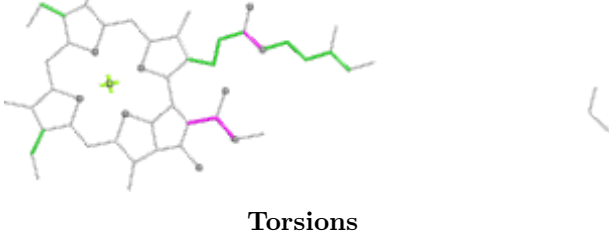
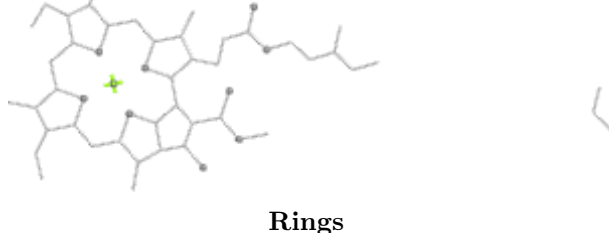


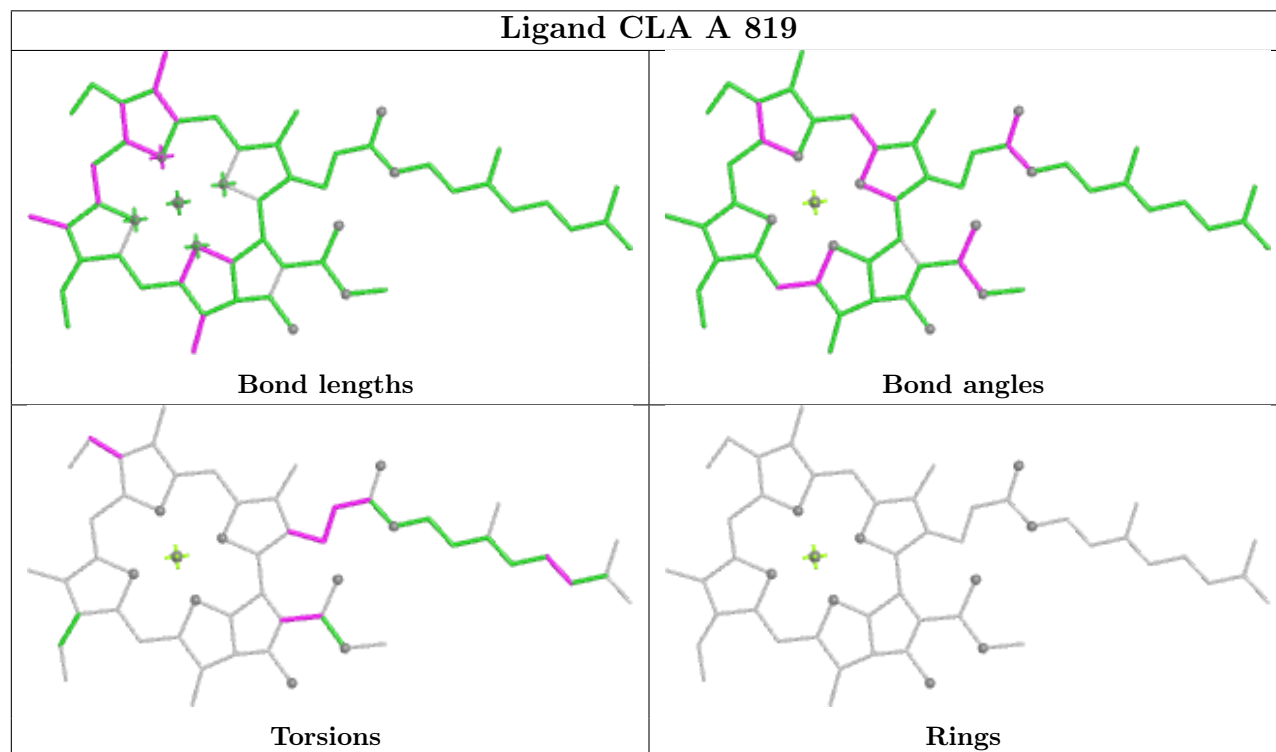
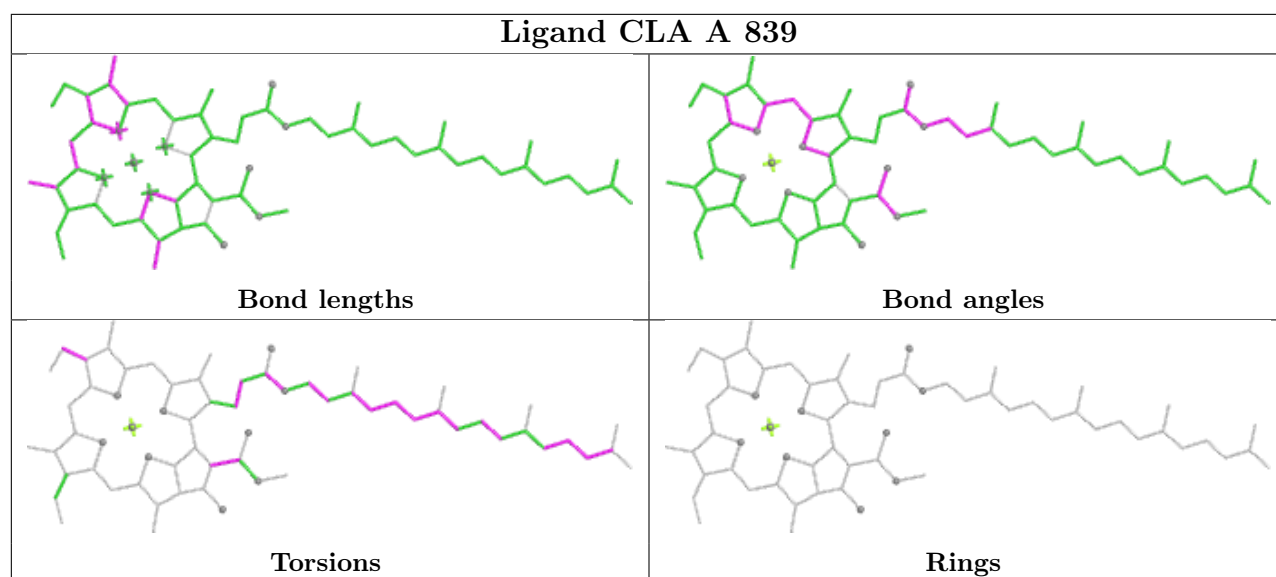
Ligand 8CT K 105	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand 0UR 5 314	
	Bond lengths
	Bond angles
	Torsions
	Rings

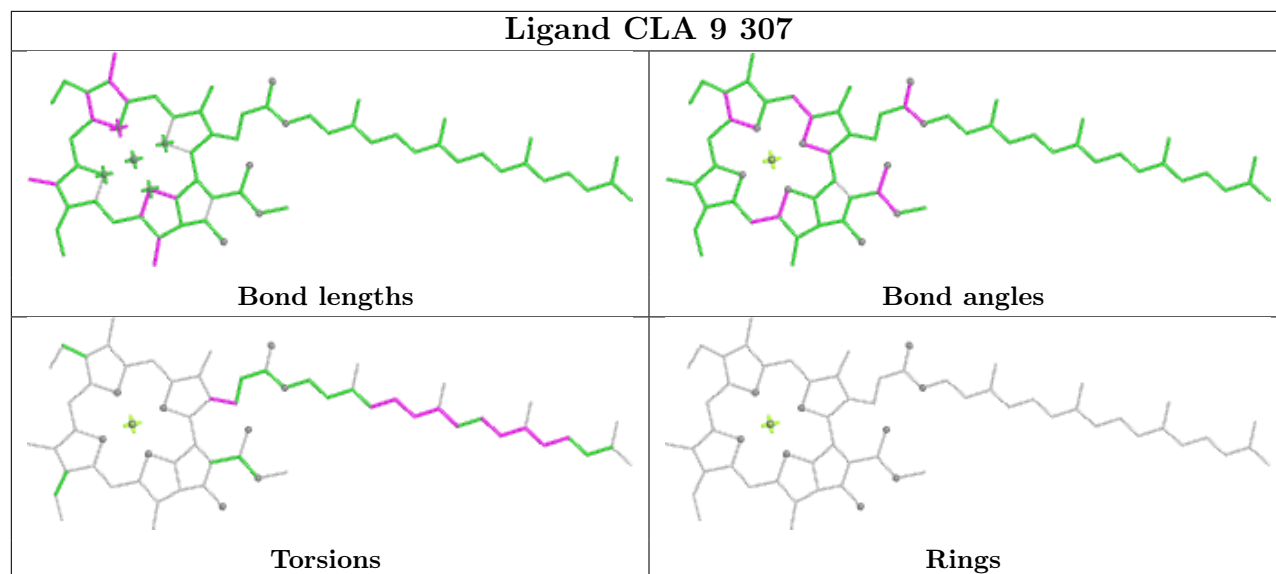


Ligand CLA 9 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

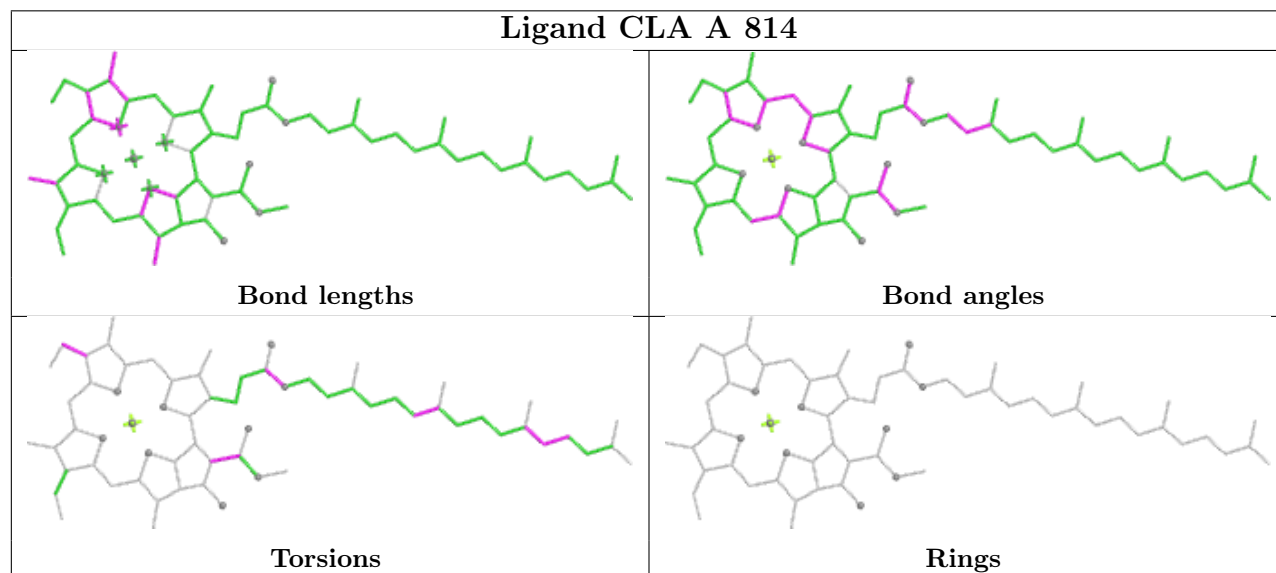
Ligand CLA A 806	
	
Bond lengths	Bond angles
	
Torsions	Rings



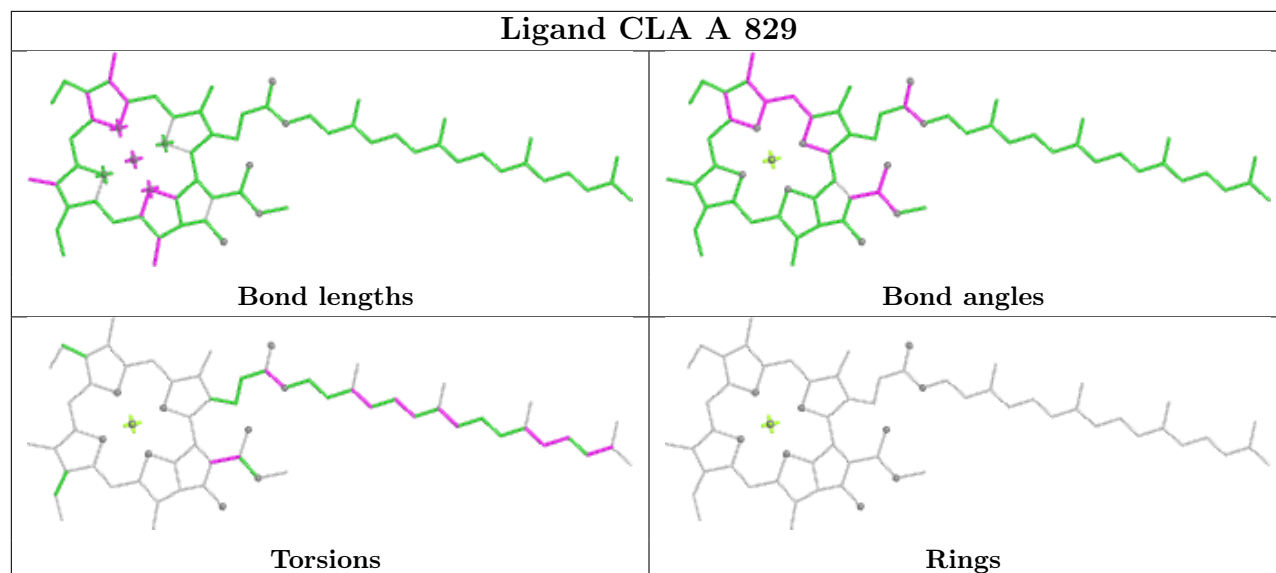
Ligand CLA 9 307

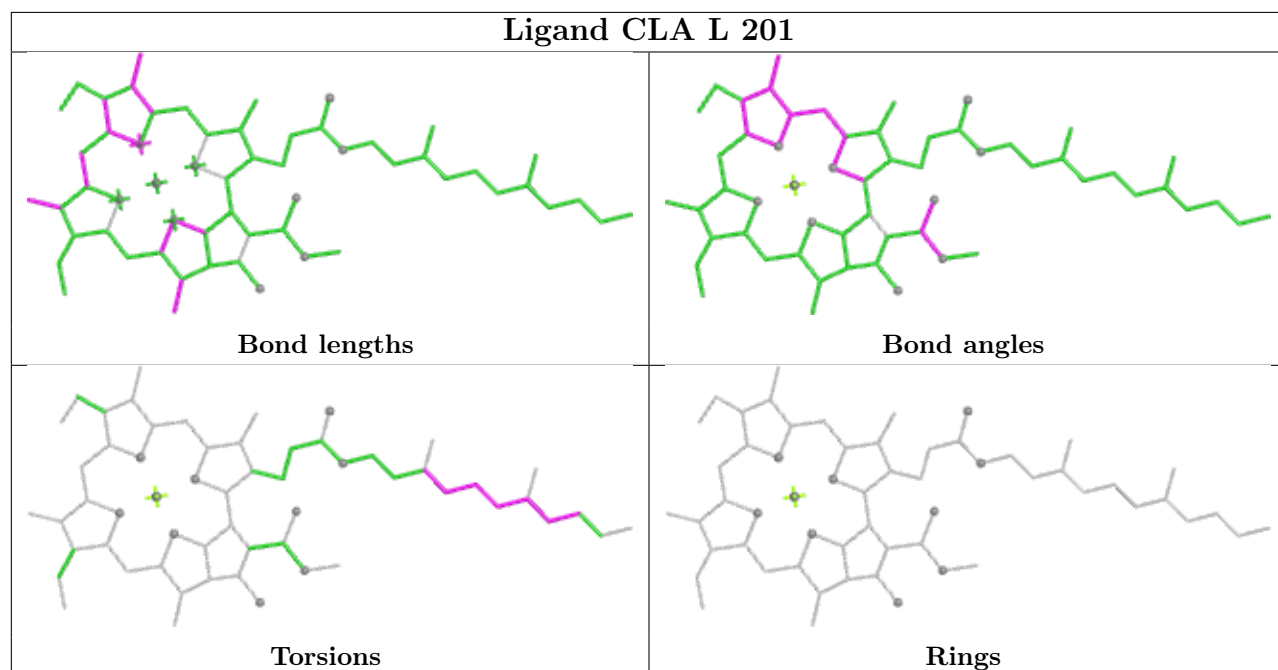
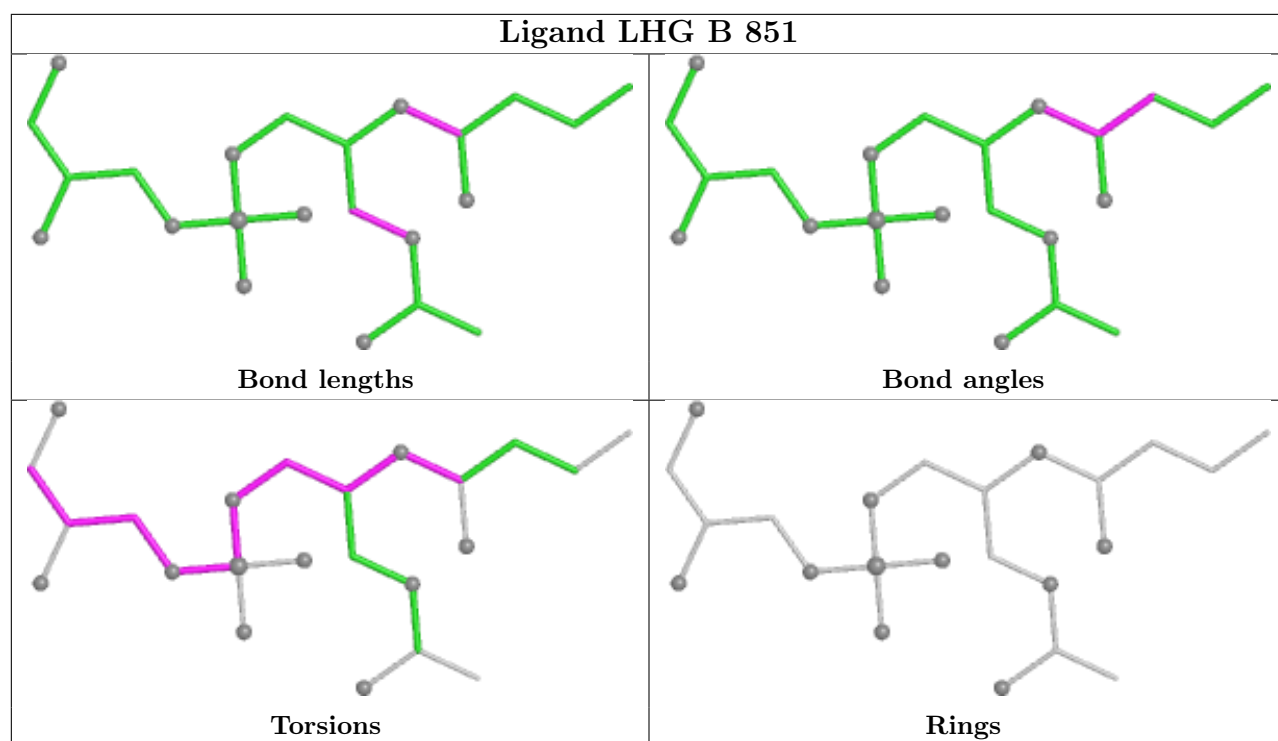


Ligand CLA A 814

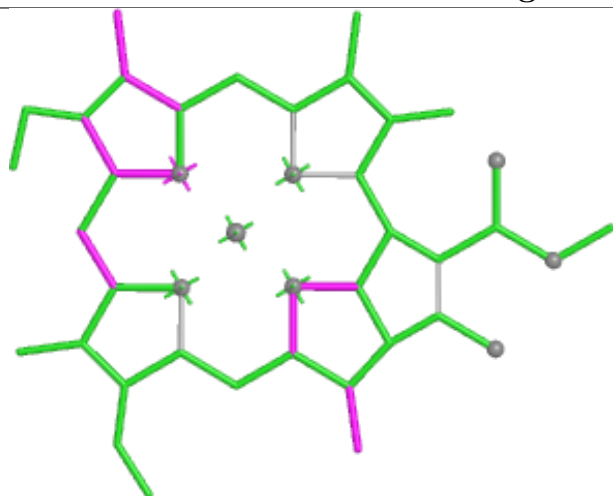


Ligand CLA A 829

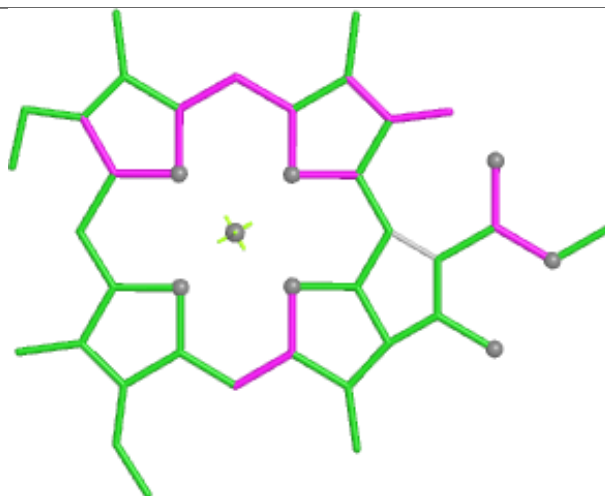




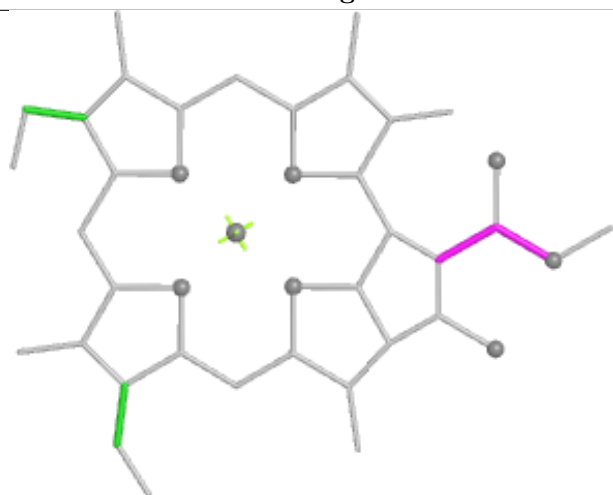
Ligand CLA 0 309



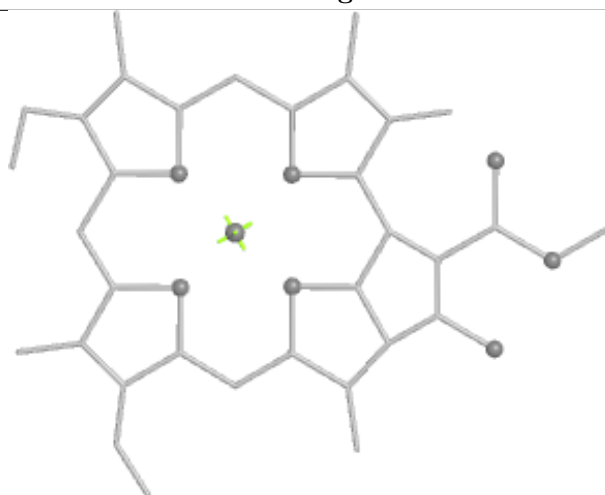
Bond lengths



Bond angles

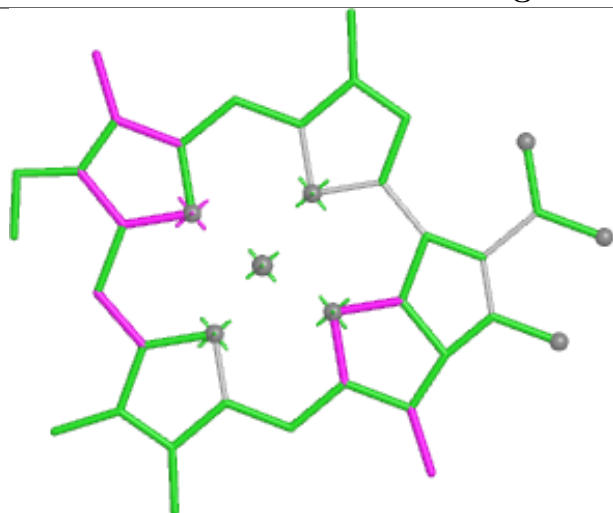


Torsions

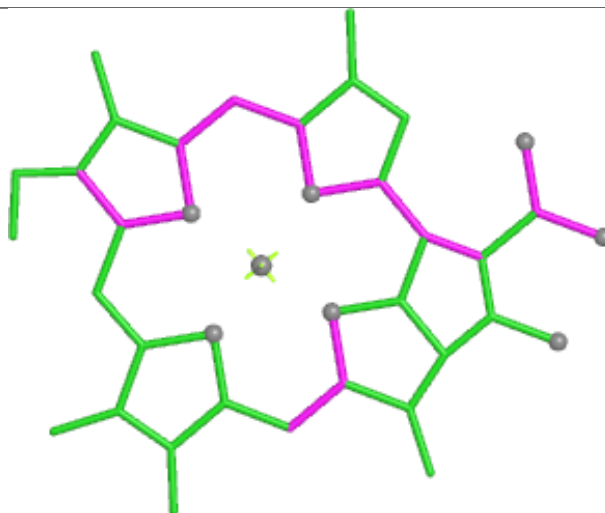


Rings

Ligand CLA O 205



Bond lengths



Bond angles

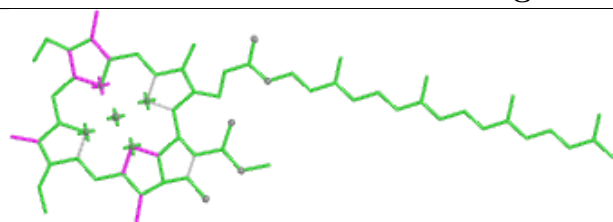


Torsions

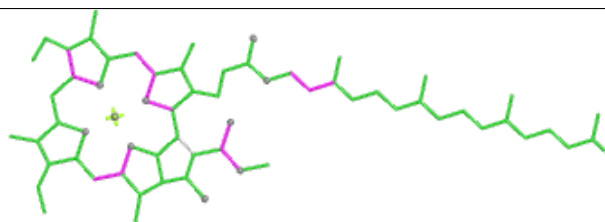


Rings

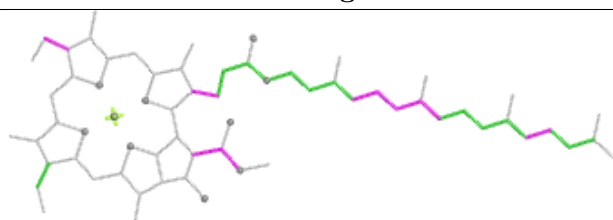
Ligand CLA A 831



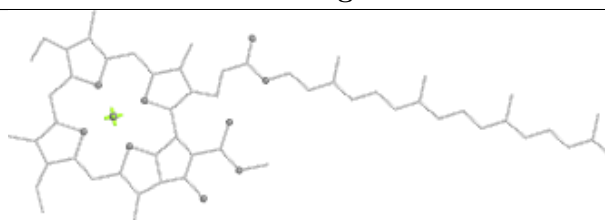
Bond lengths



Bond angles

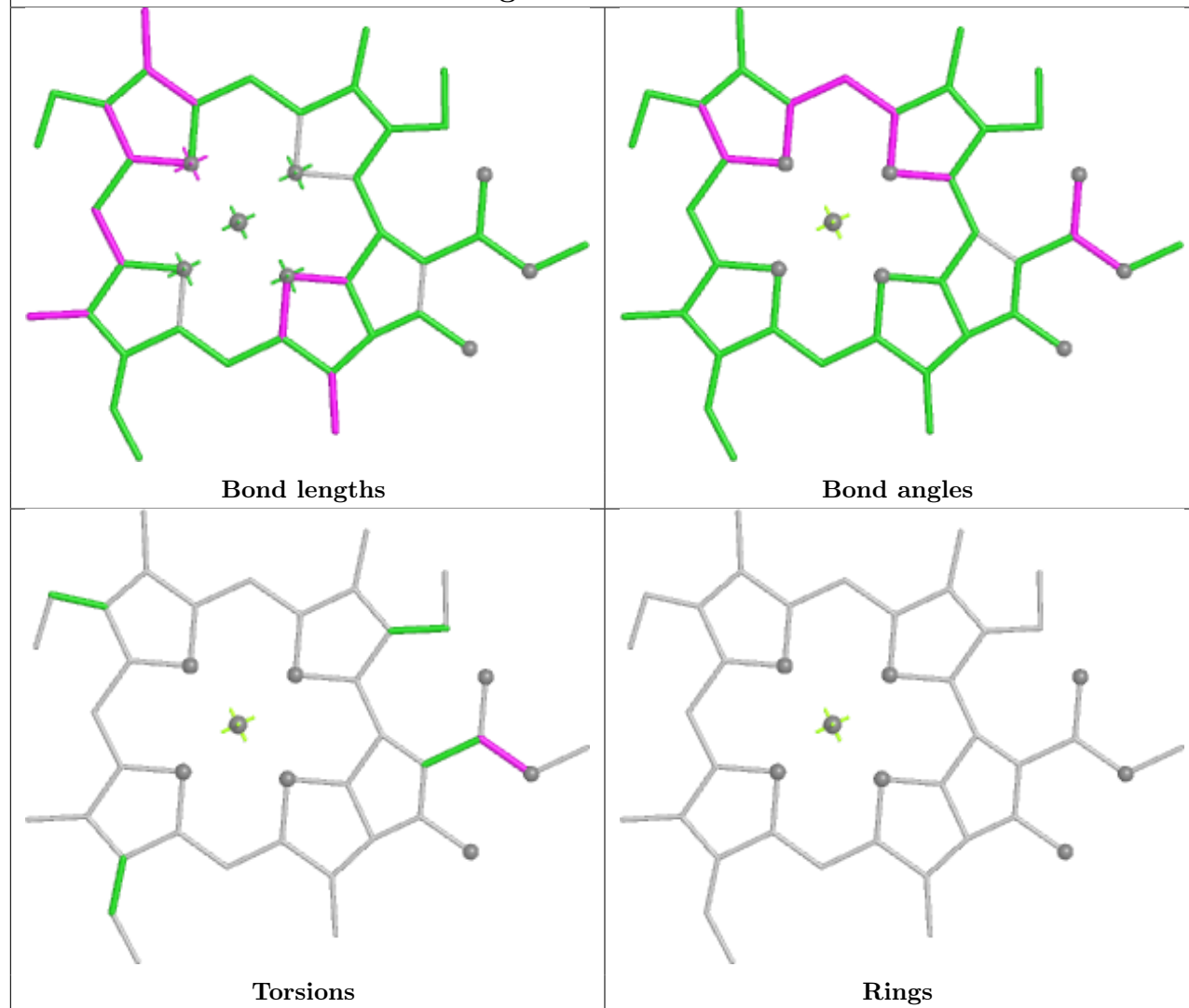


Torsions

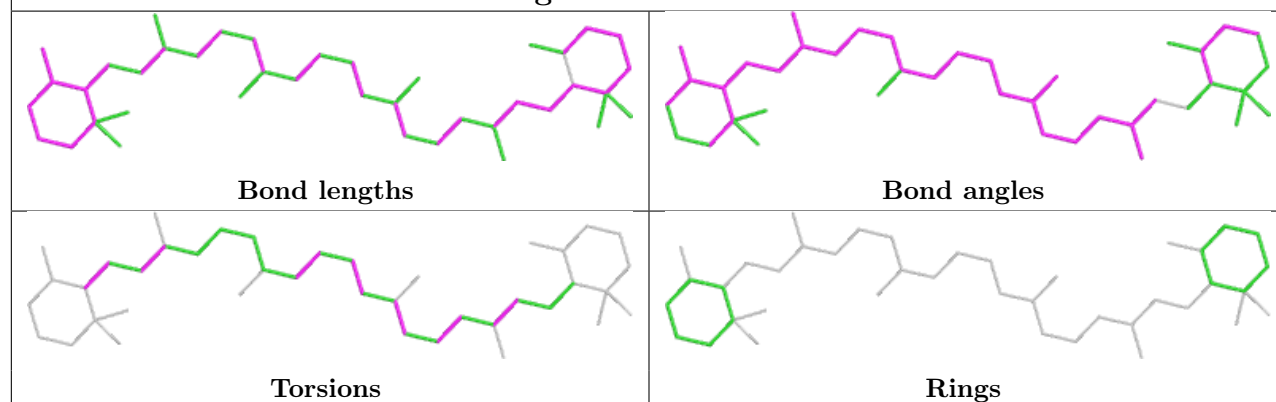


Rings

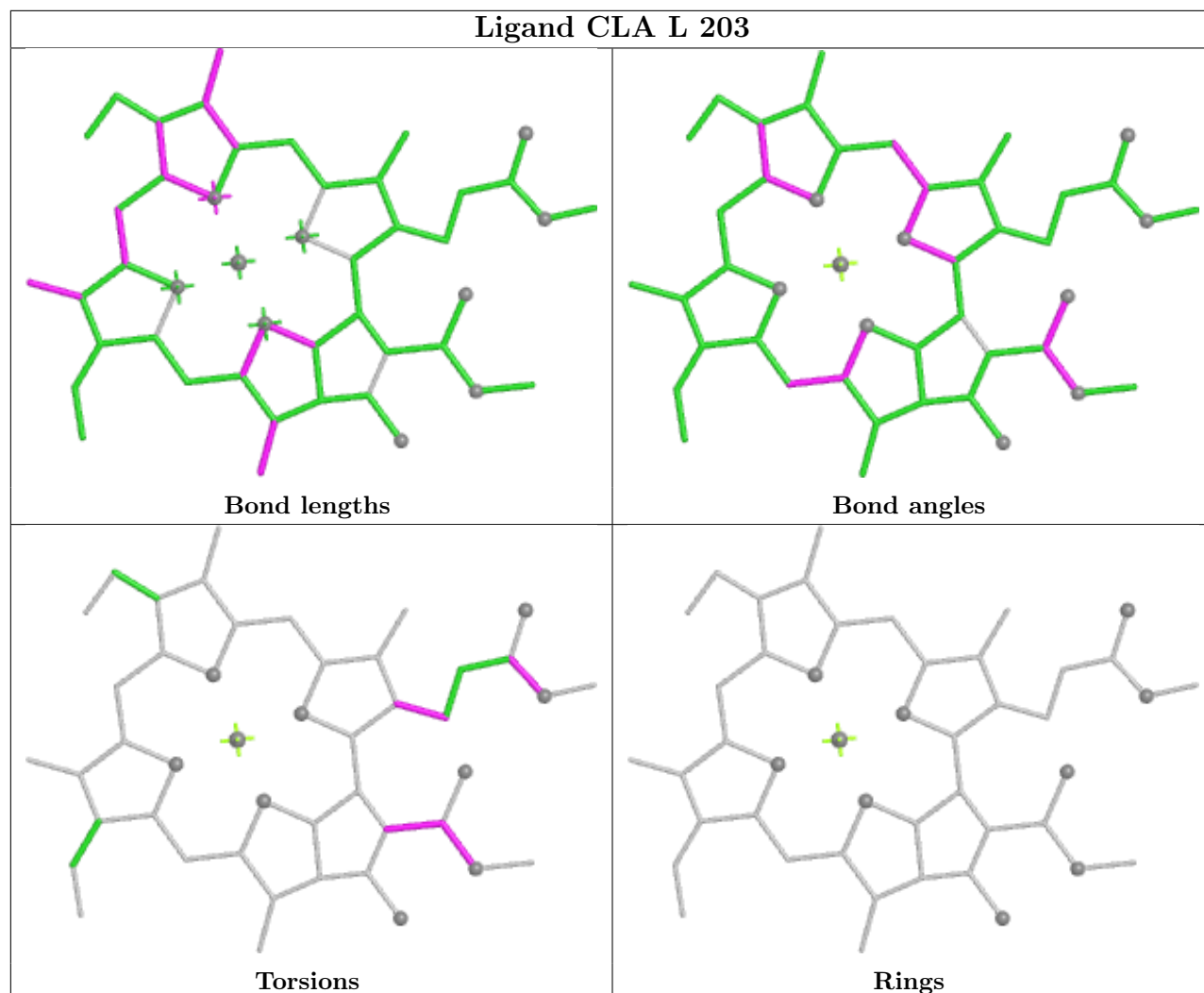
Ligand CLA J 103



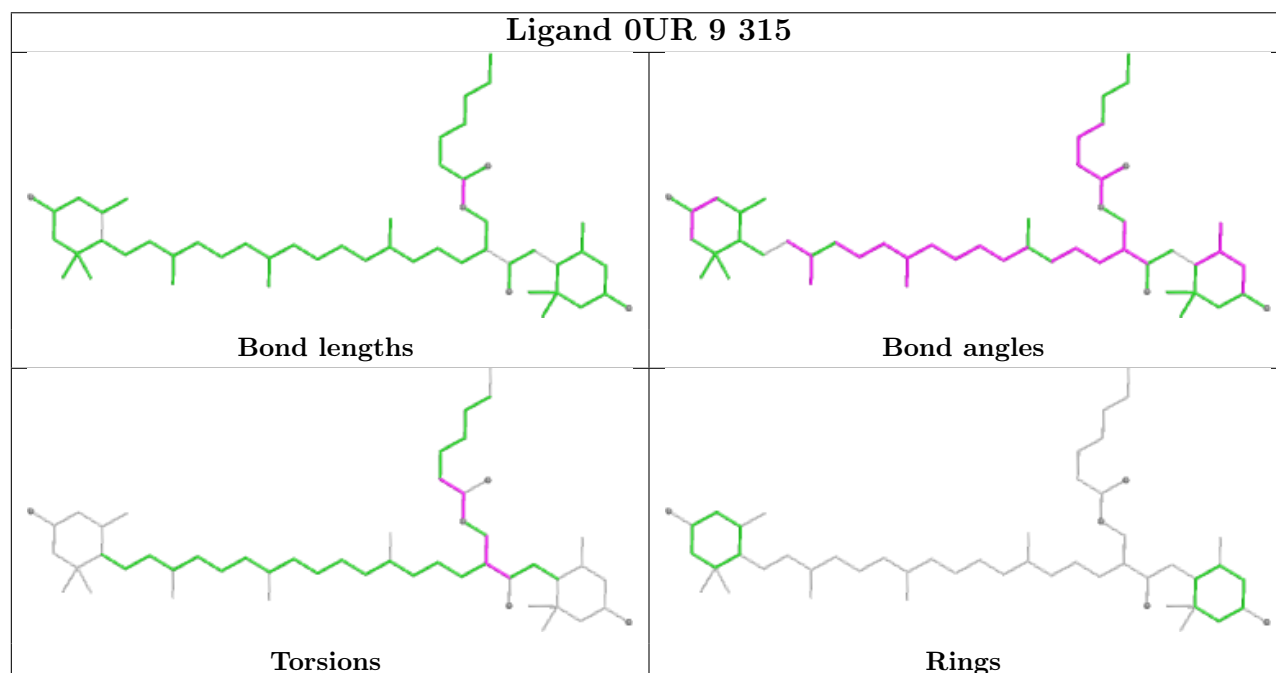
Ligand 8CT A 849

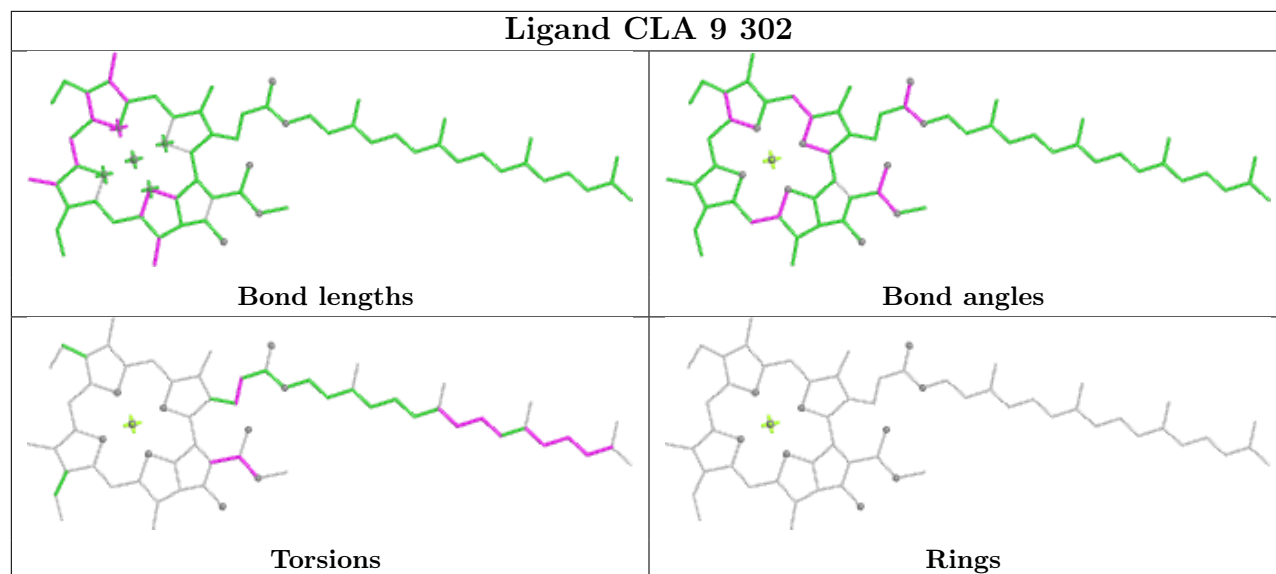
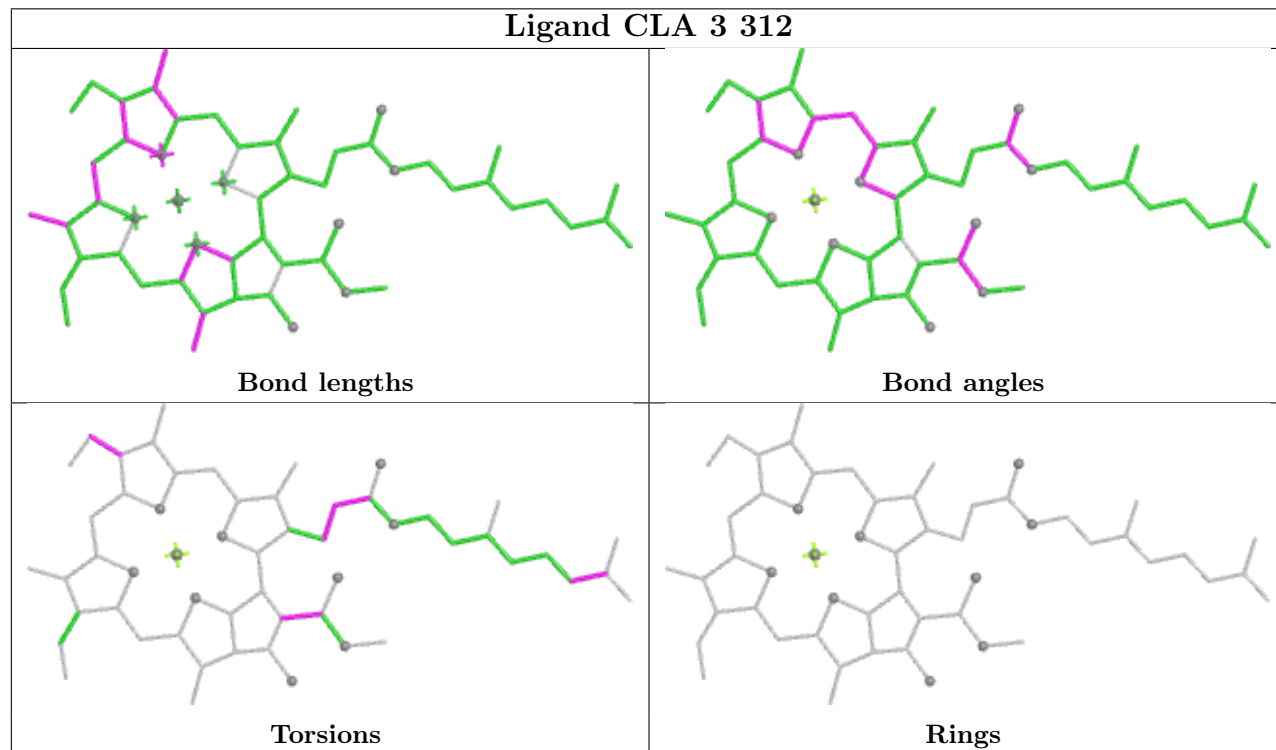


Ligand CLA L 203

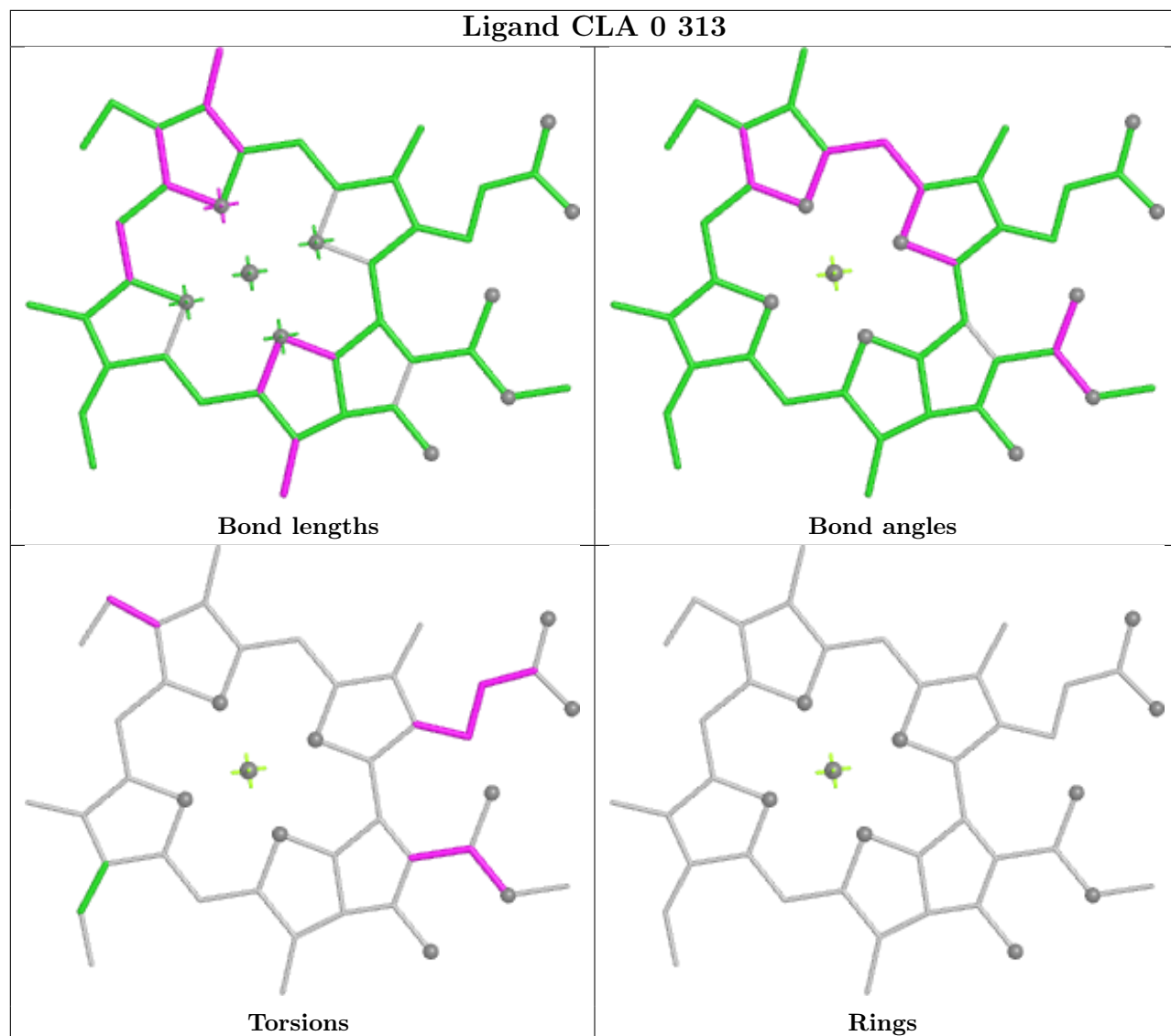


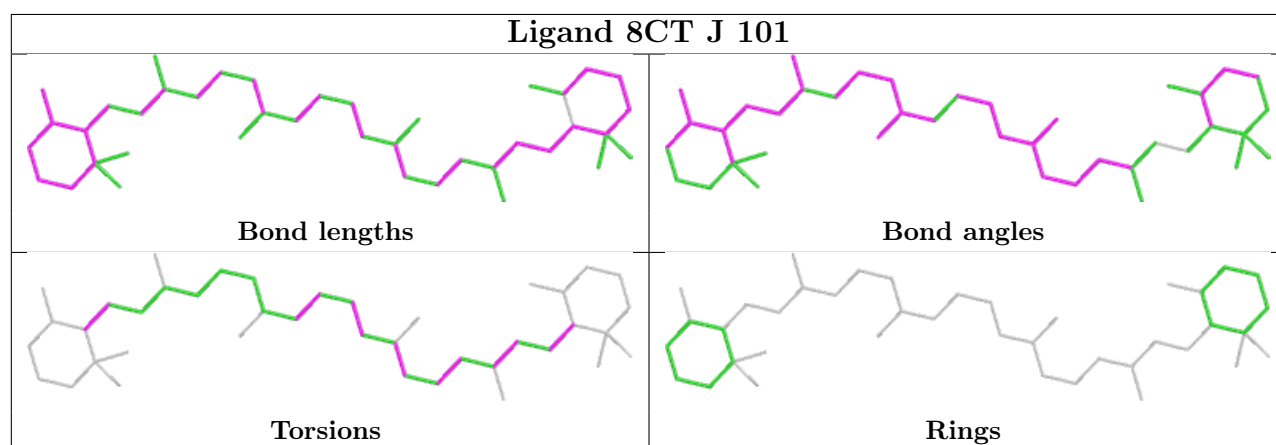
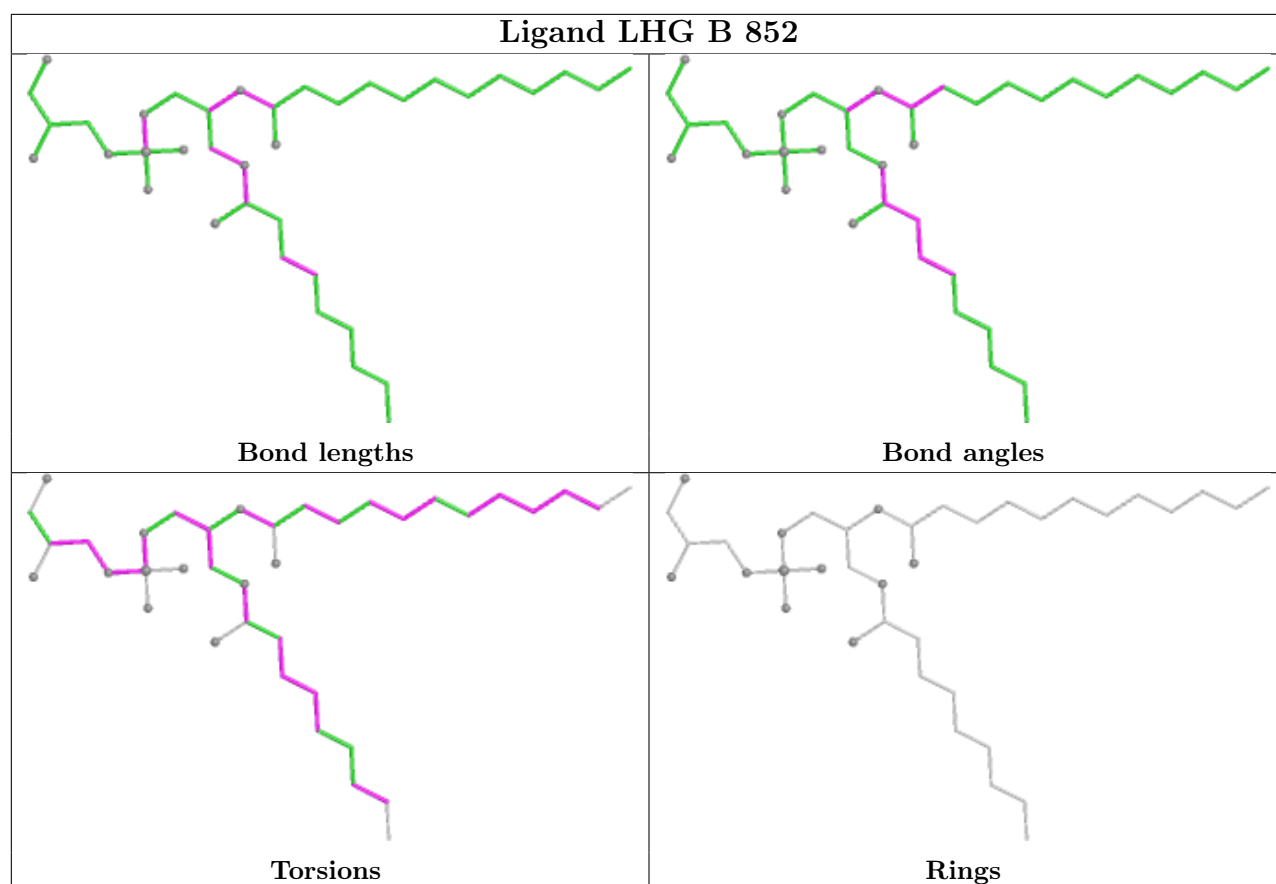
Ligand OUR 9 315

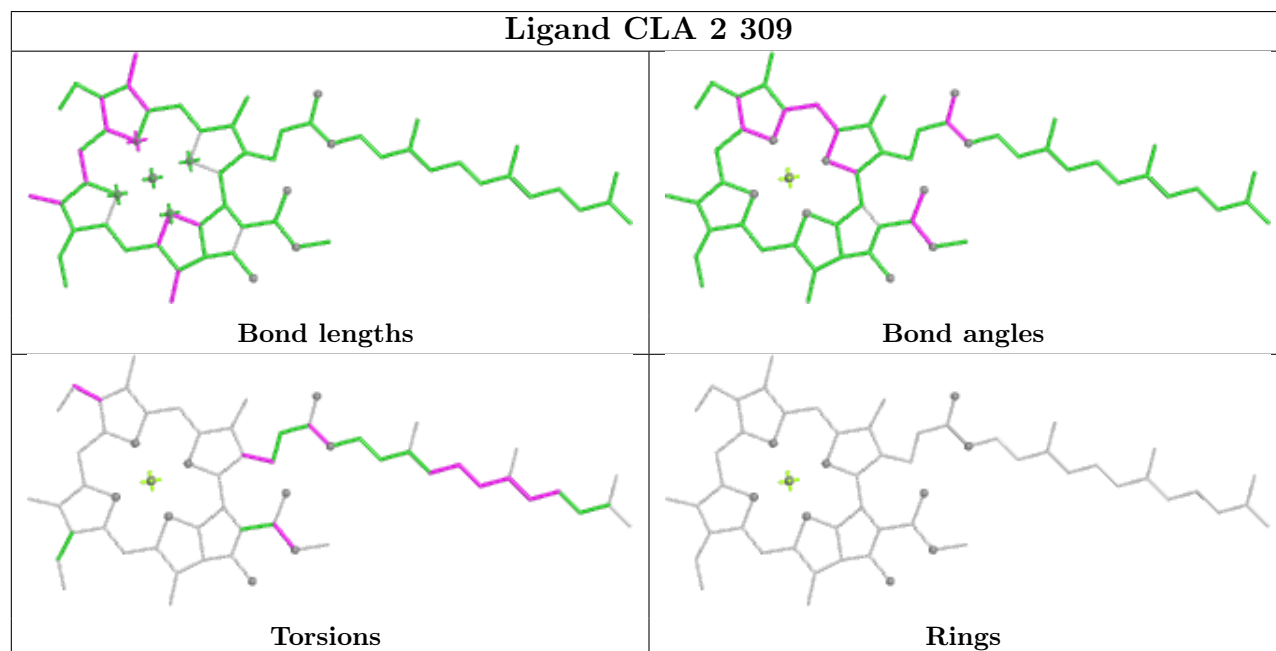
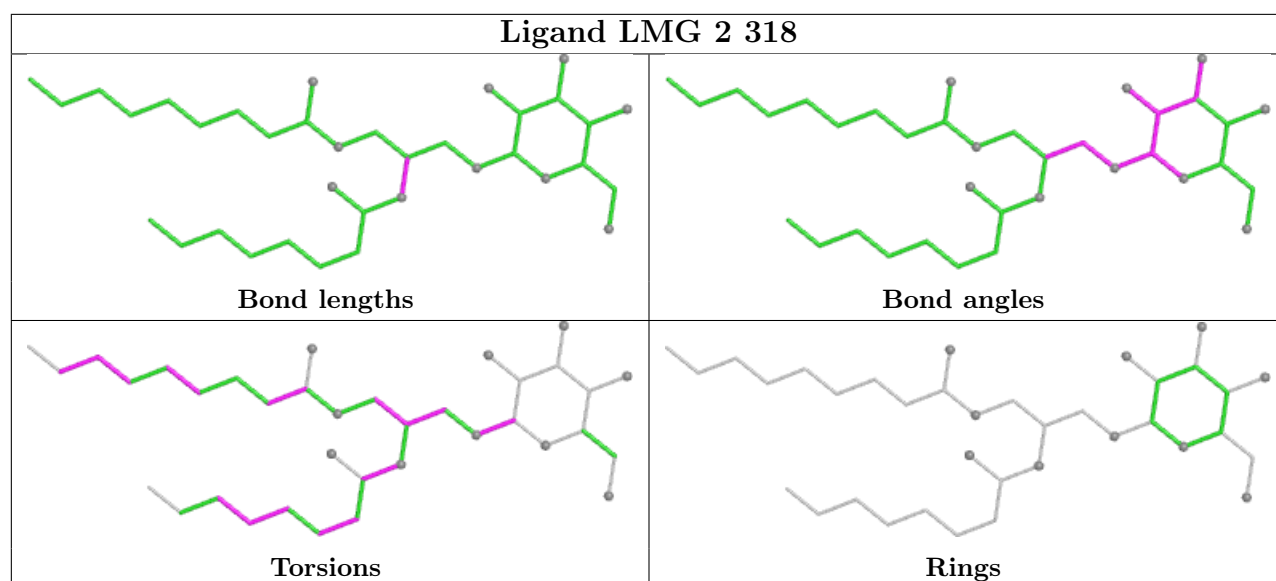


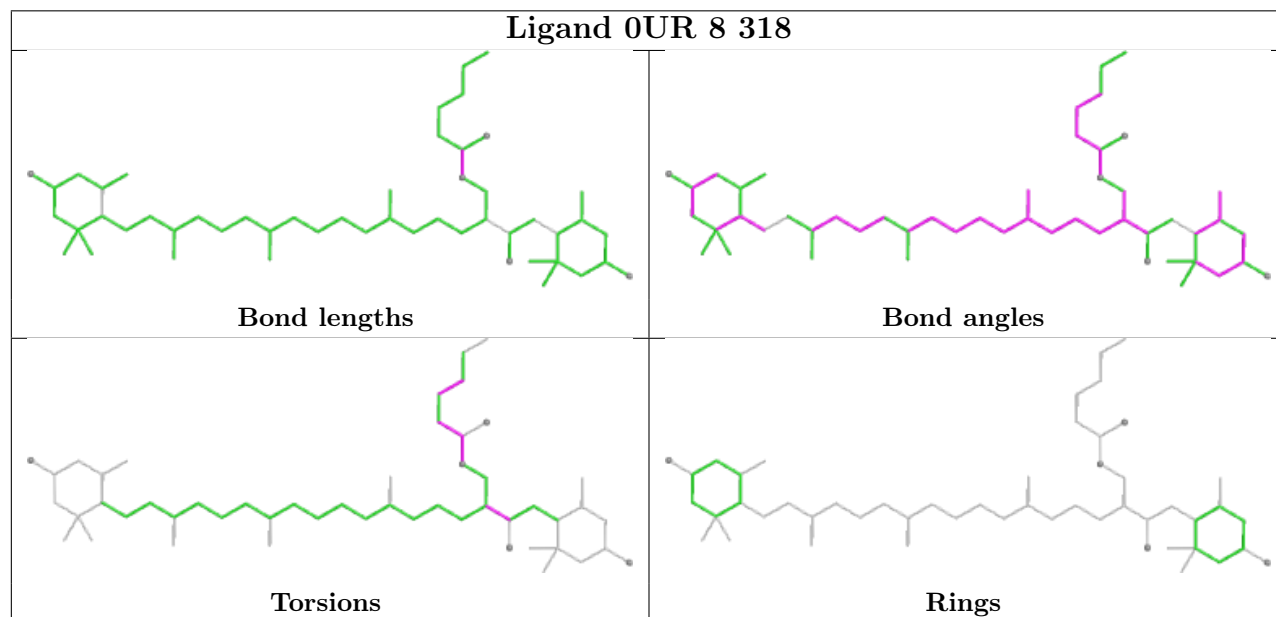
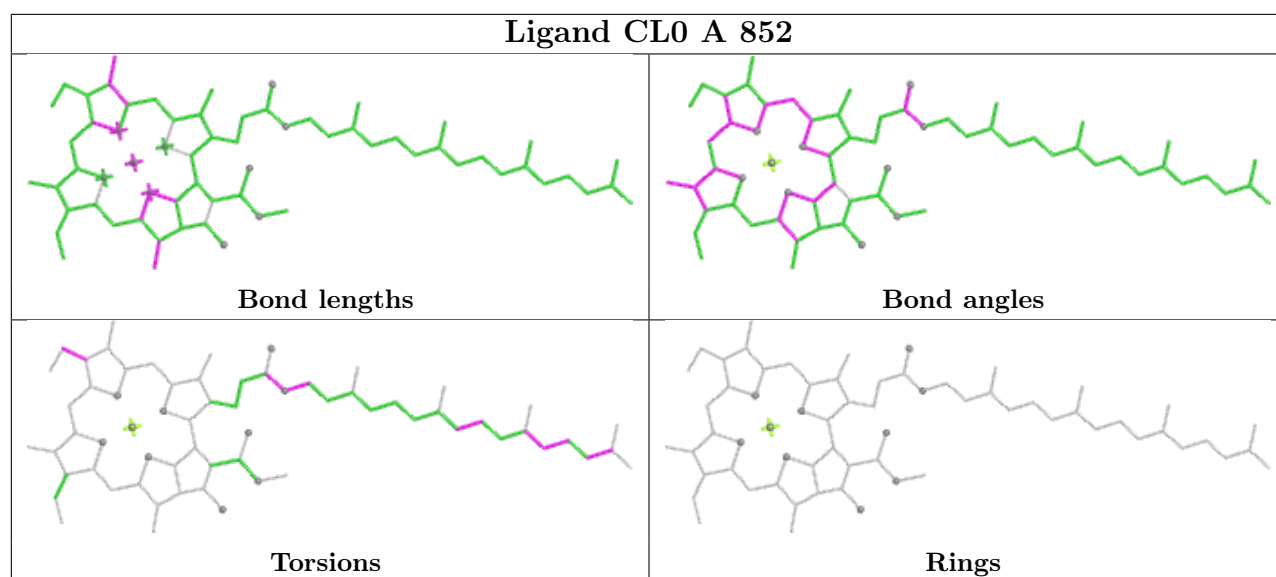
Ligand CLA 9 302**Ligand CLA 3 312**

Ligand CLA 0 313

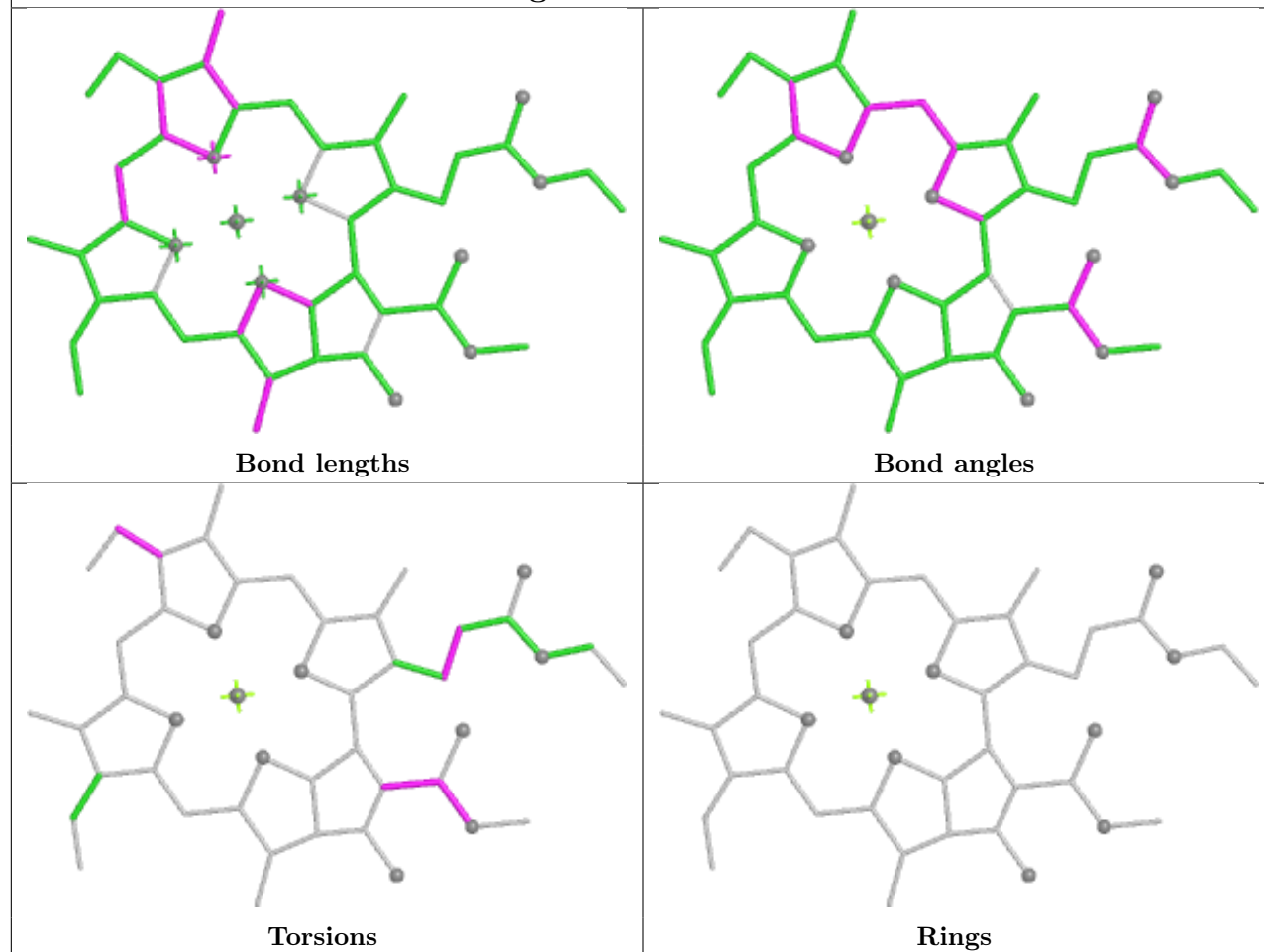




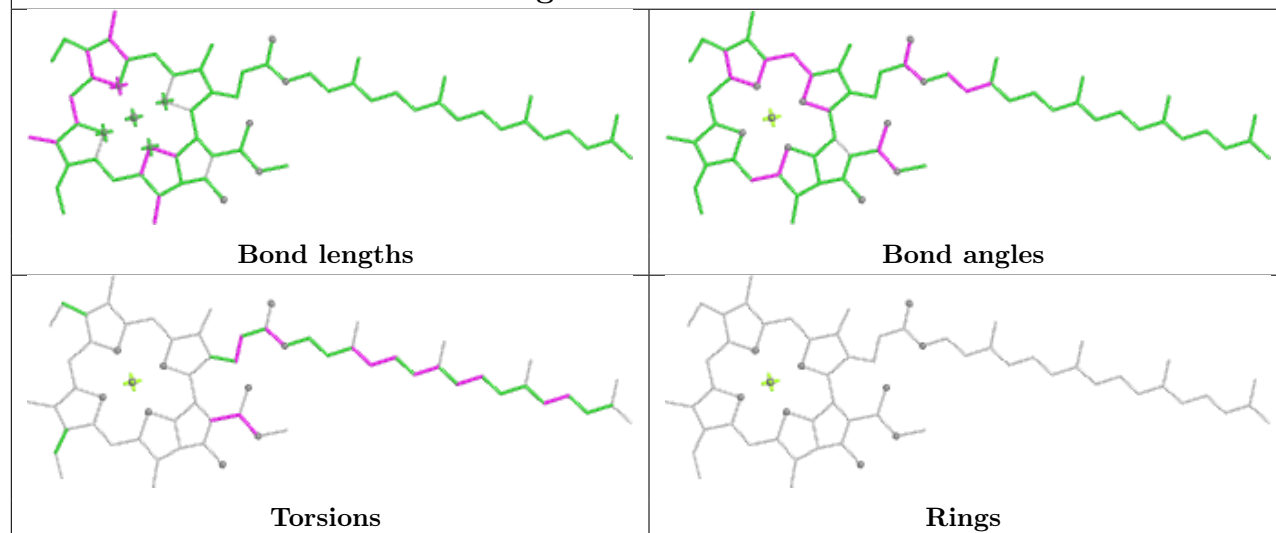




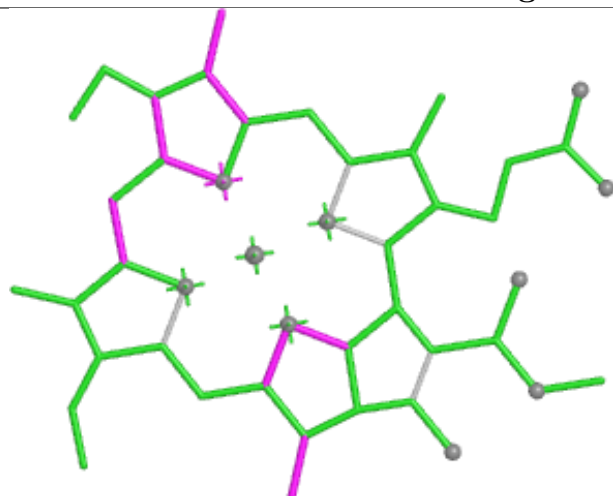
Ligand CLA L 206



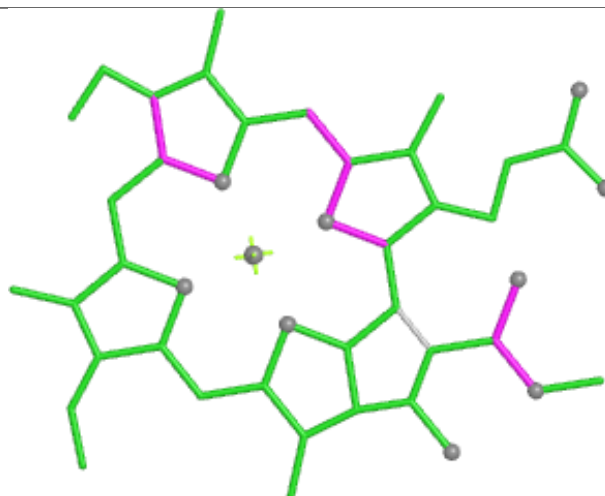
Ligand CLA 1 311



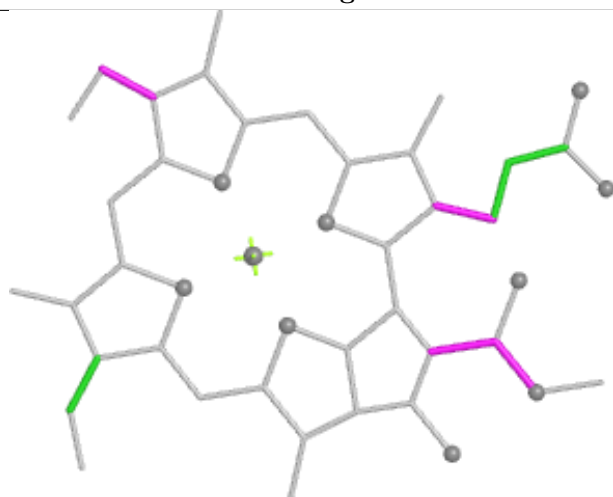
Ligand CLA 5 309



Bond lengths



Bond angles

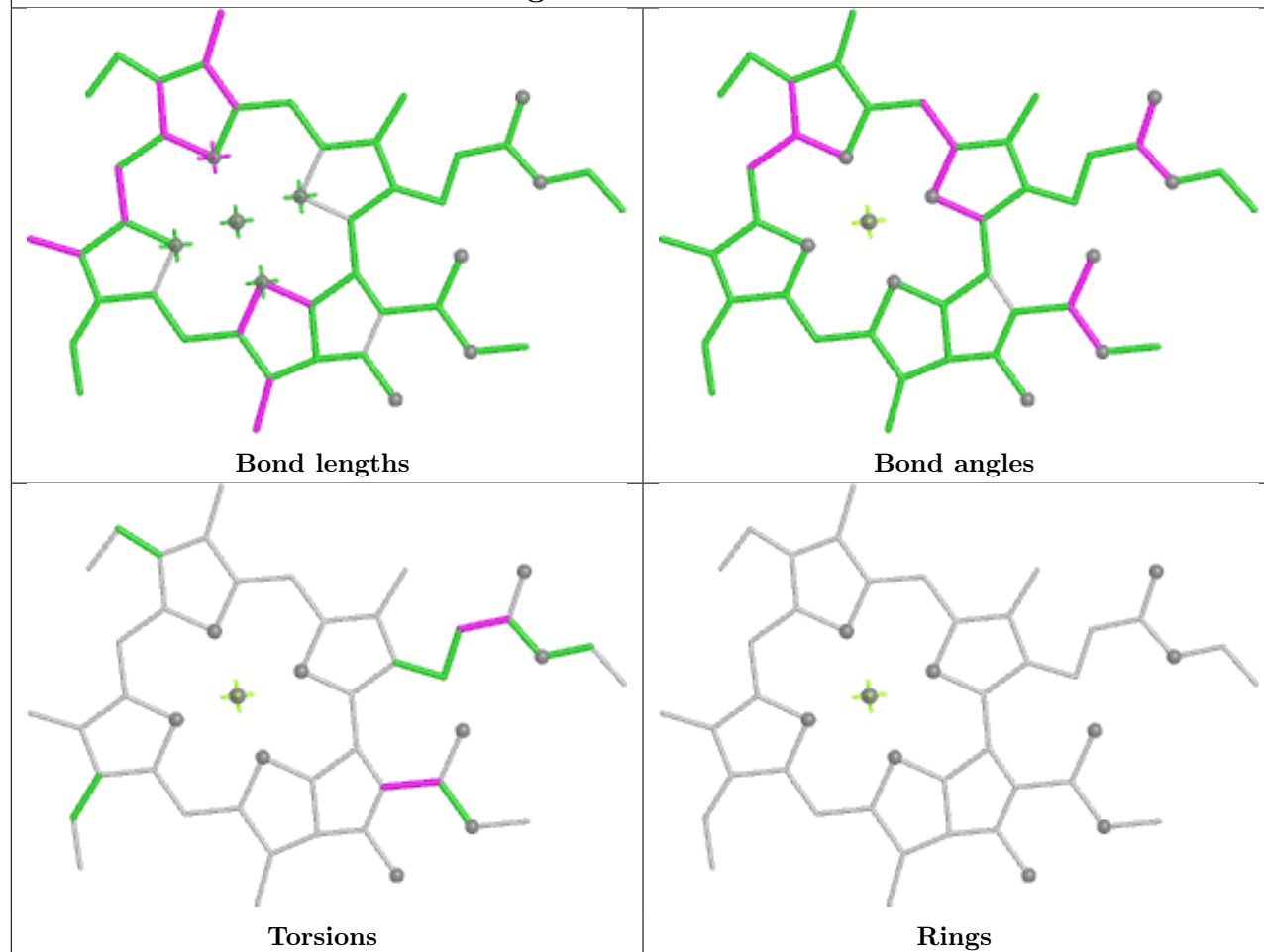


Torsions

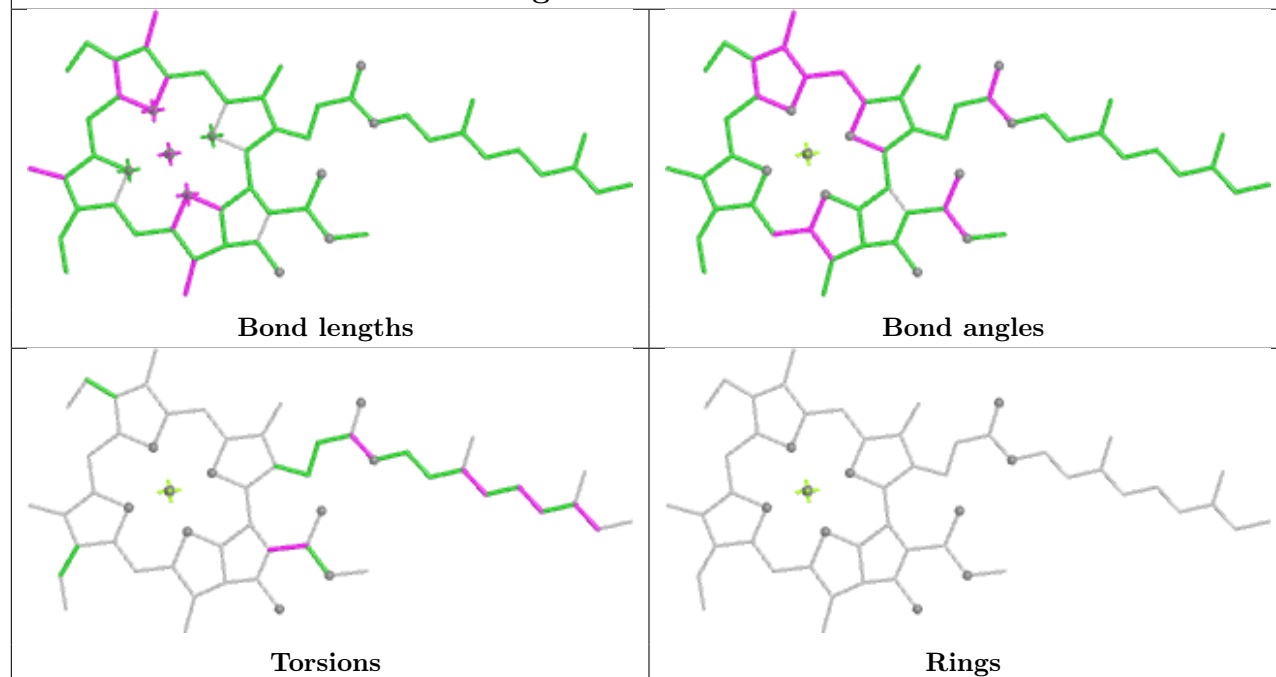


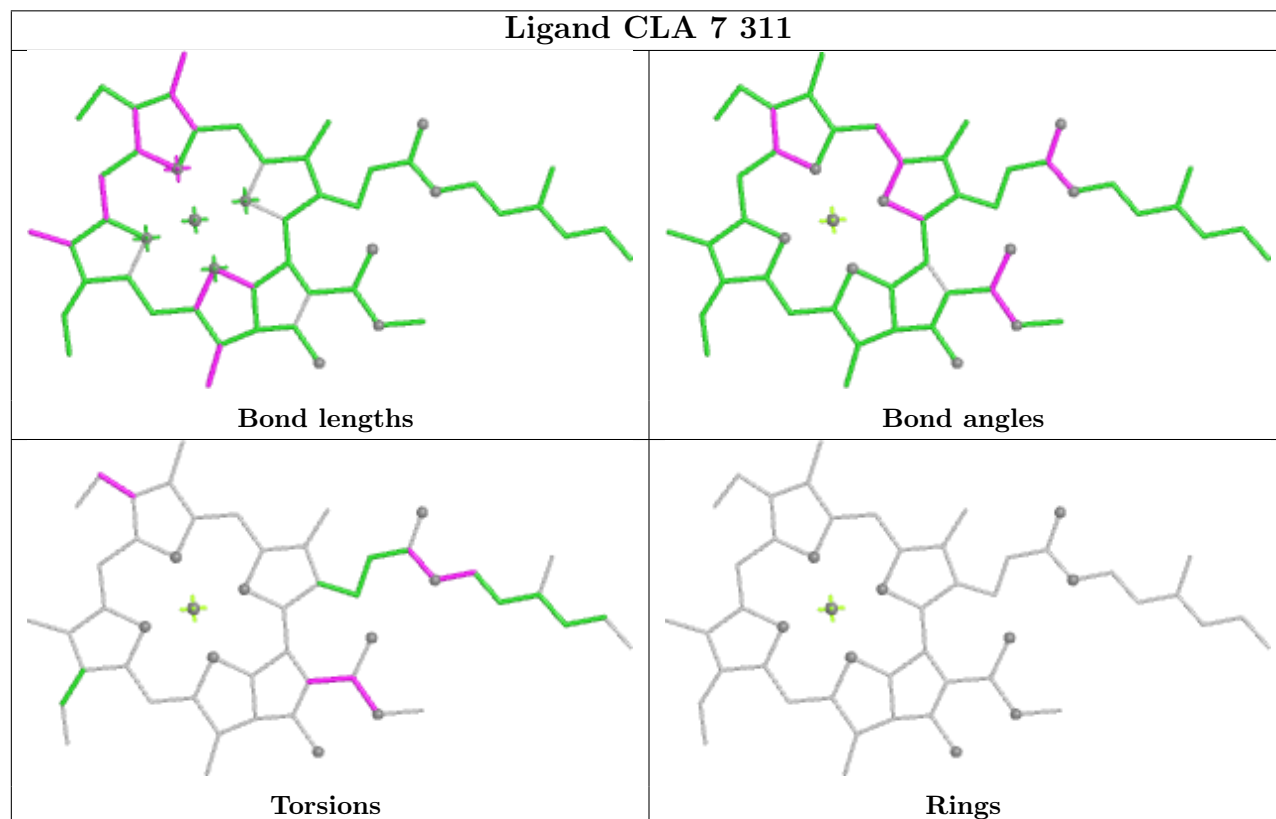
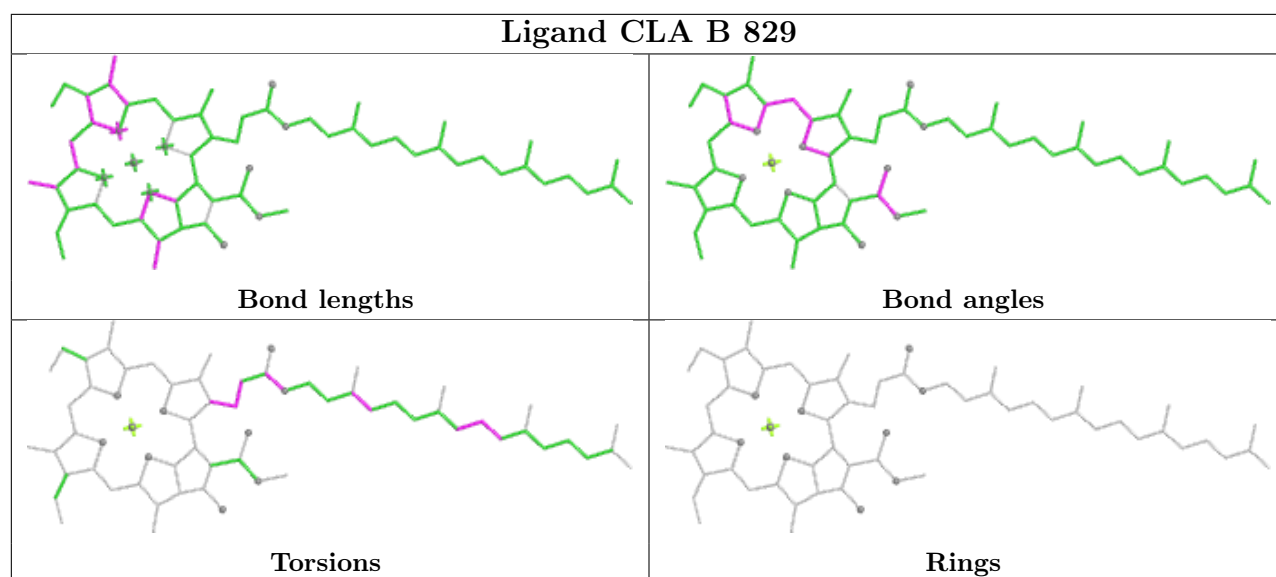
Rings

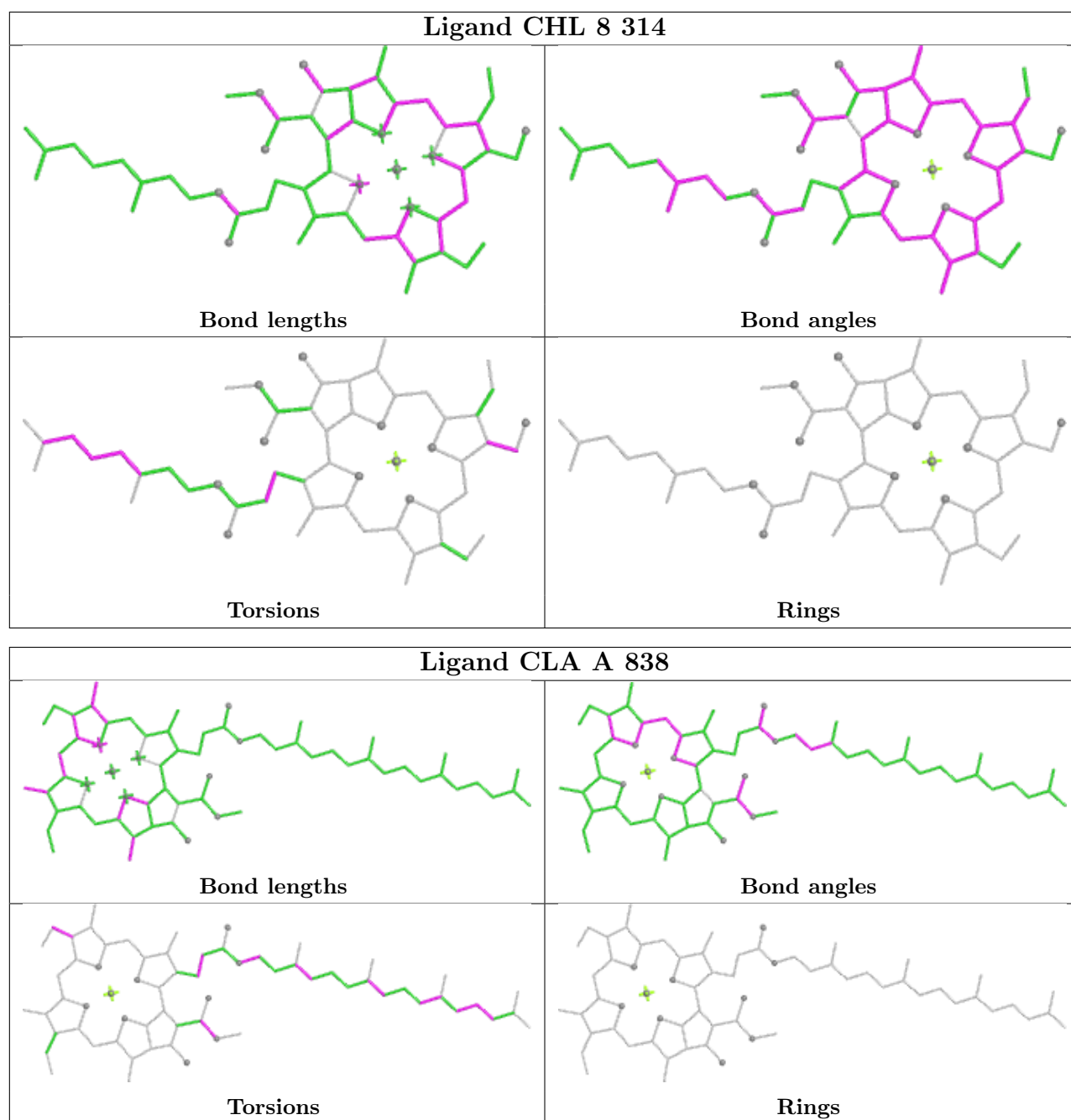
Ligand CLA B 838

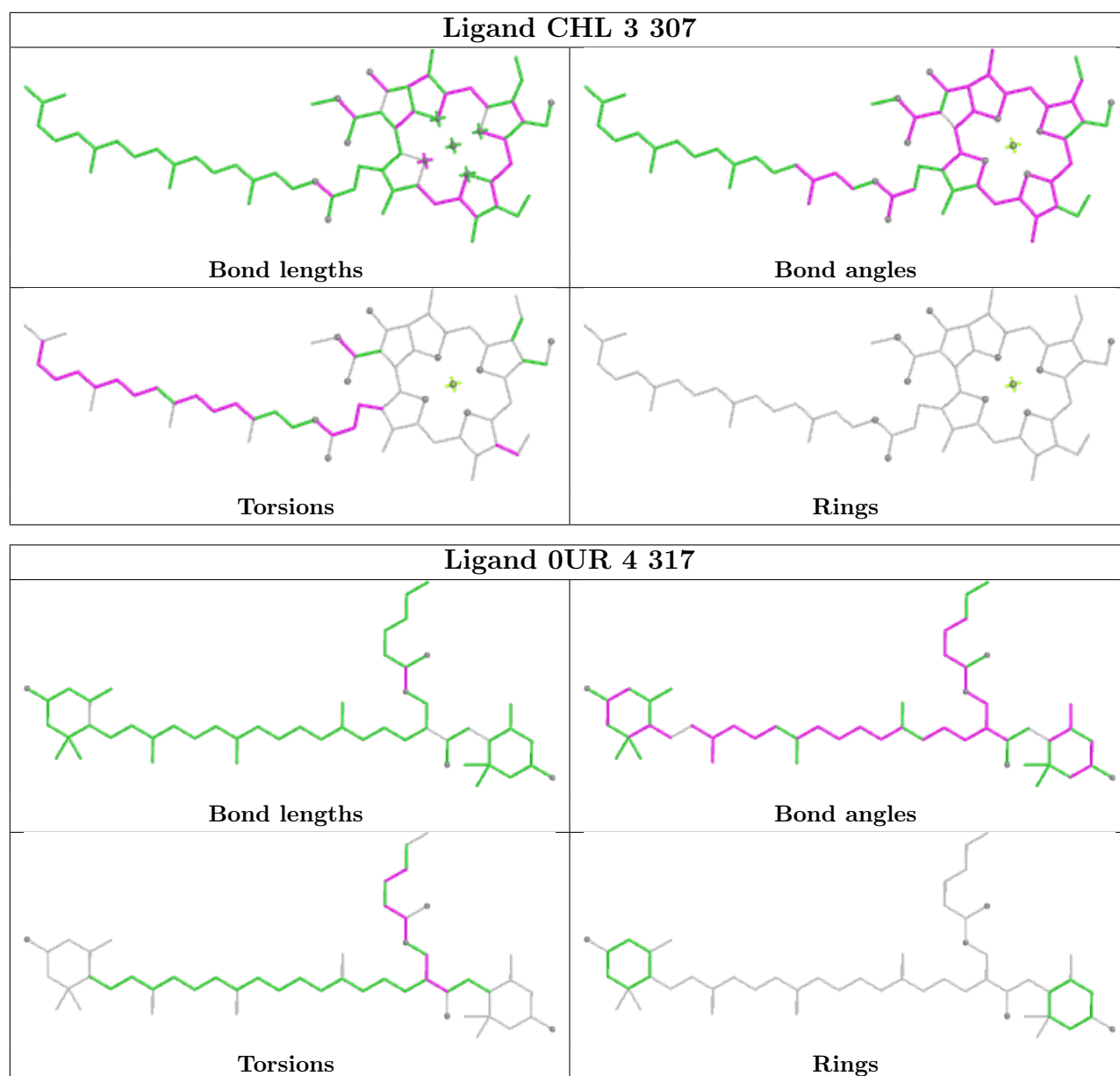


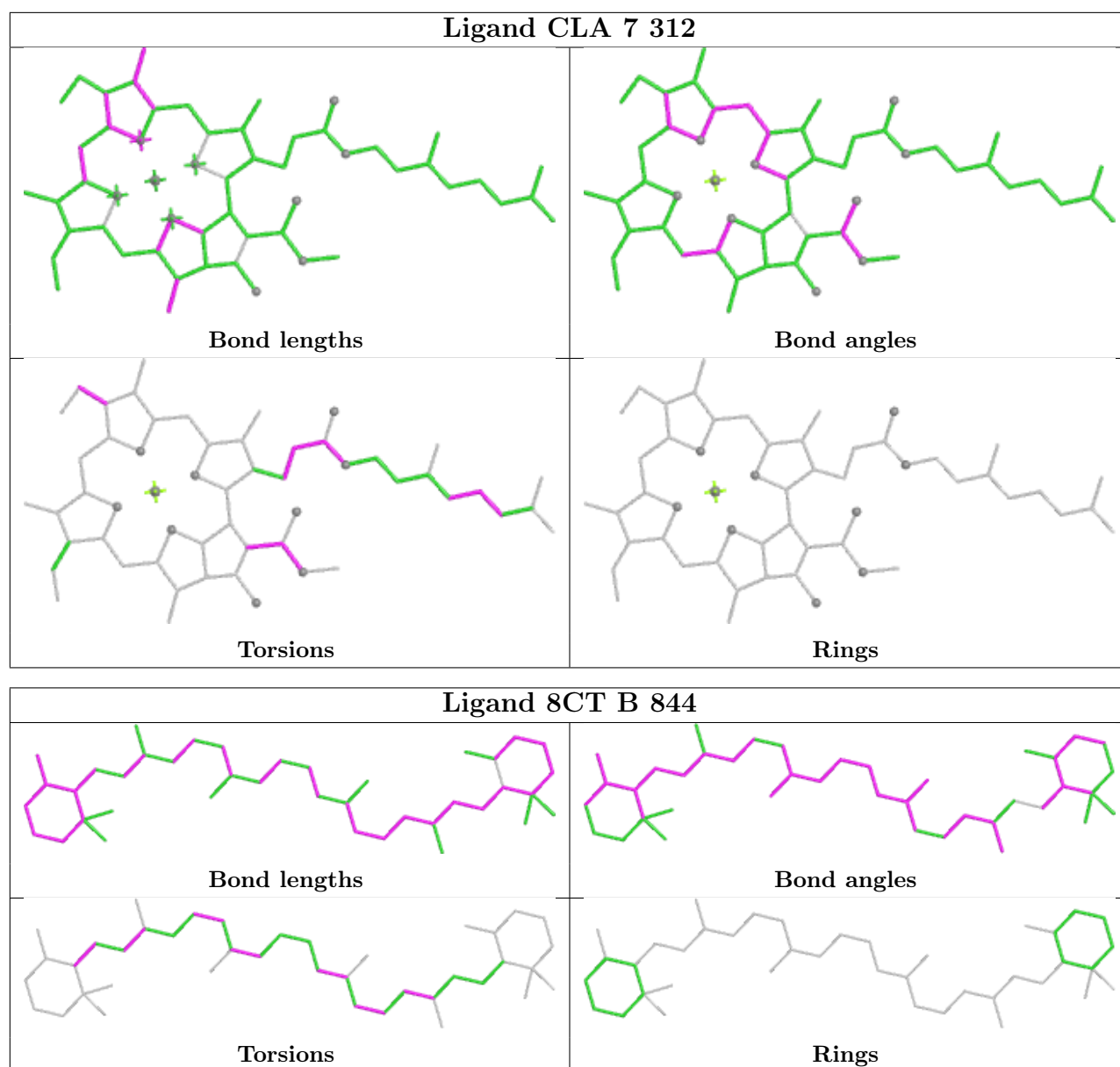
Ligand CLA B 830



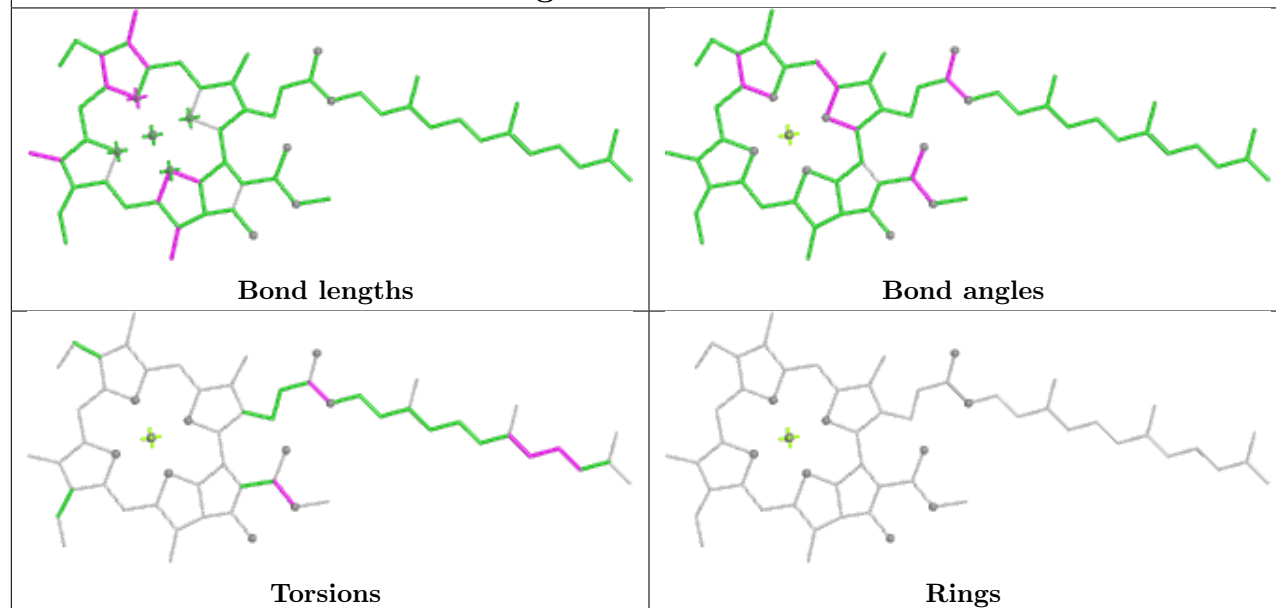




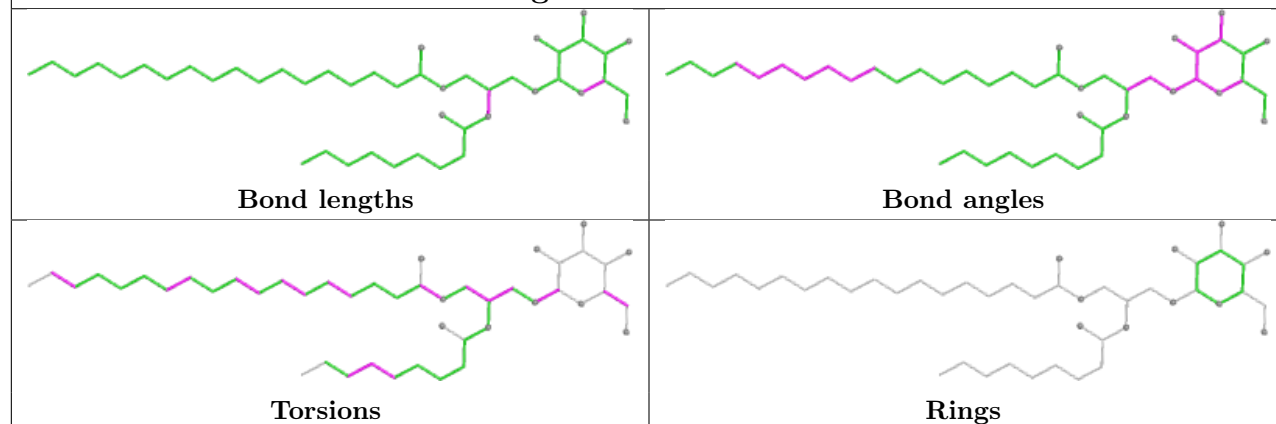




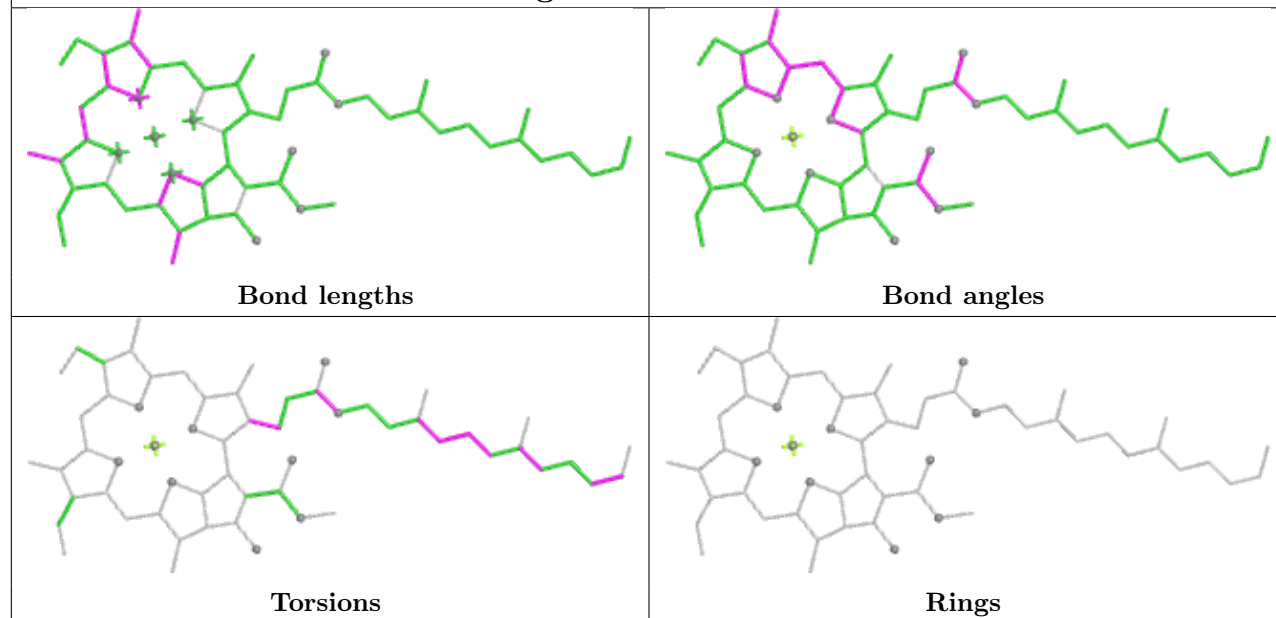
Ligand CLA 4 304

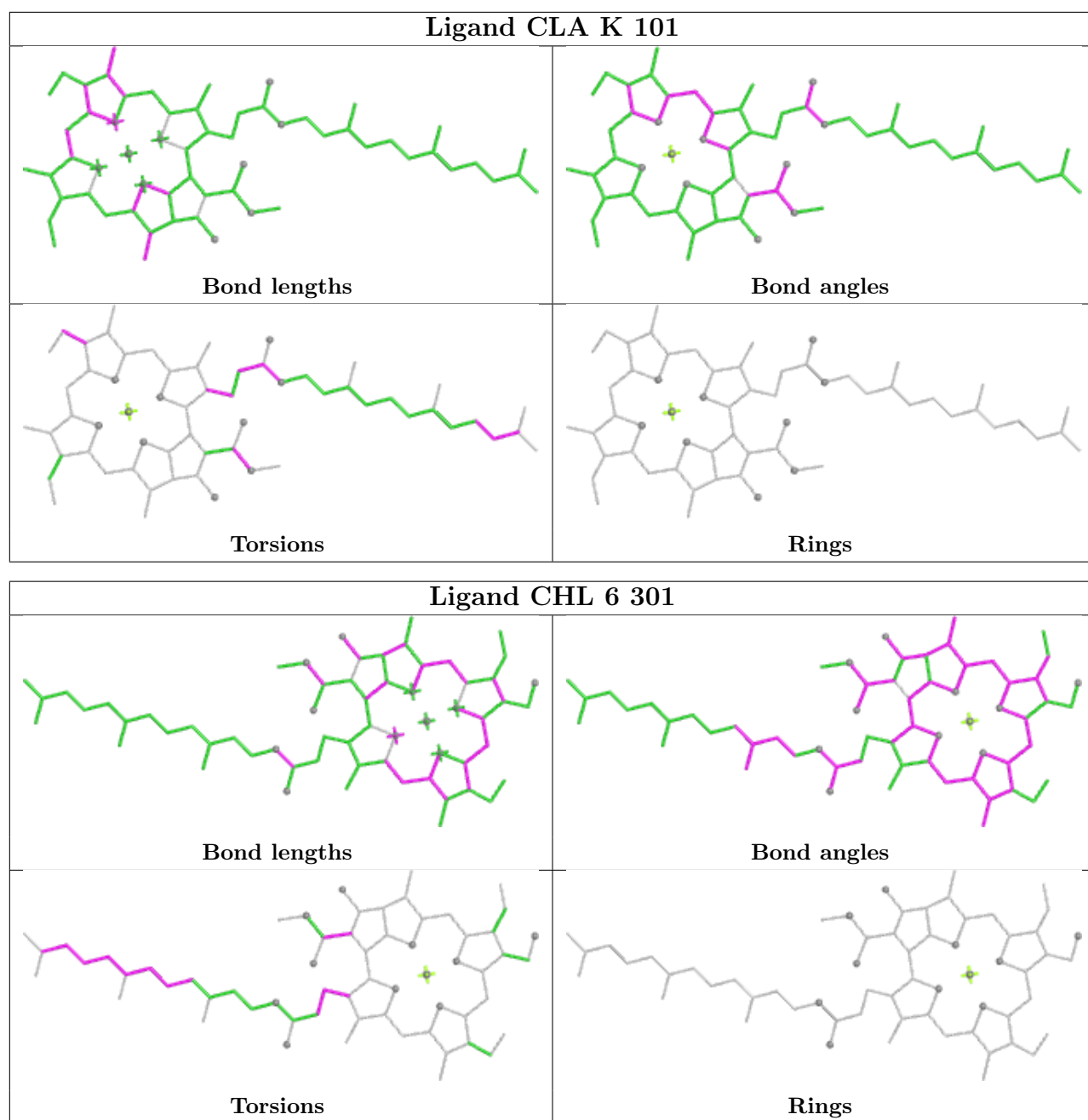


Ligand LMG J 105

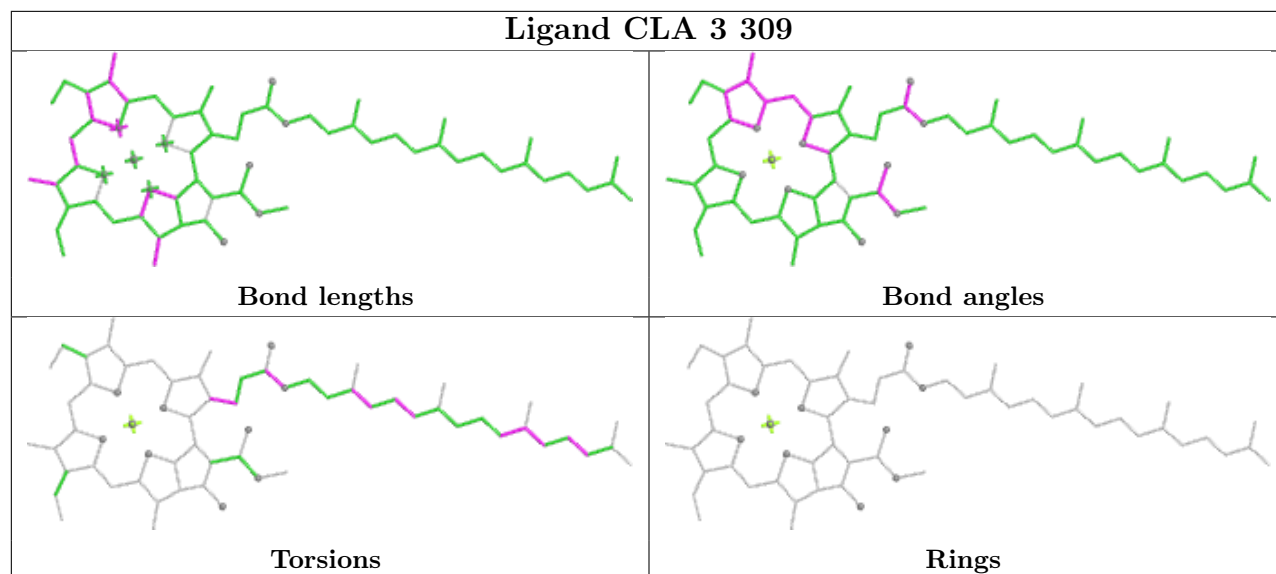


Ligand CLA 7 309

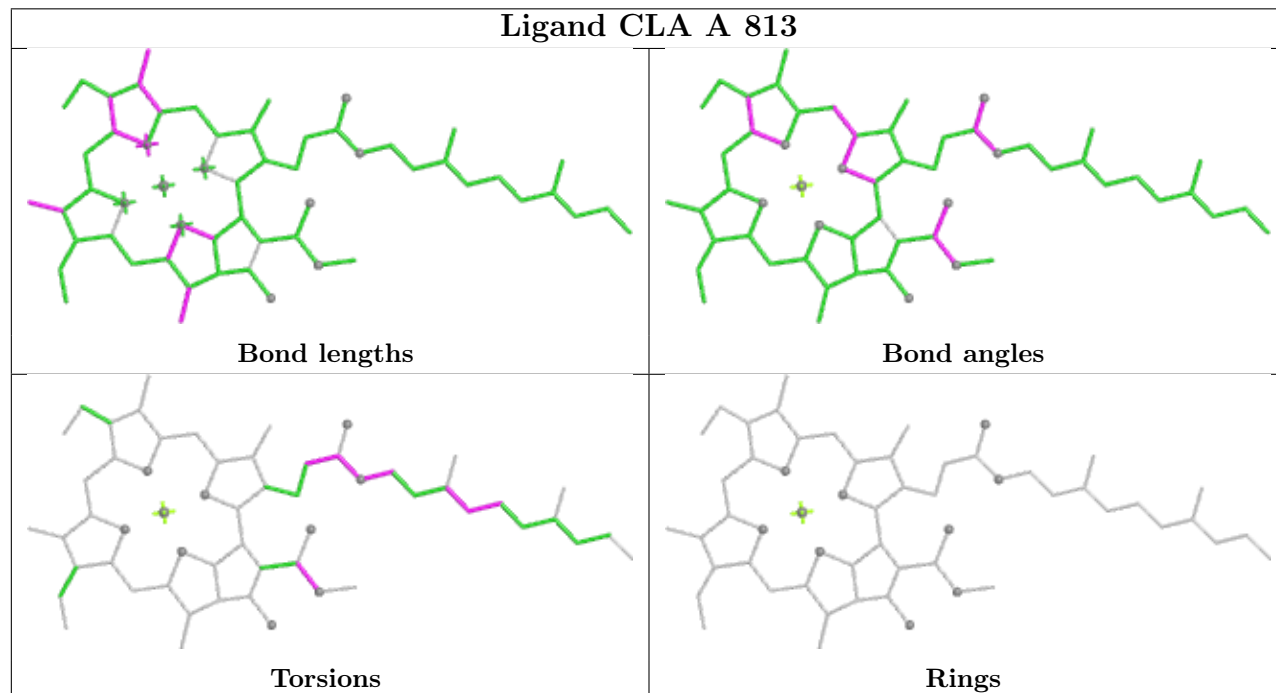


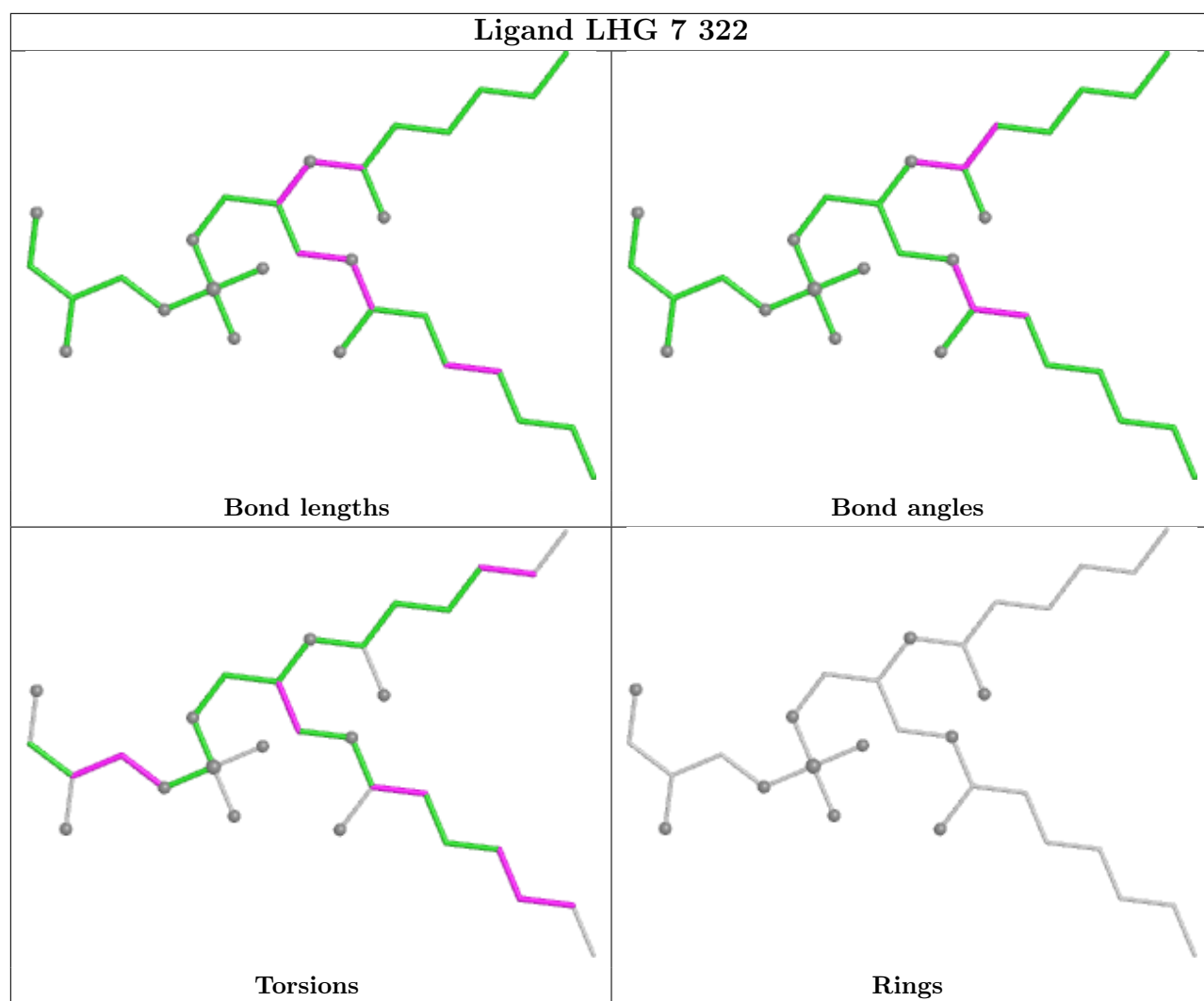


Ligand CLA 3 309

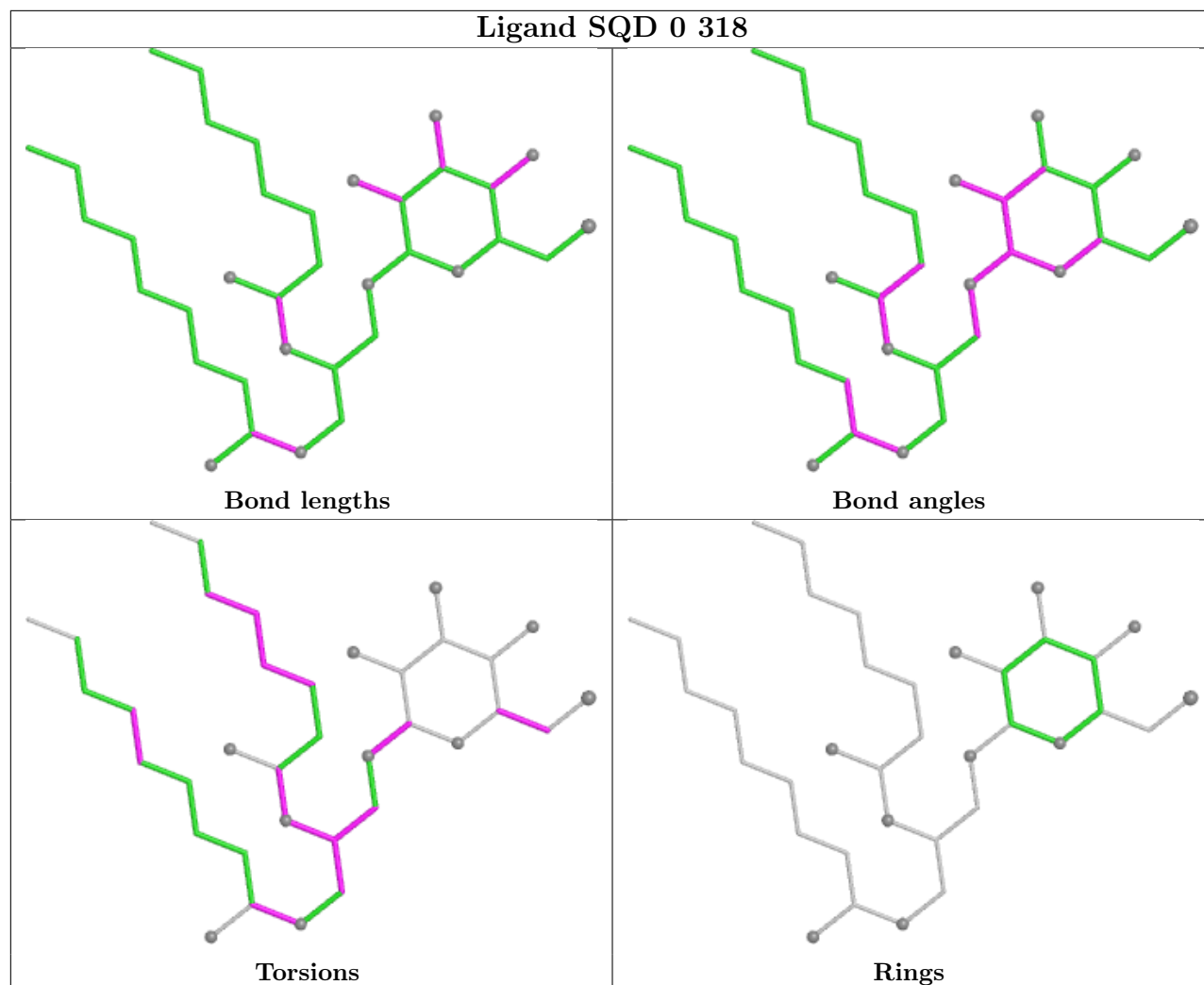


Ligand CLA A 813

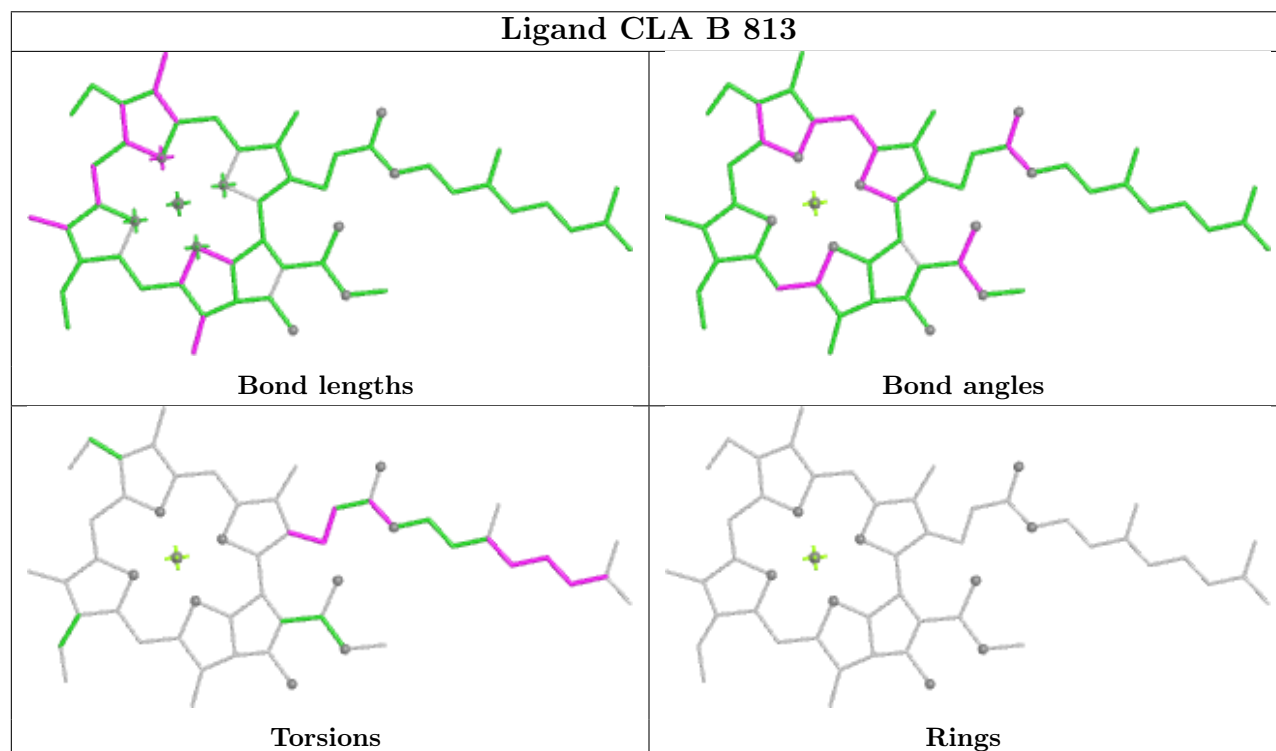




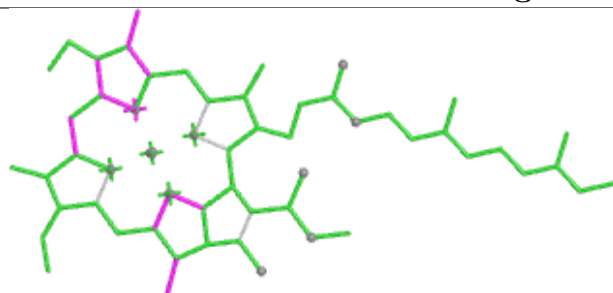
Ligand SQD 0 318



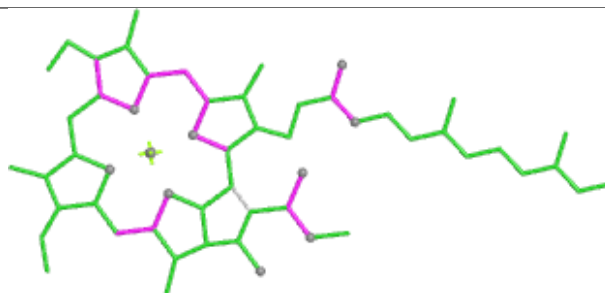
Ligand CLA B 813



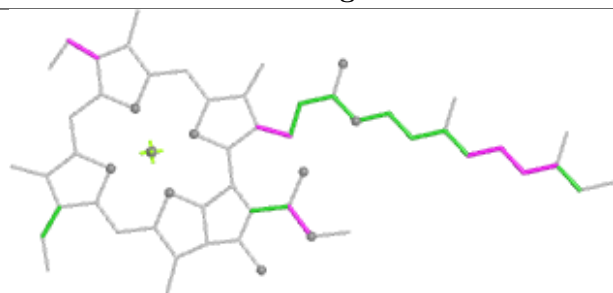
Ligand CLA B 820



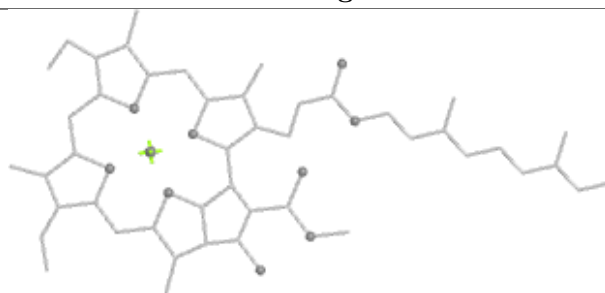
Bond lengths



Bond angles

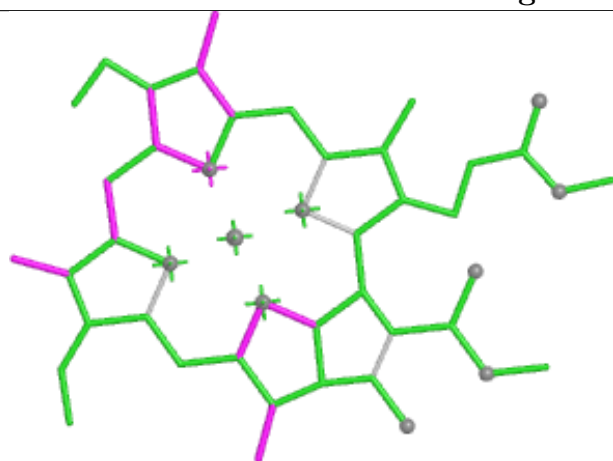


Torsions

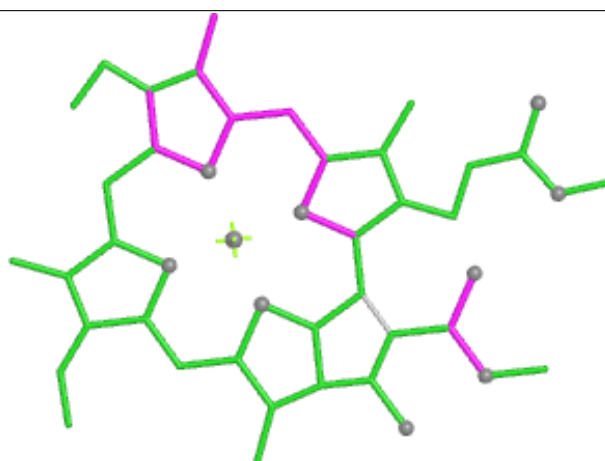


Rings

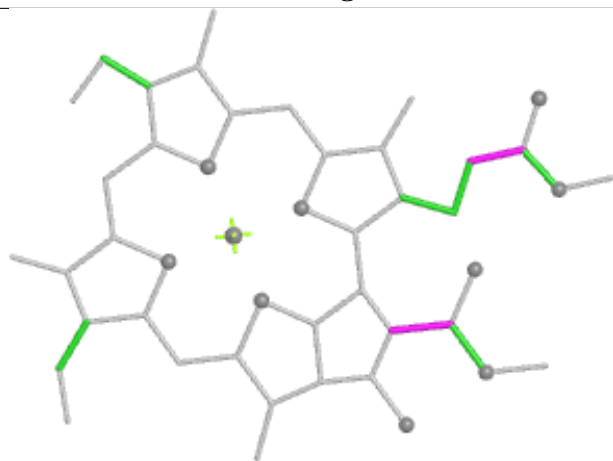
Ligand CLA 3 311



Bond lengths



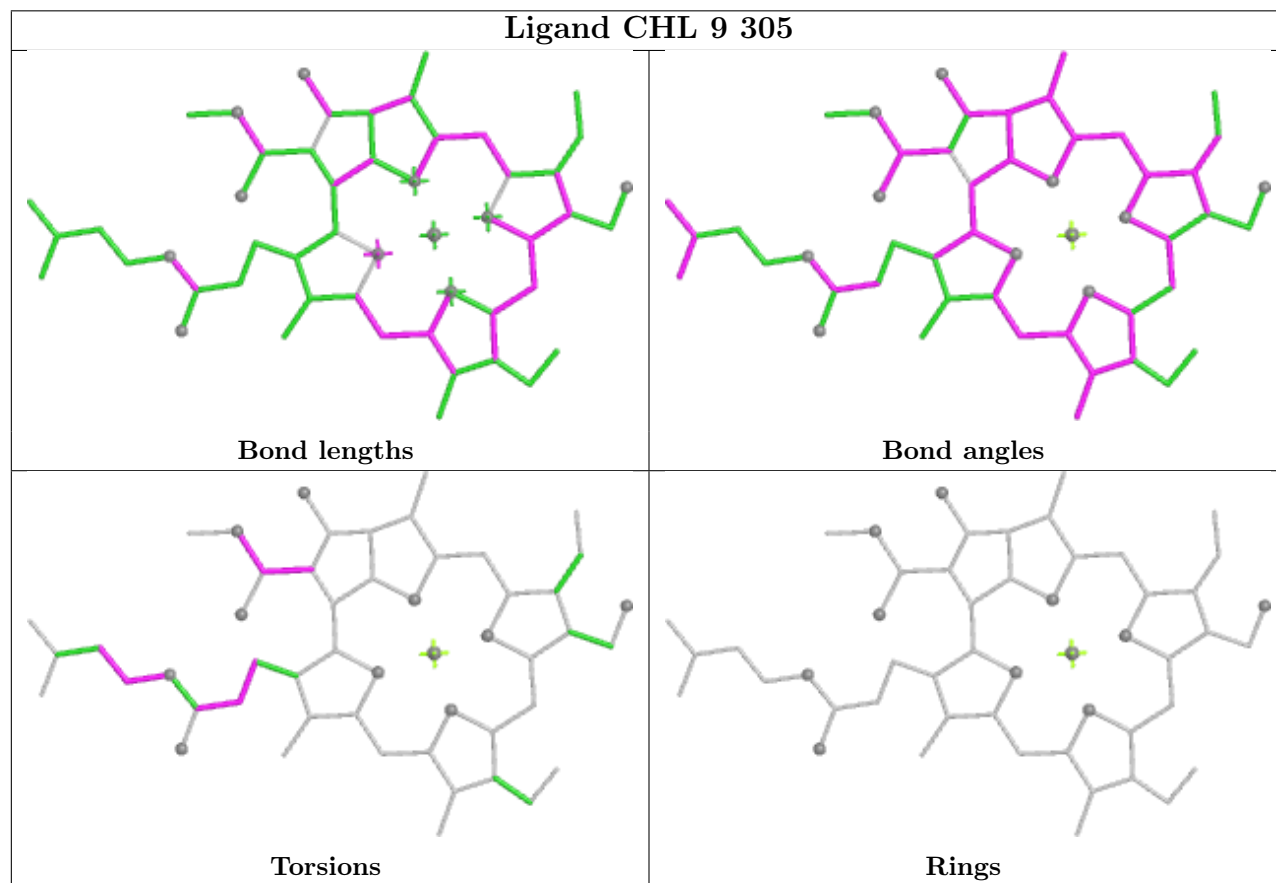
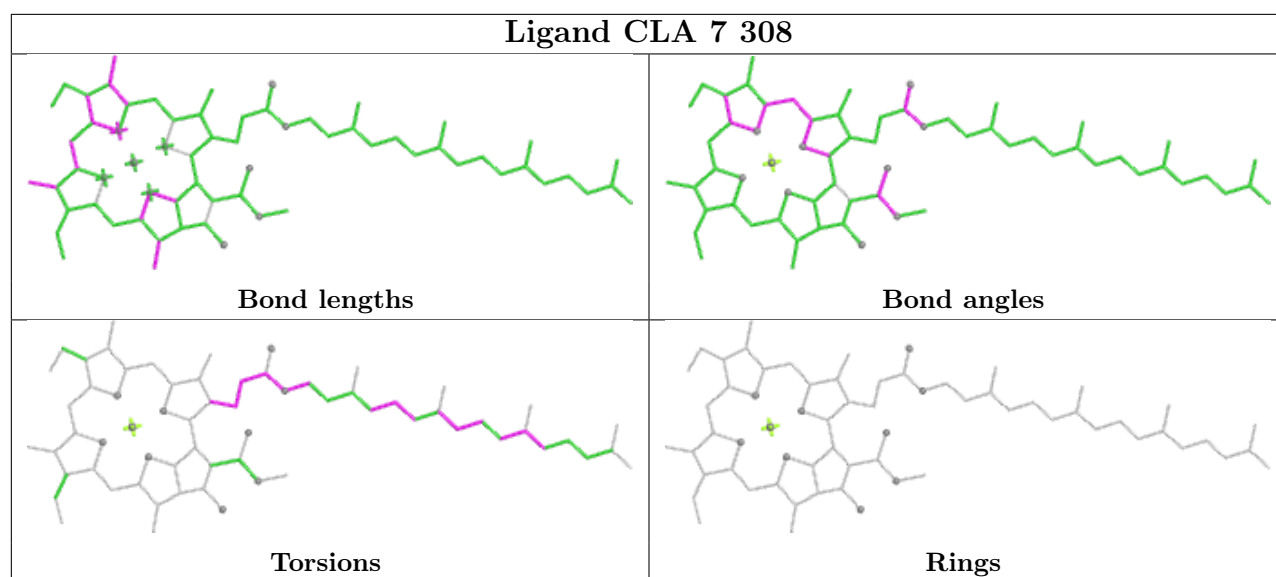
Bond angles

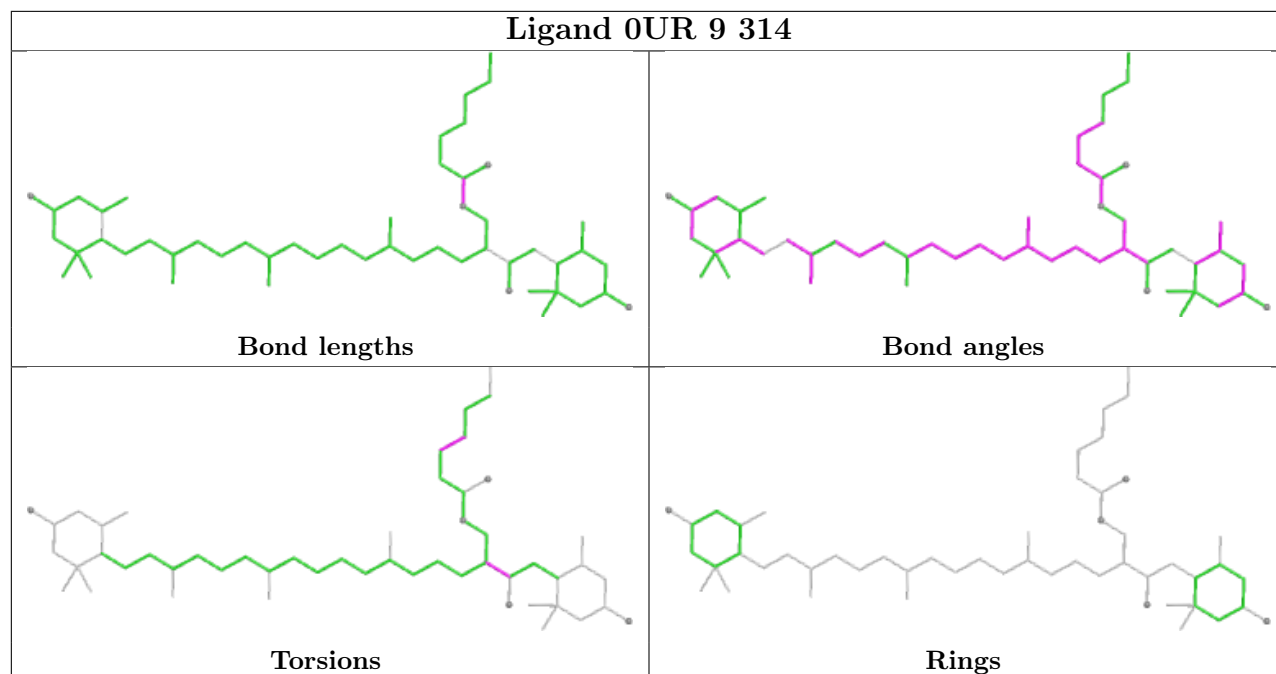
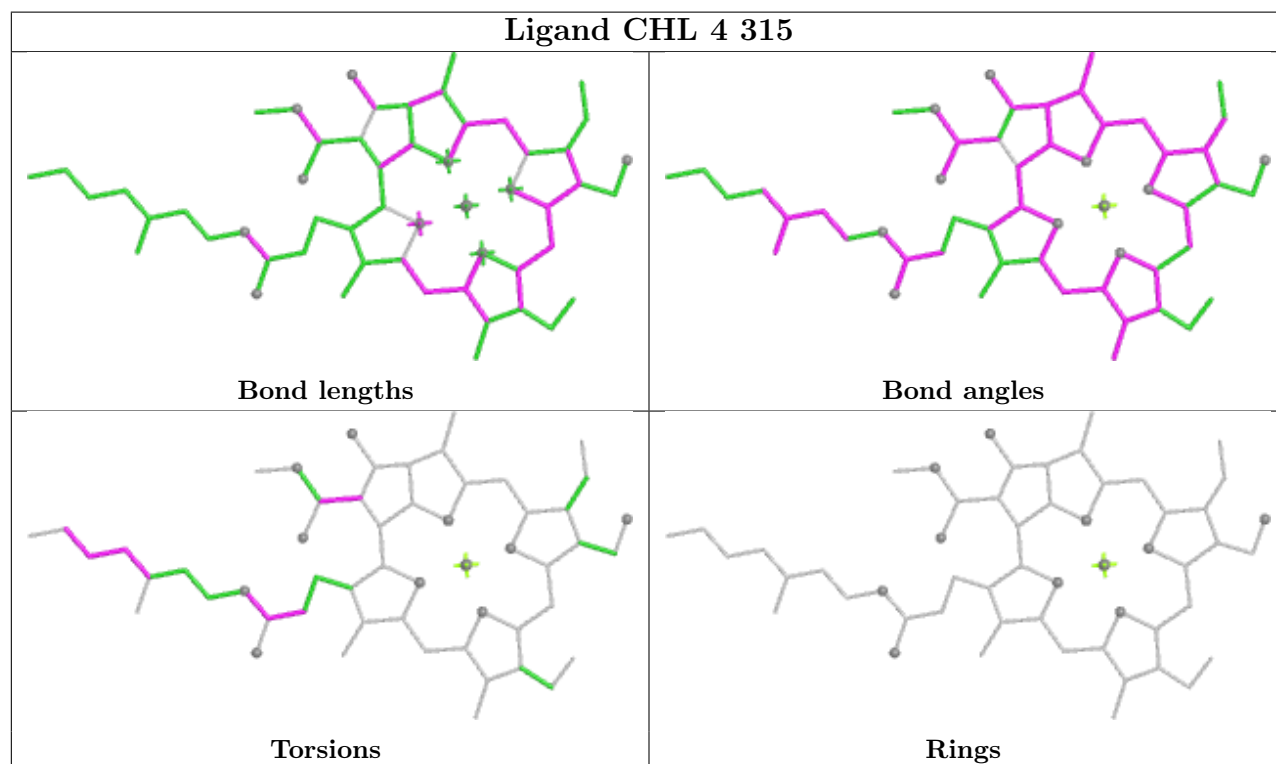


Torsions

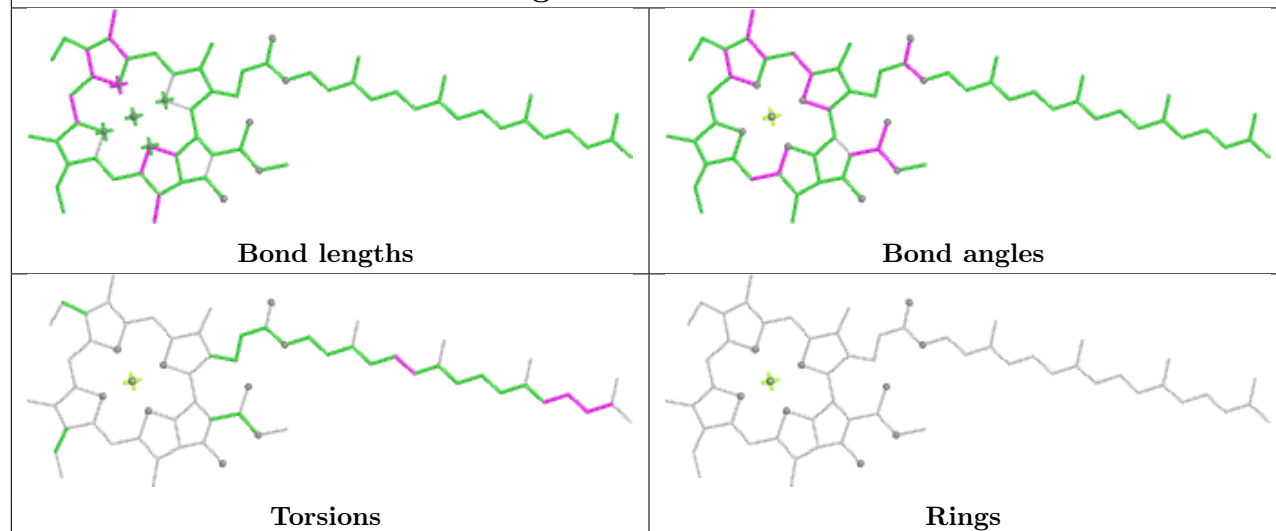


Rings

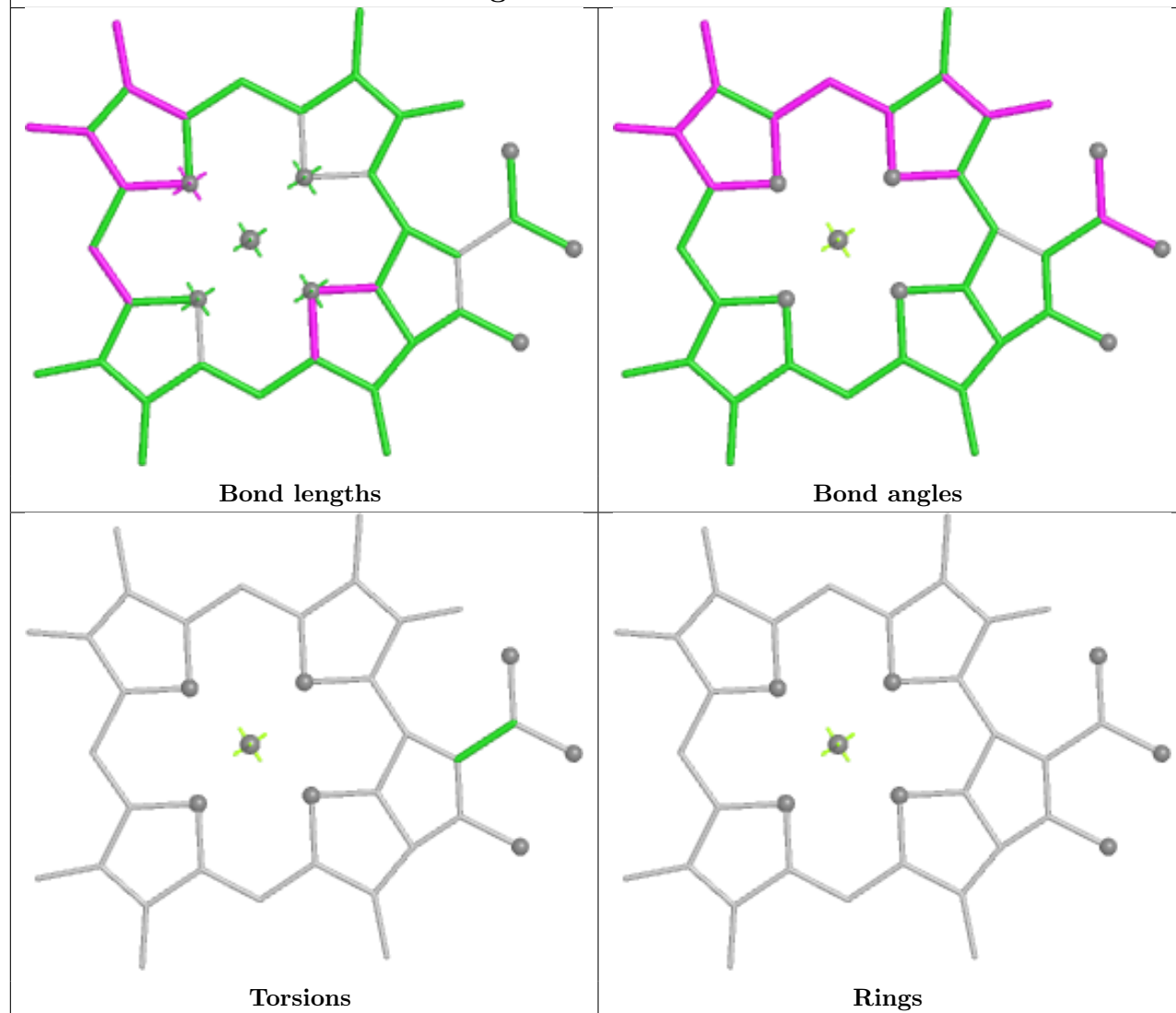


Ligand OUR 9 314**Ligand CHL 4 315**

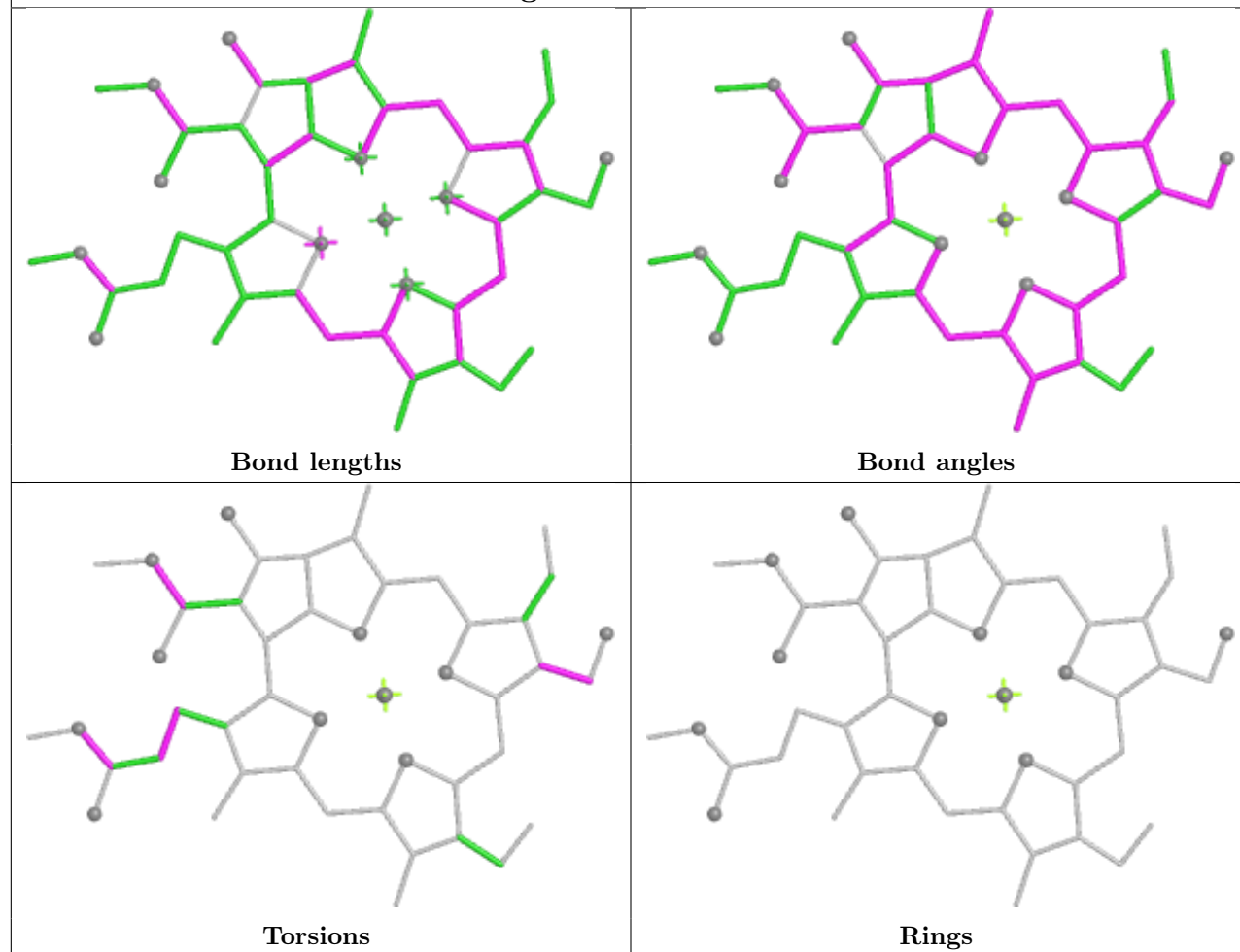
Ligand CLA B 837



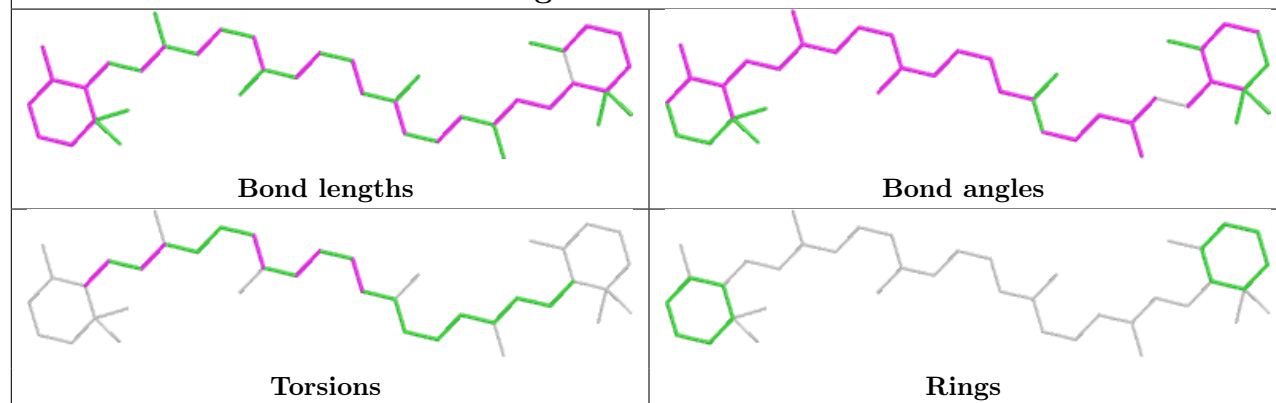
Ligand CLA O 206



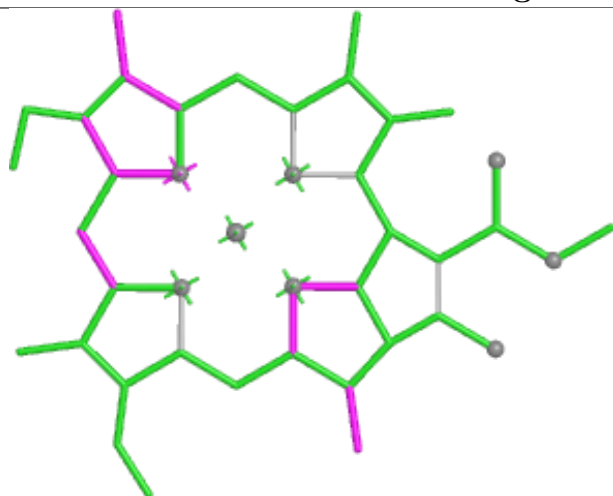
Ligand CHL 9 301



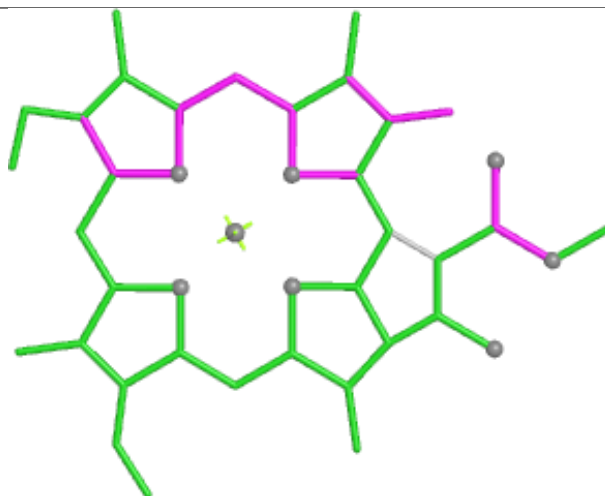
Ligand 8CT O 202



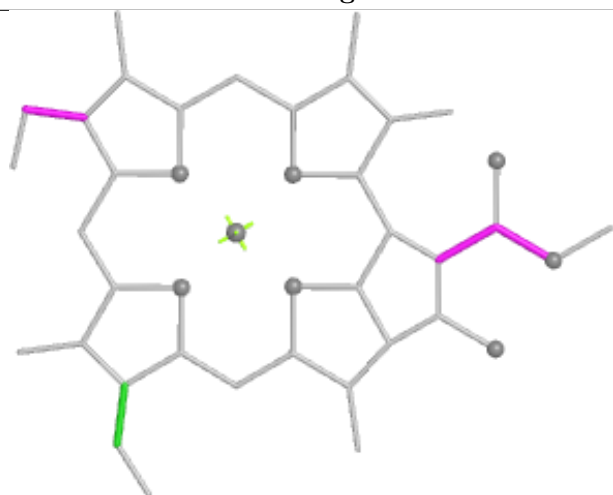
Ligand CLA O 204



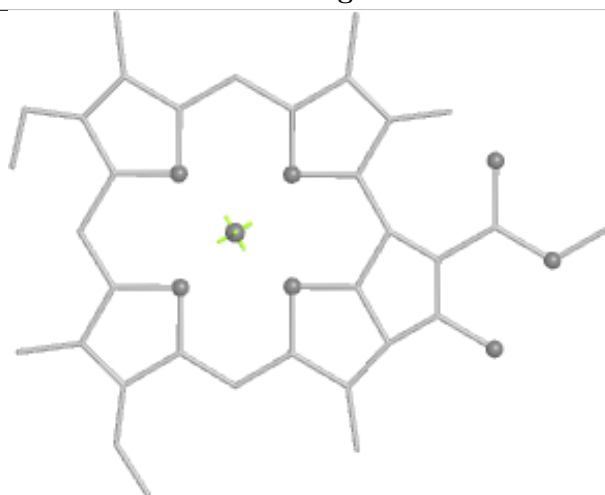
Bond lengths



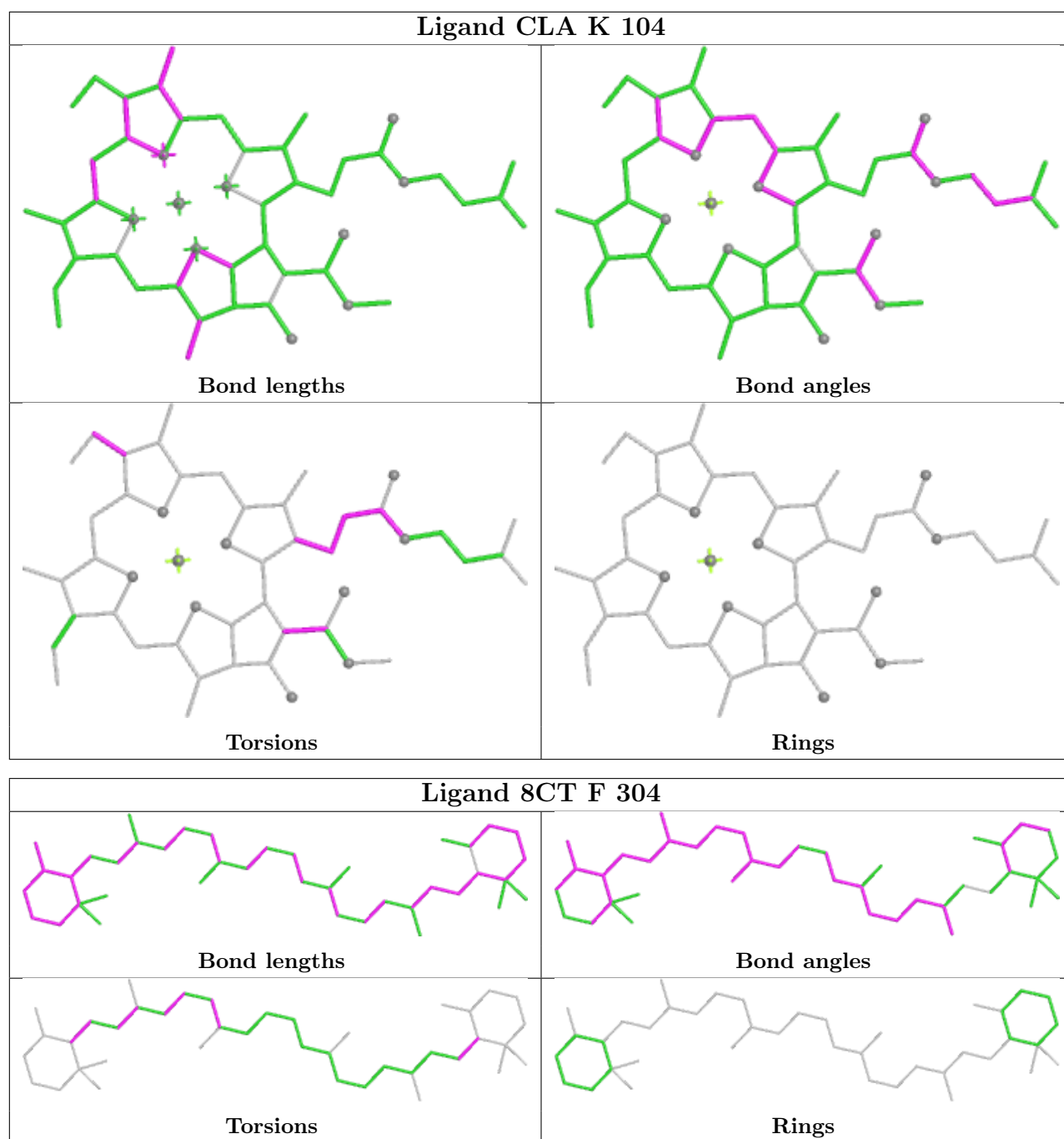
Bond angles



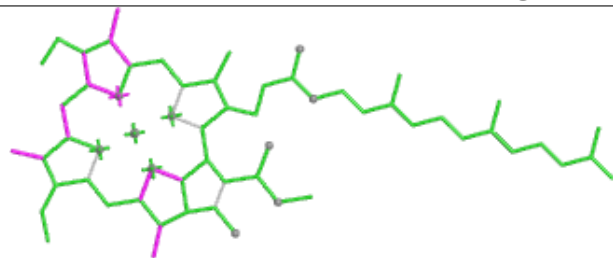
Torsions



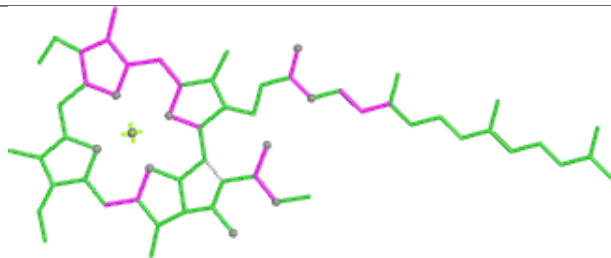
Rings



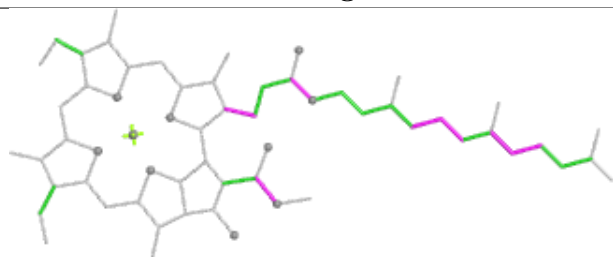
Ligand CLA B 836



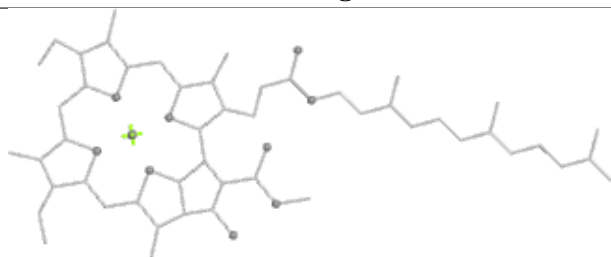
Bond lengths



Bond angles

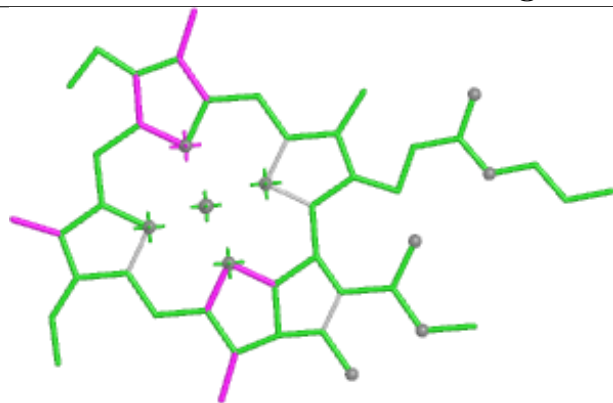


Torsions

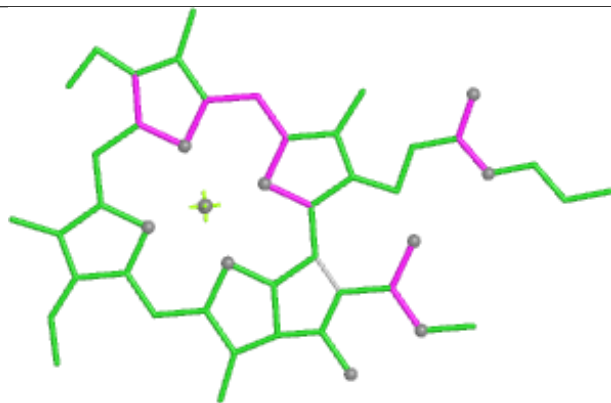


Rings

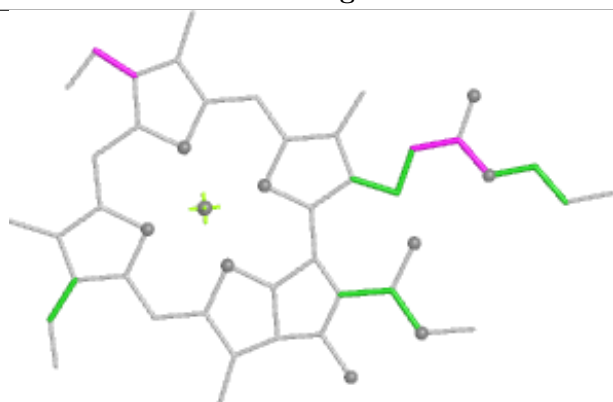
Ligand CLA 9 303



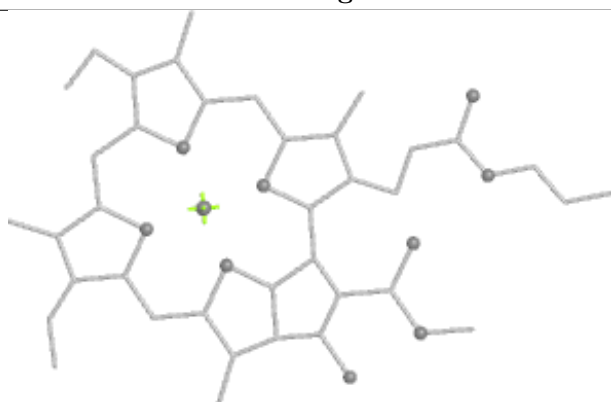
Bond lengths



Bond angles

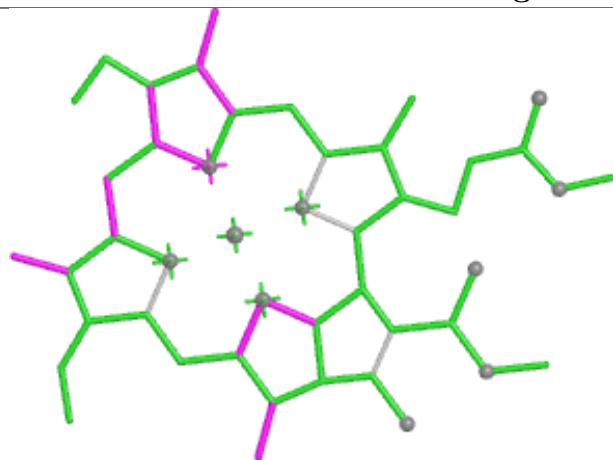


Torsions

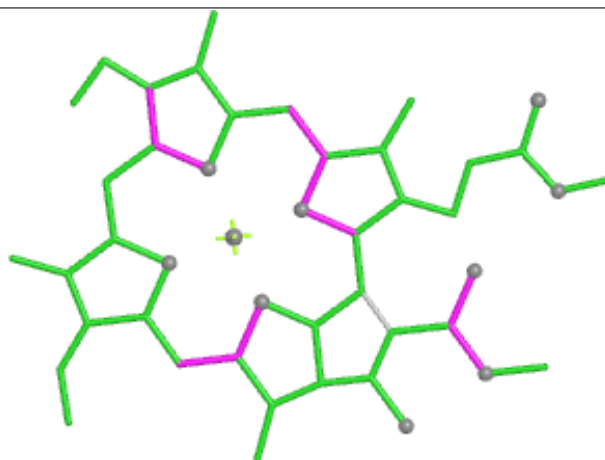


Rings

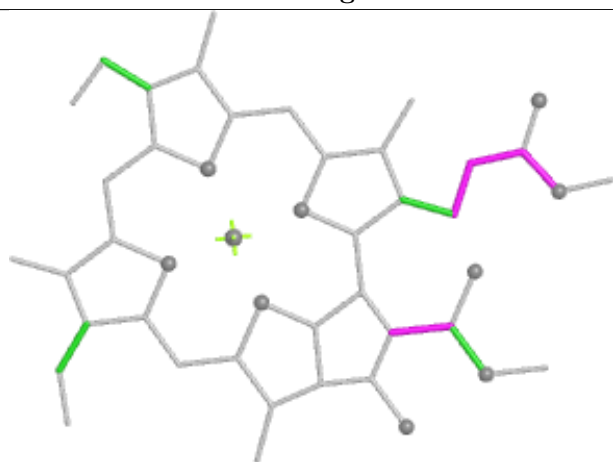
Ligand CLA K 103



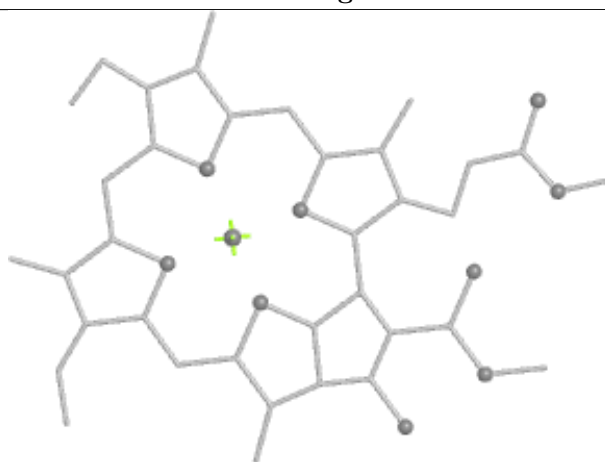
Bond lengths



Bond angles

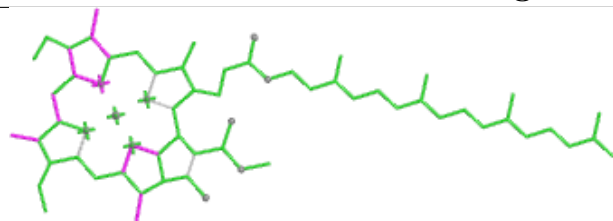


Torsions

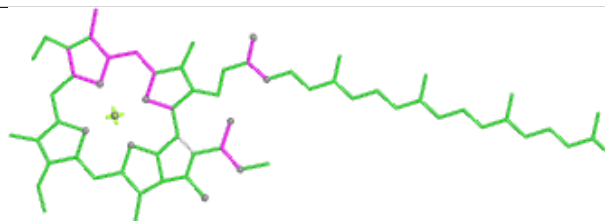


Rings

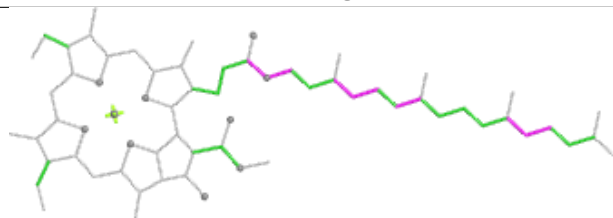
Ligand CLA A 820



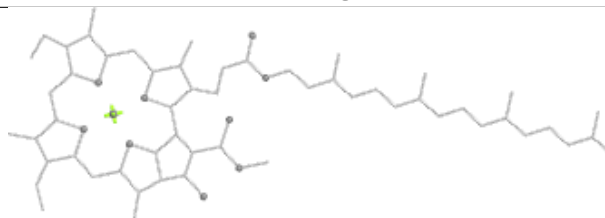
Bond lengths



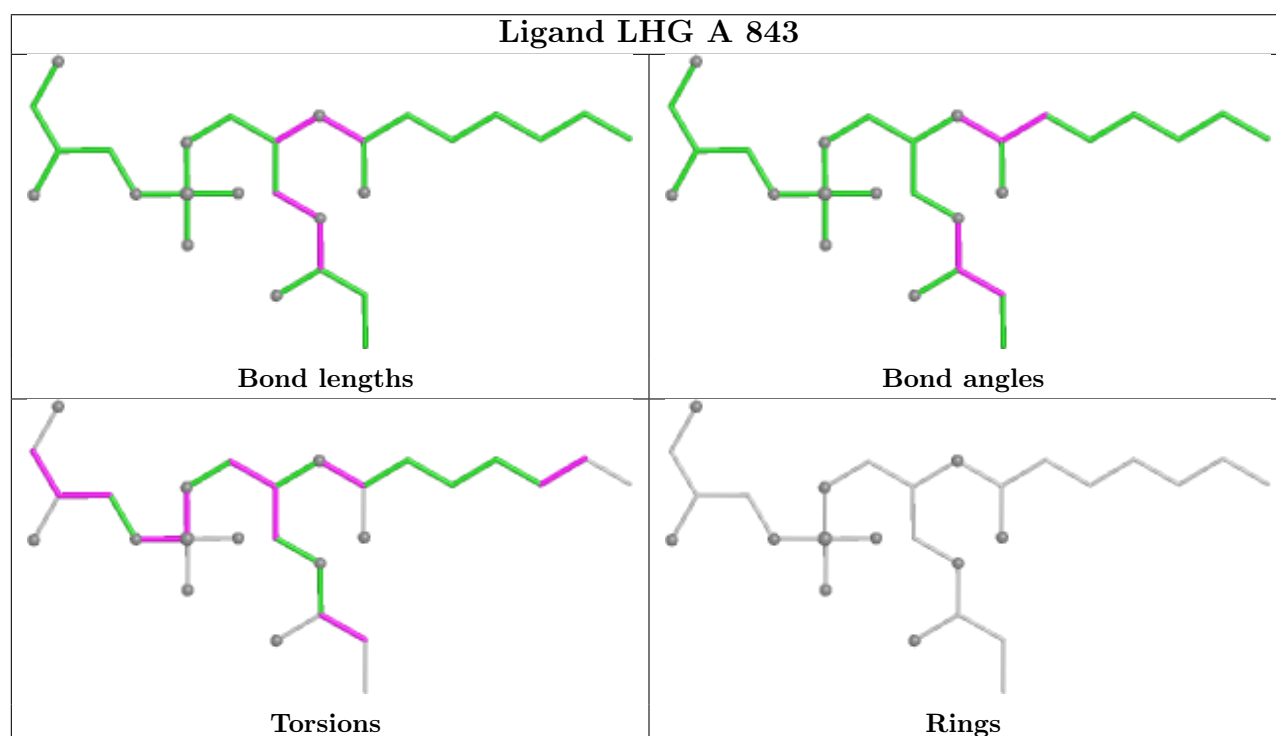
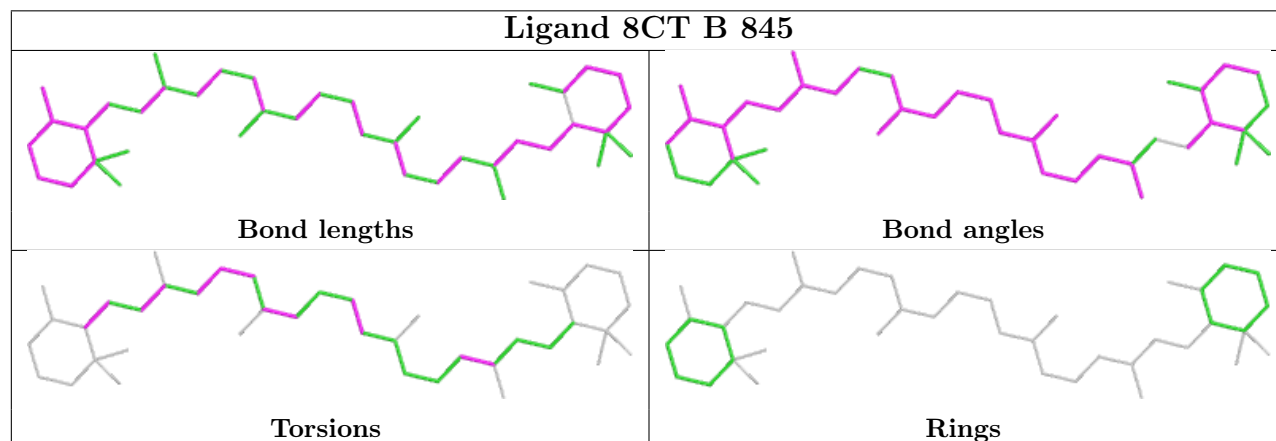
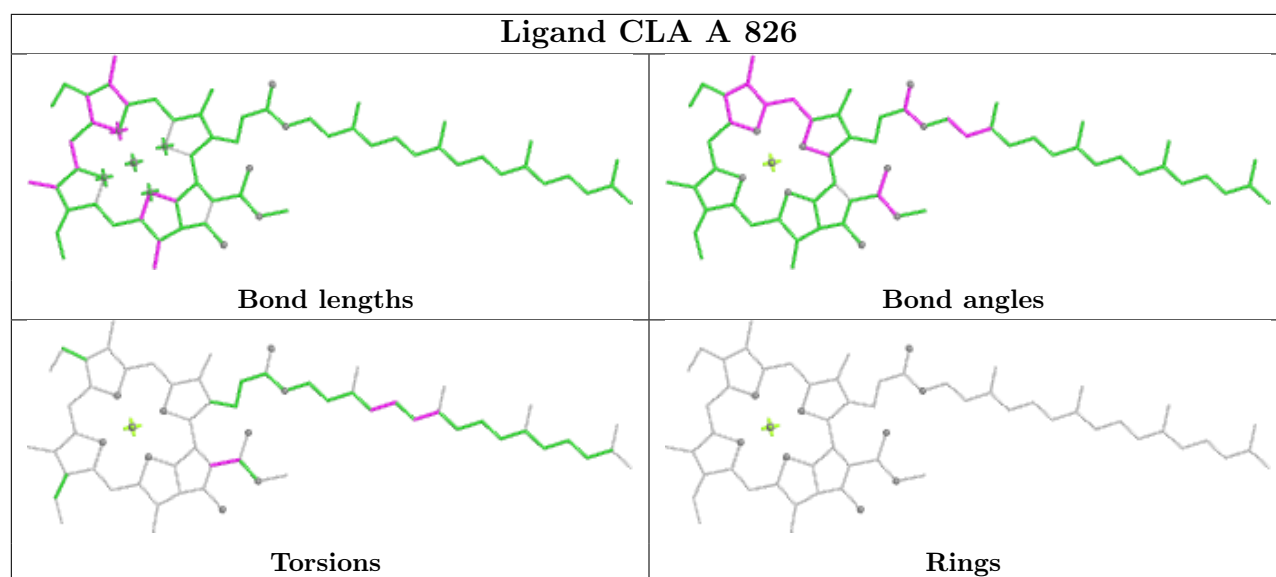
Bond angles

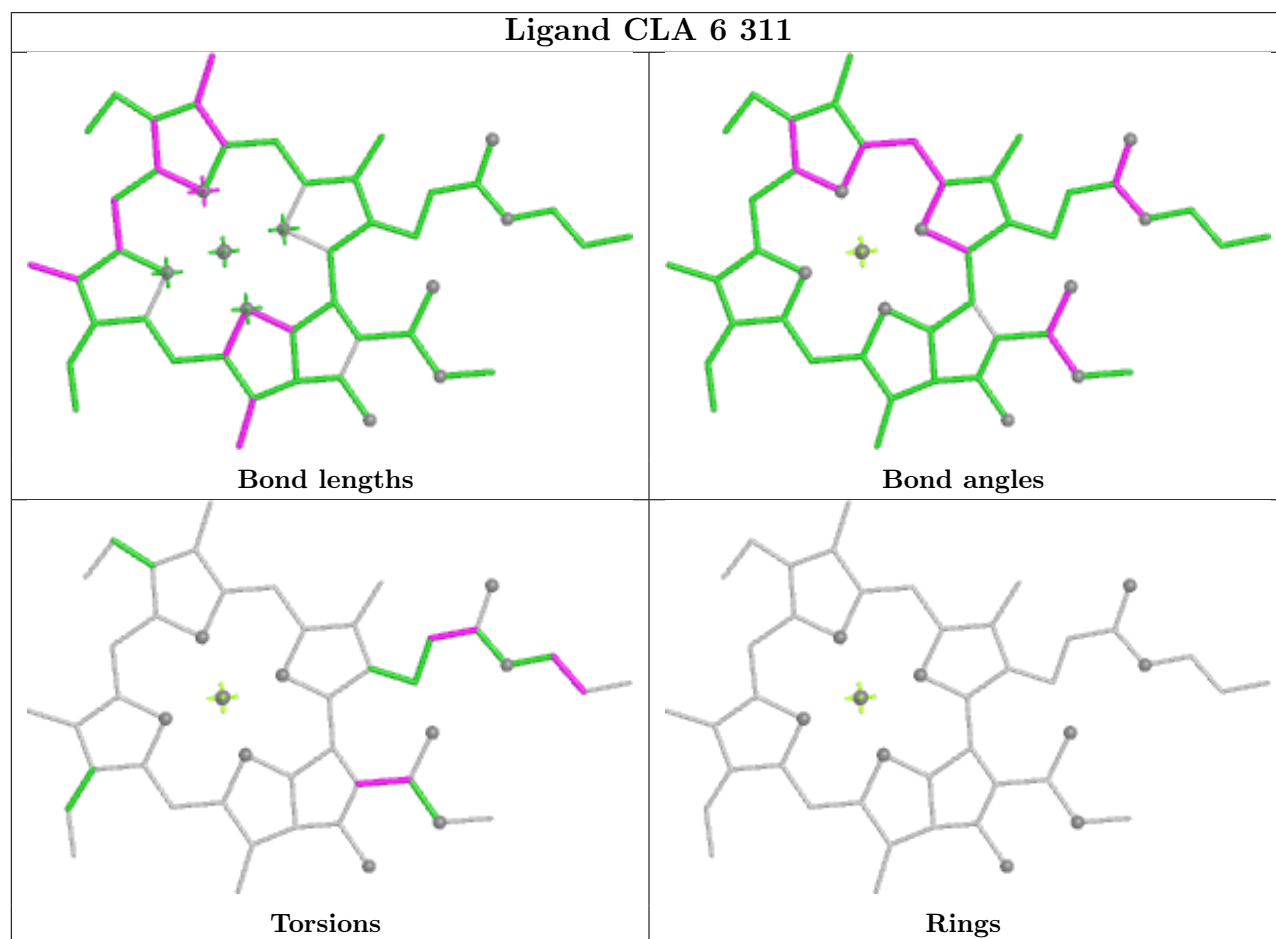
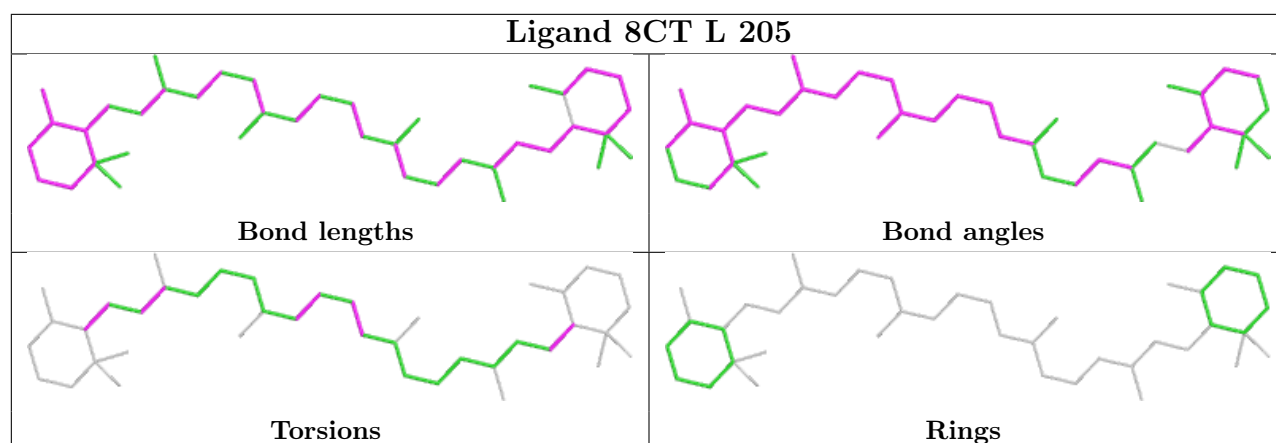


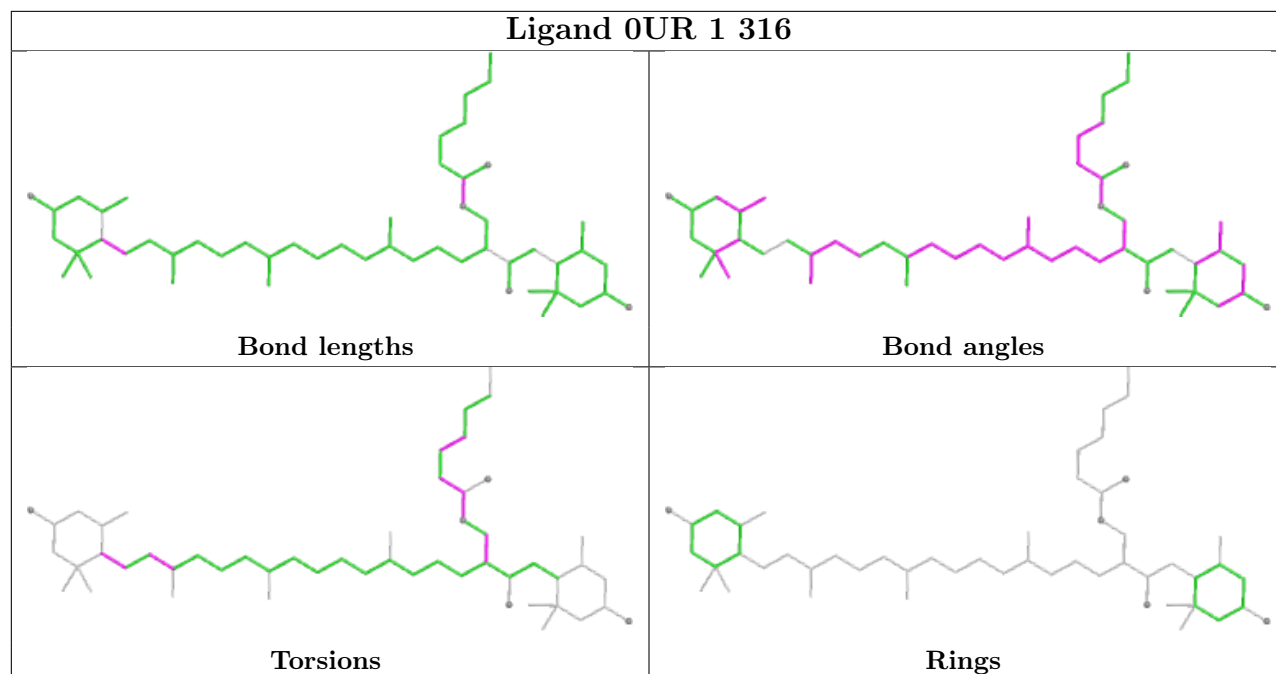
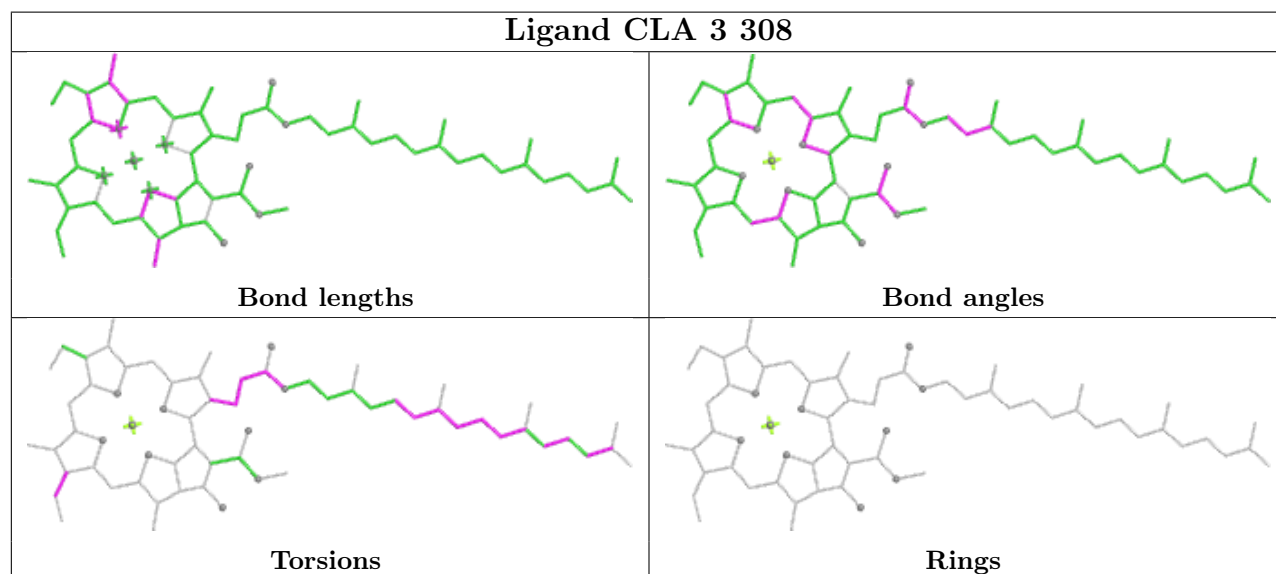
Torsions



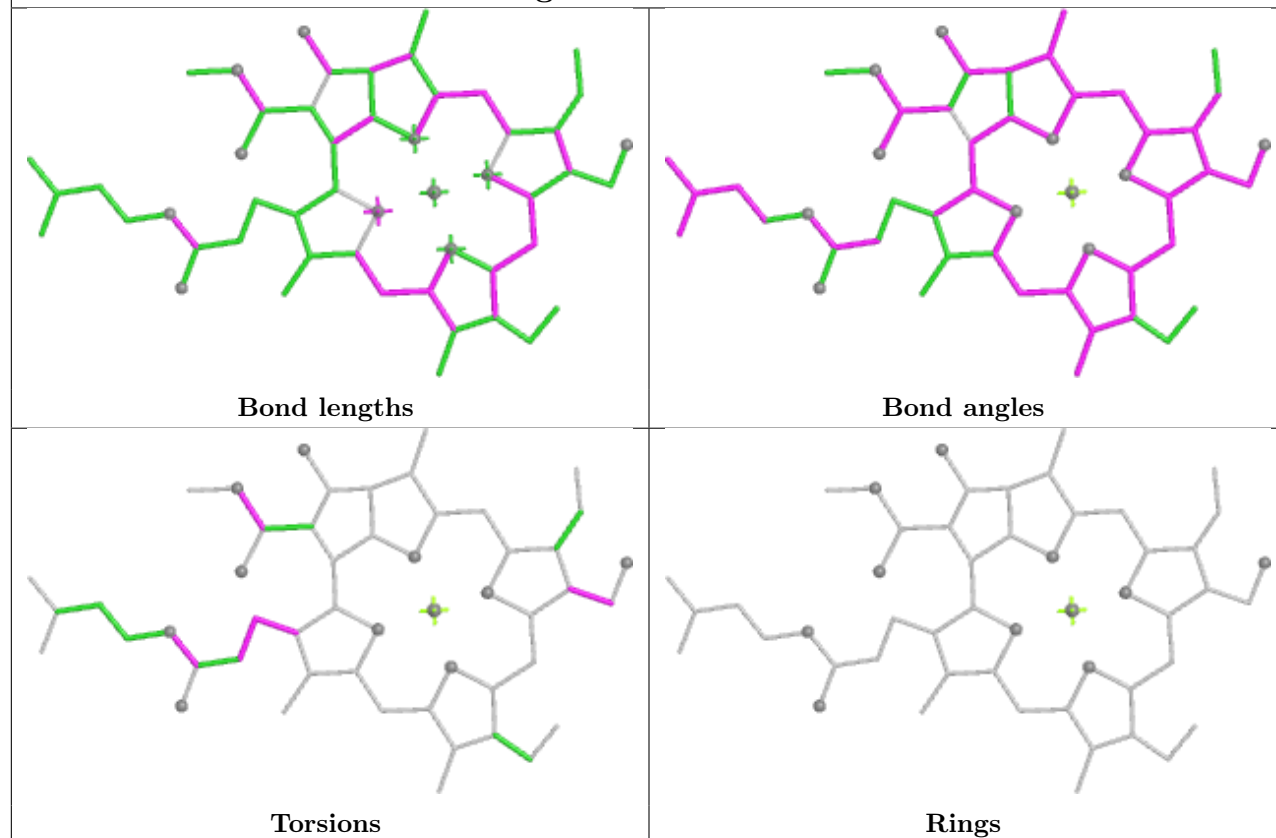
Rings



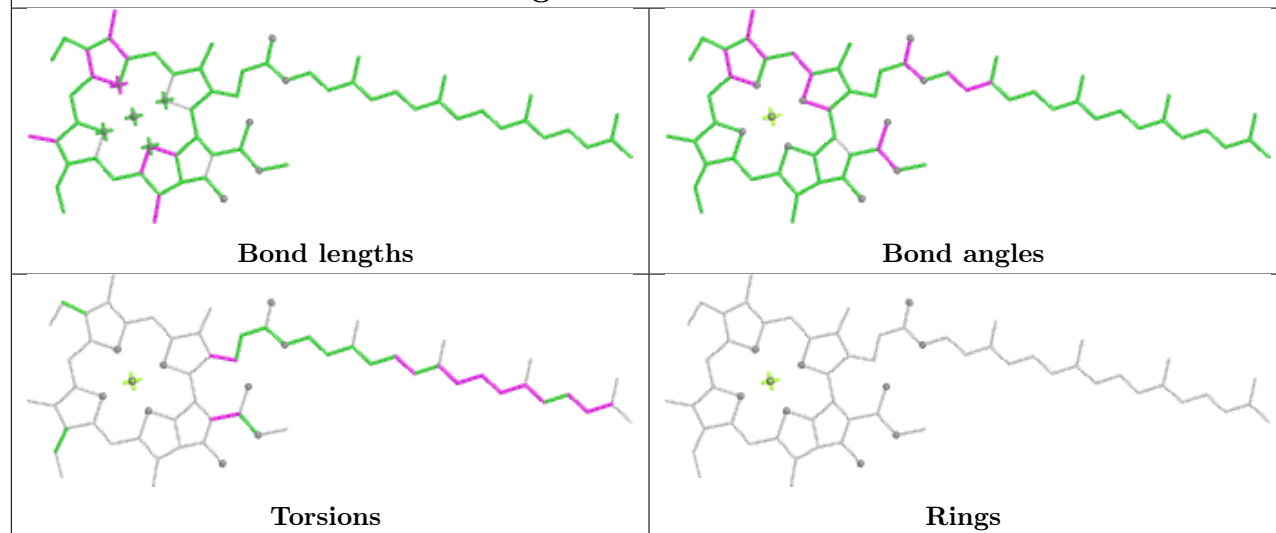


Ligand OUR 1 316**Ligand CLA 3 308**

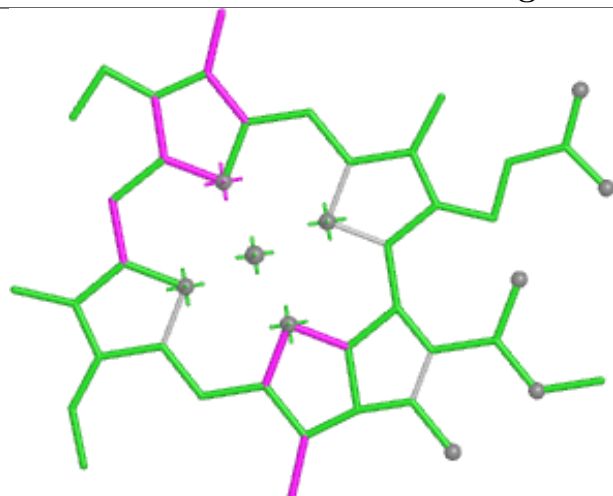
Ligand CHL 4 307



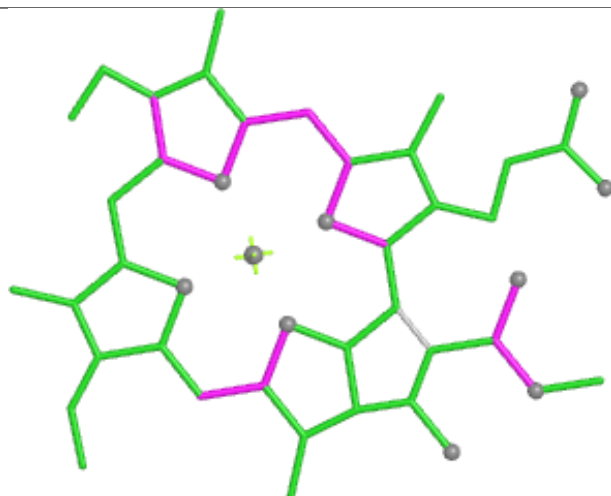
Ligand CLA B 827



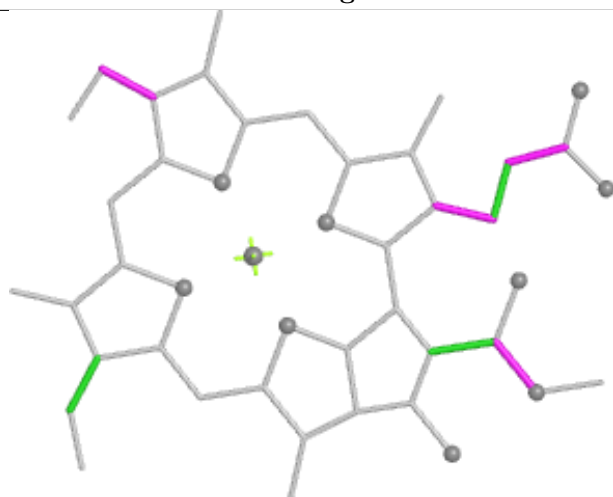
Ligand CLA 3 313



Bond lengths



Bond angles

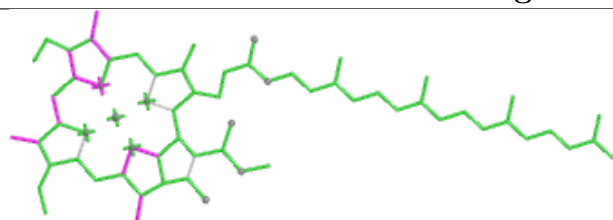


Torsions

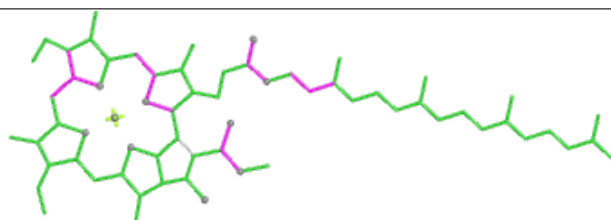


Rings

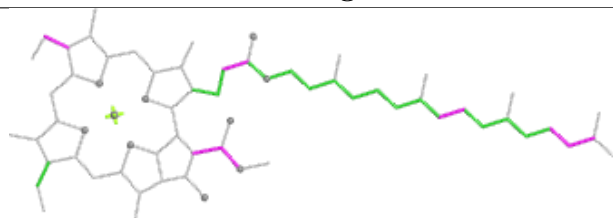
Ligand CLA B 805



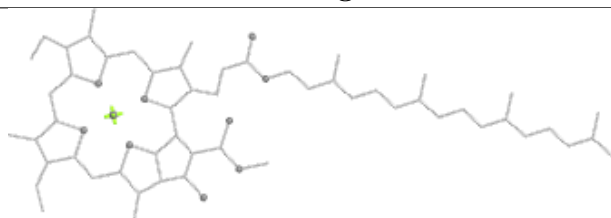
Bond lengths



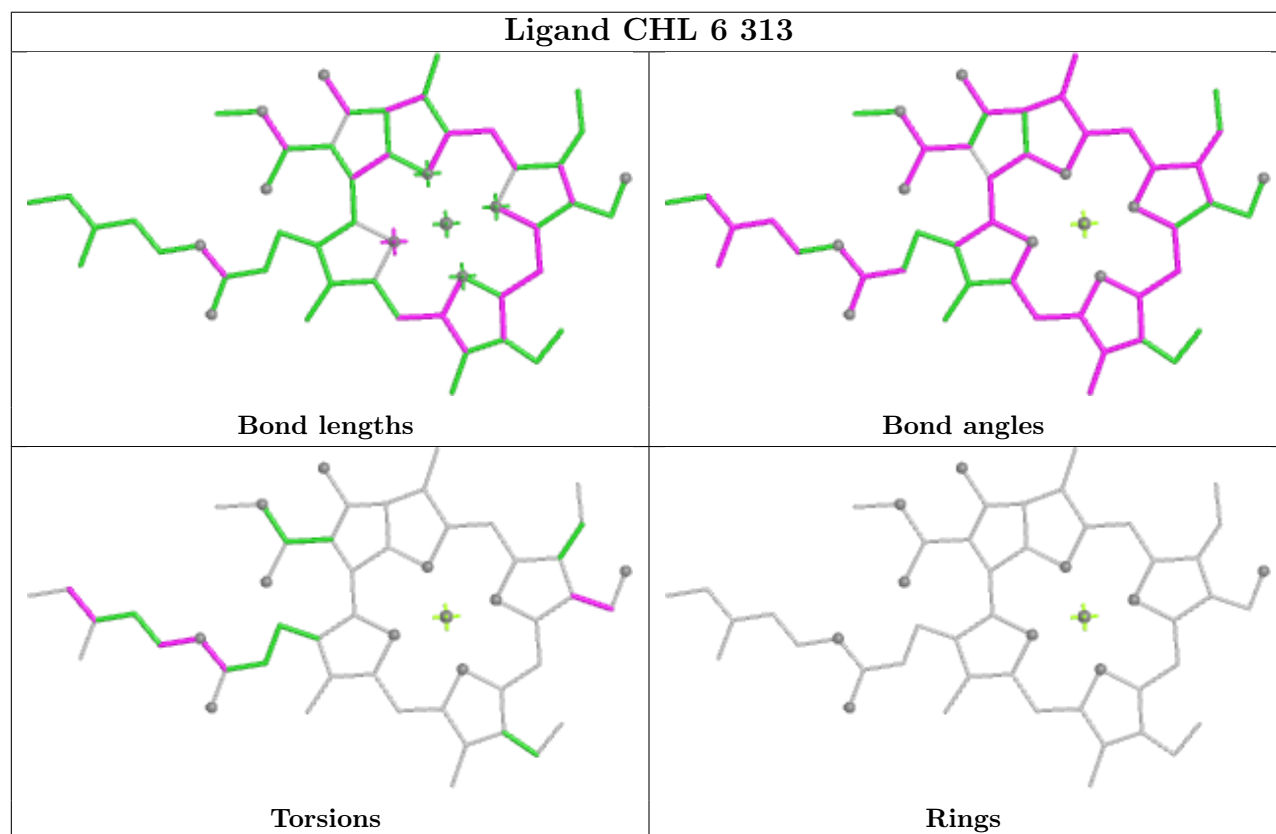
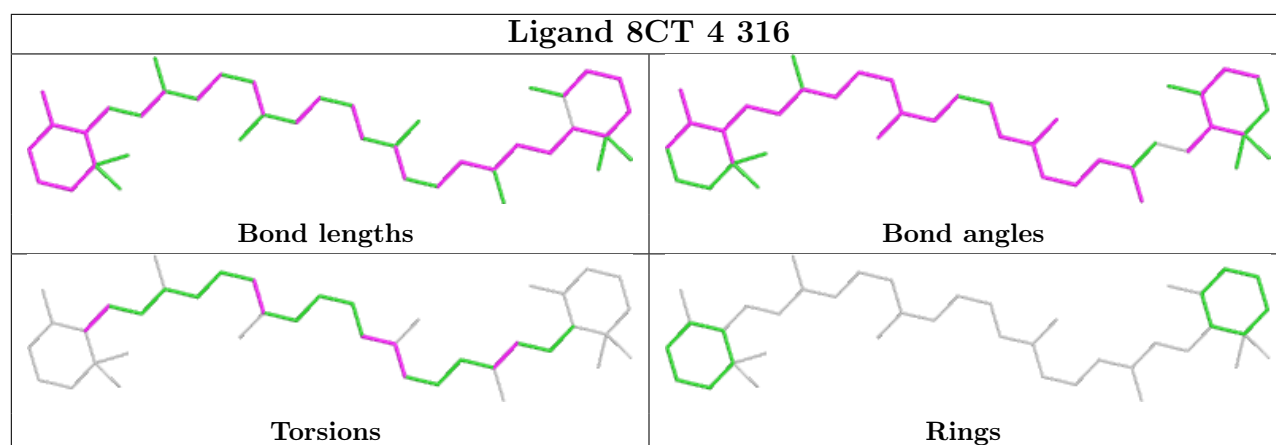
Bond angles



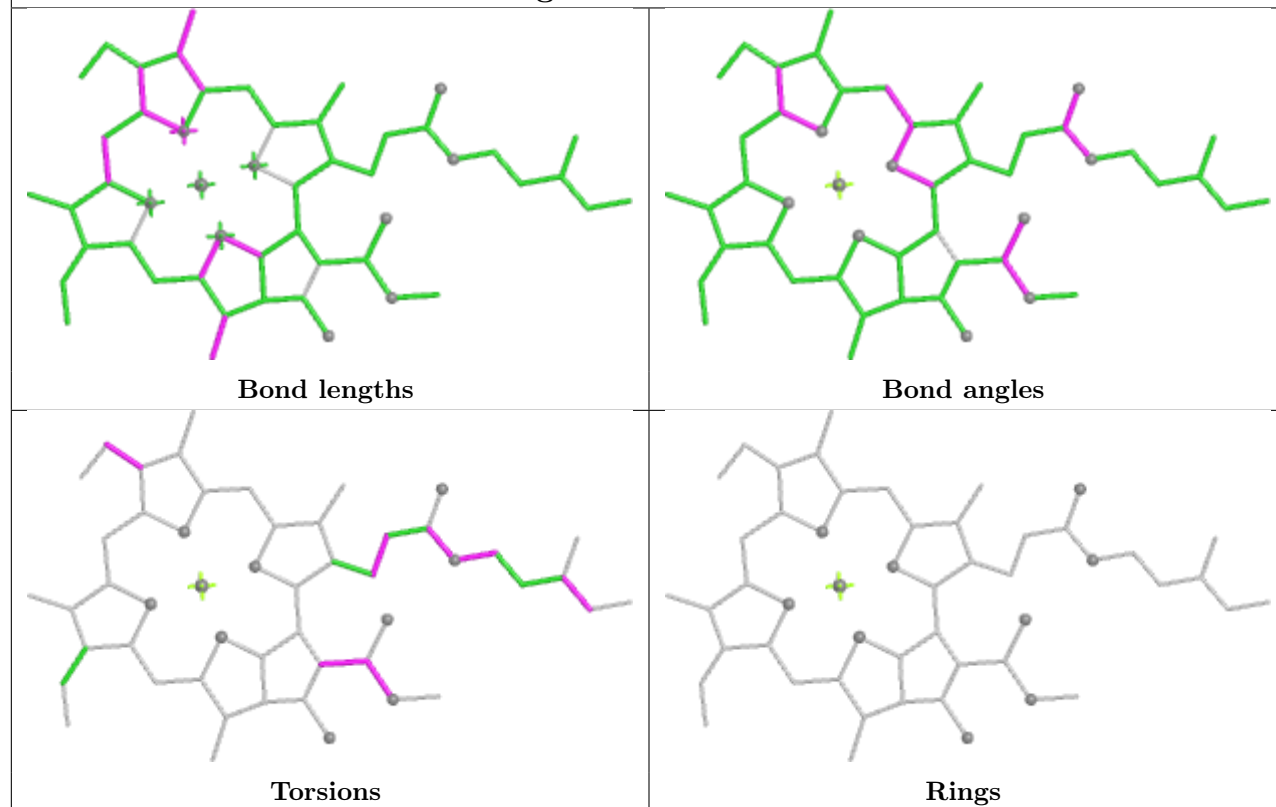
Torsions



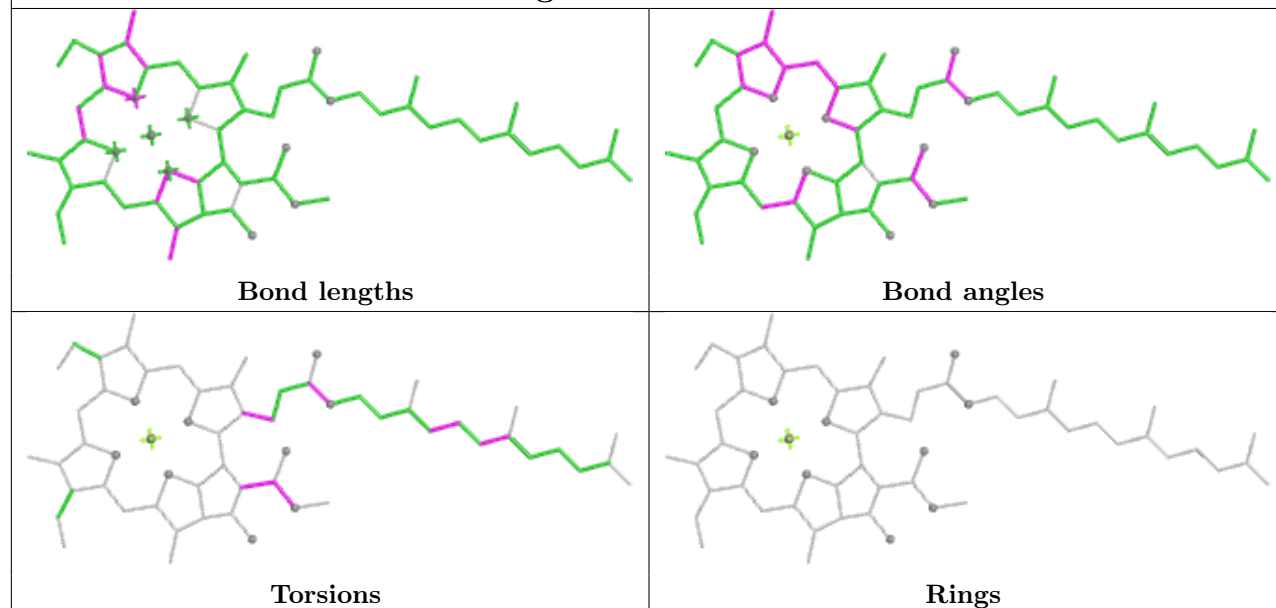
Rings



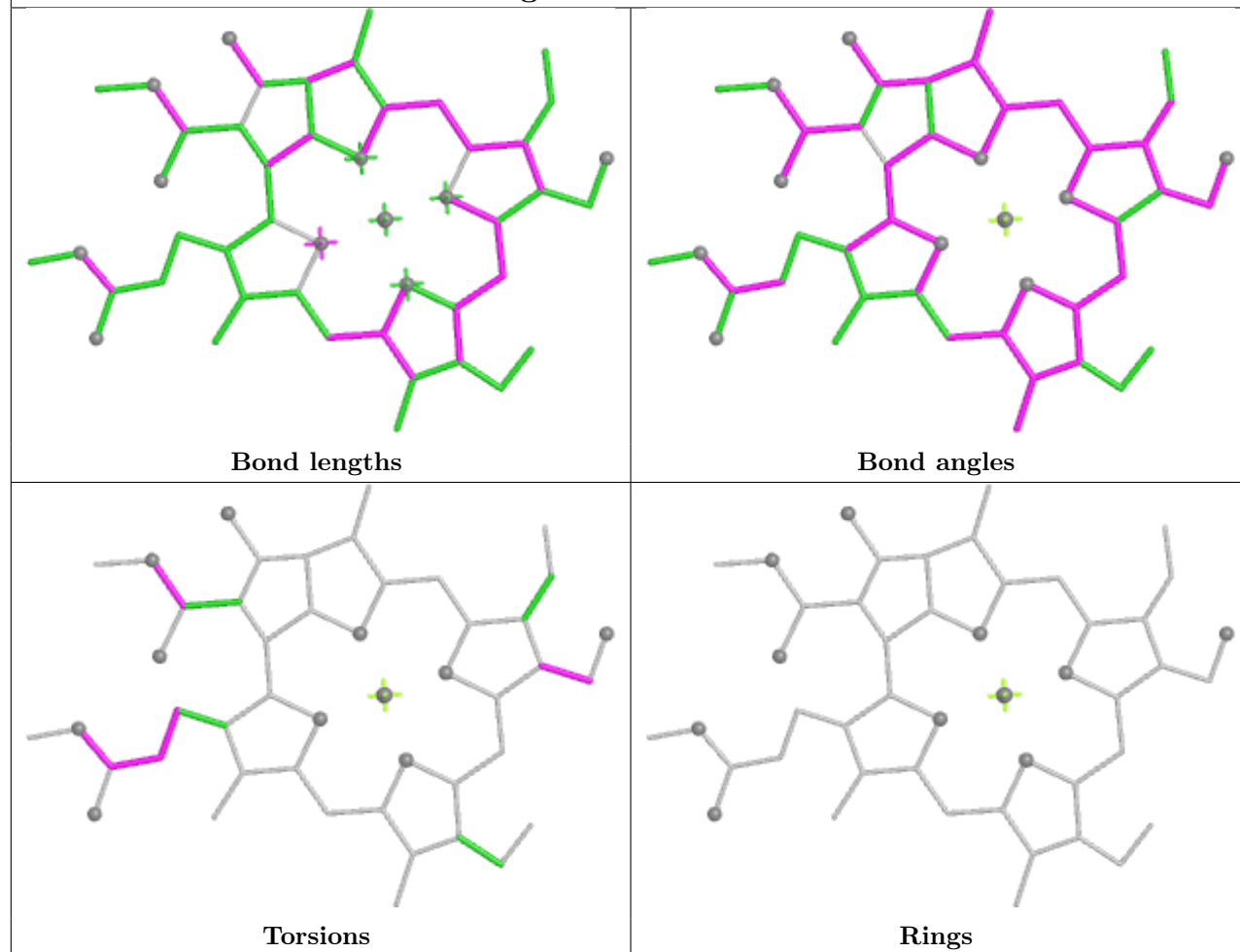
Ligand CLA 6 318



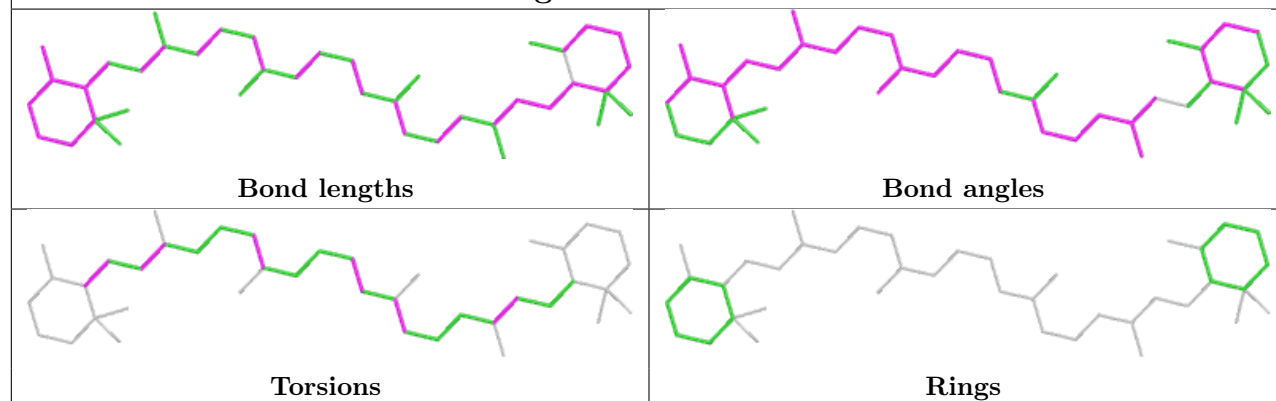
Ligand CLA 5 308



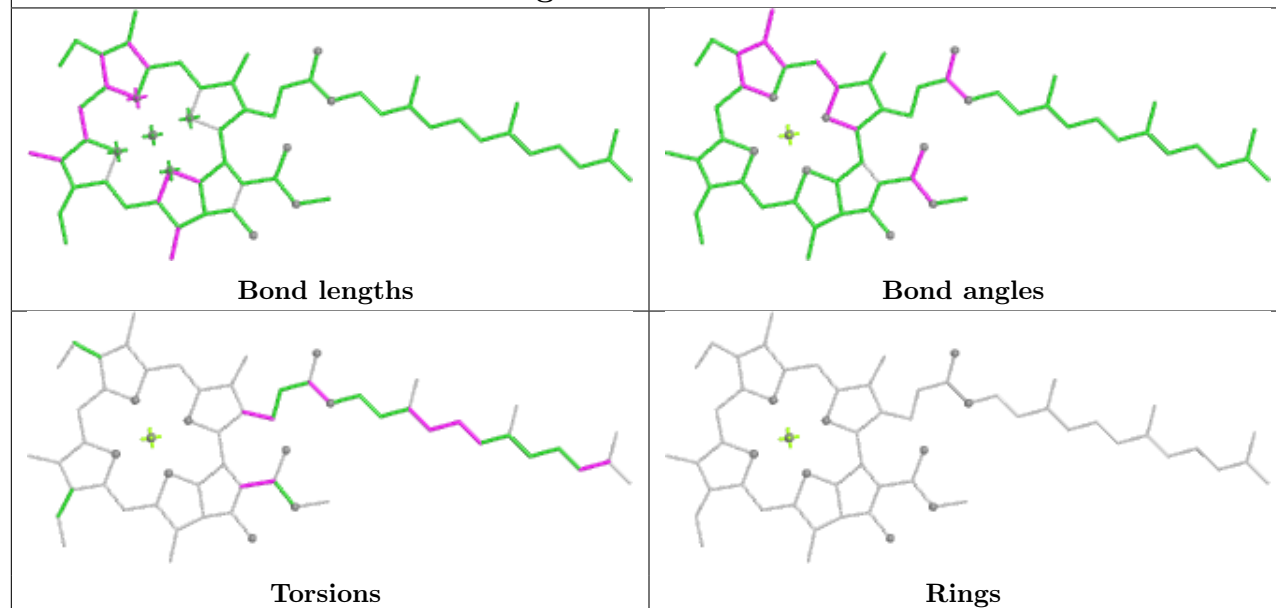
Ligand CHL 5 306



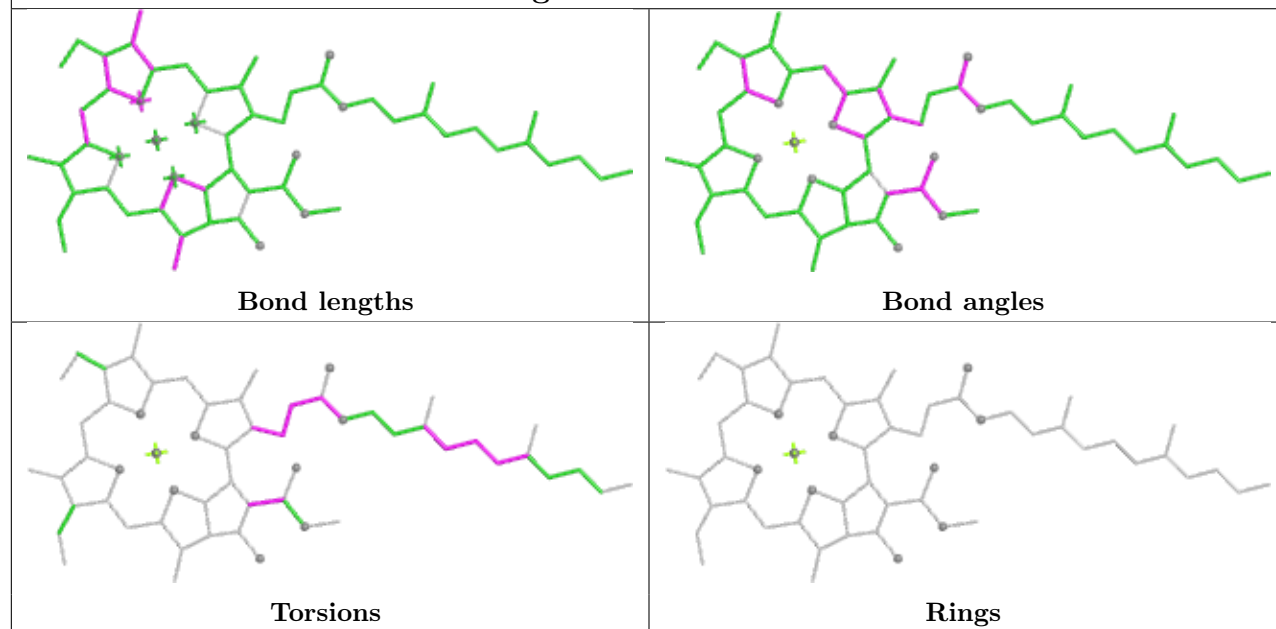
Ligand 8CT A 847



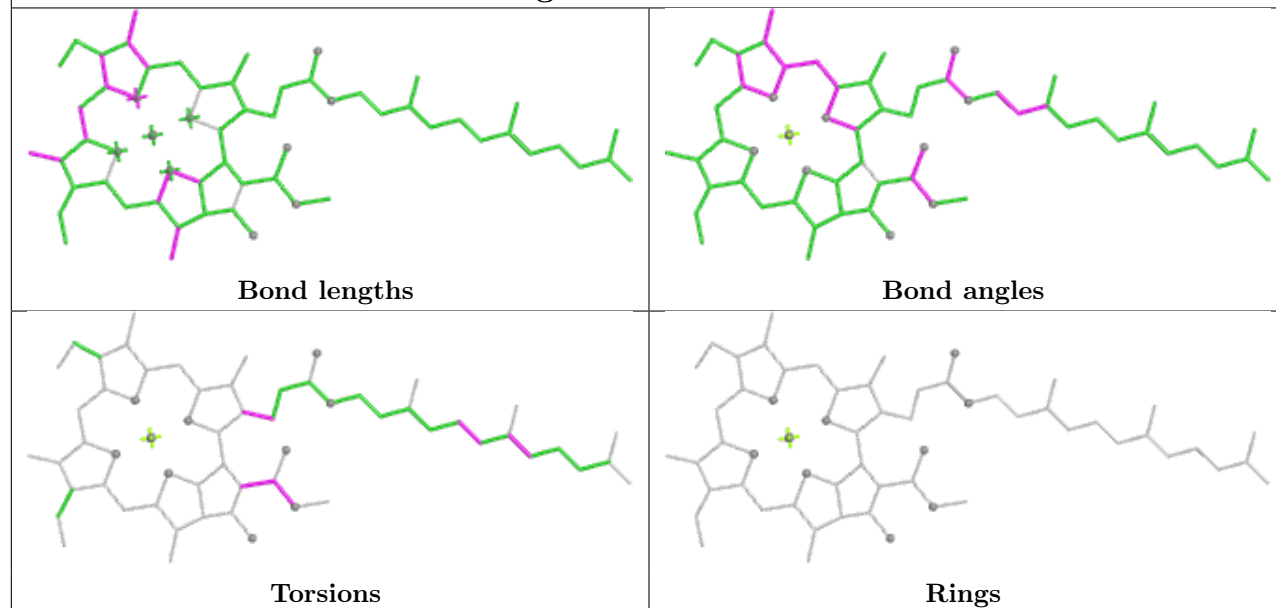
Ligand CLA 0 308



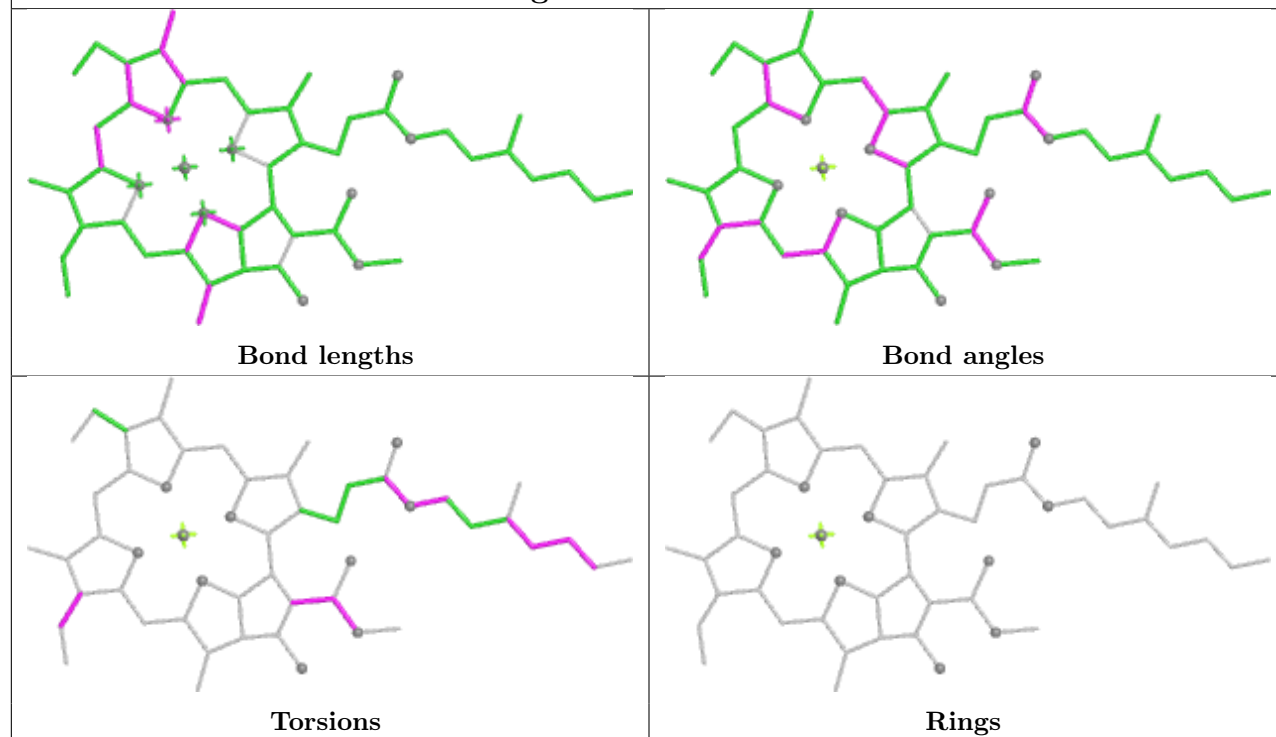
Ligand CLA B 801

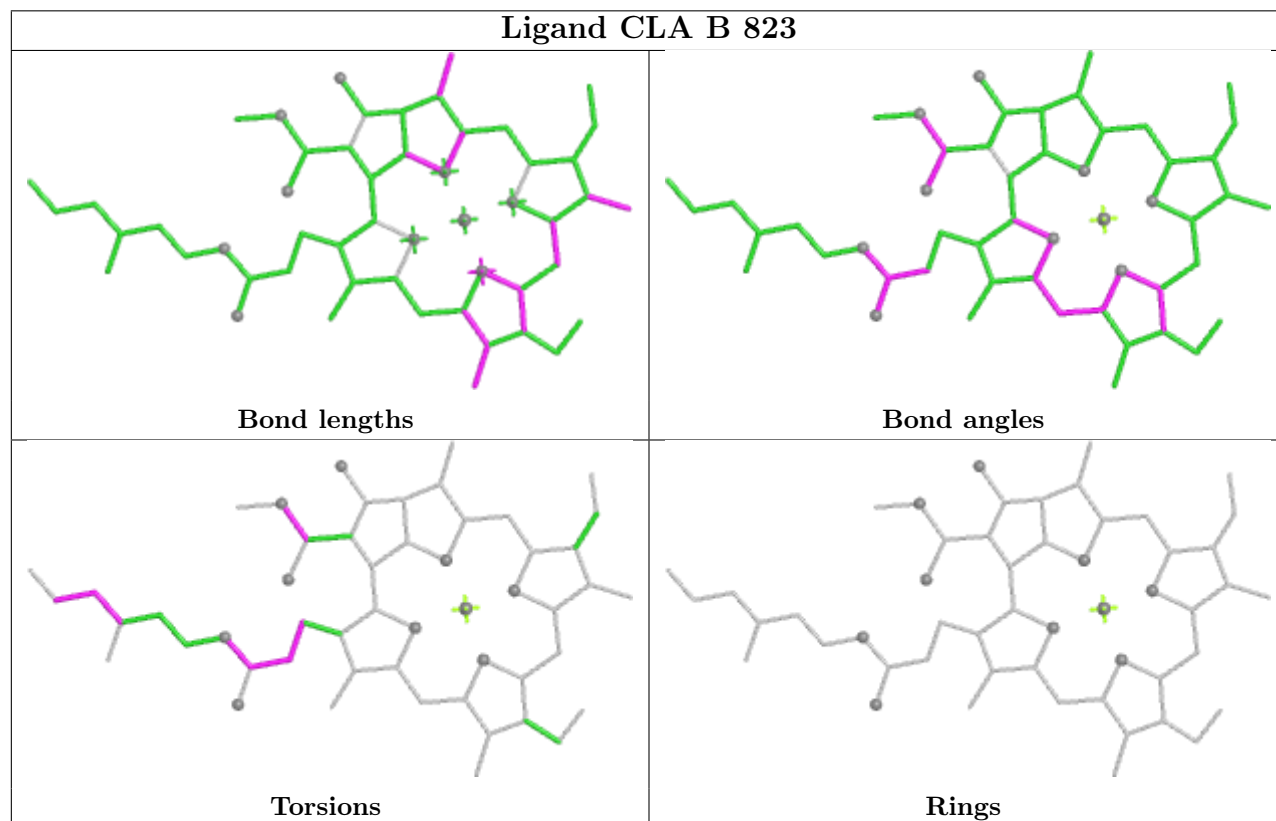
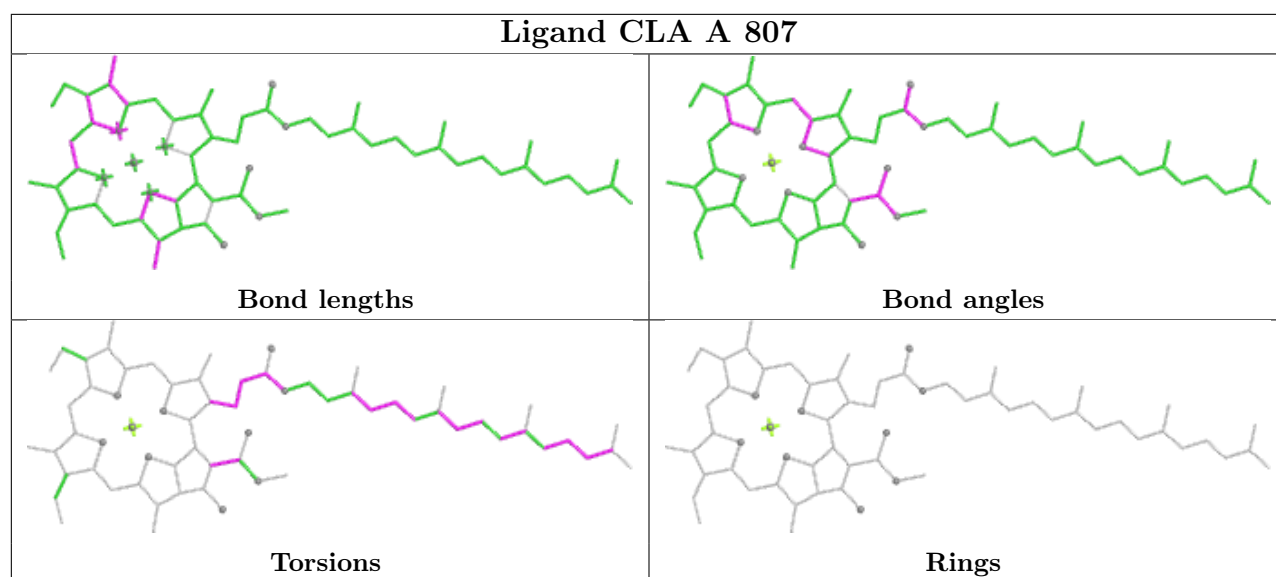


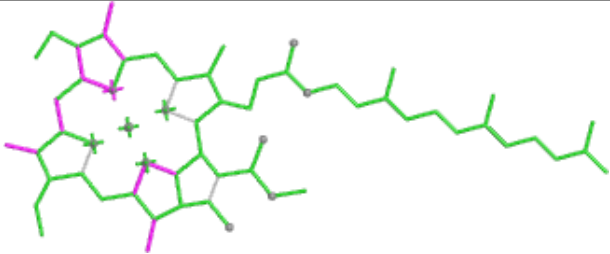
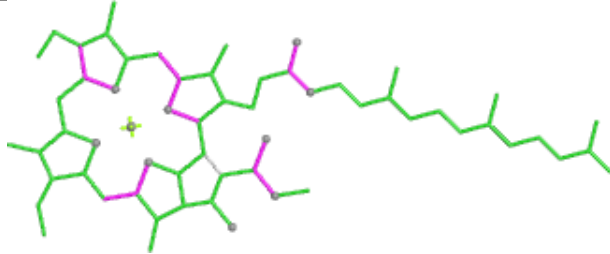
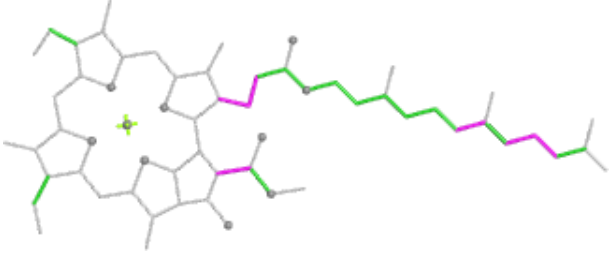
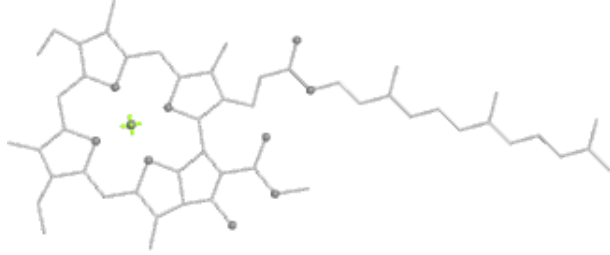
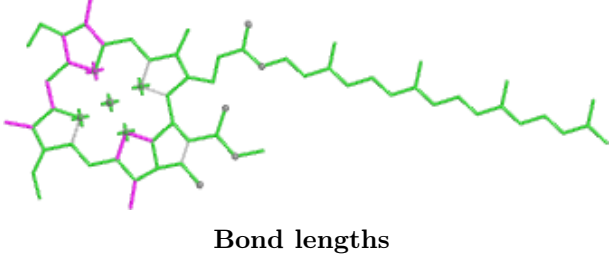
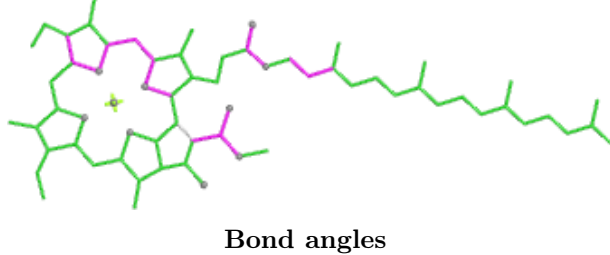
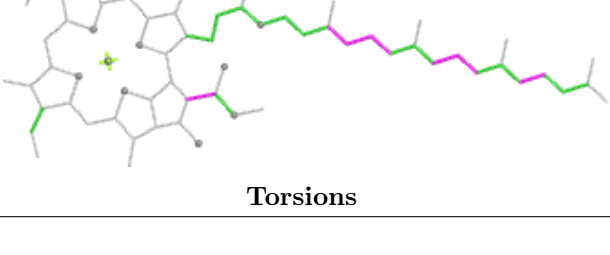
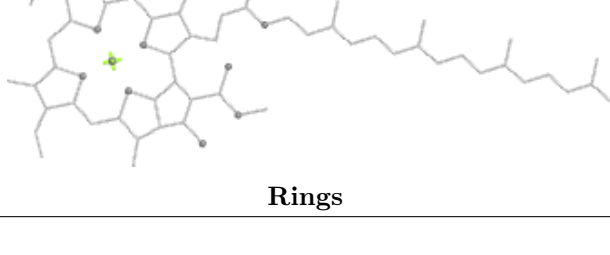
Ligand CLA 8 310

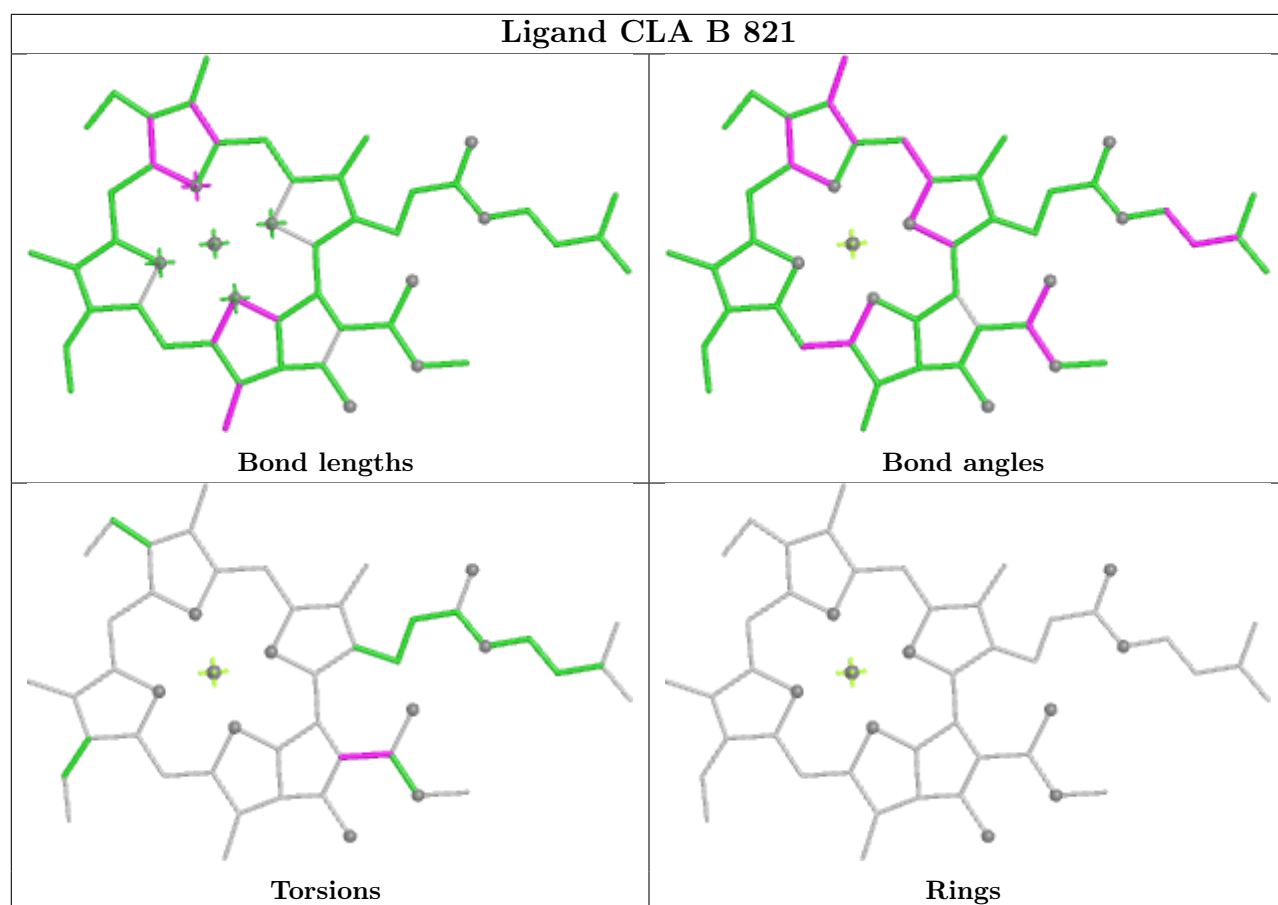


Ligand CLA K 102

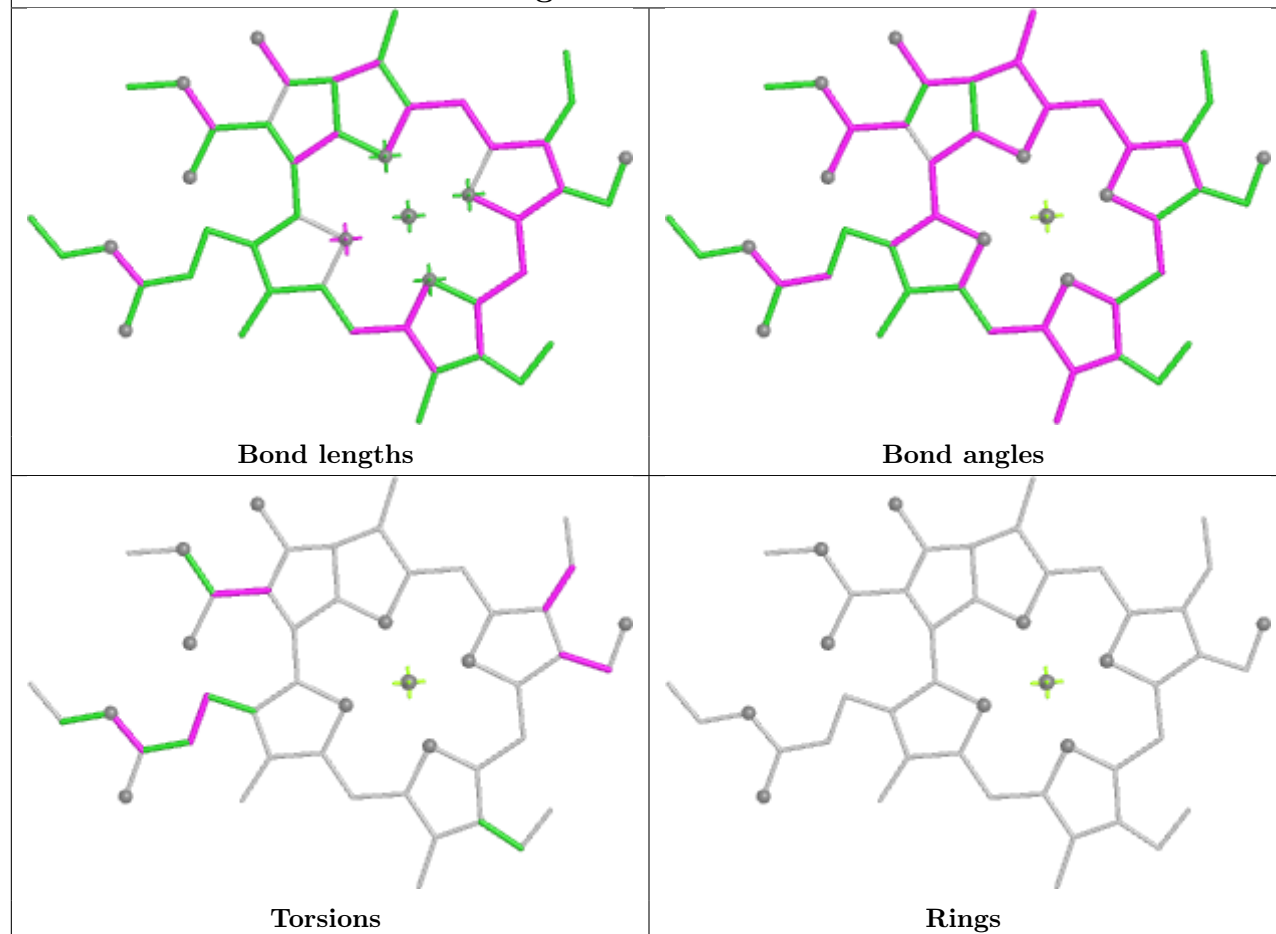




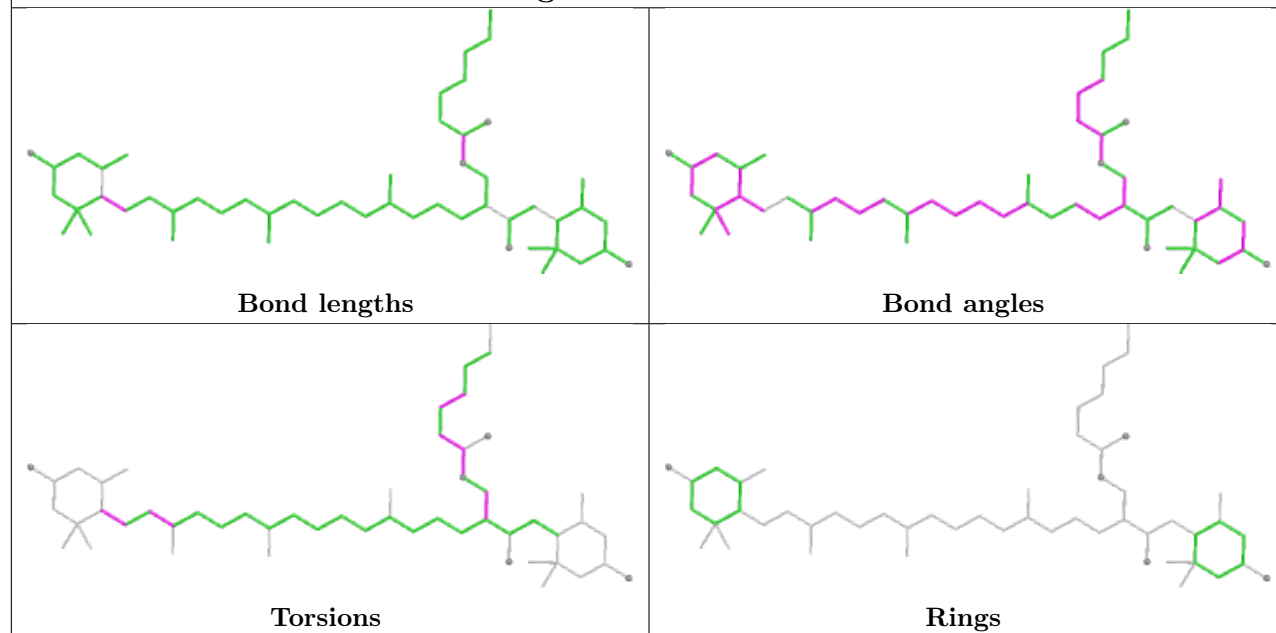
Ligand CLA B 828	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 811	
 Bond lengths	 Bond angles
 Torsions	 Rings



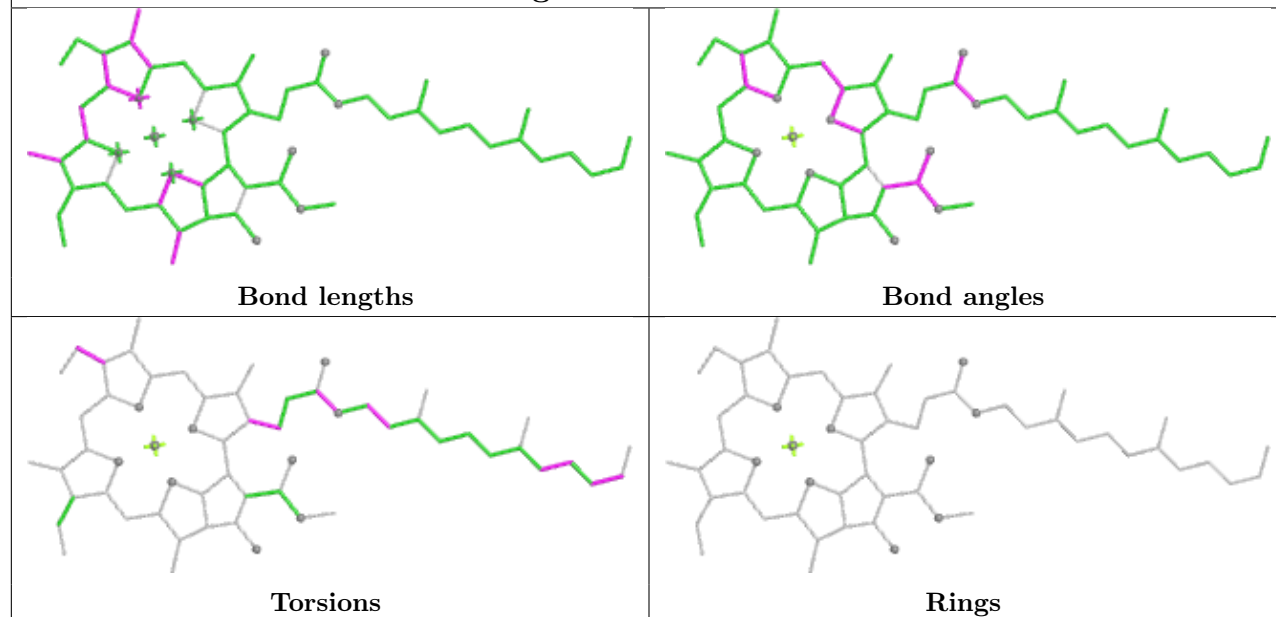
Ligand CHL 0 306



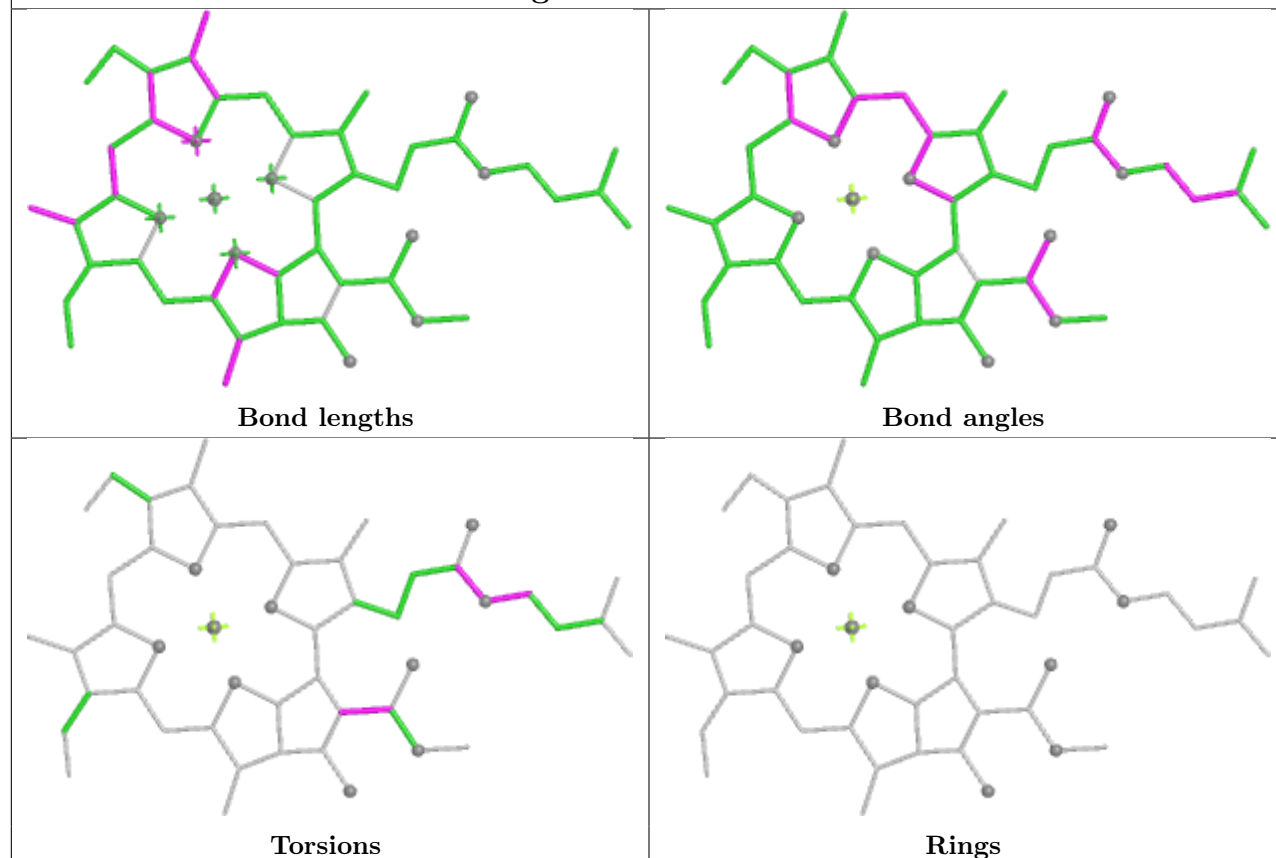
Ligand OUR 6 321



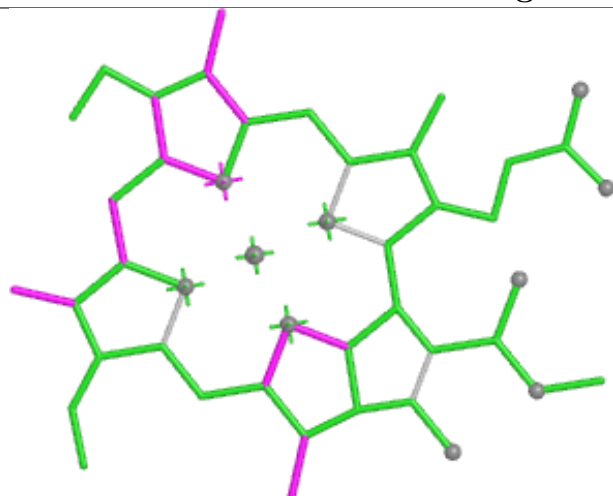
Ligand CLA B 818



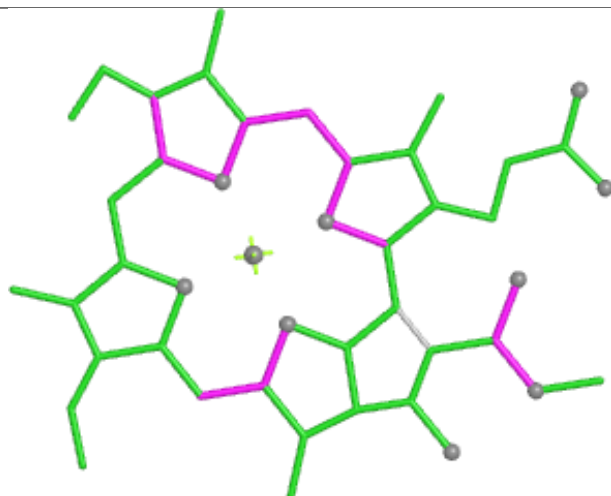
Ligand CLA A 830



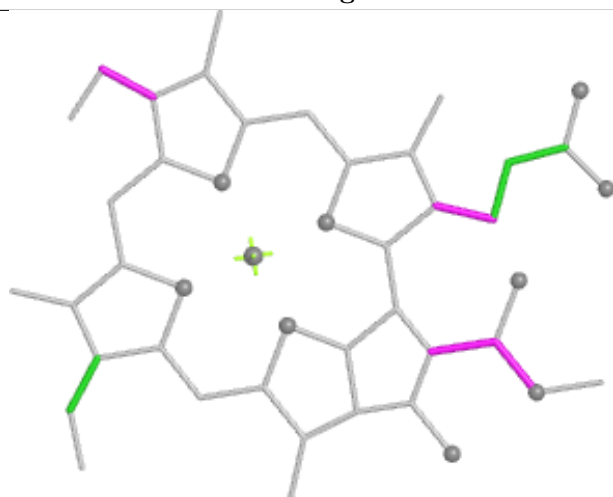
Ligand CLA F 303



Bond lengths



Bond angles

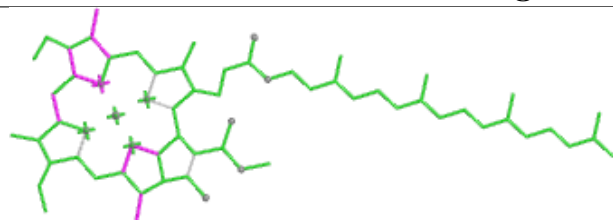


Torsions

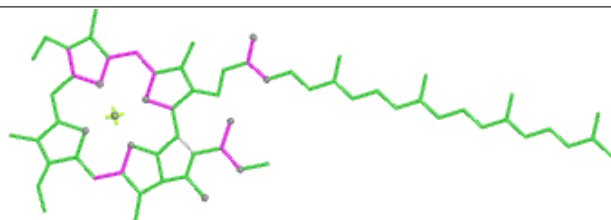


Rings

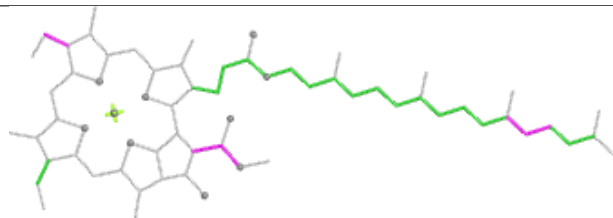
Ligand CLA B 841



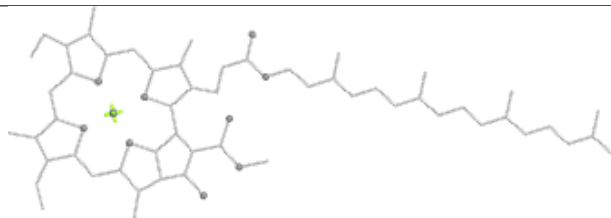
Bond lengths



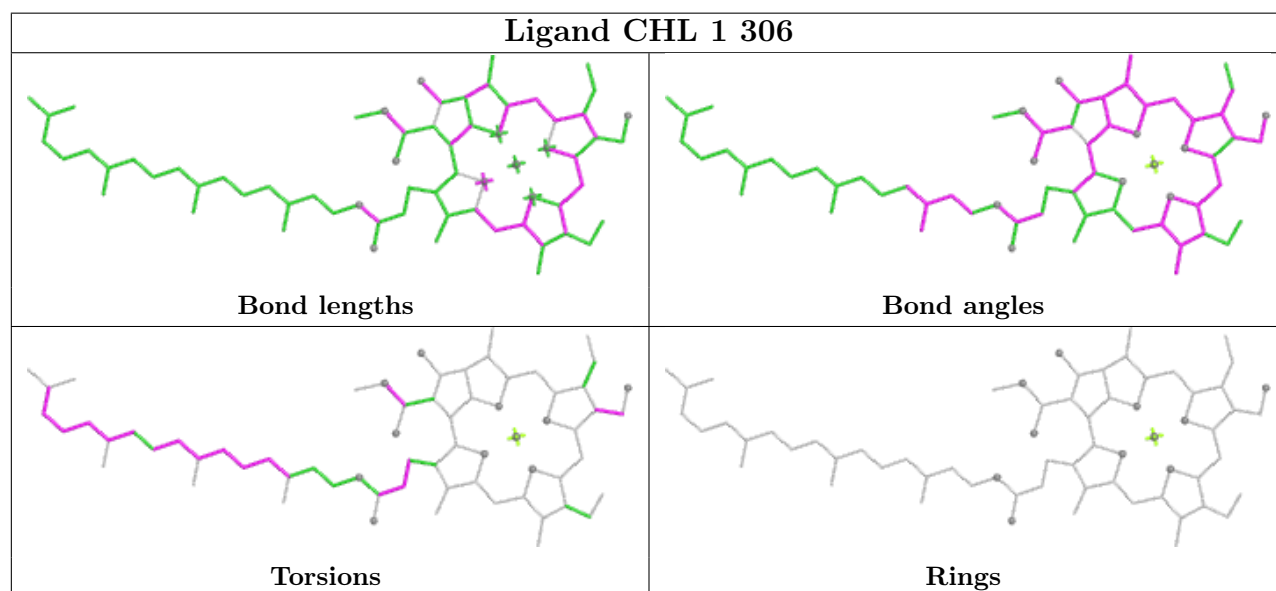
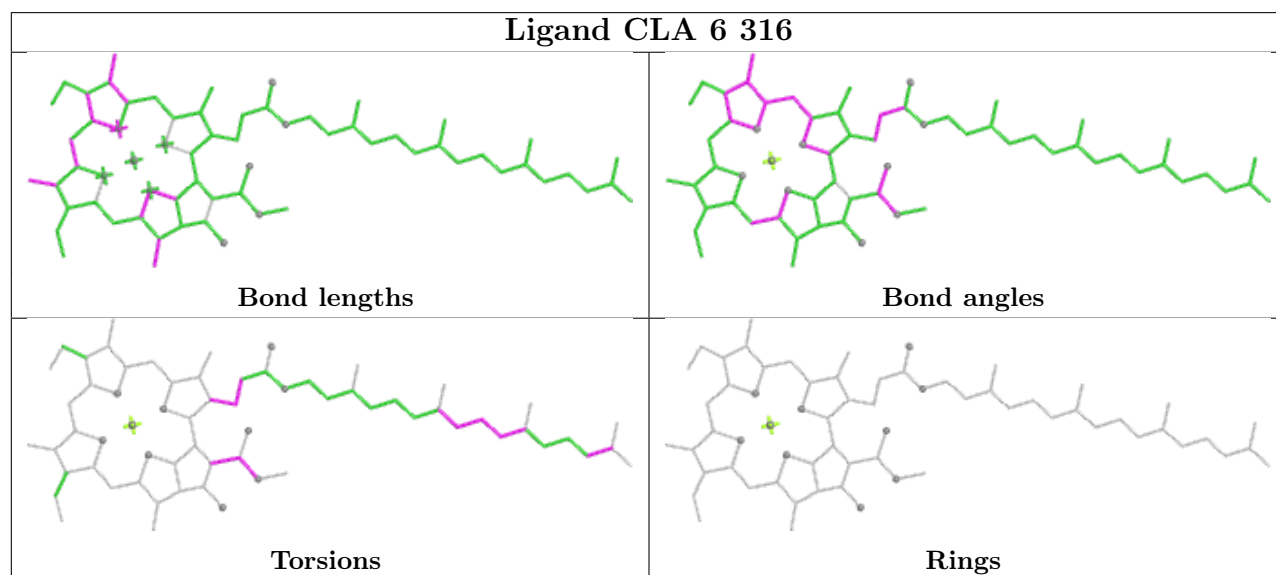
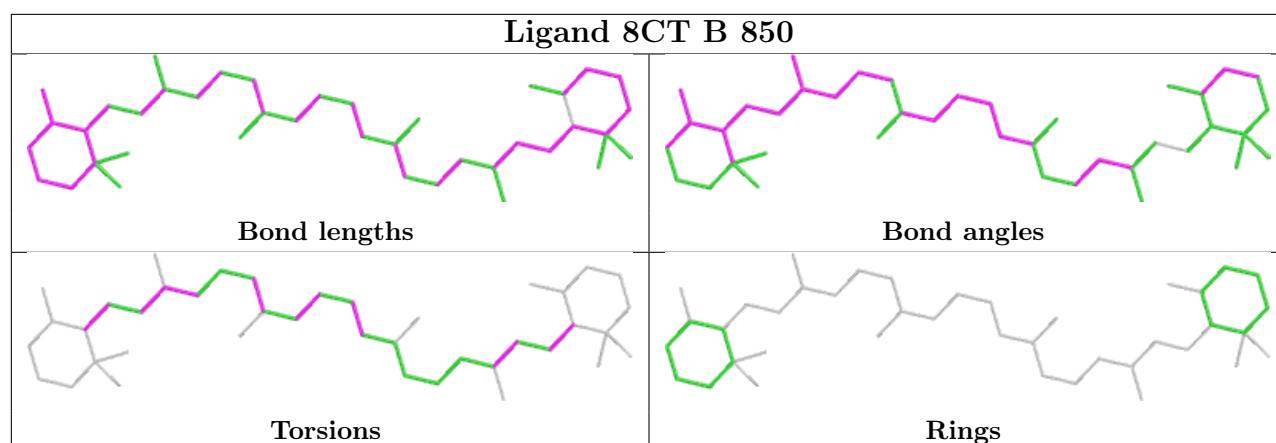
Bond angles

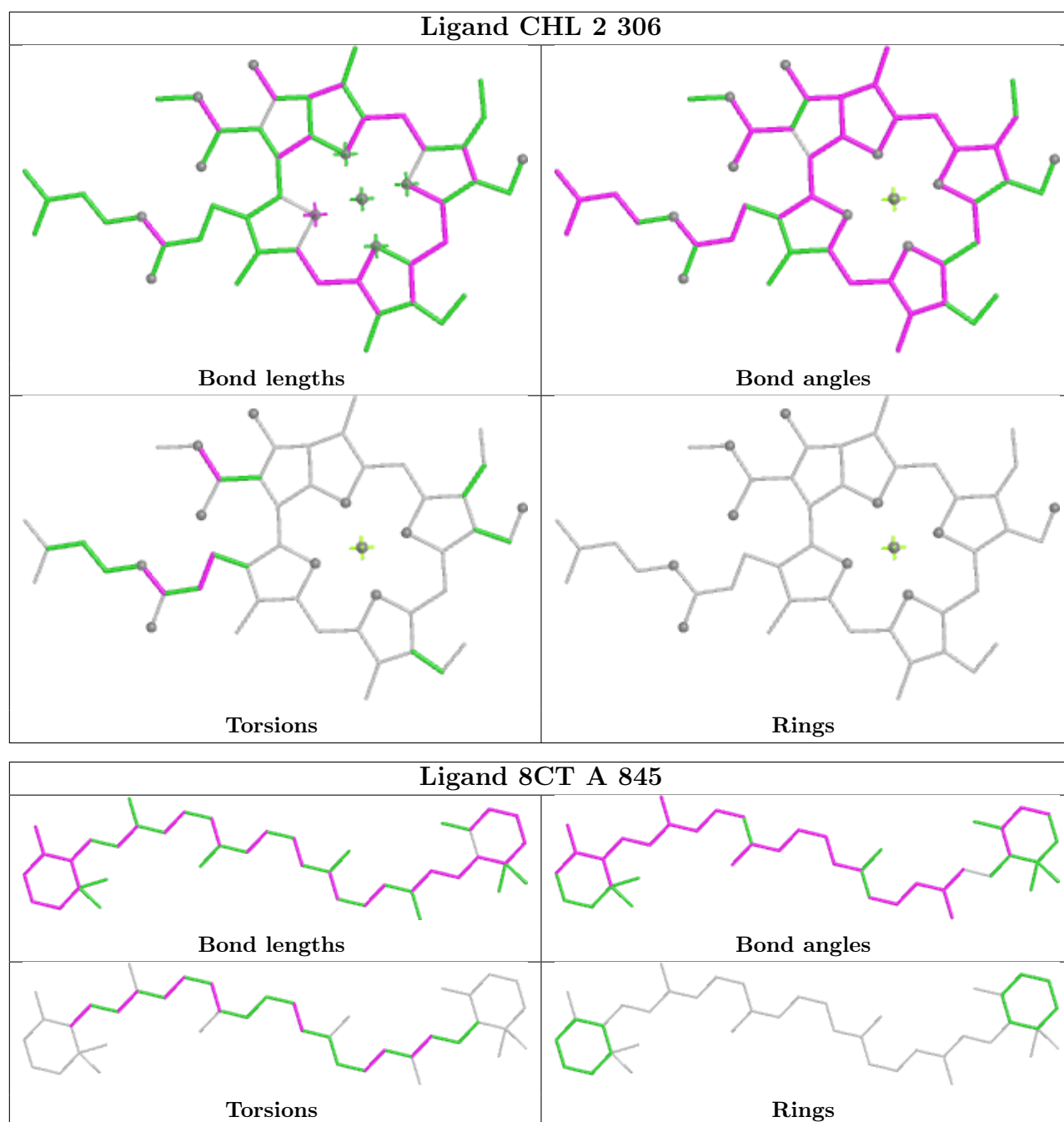


Torsions

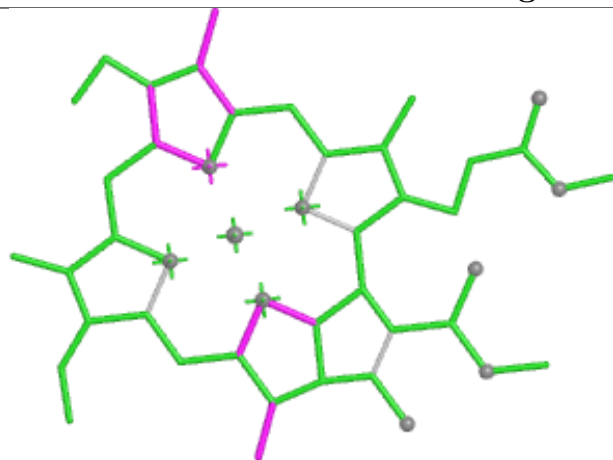


Rings

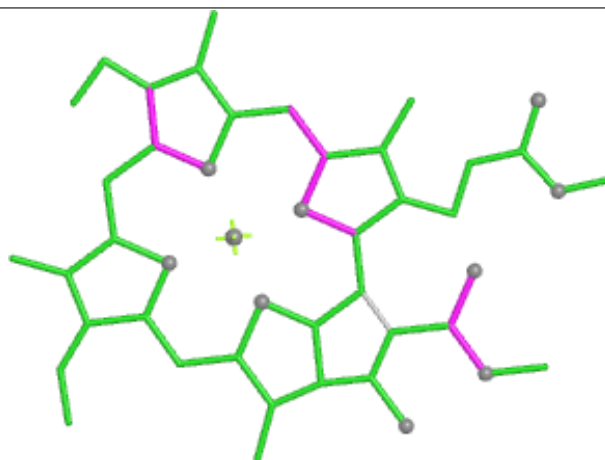




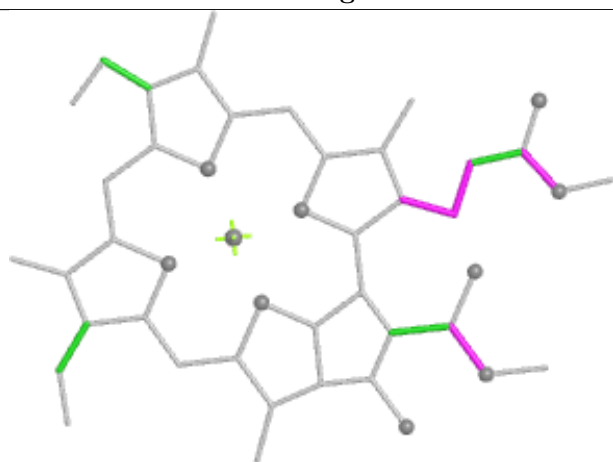
Ligand CLA 5 307



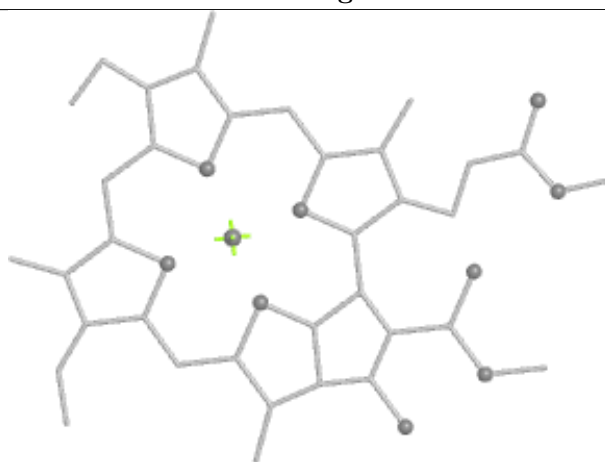
Bond lengths



Bond angles

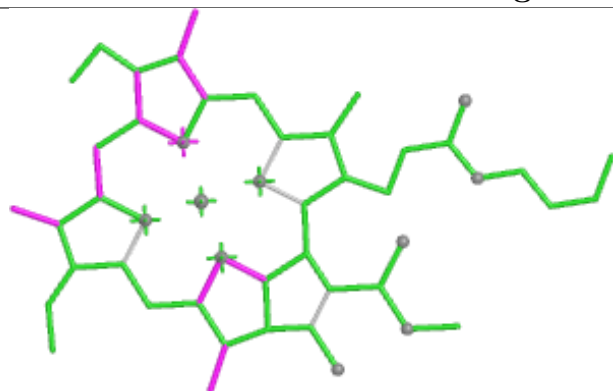


Torsions

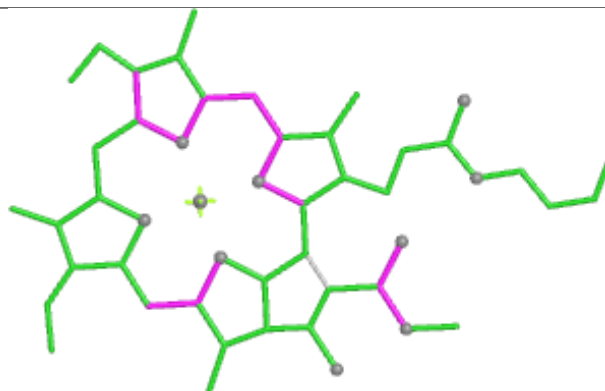


Rings

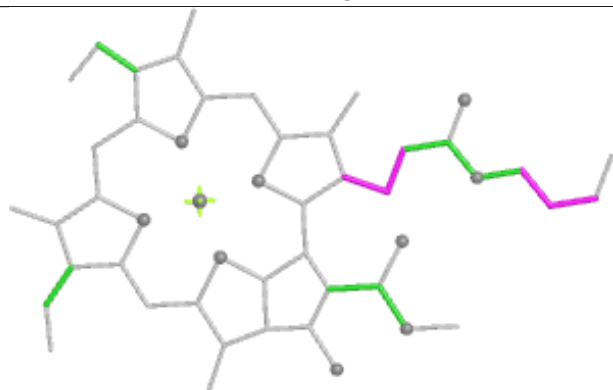
Ligand CLA A 821



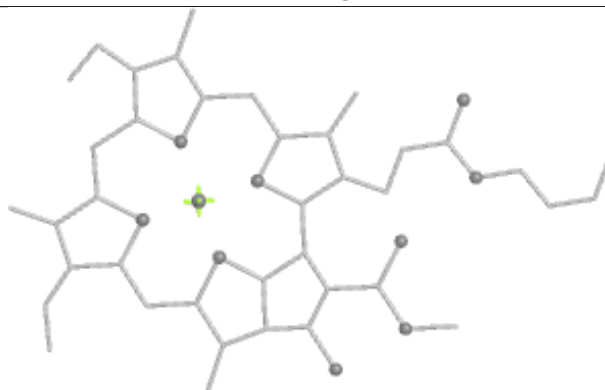
Bond lengths



Bond angles

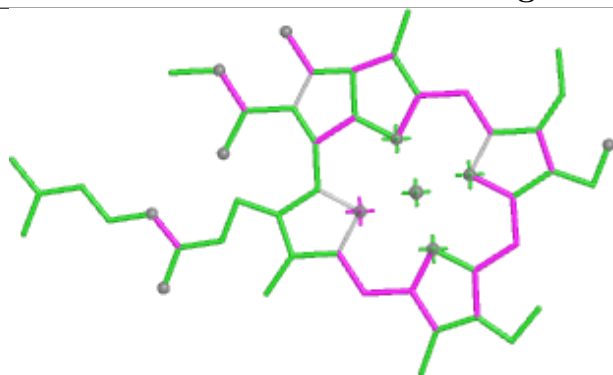


Torsions

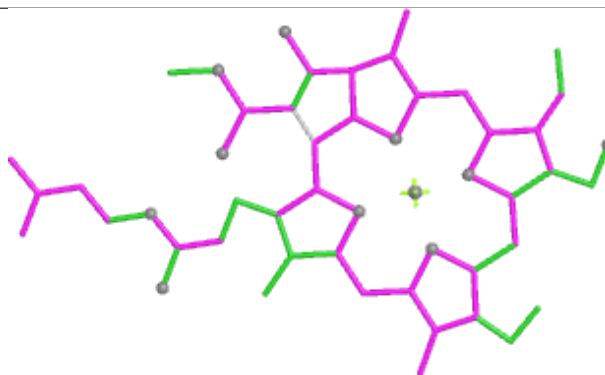


Rings

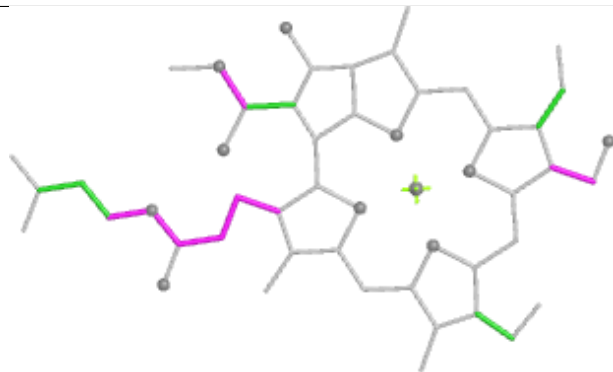
Ligand CHL 8 308



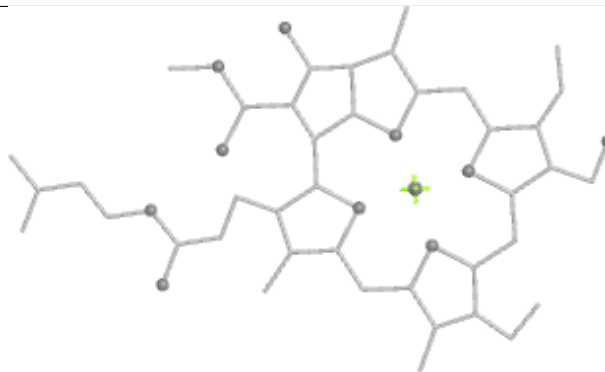
Bond lengths



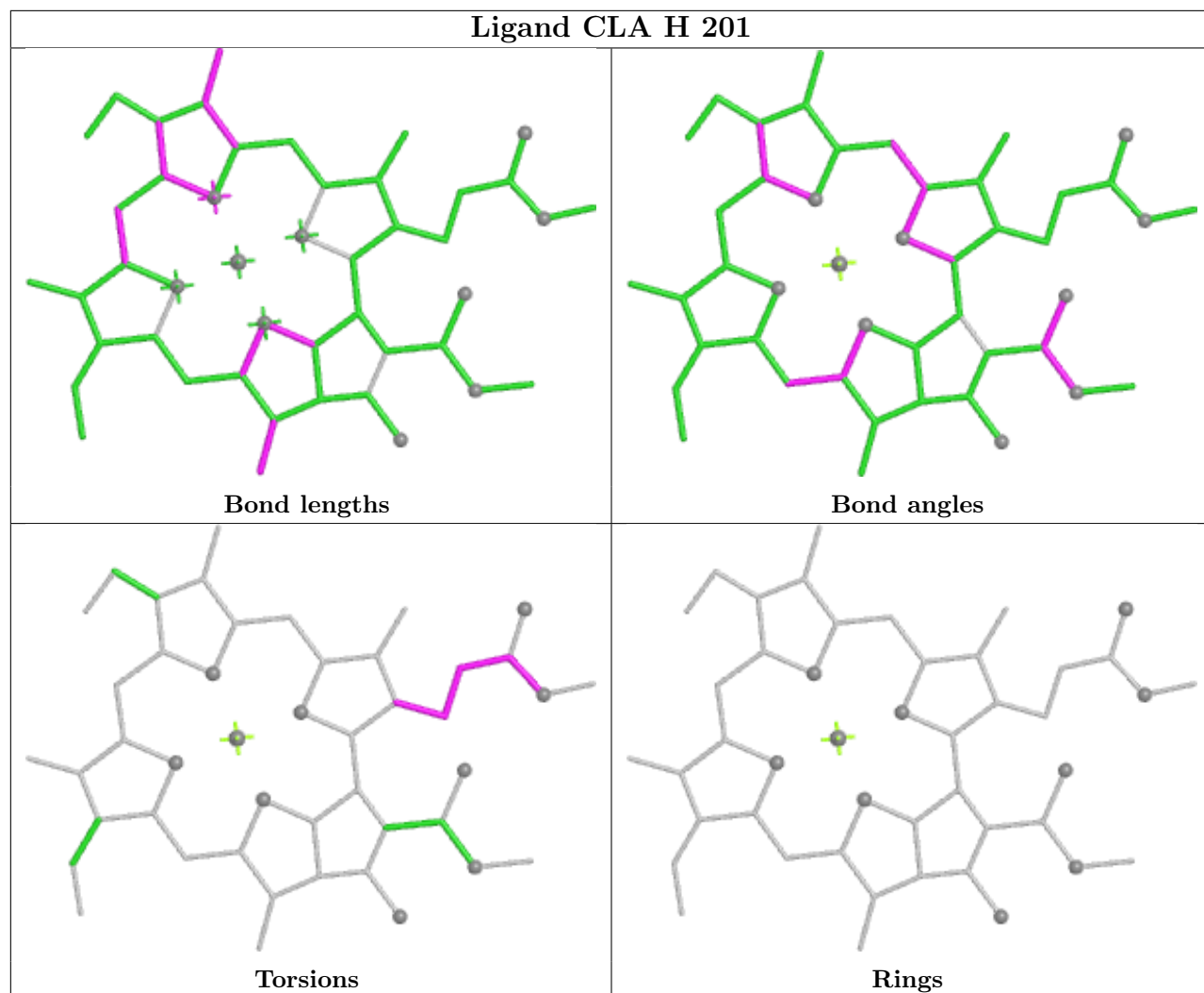
Bond angles



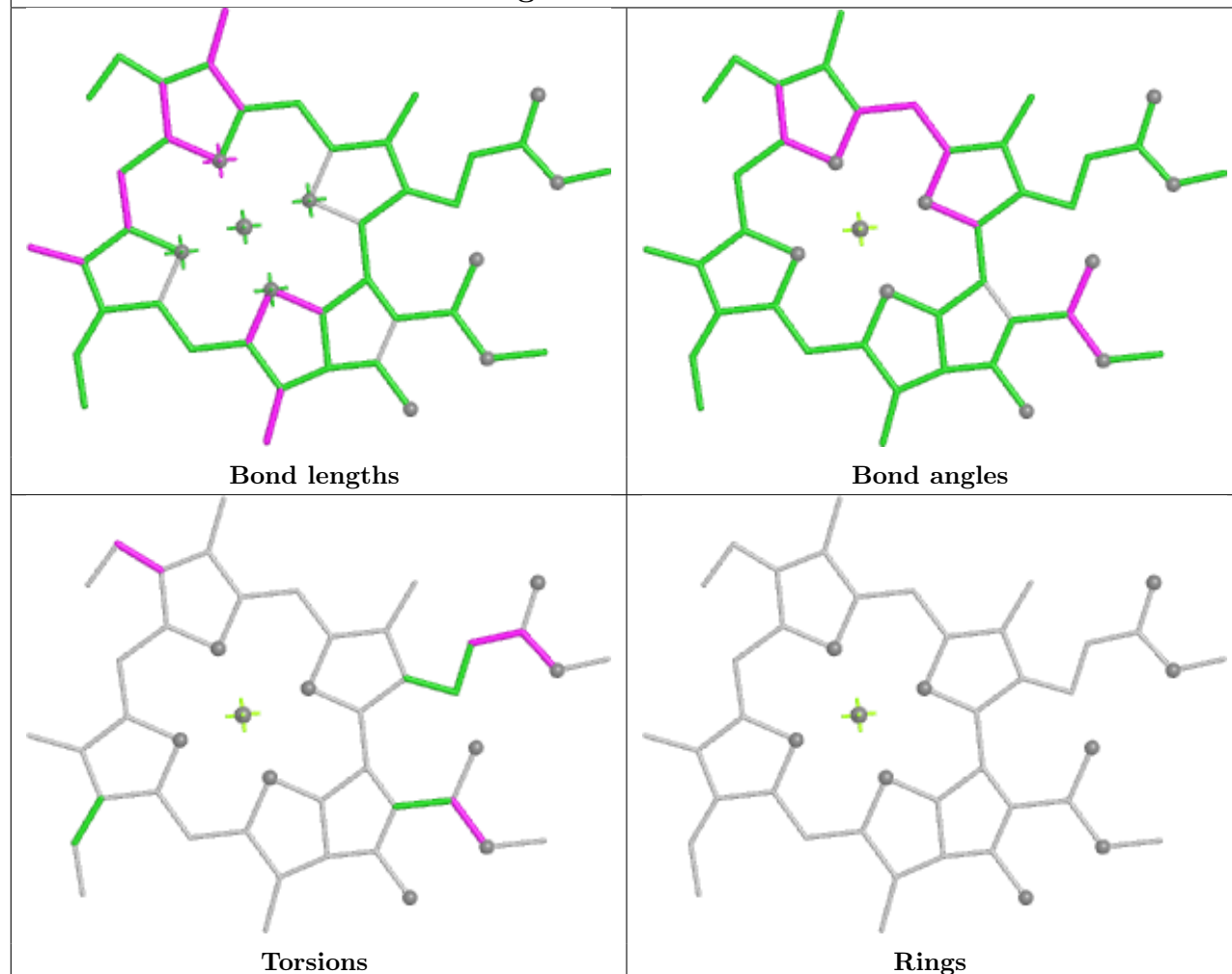
Torsions



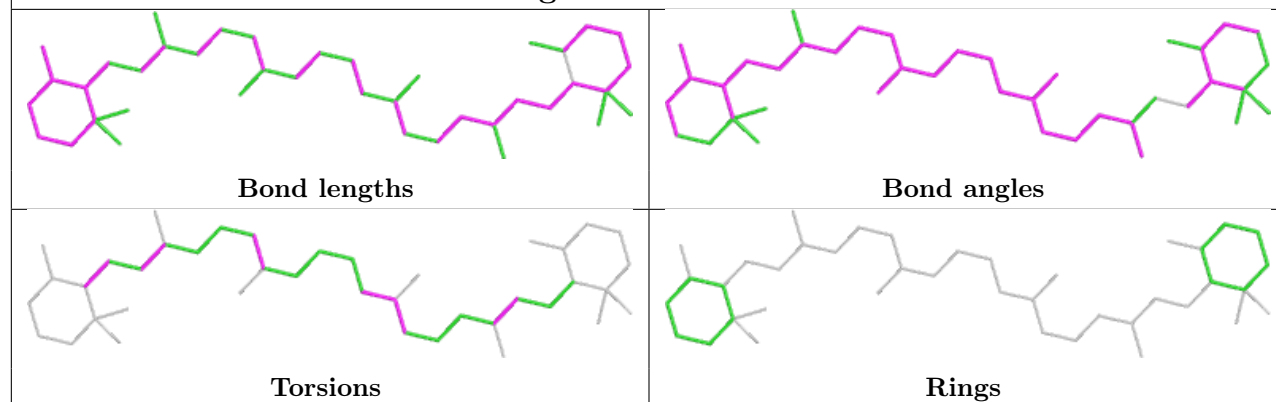
Rings

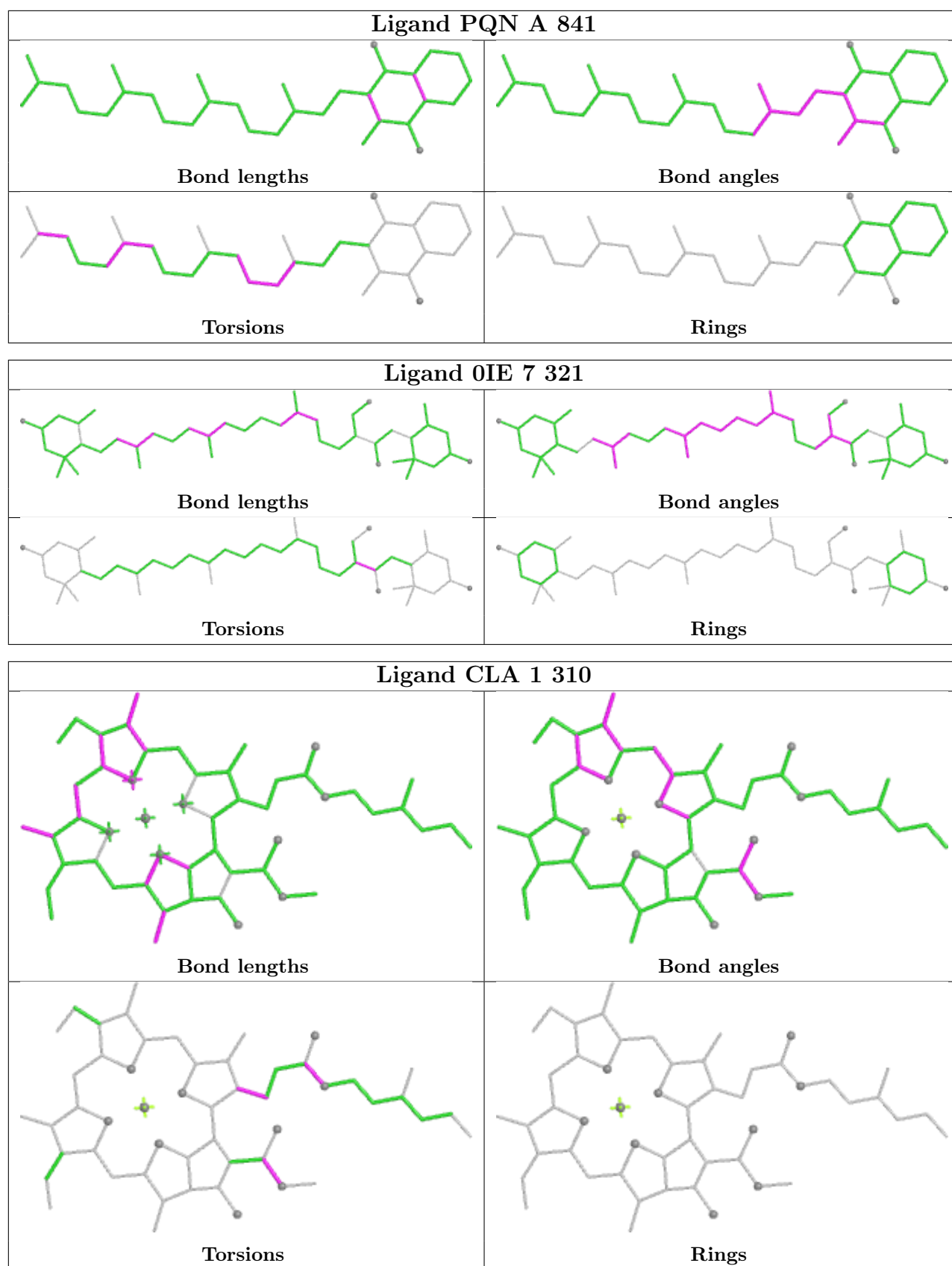


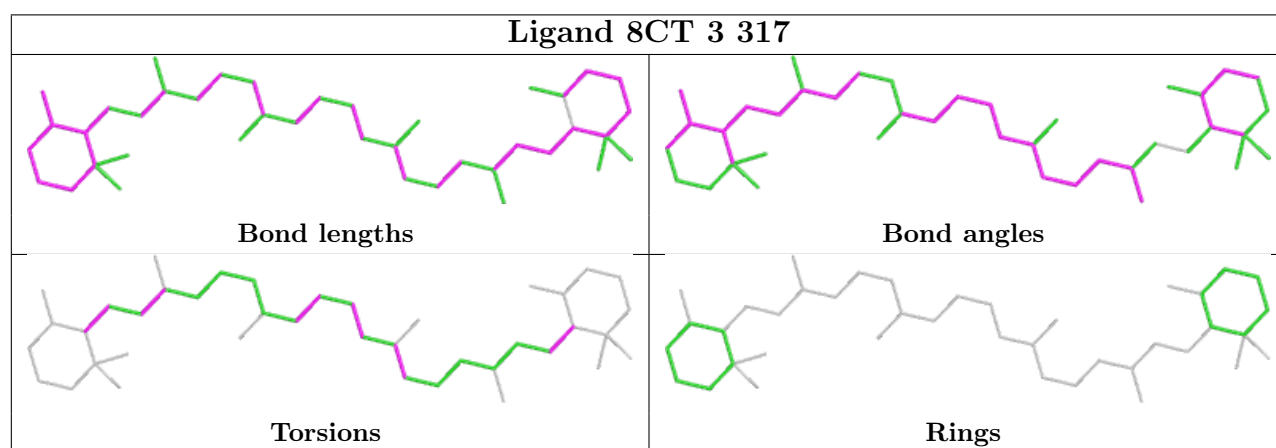
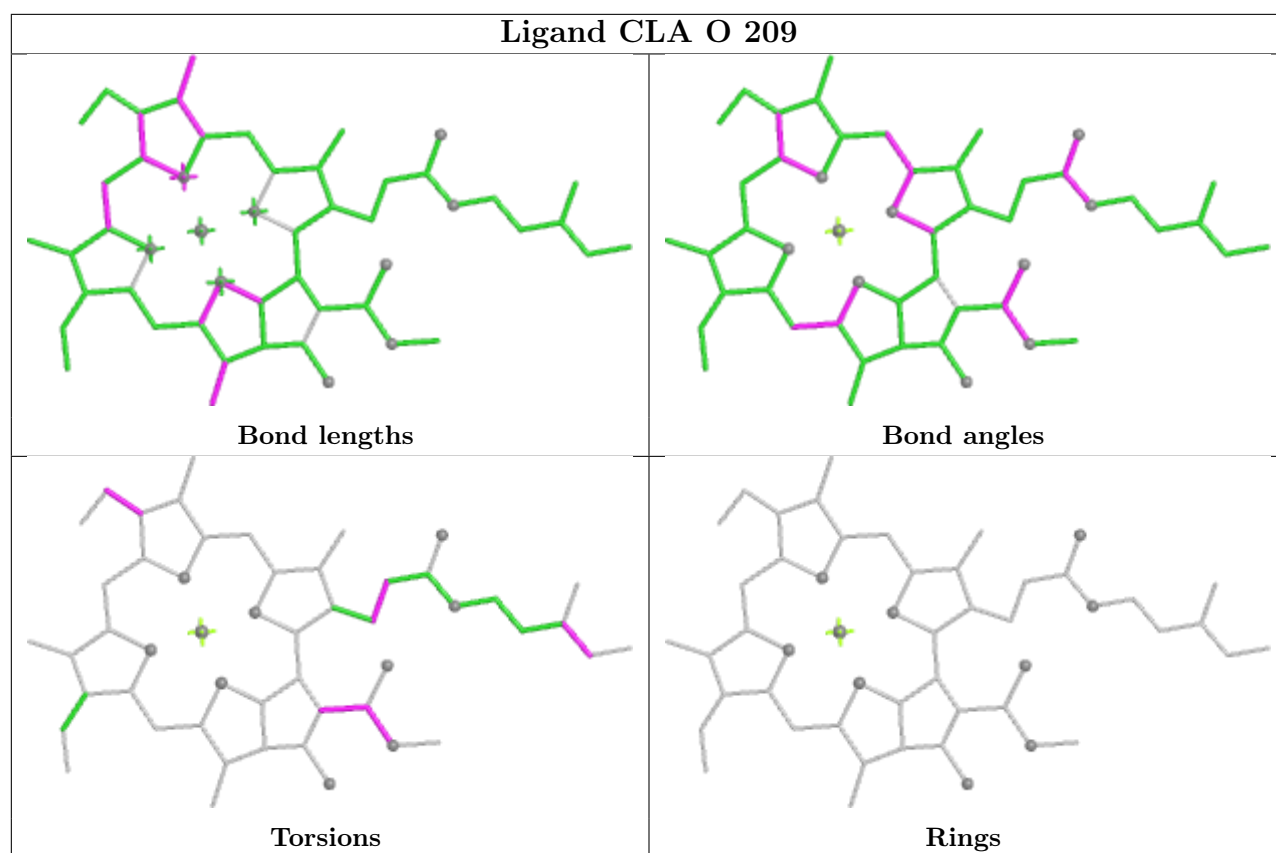
Ligand CLA 8 312



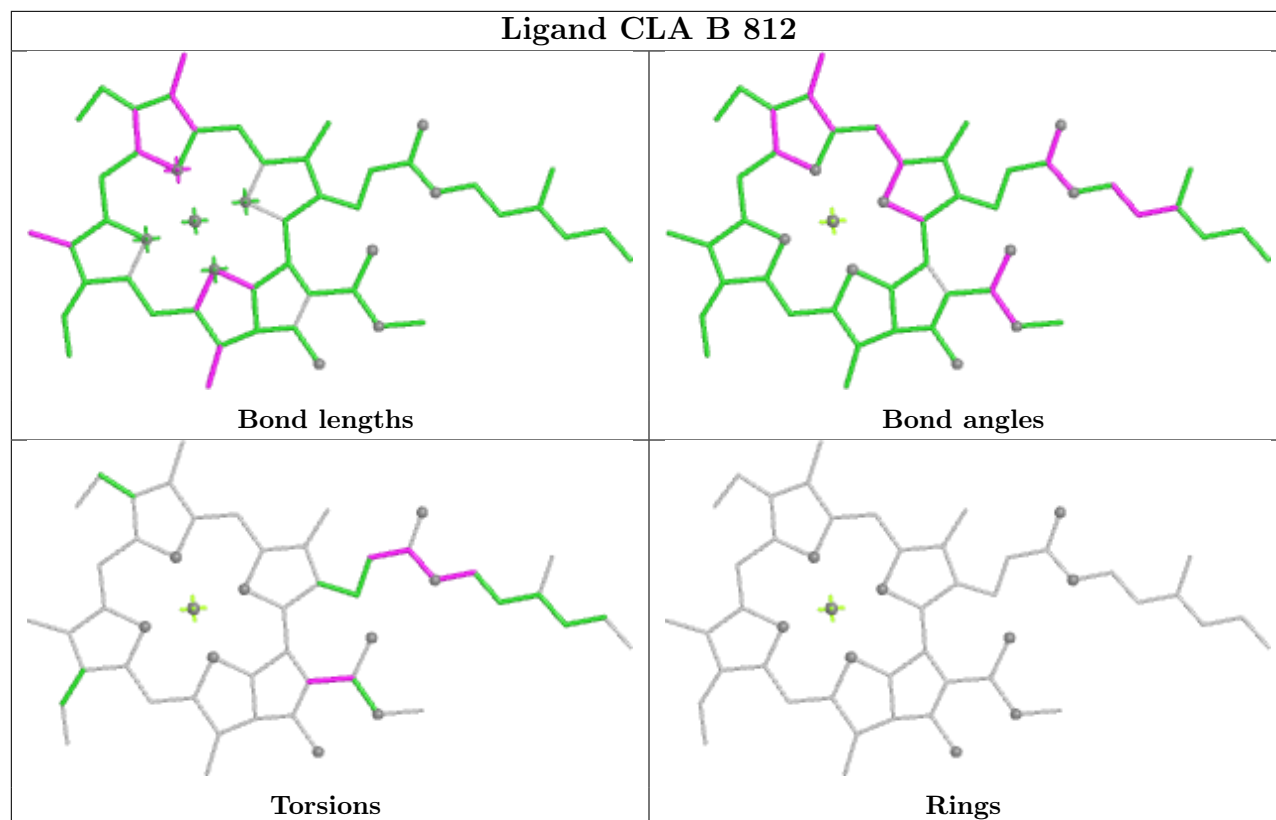
Ligand 8CT 2 314



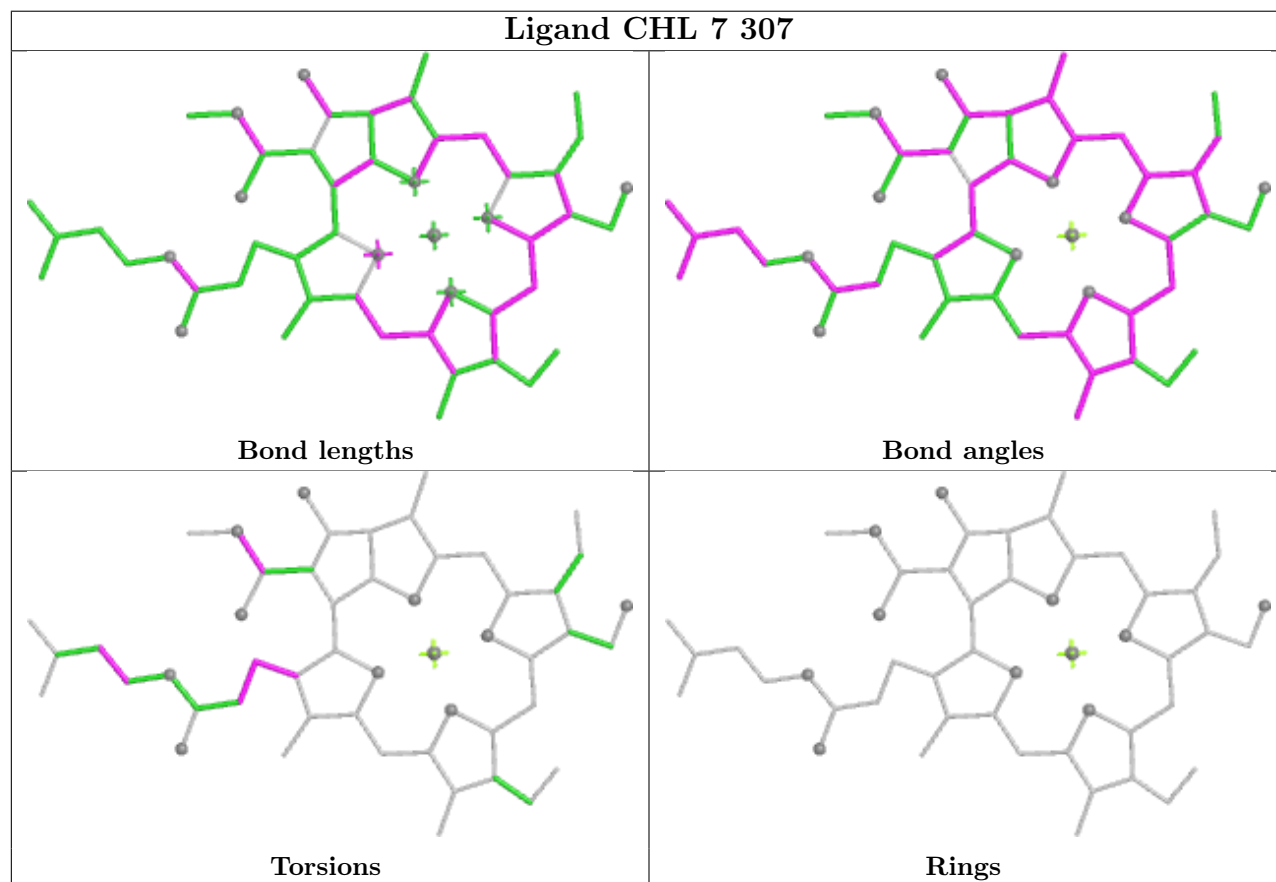


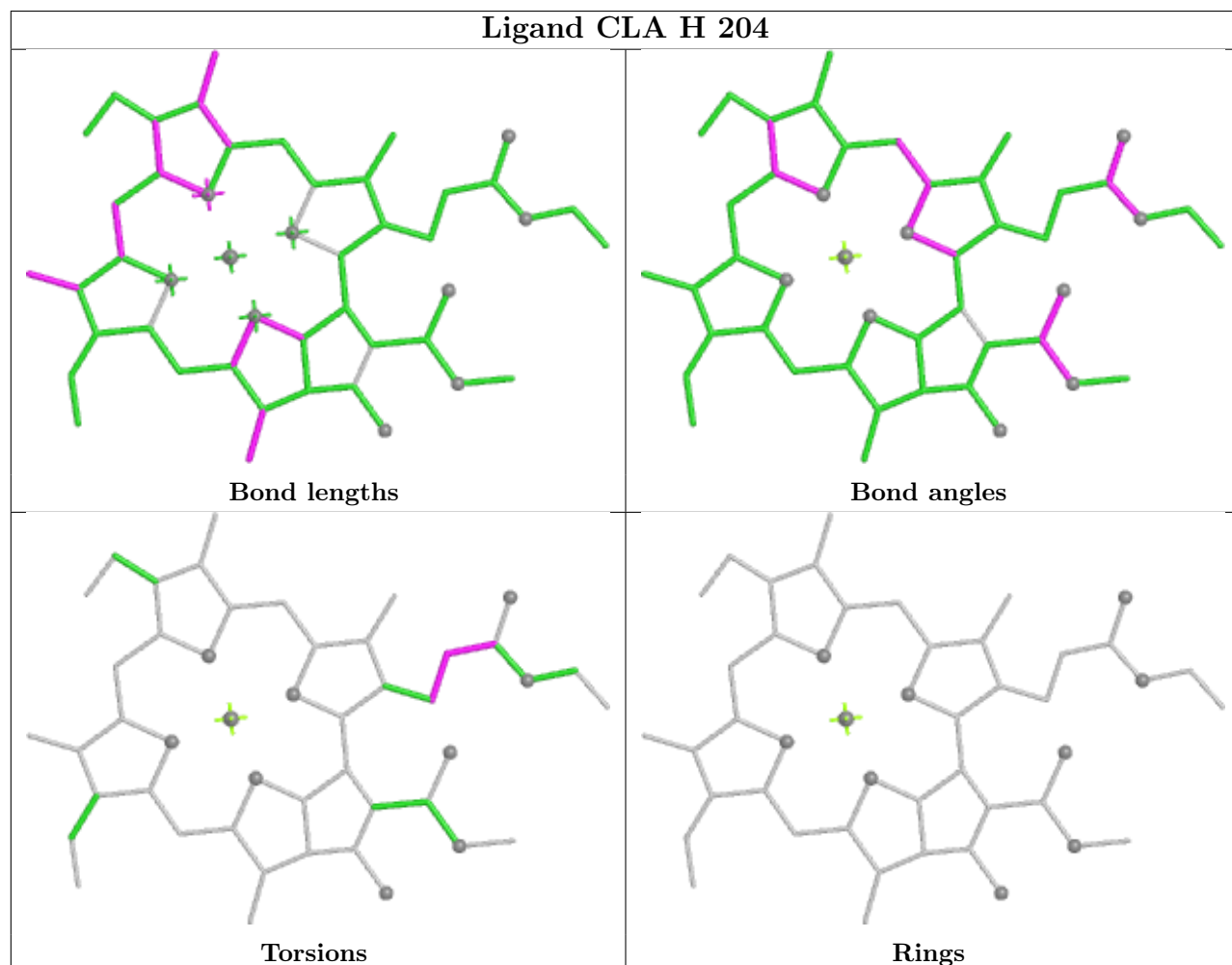
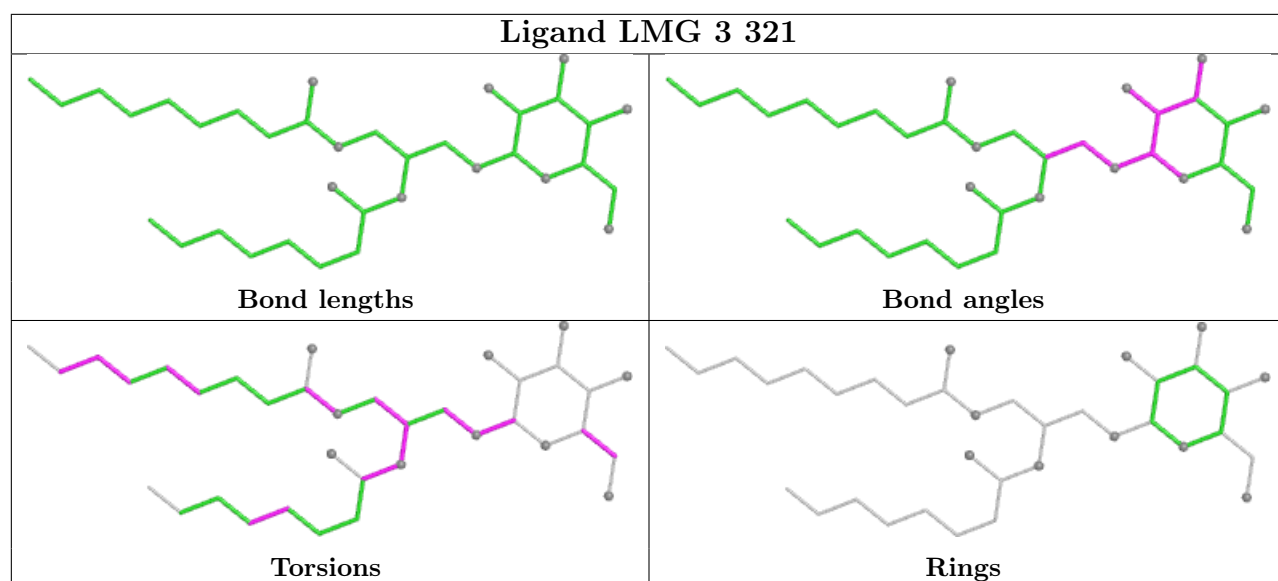


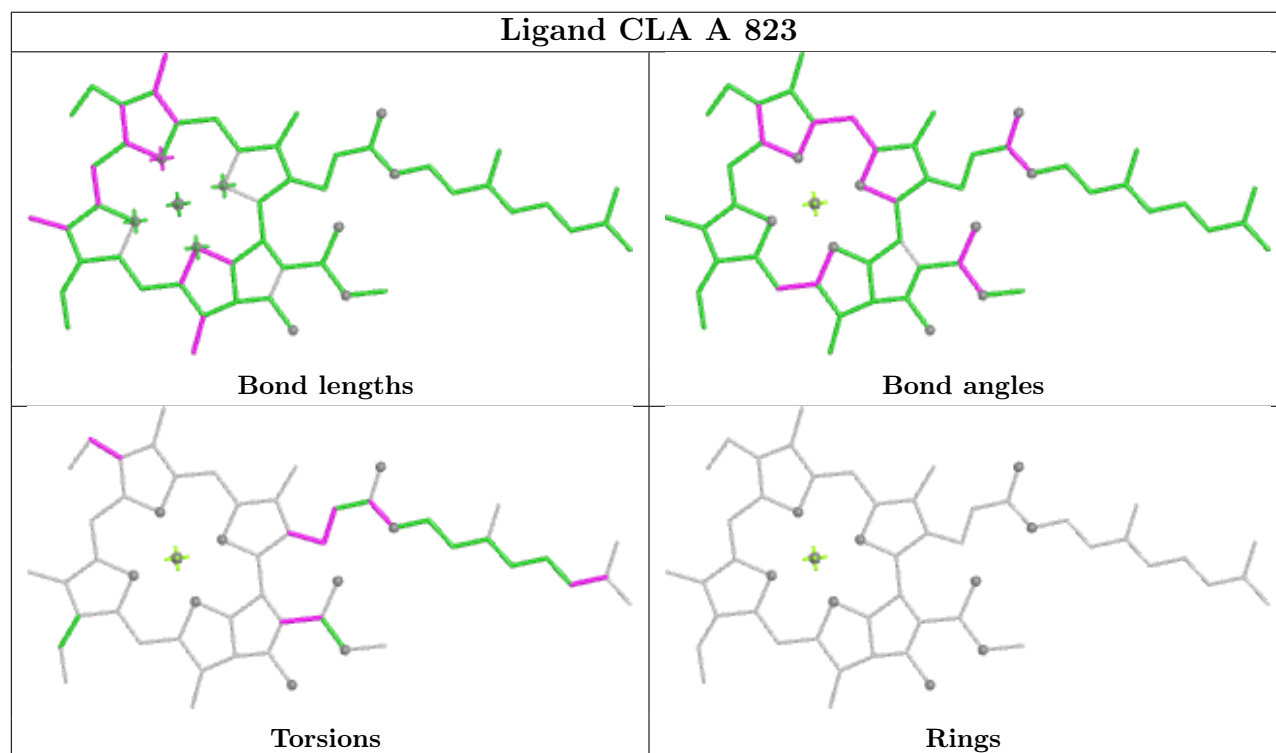
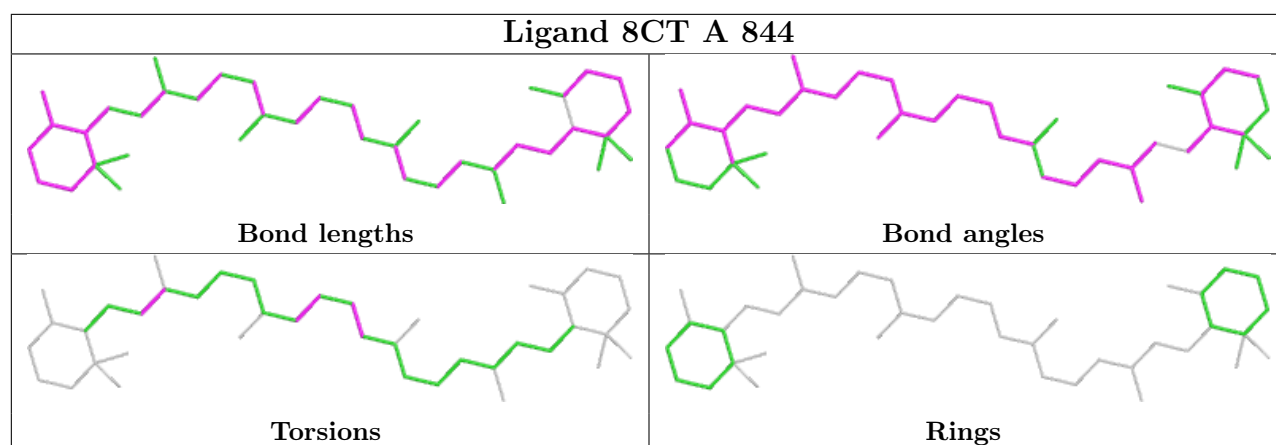
Ligand CLA B 812



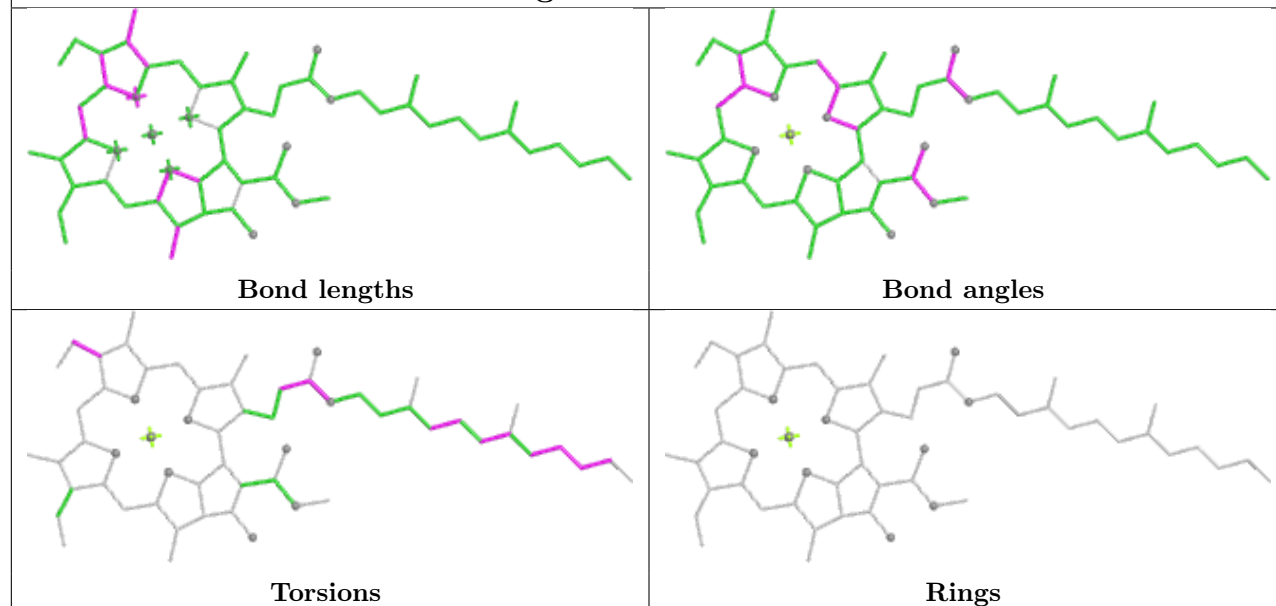
Ligand CHL 7 307



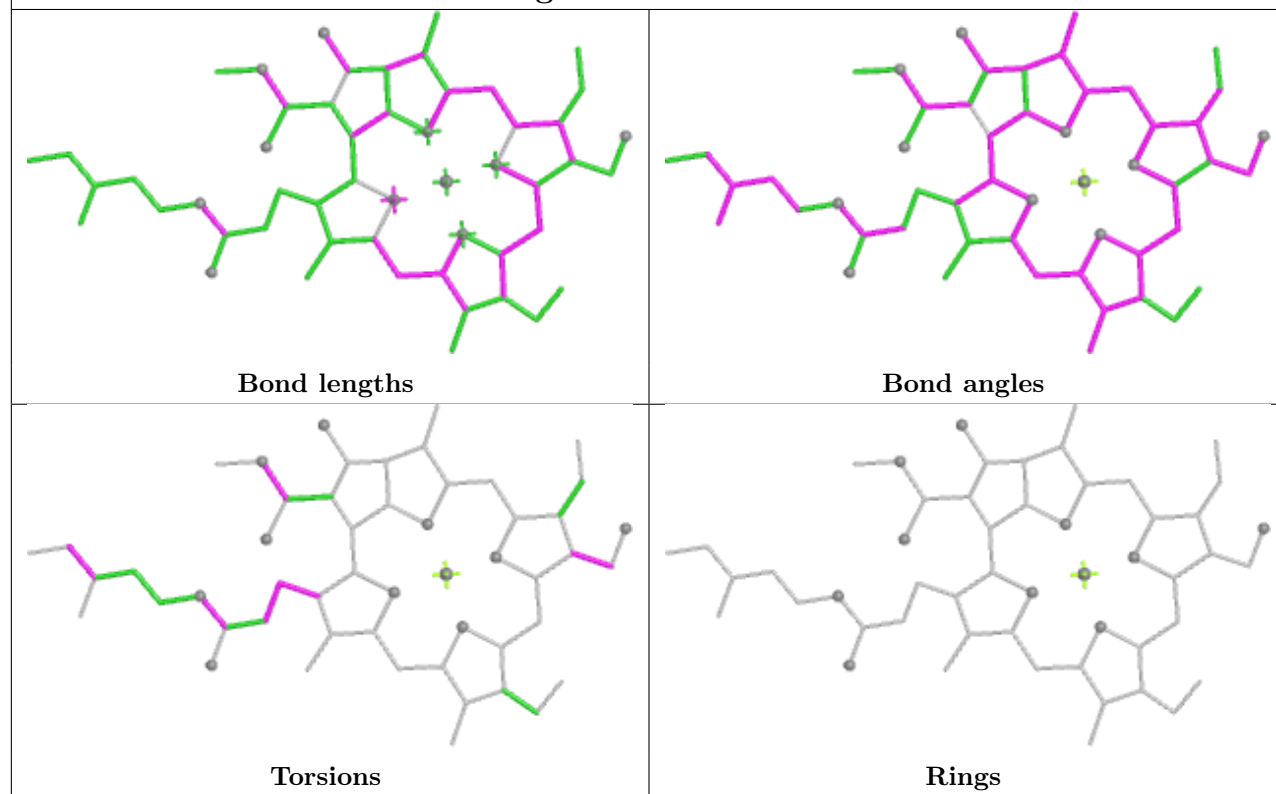


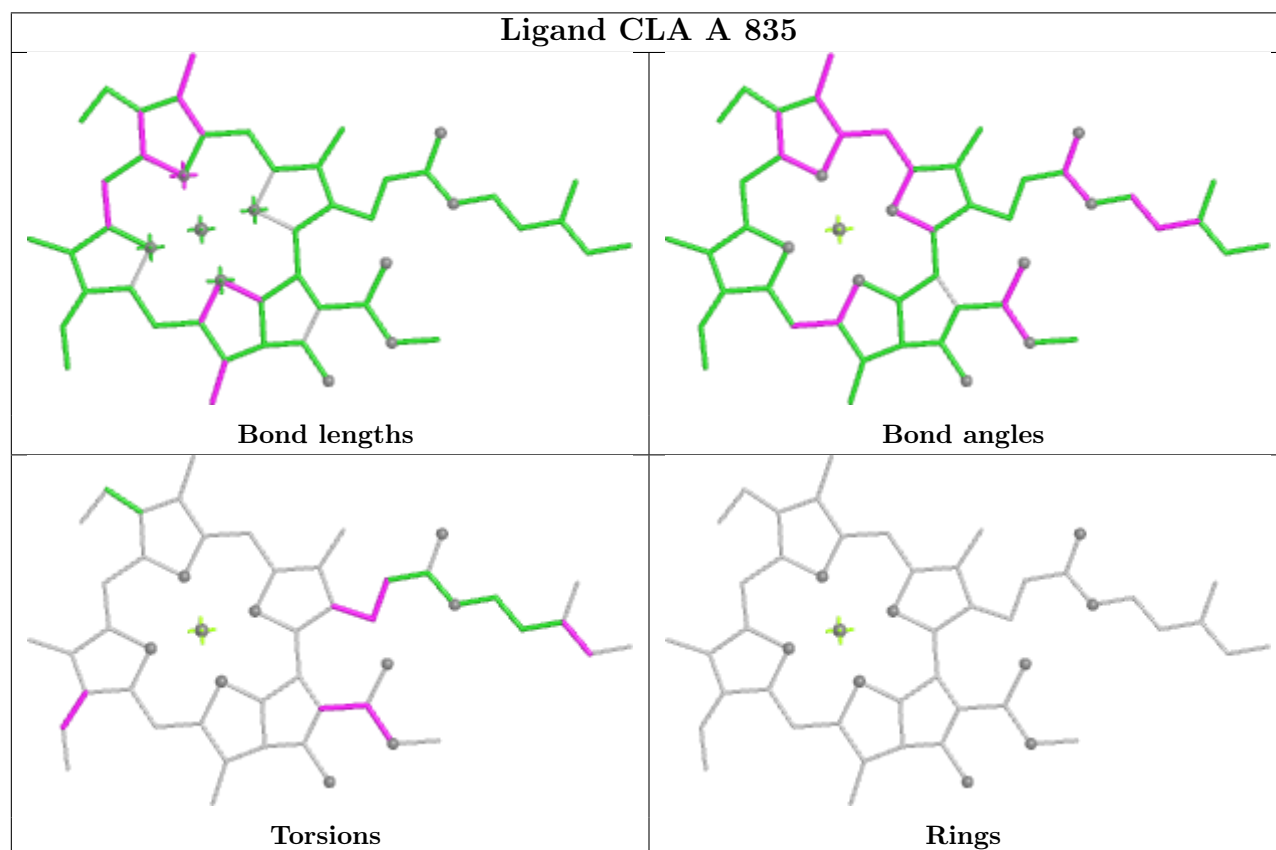
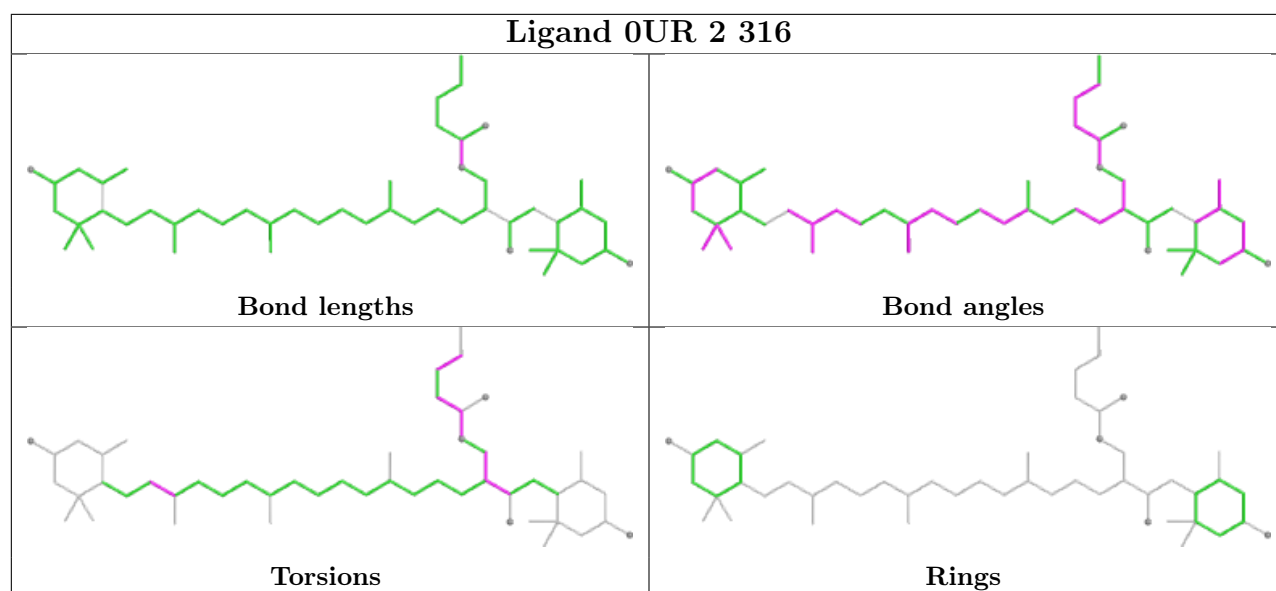


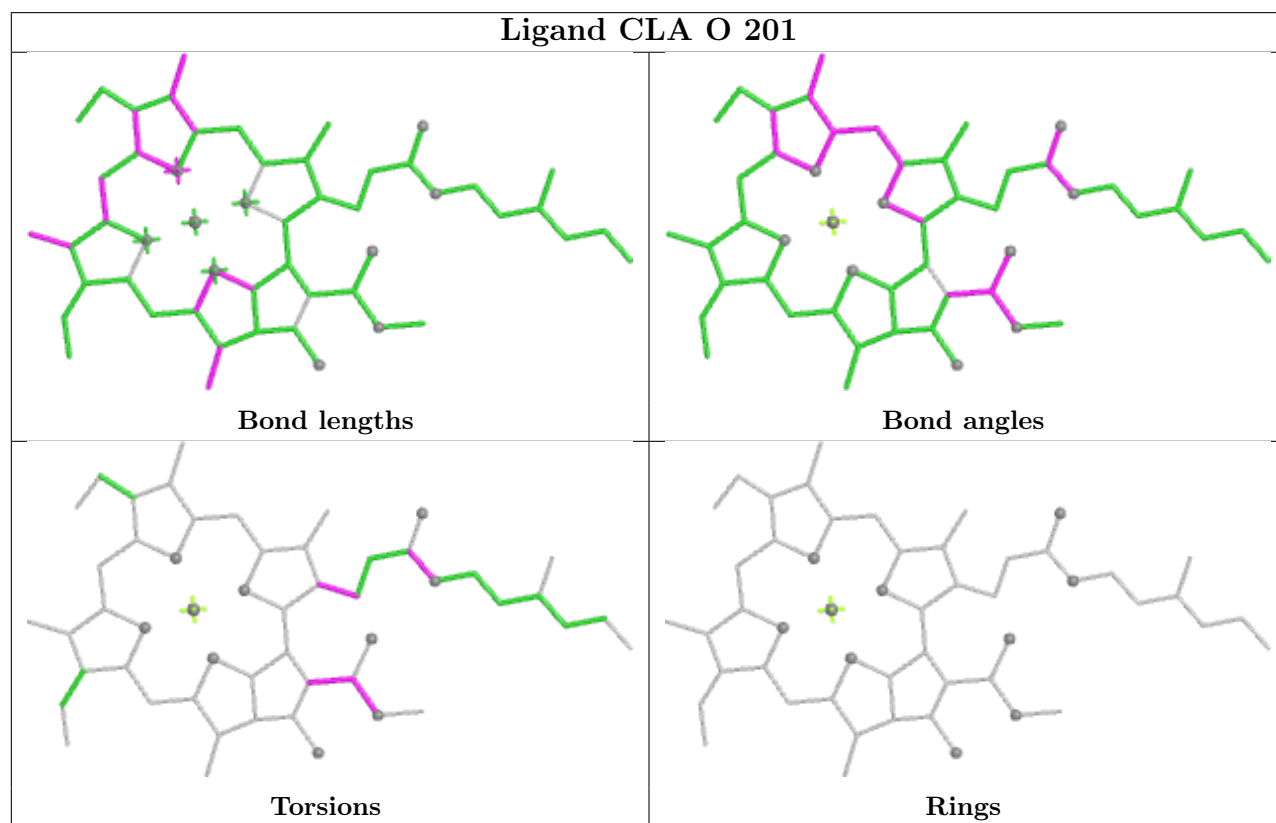
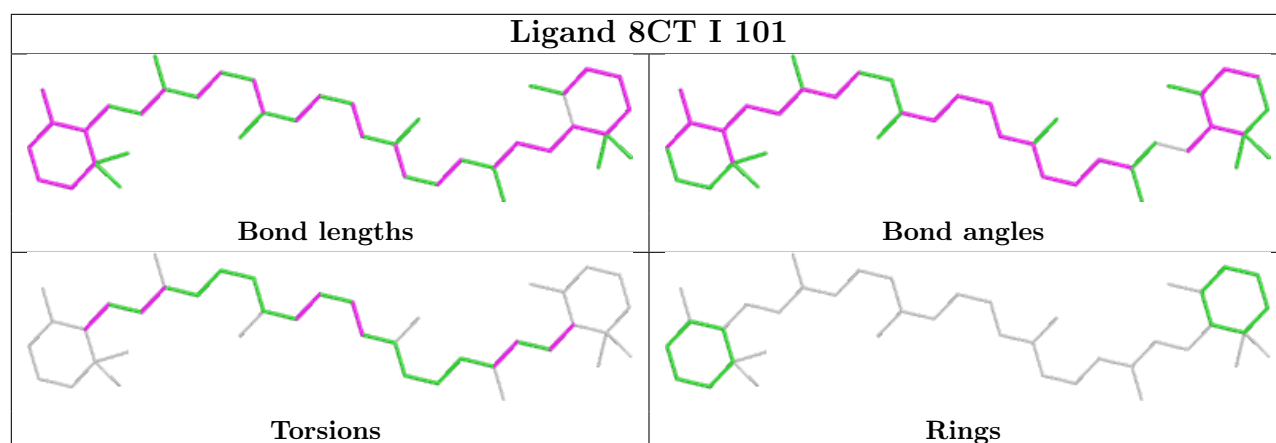
Ligand CLA 5 302



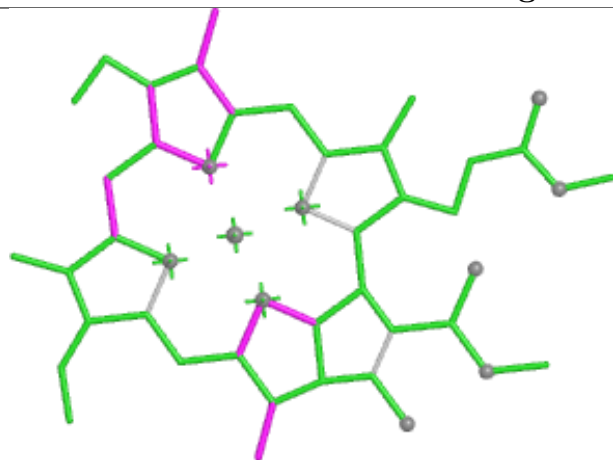
Ligand CHL 0 301



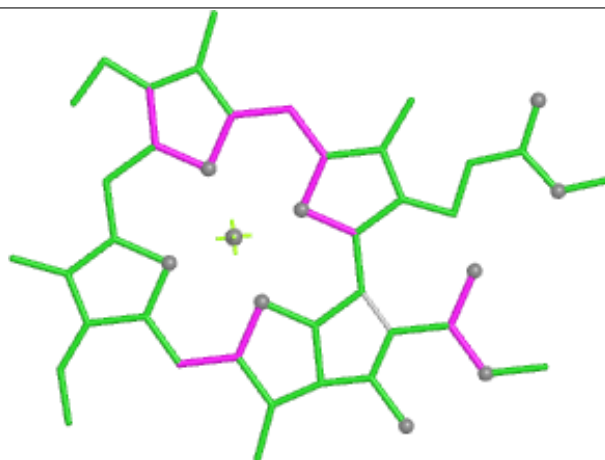




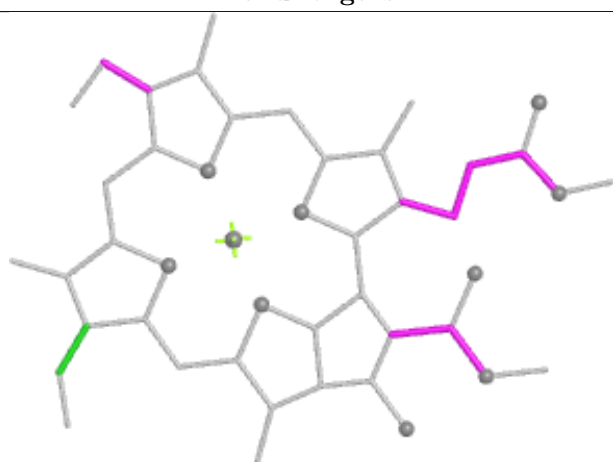
Ligand CLA 6 317



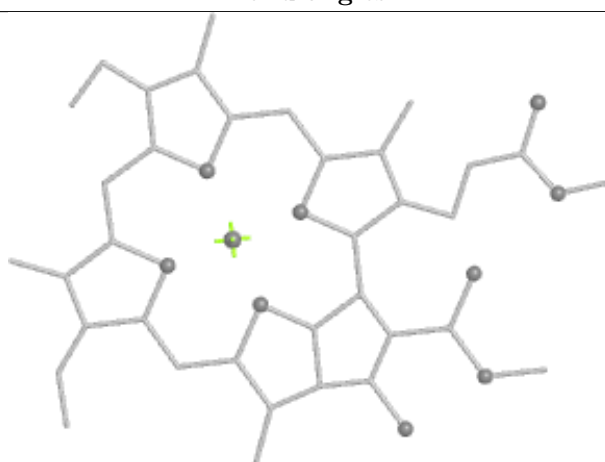
Bond lengths



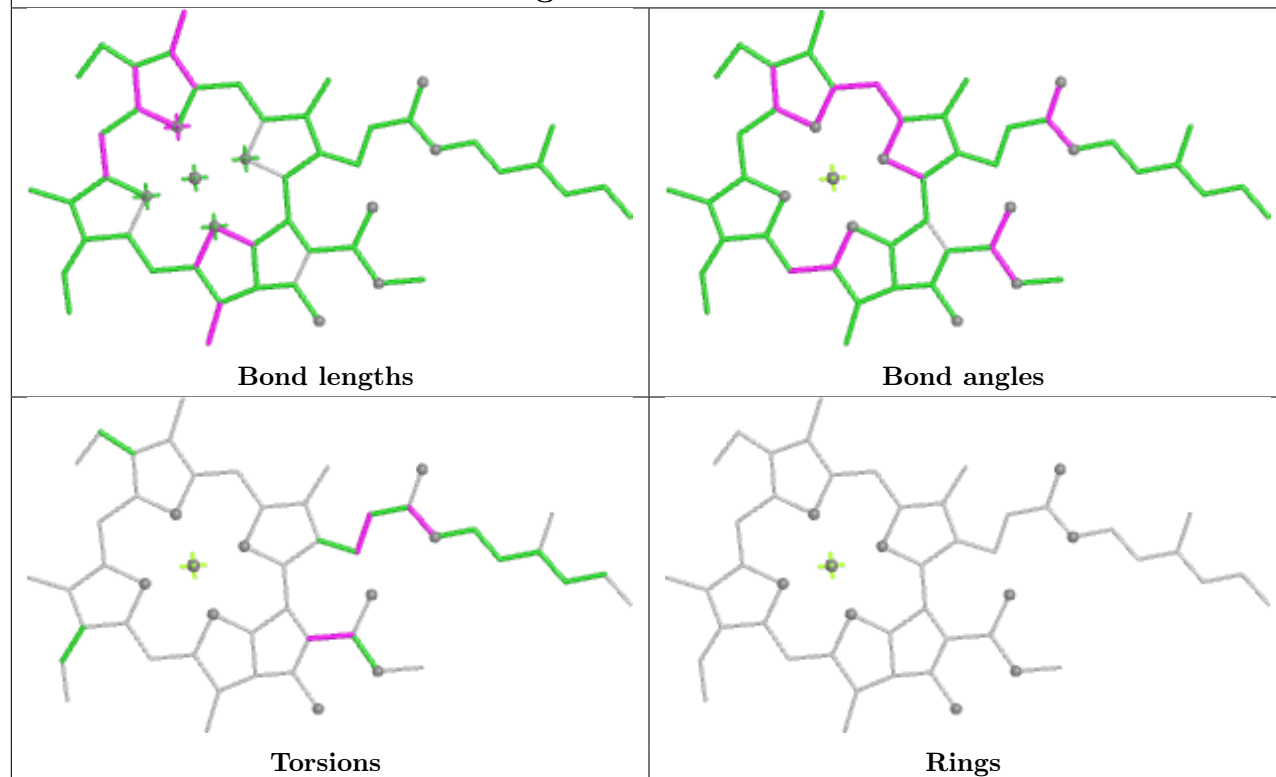
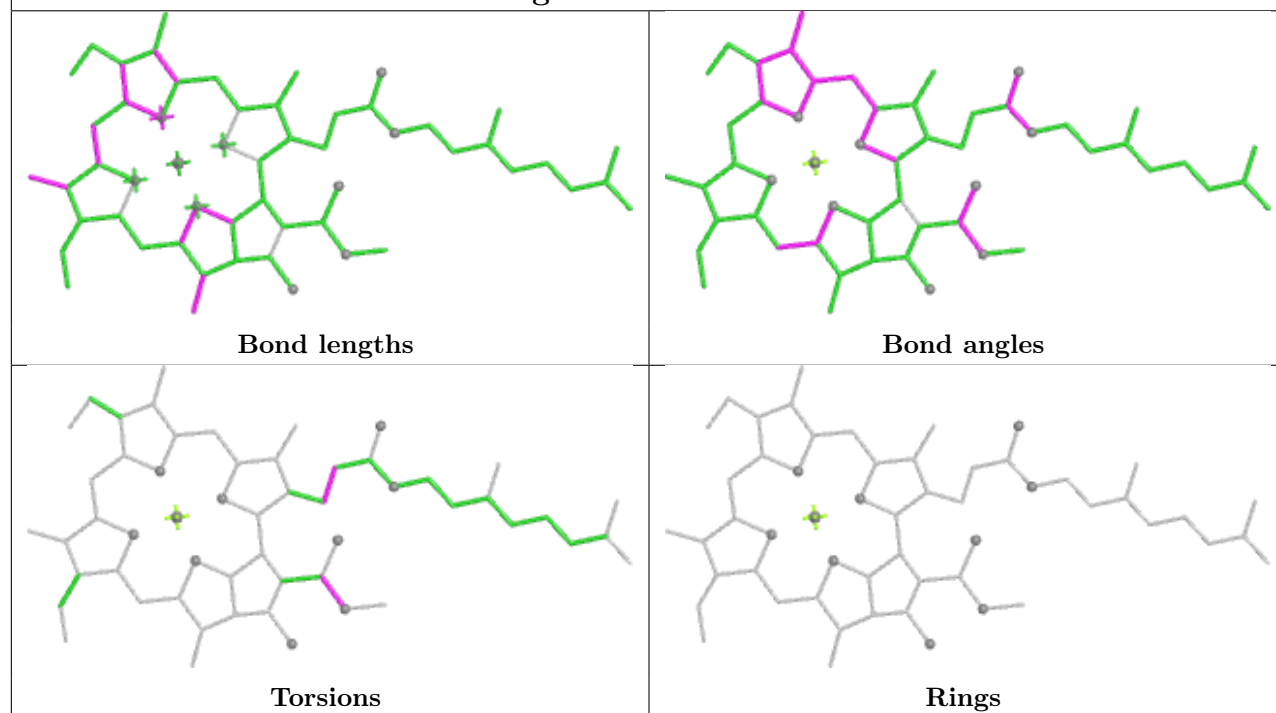
Bond angles

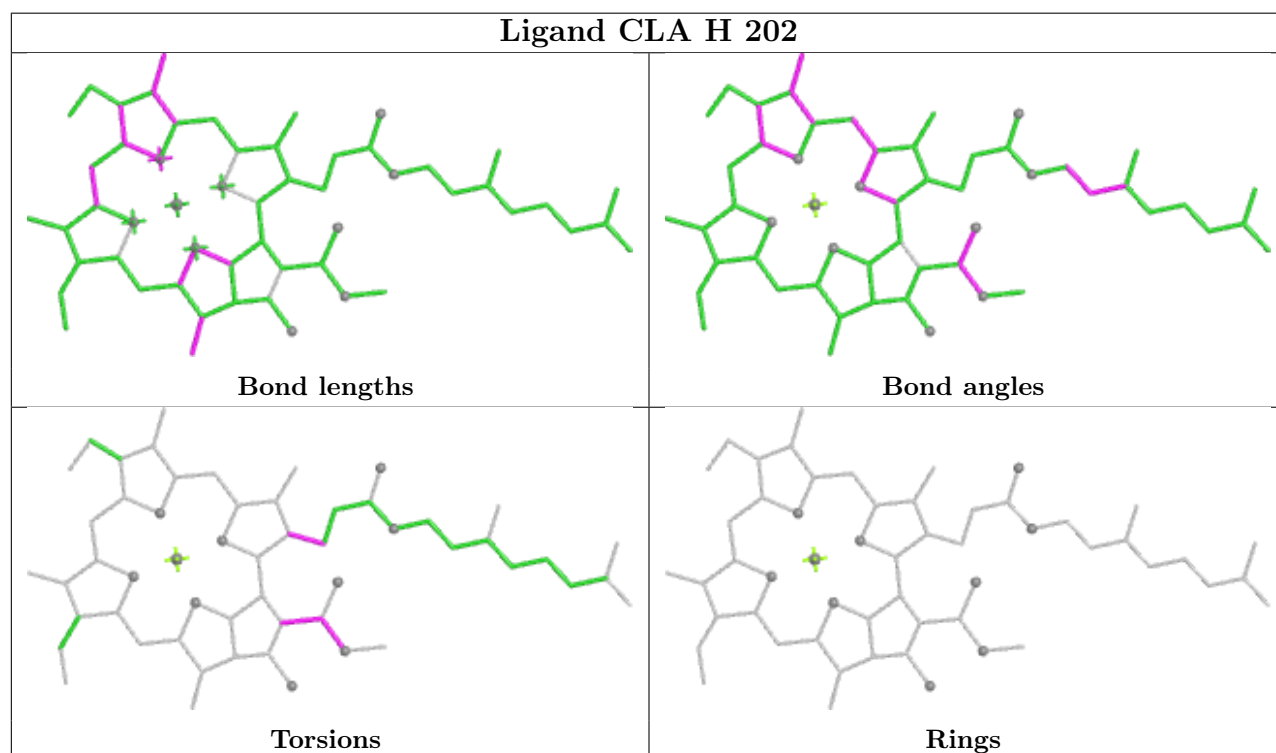
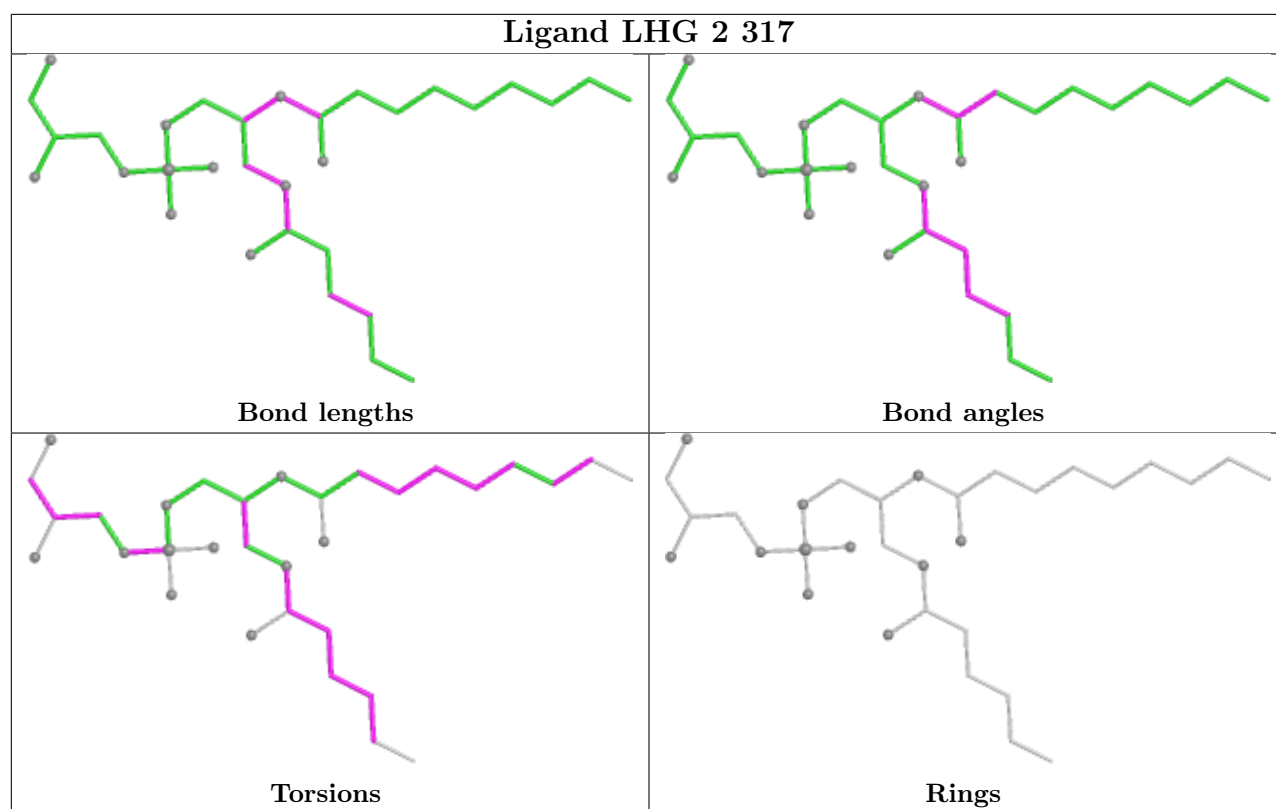


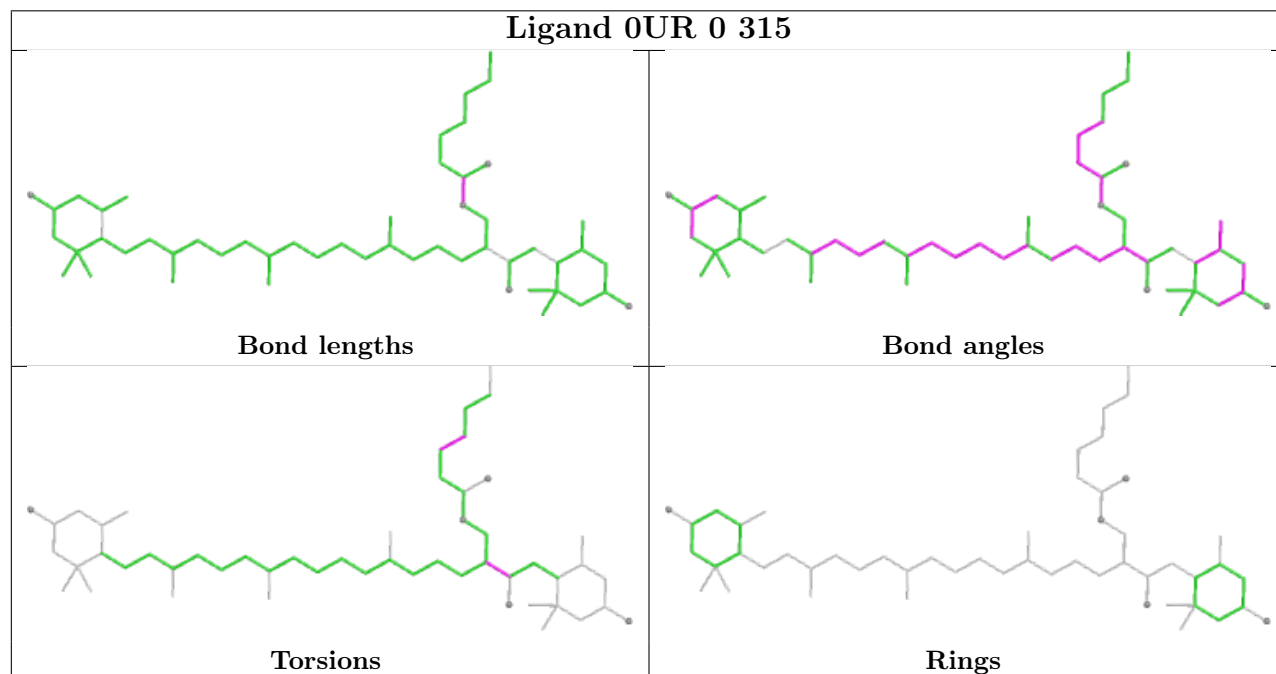
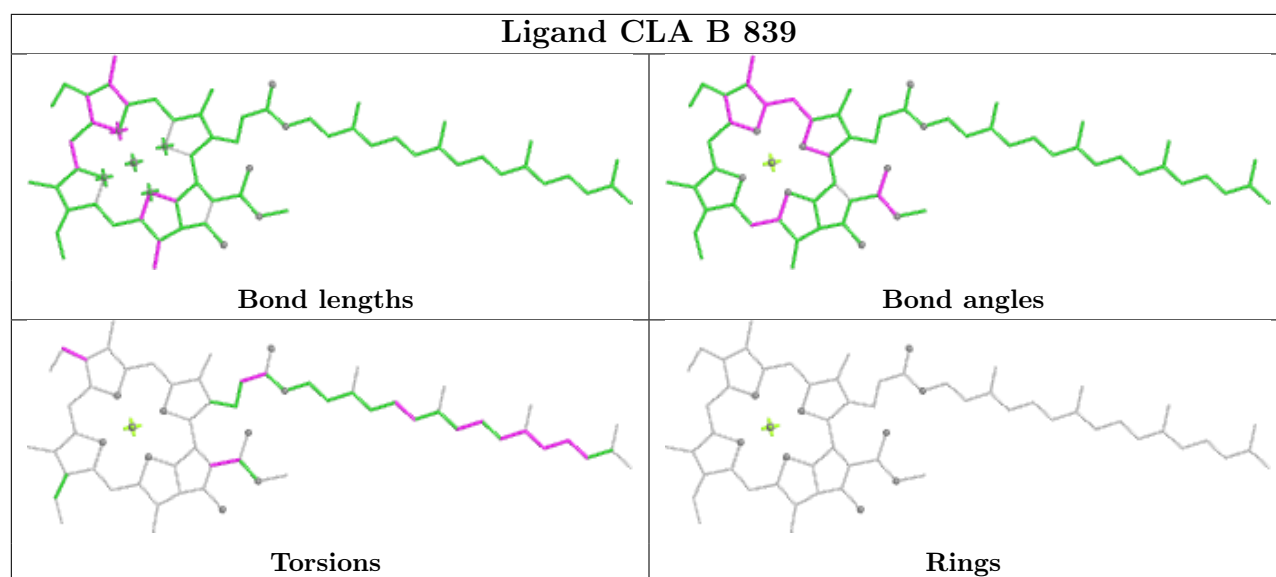
Torsions



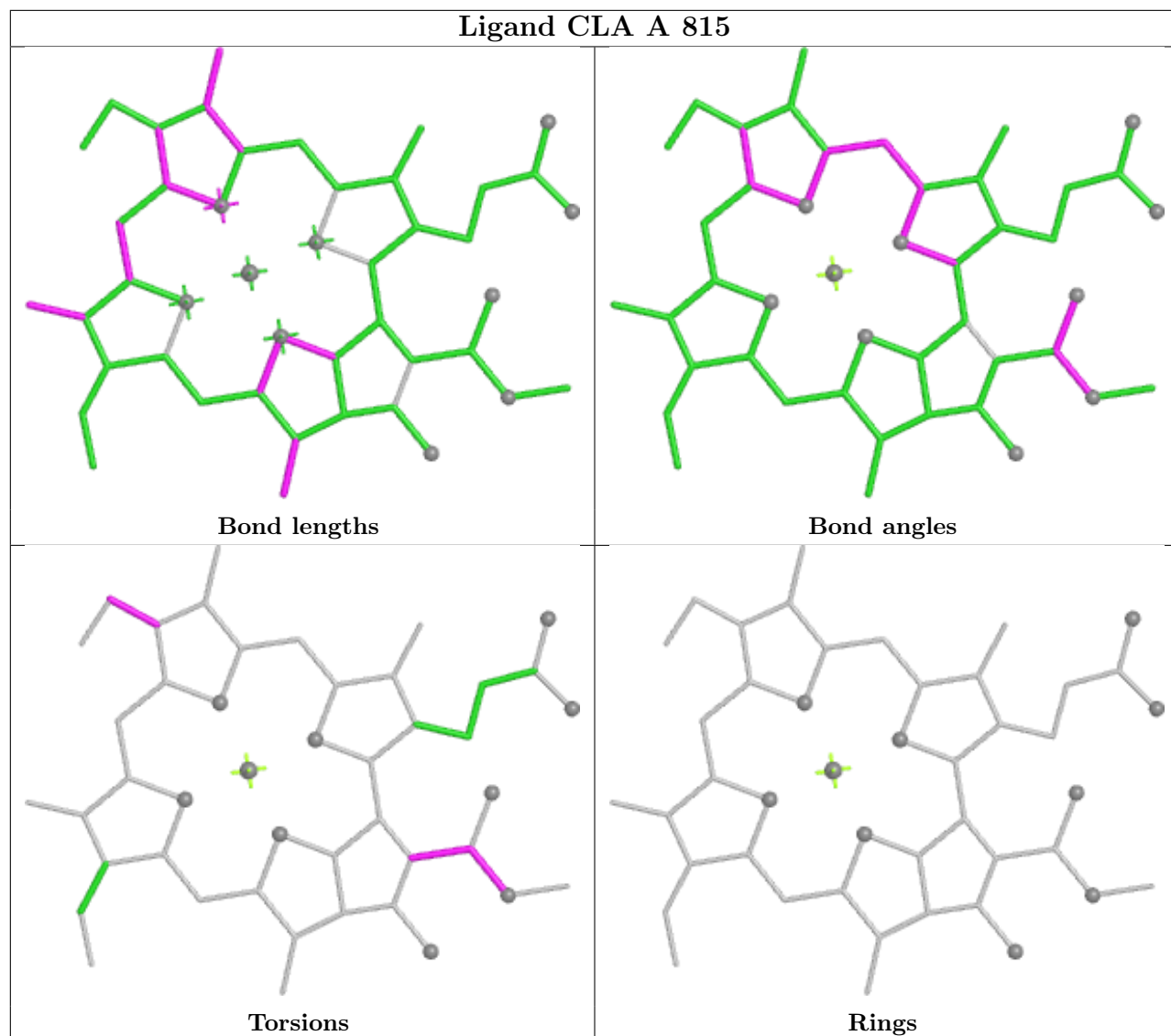
Rings

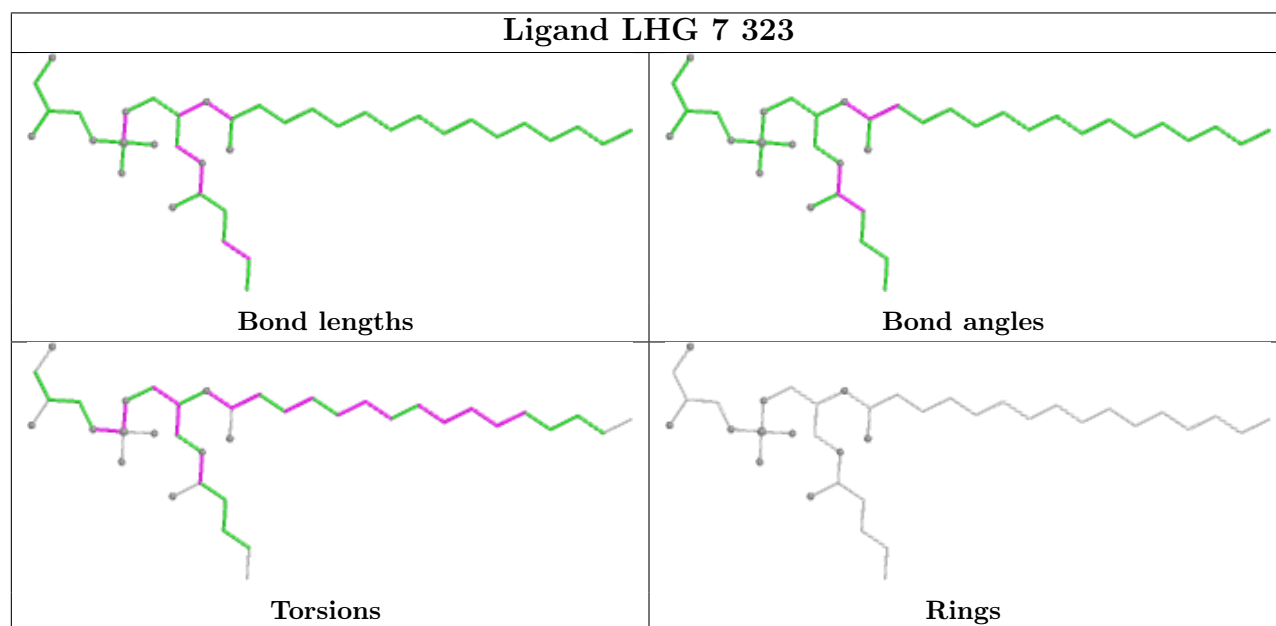
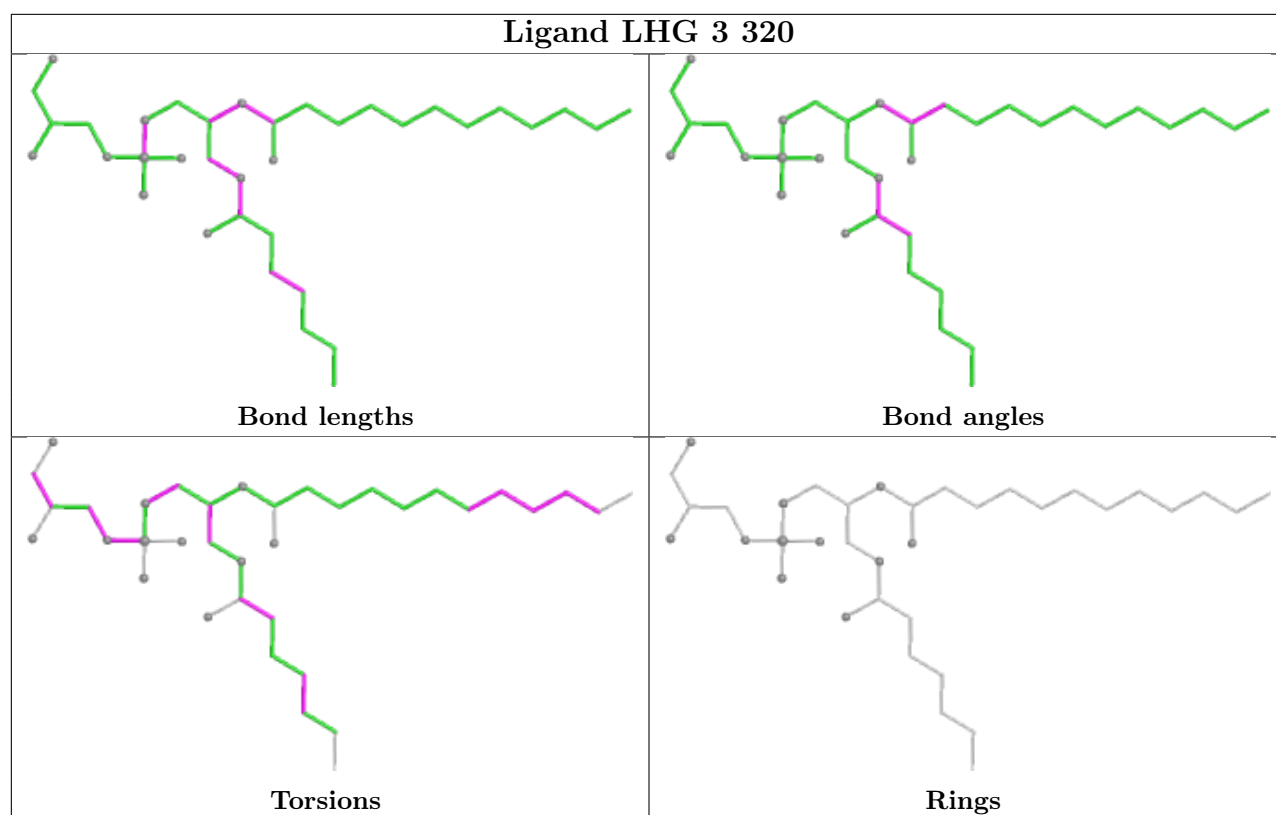
Ligand CLA 1 303**Ligand CLA B 815**

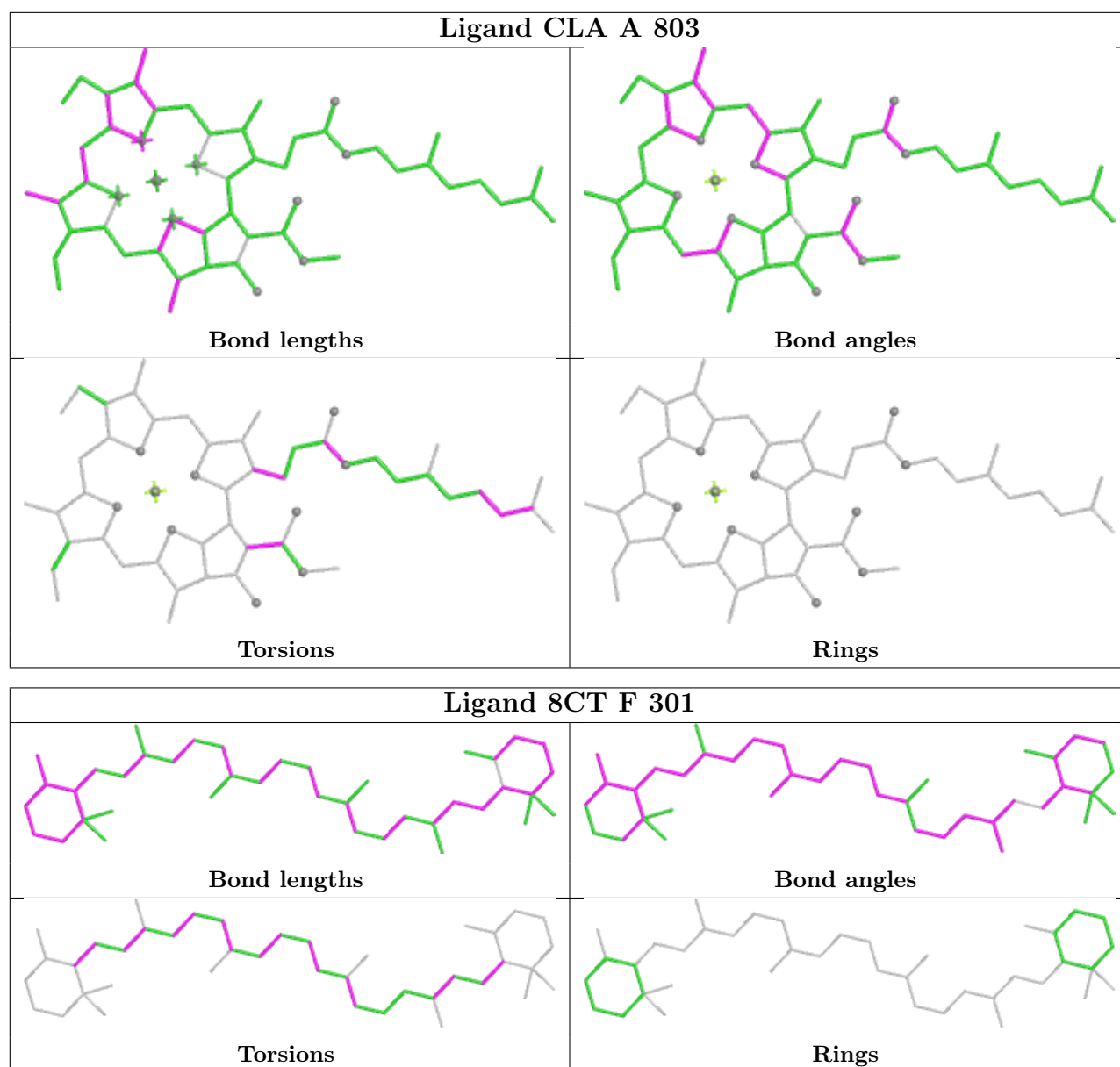


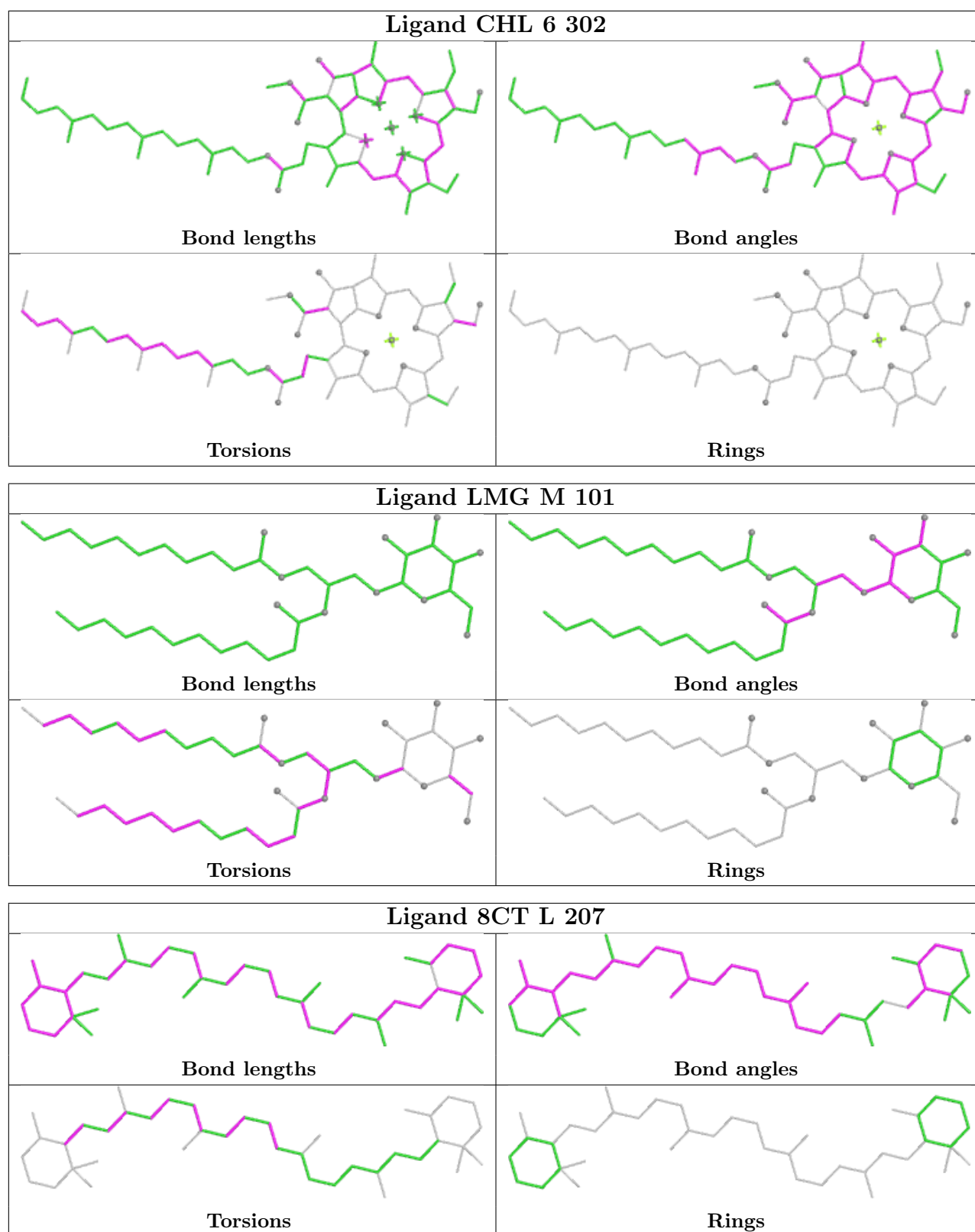


Ligand CLA A 815

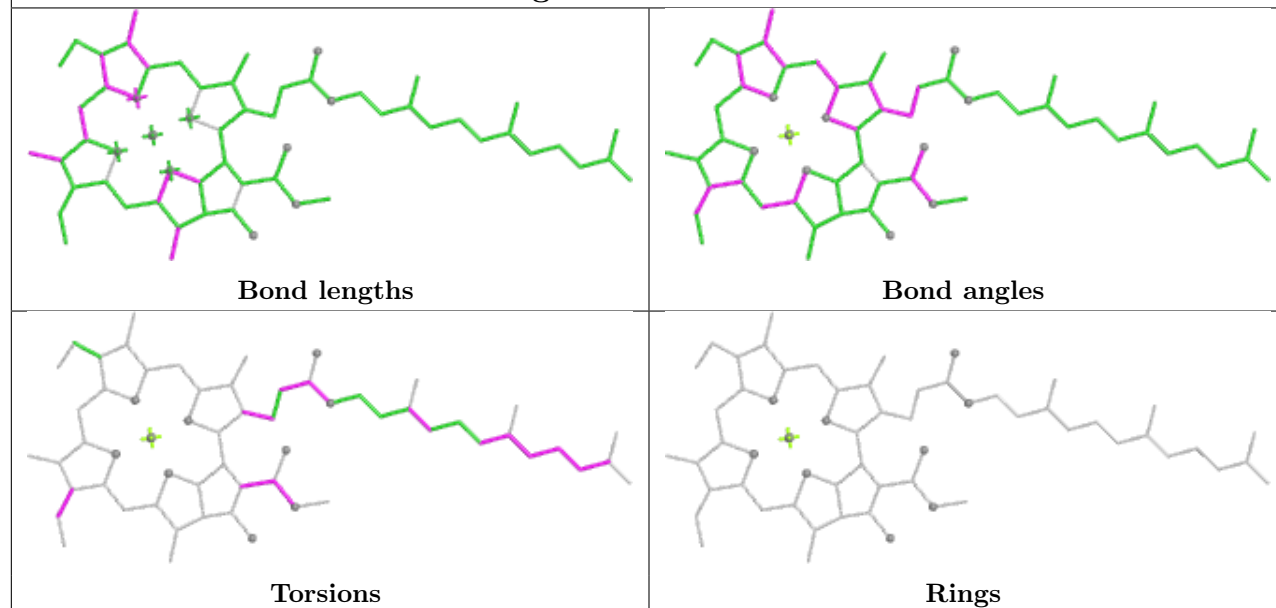




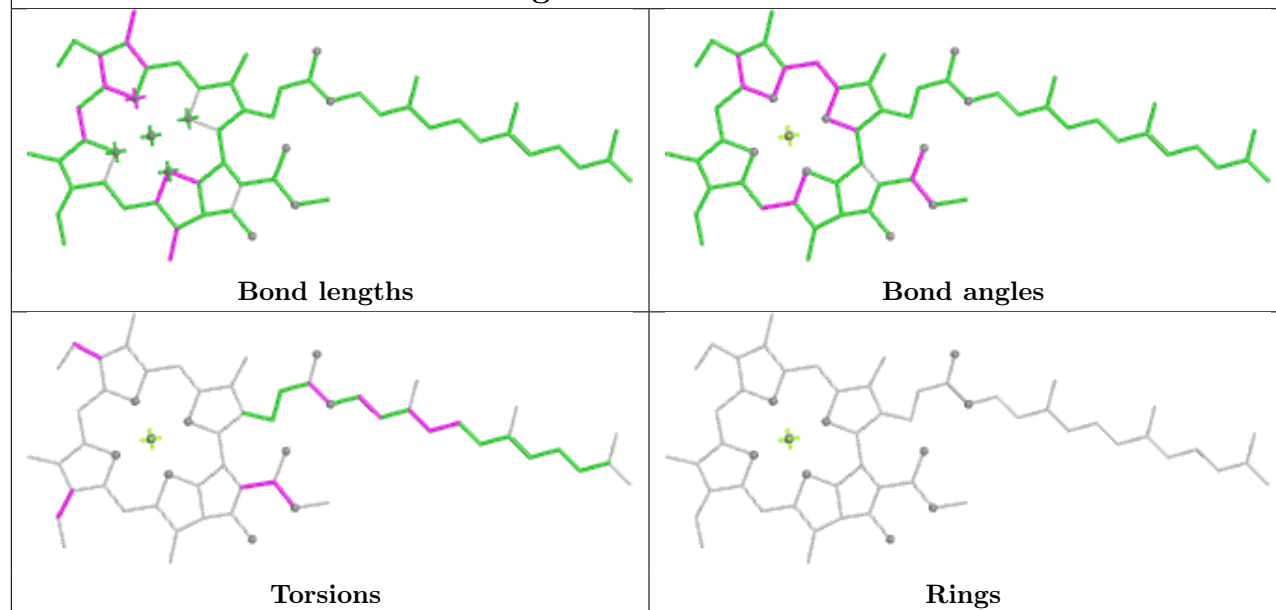




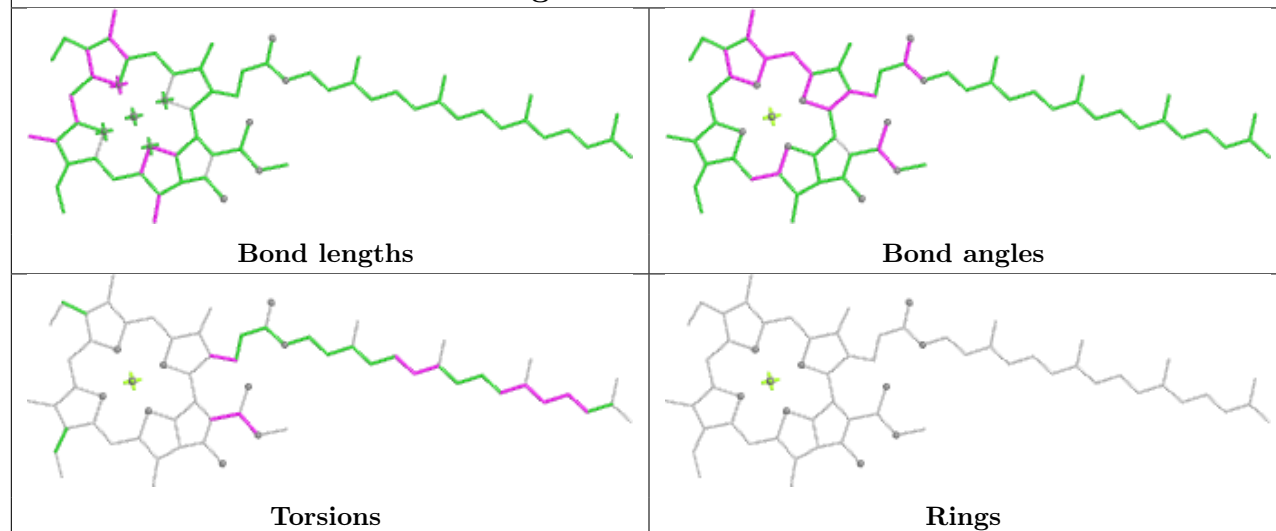
Ligand CLA B 817



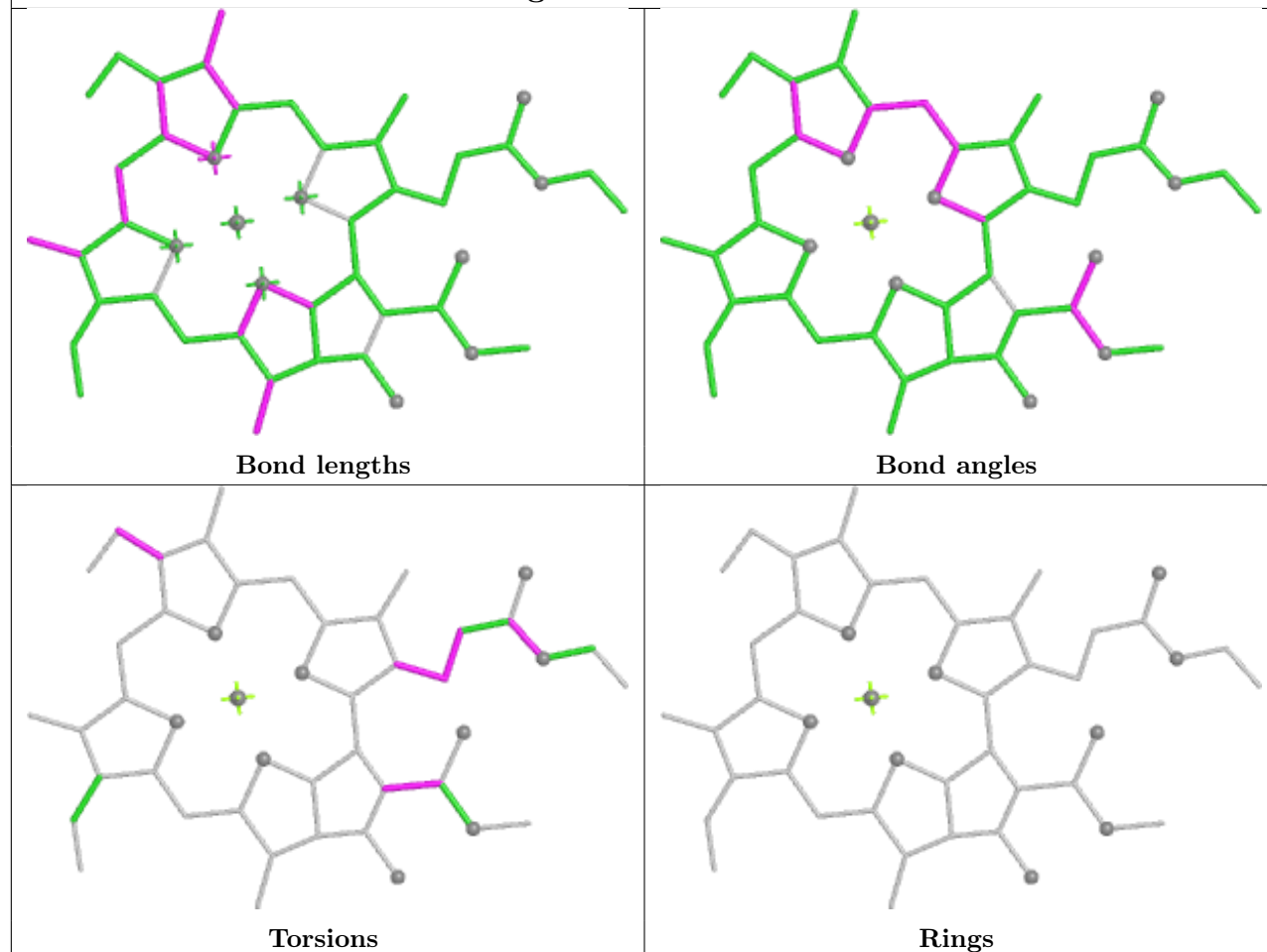
Ligand CLA B 822

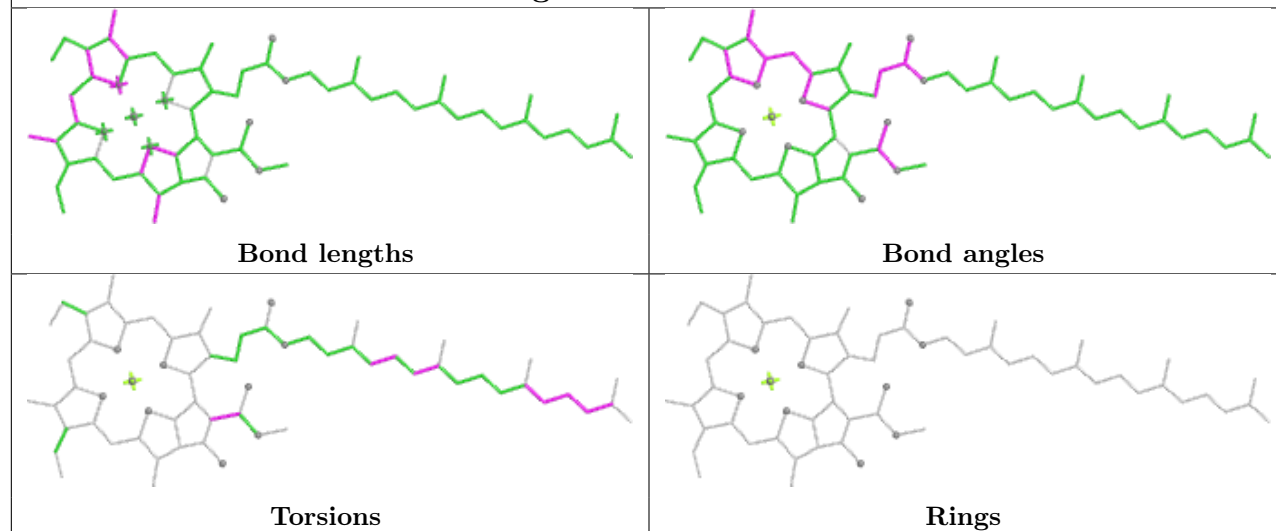
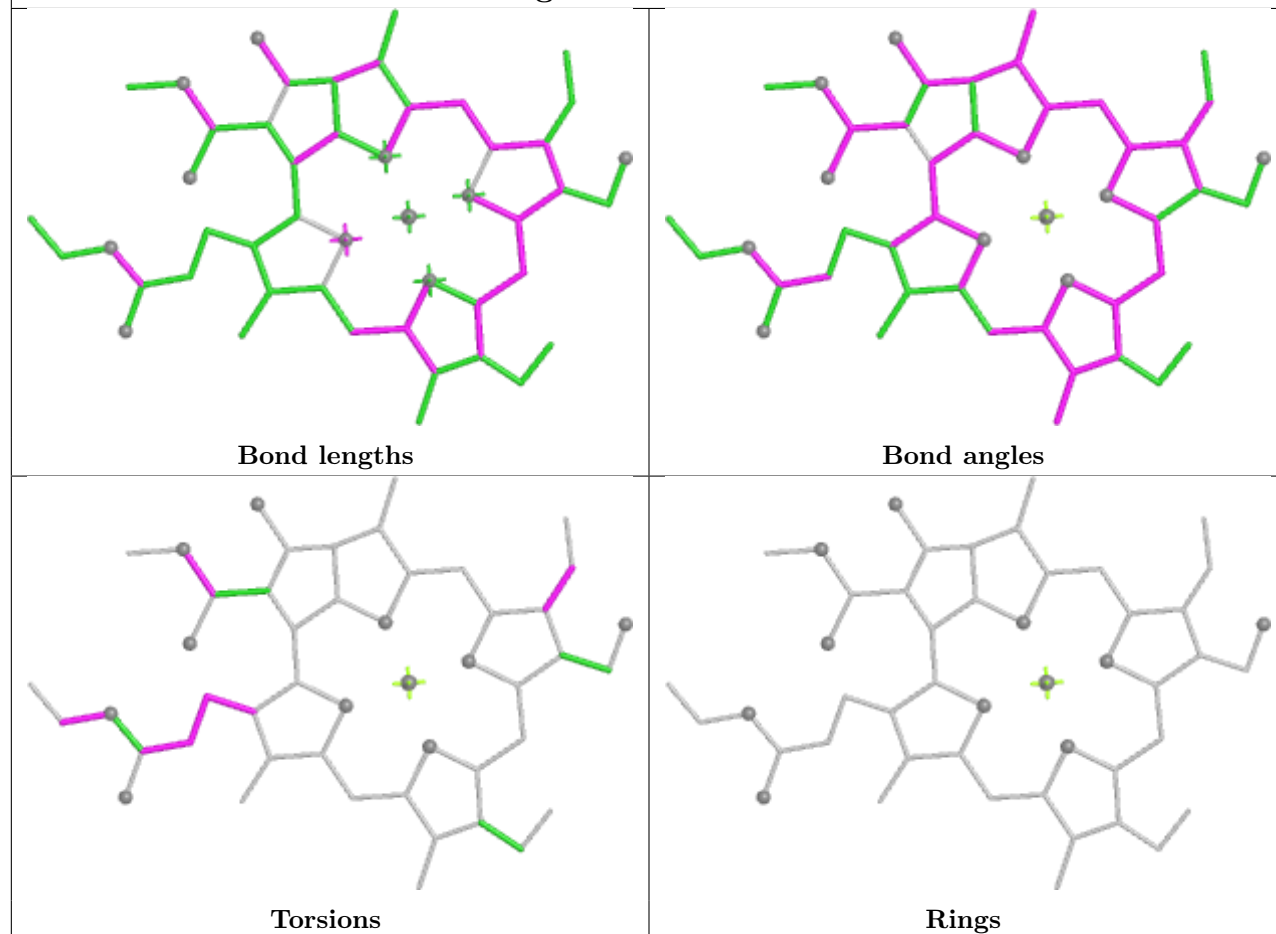


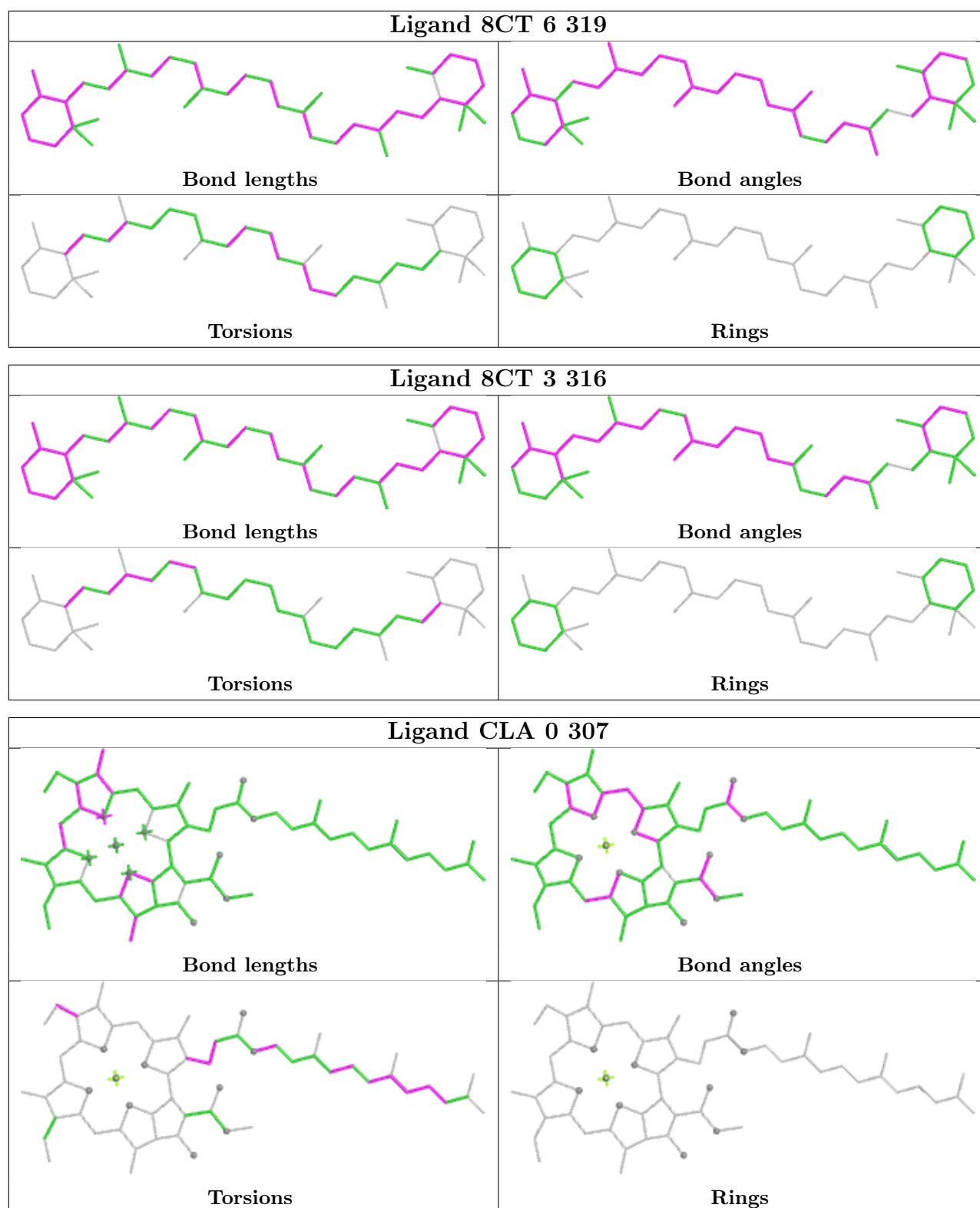
Ligand CLA A 825

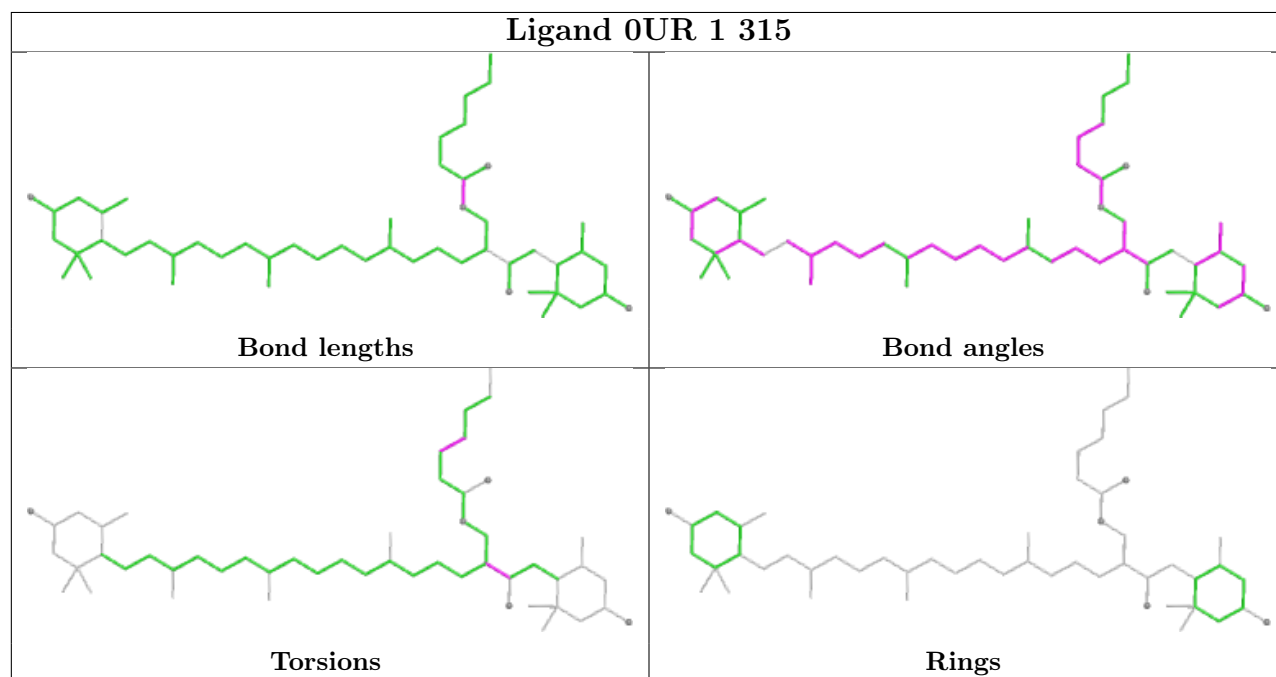
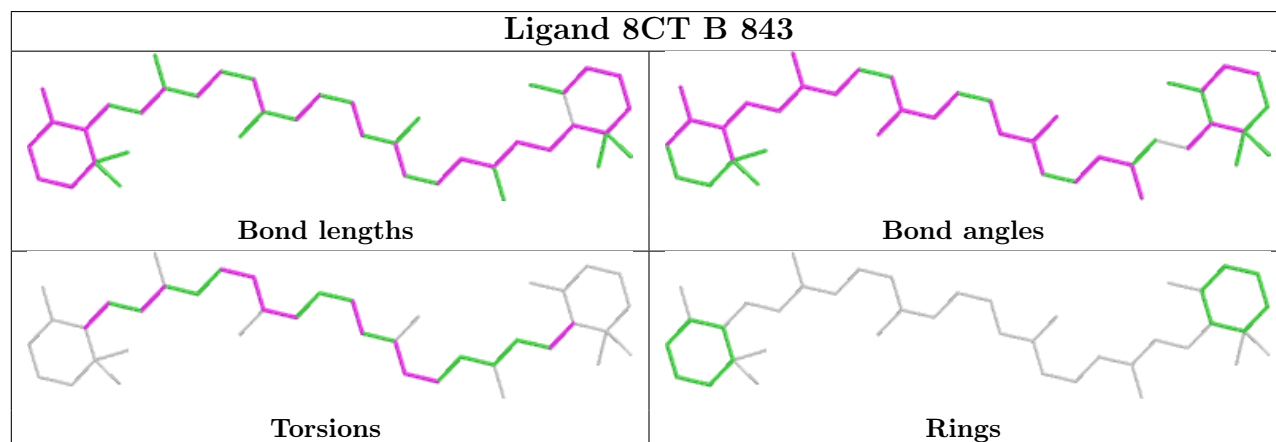
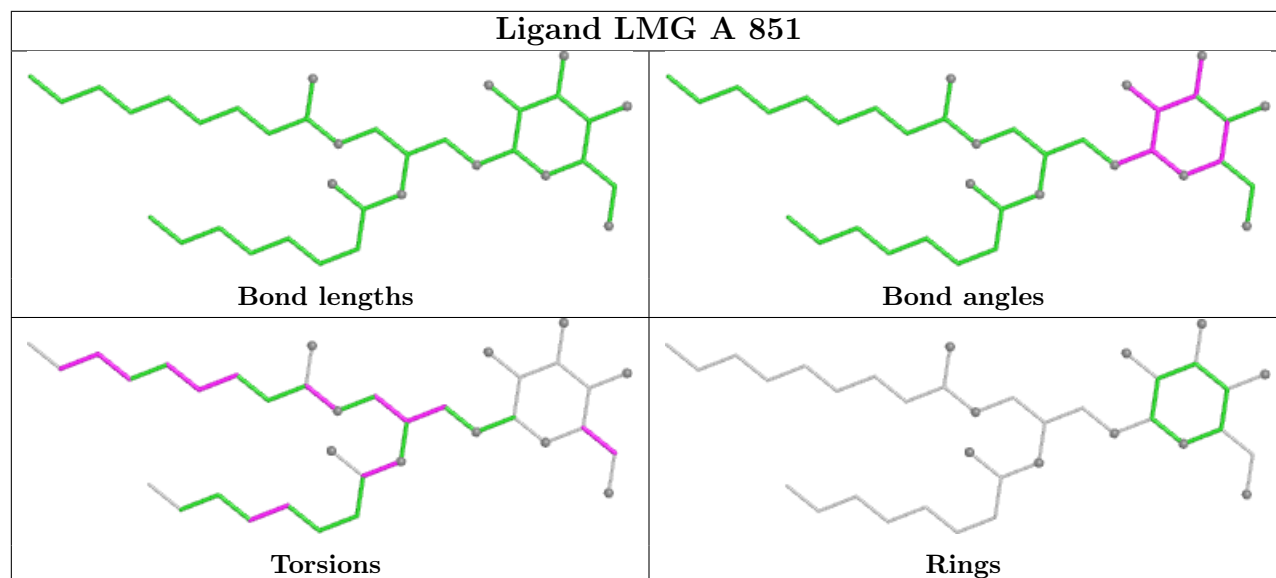


Ligand CLA H 203

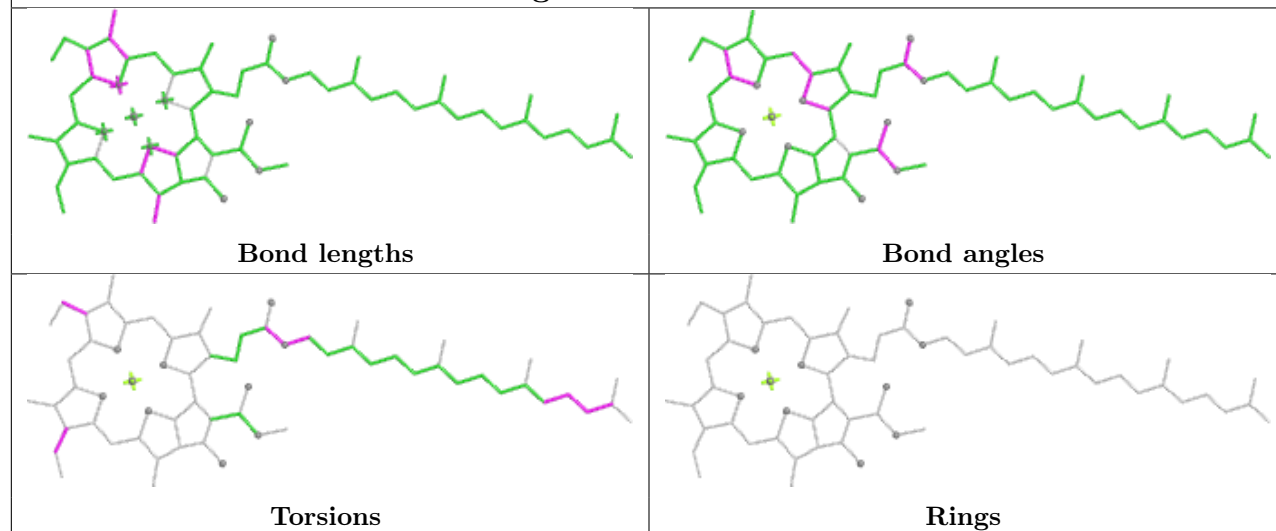


Ligand CLA B 832**Ligand CHL 5 305**

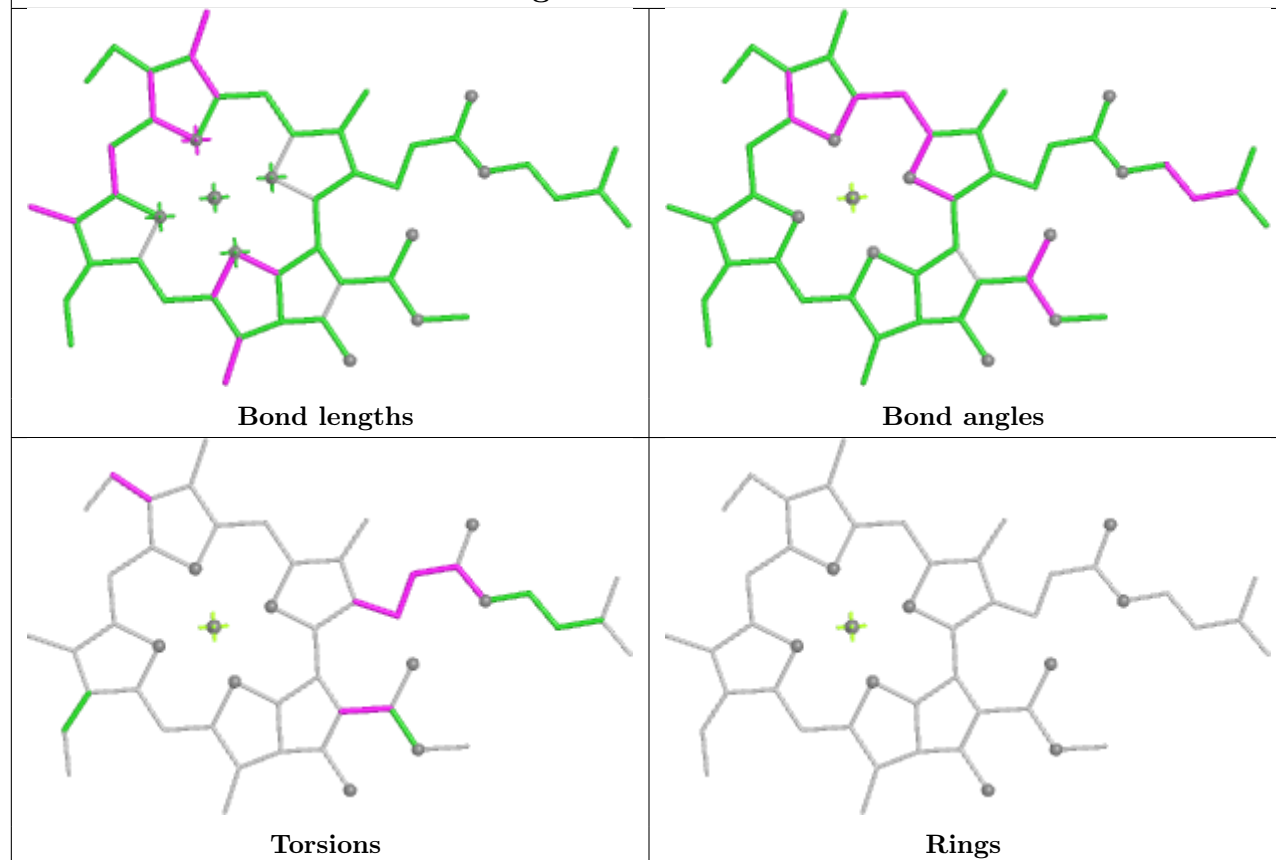




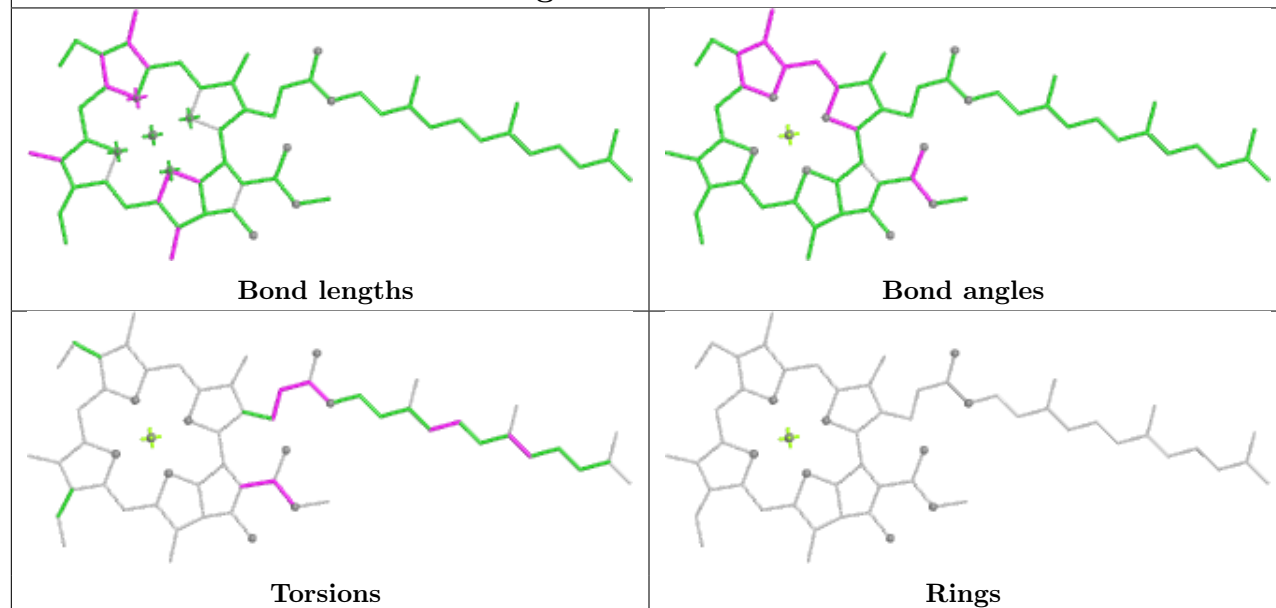
Ligand CLA B 840



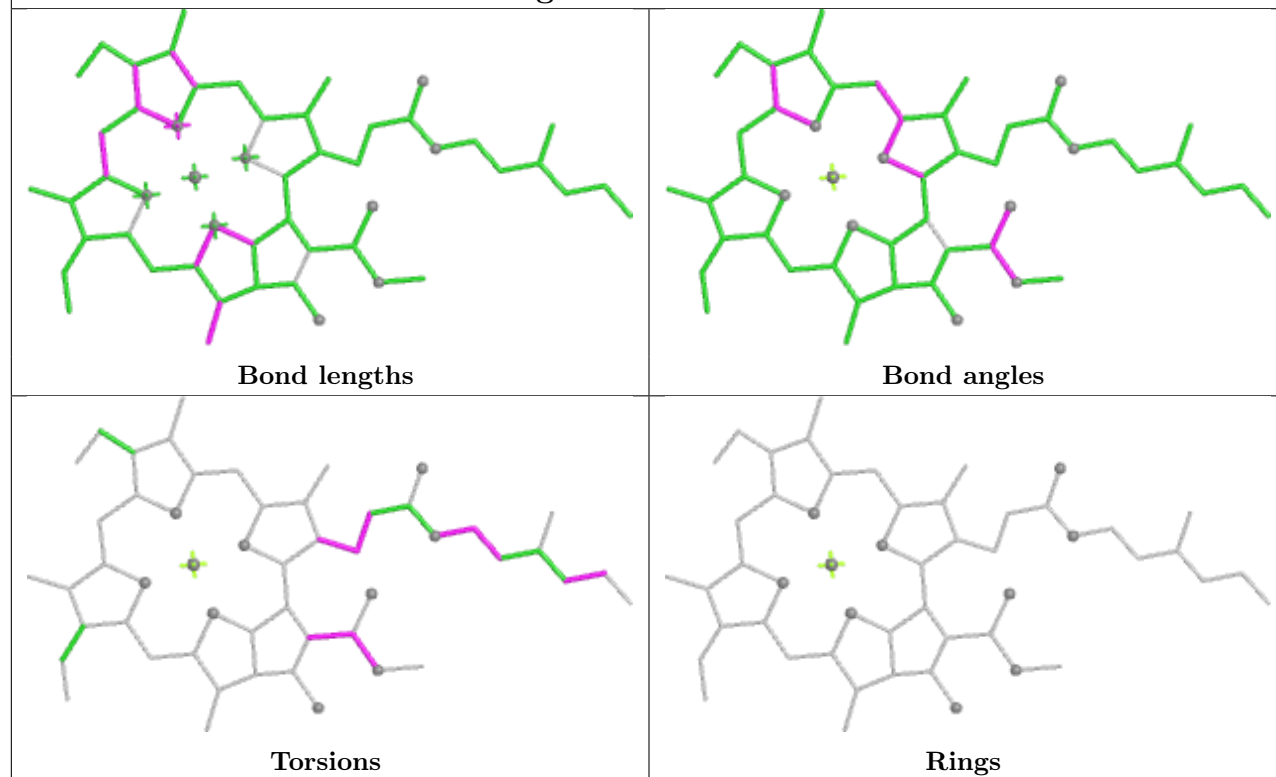
Ligand CLA B 831



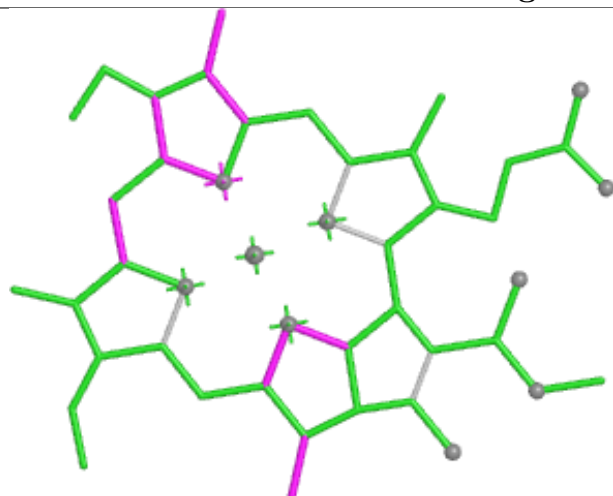
Ligand CLA 2 311



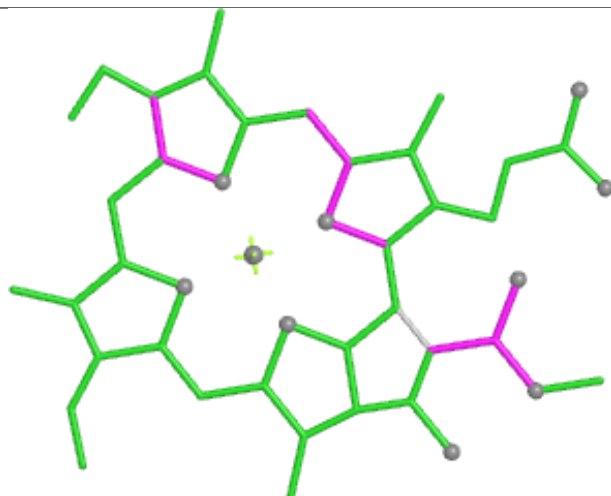
Ligand CLA 5 303



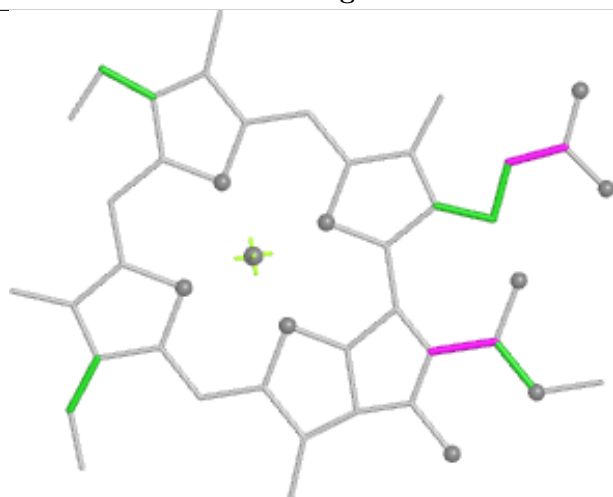
Ligand CLA 6 314



Bond lengths



Bond angles

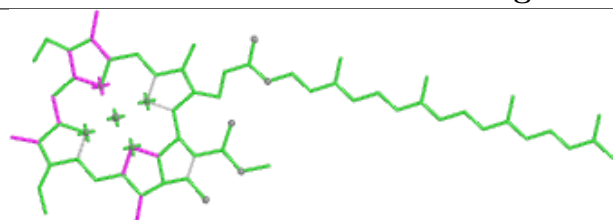


Torsions

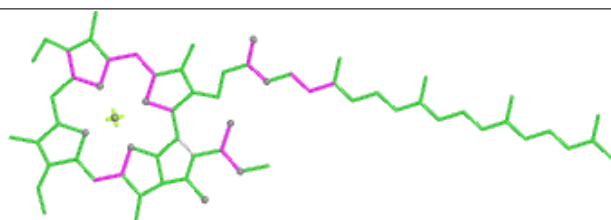


Rings

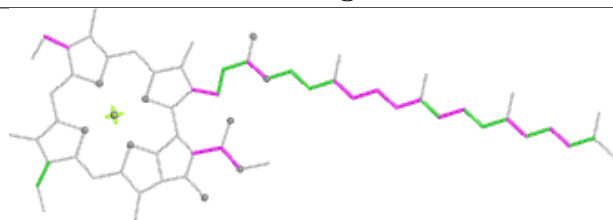
Ligand CLA A 805



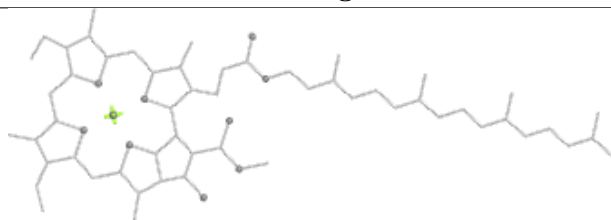
Bond lengths



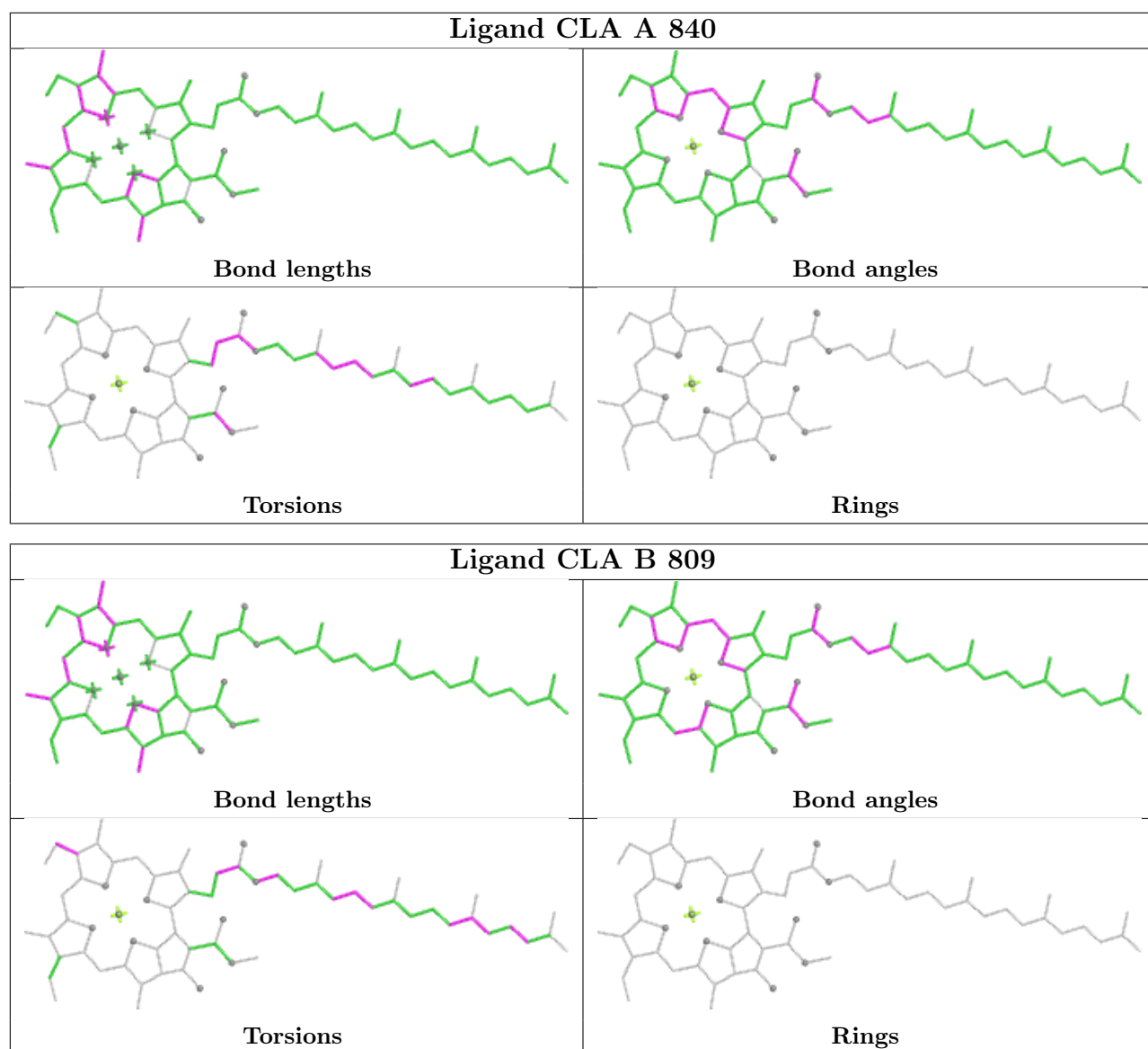
Bond angles



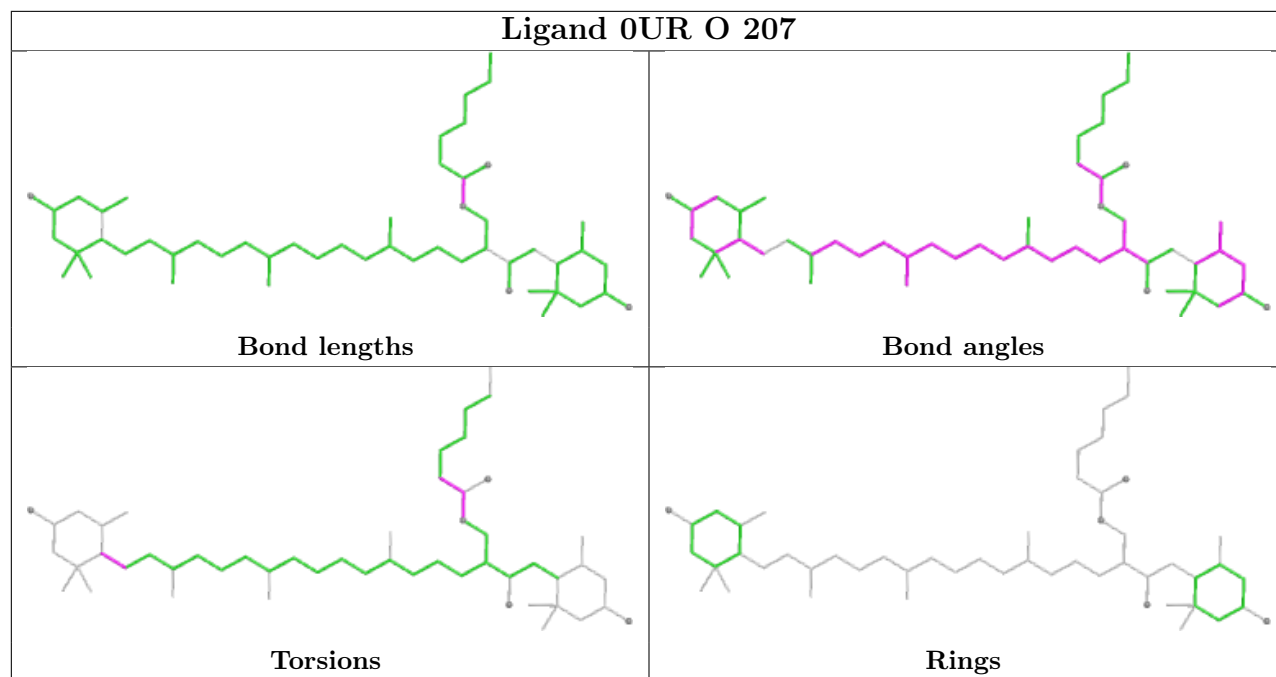
Torsions



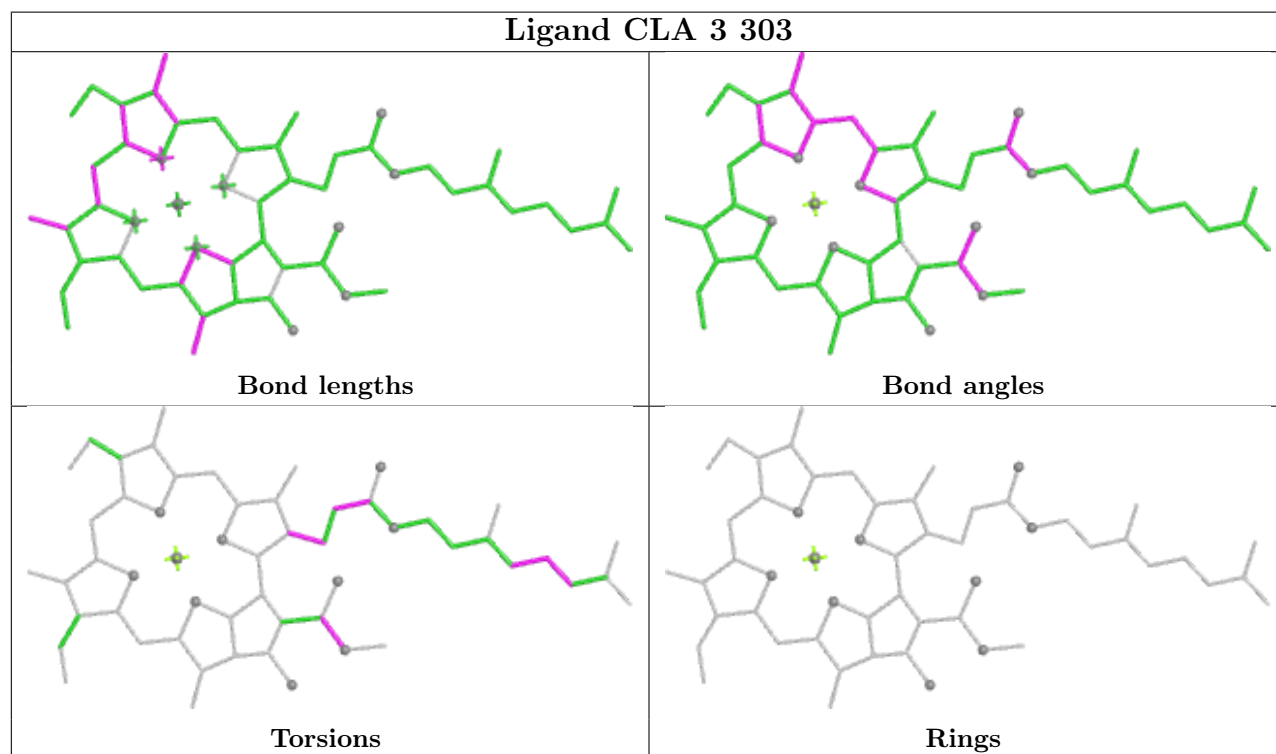
Rings



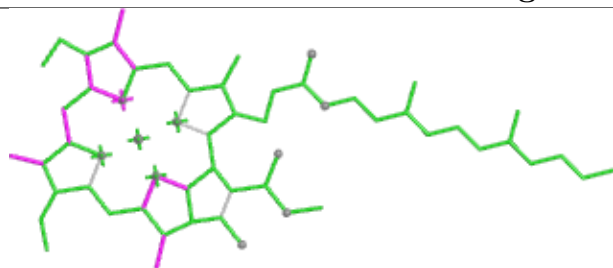
Ligand OUR O 207



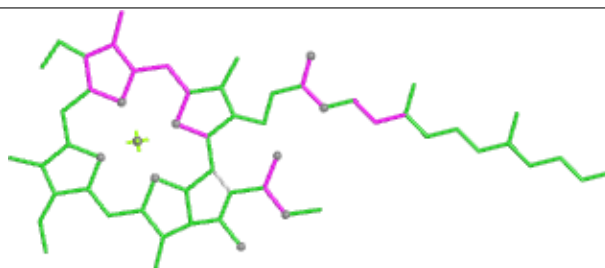
Ligand CLA 3 303



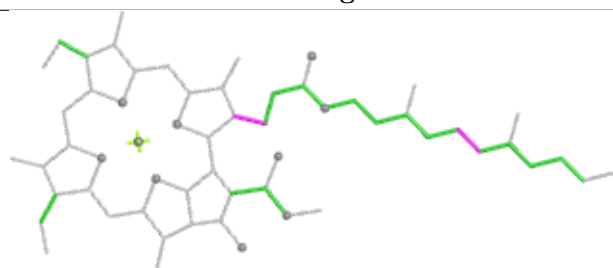
Ligand CLA 6 309



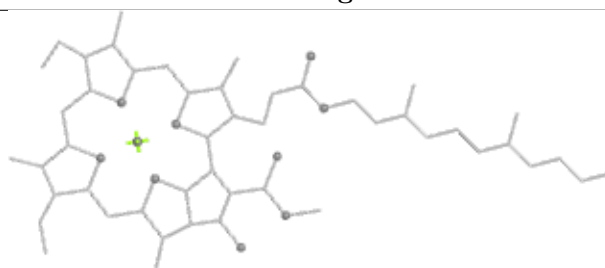
Bond lengths



Bond angles

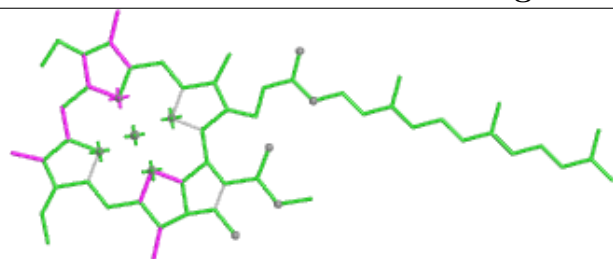


Torsions

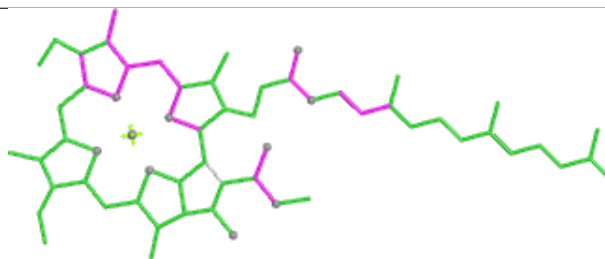


Rings

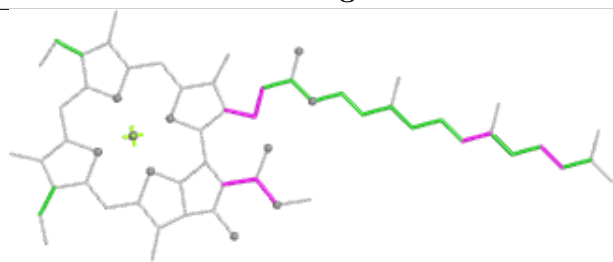
Ligand CLA B 816



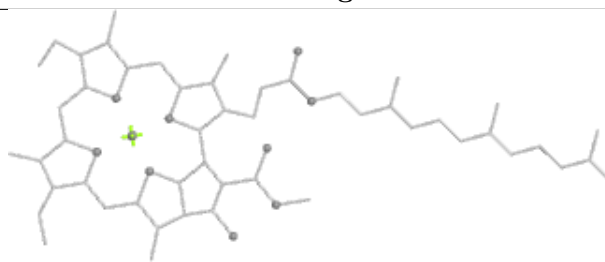
Bond lengths



Bond angles

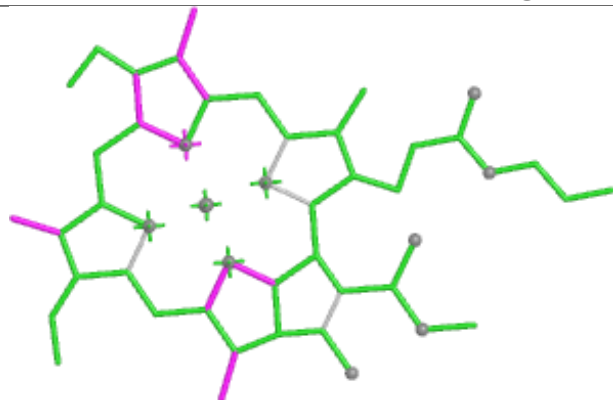


Torsions

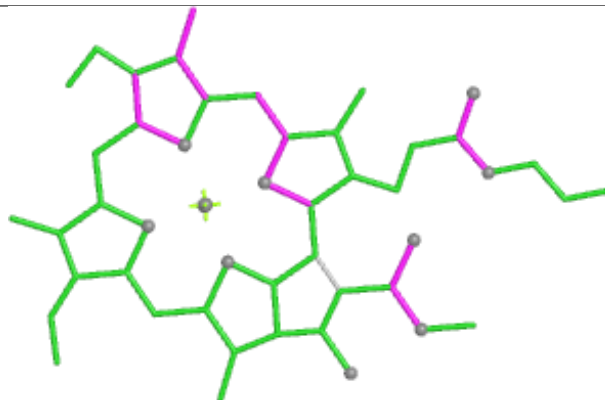


Rings

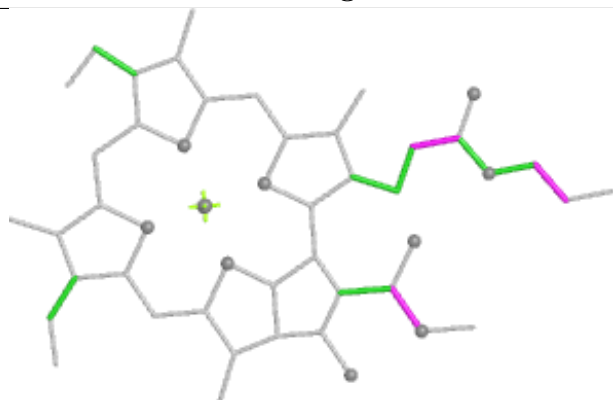
Ligand CLA 2 310



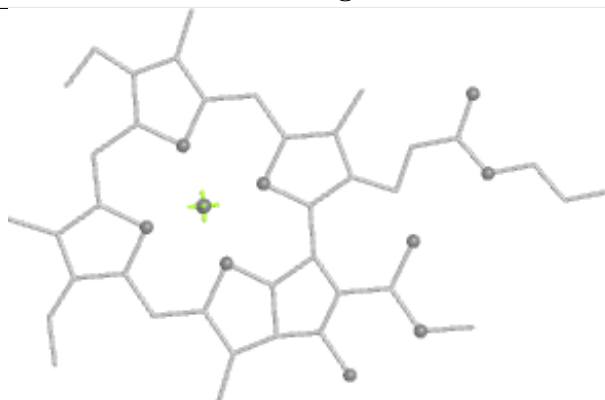
Bond lengths



Bond angles

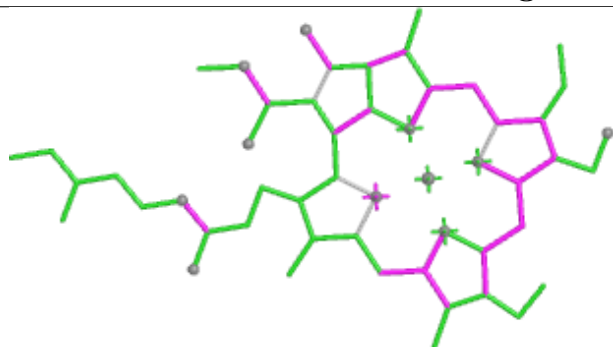


Torsions

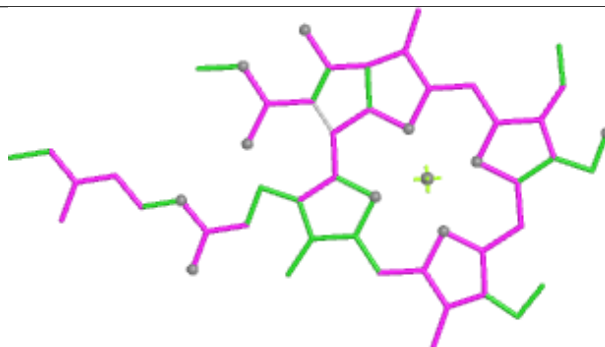


Rings

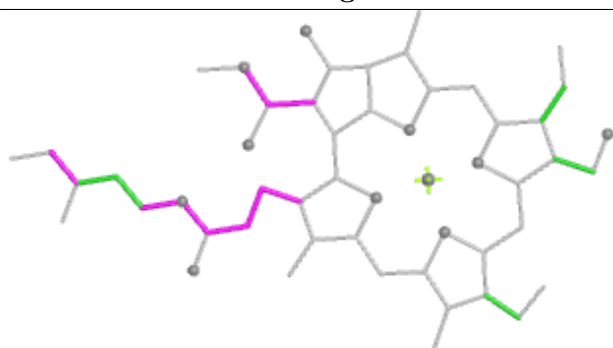
Ligand CHL 8 301



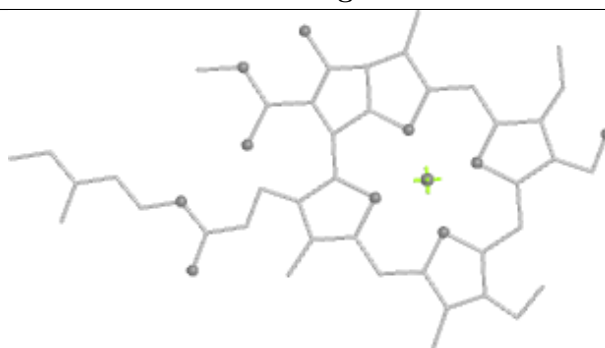
Bond lengths



Bond angles

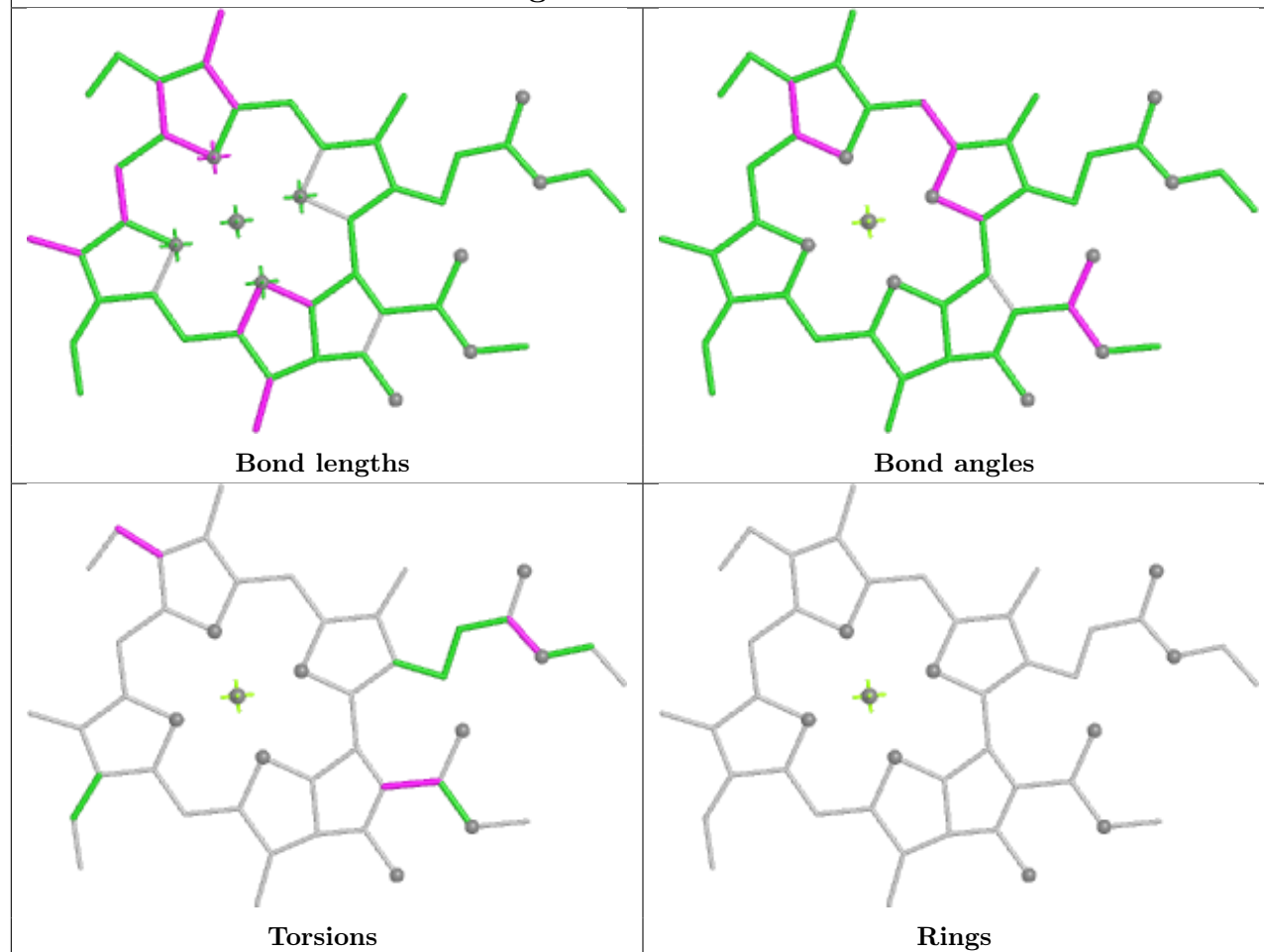


Torsions

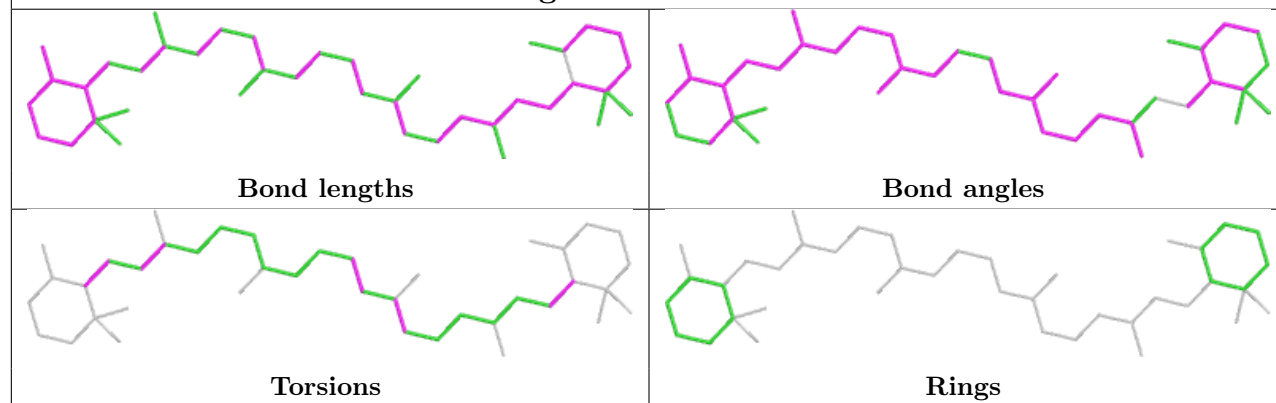


Rings

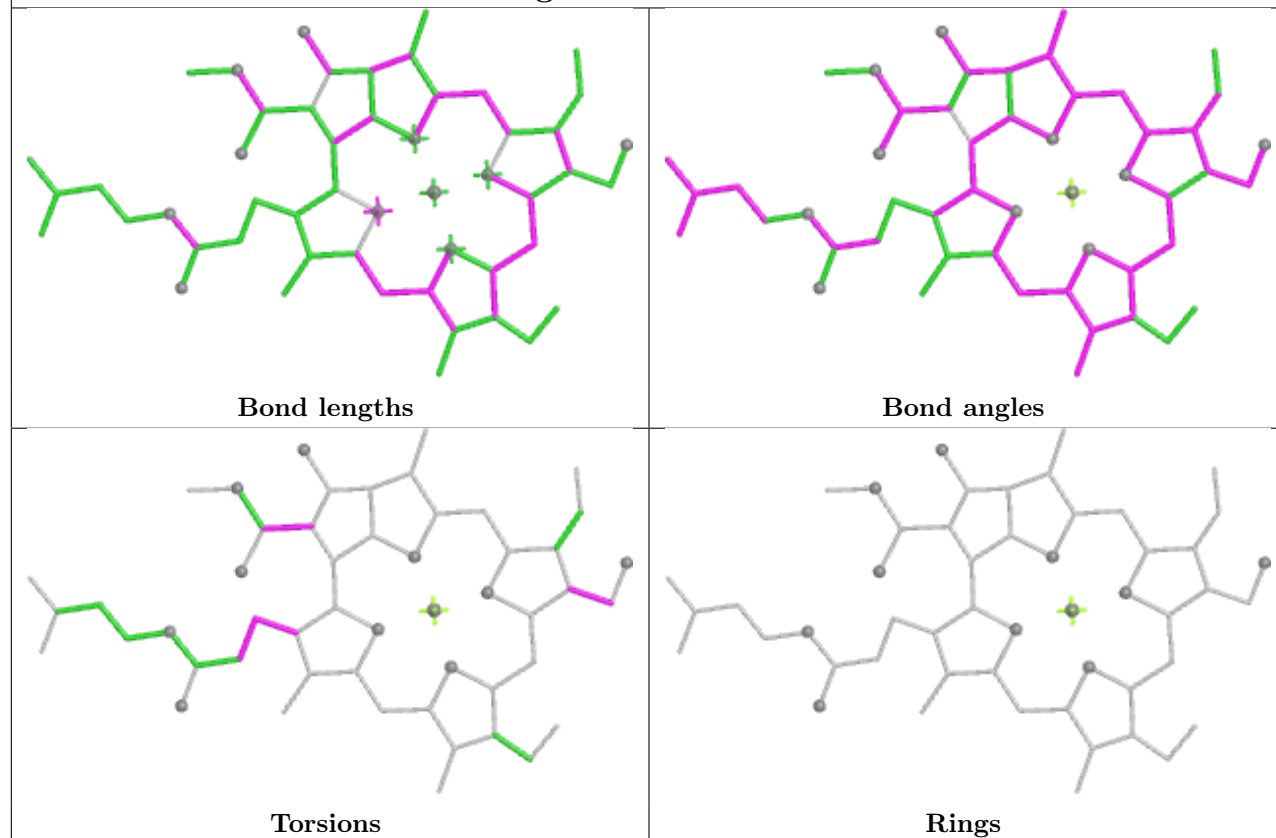
Ligand CLA F 302



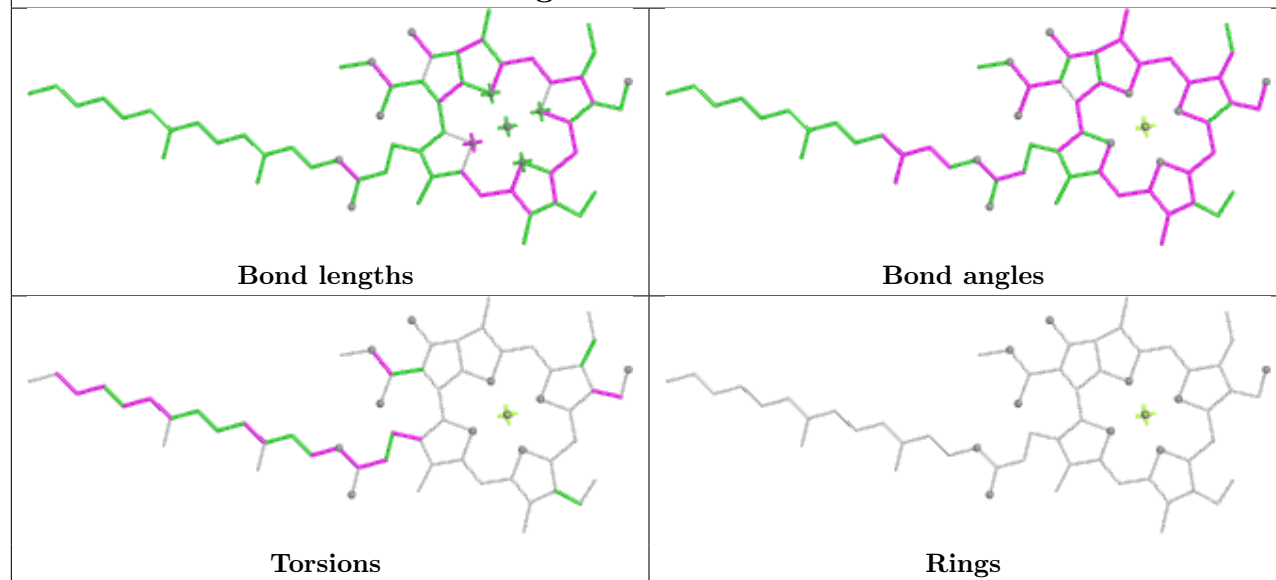
Ligand 8CT 1 314

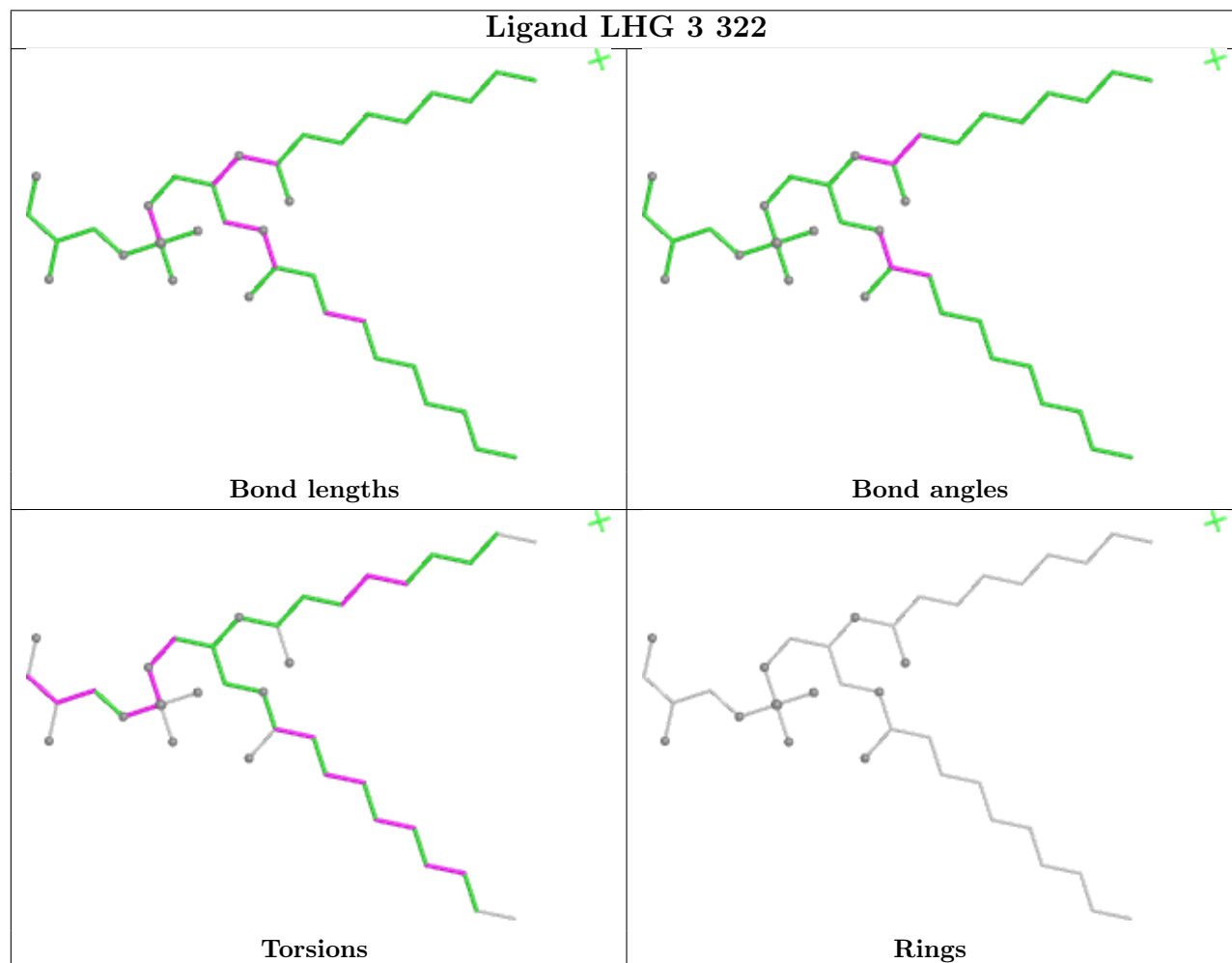
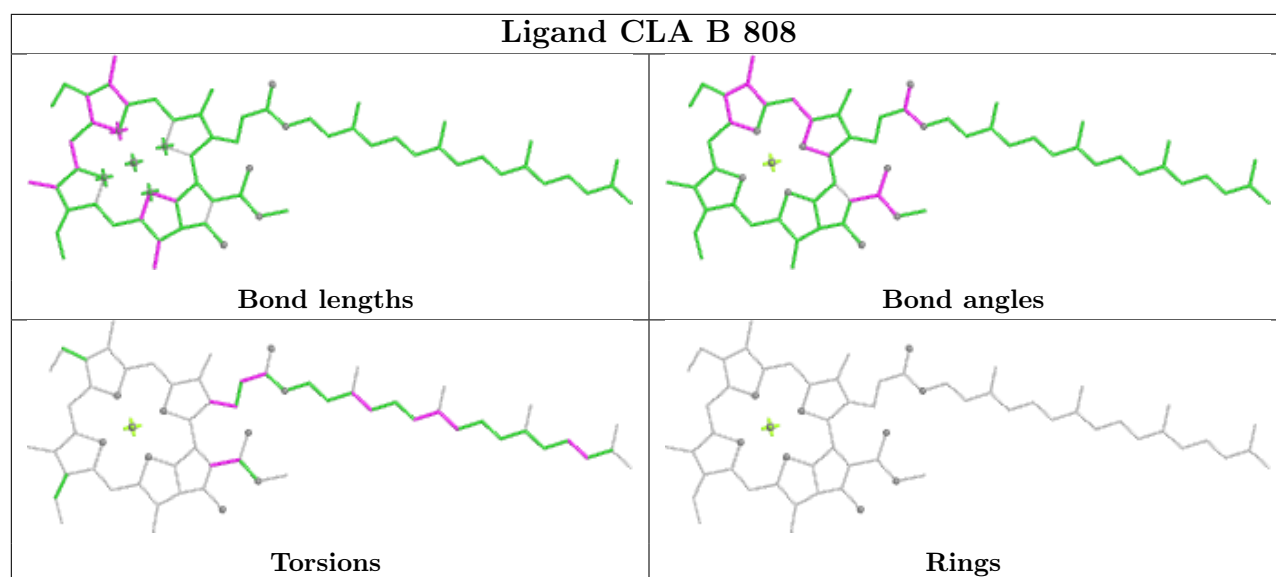


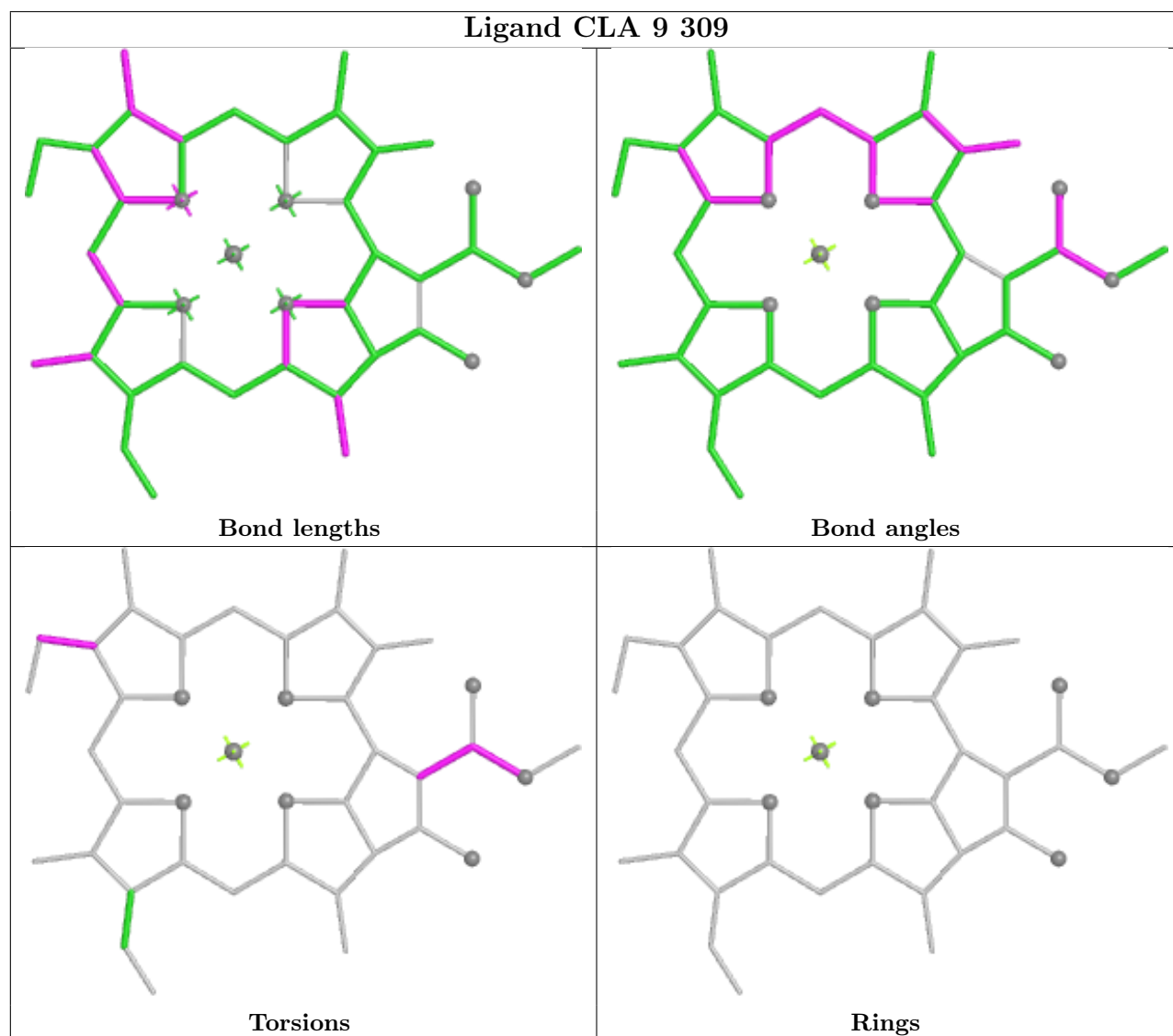
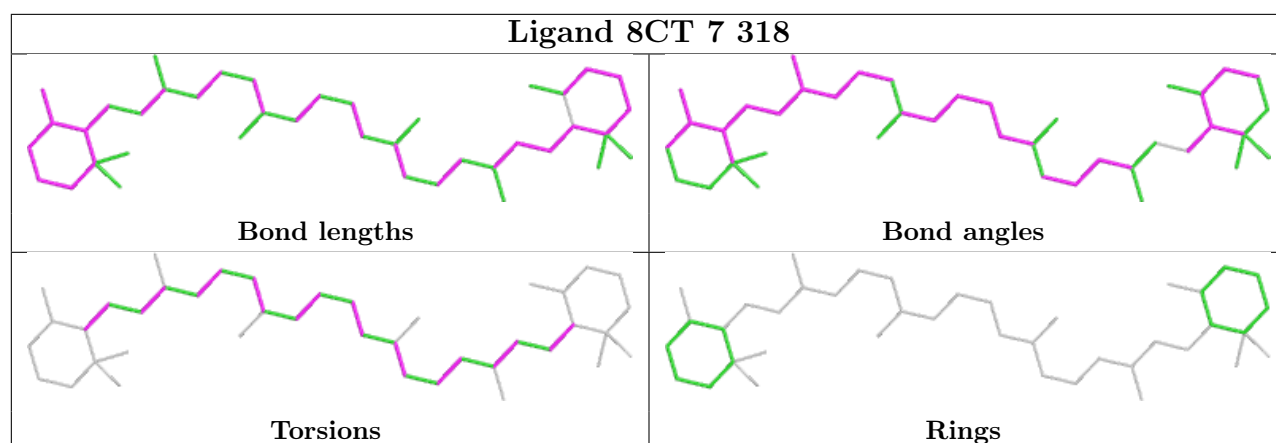
Ligand CHL 2 312

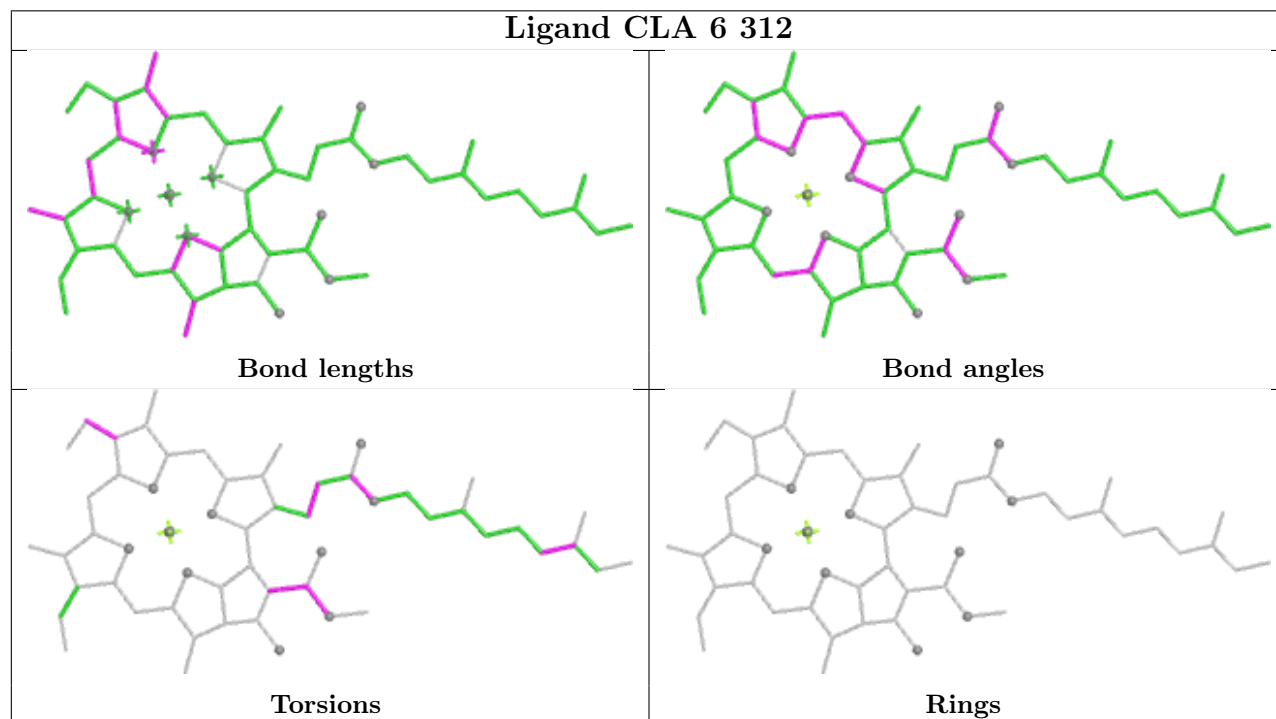
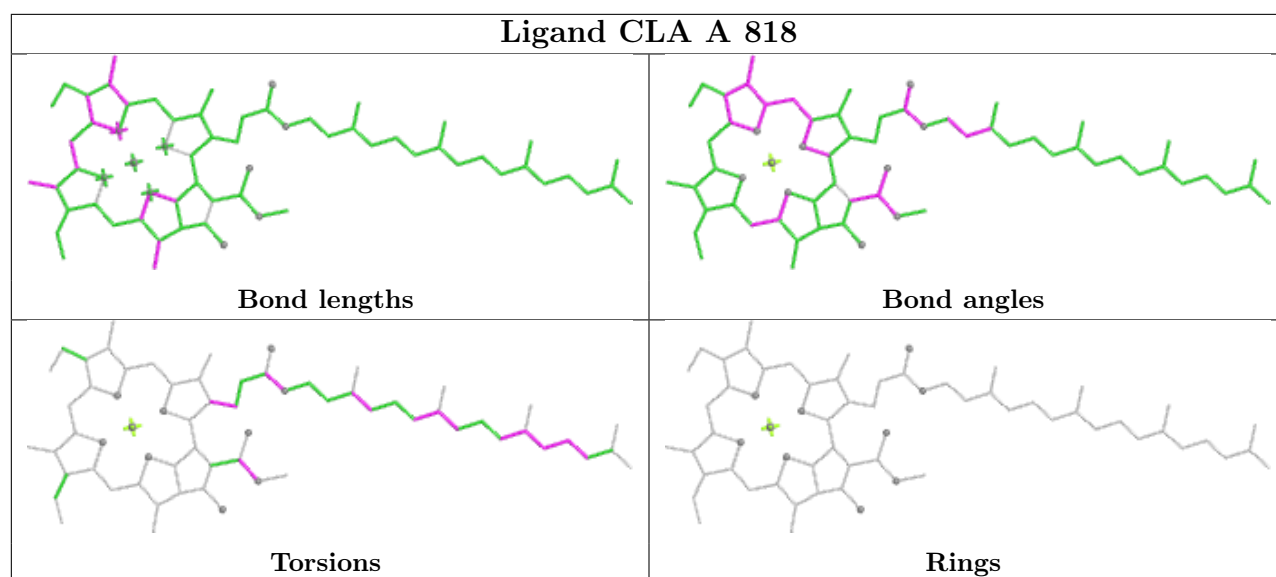


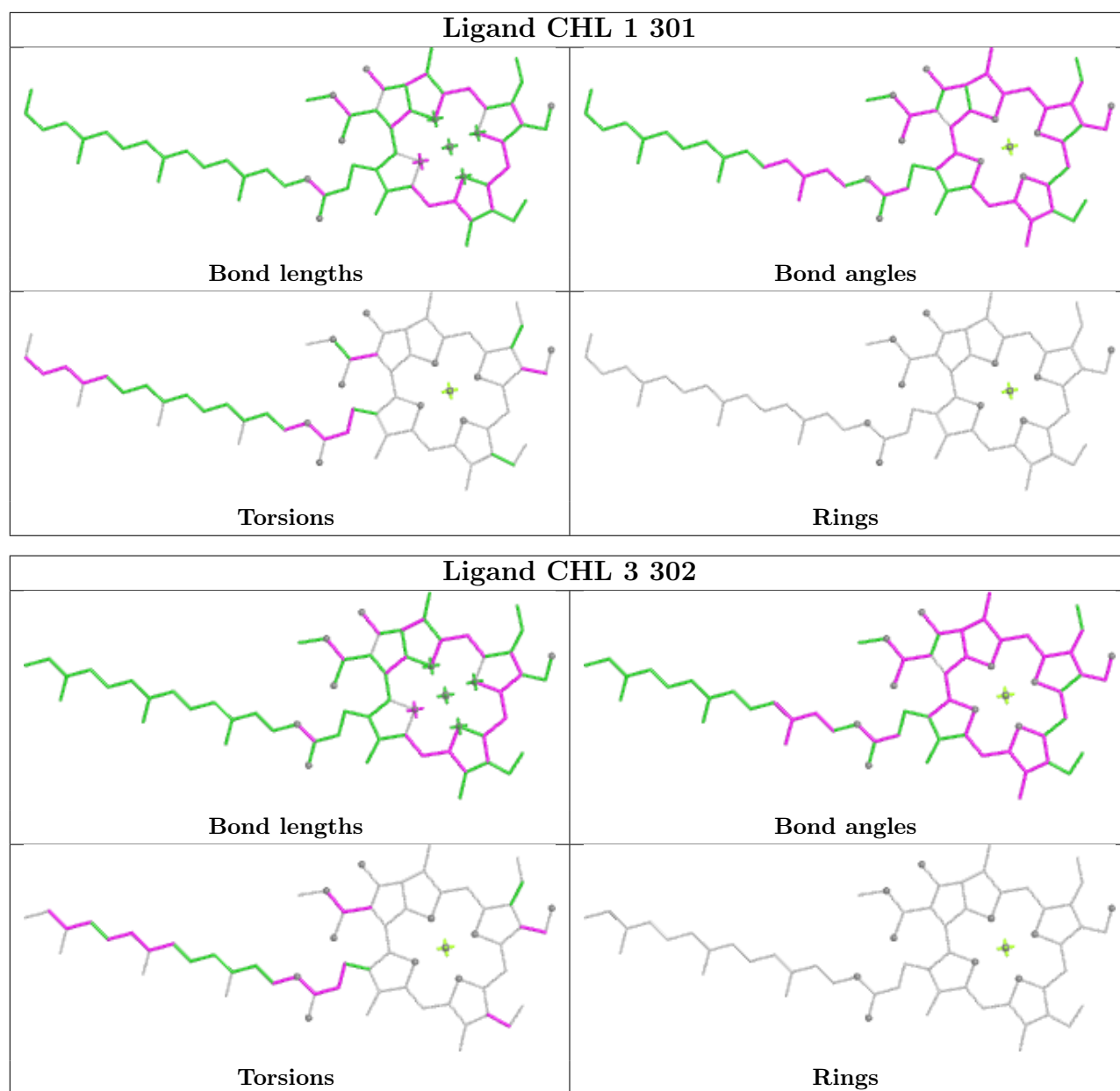
Ligand CHL 7 306



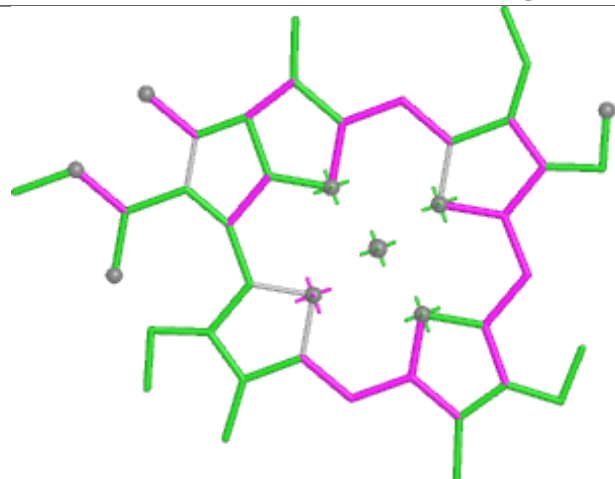




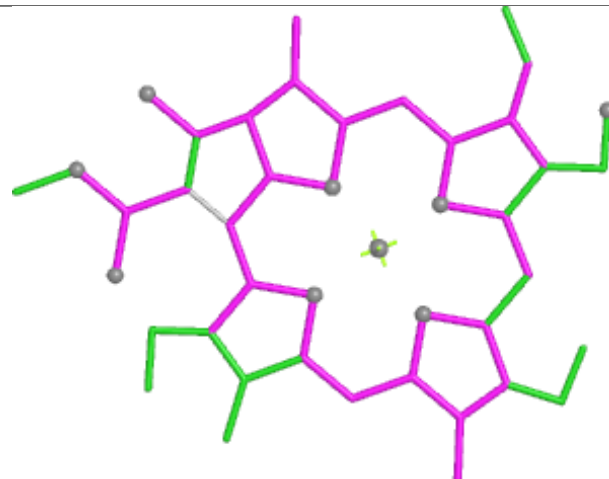




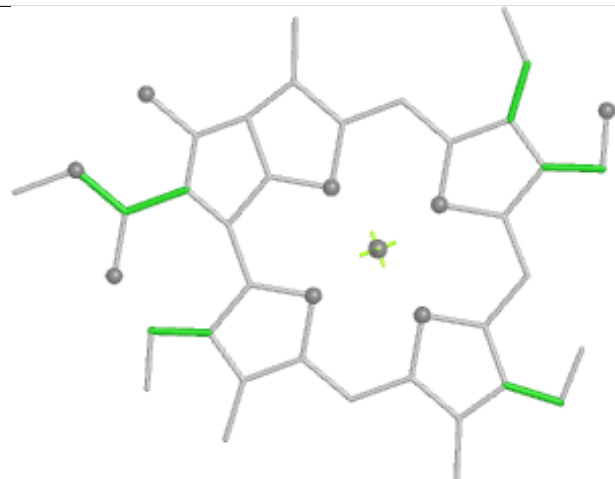
Ligand CHL 2 304



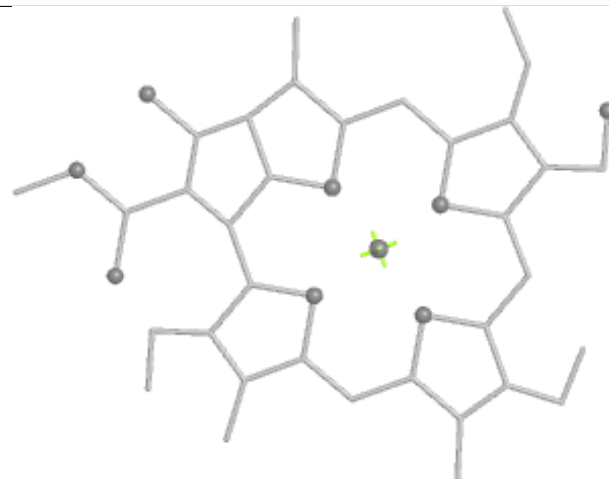
Bond lengths



Bond angles



Torsions

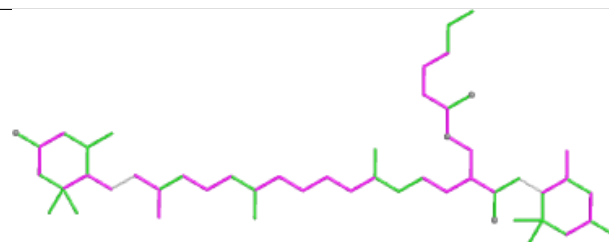


Rings

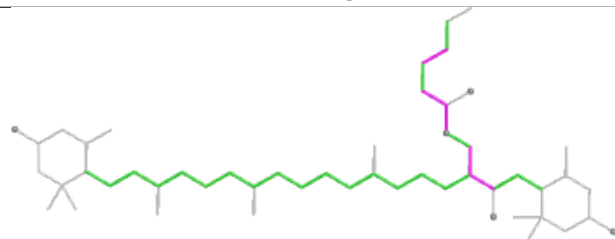
Ligand OUR 7 320



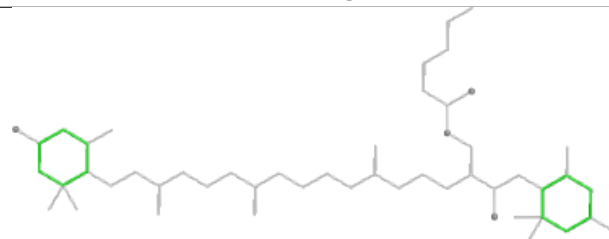
Bond lengths



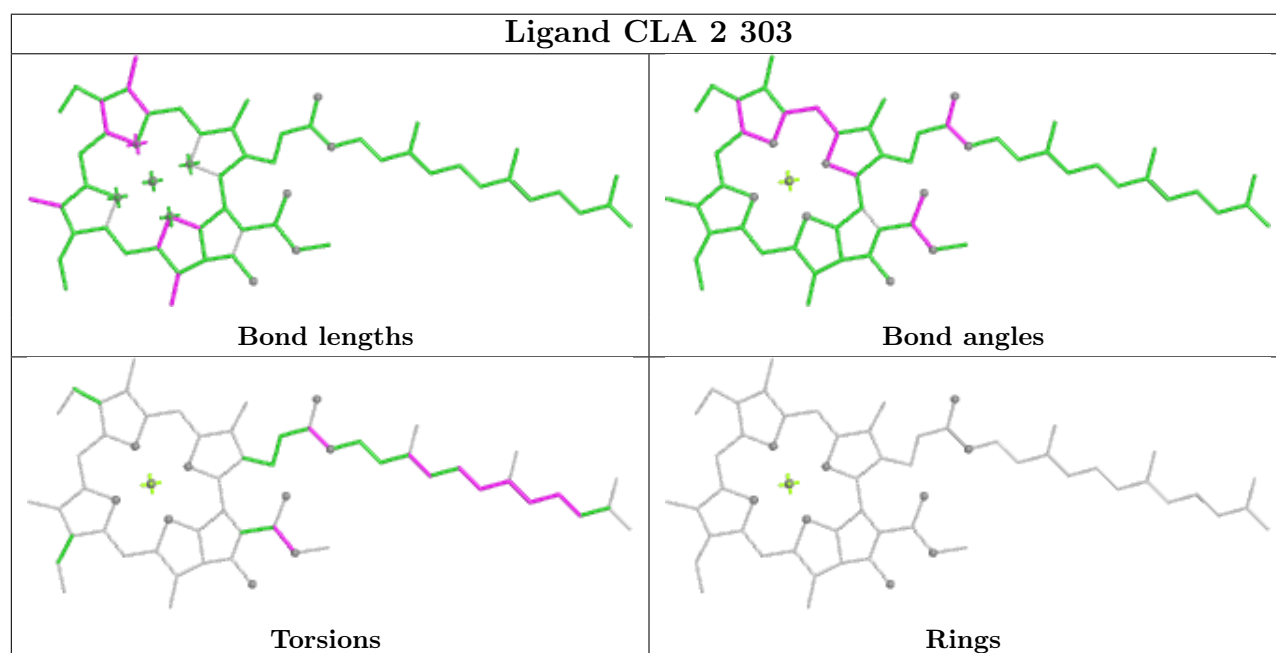
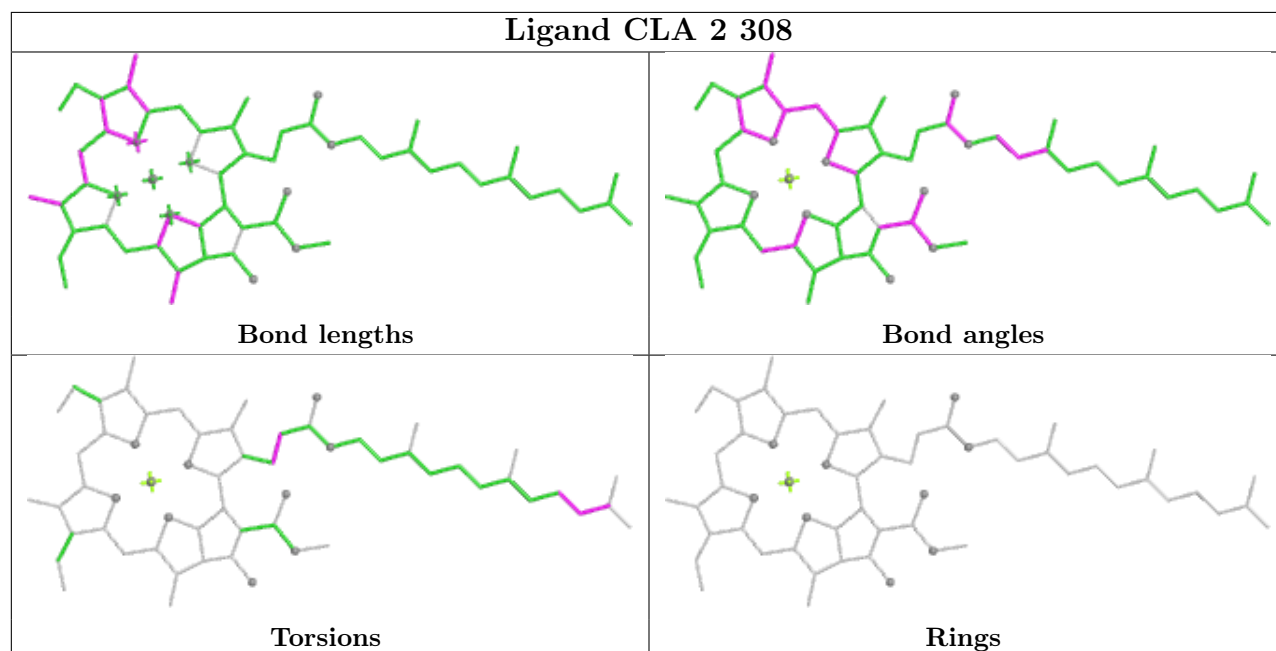
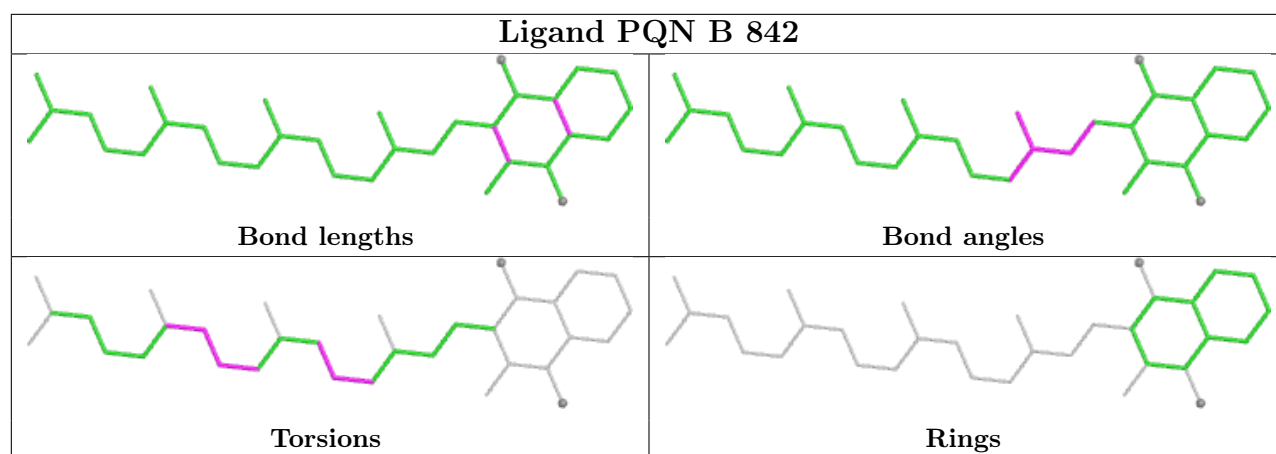
Bond angles

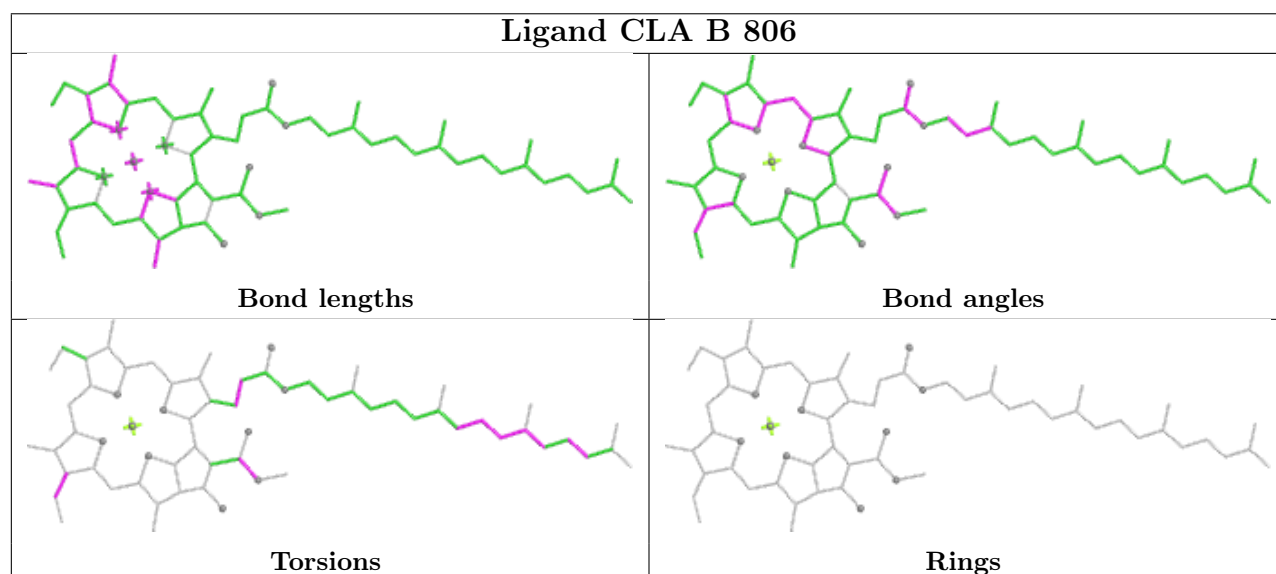
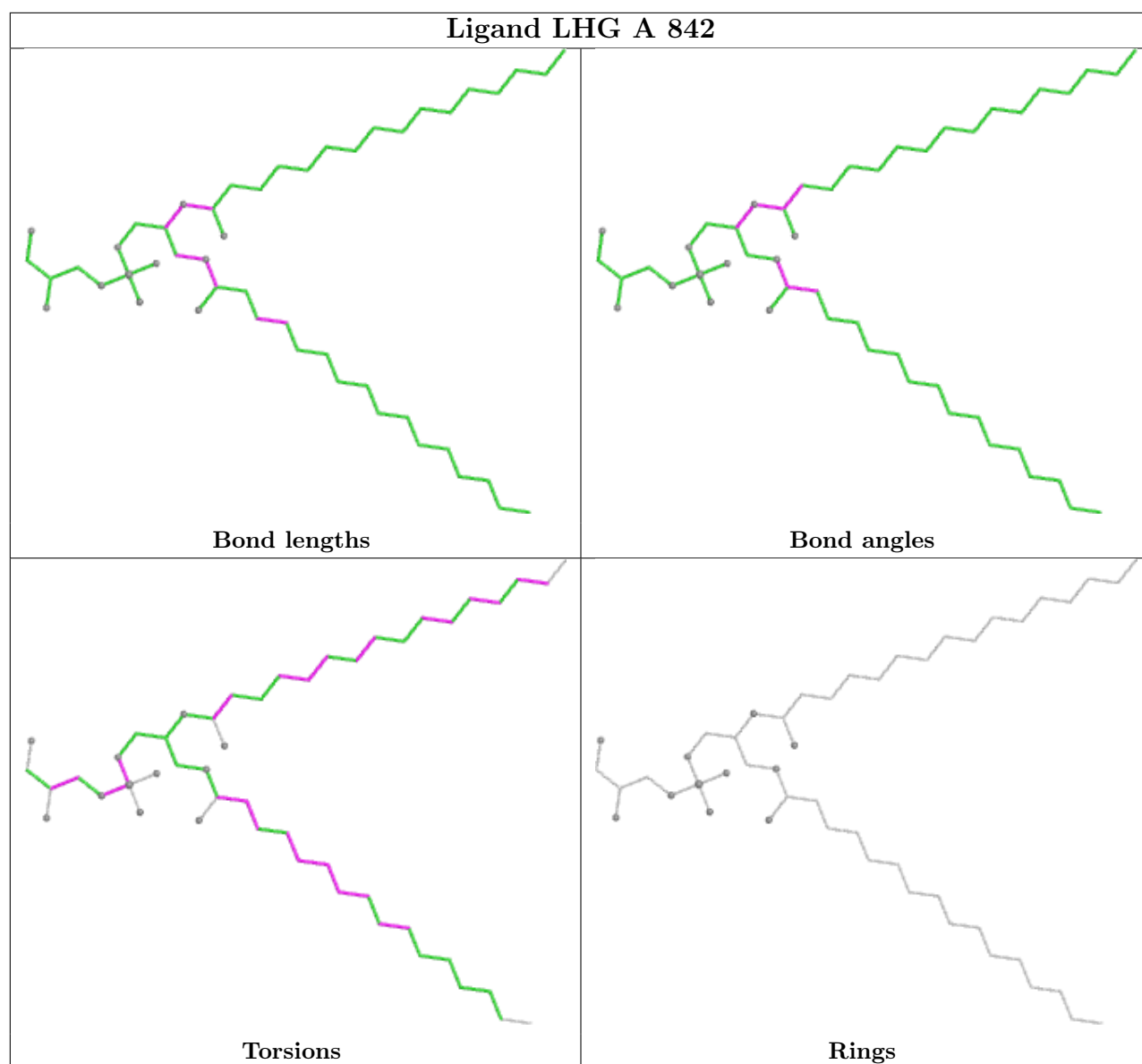


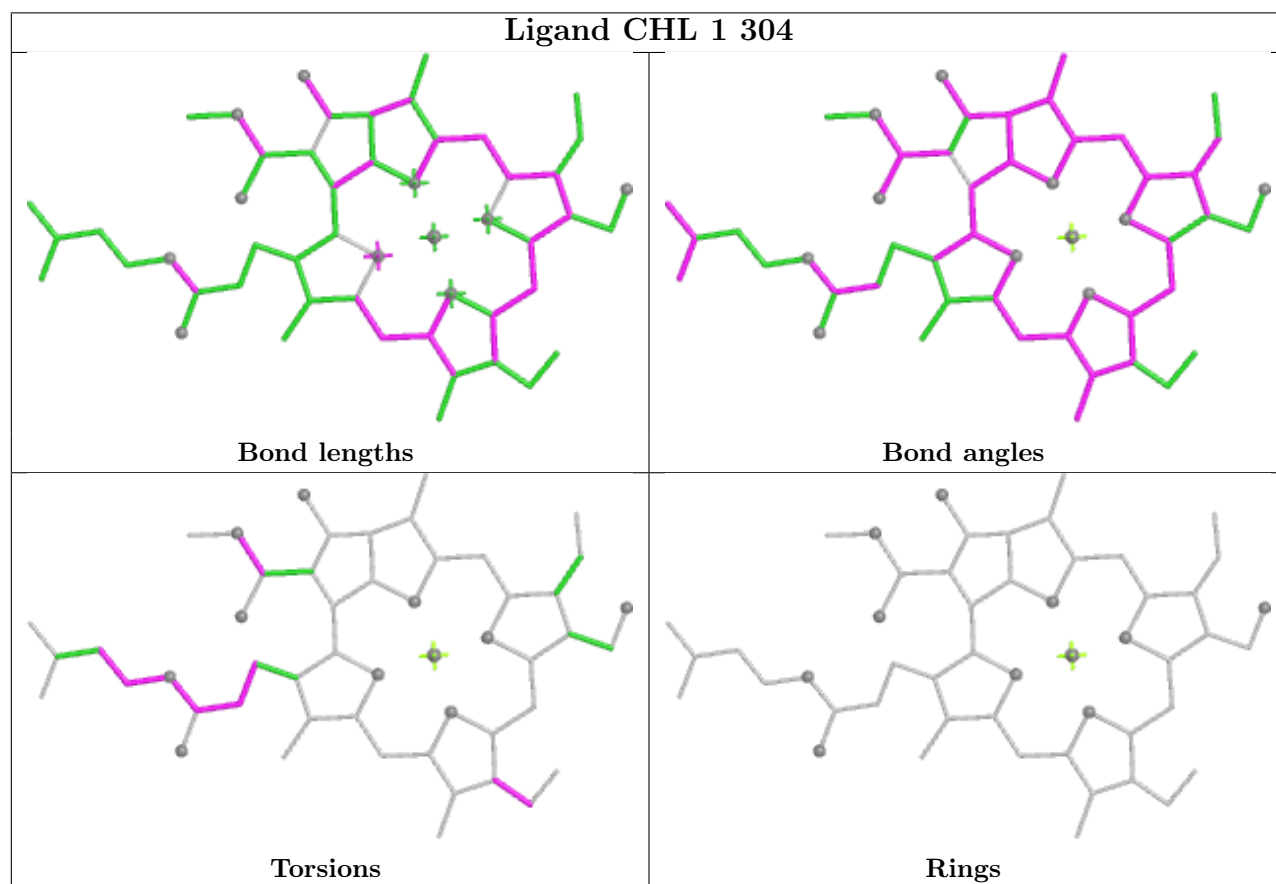
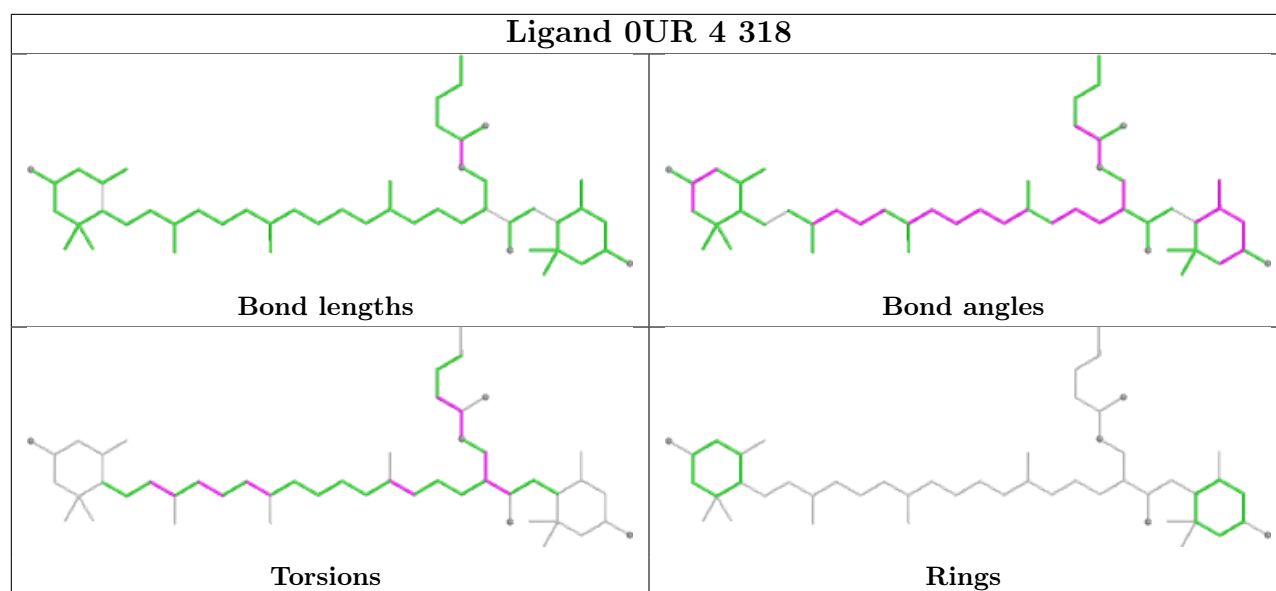
Torsions

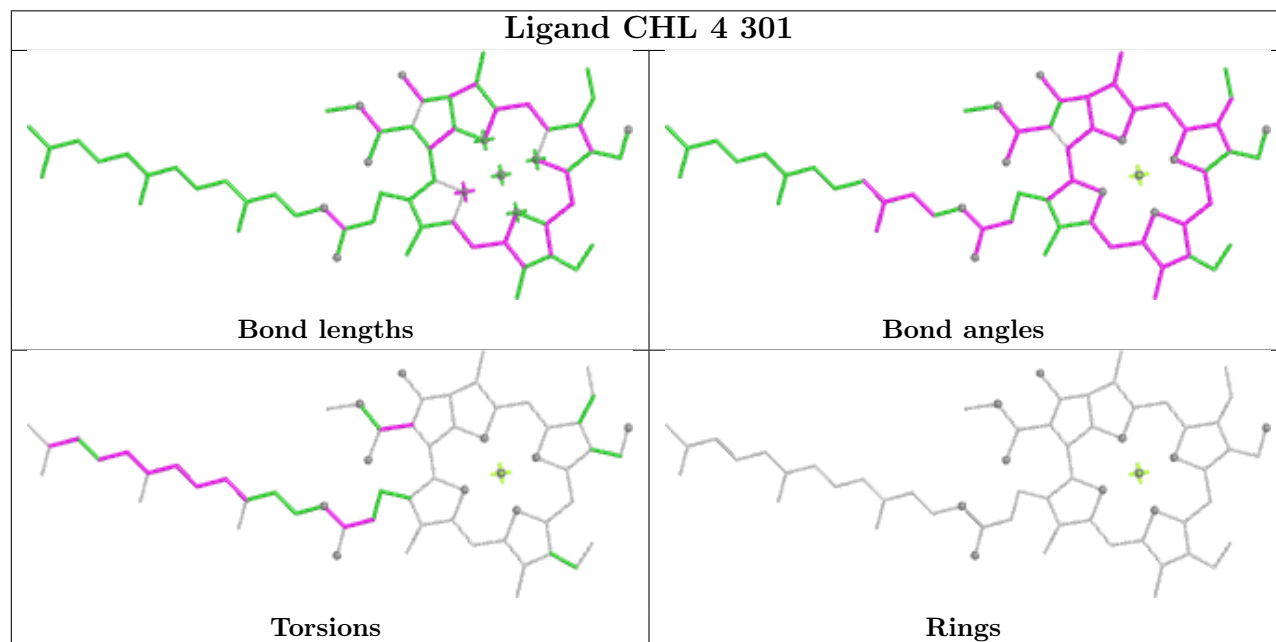
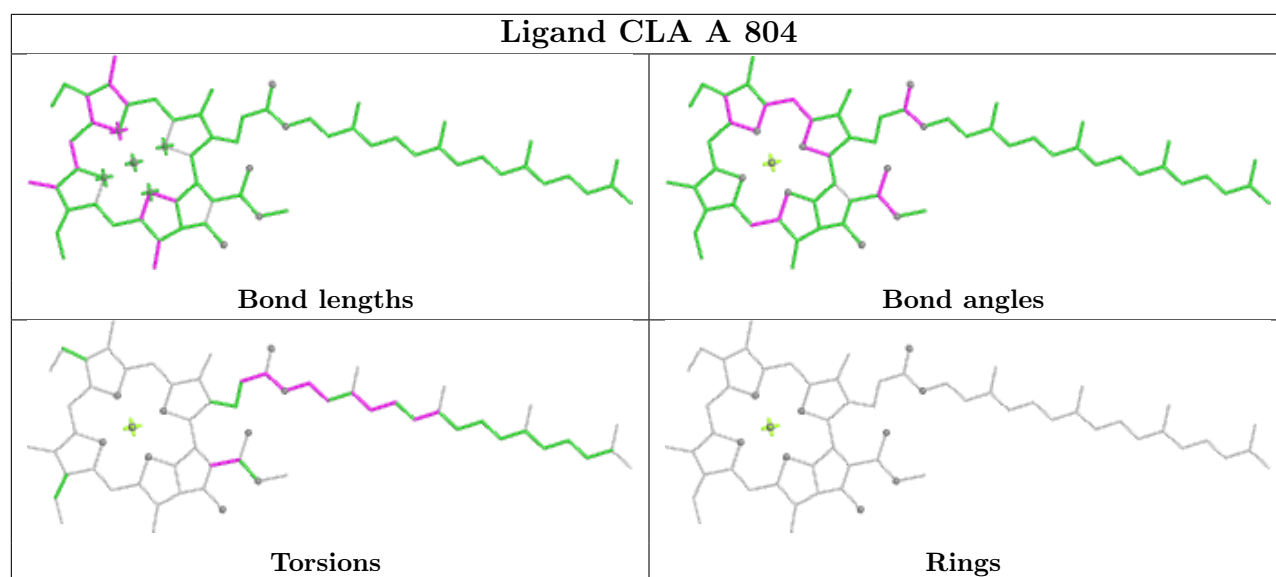


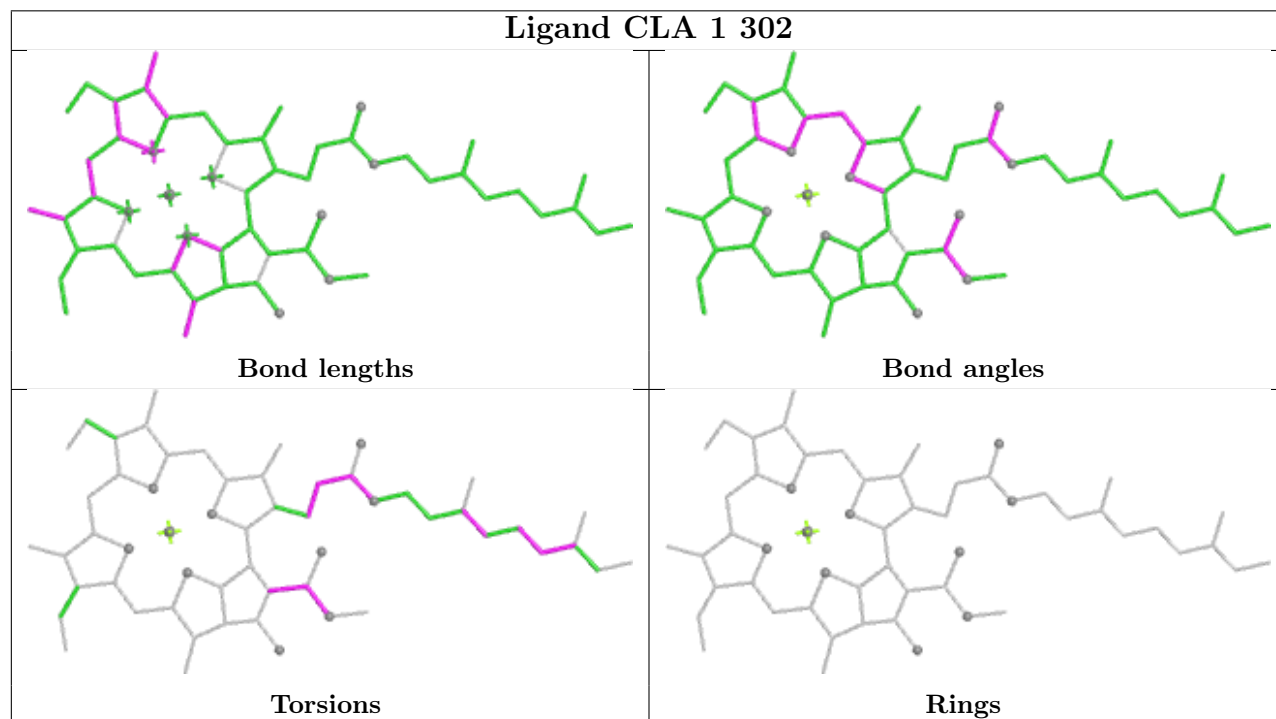
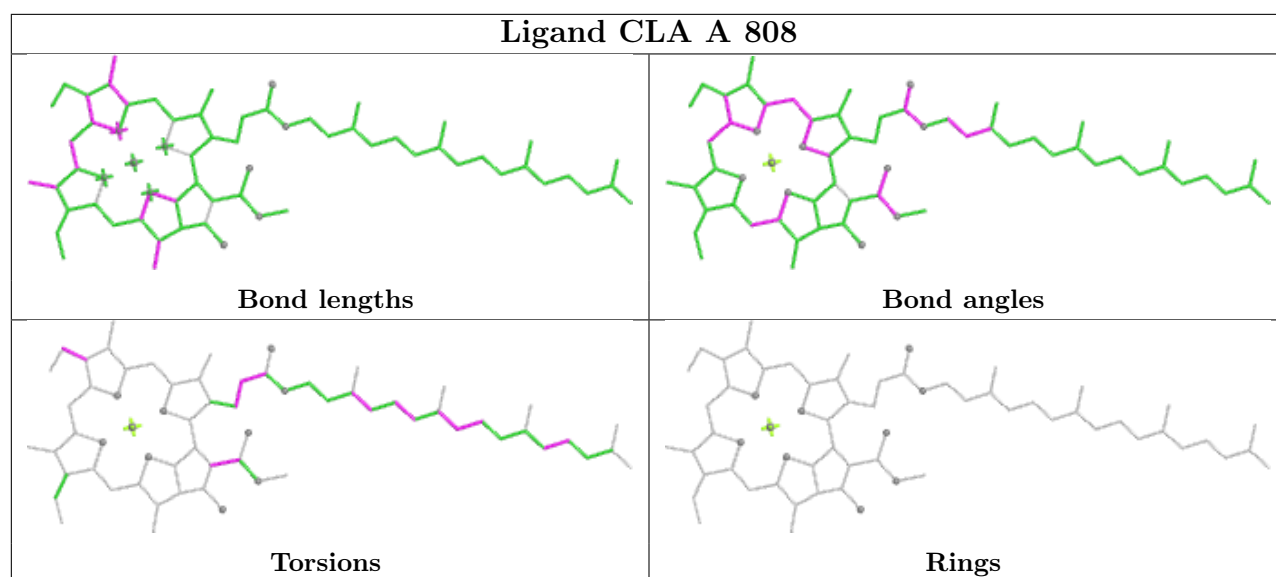
Rings



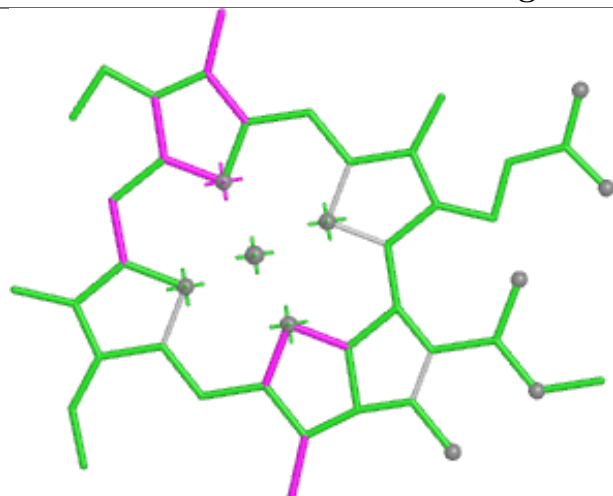




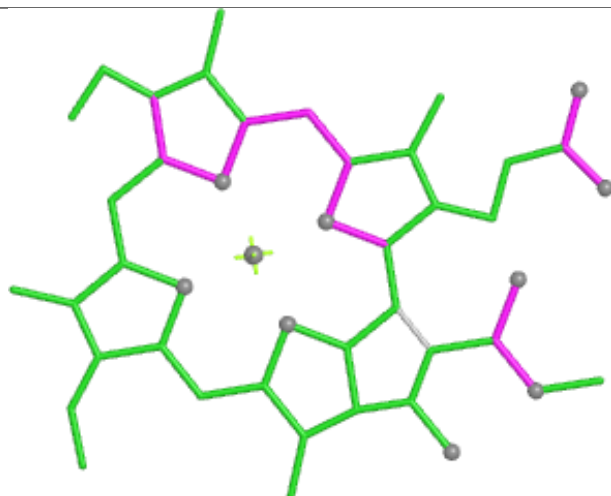




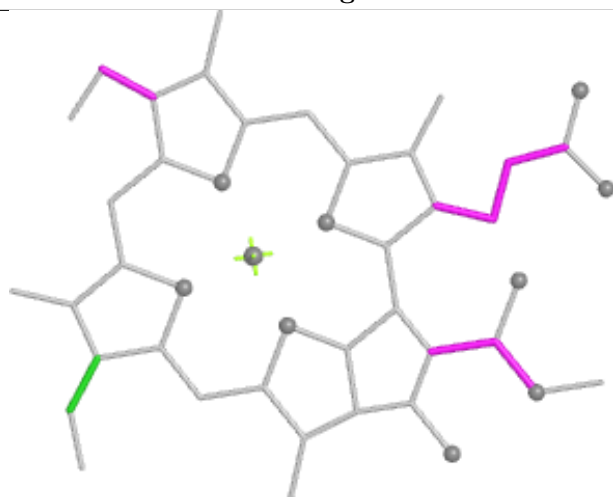
Ligand CLA 8 315



Bond lengths



Bond angles

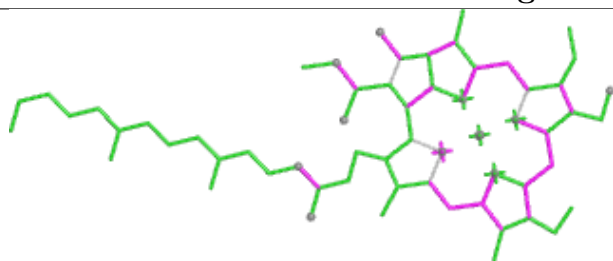


Torsions

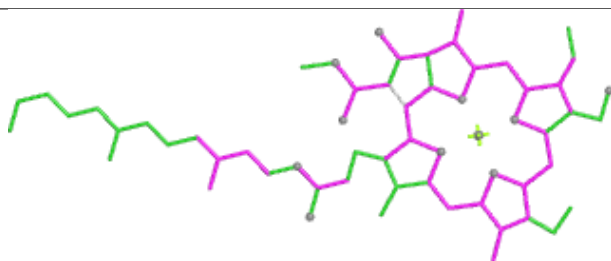


Rings

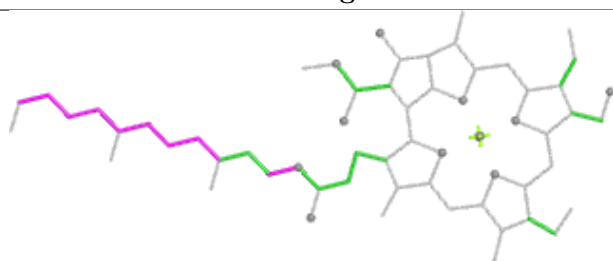
Ligand CHL 6 308



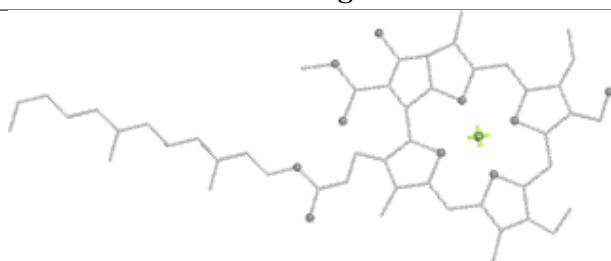
Bond lengths



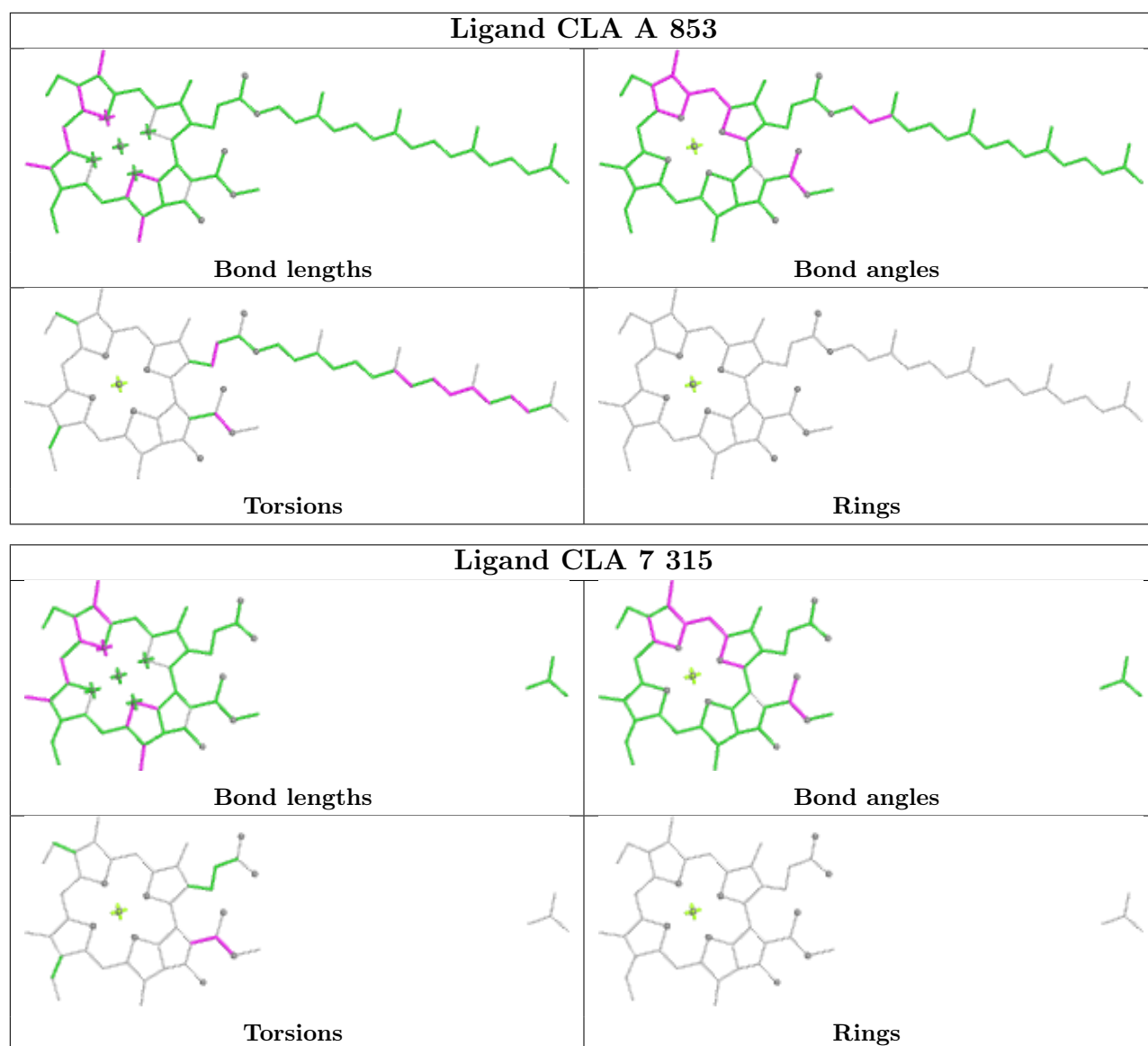
Bond angles

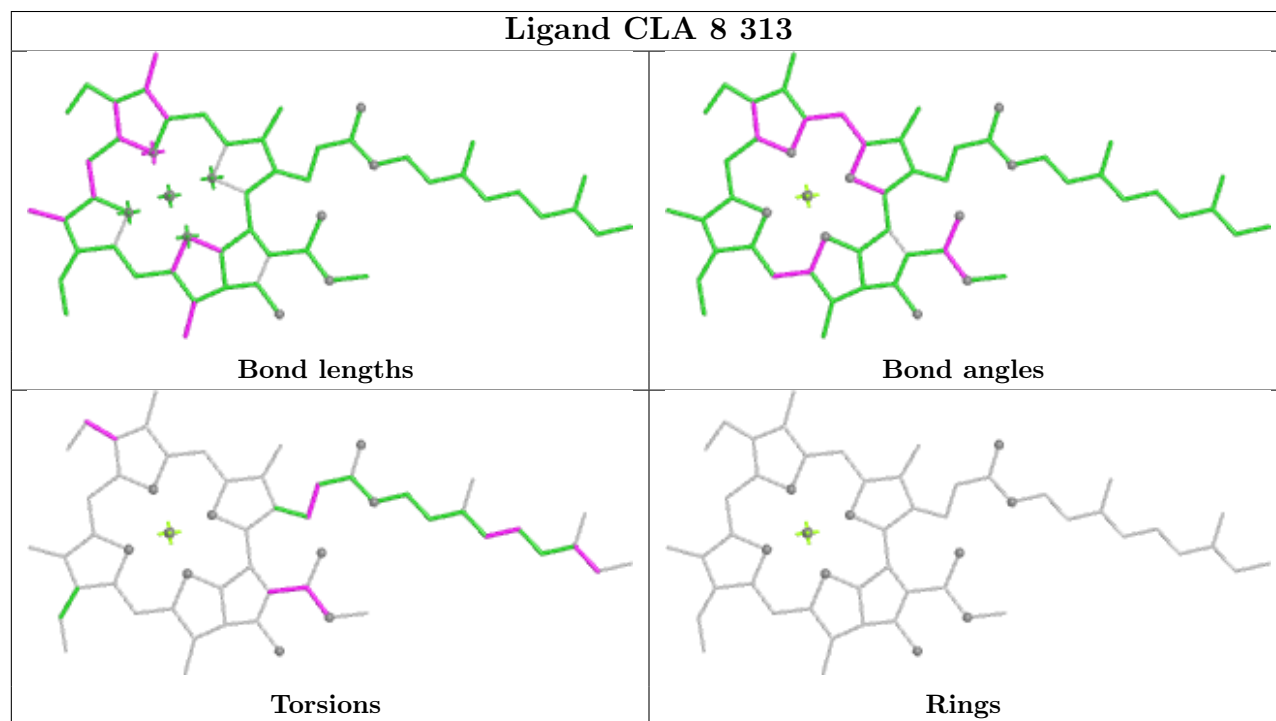
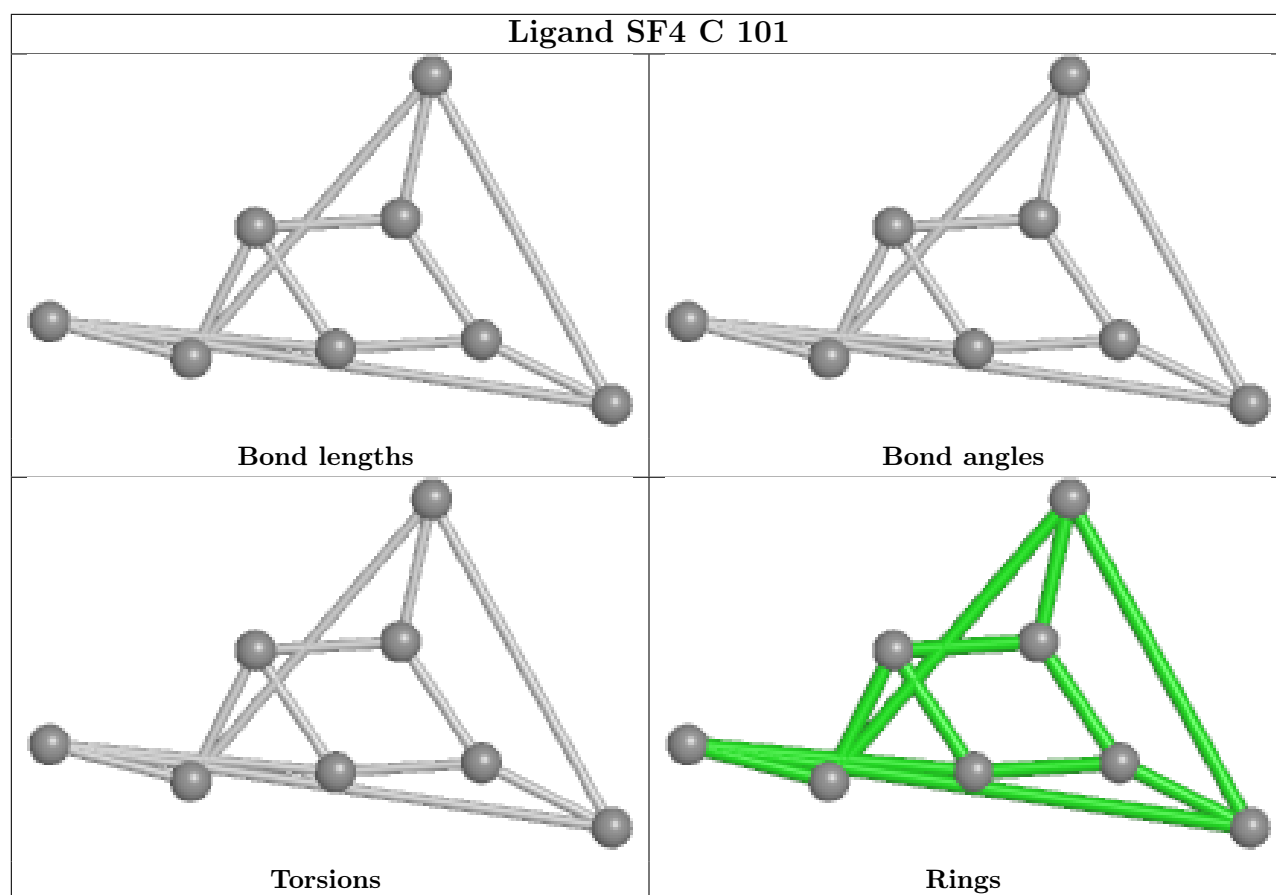


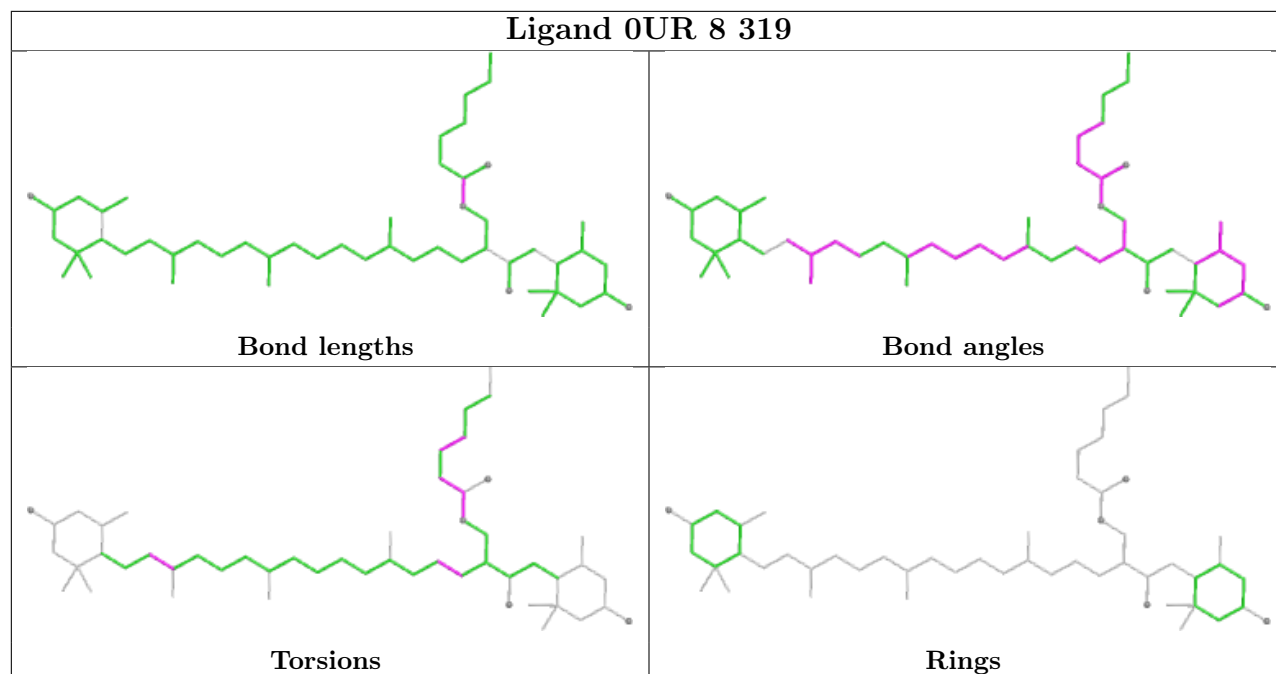
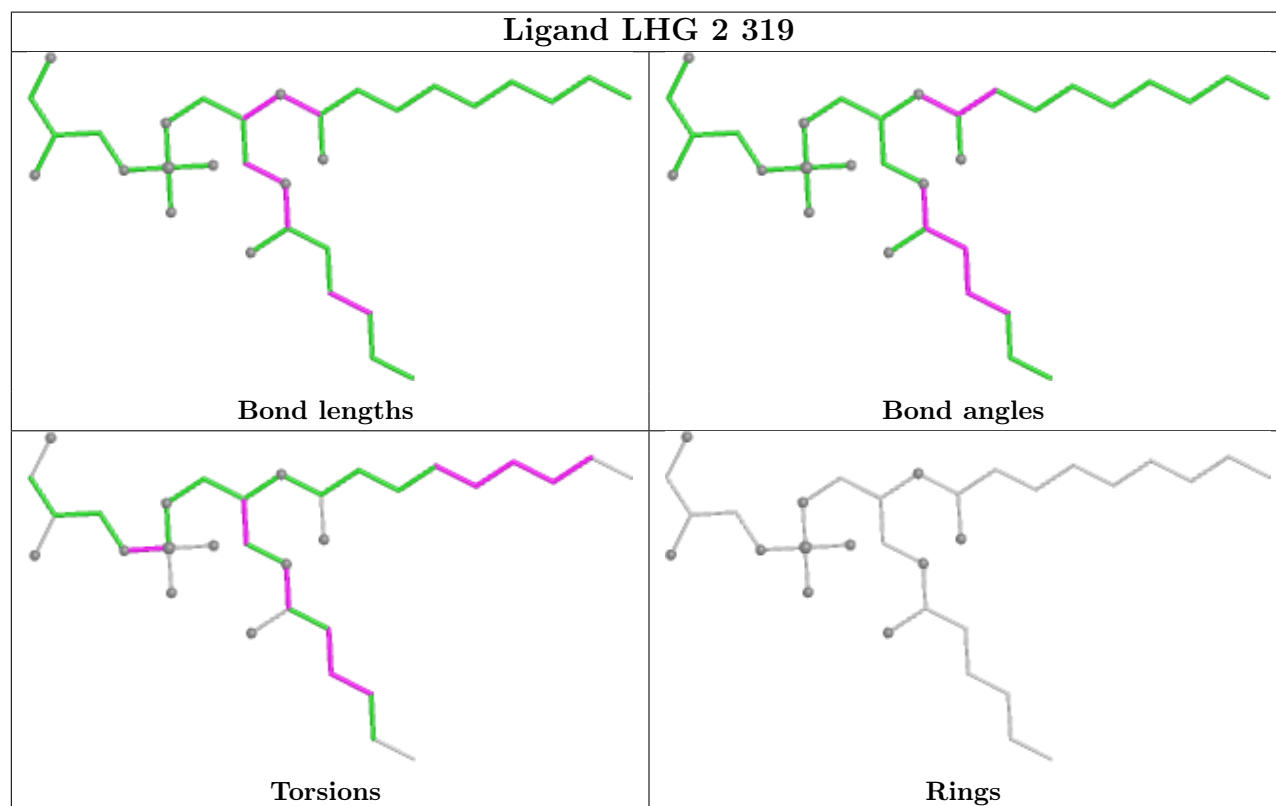
Torsions

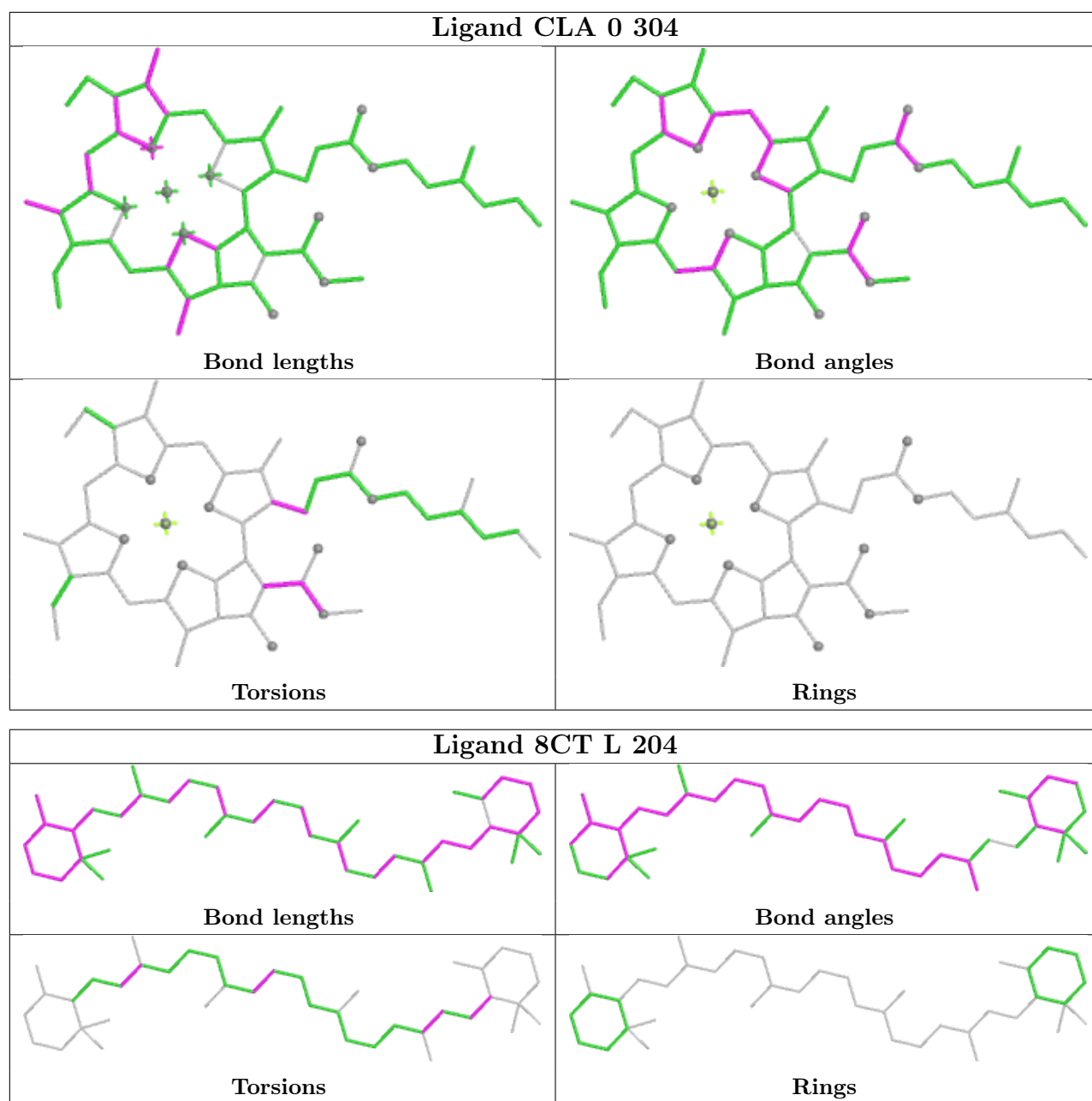


Rings

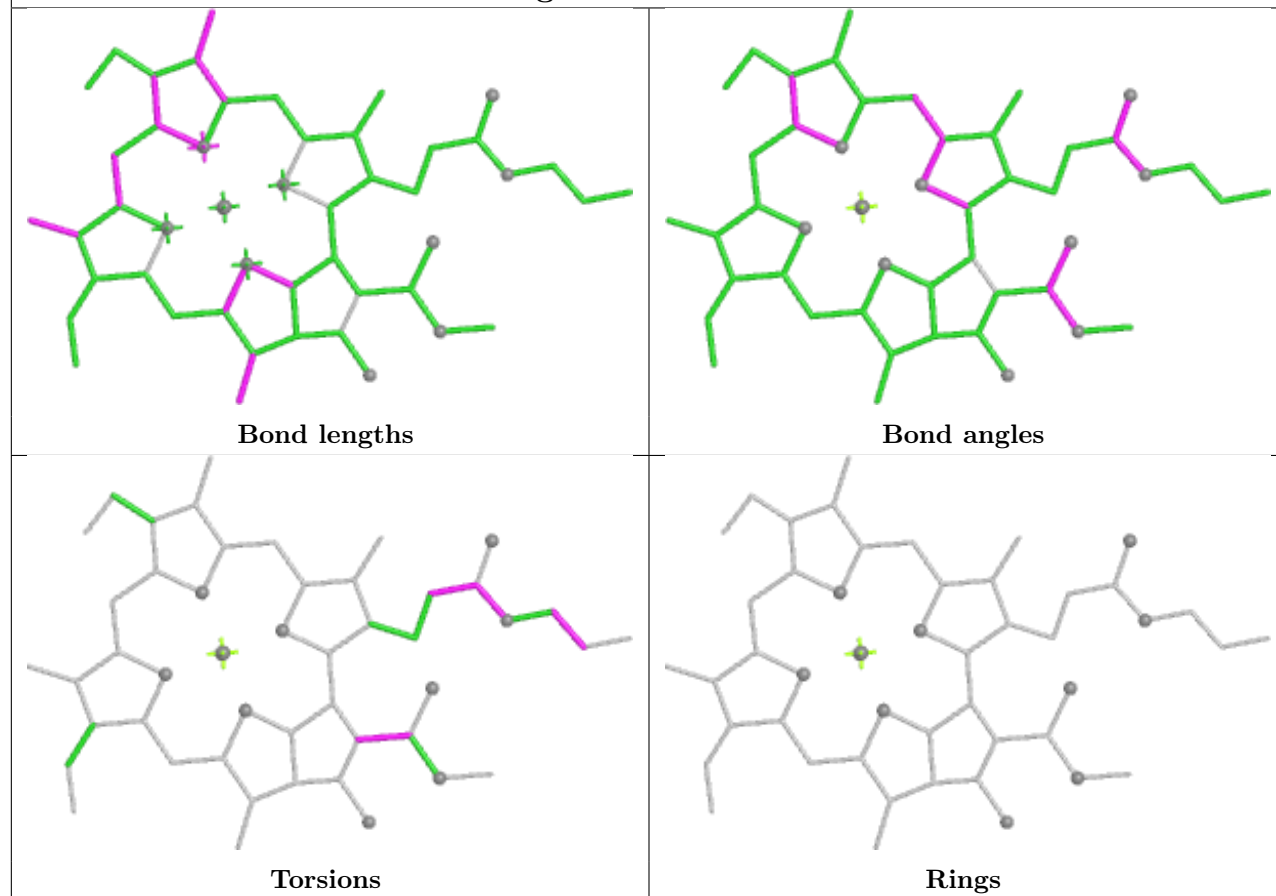




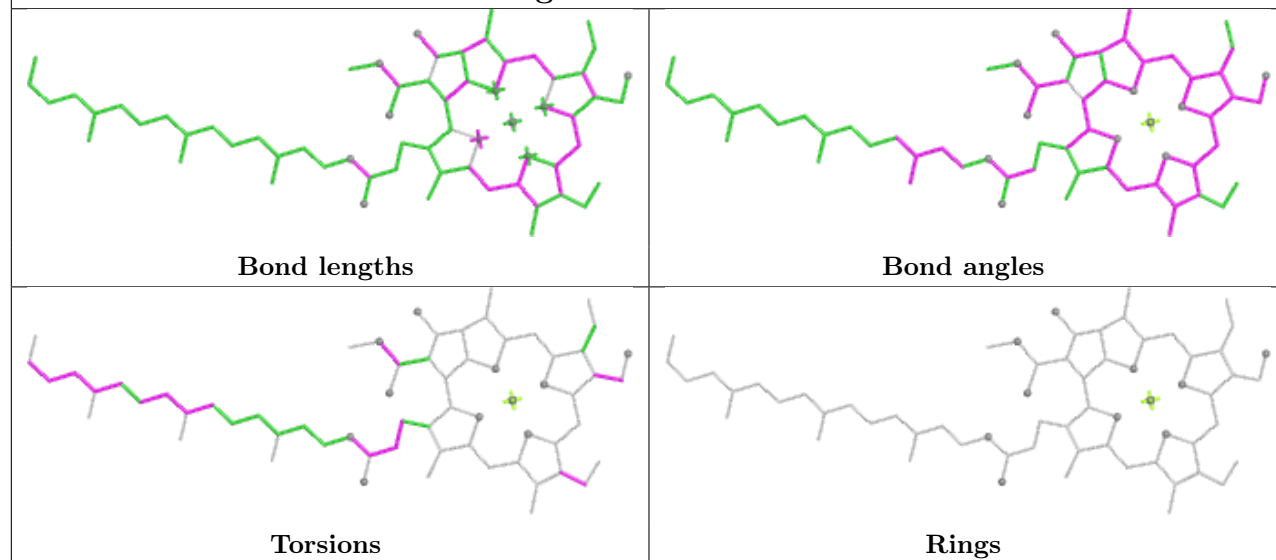
Ligand OUR 8 319**Ligand LHG 2 319**

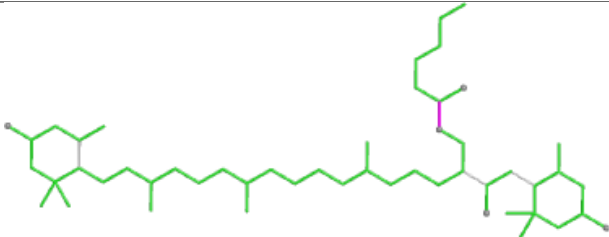
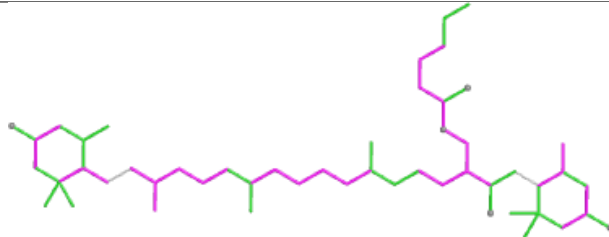
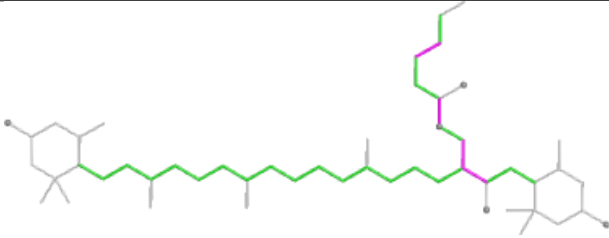
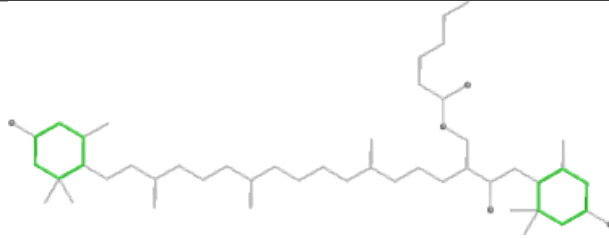


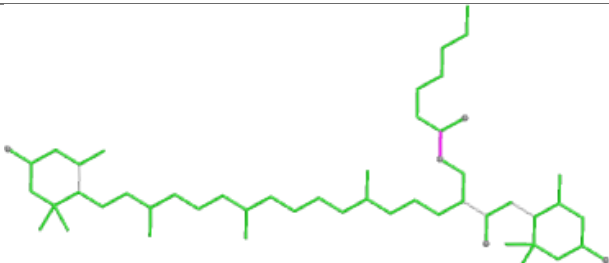
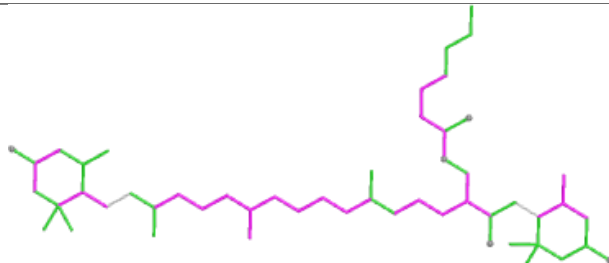
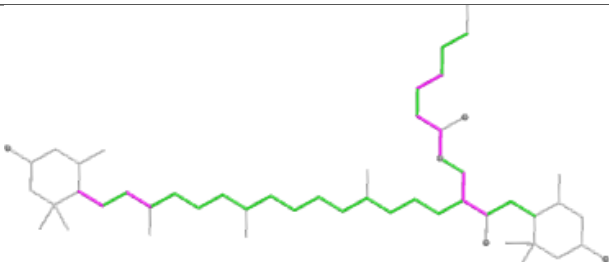
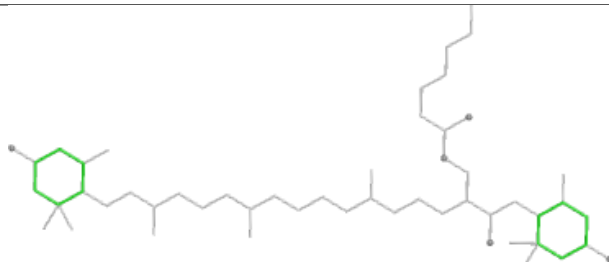
Ligand CLA 4 311

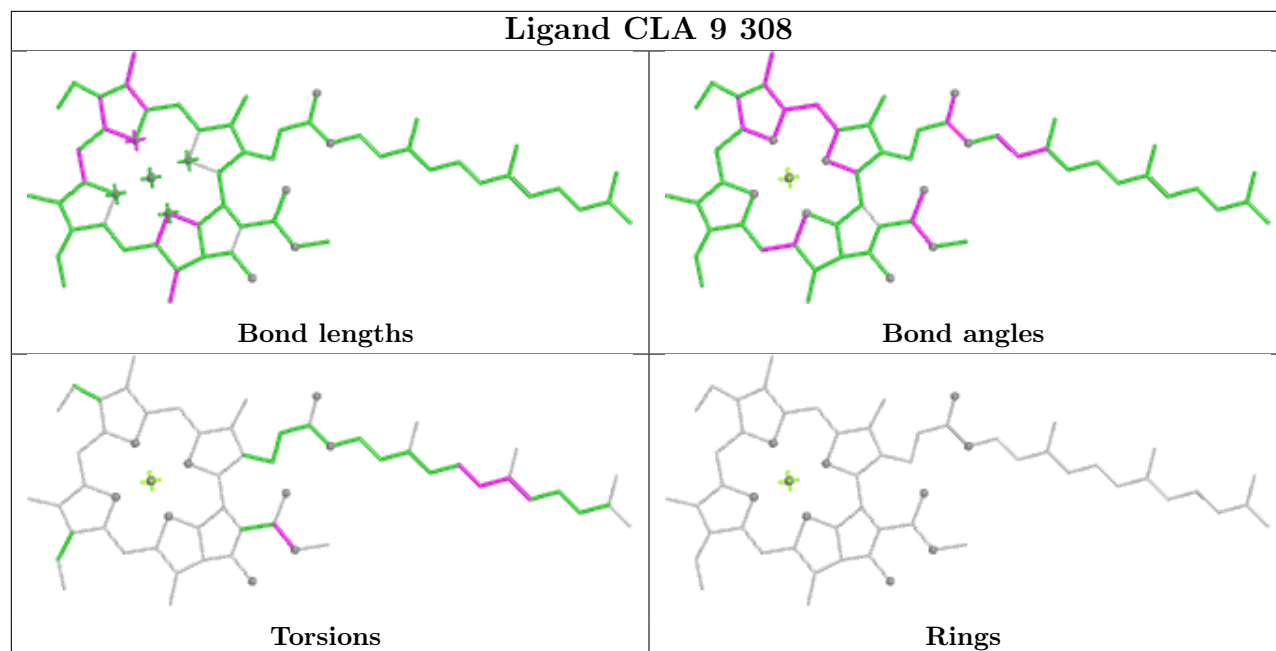
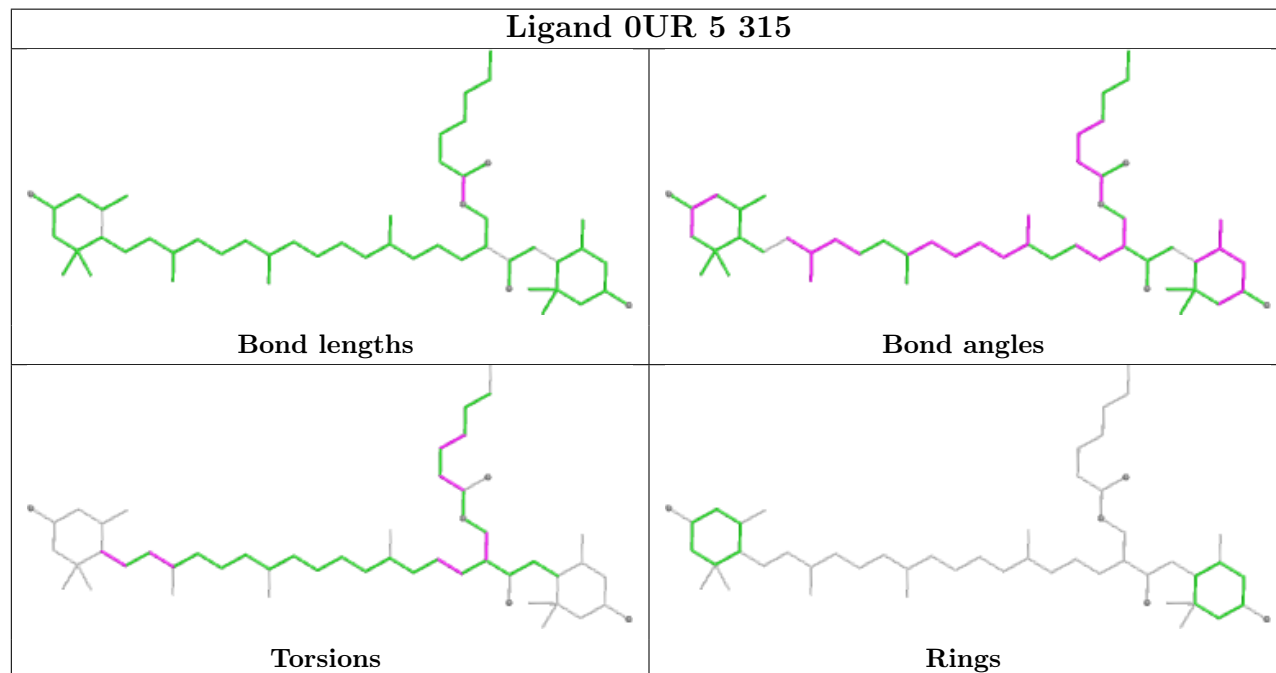


Ligand CHL 5 301

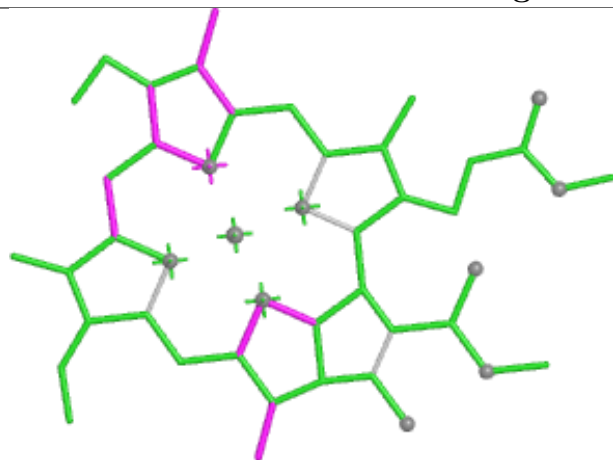


Ligand OUR 2 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

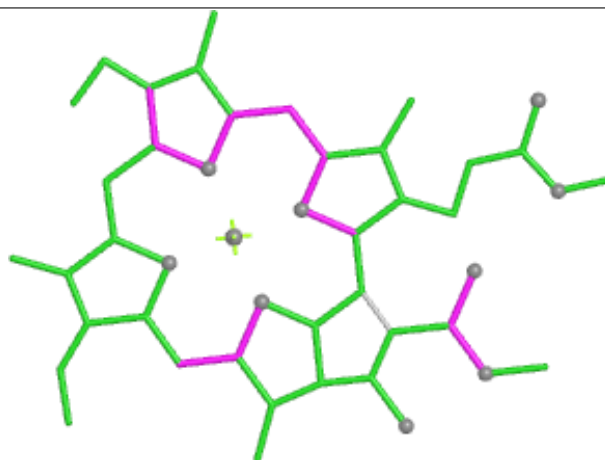
Ligand OUR 0 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 9 308**Ligand OUR 5 315**

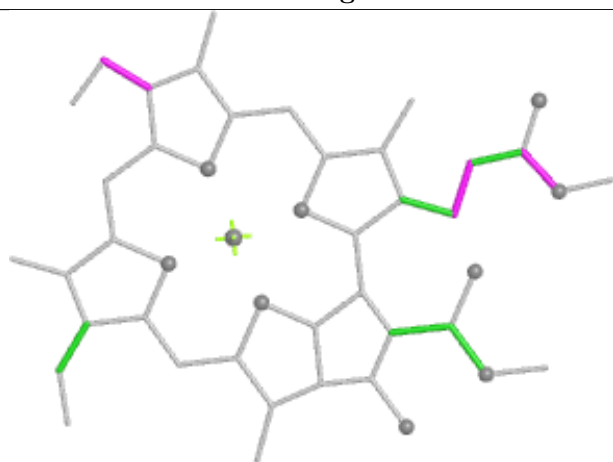
Ligand CLA G 103



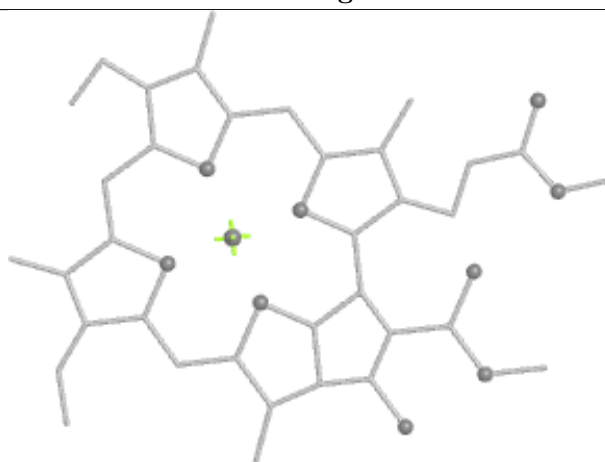
Bond lengths



Bond angles

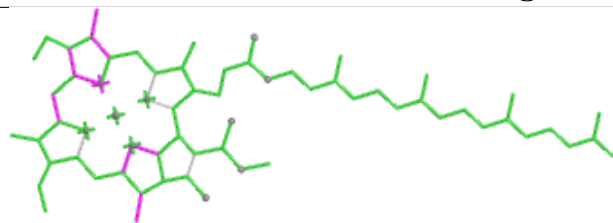


Torsions

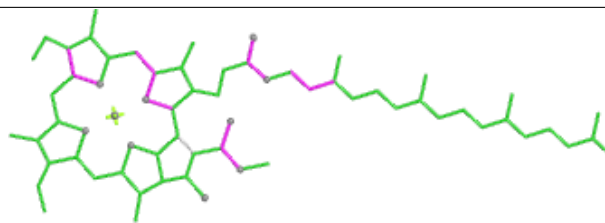


Rings

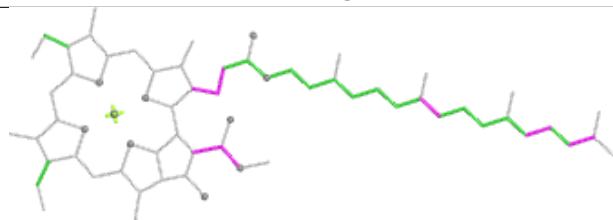
Ligand CLA 8 305



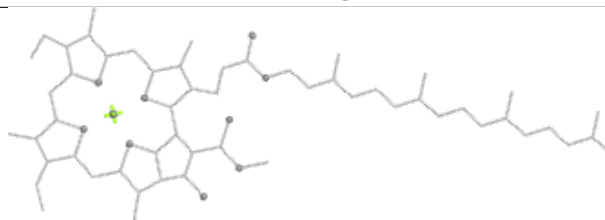
Bond lengths



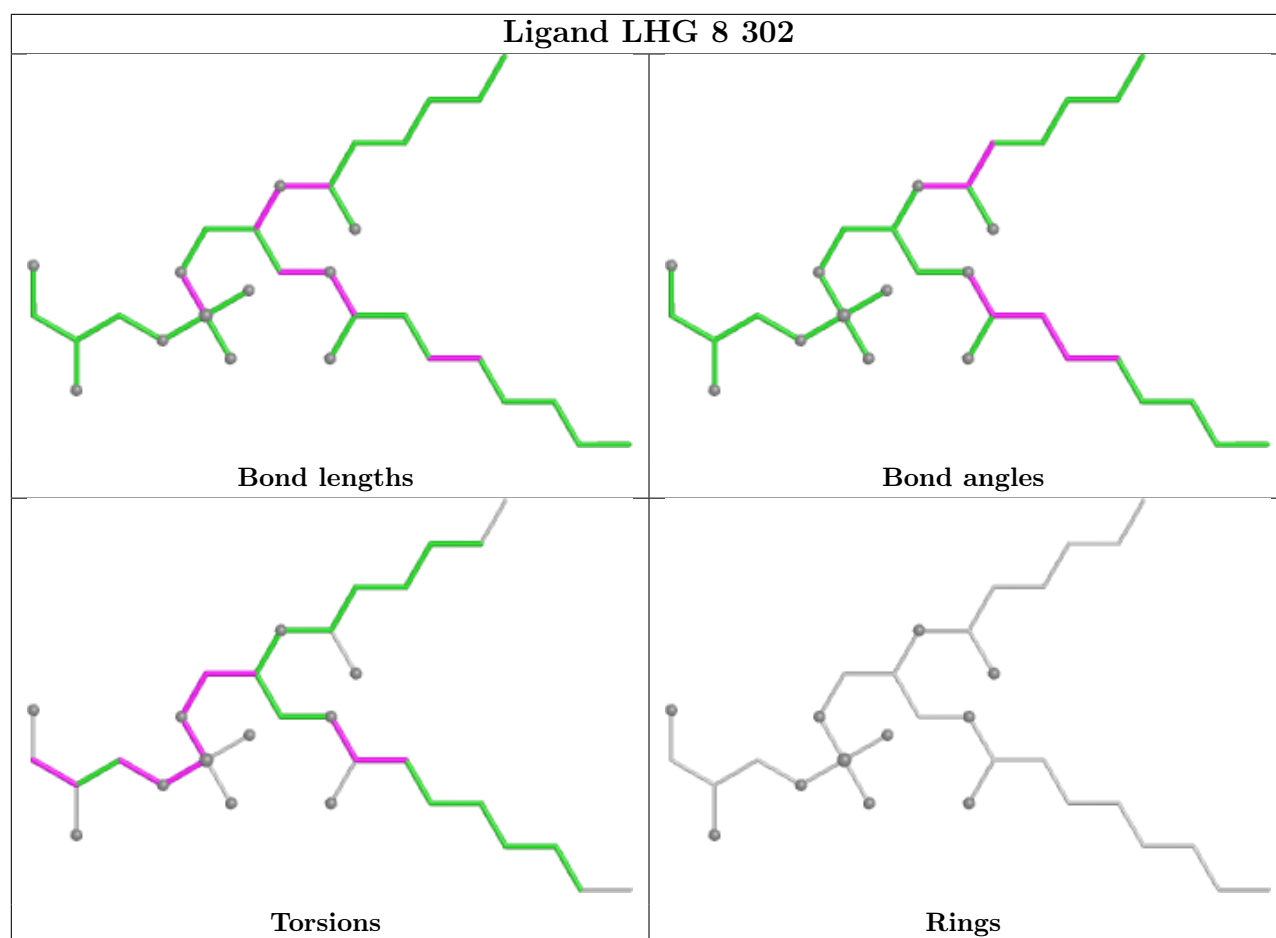
Bond angles



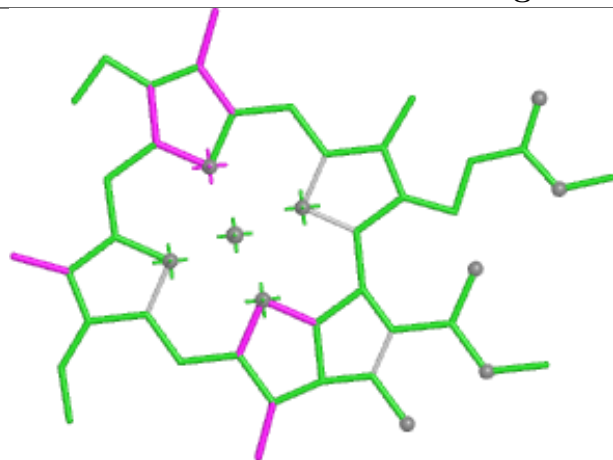
Torsions



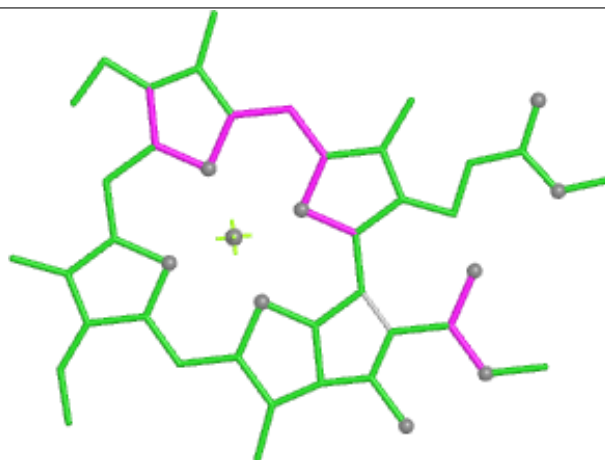
Rings



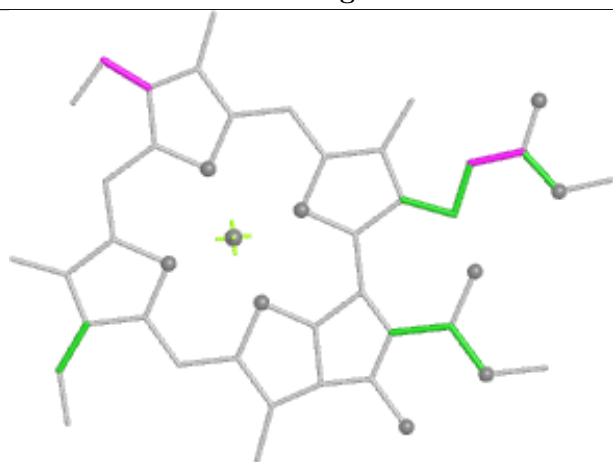
Ligand CLA A 833



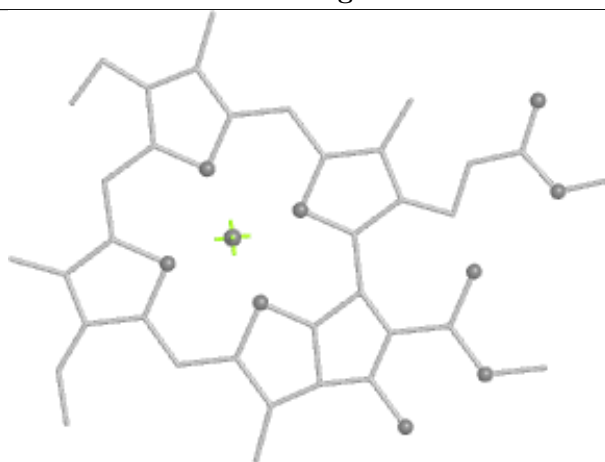
Bond lengths



Bond angles

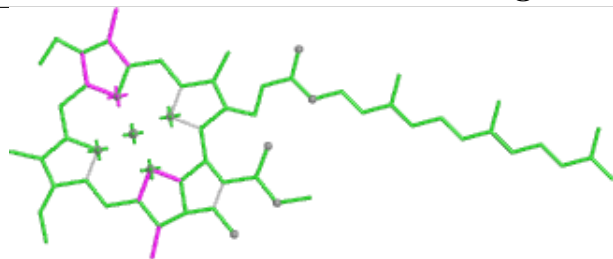


Torsions

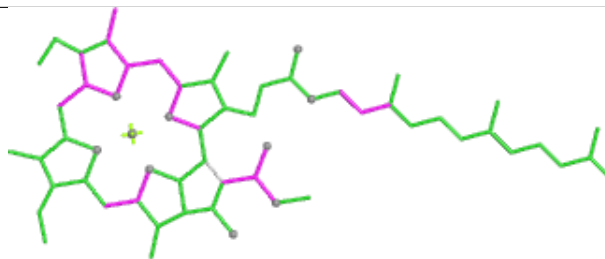


Rings

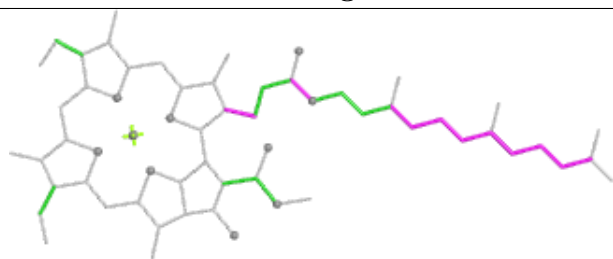
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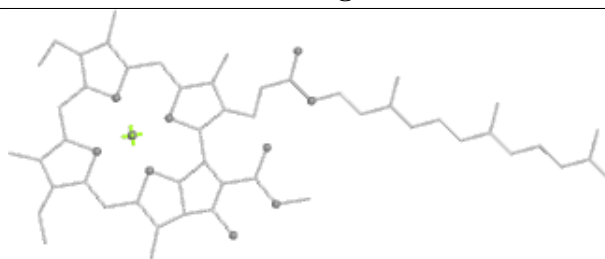
Bond lengths



Bond angles

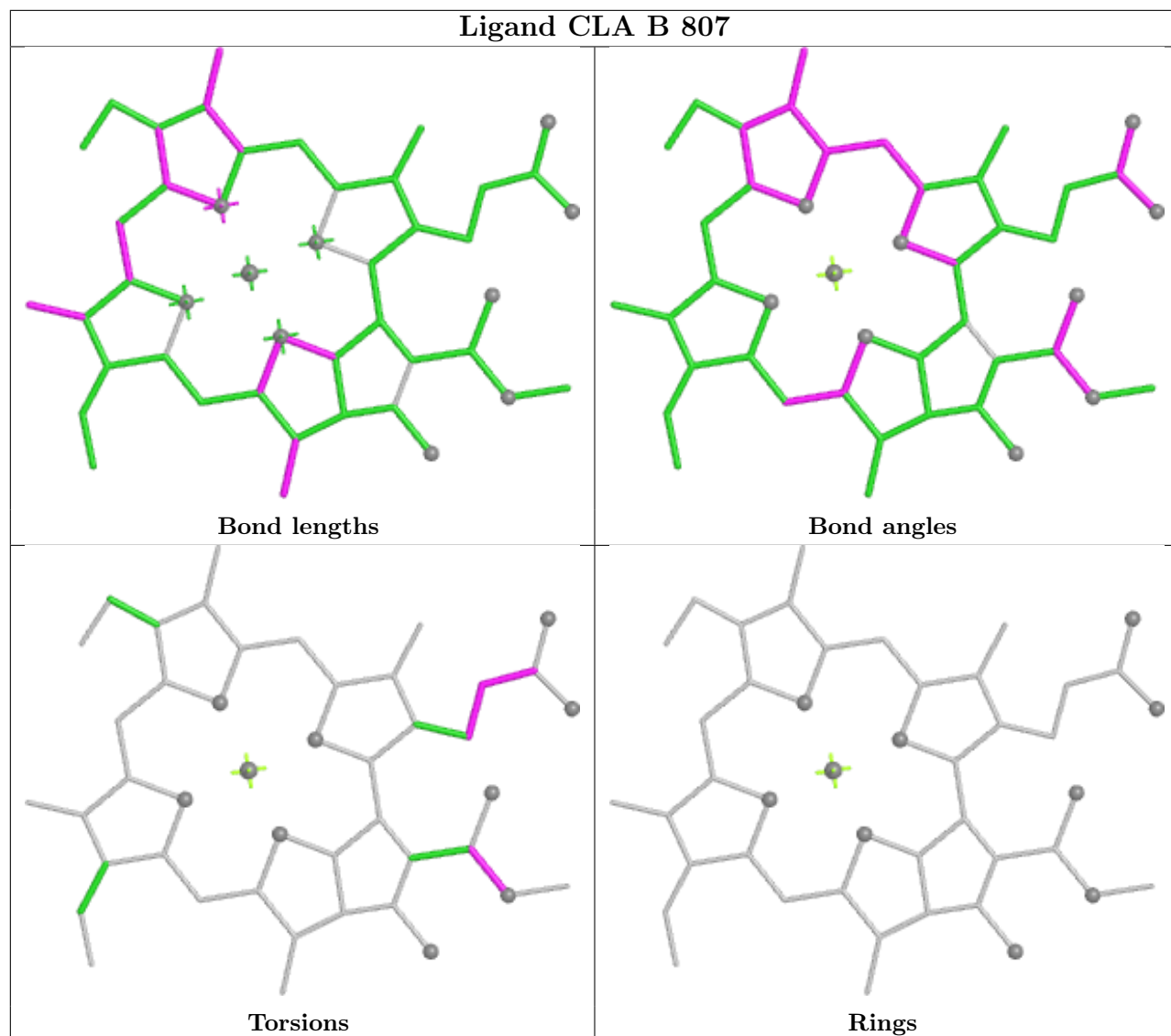


Torsions

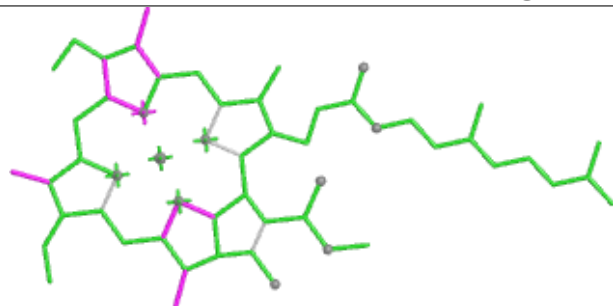


Rings

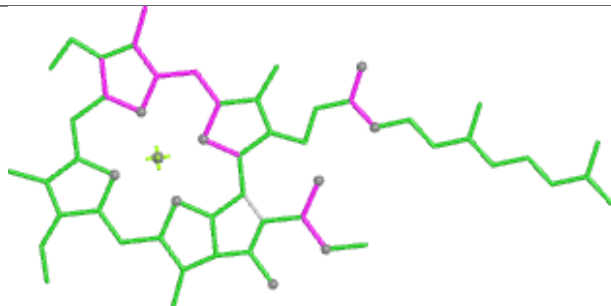
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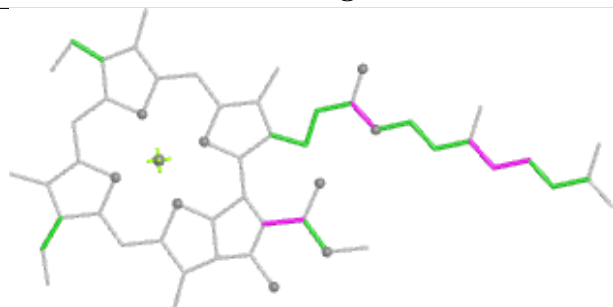
Ligand CLA 7 304



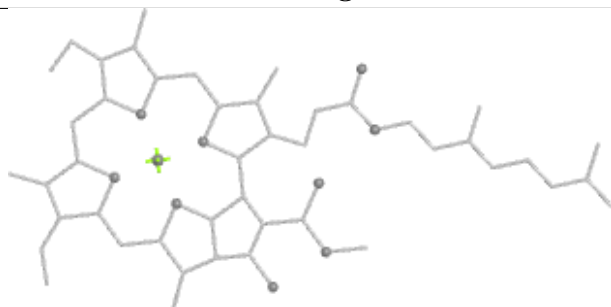
Bond lengths



Bond angles

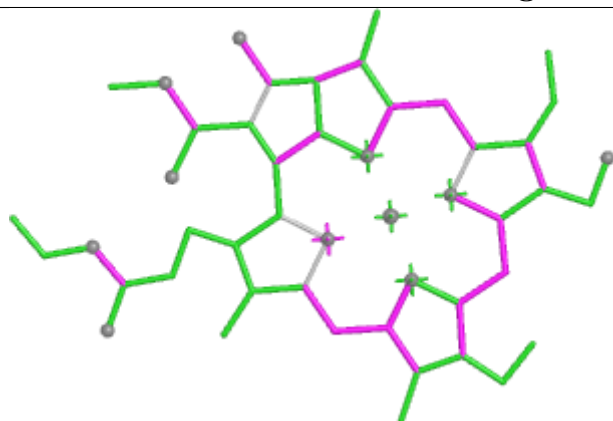


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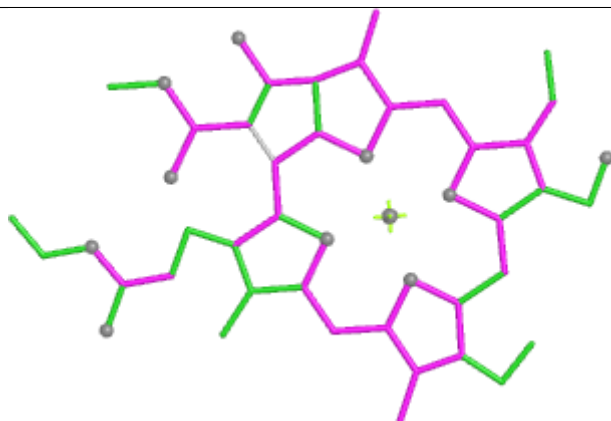


Rings

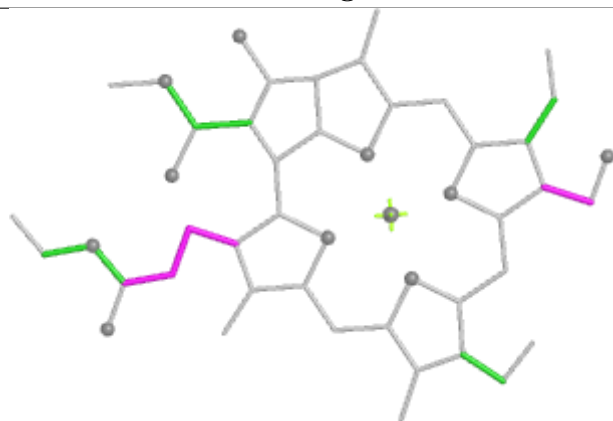
Ligand CHL 9 306



Bond lengths



Bond angles

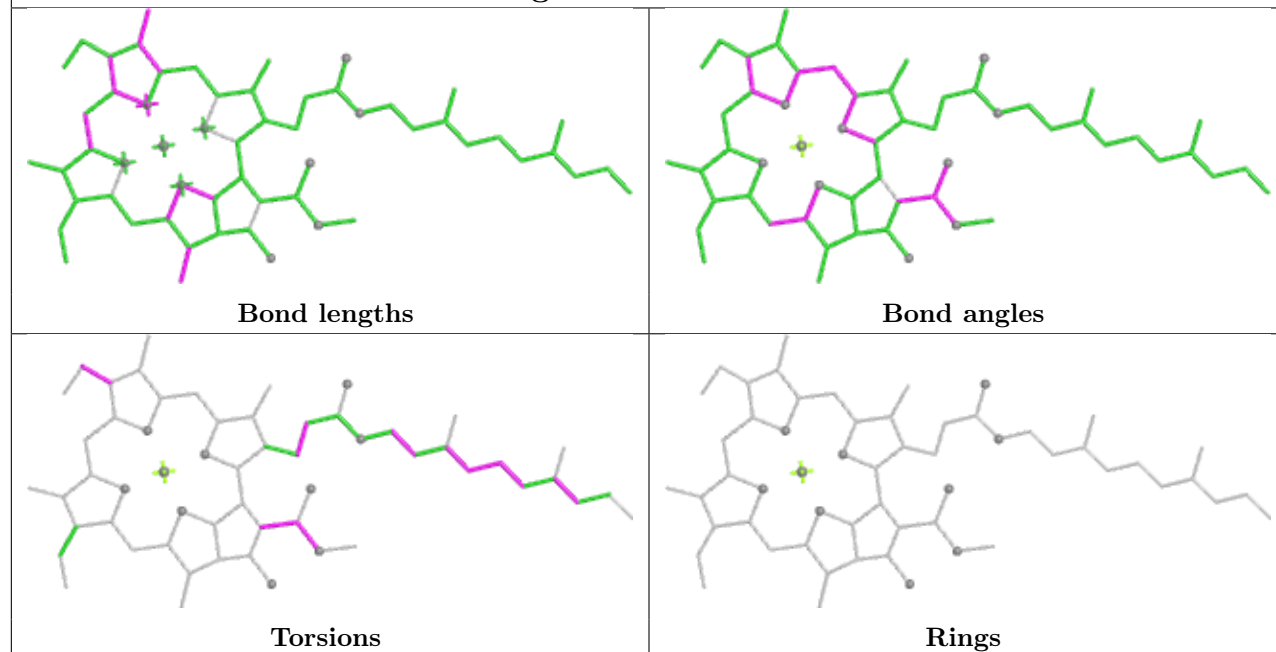


Torsions

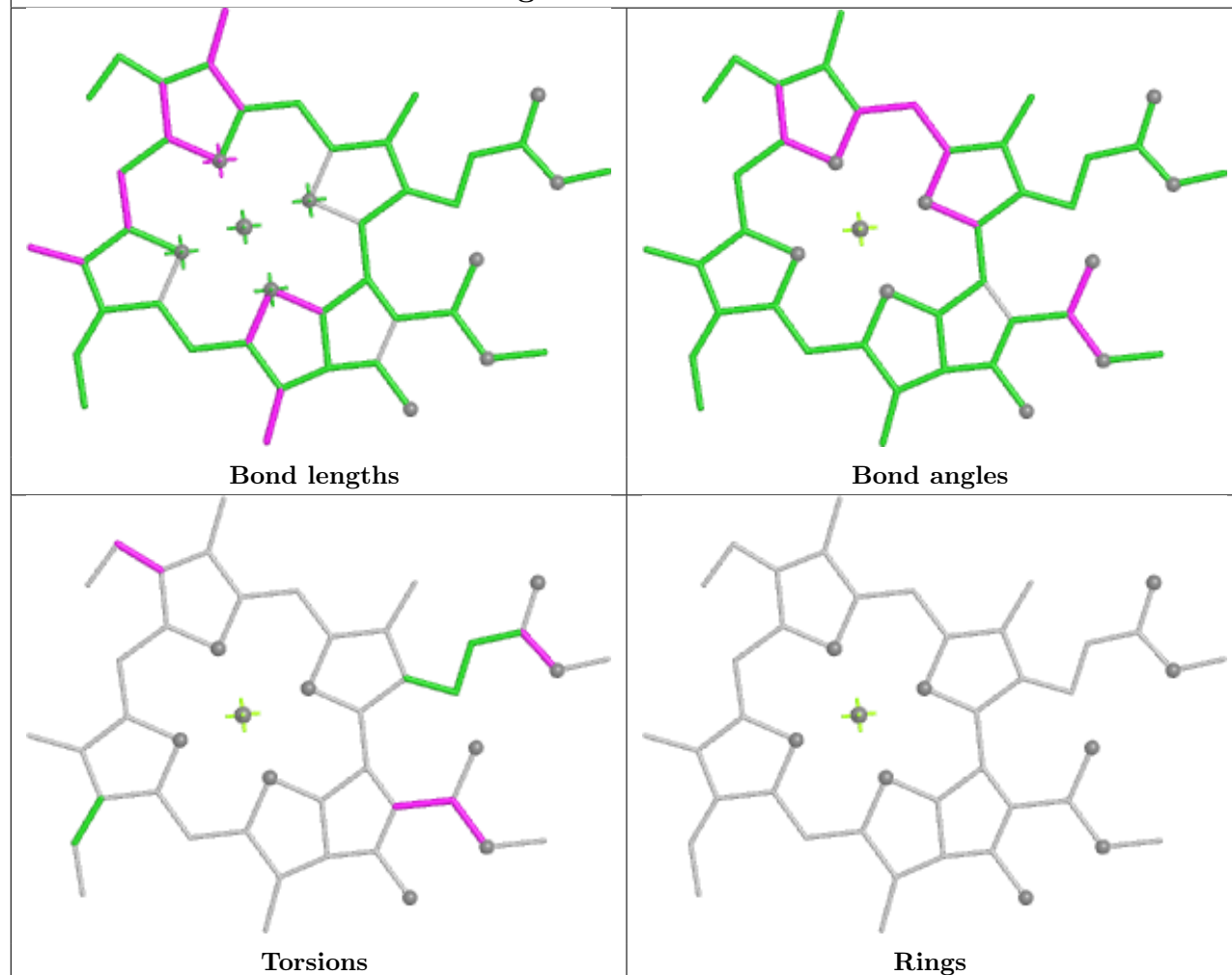


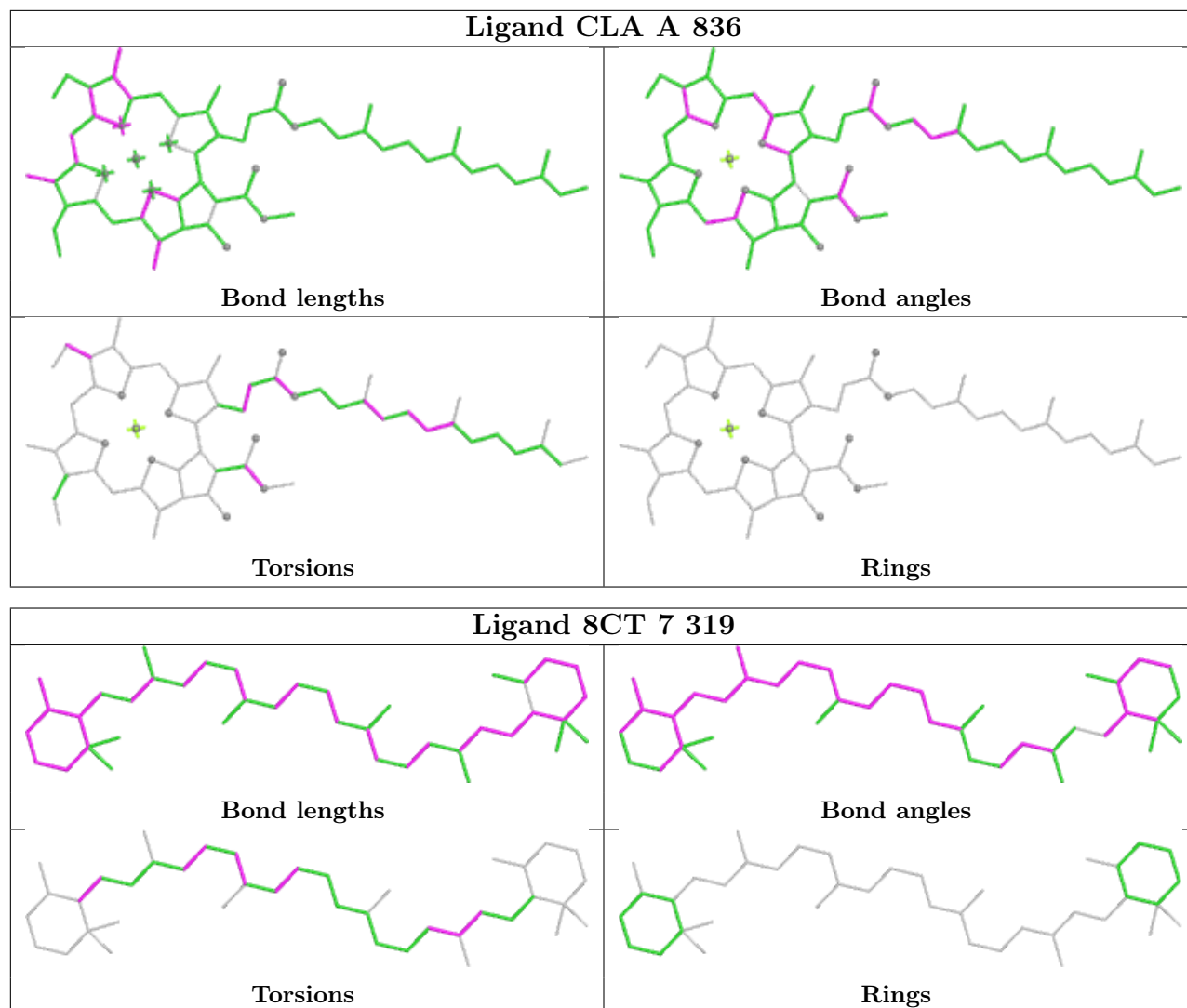
Rings

Ligand CLA A 834

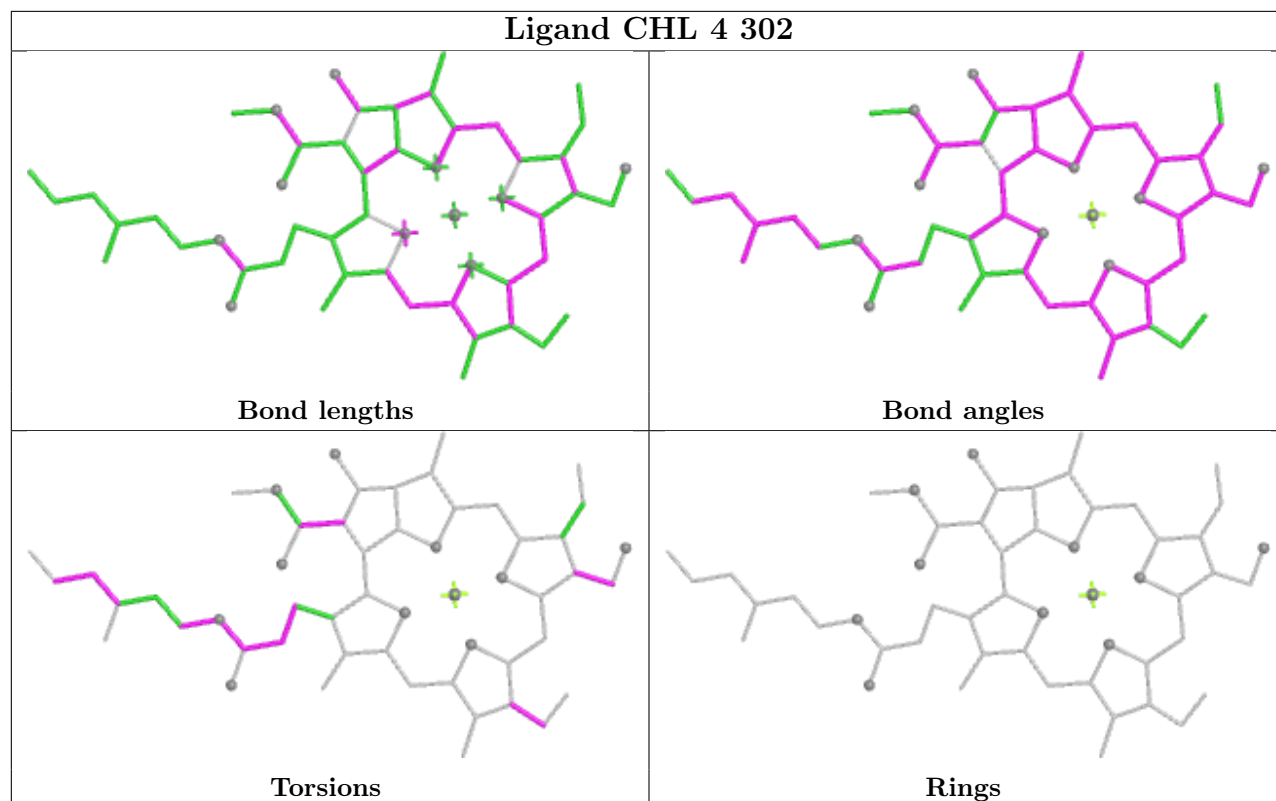


Ligand CLA 8 304

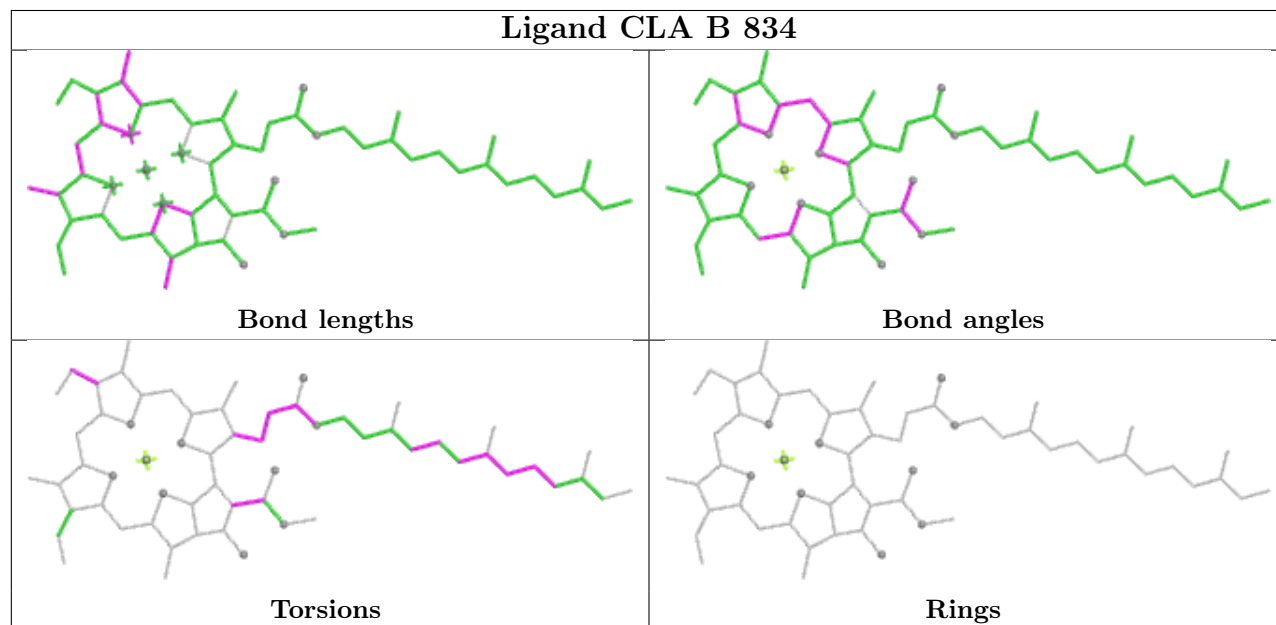


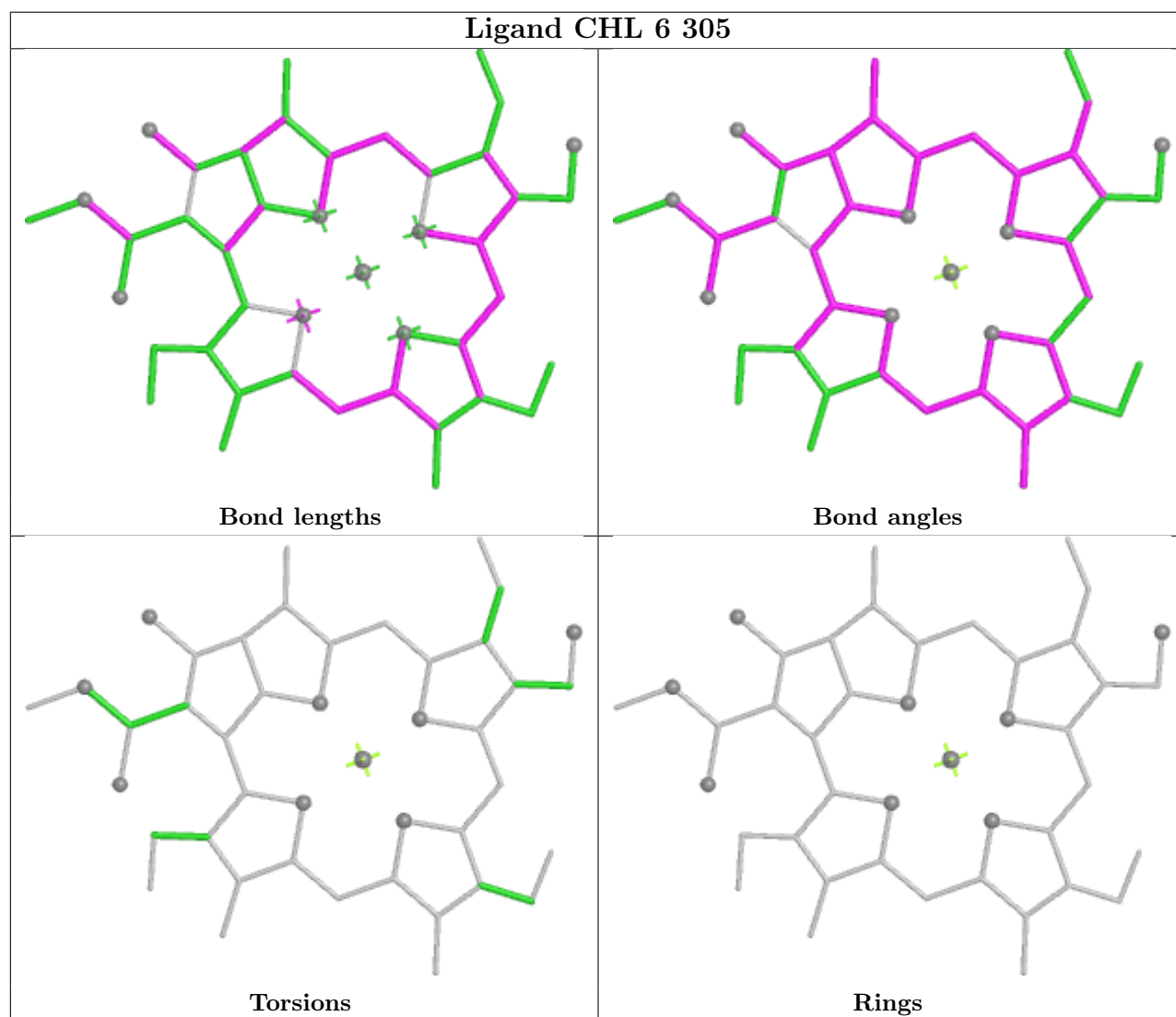
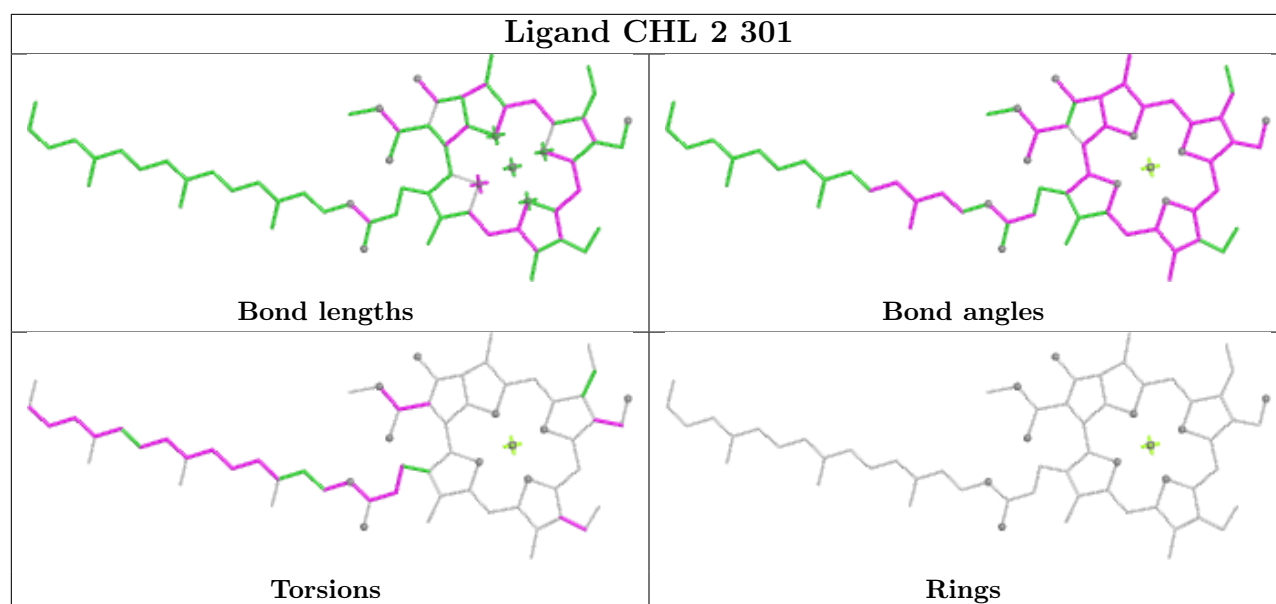


Ligand CHL 4 302

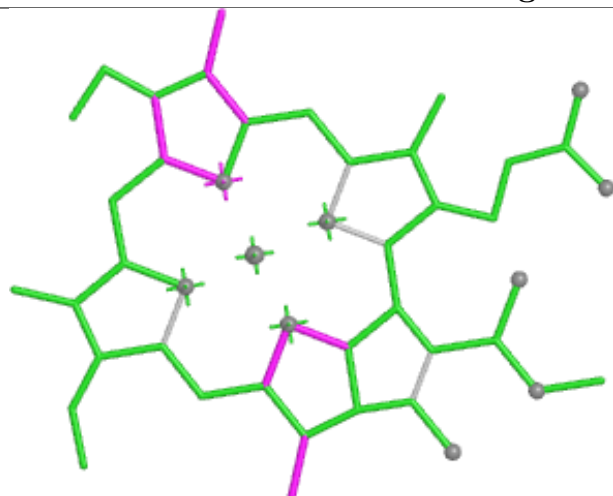


Ligand CLA B 834

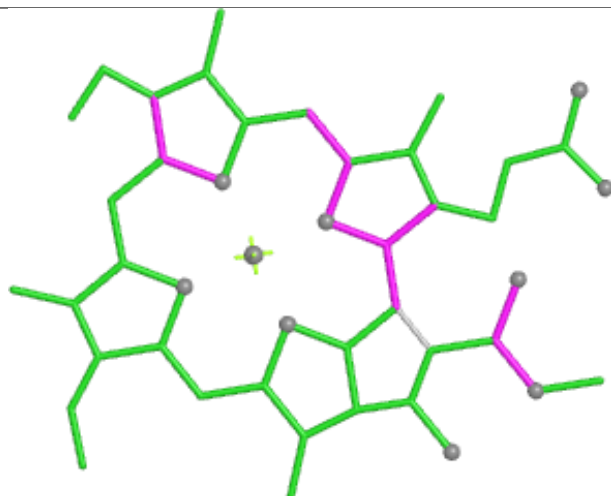




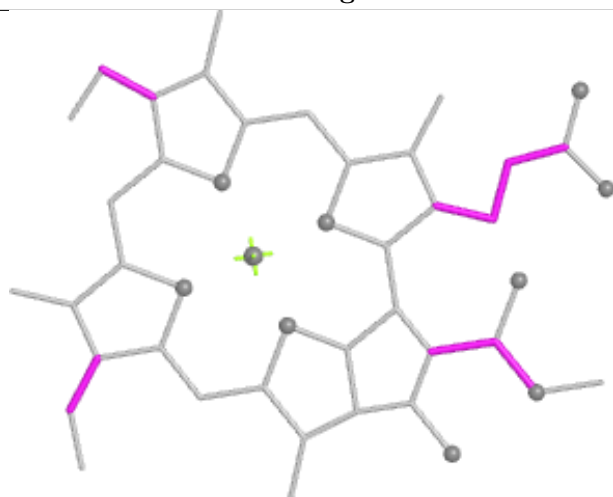
Ligand CLA 7 316



Bond lengths



Bond angles

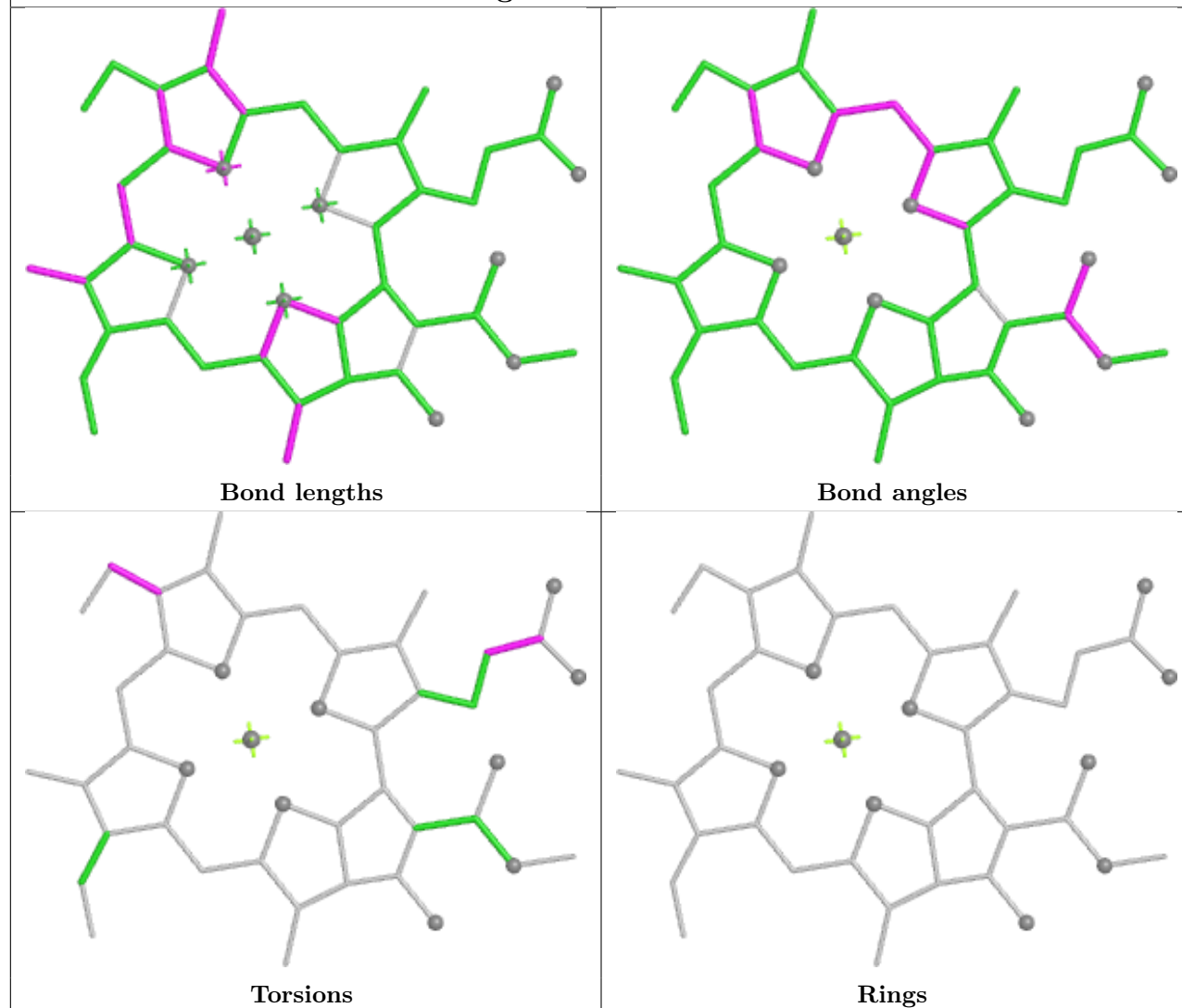


Torsions

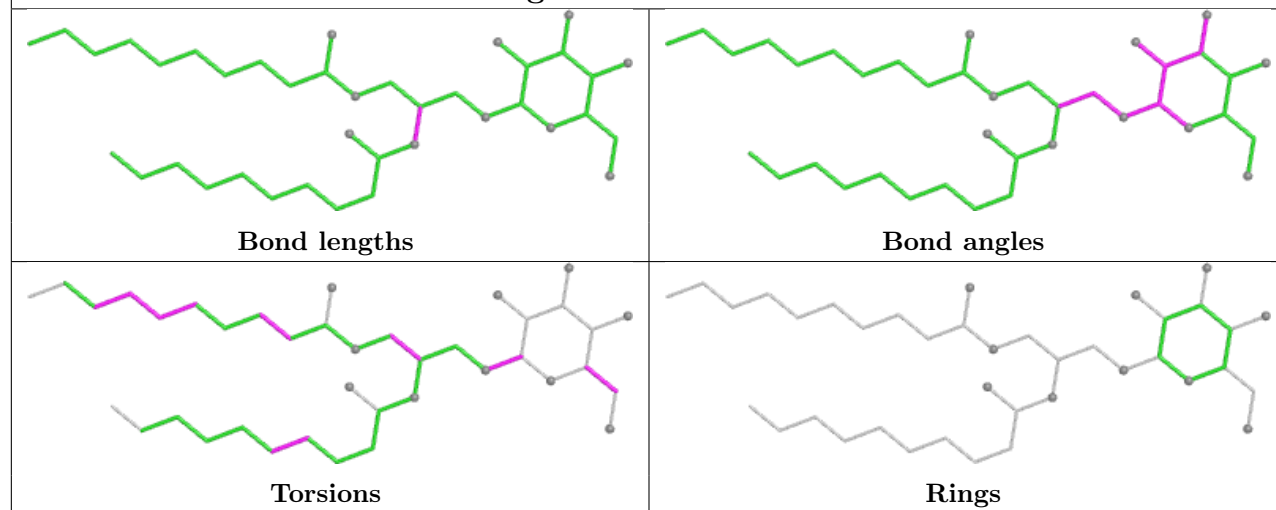


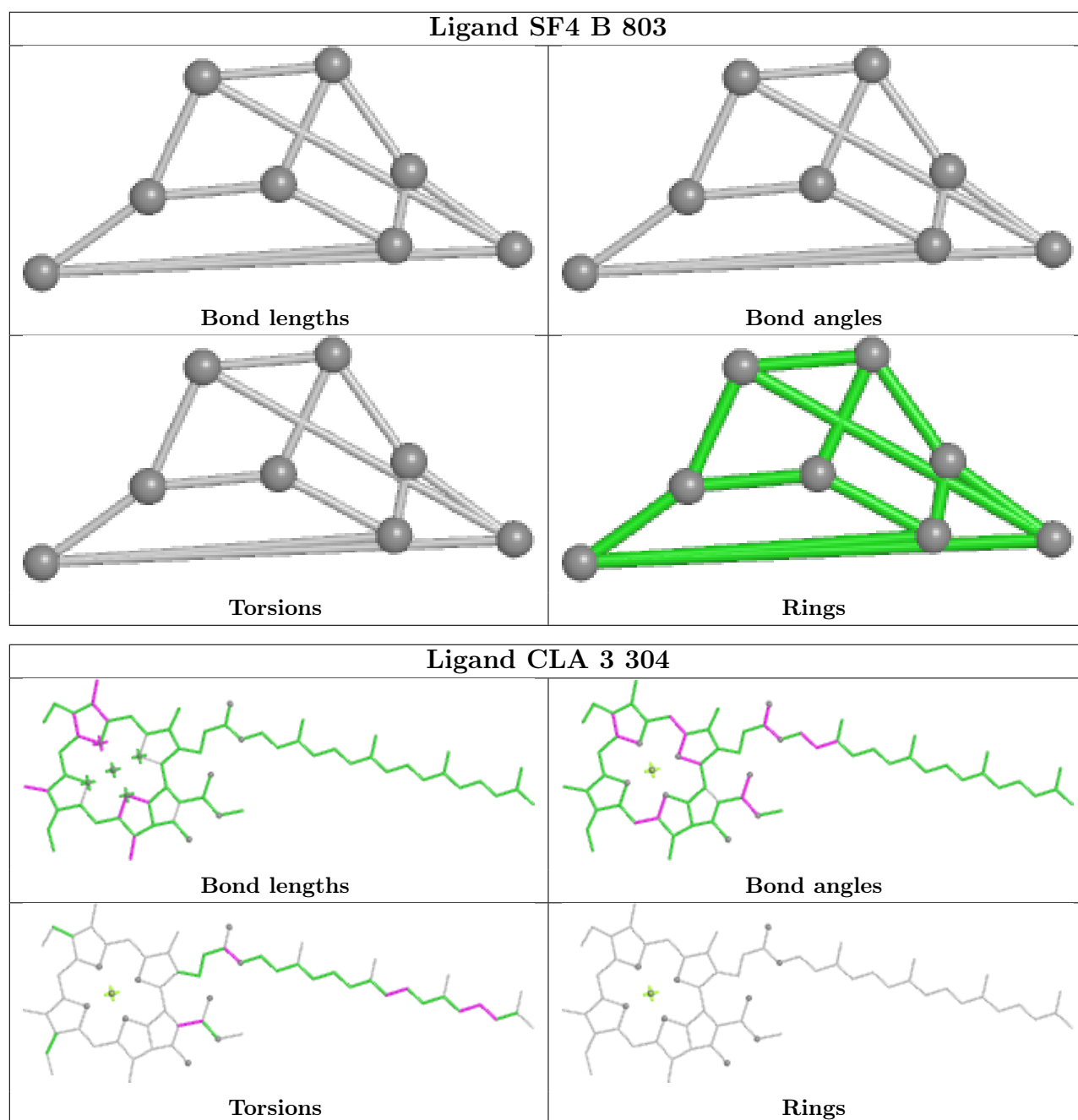
Rings

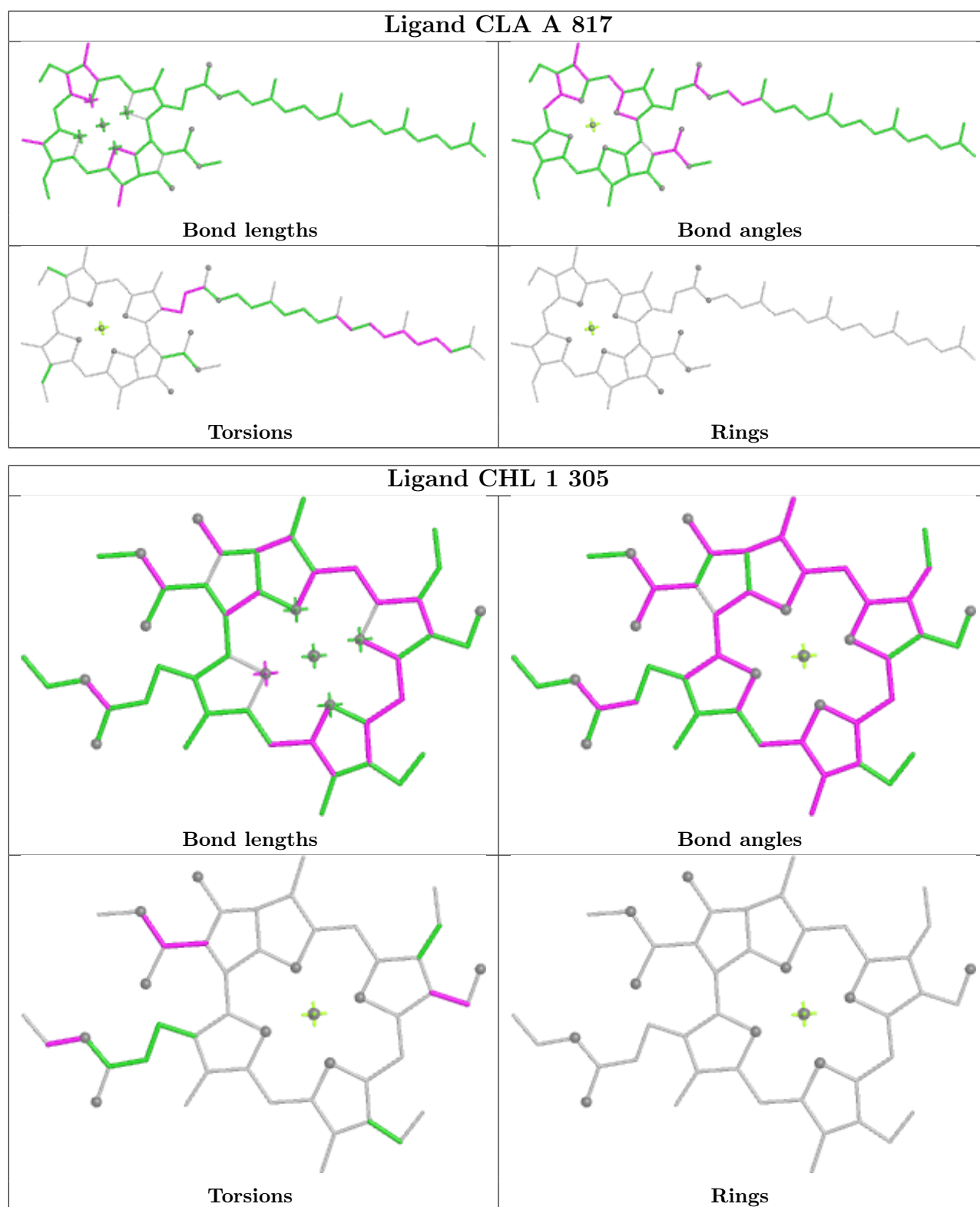
Ligand CLA 4 303



Ligand LMG O 210







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

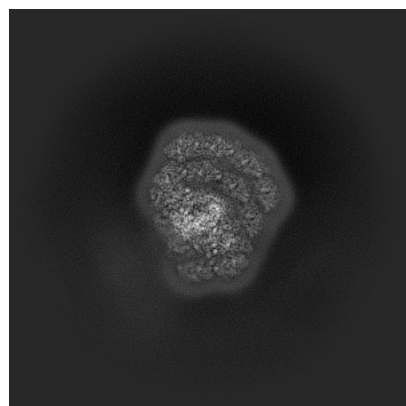
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61973. These allow visual inspection of the internal detail of the map and identification of artifacts.

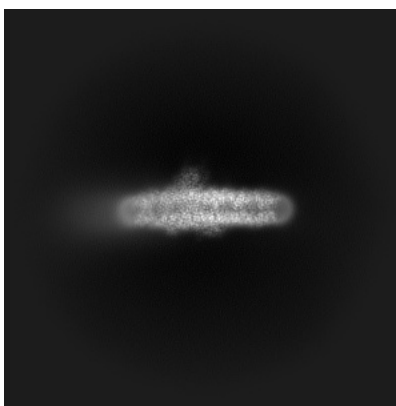
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

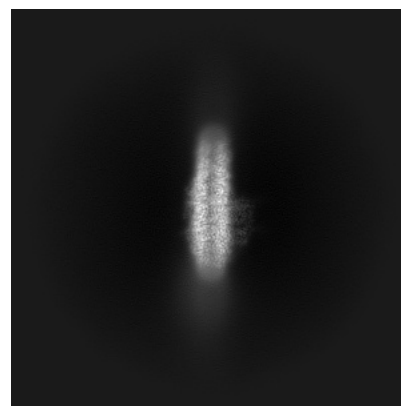
6.1.1 Primary map



X

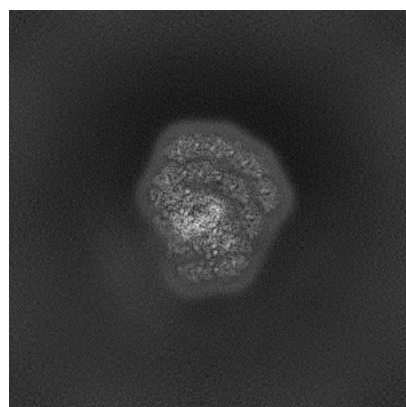


Y

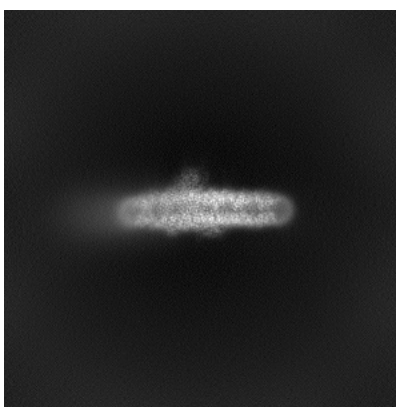


Z

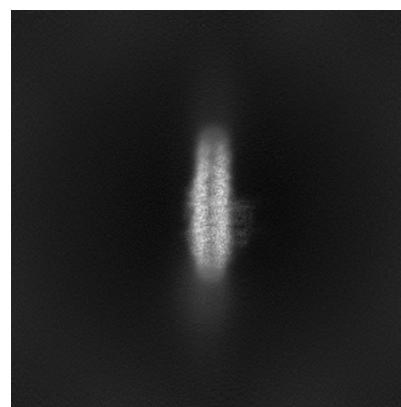
6.1.2 Raw map



X



Y

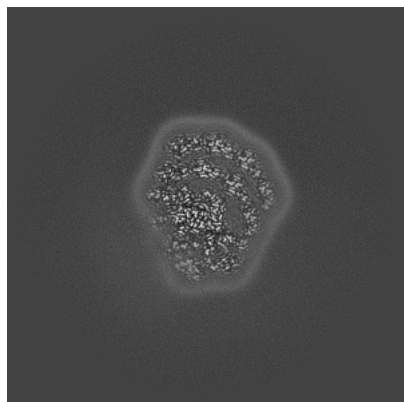


Z

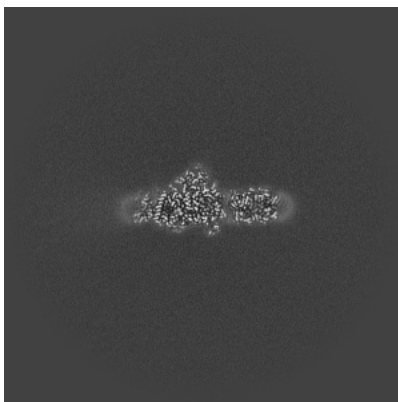
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

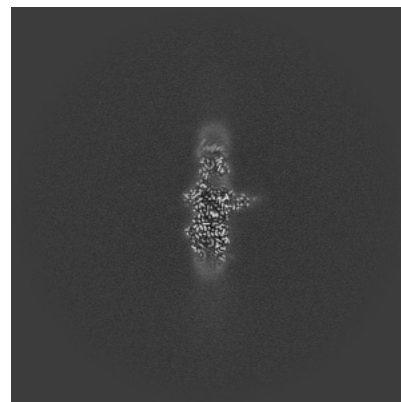
6.2.1 Primary map



X Index: 256

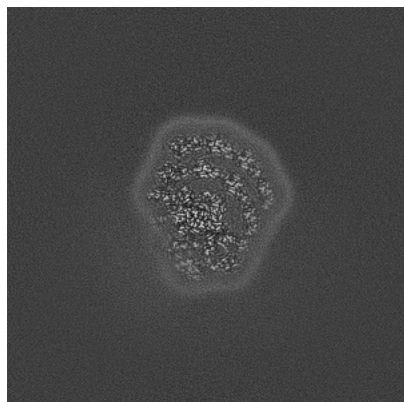


Y Index: 256

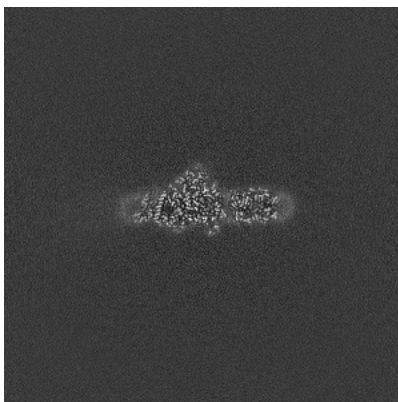


Z Index: 256

6.2.2 Raw map



X Index: 256



Y Index: 256

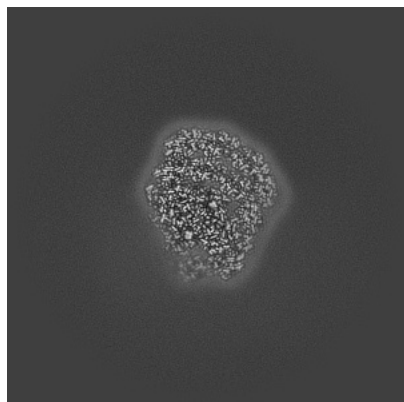


Z Index: 256

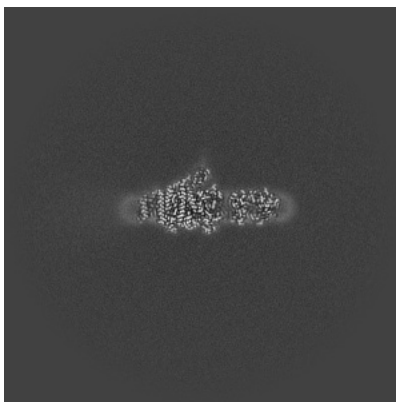
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

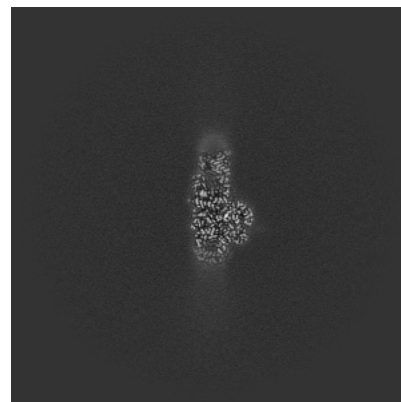
6.3.1 Primary map



X Index: 268

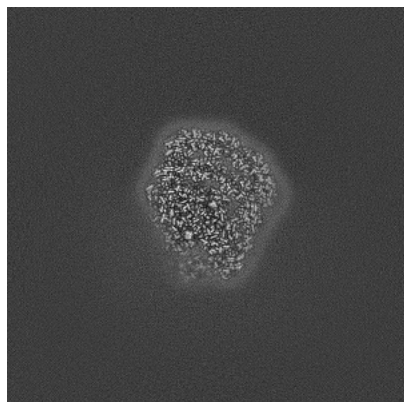


Y Index: 263

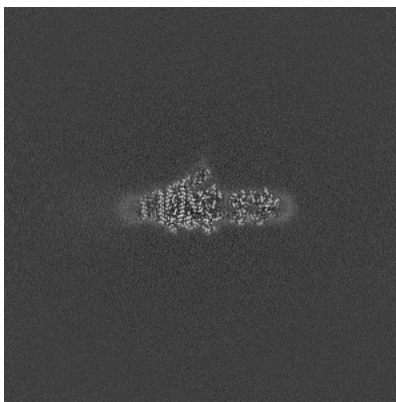


Z Index: 238

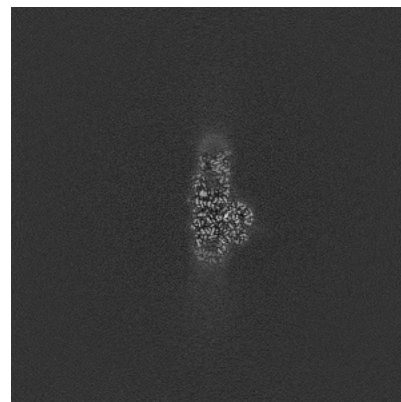
6.3.2 Raw map



X Index: 268



Y Index: 263

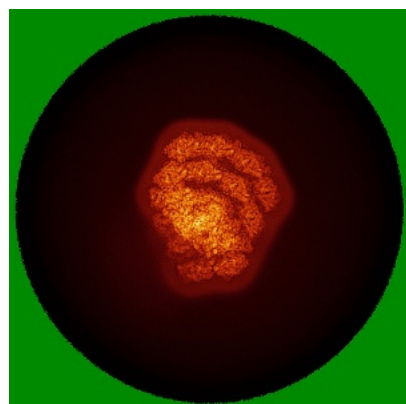


Z Index: 238

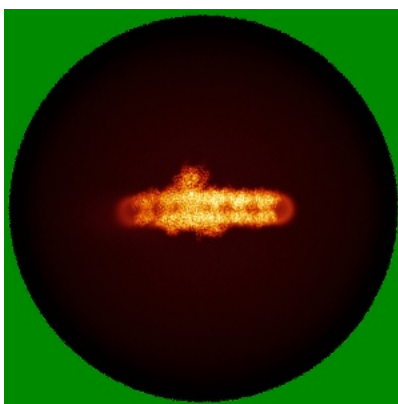
The images above show the largest variance slices of the map in three orthogonal directions.

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

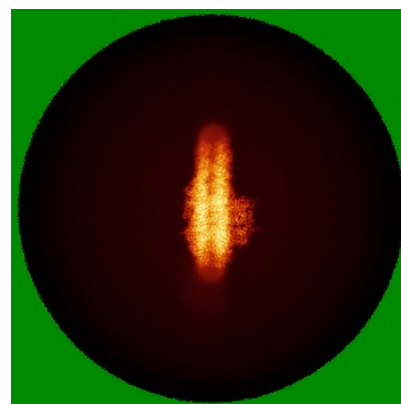
6.4.1 Primary map



X

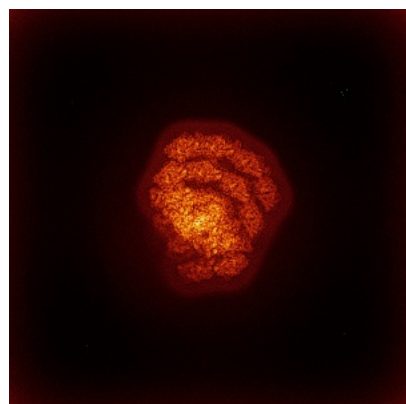


Y

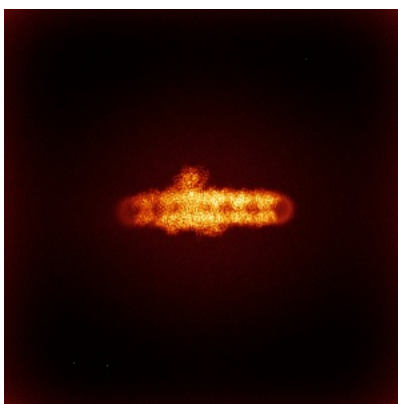


Z

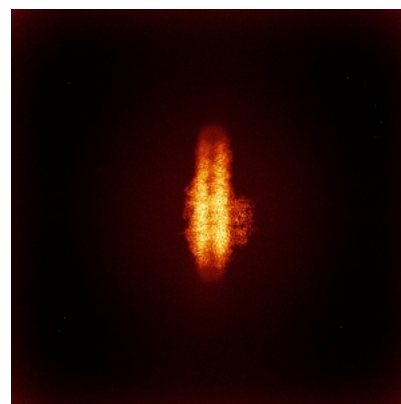
6.4.2 Raw map



X



Y

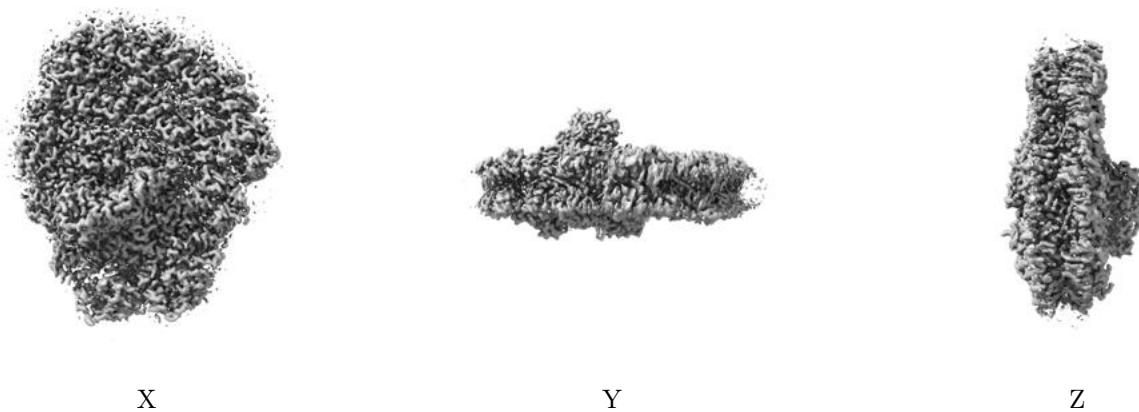


Z

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

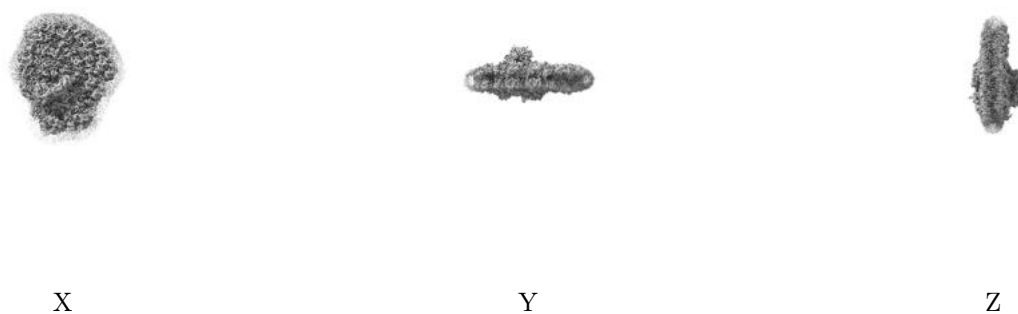
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

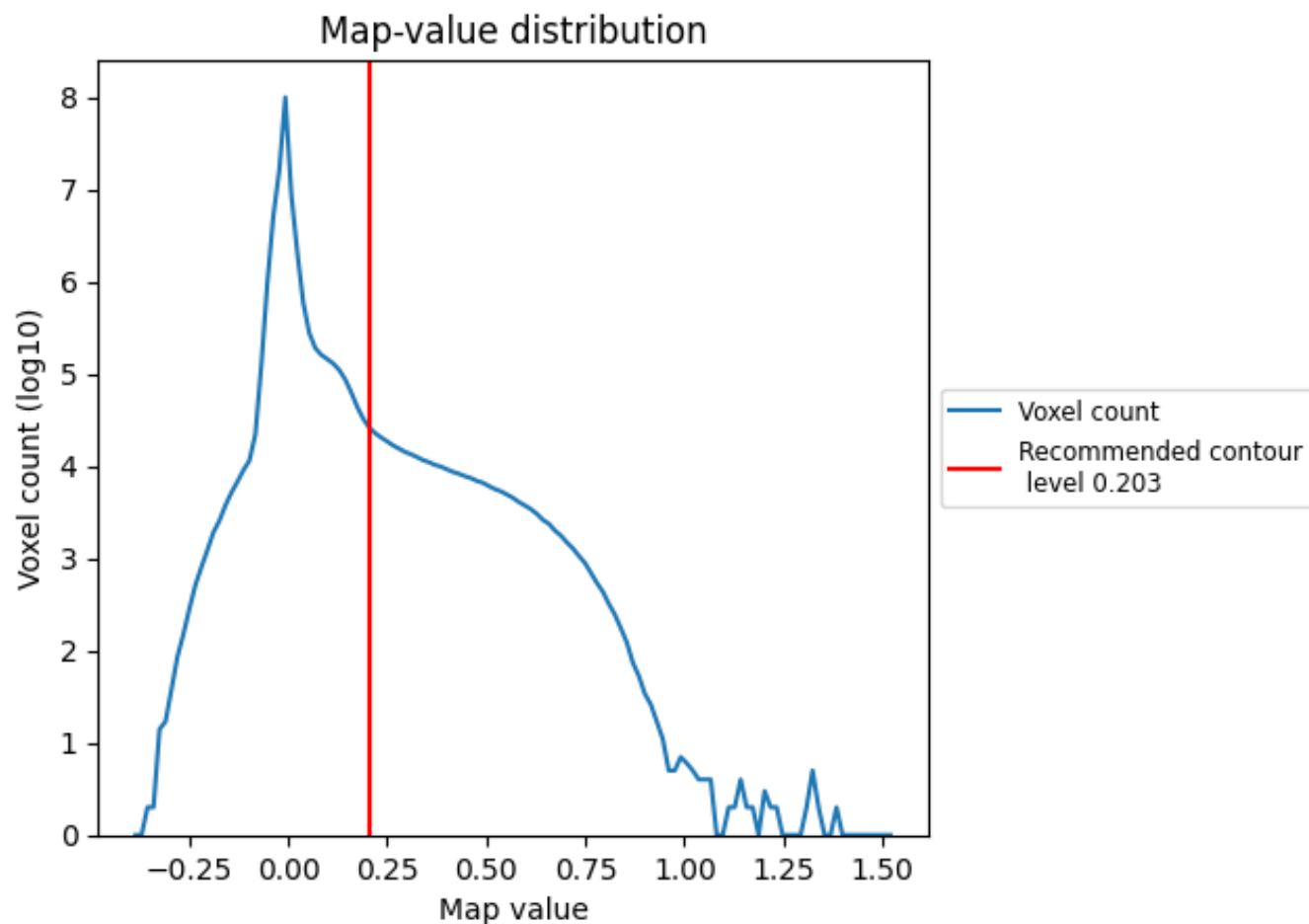
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

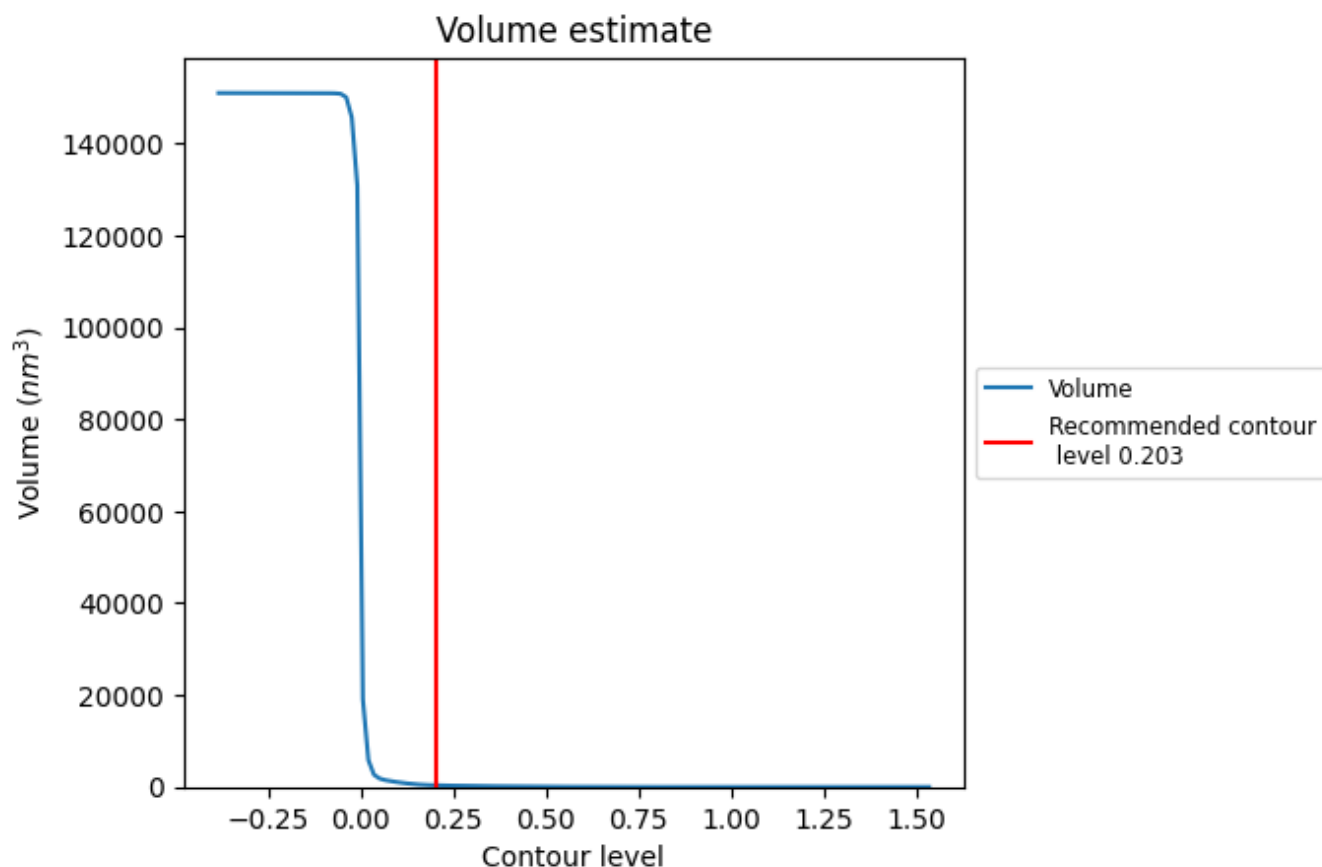
This section contains the results of statistical analysis of the map.

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.

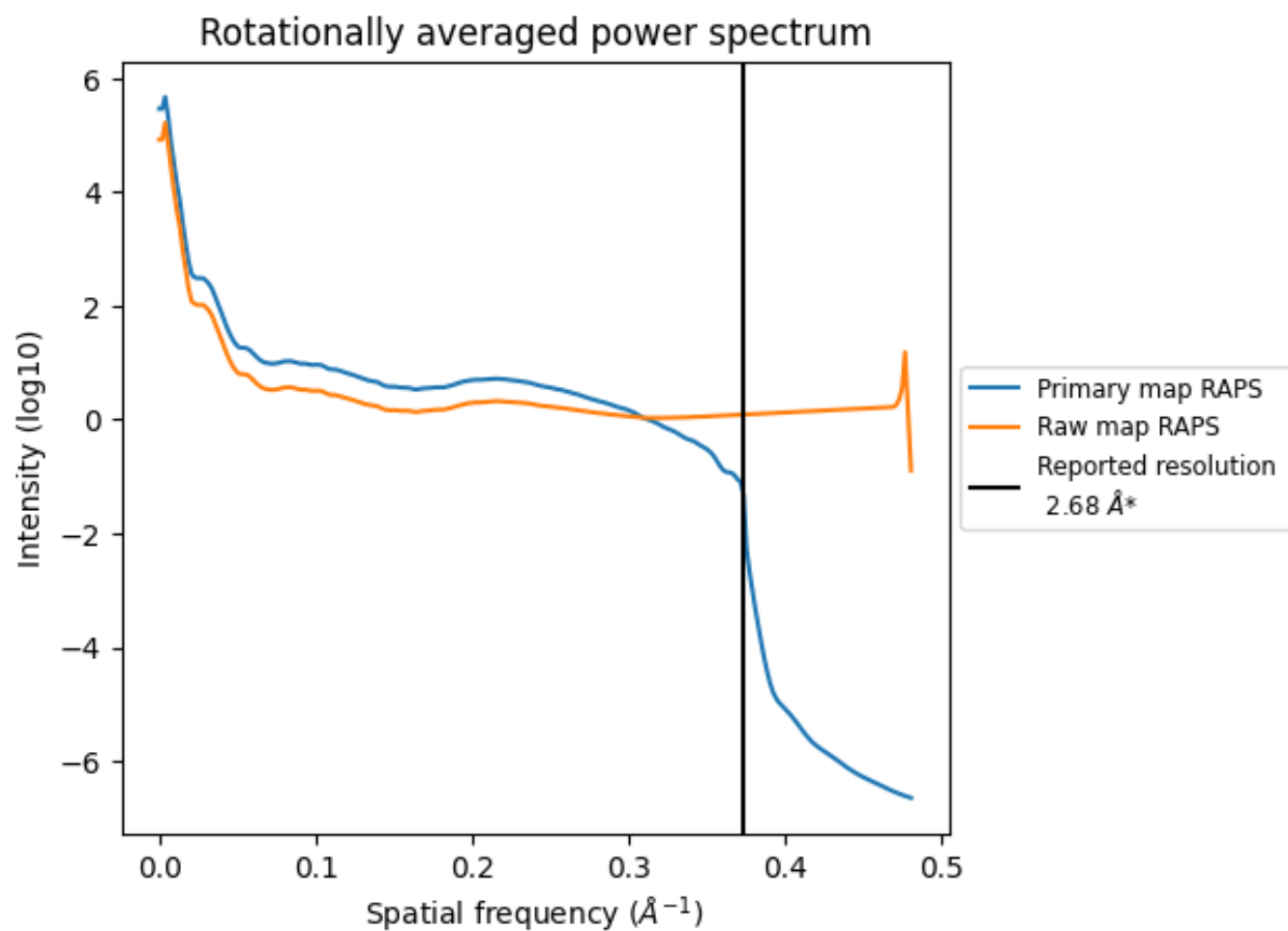
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 356 nm^3 ; this corresponds to an approximate mass of 322 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 ⓘ

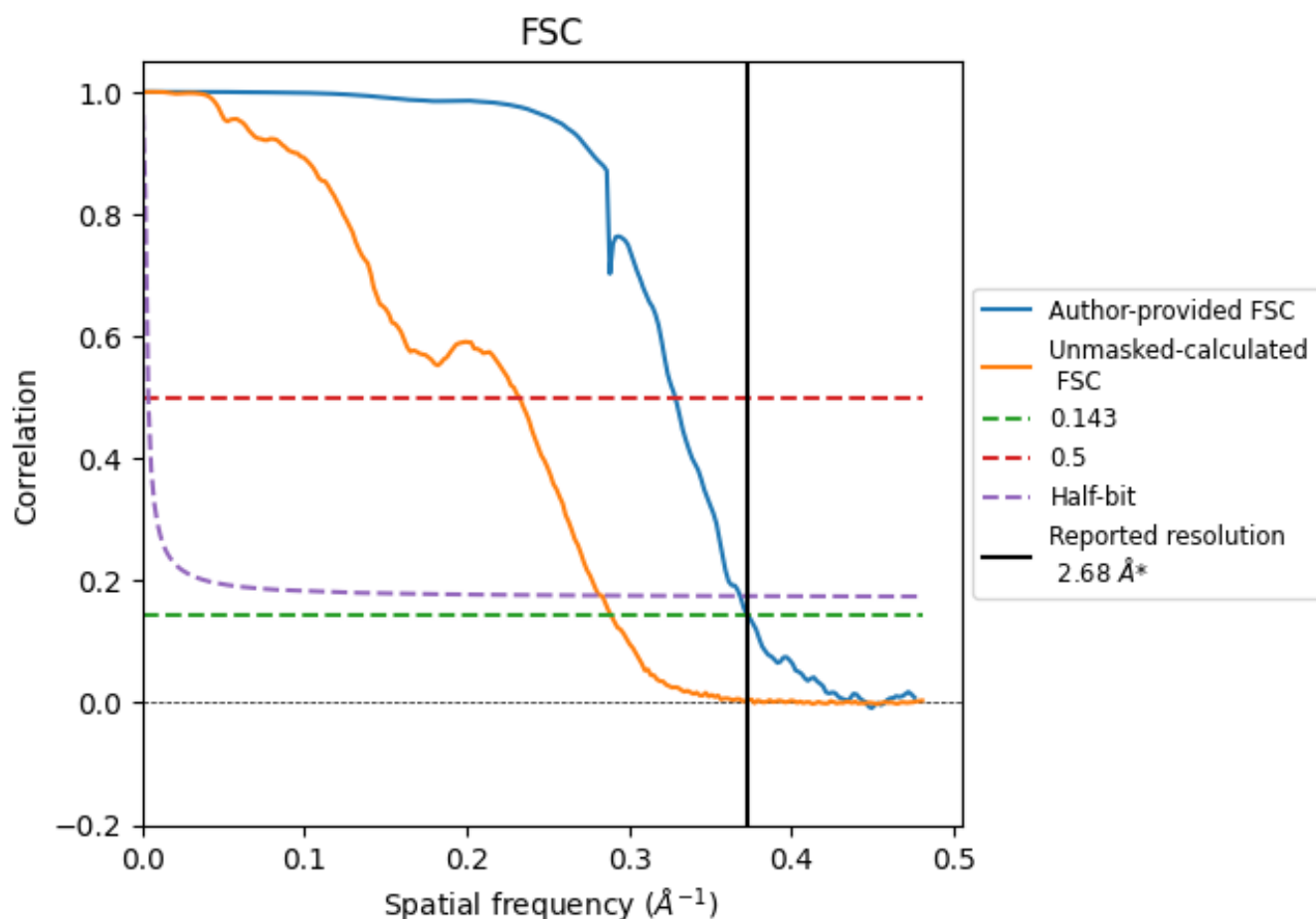


*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.373 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

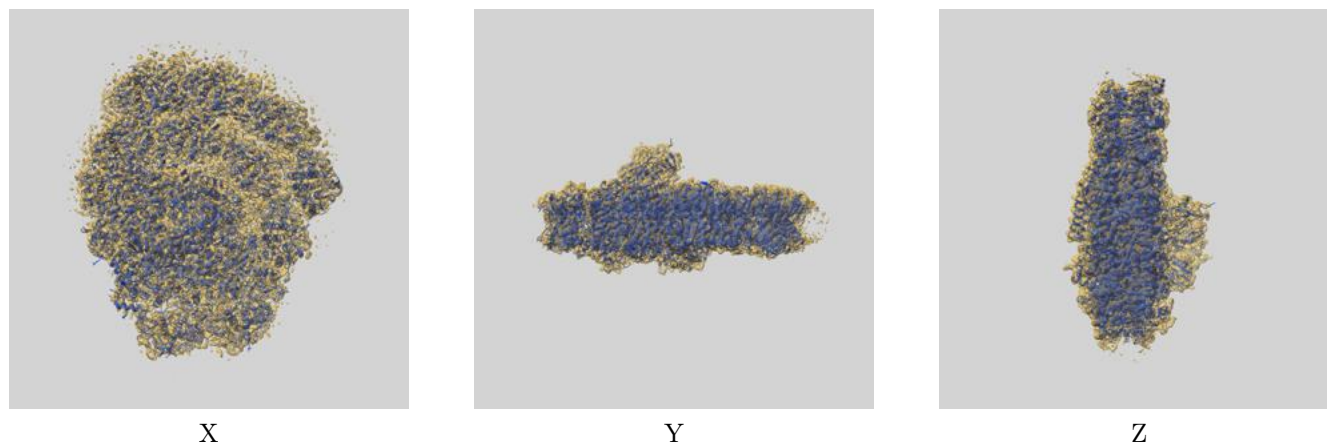
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.04	2.71
Unmasked-calculated*	3.46	4.30	3.54

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

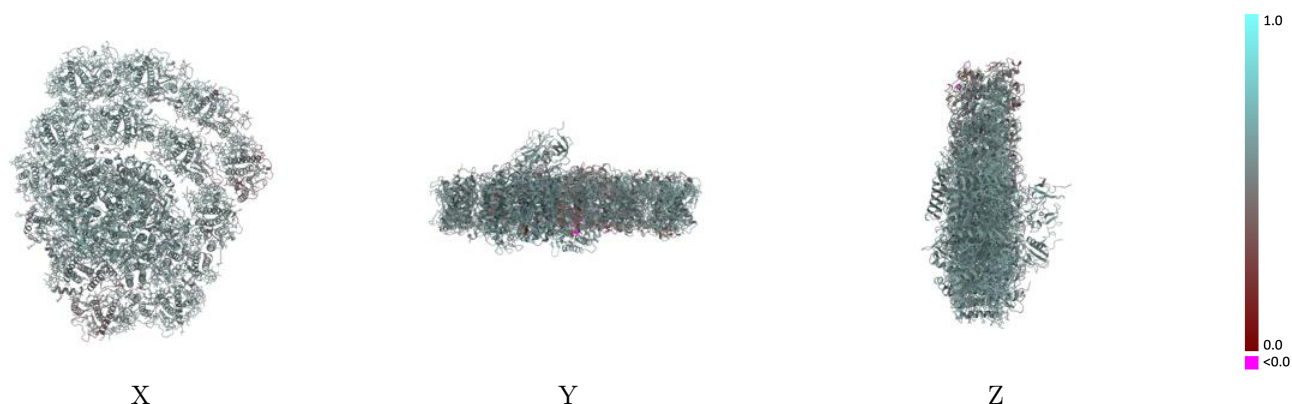
This section contains information regarding the fit between EMDB map EMD-61973 and PDB model 9K1E. Per-residue inclusion information can be found in [section 3](#) on [page 31](#).

9.1 Map-model overlay [i](#)



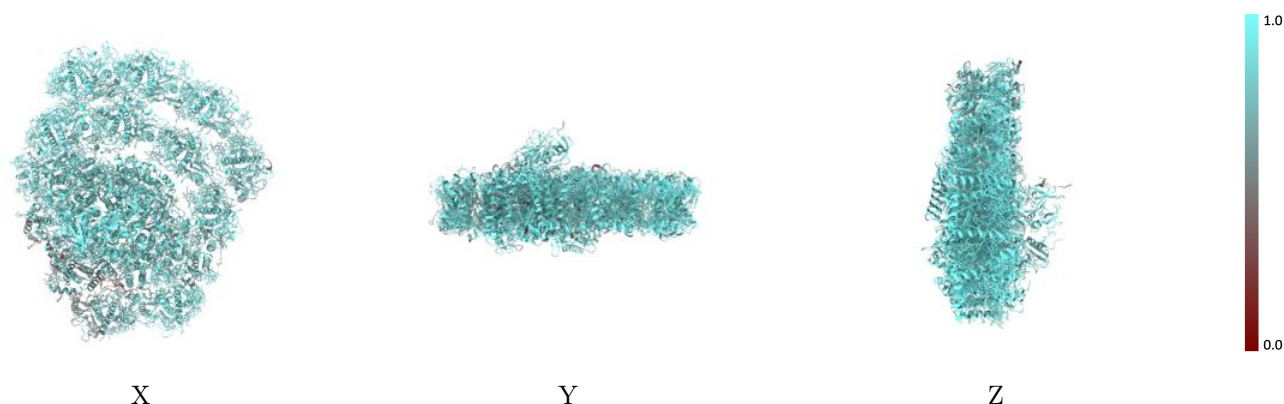
The images above show the 3D surface view of the map at the recommended contour level 0.203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



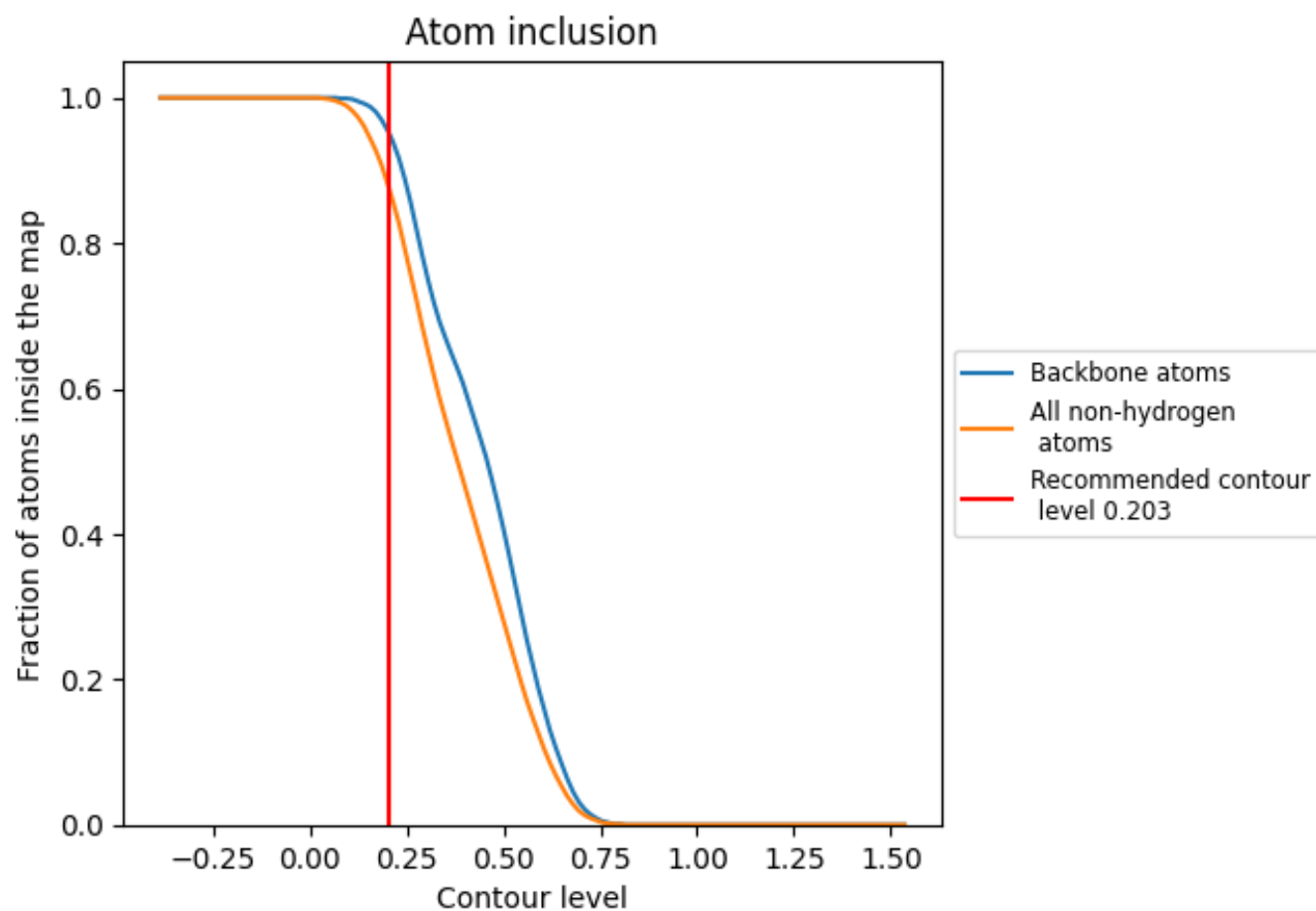
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.203).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% 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 (0.203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8780	0.5690
0	0.6840	0.4860
1	0.8580	0.5500
2	0.9240	0.5870
3	0.9240	0.5890
4	0.8710	0.5440
5	0.7850	0.4690
6	0.9090	0.5720
7	0.9070	0.5760
8	0.8660	0.5350
9	0.8650	0.5600
A	0.9370	0.6050
B	0.9420	0.6030
C	0.9600	0.5880
D	0.9110	0.5820
E	0.8580	0.5600
F	0.9030	0.5700
G	0.7840	0.5290
H	0.6250	0.5400
I	0.8210	0.5660
J	0.9140	0.5760
K	0.8720	0.5610
L	0.7190	0.5500
M	0.8900	0.5810
O	0.6960	0.5340

1.0

0.0

<0.0