



wwPDB EM Validation Summary Report ⓘ

Sep 15, 2026 – 11:13 AM JST

PDB ID : 9LUT / pdb_00009lut
EMDB ID : EMD-63404
Title : PSI-LHCI supercomplex binding with 4 Lhcas from M. polymorpha
Authors : Tsai, P.-C.; La Rocca, R.; Shen, J.-R.; Akita, F.
Deposited on : 2025-02-10
Resolution : 1.94 Å(reported)
Based on initial model : 6L35

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

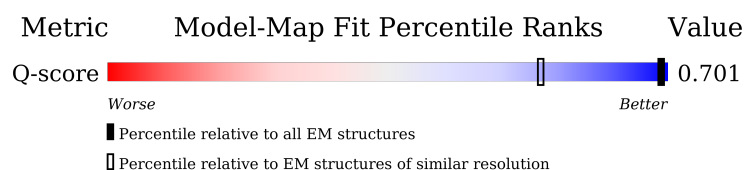
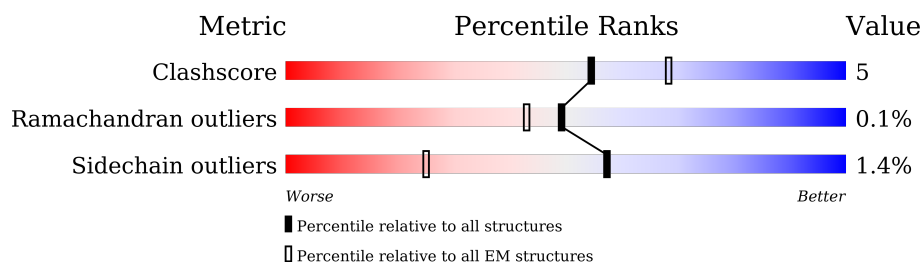
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 1.94 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.



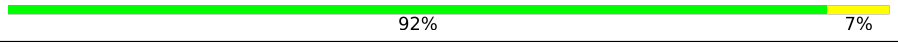
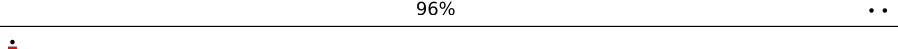
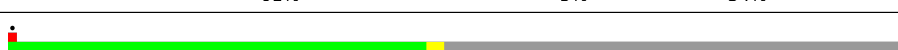
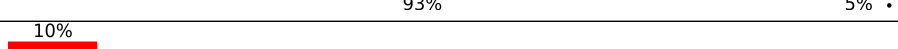
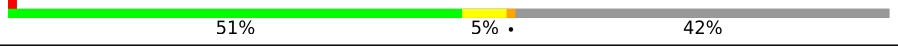
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1283 (1.45 - 2.44)

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	6	243	
2	2	267	
3	3	279	
4	5	249	

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	215	
9	E	132	
10	F	246	
11	G	161	
12	I	36	
13	J	42	
14	K	135	
15	M	32	
16	H	142	
17	L	221	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 36239 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	6	194	Total	C	N	O	S	0	0
			1496	977	248	268	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	201	Total	C	N	O	S	0	0
			1557	1025	253	274	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	220	Total	C	N	O	S	0	0
			1705	1115	277	307	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	198	Total	C	N	O	S	0	0
			1549	1022	248	275	4		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	742	Total	C	N	O	S	0	0
			5846	3837	988	1004	17		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5854	3839	998	1003	14		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			602	368	104	119	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	142	Total	C	N	O	S	0	0
			1112	719	191	199	3		

- Molecule 9 is a protein called Photosystem I reaction centre subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	64	Total	C	N	O	S	0	0
			503	319	86	96	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	161	Total	C	N	O	S	0	0
			1248	809	212	225	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	90	Total	C	N	O	S	0	0
			673	432	117	123	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	35	Total	C	N	O	S	0	0
			274	187	36	49	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	41	Total	C	N	O	S	0	0
			328	225	48	54	1		

- Molecule 14 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	80	Total	C	N	O	S	0	0
			561	354	97	106	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	30	Total	C	N	O		0	0
			235	155	36	44			

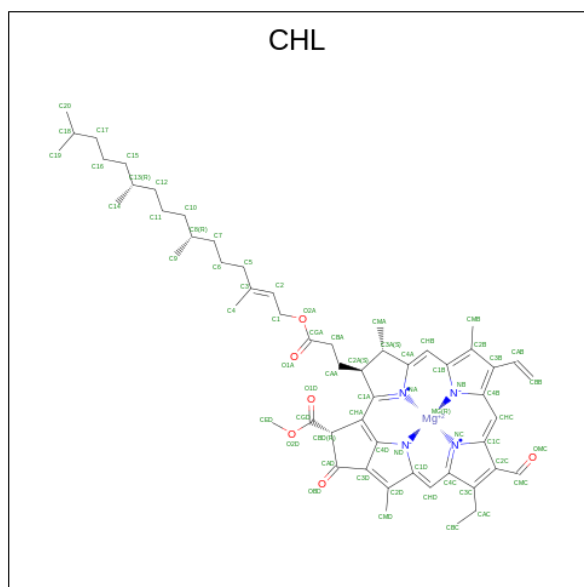
- Molecule 16 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	78	Total	C	N	O	S	0	0
			578	374	99	103	2		

- Molecule 17 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	128	Total	C	N	O	S	0	0
			958	639	150	167	2		

- Molecule 18 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



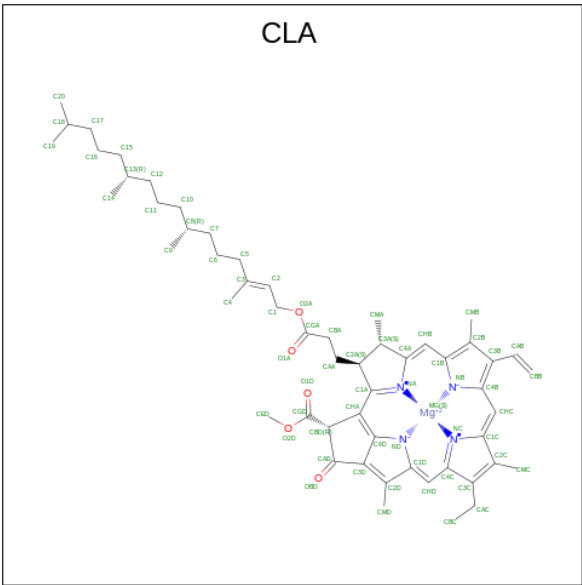
Mol	Chain	Residues	Atoms					AltConf
18	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
18	6	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	2	1	Total	C	Mg	N	O	0
			49	38	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	2	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
18	3	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
18	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
18	5	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
18	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 19 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
19	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 59	C 49	Mg 1	N 4	O 5	0
19	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	5	1	Total 44	C 34	Mg 1	N 4	O 5	0
19	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 48	C 38	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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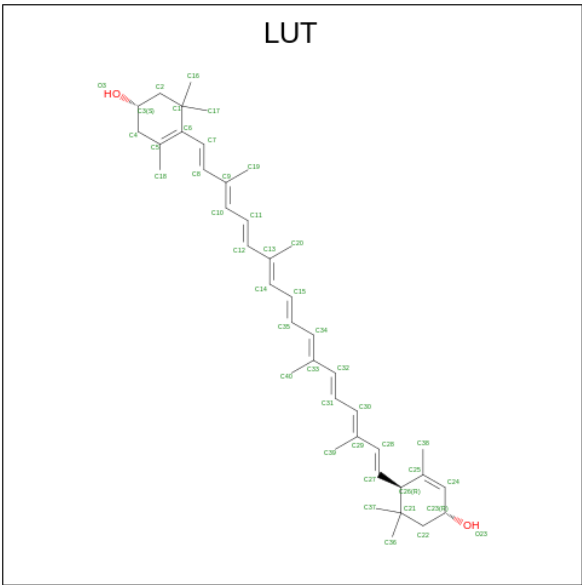
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19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
19	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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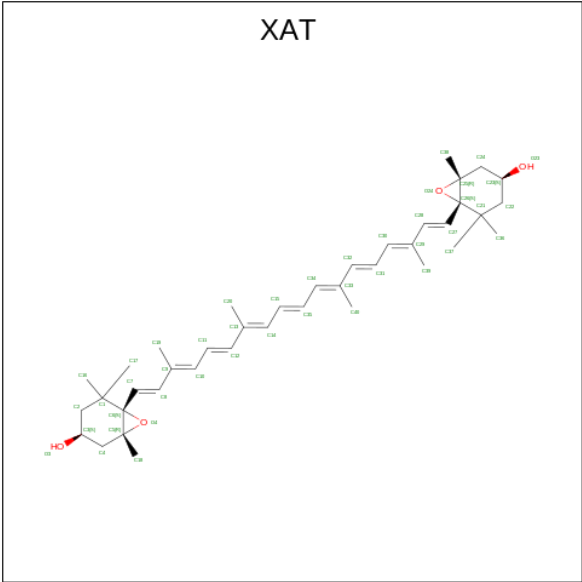
Mol	Chain	Residues	Atoms					AltConf
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19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	F	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	F	1	Total 41	C 33	Mg 1	N 4	O 3	0
19	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
19	K	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	L	1	Total 42	C 34	Mg 1	N 4	O 3	0

- Molecule 20 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).



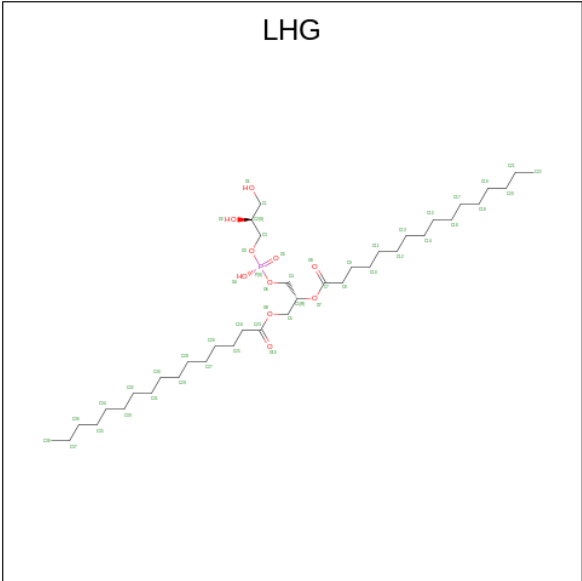
Mol	Chain	Residues	Atoms			AltConf
20	6	1	Total	C	O	0
			42	40	2	
20	6	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	2	1	Total	C	O	0
			42	40	2	
20	3	1	Total	C	O	0
			42	40	2	
20	3	1	Total	C	O	0
			42	40	2	
20	5	1	Total	C	O	0
			42	40	2	
20	5	1	Total	C	O	0
			42	40	2	
20	J	1	Total	C	O	0
			42	40	2	

- Molecule 21 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	6	1	Total	C	O	0
			44	40	4	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



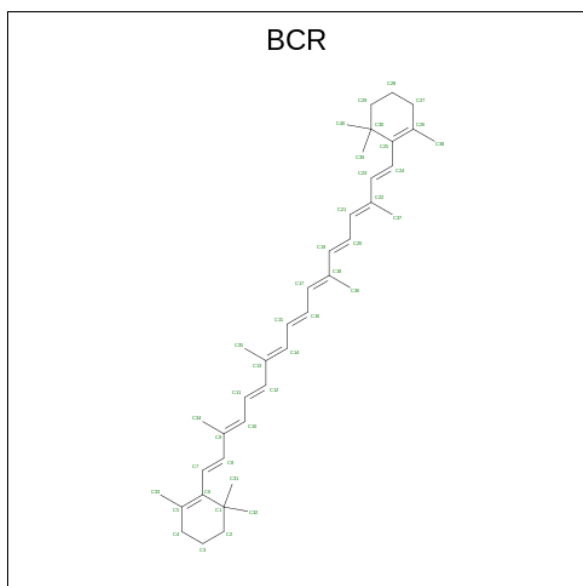
Mol	Chain	Residues	Atoms				AltConf
22	6	1	Total	C	O	P	0
			49	38	10	1	
22	6	1	Total	C	O	P	0
			27	16	10	1	

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Mol	Chain	Residues	Atoms				AltConf
22	2	1	Total	C	O	P	0
			38	27	10	1	
22	5	1	Total	C	O	P	0
			44	33	10	1	
22	A	1	Total	C	O	P	0
			49	38	10	1	
22	A	1	Total	C	O	P	0
			34	23	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



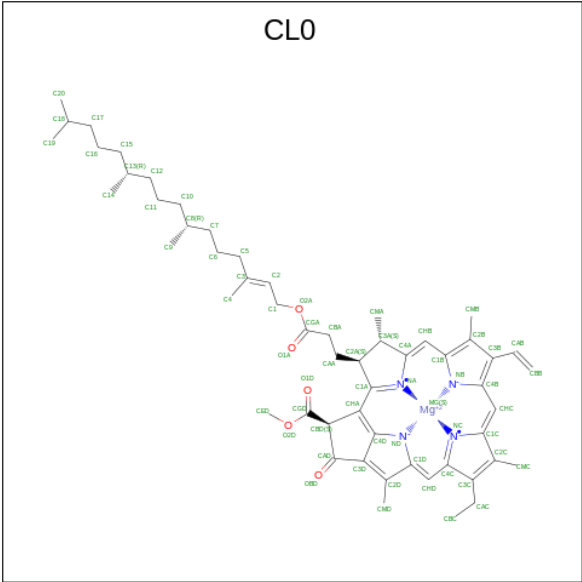
Mol	Chain	Residues	Atoms		AltConf
23	2	1	Total	C	0
			40	40	
23	3	1	Total	C	0
			40	40	
23	5	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	
23	A	1	Total	C	0
			40	40	

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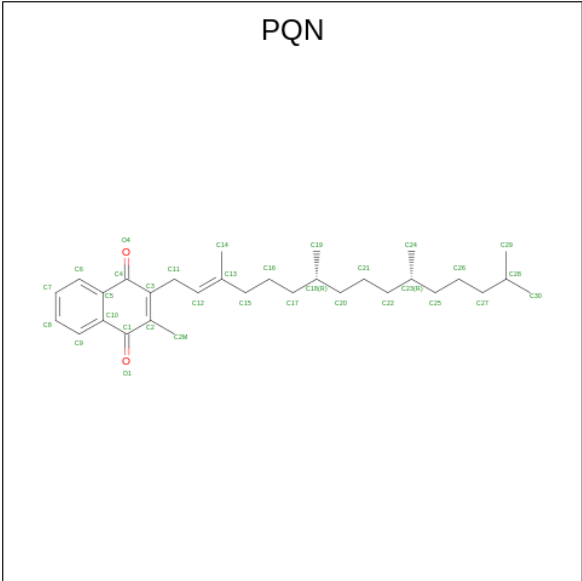
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C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

- Molecule 24 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



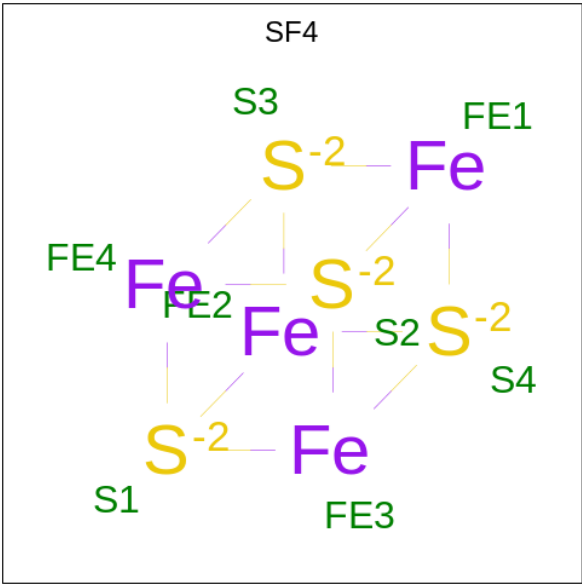
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



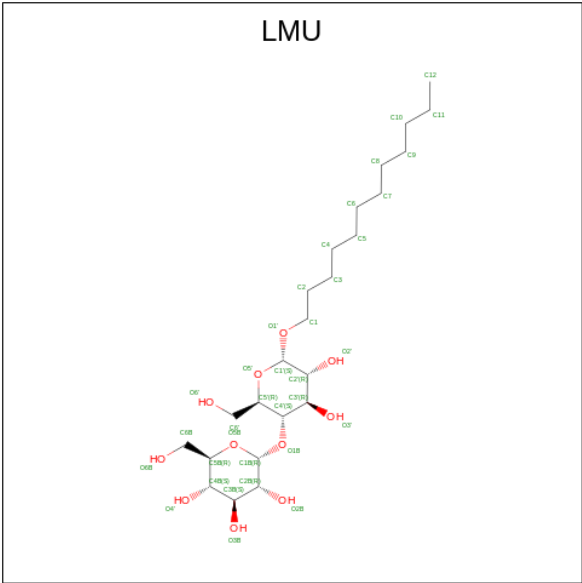
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



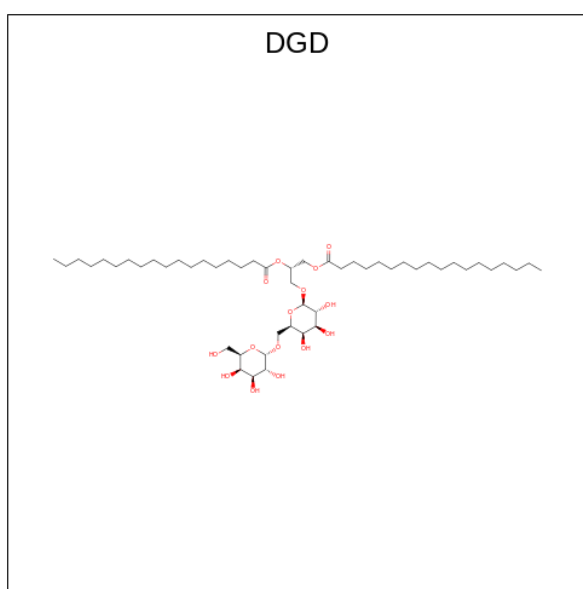
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).



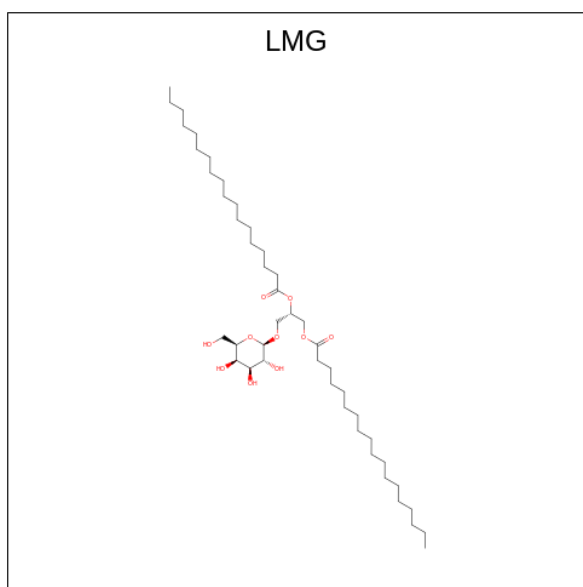
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			35	24	11	
27	G	1	Total	C	O	0
			35	24	11	

- Molecule 28 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
28	B	1	Total	C	O	0
			66	51	15	

- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			30	20	10	
29	J	1	Total	C	O	0
			41	31	10	

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		AltConf
30	6	14	Total	O	0
			14	14	
30	2	25	Total	O	0
			25	25	
30	3	37	Total	O	0
			37	37	
30	5	17	Total	O	0
			17	17	
30	A	184	Total	O	0
			184	184	
30	B	205	Total	O	0
			205	205	
30	C	45	Total	O	0
			45	45	
30	D	20	Total	O	0
			20	20	
30	E	17	Total	O	0
			17	17	
30	F	20	Total	O	0
			20	20	

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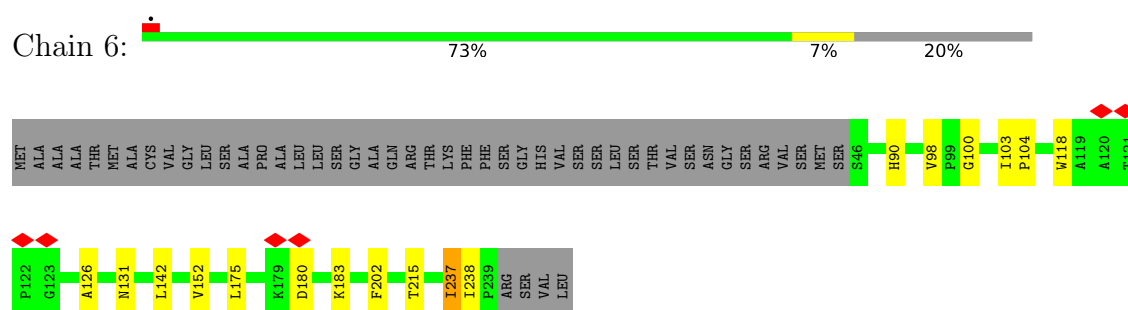
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Mol	Chain	Residues	Atoms		AltConf
30	G	2	Total 2	O 2	0
30	I	3	Total 3	O 3	0
30	J	4	Total 4	O 4	0
30	K	2	Total 2	O 2	0
30	M	2	Total 2	O 2	0
30	L	9	Total 9	O 9	0

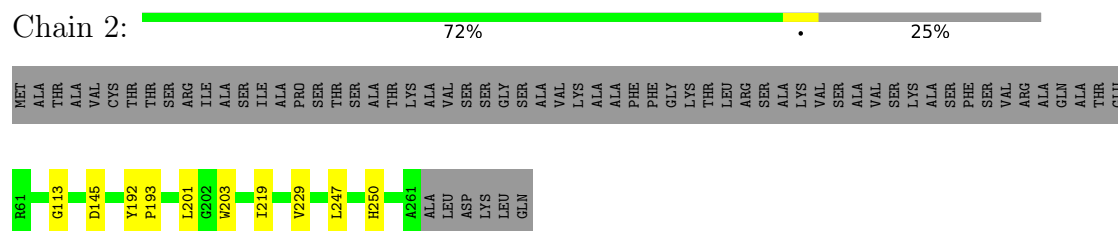
3 Residue-property plots

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

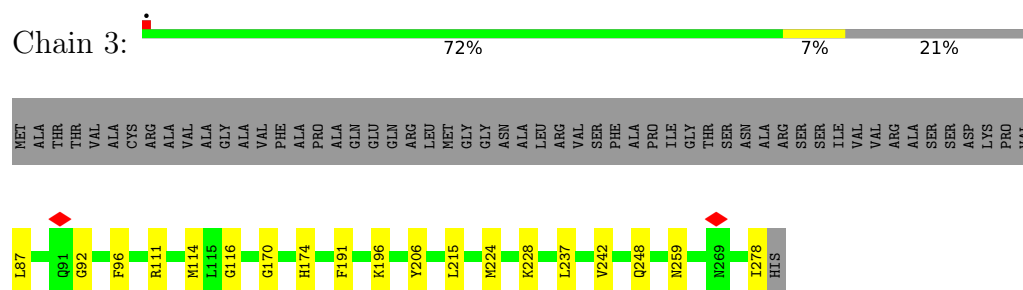
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



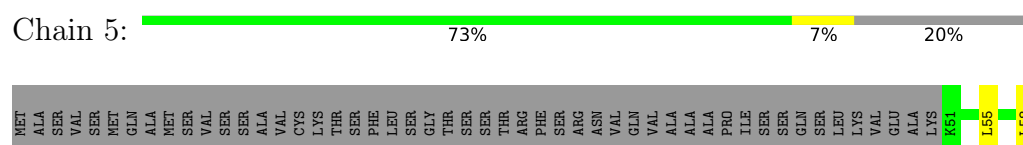
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



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



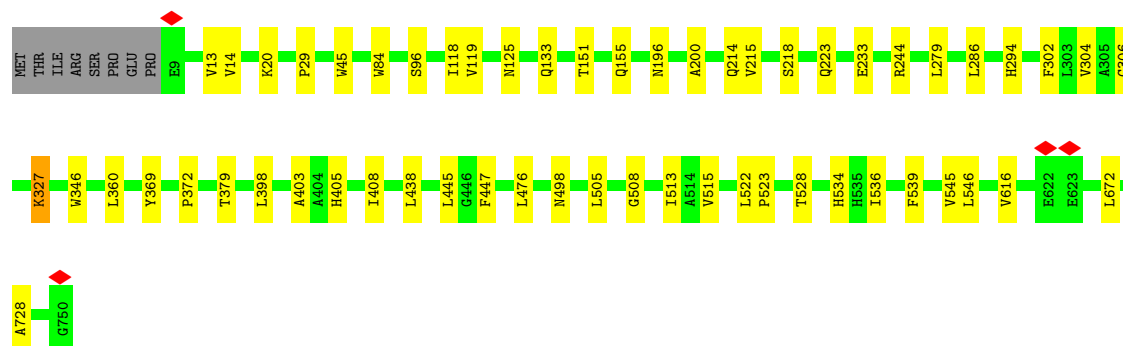
- Molecule 4: Chlorophyll a-b binding protein, chloroplastic





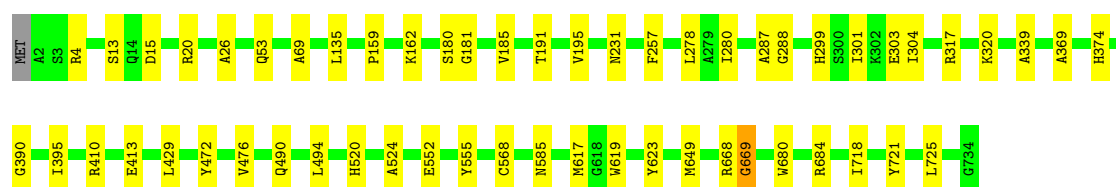
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 91% 7%



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 92% 7%



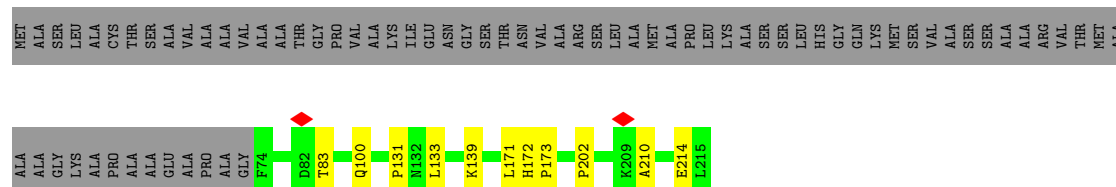
- Molecule 7: Photosystem I iron-sulfur center

Chain C: 96% 2%



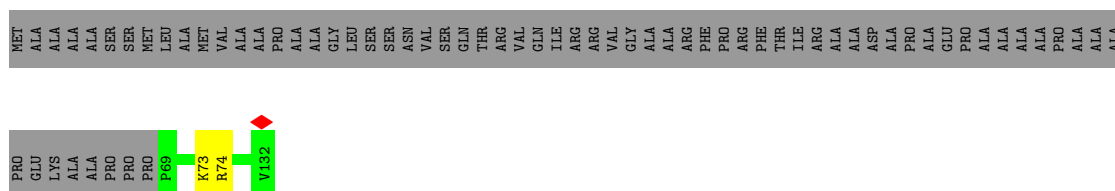
- Molecule 8: Photosystem I reaction center subunit II, chloroplastic

Chain D: 61% 5% 34%



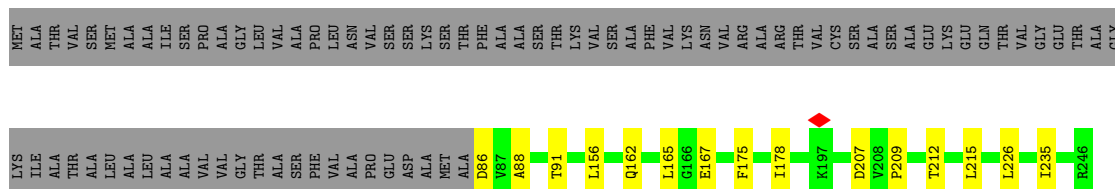
- Molecule 9: Photosystem I reaction centre subunit IV

Chain E: 47% 52%



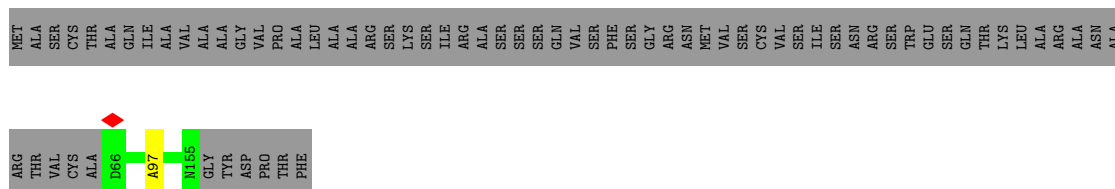
• Molecule 10: Photosystem I reaction center subunit III

Chain F: 59% 6% 35%



• Molecule 11: Photosystem I reaction center subunit V, chloroplastic

Chain G: 55% 0% 44%



• Molecule 12: Photosystem I reaction center subunit VIII

Chain I: 86% 11% 0%



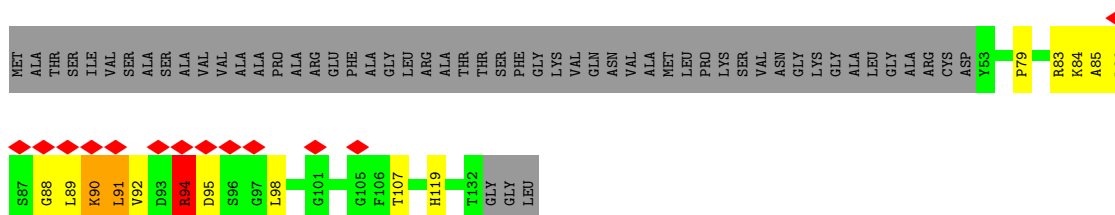
• Molecule 13: Photosystem I reaction center subunit IX

Chain J: 93% 5% 0%



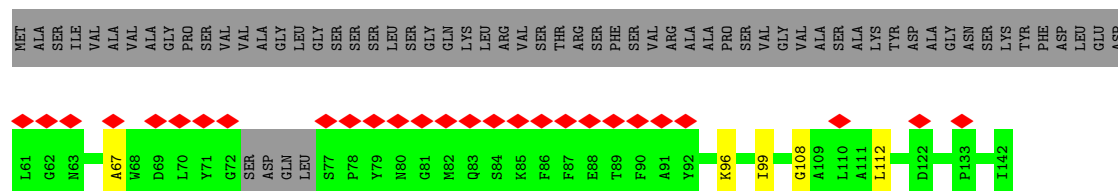
• Molecule 14: PSI-K

Chain K: 10% 48% 9% 0% 41%

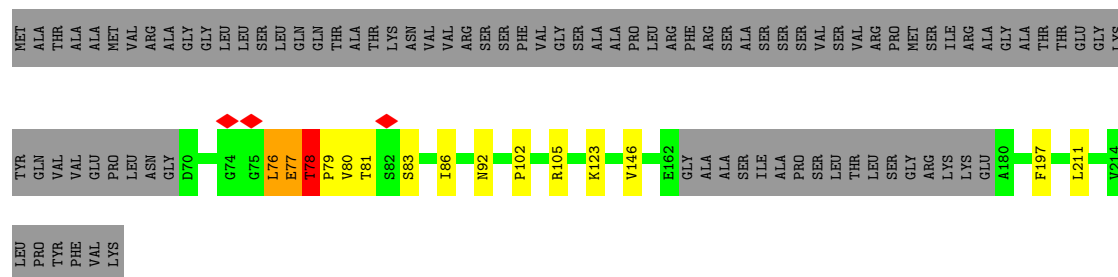


MET
THR
S3
V16
Q32

Chain H:



Chain L: 51% 5% 42%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157685	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	0.674	Depositor
Minimum map value	-0.321	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	363.5, 363.5, 363.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.727, 0.727, 0.727	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, CL0, BCR, SF4, LMU, LMG, LHG, XAT, CHL, PQN, CLA, LUT

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	6	0.25	0/1546	0.48	0/2112
2	2	0.22	0/1612	0.40	0/2203
3	3	0.24	0/1755	0.46	0/2379
4	5	0.23	0/1600	0.45	0/2185
5	A	0.28	0/6044	0.50	0/8247
6	B	0.31	0/6066	0.56	0/8277
7	C	0.36	0/612	0.58	0/829
8	D	0.20	0/1141	0.47	0/1538
9	E	0.28	0/516	0.40	0/701
10	F	0.22	0/1275	0.49	0/1725
11	G	0.19	0/686	0.42	0/931
12	I	0.30	0/281	0.64	0/384
13	J	0.18	0/338	0.42	0/462
14	K	0.42	0/567	0.59	0/766
15	M	0.21	0/236	0.41	0/317
16	H	0.20	0/591	0.45	0/796
17	L	0.32	0/987	0.55	0/1348
All	All	0.28	0/25853	0.50	0/35200

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
8	D	0	1
9	E	0	1
14	K	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	D	172	HIS	Peptide
9	E	74	ARG	Sidechain
14	K	94	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	6	1496	0	1474	11	0
2	2	1557	0	1510	9	0
3	3	1705	0	1672	14	0
4	5	1549	0	1528	16	0
5	A	5846	0	5712	39	0
6	B	5854	0	5632	36	0
7	C	602	0	575	1	0
8	D	1112	0	1128	6	0
9	E	503	0	490	0	0
10	F	1248	0	1291	9	0
11	G	673	0	678	1	0
12	I	274	0	285	2	0
13	J	328	0	339	2	0
14	K	561	0	581	11	0
15	M	235	0	259	1	0
16	H	578	0	590	2	0
17	L	958	0	956	11	0
18	2	302	0	234	11	0
18	3	112	0	101	4	0
18	5	178	0	120	1	0
18	6	97	0	68	6	0
19	2	482	0	433	12	0
19	3	618	0	535	15	0
19	5	549	0	501	11	0
19	6	626	0	548	18	0
19	A	2443	0	2417	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	B	2485	0	2516	57	0
19	F	146	0	121	4	0
19	G	90	0	66	1	0
19	J	42	0	31	1	0
19	K	140	0	104	1	0
19	L	147	0	123	4	0
20	2	126	0	168	8	0
20	3	84	0	112	11	0
20	5	84	0	112	7	0
20	6	84	0	112	4	0
20	J	42	0	56	4	0
21	6	44	0	56	3	0
22	2	38	0	46	0	0
22	5	44	0	58	5	0
22	6	76	0	98	6	0
22	A	83	0	112	3	0
23	2	40	0	56	2	0
23	3	40	0	56	2	0
23	5	40	0	56	2	0
23	A	200	0	280	17	0
23	B	200	0	280	13	0
23	F	80	0	112	6	0
23	G	80	0	112	6	0
23	I	40	0	56	2	0
23	J	40	0	56	6	0
23	K	80	0	112	4	0
23	L	80	0	112	4	0
23	M	40	0	56	3	0
24	A	65	0	72	2	0
25	A	33	0	46	2	0
25	B	33	0	46	1	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	A	35	0	46	0	0
27	B	70	0	92	4	0
27	G	35	0	46	2	0
28	B	66	0	96	4	0
29	J	71	0	85	3	0
30	2	25	0	0	0	0
30	3	37	0	0	0	0
30	5	17	0	0	0	0
30	6	14	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A	184	0	0	0	0
30	B	205	0	0	2	0
30	C	45	0	0	0	0
30	D	20	0	0	0	0
30	E	17	0	0	0	0
30	F	20	0	0	0	0
30	G	2	0	0	0	0
30	I	3	0	0	0	0
30	J	4	0	0	0	0
30	K	2	0	0	0	0
30	L	9	0	0	0	0
30	M	2	0	0	0	0
All	All	36239	0	35421	364	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 5.

The worst 5 of 364 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)
3:3:242:VAL:HG11	20:3:316:LUT:H32	1.69	0.74
3:3:191:PHE:HE2	18:3:306:CHL:HBB2	1.56	0.71
19:A:824:CLA:H2	14:K:88:GLY:HA3	1.73	0.71
19:A:811:CLA:HBB2	19:A:814:CLA:HMA3	1.75	0.68
1:6:98:VAL:HG11	20:6:315:LUT:H12	1.76	0.68

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	6	192/243 (79%)	189 (98%)	3 (2%)	0	100	100
2	2	199/267 (74%)	196 (98%)	3 (2%)	0	100	100
3	3	218/279 (78%)	210 (96%)	8 (4%)	0	100	100
4	5	196/249 (79%)	191 (97%)	5 (3%)	0	100	100
5	A	740/750 (99%)	722 (98%)	18 (2%)	0	100	100
6	B	731/734 (100%)	713 (98%)	17 (2%)	1 (0%)	48	41
7	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
8	D	140/215 (65%)	134 (96%)	5 (4%)	1 (1%)	18	9
9	E	62/132 (47%)	61 (98%)	1 (2%)	0	100	100
10	F	159/246 (65%)	156 (98%)	3 (2%)	0	100	100
11	G	88/161 (55%)	88 (100%)	0	0	100	100
12	I	33/36 (92%)	33 (100%)	0	0	100	100
13	J	39/42 (93%)	38 (97%)	1 (3%)	0	100	100
14	K	78/135 (58%)	73 (94%)	5 (6%)	0	100	100
15	M	28/32 (88%)	28 (100%)	0	0	100	100
16	H	74/142 (52%)	72 (97%)	2 (3%)	0	100	100
17	L	124/221 (56%)	117 (94%)	6 (5%)	1 (1%)	16	7
All	All	3179/3965 (80%)	3097 (97%)	79 (2%)	3 (0%)	49	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	173	PRO
17	L	78	THR
6	B	669	GLY

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	6	152/190 (80%)	146 (96%)	6 (4%)	28	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	2	155/204 (76%)	154 (99%)	1 (1%)	78	78
3	3	173/216 (80%)	172 (99%)	1 (1%)	78	78
4	5	159/202 (79%)	159 (100%)	0	100	100
5	A	603/611 (99%)	596 (99%)	7 (1%)	63	57
6	B	597/598 (100%)	593 (99%)	4 (1%)	76	74
7	C	68/69 (99%)	68 (100%)	0	100	100
8	D	116/161 (72%)	116 (100%)	0	100	100
9	E	57/99 (58%)	56 (98%)	1 (2%)	51	43
10	F	129/189 (68%)	126 (98%)	3 (2%)	44	33
11	G	70/125 (56%)	70 (100%)	0	100	100
12	I	31/32 (97%)	30 (97%)	1 (3%)	34	20
13	J	35/36 (97%)	35 (100%)	0	100	100
14	K	58/96 (60%)	52 (90%)	6 (10%)	7	1
15	M	28/30 (93%)	28 (100%)	0	100	100
16	H	58/107 (54%)	56 (97%)	2 (3%)	32	19
17	L	97/169 (57%)	94 (97%)	3 (3%)	35	21
All	All	2586/3134 (82%)	2551 (99%)	35 (1%)	57	52

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	K	94	ARG
14	K	95	ASP
17	L	76	LEU
5	A	233	GLU
5	A	223	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
7	C	37	ASN
13	J	30	ASN
9	E	123	ASN
11	G	96	GLN
16	H	131	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

207 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
23	BCR	B	846	-	41,41,41	1.81	7 (17%)	56,56,56	2.16	17 (30%)
19	CLA	B	835	6	49,53,73	1.38	6 (12%)	59,89,113	1.10	4 (6%)
23	BCR	G	205	-	41,41,41	1.75	8 (19%)	56,56,56	1.74	15 (26%)
19	CLA	F	303	30	49,53,73	1.40	6 (12%)	59,89,113	1.11	3 (5%)
27	LMU	A	853	-	36,36,36	0.25	0	47,47,47	0.71	3 (6%)
23	BCR	B	848	-	41,41,41	1.80	8 (19%)	56,56,56	2.08	15 (26%)
19	CLA	5	303	30	49,53,73	1.40	9 (18%)	59,89,113	1.09	5 (8%)
19	CLA	B	813	6	49,53,73	1.41	8 (16%)	59,89,113	1.14	4 (6%)
19	CLA	3	309	30	59,63,73	1.29	8 (13%)	71,101,113	1.06	5 (7%)
19	CLA	A	809	5	52,56,73	1.43	7 (13%)	62,92,113	1.05	4 (6%)
19	CLA	6	314	1	49,53,73	1.40	7 (14%)	59,89,113	1.17	6 (10%)
18	CHL	5	304	30	50,54,74	1.39	9 (18%)	56,90,114	1.19	6 (10%)
18	CHL	2	301	2	70,74,74	1.15	7 (10%)	80,114,114	1.05	6 (7%)
19	CLA	B	837	6	56,60,73	1.39	8 (14%)	67,97,113	1.07	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	3	305	3	50,54,73	1.39	7 (14%)	60,90,113	1.17	6 (10%)
19	CLA	2	312	2	69,73,73	1.21	8 (11%)	83,113,113	1.05	6 (7%)
19	CLA	L	302	17	64,68,73	1.23	8 (12%)	77,107,113	0.92	3 (3%)
19	CLA	A	803	-	69,73,73	1.19	7 (10%)	83,113,113	0.95	4 (4%)
23	BCR	B	845	-	41,41,41	1.71	8 (19%)	56,56,56	1.78	14 (25%)
19	CLA	3	311	3	59,63,73	1.31	9 (15%)	71,101,113	1.19	6 (8%)
19	CLA	2	302	2	69,73,73	1.16	7 (10%)	83,113,113	1.00	4 (4%)
19	CLA	3	307	3	64,68,73	1.21	7 (10%)	77,107,113	1.17	6 (7%)
19	CLA	B	801	30	69,73,73	1.22	9 (13%)	83,113,113	1.00	7 (8%)
19	CLA	A	841	5	69,73,73	1.19	7 (10%)	83,113,113	0.94	3 (3%)
19	CLA	B	807	6	69,73,73	1.22	7 (10%)	83,113,113	1.04	5 (6%)
19	CLA	B	811	6	69,73,73	1.20	7 (10%)	83,113,113	0.97	4 (4%)
19	CLA	B	816	6	69,73,73	1.22	8 (11%)	83,113,113	1.01	4 (4%)
19	CLA	A	834	5	69,73,73	1.25	8 (11%)	83,113,113	0.97	4 (4%)
19	CLA	B	833	6	69,73,73	1.22	7 (10%)	83,113,113	0.99	5 (6%)
19	CLA	6	313	1	49,53,73	1.43	7 (14%)	59,89,113	1.18	5 (8%)
24	CL0	A	802	5	69,73,73	1.48	9 (13%)	83,113,113	0.80	3 (3%)
26	SF4	A	845	5,6	0,12,12	-	-	-		
26	SF4	C	102	7	0,12,12	-	-	-		
19	CLA	A	817	30	49,53,73	1.40	7 (14%)	59,89,113	1.22	5 (8%)
19	CLA	A	842	5	69,73,73	1.23	7 (10%)	83,113,113	1.00	4 (4%)
19	CLA	3	301	3	64,68,73	1.22	8 (12%)	77,107,113	0.99	4 (5%)
19	CLA	B	825	30	69,73,73	1.18	8 (11%)	83,113,113	1.06	6 (7%)
19	CLA	B	819	6	69,73,73	1.17	7 (10%)	83,113,113	0.98	4 (4%)
19	CLA	B	838	6	69,73,73	1.18	7 (10%)	83,113,113	0.98	4 (4%)
19	CLA	5	307	4	63,67,73	1.21	6 (9%)	75,105,113	1.10	5 (6%)
19	CLA	B	820	30	61,65,73	1.28	8 (13%)	73,103,113	1.11	7 (9%)
19	CLA	B	831	6	49,53,73	1.48	7 (14%)	59,89,113	1.06	3 (5%)
20	LUT	2	316	-	42,43,43	1.61	8 (19%)	51,60,60	1.62	11 (21%)
18	CHL	3	314	3	70,74,74	1.19	8 (11%)	80,114,114	1.04	8 (10%)
23	BCR	A	852	-	41,41,41	1.73	8 (19%)	56,56,56	1.80	14 (25%)
19	CLA	B	809	6	69,73,73	1.20	7 (10%)	83,113,113	0.95	4 (4%)
19	CLA	5	314	4	49,53,73	1.51	6 (12%)	59,89,113	1.38	7 (11%)
19	CLA	B	810	6	69,73,73	1.22	8 (11%)	83,113,113	0.96	6 (7%)
19	CLA	L	301	17	49,53,73	1.42	8 (16%)	59,89,113	1.15	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	6	308	1	54,58,73	1.35	8 (14%)	65,95,113	1.09	4 (6%)
19	CLA	B	818	6	66,70,73	1.26	7 (10%)	79,109,113	1.15	8 (10%)
19	CLA	F	301	30	64,68,73	1.25	7 (10%)	77,107,113	1.07	6 (7%)
19	CLA	G	204	11	49,53,73	1.41	8 (16%)	59,89,113	1.08	4 (6%)
19	CLA	B	832	6	69,73,73	1.21	8 (11%)	83,113,113	0.98	3 (3%)
19	CLA	K	202	14	48,52,73	1.48	9 (18%)	61,88,113	1.07	3 (4%)
26	SF4	C	101	7	0,12,12	-	-	-		
19	CLA	5	310	4	48,52,73	1.40	6 (12%)	58,88,113	1.08	4 (6%)
23	BCR	F	302	-	41,41,41	1.71	8 (19%)	56,56,56	1.78	15 (26%)
20	LUT	5	316	-	42,43,43	1.62	8 (19%)	51,60,60	1.85	13 (25%)
19	CLA	B	829	6	69,73,73	1.21	7 (10%)	83,113,113	0.86	3 (3%)
19	CLA	2	313	2	54,58,73	1.36	6 (11%)	65,95,113	1.11	5 (7%)
19	CLA	A	804	30	69,73,73	1.17	7 (10%)	83,113,113	1.00	5 (6%)
19	CLA	B	841	6	69,73,73	1.28	8 (11%)	83,113,113	0.94	3 (3%)
23	BCR	5	317	-	41,41,41	1.75	8 (19%)	56,56,56	1.98	18 (32%)
19	CLA	B	834	6	64,68,73	1.25	7 (10%)	77,107,113	0.97	4 (5%)
19	CLA	A	808	5	69,73,73	1.19	8 (11%)	83,113,113	0.97	3 (3%)
19	CLA	A	823	5	49,53,73	1.42	8 (16%)	59,89,113	1.15	5 (8%)
19	CLA	A	827	30	59,63,73	1.25	6 (10%)	71,101,113	1.02	4 (5%)
23	BCR	A	850	-	41,41,41	1.71	8 (19%)	56,56,56	1.67	13 (23%)
19	CLA	A	838	5	55,59,73	1.39	8 (14%)	66,96,113	1.11	6 (9%)
19	CLA	K	203	14	49,53,73	1.39	8 (16%)	59,89,113	1.09	4 (6%)
19	CLA	A	816	5	46,50,73	1.46	7 (15%)	55,85,113	1.14	4 (7%)
19	CLA	B	815	6	69,73,73	1.21	8 (11%)	83,113,113	0.92	3 (3%)
19	CLA	A	837	5	49,53,73	1.40	8 (16%)	59,89,113	1.22	5 (8%)
19	CLA	2	308	2	49,53,73	1.36	7 (14%)	59,89,113	1.12	4 (6%)
21	XAT	6	316	-	39,47,47	0.66	2 (5%)	54,74,74	0.97	3 (5%)
19	CLA	6	309	1	69,73,73	1.14	7 (10%)	83,113,113	0.99	5 (6%)
19	CLA	B	840	30	69,73,73	1.16	6 (8%)	83,113,113	1.15	8 (9%)
19	CLA	F	304	10	45,49,73	1.50	8 (17%)	54,84,113	1.21	5 (9%)
19	CLA	2	303	2	49,53,73	1.44	7 (14%)	59,89,113	1.08	5 (8%)
18	CHL	5	305	30	47,51,74	1.39	7 (14%)	52,86,114	1.19	5 (9%)
19	CLA	A	812	5	69,73,73	1.21	8 (11%)	83,113,113	0.98	4 (4%)
20	LUT	3	315	-	42,43,43	1.62	8 (19%)	51,60,60	1.74	14 (27%)
19	CLA	A	810	5	69,73,73	1.17	8 (11%)	83,113,113	0.97	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	808	6	64,68,73	1.23	7 (10%)	77,107,113	1.00	3 (3%)
18	CHL	5	306	30	50,54,74	1.34	7 (14%)	56,90,114	1.15	5 (8%)
19	CLA	3	304	30	49,53,73	1.41	8 (16%)	59,89,113	1.14	5 (8%)
19	CLA	B	836	30	49,53,73	1.41	8 (16%)	59,89,113	1.14	4 (6%)
23	BCR	K	205	-	41,41,41	1.69	8 (19%)	56,56,56	1.56	11 (19%)
23	BCR	B	844	-	41,41,41	1.69	8 (19%)	56,56,56	1.78	15 (26%)
19	CLA	A	819	5	61,65,73	1.28	7 (11%)	73,103,113	1.11	7 (9%)
23	BCR	F	305	-	41,41,41	1.71	8 (19%)	56,56,56	1.78	15 (26%)
19	CLA	A	814	5	69,73,73	1.20	8 (11%)	83,113,113	0.99	4 (4%)
27	LMU	G	202	-	36,36,36	0.27	0	47,47,47	0.68	0
19	CLA	6	307	30	49,53,73	1.46	6 (12%)	59,89,113	1.21	7 (11%)
23	BCR	3	317	-	41,41,41	1.70	10 (24%)	56,56,56	1.84	18 (32%)
23	BCR	L	305	-	41,41,41	1.66	8 (19%)	56,56,56	1.73	15 (26%)
19	CLA	B	812	6	64,68,73	1.29	7 (10%)	77,107,113	1.00	4 (5%)
19	CLA	A	830	5	69,73,73	1.26	8 (11%)	83,113,113	0.91	3 (3%)
19	CLA	B	804	-	69,73,73	1.14	7 (10%)	83,113,113	1.02	6 (7%)
19	CLA	6	305	30	49,53,73	1.41	7 (14%)	59,89,113	1.08	3 (5%)
19	CLA	B	842	22	69,73,73	1.18	7 (10%)	83,113,113	0.95	5 (6%)
19	CLA	2	309	2	65,69,73	1.19	7 (10%)	78,108,113	1.13	6 (7%)
19	CLA	5	308	4	64,68,73	1.19	7 (10%)	77,107,113	1.01	4 (5%)
23	BCR	A	849	-	41,41,41	1.73	8 (19%)	56,56,56	1.74	15 (26%)
18	CHL	2	314	2	50,54,74	1.35	7 (14%)	56,90,114	1.17	4 (7%)
18	CHL	6	306	1	50,54,74	1.37	7 (14%)	56,90,114	1.20	5 (8%)
22	LHG	2	318	19	37,37,48	0.31	0	40,43,54	0.41	0
19	CLA	B	824	6	49,53,73	1.37	8 (16%)	59,89,113	1.11	5 (8%)
19	CLA	A	839	5	59,63,73	1.30	7 (11%)	71,101,113	0.99	3 (4%)
19	CLA	K	201	30	55,59,73	1.31	7 (12%)	66,96,113	1.14	6 (9%)
19	CLA	3	310	3	47,51,73	1.51	7 (14%)	56,86,113	1.18	5 (8%)
19	CLA	A	836	5	64,68,73	1.24	7 (10%)	77,107,113	1.00	4 (5%)
18	CHL	3	306	30	50,54,74	1.37	8 (16%)	56,90,114	1.27	7 (12%)
19	CLA	A	815	5	55,59,73	1.36	8 (14%)	66,96,113	1.07	4 (6%)
18	CHL	2	307	30	53,57,74	1.33	8 (15%)	59,93,114	1.11	6 (10%)
19	CLA	A	831	5	69,73,73	1.30	9 (13%)	83,113,113	0.86	4 (4%)
19	CLA	A	833	5	59,63,73	1.31	8 (13%)	71,101,113	1.02	5 (7%)
19	CLA	3	313	30	49,53,73	1.40	8 (16%)	59,89,113	1.19	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	K	204	-	41,41,41	1.71	8 (19%)	56,56,56	1.79	17 (30%)
23	BCR	A	848	-	41,41,41	1.73	8 (19%)	56,56,56	1.88	15 (26%)
19	CLA	A	824	5	69,73,73	1.20	6 (8%)	83,113,113	1.09	6 (7%)
20	LUT	6	318	-	42,43,43	1.67	8 (19%)	51,60,60	2.01	16 (31%)
23	BCR	L	304	-	41,41,41	1.74	9 (21%)	56,56,56	1.94	18 (32%)
19	CLA	B	826	30	57,61,73	1.27	7 (12%)	68,98,113	1.04	4 (5%)
18	CHL	5	313	4	47,51,74	1.36	7 (14%)	52,86,114	1.22	6 (11%)
19	CLA	B	822	6	50,54,73	1.42	7 (14%)	60,90,113	1.16	5 (8%)
23	BCR	B	847	-	41,41,41	1.67	9 (21%)	56,56,56	1.76	14 (25%)
19	CLA	A	807	5	69,73,73	1.16	7 (10%)	83,113,113	1.00	4 (4%)
23	BCR	J	103	-	41,41,41	1.81	8 (19%)	56,56,56	2.25	20 (35%)
19	CLA	A	825	5	69,73,73	1.22	8 (11%)	83,113,113	1.07	6 (7%)
20	LUT	2	317	-	42,43,43	1.65	8 (19%)	51,60,60	1.95	11 (21%)
19	CLA	6	310	22	60,64,73	1.29	7 (11%)	72,102,113	1.05	4 (5%)
19	CLA	A	820	5	69,73,73	1.17	8 (11%)	83,113,113	1.00	4 (4%)
19	CLA	3	308	3	69,73,73	1.14	7 (10%)	83,113,113	1.04	4 (4%)
19	CLA	6	302	1	65,69,73	1.21	8 (12%)	78,108,113	0.99	4 (5%)
19	CLA	3	303	30	51,55,73	1.37	9 (17%)	61,91,113	1.09	5 (8%)
19	CLA	A	832	5	54,58,73	1.38	7 (12%)	65,95,113	0.98	3 (4%)
29	LMG	J	105	-	41,41,55	0.53	0	49,49,63	0.69	0
19	CLA	L	303	30	46,50,73	1.44	8 (17%)	55,85,113	1.17	4 (7%)
19	CLA	A	806	5	59,63,73	1.28	7 (11%)	71,101,113	1.02	4 (5%)
19	CLA	3	302	3	59,63,73	1.38	8 (13%)	71,101,113	1.00	5 (7%)
19	CLA	B	839	6	51,55,73	1.41	7 (13%)	61,91,113	1.09	5 (8%)
19	CLA	A	826	30	69,73,73	1.26	8 (11%)	83,113,113	1.00	6 (7%)
19	CLA	B	802	30	69,73,73	1.17	8 (11%)	83,113,113	0.95	5 (6%)
20	LUT	6	315	-	42,43,43	1.65	8 (19%)	51,60,60	1.63	12 (23%)
19	CLA	A	818	5	64,68,73	1.32	8 (12%)	77,107,113	1.15	6 (7%)
19	CLA	B	830	6	64,68,73	1.24	8 (12%)	77,107,113	1.02	5 (6%)
19	CLA	6	303	1	59,63,73	1.32	7 (11%)	71,101,113	0.98	4 (5%)
19	CLA	B	817	6	69,73,73	1.24	7 (10%)	83,113,113	0.94	4 (4%)
19	CLA	6	311	1	49,53,73	1.45	7 (14%)	59,89,113	1.19	5 (8%)
22	LHG	6	319	19	26,26,48	0.36	0	29,32,54	0.48	0
25	PQN	B	843	-	34,34,34	0.39	0	42,45,45	0.59	0
19	CLA	A	805	5	69,73,73	1.18	7 (10%)	83,113,113	0.94	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CHL	2	320	4	56,60,74	1.32	8 (14%)	63,97,114	1.13	6 (9%)
23	BCR	I	101	-	41,41,41	1.68	8 (19%)	56,56,56	1.68	14 (25%)
19	CLA	2	310	22	60,64,73	1.27	7 (11%)	72,102,113	1.04	5 (6%)
27	LMU	B	850	-	36,36,36	0.25	0	47,47,47	0.41	0
23	BCR	G	201	-	41,41,41	1.69	8 (19%)	56,56,56	1.76	14 (25%)
23	BCR	A	851	-	41,41,41	1.67	9 (21%)	56,56,56	1.75	15 (26%)
19	CLA	B	828	6	69,73,73	1.21	8 (11%)	83,113,113	0.95	4 (4%)
19	CLA	B	823	6	59,63,73	1.37	8 (13%)	71,101,113	1.15	5 (7%)
19	CLA	B	827	6	69,73,73	1.26	8 (11%)	83,113,113	0.93	4 (4%)
18	CHL	2	305	30	50,54,74	1.37	9 (18%)	56,90,114	1.17	6 (10%)
19	CLA	A	811	5	59,63,73	1.32	7 (11%)	71,101,113	0.98	3 (4%)
25	PQN	A	844	-	34,34,34	0.35	0	42,45,45	0.64	1 (2%)
19	CLA	J	102	13	46,50,73	1.46	7 (15%)	55,85,113	1.25	5 (9%)
23	BCR	M	101	-	41,41,41	1.73	8 (19%)	56,56,56	1.73	13 (23%)
20	LUT	3	316	-	42,43,43	1.65	8 (19%)	51,60,60	1.83	14 (27%)
28	DGD	B	849	-	67,67,67	0.53	0	81,81,81	0.74	1 (1%)
20	LUT	2	315	-	42,43,43	1.65	8 (19%)	51,60,60	1.78	12 (23%)
19	CLA	B	821	6	47,51,73	1.43	8 (17%)	56,86,113	1.11	4 (7%)
19	CLA	5	309	30	64,68,73	1.22	7 (10%)	77,107,113	1.02	4 (5%)
19	CLA	G	203	11	49,53,73	1.48	8 (16%)	59,89,113	1.07	4 (6%)
23	BCR	2	319	-	41,41,41	1.81	8 (19%)	56,56,56	2.12	19 (33%)
19	CLA	A	822	30	69,73,73	1.18	8 (11%)	83,113,113	0.95	4 (4%)
19	CLA	2	311	2	49,53,73	1.47	8 (16%)	59,89,113	1.08	4 (6%)
20	LUT	5	315	-	42,43,43	1.65	8 (19%)	51,60,60	1.63	9 (17%)
19	CLA	A	828	5	69,73,73	1.26	8 (11%)	83,113,113	1.04	6 (7%)
22	LHG	A	847	19	33,33,48	0.31	0	36,39,54	0.39	0
22	LHG	5	318	-	43,43,48	0.28	0	46,49,54	0.35	0
29	LMG	J	104	-	30,30,55	0.62	0	38,38,63	0.70	0
27	LMU	B	851	-	36,36,36	0.22	0	47,47,47	0.41	0
19	CLA	5	311	4	65,69,73	1.20	6 (9%)	78,108,113	1.10	6 (7%)
19	CLA	6	304	30	53,57,73	1.35	7 (13%)	62,93,113	1.16	5 (8%)
19	CLA	B	814	6	69,73,73	1.23	8 (11%)	83,113,113	0.95	4 (4%)
19	CLA	A	813	5	58,62,73	1.29	8 (13%)	69,99,113	0.99	4 (5%)
19	CLA	A	840	5	54,58,73	1.40	7 (12%)	65,95,113	1.09	4 (6%)
20	LUT	J	101	-	42,43,43	1.65	8 (19%)	51,60,60	1.89	14 (27%)
19	CLA	3	312	3	46,50,73	1.47	6 (13%)	55,85,113	1.13	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	829	5	69,73,73	1.22	7 (10%)	83,113,113	1.00	3 (3%)
19	CLA	5	302	4	54,58,73	1.40	7 (12%)	65,95,113	1.05	4 (6%)
18	CHL	2	306	30	47,51,74	1.38	7 (14%)	52,86,114	1.30	8 (15%)
19	CLA	A	835	5	69,73,73	1.21	7 (10%)	83,113,113	0.95	4 (4%)
19	CLA	A	843	22	49,53,73	1.42	9 (18%)	59,89,113	1.08	4 (6%)
22	LHG	A	846	-	48,48,48	0.27	0	51,54,54	0.38	0
18	CHL	6	301	1	55,59,74	1.28	8 (14%)	62,96,114	1.12	5 (8%)
22	LHG	6	317	19	48,48,48	0.28	0	51,54,54	0.37	0
19	CLA	6	312	1	69,73,73	1.16	7 (10%)	83,113,113	1.16	6 (7%)
19	CLA	5	312	4	69,73,73	1.21	7 (10%)	83,113,113	1.07	5 (6%)
19	CLA	A	821	5	49,53,73	1.42	7 (14%)	59,89,113	1.16	5 (8%)
19	CLA	5	301	4	64,68,73	1.22	8 (12%)	77,107,113	1.00	4 (5%)
19	CLA	A	801	5	59,63,73	1.28	9 (15%)	71,101,113	1.02	4 (5%)
19	CLA	B	805	6	49,53,73	1.47	8 (16%)	59,89,113	1.09	3 (5%)
19	CLA	B	803	6	69,73,73	1.25	7 (10%)	83,113,113	0.83	4 (4%)
19	CLA	B	806	6	69,73,73	1.19	8 (11%)	83,113,113	0.95	3 (3%)
19	CLA	2	304	30	54,58,73	1.33	9 (16%)	65,95,113	1.05	5 (7%)

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
23	BCR	B	846	-	-	5/29/63/63	0/2/2/2
19	CLA	B	835	6	-	3/15/91/115	-
23	BCR	G	205	-	-	0/29/63/63	0/2/2/2
19	CLA	F	303	30	-	2/15/91/115	-
27	LMU	A	853	-	-	4/21/61/61	0/2/2/2
23	BCR	B	848	-	-	5/29/63/63	0/2/2/2
19	CLA	5	303	30	-	2/15/91/115	-
19	CLA	B	813	6	-	3/15/91/115	-
19	CLA	3	309	30	-	2/27/103/115	-
19	CLA	A	809	5	-	1/19/95/115	-
19	CLA	6	314	1	-	4/15/91/115	-
18	CHL	5	304	30	-	4/17/93/117	-
18	CHL	2	301	2	-	5/41/117/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	837	6	-	3/24/100/115	-
19	CLA	3	305	3	-	0/17/93/115	-
19	CLA	2	312	2	-	4/39/115/115	-
19	CLA	L	302	17	-	5/33/109/115	-
19	CLA	A	803	-	-	5/39/115/115	-
23	BCR	B	845	-	-	5/29/63/63	0/2/2/2
19	CLA	3	311	3	-	5/27/103/115	-
19	CLA	2	302	2	-	6/39/115/115	-
19	CLA	3	307	3	-	7/33/109/115	-
19	CLA	B	801	30	-	8/39/115/115	-
19	CLA	A	841	5	-	6/39/115/115	-
19	CLA	B	807	6	-	7/39/115/115	-
19	CLA	B	811	6	-	6/39/115/115	-
19	CLA	B	816	6	-	9/39/115/115	-
19	CLA	A	834	5	-	3/39/115/115	-
19	CLA	B	833	6	-	2/39/115/115	-
19	CLA	6	313	1	-	5/15/91/115	-
24	CL0	A	802	5	-	1/39/115/115	-
26	SF4	A	845	5,6	-	-	0/6/5/5
26	SF4	C	102	7	-	-	0/6/5/5
19	CLA	A	817	30	-	3/15/91/115	-
19	CLA	A	842	5	-	2/39/115/115	-
19	CLA	3	301	3	-	3/33/109/115	-
19	CLA	B	825	30	-	7/39/115/115	-
19	CLA	B	819	6	-	8/39/115/115	-
19	CLA	B	838	6	-	4/39/115/115	-
19	CLA	5	307	4	-	12/32/108/115	-
19	CLA	B	820	30	-	0/30/106/115	-
19	CLA	B	831	6	-	5/15/91/115	-
20	LUT	2	316	-	-	0/29/67/67	0/2/2/2
18	CHL	3	314	3	-	8/41/117/117	-
23	BCR	A	852	-	-	7/29/63/63	0/2/2/2
19	CLA	B	809	6	-	2/39/115/115	-
19	CLA	5	314	4	-	7/15/91/115	-
19	CLA	B	810	6	-	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	L	301	17	-	2/15/91/115	-
19	CLA	6	308	1	-	0/21/97/115	-
19	CLA	B	818	6	-	3/36/112/115	-
19	CLA	F	301	30	-	2/33/109/115	-
19	CLA	G	204	11	-	5/15/91/115	-
19	CLA	B	832	6	-	4/39/115/115	-
19	CLA	K	202	14	-	4/13/89/115	-
26	SF4	C	101	7	-	-	0/6/5/5
19	CLA	5	310	4	-	7/13/89/115	-
23	BCR	F	302	-	-	3/29/63/63	0/2/2/2
20	LUT	5	316	-	-	3/29/67/67	0/2/2/2
19	CLA	B	829	6	-	3/39/115/115	-
19	CLA	2	313	2	-	2/21/97/115	-
19	CLA	A	804	30	-	4/39/115/115	-
19	CLA	B	841	6	-	1/39/115/115	-
23	BCR	5	317	-	-	6/29/63/63	0/2/2/2
19	CLA	B	834	6	-	2/33/109/115	-
19	CLA	A	808	5	-	9/39/115/115	-
19	CLA	A	823	5	-	3/15/91/115	-
19	CLA	A	827	30	-	0/27/103/115	-
23	BCR	A	850	-	-	0/29/63/63	0/2/2/2
19	CLA	A	838	5	-	4/23/99/115	-
19	CLA	K	203	14	-	5/15/91/115	-
19	CLA	A	816	5	-	1/12/88/115	-
19	CLA	B	815	6	-	3/39/115/115	-
19	CLA	A	837	5	-	4/15/91/115	-
19	CLA	2	308	2	-	1/15/91/115	-
21	XAT	6	316	-	-	1/31/93/93	0/4/4/4
19	CLA	6	309	1	-	9/39/115/115	-
19	CLA	B	840	30	-	6/39/115/115	-
19	CLA	F	304	10	-	2/10/86/115	-
19	CLA	2	303	2	-	5/15/91/115	-
18	CHL	5	305	30	-	0/14/90/117	-
19	CLA	A	812	5	-	6/39/115/115	-
20	LUT	3	315	-	-	4/29/67/67	0/2/2/2
19	CLA	A	810	5	-	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	808	6	-	1/33/109/115	-
18	CHL	5	306	30	-	3/17/93/117	-
19	CLA	3	304	30	-	3/15/91/115	-
19	CLA	B	836	30	-	2/15/91/115	-
23	BCR	K	205	-	-	18/29/63/63	0/2/2/2
23	BCR	B	844	-	-	2/29/63/63	0/2/2/2
19	CLA	A	819	5	-	5/30/106/115	-
23	BCR	F	305	-	-	4/29/63/63	0/2/2/2
19	CLA	A	814	5	-	6/39/115/115	-
27	LMU	G	202	-	-	7/21/61/61	0/2/2/2
19	CLA	6	307	30	-	3/15/91/115	-
23	BCR	3	317	-	-	3/29/63/63	0/2/2/2
23	BCR	L	305	-	-	3/29/63/63	0/2/2/2
19	CLA	B	812	6	-	5/33/109/115	-
19	CLA	A	830	5	-	4/39/115/115	-
19	CLA	B	804	-	-	2/39/115/115	-
19	CLA	6	305	30	-	2/15/91/115	-
19	CLA	B	842	22	-	19/39/115/115	-
19	CLA	2	309	2	-	6/35/111/115	-
19	CLA	5	308	4	-	4/33/109/115	-
23	BCR	A	849	-	-	3/29/63/63	0/2/2/2
18	CHL	2	314	2	-	4/17/93/117	-
18	CHL	6	306	1	-	4/17/93/117	-
22	LHG	2	318	19	-	3/42/42/53	-
19	CLA	B	824	6	-	4/15/91/115	-
19	CLA	A	839	5	-	0/27/103/115	-
19	CLA	K	201	30	-	7/23/99/115	-
19	CLA	3	310	3	-	1/13/89/115	-
19	CLA	A	836	5	-	3/33/109/115	-
18	CHL	3	306	30	-	2/17/93/117	-
19	CLA	A	815	5	-	1/23/99/115	-
18	CHL	2	307	30	-	2/21/97/117	-
19	CLA	A	831	5	-	4/39/115/115	-
19	CLA	A	833	5	-	2/27/103/115	-
19	CLA	3	313	30	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	K	204	-	-	3/29/63/63	0/2/2/2
23	BCR	A	848	-	-	5/29/63/63	0/2/2/2
19	CLA	A	824	5	-	2/39/115/115	-
20	LUT	6	318	-	-	6/29/67/67	0/2/2/2
23	BCR	L	304	-	-	2/29/63/63	0/2/2/2
19	CLA	B	826	30	-	4/25/101/115	-
18	CHL	5	313	4	-	1/14/90/117	-
19	CLA	B	822	6	-	1/17/93/115	-
23	BCR	B	847	-	-	1/29/63/63	0/2/2/2
19	CLA	A	807	5	-	6/39/115/115	-
23	BCR	J	103	-	-	6/29/63/63	0/2/2/2
19	CLA	A	825	5	-	5/39/115/115	-
20	LUT	2	317	-	-	4/29/67/67	0/2/2/2
19	CLA	6	310	22	-	3/29/105/115	-
19	CLA	A	820	5	-	7/39/115/115	-
19	CLA	3	308	3	-	1/39/115/115	-
19	CLA	6	302	1	-	3/35/111/115	-
19	CLA	3	303	30	-	1/18/94/115	-
19	CLA	A	832	5	-	0/21/97/115	-
29	LMG	J	105	-	-	9/36/56/70	0/1/1/1
19	CLA	L	303	30	-	2/12/88/115	-
19	CLA	A	806	5	-	3/27/103/115	-
19	CLA	3	302	3	-	1/27/103/115	-
19	CLA	B	839	6	-	3/18/94/115	-
19	CLA	A	826	30	-	7/39/115/115	-
19	CLA	B	802	30	-	7/39/115/115	-
20	LUT	6	315	-	-	2/29/67/67	0/2/2/2
19	CLA	A	818	5	-	7/33/109/115	-
19	CLA	B	830	6	-	4/33/109/115	-
19	CLA	6	303	1	-	4/27/103/115	-
19	CLA	B	817	6	-	2/39/115/115	-
19	CLA	6	311	1	-	5/15/91/115	-
22	LHG	6	319	19	-	2/31/31/53	-
25	PQN	B	843	-	-	1/23/43/43	0/2/2/2
19	CLA	A	805	5	-	4/39/115/115	-
18	CHL	2	320	4	-	4/25/101/117	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	I	101	-	-	1/29/63/63	0/2/2/2
19	CLA	2	310	22	-	2/29/105/115	-
27	LMU	B	850	-	-	7/21/61/61	0/2/2/2
23	BCR	G	201	-	-	4/29/63/63	0/2/2/2
23	BCR	A	851	-	-	0/29/63/63	0/2/2/2
19	CLA	B	828	6	-	3/39/115/115	-
19	CLA	B	823	6	-	3/27/103/115	-
19	CLA	B	827	6	-	1/39/115/115	-
18	CHL	2	305	30	-	2/17/93/117	-
19	CLA	A	811	5	-	3/27/103/115	-
25	PQN	A	844	-	-	5/23/43/43	0/2/2/2
19	CLA	J	102	13	-	2/12/88/115	-
23	BCR	M	101	-	-	2/29/63/63	0/2/2/2
20	LUT	3	316	-	-	3/29/67/67	0/2/2/2
28	DGD	B	849	-	-	21/55/95/95	0/2/2/2
20	LUT	2	315	-	-	2/29/67/67	0/2/2/2
19	CLA	B	821	6	-	1/13/89/115	-
19	CLA	5	309	30	-	3/33/109/115	-
19	CLA	G	203	11	-	4/15/91/115	-
23	BCR	2	319	-	-	8/29/63/63	0/2/2/2
19	CLA	A	822	30	-	1/39/115/115	-
19	CLA	2	311	2	-	5/15/91/115	-
20	LUT	5	315	-	-	2/29/67/67	0/2/2/2
19	CLA	A	828	5	-	16/39/115/115	-
22	LHG	A	847	19	-	5/38/38/53	-
22	LHG	5	318	-	-	9/48/48/53	-
29	LMG	J	104	-	-	6/25/45/70	0/1/1/1
27	LMU	B	851	-	-	4/21/61/61	0/2/2/2
19	CLA	5	311	4	-	2/35/111/115	-
19	CLA	6	304	30	-	2/20/96/115	-
19	CLA	B	814	6	-	8/39/115/115	-
19	CLA	A	813	5	-	1/26/102/115	-
19	CLA	A	840	5	-	3/21/97/115	-
20	LUT	J	101	-	-	2/29/67/67	0/2/2/2
19	CLA	3	312	3	-	2/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	829	5	-	5/39/115/115	-
19	CLA	5	302	4	-	3/21/97/115	-
18	CHL	2	306	30	-	2/14/90/117	-
19	CLA	A	835	5	-	2/39/115/115	-
19	CLA	A	843	22	-	5/15/91/115	-
22	LHG	A	846	-	-	7/53/53/53	-
18	CHL	6	301	1	-	5/23/99/117	-
22	LHG	6	317	19	-	8/53/53/53	-
19	CLA	6	312	1	-	4/39/115/115	-
19	CLA	5	312	4	-	12/39/115/115	-
19	CLA	A	821	5	-	2/15/91/115	-
19	CLA	5	301	4	-	3/33/109/115	-
19	CLA	A	801	5	-	6/27/103/115	-
19	CLA	B	805	6	-	3/15/91/115	-
19	CLA	B	803	6	-	3/39/115/115	-
19	CLA	B	806	6	-	4/39/115/115	-
19	CLA	2	304	30	-	2/21/97/115	-

The worst 5 of 1428 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	802	CL0	MG-NC	5.78	2.20	2.06
23	2	319	BCR	C21-C22	5.61	1.43	1.35
24	A	802	CL0	MG-NA	5.49	2.19	2.06
19	A	831	CLA	MG-NA	4.93	2.18	2.06
23	B	848	BCR	C10-C9	4.93	1.42	1.35

The worst 5 of 1222 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	848	BCR	C11-C10-C9	6.05	135.94	127.31
23	B	848	BCR	C16-C15-C14	5.60	134.95	123.47
23	B	848	BCR	C10-C11-C12	5.49	140.34	123.22
20	2	317	LUT	C28-C29-C30	5.48	127.34	118.94
23	A	852	BCR	C15-C16-C17	5.42	134.58	123.47

There are no chirality outliers.

5 of 815 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	2	306	CHL	CBD-CGD-O2D-CED
18	2	306	CHL	O1D-CGD-O2D-CED
18	3	314	CHL	CBD-CGD-O2D-CED
18	3	314	CHL	O1D-CGD-O2D-CED
19	6	311	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

165 monomers are involved in 280 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	846	BCR	2	0
23	G	205	BCR	2	0
19	F	303	CLA	1	0
23	B	848	BCR	2	0
19	3	309	CLA	2	0
19	6	314	CLA	1	0
18	2	301	CHL	3	0
19	3	305	CLA	1	0
19	2	312	CLA	4	0
19	L	302	CLA	2	0
23	B	845	BCR	3	0
19	3	311	CLA	2	0
19	2	302	CLA	2	0
19	B	801	CLA	3	0
19	A	841	CLA	1	0
19	B	807	CLA	3	0
19	B	811	CLA	1	0
19	B	816	CLA	4	0
19	A	834	CLA	2	0
19	B	833	CLA	1	0
19	6	313	CLA	1	0
24	A	802	CL0	2	0
19	A	842	CLA	2	0
19	3	301	CLA	1	0
19	B	825	CLA	3	0
19	B	838	CLA	4	0
19	5	307	CLA	4	0
19	B	820	CLA	3	0
19	B	831	CLA	1	0
20	2	316	LUT	2	0
18	3	314	CHL	3	0
23	A	852	BCR	3	0
19	B	809	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	5	314	CLA	1	0
19	B	810	CLA	1	0
19	L	301	CLA	1	0
19	6	308	CLA	2	0
19	B	818	CLA	2	0
19	F	301	CLA	2	0
19	B	832	CLA	2	0
23	F	302	BCR	4	0
20	5	316	LUT	3	0
19	B	829	CLA	2	0
19	B	841	CLA	3	0
23	5	317	BCR	2	0
19	B	834	CLA	1	0
19	A	808	CLA	4	0
19	A	823	CLA	2	0
23	A	850	BCR	1	0
19	A	816	CLA	2	0
19	A	837	CLA	3	0
19	2	308	CLA	2	0
21	6	316	XAT	3	0
19	6	309	CLA	1	0
19	B	840	CLA	3	0
19	F	304	CLA	1	0
19	2	303	CLA	1	0
19	A	812	CLA	2	0
20	3	315	LUT	5	0
19	A	810	CLA	2	0
23	K	205	BCR	2	0
23	B	844	BCR	2	0
19	A	819	CLA	4	0
23	F	305	BCR	2	0
19	A	814	CLA	2	0
27	G	202	LMU	2	0
19	6	307	CLA	1	0
23	3	317	BCR	2	0
23	L	305	BCR	4	0
19	B	812	CLA	5	0
19	B	804	CLA	1	0
19	6	305	CLA	2	0
19	B	842	CLA	2	0
19	2	309	CLA	3	0
19	5	308	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	849	BCR	3	0
18	2	314	CHL	1	0
18	6	306	CHL	3	0
19	B	824	CLA	1	0
19	A	839	CLA	2	0
19	K	201	CLA	1	0
19	3	310	CLA	2	0
19	A	836	CLA	1	0
18	3	306	CHL	1	0
18	2	307	CHL	2	0
19	A	831	CLA	2	0
19	A	833	CLA	1	0
19	3	313	CLA	1	0
23	K	204	BCR	2	0
23	A	848	BCR	5	0
19	A	824	CLA	3	0
20	6	318	LUT	2	0
19	B	826	CLA	1	0
18	5	313	CHL	1	0
19	B	822	CLA	1	0
23	B	847	BCR	4	0
19	A	807	CLA	3	0
23	J	103	BCR	6	0
19	A	825	CLA	3	0
20	2	317	LUT	2	0
19	6	310	CLA	2	0
19	A	820	CLA	2	0
19	3	308	CLA	2	0
19	6	302	CLA	2	0
19	3	303	CLA	1	0
19	A	832	CLA	1	0
29	J	105	LMG	1	0
19	L	303	CLA	1	0
19	A	806	CLA	1	0
19	3	302	CLA	4	0
19	B	802	CLA	3	0
20	6	315	LUT	2	0
19	A	818	CLA	3	0
19	B	830	CLA	3	0
19	6	303	CLA	1	0
19	B	817	CLA	2	0
19	6	311	CLA	1	0

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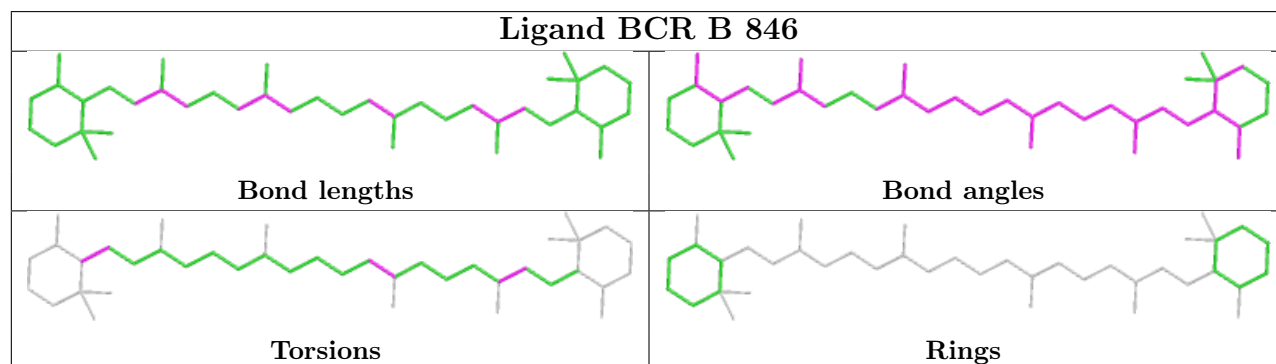
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	B	843	PQN	1	0
19	A	805	CLA	2	0
18	2	320	CHL	3	0
23	I	101	BCR	2	0
19	2	310	CLA	1	0
27	B	850	LMU	3	0
23	G	201	BCR	5	0
23	A	851	BCR	5	0
19	B	828	CLA	1	0
19	B	823	CLA	2	0
19	B	827	CLA	1	0
18	2	305	CHL	2	0
19	A	811	CLA	3	0
25	A	844	PQN	2	0
19	J	102	CLA	1	0
23	M	101	BCR	3	0
20	3	316	LUT	6	0
28	B	849	DGD	4	0
20	2	315	LUT	4	0
19	5	309	CLA	1	0
19	G	203	CLA	1	0
23	2	319	BCR	2	0
19	A	822	CLA	5	0
19	2	311	CLA	1	0
20	5	315	LUT	4	0
19	A	828	CLA	1	0
22	A	847	LHG	1	0
22	5	318	LHG	5	0
29	J	104	LMG	2	0
27	B	851	LMU	1	0
19	5	311	CLA	1	0
19	6	304	CLA	1	0
19	B	814	CLA	2	0
19	A	813	CLA	1	0
20	J	101	LUT	4	0
19	3	312	CLA	2	0
19	5	302	CLA	1	0
18	2	306	CHL	1	0
19	A	835	CLA	2	0
22	A	846	LHG	2	0
18	6	301	CHL	3	0
22	6	317	LHG	6	0

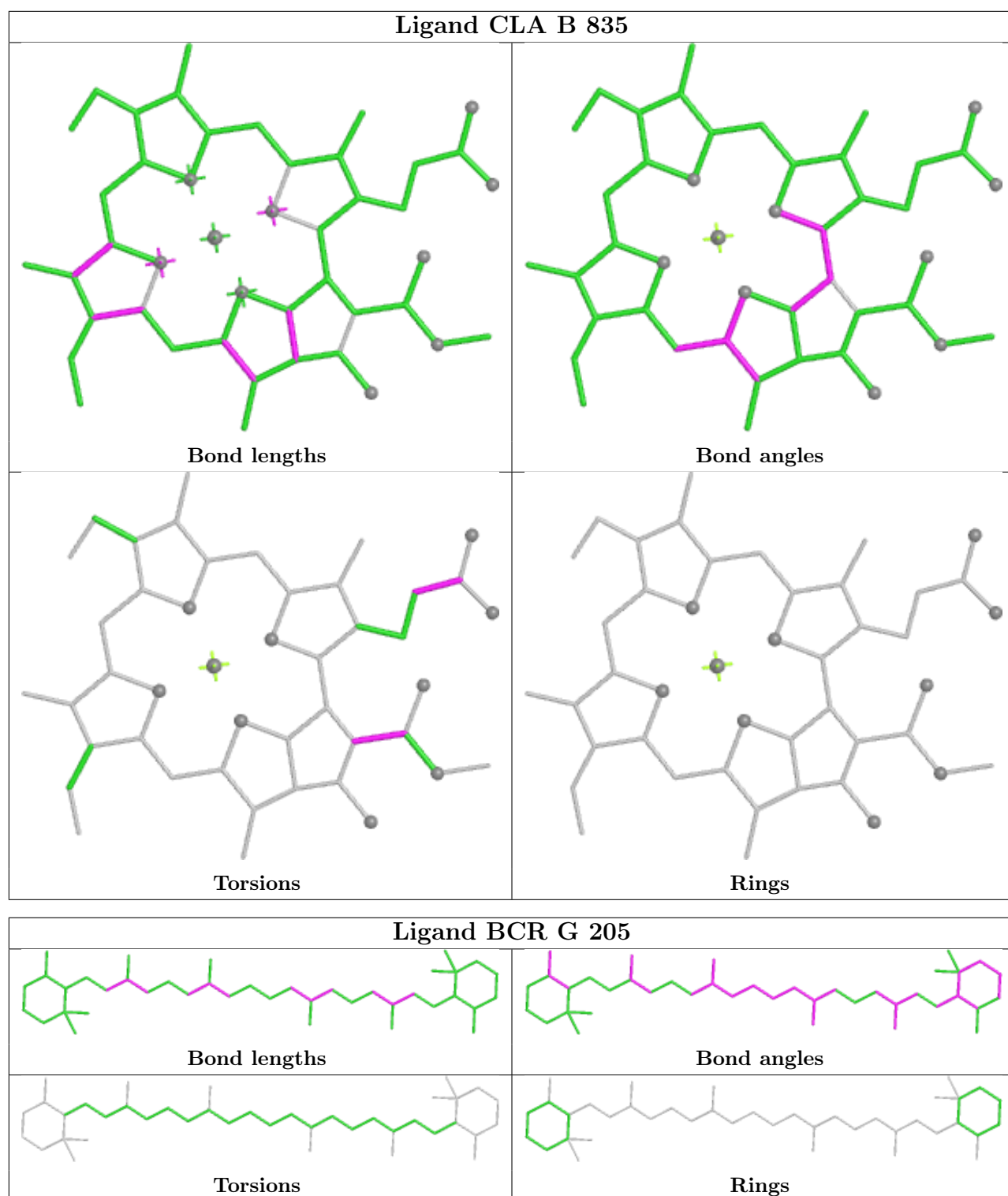
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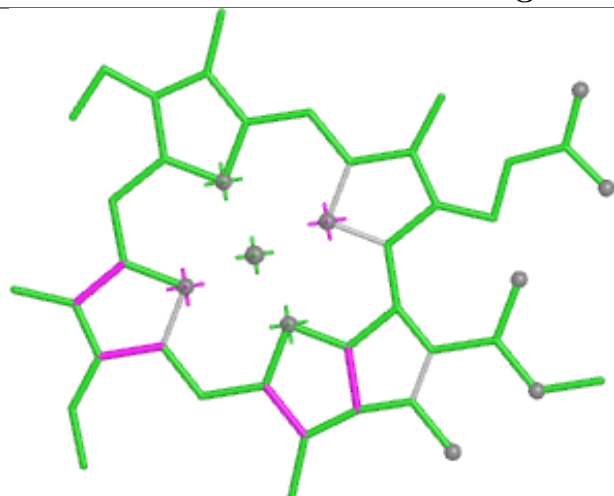
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	6	312	CLA	4	0
19	5	312	CLA	1	0
19	A	821	CLA	3	0
19	5	301	CLA	1	0
19	B	803	CLA	2	0
19	B	806	CLA	3	0

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.

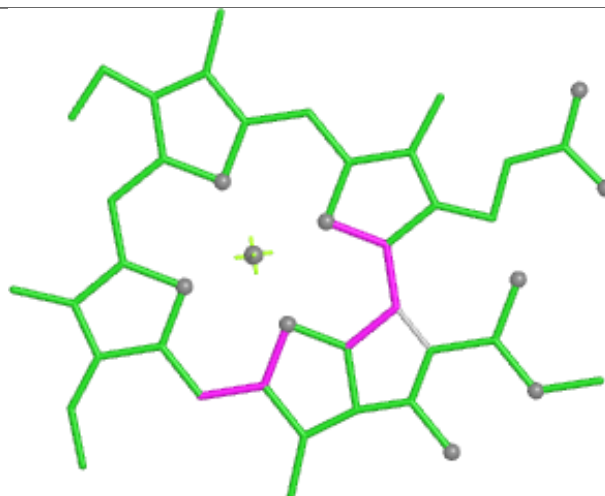




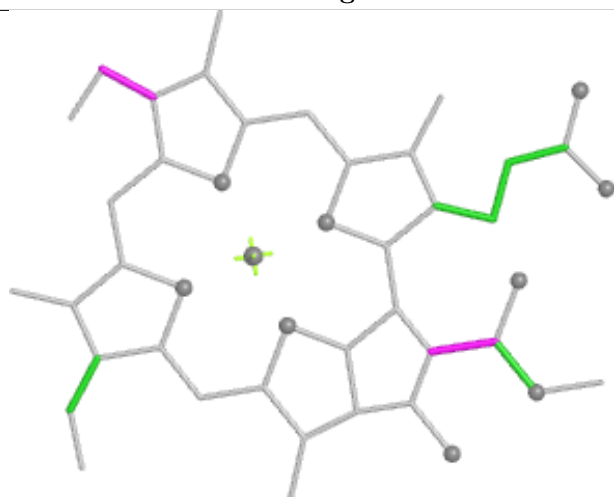
Ligand CLA F 303



Bond lengths



Bond angles

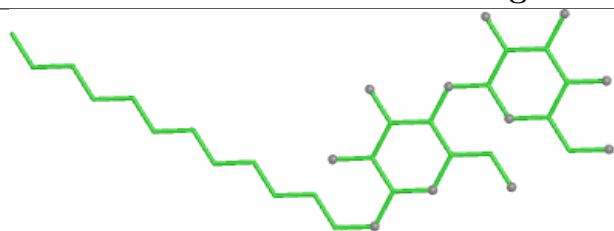


Torsions

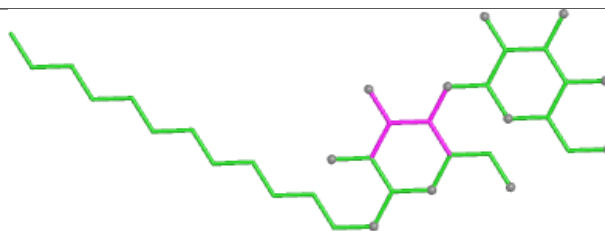


Rings

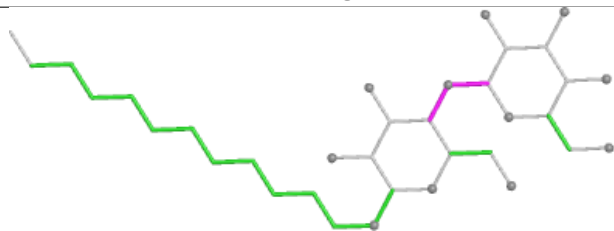
Ligand LMU A 853



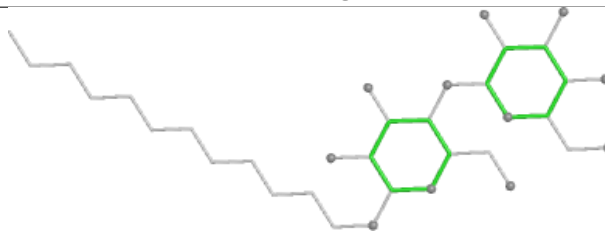
Bond lengths



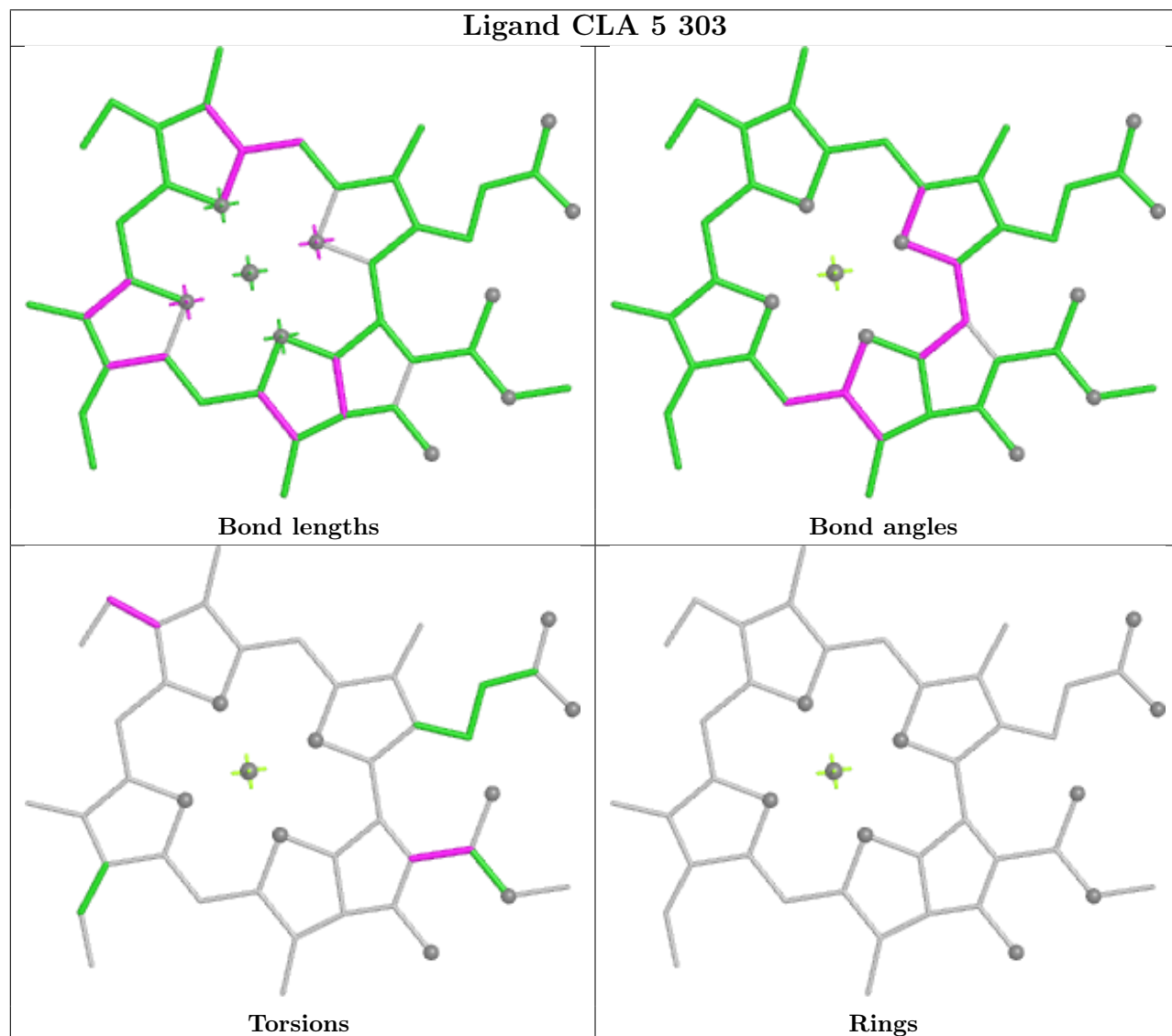
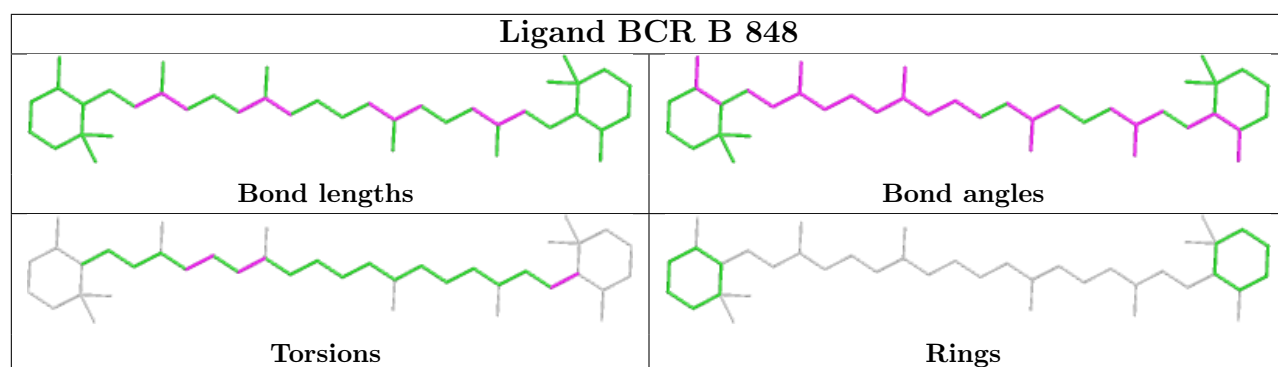
Bond angles



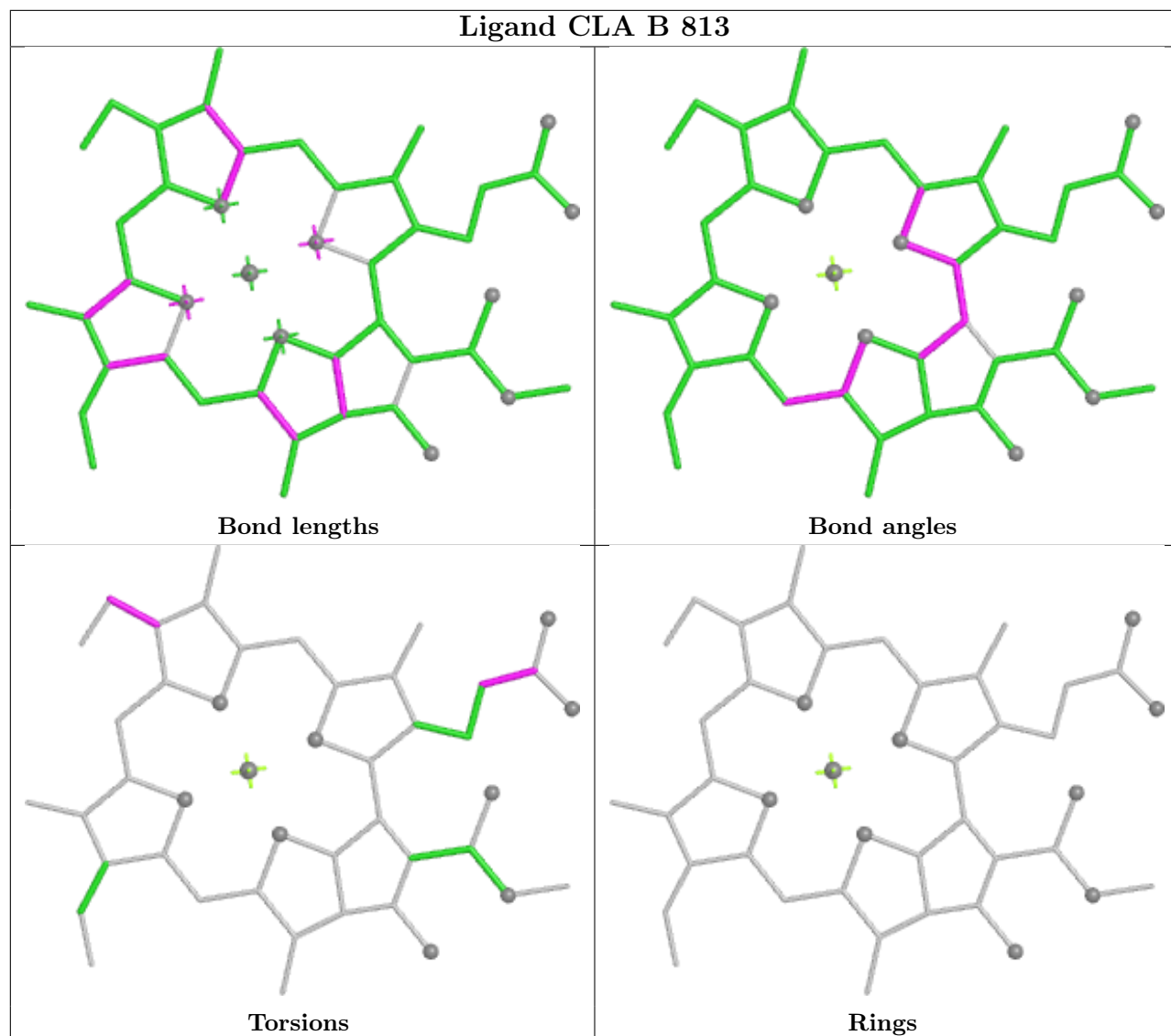
Torsions



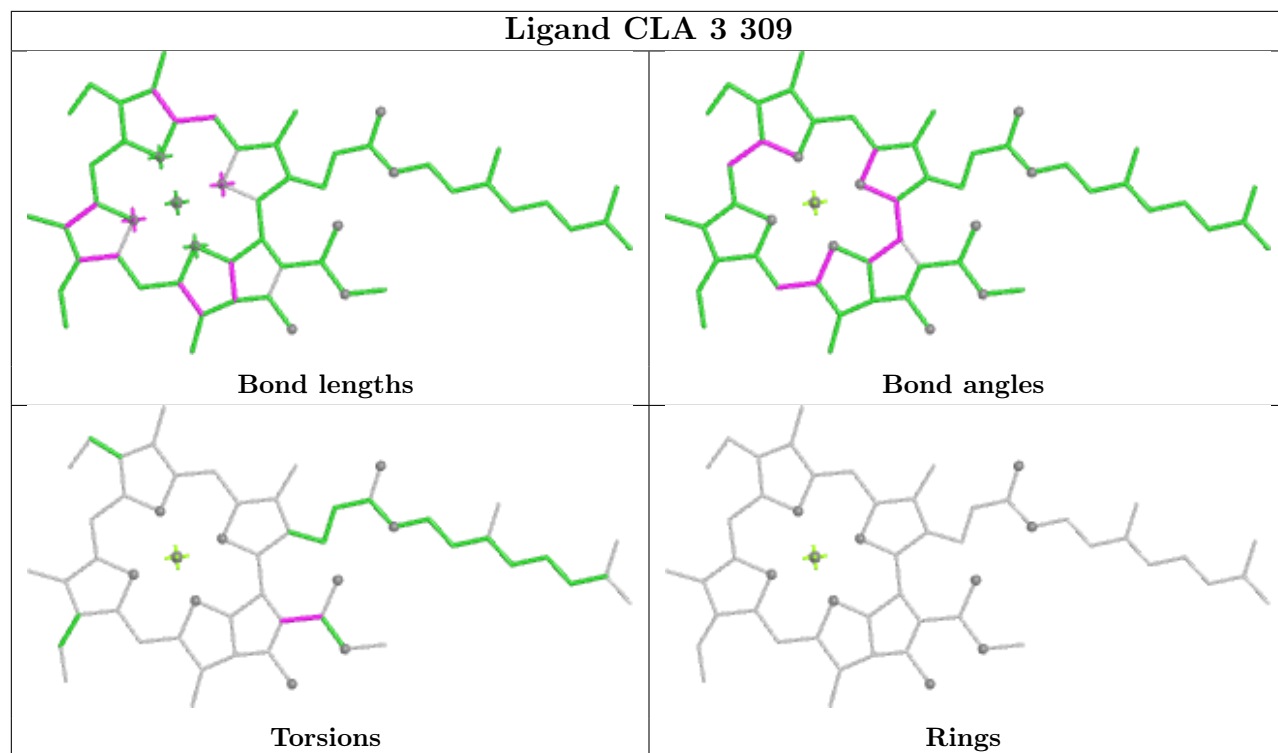
Rings



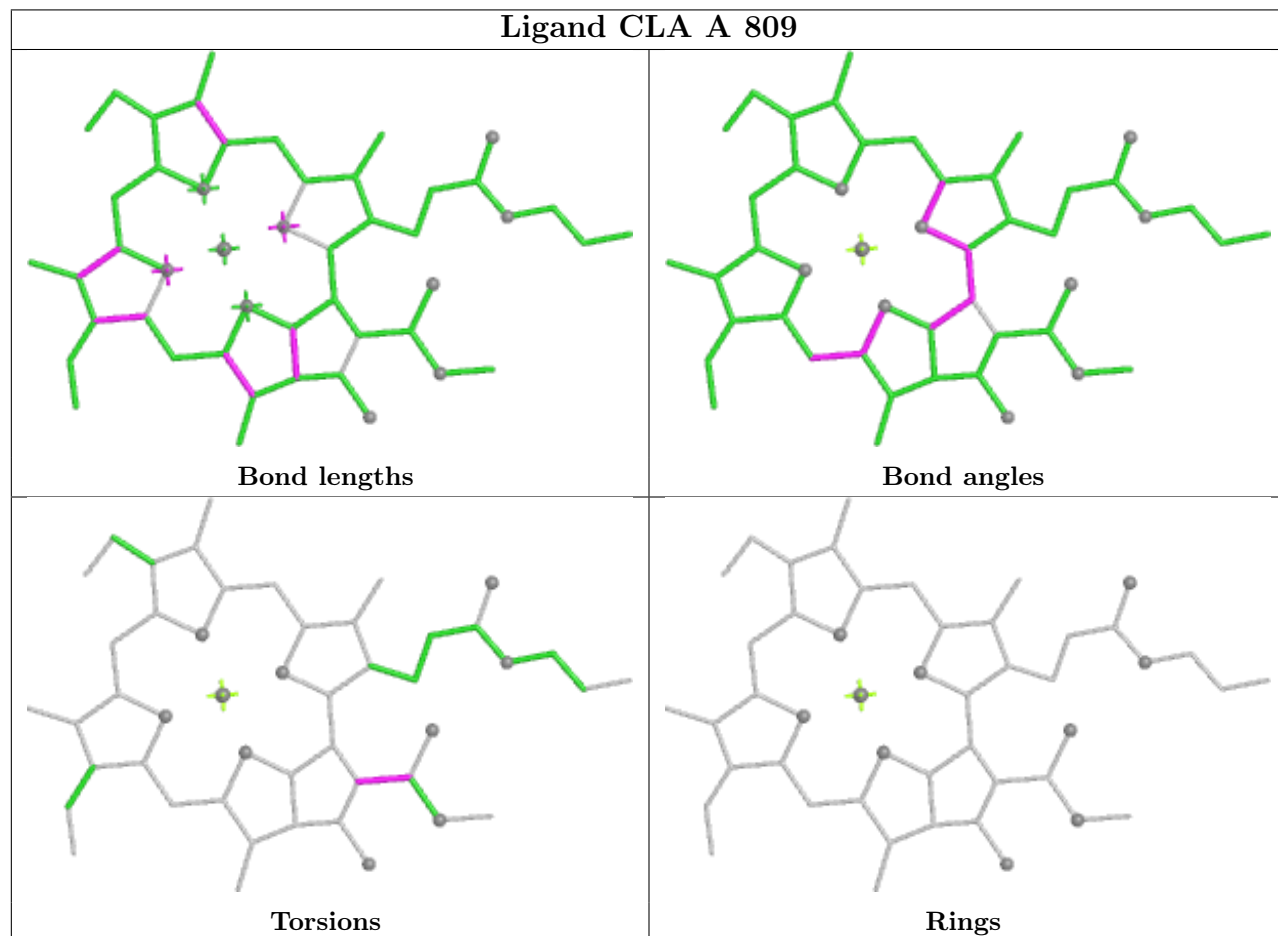
Ligand CLA B 813



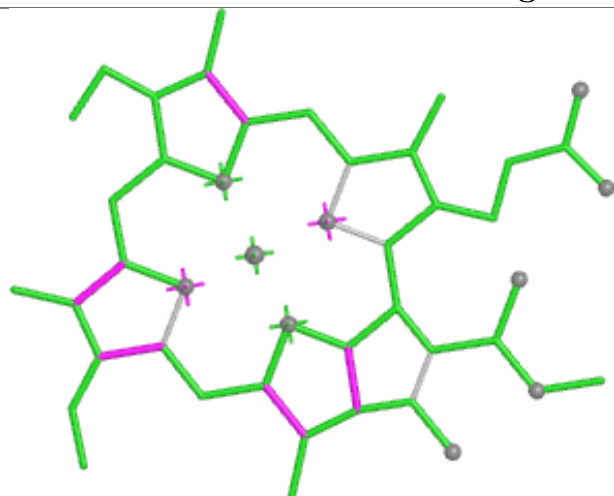
Ligand CLA 3 309



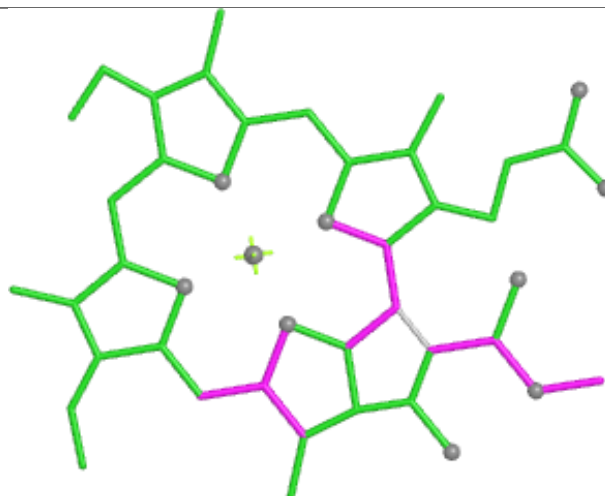
Ligand CLA A 809



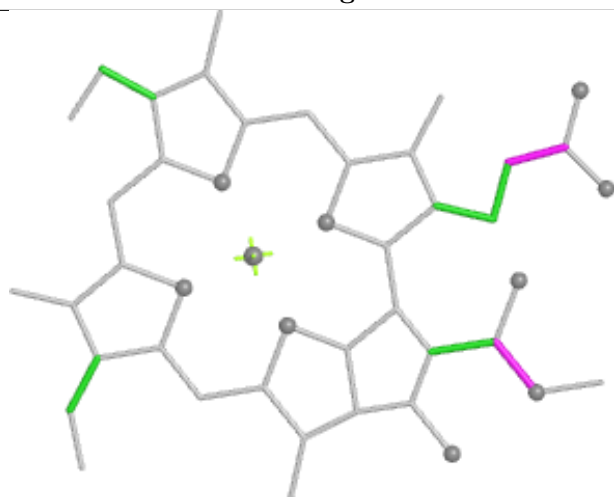
Ligand CLA 6 314



Bond lengths



Bond angles

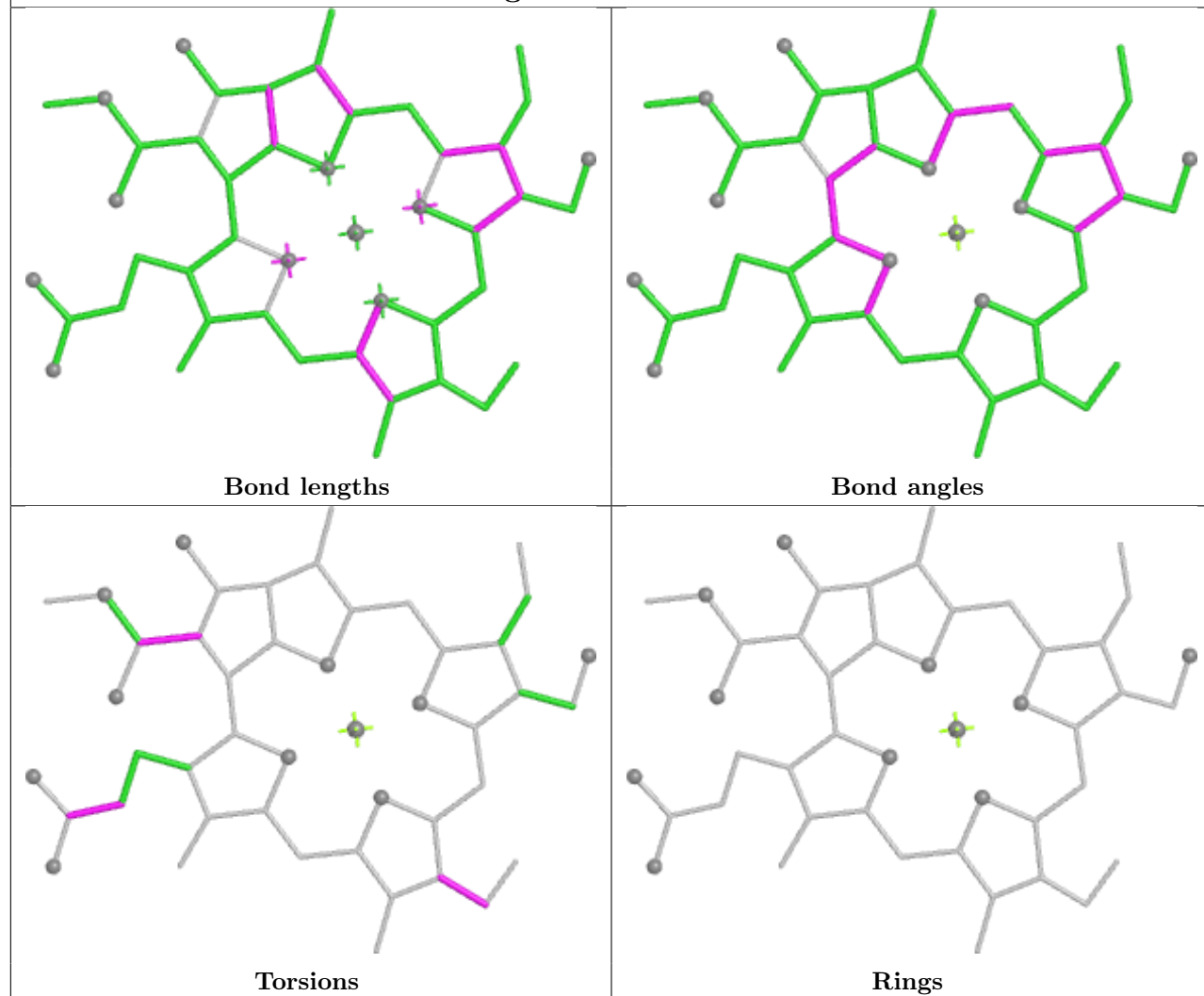


Torsions

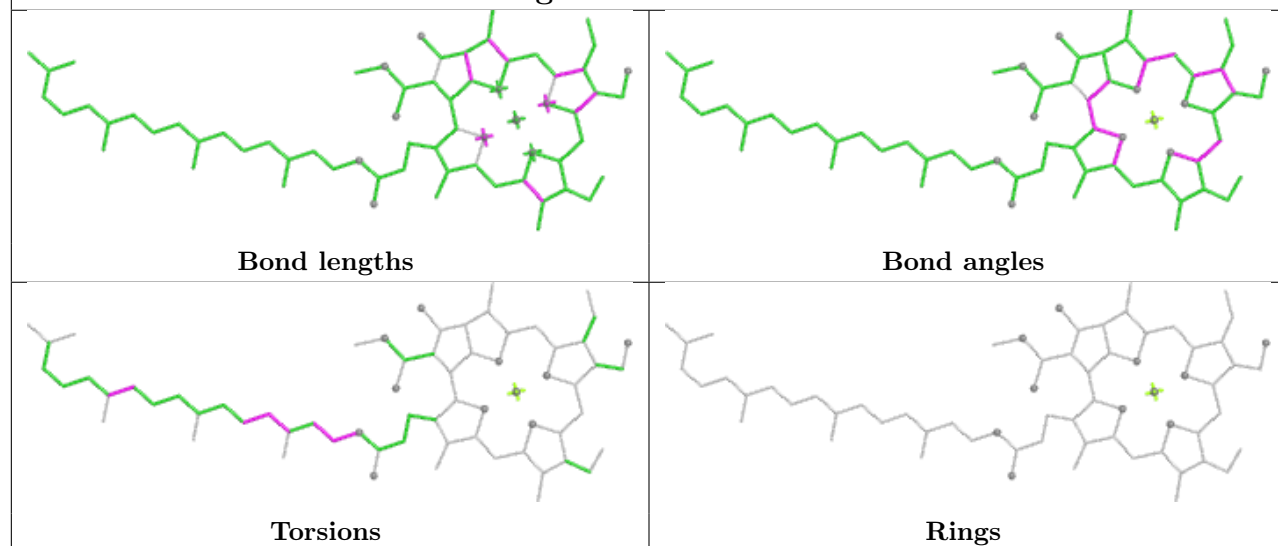


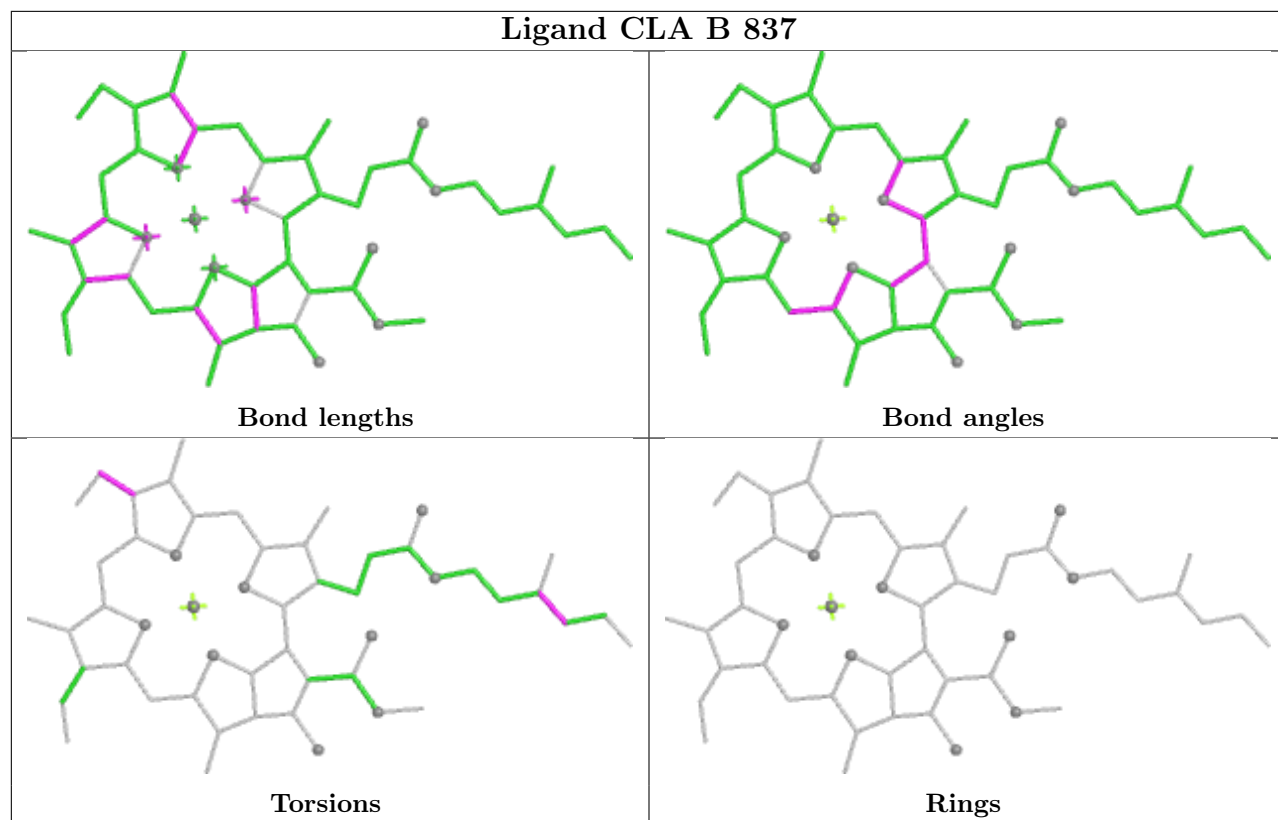
Rings

Ligand CHL 5 304

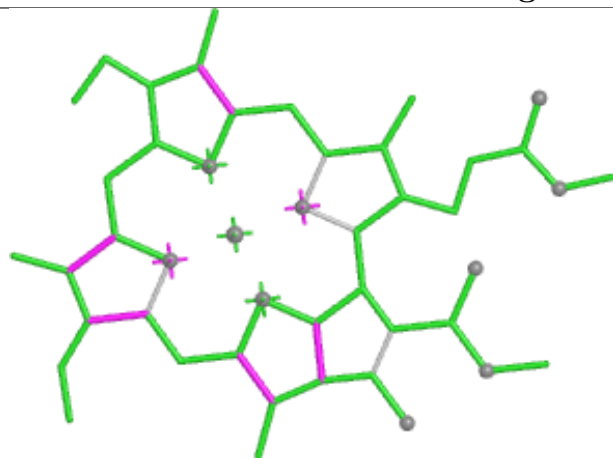


Ligand CHL 2 301

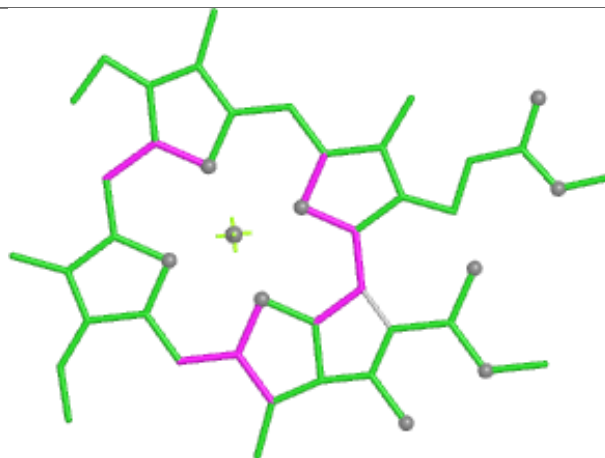




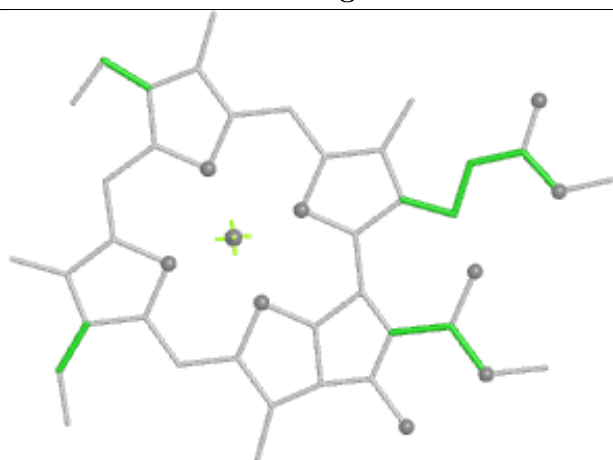
Ligand CLA 3 305



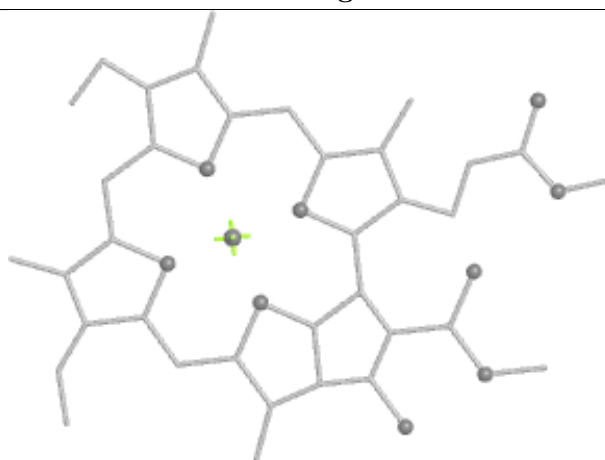
Bond lengths



Bond angles

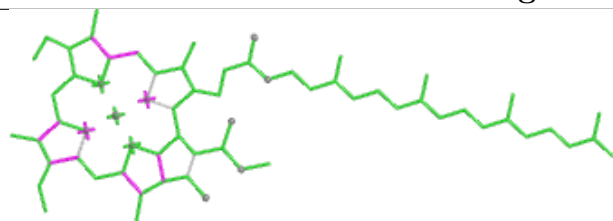


Torsions

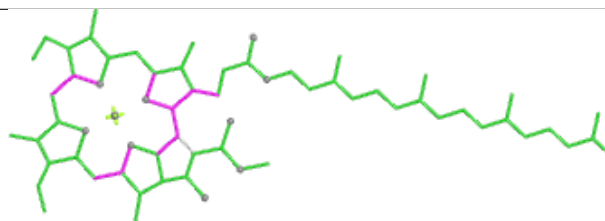


Rings

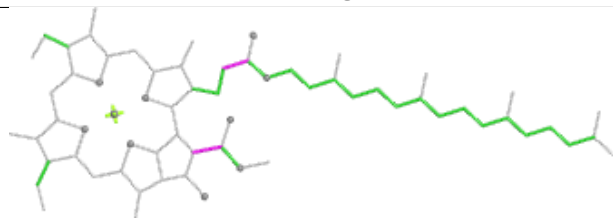
Ligand CLA 2 312



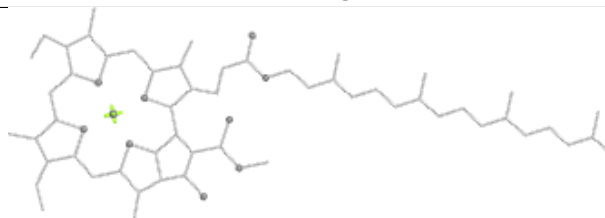
Bond lengths



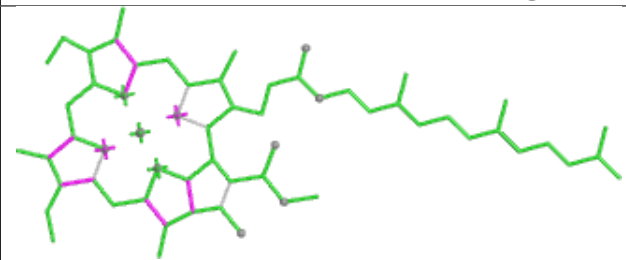
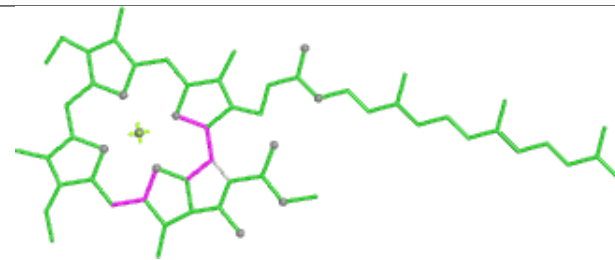
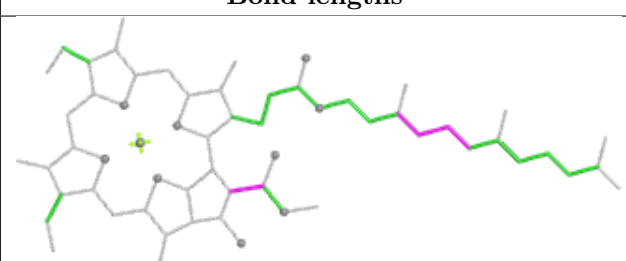
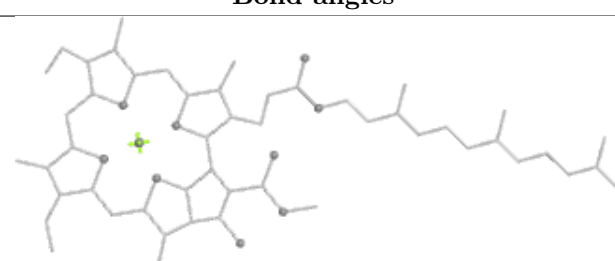
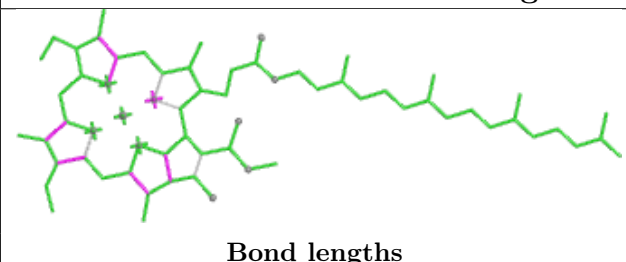
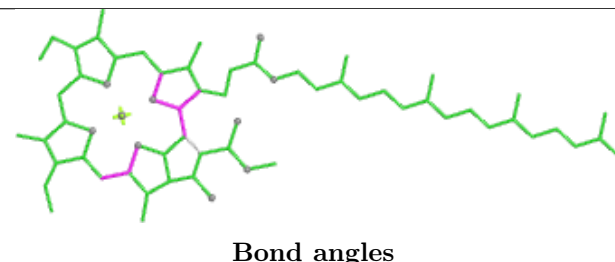
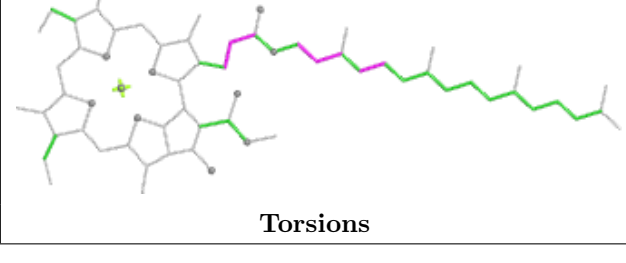
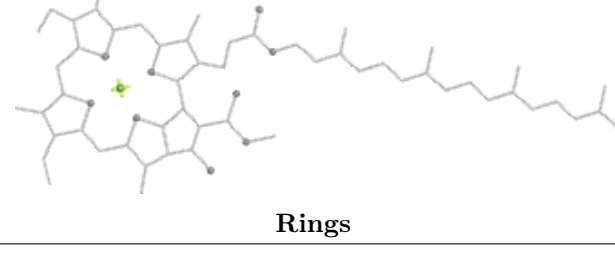
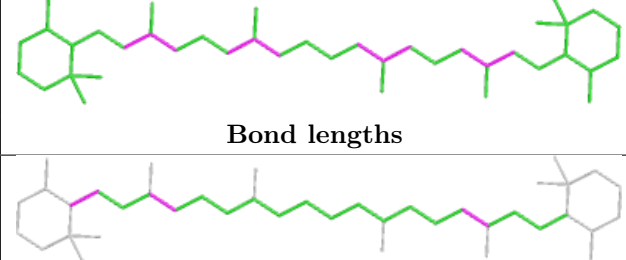
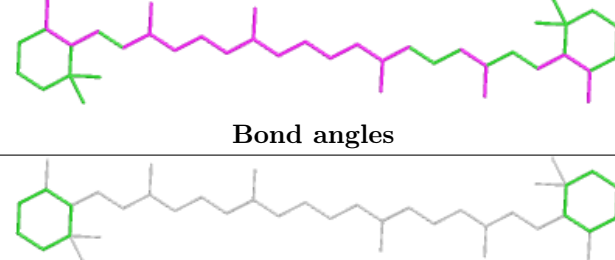
Bond angles

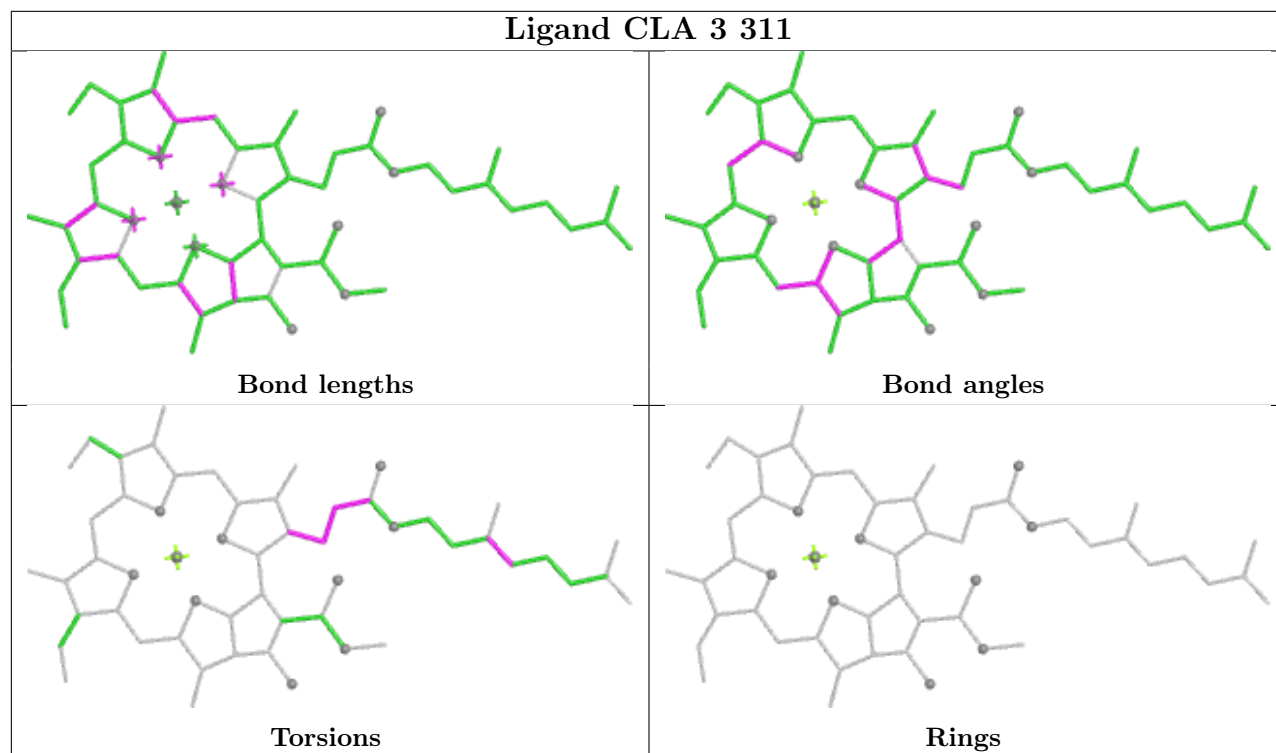
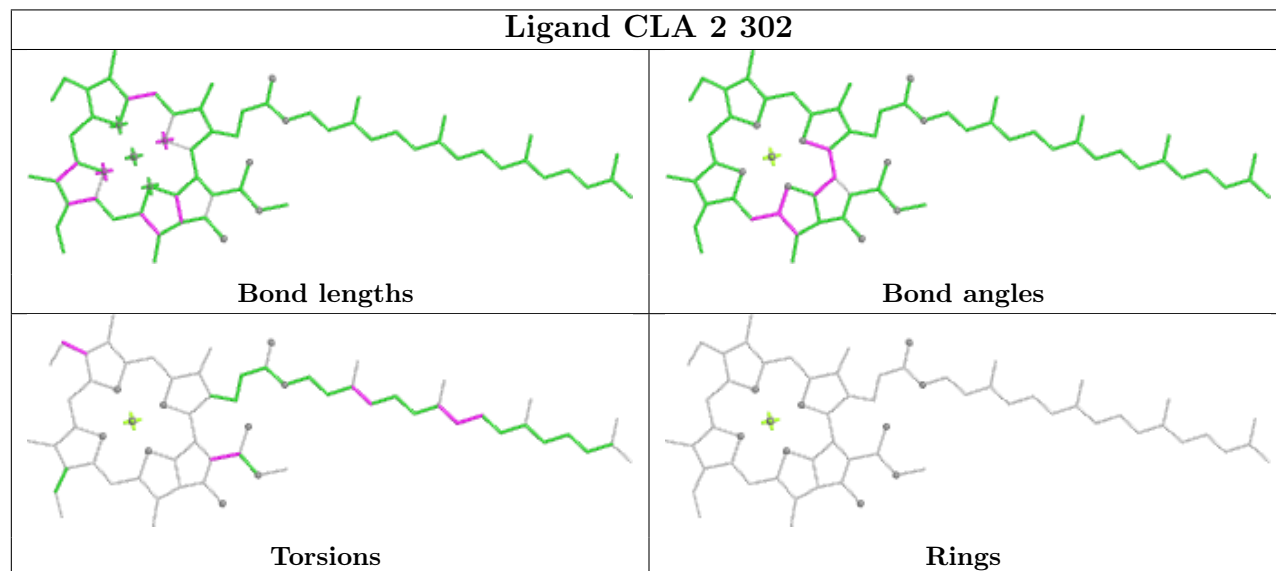


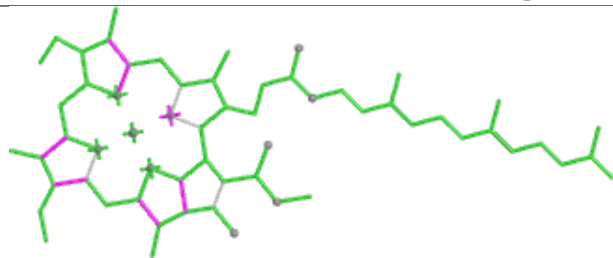
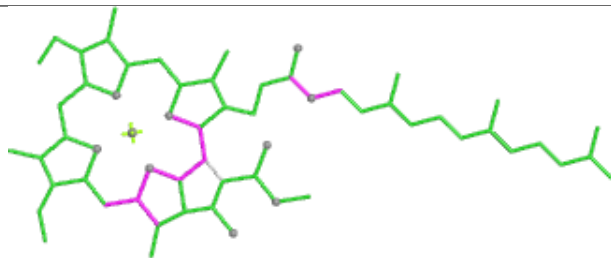
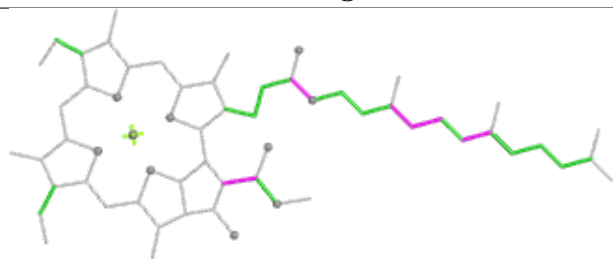
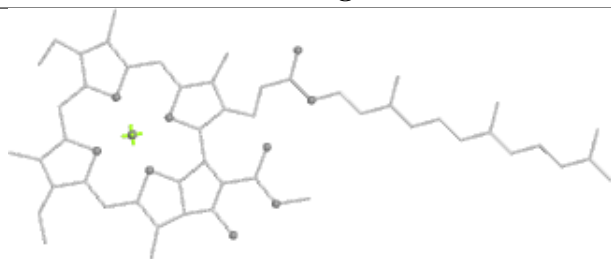
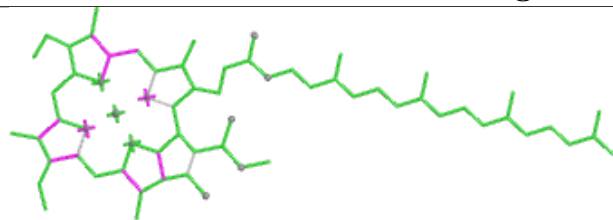
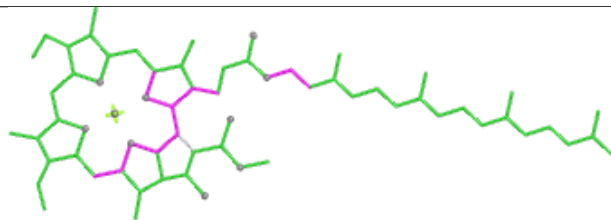
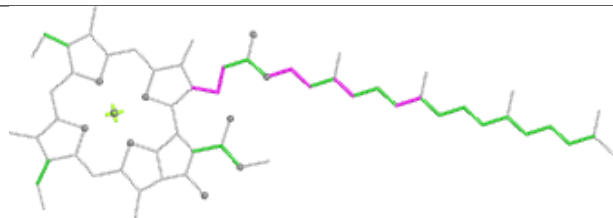
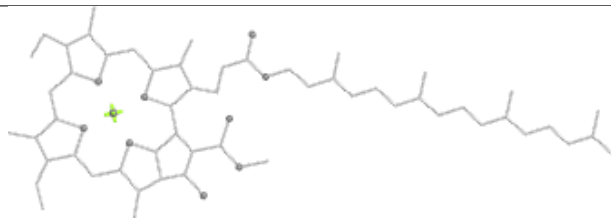
Torsions

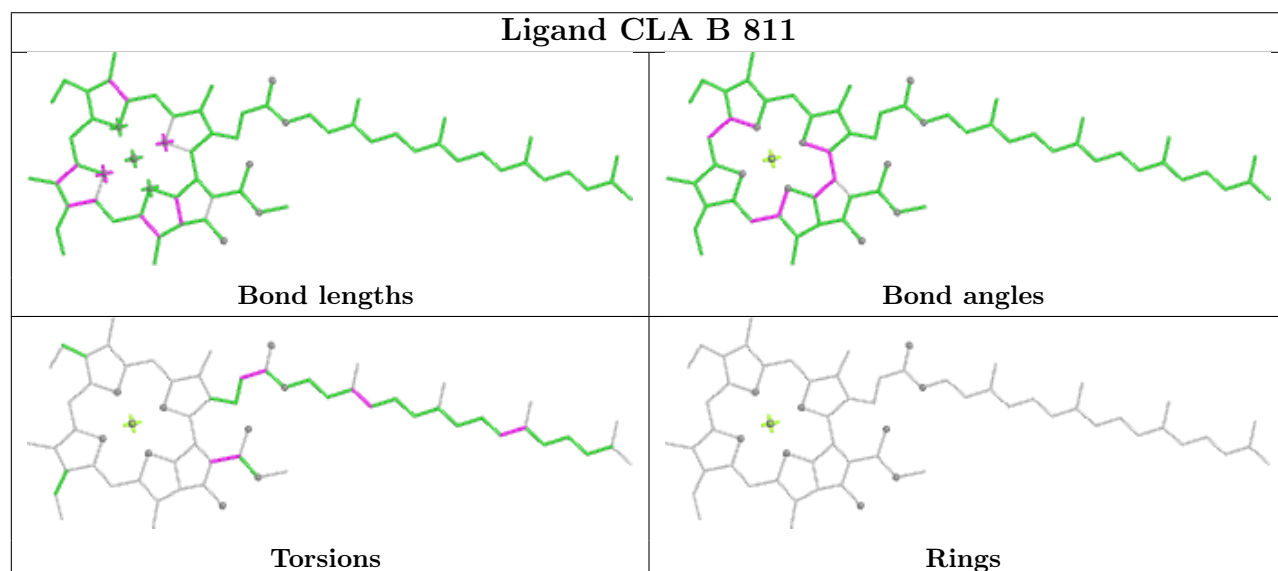
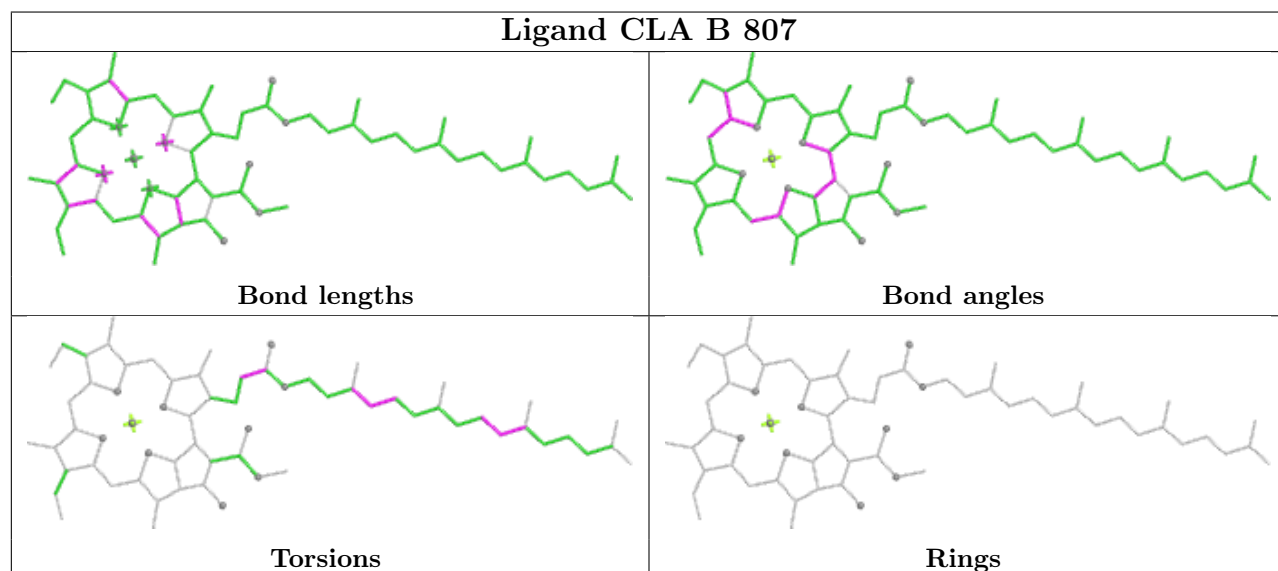
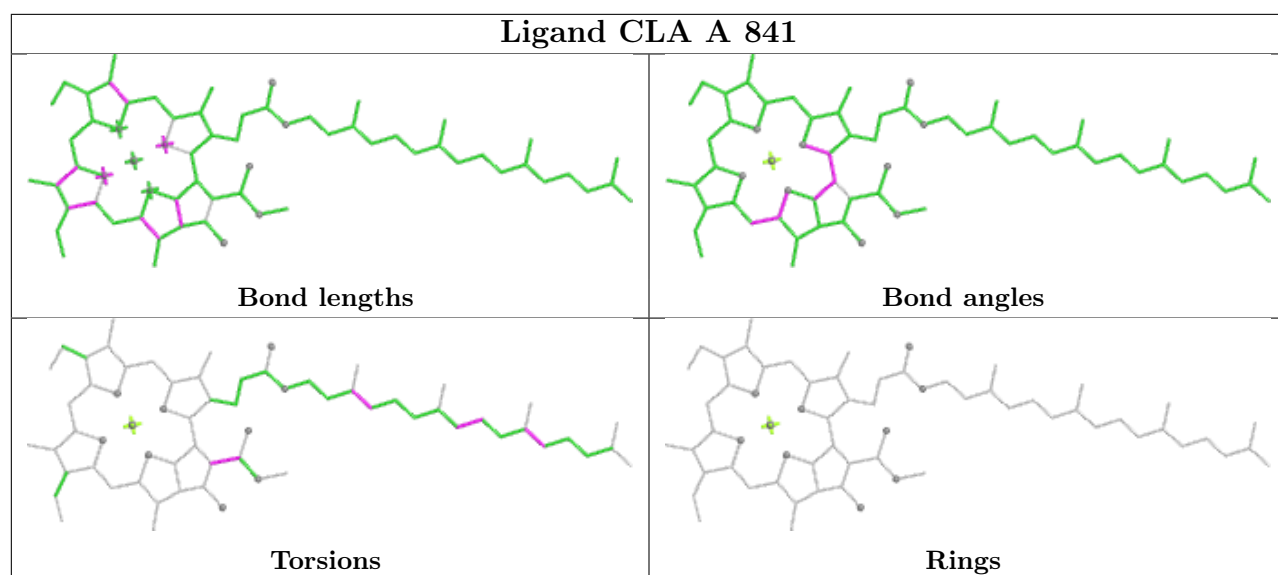


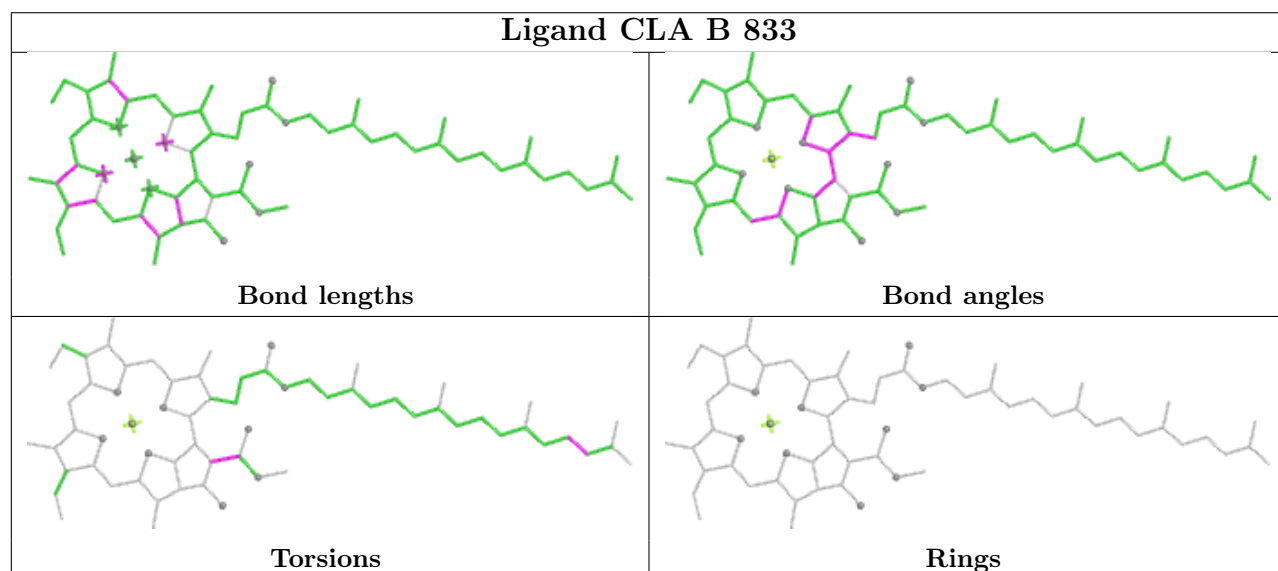
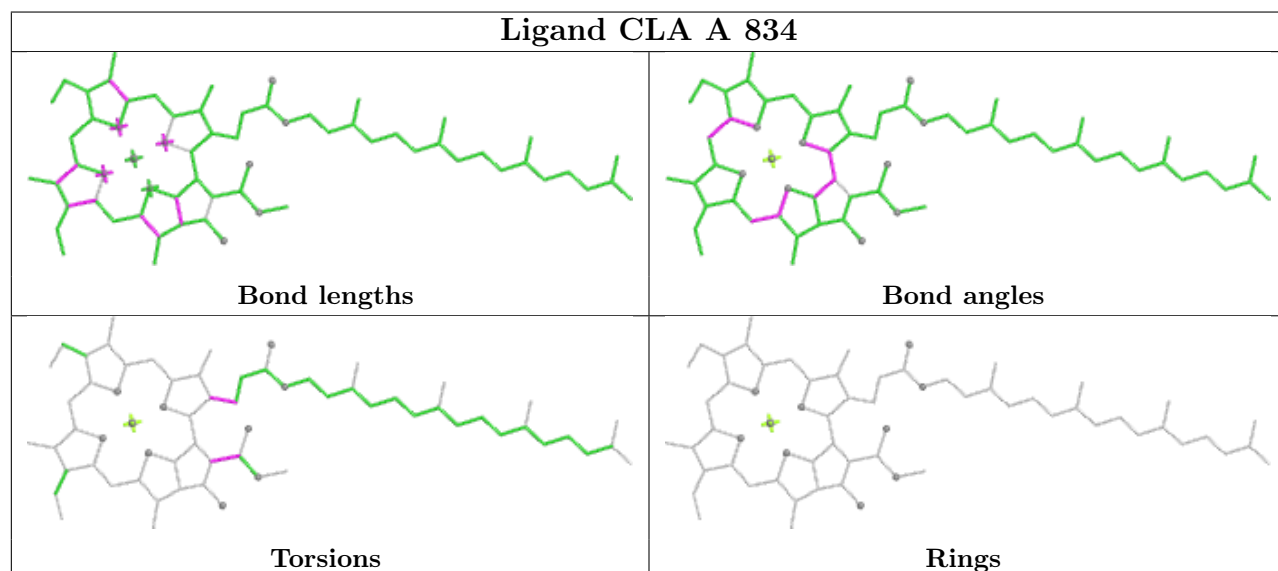
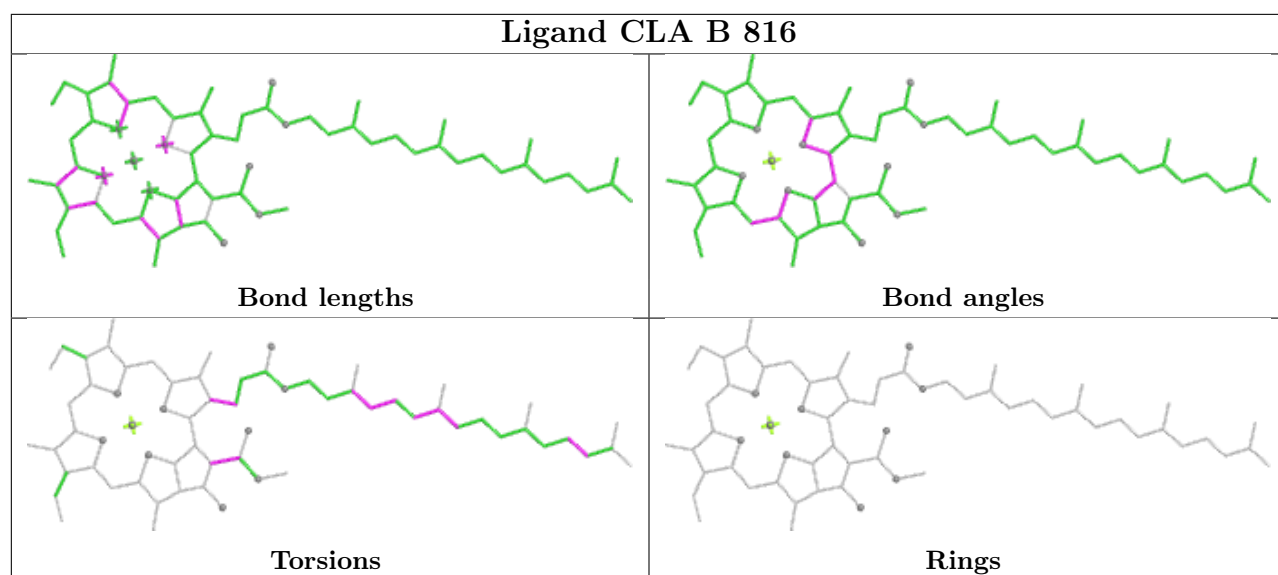
Rings

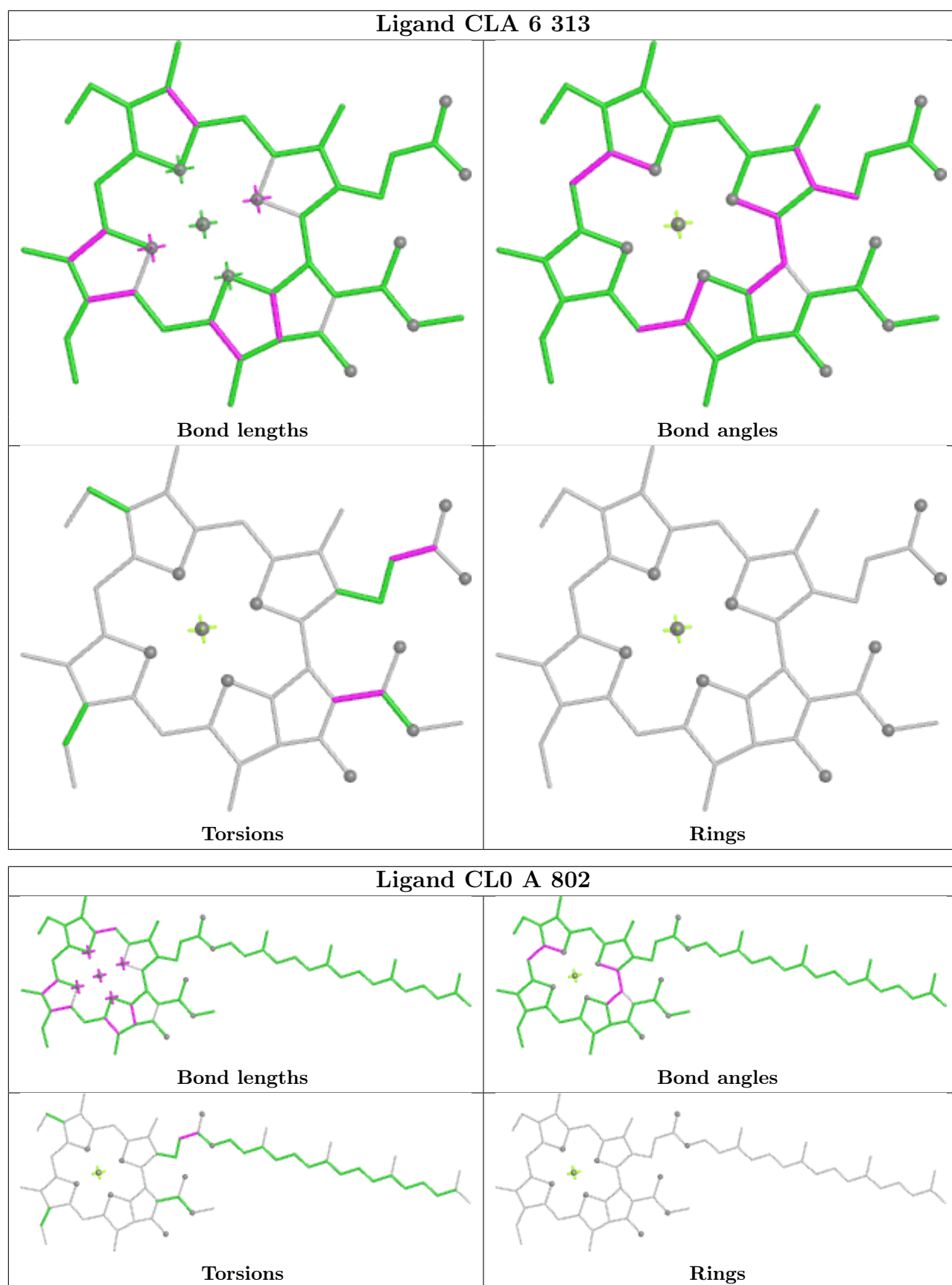
Ligand CLA L 302	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 311**Ligand CLA 2 302**

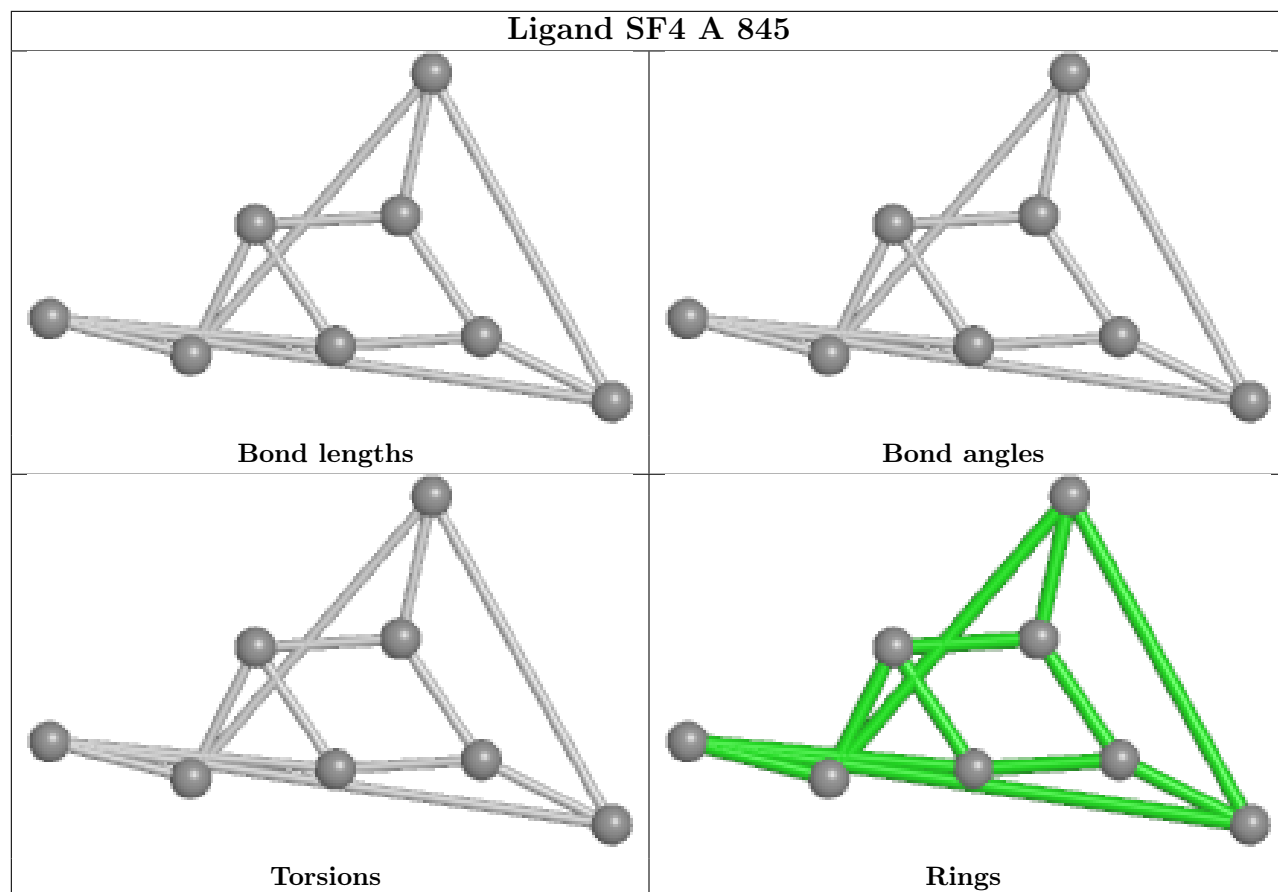
Ligand CLA 3 307**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 801****Bond lengths****Bond angles****Torsions****Rings**



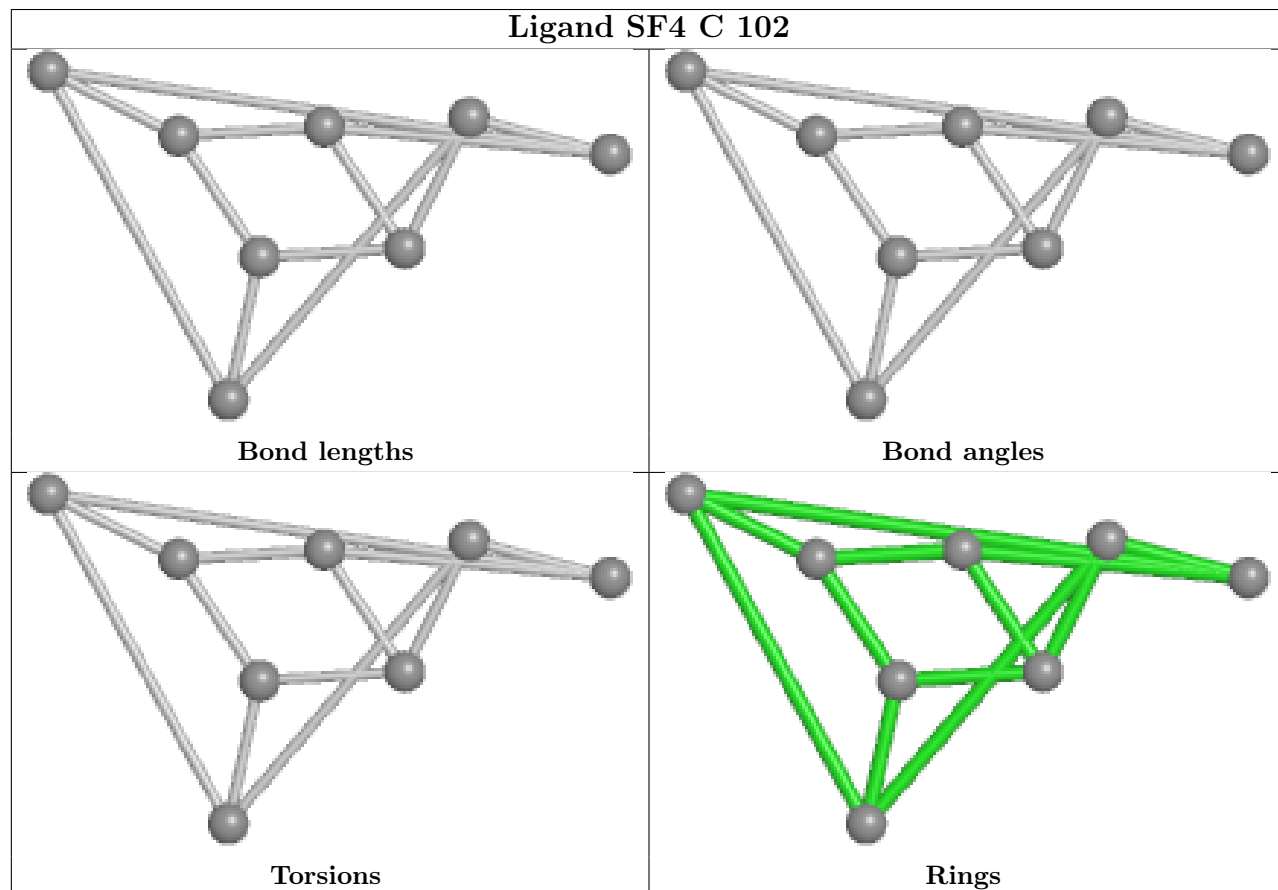


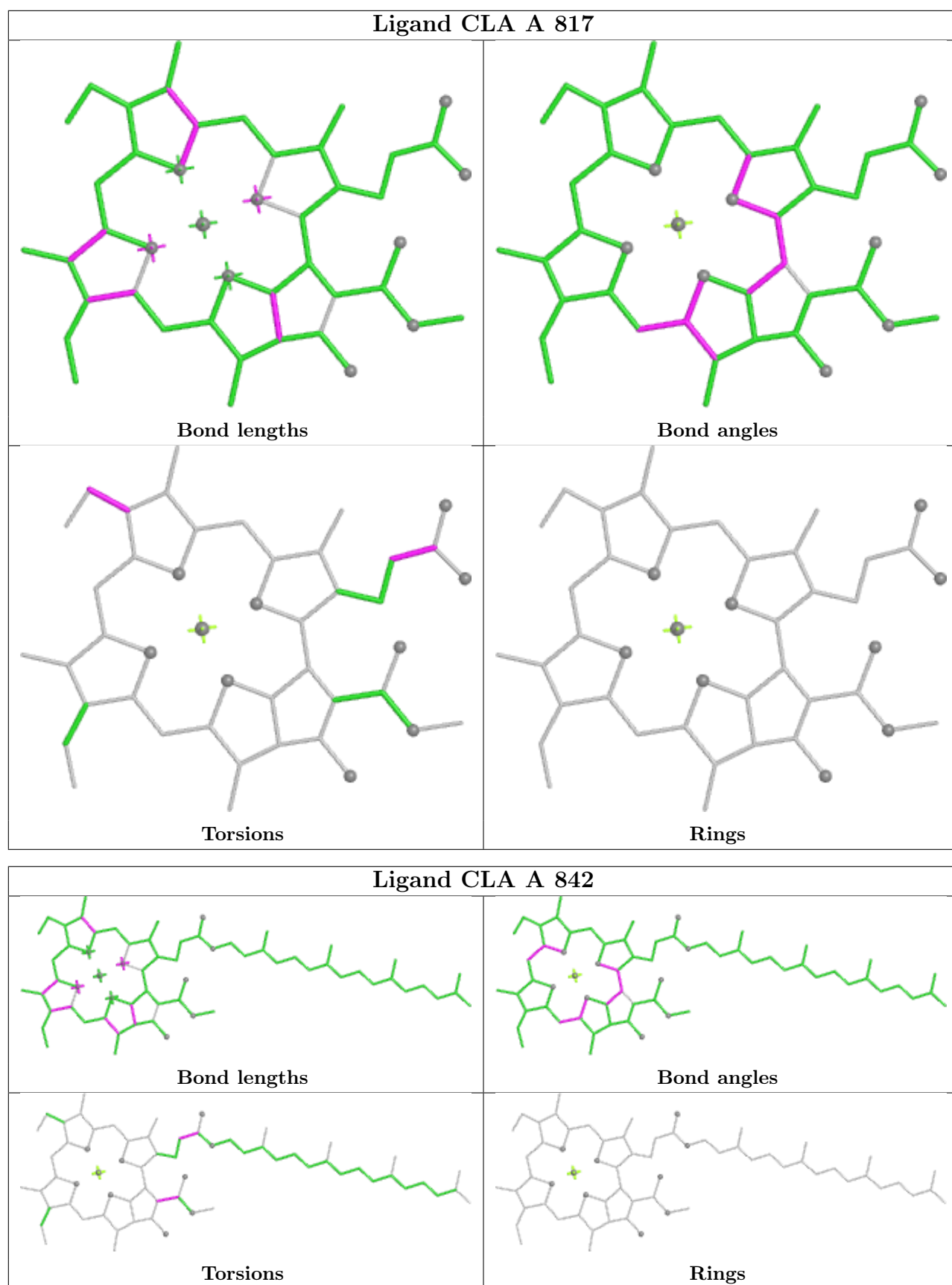


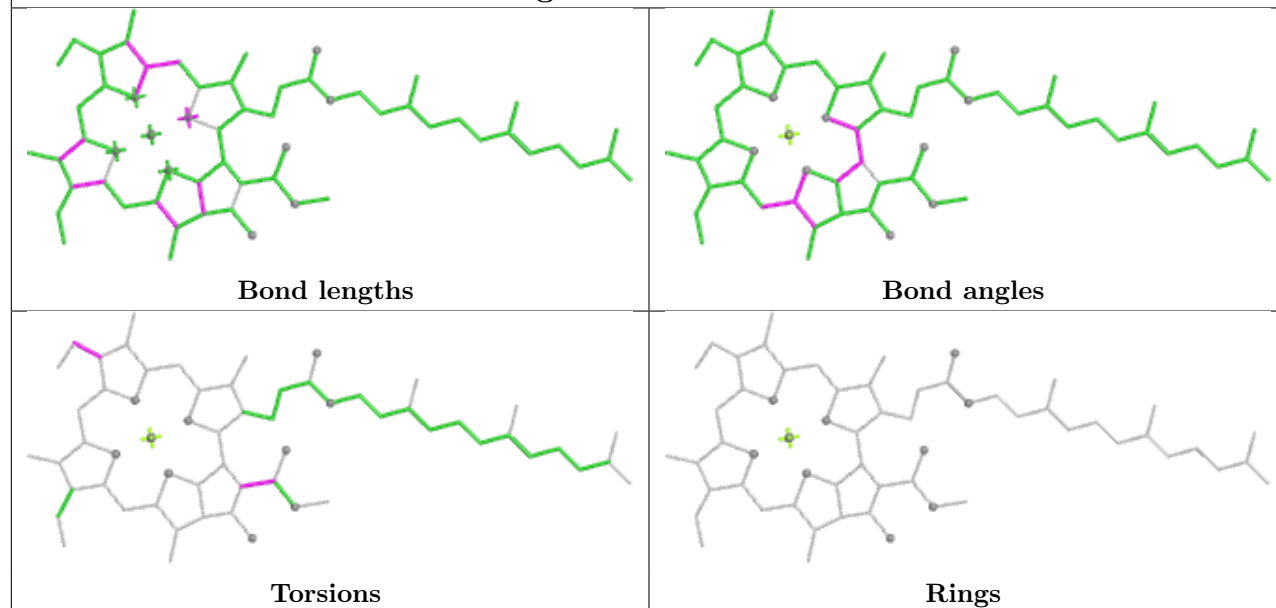
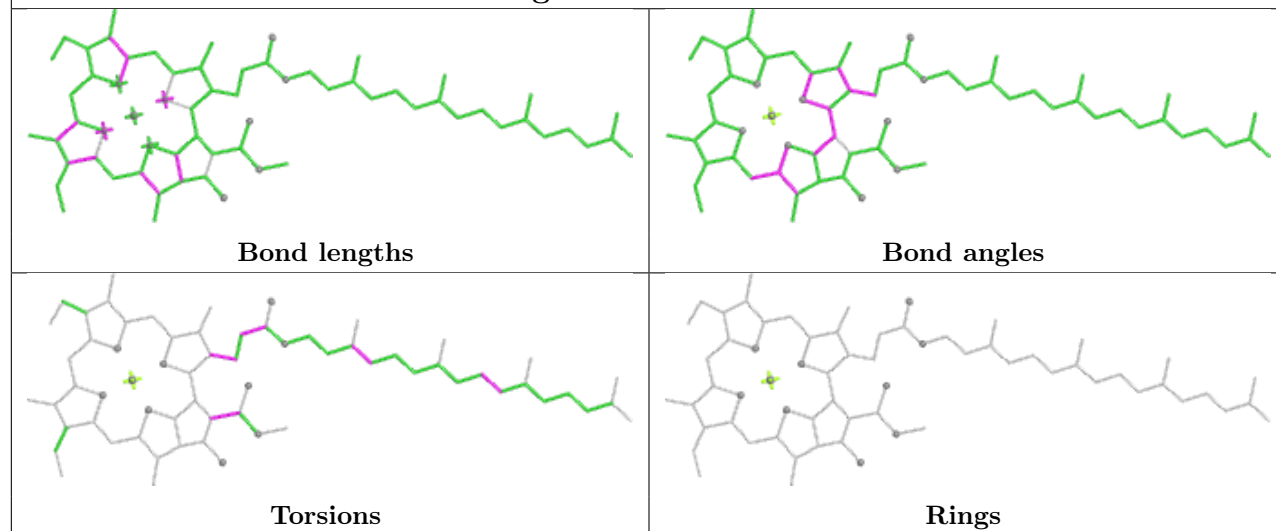
Ligand SF4 A 845

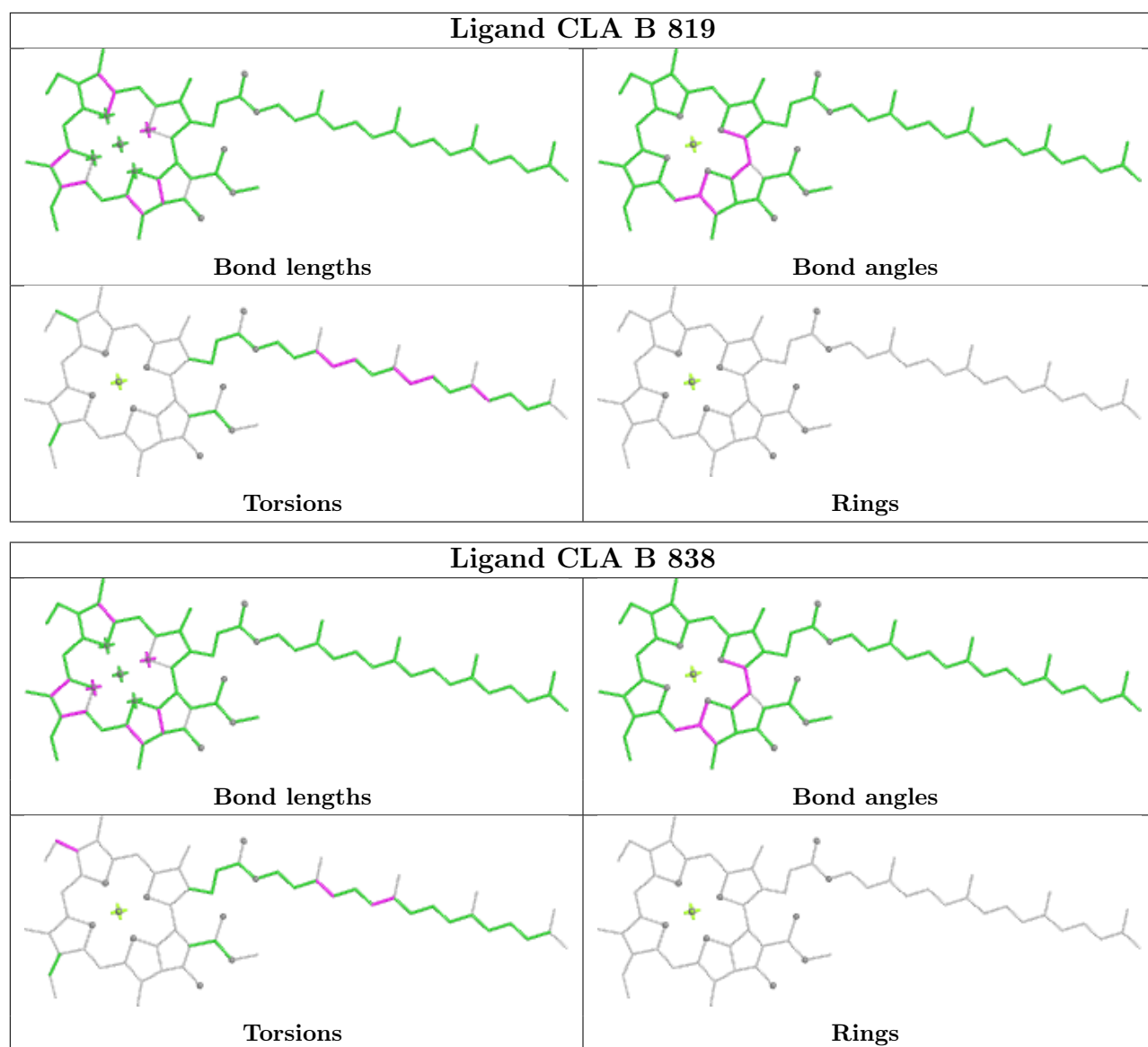


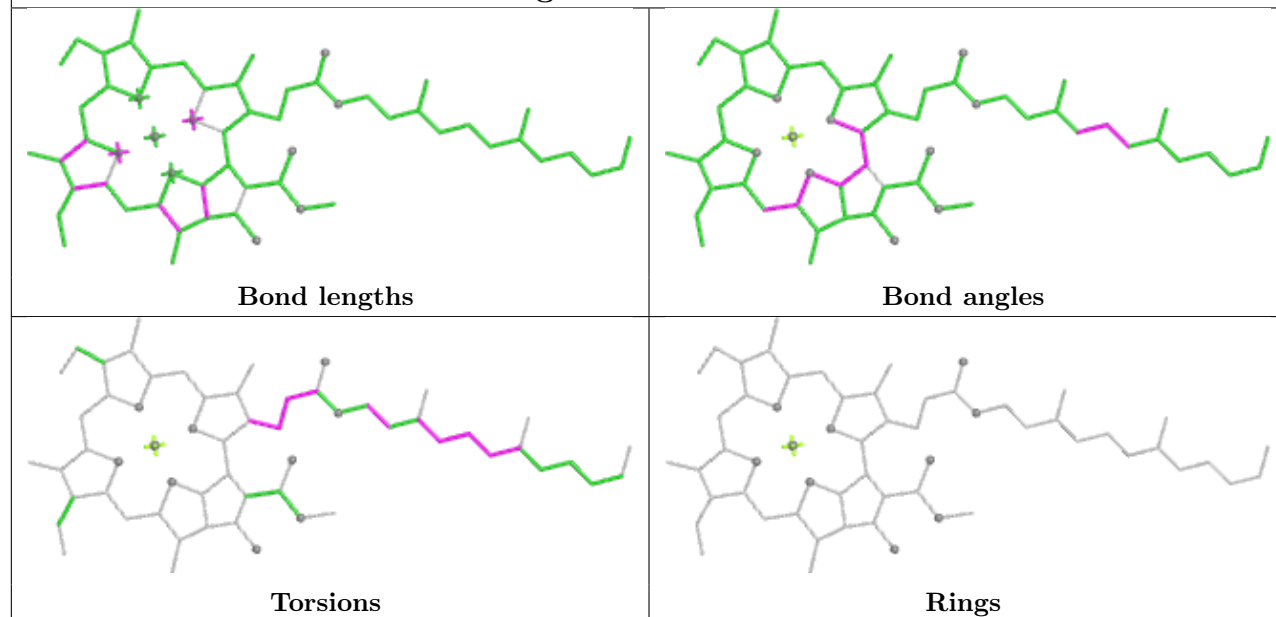
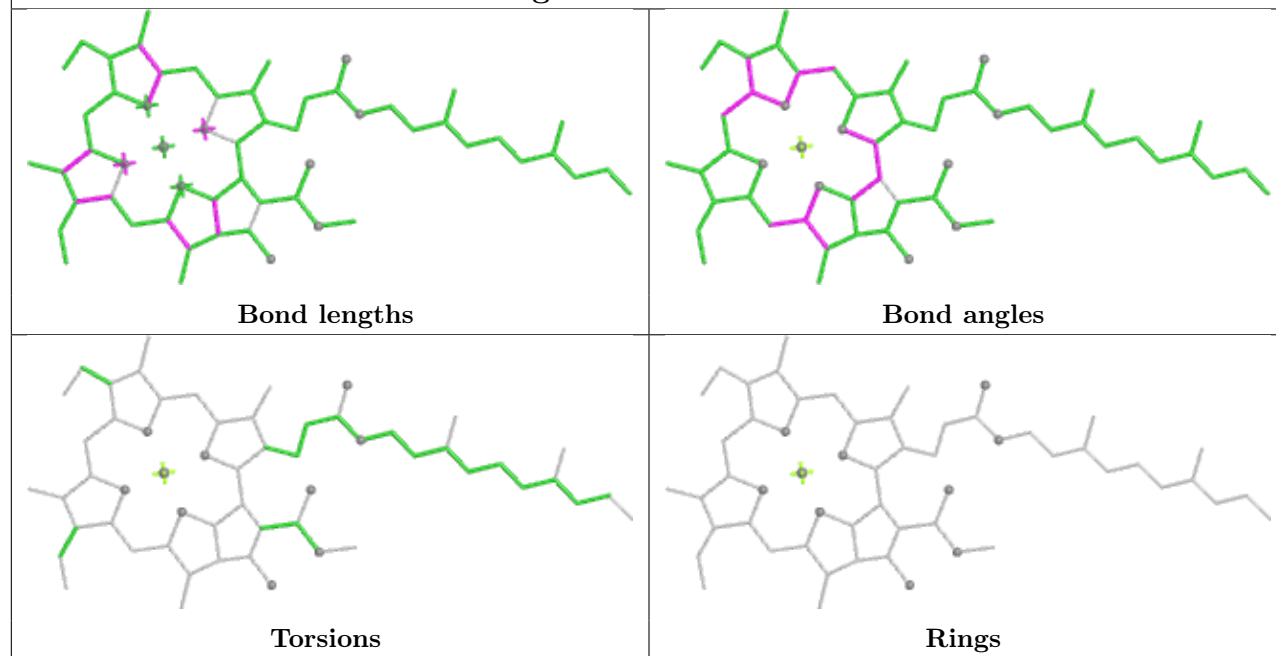
Ligand SF4 C 102



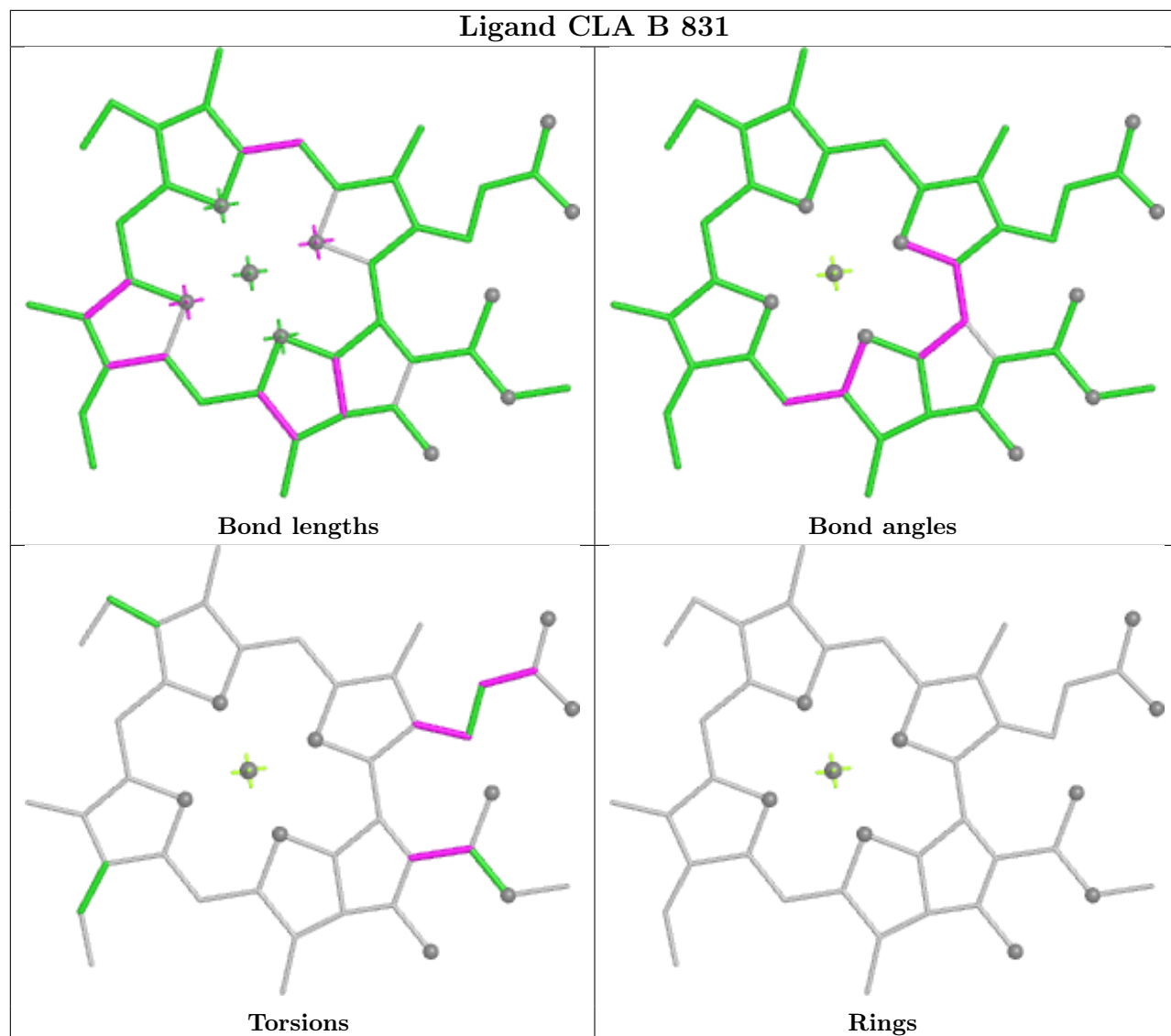


Ligand CLA 3 301**Ligand CLA B 825**

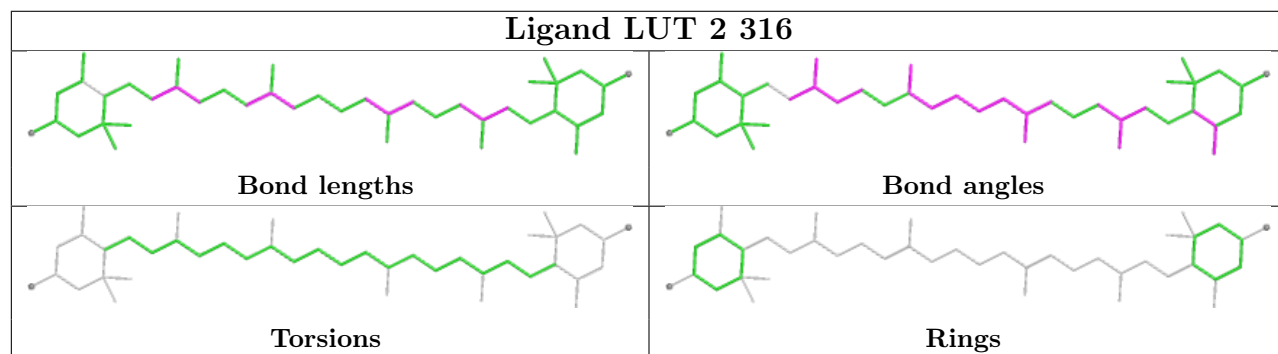


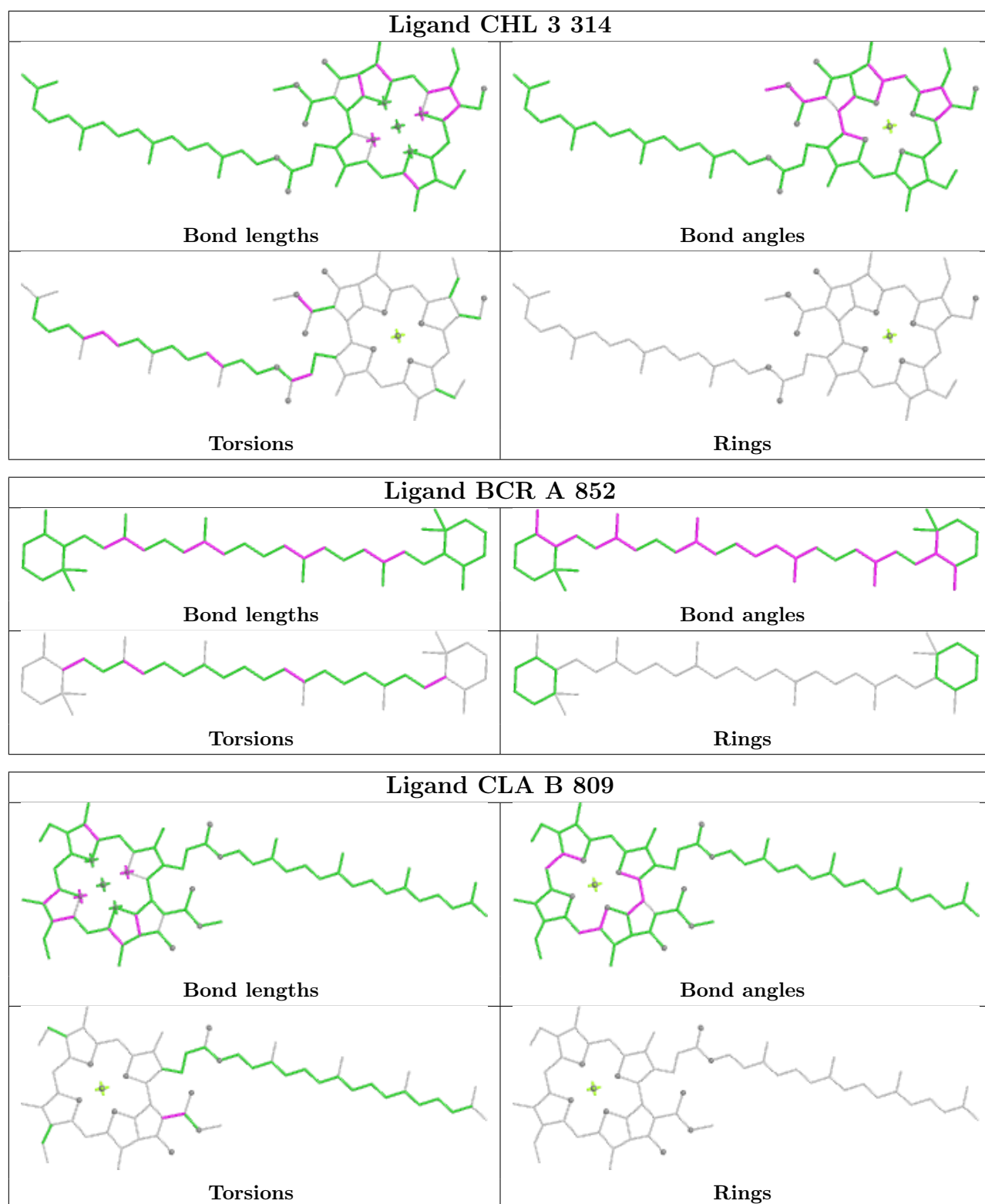
Ligand CLA 5 307**Ligand CLA B 820**

Ligand CLA B 831

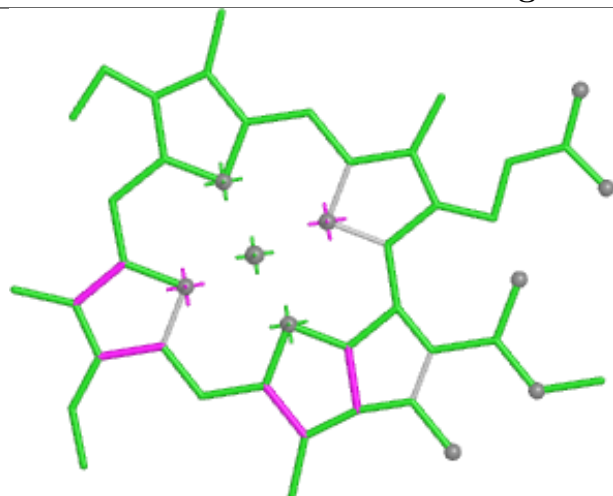


Ligand LUT 2 316

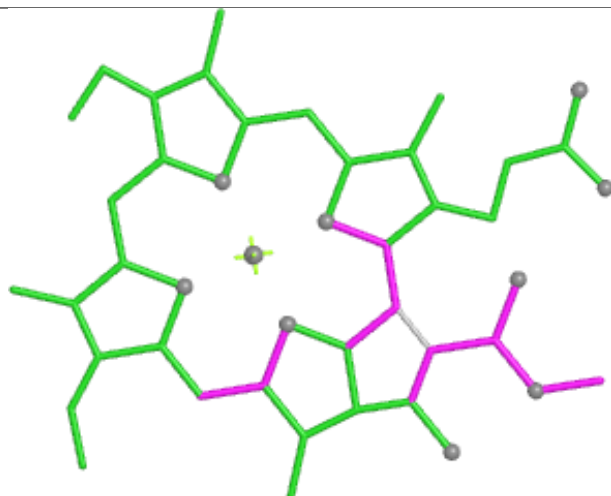




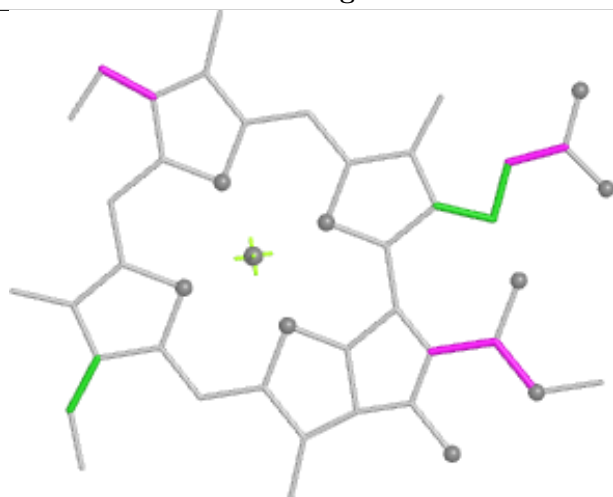
Ligand CLA 5 314



Bond lengths



Bond angles

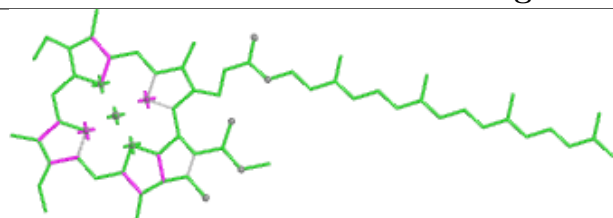


Torsions

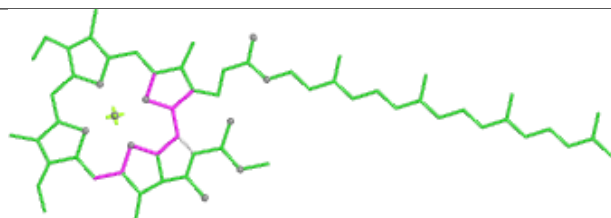


Rings

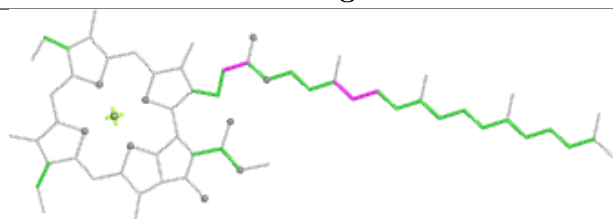
Ligand CLA B 810



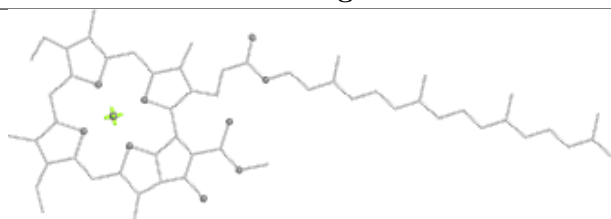
Bond lengths



Bond angles

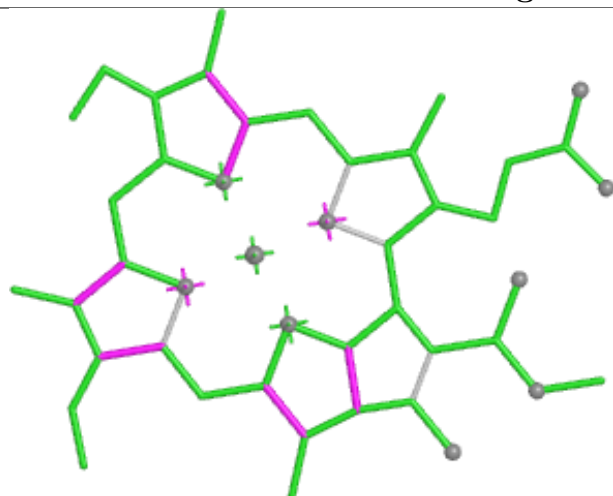


Torsions

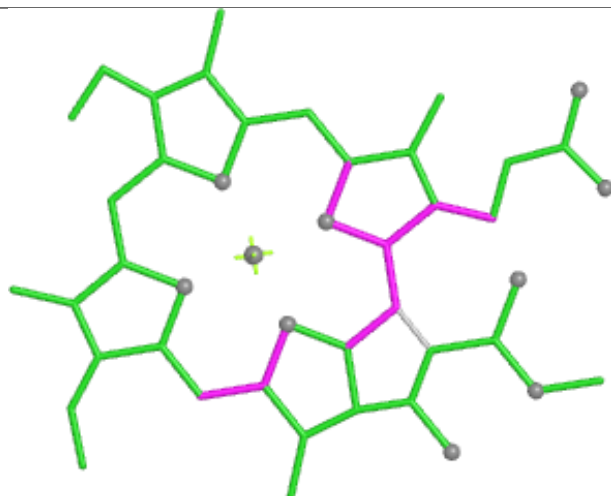


Rings

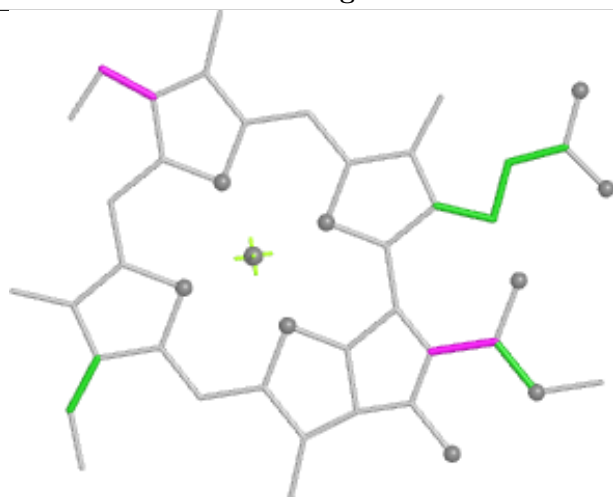
Ligand CLA L 301



Bond lengths



Bond angles

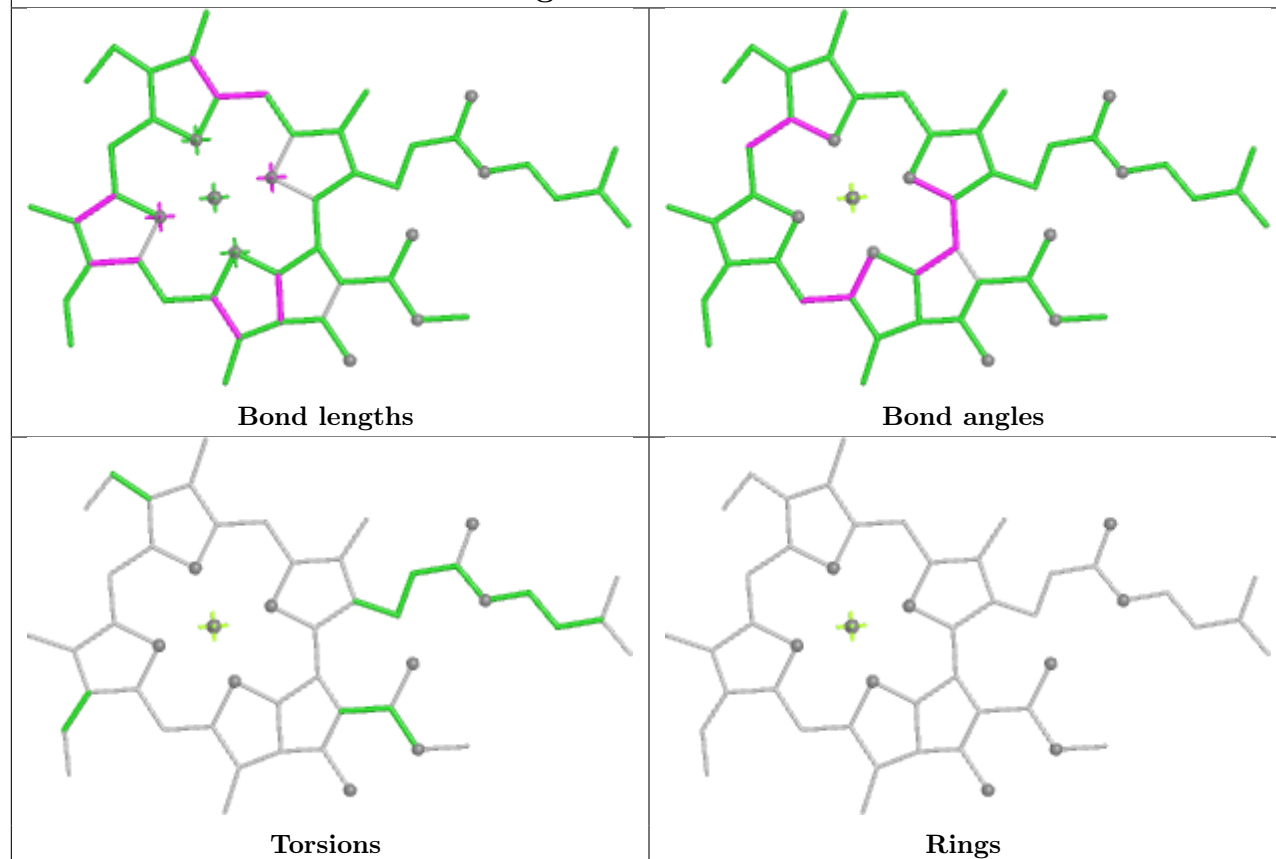


Torsions

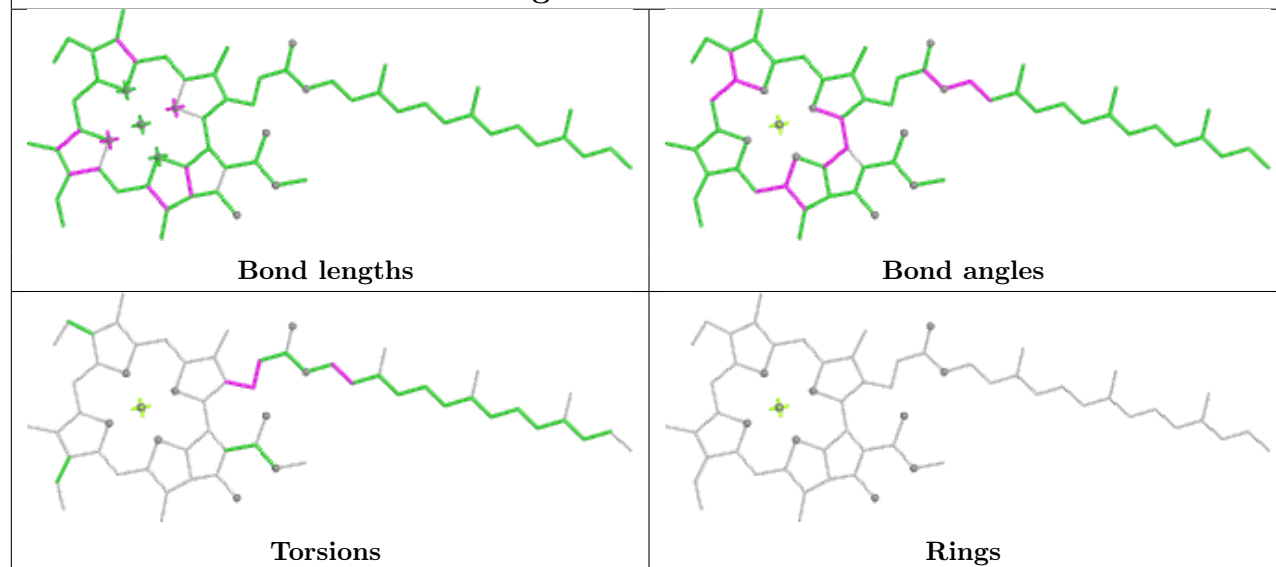


Rings

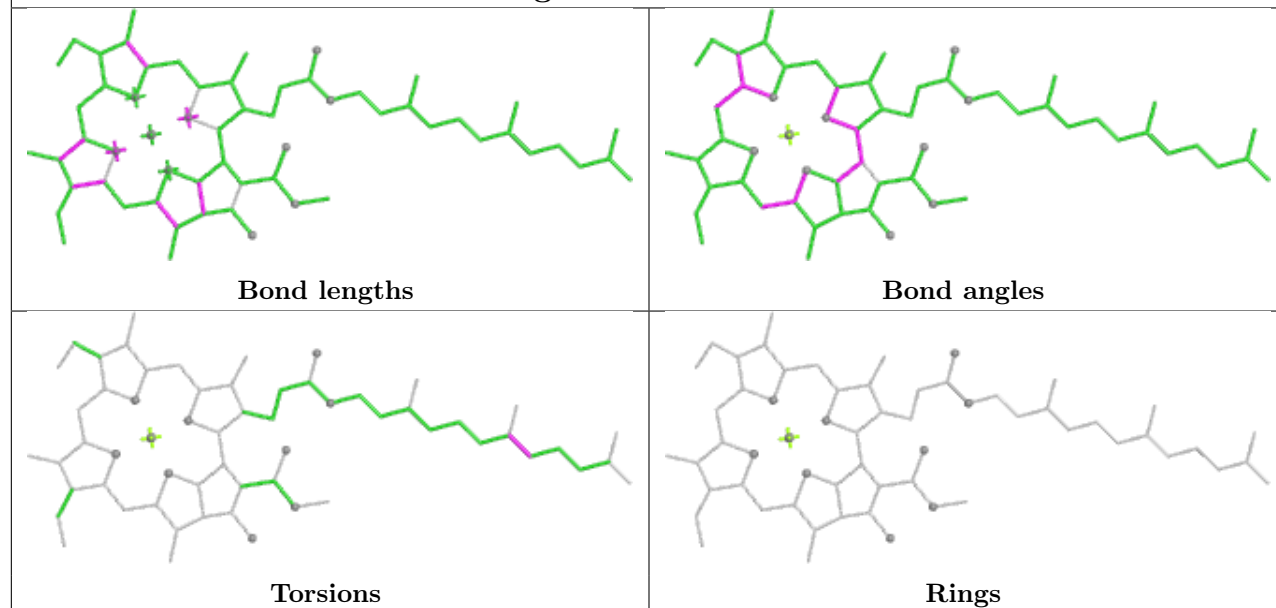
Ligand CLA 6 308



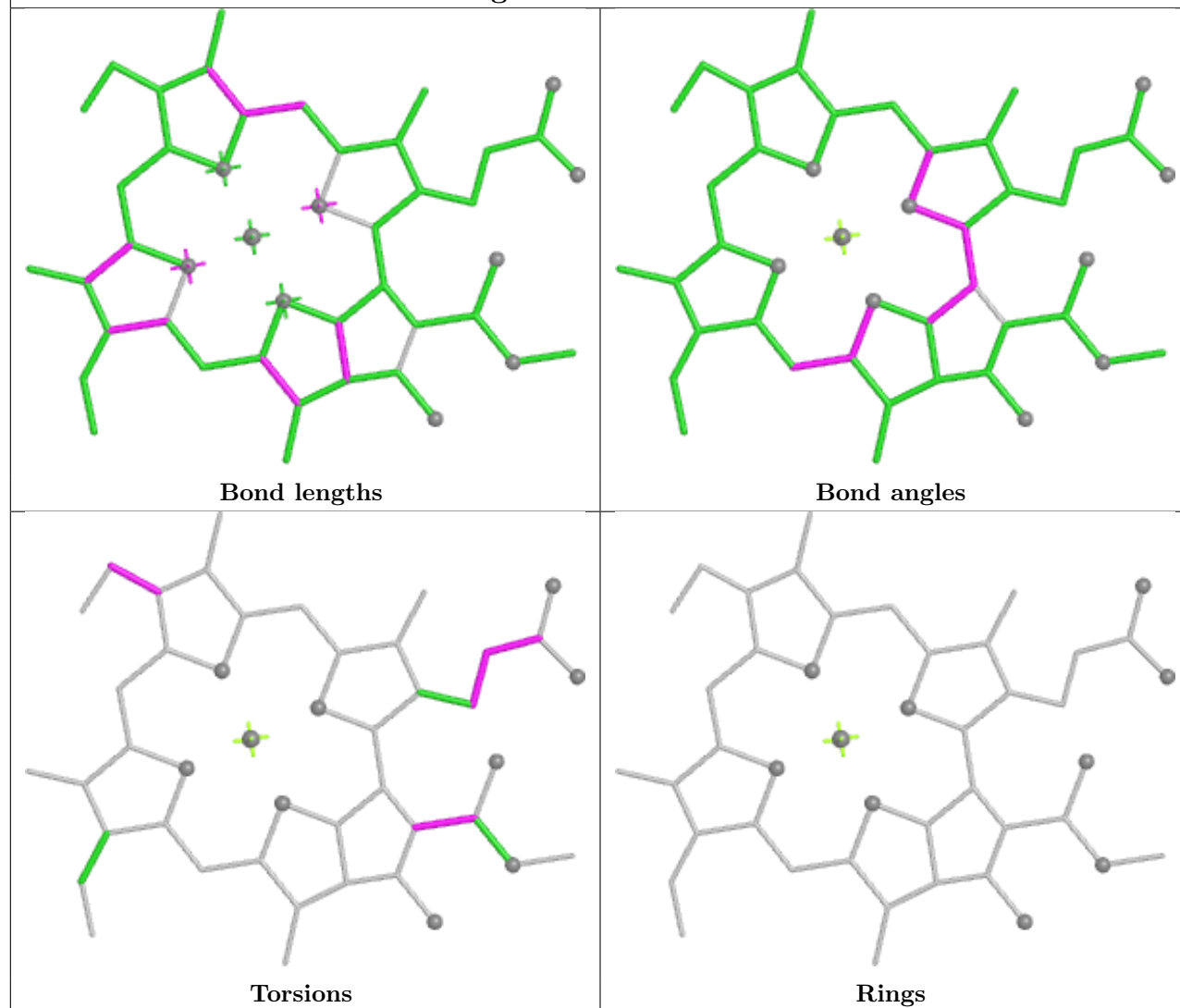
Ligand CLA B 818

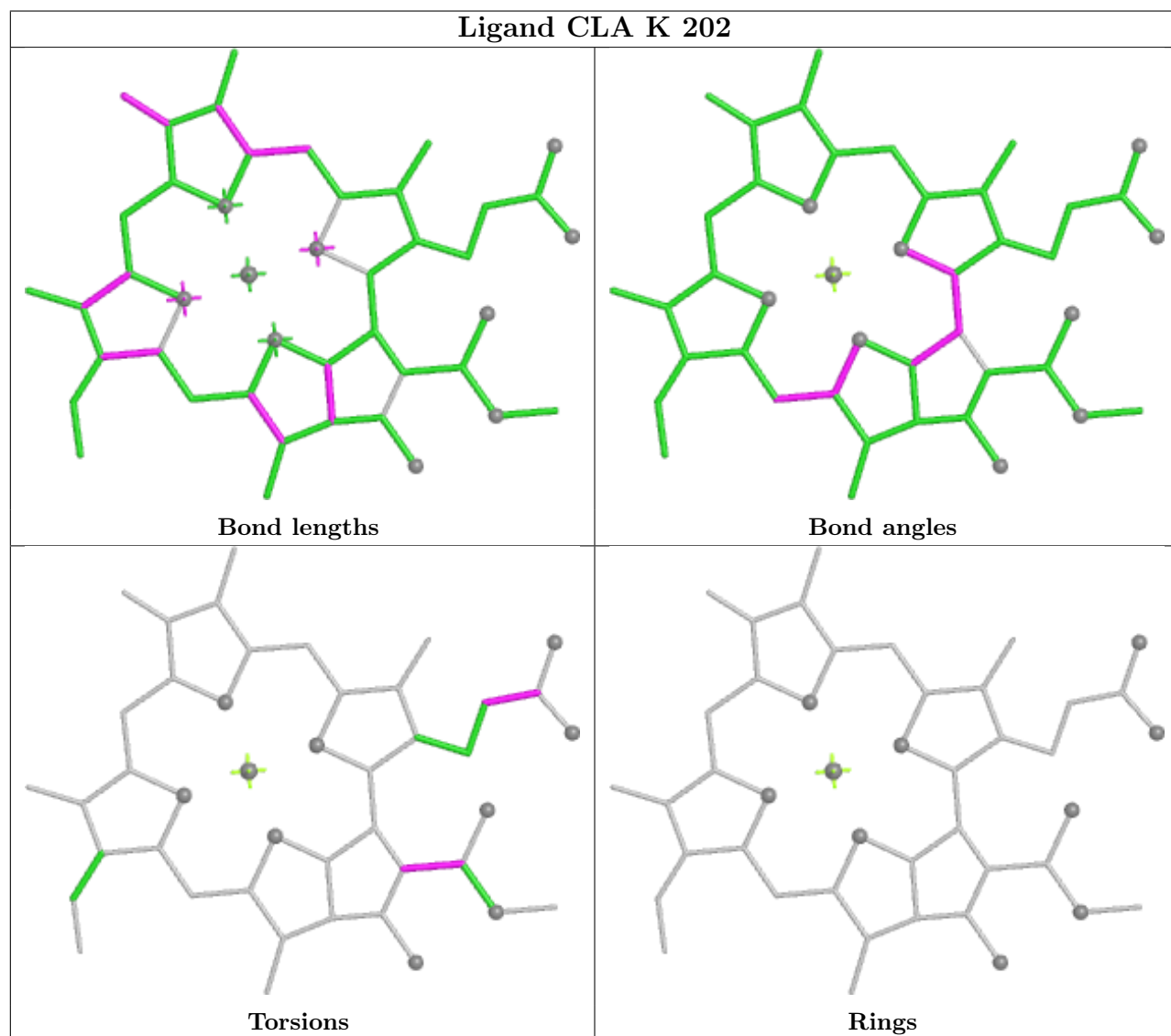
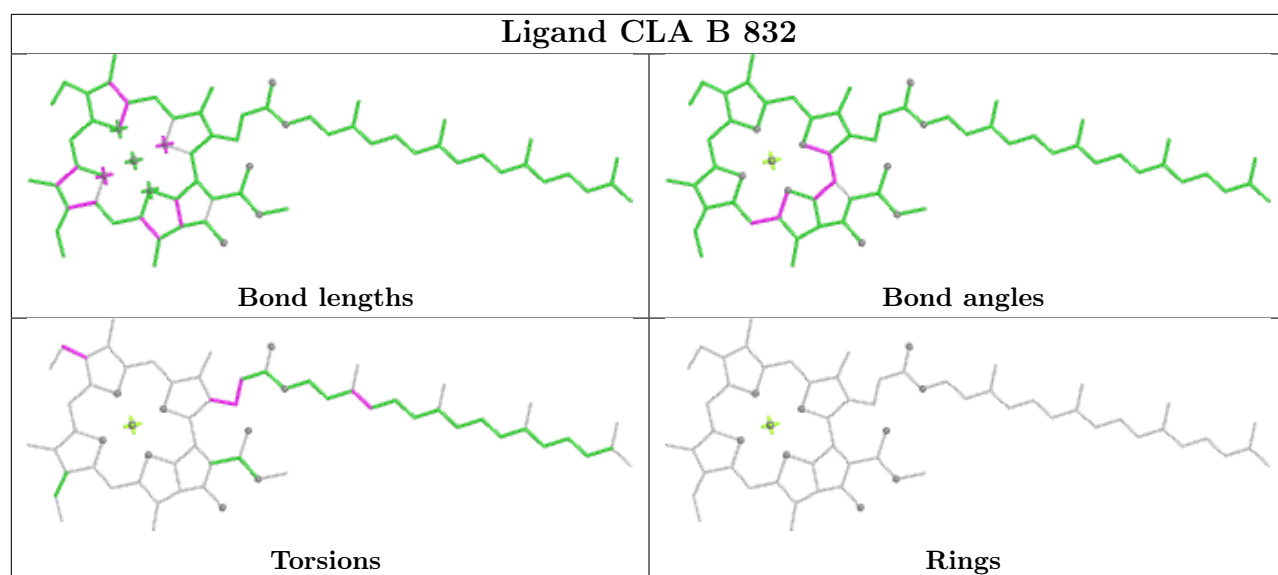


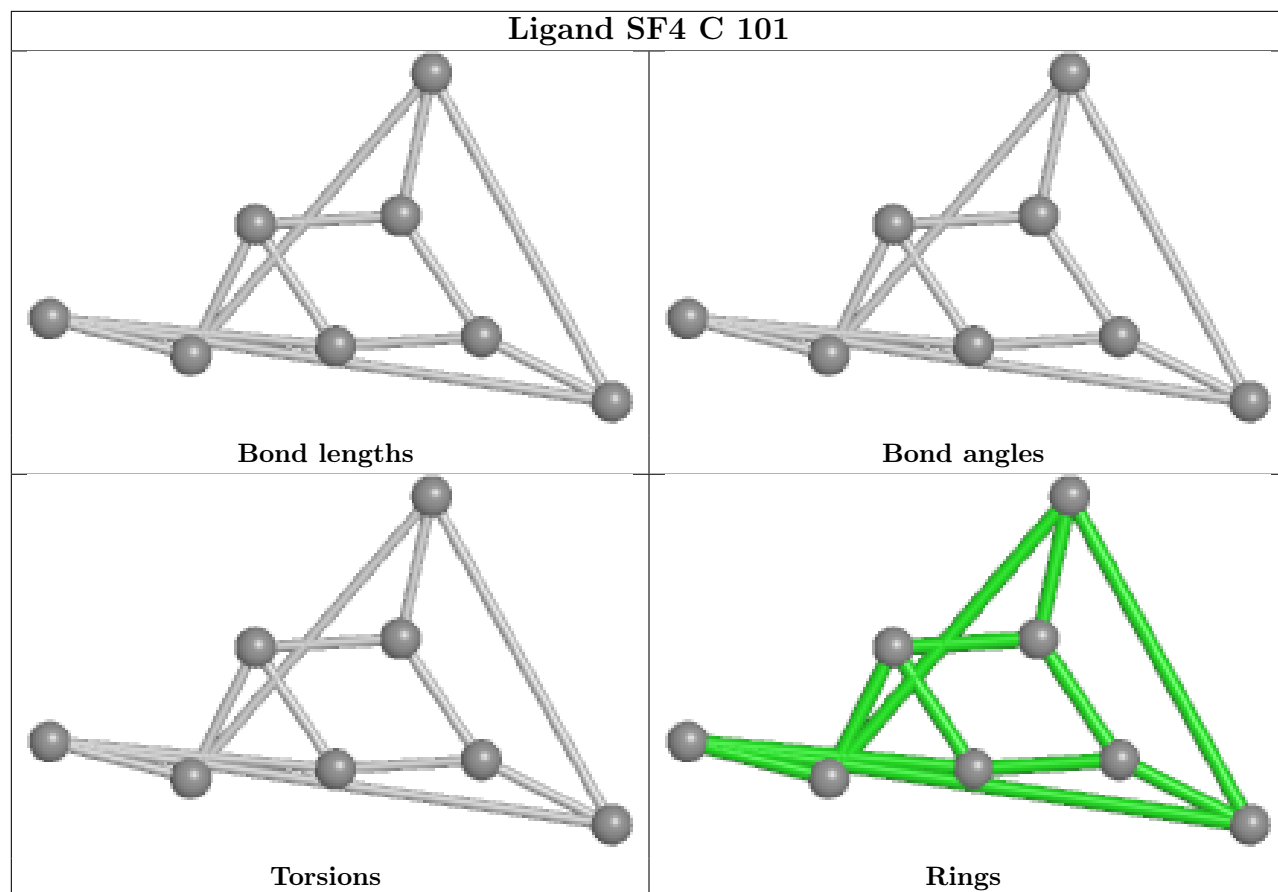
Ligand CLA F 301



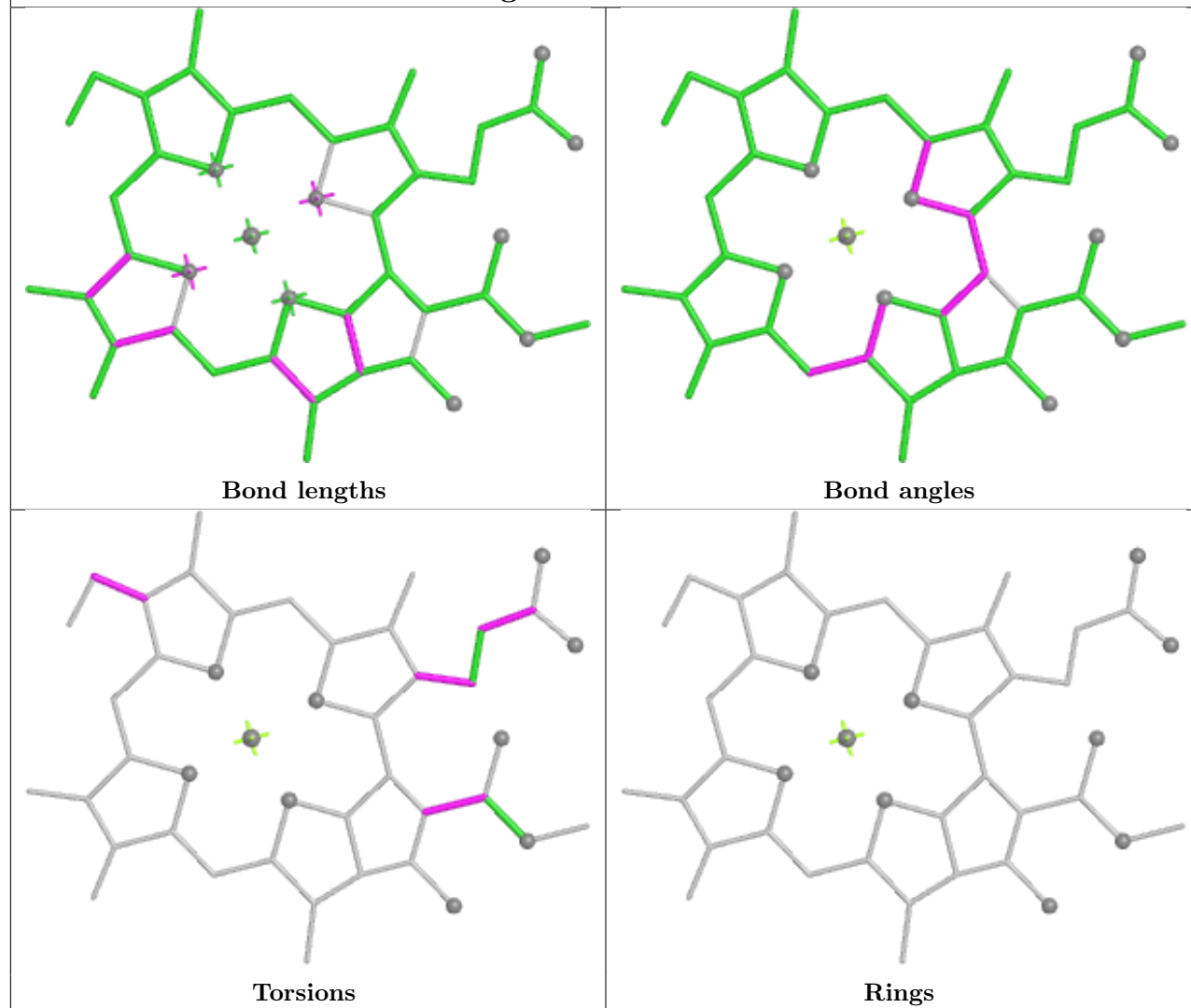
Ligand CLA G 204



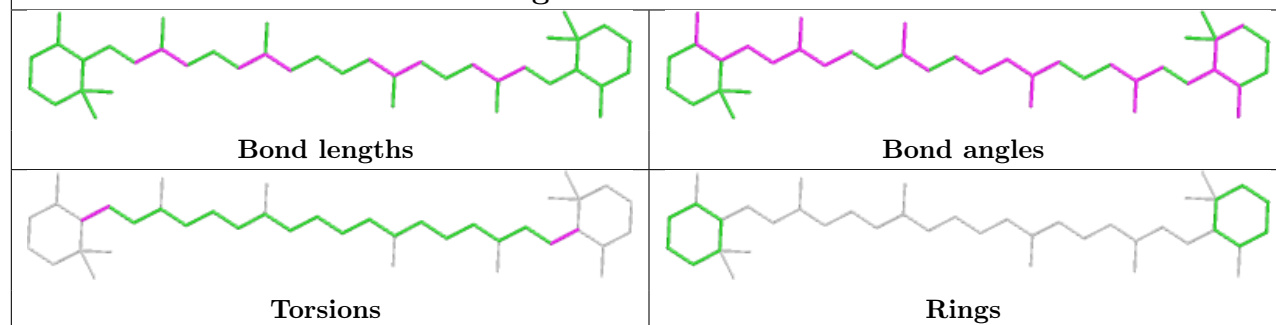


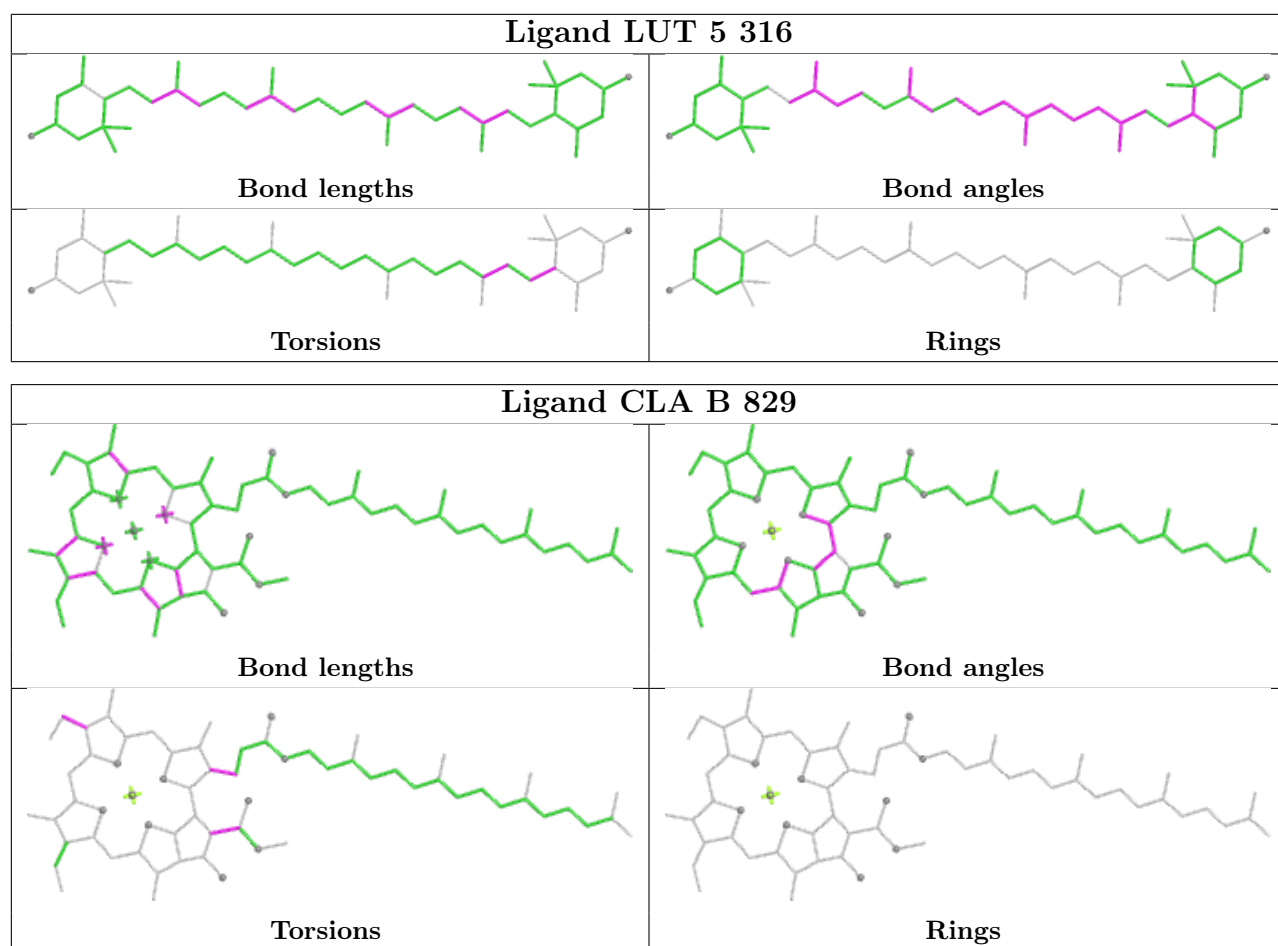


Ligand CLA 5 310

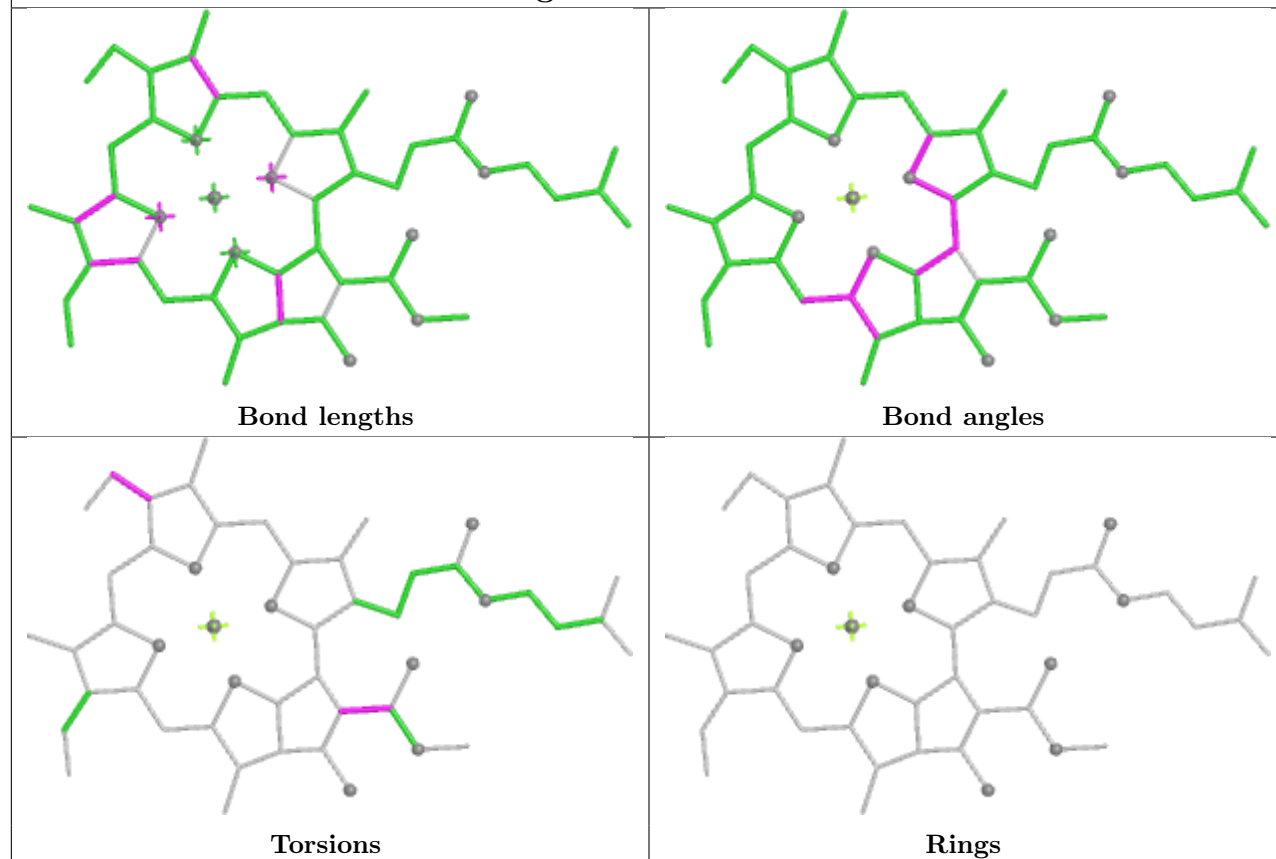


Ligand BCR F 302

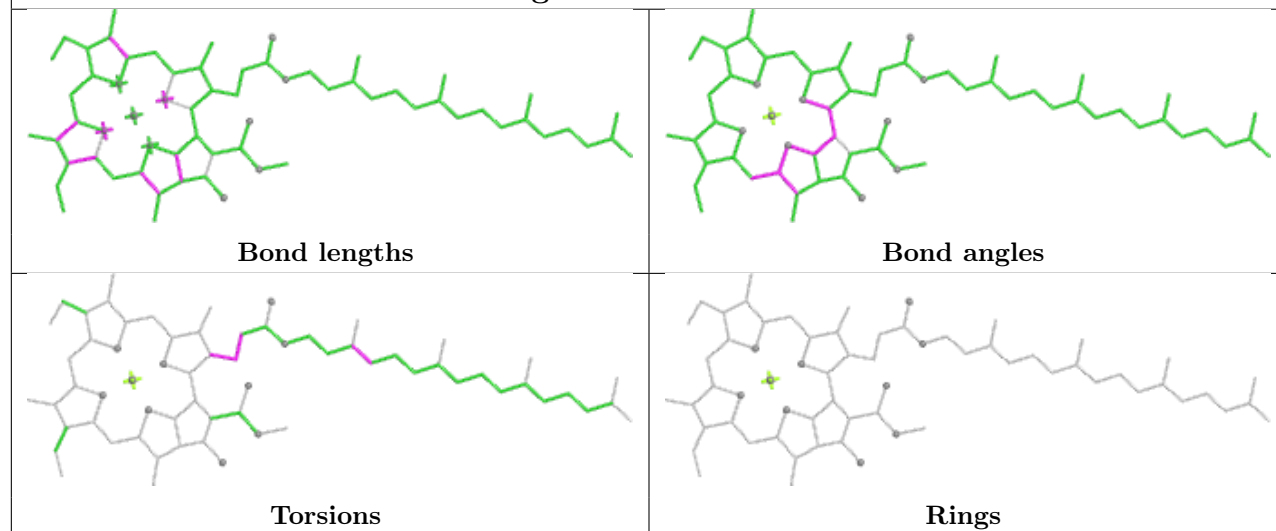


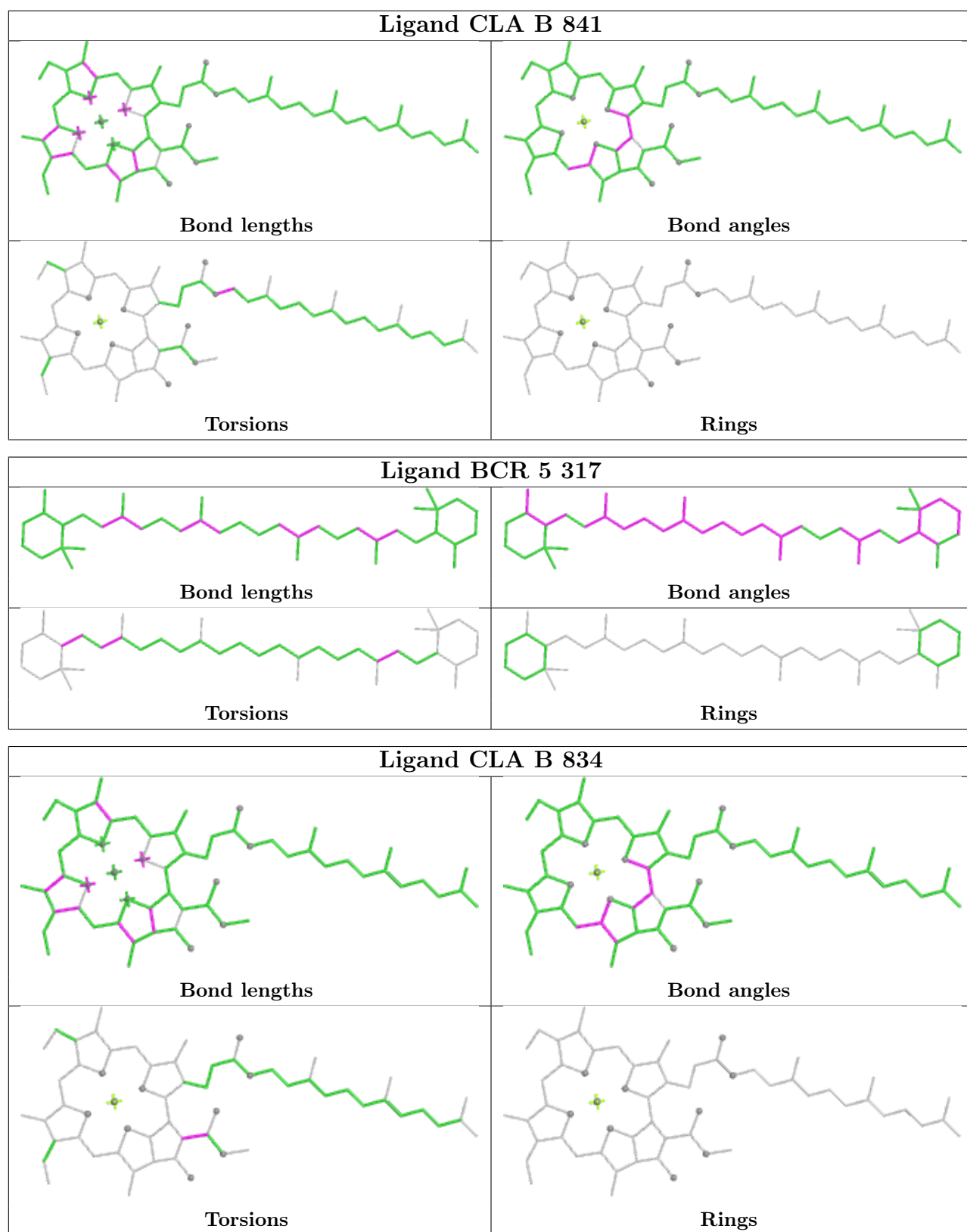


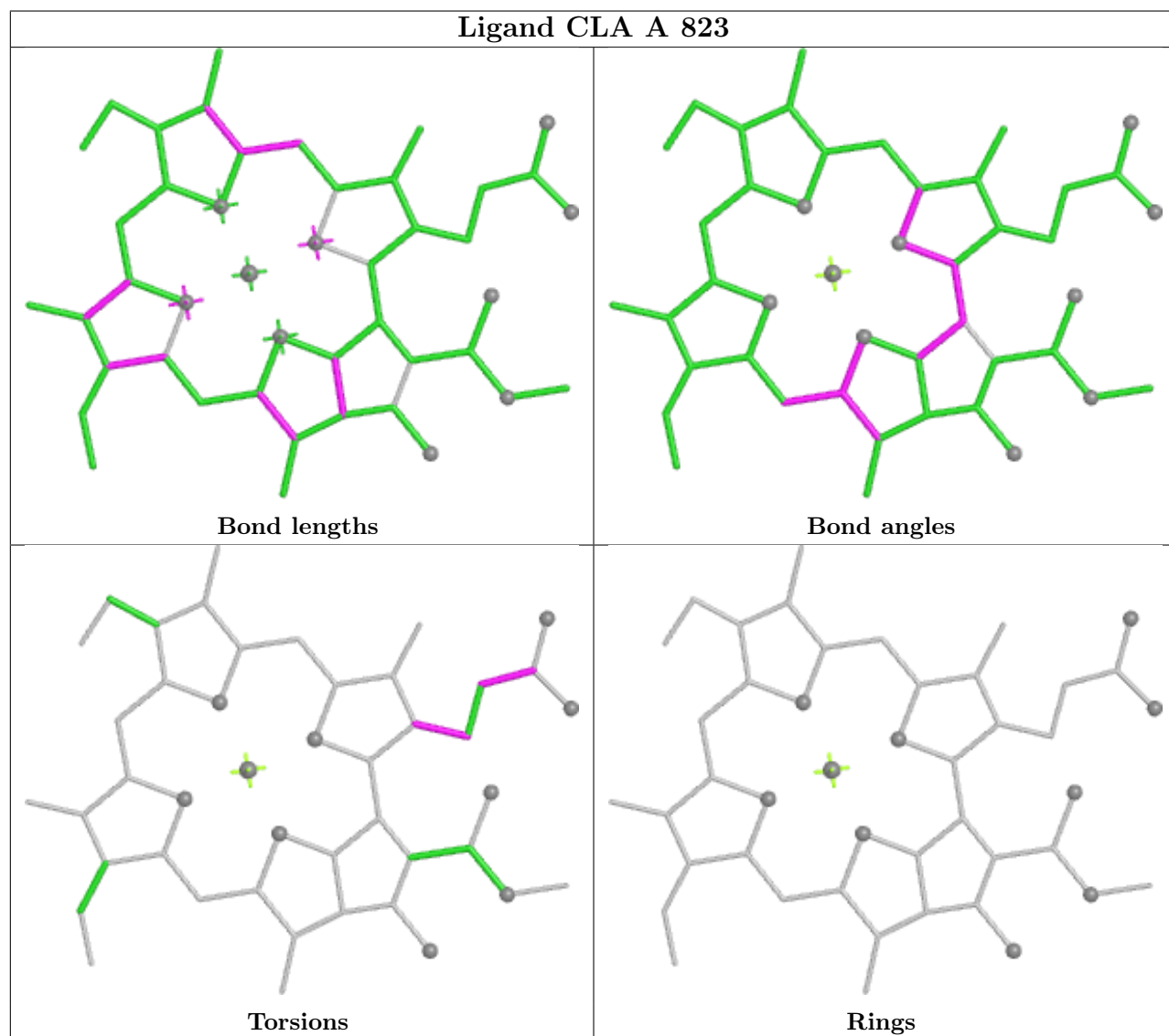
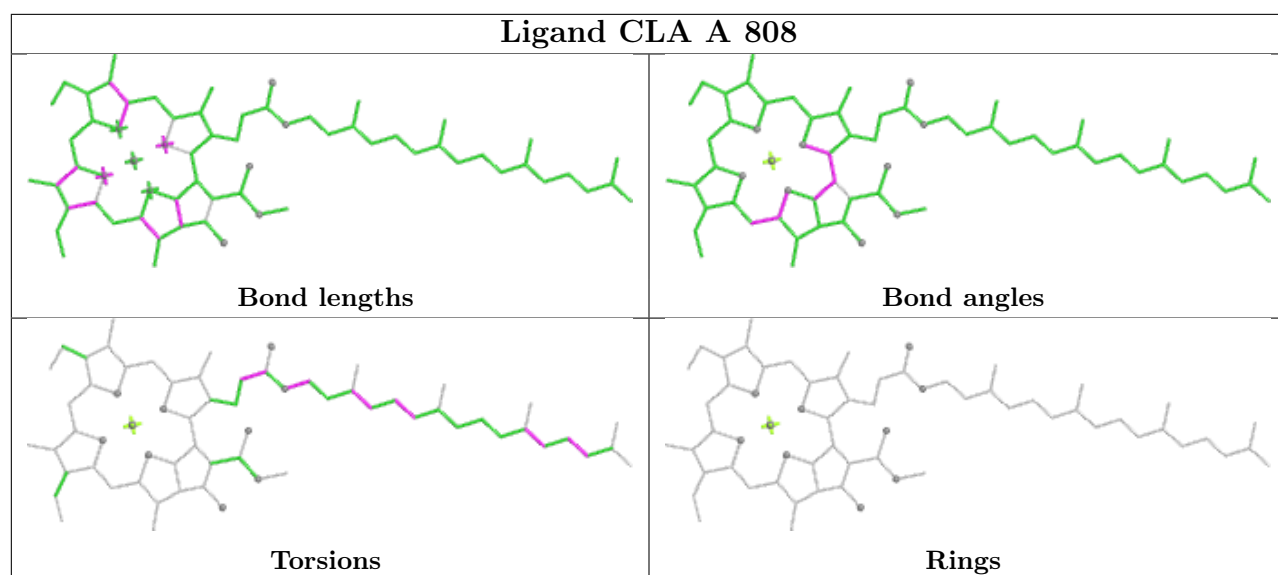
Ligand CLA 2 313

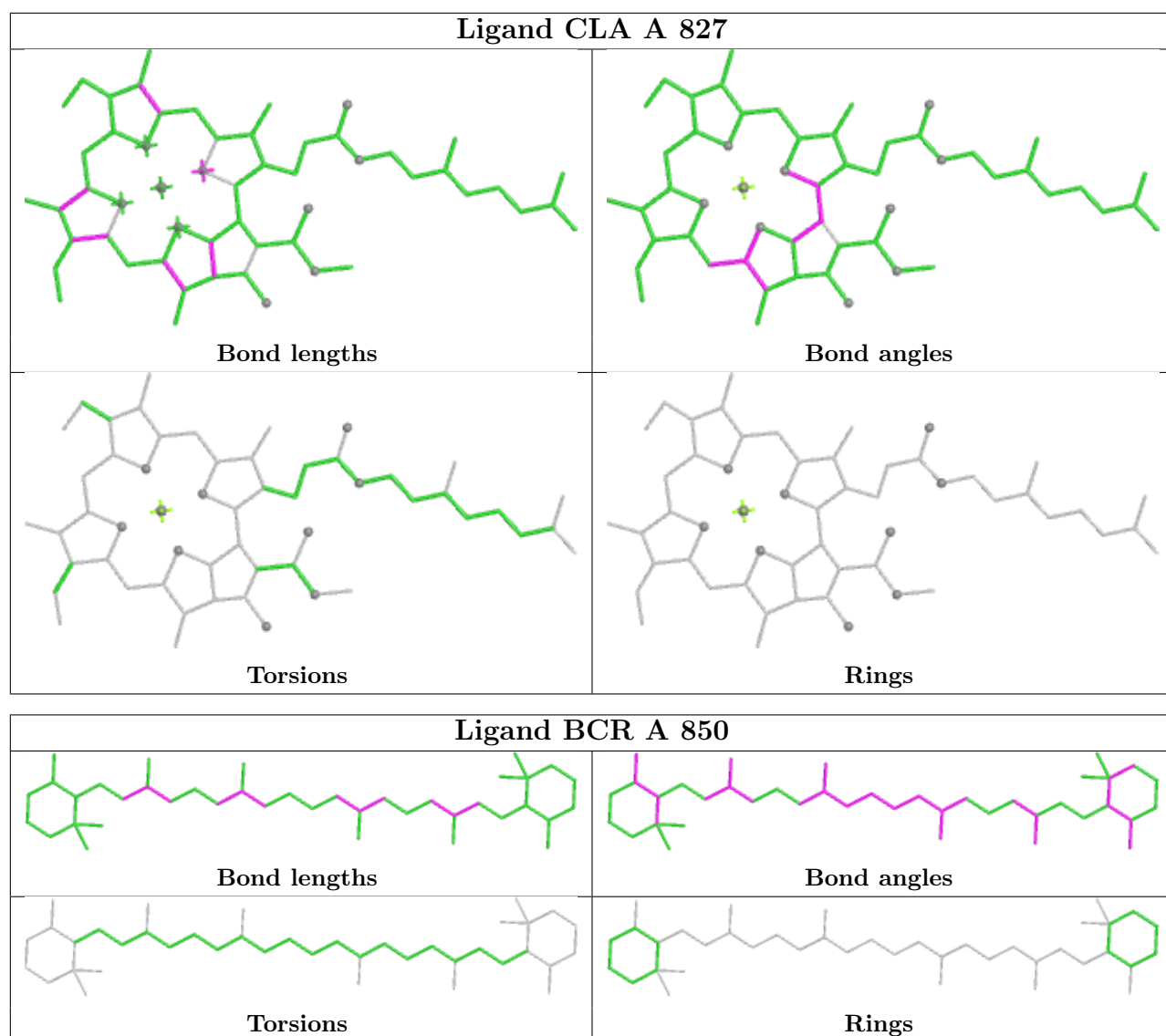


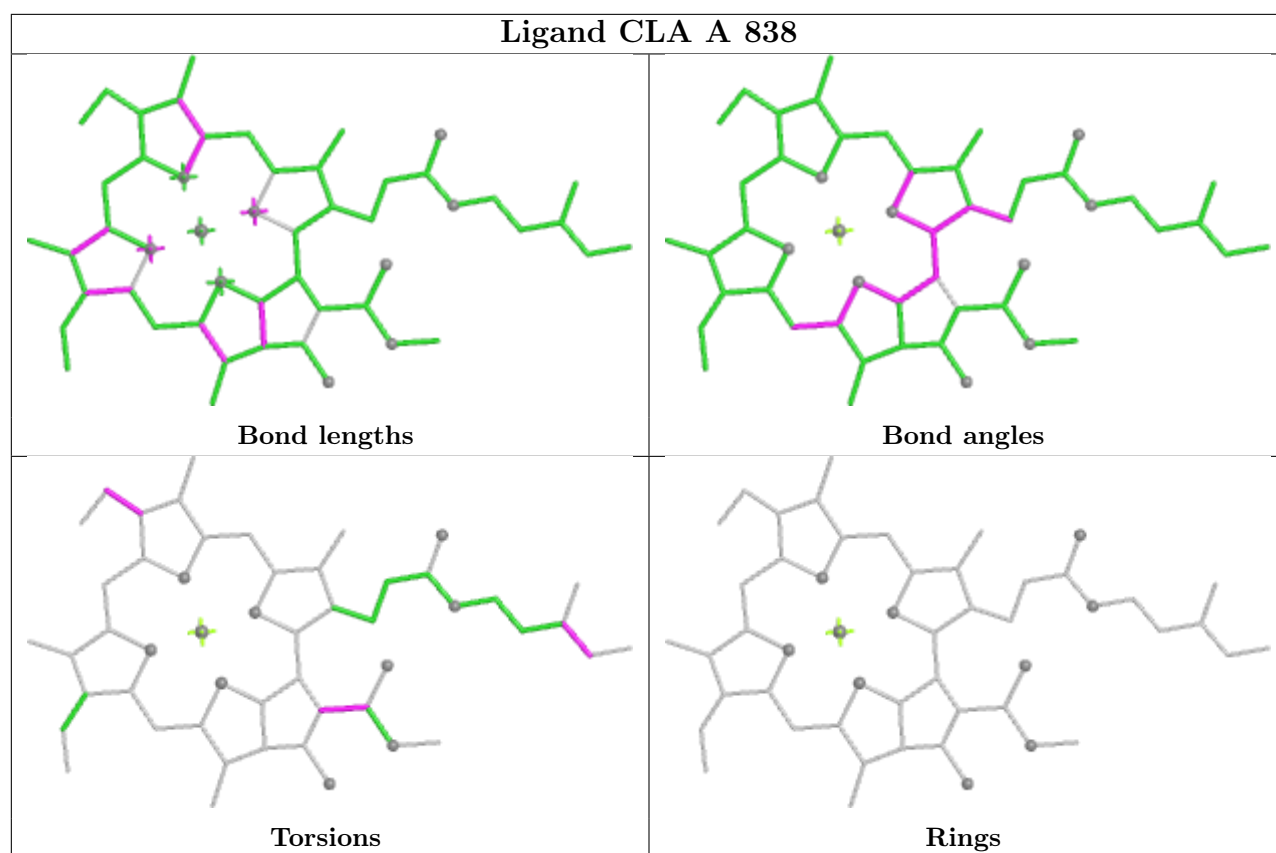
Ligand CLA A 804

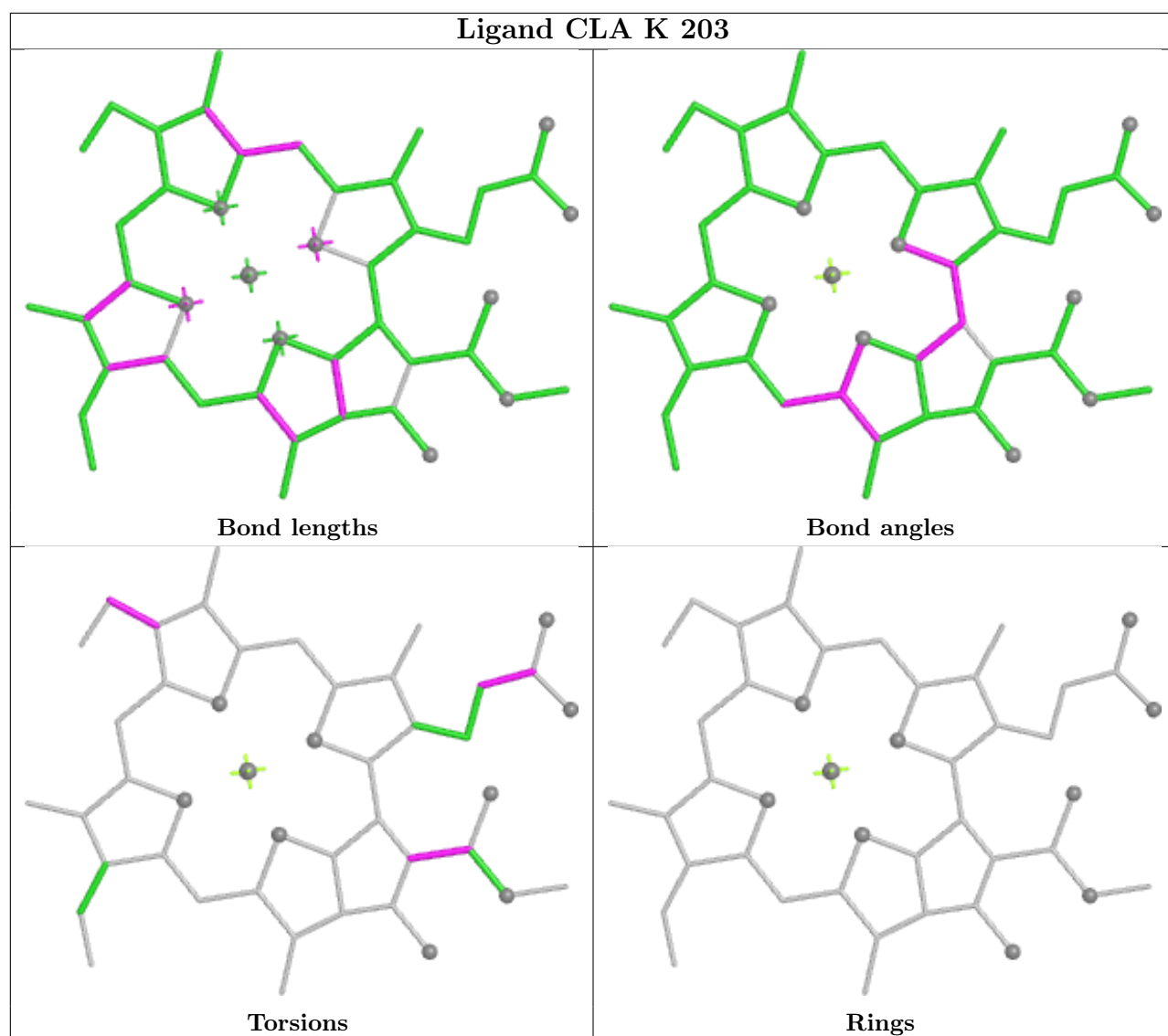


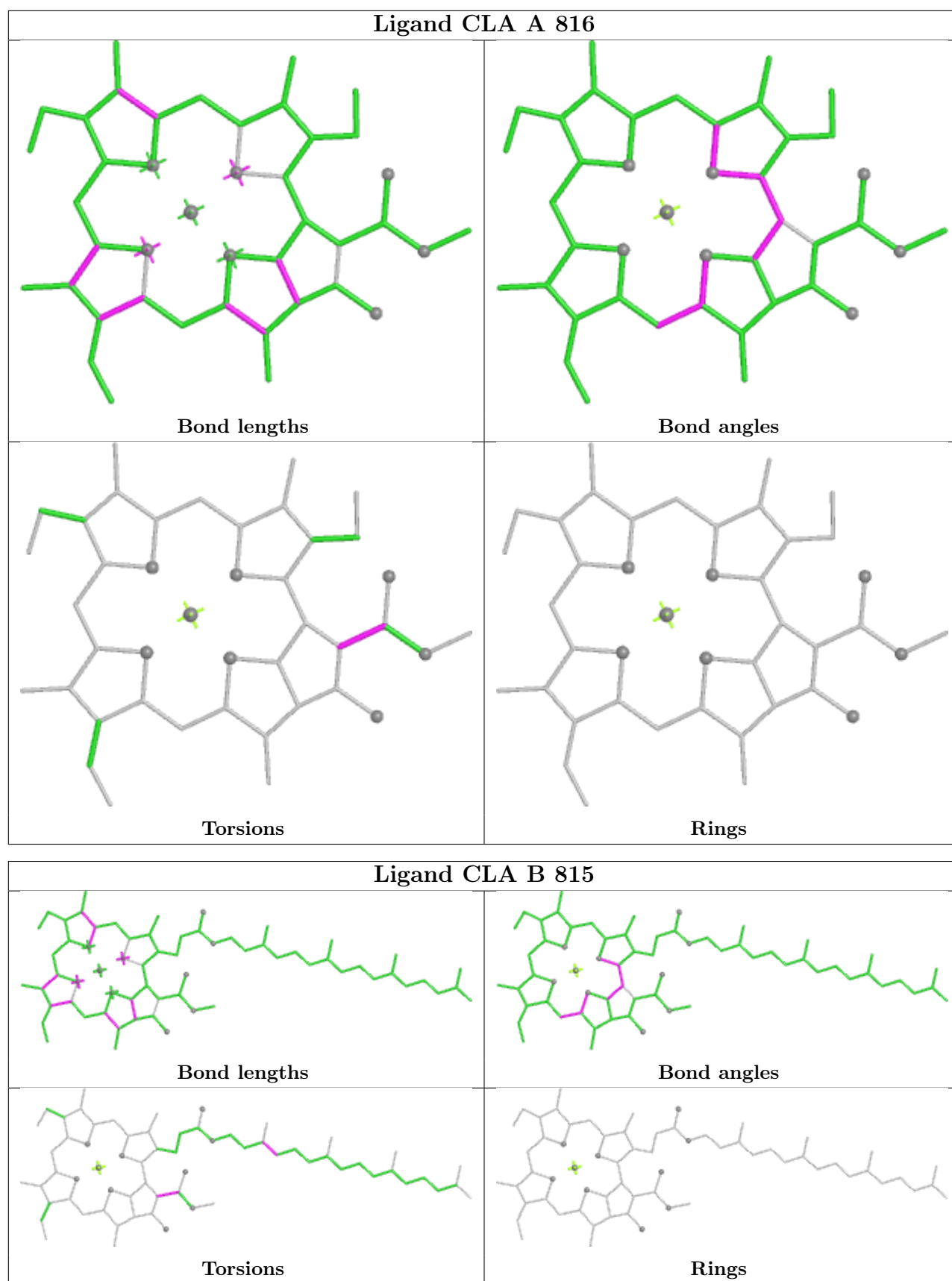




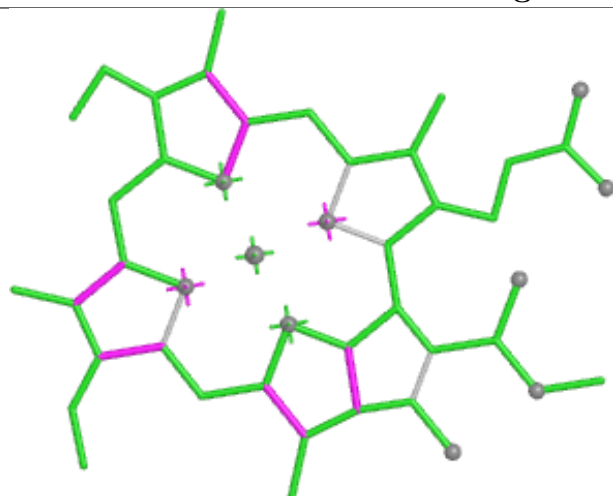




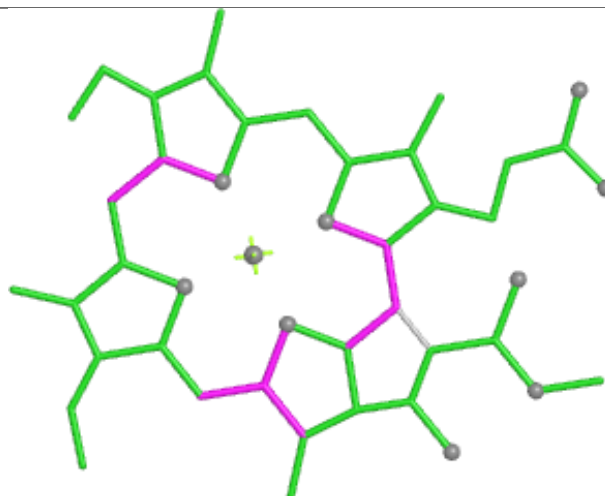




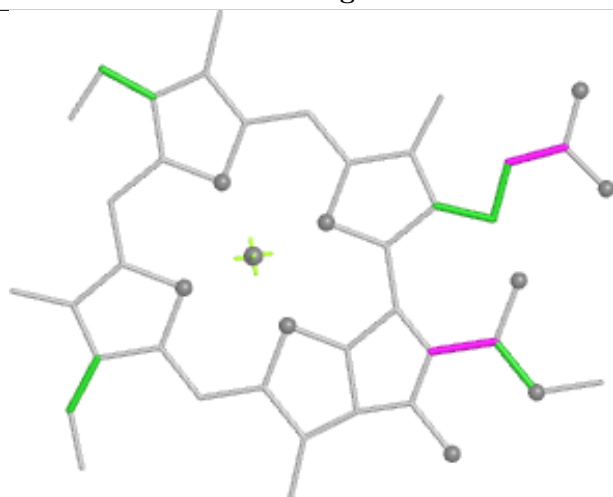
Ligand CLA A 837



Bond lengths



Bond angles

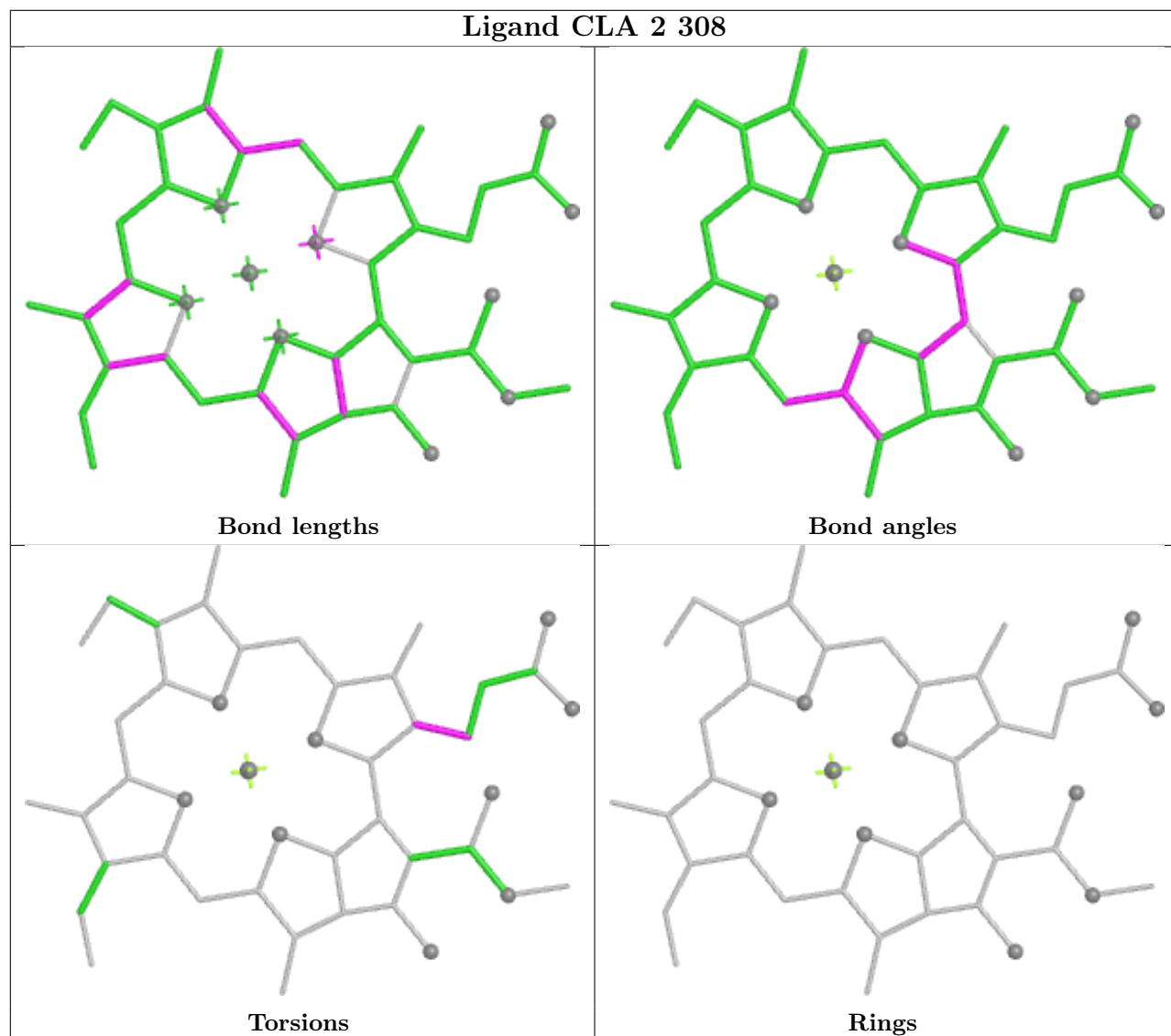


Torsions

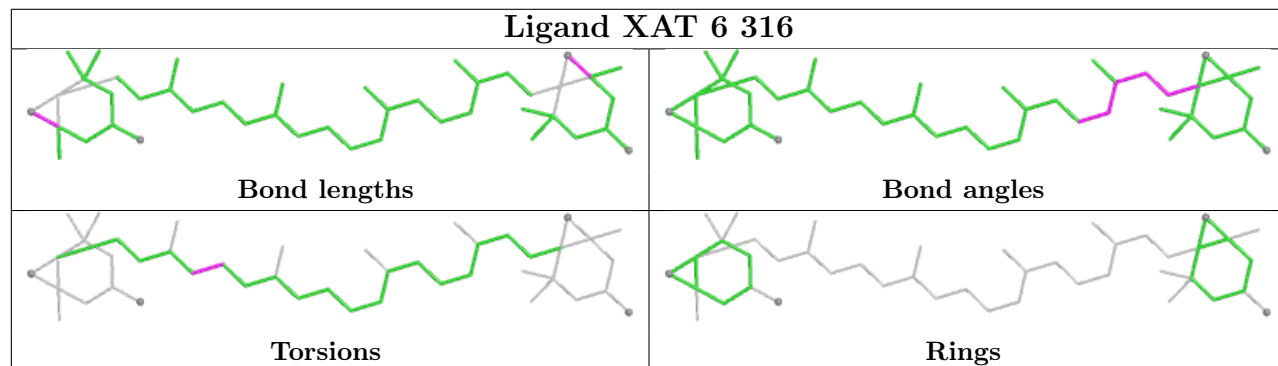


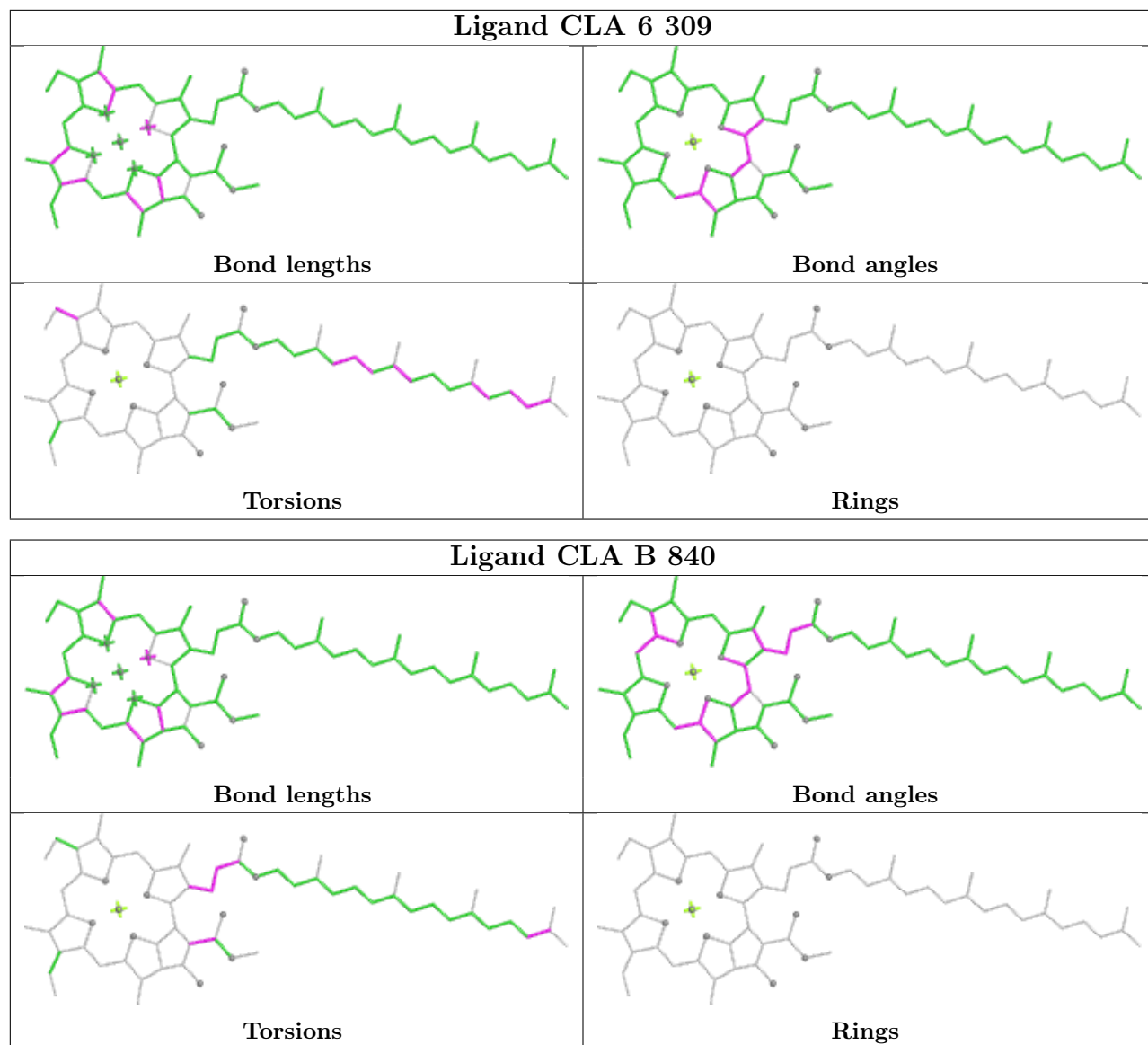
Rings

Ligand CLA 2 308

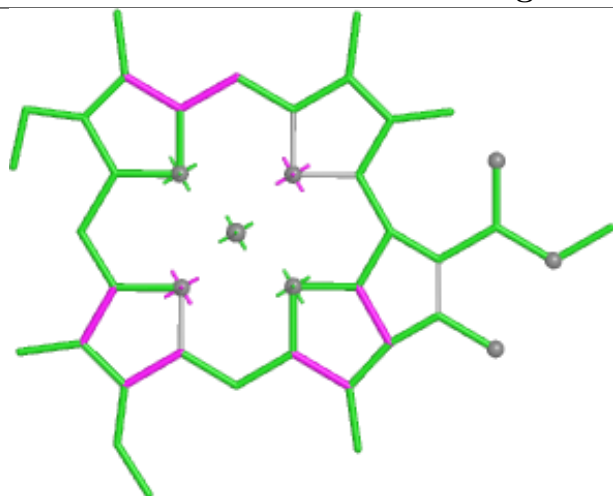


Ligand XAT 6 316

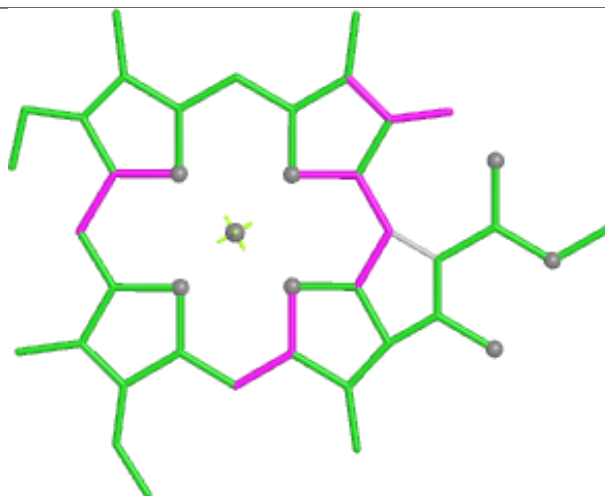




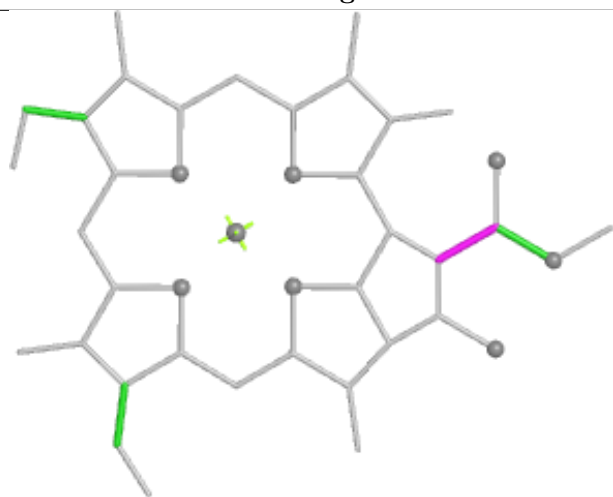
Ligand CLA F 304



Bond lengths



Bond angles

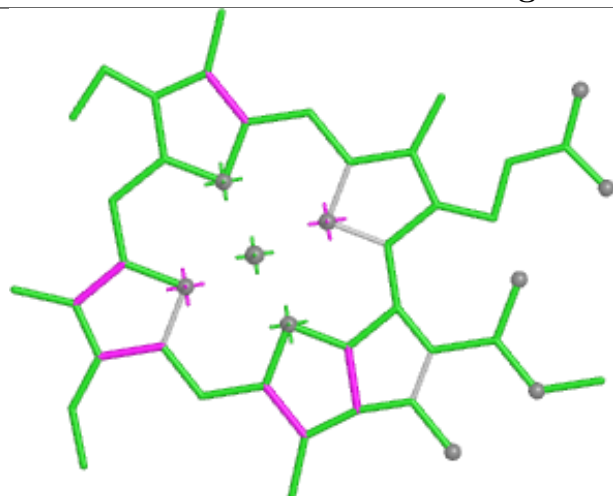


Torsions

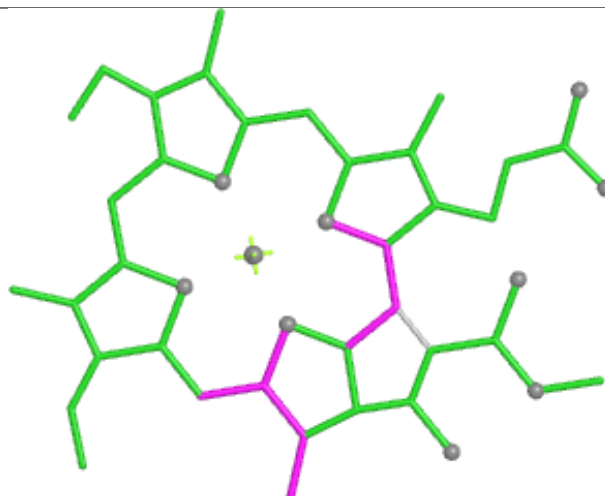


Rings

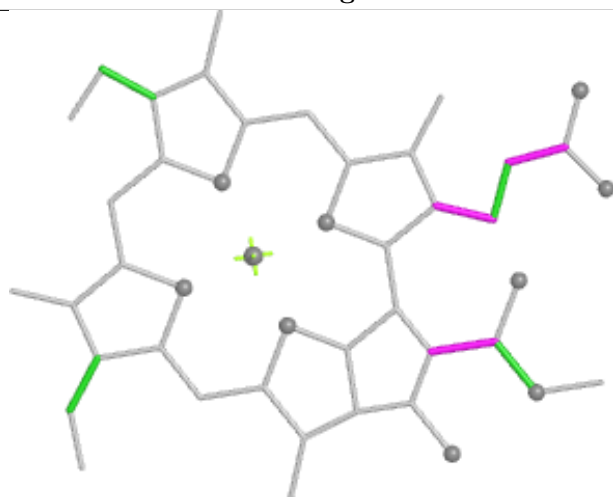
Ligand CLA 2 303



Bond lengths



Bond angles

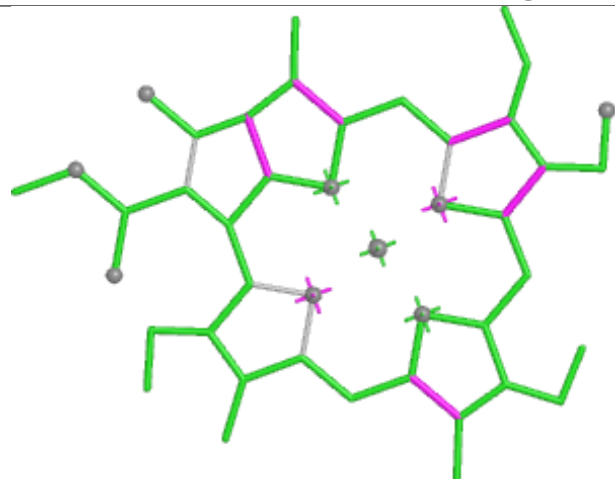


Torsions

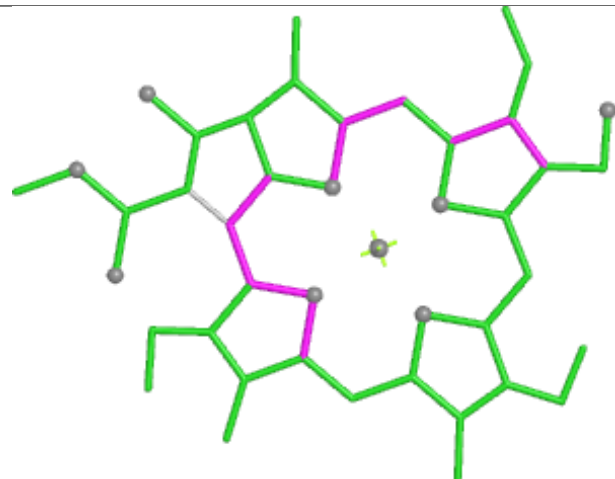


Rings

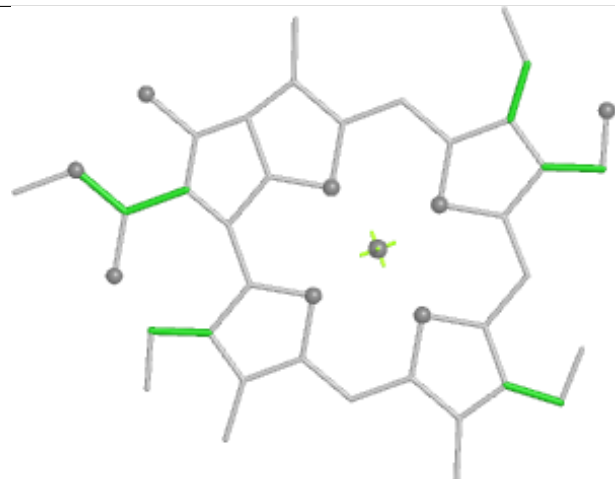
Ligand CHL 5 305



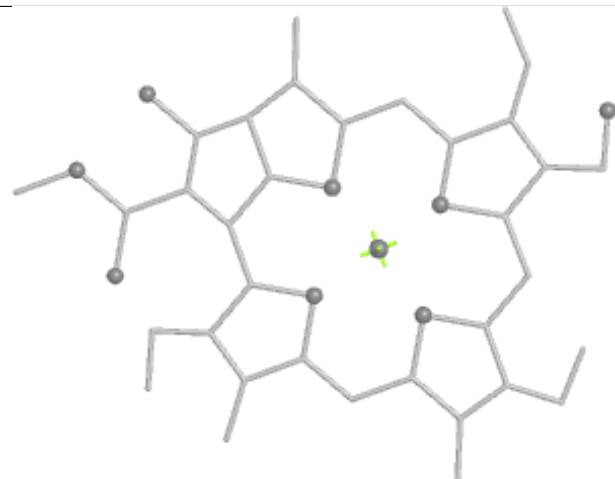
Bond lengths



Bond angles

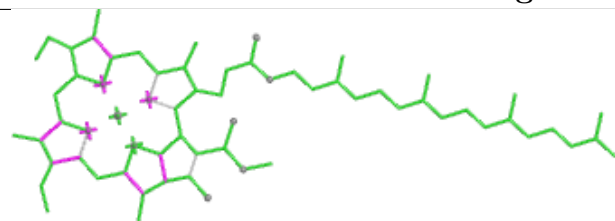


Torsions

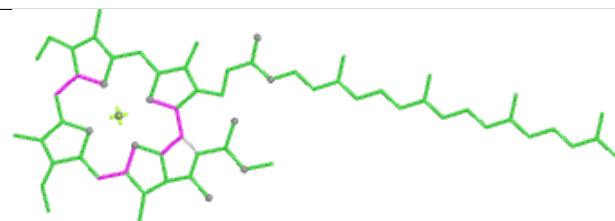


Rings

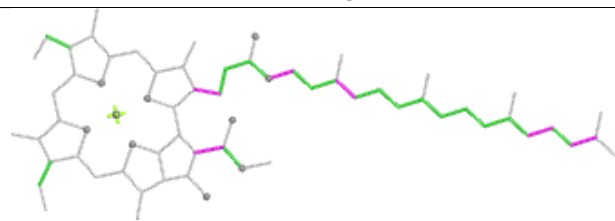
Ligand CLA A 812



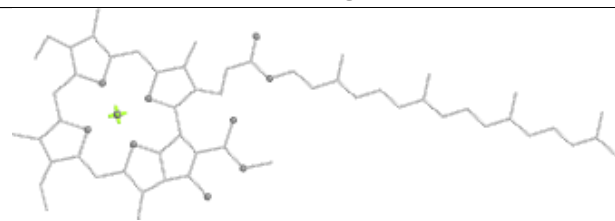
Bond lengths



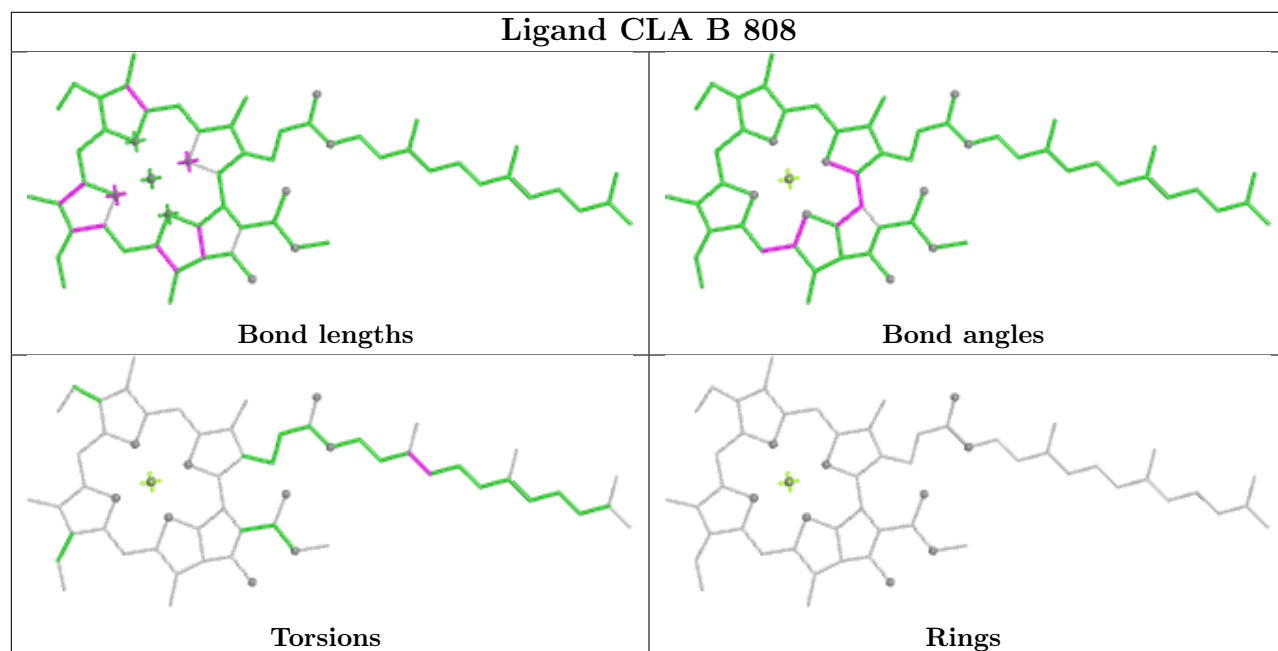
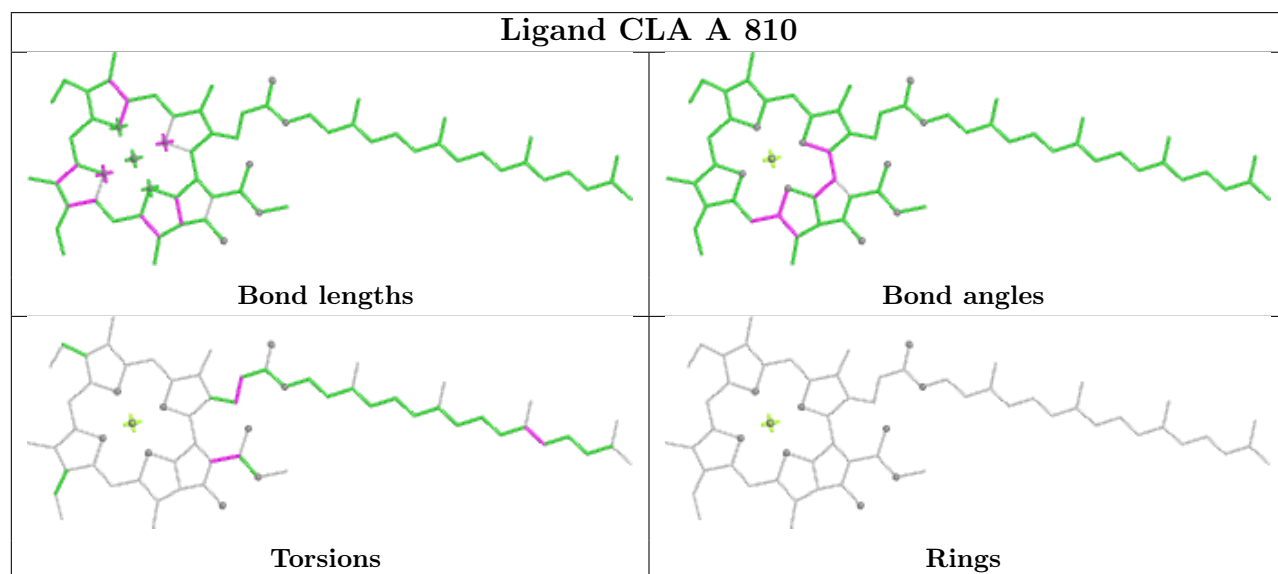
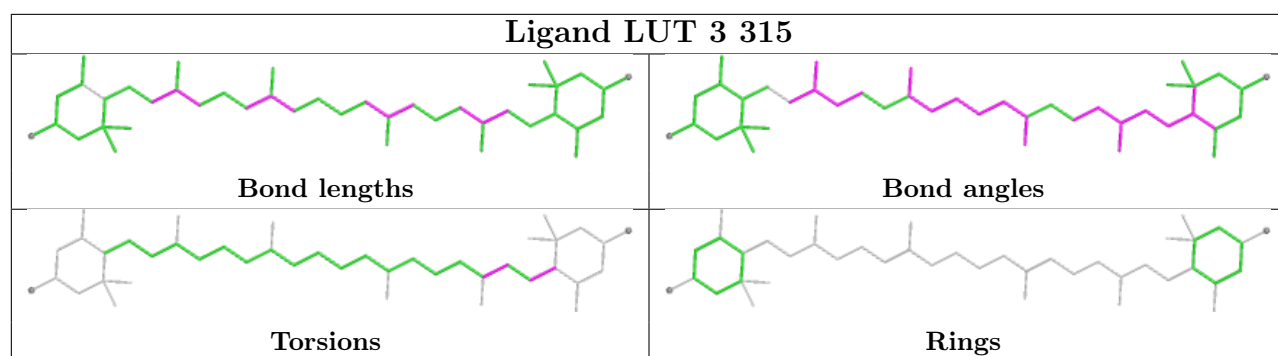
Bond angles



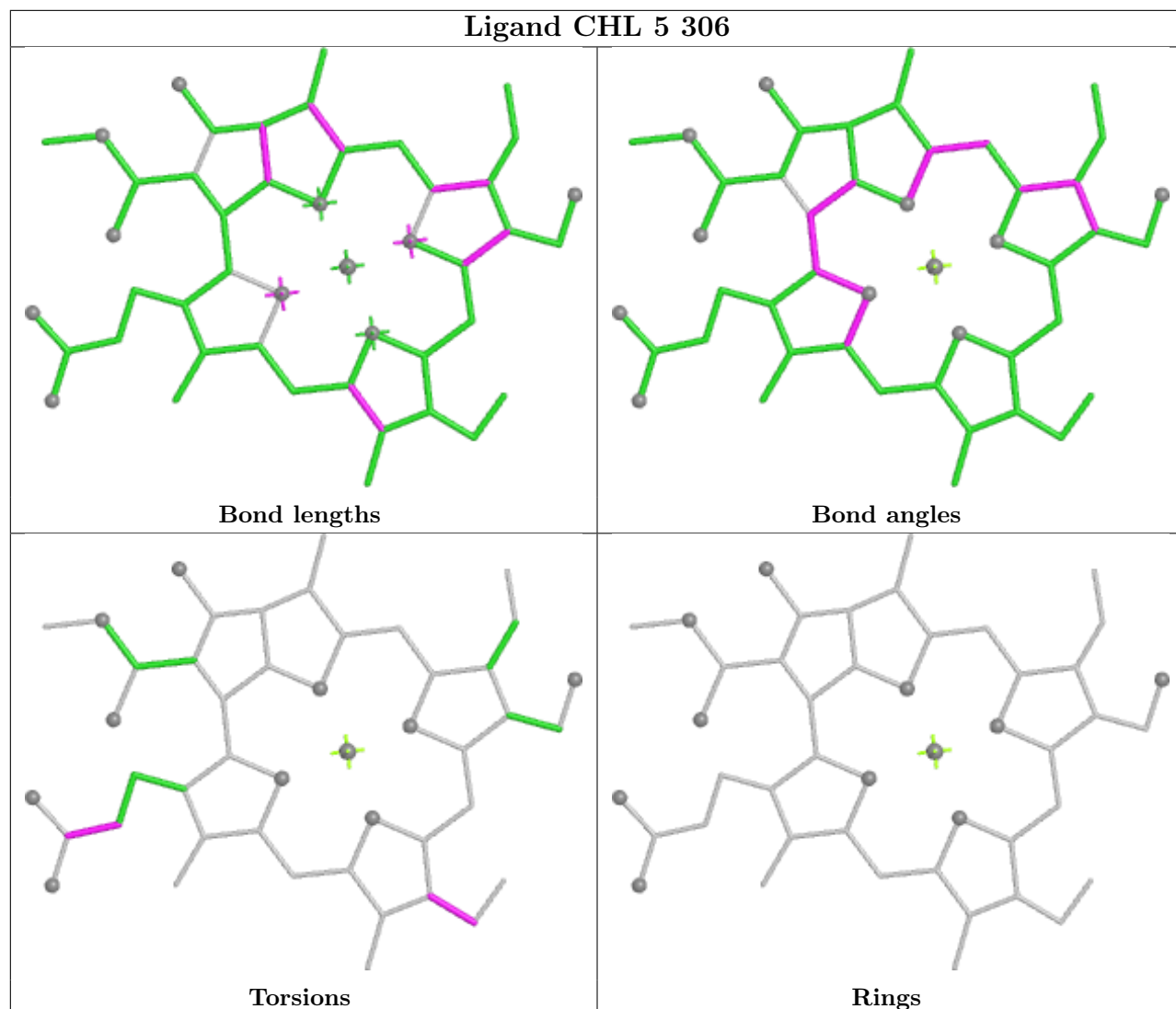
Torsions



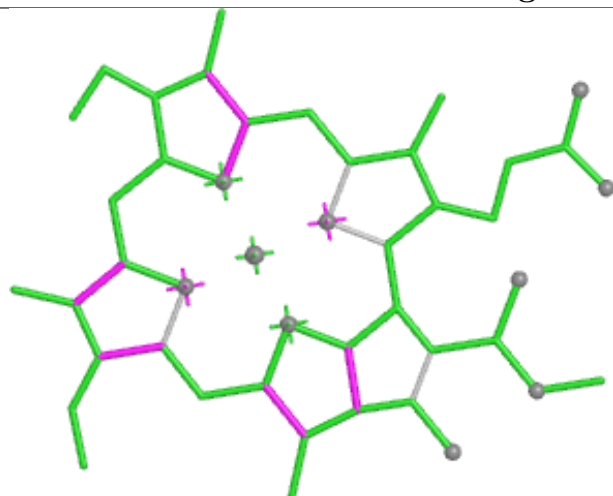
Rings



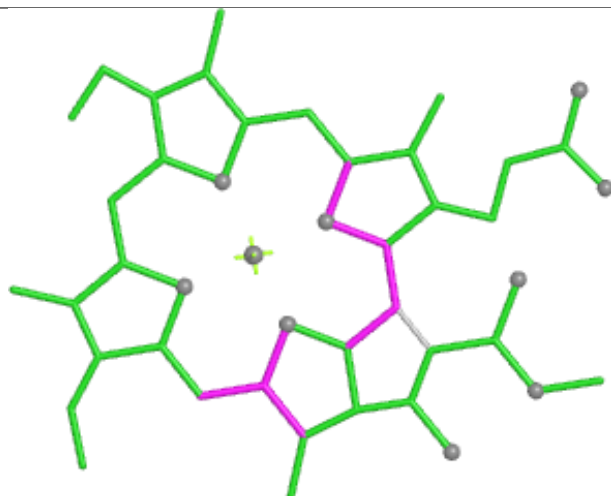
Ligand CHL 5 306



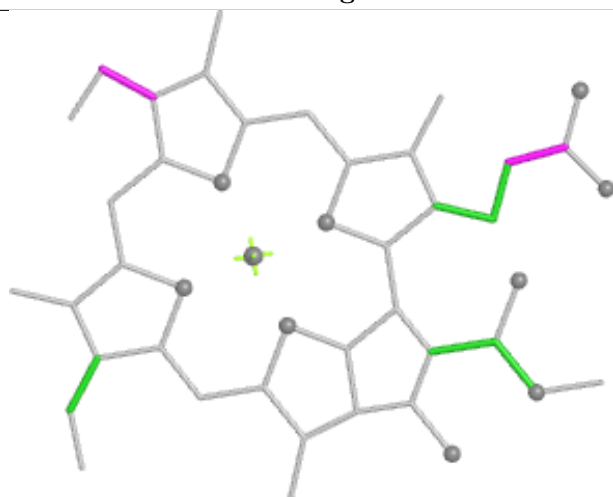
Ligand CLA 3 304



Bond lengths



Bond angles

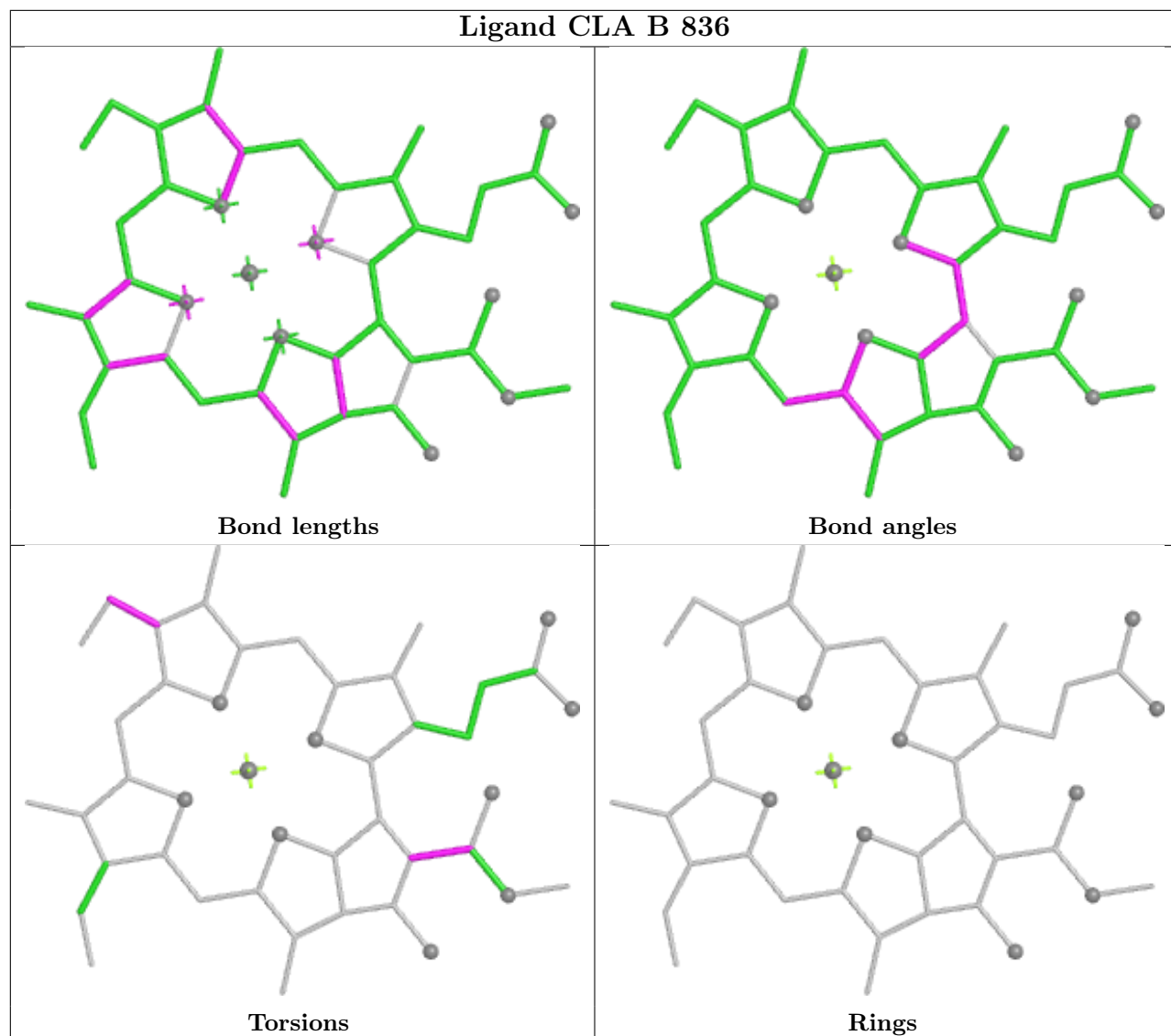


Torsions

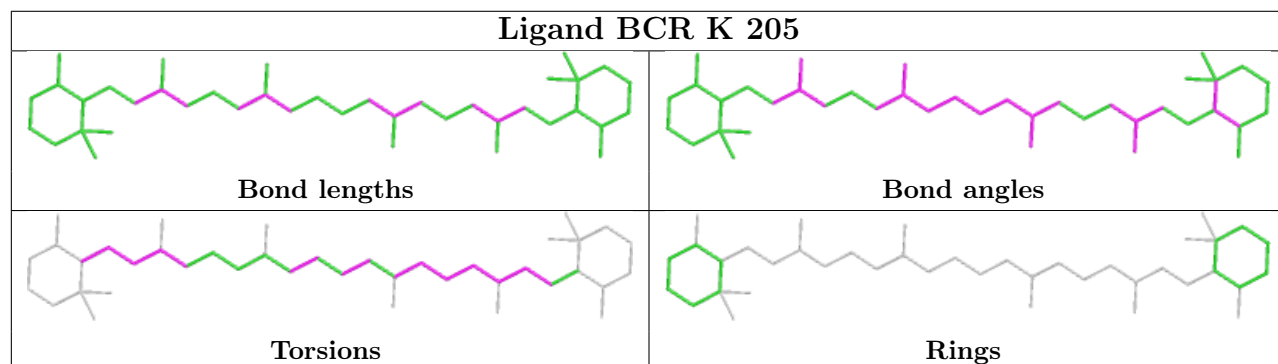


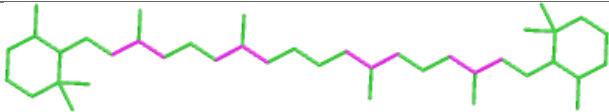
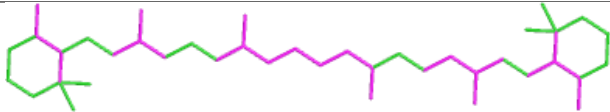
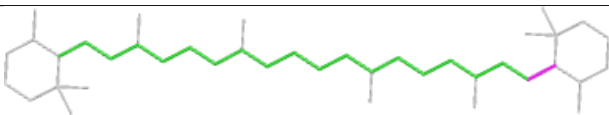
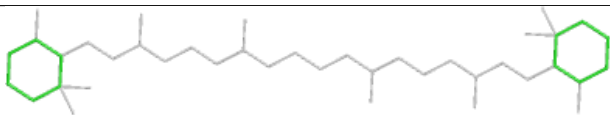
Rings

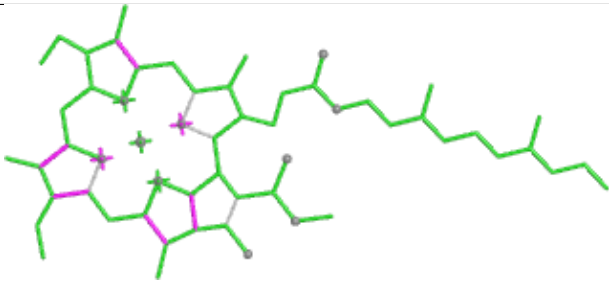
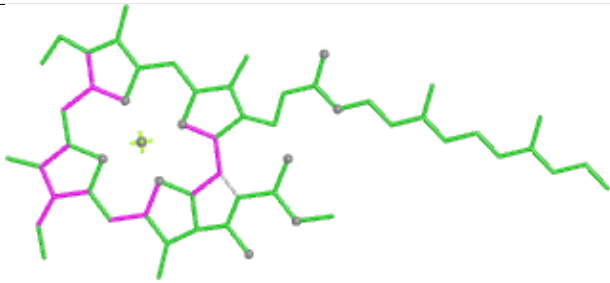
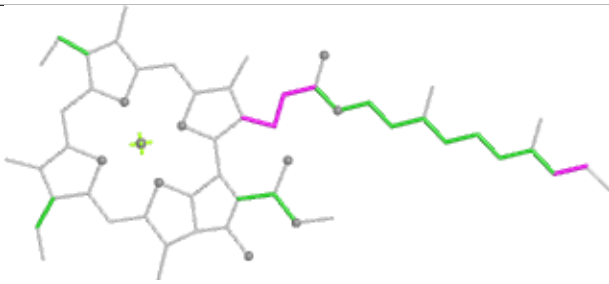
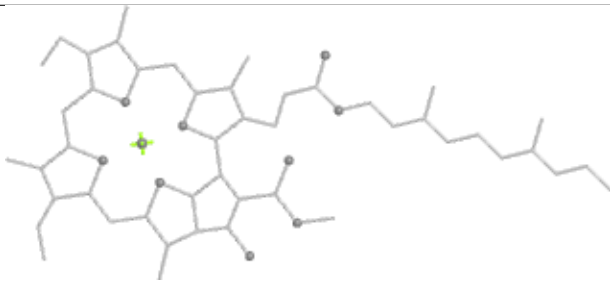
Ligand CLA B 836

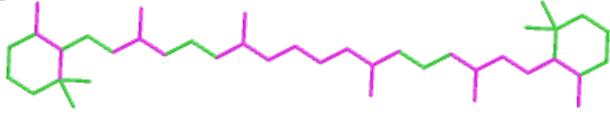
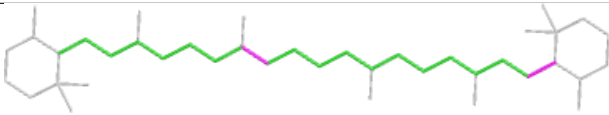
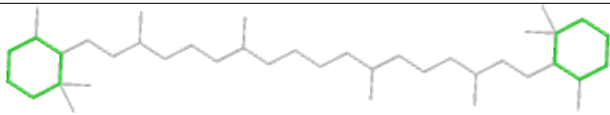


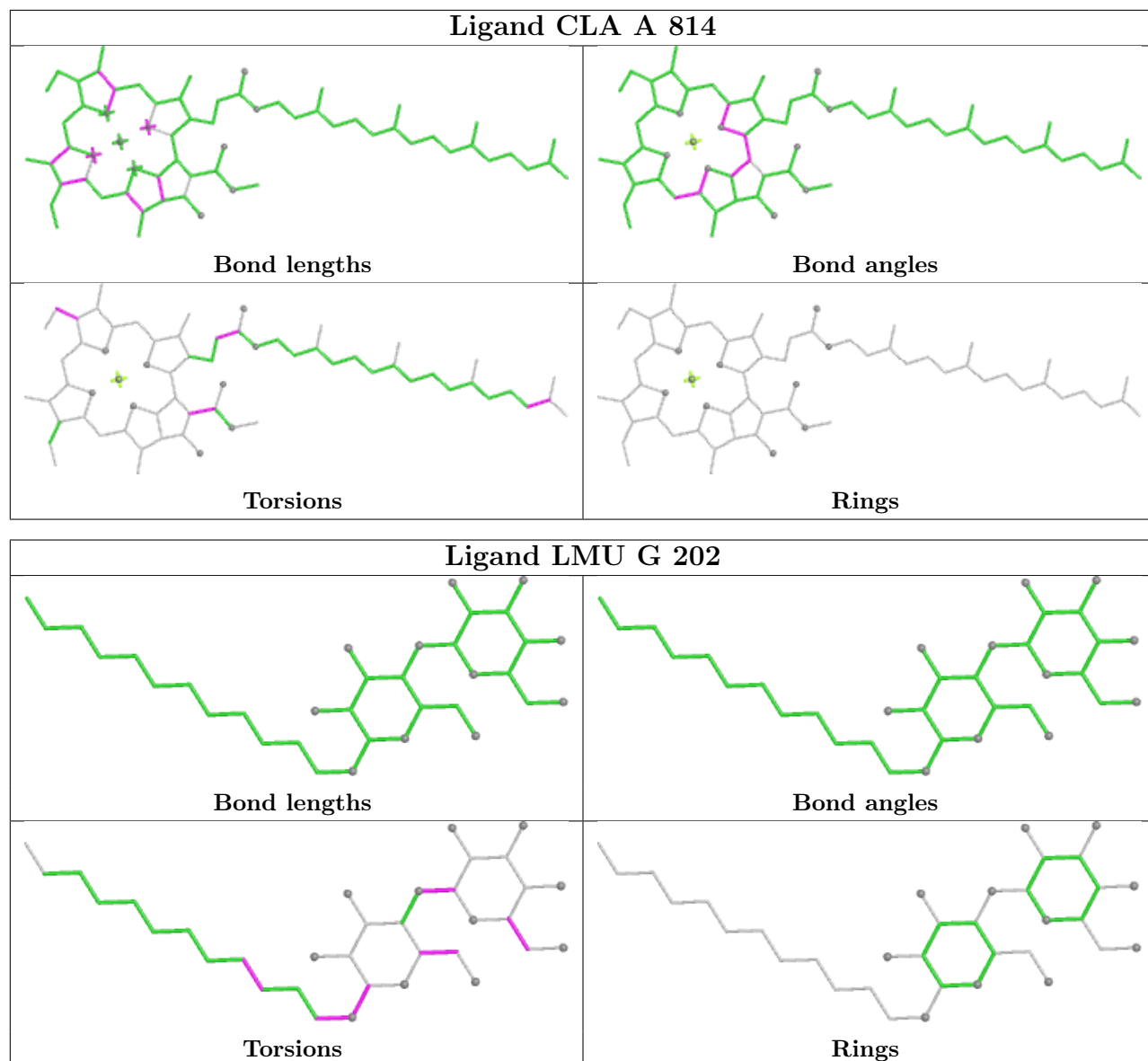
Ligand BCR K 205



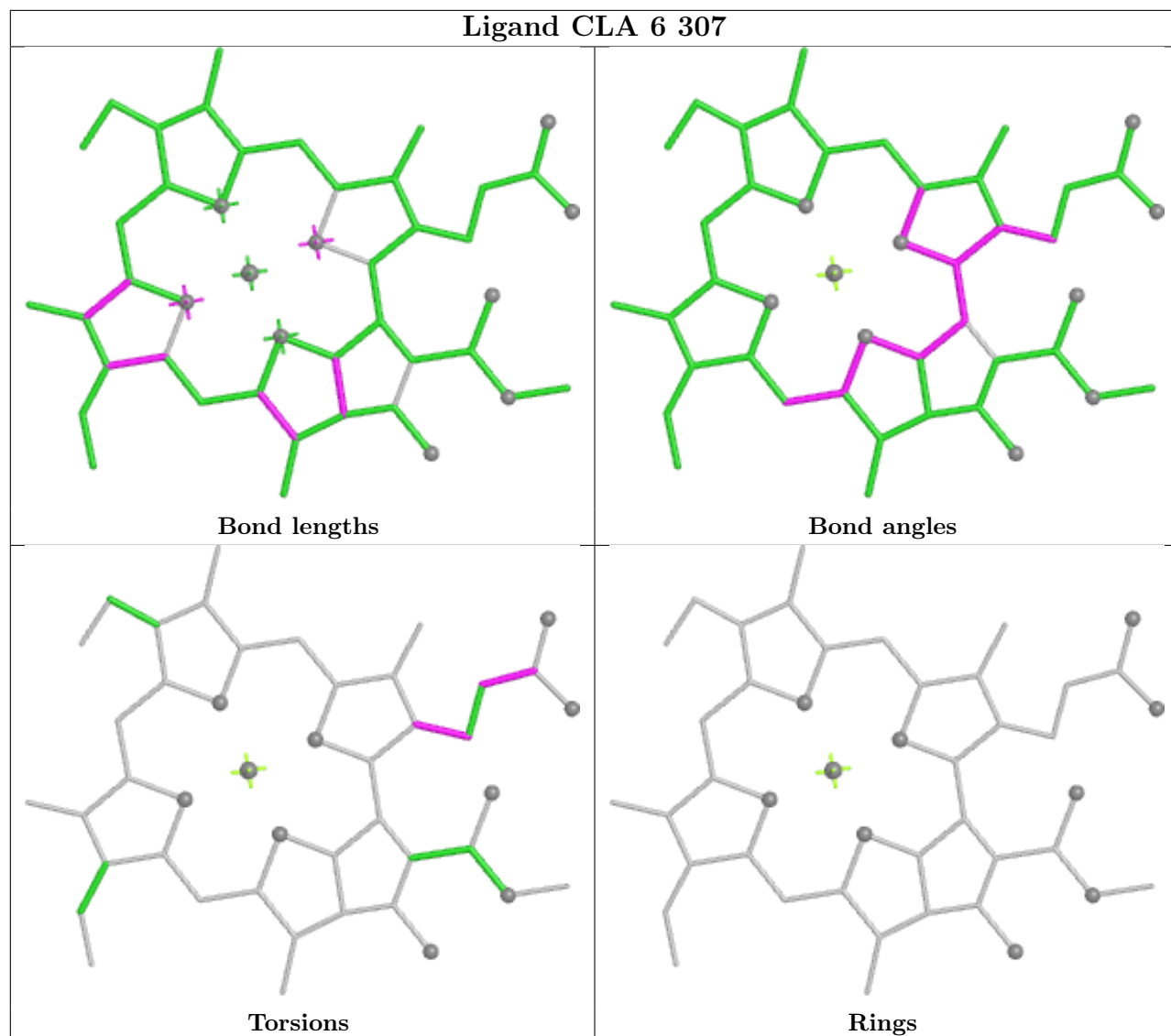
Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

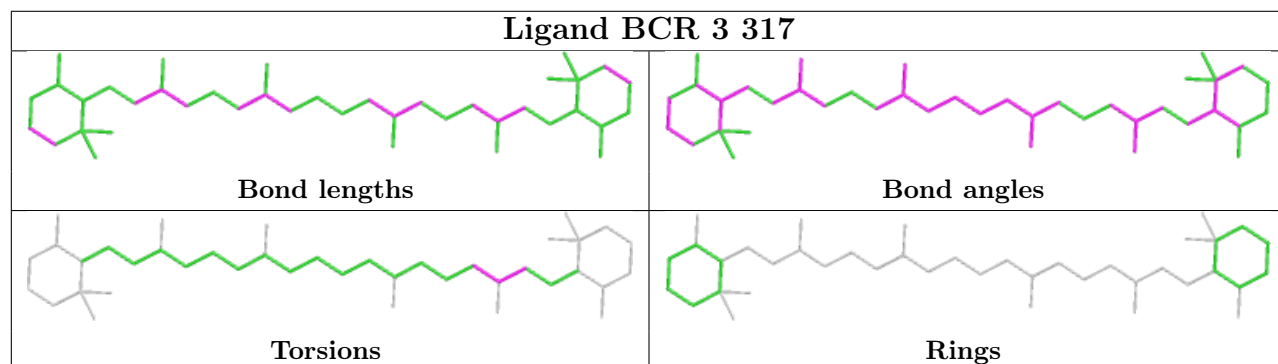
Ligand BCR F 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

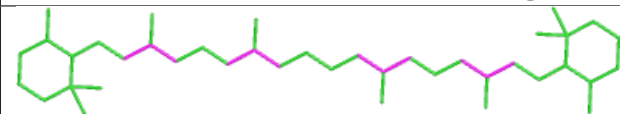
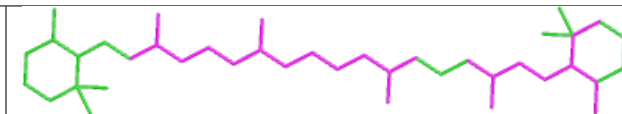
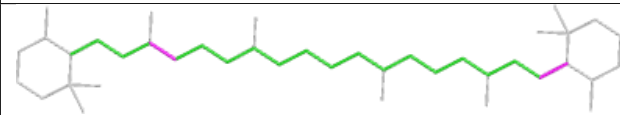
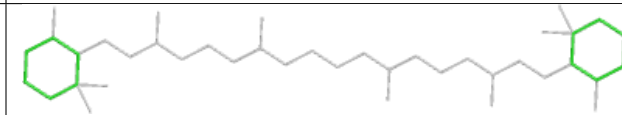


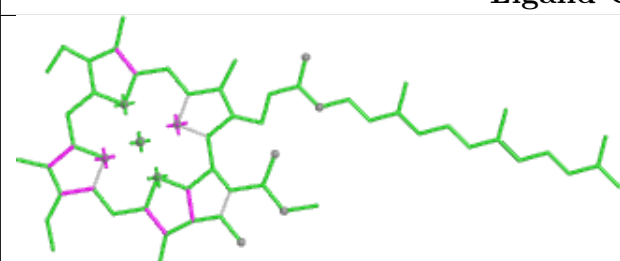
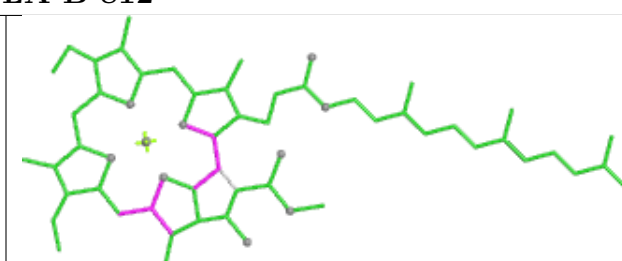
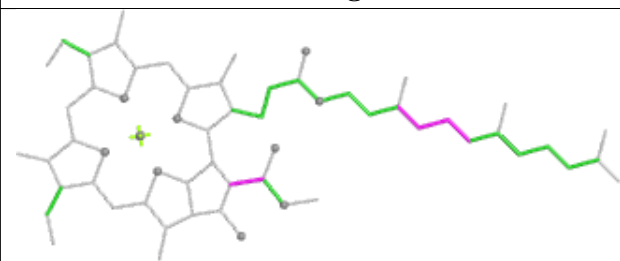
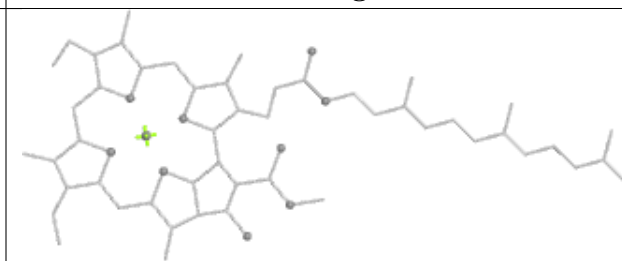
Ligand CLA 6 307

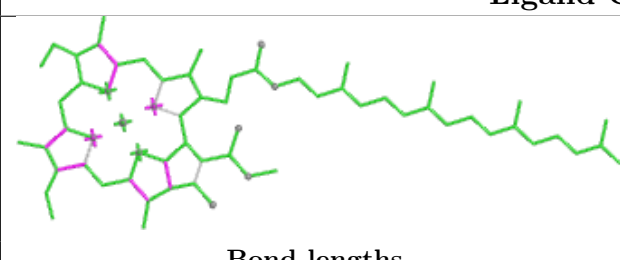
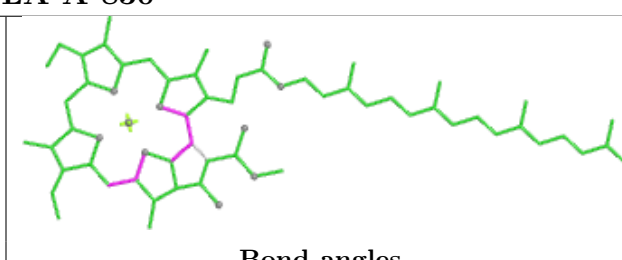
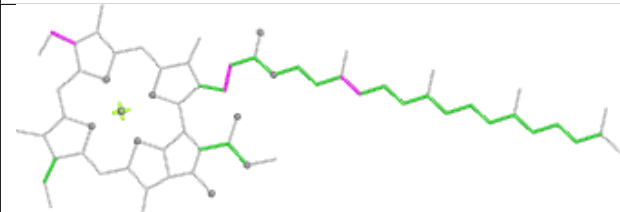
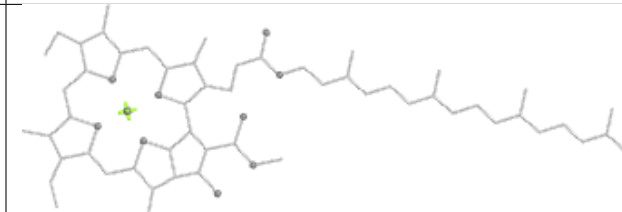


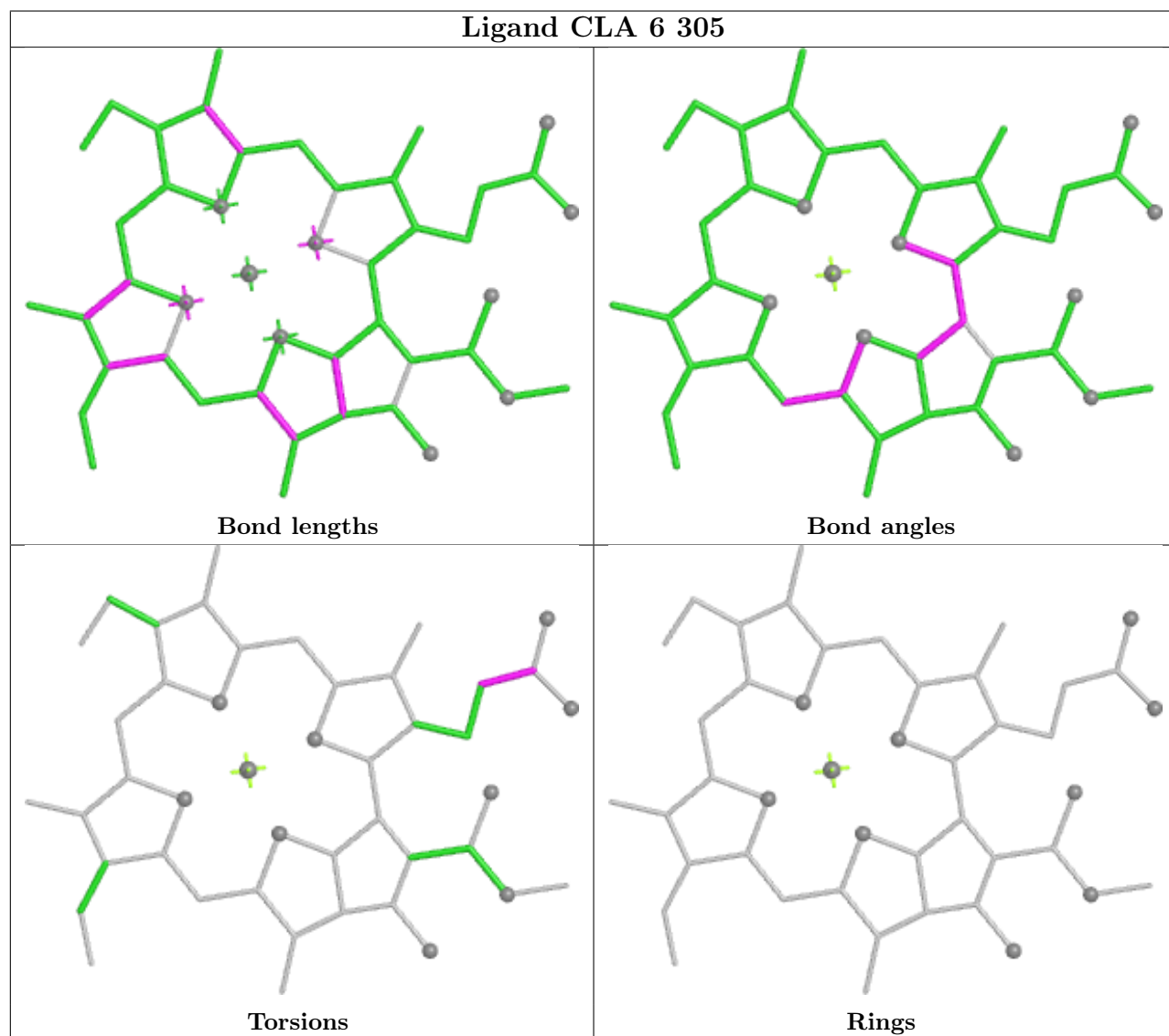
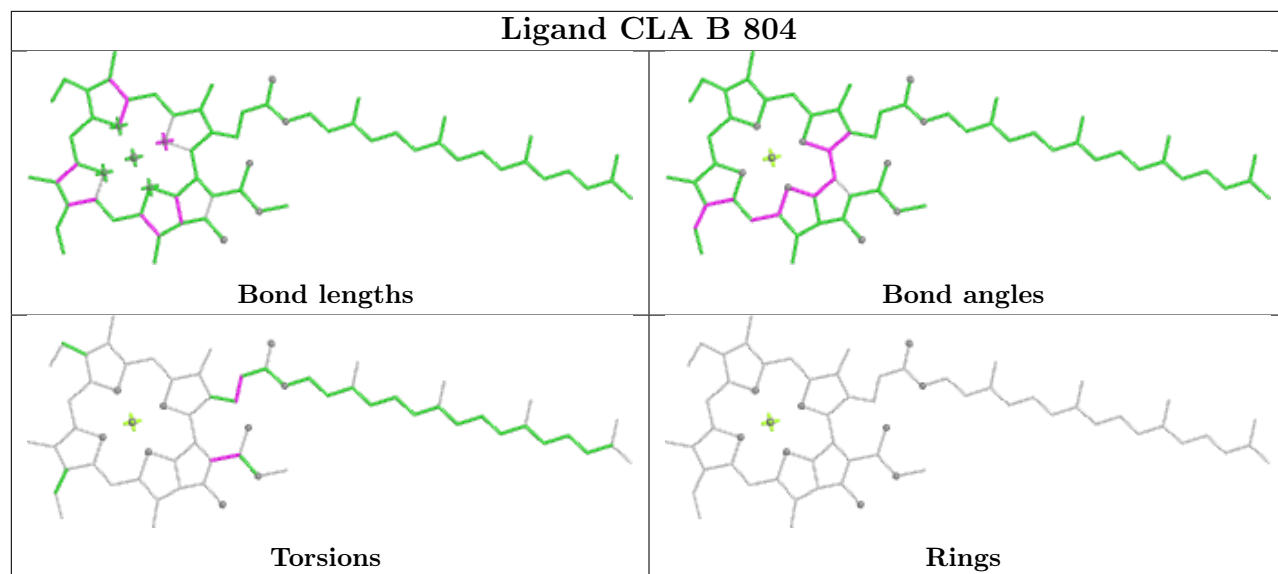
Ligand BCR 3 317

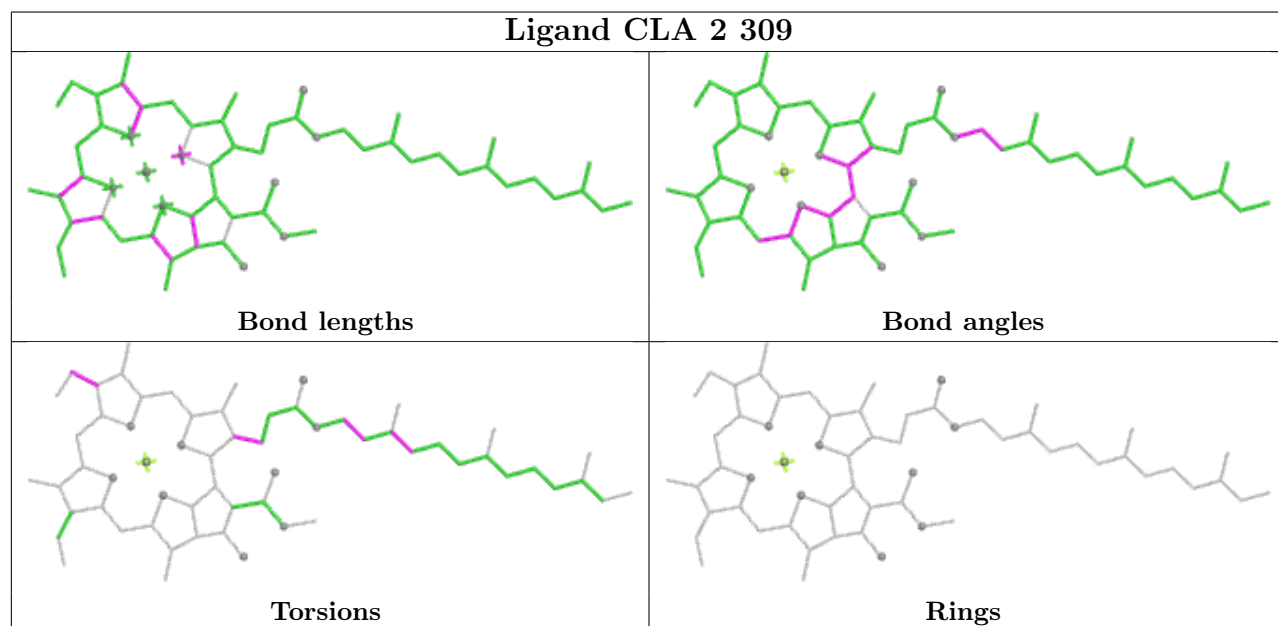
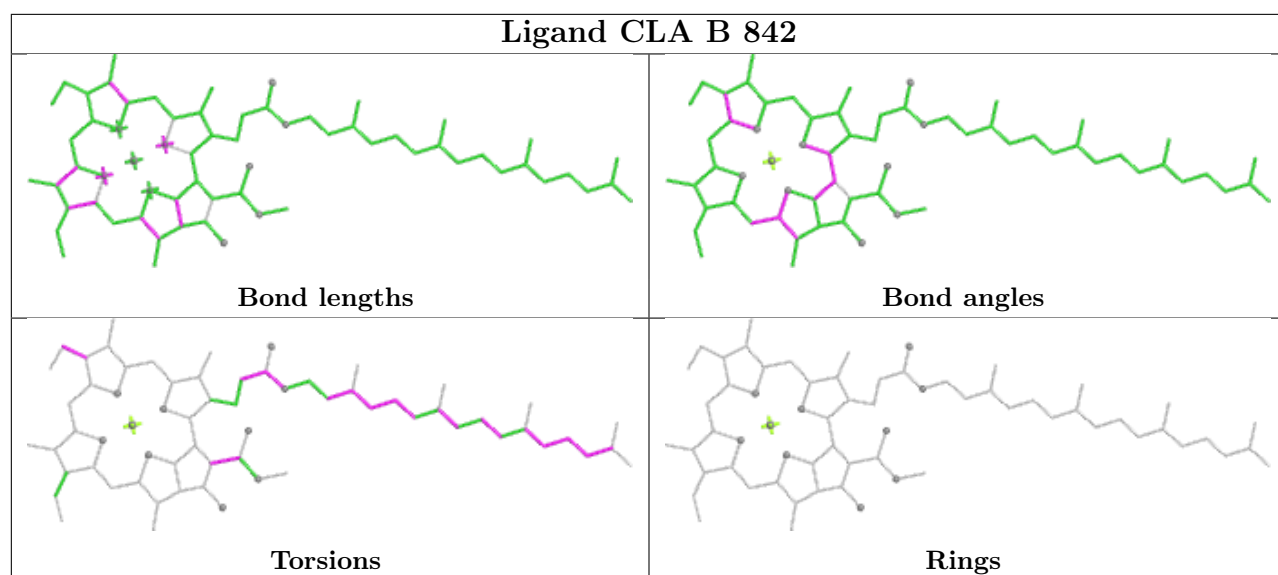


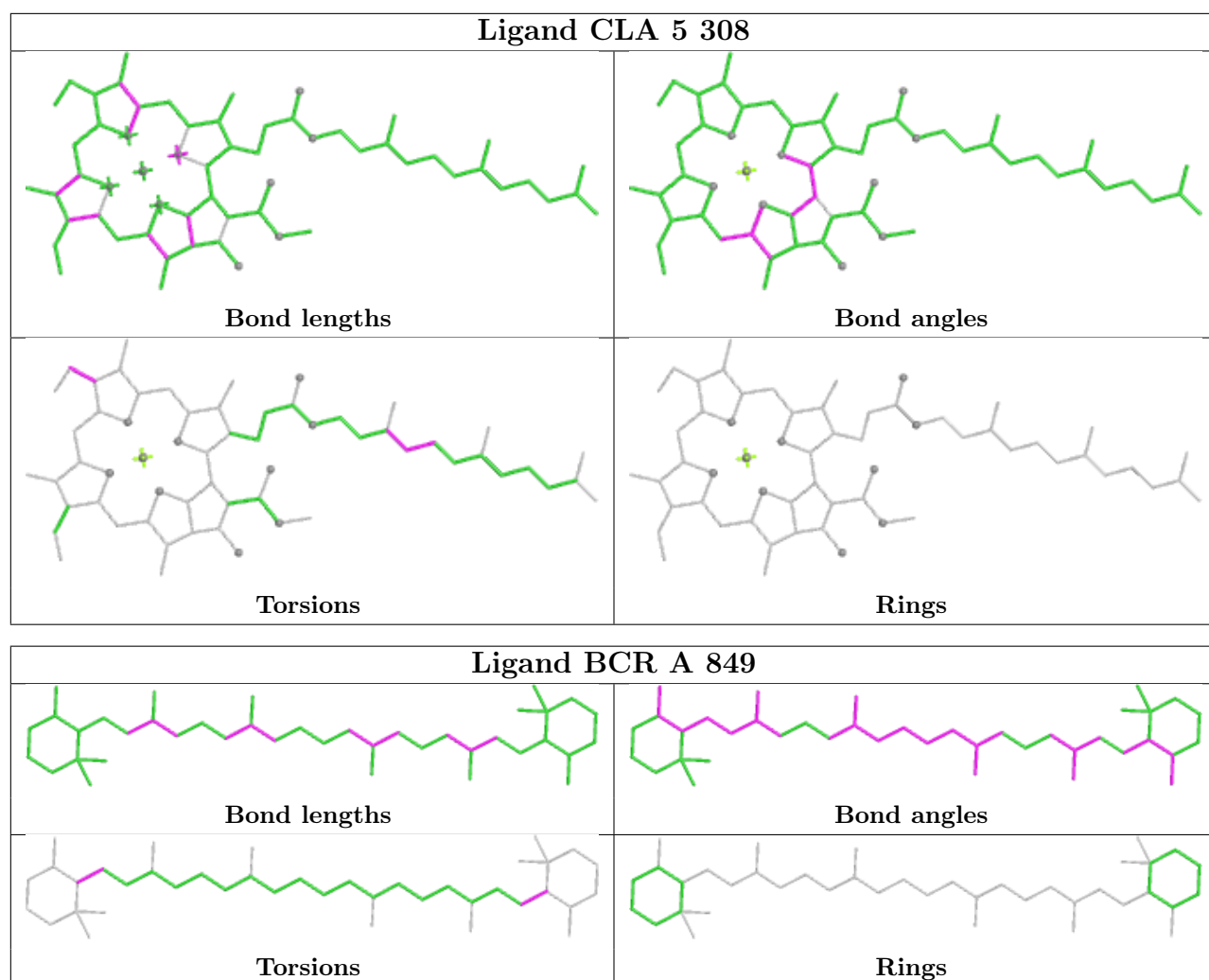
Ligand BCR L 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 812	
	
Bond lengths	Bond angles
	
Torsions	Rings

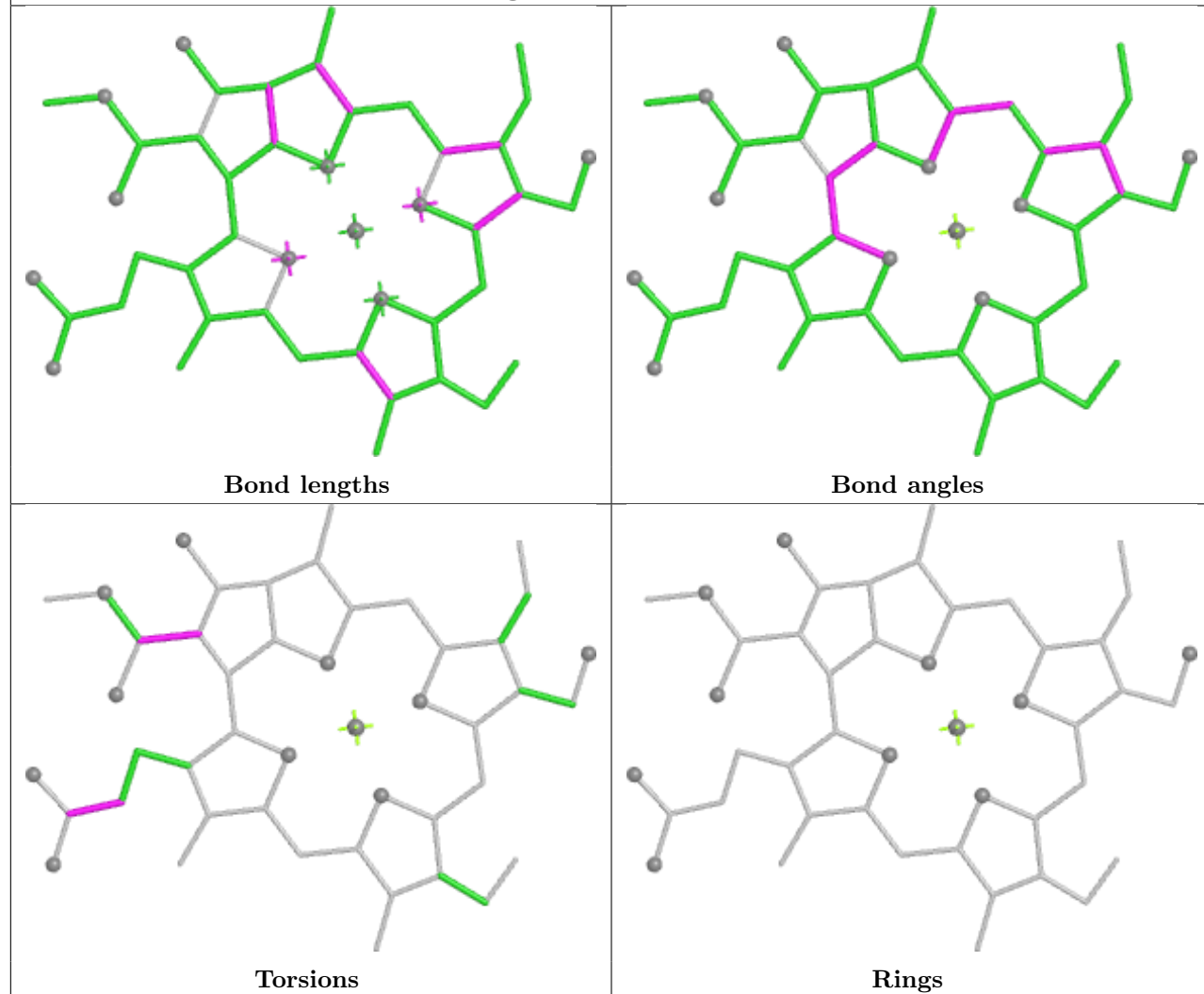
Ligand CLA A 830	
	
Bond lengths	Bond angles
	
Torsions	Rings



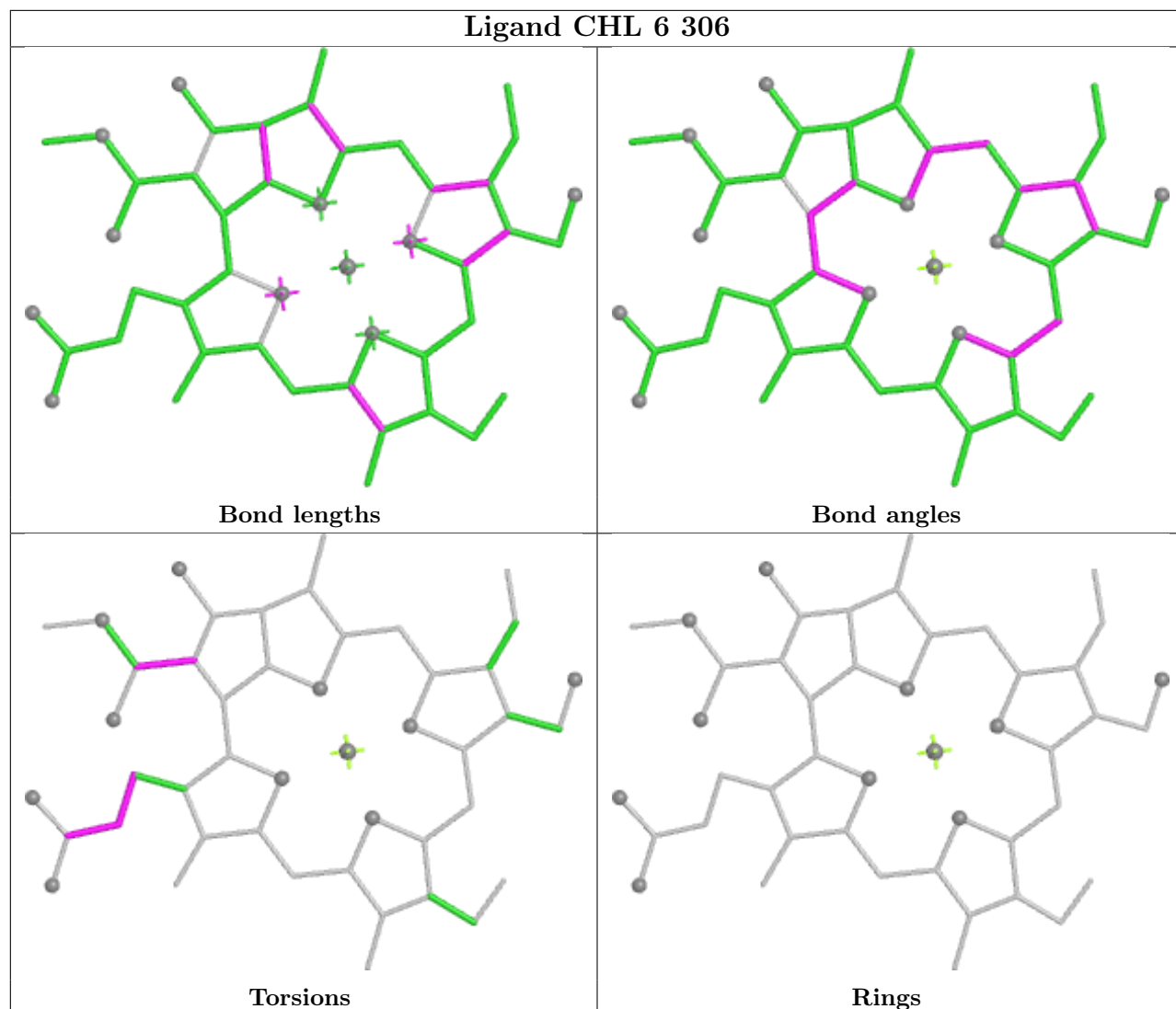


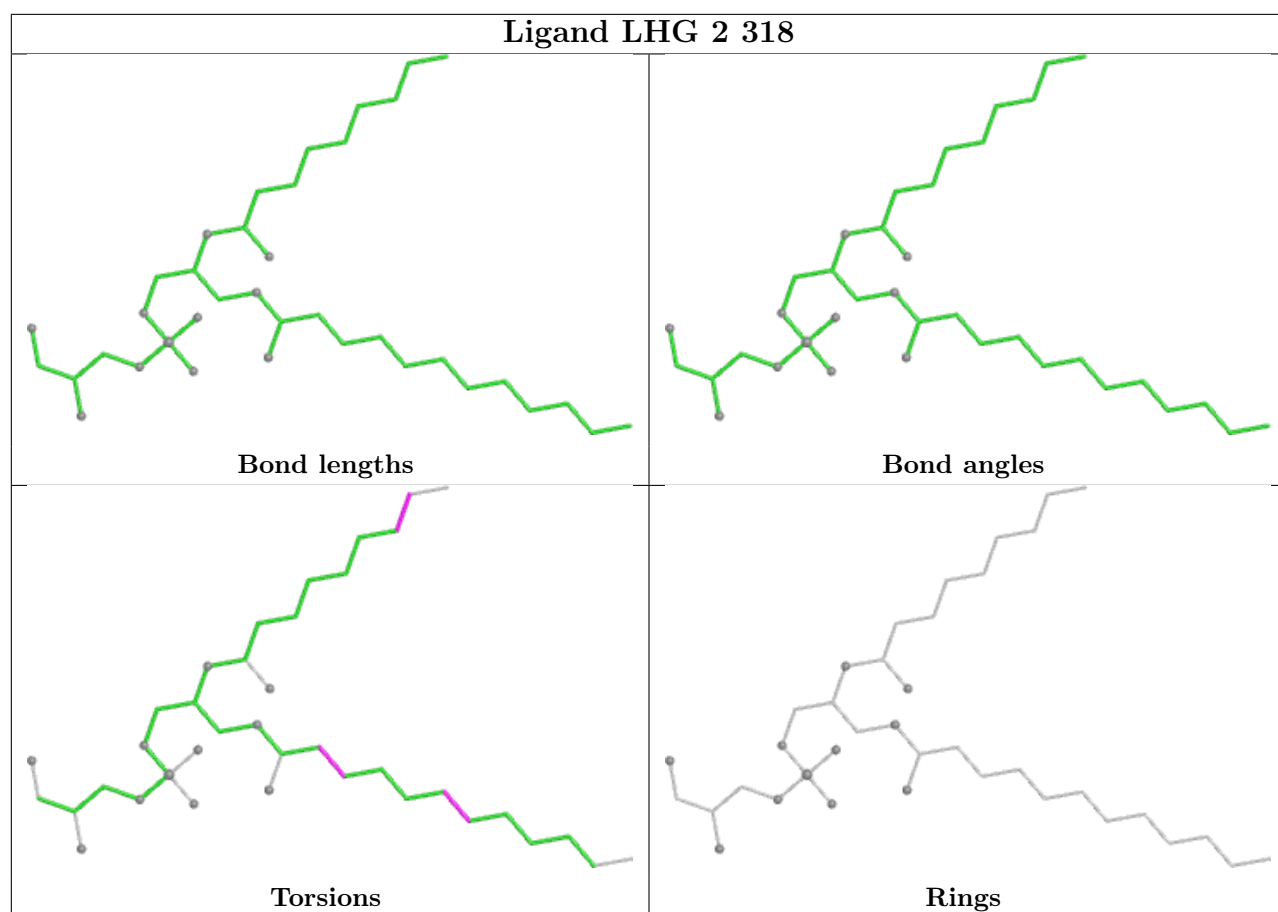


Ligand CHL 2 314

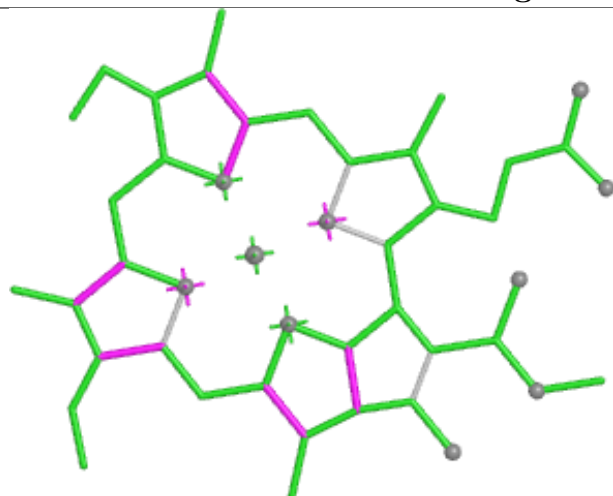


Ligand CHL 6 306

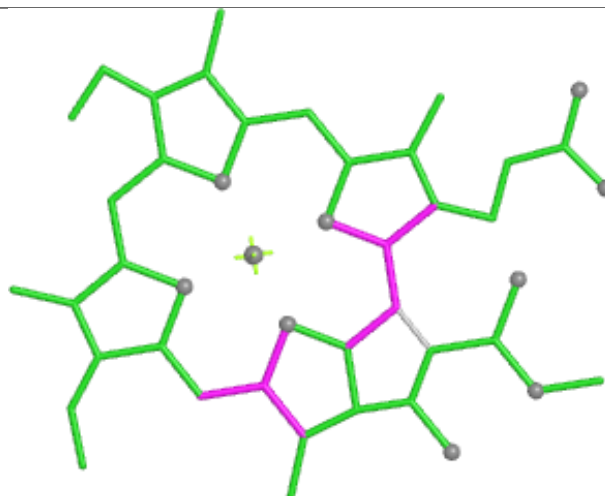




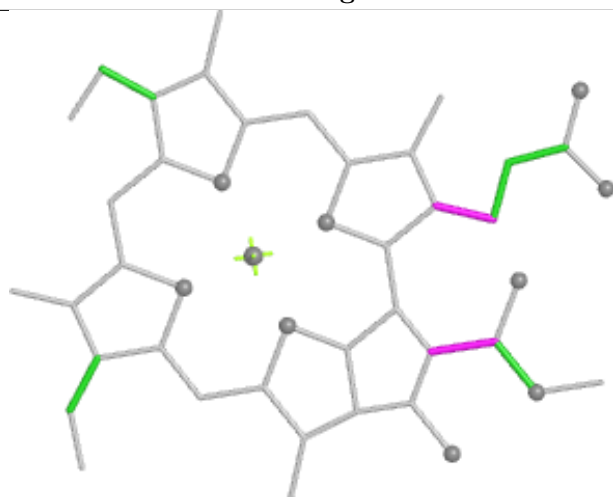
Ligand CLA B 824



Bond lengths



Bond angles

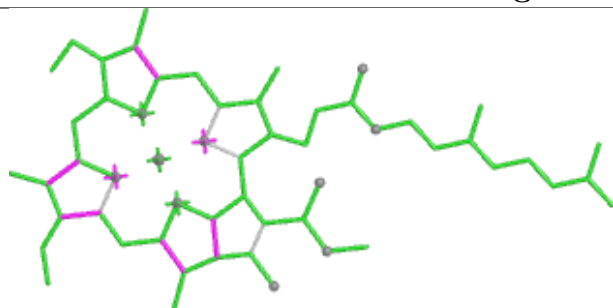


Torsions

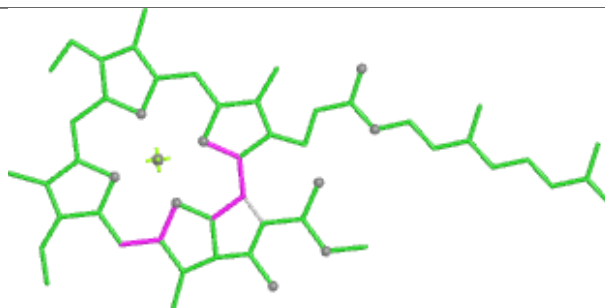


Rings

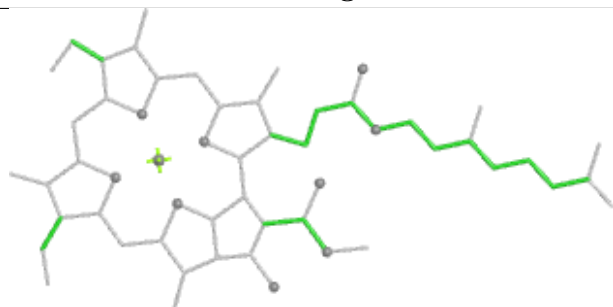
Ligand CLA A 839



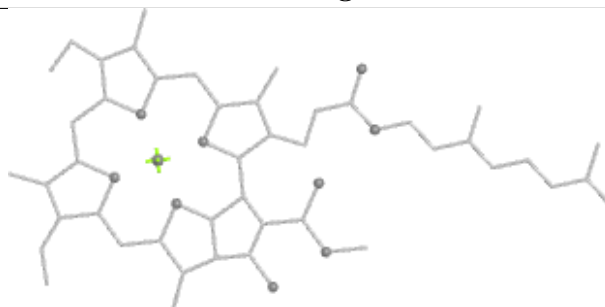
Bond lengths



Bond angles

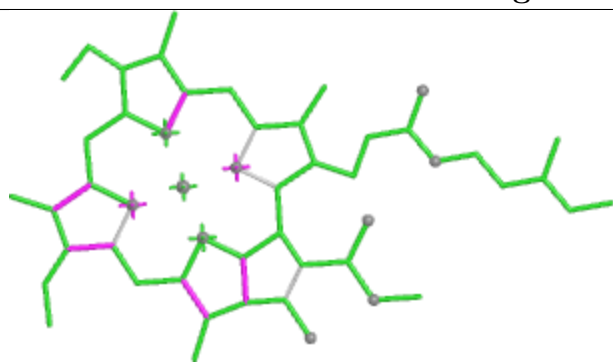


Torsions

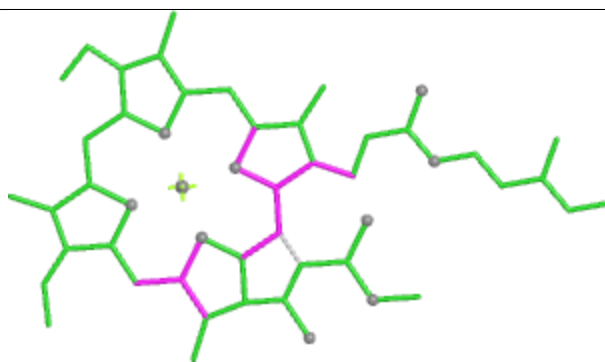


Rings

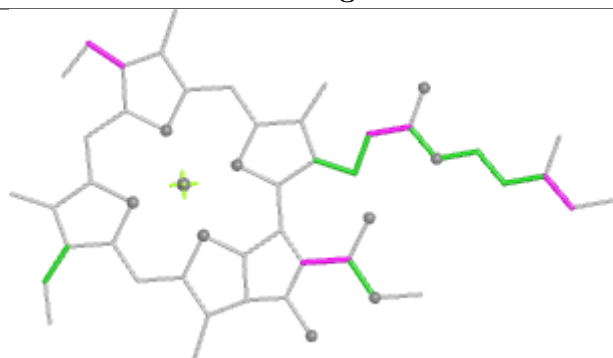
Ligand CLA K 201



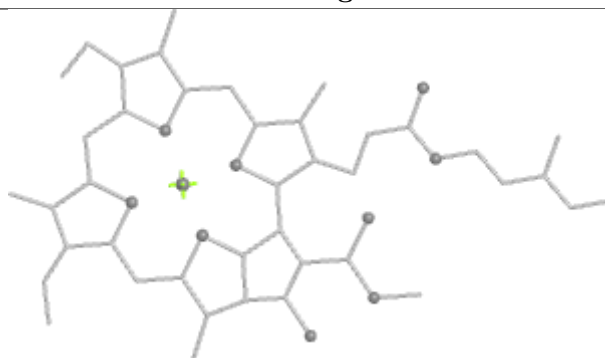
Bond lengths



Bond angles

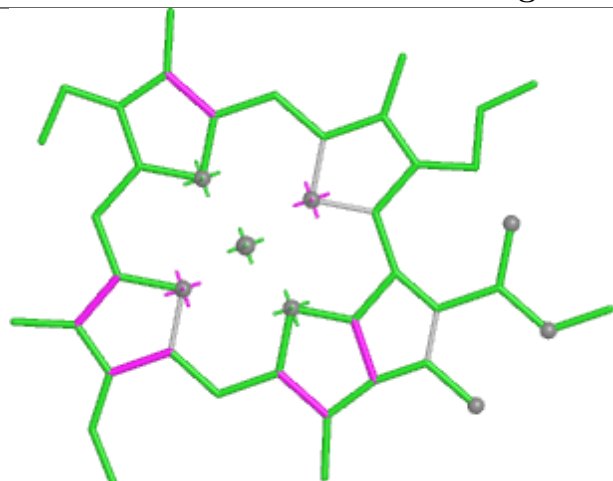


Torsions

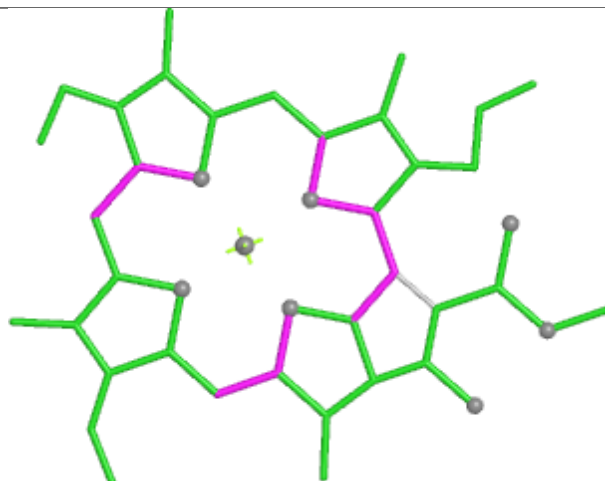


Rings

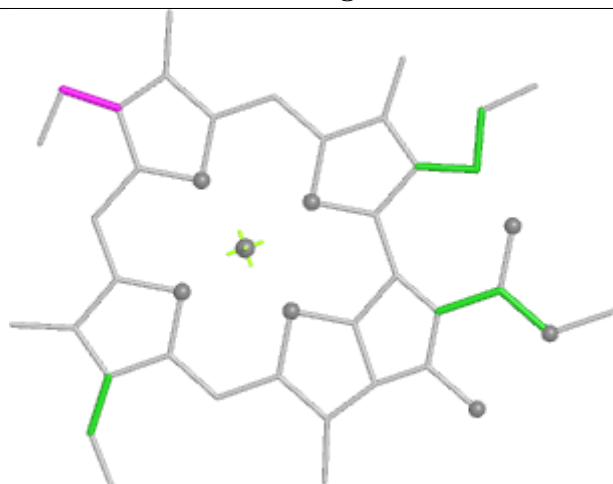
Ligand CLA 3 310



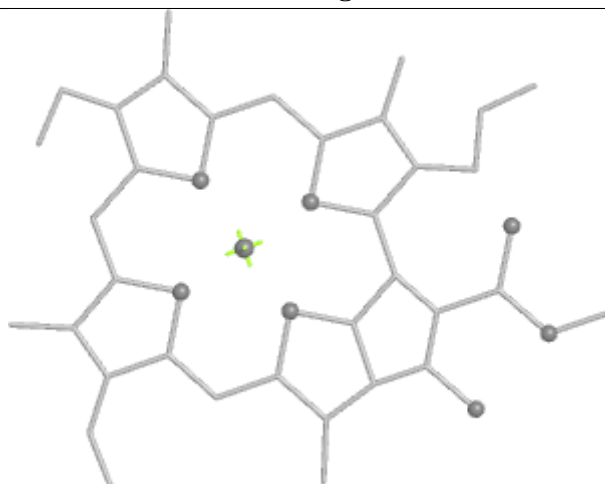
Bond lengths



Bond angles

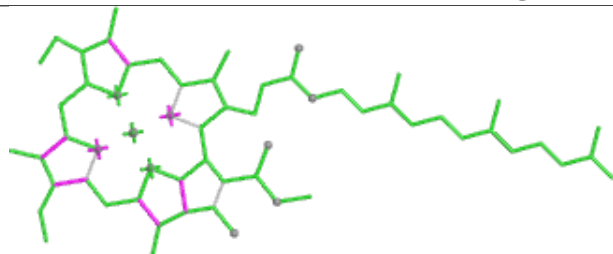


Torsions

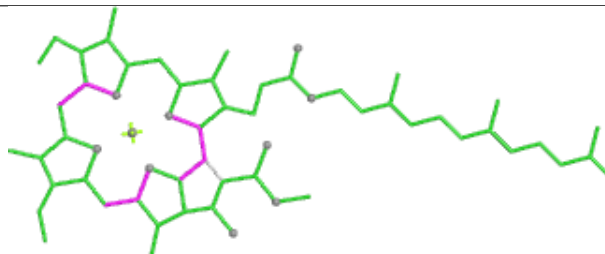


Rings

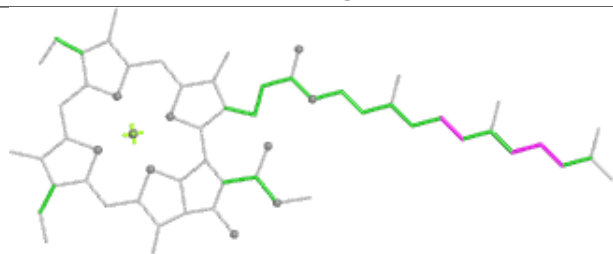
Ligand CLA A 836



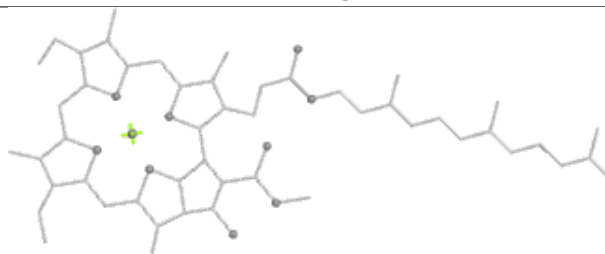
Bond lengths



Bond angles

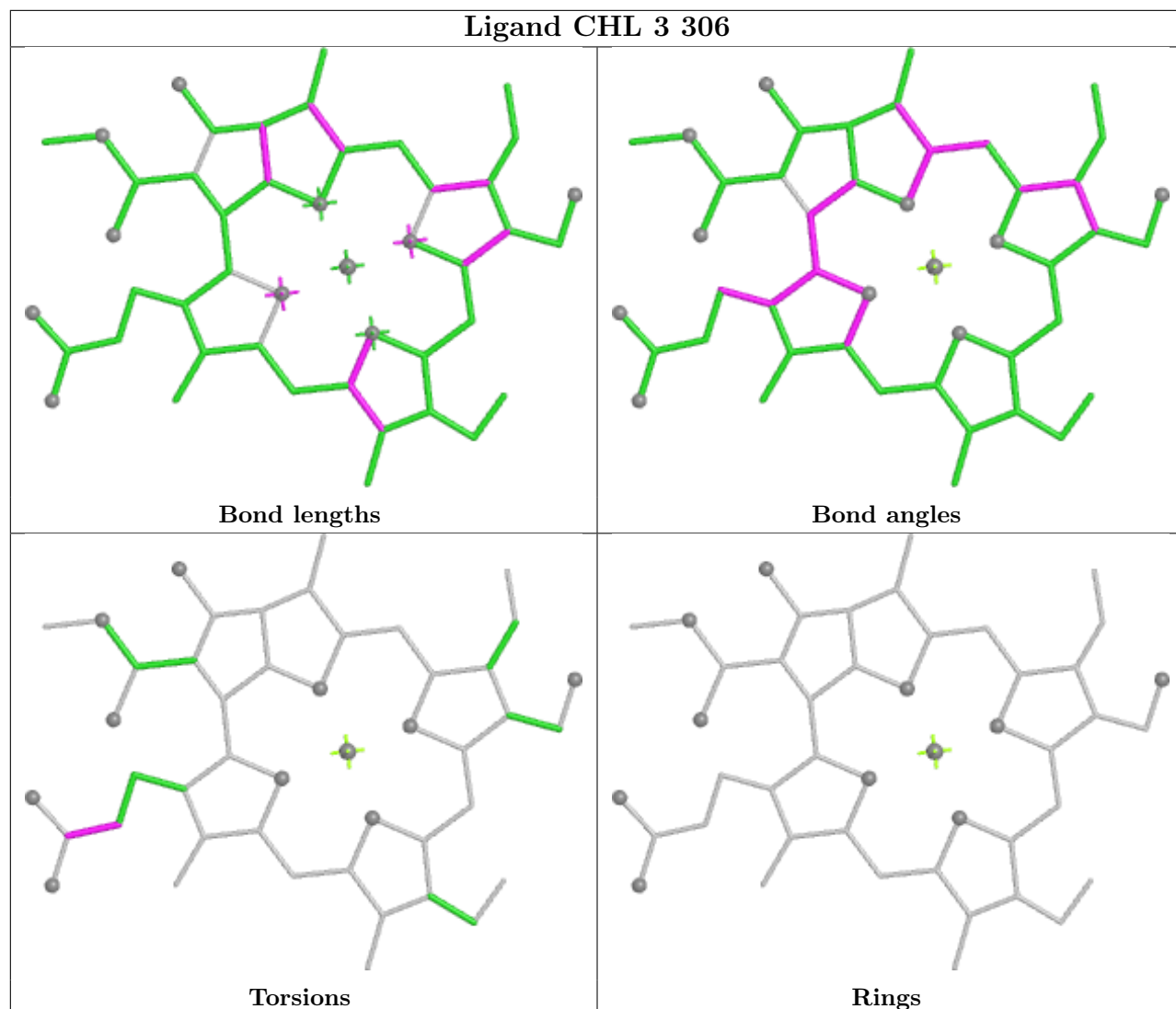


Torsions

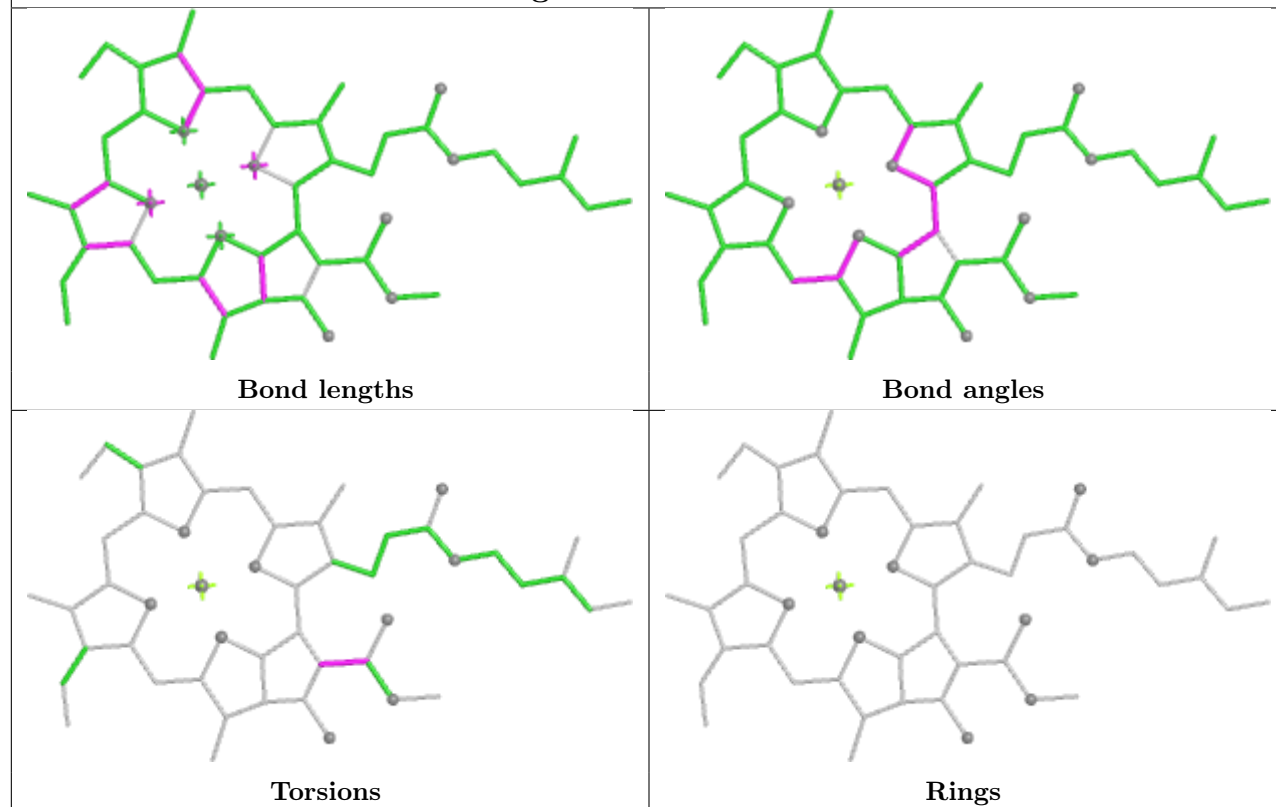


Rings

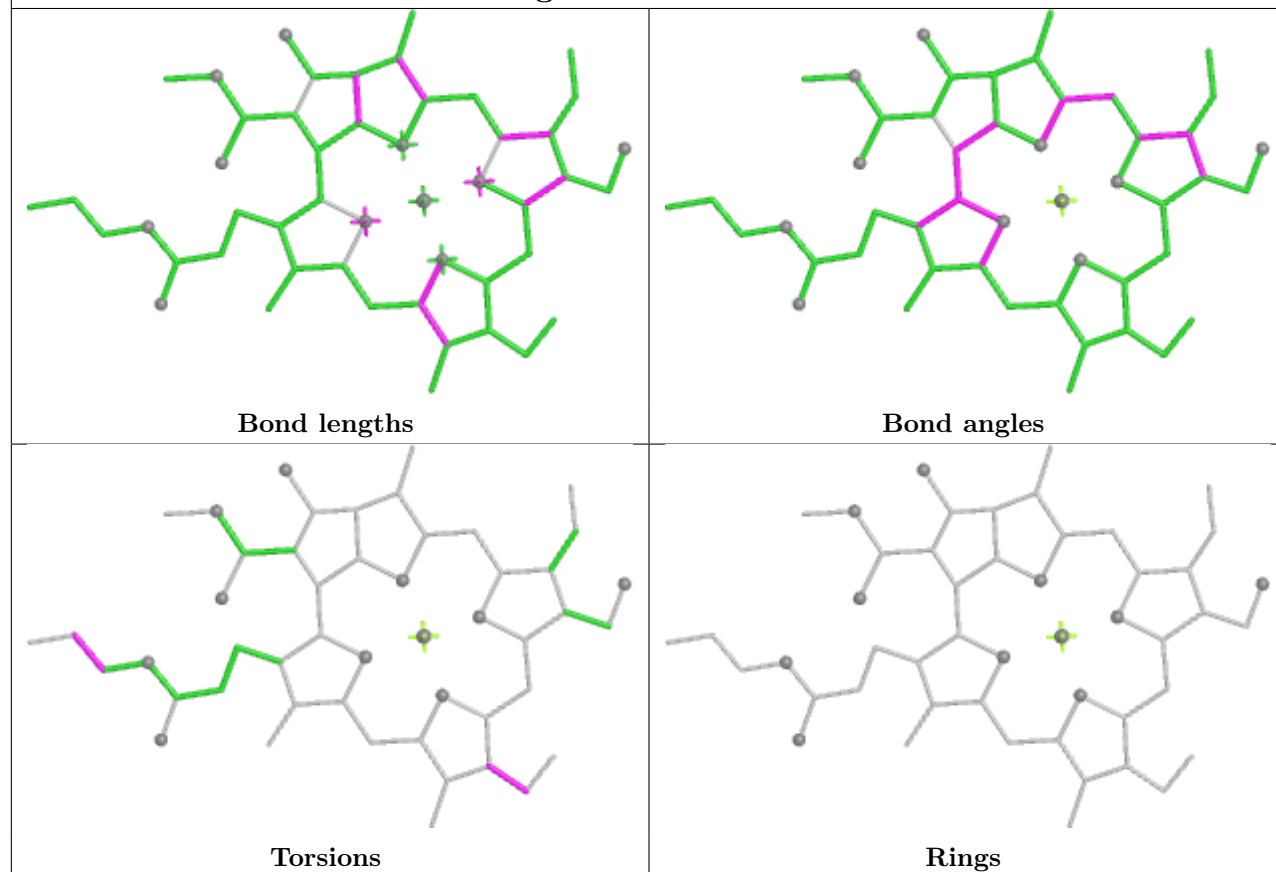
Ligand CHL 3 306

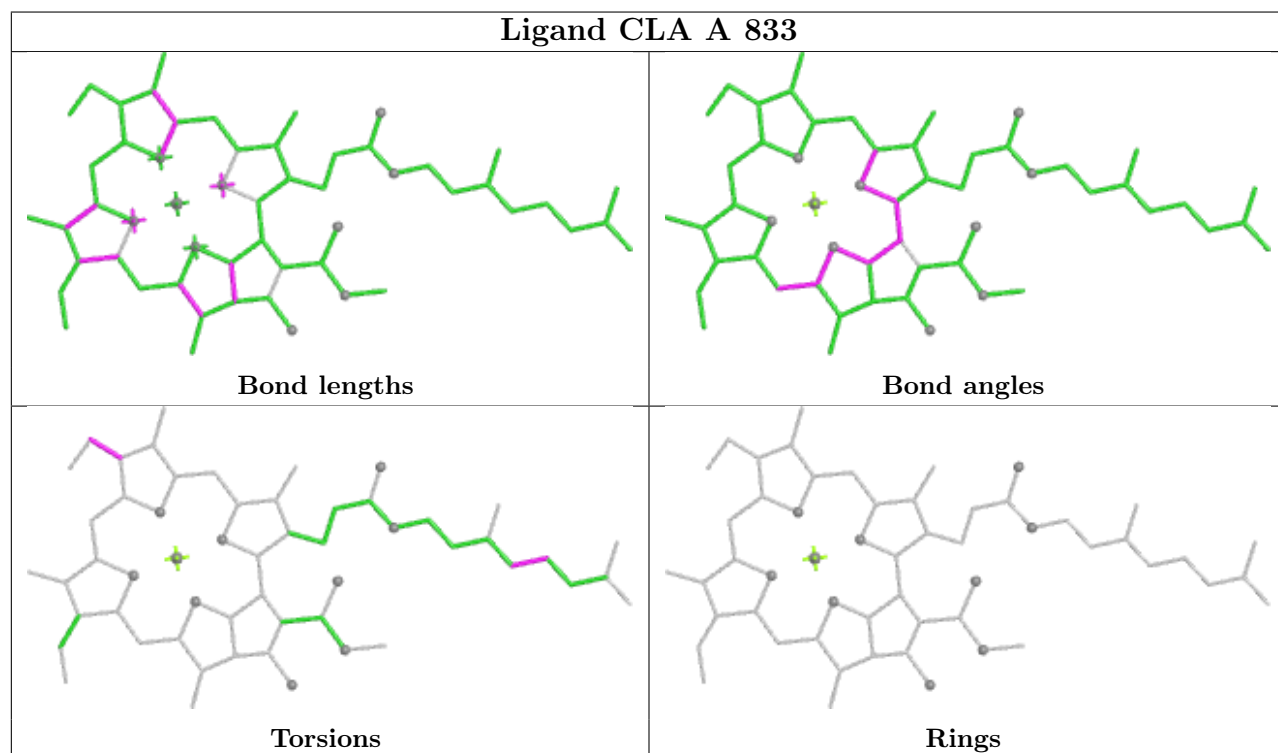
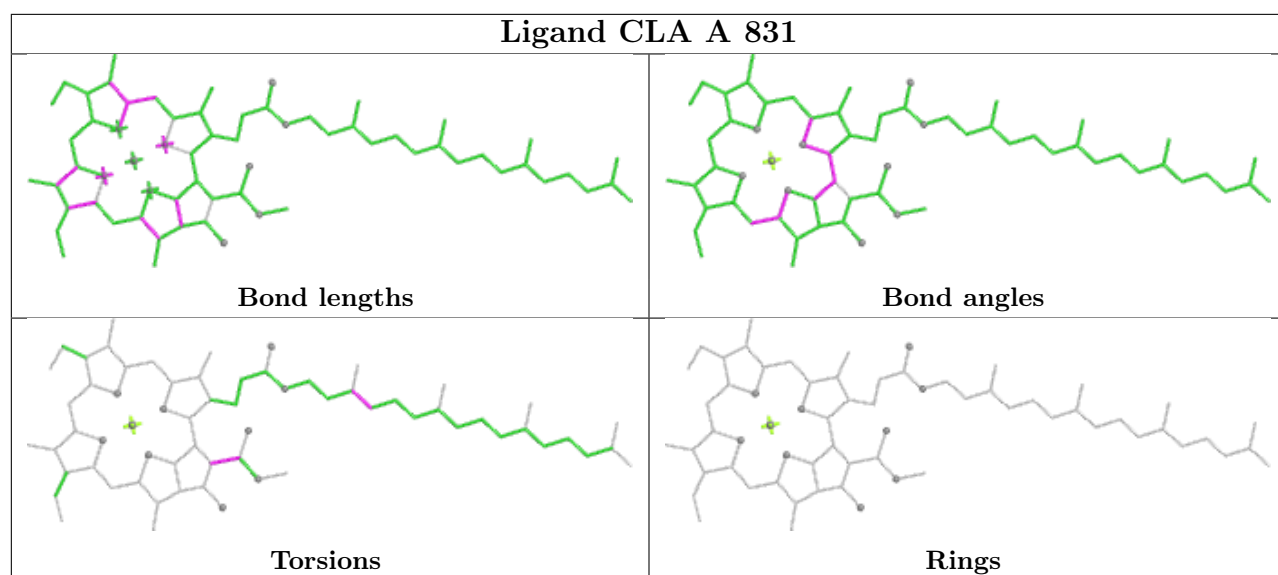


Ligand CLA A 815

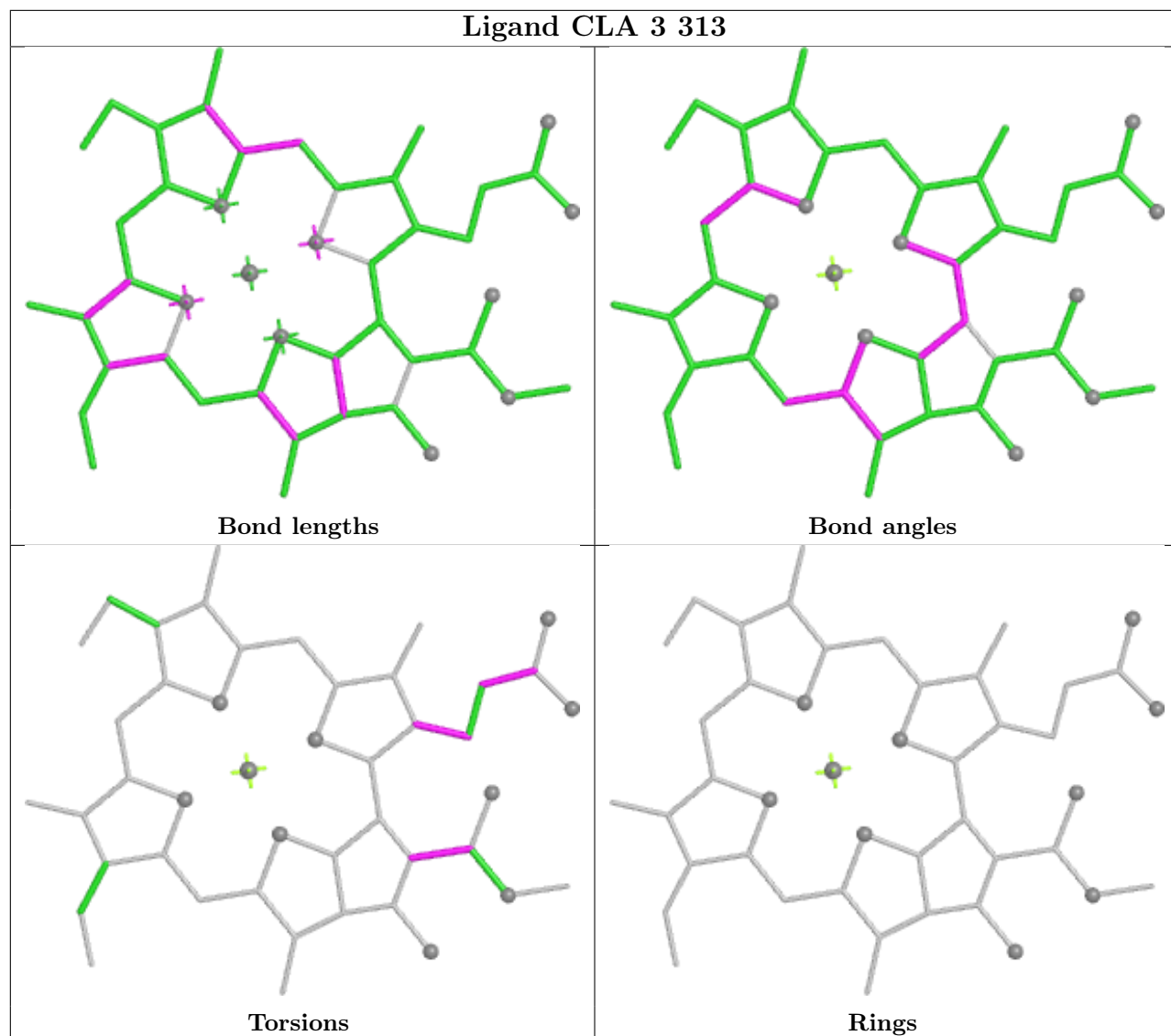


Ligand CHL 2 307

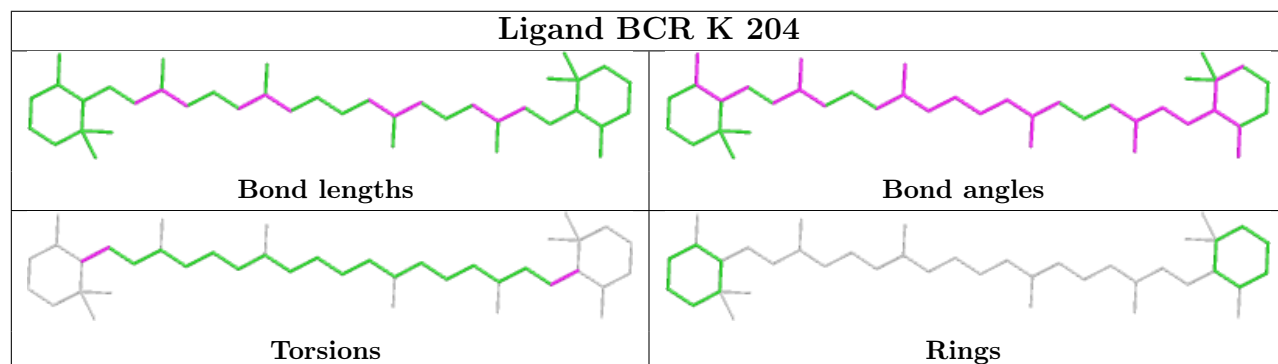


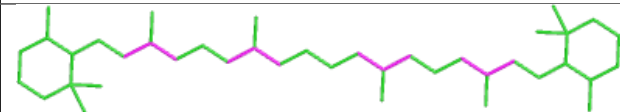
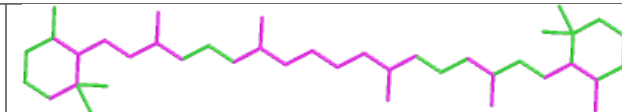
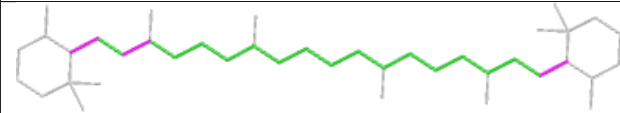
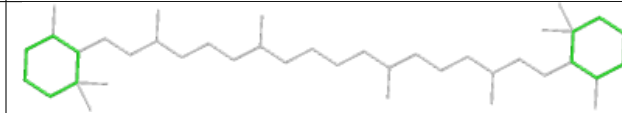
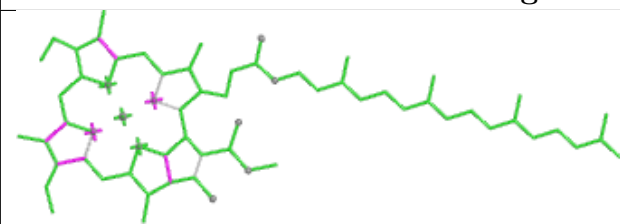
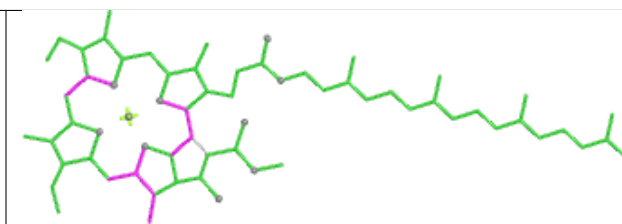
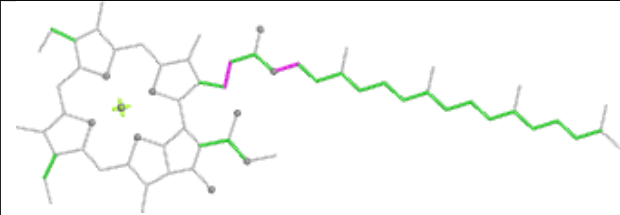
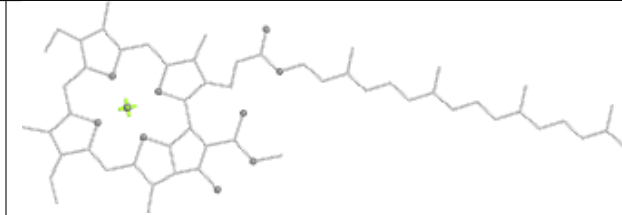
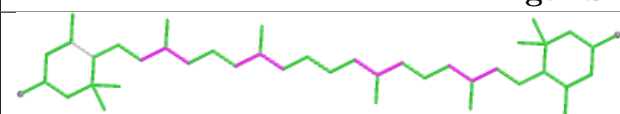
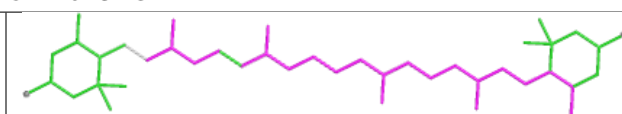
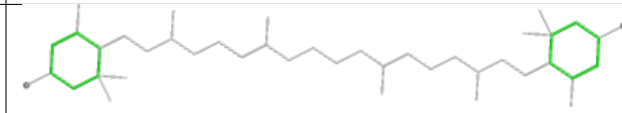
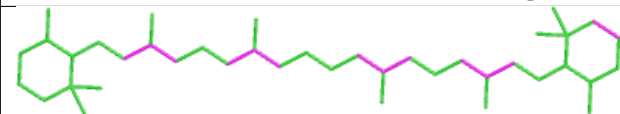
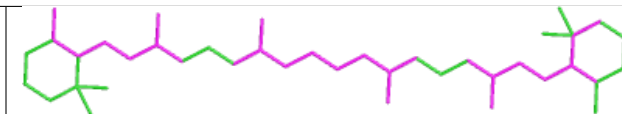
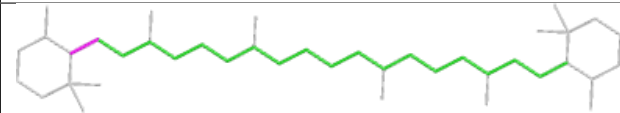
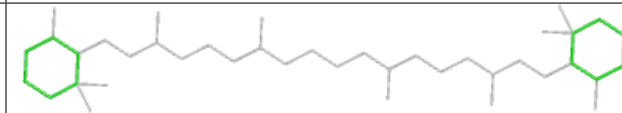


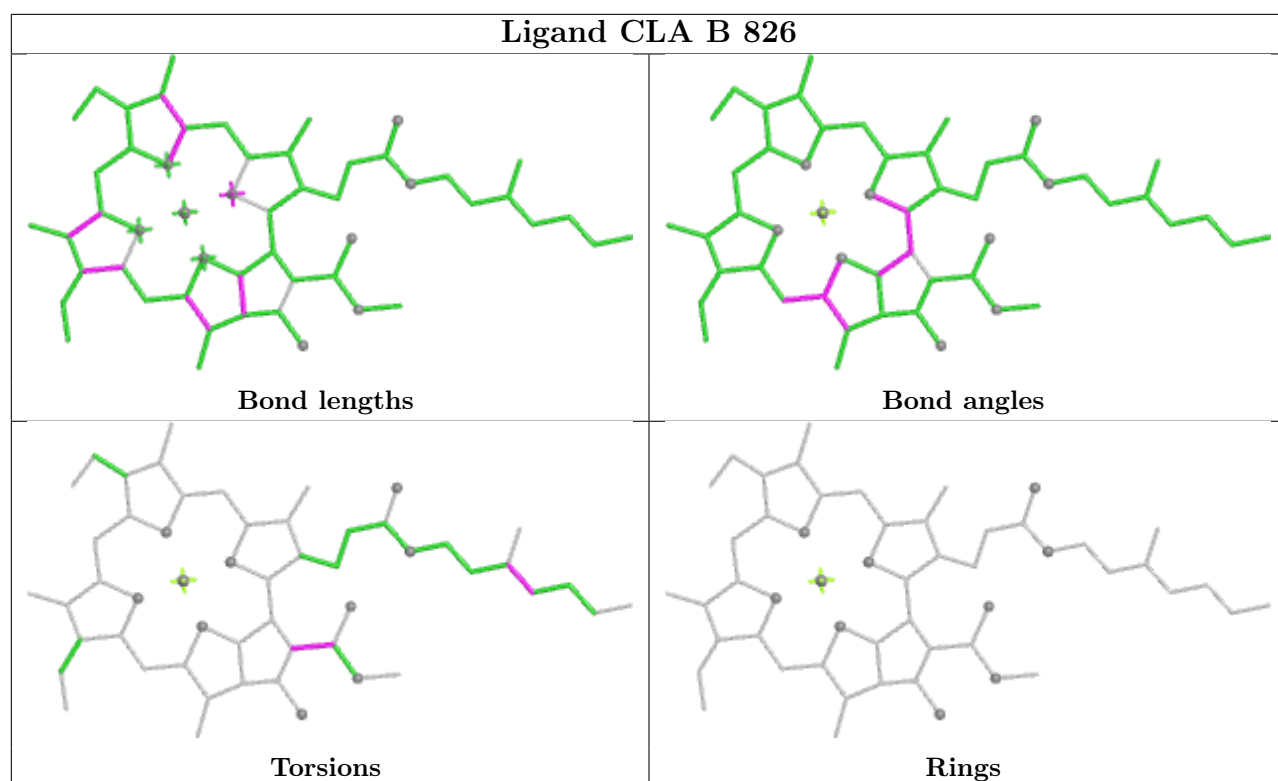
Ligand CLA 3 313



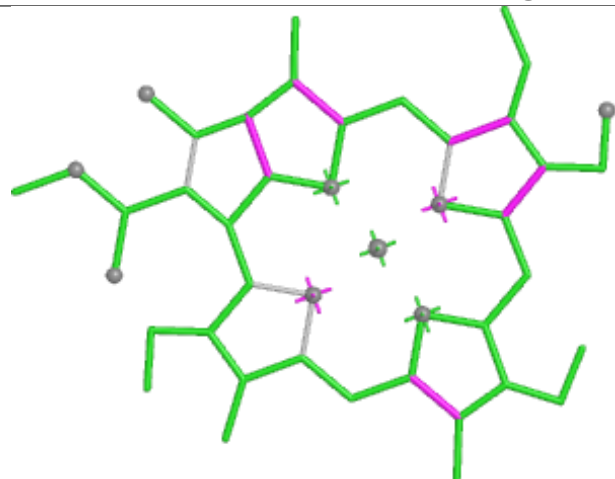
Ligand BCR K 204



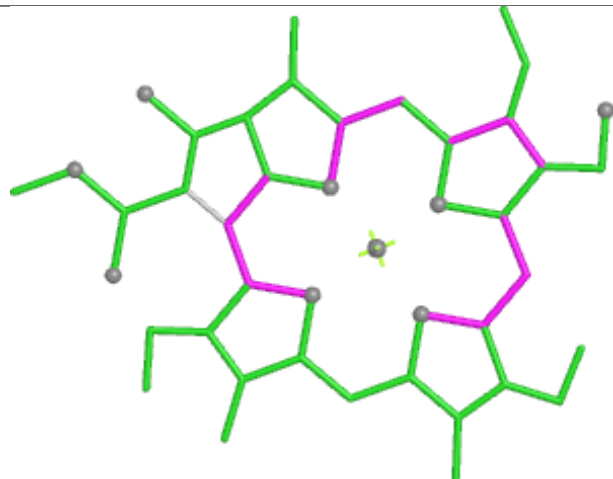
Ligand BCR A 848	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 824	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 6 318	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 304	
 Bond lengths	 Bond angles
 Torsions	 Rings



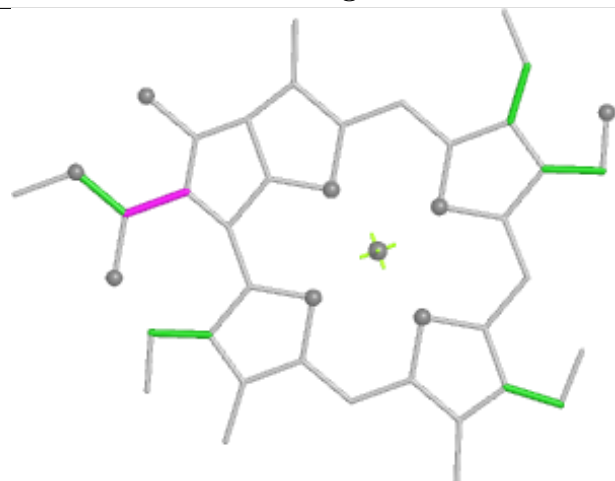
Ligand CHL 5 313



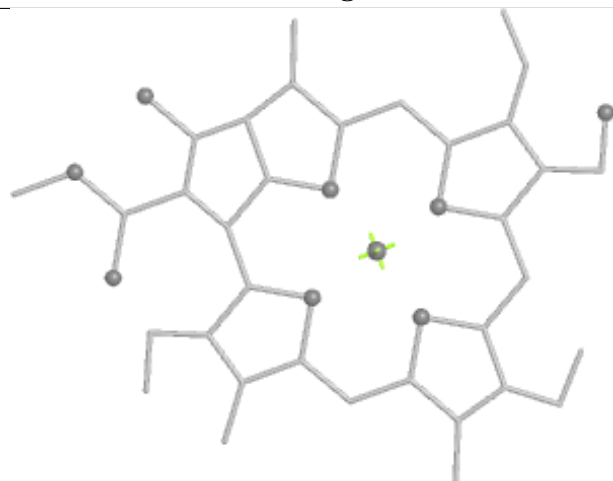
Bond lengths



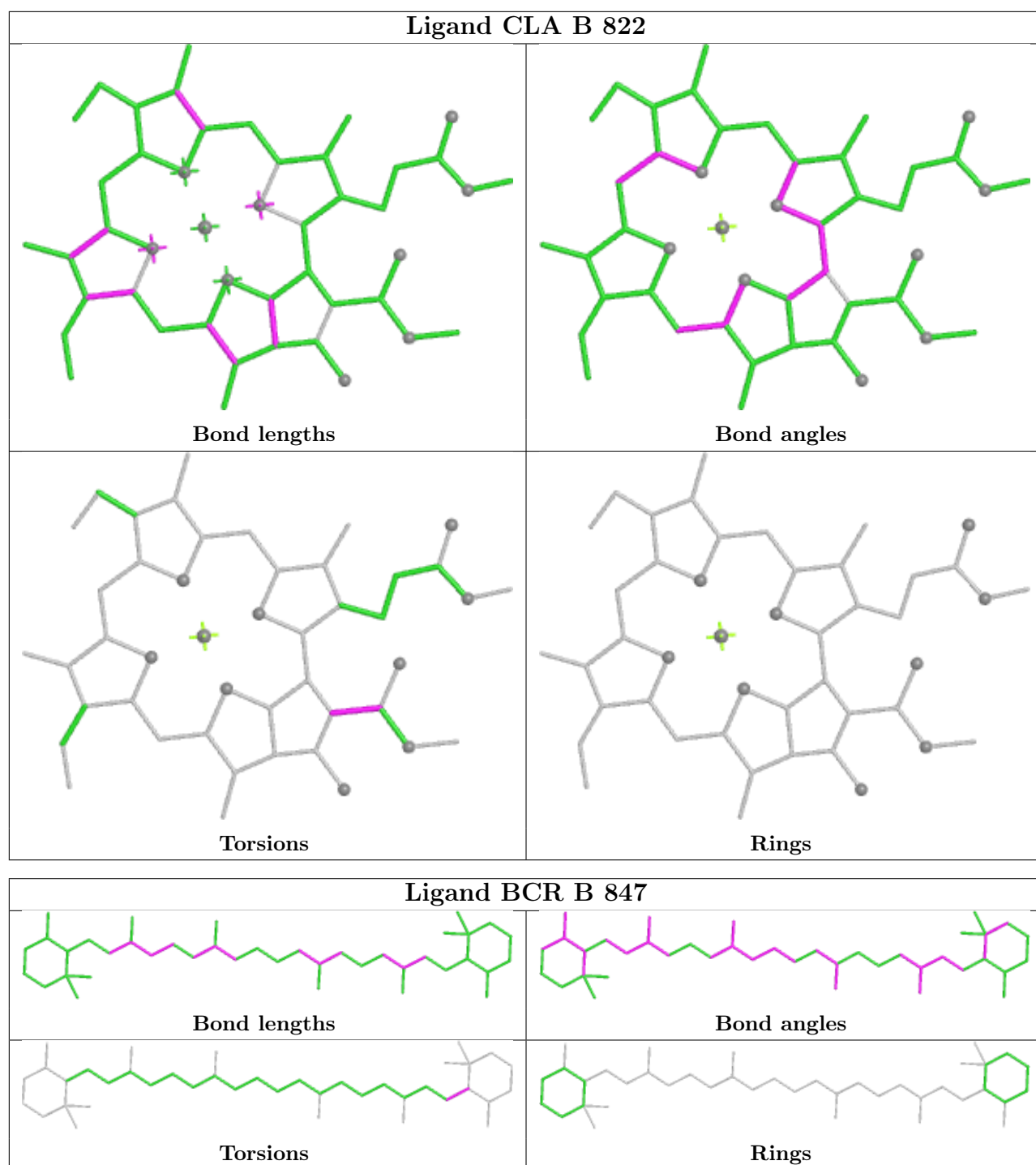
Bond angles

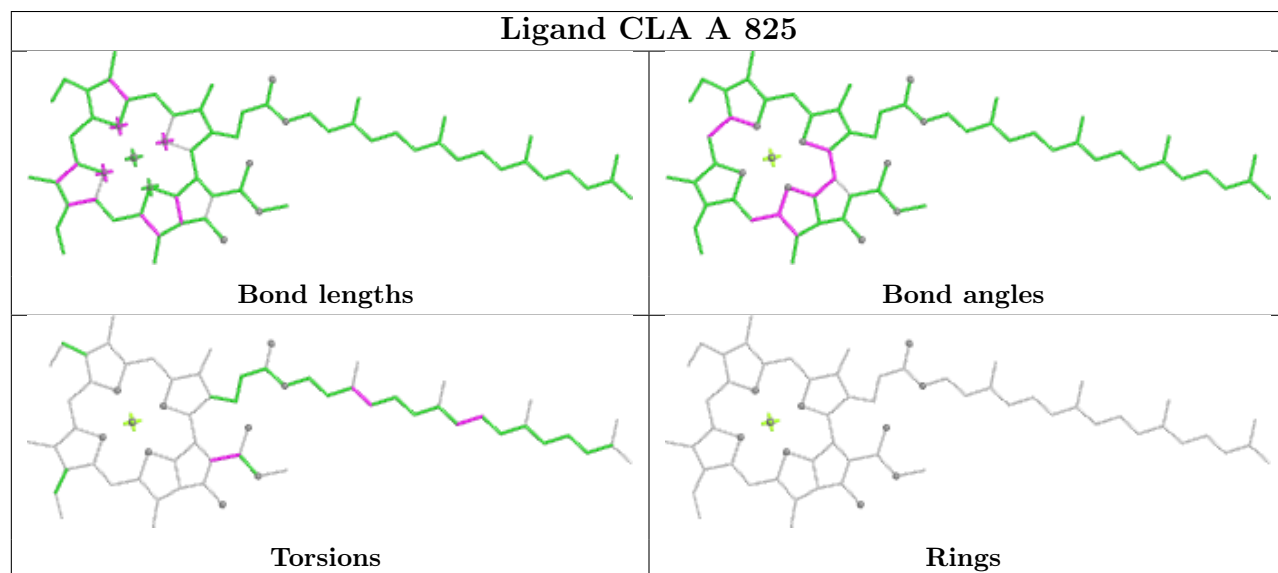
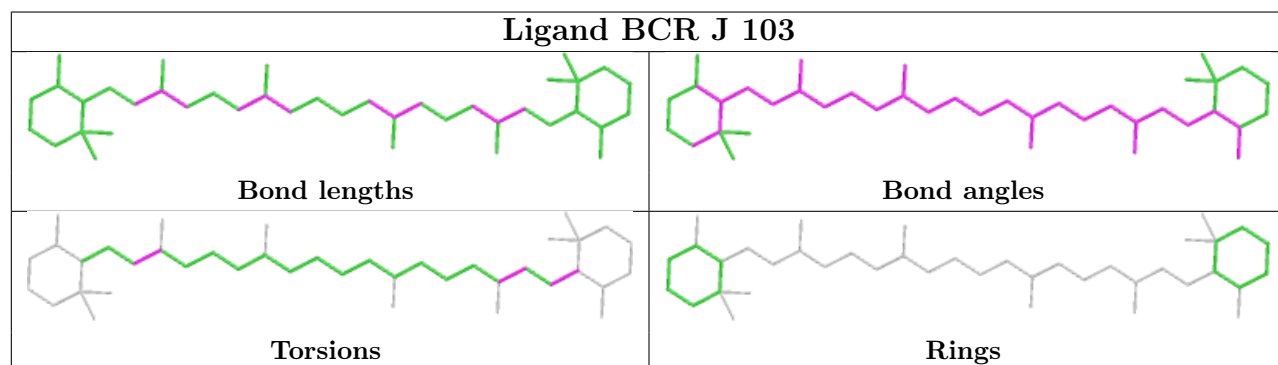
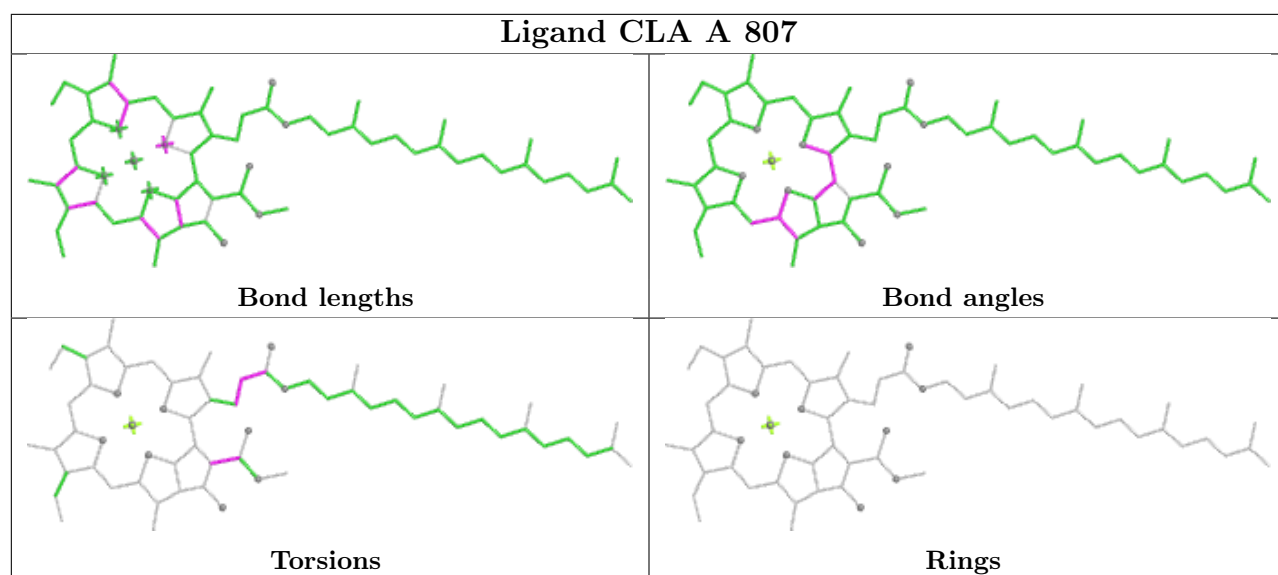


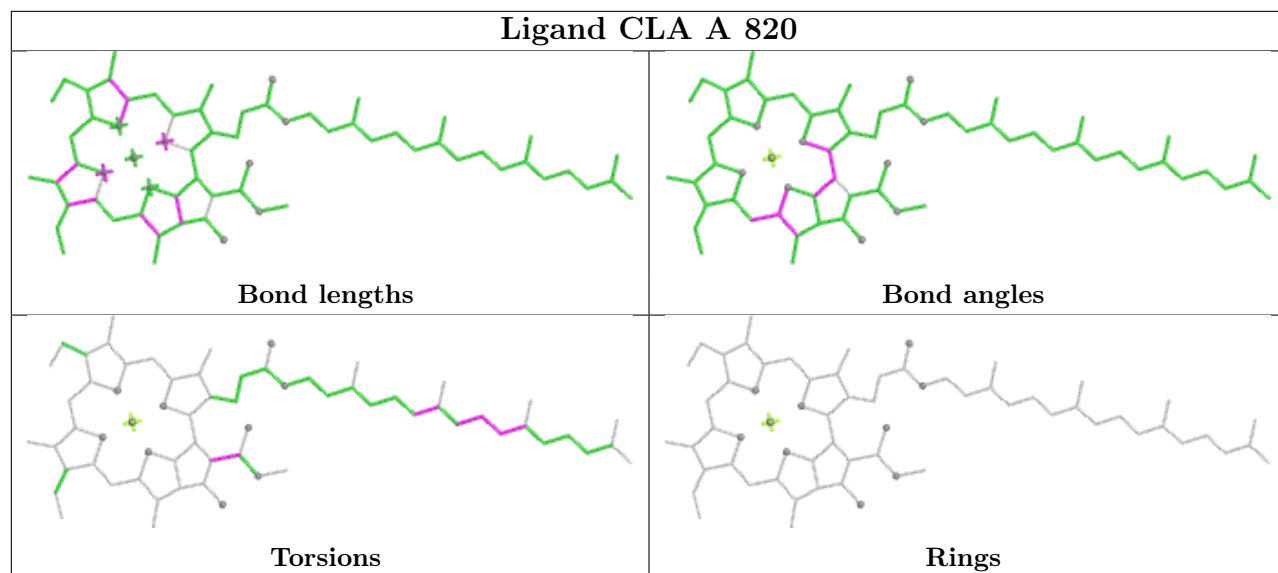
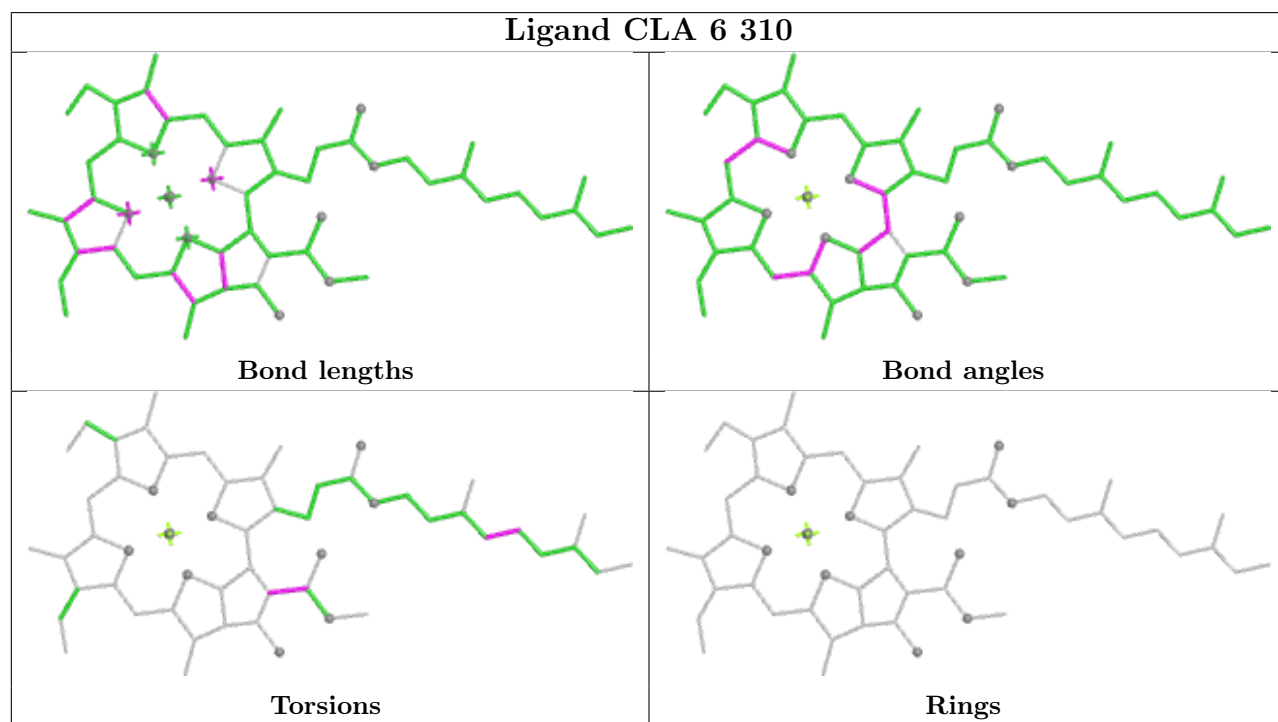
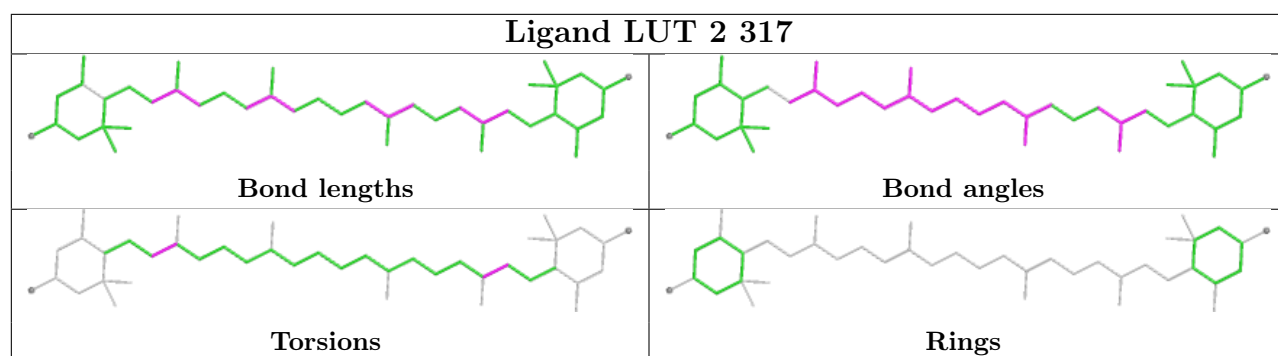
Torsions

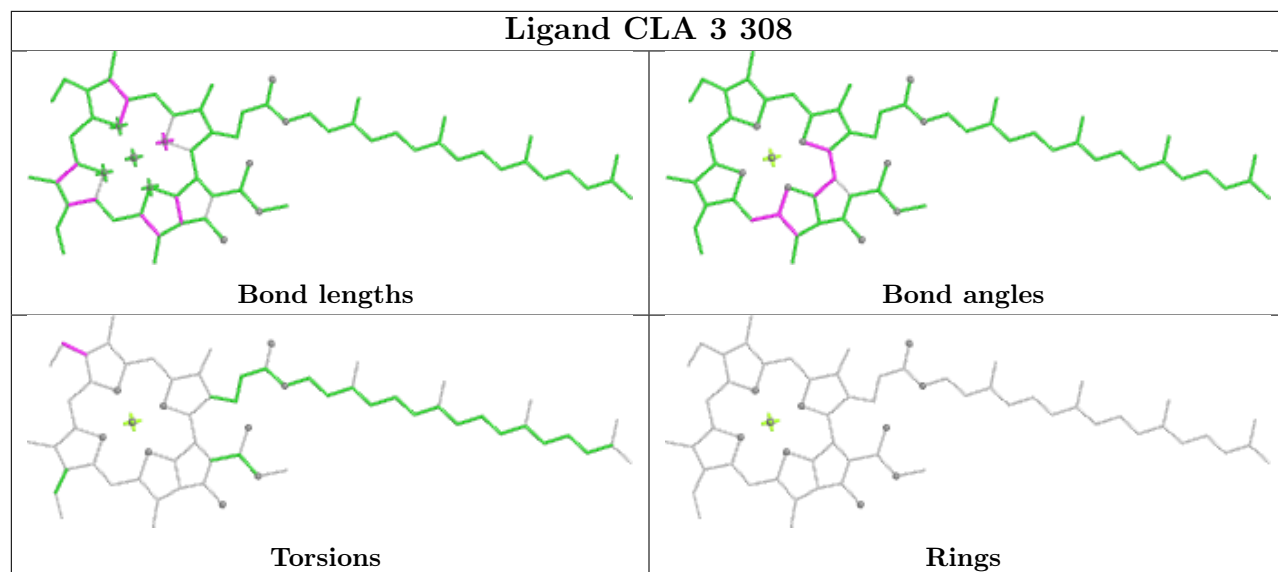
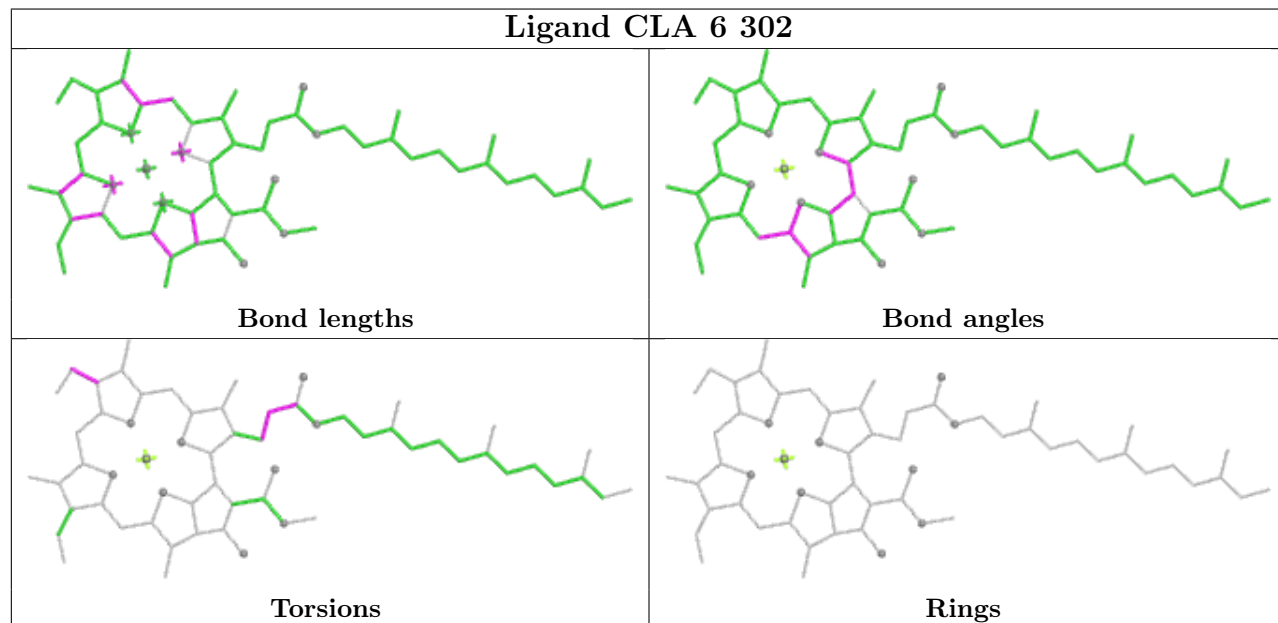


Rings

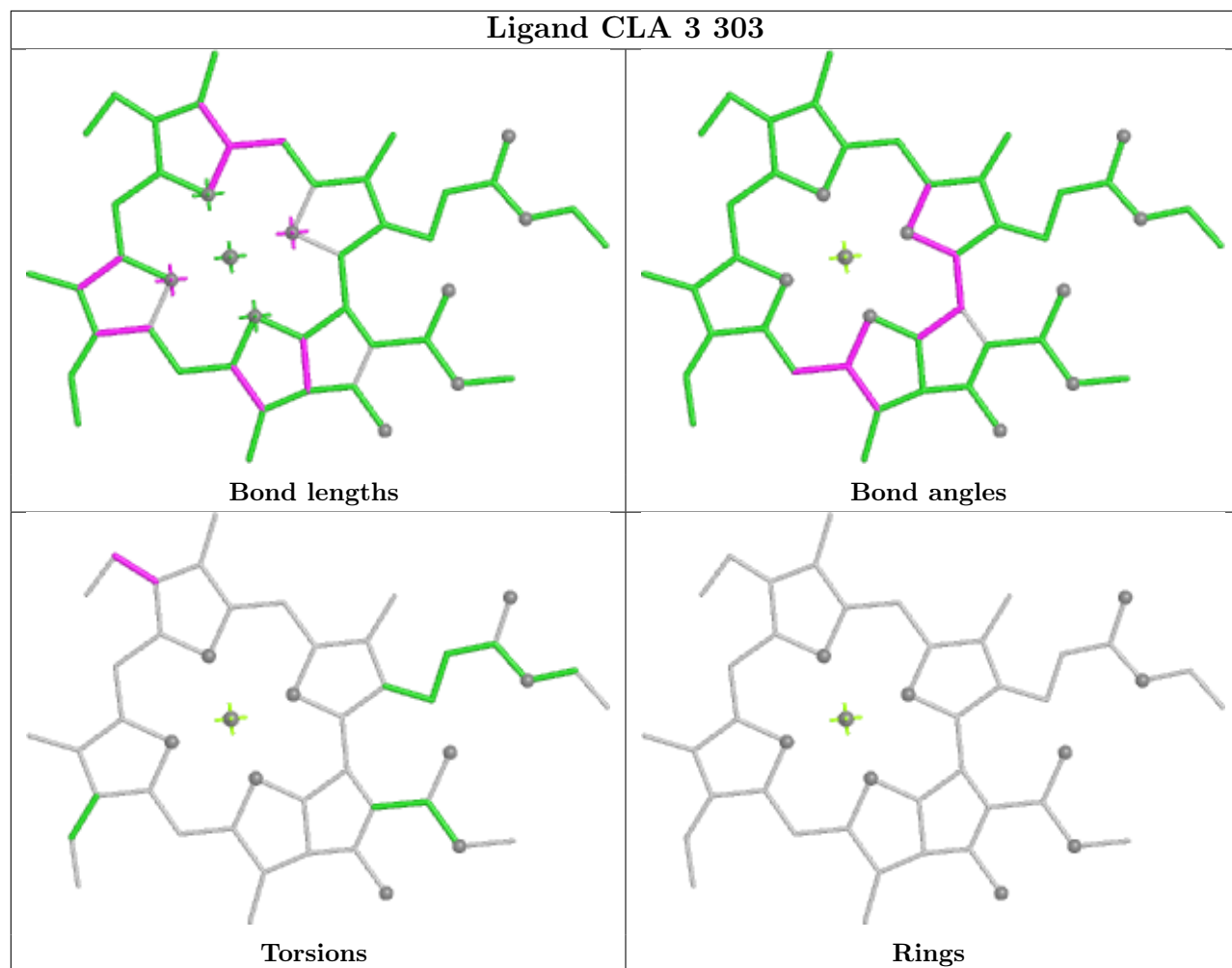




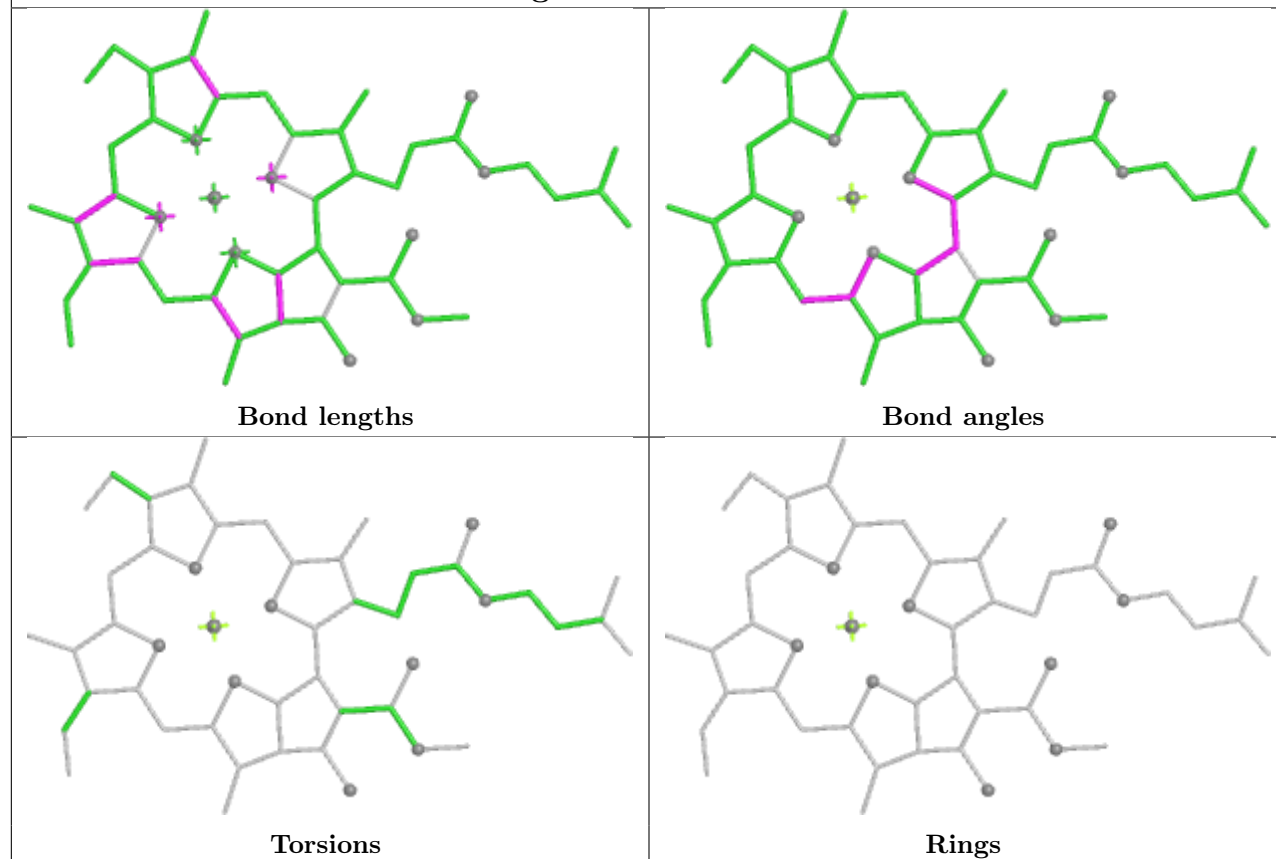


Ligand CLA 3 308**Ligand CLA 6 302**

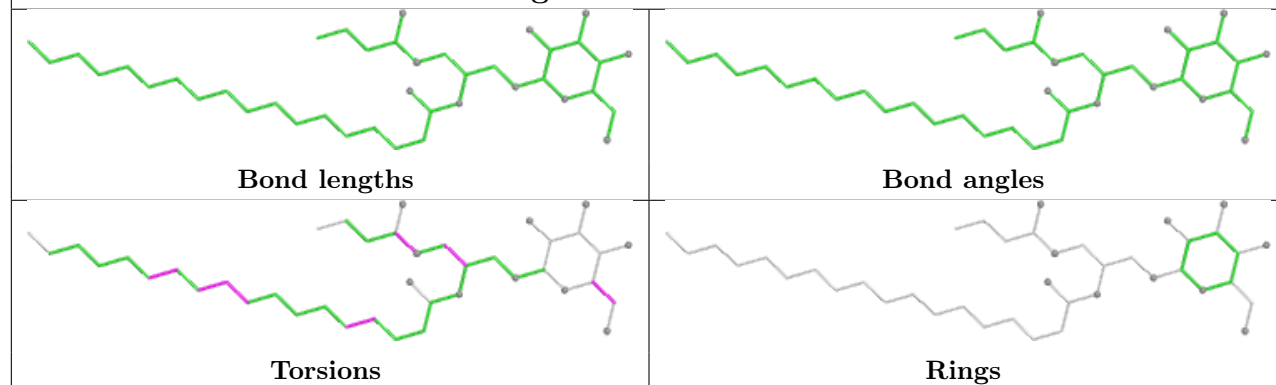
Ligand CLA 3 303



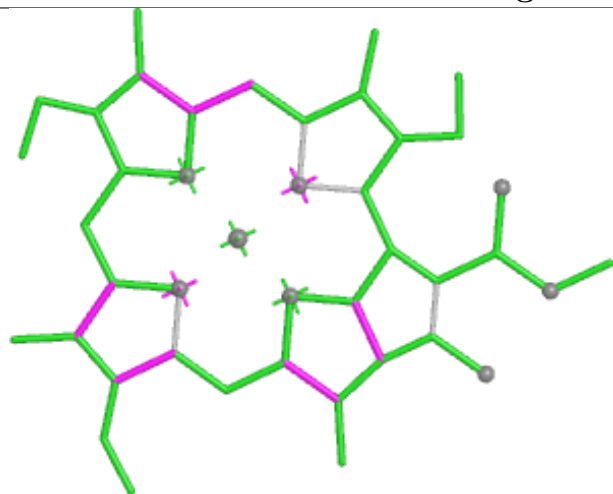
Ligand CLA A 832



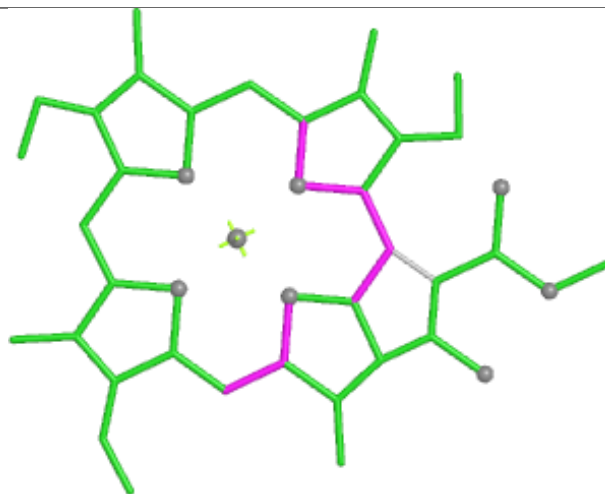
Ligand LMG J 105



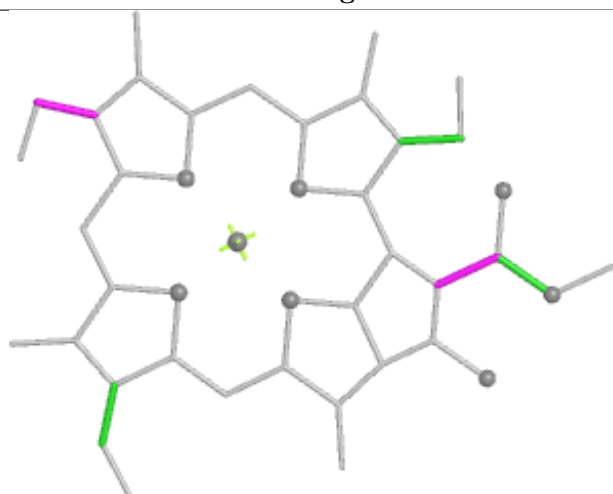
Ligand CLA L 303



Bond lengths



Bond angles

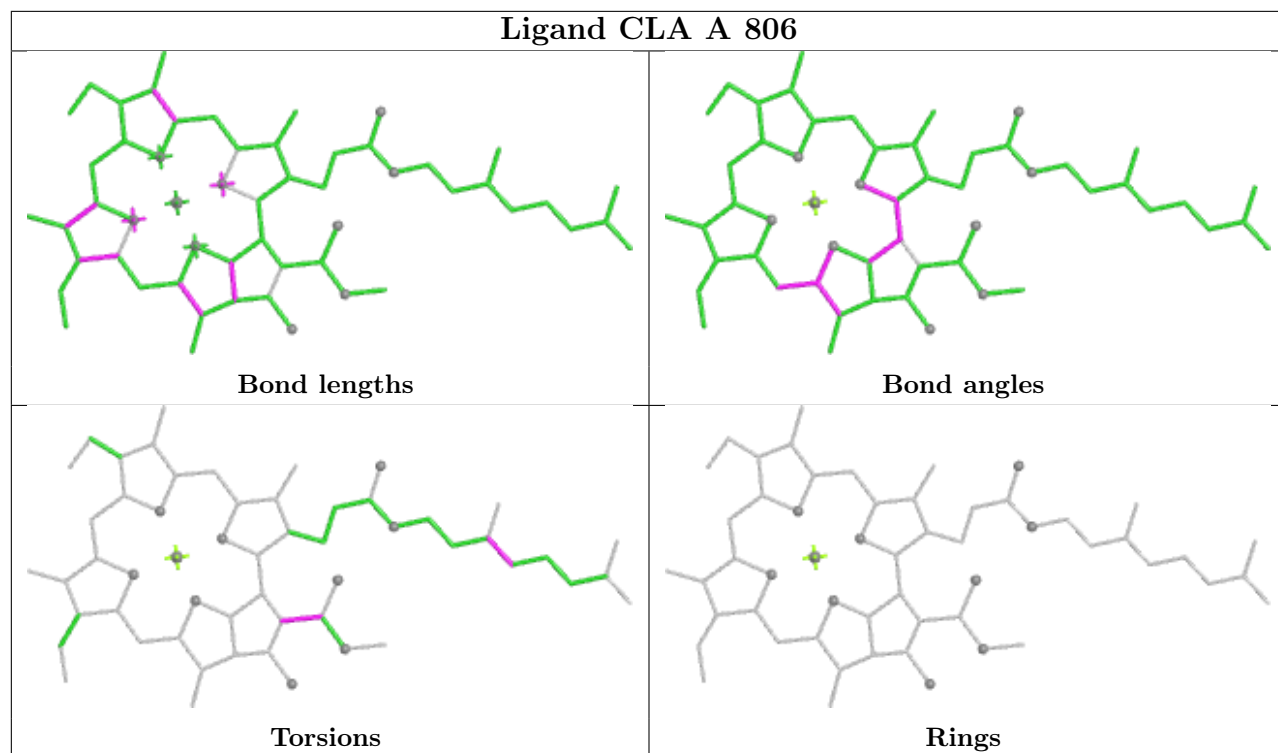


Torsions

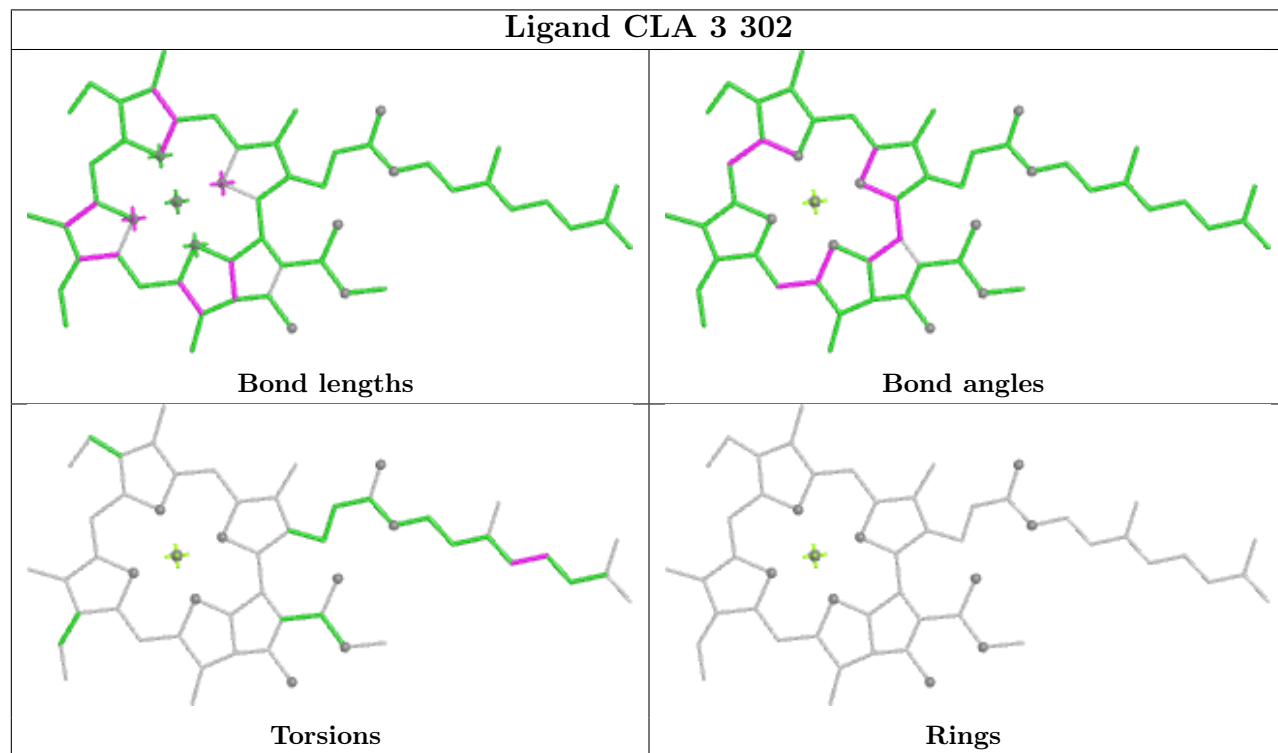


Rings

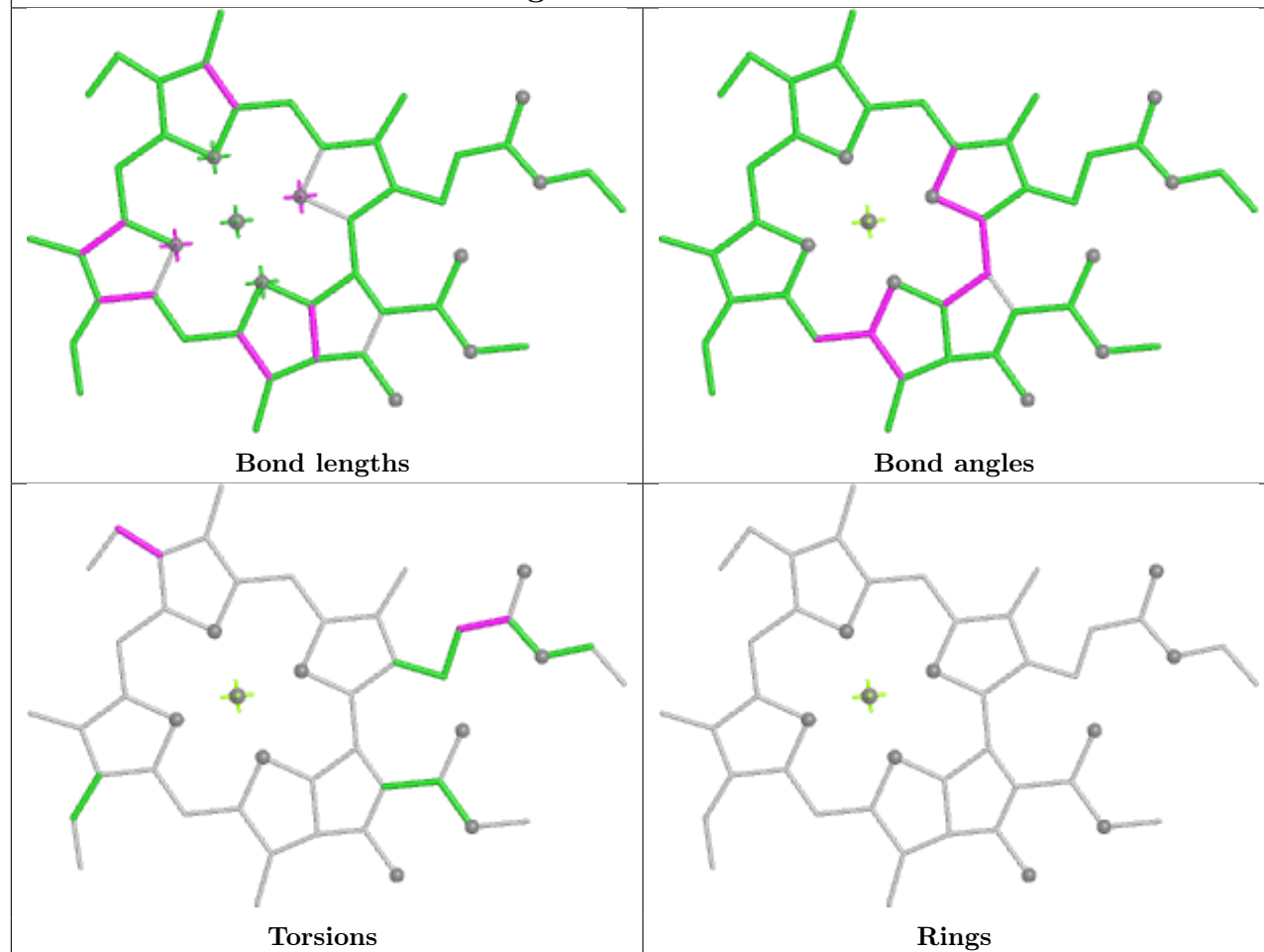
Ligand CLA A 806



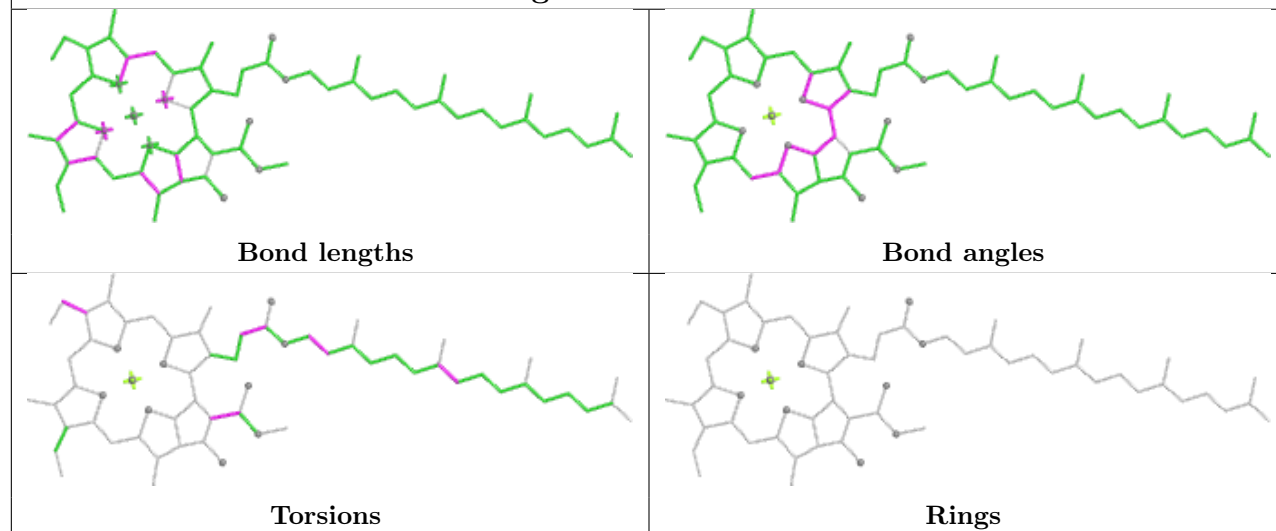
Ligand CLA 3 302

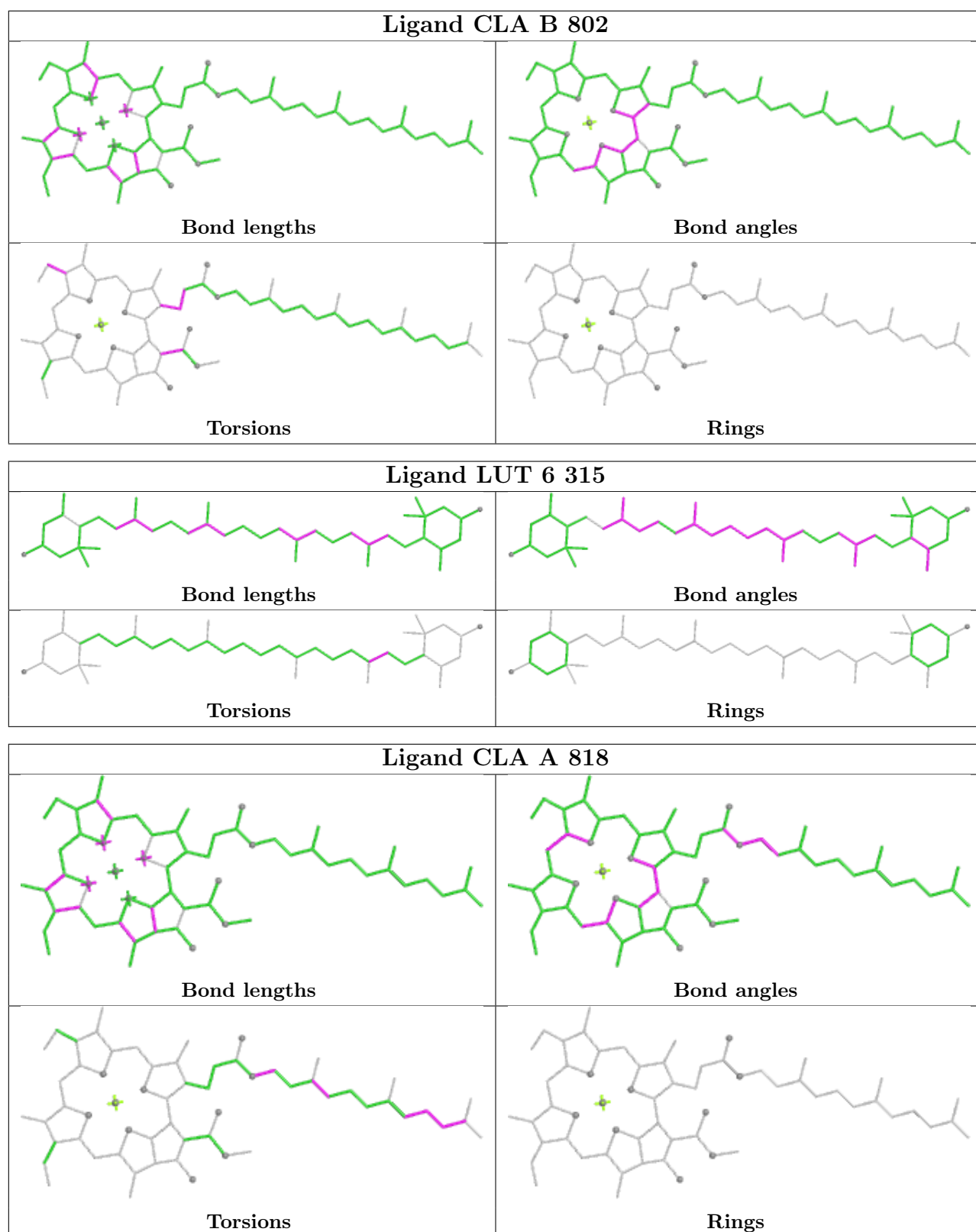


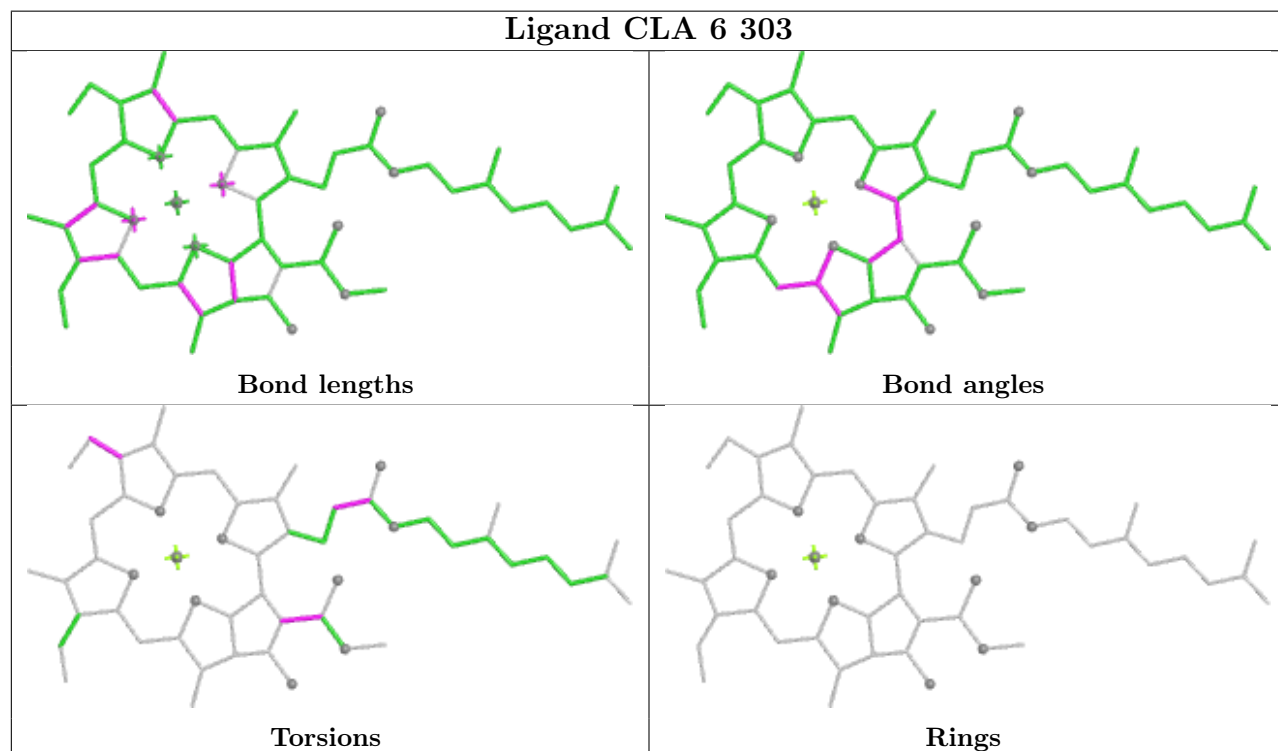
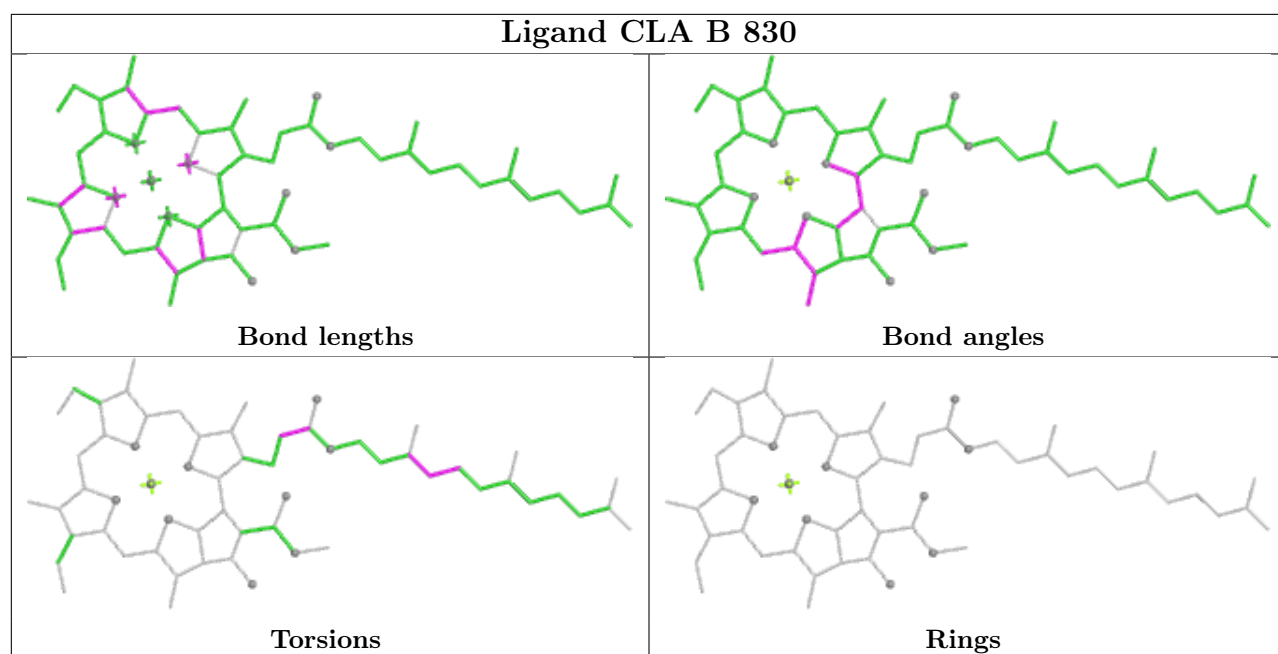
Ligand CLA B 839

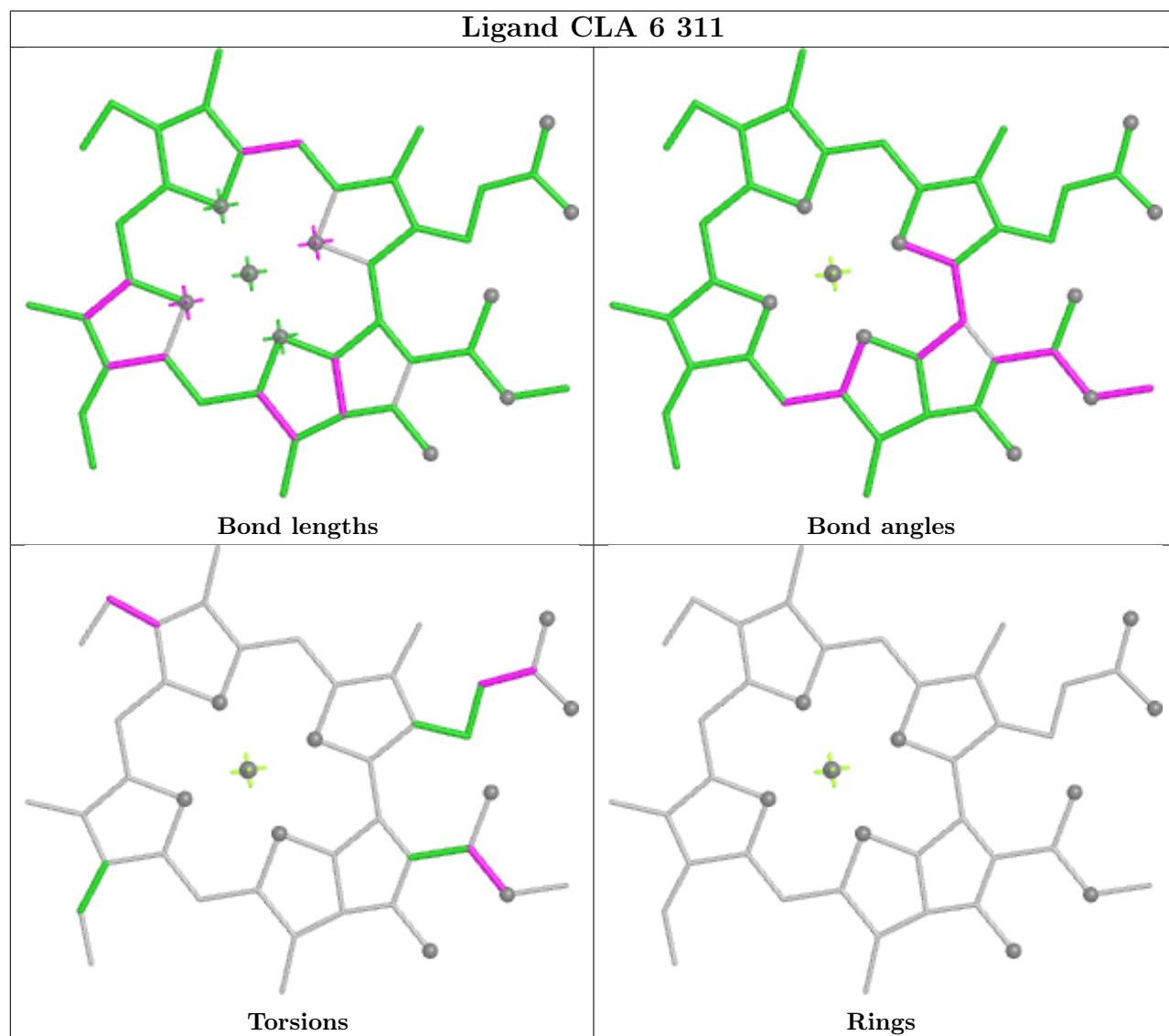
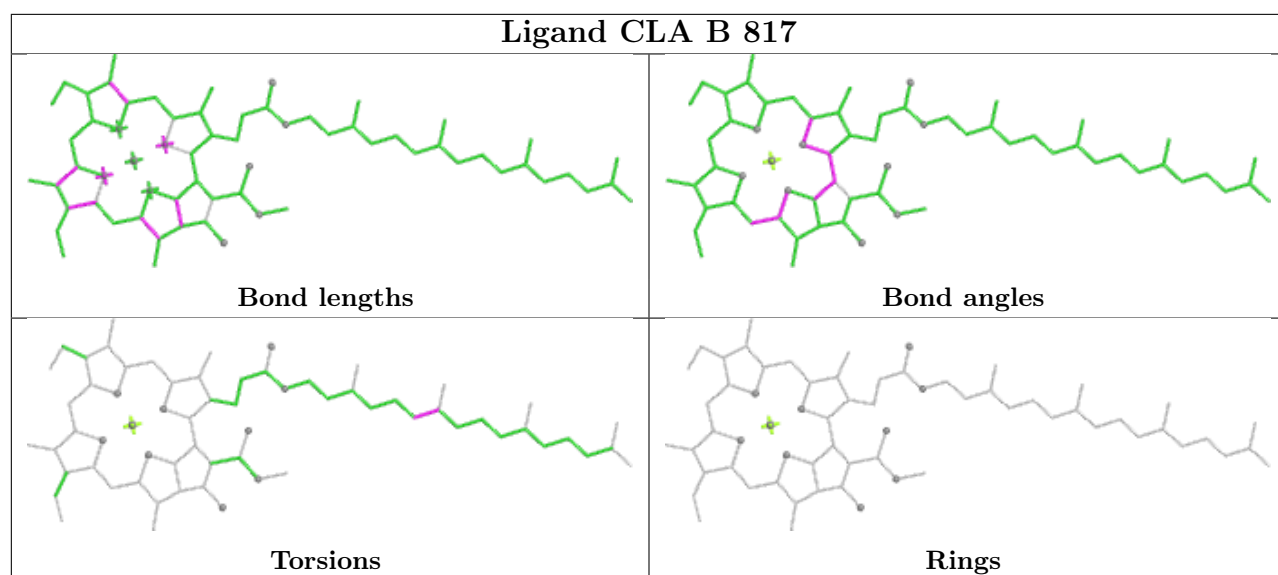


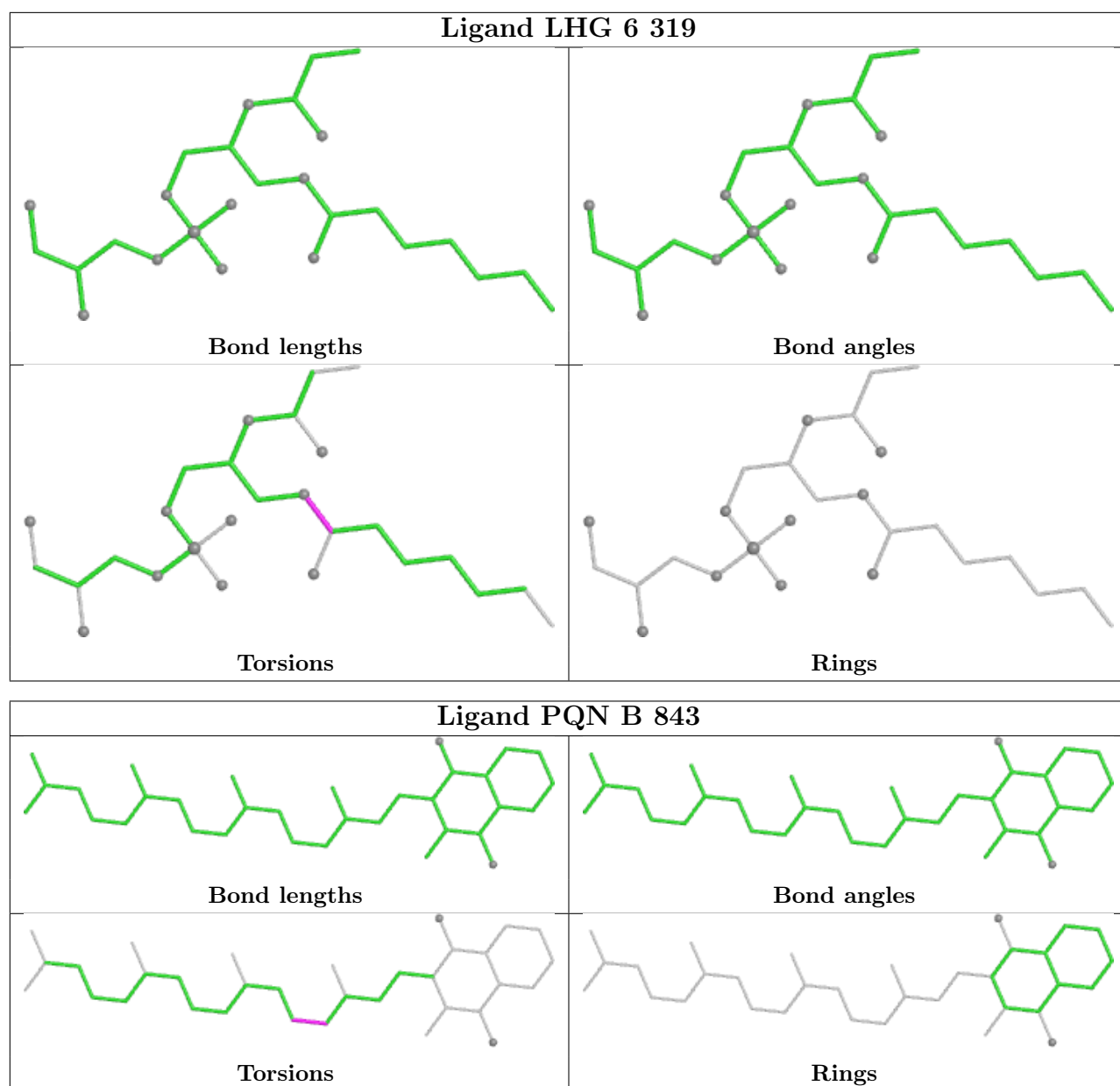
Ligand CLA A 826

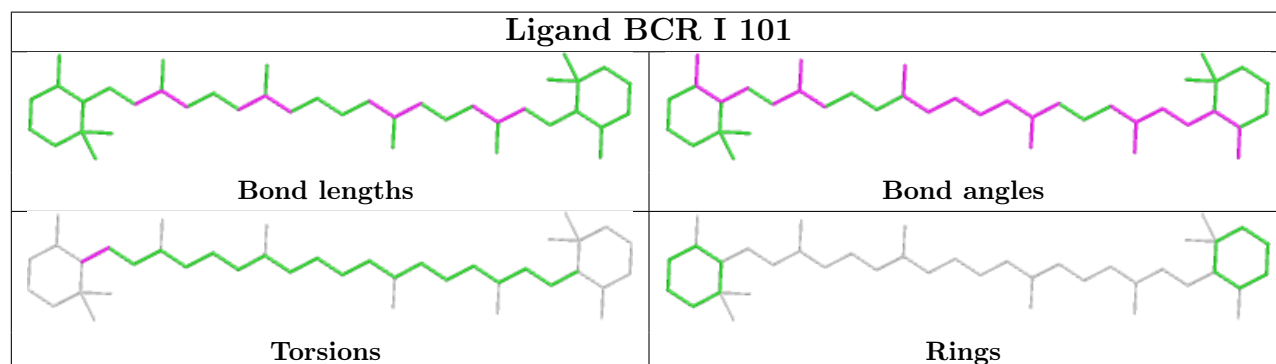
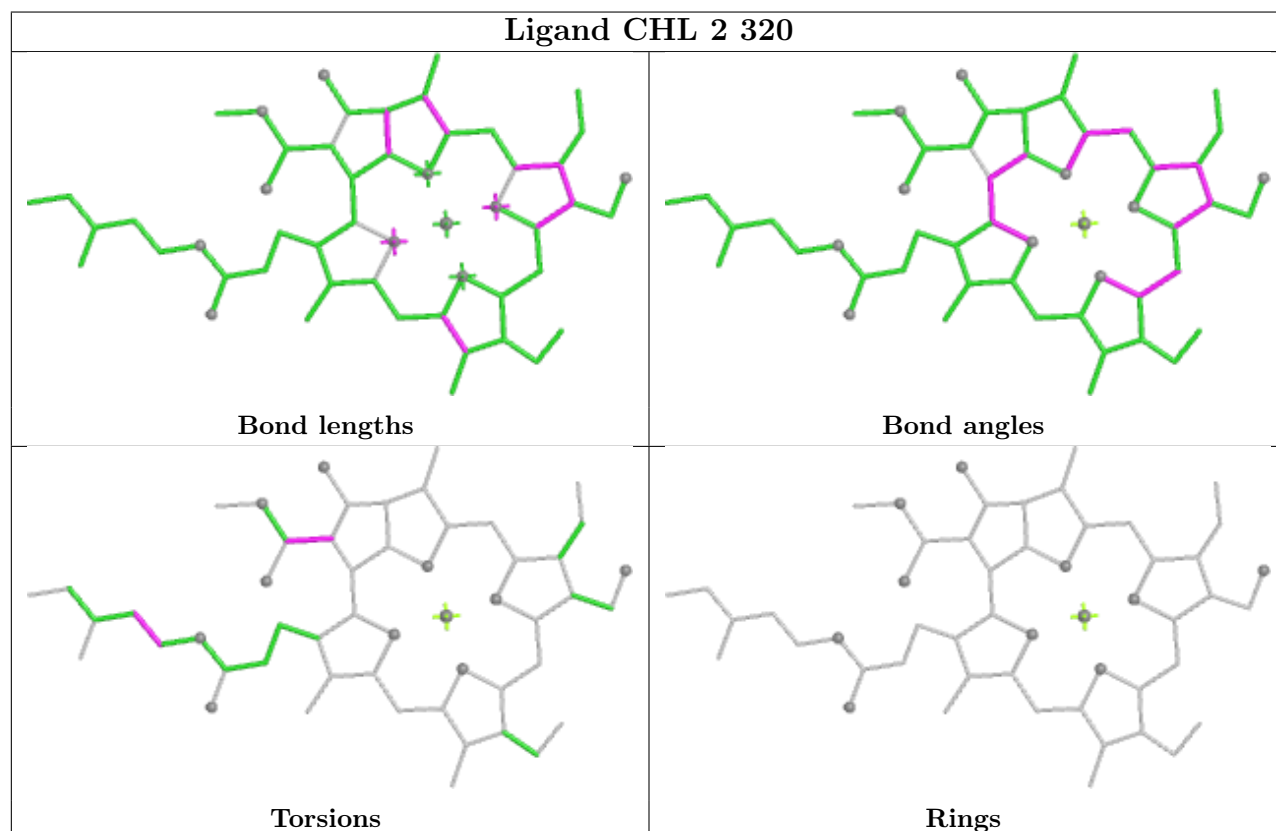
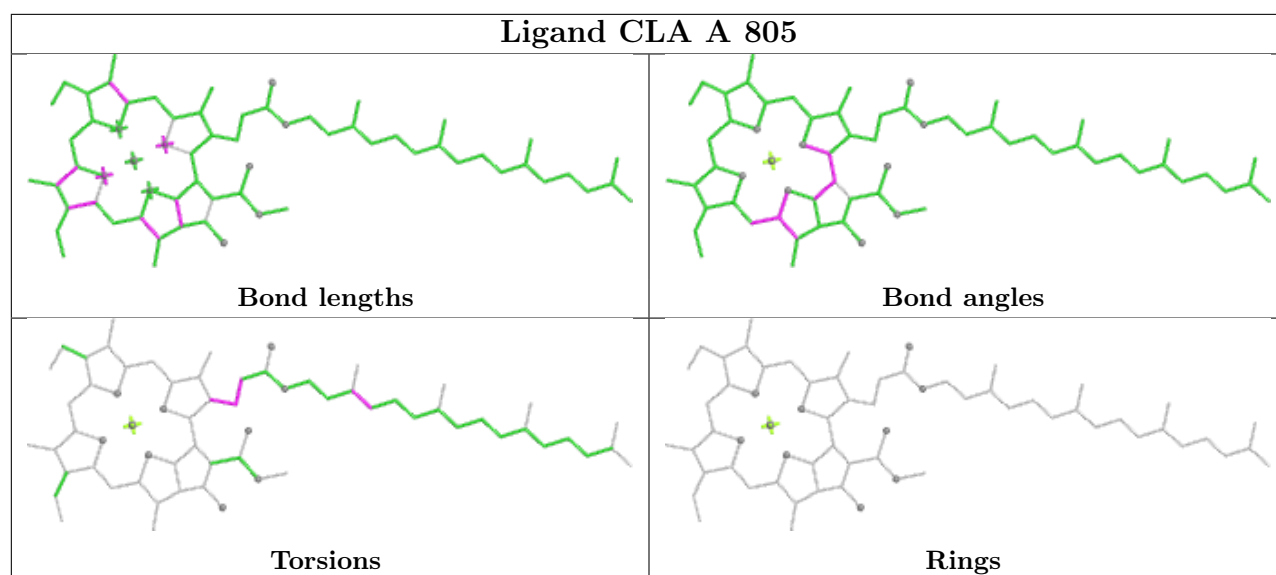


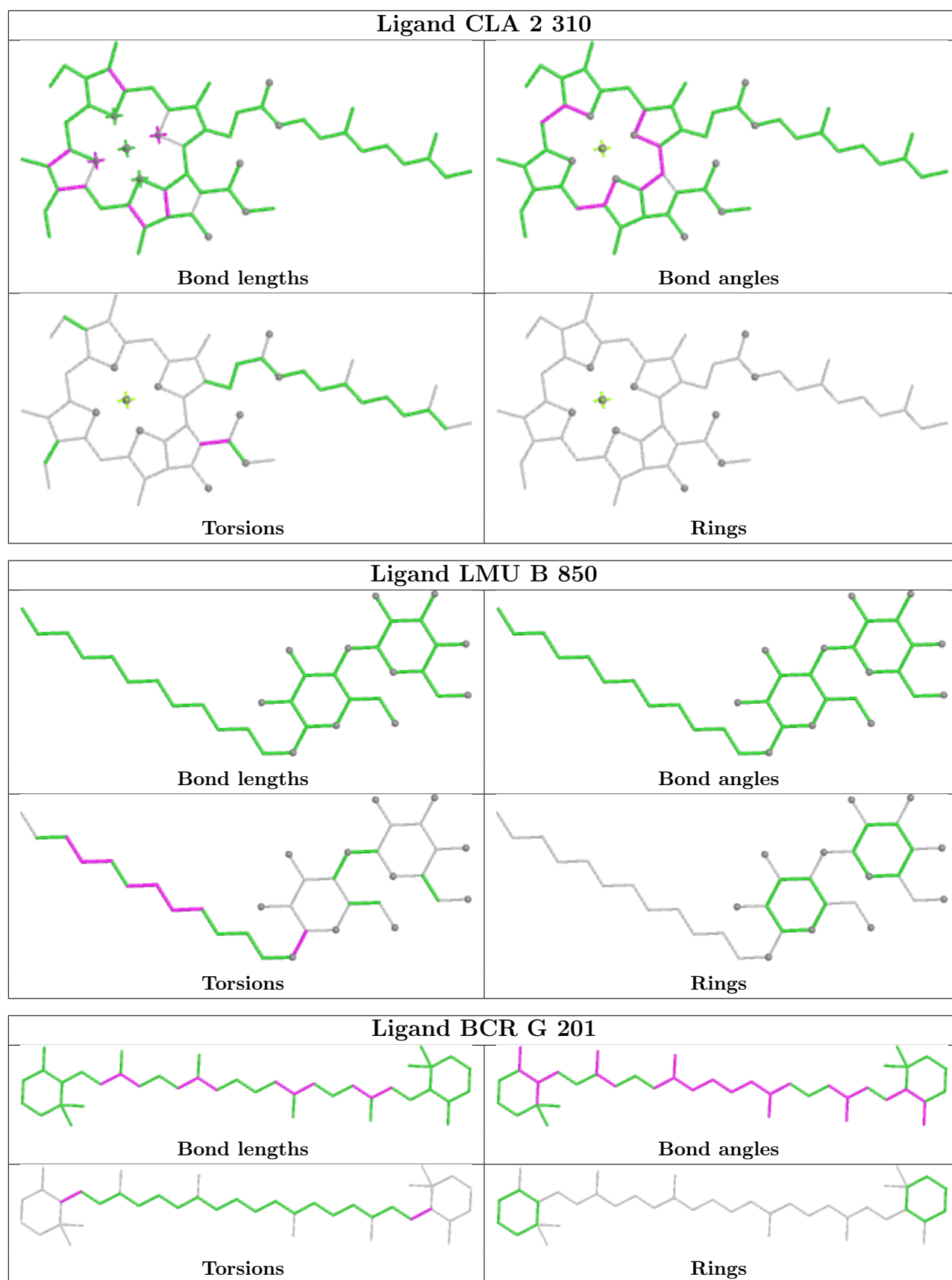


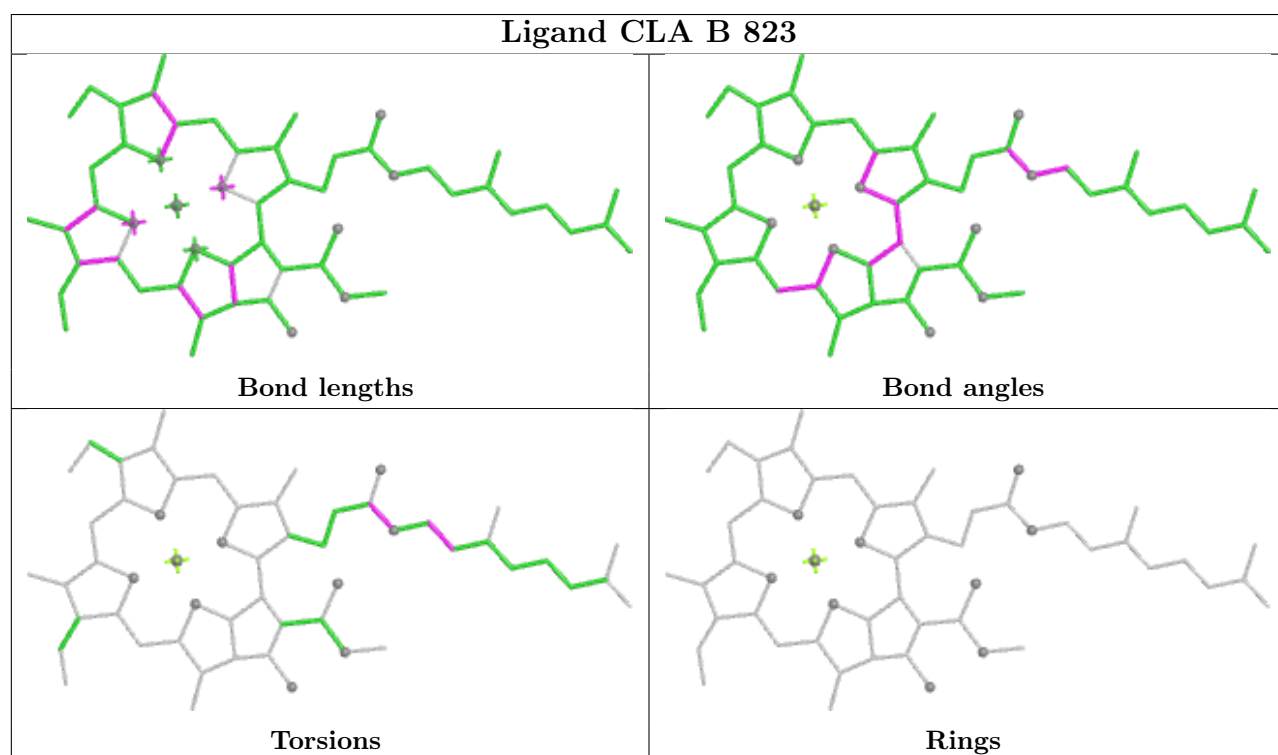
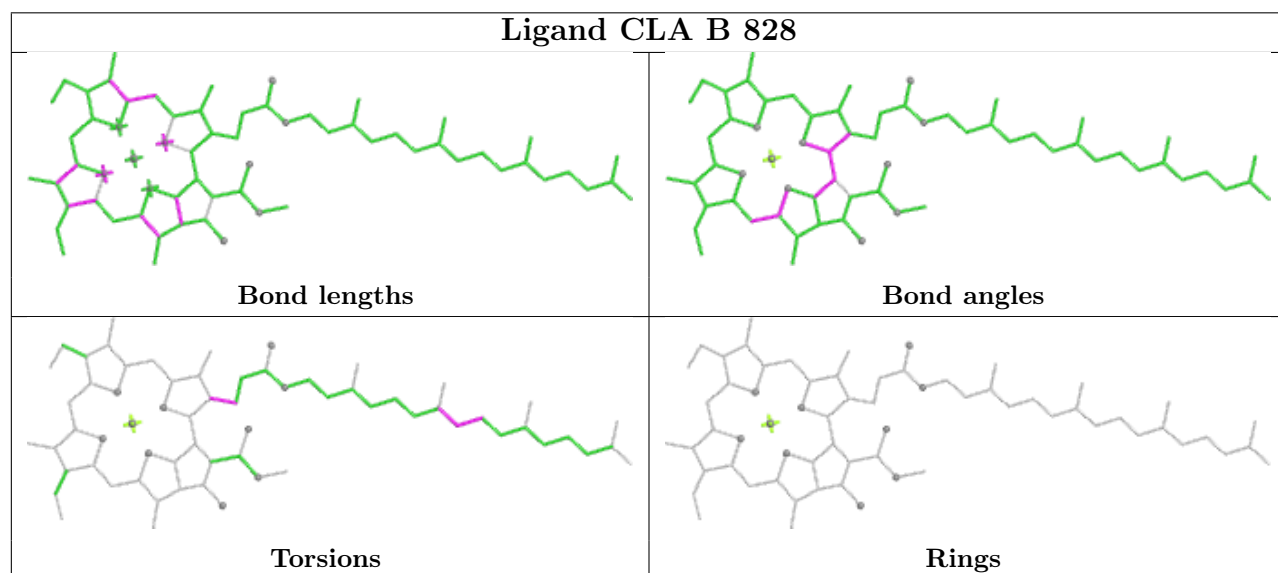
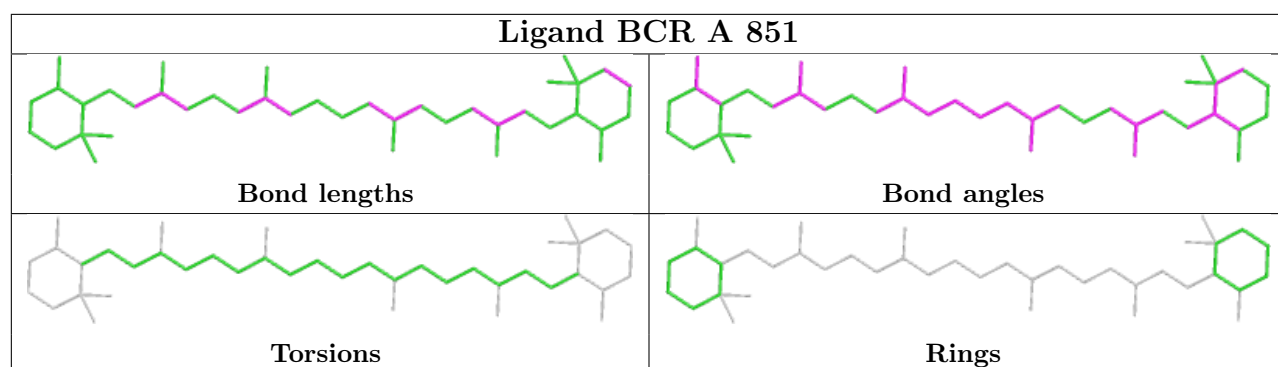


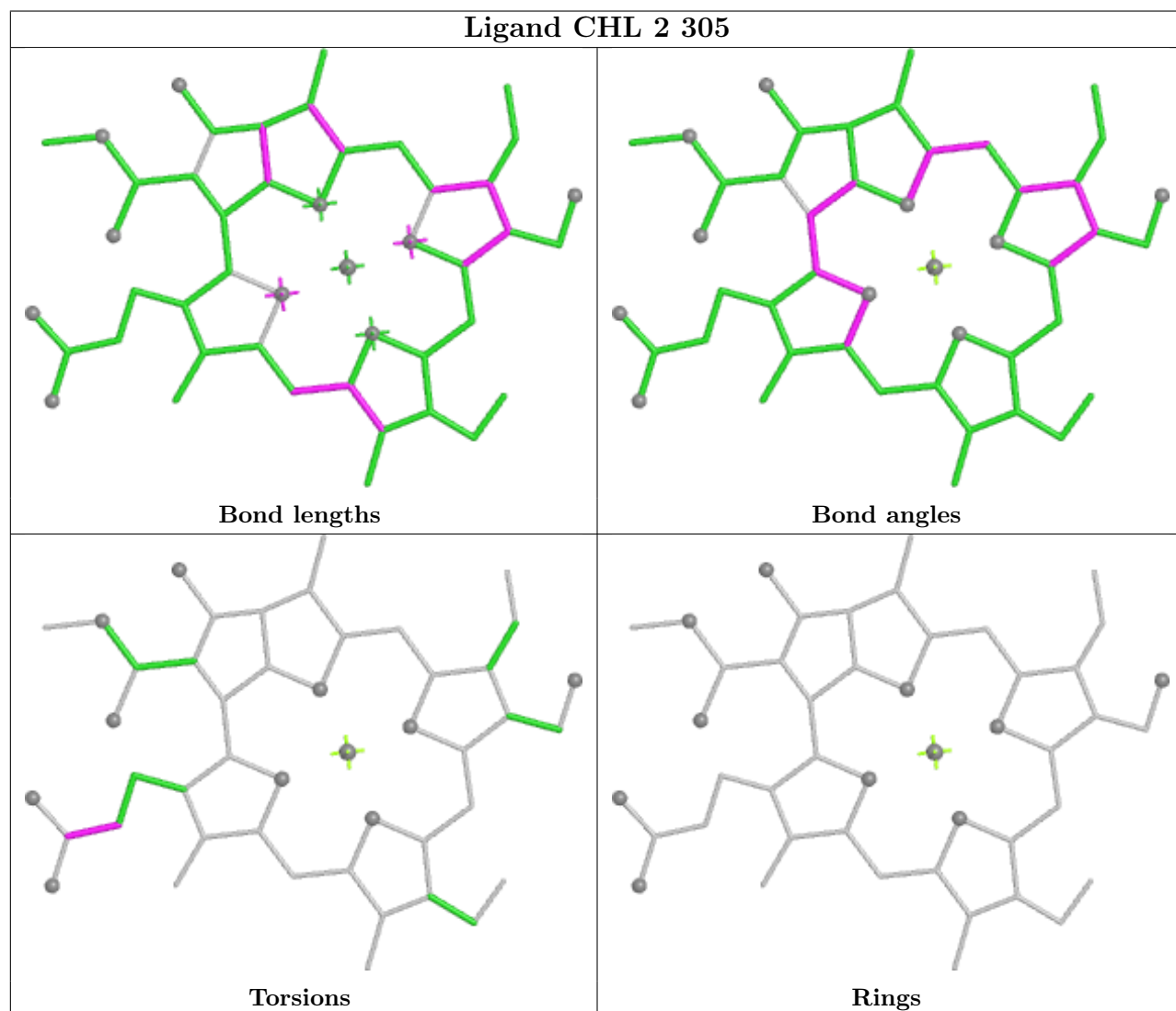
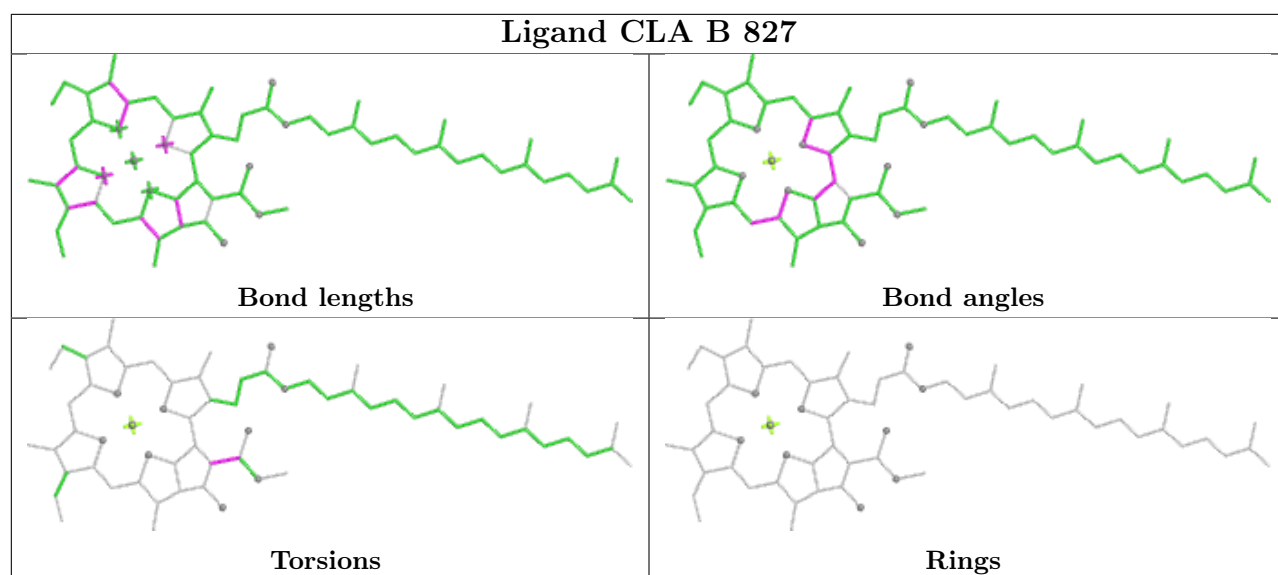


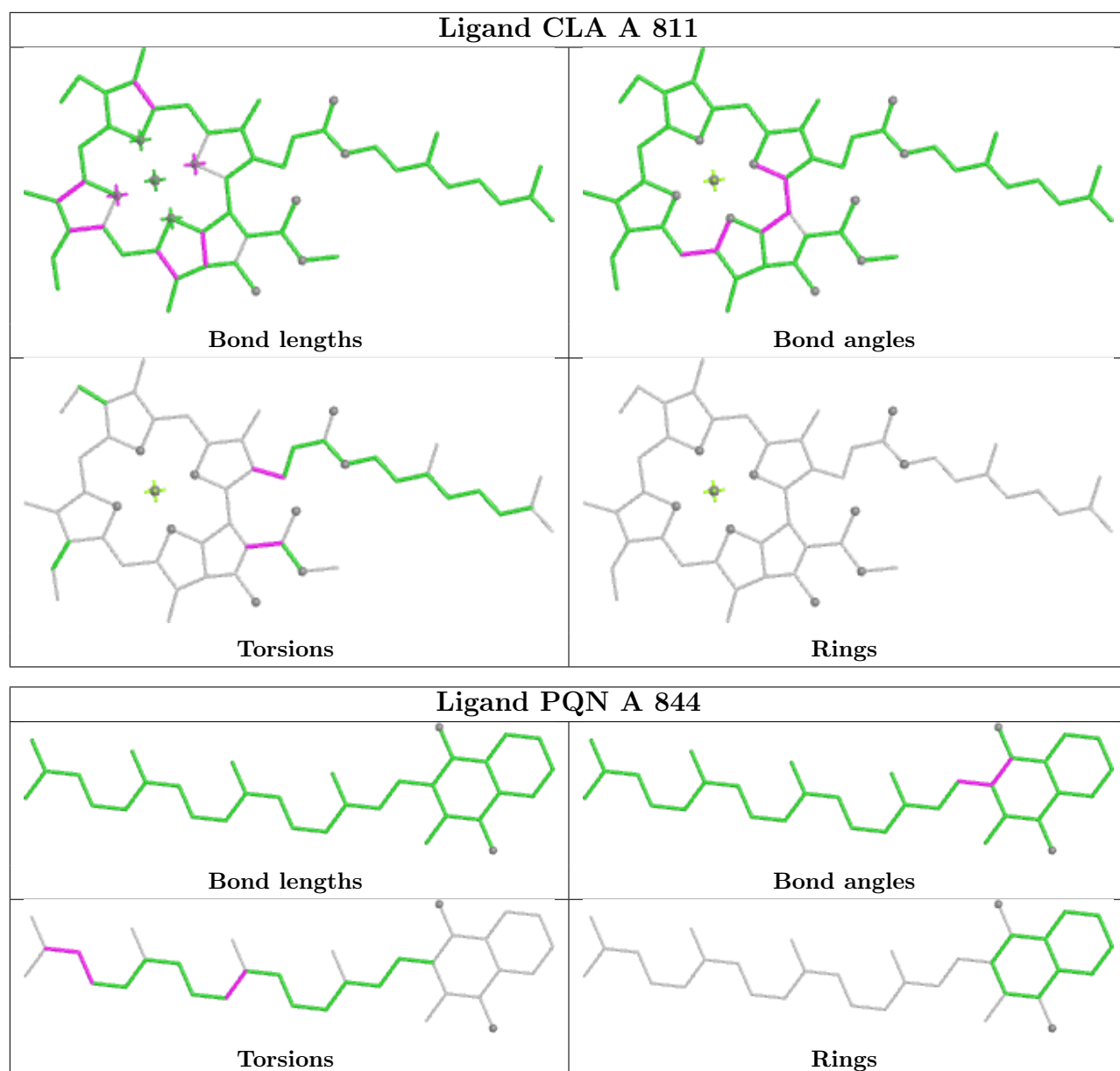




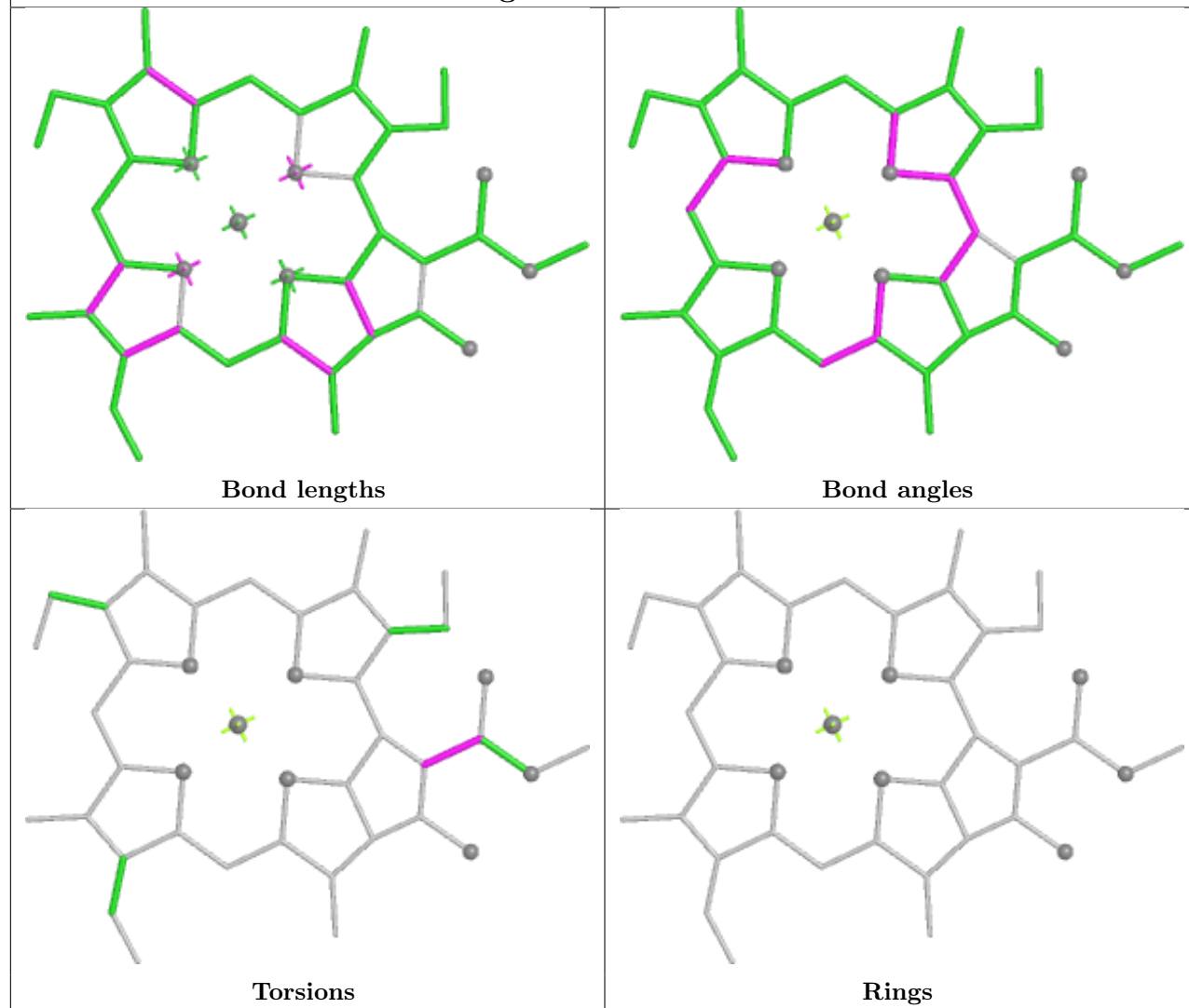




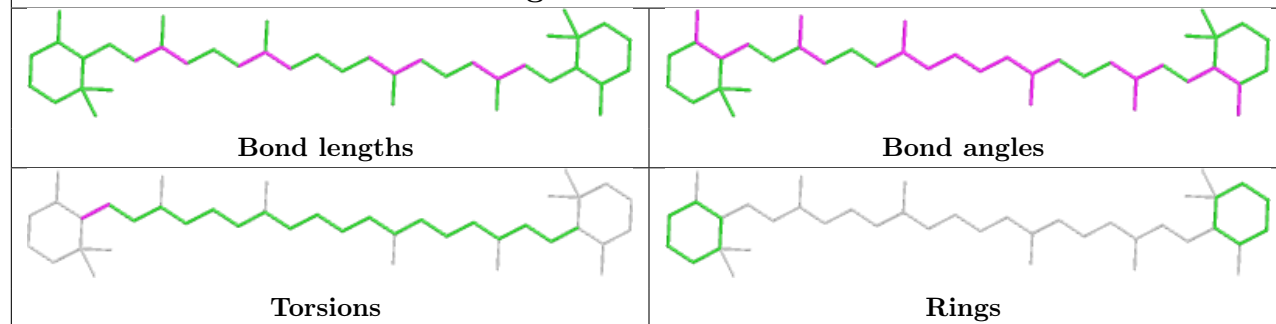


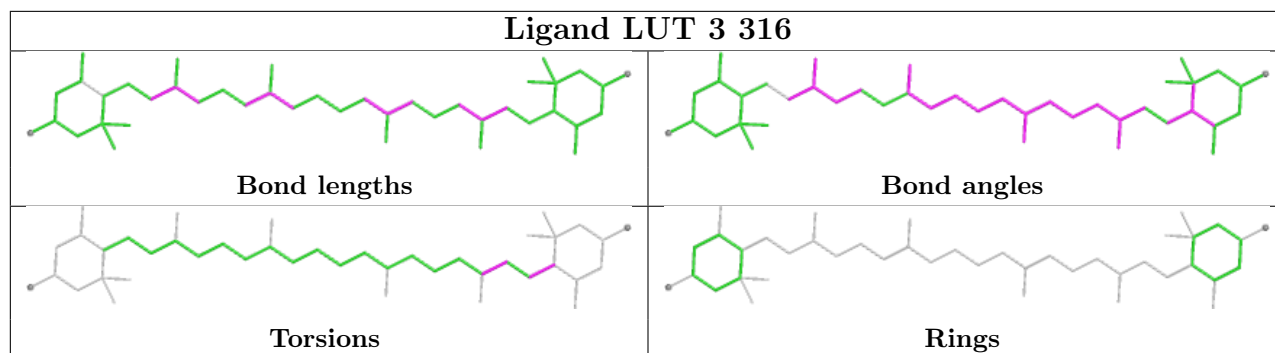
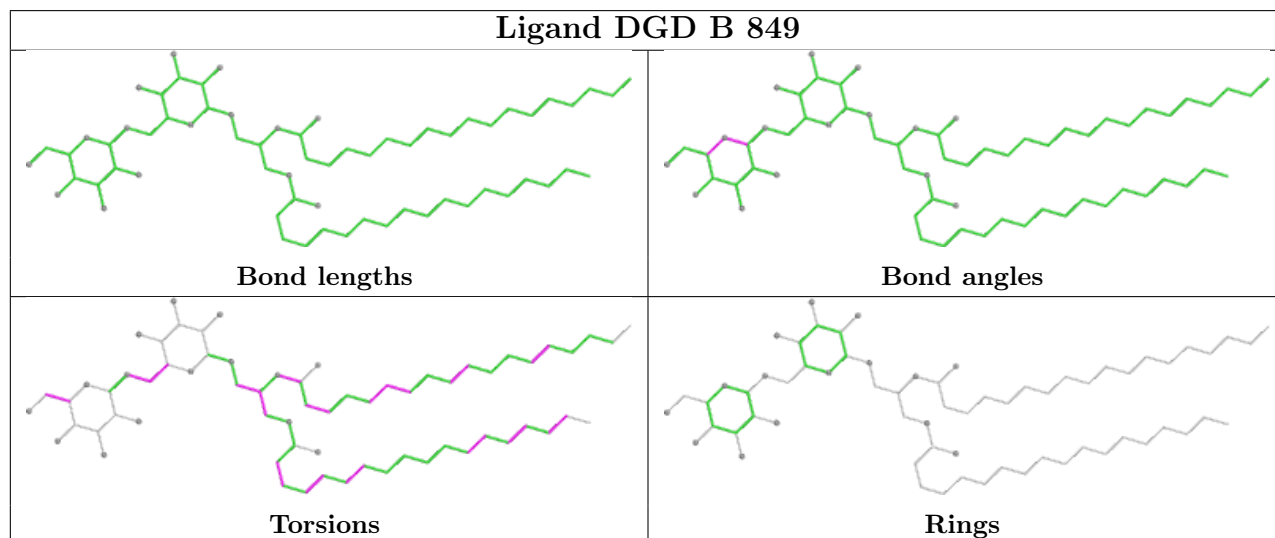
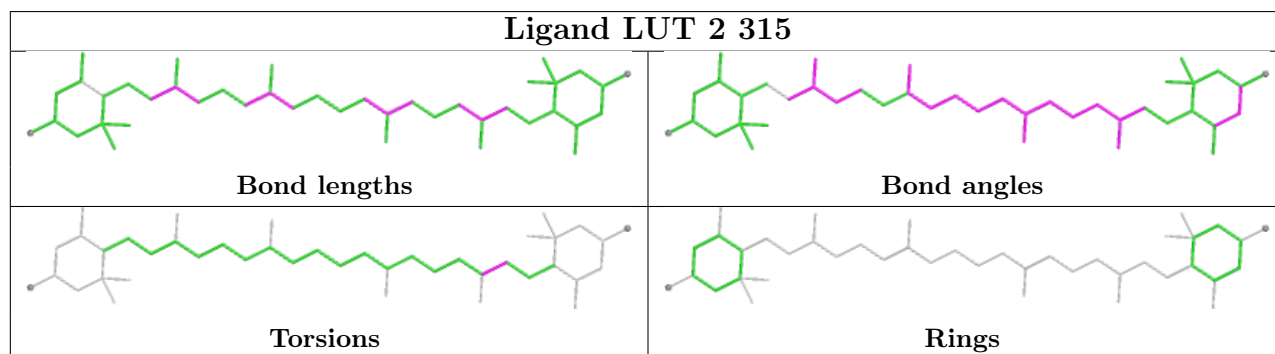


Ligand CLA J 102

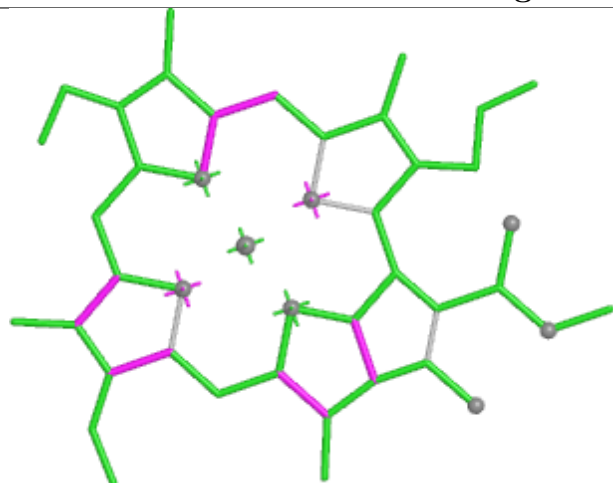


Ligand BCR M 101

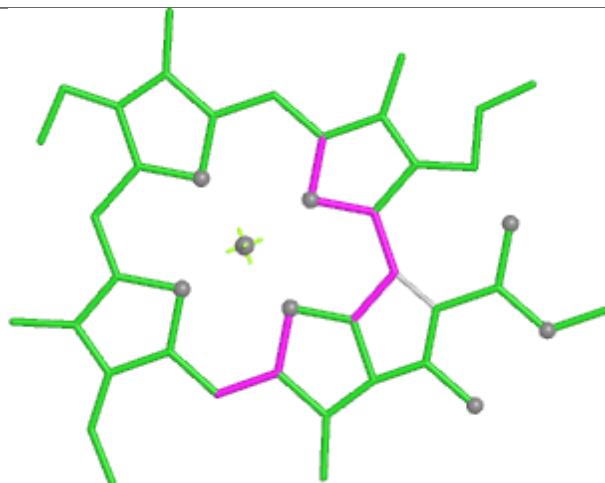


Ligand LUT 3 316**Ligand DGD B 849****Ligand LUT 2 315**

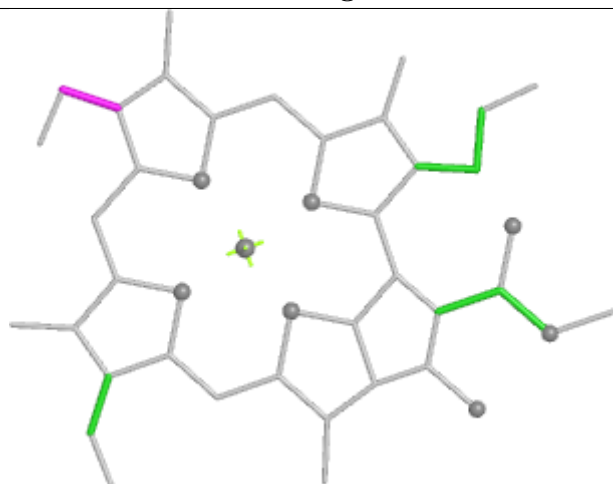
Ligand CLA B 821



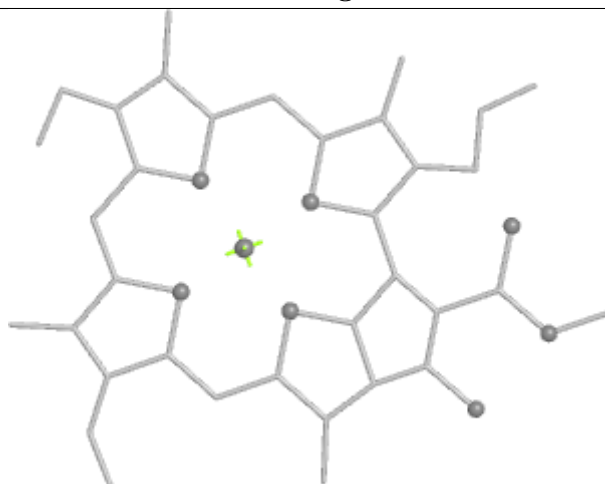
Bond lengths



Bond angles

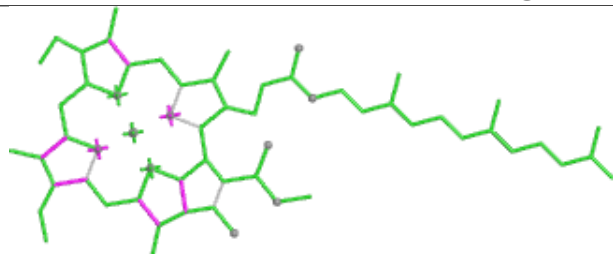


Torsions

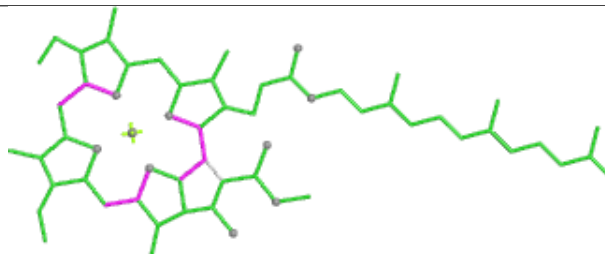


Rings

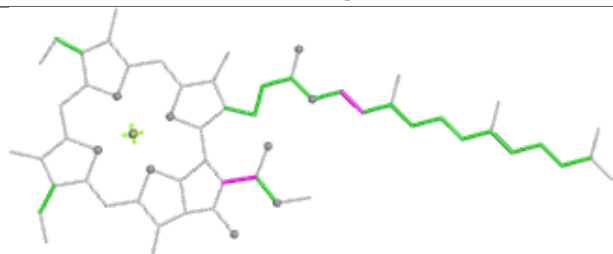
Ligand CLA 5 309



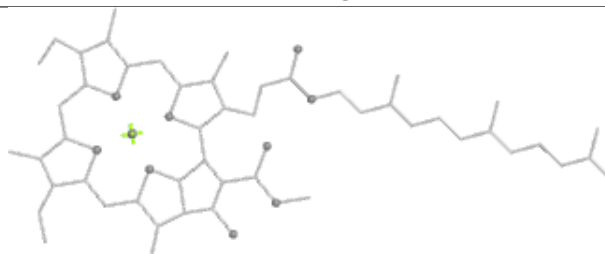
Bond lengths



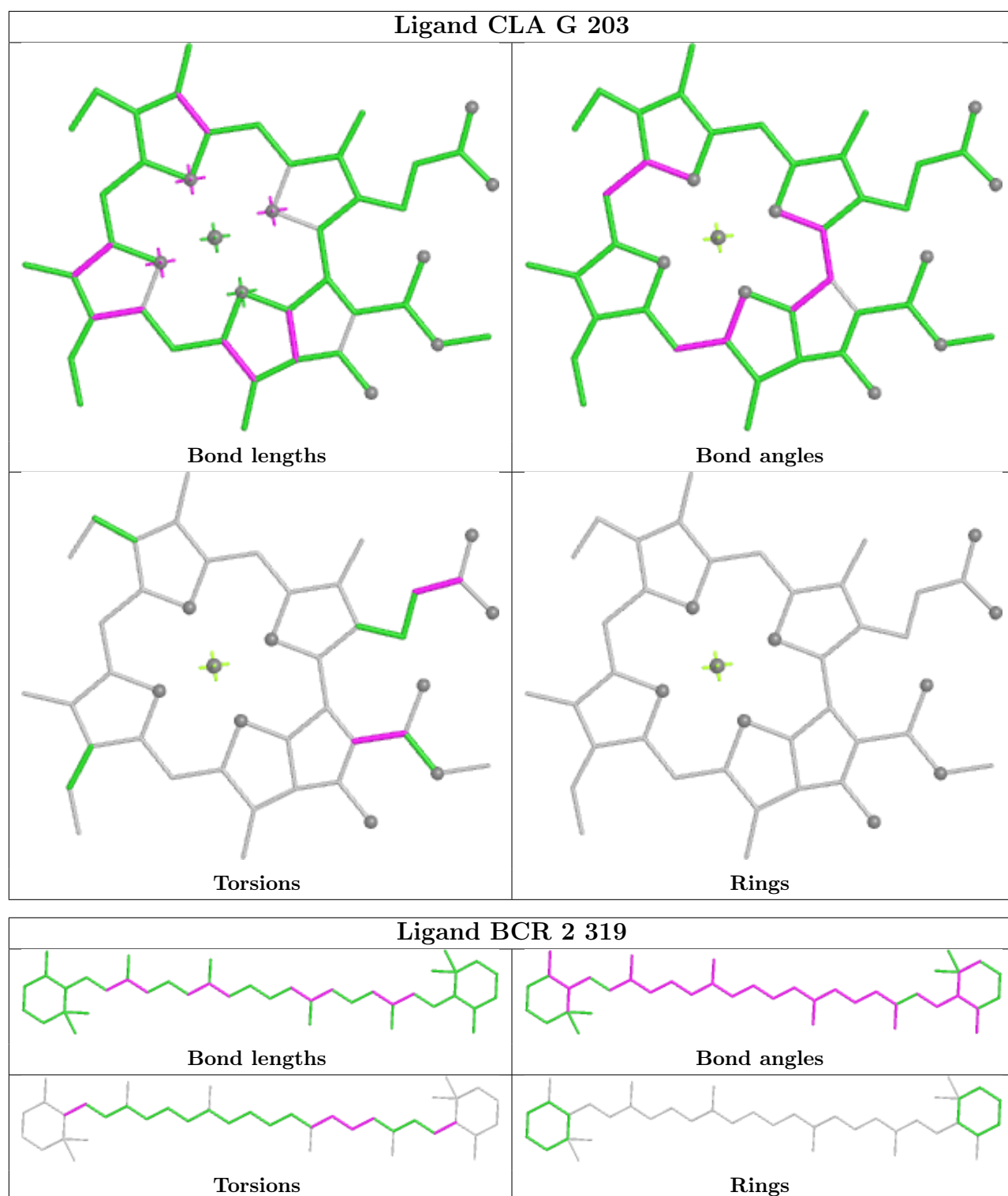
Bond angles

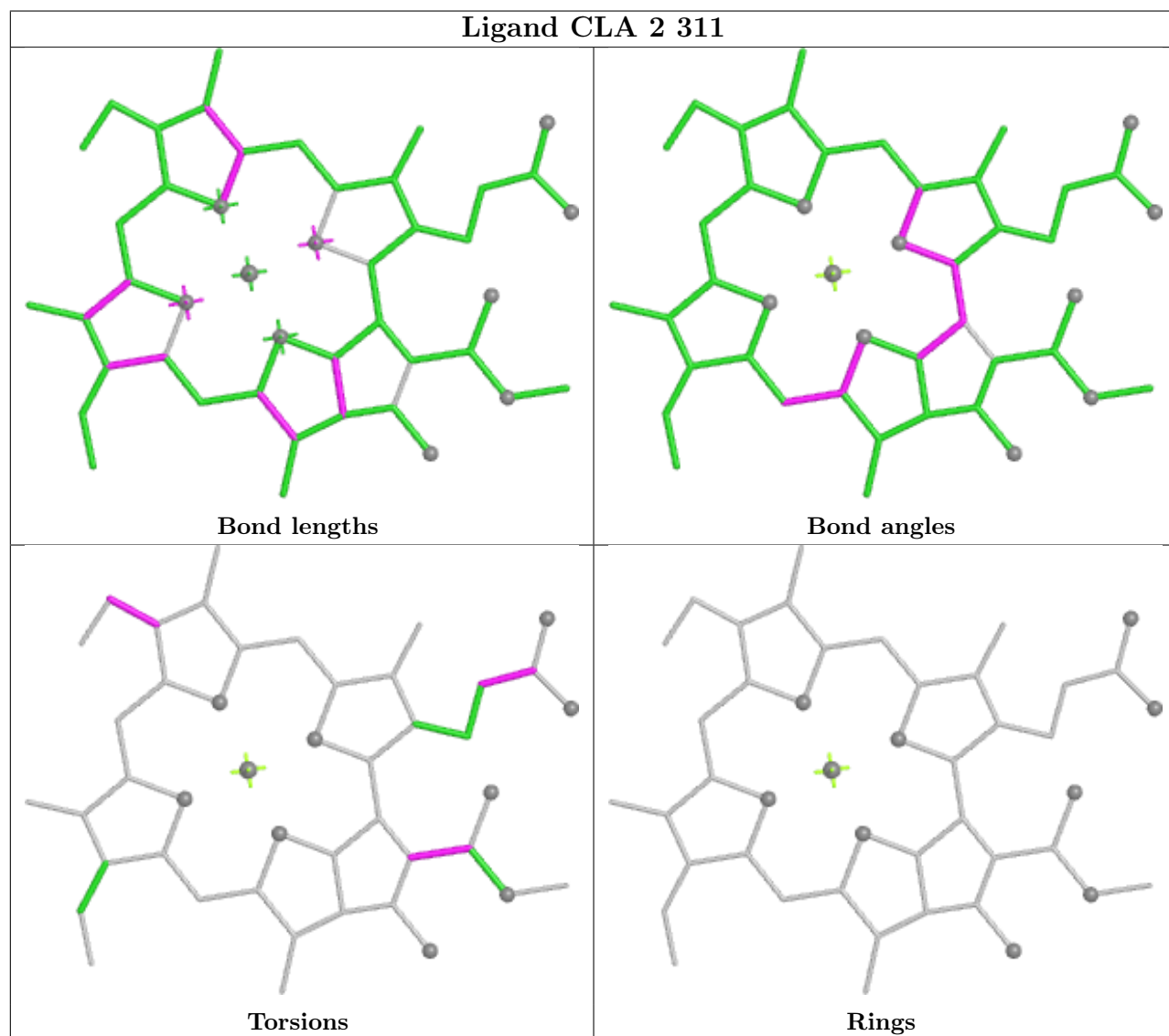
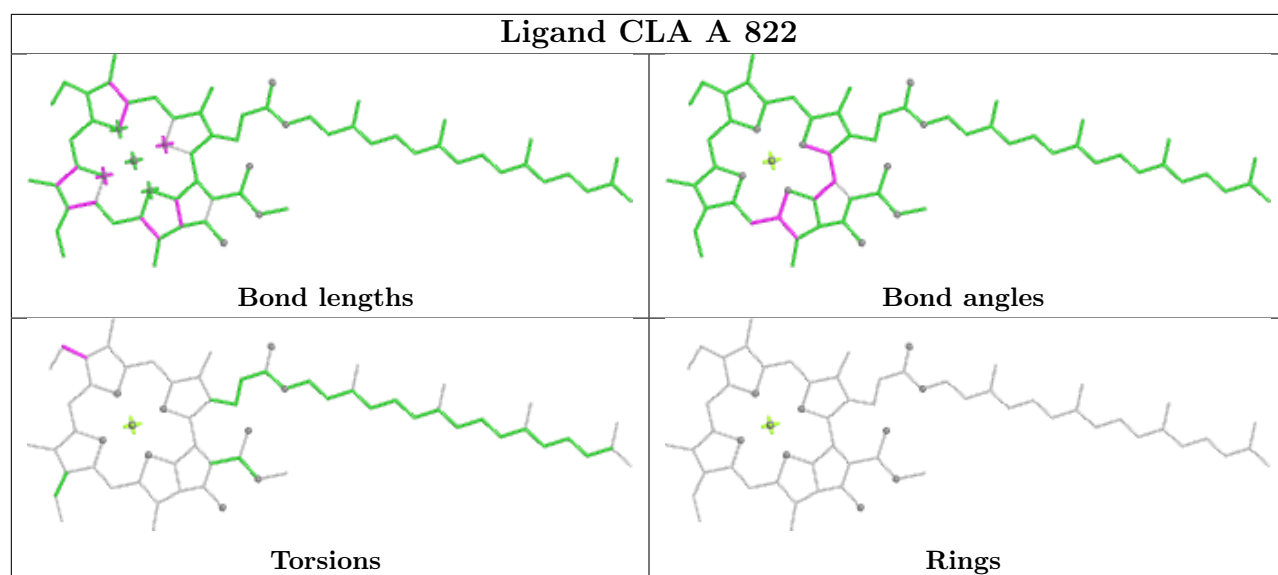


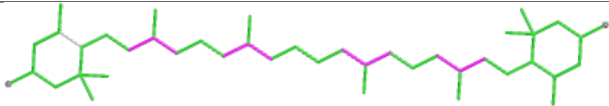
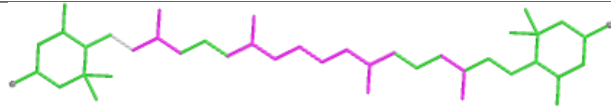
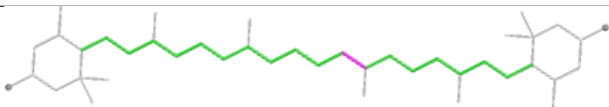
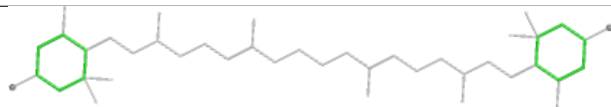
Torsions

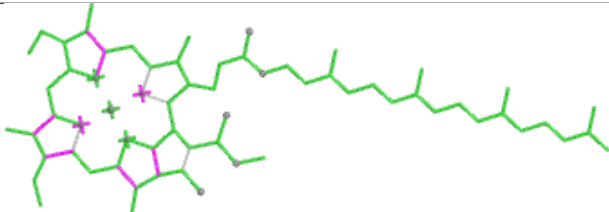
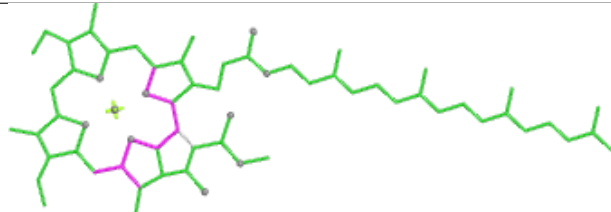
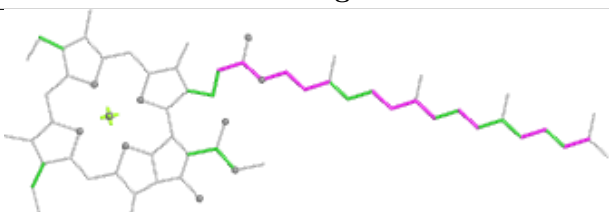
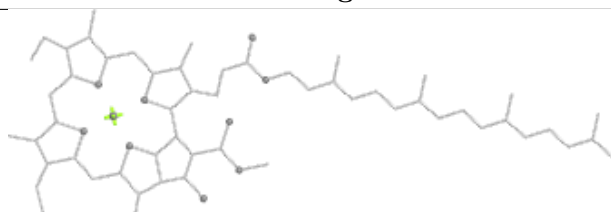


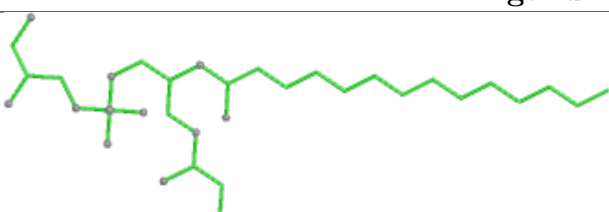
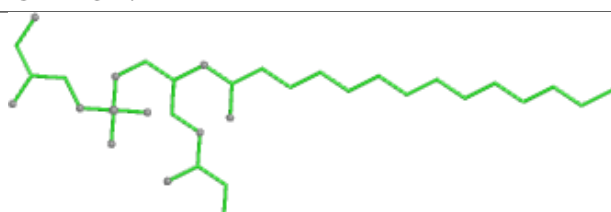
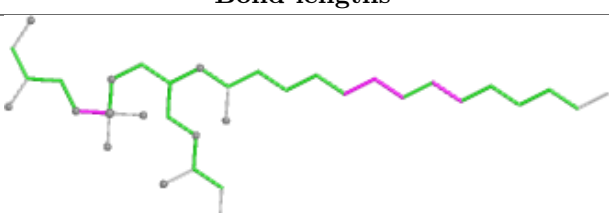
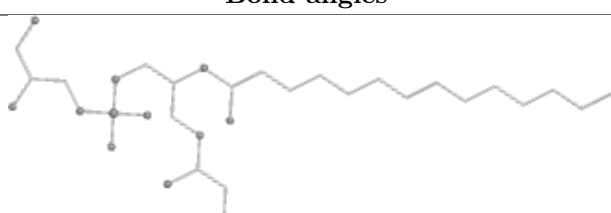
Rings

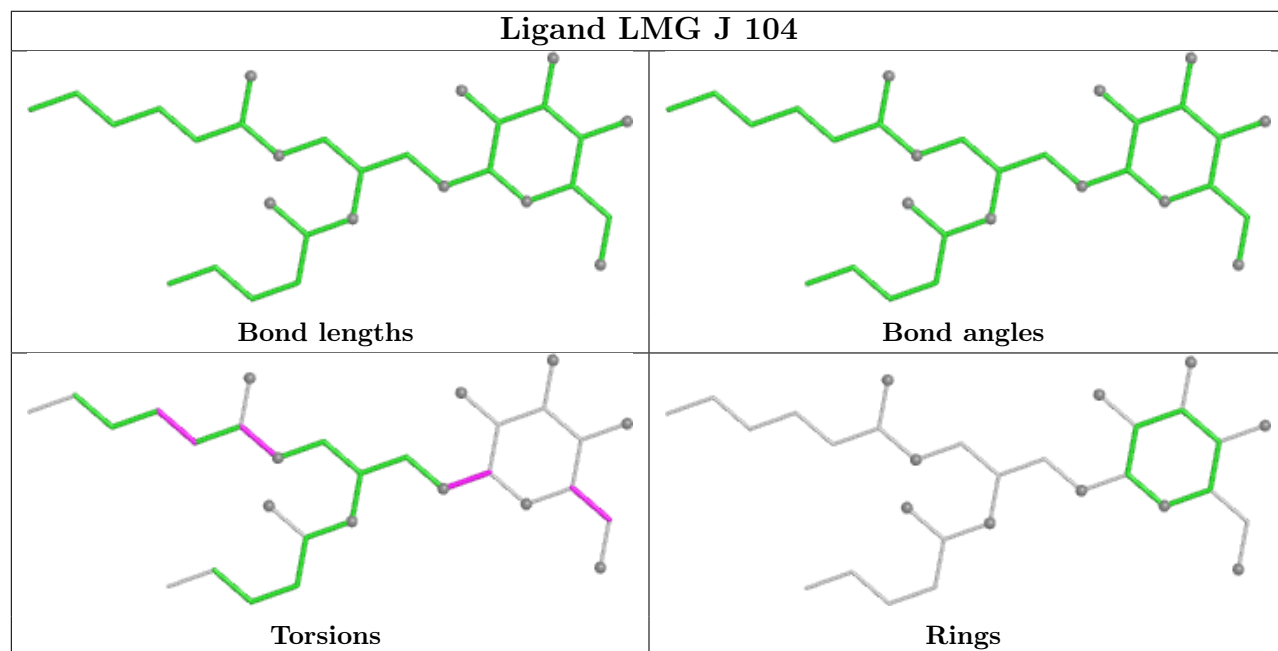
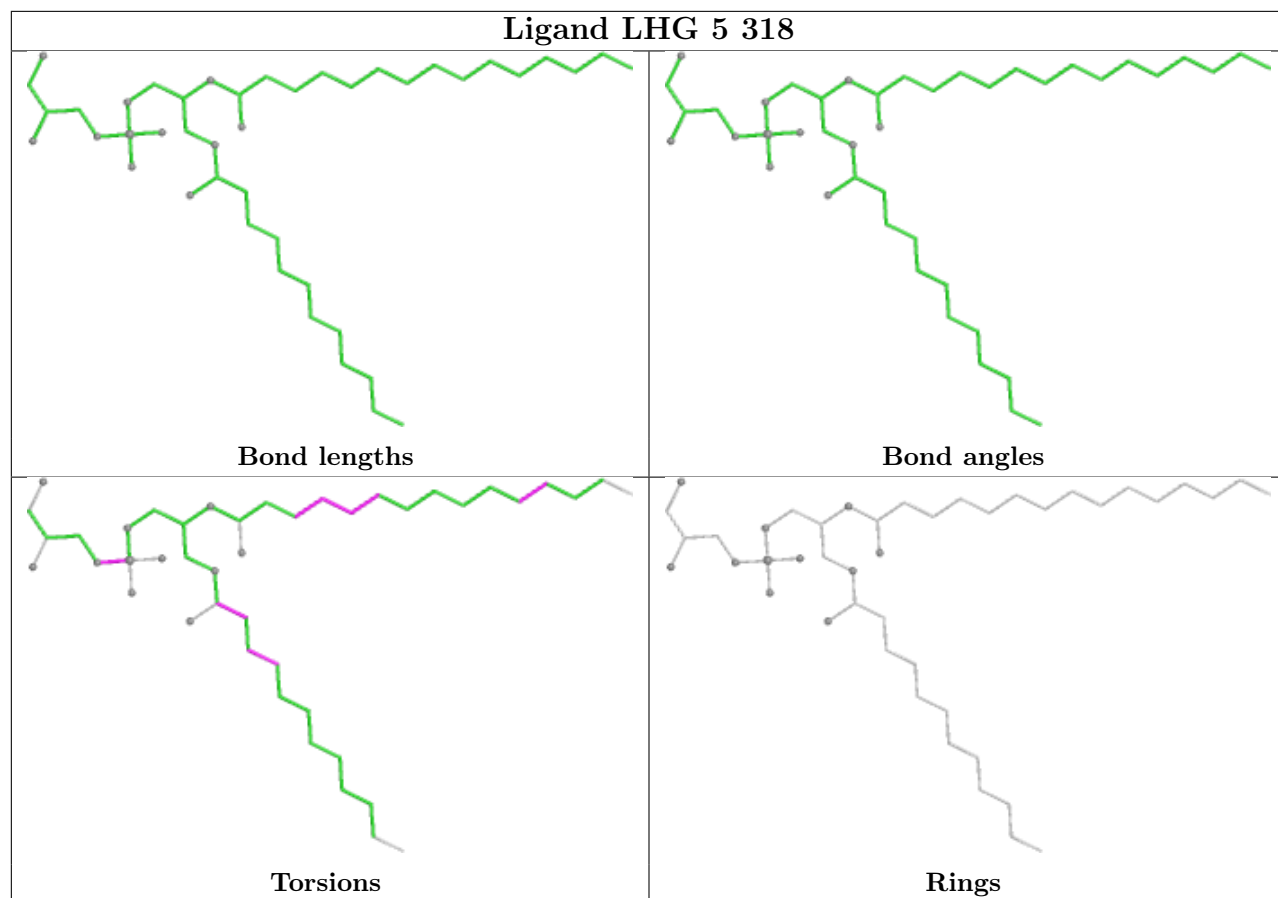


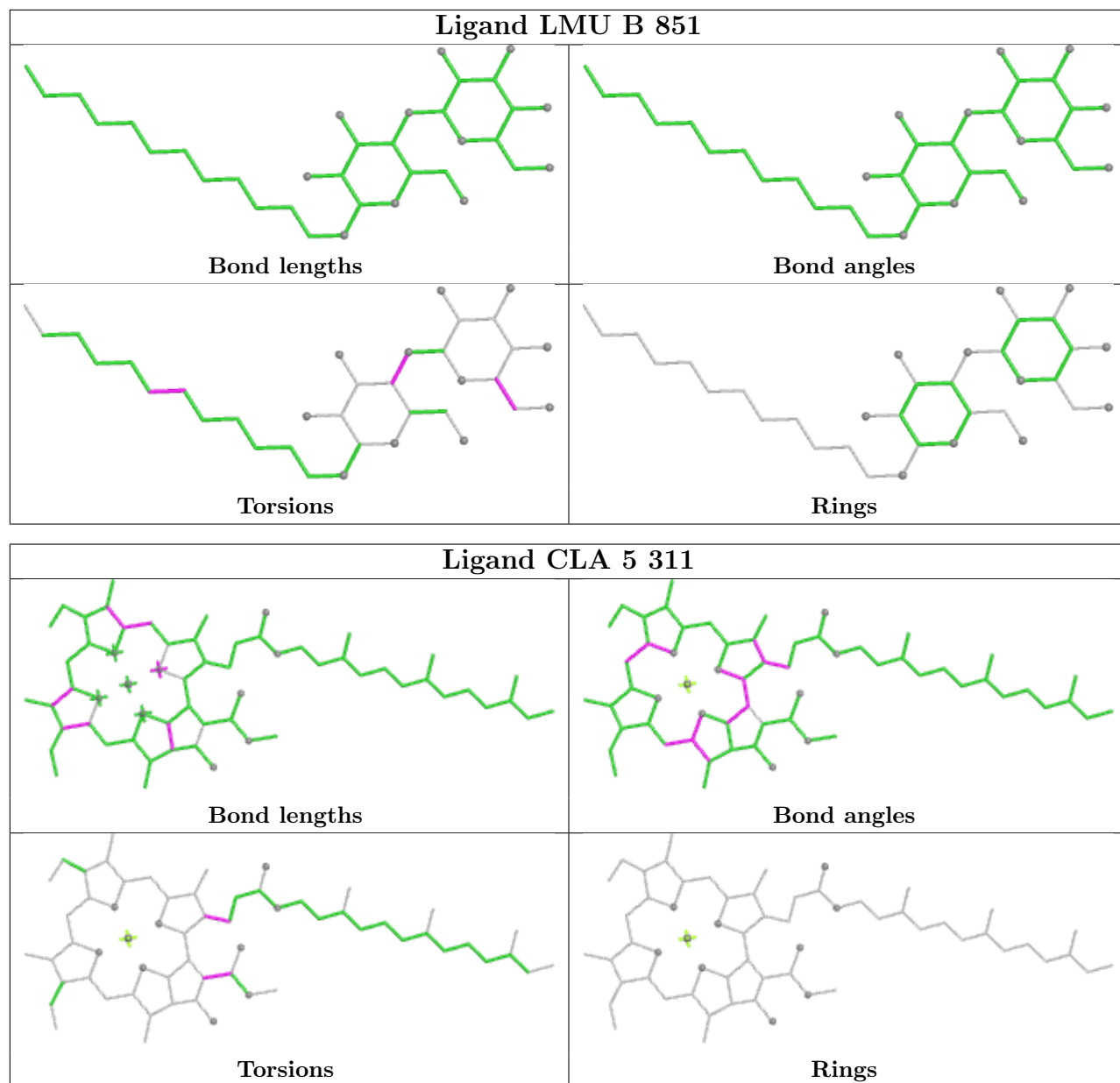


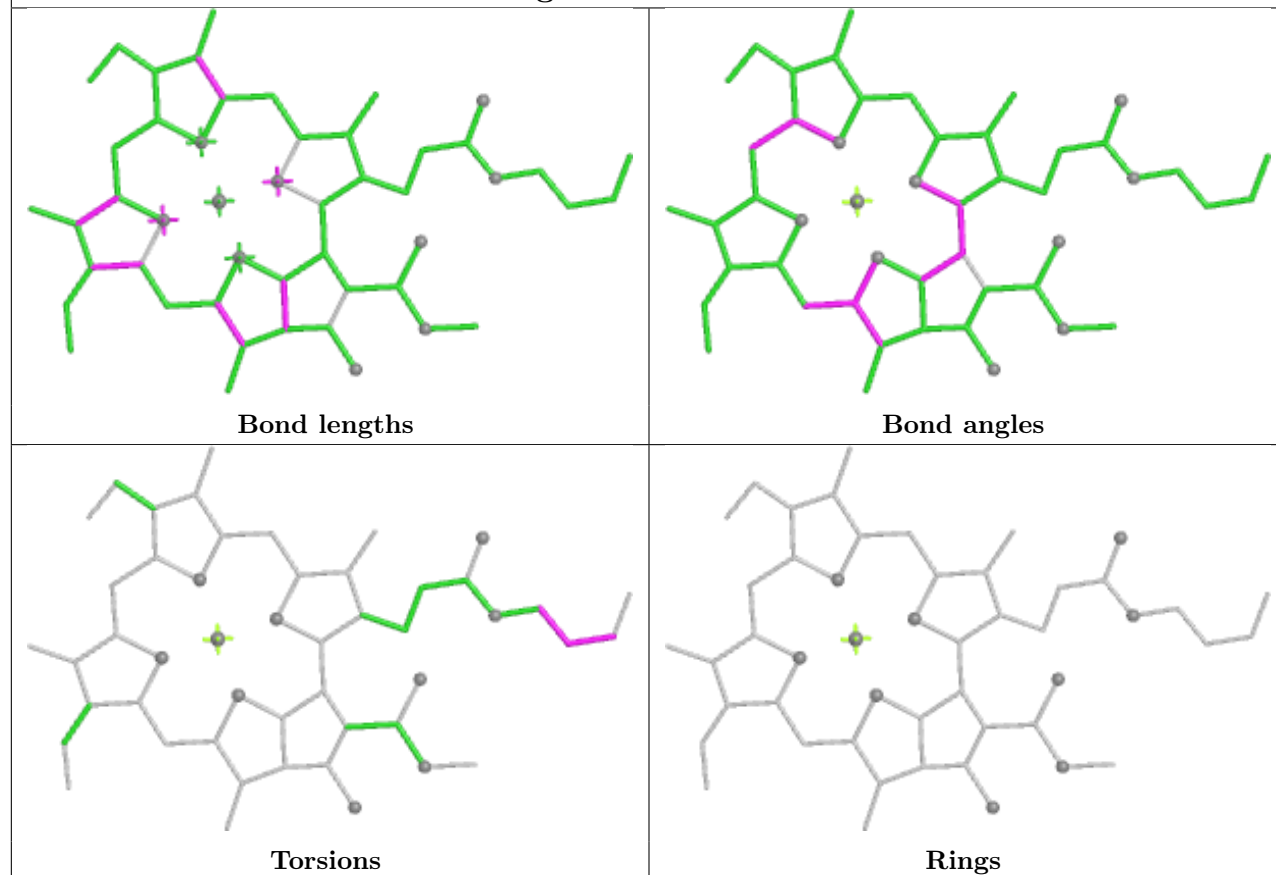
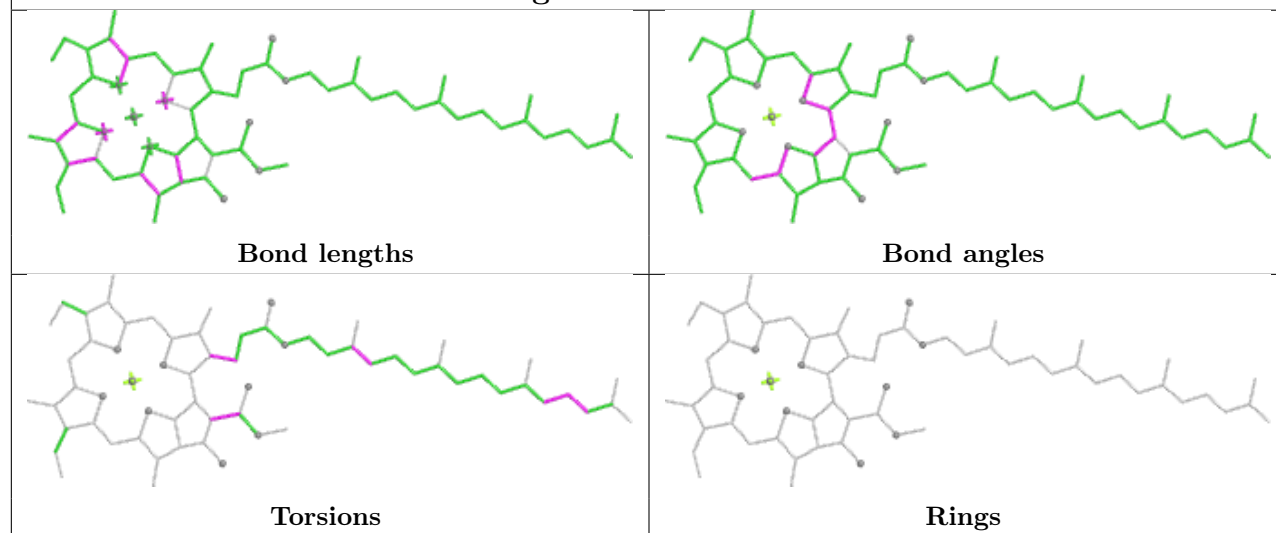
Ligand LUT 5 315	
	
Bond lengths	Bond angles
	
Torsions	Rings

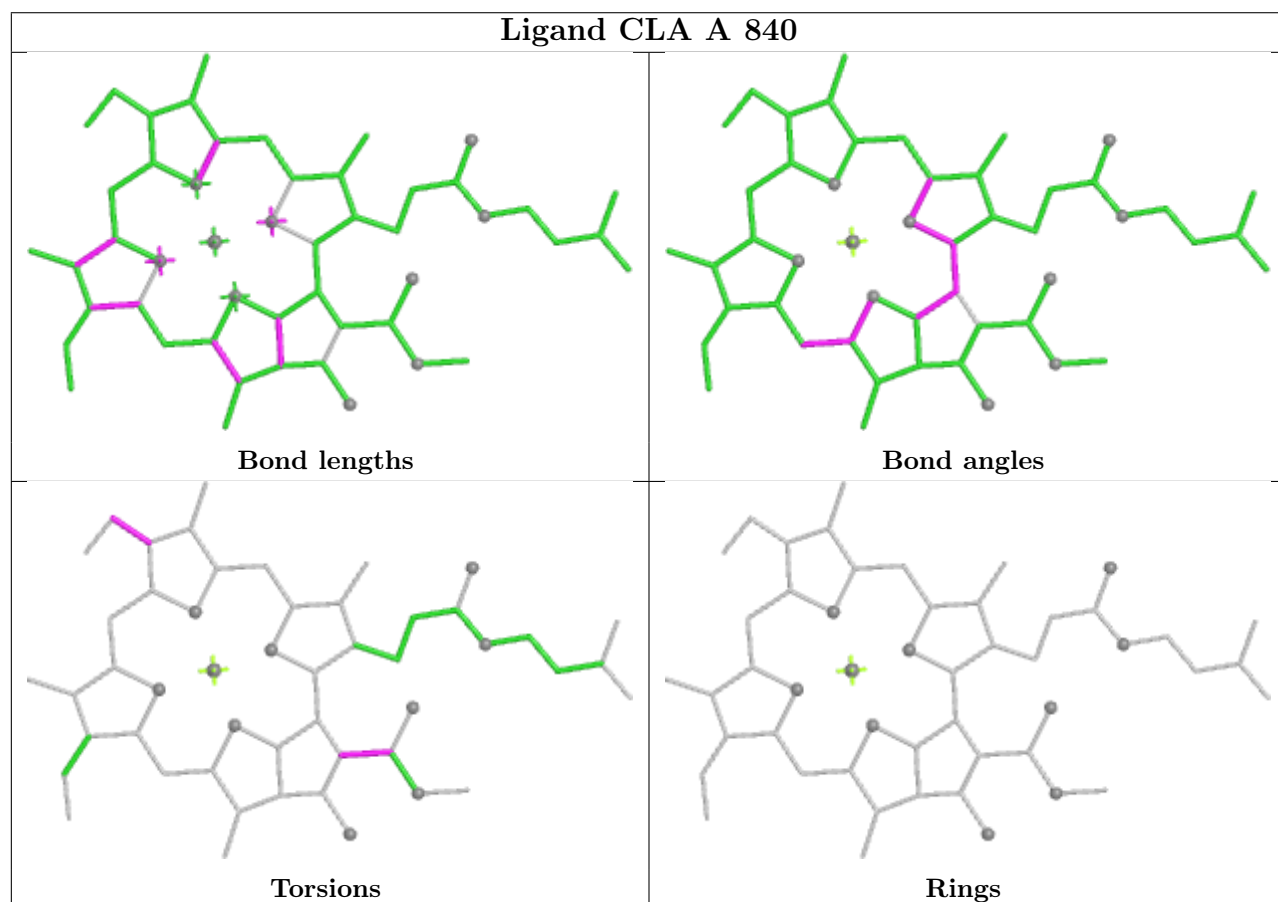
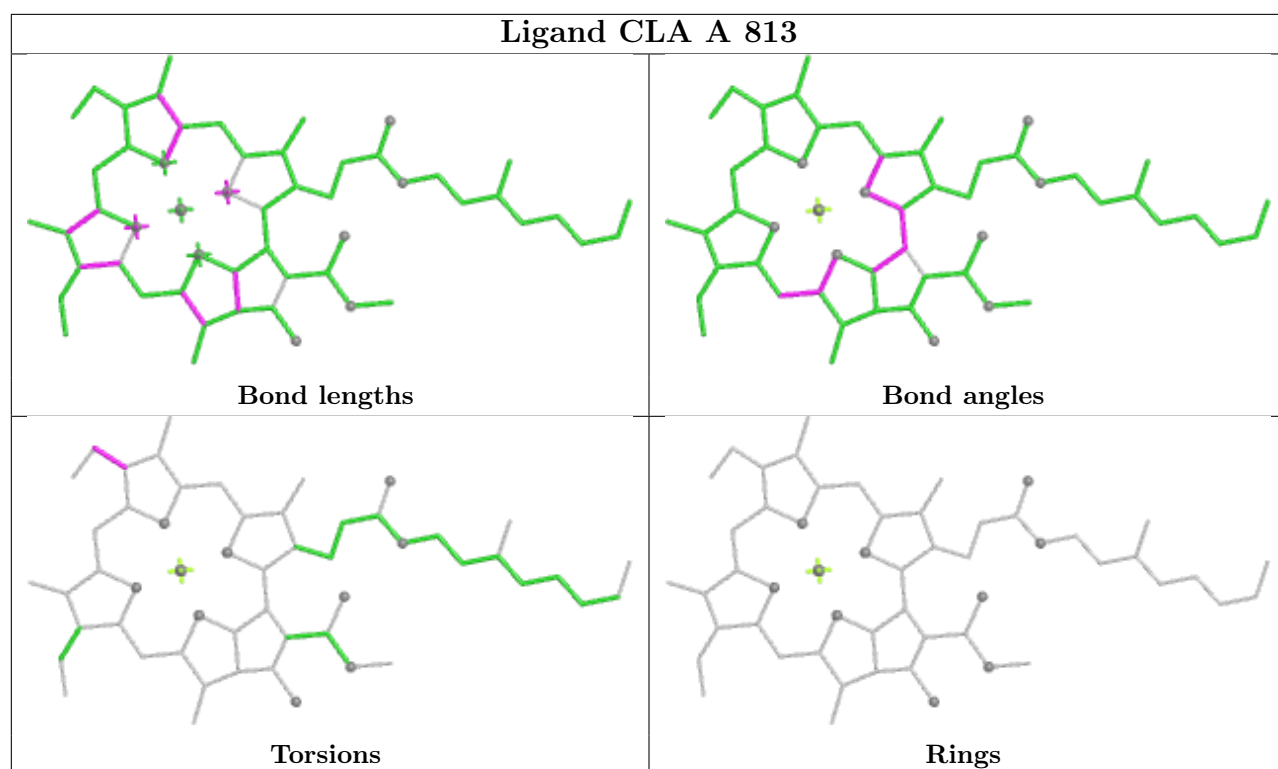
Ligand CLA A 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

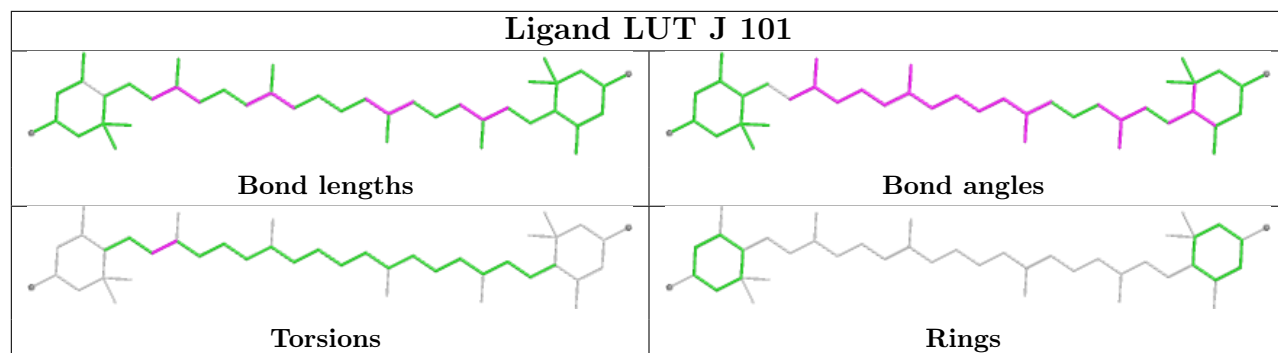
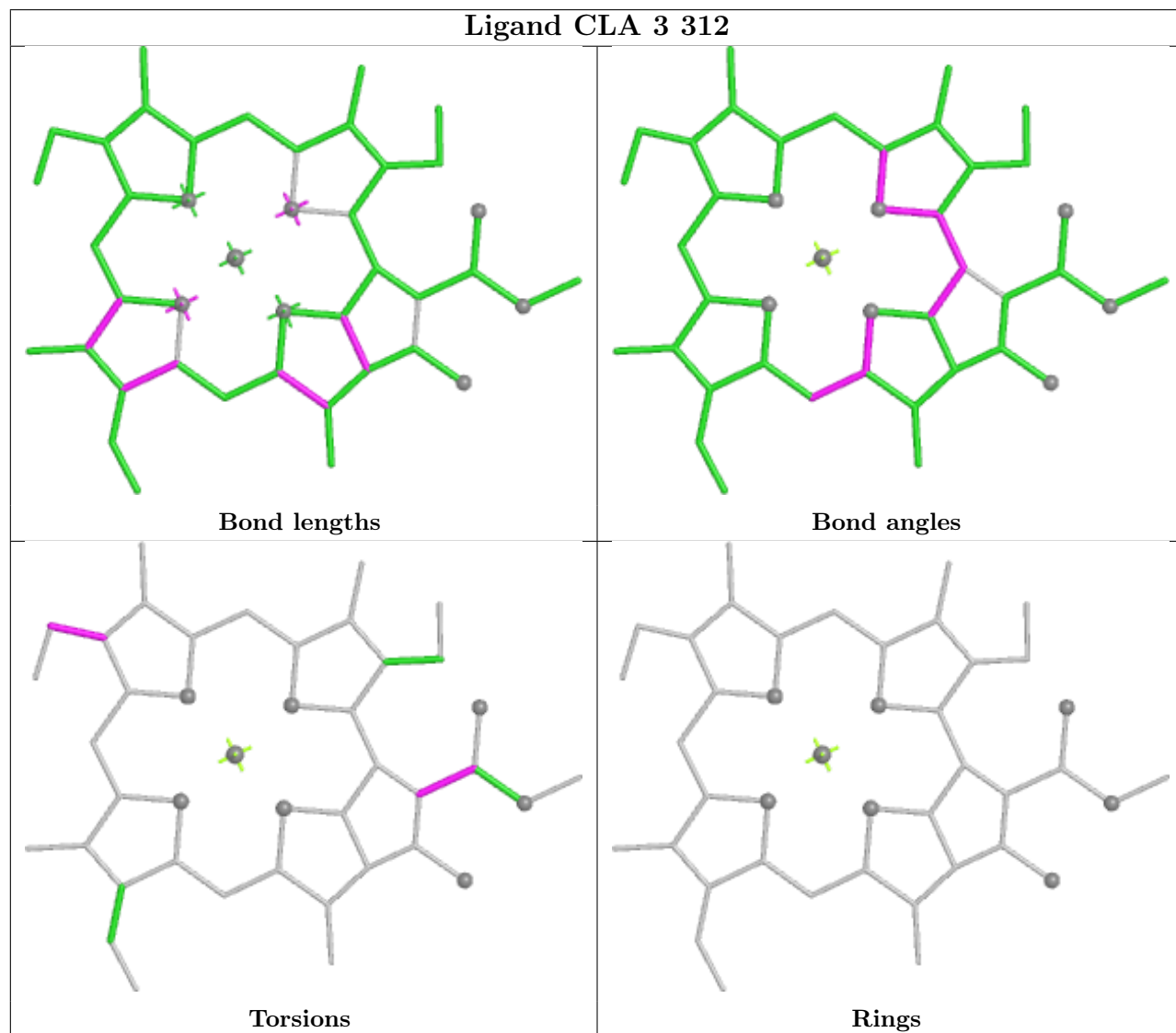
Ligand LHG A 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

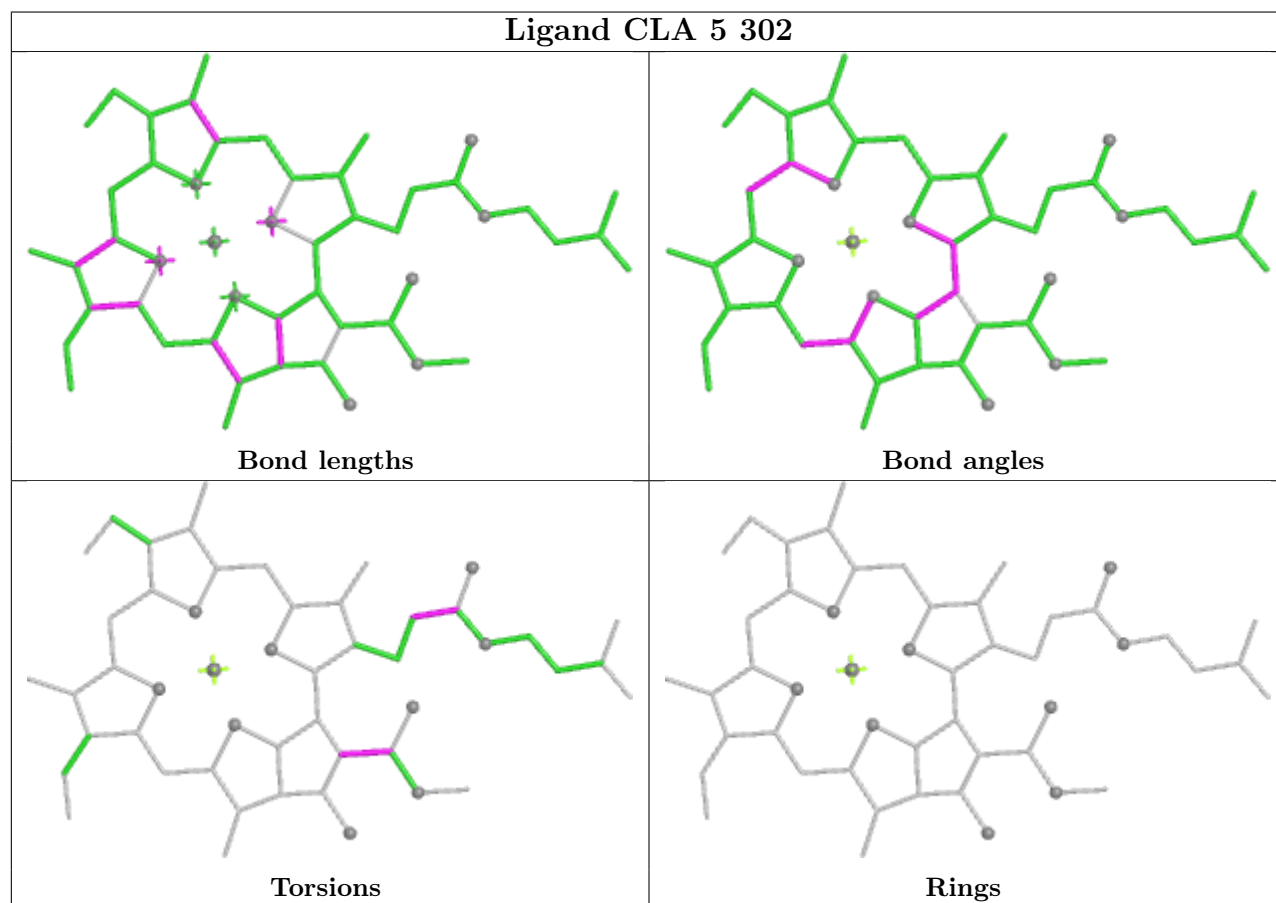
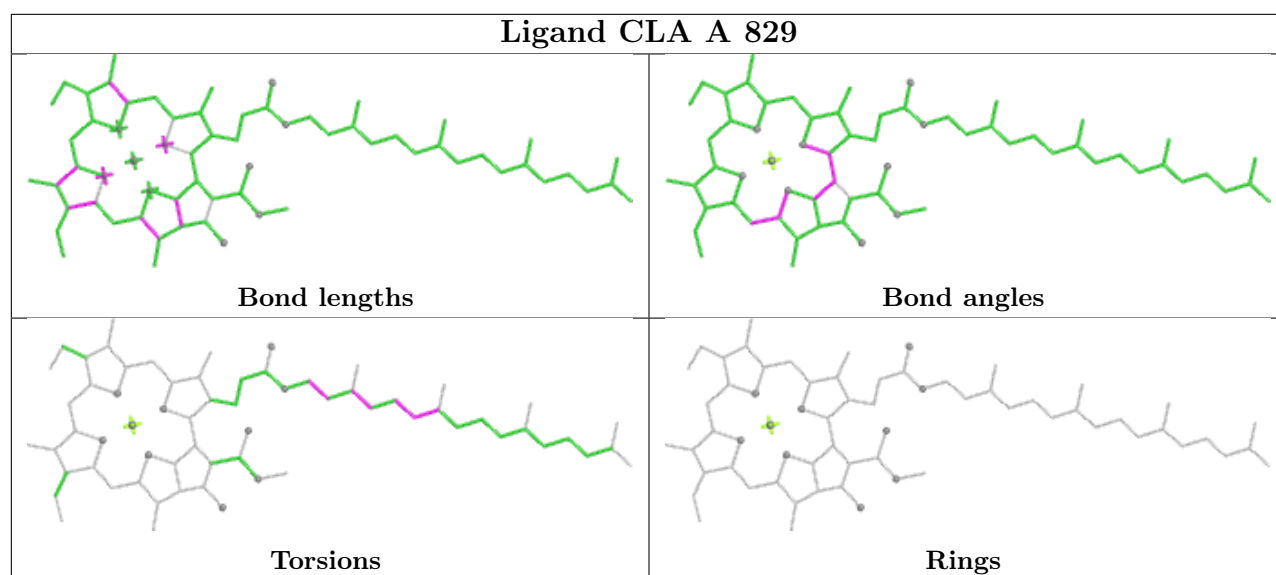


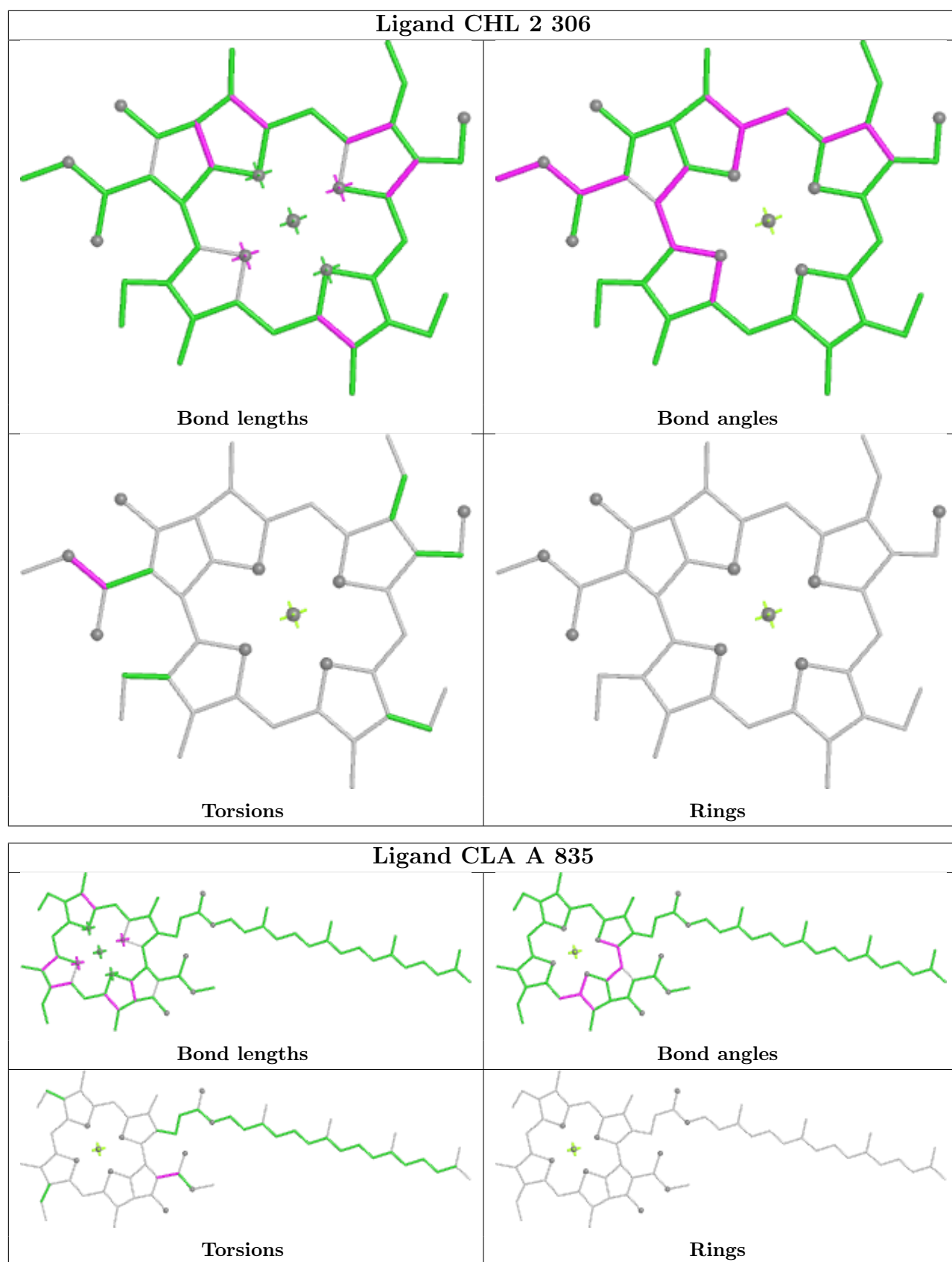


Ligand CLA 6 304**Ligand CLA B 814**

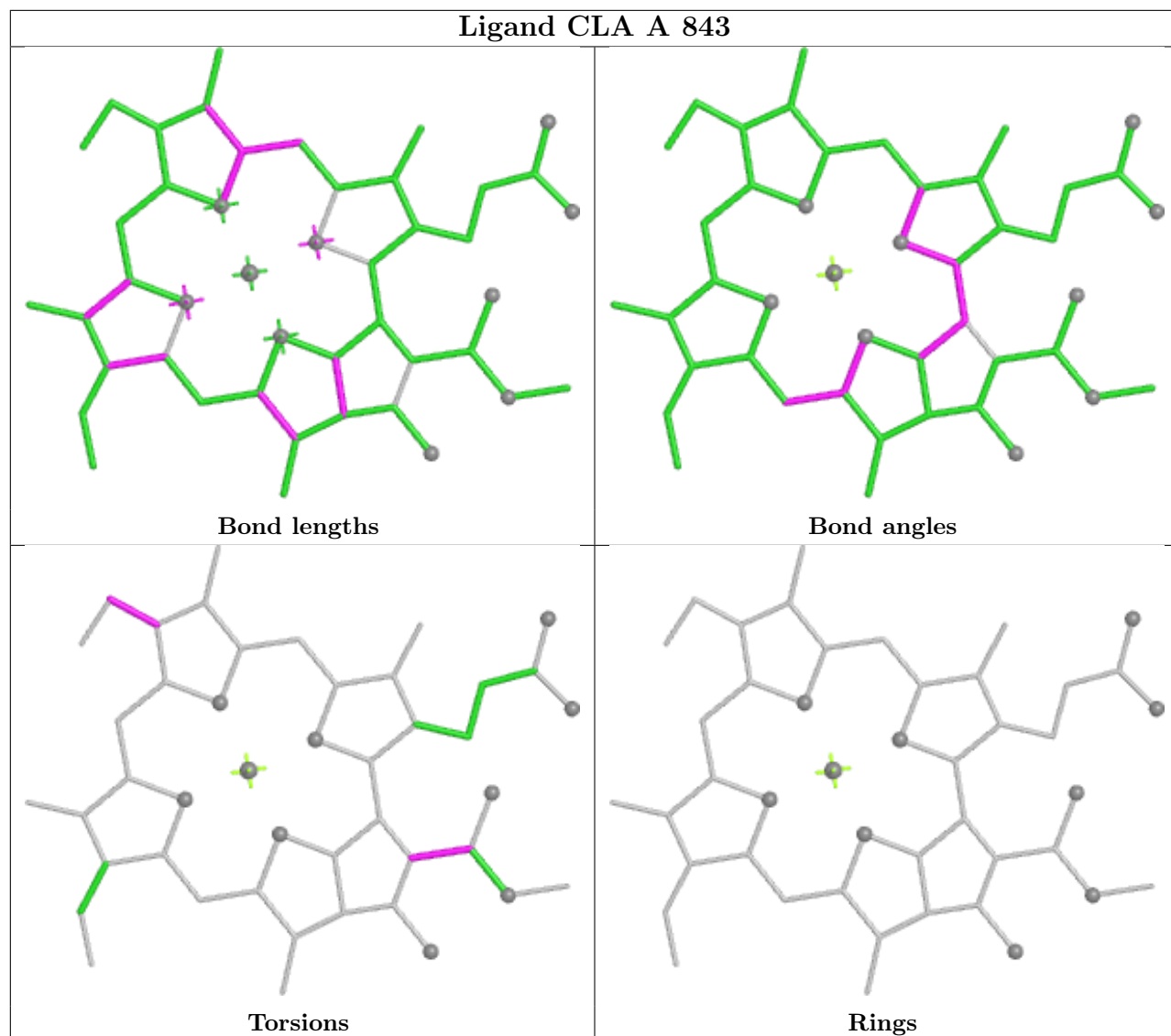


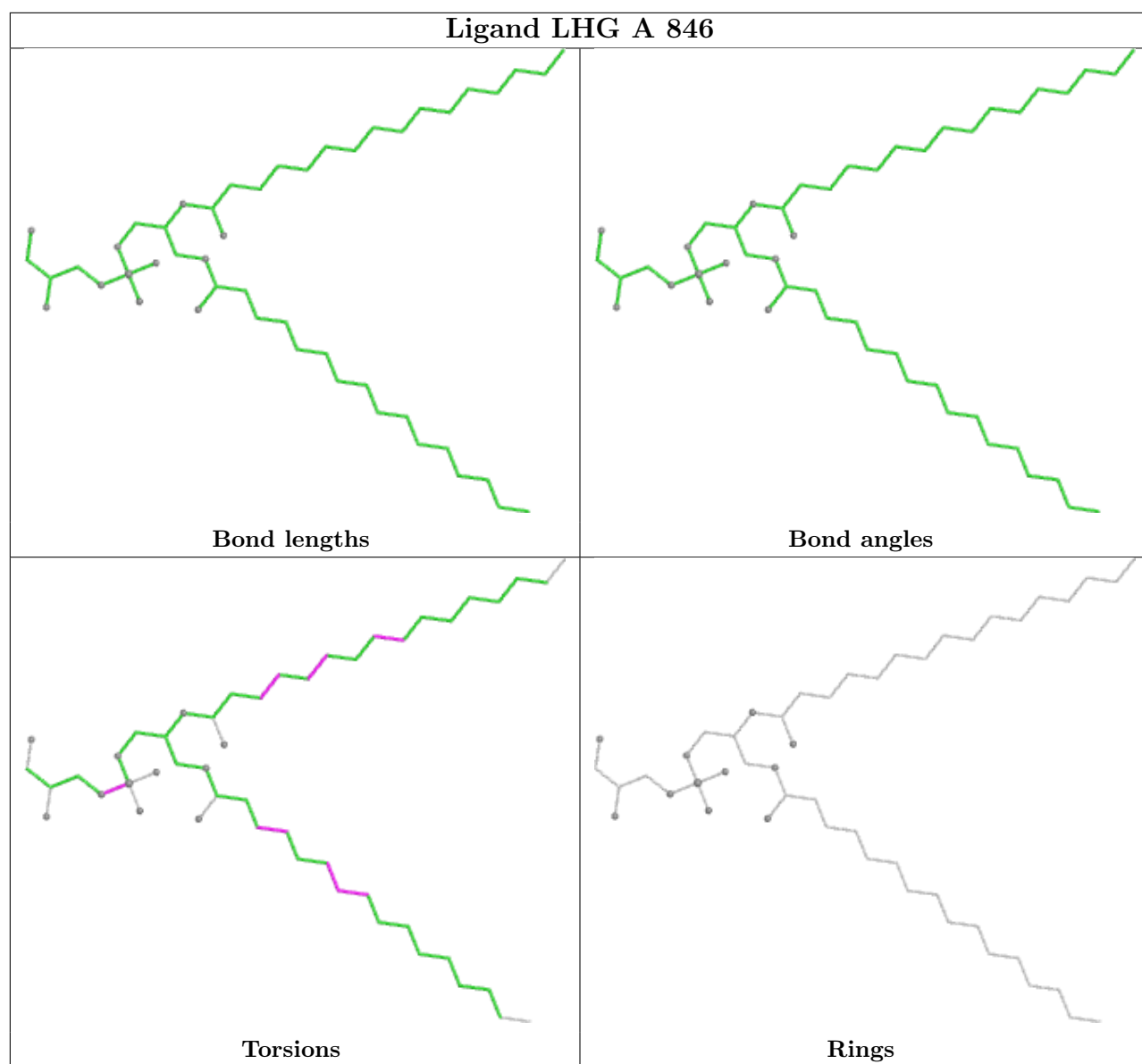
Ligand LUT J 101**Ligand CLA 3 312**

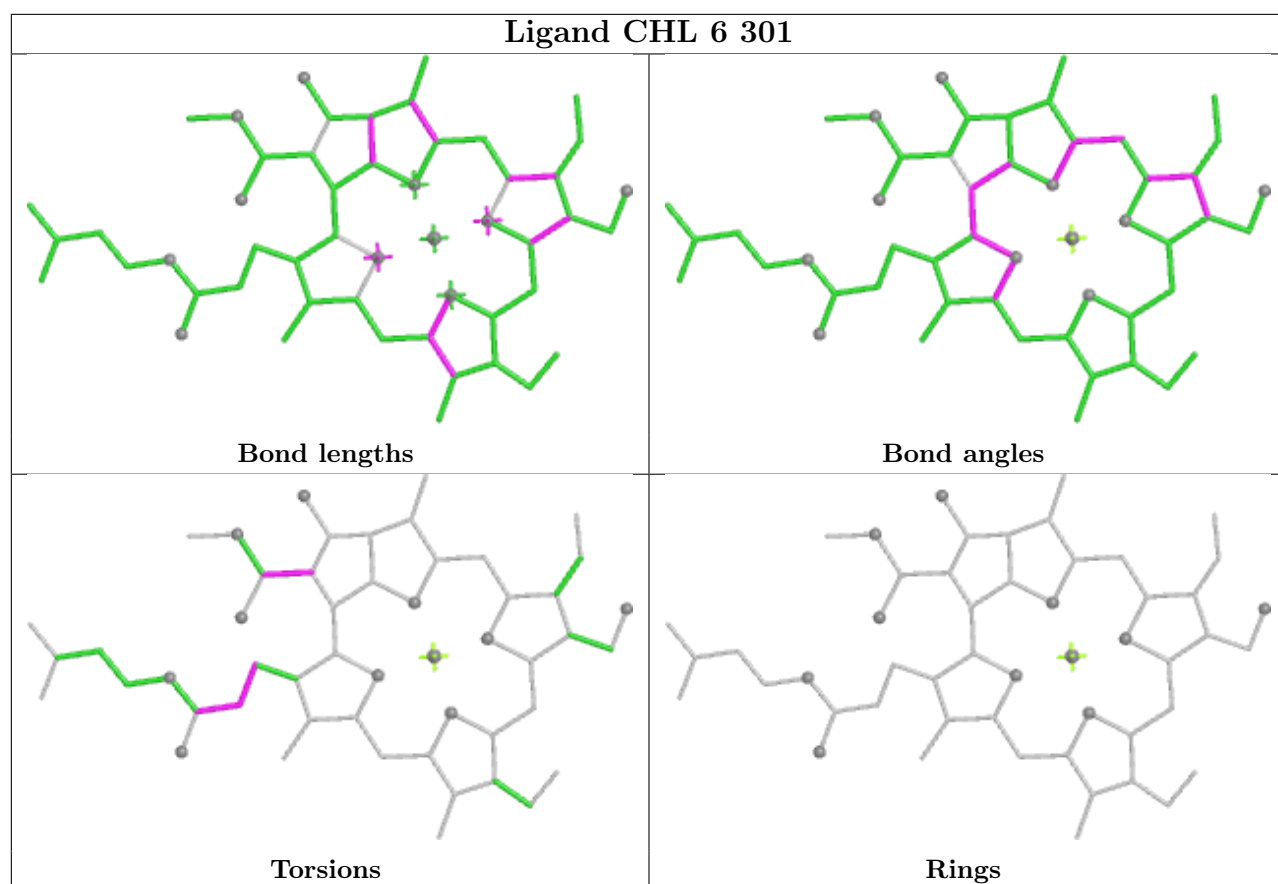


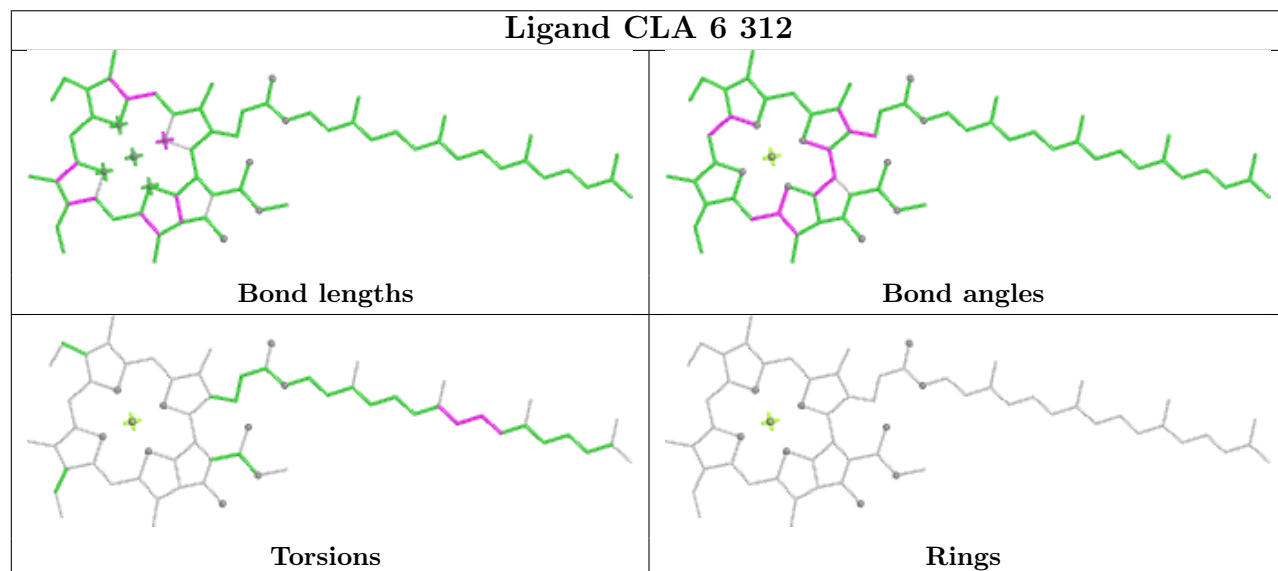
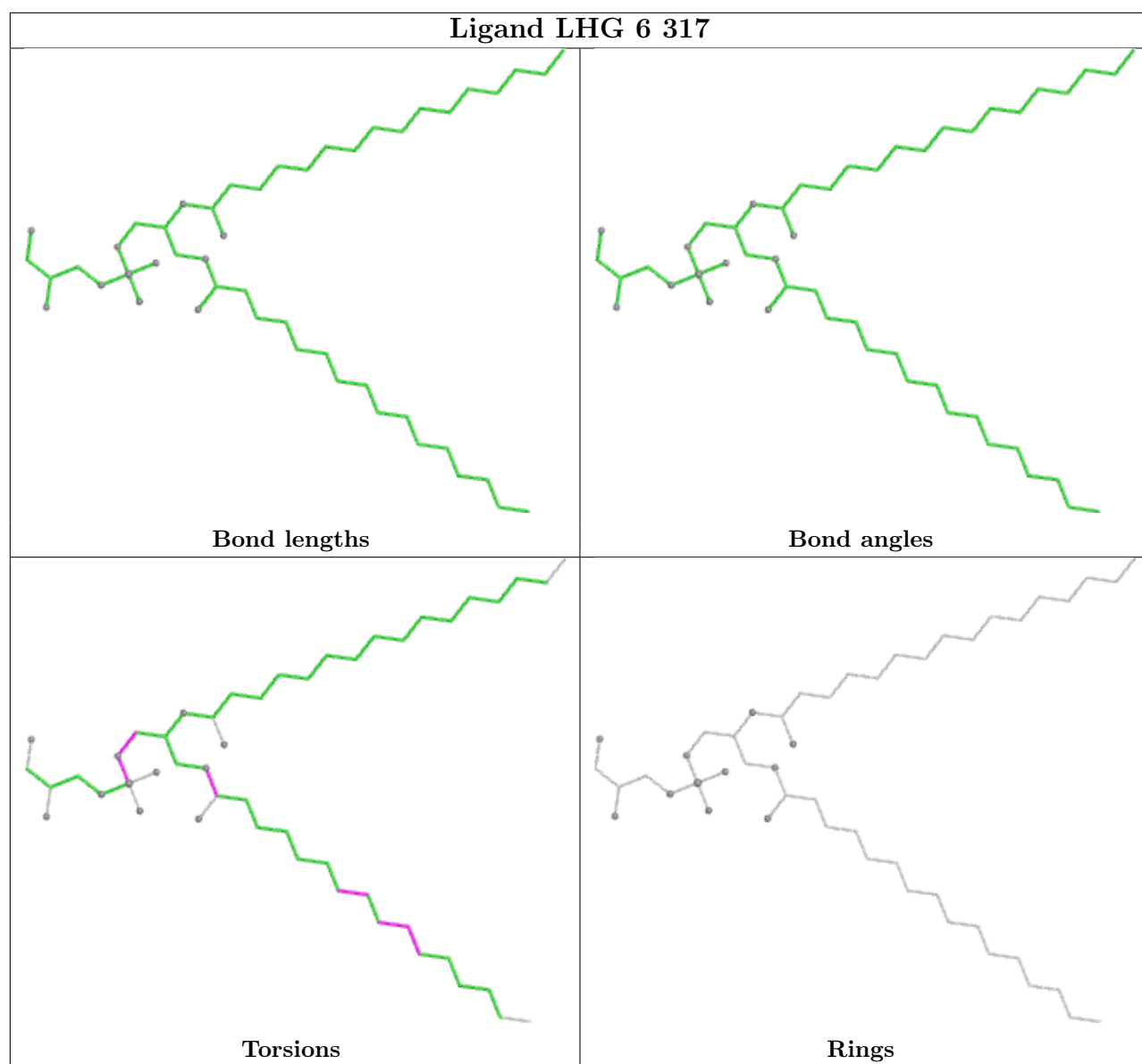


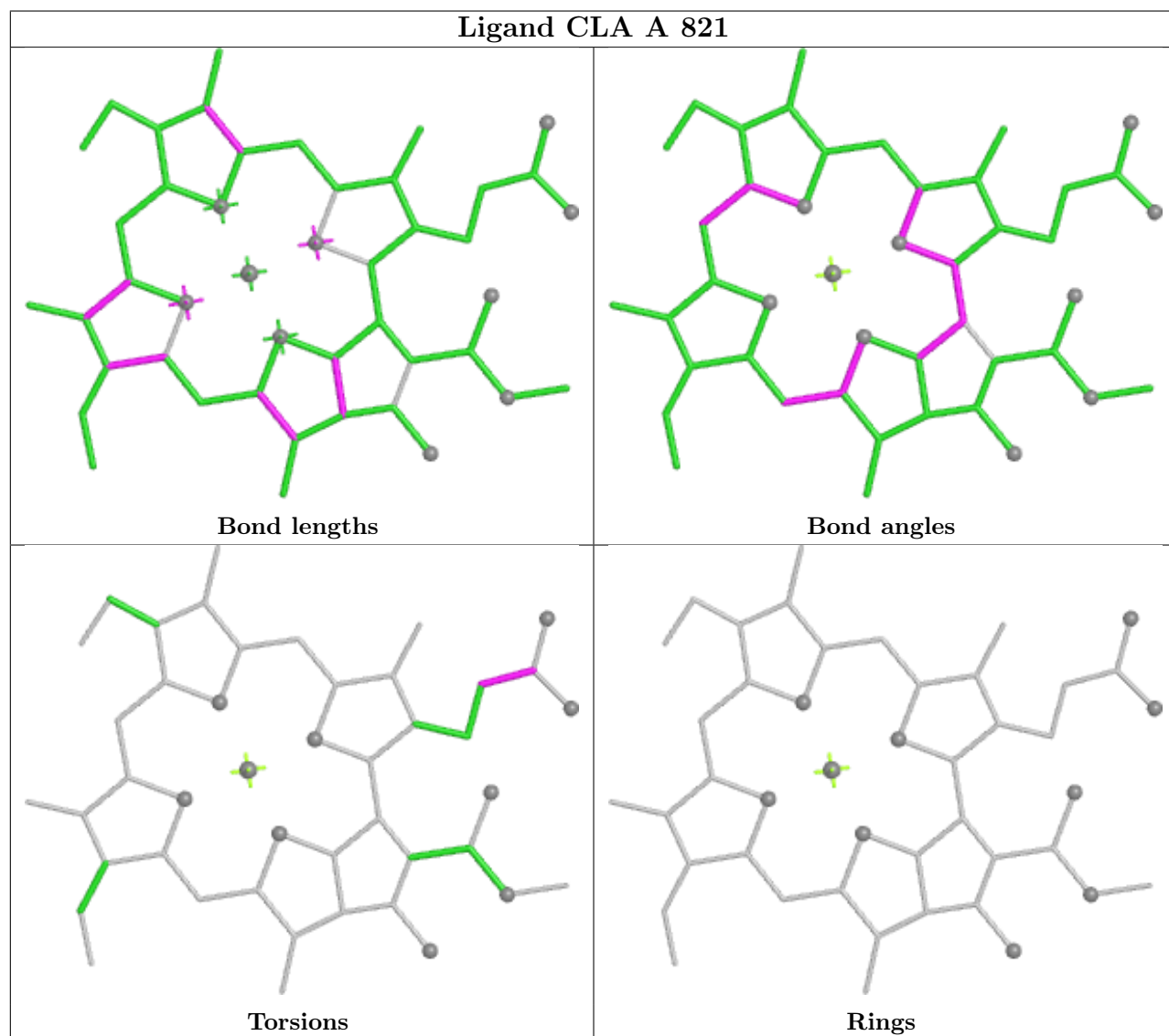
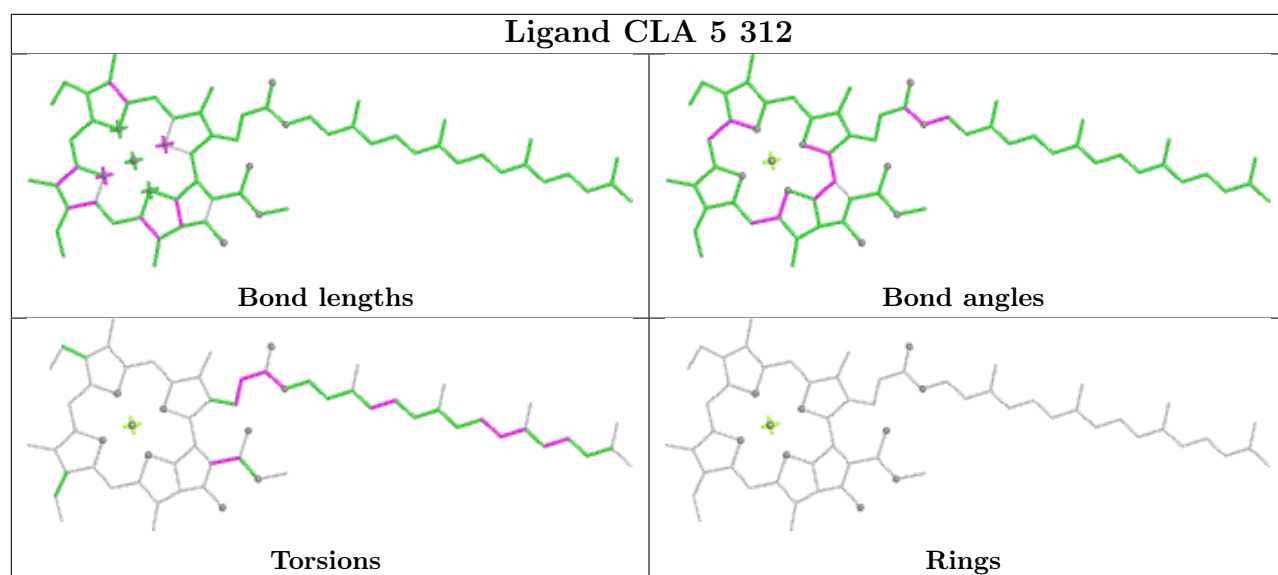
Ligand CLA A 843

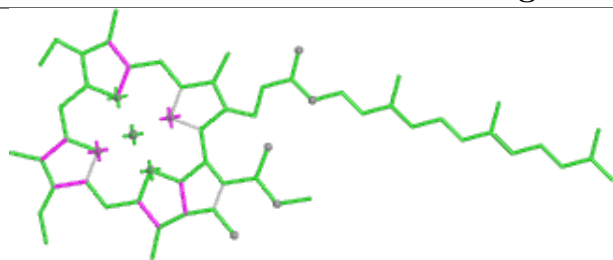
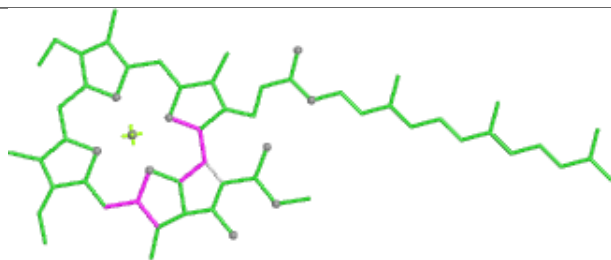
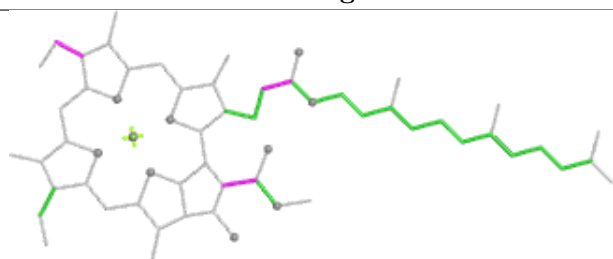
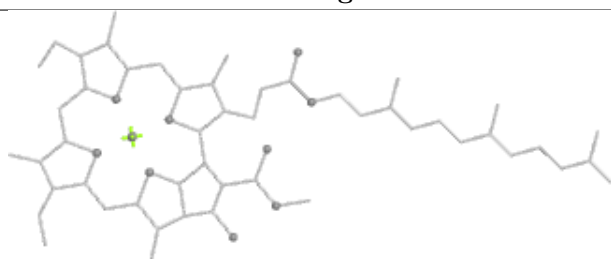
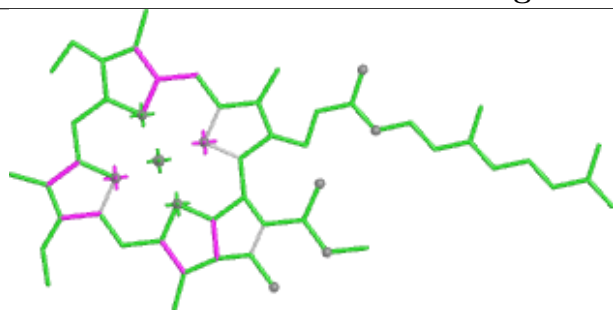
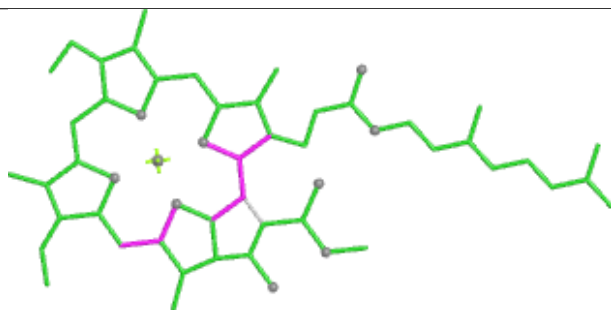
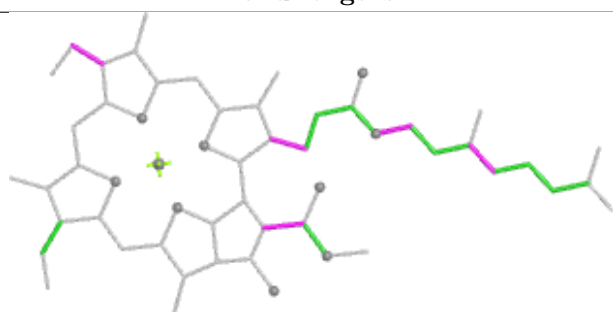
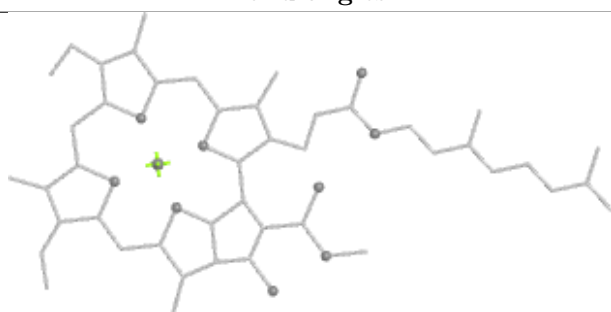




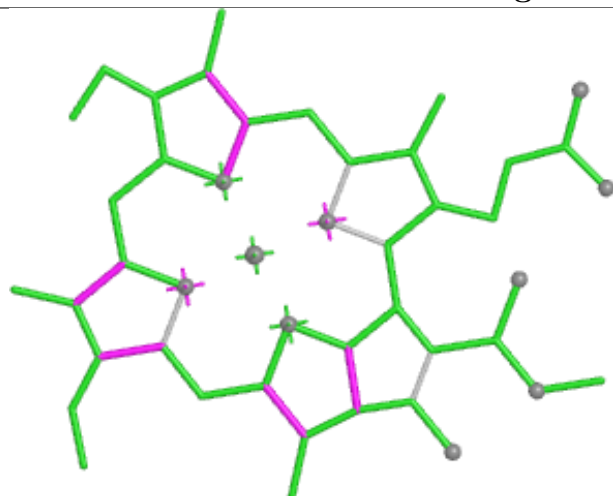




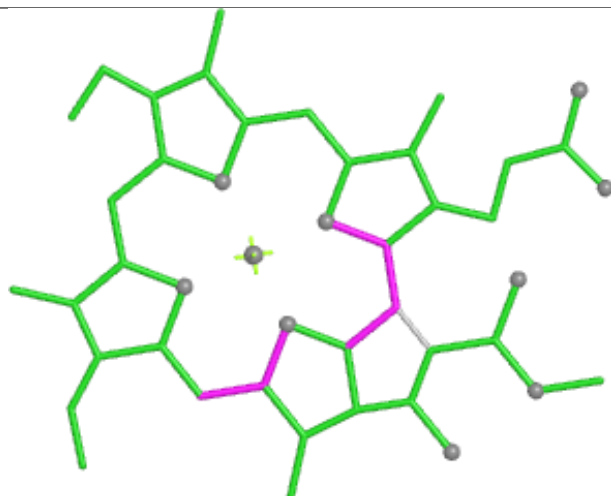


Ligand CLA 5 301**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 801****Bond lengths****Bond angles****Torsions****Rings**

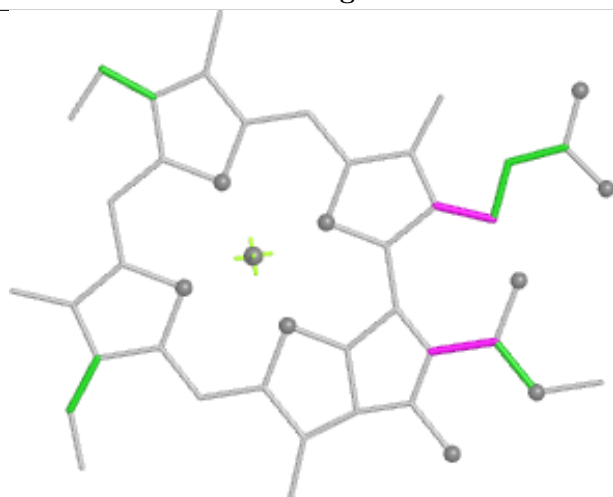
Ligand CLA B 805



Bond lengths



Bond angles

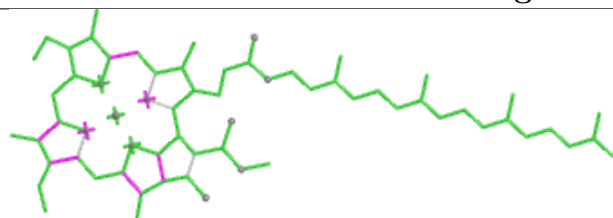


Torsions

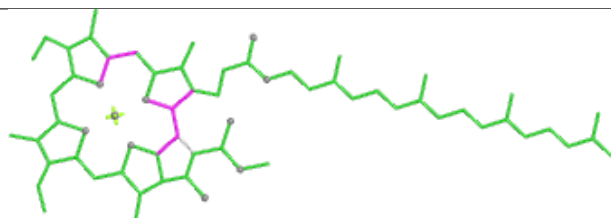


Rings

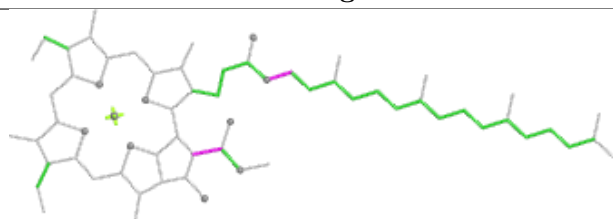
Ligand CLA B 803



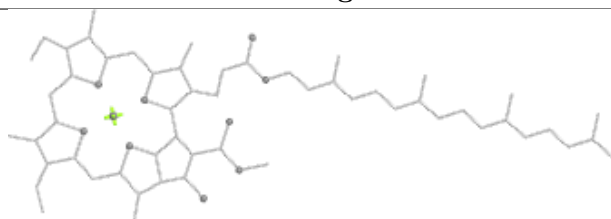
Bond lengths



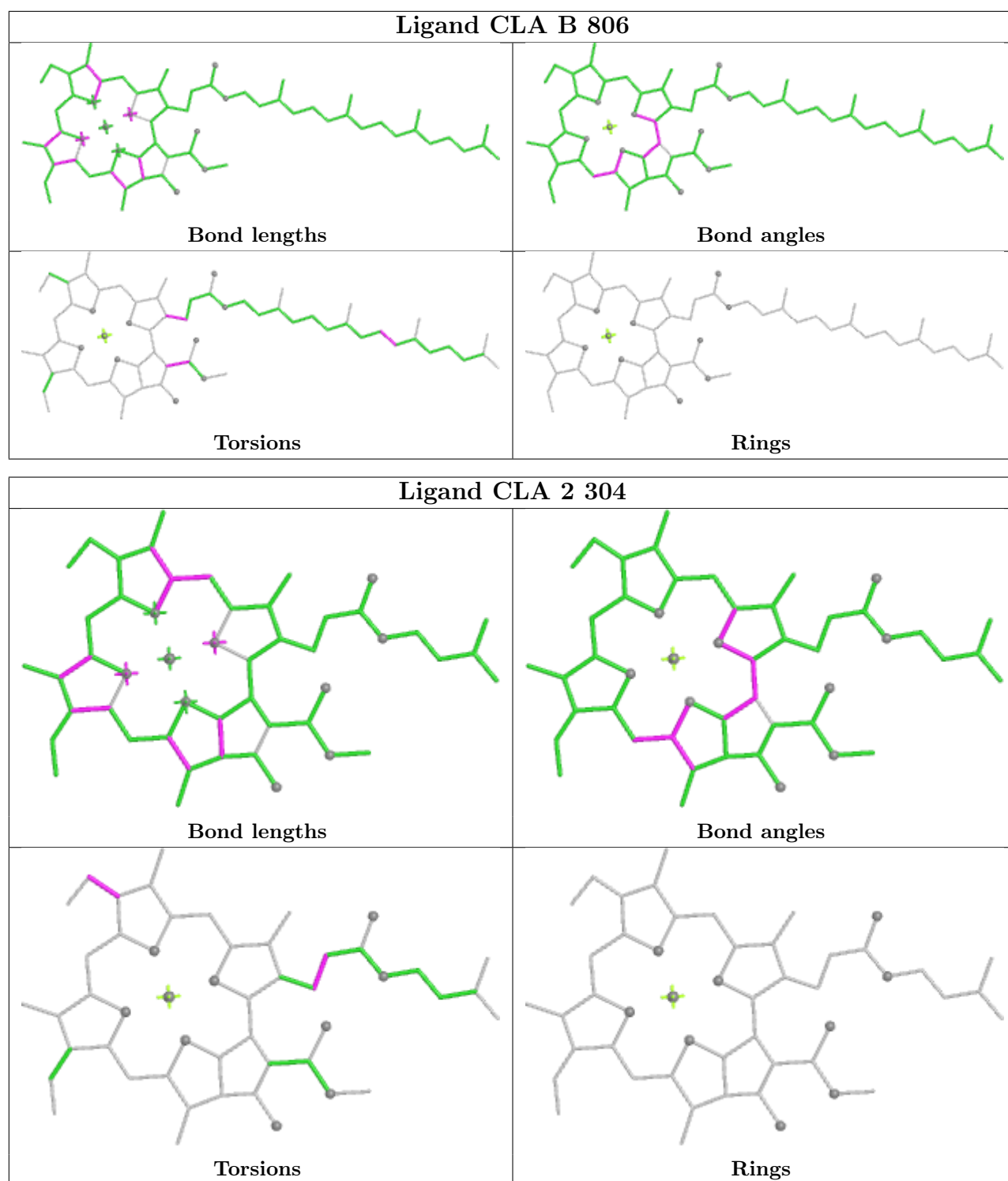
Bond angles



Torsions



Rings



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.

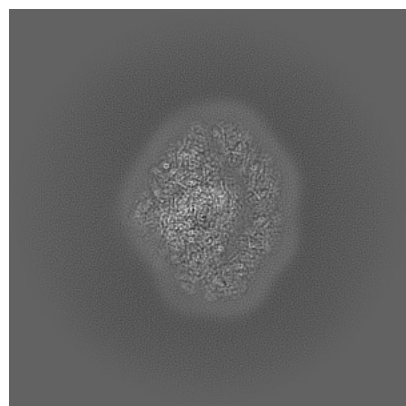
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63404. These allow visual inspection of the internal detail of the map and identification of artifacts.

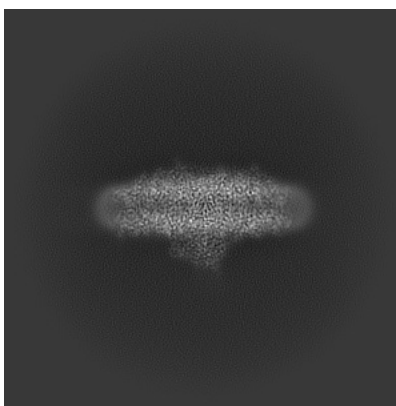
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

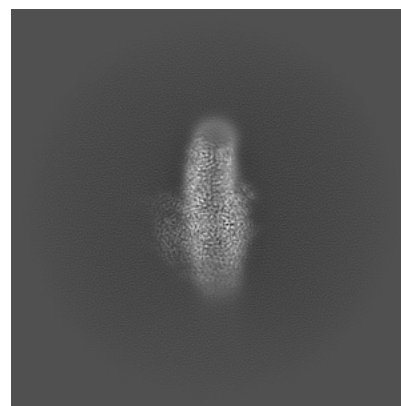
6.1.1 Primary map



X

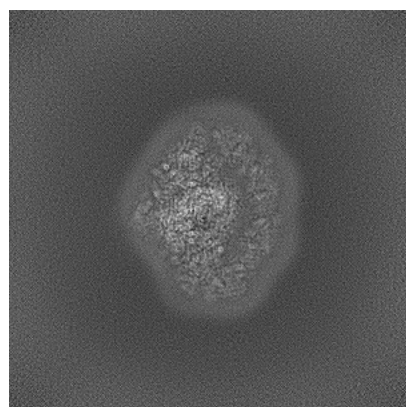


Y

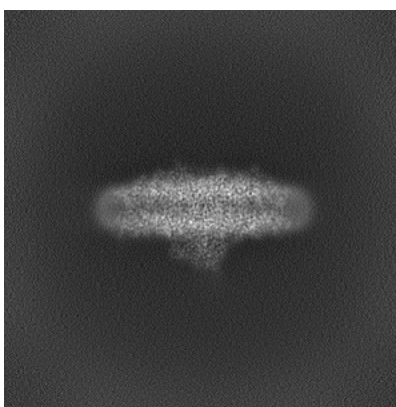


Z

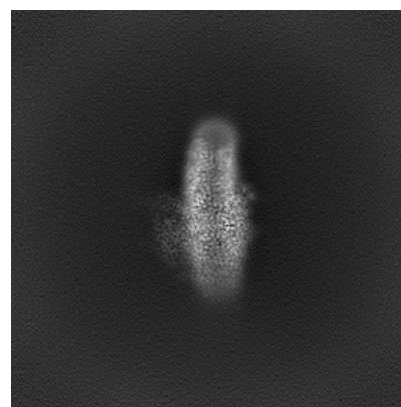
6.1.2 Raw map



X



Y

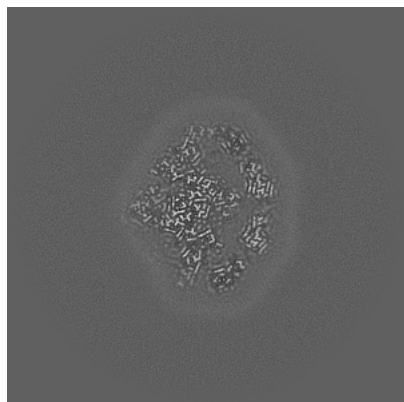


Z

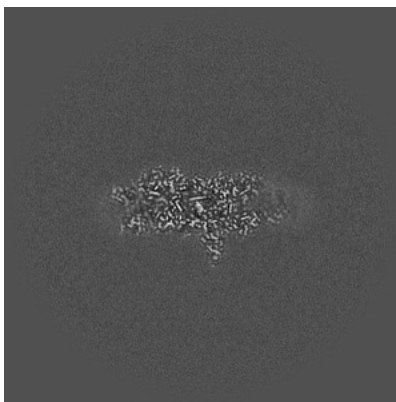
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

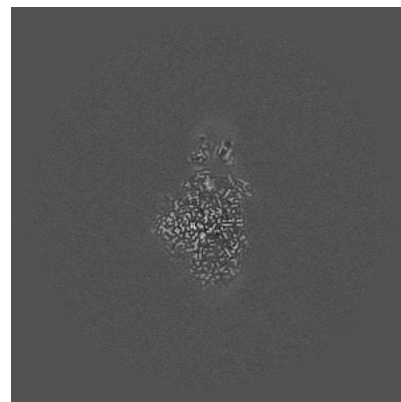
6.2.1 Primary map



X Index: 250

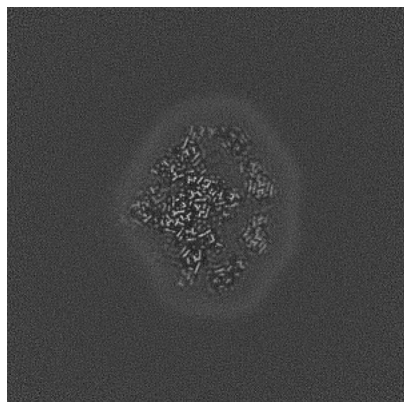


Y Index: 250

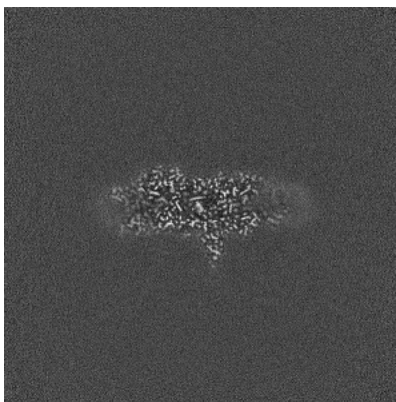


Z Index: 250

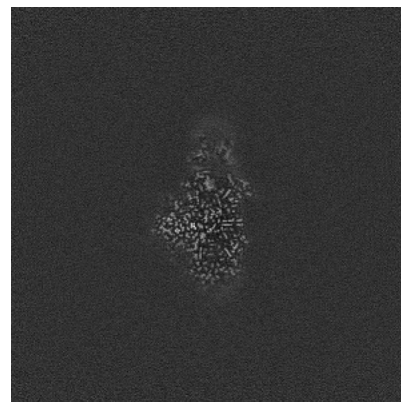
6.2.2 Raw map



X Index: 250



Y Index: 250

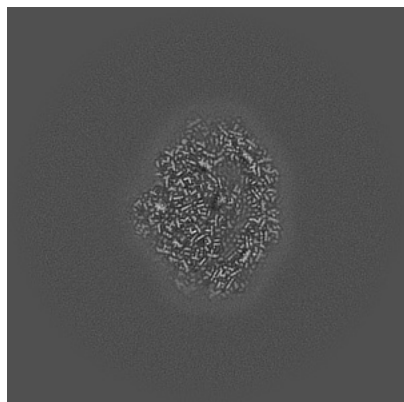


Z Index: 250

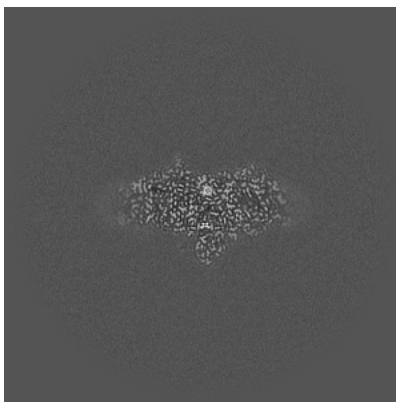
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

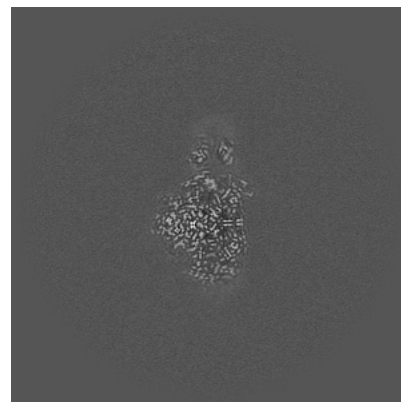
6.3.1 Primary map



X Index: 236

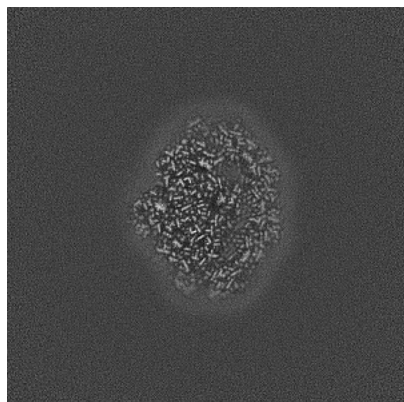


Y Index: 227

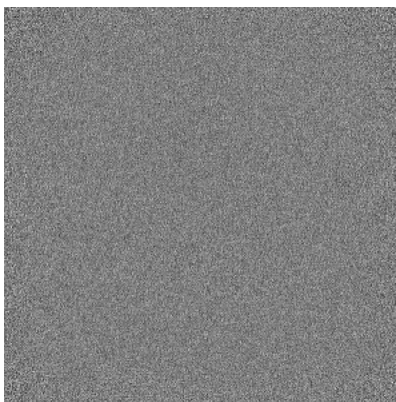


Z Index: 251

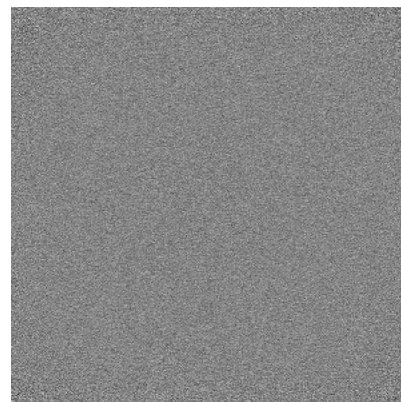
6.3.2 Raw map



X Index: 236



Y Index: 0

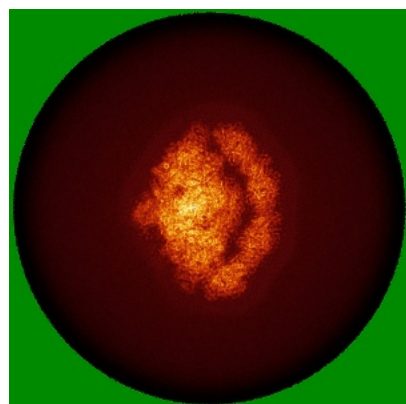


Z Index: 0

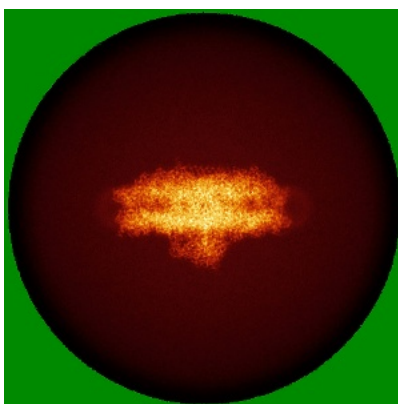
The images above show the largest variance slices of the map in three orthogonal directions.

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

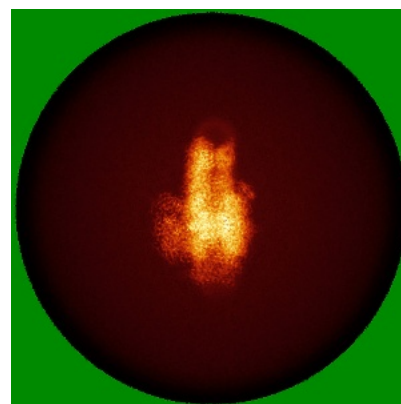
6.4.1 Primary map



X

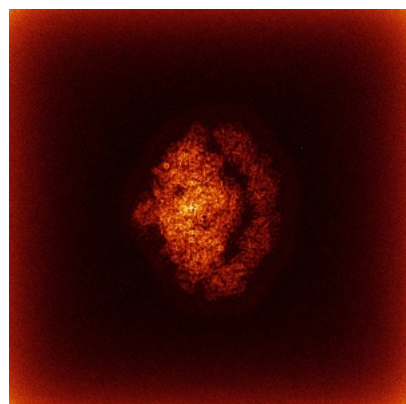


Y

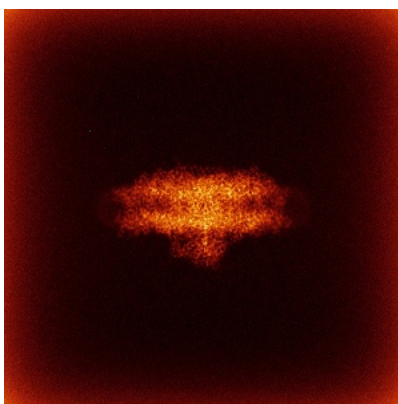


Z

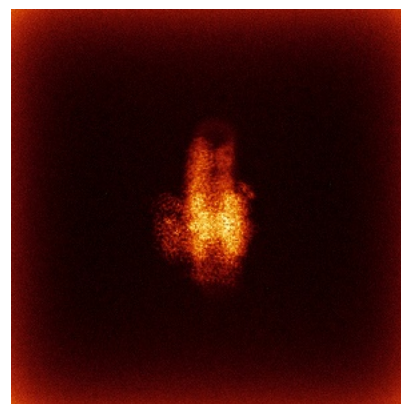
6.4.2 Raw map



X



Y

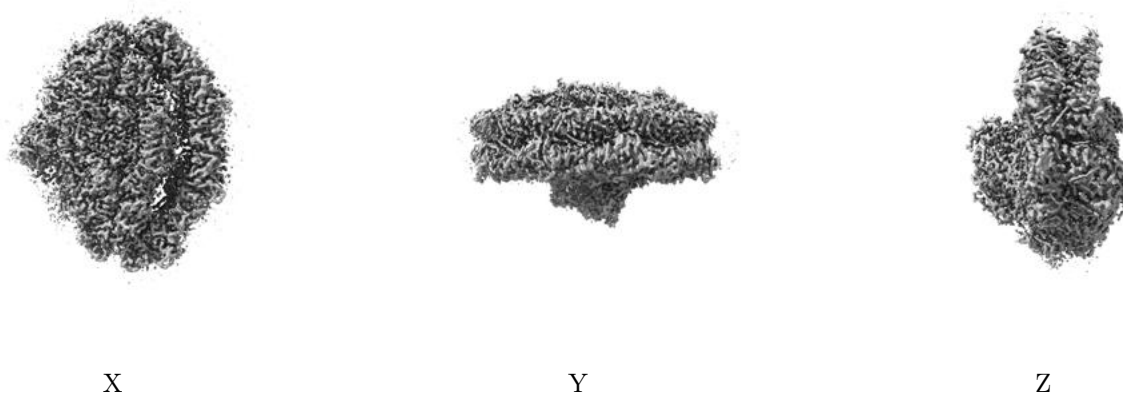


Z

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

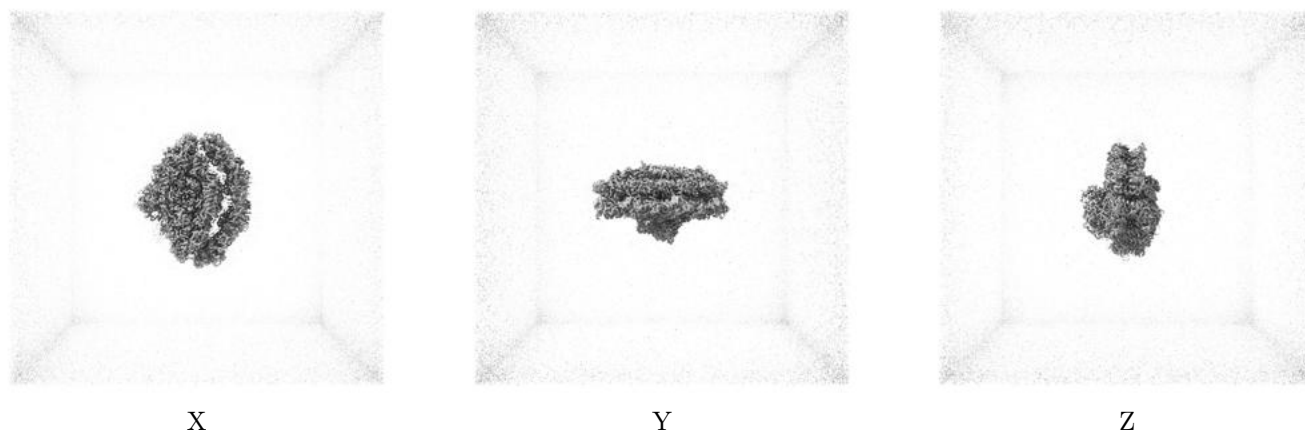
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

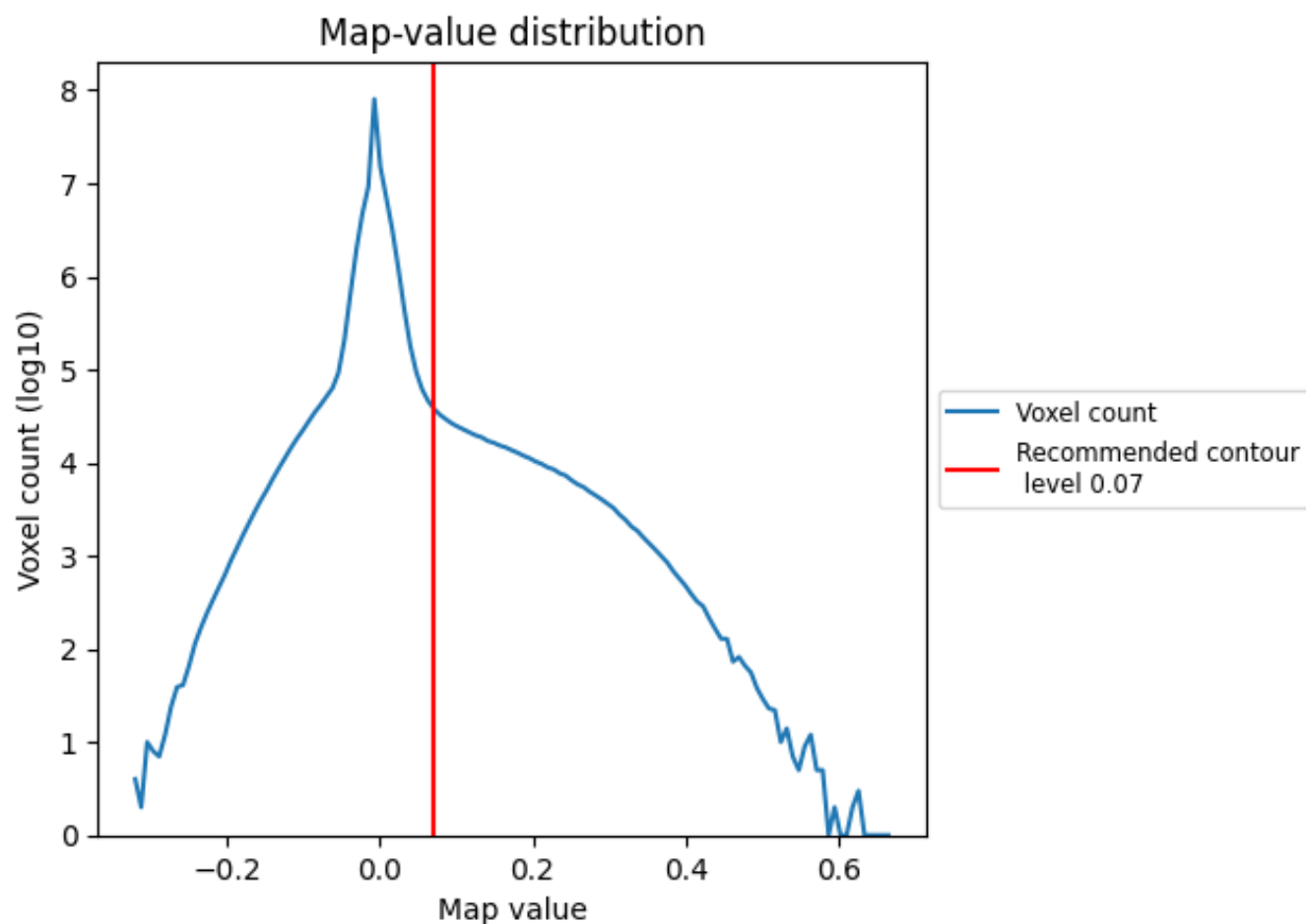
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

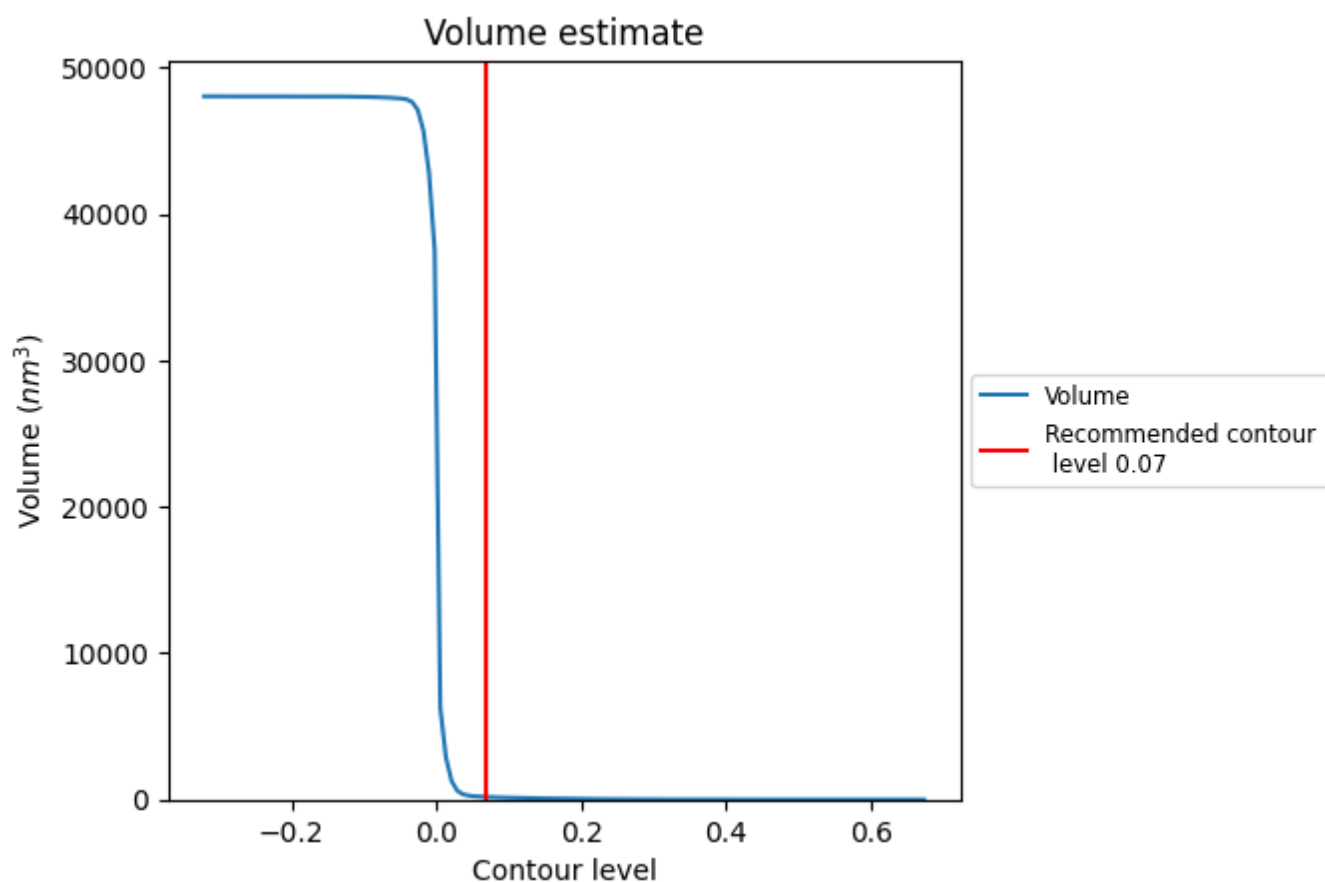
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

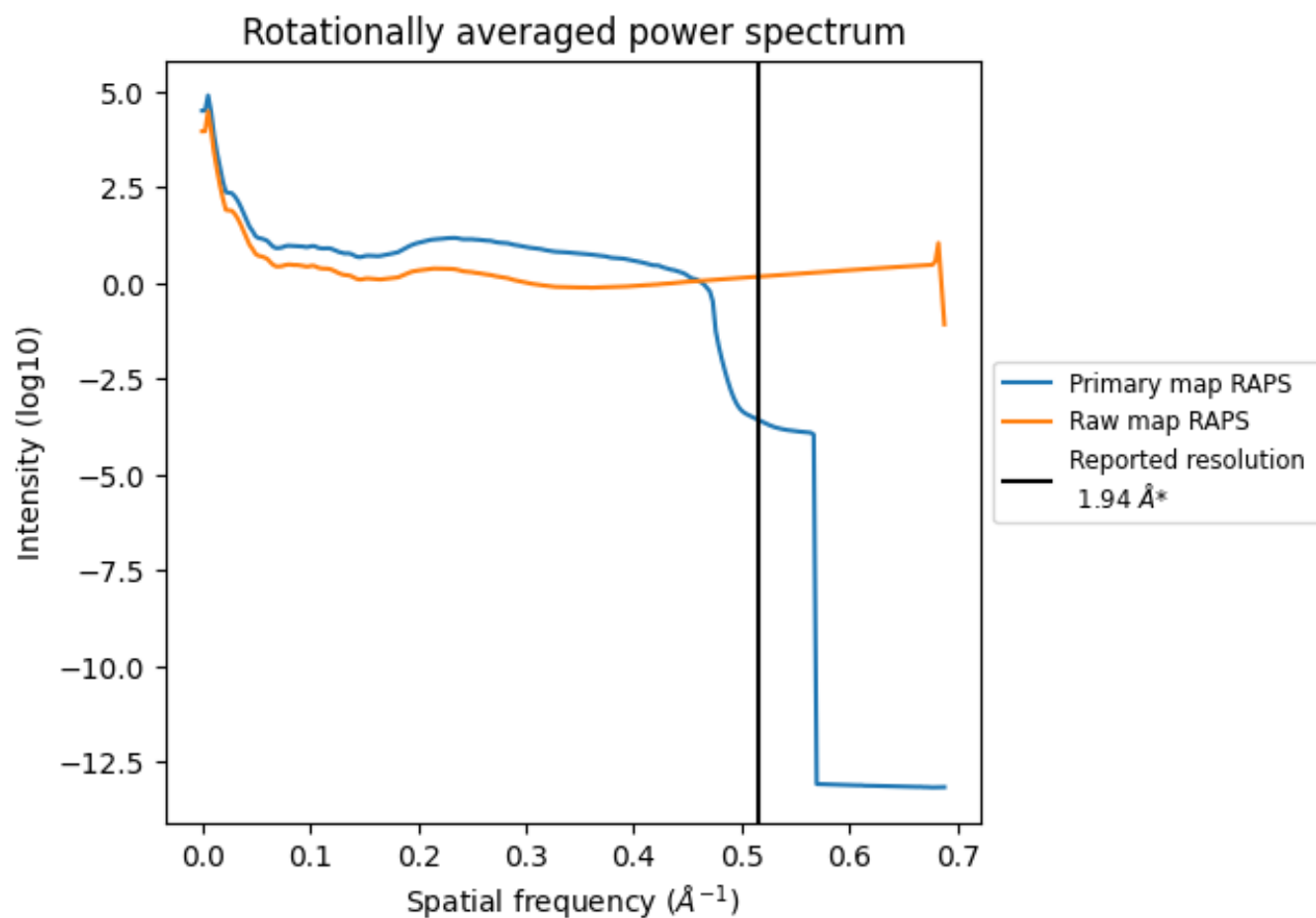
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 159 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 ⓘ

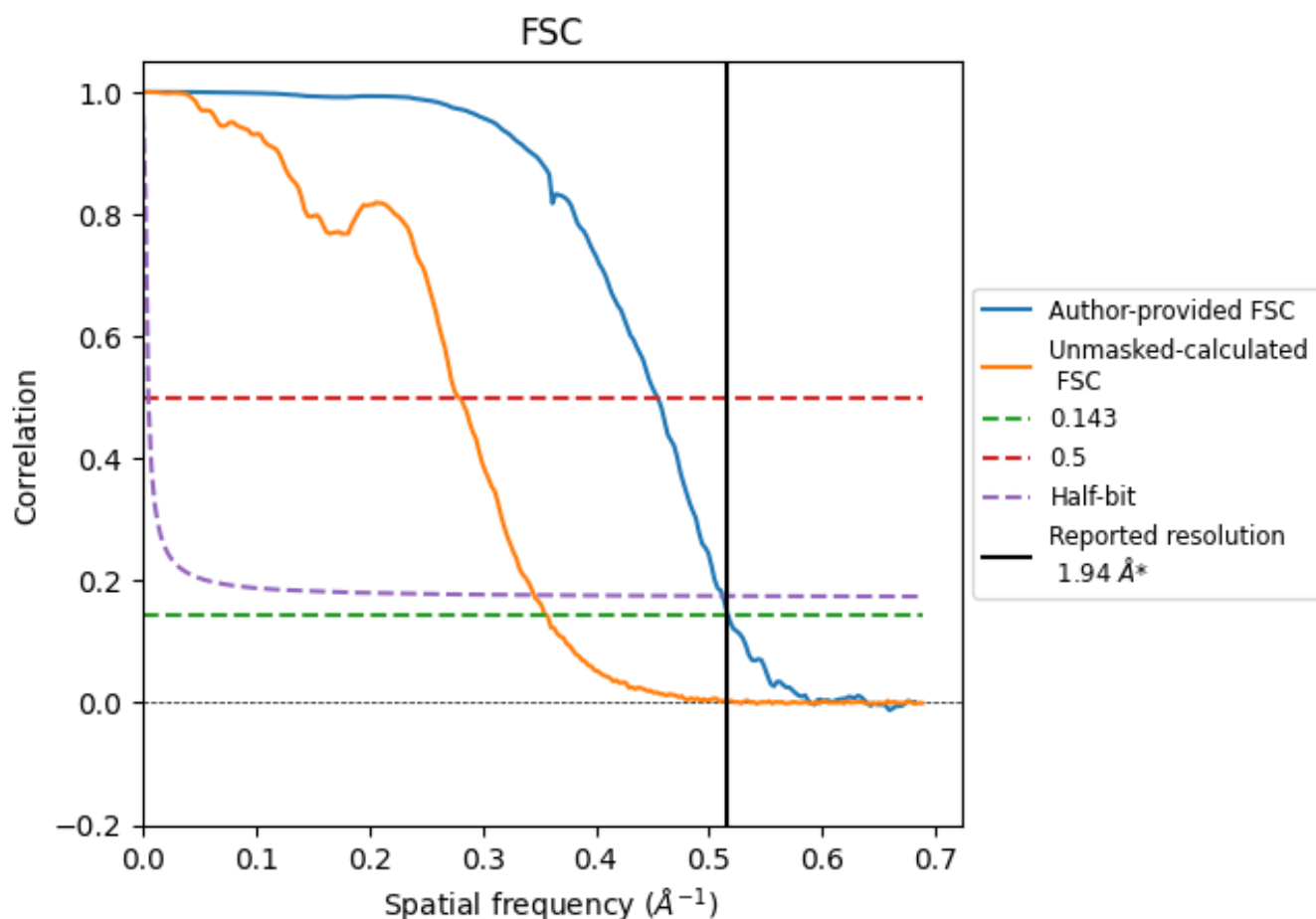


*Reported resolution corresponds to spatial frequency of 0.515 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.515 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

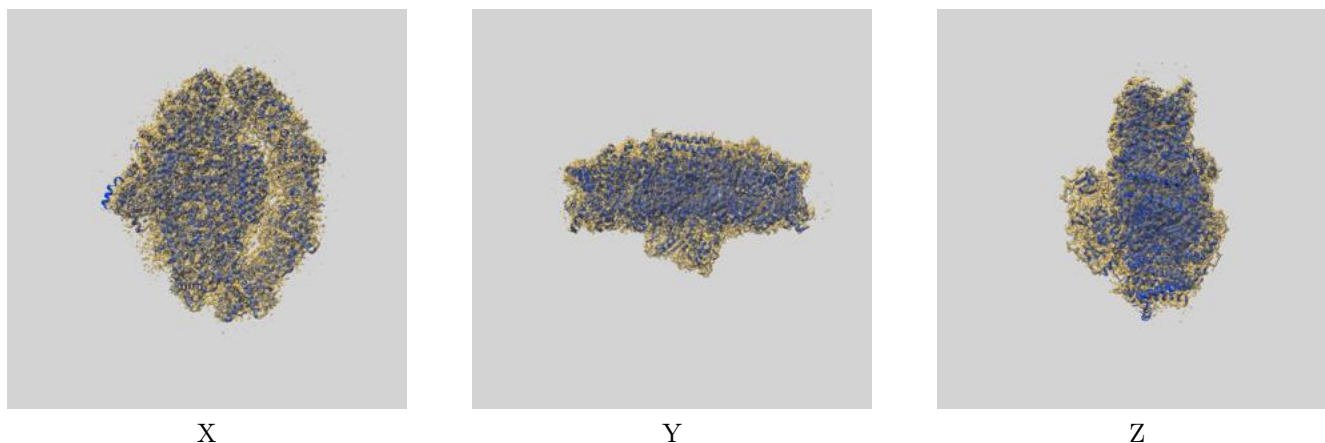
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.94	-	-
Author-provided FSC curve	1.94	2.20	1.95
Unmasked-calculated*	2.80	3.58	2.89

*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 2.80 differs from the reported value 1.94 by more than 10 %

9 Map-model fit [i](#)

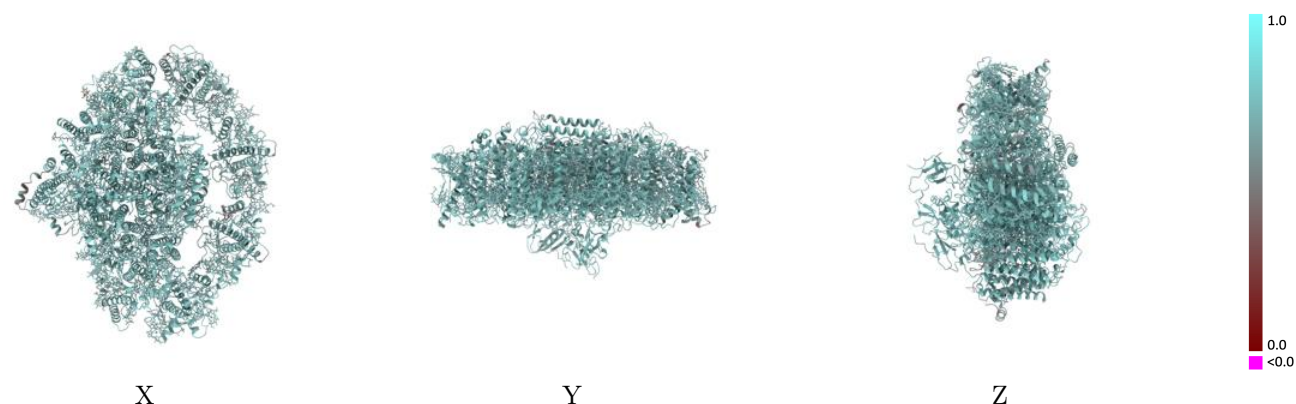
This section contains information regarding the fit between EMDB map EMD-63404 and PDB model 9LUT. Per-residue inclusion information can be found in section [3](#) on page [24](#).

9.1 Map-model overlay [i](#)



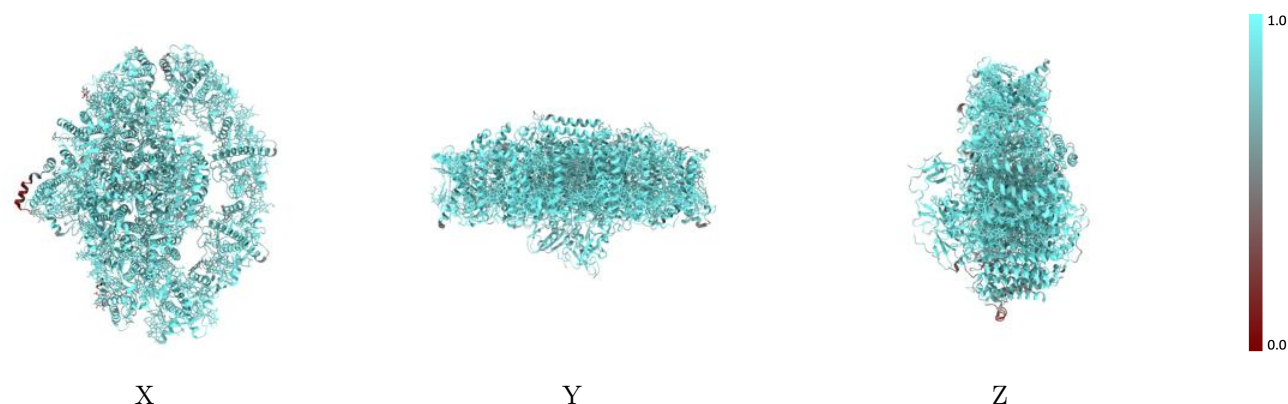
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



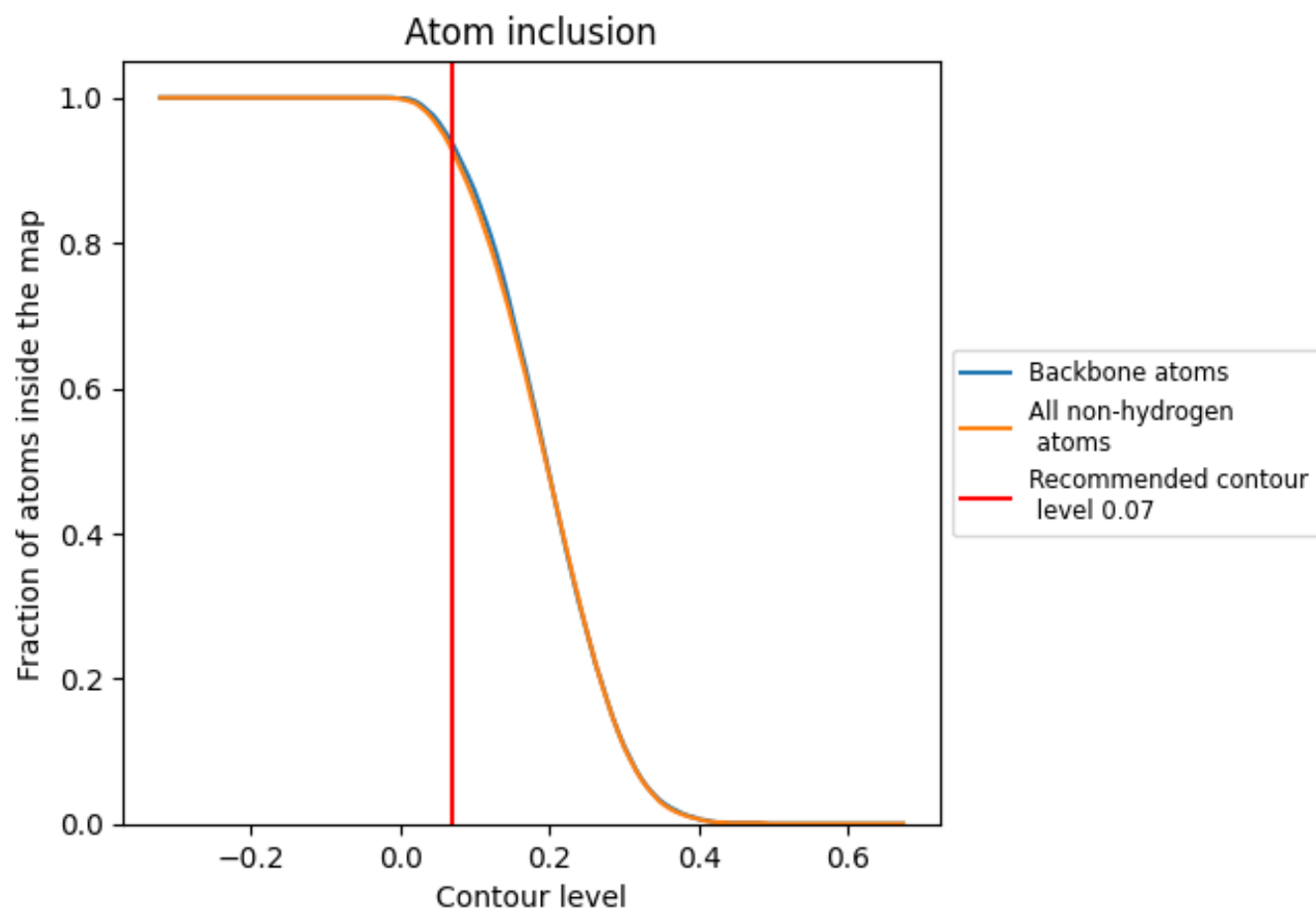
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9280	0.7010
2	0.9240	0.6830
3	0.9280	0.6930
5	0.9090	0.6680
6	0.8820	0.6520
A	0.9680	0.7270
B	0.9610	0.7210
C	0.9830	0.7350
D	0.9250	0.7020
E	0.9100	0.6980
F	0.9190	0.7020
G	0.8640	0.6730
H	0.5090	0.6040
I	0.9620	0.7000
J	0.9460	0.6980
K	0.7170	0.6180
L	0.9140	0.6820
M	0.8680	0.6720

