



wwPDB EM Validation Summary Report ⓘ

Aug 7, 2026 – 12:57 AM JST

PDB ID : 9KQP / pdb_00009kqp
EMDB ID : EMD-62511
Title : PSI-LHCI supercomplex binding with 10 Lhcas from *C. subellipsoidea*
Authors : Tsai, P.-C.; Kato, K.; Shen, J.-R.; Akita, F.
Deposited on : 2024-11-26
Resolution : 1.92 Å(reported)
Based on initial model : 6zzx

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:

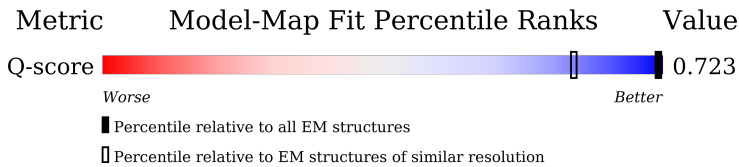
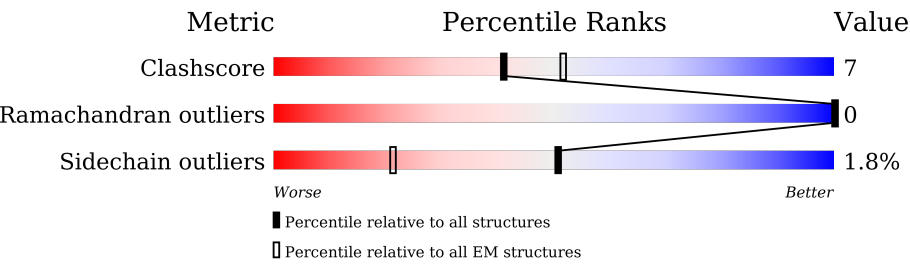
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 1.92 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	1227 (1.42 - 2.42)

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

Mol	Chain	Length	Quality of chain
1	A	751	91% 8% .
2	B	734	93% 7%
3	C	81	94% . ..
4	D	192	68% 7% 26%

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Mol	Chain	Length	Quality of chain
5	E	71	
6	F	245	
7	G	138	
8	H	133	
9	I	36	
10	J	41	
11	K	131	
12	M	31	
13	a	229	
13	b	229	
14	3	246	
15	7	259	
16	8	255	
17	9	230	
18	L	210	
19	O	142	
20	2	273	
21	4	246	
22	5	274	
23	6	272	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	UNL	3	306	-	-	X	-
36	LUT	4	302	-	X	-	-
36	LUT	6	303	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	LUT	9	302	-	X	-	-
36	LUT	9	305	-	X	-	-
36	LUT	F	304	-	X	-	-
36	LUT	a	305	-	X	-	-

2 Entry composition

There are 44 unique types of molecules in this entry. The entry contains 52991 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5814	3800	992	1004	18		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	732	Total	C	N	O	S	0	0
			5808	3812	985	998	13		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			596	365	103	117	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1110	711	193	203	3		

- Molecule 5 is a protein called Photosystem I reaction centre subunit IV/PsaE.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	60	Total	C	N	O	S	0	0
			490	316	83	90	1		

- Molecule 6 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1264	805	223	234	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	103	Total	C	N	O	S	0	0
			767	488	132	146	1		

- Molecule 8 is a protein called Photosystem I reaction centre subunit VI.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	91	Total	C	N	O	S	0	0
			706	449	120	137			

- Molecule 9 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	33	Total	C	N	O	S	0	0
			248	171	34	41	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	39	Total	C	N	O	S	0	0
			319	220	46	52	1		

- Molecule 11 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			560	356	96	107	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	31	Total	C	N	O	S	0	0
			237	160	35	41	1		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	195	Total	C	N	O	S	0	0
			1458	944	245	267	2		
13	b	126	Total	C	N	O	S	0	0
			952	606	168	176	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	203	Total	C	N	O	S	0	0
			1580	1036	255	286	3		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	7	214	Total	C	N	O	S	0	0
			1633	1059	276	296	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	8	222	Total	C	N	O	S	0	0
			1701	1112	276	310	3		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	9	184	Total	C	N	O	S	0	0
			1414	915	238	258	3		

- Molecule 18 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	148	Total	C	N	O	S	0	0
			1102	723	183	194	2		

- Molecule 19 is a protein called Photosystem I PsaO.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	O	78	Total	C	N	O	0	0
			605	403	98	104		

- Molecule 20 is a protein called Chlorophyll a-b binding protein, chloroplastic/Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	204	Total	C	N	O	S	0	0
			1606	1046	270	286	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4	193	Total	C	N	O	S	0	0
			1506	984	246	273	3		

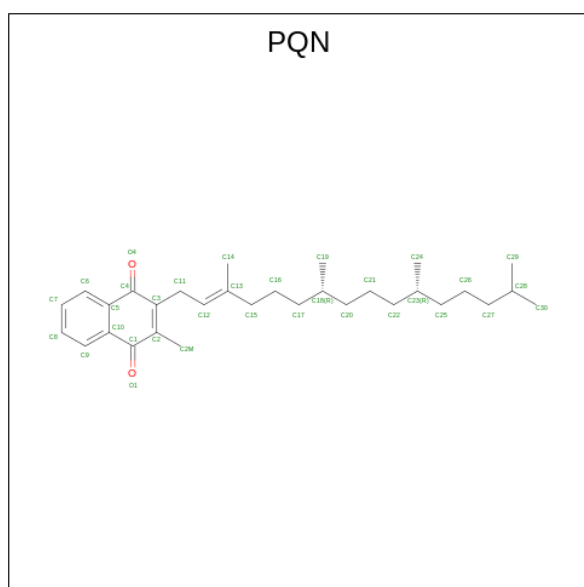
- Molecule 22 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	5	229	Total	C	N	O	S	0	0
			1766	1152	303	307	4		

- Molecule 23 is a protein called Chlorophyll a-b binding protein, chloroplastic.

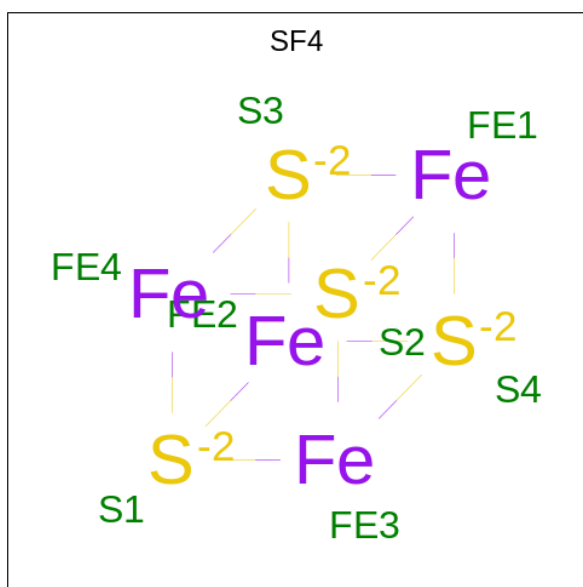
Mol	Chain	Residues	Atoms					AltConf	Trace
23	6	219	Total	C	N	O	S	0	0
			1658	1088	276	287	7		

- Molecule 24 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



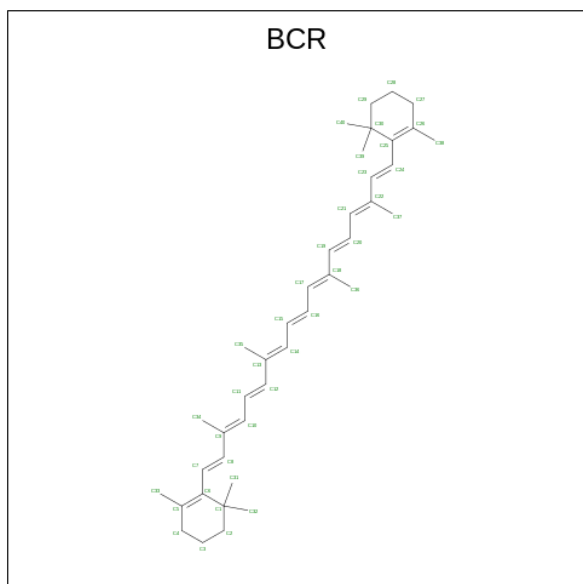
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			33	31	2	
24	B	1	Total	C	O	0
			33	31	2	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



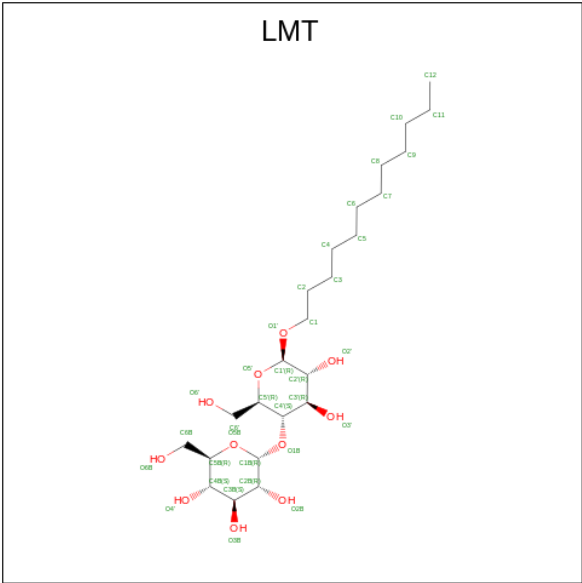
Mol	Chain	Residues	Atoms	AltConf
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	A	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	B	1	Total C 40 40	0
26	F	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	G	1	Total C 40 40	0
26	I	1	Total C 40 40	0
26	J	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	K	1	Total C 40 40	0
26	M	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	3	1	Total C 40 40	0
26	7	1	Total C 40 40	0
26	8	1	Total C 40 40	0

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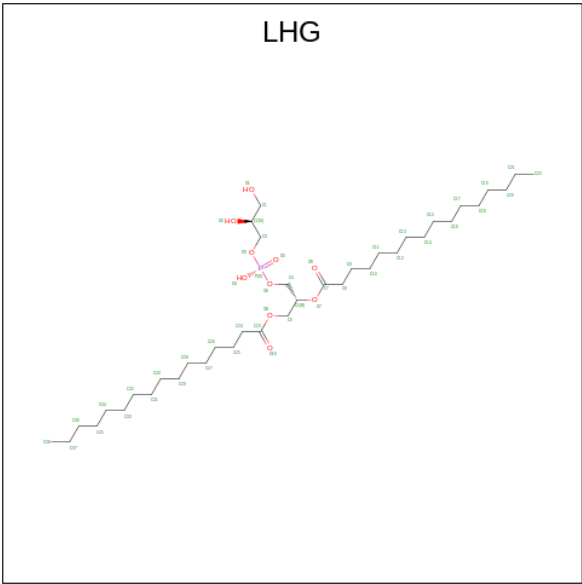
Mol	Chain	Residues	Atoms		AltConf
26	L	1	Total	C	0
			40	40	
26	L	1	Total	C	0
			40	40	
26	L	1	Total	C	0
			40	40	
26	O	1	Total	C	0
			40	40	
26	2	1	Total	C	0
			40	40	
26	5	1	Total	C	0
			40	40	
26	6	1	Total	C	0
			40	40	

- Molecule 27 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			35	24	11	
27	9	1	Total	C	O	0
			35	24	11	
27	5	1	Total	C	O	0
			35	24	11	

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).

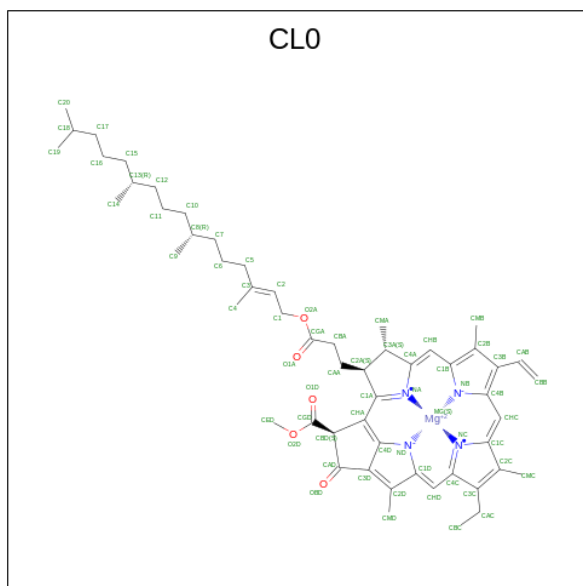


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
28	A	1	42	31	10	1	0
28	A	1	42	31	10	1	0
28	A	1	49	38	10	1	0
28	B	1	32	21	10	1	0
28	a	1	49	38	10	1	0
28	7	1	49	38	10	1	0
28	7	1	37	26	10	1	0
28	8	1	49	38	10	1	0
28	5	1	35	24	10	1	0
28	6	1	27	16	10	1	0
28	6	1	32	21	10	1	0

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

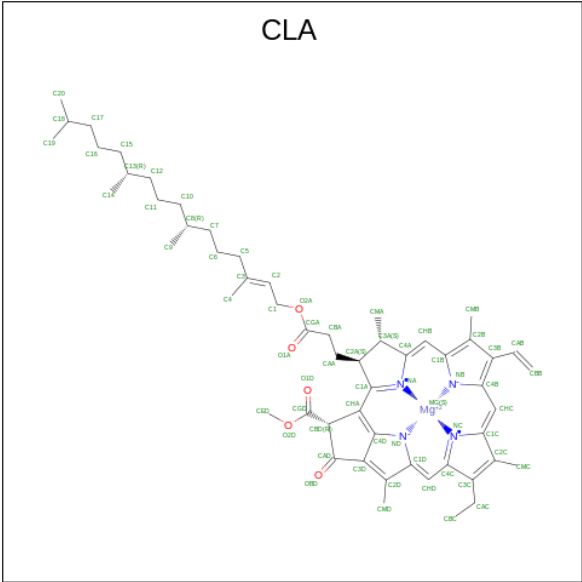
Mol	Chain	Residues	Atoms		AltConf
29	A	2	Total	C	0
			20	20	
29	B	2	Total	C	0
			24	24	
29	a	2	Total	C	0
			27	27	
29	3	1	Total	C	0
			11	11	
29	7	1	Total	C	0
			8	8	
29	8	1	Total	C	0
			18	18	
29	9	6	Total	C	0
			81	81	
29	2	1	Total	C	0
			11	11	
29	4	1	Total	C	0
			13	13	

- Molecule 30 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 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
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
31	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	3	1	Total 51	C 41	Mg 1	N 4	O 5	0
31	3	1	Total 61	C 51	Mg 1	N 4	O 5	0
31	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	7	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	7	1	Total 62	C 52	Mg 1	N 4	O 5	0
31	7	1	Total 44	C 34	Mg 1	N 4	O 5	0
31	7	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	7	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	7	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	8	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	8	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	9	1	Total 54	C 44	Mg 1	N 4	O 5	0
31	9	1	Total 50	C 40	Mg 1	N 4	O 5	0
31	9	1	Total 47	C 37	Mg 1	N 4	O 5	0
31	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
31	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	9	1	Total 56	C 46	Mg 1	N 4	O 5	0
31	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
31	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
31	O	1	Total 41	C 33	Mg 1	N 4	O 3	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
31	2	1	Total 57	C 47	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
31	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
31	4	1	Total 45	C 35	Mg 1	N 4	O 5	0

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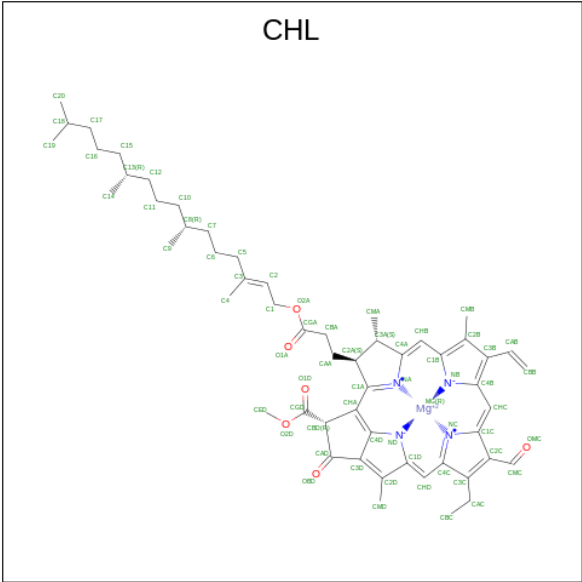
Mol	Chain	Residues	Atoms					AltConf
31	4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
31	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	5	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	5	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

- Molecule 32 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



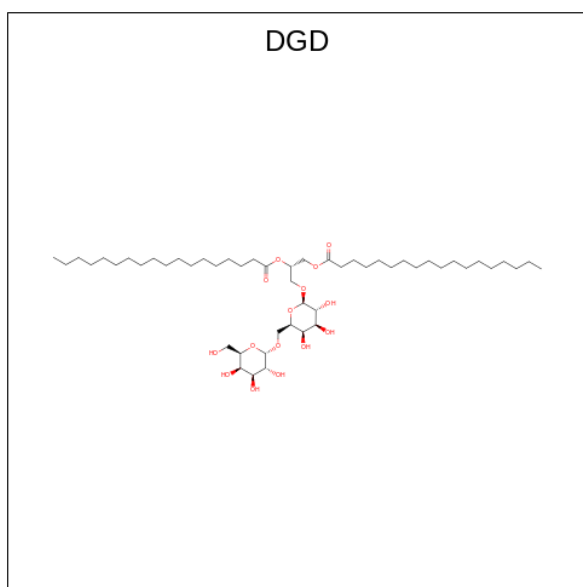
Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
32	A	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	K	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	a	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	3	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			57	46	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
32	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	8	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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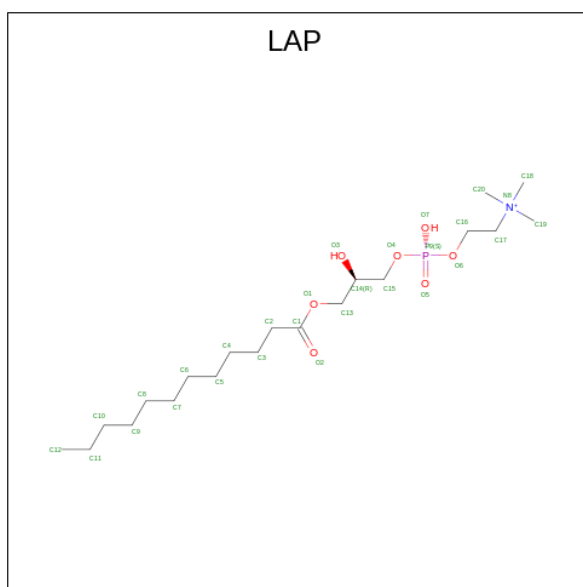
Mol	Chain	Residues	Atoms					AltConf
32	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
32	9	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	9	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	b	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
32	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	5	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
32	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



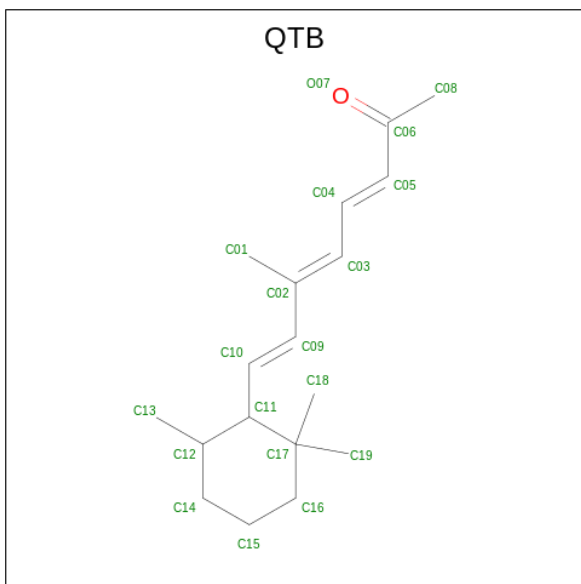
Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			61	46	15	
33	7	1	Total	C	O	0
			52	37	15	

- Molecule 34 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (CCD ID: LAP) (formula: $C_{20}H_{43}NO_7P$) (labeled as "Ligand of Interest" by depositor).



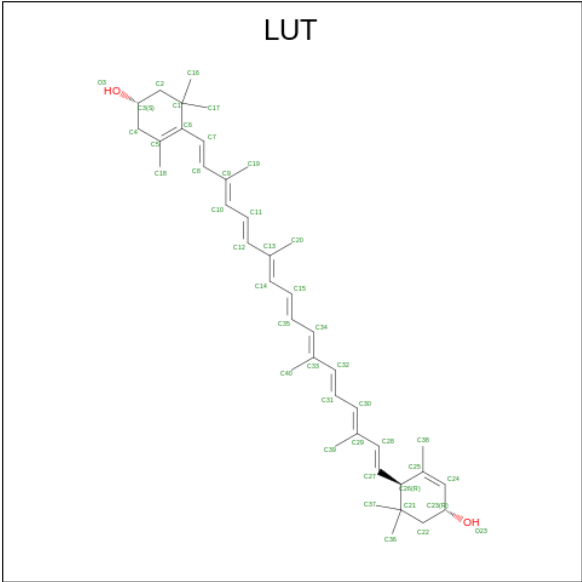
Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 35 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (CCD ID: QTB) (formula: C₁₈H₂₈O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
35	F	1	Total	C	O	0
			19	18	1	
35	a	1	Total	C	O	0
			19	18	1	
35	7	1	Total	C	O	0
			19	18	1	
35	9	1	Total	C	O	0
			19	18	1	

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



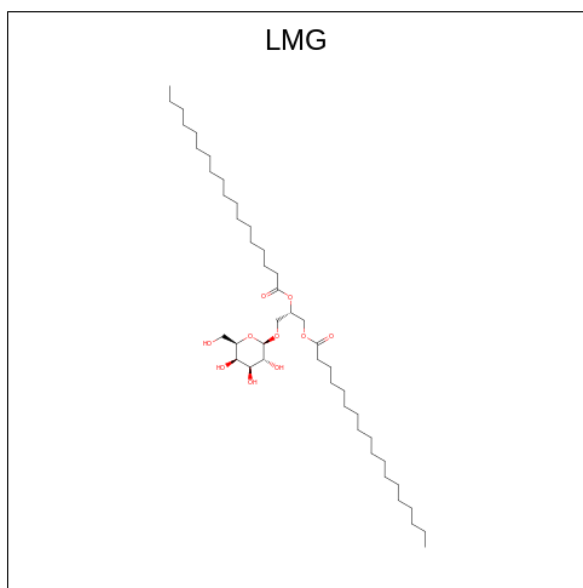
Mol	Chain	Residues	Atoms			AltConf
36	F	1	Total	C	O	0
			42	40	2	
36	J	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	a	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	7	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	9	1	Total	C	O	0
			42	40	2	
36	L	1	Total	C	O	0
			42	40	2	
36	b	1	Total	C	O	0
			42	40	2	

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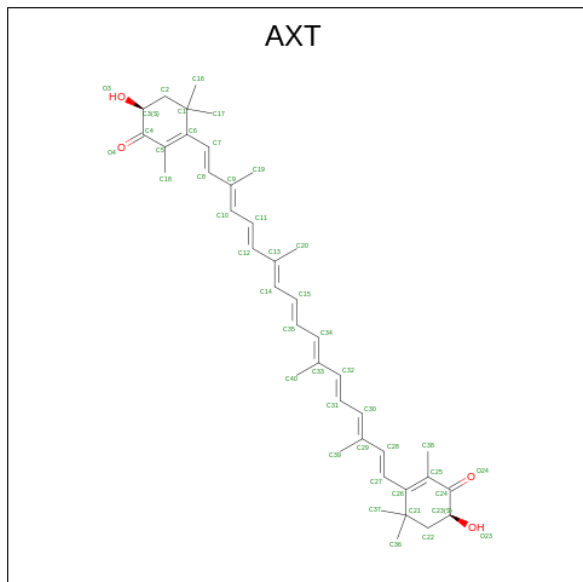
Mol	Chain	Residues	Atoms			AltConf
36	2	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



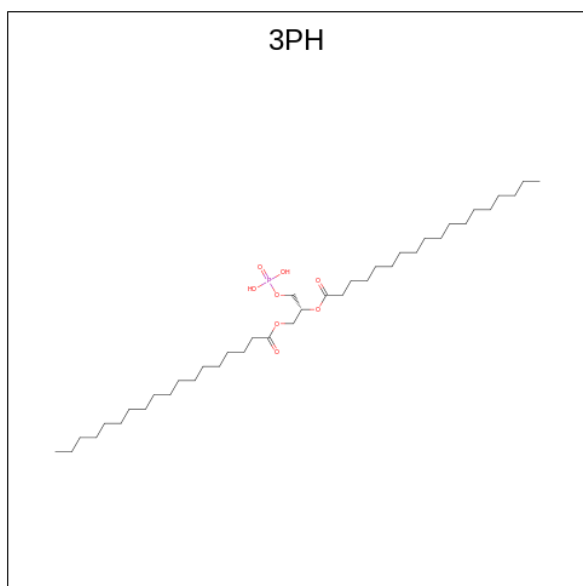
Mol	Chain	Residues	Atoms			AltConf
37	G	1	Total	C	O	0
			44	34	10	
37	J	1	Total	C	O	0
			49	39	10	
37	J	1	Total	C	O	0
			29	19	10	
37	a	1	Total	C	O	0
			42	32	10	

- Molecule 38 is ASTAXANTHIN (CCD ID: AXT) (formula: $C_{40}H_{52}O_4$) (labeled as "Ligand of Interest" by depositor).



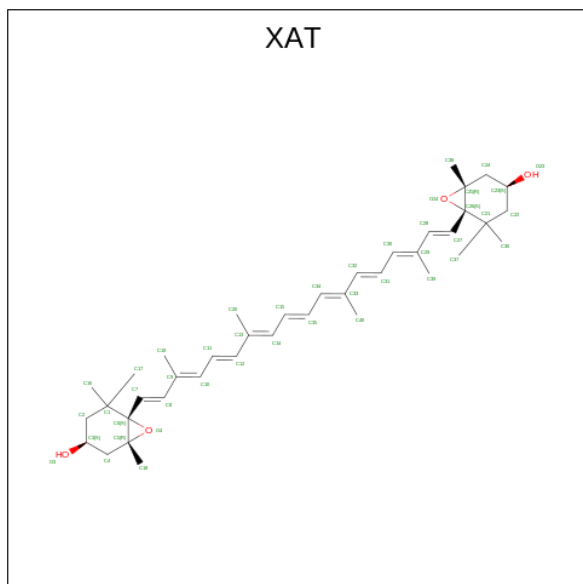
Mol	Chain	Residues	Atoms			AltConf
38	a	1	Total	C	O	0
			43	40	3	

- Molecule 39 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$) (labeled as "Ligand of Interest" by depositor).



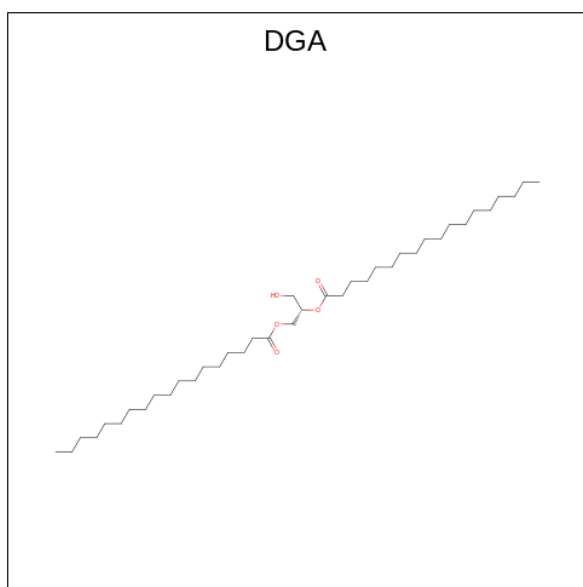
Mol	Chain	Residues	Atoms				AltConf
39	7	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 40 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$) (labeled as "Ligand of Interest" by depositor).



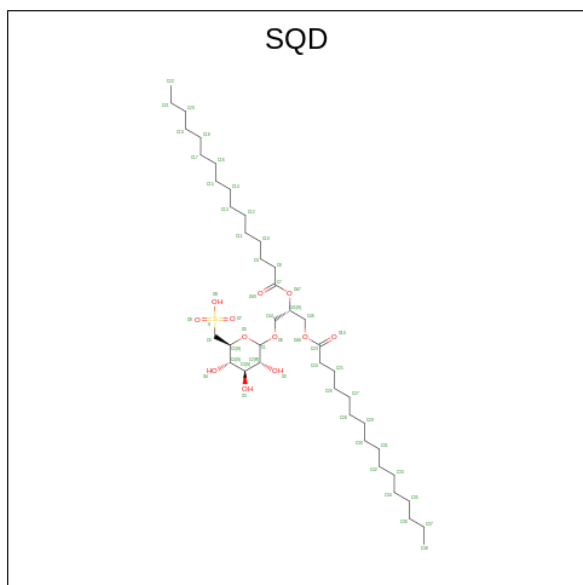
Mol	Chain	Residues	Atoms			AltConf
40	7	1	Total	C	O	0
			44	40	4	

- Molecule 41 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$) (labeled as "Ligand of Interest" by depositor).



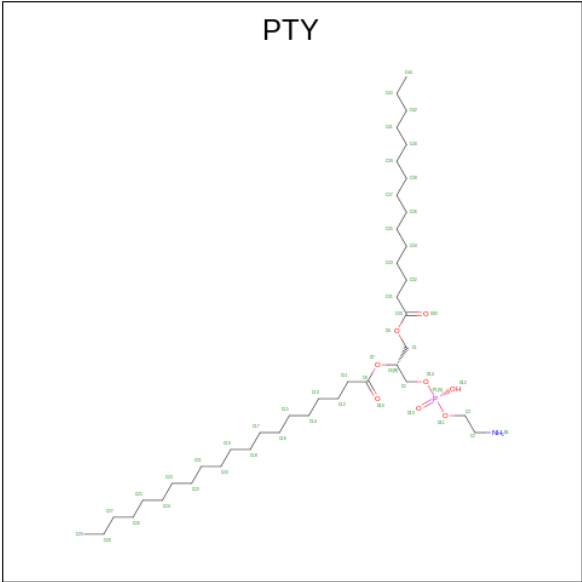
Mol	Chain	Residues	Atoms			AltConf
41	8	1	Total	C	O	0
			28	23	5	

- Molecule 42 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
42	4	1	Total	C	O	S	0
			35	22	12	1	

- Molecule 43 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
43	5	1	Total	C	N	O	P	0
			31	21	1	8	1	

- Molecule 44 is water.

Mol	Chain	Residues	Atoms		AltConf
44	A	297	Total	O	0
			297	297	
44	B	311	Total	O	0
			311	311	
44	C	60	Total	O	0
			60	60	
44	D	53	Total	O	0
			53	53	
44	E	28	Total	O	0
			28	28	
44	F	57	Total	O	0
			57	57	
44	G	18	Total	O	0
			18	18	
44	H	6	Total	O	0
			6	6	
44	I	6	Total	O	0
			6	6	
44	J	16	Total	O	0
			16	16	
44	K	2	Total	O	0
			2	2	

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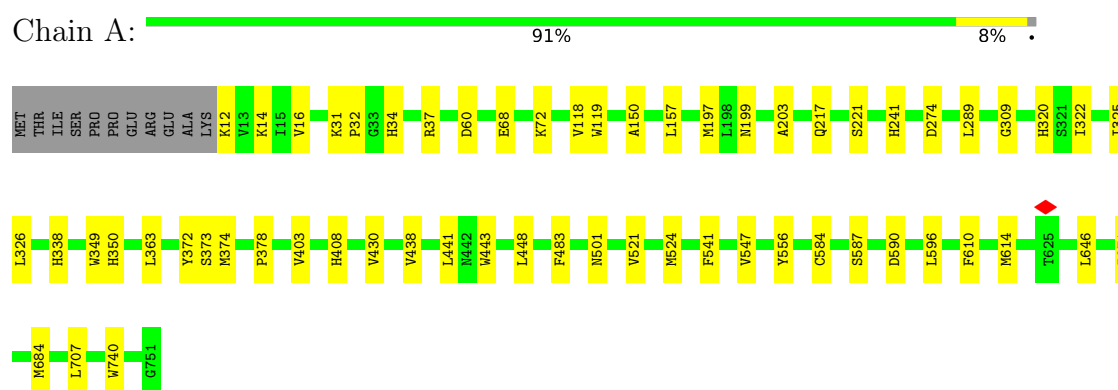
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Mol	Chain	Residues	Atoms		AltConf
44	M	5	Total 5	O 5	0
44	a	34	Total 34	O 34	0
44	3	32	Total 32	O 32	0
44	7	39	Total 39	O 39	0
44	8	37	Total 37	O 37	0
44	9	21	Total 21	O 21	0
44	L	17	Total 17	O 17	0
44	O	4	Total 4	O 4	0
44	2	3	Total 3	O 3	0
44	4	1	Total 1	O 1	0
44	5	11	Total 11	O 11	0
44	6	2	Total 2	O 2	0

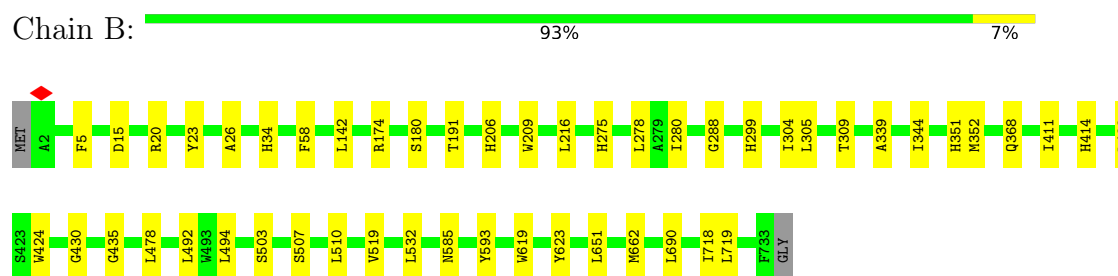
3 Residue-property plots

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.

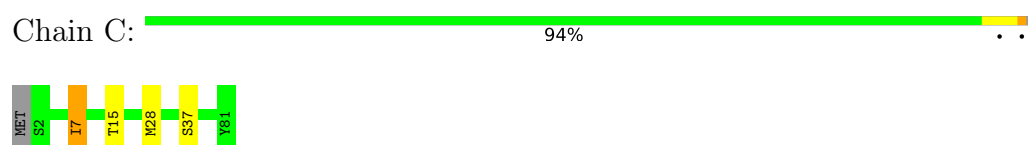
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

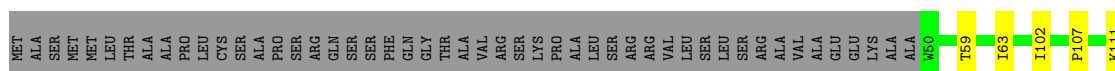


- Molecule 3: Photosystem I iron-sulfur center

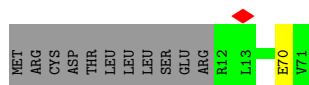
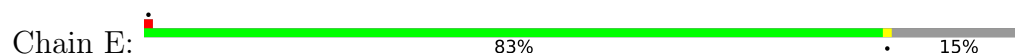


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

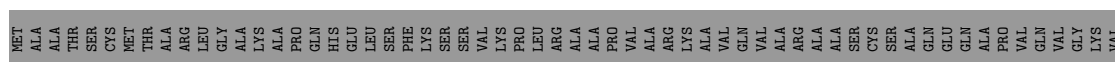




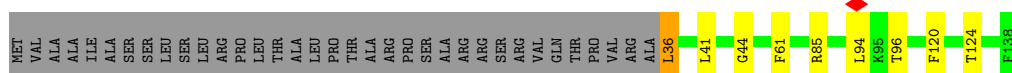
- Molecule 5: Photosystem I reaction centre subunit IV/PsaE



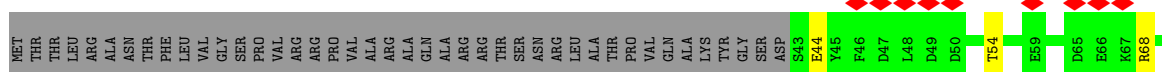
- Molecule 6: Photosystem I reaction center subunit III



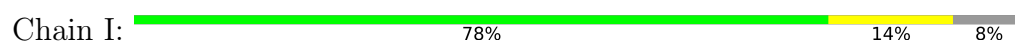
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 8: Photosystem I reaction centre subunit VI



- Molecule 9: Photosystem I reaction center subunit VIII



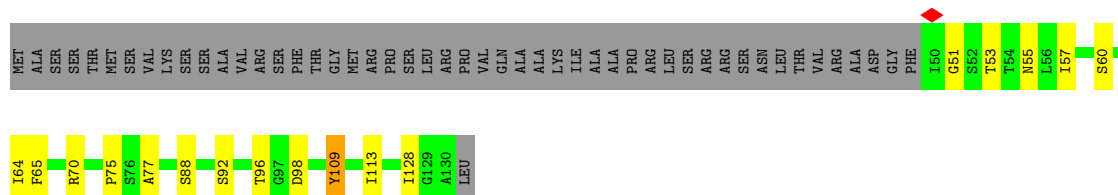
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  78% 17% 5%

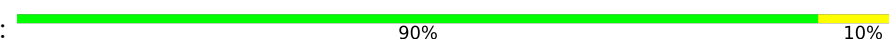


• Molecule 11: PSI-K

Chain K:  49% 12% 38%



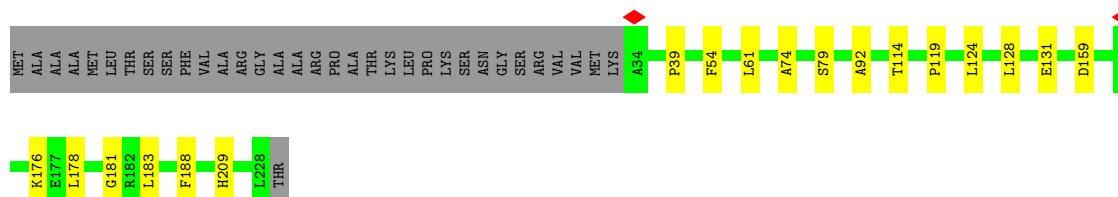
• Molecule 12: Photosystem I reaction center subunit XII

Chain M:  90% 10%

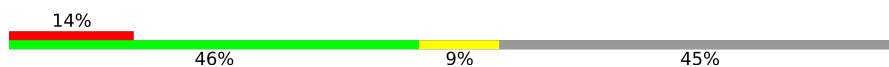


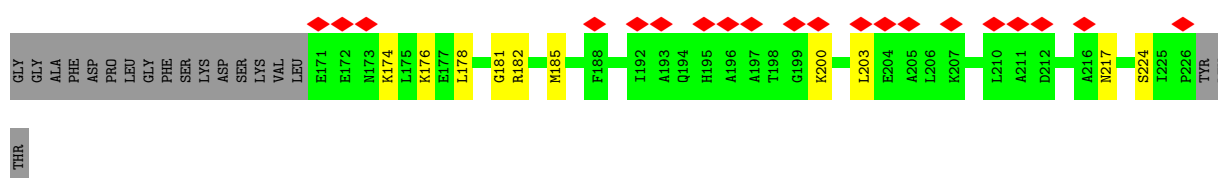
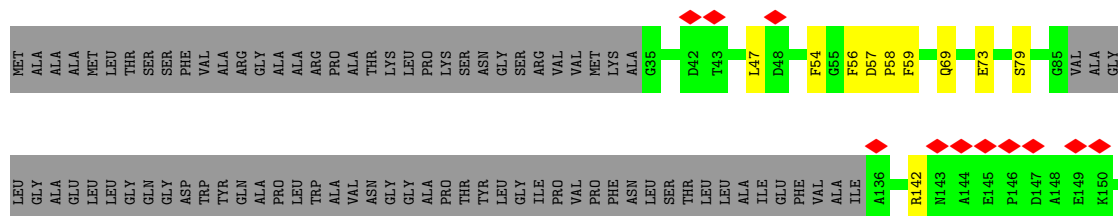
• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain a:  77% 8% 15%

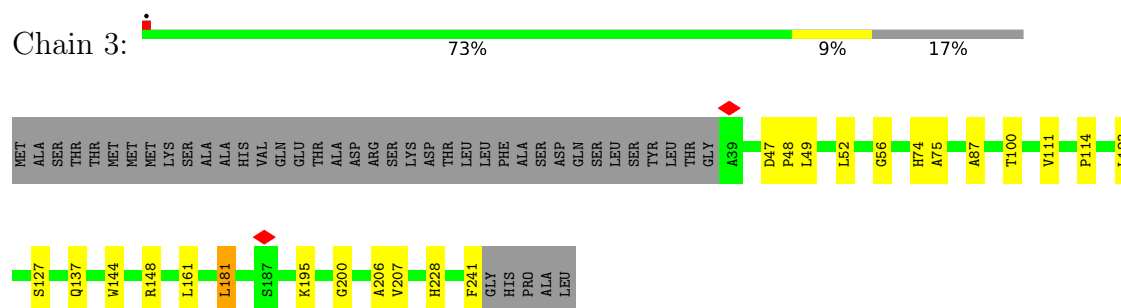


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

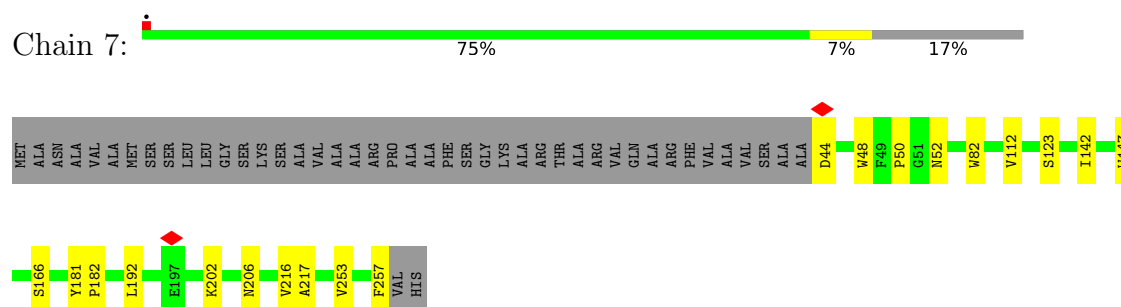
Chain b:  14% 46% 9% 45%



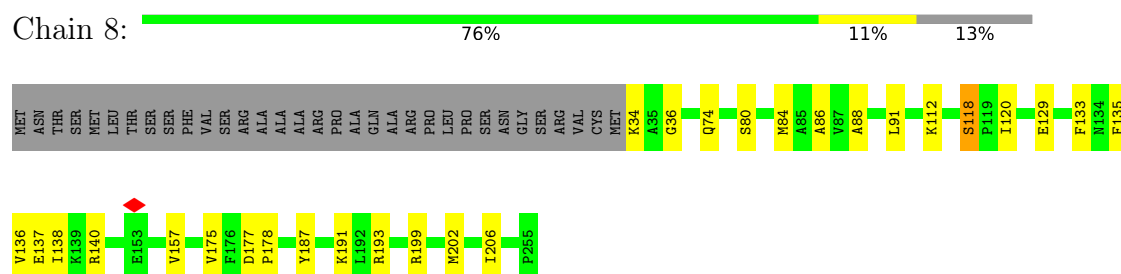
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



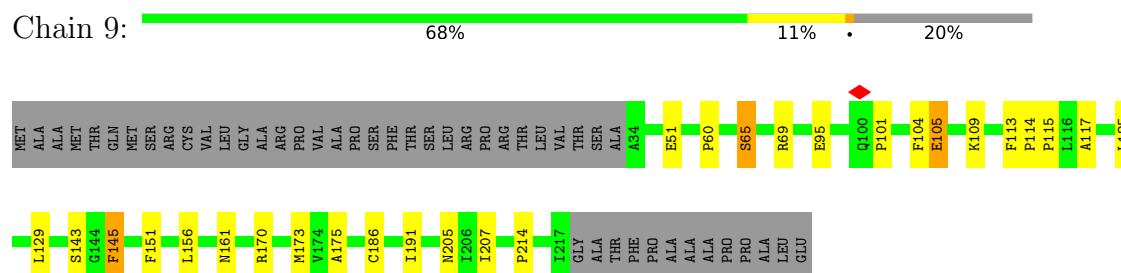
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



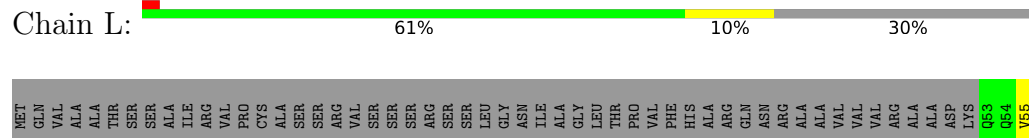
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic



- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

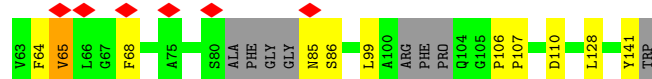
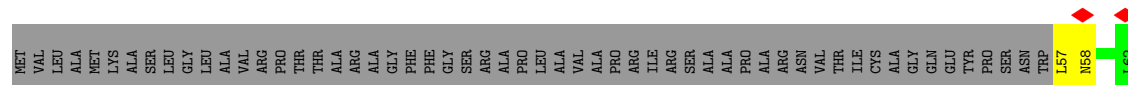


- Molecule 18: PSI subunit V

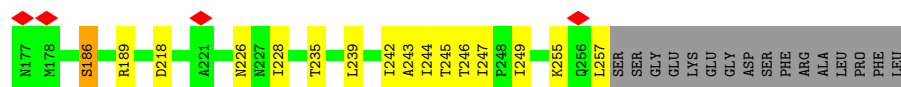
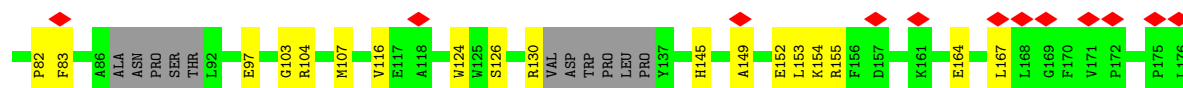




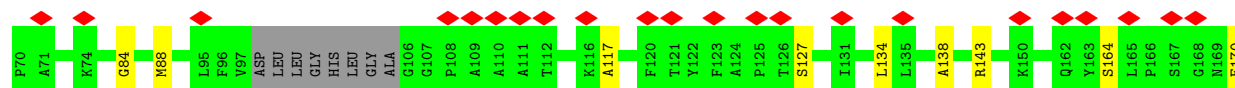
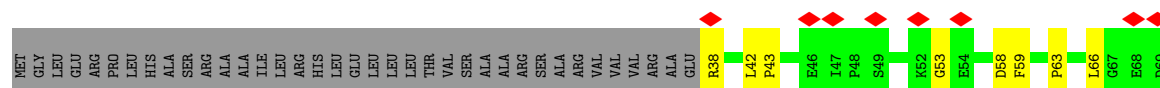
- Molecule 19: Photosystem I PsaO



- Molecule 20: Chlorophyll a-b binding protein, chloroplastic/Lhca2

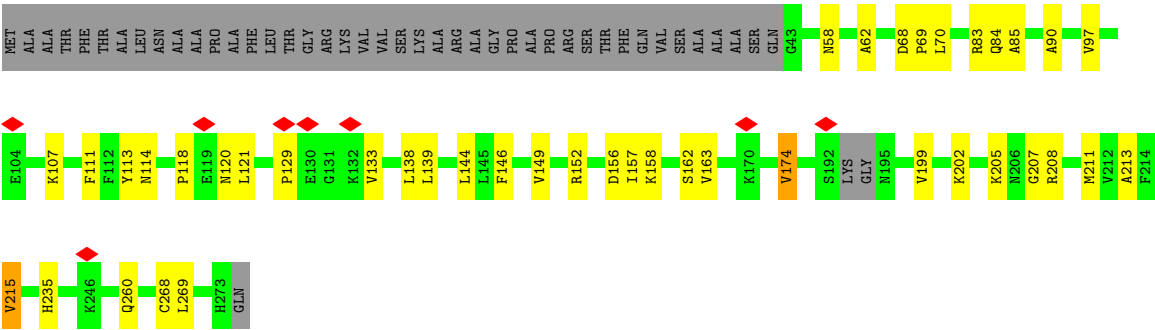


- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

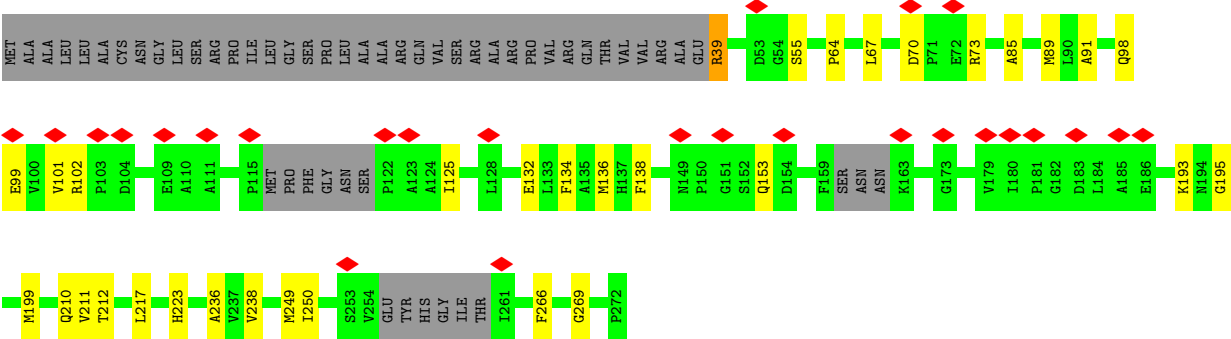


- Molecule 22: Chlorophyll a-b binding protein, chloroplastic





● Molecule 23: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	224674	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.393	Depositor
Minimum map value	-0.655	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.085	Depositor
Map size (Å)	436.2, 436.2, 436.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGA, QTB, AXT, 3PH, BCR, CHL, SF4, PTY, LAP, LMT, LHG, XAT, CL0, CLA, DGD, LMG, PQN, SQD, LUT, UNL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.24	0/6012	0.45	0/8202
2	B	0.23	0/6017	0.45	0/8218
3	C	0.30	0/606	0.58	0/822
4	D	0.18	0/1136	0.37	0/1537
5	E	0.19	0/502	0.38	0/686
6	F	0.20	0/1288	0.38	0/1737
7	G	0.18	0/783	0.39	0/1063
8	H	0.18	0/722	0.42	0/972
9	I	0.28	0/254	0.51	0/347
10	J	0.20	0/330	0.41	0/452
11	K	0.18	0/568	0.42	0/773
12	M	0.21	0/240	0.34	0/325
13	a	0.20	0/1501	0.41	0/2045
13	b	0.13	0/977	0.29	0/1322
14	3	0.26	0/1629	0.47	0/2217
15	7	0.20	0/1684	0.38	0/2298
16	8	0.21	0/1752	0.39	0/2379
17	9	0.20	0/1451	0.41	0/1964
18	L	0.19	0/1129	0.42	0/1542
19	O	0.16	0/619	0.39	0/839
20	2	0.22	0/1654	0.54	1/2254 (0.0%)
21	4	0.18	0/1553	0.37	0/2113
22	5	0.21	0/1820	0.46	1/2477 (0.0%)
23	6	0.21	0/1709	0.38	0/2328
All	All	0.22	0/35936	0.43	2/48912 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	6	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	2	66	PRO	CA-N-CD	-8.66	99.87	112.00
22	5	129	PRO	N-CD-CG	-7.27	92.30	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	6	39	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5814	0	5649	45	0
2	B	5808	0	5584	38	0
3	C	596	0	573	3	0
4	D	1110	0	1131	9	0
5	E	490	0	482	0	0
6	F	1264	0	1300	9	0
7	G	767	0	749	6	0
8	H	706	0	687	12	0
9	I	248	0	269	4	0
10	J	319	0	326	7	0
11	K	560	0	583	9	0
12	M	237	0	260	2	0
13	a	1458	0	1423	17	0
13	b	952	0	917	15	0
14	3	1580	0	1546	25	0
15	7	1633	0	1579	16	0
16	8	1701	0	1683	18	0
17	9	1414	0	1405	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L	1102	0	1129	14	0
19	O	605	0	616	7	0
20	2	1606	0	1578	34	0
21	4	1506	0	1468	25	0
22	5	1766	0	1746	34	0
23	6	1658	0	1657	28	0
24	A	33	0	46	1	0
24	B	33	0	46	2	0
25	A	8	0	0	0	0
25	C	16	0	0	0	0
26	2	40	0	56	3	0
26	3	120	0	168	7	0
26	5	40	0	56	2	0
26	6	40	0	56	2	0
26	7	40	0	56	6	0
26	8	40	0	56	4	0
26	A	160	0	224	11	0
26	B	200	0	280	16	0
26	F	40	0	56	1	0
26	G	80	0	112	1	0
26	I	40	0	56	1	0
26	J	40	0	56	1	0
26	K	80	0	112	7	0
26	L	120	0	168	6	0
26	M	40	0	56	3	0
26	O	40	0	56	2	0
27	5	35	0	44	0	0
27	9	35	0	44	0	0
27	A	70	0	89	4	0
28	5	35	0	40	1	0
28	6	59	0	58	3	0
28	7	86	0	118	8	0
28	8	49	0	74	0	0
28	A	133	0	188	7	0
28	B	32	0	34	1	0
28	a	49	0	74	9	0
29	2	11	0	0	0	0
29	3	11	0	0	4	0
29	4	13	0	0	1	0
29	7	8	0	0	0	0
29	8	18	0	0	0	0
29	9	81	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	A	20	0	0	0	0
29	B	24	0	0	0	0
29	a	27	0	0	0	0
30	A	65	0	72	3	0
31	2	574	0	442	16	0
31	3	736	0	697	19	0
31	4	685	0	550	25	0
31	5	678	0	588	21	0
31	6	545	0	436	15	0
31	7	523	0	445	11	0
31	8	692	0	606	19	0
31	9	524	0	452	4	0
31	A	2450	0	2472	93	0
31	B	2382	0	2381	63	0
31	F	161	0	144	4	0
31	G	141	0	105	8	0
31	H	138	0	99	10	0
31	J	42	0	31	1	0
31	K	142	0	105	1	0
31	L	150	0	125	6	0
31	O	134	0	98	0	0
31	a	601	0	547	18	0
31	b	520	0	389	7	0
32	3	56	0	46	1	0
32	4	141	0	92	13	0
32	5	197	0	136	15	0
32	6	296	0	217	18	0
32	7	297	0	272	25	0
32	8	111	0	99	9	0
32	9	95	0	62	5	0
32	A	180	0	165	10	0
32	K	47	0	31	1	0
32	a	157	0	120	13	0
32	b	47	0	30	1	0
33	7	52	0	65	0	0
33	B	61	0	83	4	0
34	B	29	0	42	4	0
35	7	19	0	0	0	0
35	9	19	0	0	0	0
35	F	19	0	0	0	0
35	a	19	0	0	0	0
36	2	42	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	3	84	0	111	10	0
36	4	84	0	111	11	0
36	5	84	0	111	9	0
36	6	84	0	111	5	0
36	7	42	0	56	3	0
36	8	84	0	112	7	0
36	9	126	0	165	8	0
36	F	42	0	55	2	0
36	J	42	0	54	3	0
36	L	42	0	55	1	0
36	a	84	0	109	10	0
36	b	42	0	56	5	0
37	G	44	0	58	4	0
37	J	78	0	99	4	0
37	a	42	0	54	2	0
38	a	43	0	52	1	0
39	7	33	0	39	1	0
40	7	44	0	56	0	0
41	8	28	0	38	2	0
42	4	35	0	34	1	0
43	5	31	0	35	1	0
44	2	3	0	0	0	0
44	3	32	0	0	0	0
44	4	1	0	0	0	0
44	5	11	0	0	0	0
44	6	2	0	0	0	0
44	7	39	0	0	0	0
44	8	37	0	0	0	0
44	9	21	0	0	0	0
44	A	297	0	0	1	0
44	B	311	0	0	2	0
44	C	60	0	0	0	0
44	D	53	0	0	0	0
44	E	28	0	0	0	0
44	F	57	0	0	0	0
44	G	18	0	0	0	0
44	H	6	0	0	1	0
44	I	6	0	0	0	0
44	J	16	0	0	0	0
44	K	2	0	0	0	0
44	L	17	0	0	0	0
44	M	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	O	4	0	0	0	0
44	a	34	0	0	0	0
All	All	52991	0	50690	710	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 7.

The worst 5 of 710 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)
31:H:902:CLA:HAA1	20:2:153:LEU:HD23	1.31	1.06
14:3:241:PHE:CD2	29:3:306:UNL:C2	2.39	1.05
31:A:829:CLA:HBA2	28:7:302:LHG:H242	1.39	1.02
31:H:902:CLA:O1A	20:2:153:LEU:HD21	1.61	0.99
20:2:243:ALA:O	20:2:247:ILE:HG13	1.64	0.96

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/751 (98%)	721 (98%)	17 (2%)	0	100	100
2	B	730/734 (100%)	719 (98%)	11 (2%)	0	100	100
3	C	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
4	D	141/192 (73%)	138 (98%)	3 (2%)	0	100	100
5	E	58/71 (82%)	56 (97%)	2 (3%)	0	100	100
6	F	163/245 (66%)	160 (98%)	3 (2%)	0	100	100
7	G	101/138 (73%)	99 (98%)	2 (2%)	0	100	100
8	H	89/133 (67%)	87 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	31/36 (86%)	31 (100%)	0	0	100	100
10	J	37/41 (90%)	37 (100%)	0	0	100	100
11	K	79/131 (60%)	79 (100%)	0	0	100	100
12	M	29/31 (94%)	29 (100%)	0	0	100	100
13	a	193/229 (84%)	191 (99%)	2 (1%)	0	100	100
13	b	120/229 (52%)	119 (99%)	1 (1%)	0	100	100
14	3	201/246 (82%)	194 (96%)	7 (4%)	0	100	100
15	7	212/259 (82%)	209 (99%)	3 (1%)	0	100	100
16	8	220/255 (86%)	215 (98%)	5 (2%)	0	100	100
17	9	182/230 (79%)	179 (98%)	3 (2%)	0	100	100
18	L	142/210 (68%)	139 (98%)	3 (2%)	0	100	100
19	O	72/142 (51%)	71 (99%)	1 (1%)	0	100	100
20	2	198/273 (72%)	184 (93%)	14 (7%)	0	100	100
21	4	187/246 (76%)	180 (96%)	7 (4%)	0	100	100
22	5	225/274 (82%)	216 (96%)	9 (4%)	0	100	100
23	6	211/272 (78%)	206 (98%)	5 (2%)	0	100	100
All	All	4437/5449 (81%)	4336 (98%)	101 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/613 (98%)	597 (99%)	6 (1%)	68	64
2	B	592/593 (100%)	588 (99%)	4 (1%)	76	73
3	C	68/69 (99%)	66 (97%)	2 (3%)	37	21
4	D	118/156 (76%)	117 (99%)	1 (1%)	73	71
5	E	56/67 (84%)	55 (98%)	1 (2%)	51	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	131/183 (72%)	131 (100%)	0	100	100
7	G	78/106 (74%)	75 (96%)	3 (4%)	29	14
8	H	71/105 (68%)	71 (100%)	0	100	100
9	I	26/28 (93%)	26 (100%)	0	100	100
10	J	35/37 (95%)	35 (100%)	0	100	100
11	K	59/100 (59%)	55 (93%)	4 (7%)	14	4
12	M	26/26 (100%)	25 (96%)	1 (4%)	29	14
13	a	141/166 (85%)	141 (100%)	0	100	100
13	b	92/166 (55%)	90 (98%)	2 (2%)	45	32
14	3	162/197 (82%)	160 (99%)	2 (1%)	63	57
15	7	166/195 (85%)	163 (98%)	3 (2%)	51	39
16	8	175/202 (87%)	171 (98%)	4 (2%)	44	30
17	9	143/177 (81%)	136 (95%)	7 (5%)	22	8
18	L	115/161 (71%)	112 (97%)	3 (3%)	40	24
19	O	65/110 (59%)	60 (92%)	5 (8%)	12	3
20	2	166/225 (74%)	161 (97%)	5 (3%)	36	20
21	4	155/195 (80%)	152 (98%)	3 (2%)	50	37
22	5	178/208 (86%)	172 (97%)	6 (3%)	32	16
23	6	170/212 (80%)	168 (99%)	2 (1%)	63	57
All	All	3591/4297 (84%)	3527 (98%)	64 (2%)	51	39

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	5	133	VAL
22	5	163	VAL
15	7	44	ASP
14	3	181	LEU
22	5	174	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
20	2	227	ASN

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Mol	Chain	Res	Type
23	6	210	GLN
21	4	82	GLN
22	5	125	ASN
11	K	55	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](#)

Of 354 ligands modelled in this entry, 17 are unknown - leaving 337 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
28	LHG	5	305	31	34,34,48	0.33	0	37,40,54	0.40	0
31	CLA	6	308	44	51,55,73	3.10	22 (43%)	61,91,113	2.67	23 (37%)
31	CLA	7	321	44	51,55,73	3.17	22 (43%)	61,91,113	2.72	25 (40%)
31	CLA	a	314	44	54,58,73	3.86	22 (40%)	65,95,113	2.60	26 (40%)
31	CLA	K	204	44	54,58,73	3.41	22 (40%)	65,95,113	2.60	23 (35%)
32	CHL	5	316	44	60,64,74	2.80	21 (35%)	68,102,114	2.43	26 (38%)
25	SF4	A	802	2,1	0,12,12	-	-	-	-	-
41	DGA	8	305	-	27,27,43	0.25	0	29,29,45	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	9	311	17	59,63,73	4.99	22 (37%)	71,101,113	2.47	30 (42%)
31	CLA	A	838	44	69,73,73	2.65	23 (33%)	83,113,113	2.45	24 (28%)
31	CLA	B	843	44	49,53,73	2.90	21 (42%)	59,89,113	2.71	24 (40%)
26	BCR	O	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	5 (8%)
32	CHL	6	318	44	50,54,74	3.77	22 (44%)	56,90,114	2.51	25 (44%)
31	CLA	A	820	1	59,63,73	3.00	24 (40%)	71,101,113	2.58	23 (32%)
31	CLA	5	311	22	50,54,73	2.77	21 (42%)	60,90,113	2.72	26 (43%)
32	CHL	a	318	44	52,56,74	3.03	19 (36%)	58,92,114	2.50	22 (37%)
31	CLA	3	312	44	69,73,73	2.70	21 (30%)	83,113,113	2.31	27 (32%)
33	DGD	7	308	-	53,53,67	1.05	4 (7%)	67,67,81	1.53	12 (17%)
31	CLA	3	317	44	55,59,73	3.09	21 (38%)	66,96,113	2.66	26 (39%)
31	CLA	G	204	7	54,58,73	3.13	22 (40%)	65,95,113	2.58	26 (40%)
31	CLA	b	307	-	50,54,73	5.50	23 (46%)	60,90,113	2.76	25 (41%)
31	CLA	9	321	17	60,64,73	2.59	22 (36%)	72,102,113	2.45	27 (37%)
31	CLA	A	823	1	59,63,73	3.02	20 (33%)	71,101,113	2.42	23 (32%)
31	CLA	K	205	11	50,54,73	3.19	22 (44%)	60,90,113	2.71	23 (38%)
31	CLA	7	312	15	66,70,73	2.66	24 (36%)	79,109,113	2.33	24 (30%)
36	LUT	2	301	-	42,43,43	5.53	19 (45%)	51,60,60	5.77	32 (62%)
31	CLA	a	310	13	49,53,73	3.23	22 (44%)	59,89,113	2.77	23 (38%)
31	CLA	5	308	22	50,54,73	3.76	22 (44%)	60,90,113	2.70	24 (40%)
31	CLA	A	825	1	58,62,73	2.77	24 (41%)	69,99,113	2.61	27 (39%)
31	CLA	A	845	1	60,64,73	2.59	22 (36%)	72,102,113	2.50	23 (31%)
26	BCR	2	302	-	41,41,41	1.10	3 (7%)	56,56,56	1.27	7 (12%)
31	CLA	B	834	2	69,73,73	2.86	21 (30%)	83,113,113	2.37	27 (32%)
31	CLA	5	323	22	60,64,73	3.01	19 (31%)	72,102,113	2.56	26 (36%)
31	CLA	A	835	1	59,63,73	2.85	23 (38%)	71,101,113	2.51	22 (30%)
31	CLA	A	856	44	69,73,73	2.40	21 (30%)	83,113,113	2.32	24 (28%)
31	CLA	B	823	2	59,63,73	2.68	21 (35%)	71,101,113	2.54	26 (36%)
31	CLA	2	313	20	50,54,73	3.36	20 (40%)	60,90,113	2.55	21 (35%)
31	CLA	4	318	21	49,53,73	3.74	22 (44%)	59,89,113	2.64	23 (38%)
26	BCR	K	203	-	41,41,41	1.10	2 (4%)	56,56,56	1.27	6 (10%)
31	CLA	3	318	14	55,59,73	3.48	21 (38%)	66,96,113	2.60	28 (42%)
31	CLA	B	814	2	69,73,73	3.07	23 (33%)	83,113,113	2.36	24 (28%)
38	AXT	a	304	-	44,44,45	0.70	1 (2%)	55,62,64	0.91	1 (1%)
31	CLA	b	303	-	50,54,73	4.11	23 (46%)	60,90,113	2.72	24 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	B	821	2	62,66,73	2.68	19 (30%)	74,104,113	2.42	22 (29%)
26	BCR	A	803	-	41,41,41	1.04	2 (4%)	56,56,56	1.13	3 (5%)
31	CLA	9	312	17	50,54,73	2.88	20 (40%)	60,90,113	2.68	22 (36%)
31	CLA	4	308	21	64,68,73	2.41	22 (34%)	77,107,113	2.50	27 (35%)
31	CLA	G	205	7	50,54,73	2.90	23 (46%)	60,90,113	2.66	21 (35%)
31	CLA	a	321	44	54,58,73	2.92	19 (35%)	65,95,113	2.66	30 (46%)
36	LUT	4	302	-	42,43,43	5.65	19 (45%)	51,60,60	5.74	34 (66%)
31	CLA	a	312	13	69,73,73	3.10	23 (33%)	83,113,113	2.37	24 (28%)
31	CLA	3	313	-	64,68,73	2.76	20 (31%)	77,107,113	2.50	27 (35%)
28	LHG	B	807	31	31,31,48	0.81	1 (3%)	34,37,54	1.27	4 (11%)
27	LMT	9	306	-	36,36,36	1.26	6 (16%)	47,47,47	0.95	2 (4%)
32	CHL	3	315	44	60,64,74	2.30	17 (28%)	68,102,114	2.60	25 (36%)
36	LUT	a	305	-	42,43,43	5.74	20 (47%)	51,60,60	5.70	29 (56%)
31	CLA	3	307	14	69,73,73	3.13	23 (33%)	83,113,113	2.32	27 (32%)
26	BCR	B	802	-	41,41,41	1.06	2 (4%)	56,56,56	1.16	4 (7%)
31	CLA	b	305	13	50,54,73	3.19	25 (50%)	60,90,113	2.59	25 (41%)
35	QTB	F	303	-	19,19,19	1.31	3 (15%)	20,26,26	1.32	4 (20%)
31	CLA	7	316	15	50,54,73	3.28	22 (44%)	60,90,113	2.70	24 (40%)
31	CLA	7	313	15	47,52,73	3.09	23 (48%)	56,88,113	2.64	21 (37%)
32	CHL	A	831	1	62,66,74	2.23	19 (30%)	70,104,114	2.61	28 (40%)
36	LUT	3	305	-	42,43,43	5.47	19 (45%)	51,60,60	5.76	32 (62%)
31	CLA	5	307	22	59,63,73	3.80	22 (37%)	71,101,113	2.48	28 (39%)
31	CLA	3	311	14	69,73,73	2.78	23 (33%)	83,113,113	2.33	26 (31%)
32	CHL	8	316	44	70,74,74	2.12	20 (28%)	80,114,114	2.19	25 (31%)
31	CLA	8	317	44	54,58,73	2.83	21 (38%)	65,95,113	2.71	25 (38%)
32	CHL	5	319	-	51,55,74	3.28	19 (37%)	57,91,114	2.47	22 (38%)
35	QTB	9	304	-	19,19,19	1.29	2 (10%)	20,26,26	1.46	2 (10%)
31	CLA	3	308	14	50,54,73	3.63	22 (44%)	60,90,113	2.71	22 (36%)
31	CLA	J	105	10	46,50,73	3.15	21 (45%)	55,85,113	2.85	23 (41%)
31	CLA	3	314	14	56,60,73	2.99	20 (35%)	67,97,113	2.49	26 (38%)
35	QTB	a	302	-	19,19,19	1.28	2 (10%)	20,26,26	1.69	4 (20%)
31	CLA	A	816	1	69,73,73	2.49	20 (28%)	83,113,113	2.26	25 (30%)
36	LUT	4	303	-	42,43,43	5.65	19 (45%)	51,60,60	5.53	31 (60%)
31	CLA	4	320	21	49,53,73	3.35	24 (48%)	59,89,113	2.66	24 (40%)
32	CHL	b	309	13	51,55,74	2.41	20 (39%)	57,91,114	2.43	23 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	A	814	44	69,73,73	2.69	23 (33%)	83,113,113	2.33	26 (31%)
31	CLA	A	821	1	69,73,73	2.55	20 (28%)	83,113,113	2.42	26 (31%)
31	CLA	K	206	11	50,54,73	3.36	20 (40%)	60,90,113	2.62	21 (35%)
27	LMT	A	807	-	36,36,36	1.21	6 (16%)	47,47,47	1.06	3 (6%)
31	CLA	A	830	1	64,68,73	2.90	23 (35%)	77,107,113	2.49	27 (35%)
31	CLA	7	311	15	69,73,73	2.46	21 (30%)	83,113,113	2.31	24 (28%)
31	CLA	B	838	2	50,54,73	2.99	24 (48%)	60,90,113	2.58	24 (40%)
31	CLA	4	305	21	56,60,73	2.42	22 (39%)	67,97,113	4.56	35 (52%)
26	BCR	3	303	-	41,41,41	1.08	3 (7%)	56,56,56	1.25	5 (8%)
31	CLA	8	318	16	54,58,73	2.53	20 (37%)	65,95,113	2.58	25 (38%)
36	LUT	L	304	31	42,43,43	5.64	20 (47%)	51,60,60	5.75	33 (64%)
31	CLA	A	834	44	69,73,73	2.42	21 (30%)	83,113,113	2.25	23 (27%)
31	CLA	B	847	2	69,73,73	2.79	22 (31%)	83,113,113	2.32	21 (25%)
31	CLA	H	902	44	50,54,73	3.75	22 (44%)	60,90,113	2.66	24 (40%)
31	CLA	4	314	-	49,53,73	4.21	22 (44%)	59,89,113	2.77	26 (44%)
31	CLA	8	307	16	50,54,73	3.01	23 (46%)	60,90,113	2.75	23 (38%)
31	CLA	9	317	-	51,55,73	3.44	24 (47%)	61,91,113	2.65	21 (34%)
31	CLA	A	848	1	61,65,73	2.78	21 (34%)	73,103,113	2.37	23 (31%)
31	CLA	B	833	44	59,63,73	2.41	21 (35%)	71,101,113	2.43	21 (29%)
31	CLA	3	320	14	49,53,73	3.56	23 (46%)	59,89,113	2.71	23 (38%)
31	CLA	L	306	44	49,53,73	2.76	23 (46%)	59,89,113	2.66	22 (37%)
31	CLA	A	849	1	50,54,73	3.42	22 (44%)	60,90,113	2.60	23 (38%)
31	CLA	B	832	44	69,73,73	2.37	22 (31%)	83,113,113	2.49	29 (34%)
31	CLA	7	309	15	64,68,73	2.32	21 (32%)	77,107,113	2.37	26 (33%)
31	CLA	B	849	2	54,58,73	3.07	21 (38%)	65,95,113	2.56	24 (36%)
31	CLA	A	850	1	55,59,73	2.81	22 (40%)	66,96,113	2.65	26 (39%)
32	CHL	4	317	-	50,54,74	2.62	18 (36%)	56,90,114	2.48	23 (41%)
31	CLA	8	314	44	56,60,73	2.74	21 (37%)	67,97,113	2.59	28 (41%)
31	CLA	6	322	23	50,54,73	3.10	22 (44%)	60,90,113	2.62	24 (40%)
31	CLA	4	319	-	46,50,73	4.16	22 (47%)	55,85,113	2.71	24 (43%)
32	CHL	8	319	44	49,53,74	2.62	18 (36%)	54,88,114	2.57	22 (40%)
26	BCR	M	101	-	41,41,41	1.05	2 (4%)	56,56,56	1.16	3 (5%)
32	CHL	4	313	21	52,56,74	3.66	17 (32%)	58,92,114	2.46	26 (44%)
32	CHL	4	310	-	51,55,74	3.10	20 (39%)	57,91,114	2.43	23 (40%)
36	LUT	6	304	-	42,43,43	5.62	19 (45%)	51,60,60	5.35	31 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	J	104	-	29,29,55	1.03	1 (3%)	37,37,63	1.19	3 (8%)
33	DGD	B	808	-	62,62,67	1.03	2 (3%)	76,76,81	1.29	5 (6%)
31	CLA	7	310	15	48,52,73	3.30	22 (45%)	58,88,113	2.78	25 (43%)
31	CLA	a	311	44	64,68,73	2.68	22 (34%)	77,107,113	2.47	28 (36%)
31	CLA	O	203	44	59,63,73	2.74	23 (38%)	71,101,113	2.53	28 (39%)
31	CLA	B	819	2	69,73,73	2.53	23 (33%)	83,113,113	2.48	29 (34%)
26	BCR	B	805	-	41,41,41	1.05	2 (4%)	56,56,56	1.29	5 (8%)
26	BCR	G	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	4 (7%)
31	CLA	A	837	1	69,73,73	2.50	21 (30%)	83,113,113	2.33	24 (28%)
32	CHL	9	320	44	52,56,74	2.51	19 (36%)	58,92,114	2.40	23 (39%)
31	CLA	A	826	1	69,73,73	2.53	21 (30%)	83,113,113	2.31	25 (30%)
28	LHG	a	306	31	48,48,48	0.62	1 (2%)	51,54,54	1.23	5 (9%)
31	CLA	5	309	22	51,55,73	3.84	22 (43%)	61,91,113	2.64	24 (39%)
31	CLA	B	811	2	69,73,73	2.57	21 (30%)	83,113,113	2.42	24 (28%)
31	CLA	B	837	2	59,63,73	2.94	22 (37%)	71,101,113	2.37	25 (35%)
37	LMG	G	202	-	44,44,55	0.87	1 (2%)	52,52,63	1.30	5 (9%)
31	CLA	2	314	20	50,54,73	4.80	22 (44%)	60,90,113	2.63	25 (41%)
32	CHL	7	319	15	51,55,74	2.61	20 (39%)	57,91,114	2.82	18 (31%)
32	CHL	a	317	13	65,69,74	2.20	19 (29%)	74,108,114	2.26	29 (39%)
31	CLA	b	304	13	50,54,73	4.05	24 (48%)	60,90,113	2.60	23 (38%)
31	CLA	a	322	13	50,54,73	3.20	21 (42%)	60,90,113	2.56	23 (38%)
32	CHL	7	324	16	70,74,74	1.82	20 (28%)	80,114,114	2.20	28 (35%)
31	CLA	B	826	2	54,58,73	2.83	22 (40%)	65,95,113	2.71	25 (38%)
27	LMT	A	808	-	36,36,36	1.21	5 (13%)	47,47,47	0.99	2 (4%)
31	CLA	2	311	20	49,53,73	4.96	23 (46%)	59,89,113	2.62	22 (37%)
31	CLA	A	853	1	69,73,73	2.68	22 (31%)	83,113,113	2.34	28 (33%)
31	CLA	2	309	-	50,54,73	2.69	21 (42%)	60,90,113	2.58	23 (38%)
26	BCR	F	302	-	41,41,41	0.98	2 (4%)	56,56,56	1.02	2 (3%)
35	QTB	7	303	-	19,19,19	1.28	2 (10%)	20,26,26	1.53	4 (20%)
31	CLA	A	847	1	69,73,73	2.60	20 (28%)	83,113,113	2.44	25 (30%)
31	CLA	2	304	20	50,54,73	3.19	23 (46%)	60,90,113	2.61	21 (35%)
31	CLA	A	822	1	59,63,73	2.66	23 (38%)	71,101,113	2.58	27 (38%)
36	LUT	9	305	-	42,43,43	5.68	19 (45%)	51,60,60	5.95	32 (62%)
31	CLA	A	844	1	54,58,73	3.12	22 (40%)	65,95,113	2.61	24 (36%)
31	CLA	7	314	44	58,62,73	2.76	21 (36%)	70,100,113	2.52	27 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	A	817	31,1	59,63,73	2.77	21 (35%)	71,101,113	2.54	23 (32%)
32	CHL	A	840	1	70,74,74	2.23	20 (28%)	80,114,114	2.12	24 (30%)
31	CLA	B	818	2	59,63,73	2.44	19 (32%)	71,101,113	2.50	26 (36%)
26	BCR	B	804	-	41,41,41	1.03	2 (4%)	56,56,56	1.12	3 (5%)
31	CLA	A	815	-	69,73,73	2.63	21 (30%)	83,113,113	2.31	25 (30%)
31	CLA	A	819	1	69,73,73	2.32	22 (31%)	83,113,113	2.42	29 (34%)
31	CLA	A	846	1	69,73,73	2.60	22 (31%)	83,113,113	2.38	27 (32%)
26	BCR	B	806	-	41,41,41	1.04	2 (4%)	56,56,56	1.05	5 (8%)
31	CLA	B	828	44	64,68,73	2.47	21 (32%)	77,107,113	2.35	25 (32%)
31	CLA	A	832	1	69,73,73	2.30	19 (27%)	83,113,113	2.24	24 (28%)
26	BCR	8	301	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	6 (10%)
31	CLA	4	315	44	49,53,73	5.09	23 (46%)	59,89,113	2.64	23 (38%)
31	CLA	G	206	44	49,53,73	3.45	21 (42%)	59,89,113	2.61	21 (35%)
31	CLA	B	848	28	69,73,73	2.29	22 (31%)	83,113,113	2.35	24 (28%)
31	CLA	B	824	2	61,65,73	3.09	23 (37%)	73,103,113	2.52	27 (36%)
26	BCR	K	202	-	41,41,41	1.07	2 (4%)	56,56,56	1.25	8 (14%)
31	CLA	b	313	13	64,68,73	3.42	22 (34%)	77,107,113	2.35	25 (32%)
36	LUT	J	103	-	42,43,43	5.66	20 (47%)	51,60,60	5.75	31 (60%)
31	CLA	2	307	20	61,65,73	2.89	22 (36%)	73,103,113	2.53	26 (35%)
31	CLA	2	305	20	49,53,73	4.13	22 (44%)	59,89,113	2.71	22 (37%)
31	CLA	A	836	1	64,68,73	2.58	22 (34%)	77,107,113	2.44	25 (32%)
32	CHL	6	319	-	51,55,74	4.63	20 (39%)	57,91,114	2.54	26 (45%)
31	CLA	4	321	21	54,58,73	3.73	22 (40%)	65,95,113	2.64	28 (43%)
31	CLA	2	310	20	49,53,73	6.63	23 (46%)	59,89,113	2.69	24 (40%)
36	LUT	7	305	-	42,43,43	5.55	20 (47%)	51,60,60	5.71	31 (60%)
31	CLA	4	316	-	51,55,73	3.33	24 (47%)	61,91,113	2.98	21 (34%)
28	LHG	7	307	31	36,36,48	0.77	1 (2%)	39,42,54	1.24	4 (10%)
31	CLA	F	301	44	69,73,73	2.49	23 (33%)	83,113,113	2.40	28 (33%)
36	LUT	9	302	-	42,43,43	5.49	20 (47%)	51,60,60	5.76	33 (64%)
36	LUT	3	304	-	42,43,43	5.56	20 (47%)	51,60,60	5.67	33 (64%)
31	CLA	b	308	13	50,54,73	3.61	23 (46%)	60,90,113	2.57	24 (40%)
31	CLA	5	313	28	50,54,73	3.64	25 (50%)	60,90,113	2.76	21 (35%)
27	LMT	5	301	-	36,36,36	1.22	5 (13%)	47,47,47	0.96	2 (4%)
28	LHG	A	810	31	41,41,48	0.72	1 (2%)	44,47,54	1.14	4 (9%)
31	CLA	7	315	28	59,63,73	3.78	23 (38%)	70,100,113	2.53	25 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	XAT	7	306	-	39,47,47	1.60	8 (20%)	54,74,74	1.55	9 (16%)
31	CLA	H	903	18	50,54,73	3.04	20 (40%)	60,90,113	2.56	21 (35%)
36	LUT	F	304	-	42,43,43	5.43	20 (47%)	51,60,60	6.02	35 (68%)
36	LUT	5	304	-	42,43,43	5.61	19 (45%)	51,60,60	5.48	31 (60%)
31	CLA	8	321	16	50,54,73	3.19	21 (42%)	60,90,113	2.68	20 (33%)
31	CLA	A	857	44	69,73,73	2.24	20 (28%)	83,113,113	2.42	29 (34%)
36	LUT	8	303	-	42,43,43	5.52	20 (47%)	51,60,60	5.71	34 (66%)
31	CLA	b	306	-	50,54,73	4.62	22 (44%)	60,90,113	2.63	22 (36%)
31	CLA	2	312	20	50,54,73	3.61	22 (44%)	60,90,113	2.72	24 (40%)
39	3PH	7	301	-	32,32,47	0.75	1 (3%)	36,37,52	0.73	1 (2%)
26	BCR	L	301	-	41,41,41	0.98	1 (2%)	56,56,56	1.19	5 (8%)
31	CLA	2	315	44	50,54,73	3.23	23 (46%)	60,90,113	2.70	23 (38%)
26	BCR	3	302	-	41,41,41	1.07	2 (4%)	56,56,56	1.17	4 (7%)
31	CLA	B	827	2	64,68,73	2.42	19 (29%)	77,107,113	2.45	25 (32%)
26	BCR	A	806	-	41,41,41	1.01	2 (4%)	56,56,56	1.10	5 (8%)
31	CLA	5	321	22	50,54,73	3.35	20 (40%)	60,90,113	2.70	25 (41%)
31	CLA	B	830	2	64,68,73	2.65	22 (34%)	77,107,113	2.32	27 (35%)
36	LUT	5	303	-	42,43,43	5.56	19 (45%)	51,60,60	5.70	33 (64%)
31	CLA	3	316	44	54,58,73	2.61	22 (40%)	65,95,113	2.55	25 (38%)
32	CHL	5	317	44	51,55,74	2.97	18 (35%)	57,91,114	2.55	21 (36%)
31	CLA	B	850	2	66,70,73	2.60	21 (31%)	79,109,113	2.30	24 (30%)
32	CHL	5	322	22	51,55,74	2.98	19 (37%)	57,91,114	2.46	23 (40%)
31	CLA	a	309	13	64,68,73	4.60	24 (37%)	77,107,113	2.47	29 (37%)
31	CLA	L	305	18	64,68,73	2.55	22 (34%)	77,107,113	2.41	24 (31%)
31	CLA	b	310	-	50,54,73	2.80	21 (42%)	60,90,113	2.60	23 (38%)
32	CHL	6	320	-	51,55,74	3.08	19 (37%)	57,91,114	2.41	21 (36%)
31	CLA	4	309	21	64,68,73	2.53	23 (35%)	77,107,113	2.49	31 (40%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
30	CL0	A	813	1	69,73,73	1.85	17 (24%)	83,113,113	3.26	30 (36%)
31	CLA	4	312	21	51,55,73	2.91	22 (43%)	61,91,113	2.63	25 (40%)
31	CLA	A	828	1	69,73,73	2.53	23 (33%)	83,113,113	2.38	24 (28%)
31	CLA	B	817	2	69,73,73	2.47	21 (30%)	83,113,113	2.43	25 (30%)
31	CLA	L	307	36	49,53,73	3.87	20 (40%)	59,89,113	2.67	24 (40%)
31	CLA	A	854	28	50,54,73	2.85	21 (42%)	60,90,113	2.75	21 (35%)
31	CLA	B	831	2	54,58,73	2.67	23 (42%)	65,95,113	2.60	28 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CLA	H	901	8	50,54,73	2.78	22 (44%)	60,90,113	2.59	25 (41%)
31	CLA	B	845	2	54,58,73	2.77	21 (38%)	65,95,113	2.66	25 (38%)
31	CLA	B	815	2	69,73,73	2.31	21 (30%)	83,113,113	2.35	25 (30%)
31	CLA	8	320	16	69,73,73	2.56	23 (33%)	83,113,113	2.28	27 (32%)
32	CHL	6	309	23	70,74,74	2.14	20 (28%)	80,114,114	2.11	25 (31%)
24	PQN	A	801	-	34,34,34	0.35	0	42,45,45	0.58	0
32	CHL	6	317	23	51,55,74	2.76	20 (39%)	57,91,114	2.41	22 (38%)
37	LMG	a	301	-	42,42,55	0.83	0	50,50,63	1.26	4 (8%)
32	CHL	6	321	23	47,51,74	3.60	18 (38%)	52,86,114	2.49	22 (42%)
31	CLA	F	305	6	50,54,73	2.88	23 (46%)	60,90,113	2.80	26 (43%)
31	CLA	6	314	23	51,55,73	4.15	22 (43%)	61,91,113	2.68	24 (39%)
31	CLA	6	315	28	50,54,73	5.69	24 (48%)	60,90,113	2.68	22 (36%)
31	CLA	5	314	22	49,53,73	3.34	23 (46%)	59,89,113	2.72	24 (40%)
31	CLA	B	813	2	69,73,73	2.73	24 (34%)	83,113,113	2.44	25 (30%)
26	BCR	J	102	-	41,41,41	0.99	2 (4%)	56,56,56	1.20	3 (5%)
31	CLA	a	315	28	59,63,73	2.56	22 (37%)	71,101,113	2.60	24 (33%)
43	PTY	5	306	-	30,30,49	0.54	0	33,35,54	0.80	1 (3%)
31	CLA	B	844	2	69,73,73	2.42	21 (30%)	83,113,113	2.36	25 (30%)
32	CHL	a	320	44	52,56,74	2.29	19 (36%)	58,92,114	2.52	22 (37%)
31	CLA	8	313	28	50,54,73	3.49	24 (48%)	60,90,113	2.70	23 (38%)
26	BCR	G	203	-	41,41,41	1.09	2 (4%)	56,56,56	1.18	4 (7%)
31	CLA	2	306	20	64,68,73	3.44	24 (37%)	77,107,113	2.38	26 (33%)
31	CLA	A	855	1	69,73,73	2.75	21 (30%)	83,113,113	2.36	26 (31%)
31	CLA	O	204	-	45,49,73	3.04	22 (48%)	54,84,113	2.76	25 (46%)
26	BCR	3	301	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	6 (10%)
31	CLA	3	309	14	69,73,73	2.32	22 (31%)	83,113,113	2.39	27 (32%)
31	CLA	B	840	2	69,73,73	2.48	24 (34%)	83,113,113	2.33	25 (30%)
28	LHG	A	809	-	41,41,48	0.72	2 (4%)	44,47,54	1.29	6 (13%)
28	LHG	8	304	31	48,48,48	0.63	1 (2%)	51,54,54	1.24	6 (11%)
36	LUT	9	303	-	42,43,43	5.55	19 (45%)	51,60,60	5.53	30 (58%)
26	BCR	6	302	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
31	CLA	b	312	13	50,54,73	5.15	22 (44%)	60,90,113	2.61	24 (40%)
31	CLA	B	841	2	59,63,73	2.67	21 (35%)	71,101,113	2.55	28 (39%)
31	CLA	6	316	23	54,58,73	4.63	23 (42%)	65,95,113	2.65	27 (41%)
31	CLA	4	311	28	50,54,73	6.47	23 (46%)	60,90,113	2.62	24 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	B	803	-	41,41,41	1.08	2 (4%)	56,56,56	1.16	2 (3%)
31	CLA	B	816	2	65,69,73	3.02	22 (33%)	78,108,113	2.51	26 (33%)
36	LUT	6	303	-	42,43,43	5.57	19 (45%)	51,60,60	5.78	34 (66%)
31	CLA	7	322	15	50,54,73	3.20	22 (44%)	60,90,113	2.62	22 (36%)
31	CLA	A	833	1	51,55,73	3.42	23 (45%)	61,91,113	2.78	24 (39%)
26	BCR	A	804	-	41,41,41	1.09	2 (4%)	56,56,56	1.14	4 (7%)
31	CLA	9	318	44	69,73,73	2.89	20 (28%)	83,113,113	2.30	26 (31%)
31	CLA	5	320	22	50,54,73	5.59	25 (50%)	60,90,113	2.67	26 (43%)
31	CLA	6	312	23	69,73,73	3.13	24 (34%)	83,113,113	2.34	25 (30%)
31	CLA	B	829	2	59,63,73	2.55	21 (35%)	71,101,113	2.69	25 (35%)
31	CLA	8	308	16	69,73,73	2.63	25 (36%)	83,113,113	2.35	25 (30%)
31	CLA	5	315	22	69,73,73	4.22	23 (33%)	83,113,113	4.28	28 (33%)
31	CLA	8	310	16	69,73,73	2.54	22 (31%)	83,113,113	2.40	24 (28%)
31	CLA	b	302	13	50,54,73	2.98	21 (42%)	60,90,113	2.73	25 (41%)
31	CLA	3	310	14	64,68,73	3.06	22 (34%)	77,107,113	2.46	26 (33%)
31	CLA	A	843	1	69,73,73	2.82	22 (31%)	83,113,113	2.27	24 (28%)
25	SF4	C	102	3	0,12,12	-	-	-	-	-
31	CLA	6	306	23	50,54,73	3.30	25 (50%)	60,90,113	2.70	18 (30%)
31	CLA	5	310	22	69,73,73	2.66	23 (33%)	83,113,113	2.39	29 (34%)
31	CLA	B	839	2	64,68,73	2.57	23 (35%)	77,107,113	2.37	26 (33%)
31	CLA	B	812	-	69,73,73	2.31	22 (31%)	83,113,113	2.39	26 (31%)
36	LUT	a	303	-	42,43,43	5.61	19 (45%)	51,60,60	5.48	34 (66%)
31	CLA	B	836	2	69,73,73	2.52	21 (30%)	83,113,113	2.27	24 (28%)
26	BCR	L	302	-	41,41,41	1.04	2 (4%)	56,56,56	1.14	6 (10%)
37	LMG	J	101	-	49,49,55	0.83	3 (6%)	57,57,63	1.23	2 (3%)
32	CHL	7	317	15	61,65,74	2.45	20 (32%)	69,103,114	2.30	26 (37%)
31	CLA	9	319	17	50,54,73	5.00	21 (42%)	60,90,113	2.73	25 (41%)
31	CLA	A	852	1	55,59,73	3.30	22 (40%)	66,96,113	2.68	24 (36%)
31	CLA	O	202	19	40,46,73	3.33	21 (52%)	48,80,113	2.78	22 (45%)
31	CLA	9	314	17	64,68,73	3.49	23 (35%)	77,107,113	2.44	25 (32%)
28	LHG	6	301	31	26,26,48	0.78	0	29,32,54	1.22	2 (6%)
31	CLA	A	851	1	69,73,73	2.77	22 (31%)	83,113,113	2.31	22 (26%)
31	CLA	A	827	1	59,63,73	2.84	21 (35%)	71,101,113	2.47	22 (30%)
31	CLA	8	315	16	56,60,73	2.85	23 (41%)	67,97,113	2.55	28 (41%)
31	CLA	b	311	13	50,54,73	3.86	23 (46%)	60,90,113	2.68	24 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
42	SQD	4	304	-	34,35,54	1.80	7 (20%)	43,46,65	1.54	6 (13%)
31	CLA	9	313	17	49,53,73	4.51	24 (48%)	59,89,113	2.75	22 (37%)
31	CLA	B	822	2	69,73,73	2.64	22 (31%)	83,113,113	2.27	23 (27%)
31	CLA	8	311	16	59,63,73	2.87	22 (37%)	71,101,113	2.55	25 (35%)
31	CLA	9	316	17	54,58,73	2.97	22 (40%)	65,95,113	2.61	23 (35%)
26	BCR	5	302	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
31	CLA	a	313	13	64,68,73	2.69	24 (37%)	77,107,113	2.45	24 (31%)
31	CLA	5	312	44	54,58,73	2.81	22 (40%)	65,95,113	2.66	28 (43%)
24	PQN	B	801	-	34,34,34	0.51	0	42,45,45	0.75	1 (2%)
31	CLA	6	313	23	50,54,73	2.97	24 (48%)	60,90,113	2.79	24 (40%)
31	CLA	a	319	13	69,73,73	2.50	20 (28%)	83,113,113	2.40	26 (31%)
31	CLA	F	306	44	54,58,73	2.79	21 (38%)	65,95,113	2.60	26 (40%)
26	BCR	A	805	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	5 (8%)
31	CLA	A	829	44	54,58,73	2.57	16 (29%)	65,95,113	3.22	26 (40%)
31	CLA	8	309	16	54,58,73	3.09	22 (40%)	65,95,113	2.74	30 (46%)
26	BCR	I	801	-	41,41,41	1.05	1 (2%)	56,56,56	1.18	4 (7%)
32	CHL	K	201	11	51,55,74	2.20	19 (37%)	57,91,114	3.20	22 (38%)
28	LHG	A	811	-	48,48,48	0.72	1 (2%)	51,54,54	1.26	5 (9%)
34	LAP	B	851	-	28,28,28	0.34	0	33,35,35	0.38	0
31	CLA	2	308	20	50,54,73	3.03	22 (44%)	60,90,113	2.72	25 (41%)
32	CHL	7	318	44	70,74,74	2.29	19 (27%)	80,114,114	2.32	25 (31%)
31	CLA	A	824	31,1	66,70,73	2.72	20 (30%)	79,109,113	2.38	26 (32%)
32	CHL	7	320	44	65,69,74	3.05	20 (30%)	74,108,114	2.28	27 (36%)
31	CLA	a	316	13	49,53,73	3.23	22 (44%)	59,89,113	2.66	26 (44%)
31	CLA	4	306	21	49,53,73	3.26	23 (46%)	59,89,113	2.67	25 (42%)
31	CLA	B	820	2	69,73,73	3.04	24 (34%)	83,113,113	2.32	25 (30%)
31	CLA	6	310	23	51,55,73	4.59	23 (45%)	61,91,113	2.68	26 (42%)
32	CHL	9	322	44	51,55,74	3.36	22 (43%)	57,91,114	2.45	24 (42%)
31	CLA	B	842	2	65,69,73	2.74	21 (32%)	78,108,113	2.42	29 (37%)
36	LUT	b	301	-	42,43,43	5.67	19 (45%)	51,60,60	5.69	33 (64%)
31	CLA	4	307	21	60,64,73	2.72	22 (36%)	72,102,113	2.45	29 (40%)
31	CLA	A	818	1	69,73,73	2.26	22 (31%)	83,113,113	2.35	25 (30%)
31	CLA	6	307	23	54,58,73	3.90	22 (40%)	65,95,113	2.56	27 (41%)
31	CLA	B	825	2	64,68,73	2.71	23 (35%)	77,107,113	2.46	26 (33%)
28	LHG	6	305	31	31,31,48	0.74	1 (3%)	34,37,54	1.29	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	BCR	L	303	-	41,41,41	1.05	2 (4%)	56,56,56	1.20	6 (10%)
28	LHG	7	302	-	48,48,48	0.58	0	51,54,54	1.26	5 (9%)
31	CLA	9	315	17	58,62,73	2.71	21 (36%)	69,99,113	2.62	27 (39%)
31	CLA	8	312	44	54,58,73	2.86	21 (38%)	65,95,113	2.58	25 (38%)
31	CLA	3	319	14	65,69,73	2.81	22 (33%)	78,108,113	2.47	28 (35%)
26	BCR	7	304	-	41,41,41	1.06	2 (4%)	56,56,56	1.19	4 (7%)
31	CLA	6	311	23	59,63,73	4.05	22 (37%)	71,101,113	2.53	27 (38%)
31	CLA	B	846	44	69,73,73	2.41	21 (30%)	83,113,113	2.27	25 (30%)
31	CLA	A	842	1	69,73,73	2.83	23 (33%)	83,113,113	2.43	26 (31%)
36	LUT	8	302	-	42,43,43	5.50	19 (45%)	51,60,60	5.63	31 (60%)
31	CLA	5	318	22	69,73,73	5.34	23 (33%)	83,113,113	2.32	27 (32%)
31	CLA	A	841	1	69,73,73	2.49	21 (30%)	83,113,113	2.51	28 (33%)
31	CLA	B	835	2	61,65,73	3.04	22 (36%)	73,103,113	2.51	25 (34%)
32	CHL	A	839	44	60,64,74	2.15	19 (31%)	68,102,114	2.85	27 (39%)

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
28	LHG	5	305	31	-	24/39/39/53	-
31	CLA	6	308	44	-	7/18/94/115	-
31	CLA	7	321	44	-	7/18/94/115	-
31	CLA	a	314	44	-	6/21/97/115	-
31	CLA	K	204	44	-	5/21/97/115	-
32	CHL	5	316	44	-	14/29/105/117	-
25	SF4	A	802	2,1	-	-	0/6/5/5
41	DGA	8	305	-	-	18/29/29/45	-
31	CLA	9	311	17	-	5/27/103/115	-
31	CLA	A	838	44	-	11/39/115/115	-
31	CLA	B	843	44	-	5/15/91/115	-
26	BCR	O	201	-	-	4/29/63/63	0/2/2/2
32	CHL	6	318	44	-	11/17/93/117	-
31	CLA	A	820	1	-	4/27/103/115	-
31	CLA	5	311	22	-	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	CHL	a	318	44	-	6/20/96/117	-
31	CLA	3	312	44	-	9/39/115/115	-
33	DGD	7	308	-	-	14/41/81/95	0/2/2/2
31	CLA	3	317	44	-	8/23/99/115	-
31	CLA	G	204	7	-	5/21/97/115	-
31	CLA	b	307	-	-	7/17/93/115	-
31	CLA	9	321	17	-	14/29/105/115	-
31	CLA	A	823	1	-	7/27/103/115	-
31	CLA	K	205	11	-	3/17/93/115	-
31	CLA	7	312	15	-	11/36/112/115	-
36	LUT	2	301	-	-	13/29/67/67	0/2/2/2
31	CLA	a	310	13	-	7/15/91/115	-
31	CLA	5	308	22	-	4/17/93/115	-
31	CLA	A	825	1	-	2/26/102/115	-
31	CLA	A	845	1	-	7/29/105/115	-
26	BCR	2	302	-	-	7/29/63/63	0/2/2/2
31	CLA	B	834	2	-	5/39/115/115	-
31	CLA	5	323	22	-	9/29/105/115	-
31	CLA	A	835	1	-	5/27/103/115	-
31	CLA	A	856	44	-	7/39/115/115	-
31	CLA	B	823	2	-	9/27/103/115	-
31	CLA	2	313	20	-	8/17/93/115	-
31	CLA	4	318	21	-	7/15/91/115	-
26	BCR	K	203	-	-	5/29/63/63	0/2/2/2
31	CLA	3	318	14	-	9/23/99/115	-
31	CLA	B	814	2	-	16/39/115/115	-
38	AXT	a	304	-	-	2/29/71/75	0/2/2/2
31	CLA	b	303	-	-	5/17/93/115	-
31	CLA	B	821	2	-	4/31/107/115	-
26	BCR	A	803	-	-	5/29/63/63	0/2/2/2
31	CLA	9	312	17	-	2/17/93/115	-
31	CLA	4	308	21	-	8/33/109/115	-
31	CLA	G	205	7	-	6/17/93/115	-
31	CLA	a	321	44	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LUT	4	302	-	-	16/29/67/67	0/2/2/2
31	CLA	a	312	13	-	13/39/115/115	-
31	CLA	3	313	-	-	12/33/109/115	-
28	LHG	B	807	31	-	7/36/36/53	-
27	LMT	9	306	-	-	10/21/61/61	0/2/2/2
32	CHL	3	315	44	-	7/29/105/117	-
36	LUT	a	305	-	-	22/29/67/67	0/2/2/2
31	CLA	3	307	14	-	10/39/115/115	-
26	BCR	B	802	-	-	5/29/63/63	0/2/2/2
31	CLA	b	305	13	-	6/17/93/115	-
35	QTB	F	303	-	-	7/11/28/28	1/1/1/1
31	CLA	7	316	15	-	5/17/93/115	-
31	CLA	7	313	15	-	4/13/89/115	-
32	CHL	A	831	1	-	13/32/108/117	-
36	LUT	3	305	-	-	13/29/67/67	0/2/2/2
31	CLA	5	307	22	-	5/27/103/115	-
31	CLA	3	311	14	-	11/39/115/115	-
32	CHL	8	316	44	-	12/41/117/117	-
31	CLA	8	317	44	-	2/21/97/115	-
32	CHL	5	319	-	-	4/19/95/117	-
35	QTB	9	304	-	-	6/11/28/28	0/1/1/1
31	CLA	3	308	14	-	5/17/93/115	-
31	CLA	J	105	10	-	6/12/88/115	-
31	CLA	3	314	14	-	9/24/100/115	-
35	QTB	a	302	-	-	5/11/28/28	0/1/1/1
31	CLA	A	816	1	-	6/39/115/115	-
36	LUT	4	303	-	-	16/29/67/67	0/2/2/2
31	CLA	4	320	21	-	9/15/91/115	-
32	CHL	b	309	13	-	12/19/95/117	-
31	CLA	A	814	44	-	10/39/115/115	-
31	CLA	A	821	1	-	12/39/115/115	-
31	CLA	K	206	11	-	7/17/93/115	-
27	LMT	A	807	-	-	6/21/61/61	0/2/2/2
31	CLA	A	830	1	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	7	311	15	-	12/39/115/115	-
31	CLA	B	838	2	-	3/17/93/115	-
31	CLA	4	305	21	-	7/24/100/115	-
26	BCR	3	303	-	-	9/29/63/63	0/2/2/2
31	CLA	8	318	16	-	2/21/97/115	-
36	LUT	L	304	31	-	15/29/67/67	0/2/2/2
31	CLA	A	834	44	-	10/39/115/115	-
31	CLA	B	847	2	-	11/39/115/115	-
31	CLA	H	902	44	-	3/17/93/115	-
31	CLA	4	314	-	-	6/15/91/115	-
31	CLA	8	307	16	-	3/17/93/115	-
31	CLA	9	317	-	-	8/18/94/115	-
31	CLA	A	848	1	-	13/30/106/115	-
31	CLA	B	833	44	-	7/27/103/115	-
31	CLA	3	320	14	-	4/15/91/115	-
31	CLA	L	306	44	-	4/15/91/115	-
31	CLA	A	849	1	-	9/17/93/115	-
31	CLA	B	832	44	-	9/39/115/115	-
31	CLA	7	309	15	-	4/33/109/115	-
31	CLA	B	849	2	-	4/21/97/115	-
31	CLA	A	850	1	-	8/23/99/115	-
32	CHL	4	317	-	-	10/17/93/117	-
31	CLA	8	314	44	-	4/24/100/115	-
31	CLA	6	322	23	-	7/17/93/115	-
31	CLA	4	319	-	-	7/12/88/115	-
32	CHL	8	319	44	-	3/16/92/117	-
26	BCR	M	101	-	-	7/29/63/63	0/2/2/2
32	CHL	4	313	21	-	10/20/96/117	-
32	CHL	4	310	-	-	6/19/95/117	-
36	LUT	6	304	-	-	16/29/67/67	0/2/2/2
37	LMG	J	104	-	-	11/24/44/70	0/1/1/1
33	DGD	B	808	-	-	22/50/90/95	0/2/2/2
31	CLA	7	310	15	-	4/13/89/115	-
31	CLA	a	311	44	-	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	O	203	44	-	14/27/103/115	-
31	CLA	B	819	2	-	6/39/115/115	-
26	BCR	B	805	-	-	7/29/63/63	0/2/2/2
26	BCR	G	201	-	-	8/29/63/63	0/2/2/2
31	CLA	A	837	1	-	18/39/115/115	-
32	CHL	9	320	44	-	9/20/96/117	-
31	CLA	A	826	1	-	14/39/115/115	-
28	LHG	a	306	31	-	19/53/53/53	-
31	CLA	5	309	22	-	7/18/94/115	-
31	CLA	B	811	2	-	6/39/115/115	-
31	CLA	B	837	2	-	6/27/103/115	-
37	LMG	G	202	-	-	23/39/59/70	0/1/1/1
31	CLA	2	314	20	-	2/17/93/115	-
32	CHL	7	319	15	-	1/19/95/117	-
32	CHL	a	317	13	-	15/35/111/117	-
31	CLA	b	304	13	-	5/17/93/115	-
31	CLA	a	322	13	-	7/17/93/115	-
32	CHL	7	324	16	-	14/41/117/117	-
31	CLA	B	826	2	-	9/21/97/115	-
27	LMT	A	808	-	-	6/21/61/61	0/2/2/2
31	CLA	2	311	20	-	8/15/91/115	-
31	CLA	A	853	1	-	12/39/115/115	-
31	CLA	2	309	-	-	5/17/93/115	-
26	BCR	F	302	-	-	7/29/63/63	0/2/2/2
35	QTB	7	303	-	-	10/11/28/28	1/1/1/1
31	CLA	A	847	1	-	7/39/115/115	-
31	CLA	2	304	20	-	11/17/93/115	-
31	CLA	A	822	1	-	9/27/103/115	-
36	LUT	9	305	-	-	18/29/67/67	0/2/2/2
31	CLA	A	844	1	-	3/21/97/115	-
31	CLA	7	314	44	-	7/25/101/115	-
31	CLA	A	817	31,1	-	6/27/103/115	-
32	CHL	A	840	1	-	13/41/117/117	-
31	CLA	B	818	2	-	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	804	-	-	5/29/63/63	0/2/2/2
31	CLA	A	815	-	-	5/39/115/115	-
31	CLA	A	819	1	-	10/39/115/115	-
31	CLA	A	846	1	-	7/39/115/115	-
26	BCR	B	806	-	-	6/29/63/63	0/2/2/2
31	CLA	B	828	44	-	4/33/109/115	-
31	CLA	A	832	1	-	6/39/115/115	-
26	BCR	8	301	-	-	6/29/63/63	0/2/2/2
31	CLA	4	315	44	-	5/15/91/115	-
31	CLA	G	206	44	-	2/15/91/115	-
31	CLA	B	848	28	-	9/39/115/115	-
31	CLA	B	824	2	-	10/30/106/115	-
26	BCR	K	202	-	-	9/29/63/63	0/2/2/2
36	LUT	J	103	-	-	16/29/67/67	0/2/2/2
31	CLA	b	313	13	-	12/33/109/115	-
31	CLA	2	307	20	-	9/30/106/115	-
31	CLA	2	305	20	-	7/15/91/115	-
31	CLA	A	836	1	-	8/33/109/115	-
32	CHL	6	319	-	-	8/19/95/117	-
31	CLA	4	321	21	-	8/21/97/115	-
31	CLA	2	310	20	-	6/15/91/115	-
36	LUT	7	305	-	-	14/29/67/67	0/2/2/2
31	CLA	4	316	-	-	6/18/94/115	-
28	LHG	7	307	31	-	21/41/41/53	-
31	CLA	F	301	44	-	9/39/115/115	-
36	LUT	9	302	-	-	17/29/67/67	0/2/2/2
36	LUT	3	304	-	-	13/29/67/67	0/2/2/2
31	CLA	b	308	13	-	7/17/93/115	-
31	CLA	5	313	28	-	6/17/93/115	-
27	LMT	5	301	-	-	9/21/61/61	0/2/2/2
28	LHG	A	810	31	-	18/46/46/53	-
31	CLA	7	315	28	-	8/27/103/115	-
40	XAT	7	306	-	-	4/31/93/93	0/4/4/4
31	CLA	H	903	18	-	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	LUT	F	304	-	-	17/29/67/67	0/2/2/2
36	LUT	5	304	-	-	16/29/67/67	0/2/2/2
31	CLA	8	321	16	-	3/17/93/115	-
31	CLA	A	857	44	-	16/39/115/115	-
36	LUT	8	303	-	-	14/29/67/67	0/2/2/2
31	CLA	b	306	-	-	7/17/93/115	-
31	CLA	2	312	20	-	6/17/93/115	-
39	3PH	7	301	-	-	15/34/34/49	-
26	BCR	L	301	-	-	9/29/63/63	0/2/2/2
31	CLA	2	315	44	-	8/17/93/115	-
26	BCR	3	302	-	-	8/29/63/63	0/2/2/2
31	CLA	B	827	2	-	9/33/109/115	-
26	BCR	A	806	-	-	7/29/63/63	0/2/2/2
31	CLA	5	321	22	-	6/17/93/115	-
31	CLA	B	830	2	-	7/33/109/115	-
36	LUT	5	303	-	-	13/29/67/67	0/2/2/2
31	CLA	3	316	44	-	4/21/97/115	-
32	CHL	5	317	44	-	6/19/95/117	-
31	CLA	B	850	2	-	8/36/112/115	-
32	CHL	5	322	22	-	5/19/95/117	-
31	CLA	a	309	13	-	6/33/109/115	-
31	CLA	L	305	18	-	10/33/109/115	-
31	CLA	b	310	-	-	6/17/93/115	-
32	CHL	6	320	-	-	11/19/95/117	-
31	CLA	4	309	21	-	12/33/109/115	-
25	SF4	C	101	3	-	-	0/6/5/5
30	CL0	A	813	1	-	9/39/115/115	-
31	CLA	4	312	21	-	9/18/94/115	-
31	CLA	A	828	1	-	7/39/115/115	-
31	CLA	B	817	2	-	13/39/115/115	-
31	CLA	L	307	36	-	9/15/91/115	-
31	CLA	A	854	28	-	6/17/93/115	-
31	CLA	B	831	2	-	6/21/97/115	-
31	CLA	H	901	8	-	9/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	845	2	-	3/21/97/115	-
31	CLA	B	815	2	-	17/39/115/115	-
31	CLA	8	320	16	-	12/39/115/115	-
32	CHL	6	309	23	-	18/41/117/117	-
24	PQN	A	801	-	-	2/23/43/43	0/2/2/2
32	CHL	6	317	23	-	10/19/95/117	-
37	LMG	a	301	-	-	21/37/57/70	0/1/1/1
32	CHL	6	321	23	-	9/14/90/117	-
31	CLA	F	305	6	-	6/17/93/115	-
31	CLA	6	314	23	-	6/18/94/115	-
31	CLA	6	315	28	-	3/17/93/115	-
31	CLA	5	314	22	-	7/15/91/115	-
31	CLA	B	813	2	-	8/39/115/115	-
26	BCR	J	102	-	-	6/29/63/63	0/2/2/2
31	CLA	a	315	28	-	7/27/103/115	-
43	PTY	5	306	-	-	17/34/34/53	-
31	CLA	B	844	2	-	10/39/115/115	-
32	CHL	a	320	44	-	7/20/96/117	-
31	CLA	8	313	28	-	8/17/93/115	-
26	BCR	G	203	-	-	11/29/63/63	0/2/2/2
31	CLA	2	306	20	-	11/33/109/115	-
31	CLA	A	855	1	-	15/39/115/115	-
31	CLA	O	204	-	-	4/10/86/115	-
26	BCR	3	301	-	-	9/29/63/63	0/2/2/2
31	CLA	3	309	14	-	16/39/115/115	-
31	CLA	B	840	2	-	12/39/115/115	-
28	LHG	A	809	-	-	20/46/46/53	-
28	LHG	8	304	31	-	15/53/53/53	-
36	LUT	9	303	-	-	16/29/67/67	0/2/2/2
26	BCR	6	302	-	-	15/29/63/63	0/2/2/2
31	CLA	b	312	13	-	5/17/93/115	-
31	CLA	B	841	2	-	10/27/103/115	-
31	CLA	6	316	23	-	3/21/97/115	-
31	CLA	4	311	28	-	8/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	BCR	B	803	-	-	9/29/63/63	0/2/2/2
31	CLA	B	816	2	-	5/35/111/115	-
36	LUT	6	303	-	-	18/29/67/67	0/2/2/2
31	CLA	7	322	15	-	6/17/93/115	-
31	CLA	A	833	1	-	9/18/94/115	-
26	BCR	A	804	-	-	9/29/63/63	0/2/2/2
31	CLA	9	318	44	-	10/39/115/115	-
31	CLA	5	320	22	-	3/17/93/115	-
31	CLA	6	312	23	-	10/39/115/115	-
31	CLA	B	829	2	-	5/27/103/115	-
31	CLA	8	308	16	-	13/39/115/115	-
31	CLA	5	315	22	-	11/39/115/115	-
31	CLA	8	310	16	-	10/39/115/115	-
31	CLA	b	302	13	-	6/17/93/115	-
31	CLA	3	310	14	-	10/33/109/115	-
31	CLA	A	843	1	-	9/39/115/115	-
25	SF4	C	102	3	-	-	0/6/5/5
31	CLA	6	306	23	-	5/17/93/115	-
31	CLA	5	310	22	-	6/39/115/115	-
31	CLA	B	839	2	-	10/33/109/115	-
31	CLA	B	812	-	-	9/39/115/115	-
36	LUT	a	303	-	-	14/29/67/67	0/2/2/2
31	CLA	B	836	2	-	6/39/115/115	-
26	BCR	L	302	-	-	6/29/63/63	0/2/2/2
37	LMG	J	101	-	-	20/44/64/70	0/1/1/1
32	CHL	7	317	15	-	12/31/107/117	-
31	CLA	9	319	17	-	9/17/93/115	-
31	CLA	A	852	1	-	2/23/99/115	-
31	CLA	O	202	19	-	3/6/78/115	-
31	CLA	9	314	17	-	10/33/109/115	-
28	LHG	6	301	31	-	16/31/31/53	-
31	CLA	A	851	1	-	9/39/115/115	-
31	CLA	A	827	1	-	9/27/103/115	-
31	CLA	8	315	16	-	7/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	311	13	-	7/17/93/115	-
42	SQD	4	304	-	-	12/30/50/69	0/1/1/1
31	CLA	9	313	17	-	6/15/91/115	-
31	CLA	B	822	2	-	17/39/115/115	-
31	CLA	8	311	16	-	11/27/103/115	-
31	CLA	9	316	17	-	5/21/97/115	-
26	BCR	5	302	-	-	13/29/63/63	0/2/2/2
31	CLA	a	313	13	-	7/33/109/115	-
31	CLA	5	312	44	-	10/21/97/115	-
24	PQN	B	801	-	-	4/23/43/43	0/2/2/2
31	CLA	6	313	23	-	5/17/93/115	-
31	CLA	a	319	13	-	13/39/115/115	-
31	CLA	F	306	44	-	4/21/97/115	-
26	BCR	A	805	-	-	8/29/63/63	0/2/2/2
31	CLA	A	829	44	-	5/21/97/115	-
31	CLA	8	309	16	-	6/21/97/115	-
26	BCR	I	801	-	-	6/29/63/63	0/2/2/2
32	CHL	K	201	11	-	9/19/95/117	-
28	LHG	A	811	-	-	19/53/53/53	-
34	LAP	B	851	-	-	16/30/30/30	-
31	CLA	2	308	20	-	3/17/93/115	-
32	CHL	7	318	44	-	23/41/117/117	-
31	CLA	A	824	31,1	-	8/36/112/115	-
32	CHL	7	320	44	-	12/35/111/117	-
31	CLA	a	316	13	-	11/15/91/115	-
31	CLA	4	306	21	-	4/15/91/115	-
31	CLA	B	820	2	-	11/39/115/115	-
31	CLA	6	310	23	-	4/18/94/115	-
32	CHL	9	322	44	-	4/19/95/117	-
31	CLA	B	842	2	-	10/35/111/115	-
36	LUT	b	301	-	-	14/29/67/67	0/2/2/2
31	CLA	4	307	21	-	10/29/105/115	-
31	CLA	A	818	1	-	10/39/115/115	-
31	CLA	6	307	23	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	825	2	-	8/33/109/115	-
28	LHG	6	305	31	-	8/36/36/53	-
26	BCR	L	303	-	-	7/29/63/63	0/2/2/2
28	LHG	7	302	-	-	32/53/53/53	-
31	CLA	9	315	17	-	9/26/102/115	-
31	CLA	8	312	44	-	4/21/97/115	-
31	CLA	3	319	14	-	7/35/111/115	-
26	BCR	7	304	-	-	7/29/63/63	0/2/2/2
31	CLA	6	311	23	-	12/27/103/115	-
31	CLA	B	846	44	-	10/39/115/115	-
31	CLA	A	842	1	-	5/39/115/115	-
36	LUT	8	302	-	-	16/29/67/67	0/2/2/2
31	CLA	5	318	22	-	11/39/115/115	-
31	CLA	A	841	1	-	13/39/115/115	-
31	CLA	B	835	2	-	8/30/106/115	-
32	CHL	A	839	44	-	6/29/105/117	-

The worst 5 of 5939 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	310	CLA	MG-NA	30.68	2.79	2.06
31	b	307	CLA	MG-NA	29.70	2.76	2.06
31	6	315	CLA	MG-NA	29.56	2.76	2.06
31	5	318	CLA	MG-ND	-28.84	1.48	2.05
31	9	319	CLA	MG-NA	28.29	2.73	2.06

The worst 5 of 7142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	5	315	CLA	C4-C3-C5	-19.91	81.78	115.27
31	5	315	CLA	C5-C3-C2	19.18	159.93	121.12
31	5	315	CLA	C4-C3-C2	-17.67	78.34	123.68
36	7	305	LUT	C15-C14-C13	-17.12	102.87	127.31
36	2	301	LUT	C15-C14-C13	-16.15	104.26	127.31

There are no chirality outliers.

5 of 2970 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	A	804	BCR	C7-C8-C9-C10
26	A	804	BCR	C7-C8-C9-C34
26	A	804	BCR	C20-C21-C22-C23
26	A	805	BCR	C7-C8-C9-C34
26	A	805	BCR	C20-C21-C22-C37

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	F	303	QTB	C11-C12-C14-C15-C16-C17
35	7	303	QTB	C11-C12-C14-C15-C16-C17

268 monomers are involved in 540 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	5	305	LHG	1	0
31	6	308	CLA	1	0
31	7	321	CLA	1	0
31	a	314	CLA	2	0
32	5	316	CHL	6	0
41	8	305	DGA	2	0
31	A	838	CLA	1	0
31	B	843	CLA	2	0
26	O	201	BCR	2	0
32	6	318	CHL	5	0
31	A	820	CLA	2	0
31	5	311	CLA	2	0
32	a	318	CHL	4	0
31	G	204	CLA	1	0
31	A	823	CLA	4	0
36	2	301	LUT	4	0
31	a	310	CLA	1	0
31	5	308	CLA	1	0
31	A	825	CLA	4	0
31	A	845	CLA	4	0
26	2	302	BCR	3	0
31	B	834	CLA	3	0
31	5	323	CLA	3	0
31	A	835	CLA	3	0
31	A	856	CLA	3	0
31	B	823	CLA	1	0
31	2	313	CLA	2	0
31	4	318	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	K	203	BCR	3	0
31	3	318	CLA	1	0
31	B	814	CLA	3	0
38	a	304	AXT	1	0
26	A	803	BCR	3	0
31	4	308	CLA	1	0
31	G	205	CLA	1	0
31	a	321	CLA	1	0
36	4	302	LUT	7	0
31	a	312	CLA	2	0
31	3	313	CLA	2	0
28	B	807	LHG	1	0
32	3	315	CHL	1	0
36	a	305	LUT	6	0
26	B	802	BCR	4	0
31	b	305	CLA	1	0
31	7	313	CLA	1	0
32	A	831	CHL	2	0
36	3	305	LUT	7	0
31	5	307	CLA	2	0
31	3	311	CLA	2	0
32	8	316	CHL	8	0
31	8	317	CLA	1	0
32	5	319	CHL	4	0
31	3	308	CLA	2	0
31	J	105	CLA	1	0
31	3	314	CLA	1	0
31	A	816	CLA	2	0
36	4	303	LUT	4	0
32	b	309	CHL	1	0
31	A	814	CLA	5	0
31	A	821	CLA	3	0
31	K	206	CLA	1	0
27	A	807	LMT	4	0
31	A	830	CLA	2	0
31	7	311	CLA	3	0
31	B	838	CLA	1	0
31	4	305	CLA	5	0
26	3	303	BCR	2	0
36	L	304	LUT	1	0
31	A	834	CLA	6	0
31	B	847	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	H	902	CLA	6	0
31	4	314	CLA	5	0
31	8	307	CLA	1	0
31	A	848	CLA	1	0
31	B	833	CLA	1	0
31	3	320	CLA	2	0
31	A	849	CLA	1	0
31	B	832	CLA	2	0
31	7	309	CLA	1	0
31	A	850	CLA	2	0
32	4	317	CHL	7	0
31	8	314	CLA	1	0
31	6	322	CLA	3	0
31	4	319	CLA	1	0
32	8	319	CHL	1	0
26	M	101	BCR	3	0
32	4	313	CHL	3	0
32	4	310	CHL	7	0
36	6	304	LUT	3	0
33	B	808	DGD	4	0
31	a	311	CLA	1	0
31	B	819	CLA	2	0
26	B	805	BCR	5	0
26	G	201	BCR	1	0
31	A	837	CLA	4	0
32	9	320	CHL	3	0
31	A	826	CLA	3	0
28	a	306	LHG	9	0
31	5	309	CLA	1	0
31	B	811	CLA	1	0
31	B	837	CLA	4	0
37	G	202	LMG	4	0
31	2	314	CLA	3	0
32	7	319	CHL	3	0
32	a	317	CHL	6	0
32	7	324	CHL	3	0
31	B	826	CLA	1	0
31	2	311	CLA	1	0
31	A	853	CLA	4	0
26	F	302	BCR	1	0
31	2	304	CLA	4	0
31	A	822	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	9	305	LUT	1	0
32	A	840	CHL	5	0
31	B	818	CLA	2	0
26	B	804	BCR	4	0
31	A	815	CLA	3	0
31	A	819	CLA	3	0
31	A	846	CLA	3	0
26	B	806	BCR	2	0
31	A	832	CLA	2	0
26	8	301	BCR	4	0
31	4	315	CLA	2	0
31	G	206	CLA	6	0
31	B	848	CLA	2	0
26	K	202	BCR	4	0
31	b	313	CLA	3	0
36	J	103	LUT	3	0
31	A	836	CLA	3	0
32	6	319	CHL	2	0
31	4	321	CLA	1	0
31	2	310	CLA	1	0
36	7	305	LUT	3	0
31	4	316	CLA	4	0
28	7	307	LHG	4	0
31	F	301	CLA	3	0
36	9	302	LUT	1	0
36	3	304	LUT	3	0
31	b	308	CLA	1	0
31	5	313	CLA	1	0
28	A	810	LHG	2	0
31	7	315	CLA	4	0
31	H	903	CLA	2	0
36	F	304	LUT	2	0
36	5	304	LUT	6	0
31	8	321	CLA	2	0
31	A	857	CLA	3	0
36	8	303	LUT	2	0
31	2	312	CLA	1	0
39	7	301	3PH	1	0
26	L	301	BCR	1	0
31	2	315	CLA	1	0
26	3	302	BCR	4	0
26	A	806	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	303	LUT	3	0
32	5	317	CHL	4	0
31	B	850	CLA	4	0
32	5	322	CHL	4	0
31	a	309	CLA	3	0
31	L	305	CLA	6	0
32	6	320	CHL	1	0
30	A	813	CL0	3	0
31	4	312	CLA	1	0
31	A	828	CLA	2	0
31	B	817	CLA	2	0
31	A	854	CLA	1	0
31	B	831	CLA	2	0
31	H	901	CLA	2	0
31	B	845	CLA	4	0
31	B	815	CLA	1	0
31	8	320	CLA	1	0
32	6	309	CHL	7	0
24	A	801	PQN	1	0
32	6	317	CHL	3	0
37	a	301	LMG	2	0
32	6	321	CHL	2	0
31	6	314	CLA	2	0
31	6	315	CLA	1	0
31	B	813	CLA	4	0
26	J	102	BCR	1	0
31	a	315	CLA	3	0
43	5	306	PTY	1	0
31	B	844	CLA	2	0
32	a	320	CHL	3	0
31	8	313	CLA	1	0
31	2	306	CLA	3	0
31	A	855	CLA	3	0
26	3	301	BCR	1	0
31	3	309	CLA	6	0
31	B	840	CLA	2	0
28	A	809	LHG	2	0
36	9	303	LUT	6	0
26	6	302	BCR	2	0
31	B	841	CLA	3	0
31	6	316	CLA	1	0
31	4	311	CLA	1	0

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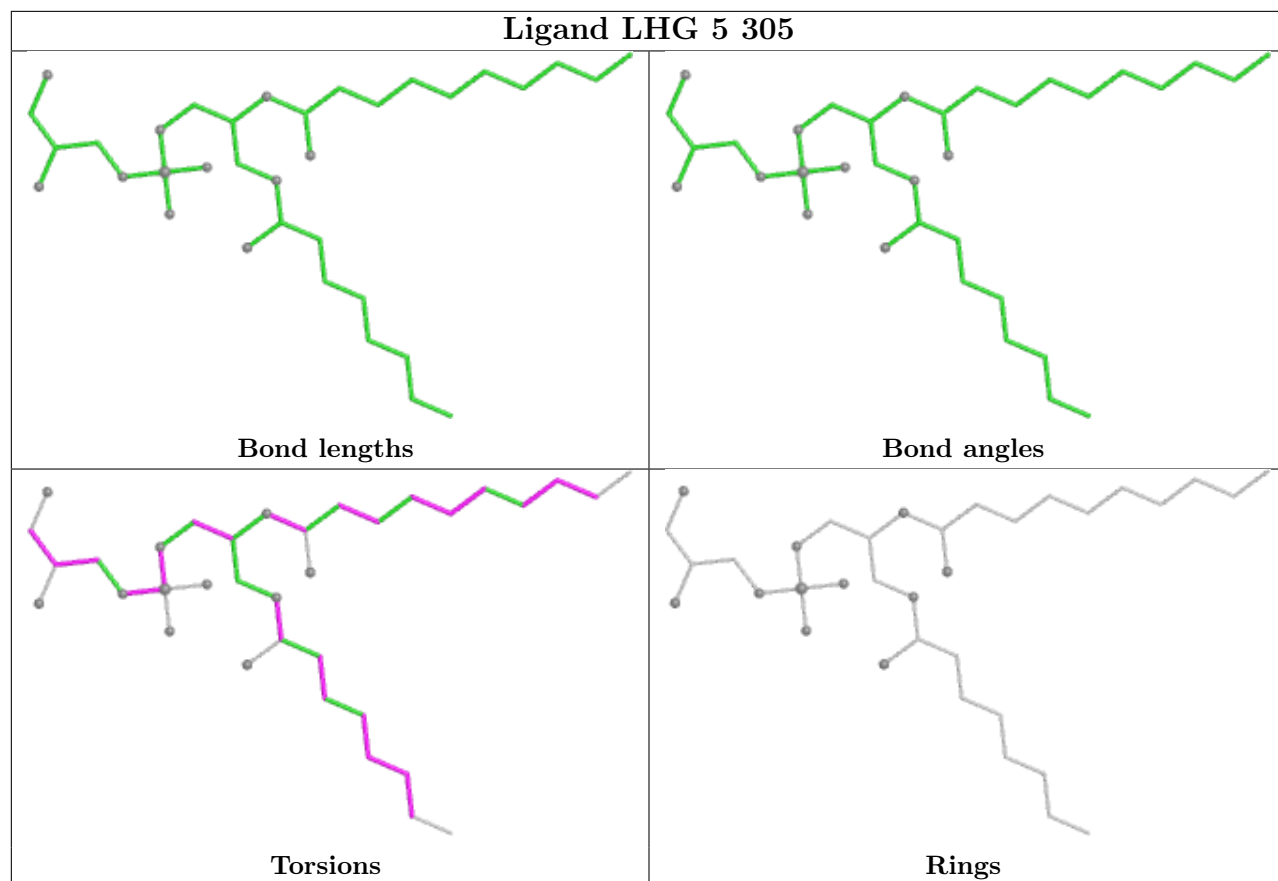
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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31	B	816	CLA	2	0
36	6	303	LUT	2	0
31	7	322	CLA	1	0
31	A	833	CLA	3	0
26	A	804	BCR	2	0
31	5	320	CLA	1	0
31	6	312	CLA	1	0
31	8	308	CLA	3	0
31	5	315	CLA	1	0
31	8	310	CLA	3	0
31	b	302	CLA	1	0
31	3	310	CLA	1	0
31	A	843	CLA	2	0
31	6	306	CLA	5	0
31	5	310	CLA	4	0
31	B	839	CLA	2	0
31	B	812	CLA	2	0
36	a	303	LUT	4	0
31	B	836	CLA	1	0
26	L	302	BCR	2	0
37	J	101	LMG	4	0
32	7	317	CHL	6	0
31	A	852	CLA	1	0
31	9	314	CLA	2	0
28	6	301	LHG	2	0
31	A	851	CLA	3	0
31	A	827	CLA	2	0
31	8	315	CLA	1	0
31	b	311	CLA	1	0
42	4	304	SQD	1	0
31	9	313	CLA	1	0
31	B	822	CLA	3	0
31	8	311	CLA	4	0
26	5	302	BCR	2	0
31	a	313	CLA	1	0
24	B	801	PQN	2	0
31	6	313	CLA	1	0
31	a	319	CLA	3	0
31	F	306	CLA	1	0
26	A	805	BCR	2	0
31	A	829	CLA	10	0

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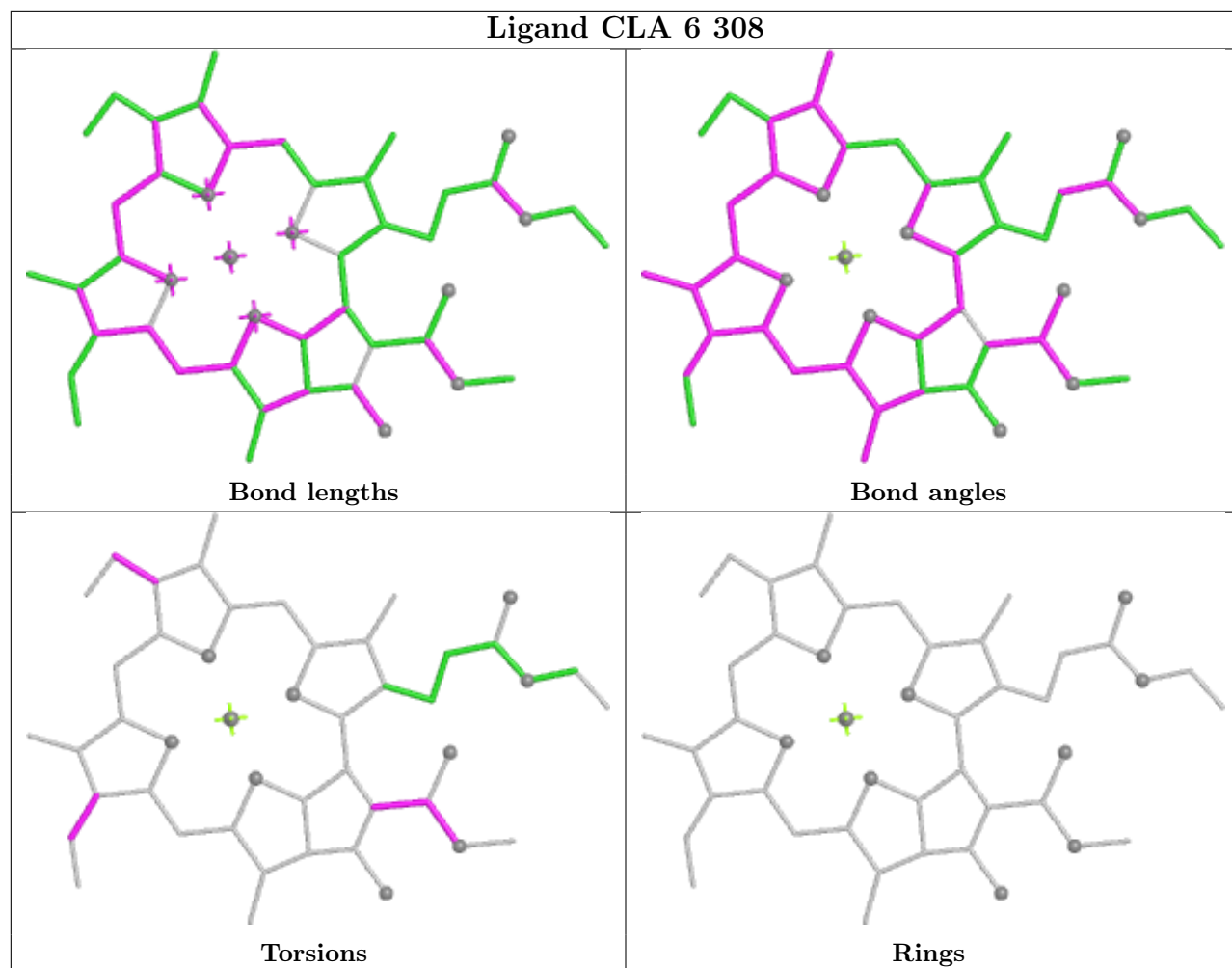
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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26	I	801	BCR	1	0
32	K	201	CHL	1	0
28	A	811	LHG	3	0
34	B	851	LAP	4	0
31	2	308	CLA	1	0
32	7	318	CHL	9	0
31	A	824	CLA	1	0
32	7	320	CHL	6	0
31	a	316	CLA	1	0
31	B	820	CLA	3	0
32	9	322	CHL	3	0
31	B	842	CLA	4	0
36	b	301	LUT	5	0
31	A	818	CLA	3	0
31	6	307	CLA	2	0
31	B	825	CLA	4	0
28	6	305	LHG	1	0
26	L	303	BCR	3	0
28	7	302	LHG	4	0
31	9	315	CLA	1	0
31	3	319	CLA	4	0
26	7	304	BCR	6	0
31	6	311	CLA	1	0
31	B	846	CLA	3	0
36	8	302	LUT	5	0
31	5	318	CLA	5	0
31	A	841	CLA	5	0
31	B	835	CLA	2	0
32	A	839	CHL	4	0

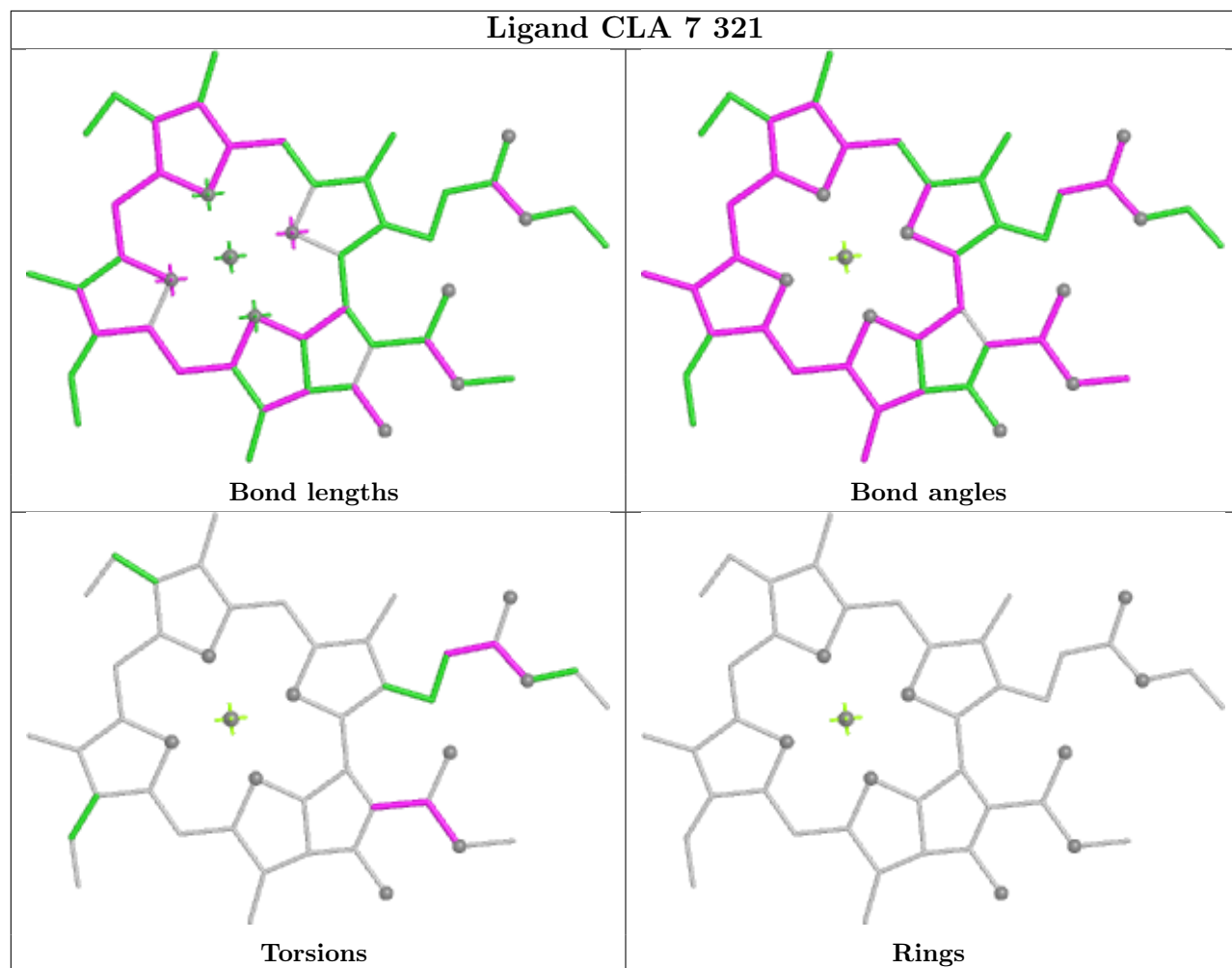
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

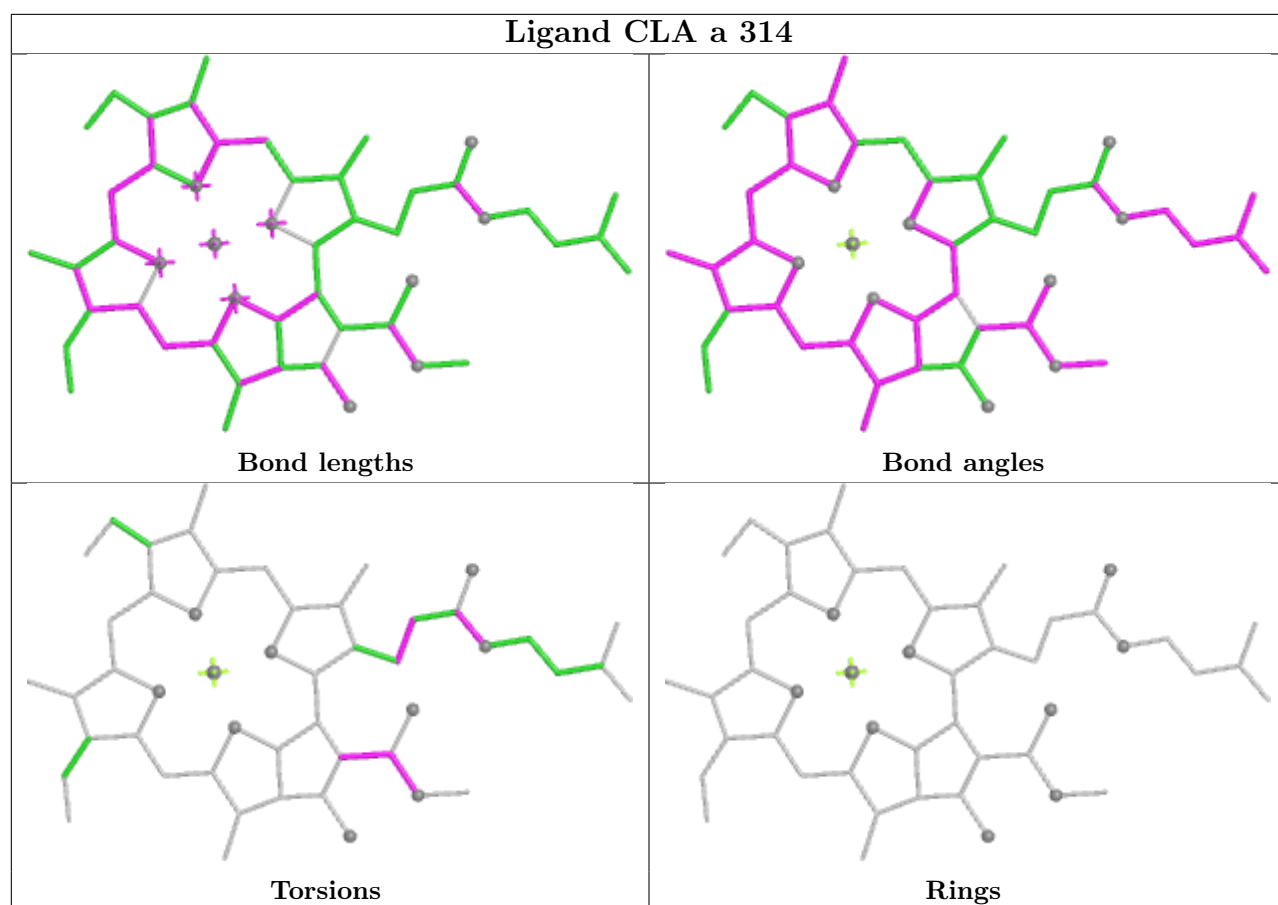


Ligand CLA 6 308

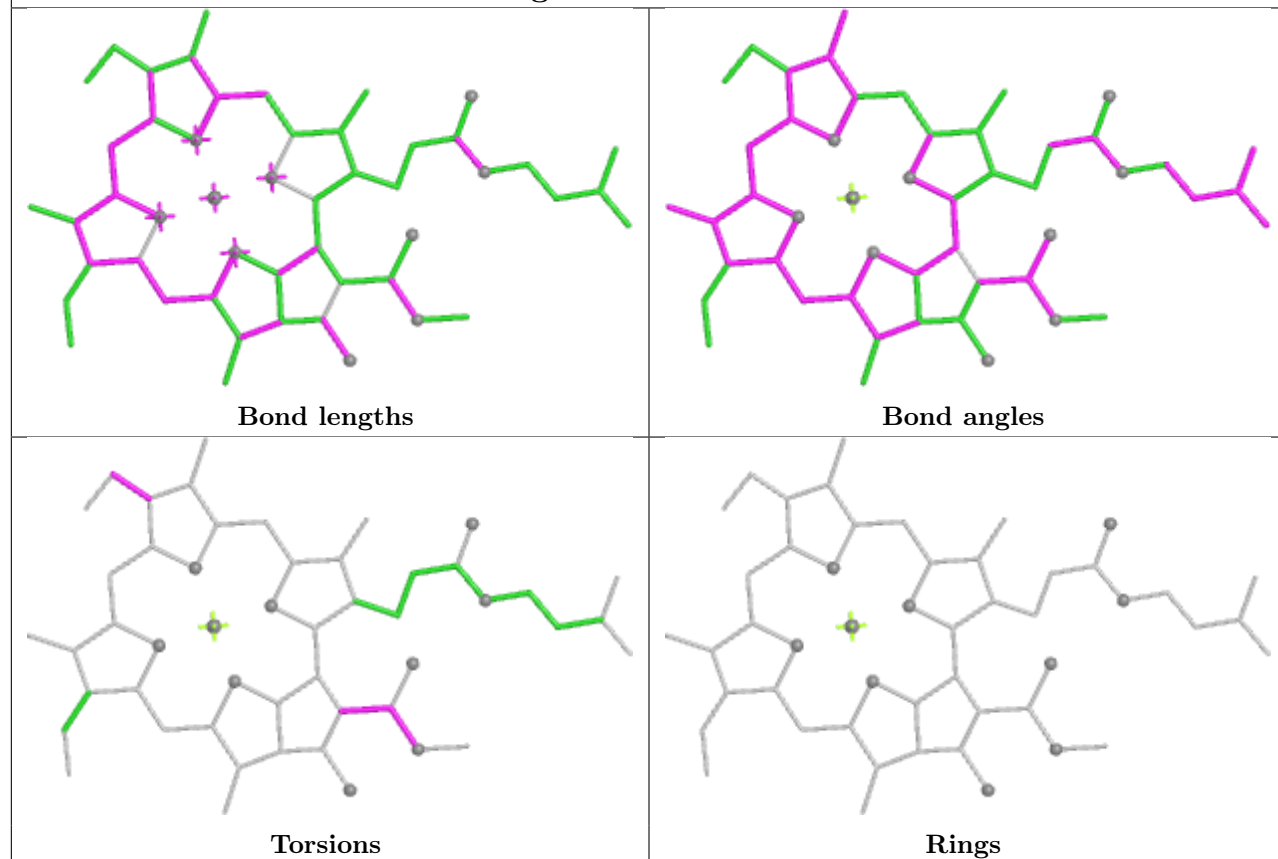


Ligand CLA 7 321

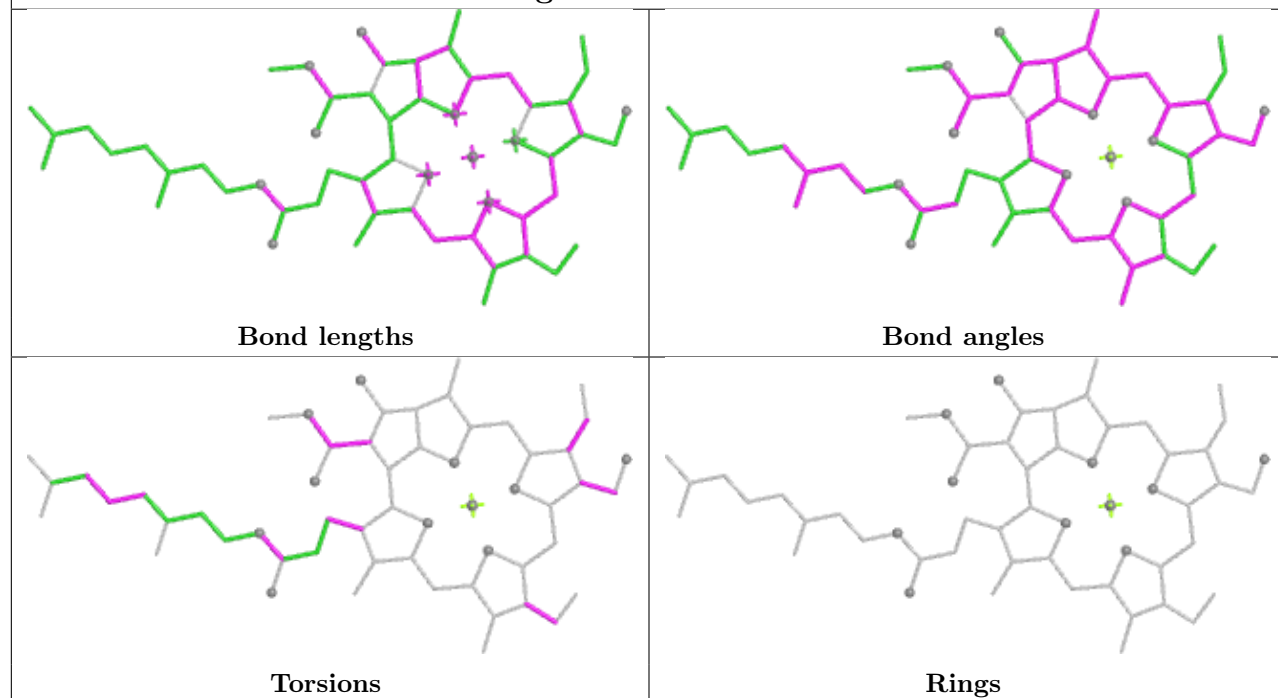


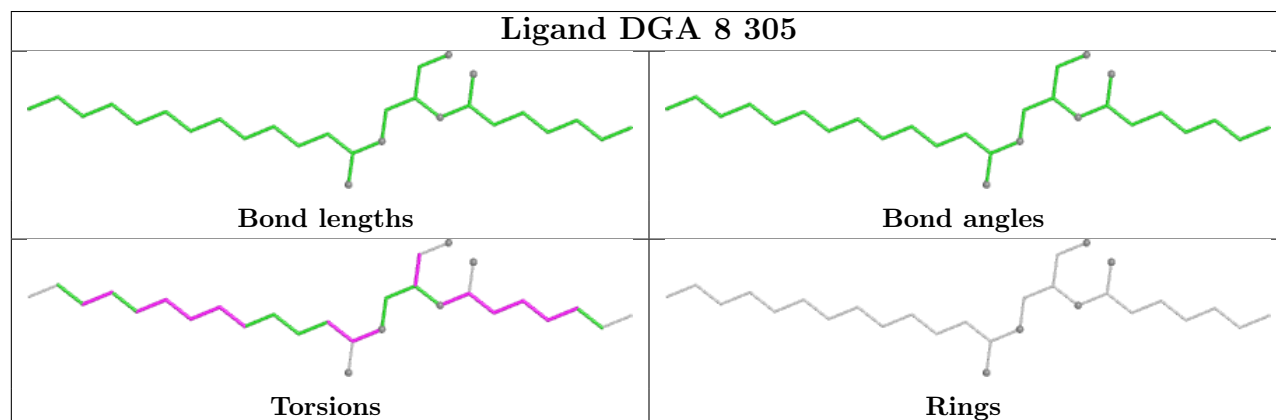
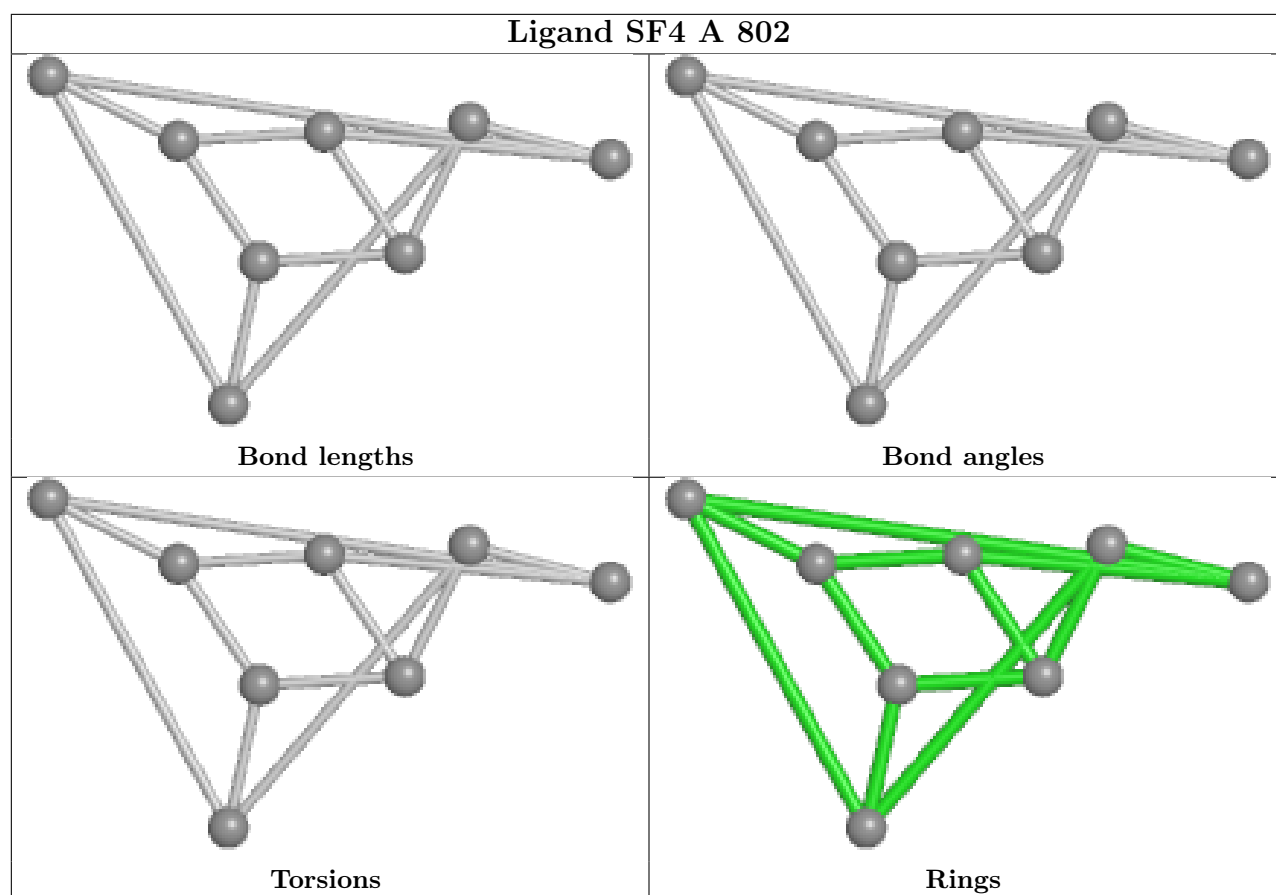


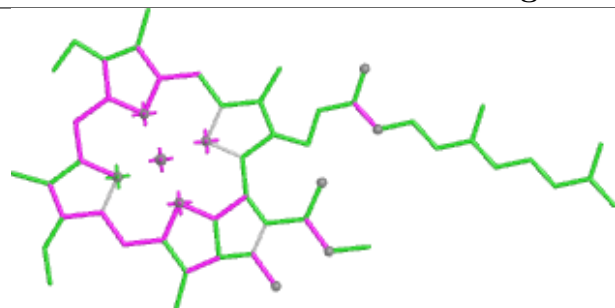
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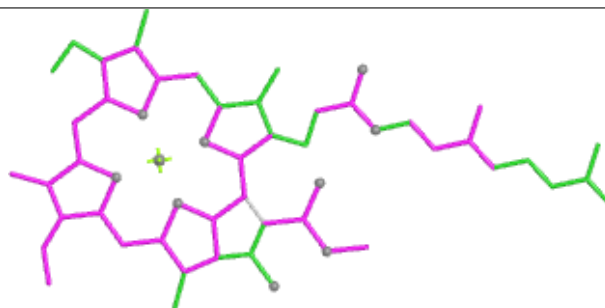
Ligand CHL 5 316



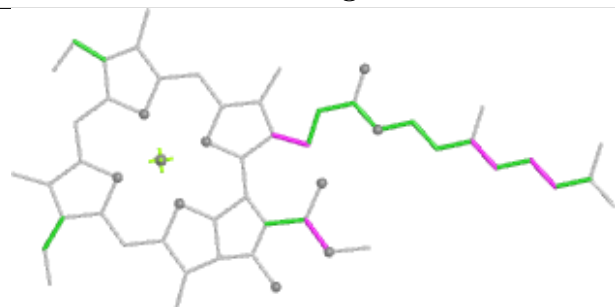


Ligand CLA 9 311

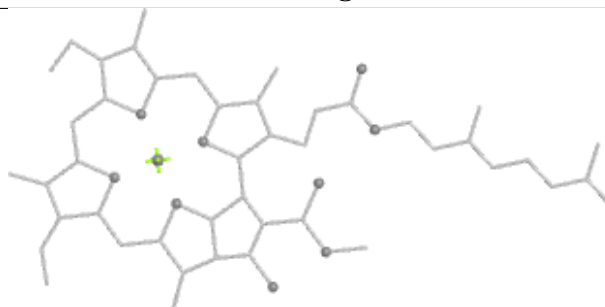
Bond lengths



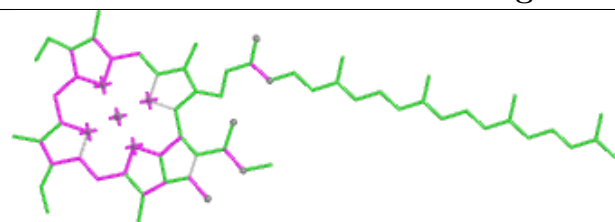
Bond angles



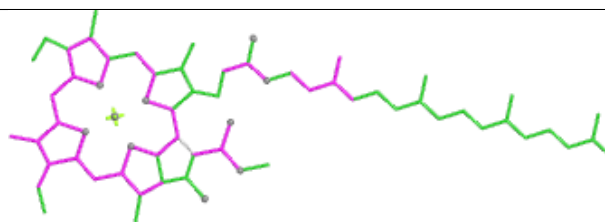
Torsions



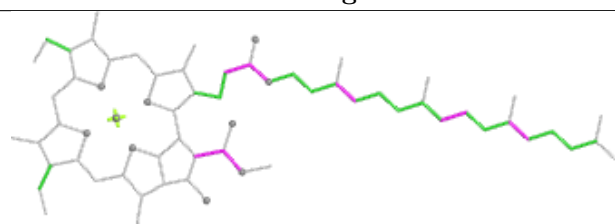
Rings

Ligand CLA A 838

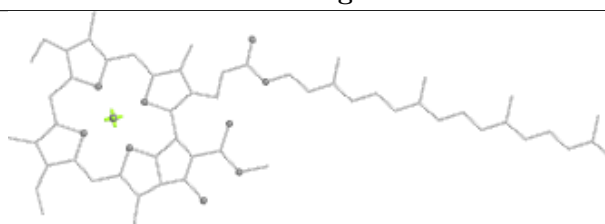
Bond lengths



Bond angles

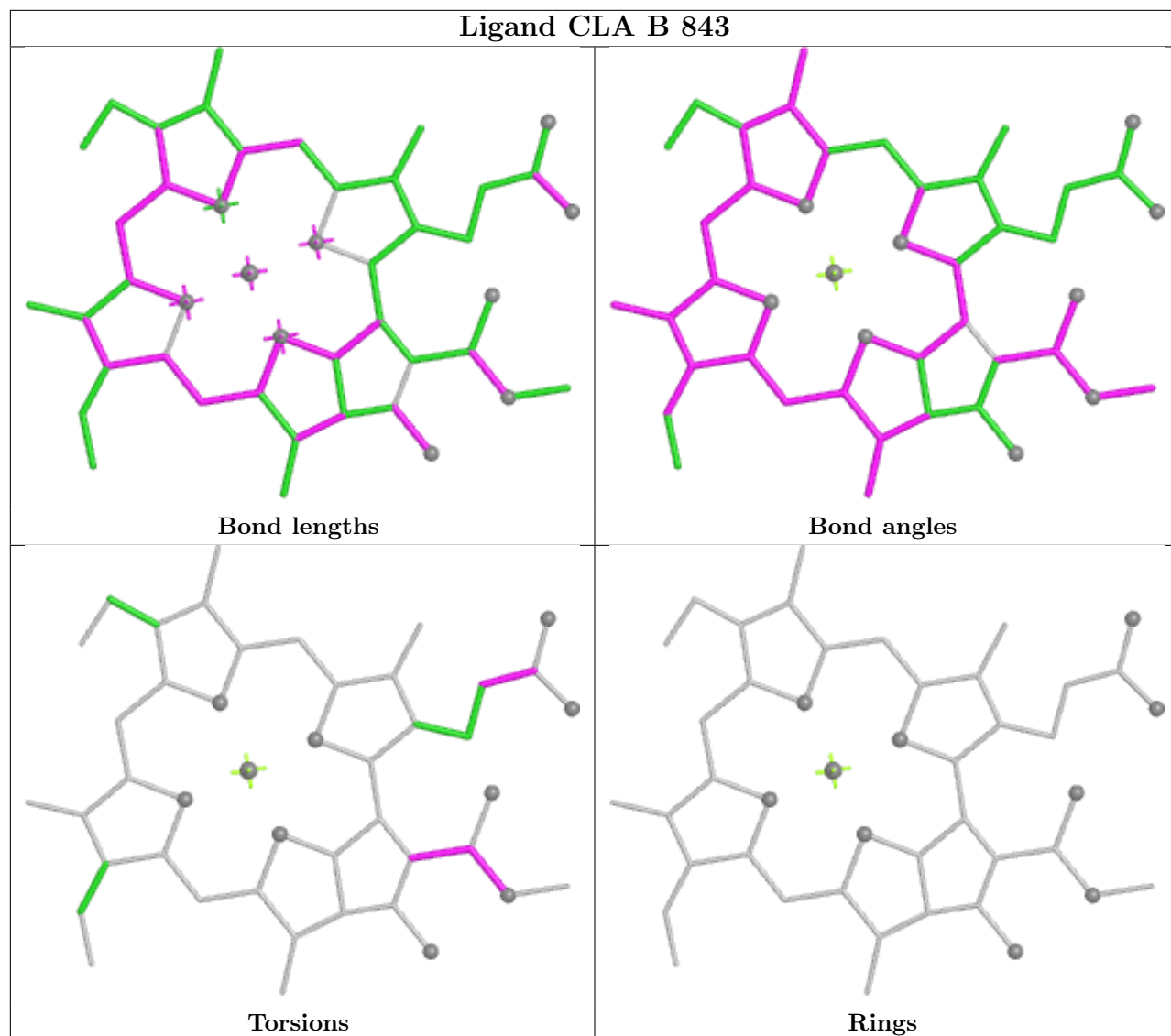


Torsions

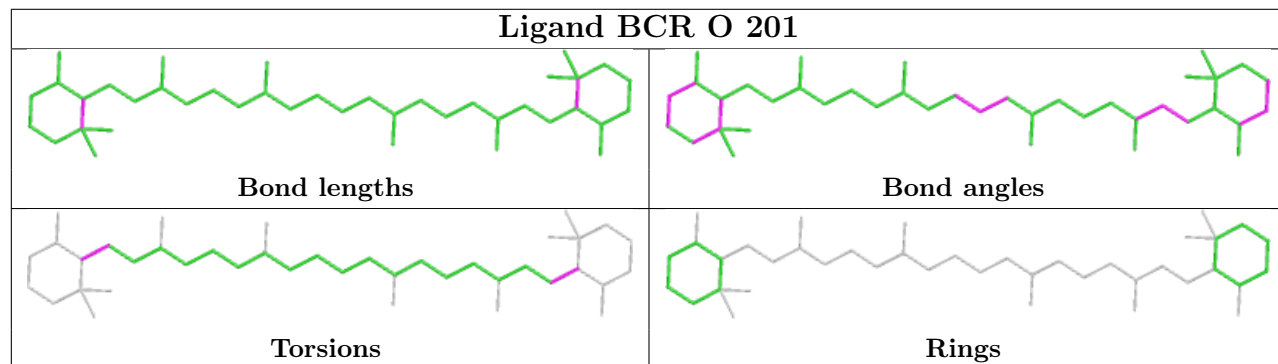


Rings

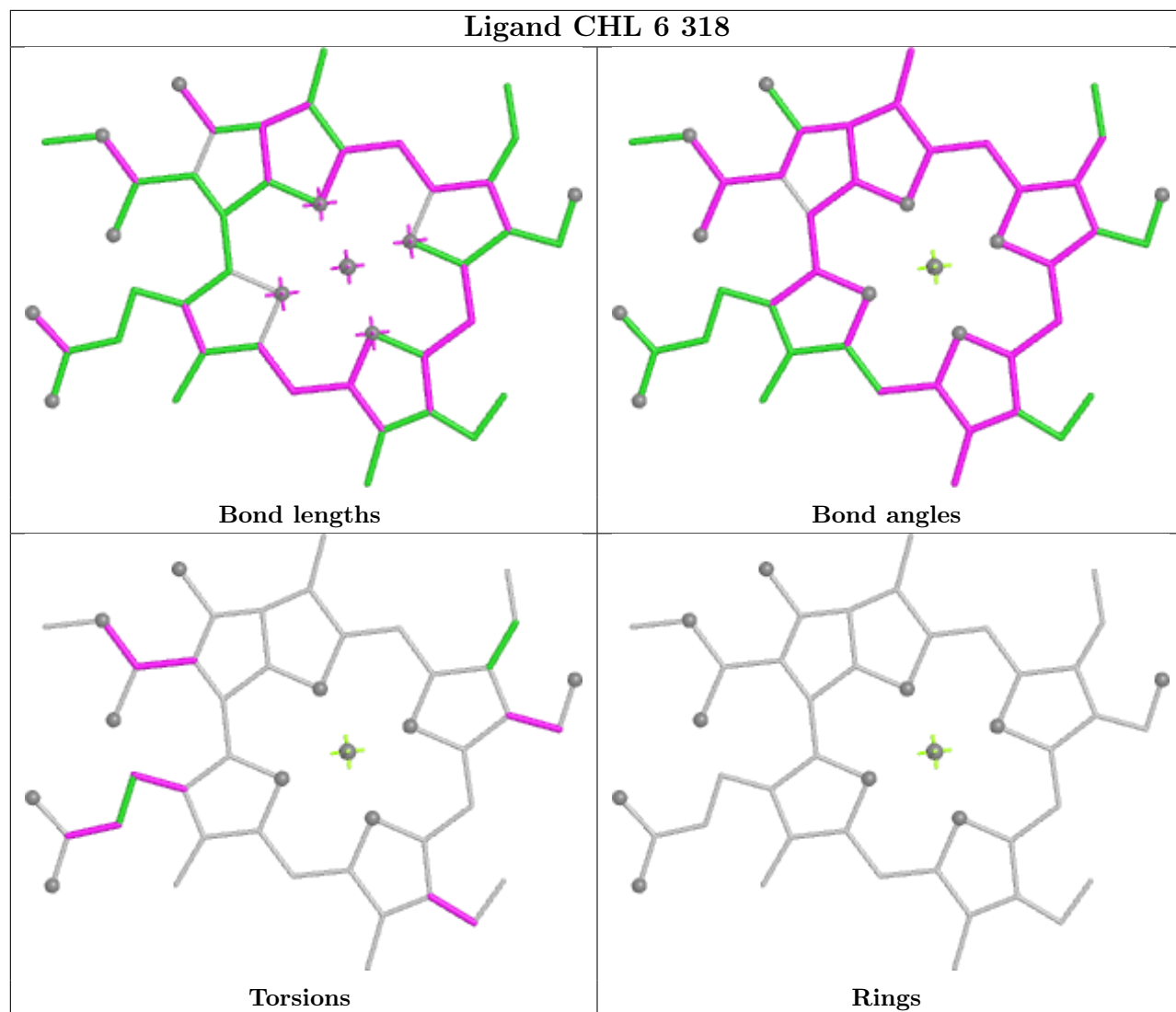
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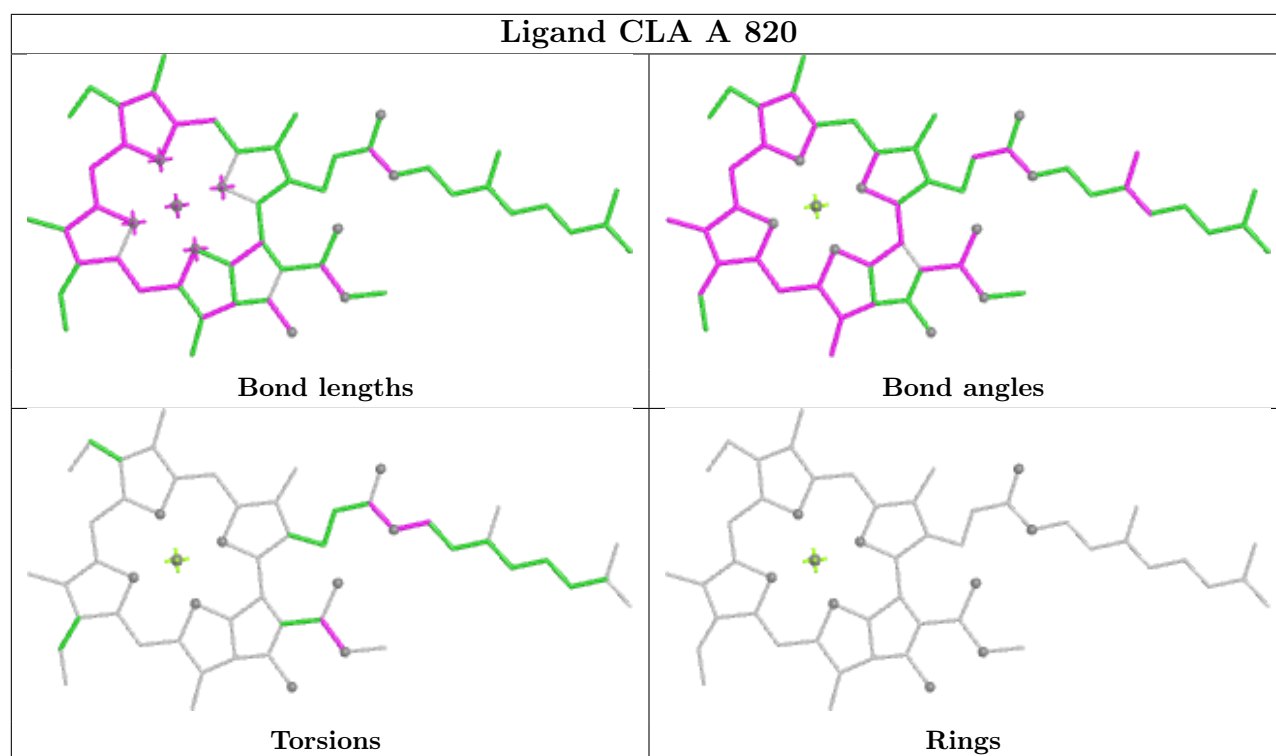


Ligand BCR O 201

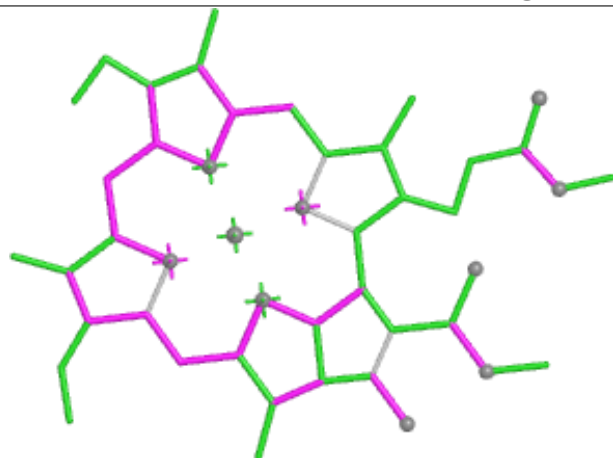


Ligand CHL 6 318

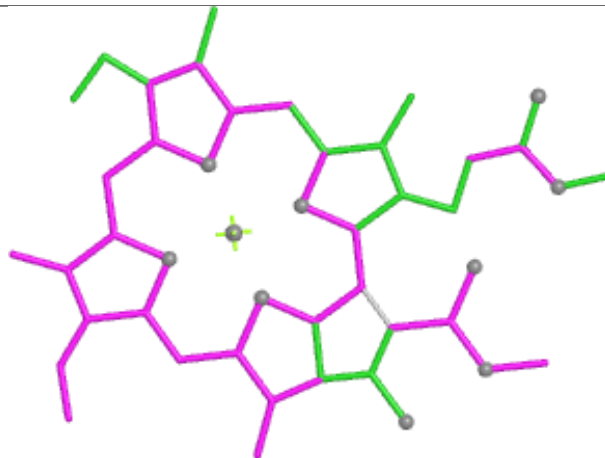




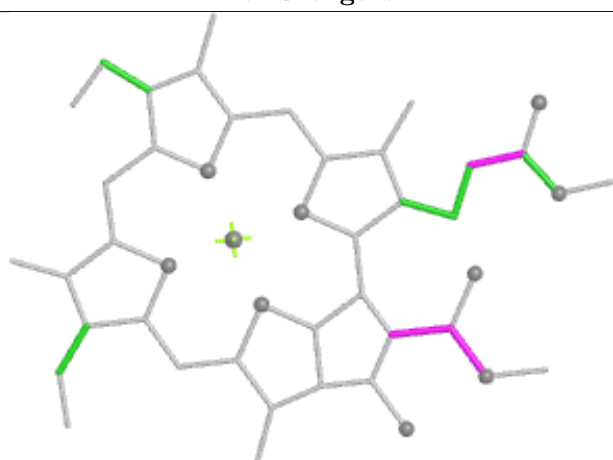
Ligand CLA 5 311



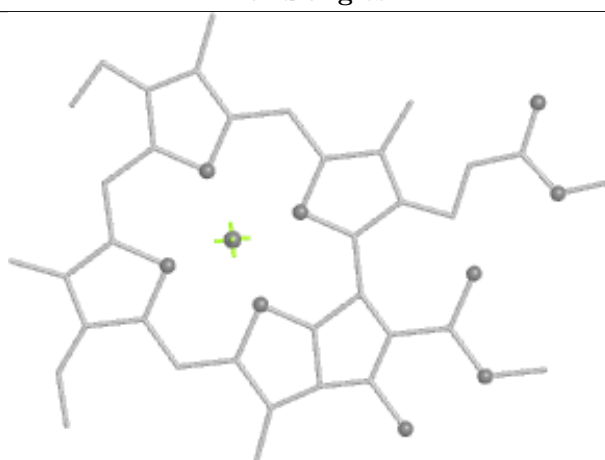
Bond lengths



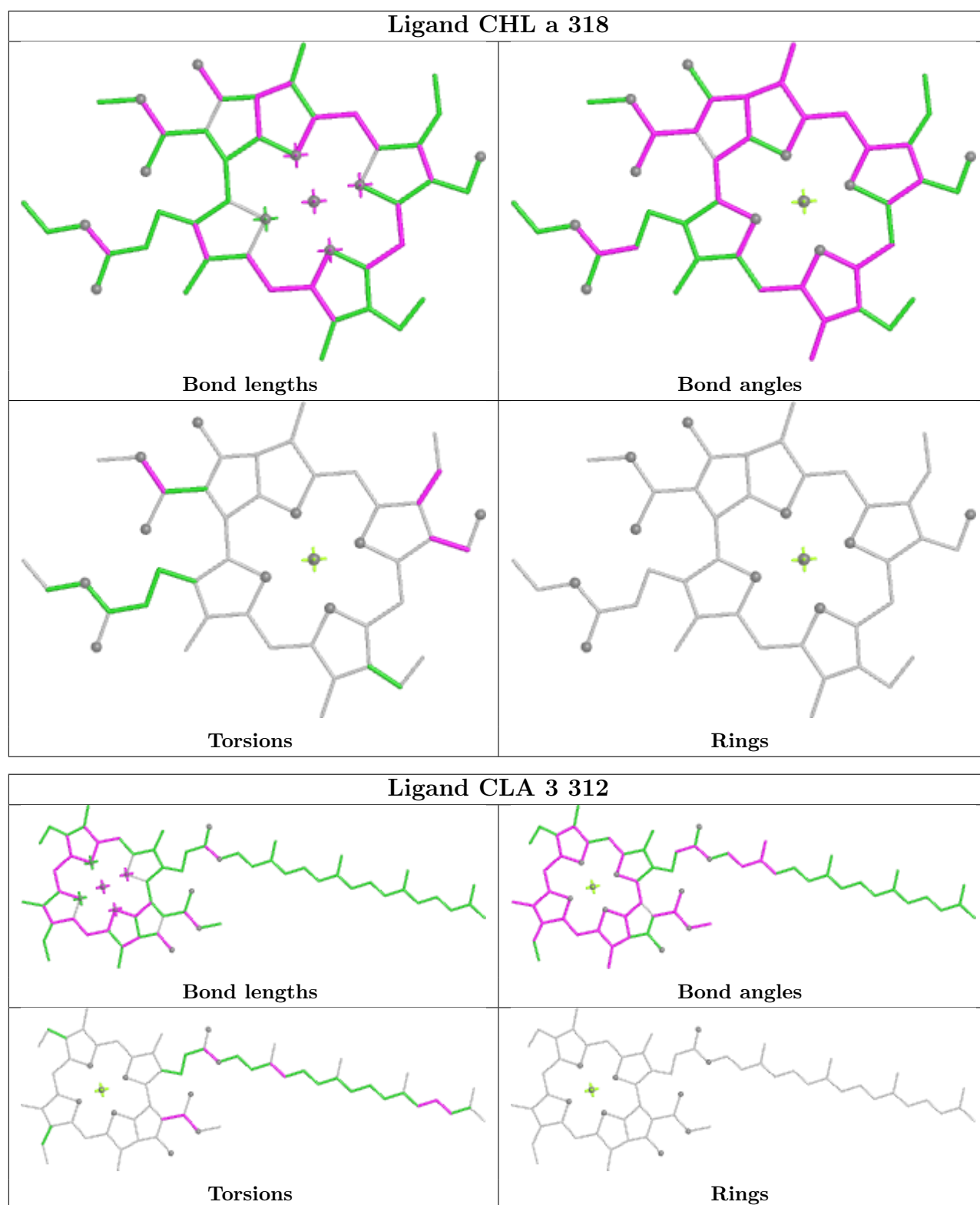
Bond angles

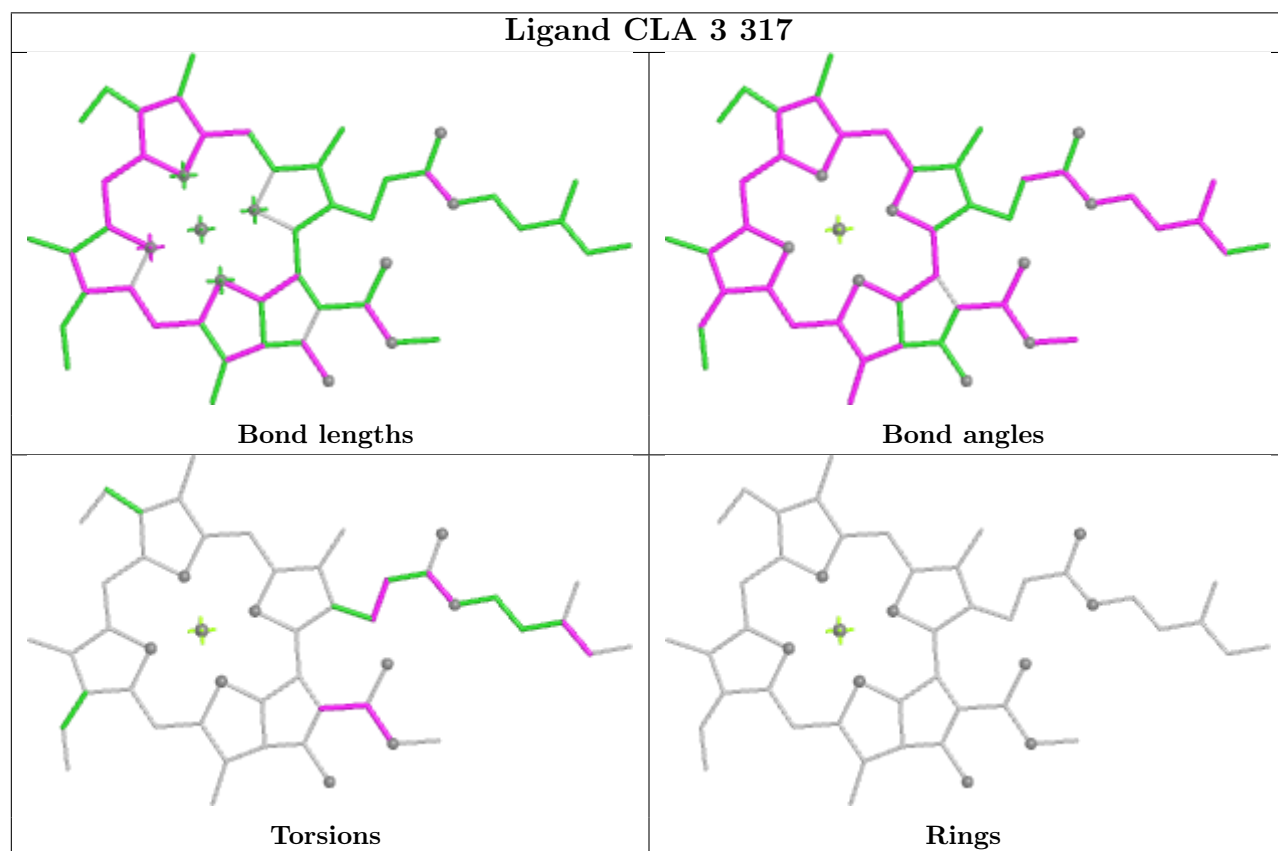
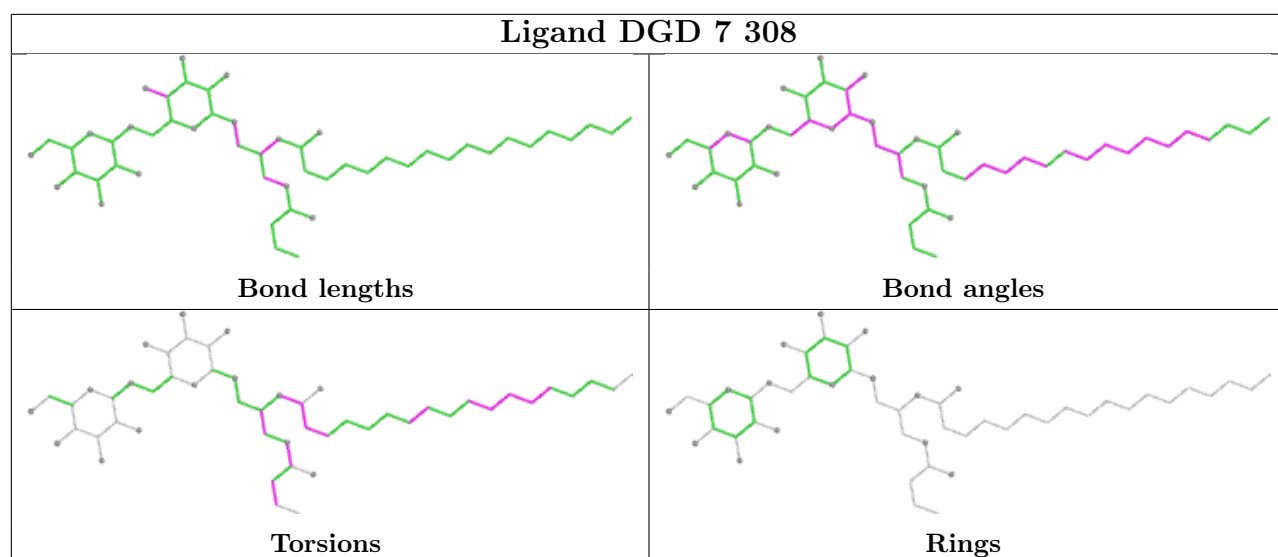


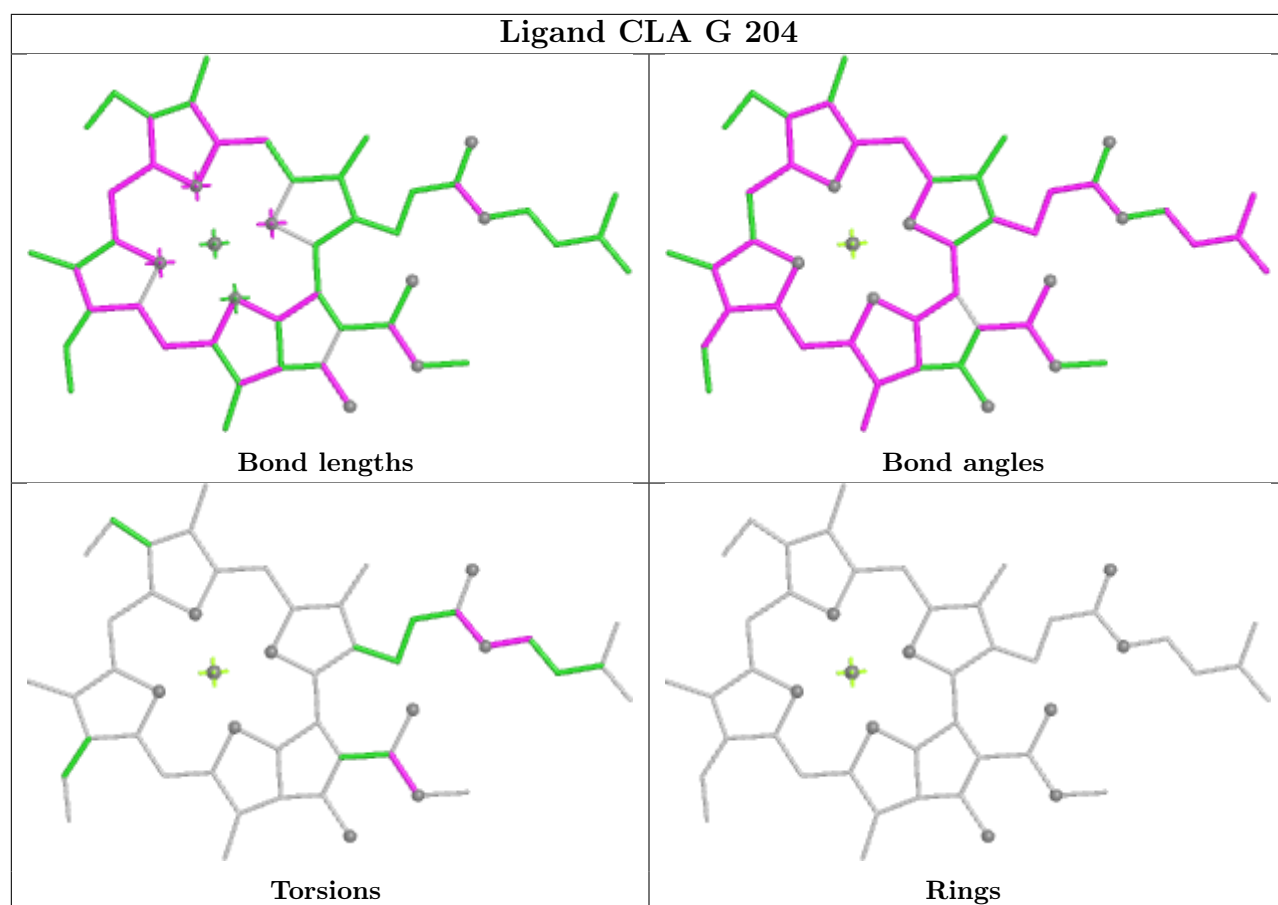
Torsions



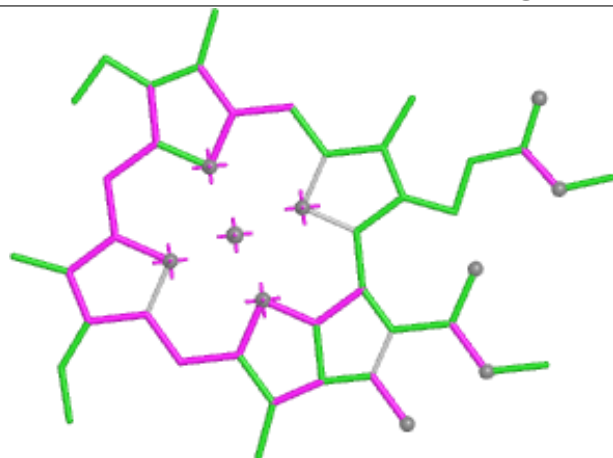
Rings



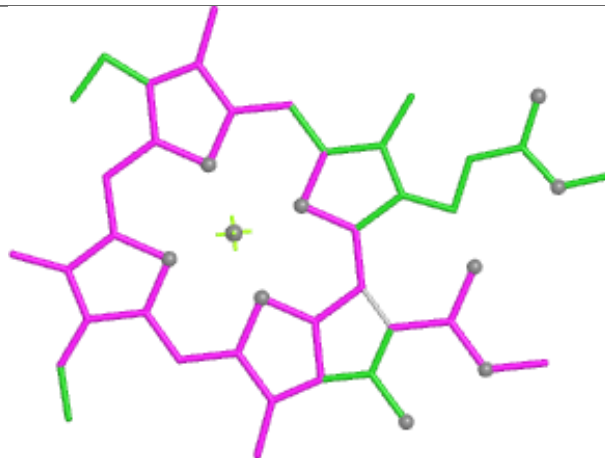




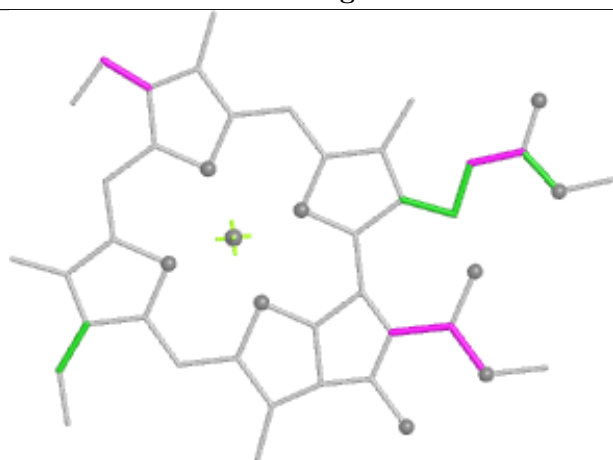
Ligand CLA b 307



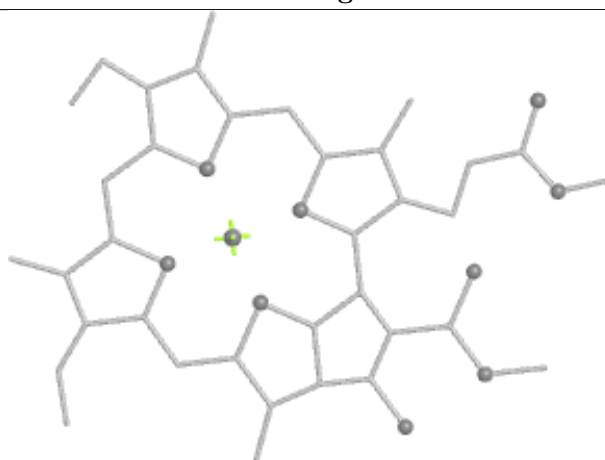
Bond lengths



Bond angles

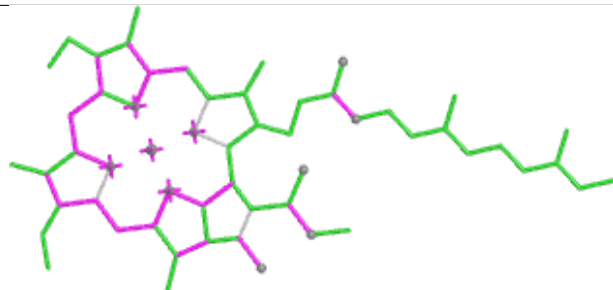


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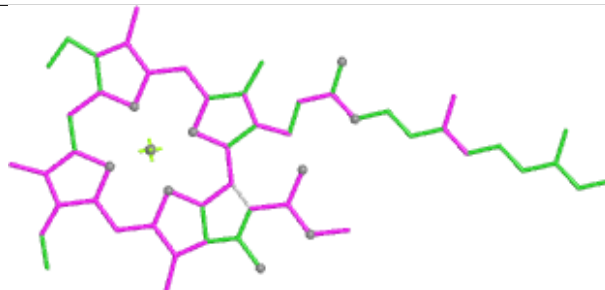


Rings

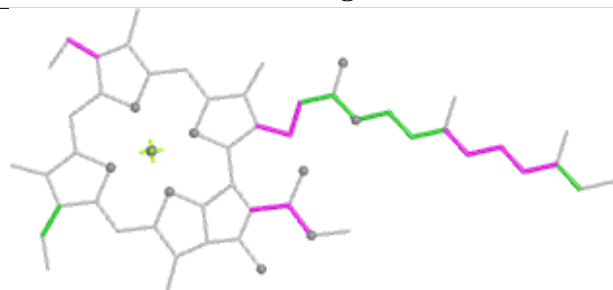
Ligand CLA 9 321



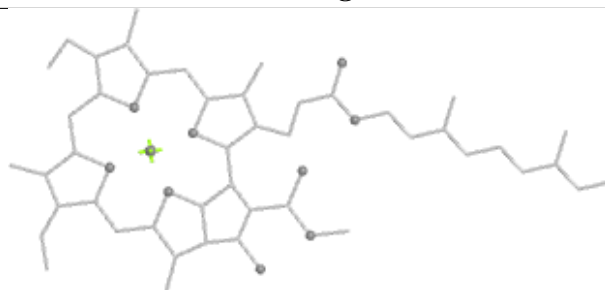
Bond lengths



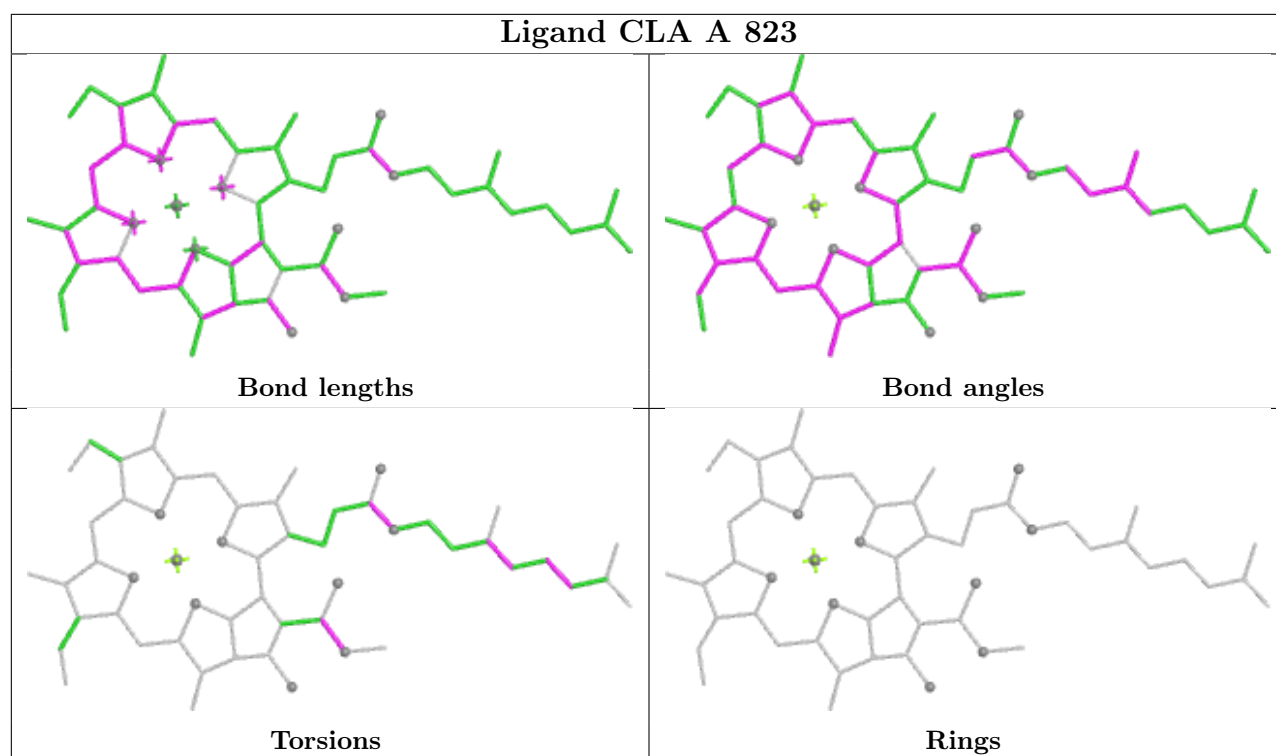
Bond angles



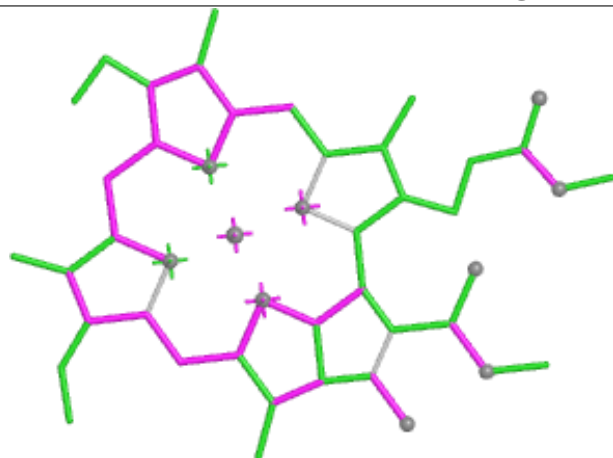
Torsions



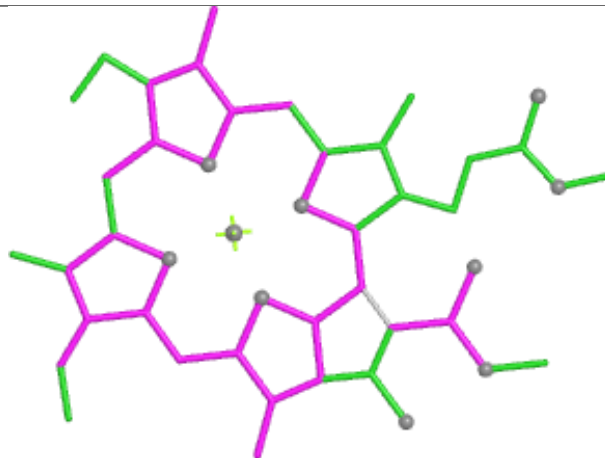
Rings



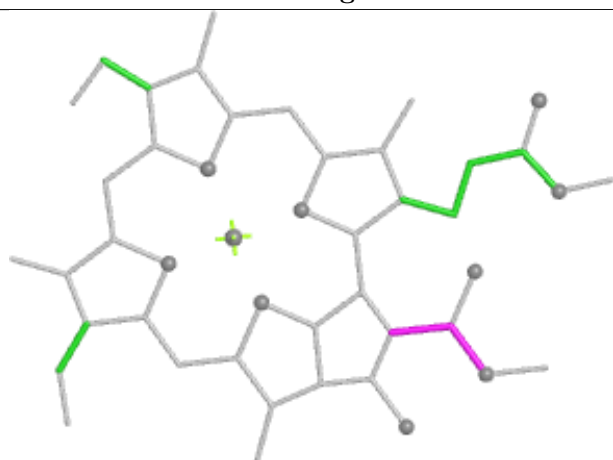
Ligand CLA K 205



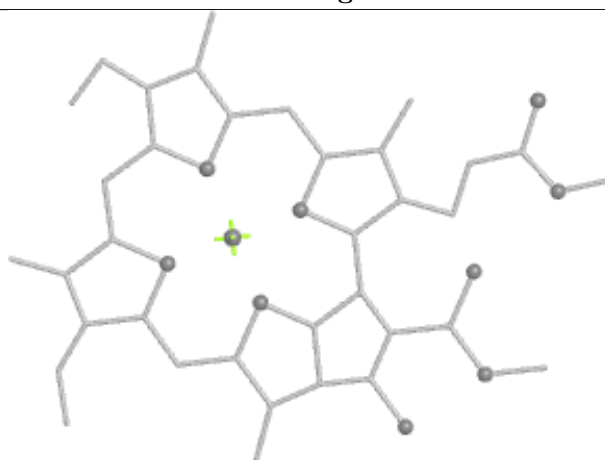
Bond lengths



Bond angles

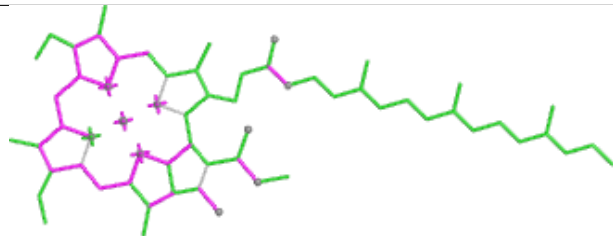


Torsions

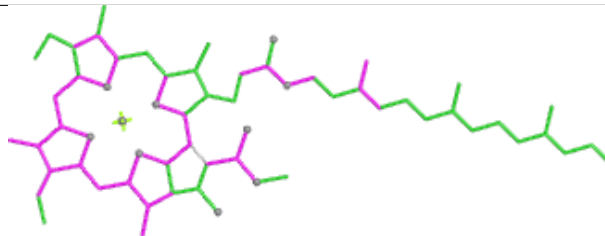


Rings

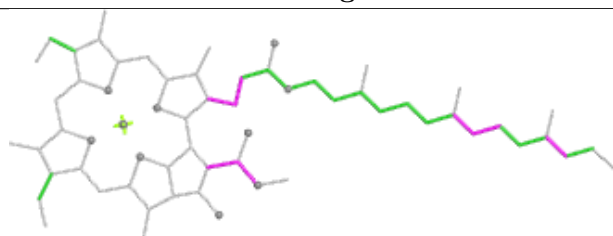
Ligand CLA 7 312



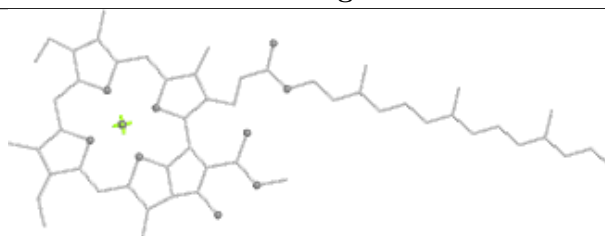
Bond lengths



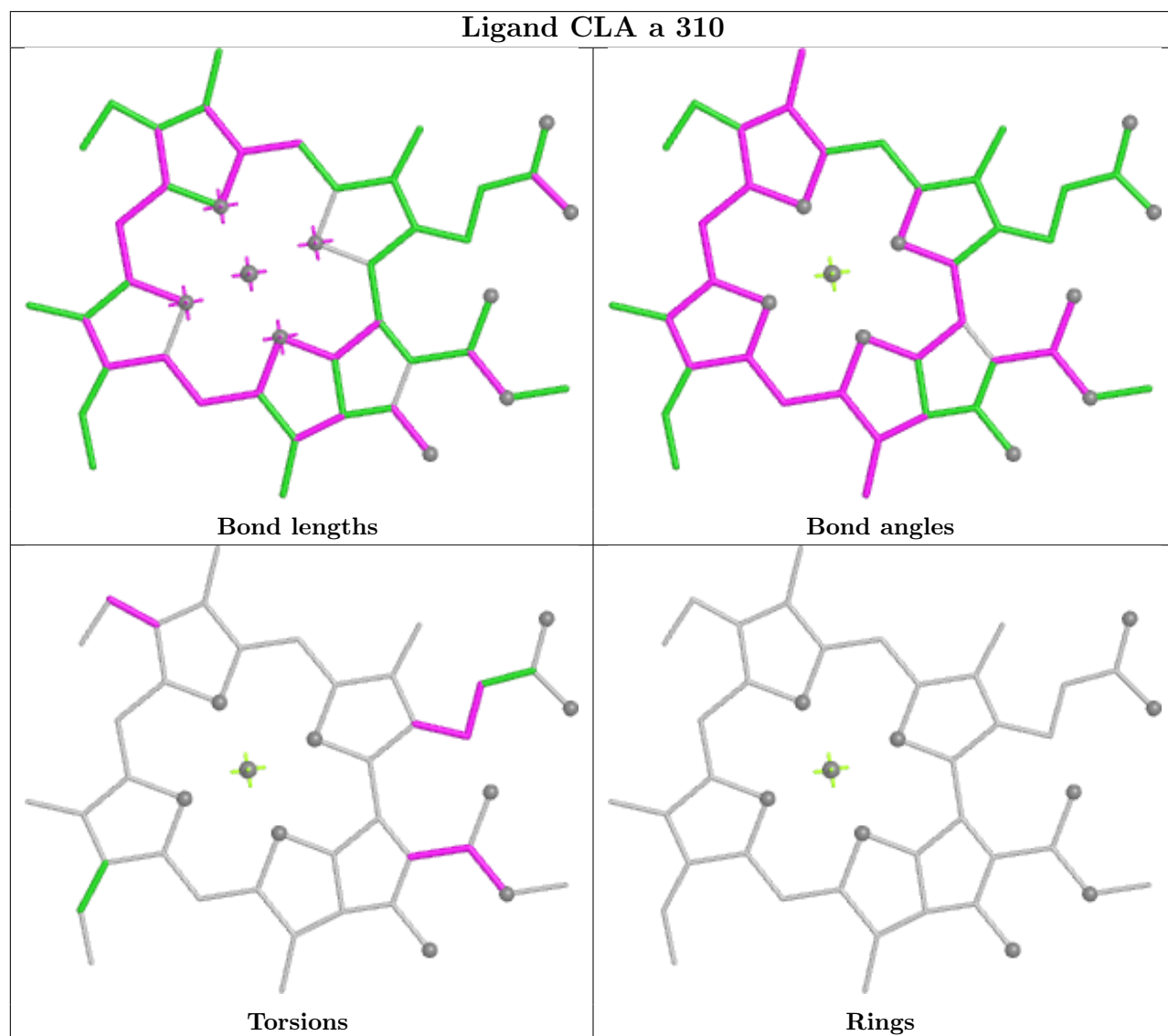
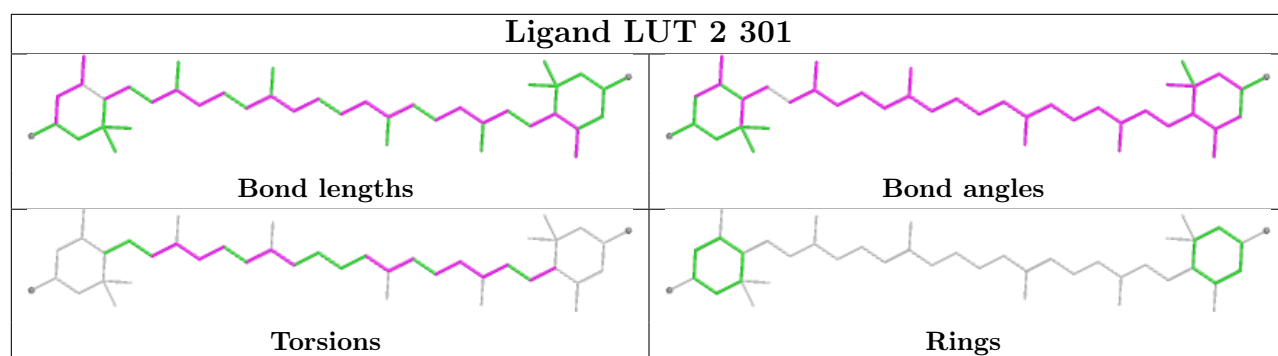
Bond angles



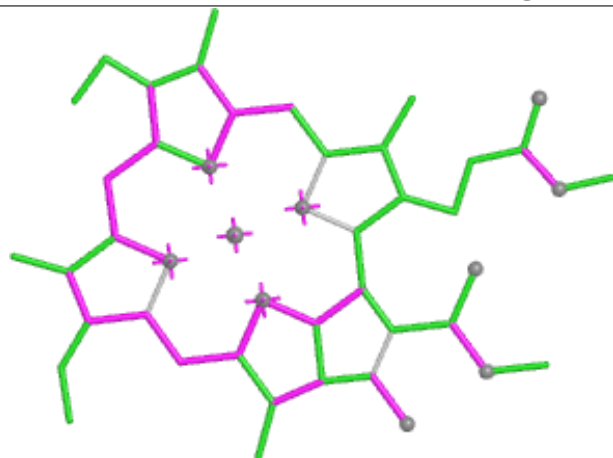
Torsions



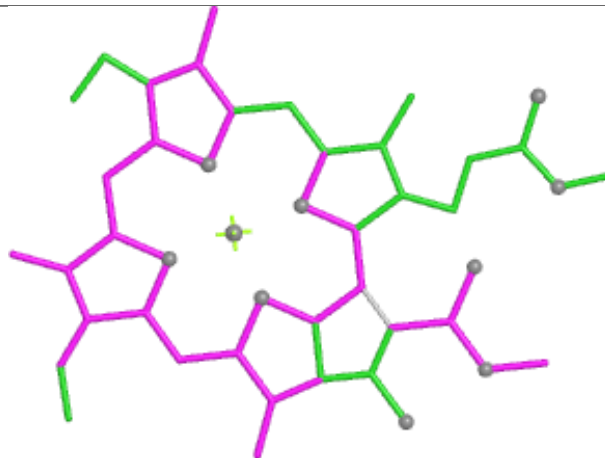
Rings



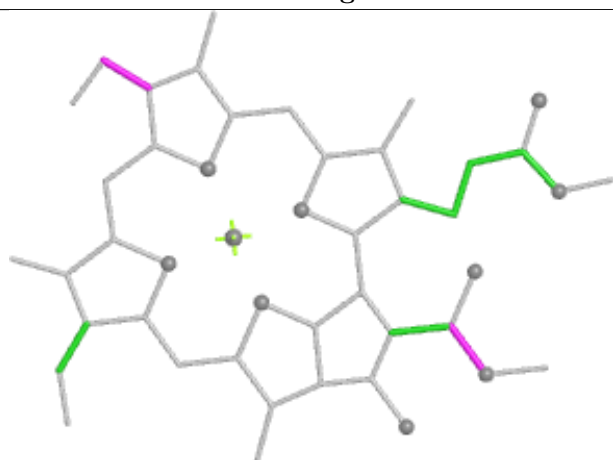
Ligand CLA 5 308



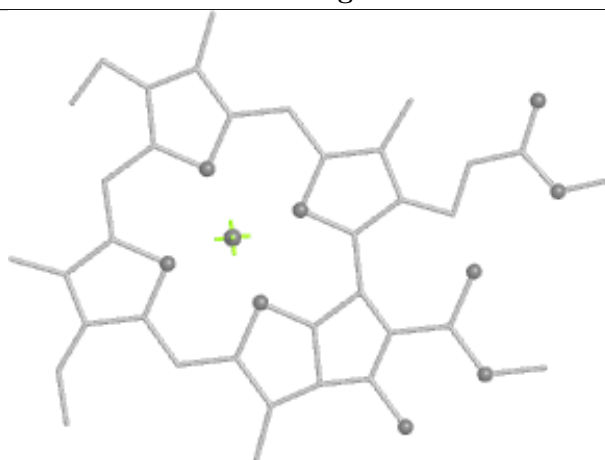
Bond lengths



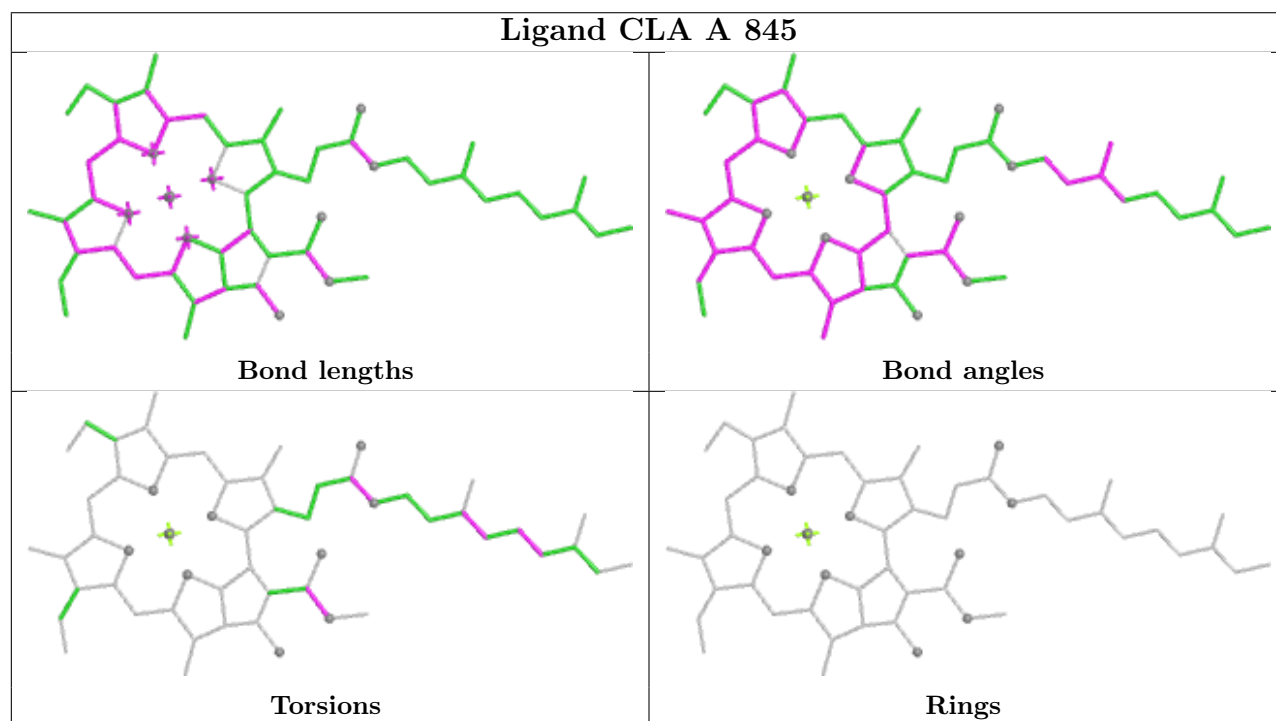
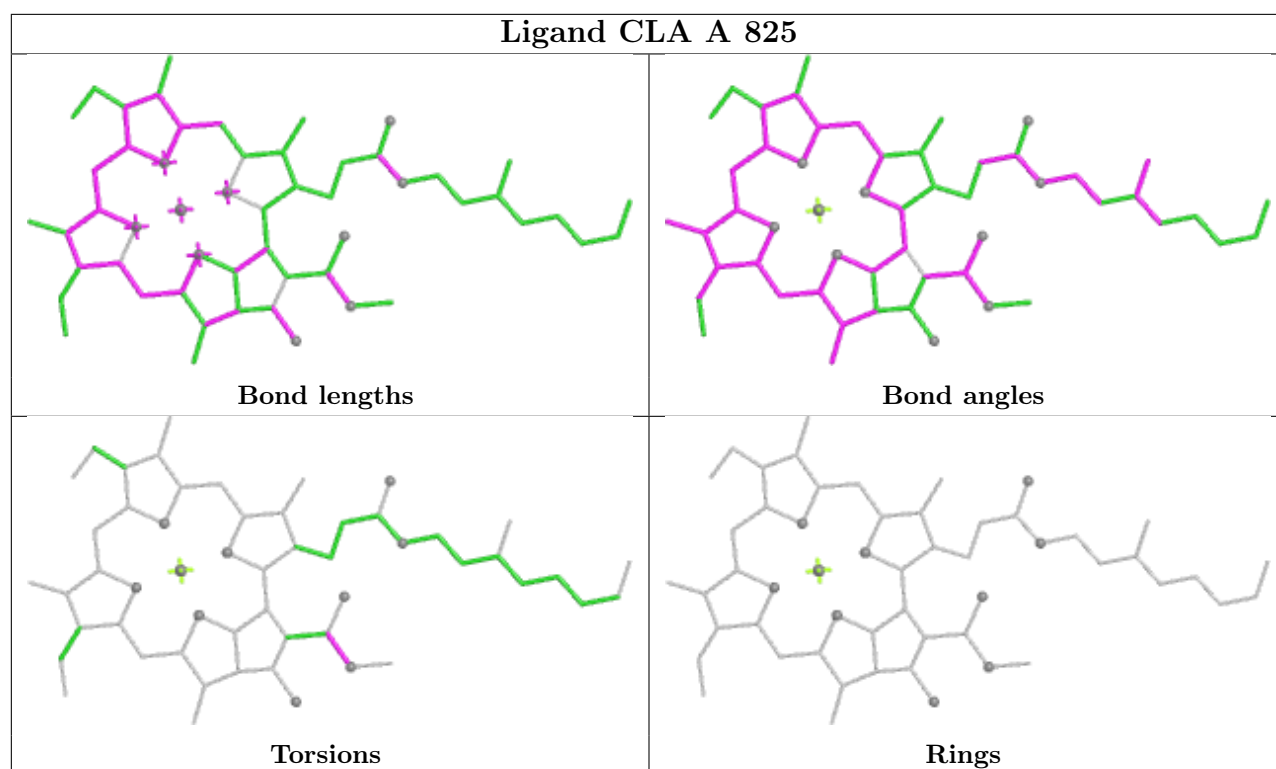
Bond angles

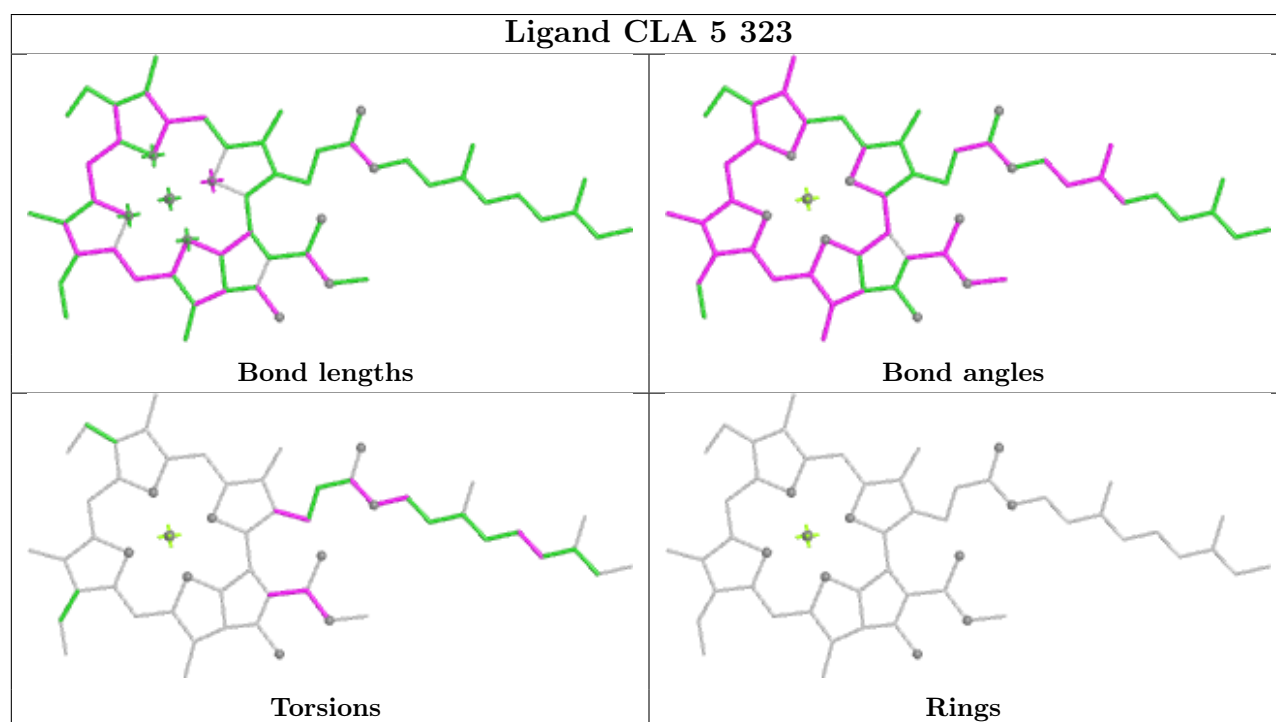
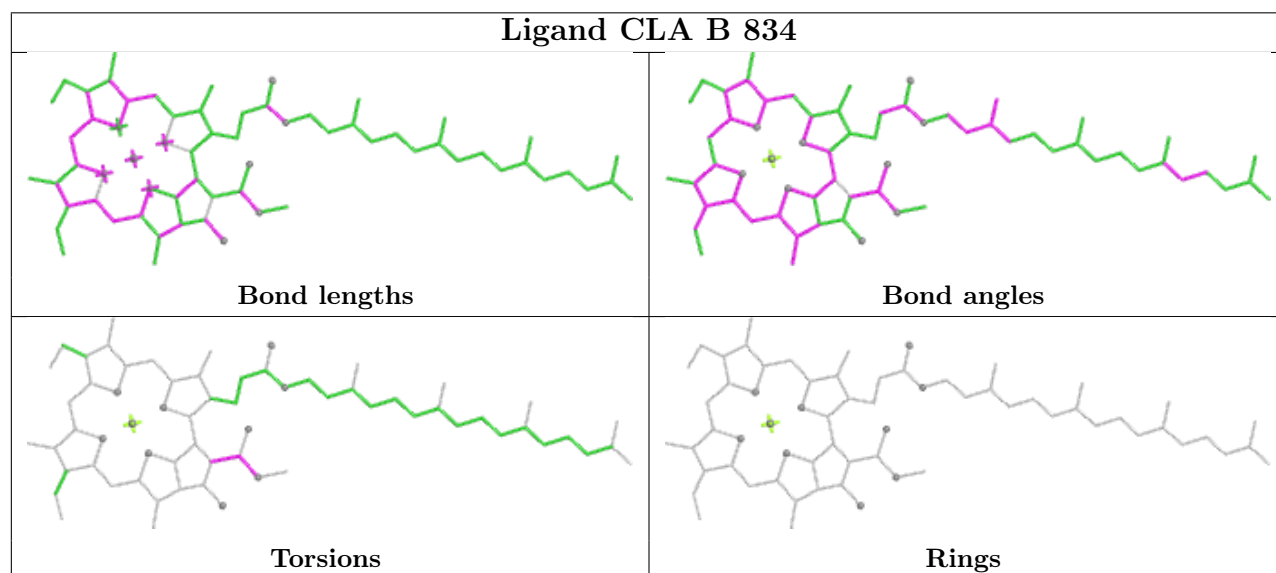
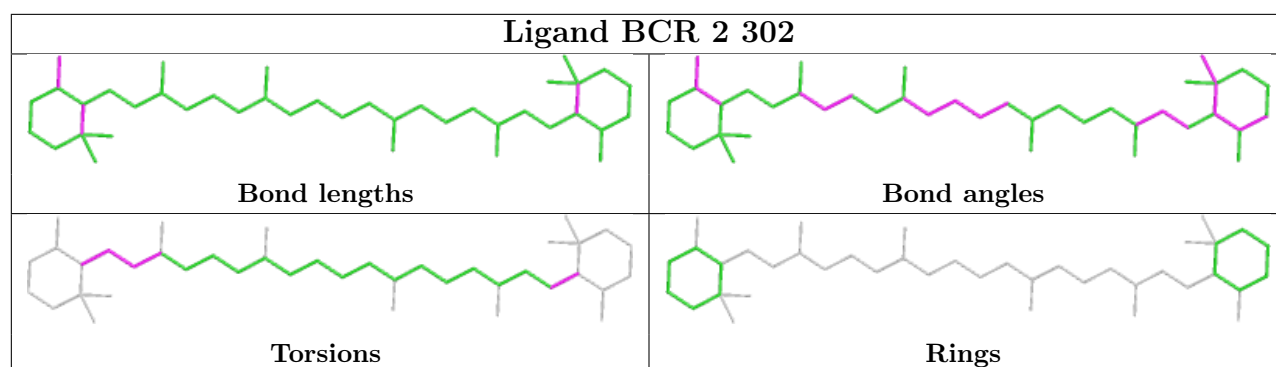


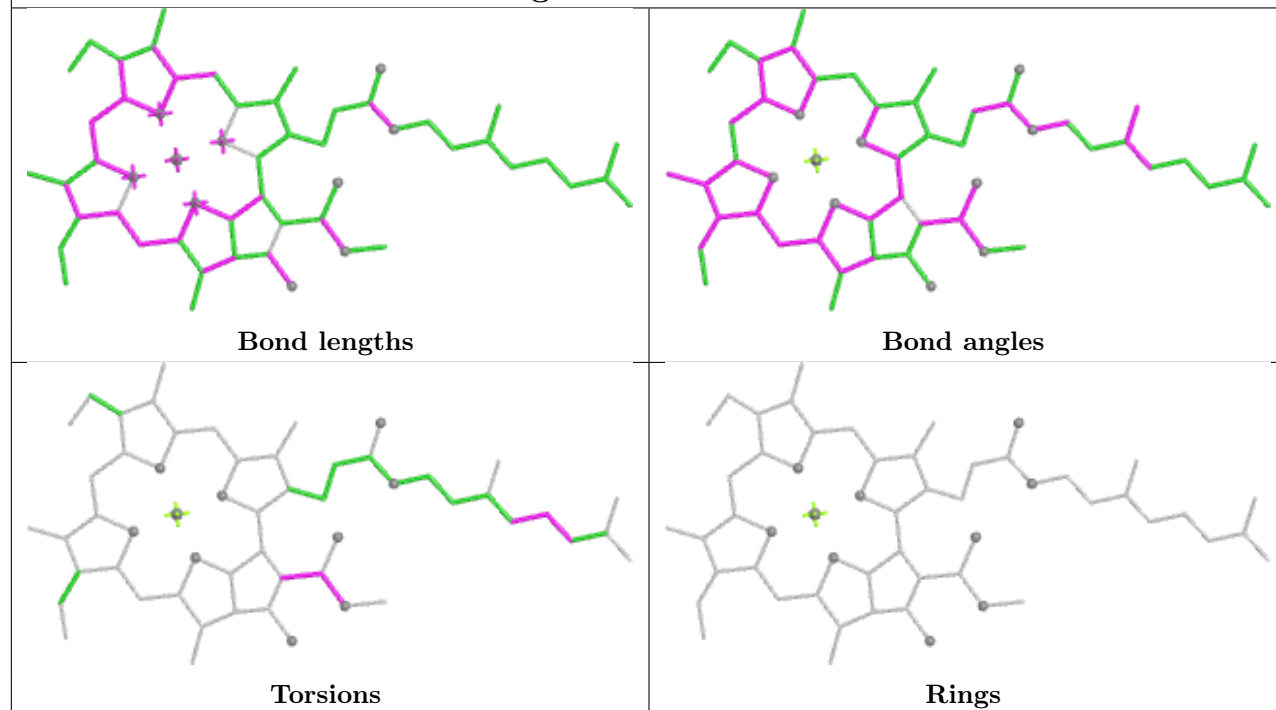
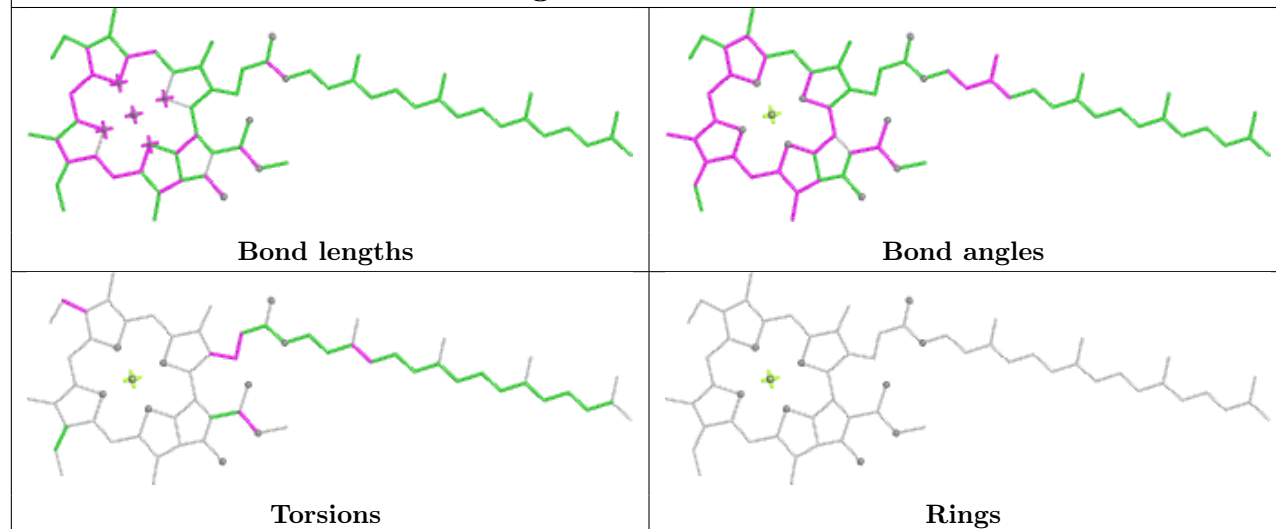
Torsions

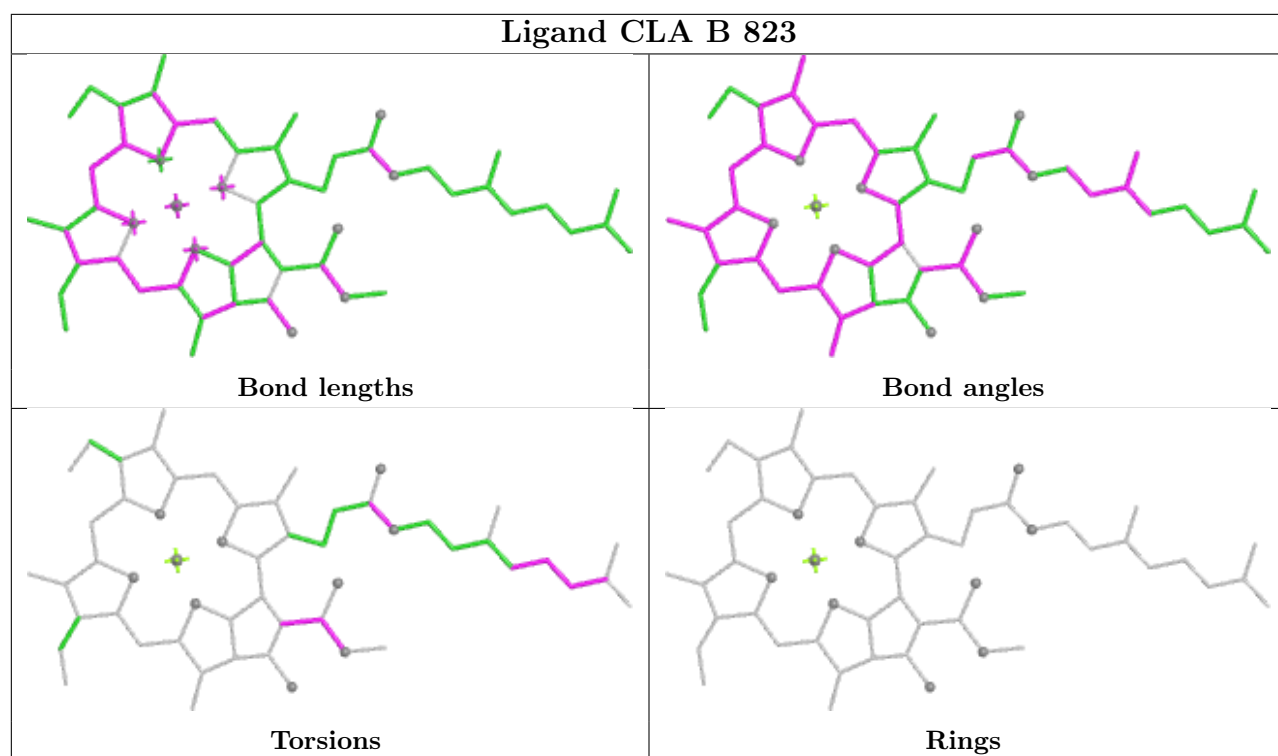


Rings

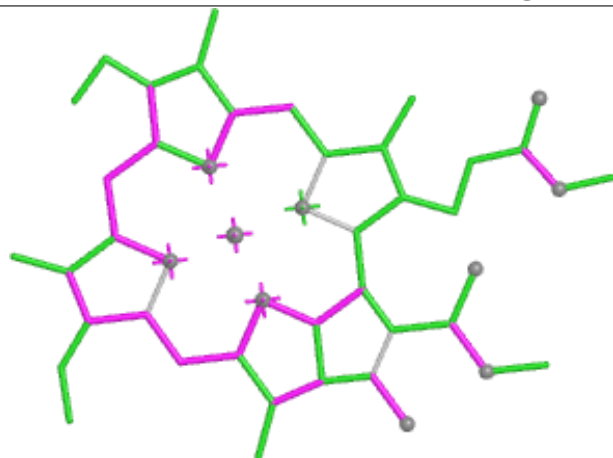




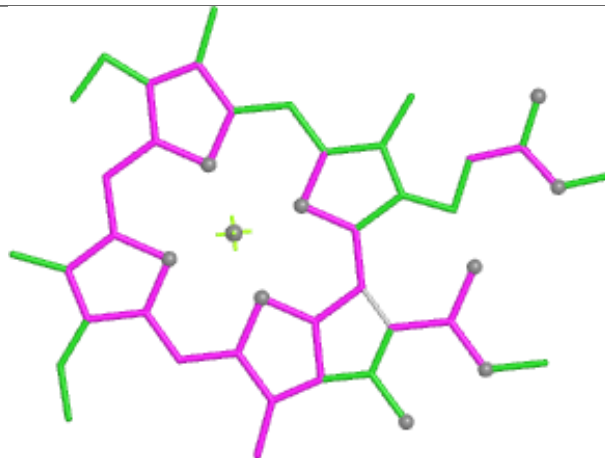
Ligand CLA A 835**Ligand CLA A 856**



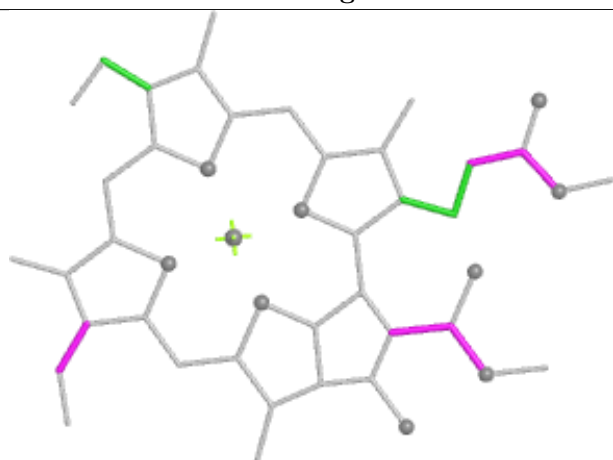
Ligand CLA 2 313



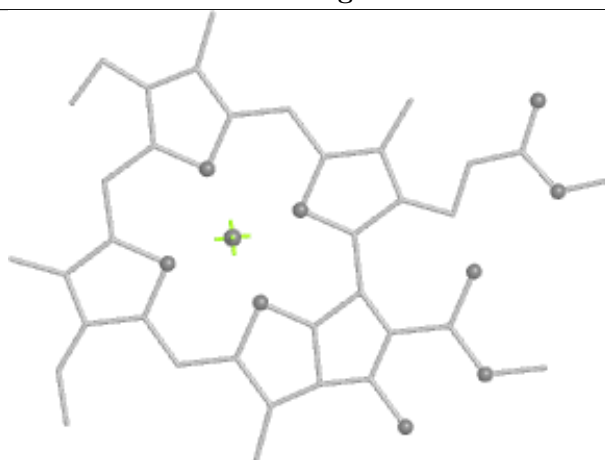
Bond lengths



Bond angles

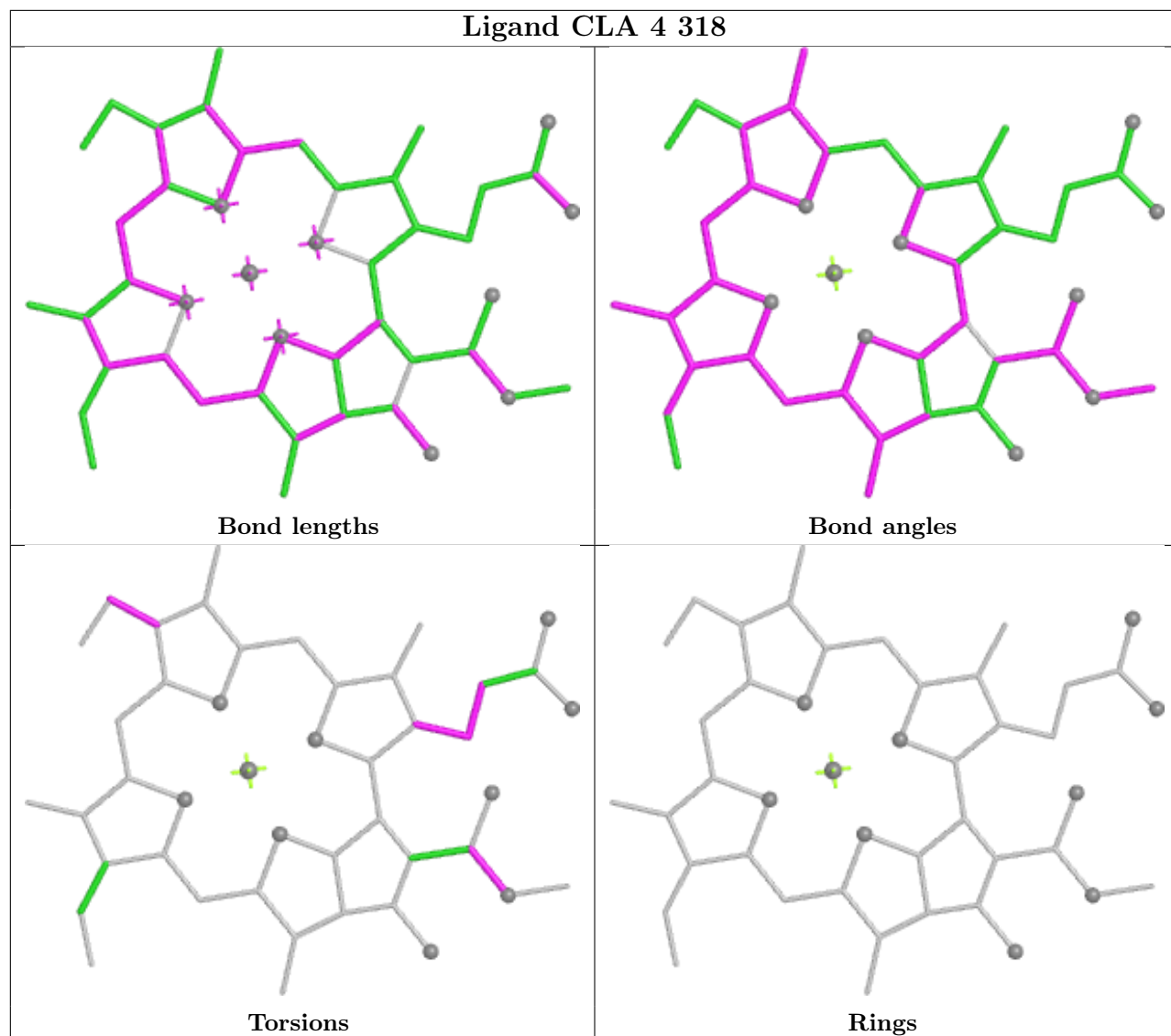


Torsions

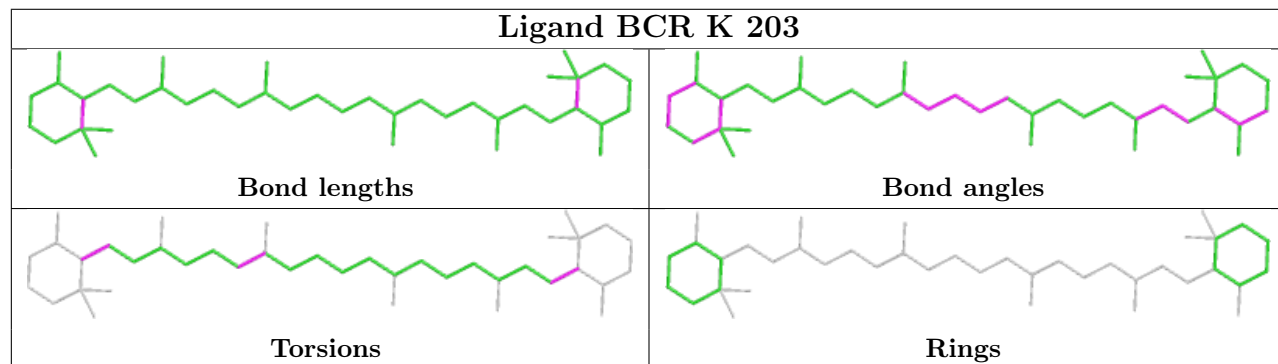


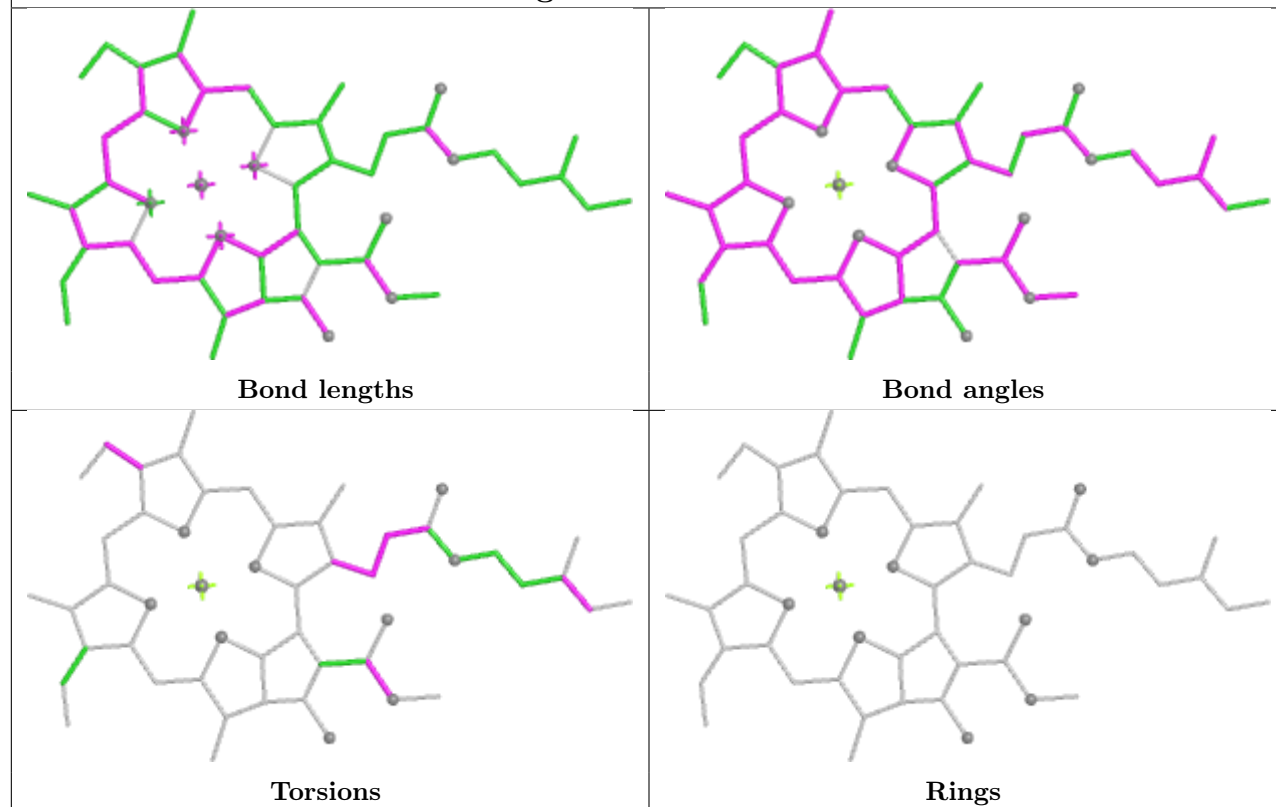
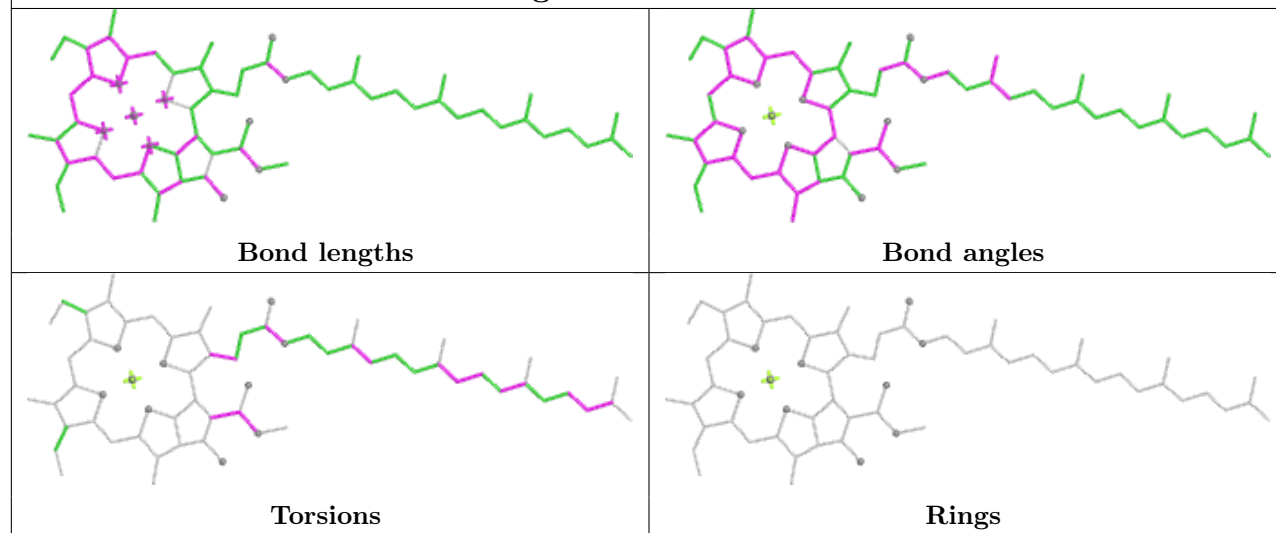
Rings

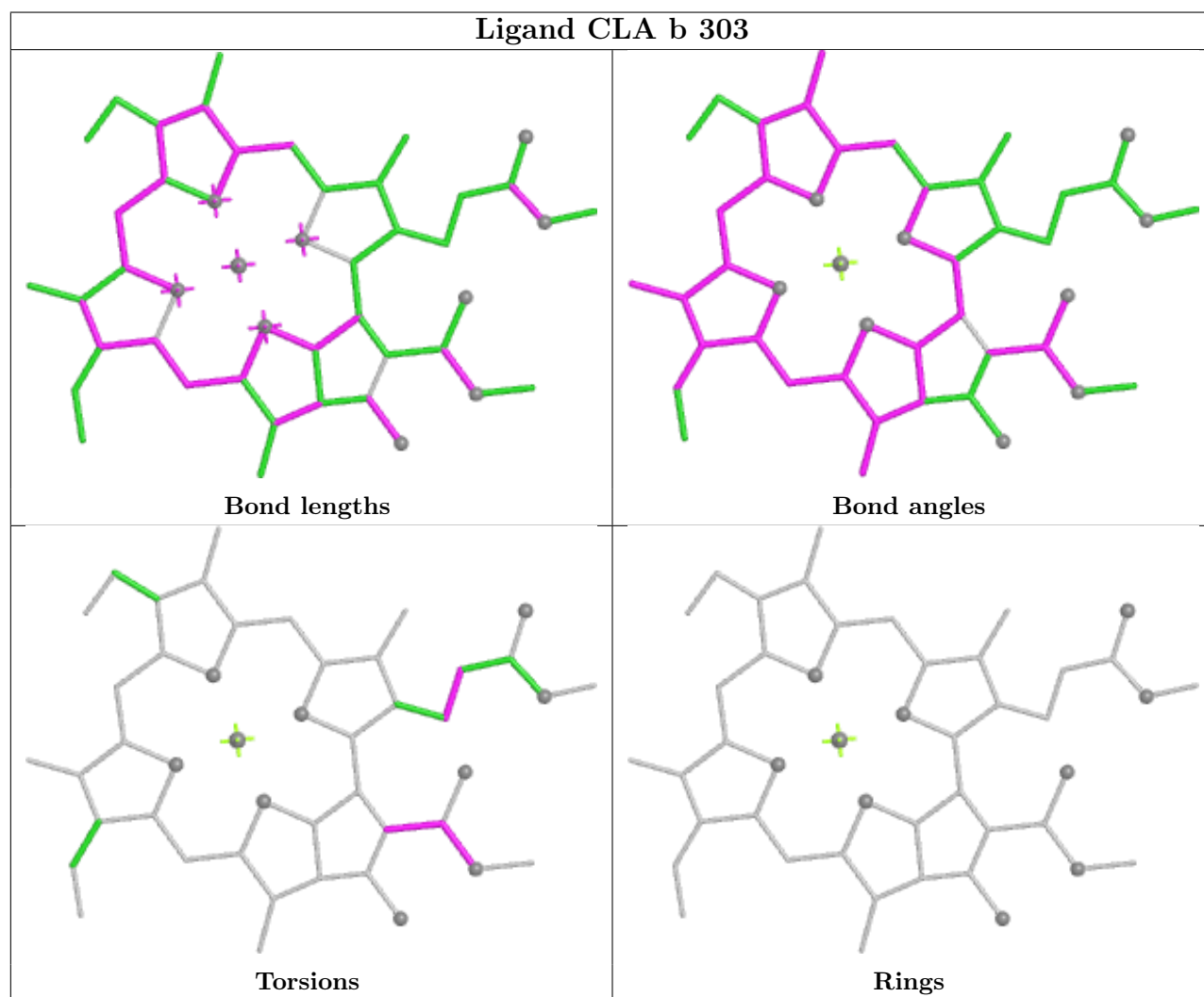
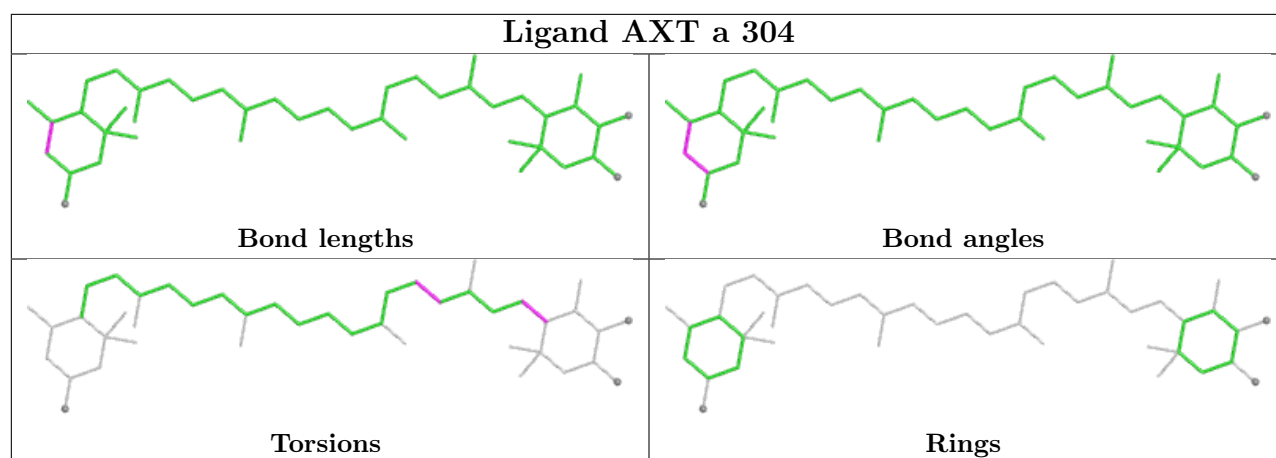
Ligand CLA 4 318

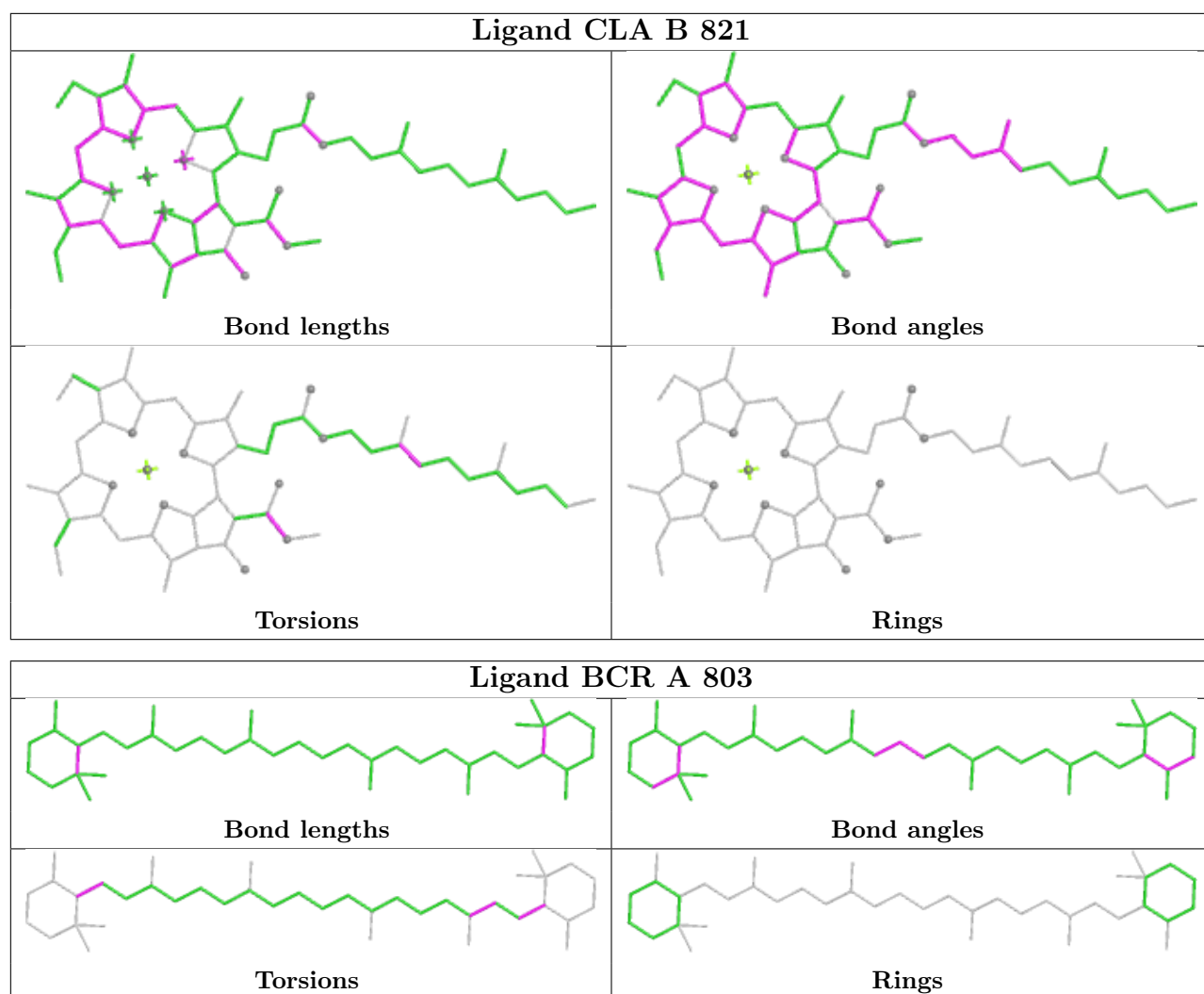


Ligand BCR K 203

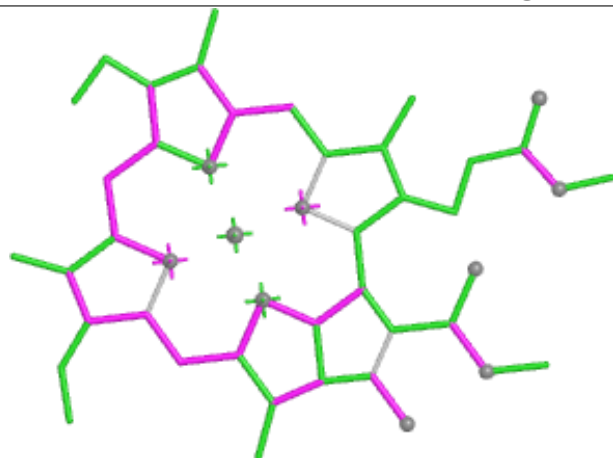


Ligand CLA 3 318**Ligand CLA B 814**

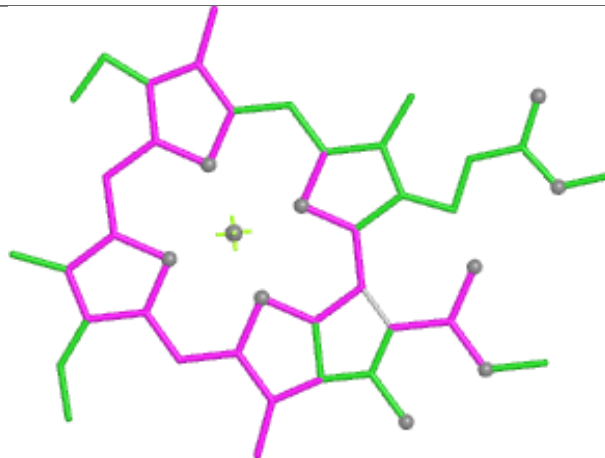




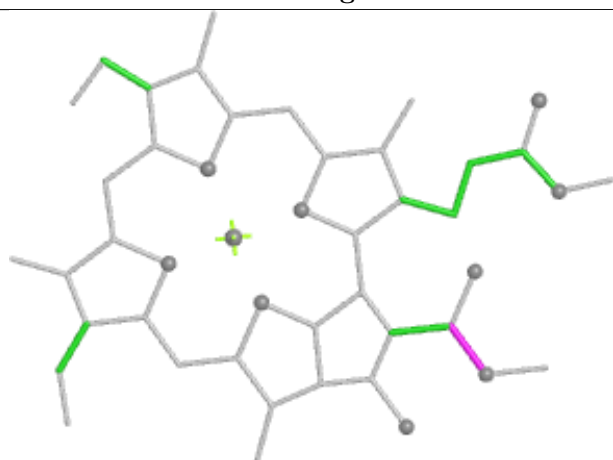
Ligand CLA 9 312



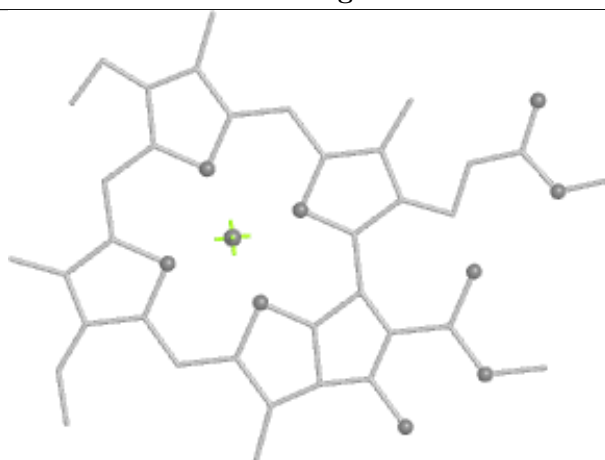
Bond lengths



Bond angles

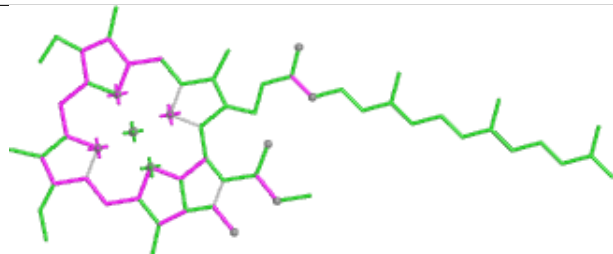


Torsions

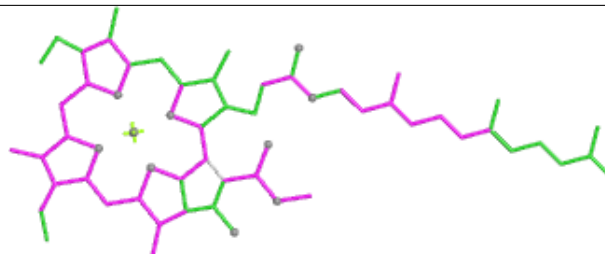


Rings

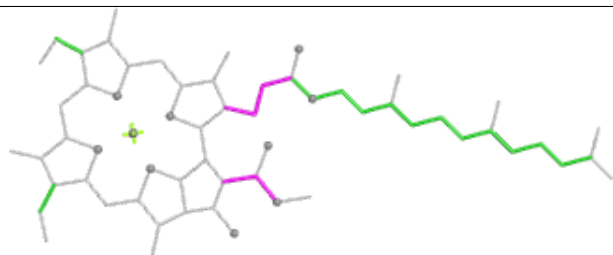
Ligand CLA 4 308



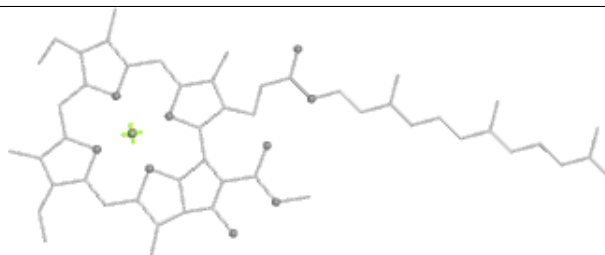
Bond lengths



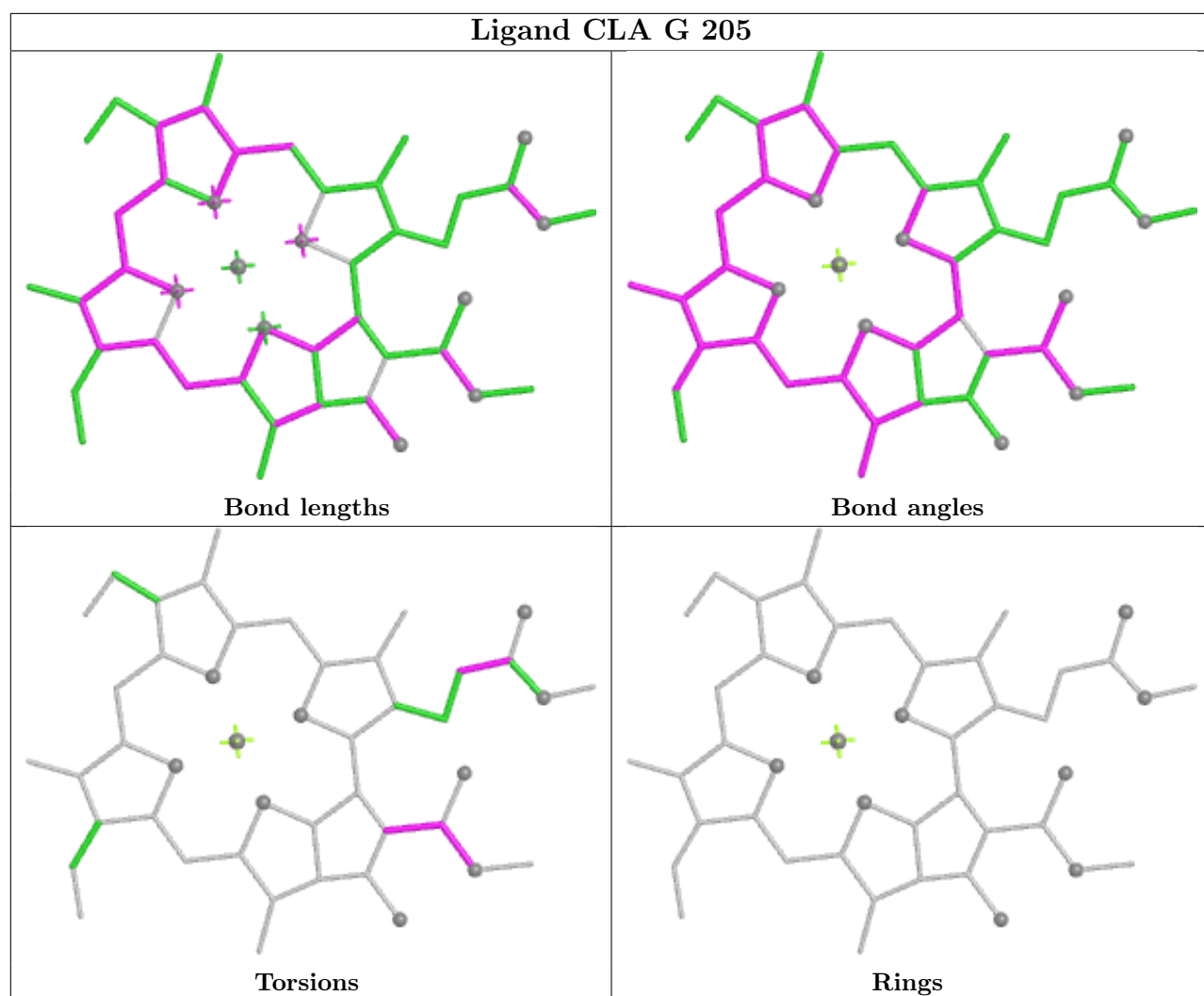
Bond angles

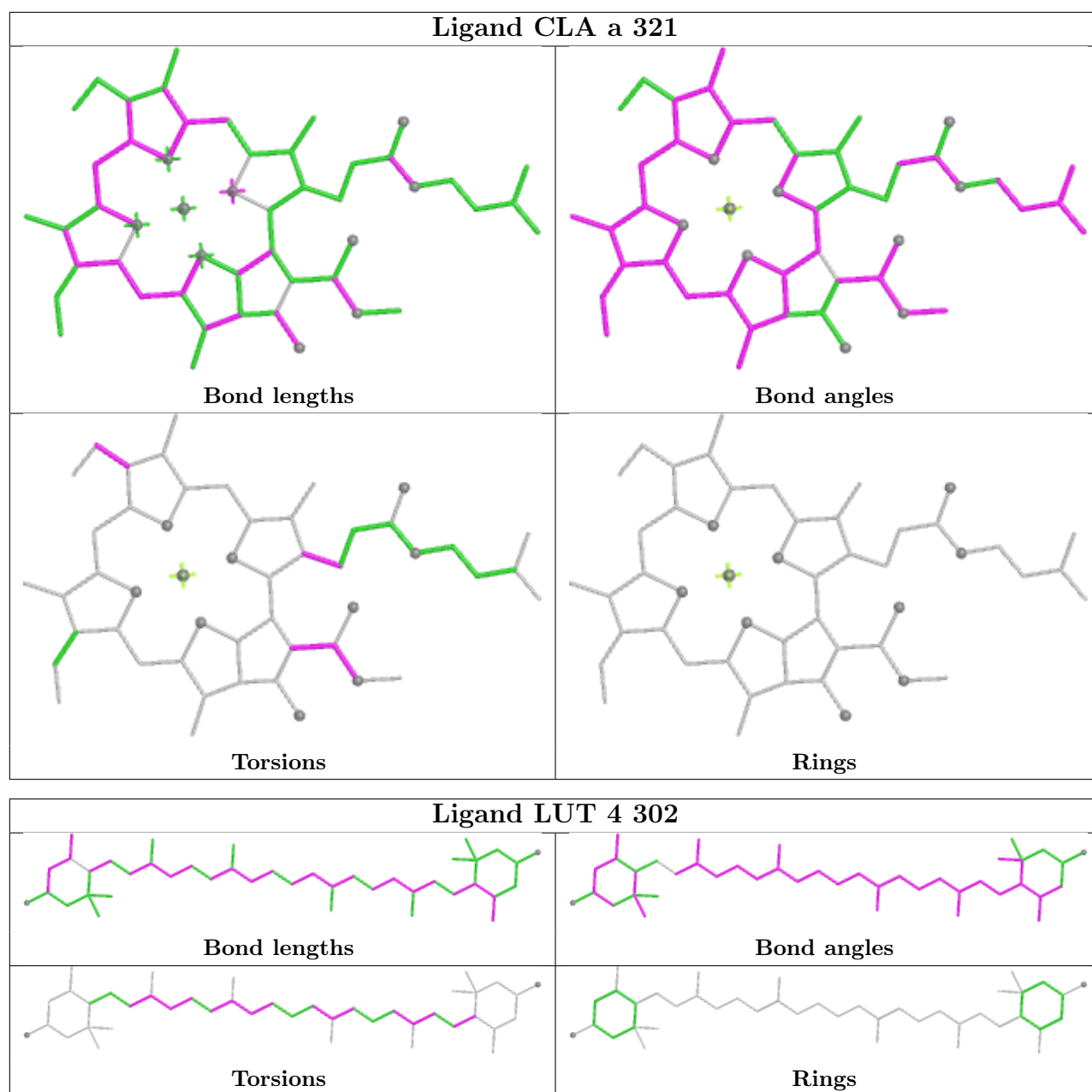


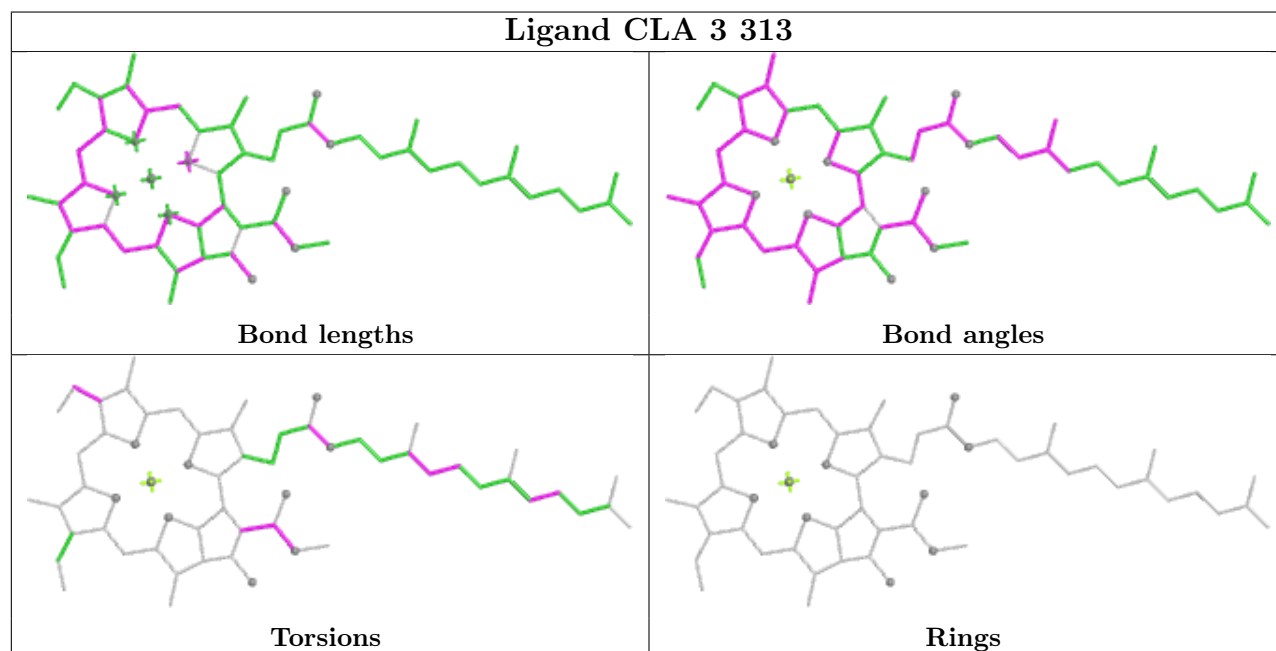
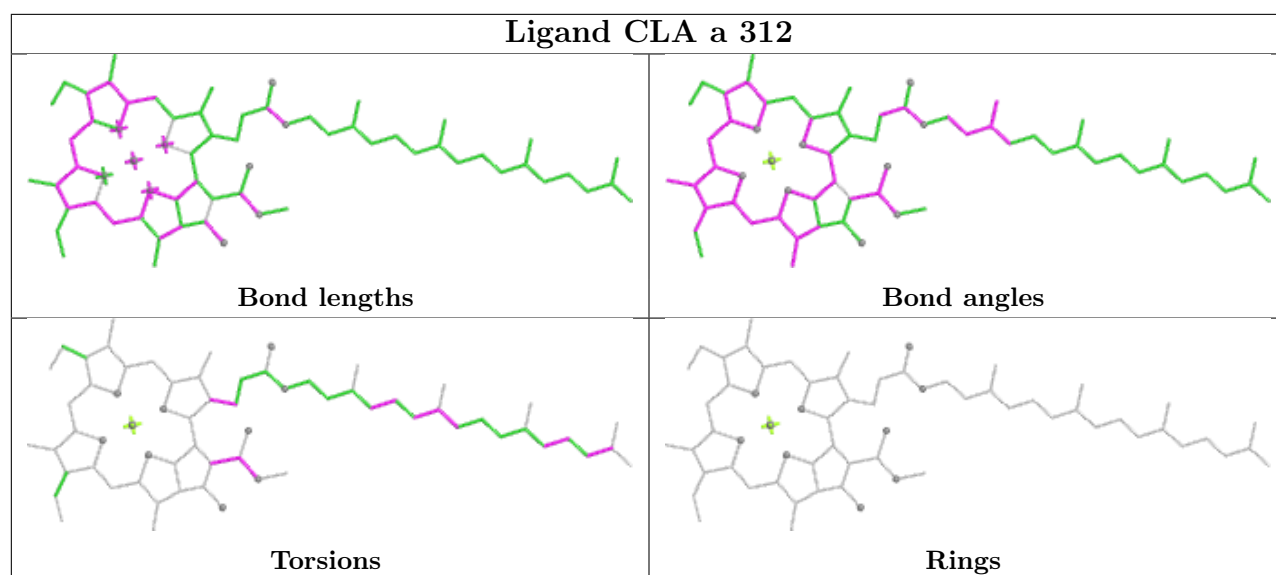
Torsions

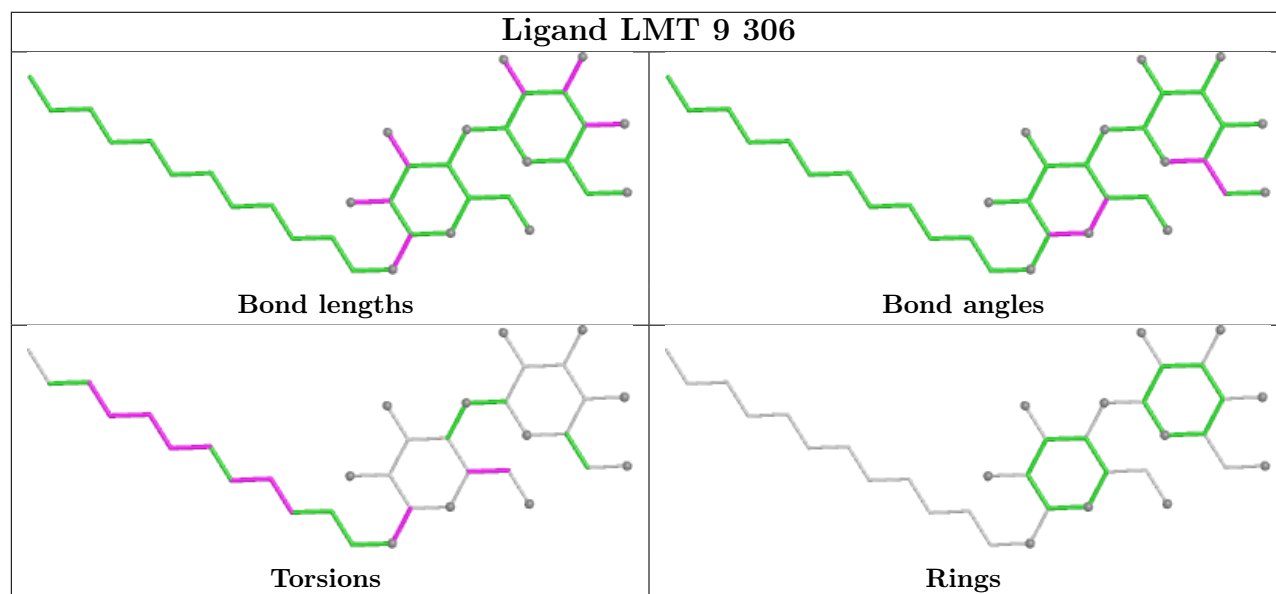
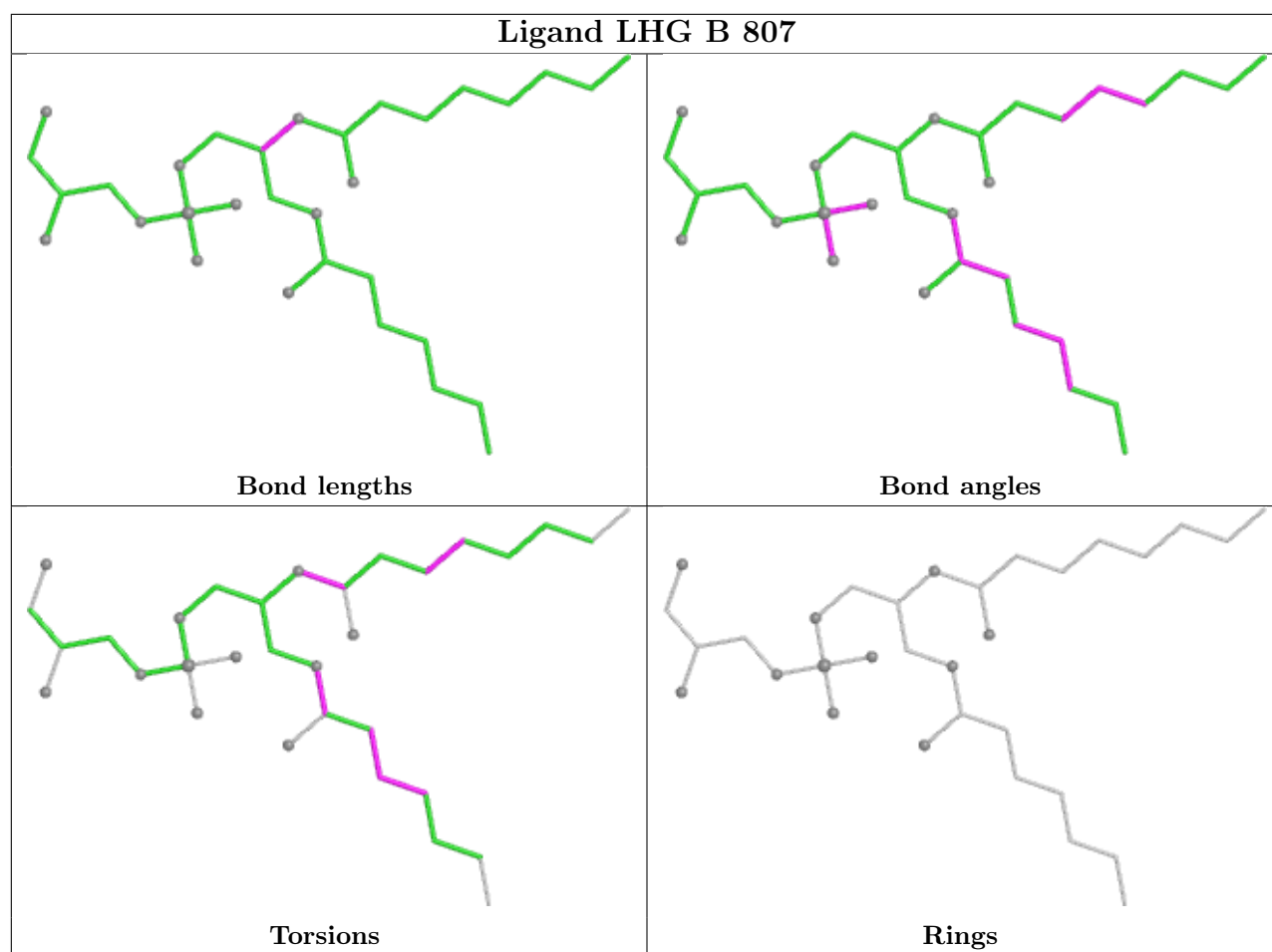


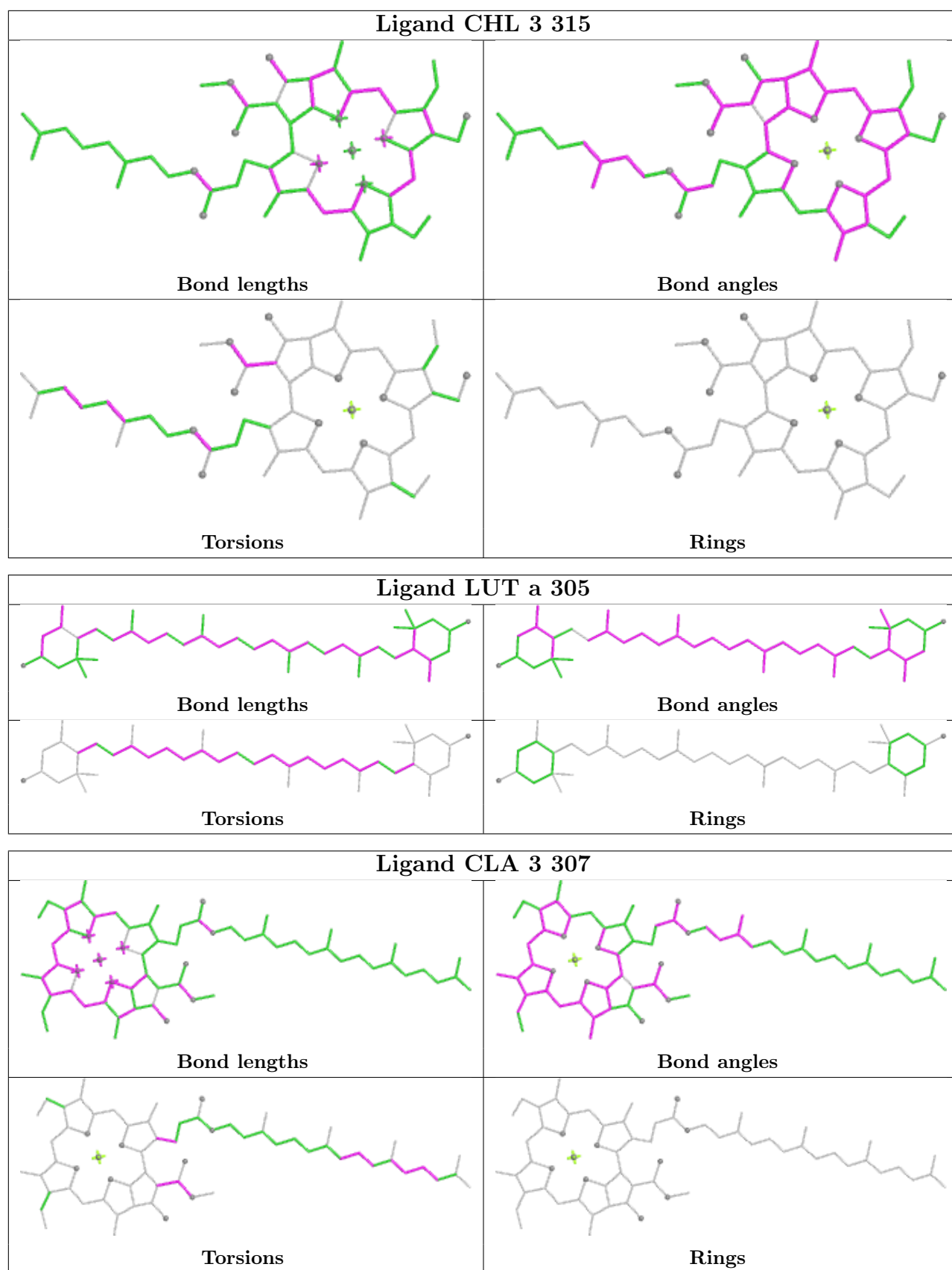
Rings

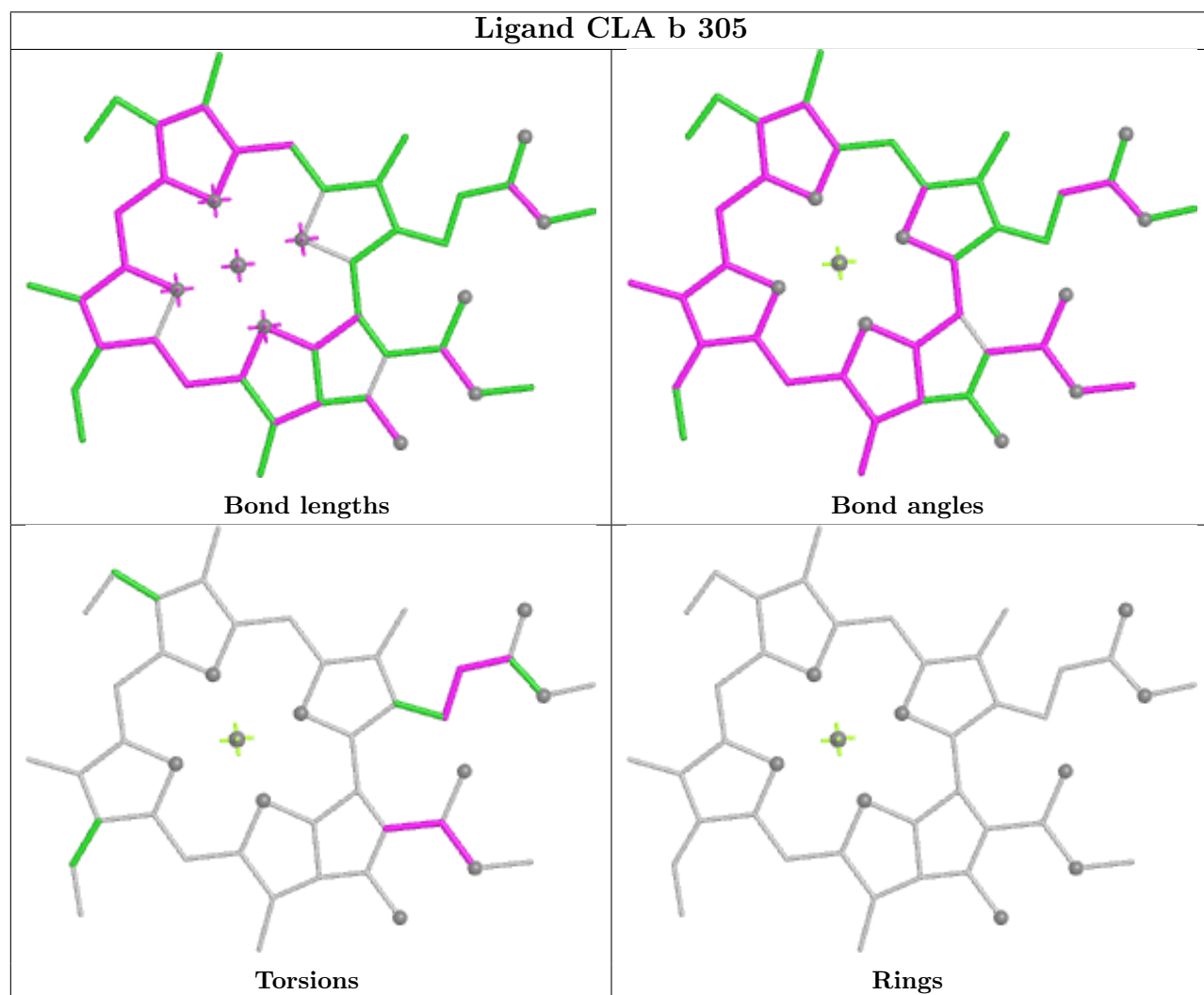
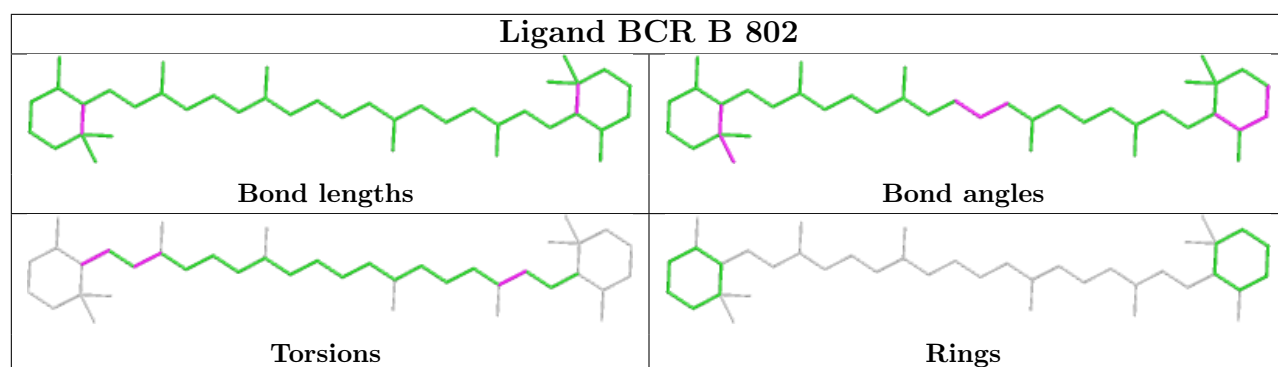


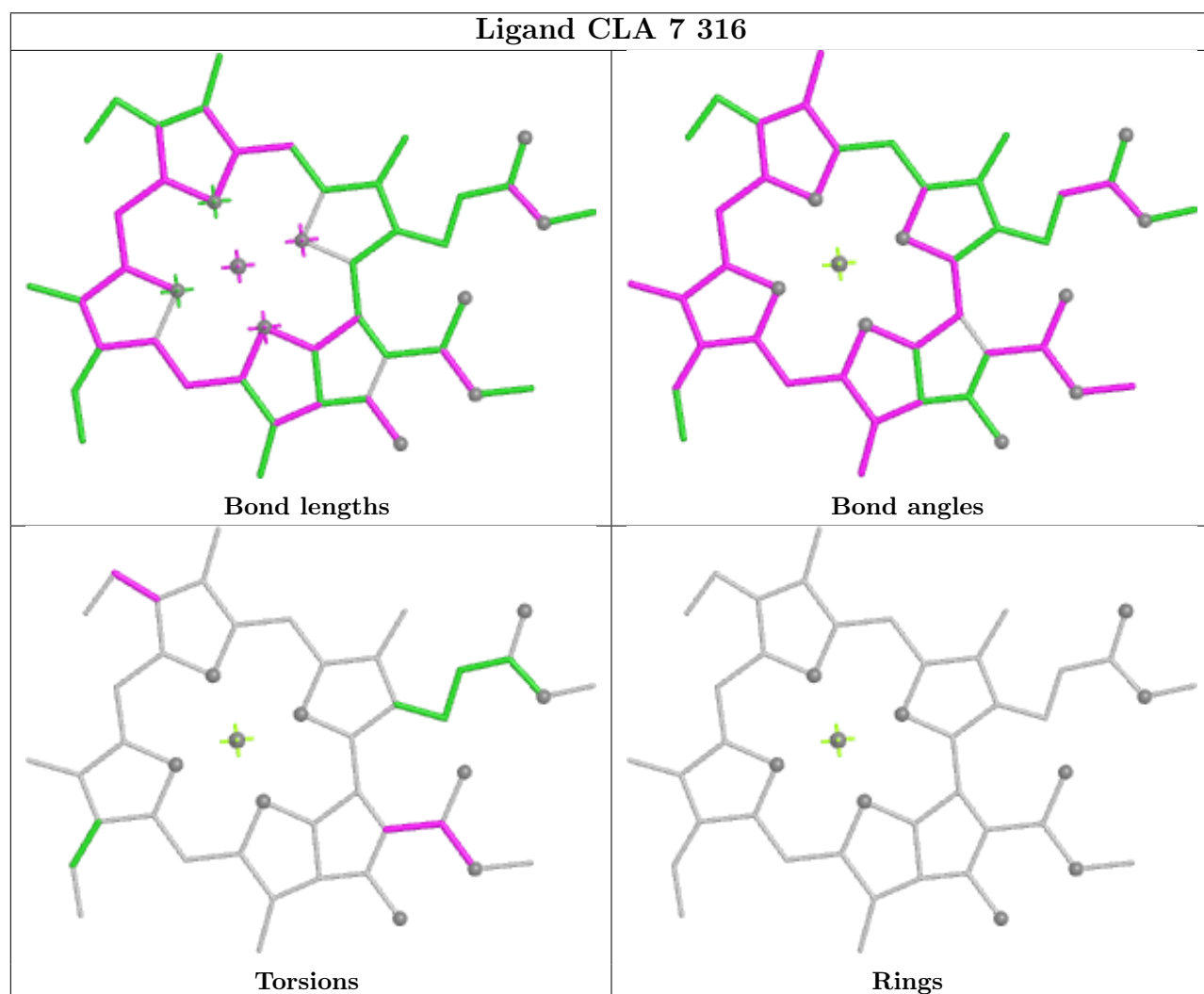
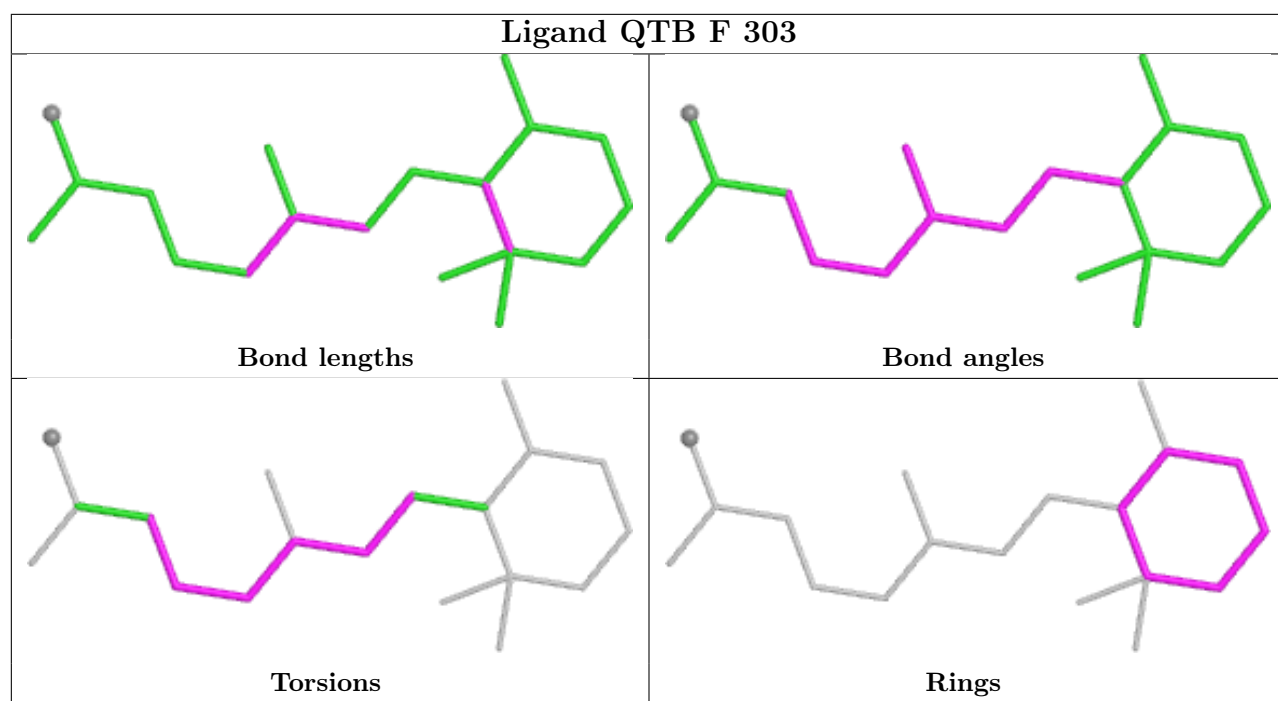




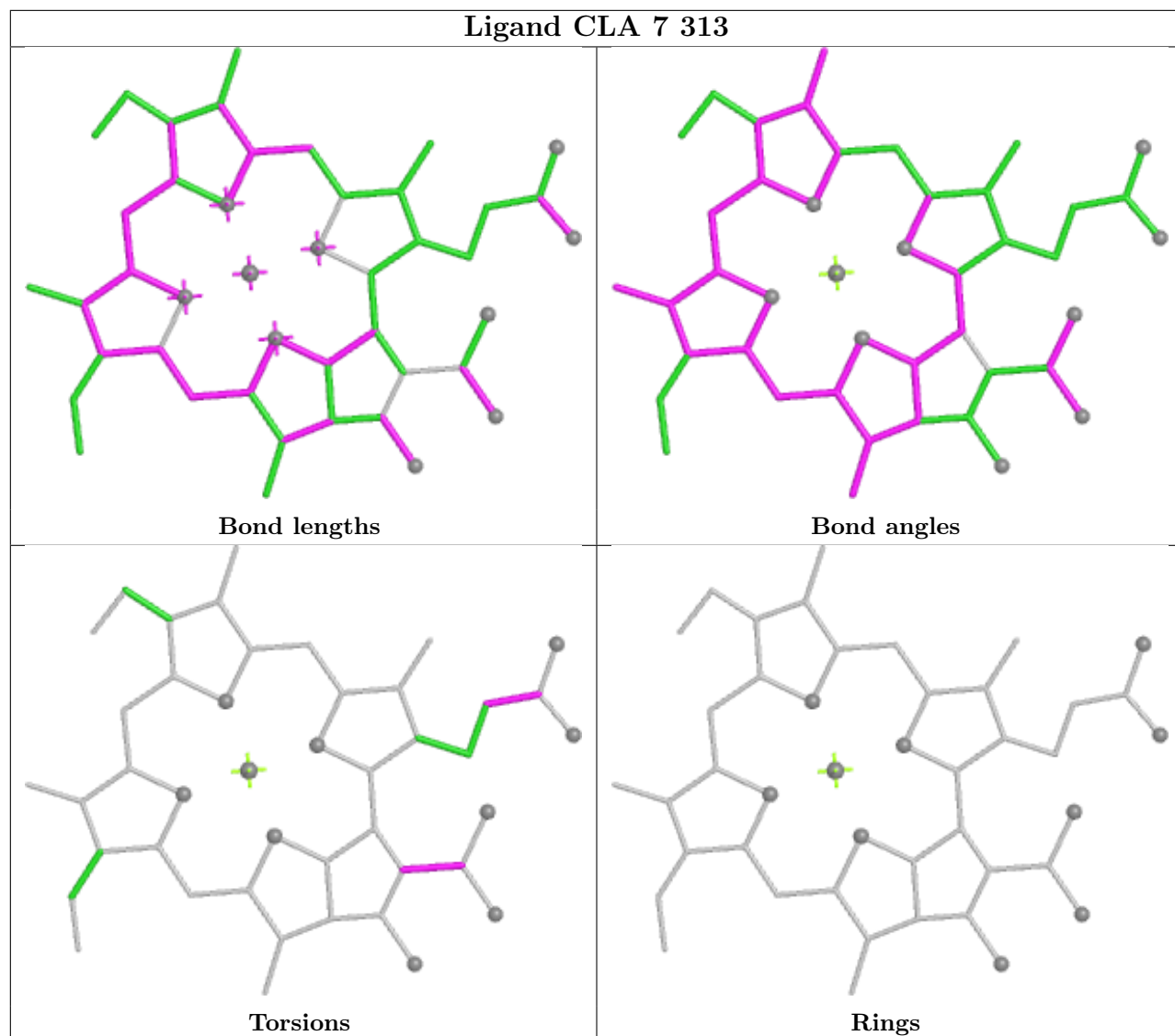


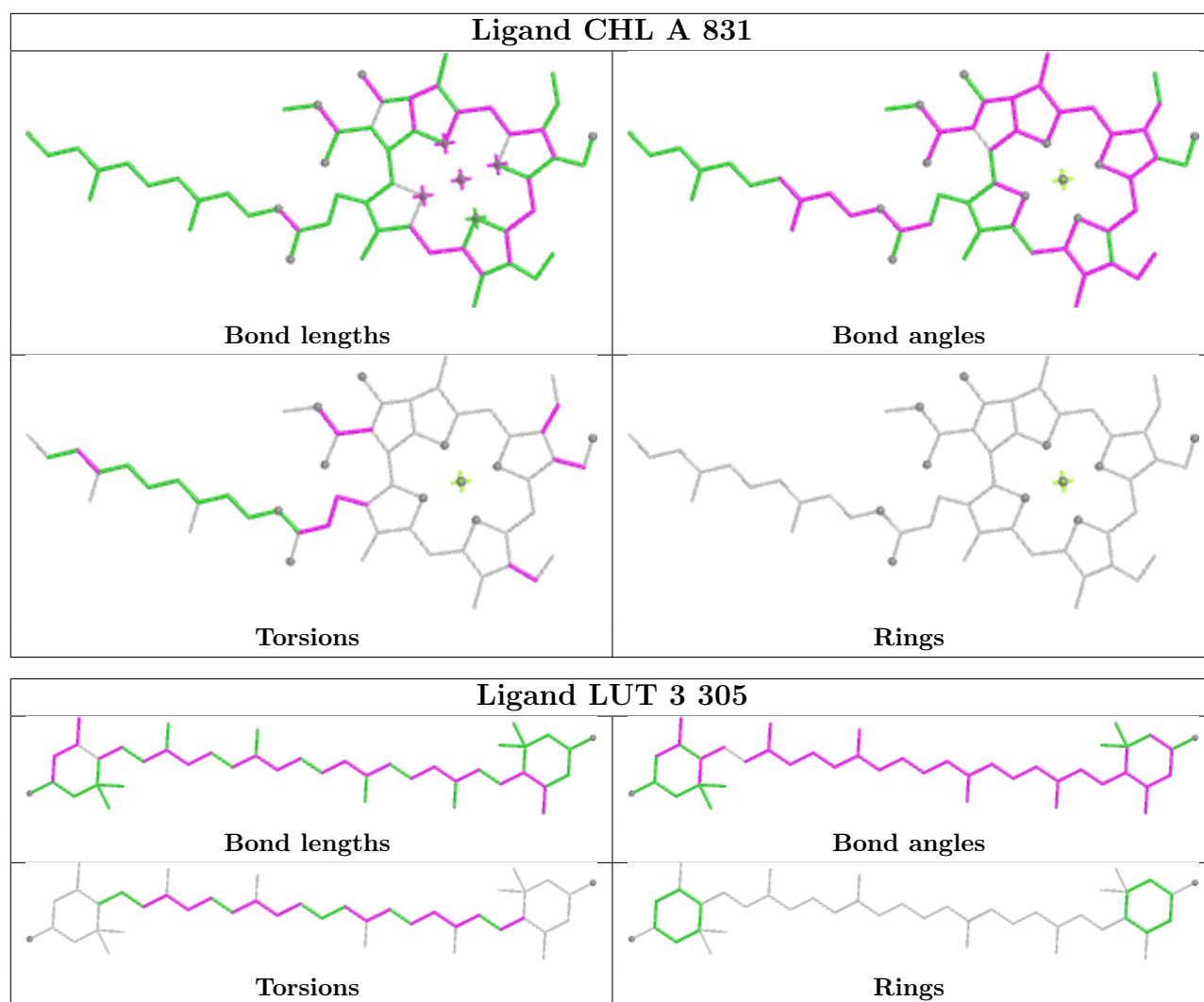




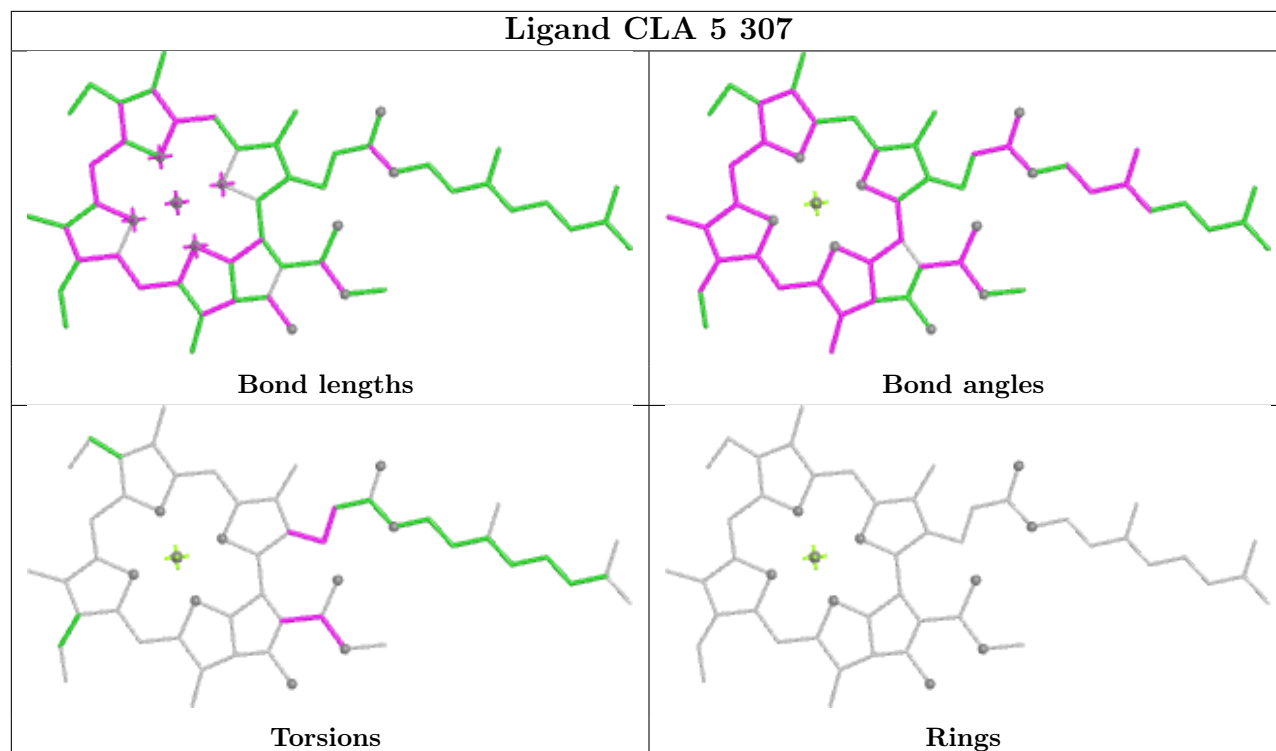


Ligand CLA 7 313

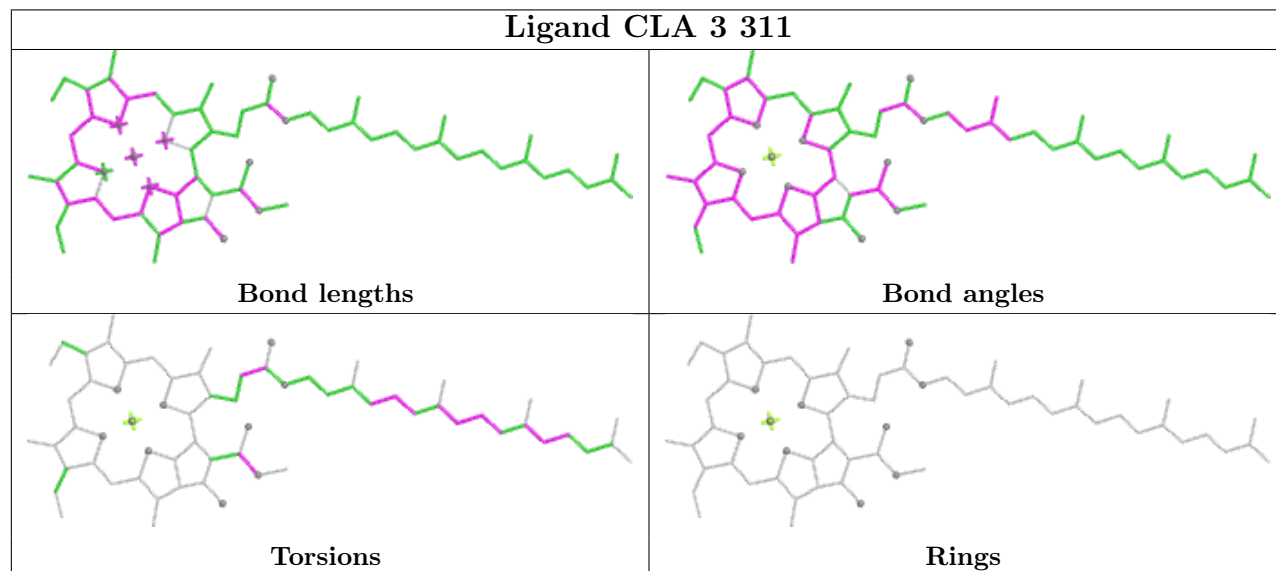


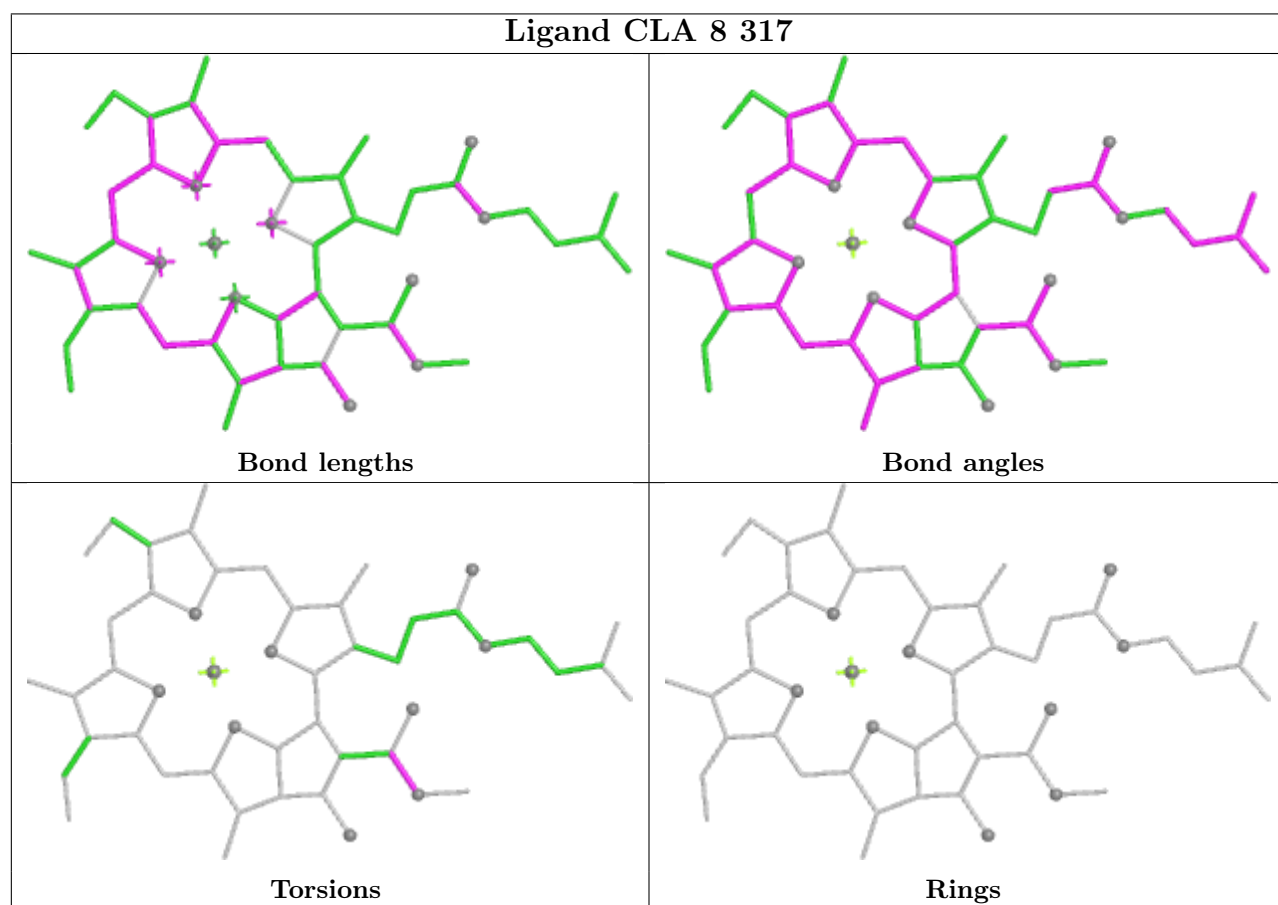
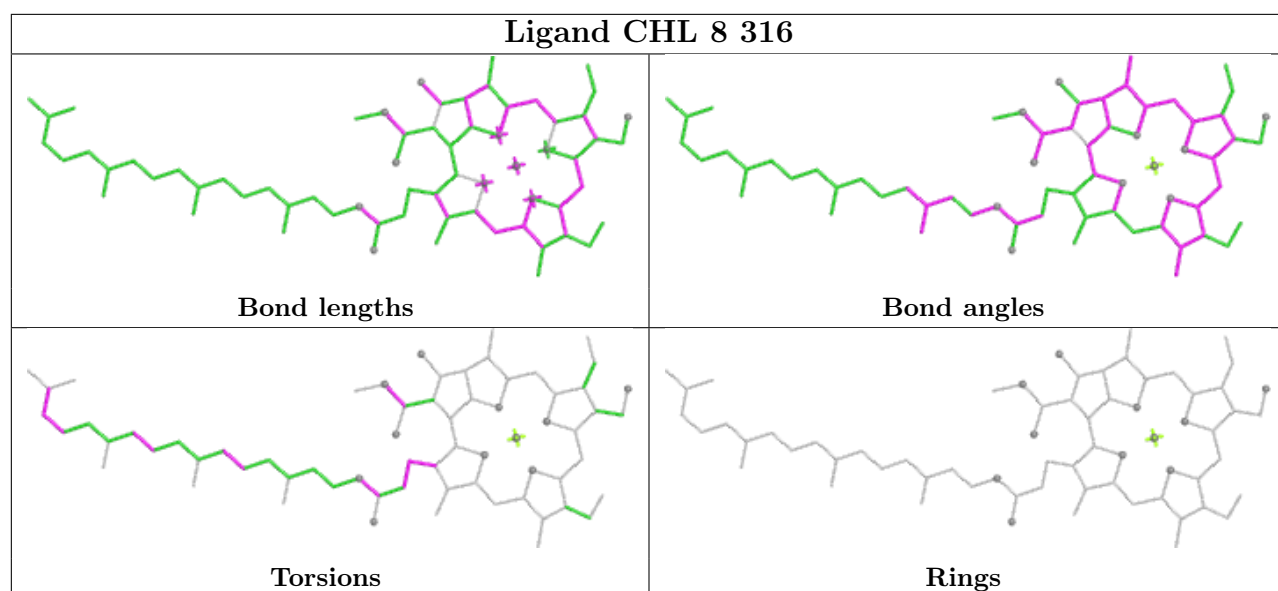


Ligand CLA 5 307

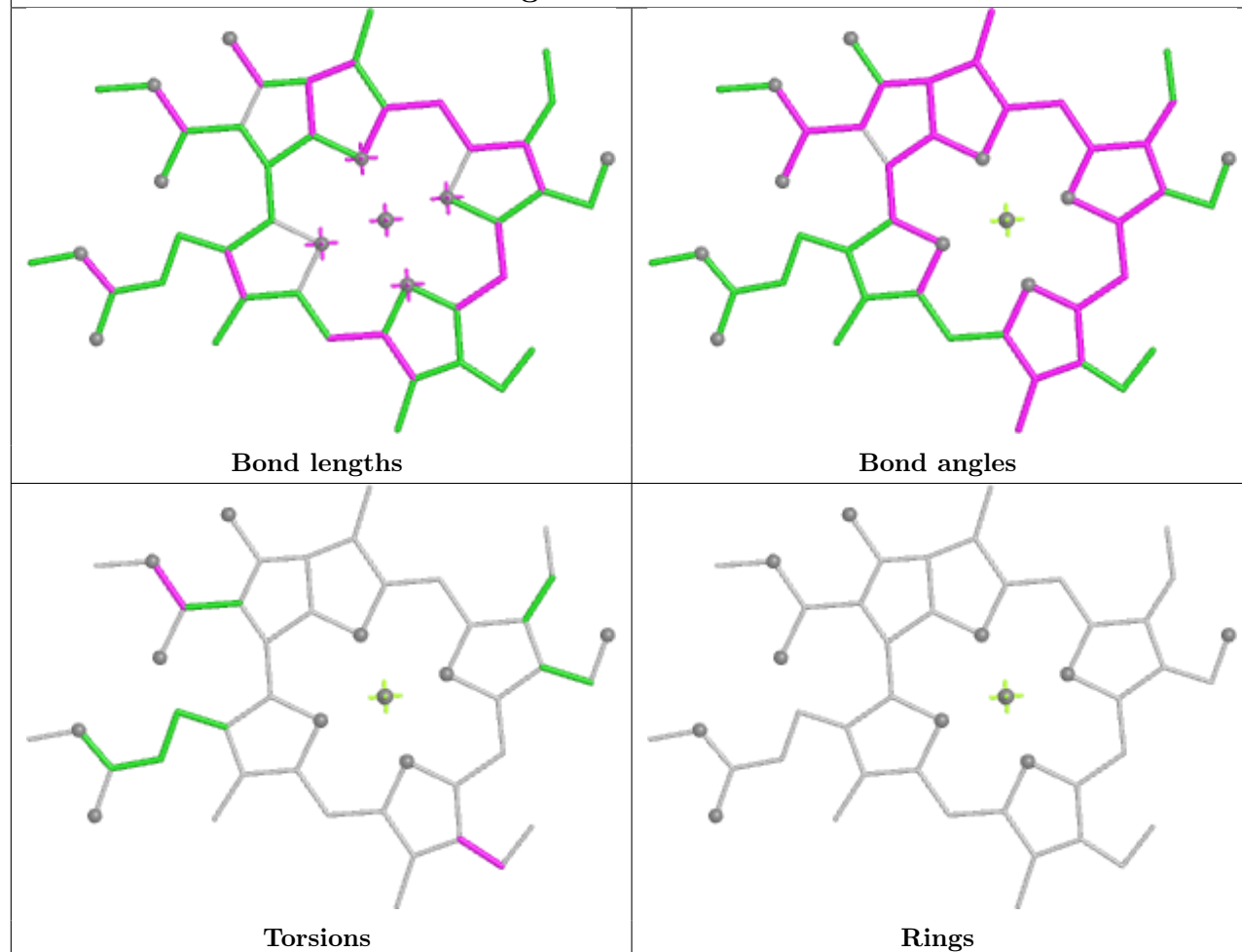


Ligand CLA 3 311

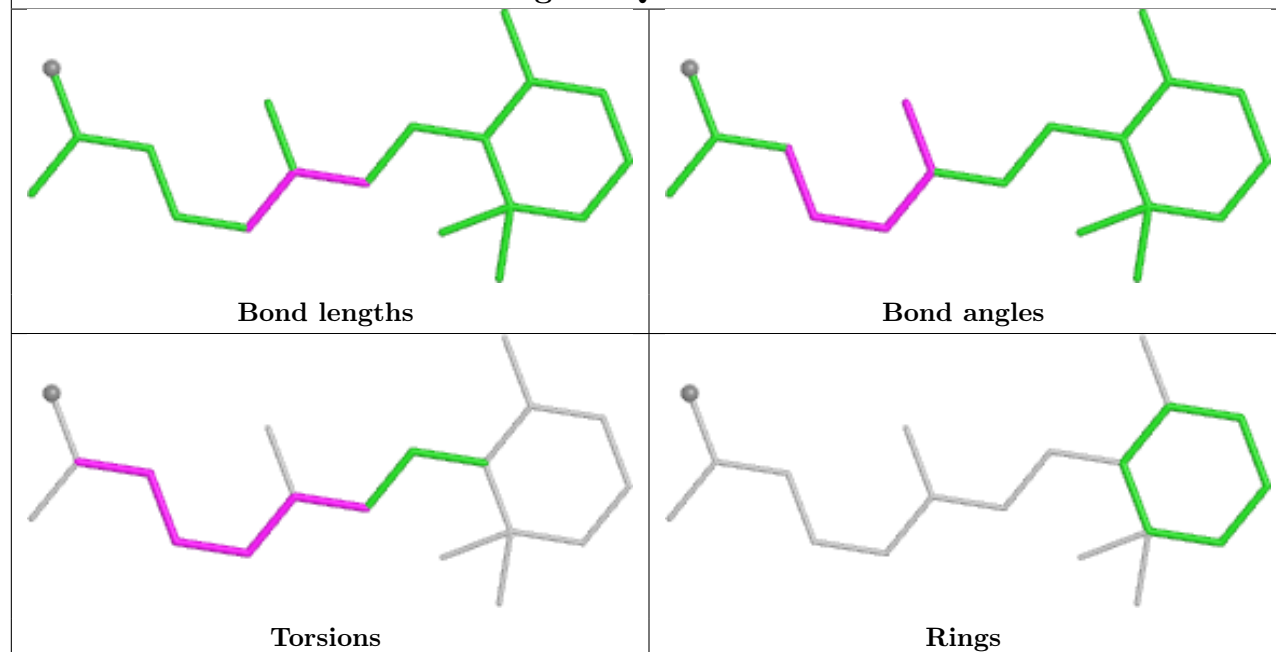




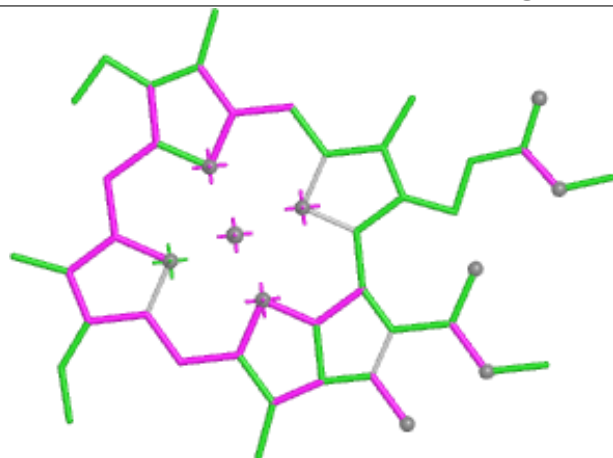
Ligand CHL 5 319



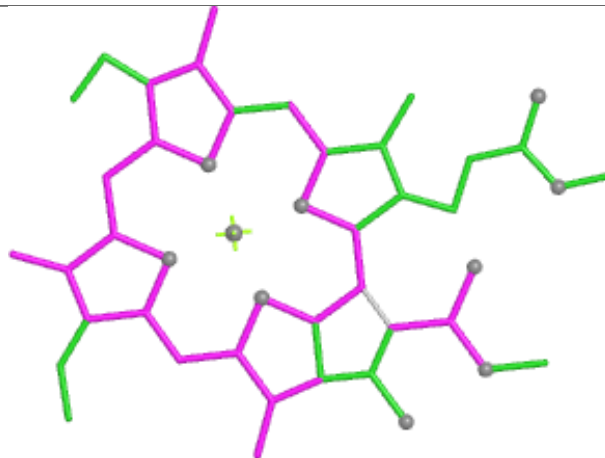
Ligand QTB 9 304



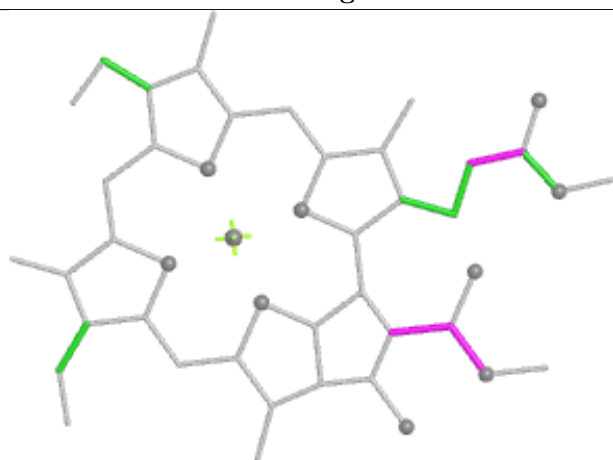
Ligand CLA 3 308



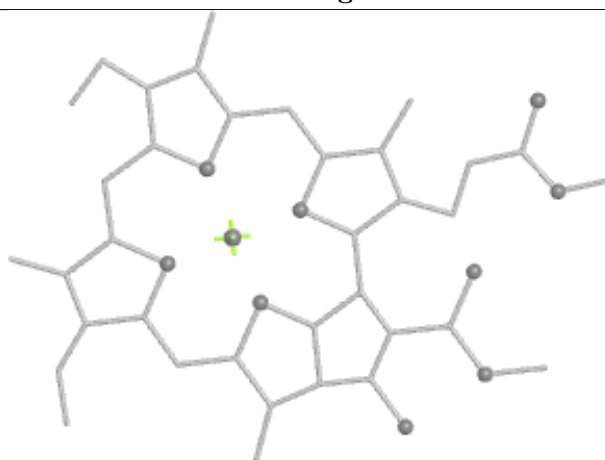
Bond lengths



Bond angles

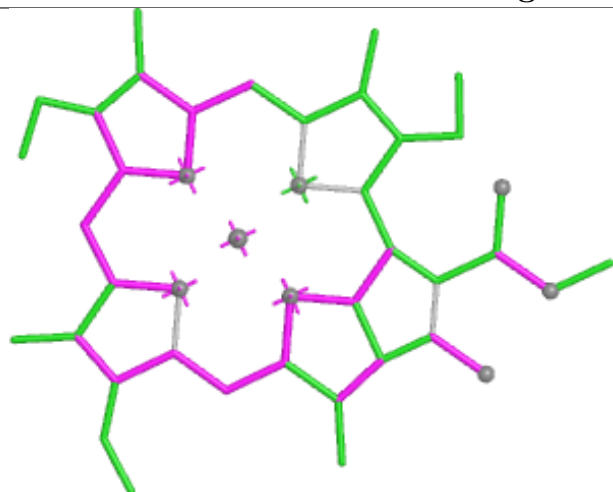


Torsions

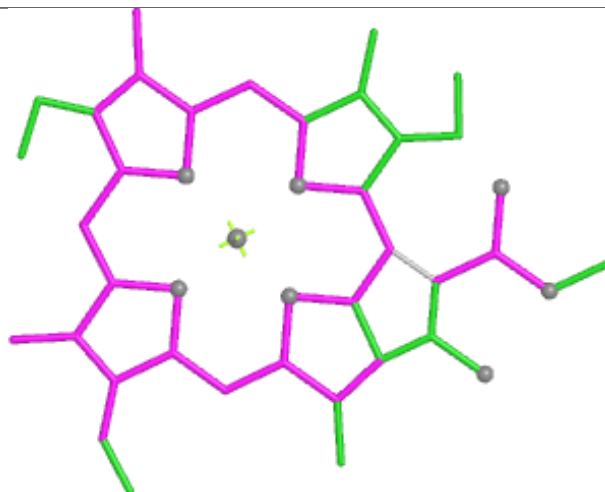


Rings

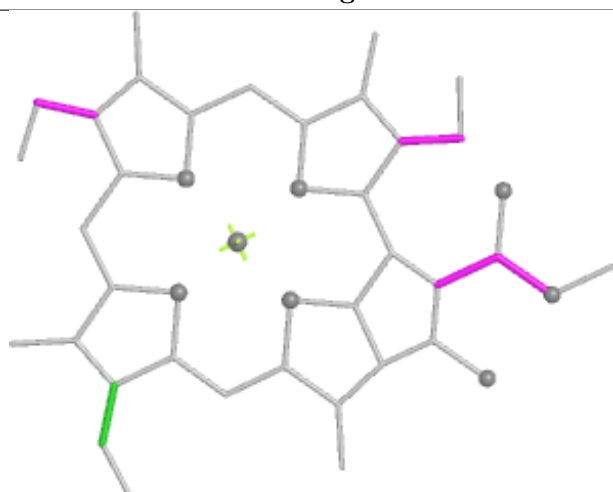
Ligand CLA J 105



Bond lengths



Bond angles

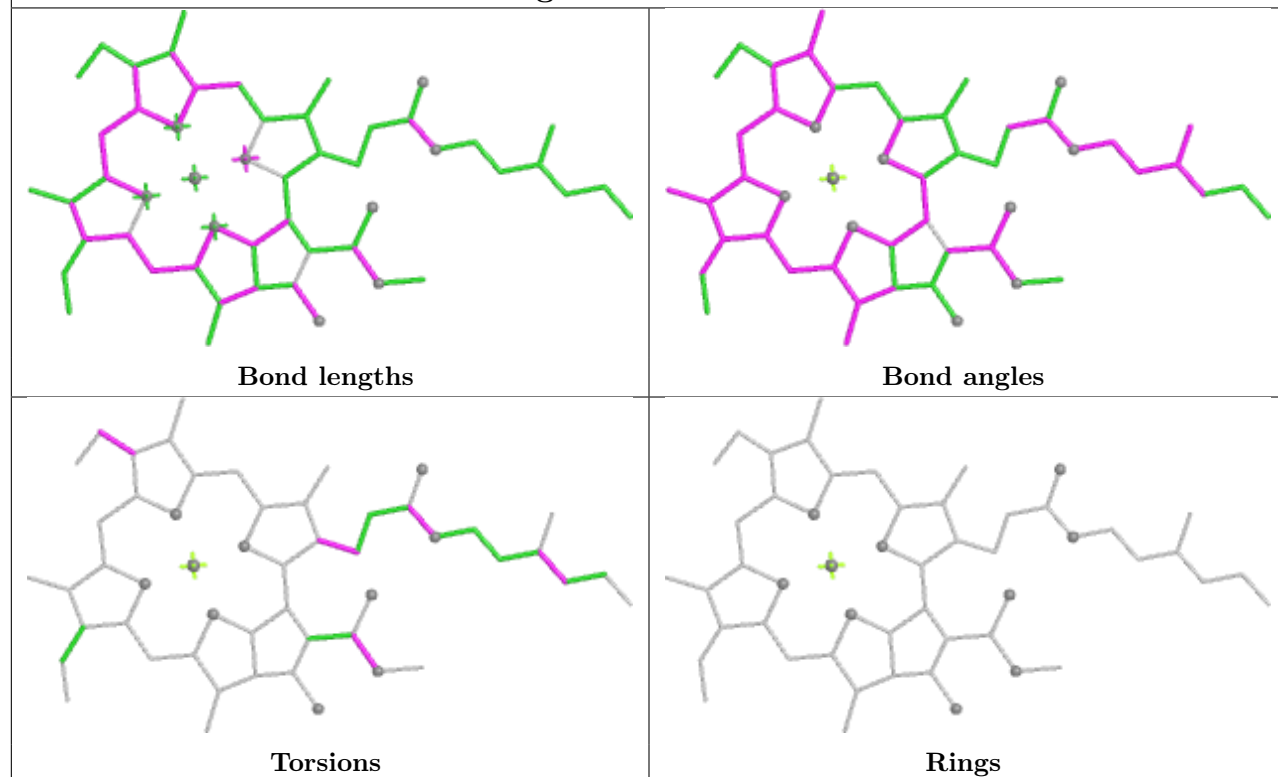


Torsions

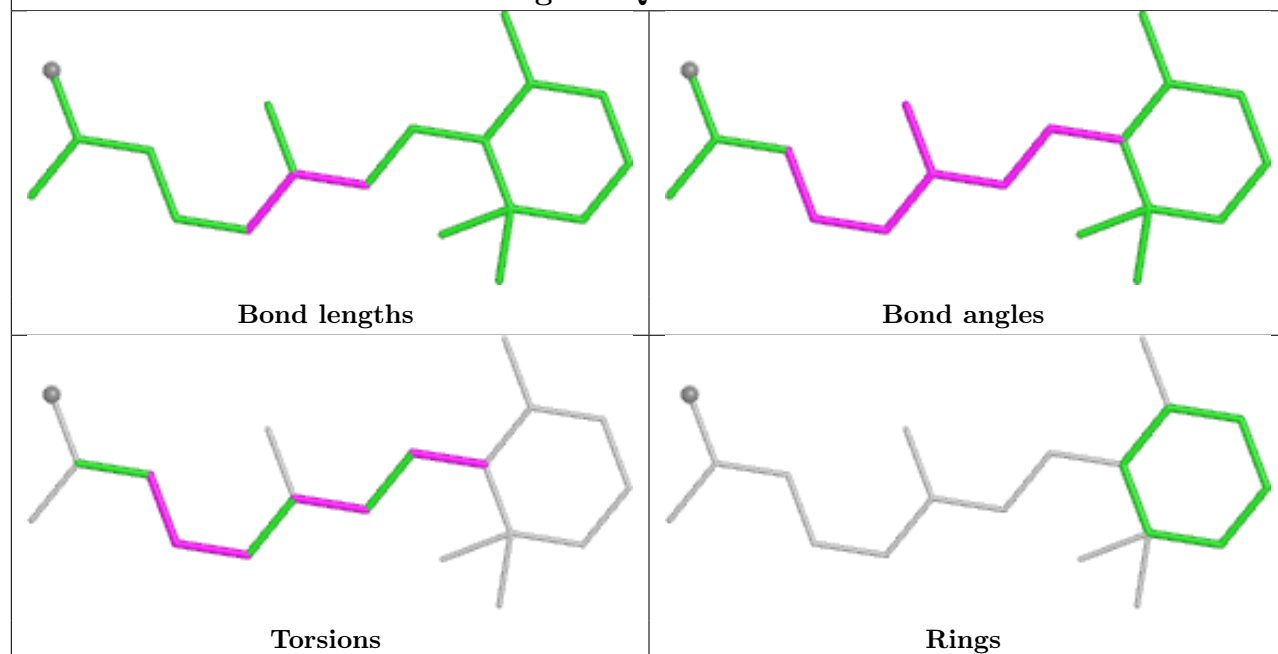


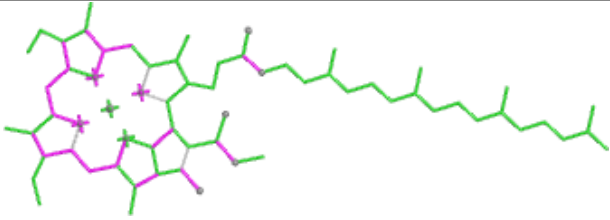
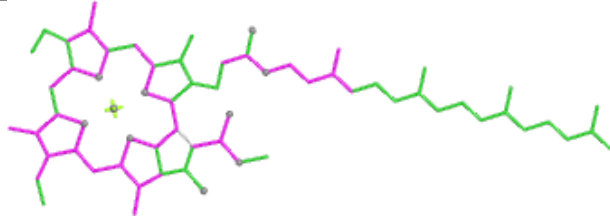
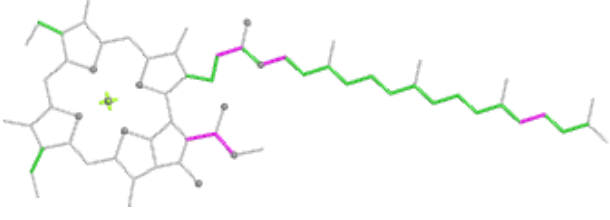
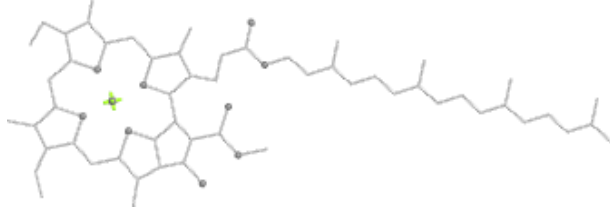
Rings

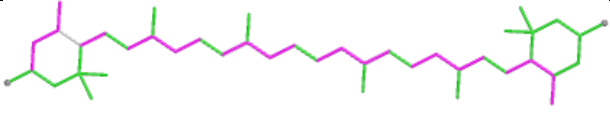
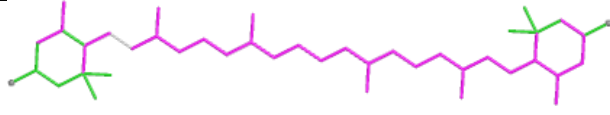
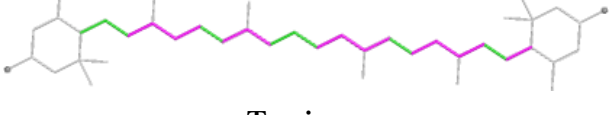
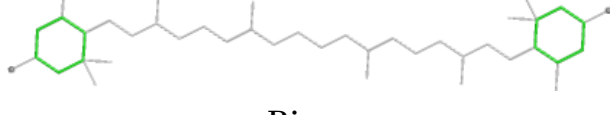
Ligand CLA 3 314



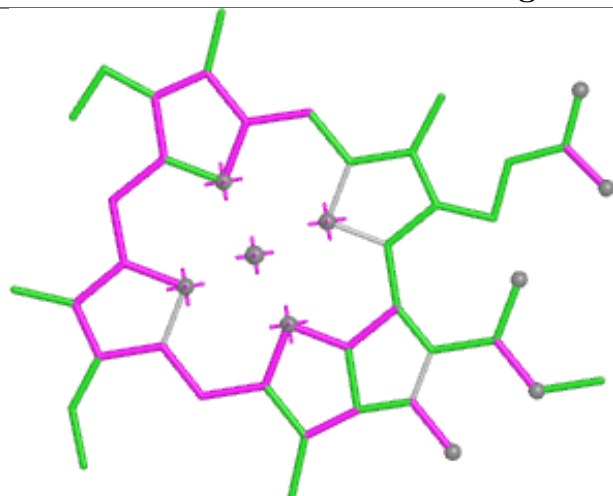
Ligand QTB a 302



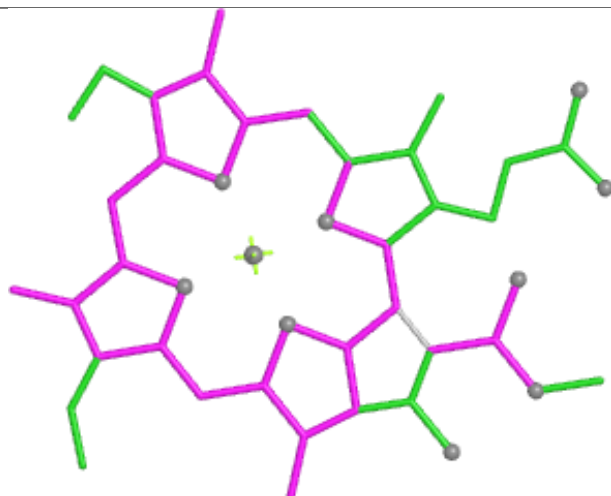
Ligand CLA A 816			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand LUT 4 303			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand CLA 4 320



Bond lengths



Bond angles

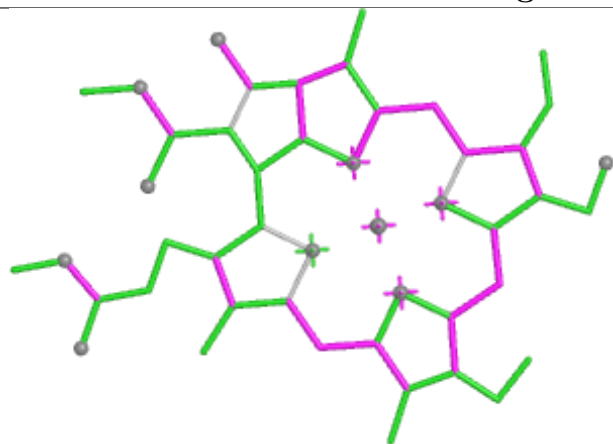


Torsions

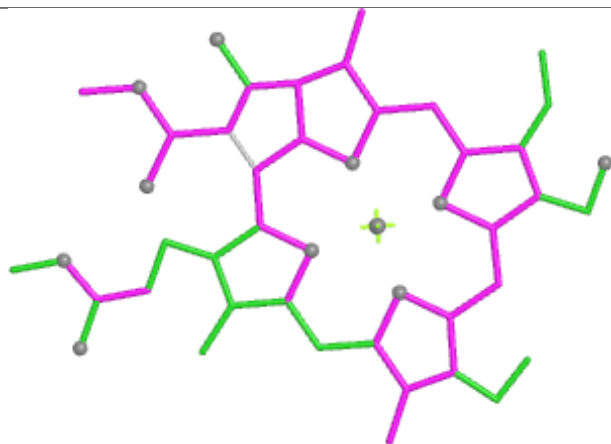


Rings

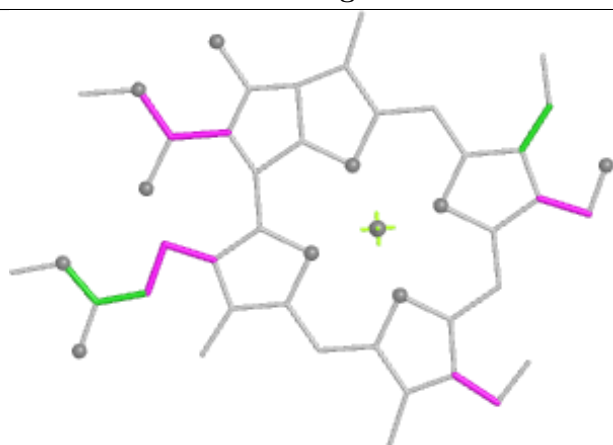
Ligand CHL b 309



Bond lengths



Bond angles

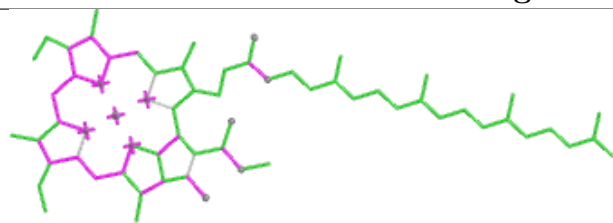


Torsions

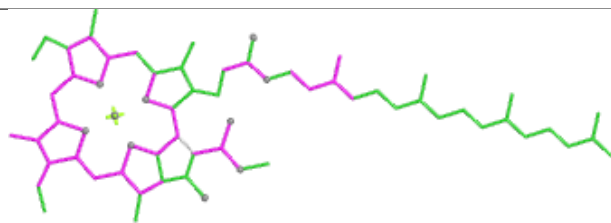


Rings

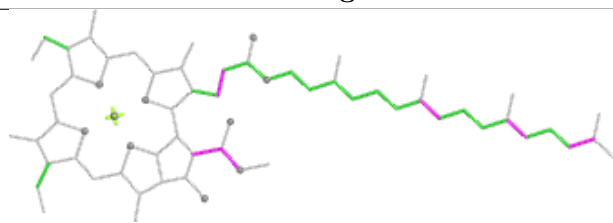
Ligand CLA A 814



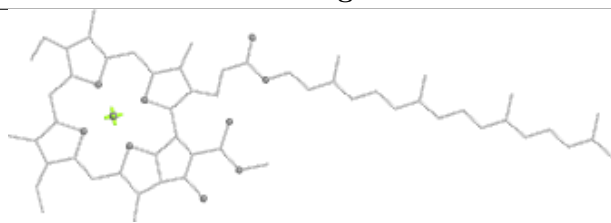
Bond lengths



Bond angles

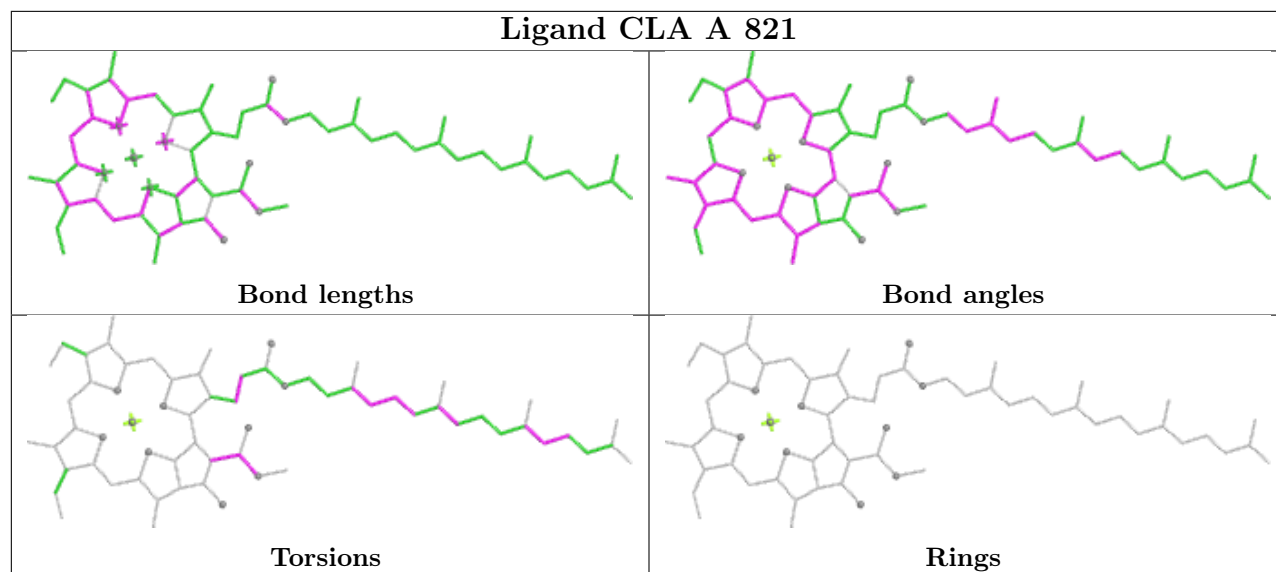


Torsions

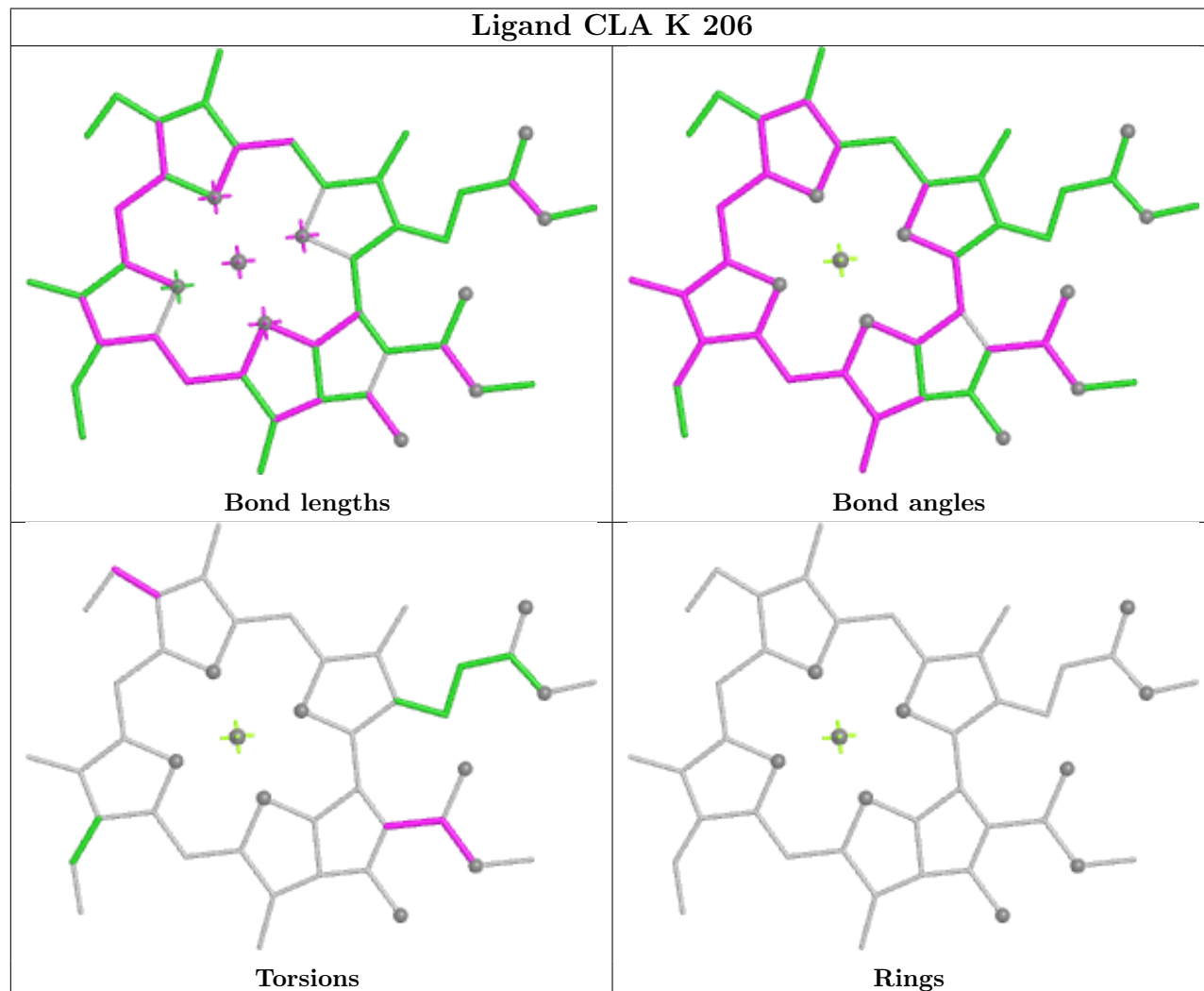


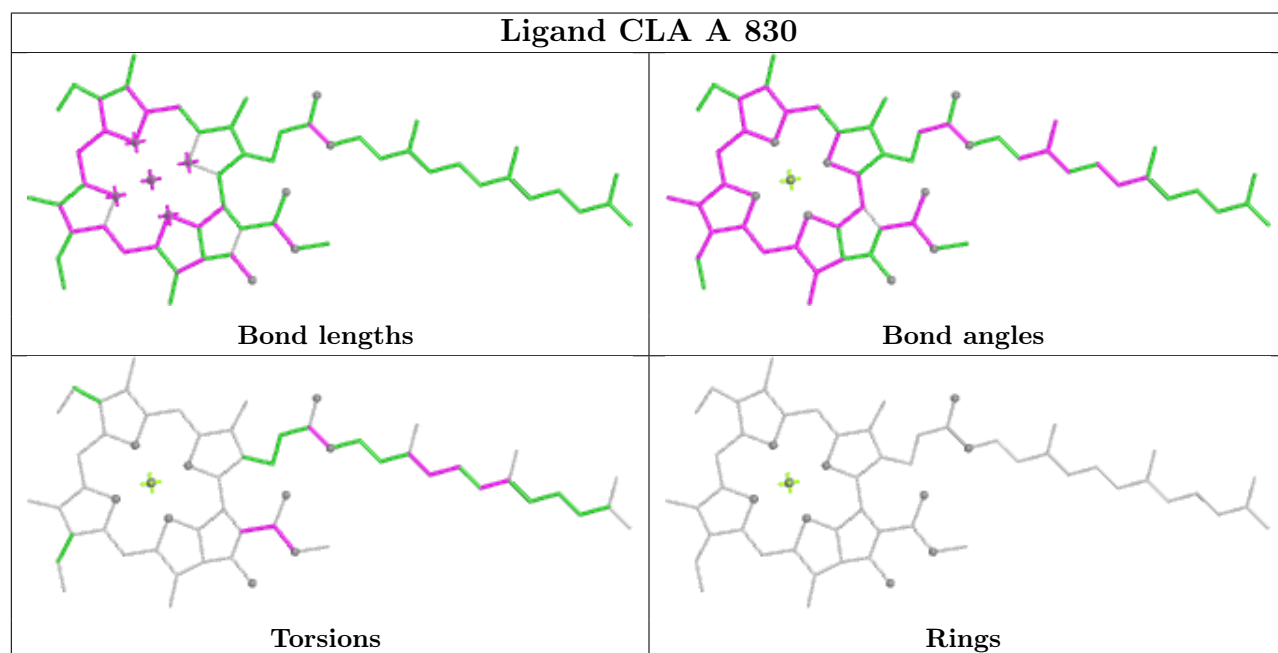
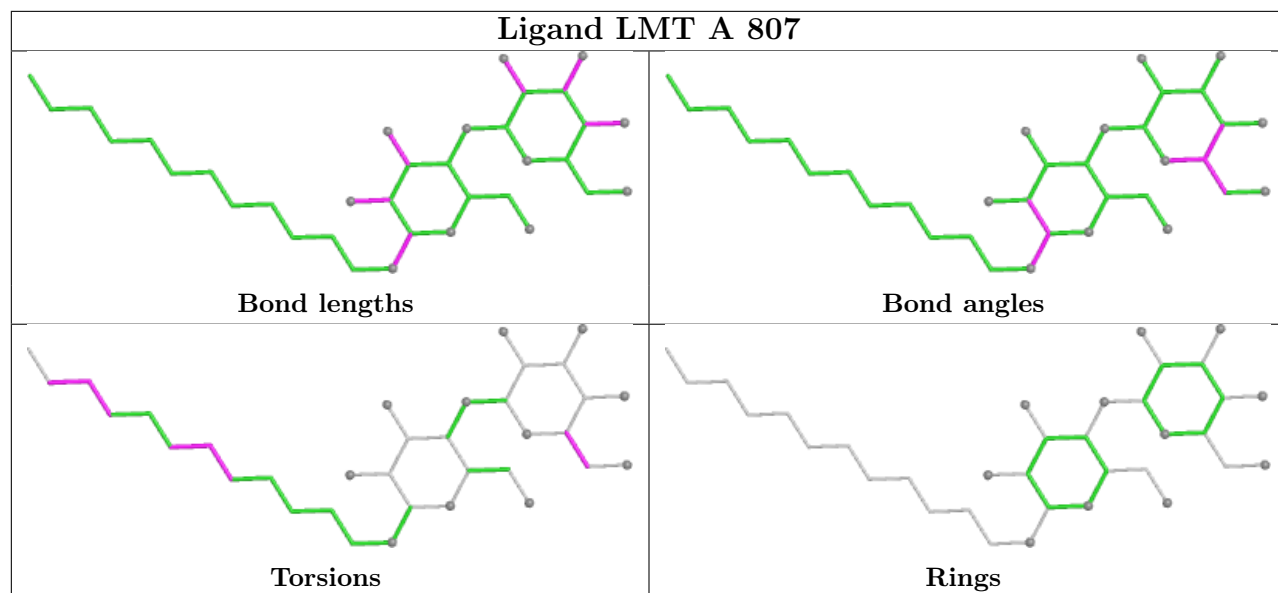
Rings

Ligand CLA A 821

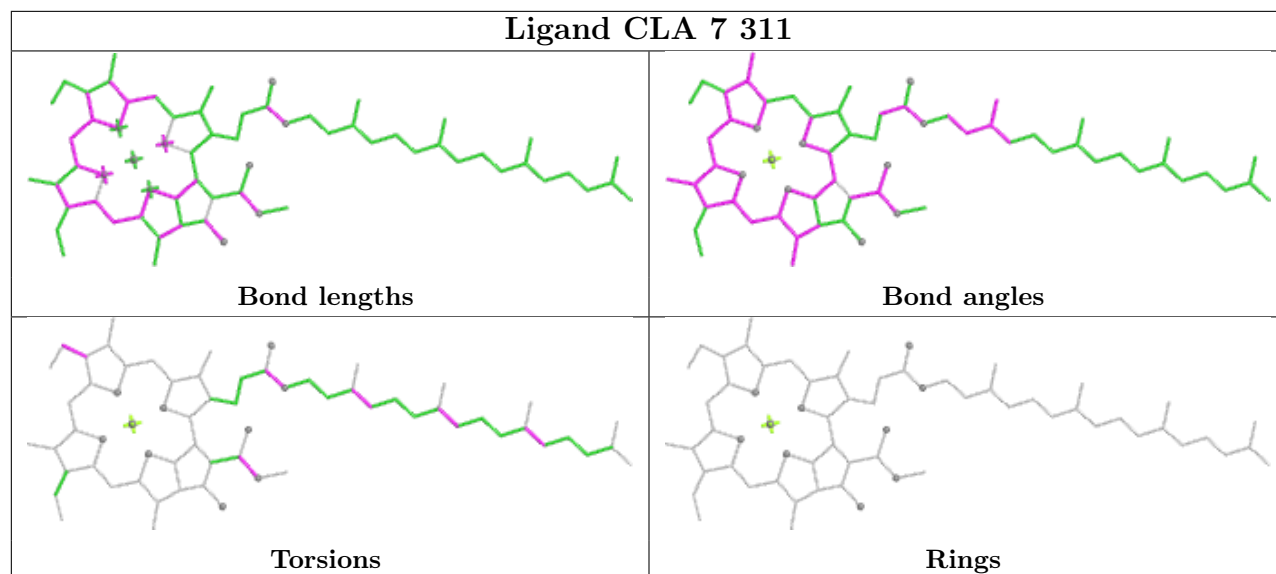


Ligand CLA K 206

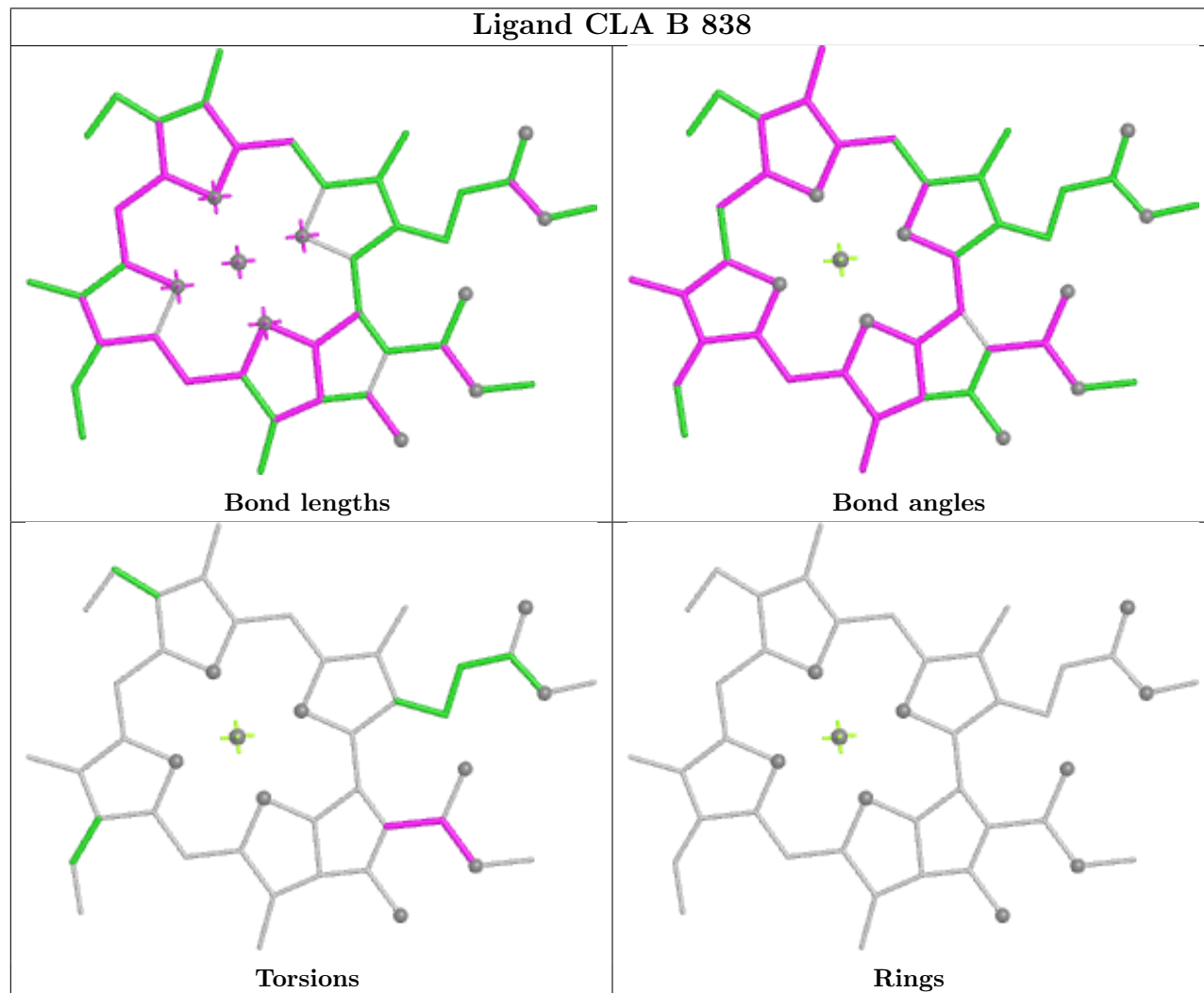


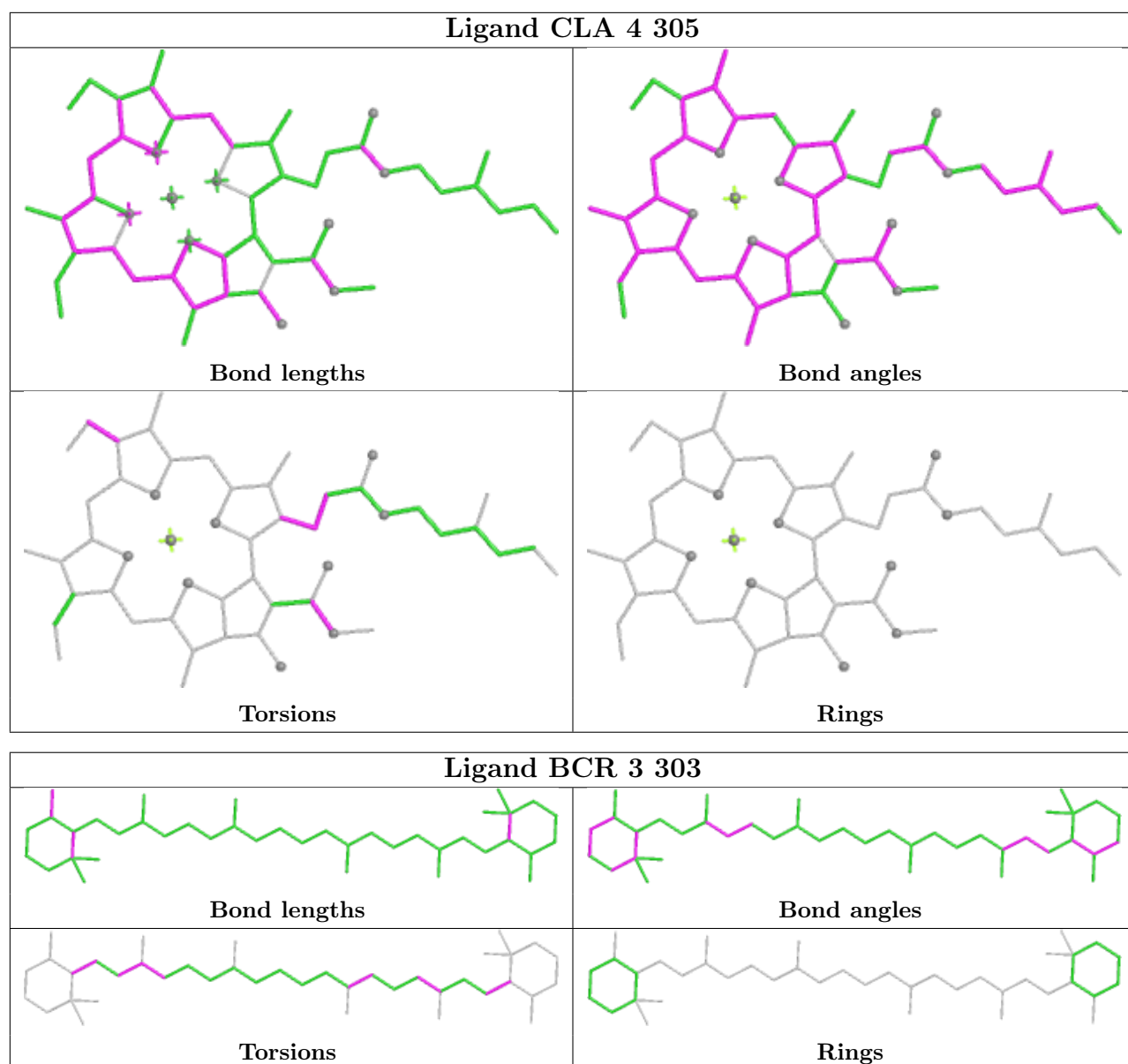


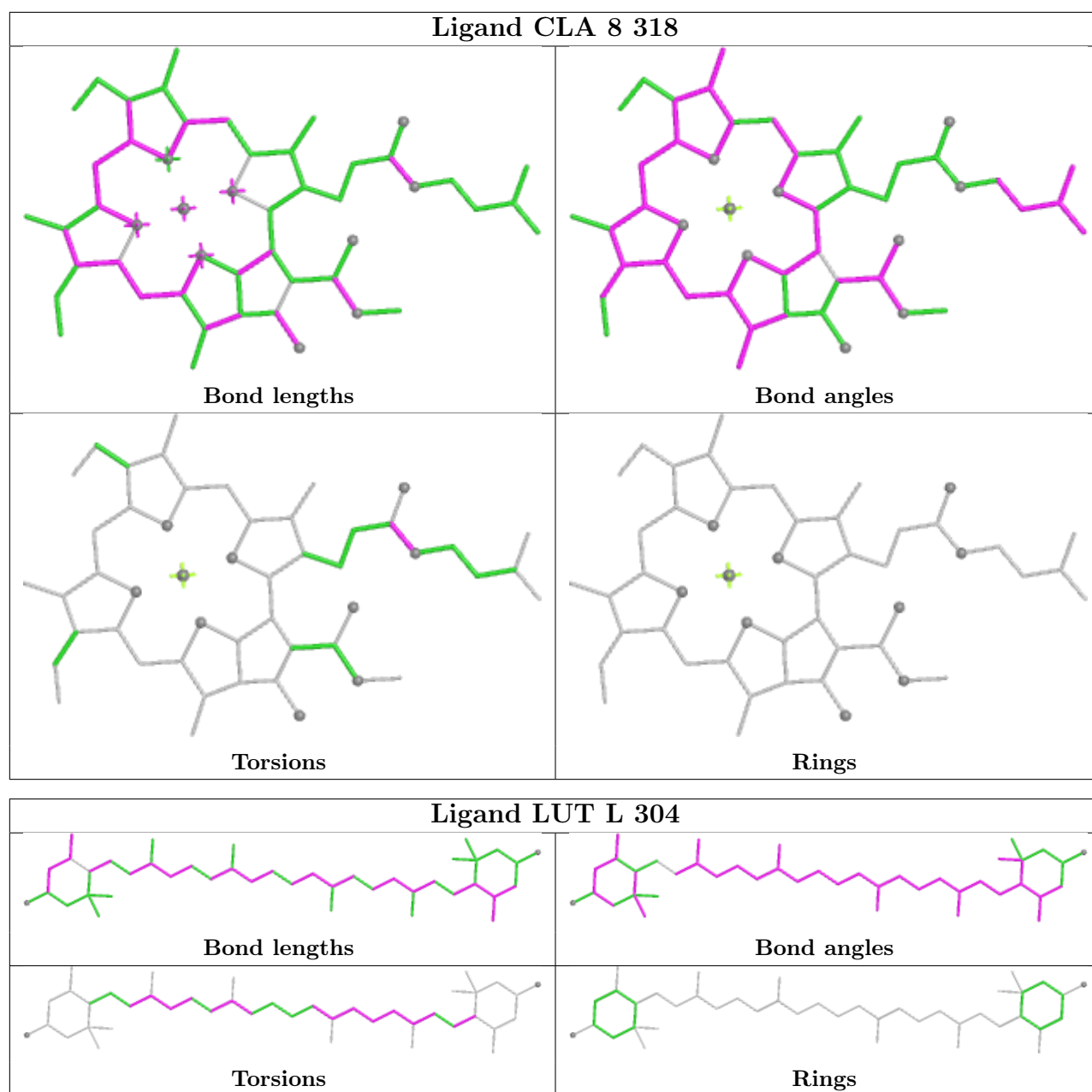
Ligand CLA 7 311

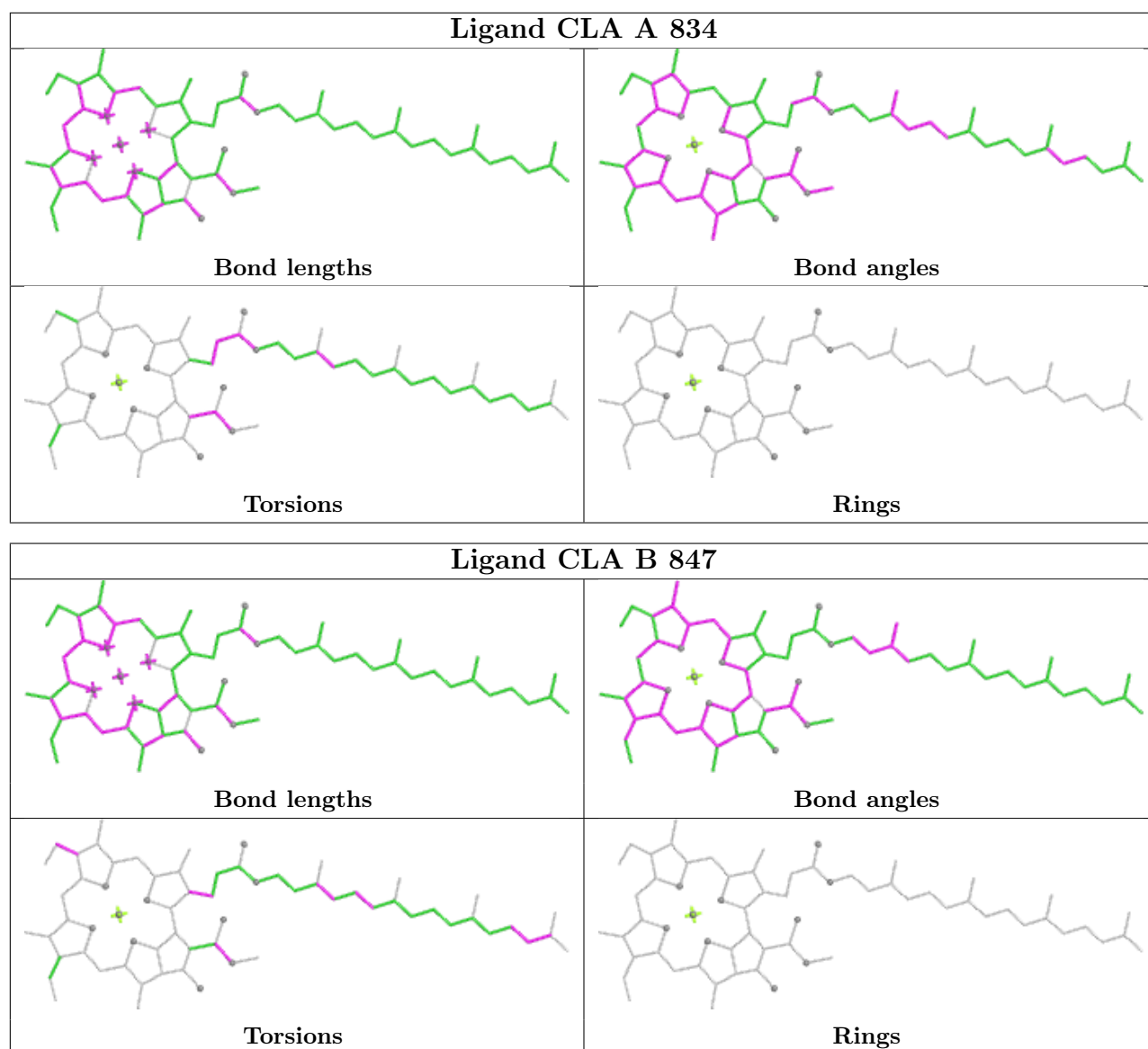


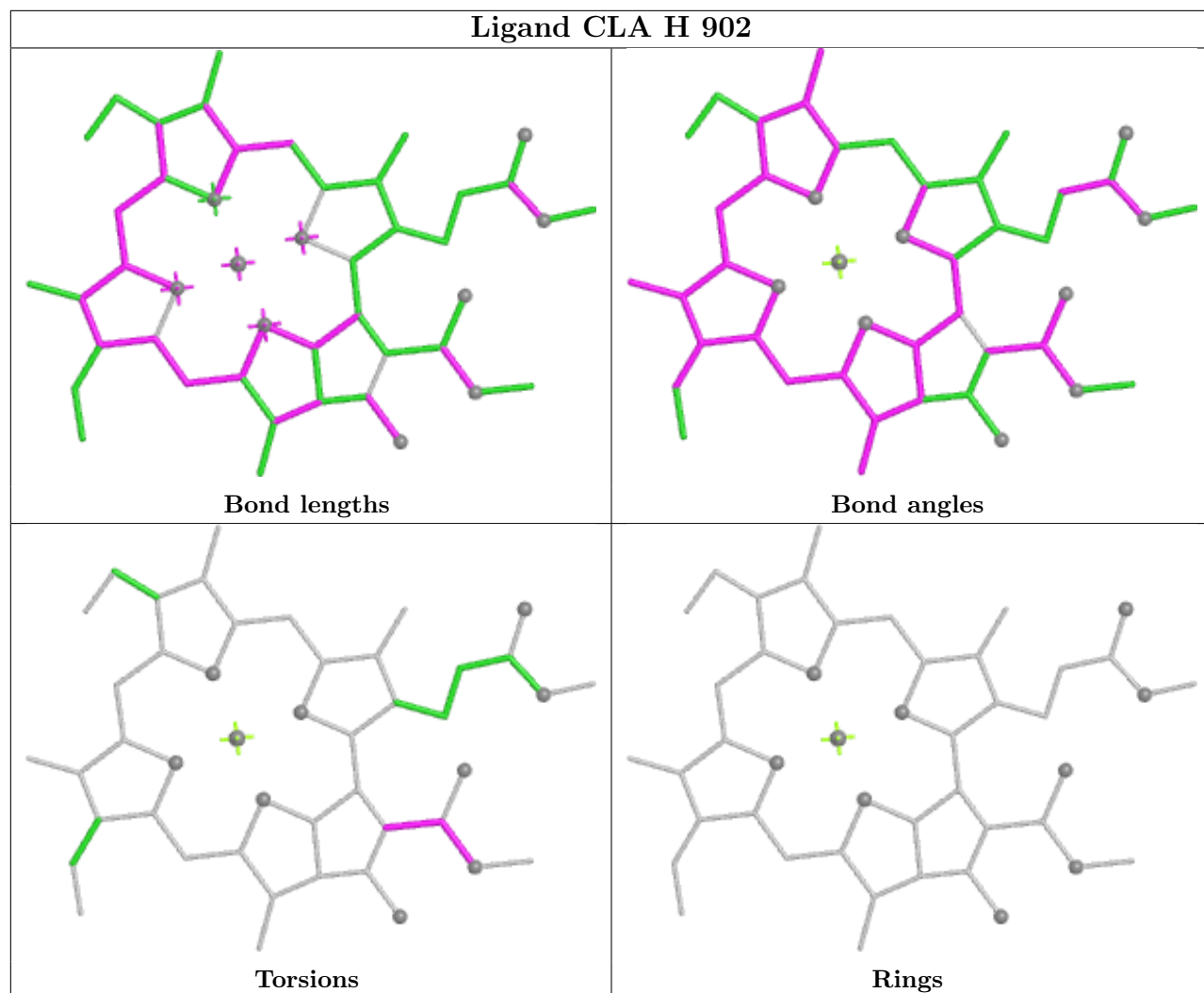
Ligand CLA B 838



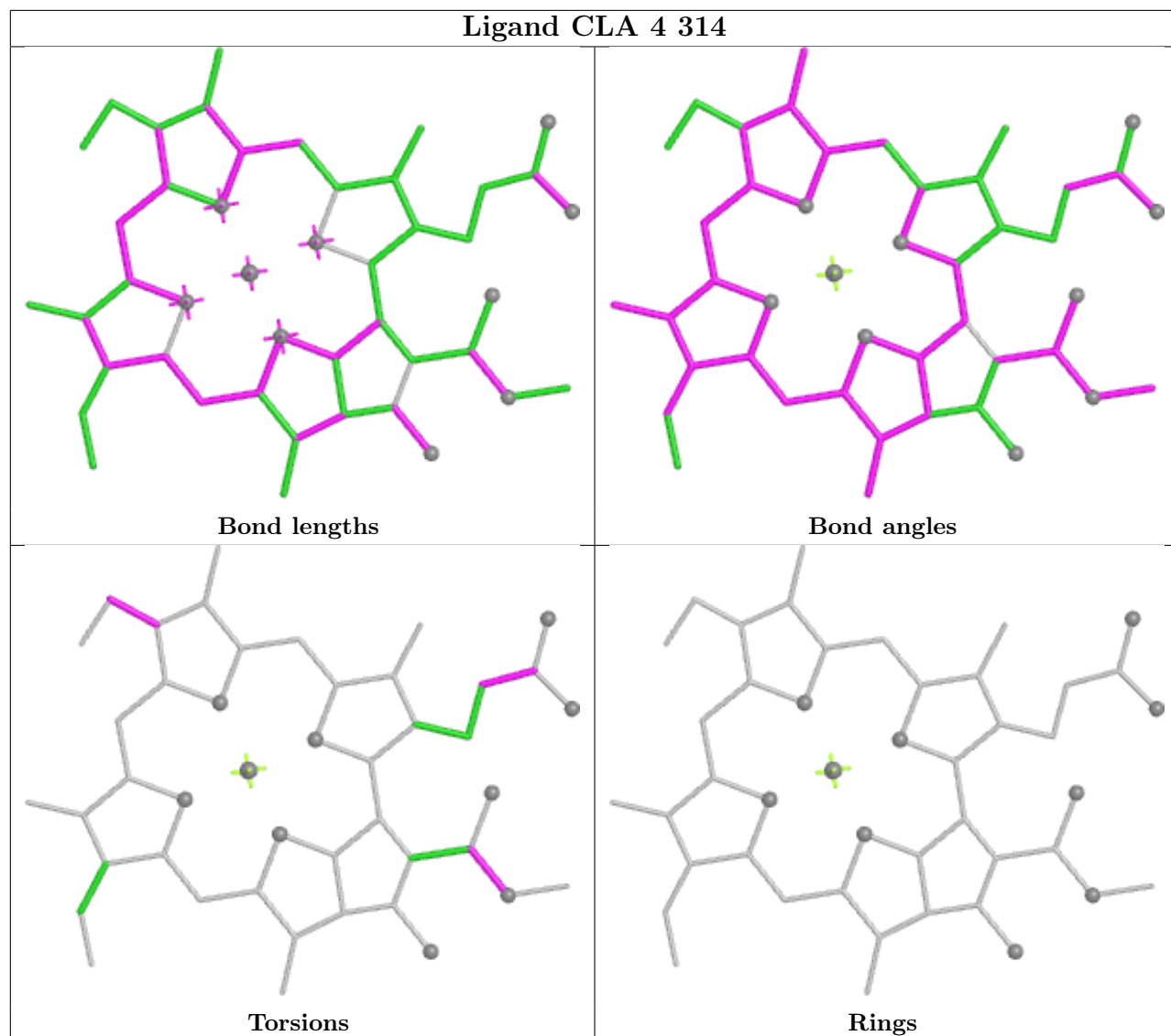




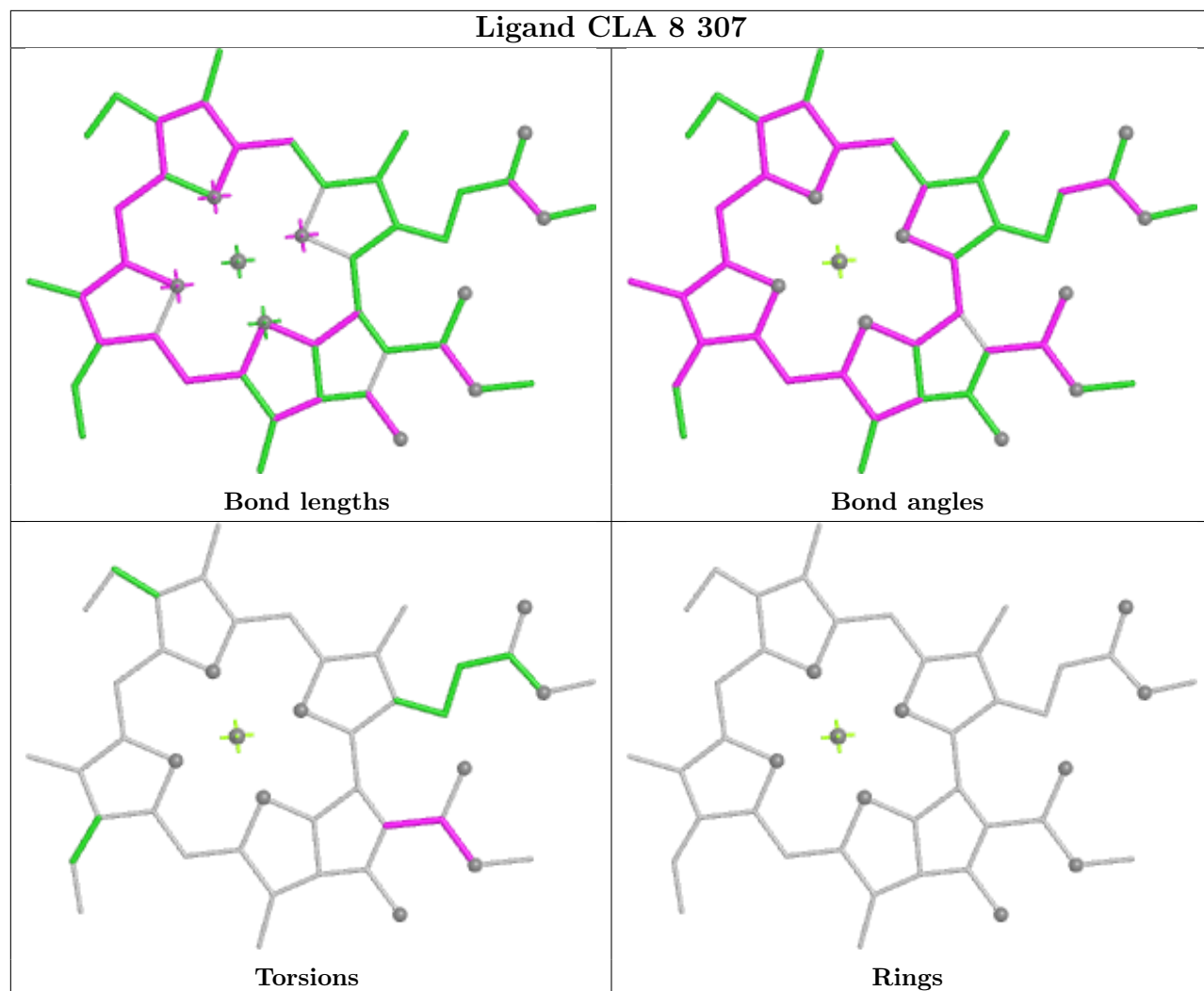




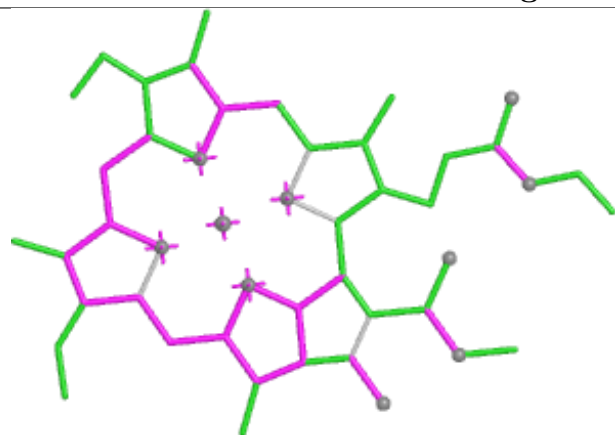
Ligand CLA 4 314



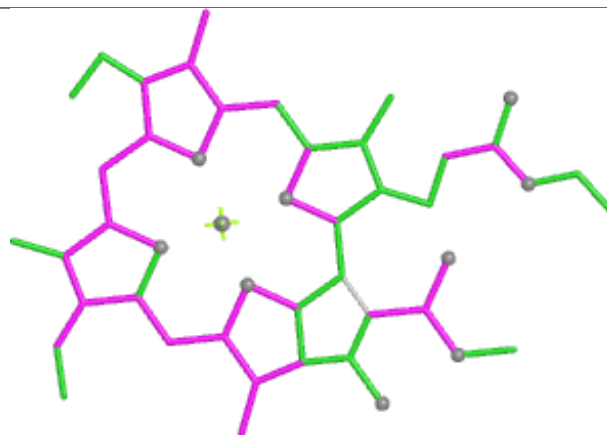
Ligand CLA 8 307



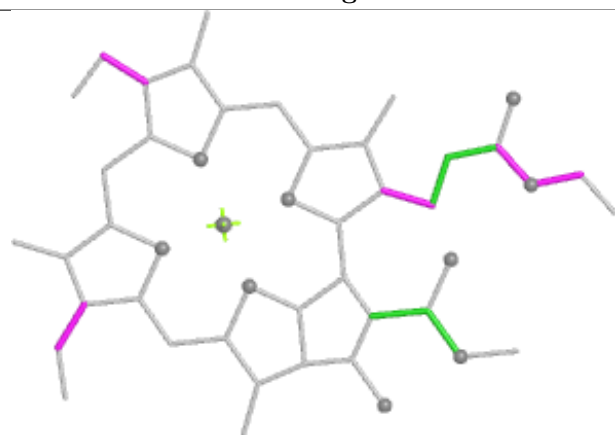
Ligand CLA 9 317



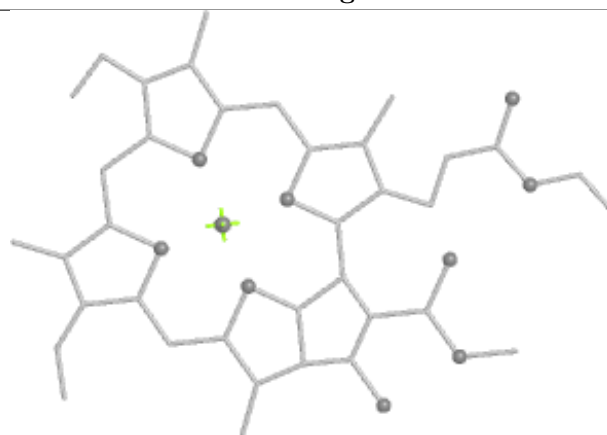
Bond lengths



Bond angles

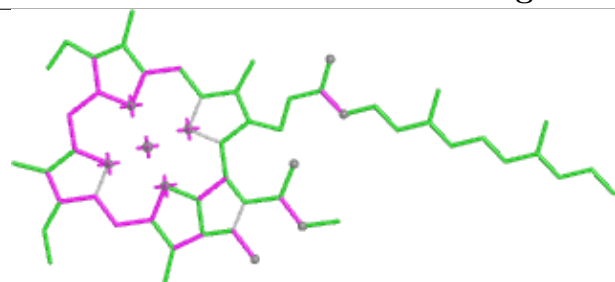


Torsions

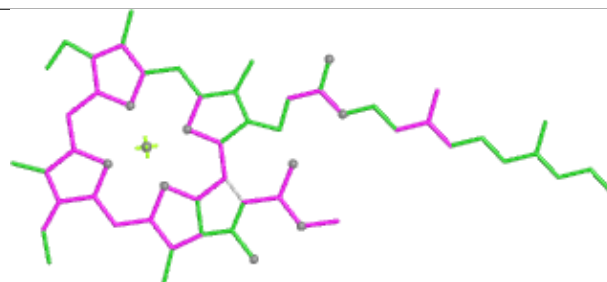


Rings

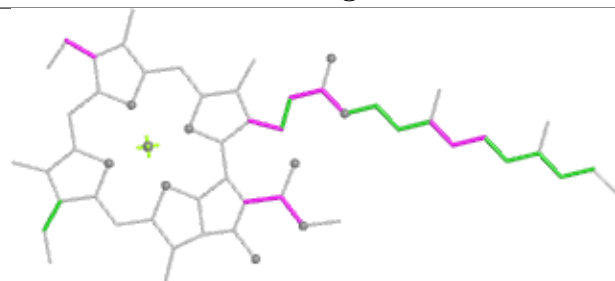
Ligand CLA A 848



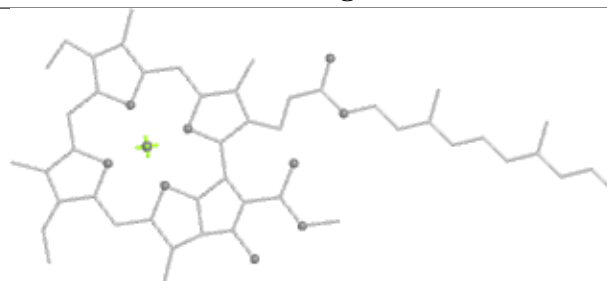
Bond lengths



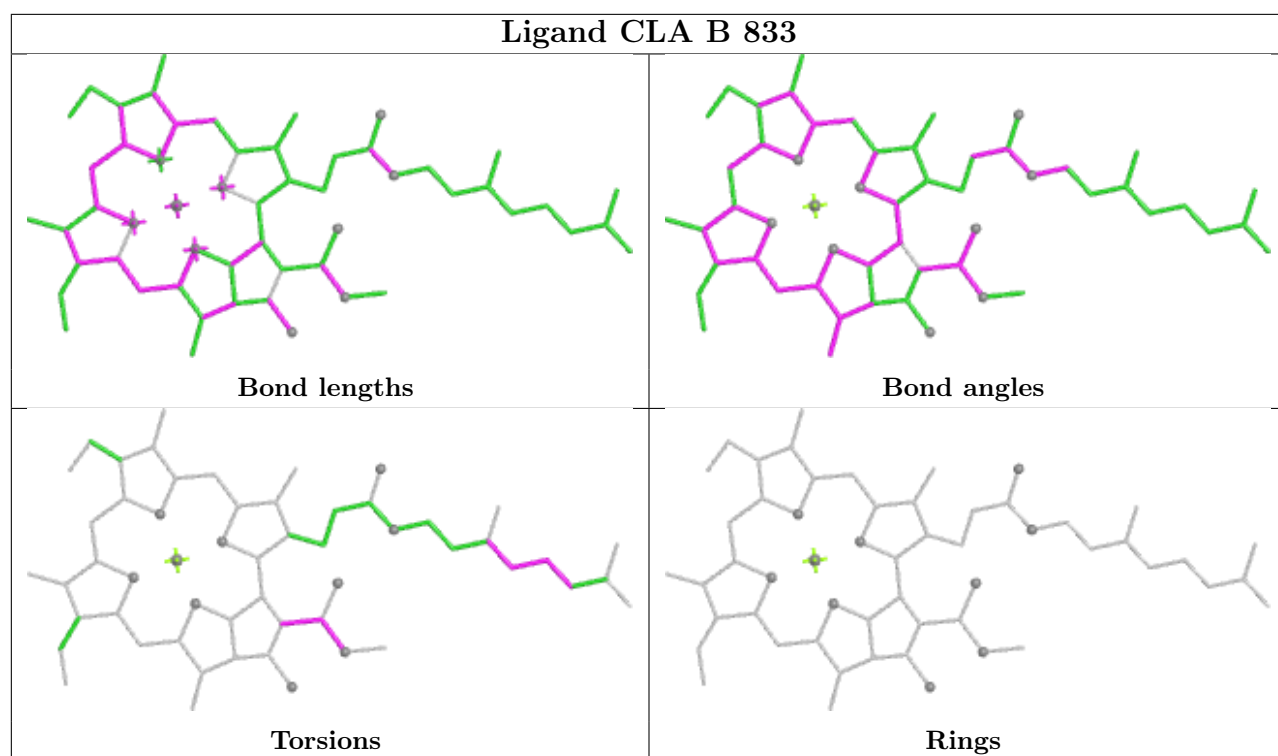
Bond angles



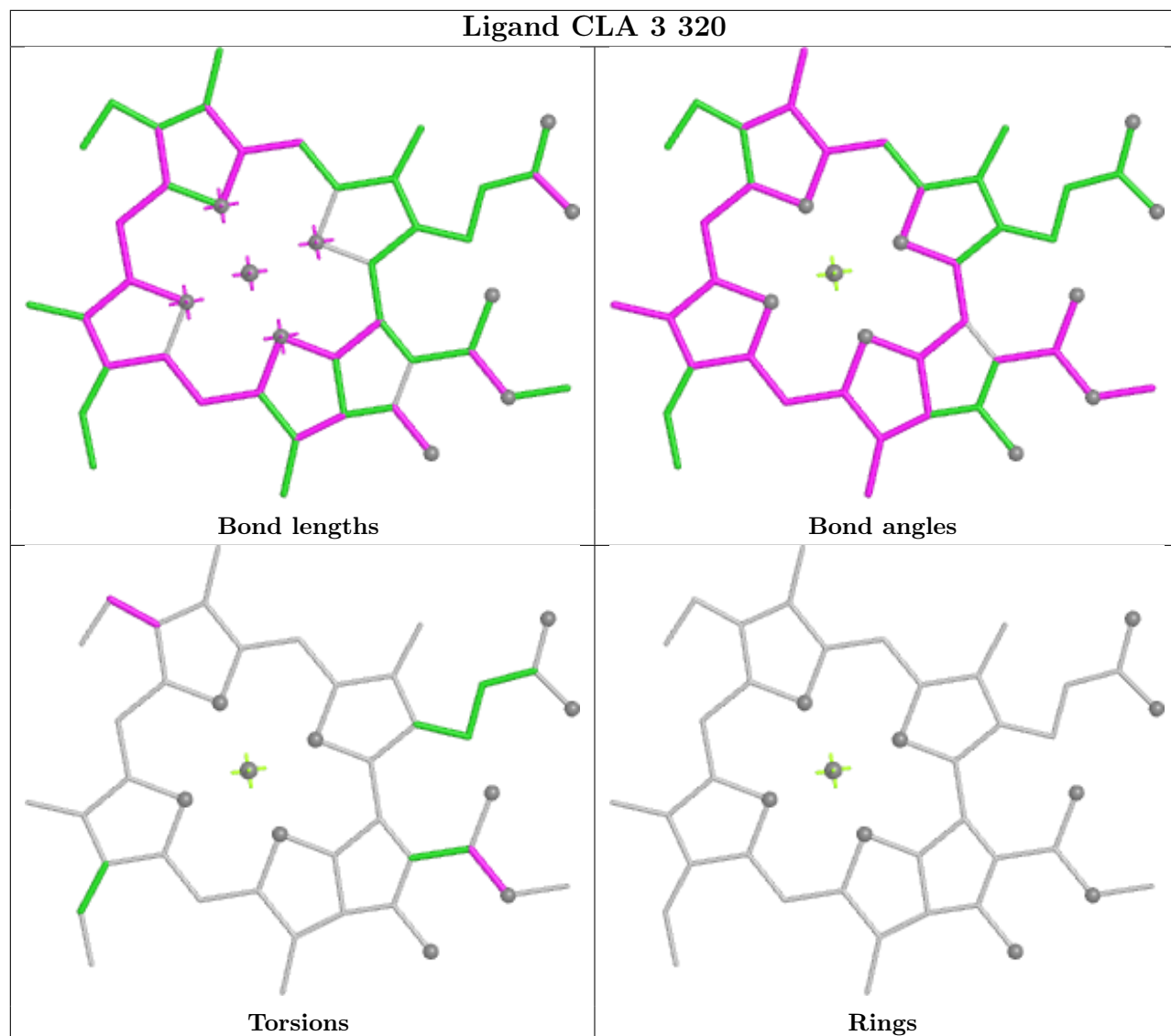
Torsions



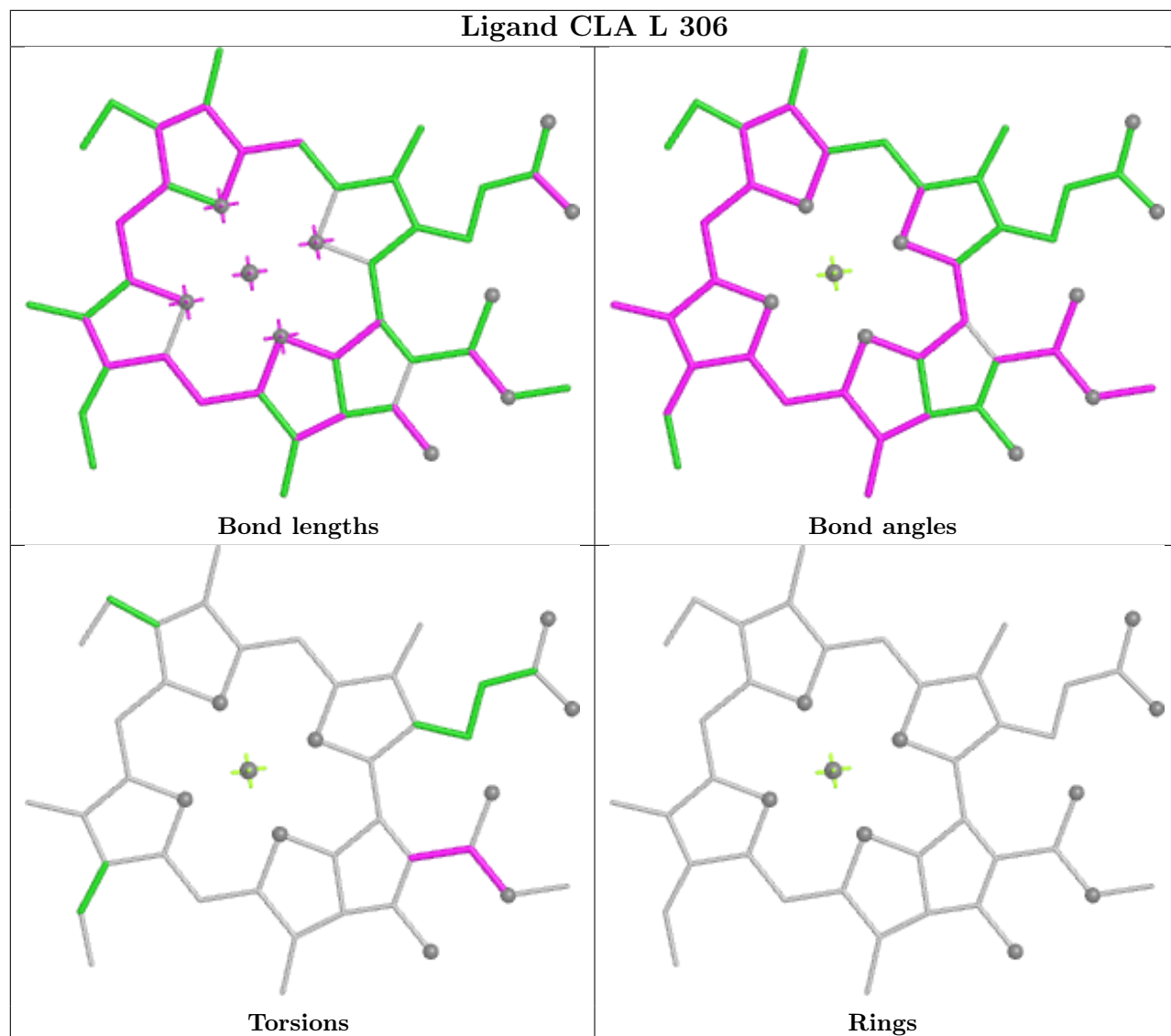
Rings



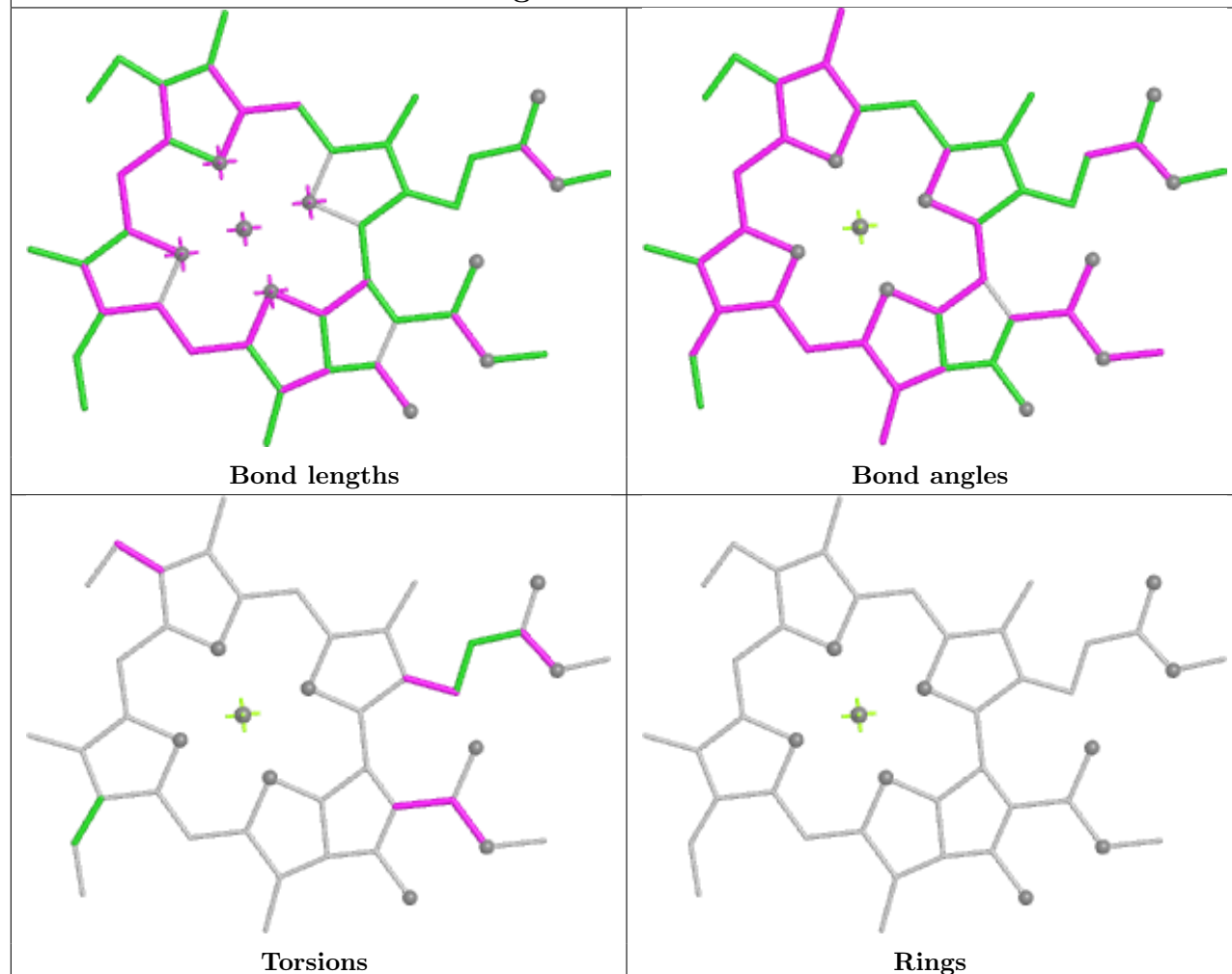
Ligand CLA 3 320



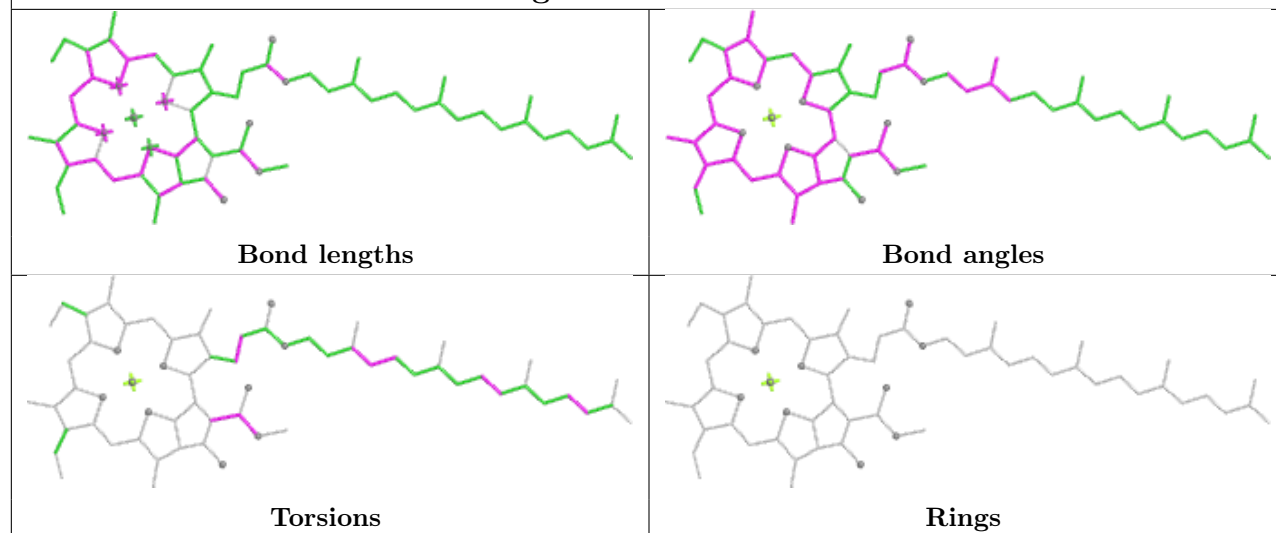
Ligand CLA L 306



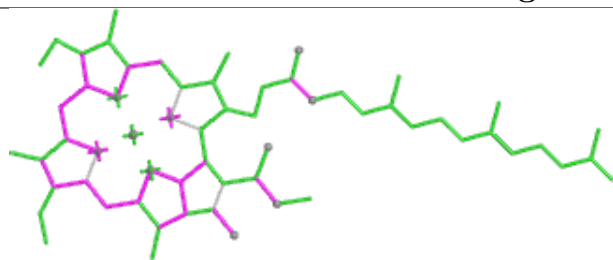
Ligand CLA A 849



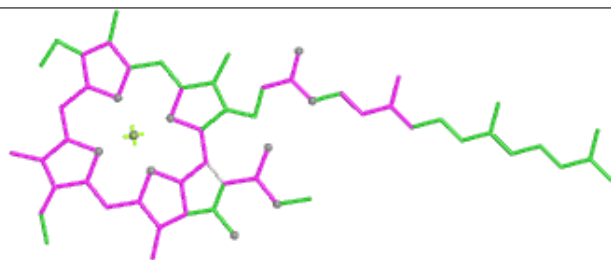
Ligand CLA B 832



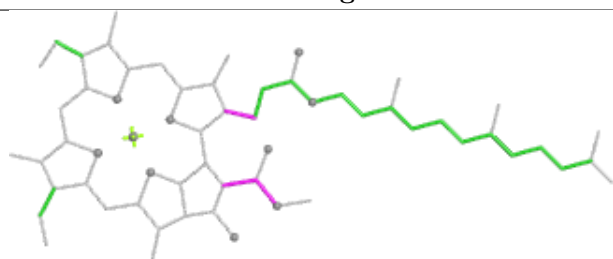
Ligand CLA 7 309



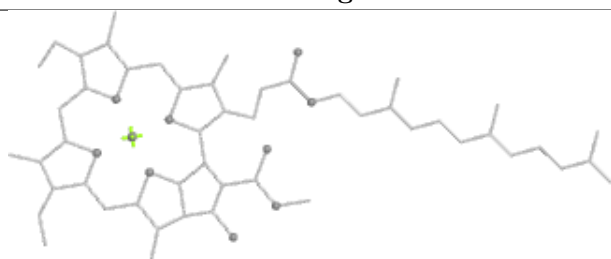
Bond lengths



Bond angles

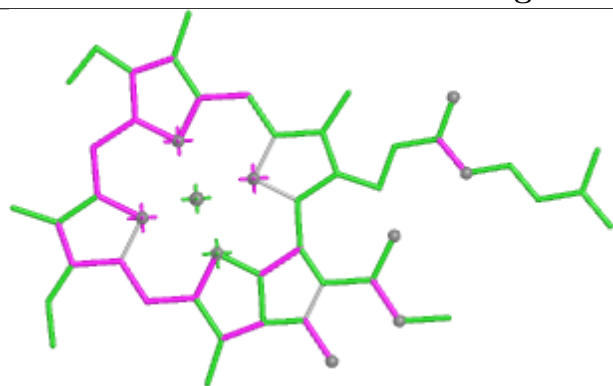


Torsions

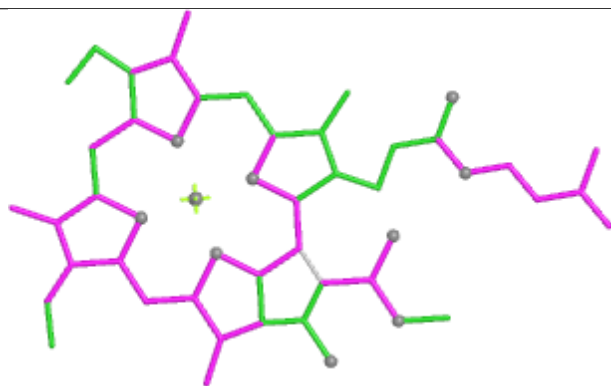


Rings

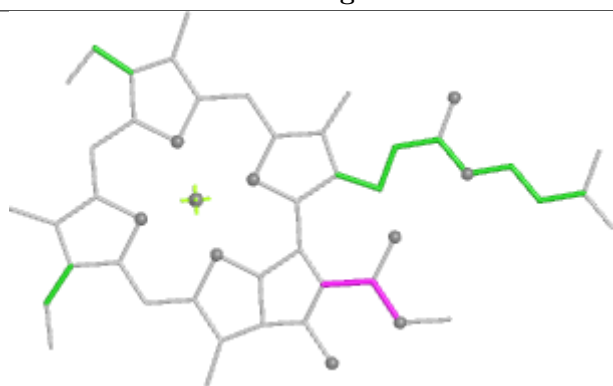
Ligand CLA B 849



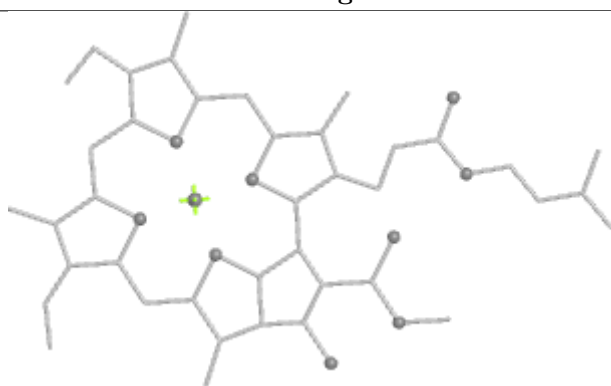
Bond lengths



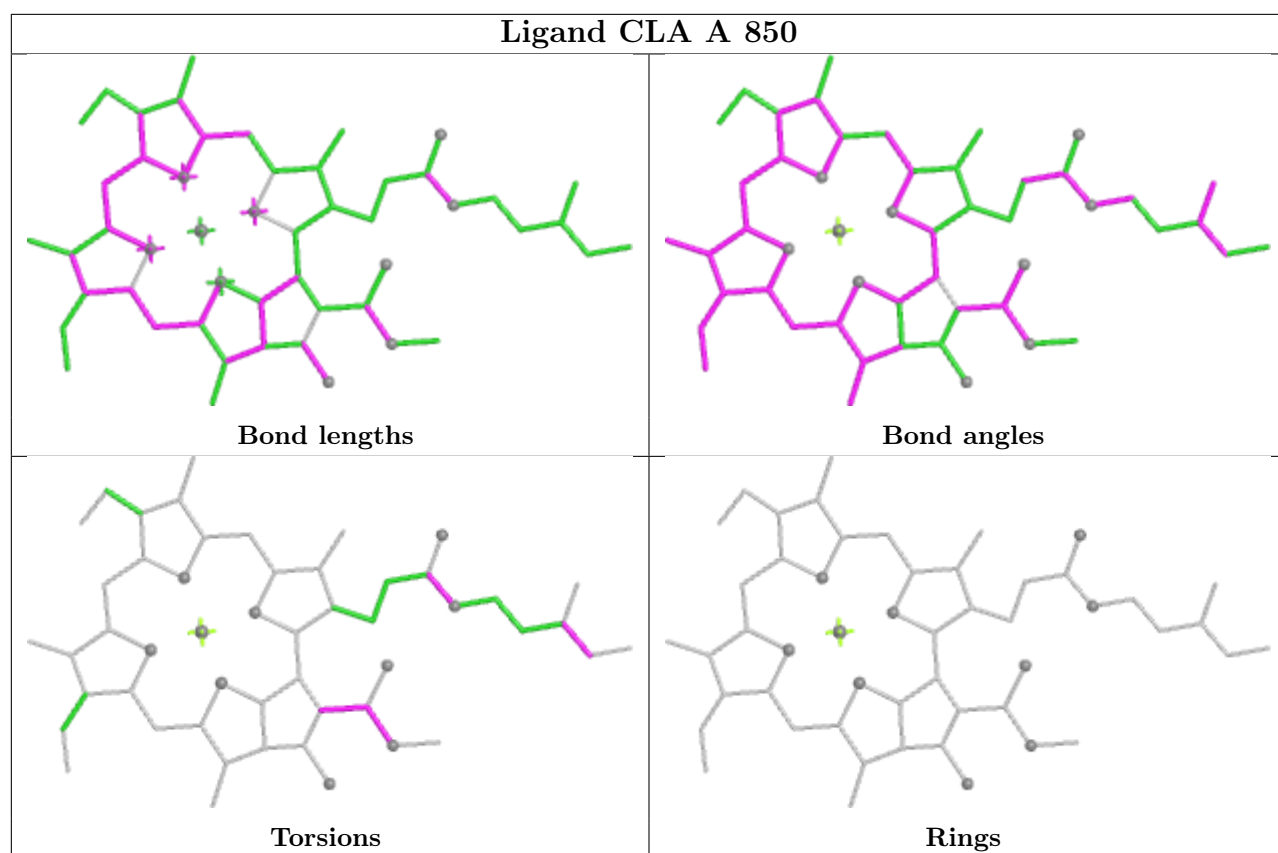
Bond angles



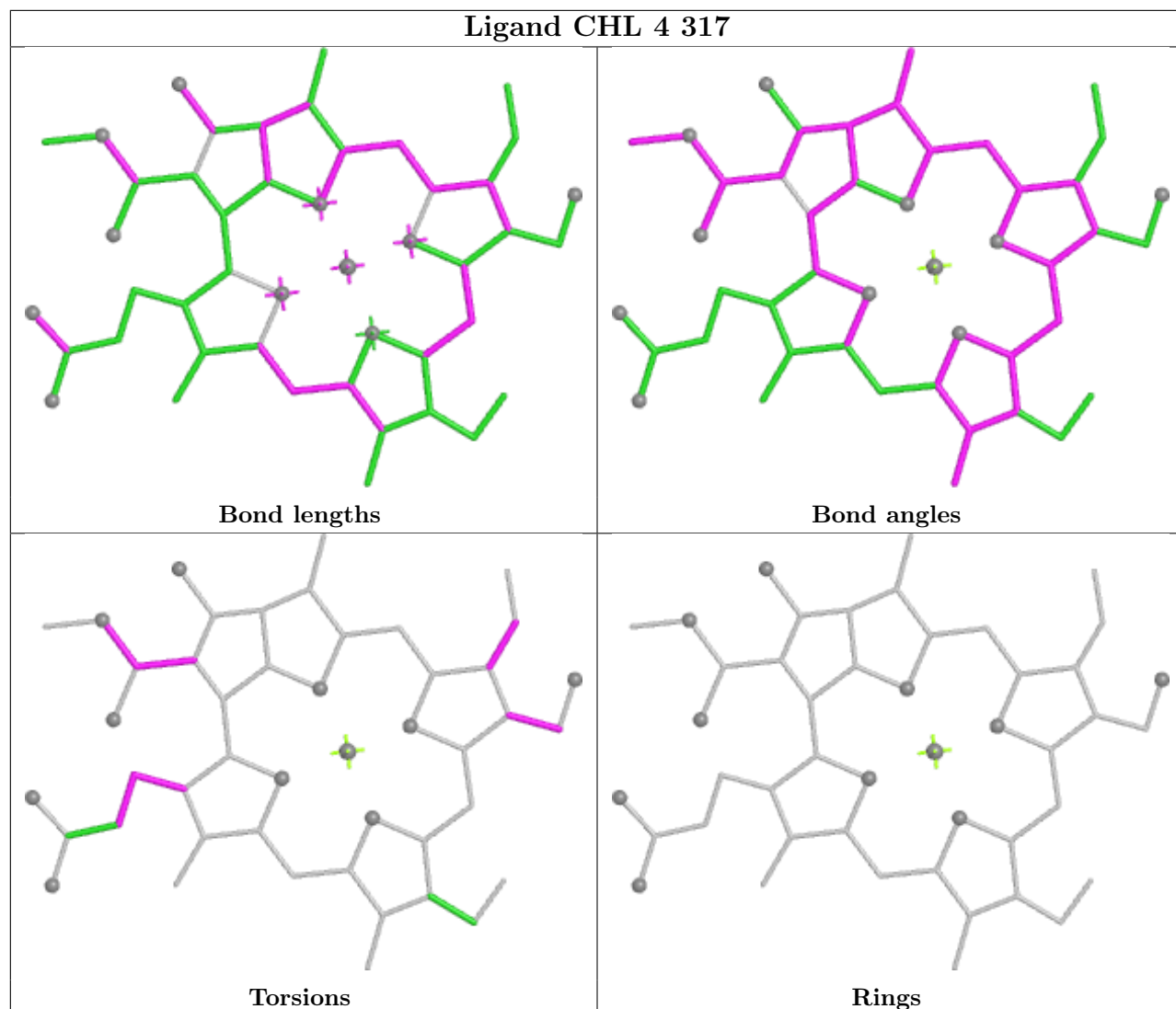
Torsions

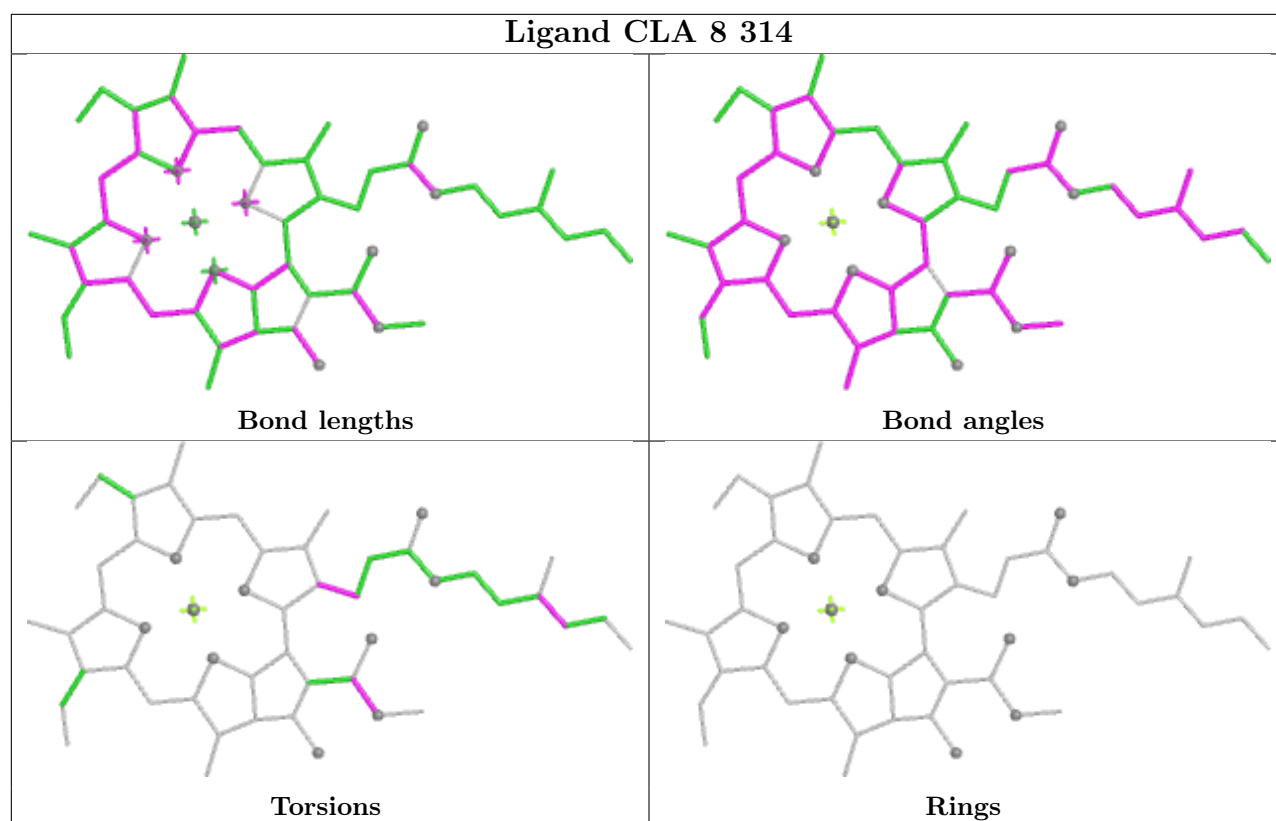


Rings

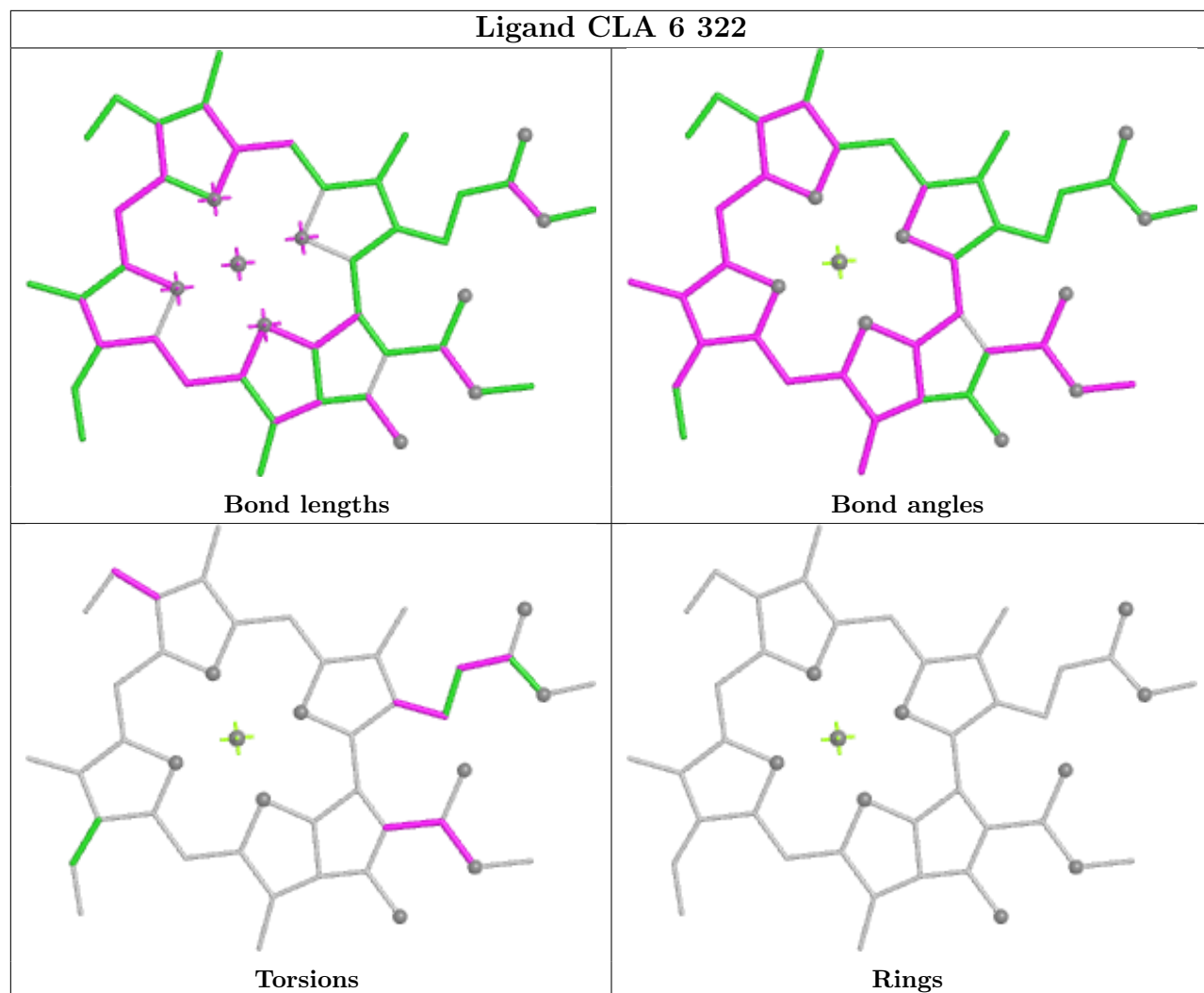


Ligand CHL 4 317

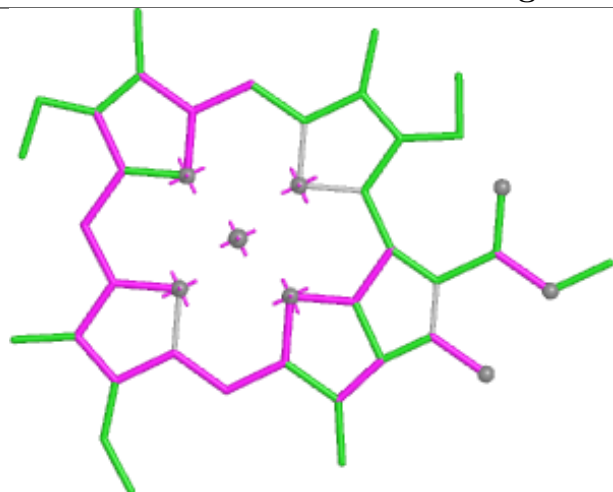




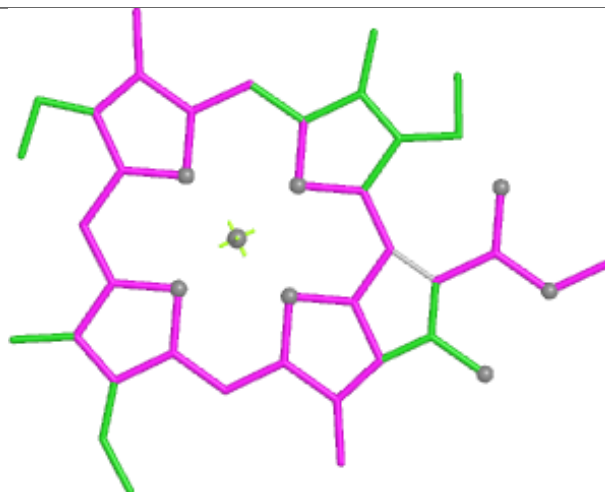
Ligand CLA 6 322



Ligand CLA 4 319



Bond lengths



Bond angles

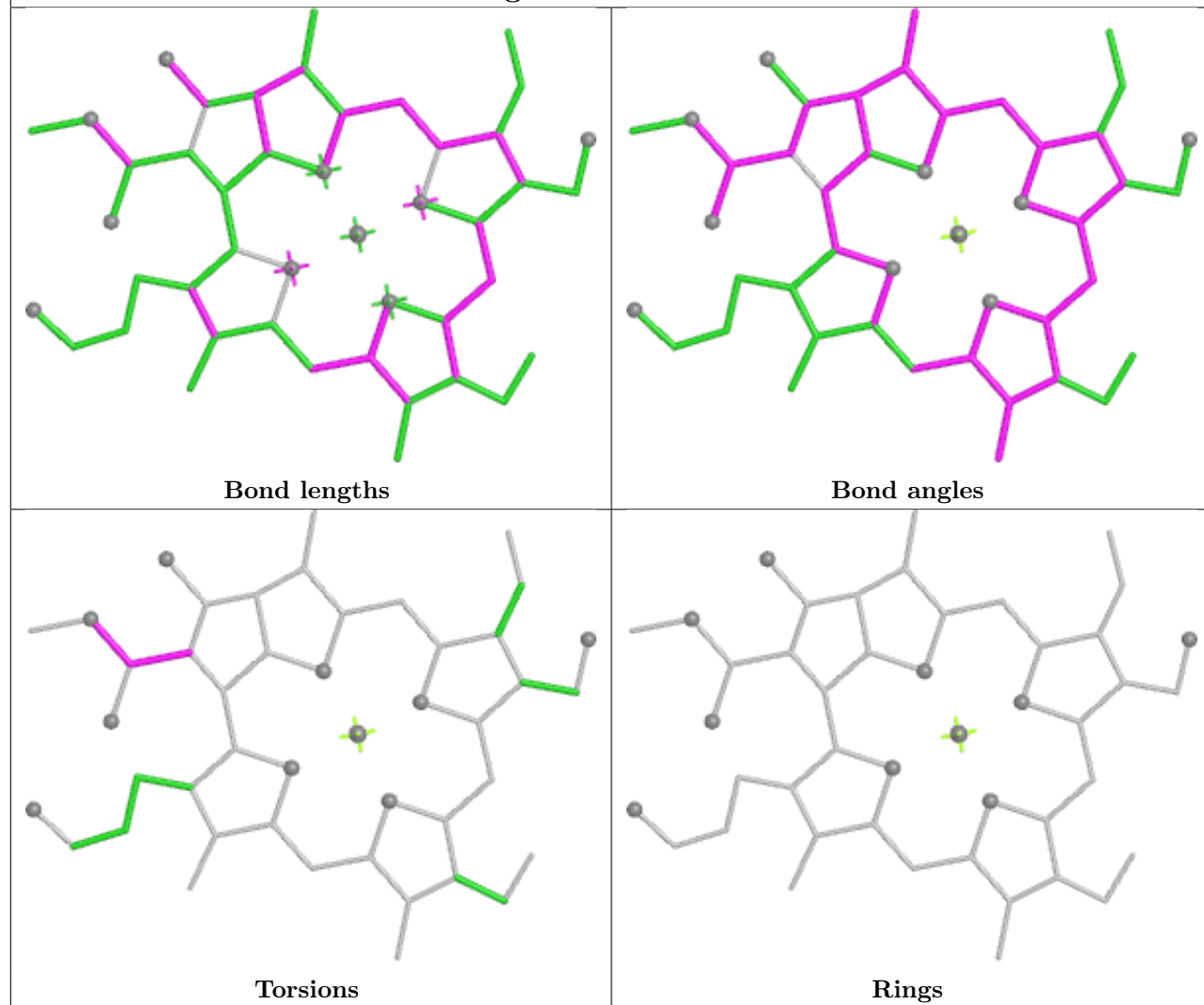


Torsions

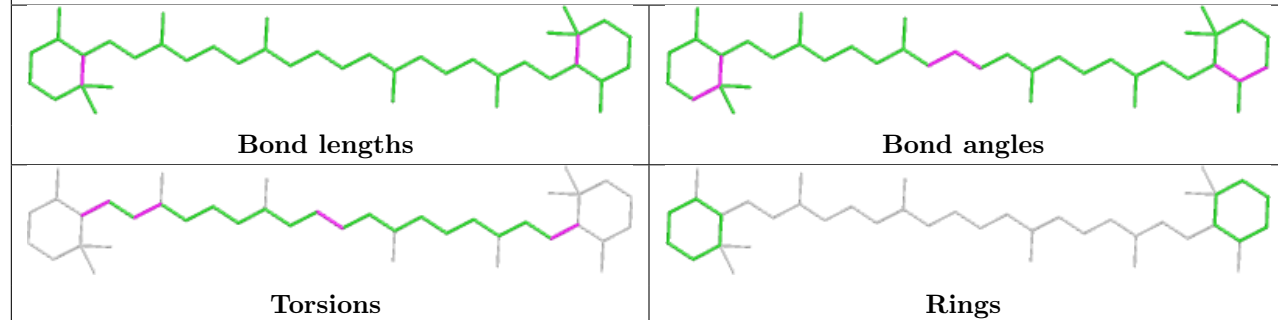


Rings

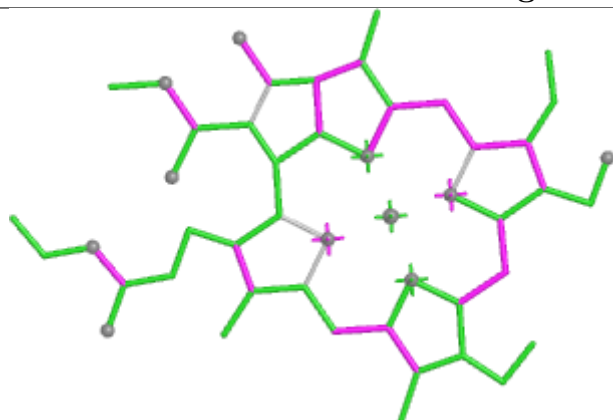
Ligand CHL 8 319



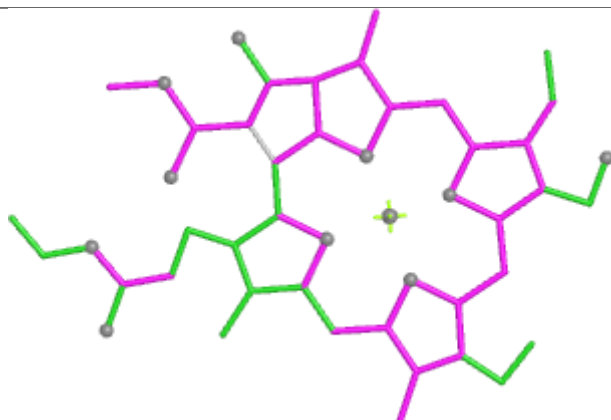
Ligand BCR M 101



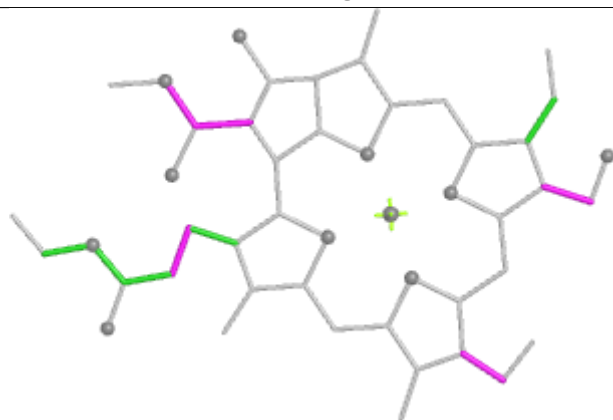
Ligand CHL 4 313



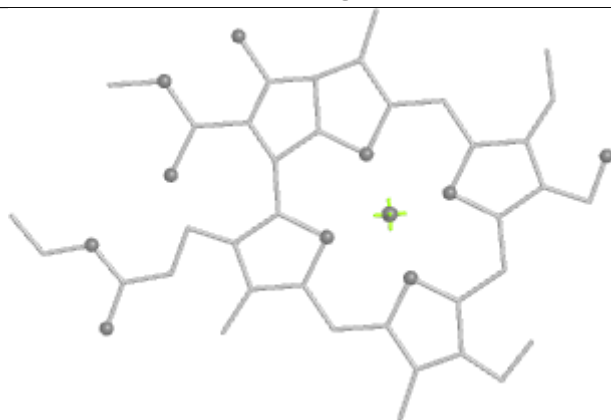
Bond lengths



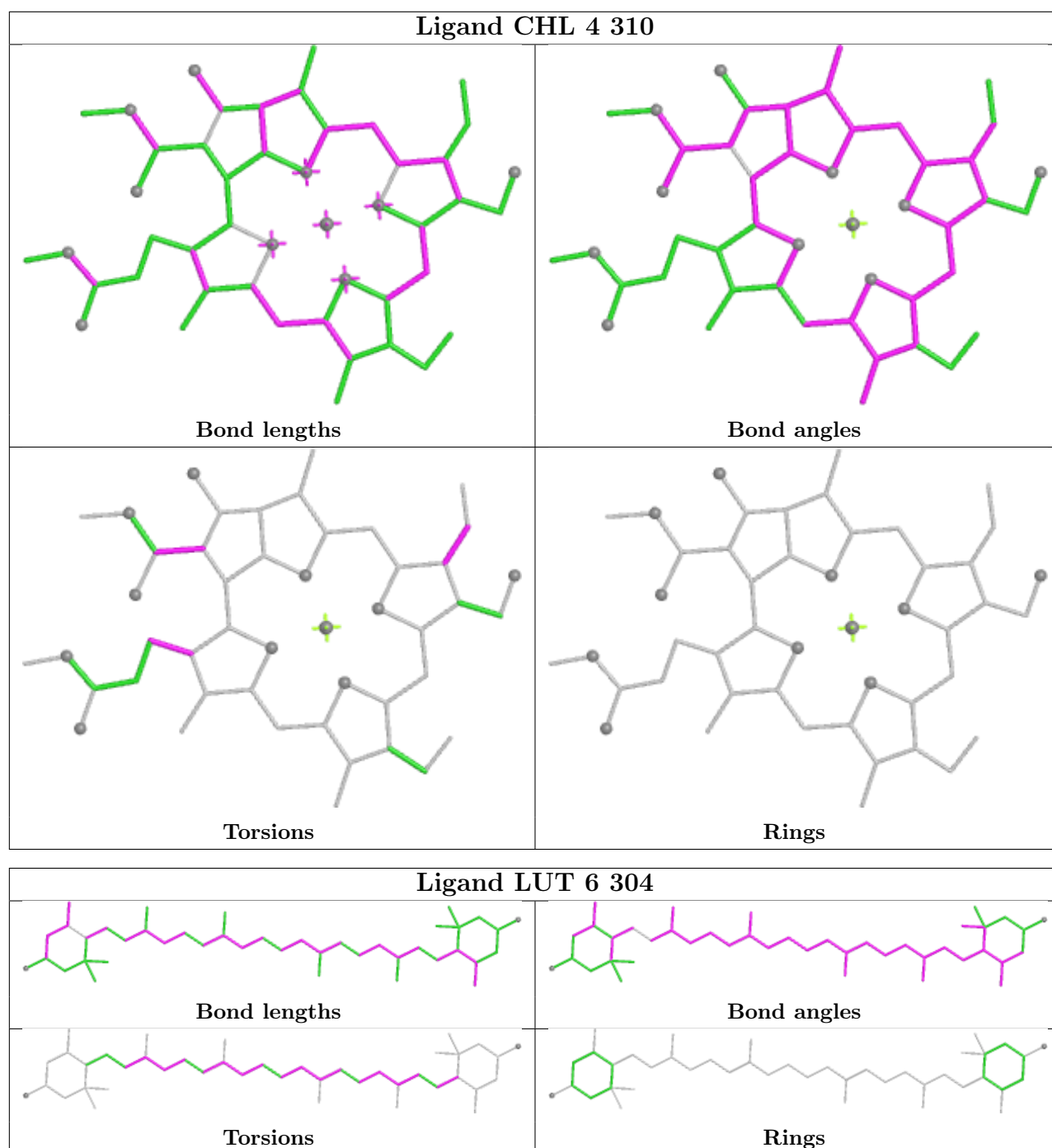
Bond angles

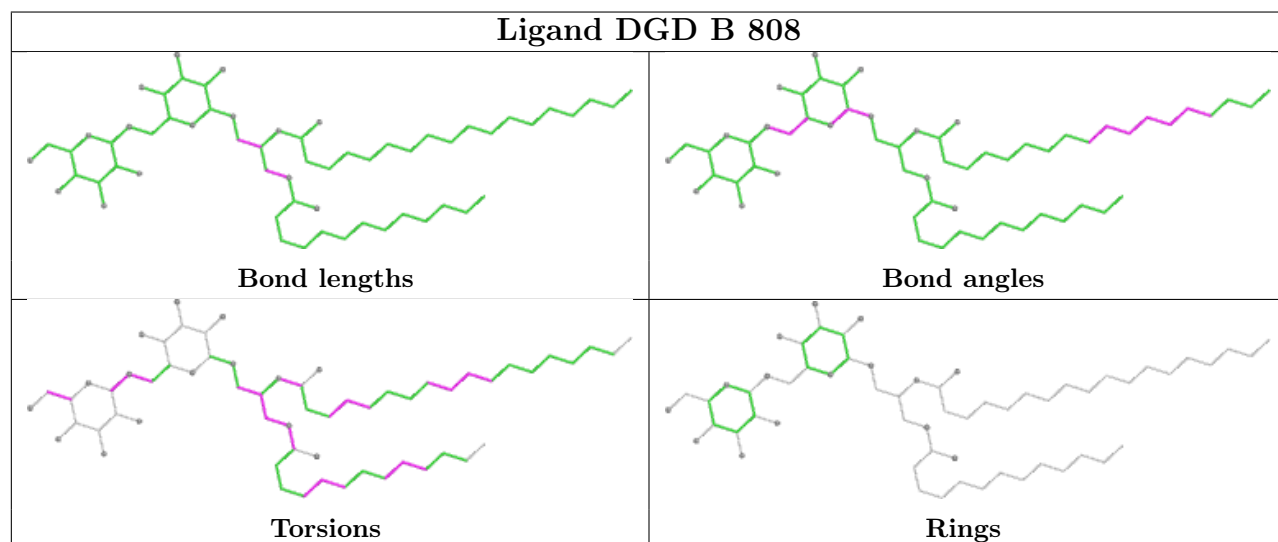
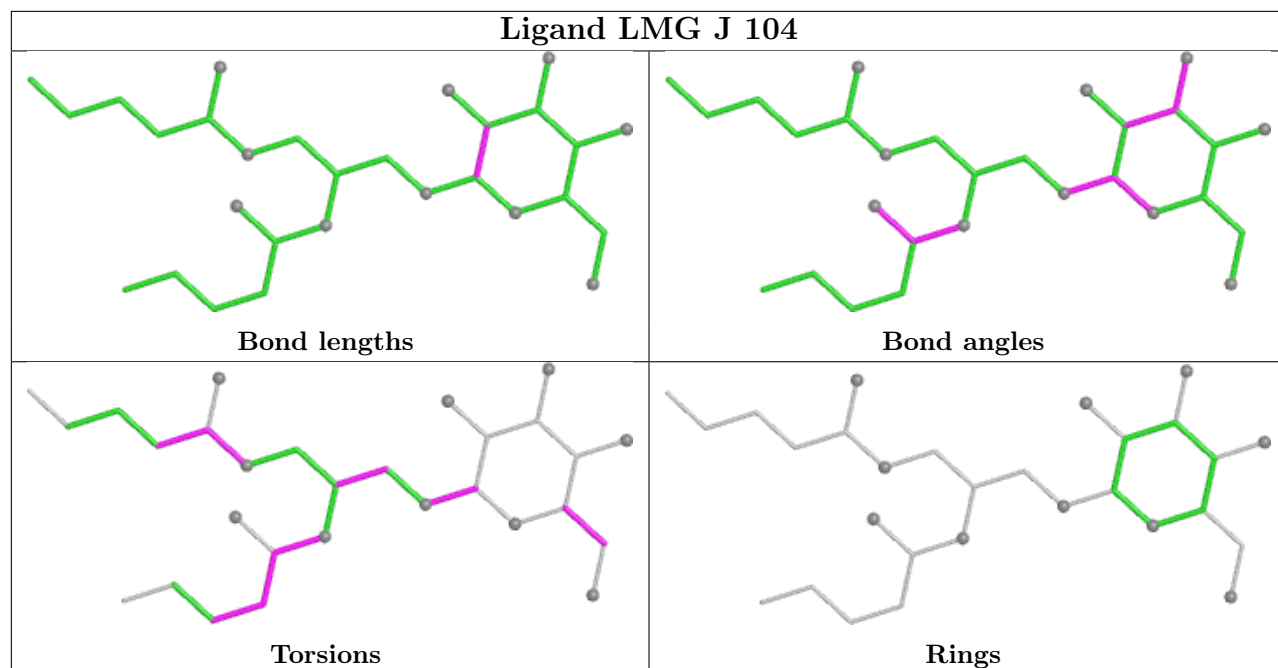


Torsions

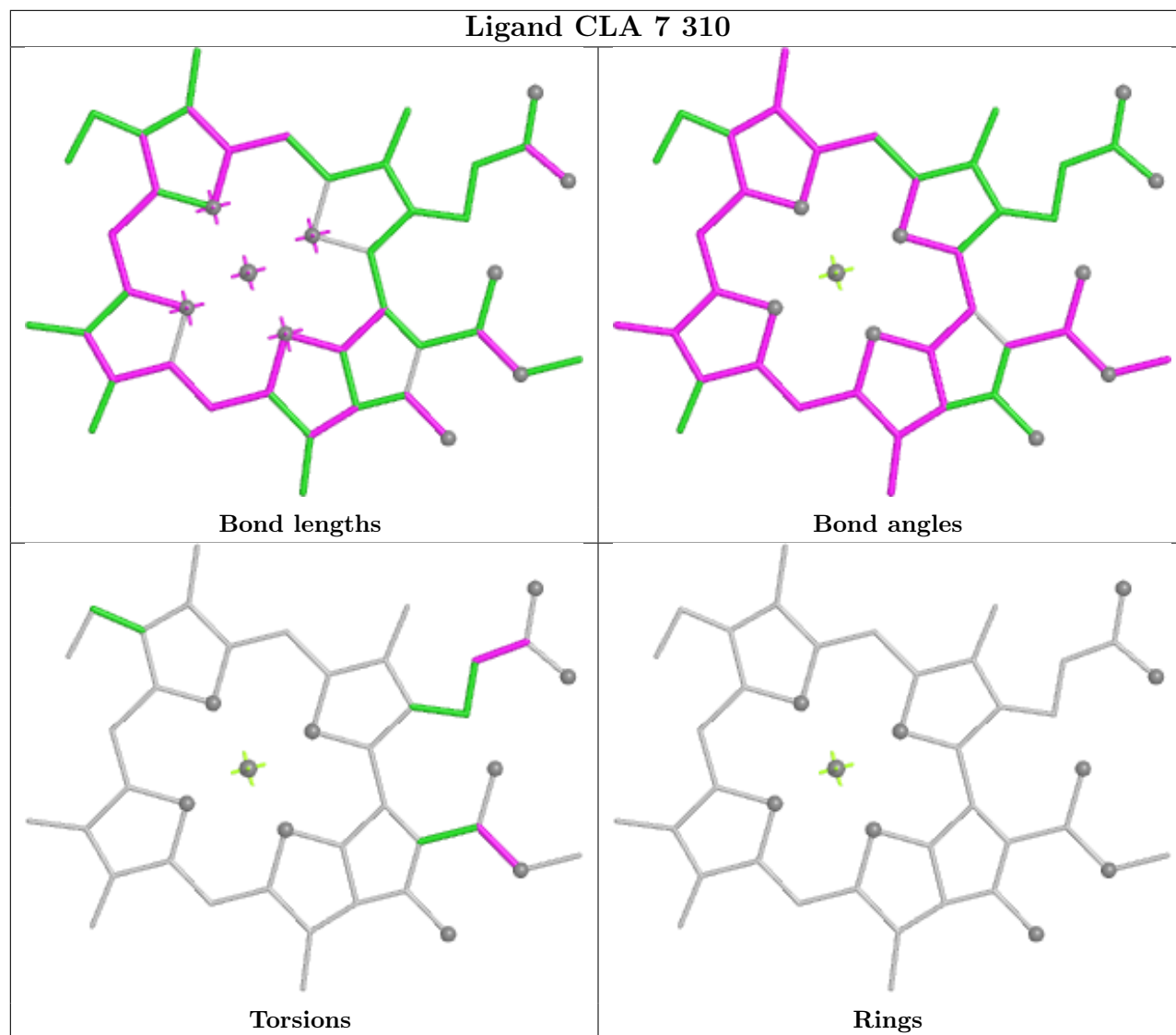


Rings

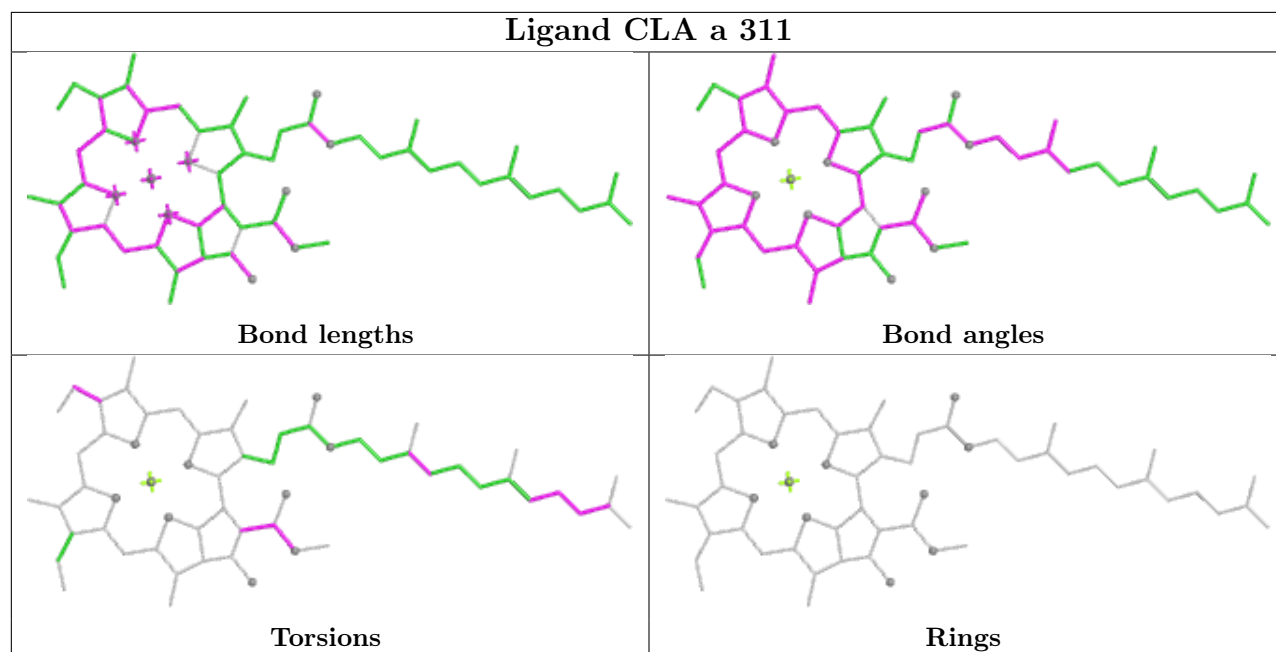


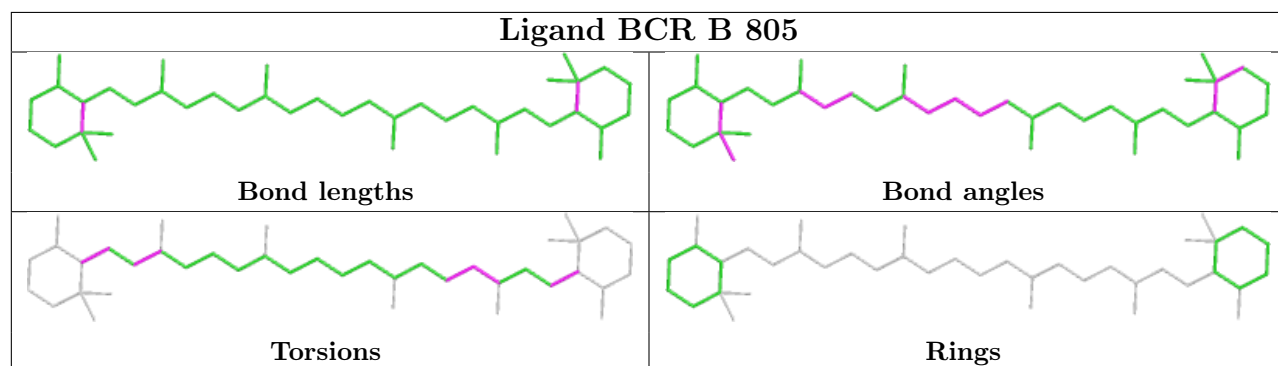
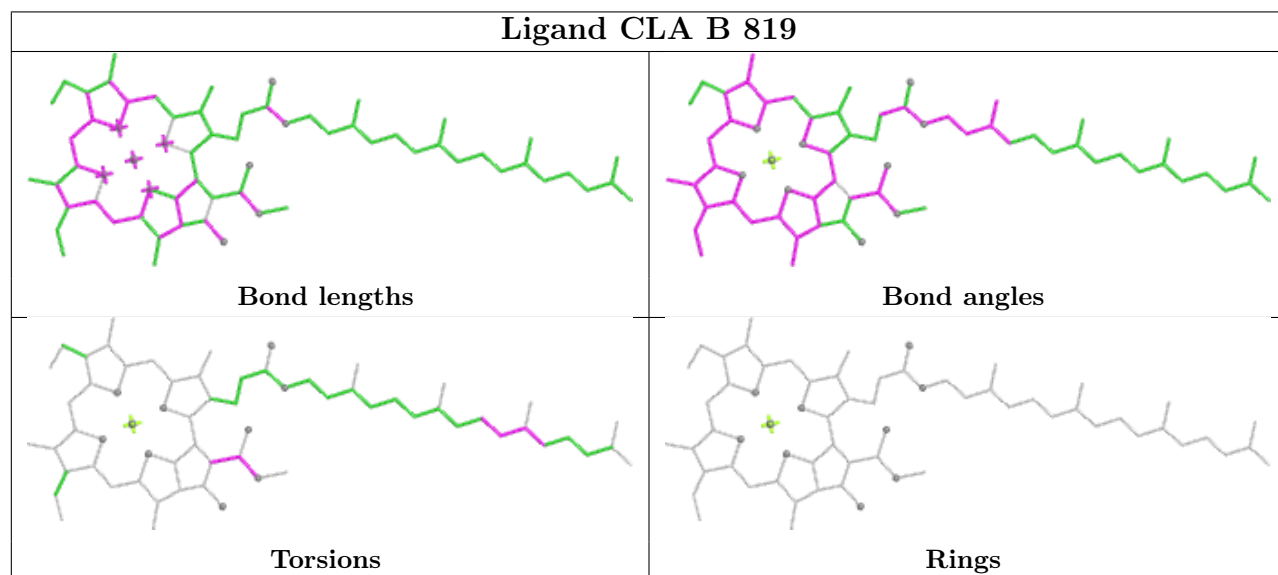
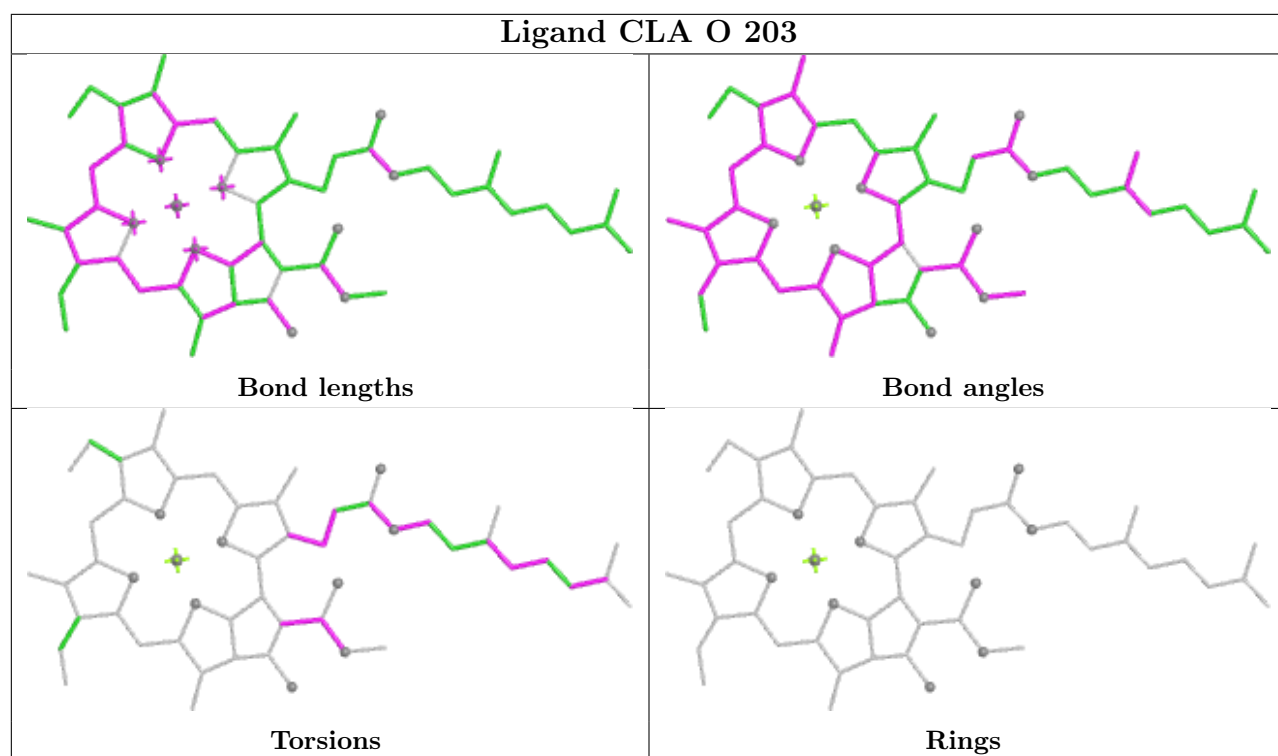


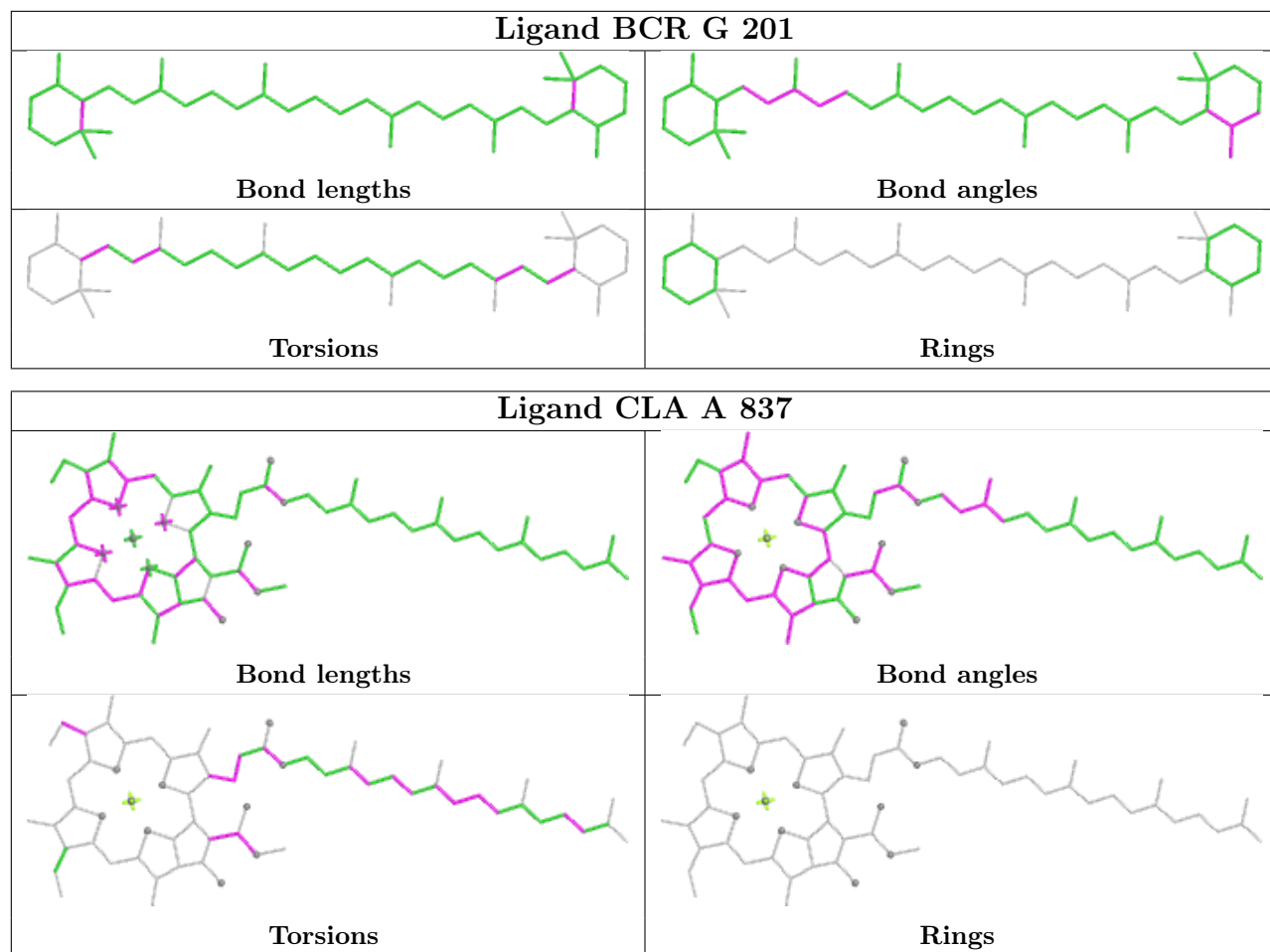
Ligand CLA 7 310



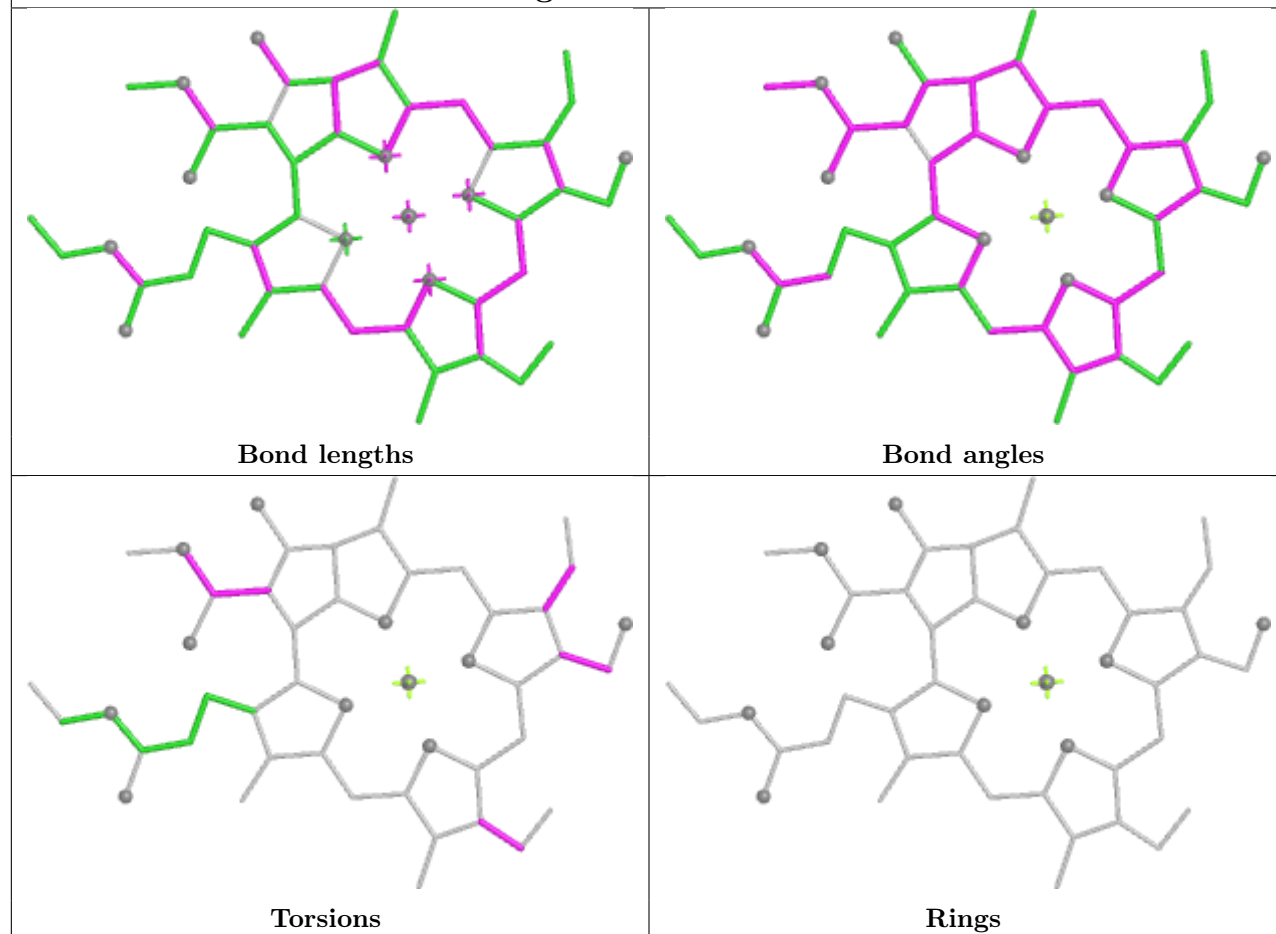
Ligand CLA a 311



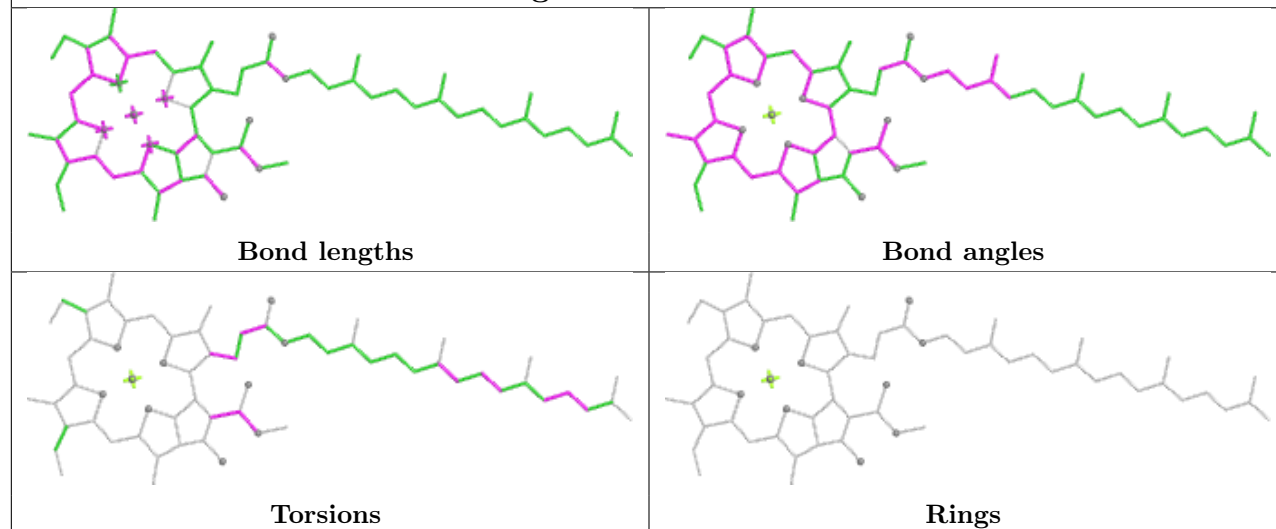


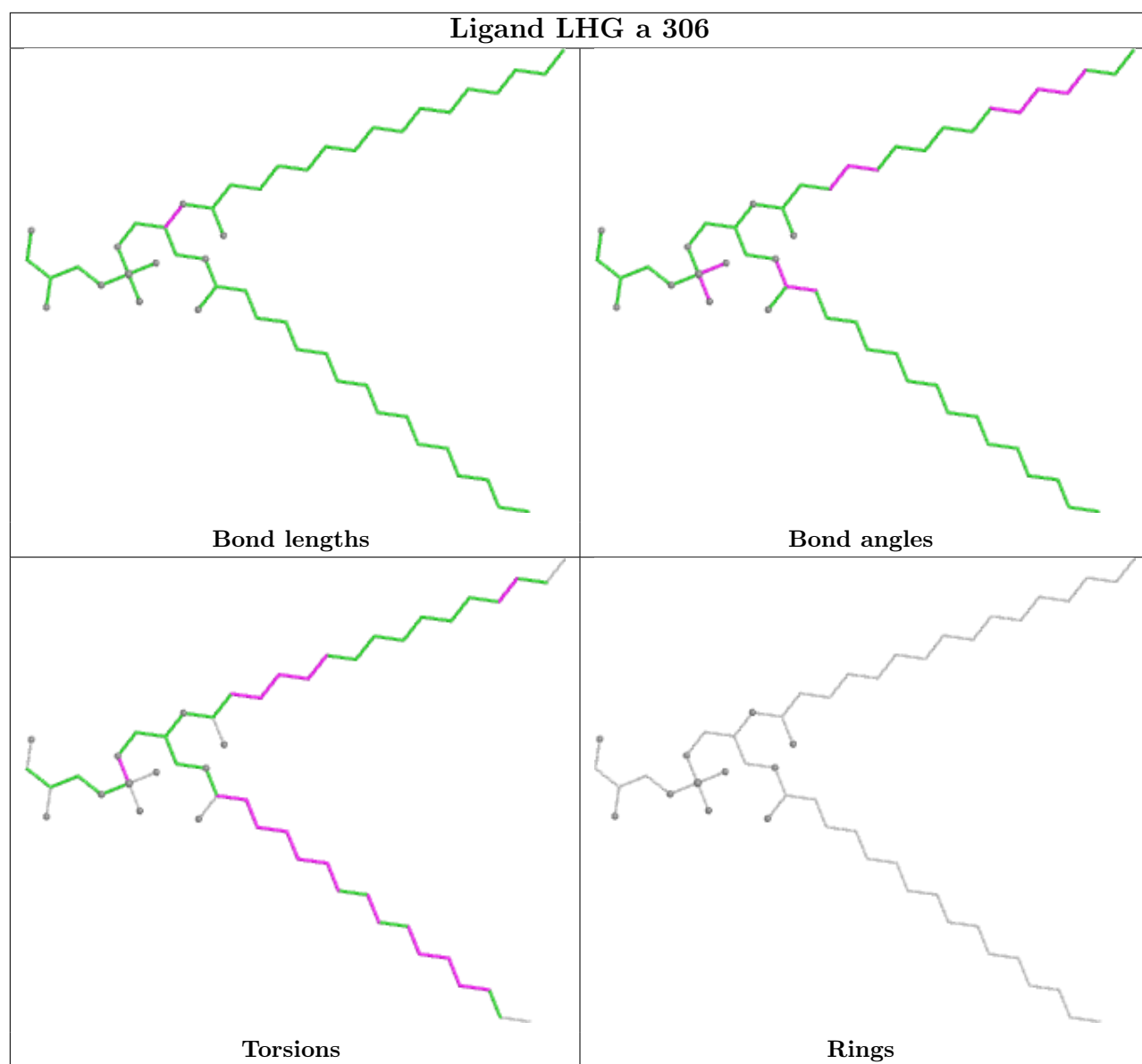


Ligand CHL 9 320

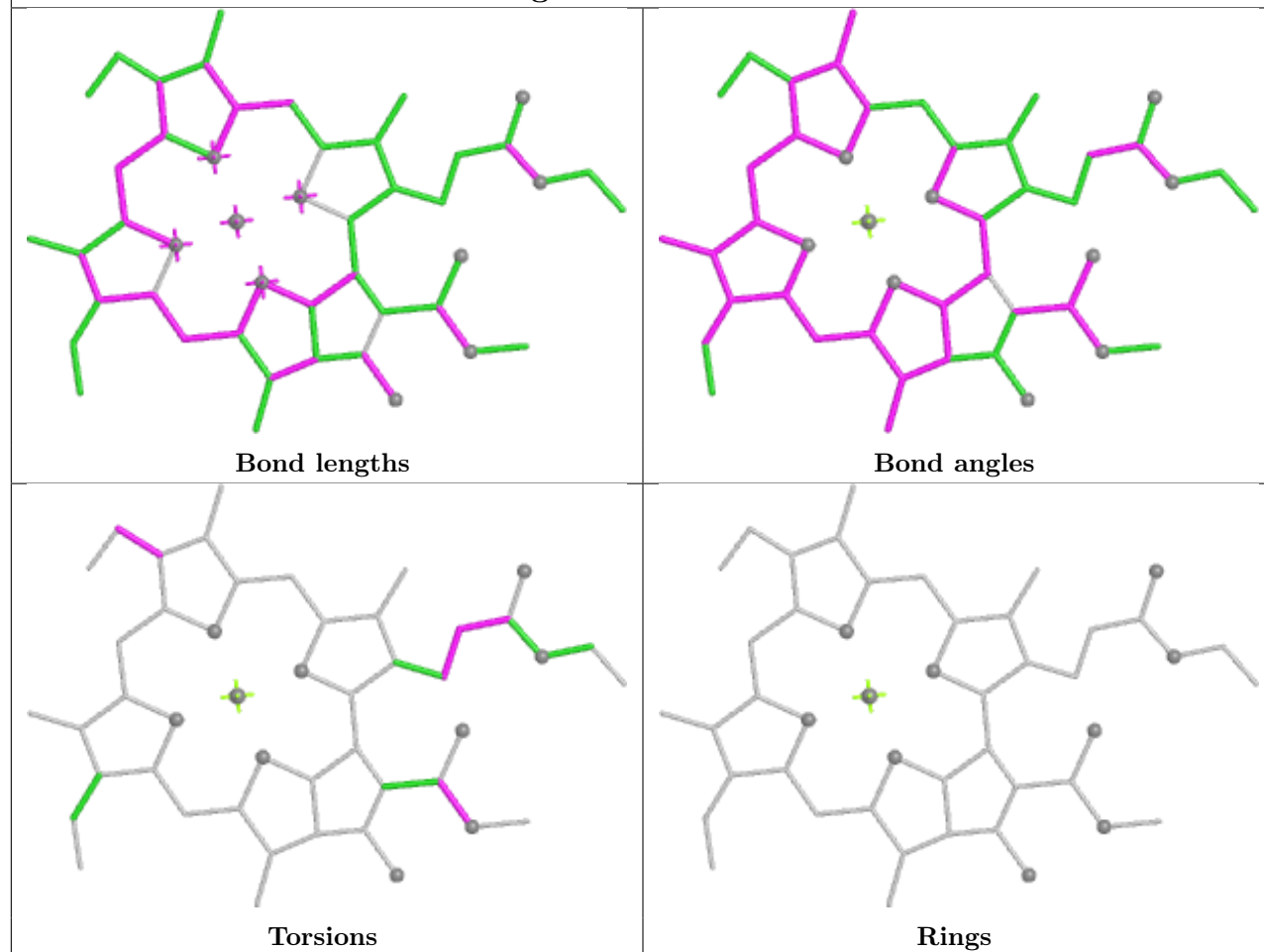


Ligand CLA A 826

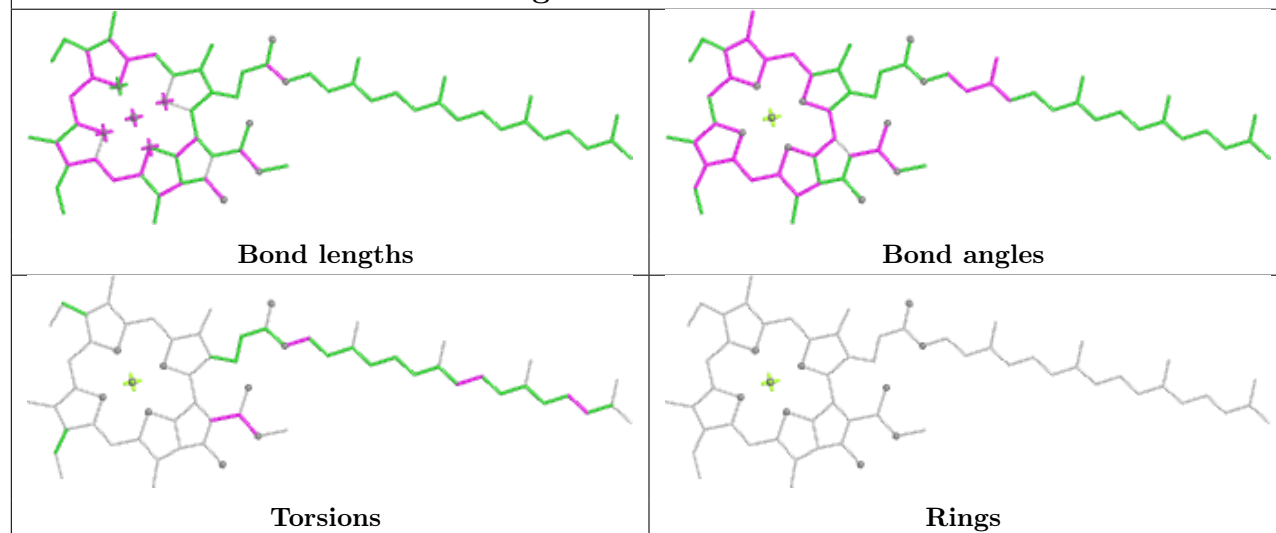


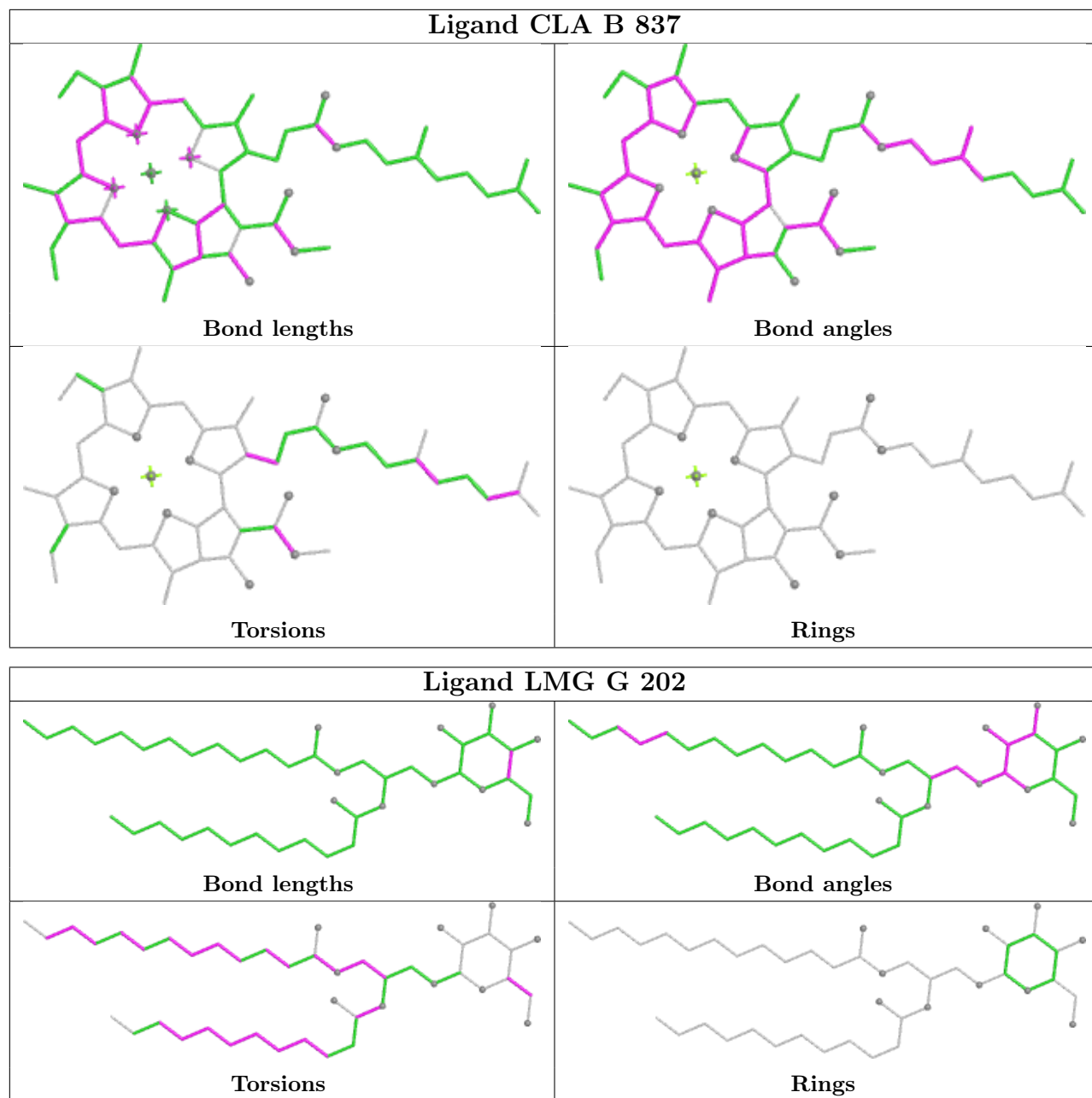


Ligand CLA 5 309

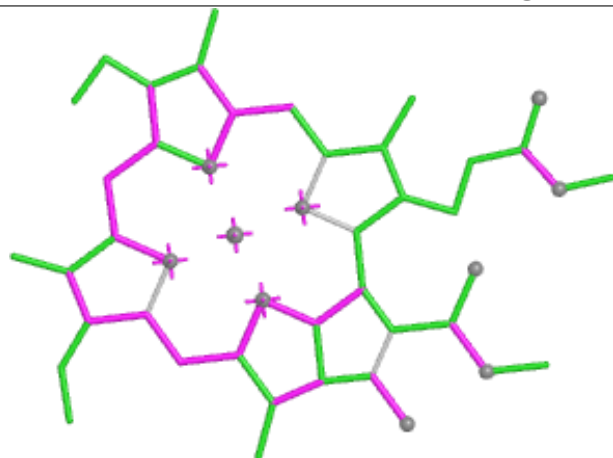


Ligand CLA B 811

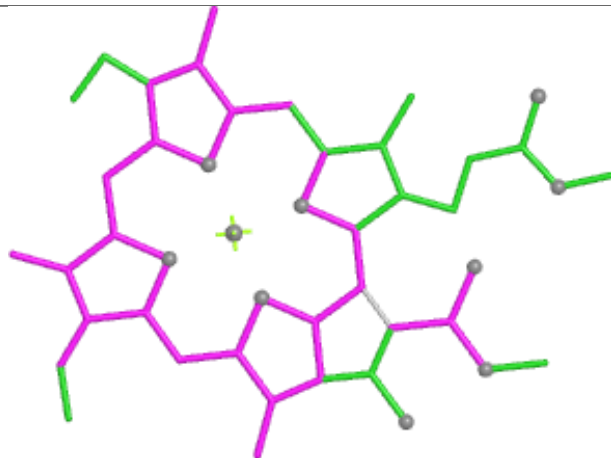




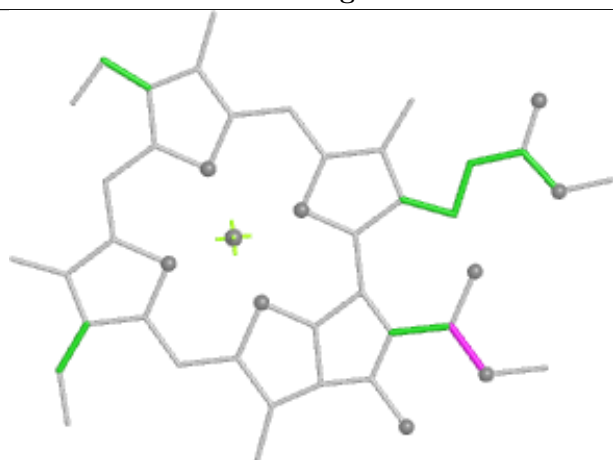
Ligand CLA 2 314



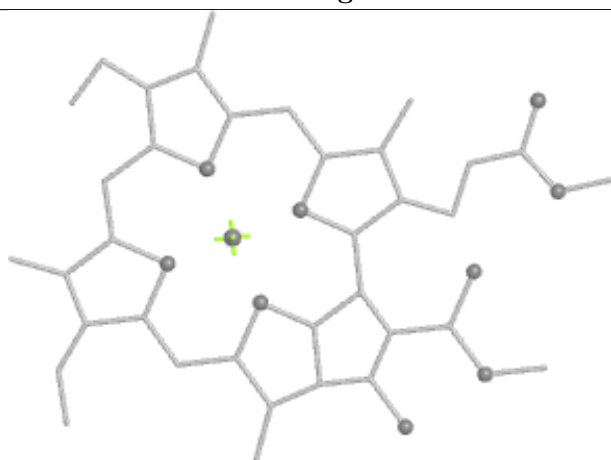
Bond lengths



Bond angles

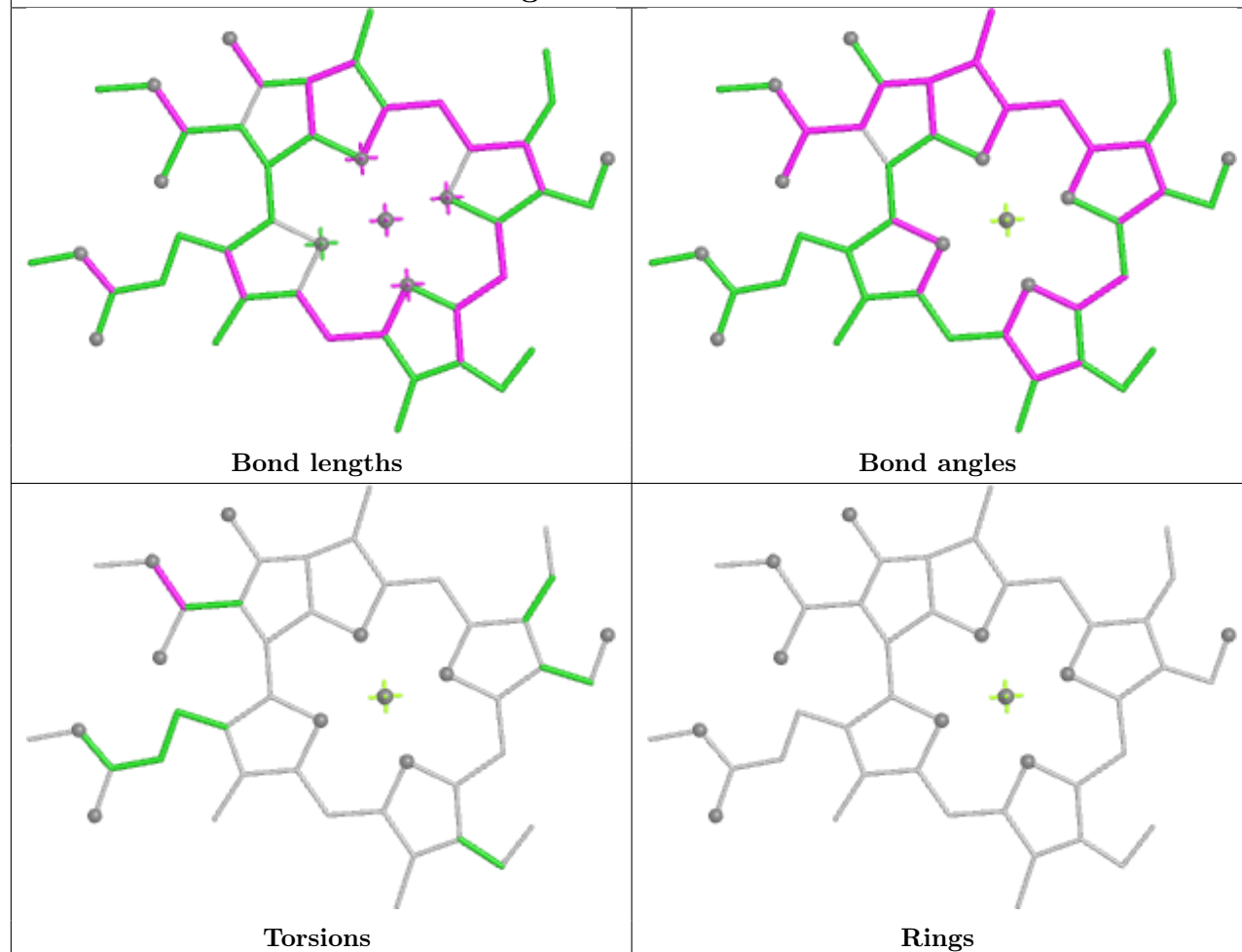


Torsions

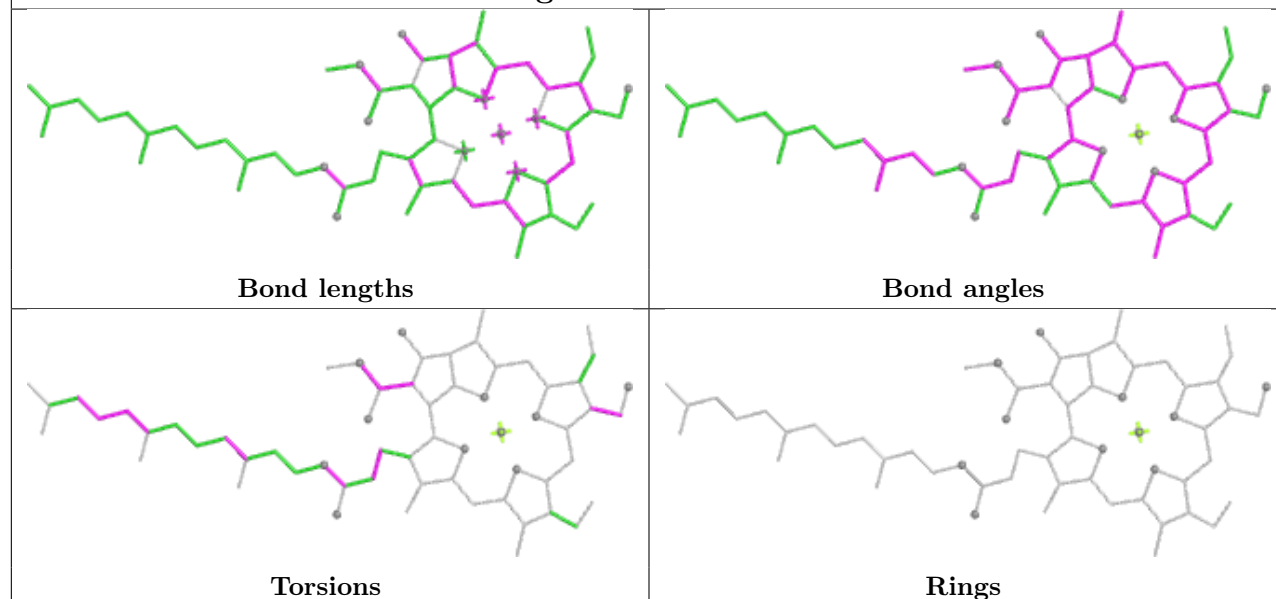


Rings

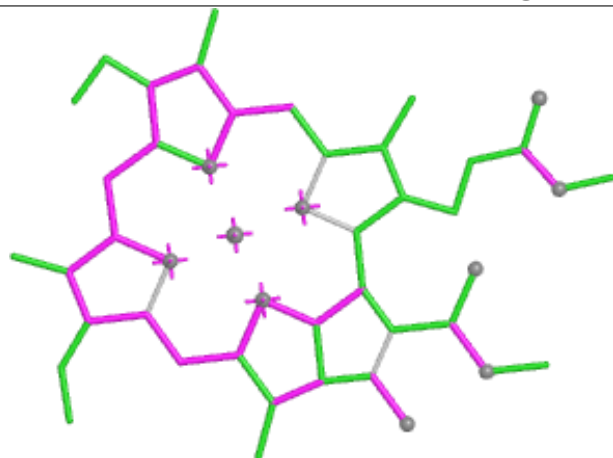
Ligand CHL 7 319



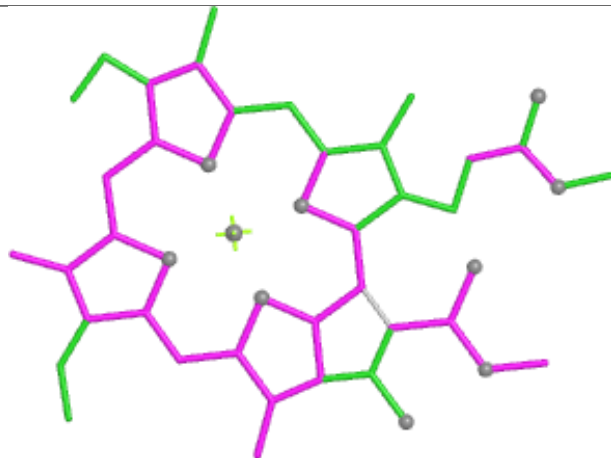
Ligand CHL a 317



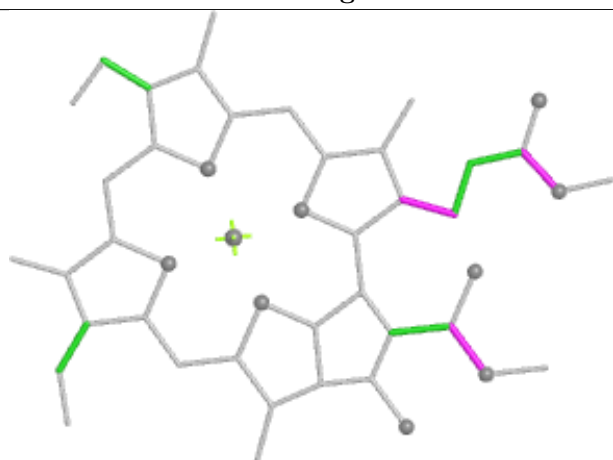
Ligand CLA b 304



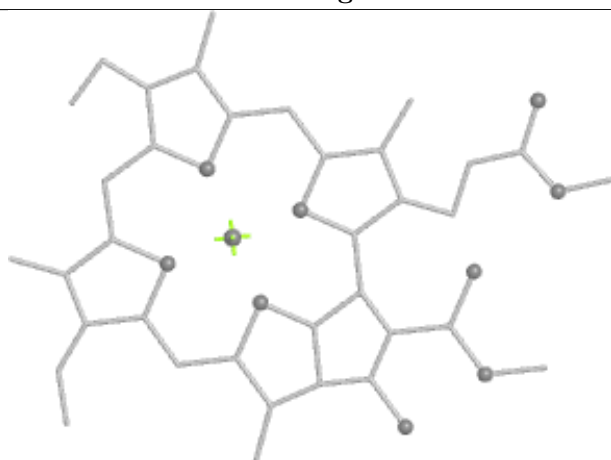
Bond lengths



Bond angles

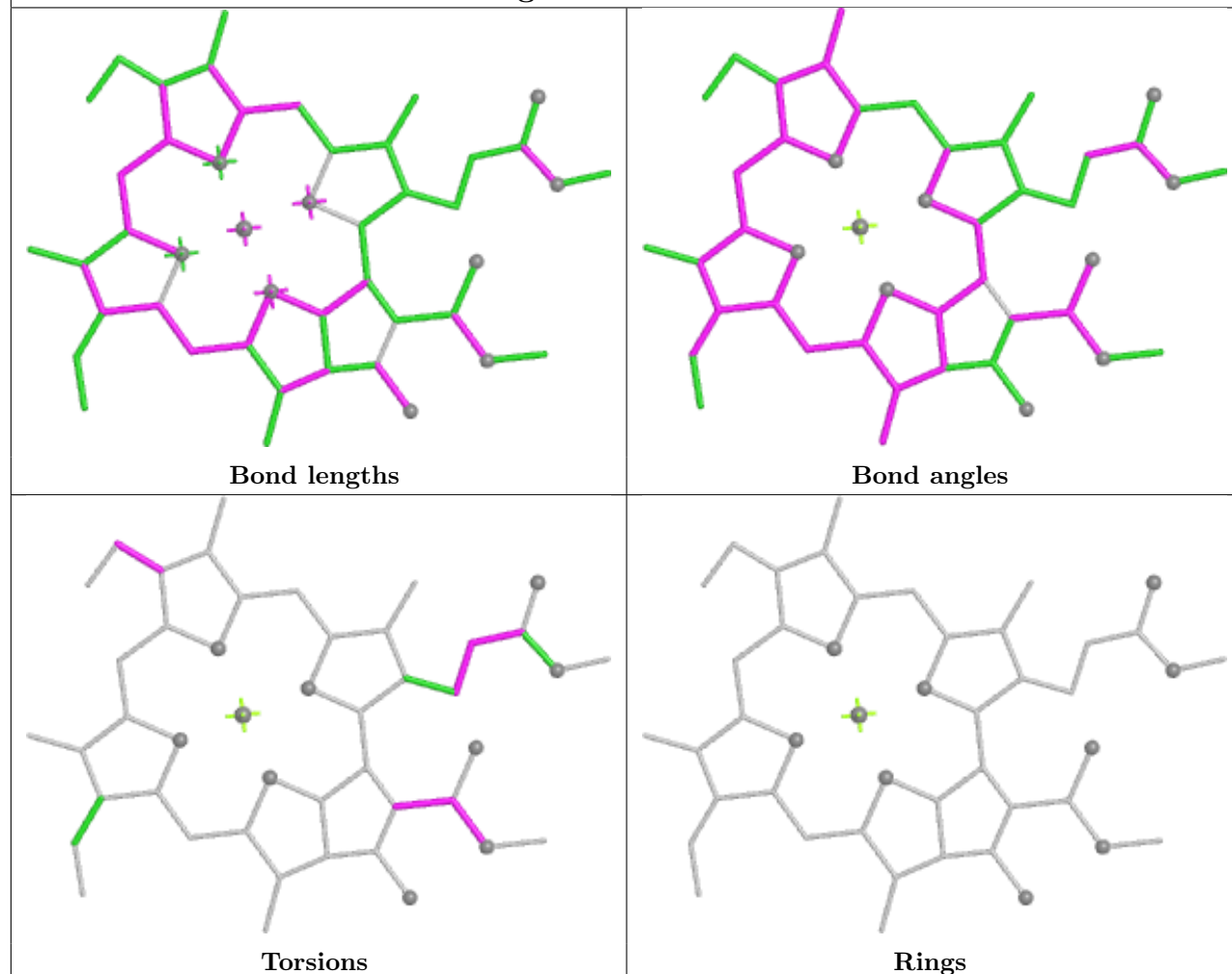


Torsions

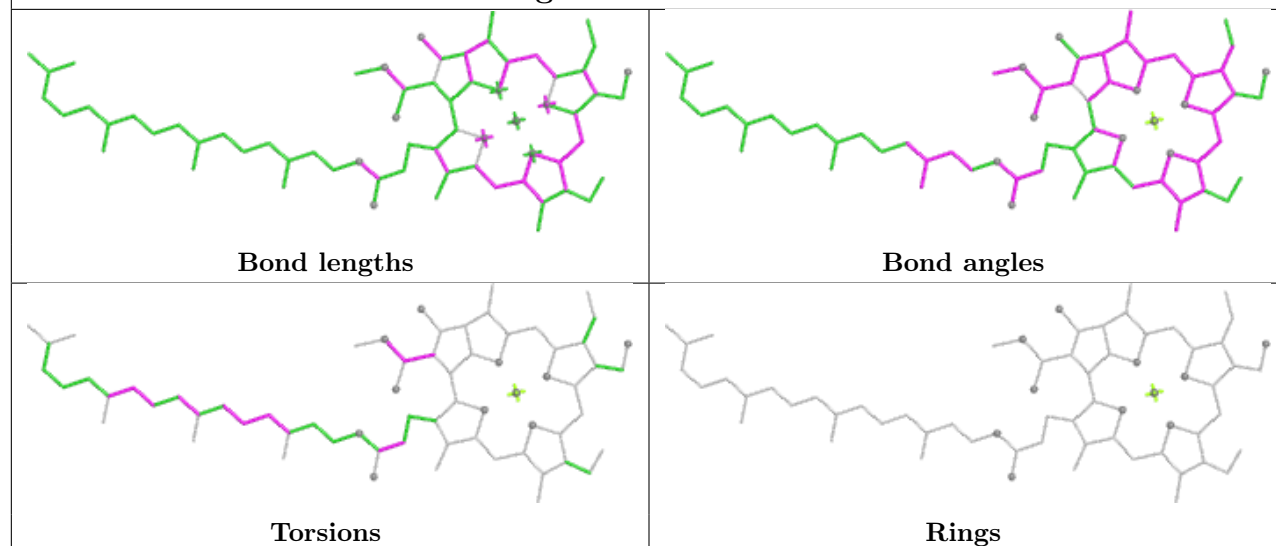


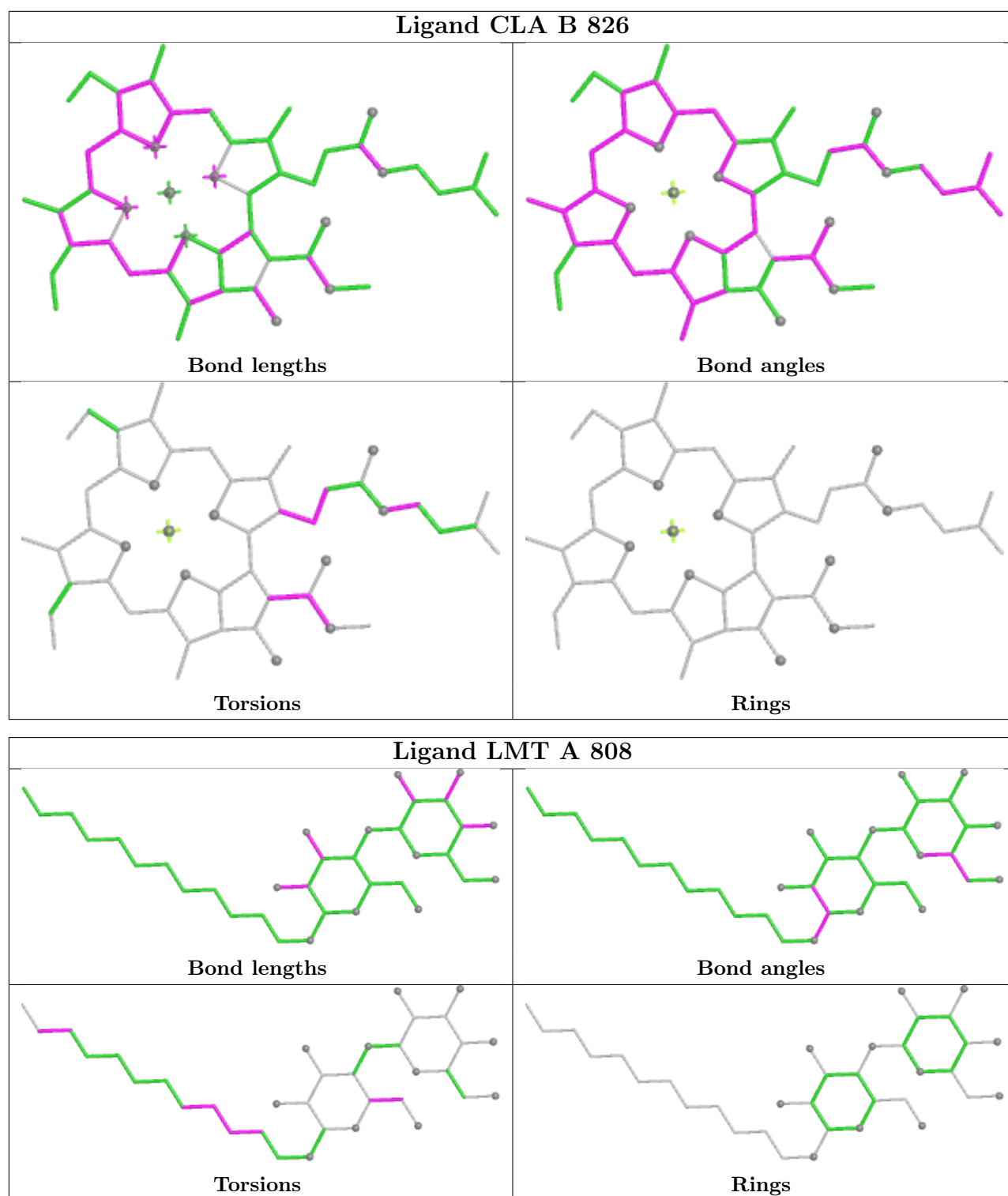
Rings

Ligand CLA a 322

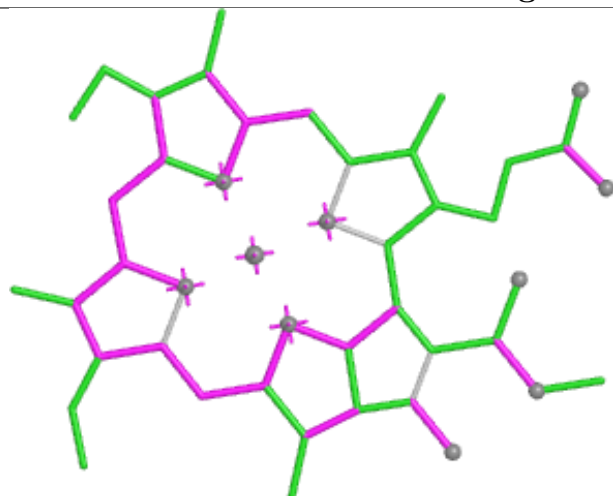


Ligand CHL 7 324

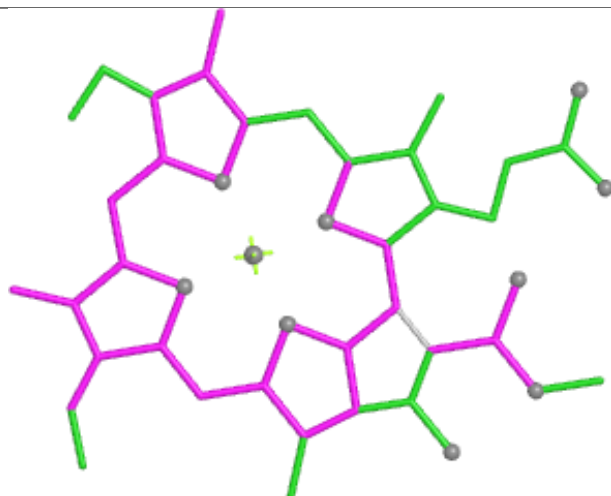




Ligand CLA 2 311



Bond lengths



Bond angles

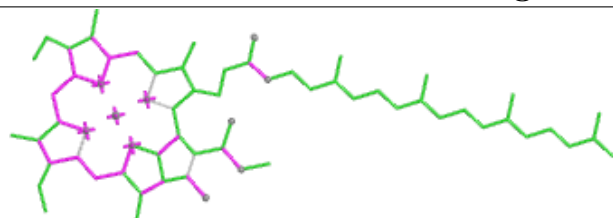


Torsions

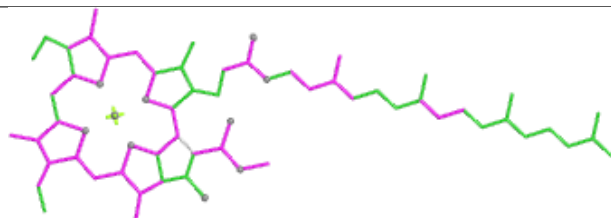


Rings

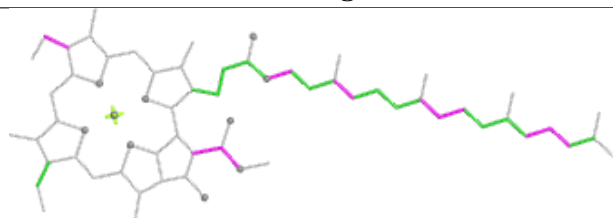
Ligand CLA A 853



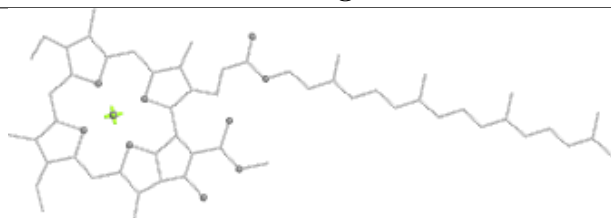
Bond lengths



Bond angles

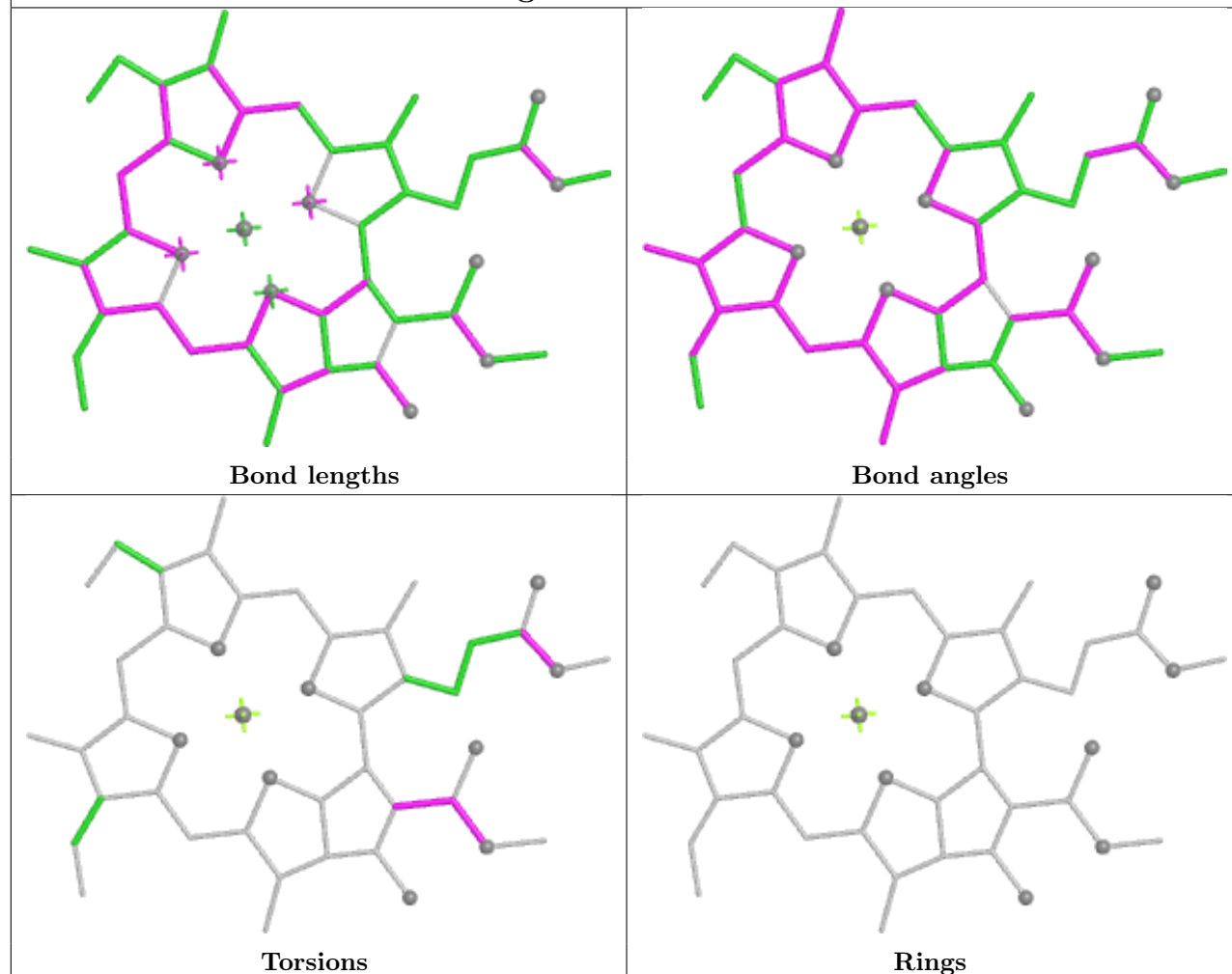


Torsions

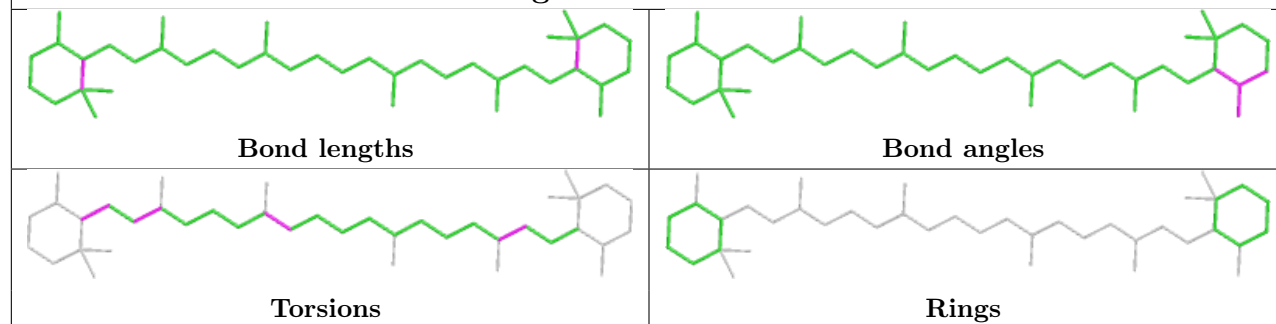


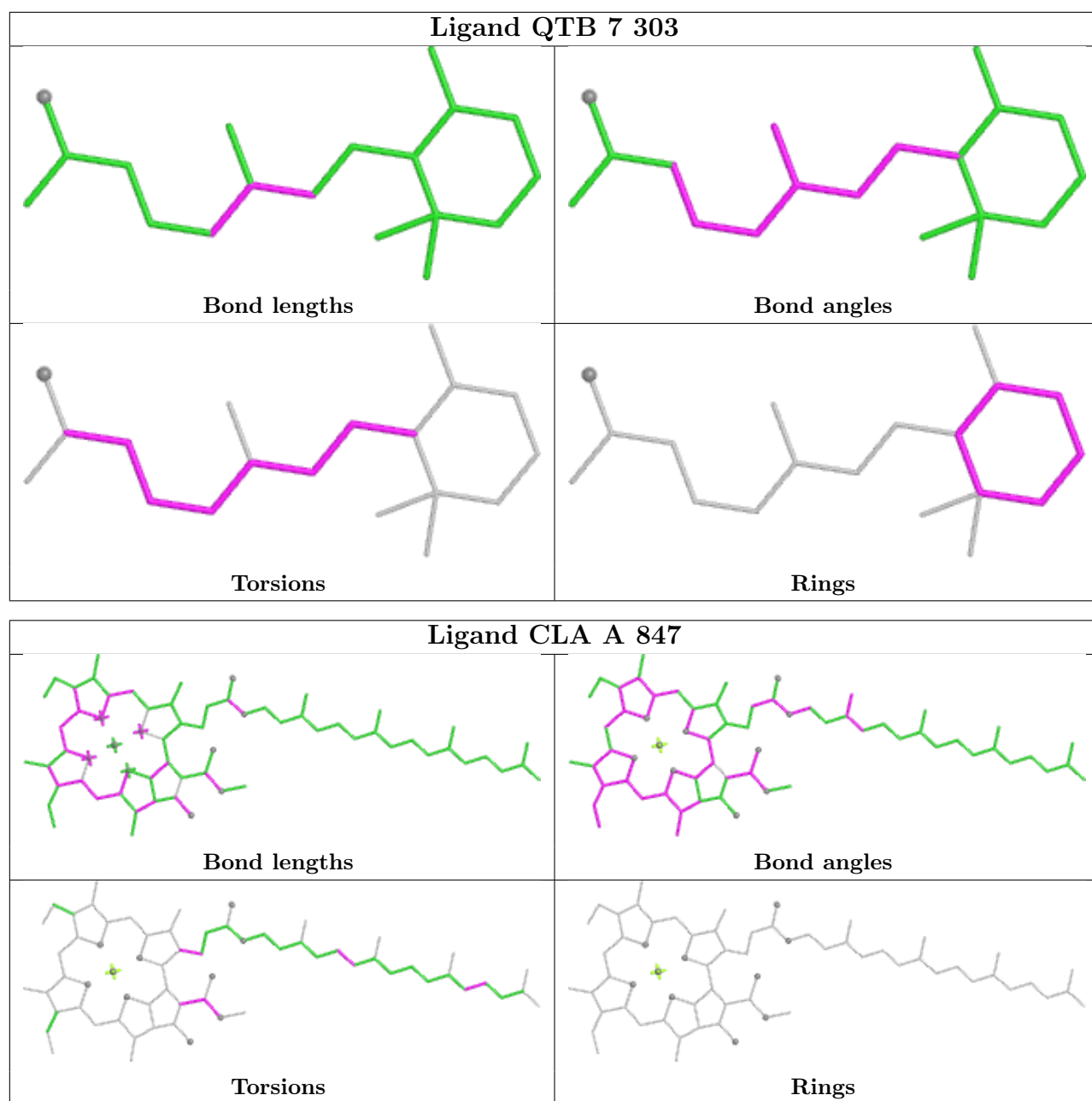
Rings

Ligand CLA 2 309

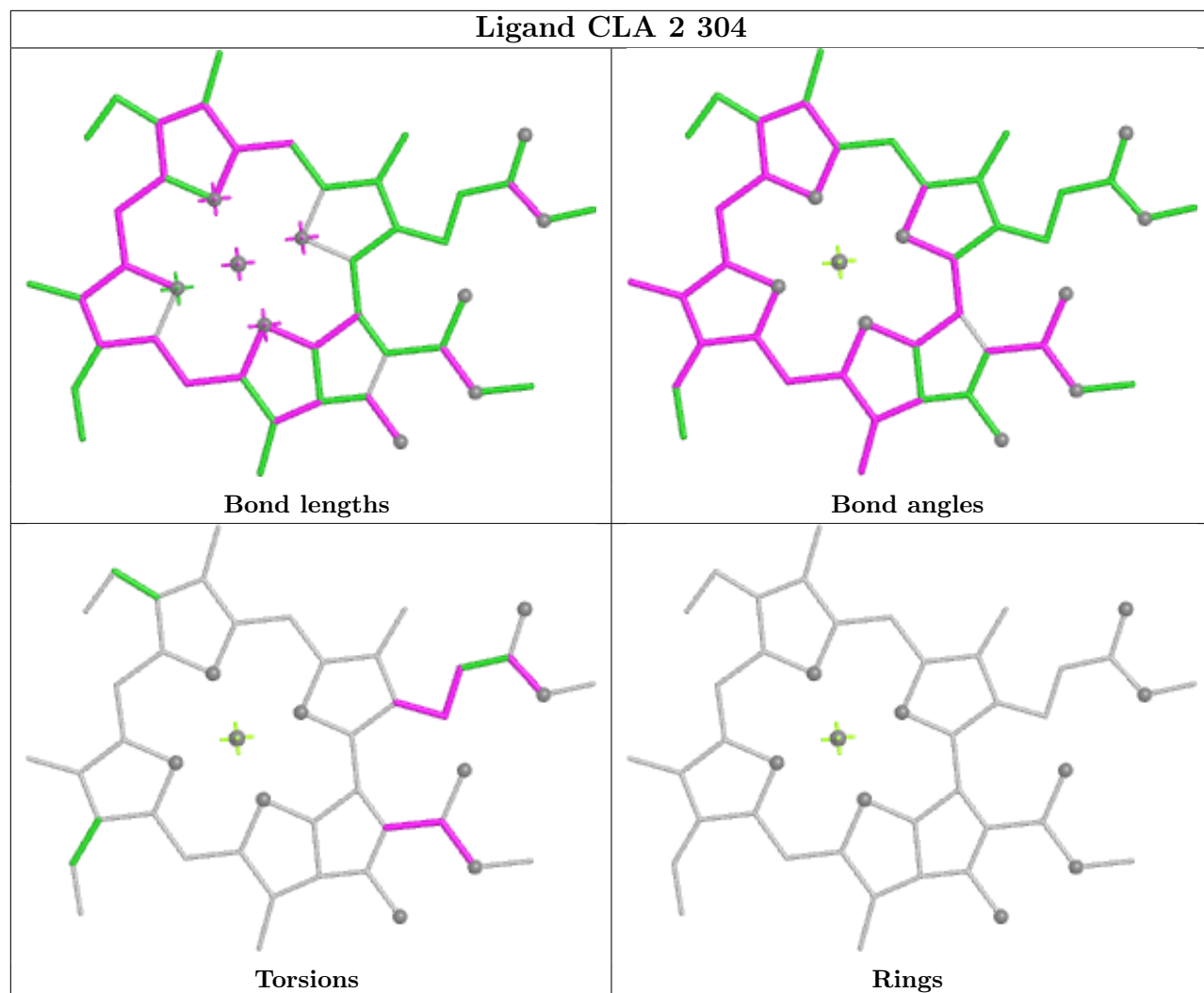


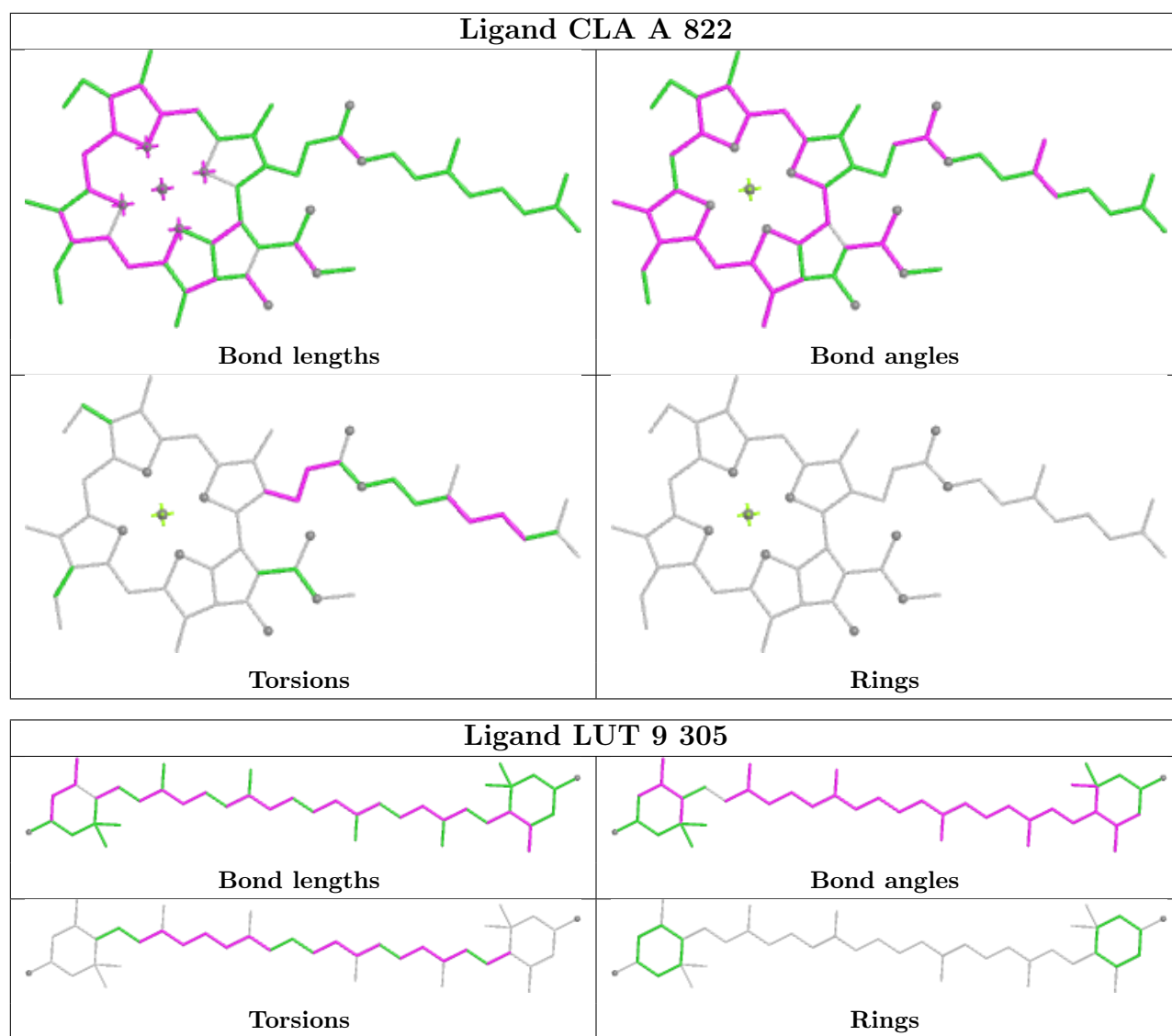
Ligand BCR F 302



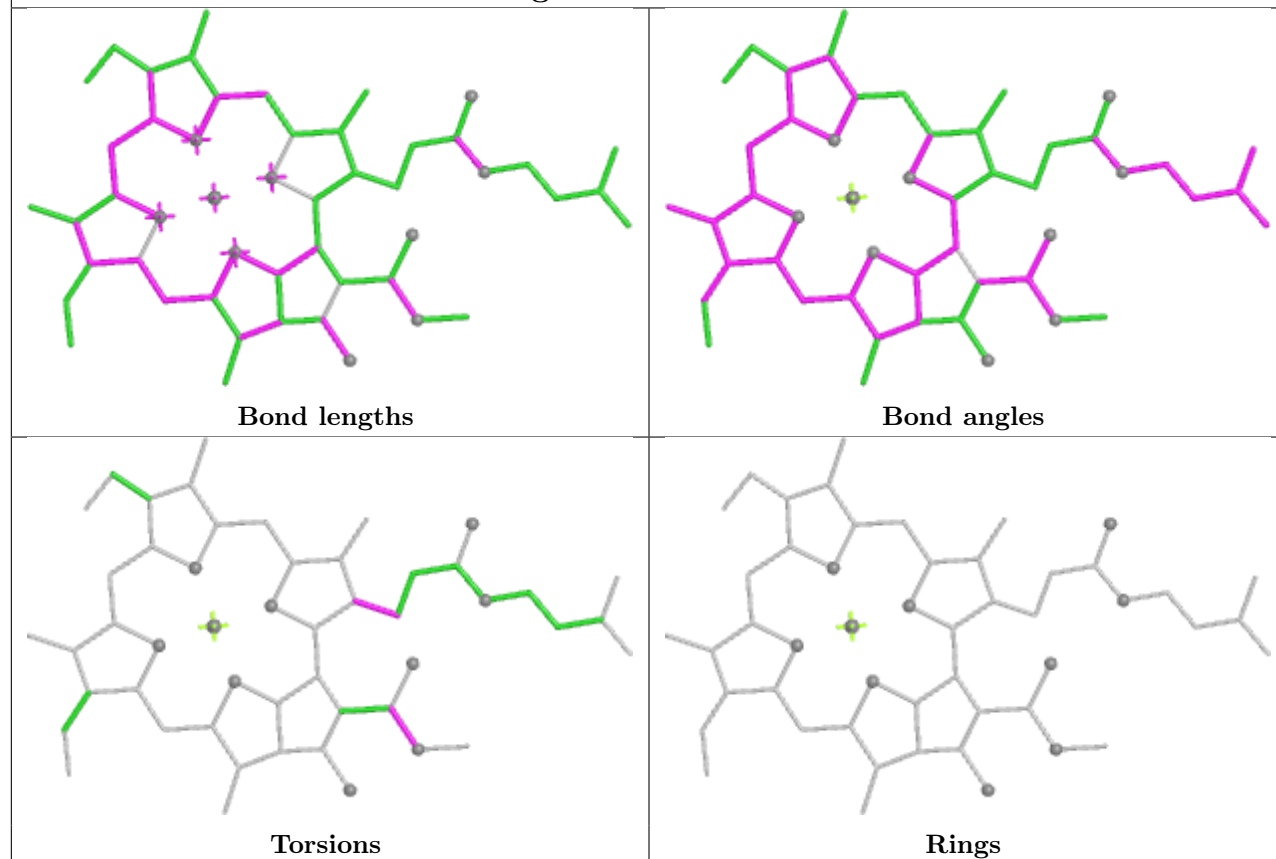


Ligand CLA 2 304

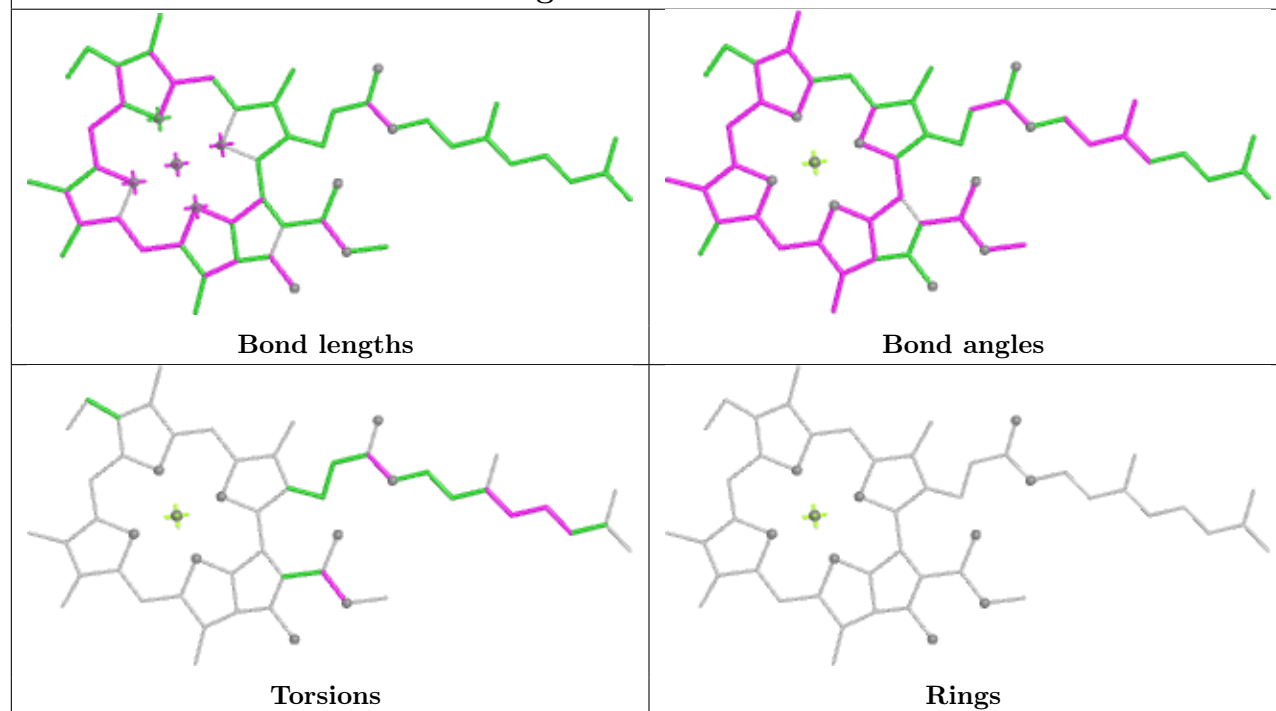


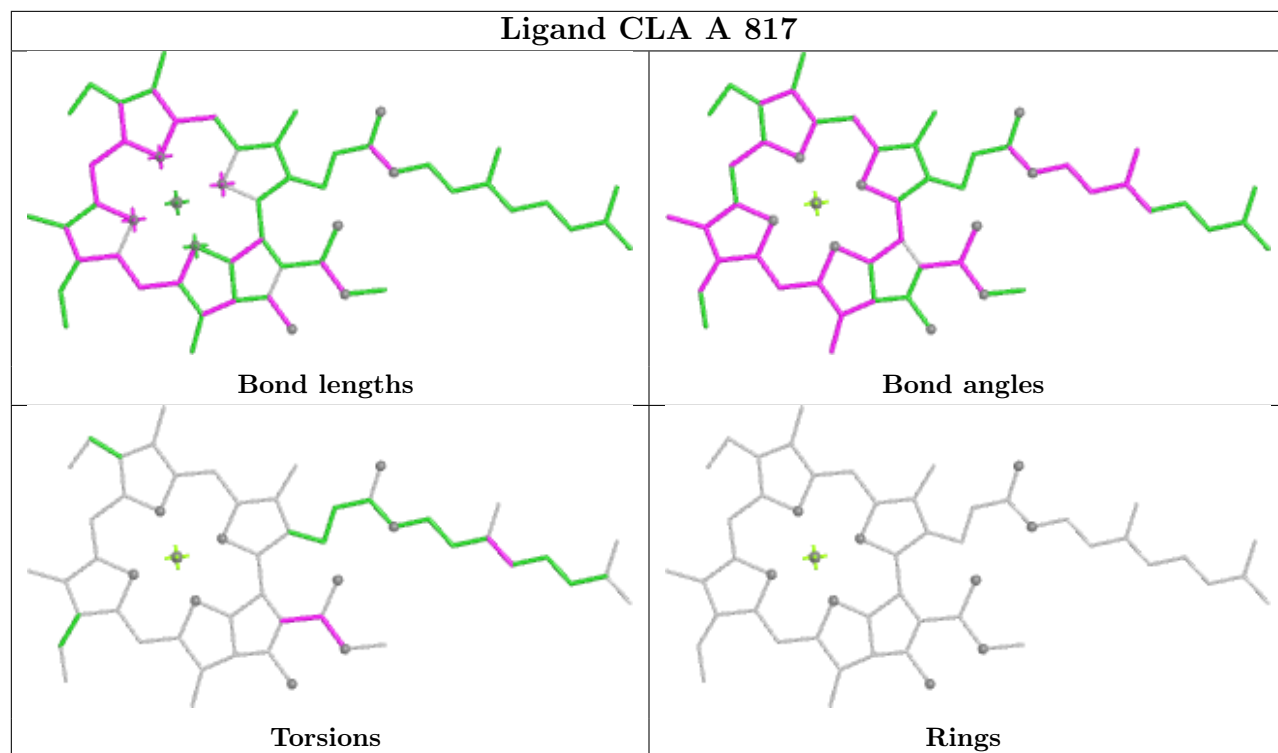
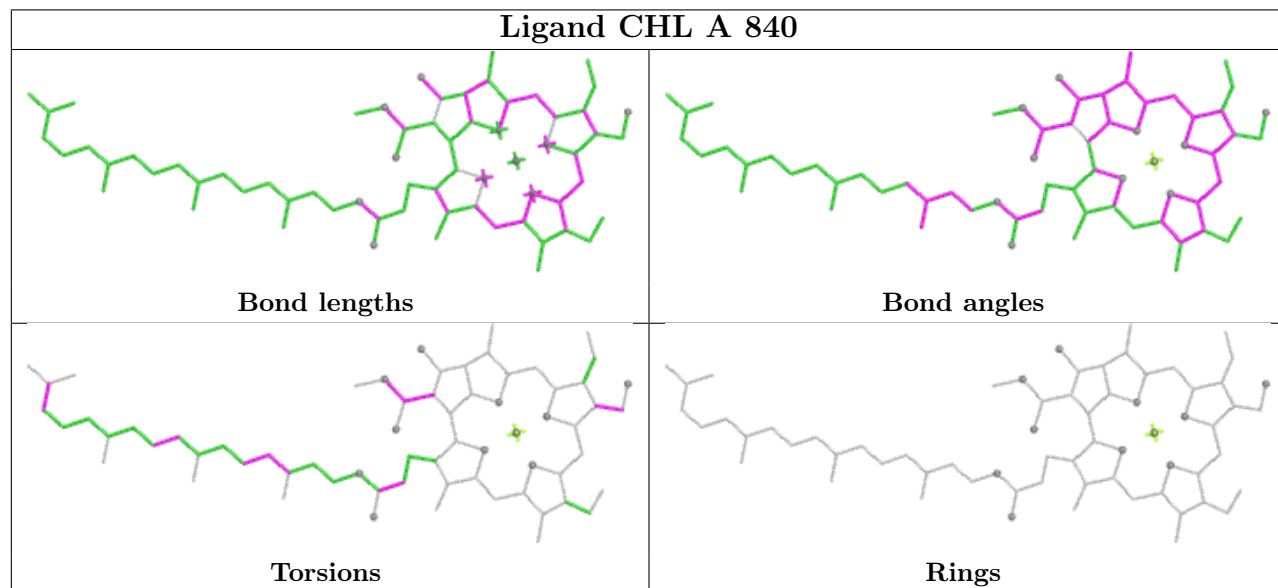


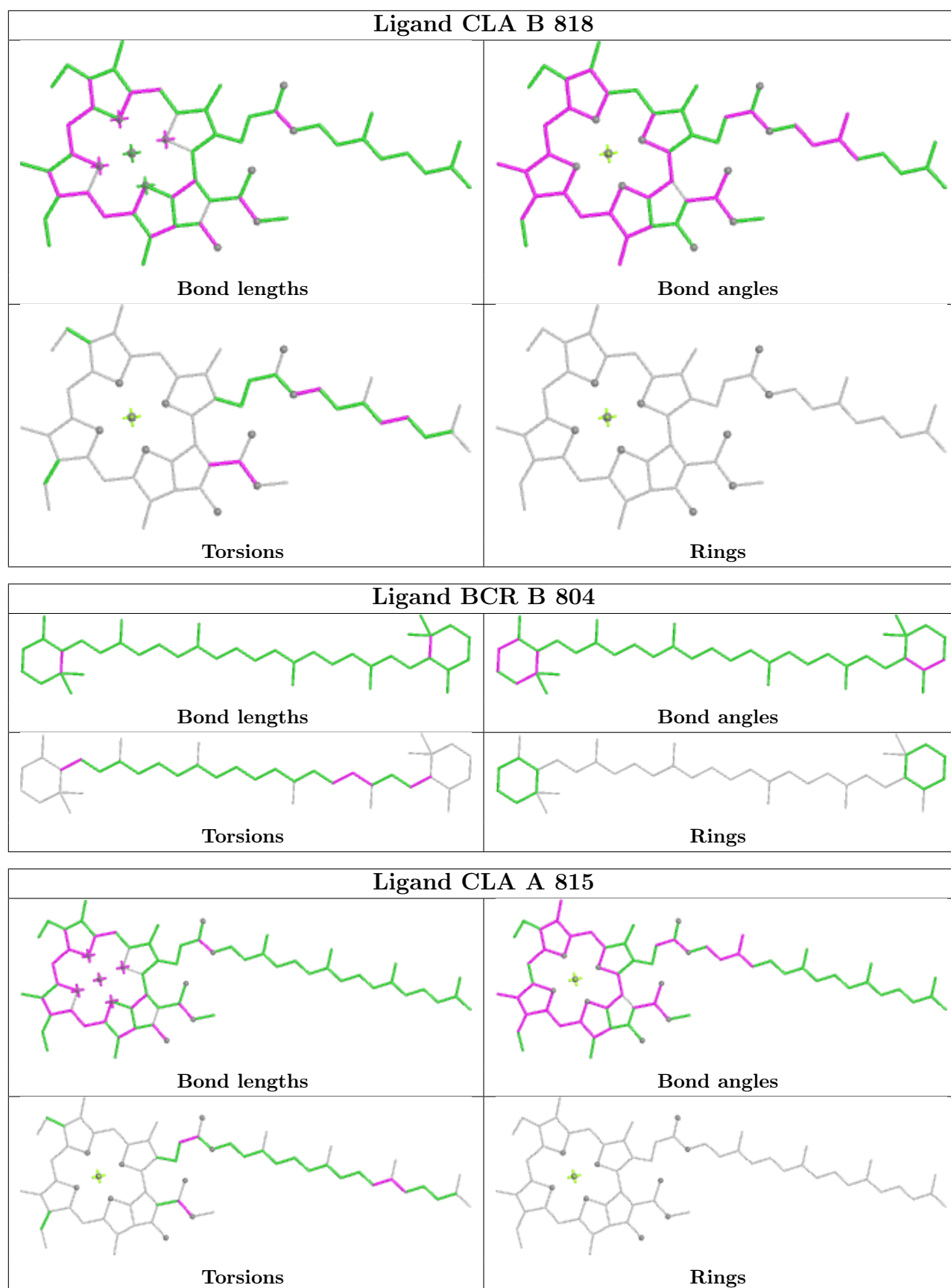
Ligand CLA A 844

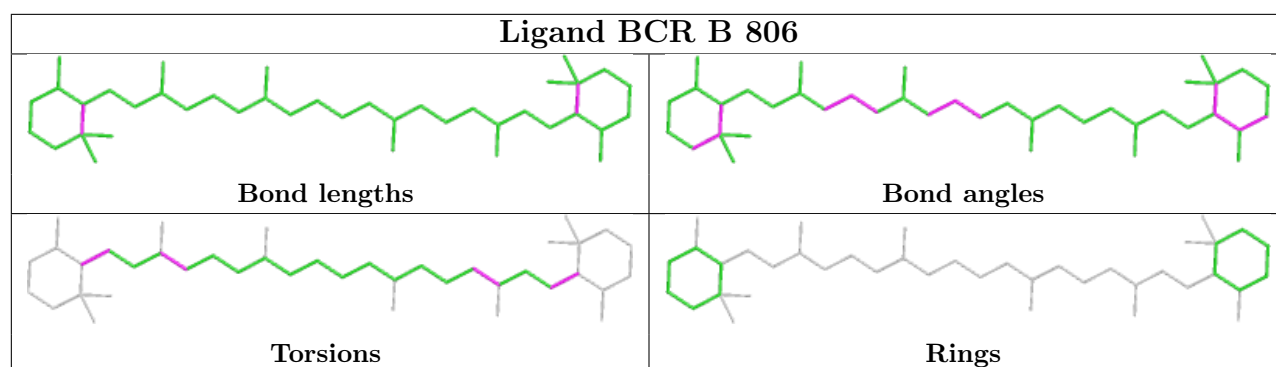
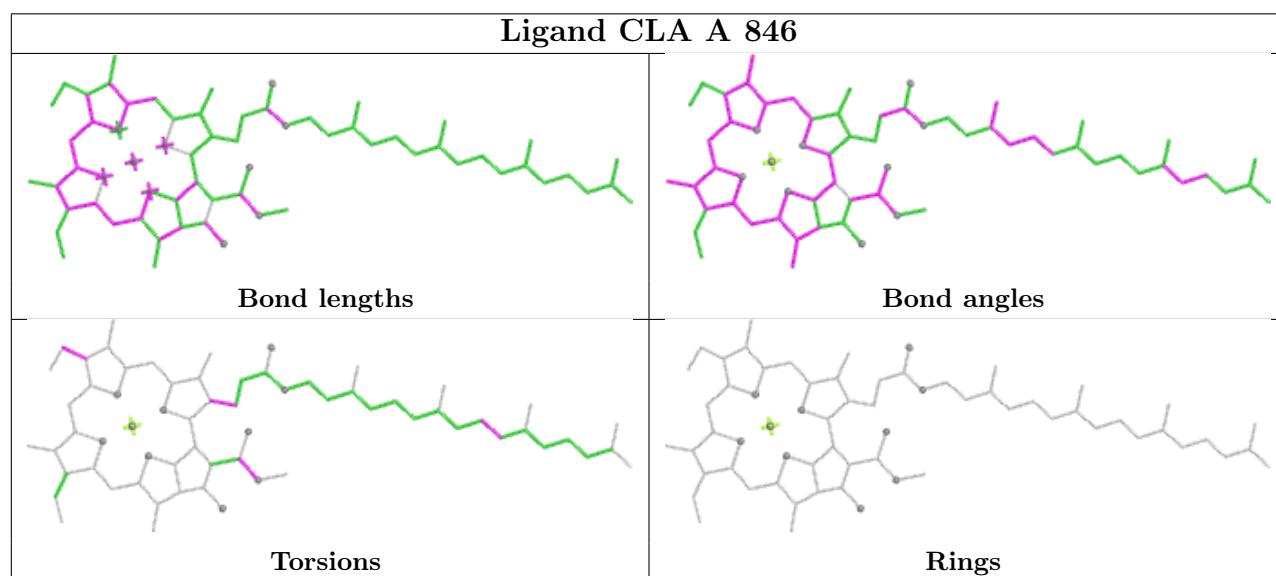
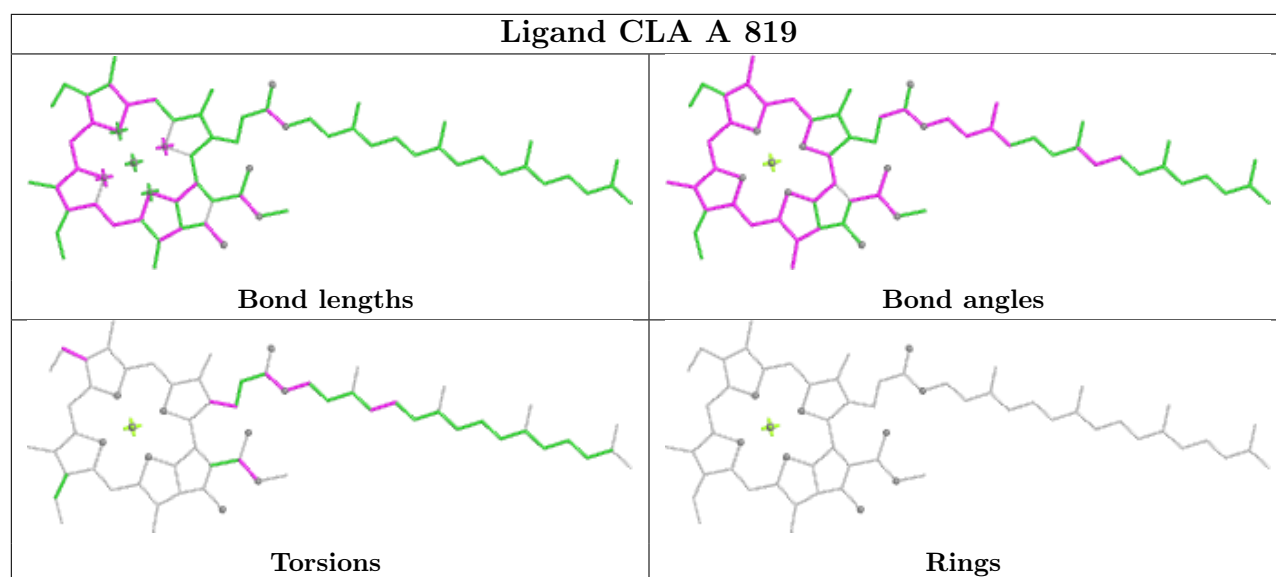


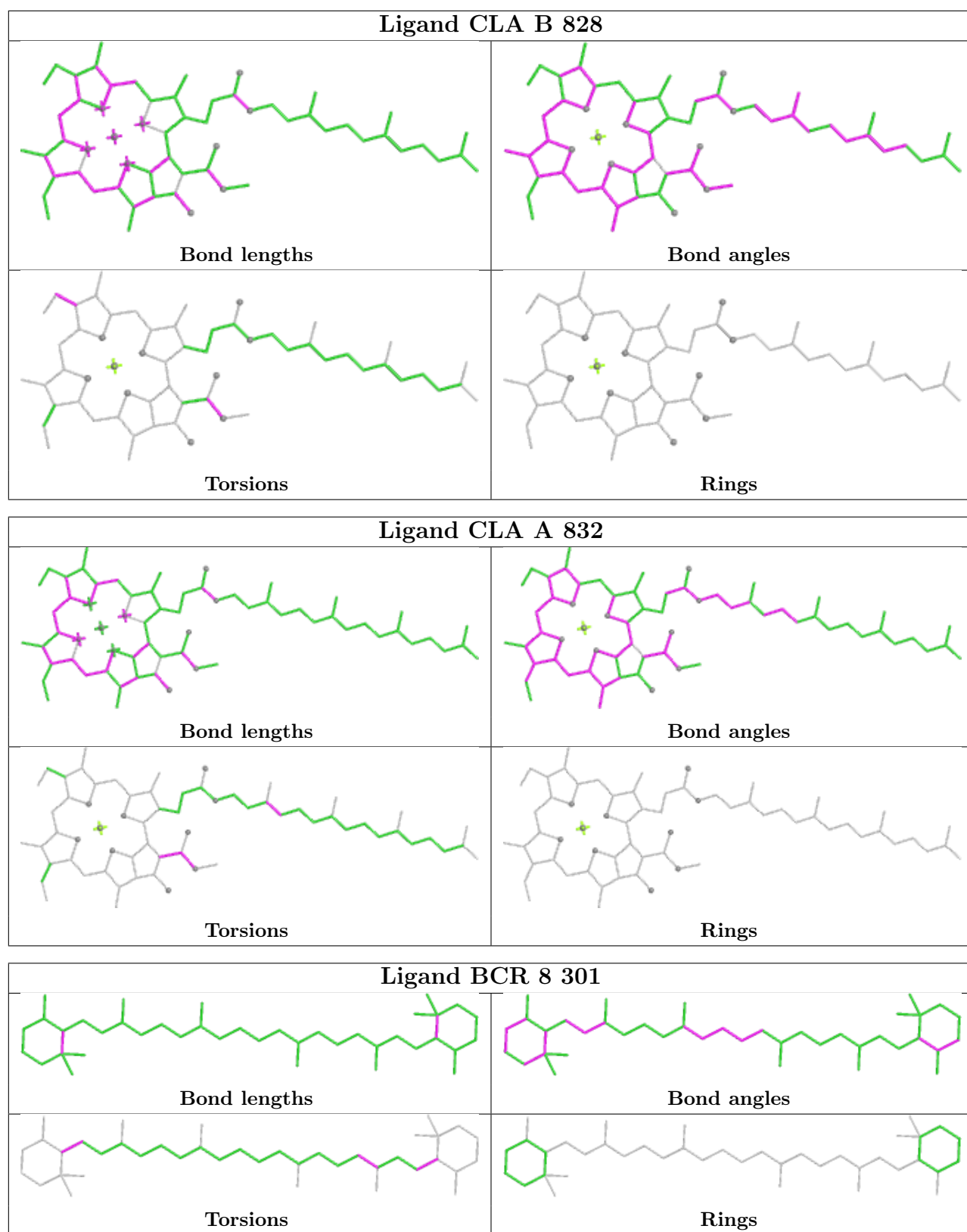
Ligand CLA 7 314



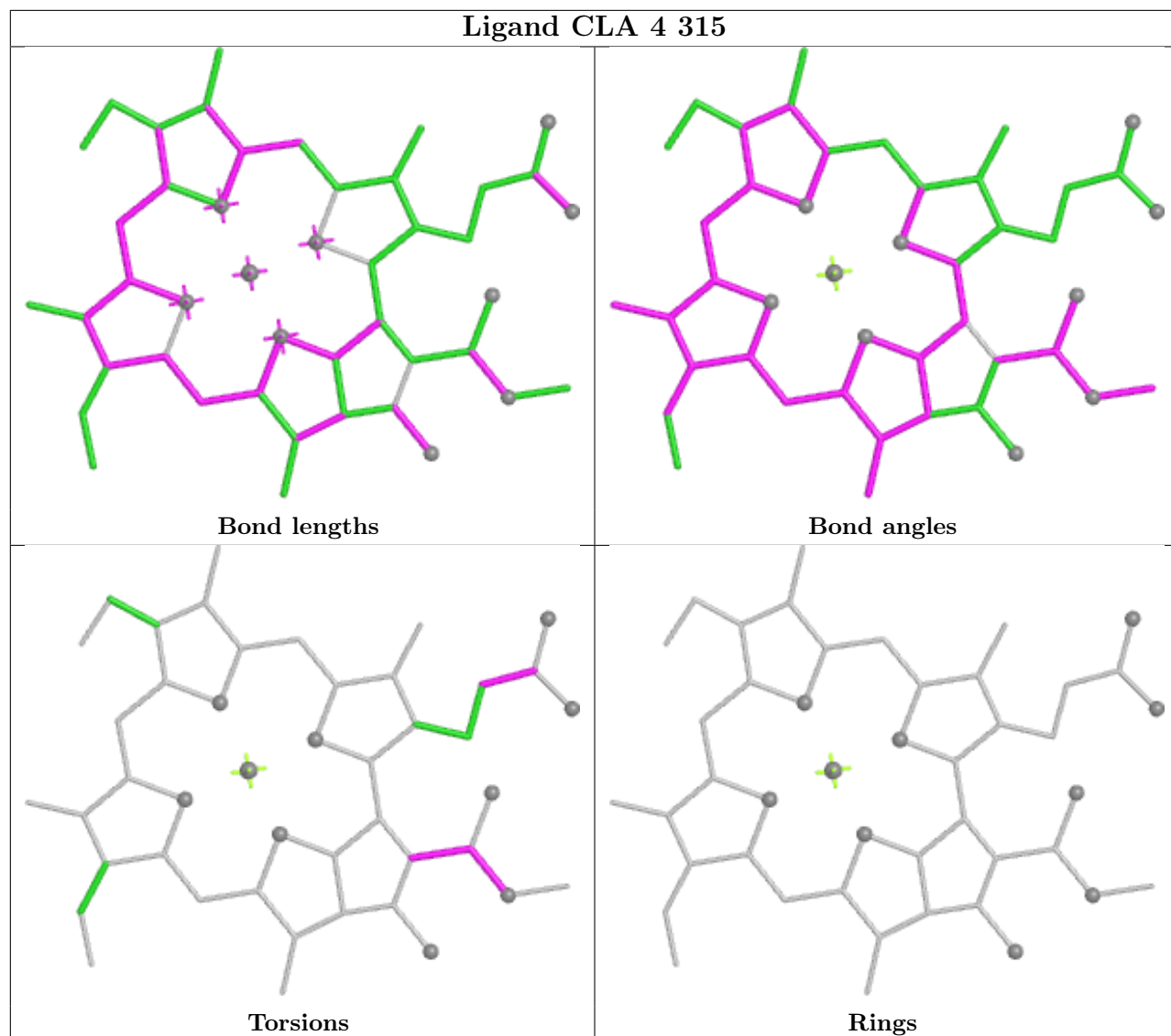
Ligand CLA A 817**Ligand CHL A 840**

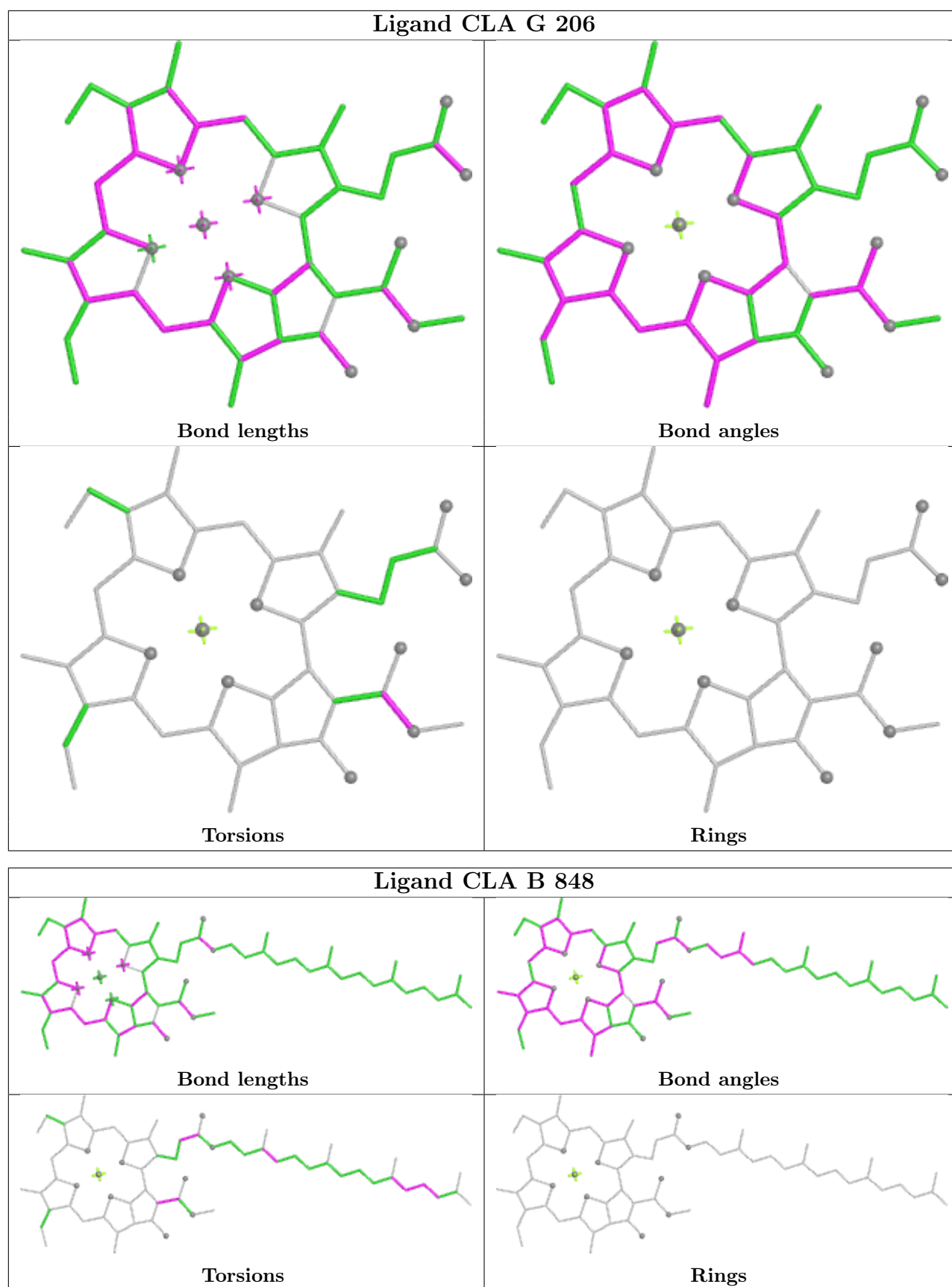


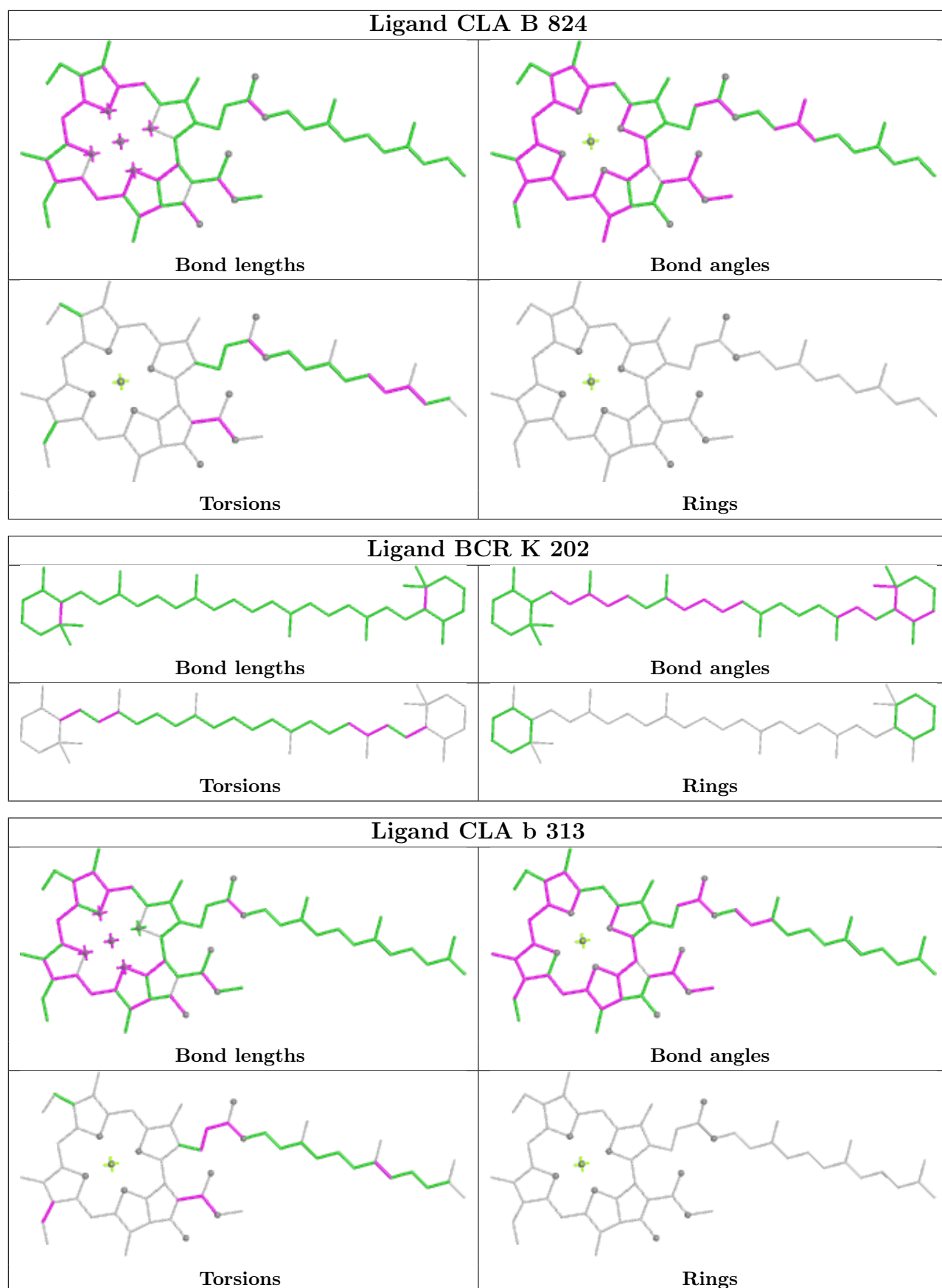


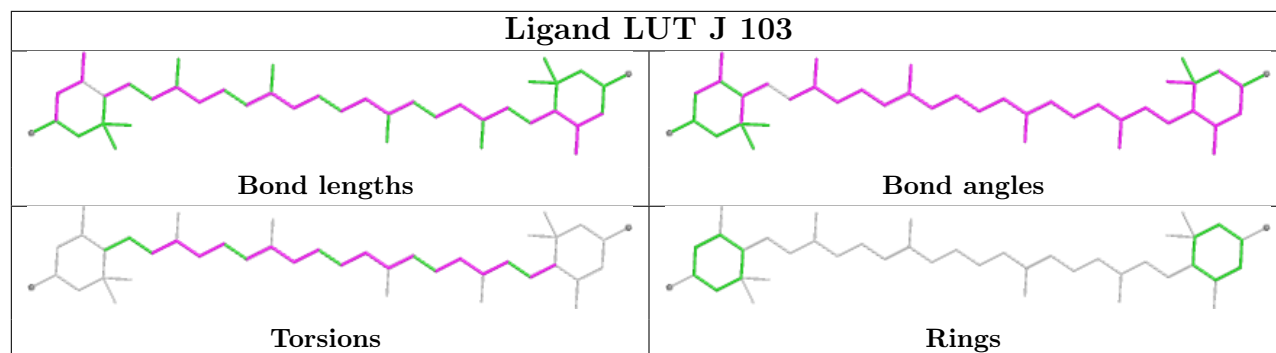
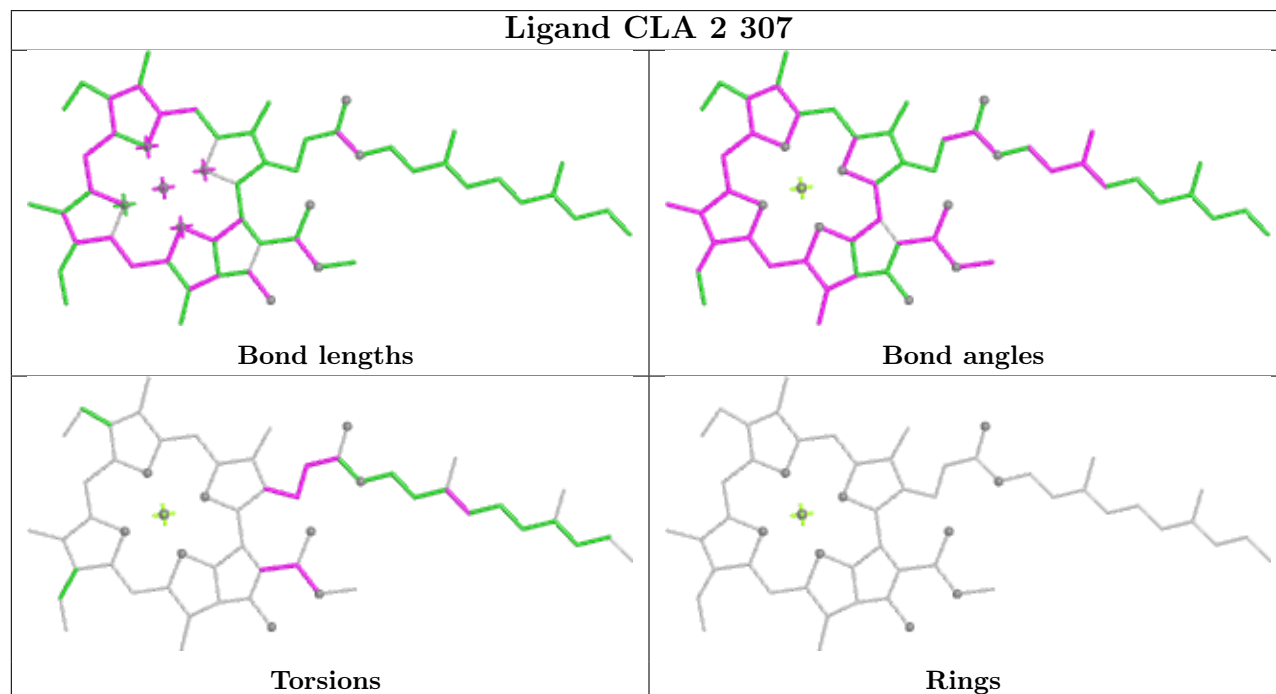


Ligand CLA 4 315

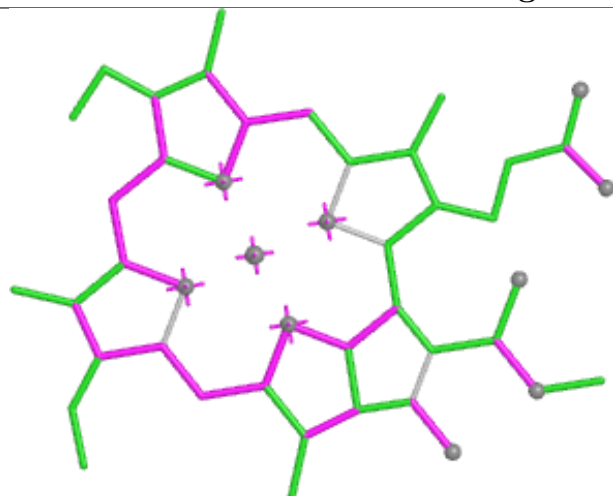




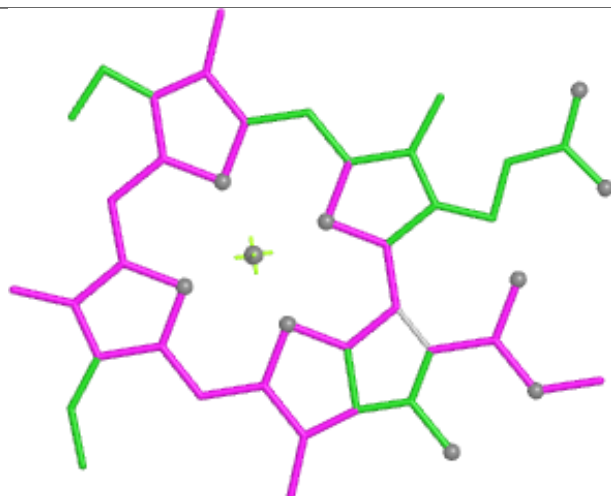


Ligand LUT J 103**Ligand CLA 2 307**

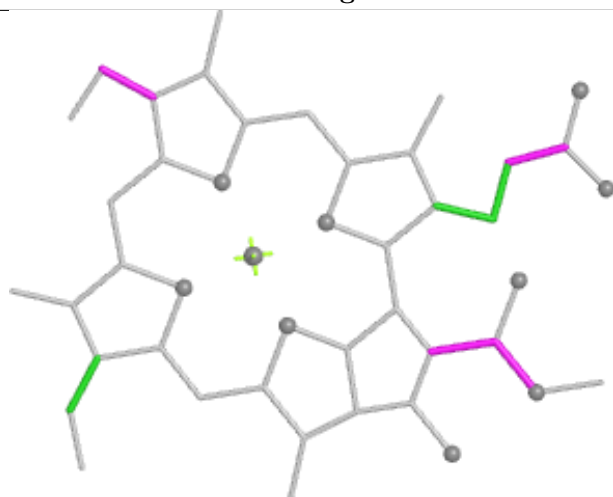
Ligand CLA 2 305



Bond lengths



Bond angles

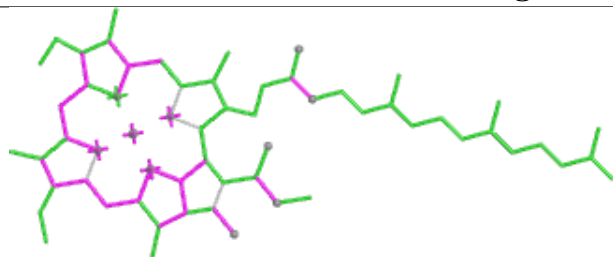


Torsions

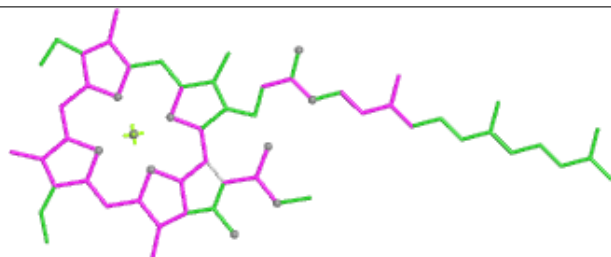


Rings

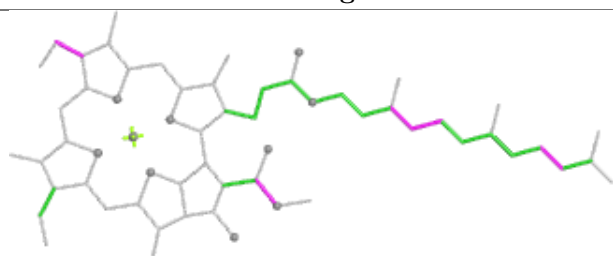
Ligand CLA A 836



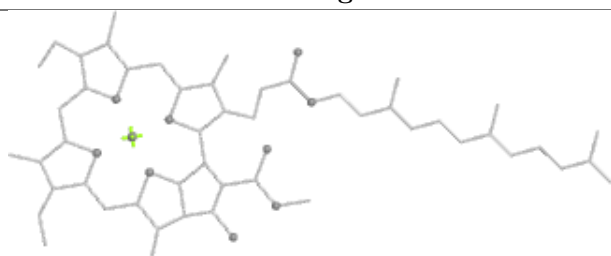
Bond lengths



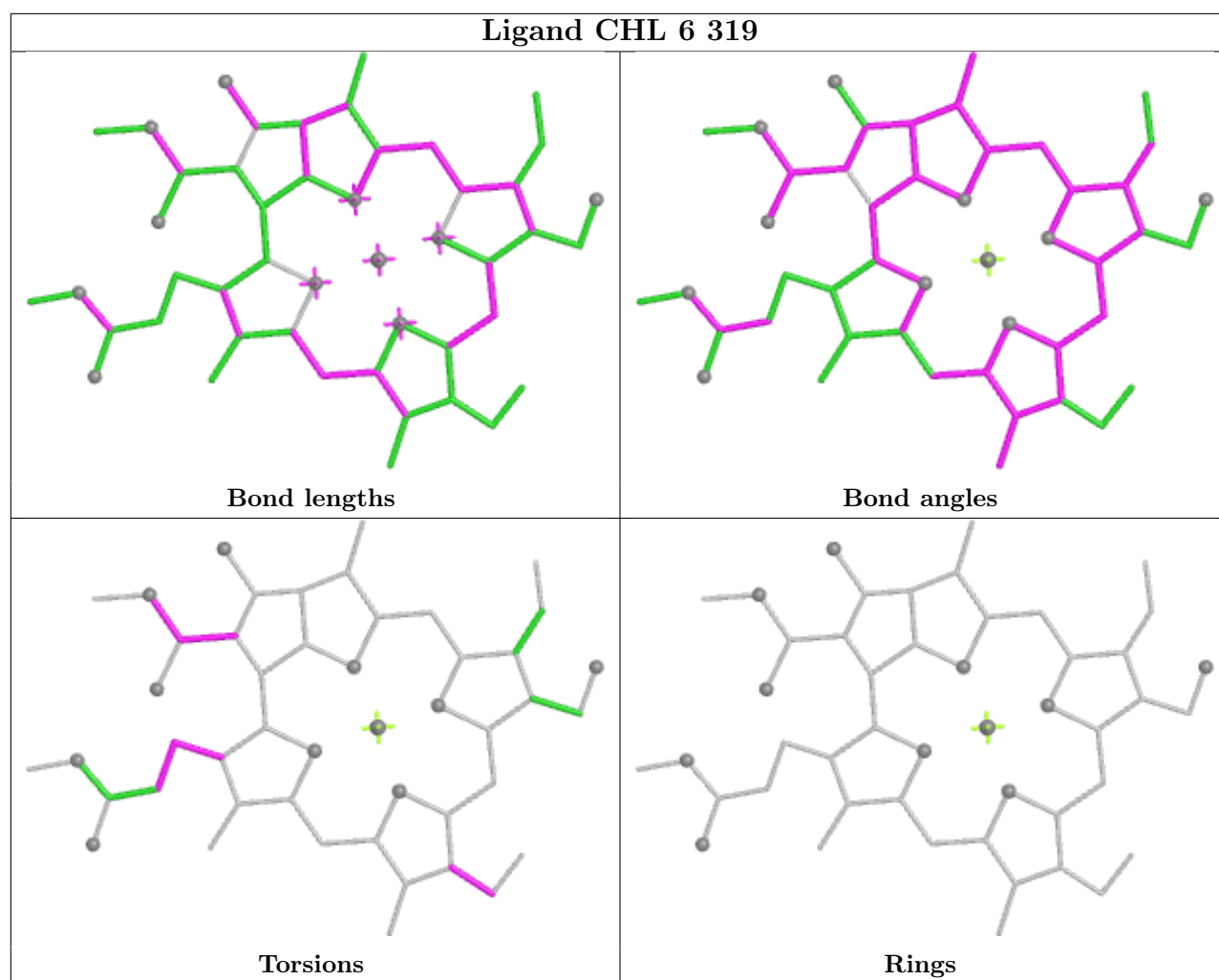
Bond angles

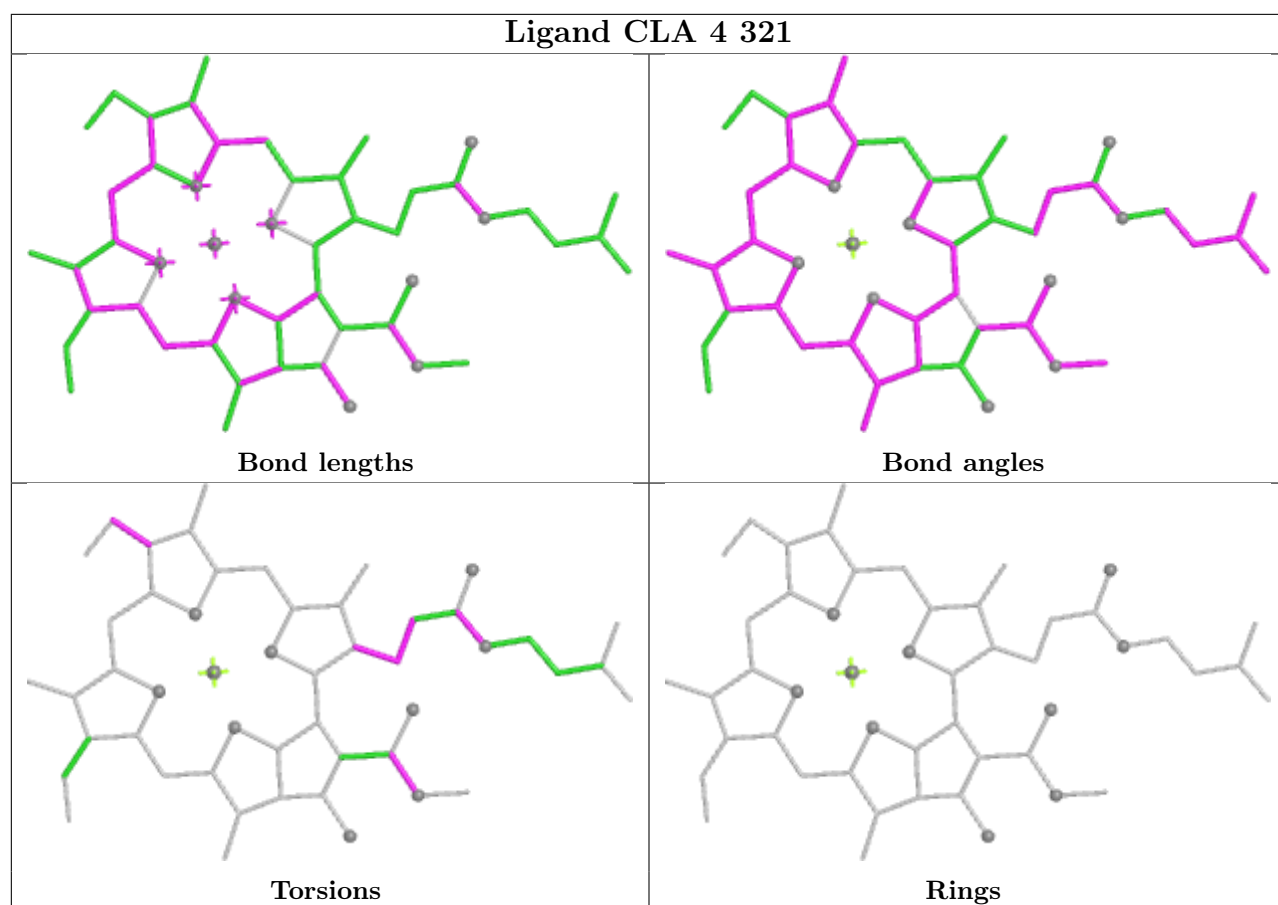


Torsions

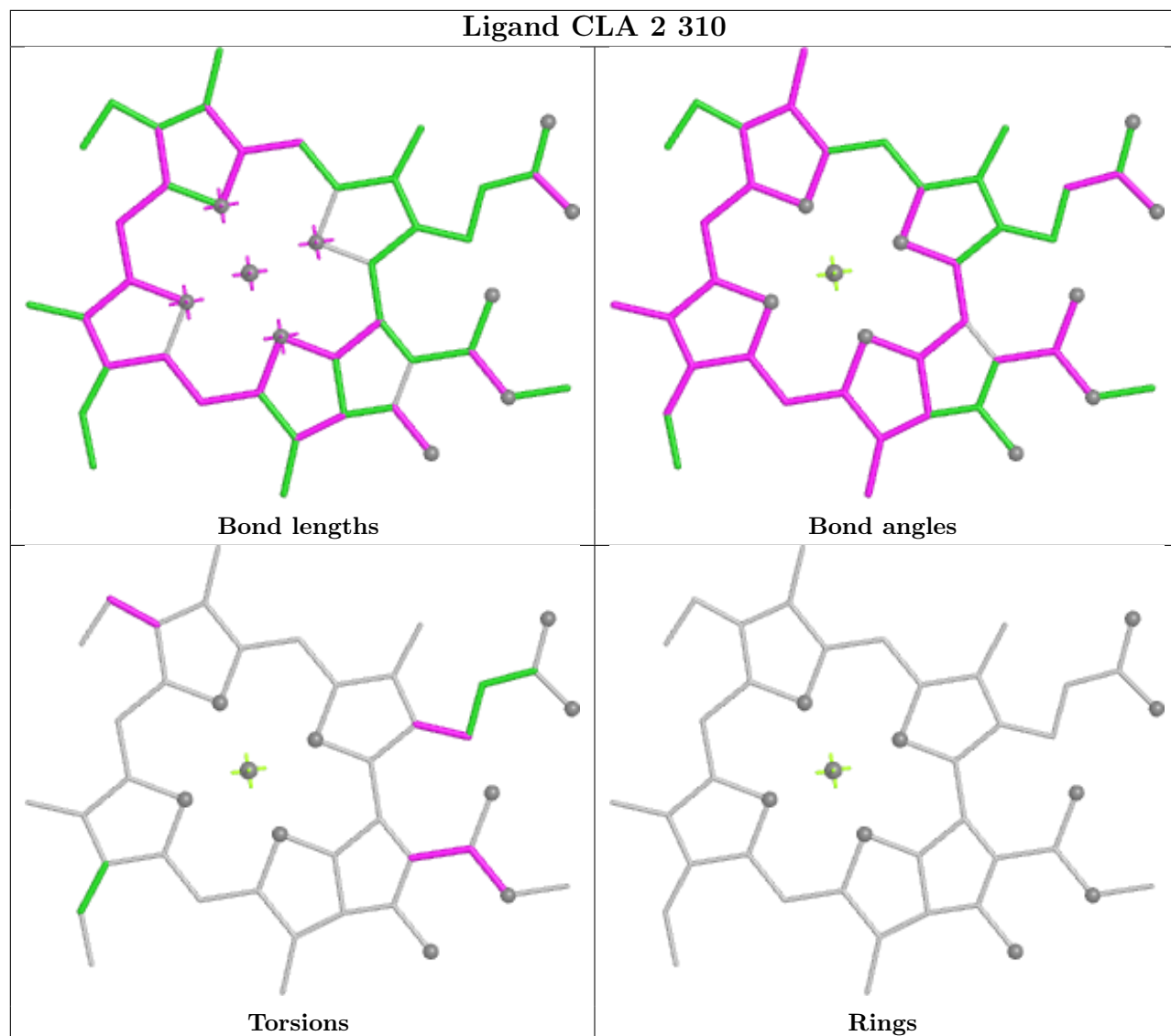


Rings

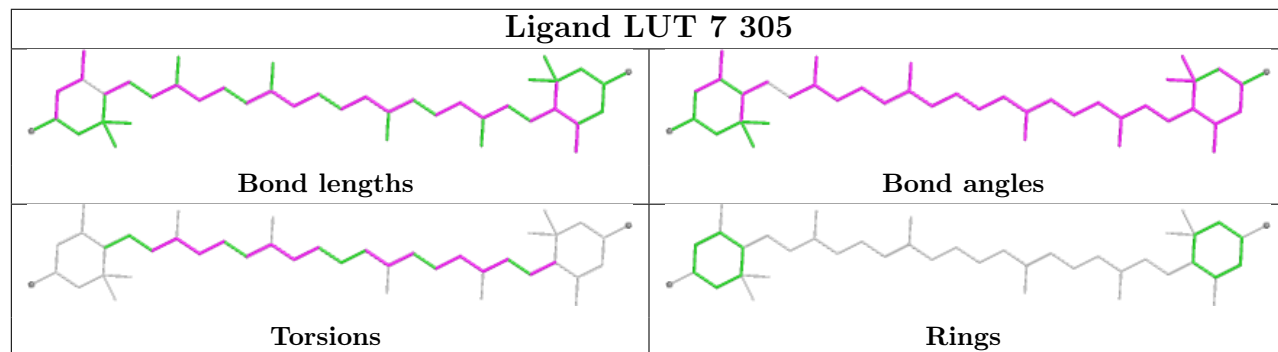




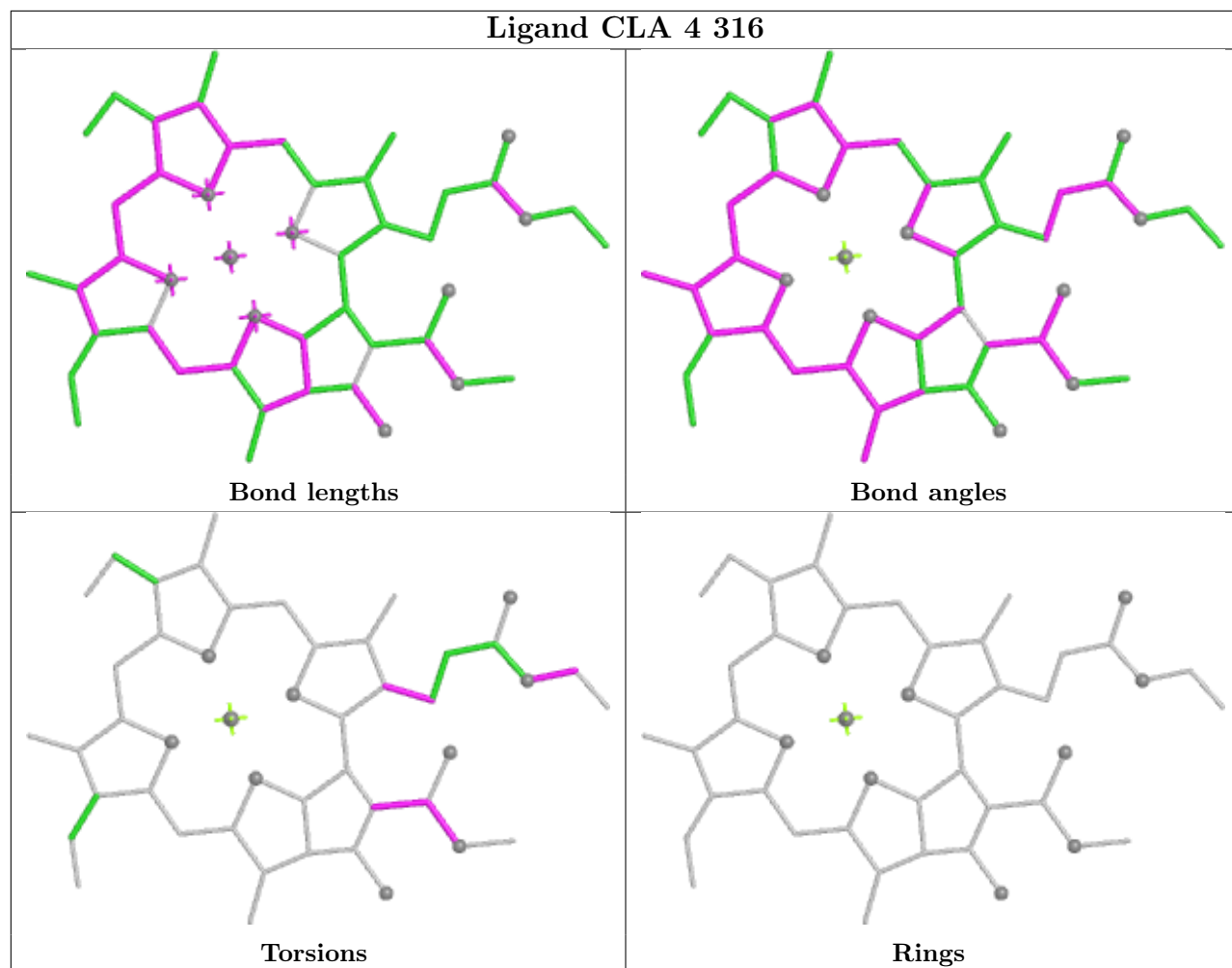
Ligand CLA 2 310



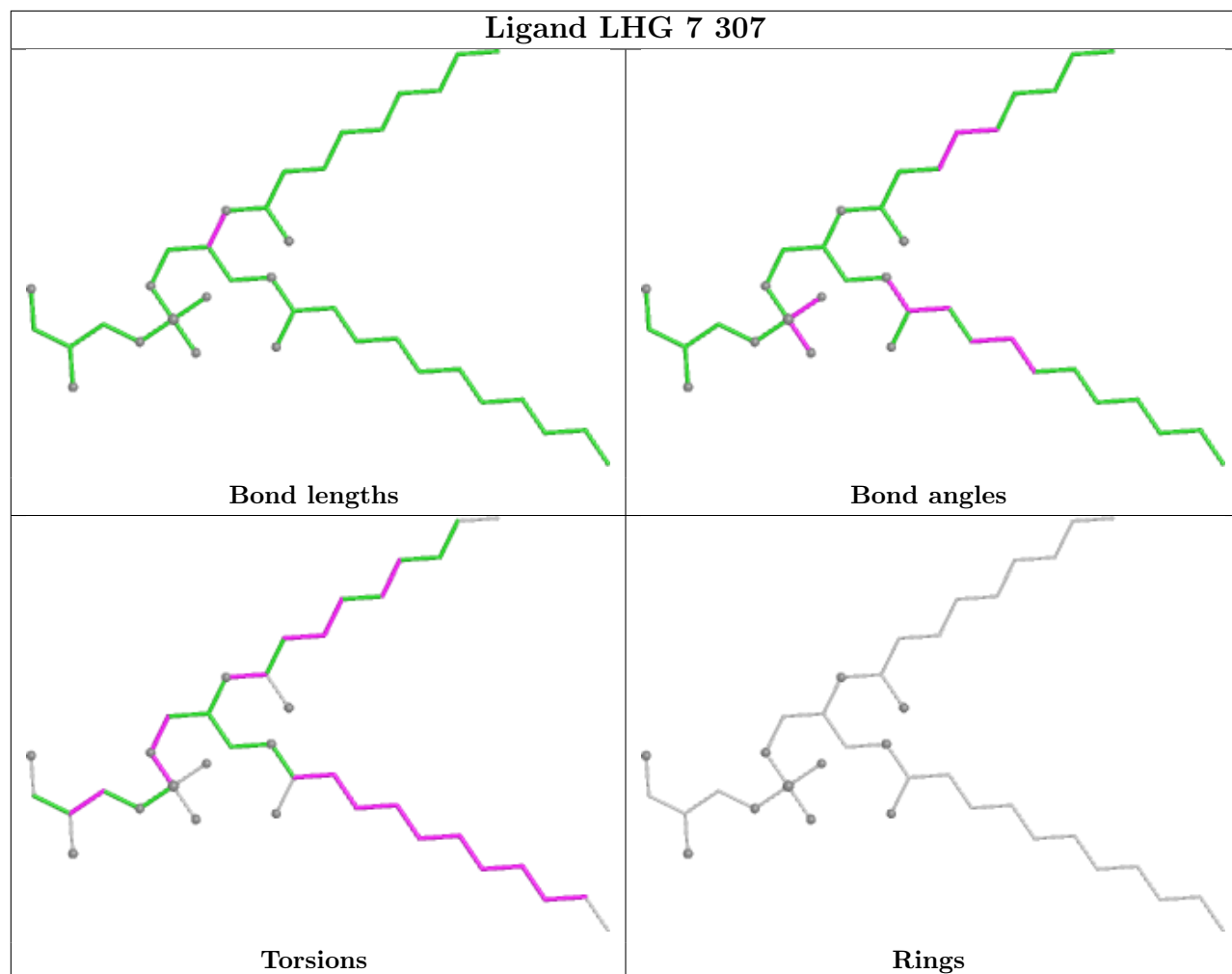
Ligand LUT 7 305



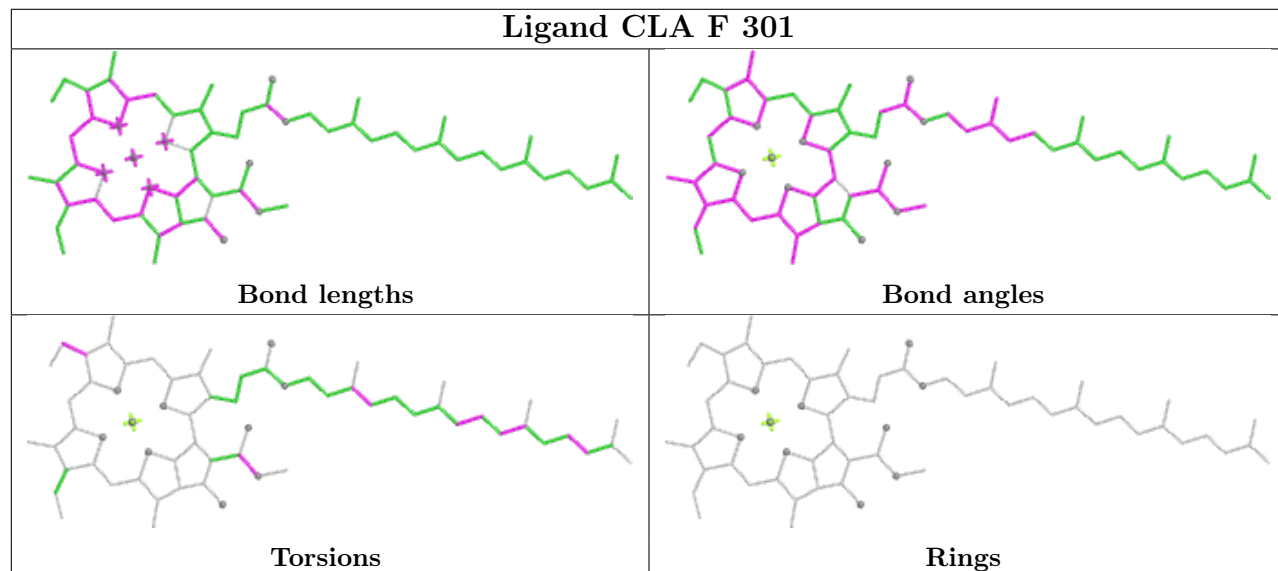
Ligand CLA 4 316

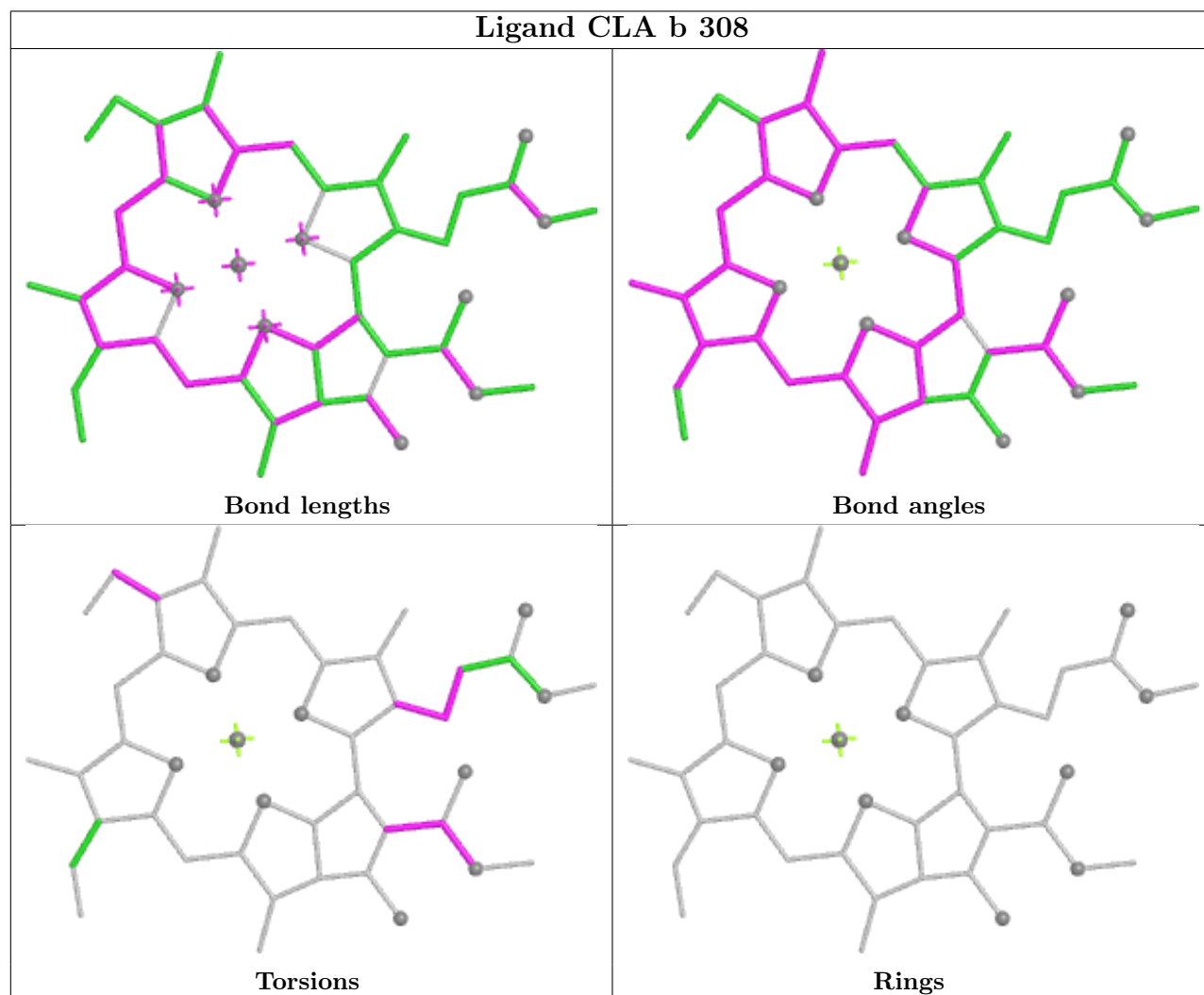
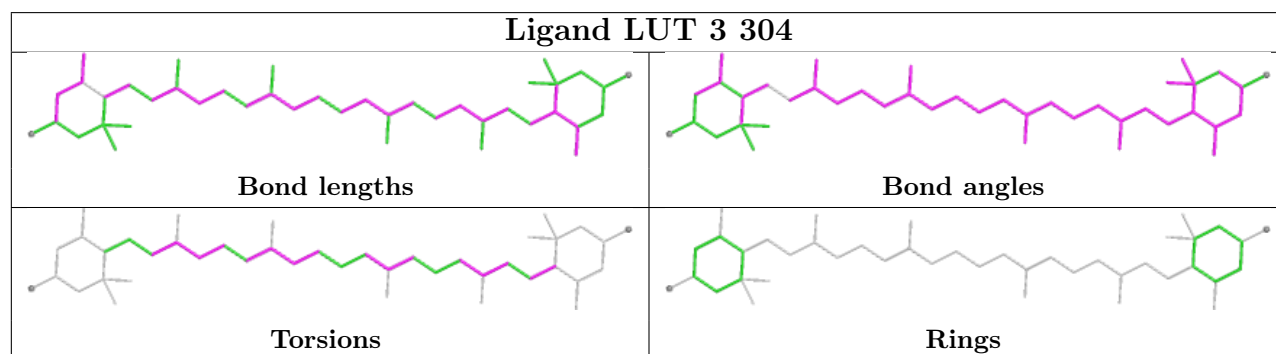
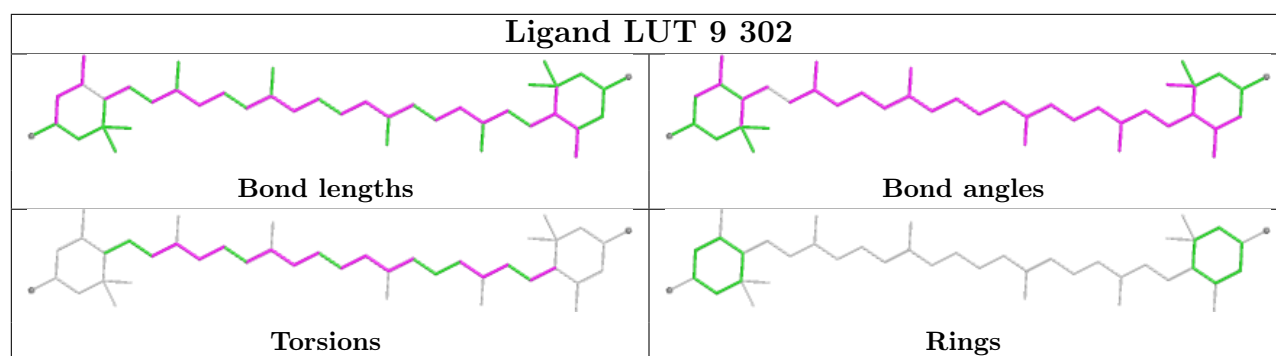


Ligand LHG 7 307

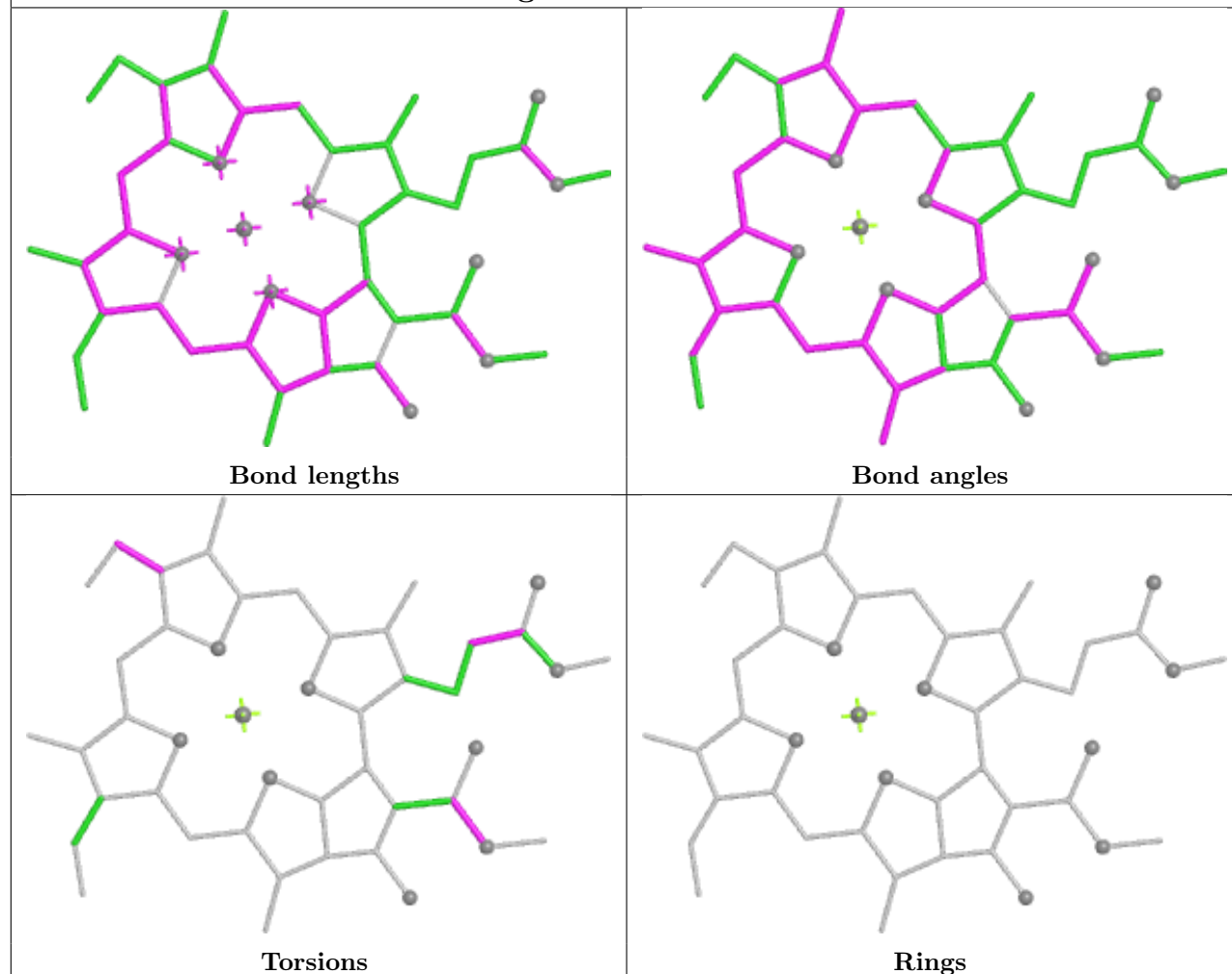


Ligand CLA F 301

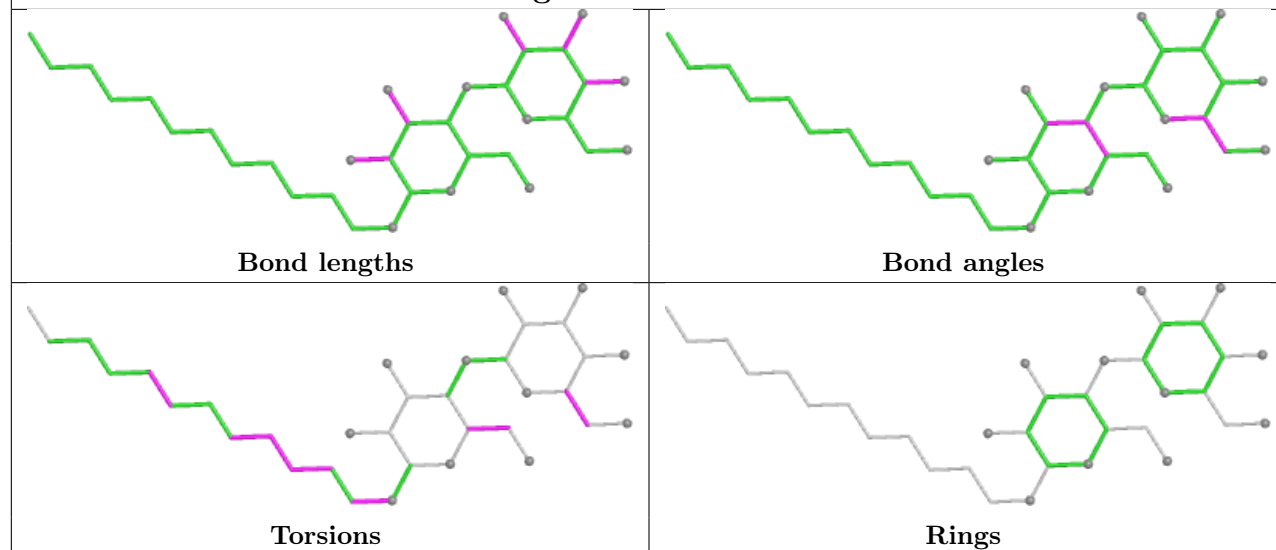


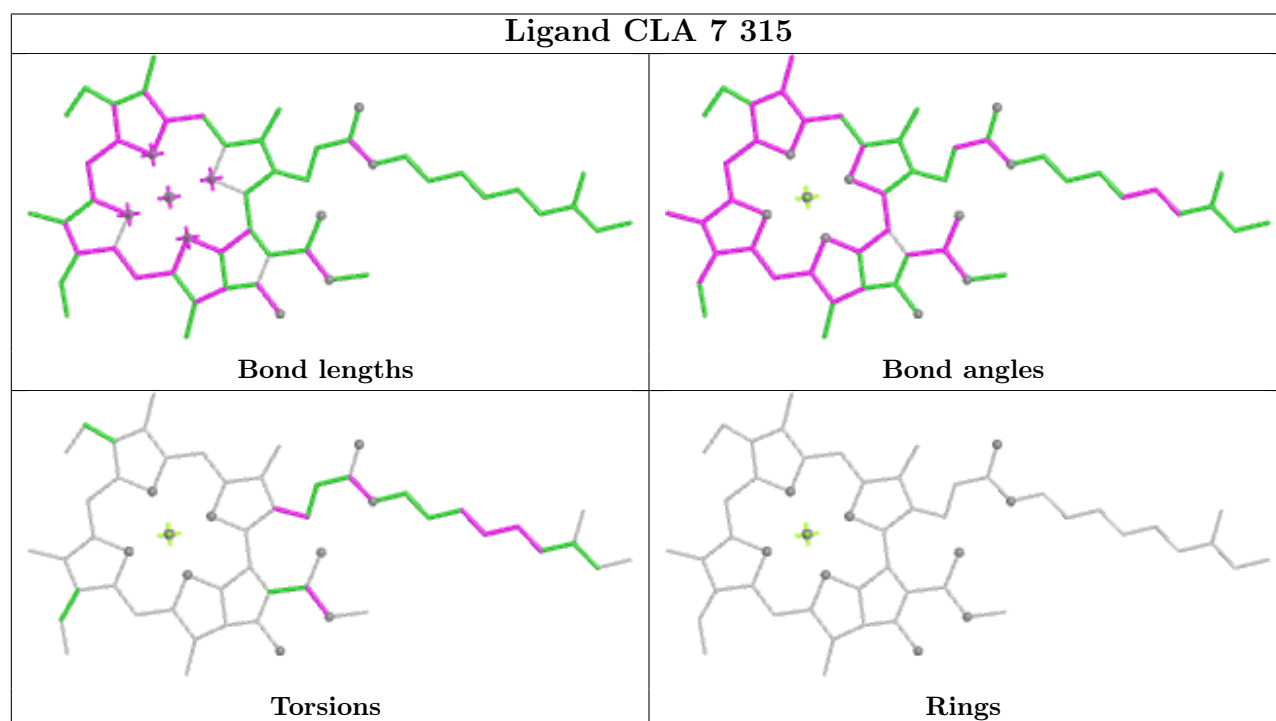
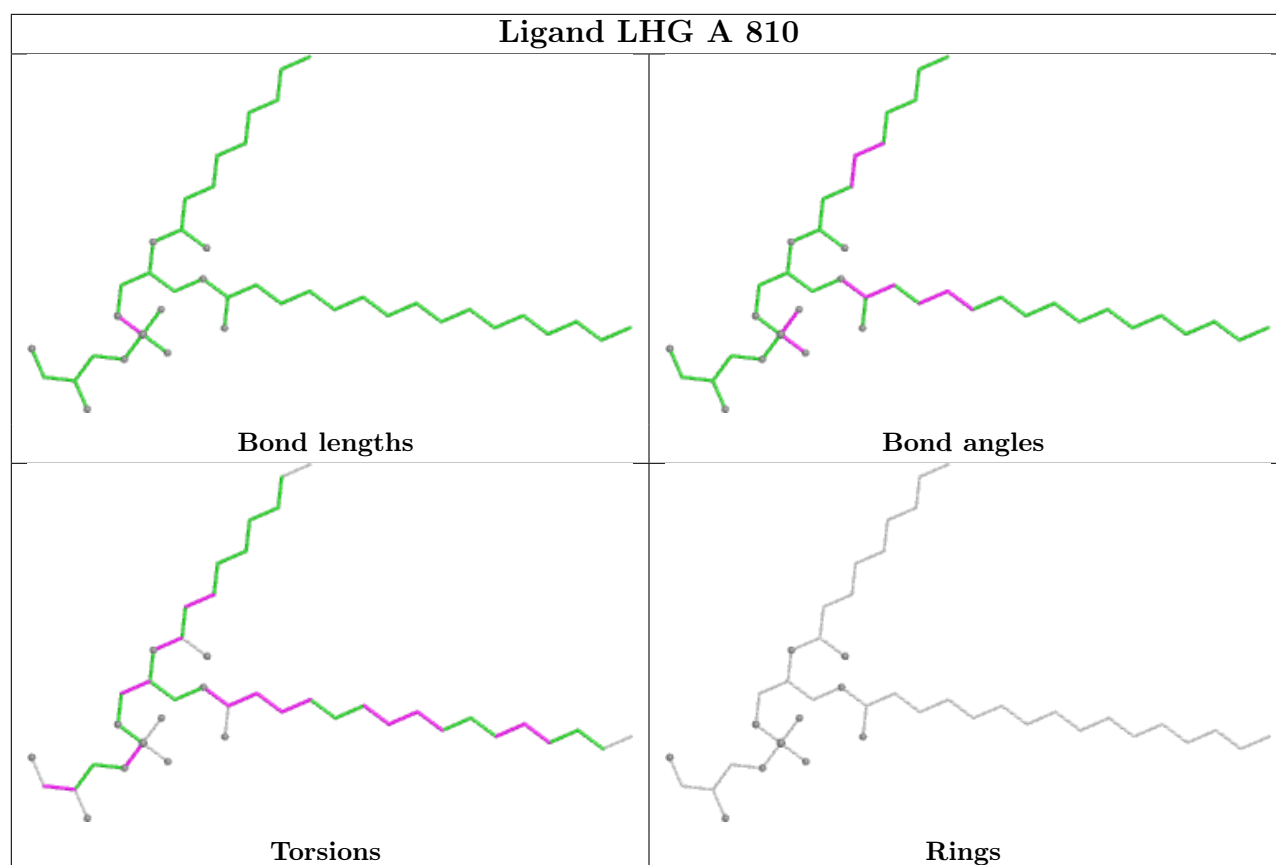


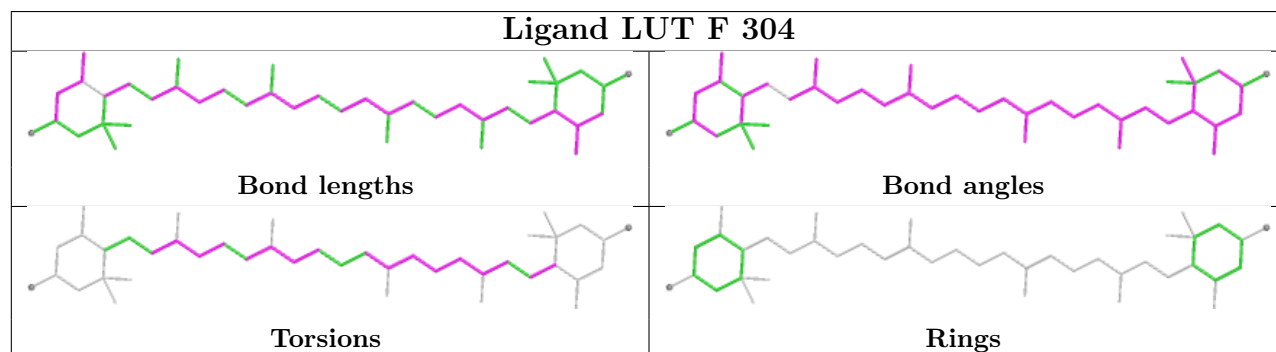
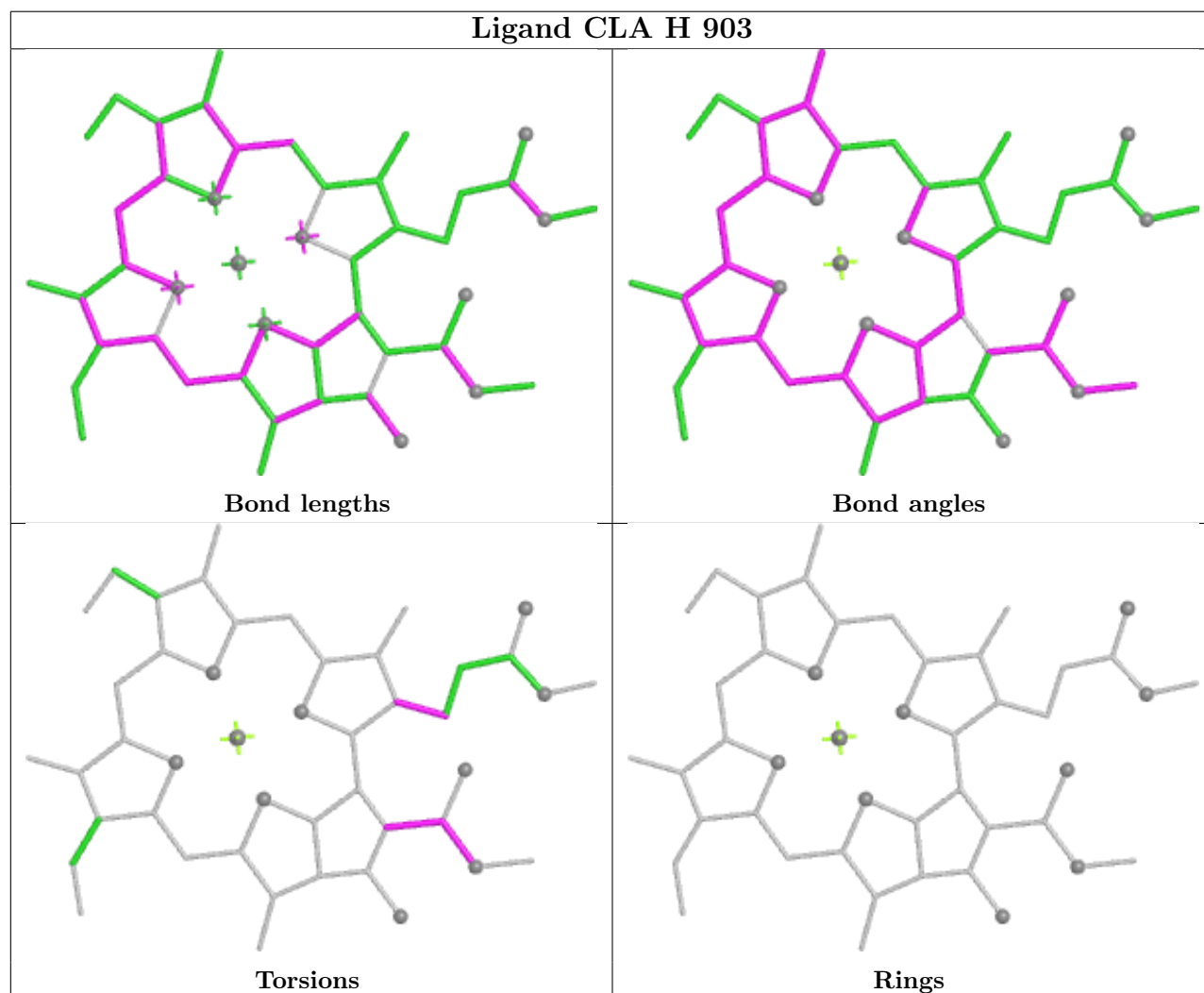
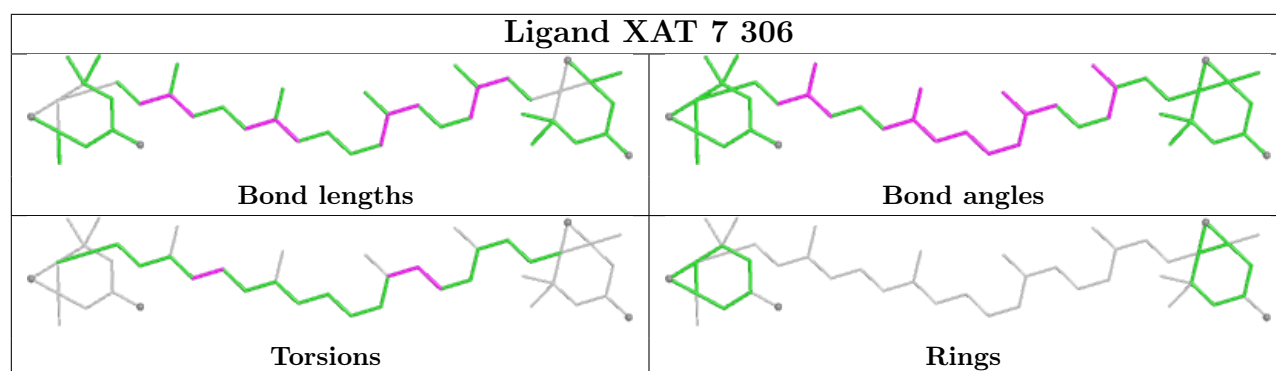
Ligand CLA 5 313

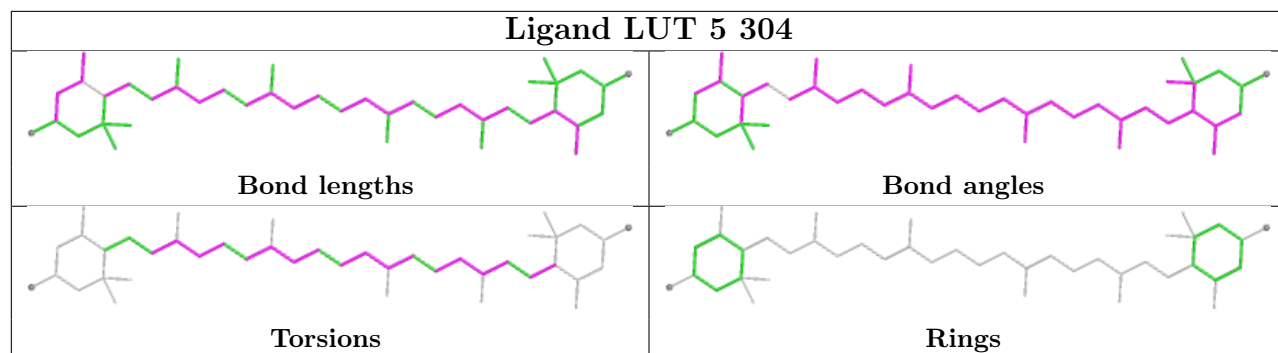
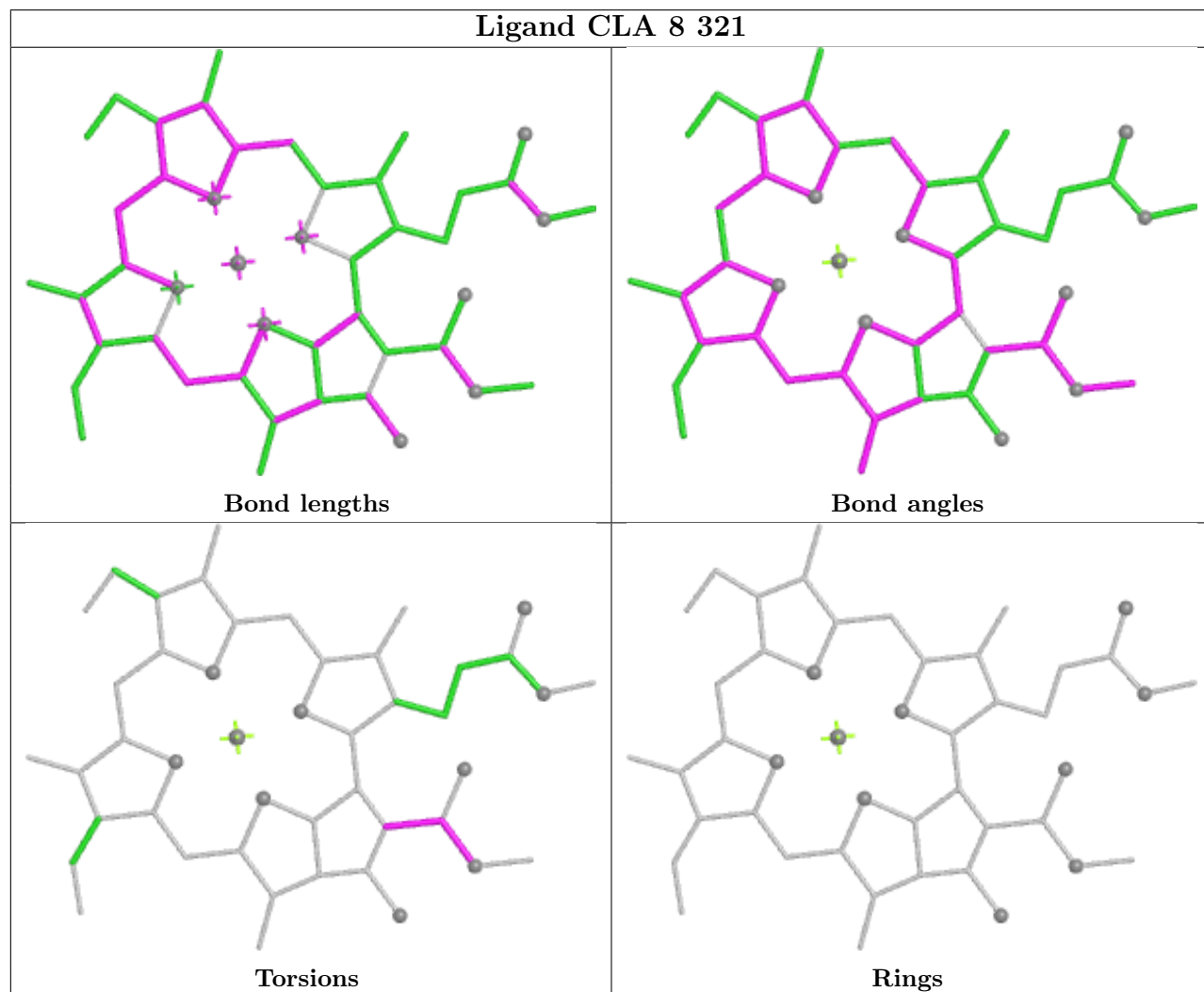


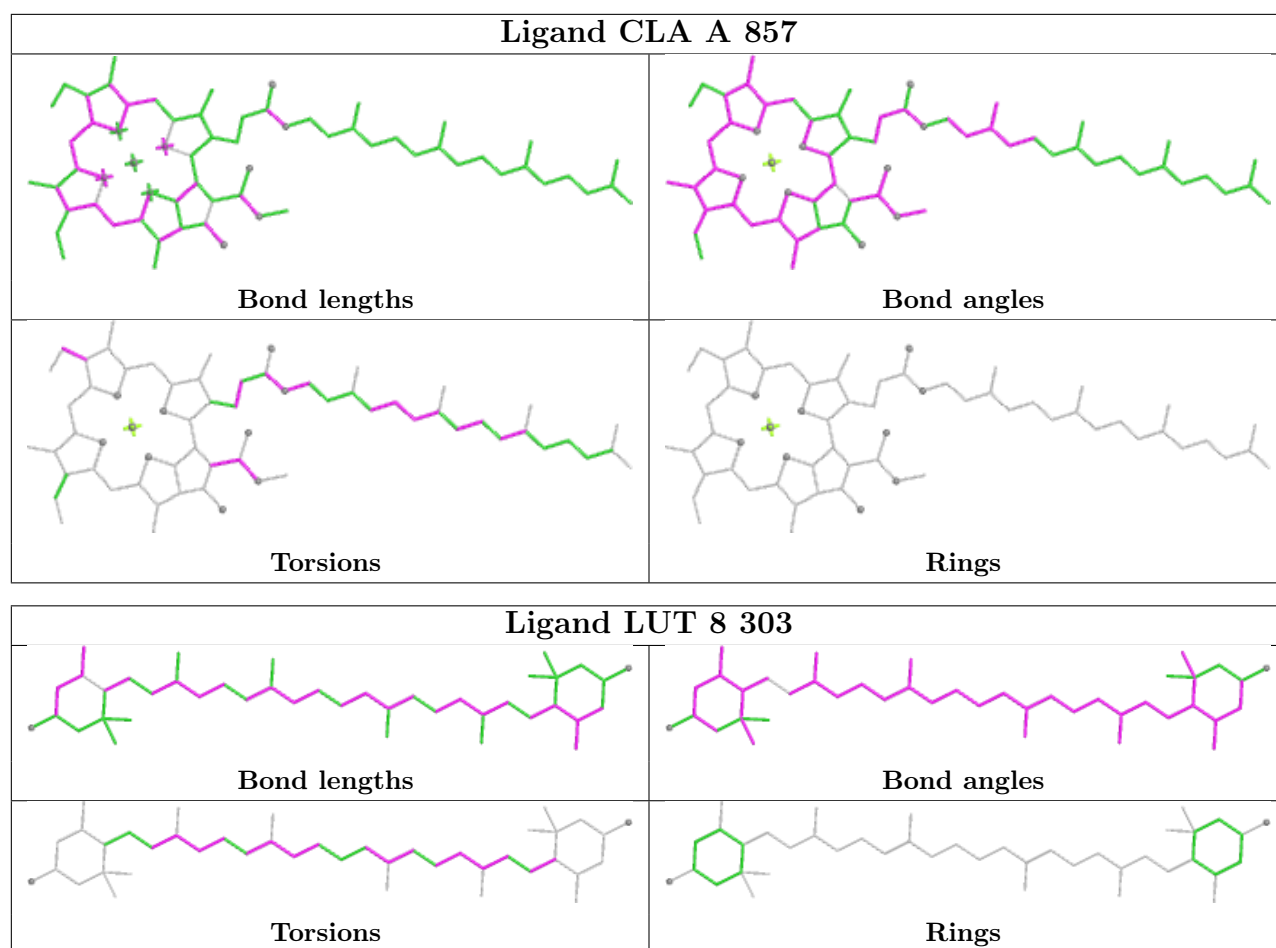
Ligand LMT 5 301



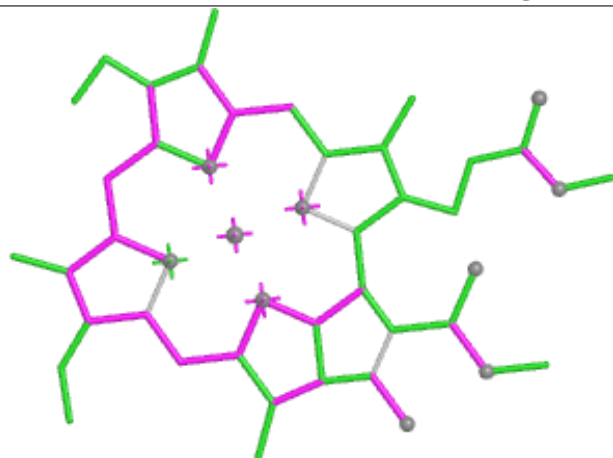




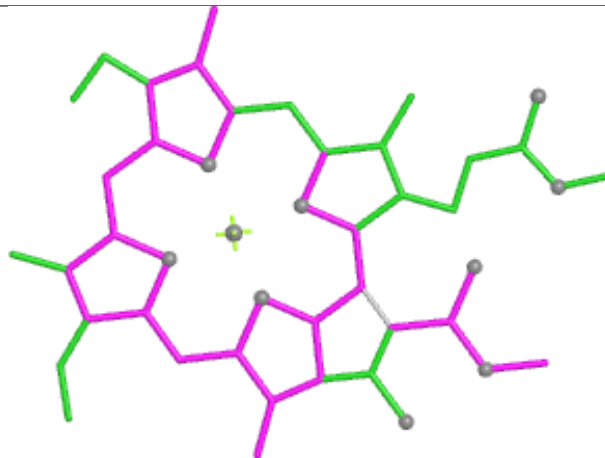
Ligand LUT 5 304**Ligand CLA 8 321**



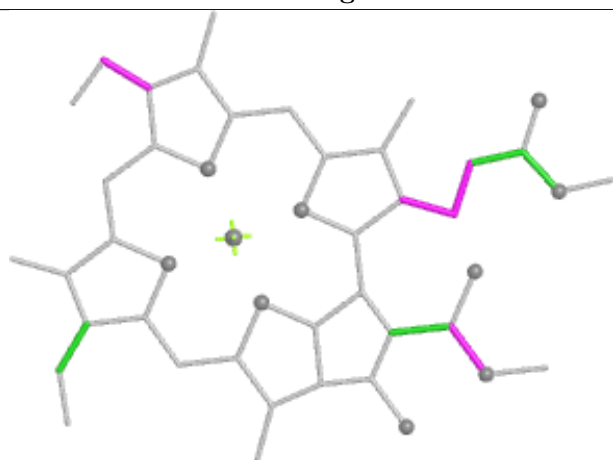
Ligand CLA b 306



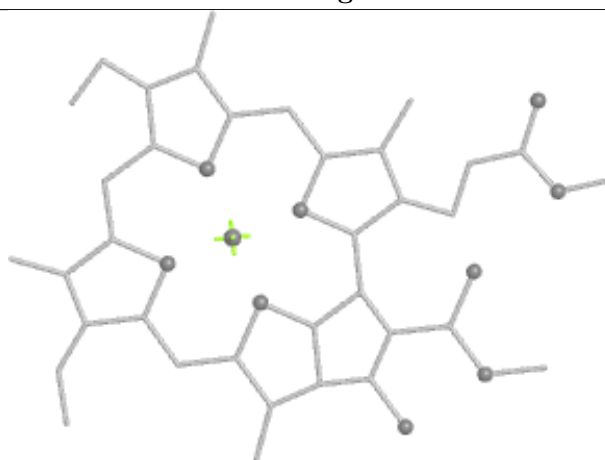
Bond lengths



Bond angles

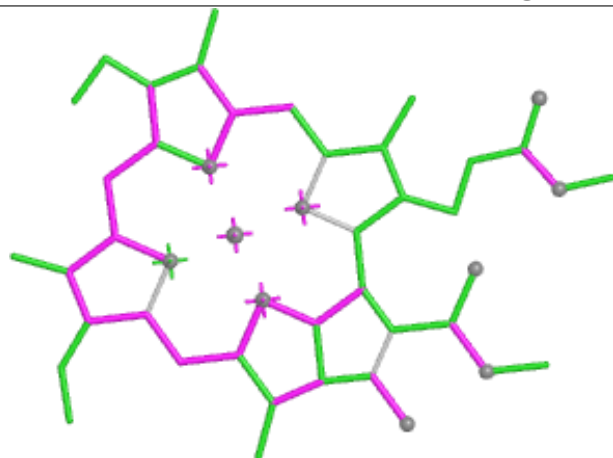


Torsions

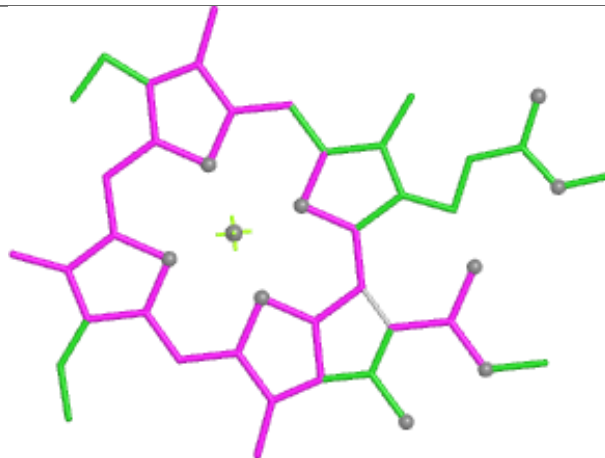


Rings

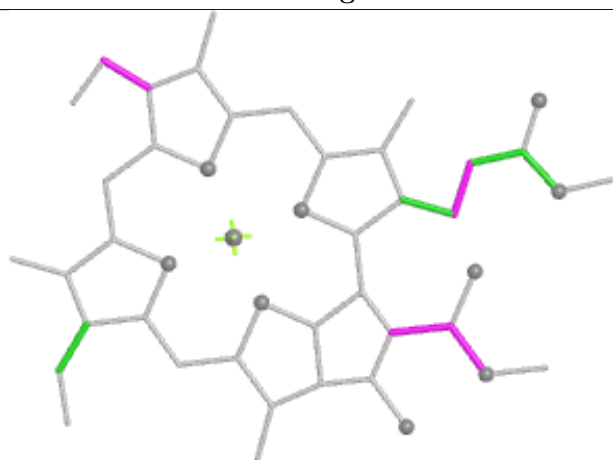
Ligand CLA 2 312



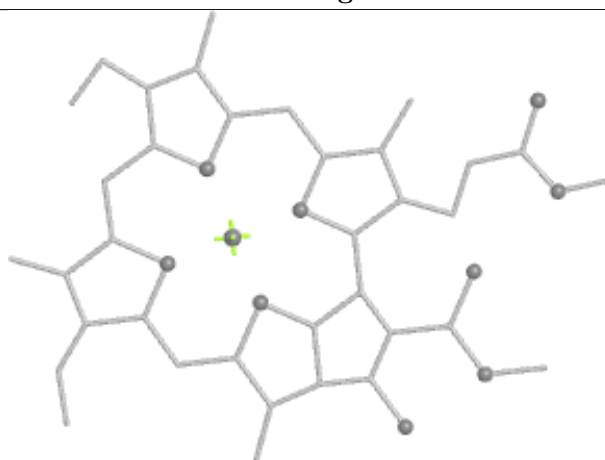
Bond lengths



Bond angles

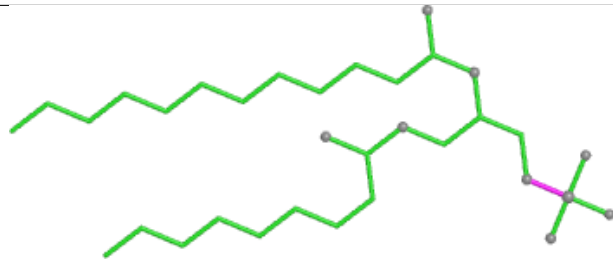


Torsions

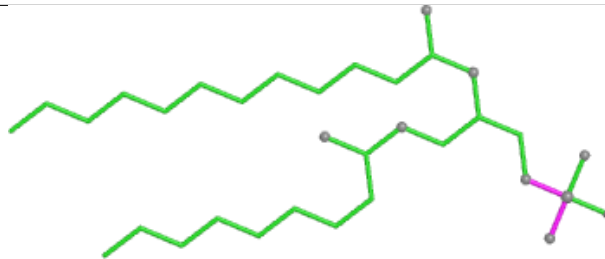


Rings

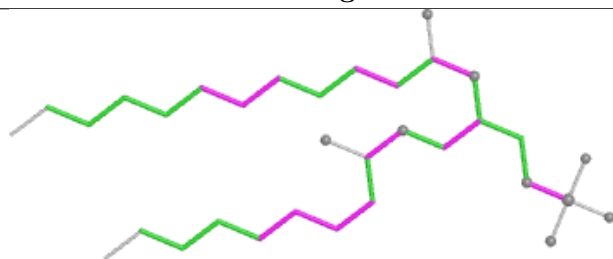
Ligand 3PH 7 301



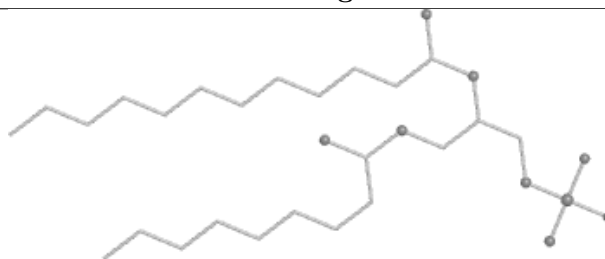
Bond lengths



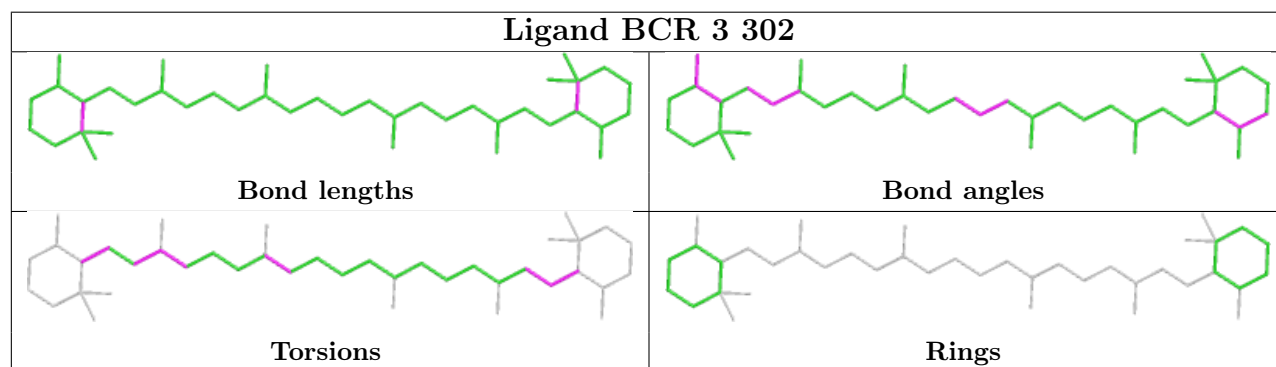
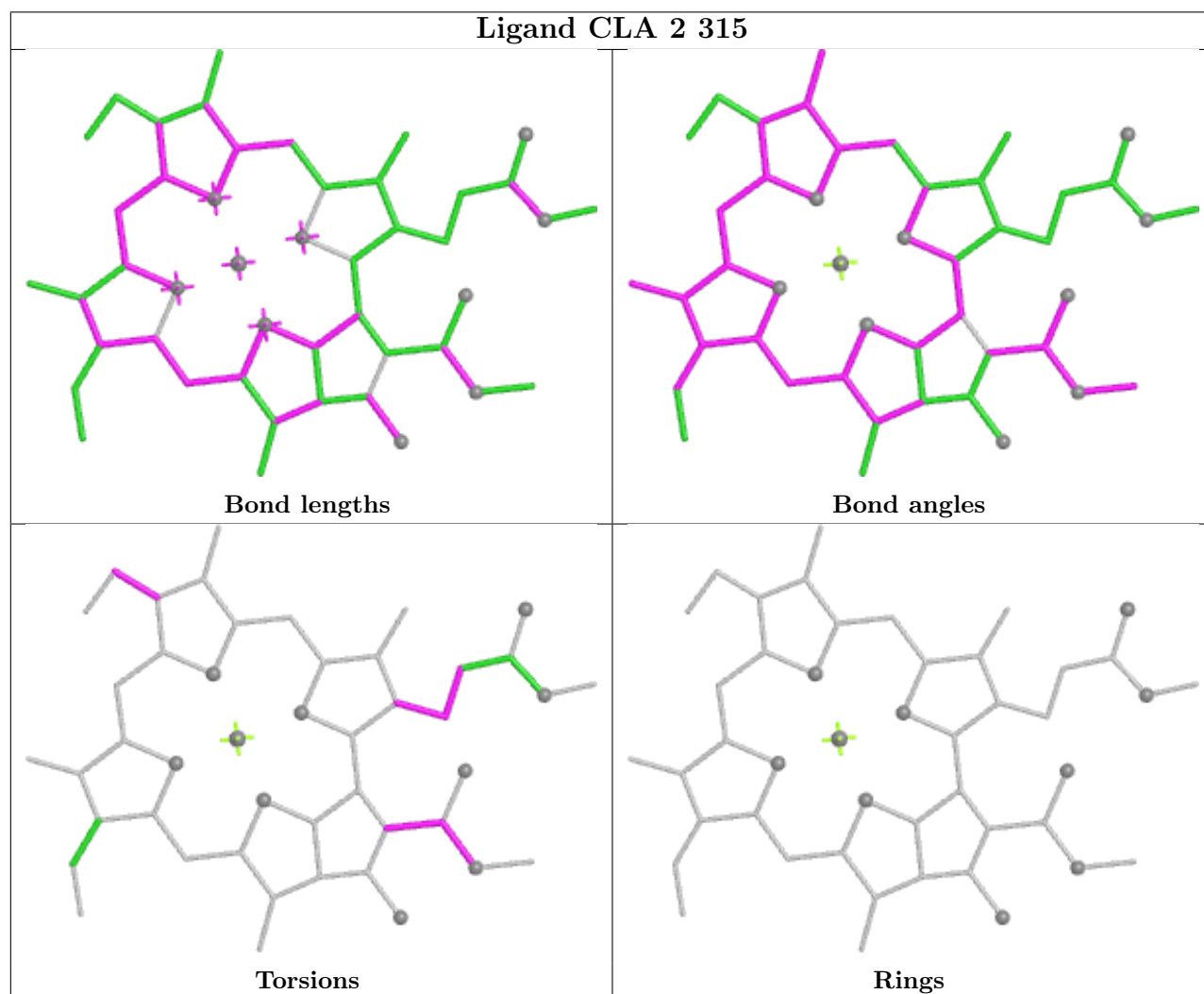
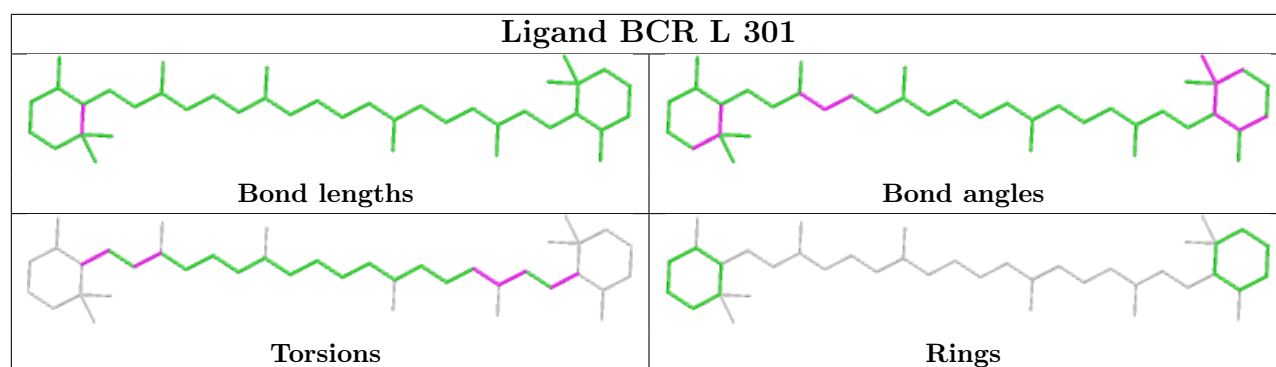
Bond angles

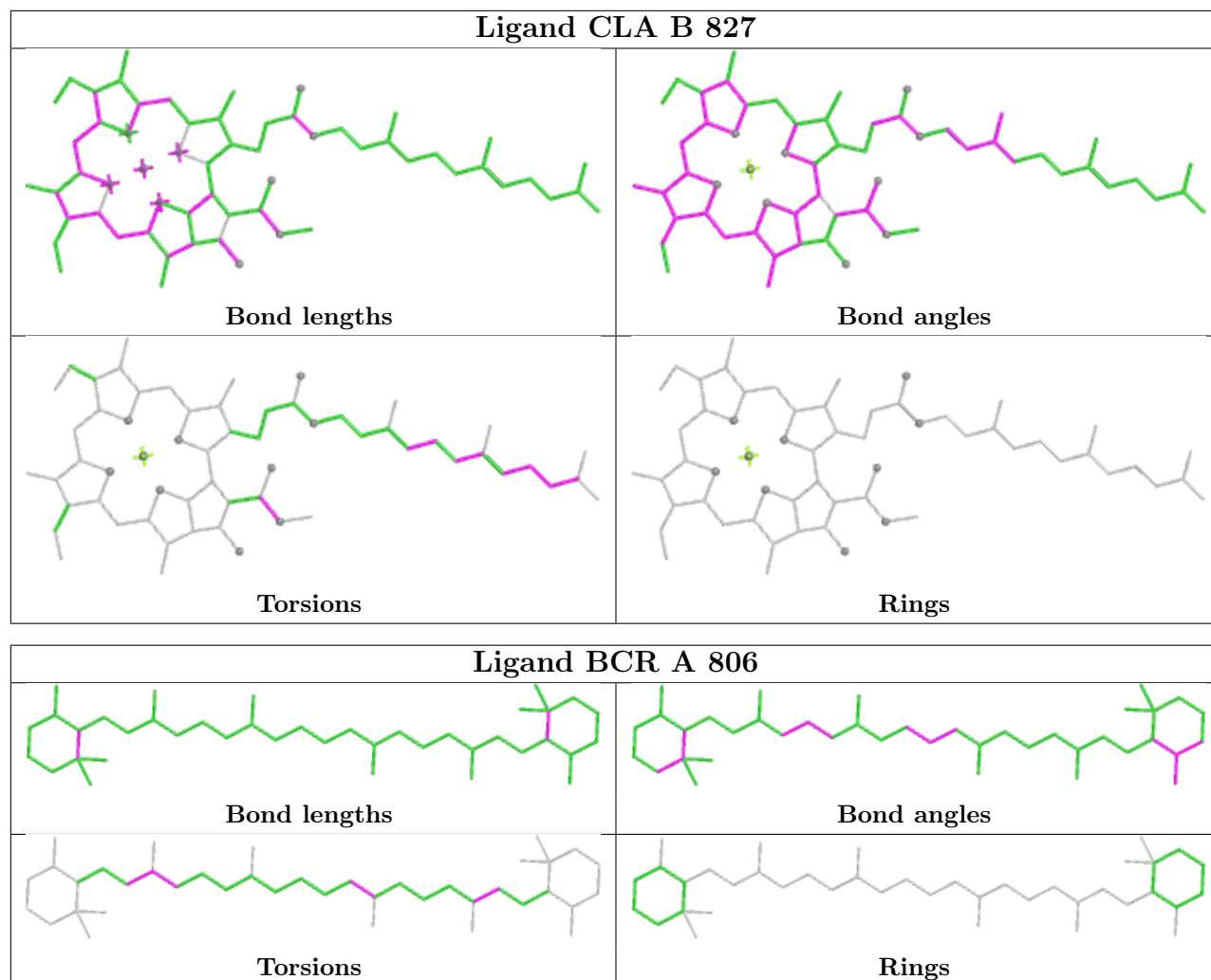


Torsions

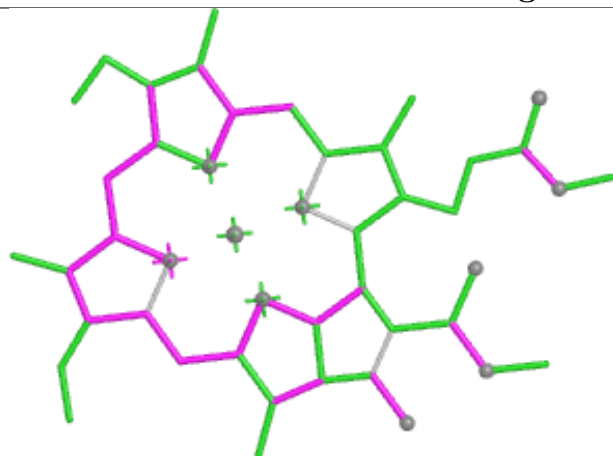


Rings

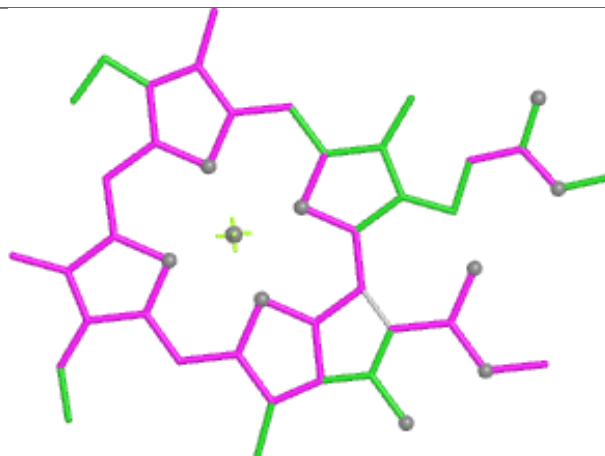




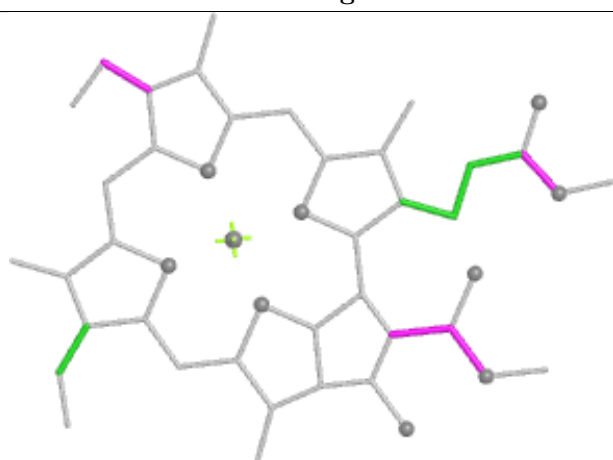
Ligand CLA 5 321



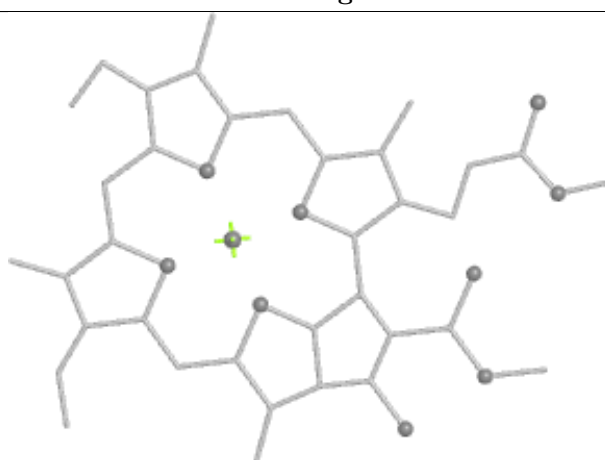
Bond lengths



Bond angles

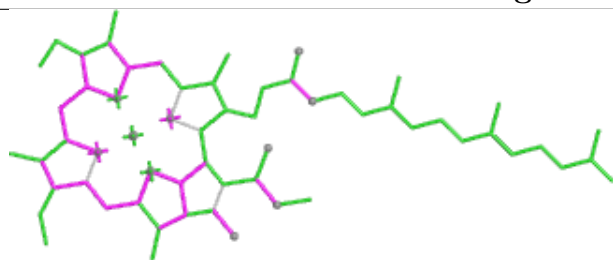


Torsions

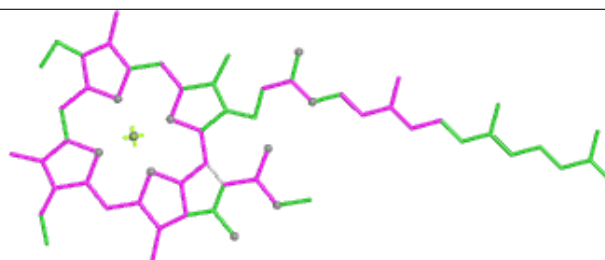


Rings

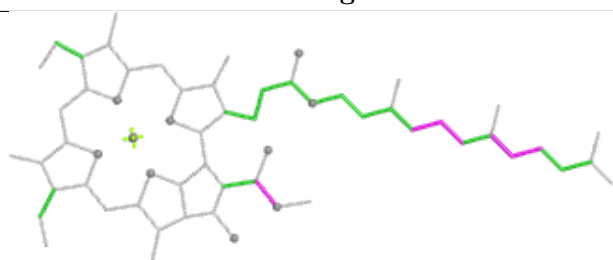
Ligand CLA B 830



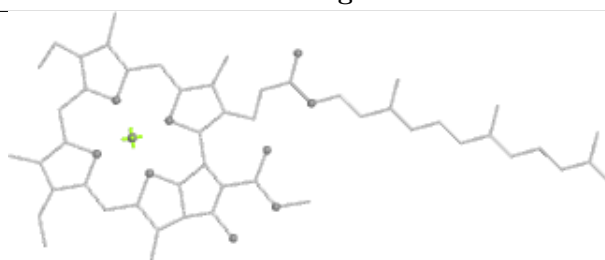
Bond lengths



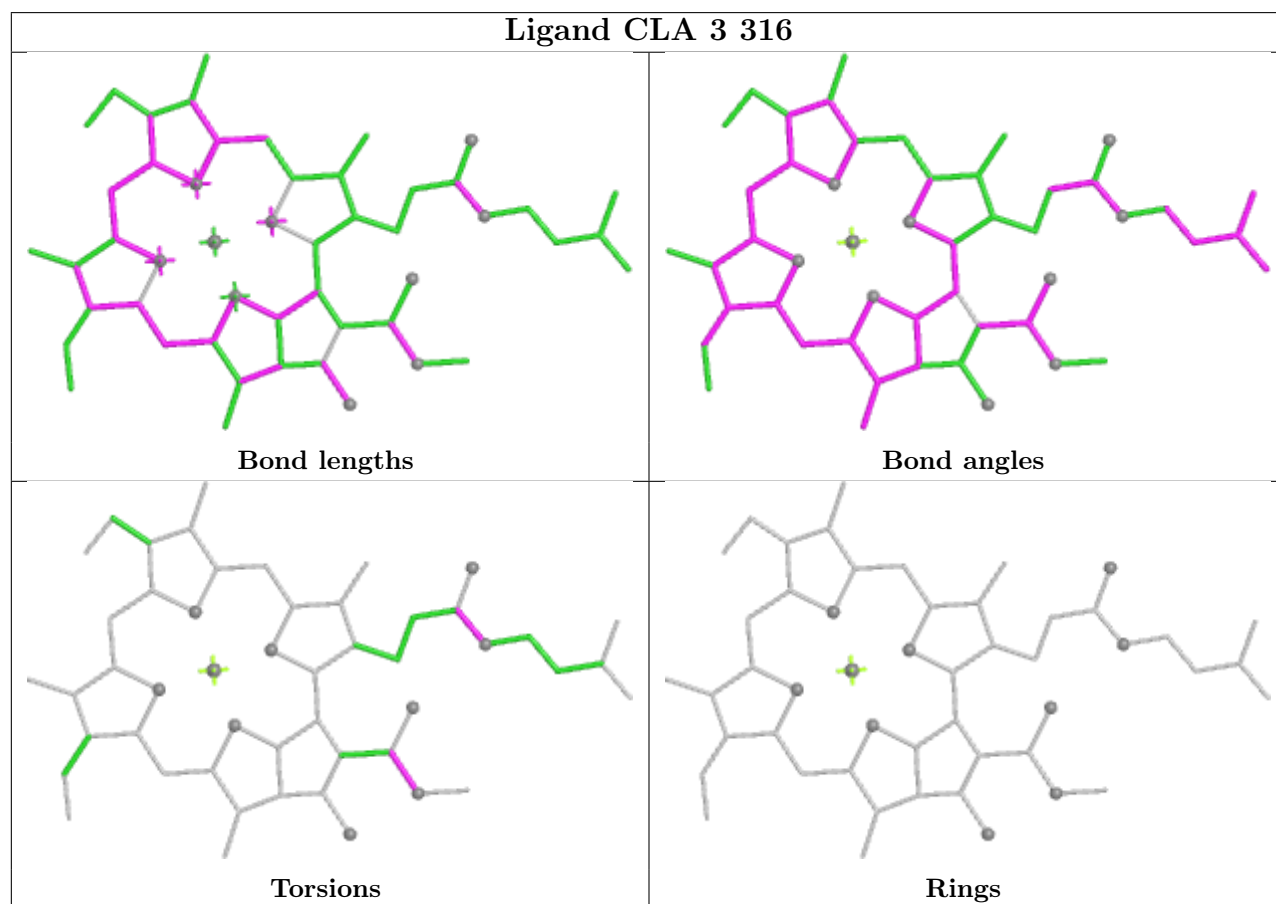
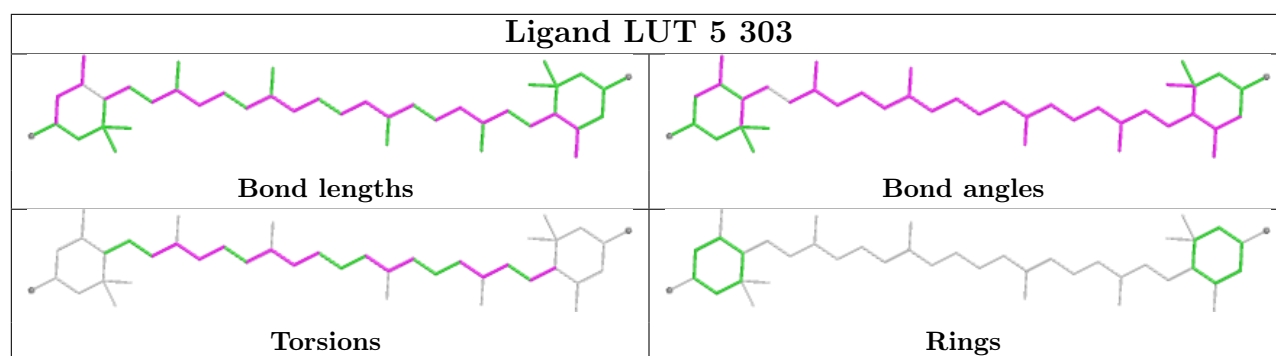
Bond angles



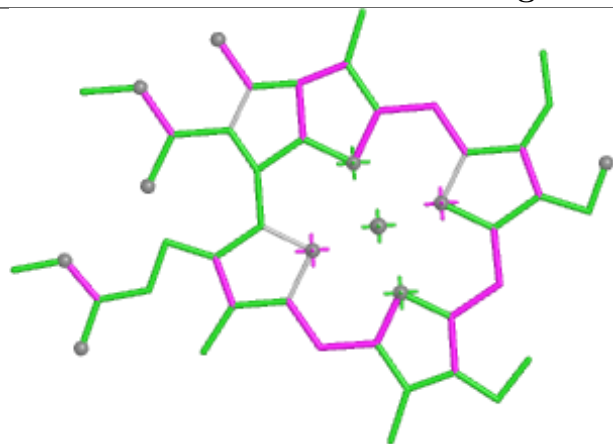
Torsions



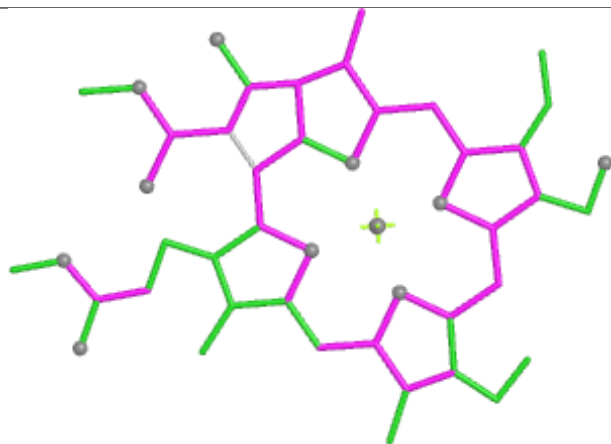
Rings



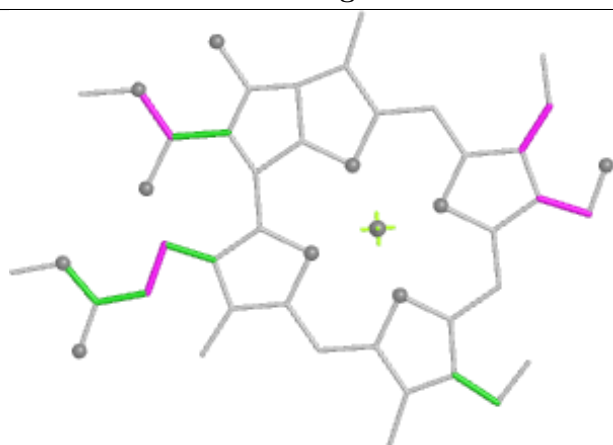
Ligand CHL 5 317



Bond lengths



Bond angles

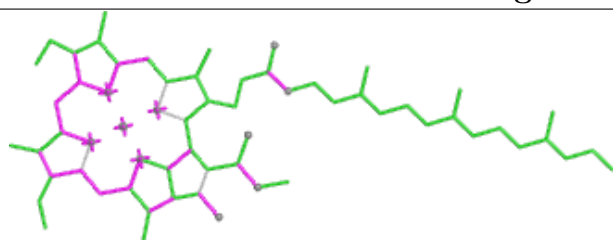


Torsions

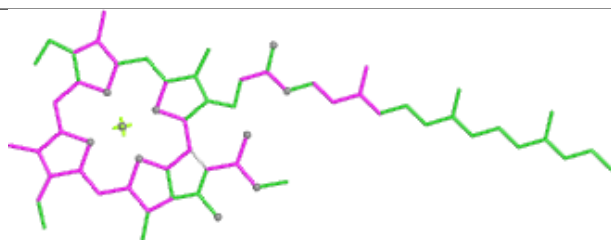


Rings

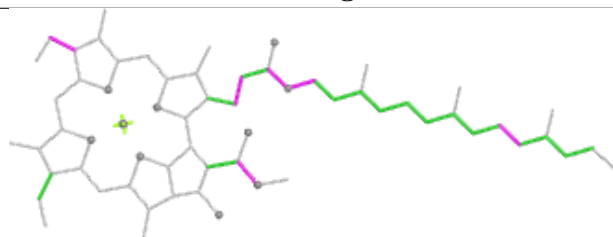
Ligand CLA B 850



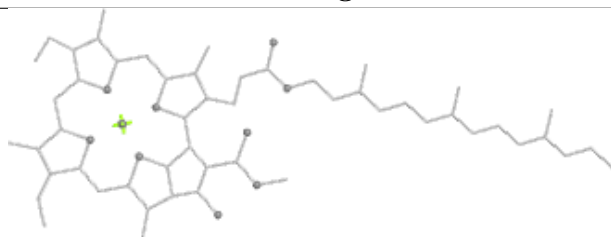
Bond lengths



Bond angles

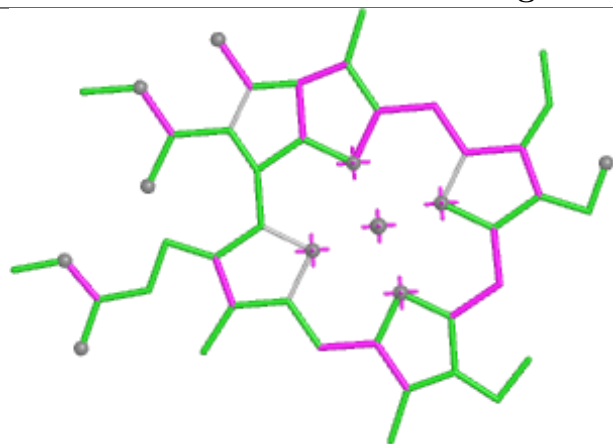


Torsions

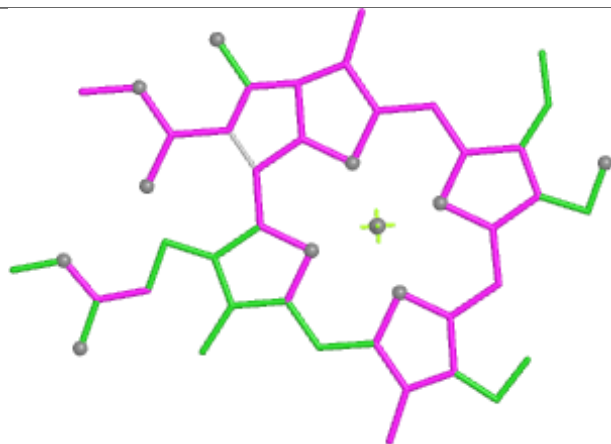


Rings

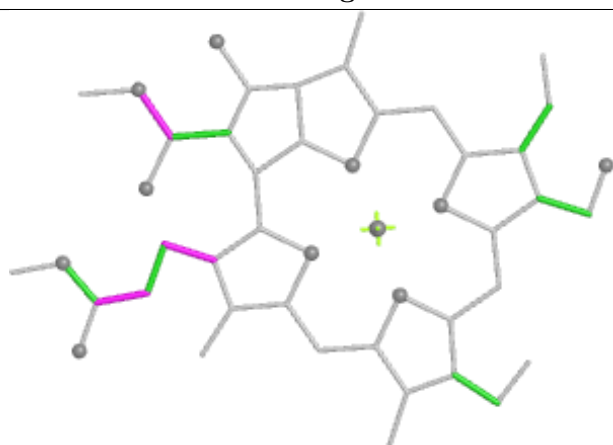
Ligand CHL 5 322



Bond lengths



Bond angles

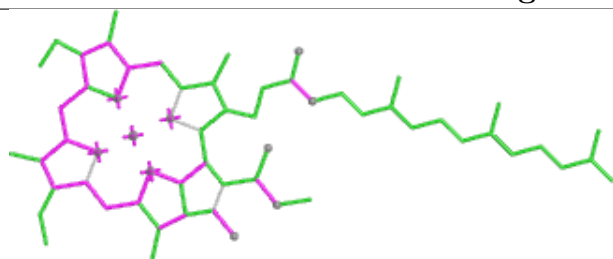


Torsions

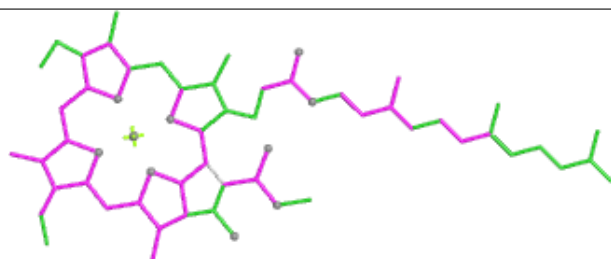


Rings

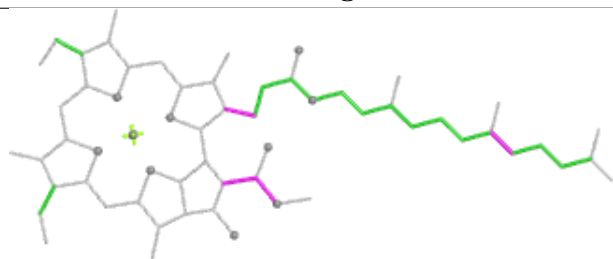
Ligand CLA a 309



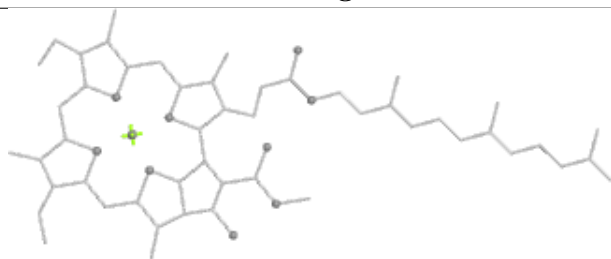
Bond lengths



Bond angles

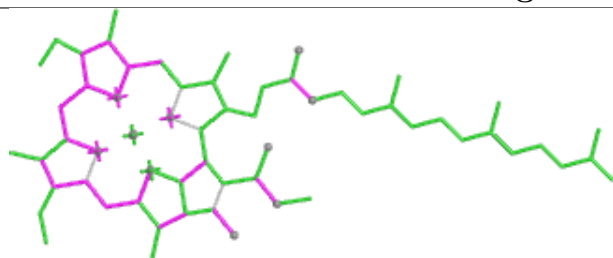


Torsions

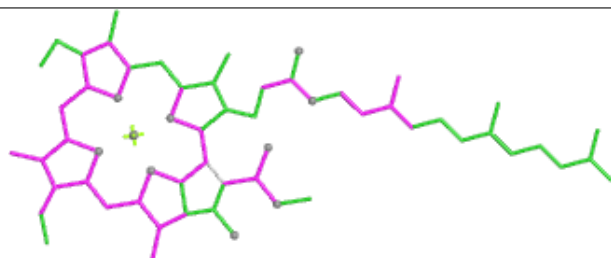


Rings

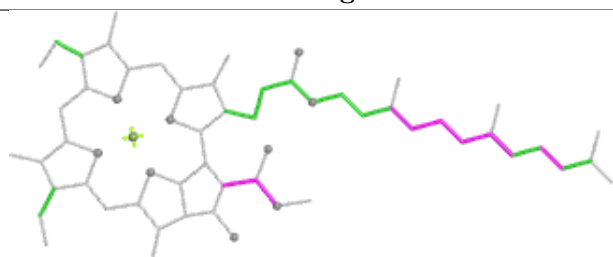
Ligand CLA L 305



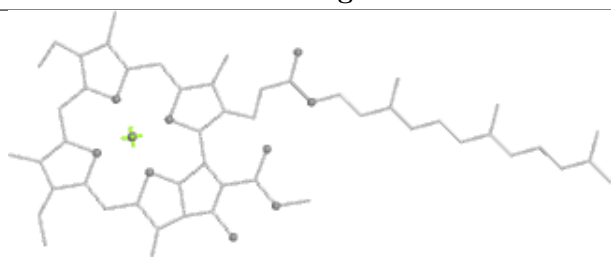
Bond lengths



Bond angles

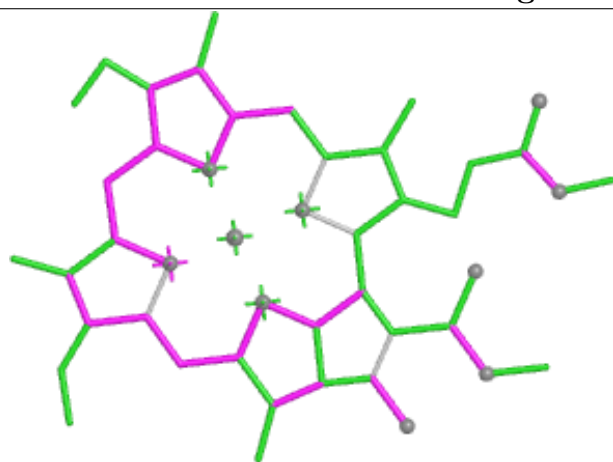


Torsions

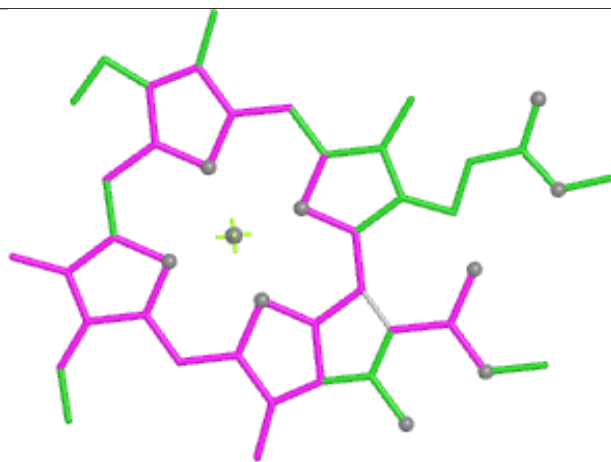


Rings

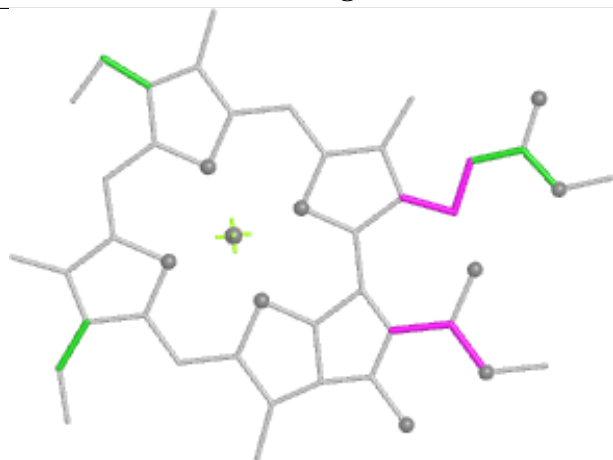
Ligand CLA b 310



Bond lengths



Bond angles

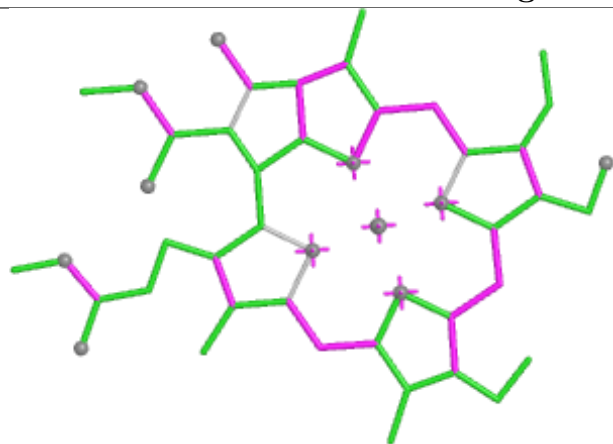


Torsions

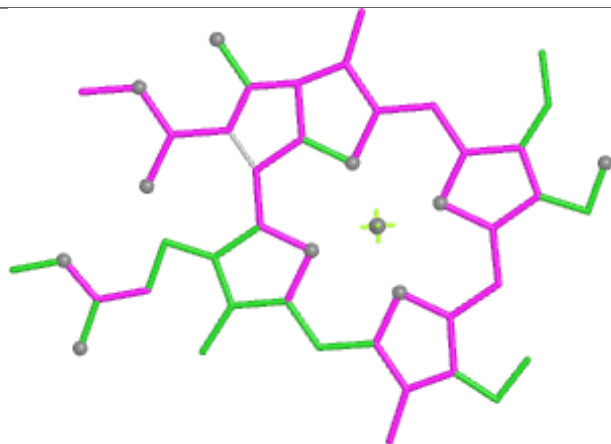


Rings

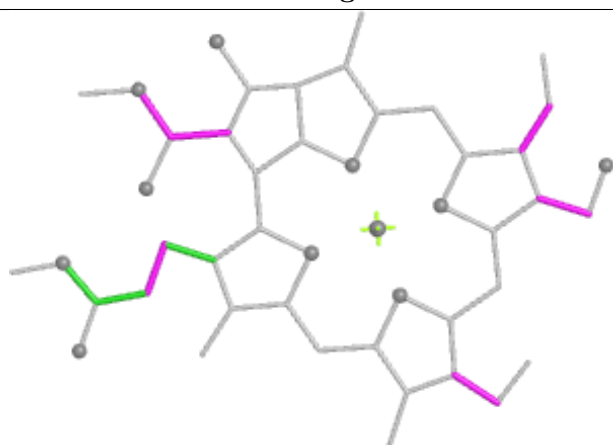
Ligand CHL 6 320



Bond lengths



Bond angles

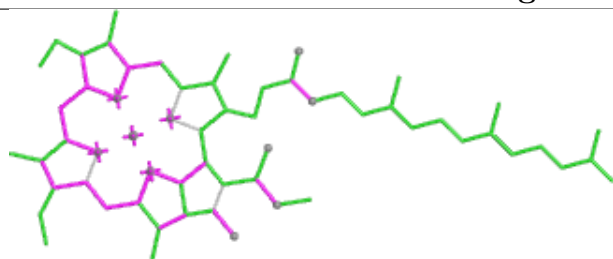


Torsions

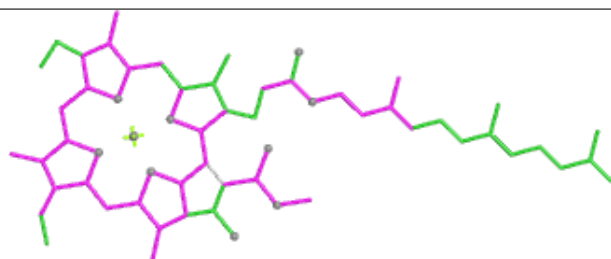


Rings

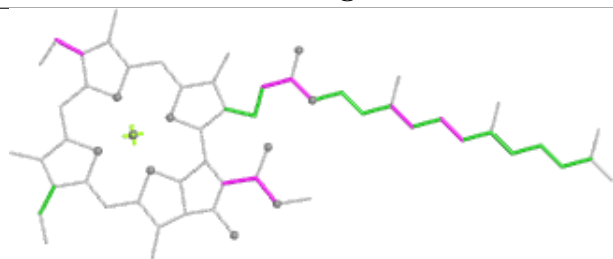
Ligand CLA 4 309



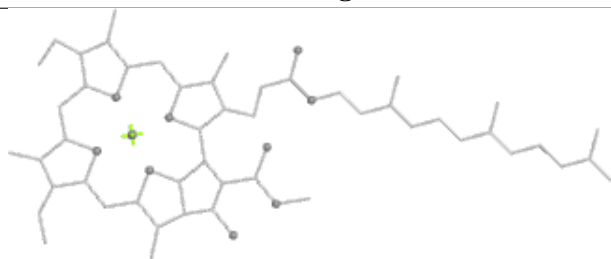
Bond lengths



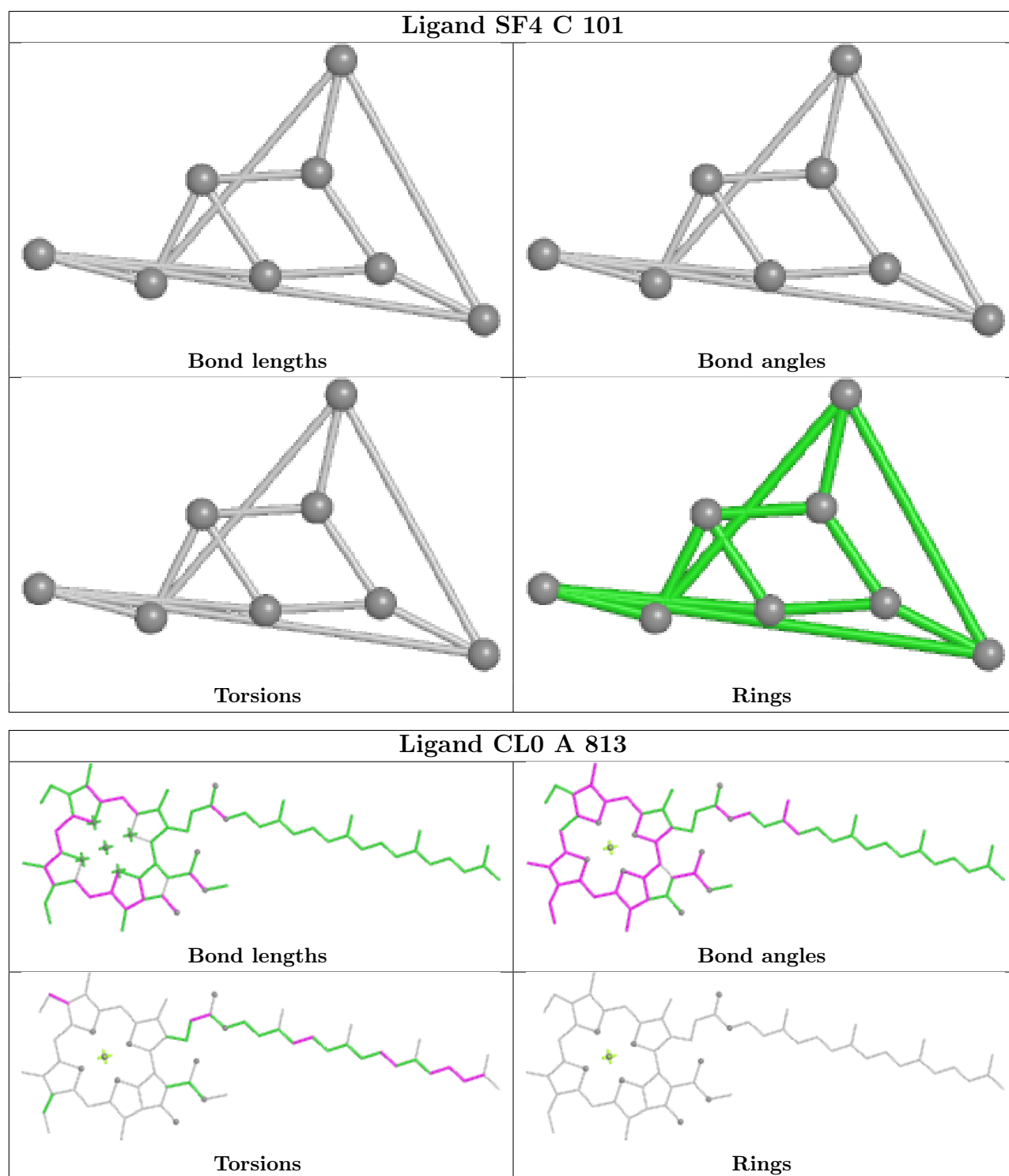
Bond angles



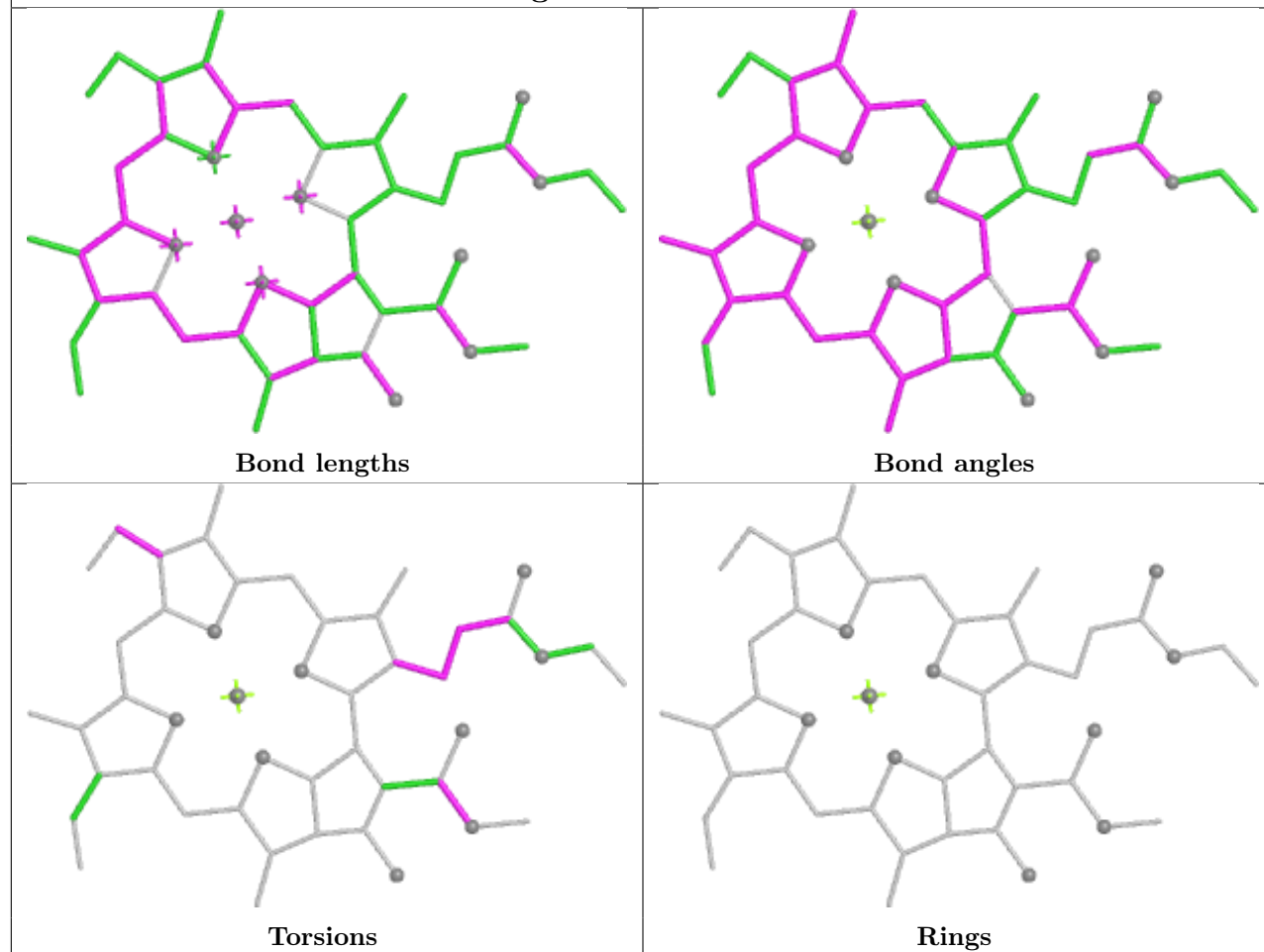
Torsions



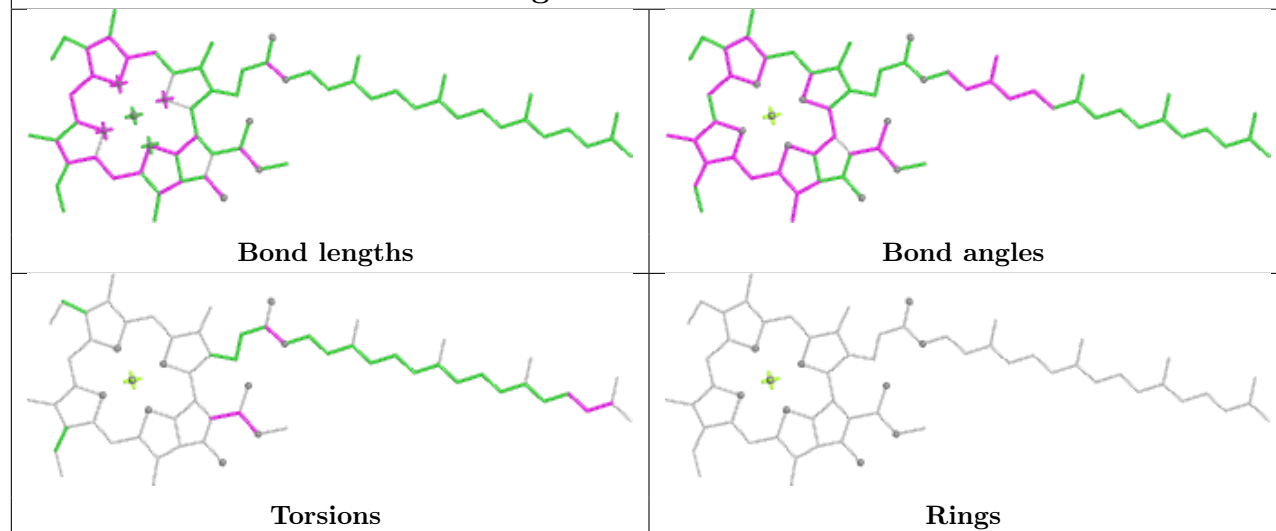
Rings



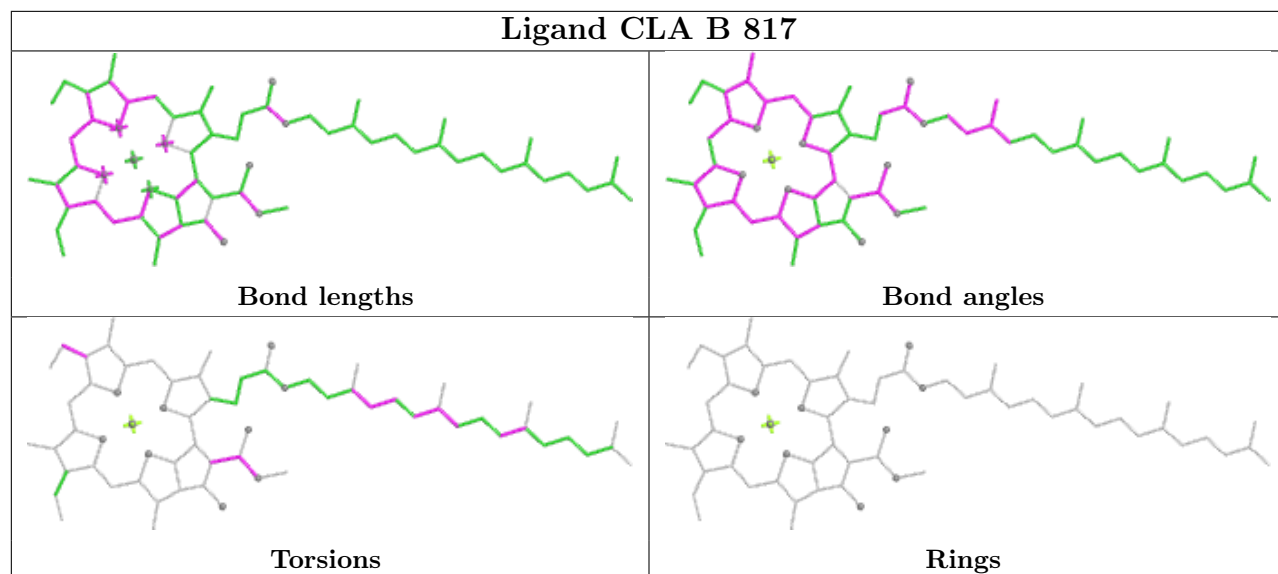
Ligand CLA 4 312



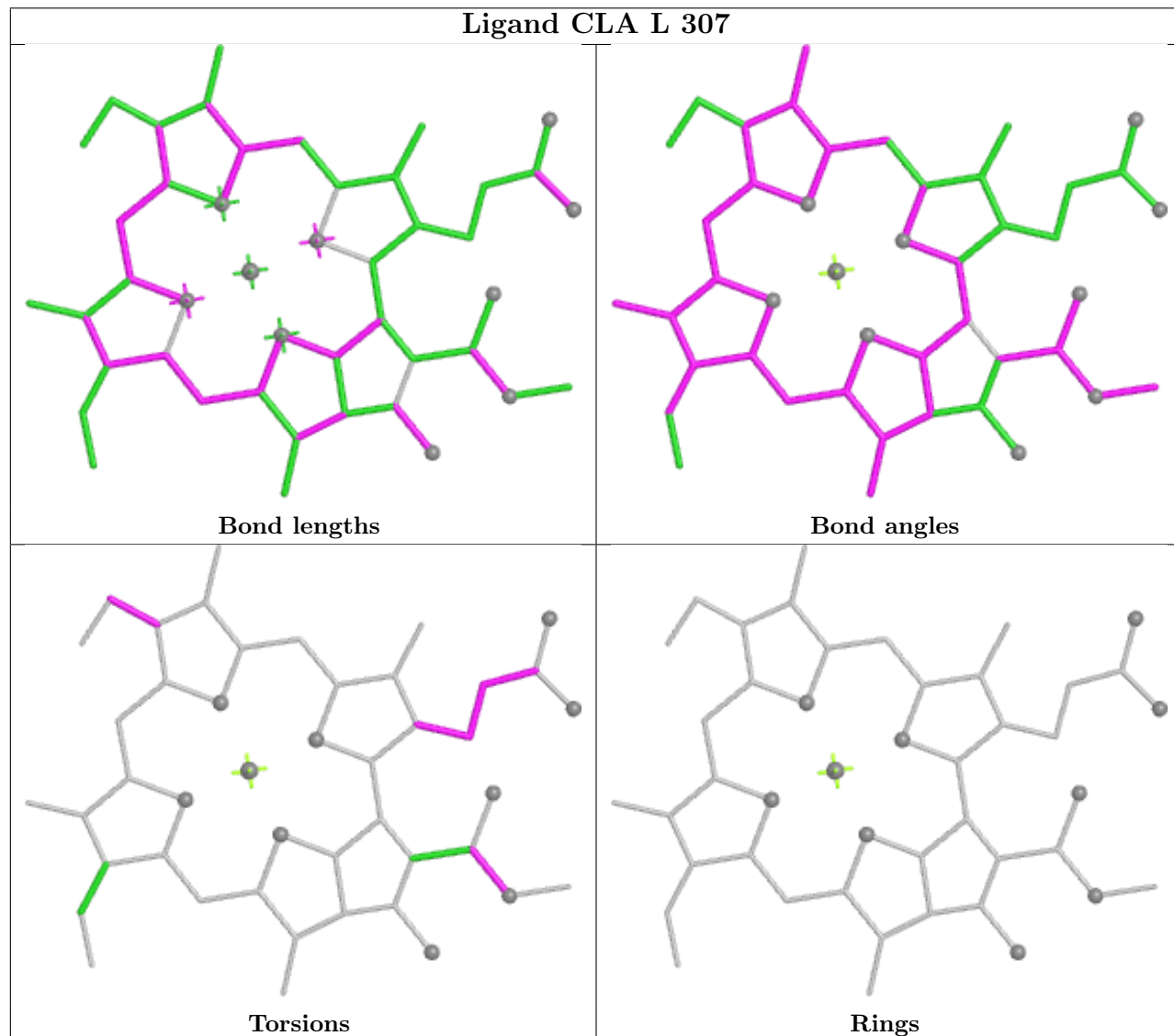
Ligand CLA A 828



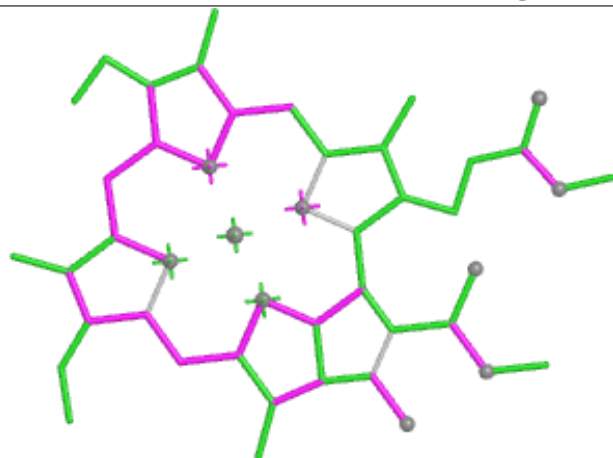
Ligand CLA B 817



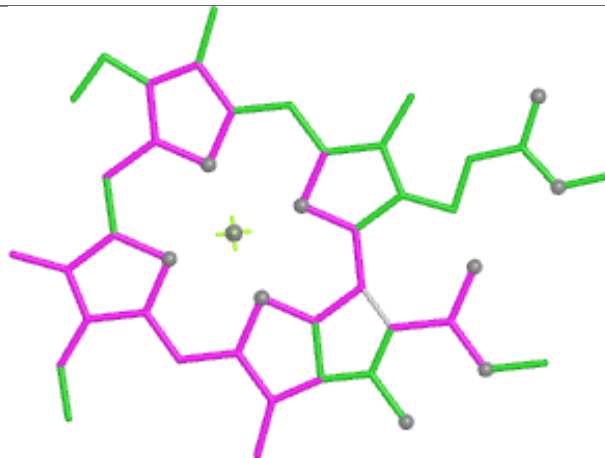
Ligand CLA L 307



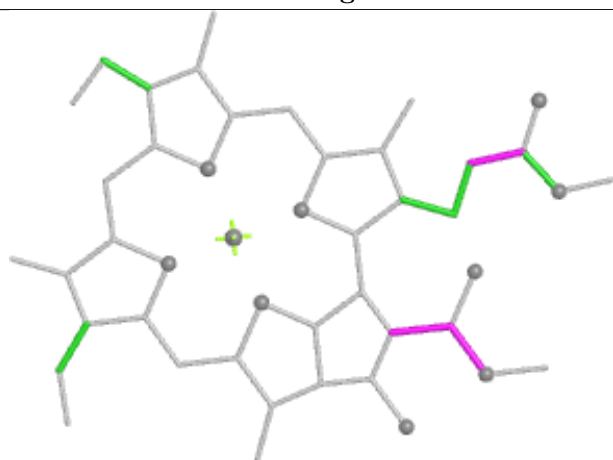
Ligand CLA A 854



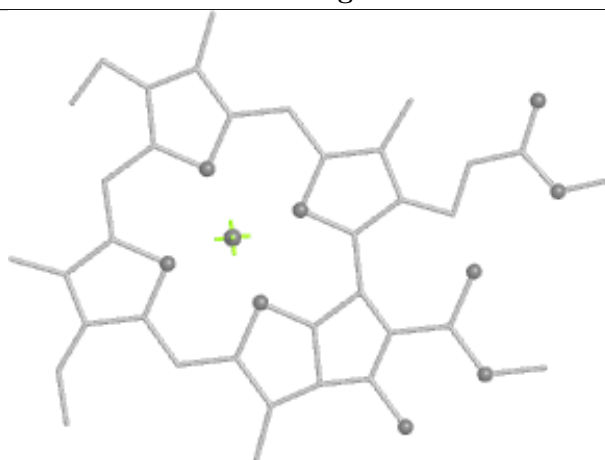
Bond lengths



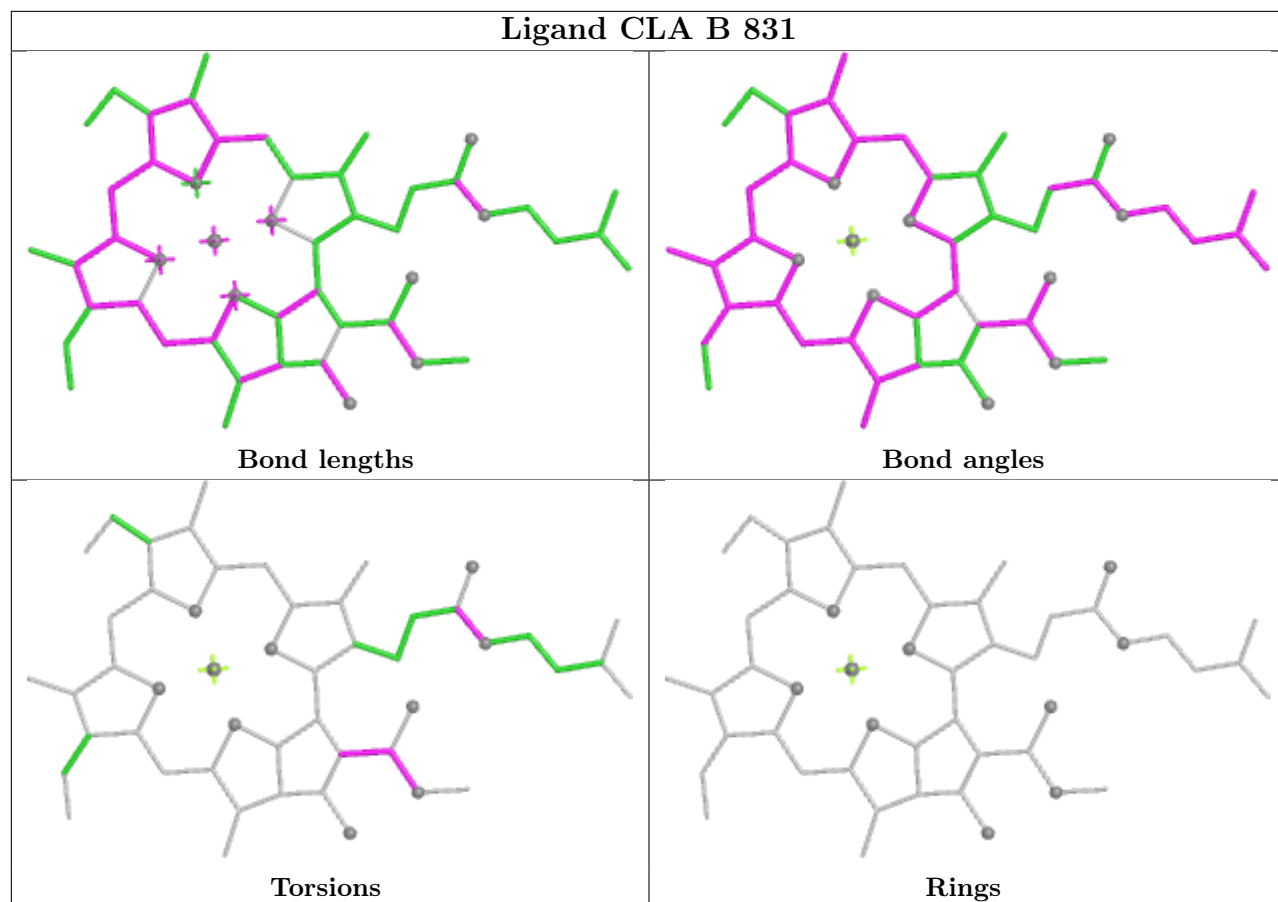
Bond angles

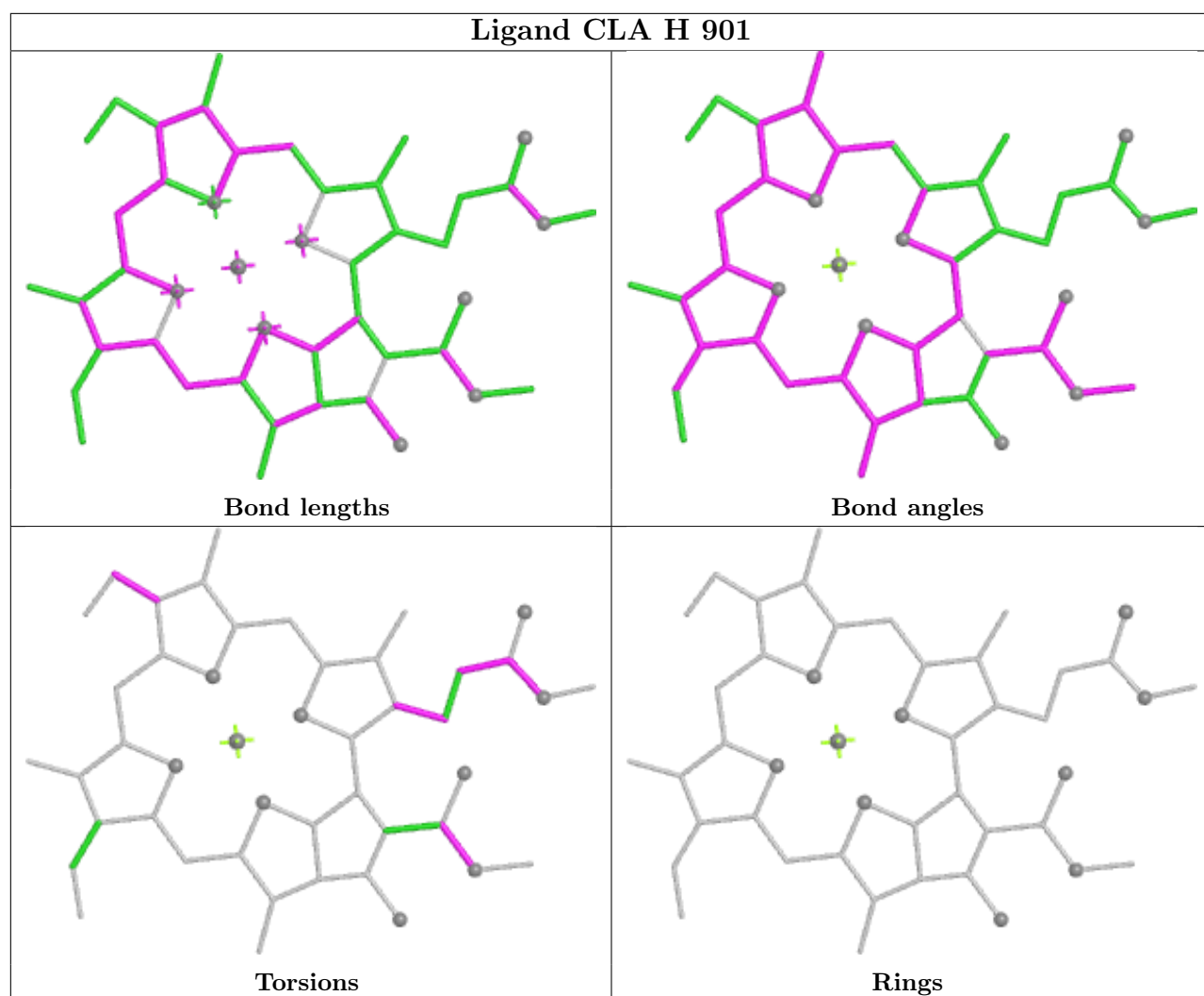


Torsions

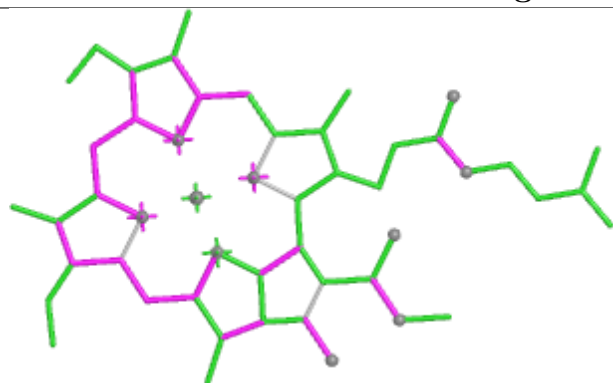


Rings

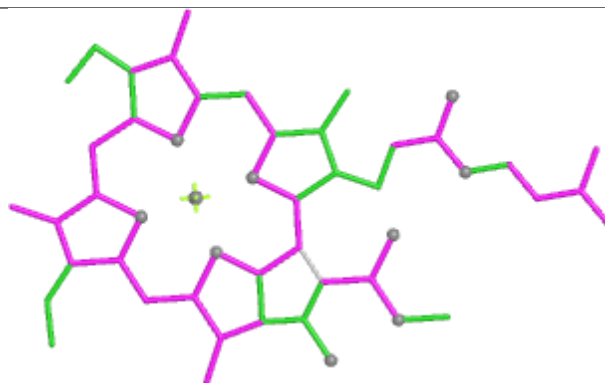




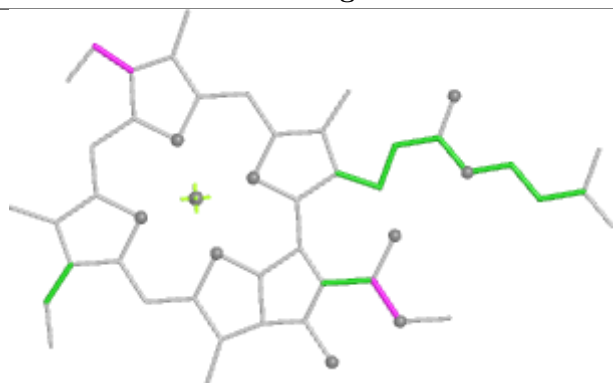
Ligand CLA B 845



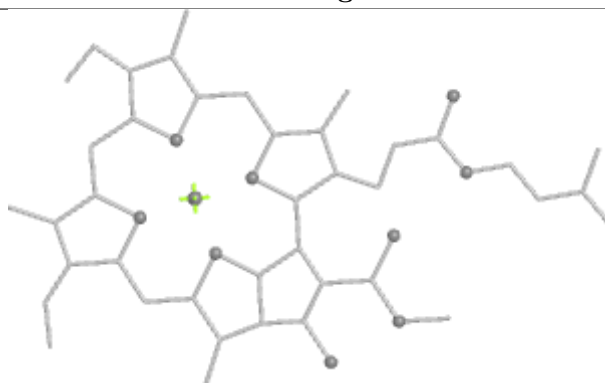
Bond lengths



Bond angles

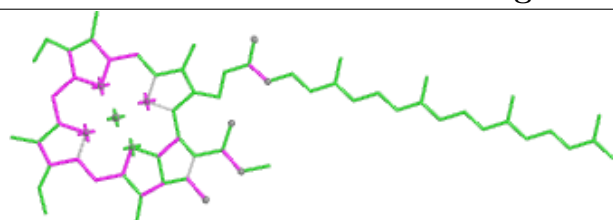


Torsions

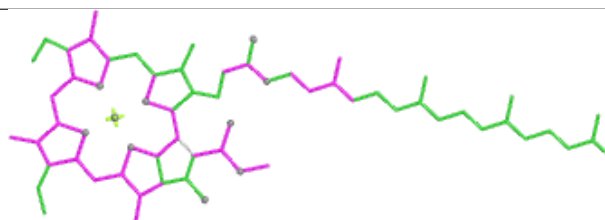


Rings

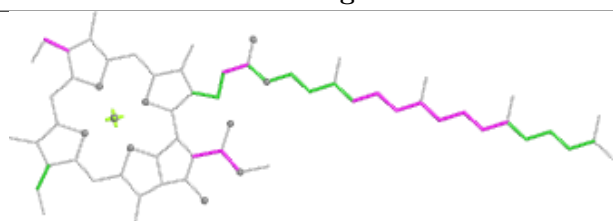
Ligand CLA B 815



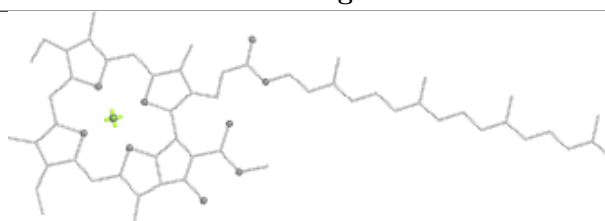
Bond lengths



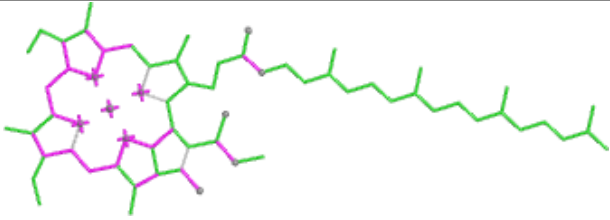
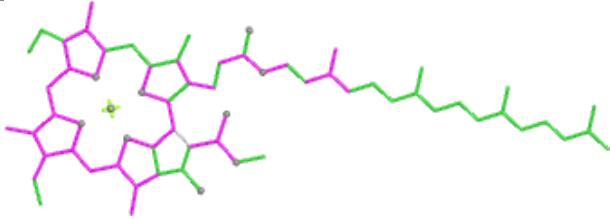
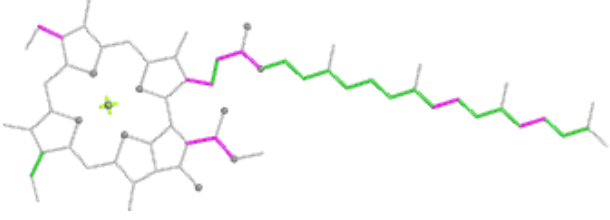
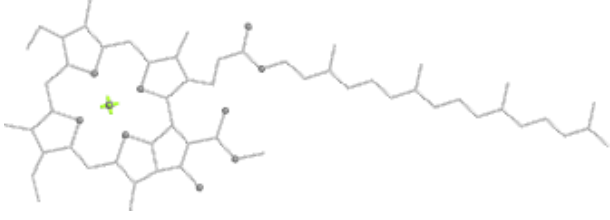
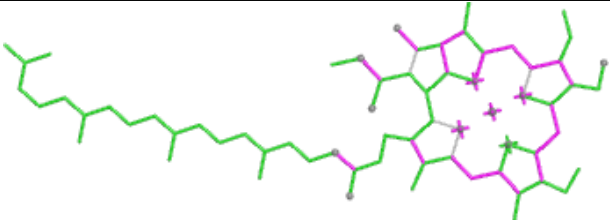
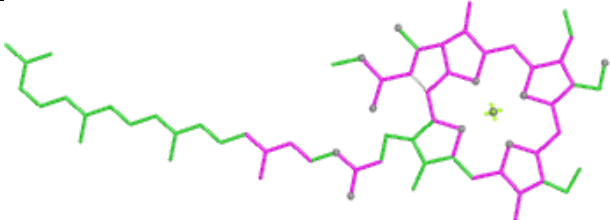
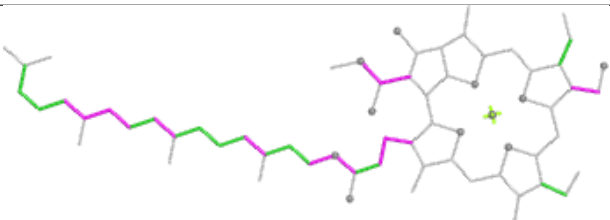
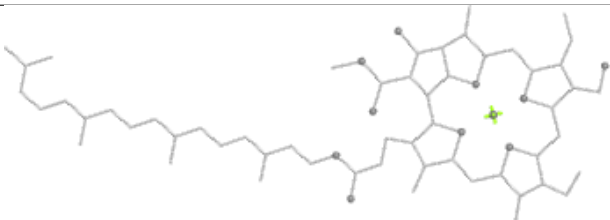
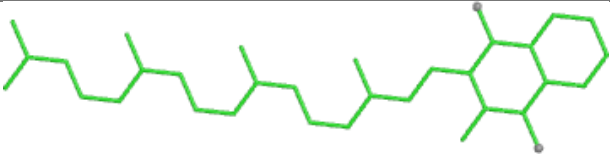
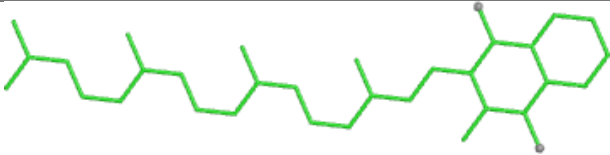
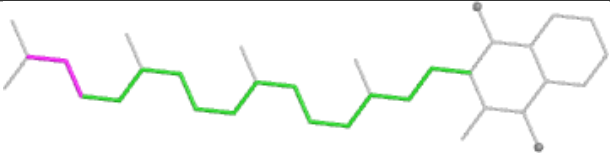
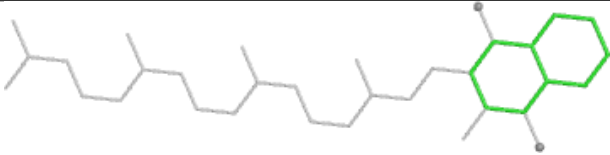
Bond angles



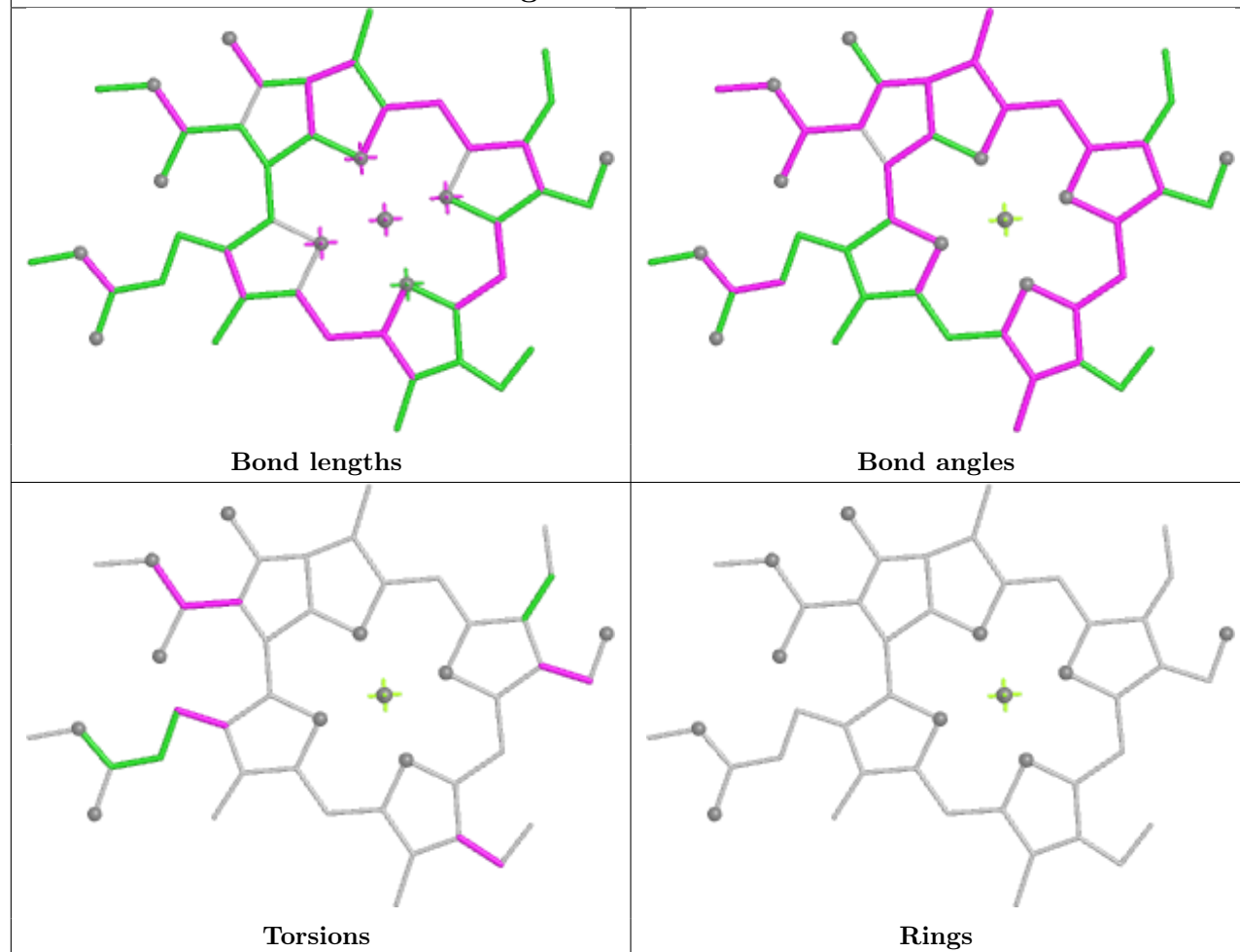
Torsions



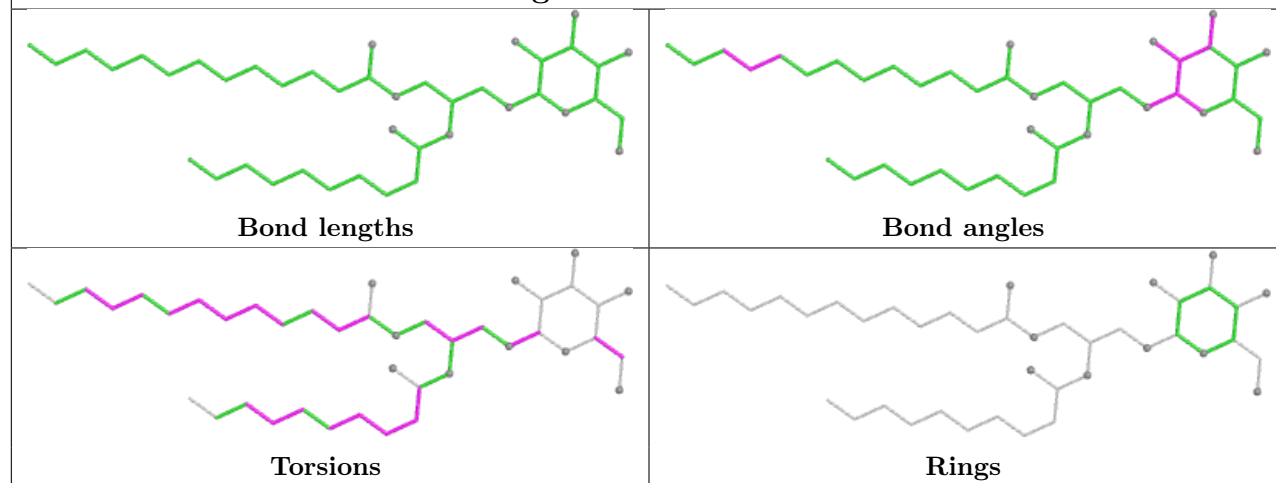
Rings

Ligand CLA 8 320	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CHL 6 309	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PQN A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

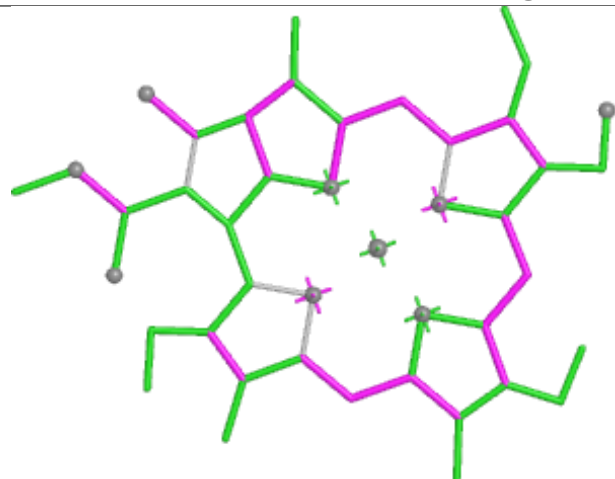
Ligand CHL 6 317



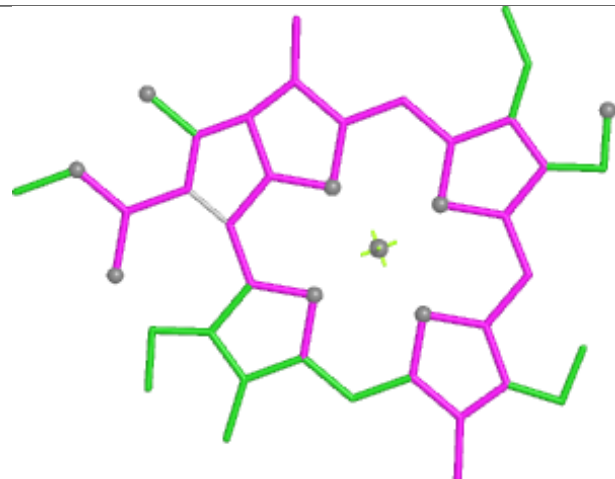
Ligand LMG a 301



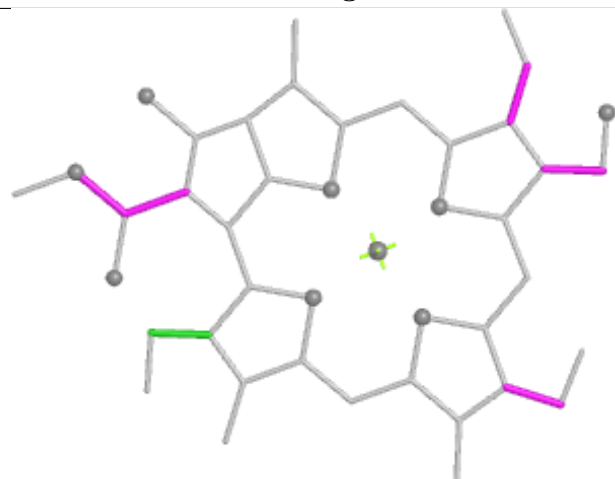
Ligand CHL 6 321



Bond lengths



Bond angles

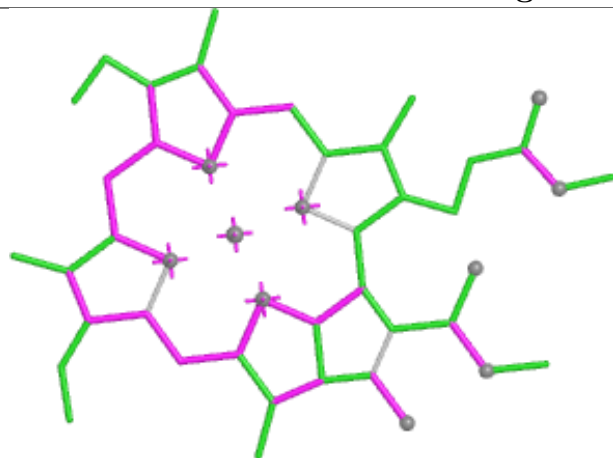


Torsions

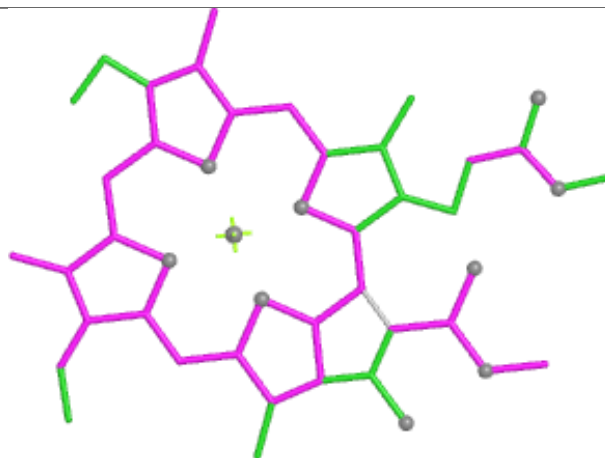


Rings

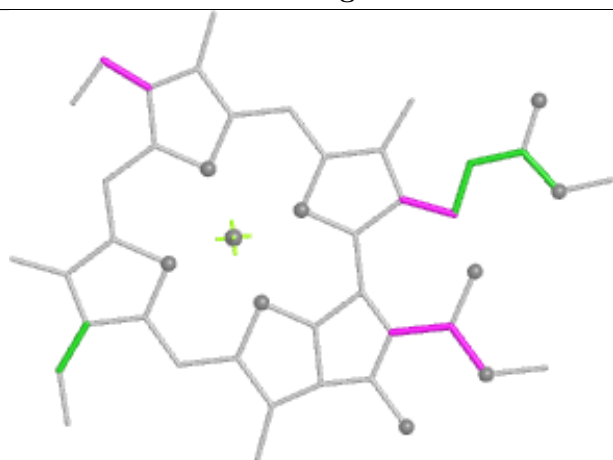
Ligand CLA F 305



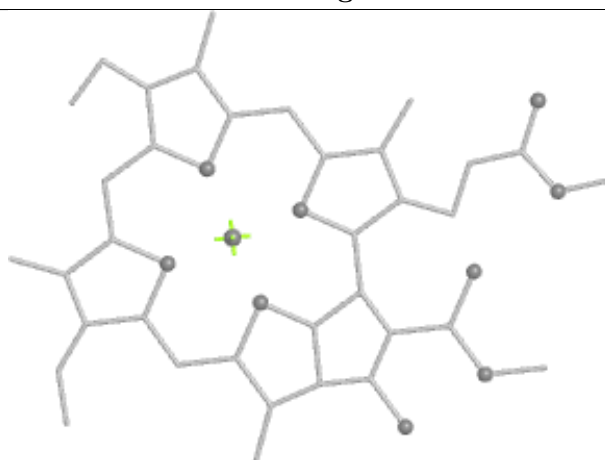
Bond lengths



Bond angles

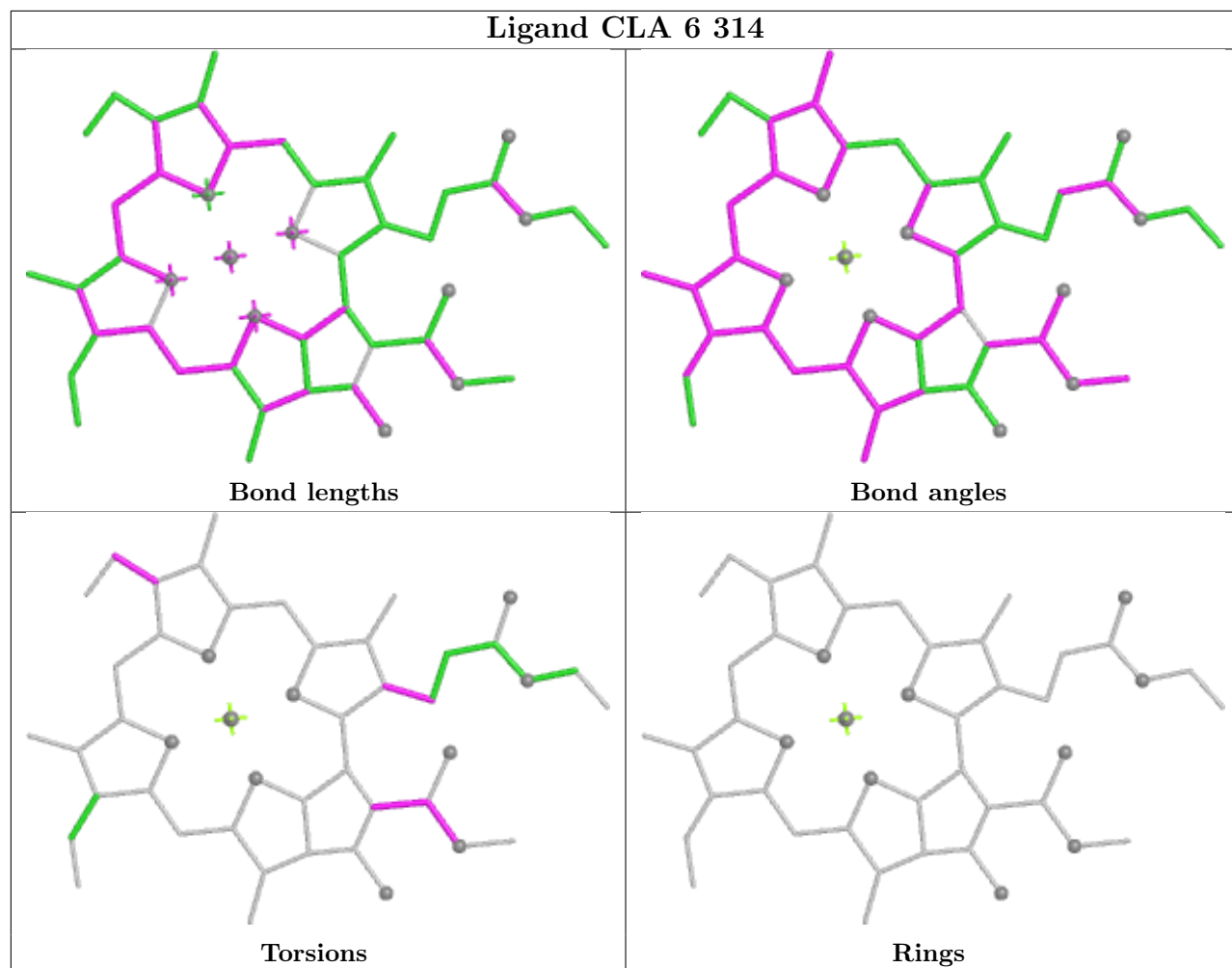


Torsions

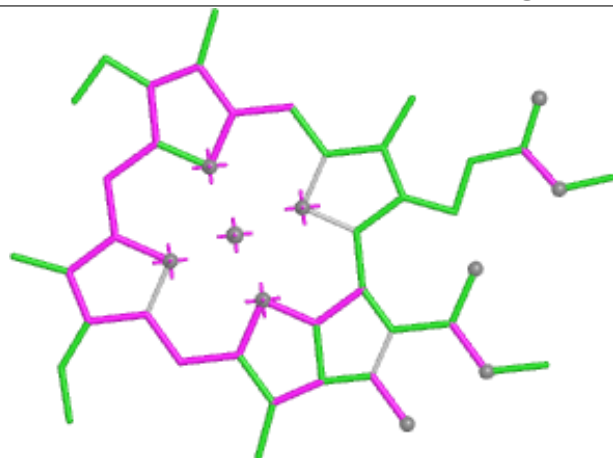


Rings

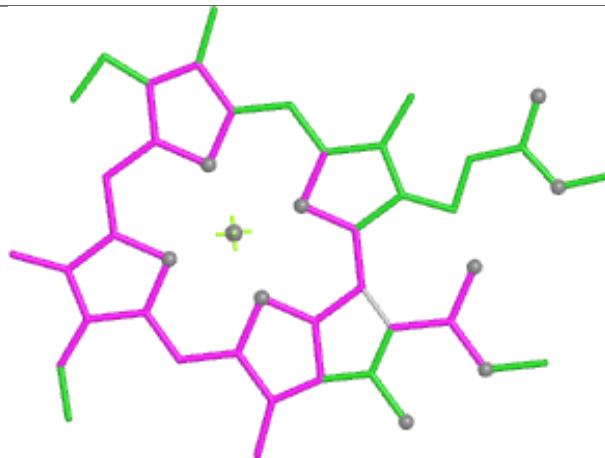
Ligand CLA 6 314



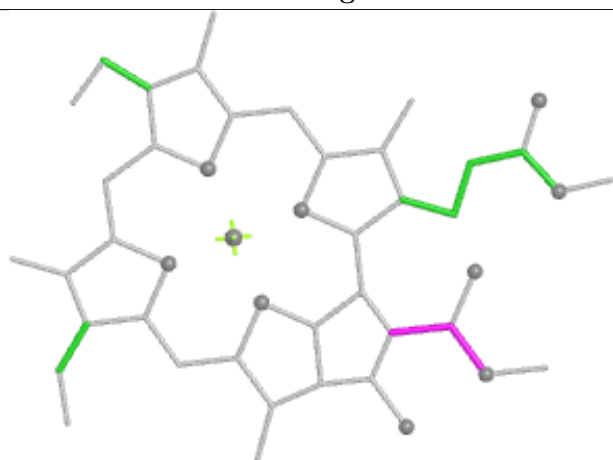
Ligand CLA 6 315



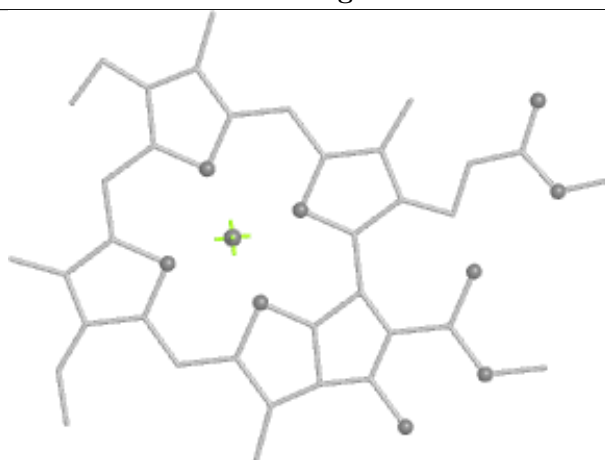
Bond lengths



Bond angles

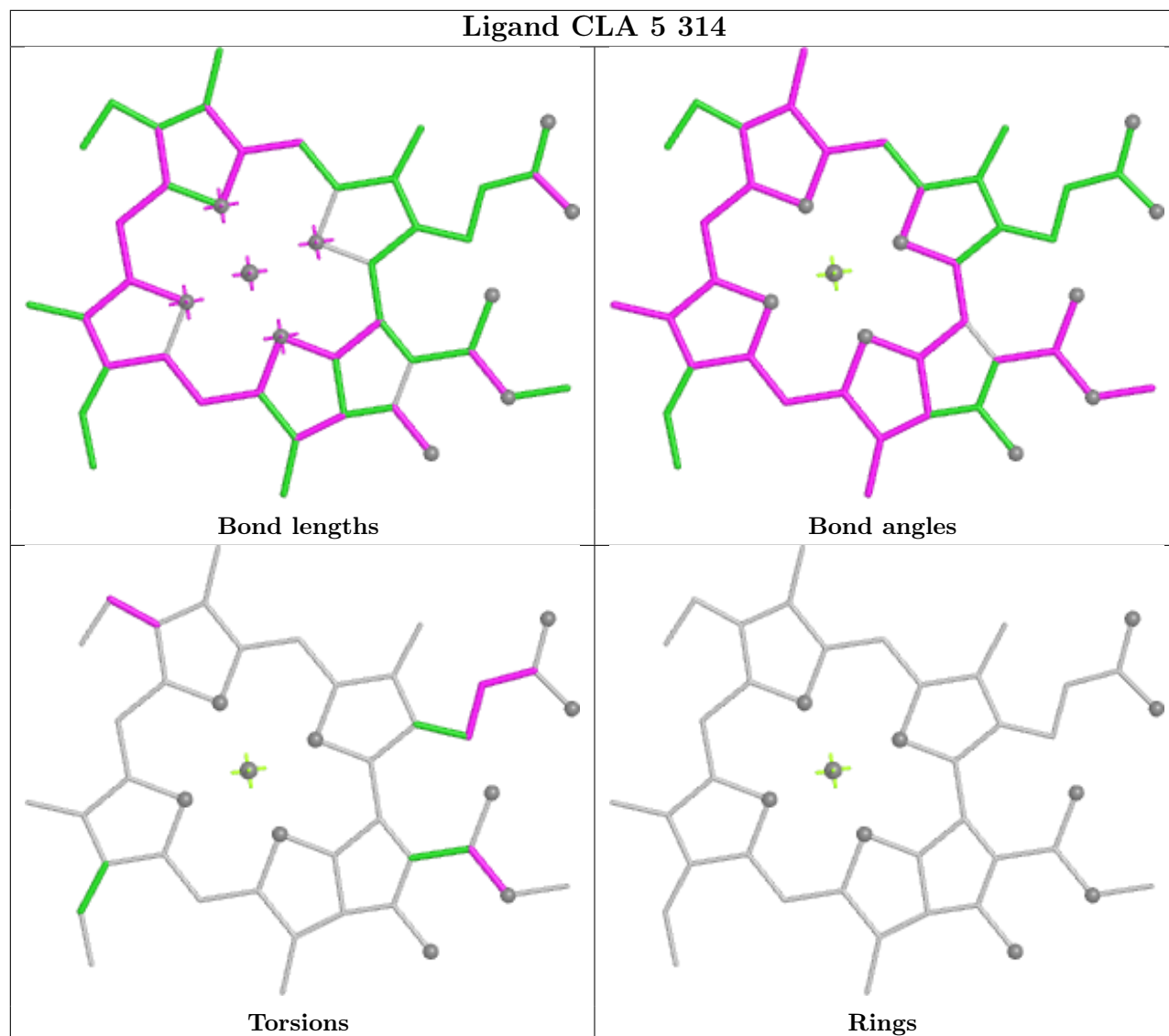


Torsions

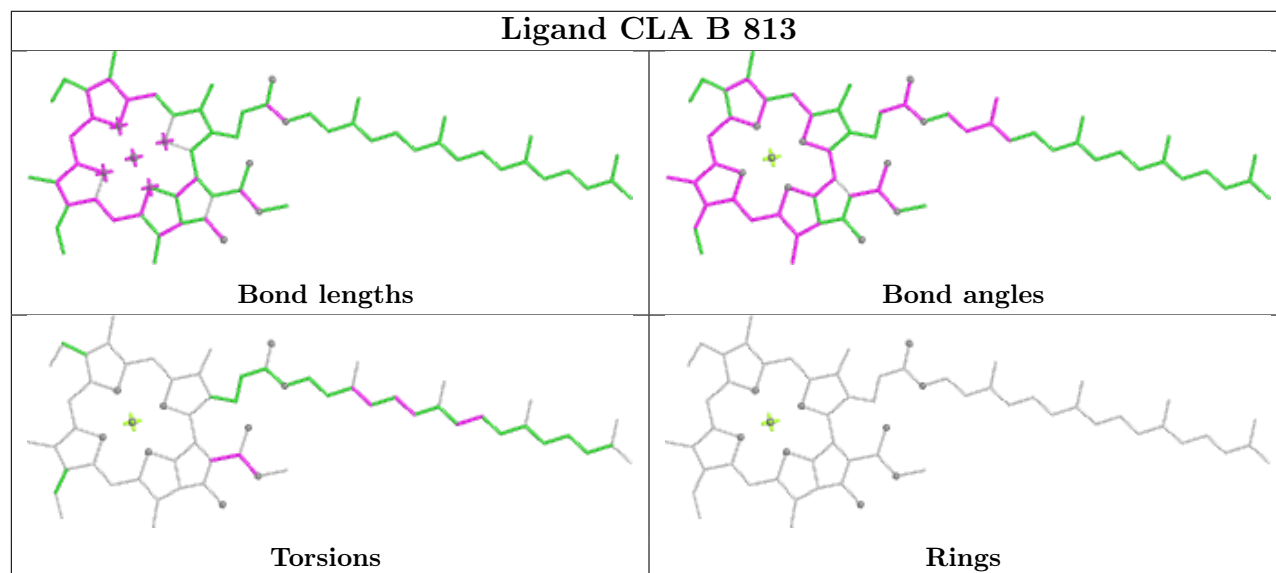


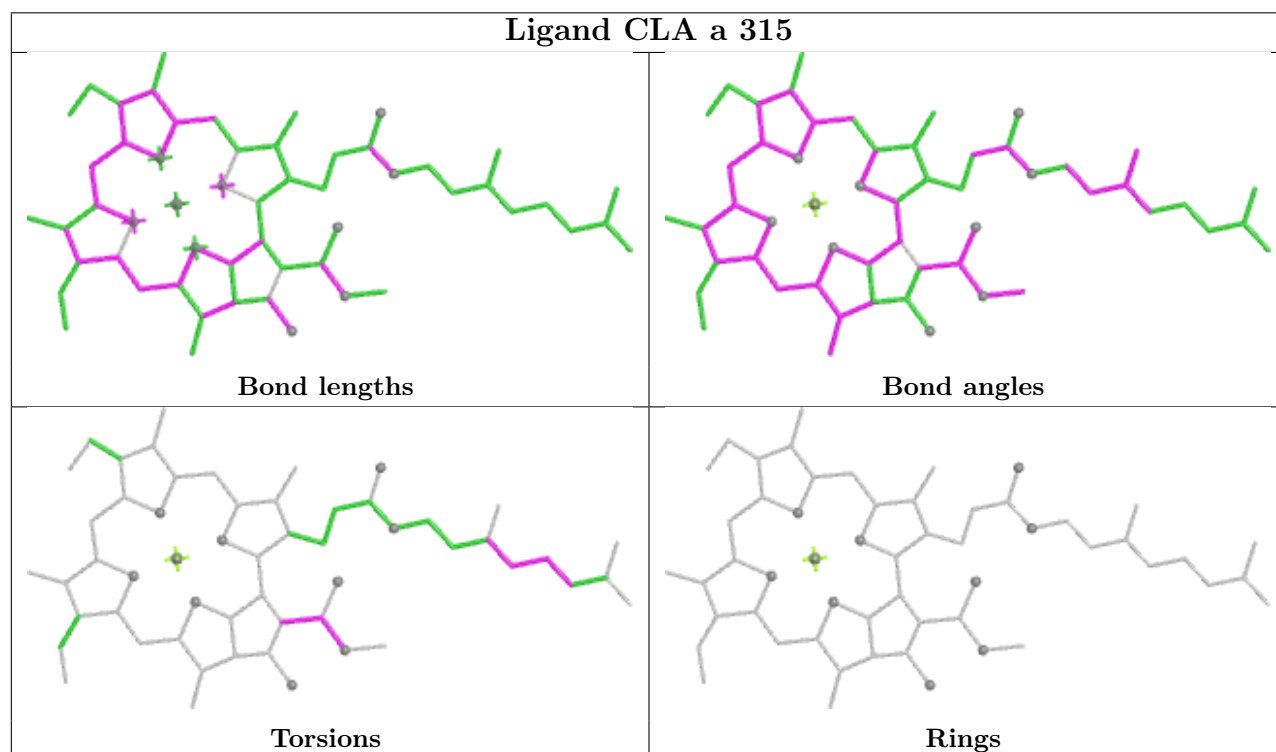
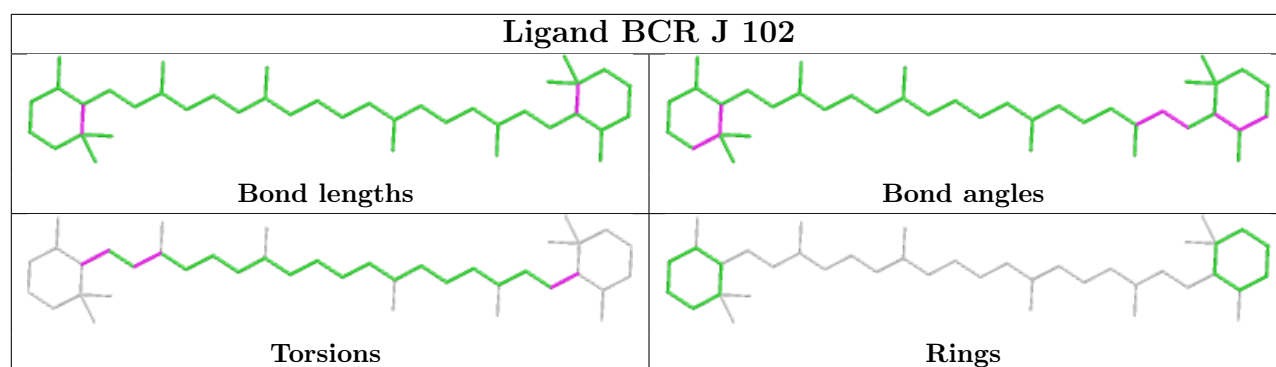
Rings

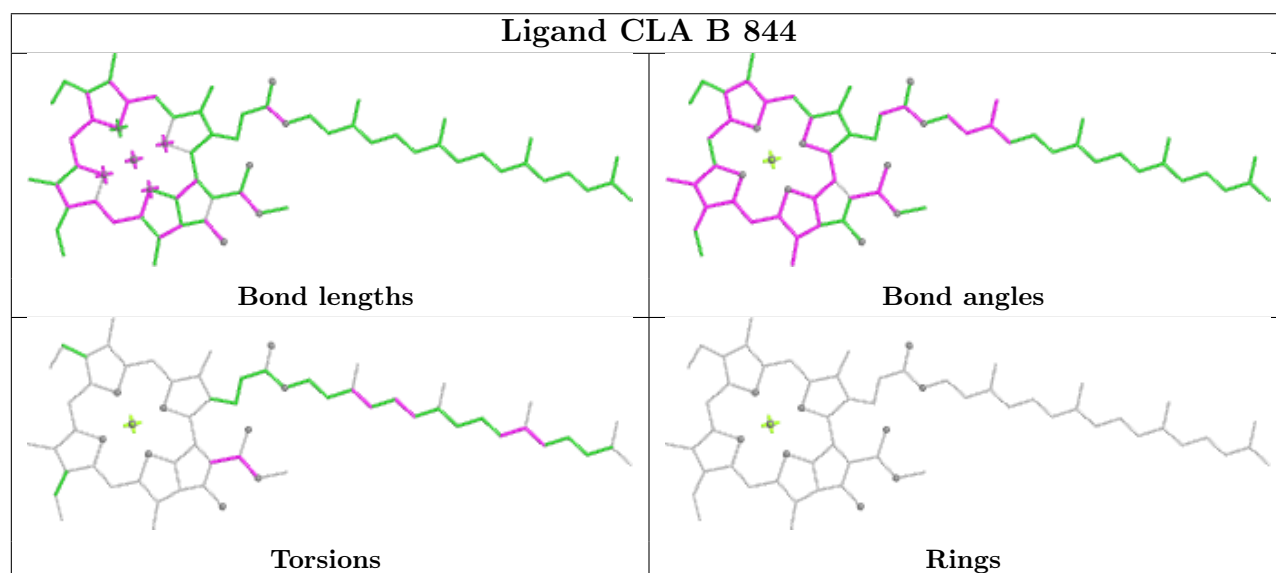
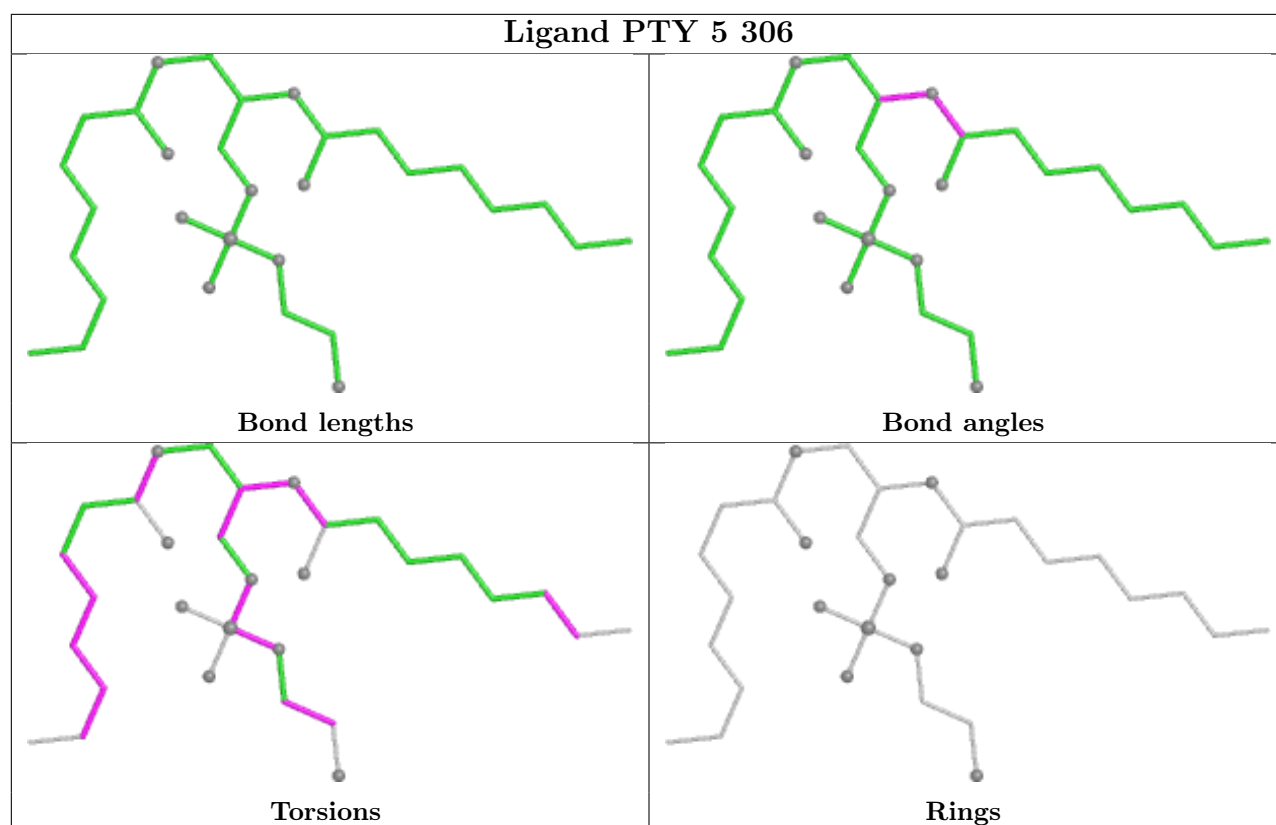
Ligand CLA 5 314



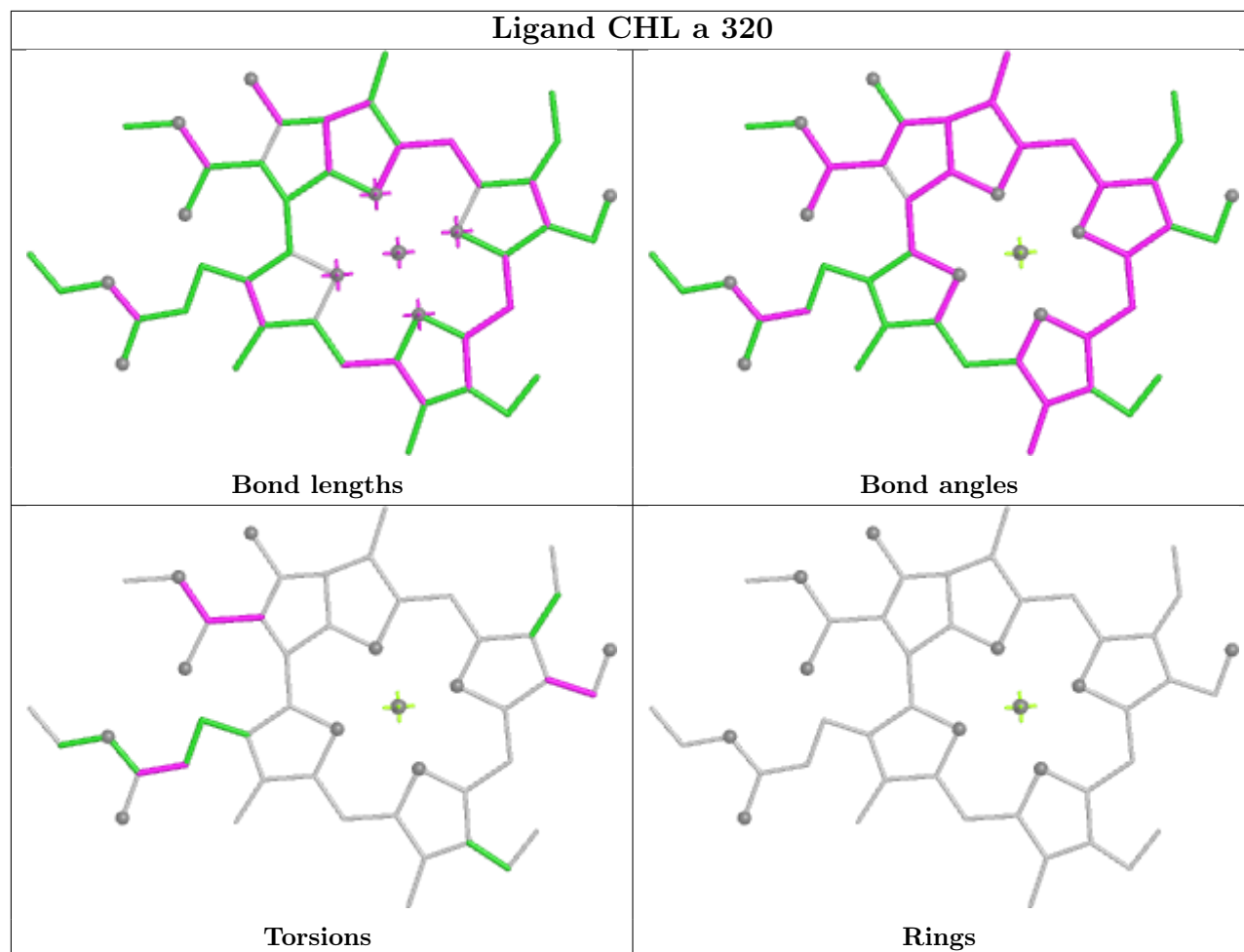
Ligand CLA B 813



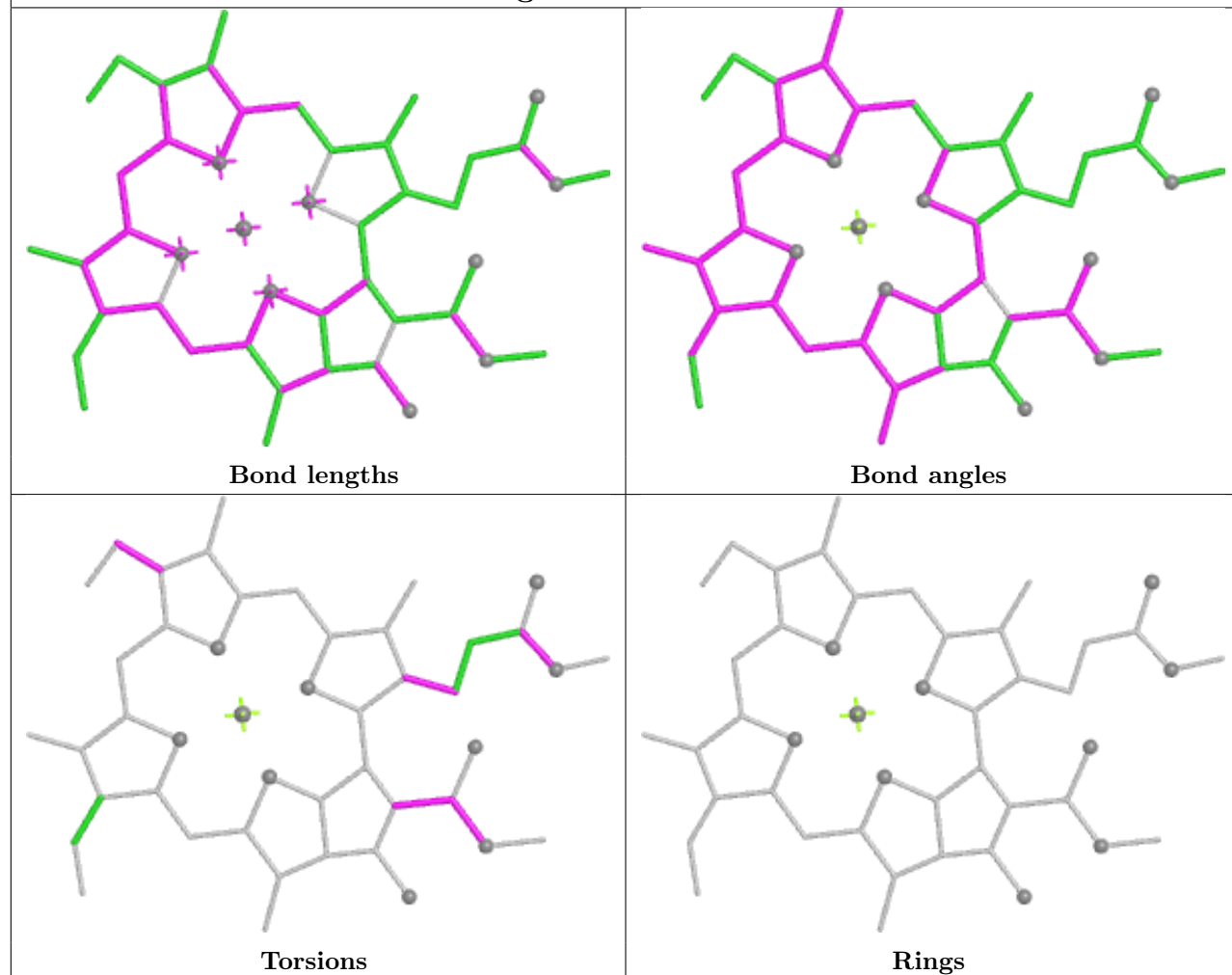




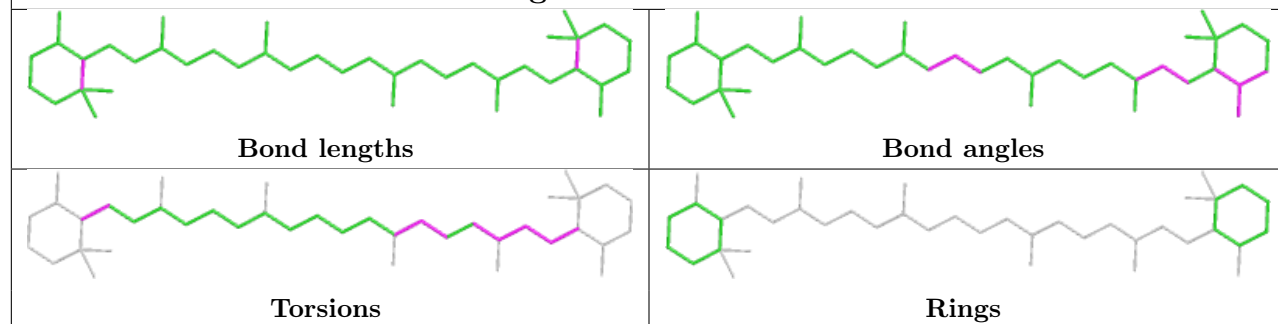
Ligand CHL a 320

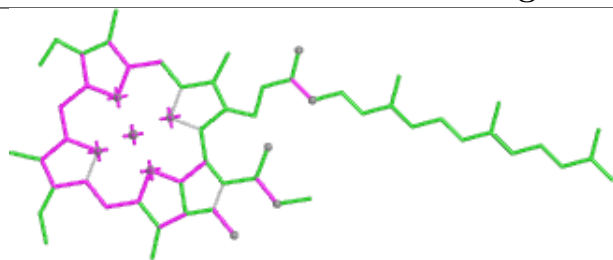
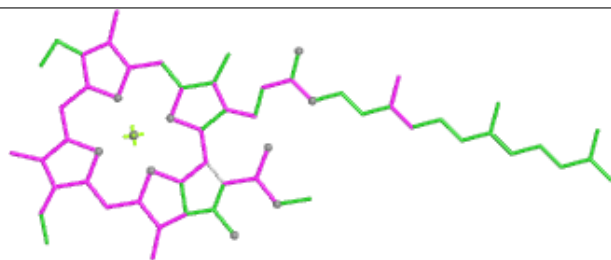
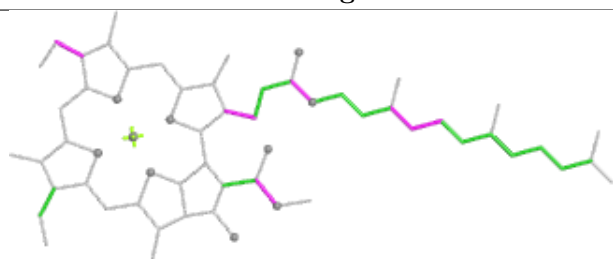
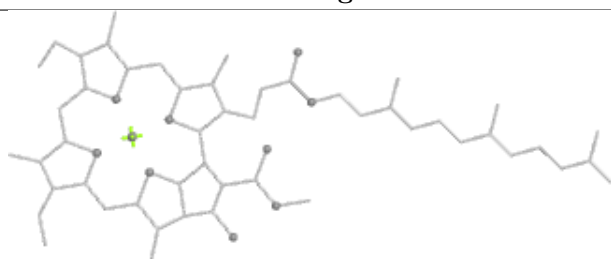
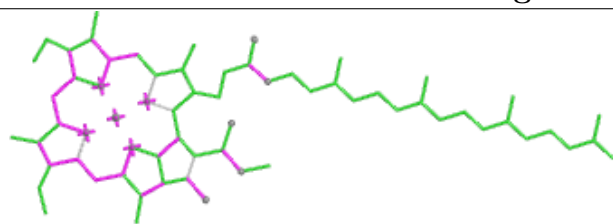
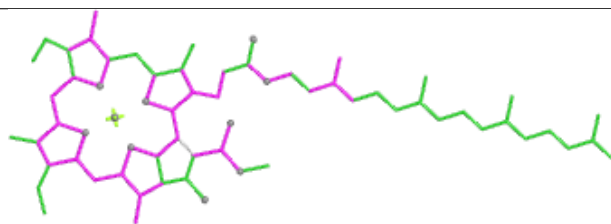
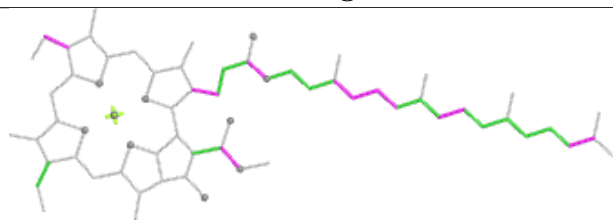
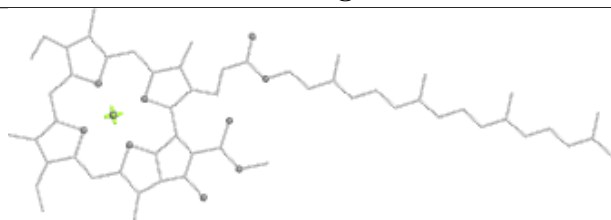


Ligand CLA 8 313

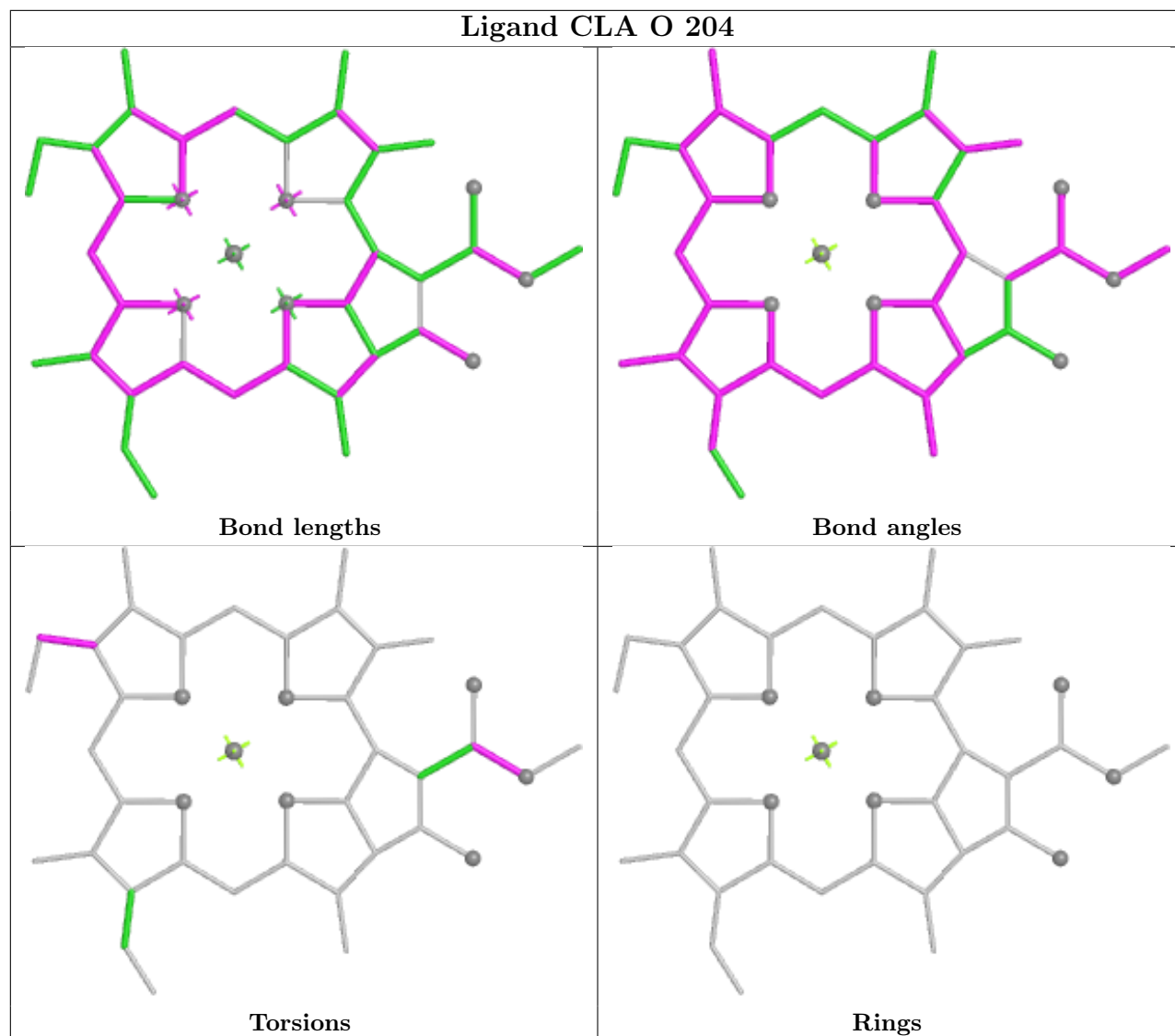


Ligand BCR G 203

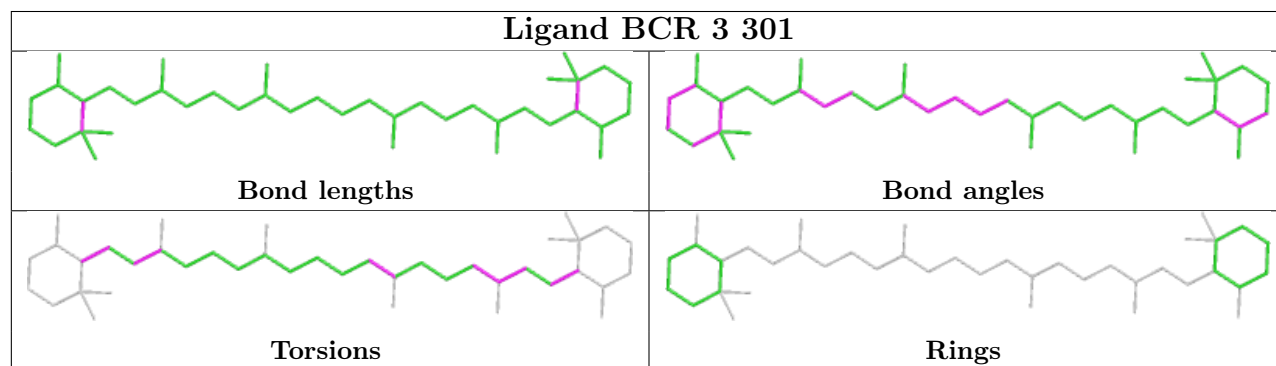


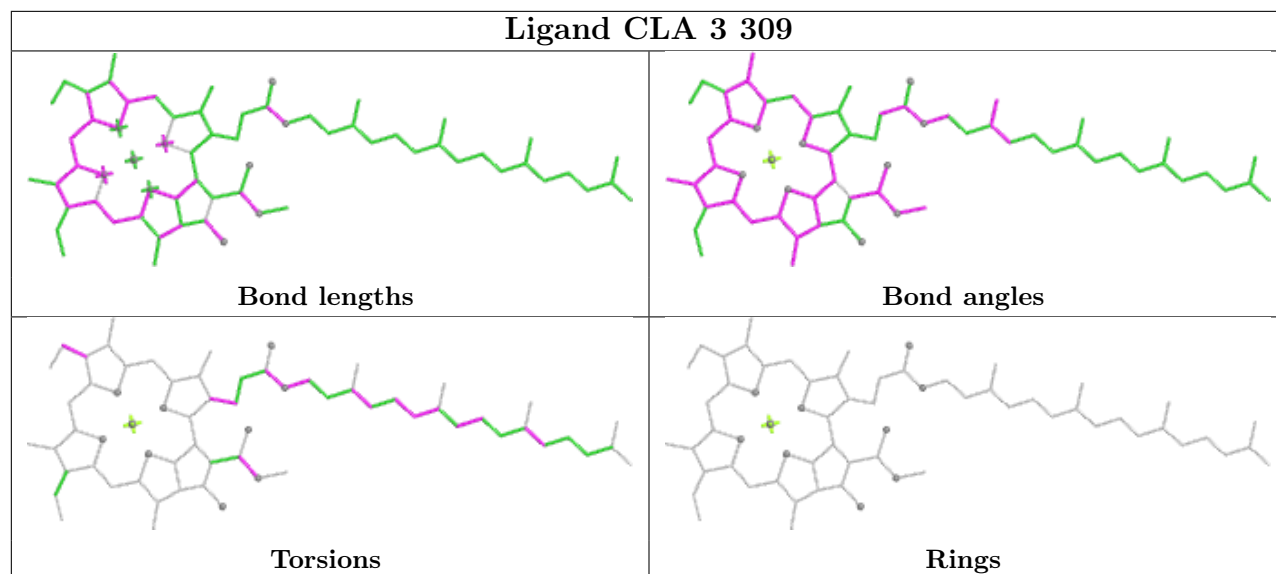
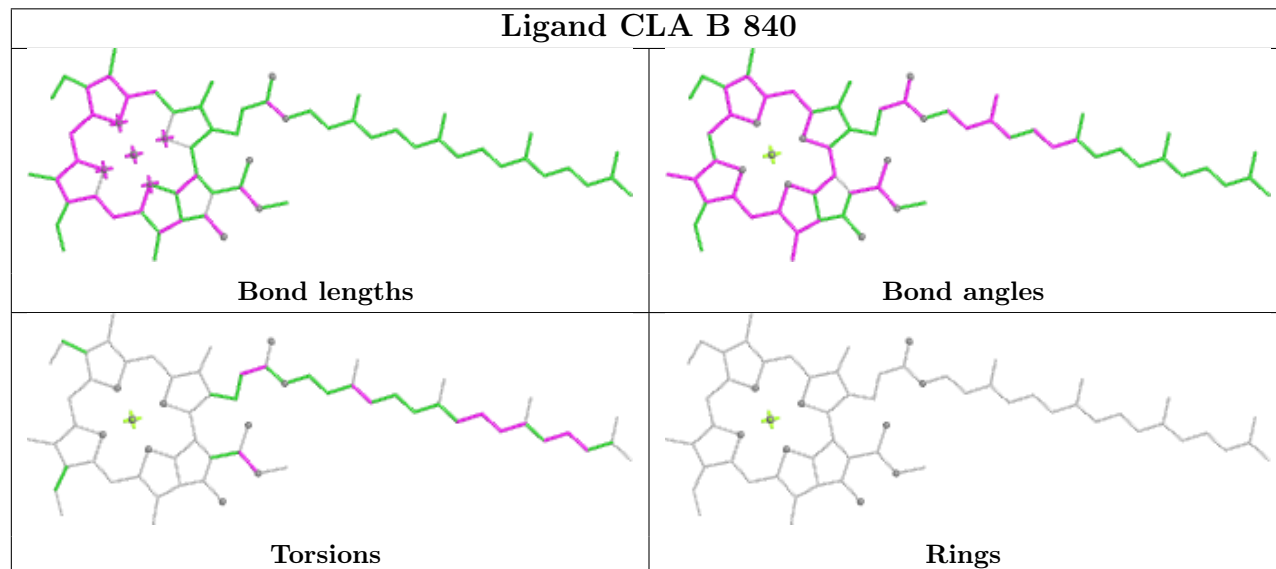
Ligand CLA 2 306**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 855****Bond lengths****Bond angles****Torsions****Rings**

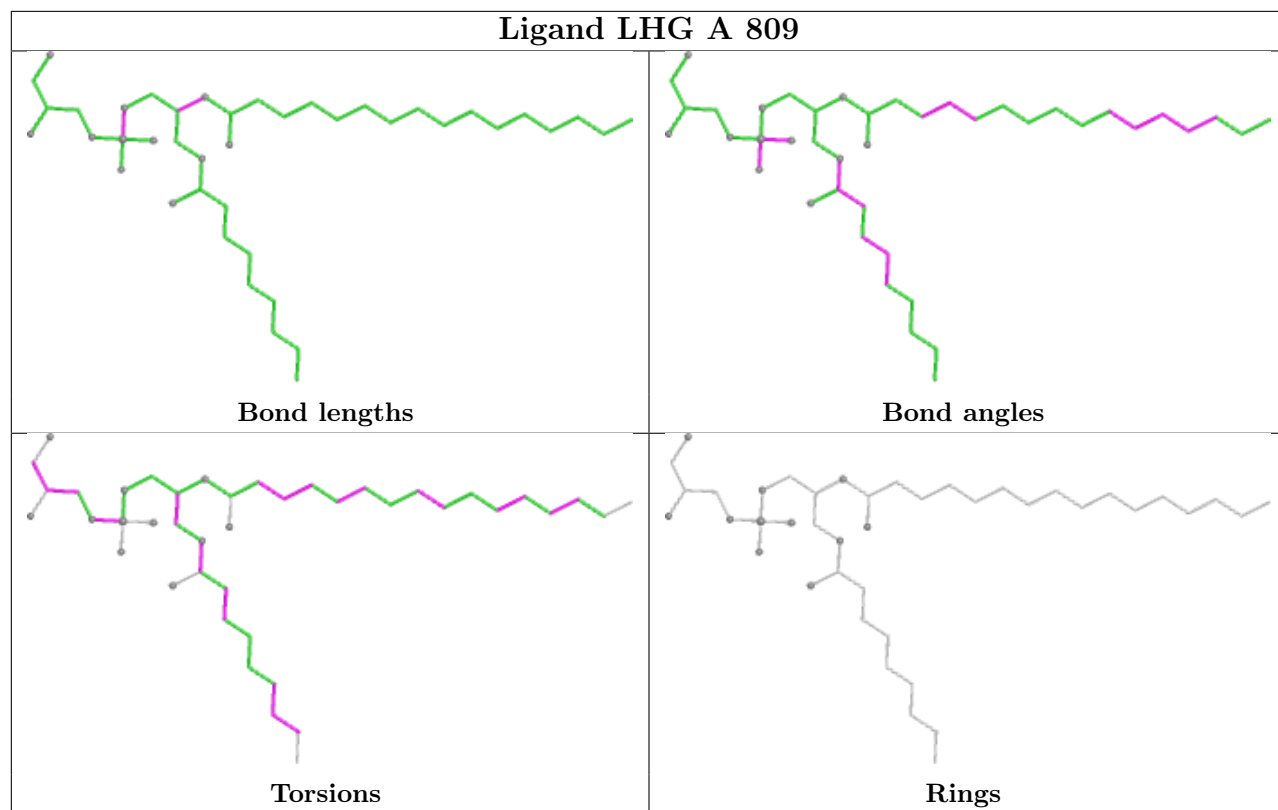
Ligand CLA O 204

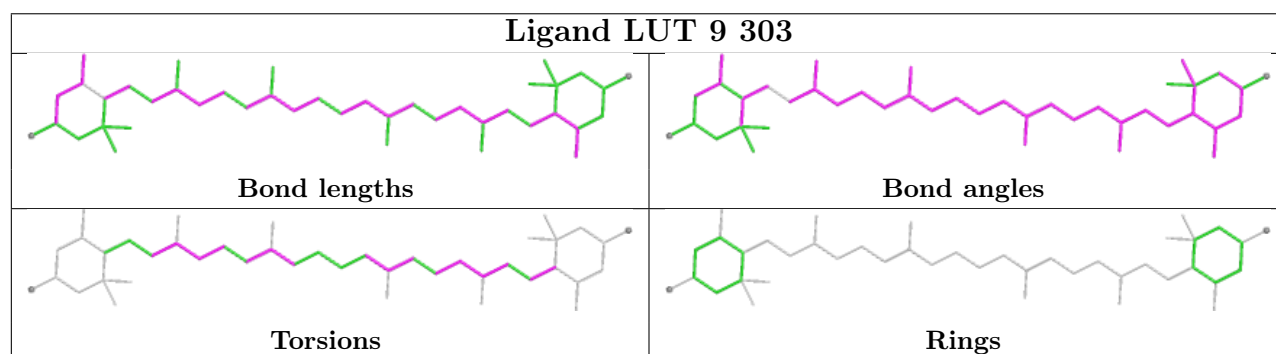
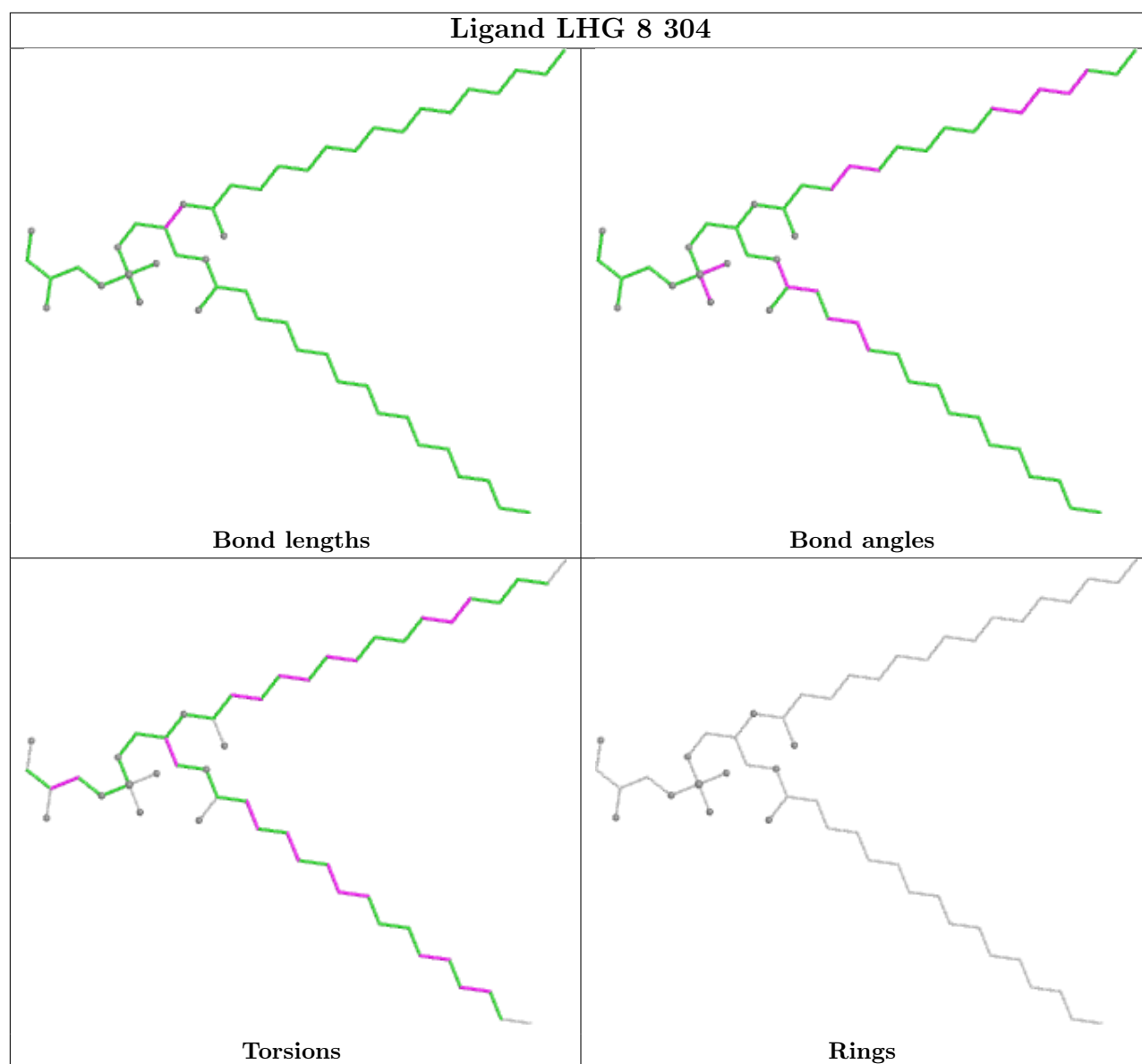


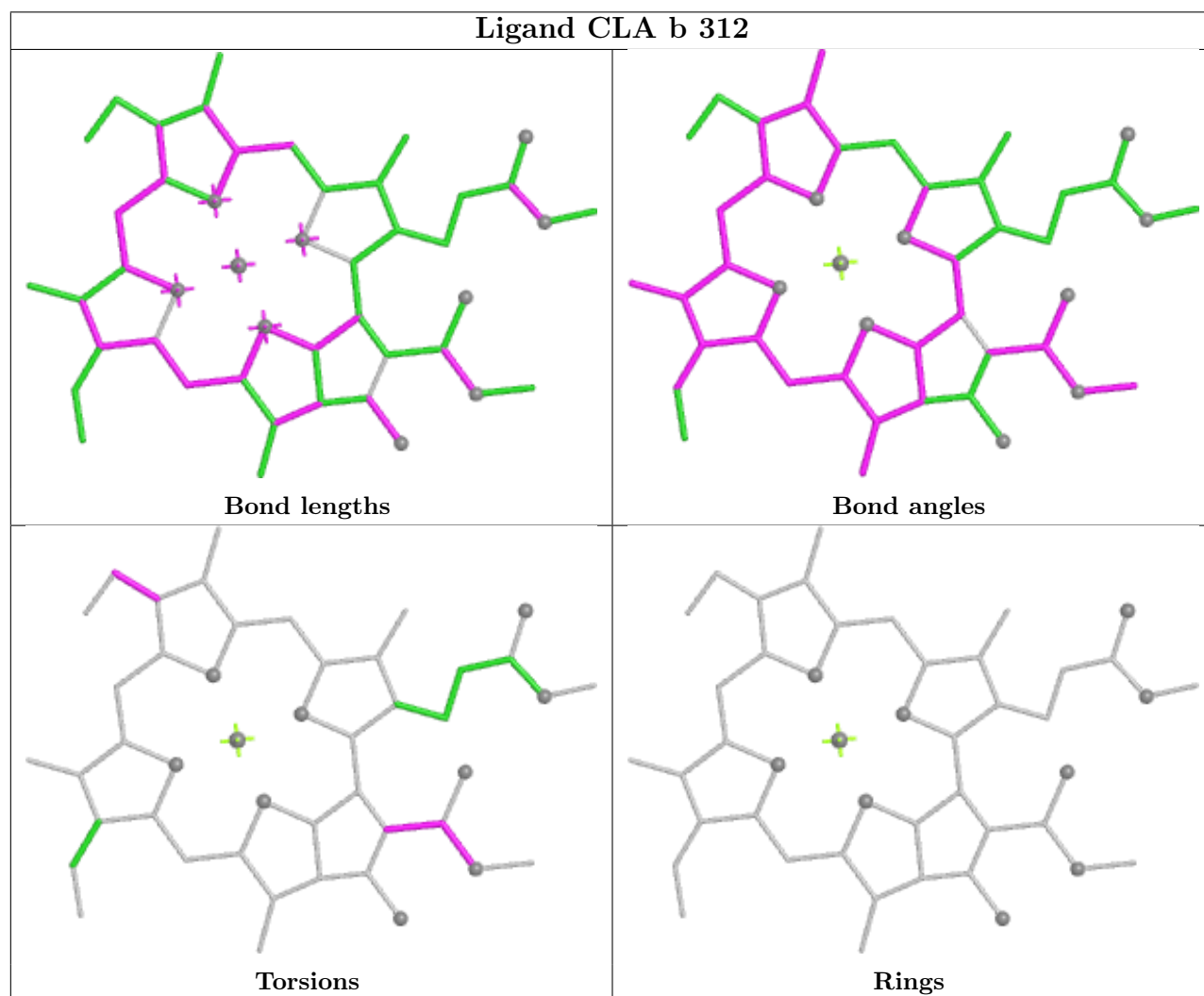
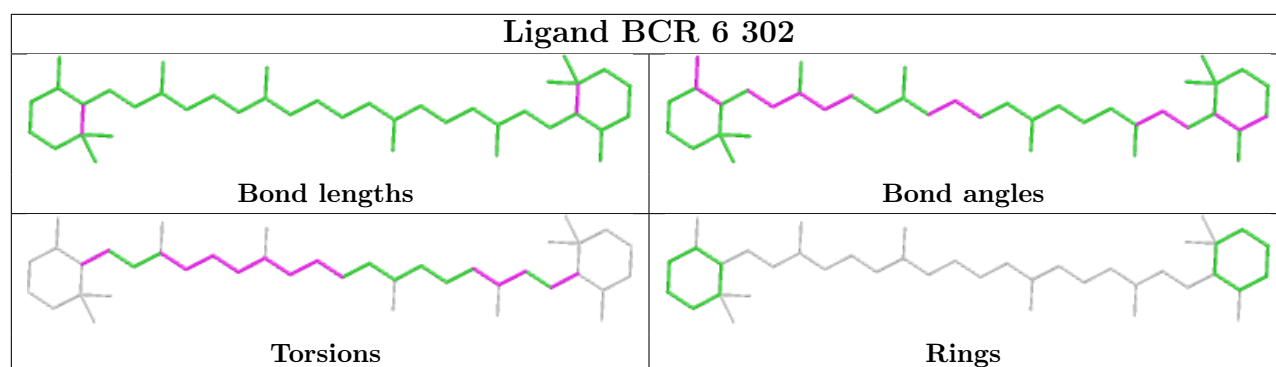
Ligand BCR 3 301



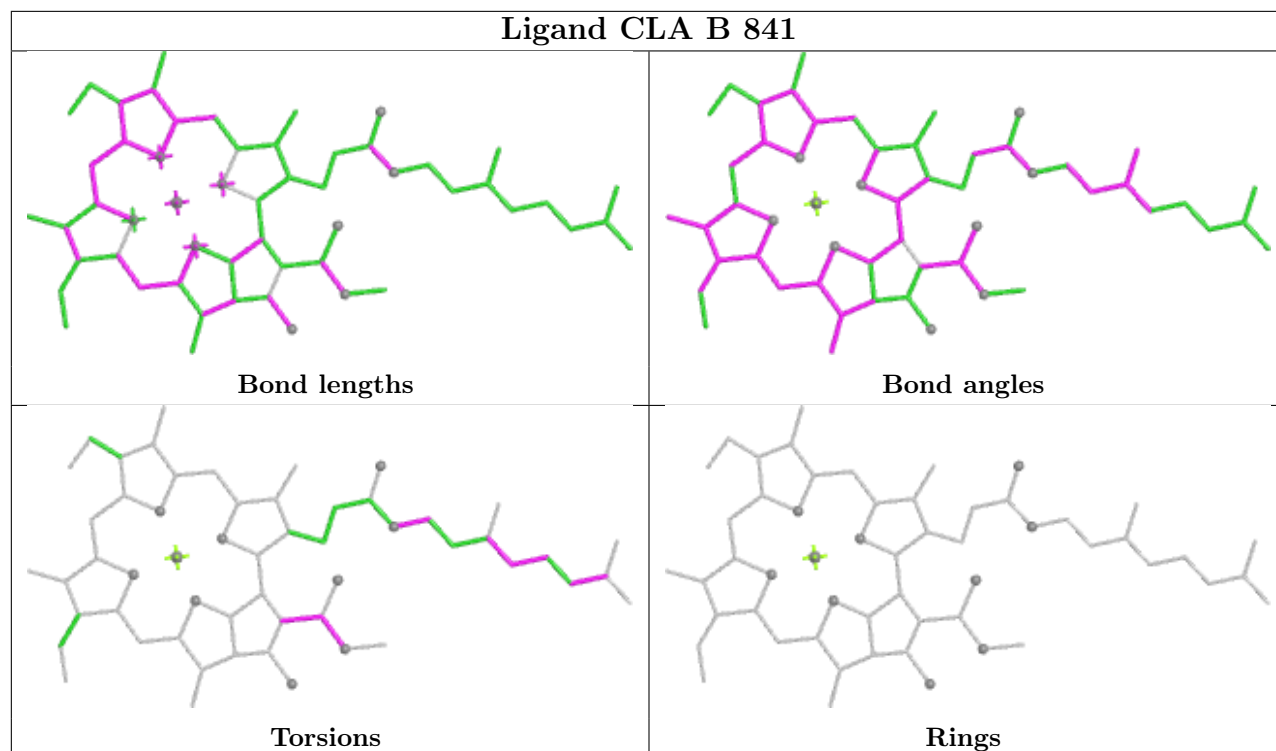
Ligand CLA 3 309**Ligand CLA B 840**



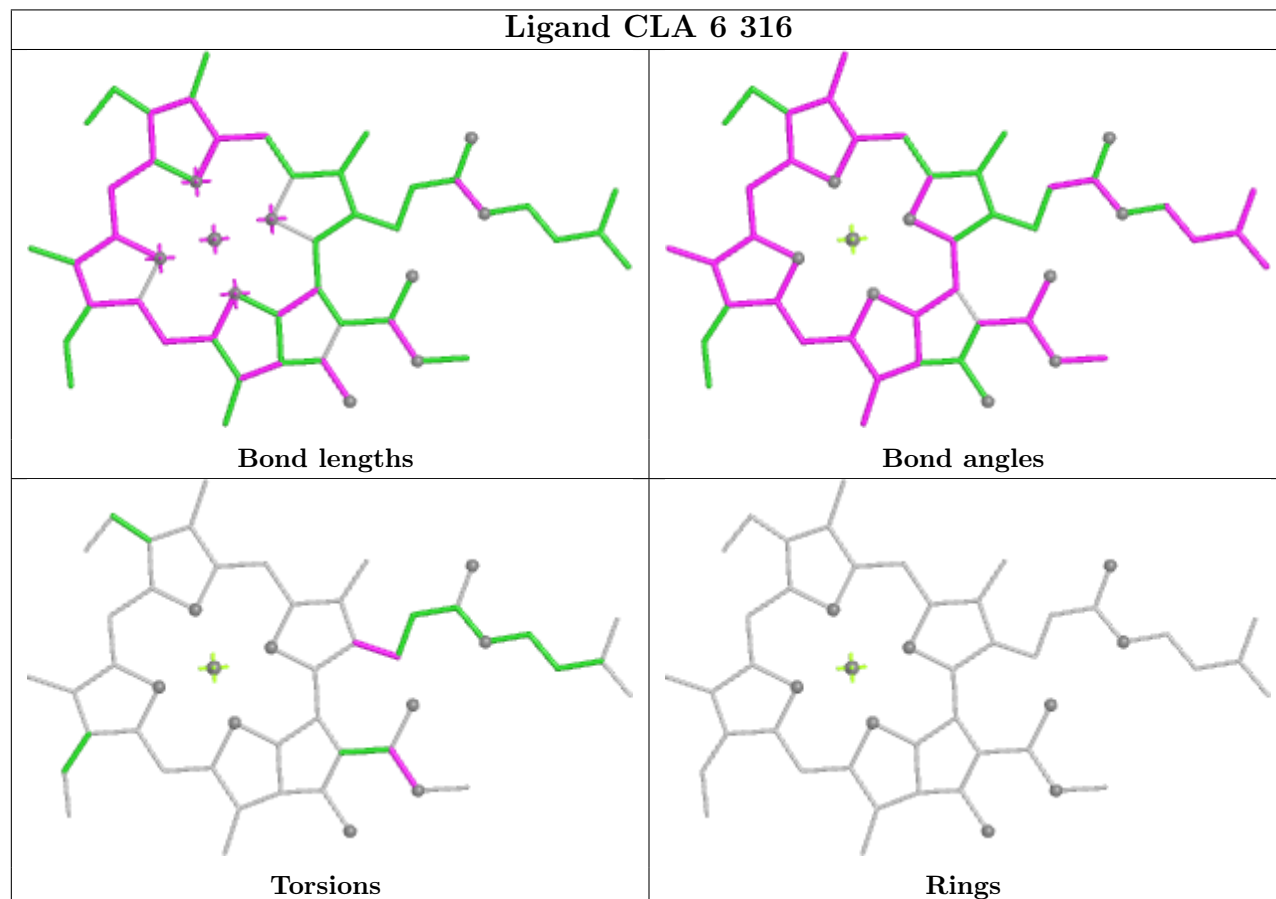


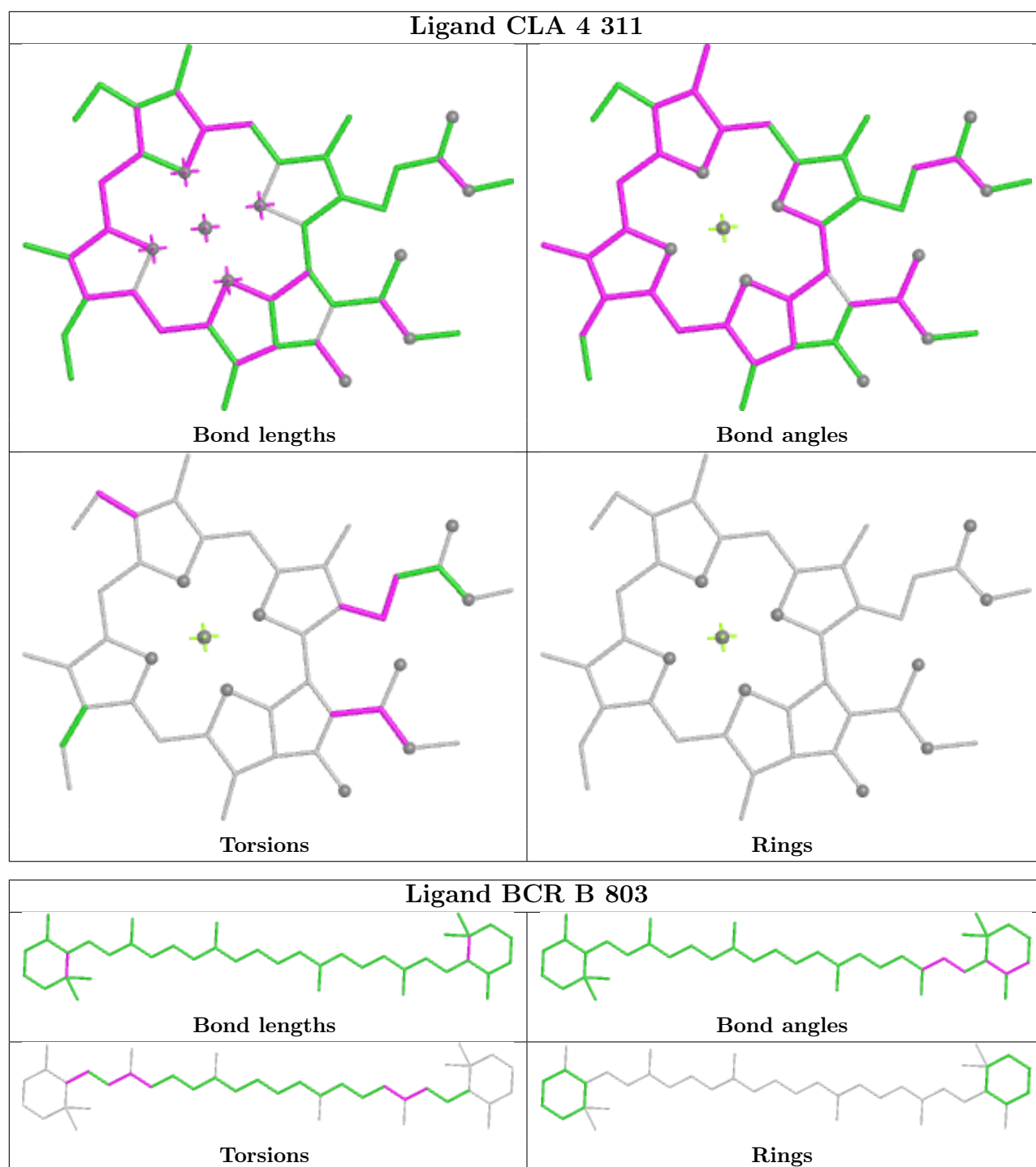


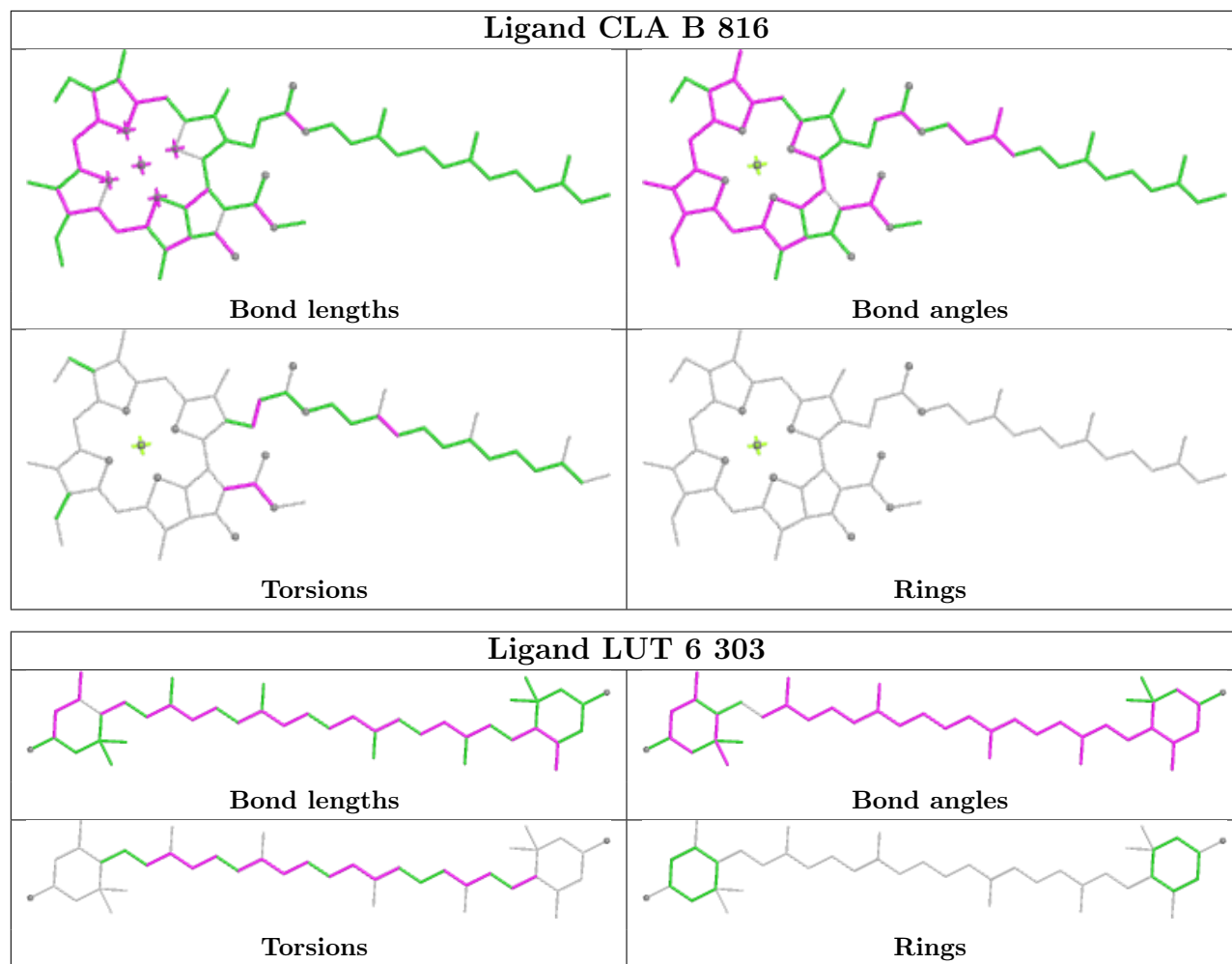
Ligand CLA B 841



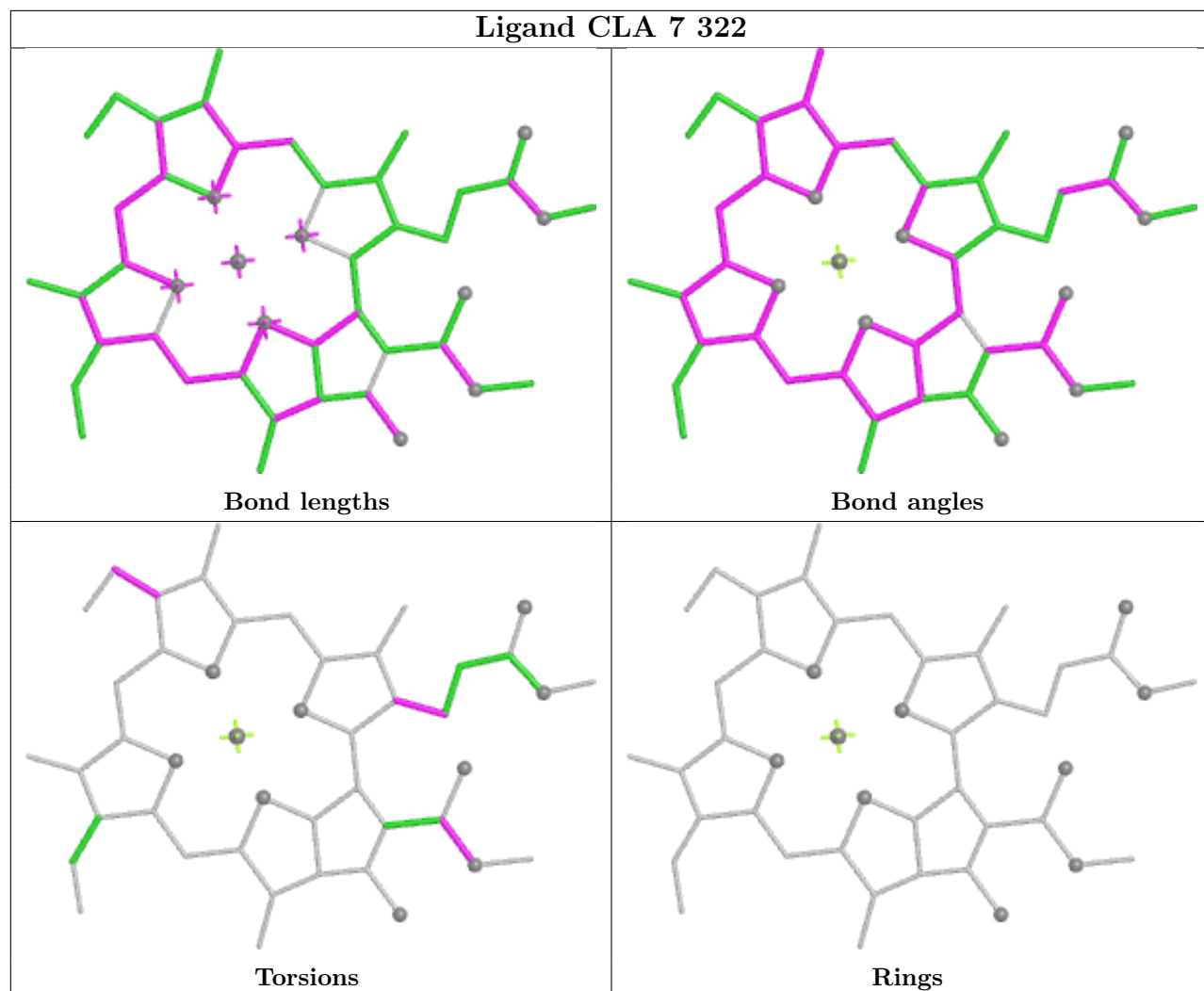
Ligand CLA 6 316



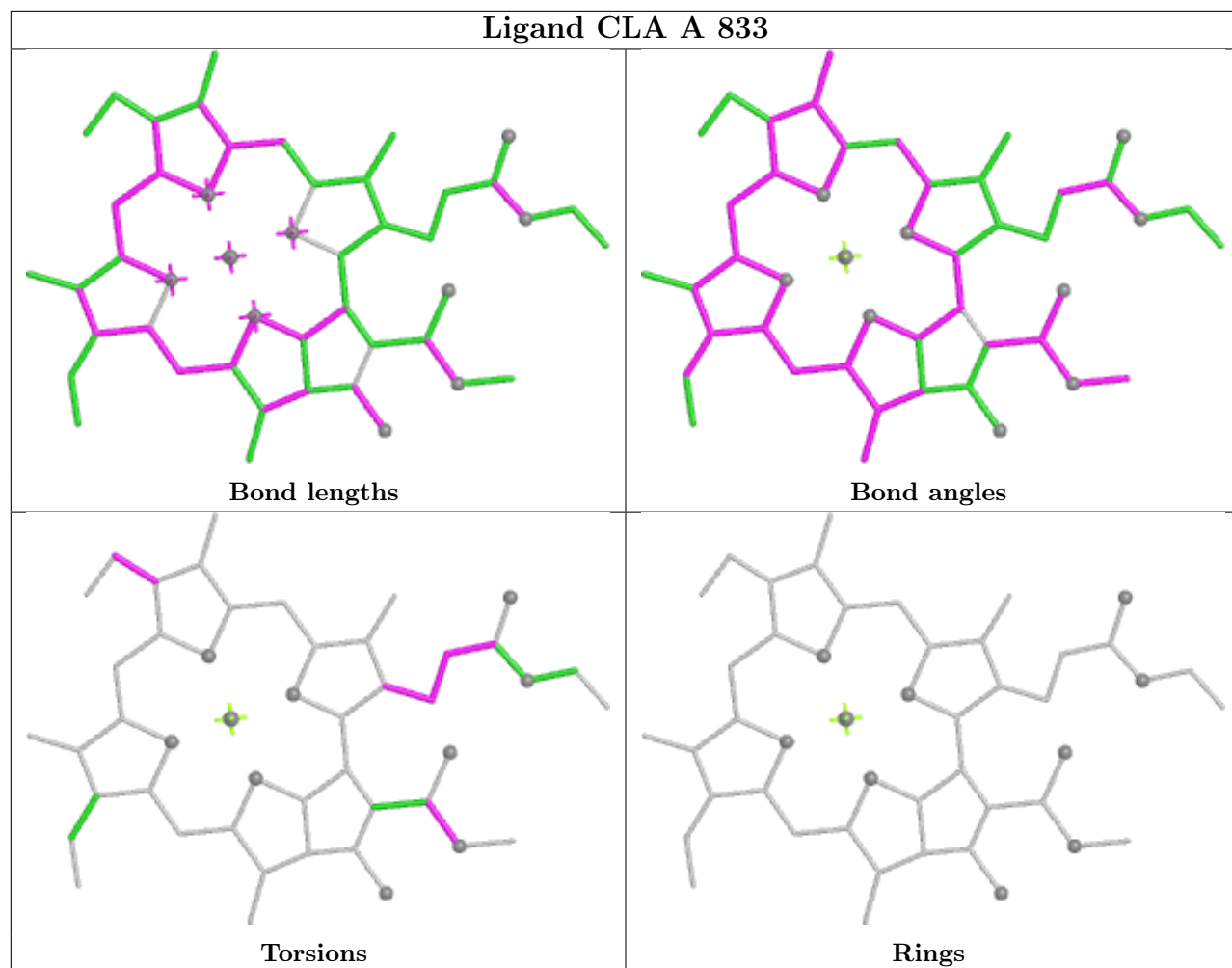




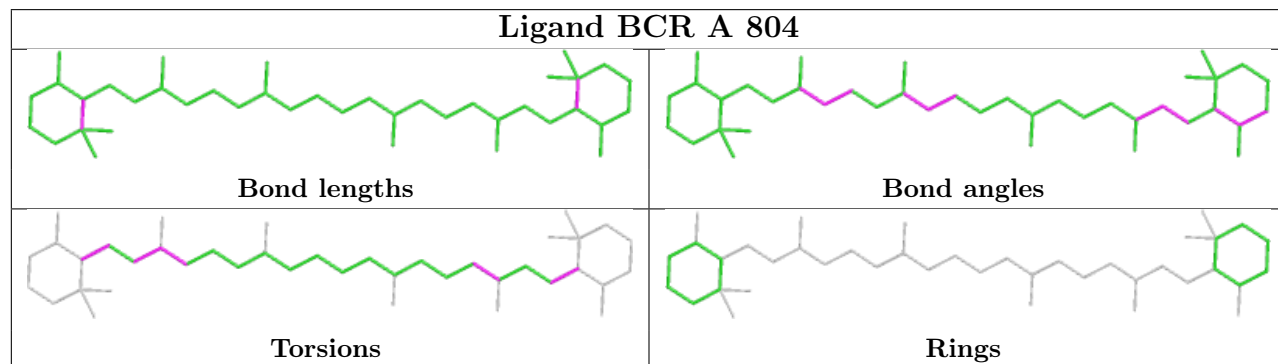
Ligand CLA 7 322



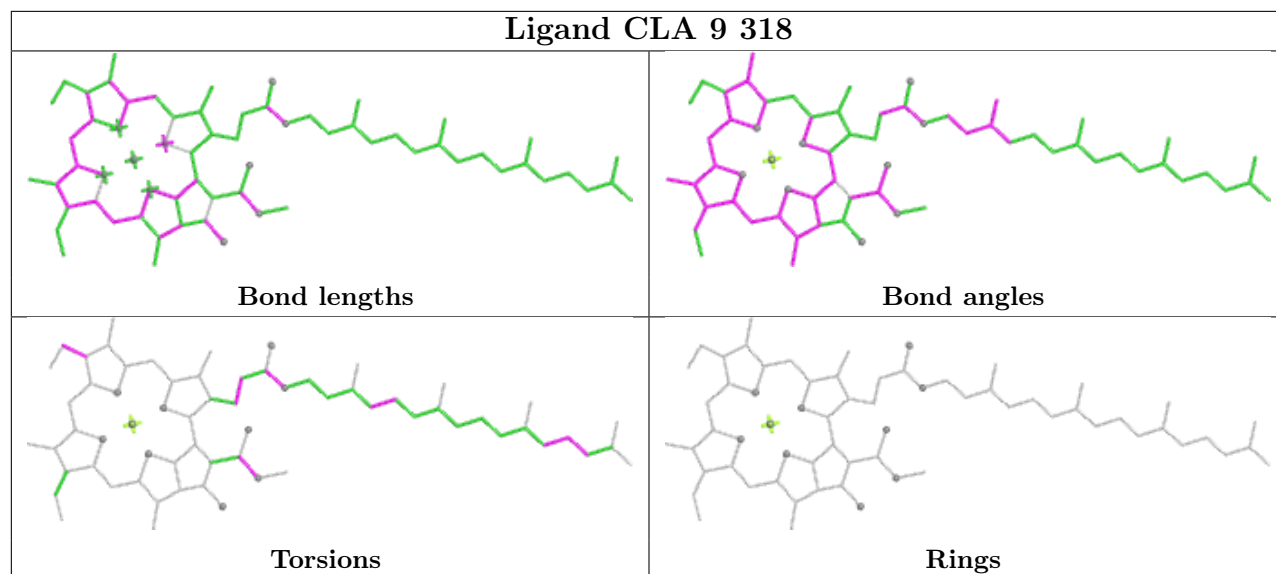
Ligand CLA A 833



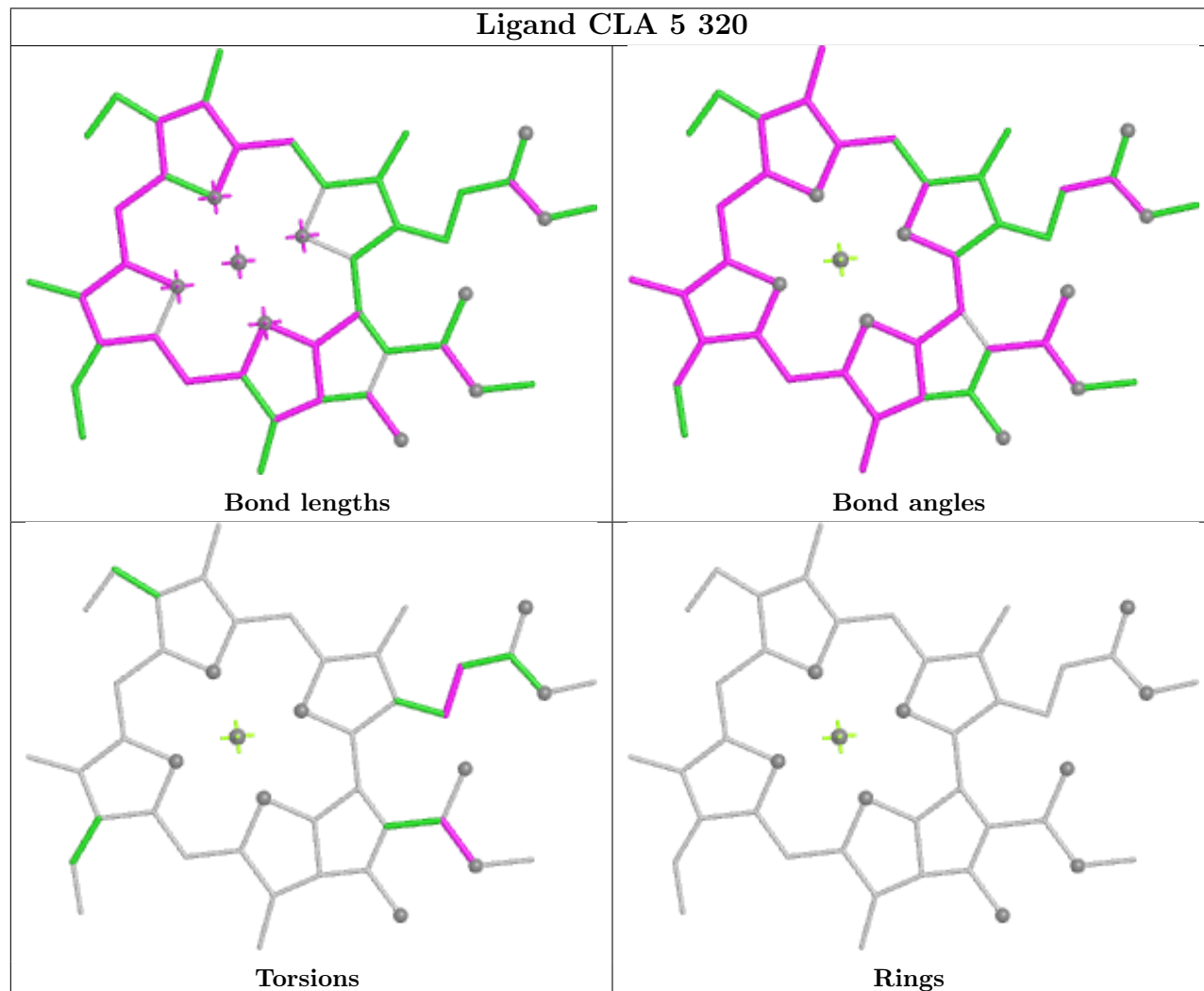
Ligand BCR A 804

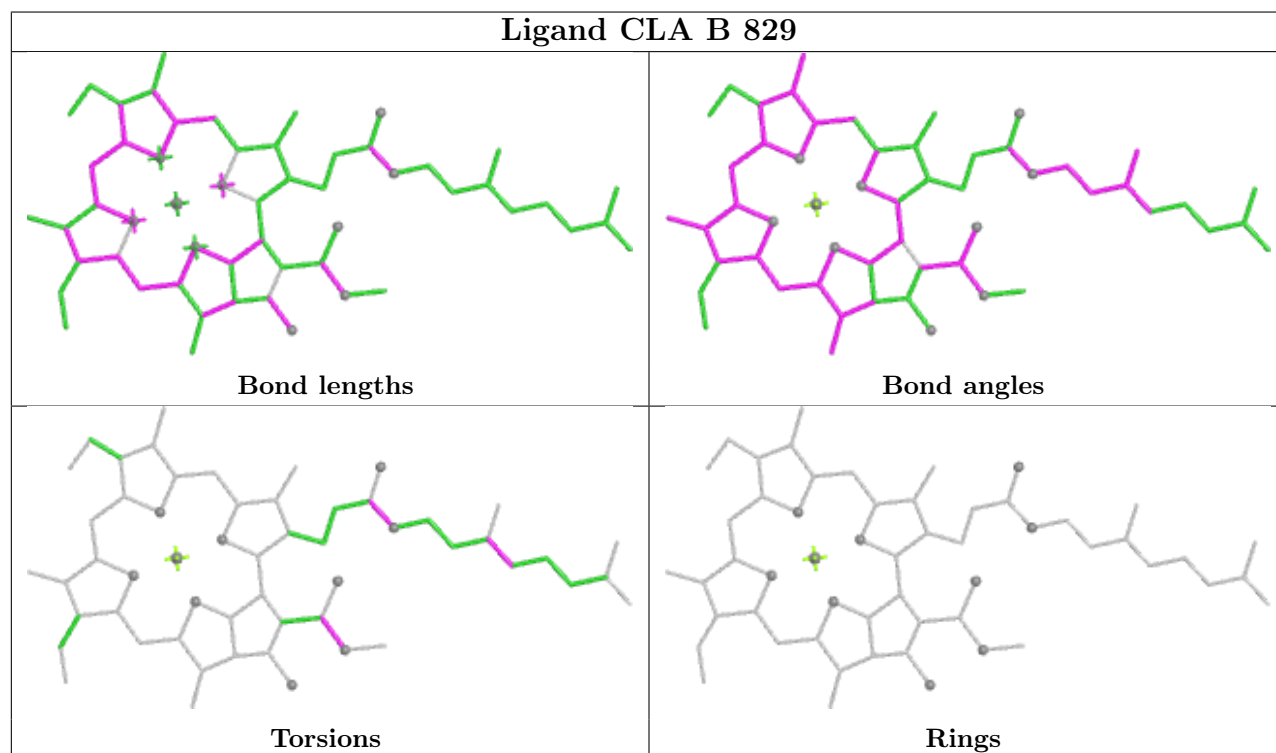
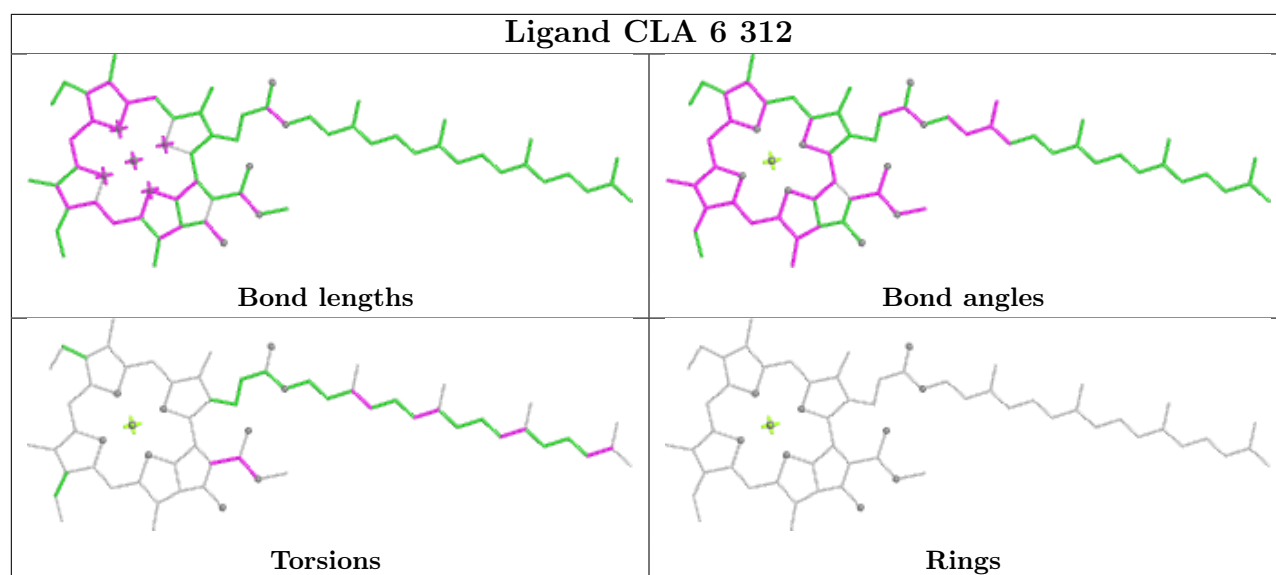


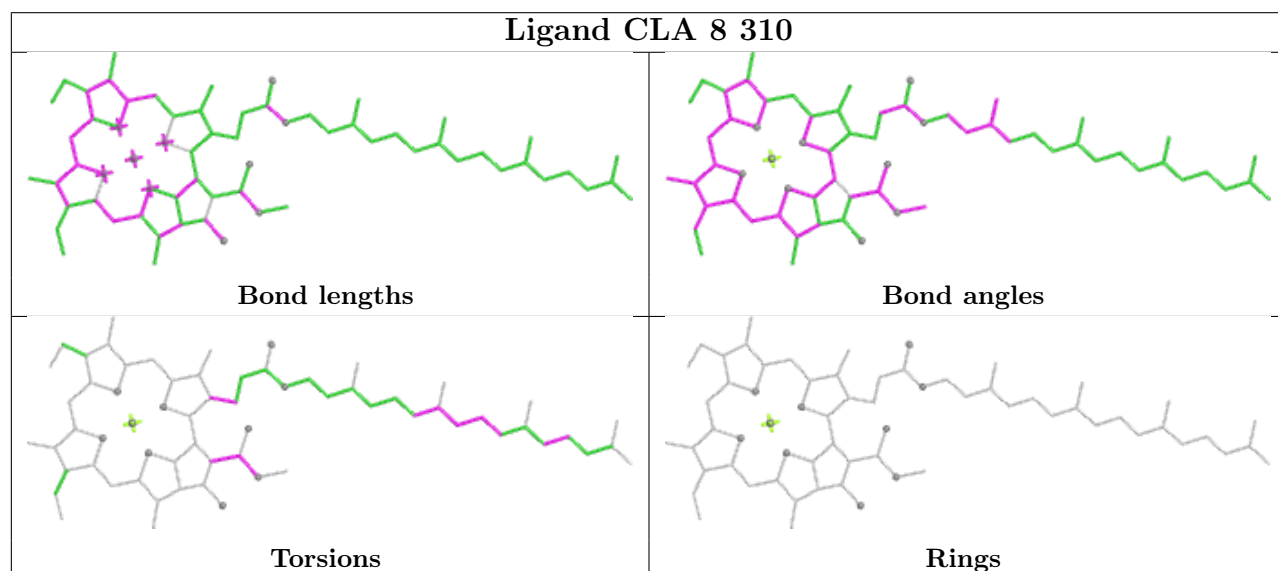
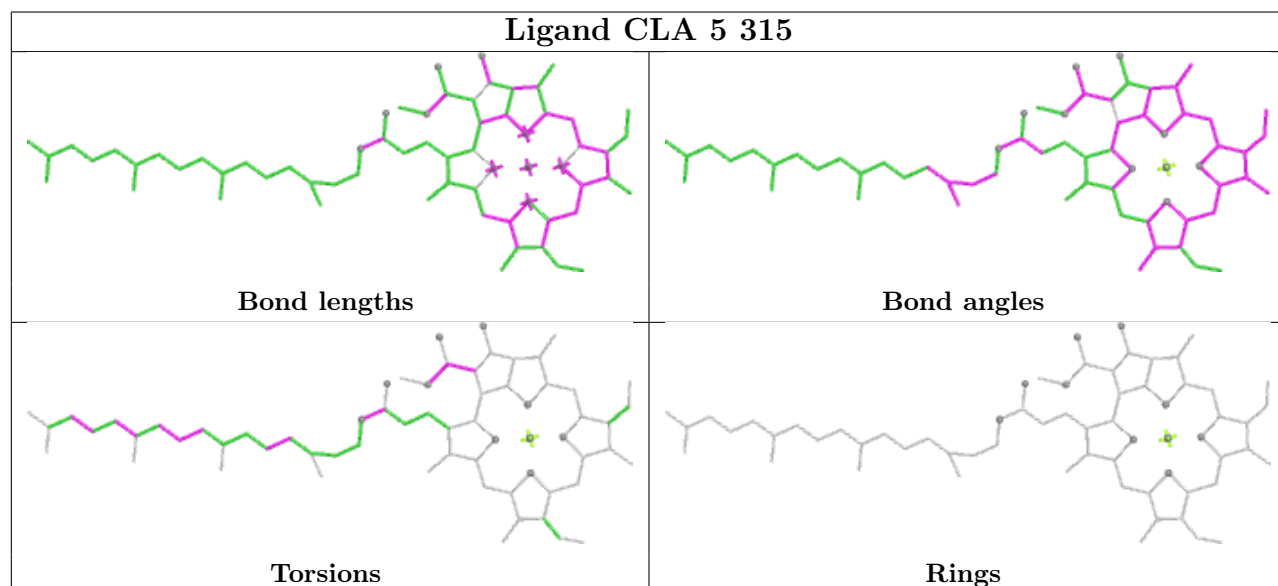
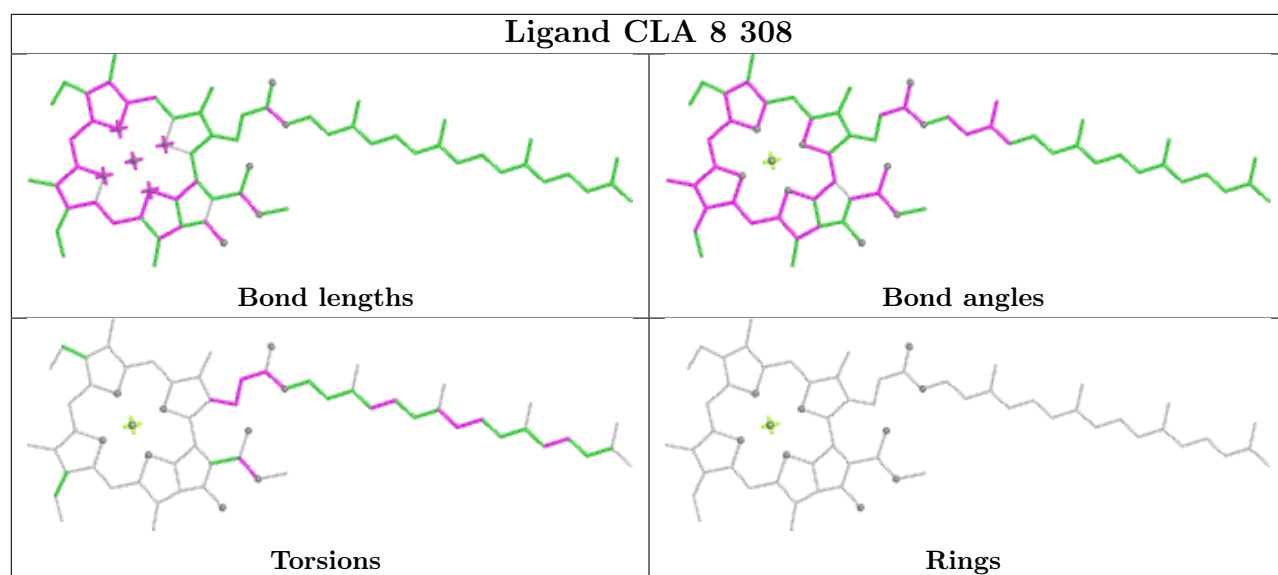
Ligand CLA 9 318



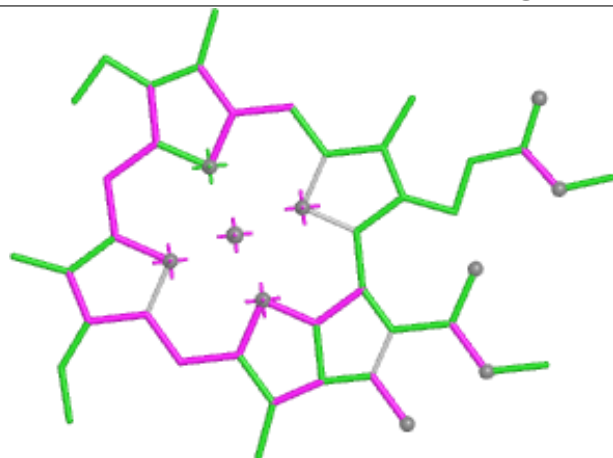
Ligand CLA 5 320



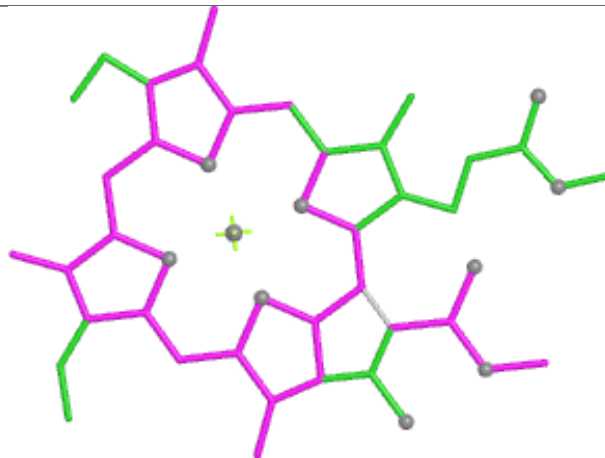




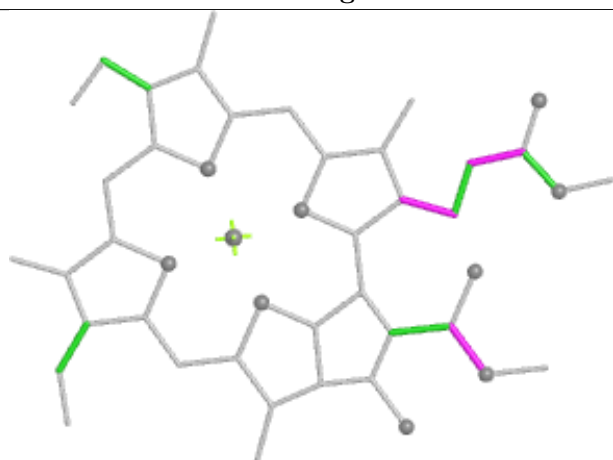
Ligand CLA b 302



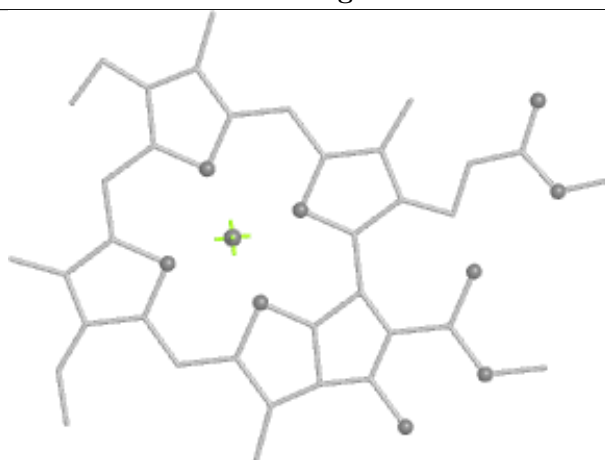
Bond lengths



Bond angles

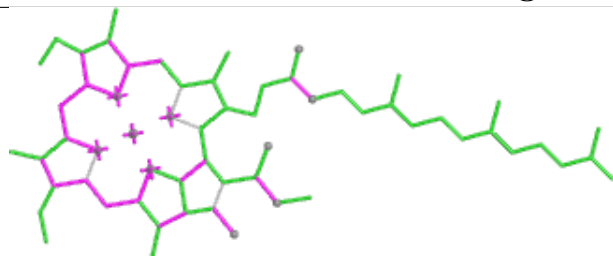


Torsions

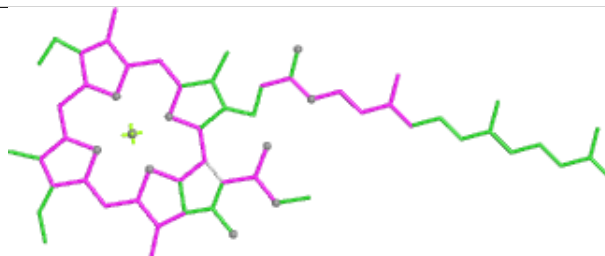


Rings

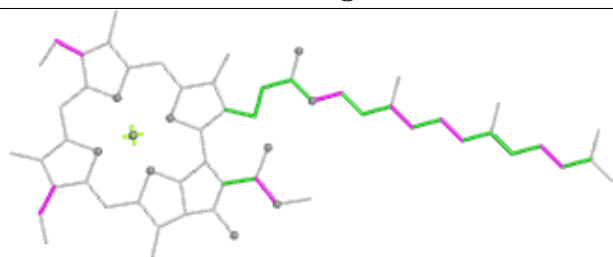
Ligand CLA 3 310



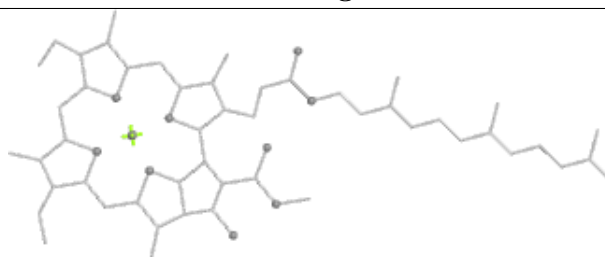
Bond lengths



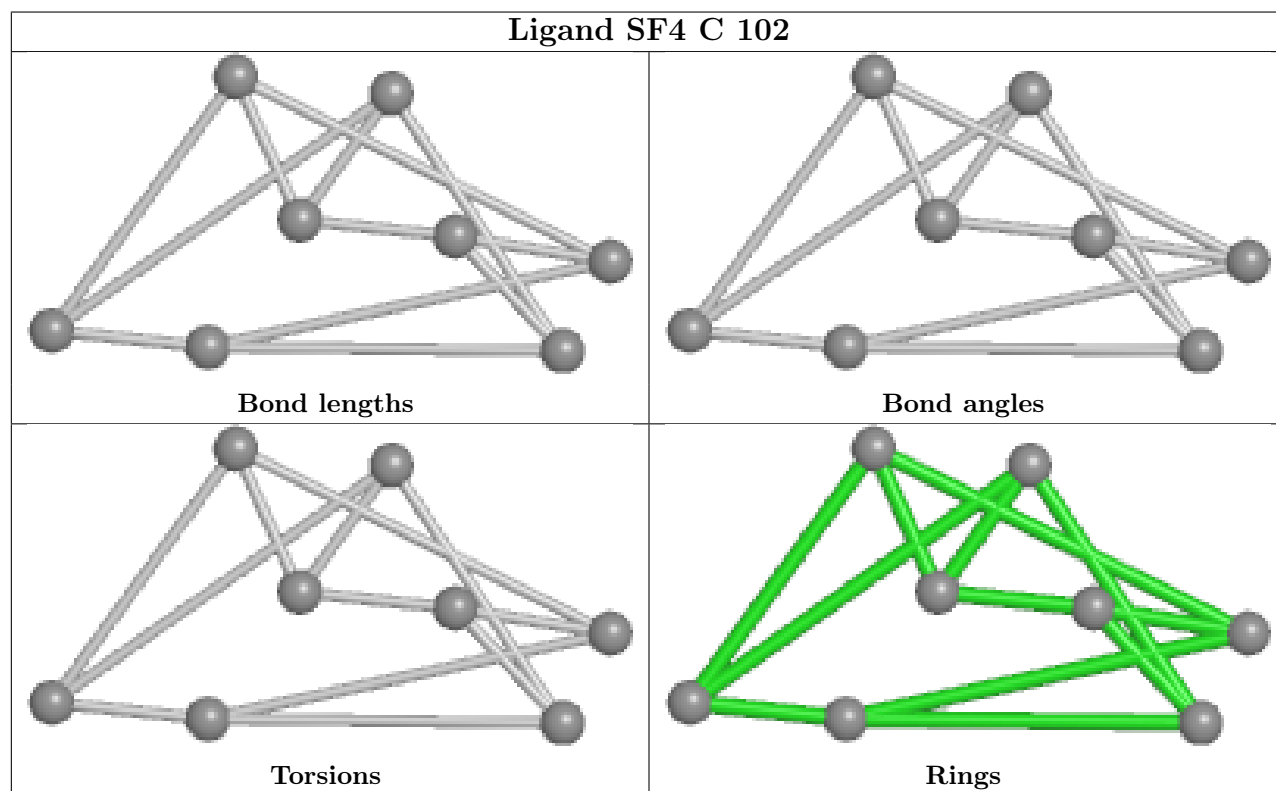
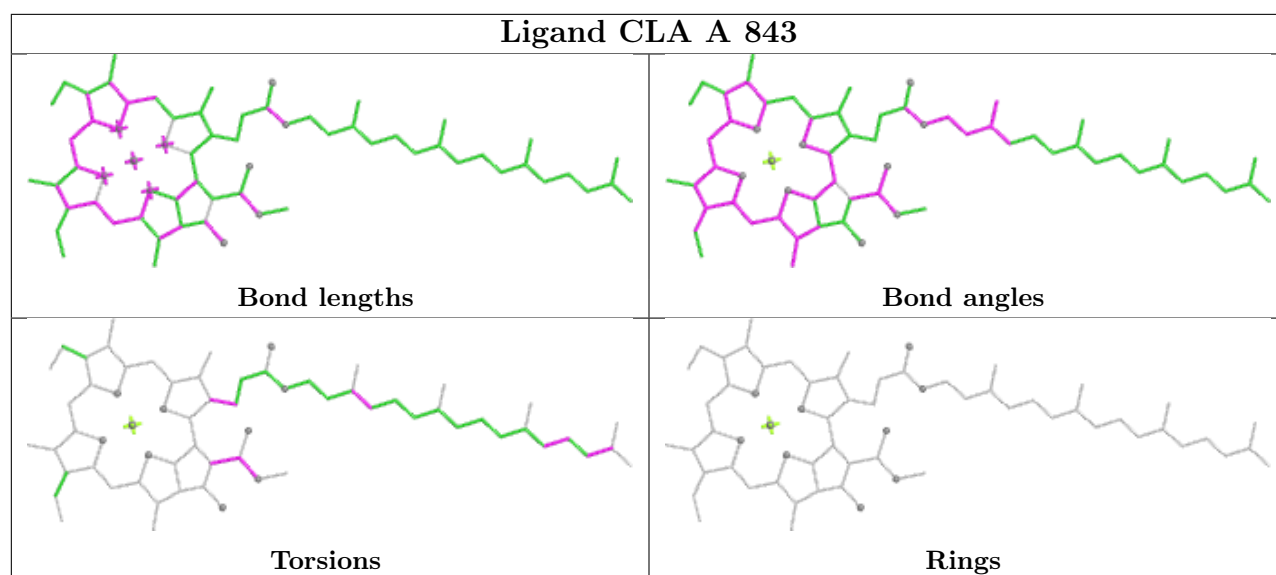
Bond angles



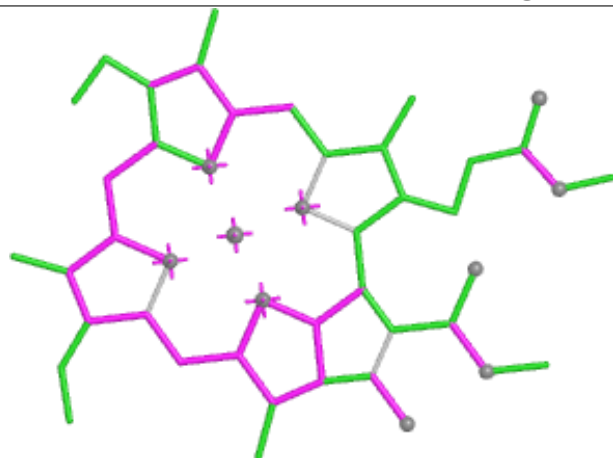
Torsions



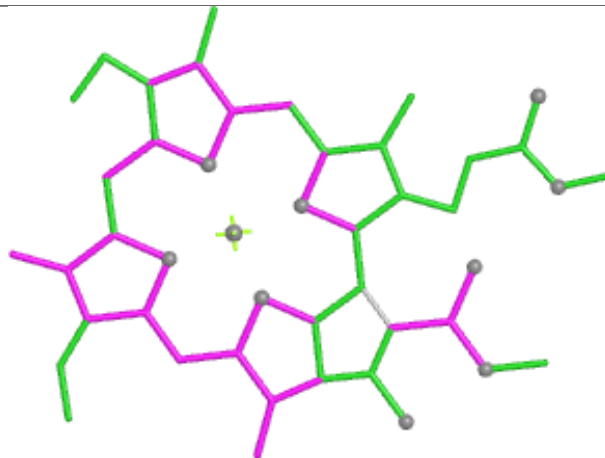
Rings



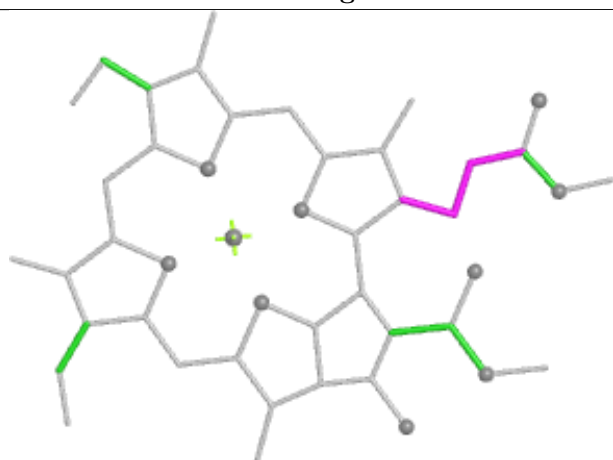
Ligand CLA 6 306



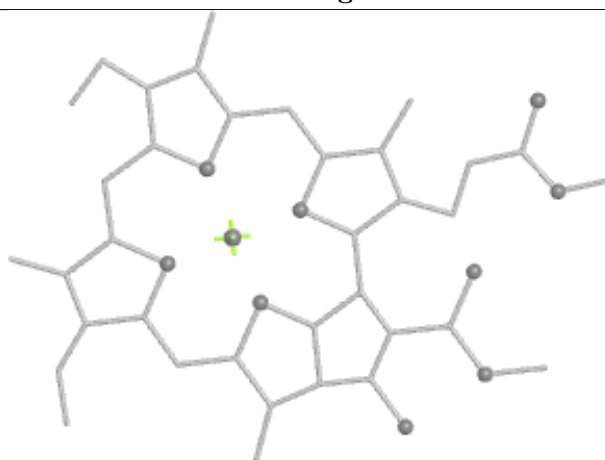
Bond lengths



Bond angles

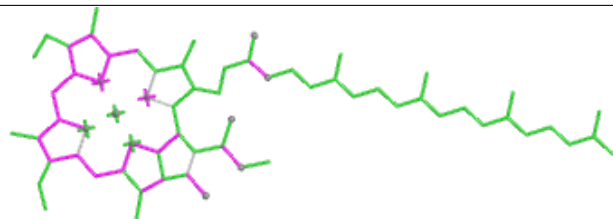


Torsions

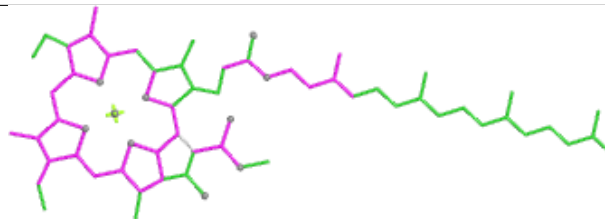


Rings

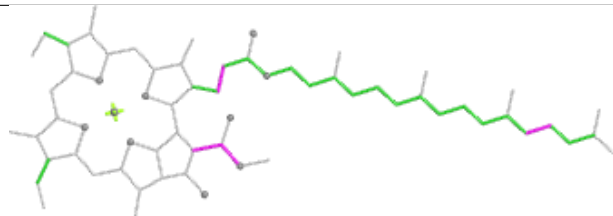
Ligand CLA 5 310



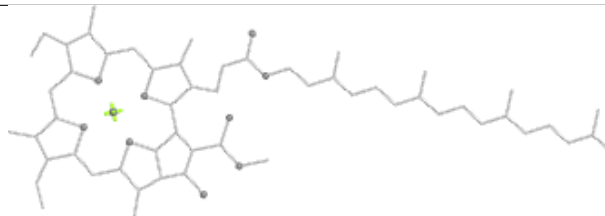
Bond lengths



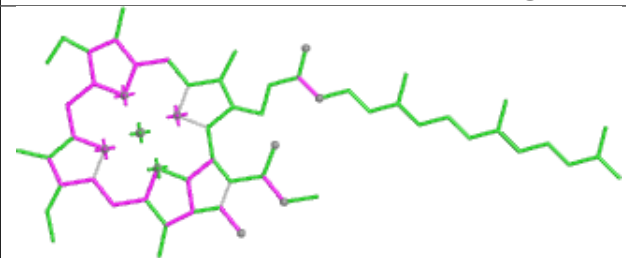
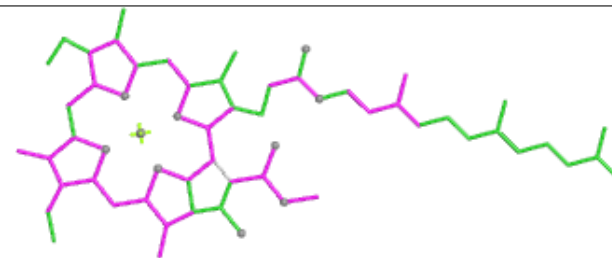
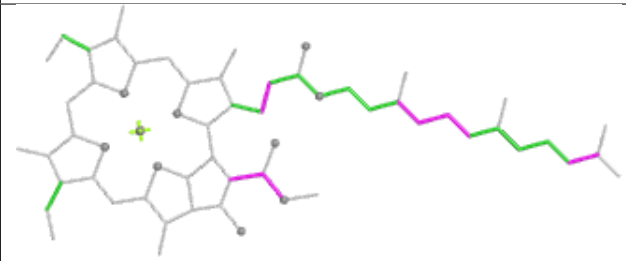
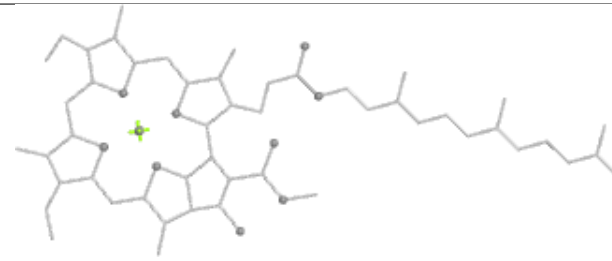
Bond angles

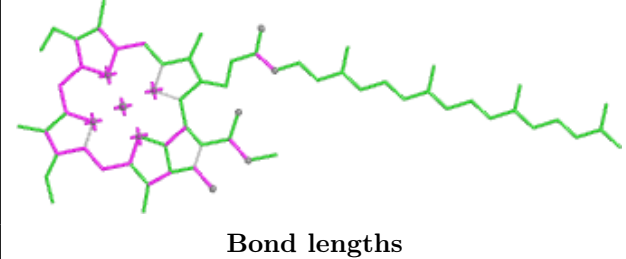
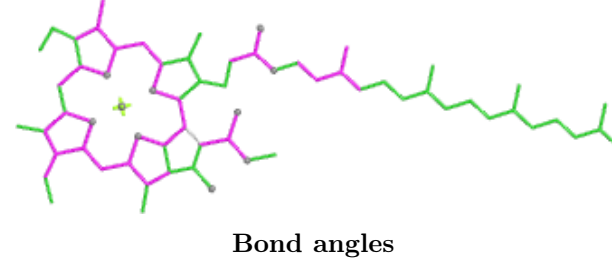
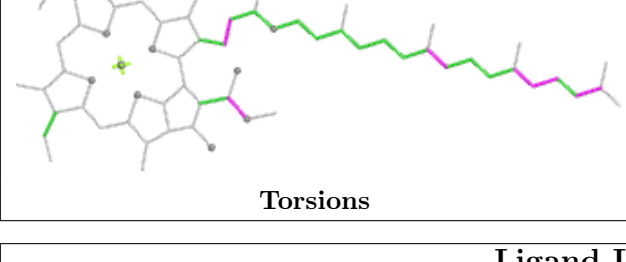
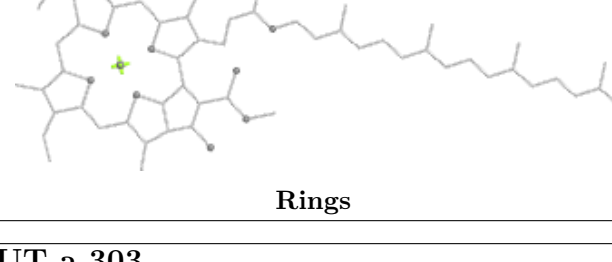


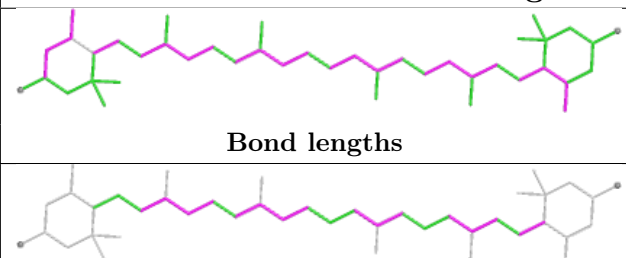
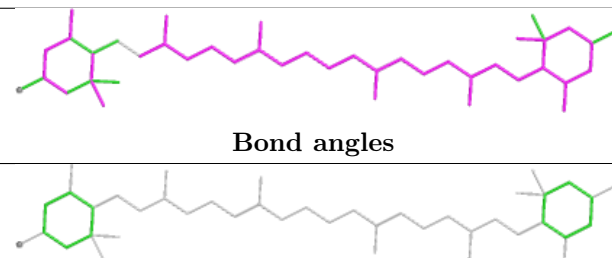
Torsions

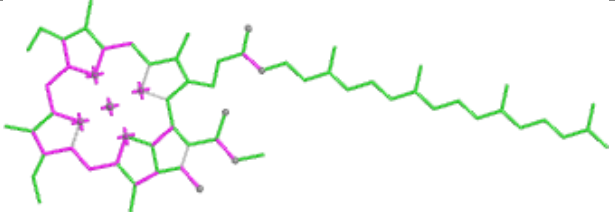
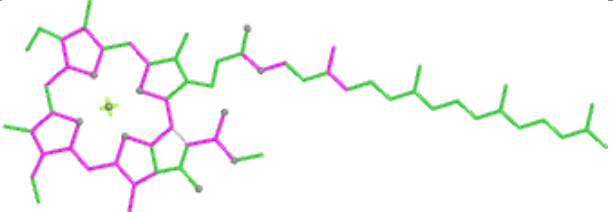
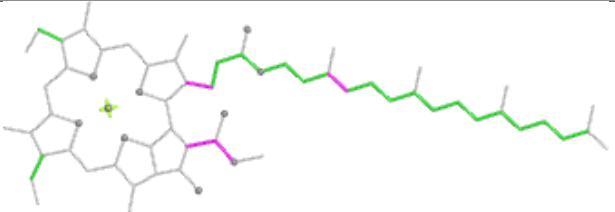
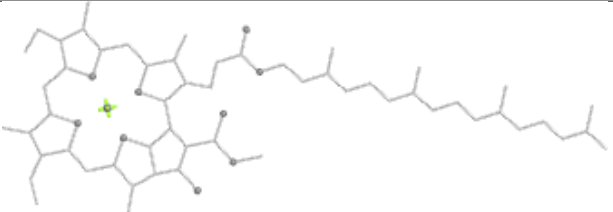
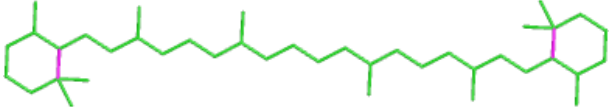
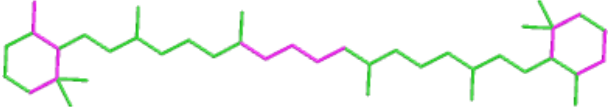
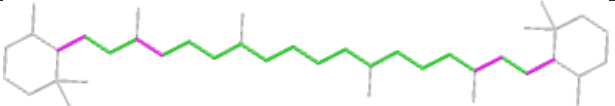
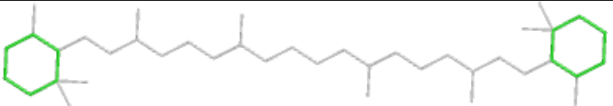
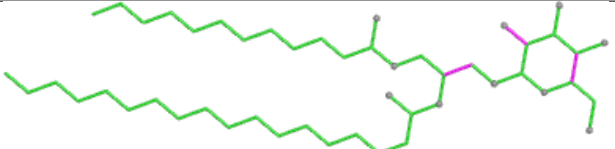
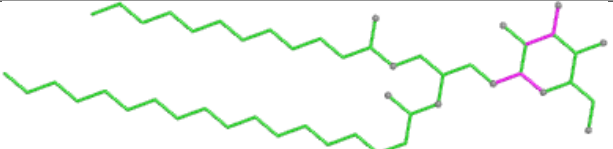
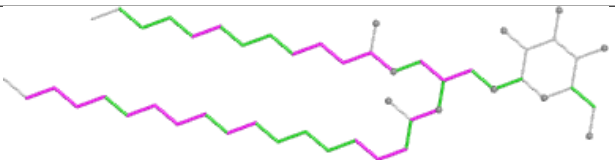
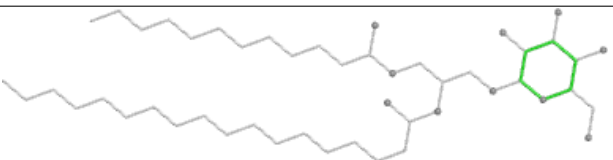


Rings

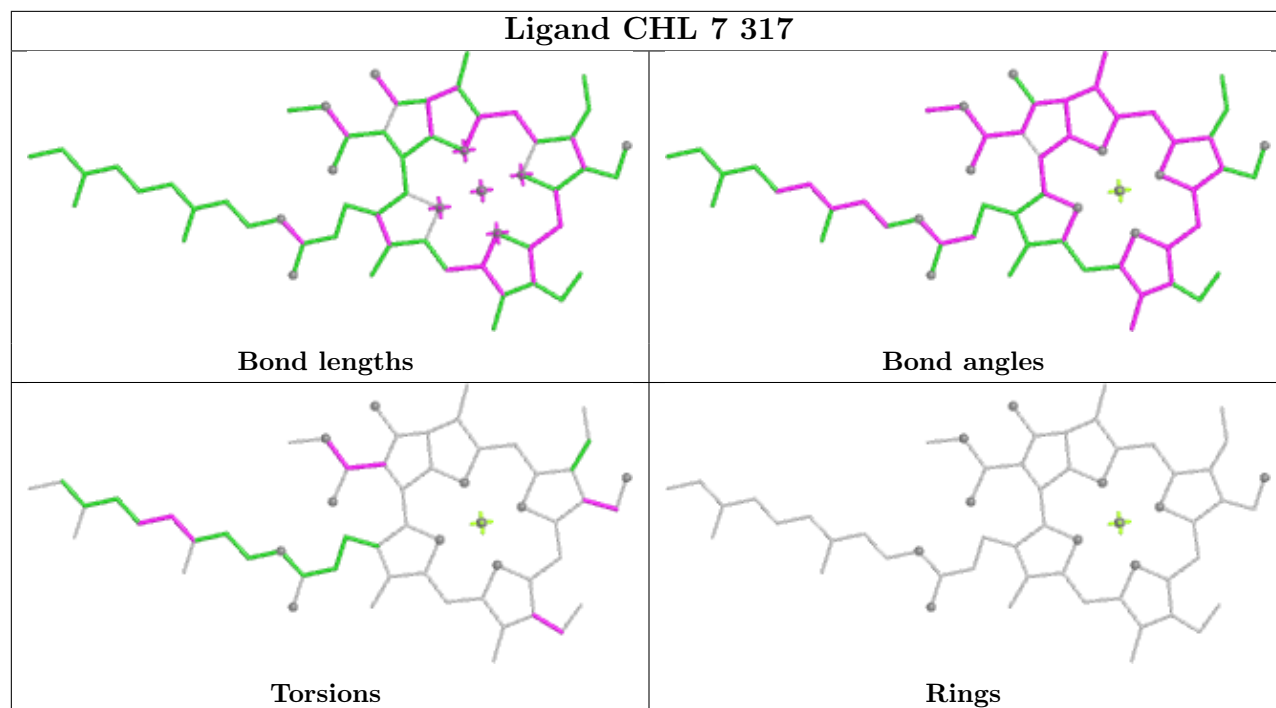
Ligand CLA B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

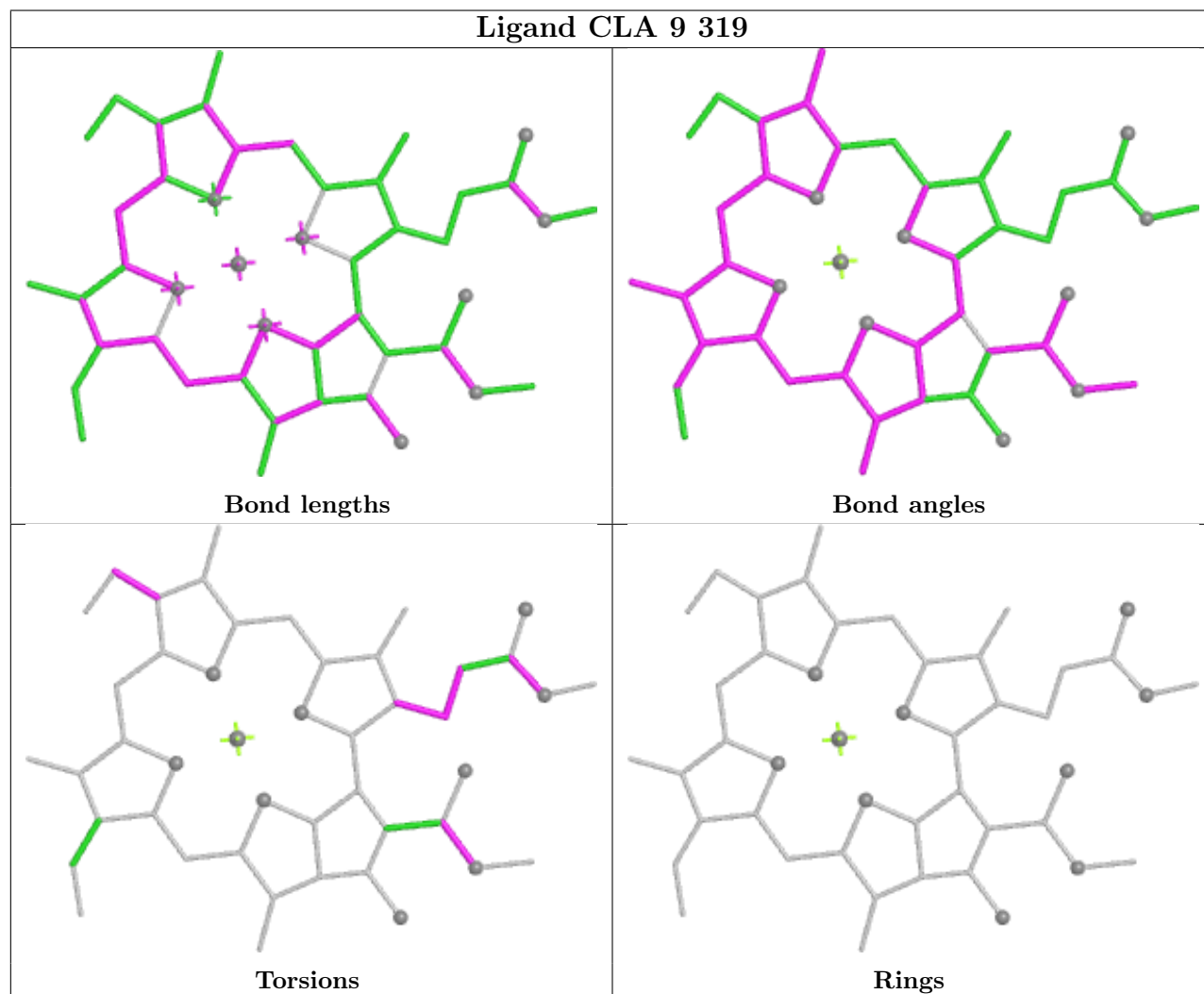
Ligand LUT a 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

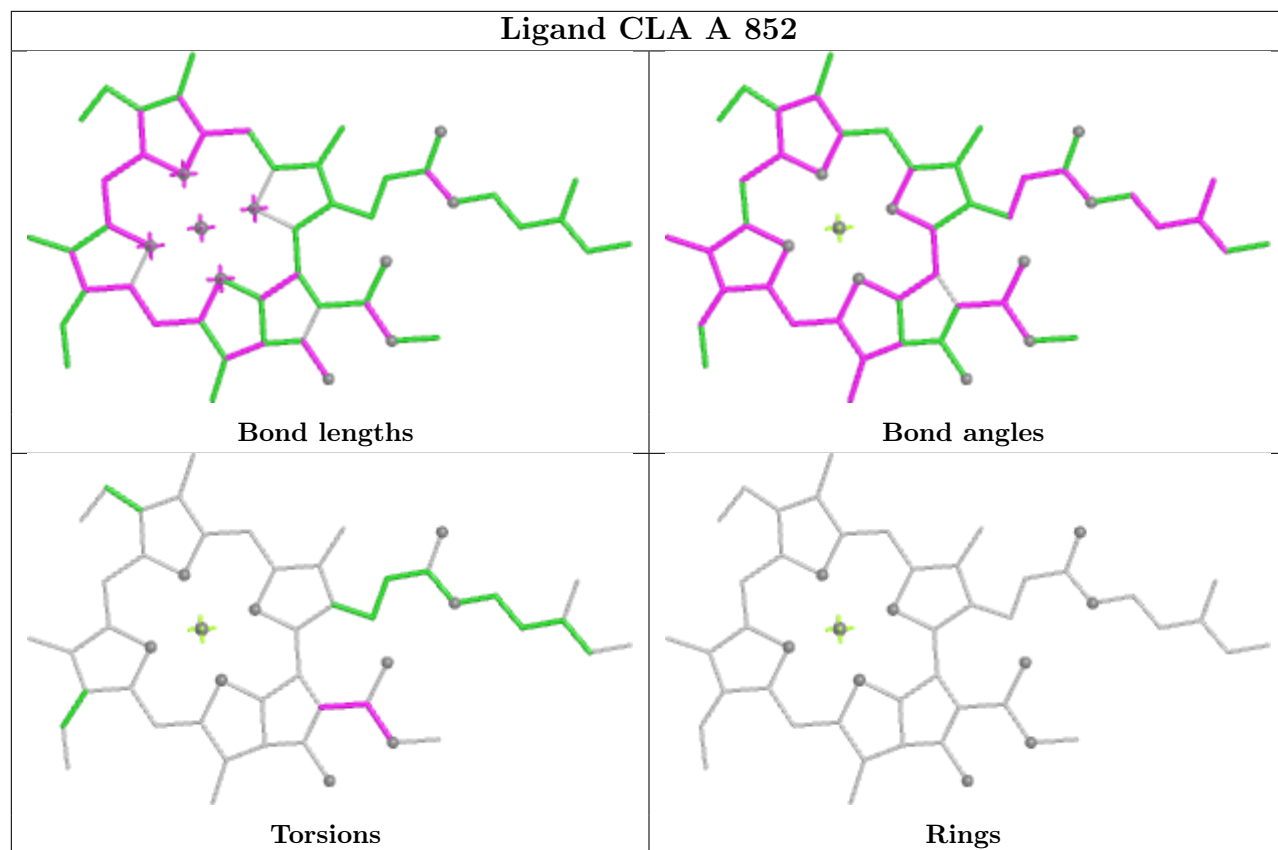
Ligand CLA B 836	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 302	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG J 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 7 317

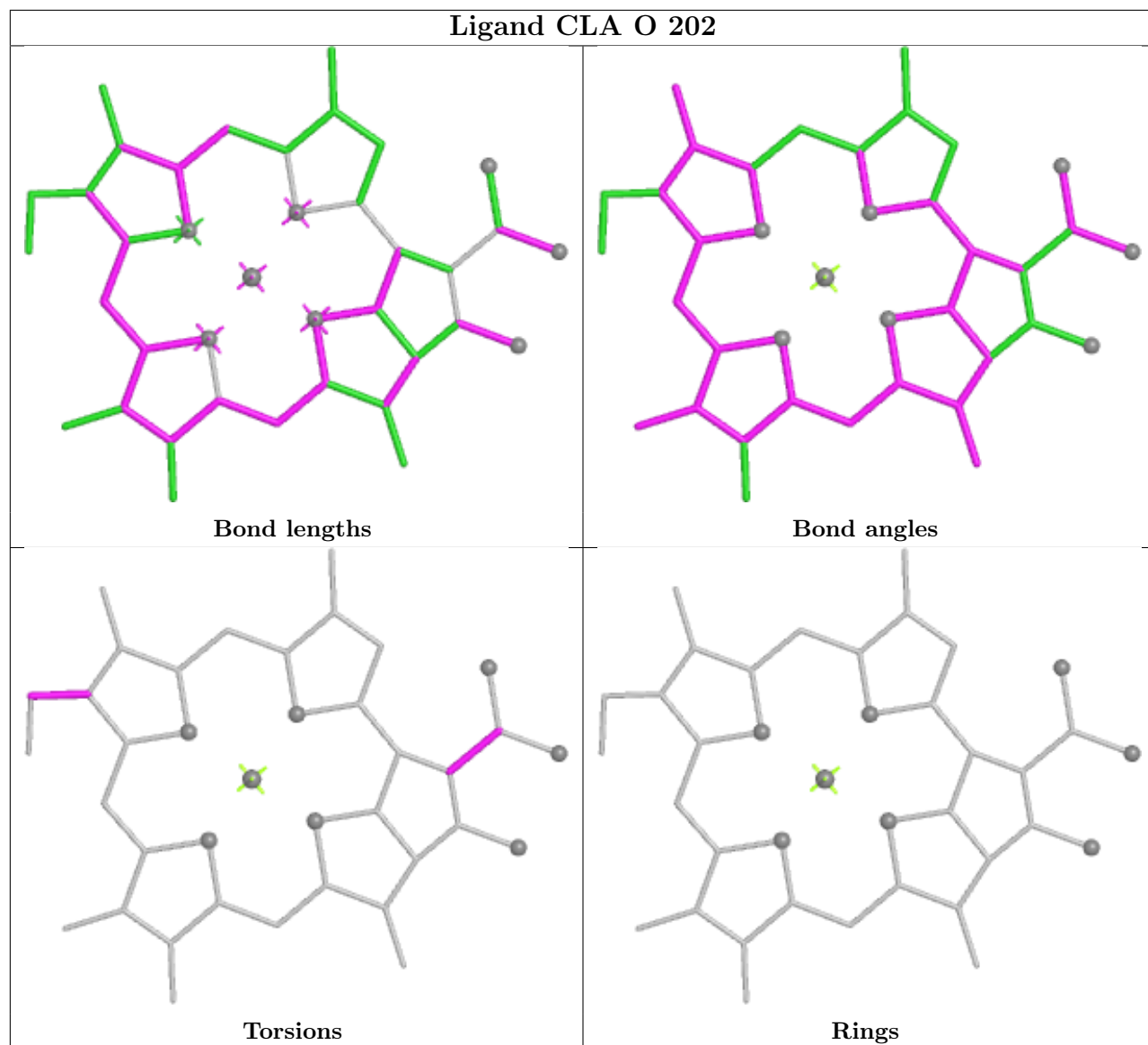


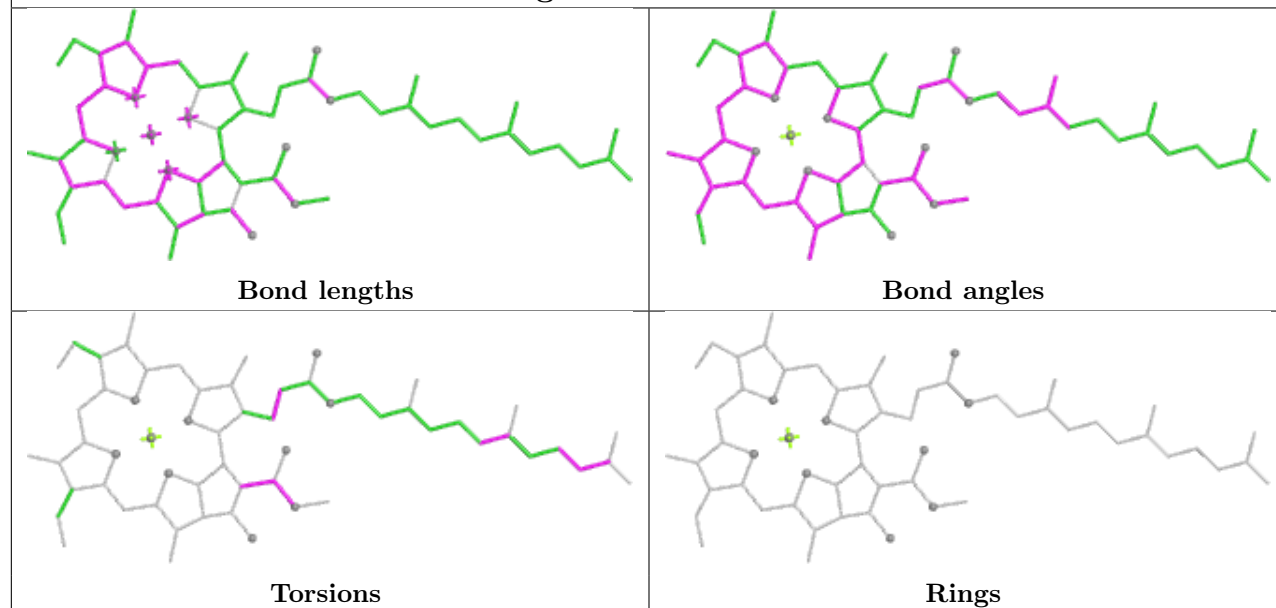
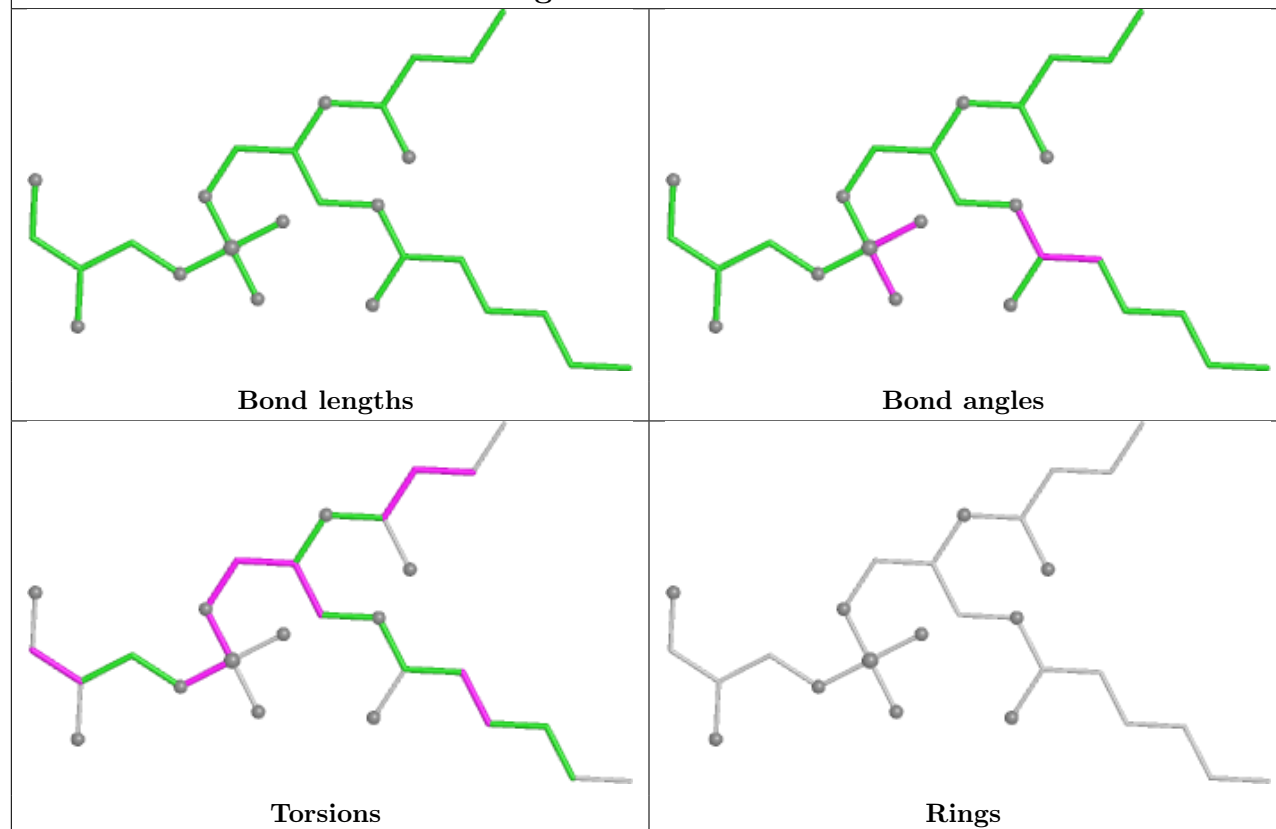
Ligand CLA 9 319

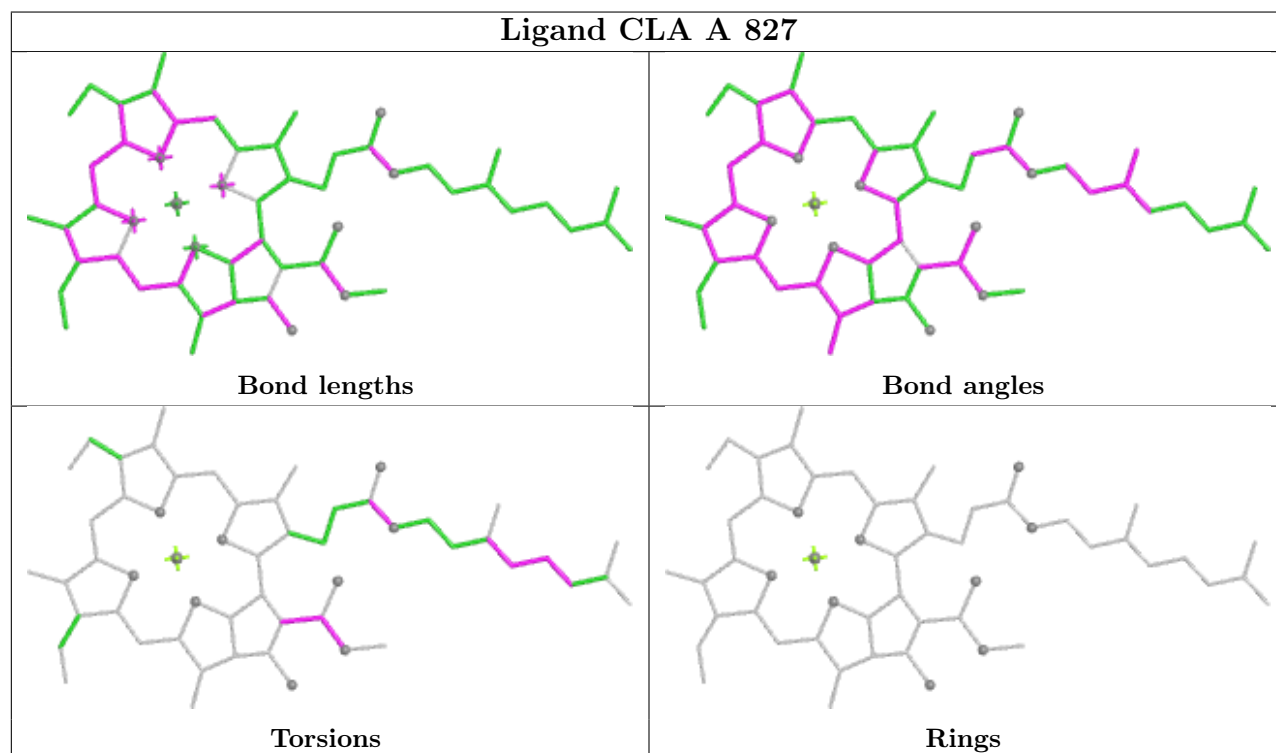
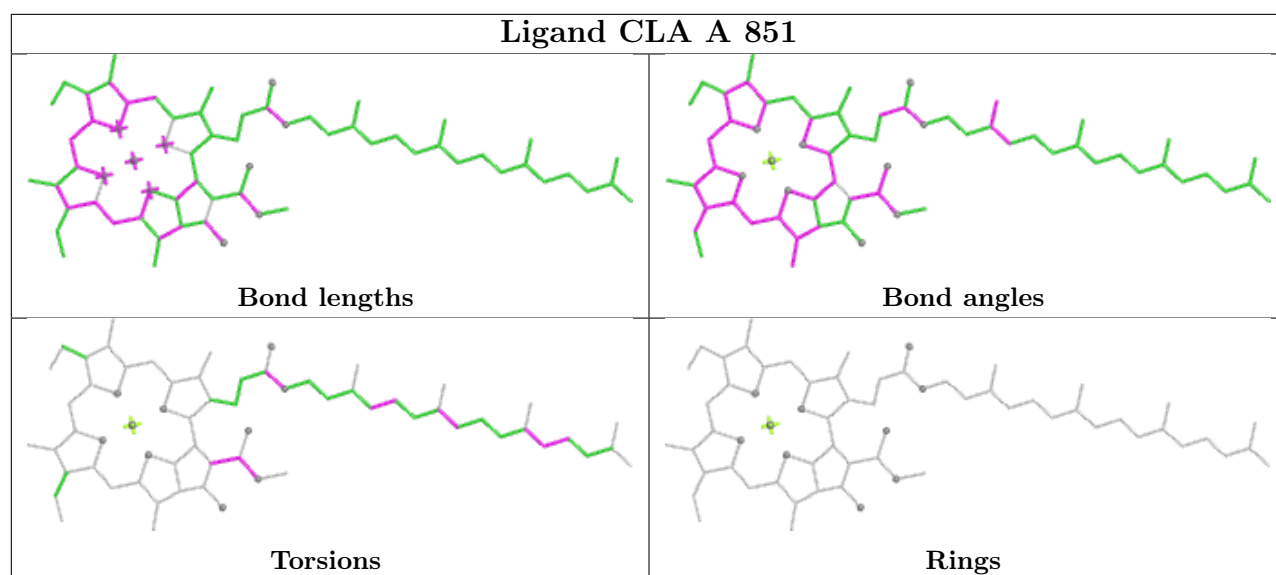


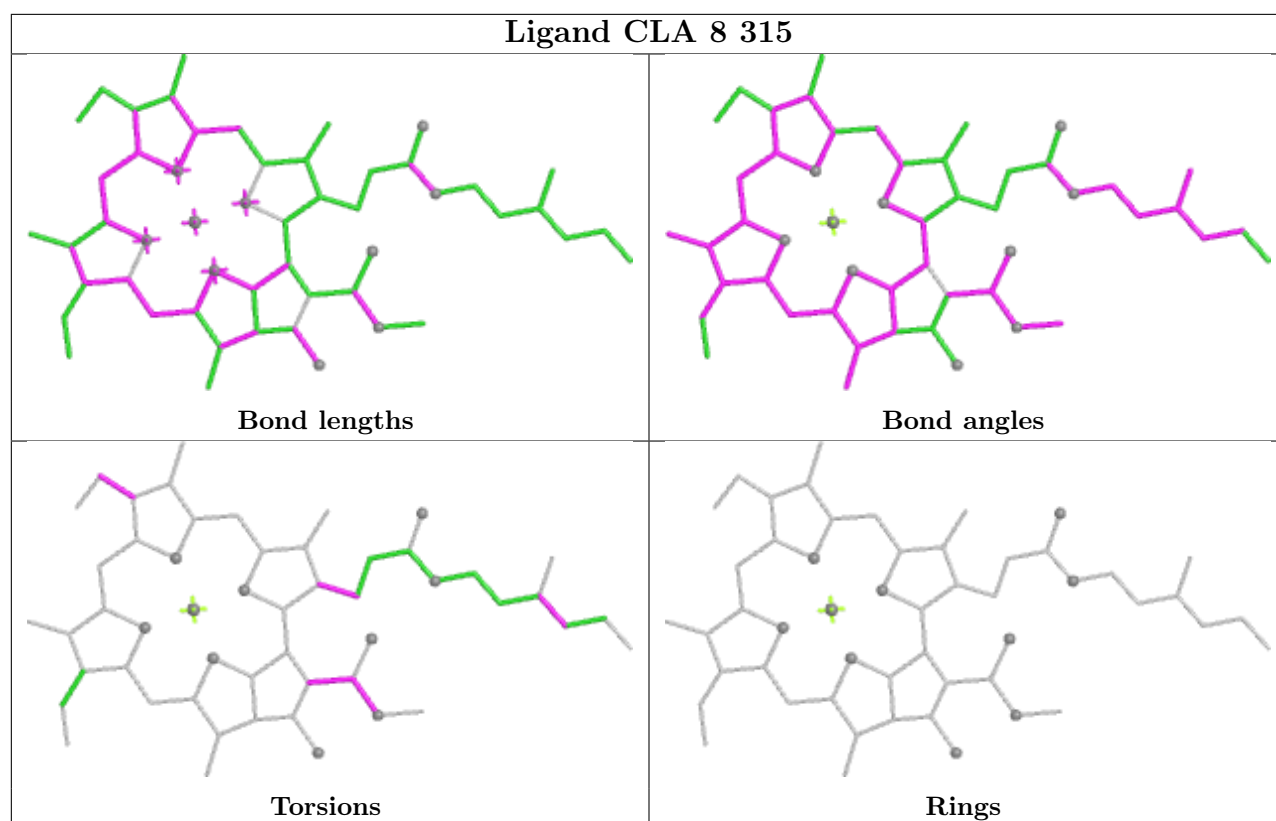


Ligand CLA O 202

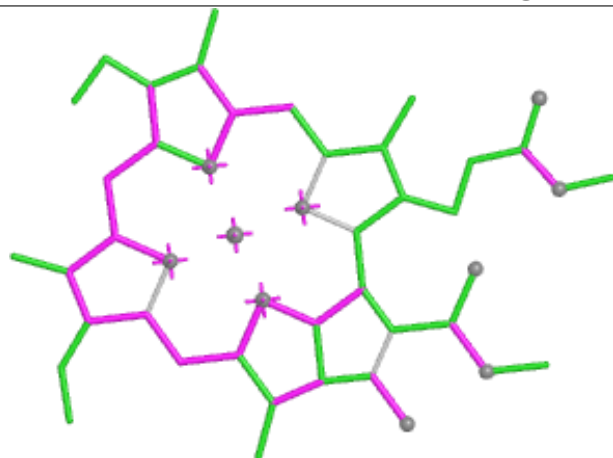


Ligand CLA 9 314**Ligand LHG 6 301**

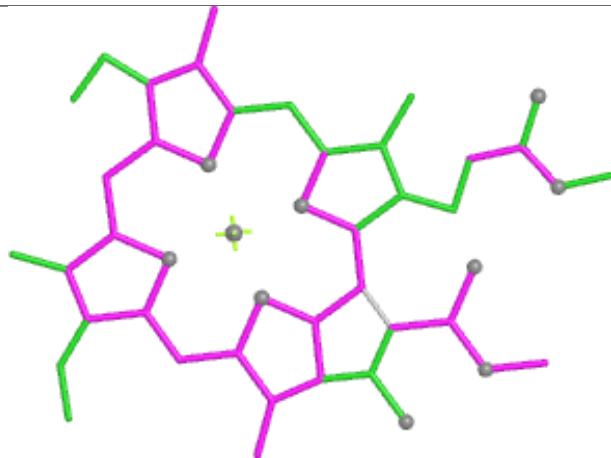




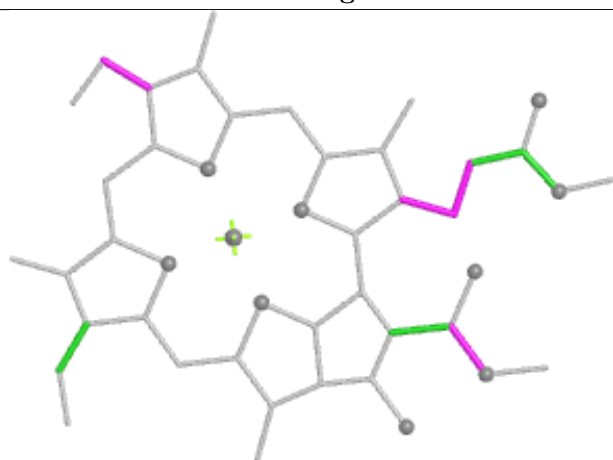
Ligand CLA b 311



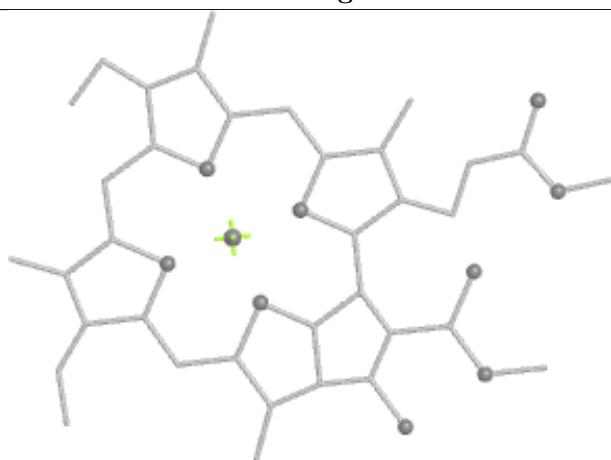
Bond lengths



Bond angles

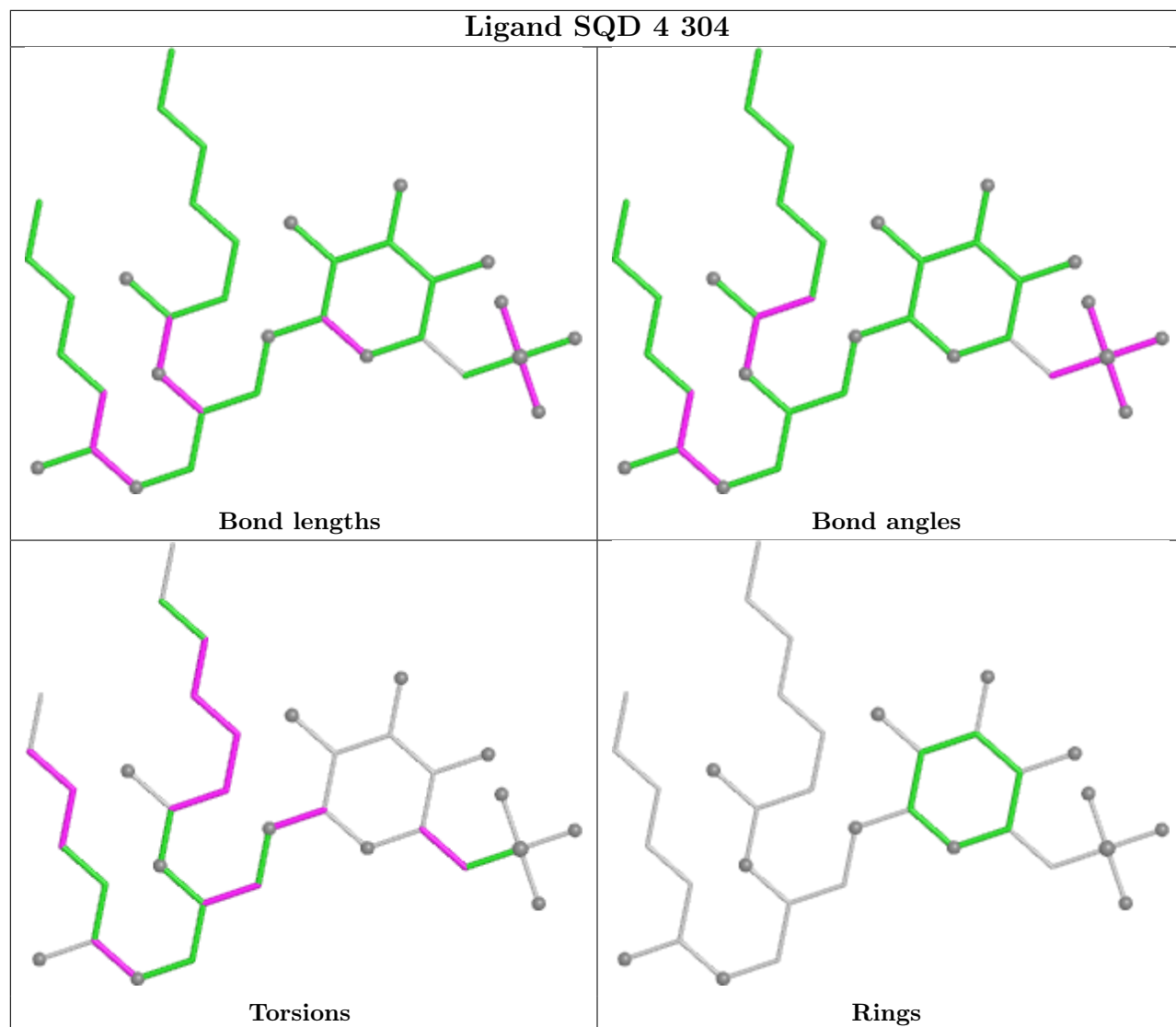


Torsions

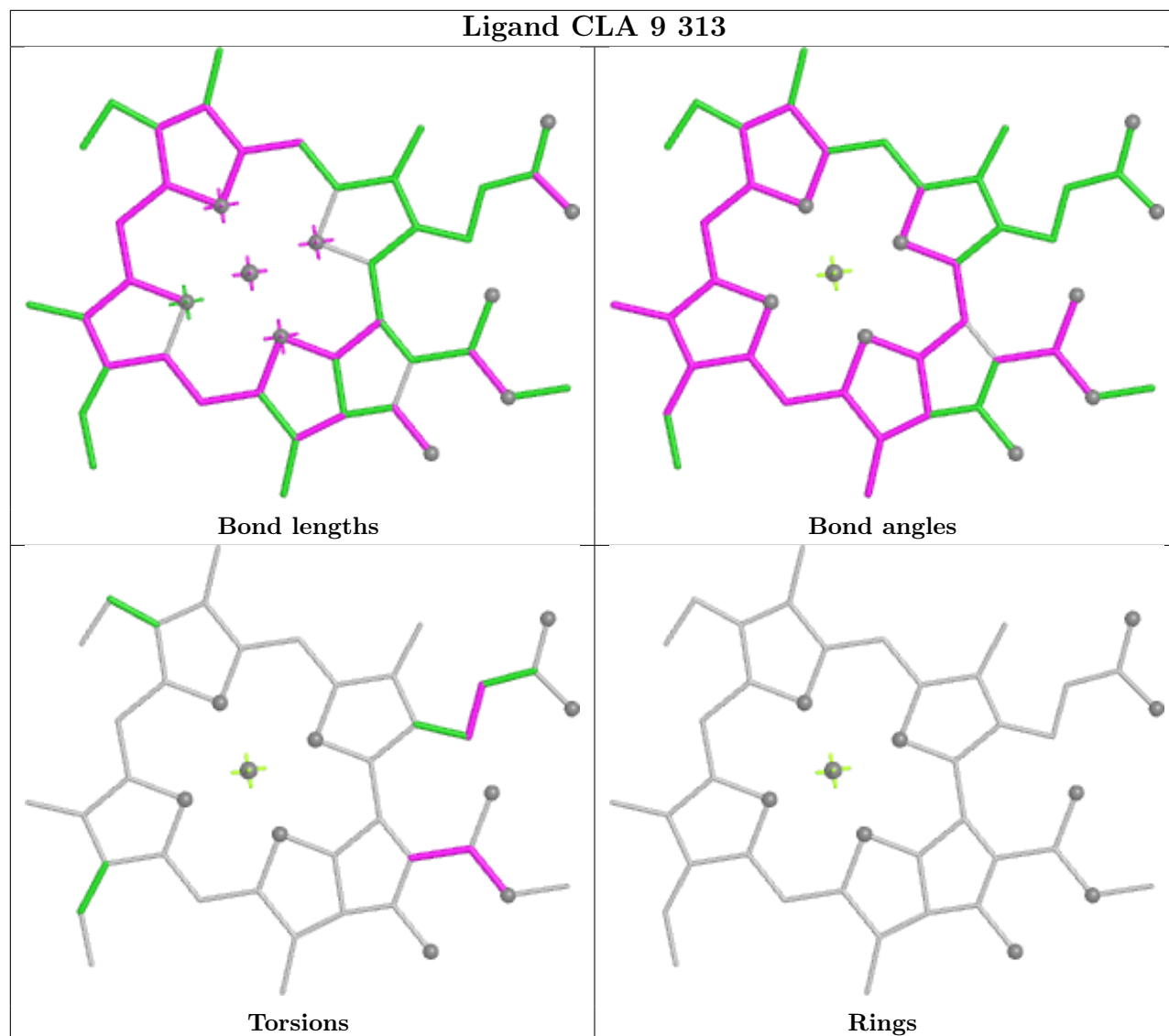


Rings

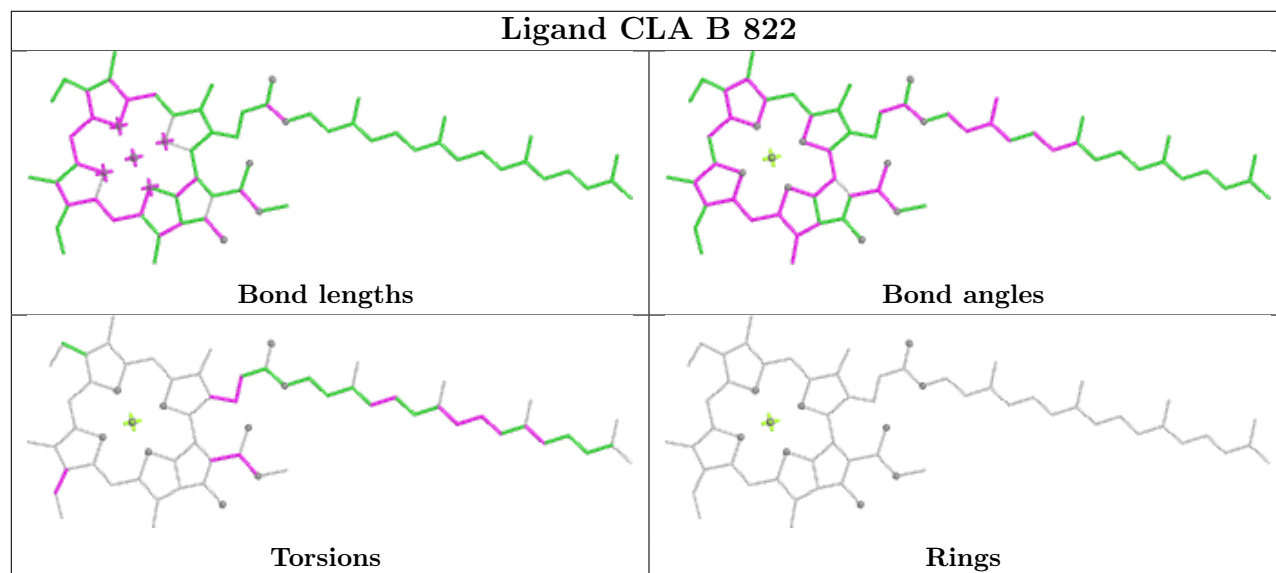
Ligand SQD 4 304



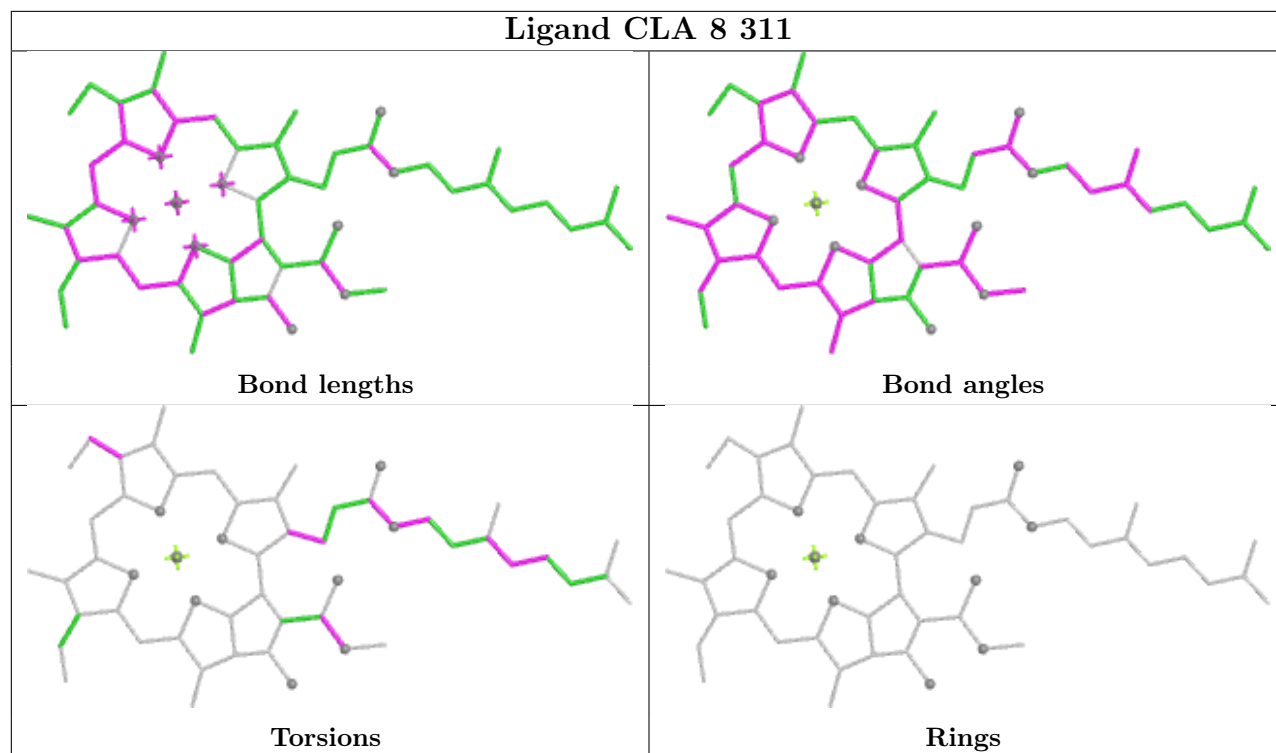
Ligand CLA 9 313



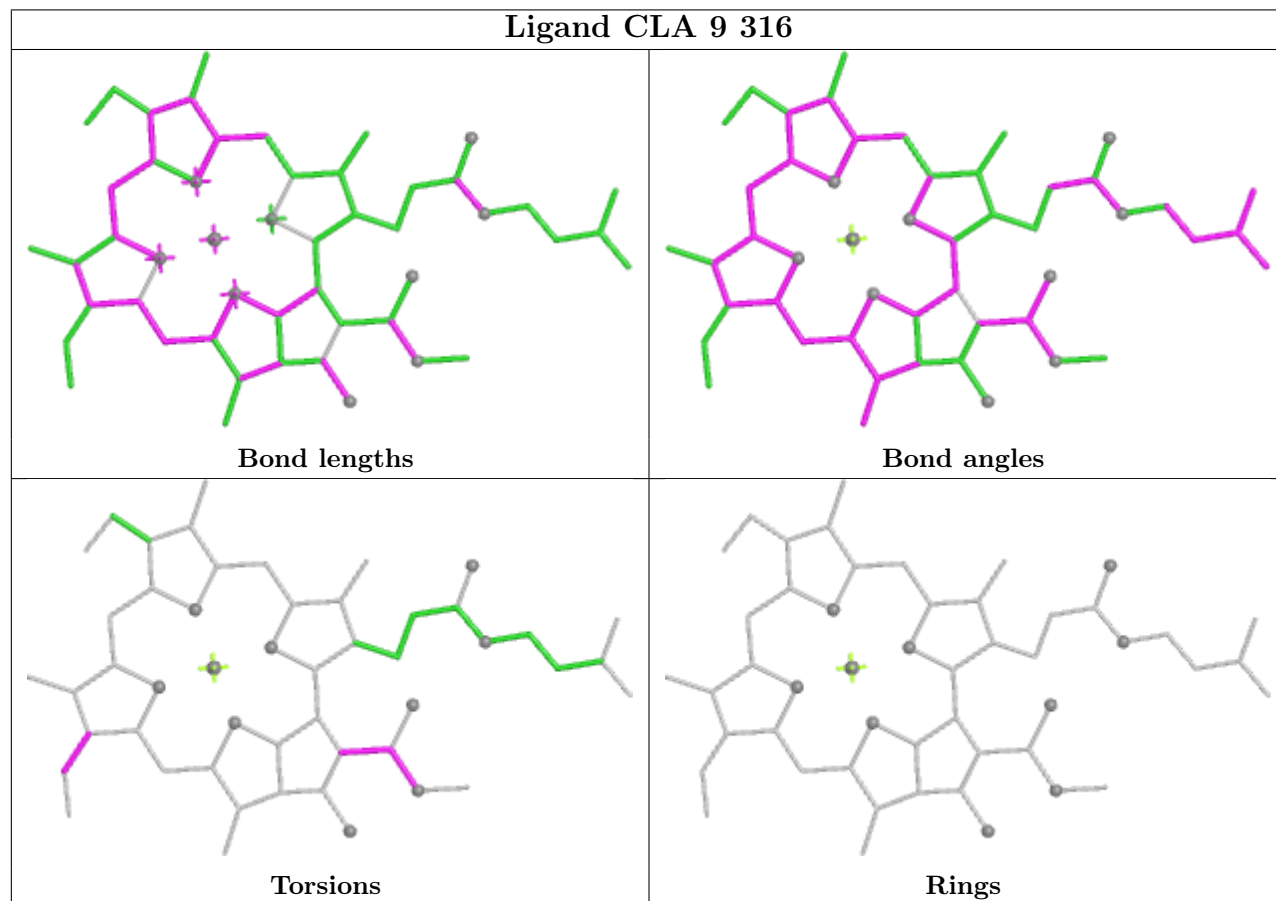
Ligand CLA B 822

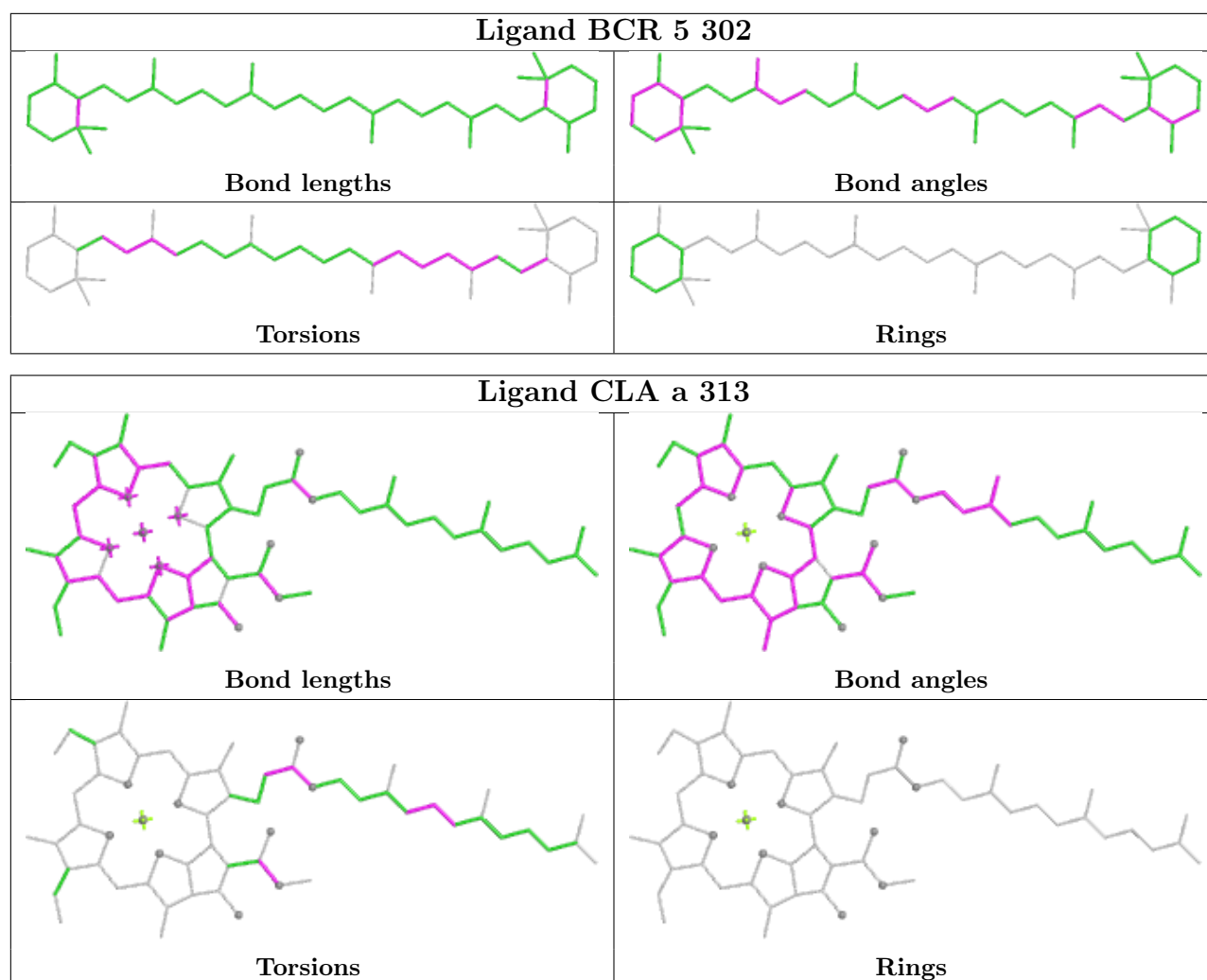


Ligand CLA 8 311

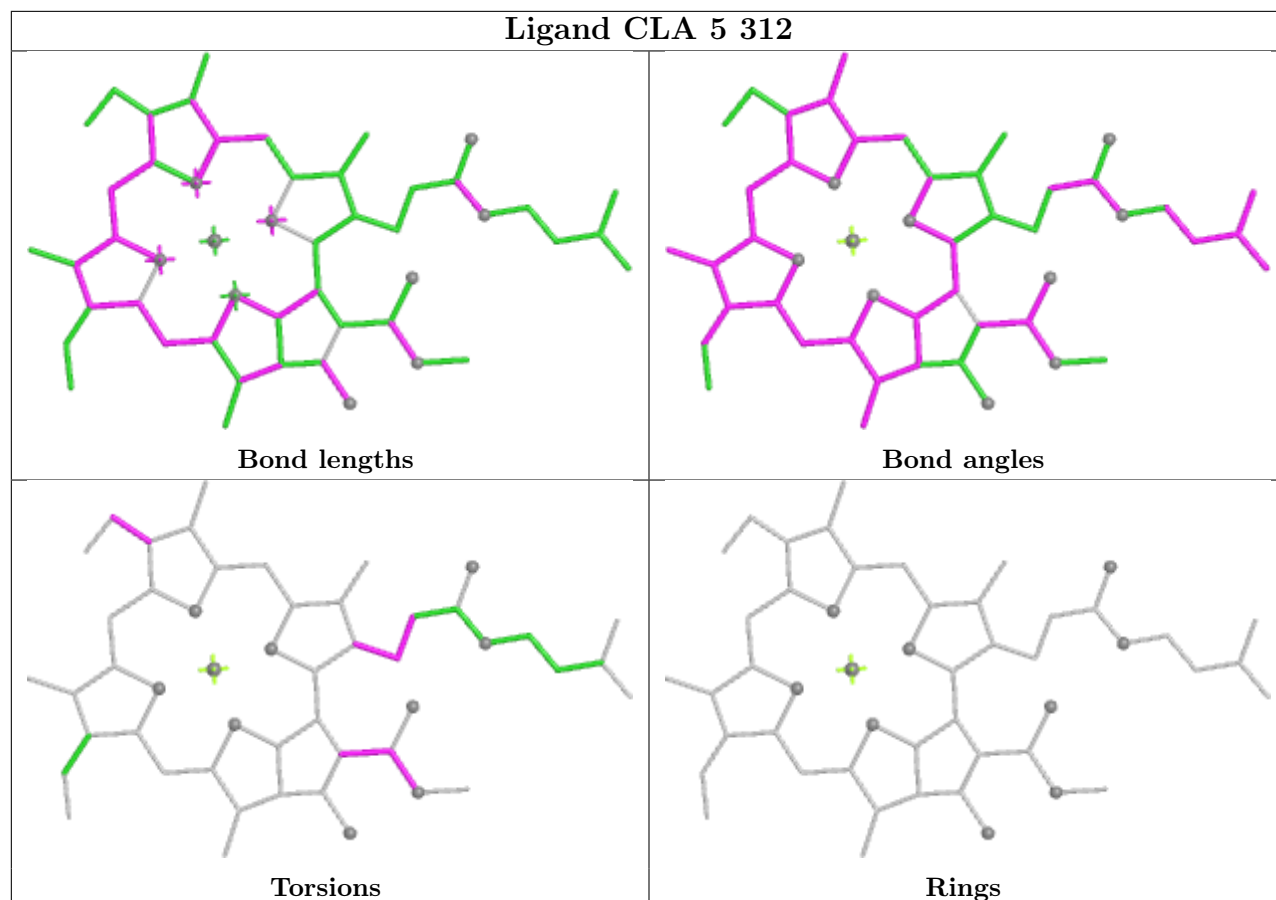


Ligand CLA 9 316

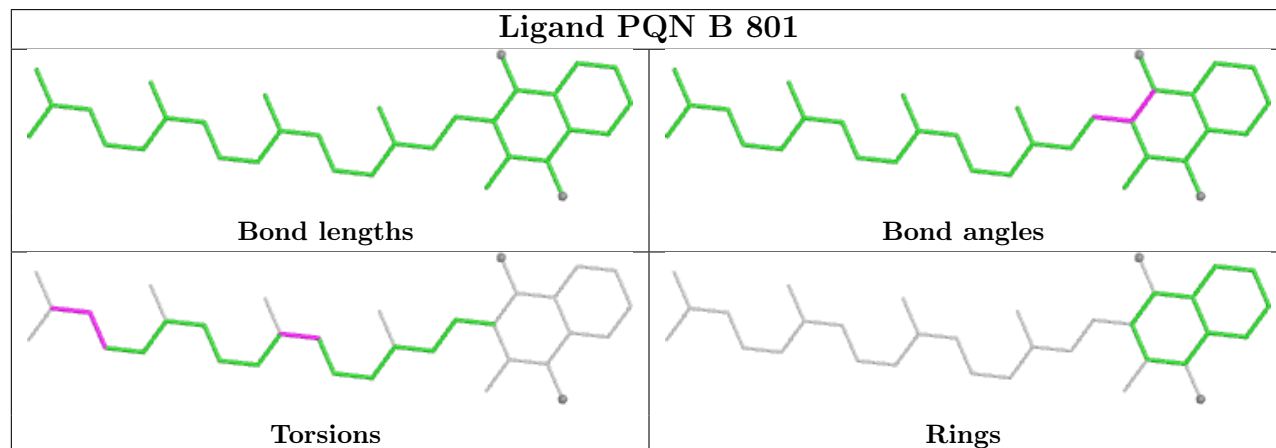




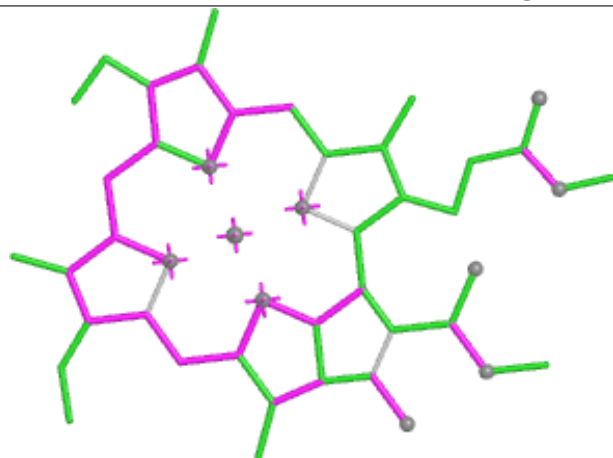
Ligand CLA 5 312



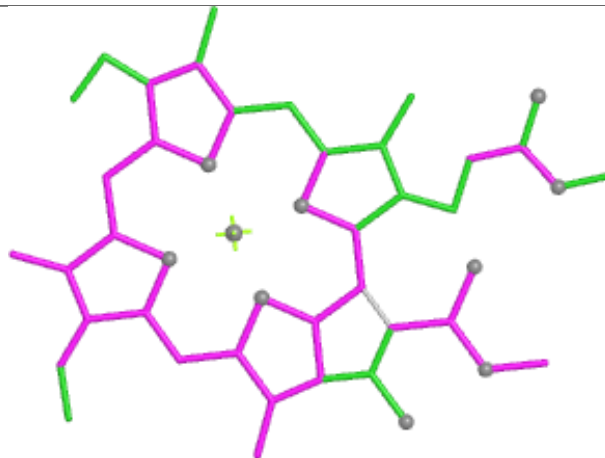
Ligand PQN B 801



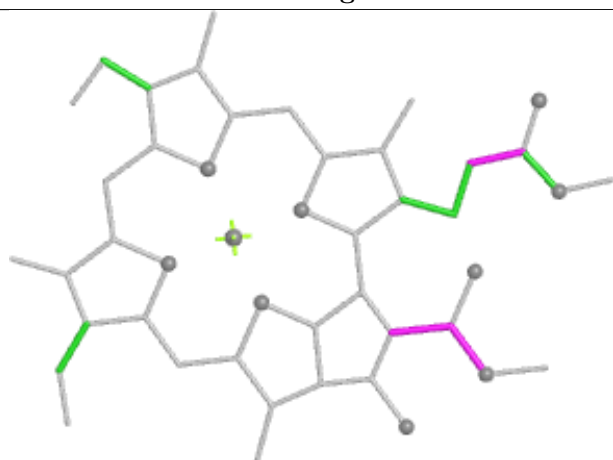
Ligand CLA 6 313



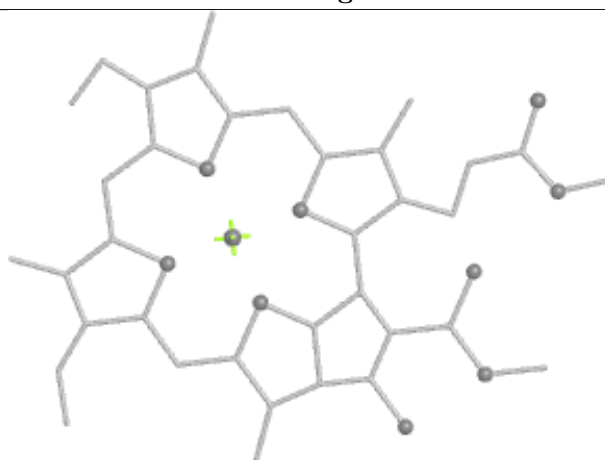
Bond lengths



Bond angles

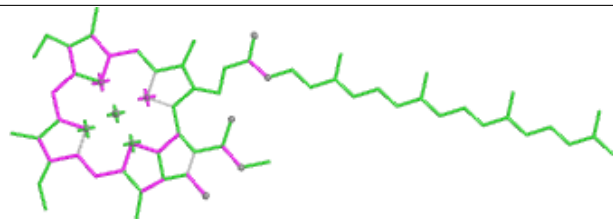


Torsions

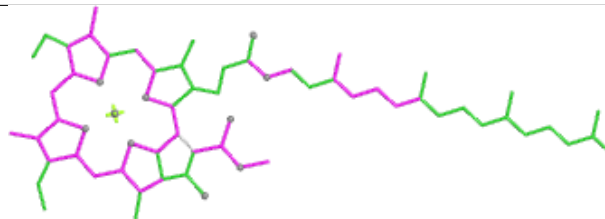


Rings

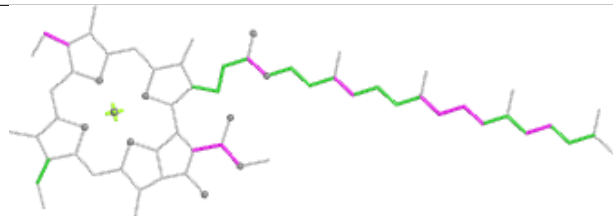
Ligand CLA a 319



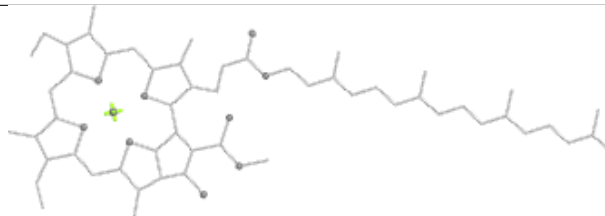
Bond lengths



Bond angles

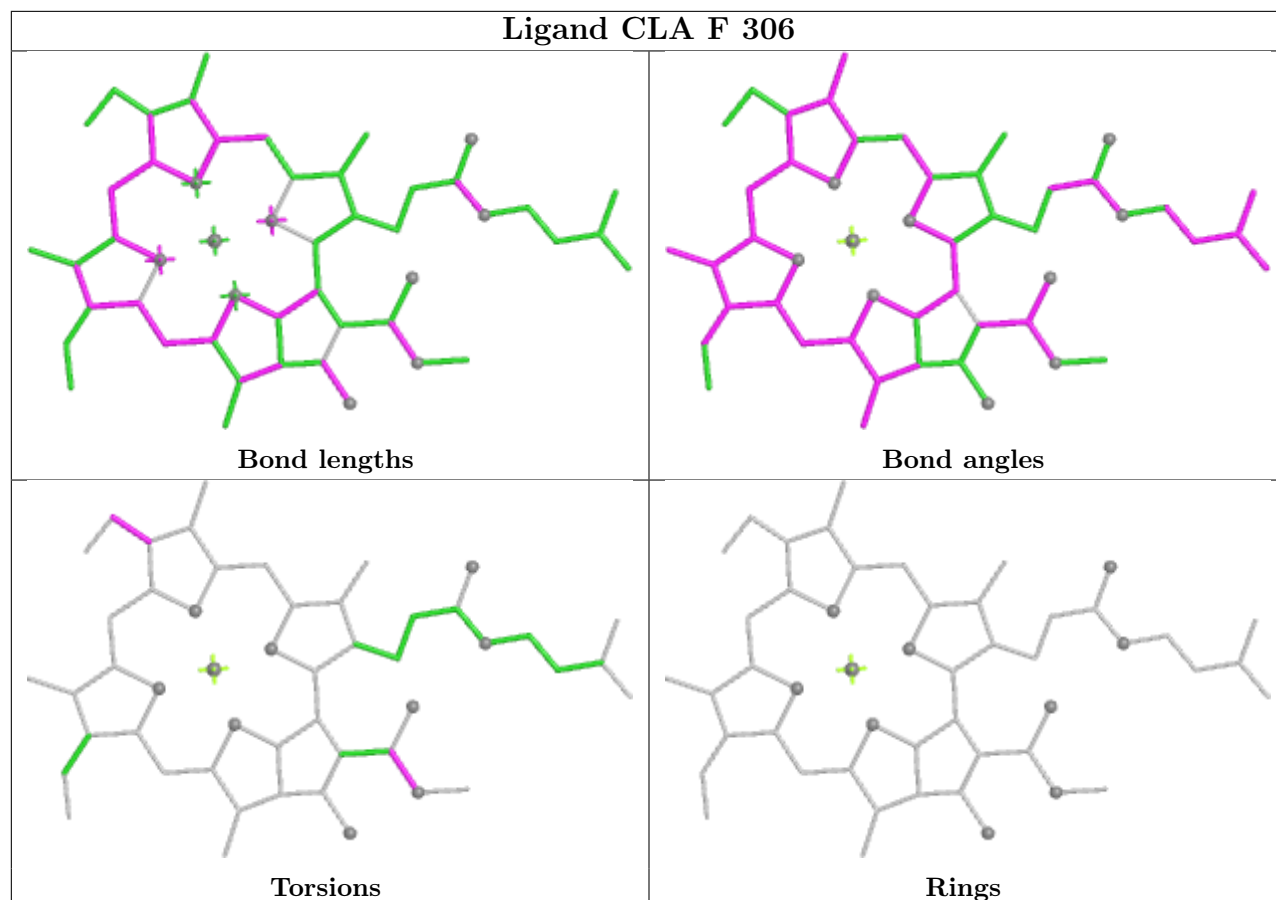


Torsions

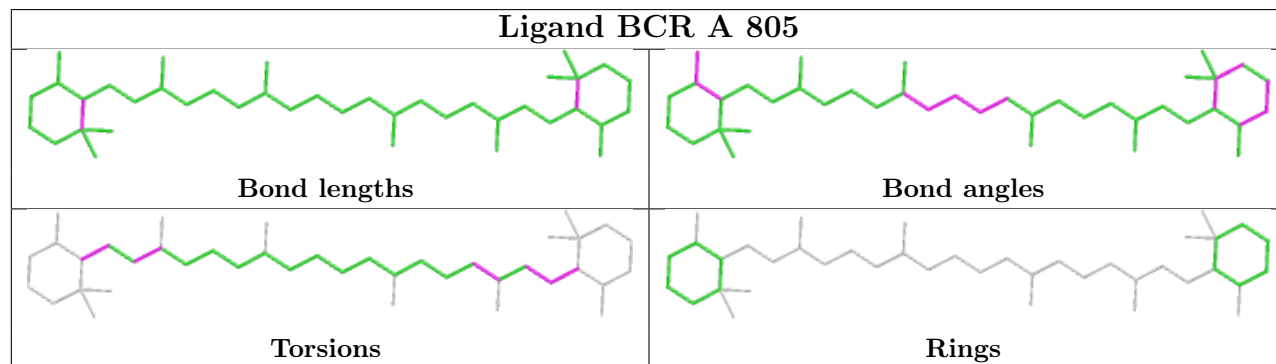


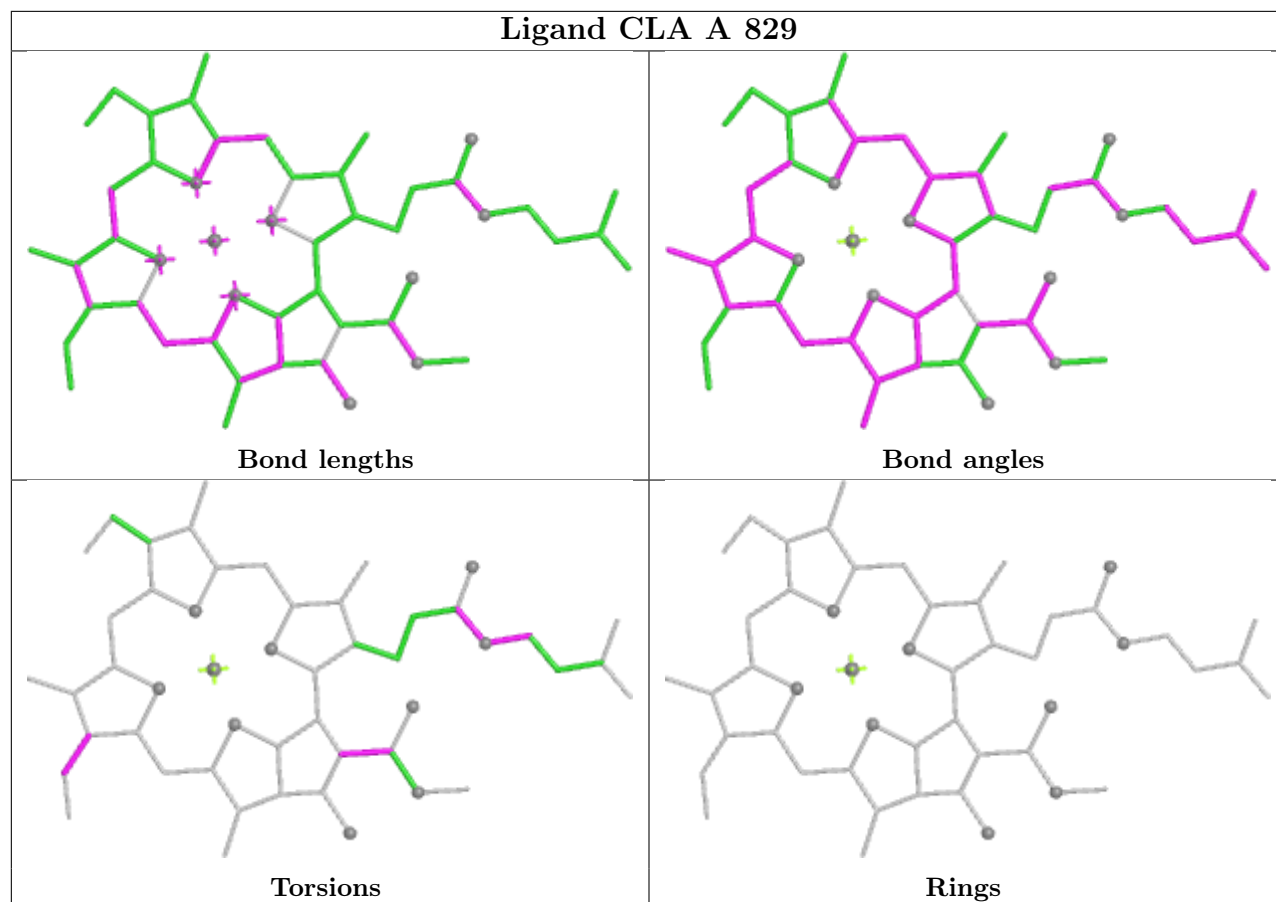
Rings

Ligand CLA F 306

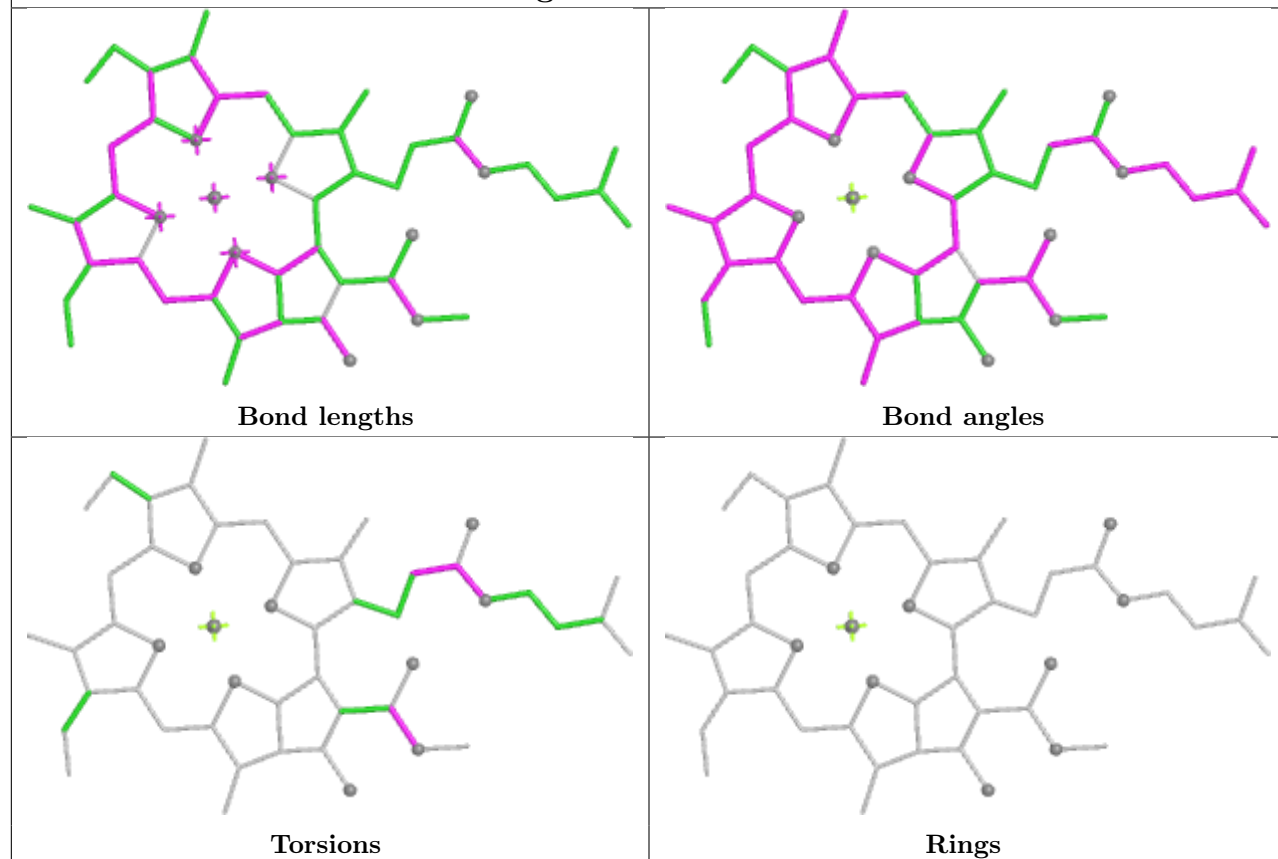


Ligand BCR A 805

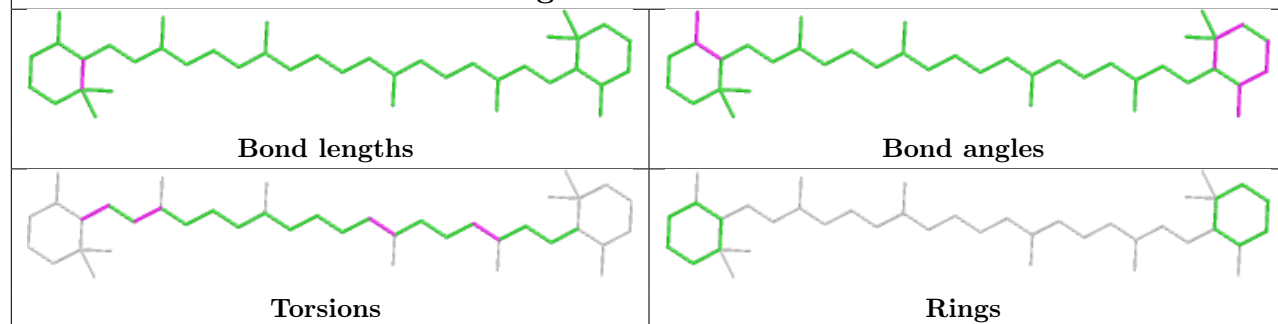




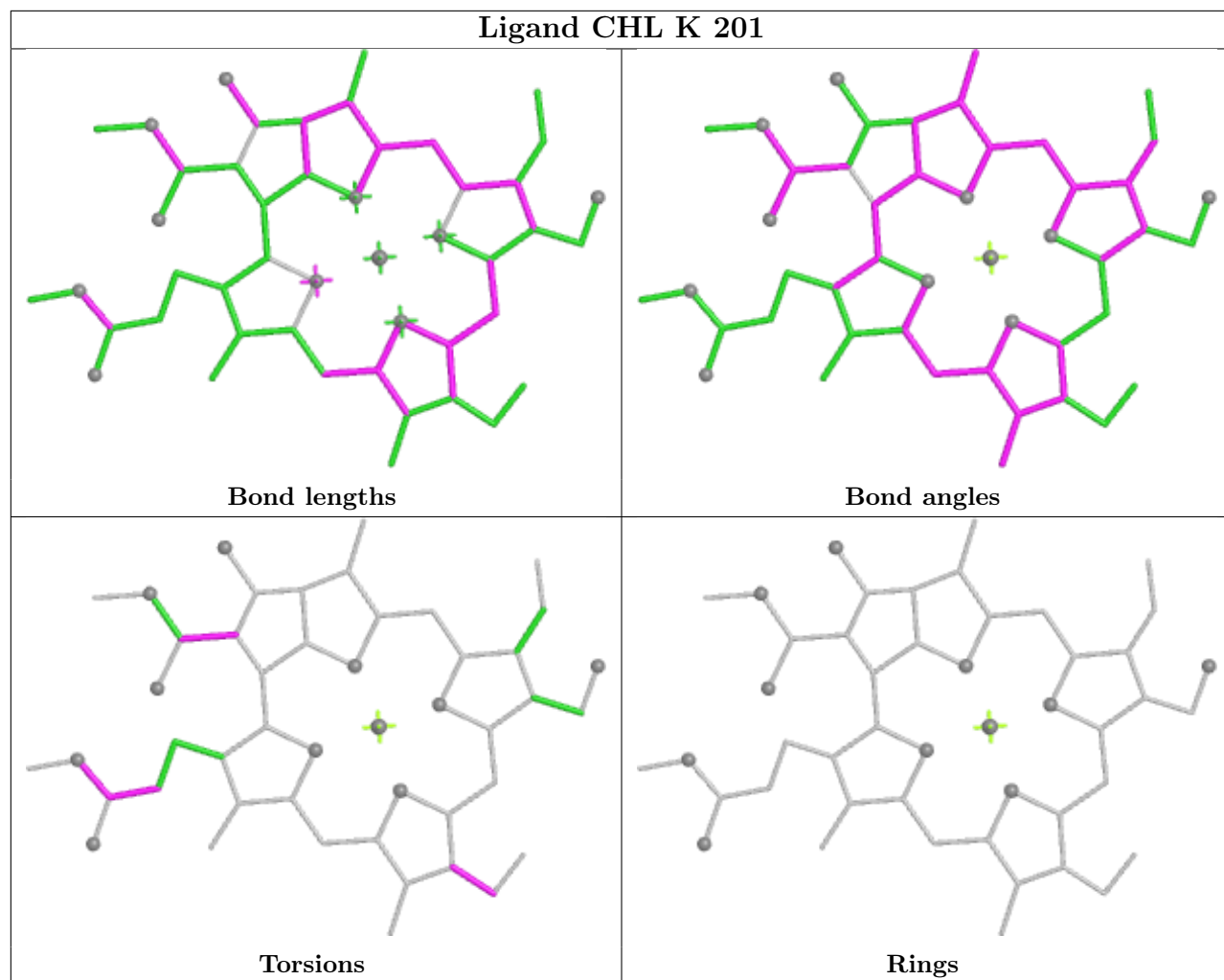
Ligand CLA 8 309

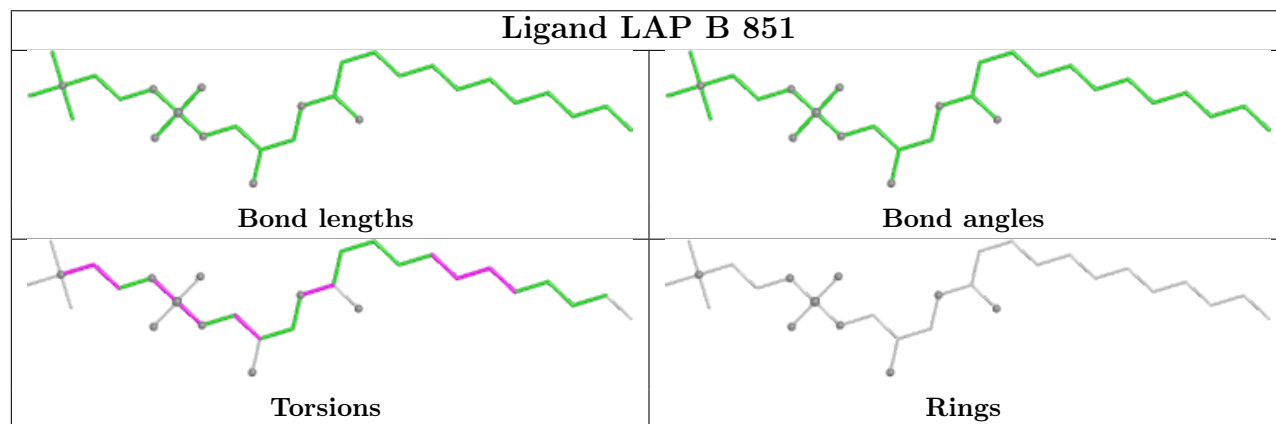
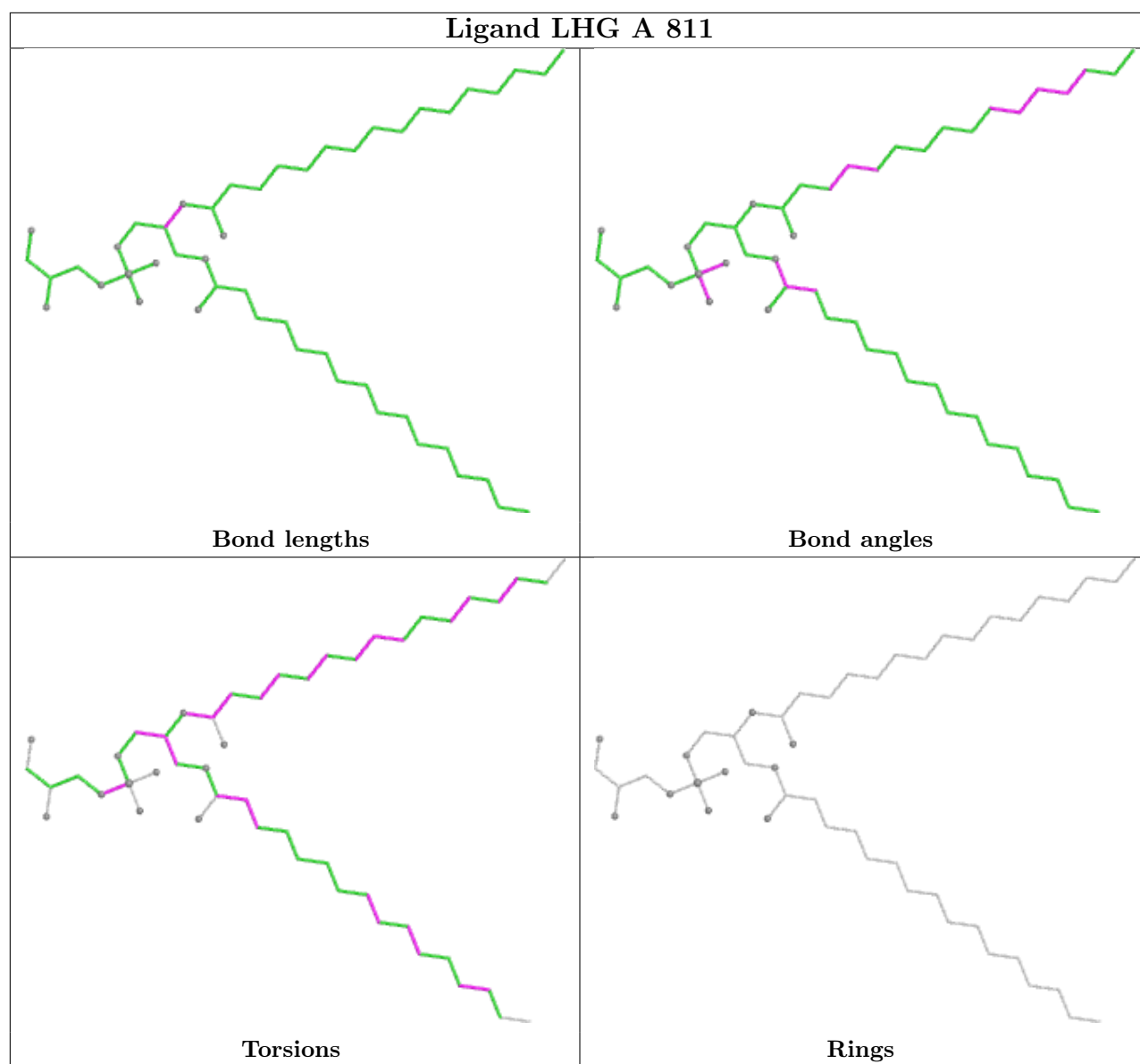


Ligand BCR I 801

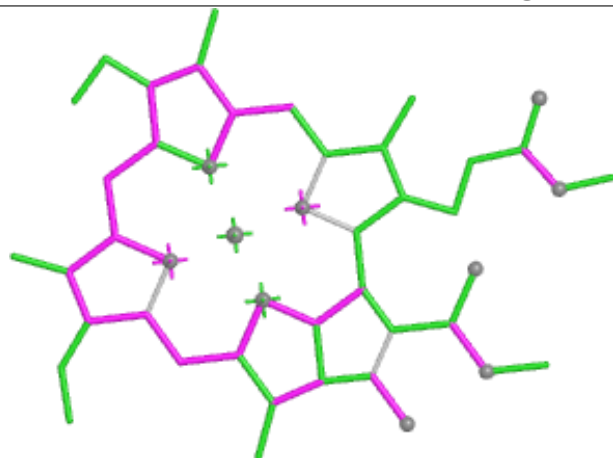


Ligand CHL K 201

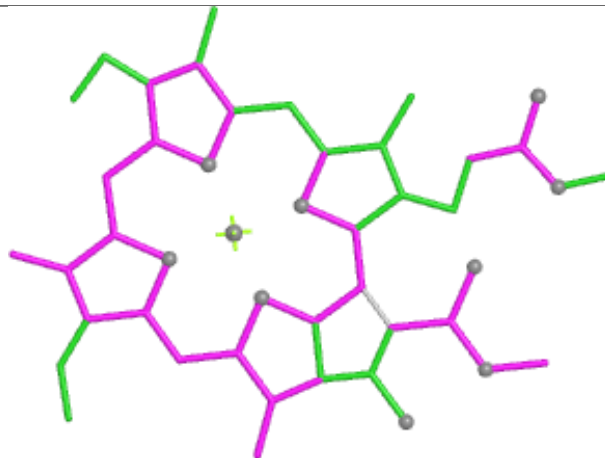




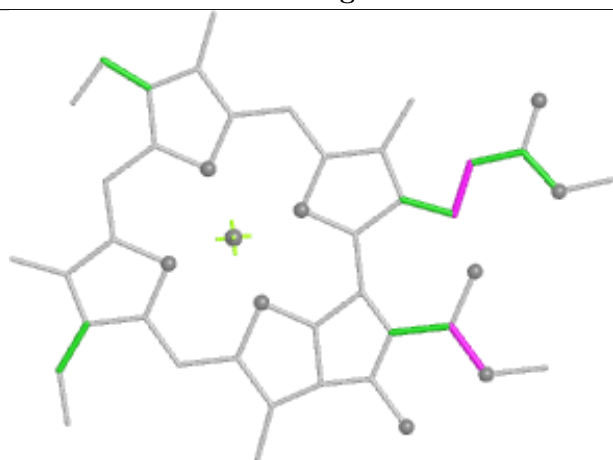
Ligand CLA 2 308



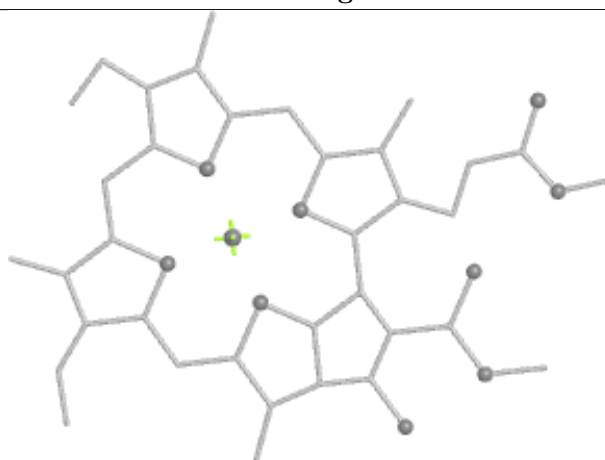
Bond lengths



Bond angles

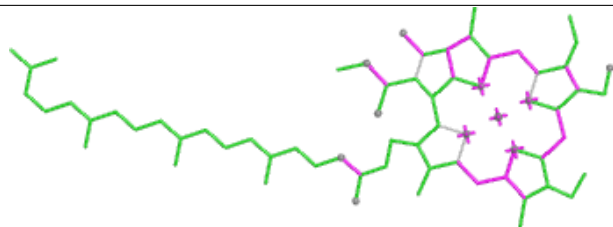


Torsions

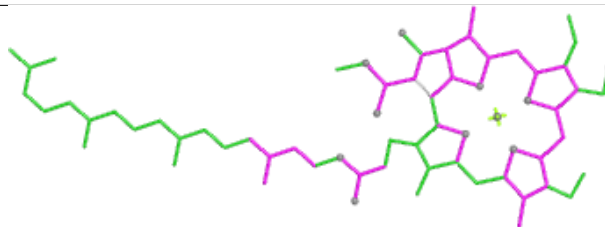


Rings

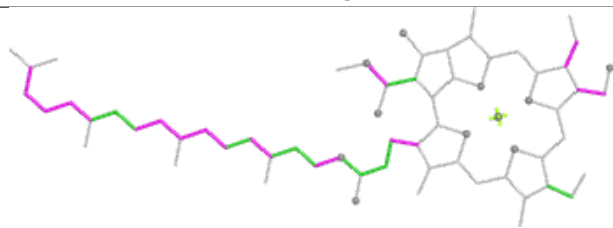
Ligand CHL 7 318



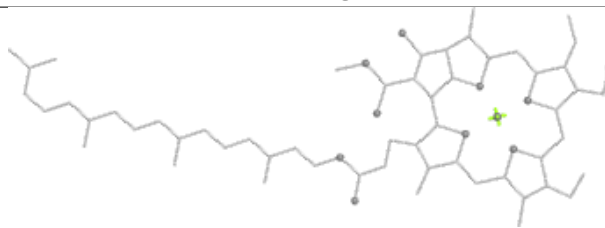
Bond lengths



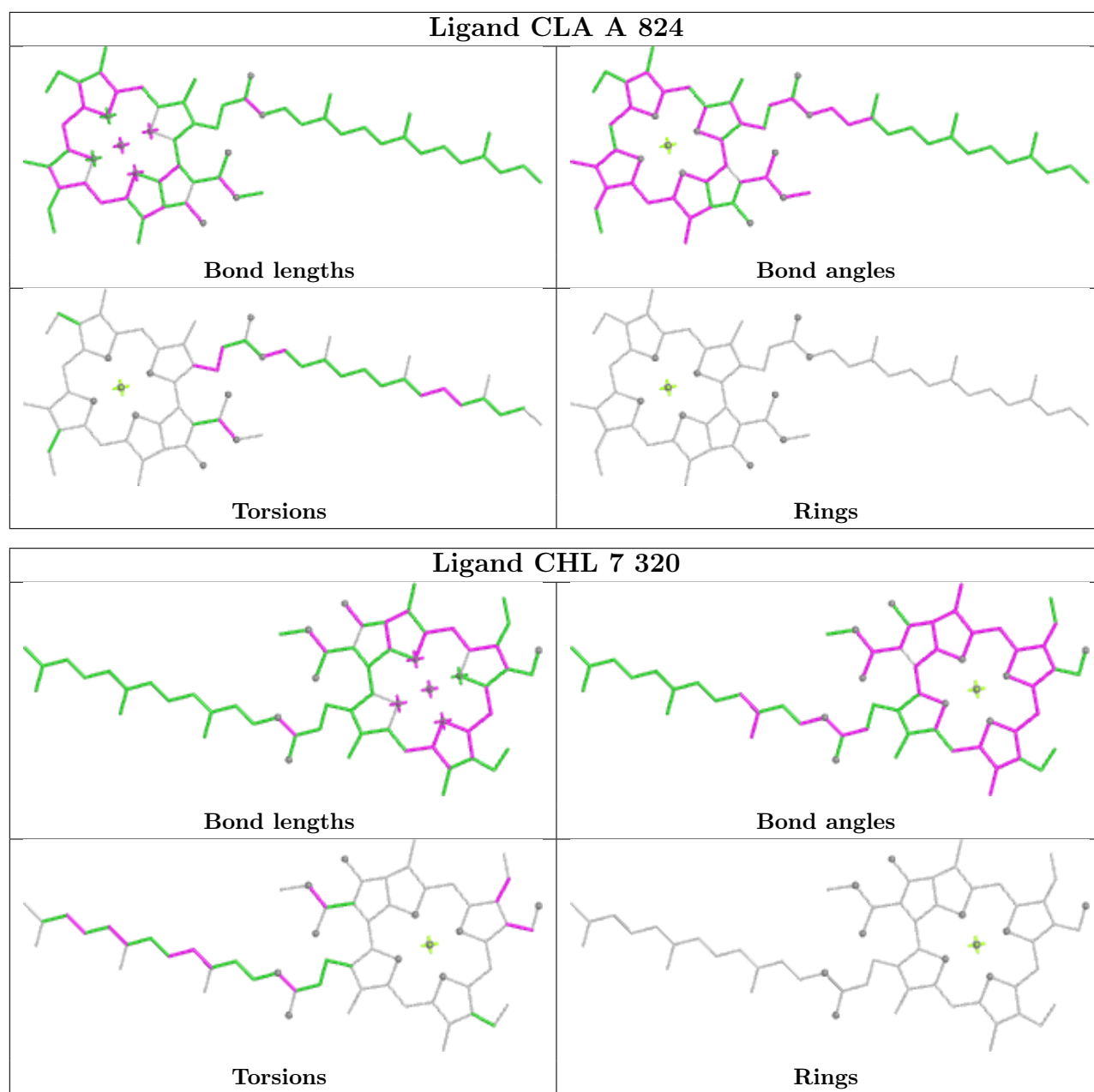
Bond angles



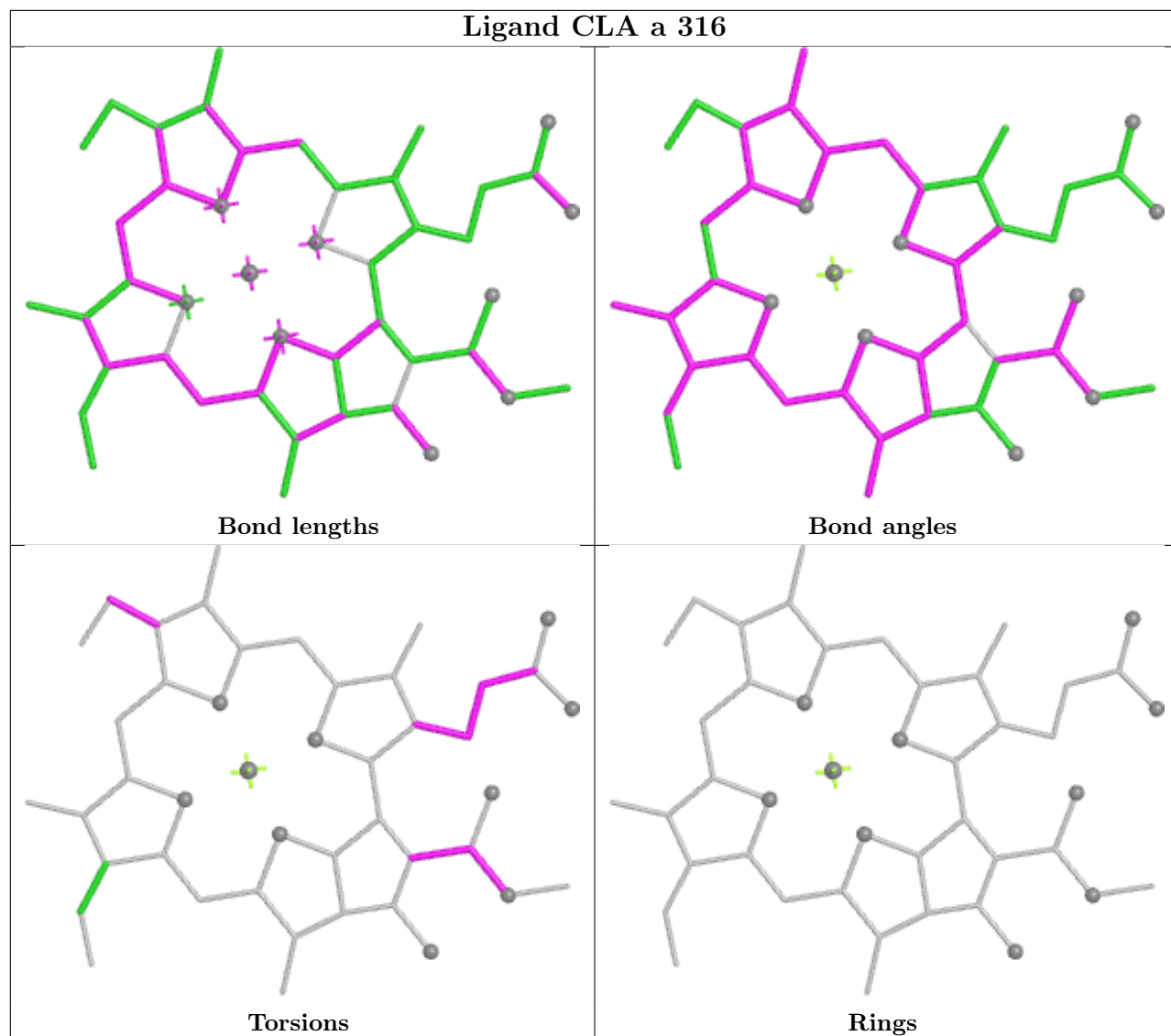
Torsions



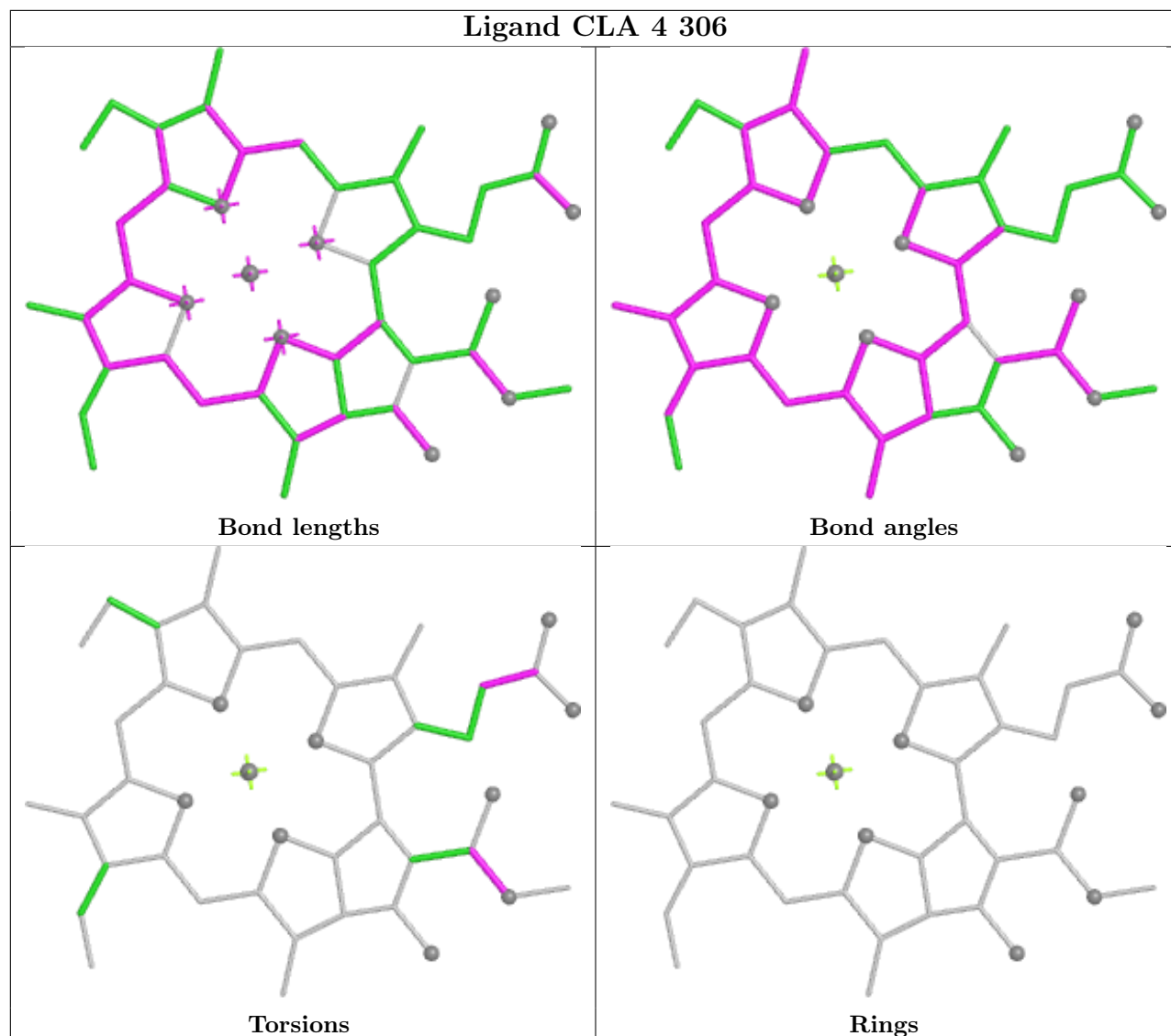
Rings



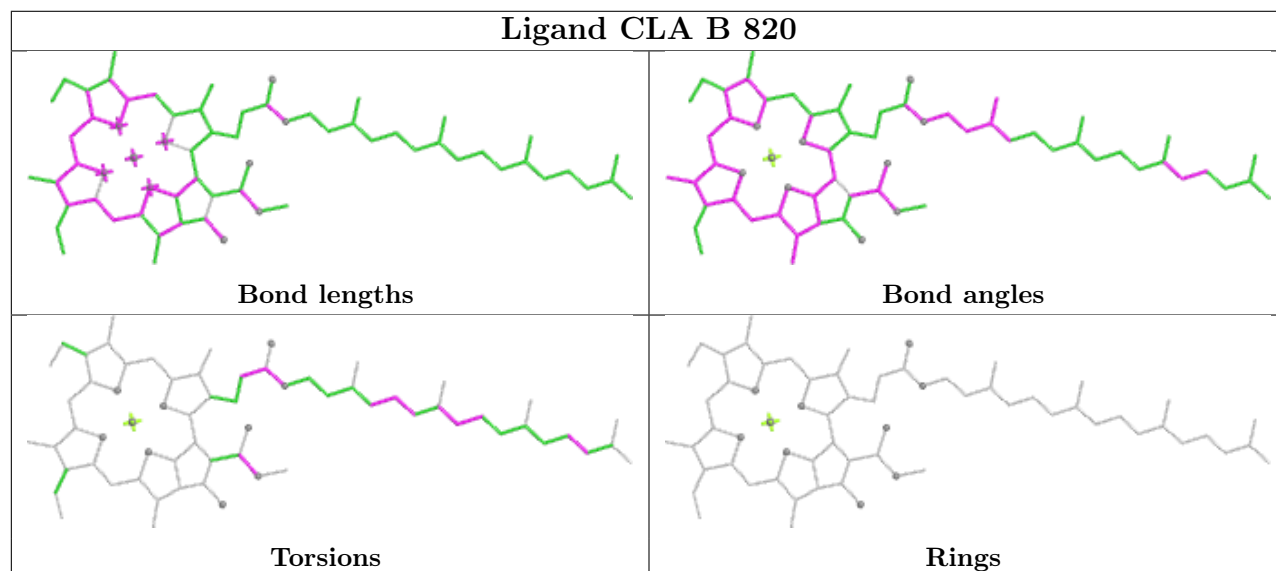
Ligand CLA a 316



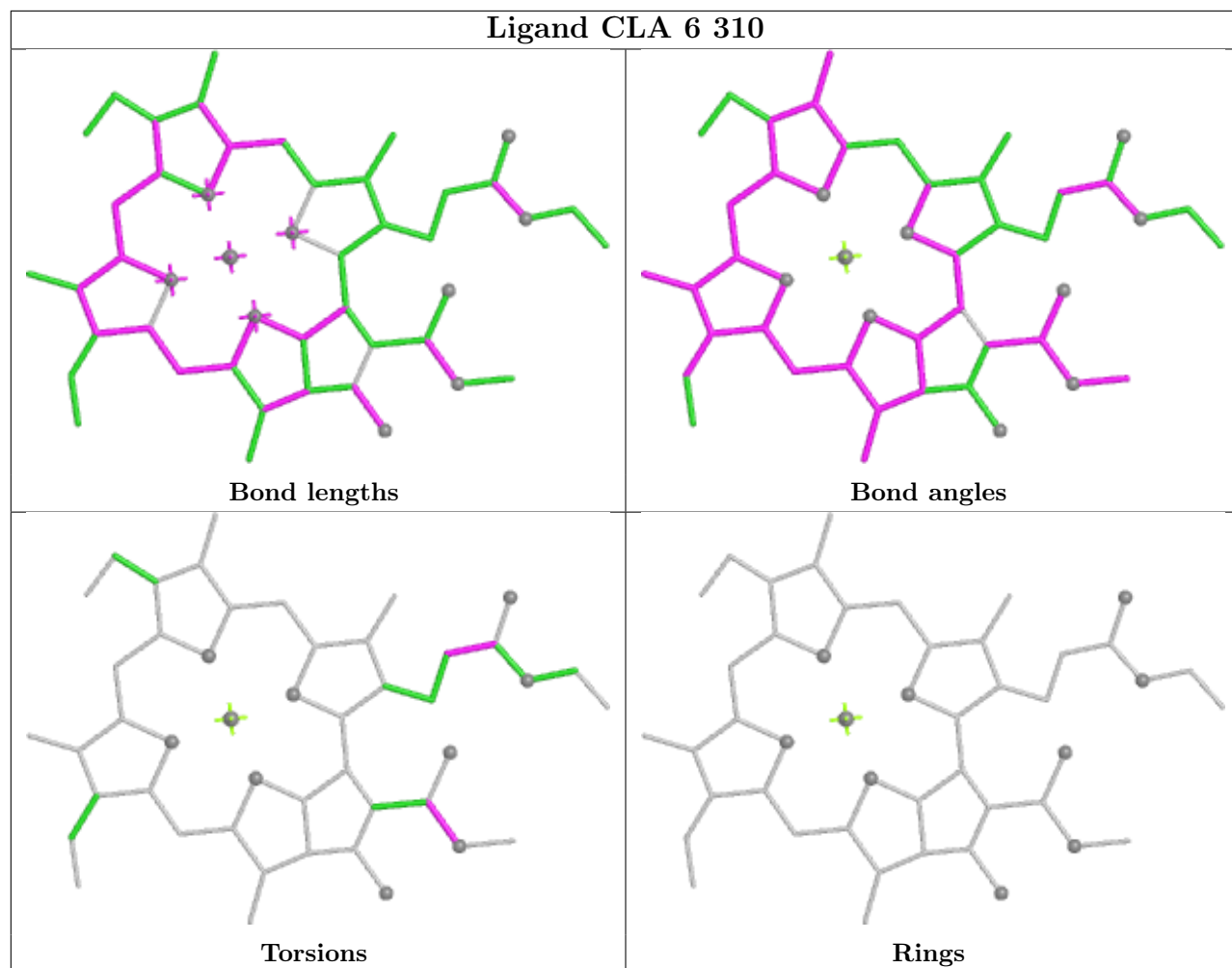
Ligand CLA 4 306



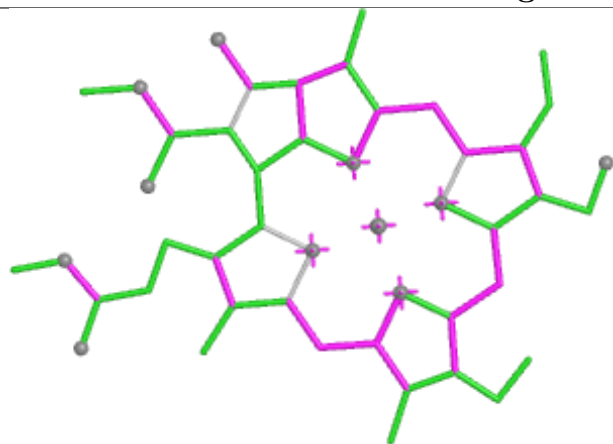
Ligand CLA B 820



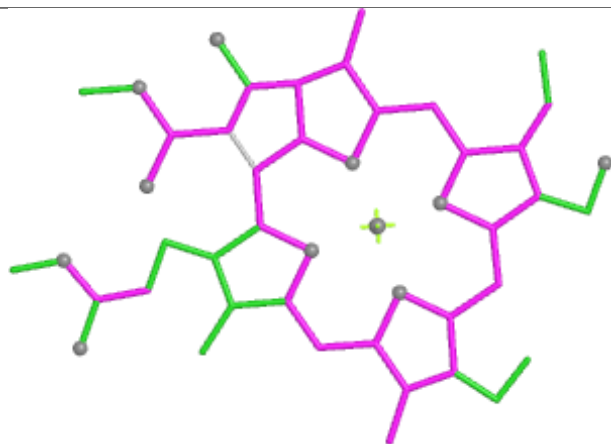
Ligand CLA 6 310



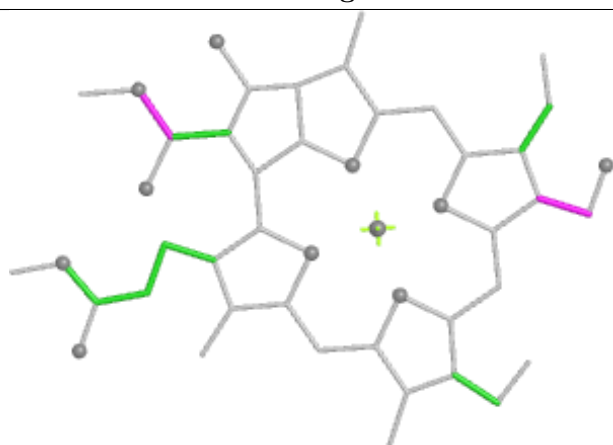
Ligand CHL 9 322



Bond lengths



Bond angles

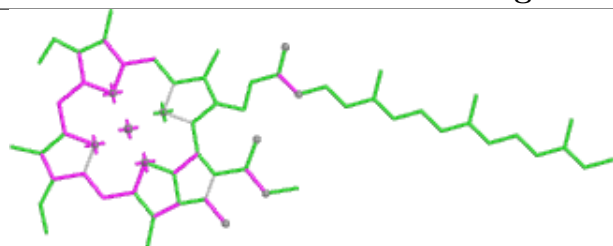


Torsions

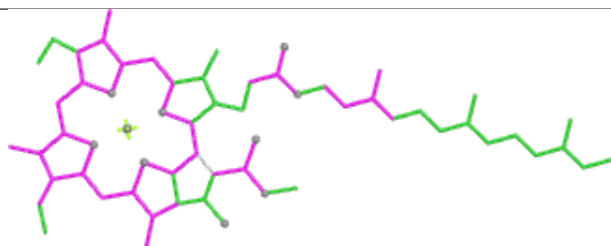


Rings

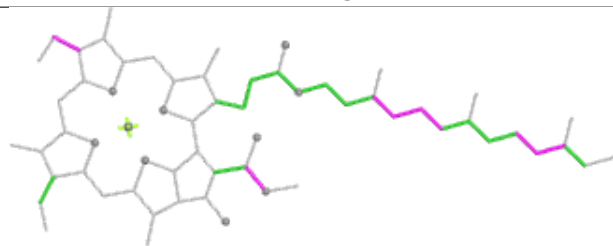
Ligand CLA B 842



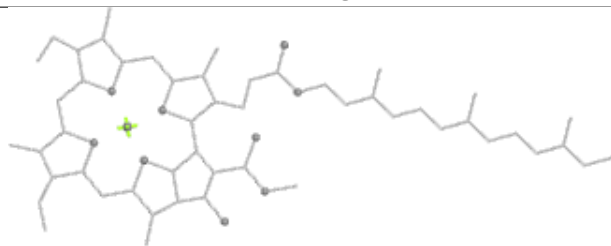
Bond lengths



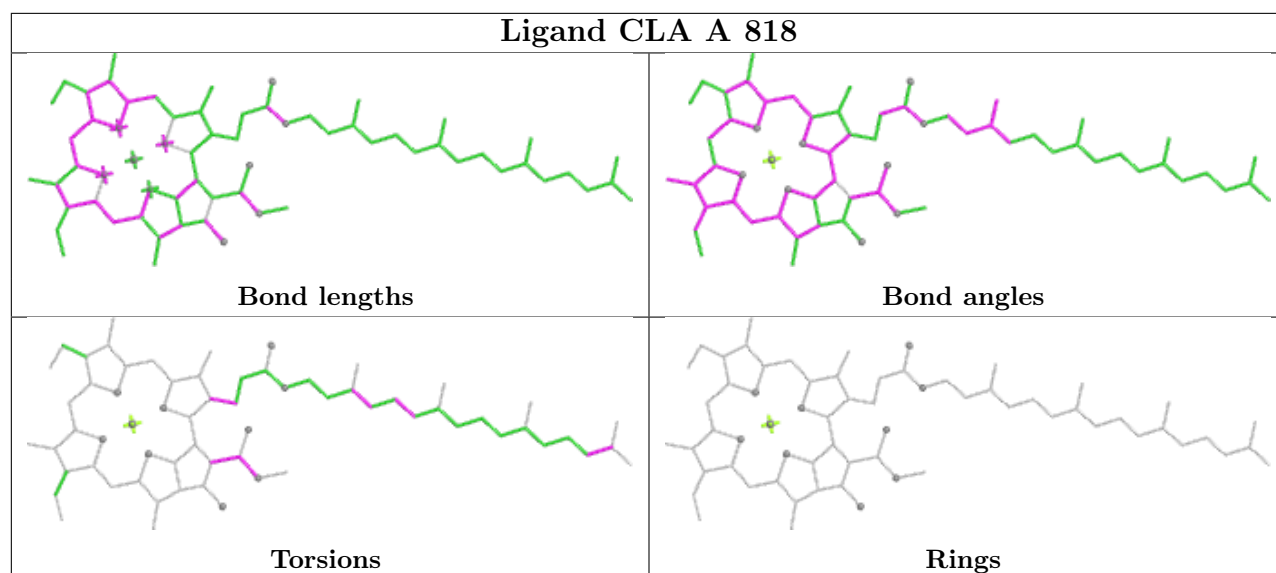
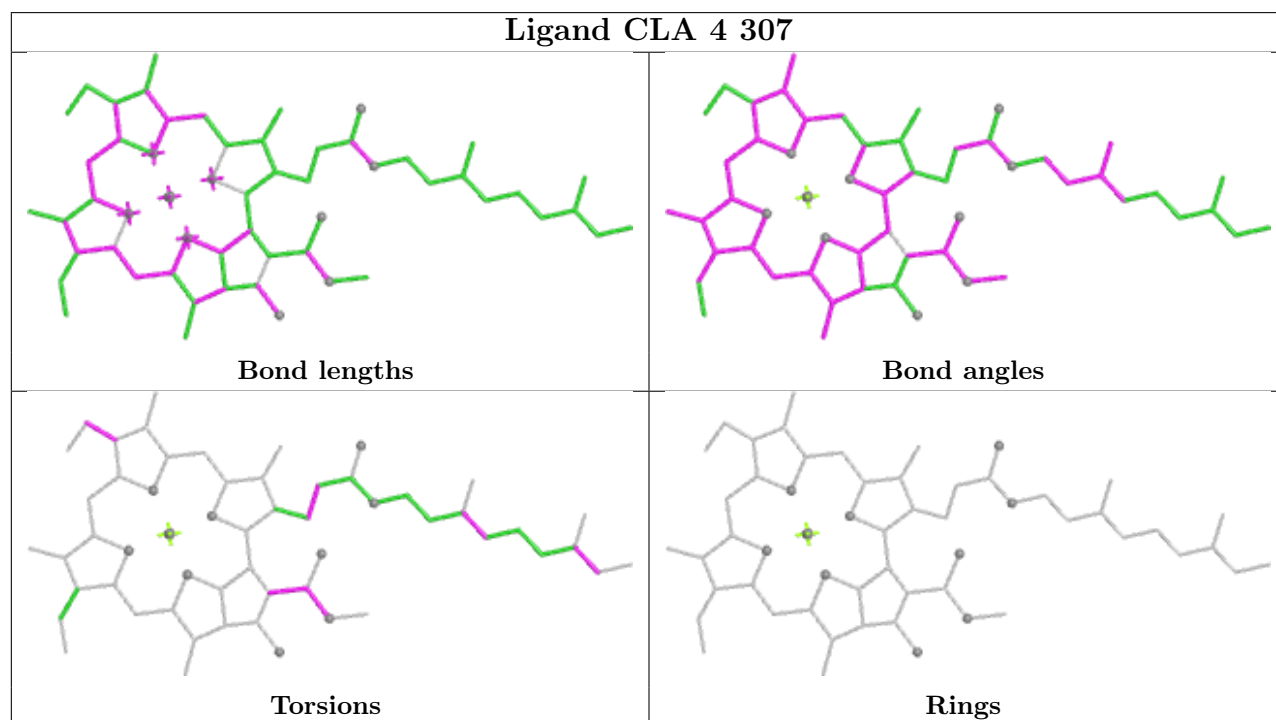
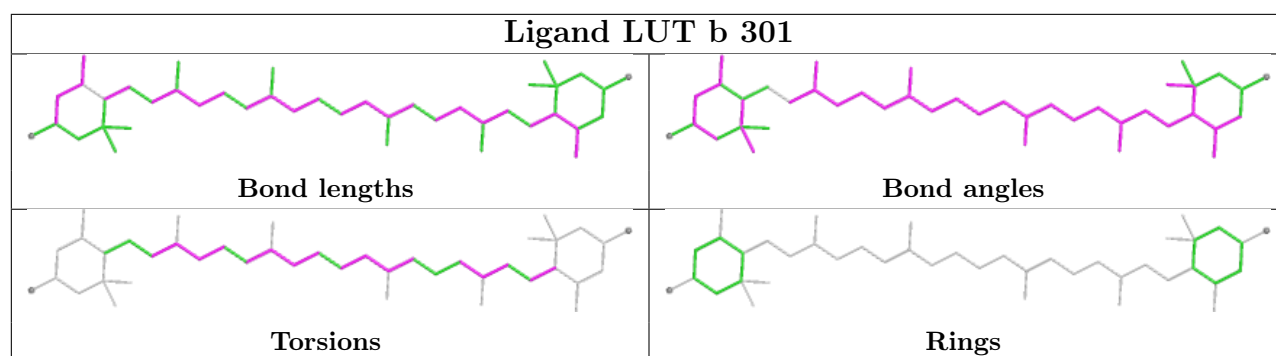
Bond angles



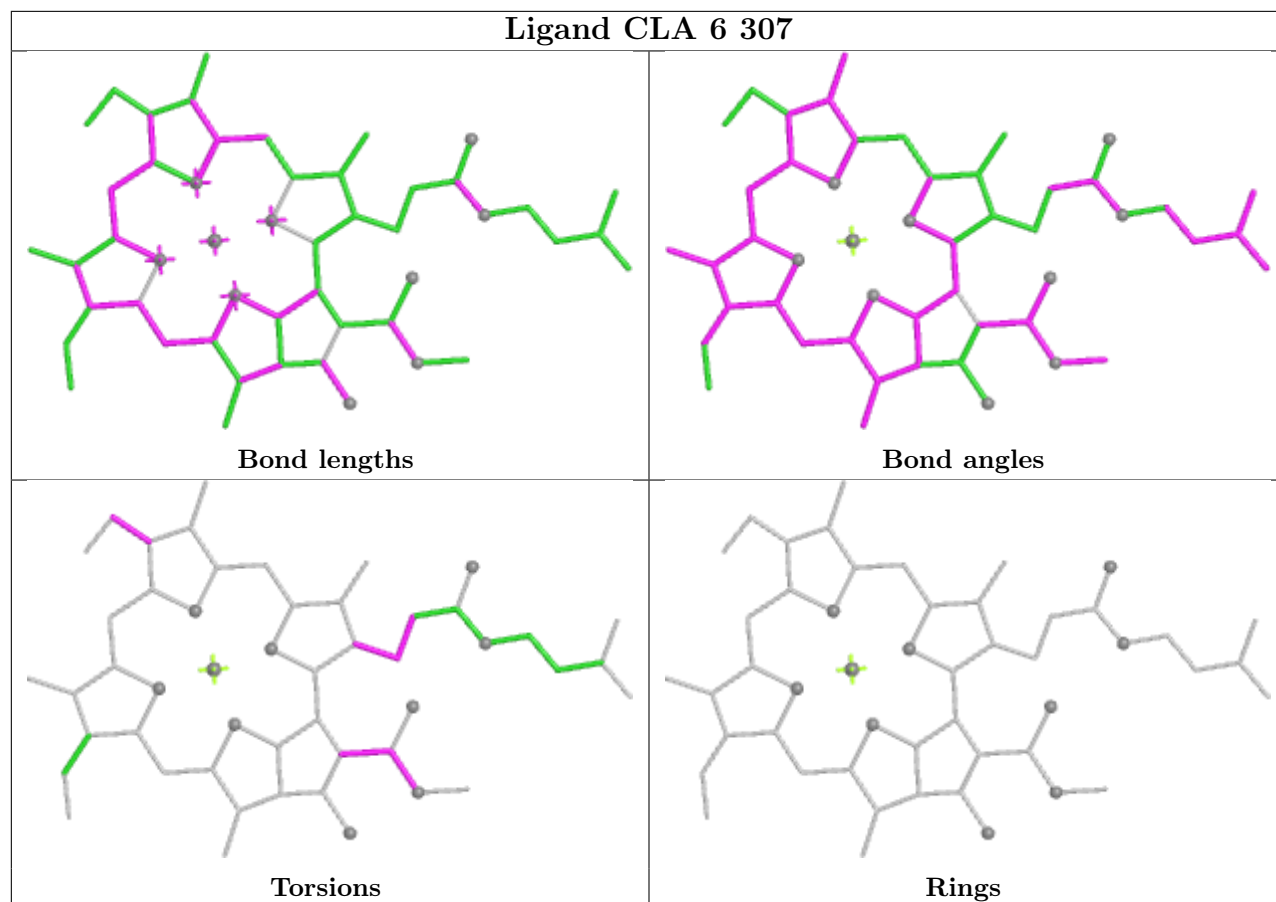
Torsions



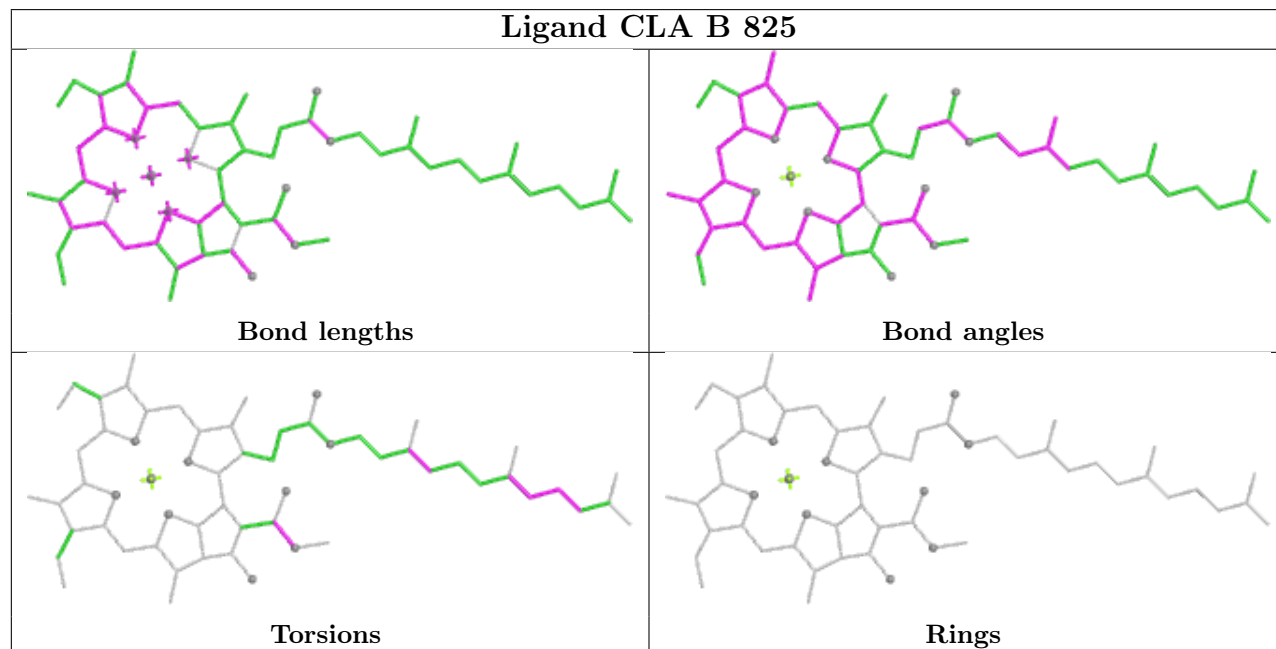
Rings

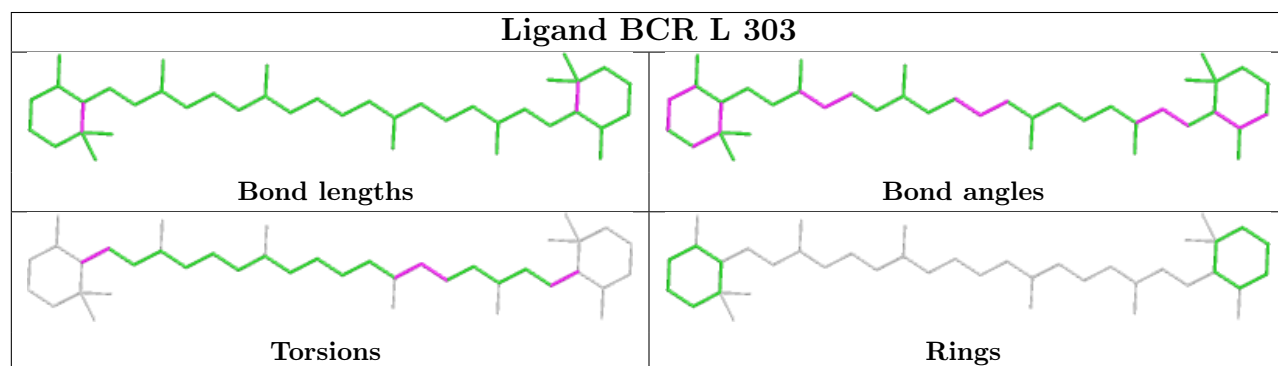
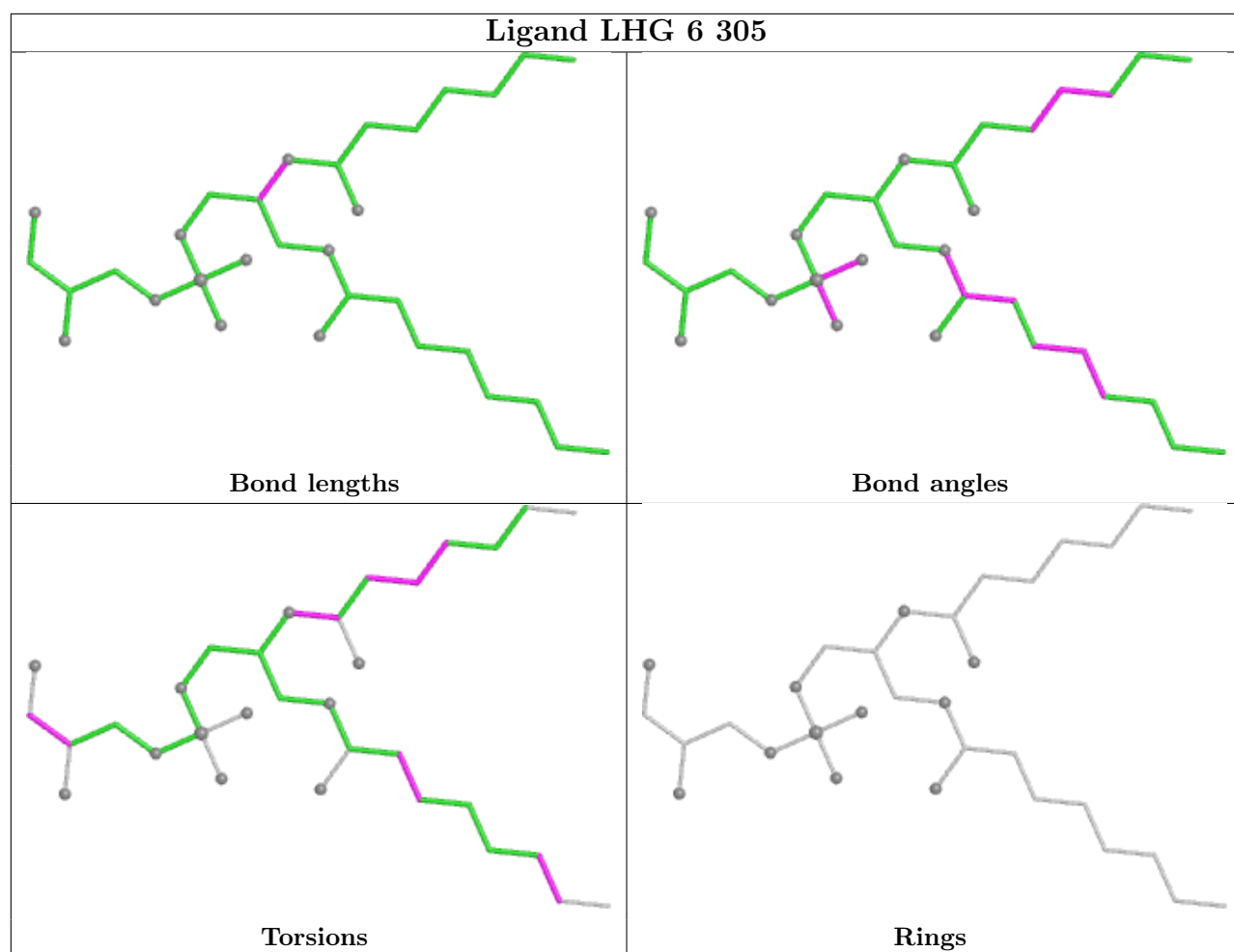


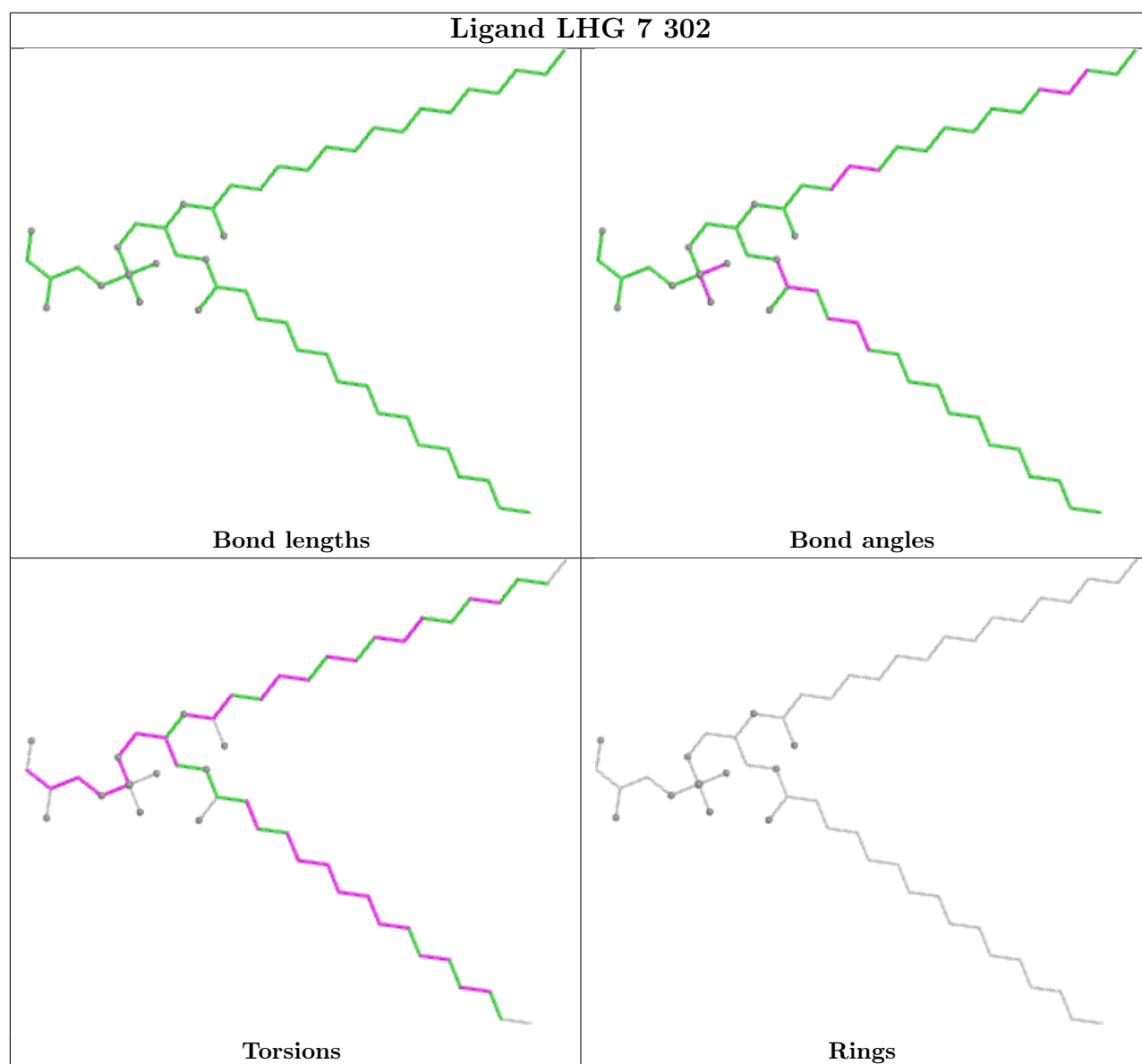
Ligand CLA 6 307



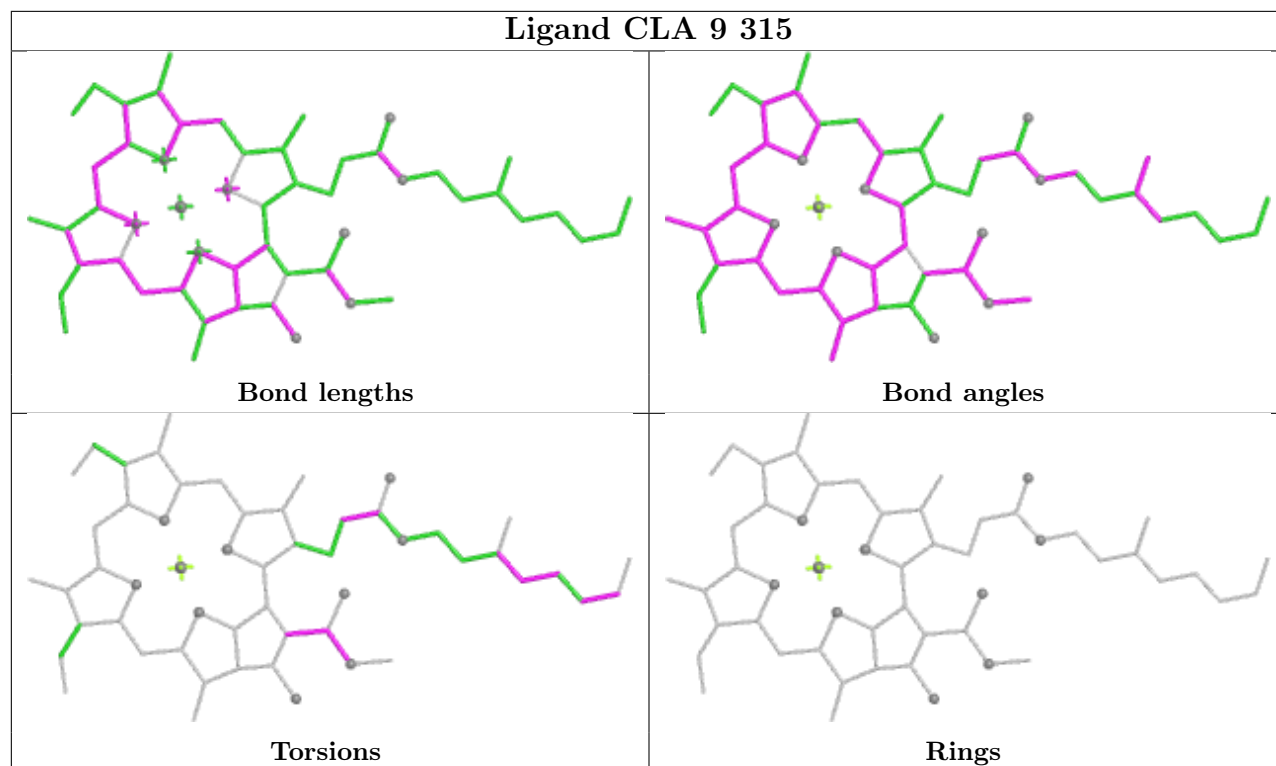
Ligand CLA B 825



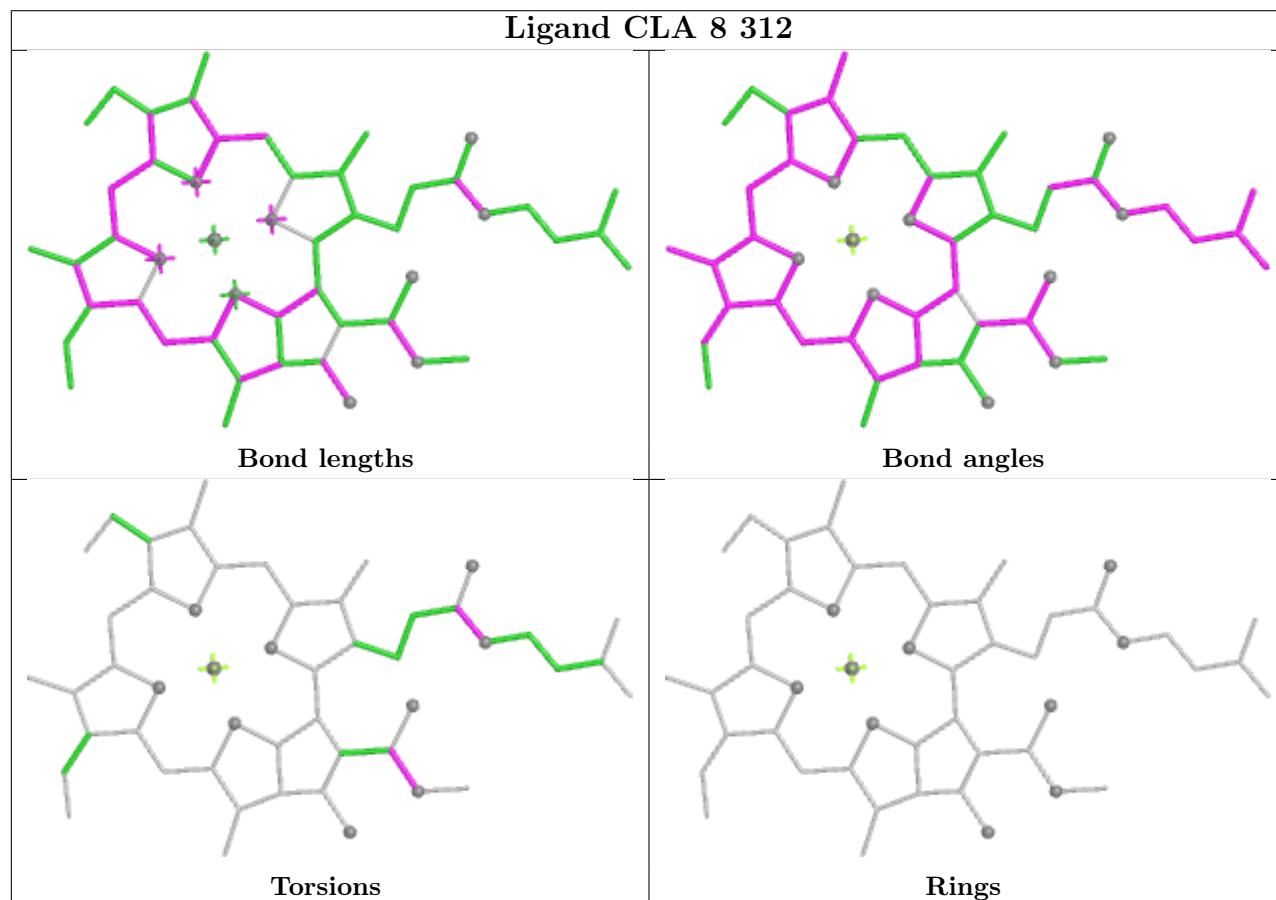


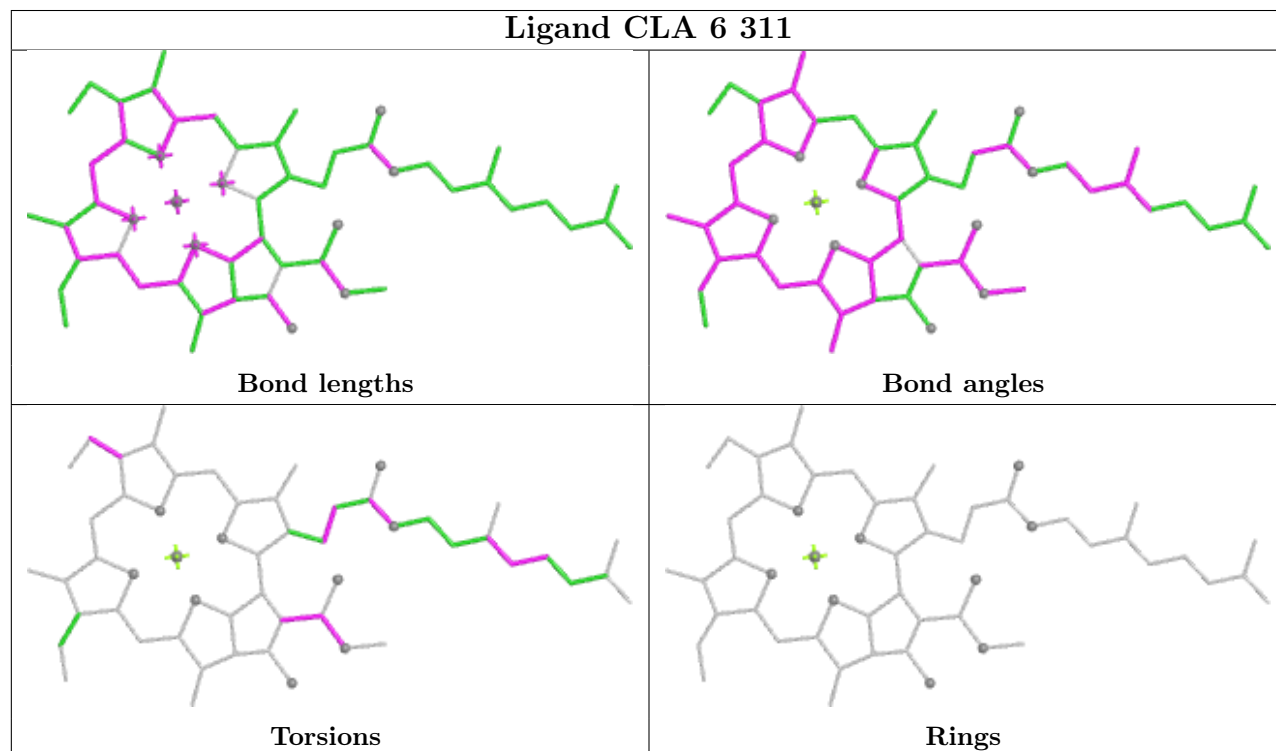
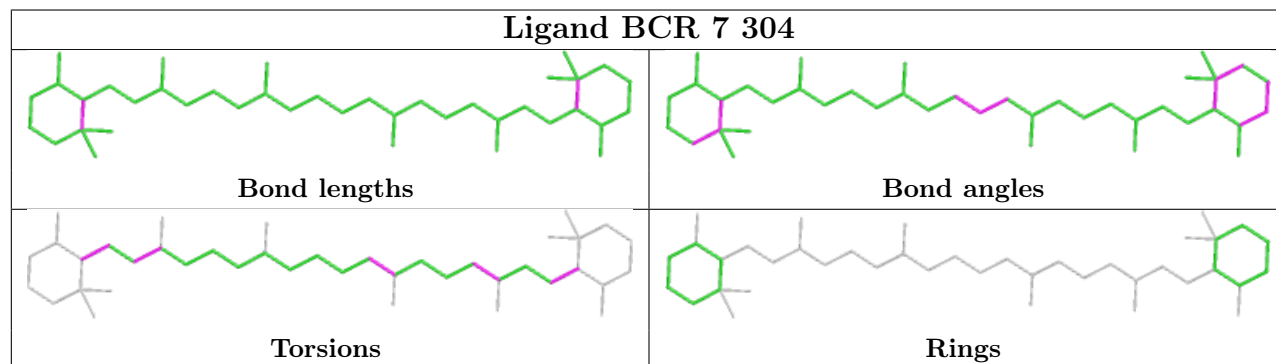
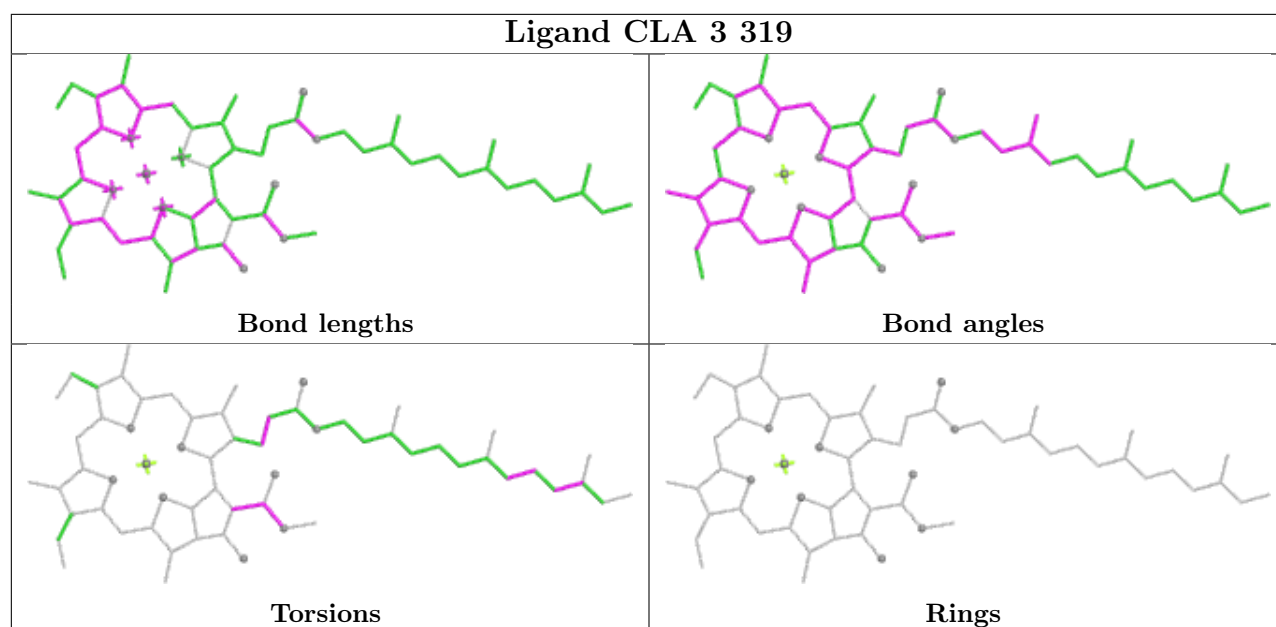


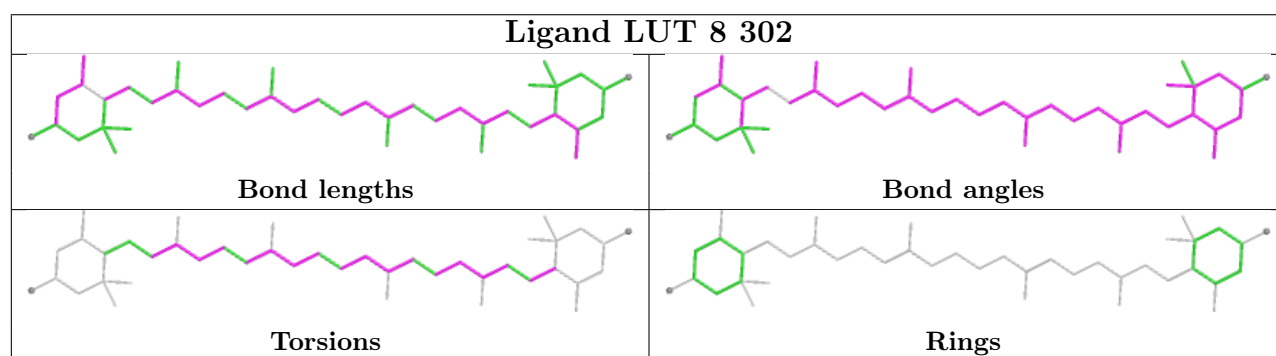
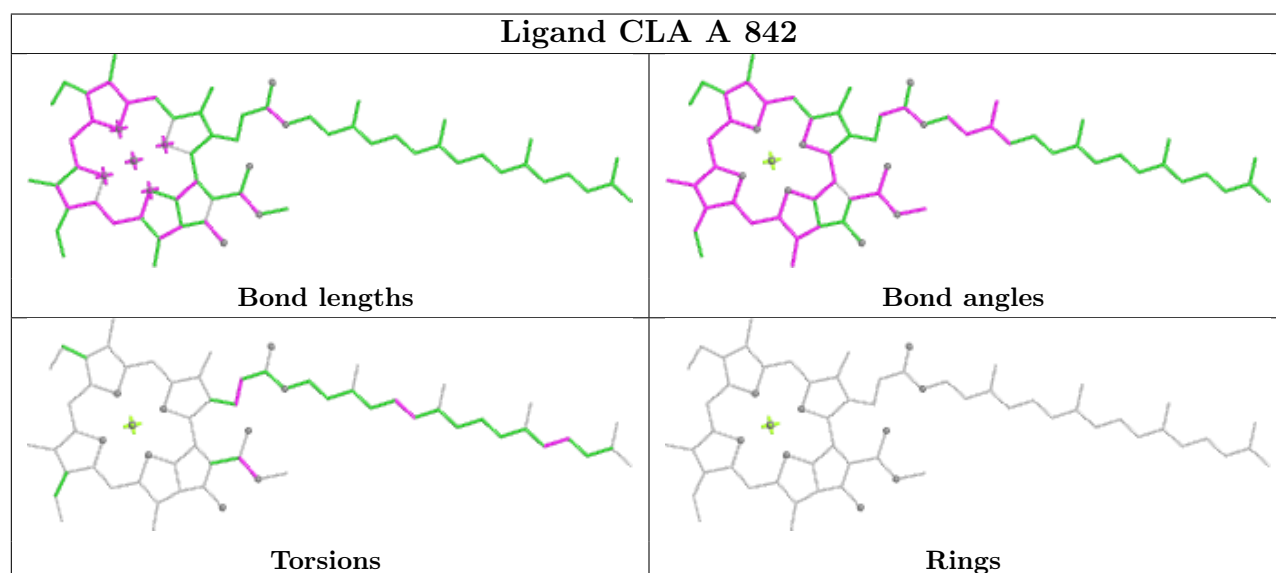
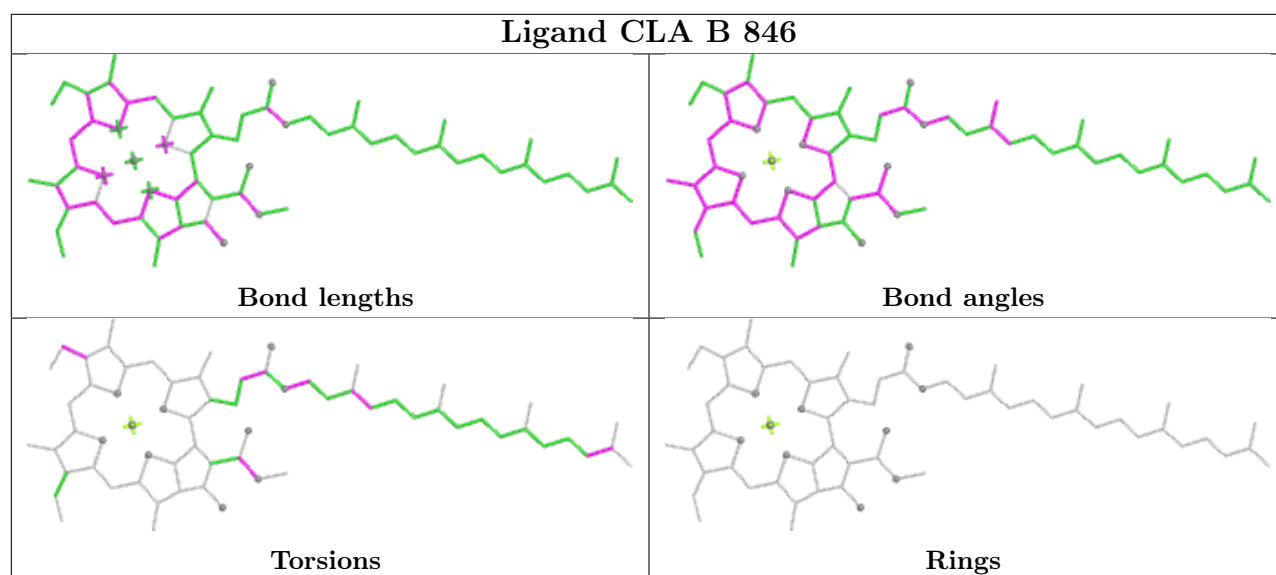
Ligand CLA 9 315

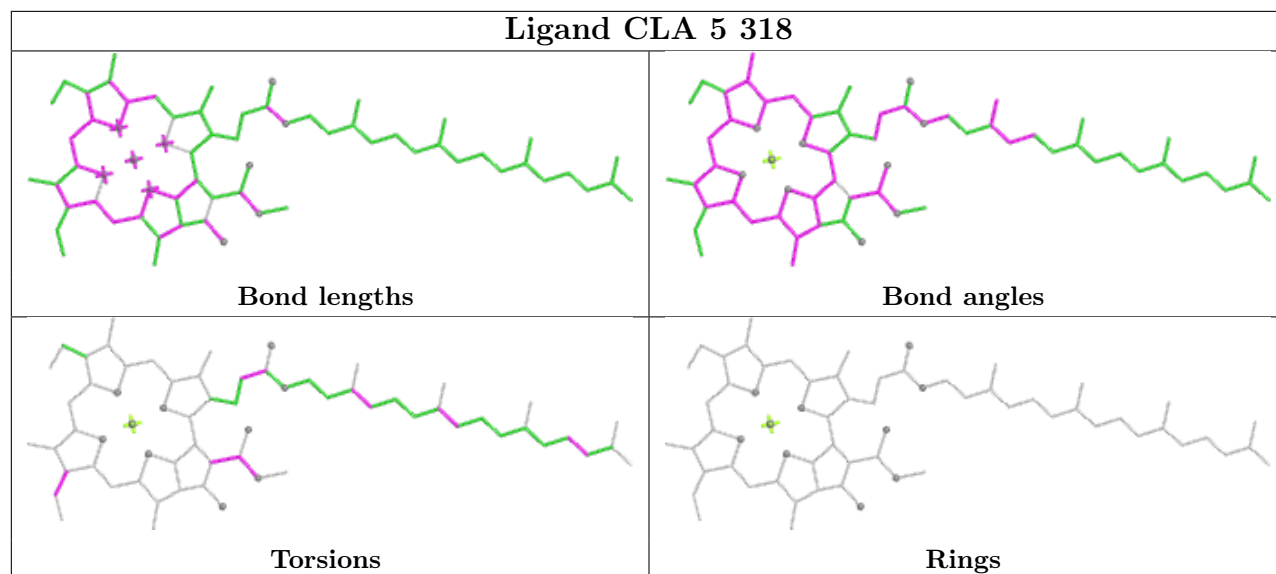
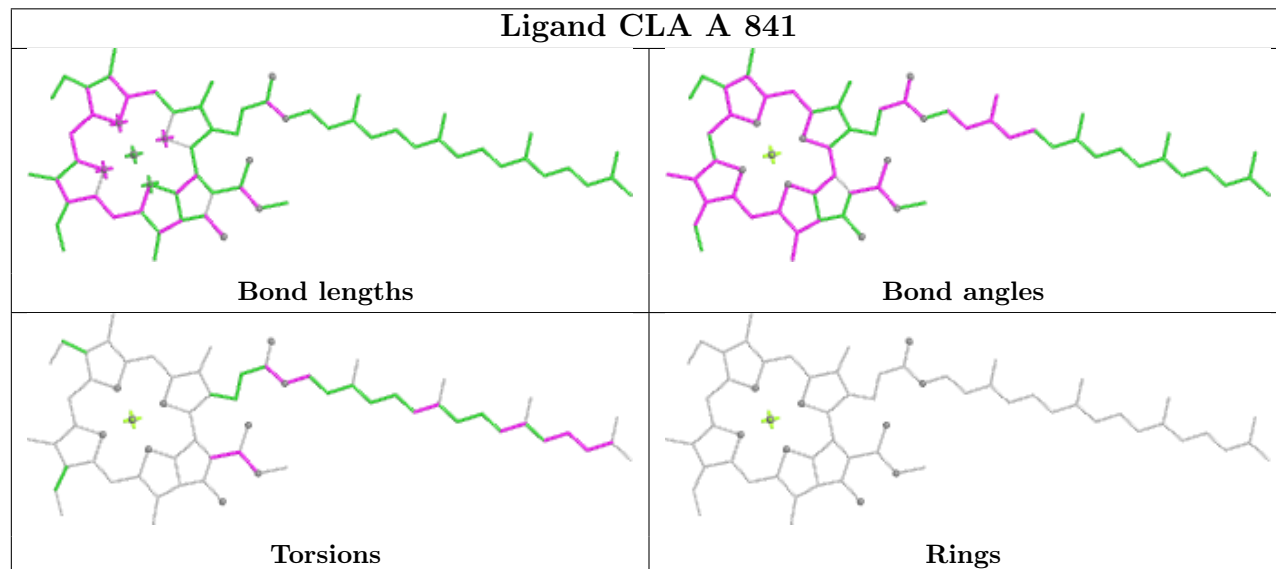


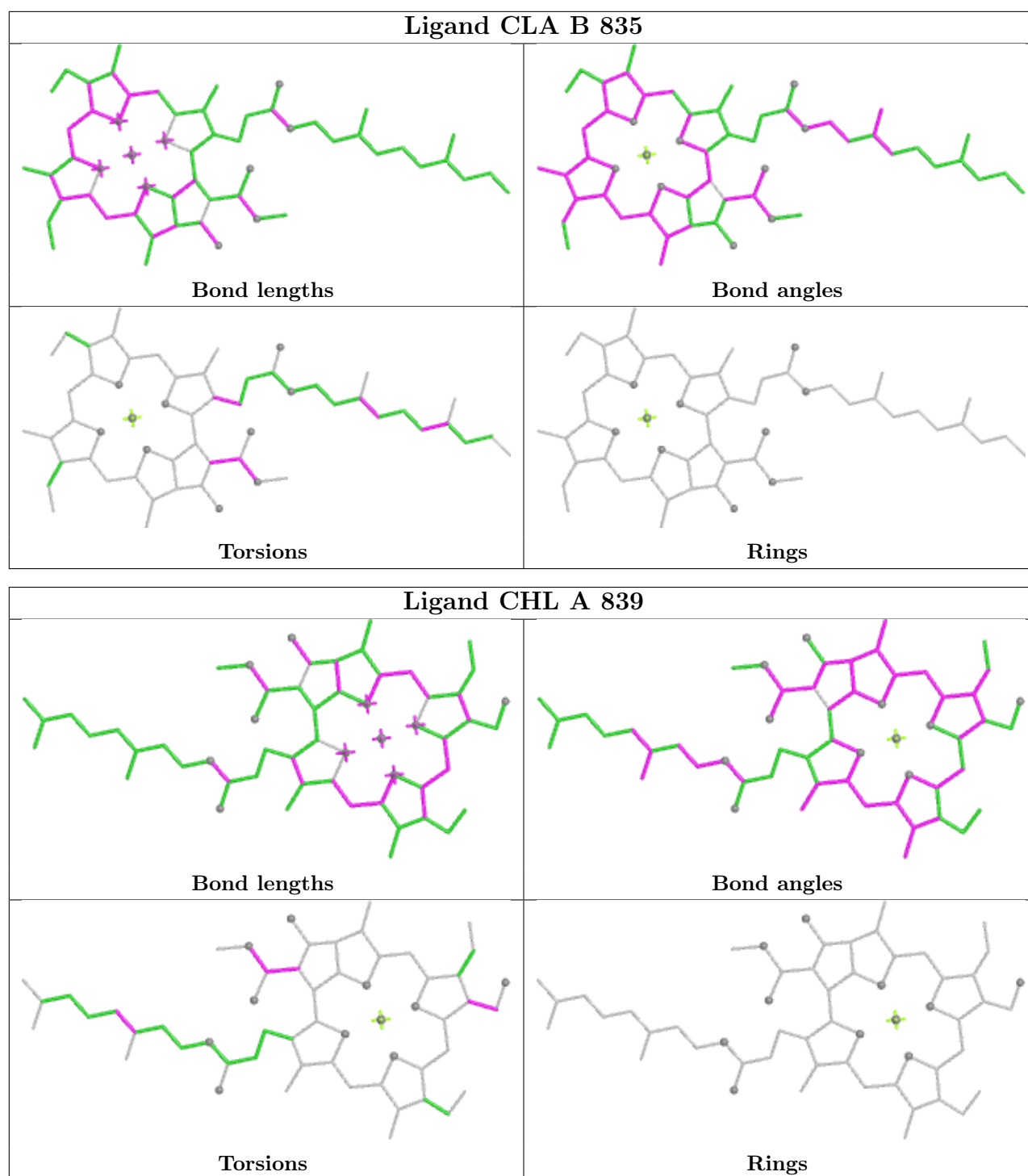
Ligand CLA 8 312







Ligand CLA 5 318**Ligand CLA A 841**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

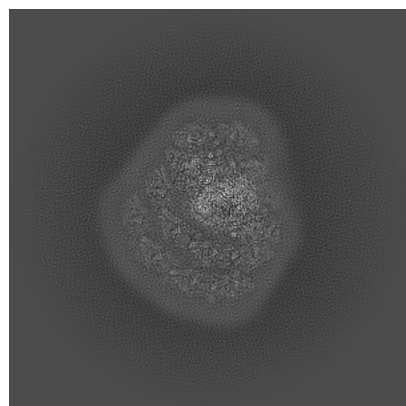
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62511. These allow visual inspection of the internal detail of the map and identification of artifacts.

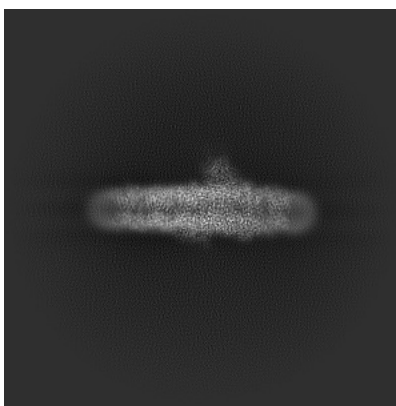
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

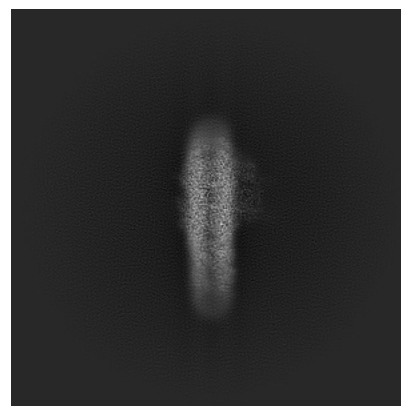
6.1.1 Primary map



X

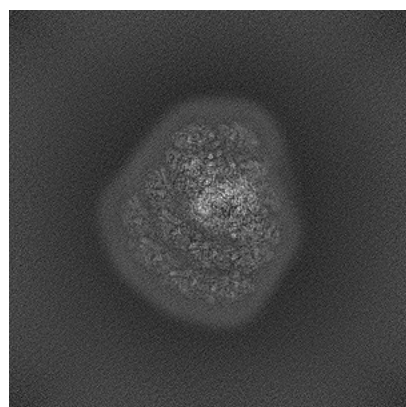


Y

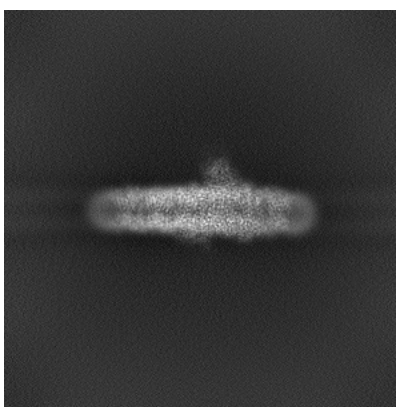


Z

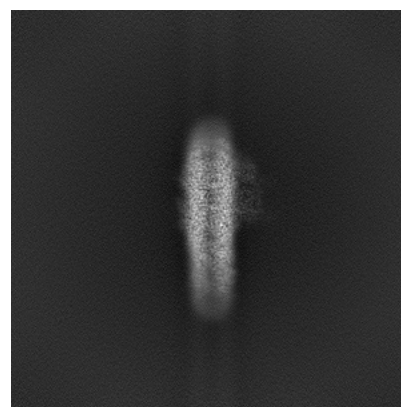
6.1.2 Raw map



X



Y

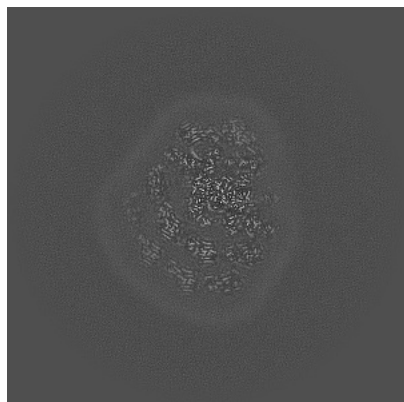


Z

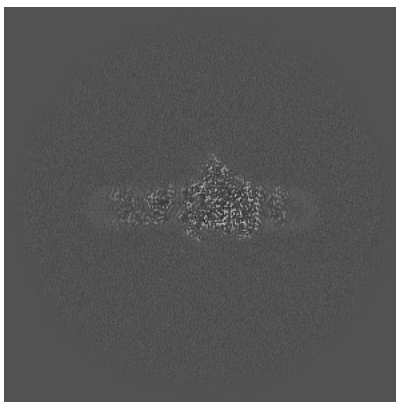
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

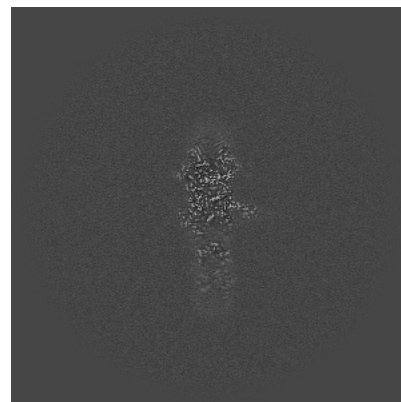
6.2.1 Primary map



X Index: 300

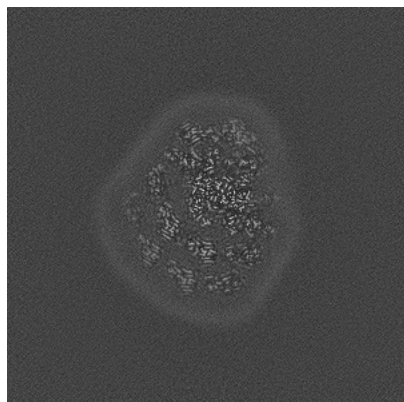


Y Index: 300

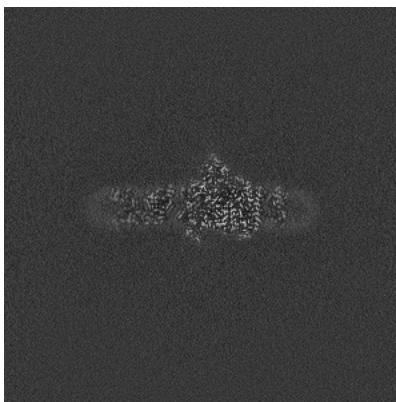


Z Index: 300

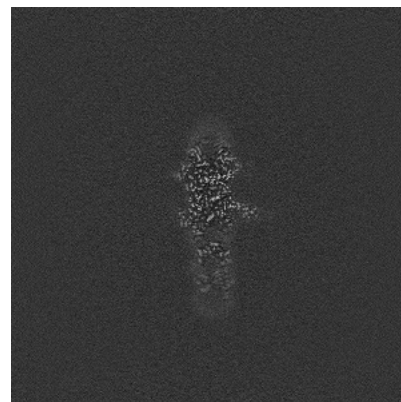
6.2.2 Raw map



X Index: 300



Y Index: 300

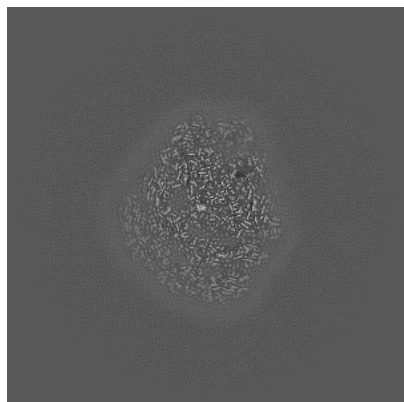


Z Index: 300

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

6.3 Largest variance slices [i](#)

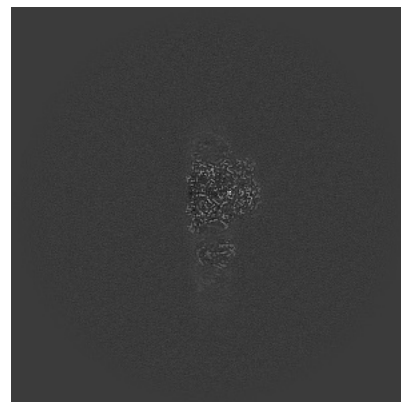
6.3.1 Primary map



X Index: 316

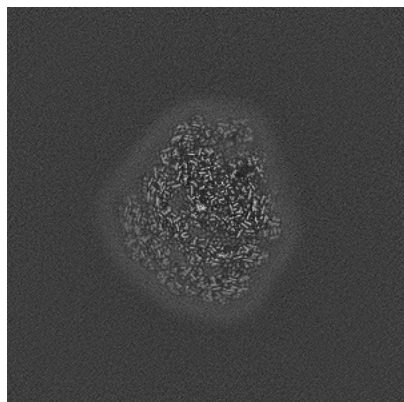


Y Index: 307

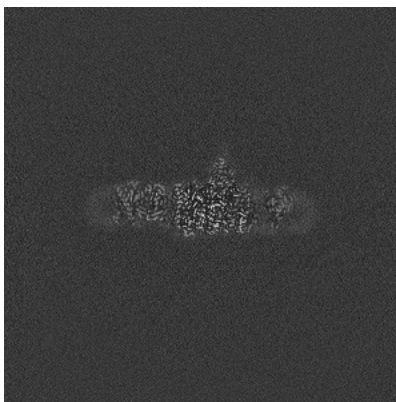


Z Index: 320

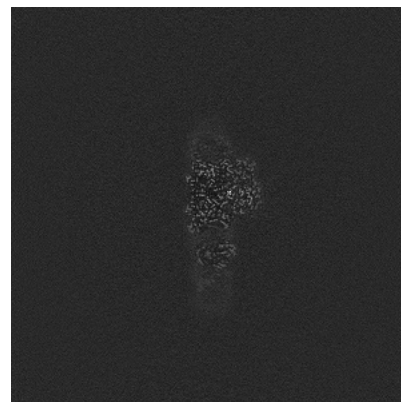
6.3.2 Raw map



X Index: 316



Y Index: 339

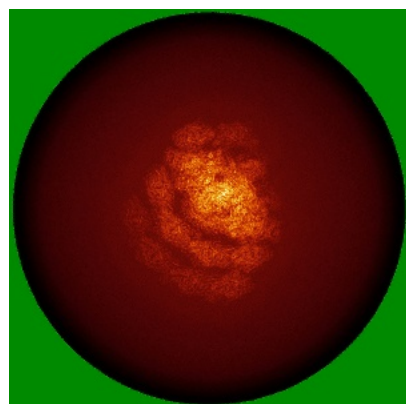


Z Index: 320

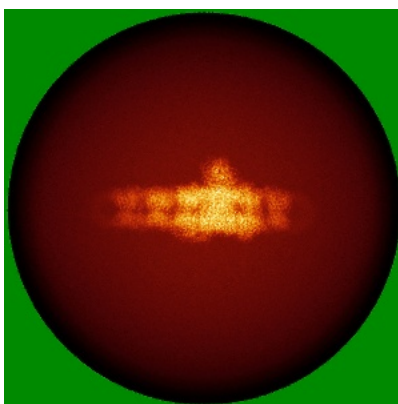
The images above show the largest variance slices of the map in three orthogonal directions.

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

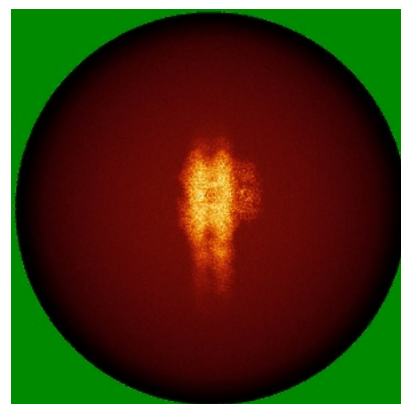
6.4.1 Primary map



X

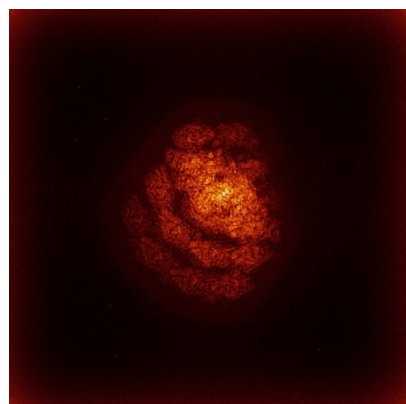


Y

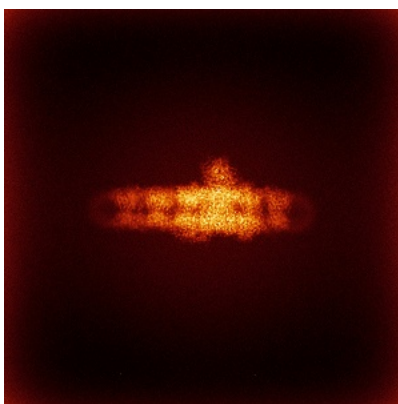


Z

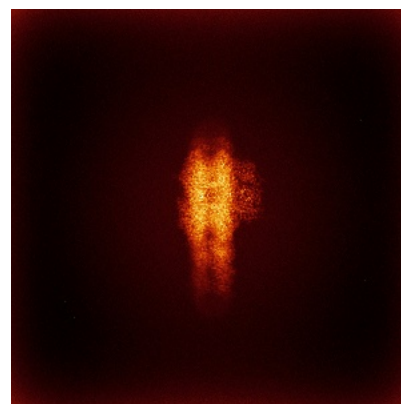
6.4.2 Raw map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.085. 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



X



Y



Z

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

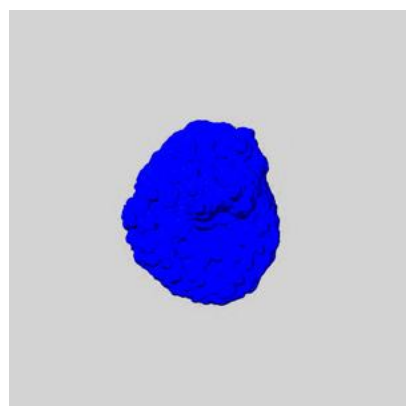
6.6 Mask visualisation [i](#)

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

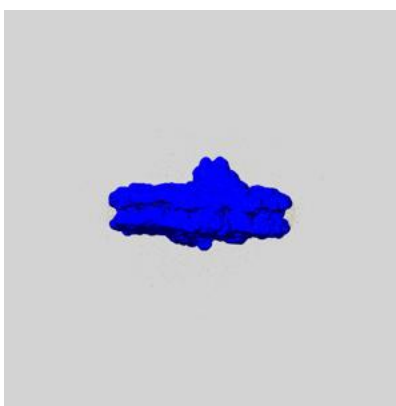
A mask typically either:

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

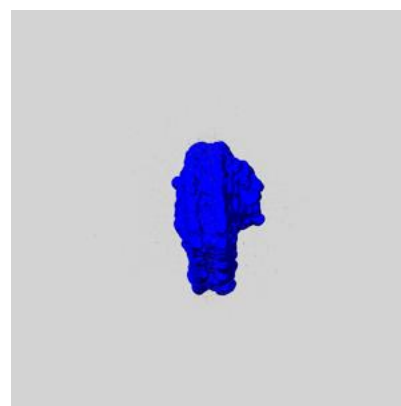
6.6.1 emd_62511_msk_1.map [i](#)



X



Y

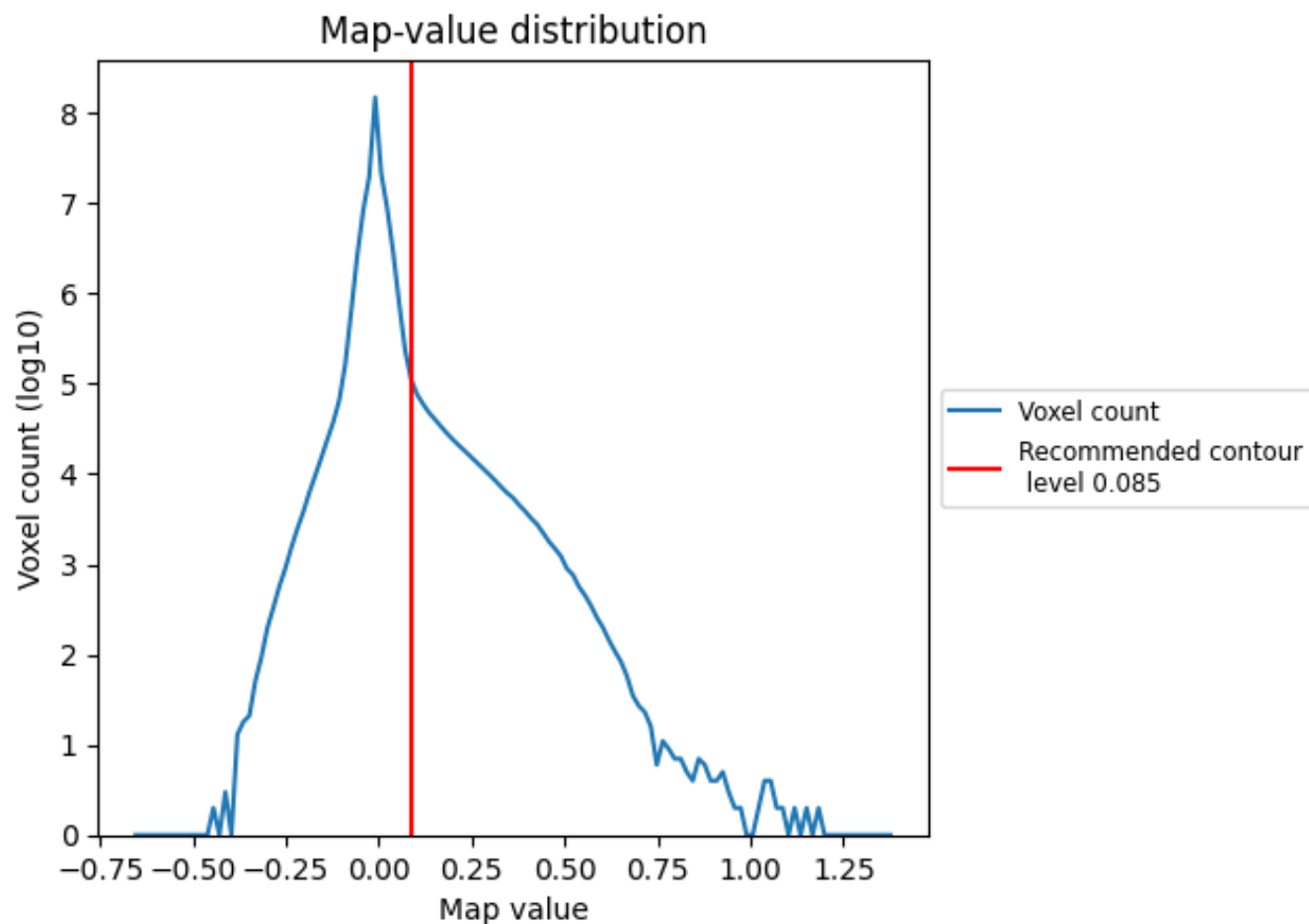


Z

7 Map analysis [i](#)

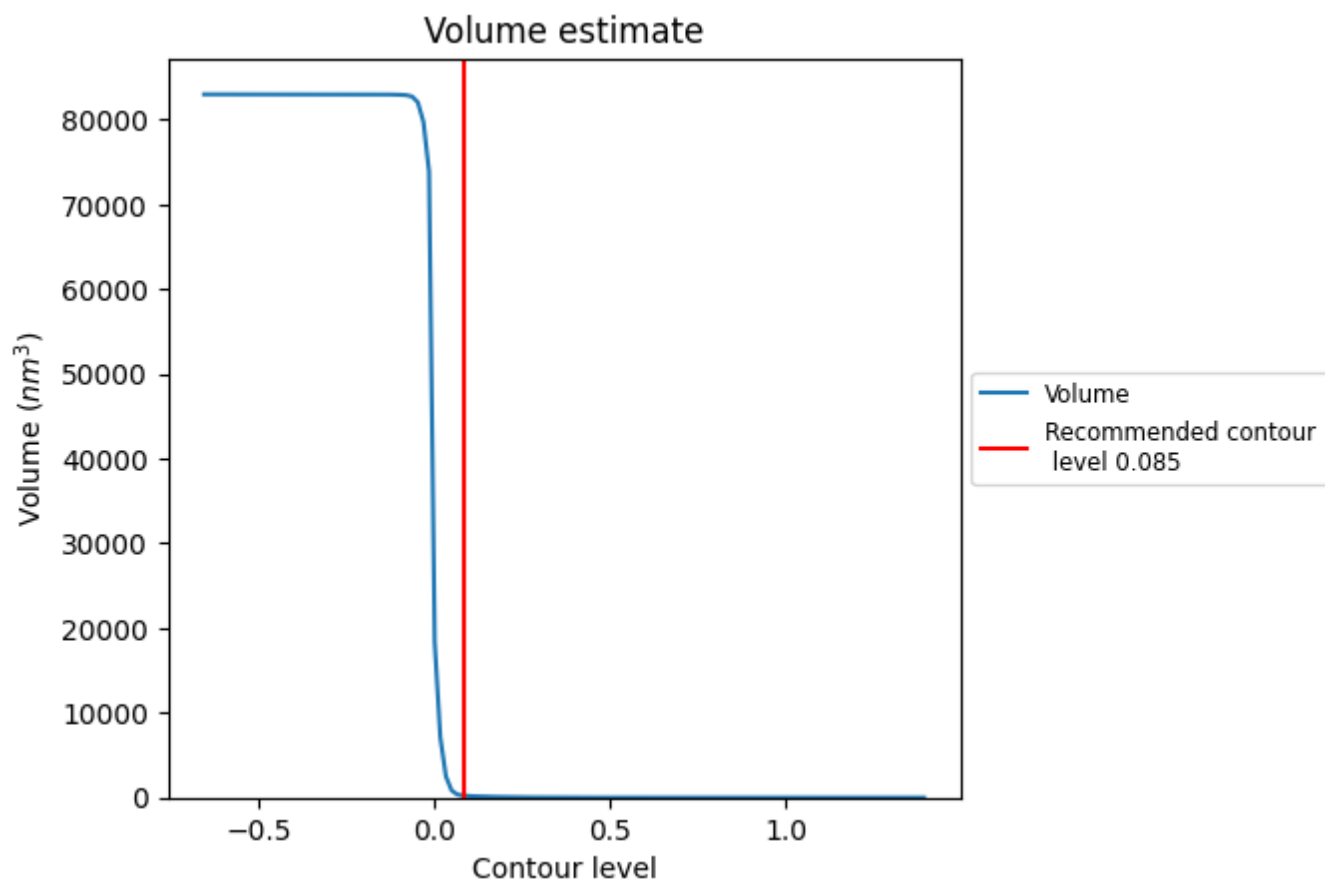
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

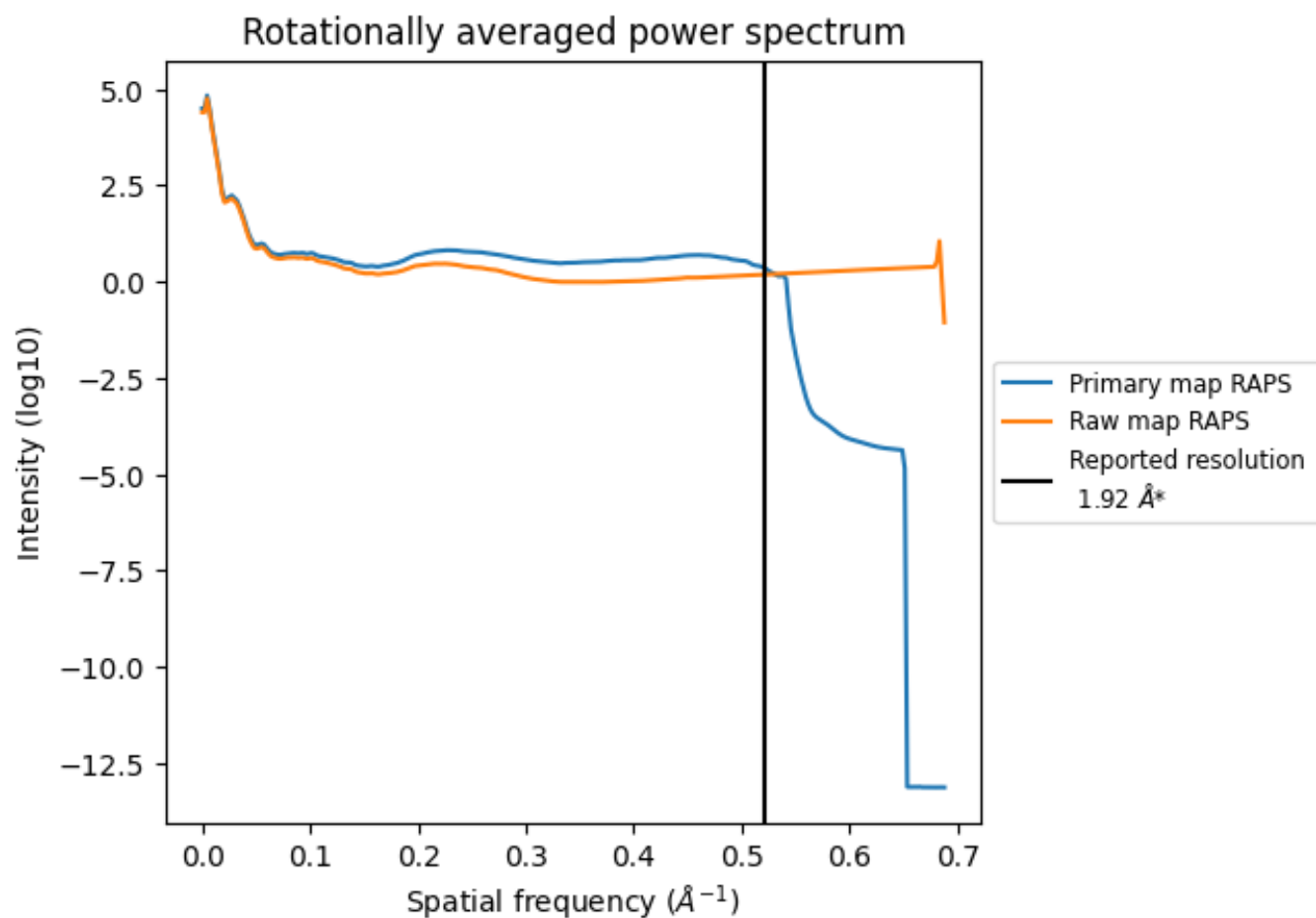
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 227 nm³; this corresponds to an approximate mass of 205 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 ⓘ

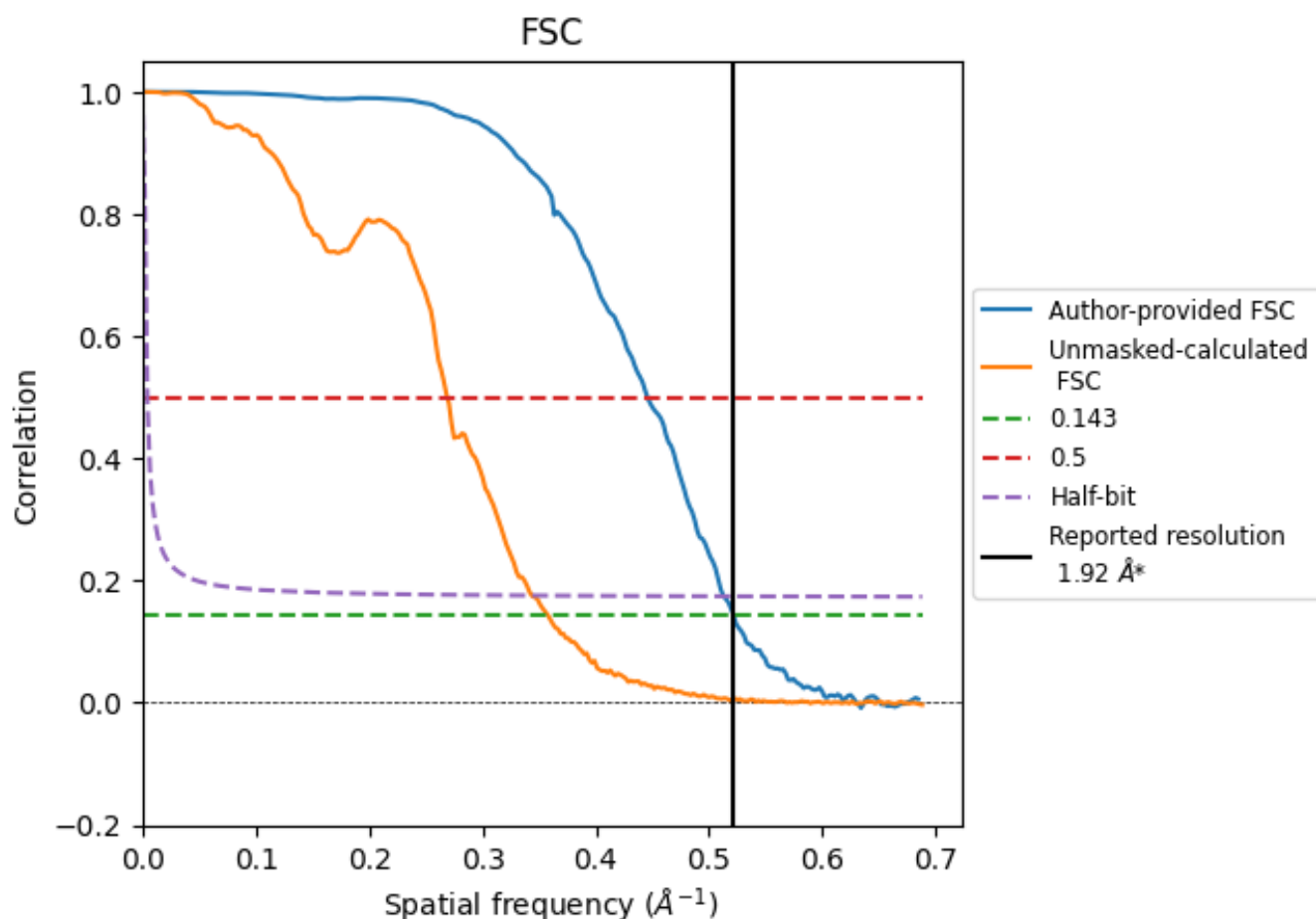


*Reported resolution corresponds to spatial frequency of 0.521 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.521 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

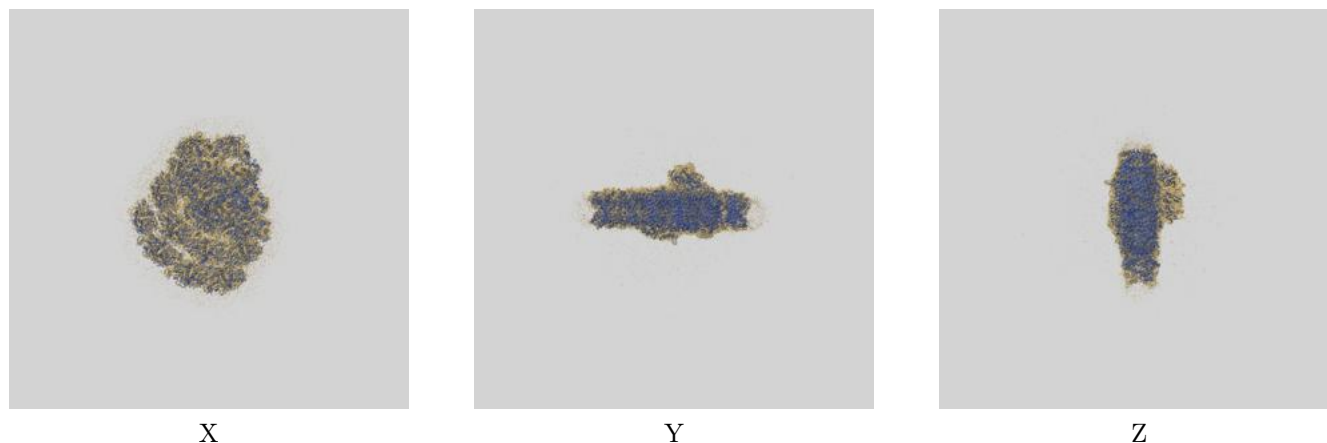
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.92	-	-
Author-provided FSC curve	1.92	2.24	1.95
Unmasked-calculated*	2.79	3.72	2.91

*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 2.79 differs from the reported value 1.92 by more than 10 %

9 Map-model fit [i](#)

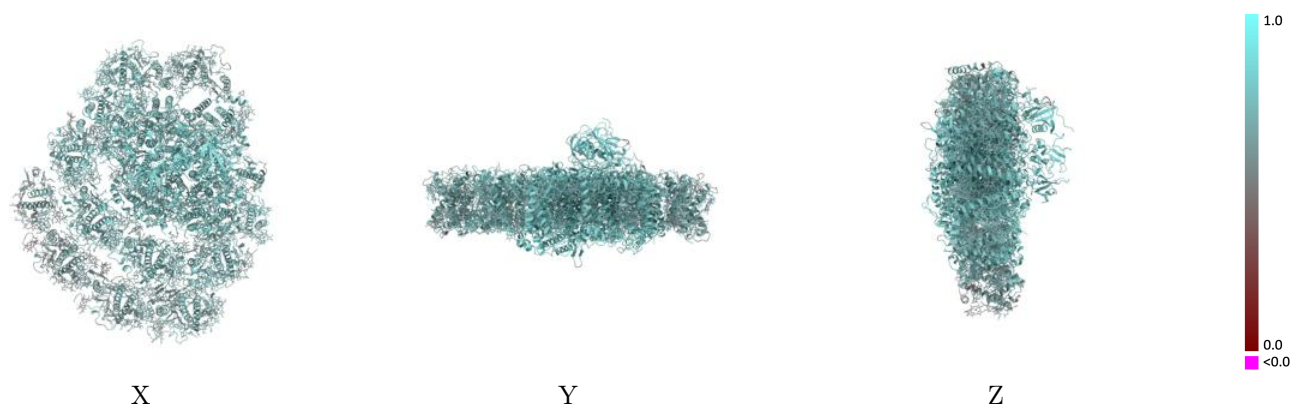
This section contains information regarding the fit between EMDB map EMD-62511 and PDB model 9KQP. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



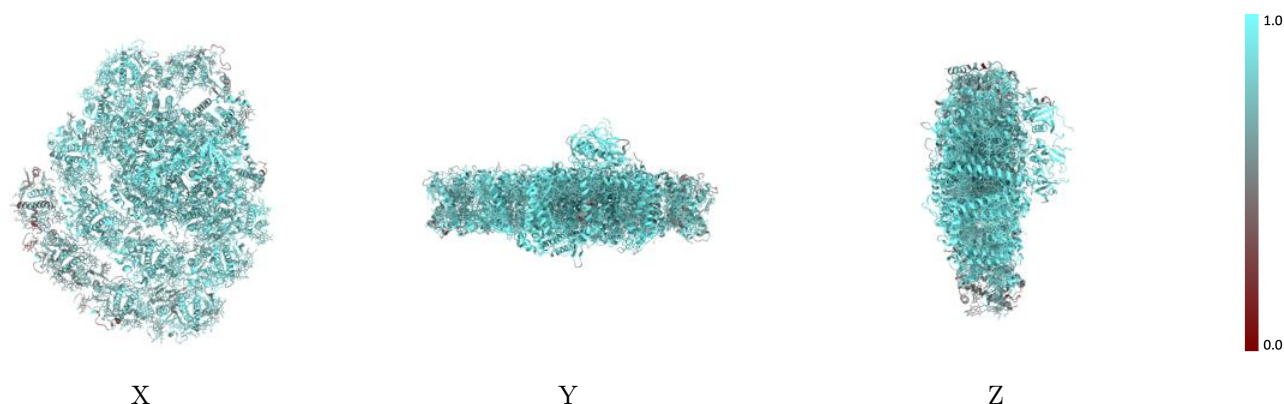
The images above show the 3D surface view of the map at the recommended contour level 0.085 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



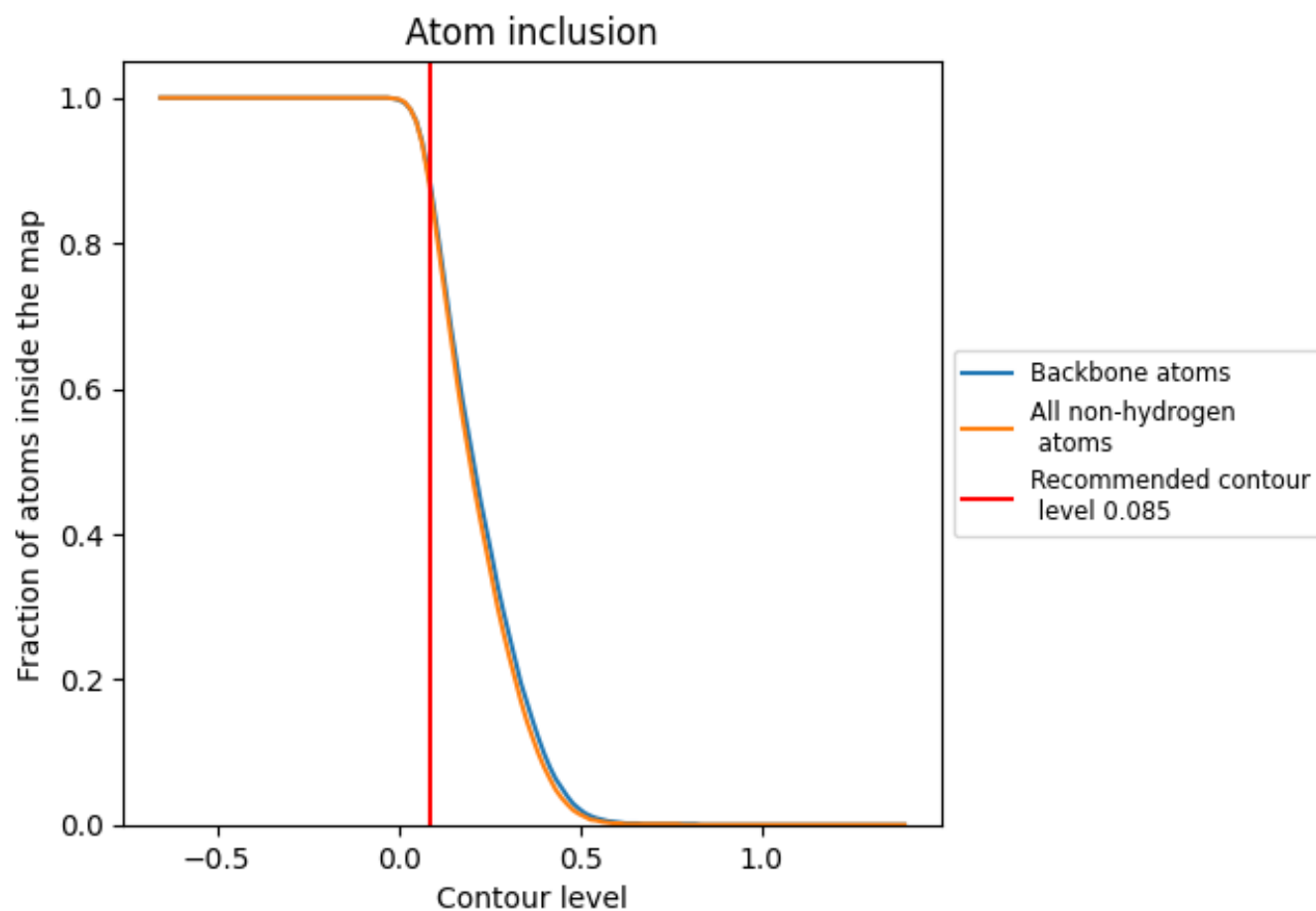
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.085).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% 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 (0.085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8820	0.7230
2	0.7470	0.6320
3	0.9070	0.7070
4	0.6450	0.5770
5	0.7930	0.6420
6	0.7360	0.6210
7	0.9190	0.7280
8	0.9100	0.7290
9	0.8830	0.6910
A	0.9650	0.7910
B	0.9690	0.7950
C	0.9920	0.8120
D	0.9590	0.7800
E	0.9200	0.7700
F	0.9490	0.7810
G	0.9090	0.7300
H	0.7620	0.6860
I	0.9760	0.7770
J	0.9690	0.7790
K	0.8840	0.6980
L	0.9000	0.7320
M	0.9530	0.7720
O	0.6770	0.6560
a	0.8890	0.7080
b	0.5990	0.5800

1.0

0.0

<0.0