



wwPDB EM Validation Summary Report ⓘ

Jun 10, 2026 – 02:44 PM EDT

PDB ID : 9YGV / pdb_00009ygv
EMDB ID : EMD-72770
Title : Photosystem I FCP Supercomplex from *Macrocystis pyrifera*
Authors : Maturana, P.; Maldonado, M.
Deposited on : 2025-09-29
Resolution : 2.47 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

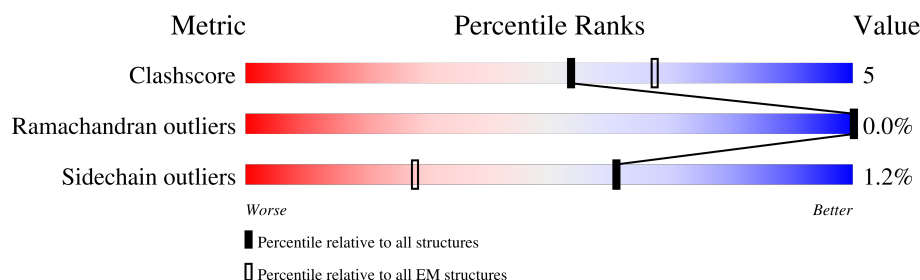
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.47 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	1	230	<div> <div>55%</div> <div> <div>73%</div> <div>23%</div> </div> </div>
2	3	191	<div> <div>61%</div> <div> <div>77%</div> <div>6%</div> <div>16%</div> </div> </div>
3	5	222	<div> <div>46%</div> <div> <div>71%</div> <div>7%</div> <div>21%</div> </div> </div>
4	7	169	<div> <div>61%</div> <div> <div>90%</div> <div>10%</div> </div> </div>
5	8	215	<div> <div>55%</div> <div> <div>75%</div> <div>7%</div> <div>18%</div> </div> </div>
6	A	749	<div> <div>61%</div> <div> <div>93%</div> <div>5%</div> </div> </div>
7	B	734	<div> <div>61%</div> <div> <div>92%</div> <div>7%</div> </div> </div>
8	C	81	<div> <div>65%</div> <div> <div>95%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
9	D	132	
10	E	61	
11	F	202	
12	I	36	
13	J	42	
14	M	30	
15	R	132	
16	b	141	
17	10	212	
17	6	212	
18	11	213	
19	13	216	
19	9	216	
20	15	155	
21	16	163	
22	17	218	
23	19	150	
24	2	104	
25	4	237	
26	L	145	
27	a	151	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 52767 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 FCP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	178	Total	C	N	O	S	0	0
			1336	860	218	250	8		

- Molecule 2 is a protein called FCP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	161	Total	C	N	O	S	0	0
			1236	782	211	235	8		

- Molecule 3 is a protein called FCP5.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	175	Total	C	N	O	S	0	0
			1299	828	219	240	12		

- Molecule 4 is a protein called FCP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	7	169	Total	C	N	O	S	0	0
			1288	832	215	229	12		

- Molecule 5 is a protein called FCP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	8	176	Total	C	N	O	S	0	0
			1328	855	222	242	9		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	742	Total	C	N	O	S	0	0
			5834	3824	989	997	24		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	730	Total	C	N	O	S	0	0
			5834	3839	980	997	18		

- Molecule 8 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	80	Total	C	N	O	S	0	0
			596	364	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	125	Total	C	N	O	S	0	0
			1002	649	170	179	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	E	60	Total	C	N	O	0	0
			482	311	82	89		

- Molecule 11 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	161	Total	C	N	O	S	0	0
			1271	817	212	237	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	34	Total	C	N	O	S	0	0
			264	184	36	43	1		

- 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
			333	227	48	56	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	30	Total	C	N	O	S	0	0
			228	152	36	39	1		

- Molecule 15 is a protein called Psar.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	85	Total	C	N	O	S	0	0
			627	410	102	113	2		

- Molecule 16 is a protein called FCPB.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	b	141	Total	C	N	O	S	0	0
			706	423	141	142			

- Molecule 17 is a protein called FCP6 and FCP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	173	Total	C	N	O	S	0	0
			1275	818	210	236	11		
17	10	172	Total	C	N	O	S	0	0
			1270	815	209	235	11		

- Molecule 18 is a protein called FCP11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	11	167	Total	C	N	O	S	0	0
			1283	833	208	235	7		

- Molecule 19 is a protein called FCP9 and FCP13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	13	141	Total	C	N	O	S	0	0
			1107	719	184	196	8		
19	9	136	Total	C	N	O	S	0	0
			1060	685	178	189	8		

- Molecule 20 is a protein called FCP15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	15	155	Total	C	N	O	S	0	0
			775	465	155	155			

- Molecule 21 is a protein called FCP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	16	163	Total	C	N	O	0	0
			815	489	163	163		

- Molecule 22 is a protein called FCP17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	17	146	Total	C	N	O	S	0	0
			1107	702	195	204	6		

- Molecule 23 is a protein called FCP19.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	19	150	Total	C	N	O	0	0
			750	450	150	150		

- Molecule 24 is a protein called FCP2.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	2	104	Total	C	N	O	0	0
			520	312	104	104		

- Molecule 25 is a protein called FCP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	4	180	Total	C	N	O	S	0	0
			1337	853	223	250	11		

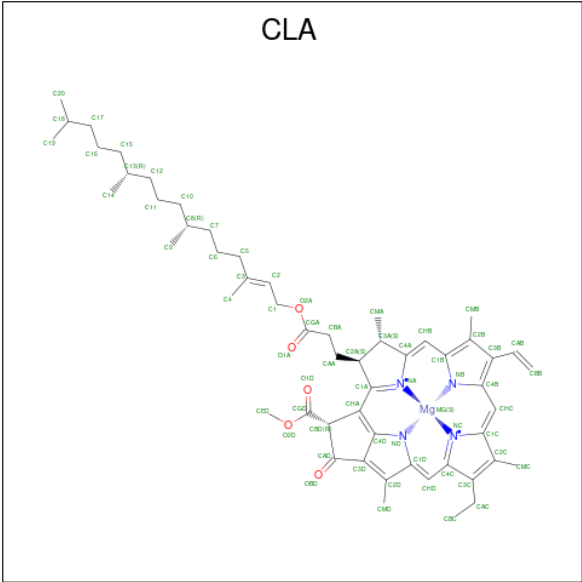
- Molecule 26 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L	134	Total	C	N	O	S	0	0
			1015	670	161	181	3		

- Molecule 27 is a protein called FCPA.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	a	151	Total	C	N	O	0	0
			755	453	151	151		

- Molecule 28 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
28	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
28	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	5	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	5	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	5	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	8	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	8	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	8	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
28	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
28	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
28	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
28	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
28	B	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 64	C 54	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	F	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	J	1	Total 58	C 48	Mg 1	N 4	O 5	0
28	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	R	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	R	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
28	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	6	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
28	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	10	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	10	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	10	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	10	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	10	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	10	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	10	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	10	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	10	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	11	1	Total 65	C 55	Mg 1	N 4	O 5	0
28	11	1	Total 57	C 47	Mg 1	N 4	O 5	0
28	11	1	Total 60	C 50	Mg 1	N 4	O 5	0
28	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	11	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	11	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	13	1	Total 56	C 46	Mg 1	N 4	O 5	0
28	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	13	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	13	1	Total 42	C 34	Mg 1	N 4	O 3	0

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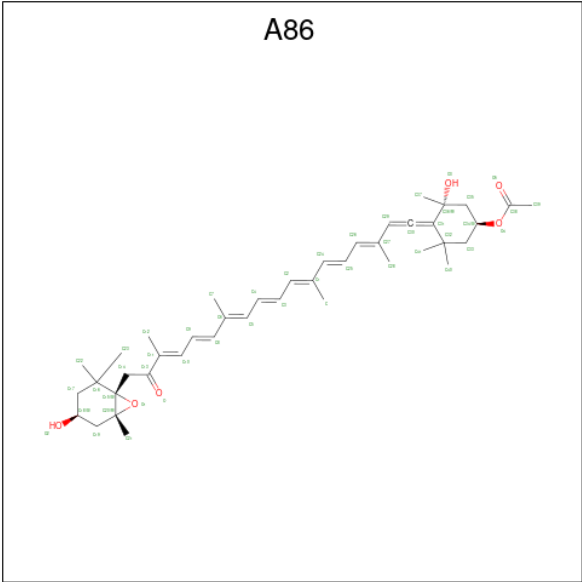
Mol	Chain	Residues	Atoms					AltConf
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28	15	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	16	1	Total 45	C 35	Mg 1	N 4	O 5	0
28	16	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	16	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	16	1	Total 41	C 33	Mg 1	N 4	O 3	0
28	16	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	17	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	17	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	17	1	Total 48	C 38	Mg 1	N 4	O 5	0
28	17	1	Total 49	C 39	Mg 1	N 4	O 5	0
28	17	1	Total 50	C 40	Mg 1	N 4	O 5	0
28	17	1	Total 47	C 37	Mg 1	N 4	O 5	0
28	17	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	19	1	Total 46	C 36	Mg 1	N 4	O 5	0
28	19	1	Total 43	C 35	Mg 1	N 4	O 3	0
28	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
28	4	1	Total 42	C 34	Mg 1	N 4	O 3	0
28	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
28	4	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
28	4	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
28	4	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
28	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
28	a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
28	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
28	a	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 29 is (3S,3'S,5R,5'R,6S,6'R,8'R)-3,5'-dihydroxy-8-oxo-6',7'-didehydro-5,5',6,6',7,8-hexahydro-5,6-epoxy-beta,beta-caroten-3'-yl acetate (CCD ID: A86) (formula: C₄₂H₅₈O₆).



Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			48	42	6	
29	1	1	Total	C	O	0
			48	42	6	
29	3	1	Total	C	O	0
			48	42	6	
29	3	1	Total	C	O	0
			48	42	6	
29	3	1	Total	C	O	0
			48	42	6	
29	5	1	Total	C	O	0
			48	42	6	
29	8	1	Total	C	O	0
			48	42	6	
29	J	1	Total	C	O	0
			48	42	6	
29	R	1	Total	C	O	0
			48	42	6	
29	R	1	Total	C	O	0
			48	42	6	
29	6	1	Total	C	O	0
			48	42	6	
29	10	1	Total	C	O	0
			48	42	6	
29	10	1	Total	C	O	0
			48	42	6	
29	11	1	Total	C	O	0
			48	42	6	

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Mol	Chain	Residues	Atoms			AltConf
29	17	1	Total 48	C 42	O 6	0
29	4	1	Total 48	C 42	O 6	0
29	4	1	Total 48	C 42	O 6	0
29	9	1	Total 48	C 42	O 6	0

- # KC1

Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	7	1	Total 45	C 35	Mg 1	N 4	O 5	0

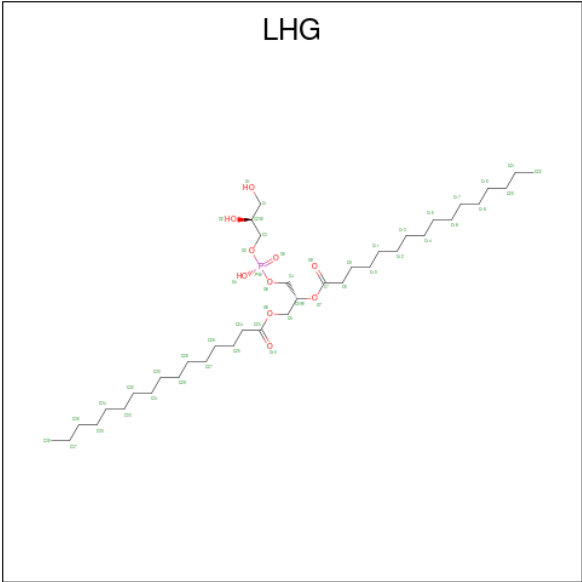


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PDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					AltConf
30	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	10	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	11	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	13	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	17	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
30	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 31 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



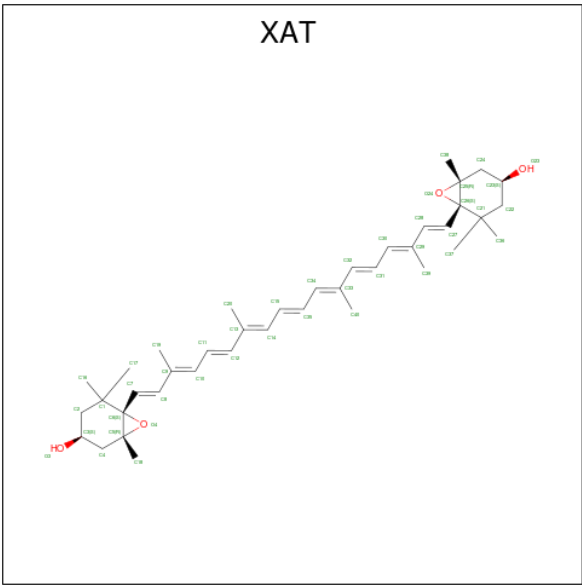
Mol	Chain	Residues	Atoms				AltConf
31	1	1	Total	C	O	P	0
			44	33	10	1	
31	5	1	Total	C	O	P	0
			24	13	10	1	
31	5	1	Total	C	O	P	0
			27	16	10	1	
31	7	1	Total	C	O	P	0
			27	16	10	1	
31	A	1	Total	C	O	P	0
			48	37	10	1	
31	A	1	Total	C	O	P	0
			27	16	10	1	
31	A	1	Total	C	O	P	0
			27	16	10	1	
31	B	1	Total	C	O	P	0
			27	16	10	1	
31	B	1	Total	C	O	P	0
			49	38	10	1	
31	I	1	Total	C	O	P	0
			49	38	10	1	
31	11	1	Total	C	O	P	0
			37	26	10	1	
31	4	1	Total	C	O	P	0
			25	14	10	1	
31	9	1	Total	C	O	P	0
			28	17	10	1	
31	9	1	Total	C	O	P	0
			30	19	10	1	

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Mol	Chain	Residues	Atoms				AltConf
31	9	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 32 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



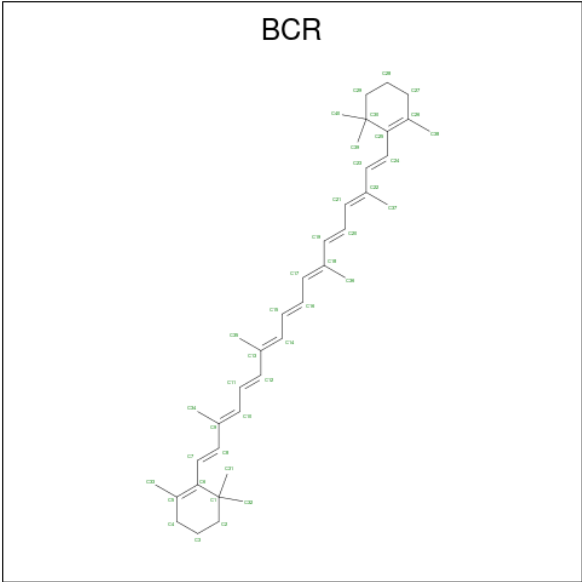
Mol	Chain	Residues	Atoms			AltConf
32	1	1	Total	C	O	0
			44	40	4	
32	3	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	5	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	
32	7	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
32	7	1	Total	C	O	0
			44	40	4	
32	8	1	Total	C	O	0
			44	40	4	
32	8	1	Total	C	O	0
			44	40	4	
32	J	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	6	1	Total	C	O	0
			44	40	4	
32	10	1	Total	C	O	0
			44	40	4	
32	10	1	Total	C	O	0
			44	40	4	
32	10	1	Total	C	O	0
			44	40	4	
32	11	1	Total	C	O	0
			44	40	4	
32	13	1	Total	C	O	0
			44	40	4	
32	13	1	Total	C	O	0
			44	40	4	
32	17	1	Total	C	O	0
			44	40	4	
32	4	1	Total	C	O	0
			44	40	4	
32	4	1	Total	C	O	0
			44	40	4	
32	9	1	Total	C	O	0
			43	39	4	

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



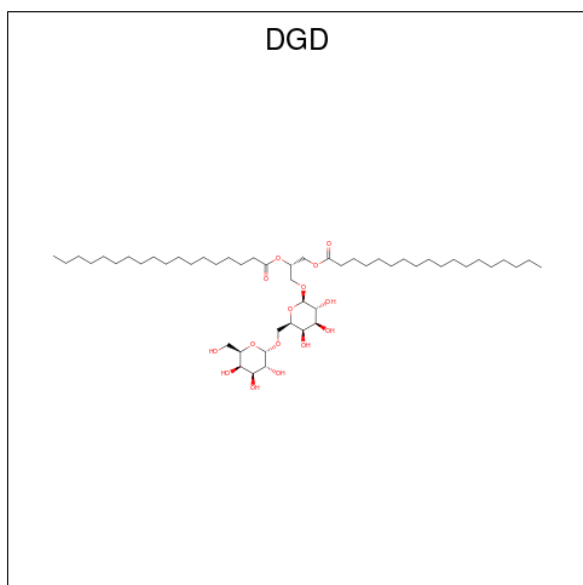
Mol	Chain	Residues	Atoms		AltConf
33	1	1	Total	C	0
			40	40	
33	8	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	A	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	
33	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
33	B	1	Total C 40 40	0
33	F	1	Total C 40 40	0
33	F	1	Total C 40 40	0
33	I	1	Total C 40 40	0
33	J	1	Total C 40 40	0
33	M	1	Total C 40 40	0
33	17	1	Total C 40 40	0
33	L	1	Total C 40 40	0
33	L	1	Total C 40 40	0

- Molecule 34 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



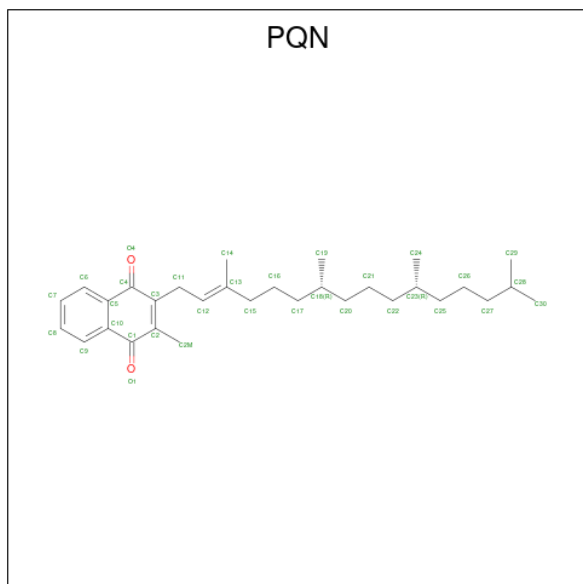
Mol	Chain	Residues	Atoms	AltConf
34	8	1	Total C O 31 17 14	0
34	4	1	Total C O 39 24 15	0

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Mol	Chain	Residues	Atoms			AltConf
34	4	1	Total	C	O	0
			29	17	12	

- Molecule 35 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



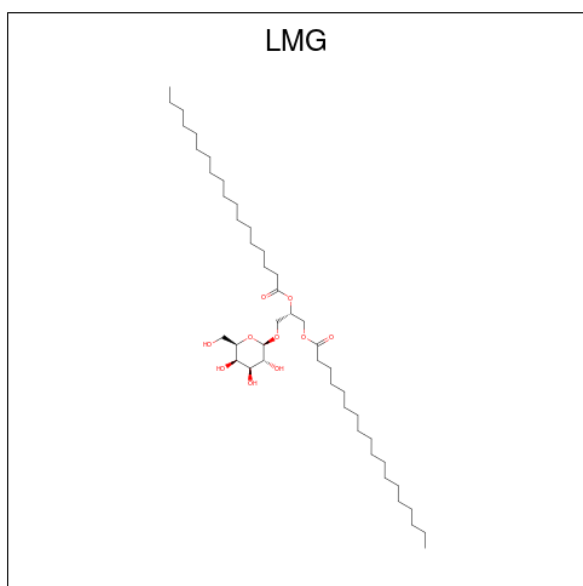
Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			33	31	2	
35	B	1	Total	C	O	0
			33	31	2	

- Molecule 36 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

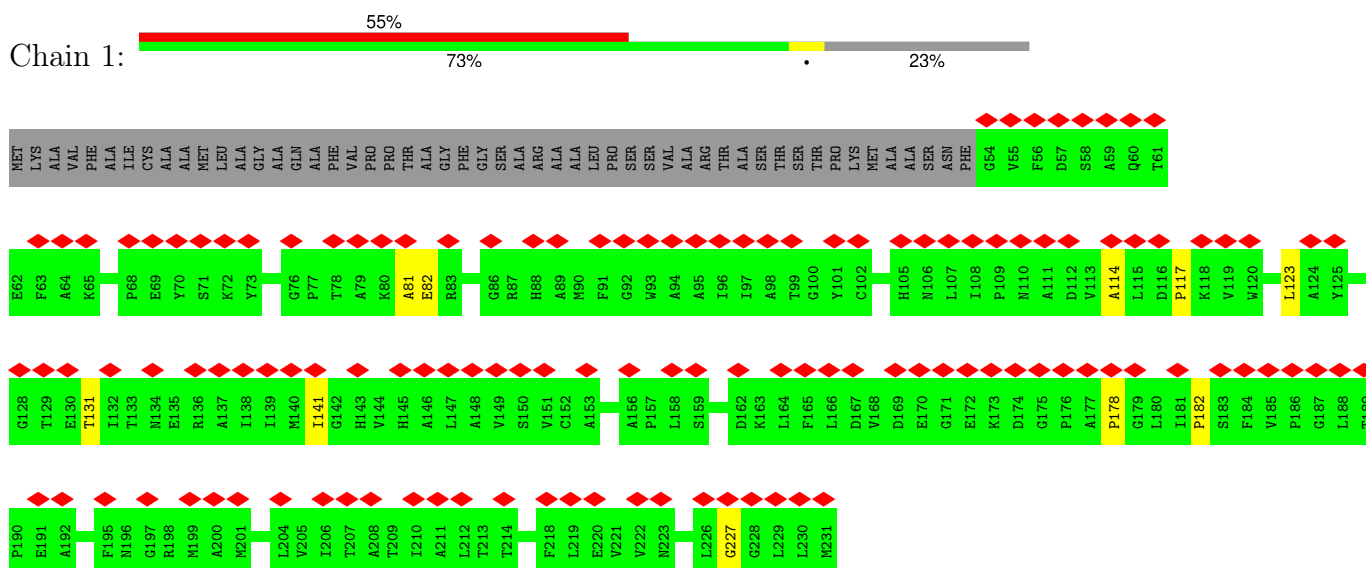


Mol	Chain	Residues	Atoms			AltConf
37	F	1	Total	C	O	0
			41	31	10	

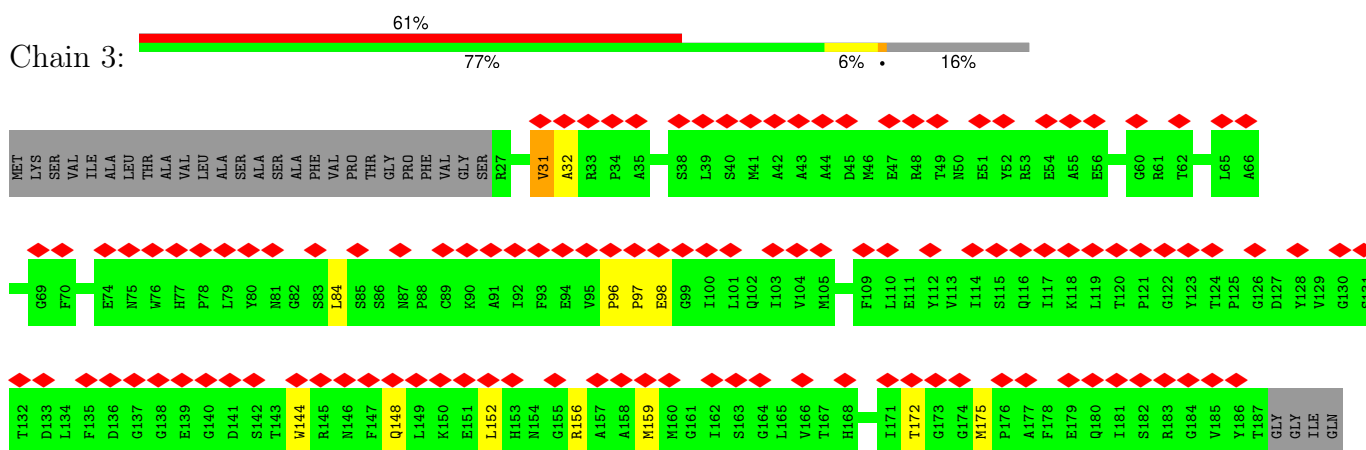
3 Residue-property plots

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: FCP1

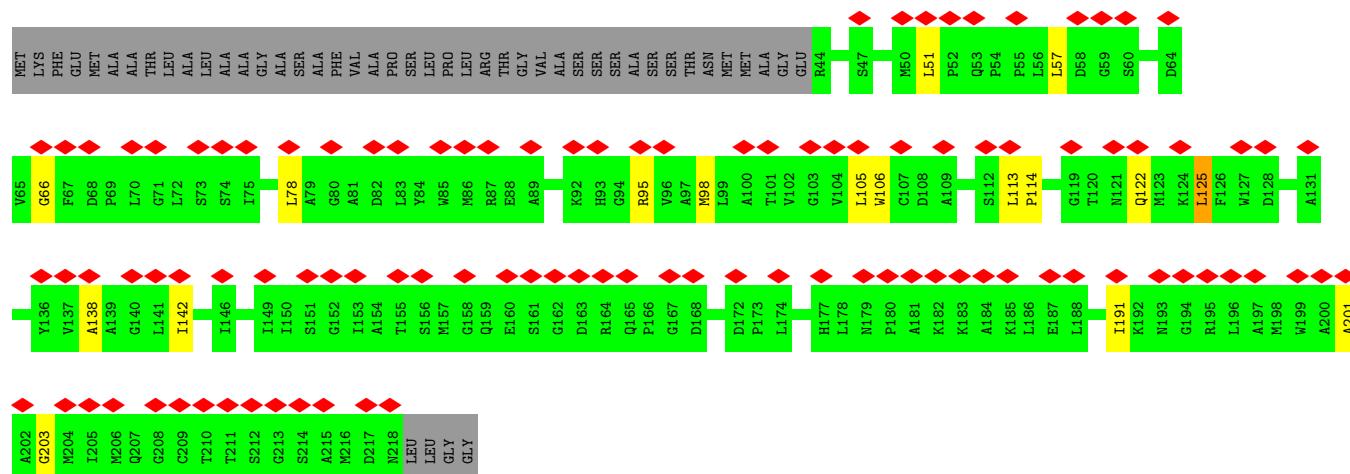


• Molecule 2: FCP3

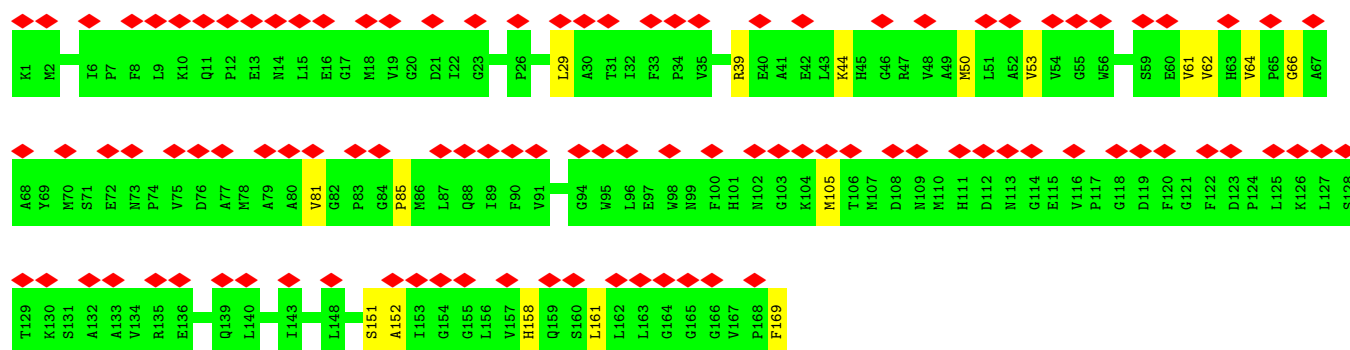
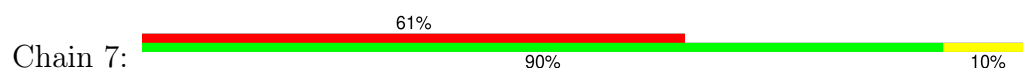


• Molecule 3: FCP5

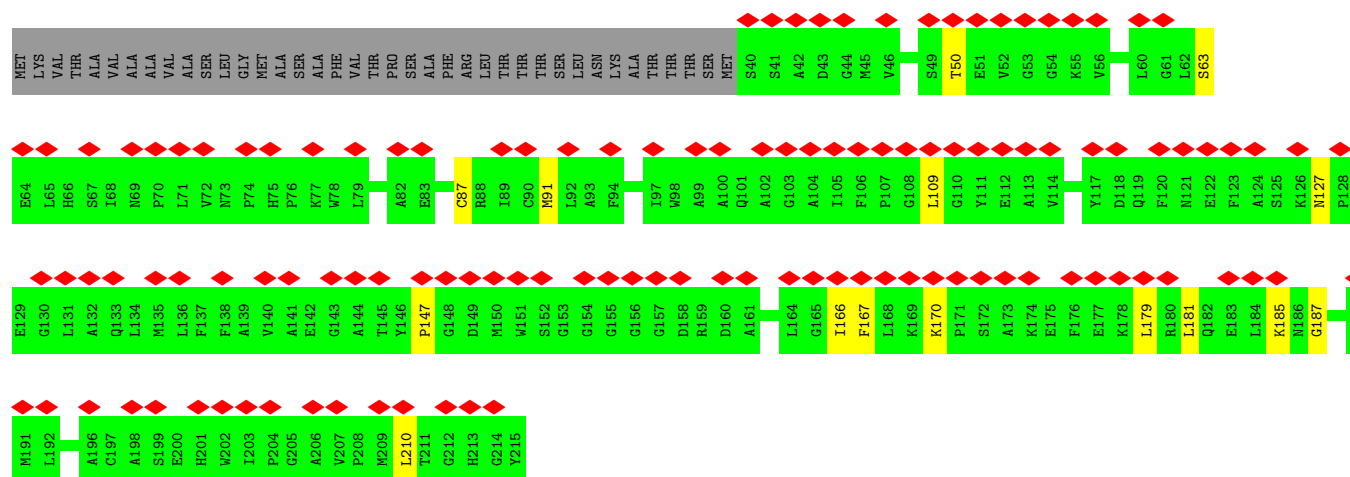
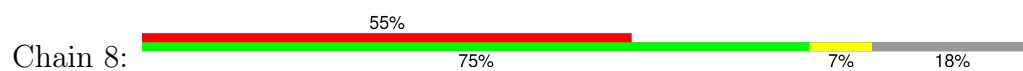




- Molecule 4: FCP7

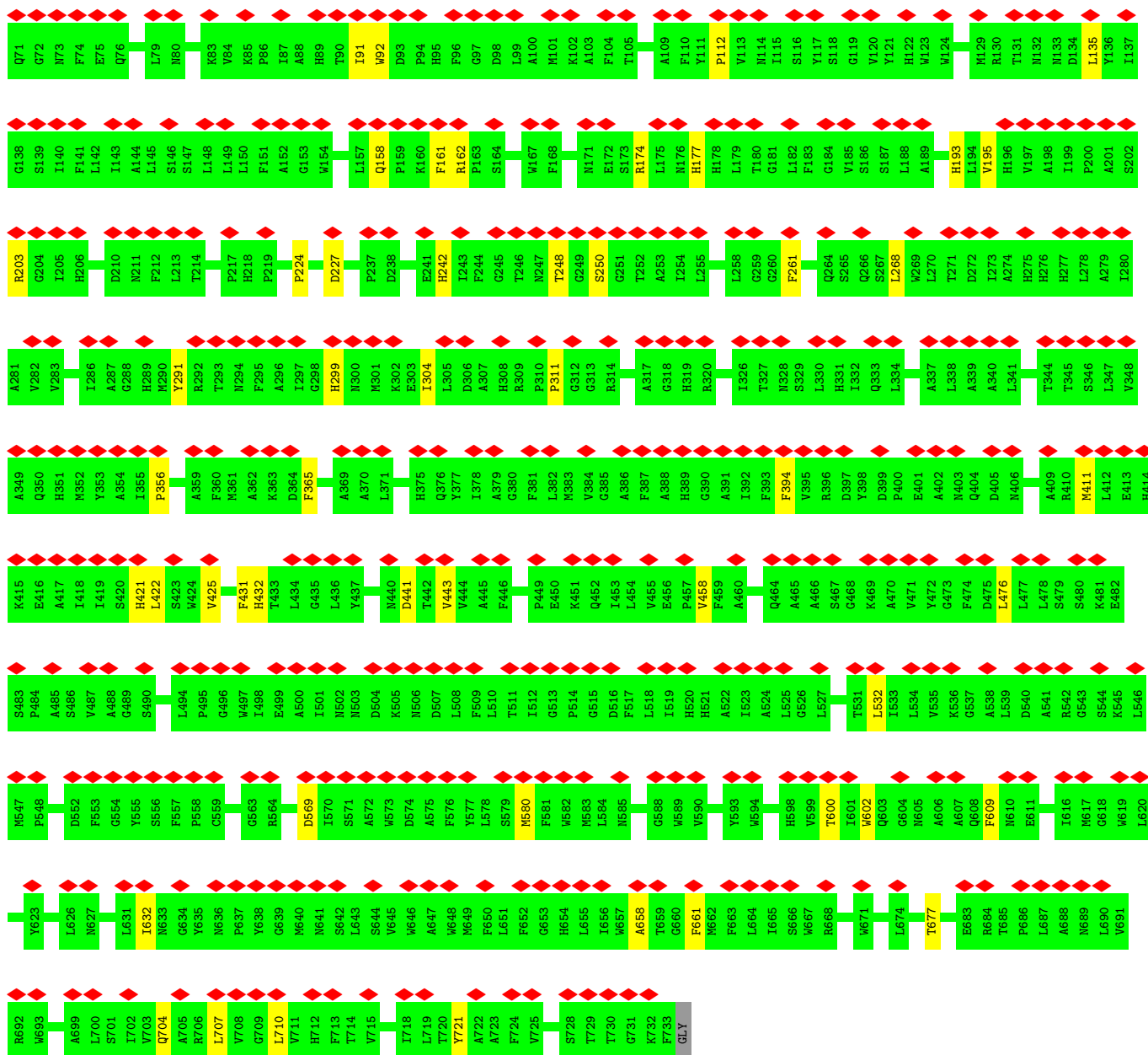


- Molecule 5: FCP8

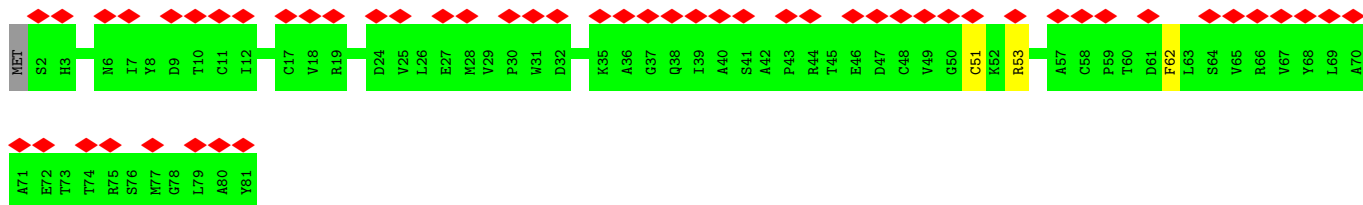


- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A1

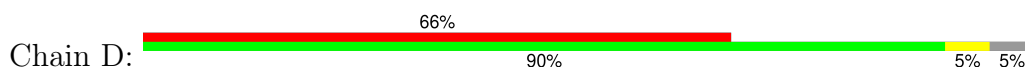


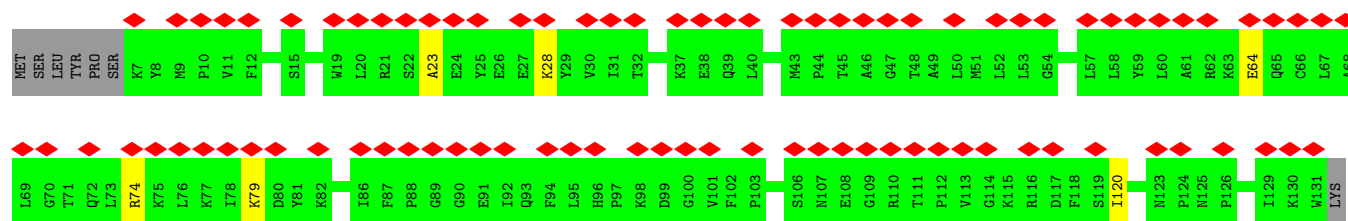


• Molecule 8: Photosystem I iron-sulfur center

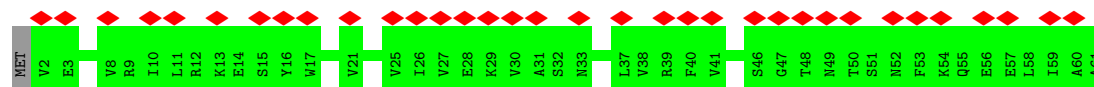


• Molecule 9: Photosystem I reaction center subunit II

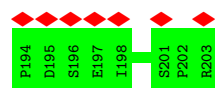
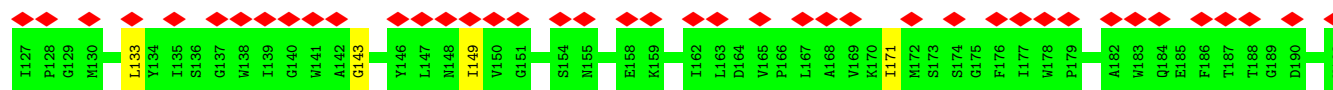
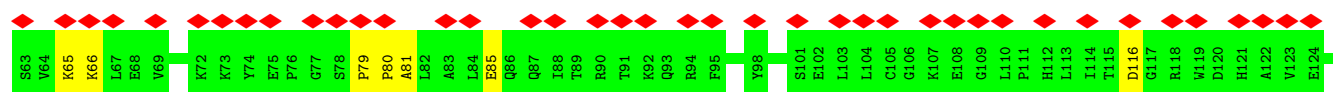
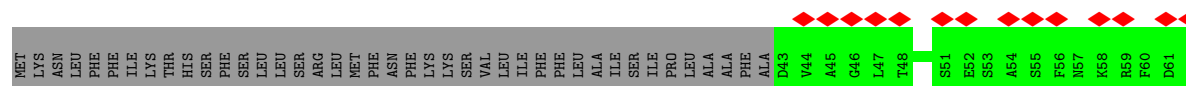
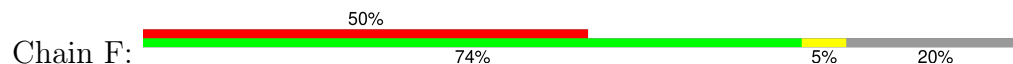




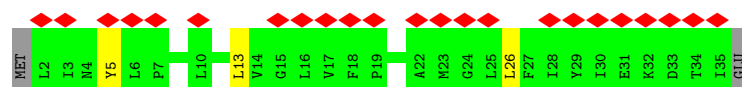
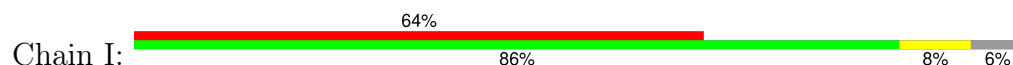
• Molecule 10: Photosystem I reaction center subunit IV



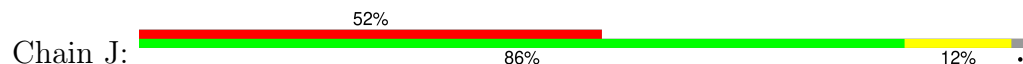
• Molecule 11: Photosystem I reaction center subunit III



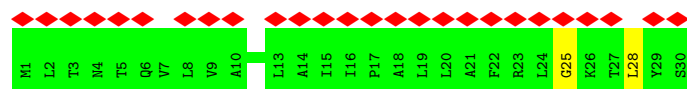
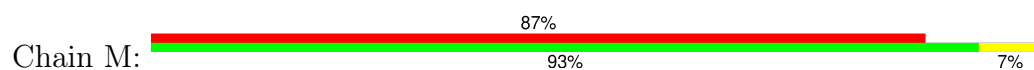
• Molecule 12: Photosystem I reaction center subunit VIII



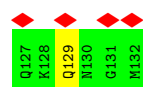
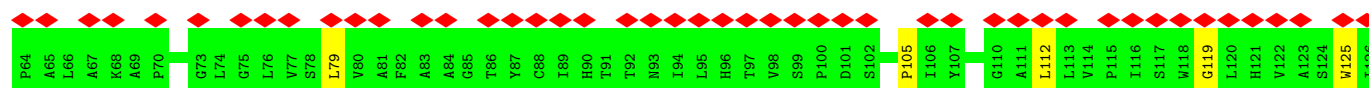
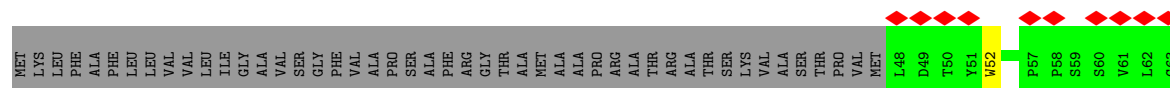
• Molecule 13: Photosystem I reaction center subunit IX



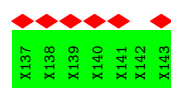
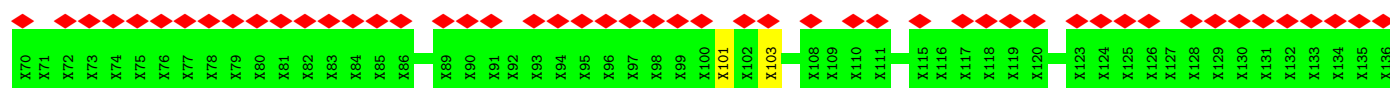
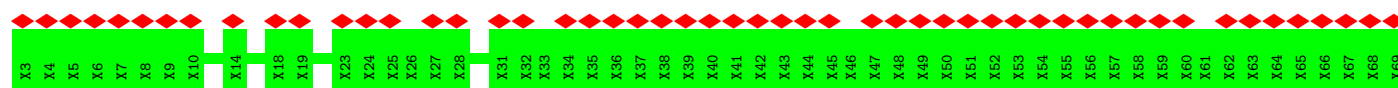
• Molecule 14: Photosystem I reaction center subunit XII



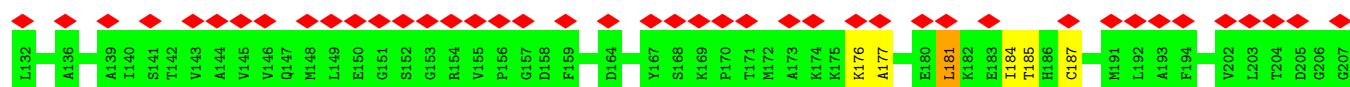
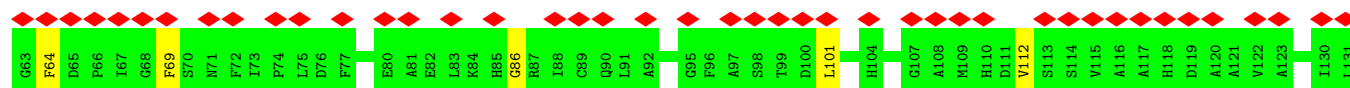
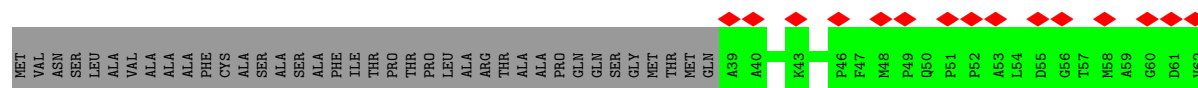
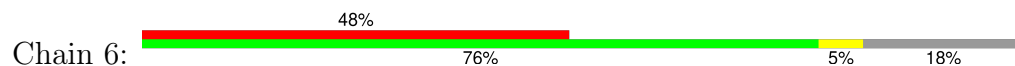
• Molecule 15: PsaR



• Molecule 16: FCPB

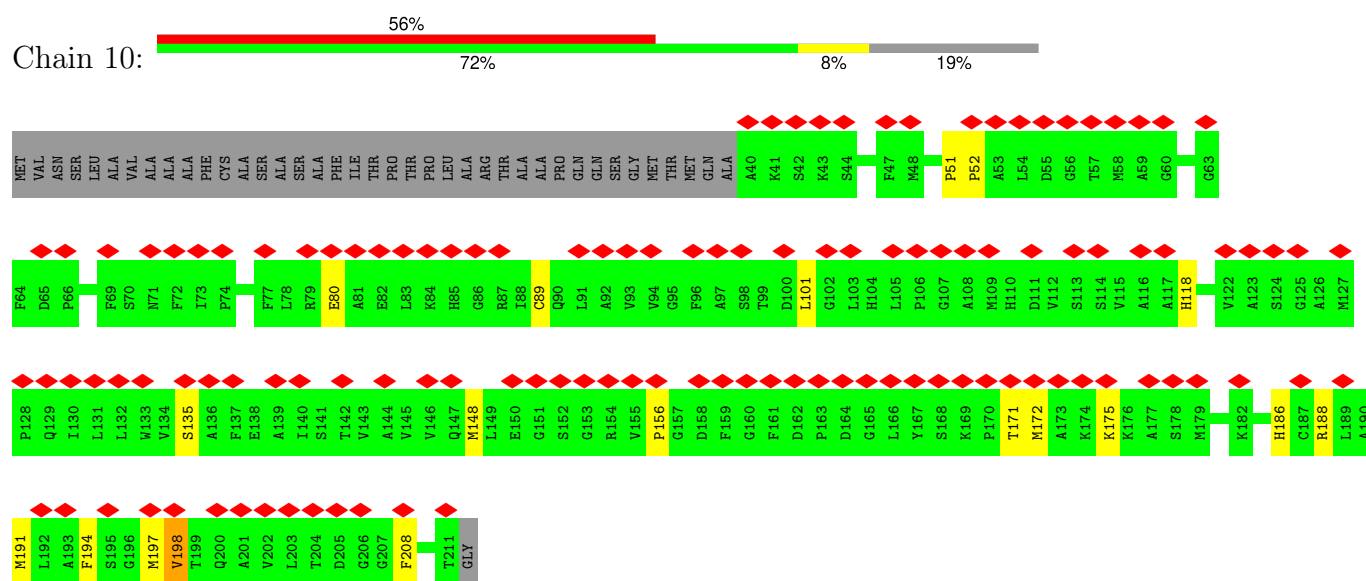


• Molecule 17: FCP6 and FCP10

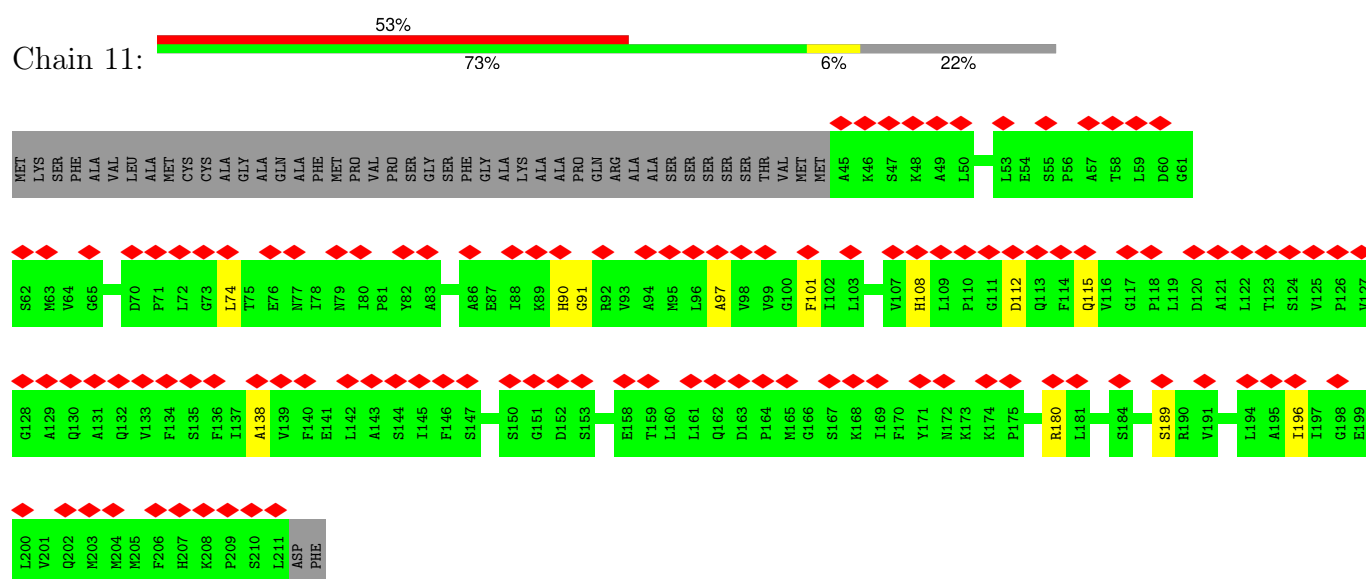




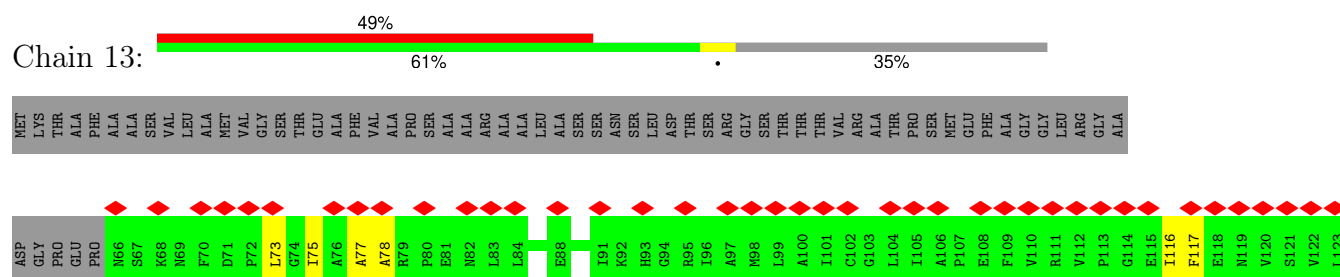
- Molecule 17: FCP6 and FCP10

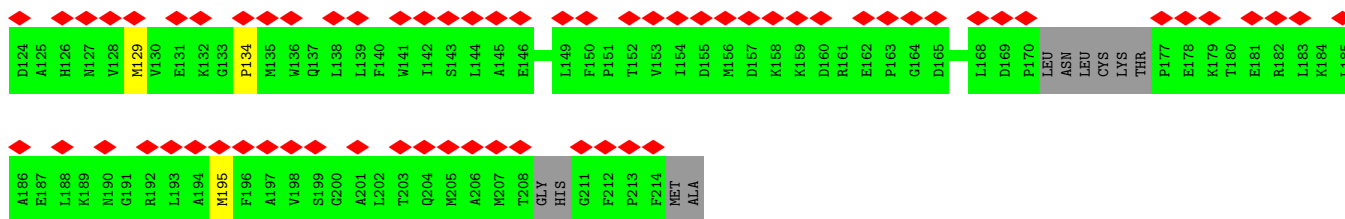


- Molecule 18: FCP11

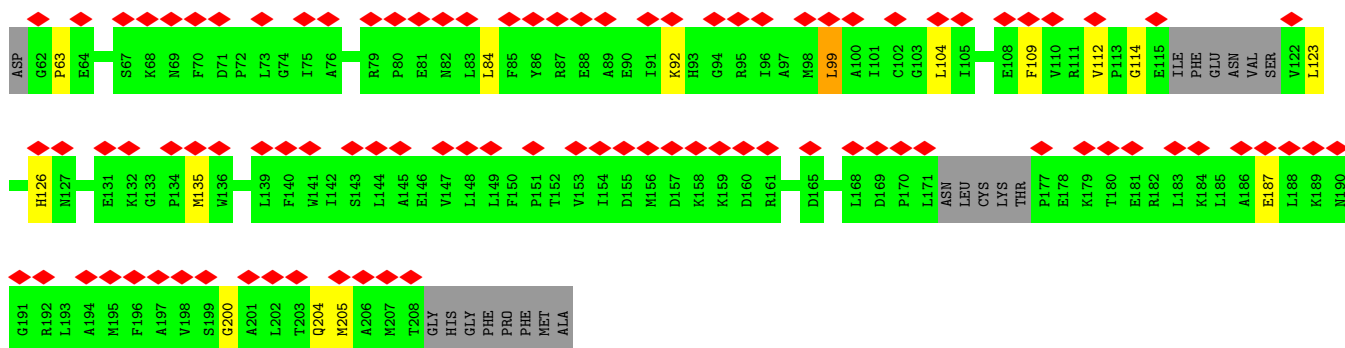
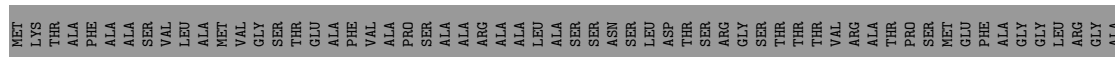
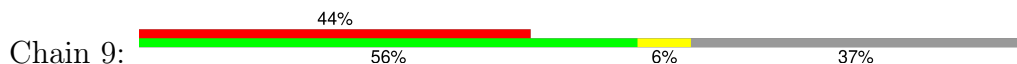


- Molecule 19: FCP9 and FCP13

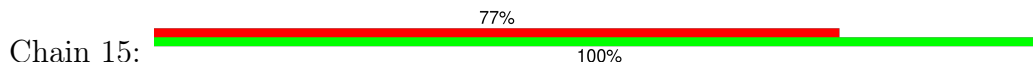




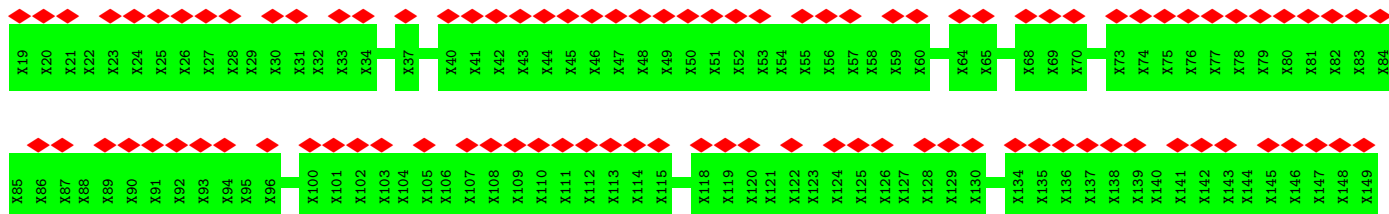
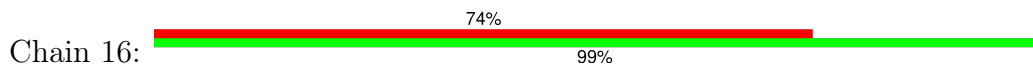
• Molecule 19: FCP9 and FCP13

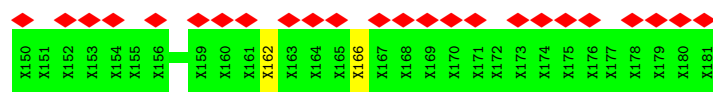


• Molecule 20: FCP15

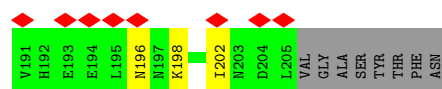
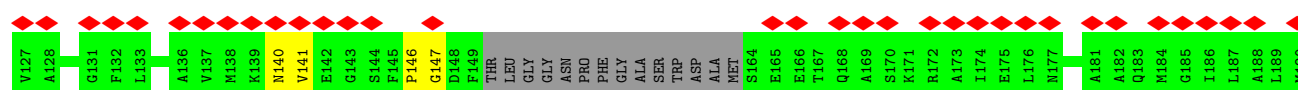
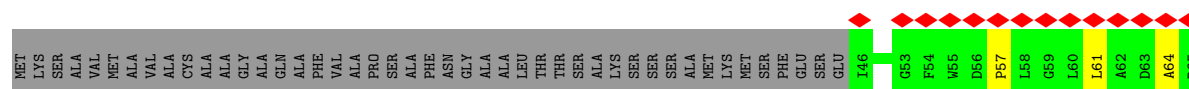
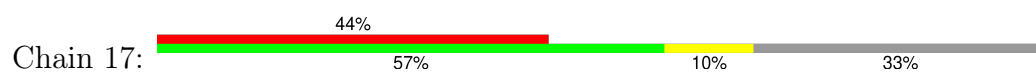


• Molecule 21: FCP16

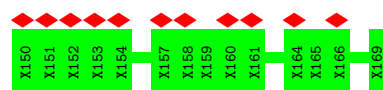
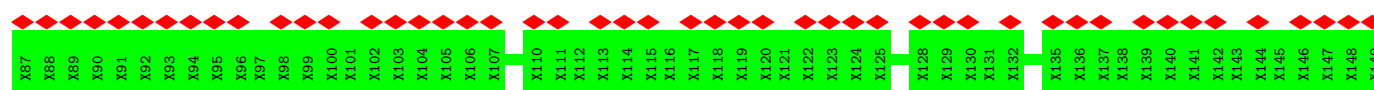
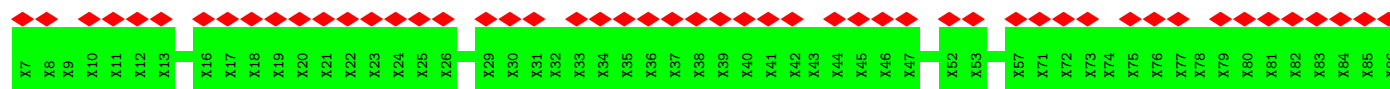
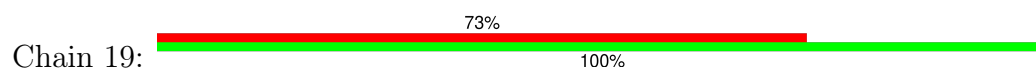




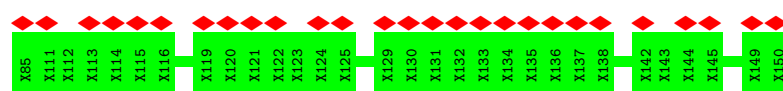
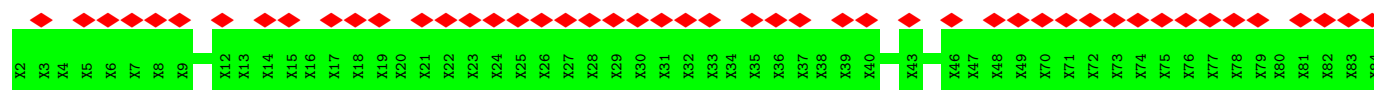
- Molecule 22: FCP17



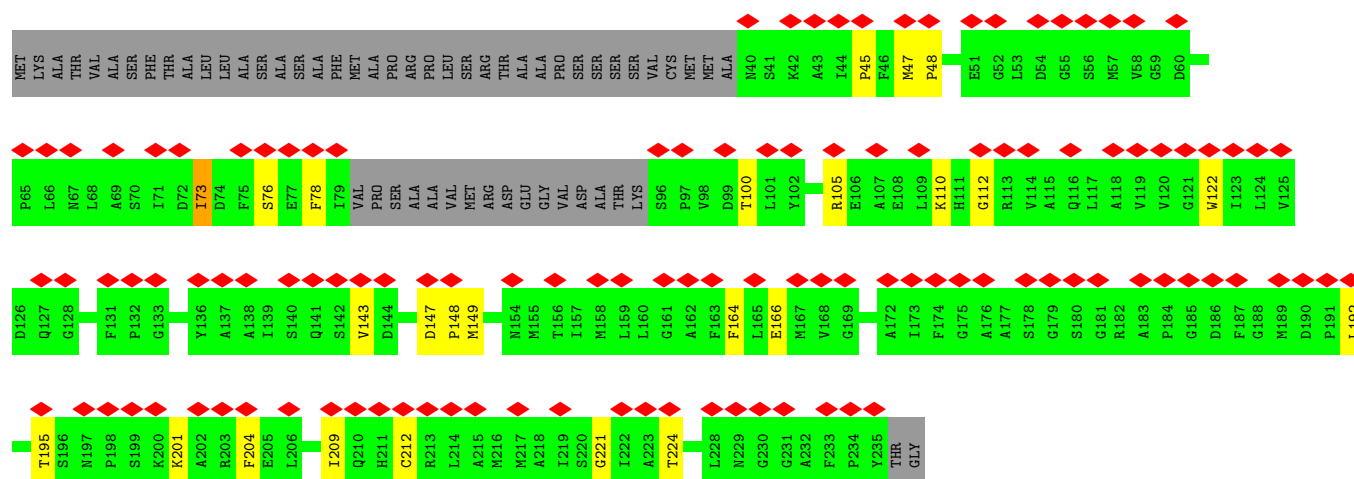
- Molecule 23: FCP19



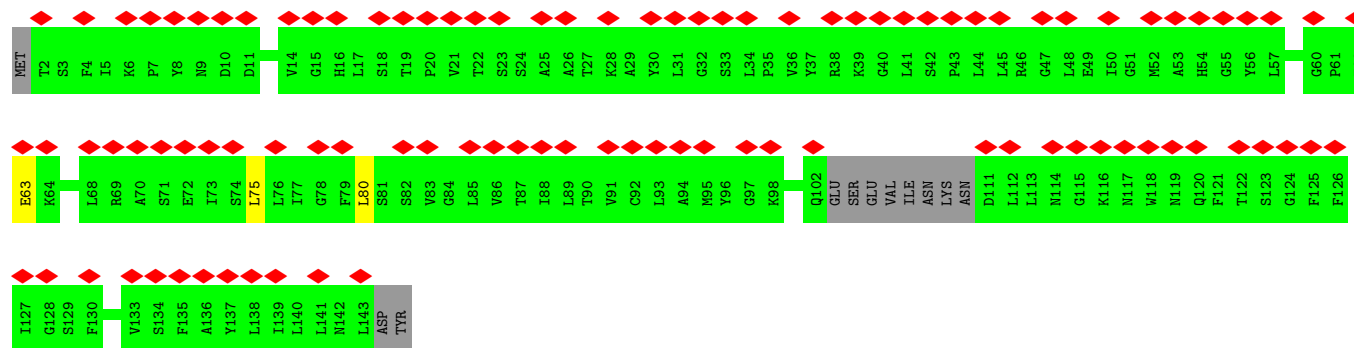
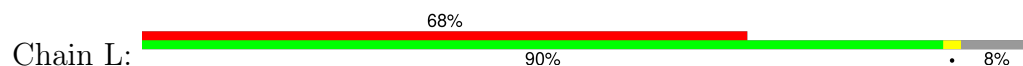
- Molecule 24: FCP2



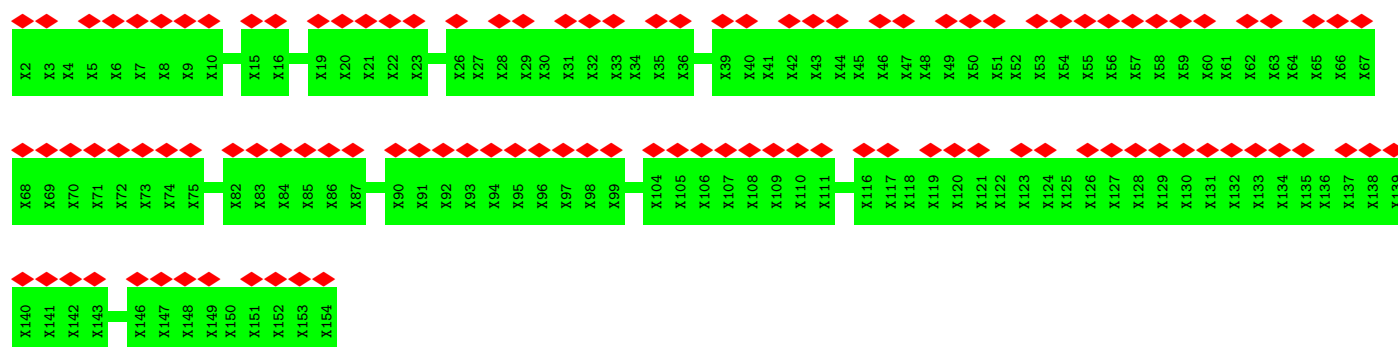
- Molecule 25: FCP4



• Molecule 26: Photosystem I reaction center subunit XI



• Molecule 27: FCPA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133000	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)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	7.047	Depositor
Minimum map value	-4.430	Depositor
Average map value	0.081	Depositor
Map value standard deviation	0.467	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	119.266, 233.664, 260.438	wwPDB
Map dimensions	214, 192, 98	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.217, 1.217, 1.2169999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DGD, LHG, KC1, SF4, LMG, CLA, BCR, A86, PQN, XAT

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	1	0.13	0/1370	0.24	0/1868
2	3	0.15	0/1264	0.31	0/1713
3	5	0.13	0/1329	0.28	0/1799
4	7	0.15	0/1322	0.27	0/1786
5	8	0.10	0/1366	0.22	0/1850
6	A	0.18	0/6027	0.34	0/8202
7	B	0.18	0/6045	0.33	0/8254
8	C	0.16	0/606	0.38	0/823
9	D	0.12	0/1028	0.28	0/1386
10	E	0.14	0/490	0.26	0/663
11	F	0.15	0/1304	0.31	0/1769
12	I	0.15	0/270	0.29	0/370
13	J	0.18	0/345	0.40	0/471
14	M	0.13	0/230	0.25	0/312
15	R	0.13	0/646	0.27	0/888
17	10	0.10	0/1301	0.25	0/1764
17	6	0.15	0/1306	0.28	0/1771
18	11	0.11	0/1314	0.24	0/1781
19	13	0.12	0/1131	0.28	0/1526
19	9	0.12	0/1082	0.31	0/1461
22	17	0.11	0/1126	0.30	0/1522
25	4	0.14	0/1367	0.31	1/1851 (0.1%)
26	L	0.15	0/1039	0.30	0/1409
All	All	0.15	0/33308	0.30	1/45239 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	76	SER	CB-CA-C	-5.34	110.43	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1336	0	1313	8	0
2	3	1236	0	1208	8	0
3	5	1299	0	1294	14	0
4	7	1288	0	1281	14	0
5	8	1328	0	1291	9	0
6	A	5834	0	5736	26	0
7	B	5834	0	5639	38	0
8	C	596	0	568	2	0
9	D	1002	0	1013	3	0
10	E	482	0	494	0	0
11	F	1271	0	1262	7	0
12	I	264	0	290	3	0
13	J	333	0	327	4	0
14	M	228	0	260	2	0
15	R	627	0	635	4	0
16	b	706	0	154	1	0
17	10	1270	0	1265	14	0
17	6	1275	0	1270	7	0
18	11	1283	0	1293	11	0
19	13	1107	0	1122	7	0
19	9	1060	0	1082	11	0
20	15	775	0	160	0	0
21	16	815	0	169	1	0
22	17	1107	0	1113	14	0
23	19	750	0	157	0	0
24	2	520	0	111	0	0
25	4	1337	0	1309	18	0
26	L	1015	0	1044	2	0
27	a	755	0	159	0	0
28	1	445	0	416	12	0
28	10	470	0	407	16	0
28	11	516	0	460	10	0
28	13	279	0	214	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	15	46	0	33	0	0
28	16	218	0	161	1	0
28	17	333	0	254	8	0
28	19	89	0	66	1	0
28	3	430	0	452	9	0
28	4	379	0	339	16	0
28	5	436	0	400	14	0
28	6	444	0	416	18	0
28	7	574	0	570	19	0
28	8	378	0	344	16	0
28	9	333	0	251	9	0
28	A	2540	0	2542	74	0
28	B	2474	0	2597	60	0
28	F	108	0	104	4	0
28	J	100	0	86	2	0
28	L	245	0	255	4	0
28	R	106	0	90	1	0
28	a	173	0	128	1	0
29	1	96	0	0	0	0
29	10	96	0	0	0	0
29	11	48	0	0	0	0
29	17	48	0	0	0	0
29	3	144	0	0	1	0
29	4	96	0	0	0	0
29	5	48	0	0	0	0
29	6	48	0	0	0	0
29	8	48	0	0	0	0
29	9	48	0	0	0	0
29	J	48	0	0	0	0
29	R	96	0	0	0	0
30	1	45	0	0	0	0
30	10	135	0	0	0	0
30	11	45	0	0	0	0
30	13	45	0	0	0	0
30	17	90	0	0	1	0
30	3	135	0	0	0	0
30	4	180	0	0	0	0
30	5	45	0	0	1	0
30	6	180	0	0	0	0
30	7	90	0	0	0	0
30	8	90	0	0	0	0
30	9	90	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	a	45	0	0	0	0
31	1	44	0	61	1	0
31	11	37	0	44	1	0
31	4	25	0	20	0	0
31	5	51	0	42	1	0
31	7	27	0	24	0	0
31	9	91	0	92	2	0
31	A	102	0	117	1	0
31	B	76	0	96	9	0
31	I	49	0	74	1	0
32	1	44	0	56	1	0
32	10	132	0	168	11	0
32	11	44	0	56	7	0
32	13	88	0	112	6	0
32	17	44	0	56	3	0
32	3	44	0	56	1	0
32	4	88	0	112	10	0
32	5	176	0	224	15	0
32	6	132	0	168	14	0
32	7	220	0	280	17	0
32	8	88	0	112	6	0
32	9	43	0	53	5	0
32	J	44	0	56	2	0
33	1	40	0	56	1	0
33	17	40	0	56	1	0
33	8	40	0	56	1	0
33	A	200	0	280	11	0
33	B	320	0	448	16	0
33	F	80	0	112	7	0
33	I	40	0	56	2	0
33	J	40	0	56	4	0
33	L	80	0	112	5	0
33	M	40	0	56	0	0
34	4	68	0	58	2	0
34	8	31	0	26	0	0
35	A	33	0	46	0	0
35	B	33	0	46	0	0
36	A	8	0	0	0	0
36	C	16	0	0	0	0
37	F	41	0	52	1	0
All	All	52767	0	47199	523	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 523 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)
28:9:303:CLA:HHC	32:9:313:XAT:H28	1.59	0.85
28:3:301:CLA:HHB	28:3:301:CLA:H2	1.63	0.81
7:B:704:GLN:HG3	31:B:844:LHG:H252	1.62	0.80
17:10:101:LEU:HD21	17:10:208:PHE:HB2	1.71	0.72
32:7:315:XAT:H30	32:7:315:XAT:H402	1.71	0.72

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	1	176/230 (76%)	172 (98%)	4 (2%)	0	100	100
2	3	159/191 (83%)	154 (97%)	4 (2%)	1 (1%)	21	35
3	5	173/222 (78%)	169 (98%)	4 (2%)	0	100	100
4	7	167/169 (99%)	163 (98%)	4 (2%)	0	100	100
5	8	174/215 (81%)	168 (97%)	6 (3%)	0	100	100
6	A	740/749 (99%)	725 (98%)	15 (2%)	0	100	100
7	B	728/734 (99%)	707 (97%)	21 (3%)	0	100	100
8	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
9	D	123/132 (93%)	123 (100%)	0	0	100	100
10	E	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
11	F	159/202 (79%)	157 (99%)	2 (1%)	0	100	100
12	I	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
13	J	39/42 (93%)	39 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	M	28/30 (93%)	28 (100%)	0	0	100	100
15	R	83/132 (63%)	83 (100%)	0	0	100	100
17	10	170/212 (80%)	163 (96%)	7 (4%)	0	100	100
17	6	171/212 (81%)	166 (97%)	5 (3%)	0	100	100
18	11	165/213 (78%)	164 (99%)	1 (1%)	0	100	100
19	13	135/216 (62%)	126 (93%)	9 (7%)	0	100	100
19	9	130/216 (60%)	125 (96%)	4 (3%)	1 (1%)	16	28
22	17	142/218 (65%)	133 (94%)	9 (6%)	0	100	100
25	4	176/237 (74%)	170 (97%)	6 (3%)	0	100	100
26	L	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
All	All	4136/4895 (84%)	4026 (97%)	108 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	3	31	VAL
19	9	109	PHE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	136/170 (80%)	136 (100%)	0	100	100
2	3	132/153 (86%)	132 (100%)	0	100	100
3	5	133/164 (81%)	131 (98%)	2 (2%)	57	78
4	7	135/135 (100%)	134 (99%)	1 (1%)	76	88
5	8	133/163 (82%)	130 (98%)	3 (2%)	44	69
6	A	607/613 (99%)	597 (98%)	10 (2%)	55	77
7	B	600/603 (100%)	594 (99%)	6 (1%)	68	84
8	C	67/68 (98%)	67 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	D	106/113 (94%)	105 (99%)	1 (1%)	70	86
10	E	53/54 (98%)	53 (100%)	0	100	100
11	F	140/177 (79%)	139 (99%)	1 (1%)	76	88
12	I	30/32 (94%)	30 (100%)	0	100	100
13	J	35/36 (97%)	35 (100%)	0	100	100
14	M	25/25 (100%)	25 (100%)	0	100	100
15	R	67/101 (66%)	65 (97%)	2 (3%)	36	61
17	10	134/161 (83%)	132 (98%)	2 (2%)	57	78
17	6	134/161 (83%)	131 (98%)	3 (2%)	45	70
18	11	139/172 (81%)	139 (100%)	0	100	100
19	13	117/170 (69%)	116 (99%)	1 (1%)	70	86
19	9	112/170 (66%)	108 (96%)	4 (4%)	31	55
22	17	113/162 (70%)	110 (97%)	3 (3%)	39	64
25	4	138/180 (77%)	135 (98%)	3 (2%)	45	70
26	L	111/122 (91%)	111 (100%)	0	100	100
All	All	3397/3905 (87%)	3355 (99%)	42 (1%)	61	81

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	6	181	LEU
25	4	73	ILE
17	10	171	THR
22	17	84	MET
25	4	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
22	17	94	GLN
22	17	183	GLN
19	9	204	GLN
7	B	158	GLN
6	A	712	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

318 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
28	CLA	B	823	7	69,73,73	0.97	4 (5%)	82,113,113	1.10	3 (3%)
36	SF4	C	102	8	0,12,12	-	-	-		
28	CLA	B	807	7	69,73,73	0.86	4 (5%)	82,113,113	1.08	5 (6%)
28	CLA	J	102	-	62,66,73	0.89	4 (6%)	73,104,113	1.20	4 (5%)
31	LHG	1	309	-	43,43,48	0.31	0	46,49,54	0.30	0
28	CLA	B	805	7	69,73,73	0.93	4 (5%)	82,113,113	1.06	6 (7%)
31	LHG	A	851	-	26,26,48	0.38	0	29,32,54	0.34	0
28	CLA	11	312	18	47,51,73	1.03	3 (6%)	55,86,113	1.62	8 (14%)
36	SF4	A	848	7,6	0,12,12	-	-	-		
28	CLA	15	201	-	50,54,73	0.95	4 (8%)	59,90,113	1.33	8 (13%)
28	CLA	A	845	-	69,73,73	0.99	4 (5%)	82,113,113	1.04	5 (6%)
28	CLA	1	305	1	56,60,73	0.82	3 (5%)	65,97,113	1.27	9 (13%)
32	XAT	10	313	-	41,47,47	0.65	2 (4%)	54,74,74	0.67	2 (3%)
28	CLA	A	831	6	54,58,73	0.99	4 (7%)	64,95,113	1.13	3 (4%)
28	CLA	9	311	19	49,53,73	0.95	4 (8%)	58,89,113	1.46	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	KC1	7	307	4	49,53,53	1.30	3 (6%)	61,89,89	1.42	13 (21%)
28	CLA	A	828	6	69,73,73	0.92	4 (5%)	82,113,113	1.02	5 (6%)
28	CLA	9	305	-	54,58,73	0.87	4 (7%)	64,95,113	1.30	9 (14%)
32	XAT	9	313	-	42,46,47	0.66	2 (4%)	52,71,74	0.82	2 (3%)
33	BCR	A	842	-	41,41,41	0.14	0	56,56,56	0.22	0
29	A86	R	203	-	47,50,50	0.44	1 (2%)	51,76,76	0.60	0
28	CLA	7	305	4	69,73,73	0.85	4 (5%)	82,113,113	1.05	6 (7%)
28	CLA	A	812	6	56,60,73	1.06	4 (7%)	65,97,113	1.15	5 (7%)
28	CLA	5	309	3	54,58,73	1.02	4 (7%)	64,95,113	1.46	9 (14%)
30	KC1	7	309	4	49,53,53	1.18	4 (8%)	61,89,89	1.43	10 (16%)
28	CLA	16	204	-	45,49,73	0.85	3 (6%)	54,84,113	1.51	9 (16%)
33	BCR	8	309	-	41,41,41	0.17	0	56,56,56	1.20	5 (8%)
31	LHG	5	314	-	23,23,48	0.41	0	26,29,54	0.36	0
32	XAT	3	313	-	41,47,47	0.67	2 (4%)	54,74,74	0.70	1 (1%)
32	XAT	5	307	-	41,47,47	0.42	0	54,74,74	1.54	7 (12%)
31	LHG	9	301	-	27,27,48	0.39	0	30,33,54	0.35	0
29	A86	4	314	-	47,50,50	0.43	1 (2%)	51,76,76	0.62	0
28	CLA	B	806	7	69,73,73	0.96	4 (5%)	82,113,113	1.01	3 (3%)
32	XAT	J	105	-	41,47,47	0.47	1 (2%)	54,74,74	1.23	5 (9%)
33	BCR	A	850	-	41,41,41	0.24	0	56,56,56	1.20	7 (12%)
28	CLA	10	305	17	50,54,73	0.94	4 (8%)	59,90,113	1.32	4 (6%)
29	A86	4	313	-	47,50,50	0.41	1 (2%)	51,76,76	0.53	0
28	CLA	11	304	18	64,68,73	0.81	4 (6%)	76,107,113	1.31	8 (10%)
28	CLA	B	813	-	64,68,73	0.94	4 (6%)	76,107,113	1.32	6 (7%)
28	CLA	A	849	6	69,73,73	0.83	4 (5%)	82,113,113	1.15	6 (7%)
28	CLA	6	301	17	69,73,73	0.83	4 (5%)	82,113,113	1.10	6 (7%)
32	XAT	7	316	-	41,47,47	0.62	2 (4%)	54,74,74	1.35	6 (11%)
28	CLA	16	201	-	49,53,73	0.82	3 (6%)	58,89,113	1.40	9 (15%)
30	KC1	17	306	-	49,53,53	1.11	4 (8%)	61,89,89	1.67	11 (18%)
30	KC1	3	309	2	49,53,53	1.15	4 (8%)	61,89,89	1.60	8 (13%)
28	CLA	19	201	-	50,54,73	0.73	2 (4%)	59,90,113	1.42	10 (16%)
28	CLA	4	305	-	46,50,73	0.85	3 (6%)	53,85,113	1.43	7 (13%)
32	XAT	6	312	-	41,47,47	0.47	1 (2%)	54,74,74	1.26	3 (5%)
34	DGD	4	301	-	40,40,67	0.19	0	54,54,81	0.23	0
28	CLA	6	304	17	46,50,73	0.99	3 (6%)	53,85,113	1.56	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	KC1	3	308	2	49,53,53	1.20	3 (6%)	61,89,89	1.54	10 (16%)
32	XAT	7	317	-	41,47,47	0.40	1 (2%)	54,74,74	1.44	7 (12%)
34	DGD	8	314	-	32,32,67	0.22	0	45,45,81	0.50	0
30	KC1	4	312	-	49,53,53	1.11	4 (8%)	61,89,89	1.34	9 (14%)
28	CLA	3	301	2	69,73,73	0.85	4 (5%)	82,113,113	1.13	4 (4%)
33	BCR	L	205	-	41,41,41	0.13	0	56,56,56	0.24	0
29	A86	J	101	-	47,50,50	0.47	1 (2%)	51,76,76	0.71	0
28	CLA	6	313	-	69,73,73	0.85	4 (5%)	82,113,113	1.21	7 (8%)
32	XAT	7	313	-	41,47,47	0.44	1 (2%)	54,74,74	1.19	4 (7%)
28	CLA	B	833	-	65,69,73	0.94	4 (6%)	77,108,113	1.09	3 (3%)
29	A86	1	313	28	47,50,50	0.40	1 (2%)	51,76,76	0.61	1 (1%)
28	CLA	A	830	6	69,73,73	0.93	4 (5%)	82,113,113	1.12	4 (4%)
28	CLA	A	803	6	59,63,73	0.88	4 (6%)	70,101,113	1.11	5 (7%)
32	XAT	6	315	-	41,47,47	0.47	0	54,74,74	1.00	5 (9%)
28	CLA	a	201	-	47,51,73	0.82	3 (6%)	55,86,113	1.56	6 (10%)
30	KC1	6	305	17	49,53,53	1.23	4 (8%)	61,89,89	1.47	9 (14%)
28	CLA	10	301	17	59,63,73	0.82	3 (5%)	70,101,113	1.23	7 (10%)
28	CLA	A	852	6	69,73,73	0.98	4 (5%)	82,113,113	1.08	5 (6%)
29	A86	8	308	-	47,50,50	0.49	1 (2%)	51,76,76	0.65	0
28	CLA	10	307	-	61,65,73	0.80	3 (4%)	72,103,113	1.27	7 (9%)
28	CLA	A	827	6	69,73,73	1.00	4 (5%)	82,113,113	1.26	6 (7%)
28	CLA	a	203	-	50,54,73	0.81	3 (6%)	59,90,113	1.61	8 (13%)
32	XAT	6	316	-	41,47,47	0.62	2 (4%)	54,74,74	0.78	1 (1%)
28	CLA	11	305	-	49,53,73	0.96	3 (6%)	58,89,113	1.46	8 (13%)
28	CLA	5	305	3	60,64,73	0.84	4 (6%)	71,102,113	1.12	5 (7%)
30	KC1	17	312	22	49,53,53	1.19	4 (8%)	61,89,89	1.56	6 (9%)
28	CLA	1	301	1	54,58,73	0.79	2 (3%)	64,95,113	1.51	11 (17%)
28	CLA	11	309	18	47,51,73	1.02	4 (8%)	55,86,113	1.37	4 (7%)
28	CLA	A	807	6	69,73,73	1.00	4 (5%)	82,113,113	1.04	4 (4%)
31	LHG	4	302	-	24,24,48	0.40	0	27,30,54	0.35	0
28	CLA	A	847	6	69,73,73	0.79	4 (5%)	82,113,113	1.28	7 (8%)
29	A86	3	310	-	47,50,50	0.42	1 (2%)	51,76,76	0.73	2 (3%)
28	CLA	B	831	7	69,73,73	0.86	4 (5%)	82,113,113	1.04	6 (7%)
33	BCR	F	804	-	41,41,41	0.13	0	56,56,56	0.27	0
28	CLA	A	820	6	53,57,73	1.06	4 (7%)	61,93,113	1.14	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	17	305	-	54,58,73	0.92	3 (5%)	64,95,113	1.50	8 (12%)
28	CLA	17	302	22	47,51,73	1.06	3 (6%)	55,86,113	1.33	7 (12%)
28	CLA	6	307	-	59,63,73	0.91	3 (5%)	70,101,113	1.22	4 (5%)
31	LHG	A	839	-	47,47,48	0.31	0	50,53,54	0.35	0
28	CLA	17	309	22	50,54,73	0.76	2 (4%)	59,90,113	1.62	11 (18%)
28	CLA	8	304	5	61,65,73	0.83	4 (6%)	72,103,113	1.31	7 (9%)
28	CLA	B	815	-	63,67,73	0.83	3 (4%)	74,105,113	1.21	4 (5%)
28	CLA	a	204	-	46,50,73	0.98	4 (8%)	53,85,113	1.64	7 (13%)
29	A86	R	201	-	47,50,50	0.42	1 (2%)	51,76,76	0.51	0
28	CLA	7	318	-	49,53,73	0.96	4 (8%)	58,89,113	1.54	9 (15%)
28	CLA	B	802	-	69,73,73	1.04	4 (5%)	82,113,113	1.07	4 (4%)
28	CLA	11	306	18	49,53,73	0.94	4 (8%)	58,89,113	1.25	6 (10%)
28	CLA	7	303	-	69,73,73	0.80	4 (5%)	82,113,113	1.15	8 (9%)
31	LHG	11	311	-	36,36,48	0.34	0	39,42,54	0.35	0
28	CLA	A	809	6	60,64,73	0.90	4 (6%)	71,102,113	1.23	5 (7%)
29	A86	10	317	-	47,50,50	0.53	1 (2%)	51,76,76	0.67	1 (1%)
31	LHG	A	840	28	26,26,48	0.41	0	29,32,54	0.31	0
31	LHG	I	102	-	48,48,48	0.29	0	51,54,54	0.29	0
28	CLA	L	201	-	69,73,73	0.81	4 (5%)	82,113,113	1.18	4 (4%)
30	KC1	8	307	5	49,53,53	1.25	4 (8%)	61,89,89	1.39	12 (19%)
30	KC1	4	311	25	49,53,53	1.03	3 (6%)	61,89,89	1.47	9 (14%)
28	CLA	B	804	-	69,73,73	0.78	3 (4%)	82,113,113	1.23	5 (6%)
28	CLA	L	204	-	54,58,73	0.94	4 (7%)	64,95,113	1.34	7 (10%)
28	CLA	9	304	19	54,58,73	0.97	4 (7%)	64,95,113	1.24	8 (12%)
32	XAT	10	314	-	41,47,47	0.60	2 (4%)	54,74,74	0.85	1 (1%)
28	CLA	B	821	-	69,73,73	0.91	4 (5%)	82,113,113	1.08	4 (4%)
28	CLA	7	312	4	69,73,73	0.78	3 (4%)	82,113,113	1.35	5 (6%)
28	CLA	F	803	11	47,51,73	1.13	4 (8%)	55,86,113	1.27	5 (9%)
28	CLA	B	814	7	63,67,73	1.00	4 (6%)	74,105,113	1.18	5 (6%)
28	CLA	A	805	6	69,73,73	1.07	4 (5%)	82,113,113	1.08	8 (9%)
28	CLA	8	313	-	60,64,73	0.80	4 (6%)	71,102,113	1.21	7 (9%)
28	CLA	8	302	5	60,64,73	0.93	4 (6%)	71,102,113	1.29	8 (11%)
30	KC1	10	311	-	49,53,53	1.26	3 (6%)	61,89,89	1.27	9 (14%)
28	CLA	A	808	6	69,73,73	1.02	4 (5%)	82,113,113	1.12	5 (6%)
28	CLA	1	307	1	59,63,73	0.95	4 (6%)	70,101,113	1.14	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	8	301	5	69,73,73	0.83	4 (5%)	82,113,113	1.12	8 (9%)
28	CLA	A	836	6	69,73,73	0.87	4 (5%)	82,113,113	1.21	9 (10%)
28	CLA	B	818	7	50,54,73	1.13	4 (8%)	59,90,113	1.33	4 (6%)
32	XAT	8	311	-	41,47,47	0.62	2 (4%)	54,74,74	0.85	2 (3%)
32	XAT	5	311	-	41,47,47	0.60	2 (4%)	54,74,74	0.83	2 (3%)
28	CLA	A	824	-	69,73,73	1.02	4 (5%)	82,113,113	1.15	5 (6%)
28	CLA	5	306	3	45,49,73	0.93	3 (6%)	54,84,113	1.46	9 (16%)
28	CLA	B	826	7	69,73,73	0.90	4 (5%)	82,113,113	1.15	5 (6%)
34	DGD	4	317	30	30,30,67	0.20	0	42,42,81	0.36	0
28	CLA	B	825	7	69,73,73	0.96	4 (5%)	82,113,113	1.02	5 (6%)
28	CLA	19	202	-	47,51,73	0.99	4 (8%)	55,86,113	1.52	8 (14%)
28	CLA	5	302	3	59,63,73	0.89	4 (6%)	70,101,113	1.16	6 (8%)
28	CLA	4	303	-	59,63,73	0.80	3 (5%)	70,101,113	1.31	7 (10%)
28	CLA	B	834	7	69,73,73	0.94	4 (5%)	82,113,113	1.14	6 (7%)
32	XAT	5	310	-	41,47,47	0.53	1 (2%)	54,74,74	0.92	2 (3%)
28	CLA	3	305	2	64,68,73	0.88	4 (6%)	76,107,113	1.19	7 (9%)
28	CLA	5	301	3	69,73,73	0.81	4 (5%)	82,113,113	1.06	5 (6%)
28	CLA	9	307	19	54,58,73	0.84	3 (5%)	64,95,113	1.41	7 (10%)
28	CLA	A	813	6	54,58,73	1.09	4 (7%)	64,95,113	1.18	5 (7%)
28	CLA	A	832	6	49,53,73	1.02	4 (8%)	58,89,113	1.39	5 (8%)
28	CLA	A	815	6	69,73,73	0.91	4 (5%)	82,113,113	1.02	6 (7%)
31	LHG	B	842	28	25,25,48	0.42	0	28,31,54	0.46	0
28	CLA	L	206	26	69,73,73	0.84	3 (4%)	82,113,113	1.35	7 (8%)
28	CLA	B	829	-	49,53,73	1.17	4 (8%)	58,89,113	1.33	7 (12%)
30	KC1	1	306	1	49,53,53	1.15	4 (8%)	61,89,89	1.46	9 (14%)
28	CLA	A	822	6	59,63,73	0.97	4 (6%)	70,101,113	1.05	5 (7%)
28	CLA	13	302	19	49,53,73	0.99	4 (8%)	58,89,113	1.42	8 (13%)
29	A86	3	312	-	47,50,50	0.52	1 (2%)	51,76,76	0.59	1 (1%)
28	CLA	B	801	7	69,73,73	0.85	4 (5%)	82,113,113	1.17	6 (7%)
32	XAT	7	314	-	41,47,47	0.62	2 (4%)	54,74,74	0.66	3 (5%)
30	KC1	5	308	-	49,53,53	1.14	3 (6%)	61,89,89	1.20	8 (13%)
28	CLA	17	303	22	52,56,73	0.88	3 (5%)	61,92,113	1.41	6 (9%)
32	XAT	11	313	-	41,47,47	0.58	2 (4%)	54,74,74	0.71	2 (3%)
28	CLA	10	302	17	50,54,73	0.97	4 (8%)	59,90,113	1.30	7 (11%)
32	XAT	13	309	-	41,47,47	0.67	2 (4%)	54,74,74	0.71	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	J	103	13	46,50,73	0.99	4 (8%)	53,85,113	1.56	5 (9%)
33	BCR	B	841	-	41,41,41	0.18	0	56,56,56	0.34	0
28	CLA	13	301	19	60,64,73	0.91	4 (6%)	71,102,113	1.40	10 (14%)
28	CLA	3	306	2	69,73,73	0.89	4 (5%)	82,113,113	0.99	5 (6%)
28	CLA	B	810	7	58,62,73	0.96	4 (6%)	71,100,113	1.17	4 (5%)
28	CLA	1	304	1	49,53,73	0.89	4 (8%)	58,89,113	1.29	8 (13%)
28	CLA	4	306	25	59,63,73	1.05	4 (6%)	70,101,113	1.13	5 (7%)
28	CLA	13	307	19	49,53,73	0.79	3 (6%)	58,89,113	1.52	8 (13%)
28	CLA	13	303	-	49,53,73	0.80	3 (6%)	58,89,113	1.55	7 (12%)
28	CLA	B	811	7	59,63,73	1.06	4 (6%)	70,101,113	1.24	5 (7%)
28	CLA	5	303	-	69,73,73	0.91	4 (5%)	82,113,113	1.17	5 (6%)
28	CLA	8	303	-	61,65,73	0.95	4 (6%)	72,103,113	1.18	4 (5%)
28	CLA	B	819	7	59,63,73	0.93	4 (6%)	70,101,113	1.13	5 (7%)
28	CLA	B	843	7	69,73,73	0.95	4 (5%)	82,113,113	1.04	3 (3%)
28	CLA	L	203	26	69,73,73	0.93	4 (5%)	82,113,113	1.09	3 (3%)
28	CLA	B	817	-	69,73,73	0.88	4 (5%)	82,113,113	1.05	5 (6%)
28	CLA	10	306	17	60,64,73	0.87	4 (6%)	71,102,113	1.21	5 (7%)
33	BCR	B	846	-	41,41,41	0.21	0	56,56,56	0.56	0
33	BCR	1	312	-	41,41,41	0.12	0	56,56,56	0.35	0
28	CLA	A	846	6	51,55,73	1.02	4 (7%)	60,91,113	1.42	4 (6%)
29	A86	6	314	-	47,50,50	0.45	1 (2%)	51,76,76	0.83	2 (3%)
28	CLA	B	845	7	69,73,73	0.91	4 (5%)	82,113,113	1.04	3 (3%)
28	CLA	11	314	-	47,51,73	0.92	4 (8%)	55,86,113	1.44	5 (9%)
28	CLA	4	304	25	55,59,73	0.91	4 (7%)	64,96,113	1.41	7 (10%)
28	CLA	B	816	7	69,73,73	0.98	4 (5%)	82,113,113	1.04	3 (3%)
28	CLA	7	306	31	69,73,73	0.83	4 (5%)	82,113,113	1.22	7 (8%)
28	CLA	10	308	17	51,55,73	0.94	4 (7%)	60,91,113	1.26	5 (8%)
28	CLA	6	303	-	59,63,73	0.88	4 (6%)	70,101,113	1.27	7 (10%)
28	CLA	7	302	4	54,58,73	1.10	4 (7%)	64,95,113	1.29	5 (7%)
28	CLA	B	812	7	69,73,73	1.06	4 (5%)	82,113,113	0.96	4 (4%)
28	CLA	A	853	-	69,73,73	1.06	4 (5%)	82,113,113	1.10	5 (6%)
31	LHG	9	314	-	32,32,48	0.35	0	35,38,54	0.33	0
36	SF4	C	101	8	0,12,12	-	-	-	-	-
28	CLA	9	310	-	49,53,73	1.06	4 (8%)	58,89,113	1.42	7 (12%)
30	KC1	9	306	19	49,53,53	1.15	3 (6%)	61,89,89	1.47	11 (18%)
28	CLA	4	316	25	65,69,73	0.65	3 (4%)	77,108,113	1.19	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	833	6	55,59,73	1.13	3 (5%)	64,96,113	1.36	5 (7%)
32	XAT	17	311	-	41,47,47	0.48	1 (2%)	54,74,74	0.96	6 (11%)
28	CLA	A	835	6	69,73,73	0.99	4 (5%)	82,113,113	1.15	7 (8%)
31	LHG	B	844	-	48,48,48	0.30	0	51,54,54	0.30	0
32	XAT	4	315	-	41,47,47	0.50	1 (2%)	54,74,74	0.95	3 (5%)
28	CLA	7	304	4	69,73,73	0.84	4 (5%)	82,113,113	1.01	2 (2%)
28	CLA	B	827	7	54,58,73	1.05	4 (7%)	64,95,113	1.24	6 (9%)
28	CLA	R	202	15	59,63,73	0.91	4 (6%)	70,101,113	1.25	5 (7%)
28	CLA	B	849	7	69,73,73	0.93	4 (5%)	82,113,113	0.91	5 (6%)
32	XAT	13	308	-	41,47,47	0.70	2 (4%)	54,74,74	0.53	0
29	A86	10	312	-	47,50,50	0.51	1 (2%)	51,76,76	1.03	5 (9%)
28	CLA	B	824	-	69,73,73	0.76	3 (4%)	82,113,113	1.18	8 (9%)
30	KC1	11	307	18	49,53,53	1.23	4 (8%)	61,89,89	1.51	10 (16%)
33	BCR	B	839	-	41,41,41	0.20	0	56,56,56	1.22	6 (10%)
28	CLA	A	806	6	59,63,73	1.02	4 (6%)	70,101,113	1.30	5 (7%)
28	CLA	3	314	31	69,73,73	0.85	4 (5%)	82,113,113	1.18	5 (6%)
28	CLA	8	305	5	49,53,73	1.04	4 (8%)	58,89,113	1.21	3 (5%)
30	KC1	13	304	19	49,53,53	1.02	3 (6%)	61,89,89	1.37	10 (16%)
28	CLA	1	314	-	69,73,73	0.82	4 (5%)	82,113,113	1.20	6 (7%)
31	LHG	7	310	28	26,26,48	0.40	0	29,32,54	0.37	0
28	CLA	11	303	18	61,65,73	0.84	4 (6%)	72,103,113	1.31	6 (8%)
33	BCR	J	104	-	41,41,41	0.23	0	56,56,56	0.29	0
28	CLA	6	311	17	51,57,73	1.67	4 (7%)	55,88,113	2.63	7 (12%)
28	CLA	16	205	-	47,51,73	0.86	3 (6%)	55,86,113	1.42	8 (14%)
33	BCR	17	310	-	41,41,41	0.12	0	56,56,56	0.61	1 (1%)
29	A86	1	302	-	47,50,50	0.54	1 (2%)	51,76,76	0.80	2 (3%)
30	KC1	6	308	17	49,53,53	1.08	4 (8%)	61,89,89	1.46	8 (13%)
28	CLA	A	804	6	69,73,73	0.82	4 (5%)	82,113,113	1.00	6 (7%)
28	CLA	4	310	-	59,63,73	0.99	4 (6%)	70,101,113	1.29	5 (7%)
33	BCR	B	840	-	41,41,41	0.26	0	56,56,56	0.50	1 (1%)
33	BCR	B	850	-	41,41,41	0.27	0	56,56,56	0.50	0
28	CLA	A	837	-	69,73,73	0.83	4 (5%)	82,113,113	1.02	7 (8%)
33	BCR	I	101	-	41,41,41	0.16	0	56,56,56	0.28	0
28	CLA	3	304	2	49,53,73	1.06	4 (8%)	58,89,113	1.20	4 (6%)
28	CLA	16	203	-	51,55,73	1.04	4 (7%)	60,91,113	1.44	7 (11%)
28	CLA	8	310	5	46,50,73	0.88	4 (8%)	53,85,113	1.29	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	814	-	49,53,73	1.12	4 (8%)	58,89,113	1.33	4 (6%)
30	KC1	3	302	2	49,53,53	1.08	4 (8%)	61,89,89	1.45	10 (16%)
32	XAT	8	312	-	41,47,47	0.61	2 (4%)	54,74,74	0.75	1 (1%)
28	CLA	10	303	-	59,63,73	0.80	4 (6%)	70,101,113	1.24	7 (10%)
28	CLA	16	202	-	46,50,73	1.02	4 (8%)	53,85,113	1.53	8 (15%)
28	CLA	B	830	7	62,66,73	1.15	4 (6%)	73,104,113	1.13	2 (2%)
28	CLA	6	306	17	62,66,73	0.82	4 (6%)	73,104,113	1.27	6 (8%)
28	CLA	13	305	-	50,54,73	0.83	3 (6%)	59,90,113	1.49	6 (10%)
30	KC1	10	304	17	49,53,53	1.20	4 (8%)	61,89,89	1.35	9 (14%)
28	CLA	R	204	15	55,59,73	0.84	4 (7%)	64,96,113	1.21	6 (9%)
28	CLA	6	302	17	57,61,73	1.00	4 (7%)	67,98,113	1.05	4 (5%)
37	LMG	F	805	-	41,41,55	0.19	0	49,49,63	0.18	0
28	CLA	B	828	-	69,73,73	0.91	4 (5%)	82,113,113	1.07	5 (6%)
28	CLA	11	302	18	69,73,73	0.83	4 (5%)	82,113,113	1.06	7 (8%)
31	LHG	5	315	-	26,26,48	0.39	0	29,32,54	0.44	0
28	CLA	B	808	7	69,73,73	0.87	4 (5%)	82,113,113	1.03	6 (7%)
33	BCR	A	843	-	41,41,41	0.12	0	56,56,56	0.20	0
28	CLA	7	308	4	47,51,73	0.96	4 (8%)	55,86,113	1.15	3 (5%)
28	CLA	11	301	18	69,73,73	0.76	4 (5%)	82,113,113	1.03	5 (6%)
31	LHG	9	302	-	29,29,48	0.34	0	32,35,54	0.34	0
30	KC1	a	205	-	49,53,53	1.06	4 (8%)	61,89,89	1.34	10 (16%)
30	KC1	8	306	5	49,53,53	1.26	4 (8%)	61,89,89	1.43	10 (16%)
28	CLA	A	825	6	69,73,73	0.95	4 (5%)	82,113,113	1.17	6 (7%)
30	KC1	6	309	17	49,53,53	1.20	4 (8%)	61,89,89	1.31	8 (13%)
28	CLA	10	309	17	47,51,73	1.00	4 (8%)	55,86,113	1.47	5 (9%)
33	BCR	F	801	-	41,41,41	0.13	0	56,56,56	0.40	0
29	A86	17	308	-	47,50,50	0.40	1 (2%)	51,76,76	0.62	1 (1%)
33	BCR	B	838	-	41,41,41	0.18	0	56,56,56	0.34	0
30	KC1	4	308	34	49,53,53	1.12	4 (8%)	61,89,89	1.29	9 (14%)
28	CLA	1	308	1	52,56,73	1.08	4 (7%)	61,92,113	1.38	6 (9%)
28	CLA	A	834	6	59,63,73	0.99	4 (6%)	70,101,113	1.28	4 (5%)
28	CLA	A	818	6	49,53,73	0.94	4 (8%)	58,89,113	1.33	4 (6%)
28	CLA	9	308	-	50,54,73	0.74	2 (4%)	59,90,113	1.47	10 (16%)
28	CLA	B	835	31	69,73,73	0.84	4 (5%)	82,113,113	1.08	4 (4%)
30	KC1	6	310	17	49,53,53	1.20	4 (8%)	61,89,89	1.42	10 (16%)
32	XAT	4	318	-	41,47,47	0.31	0	54,74,74	1.09	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	B	847	7	69,73,73	0.93	4 (5%)	82,113,113	1.16	6 (7%)
28	CLA	F	802	-	69,73,73	1.08	4 (5%)	82,113,113	1.28	5 (6%)
33	BCR	B	851	-	41,41,41	0.16	0	56,56,56	0.32	0
28	CLA	A	821	6	55,59,73	1.02	4 (7%)	64,96,113	1.21	4 (6%)
28	CLA	A	829	6	54,58,73	0.98	4 (7%)	64,95,113	1.11	6 (9%)
28	CLA	13	306	19	46,50,73	0.93	3 (6%)	53,85,113	1.48	7 (13%)
33	BCR	A	844	-	41,41,41	0.18	0	56,56,56	0.36	0
32	XAT	1	311	-	41,47,47	0.57	2 (4%)	54,74,74	1.26	3 (5%)
28	CLA	1	310	29	69,73,73	0.94	4 (5%)	82,113,113	1.10	3 (3%)
28	CLA	A	801	6	69,73,73	0.84	4 (5%)	82,113,113	1.07	6 (7%)
30	KC1	10	310	17	49,53,53	1.08	4 (8%)	61,89,89	1.42	9 (14%)
28	CLA	A	826	-	66,70,73	0.84	4 (6%)	78,109,113	1.17	6 (7%)
28	CLA	B	832	7	69,73,73	0.91	4 (5%)	82,113,113	1.10	4 (4%)
28	CLA	B	848	7	69,73,73	1.00	4 (5%)	82,113,113	1.18	6 (7%)
32	XAT	7	315	-	41,47,47	0.36	0	54,74,74	1.06	6 (11%)
30	KC1	9	309	19	49,53,53	1.15	4 (8%)	61,89,89	1.50	8 (13%)
33	BCR	L	202	-	41,41,41	0.31	0	56,56,56	1.60	9 (16%)
28	CLA	5	304	3	51,55,73	0.94	4 (7%)	60,91,113	1.27	5 (8%)
33	BCR	A	841	-	41,41,41	0.23	0	56,56,56	0.38	0
28	CLA	B	822	-	68,72,73	0.85	4 (5%)	80,111,113	1.01	5 (6%)
28	CLA	A	810	6	66,70,73	0.95	4 (6%)	78,109,113	1.07	6 (7%)
28	CLA	11	310	-	54,58,73	1.01	4 (7%)	64,95,113	1.42	6 (9%)
28	CLA	17	304	22	53,57,73	0.79	3 (5%)	61,93,113	1.31	7 (11%)
29	A86	11	308	-	47,50,50	0.51	1 (2%)	51,76,76	0.58	0
33	BCR	M	101	-	41,41,41	0.15	0	56,56,56	0.22	0
28	CLA	3	307	-	69,73,73	0.93	4 (5%)	82,113,113	1.19	7 (8%)
32	XAT	5	316	-	41,47,47	0.57	2 (4%)	54,74,74	0.90	2 (3%)
28	CLA	4	307	25	64,68,73	0.83	3 (4%)	76,107,113	1.31	7 (9%)
35	PQN	B	836	-	34,34,34	0.27	0	43,45,45	0.44	1 (2%)
28	CLA	3	303	2	69,73,73	0.80	4 (5%)	82,113,113	1.03	6 (7%)
29	A86	9	312	-	47,50,50	0.49	1 (2%)	51,76,76	0.64	0
28	CLA	A	811	6	58,62,73	1.06	4 (6%)	68,99,113	1.29	3 (4%)
28	CLA	B	809	7	69,73,73	0.89	4 (5%)	82,113,113	1.08	6 (7%)
28	CLA	A	819	-	69,73,73	0.87	4 (5%)	82,113,113	1.12	5 (6%)
28	CLA	7	311	4	50,54,73	0.81	2 (4%)	59,90,113	1.30	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CLA	A	817	6	69,73,73	0.92	4 (5%)	82,113,113	1.02	3 (3%)
33	BCR	B	837	-	41,41,41	0.24	0	56,56,56	0.37	0
28	CLA	B	803	7	69,73,73	0.89	4 (5%)	82,113,113	1.10	6 (7%)
28	CLA	A	802	-	69,73,73	0.89	4 (5%)	82,113,113	1.11	6 (7%)
35	PQN	A	838	-	34,34,34	0.26	0	43,45,45	0.44	1 (2%)
28	CLA	A	823	-	69,73,73	0.99	4 (5%)	82,113,113	1.08	6 (7%)
28	CLA	B	820	7	57,61,73	0.93	4 (7%)	67,98,113	1.10	3 (4%)
28	CLA	9	303	19	51,55,73	0.81	3 (5%)	60,91,113	1.49	9 (15%)
29	A86	5	312	-	47,50,50	0.55	1 (2%)	51,76,76	0.88	4 (7%)
28	CLA	7	301	4	69,73,73	0.83	4 (5%)	82,113,113	1.09	7 (8%)
32	XAT	10	315	-	41,47,47	0.48	1 (2%)	54,74,74	1.61	5 (9%)
29	A86	3	311	-	47,50,50	0.57	1 (2%)	51,76,76	1.15	3 (5%)
28	CLA	5	313	3	61,65,73	0.99	4 (6%)	72,103,113	1.24	4 (5%)
28	CLA	17	301	22	54,58,73	1.07	4 (7%)	64,95,113	1.49	10 (15%)
28	CLA	A	816	-	60,64,73	0.88	4 (6%)	71,102,113	1.36	5 (7%)
30	KC1	4	309	25	49,53,53	1.39	4 (8%)	61,89,89	1.27	9 (14%)
28	CLA	a	202	-	46,50,73	1.02	4 (8%)	53,85,113	1.52	7 (13%)
28	CLA	1	303	1	69,73,73	0.65	2 (2%)	82,113,113	1.23	8 (9%)
28	CLA	10	316	17	69,73,73	0.81	4 (5%)	82,113,113	1.16	7 (8%)
28	CLA	17	307	22	51,55,73	0.89	3 (5%)	60,91,113	1.44	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	B	823	7	-	5/39/115/115	-
36	SF4	C	102	8	-	-	0/6/5/5
28	CLA	B	807	7	-	17/39/115/115	-
28	CLA	J	102	-	-	13/31/107/115	-
31	LHG	1	309	-	-	15/48/48/53	-
28	CLA	B	805	7	-	10/39/115/115	-
31	LHG	A	851	-	-	6/31/31/53	-
28	CLA	11	312	18	-	7/13/89/115	-
36	SF4	A	848	7,6	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	15	201	-	-	3/17/93/115	-
28	CLA	A	845	-	-	5/39/115/115	-
28	CLA	1	305	1	-	10/24/100/115	-
32	XAT	10	313	-	-	1/31/93/93	0/4/4/4
28	CLA	A	831	6	-	9/21/97/115	-
28	CLA	9	311	19	-	3/15/91/115	-
30	KC1	7	307	4	-	3/15/71/71	-
28	CLA	A	828	6	-	5/39/115/115	-
28	CLA	9	305	-	-	8/21/97/115	-
32	XAT	9	313	-	-	5/31/88/93	0/4/4/4
33	BCR	A	842	-	-	0/29/63/63	0/2/2/2
29	A86	R	203	-	-	4/34/90/90	0/3/3/3
28	CLA	7	305	4	-	12/39/115/115	-
28	CLA	A	812	6	-	7/24/100/115	-
28	CLA	5	309	3	-	7/21/97/115	-
30	KC1	7	309	4	-	7/15/71/71	-
28	CLA	16	204	-	-	4/10/86/115	-
33	BCR	8	309	-	-	11/29/63/63	0/2/2/2
31	LHG	5	314	-	-	3/28/28/53	-
32	XAT	3	313	-	-	0/31/93/93	0/4/4/4
32	XAT	5	307	-	-	5/31/93/93	0/4/4/4
31	LHG	9	301	-	-	10/32/32/53	-
29	A86	4	314	-	-	5/34/90/90	0/3/3/3
28	CLA	B	806	7	-	10/39/115/115	-
32	XAT	J	105	-	-	4/31/93/93	0/4/4/4
33	BCR	A	850	-	-	6/29/63/63	0/2/2/2
28	CLA	10	305	17	-	5/17/93/115	-
29	A86	4	313	-	-	7/34/90/90	0/3/3/3
28	CLA	11	304	18	-	15/33/109/115	-
28	CLA	B	813	-	-	9/33/109/115	-
28	CLA	A	849	6	-	12/39/115/115	-
28	CLA	6	301	17	-	15/39/115/115	-
32	XAT	7	316	-	-	4/31/93/93	0/4/4/4
28	CLA	16	201	-	-	3/15/91/115	-
30	KC1	17	306	-	-	5/15/71/71	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	KC1	3	309	2	-	6/15/71/71	-
28	CLA	19	201	-	-	5/17/93/115	-
28	CLA	4	305	-	-	5/12/88/115	-
32	XAT	6	312	-	-	9/31/93/93	0/4/4/4
34	DGD	4	301	-	-	12/28/68/95	0/2/2/2
28	CLA	6	304	17	-	3/12/88/115	-
30	KC1	3	308	2	-	3/15/71/71	-
32	XAT	7	317	-	-	7/31/93/93	0/4/4/4
34	DGD	8	314	-	-	8/17/57/95	0/2/2/2
30	KC1	4	312	-	-	7/15/71/71	-
28	CLA	3	301	2	-	10/39/115/115	-
33	BCR	L	205	-	-	2/29/63/63	0/2/2/2
29	A86	J	101	-	-	15/34/90/90	0/3/3/3
28	CLA	6	313	-	-	16/39/115/115	-
32	XAT	7	313	-	-	4/31/93/93	0/4/4/4
28	CLA	B	833	-	-	5/35/111/115	-
29	A86	1	313	28	-	5/34/90/90	0/3/3/3
28	CLA	A	830	6	-	16/39/115/115	-
28	CLA	A	803	6	-	7/27/103/115	-
32	XAT	6	315	-	-	5/31/93/93	0/4/4/4
28	CLA	a	201	-	-	3/13/89/115	-
30	KC1	6	305	17	-	7/15/71/71	-
28	CLA	10	301	17	-	8/27/103/115	-
28	CLA	A	852	6	-	9/39/115/115	-
29	A86	8	308	-	-	4/34/90/90	0/3/3/3
28	CLA	10	307	-	-	15/30/106/115	-
28	CLA	A	827	6	-	8/39/115/115	-
28	CLA	a	203	-	-	5/17/93/115	-
32	XAT	6	316	-	-	4/31/93/93	0/4/4/4
28	CLA	11	305	-	-	2/15/91/115	-
28	CLA	5	305	3	-	11/29/105/115	-
30	KC1	17	312	22	-	3/15/71/71	-
28	CLA	1	301	1	-	5/21/97/115	-
28	CLA	11	309	18	-	5/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	A	807	6	-	13/39/115/115	-
31	LHG	4	302	-	-	11/29/29/53	-
28	CLA	A	847	6	-	15/39/115/115	-
29	A86	3	310	-	-	5/34/90/90	0/3/3/3
28	CLA	B	831	7	-	10/39/115/115	-
33	BCR	F	804	-	-	2/29/63/63	0/2/2/2
28	CLA	A	820	6	-	8/20/96/115	-
28	CLA	17	305	-	-	7/21/97/115	-
28	CLA	17	302	22	-	4/13/89/115	-
28	CLA	6	307	-	-	9/27/103/115	-
31	LHG	A	839	-	-	7/52/52/53	-
28	CLA	17	309	22	-	6/17/93/115	-
28	CLA	8	304	5	-	14/30/106/115	-
28	CLA	B	815	-	-	13/32/108/115	-
28	CLA	a	204	-	-	2/12/88/115	-
29	A86	R	201	-	-	4/34/90/90	0/3/3/3
28	CLA	7	318	-	-	9/15/91/115	-
28	CLA	B	802	-	-	2/39/115/115	-
28	CLA	11	306	18	-	2/15/91/115	-
28	CLA	7	303	-	-	21/39/115/115	-
31	LHG	11	311	-	-	13/41/41/53	-
28	CLA	A	809	6	-	9/29/105/115	-
29	A86	10	317	-	-	11/34/90/90	0/3/3/3
31	LHG	A	840	28	-	6/31/31/53	-
31	LHG	I	102	-	-	23/53/53/53	-
28	CLA	L	201	-	-	7/39/115/115	-
30	KC1	8	307	5	-	2/15/71/71	-
30	KC1	4	311	25	-	5/15/71/71	-
28	CLA	B	804	-	-	11/39/115/115	-
28	CLA	L	204	-	-	6/21/97/115	-
28	CLA	9	304	19	-	10/21/97/115	-
32	XAT	10	314	-	-	4/31/93/93	0/4/4/4
28	CLA	B	821	-	-	9/39/115/115	-
28	CLA	7	312	4	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	F	803	11	-	5/13/89/115	-
28	CLA	B	814	7	-	9/32/108/115	-
28	CLA	A	805	6	-	12/39/115/115	-
28	CLA	8	313	-	-	7/29/105/115	-
28	CLA	8	302	5	-	8/29/105/115	-
30	KC1	10	311	-	-	5/15/71/71	-
28	CLA	A	808	6	-	15/39/115/115	-
28	CLA	1	307	1	-	10/27/103/115	-
28	CLA	8	301	5	-	15/39/115/115	-
28	CLA	A	836	6	-	14/39/115/115	-
28	CLA	B	818	7	-	3/17/93/115	-
32	XAT	8	311	-	-	2/31/93/93	0/4/4/4
32	XAT	5	311	-	-	7/31/93/93	0/4/4/4
28	CLA	A	824	-	-	8/39/115/115	-
28	CLA	5	306	3	-	2/10/86/115	-
28	CLA	B	826	7	-	6/39/115/115	-
34	DGD	4	317	30	-	7/16/52/95	0/2/2/2
28	CLA	B	825	7	-	2/39/115/115	-
28	CLA	19	202	-	-	3/13/89/115	-
28	CLA	5	302	3	-	10/27/103/115	-
28	CLA	4	303	-	-	13/27/103/115	-
28	CLA	B	834	7	-	16/39/115/115	-
32	XAT	5	310	-	-	4/31/93/93	0/4/4/4
28	CLA	3	305	2	-	13/33/109/115	-
28	CLA	5	301	3	-	13/39/115/115	-
28	CLA	9	307	19	-	7/21/97/115	-
28	CLA	A	813	6	-	5/21/97/115	-
28	CLA	A	832	6	-	2/15/91/115	-
28	CLA	A	815	6	-	20/39/115/115	-
31	LHG	B	842	28	-	10/30/30/53	-
28	CLA	L	206	26	-	15/39/115/115	-
28	CLA	B	829	-	-	4/15/91/115	-
30	KC1	1	306	1	-	6/15/71/71	-
28	CLA	A	822	6	-	12/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	13	302	19	-	4/15/91/115	-
29	A86	3	312	-	-	5/34/90/90	1/3/3/3
28	CLA	B	801	7	-	9/39/115/115	-
32	XAT	7	314	-	-	0/31/93/93	0/4/4/4
30	KC1	5	308	-	-	7/15/71/71	-
28	CLA	17	303	22	-	7/19/95/115	-
32	XAT	11	313	-	-	4/31/93/93	0/4/4/4
28	CLA	10	302	17	-	6/17/93/115	-
32	XAT	13	309	-	-	7/31/93/93	0/4/4/4
28	CLA	J	103	13	-	1/12/88/115	-
33	BCR	B	841	-	-	0/29/63/63	0/2/2/2
28	CLA	13	301	19	-	14/29/105/115	-
28	CLA	3	306	2	-	8/39/115/115	-
28	CLA	B	810	7	-	10/25/101/115	-
28	CLA	1	304	1	-	6/15/91/115	-
28	CLA	4	306	25	-	14/27/103/115	-
28	CLA	13	307	19	-	4/15/91/115	-
28	CLA	13	303	-	-	6/15/91/115	-
28	CLA	B	811	7	-	13/27/103/115	-
28	CLA	5	303	-	-	11/39/115/115	-
28	CLA	8	303	-	-	14/30/106/115	-
28	CLA	B	819	7	-	5/27/103/115	-
28	CLA	B	843	7	-	14/39/115/115	-
28	CLA	L	203	26	-	5/39/115/115	-
28	CLA	B	817	-	-	17/39/115/115	-
28	CLA	10	306	17	-	11/29/105/115	-
33	BCR	B	846	-	-	2/29/63/63	0/2/2/2
33	BCR	1	312	-	-	4/29/63/63	0/2/2/2
28	CLA	A	846	6	-	5/18/94/115	-
29	A86	6	314	-	-	8/34/90/90	0/3/3/3
28	CLA	B	845	7	-	18/39/115/115	-
28	CLA	11	314	-	-	6/13/89/115	-
28	CLA	4	304	25	-	5/23/99/115	-
28	CLA	B	816	7	-	11/39/115/115	-
28	CLA	7	306	31	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	10	308	17	-	4/18/94/115	-
28	CLA	6	303	-	-	6/27/103/115	-
28	CLA	7	302	4	-	5/21/97/115	-
28	CLA	B	812	7	-	10/39/115/115	-
28	CLA	A	853	-	-	6/39/115/115	-
31	LHG	9	314	-	-	10/37/37/53	-
36	SF4	C	101	8	-	-	0/6/5/5
28	CLA	9	310	-	-	7/15/91/115	-
30	KC1	9	306	19	-	7/15/71/71	-
28	CLA	4	316	25	-	13/35/111/115	-
28	CLA	A	833	6	-	7/23/99/115	-
32	XAT	17	311	-	-	5/31/93/93	0/4/4/4
28	CLA	A	835	6	-	5/39/115/115	-
31	LHG	B	844	-	-	10/53/53/53	-
32	XAT	4	315	-	-	10/31/93/93	0/4/4/4
28	CLA	7	304	4	-	12/39/115/115	-
28	CLA	B	827	7	-	5/21/97/115	-
28	CLA	R	202	15	-	9/27/103/115	-
28	CLA	B	849	7	-	7/39/115/115	-
32	XAT	13	308	-	-	1/31/93/93	0/4/4/4
29	A86	10	312	-	-	12/34/90/90	0/3/3/3
28	CLA	B	824	-	-	9/39/115/115	-
30	KC1	11	307	18	-	5/15/71/71	-
33	BCR	B	839	-	-	1/29/63/63	0/2/2/2
28	CLA	A	806	6	-	12/27/103/115	-
28	CLA	3	314	31	-	9/39/115/115	-
28	CLA	8	305	5	-	7/15/91/115	-
30	KC1	13	304	19	-	7/15/71/71	-
28	CLA	1	314	-	-	12/39/115/115	-
31	LHG	7	310	28	-	8/31/31/53	-
28	CLA	11	303	18	-	11/30/106/115	-
33	BCR	J	104	-	-	1/29/63/63	0/2/2/2
28	CLA	6	311	17	-	14/30/92/115	-
28	CLA	16	205	-	-	7/13/89/115	-
33	BCR	17	310	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	A86	1	302	-	-	10/34/90/90	0/3/3/3
30	KC1	6	308	17	-	4/15/71/71	-
28	CLA	A	804	6	-	9/39/115/115	-
28	CLA	4	310	-	-	11/27/103/115	-
33	BCR	B	840	-	-	4/29/63/63	0/2/2/2
33	BCR	B	850	-	-	2/29/63/63	0/2/2/2
28	CLA	A	837	-	-	20/39/115/115	-
33	BCR	I	101	-	-	0/29/63/63	0/2/2/2
28	CLA	3	304	2	-	6/15/91/115	-
28	CLA	16	203	-	-	9/18/94/115	-
28	CLA	8	310	5	-	4/12/88/115	-
28	CLA	A	814	-	-	7/15/91/115	-
30	KC1	3	302	2	-	2/15/71/71	-
32	XAT	8	312	-	-	6/31/93/93	0/4/4/4
28	CLA	10	303	-	-	13/27/103/115	-
28	CLA	16	202	-	-	3/12/88/115	-
28	CLA	B	830	7	-	5/31/107/115	-
28	CLA	6	306	17	-	10/31/107/115	-
28	CLA	13	305	-	-	7/17/93/115	-
30	KC1	10	304	17	-	5/15/71/71	-
28	CLA	R	204	15	-	7/23/99/115	-
28	CLA	6	302	17	-	7/25/101/115	-
37	LMG	F	805	-	-	3/36/56/70	0/1/1/1
28	CLA	B	828	-	-	10/39/115/115	-
28	CLA	11	302	18	-	17/39/115/115	-
31	LHG	5	315	-	-	11/31/31/53	-
28	CLA	B	808	7	-	17/39/115/115	-
33	BCR	A	843	-	-	0/29/63/63	0/2/2/2
28	CLA	7	308	4	-	8/13/89/115	-
28	CLA	11	301	18	-	14/39/115/115	-
31	LHG	9	302	-	-	8/33/33/53	-
30	KC1	a	205	-	-	2/15/71/71	-
30	KC1	8	306	5	-	2/15/71/71	-
28	CLA	A	825	6	-	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	KC1	6	309	17	-	7/15/71/71	-
28	CLA	10	309	17	-	5/13/89/115	-
33	BCR	F	801	-	-	0/29/63/63	0/2/2/2
29	A86	17	308	-	-	2/34/90/90	0/3/3/3
33	BCR	B	838	-	-	0/29/63/63	0/2/2/2
30	KC1	4	308	34	-	6/15/71/71	-
28	CLA	1	308	1	-	5/19/95/115	-
28	CLA	A	834	6	-	10/27/103/115	-
28	CLA	A	818	6	-	5/15/91/115	-
28	CLA	9	308	-	-	2/17/93/115	-
28	CLA	B	835	31	-	8/39/115/115	-
30	KC1	6	310	17	-	7/15/71/71	-
32	XAT	4	318	-	-	5/31/93/93	0/4/4/4
28	CLA	B	847	7	-	12/39/115/115	-
28	CLA	F	802	-	-	12/39/115/115	-
33	BCR	B	851	-	-	3/29/63/63	0/2/2/2
28	CLA	A	821	6	-	7/23/99/115	-
28	CLA	A	829	6	-	8/21/97/115	-
28	CLA	13	306	19	-	6/12/88/115	-
33	BCR	A	844	-	-	3/29/63/63	0/2/2/2
32	XAT	1	311	-	-	2/31/93/93	0/4/4/4
28	CLA	1	310	29	-	11/39/115/115	-
28	CLA	A	801	6	-	3/39/115/115	-
30	KC1	10	310	17	-	5/15/71/71	-
28	CLA	A	826	-	-	7/36/112/115	-
28	CLA	B	832	7	-	15/39/115/115	-
28	CLA	B	848	7	-	5/39/115/115	-
32	XAT	7	315	-	-	8/31/93/93	0/4/4/4
30	KC1	9	309	19	-	4/15/71/71	-
33	BCR	L	202	-	-	6/29/63/63	0/2/2/2
28	CLA	5	304	3	-	7/18/94/115	-
33	BCR	A	841	-	-	4/29/63/63	0/2/2/2
28	CLA	B	822	-	-	9/38/114/115	-
28	CLA	A	810	6	-	12/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CLA	11	310	-	-	10/21/97/115	-
28	CLA	17	304	22	-	6/20/96/115	-
29	A86	11	308	-	-	4/34/90/90	0/3/3/3
33	BCR	M	101	-	-	0/29/63/63	0/2/2/2
28	CLA	3	307	-	-	15/39/115/115	-
32	XAT	5	316	-	-	0/31/93/93	0/4/4/4
28	CLA	4	307	25	-	13/33/109/115	-
35	PQN	B	836	-	-	5/23/43/43	0/2/2/2
28	CLA	3	303	2	-	16/39/115/115	-
29	A86	9	312	-	-	13/34/90/90	0/3/3/3
28	CLA	A	811	6	-	7/26/102/115	-
28	CLA	B	809	7	-	7/39/115/115	-
28	CLA	A	819	-	-	4/39/115/115	-
28	CLA	7	311	4	-	7/17/93/115	-
28	CLA	A	817	6	-	15/39/115/115	-
33	BCR	B	837	-	-	3/29/63/63	0/2/2/2
28	CLA	B	803	7	-	13/39/115/115	-
28	CLA	A	802	-	-	12/39/115/115	-
35	PQN	A	838	-	-	3/23/43/43	0/2/2/2
28	CLA	A	823	-	-	16/39/115/115	-
28	CLA	B	820	7	-	10/25/101/115	-
28	CLA	9	303	19	-	5/18/94/115	-
29	A86	5	312	-	-	7/34/90/90	0/3/3/3
28	CLA	7	301	4	-	13/39/115/115	-
32	XAT	10	315	-	-	4/31/93/93	0/4/4/4
29	A86	3	311	-	-	11/34/90/90	0/3/3/3
28	CLA	5	313	3	-	13/30/106/115	-
28	CLA	17	301	22	-	5/21/97/115	-
28	CLA	A	816	-	-	9/29/105/115	-
30	KC1	4	309	25	-	7/15/71/71	-
28	CLA	a	202	-	-	6/12/88/115	-
28	CLA	1	303	1	-	16/39/115/115	-
28	CLA	10	316	17	-	12/39/115/115	-
28	CLA	17	307	22	-	5/18/94/115	-

The worst 5 of 907 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	6	311	CLA	C2D-C1D	-9.74	1.37	1.50
30	4	309	KC1	MG-NA	6.51	2.21	2.06
30	8	306	KC1	MG-NA	6.05	2.20	2.06
30	10	311	KC1	MG-NA	6.00	2.20	2.06
30	7	307	KC1	MG-NA	5.80	2.20	2.06

The worst 5 of 1566 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	311	CLA	C2D-C1D-ND	-15.97	109.53	120.88
28	7	312	CLA	C4A-NA-C1A	8.72	110.66	106.68
28	6	311	CLA	CMD-C2D-C1D	8.23	126.54	113.05
28	a	203	CLA	C4A-NA-C1A	7.92	110.29	106.68
28	17	301	CLA	C4A-NA-C1A	7.66	110.17	106.68

There are no chirality outliers.

5 of 2406 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	1	301	CLA	C1-C2-C3-C4
28	1	301	CLA	C1-C2-C3-C5
28	1	303	CLA	CBA-CGA-O2A-C1
28	1	303	CLA	O1A-CGA-O2A-C1
28	1	303	CLA	CBD-CGD-O2D-CED

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	3	312	A86	C31-C32-C33-C34-C35-C36

222 monomers are involved in 418 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	B	823	CLA	1	0
28	B	807	CLA	2	0
28	J	102	CLA	2	0
31	1	309	LHG	1	0
28	11	312	CLA	4	0
28	1	305	CLA	1	0
28	A	831	CLA	3	0
28	9	311	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	828	CLA	2	0
28	9	305	CLA	1	0
32	9	313	XAT	5	0
33	A	842	BCR	1	0
28	7	305	CLA	3	0
28	A	812	CLA	1	0
28	5	309	CLA	2	0
33	8	309	BCR	1	0
32	3	313	XAT	1	0
32	5	307	XAT	5	0
31	9	301	LHG	1	0
28	B	806	CLA	3	0
32	J	105	XAT	2	0
33	A	850	BCR	3	0
28	10	305	CLA	1	0
28	11	304	CLA	3	0
28	B	813	CLA	1	0
28	A	849	CLA	1	0
28	6	301	CLA	5	0
32	7	316	XAT	3	0
28	19	201	CLA	1	0
28	4	305	CLA	1	0
32	6	312	XAT	6	0
34	4	301	DGD	1	0
32	7	317	XAT	5	0
28	3	301	CLA	3	0
33	L	205	BCR	1	0
28	6	313	CLA	2	0
32	7	313	XAT	6	0
28	A	830	CLA	3	0
28	A	803	CLA	2	0
32	6	315	XAT	7	0
28	10	301	CLA	3	0
28	A	852	CLA	4	0
28	10	307	CLA	2	0
28	A	827	CLA	2	0
32	6	316	XAT	1	0
28	11	305	CLA	1	0
28	5	305	CLA	2	0
30	17	312	KC1	1	0
28	1	301	CLA	1	0
28	A	847	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	3	310	A86	1	0
28	B	831	CLA	3	0
33	F	804	BCR	2	0
28	A	820	CLA	1	0
28	17	302	CLA	2	0
28	6	307	CLA	1	0
28	17	309	CLA	1	0
28	8	304	CLA	3	0
28	B	815	CLA	2	0
28	7	303	CLA	3	0
31	11	311	LHG	1	0
28	A	809	CLA	1	0
31	A	840	LHG	1	0
31	I	102	LHG	1	0
28	L	201	CLA	1	0
28	B	804	CLA	1	0
28	L	204	CLA	1	0
28	9	304	CLA	1	0
32	10	314	XAT	5	0
28	B	821	CLA	2	0
28	7	312	CLA	2	0
28	A	805	CLA	2	0
28	8	313	CLA	1	0
28	8	302	CLA	1	0
28	A	808	CLA	6	0
28	1	307	CLA	2	0
28	8	301	CLA	5	0
28	A	836	CLA	2	0
28	B	818	CLA	3	0
32	8	311	XAT	1	0
32	5	311	XAT	6	0
28	A	824	CLA	3	0
28	5	306	CLA	2	0
28	B	826	CLA	4	0
34	4	317	DGD	1	0
28	B	825	CLA	2	0
28	5	302	CLA	1	0
28	4	303	CLA	3	0
32	5	310	XAT	2	0
28	3	305	CLA	1	0
28	9	307	CLA	1	0
28	A	813	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	A	832	CLA	1	0
28	A	815	CLA	3	0
31	B	842	LHG	4	0
28	L	206	CLA	1	0
28	B	829	CLA	2	0
28	A	822	CLA	1	0
28	13	302	CLA	2	0
28	B	801	CLA	1	0
32	7	314	XAT	1	0
30	5	308	KC1	1	0
28	17	303	CLA	2	0
32	11	313	XAT	7	0
32	13	309	XAT	1	0
33	B	841	BCR	2	0
28	13	301	CLA	4	0
28	3	306	CLA	2	0
28	B	810	CLA	2	0
28	1	304	CLA	1	0
28	4	306	CLA	3	0
28	13	303	CLA	1	0
28	B	811	CLA	3	0
28	5	303	CLA	2	0
28	8	303	CLA	3	0
28	B	819	CLA	4	0
28	B	843	CLA	3	0
28	L	203	CLA	1	0
28	B	817	CLA	5	0
28	10	306	CLA	4	0
33	B	846	BCR	5	0
33	1	312	BCR	1	0
28	A	846	CLA	2	0
28	B	845	CLA	2	0
28	11	314	CLA	1	0
28	4	304	CLA	2	0
28	B	816	CLA	3	0
28	7	306	CLA	1	0
28	10	308	CLA	1	0
28	6	303	CLA	1	0
28	B	812	CLA	2	0
28	A	853	CLA	1	0
31	9	314	LHG	1	0
28	9	310	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	4	316	CLA	1	0
32	17	311	XAT	3	0
28	A	835	CLA	1	0
31	B	844	LHG	5	0
32	4	315	XAT	2	0
28	7	304	CLA	4	0
28	B	827	CLA	2	0
28	R	202	CLA	1	0
28	B	849	CLA	1	0
32	13	308	XAT	5	0
28	B	824	CLA	2	0
28	A	806	CLA	2	0
28	8	305	CLA	2	0
28	1	314	CLA	5	0
28	11	303	CLA	1	0
33	J	104	BCR	4	0
28	6	311	CLA	1	0
33	17	310	BCR	1	0
28	A	804	CLA	1	0
28	4	310	CLA	4	0
33	B	840	BCR	1	0
33	B	850	BCR	4	0
28	A	837	CLA	4	0
33	I	101	BCR	2	0
28	3	304	CLA	1	0
28	16	203	CLA	1	0
28	8	310	CLA	1	0
28	A	814	CLA	1	0
32	8	312	XAT	5	0
28	10	303	CLA	1	0
28	6	306	CLA	4	0
28	13	305	CLA	1	0
28	6	302	CLA	5	0
37	F	805	LMG	1	0
28	B	828	CLA	4	0
31	5	315	LHG	1	0
28	B	808	CLA	1	0
33	A	843	BCR	2	0
28	7	308	CLA	1	0
28	11	301	CLA	2	0
28	A	825	CLA	1	0
33	F	801	BCR	5	0

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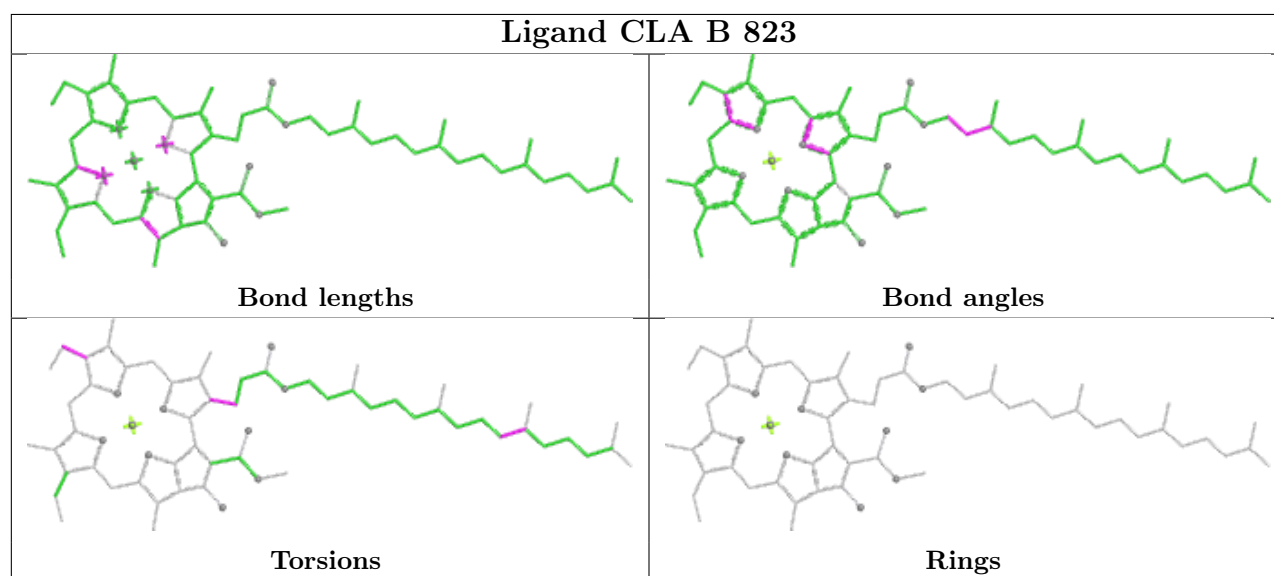
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28	A	834	CLA	3	0
28	A	818	CLA	2	0
28	B	835	CLA	1	0
32	4	318	XAT	8	0
28	B	847	CLA	2	0
28	F	802	CLA	4	0
33	B	851	BCR	1	0
28	A	821	CLA	1	0
28	A	829	CLA	2	0
33	A	844	BCR	3	0
32	1	311	XAT	1	0
28	1	310	CLA	2	0
28	A	801	CLA	1	0
28	A	826	CLA	2	0
28	B	832	CLA	2	0
28	B	848	CLA	1	0
32	7	315	XAT	3	0
33	L	202	BCR	4	0
28	5	304	CLA	1	0
33	A	841	BCR	5	0
28	B	822	CLA	2	0
28	A	810	CLA	3	0
28	11	310	CLA	1	0
32	5	316	XAT	2	0
28	4	307	CLA	3	0
28	3	303	CLA	2	0
28	A	811	CLA	1	0
28	B	809	CLA	2	0
28	A	819	CLA	3	0
28	7	311	CLA	1	0
28	A	817	CLA	7	0
33	B	837	BCR	3	0
28	B	803	CLA	1	0
28	A	802	CLA	6	0
28	A	823	CLA	2	0
28	B	820	CLA	2	0
28	9	303	CLA	2	0
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28	17	301	CLA	2	0

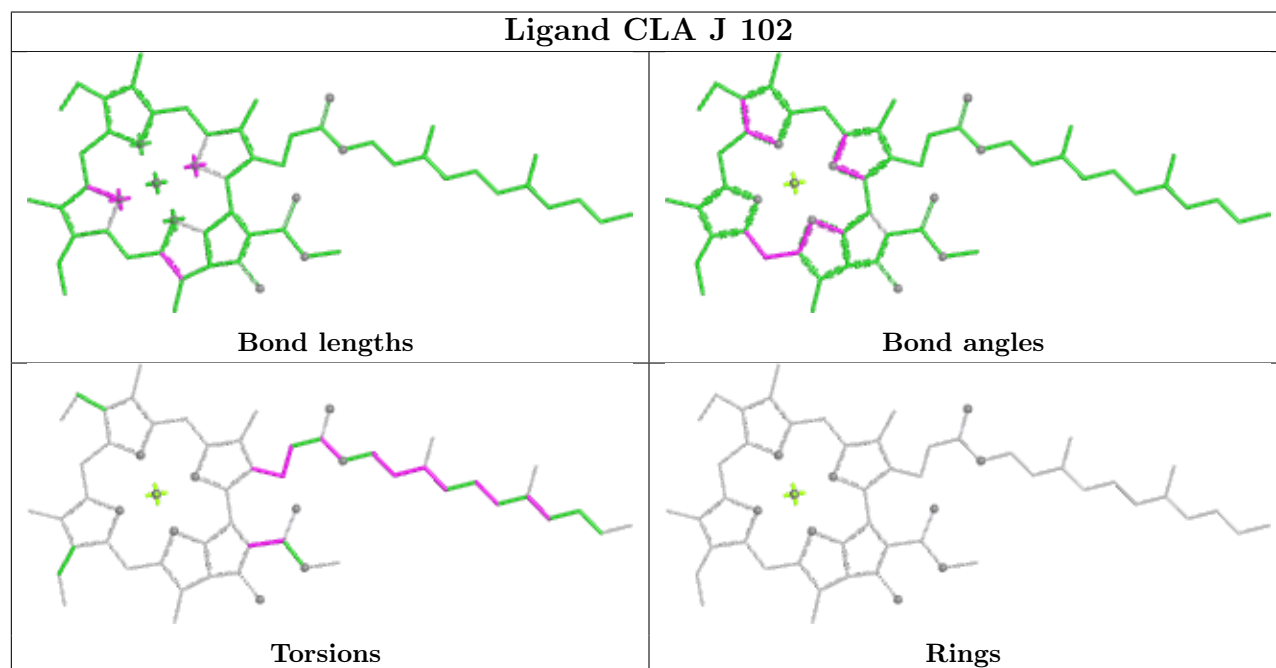
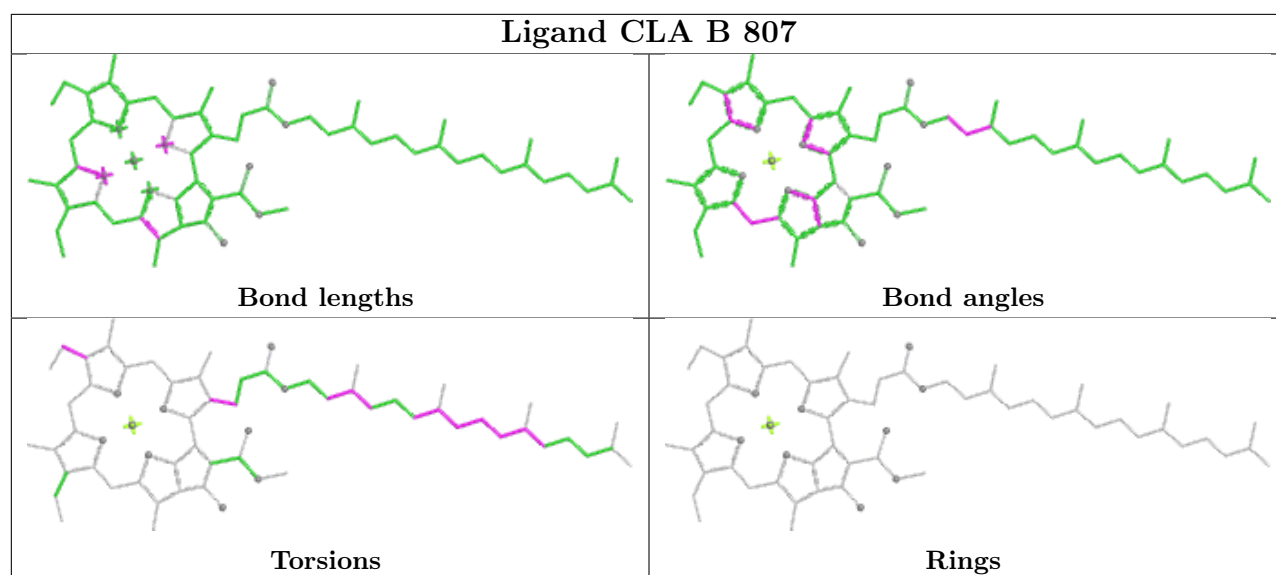
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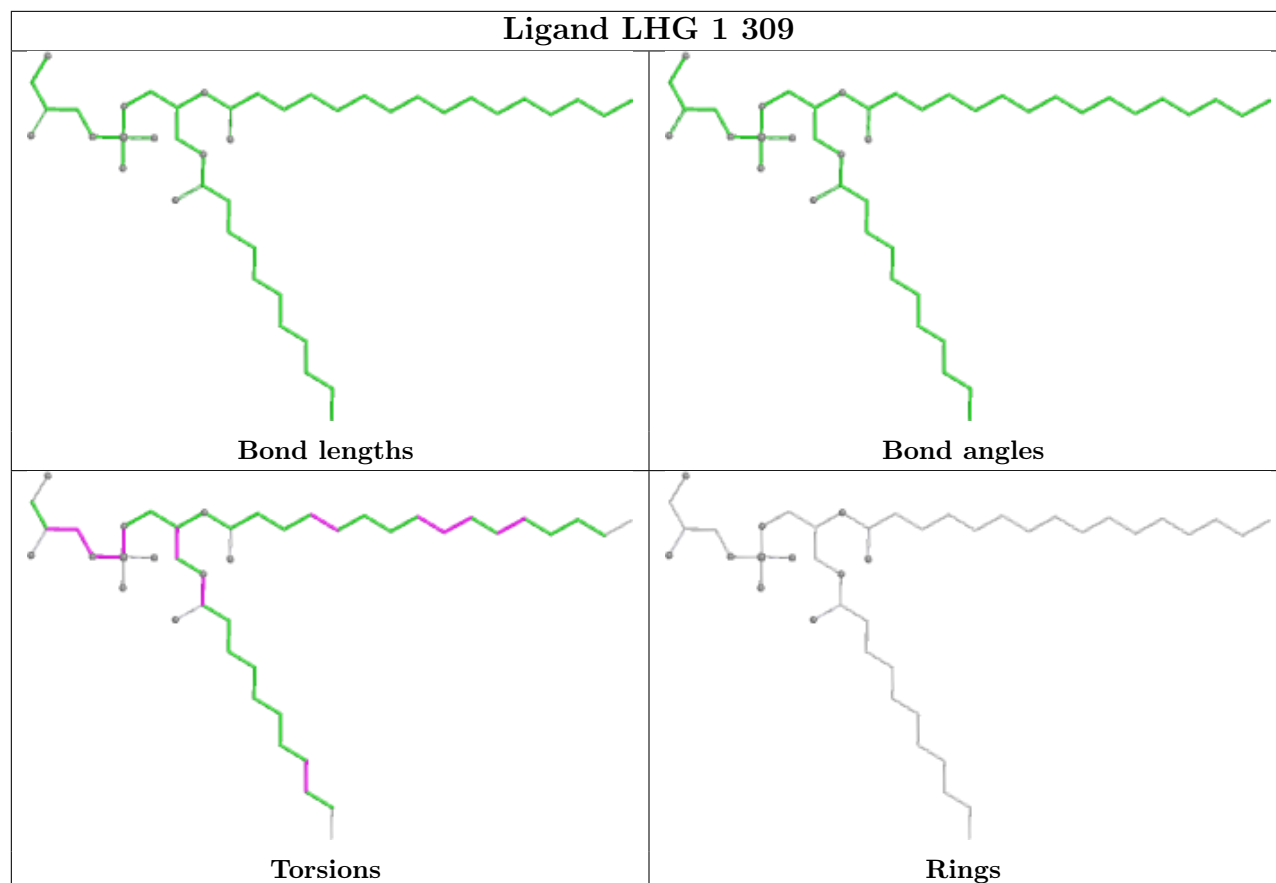
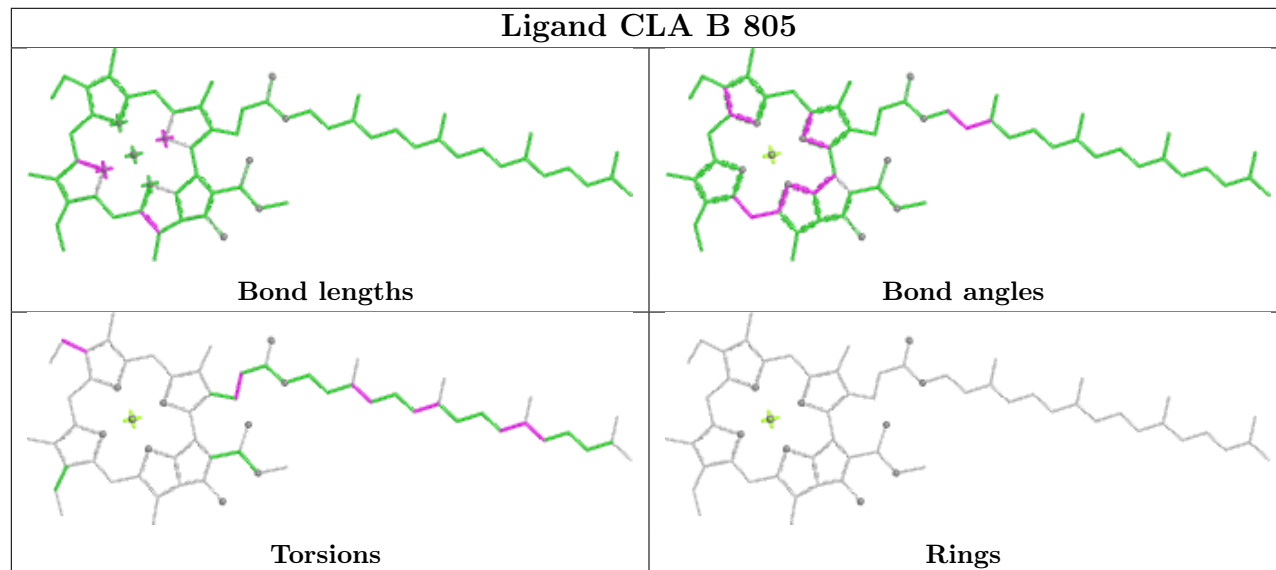
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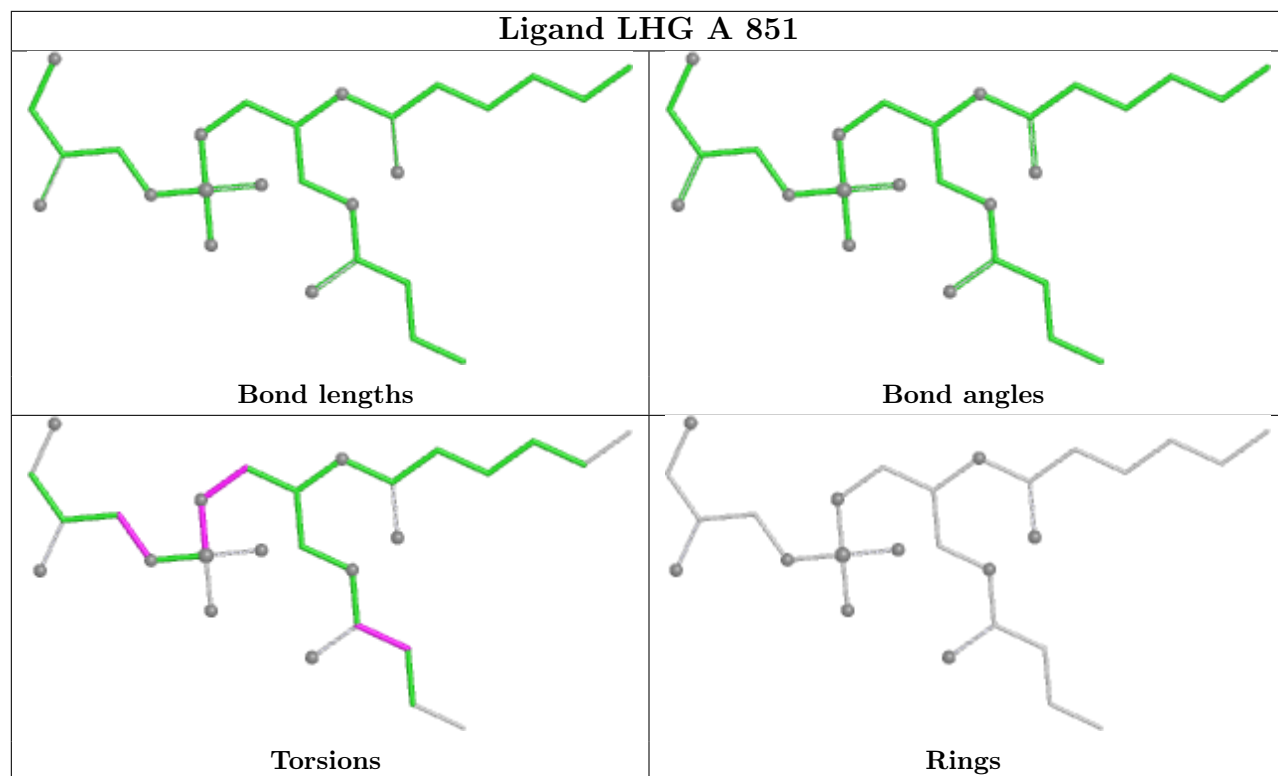
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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28	1	303	CLA	2	0
28	10	316	CLA	4	0
28	17	307	CLA	1	0

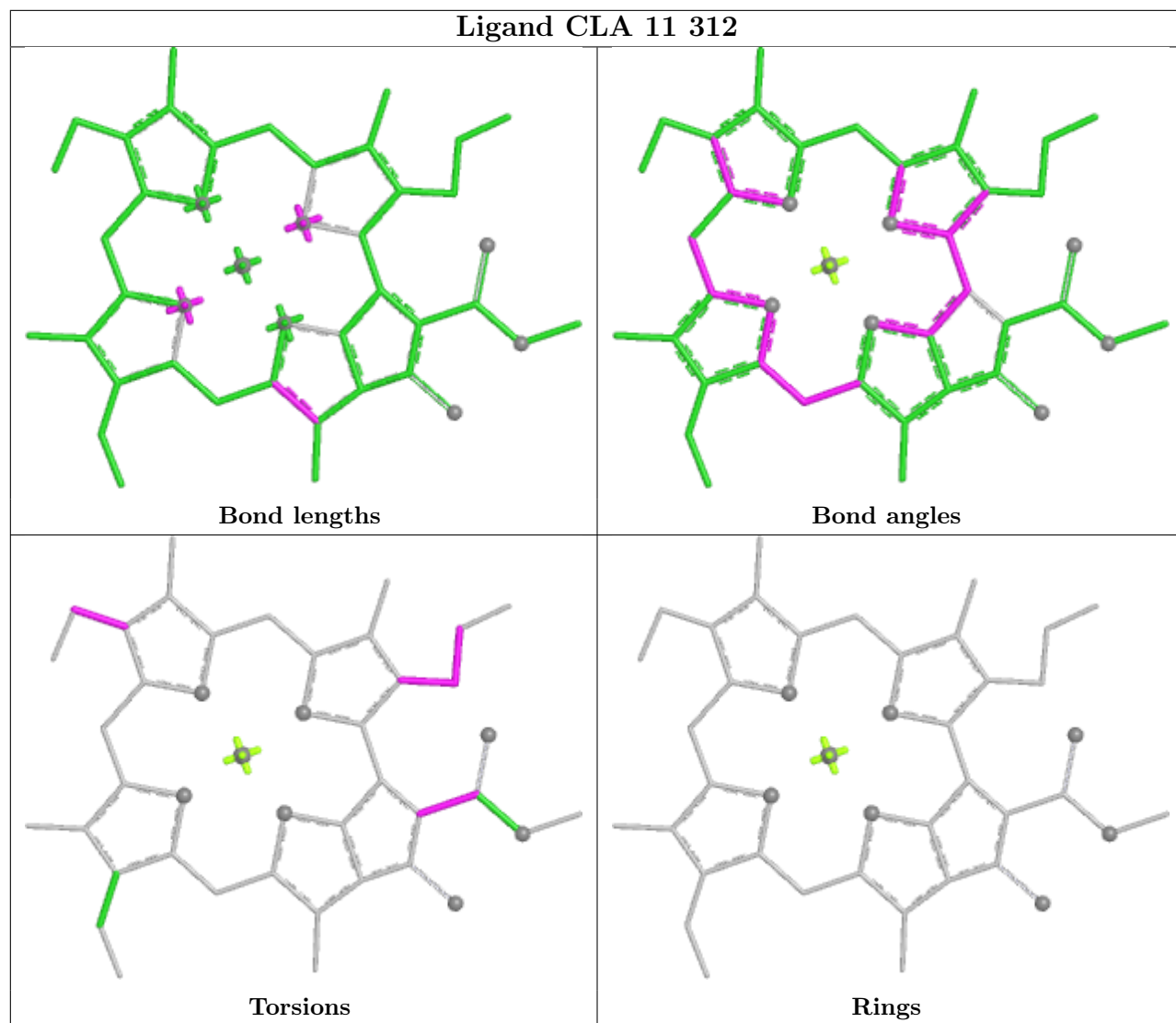
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



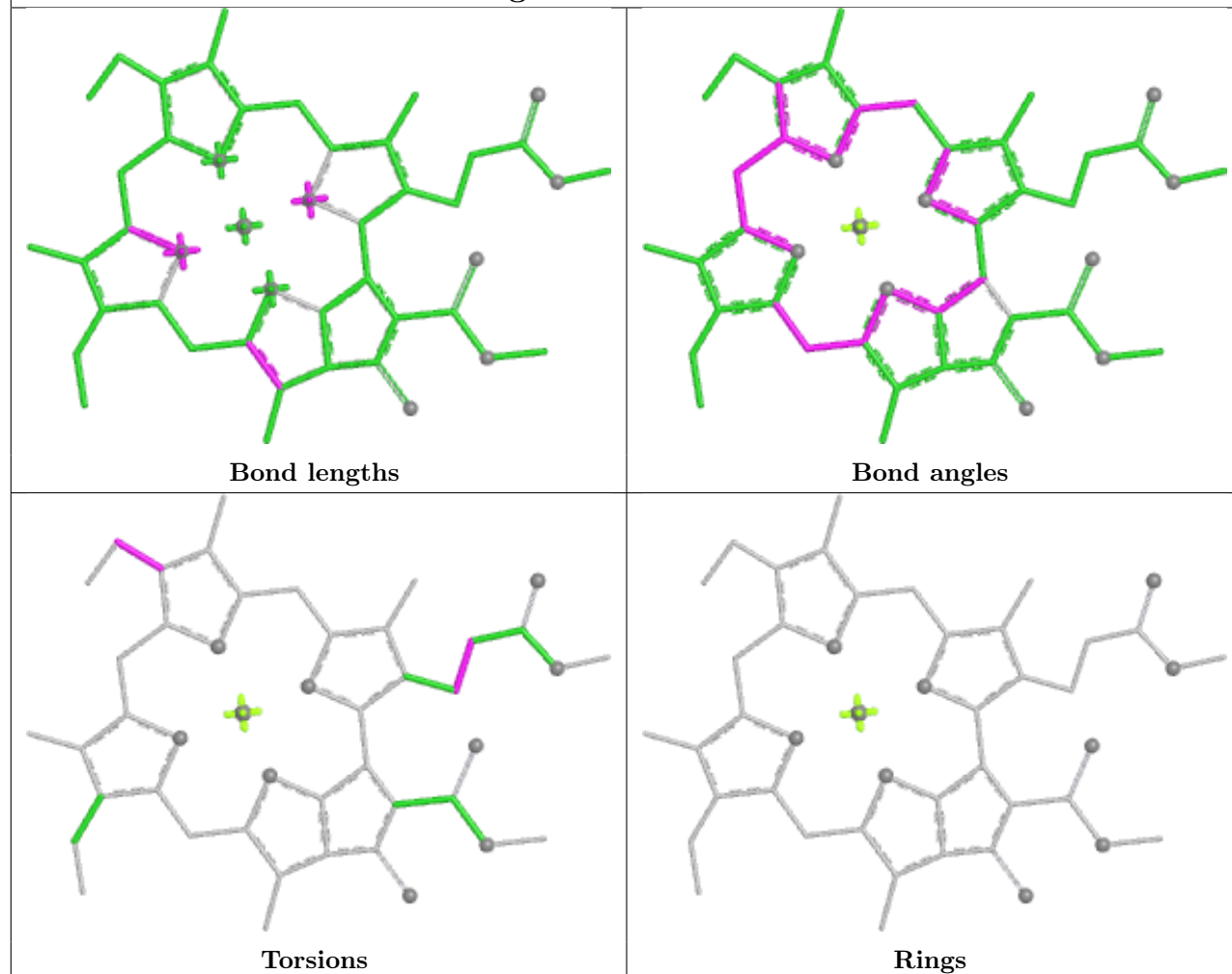


Ligand LHG 1 309**Ligand CLA B 805**

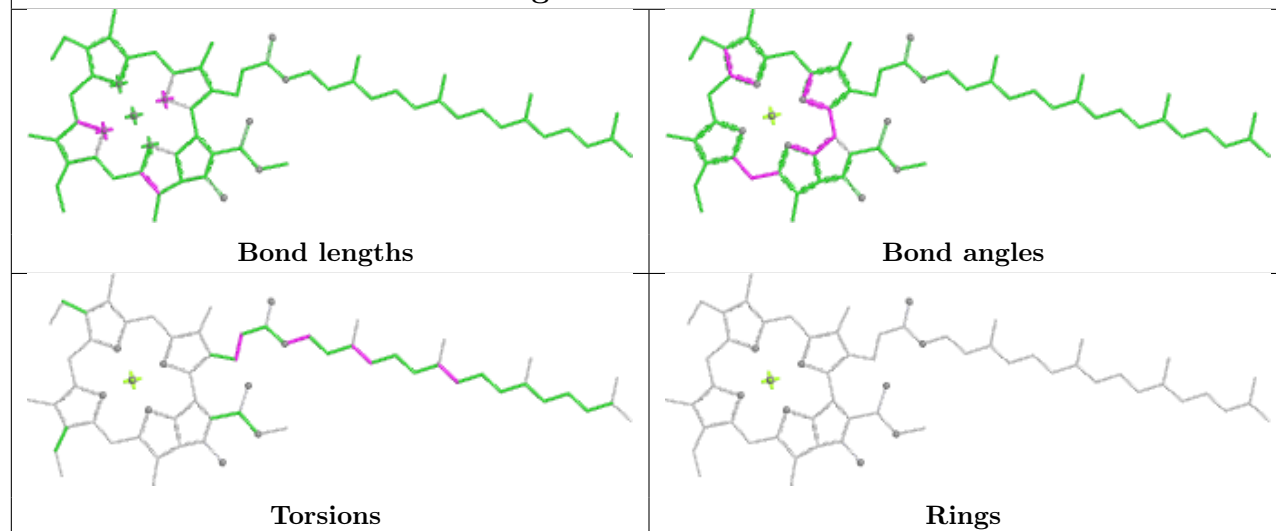


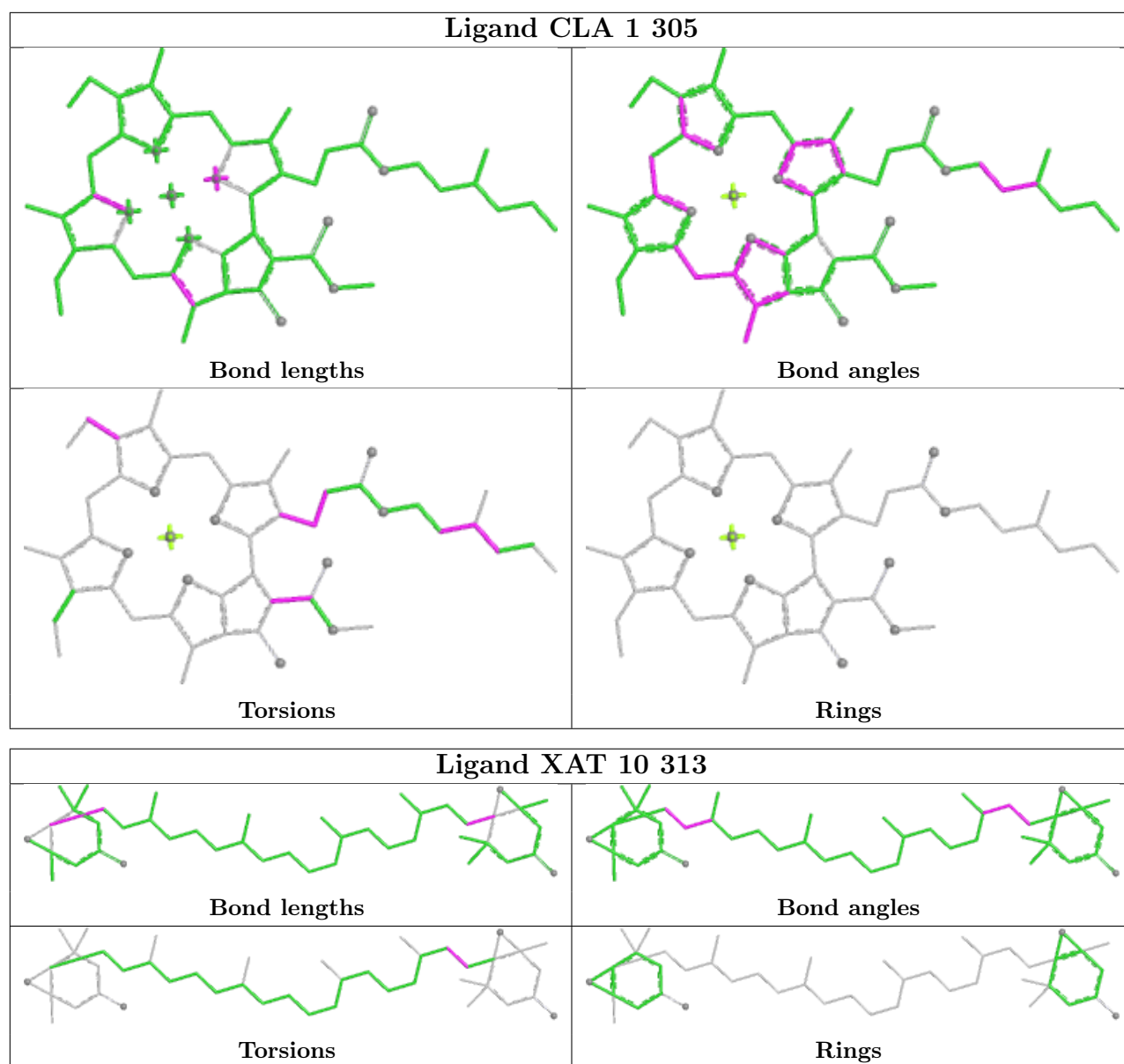


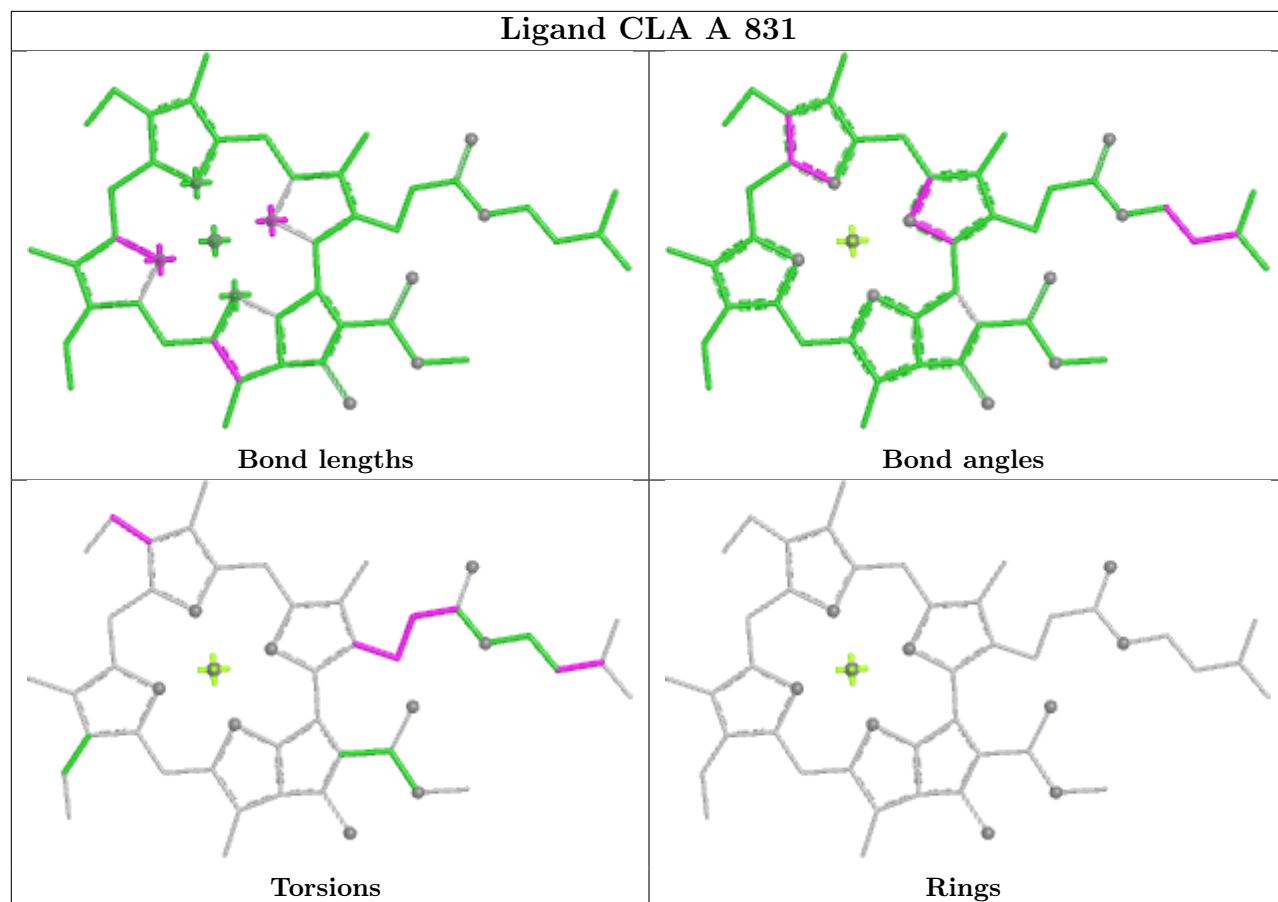
Ligand CLA 15 201



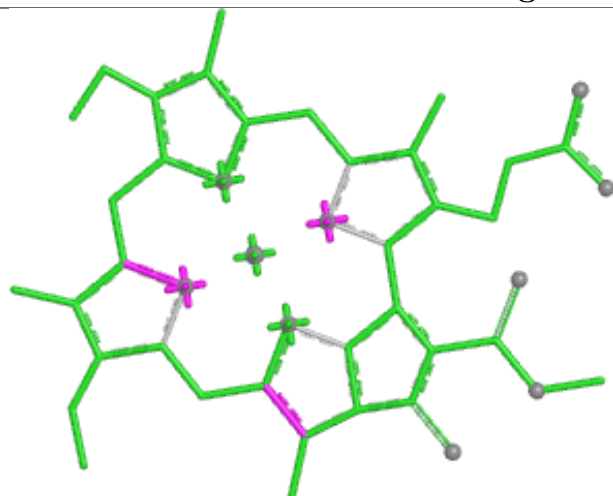
Ligand CLA A 845



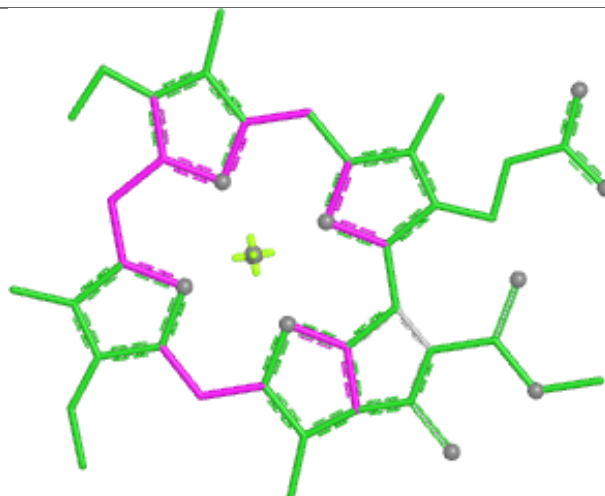




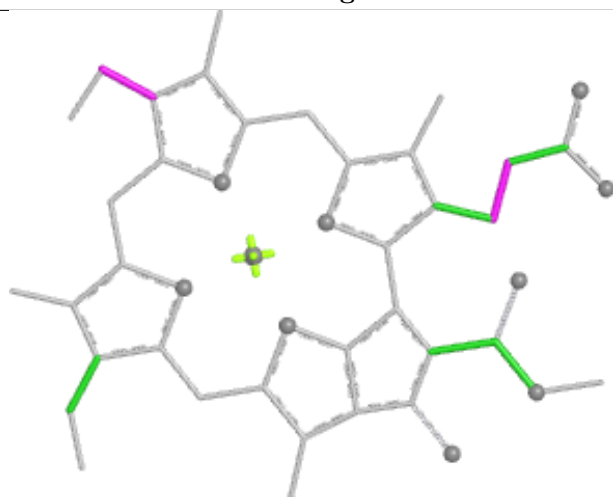
Ligand CLA 9 311



Bond lengths



Bond angles

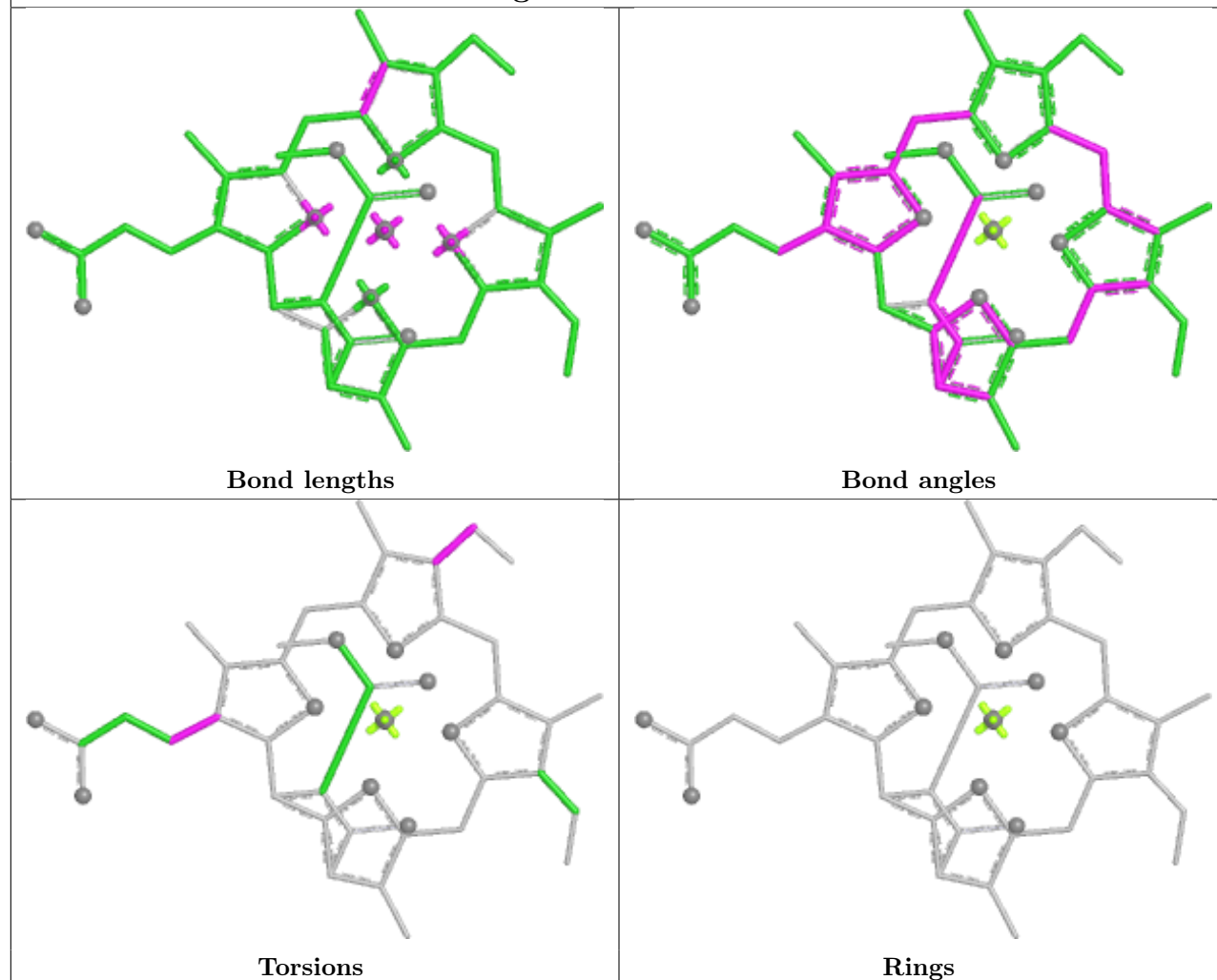


Torsions

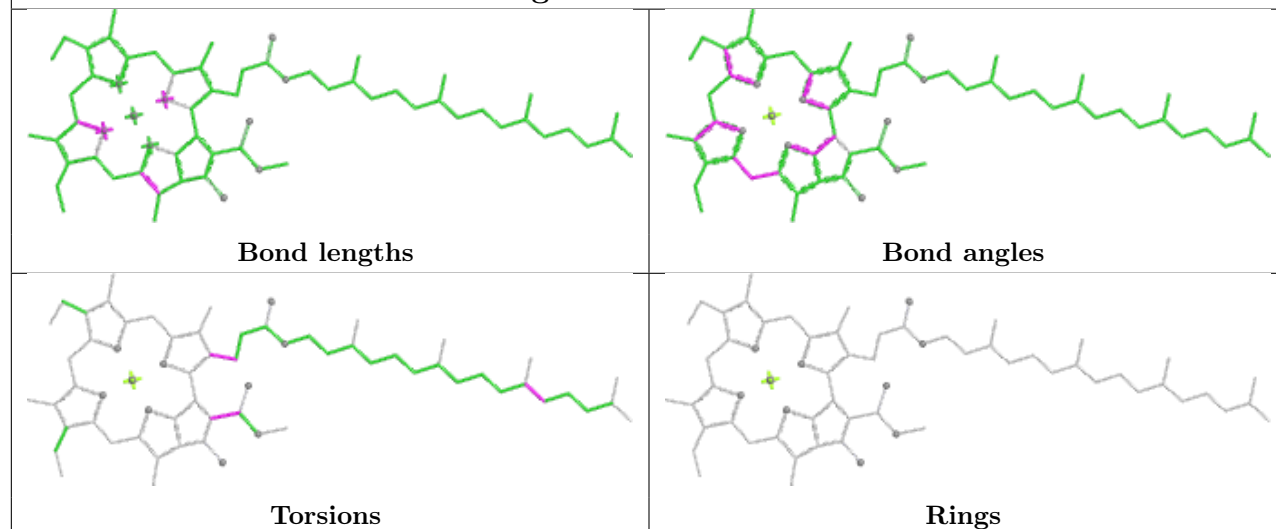


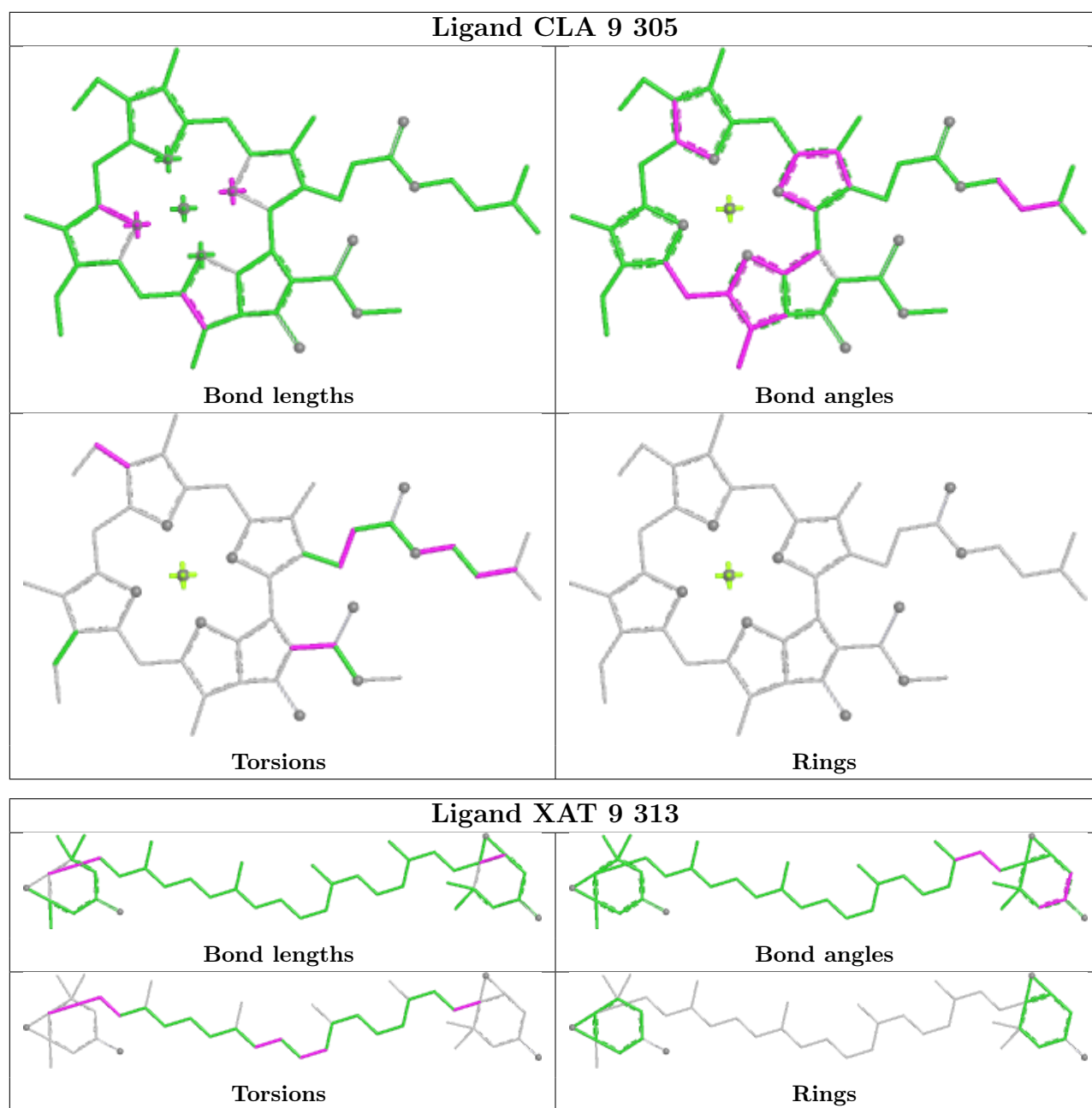
Rings

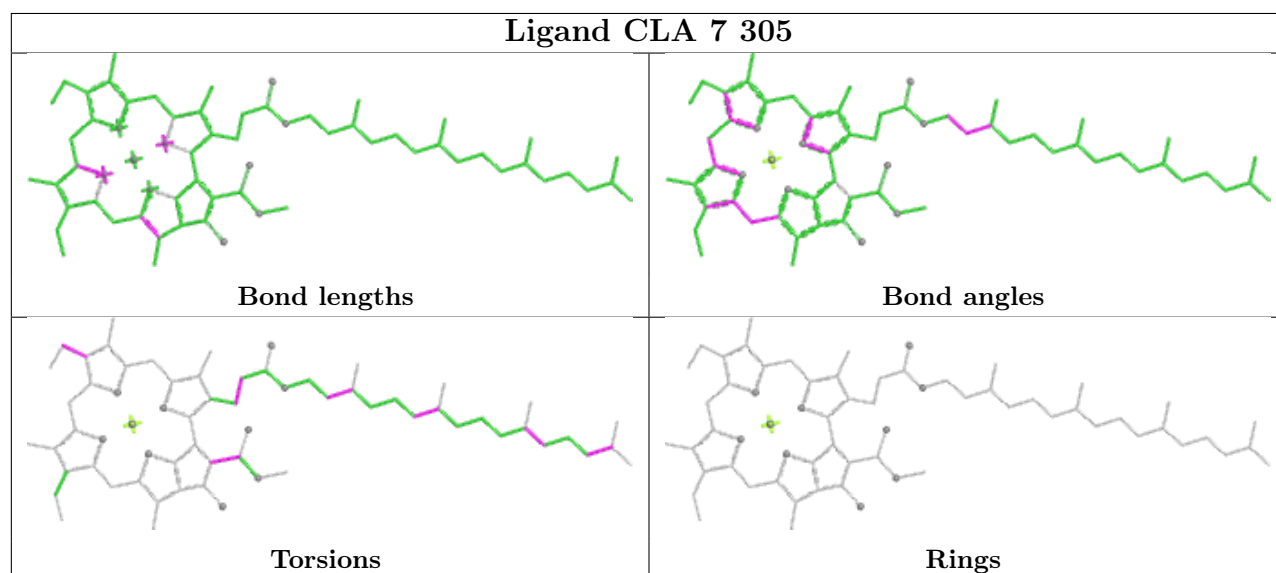
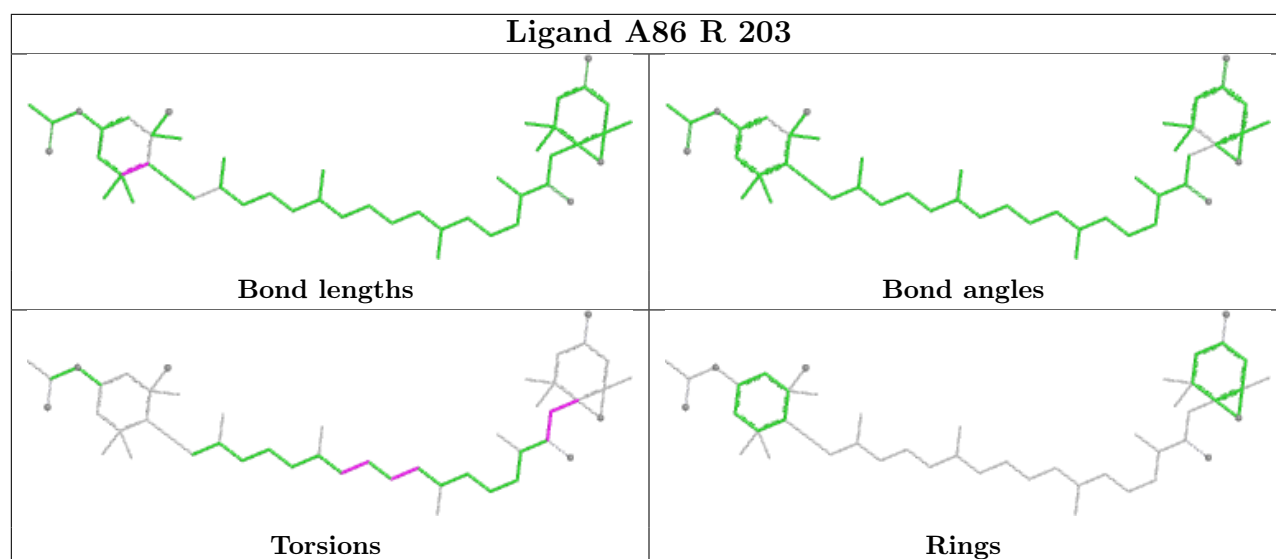
Ligand KC1 7 307



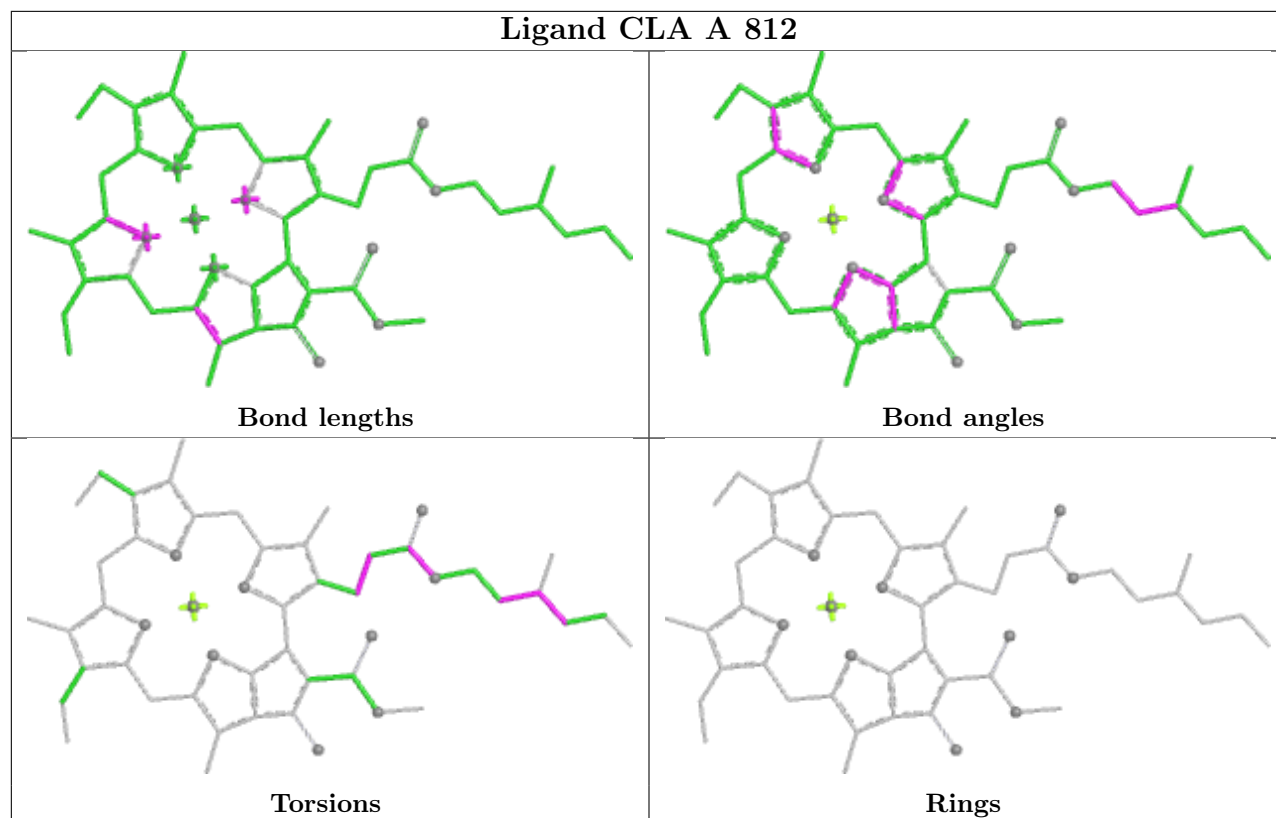
Ligand CLA A 828



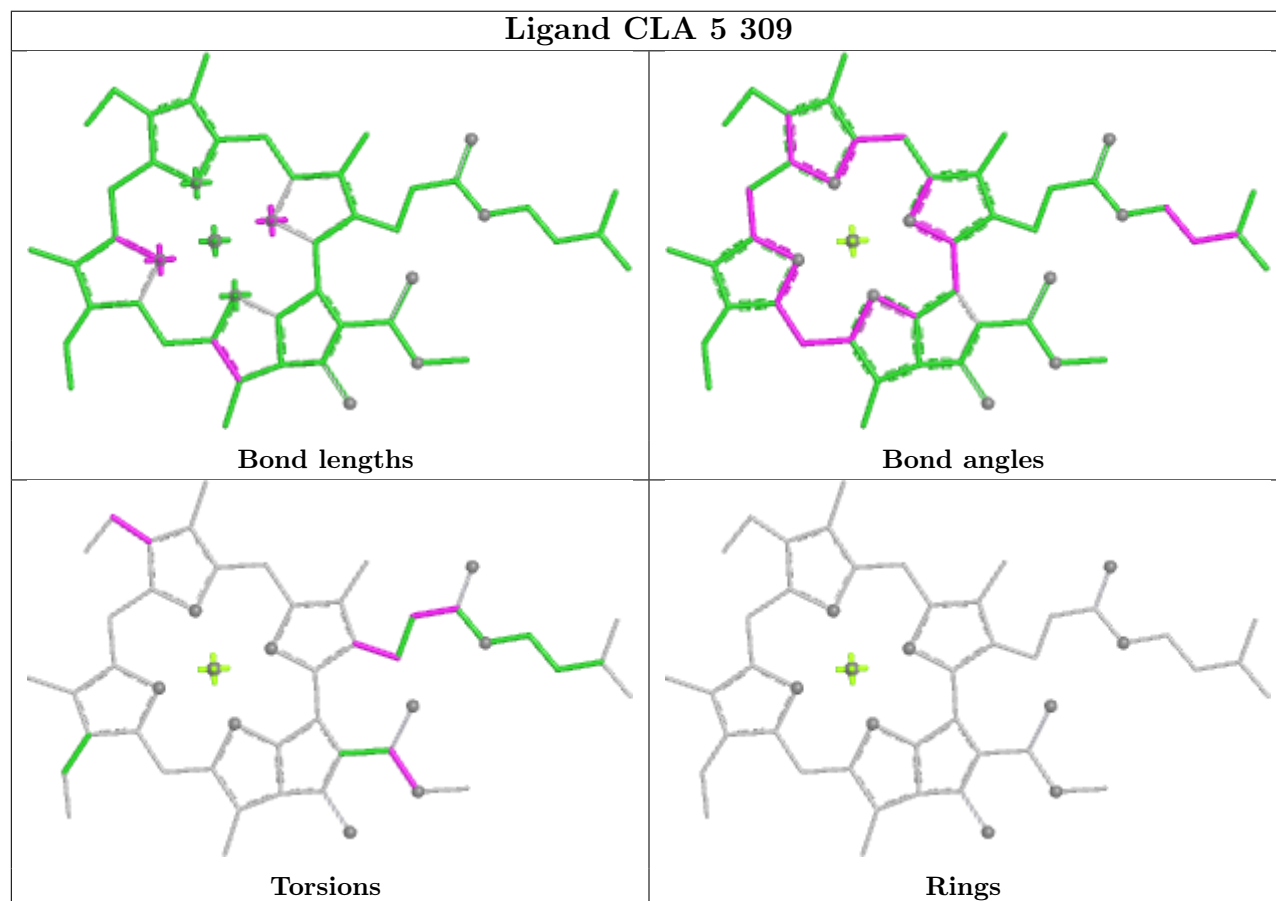




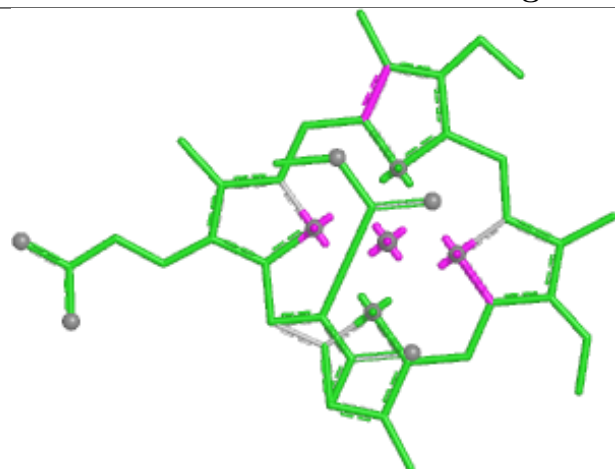
Ligand CLA A 812



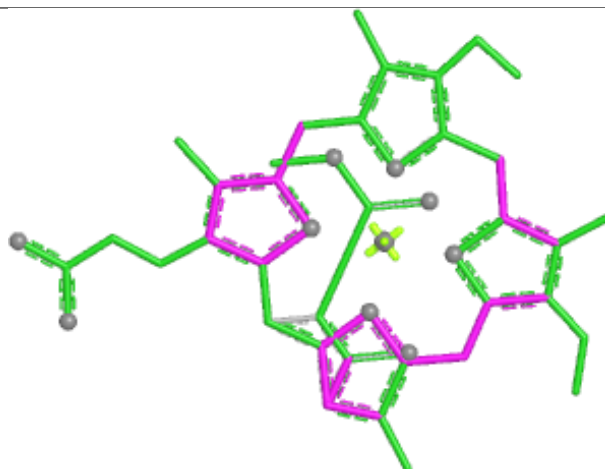
Ligand CLA 5 309



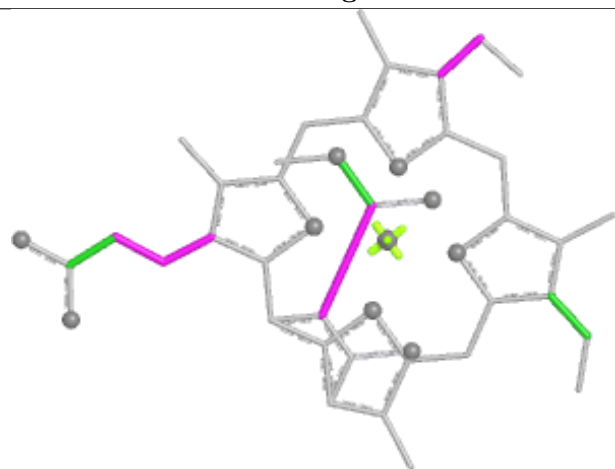
Ligand KC1 7 309



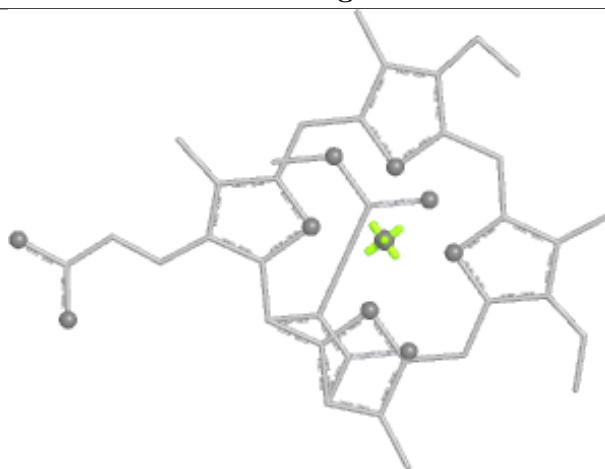
Bond lengths



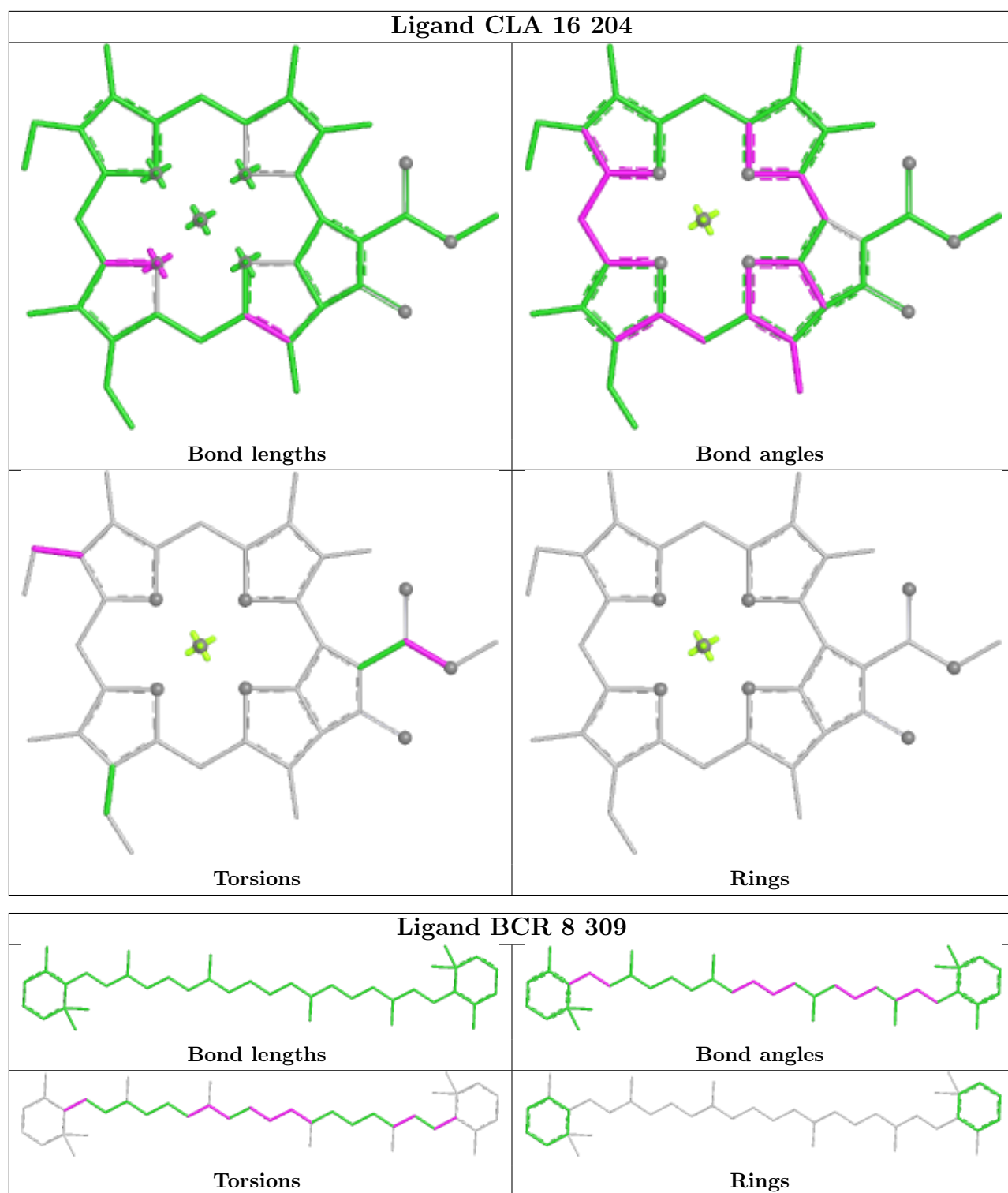
Bond angles

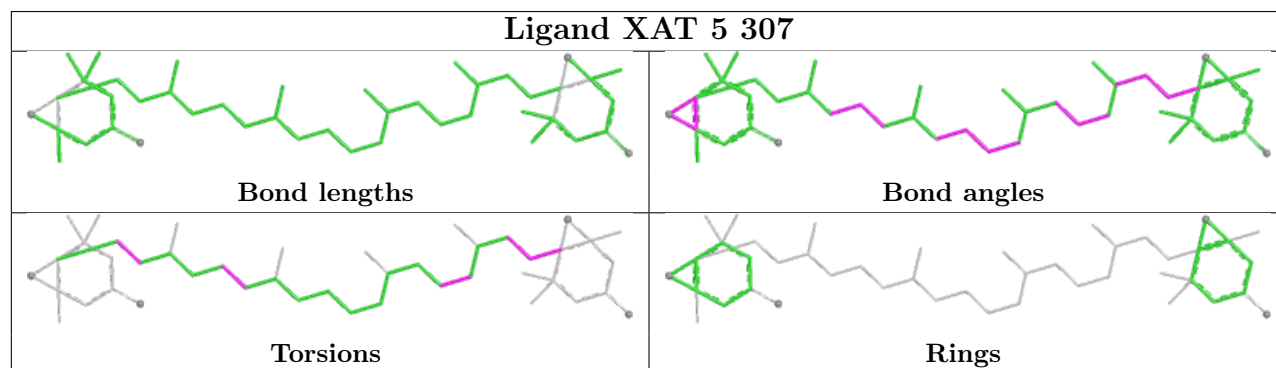
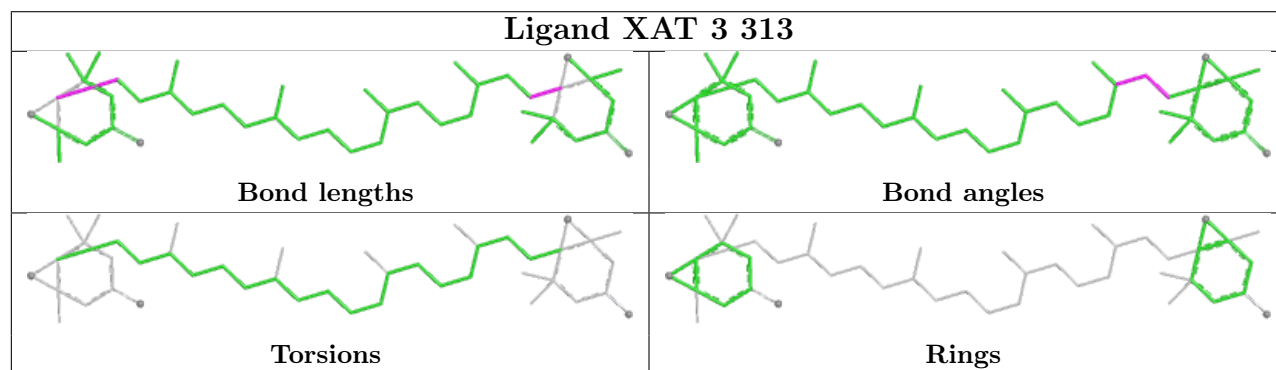
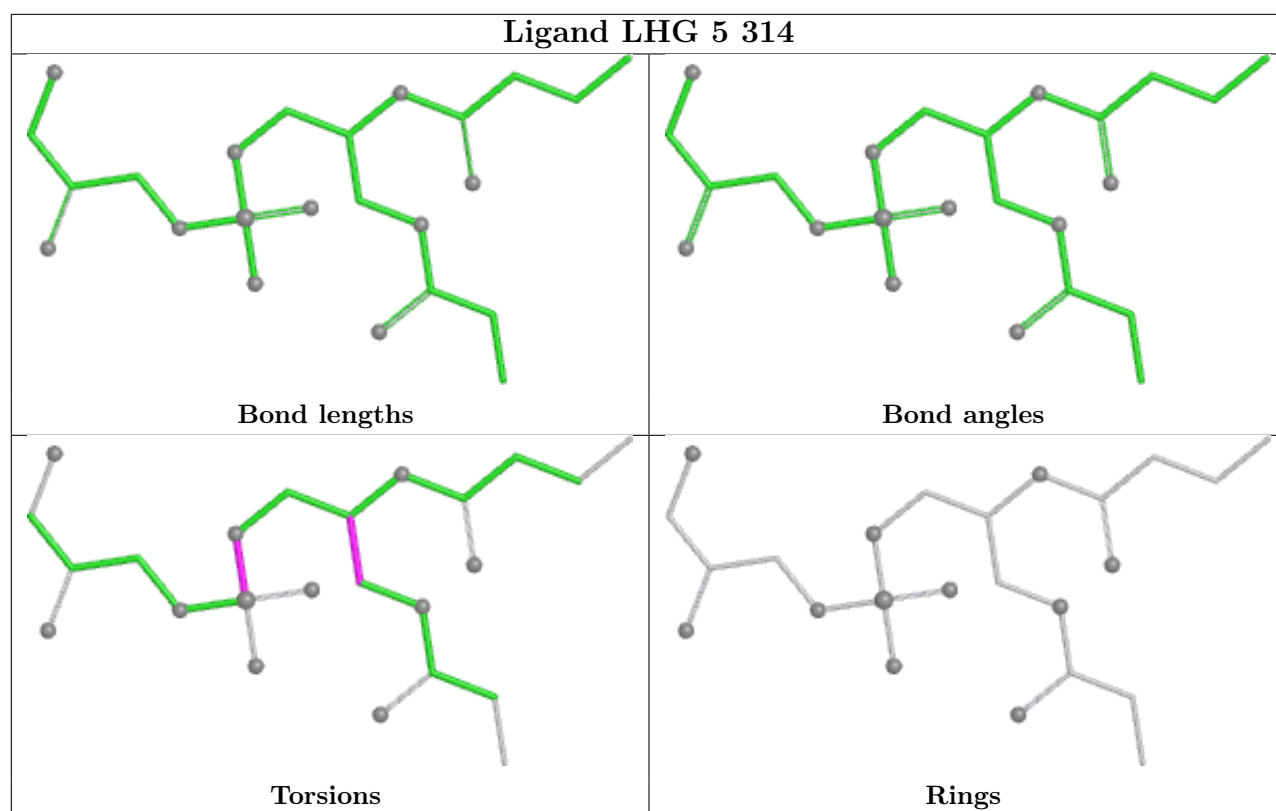


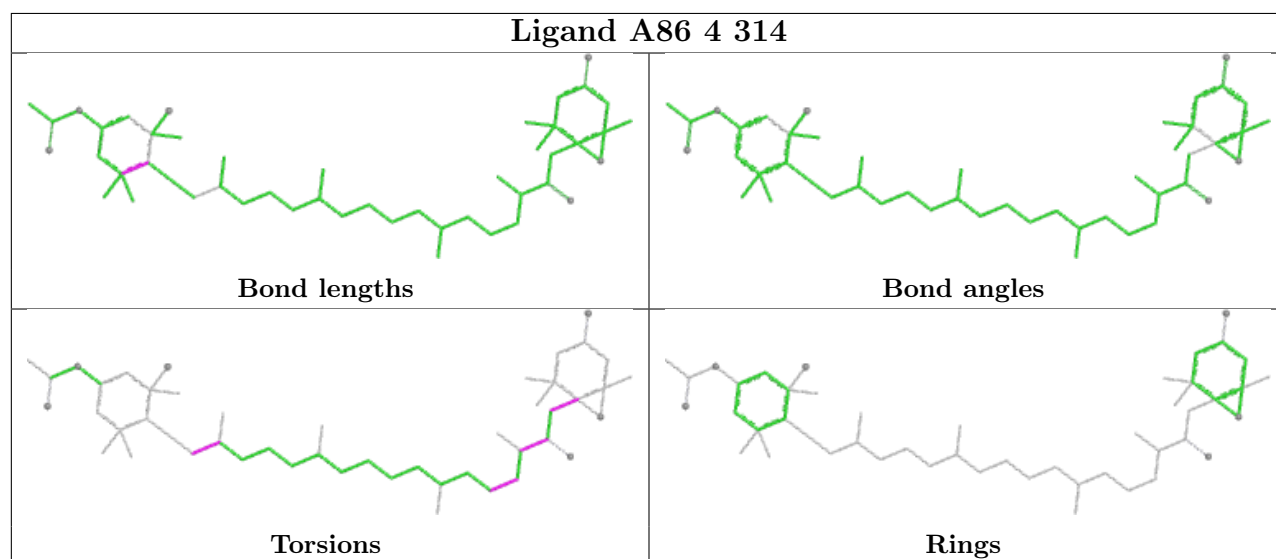
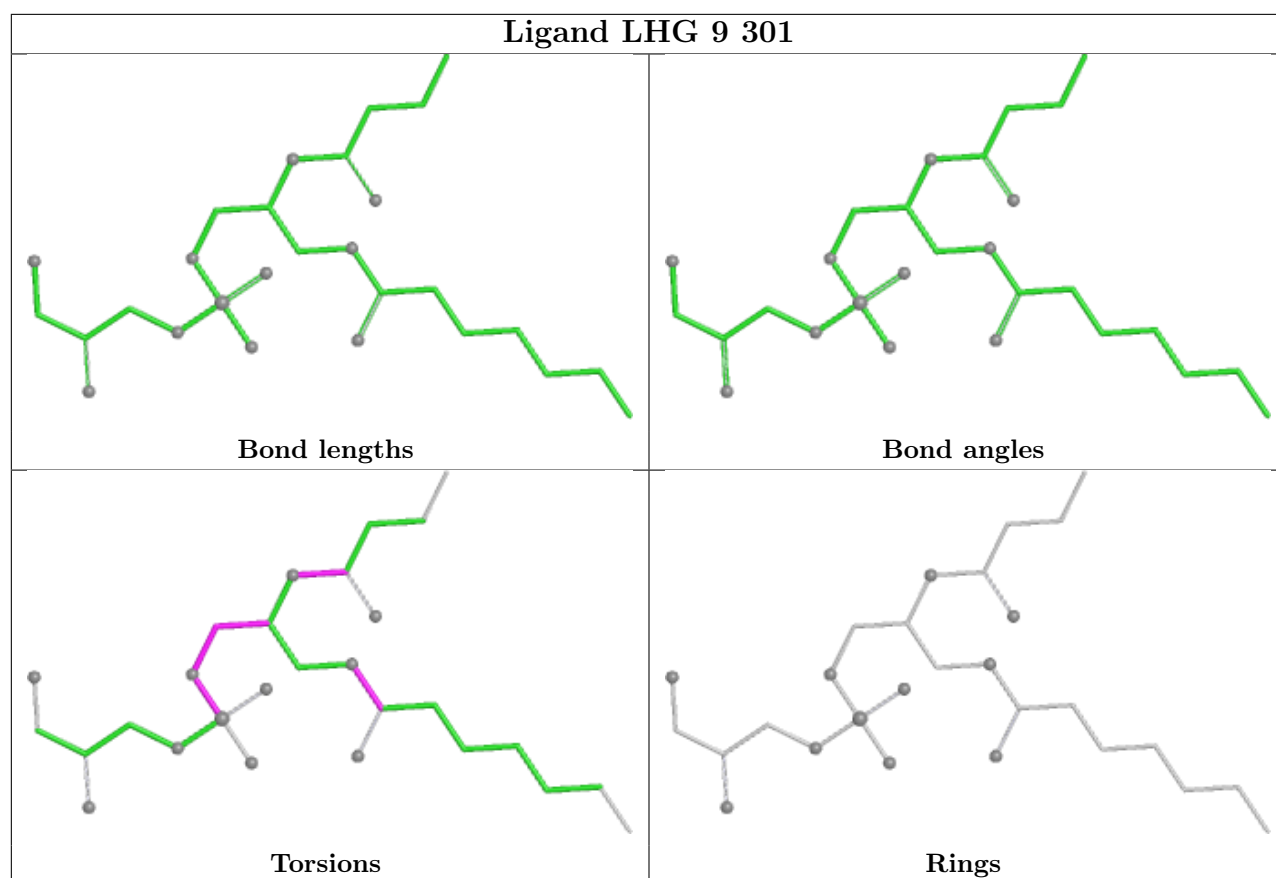
Torsions

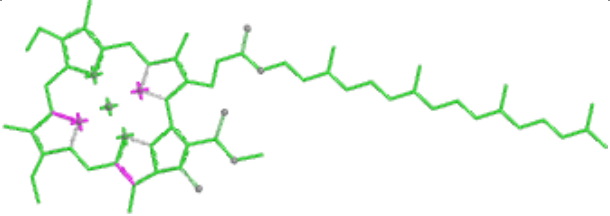
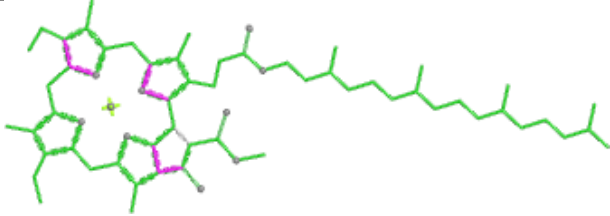
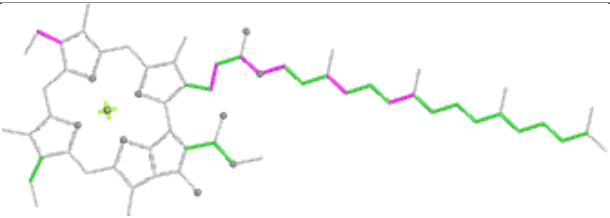
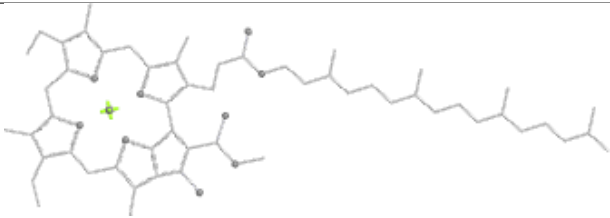
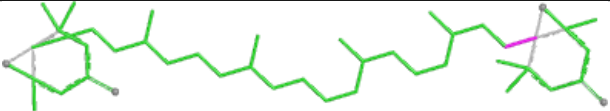
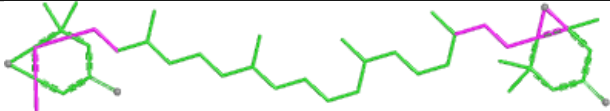
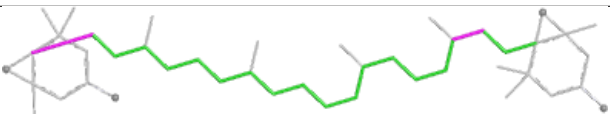
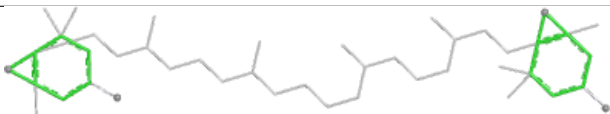
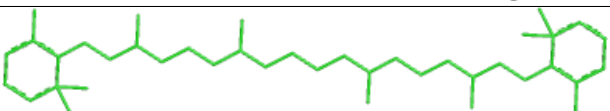
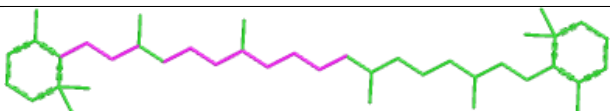
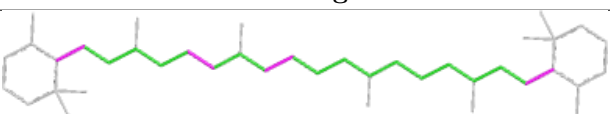
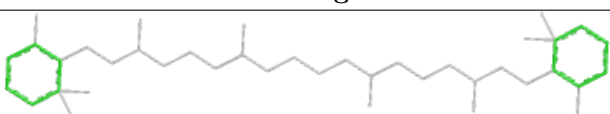


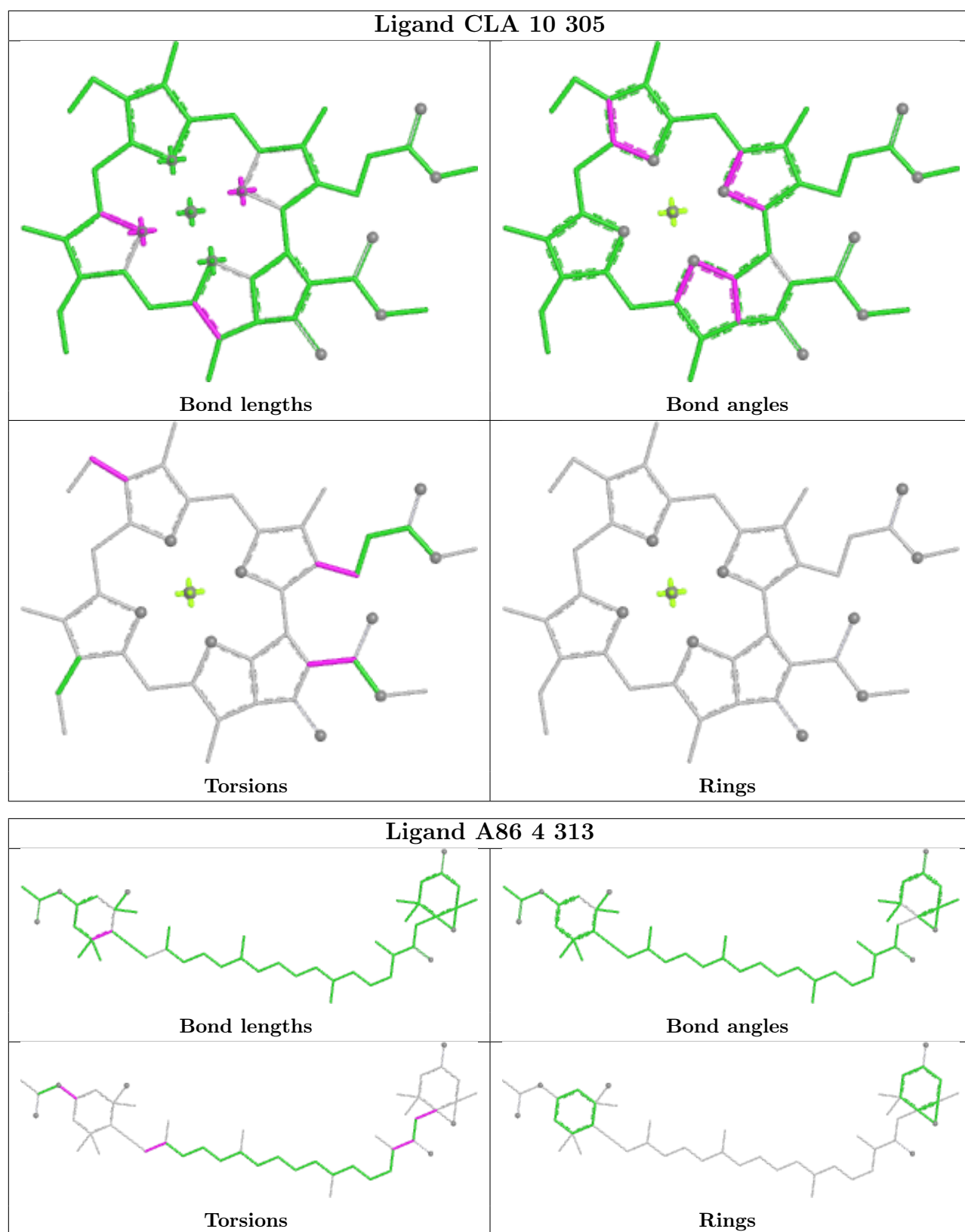
Rings

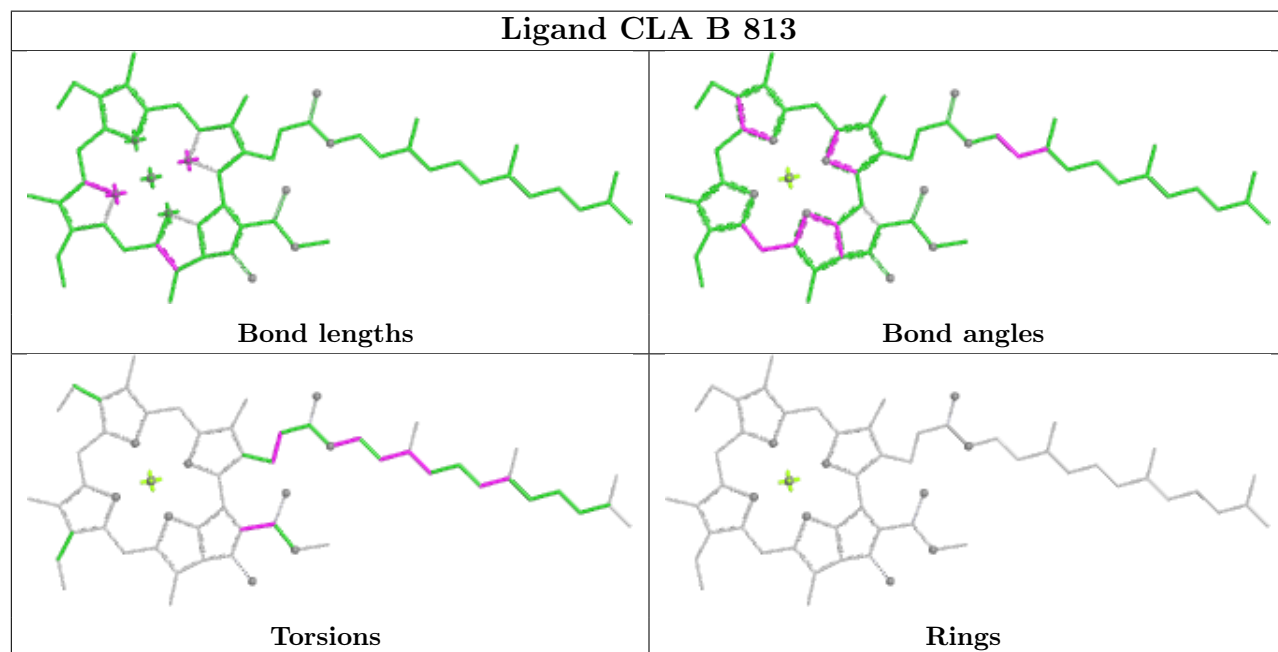
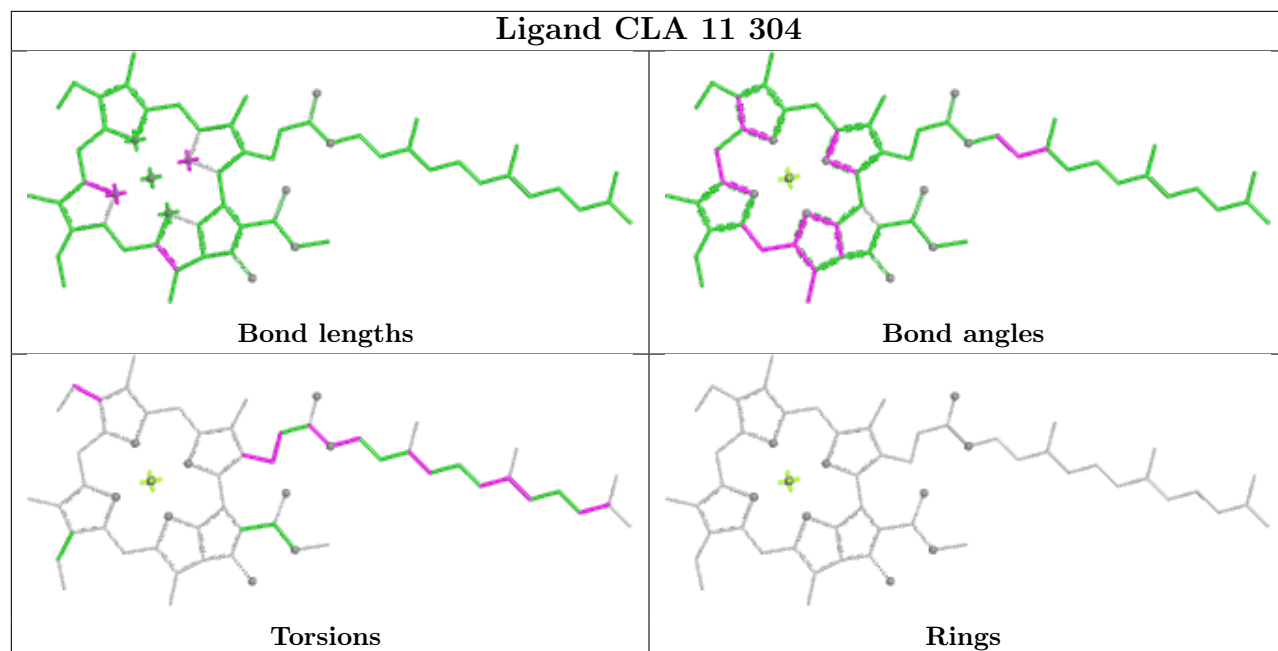


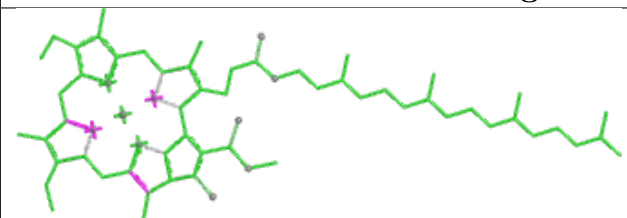
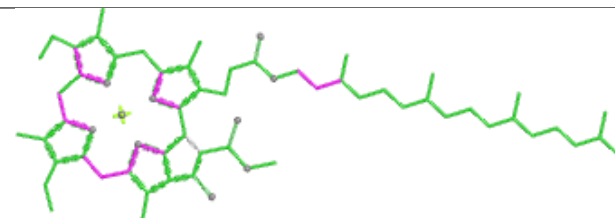
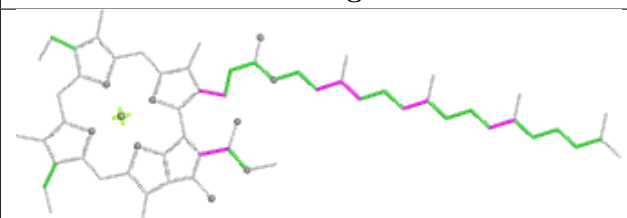
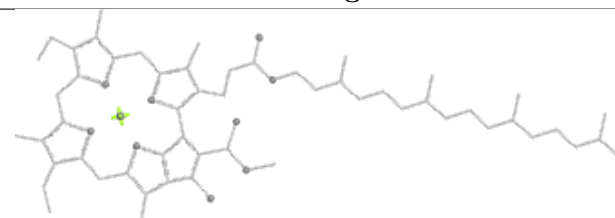


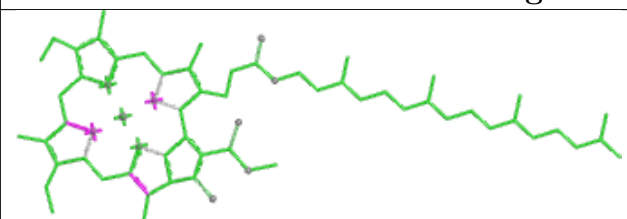
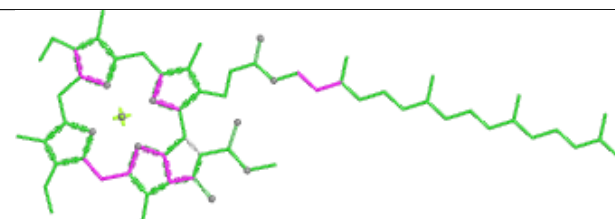
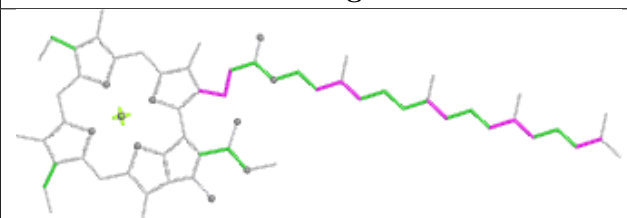
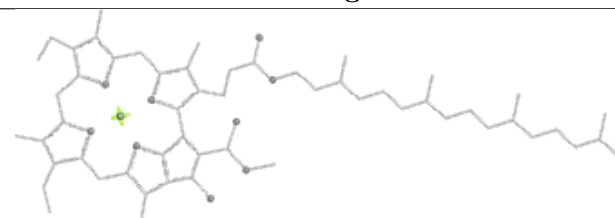


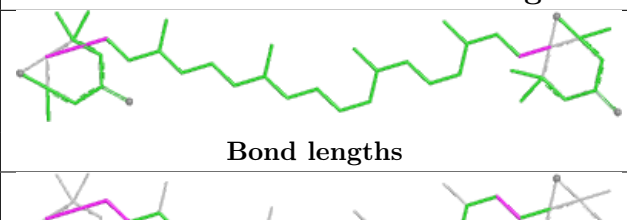
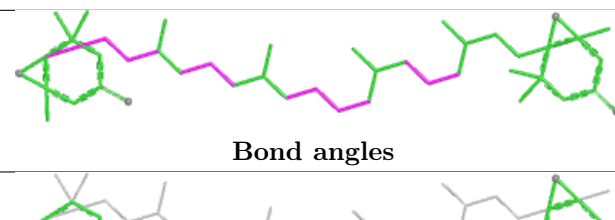


Ligand CLA B 806	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand XAT J 105	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 850	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

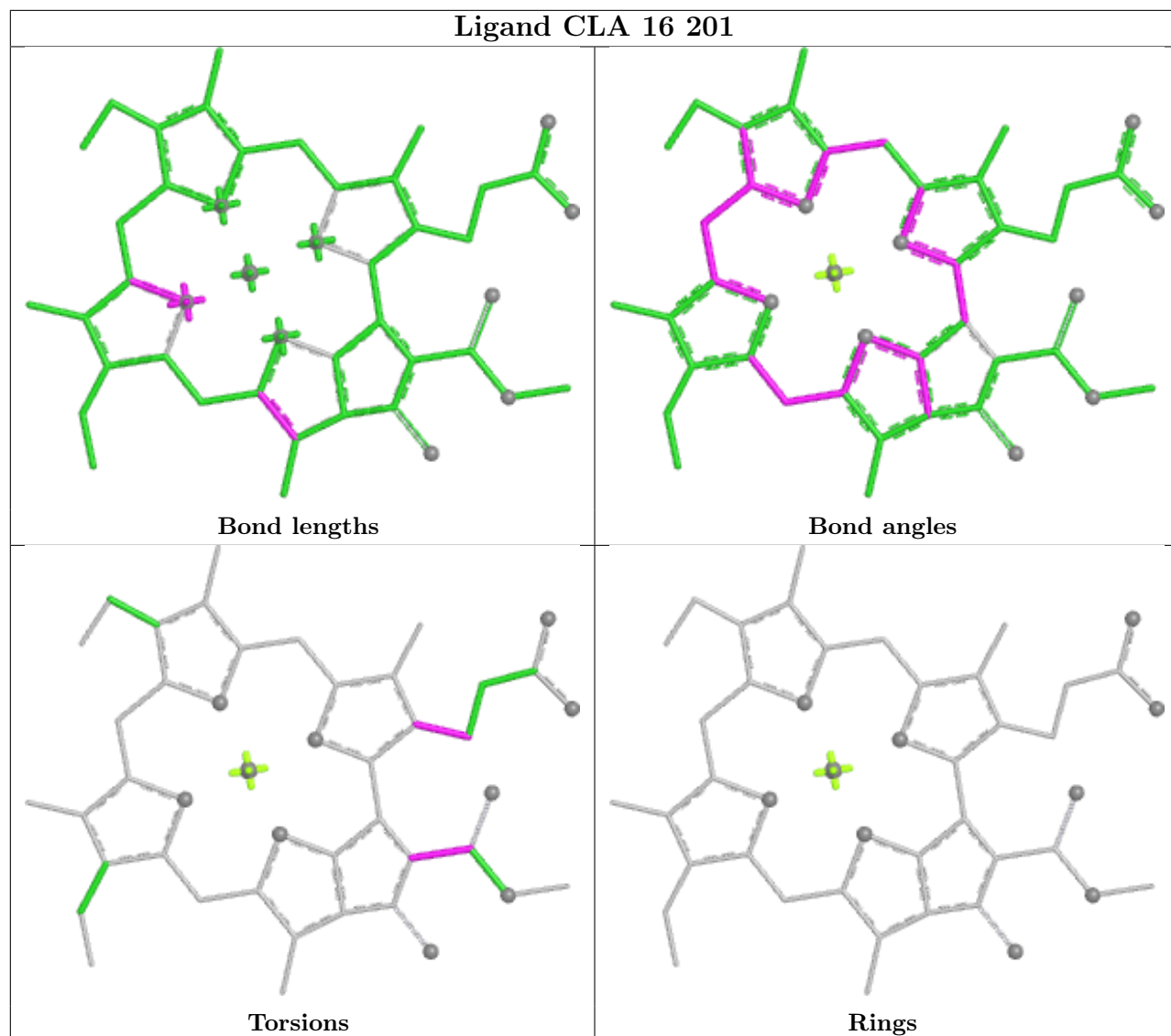


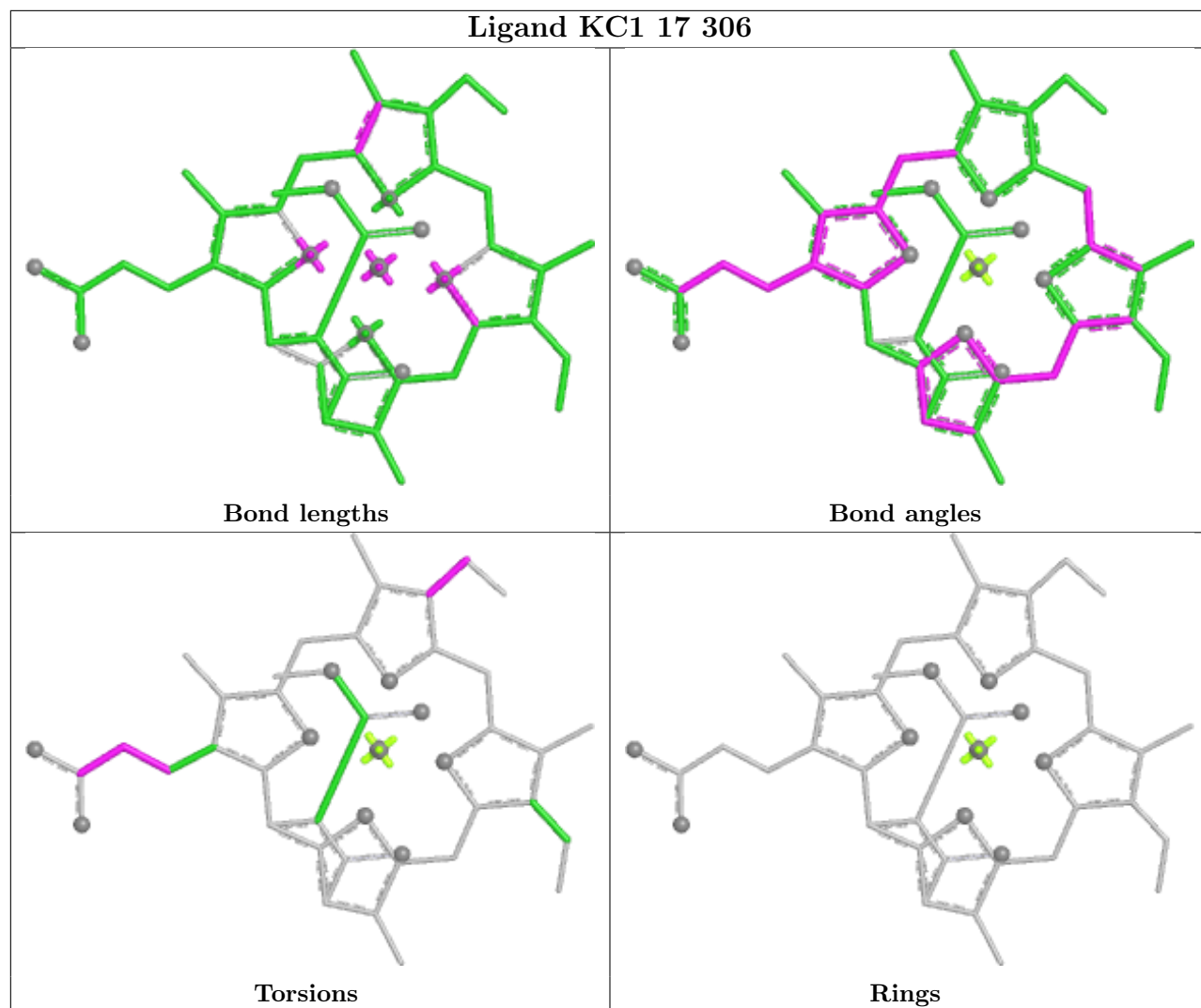


Ligand CLA A 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

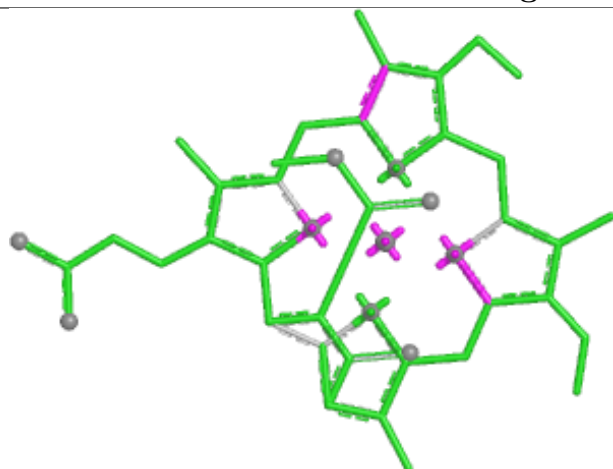
Ligand CLA 6 301	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand XAT 7 316	
	
Bond lengths	Bond angles
	
Torsions	Rings

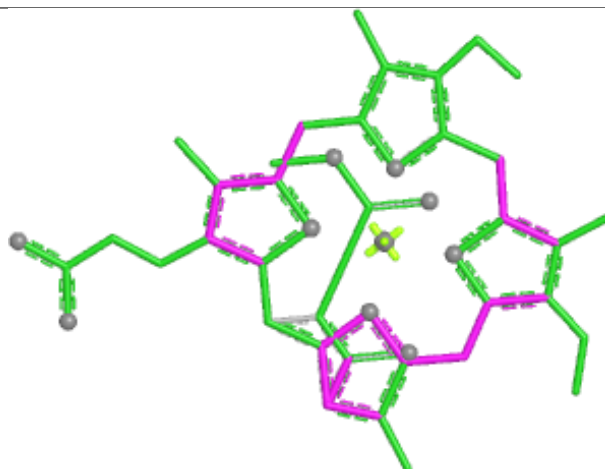




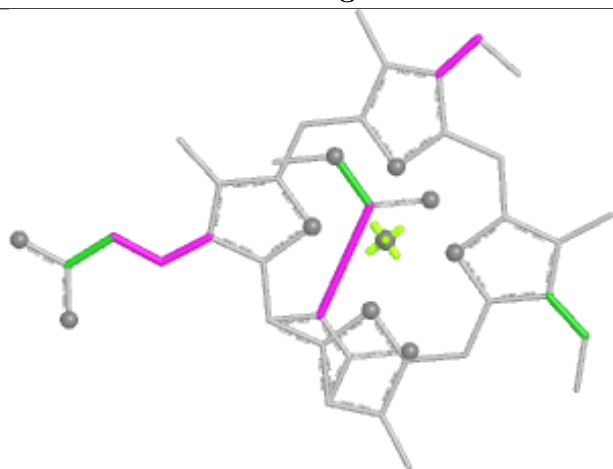
Ligand KC1 3 309



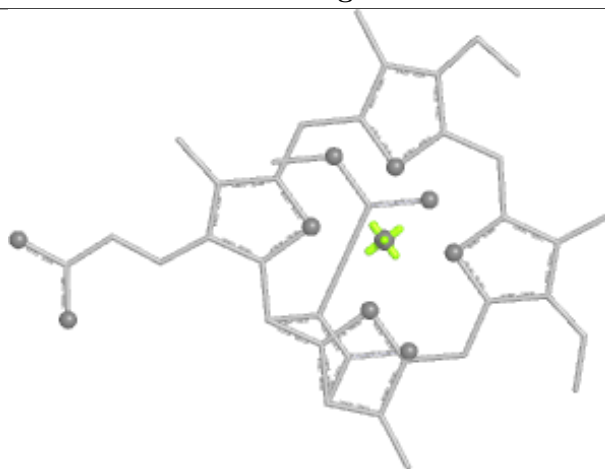
Bond lengths



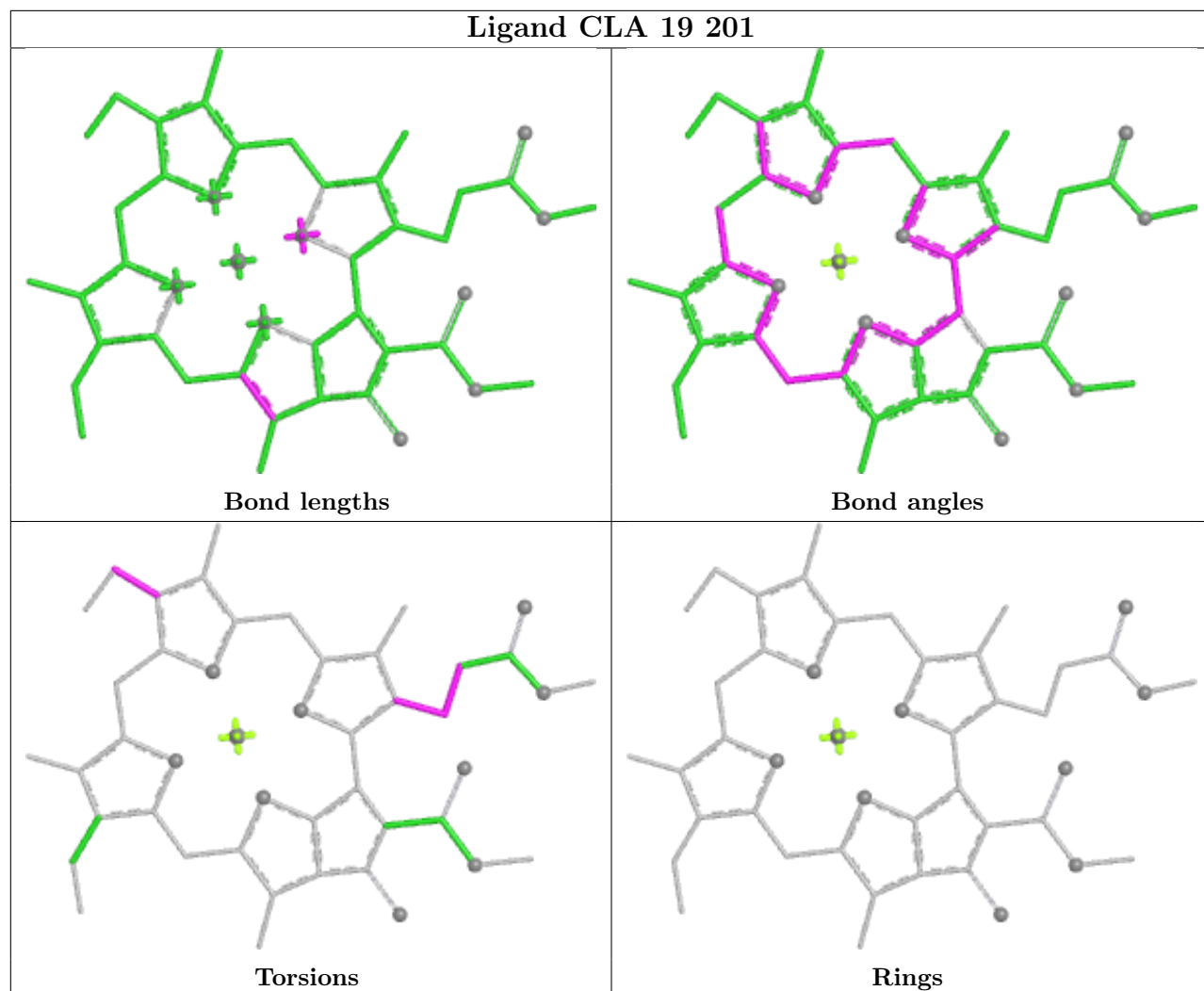
Bond angles



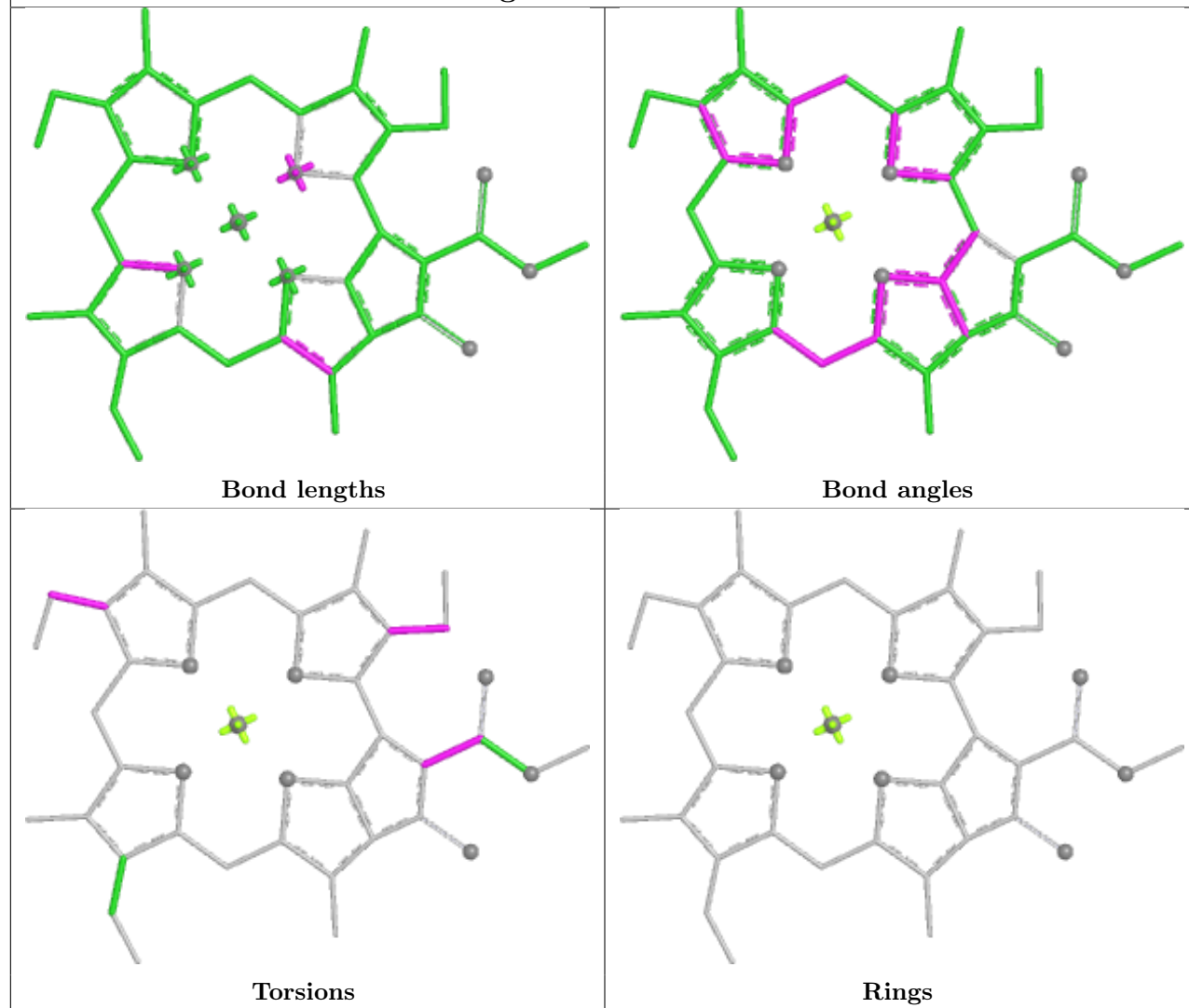
Torsions



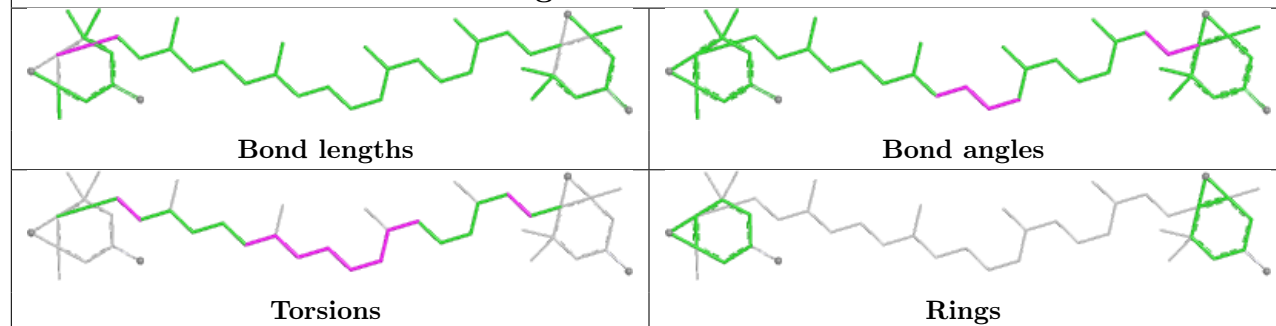
Rings

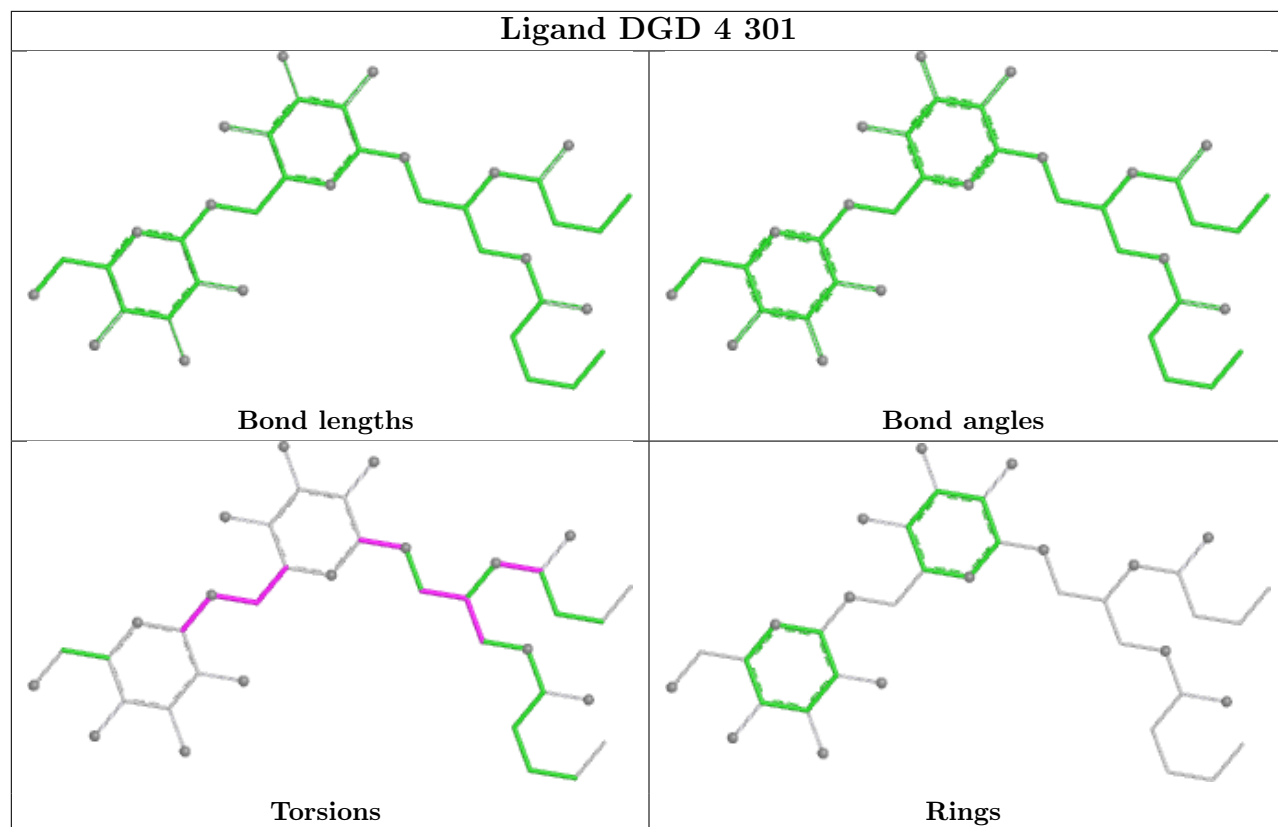


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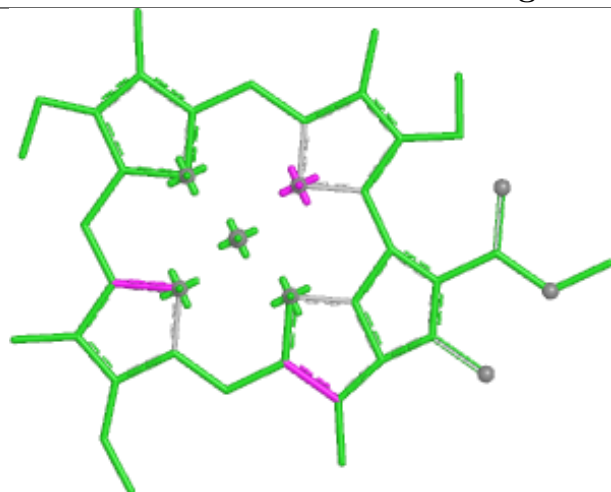


Ligand XAT 6 312

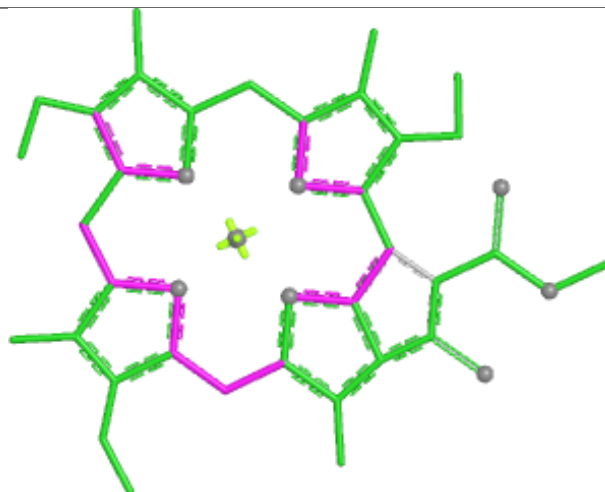




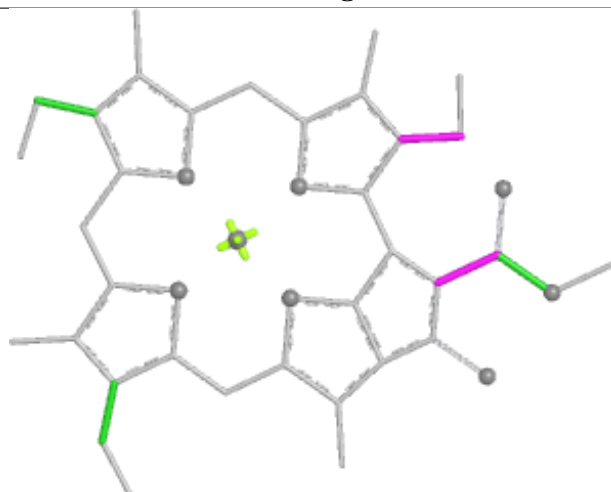
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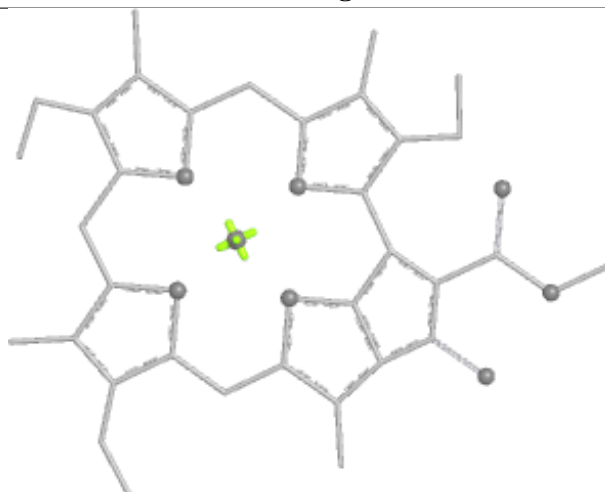
Bond lengths



Bond angles

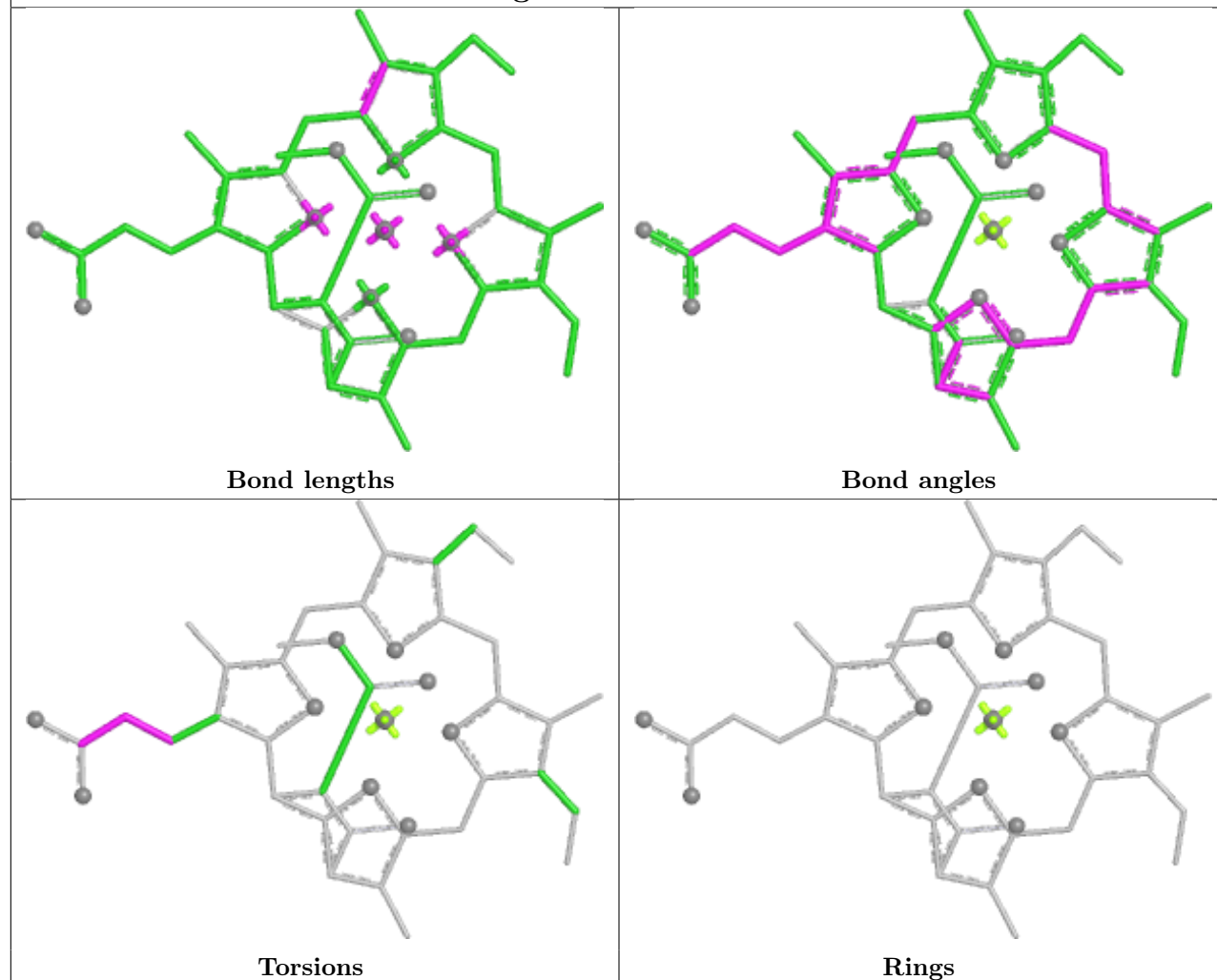


Torsions

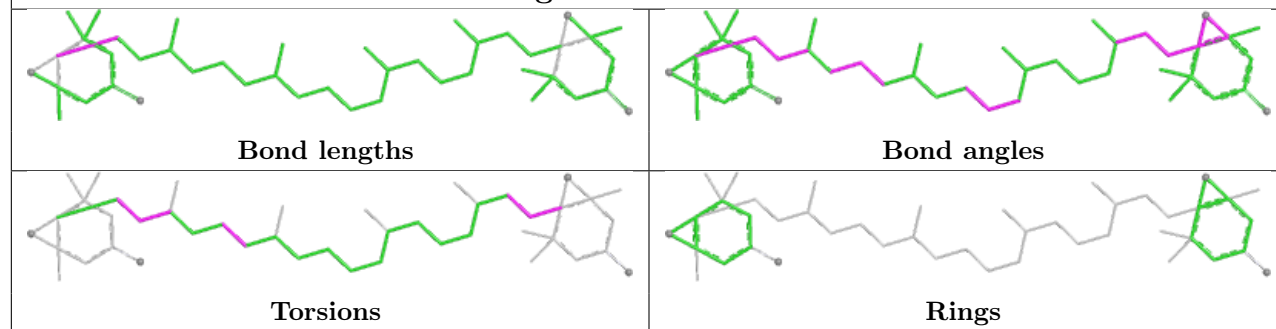


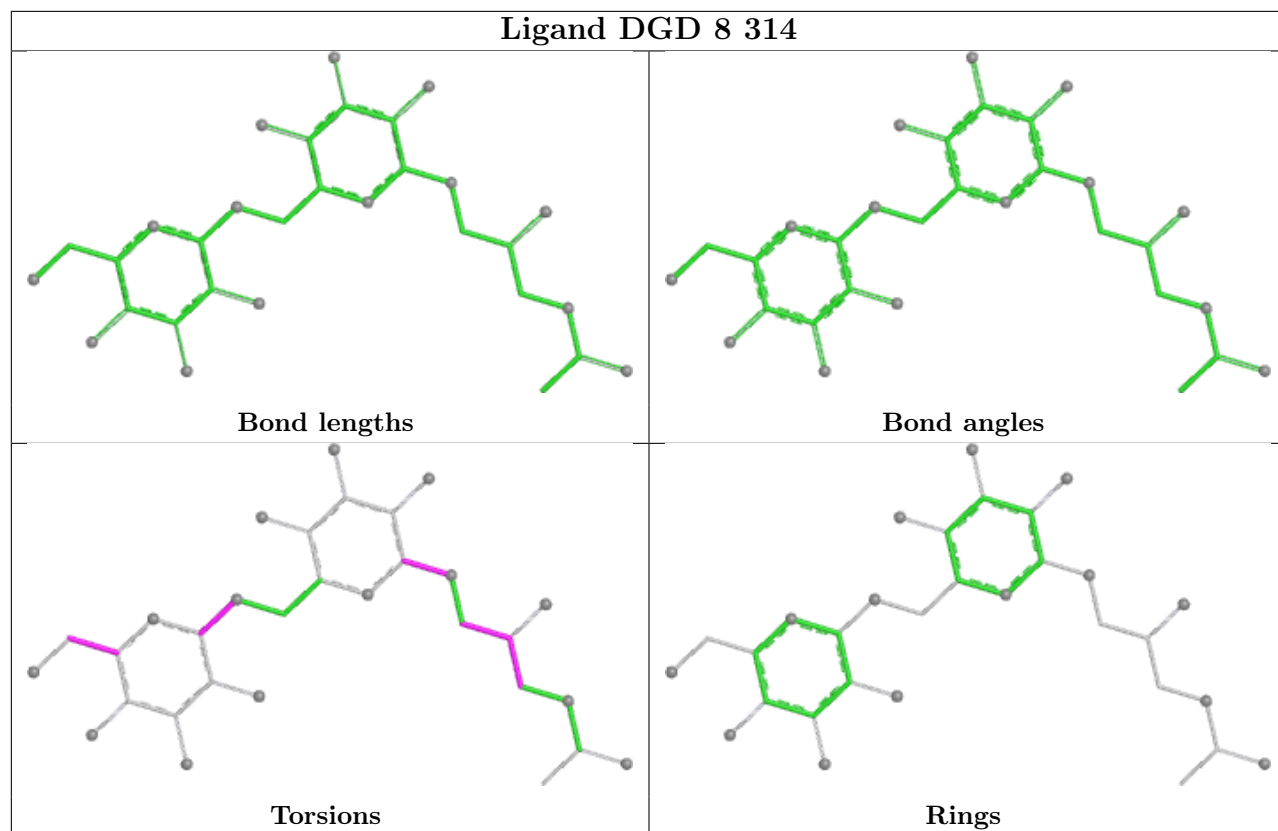
Rings

Ligand KC1 3 308

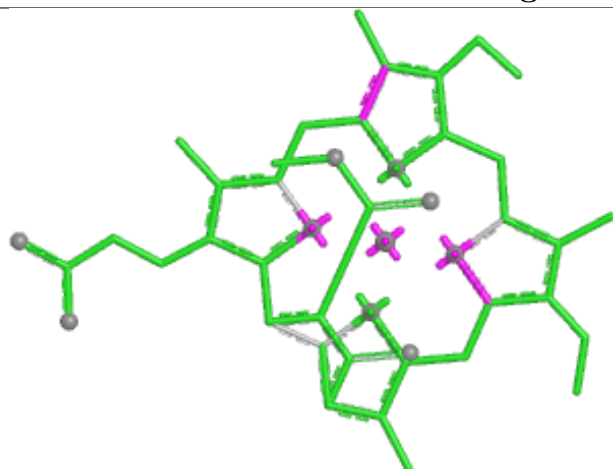


Ligand XAT 7 317

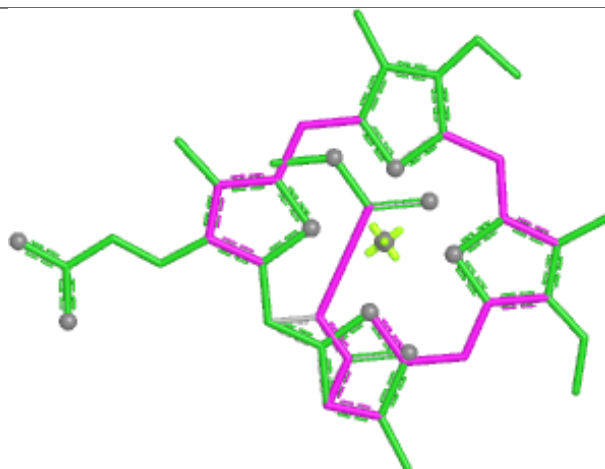




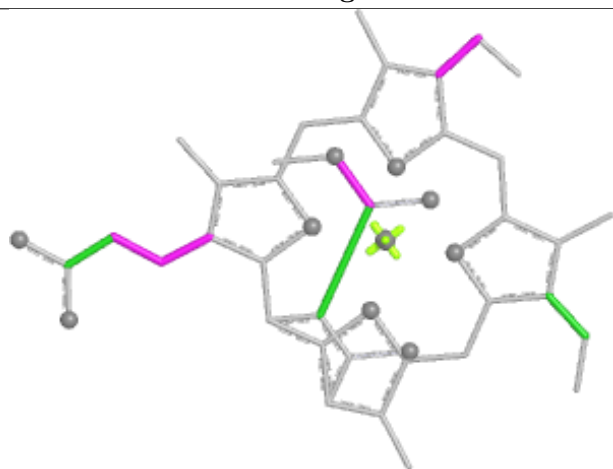
Ligand KC1 4 312



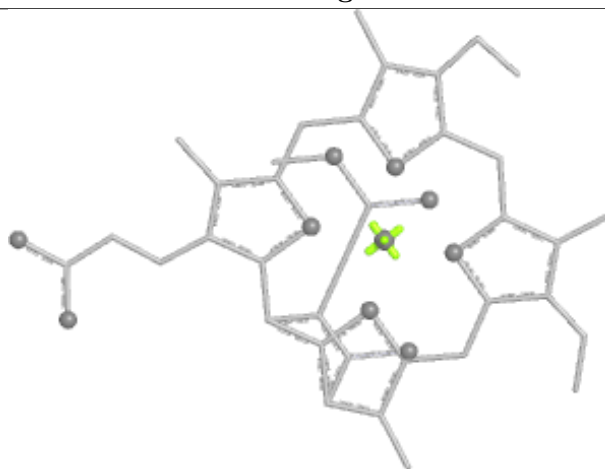
Bond lengths



Bond angles

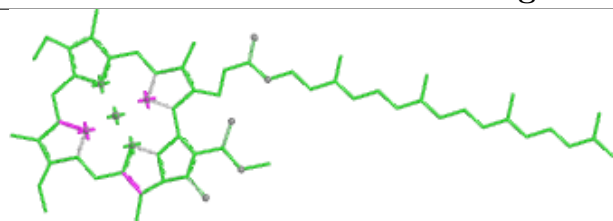


Torsions

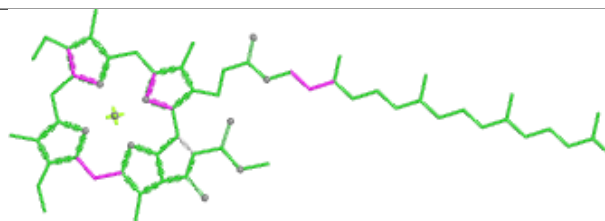


Rings

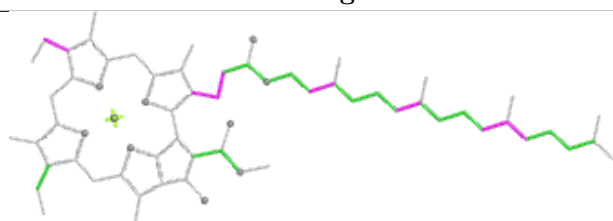
Ligand CLA 3 301



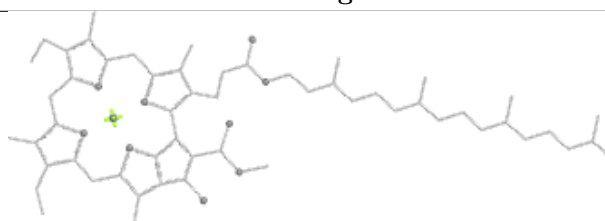
Bond lengths



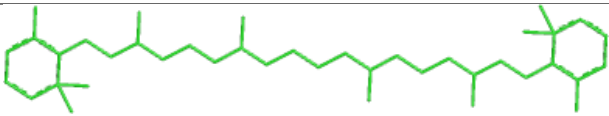
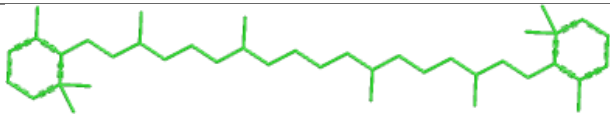
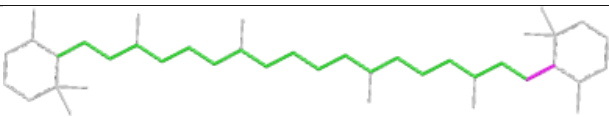
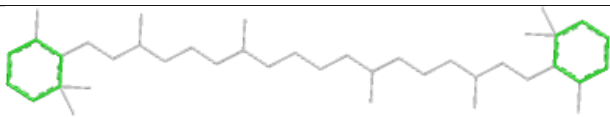
Bond angles



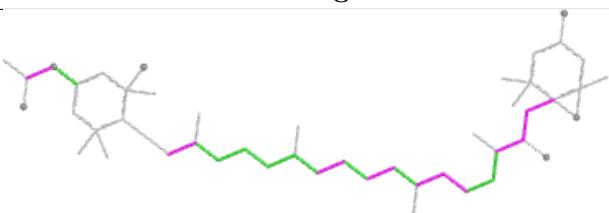
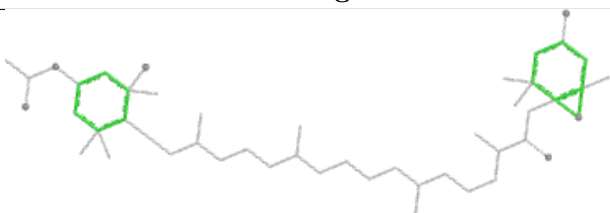


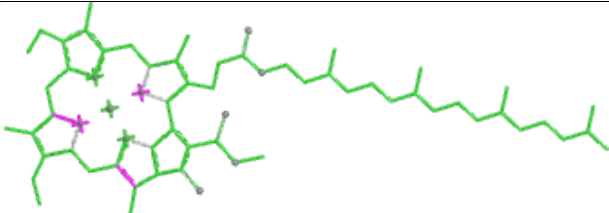
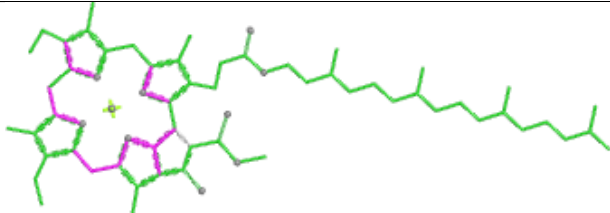
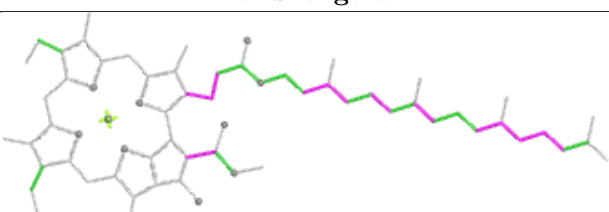
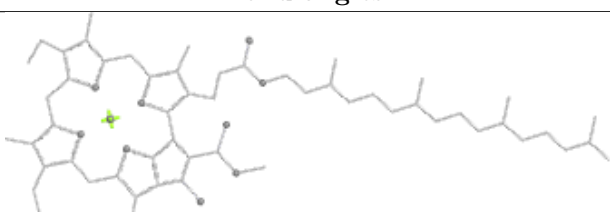
Torsions

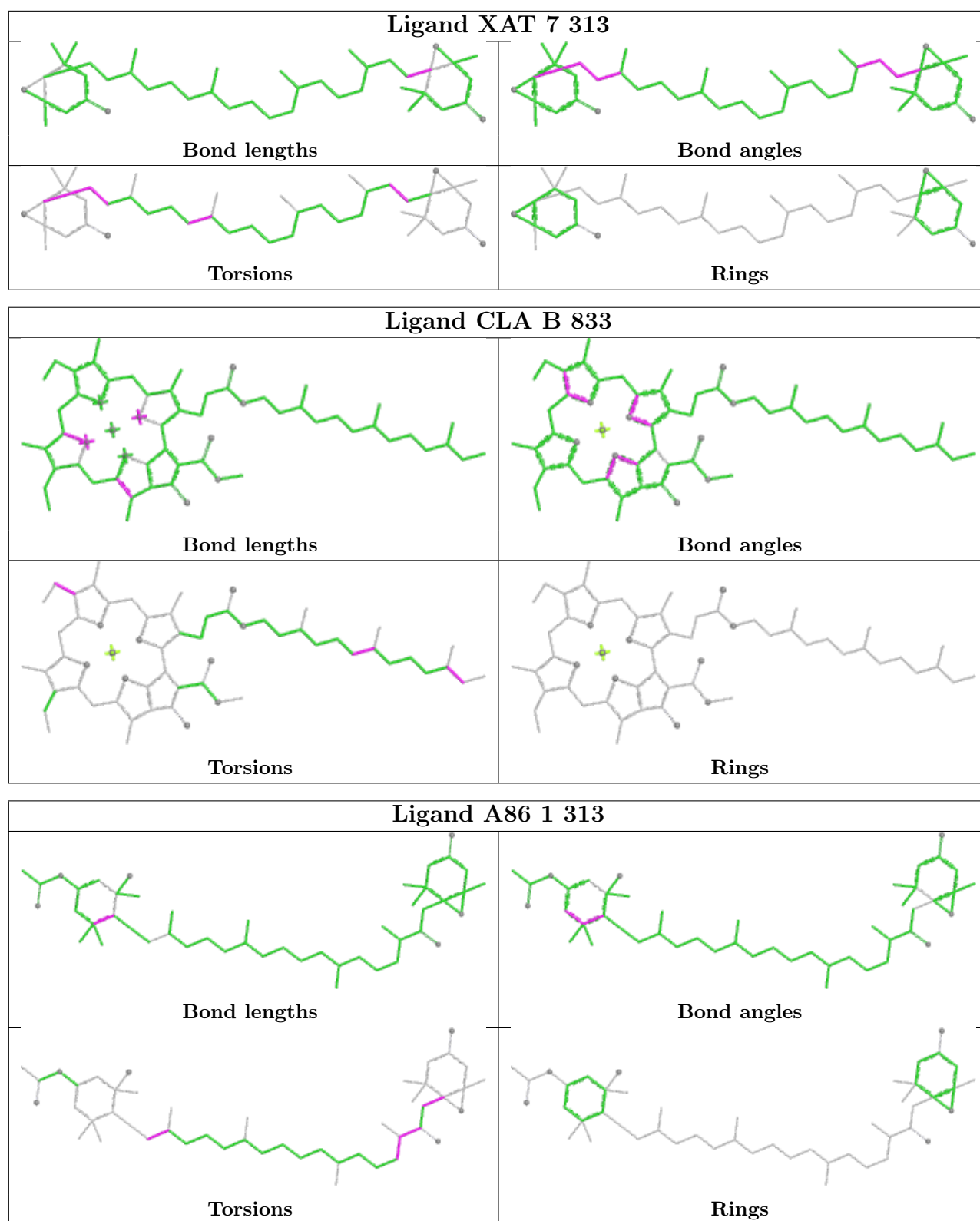


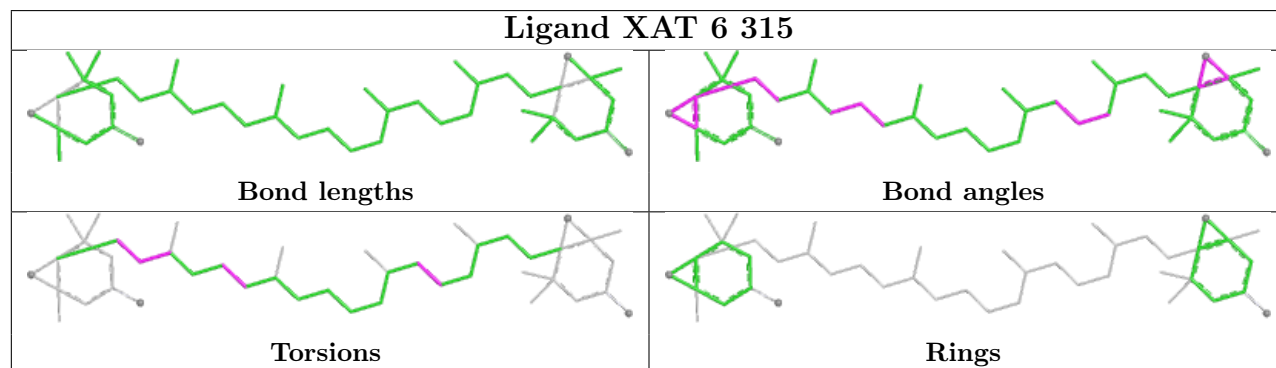
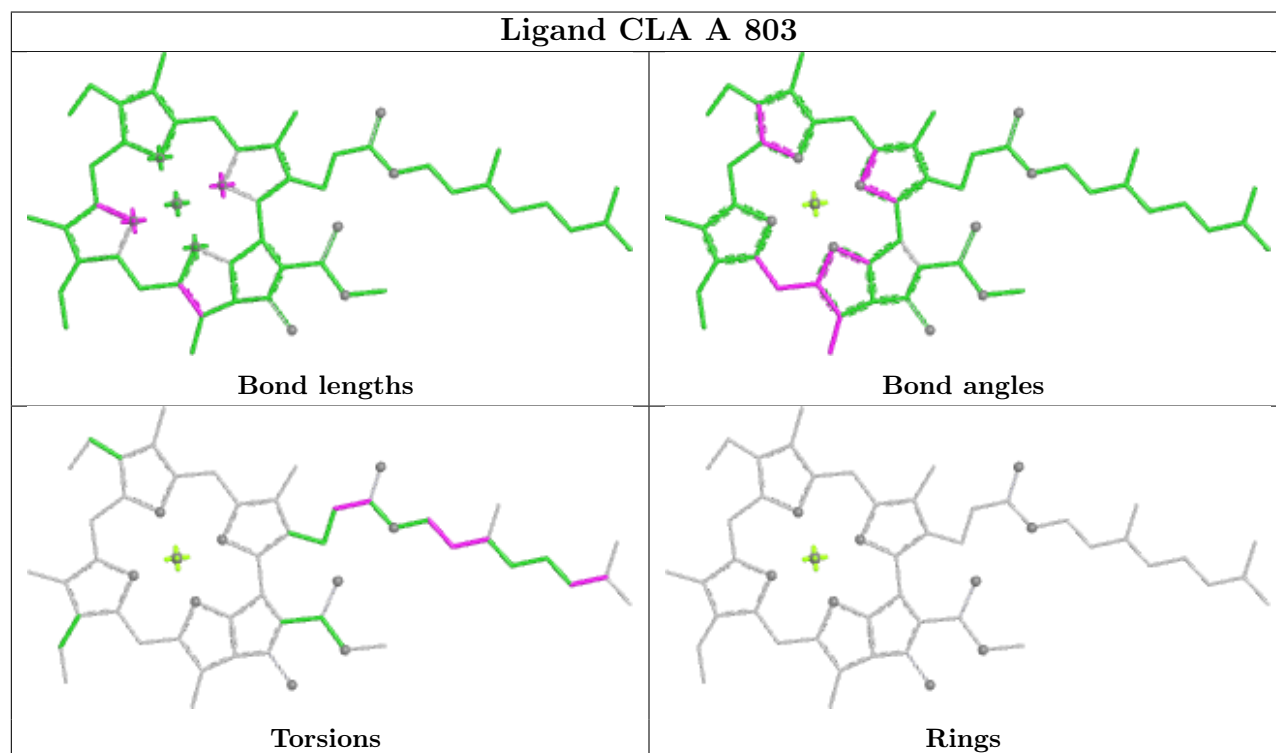
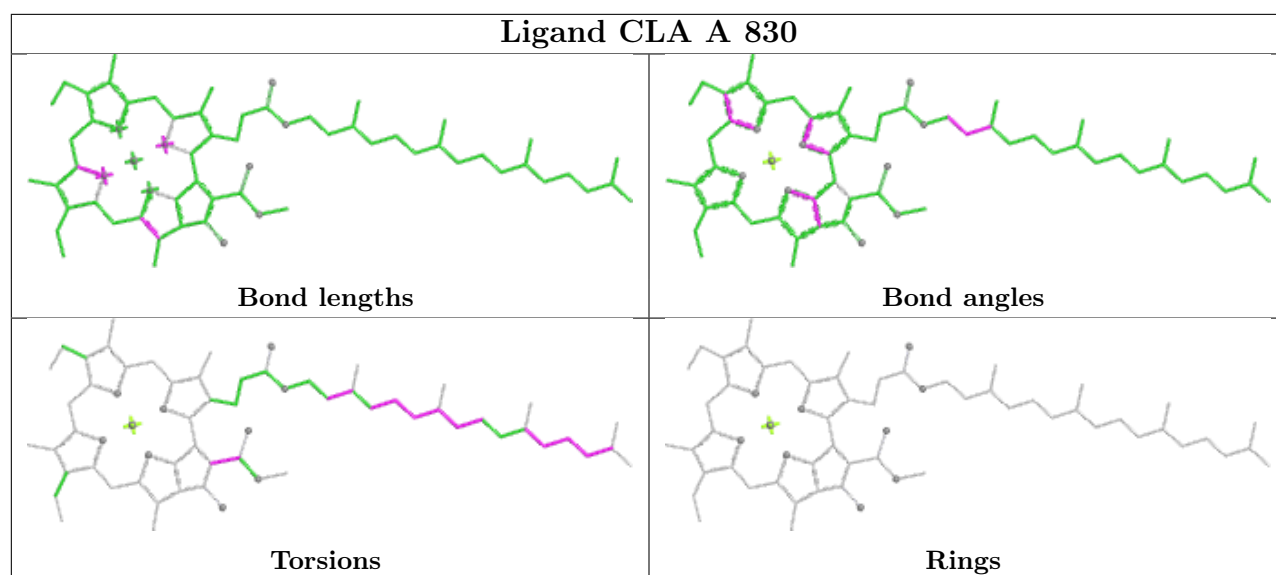
Rings

Ligand BCR L 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

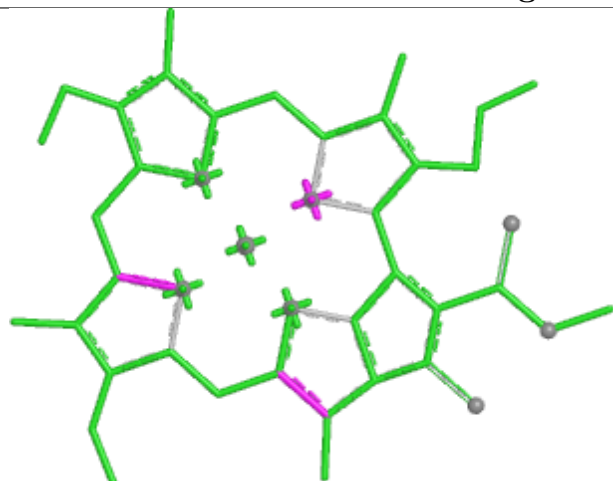
Ligand A86 J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 313	
	
Bond lengths	Bond angles
	
Torsions	Rings

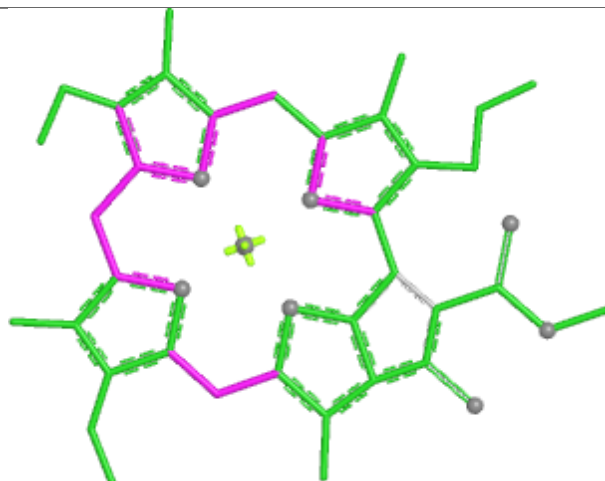




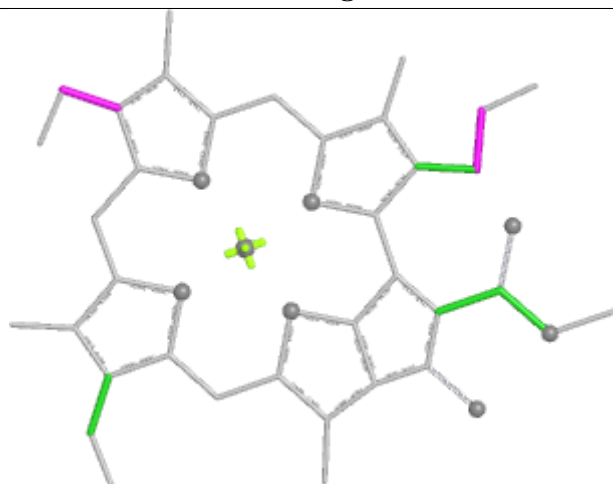
Ligand CLA a 201



Bond lengths



Bond angles

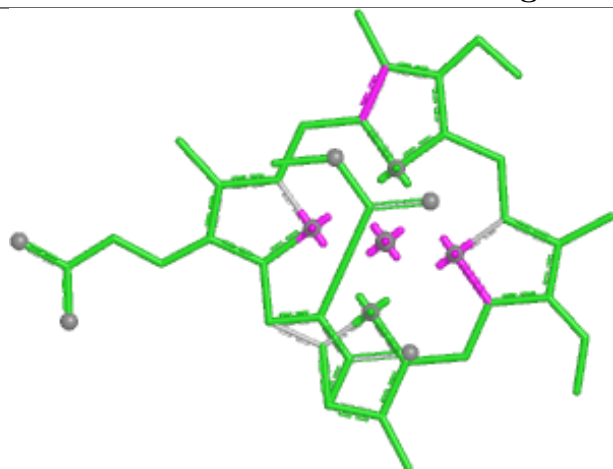


Torsions

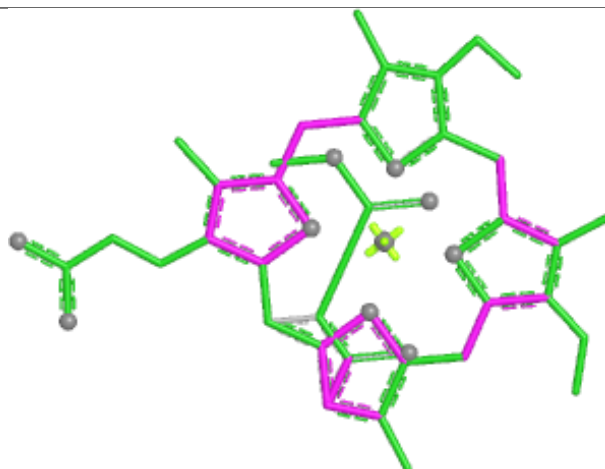


Rings

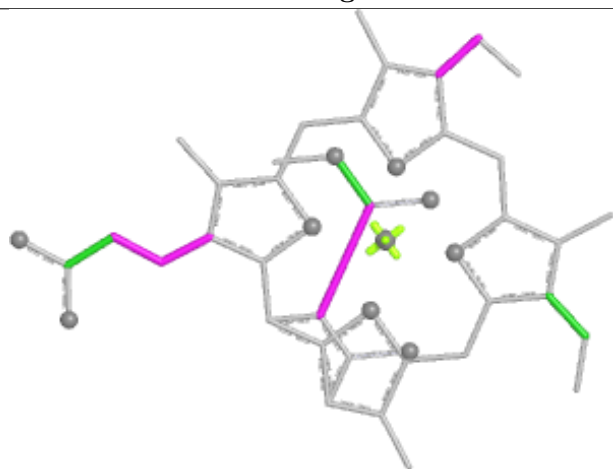
Ligand KC1 6 305



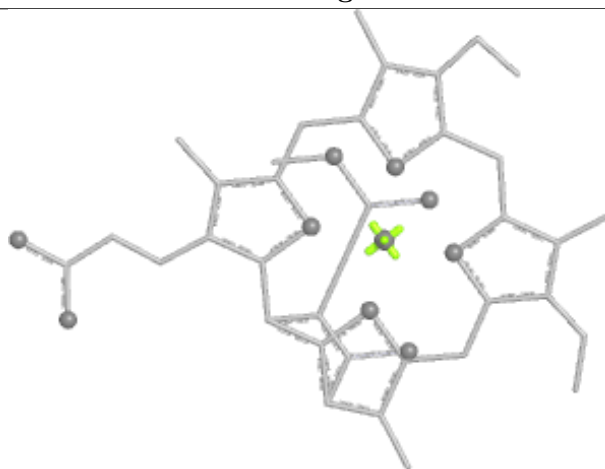
Bond lengths



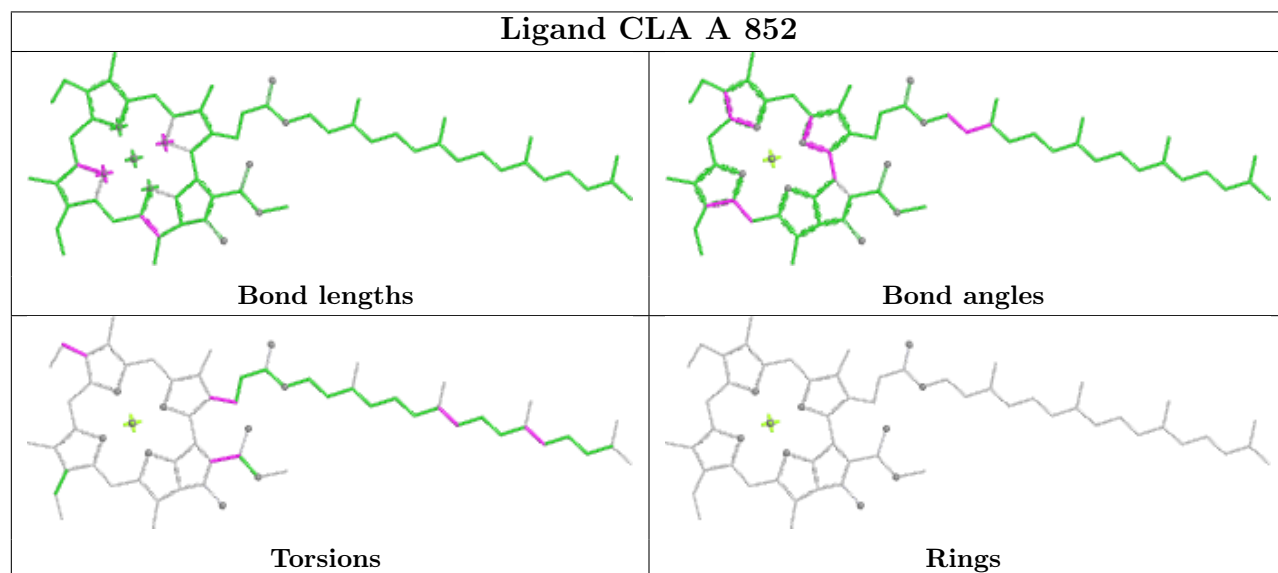
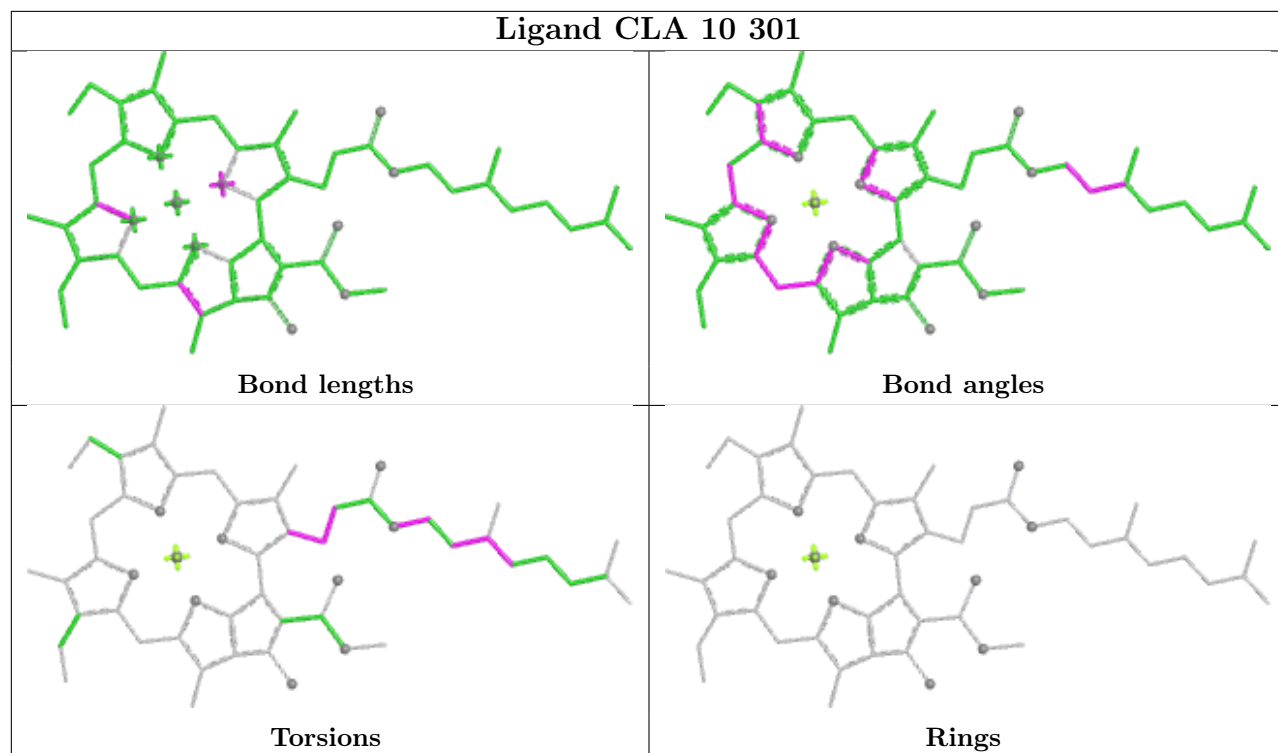
Bond angles

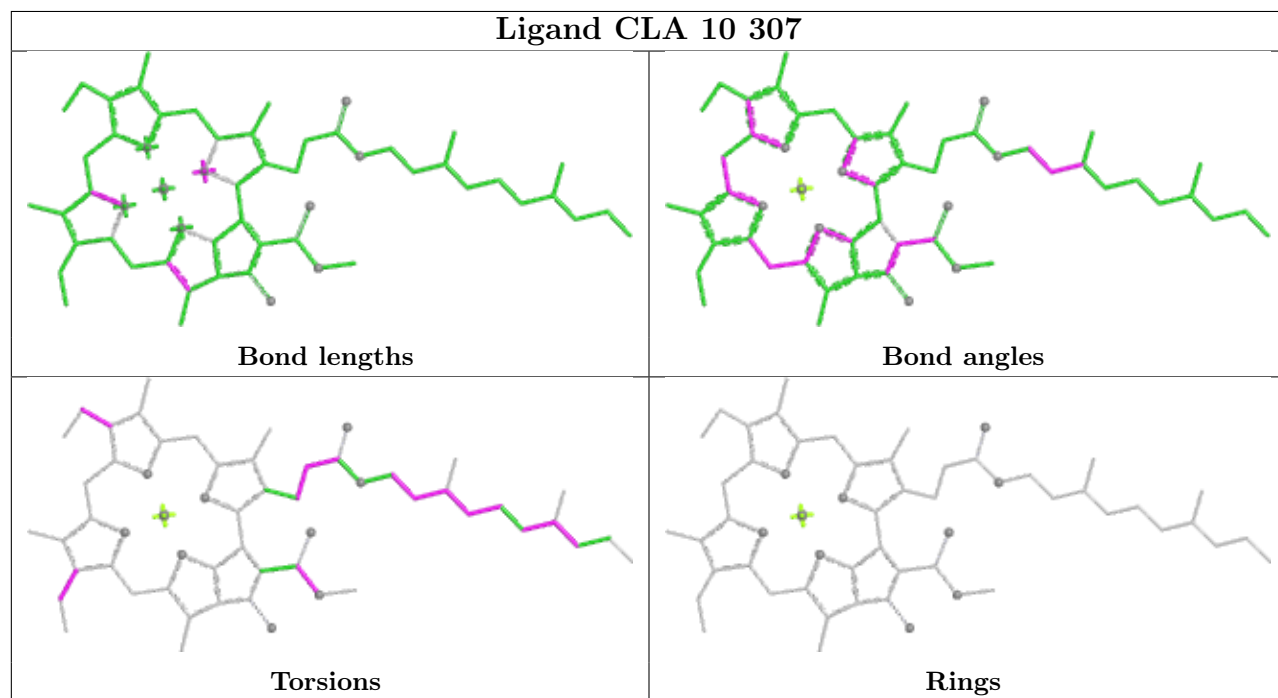
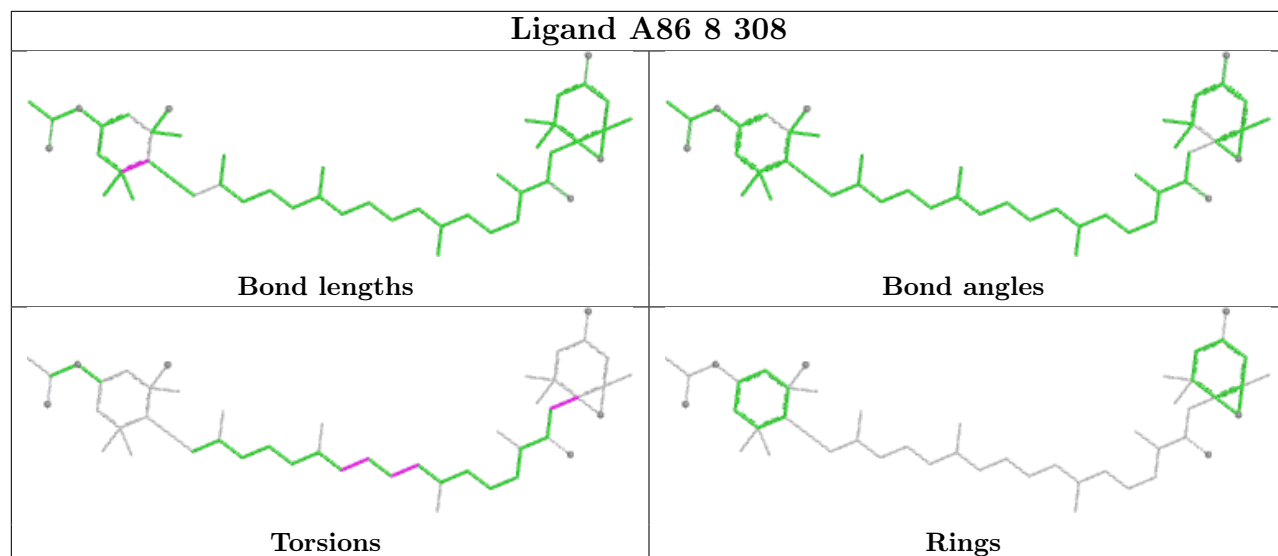


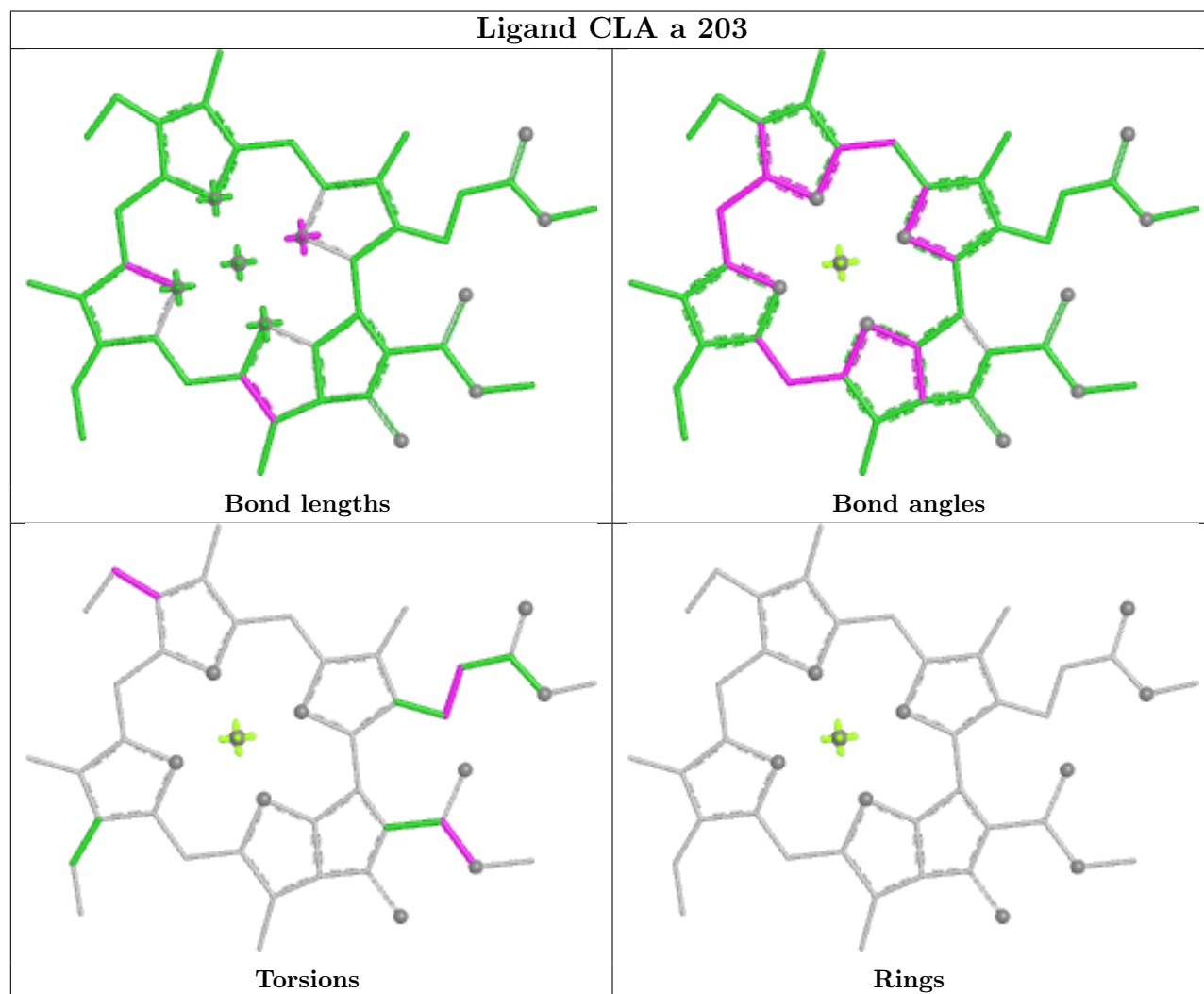
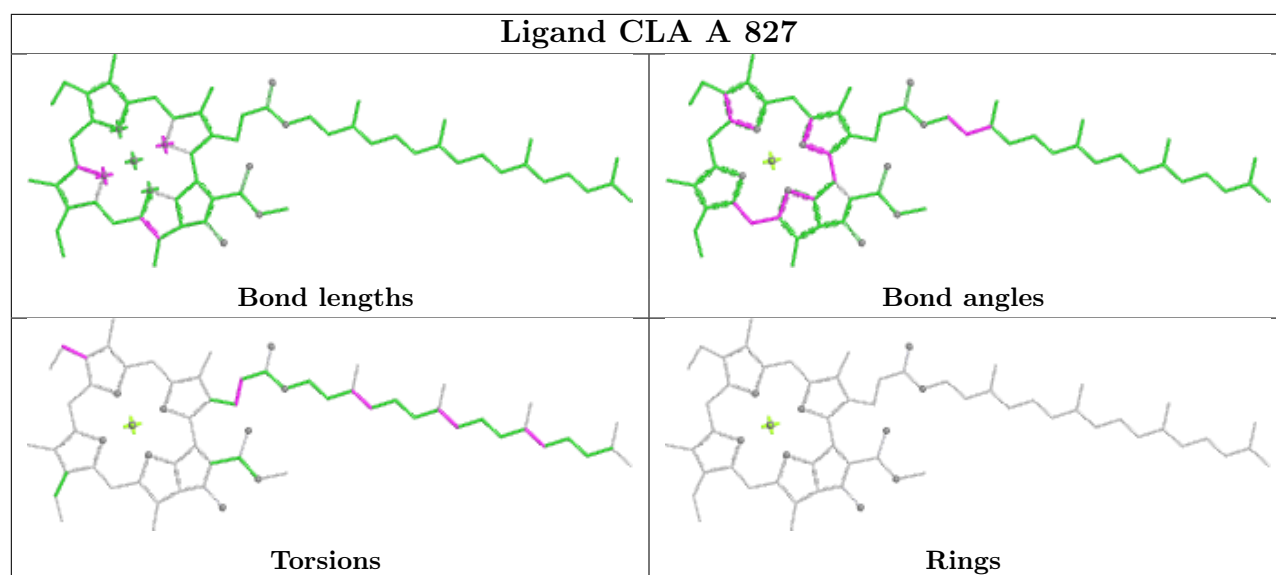
Torsions

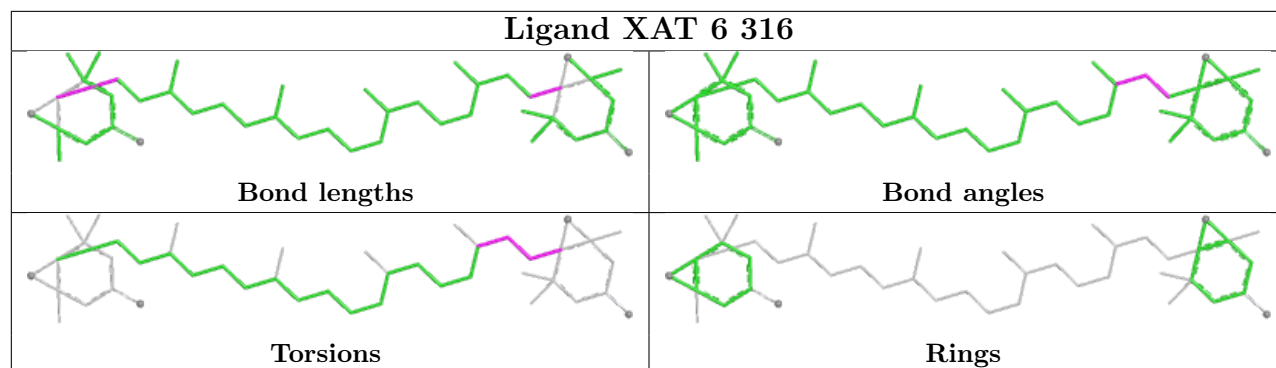
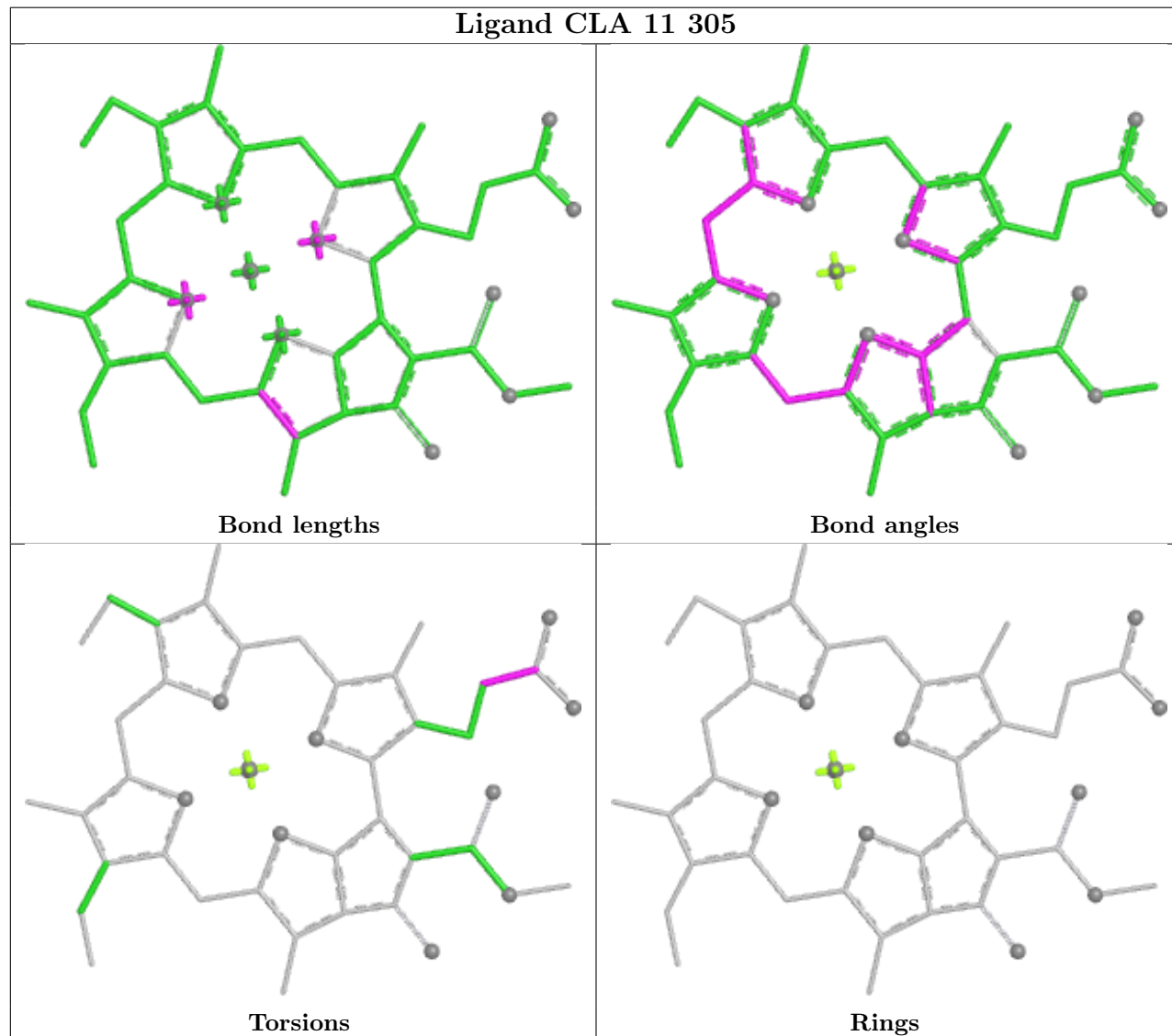


Rings

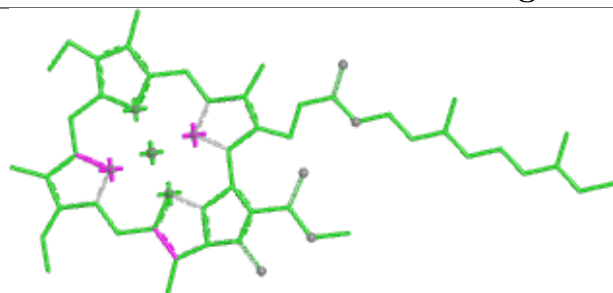




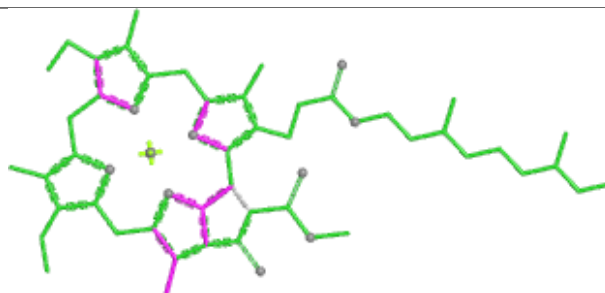


Ligand XAT 6 316**Ligand CLA 11 305**

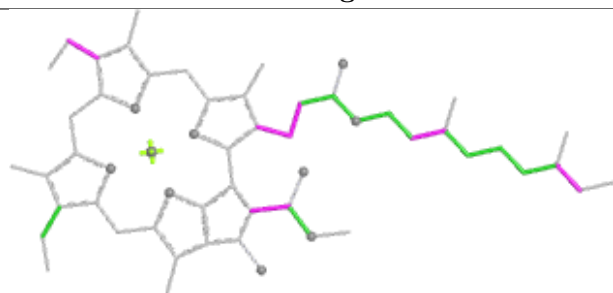
Ligand CLA 5 305



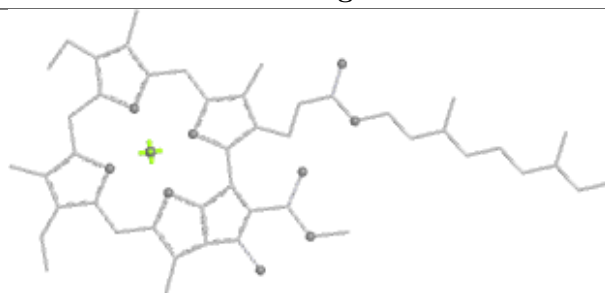
Bond lengths



Bond angles

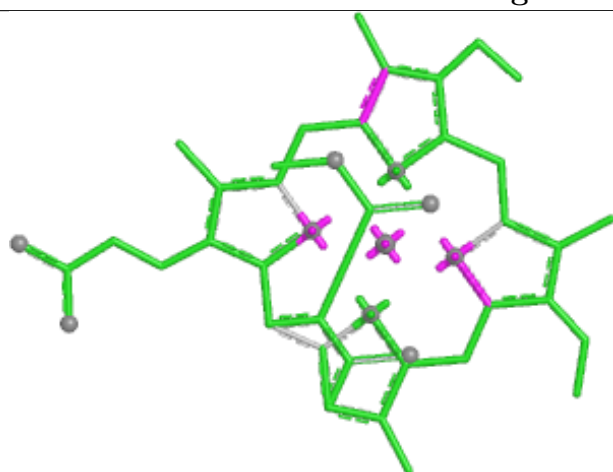


Torsions

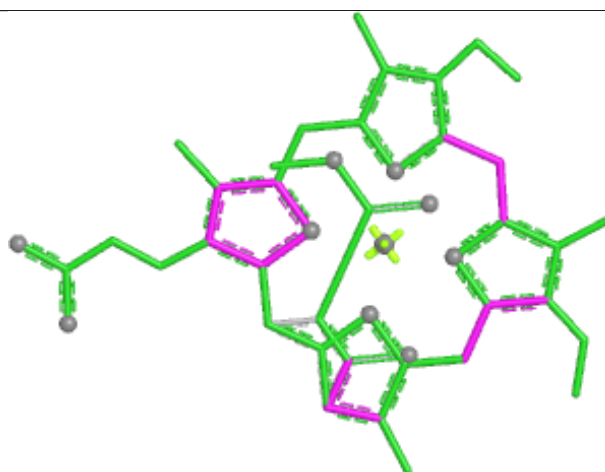


Rings

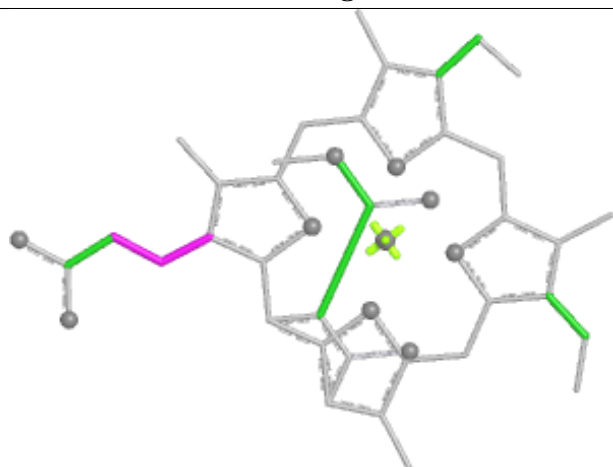
Ligand KC1 17 312



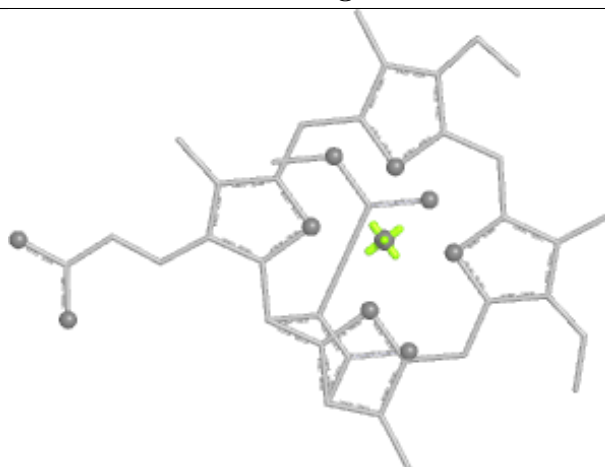
Bond lengths



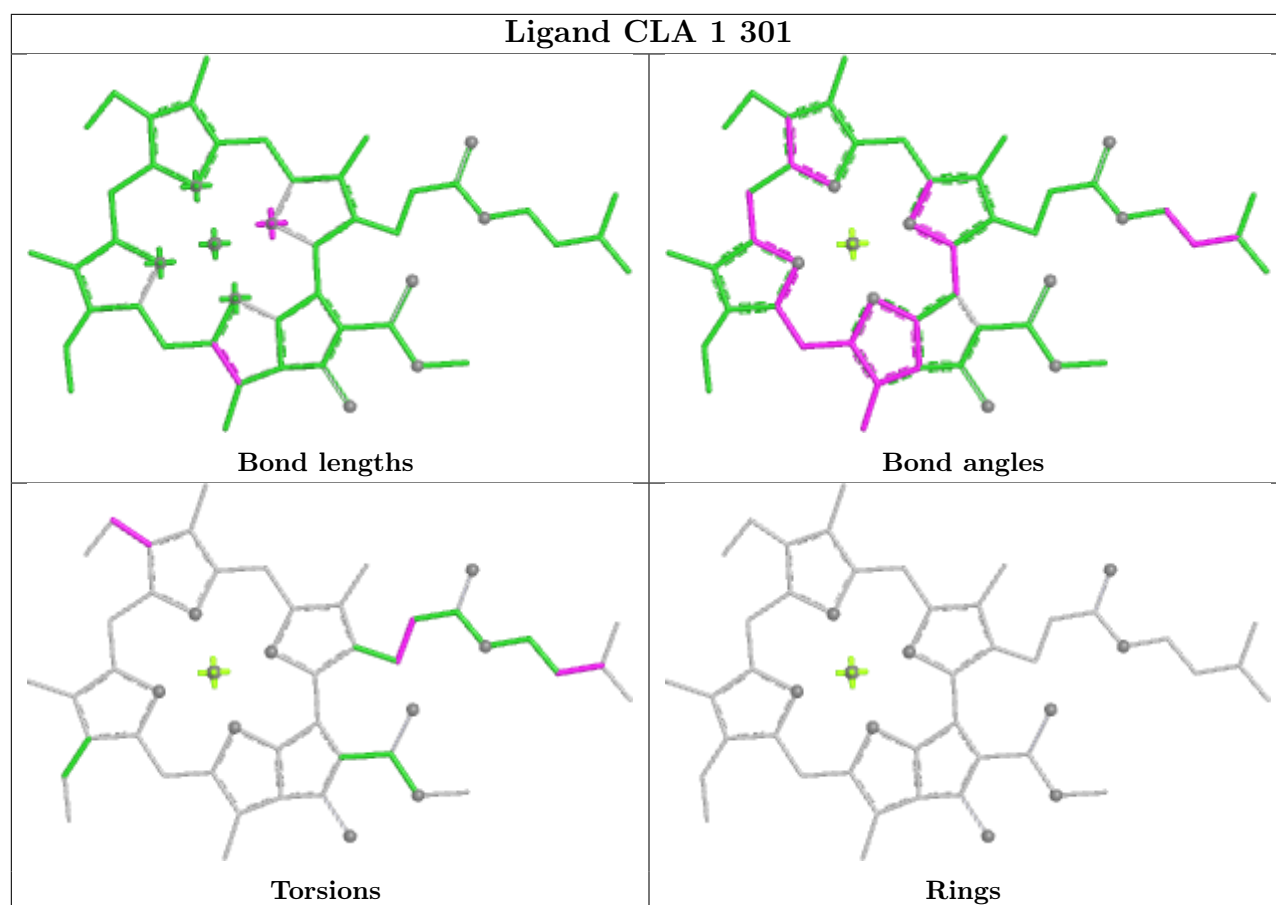
Bond angles

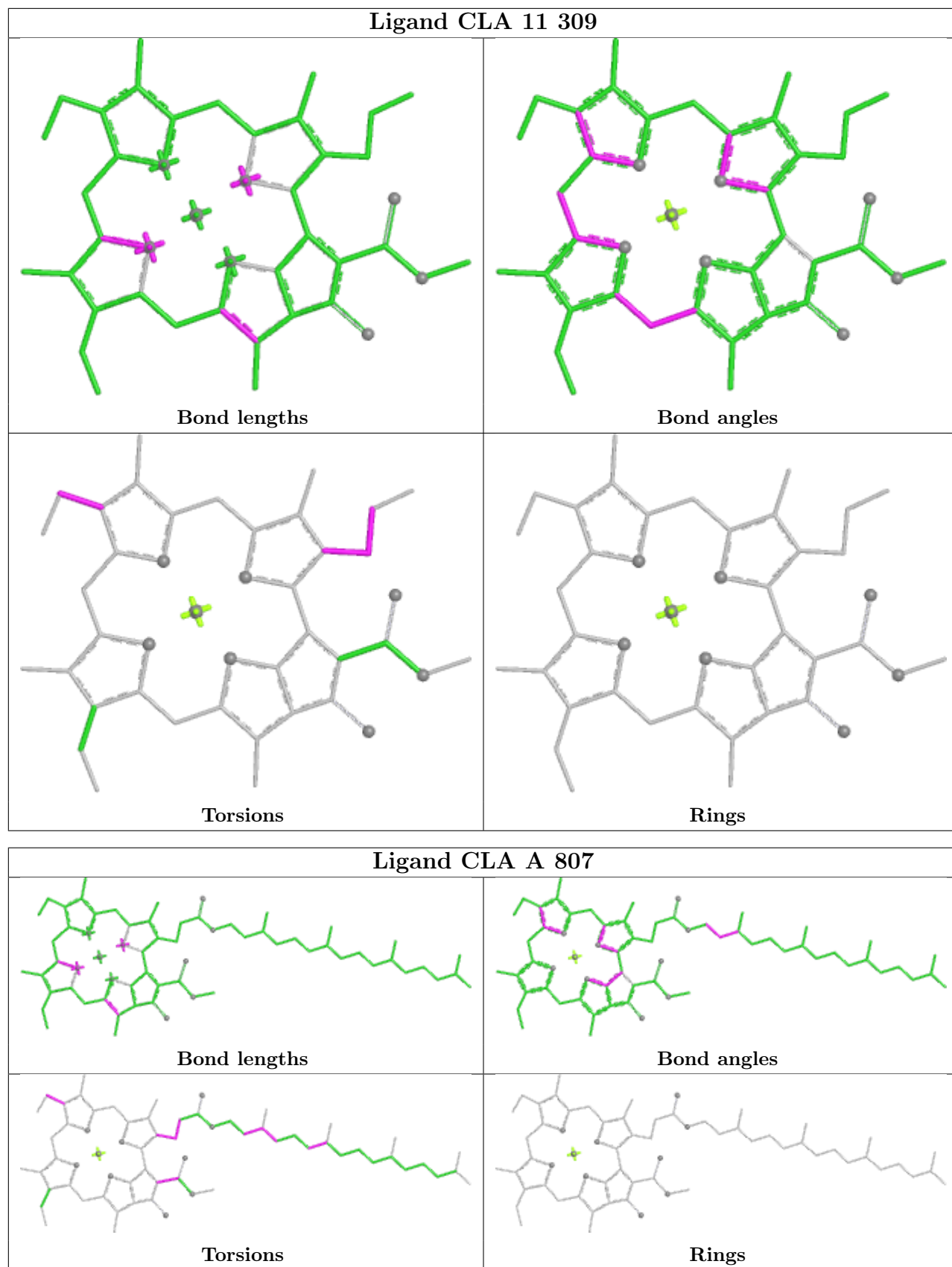


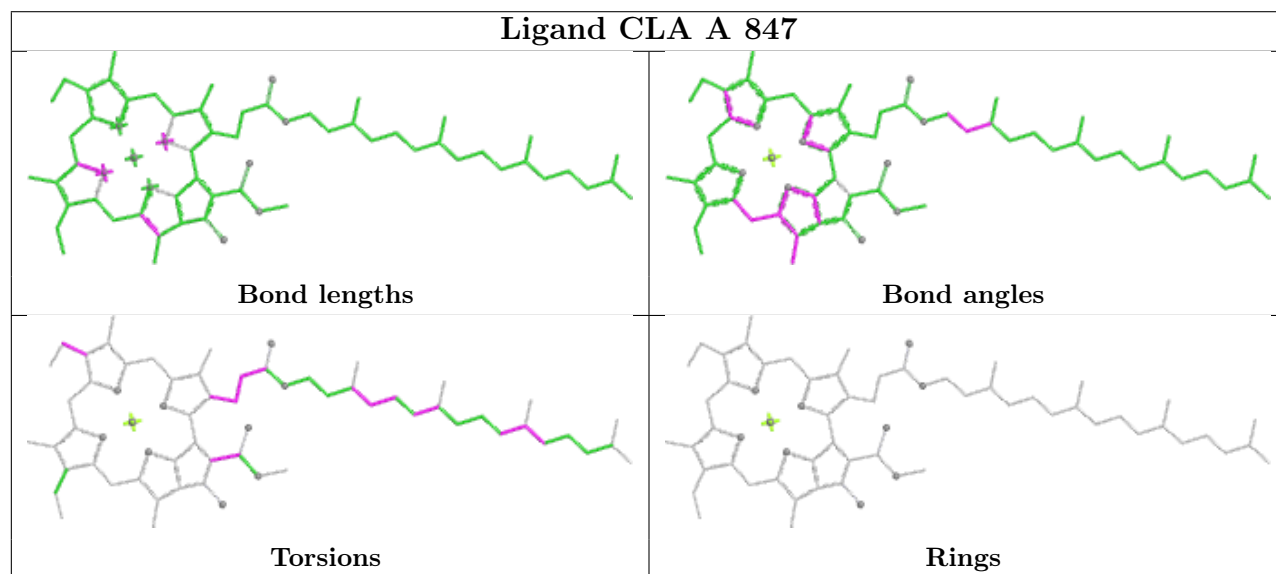
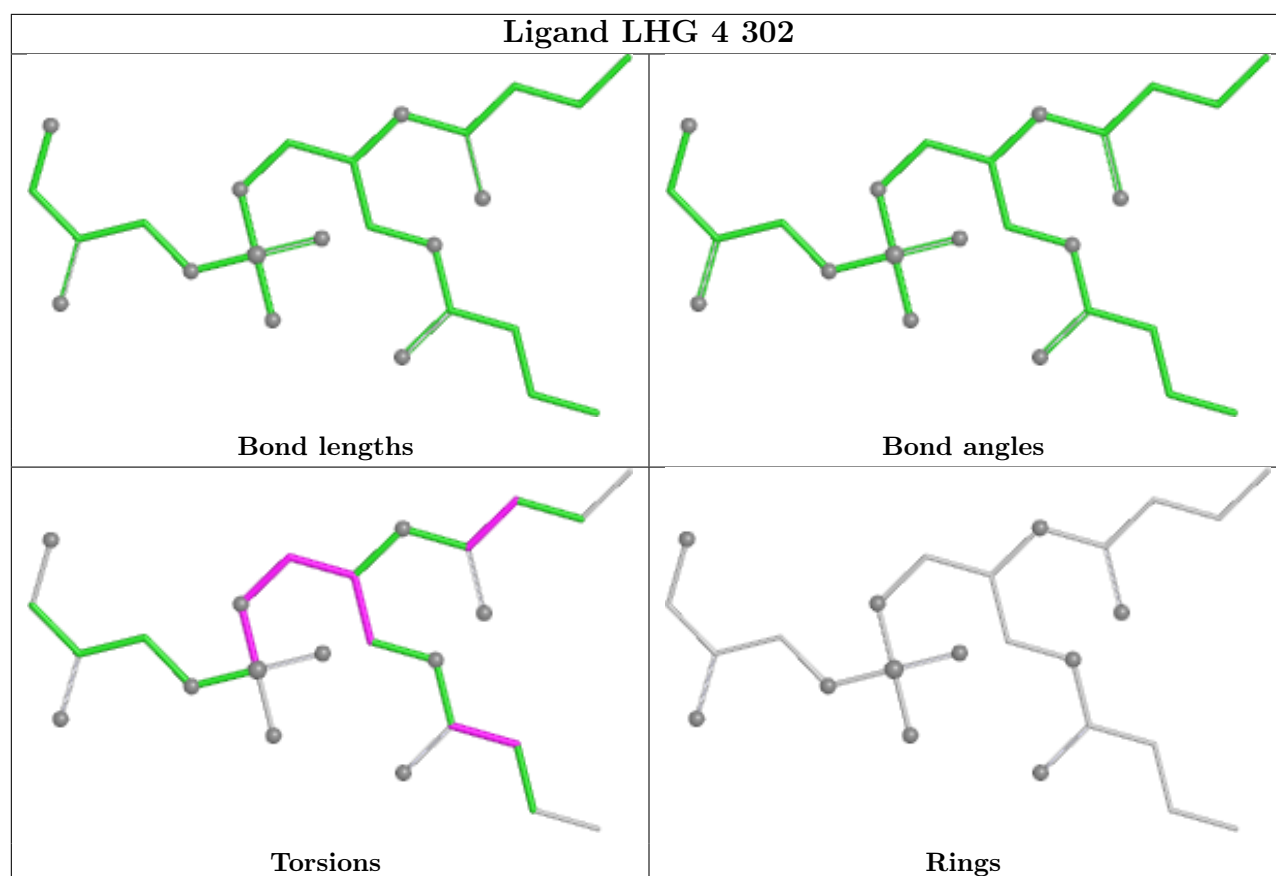
Torsions

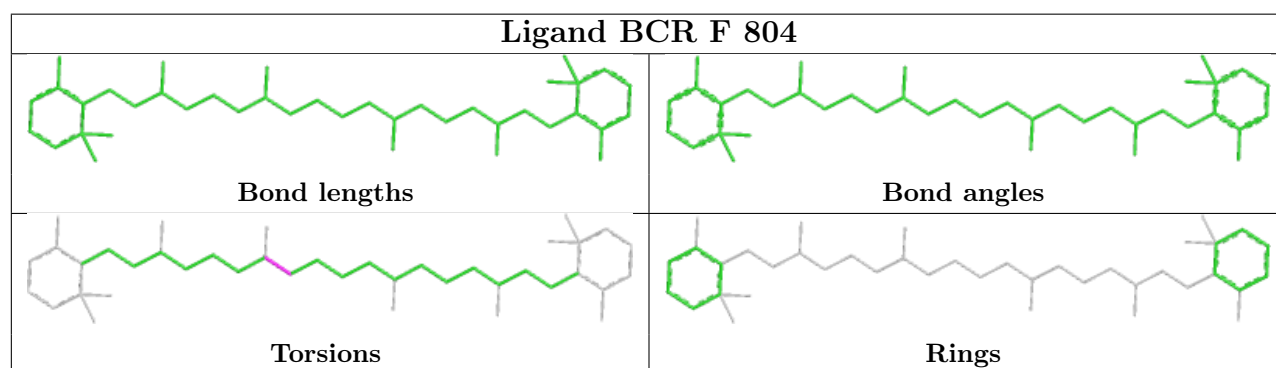
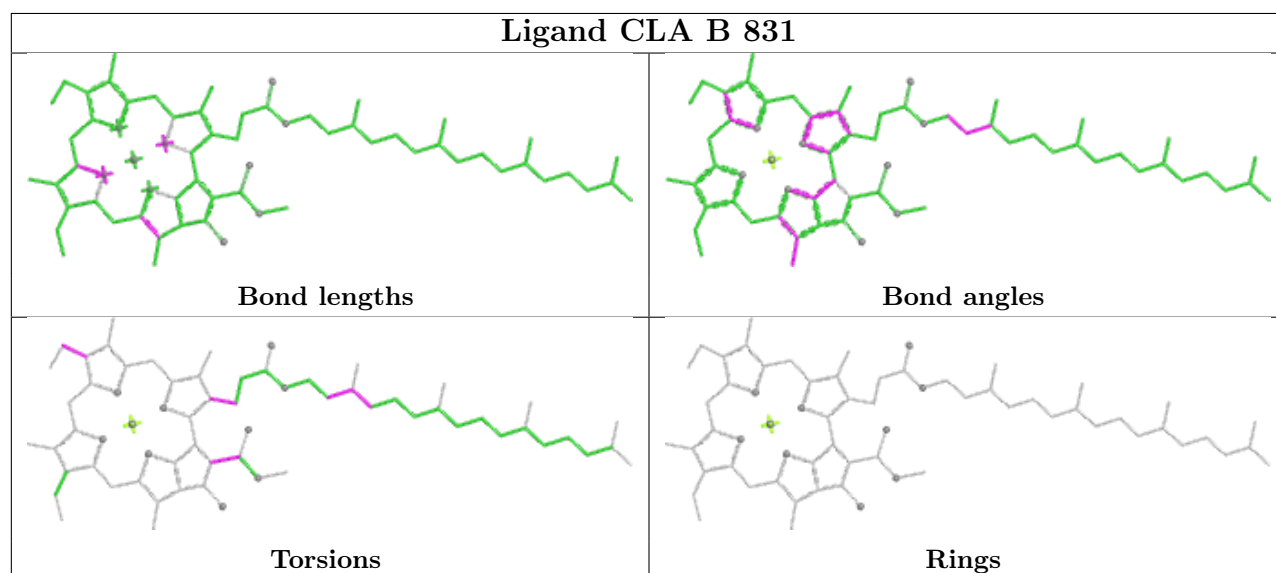
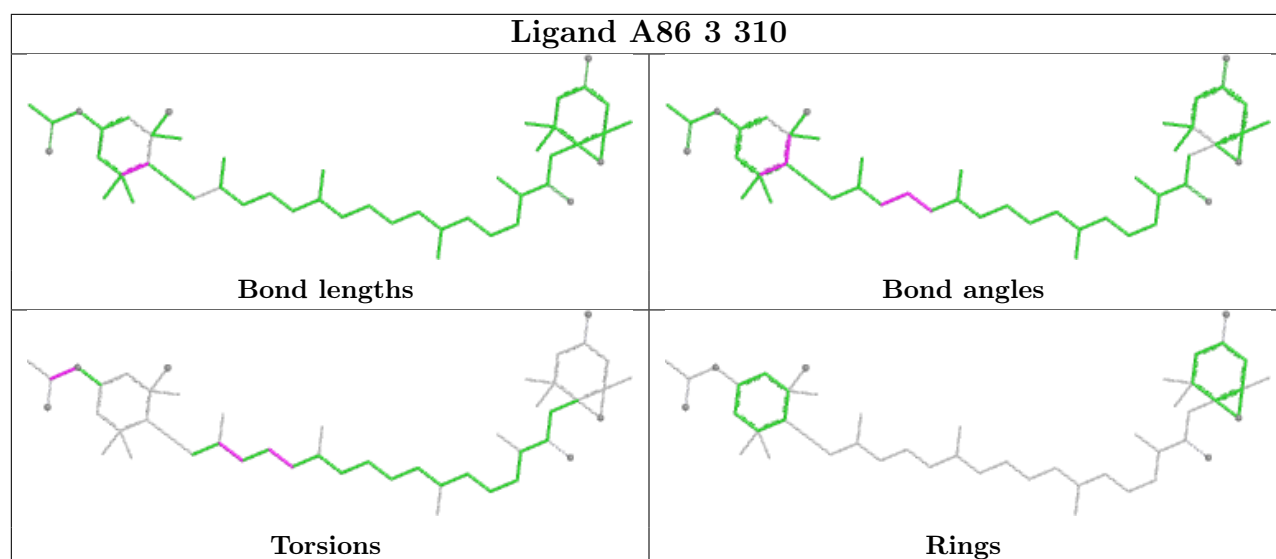


Rings

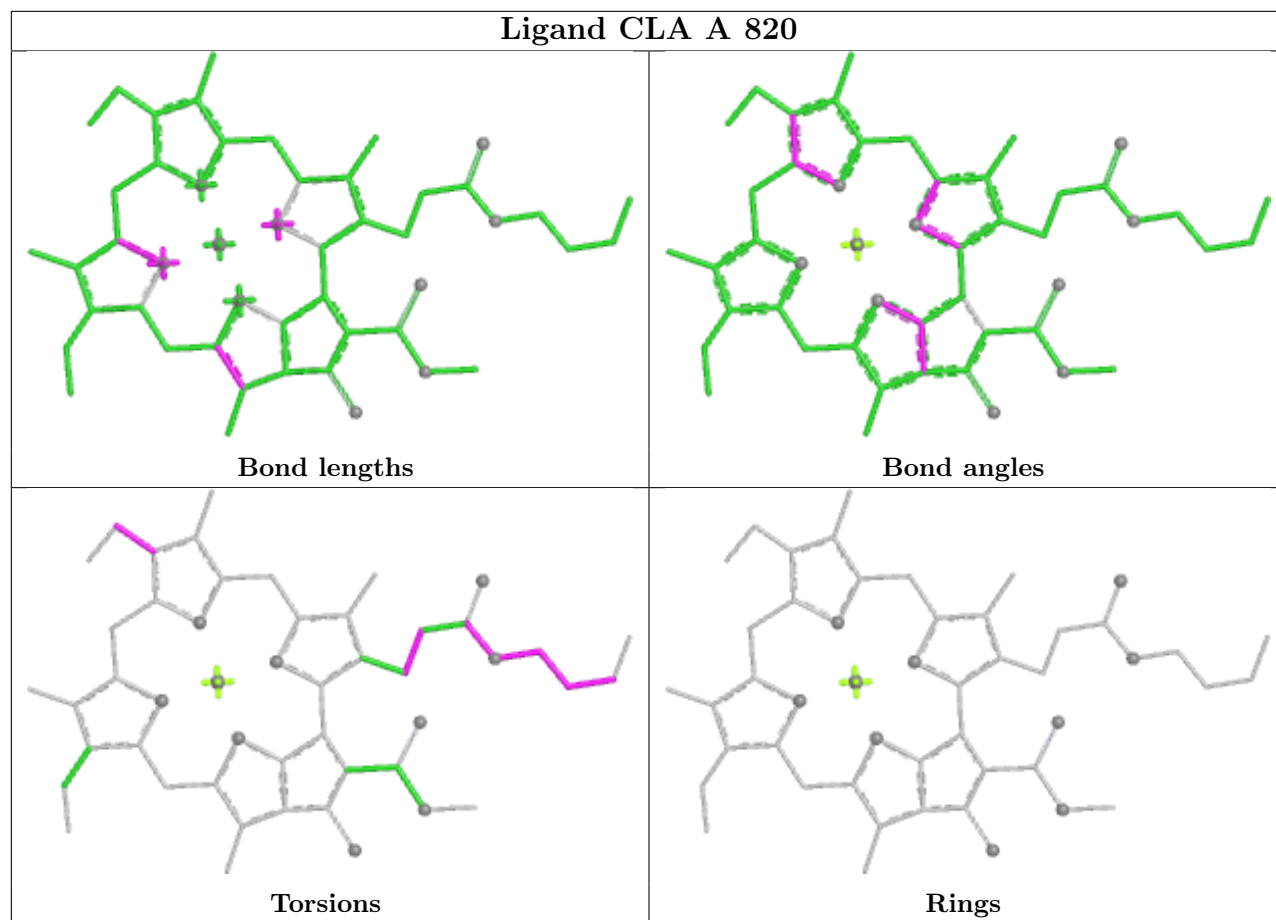


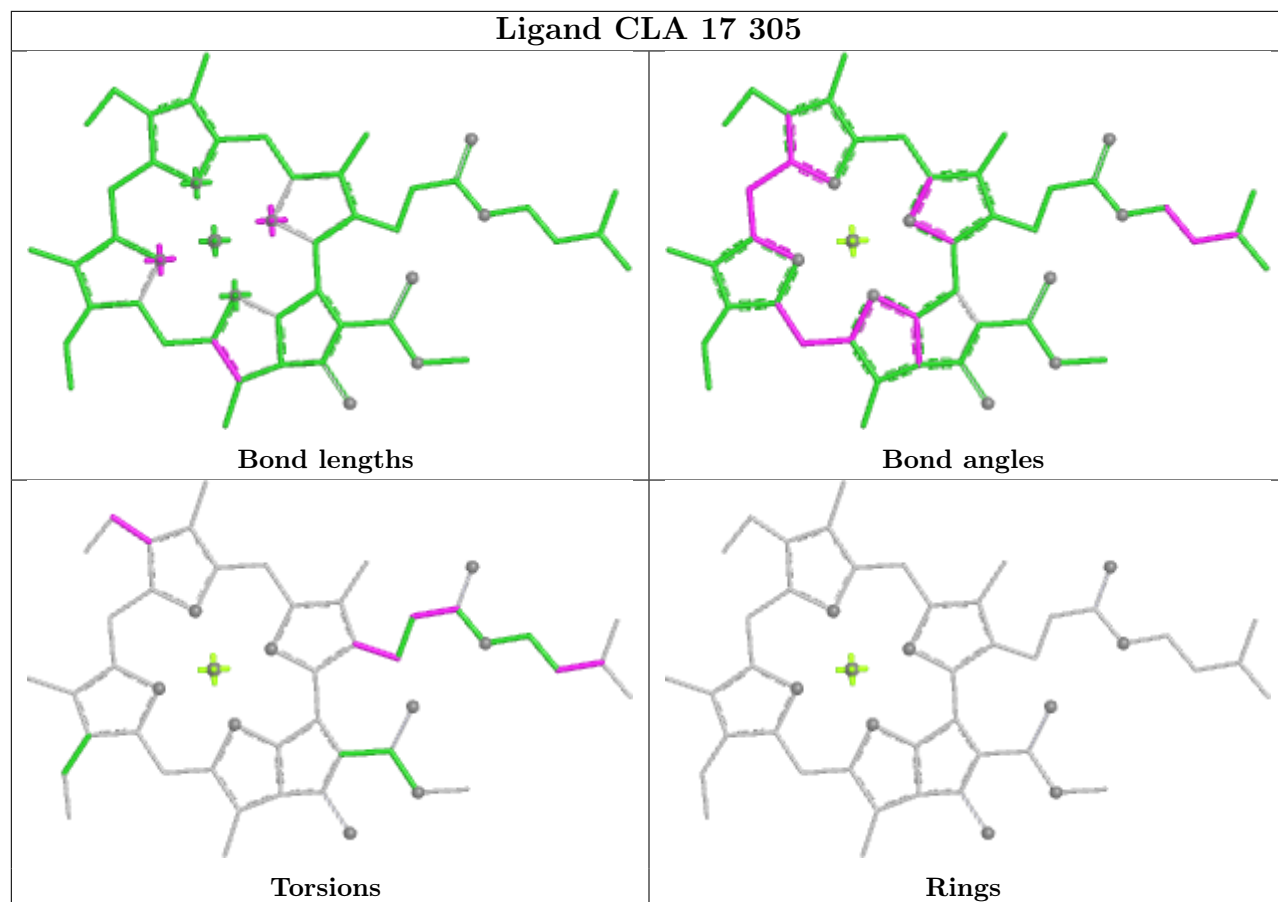


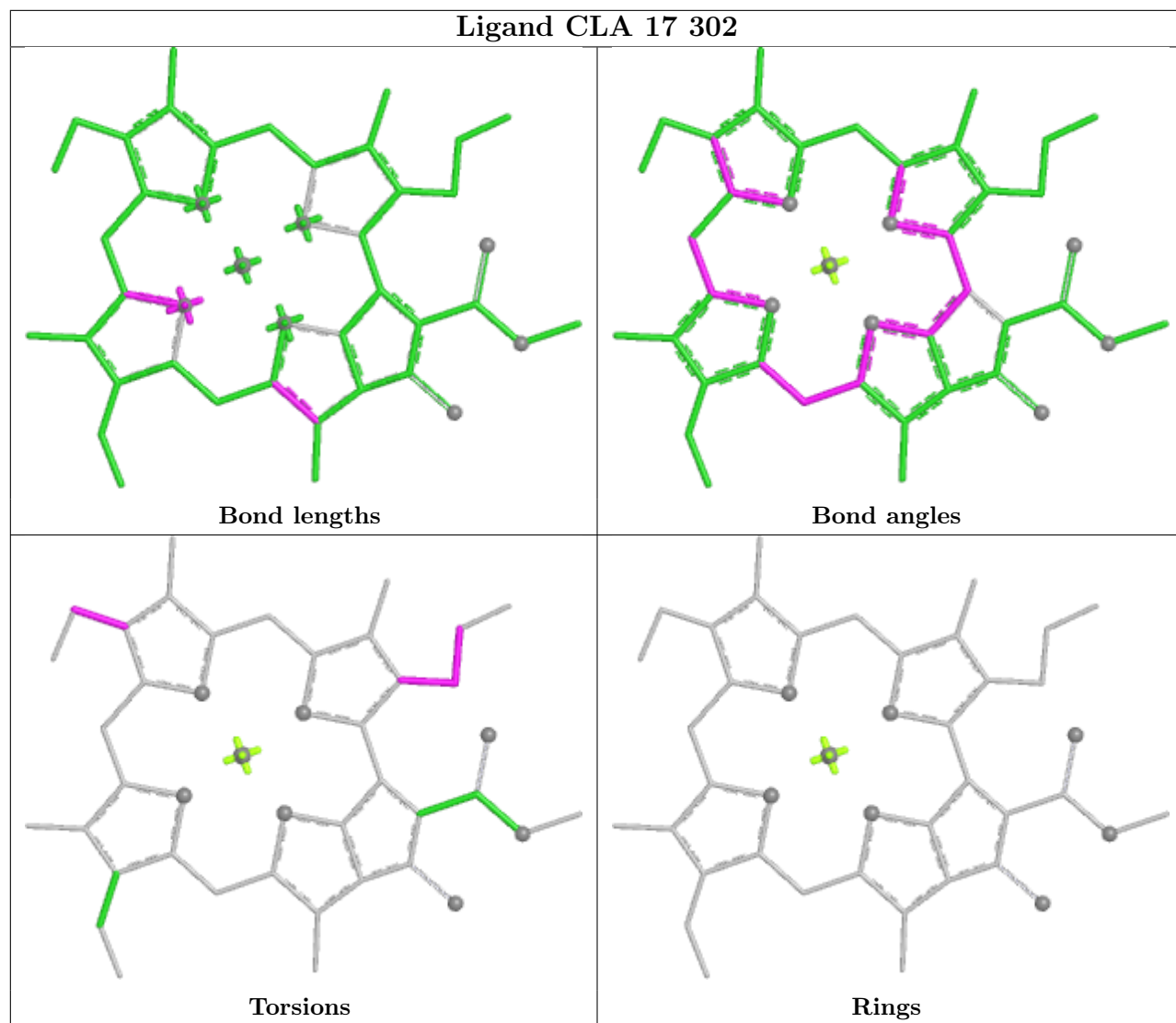


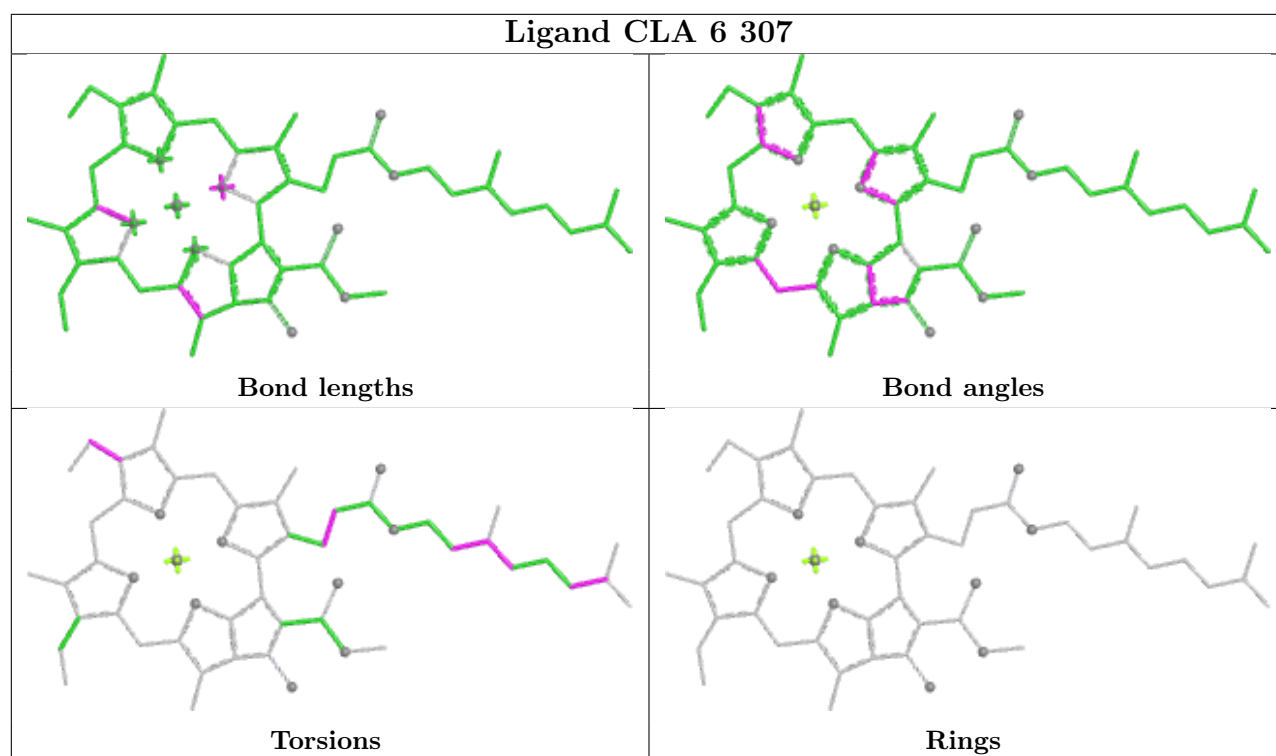


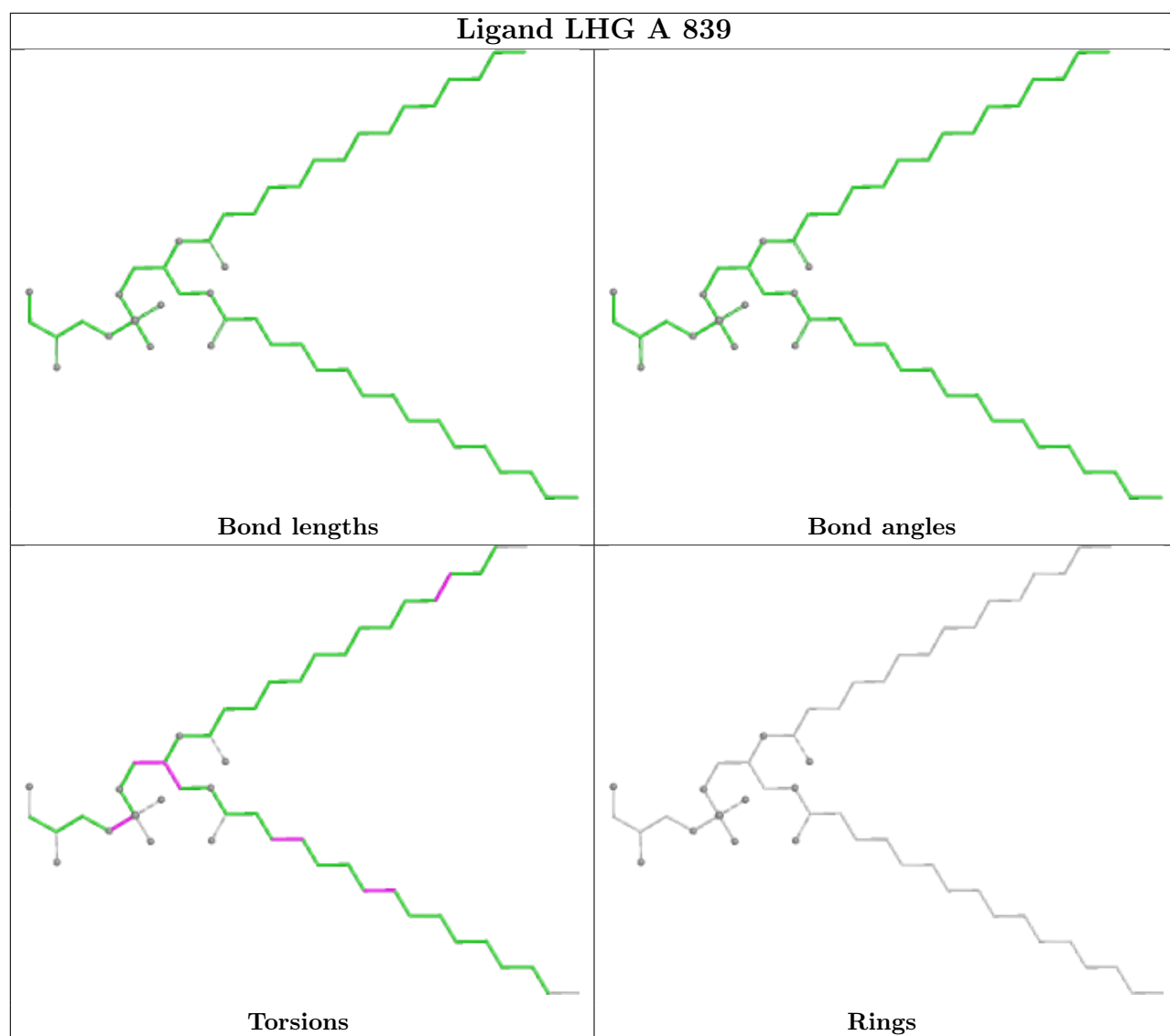
Ligand CLA A 820



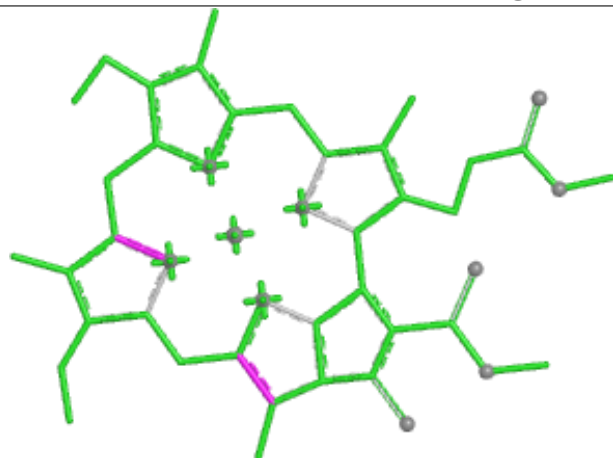




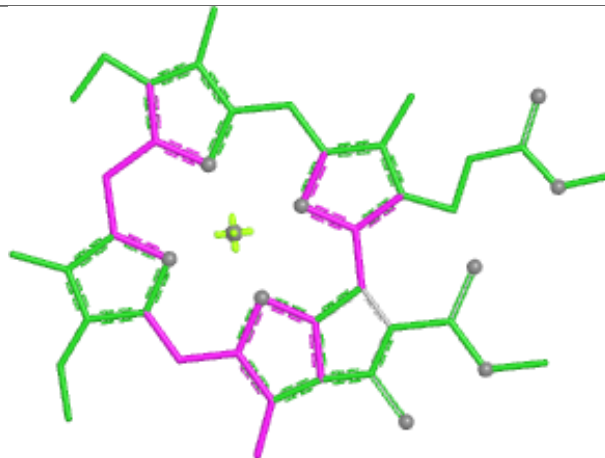




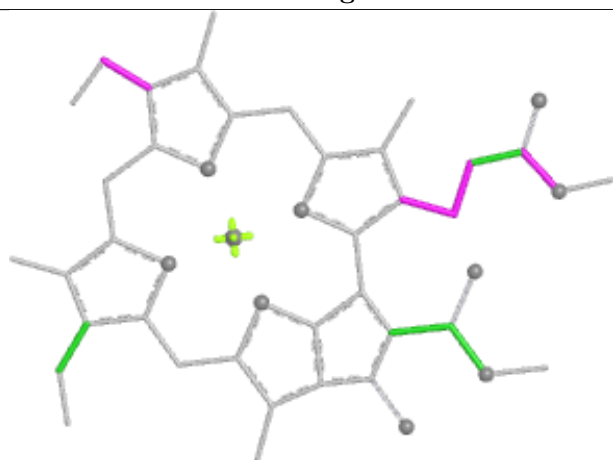
Ligand CLA 17 309



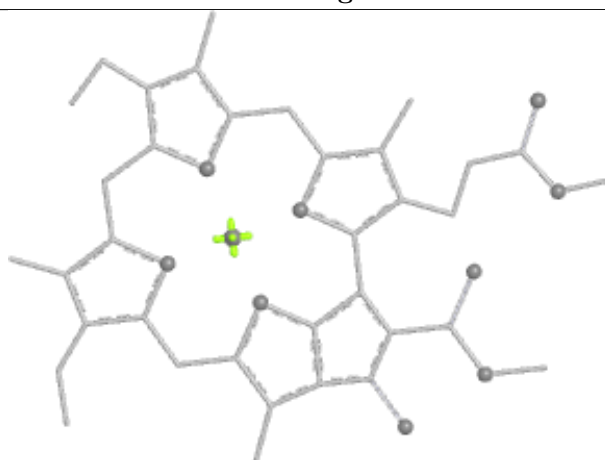
Bond lengths



Bond angles

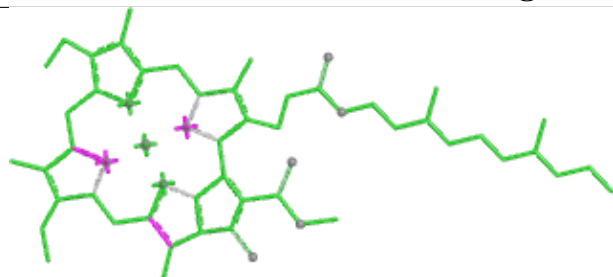


Torsions

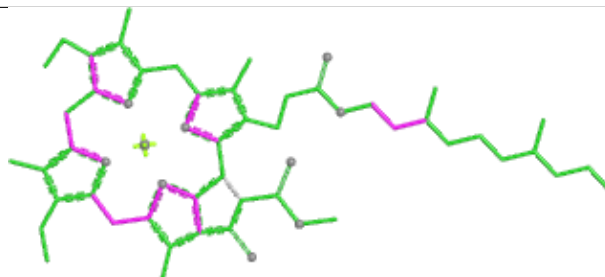


Rings

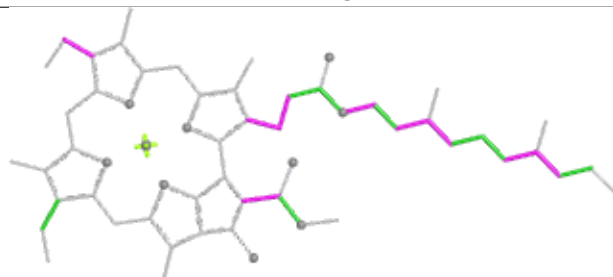
Ligand CLA 8 304



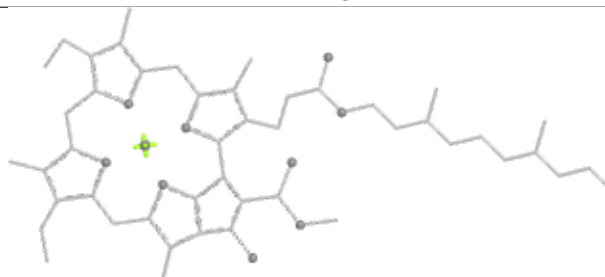
Bond lengths



Bond angles

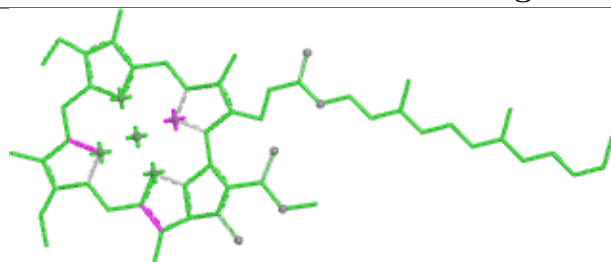


Torsions

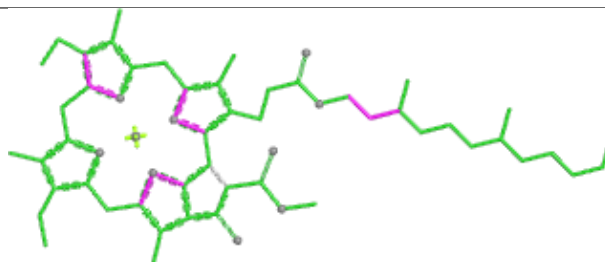


Rings

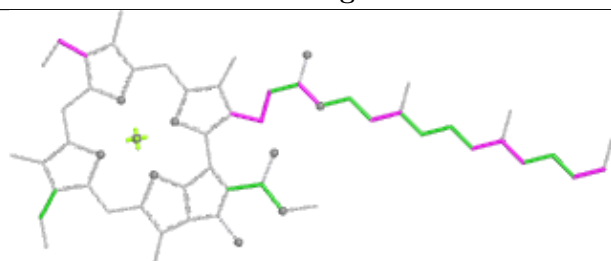
Ligand CLA B 815



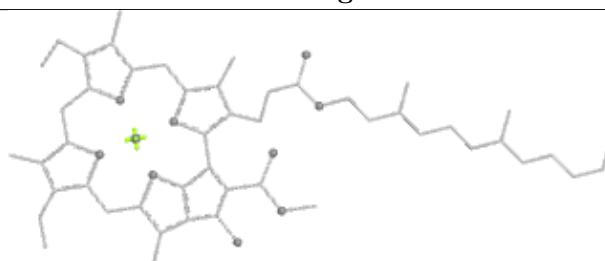
Bond lengths



Bond angles

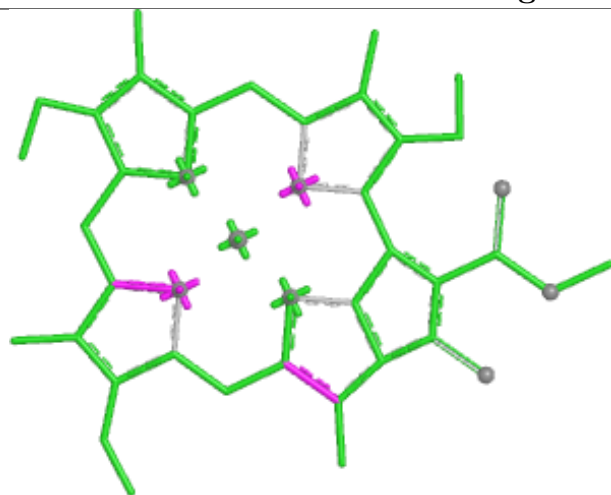


Torsions

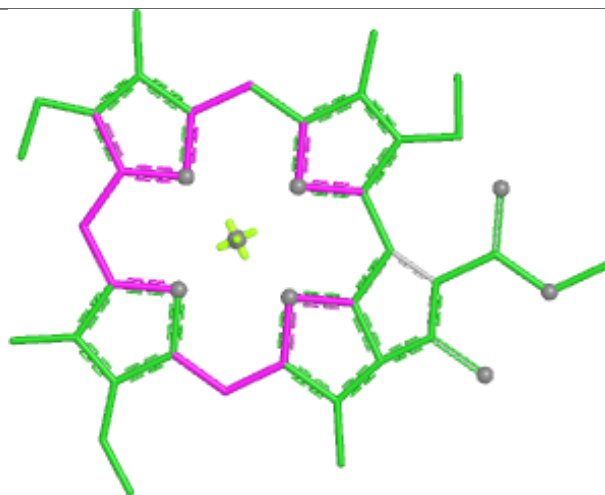


Rings

Ligand CLA a 204



Bond lengths



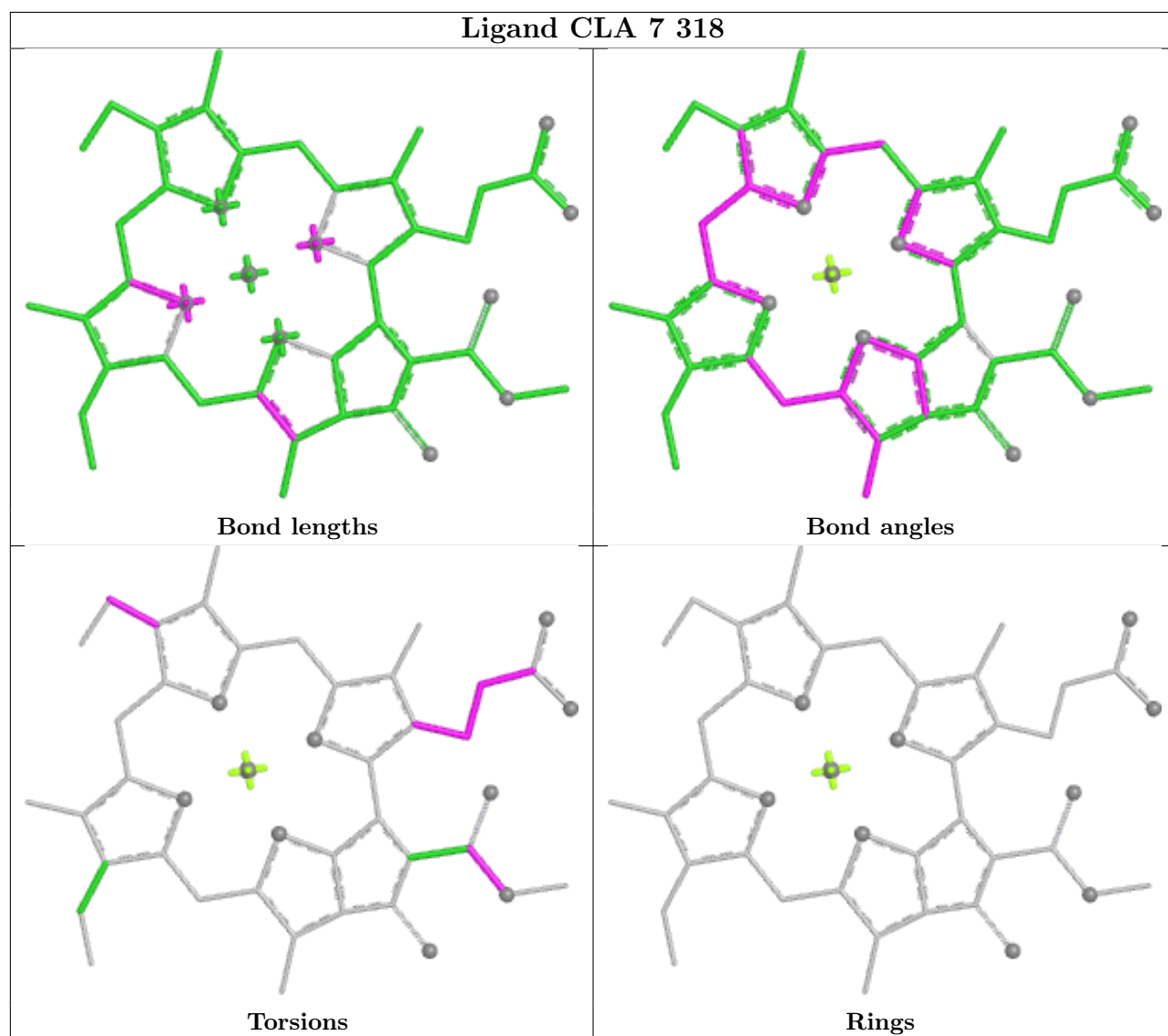
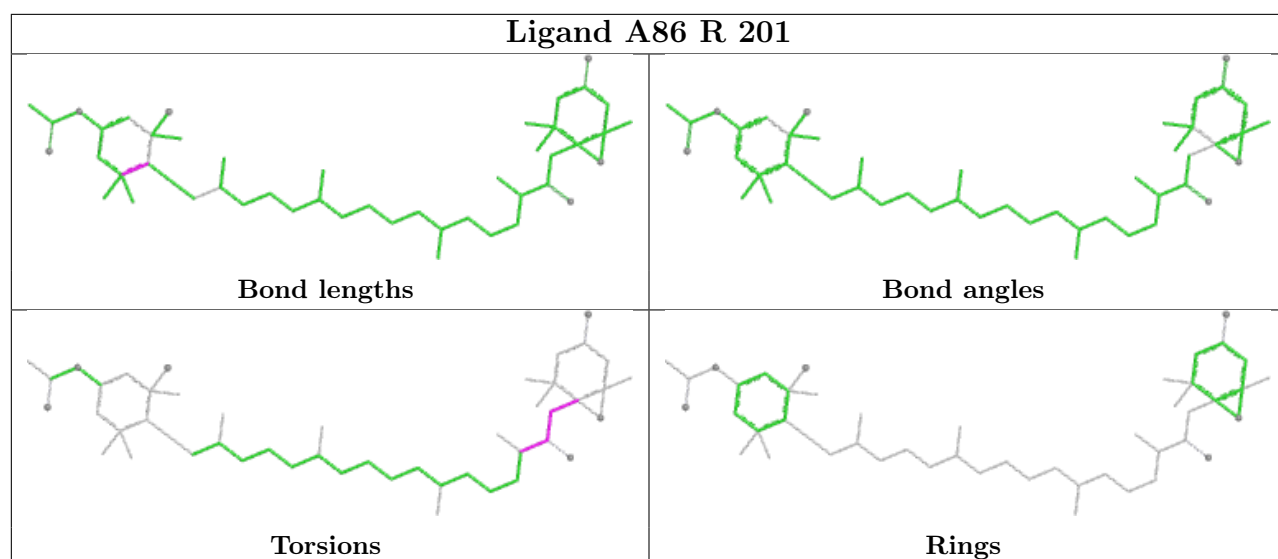
Bond angles

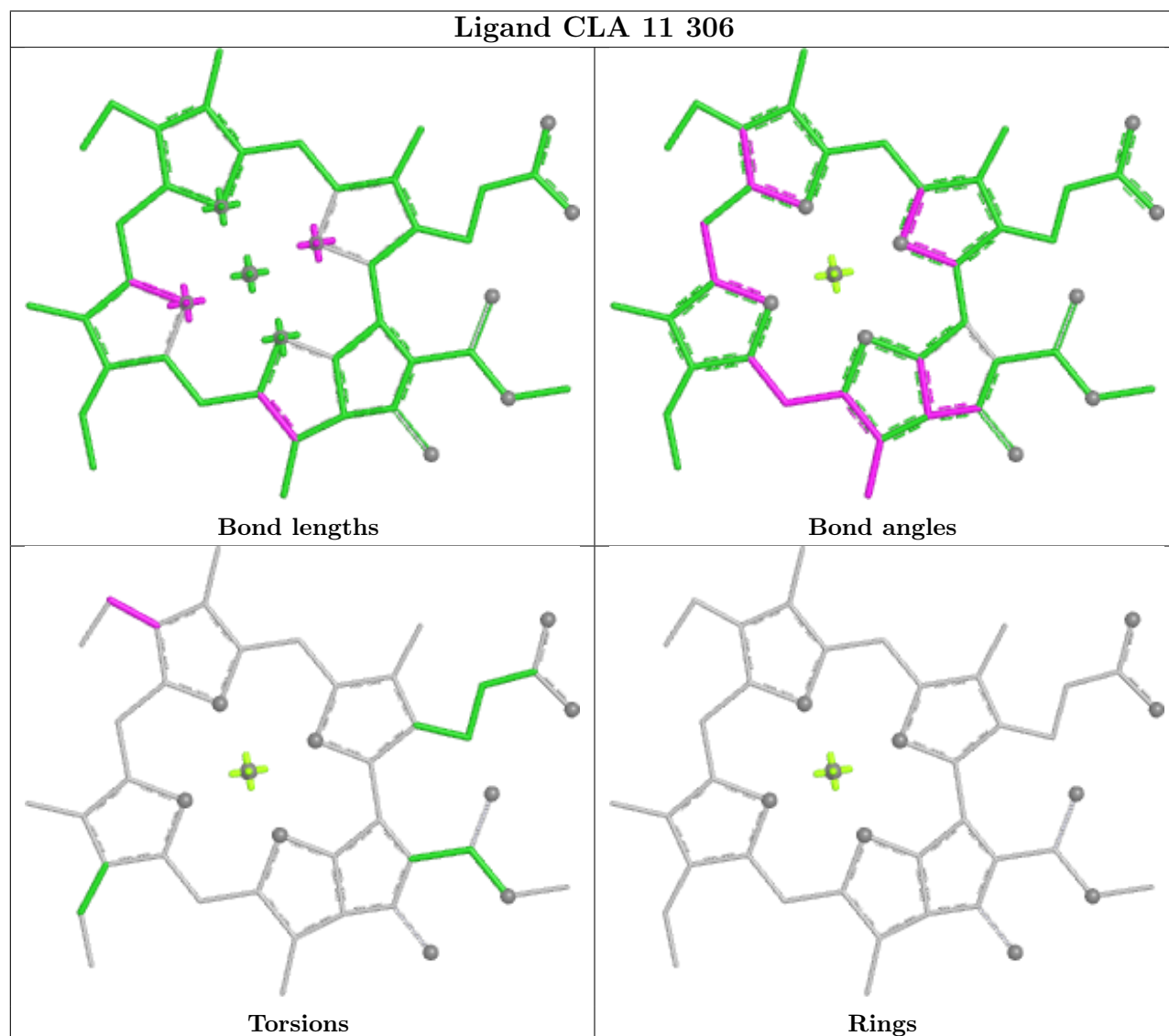
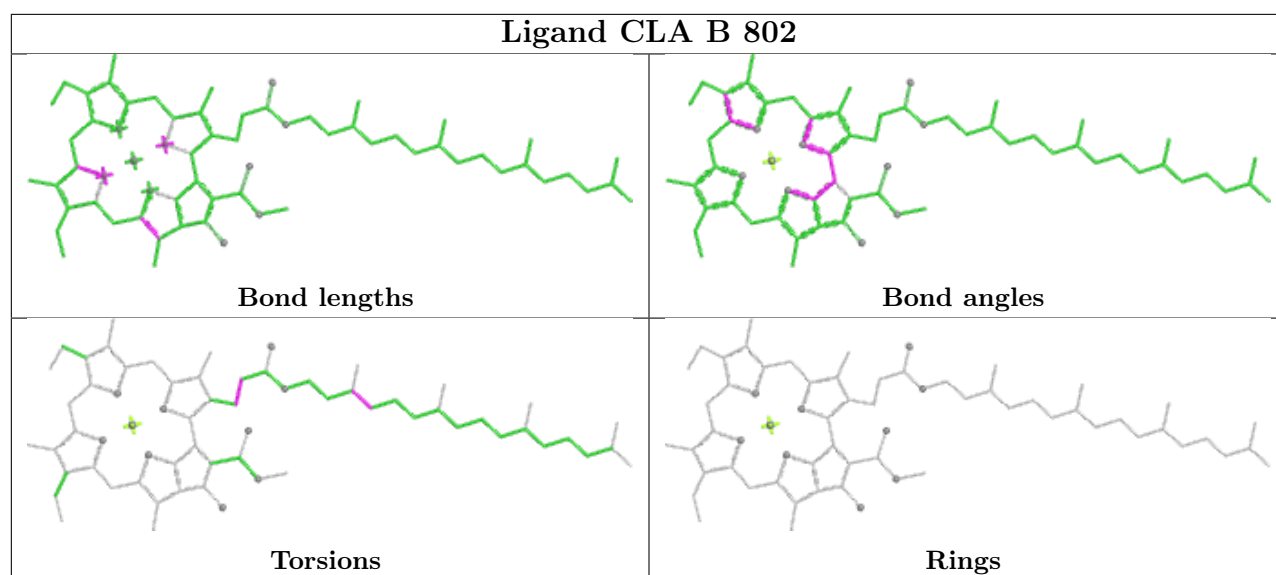


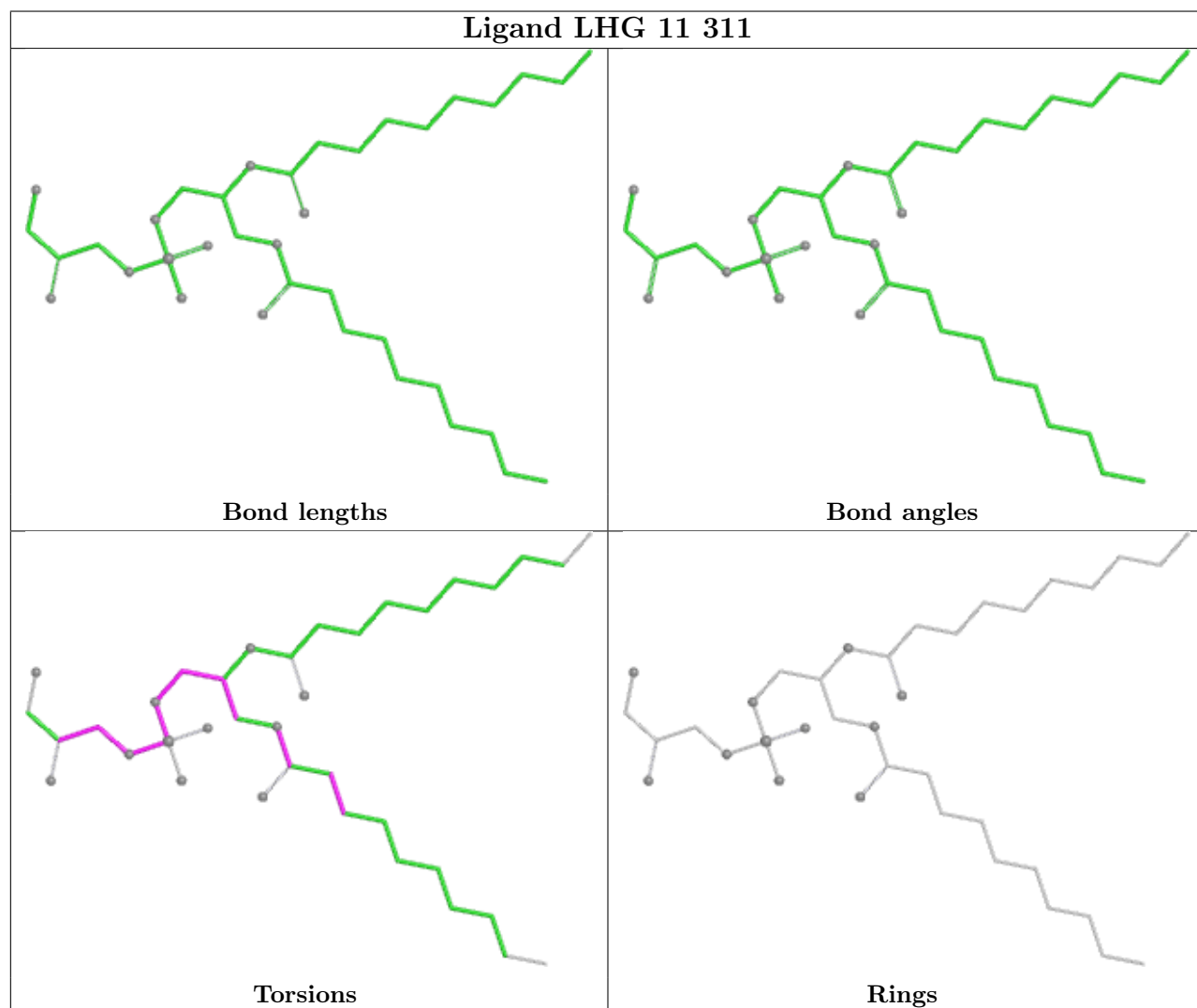
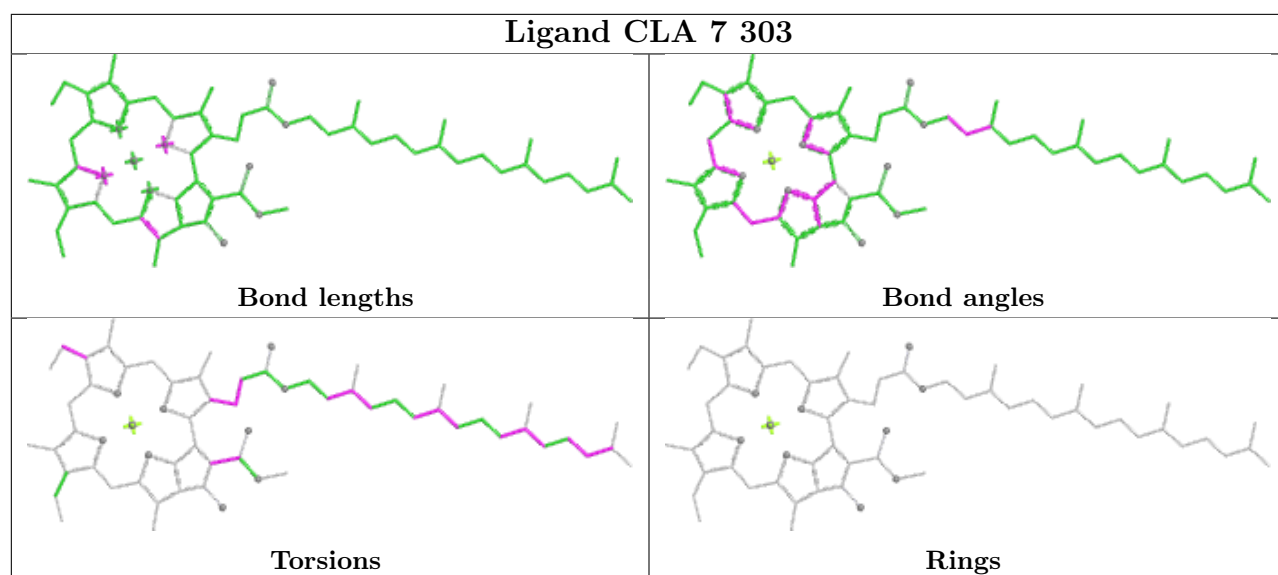
Torsions

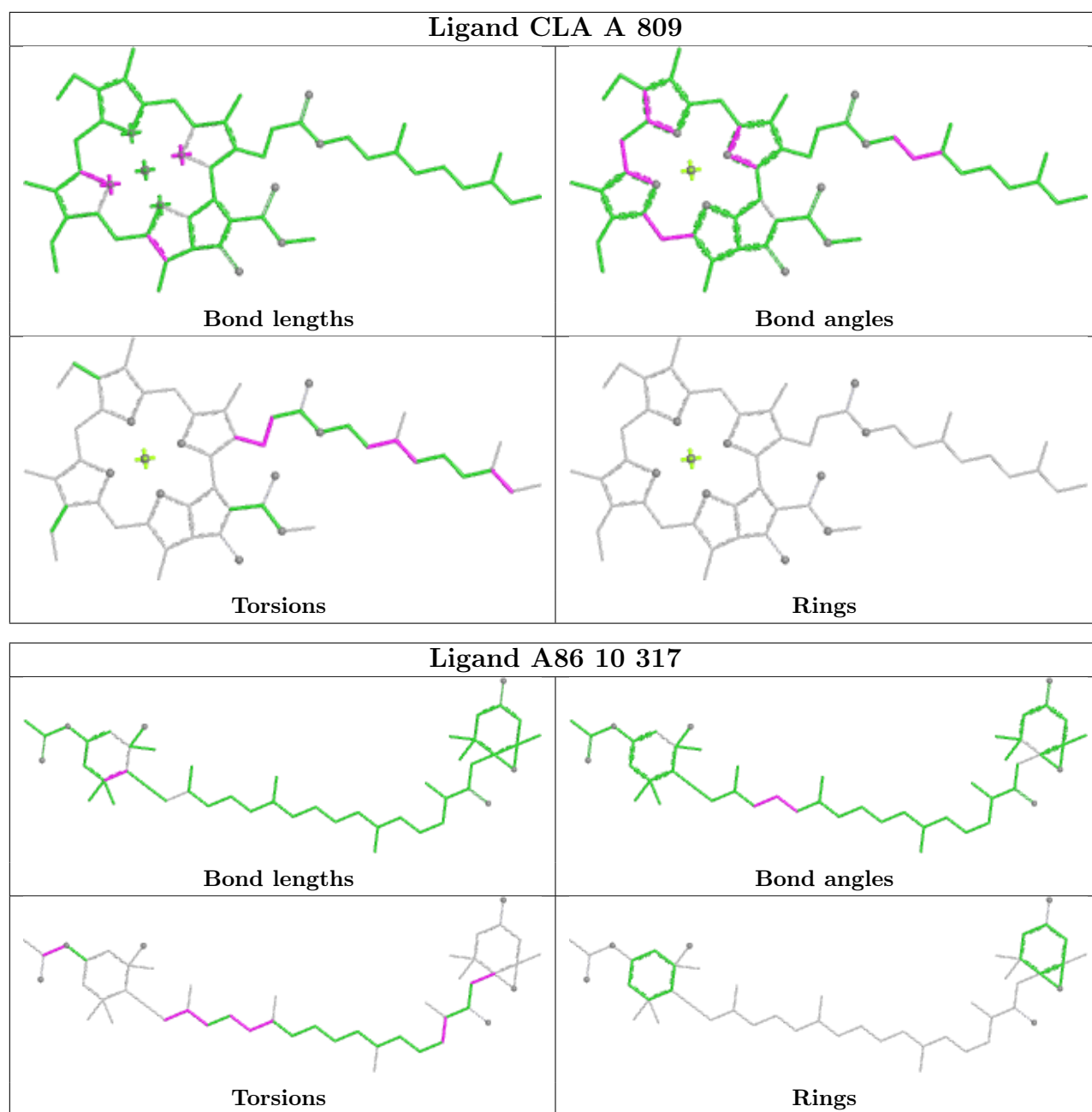


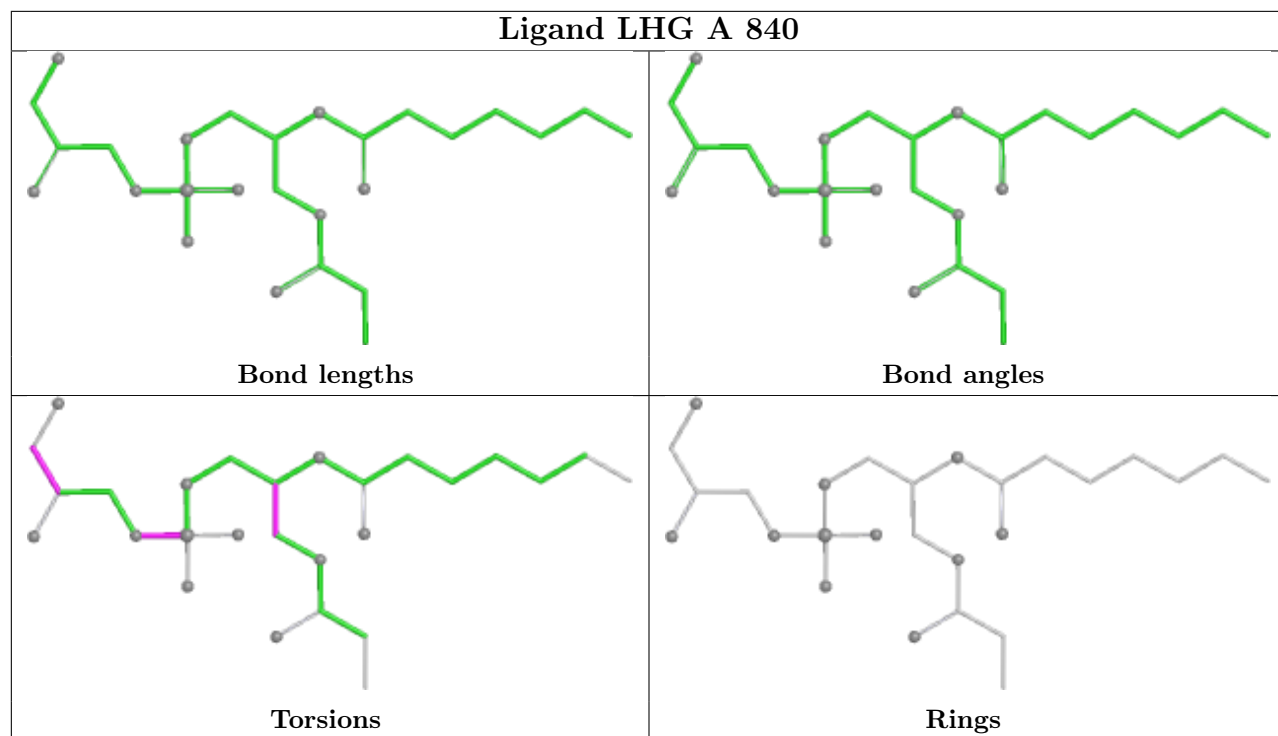
Rings

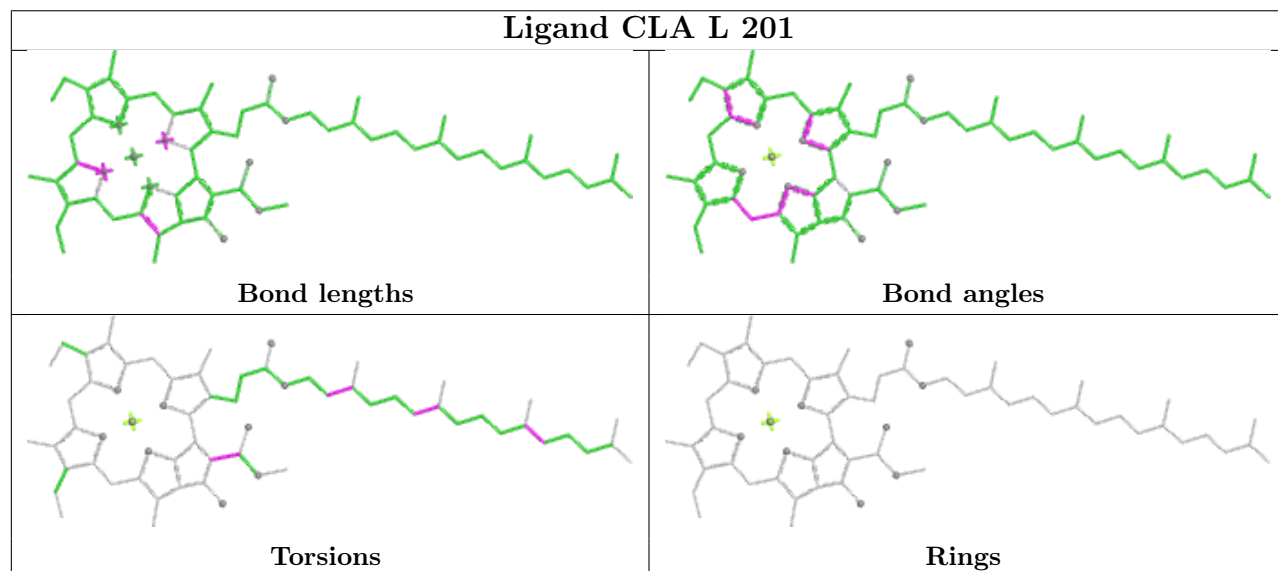
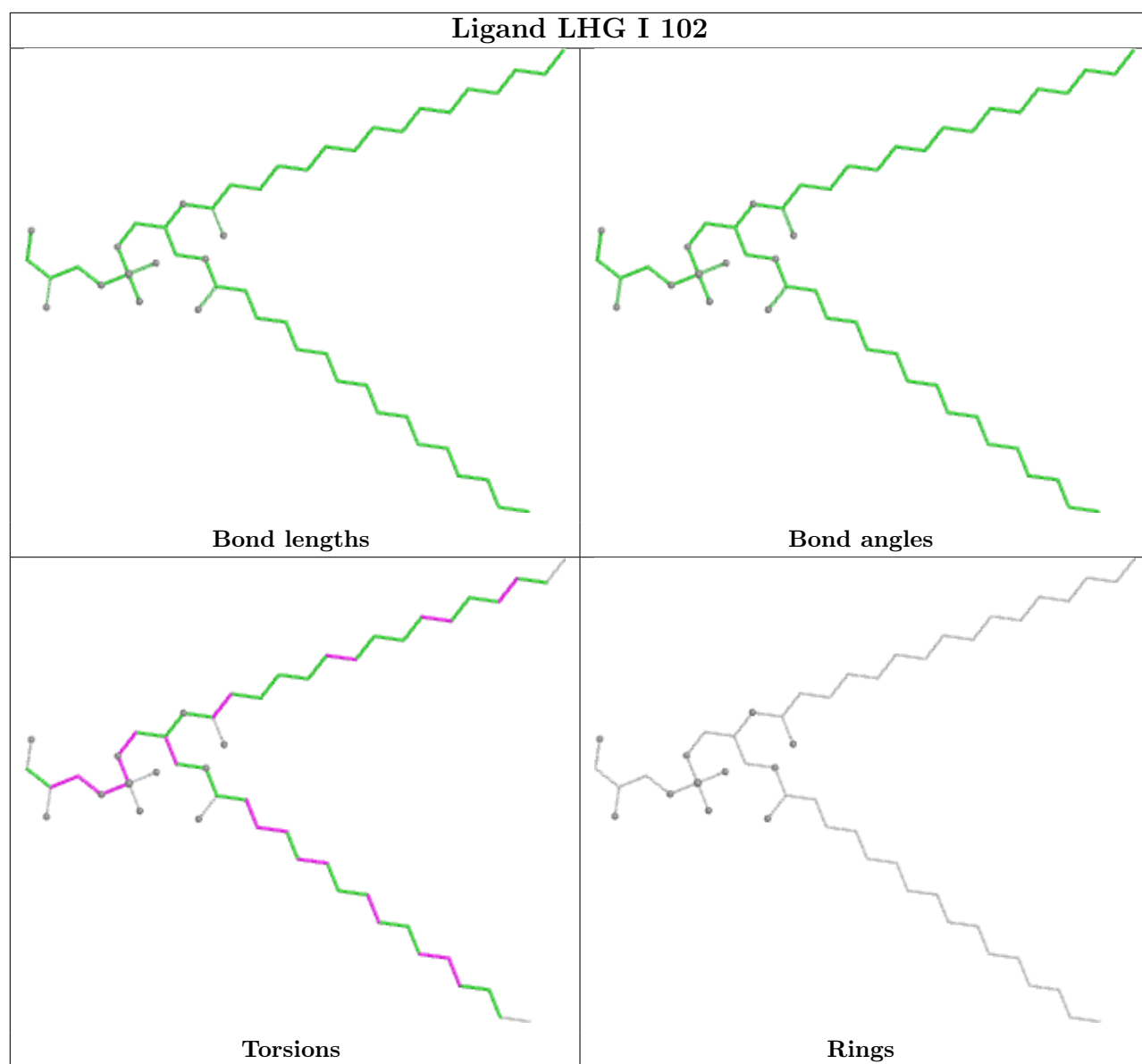




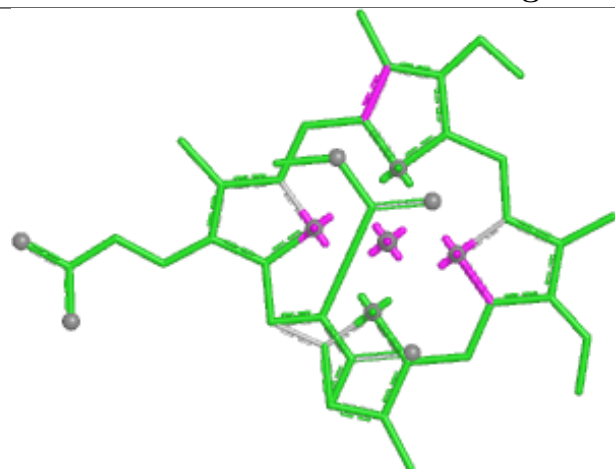




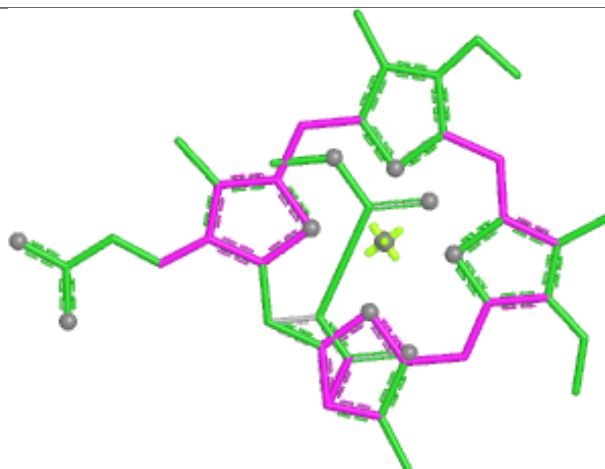




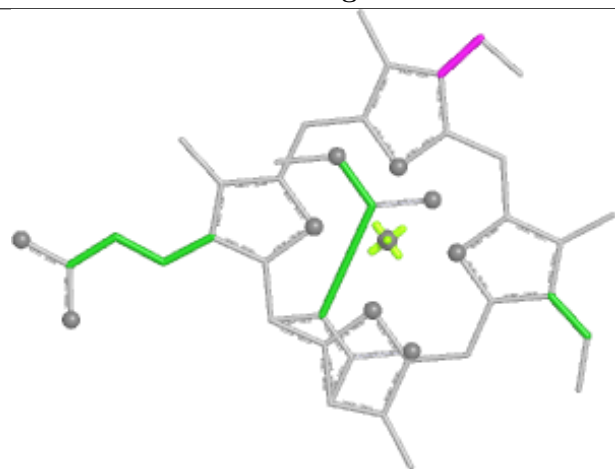
Ligand KC1 8 307



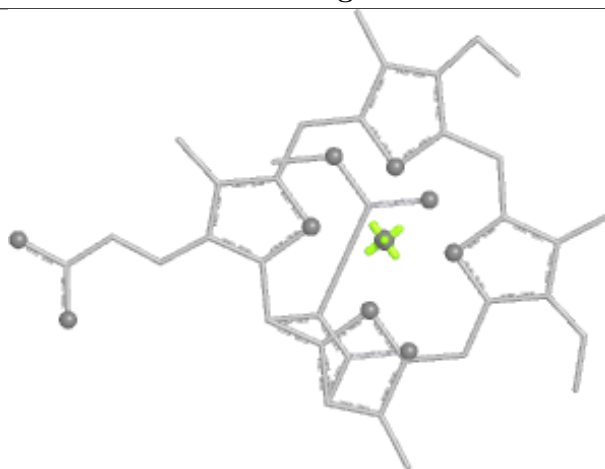
Bond lengths



Bond angles

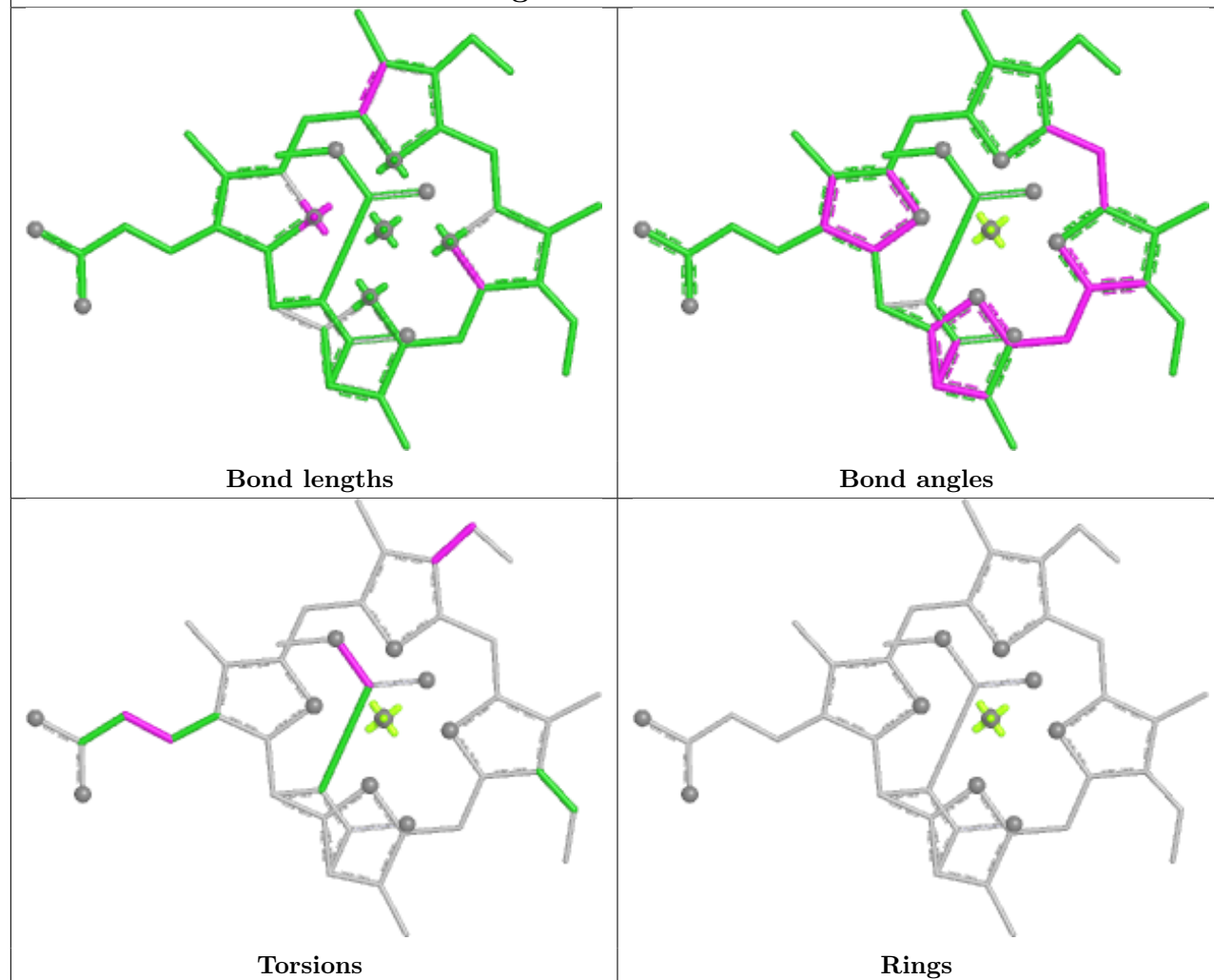


Torsions

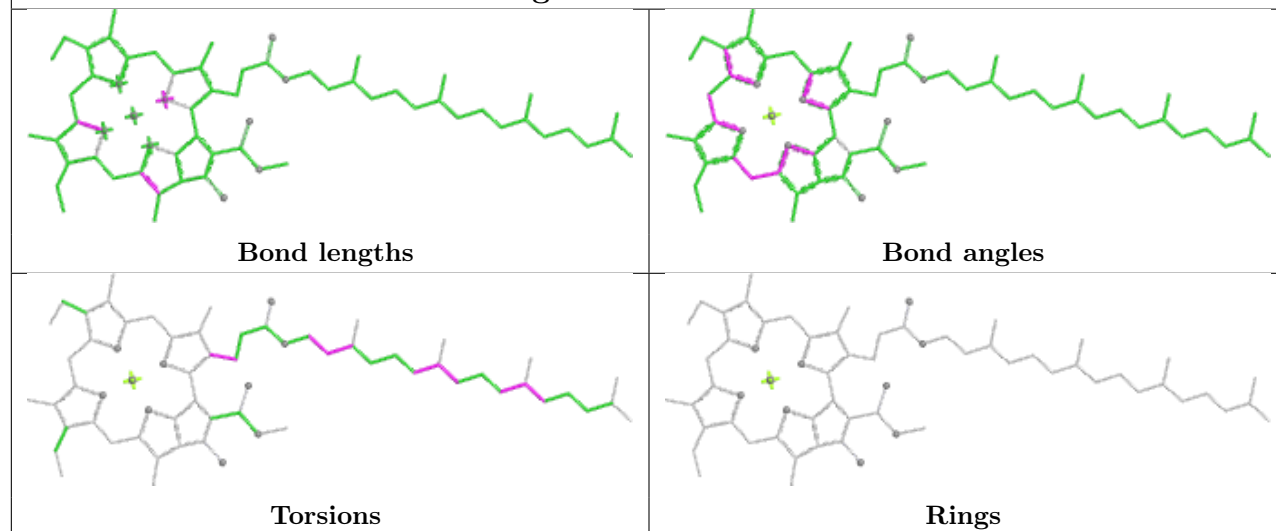


Rings

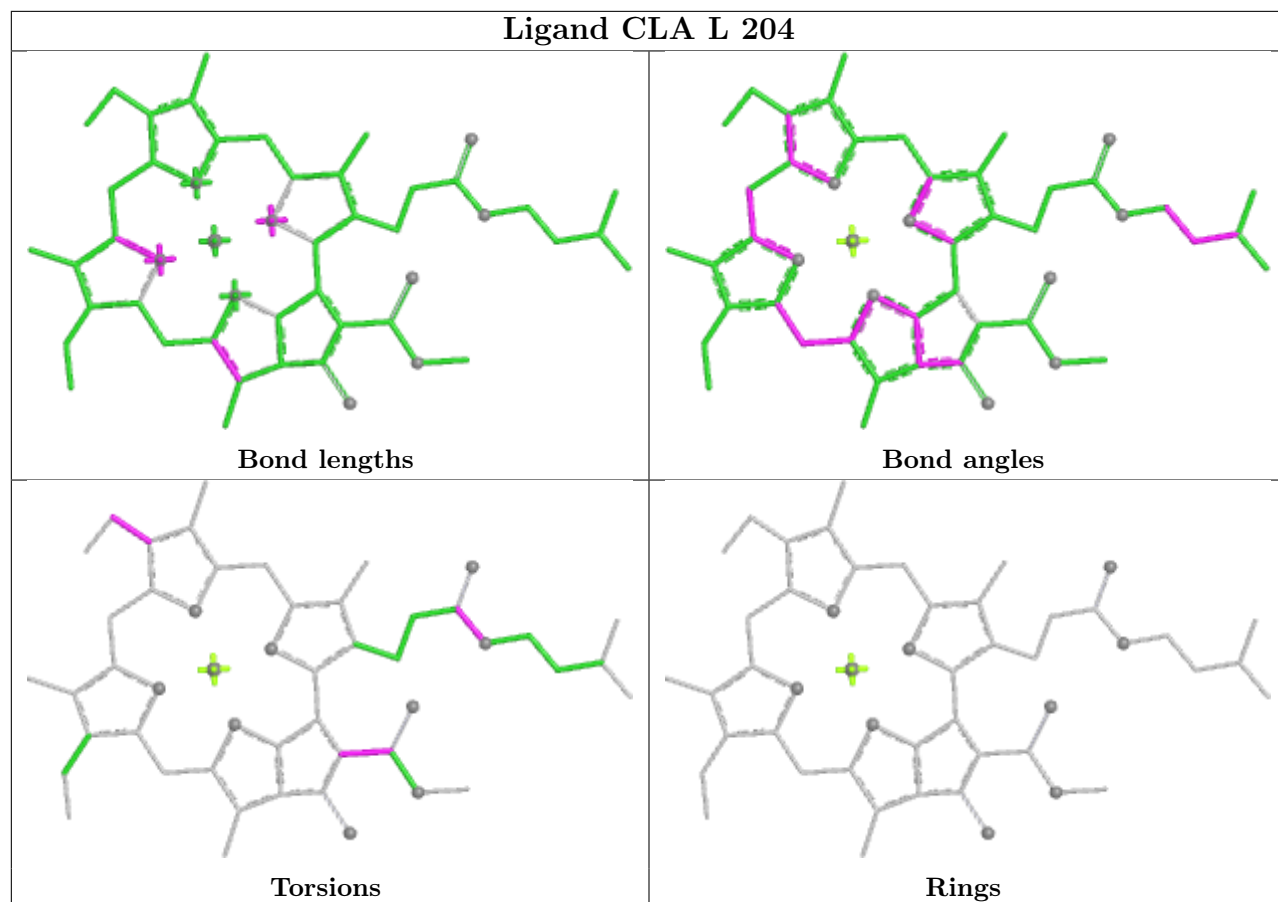
Ligand KC1 4 311



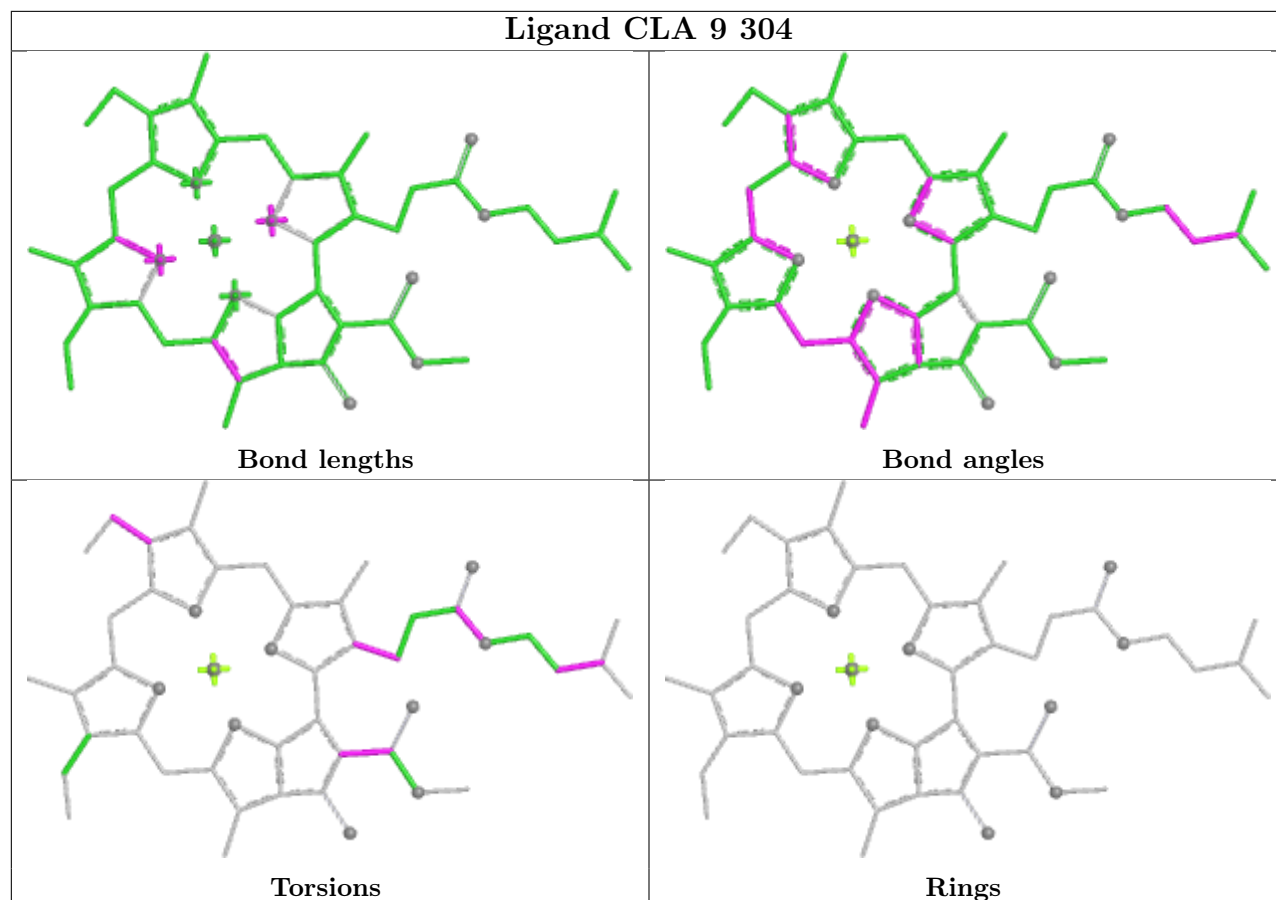
Ligand CLA B 804



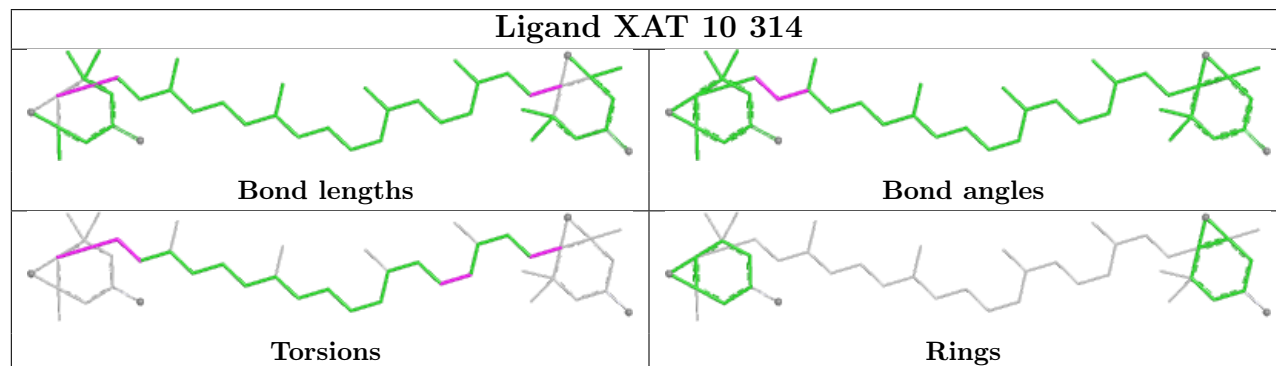
Ligand CLA L 204

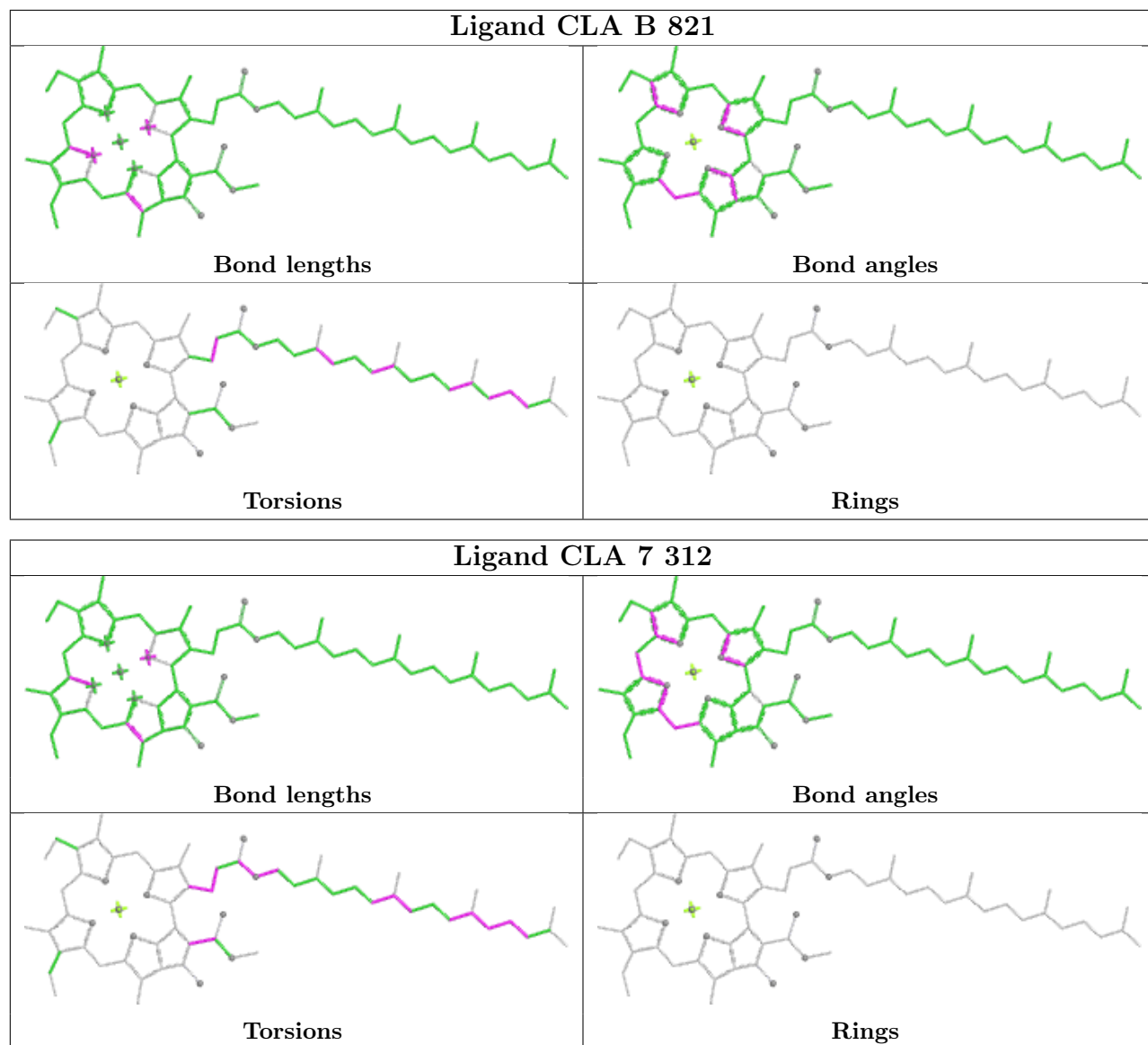


Ligand CLA 9 304

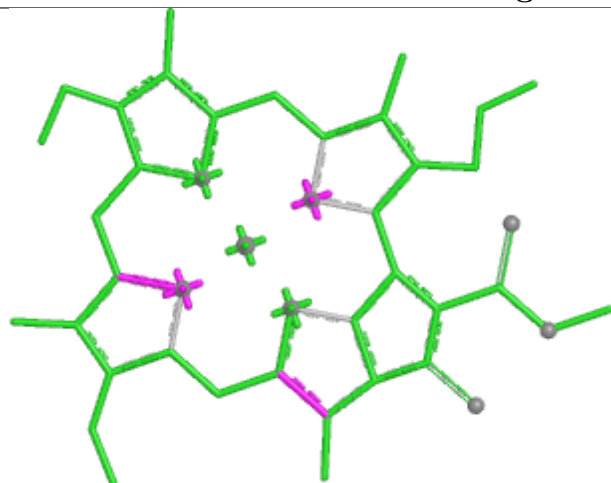


Ligand XAT 10 314

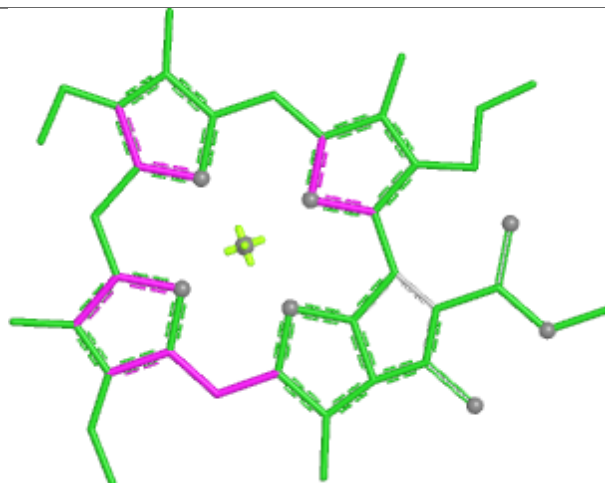




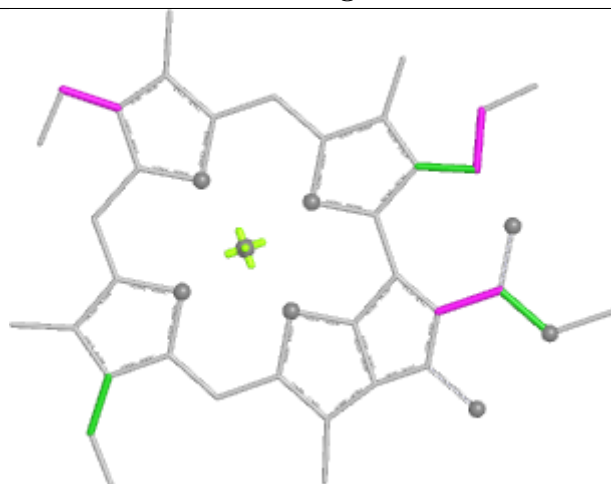
Ligand CLA F 803



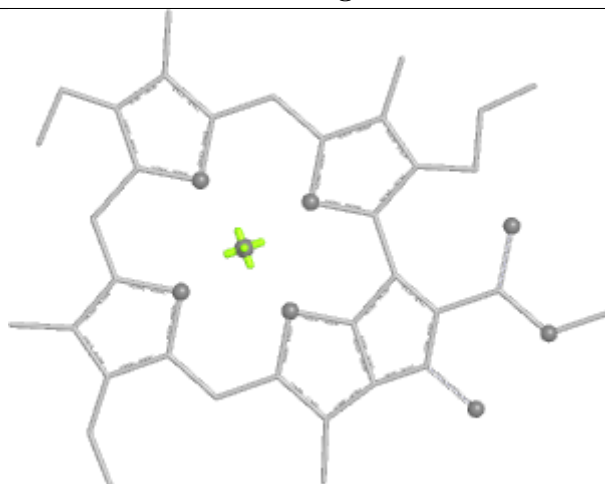
Bond lengths



Bond angles

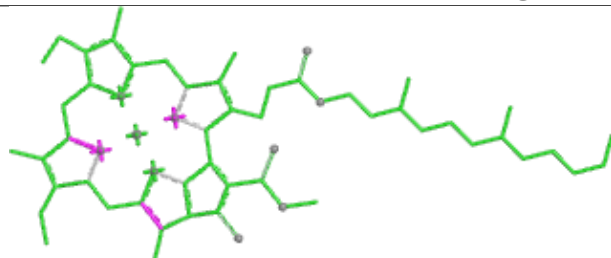


Torsions

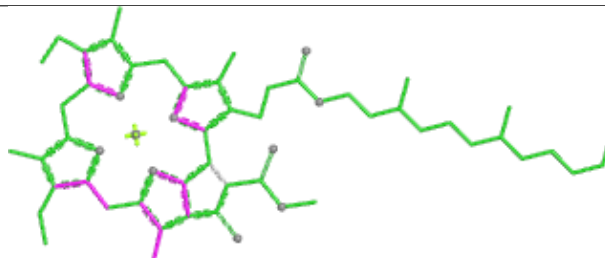


Rings

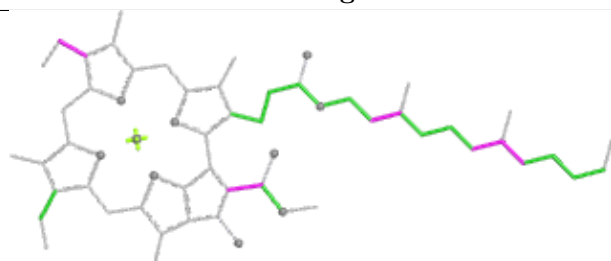
Ligand CLA B 814



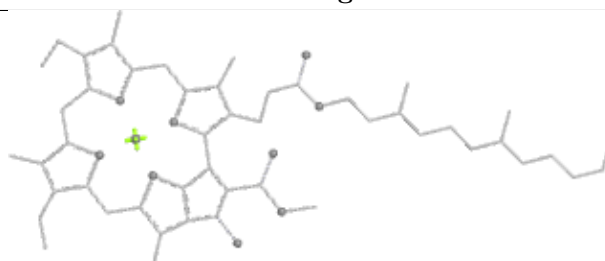
Bond lengths



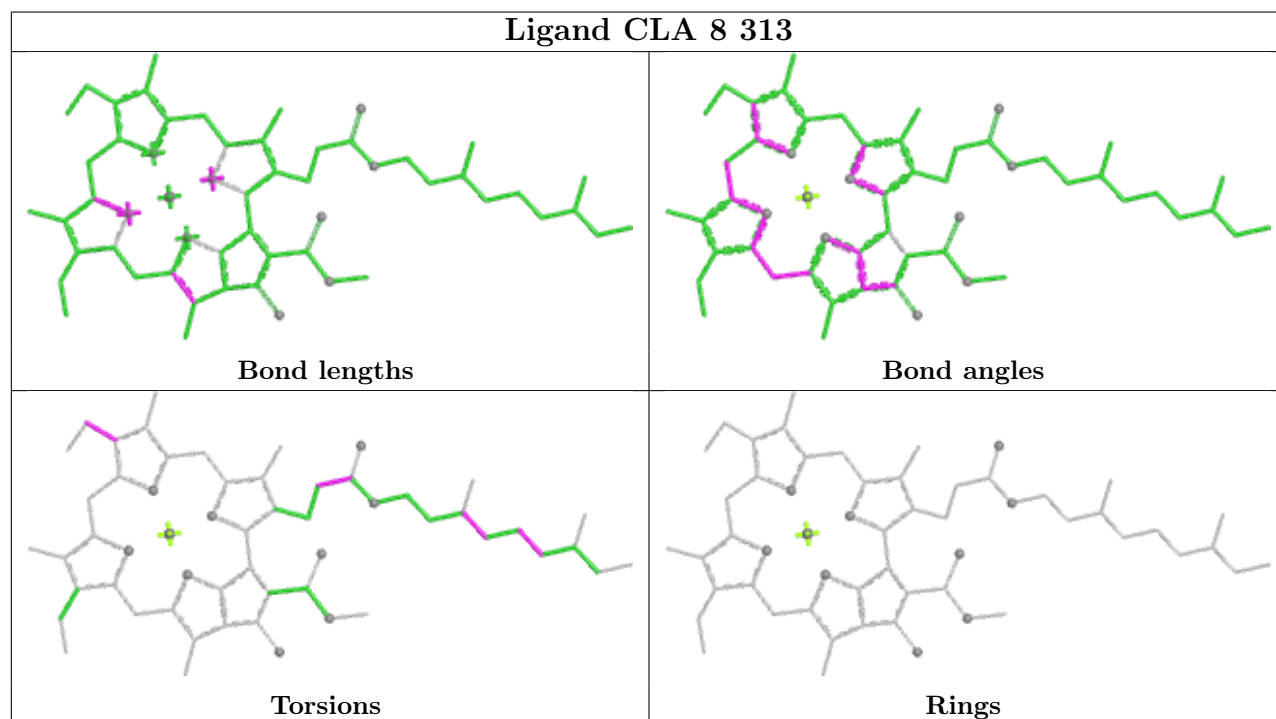
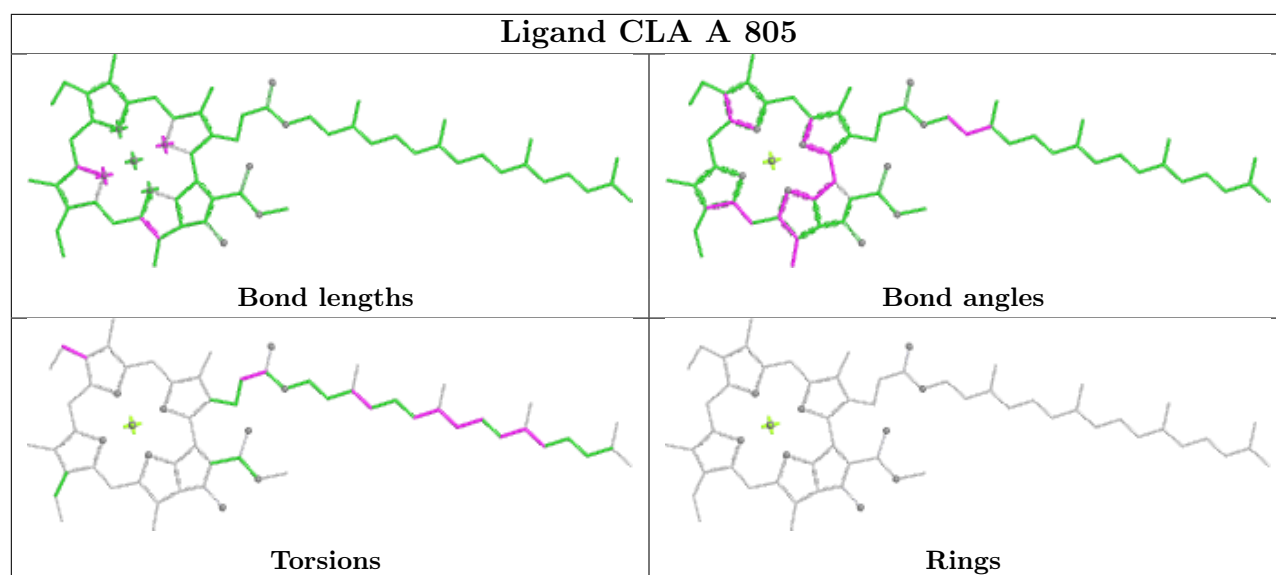
Bond angles



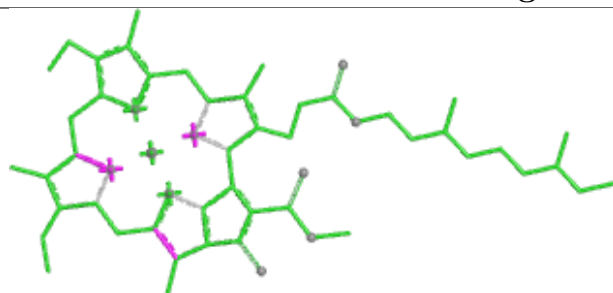
Torsions



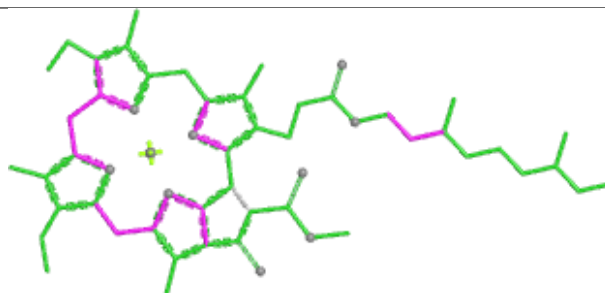
Rings



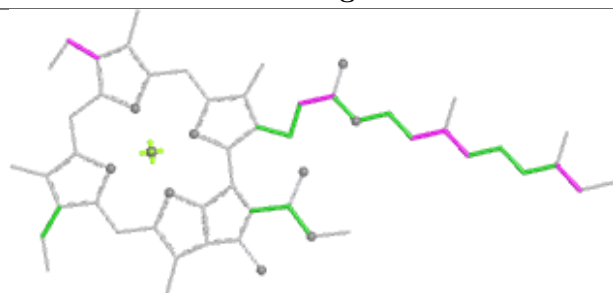
Ligand CLA 8 302



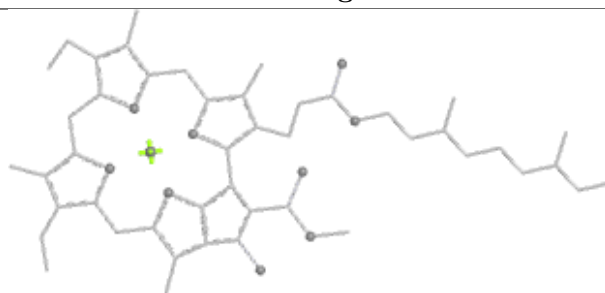
Bond lengths



Bond angles

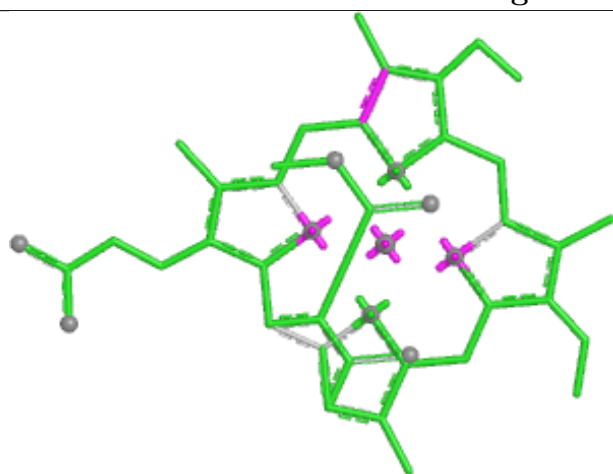


Torsions

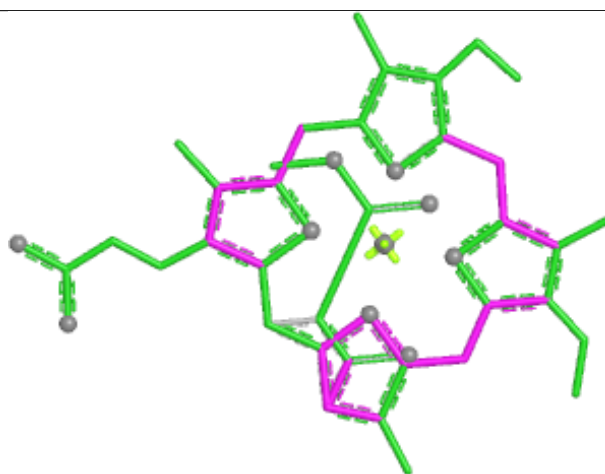


Rings

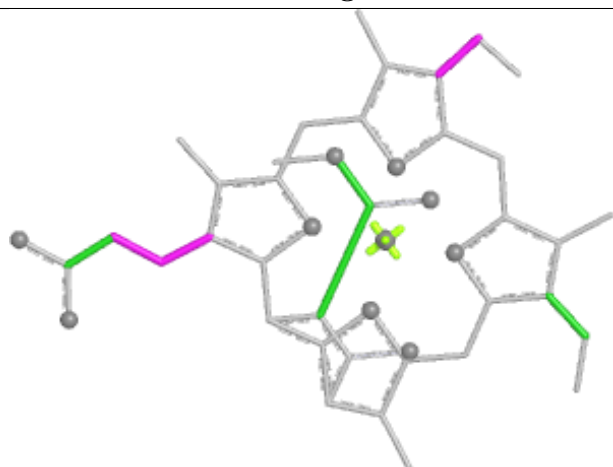
Ligand KC1 10 311



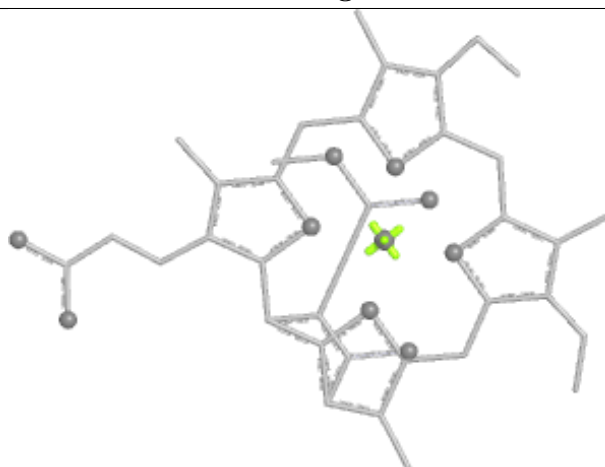
Bond lengths



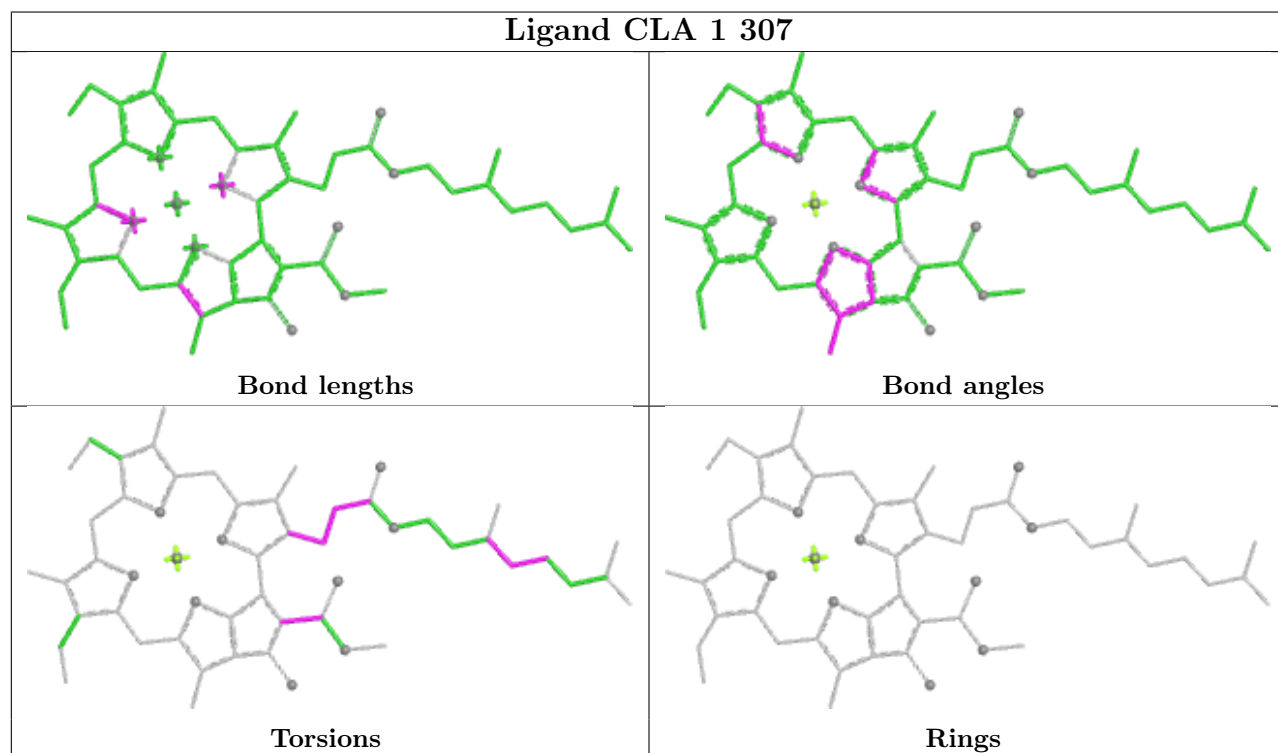
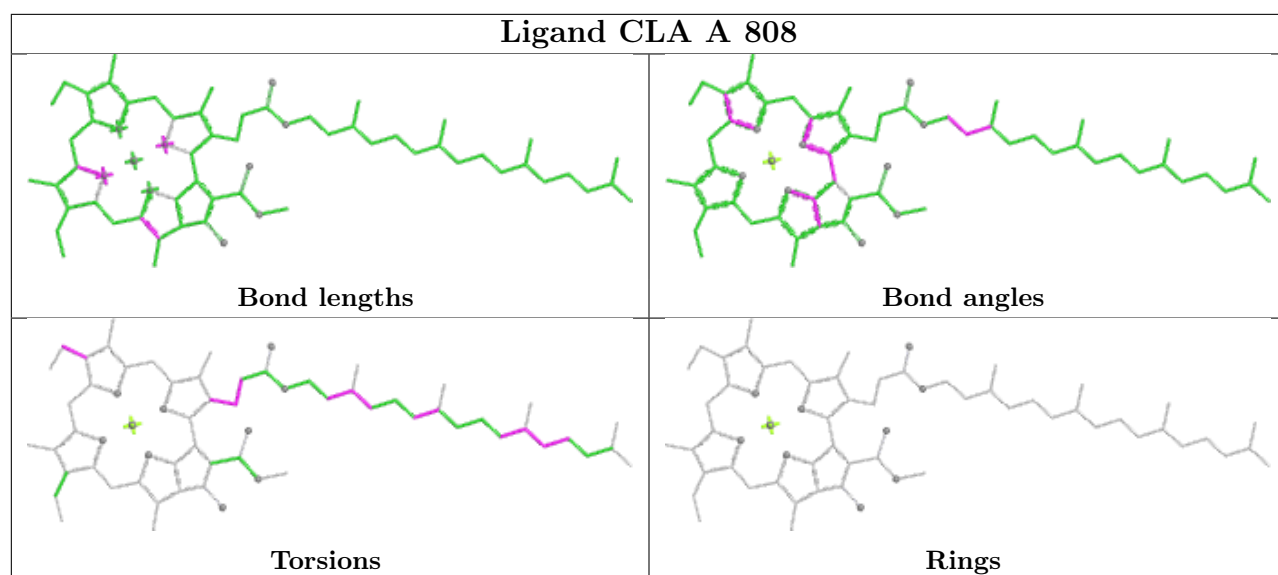
Bond angles

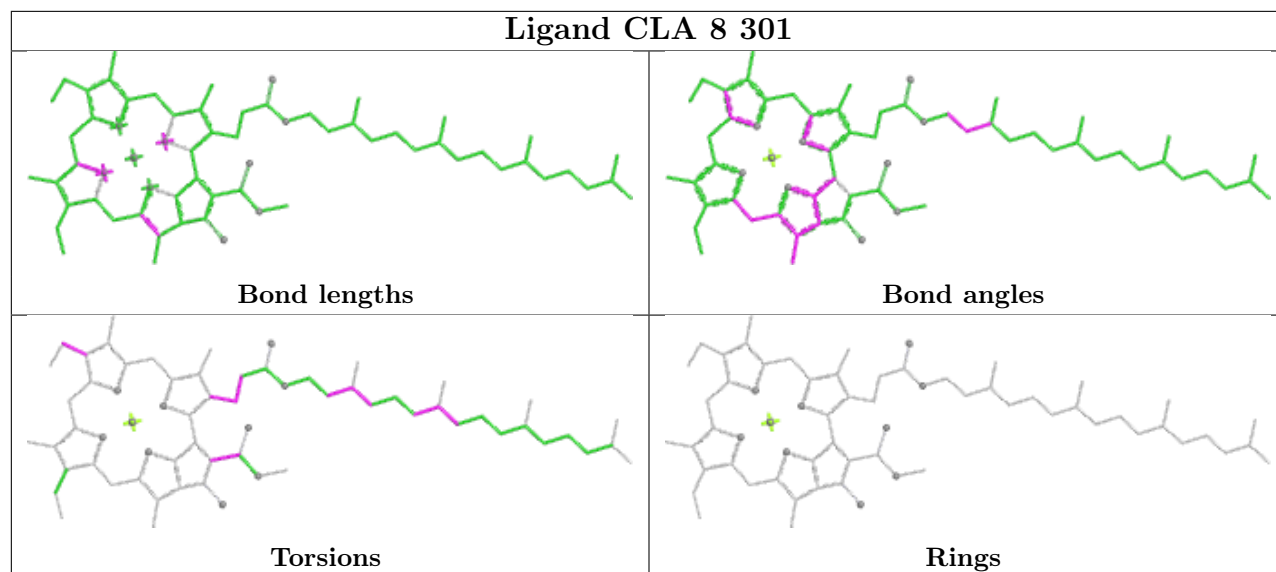
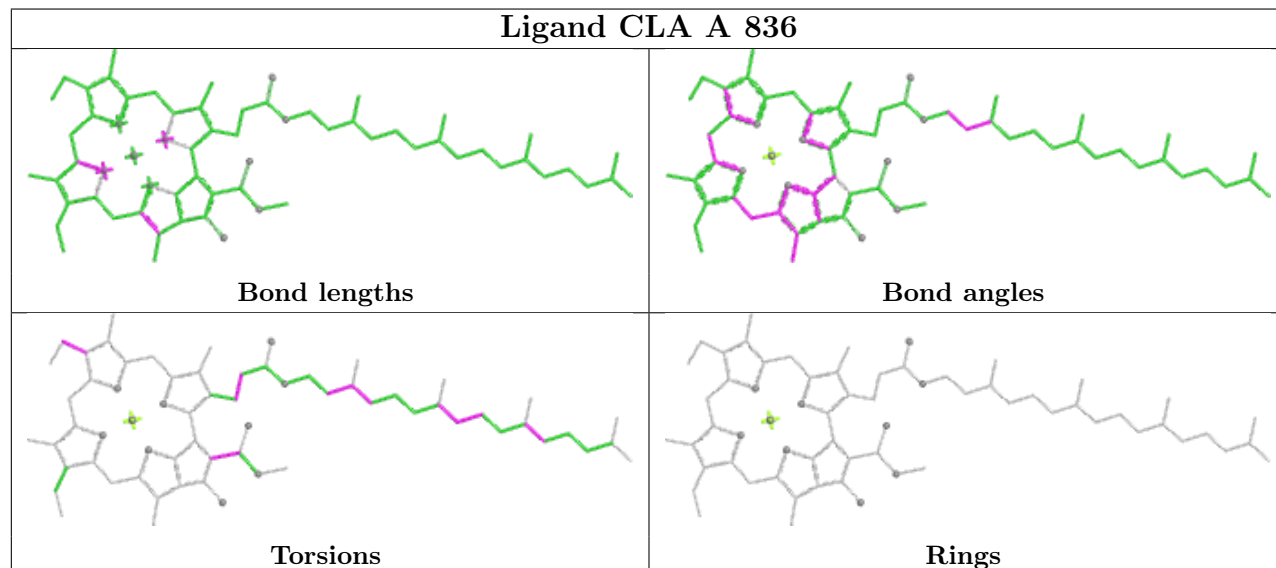


Torsions

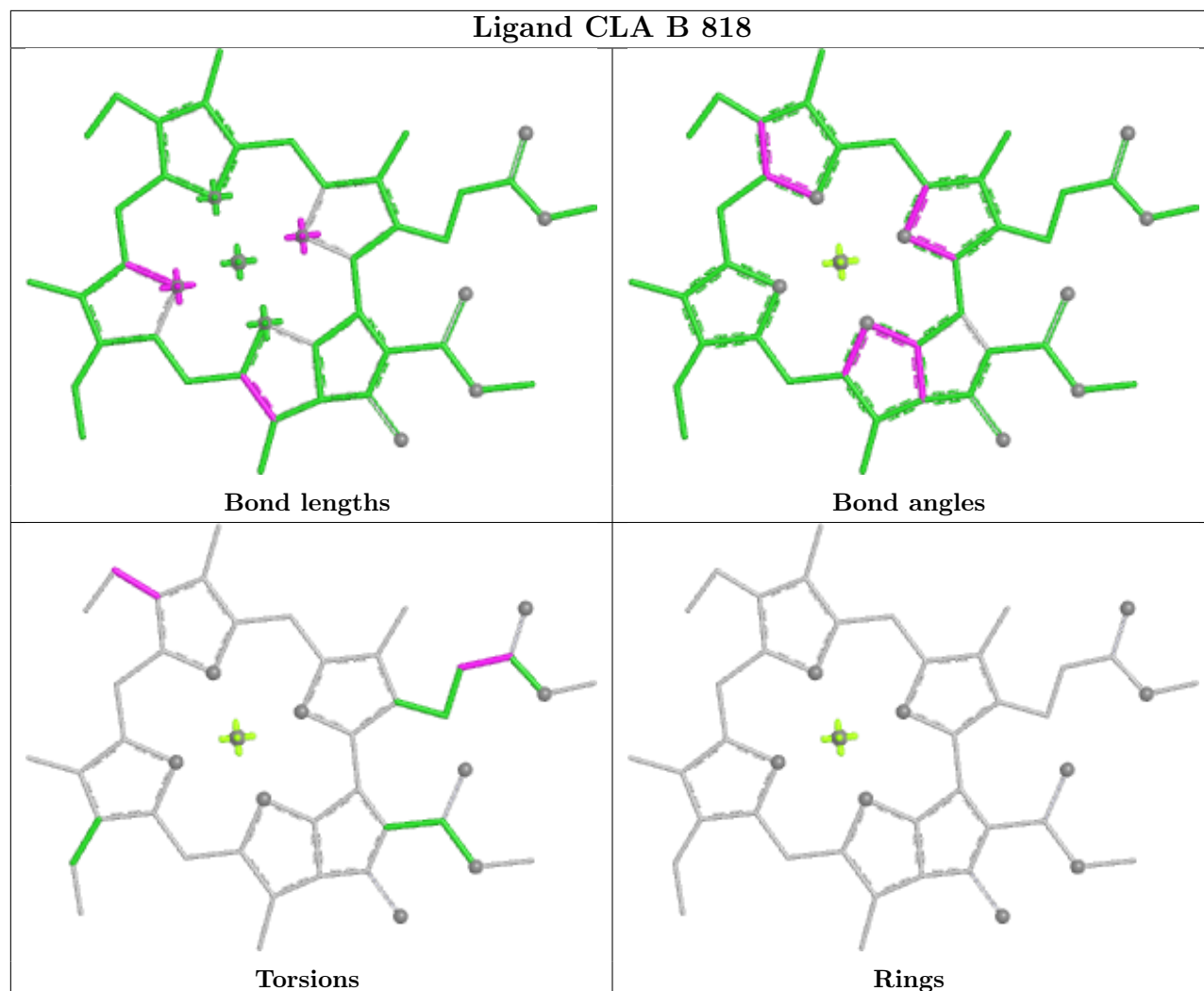


Rings

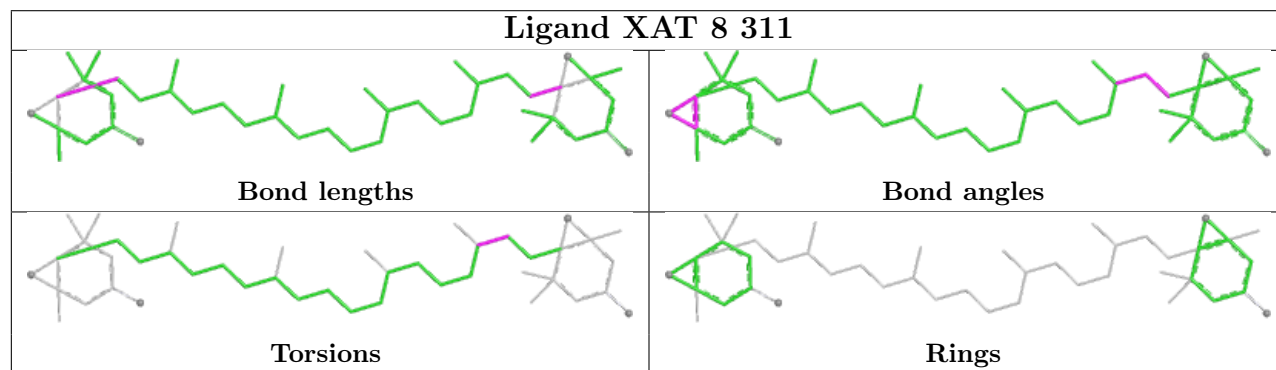


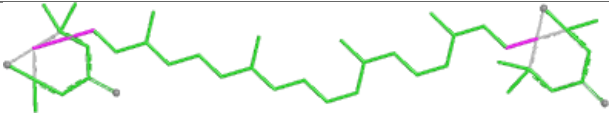
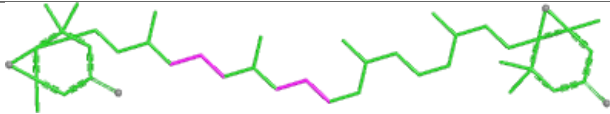
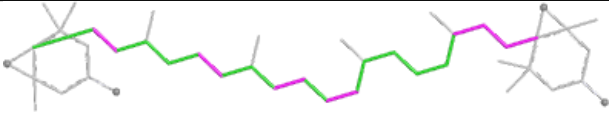
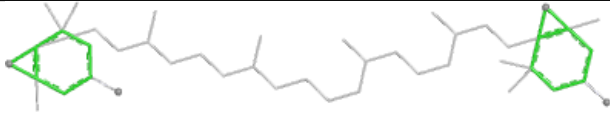
Ligand CLA 8 301**Ligand CLA A 836**

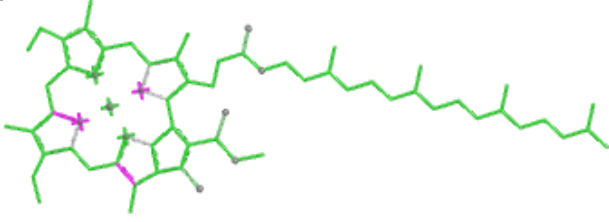
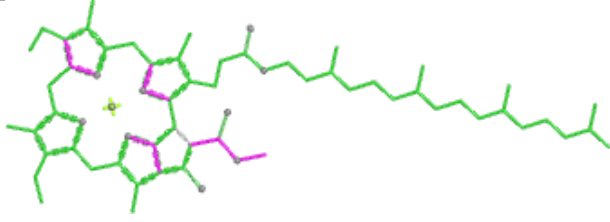
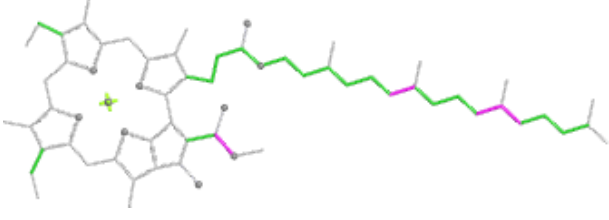
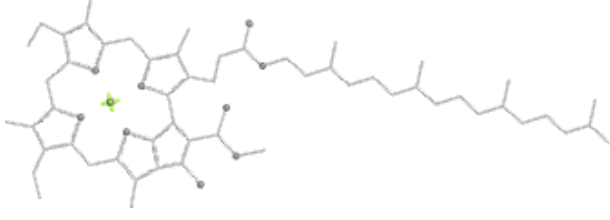
Ligand CLA B 818



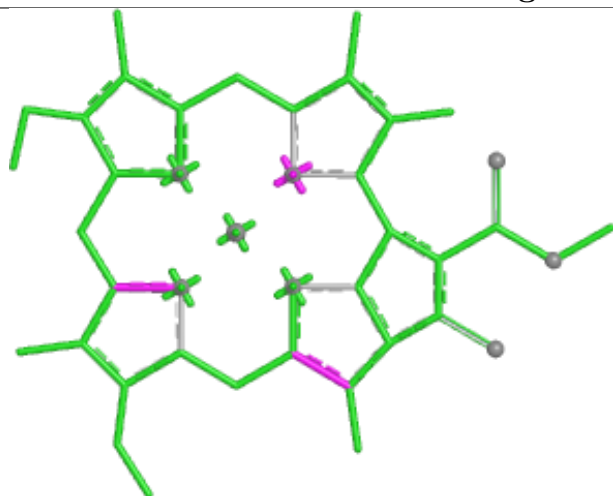
Ligand XAT 8 311



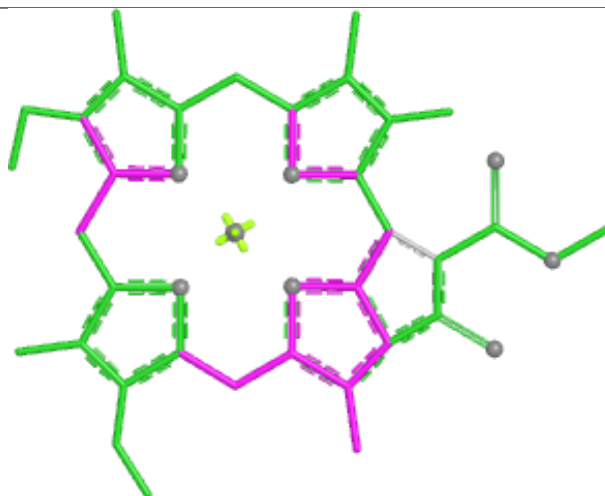
Ligand XAT 5 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

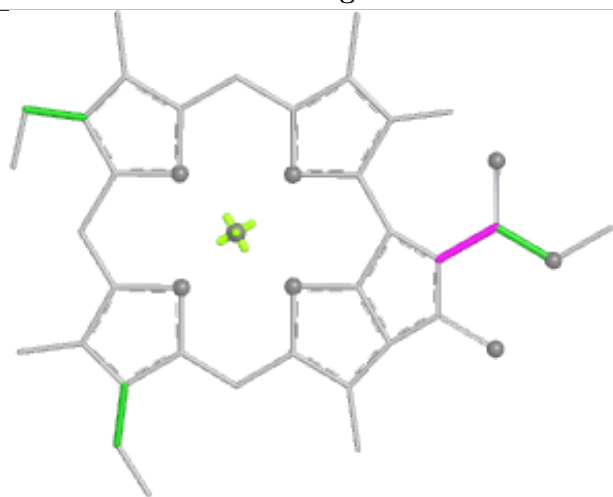
Ligand CLA 5 306



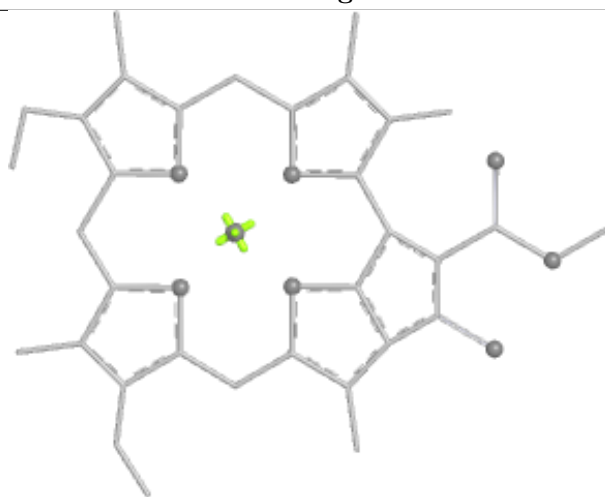
Bond lengths



Bond angles

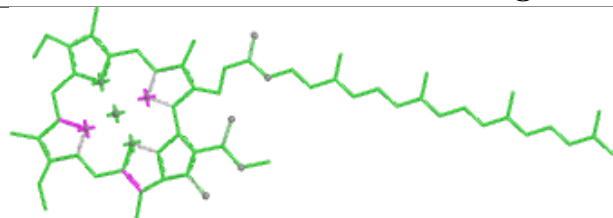


Torsions

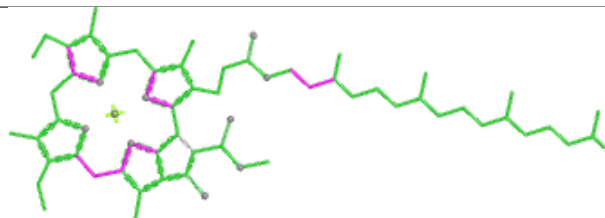


Rings

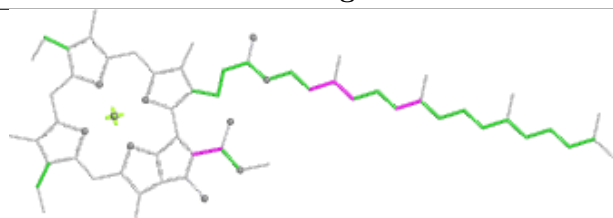
Ligand CLA B 826



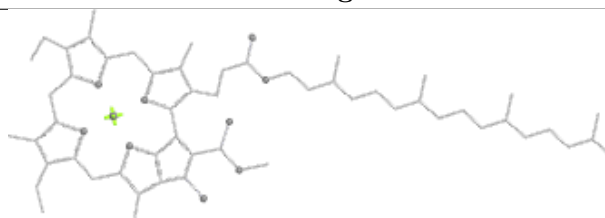
Bond lengths



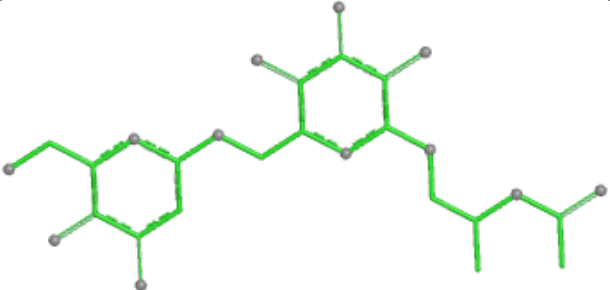
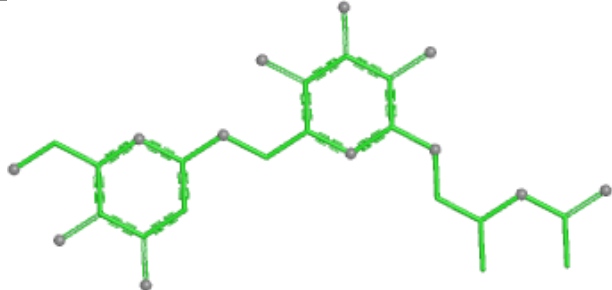
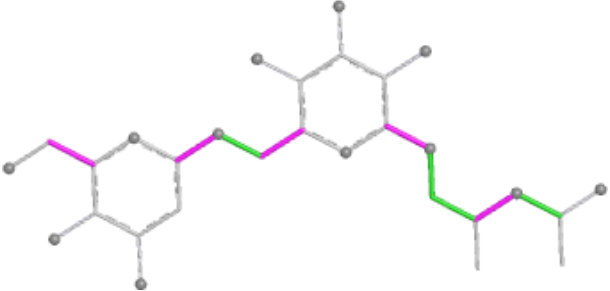
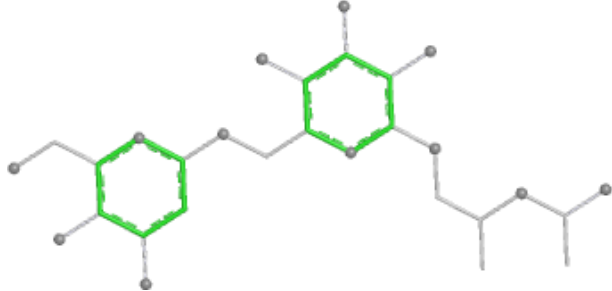
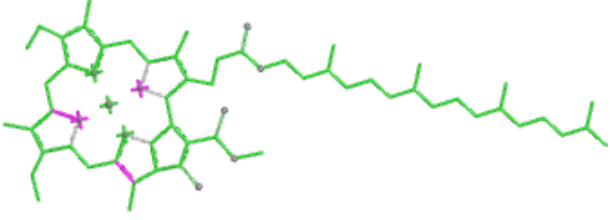
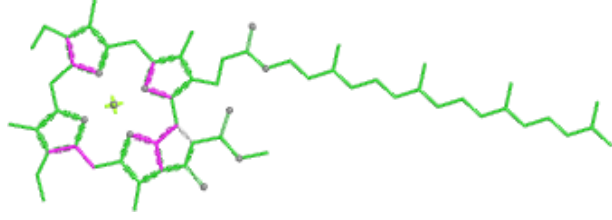
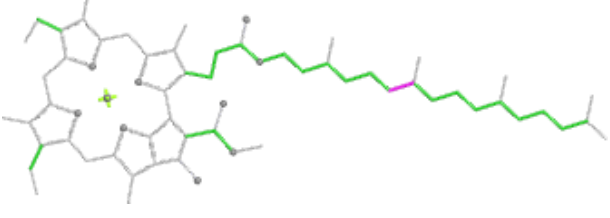
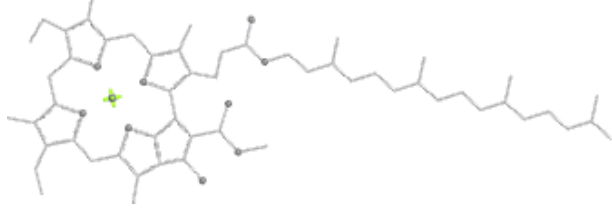
Bond angles

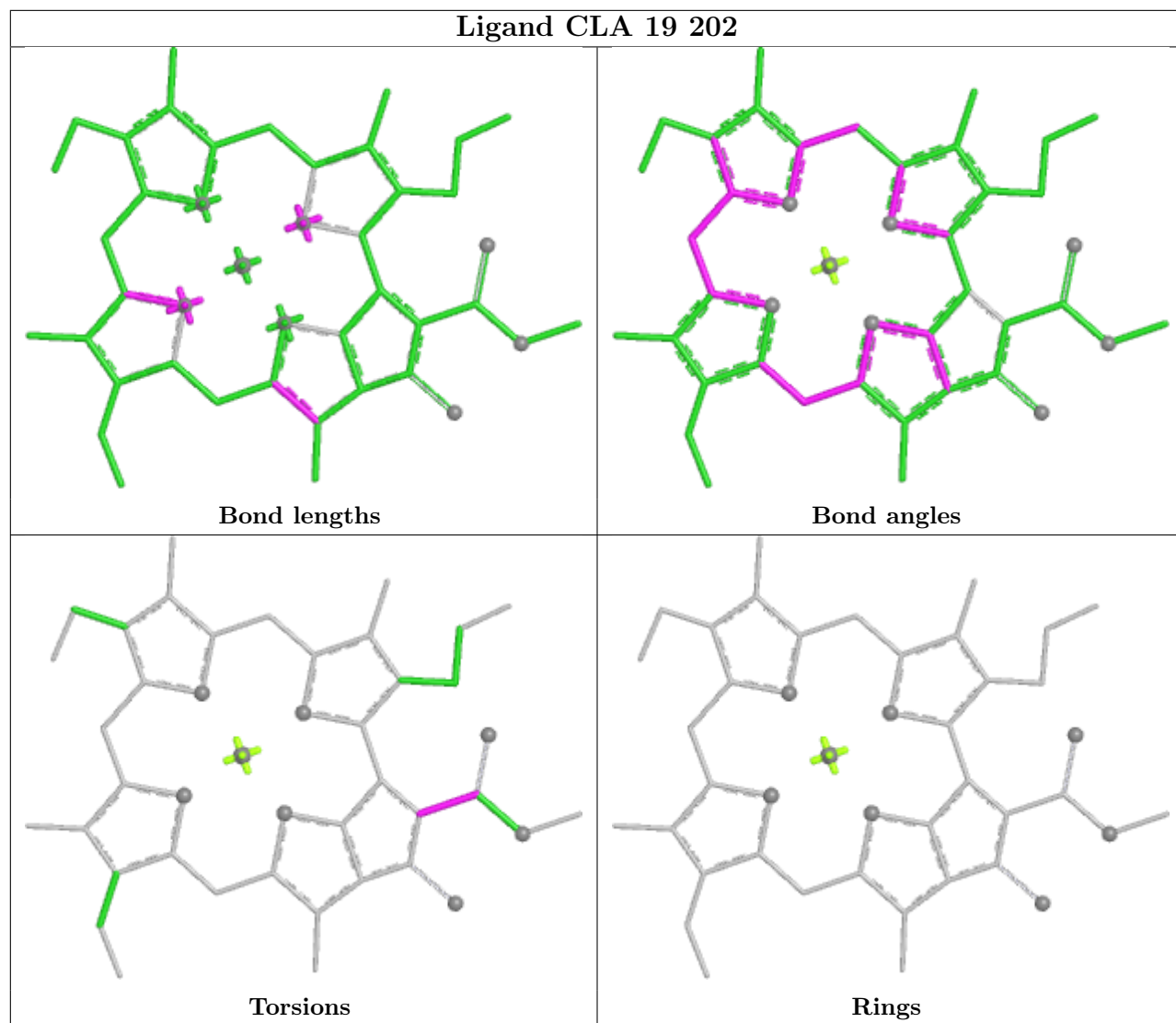


Torsions

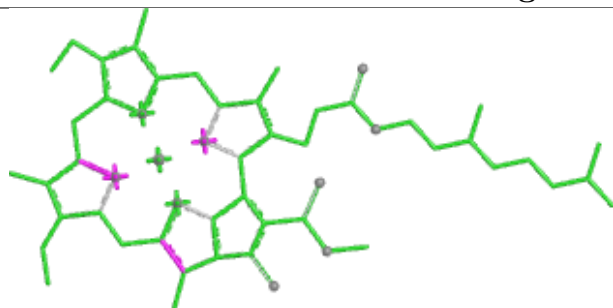


Rings

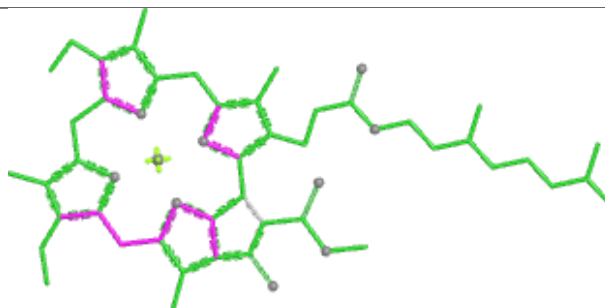
Ligand DGD 4 317	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA B 825	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



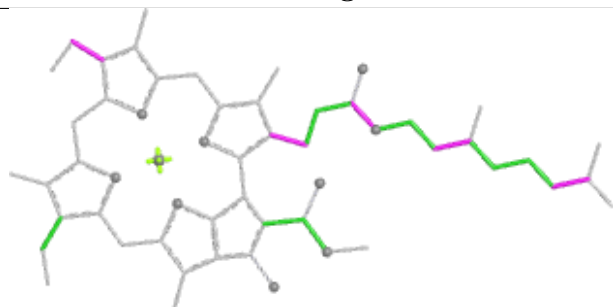
Ligand CLA 5 302



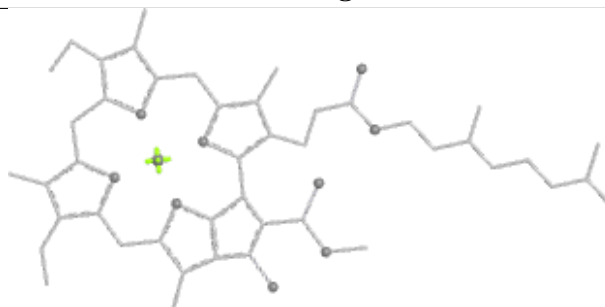
Bond lengths



Bond angles

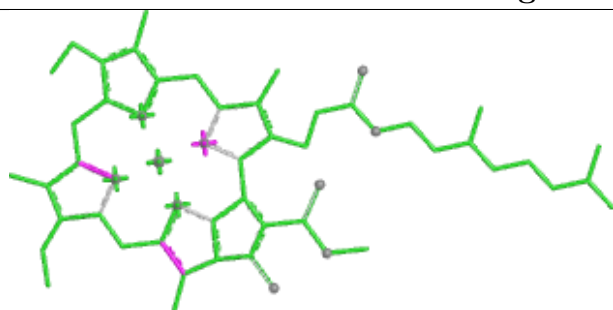


Torsions

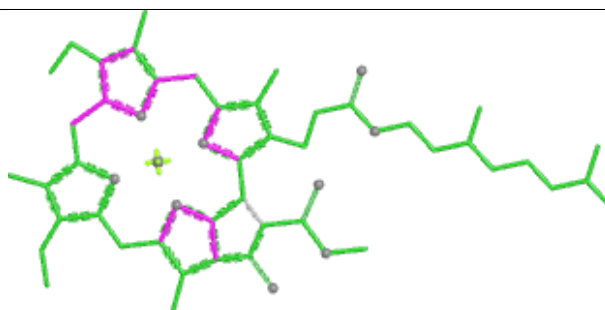


Rings

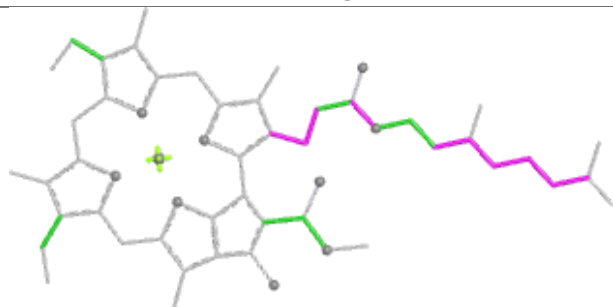
Ligand CLA 4 303



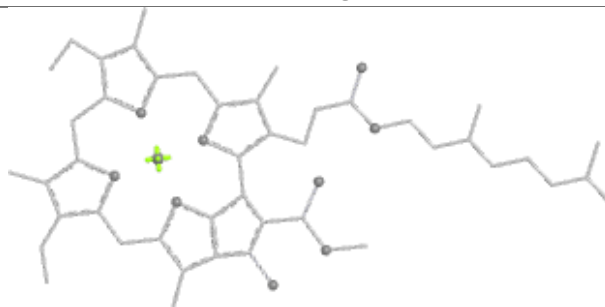
Bond lengths



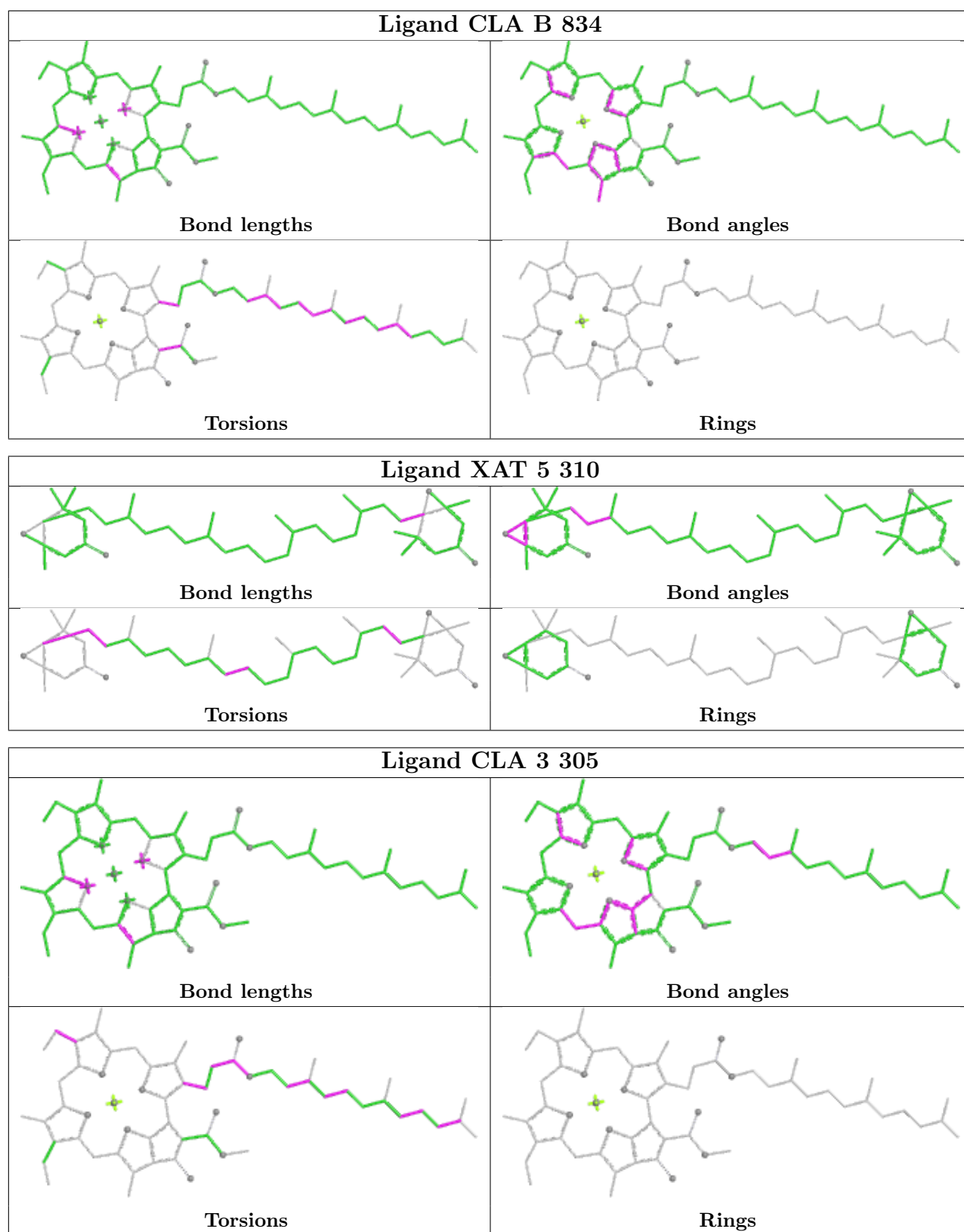
Bond angles

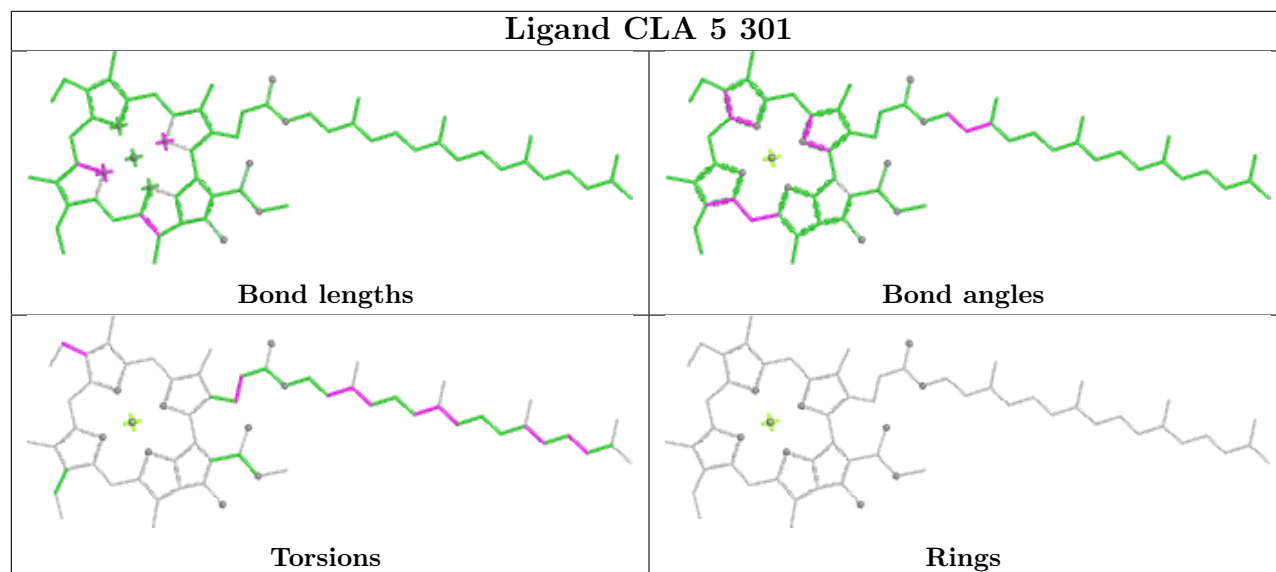
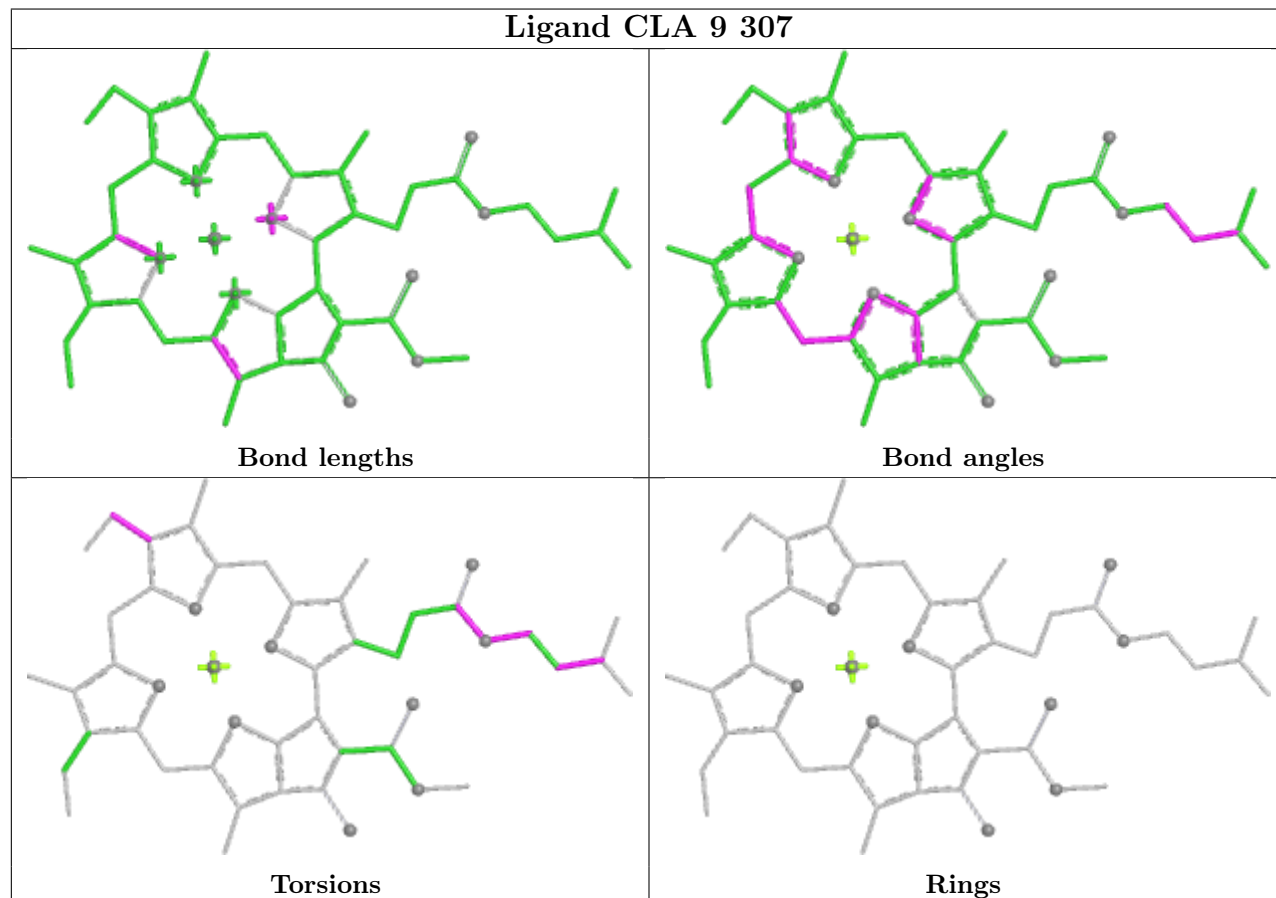


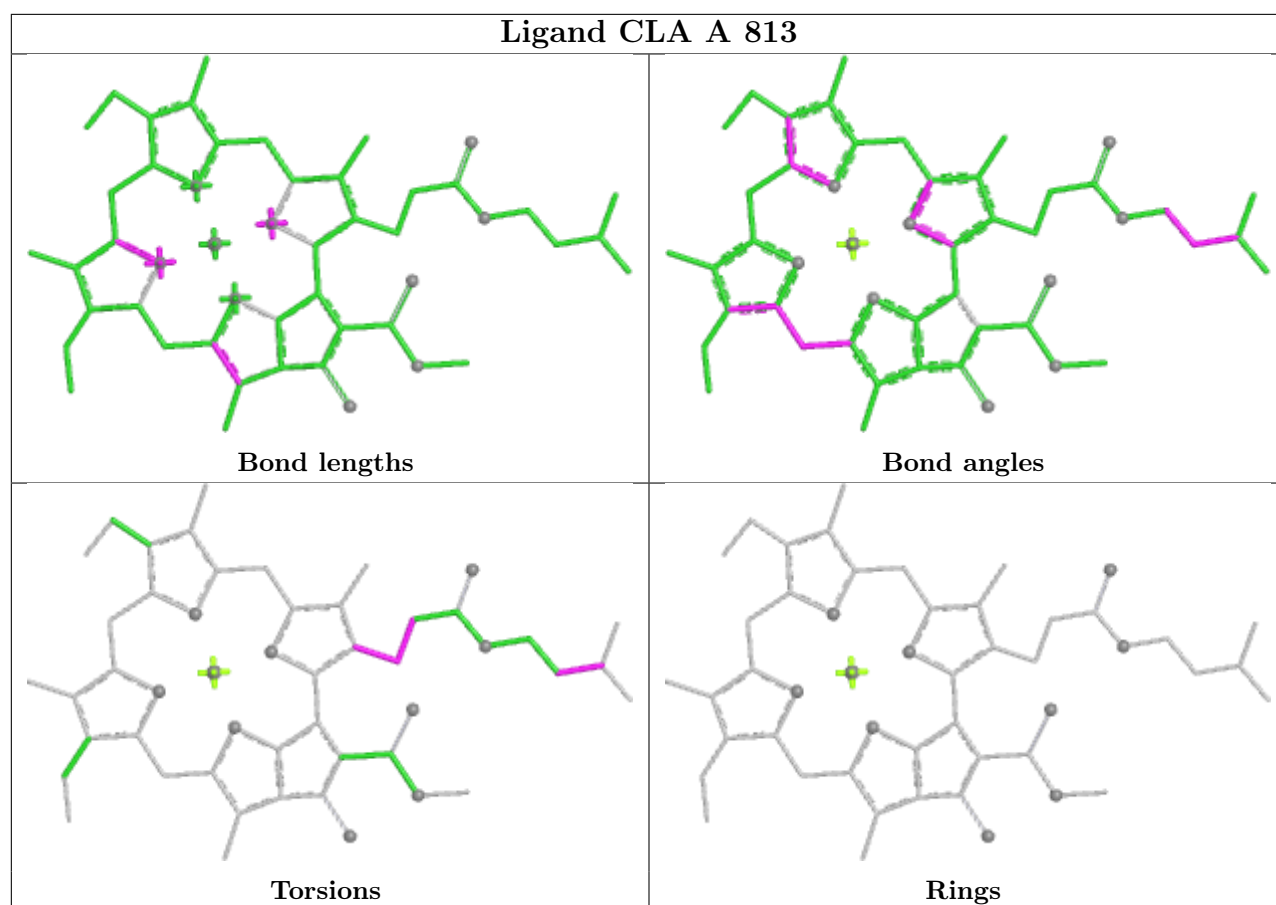
Torsions



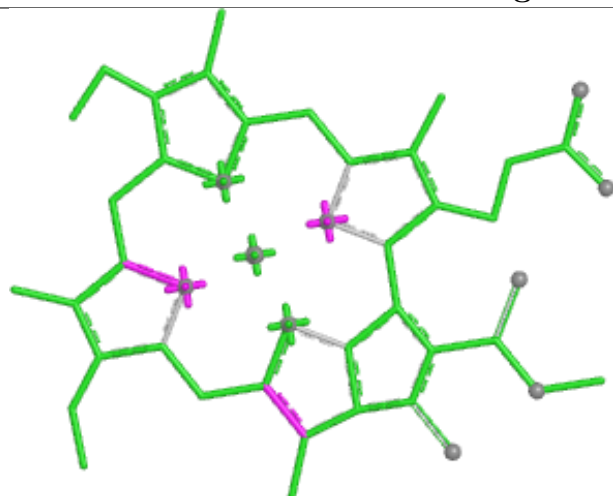
Rings



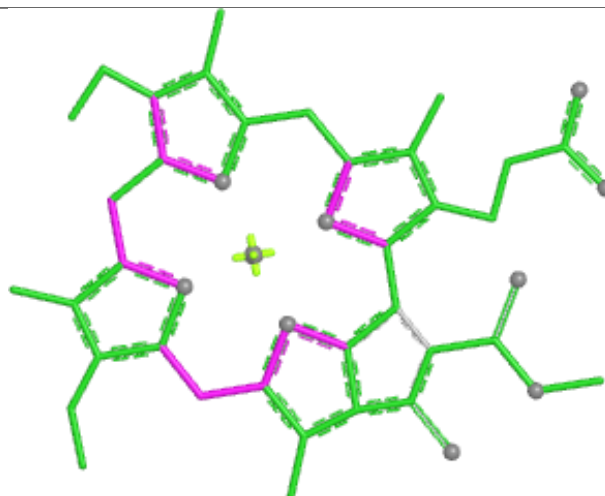
Ligand CLA 5 301**Ligand CLA 9 307**



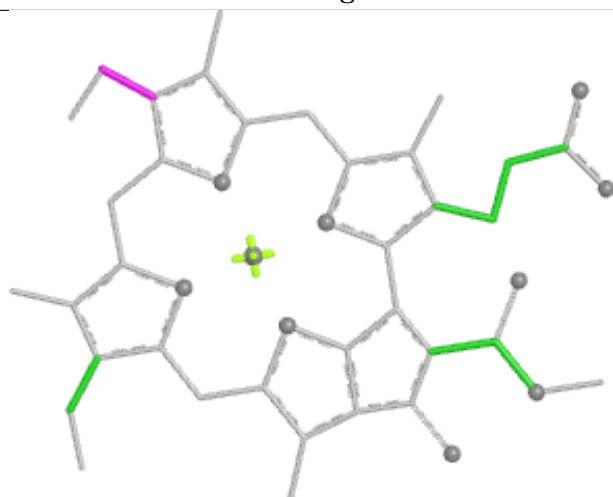
Ligand CLA A 832



Bond lengths



Bond angles

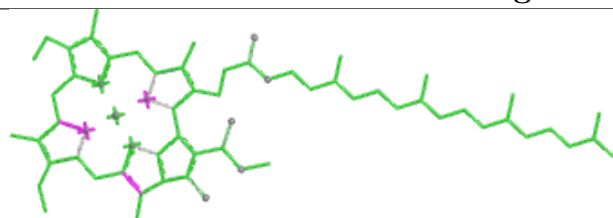


Torsions

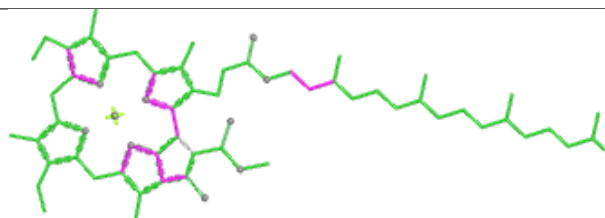


Rings

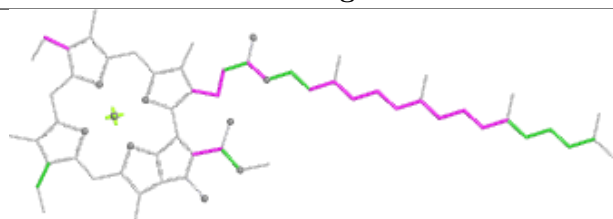
Ligand CLA A 815



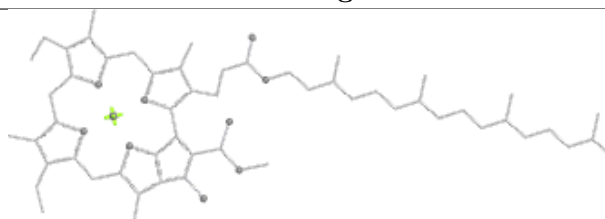
Bond lengths



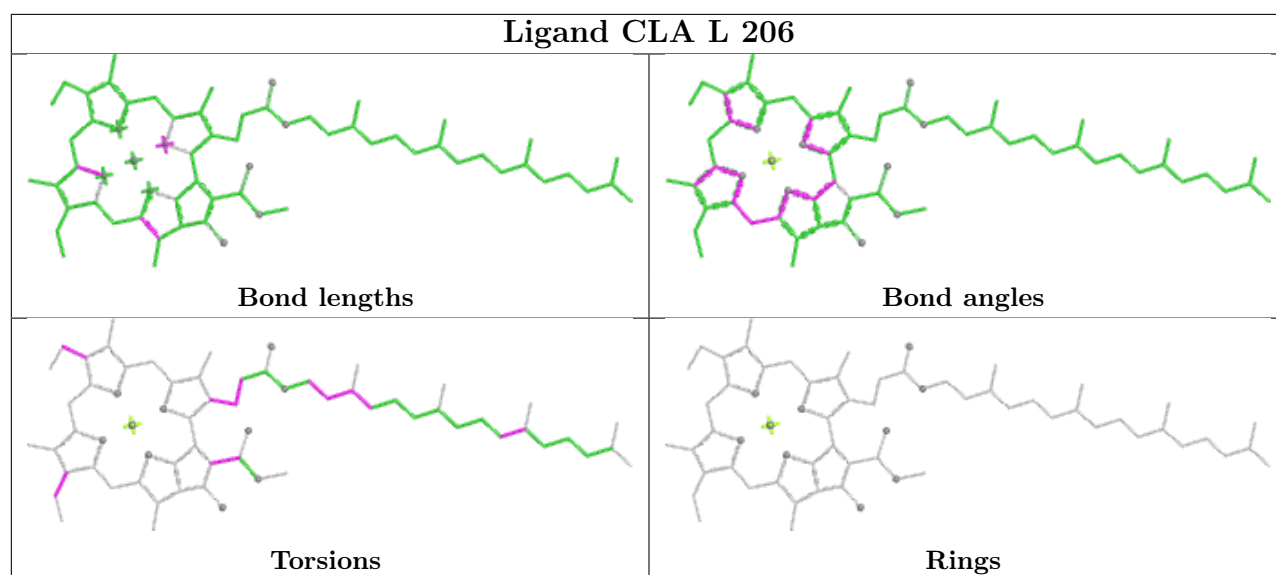
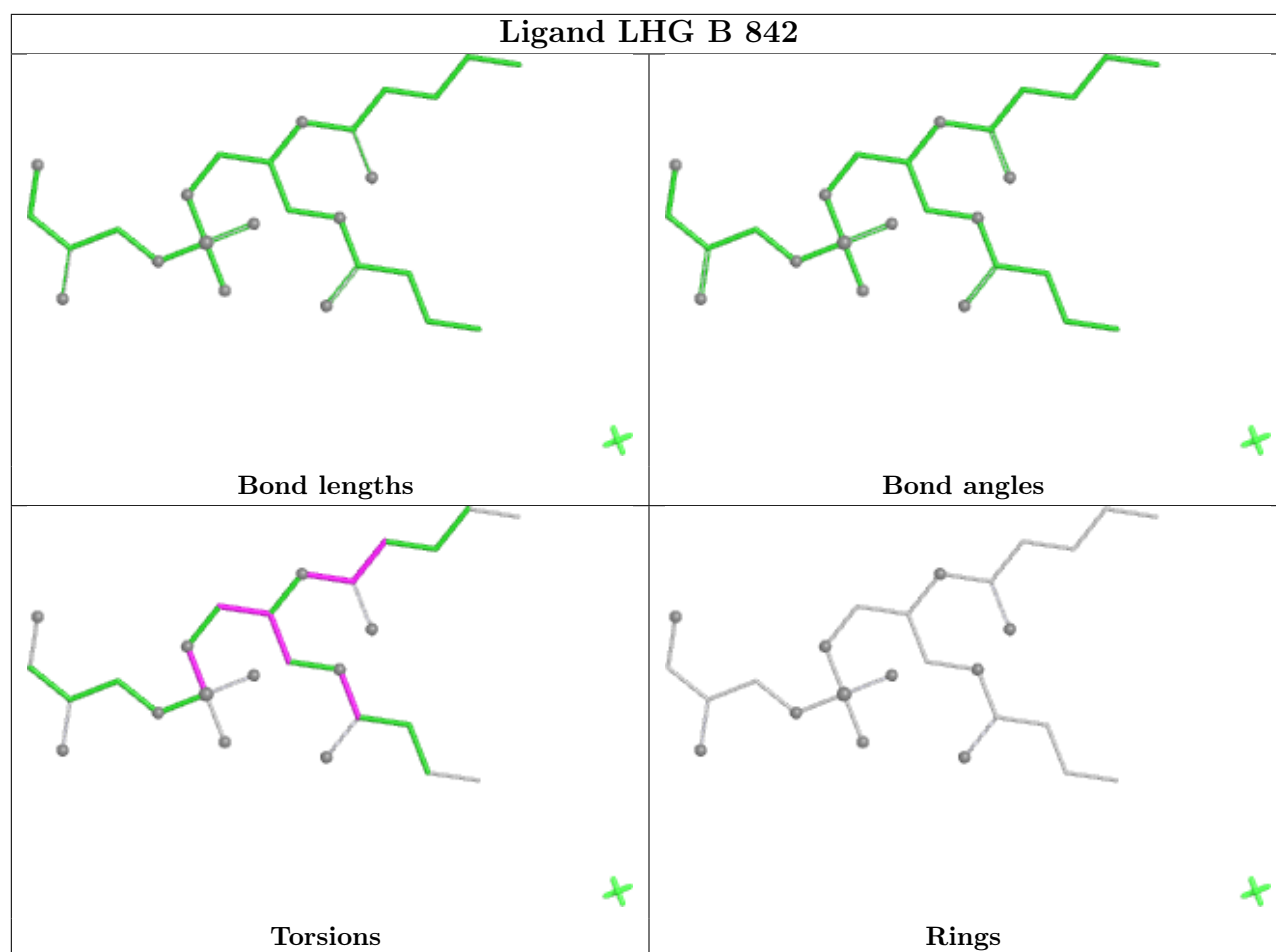
Bond angles



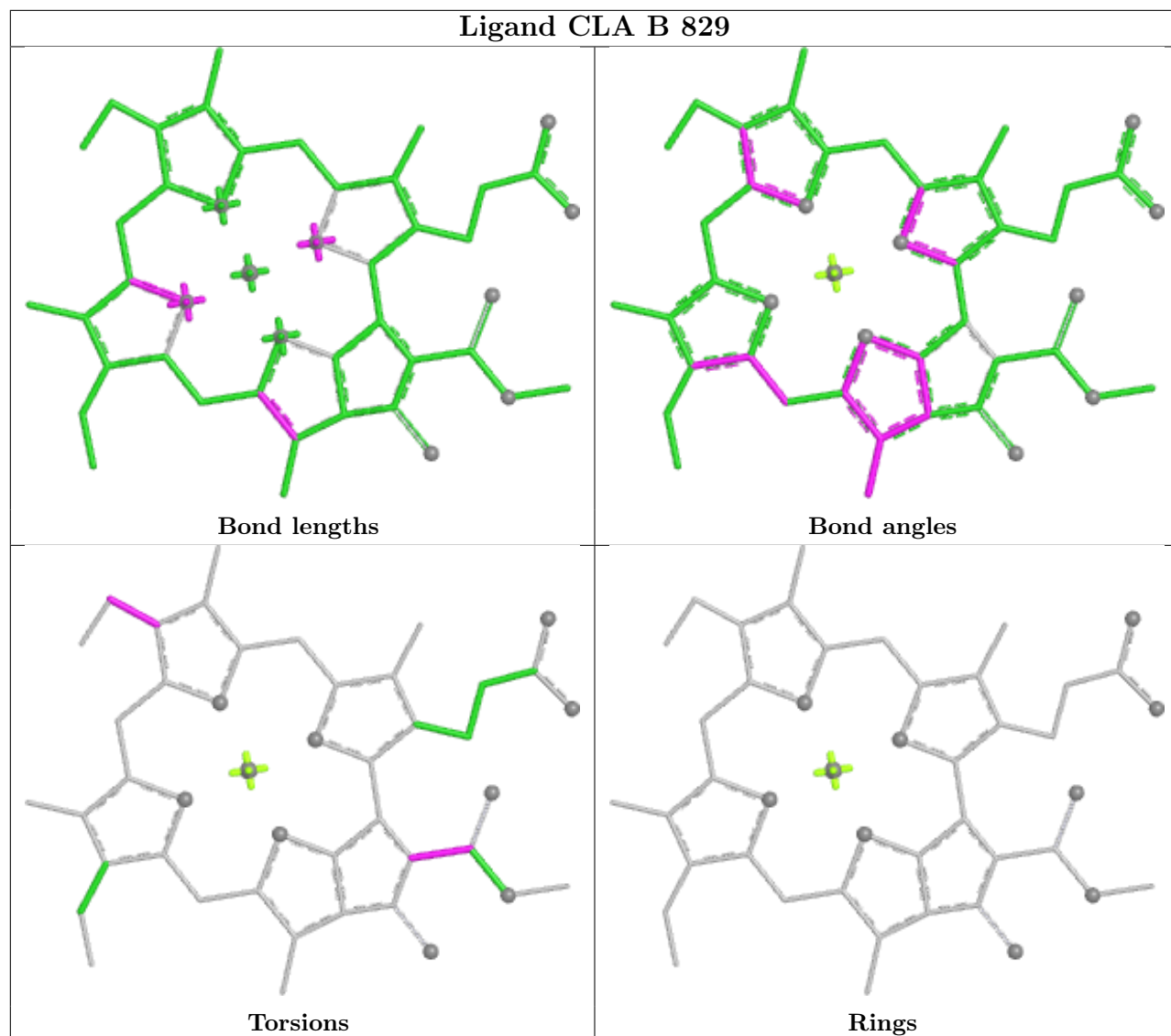
Torsions



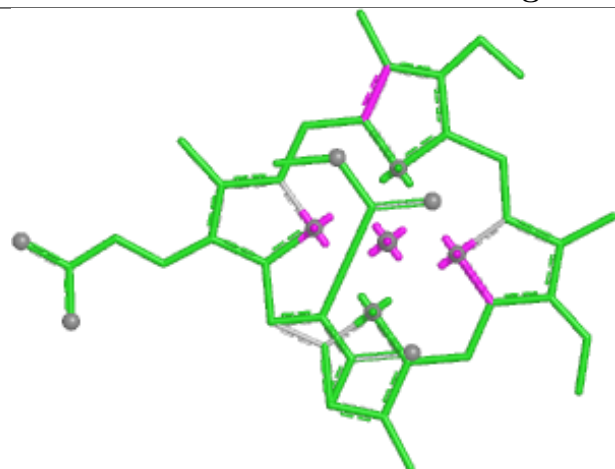
Rings



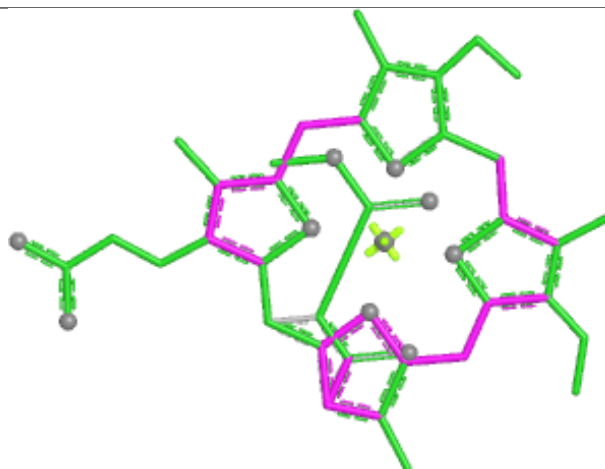
Ligand CLA B 829



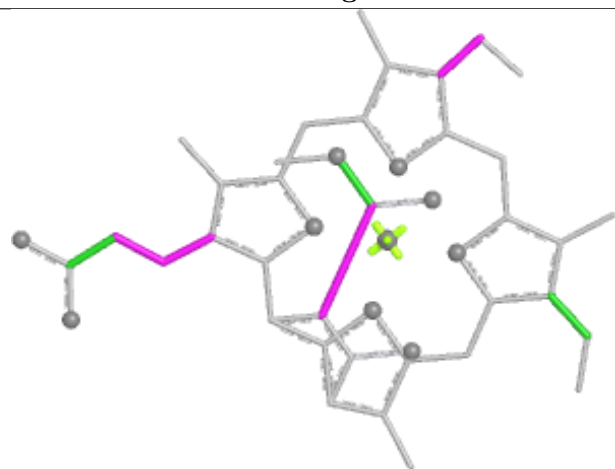
Ligand KC1 1 306



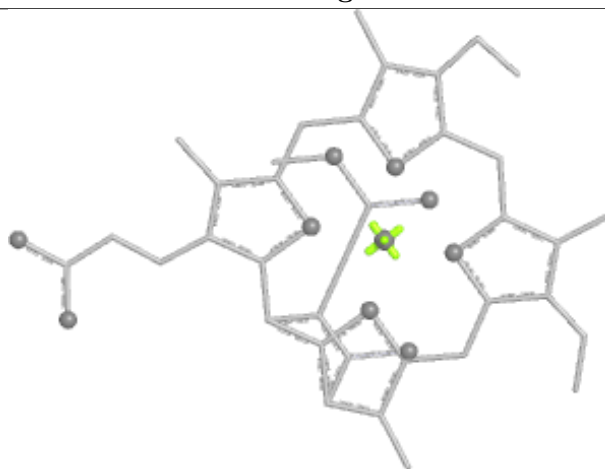
Bond lengths



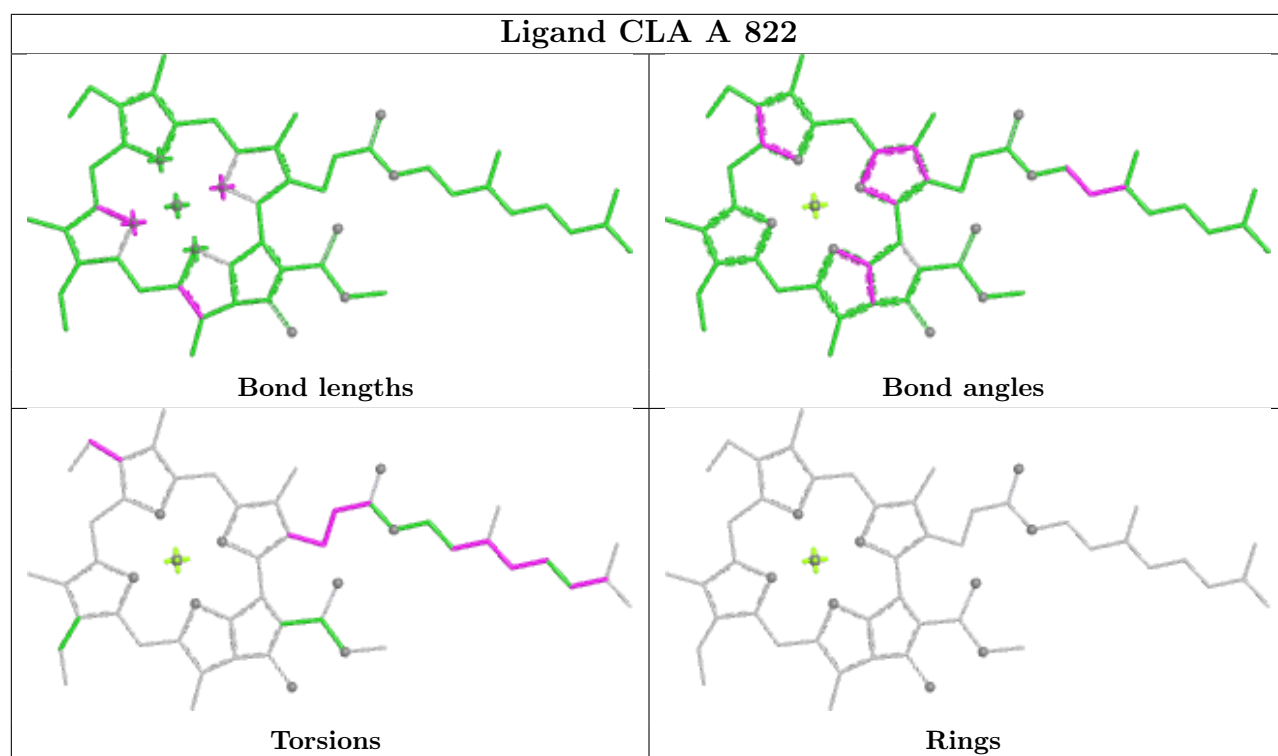
Bond angles

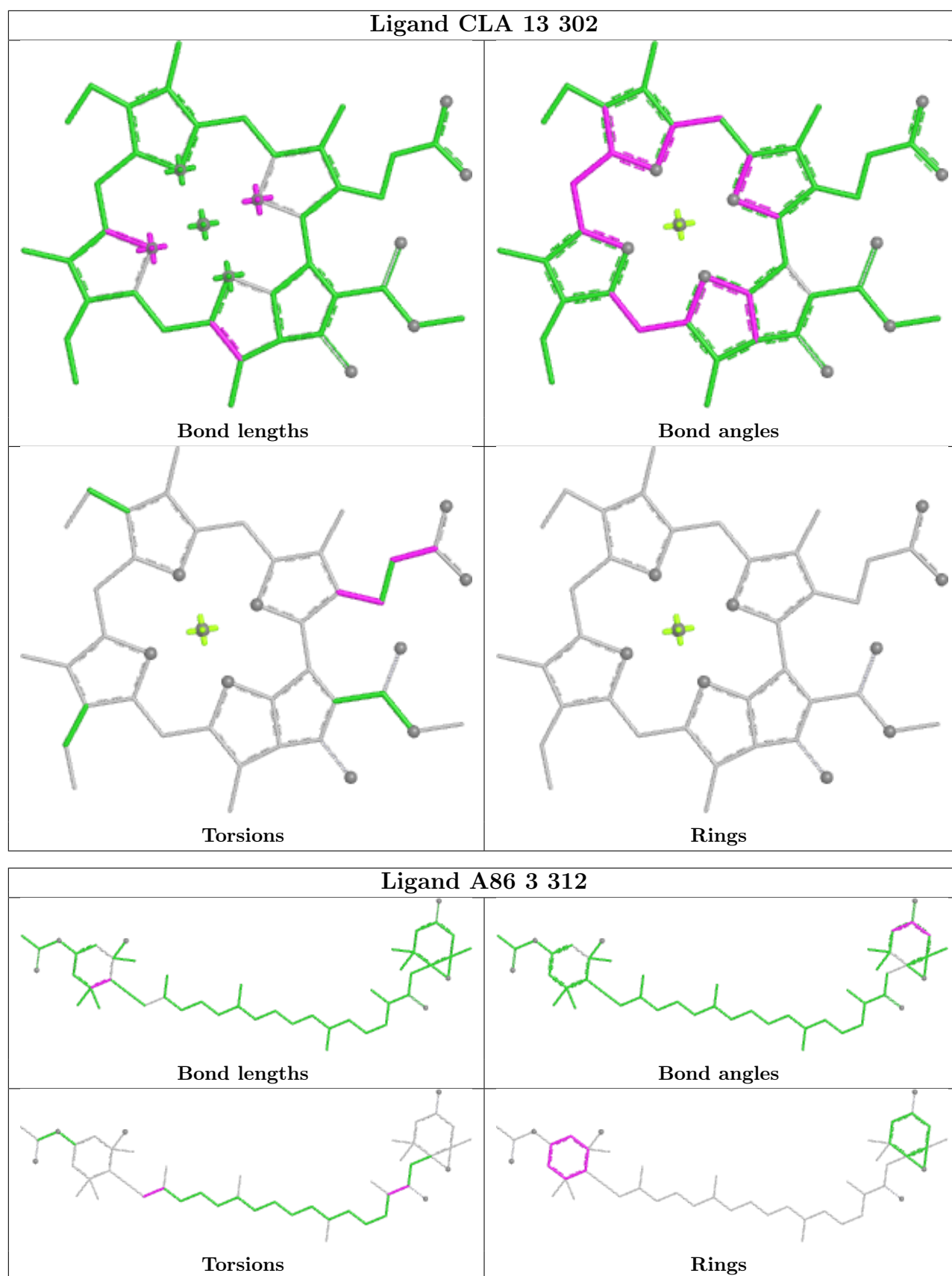


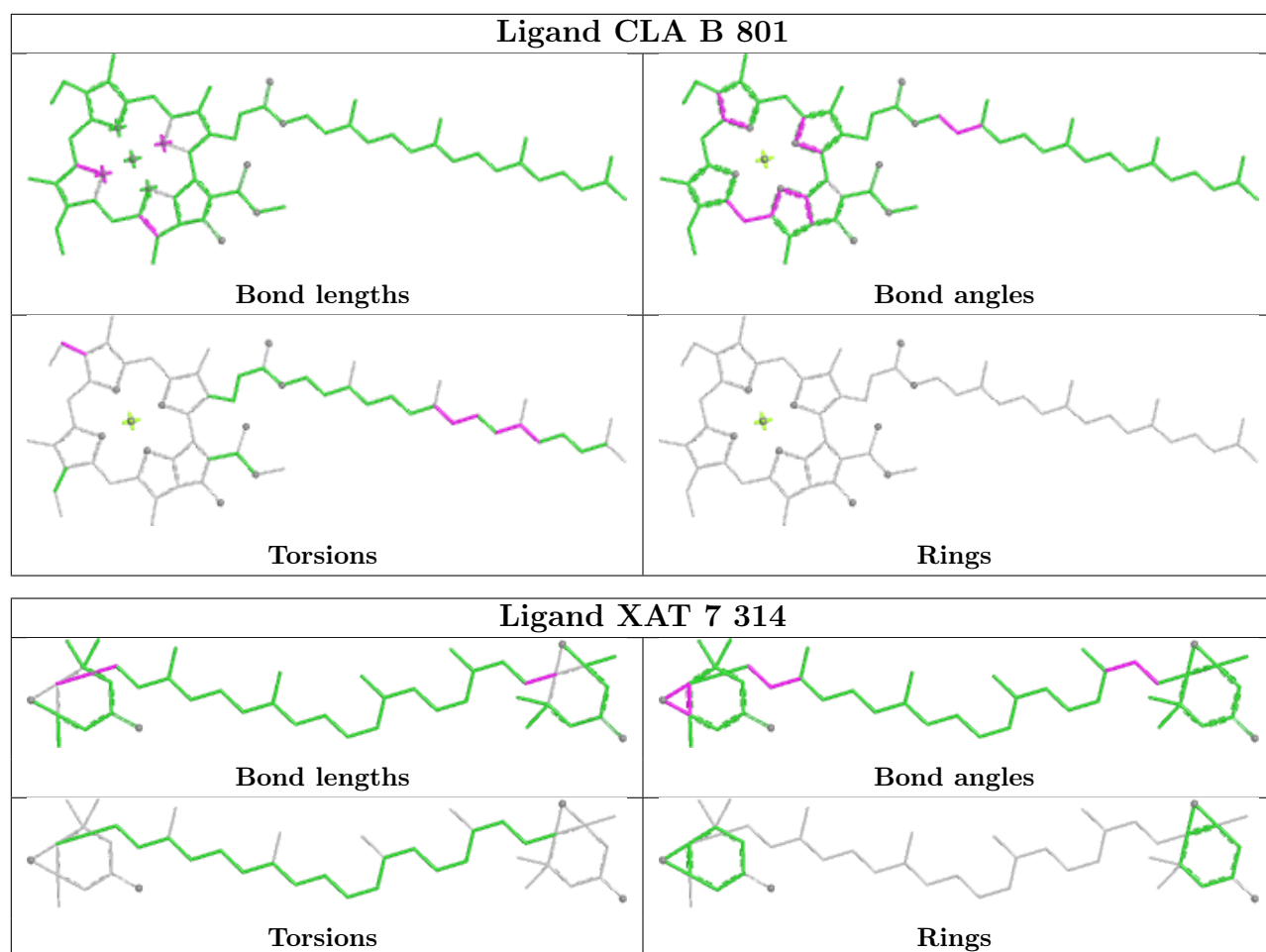
Torsions



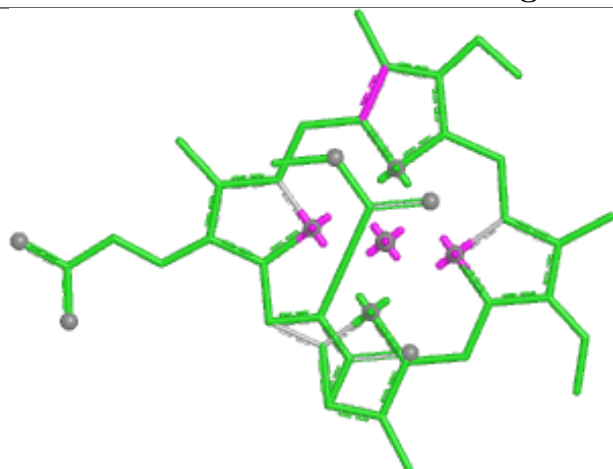
Rings



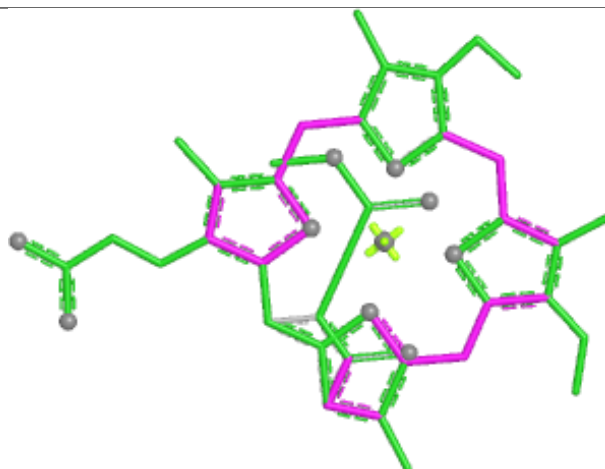




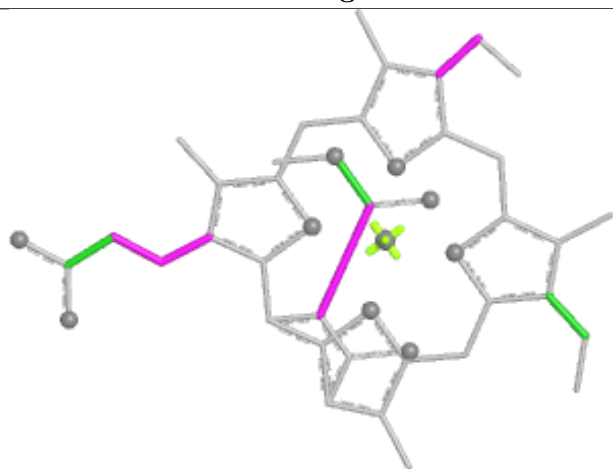
Ligand KC1 5 308



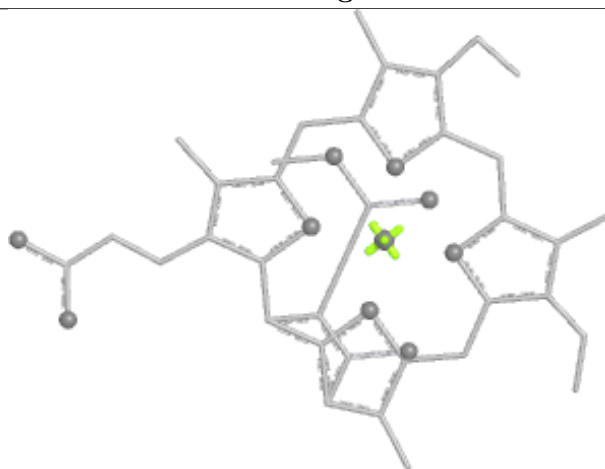
Bond lengths



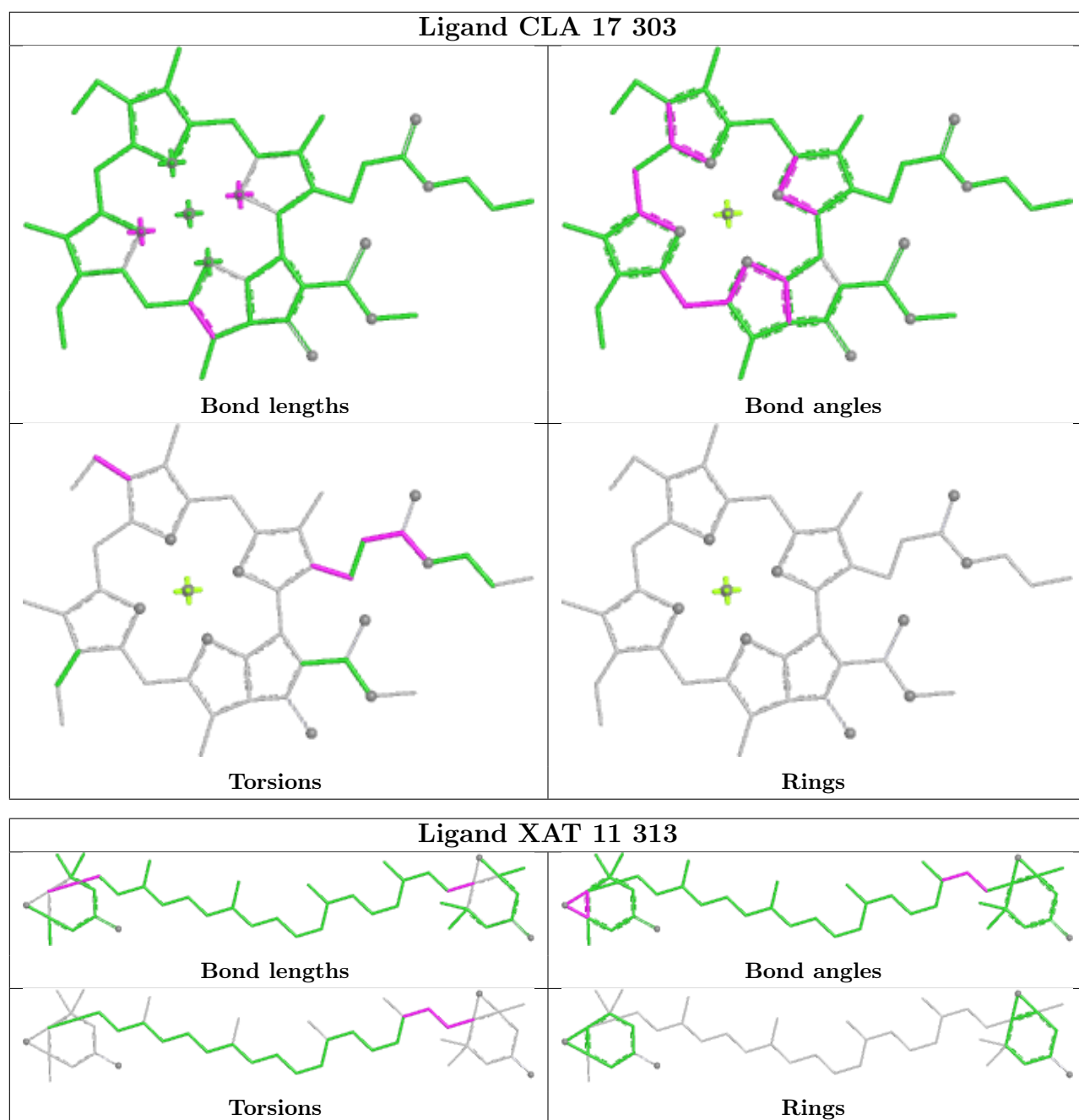
Bond angles

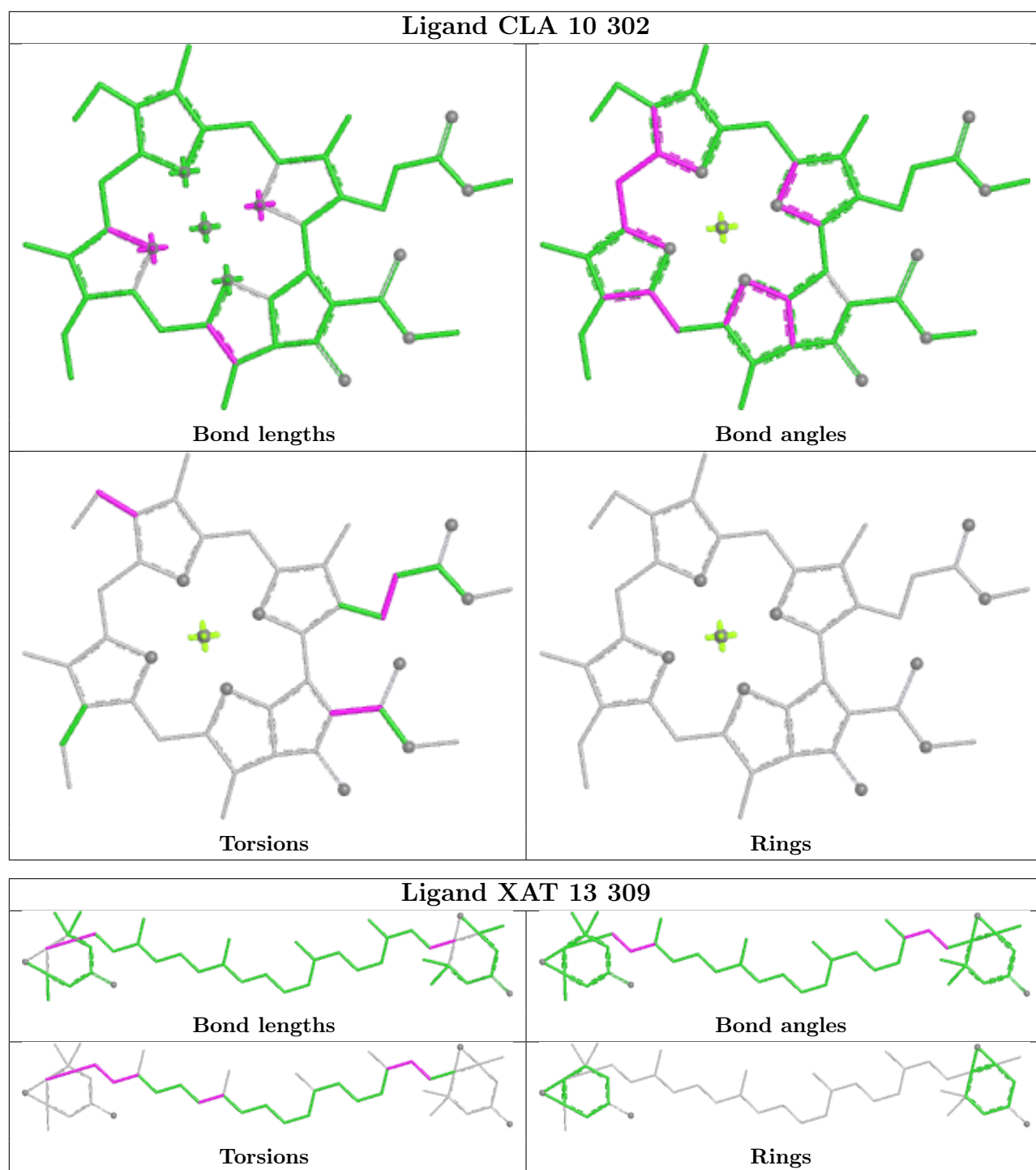


Torsions

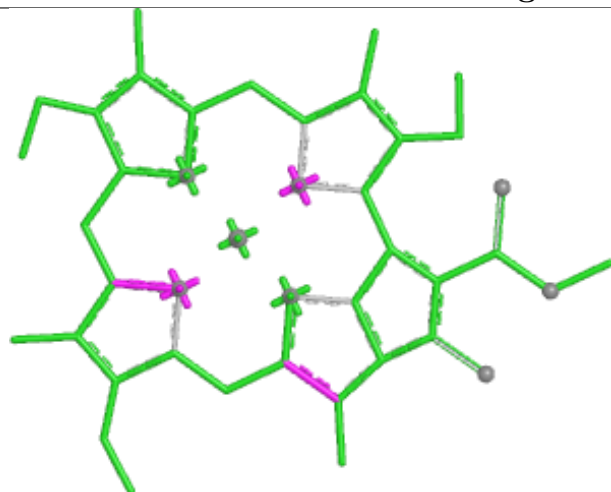


Rings

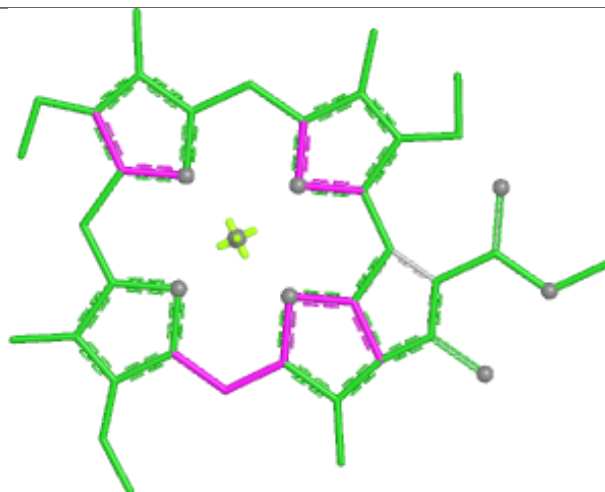




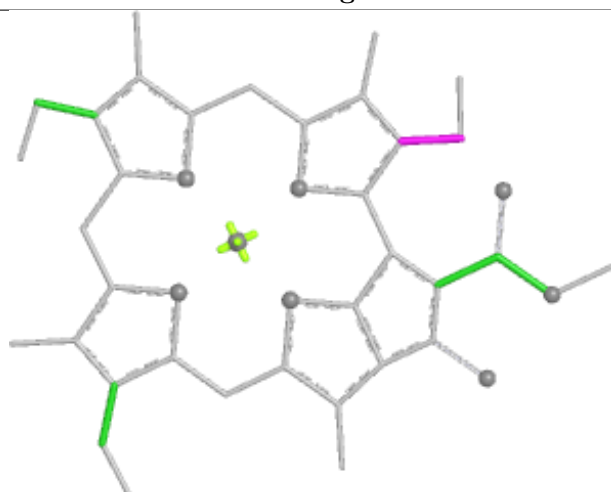
Ligand CLA J 103



Bond lengths



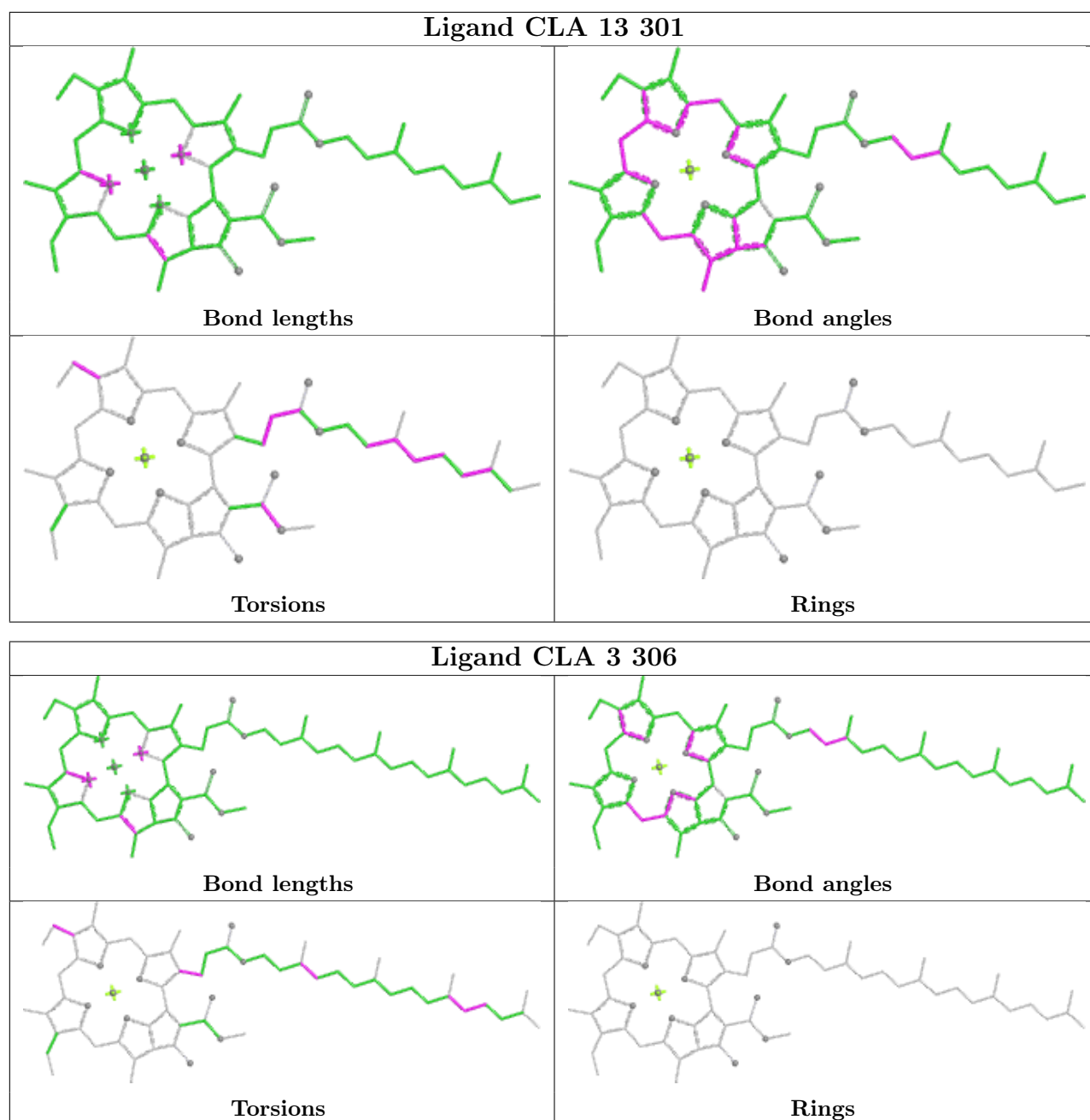
Bond angles

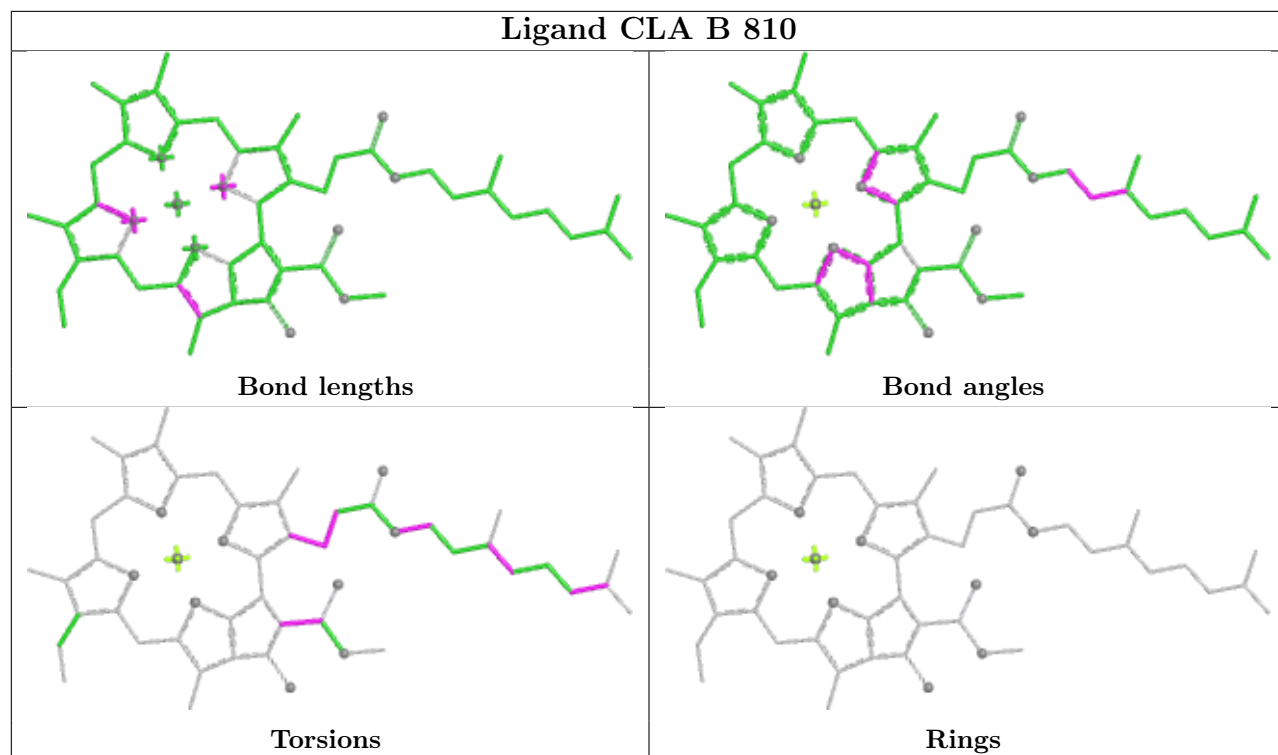


Torsions

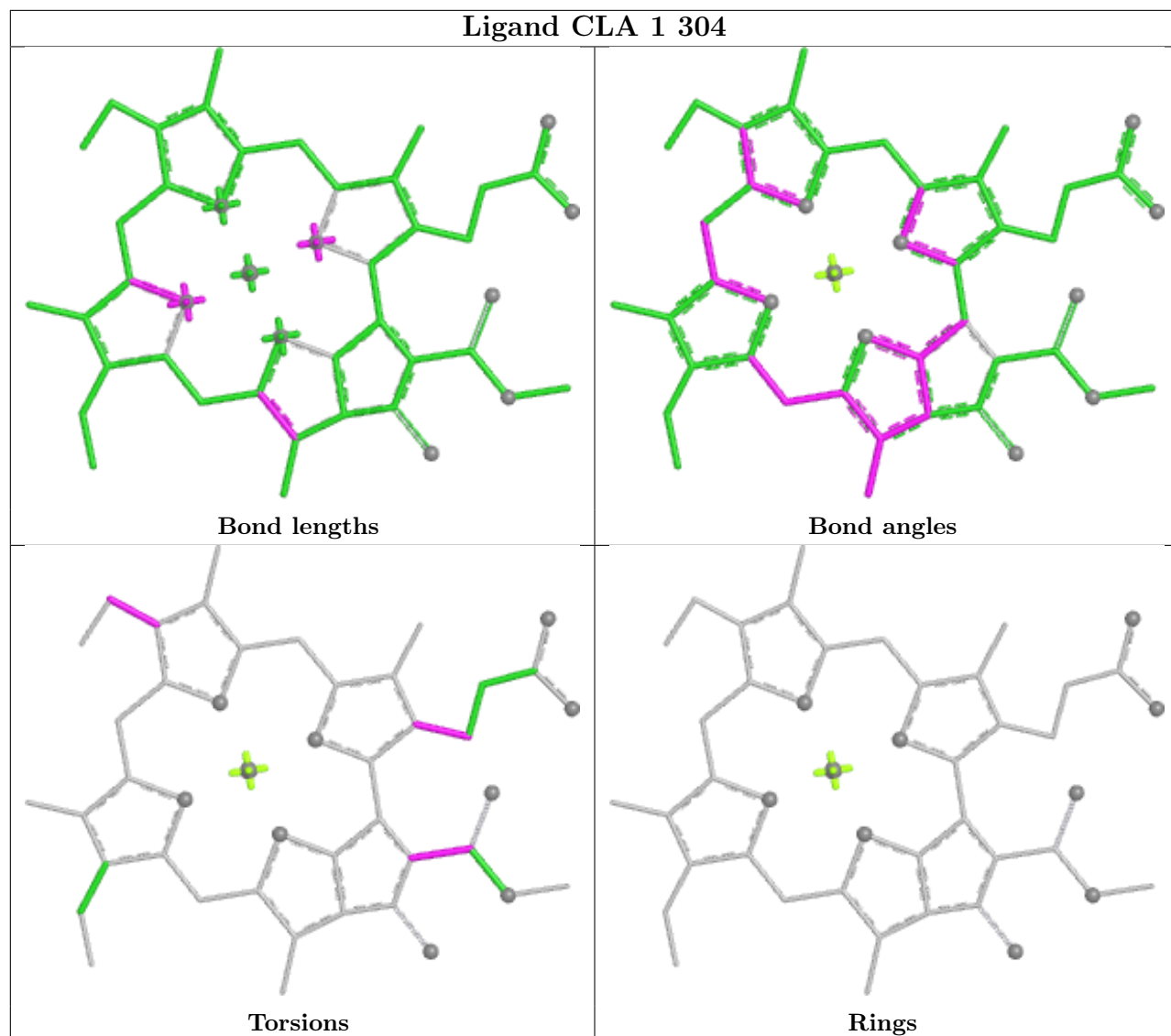


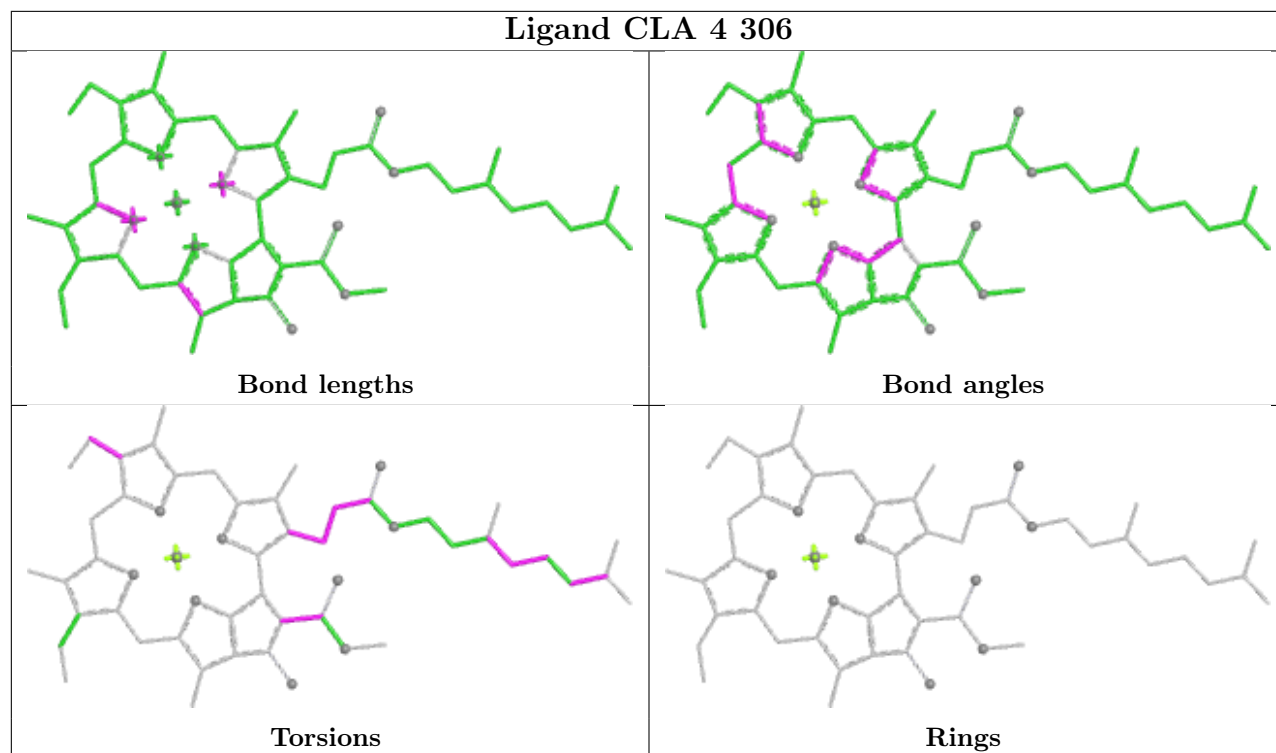
Rings

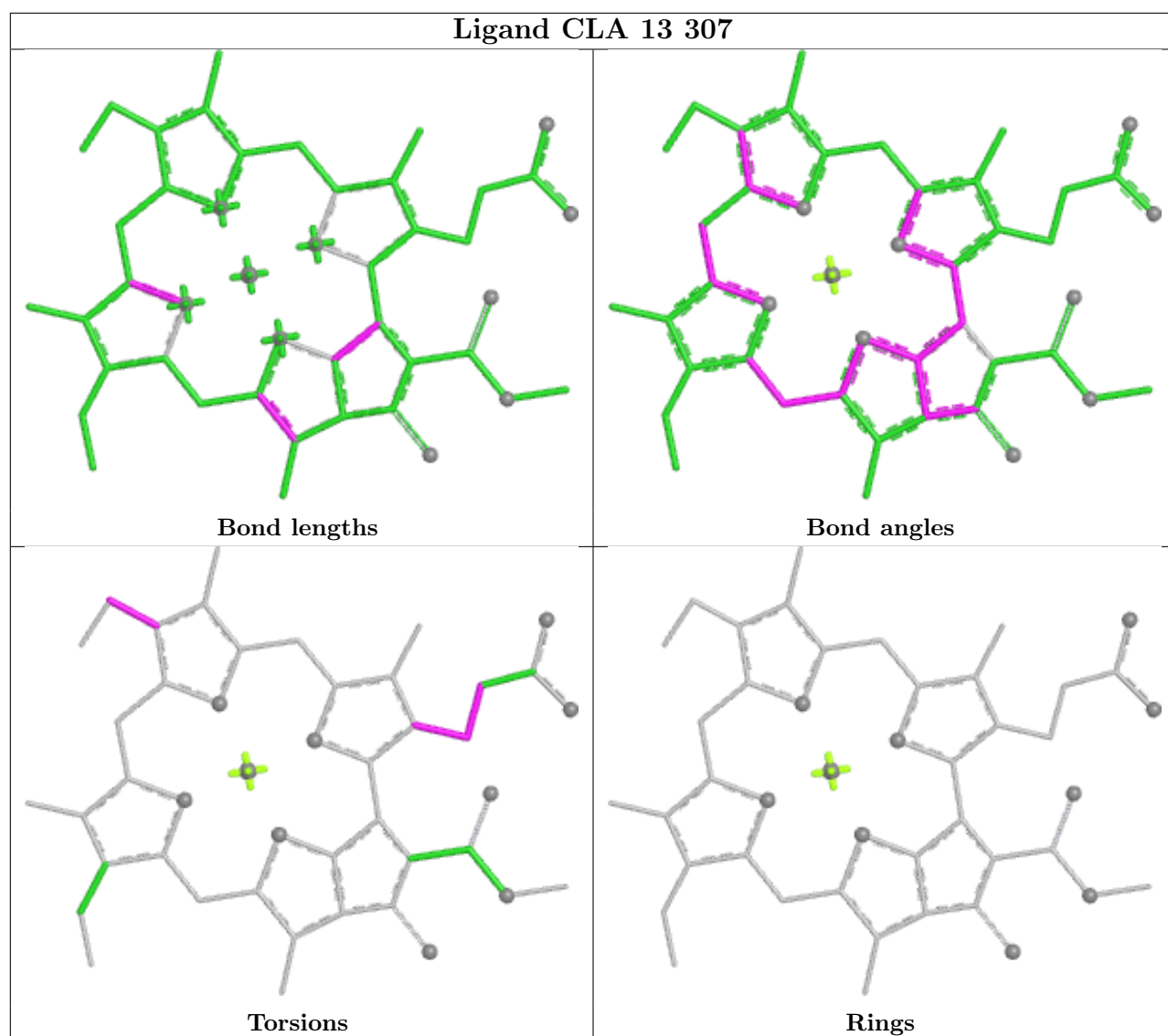


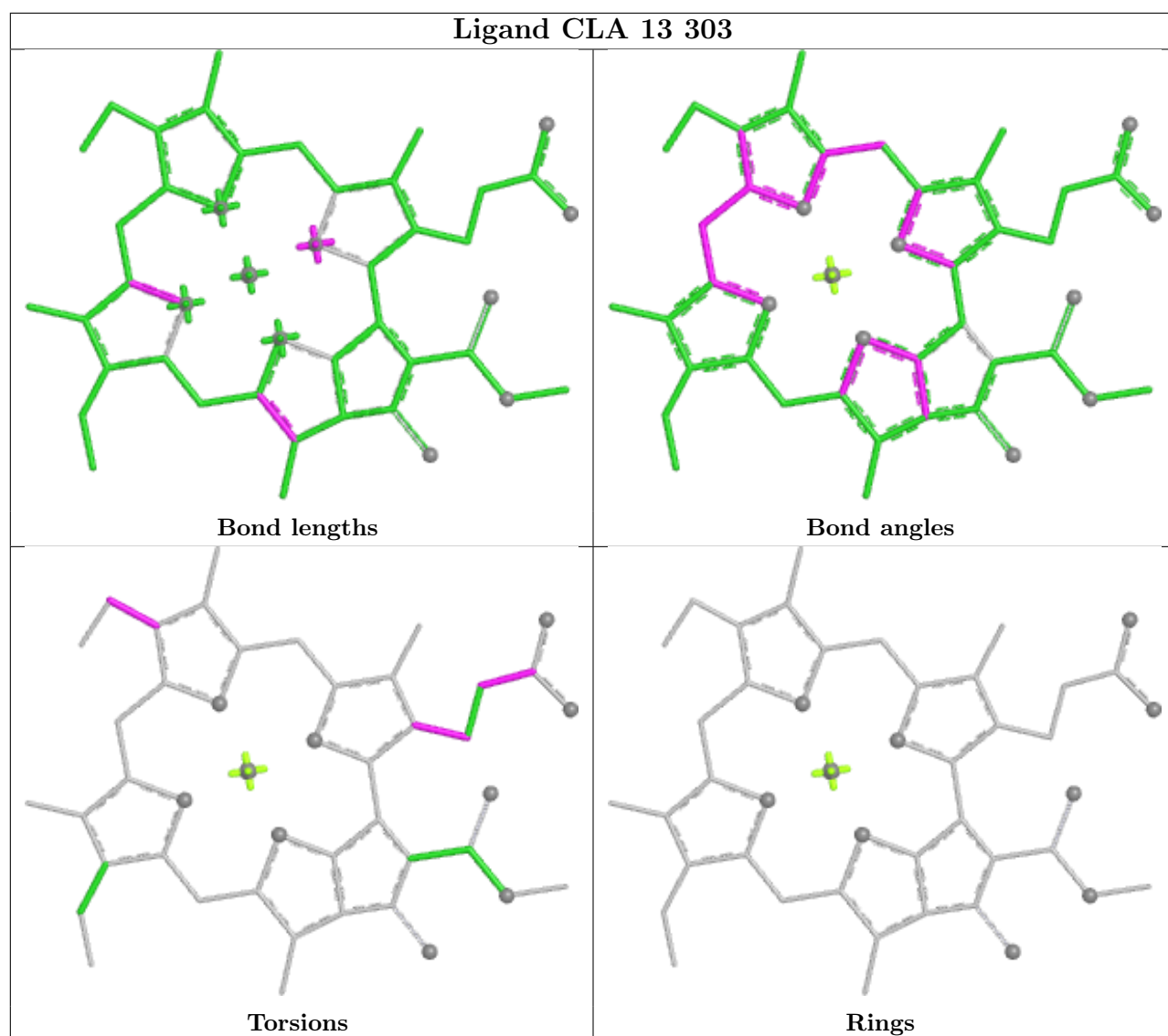


Ligand CLA 1 304

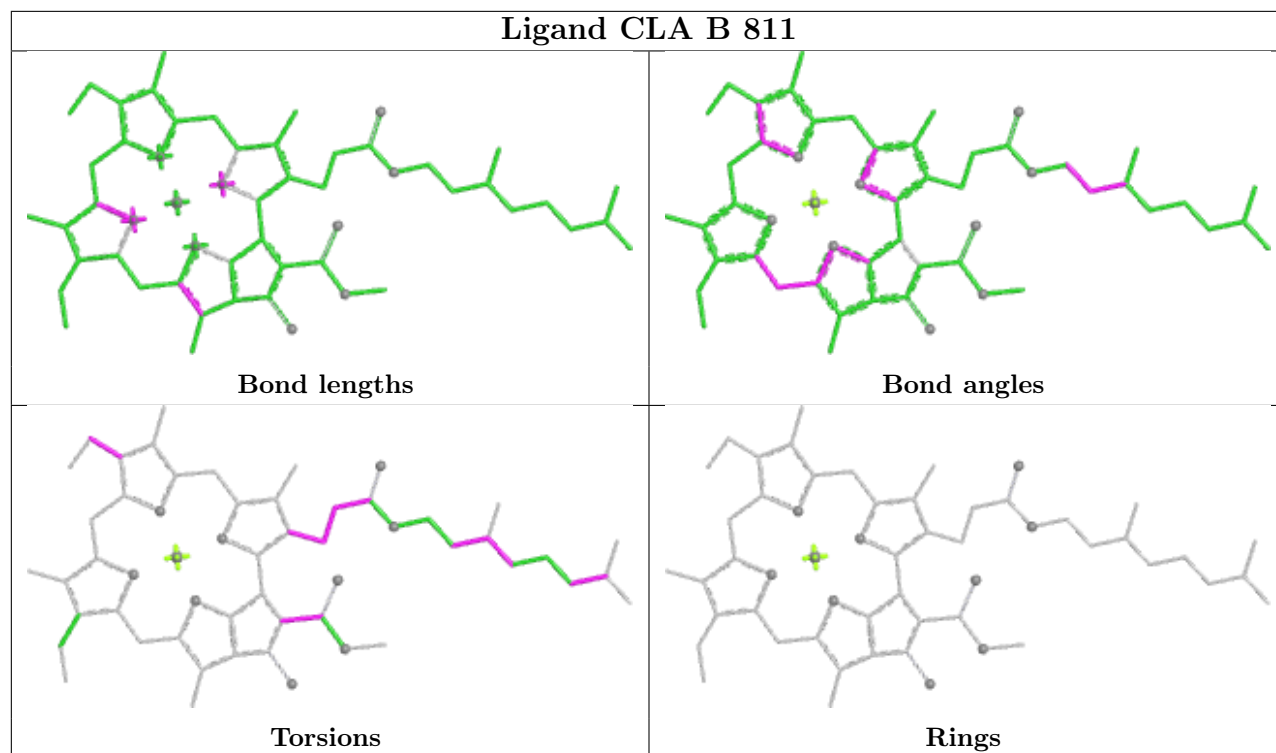




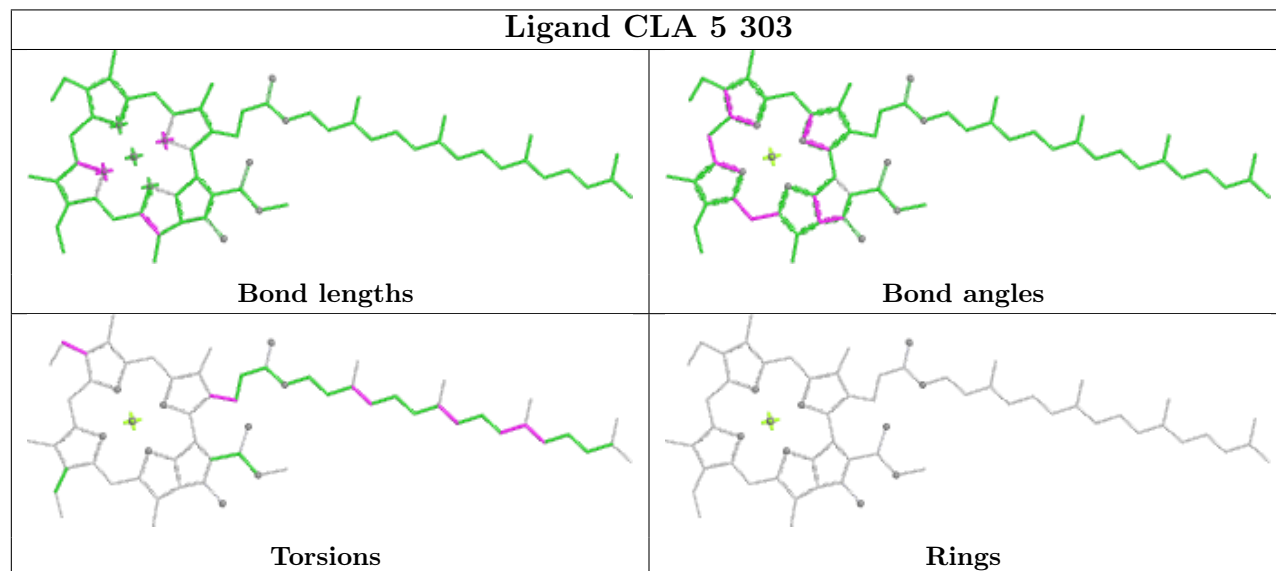


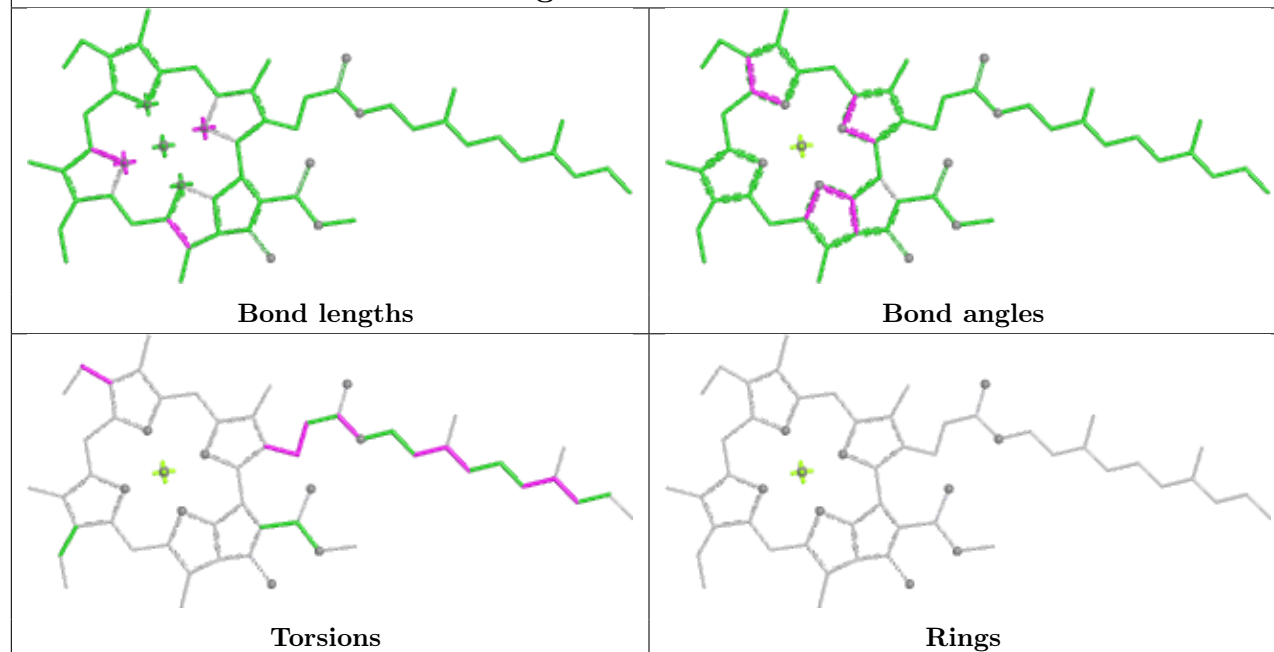
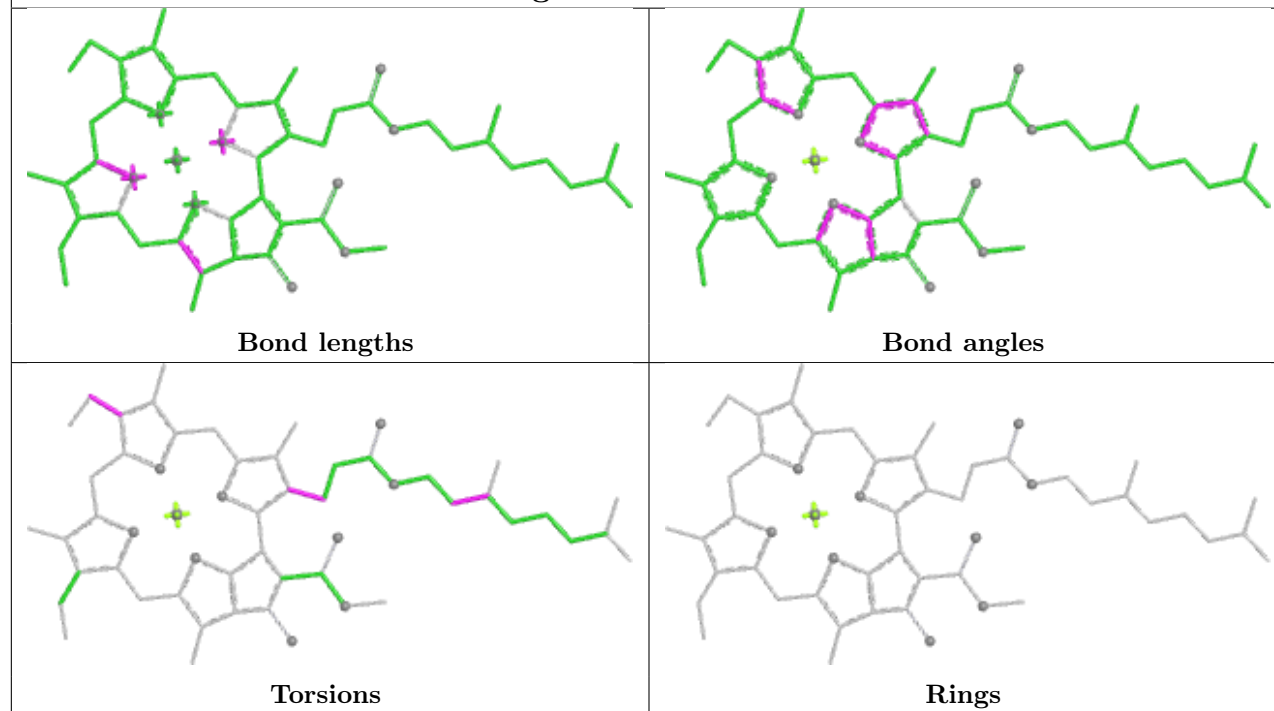


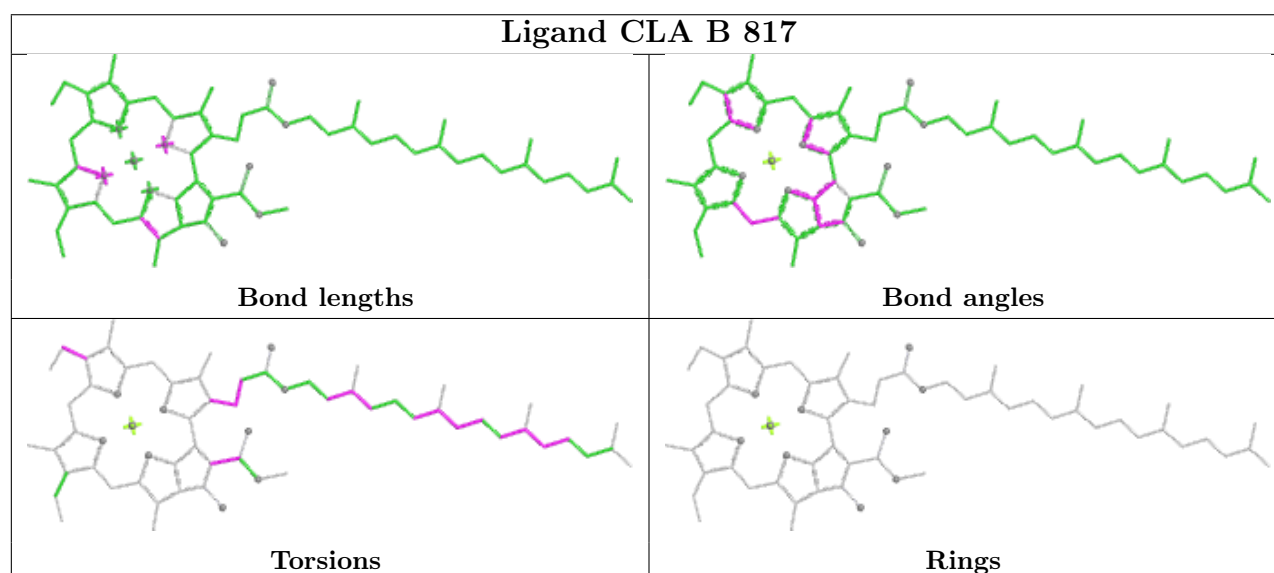
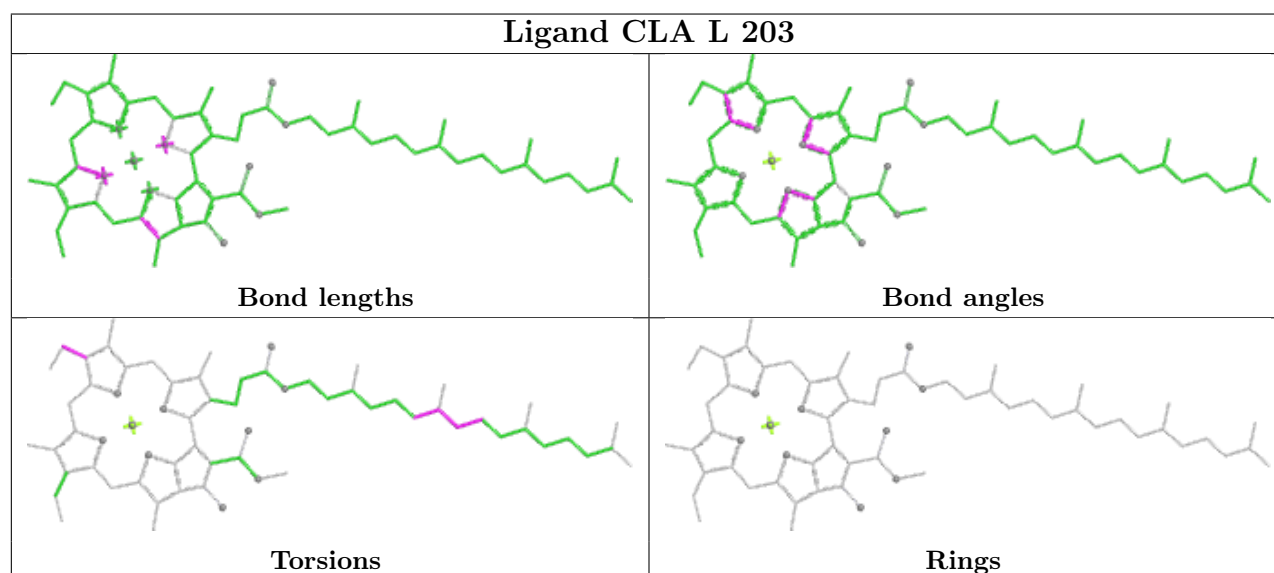
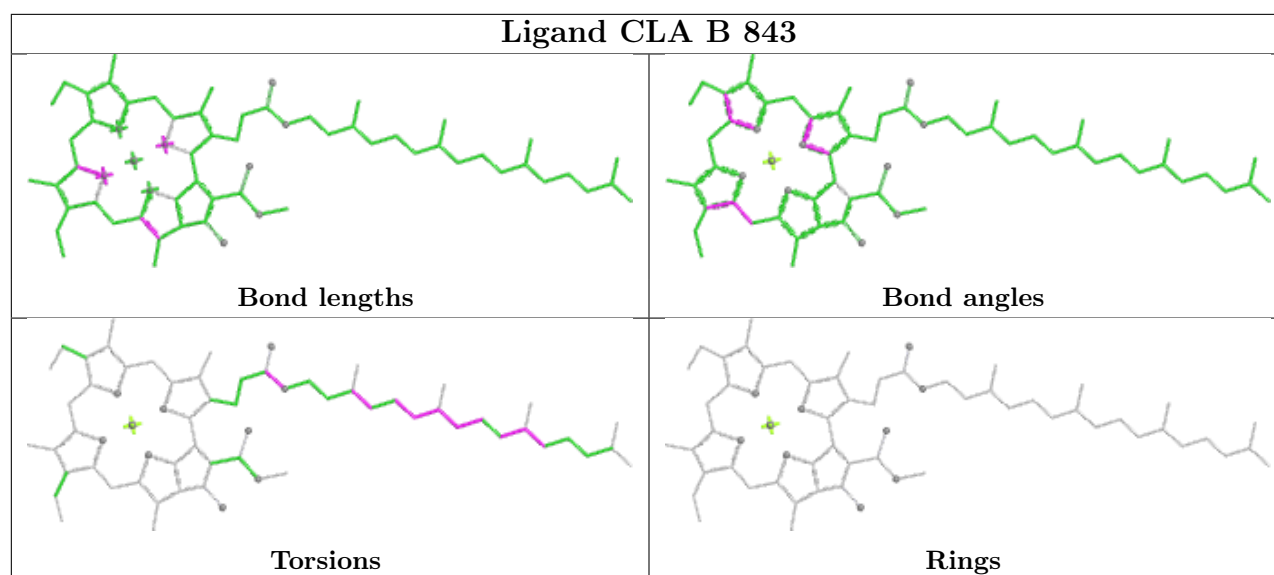
Ligand CLA B 811

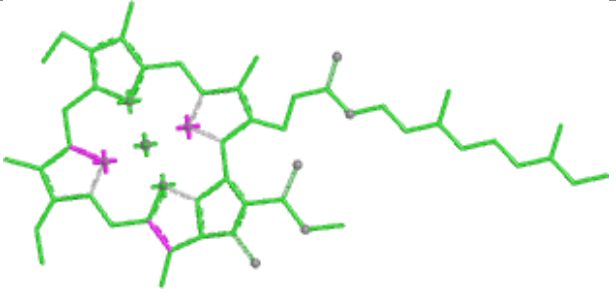
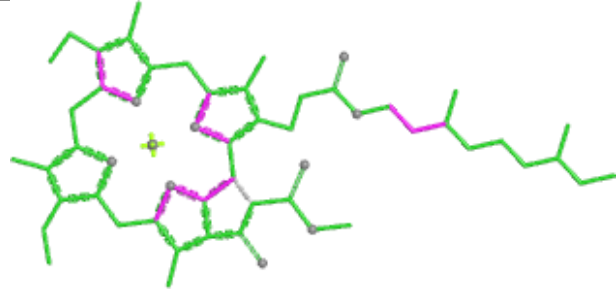
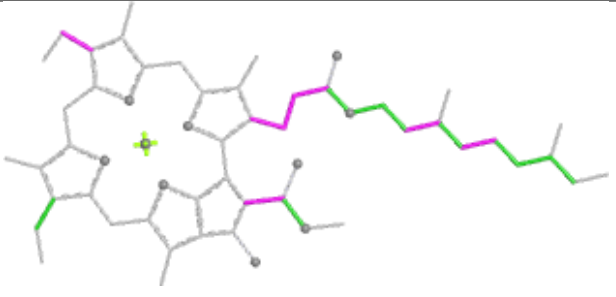
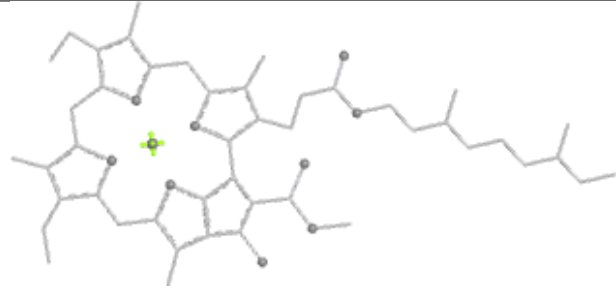


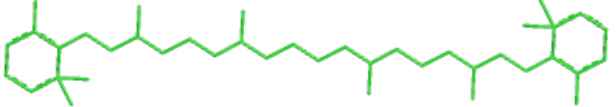
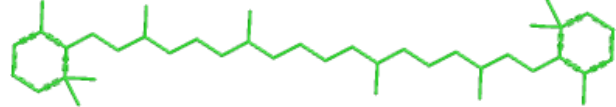

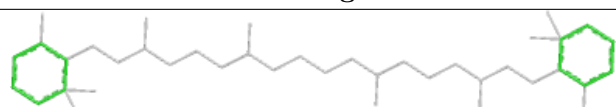
Ligand CLA 5 303

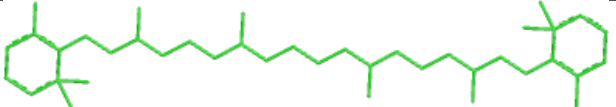
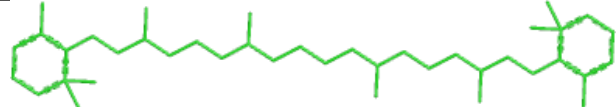
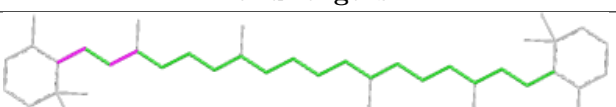
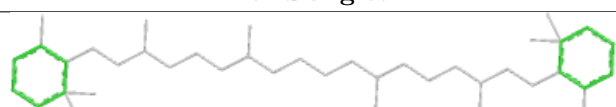


Ligand CLA 8 303**Ligand CLA B 819**

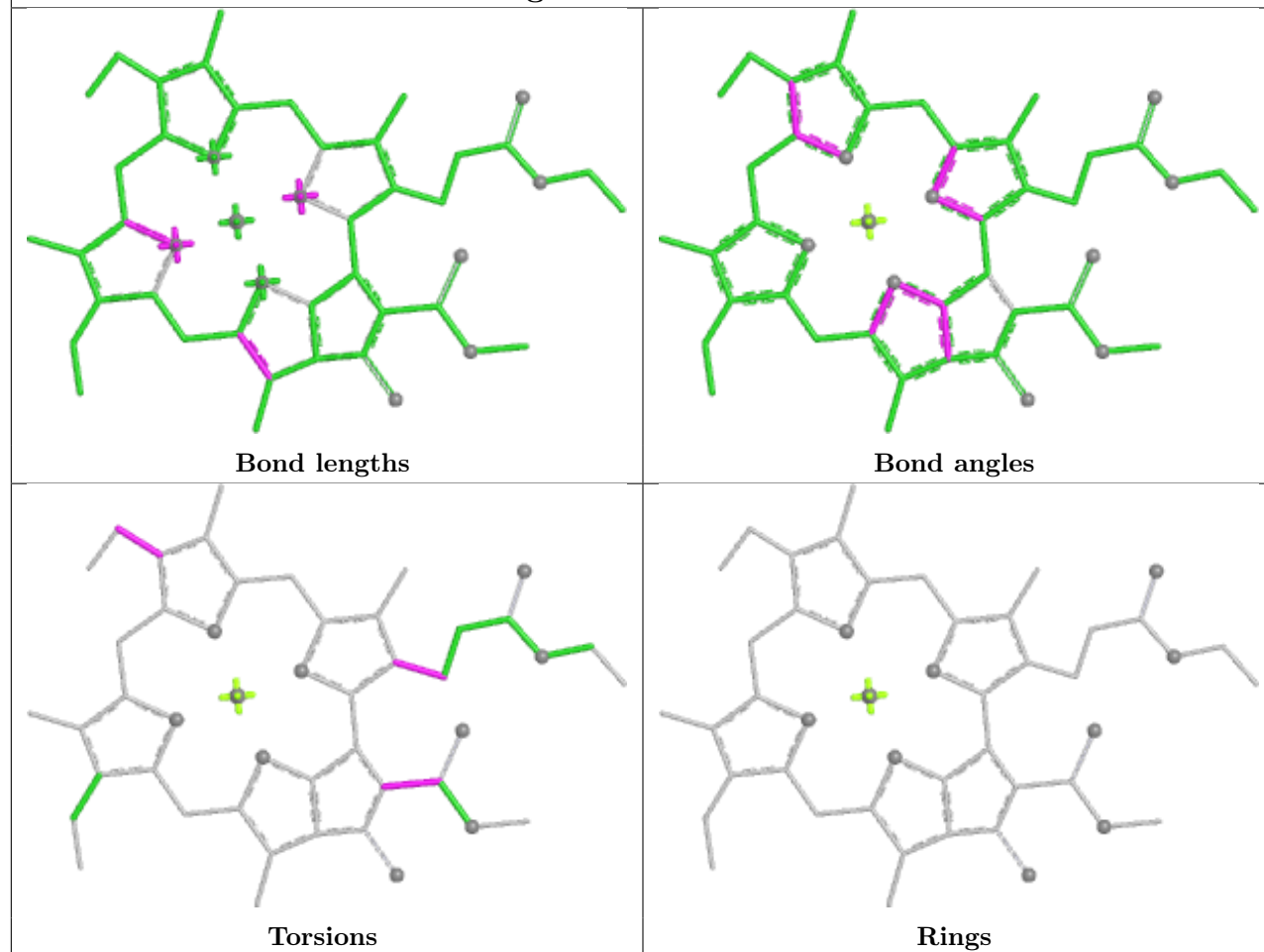


Ligand CLA 10 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

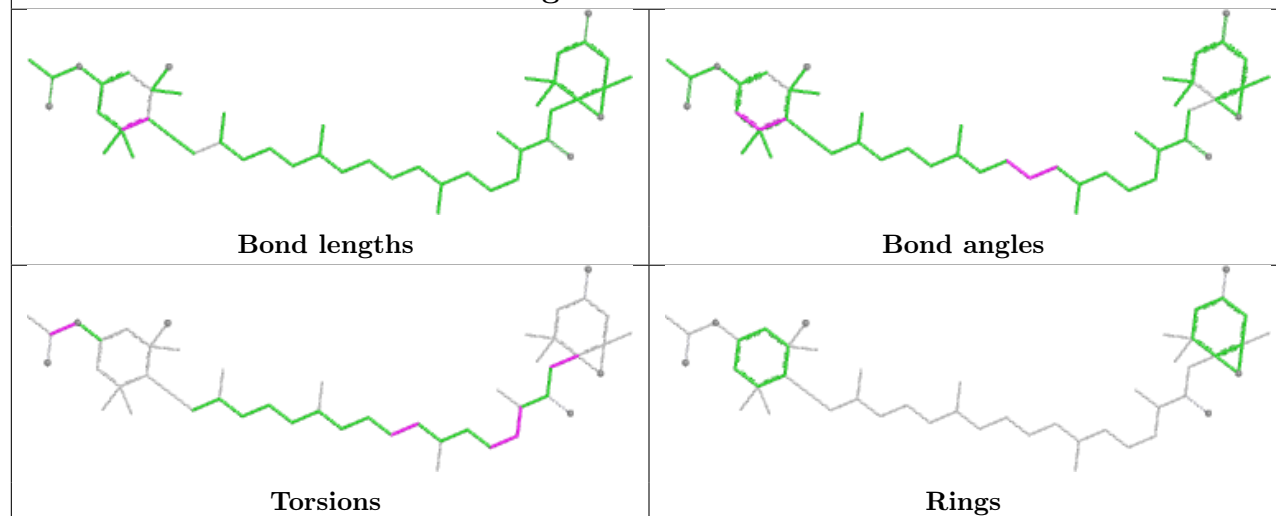
Ligand BCR B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

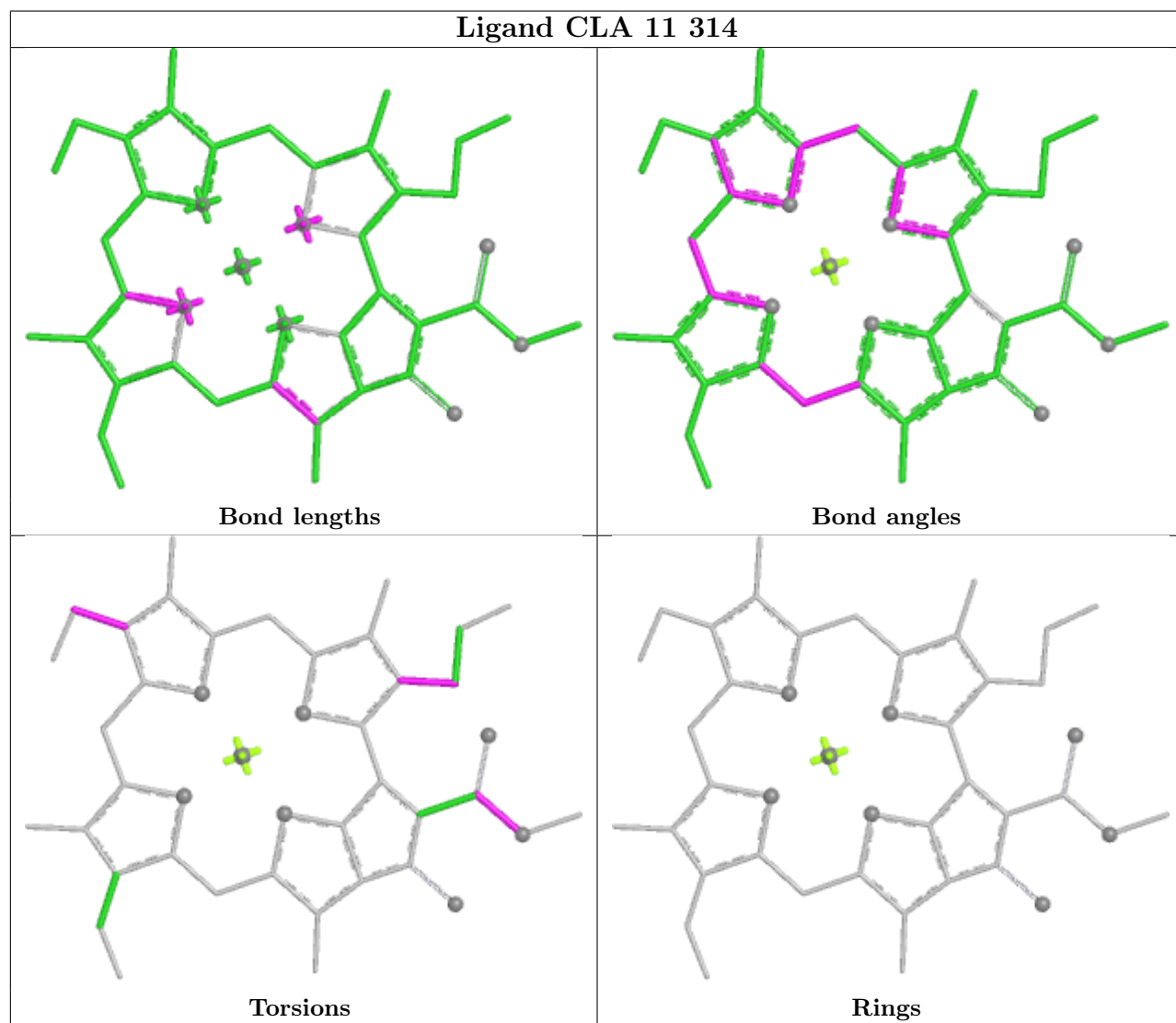
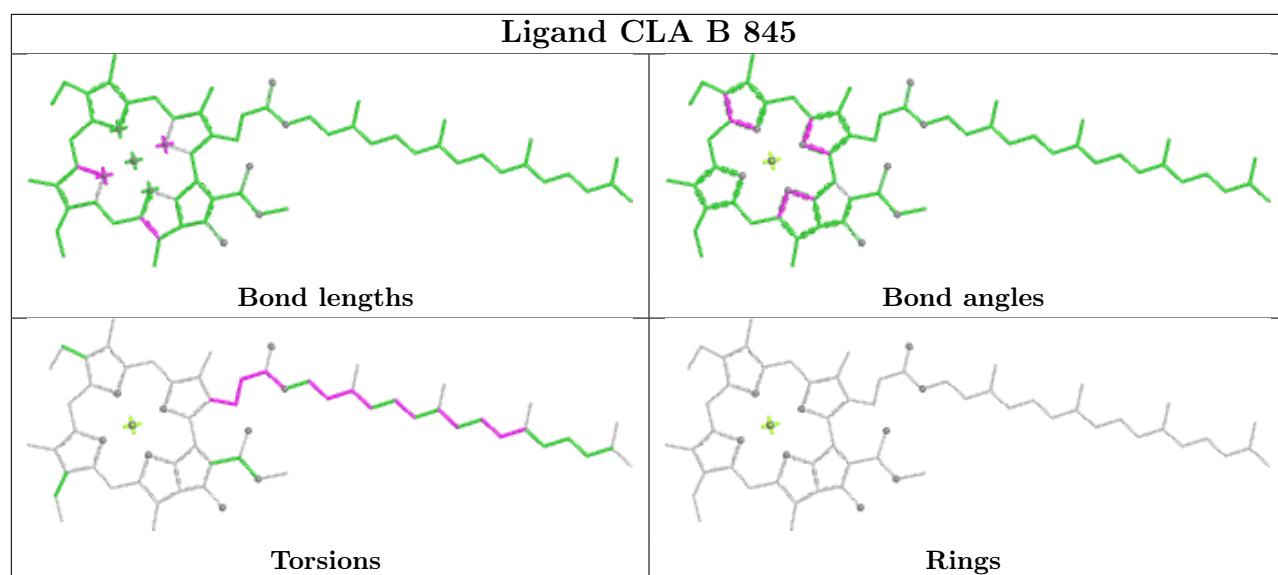
Ligand BCR 1 312	
	
Bond lengths	Bond angles
	
Torsions	Rings

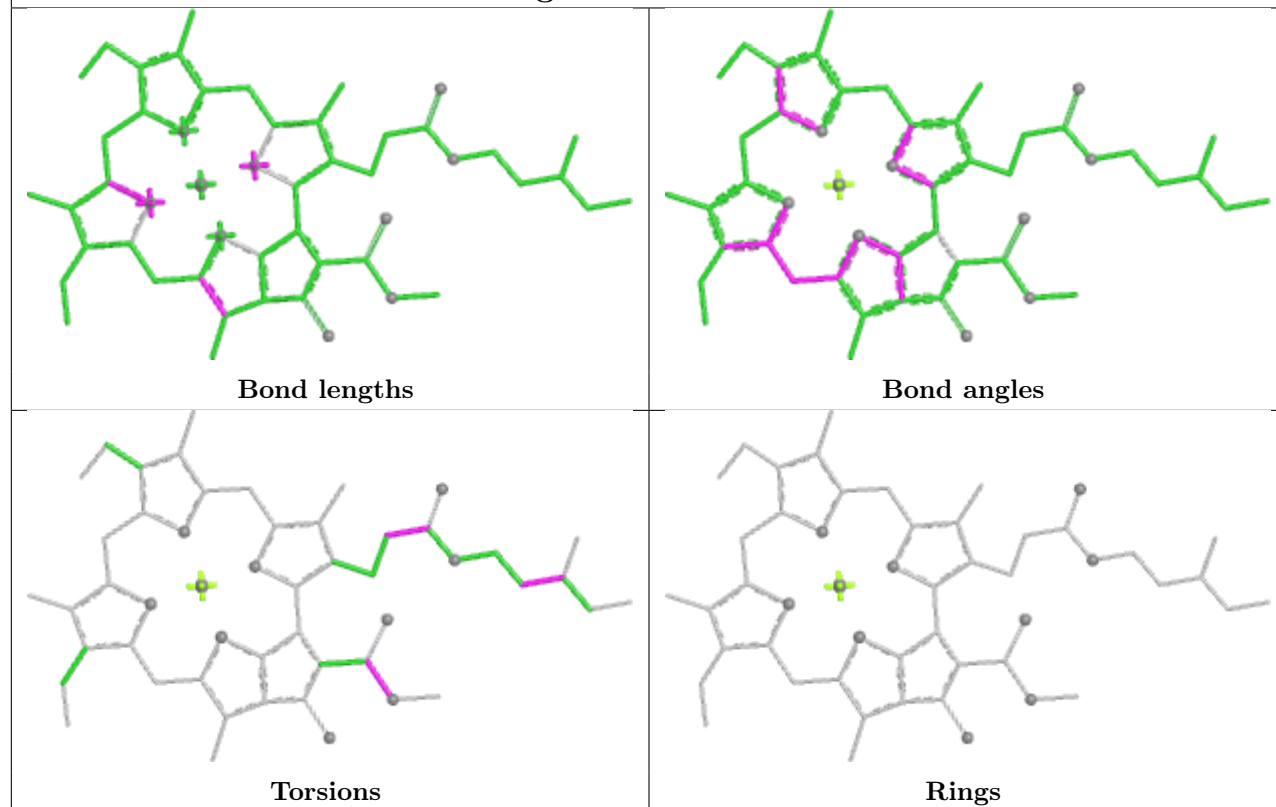
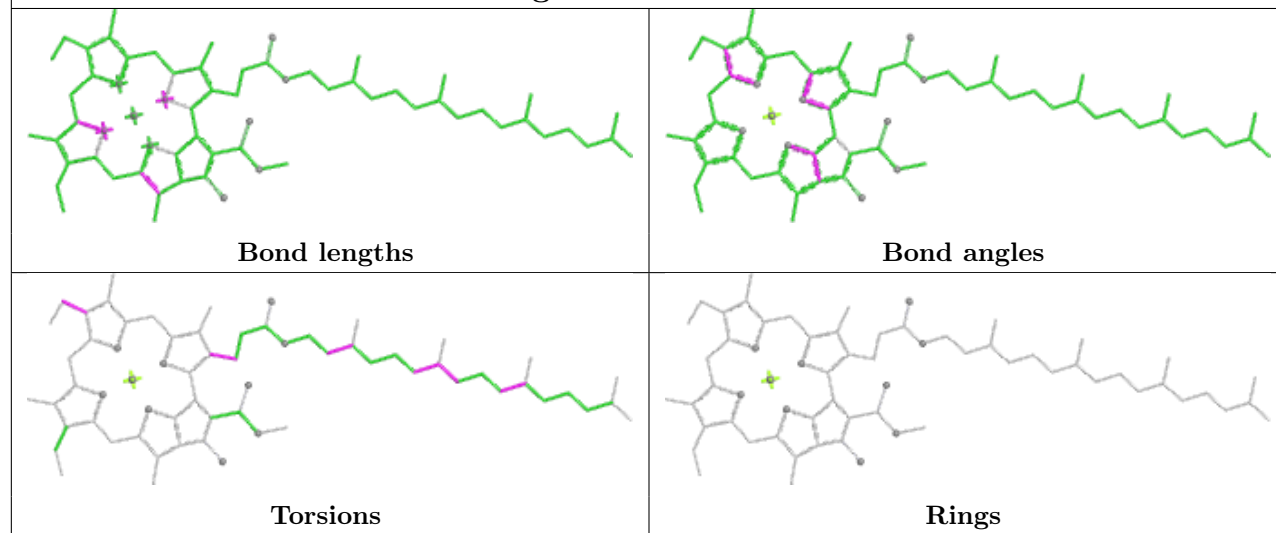
Ligand CLA A 846



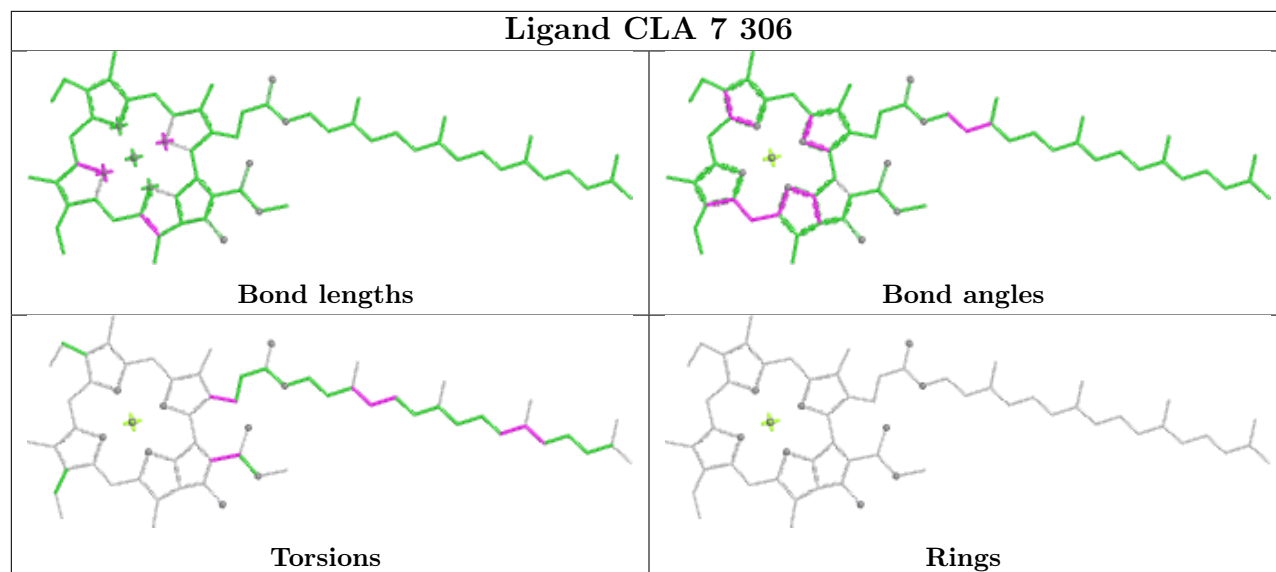
Ligand A86 6 314



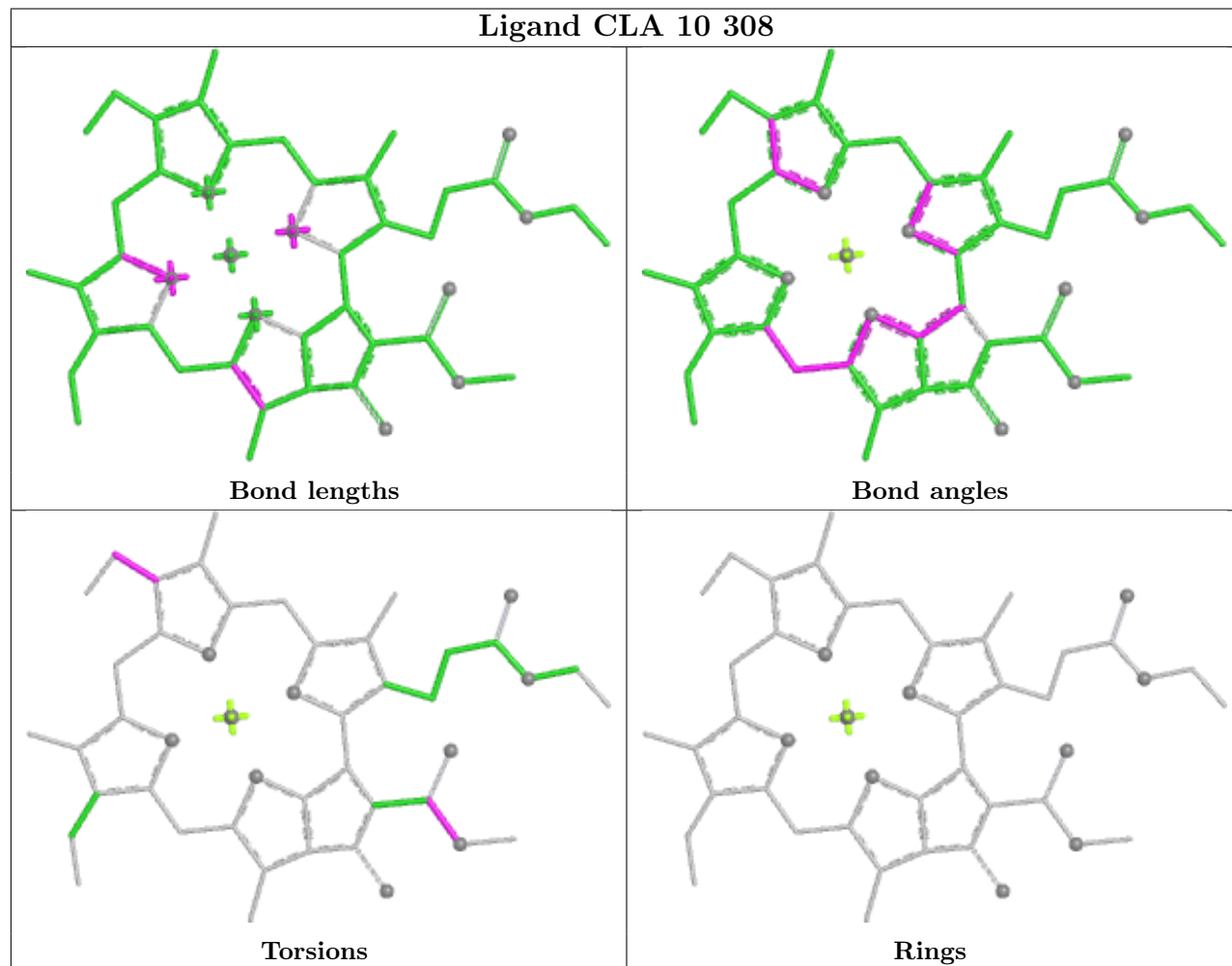


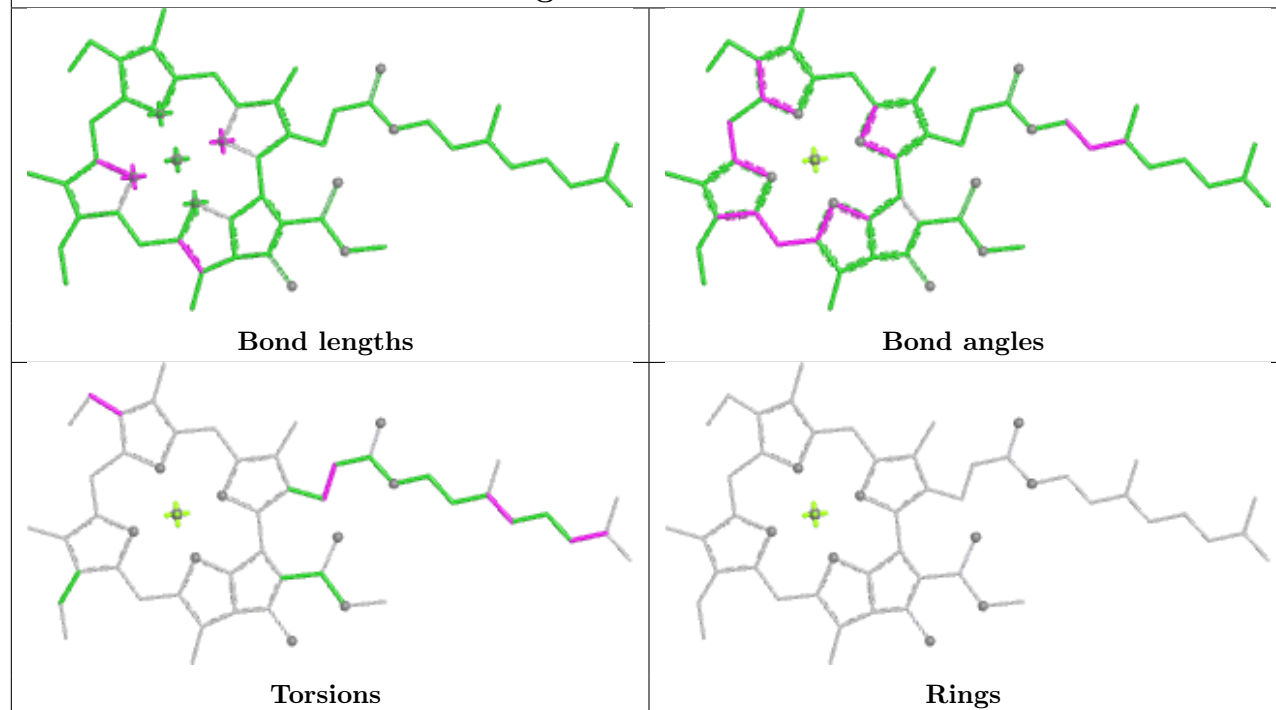
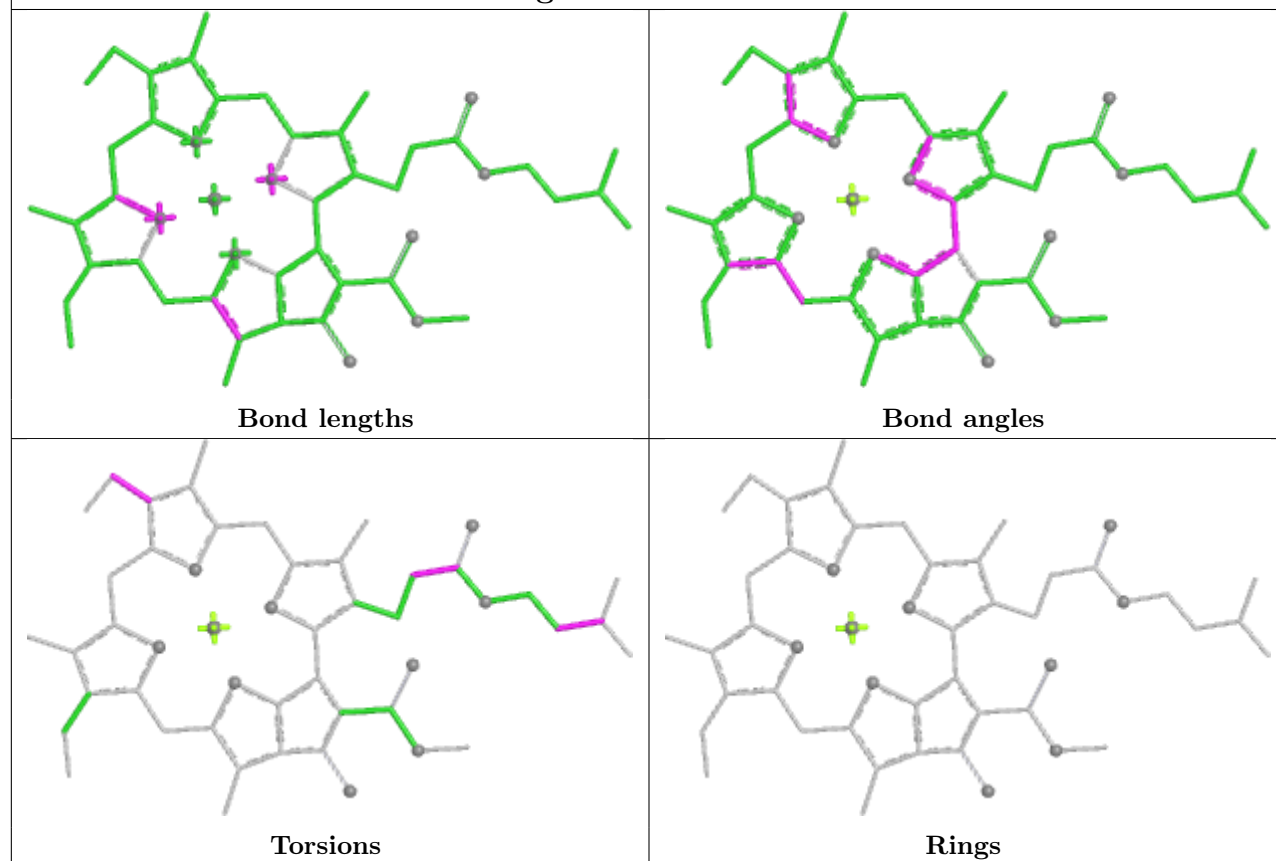
Ligand CLA 4 304**Ligand CLA B 816**

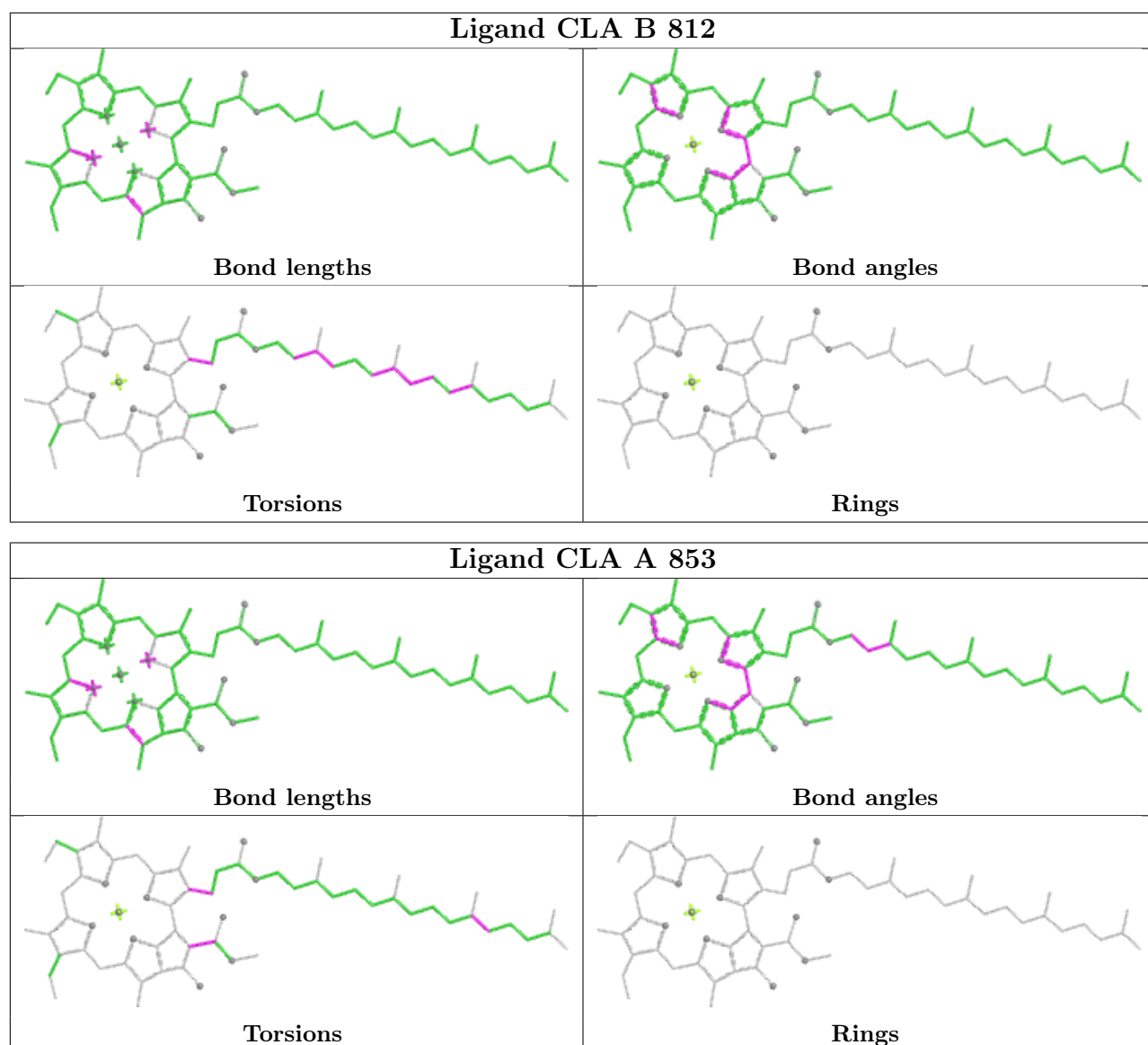
Ligand CLA 7 306

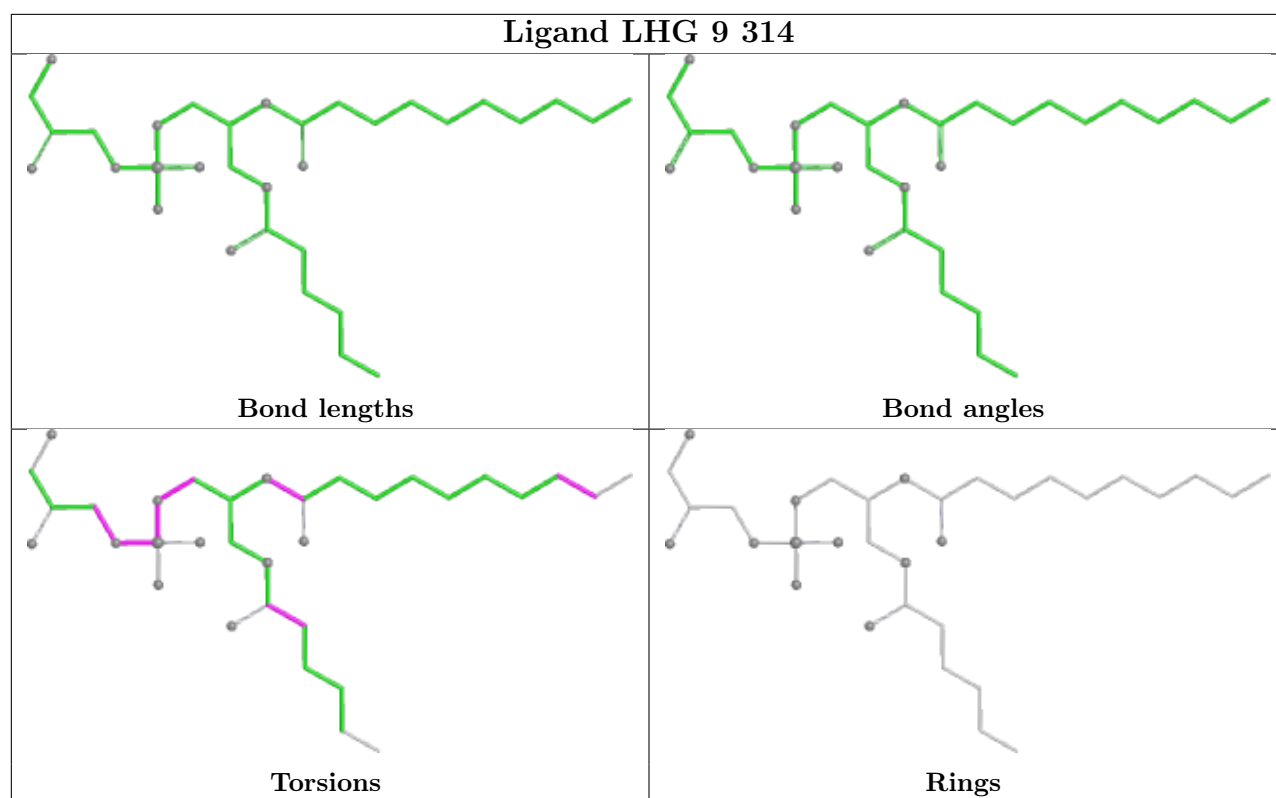


Ligand CLA 10 308

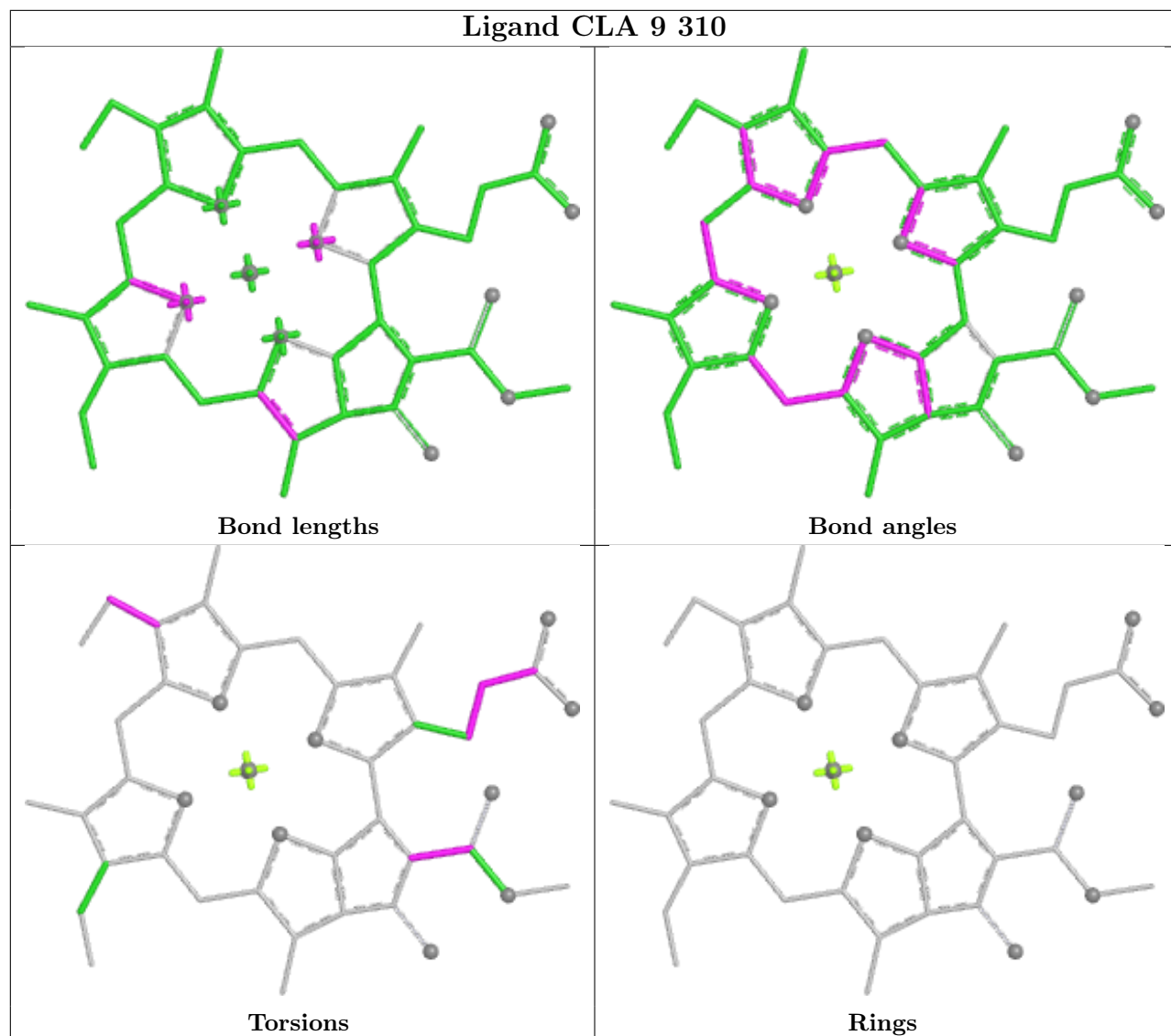


Ligand CLA 6 303**Ligand CLA 7 302**

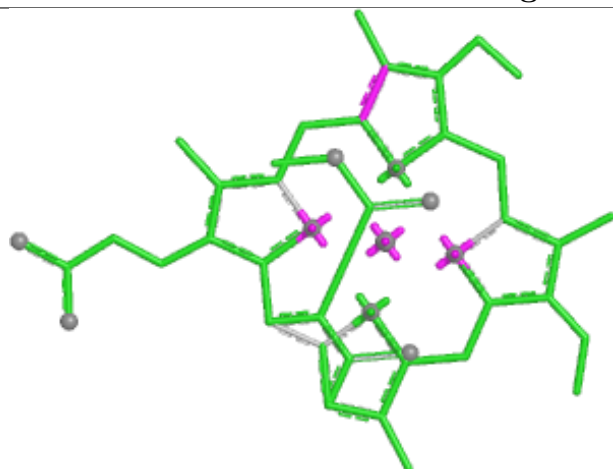




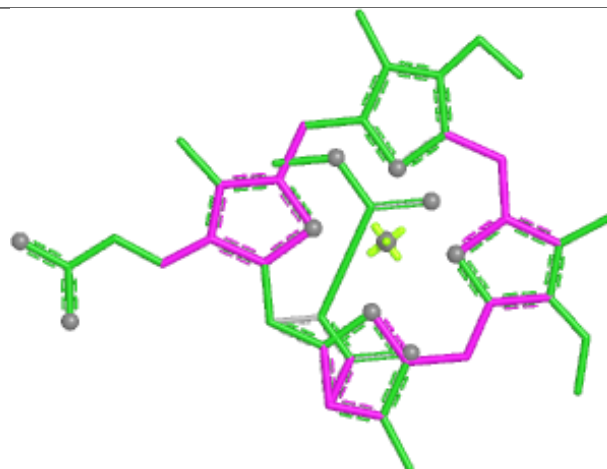
Ligand CLA 9 310



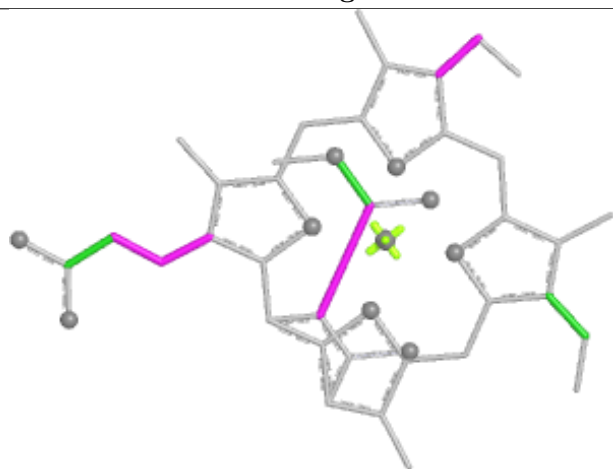
Ligand KC1 9 306



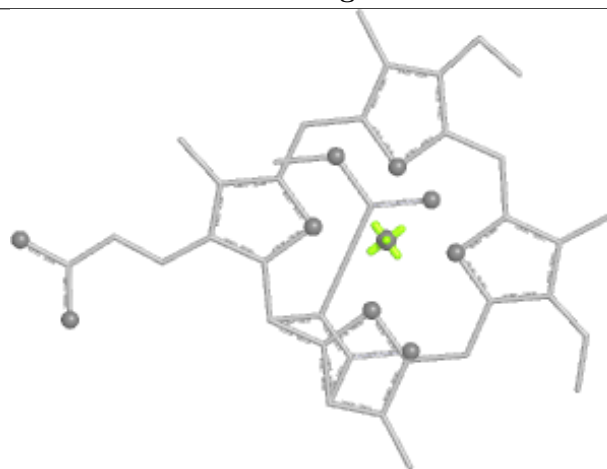
Bond lengths



Bond angles

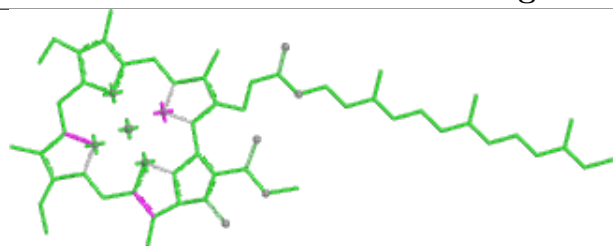


Torsions

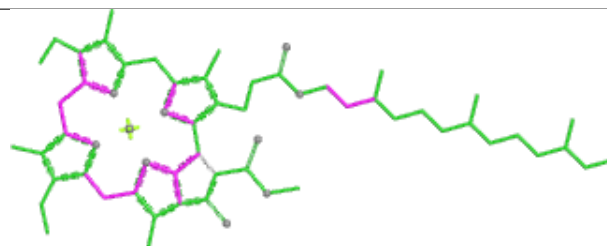


Rings

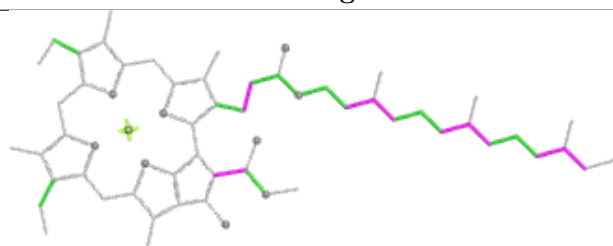
Ligand CLA 4 316



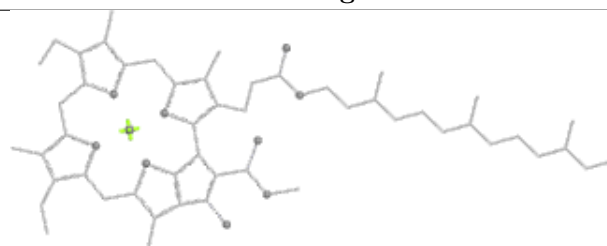
Bond lengths



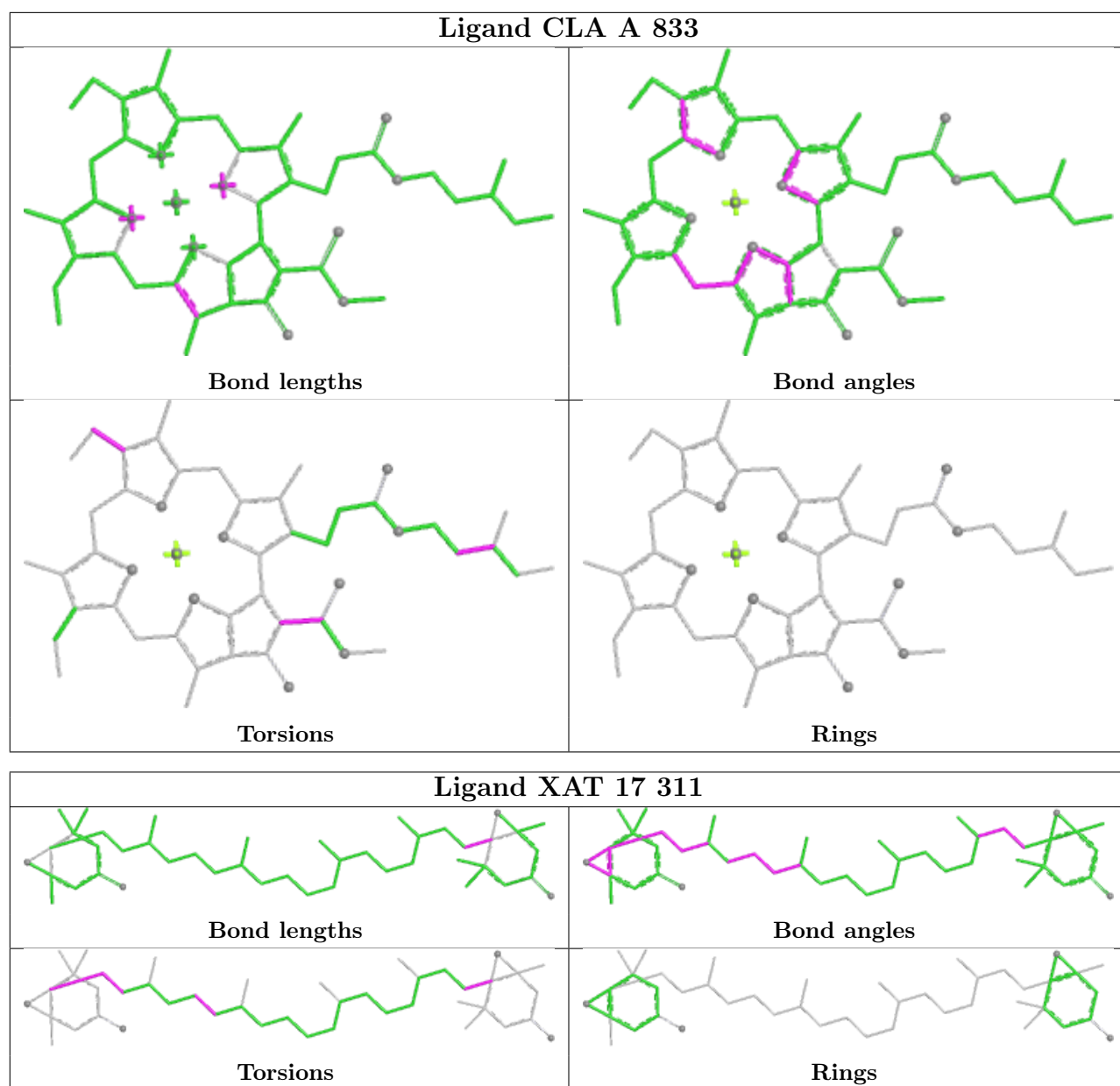
Bond angles

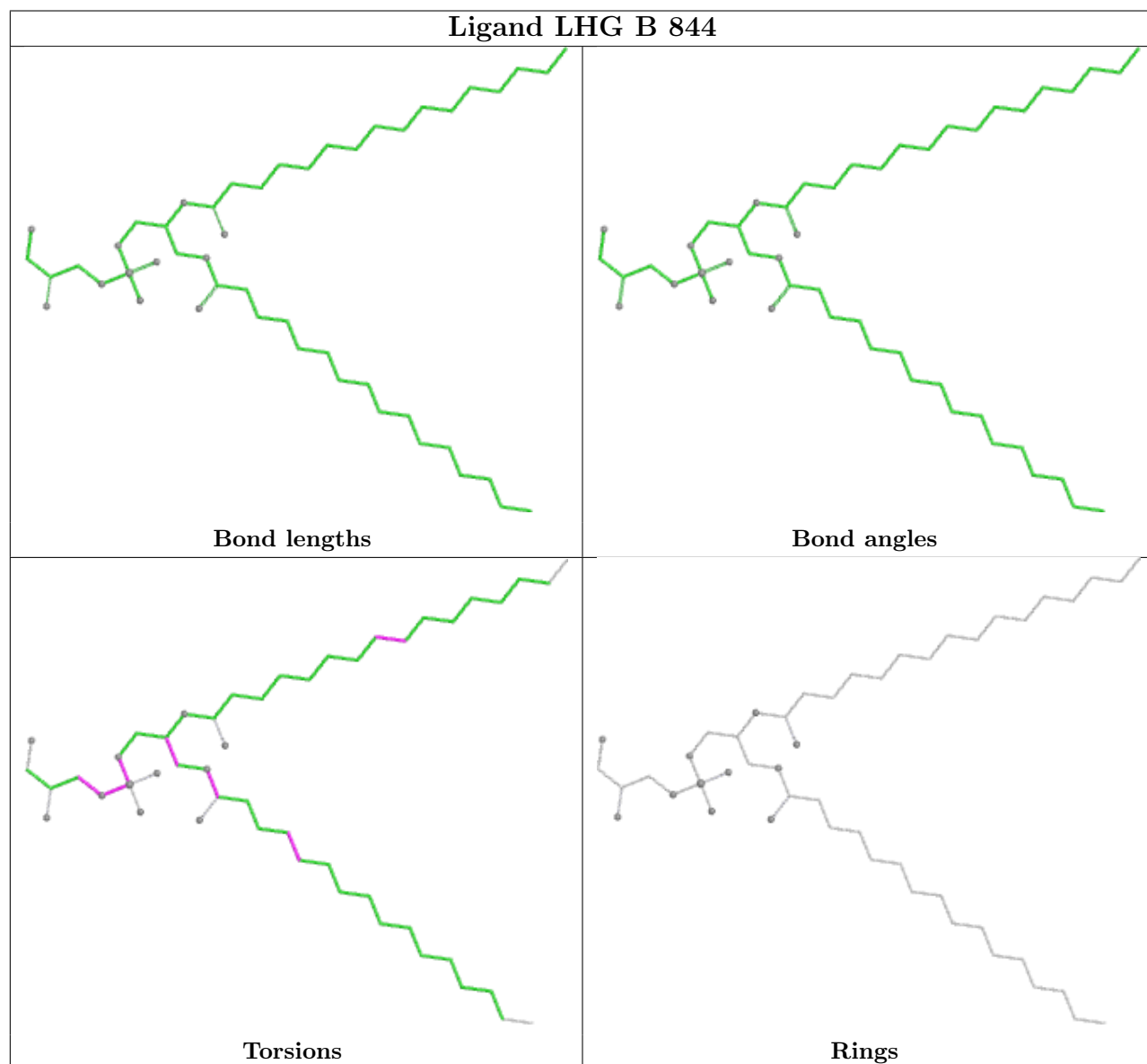
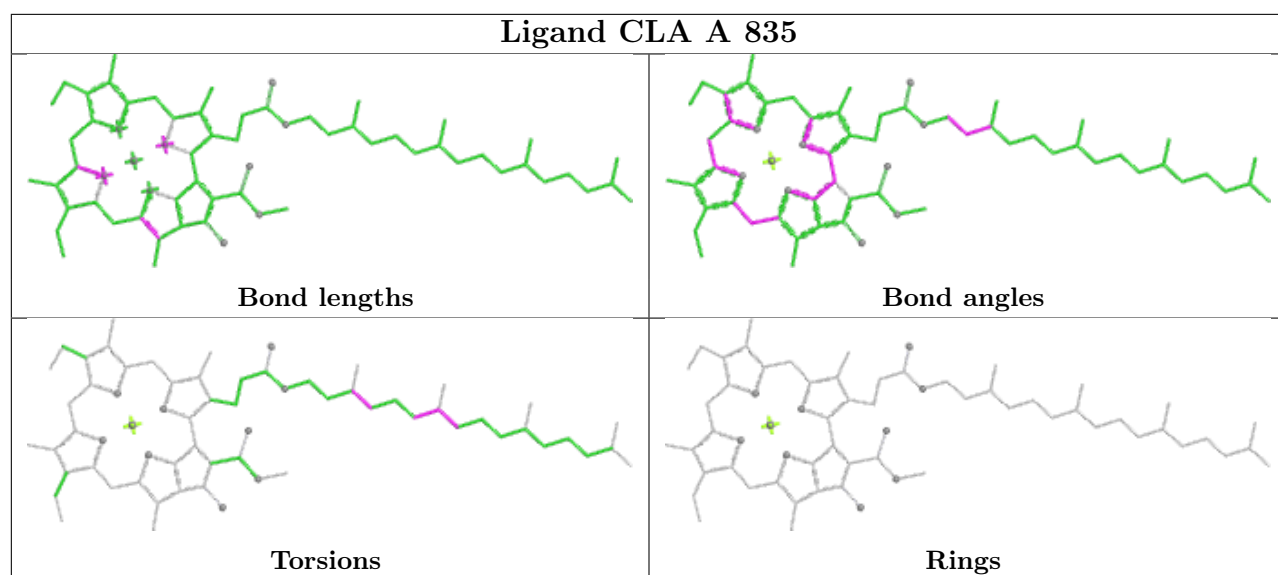


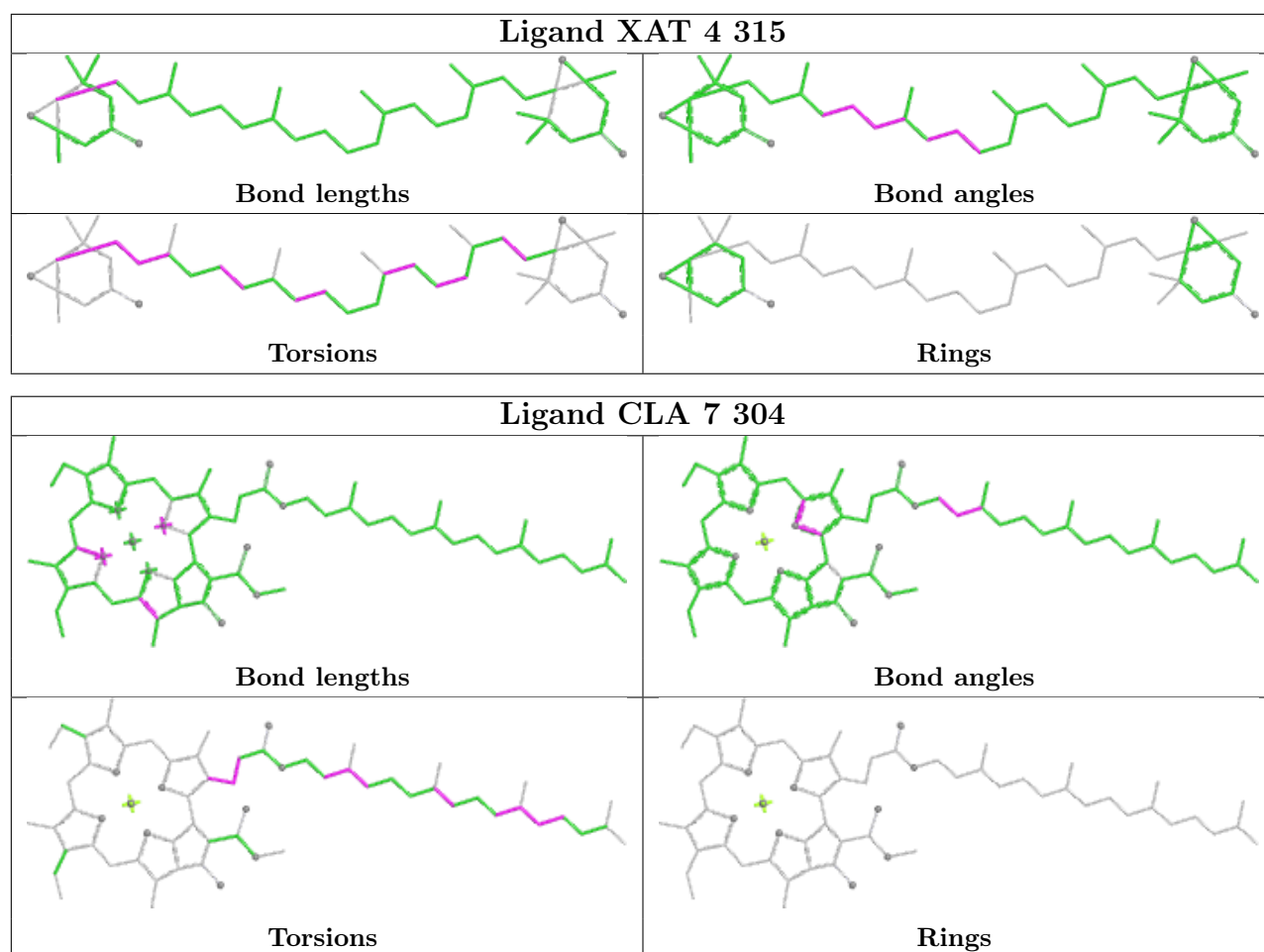
Torsions



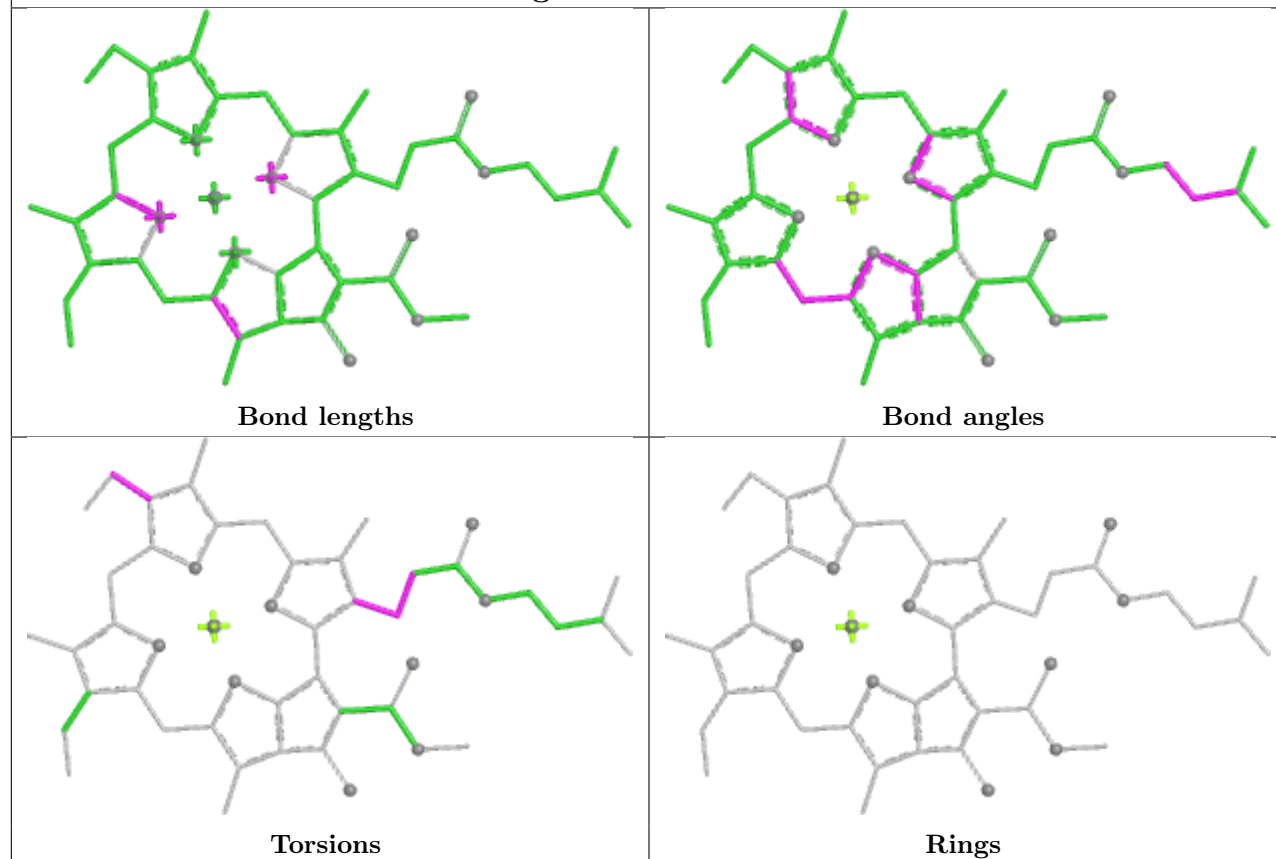
Rings



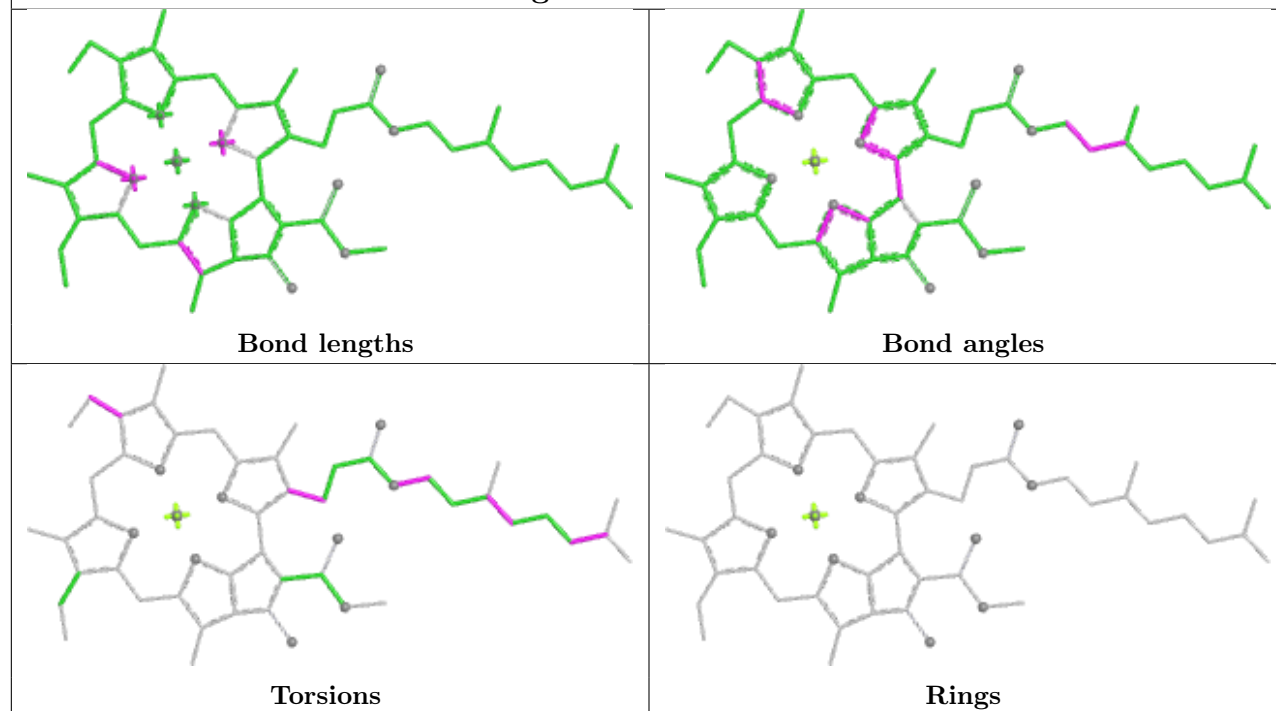


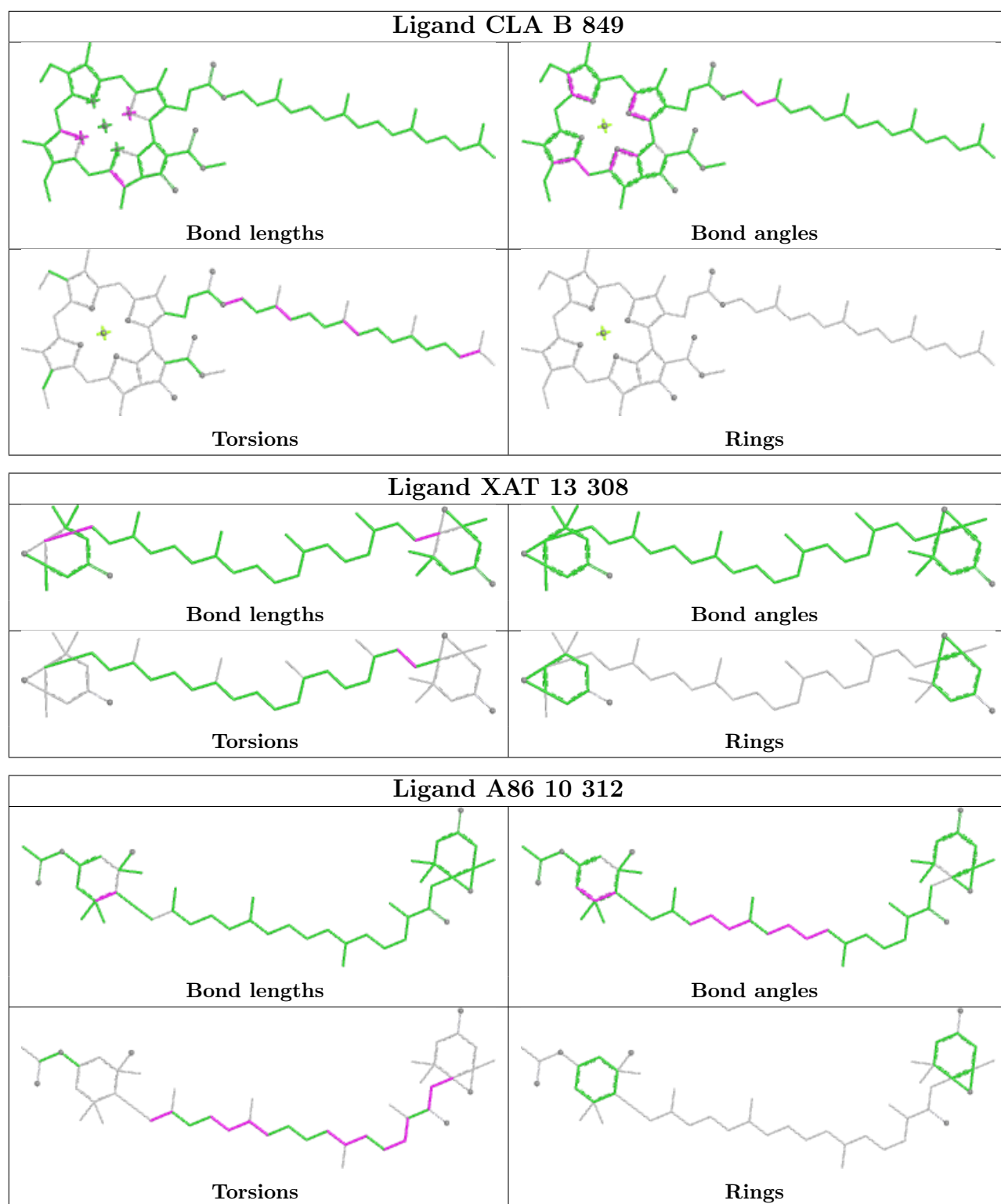


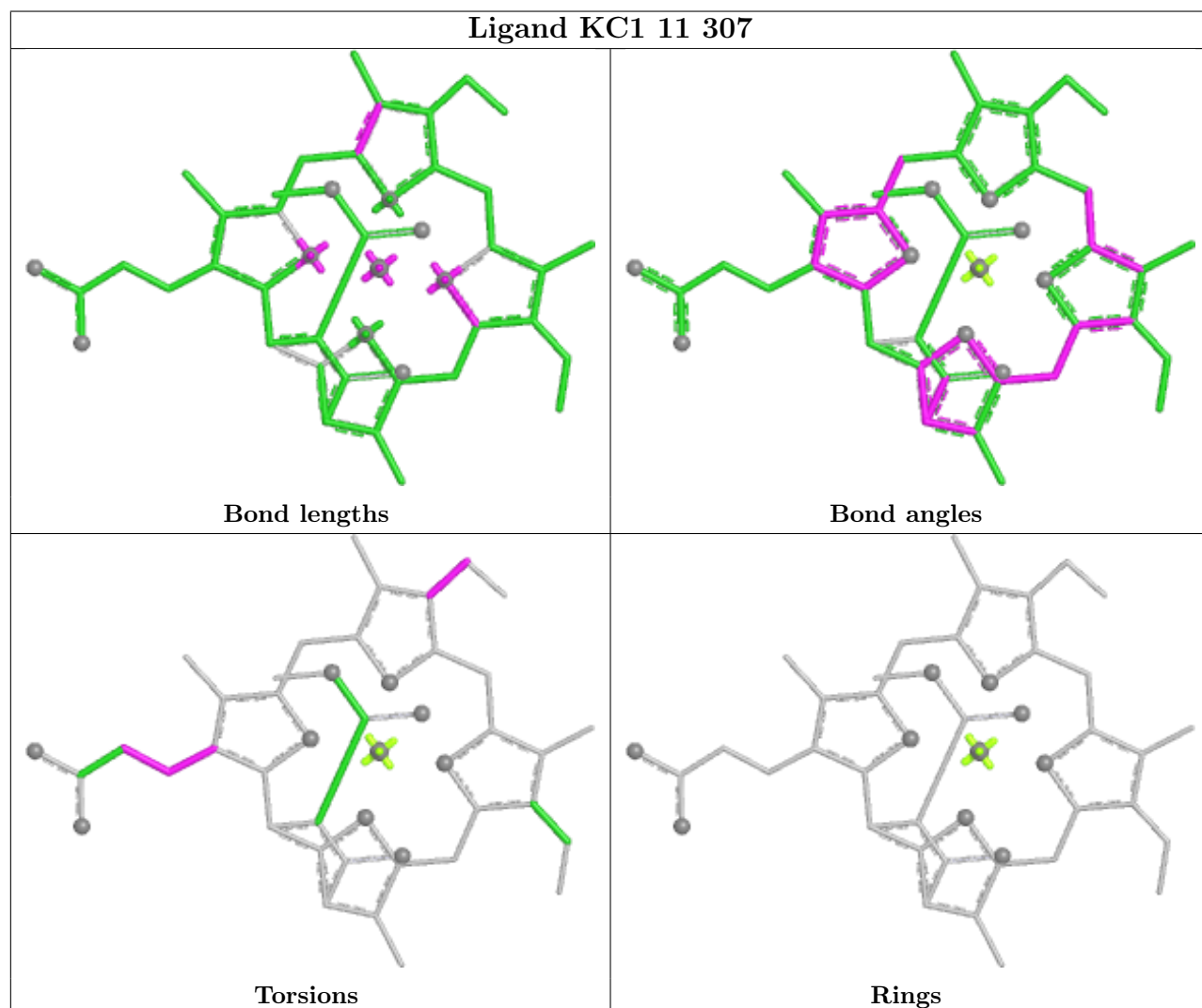
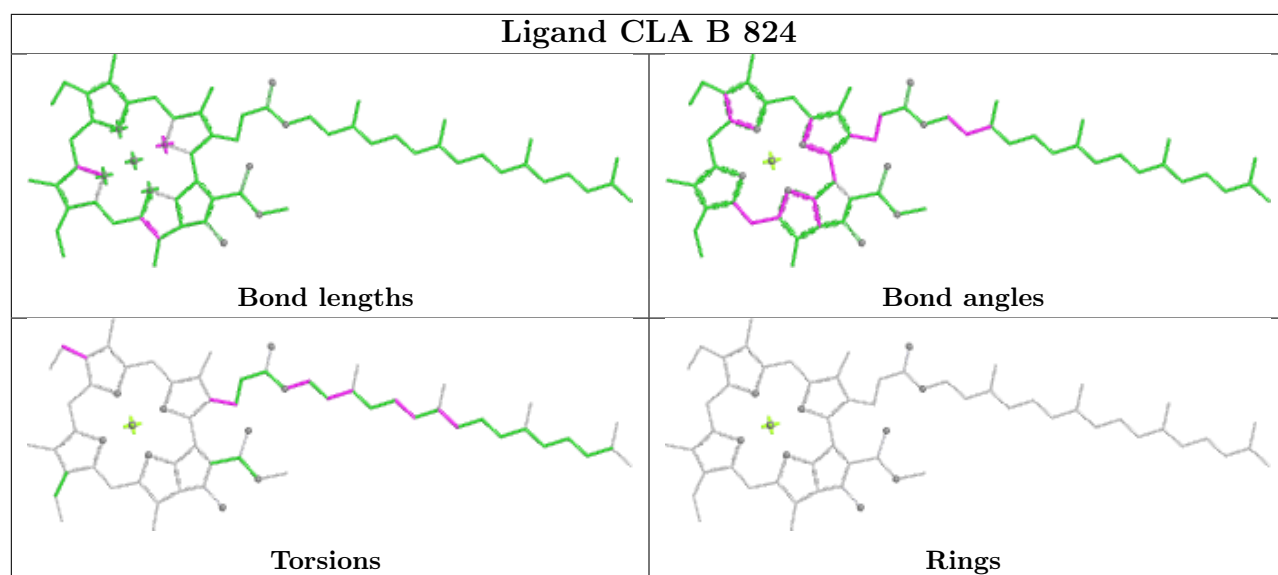
Ligand CLA B 827

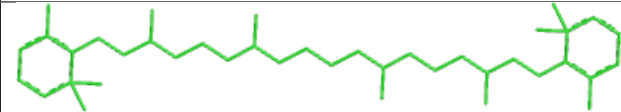
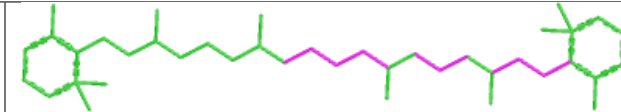
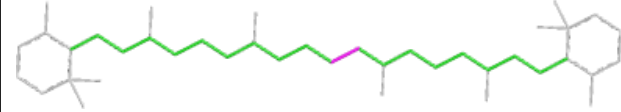
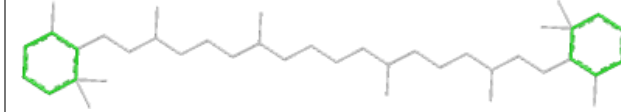


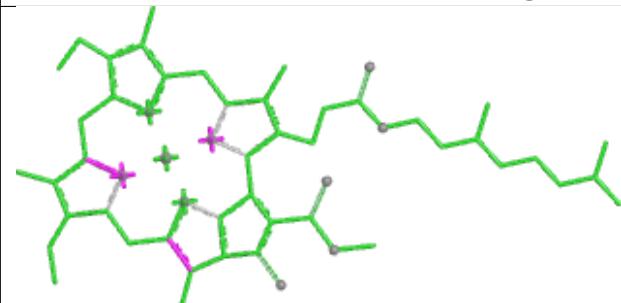
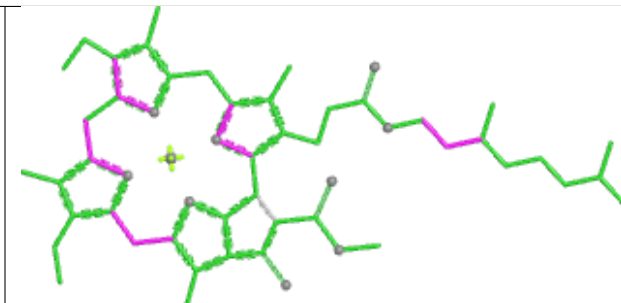
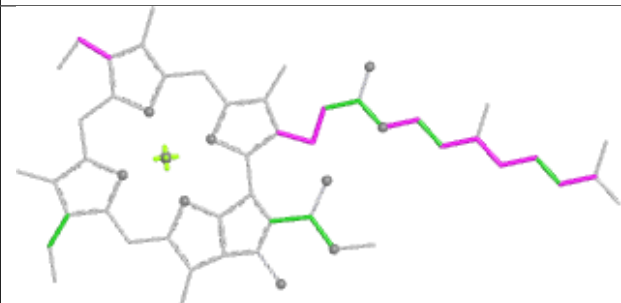
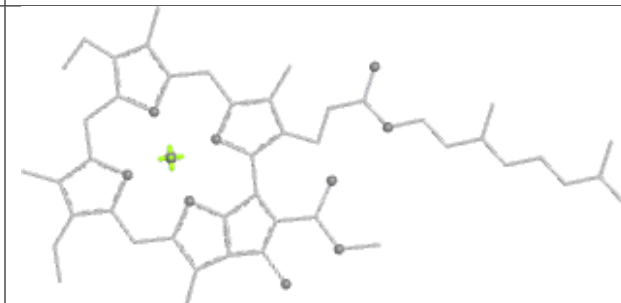
Ligand CLA R 202

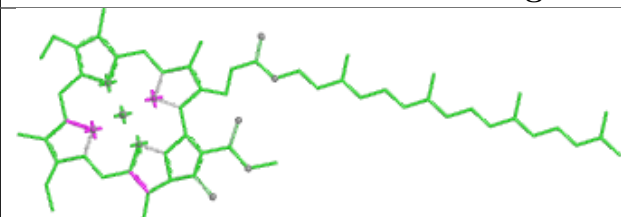
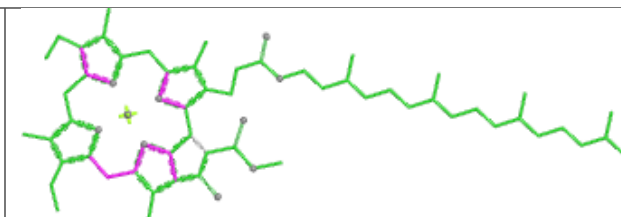
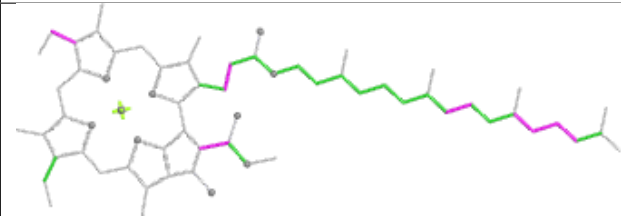
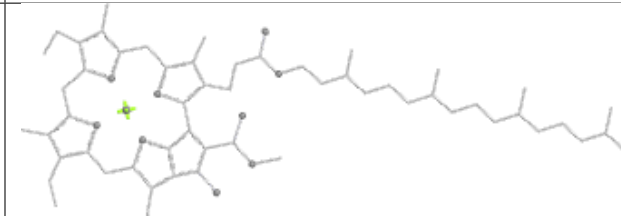




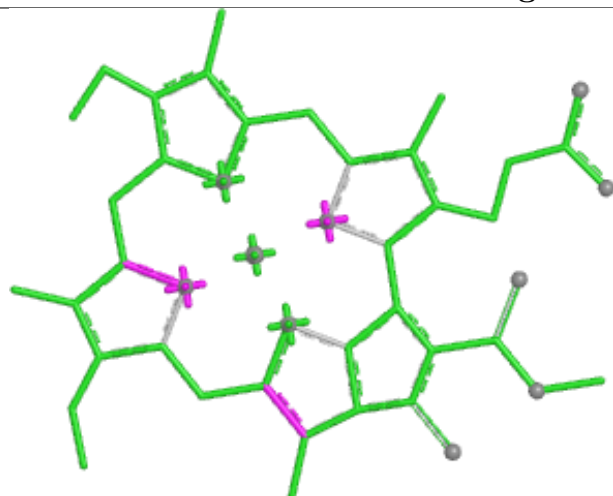


Ligand BCR B 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

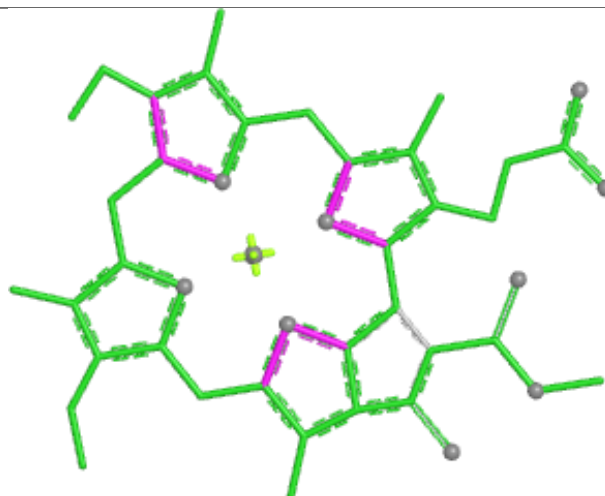
Ligand CLA A 806	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 3 314	
	
Bond lengths	Bond angles
	
Torsions	Rings

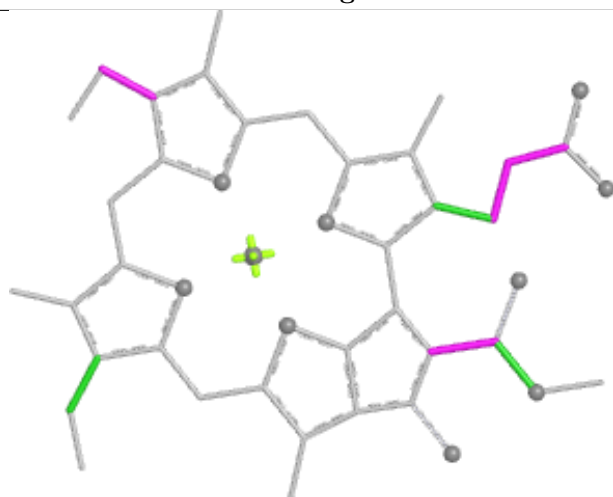
Ligand CLA 8 305



Bond lengths



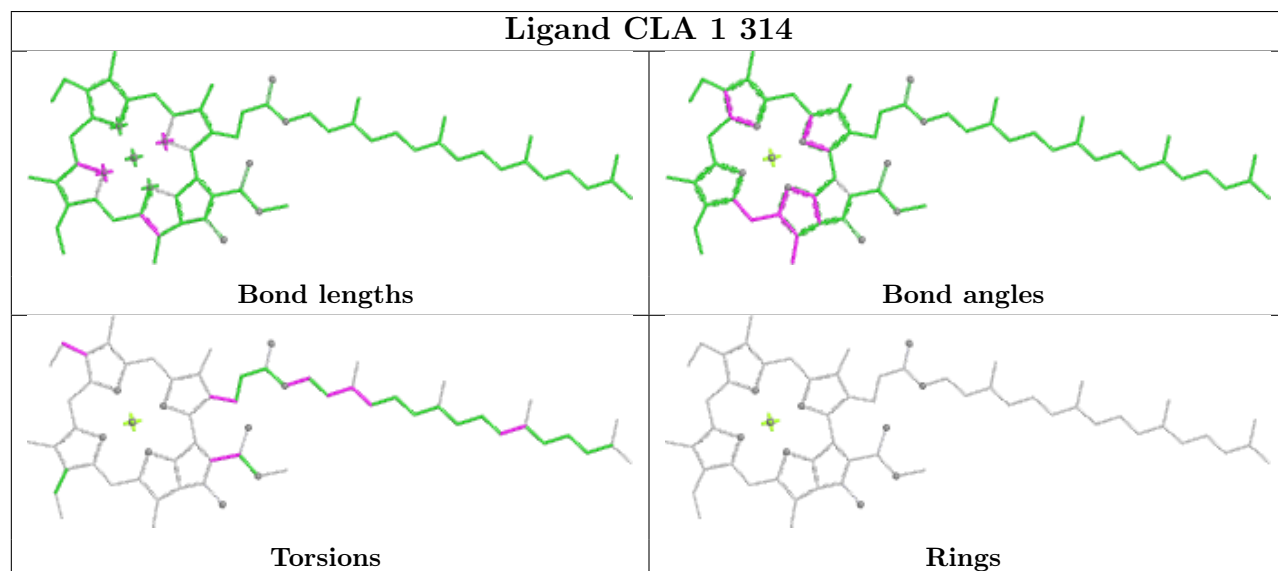
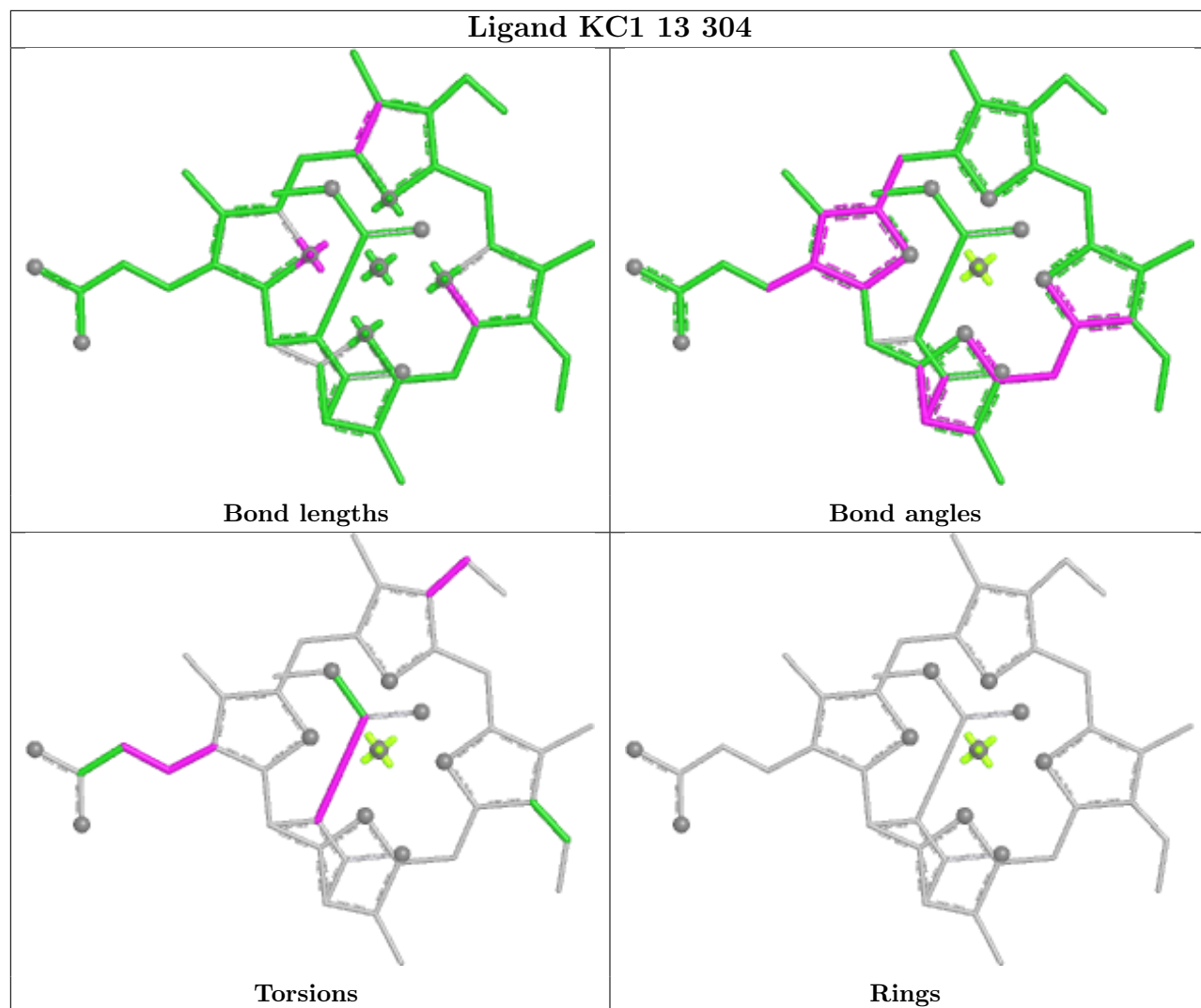
Bond angles



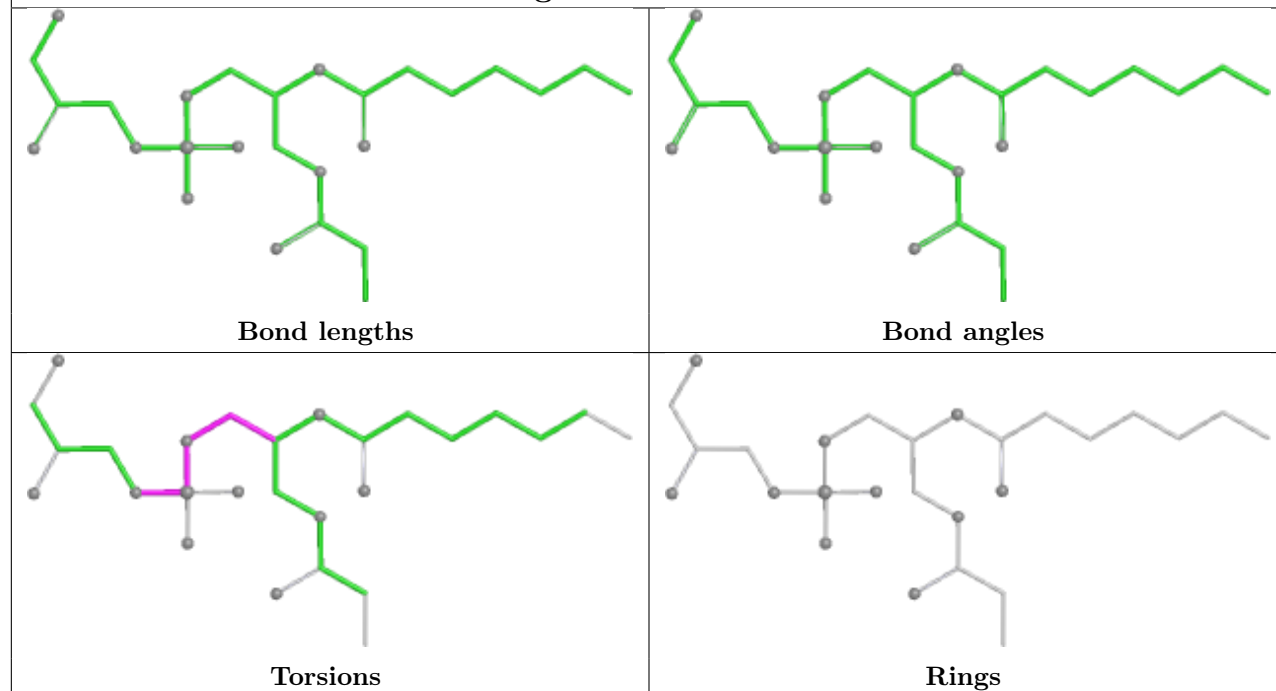
Torsions



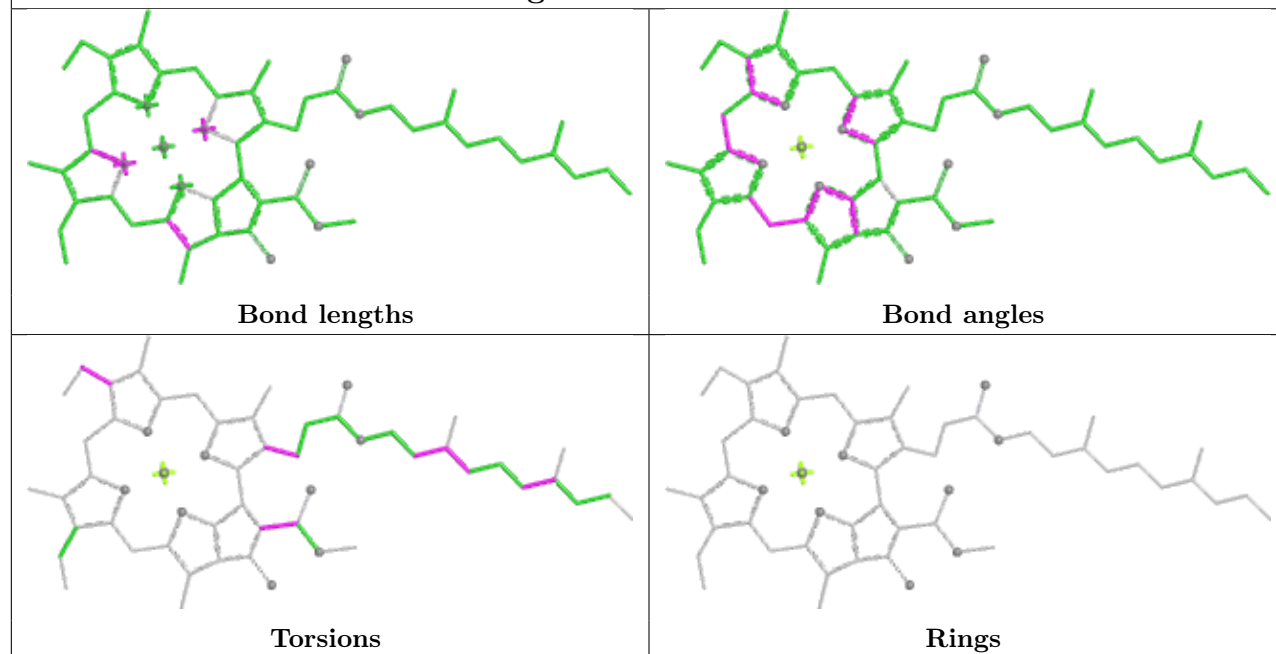
Rings

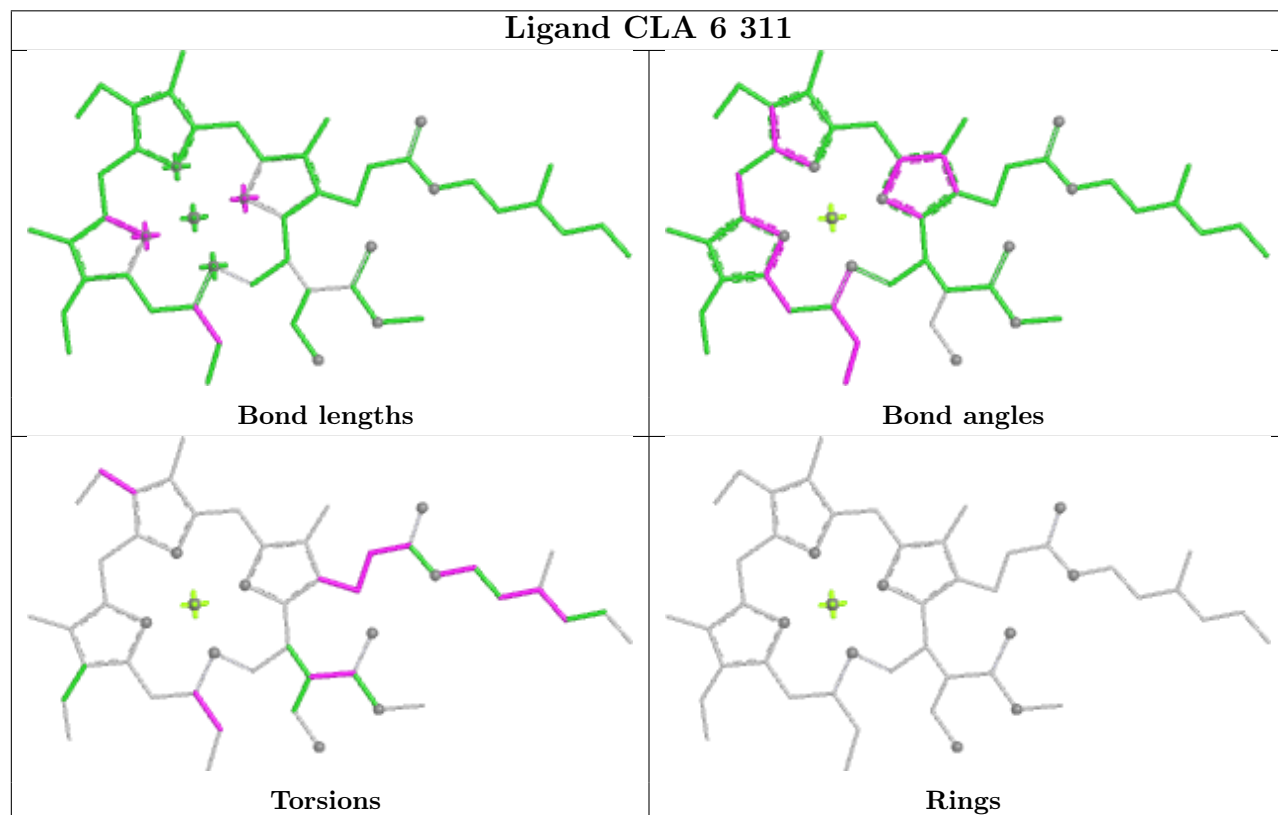
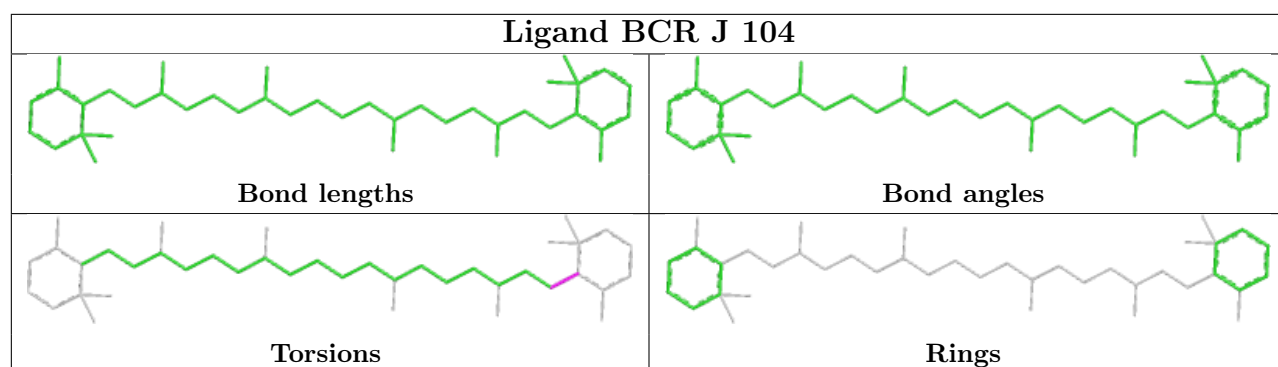


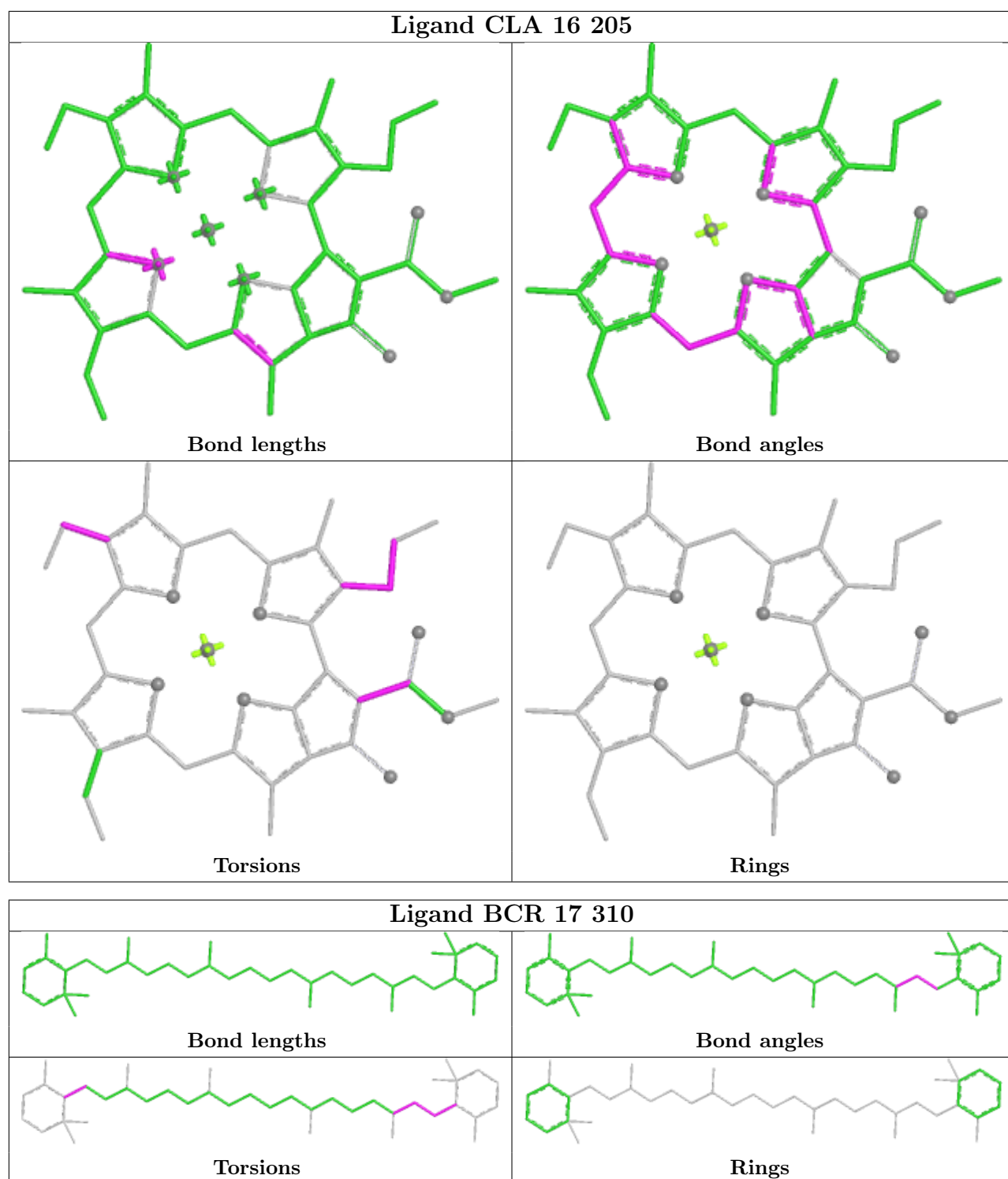
Ligand LHG 7 310

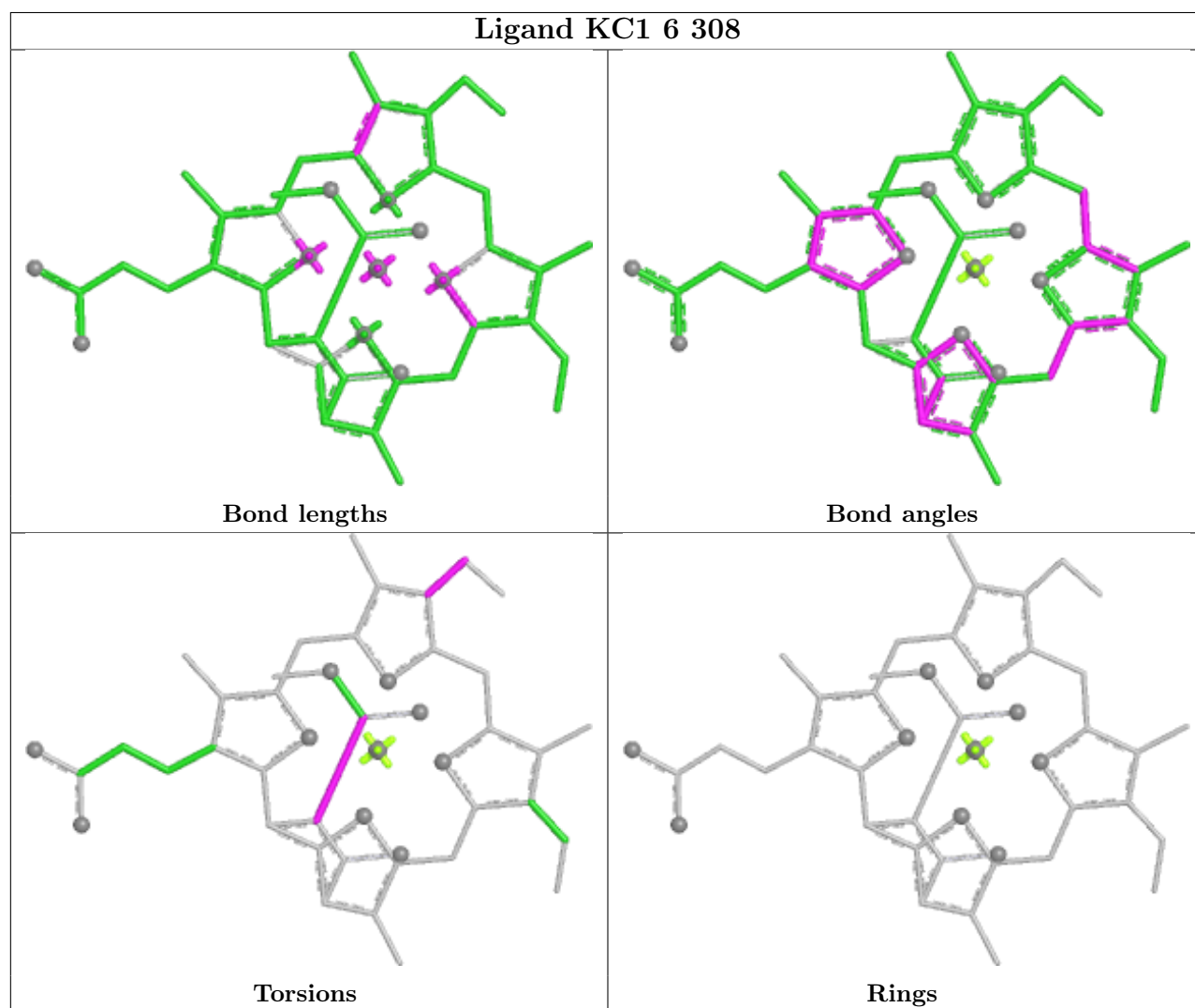
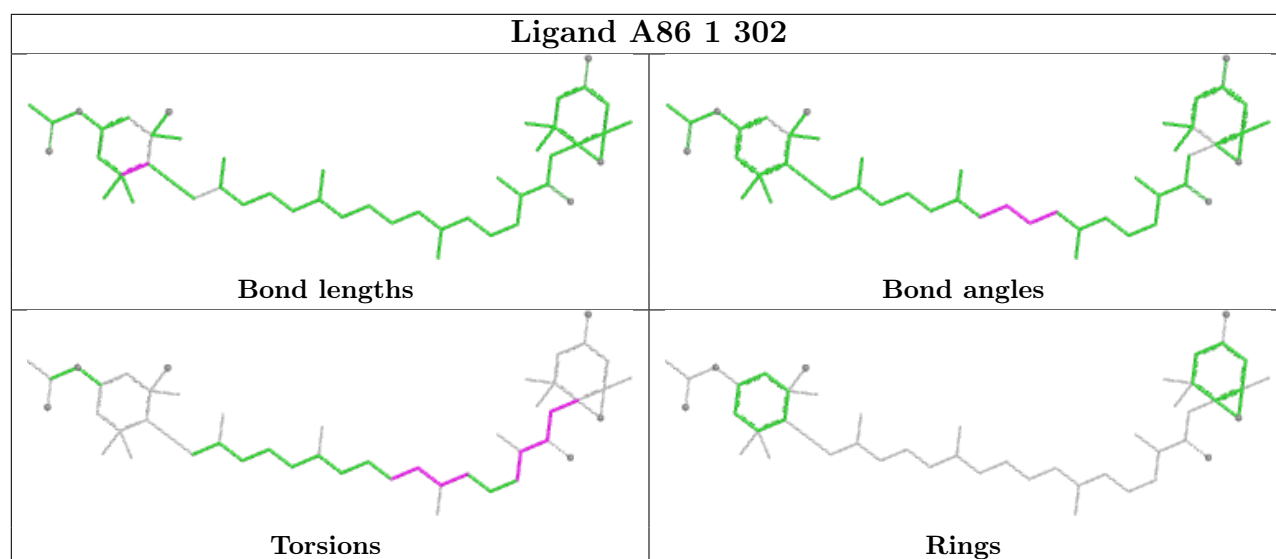


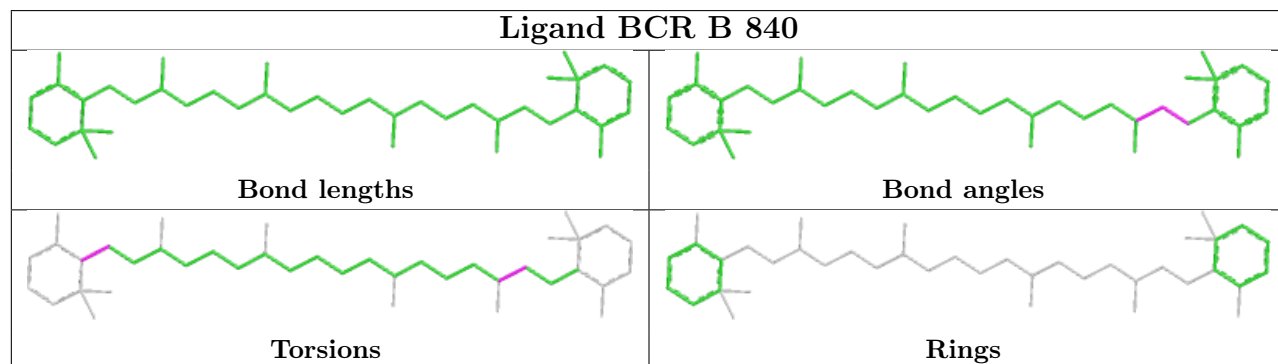
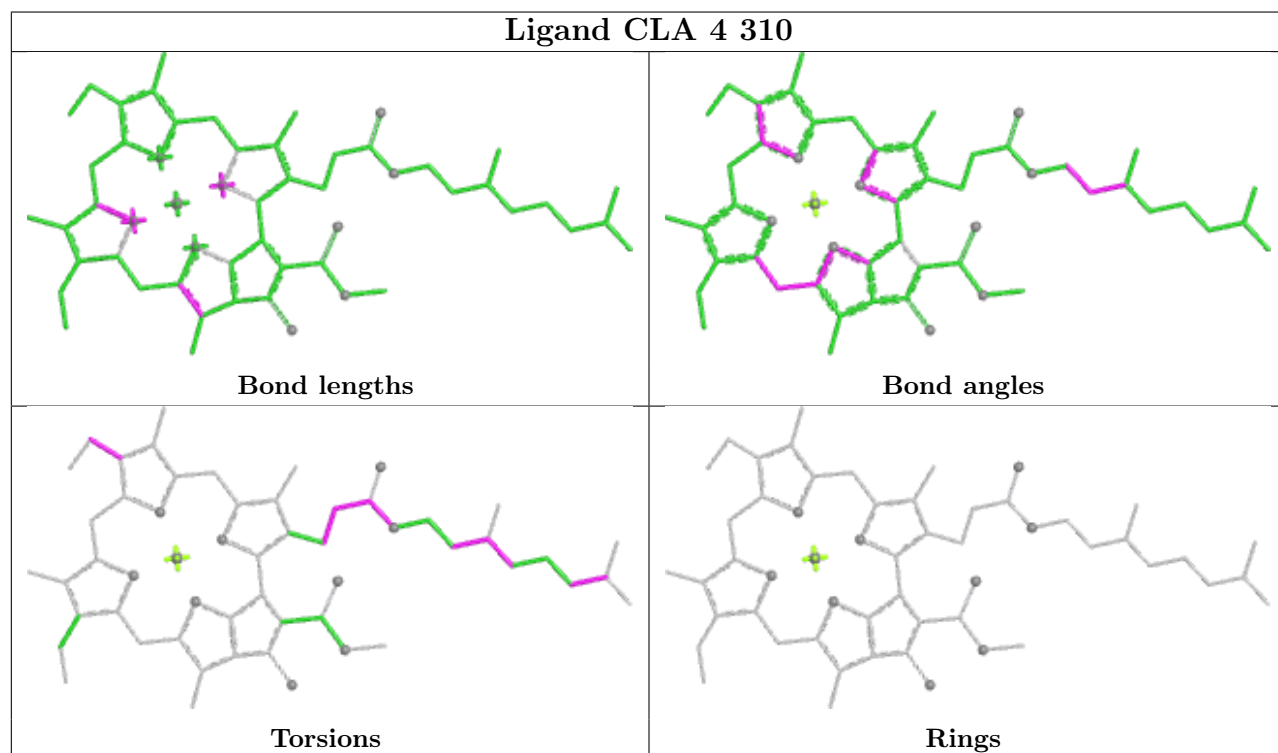
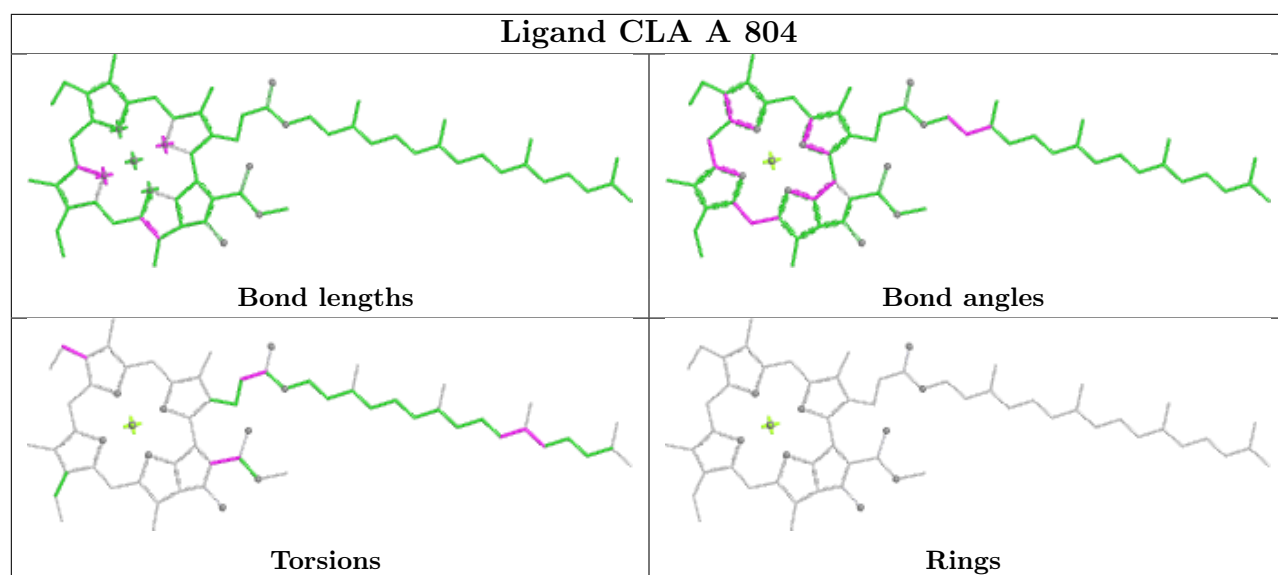
Ligand CLA 11 303

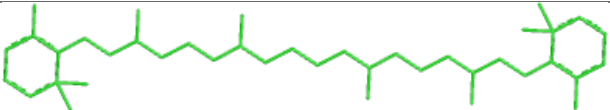
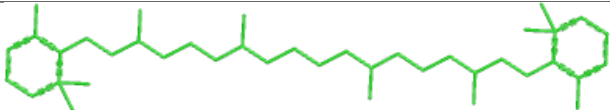
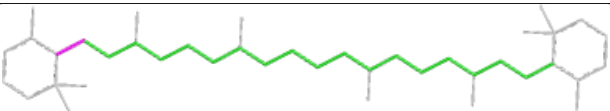
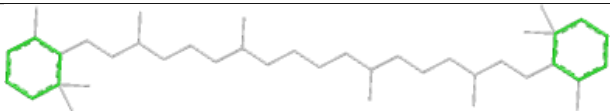


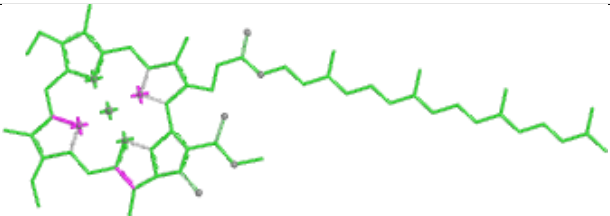
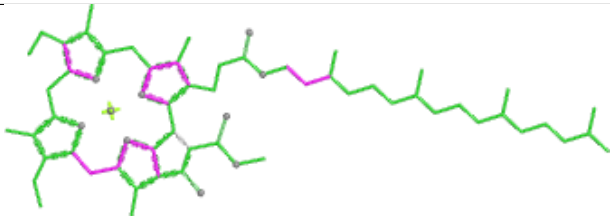
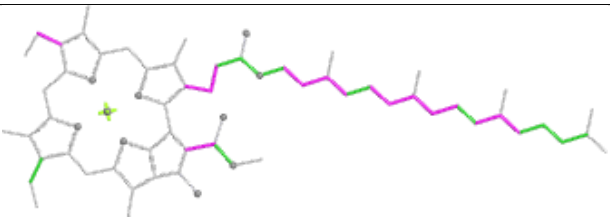
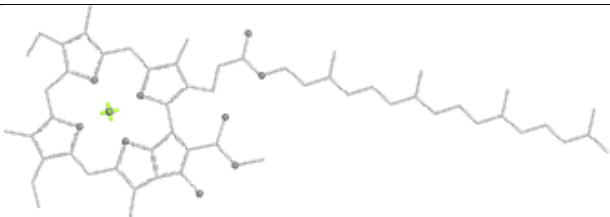




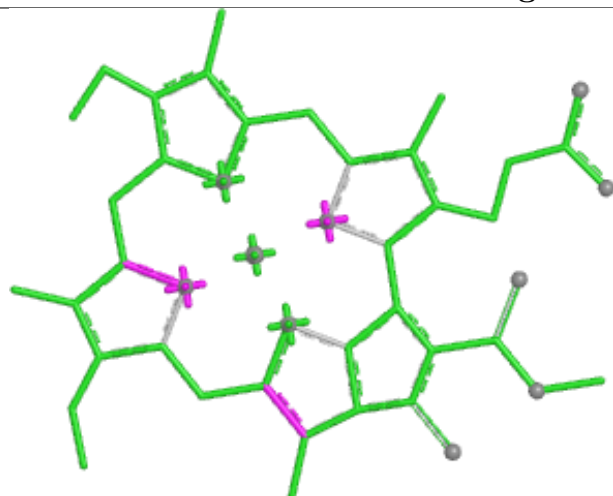




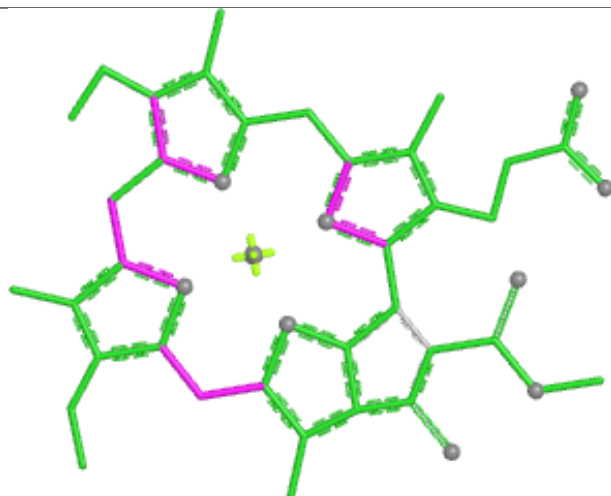
Ligand BCR B 850			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand CLA A 837			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

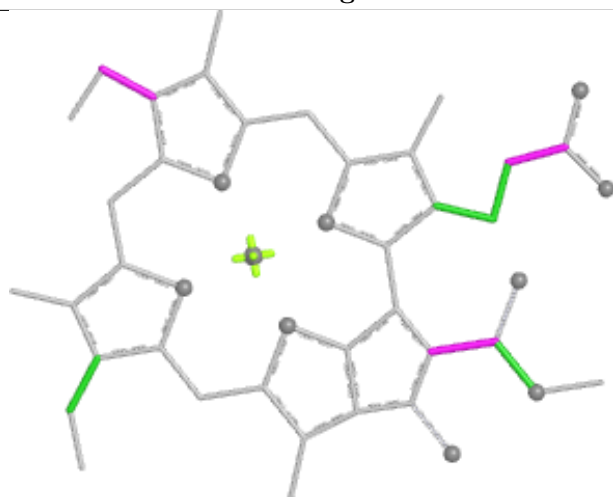
Ligand CLA 3 304



Bond lengths



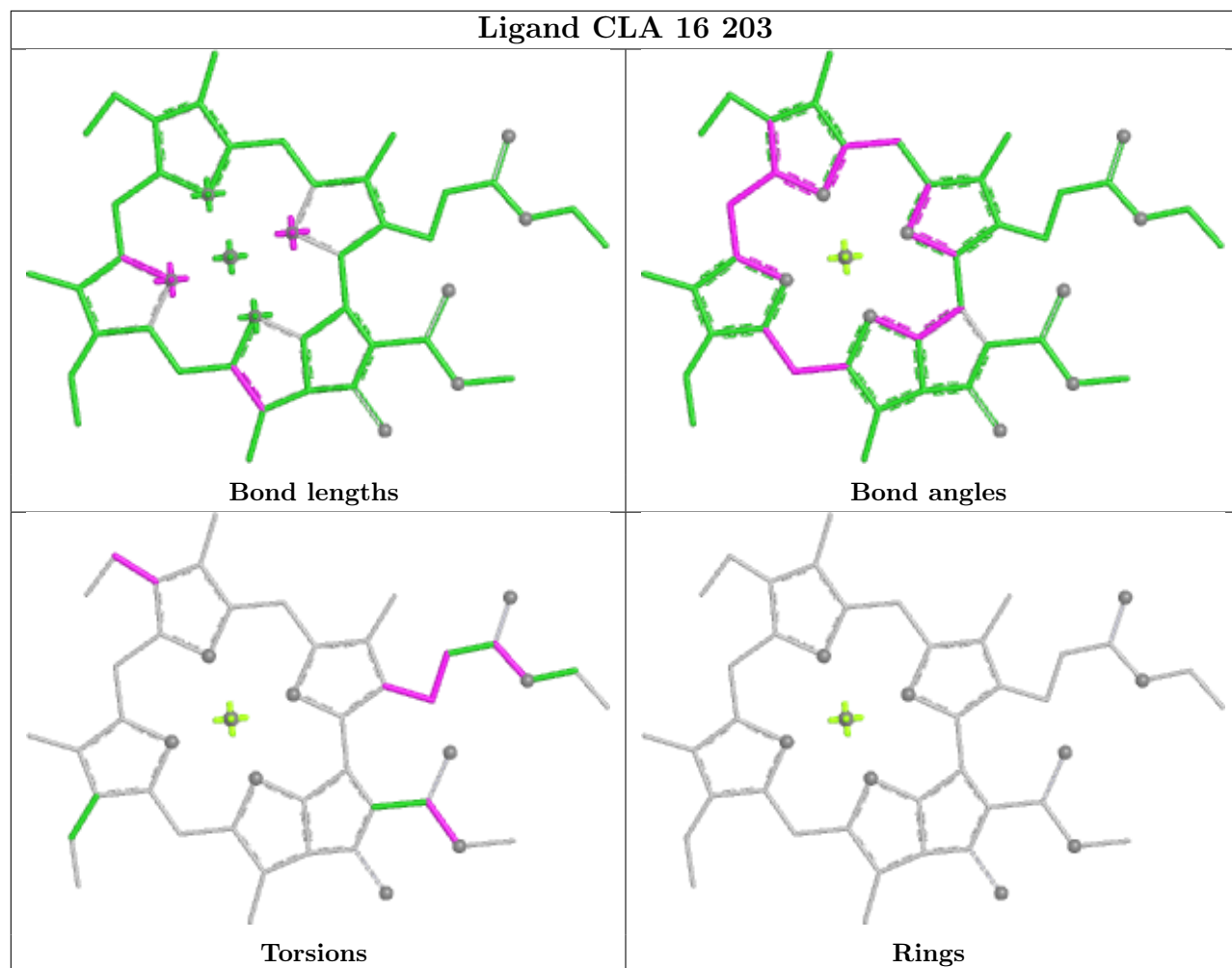
Bond angles



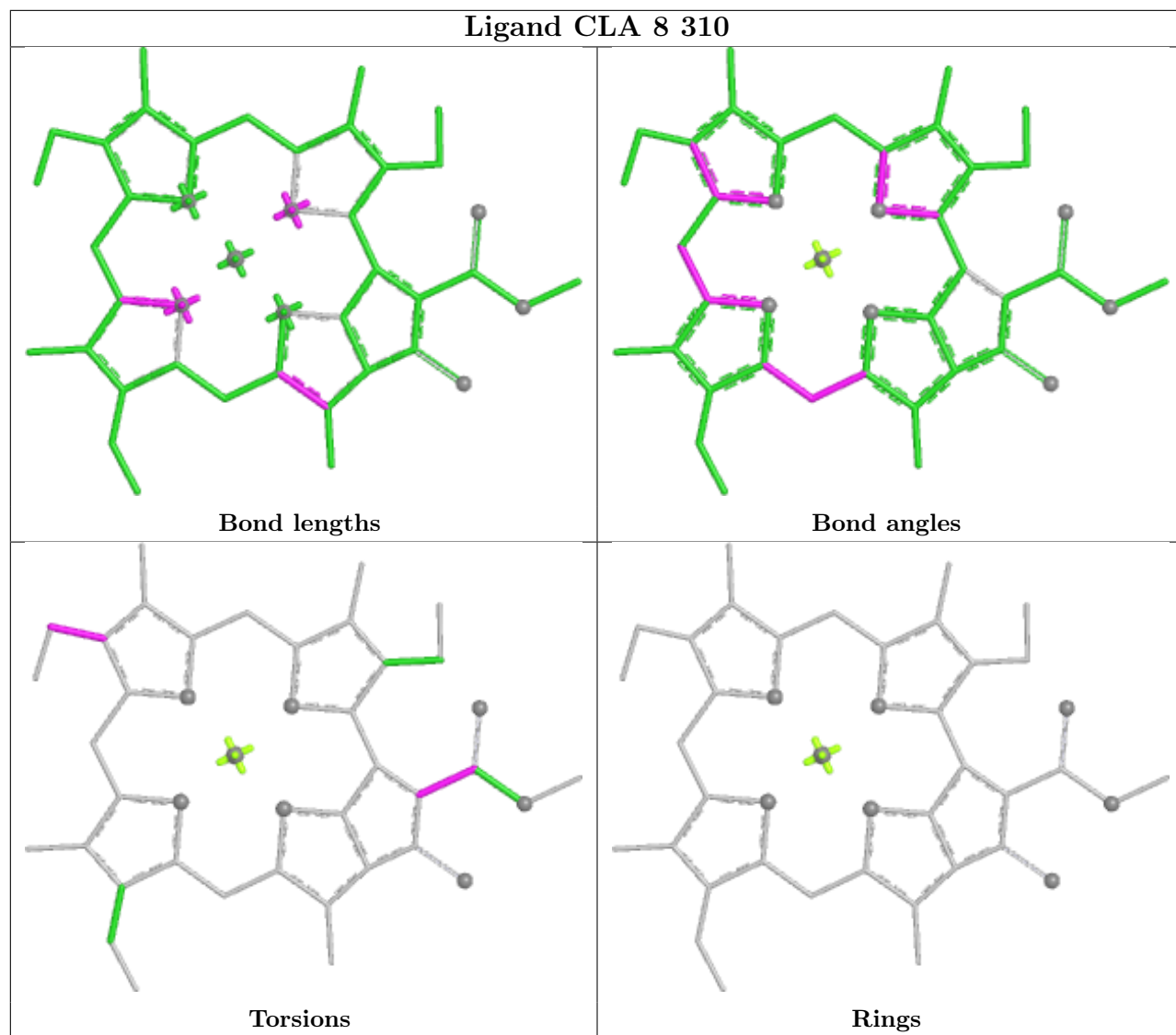
Torsions



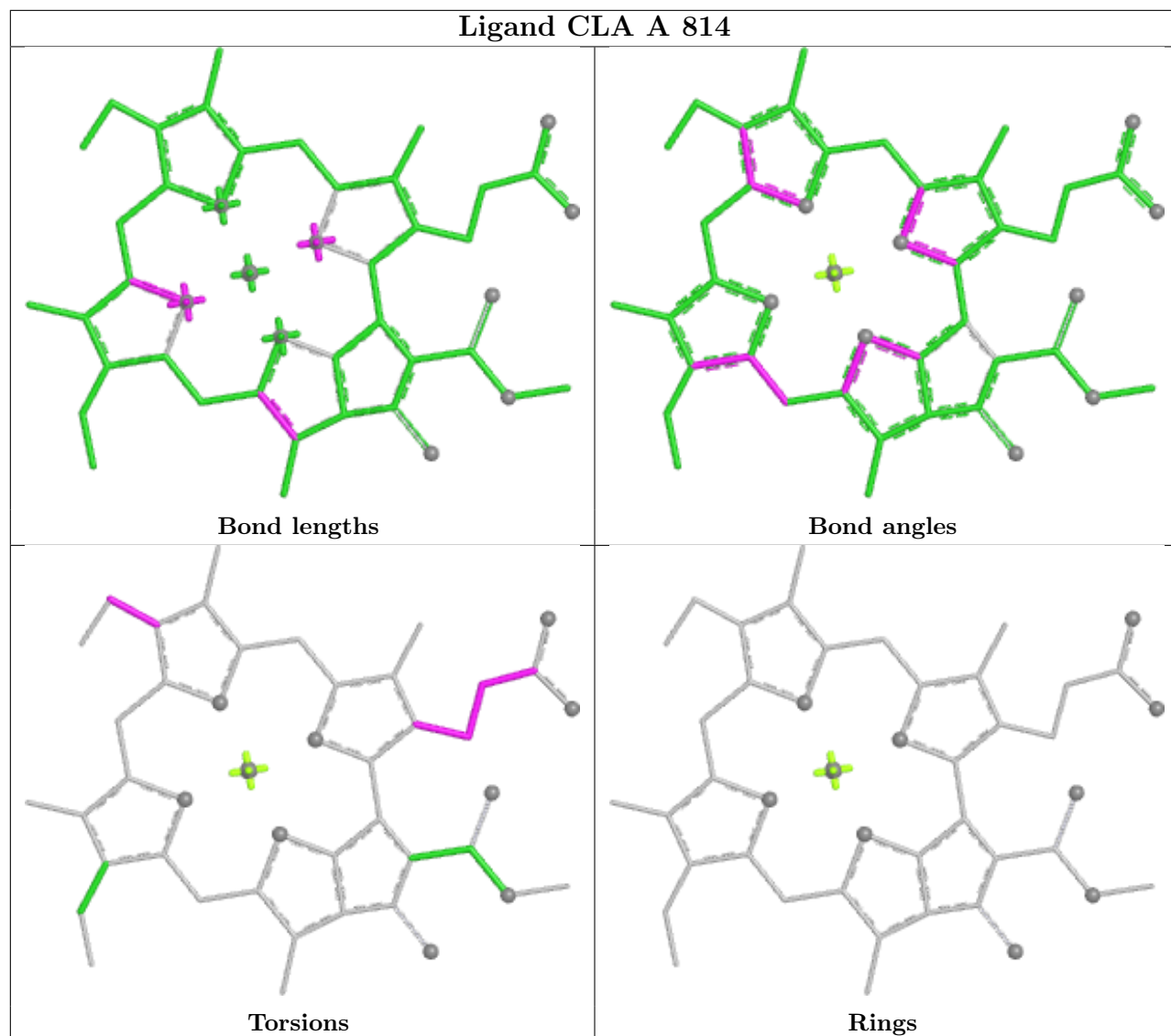
Rings



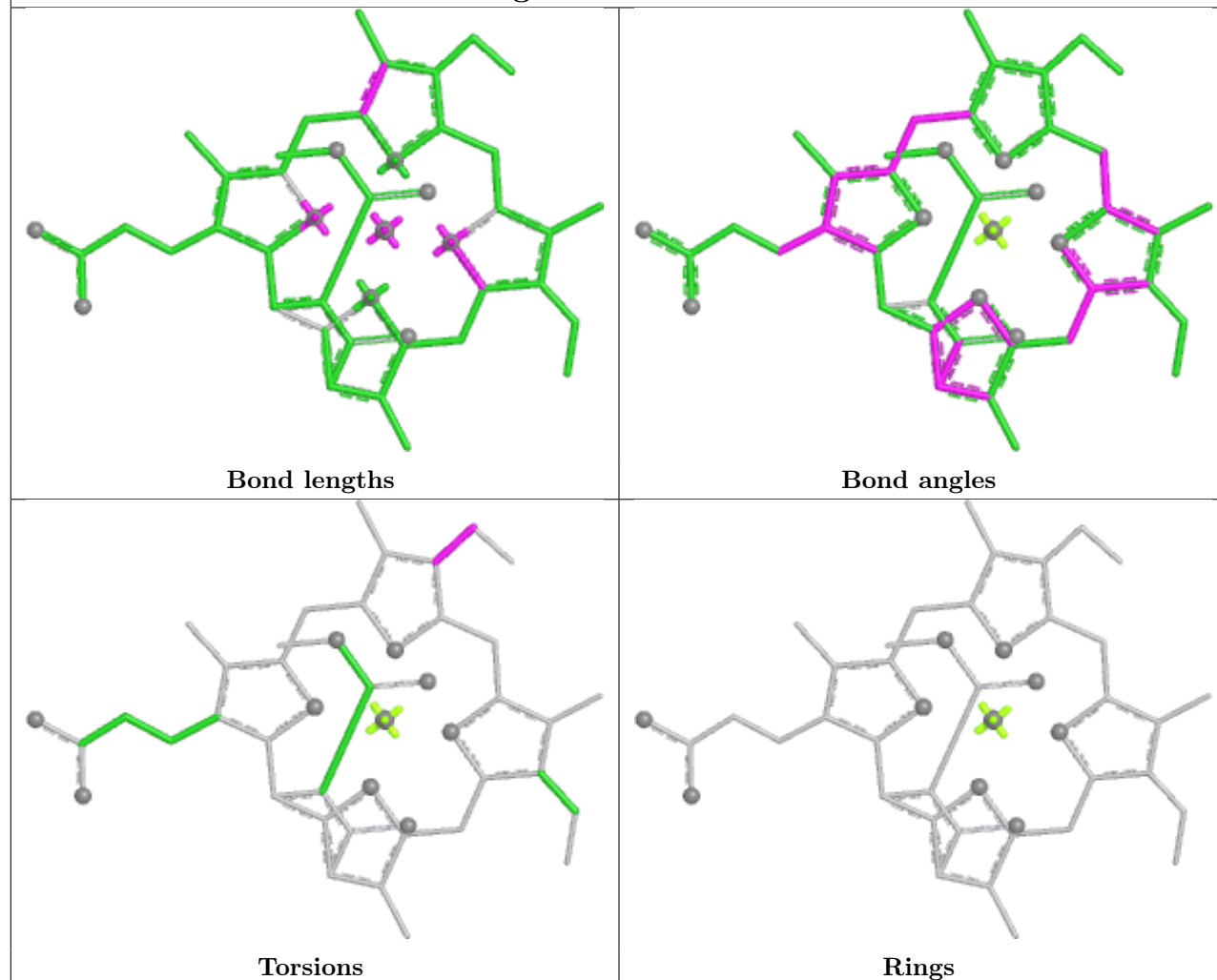
Ligand CLA 8 310



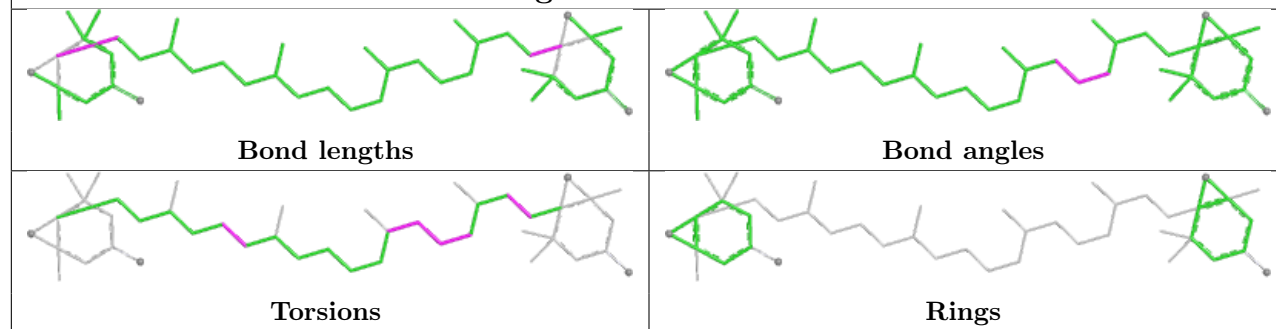
Ligand CLA A 814

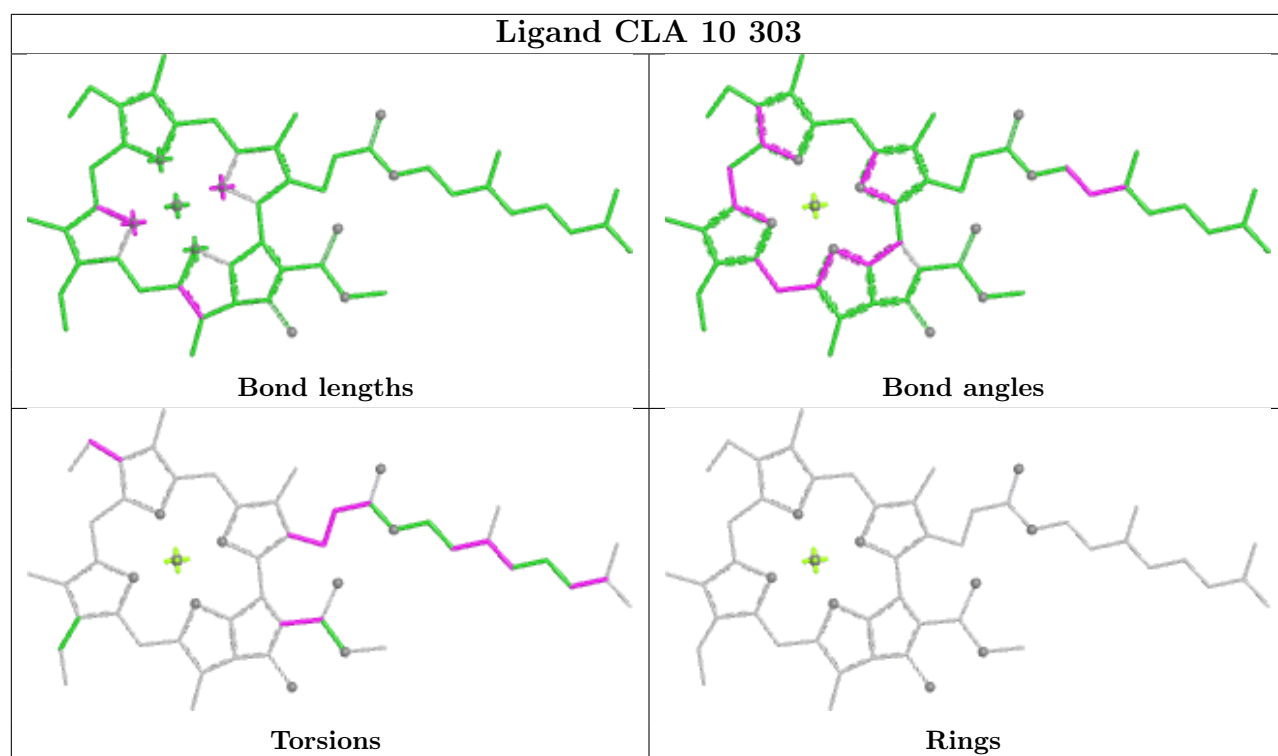


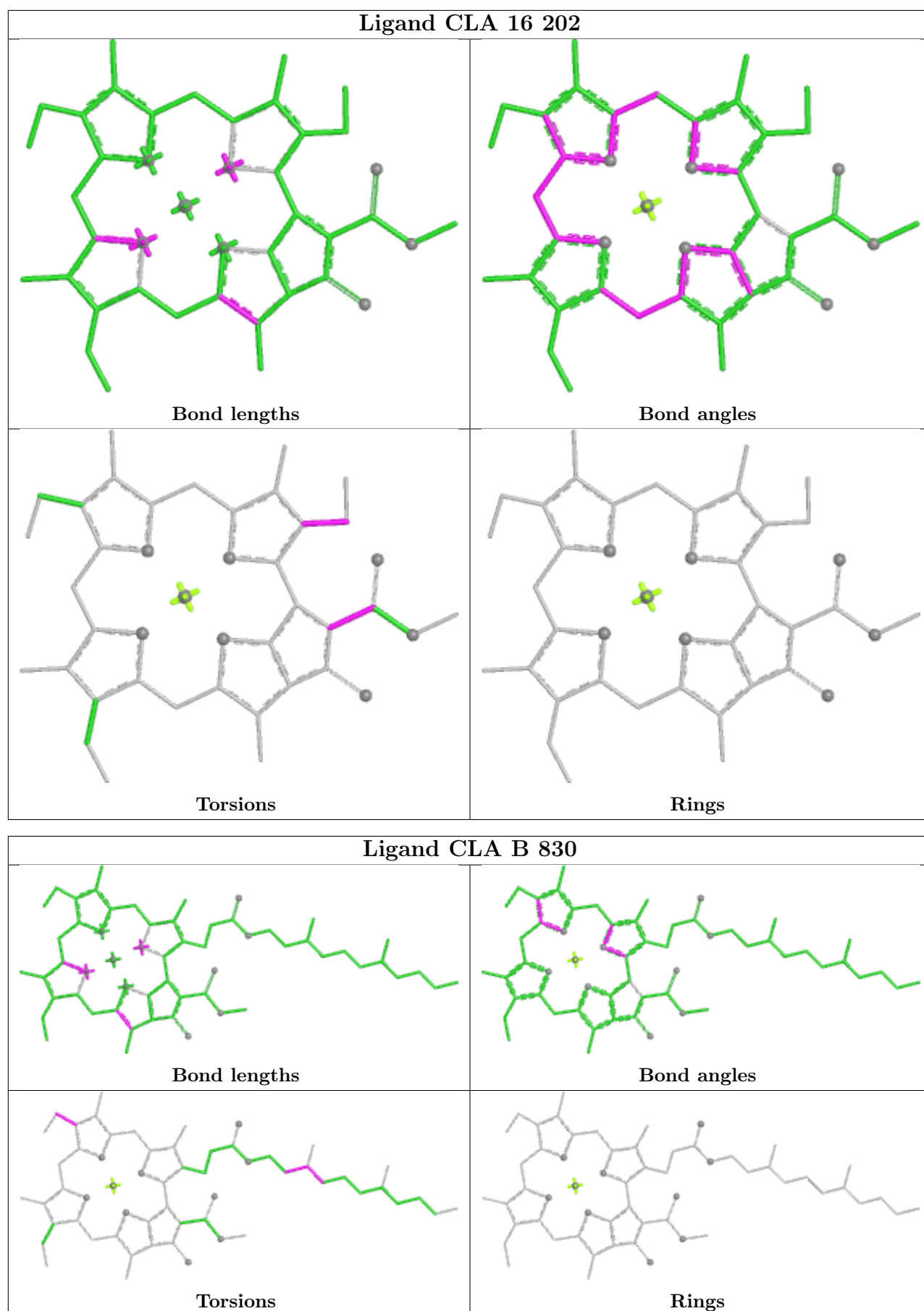
Ligand KC1 3 302



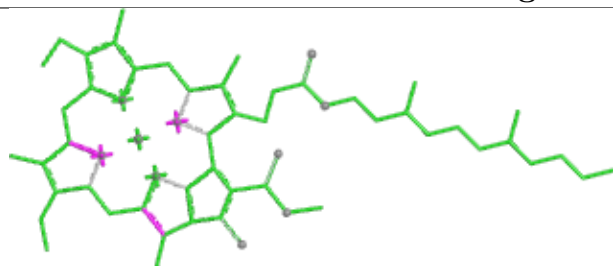
Ligand XAT 8 312



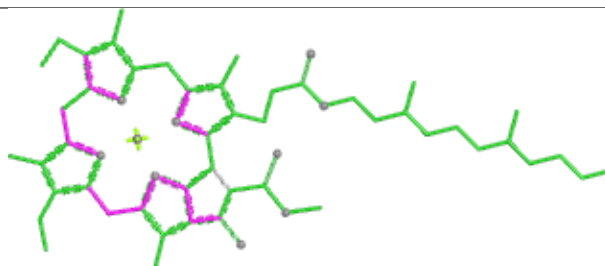




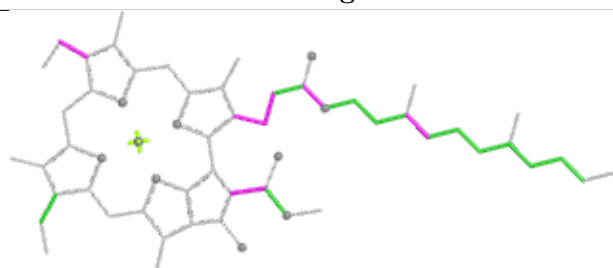
Ligand CLA 6 306



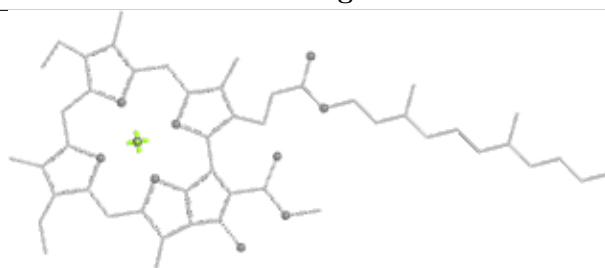
Bond lengths



Bond angles

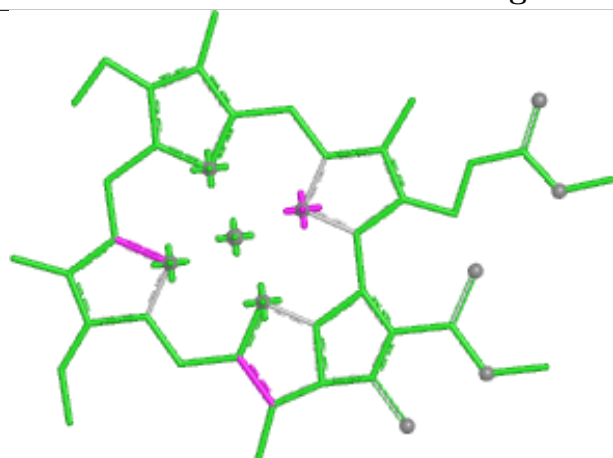


Torsions

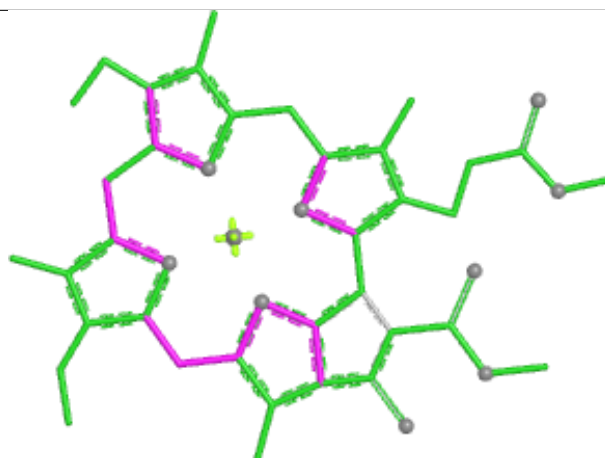


Rings

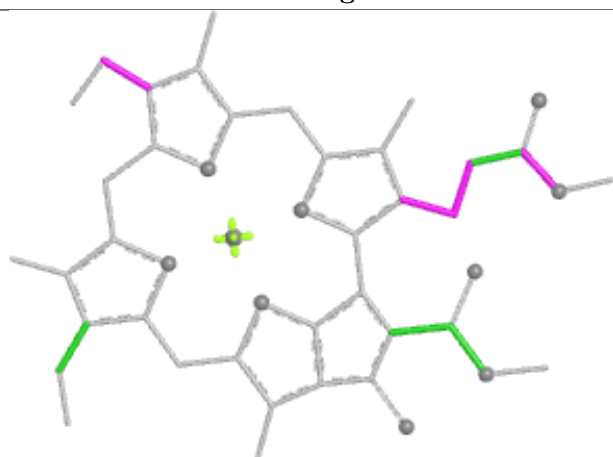
Ligand CLA 13 305



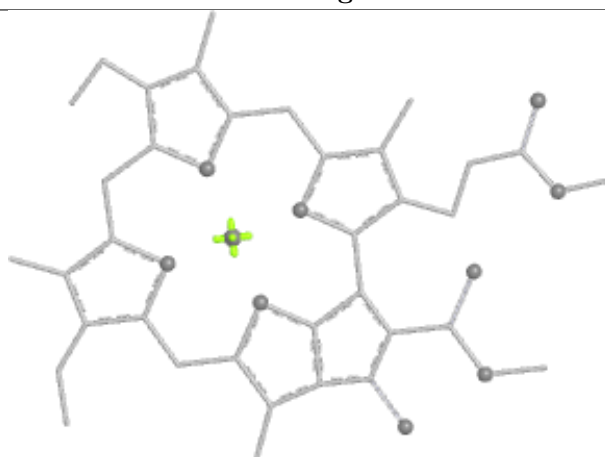
Bond lengths



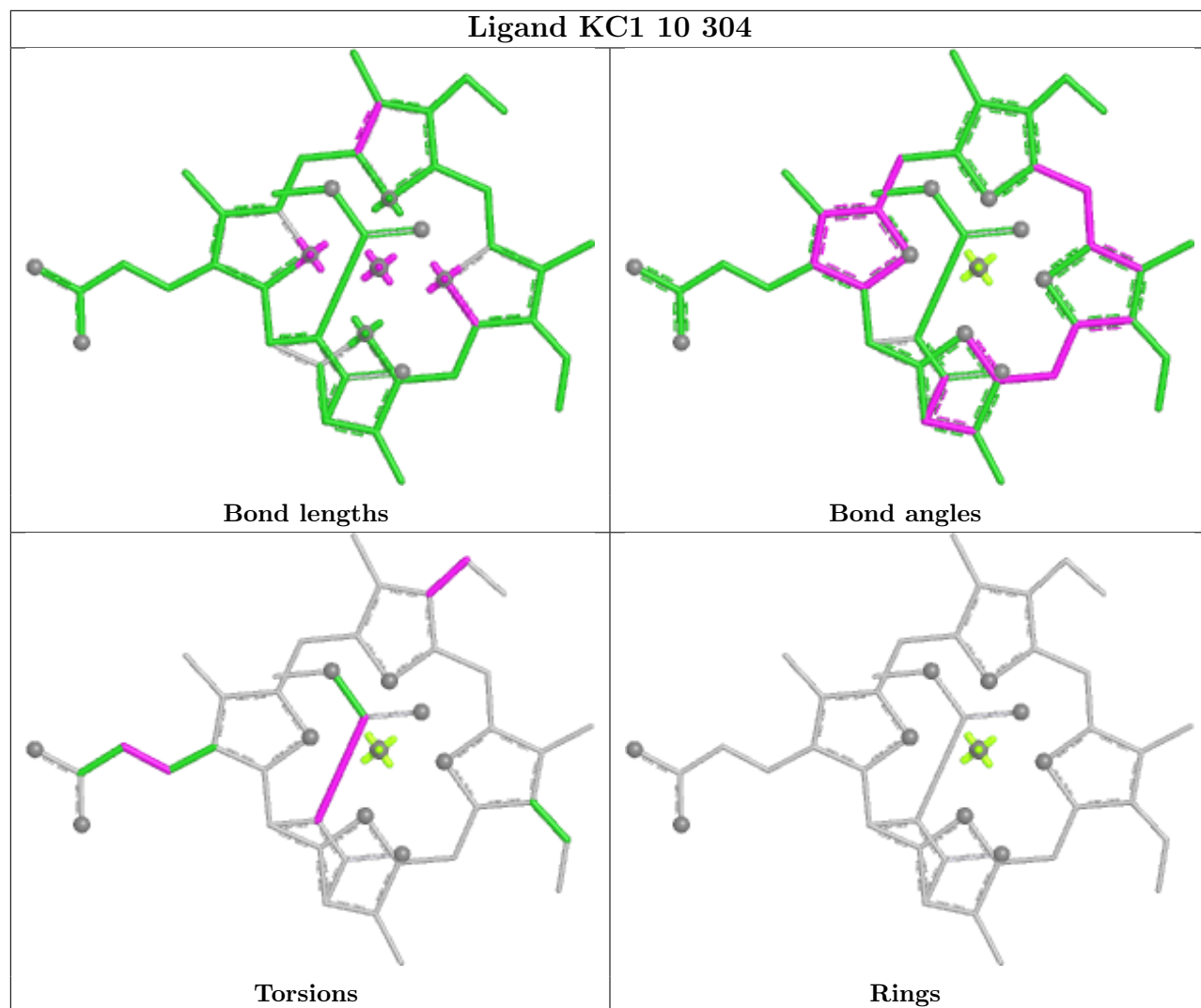
Bond angles



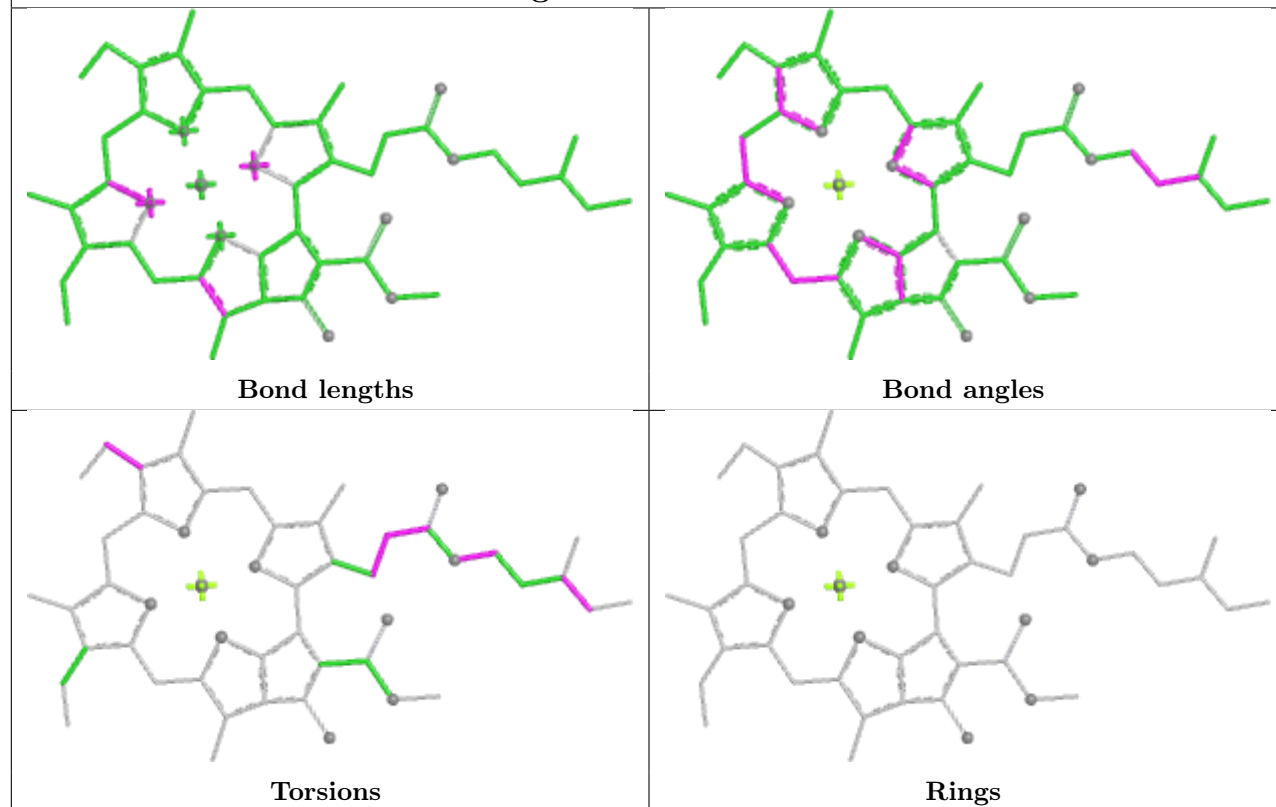
Torsions



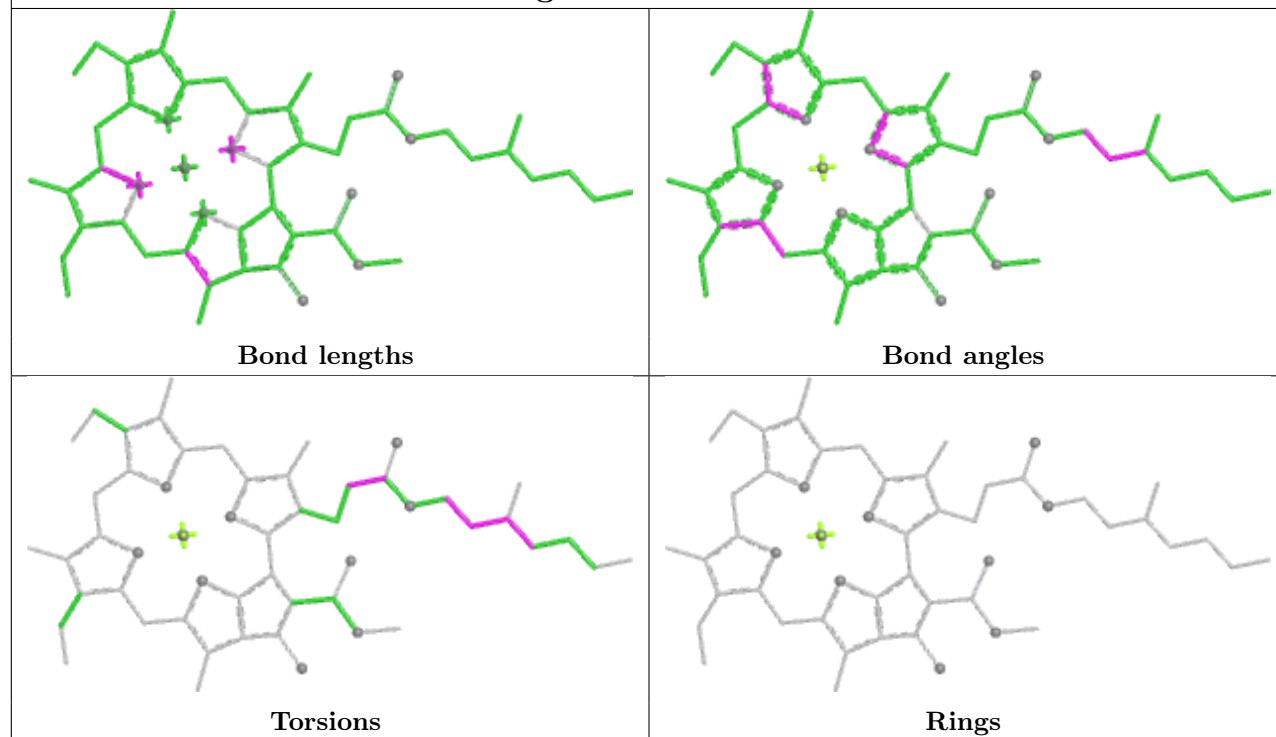
Rings

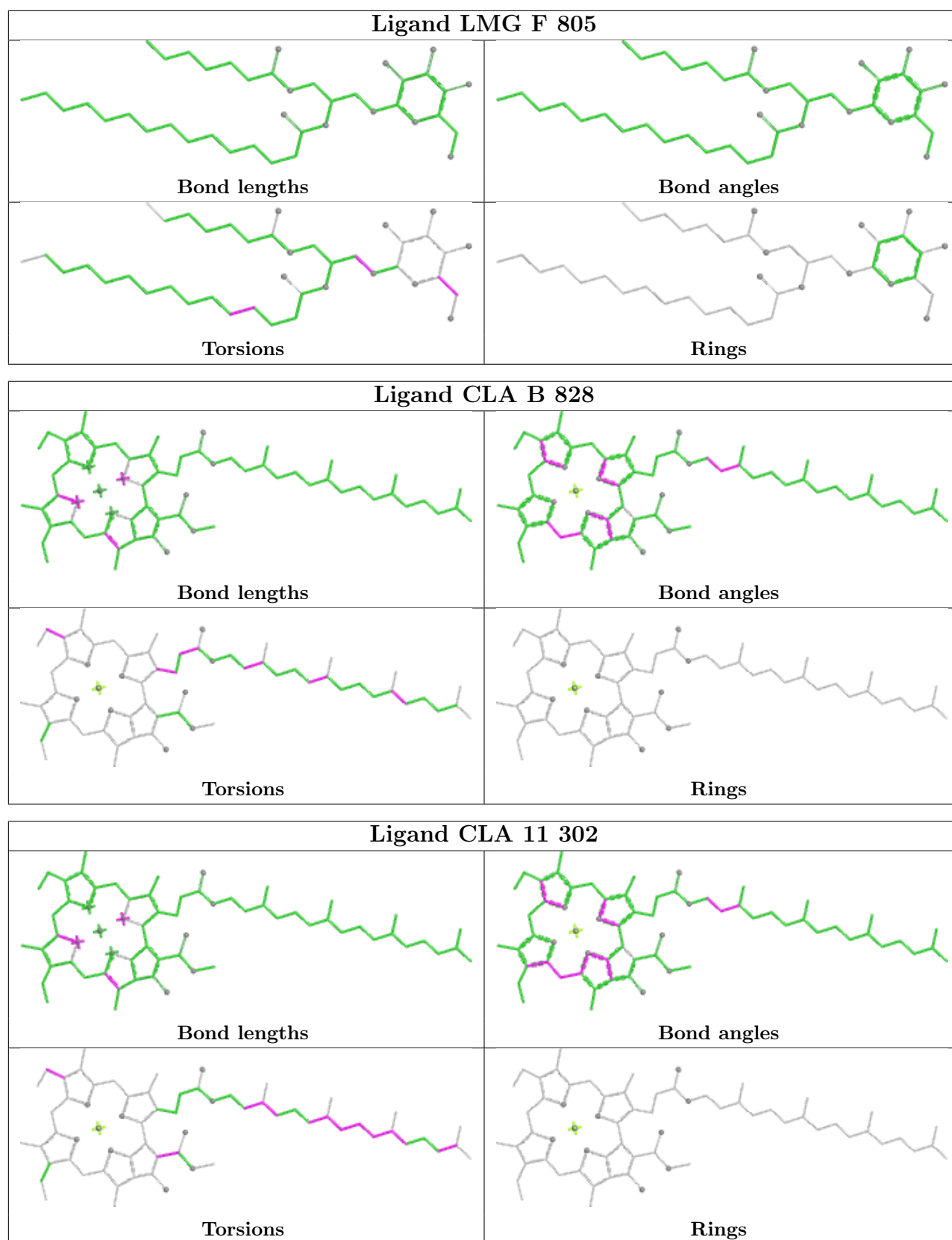


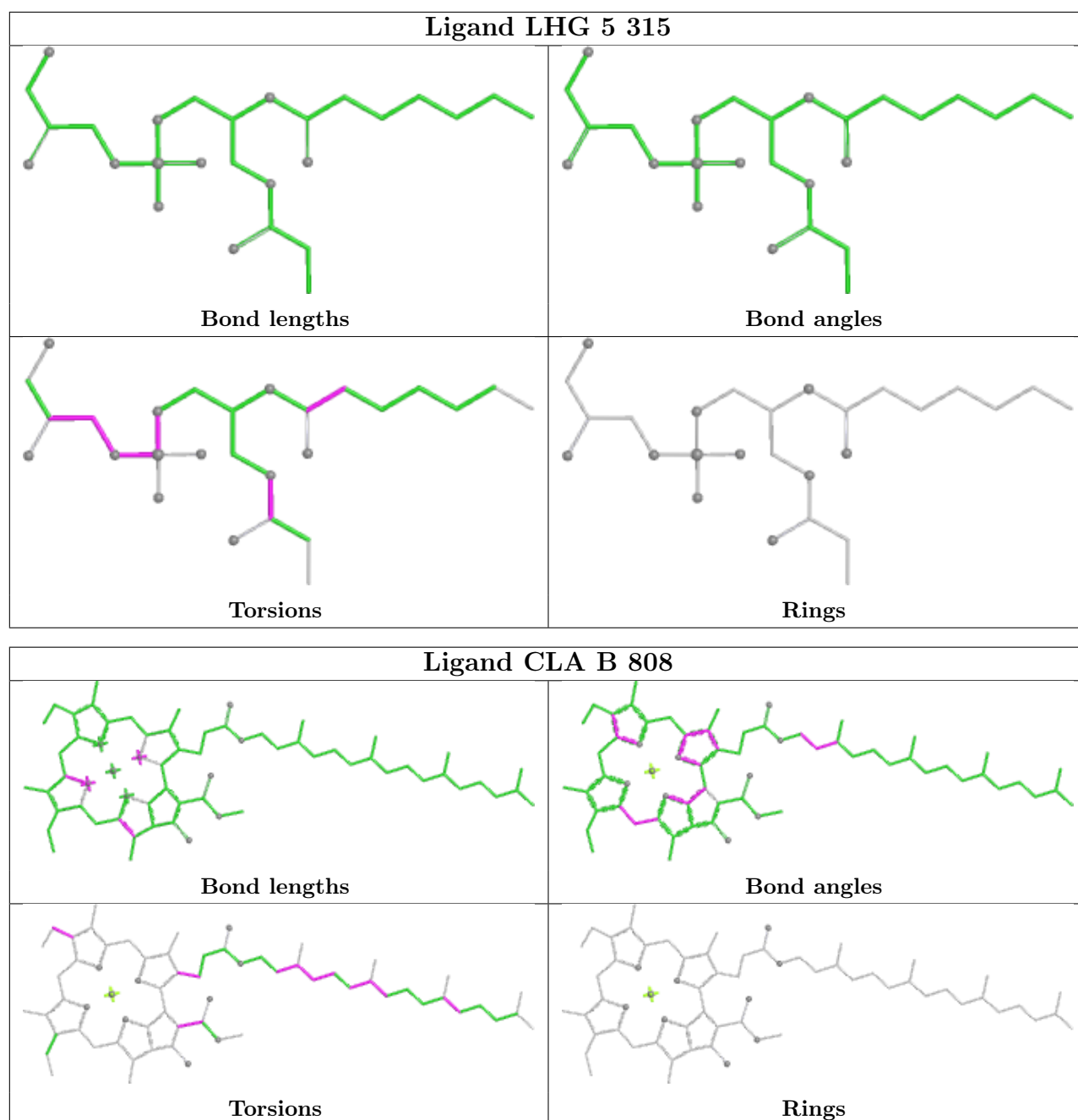
Ligand CLA R 204



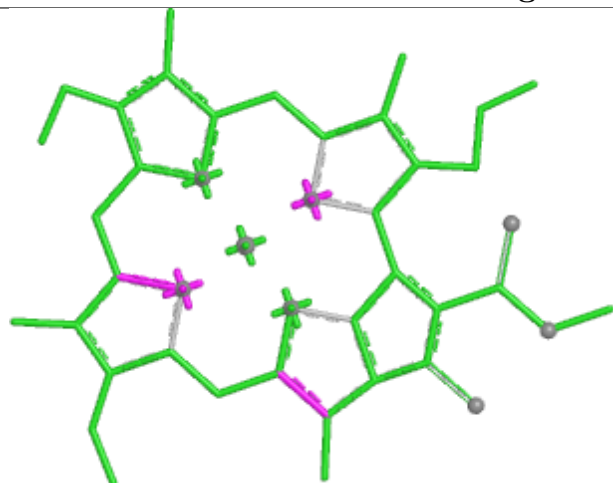
Ligand CLA 6 302



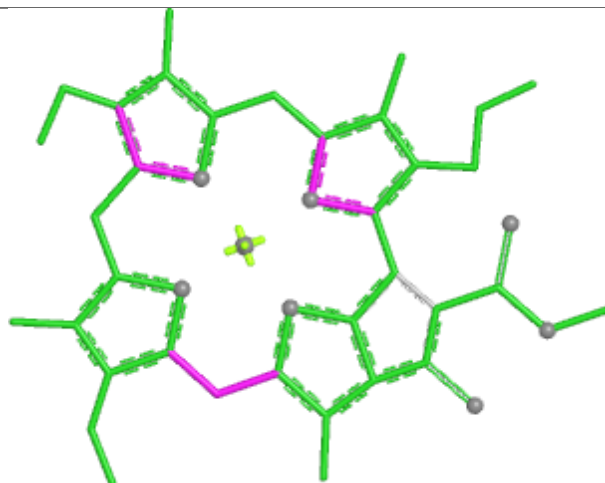




Ligand CLA 7 308



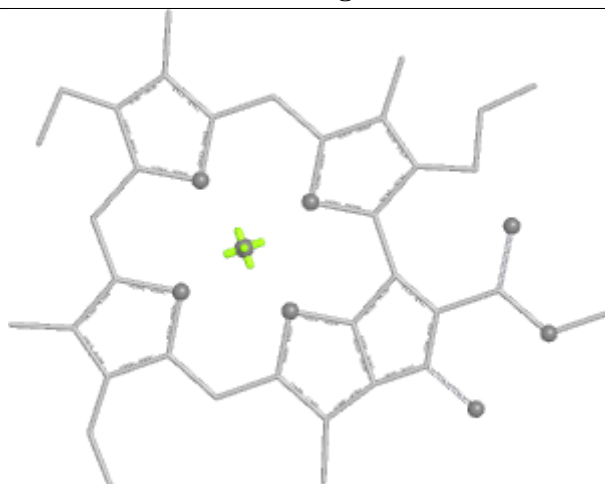
Bond lengths



Bond angles

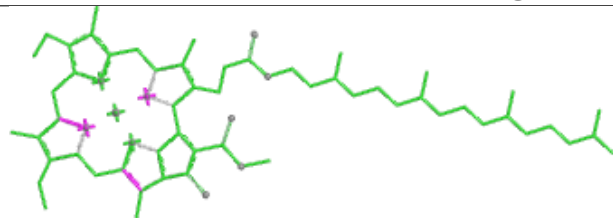


Torsions

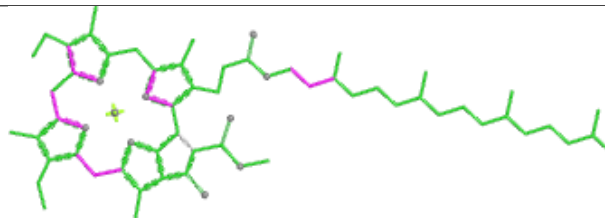


Rings

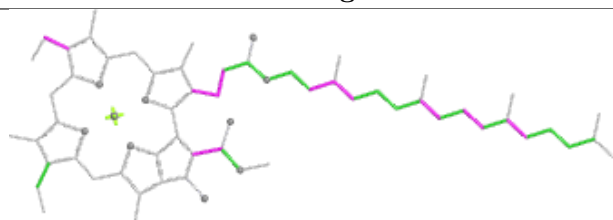
Ligand CLA 11 301



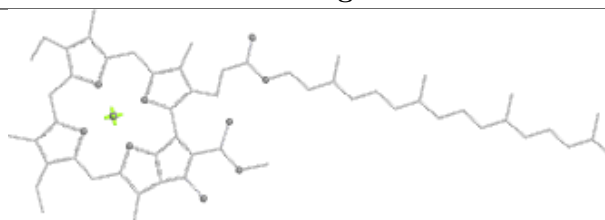
Bond lengths



Bond angles

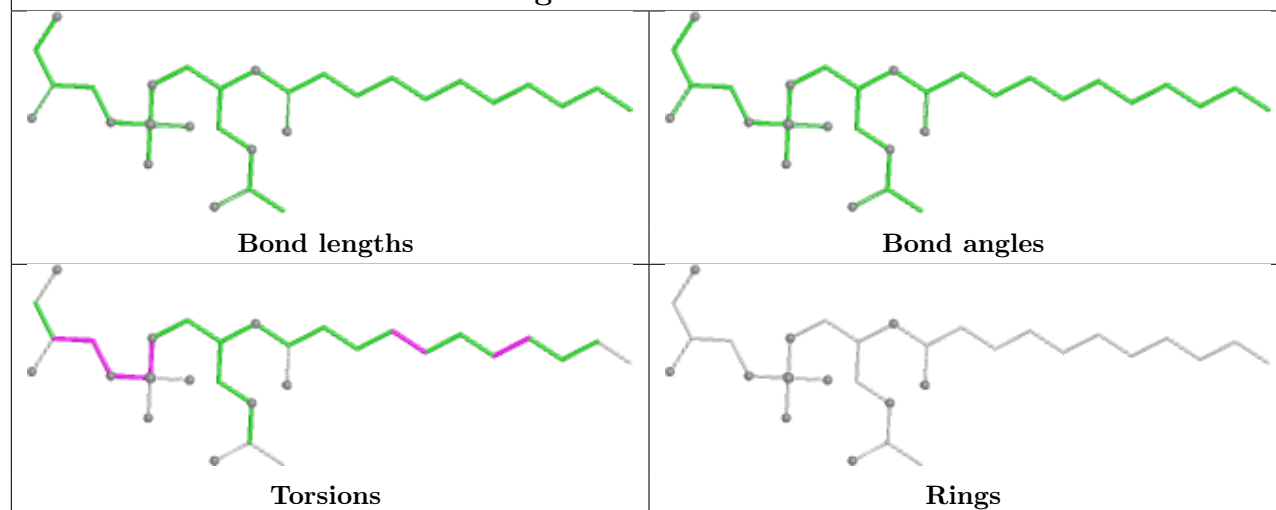


Torsions

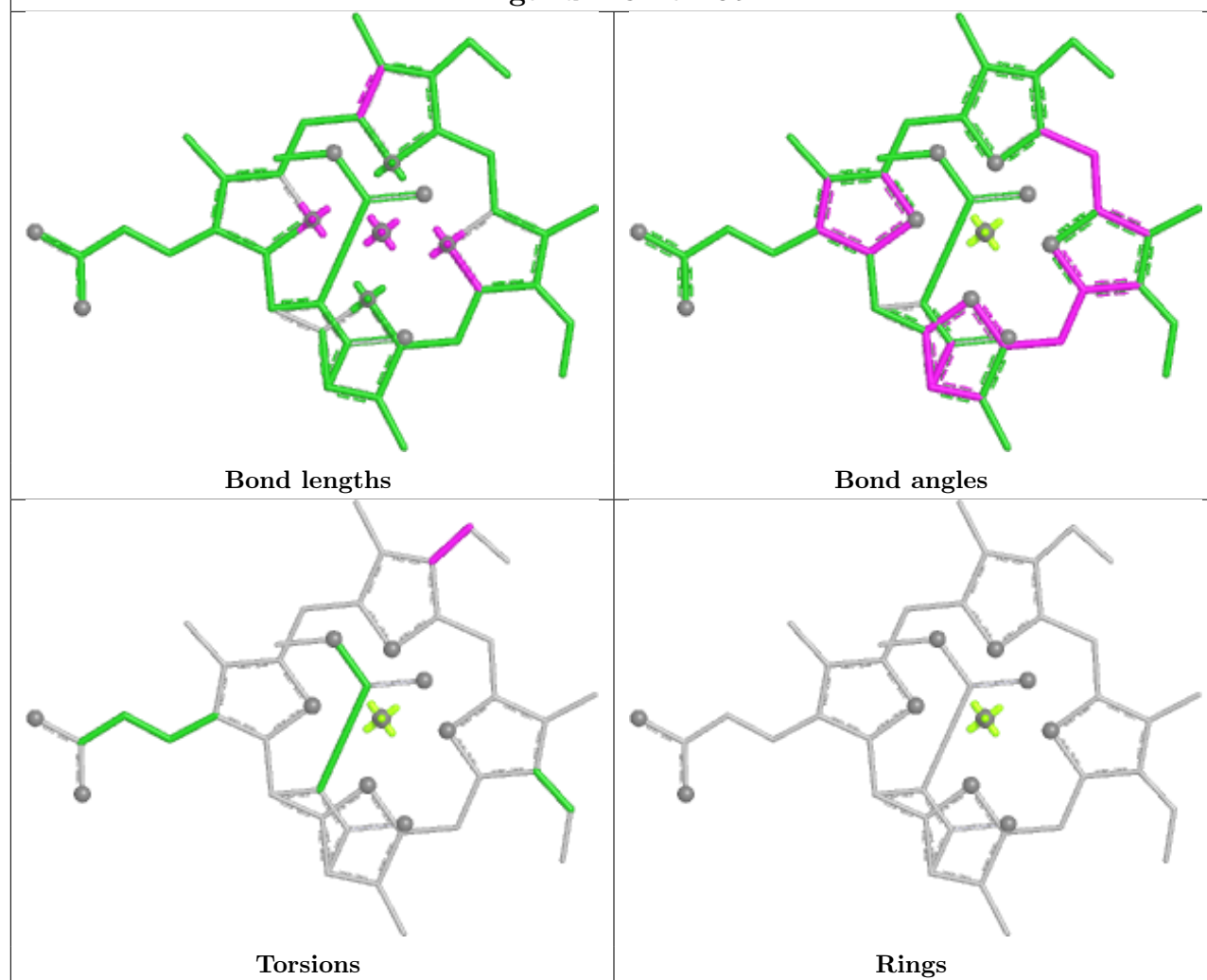


Rings

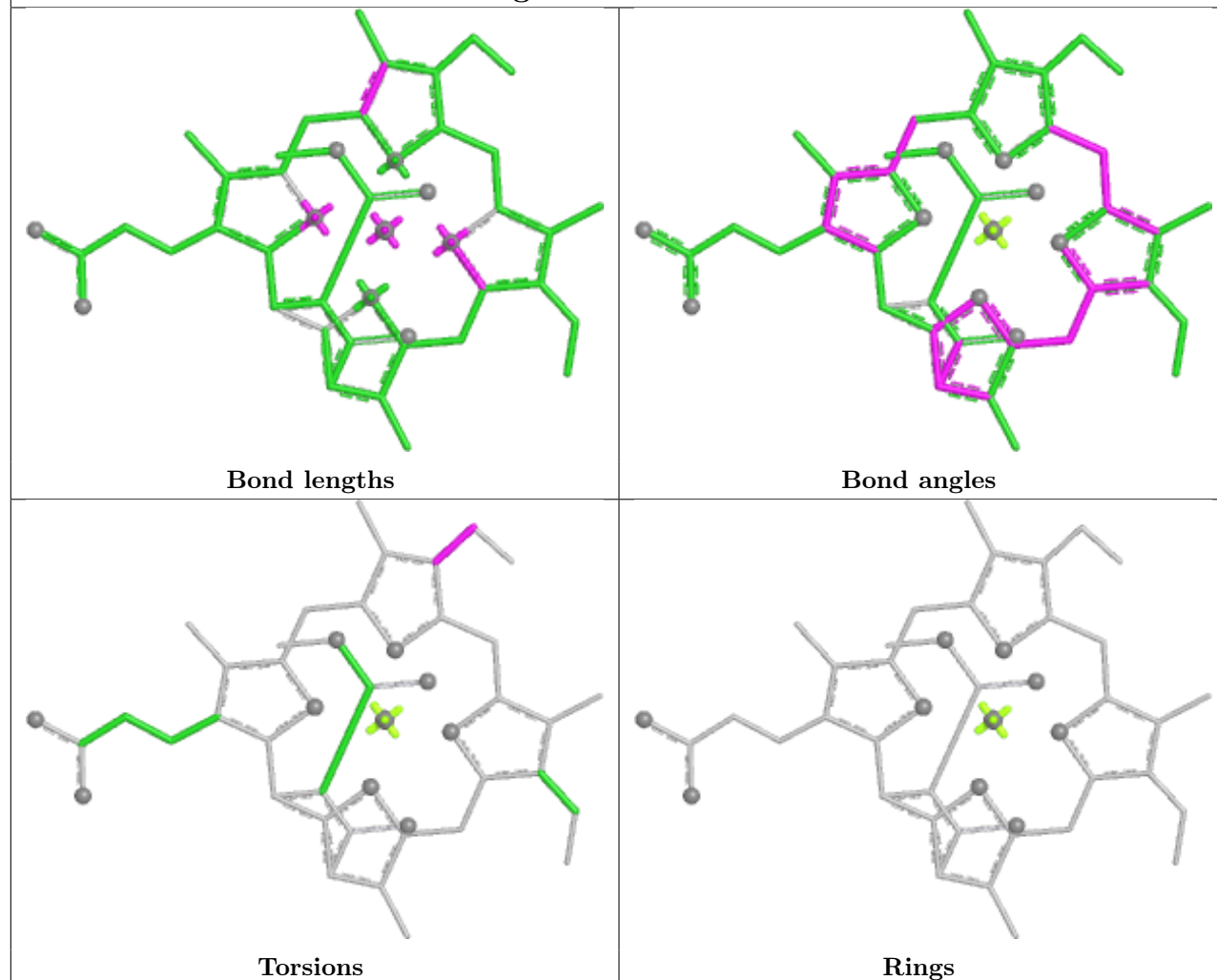
Ligand LHG 9 302



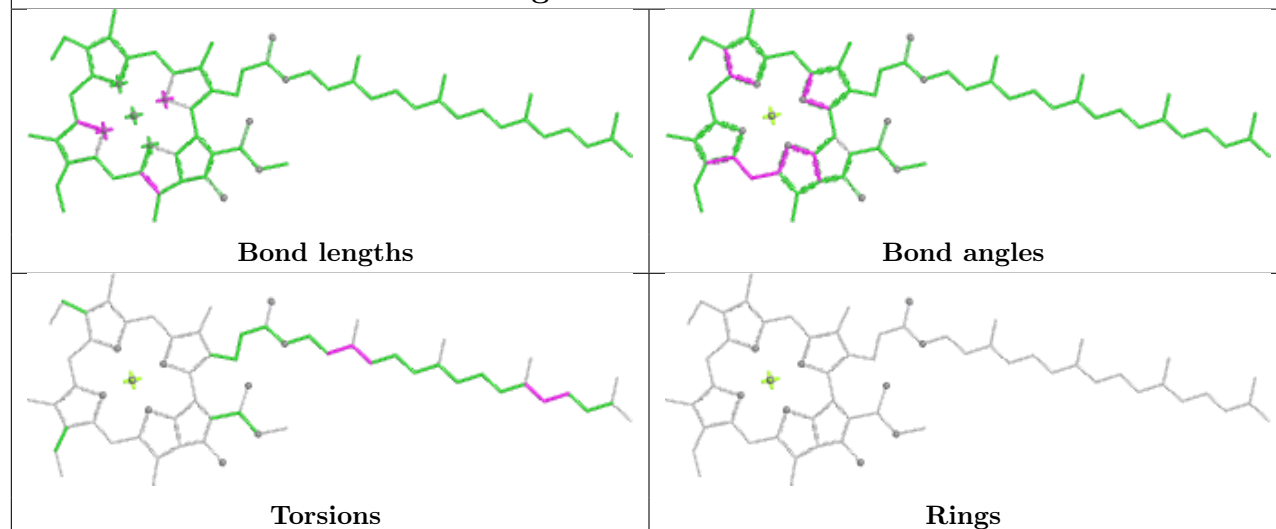
Ligand KC1 a 205



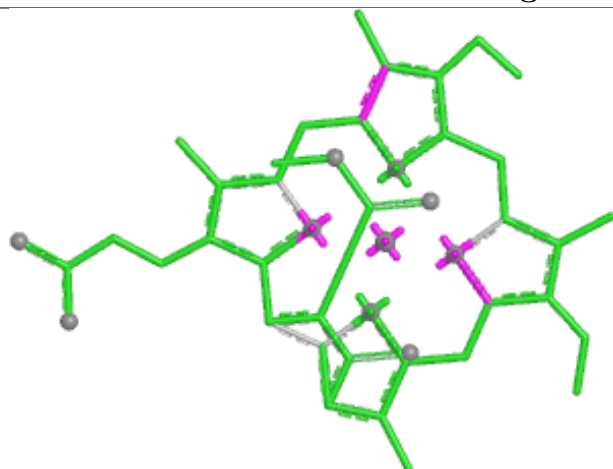
Ligand KC1 8 306



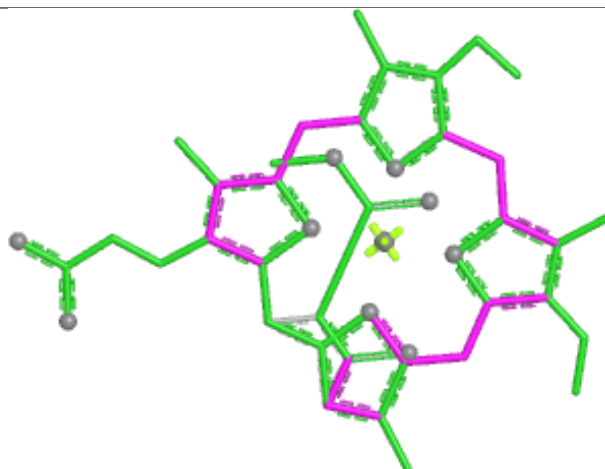
Ligand CLA A 825



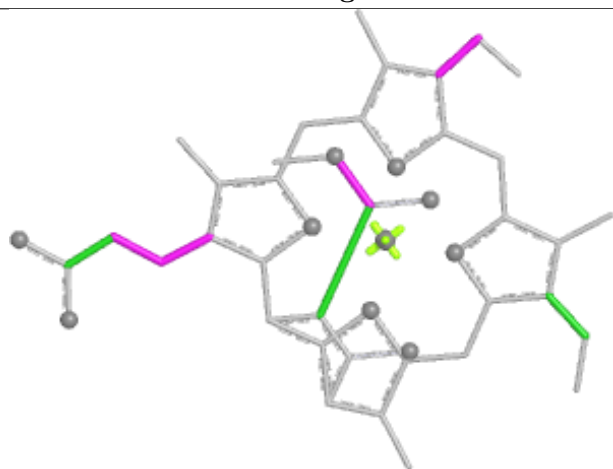
Ligand KC1 6 309



Bond lengths



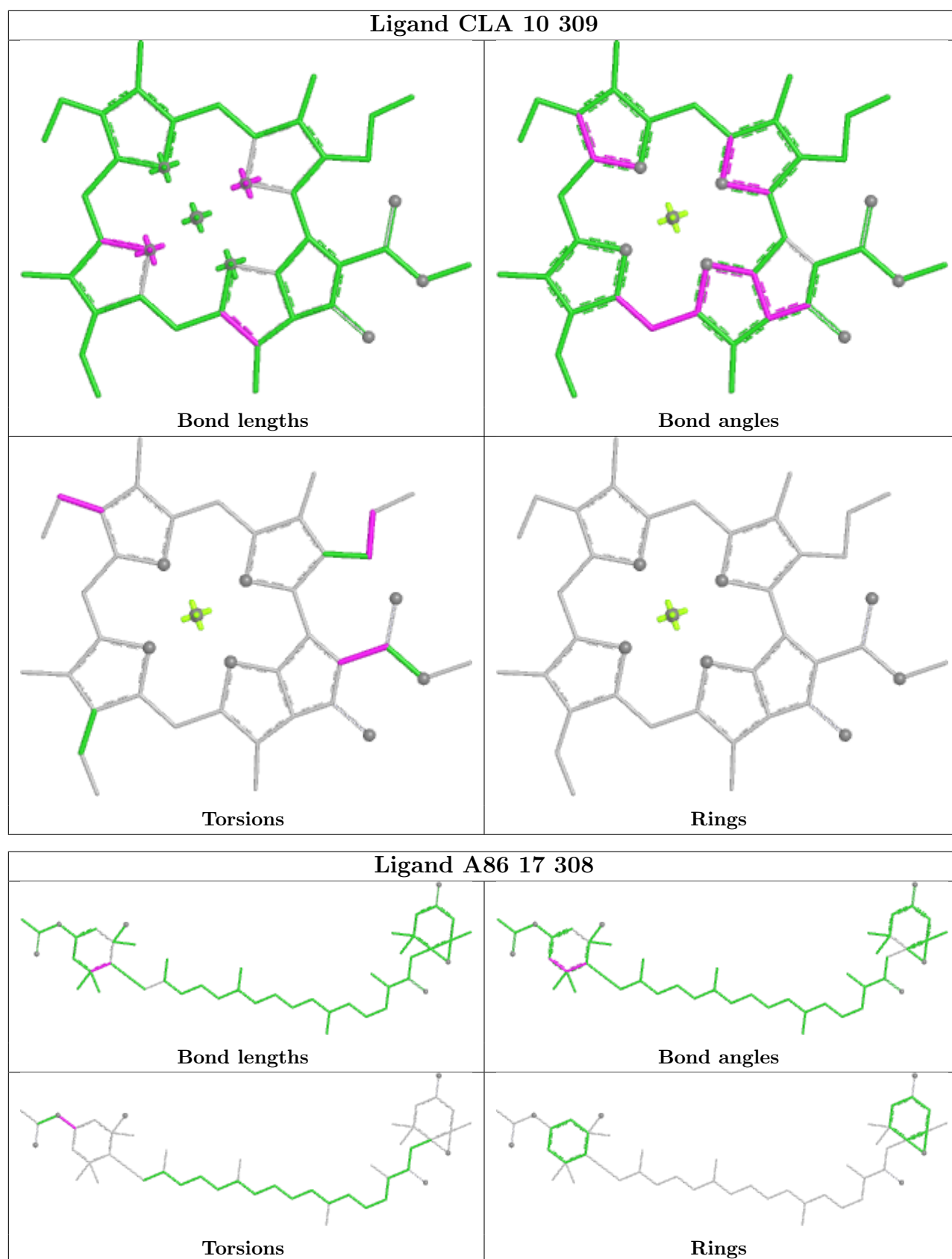
Bond angles



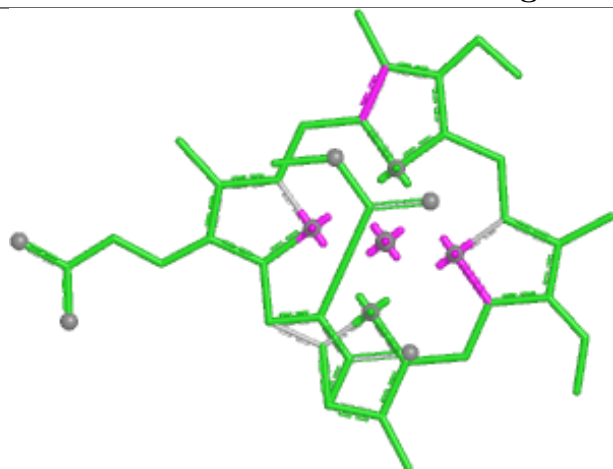
Torsions



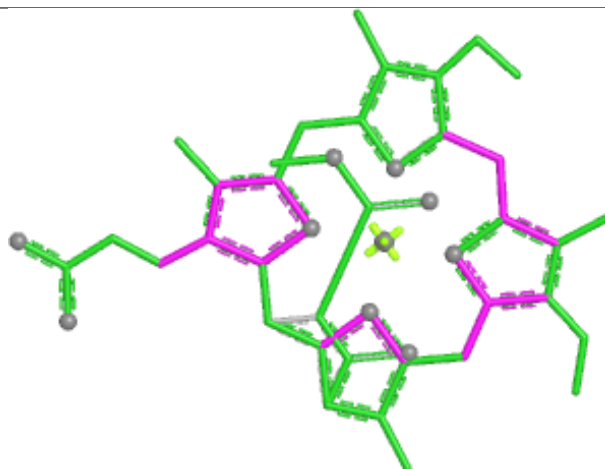
Rings



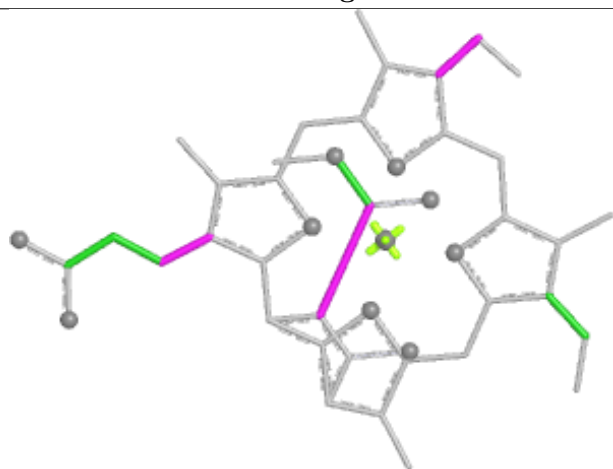
Ligand KC1 4 308



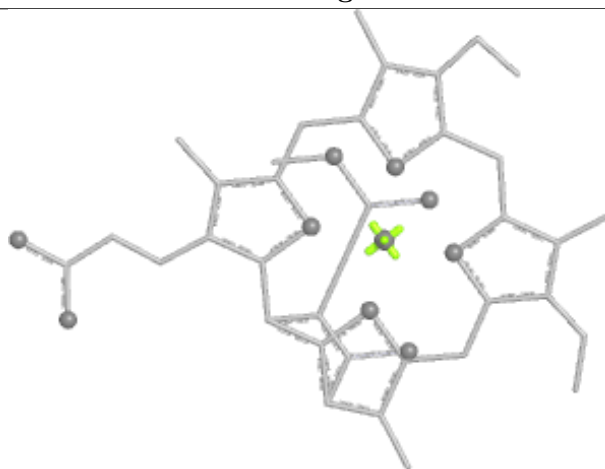
Bond lengths



Bond angles

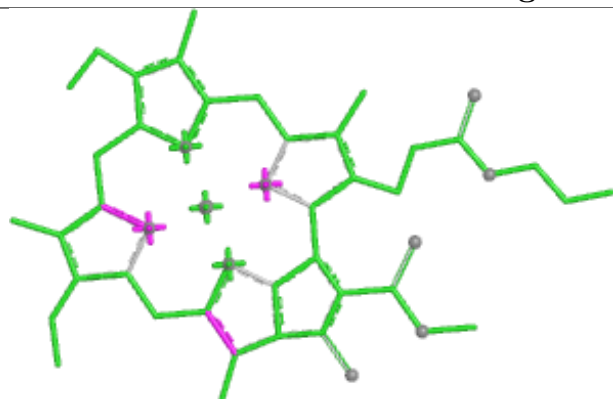


Torsions

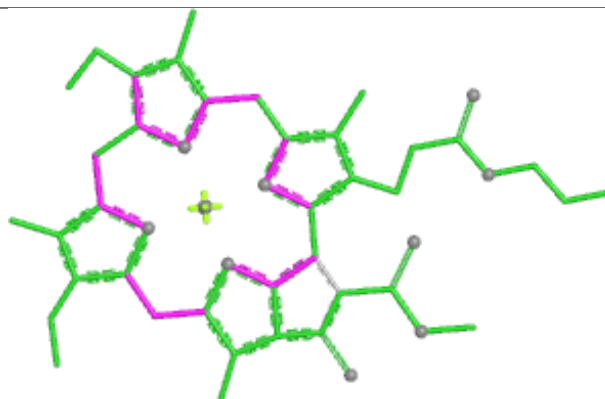


Rings

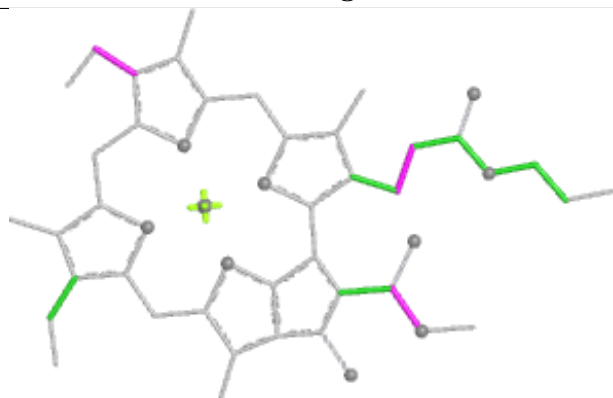
Ligand CLA 1 308



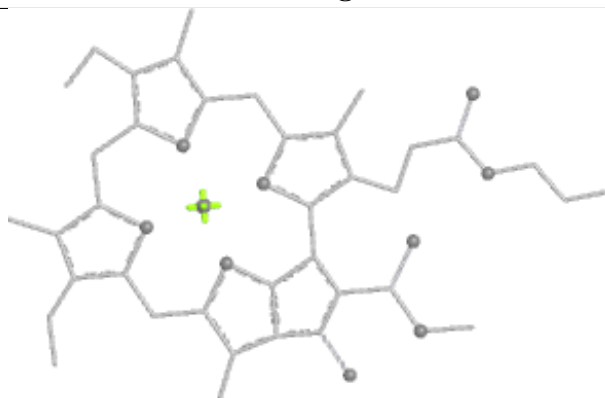
Bond lengths



Bond angles

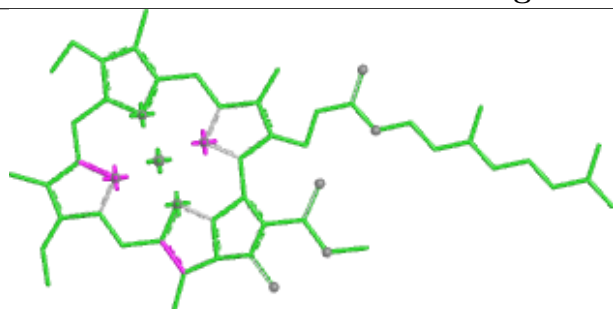


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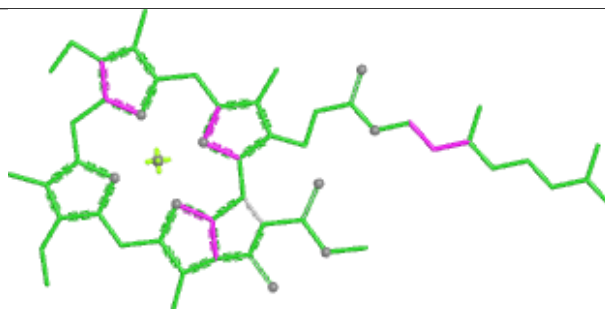


Rings

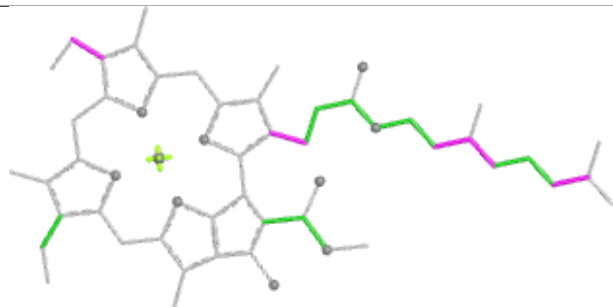
Ligand CLA A 834



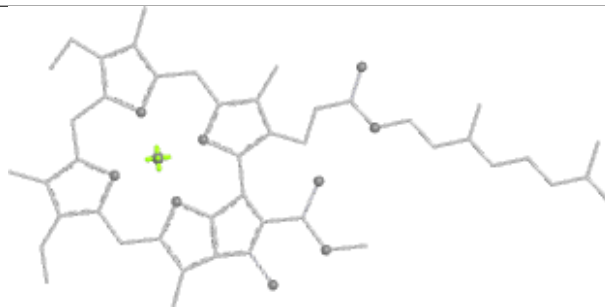
Bond lengths



Bond angles

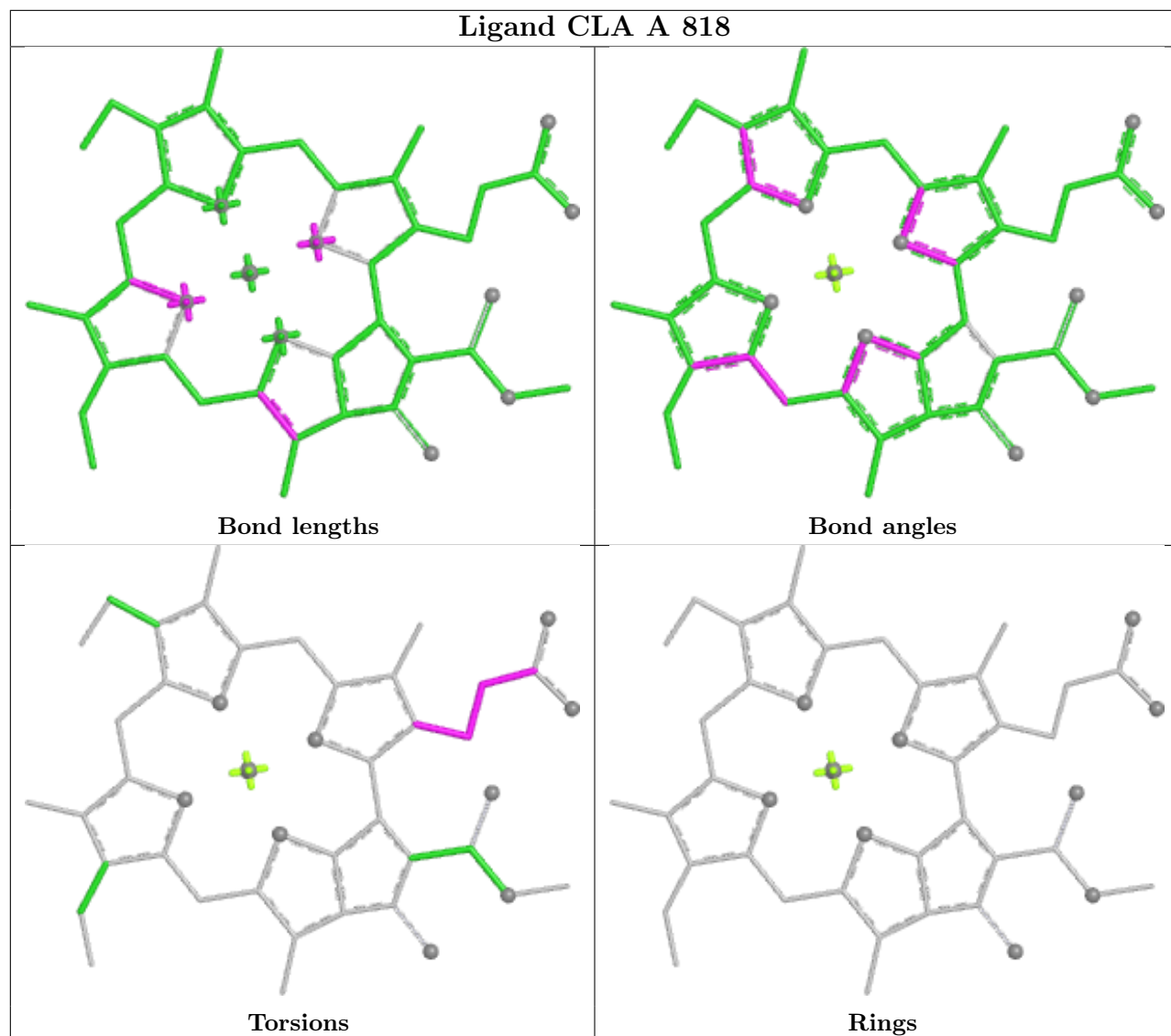


Torsions

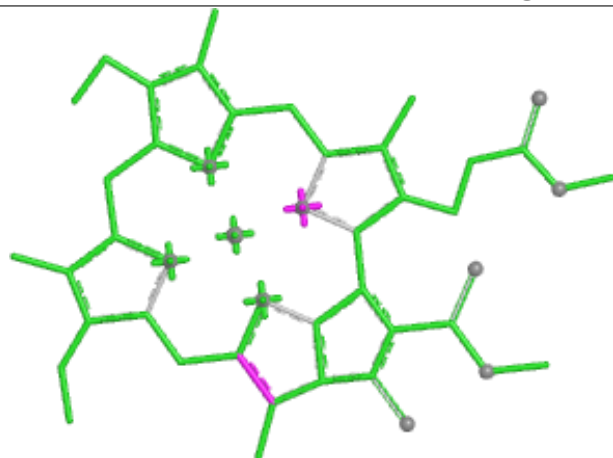


Rings

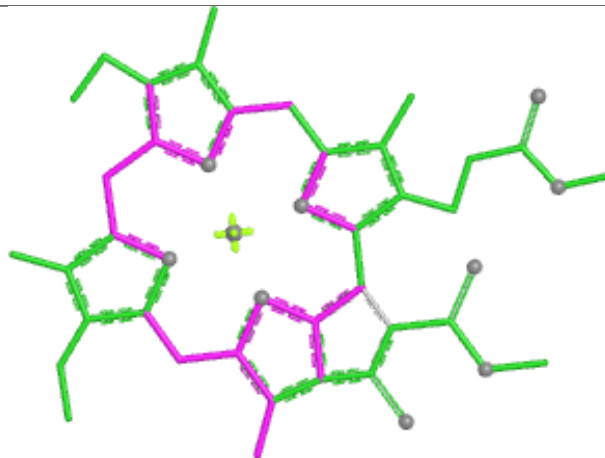
Ligand CLA A 818



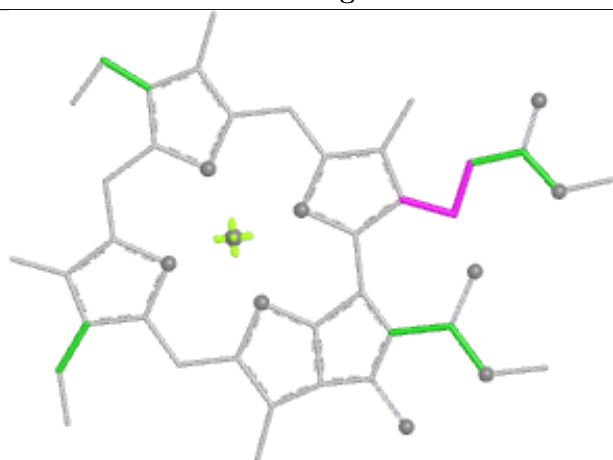
Ligand CLA 9 308



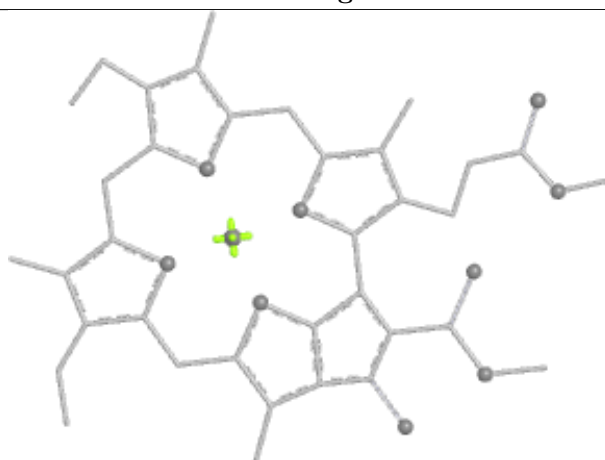
Bond lengths



Bond angles

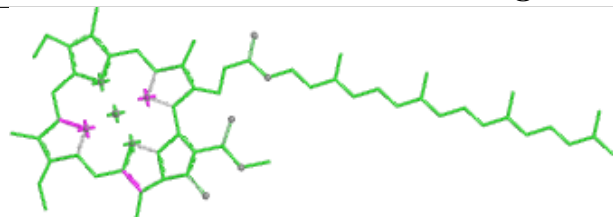


Torsions

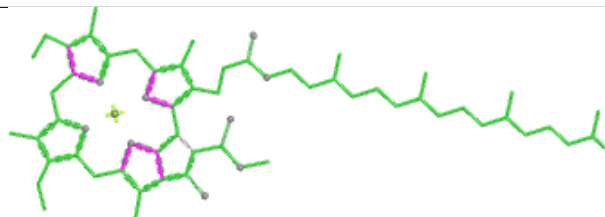


Rings

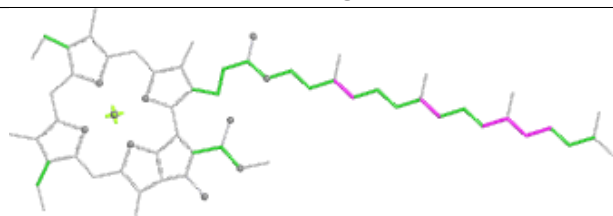
Ligand CLA B 835



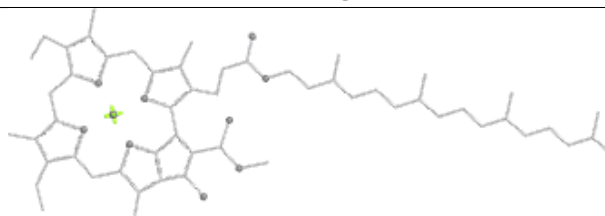
Bond lengths



Bond angles

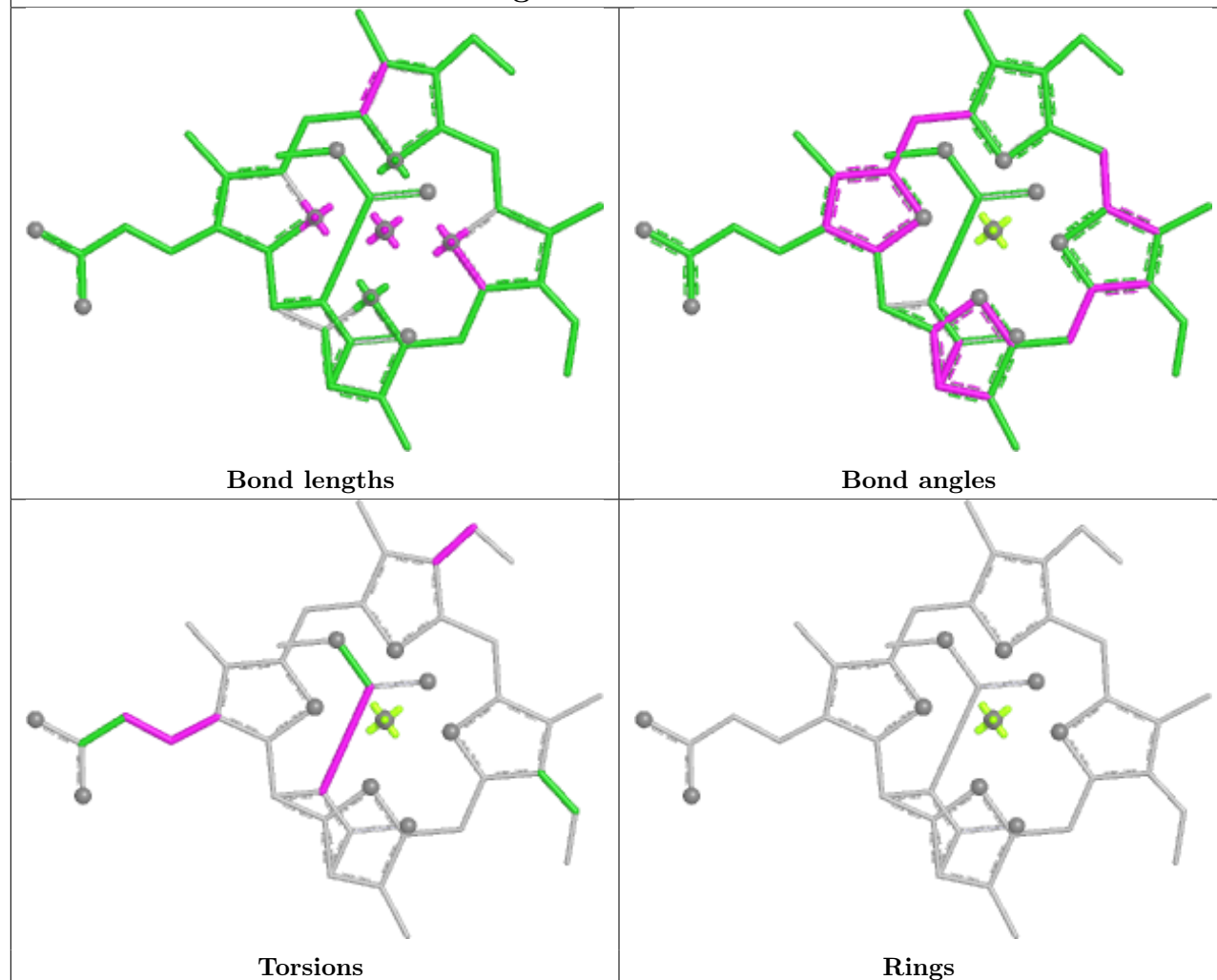


Torsions

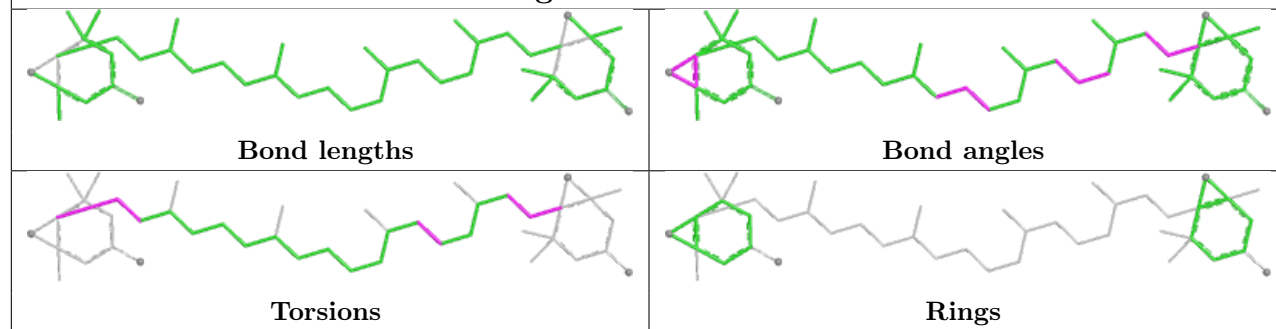


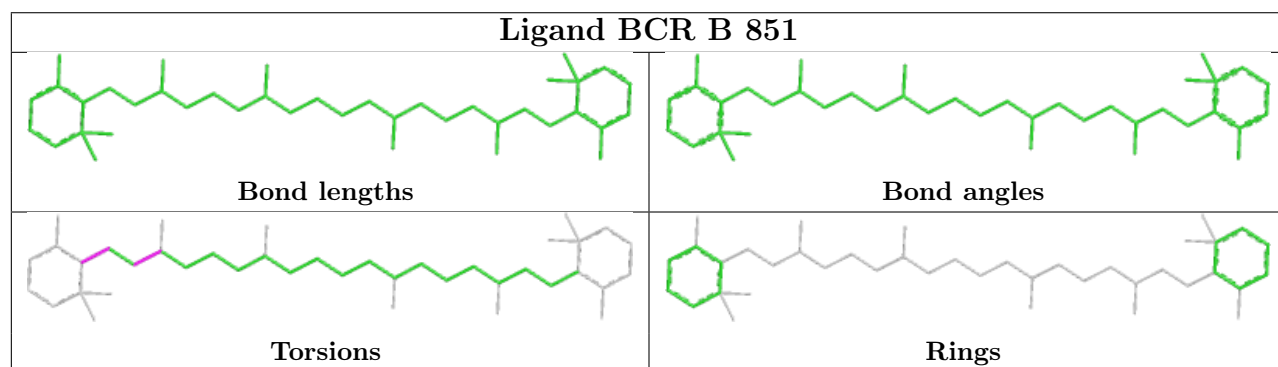
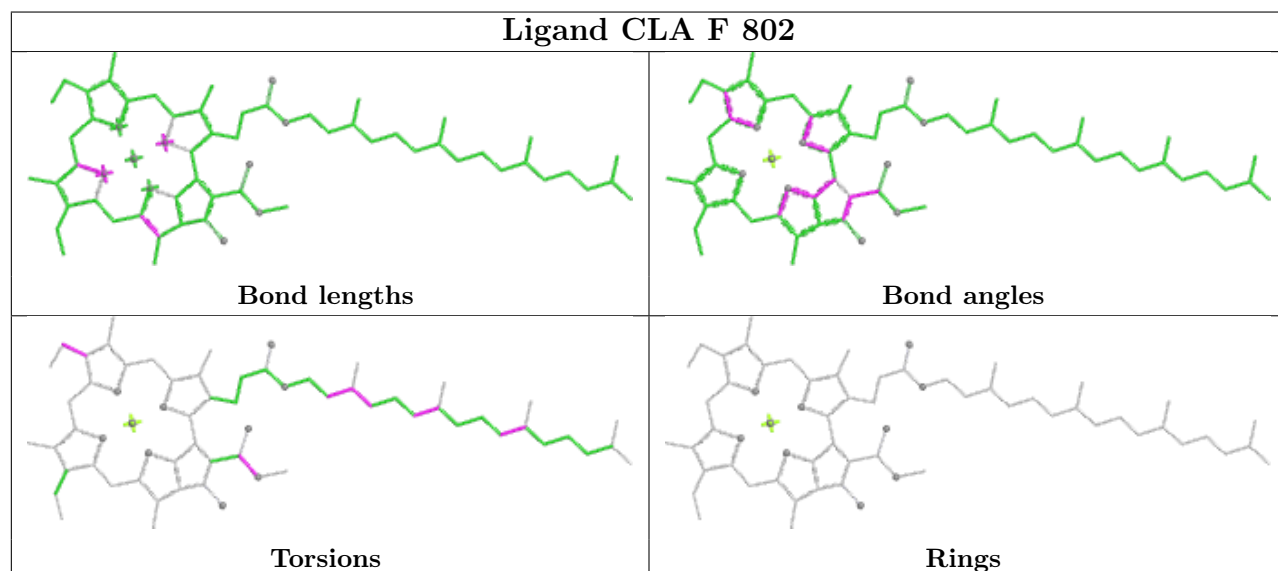
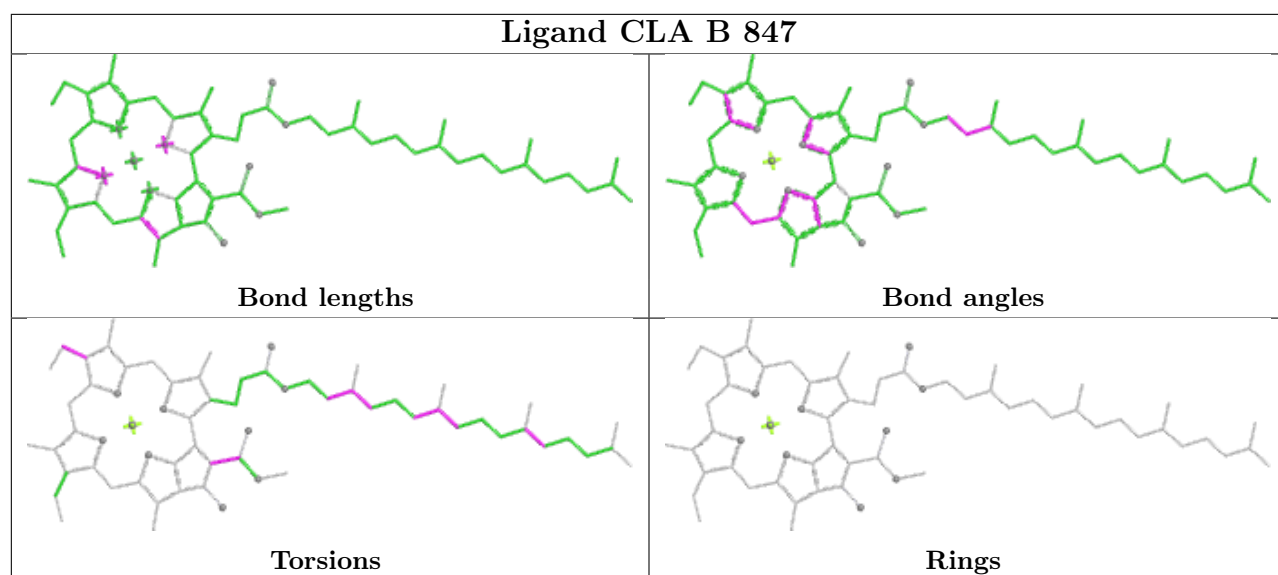
Rings

Ligand KC1 6 310

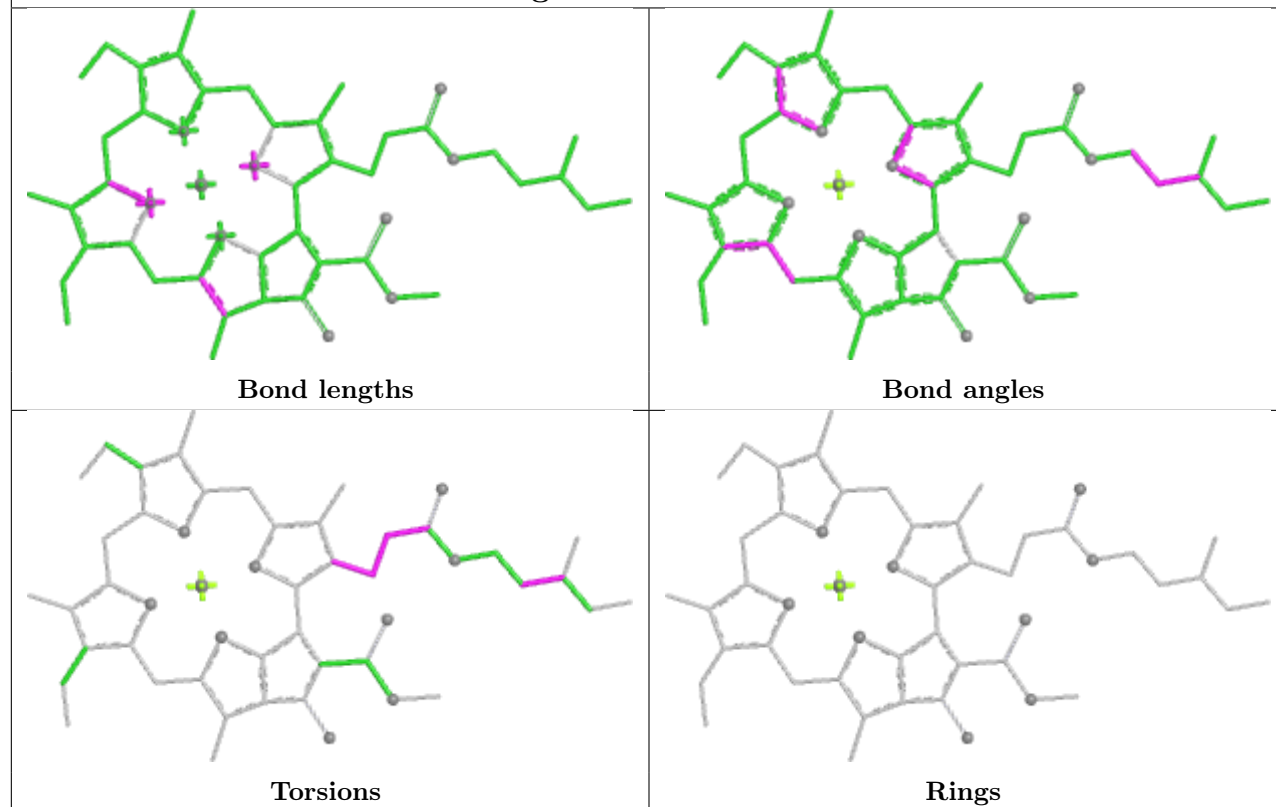


Ligand XAT 4 318

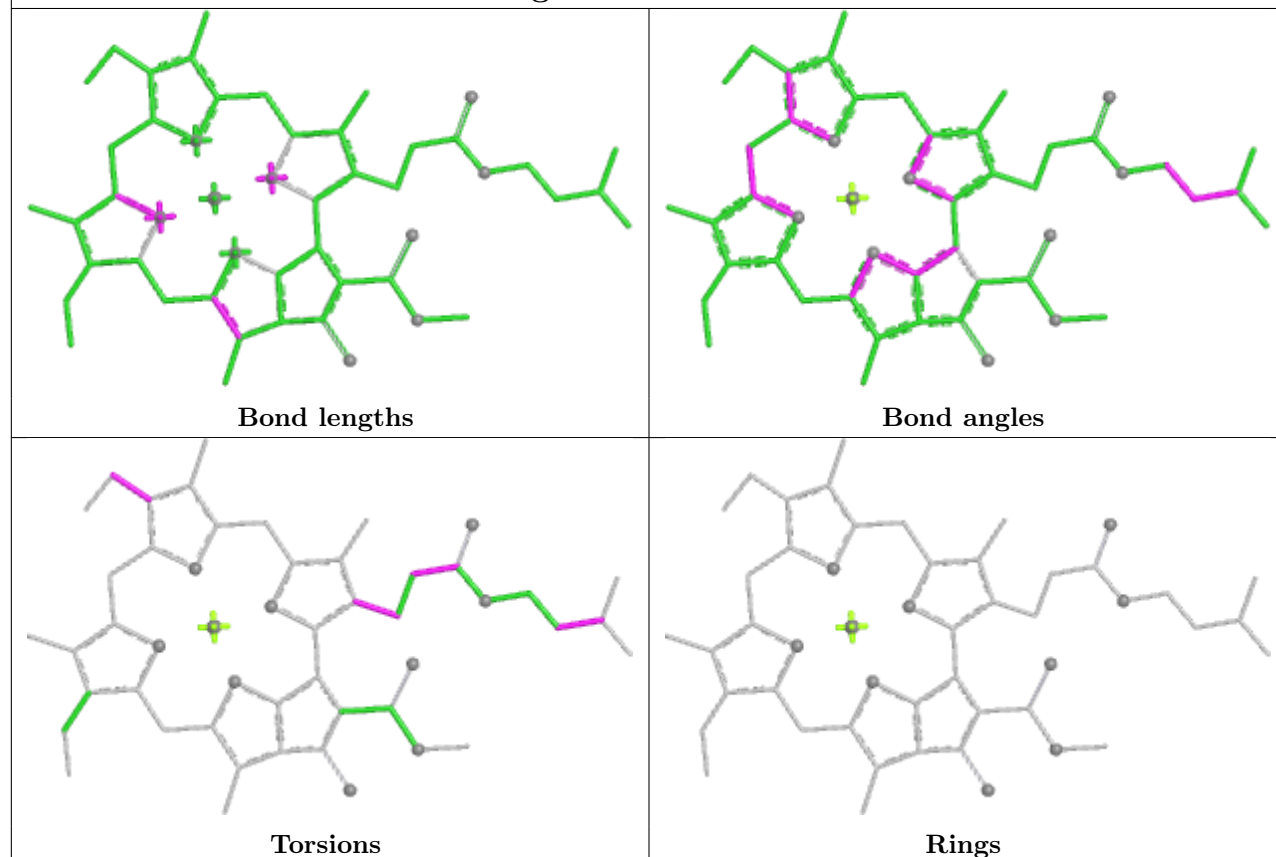




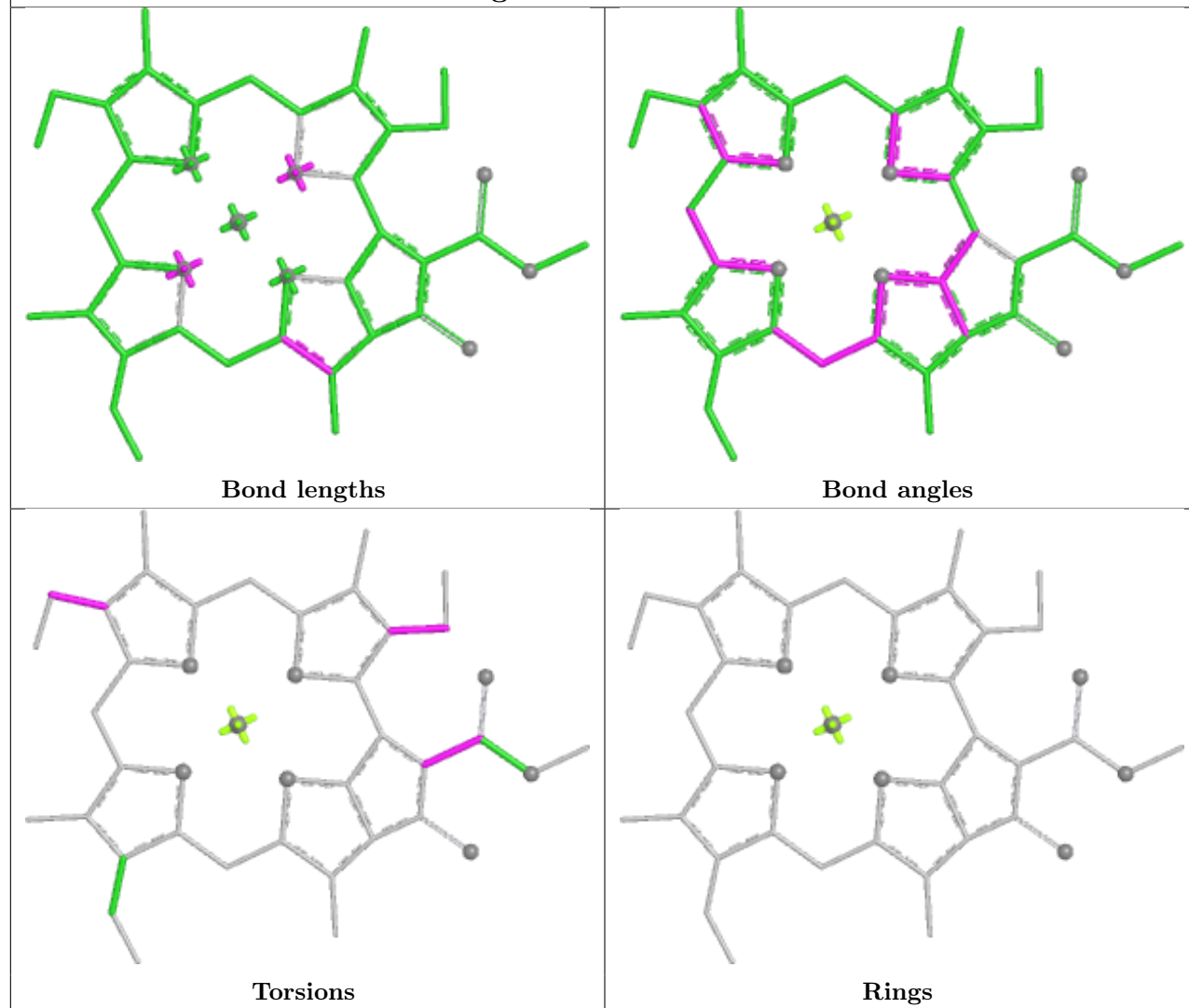
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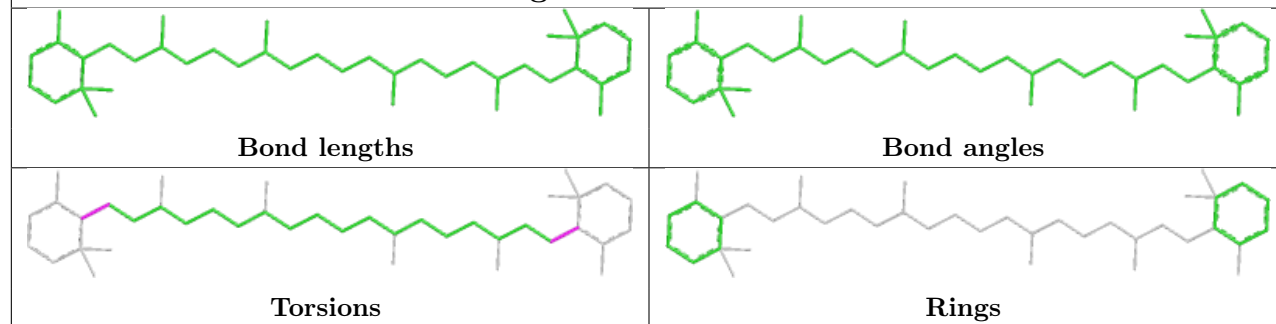
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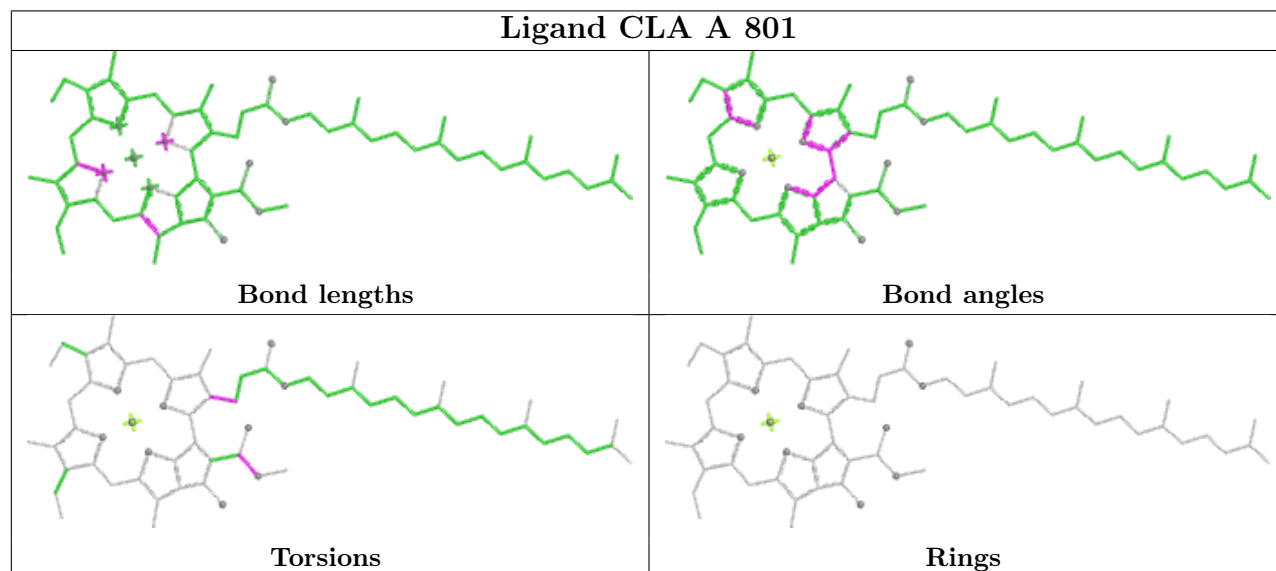
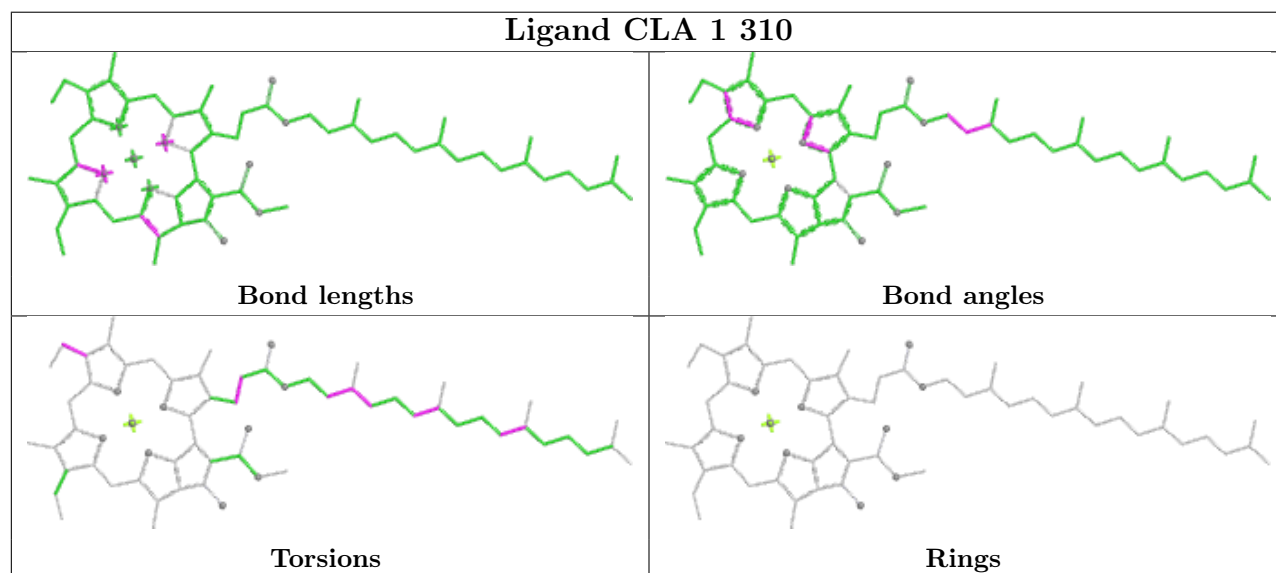
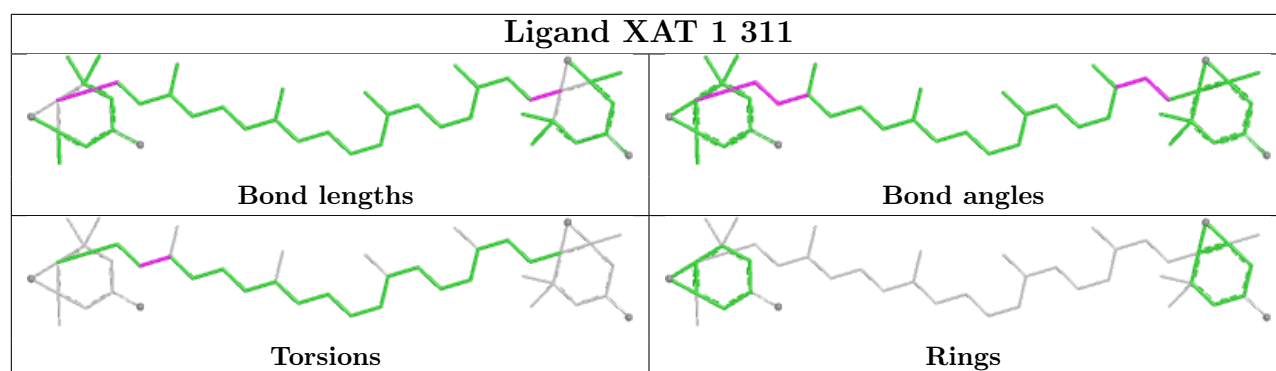


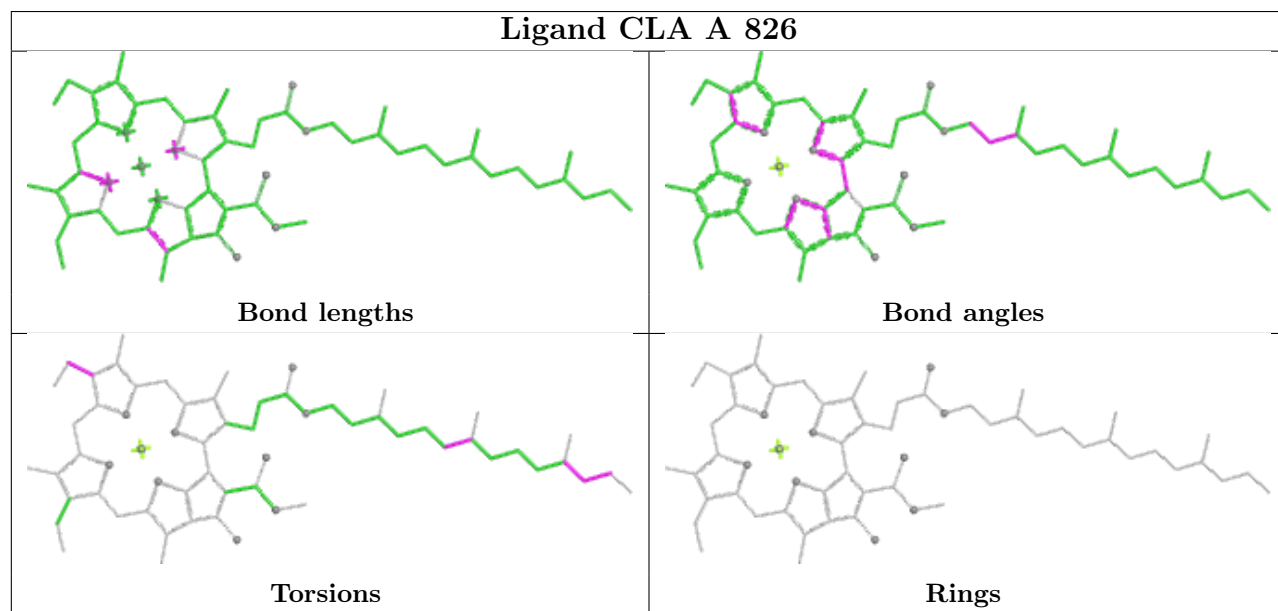
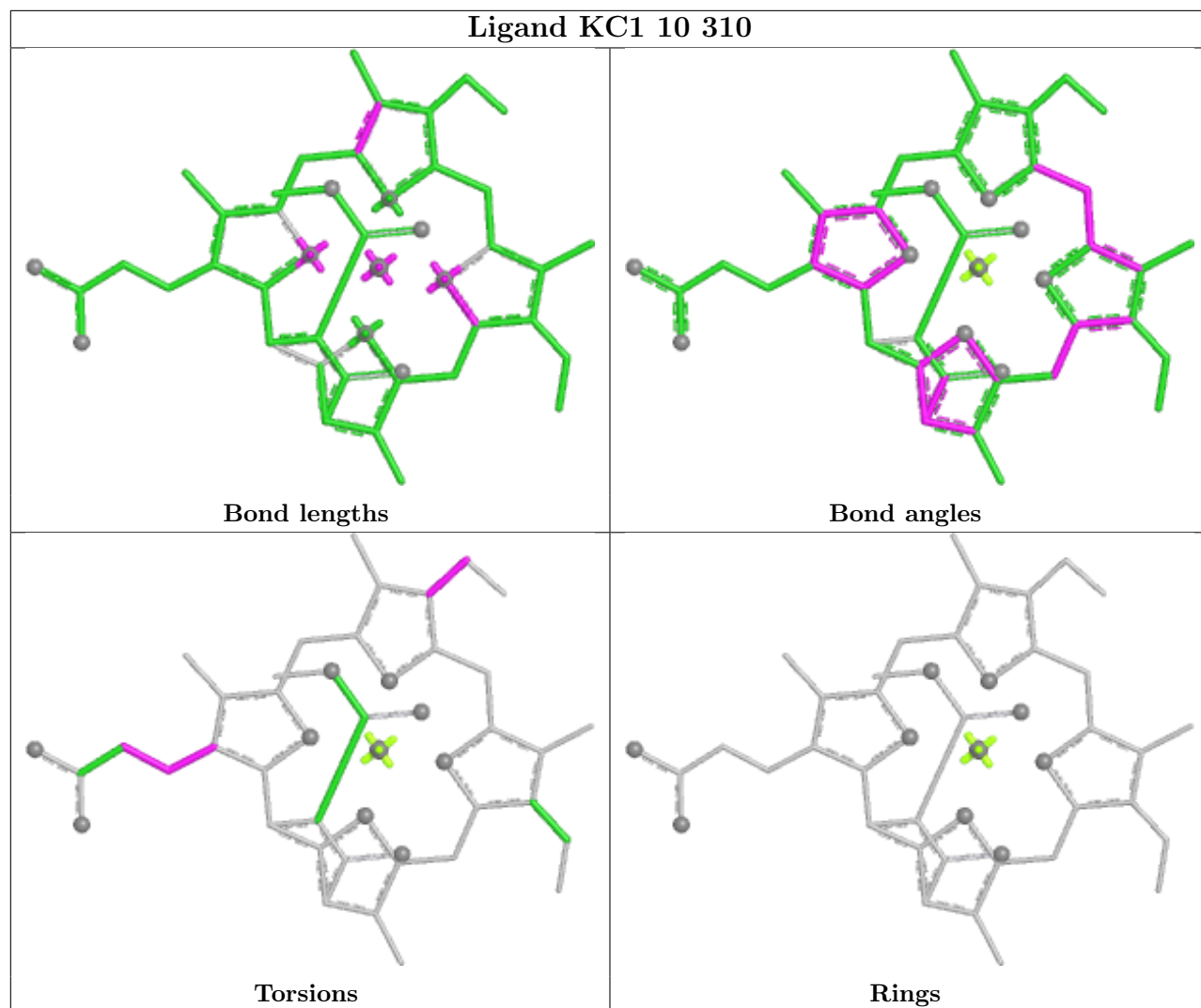
Ligand CLA 13 306

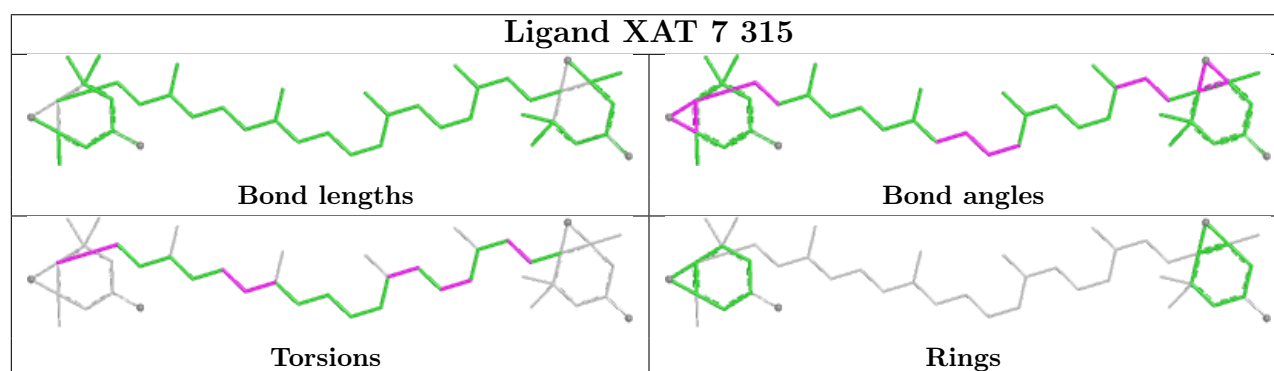
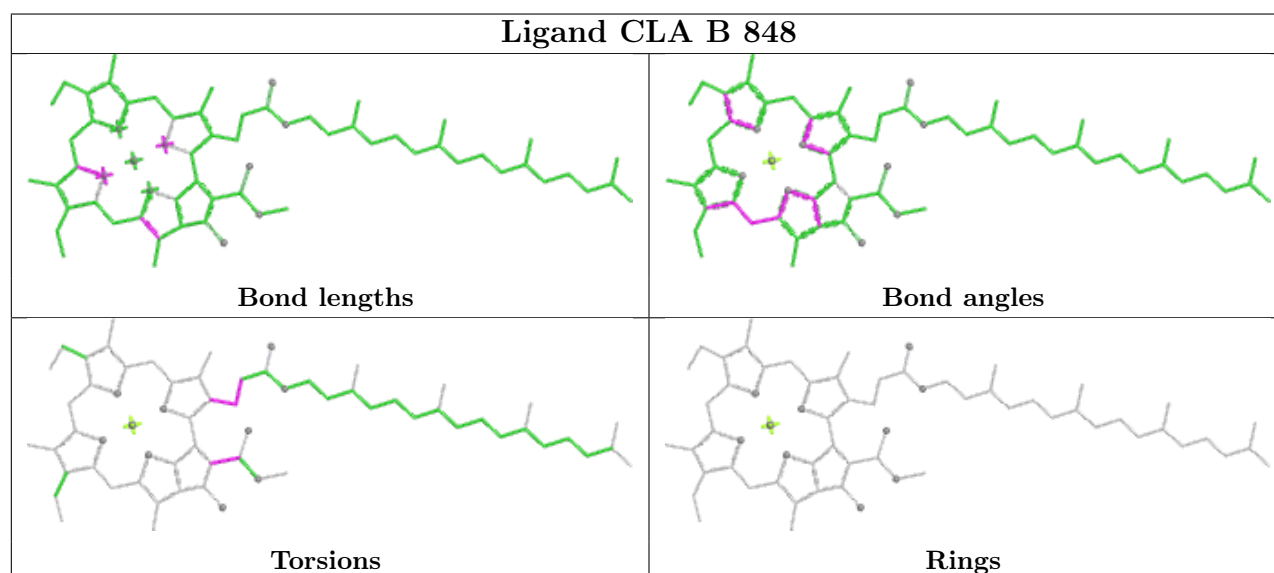
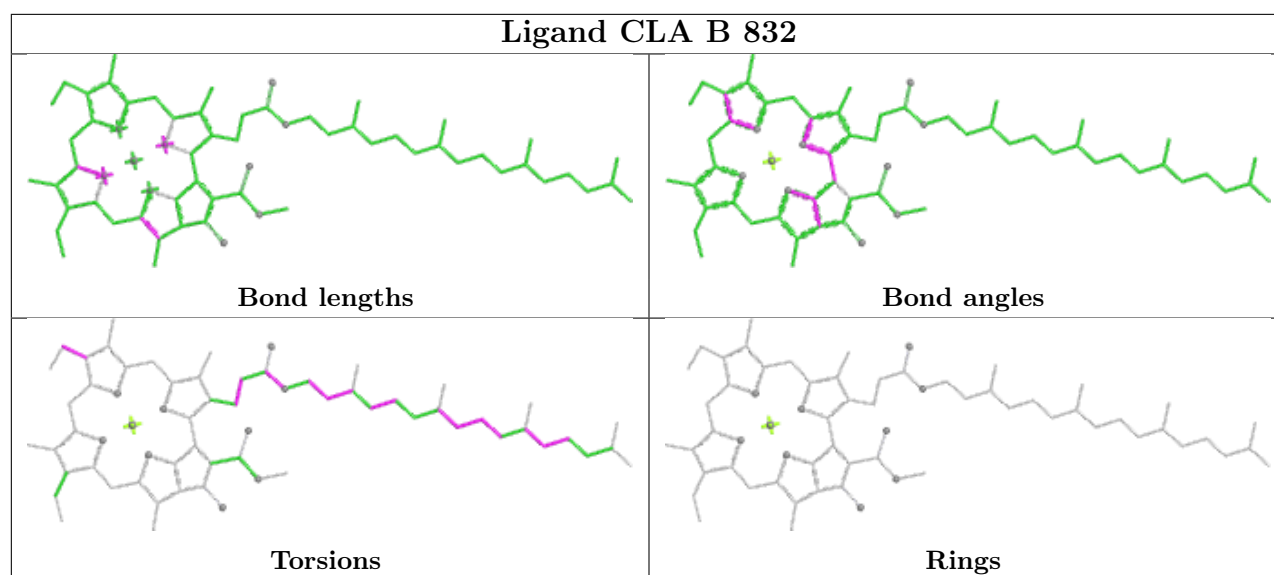


Ligand BCR A 844

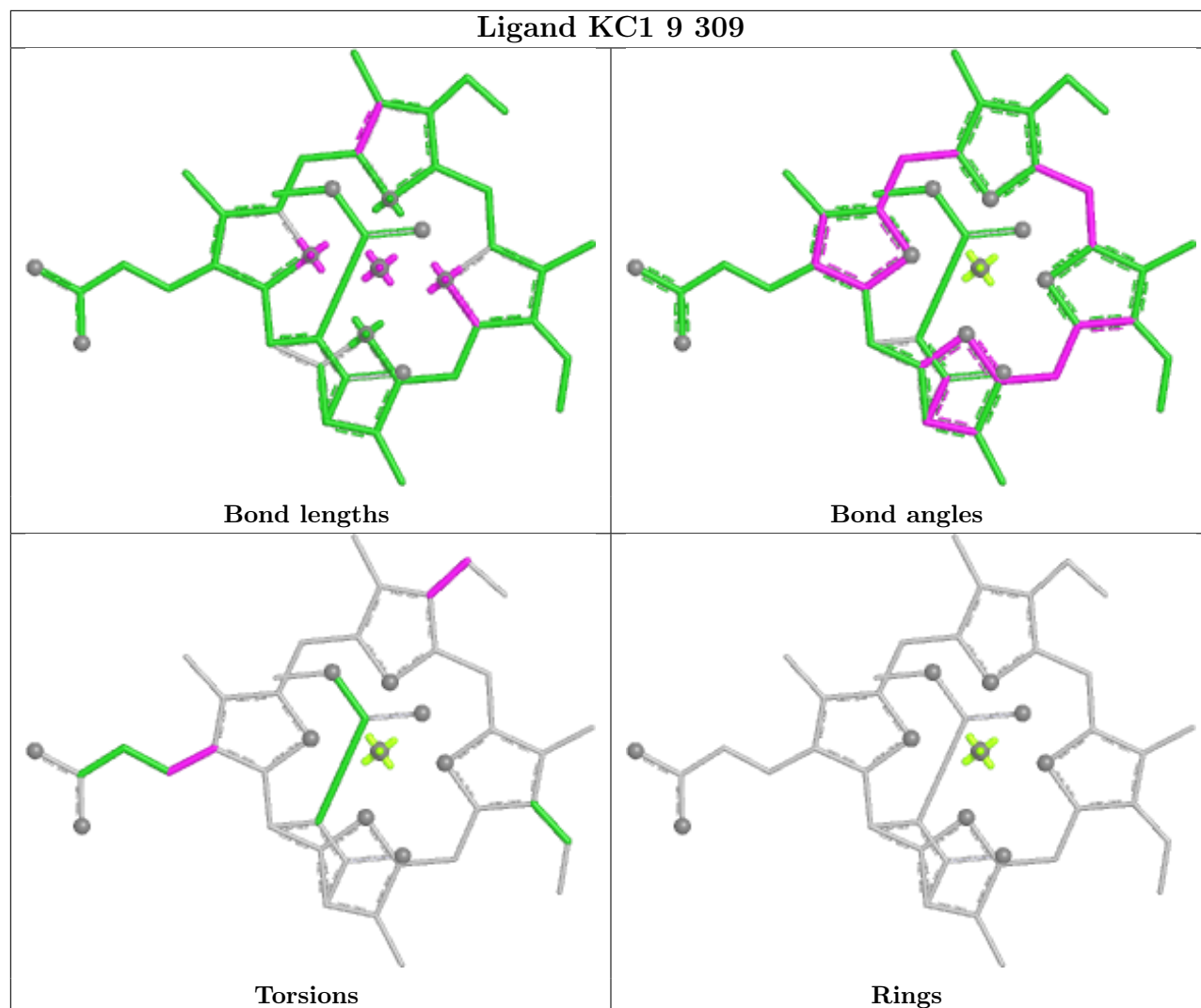




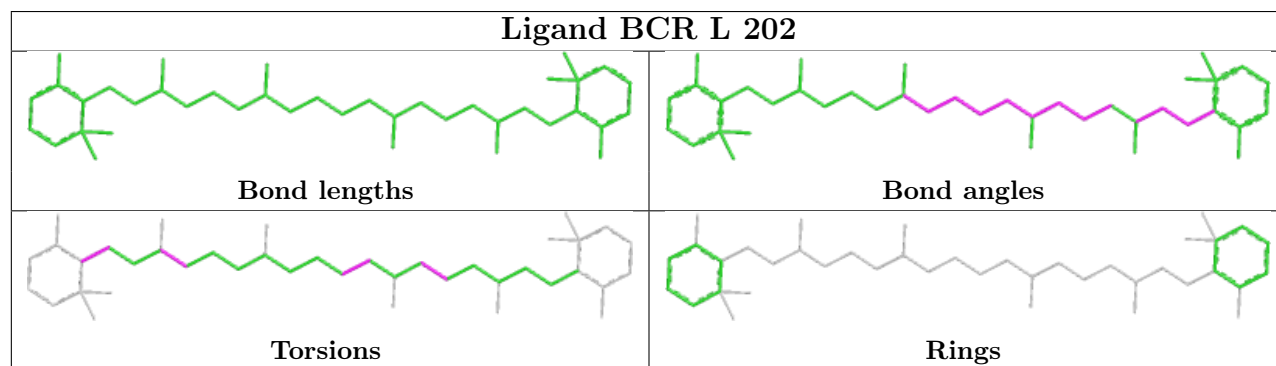




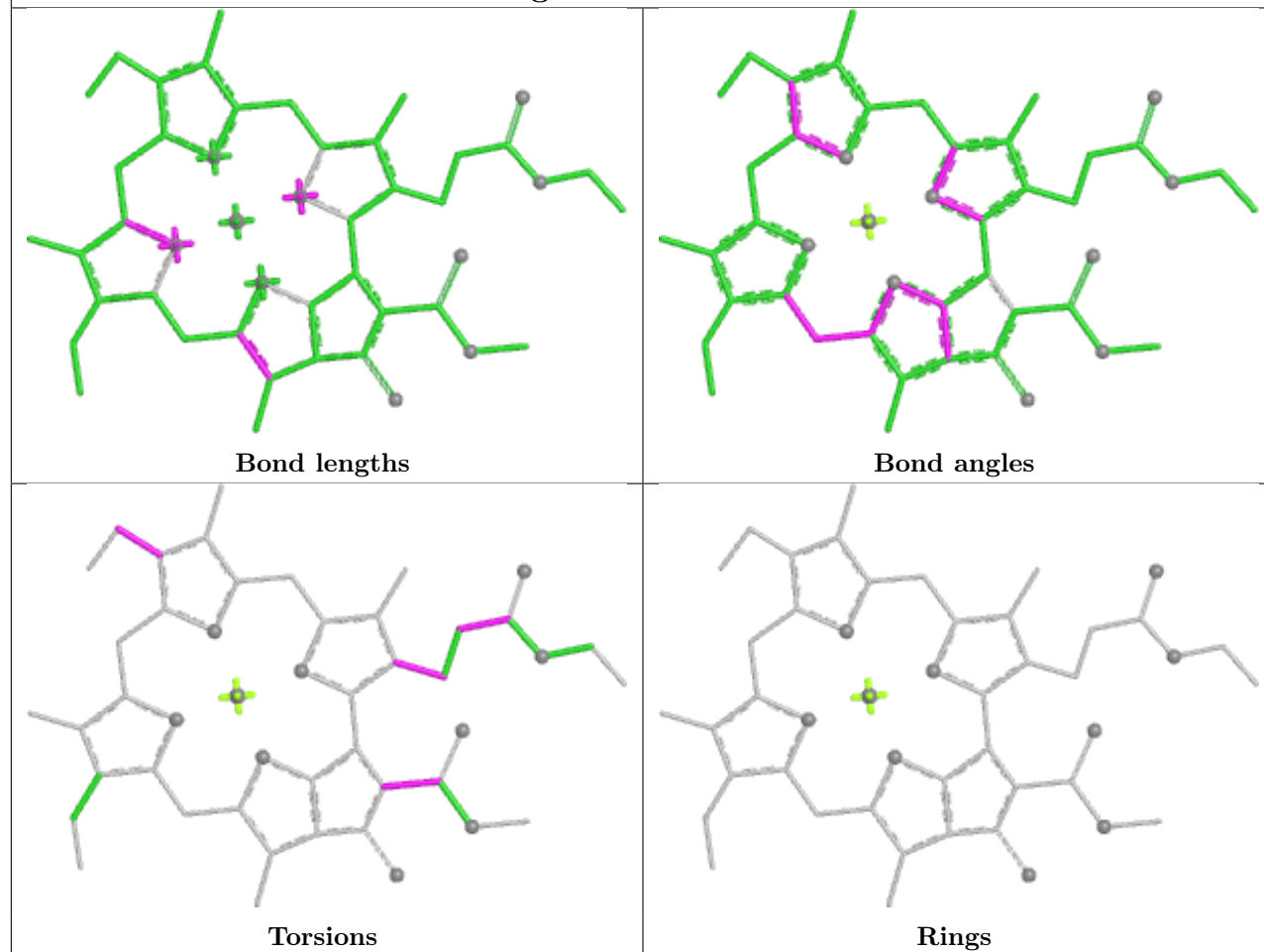
Ligand KC1 9 309



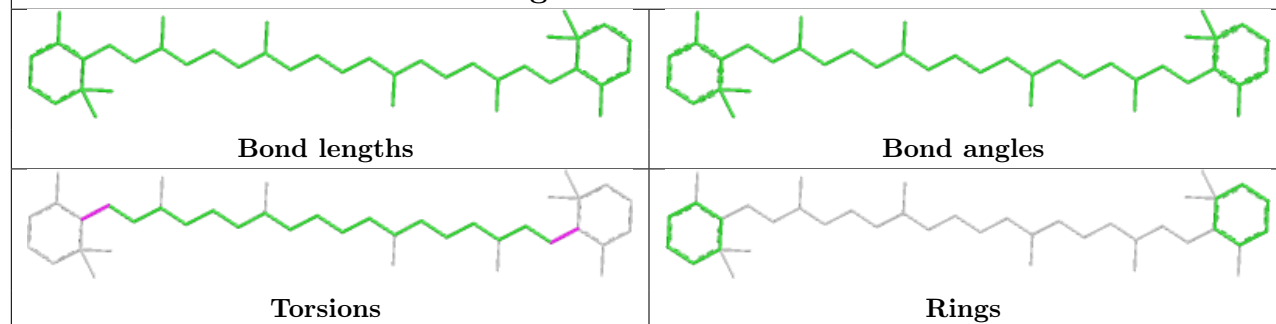
Ligand BCR L 202

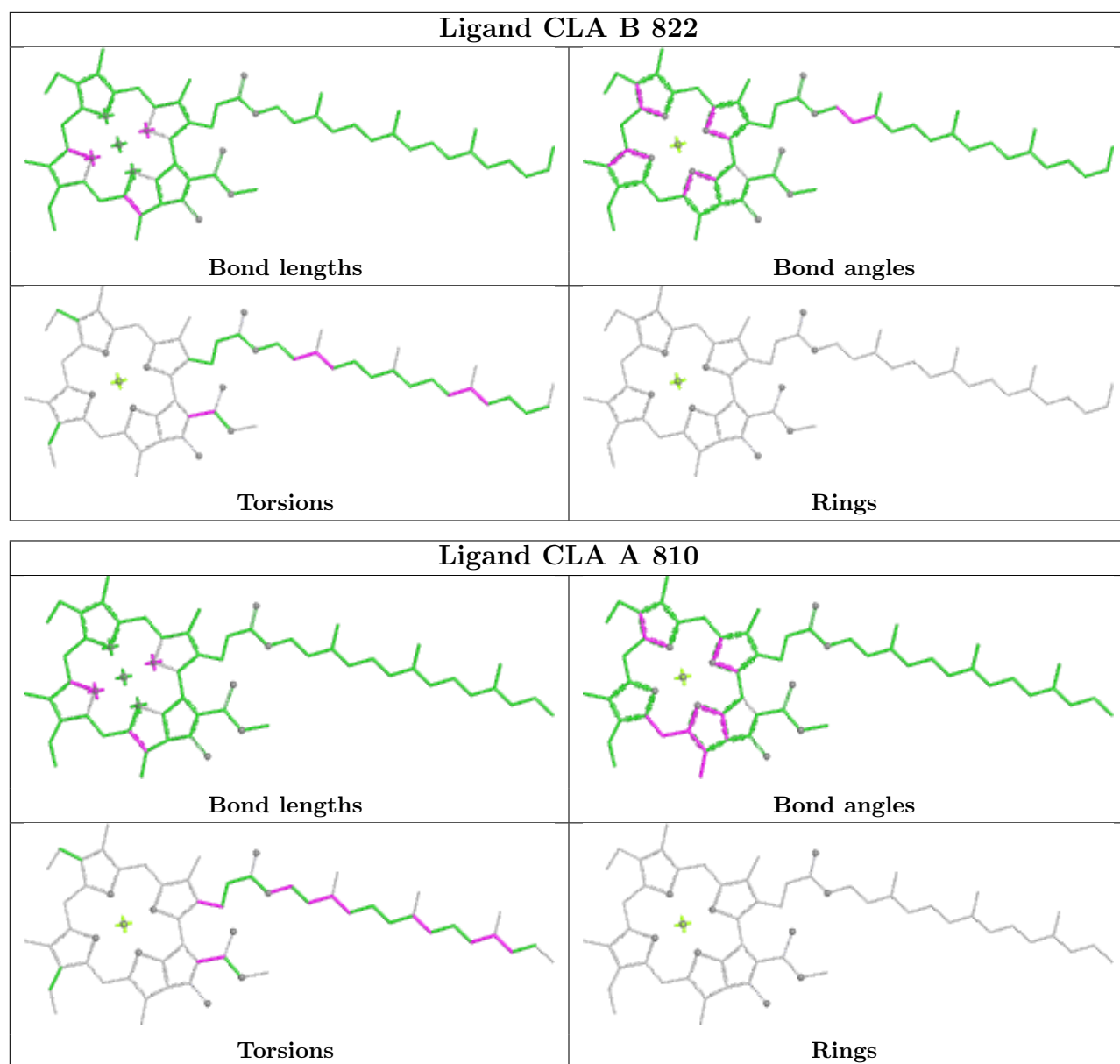


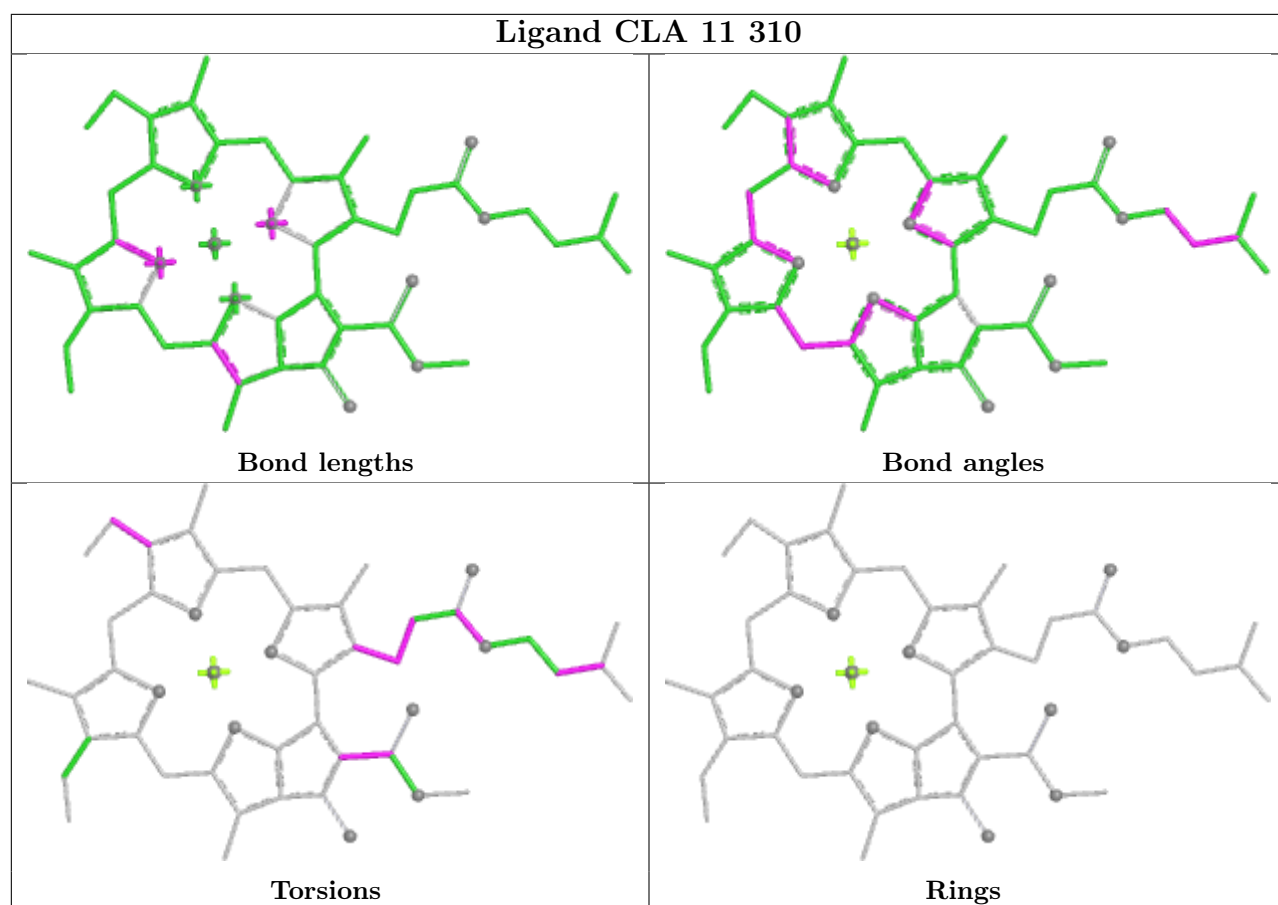
Ligand CLA 5 304

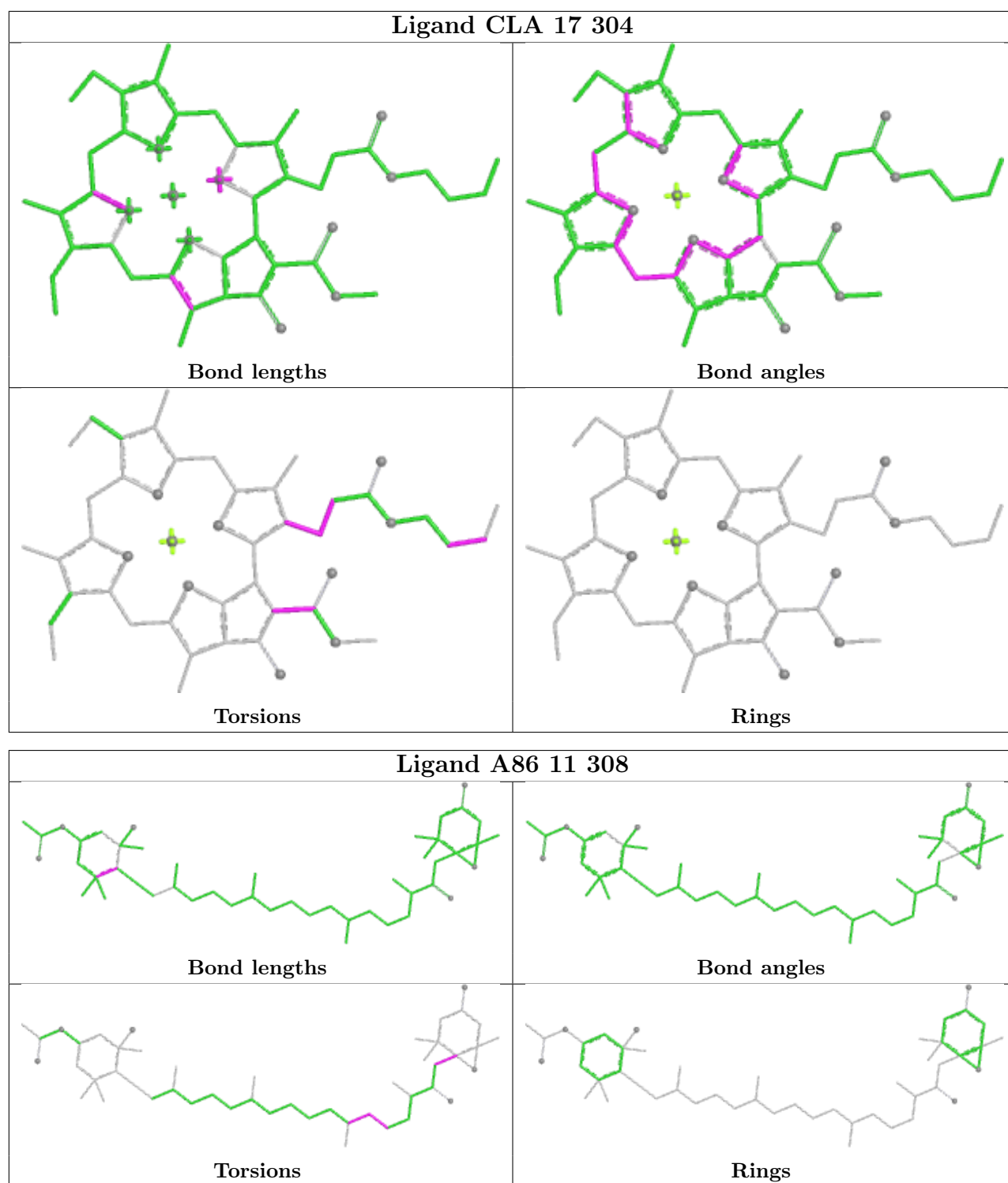


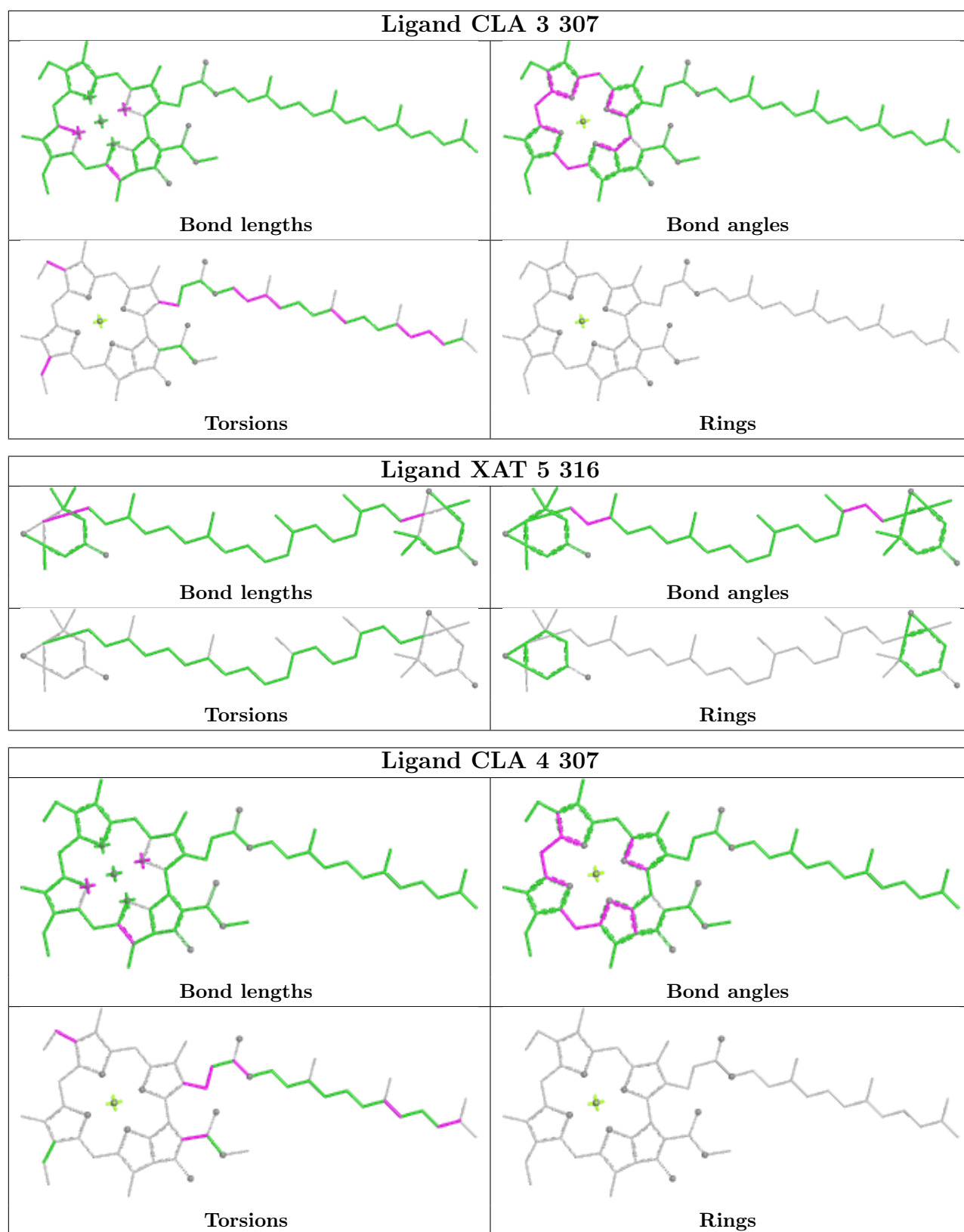
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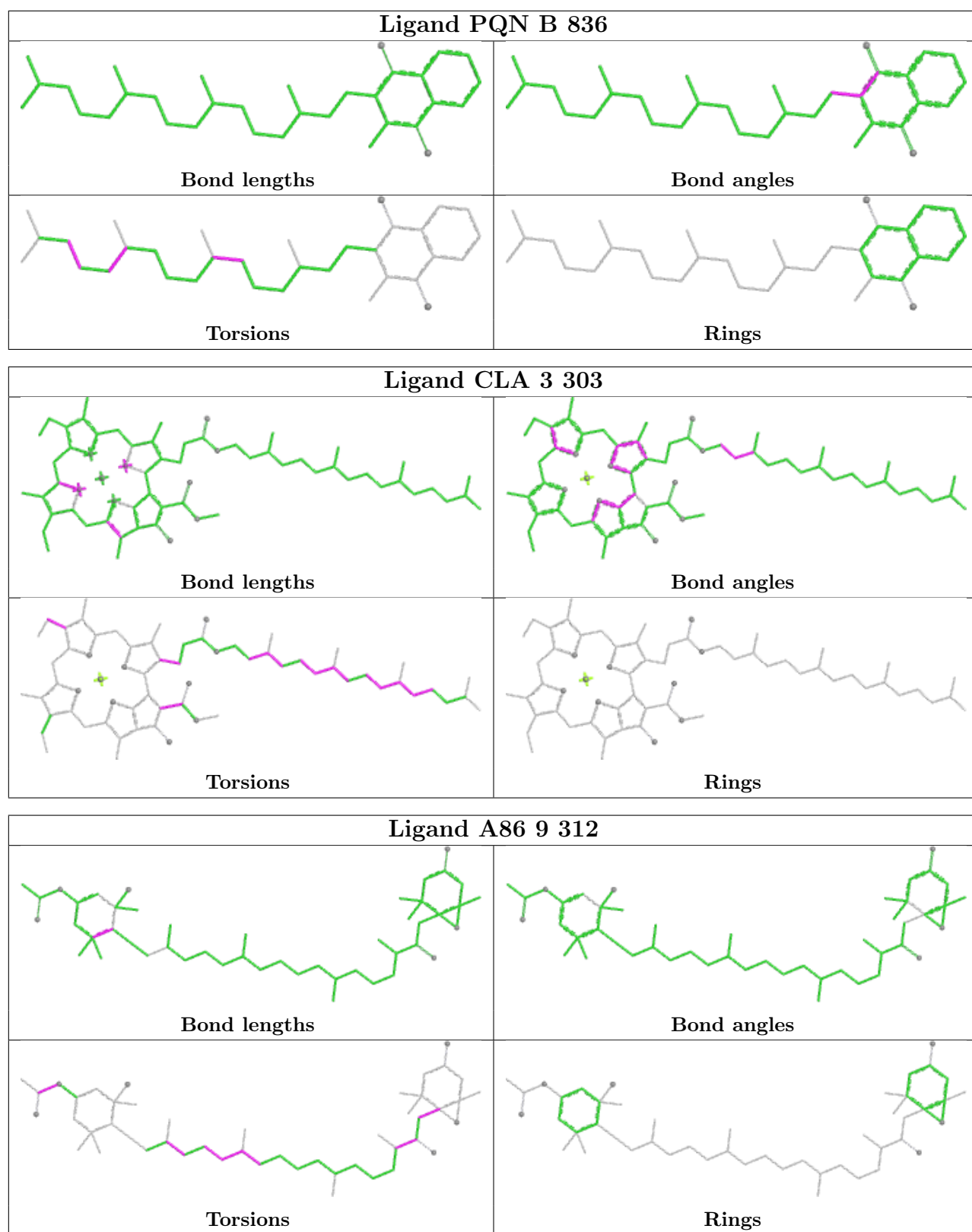


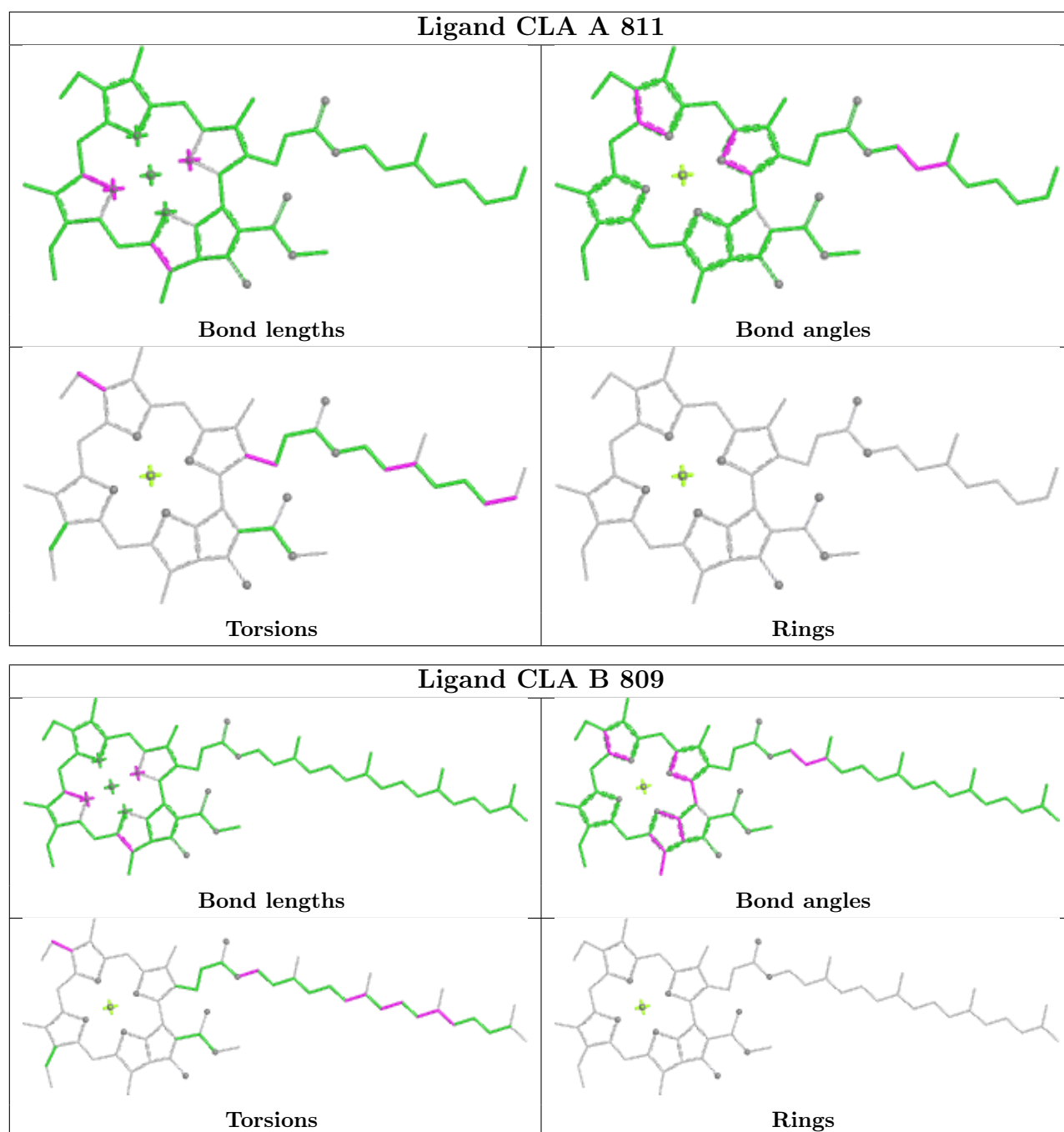




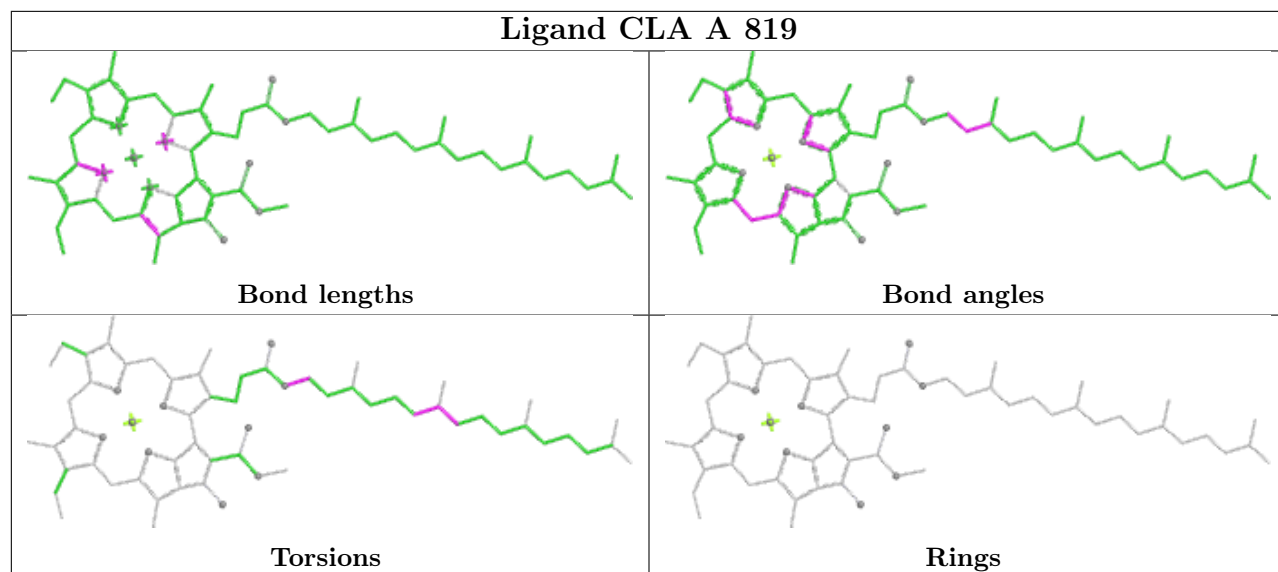




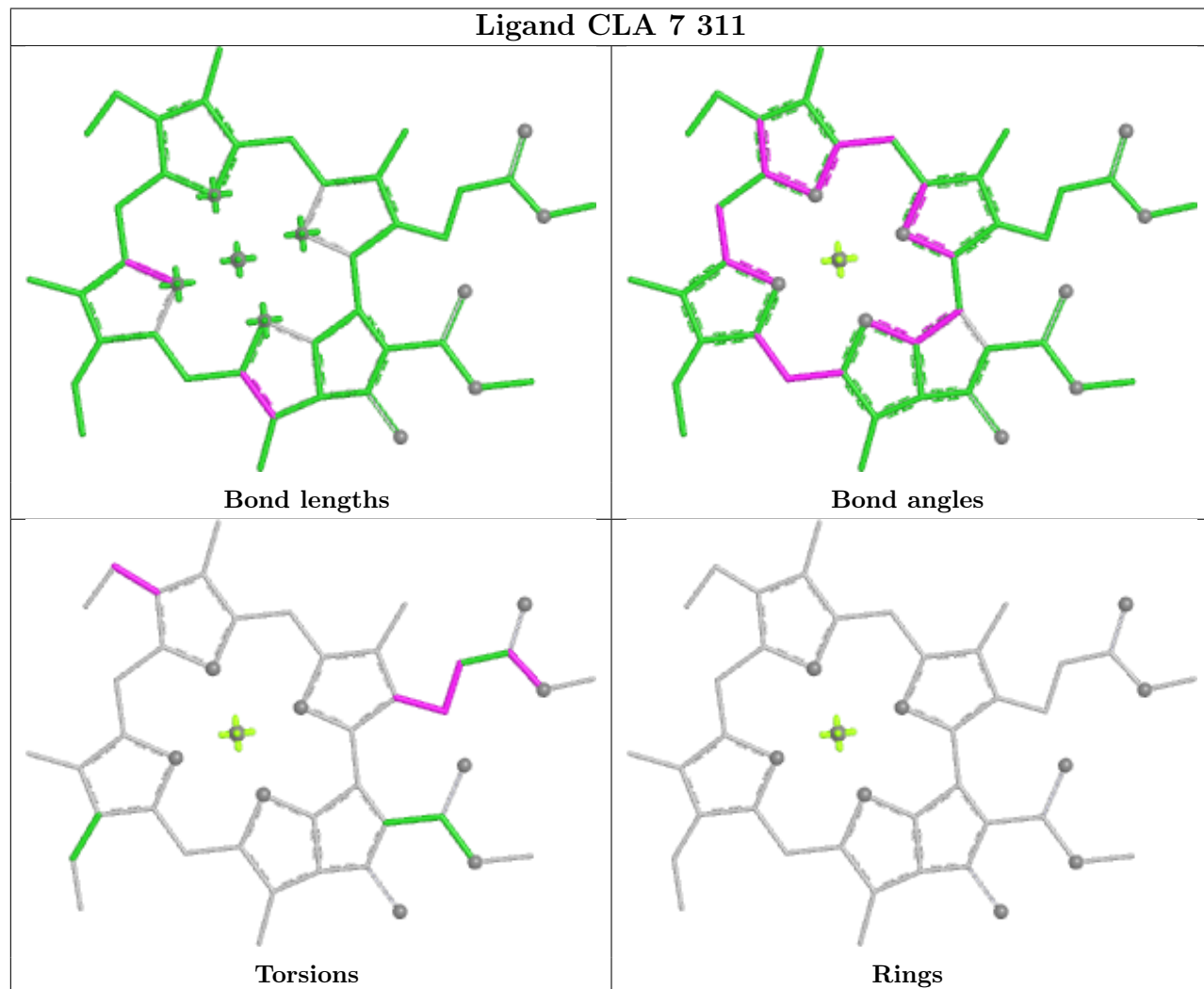


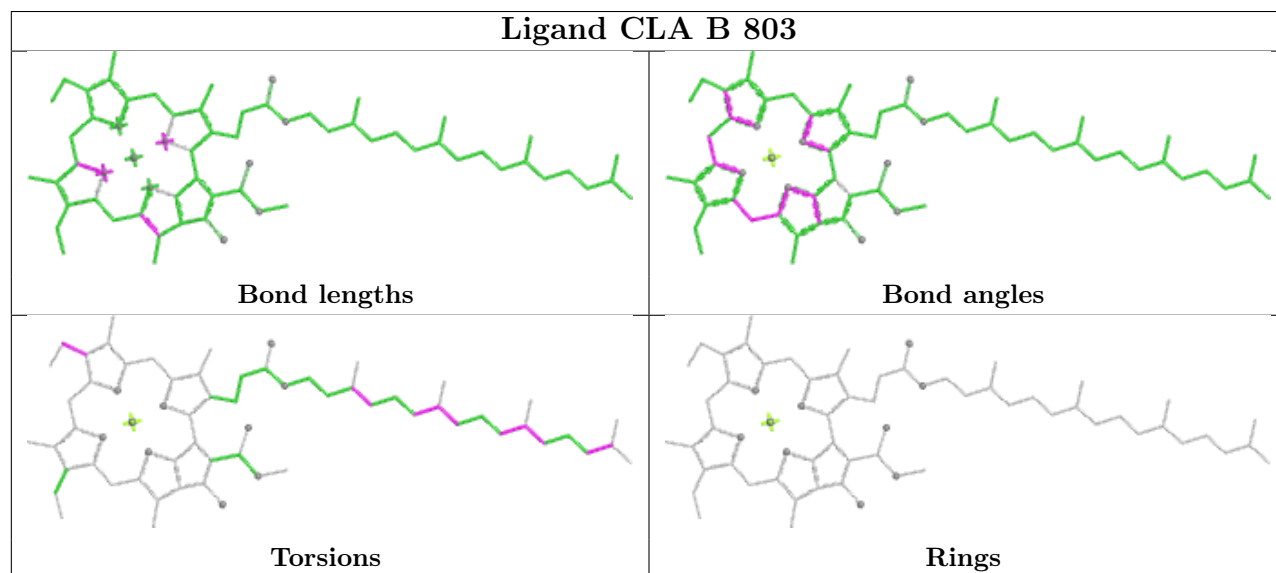
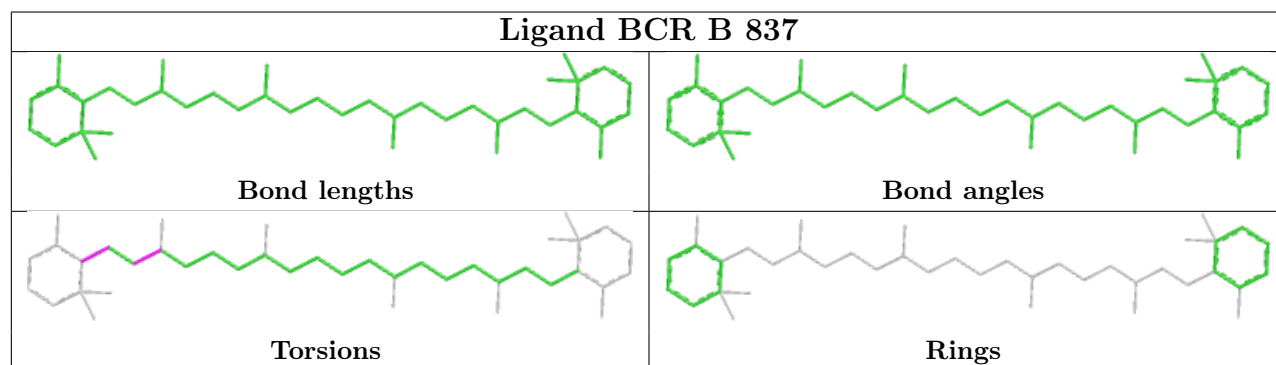
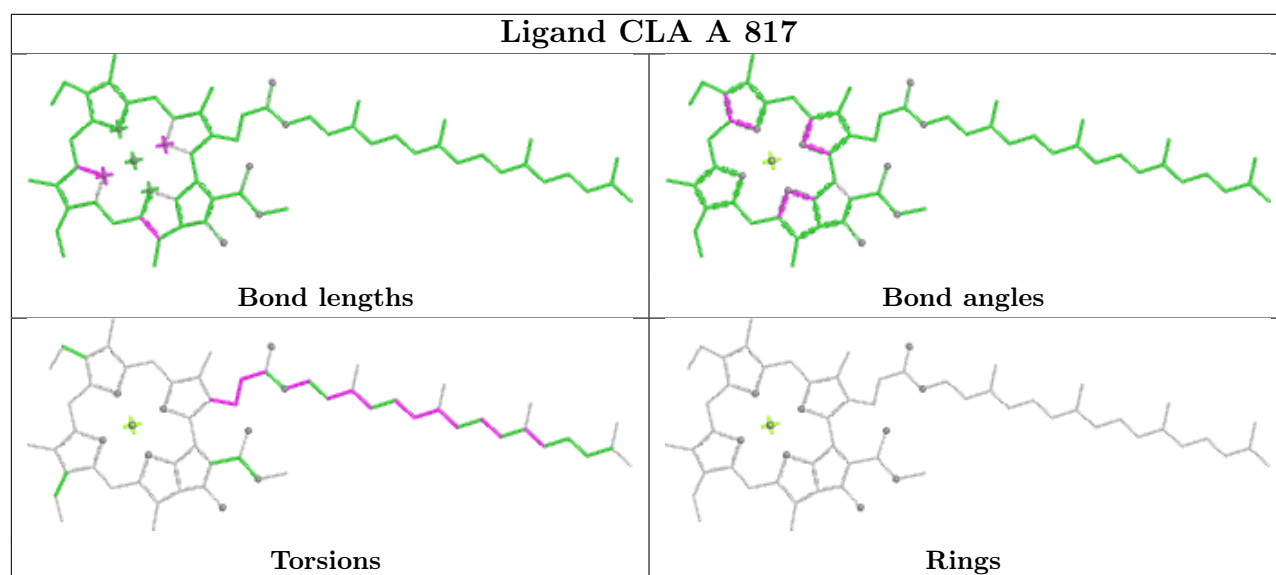


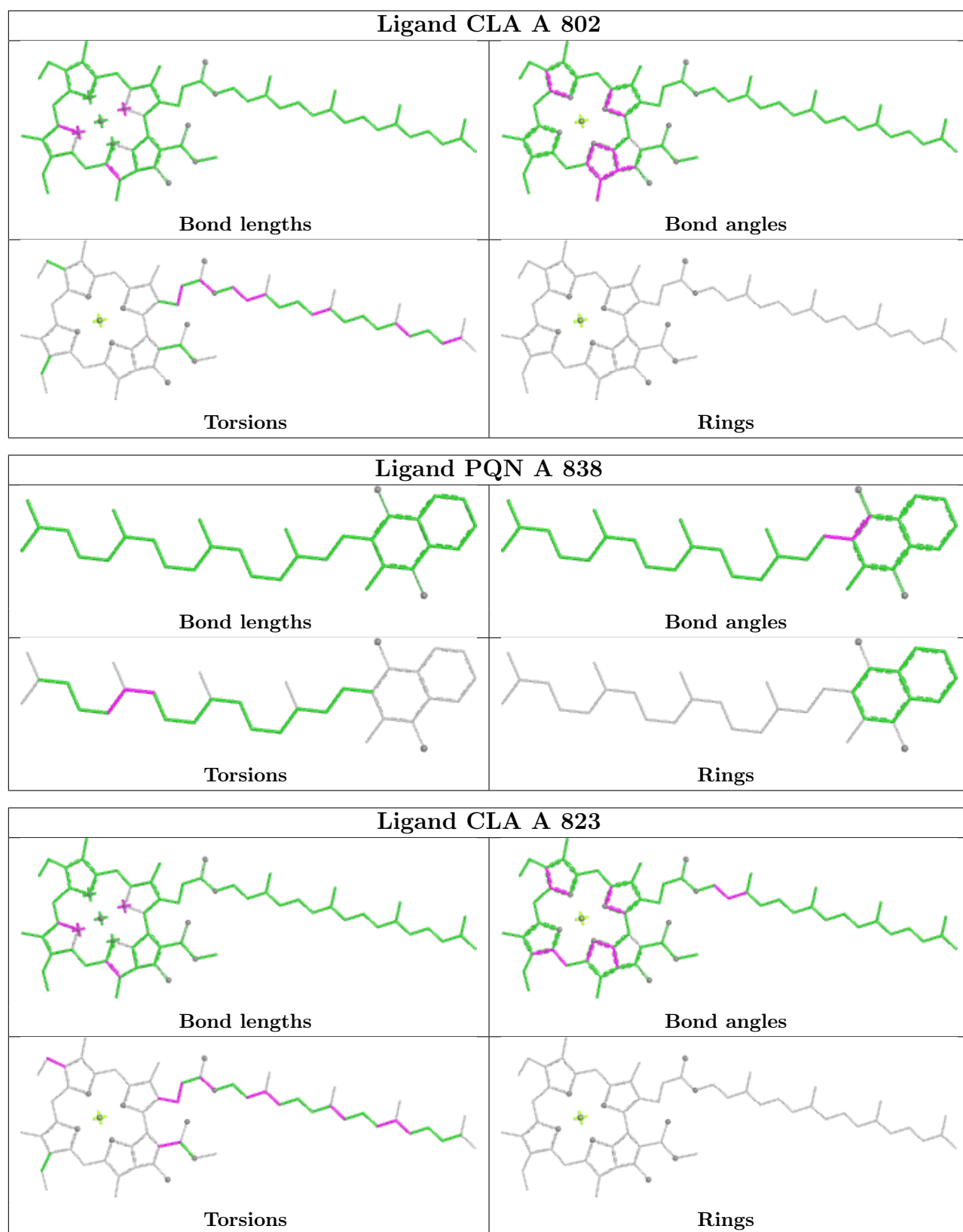
Ligand CLA A 819



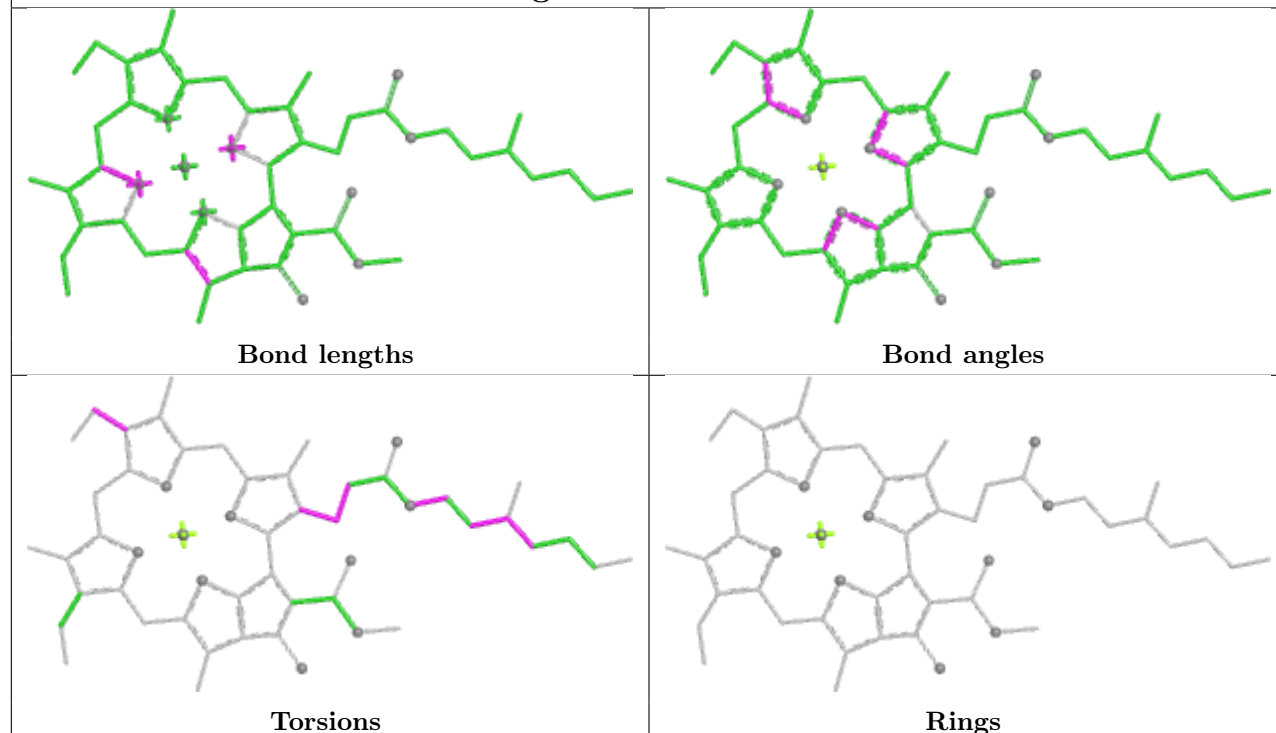
Ligand CLA 7 311



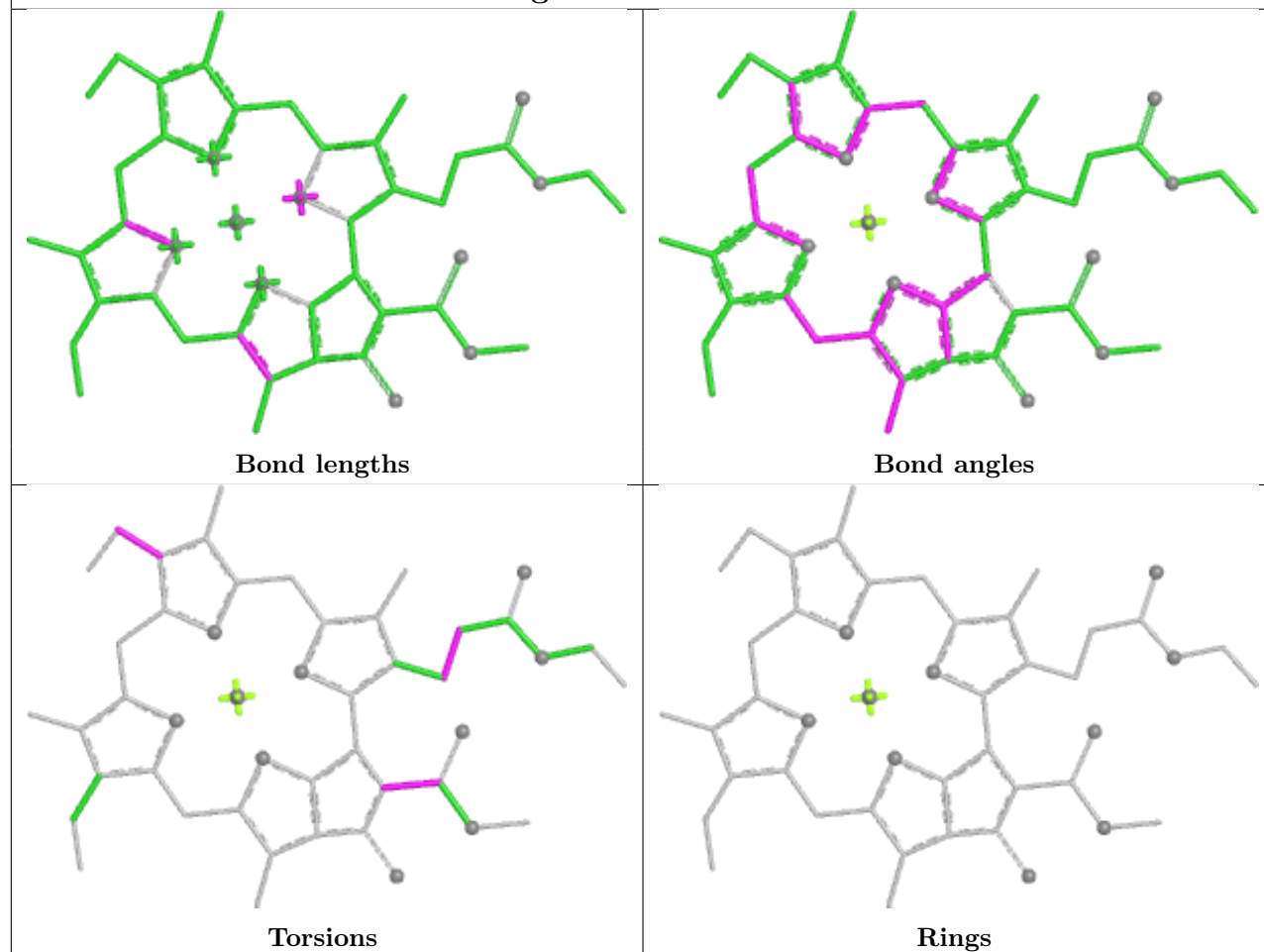


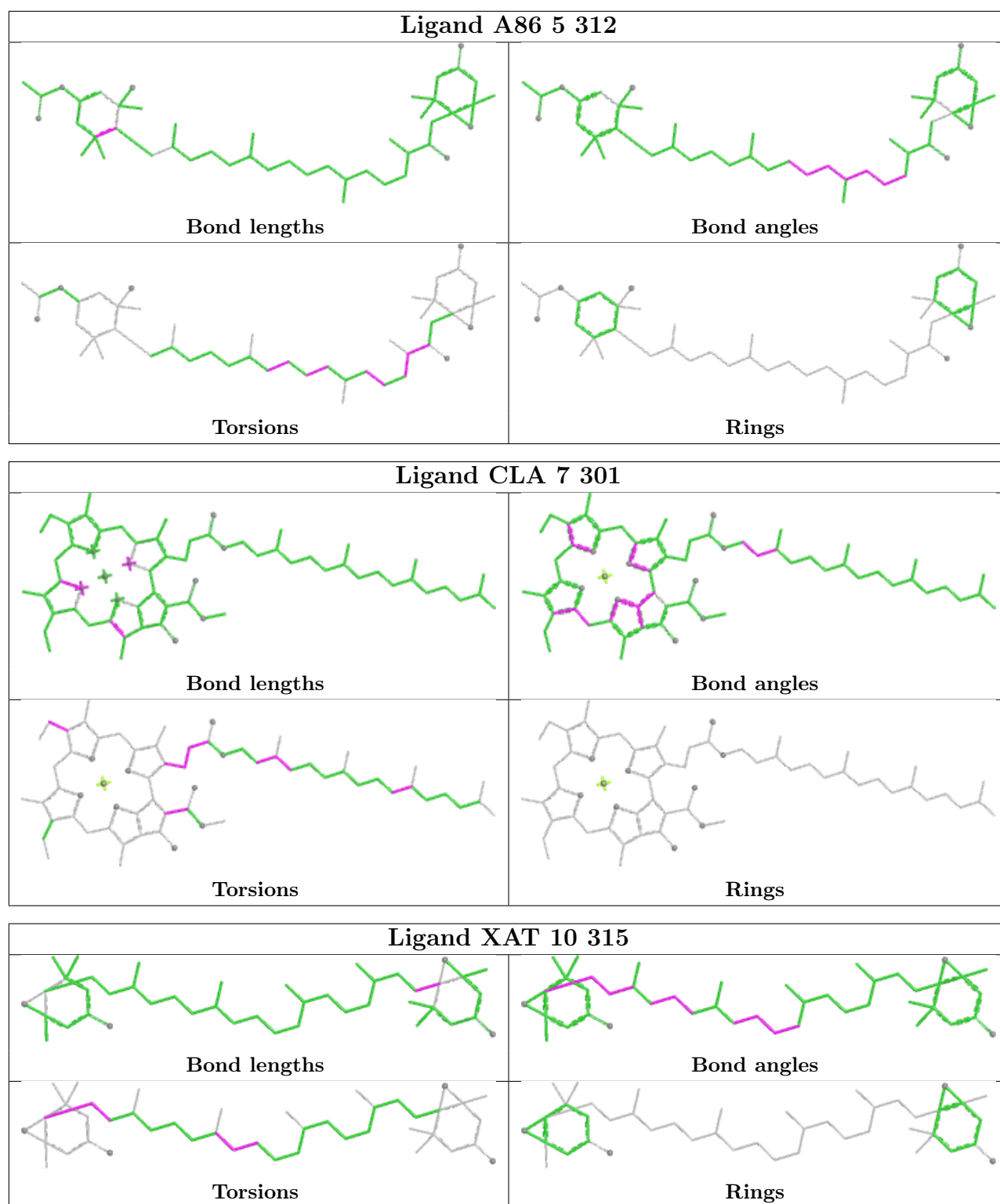


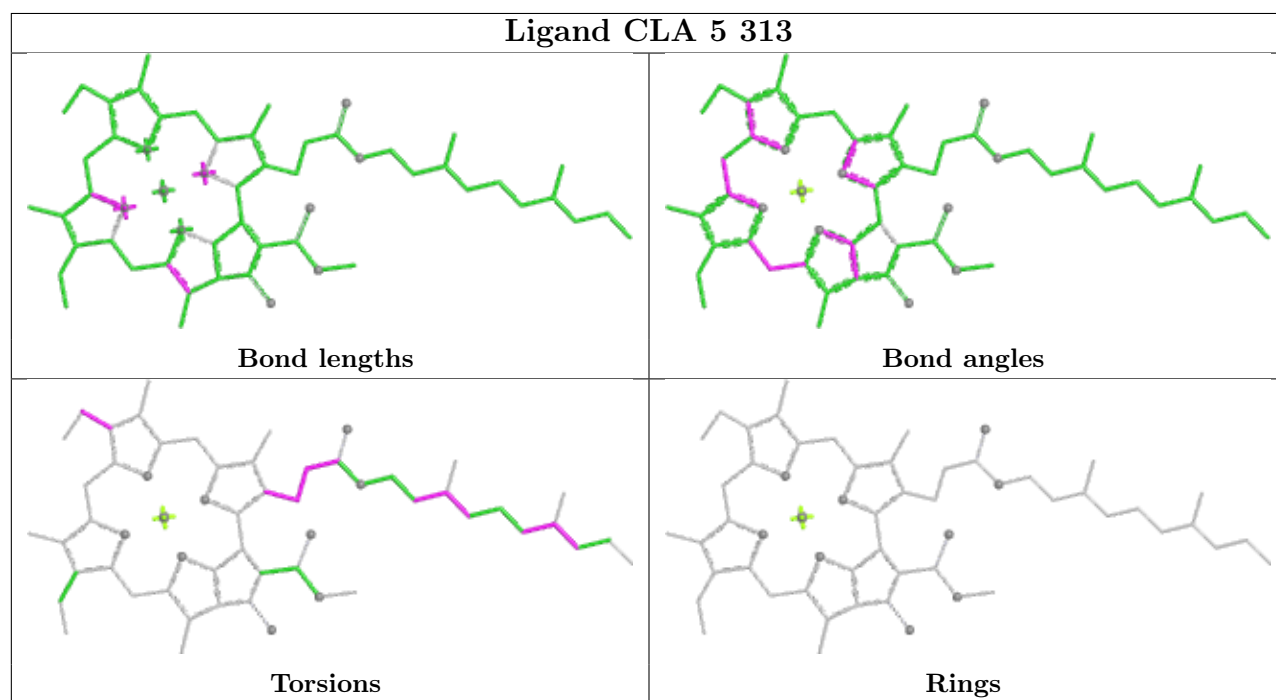
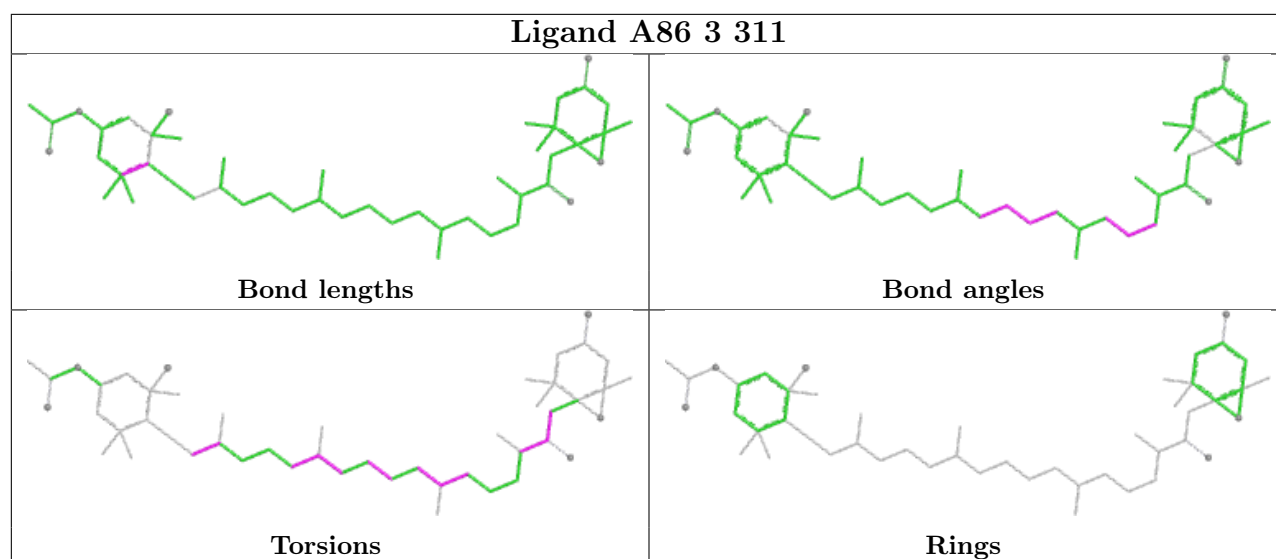
Ligand CLA B 820

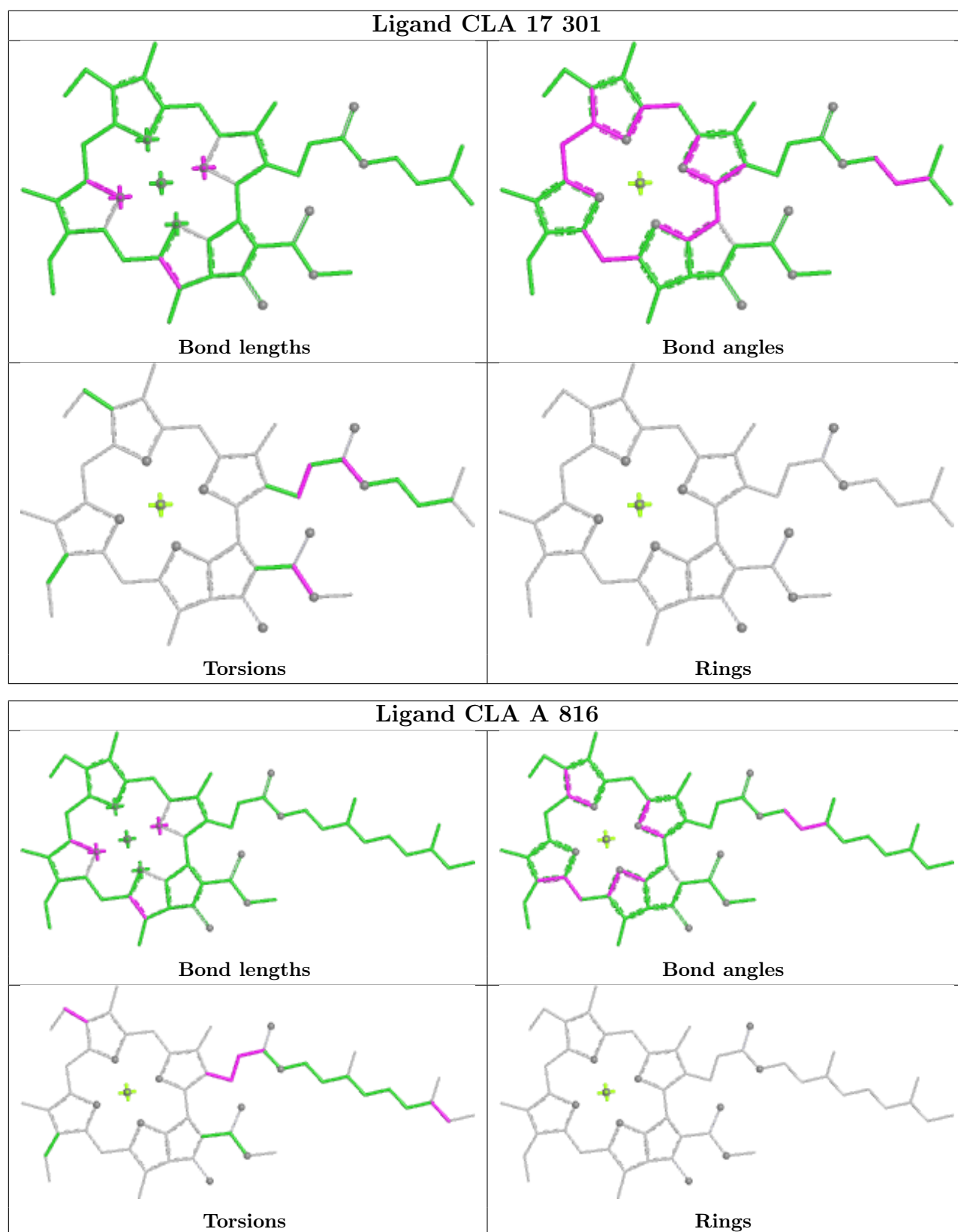


Ligand CLA 9 303

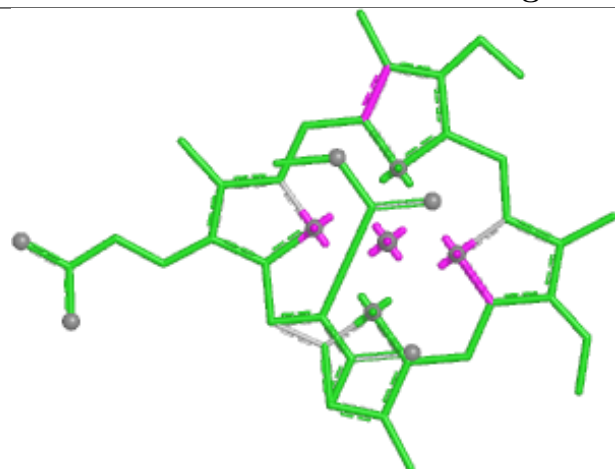




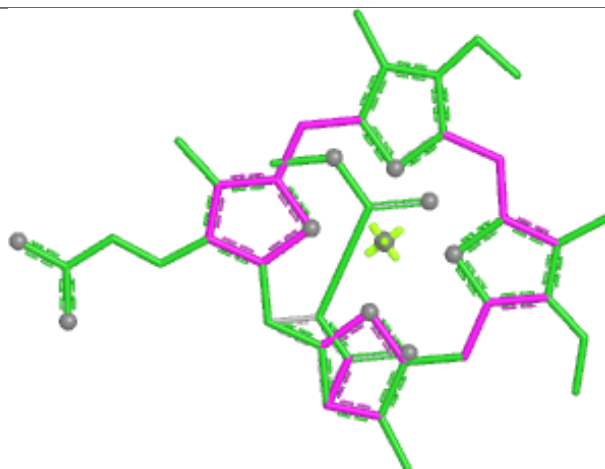




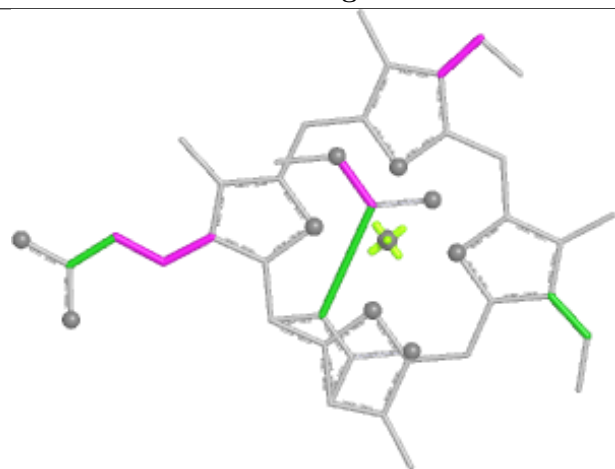
Ligand KC1 4 309



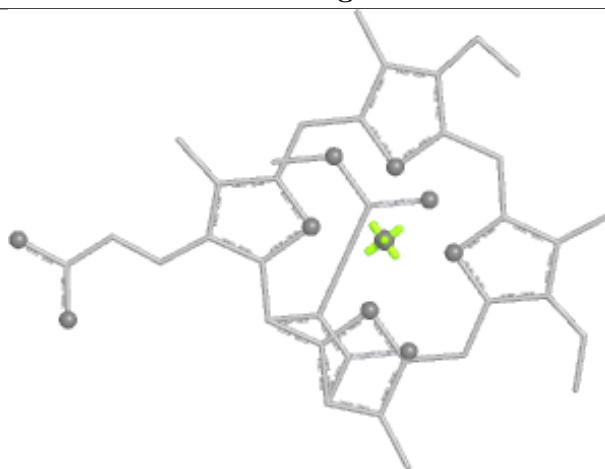
Bond lengths



Bond angles

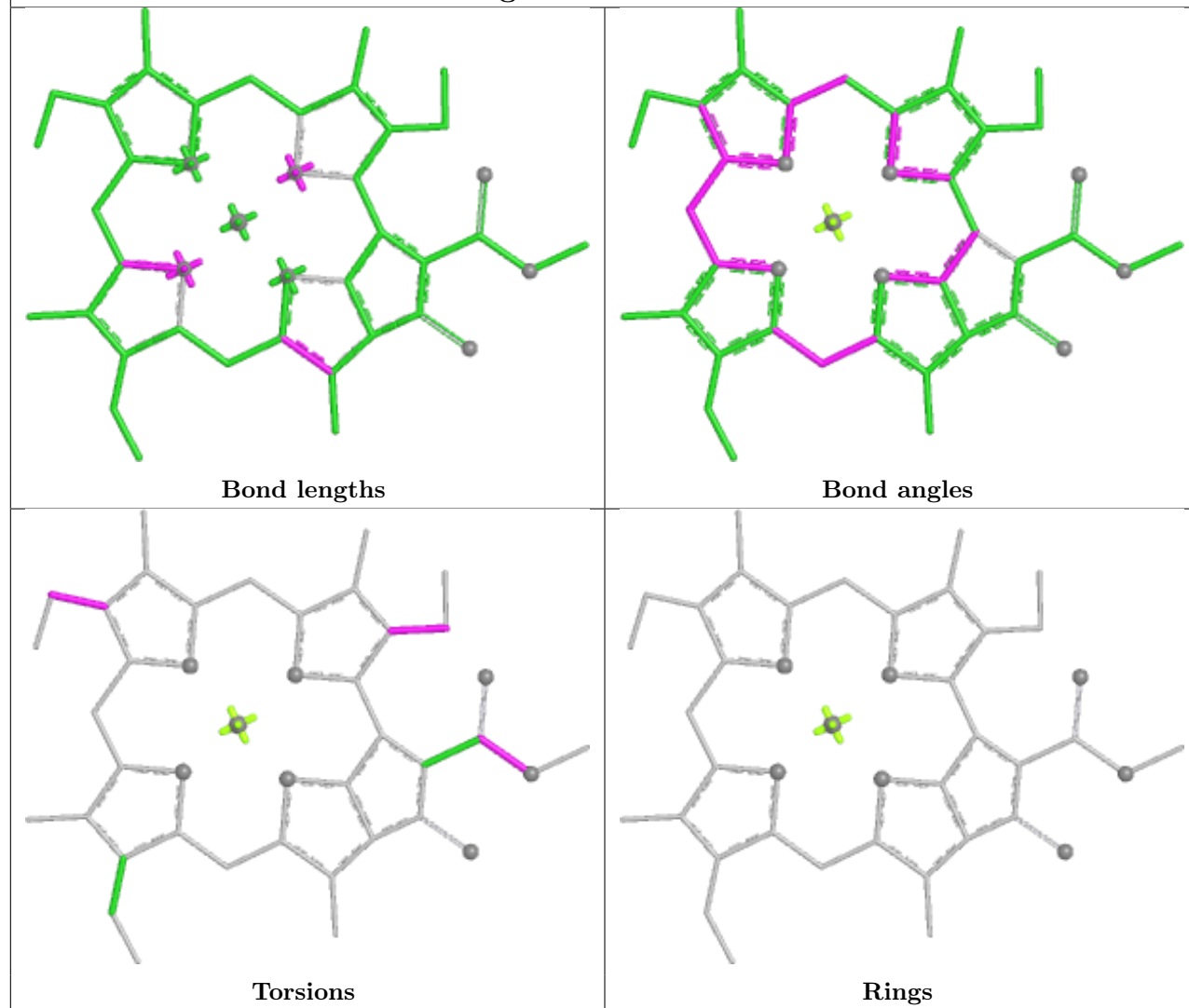


Torsions

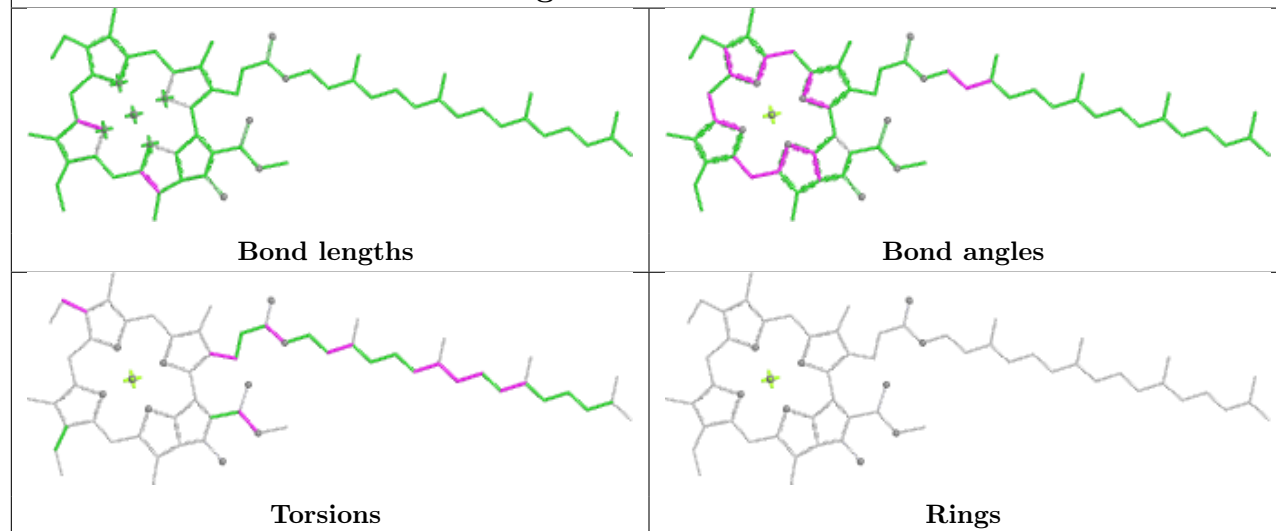


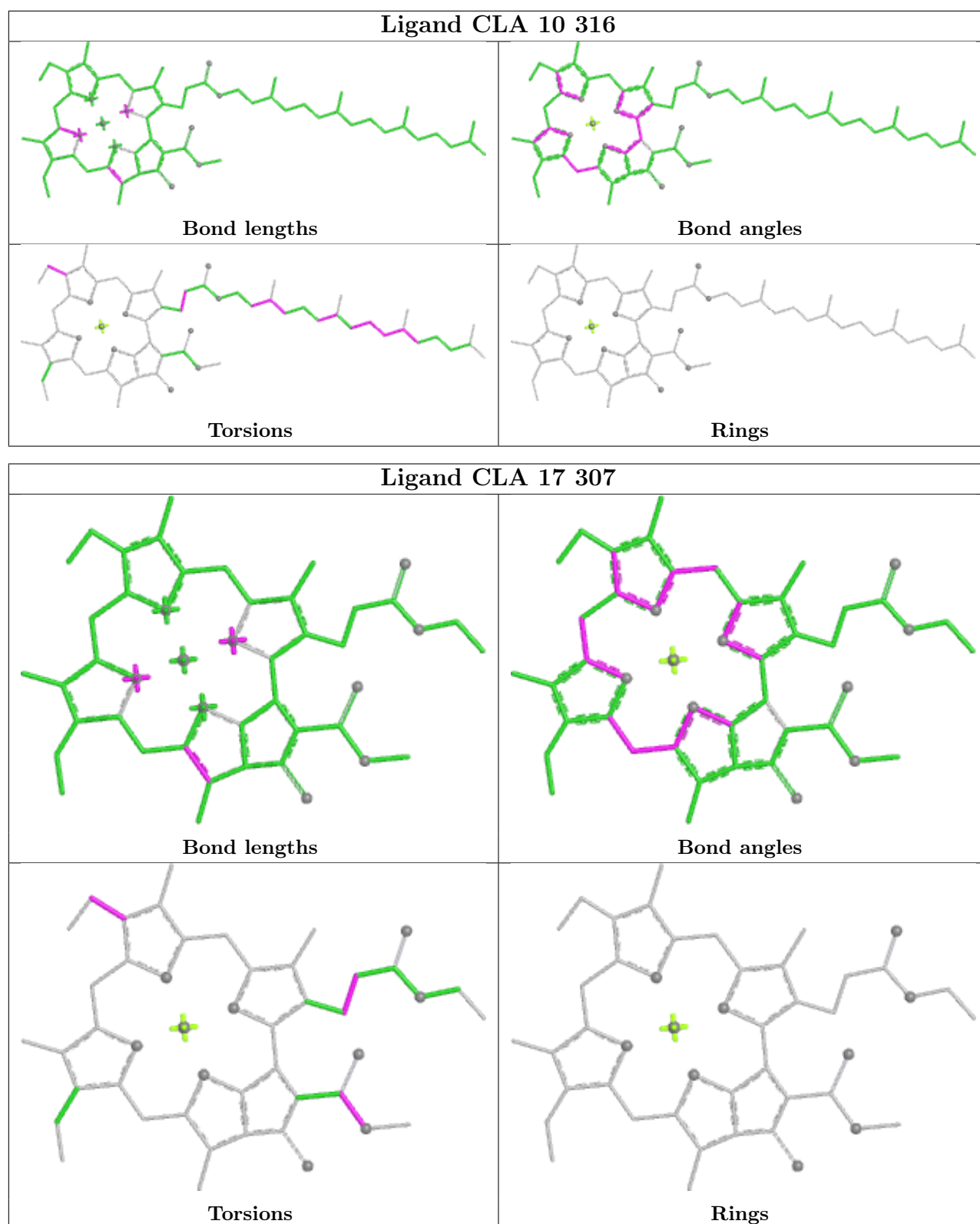
Rings

Ligand CLA a 202



Ligand CLA 1 303





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	2	2
20	15	1
23	19	1
27	a	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	49:UNK	C	70:UNK	N	27.51
1	2	85:UNK	C	111:UNK	N	21.06
1	15	55:UNK	C	61:UNK	N	20.22
1	19	57:UNK	C	71:UNK	N	7.85
1	a	99:UNK	C	102:UNK	N	5.58

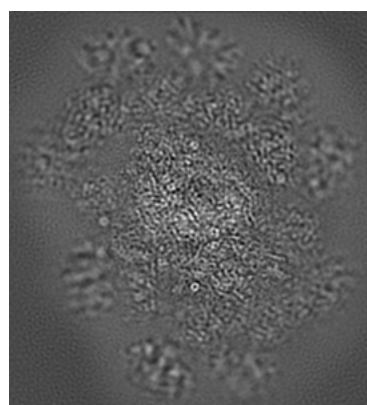
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-72770. These allow visual inspection of the internal detail of the map and identification of artifacts.

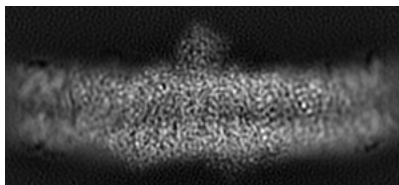
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

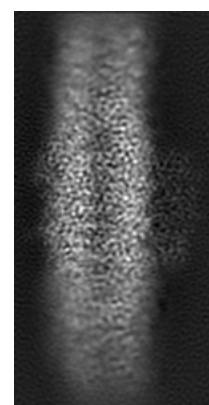
6.1.1 Primary map



X



Y

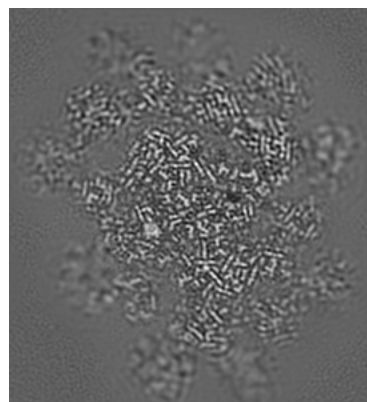


Z

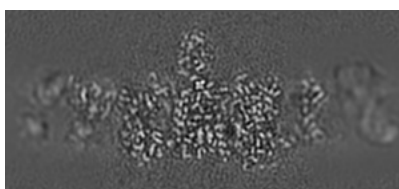
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

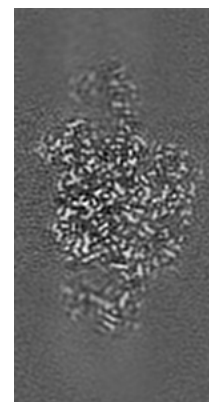
6.2.1 Primary map



X Index: 49



Y Index: 96

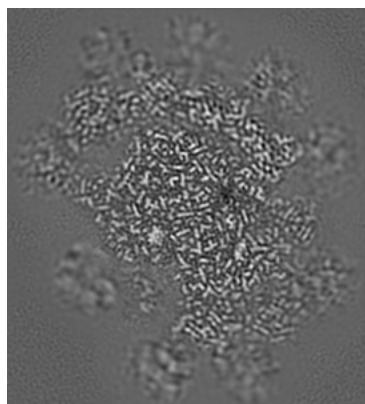


Z Index: 107

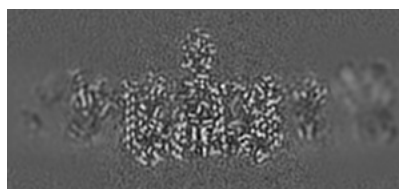
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

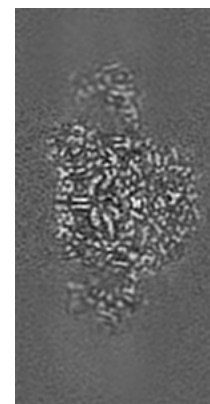
6.3.1 Primary map



X Index: 52



Y Index: 99

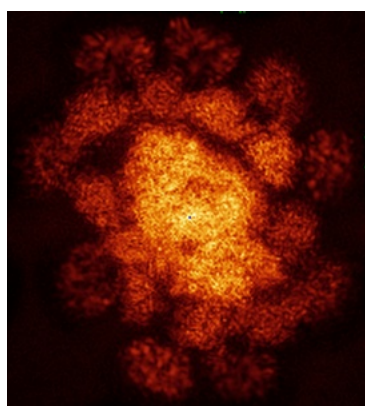


Z Index: 104

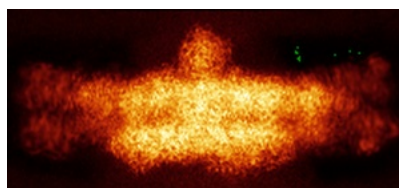
The images above show the largest variance slices of the map in three orthogonal directions.

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

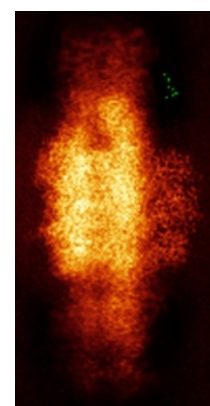
6.4.1 Primary map



X



Y

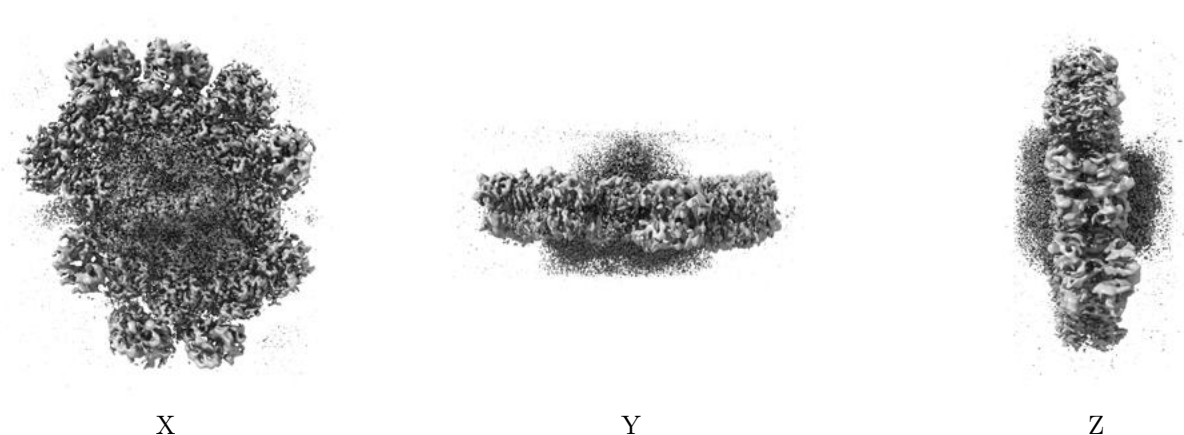


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

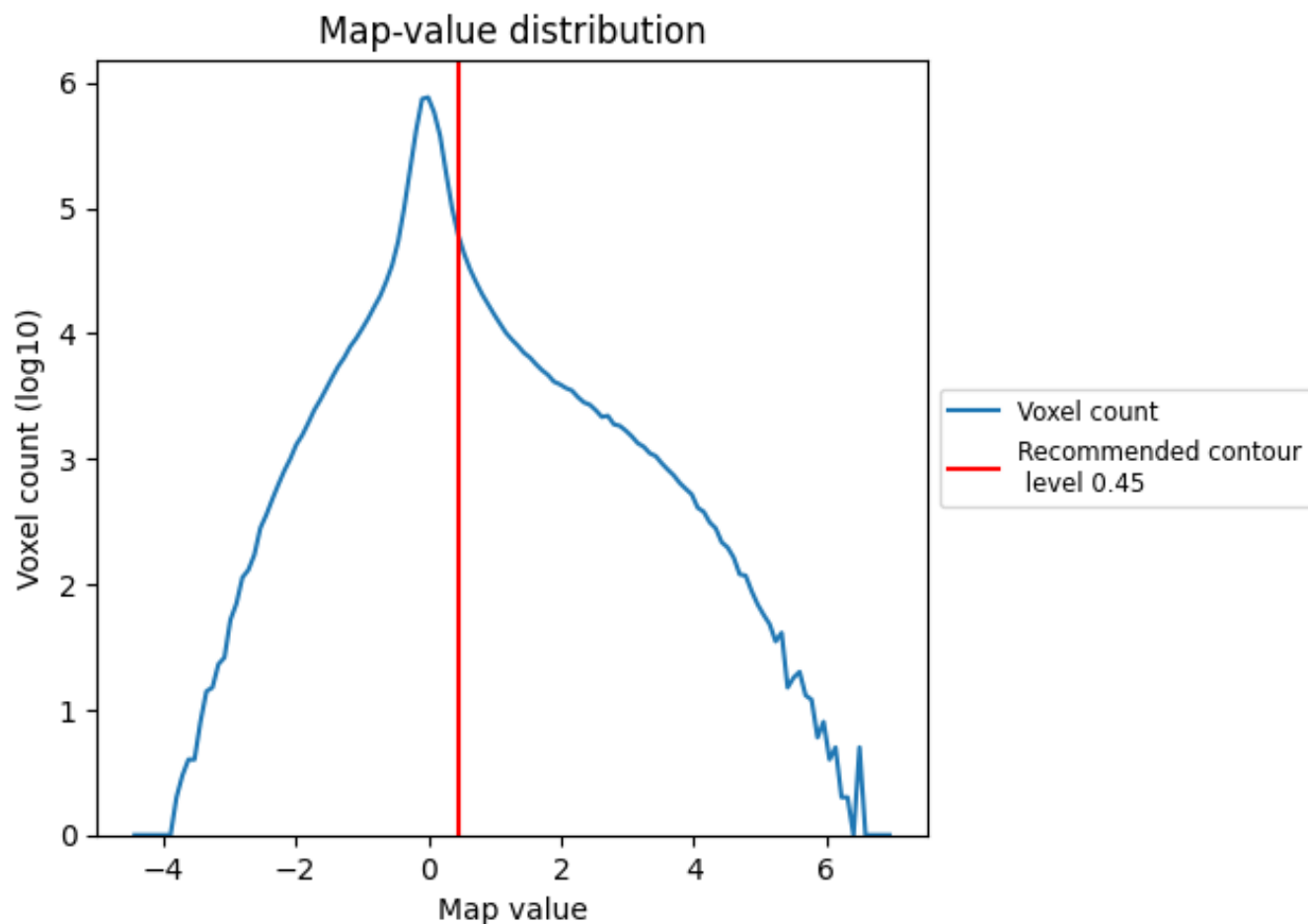
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

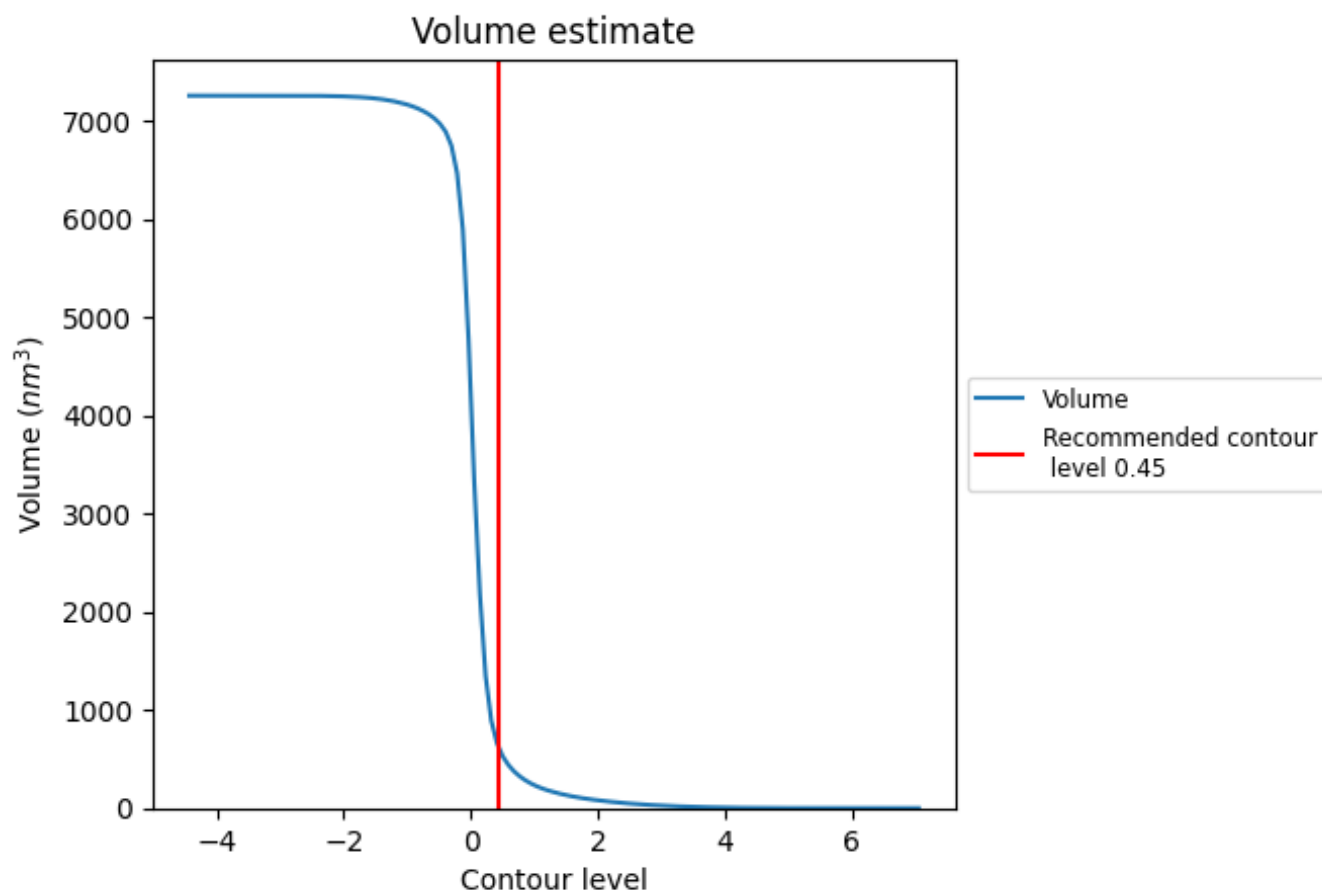
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 604 nm³; this corresponds to an approximate mass of 546 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 [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

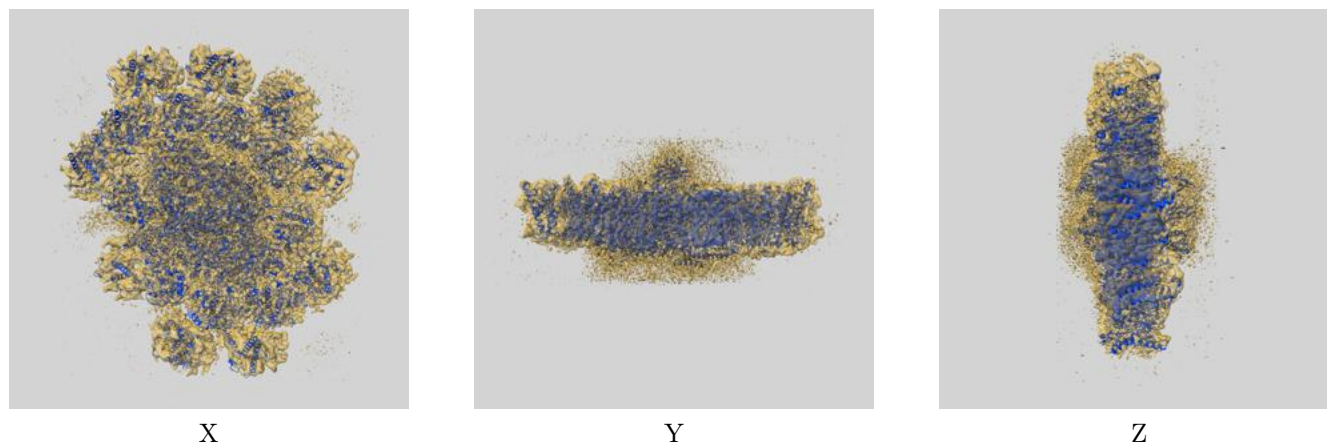
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

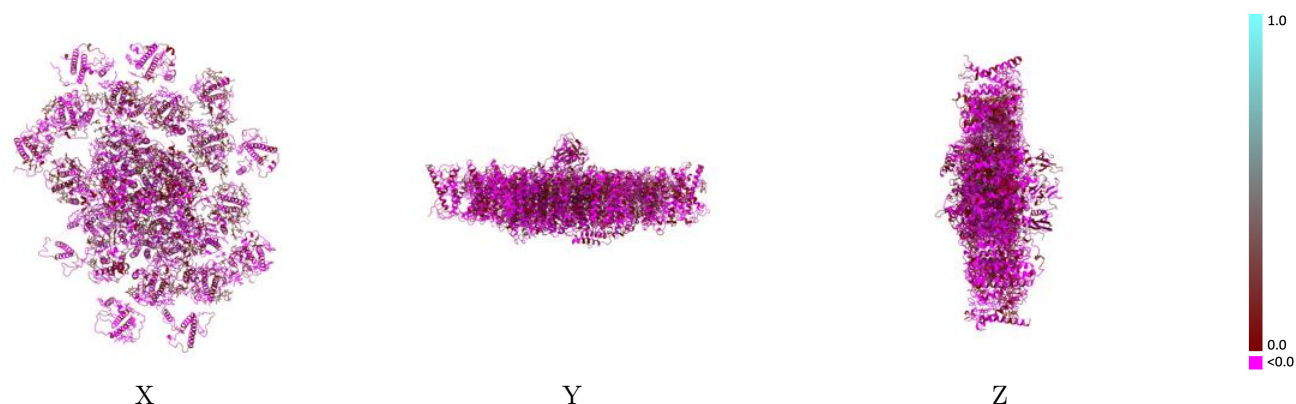
This section contains information regarding the fit between EMDB map EMD-72770 and PDB model 9YGV. Per-residue inclusion information can be found in section [3](#) on page [29](#).

9.1 Map-model overlay [i](#)



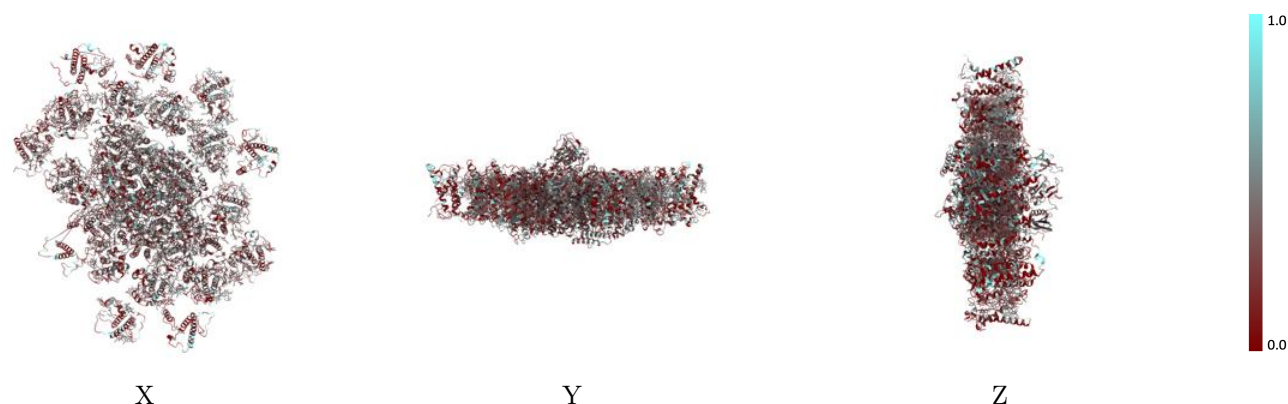
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



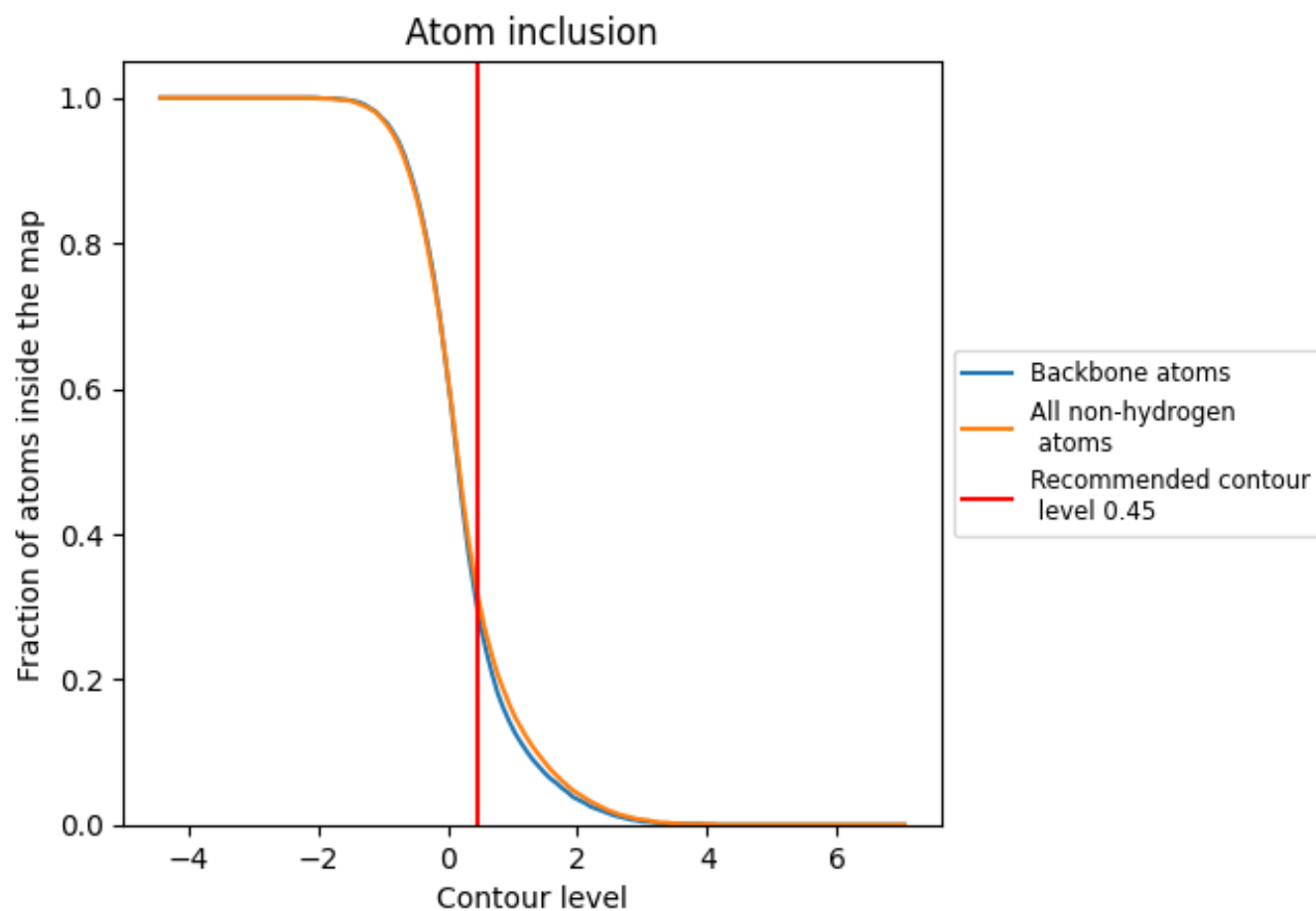
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).





























































9.4 Atom inclusion [i](#)



At the recommended contour level, 30% of all backbone atoms, 32% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3210	 -0.0080
1	 0.2830	 -0.0090
10	 0.3030	 0.0020
11	 0.3100	 -0.0050
13	 0.2660	 -0.0010
15	 0.2510	 -0.0300
16	 0.2700	 -0.0600
17	 0.3330	 0.0360
19	 0.3170	 -0.0250
2	 0.3190	 -0.0170
3	 0.2980	 0.0110
4	 0.3030	 -0.0250
5	 0.3330	 0.0140
6	 0.3680	 0.0300
7	 0.3600	 0.0230
8	 0.3110	 0.0270
9	 0.2830	 -0.0220
A	 0.3430	 -0.0160
B	 0.3490	 -0.0100
C	 0.3280	 -0.0490
D	 0.2890	 -0.0160
E	 0.3890	 0.0370
F	 0.3510	 -0.0030
I	 0.2560	 -0.0410
J	 0.3040	 -0.0400
L	 0.2840	 -0.0320
M	 0.2450	 -0.0070
R	 0.2790	 -0.0530
a	 0.2950	 -0.0730
b	 0.2420	 -0.0390

