



wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 03:28 AM UTC

PDB ID : 6SL5 / pdb_00006sl5
EMDB ID : EMD-10236
Title : Dunaliella Photosystem I Supercomplex
Authors : Nelson, N.; Caspy, I.; Malavath, T.; Klaiman, D.; Shkolinsky, Y.
Deposited on : 2019-08-18
Resolution : 2.84 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:

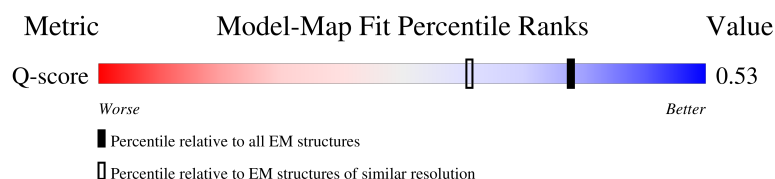
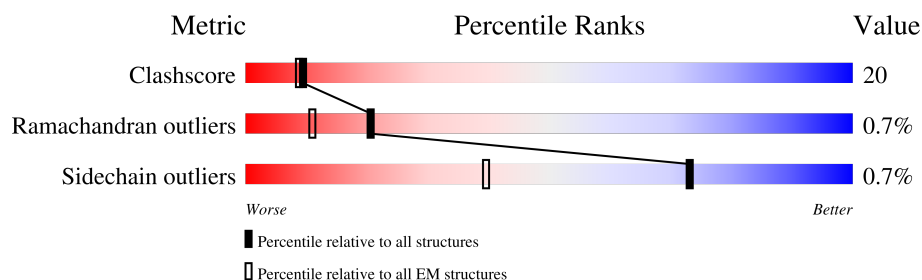
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.84 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11884 (2.34 - 3.34)

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

Mol	Chain	Length	Quality of chain
1	A	740	
2	B	733	
3	C	80	
4	D	144	

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Mol	Chain	Length	Quality of chain
5	E	64	
6	F	162	
7	J	41	
8	G	101	
9	H	92	
10	I	39	
11	K	84	
12	L	155	
13	O	86	
14	1	197	
15	2	208	
16	3	228	
17	4	211	
18	5	202	
19	6	178	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CL0	A	1011	X	-	-	-
21	CLA	1	601	X	-	X	-
21	CLA	1	602	X	-	-	-
21	CLA	1	603	X	-	-	-
21	CLA	1	604	X	-	-	-
21	CLA	1	605	X	-	-	-
21	CLA	1	606	X	-	-	-
21	CLA	1	607	X	-	-	-
21	CLA	1	608	X	-	-	-
21	CLA	1	611	X	-	-	-
21	CLA	1	612	X	-	-	-
21	CLA	1	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	1	615	X	-	-	-
21	CLA	2	601	X	-	-	-
21	CLA	2	602	X	-	-	-
21	CLA	2	603	X	-	-	-
21	CLA	2	604	X	-	-	-
21	CLA	2	605	X	-	-	-
21	CLA	2	606	X	-	-	-
21	CLA	2	607	X	-	-	-
21	CLA	2	608	X	-	-	-
21	CLA	2	612	X	-	-	-
21	CLA	2	615	X	-	-	-
21	CLA	3	601	X	-	-	-
21	CLA	3	602	X	-	-	-
21	CLA	3	603	X	-	-	-
21	CLA	3	605	X	-	-	-
21	CLA	3	606	X	-	-	-
21	CLA	3	607	X	-	-	-
21	CLA	3	608	X	-	-	-
21	CLA	3	610	X	-	-	-
21	CLA	3	611	X	-	-	-
21	CLA	3	612	X	-	-	-
21	CLA	3	613	X	-	-	-
21	CLA	3	614	X	-	-	-
21	CLA	3	615	X	-	-	-
21	CLA	4	601	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	605	X	-	-	-
21	CLA	4	606	X	-	-	-
21	CLA	4	607	X	-	-	-
21	CLA	4	608	X	-	-	-
21	CLA	4	609	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	615	X	-	-	-
21	CLA	5	601	X	-	-	-
21	CLA	5	602	X	-	-	-
21	CLA	5	603	X	-	-	-
21	CLA	5	604	X	-	X	-
21	CLA	5	605	X	-	-	-
21	CLA	5	606	X	-	X	-
21	CLA	5	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	5	608	X	-	-	-
21	CLA	5	612	X	-	-	-
21	CLA	5	613	X	-	-	-
21	CLA	5	614	X	-	-	-
21	CLA	6	601	X	-	X	-
21	CLA	6	602	X	-	-	-
21	CLA	6	603	X	-	-	-
21	CLA	6	604	X	-	-	-
21	CLA	6	605	X	-	-	-
21	CLA	6	606	X	-	-	-
21	CLA	6	607	X	-	-	-
21	CLA	6	608	X	-	-	-
21	CLA	6	609	X	-	-	-
21	CLA	6	612	X	-	-	-
21	CLA	6	613	X	-	-	-
21	CLA	A	1012	X	-	-	-
21	CLA	A	1013	X	-	-	-
21	CLA	A	1101	X	-	-	-
21	CLA	A	1102	X	-	-	-
21	CLA	A	1103	X	-	-	-
21	CLA	A	1104	X	-	-	-
21	CLA	A	1105	X	-	-	-
21	CLA	A	1106	X	-	-	-
21	CLA	A	1107	X	-	-	-
21	CLA	A	1108	X	-	-	-
21	CLA	A	1109	X	-	-	-
21	CLA	A	1110	X	-	-	-
21	CLA	A	1111	X	-	-	-
21	CLA	A	1112	X	-	-	-
21	CLA	A	1113	X	-	-	-
21	CLA	A	1114	X	-	-	-
21	CLA	A	1115	X	-	-	-
21	CLA	A	1116	X	-	-	-
21	CLA	A	1117	X	-	-	-
21	CLA	A	1118	X	-	-	-
21	CLA	A	1119	X	-	-	-
21	CLA	A	1120	X	-	-	-
21	CLA	A	1121	X	-	X	-
21	CLA	A	1122	X	-	-	-
21	CLA	A	1123	X	-	-	-
21	CLA	A	1124	X	-	-	-
21	CLA	A	1125	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	1126	X	-	-	-
21	CLA	A	1127	X	-	-	-
21	CLA	A	1128	X	-	-	-
21	CLA	A	1129	X	-	-	-
21	CLA	A	1130	X	-	-	-
21	CLA	A	1131	X	-	-	-
21	CLA	A	1132	X	-	-	-
21	CLA	A	1133	X	-	-	-
21	CLA	A	1134	X	-	-	-
21	CLA	A	1135	X	-	-	-
21	CLA	A	1136	X	-	-	-
21	CLA	A	1137	X	-	-	-
21	CLA	A	1138	X	-	-	-
21	CLA	A	1139	X	-	-	-
21	CLA	A	1140	X	-	-	-
21	CLA	A	1141	X	-	-	-
21	CLA	B	1021	X	-	-	-
21	CLA	B	1022	X	-	-	-
21	CLA	B	1023	X	-	X	-
21	CLA	B	1201	X	-	-	-
21	CLA	B	1202	X	-	-	-
21	CLA	B	1203	X	-	-	-
21	CLA	B	1204	X	-	-	-
21	CLA	B	1205	X	-	-	-
21	CLA	B	1206	X	-	-	-
21	CLA	B	1207	X	-	-	-
21	CLA	B	1208	X	-	-	-
21	CLA	B	1209	X	-	-	-
21	CLA	B	1210	X	-	-	-
21	CLA	B	1211	X	-	-	-
21	CLA	B	1212	X	-	-	-
21	CLA	B	1213	X	-	-	-
21	CLA	B	1214	X	-	-	-
21	CLA	B	1215	X	-	-	-
21	CLA	B	1216	X	-	-	-
21	CLA	B	1217	X	-	-	-
21	CLA	B	1218	X	-	-	-
21	CLA	B	1219	X	-	-	-
21	CLA	B	1220	X	-	-	-
21	CLA	B	1221	X	-	-	-
21	CLA	B	1222	X	-	-	-
21	CLA	B	1223	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B	1224	X	-	-	-
21	CLA	B	1225	X	-	-	-
21	CLA	B	1226	X	-	-	-
21	CLA	B	1227	X	-	-	-
21	CLA	B	1228	X	-	-	-
21	CLA	B	1229	X	-	-	-
21	CLA	B	1230	X	-	-	-
21	CLA	B	1231	X	-	-	-
21	CLA	B	1232	X	-	-	-
21	CLA	B	1234	X	-	-	-
21	CLA	B	1235	X	-	-	-
21	CLA	B	1236	X	-	-	-
21	CLA	B	1237	X	-	-	-
21	CLA	B	1238	X	-	-	-
21	CLA	B	1239	X	-	-	-
21	CLA	B	1240	X	-	-	-
21	CLA	F	1301	X	-	-	-
21	CLA	F	1302	X	-	-	-
21	CLA	G	1601	X	-	-	-
21	CLA	G	1602	X	-	-	-
21	CLA	G	1603	X	-	-	-
21	CLA	H	1701	X	-	-	-
21	CLA	H	1702	X	-	-	-
21	CLA	J	1901	X	-	-	-
21	CLA	K	1401	X	-	-	-
21	CLA	K	1402	X	-	-	-
21	CLA	K	1403	X	-	-	-
21	CLA	K	1404	X	-	-	-
21	CLA	L	1501	X	-	-	-
21	CLA	L	1502	X	-	-	-
21	CLA	L	1503	X	-	-	-
21	CLA	L	1504	X	-	-	-
21	CLA	O	1801	X	-	-	-
21	CLA	O	1802	X	-	-	-
21	CLA	O	1803	X	-	-	-
34	LUT	4	501	X	-	-	-
34	LUT	5	501	X	-	-	-
34	LUT	5	504	X	-	-	-
34	LUT	6	501	X	-	X	-
35	XAT	1	502	X	-	-	-
35	XAT	2	502	X	-	-	-
35	XAT	3	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	XAT	4	502	X	-	-	-
35	XAT	6	502	X	-	-	-
35	XAT	6	504	X	-	-	-
36	CHL	1	609	X	-	-	-
36	CHL	1	610	X	-	-	-
36	CHL	2	609	X	-	-	-
36	CHL	2	610	X	-	-	-
36	CHL	2	611	X	-	-	-
36	CHL	2	613	X	-	-	-
36	CHL	3	604	X	-	-	-
36	CHL	4	610	X	-	-	-
36	CHL	4	611	X	-	-	-
36	CHL	4	613	X	-	-	-
36	CHL	5	609	X	-	X	-
36	CHL	5	610	X	-	-	-
36	CHL	6	610	X	-	-	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 43789 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	740	Total	C	N	O	S	0	0
			5808	3795	993	1002	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5808	3815	974	1006	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1134	727	197	204	6		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			515	327	89	99		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	162	Total	C	N	O	S	0	0
			1278	823	217	236	2		

- Molecule 7 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	41	Total	C	N	O	S	0	0
			327	223	47	56	1		

- Molecule 8 is a protein called PsaG.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	101	Total	C	N	O	S	0	0
			773	500	135	136	2		

- Molecule 9 is a protein called PsaH.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	92	Total	C	N	O	S	0	0
			704	445	120	137	2		

- Molecule 10 is a protein called PsaI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	39	Total	C	N	O	S	0	0
			301	208	43	49	1		

- Molecule 11 is a protein called PsaK.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	84	Total	C	N	O	S	0	0
			573	354	106	110	3		

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	155	Total	C	N	O	S	0	0
			1137	736	191	203	7		

- Molecule 13 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	86	Total	C	N	O	S	0	0
			684	456	108	118	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1	197	Total	C	N	O	S	0	0
			1501	963	255	276	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	204	ALA	GLU	conflict	UNP C1K003

- Molecule 15 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	2	208	Total	C	N	O	S	0	0
			1609	1033	272	297	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	3	228	Total	C	N	O	S	0	0
			1740	1134	284	317	5		

- Molecule 17 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	4	211	Total	C	N	O	S	0	0
			1637	1058	272	303	4		

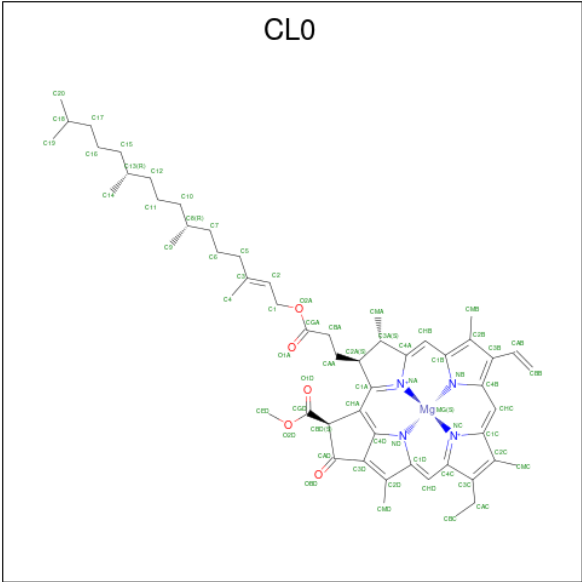
- Molecule 18 is a protein called Lhca5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	5	202	Total	C	N	O	S	0	0
			1525	977	257	284	7		

- Molecule 19 is a protein called Lhca6.

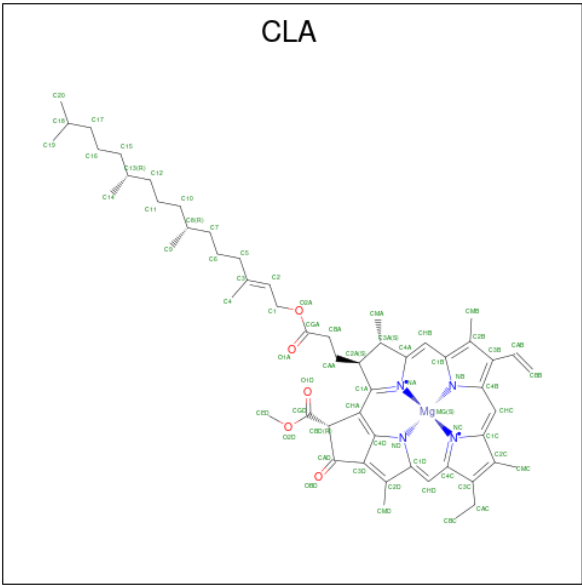
Mol	Chain	Residues	Atoms					AltConf	Trace
19	6	178	Total	C	N	O	S	0	0
			1378	896	230	245	7		

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
21	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 48	C 38	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	B	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
21	F	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
21	J	1	Total 49	C 39	Mg 1	N 4	O 5	0
21	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
21	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	H	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	K	1	Total 48	C 38	Mg 1	N 4	O 5	0
21	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 38	C 30	Mg 1	N 4	O 3	0
21	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
21	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
21	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	4	1	Total 51	C 41	Mg 1	N 4	O 5	0

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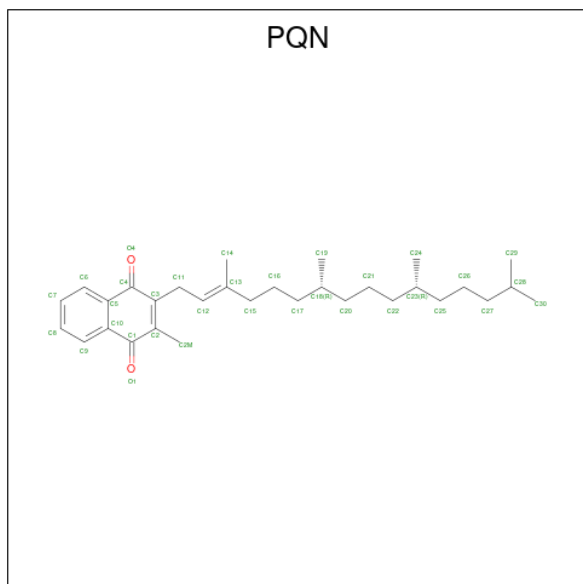
Mol	Chain	Residues	Atoms					AltConf
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
21	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
21	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
21	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
21	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
21	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
21	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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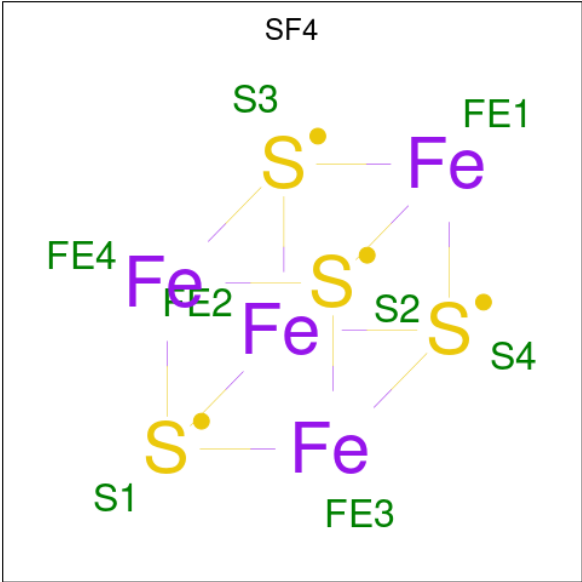
Mol	Chain	Residues	Atoms					AltConf
21	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



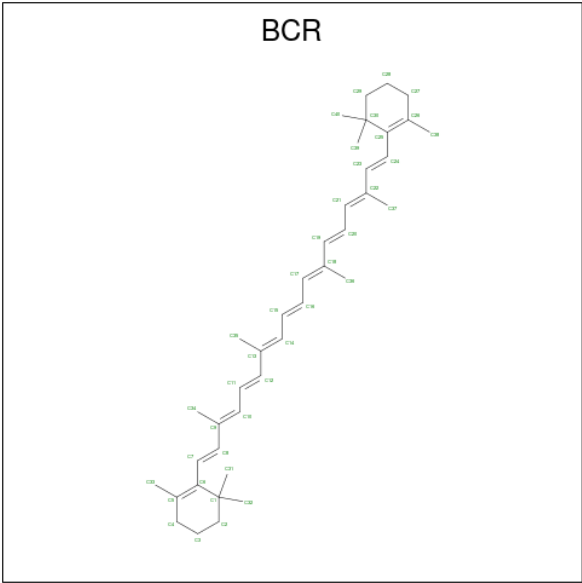
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	C	O	0
			33	31	2	
22	B	1	Total	C	O	0
			33	31	2	

- Molecule 23 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			40	40	

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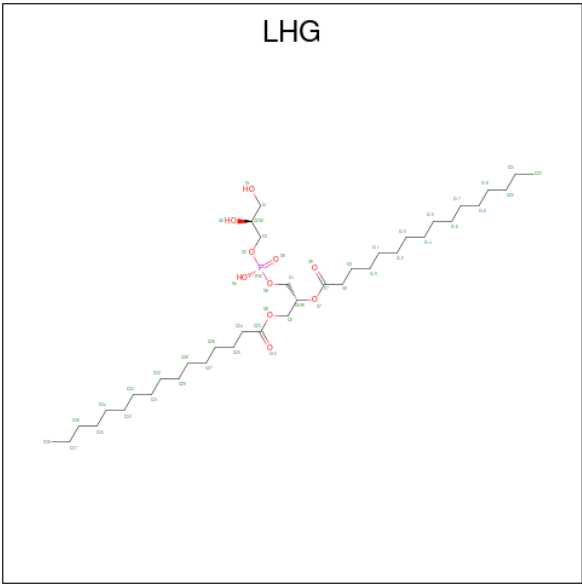
Mol	Chain	Residues	Atoms	AltConf
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	A	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	B	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	F	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	J	1	Total C 40 40	0
24	G	1	Total C 40 40	0
24	H	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	I	1	Total C 40 40	0
24	K	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
24	L	1	Total	C	0
			40	40	
24	L	1	Total	C	0
			40	40	
24	O	1	Total	C	0
			40	40	
24	1	1	Total	C	0
			40	40	
24	2	1	Total	C	0
			40	40	
24	3	1	Total	C	0
			40	40	
24	3	1	Total	C	0
			40	40	
24	3	1	Total	C	0
			40	40	
24	4	1	Total	C	0
			40	40	

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



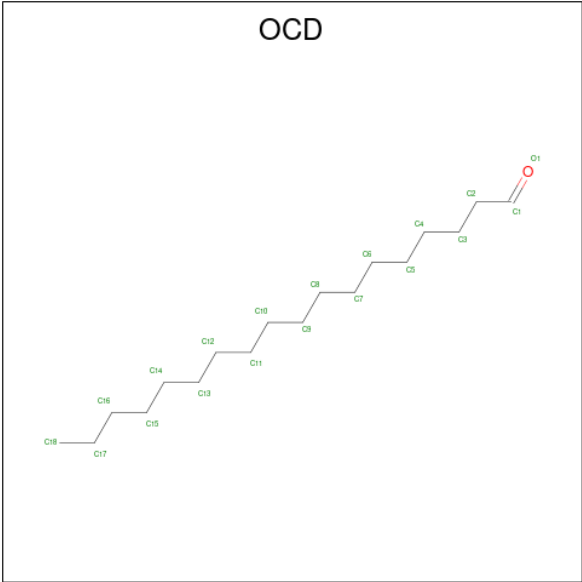
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			49	38	10	1	
25	A	1	Total	C	O	P	0
			49	38	10	1	

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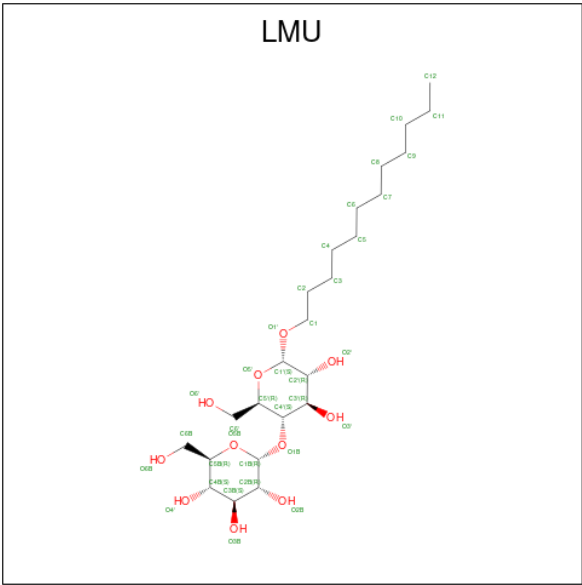
Mol	Chain	Residues	Atoms				AltConf
25	B	1	Total	C	O	P	0
			42	31	10	1	
25	F	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			49	38	10	1	
25	1	1	Total	C	O	P	0
			26	15	10	1	
25	1	1	Total	C	O	P	0
			31	20	10	1	
25	2	1	Total	C	O	P	0
			35	24	10	1	
25	2	1	Total	C	O	P	0
			43	32	10	1	
25	2	1	Total	C	O	P	0
			36	25	10	1	
25	3	1	Total	C	O	P	0
			17	8	8	1	
25	4	1	Total	C	O	P	0
			29	18	10	1	
25	5	1	Total	C	O	P	0
			43	32	10	1	
25	5	1	Total	C	O	P	0
			24	13	10	1	
25	6	1	Total	C	O	P	0
			25	14	10	1	

- Molecule 26 is octadecanal (CCD ID: OCD) (formula: C₁₈H₃₆O).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			19	18	1	

- Molecule 27 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



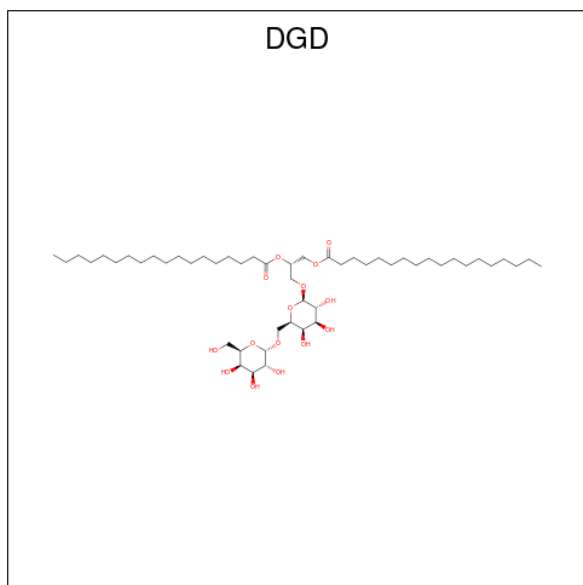
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			35	24	11	
27	A	1	Total	C	O	0
			35	24	11	
27	B	1	Total	C	O	0
			35	24	11	

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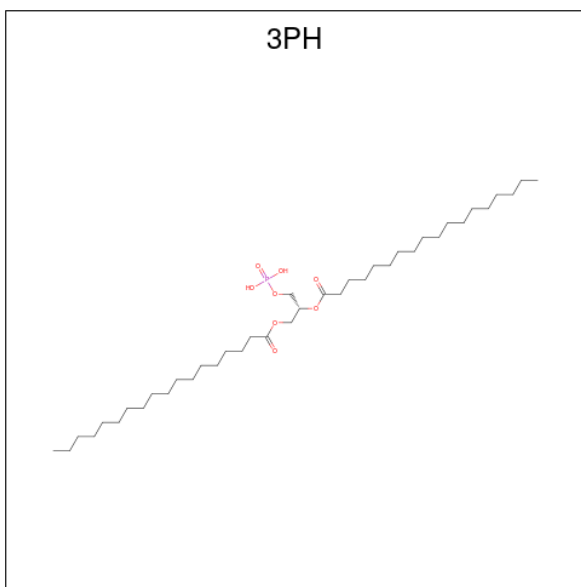
Mol	Chain	Residues	Atoms			AltConf
27	6	1	Total	C	O	0
			35	24	11	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			61	46	15	
28	2	1	Total	C	O	0
			39	24	15	
28	3	1	Total	C	O	0
			39	24	15	
28	3	1	Total	C	O	0
			45	30	15	

- Molecule 29 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).

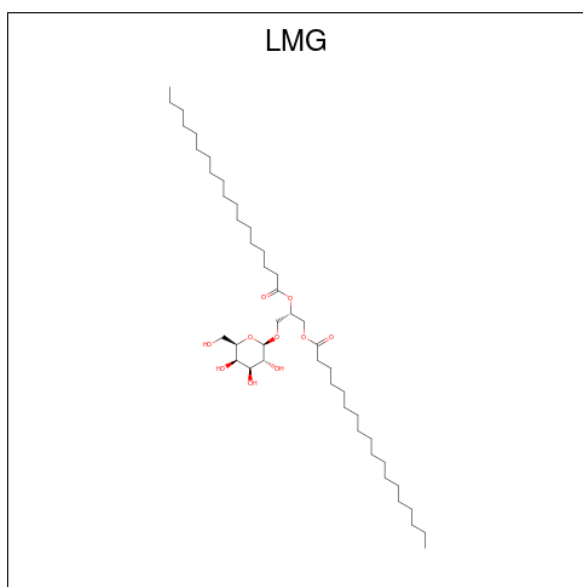


Mol	Chain	Residues	Atoms				AltConf
29	B	1	Total	C	O	P	0
			31	22	8	1	
29	F	1	Total	C	O	P	0
			34	25	8	1	
29	5	1	Total	C	O	P	0
			28	19	8	1	
29	5	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 30 is CALCIUM ION (CCD ID: CA) (formula: Ca).

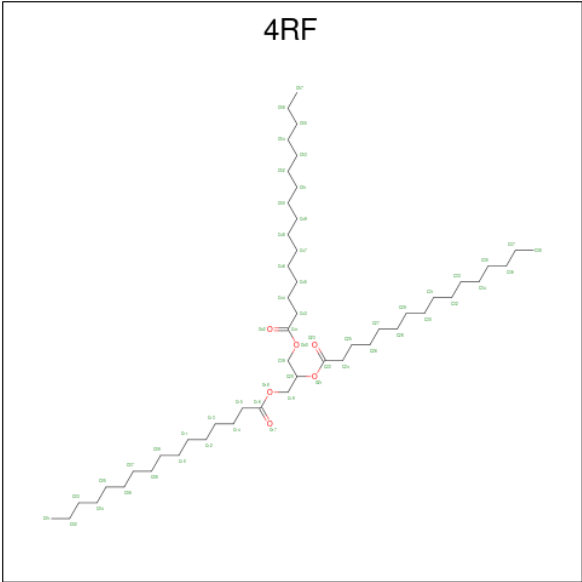
Mol	Chain	Residues	Atoms		AltConf
30	B	1	Total	Ca	0
			1	1	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



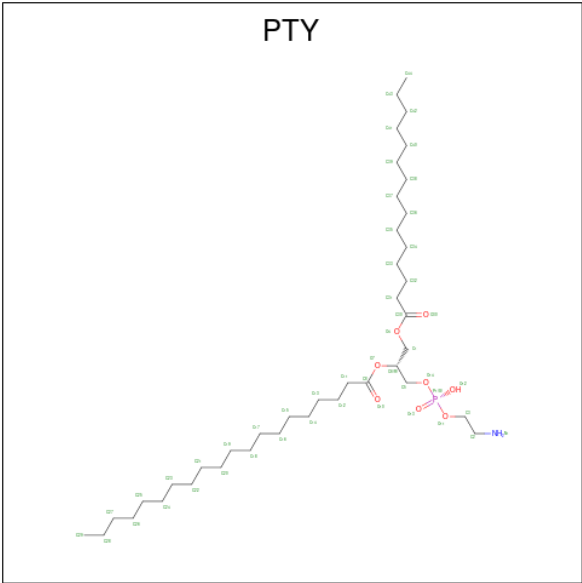
Mol	Chain	Residues	Atoms			AltConf
31	F	1	Total	C	O	0
			50	40	10	
31	1	1	Total	C	O	0
			32	22	10	
31	2	1	Total	C	O	0
			50	40	10	
31	3	1	Total	C	O	0
			32	22	10	
31	3	1	Total	C	O	0
			50	40	10	
31	4	1	Total	C	O	0
			46	36	10	
31	4	1	Total	C	O	0
			39	29	10	
31	6	1	Total	C	O	0
			37	27	10	

- Molecule 32 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



Mol	Chain	Residues	Atoms			AltConf
32	L	1	Total	C	O	0
			39	33	6	
32	5	1	Total	C	O	0
			32	26	6	

- Molecule 33 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



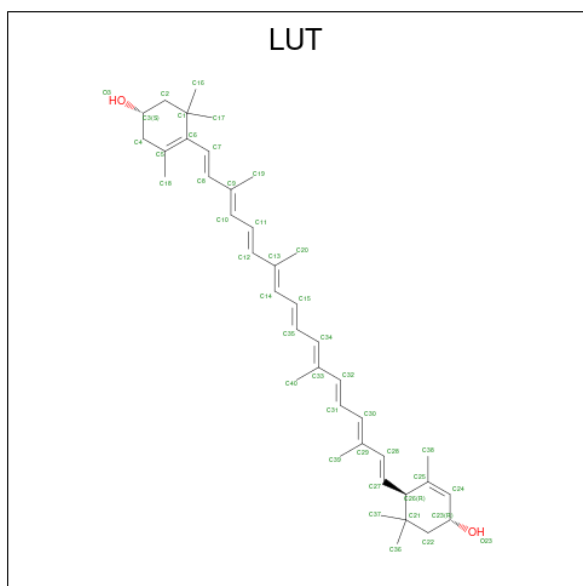
Mol	Chain	Residues	Atoms					AltConf
33	L	1	Total	C	N	O	P	0
			20	10	1	8	1	
33	O	1	Total	C	N	O	P	0
			22	12	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
33	1	1	Total	C	N	O	P	0
			40	30	1	8	1	
33	1	1	Total	C	N	O	P	0
			18	8	1	8	1	
33	3	1	Total	C	N	O	P	0
			26	16	1	8	1	
33	3	1	Total	C	N	O	P	0
			20	10	1	8	1	
33	4	1	Total	C	N	O	P	0
			35	25	1	8	1	
33	5	1	Total	C	N	O	P	0
			36	26	1	8	1	
33	6	1	Total	C	N	O	P	0
			24	14	1	8	1	

- Molecule 34 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



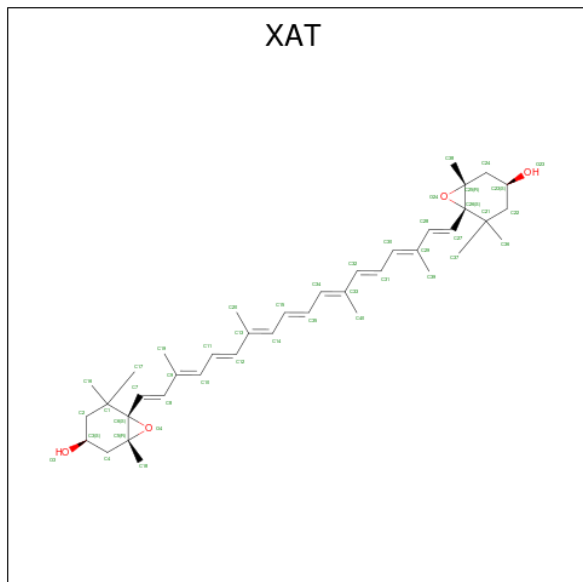
Mol	Chain	Residues	Atoms			AltConf
34	1	1	Total	C	O	0
			42	40	2	
34	2	1	Total	C	O	0
			42	40	2	
34	3	1	Total	C	O	0
			42	40	2	
34	4	1	Total	C	O	0
			42	40	2	

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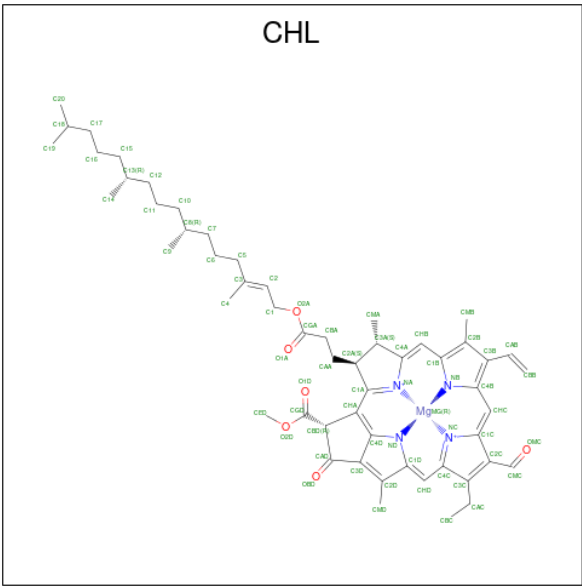
Mol	Chain	Residues	Atoms			AltConf
34	5	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	
34	6	1	Total	C	O	0
			42	40	2	

- Molecule 35 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).



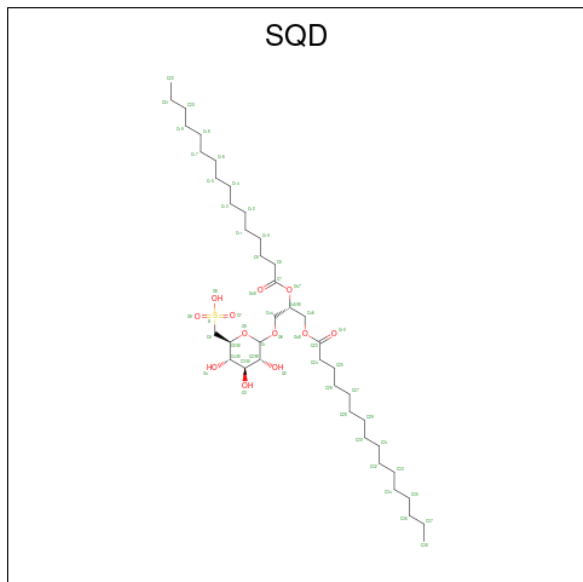
Mol	Chain	Residues	Atoms			AltConf
35	1	1	Total	C	O	0
			44	40	4	
35	2	1	Total	C	O	0
			44	40	4	
35	3	1	Total	C	O	0
			44	40	4	
35	4	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	
35	6	1	Total	C	O	0
			44	40	4	

- Molecule 36 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



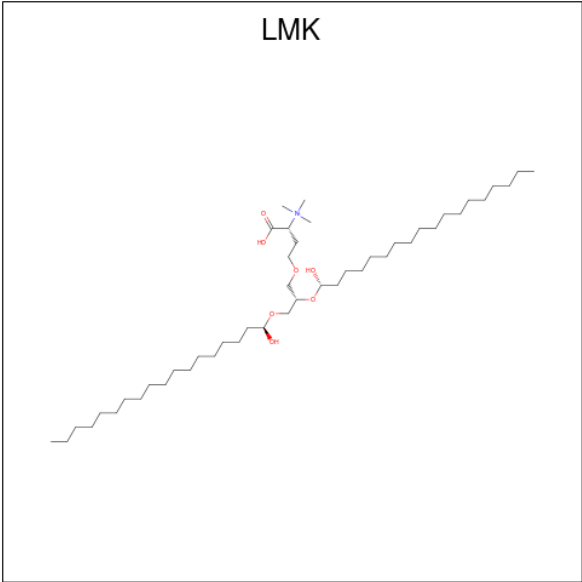
Mol	Chain	Residues	Atoms						AltConf
36	1	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
36	1	1	Total	C	Mg	N	O		0
			47	36	1	4	6		
36	2	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
36	2	1	Total	C	Mg	N	O		0
			56	45	1	4	6		
36	2	1	Total	C	Mg	N	O		0
			48	37	1	4	6		
36	2	1	Total	C	Mg	N	O		0
			46	35	1	4	6		
36	3	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
36	4	1	Total	C	Mg	N	O		0
			47	36	1	4	6		
36	4	1	Total	C	Mg	N	O		0
			51	40	1	4	6		
36	4	1	Total	C	Mg	N	O		0
			61	50	1	4	6		
36	5	1	Total	C	Mg	N	O		0
			66	55	1	4	6		
36	5	1	Total	C	Mg	N	O		0
			47	36	1	4	6		
36	6	1	Total	C	Mg	N	O		0
			47	36	1	4	6		

- Molecule 37 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



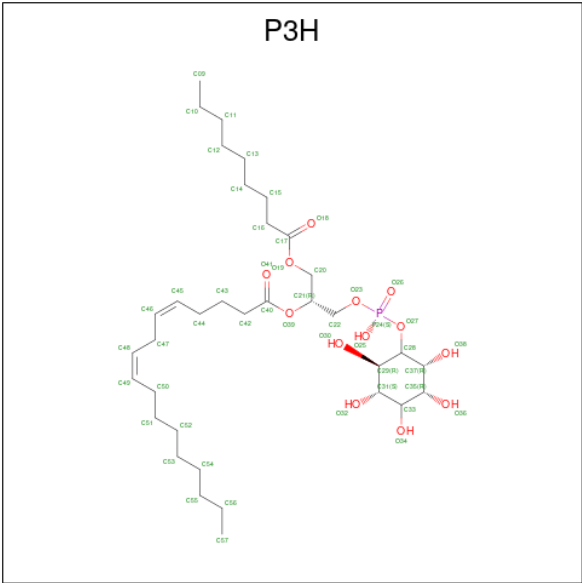
Mol	Chain	Residues	Atoms				AltConf
37	2	1	Total	C	O	S	0
			40	27	12	1	
37	3	1	Total	C	O	S	0
			35	22	12	1	
37	6	1	Total	C	O	S	0
			32	19	12	1	

- Molecule 38 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanum (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$).



Mol	Chain	Residues	Atoms				AltConf
38	2	1	Total	C	N	O	0
			31	23	1	7	
38	4	1	Total	C	N	O	0
			35	27	1	7	

- Molecule 39 is [(2 {R})-1-nonanoyloxy-3-[oxidanyl-[(2 {R},3 {S},5 {R},6 {R})-2,3,4,5,6-pentakis(oxidanyl)cyclohexyl]oxy-phosphoryl]oxy-propan-2-yl] (5 {Z},8 {Z})-heptadeca-5,8-dienoate (CCD ID: P3H) (formula: C₃₅H₆₃O₁₃P).



Mol	Chain	Residues	Atoms				AltConf
39	2	1	Total	C	O	P	0
			49	35	13	1	

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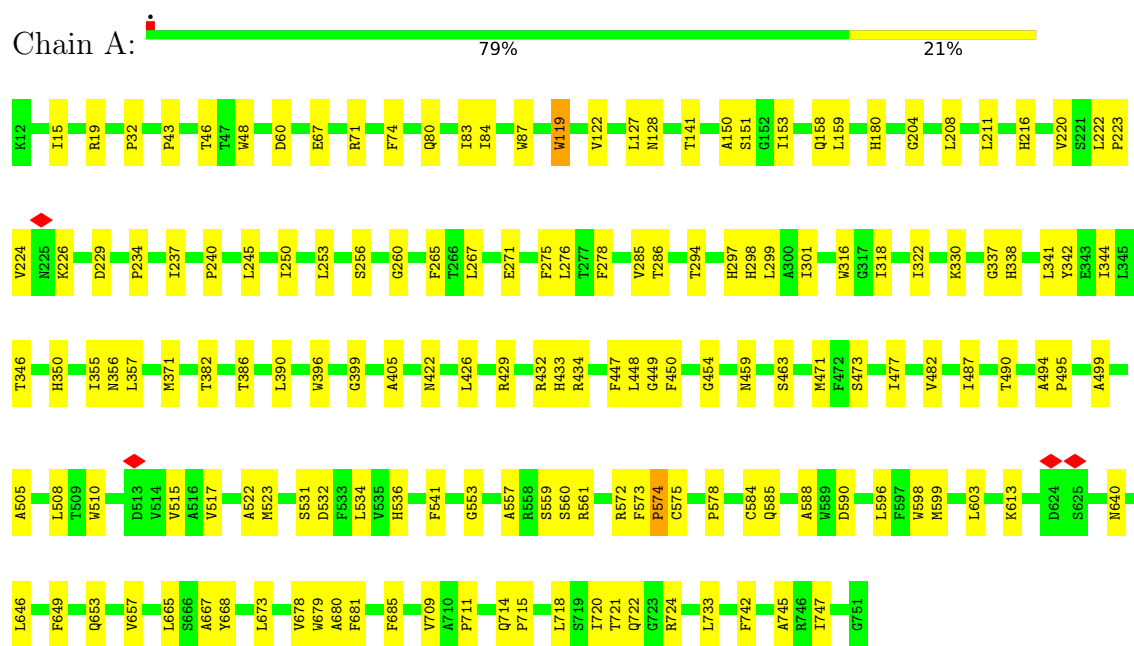
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
39	5	1	32	18	13	1	0

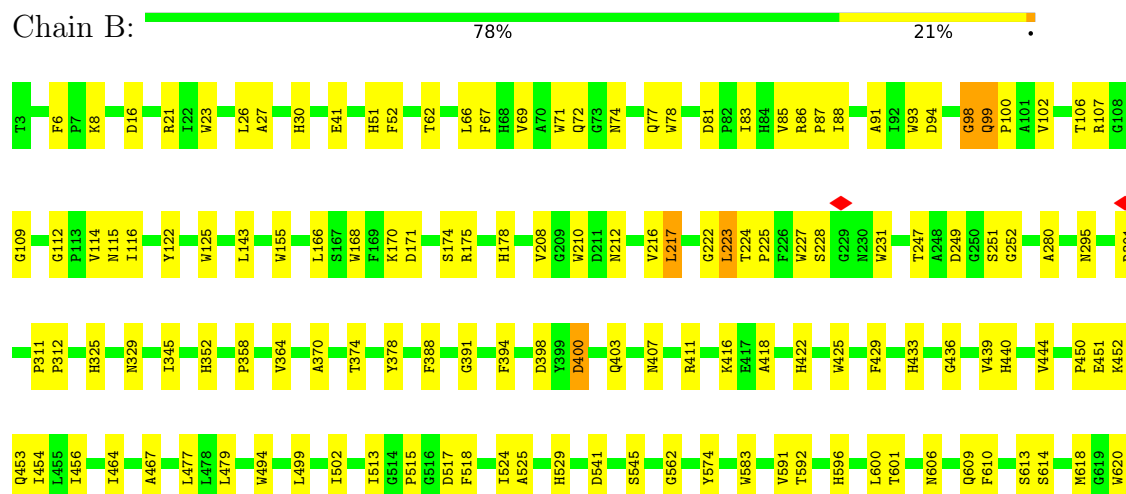
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





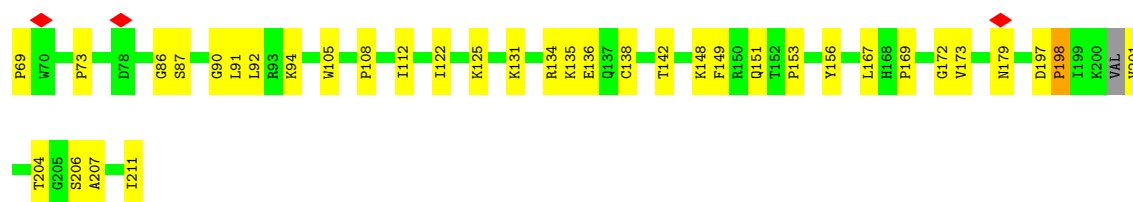
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 78% 22%



• Molecule 4: Psad

Chain D: 74% 24% ..



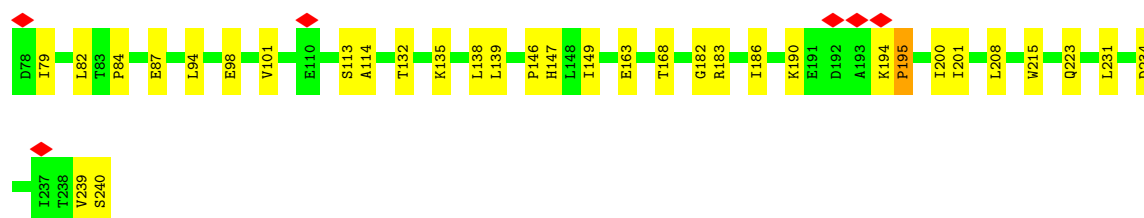
• Molecule 5: Psae

Chain E: 75% 25%



• Molecule 6: Psaf

Chain F: 80% 20%



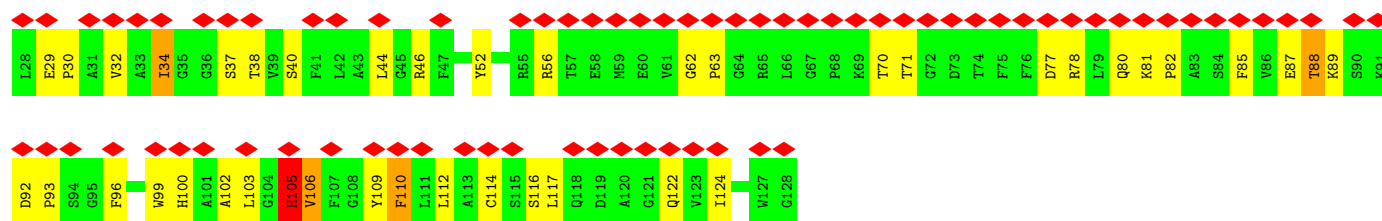
• Molecule 7: Photosystem I reaction center subunit IX

Chain J: 5% 66% 27% 7%

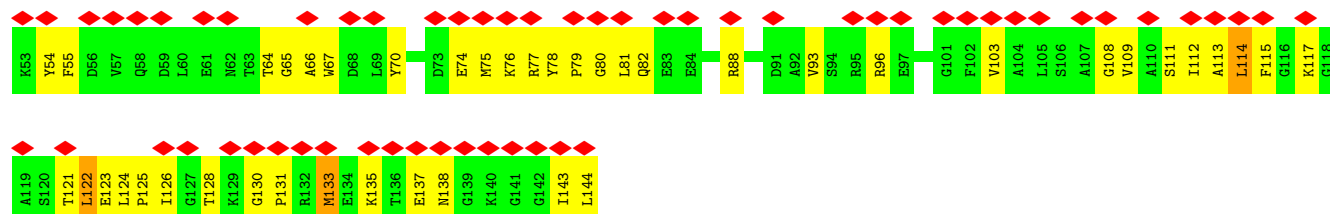


• Molecule 8: Psag

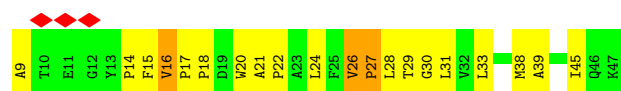
Chain G: 73% 59% 36% ..



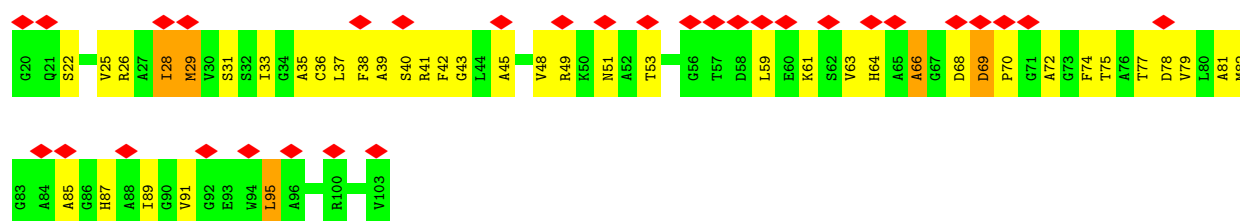
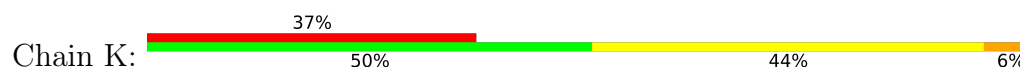
• Molecule 9: PsaH



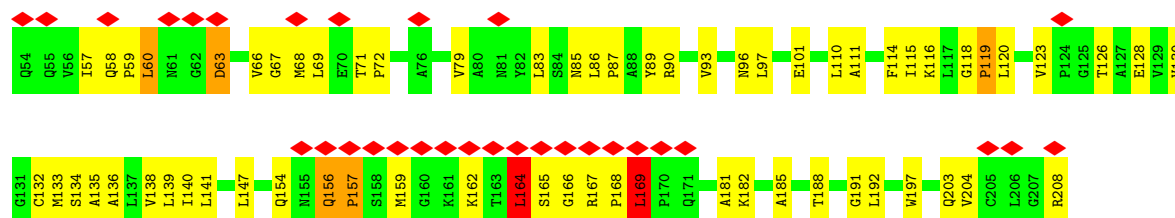
• Molecule 10: PsaI



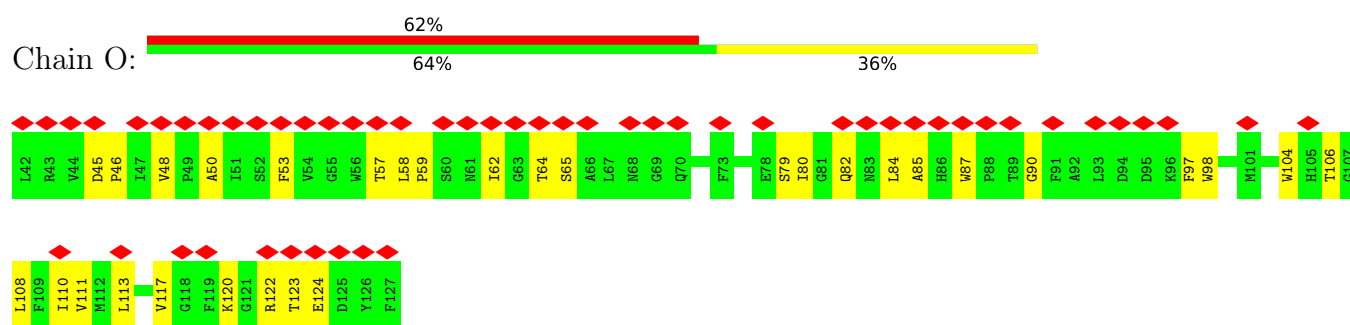
• Molecule 11: PsaK



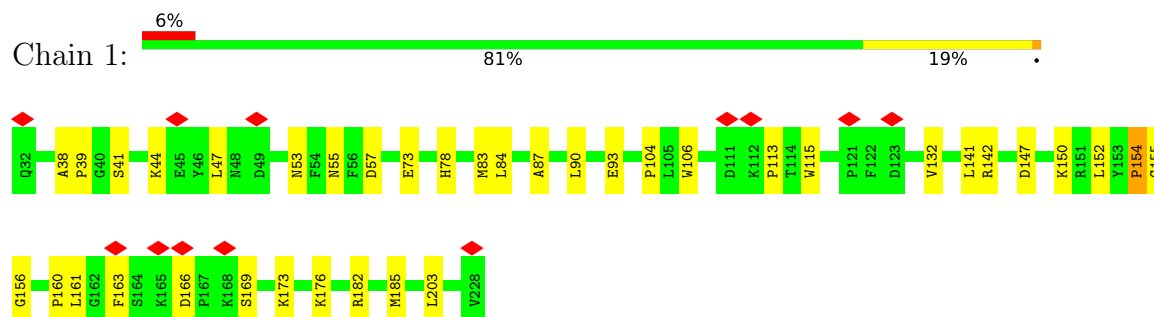
• Molecule 12: PsaL



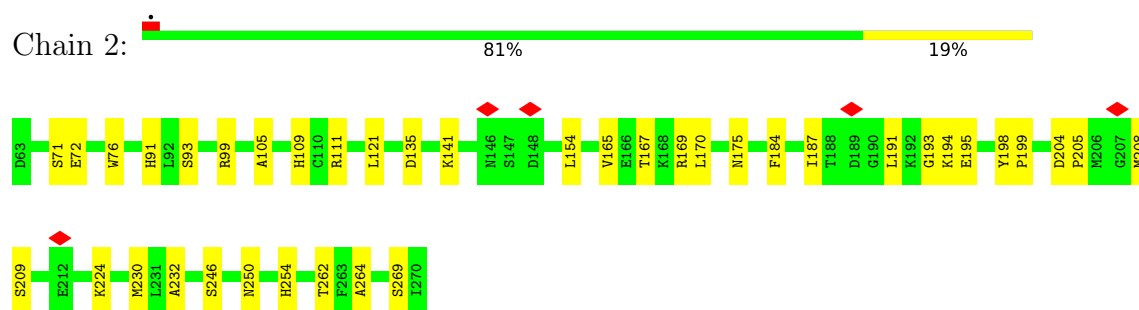
• Molecule 13: PsaO



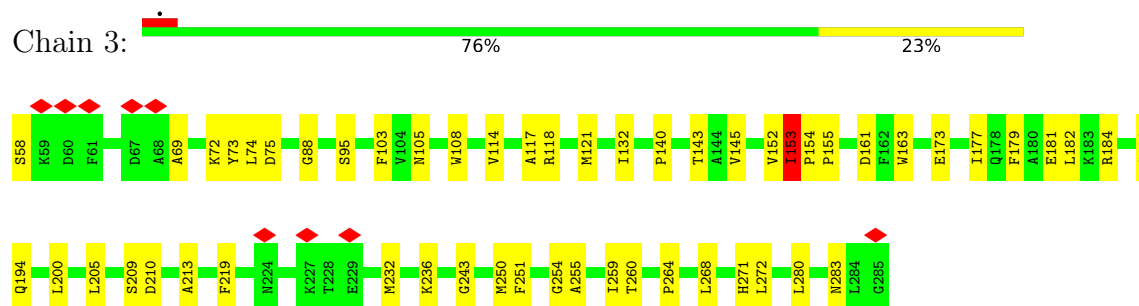
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



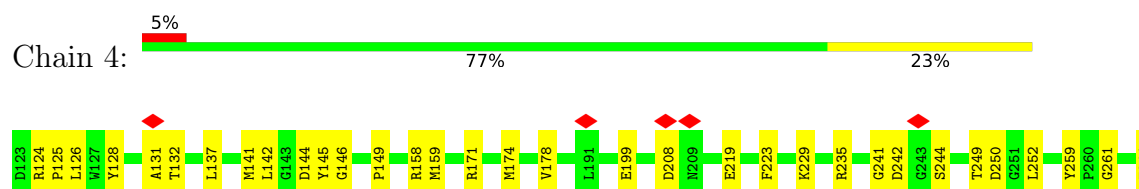
- Molecule 15: Lhca2



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

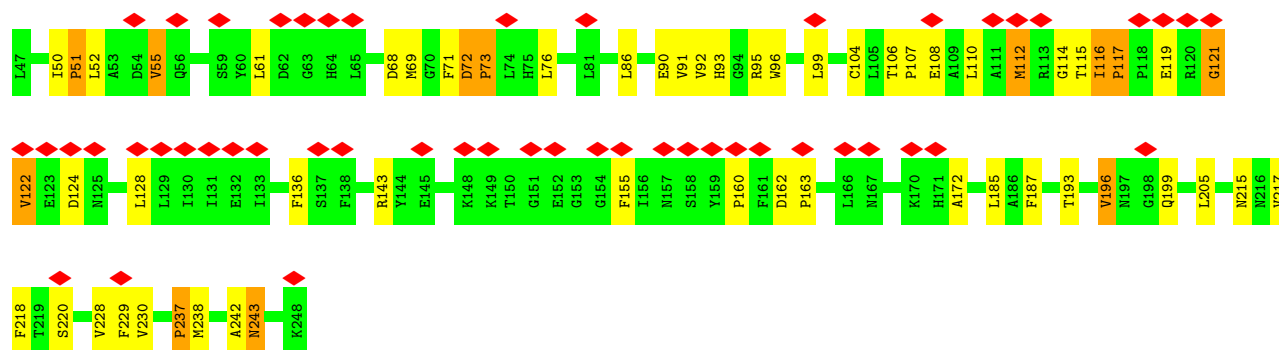
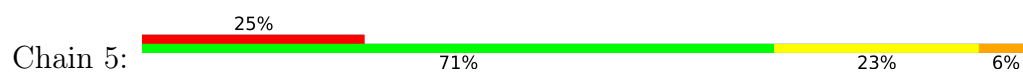


- Molecule 17: Lhca4

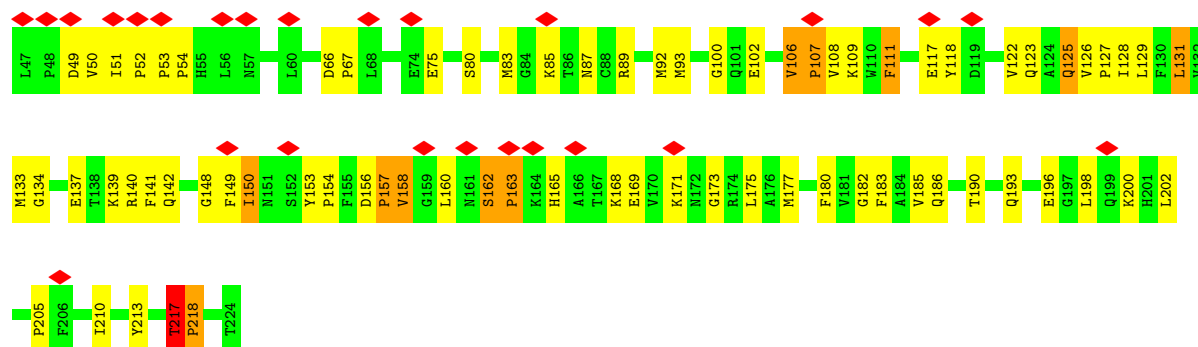




• Molecule 18: Lhca5



• Molecule 19: Lhca6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	189006	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42.68	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.155	Depositor
Minimum map value	-0.071	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0247	Depositor
Map size ($\text{\AA}$)	384.12003, 384.12003, 384.12003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LUT, CLA, DGD, BCR, CL0, OCD, P3H, 3PH, PQN, LMG, XAT, 4RF, PTY, SF4, CA, CHL, LMU, SQD, LMK, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.56	4/6004 (0.1%)	0.77	7/8190 (0.1%)
2	B	0.58	3/6021 (0.0%)	0.79	8/8230 (0.1%)
3	C	0.43	0/610	0.67	0/828
4	D	0.77	2/1164 (0.2%)	1.03	3/1570 (0.2%)
5	E	0.50	0/525	0.62	0/712
6	F	0.78	2/1305 (0.2%)	1.02	3/1764 (0.2%)
7	J	1.15	2/338 (0.6%)	1.39	3/461 (0.7%)
8	G	0.76	1/796 (0.1%)	1.14	8/1077 (0.7%)
9	H	0.75	0/716	1.16	2/963 (0.2%)
10	I	1.55	3/315 (1.0%)	1.97	6/437 (1.4%)
11	K	0.96	1/581 (0.2%)	1.47	7/785 (0.9%)
12	L	1.32	8/1164 (0.7%)	1.71	13/1589 (0.8%)
13	O	0.69	0/708	0.93	1/966 (0.1%)
14	1	0.42	0/1540	0.68	0/2088
15	2	0.37	0/1656	0.59	0/2243
16	3	0.46	0/1790	0.67	1/2432 (0.0%)
17	4	0.46	0/1687	0.73	1/2300 (0.0%)
18	5	0.96	3/1561 (0.2%)	1.25	7/2123 (0.3%)
19	6	0.92	2/1417 (0.1%)	1.31	10/1929 (0.5%)
All	All	0.70	31/29898 (0.1%)	0.96	80/40687 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
11	K	0	2
16	3	0	1
All	All	0	3

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	L	157	PRO	N-CA	22.30	1.70	1.47
18	5	73	PRO	N-CA	19.88	1.70	1.47
7	J	36	PRO	N-CA	18.05	1.70	1.47
6	F	195	PRO	N-CA	18.00	1.70	1.47
1	A	574	PRO	N-CA	17.69	1.70	1.47

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	5	72	ASP	CA-C-N	19.41	139.70	119.90
18	5	72	ASP	C-N-CA	19.41	139.70	119.90
19	6	217	THR	CA-C-N	19.13	139.07	119.56
19	6	217	THR	C-N-CA	19.13	139.07	119.56
12	L	169	LEU	CA-C-N	18.37	138.31	120.31

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
16	3	153	ILE	Mainchain
11	K	66	ALA	Mainchain
11	K	68	ASP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5808	0	5642	142	0
2	B	5808	0	5560	189	0
3	C	600	0	582	13	0
4	D	1134	0	1142	26	0
5	E	515	0	508	10	0
6	F	1278	0	1299	41	0
7	J	327	0	328	18	0
8	G	773	0	756	45	0
9	H	704	0	693	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	I	301	0	297	41	0
11	K	573	0	567	55	0
12	L	1137	0	1165	80	0
13	O	684	0	661	33	0
14	1	1501	0	1469	38	0
15	2	1609	0	1556	31	0
16	3	1740	0	1698	54	0
17	4	1637	0	1579	47	0
18	5	1525	0	1517	91	0
19	6	1378	0	1382	96	0
20	A	65	0	72	10	0
21	1	682	0	648	52	0
21	2	602	0	609	13	0
21	3	746	0	722	49	0
21	4	632	0	600	28	0
21	5	602	0	549	100	0
21	6	602	0	542	98	0
21	A	2658	0	2762	220	0
21	B	2619	0	2762	200	0
21	F	96	0	74	2	0
21	G	138	0	99	18	0
21	H	106	0	92	4	0
21	J	49	0	38	3	0
21	K	193	0	148	35	0
21	L	230	0	219	24	0
21	O	136	0	95	3	0
22	A	33	0	46	3	0
22	B	33	0	46	7	0
23	A	8	0	0	0	0
23	C	16	0	0	0	0
24	1	40	0	53	5	0
24	2	40	0	53	1	0
24	3	120	0	159	15	0
24	4	40	0	53	1	0
24	A	280	0	367	41	0
24	B	240	0	317	38	0
24	F	80	0	106	24	0
24	G	40	0	53	20	0
24	H	40	0	53	5	0
24	I	80	0	106	16	0
24	J	80	0	105	7	0
24	K	40	0	53	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	L	80	0	106	5	0
24	O	40	0	52	7	0
25	1	106	0	128	5	0
25	2	114	0	141	8	0
25	3	17	0	12	0	0
25	4	29	0	28	0	0
25	5	67	0	77	11	0
25	6	25	0	20	0	0
25	A	98	0	148	6	0
25	B	42	0	57	3	0
25	F	49	0	74	2	0
26	A	19	0	0	0	0
27	6	35	0	46	1	0
27	A	70	0	92	2	0
27	B	35	0	46	2	0
28	2	39	0	36	2	0
28	3	84	0	84	6	0
28	B	61	0	83	5	0
29	5	57	0	60	5	0
29	B	31	0	35	2	0
29	F	34	0	41	0	0
30	B	1	0	0	0	0
31	1	32	0	34	1	0
31	2	50	0	73	0	0
31	3	82	0	107	19	0
31	4	85	0	113	2	0
31	6	37	0	44	12	0
31	F	50	0	73	3	0
32	5	32	0	39	1	0
32	L	39	0	53	2	0
33	1	58	0	64	0	0
33	3	46	0	38	0	0
33	4	35	0	43	0	0
33	5	36	0	48	10	0
33	6	24	0	21	1	0
33	L	20	0	13	0	0
33	O	22	0	17	5	0
34	1	42	0	55	7	0
34	2	42	0	55	6	0
34	3	42	0	55	9	0
34	4	42	0	55	4	0
34	5	168	0	220	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	6	42	0	55	22	0
35	1	44	0	56	2	0
35	2	44	0	56	3	0
35	3	44	0	56	7	0
35	4	44	0	56	3	0
35	6	88	0	112	14	0
36	1	113	0	100	7	0
36	2	216	0	180	8	0
36	3	66	0	69	3	0
36	4	159	0	124	1	0
36	5	113	0	100	40	0
36	6	47	0	30	7	0
37	2	40	0	46	2	0
37	3	35	0	33	2	0
37	6	32	0	27	1	0
38	2	31	0	0	0	0
38	4	35	0	0	0	0
39	2	49	0	0	0	0
39	5	32	0	0	1	0
All	All	43789	0	43688	1758	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 20.

The worst 5 of 1758 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)
10:I:27:PRO:N	10:I:27:PRO:CA	1.69	1.49
12:L:157:PRO:N	12:L:157:PRO:CA	1.69	1.47
1:A:574:PRO:N	1:A:574:PRO:CA	1.70	1.45
6:F:195:PRO:N	6:F:195:PRO:CA	1.70	1.42
18:5:73:PRO:N	18:5:73:PRO:CA	1.70	1.42

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/740 (100%)	693 (94%)	43 (6%)	2 (0%)	36	55
2	B	731/733 (100%)	693 (95%)	37 (5%)	1 (0%)	48	69
3	C	78/80 (98%)	71 (91%)	7 (9%)	0	100	100
4	D	141/144 (98%)	125 (89%)	16 (11%)	0	100	100
5	E	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
6	F	160/162 (99%)	143 (89%)	16 (10%)	1 (1%)	21	39
7	J	39/41 (95%)	33 (85%)	6 (15%)	0	100	100
8	G	99/101 (98%)	86 (87%)	11 (11%)	2 (2%)	6	12
9	H	90/92 (98%)	81 (90%)	9 (10%)	0	100	100
10	I	37/39 (95%)	32 (86%)	4 (11%)	1 (3%)	4	8
11	K	82/84 (98%)	75 (92%)	6 (7%)	1 (1%)	10	22
12	L	153/155 (99%)	143 (94%)	6 (4%)	4 (3%)	4	9
13	O	84/86 (98%)	74 (88%)	10 (12%)	0	100	100
14	1	195/197 (99%)	177 (91%)	16 (8%)	2 (1%)	12	24
15	2	206/208 (99%)	193 (94%)	13 (6%)	0	100	100
16	3	226/228 (99%)	213 (94%)	13 (6%)	0	100	100
17	4	209/211 (99%)	188 (90%)	21 (10%)	0	100	100
18	5	200/202 (99%)	177 (88%)	17 (8%)	6 (3%)	3	7
19	6	176/178 (99%)	152 (86%)	17 (10%)	7 (4%)	2	3
All	All	3706/3745 (99%)	3409 (92%)	270 (7%)	27 (1%)	20	35

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	5	122	VAL
18	5	160	PRO

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Mol	Chain	Res	Type
19	6	107	PRO
6	F	135	LYS
8	G	82	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	599/599 (100%)	599 (100%)	0	100	100
2	B	593/593 (100%)	591 (100%)	2 (0%)	86	94
3	C	68/68 (100%)	68 (100%)	0	100	100
4	D	122/123 (99%)	122 (100%)	0	100	100
5	E	57/57 (100%)	57 (100%)	0	100	100
6	F	135/135 (100%)	135 (100%)	0	100	100
7	J	36/36 (100%)	35 (97%)	1 (3%)	38	62
8	G	78/78 (100%)	76 (97%)	2 (3%)	40	65
9	H	71/71 (100%)	68 (96%)	3 (4%)	26	51
10	I	30/30 (100%)	30 (100%)	0	100	100
11	K	53/53 (100%)	51 (96%)	2 (4%)	29	54
12	L	119/119 (100%)	116 (98%)	3 (2%)	42	66
13	O	71/71 (100%)	71 (100%)	0	100	100
14	1	152/152 (100%)	152 (100%)	0	100	100
15	2	167/167 (100%)	167 (100%)	0	100	100
16	3	173/173 (100%)	173 (100%)	0	100	100
17	4	169/169 (100%)	169 (100%)	0	100	100
18	5	163/163 (100%)	160 (98%)	3 (2%)	51	74
19	6	147/147 (100%)	141 (96%)	6 (4%)	27	52
All	All	3003/3004 (100%)	2981 (99%)	22 (1%)	73	88

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	5	112	MET
19	6	107	PRO
19	6	87	ASN
19	6	108	VAL
9	H	122	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
17	4	309	GLN
17	4	311	HIS
4	D	187	GLN
4	D	137	GLN
19	6	73	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 292 ligands modelled in this entry, 1 is monoatomic - leaving 291 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	A	5001	21	48,48,48	0.46	0	51,54,54	1.12	3 (5%)
24	BCR	B	4004	-	41,41,41	1.61	4 (9%)	56,56,56	4.39	13 (23%)
33	PTY	6	804	-	23,23,49	1.14	3 (13%)	26,28,54	1.26	2 (7%)
21	CLA	A	1129	-	59,63,73	1.49	7 (11%)	70,101,113	2.23	19 (27%)
21	CLA	B	1221	-	69,73,73	1.36	7 (10%)	82,113,113	2.04	20 (24%)
24	BCR	I	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.32	17 (30%)
38	LMK	4	805	-	34,34,53	1.69	4 (11%)	34,41,60	1.49	2 (5%)
21	CLA	A	1104	-	69,73,73	1.43	7 (10%)	82,113,113	2.08	20 (24%)
21	CLA	4	608	-	50,54,73	1.60	7 (14%)	59,90,113	2.11	16 (27%)
31	LMG	3	802	-	32,32,55	0.75	1 (3%)	40,40,63	0.99	1 (2%)
34	LUT	5	503	-	42,43,43	2.51	2 (4%)	51,60,60	4.40	19 (37%)
21	CLA	A	1102	-	69,73,73	1.37	7 (10%)	82,113,113	1.99	20 (24%)
22	PQN	A	2001	-	34,34,34	0.35	0	43,45,45	1.17	2 (4%)
21	CLA	H	1701	-	64,68,73	1.45	7 (10%)	76,107,113	2.25	21 (27%)
21	CLA	6	609	-	50,54,73	1.60	6 (12%)	59,90,113	2.03	16 (27%)
25	LHG	6	801	-	24,24,48	0.55	0	27,30,54	1.22	3 (11%)
32	4RF	L	5002	-	38,38,56	1.06	6 (15%)	41,41,59	0.99	3 (7%)
34	LUT	3	501	-	42,43,43	2.38	2 (4%)	51,60,60	1.87	11 (21%)
24	BCR	L	4002	-	41,41,41	1.75	7 (17%)	56,56,56	4.50	15 (26%)
21	CLA	A	1141	25	64,68,73	1.44	7 (10%)	76,107,113	2.04	20 (26%)
36	CHL	2	610	-	50,64,74	1.67	9 (18%)	46,102,114	1.82	11 (23%)
34	LUT	6	501	-	42,43,43	2.48	2 (4%)	51,60,60	2.13	14 (27%)
21	CLA	3	602	-	56,60,73	1.53	6 (10%)	65,97,113	2.10	18 (27%)
21	CLA	B	1021	-	69,73,73	1.40	7 (10%)	82,113,113	2.04	22 (26%)
21	CLA	1	607	-	50,54,73	1.62	7 (14%)	59,90,113	2.04	14 (23%)
21	CLA	3	613	-	50,54,73	1.59	7 (14%)	59,90,113	2.25	15 (25%)
21	CLA	A	1113	-	69,73,73	1.40	7 (10%)	82,113,113	1.78	18 (21%)
21	CLA	L	1503	-	54,58,73	1.56	6 (11%)	64,95,113	2.10	18 (28%)
21	CLA	A	1126	-	69,73,73	1.41	7 (10%)	82,113,113	1.95	20 (24%)
21	CLA	5	603	-	64,68,73	1.47	7 (10%)	76,107,113	2.14	22 (28%)
21	CLA	A	1136	-	69,73,73	1.40	8 (11%)	82,113,113	1.90	23 (28%)
21	CLA	F	1301	-	51,55,73	1.60	7 (13%)	60,91,113	2.10	18 (30%)
21	CLA	2	606	-	54,58,73	1.55	7 (12%)	64,95,113	2.15	20 (31%)
21	CLA	4	615	17	55,59,73	1.56	7 (12%)	64,96,113	2.06	16 (25%)
21	CLA	5	607	-	64,68,73	1.46	6 (9%)	76,107,113	2.14	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	6	607	-	64,68,73	1.42	7 (10%)	76,107,113	1.98	18 (23%)
21	CLA	A	1137	-	64,68,73	1.45	6 (9%)	76,107,113	2.03	23 (30%)
21	CLA	2	612	-	69,73,73	1.37	7 (10%)	82,113,113	1.96	20 (24%)
21	CLA	B	1216	-	69,73,73	1.37	7 (10%)	82,113,113	1.81	17 (20%)
21	CLA	B	1212	-	59,63,73	1.45	6 (10%)	70,101,113	2.04	19 (27%)
21	CLA	B	1230	-	69,73,73	1.38	7 (10%)	82,113,113	2.03	22 (26%)
21	CLA	1	615	-	64,68,73	1.44	8 (12%)	76,107,113	1.96	20 (26%)
21	CLA	B	1238	-	69,73,73	1.39	7 (10%)	82,113,113	1.99	18 (21%)
28	DGD	3	804	-	40,40,67	0.90	1 (2%)	54,54,81	1.21	4 (7%)
34	LUT	4	501	-	42,43,43	2.40	2 (4%)	51,60,60	2.20	17 (33%)
36	CHL	1	610	-	41,55,74	2.19	8 (19%)	35,91,114	2.17	11 (31%)
21	CLA	5	614	-	69,73,73	1.33	7 (10%)	82,113,113	2.62	23 (28%)
24	BCR	A	4007	-	41,41,41	1.64	4 (9%)	56,56,56	4.77	16 (28%)
28	DGD	3	805	-	46,46,67	0.90	2 (4%)	60,60,81	1.03	3 (5%)
24	BCR	A	4003	-	41,41,41	1.68	4 (9%)	56,56,56	4.38	18 (32%)
21	CLA	A	1108	-	59,63,73	1.49	7 (11%)	70,101,113	2.05	17 (24%)
21	CLA	A	1122	-	69,73,73	1.37	7 (10%)	82,113,113	1.94	21 (25%)
21	CLA	B	1213	-	64,68,73	1.44	7 (10%)	76,107,113	2.01	21 (27%)
21	CLA	4	602	-	54,58,73	1.57	7 (12%)	64,95,113	2.13	17 (26%)
24	BCR	B	4005	-	41,41,41	1.61	5 (12%)	56,56,56	4.44	10 (17%)
21	CLA	A	1128	-	69,73,73	1.41	7 (10%)	82,113,113	1.88	16 (19%)
21	CLA	5	605	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	19 (23%)
24	BCR	J	4002	-	41,41,41	1.79	6 (14%)	56,56,56	4.60	19 (33%)
33	PTY	5	803	-	35,35,49	1.03	4 (11%)	38,40,54	1.14	2 (5%)
36	CHL	2	609	15	60,74,74	1.51	9 (15%)	58,114,114	1.63	12 (20%)
35	XAT	6	504	-	41,47,47	0.88	2 (4%)	54,74,74	6.46	17 (31%)
21	CLA	B	1236	-	59,63,73	1.50	7 (11%)	70,101,113	2.06	19 (27%)
25	LHG	2	803	-	35,35,48	0.47	0	38,41,54	1.21	4 (10%)
21	CLA	1	612	-	64,68,73	1.41	7 (10%)	76,107,113	2.04	17 (22%)
21	CLA	B	1214	-	69,73,73	1.38	7 (10%)	82,113,113	1.95	19 (23%)
34	LUT	2	501	-	42,43,43	2.40	1 (2%)	51,60,60	2.10	19 (37%)
31	LMG	4	802	-	46,46,55	1.05	4 (8%)	54,54,63	1.45	5 (9%)
21	CLA	5	601	-	49,53,73	1.87	11 (22%)	58,89,113	2.91	19 (32%)
21	CLA	A	1103	-	69,73,73	1.34	7 (10%)	82,113,113	2.06	20 (24%)
21	CLA	B	1204	-	69,73,73	1.38	7 (10%)	82,113,113	2.02	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CL0	A	1011	-	58,73,73	3.20	17 (29%)	60,113,113	2.87	17 (28%)
21	CLA	2	602	-	56,60,73	1.53	7 (12%)	65,97,113	2.03	18 (27%)
21	CLA	1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
21	CLA	A	1105	-	64,68,73	1.47	8 (12%)	76,107,113	2.07	22 (28%)
24	BCR	I	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.56	17 (30%)
24	BCR	B	4003	-	41,41,41	1.71	5 (12%)	56,56,56	4.54	23 (41%)
33	PTY	1	806	-	17,17,49	1.29	2 (11%)	18,21,54	1.25	2 (11%)
21	CLA	6	612	-	69,73,73	1.37	6 (8%)	82,113,113	2.01	21 (25%)
21	CLA	A	1116	-	60,64,73	1.45	7 (11%)	71,102,113	2.08	18 (25%)
21	CLA	A	1123	-	69,73,73	1.43	8 (11%)	82,113,113	1.88	18 (21%)
36	CHL	4	613	-	55,69,74	1.64	9 (16%)	52,108,114	1.92	9 (17%)
21	CLA	L	1502	-	69,73,73	1.43	8 (11%)	82,113,113	2.22	26 (31%)
21	CLA	B	1218	-	69,73,73	1.44	8 (11%)	82,113,113	2.01	18 (21%)
34	LUT	5	502	-	42,43,43	2.51	2 (4%)	51,60,60	2.08	14 (27%)
21	CLA	B	1240	-	69,73,73	1.38	7 (10%)	82,113,113	1.88	16 (19%)
31	LMG	2	804	-	50,50,55	1.17	5 (10%)	58,58,63	1.20	2 (3%)
35	XAT	4	502	-	41,47,47	0.76	1 (2%)	54,74,74	1.72	12 (22%)
21	CLA	B	1226	-	69,73,73	1.43	7 (10%)	82,113,113	1.98	19 (23%)
21	CLA	A	1120	-	64,68,73	1.45	7 (10%)	76,107,113	2.05	20 (26%)
25	LHG	5	802	-	23,23,48	0.55	0	26,29,54	1.54	4 (15%)
33	PTY	O	5002	-	21,21,49	1.32	4 (19%)	24,26,54	1.47	2 (8%)
24	BCR	G	4001	-	41,41,41	1.64	4 (9%)	56,56,56	4.29	21 (37%)
39	P3H	5	806	-	32,32,49	1.45	7 (21%)	41,44,61	1.05	2 (4%)
21	CLA	K	1401	-	49,53,73	1.66	7 (14%)	58,89,113	2.69	20 (34%)
21	CLA	B	1234	-	59,63,73	1.50	7 (11%)	70,101,113	2.08	20 (28%)
21	CLA	J	1901	-	53,57,73	1.66	7 (13%)	61,93,113	2.55	21 (34%)
35	XAT	2	502	-	41,47,47	0.78	1 (2%)	54,74,74	1.74	13 (24%)
36	CHL	4	610	-	41,55,74	1.62	8 (19%)	35,91,114	2.33	12 (34%)
33	PTY	3	808	-	19,19,49	1.37	4 (21%)	22,24,54	1.50	2 (9%)
36	CHL	4	611	-	45,59,74	1.83	9 (20%)	40,96,114	2.11	11 (27%)
32	4RF	5	805	-	31,31,56	1.21	5 (16%)	34,34,59	1.29	4 (11%)
35	XAT	6	502	-	41,47,47	0.85	1 (2%)	54,74,74	1.75	12 (22%)
21	CLA	4	612	-	69,73,73	1.37	7 (10%)	82,113,113	1.85	19 (23%)
21	CLA	A	1121	-	64,68,73	1.39	6 (9%)	76,107,113	1.94	19 (25%)
25	LHG	1	802	-	25,25,48	0.50	0	28,31,54	1.31	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	5	604	18	69,73,73	1.36	6 (8%)	82,113,113	1.96	19 (23%)
23	SF4	C	3002	3	0,12,12	-	-	-		
29	3PH	5	807	-	28,28,47	1.10	4 (14%)	31,33,52	1.43	3 (9%)
21	CLA	6	608	-	50,54,73	1.57	6 (12%)	59,90,113	2.10	17 (28%)
21	CLA	1	605	-	69,73,73	1.36	7 (10%)	82,113,113	1.94	21 (25%)
21	CLA	3	603	-	69,73,73	1.45	7 (10%)	82,113,113	2.02	22 (26%)
23	SF4	C	3003	3	0,12,12	-	-	-		
21	CLA	A	1132	-	69,73,73	1.35	6 (8%)	82,113,113	1.93	20 (24%)
27	LMU	6	805	-	36,36,36	0.47	0	47,47,47	0.94	4 (8%)
24	BCR	A	4005	-	41,41,41	1.60	5 (12%)	56,56,56	4.36	9 (16%)
33	PTY	1	805	-	39,39,49	0.98	3 (7%)	42,44,54	1.15	2 (4%)
36	CHL	6	610	-	41,55,74	1.46	9 (21%)	35,91,114	2.06	11 (31%)
22	PQN	B	2002	-	34,34,34	0.37	0	43,45,45	1.23	2 (4%)
36	CHL	2	611	-	42,56,74	1.75	9 (21%)	36,92,114	2.16	11 (30%)
37	SQD	3	806	-	33,35,54	0.91	0	43,46,65	1.10	4 (9%)
21	CLA	A	1138	-	69,73,73	1.38	7 (10%)	82,113,113	1.99	16 (19%)
21	CLA	B	1228	-	64,68,73	1.41	7 (10%)	76,107,113	1.95	18 (23%)
25	LHG	F	5001	-	48,48,48	0.40	0	51,54,54	0.96	3 (5%)
21	CLA	1	608	-	59,63,73	1.50	7 (11%)	70,101,113	2.05	21 (30%)
21	CLA	1	604	-	69,73,73	1.40	8 (11%)	82,113,113	2.05	23 (28%)
21	CLA	5	608	-	59,63,73	1.53	7 (11%)	70,101,113	2.10	18 (25%)
31	LMG	1	804	-	32,32,55	0.60	0	40,40,63	1.49	7 (17%)
28	DGD	B	5002	-	62,62,67	1.22	6 (9%)	76,76,81	1.07	4 (5%)
21	CLA	B	1222	-	69,73,73	1.40	7 (10%)	82,113,113	1.96	22 (26%)
36	CHL	3	604	-	60,74,74	1.79	10 (16%)	58,114,114	1.73	10 (17%)
21	CLA	5	606	-	54,58,73	1.53	7 (12%)	64,95,113	2.08	19 (29%)
33	PTY	4	804	-	34,34,49	1.04	4 (11%)	37,39,54	1.14	2 (5%)
25	LHG	3	801	-	16,16,48	0.83	1 (6%)	17,20,54	0.74	0
35	XAT	3	502	-	41,47,47	0.82	1 (2%)	54,74,74	2.05	15 (27%)
21	CLA	A	1112	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	20 (24%)
21	CLA	6	606	-	54,58,73	1.51	5 (9%)	64,95,113	2.10	19 (29%)
21	CLA	B	1239	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	20 (24%)
23	SF4	A	3001	2,1	0,12,12	-	-	-		
31	LMG	6	802	-	37,37,55	0.63	1 (2%)	45,45,63	1.08	3 (6%)
21	CLA	A	1110	-	59,63,73	1.50	7 (11%)	70,101,113	2.11	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	F	4001	-	41,41,41	1.60	4 (9%)	56,56,56	4.55	17 (30%)
26	OCD	A	5003	-	17,18,18	0.26	0	16,17,17	0.94	0
21	CLA	B	1207	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	19 (23%)
21	CLA	3	601	-	64,68,73	1.45	7 (10%)	76,107,113	2.06	17 (22%)
21	CLA	A	1124	-	64,68,73	1.45	7 (10%)	76,107,113	1.96	22 (28%)
29	3PH	F	5003	-	33,33,47	1.01	4 (12%)	36,38,52	1.20	2 (5%)
36	CHL	5	610	-	41,55,74	1.51	9 (21%)	35,91,114	2.21	10 (28%)
21	CLA	A	1119	-	69,73,73	1.40	7 (10%)	82,113,113	1.86	19 (23%)
21	CLA	B	1217	-	69,73,73	1.40	7 (10%)	82,113,113	1.87	18 (21%)
21	CLA	K	1404	-	49,53,73	1.59	7 (14%)	58,89,113	2.07	15 (25%)
27	LMU	A	5004	-	36,36,36	0.44	0	47,47,47	1.09	2 (4%)
21	CLA	A	1117	-	69,73,73	1.36	6 (8%)	82,113,113	1.94	17 (20%)
21	CLA	B	1223	-	69,73,73	1.39	7 (10%)	82,113,113	1.96	18 (21%)
21	CLA	A	1135	-	55,59,73	1.61	7 (12%)	64,96,113	2.16	18 (28%)
25	LHG	4	801	-	28,28,48	0.56	1 (3%)	31,34,54	1.30	4 (12%)
21	CLA	6	613	-	49,53,73	1.60	6 (12%)	58,89,113	2.16	14 (24%)
21	CLA	B	1227	-	69,73,73	1.36	7 (10%)	82,113,113	1.96	22 (26%)
21	CLA	A	1127	-	69,73,73	1.41	7 (10%)	82,113,113	1.89	18 (21%)
21	CLA	B	1215	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	18 (21%)
21	CLA	B	1022	-	69,73,73	1.34	6 (8%)	82,113,113	1.93	19 (23%)
21	CLA	O	1803	-	64,68,73	1.50	8 (12%)	76,107,113	1.99	21 (27%)
21	CLA	3	606	-	59,63,73	1.50	7 (11%)	70,101,113	2.08	22 (31%)
21	CLA	4	607	-	64,68,73	1.43	7 (10%)	76,107,113	1.98	19 (25%)
24	BCR	K	4001	-	41,41,41	1.61	4 (9%)	56,56,56	4.49	17 (30%)
21	CLA	A	1106	-	69,73,73	1.40	7 (10%)	82,113,113	1.93	17 (20%)
21	CLA	A	1012	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
21	CLA	L	1504	-	54,58,73	1.52	6 (11%)	64,95,113	2.11	19 (29%)
21	CLA	1	613	-	49,53,73	1.64	7 (14%)	58,89,113	2.03	17 (29%)
21	CLA	4	601	-	64,68,73	1.44	7 (10%)	76,107,113	2.23	23 (30%)
24	BCR	A	4001	-	41,41,41	1.61	4 (9%)	56,56,56	5.22	22 (39%)
21	CLA	2	608	-	54,58,73	1.56	7 (12%)	64,95,113	2.19	19 (29%)
21	CLA	A	1107	-	69,73,73	1.34	5 (7%)	82,113,113	1.93	19 (23%)
21	CLA	1	603	-	64,68,73	1.42	8 (12%)	76,107,113	2.13	21 (27%)
21	CLA	3	615	-	60,64,73	1.48	8 (13%)	71,102,113	2.06	21 (29%)
21	CLA	B	1220	-	59,63,73	1.52	7 (11%)	70,101,113	2.05	22 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	2	607	25	64,68,73	1.43	7 (10%)	76,107,113	2.11	21 (27%)
21	CLA	B	1206	2	69,73,73	1.34	6 (8%)	82,113,113	1.90	18 (21%)
21	CLA	A	1125	-	69,73,73	1.42	7 (10%)	82,113,113	1.92	17 (20%)
21	CLA	B	1023	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	19 (23%)
21	CLA	O	1802	-	41,46,73	1.62	6 (14%)	51,81,113	2.09	15 (29%)
27	LMU	B	5004	-	36,36,36	0.44	0	47,47,47	0.91	2 (4%)
34	LUT	5	501	-	42,43,43	2.63	1 (2%)	51,60,60	4.52	20 (39%)
37	SQD	6	803	-	30,32,54	0.98	1 (3%)	40,43,65	0.99	2 (5%)
21	CLA	5	613	-	49,53,73	1.71	8 (16%)	58,89,113	2.28	18 (31%)
21	CLA	B	1211	-	69,73,73	1.42	7 (10%)	82,113,113	1.94	17 (20%)
24	BCR	B	4002	-	41,41,41	1.60	4 (9%)	56,56,56	4.39	11 (19%)
21	CLA	4	609	17	64,68,73	1.40	6 (9%)	76,107,113	2.20	21 (27%)
35	XAT	1	502	-	41,47,47	0.78	1 (2%)	54,74,74	2.05	12 (22%)
38	LMK	2	807	-	30,30,53	1.76	2 (6%)	30,37,60	1.71	4 (13%)
21	CLA	3	614	-	46,50,73	1.61	6 (13%)	53,85,113	2.11	13 (24%)
24	BCR	B	4001	-	41,41,41	1.71	4 (9%)	56,56,56	4.61	16 (28%)
31	LMG	F	5002	-	50,50,55	1.15	5 (10%)	58,58,63	1.09	2 (3%)
24	BCR	3	504	-	41,41,41	1.64	5 (12%)	56,56,56	4.49	18 (32%)
21	CLA	G	1602	-	50,54,73	1.58	6 (12%)	59,90,113	2.08	16 (27%)
21	CLA	3	612	-	69,73,73	1.38	7 (10%)	82,113,113	1.92	16 (19%)
37	SQD	2	805	-	38,40,54	0.88	0	48,51,65	0.91	2 (4%)
21	CLA	3	610	16	54,58,73	1.53	6 (11%)	64,95,113	2.14	19 (29%)
21	CLA	A	1109	-	69,73,73	1.37	7 (10%)	82,113,113	2.00	18 (21%)
25	LHG	1	803	-	30,30,48	0.44	0	33,36,54	1.21	4 (12%)
34	LUT	1	501	-	42,43,43	2.51	2 (4%)	51,60,60	5.01	23 (45%)
21	CLA	A	1131	-	69,73,73	1.39	6 (8%)	82,113,113	2.06	16 (19%)
21	CLA	6	605	-	69,73,73	1.39	7 (10%)	82,113,113	2.12	24 (29%)
21	CLA	F	1302	-	53,57,73	1.57	7 (13%)	61,93,113	2.25	18 (29%)
21	CLA	1	601	-	69,73,73	1.35	6 (8%)	82,113,113	1.93	20 (24%)
24	BCR	A	4004	-	41,41,41	1.67	5 (12%)	56,56,56	4.68	17 (30%)
21	CLA	1	602	-	50,54,73	1.60	7 (14%)	59,90,113	2.04	15 (25%)
24	BCR	O	4001	-	41,41,41	1.71	6 (14%)	56,56,56	5.23	22 (39%)
21	CLA	A	1111	-	69,73,73	1.41	7 (10%)	82,113,113	1.98	20 (24%)
21	CLA	2	615	-	69,73,73	1.38	7 (10%)	82,113,113	1.86	19 (23%)
21	CLA	A	1118	-	54,58,73	1.67	9 (16%)	64,95,113	2.20	20 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	LUT	5	504	-	42,43,43	2.59	2 (4%)	51,60,60	4.71	21 (41%)
24	BCR	L	4001	-	41,41,41	1.67	6 (14%)	56,56,56	4.45	14 (25%)
21	CLA	3	607	-	64,68,73	1.43	7 (10%)	76,107,113	1.97	21 (27%)
29	3PH	5	804	-	27,27,47	1.13	4 (14%)	30,32,52	1.23	2 (6%)
21	CLA	2	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
21	CLA	3	611	-	69,73,73	1.43	7 (10%)	82,113,113	1.89	17 (20%)
21	CLA	4	605	-	69,73,73	1.38	7 (10%)	82,113,113	2.00	22 (26%)
24	BCR	2	503	-	41,41,41	1.59	4 (9%)	56,56,56	4.43	16 (28%)
25	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.02	2 (3%)
21	CLA	G	1603	-	49,53,73	1.56	7 (14%)	58,89,113	2.66	19 (32%)
21	CLA	6	604	-	64,68,73	1.46	8 (12%)	76,107,113	1.95	22 (28%)
21	CLA	A	1130	-	59,63,73	1.58	7 (11%)	70,101,113	2.09	24 (34%)
21	CLA	H	1702	-	50,54,73	1.72	8 (16%)	59,90,113	2.23	22 (37%)
31	LMG	3	803	-	50,50,55	1.18	5 (10%)	58,58,63	1.11	3 (5%)
21	CLA	K	1403	-	52,56,73	1.53	8 (15%)	61,92,113	2.40	18 (29%)
21	CLA	B	1208	-	64,68,73	1.40	7 (10%)	76,107,113	1.96	18 (23%)
25	LHG	2	801	21	34,34,48	0.48	0	37,40,54	1.20	4 (10%)
36	CHL	2	613	-	40,54,74	1.89	10 (25%)	34,90,114	2.09	12 (35%)
21	CLA	A	1133	-	69,73,73	1.46	8 (11%)	82,113,113	1.77	16 (19%)
21	CLA	A	1013	-	69,73,73	1.41	7 (10%)	82,113,113	1.89	18 (21%)
21	CLA	3	605	-	69,73,73	1.39	7 (10%)	82,113,113	1.88	13 (15%)
21	CLA	A	1101	-	69,73,73	1.40	8 (11%)	82,113,113	1.88	19 (23%)
21	CLA	A	1139	-	69,73,73	1.42	7 (10%)	82,113,113	2.03	20 (24%)
21	CLA	O	1801	-	41,46,73	1.73	8 (19%)	47,80,113	2.93	13 (27%)
21	CLA	B	1205	-	69,73,73	1.37	7 (10%)	82,113,113	2.00	18 (21%)
21	CLA	B	1224	-	69,73,73	1.38	7 (10%)	82,113,113	1.89	19 (23%)
21	CLA	2	601	-	69,73,73	1.45	7 (10%)	82,113,113	1.94	17 (20%)
24	BCR	3	503	-	41,41,41	1.61	4 (9%)	56,56,56	4.35	14 (25%)
21	CLA	B	1209	-	50,54,73	1.61	7 (14%)	59,90,113	2.12	16 (27%)
21	CLA	B	1229	-	69,73,73	1.41	8 (11%)	82,113,113	2.04	27 (32%)
33	PTY	L	5003	-	19,19,49	1.40	4 (21%)	22,24,54	1.46	2 (9%)
24	BCR	1	504	-	41,41,41	1.60	4 (9%)	56,56,56	4.26	20 (35%)
21	CLA	B	1237	-	69,73,73	1.39	6 (8%)	82,113,113	1.98	21 (25%)
21	CLA	4	606	-	54,58,73	1.55	7 (12%)	64,95,113	2.05	15 (23%)
21	CLA	L	1501	-	69,73,73	1.35	9 (13%)	82,113,113	2.12	23 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	B	4006	-	41,41,41	1.68	5 (12%)	56,56,56	4.41	13 (23%)
21	CLA	B	1232	-	59,63,73	1.52	7 (11%)	70,101,113	2.04	18 (25%)
21	CLA	A	1134	1	59,63,73	1.45	6 (10%)	70,101,113	2.02	19 (27%)
33	PTY	3	807	-	25,25,49	1.22	3 (12%)	28,30,54	1.29	2 (7%)
24	BCR	H	4001	-	41,41,41	1.69	5 (12%)	56,56,56	4.59	18 (32%)
24	BCR	J	4001	-	41,41,41	1.69	6 (14%)	56,56,56	4.68	23 (41%)
21	CLA	A	1140	-	65,69,73	1.43	7 (10%)	77,108,113	1.96	19 (24%)
21	CLA	3	608	-	69,73,73	1.38	8 (11%)	82,113,113	1.82	19 (23%)
21	CLA	A	1115	-	64,68,73	1.41	7 (10%)	76,107,113	1.95	19 (25%)
21	CLA	B	1203	-	69,73,73	1.38	7 (10%)	82,113,113	1.88	19 (23%)
21	CLA	B	1235	-	64,68,73	1.40	7 (10%)	76,107,113	2.00	20 (26%)
21	CLA	6	602	-	54,58,73	1.52	6 (11%)	64,95,113	2.13	20 (31%)
24	BCR	A	4002	-	41,41,41	1.61	4 (9%)	56,56,56	4.56	21 (37%)
25	LHG	B	5001	-	41,41,48	0.44	0	44,47,54	1.13	3 (6%)
25	LHG	2	802	-	42,42,48	0.44	0	45,48,54	1.20	4 (8%)
21	CLA	B	1201	-	52,56,73	1.55	7 (13%)	61,92,113	2.32	21 (34%)
21	CLA	4	604	-	64,68,73	1.40	6 (9%)	76,107,113	1.95	19 (25%)
24	BCR	A	4006	-	41,41,41	1.64	4 (9%)	56,56,56	4.31	13 (23%)
28	DGD	2	806	-	40,40,67	0.90	2 (5%)	54,54,81	1.10	2 (3%)
21	CLA	5	612	18	50,54,73	1.85	10 (20%)	59,90,113	2.28	21 (35%)
24	BCR	3	506	-	41,41,41	1.68	4 (9%)	56,56,56	4.09	22 (39%)
29	3PH	B	5003	-	30,30,47	1.09	4 (13%)	33,35,52	1.31	2 (6%)
36	CHL	5	609	-	60,74,74	1.24	9 (15%)	58,114,114	1.64	11 (18%)
21	CLA	G	1601	-	51,55,73	1.56	6 (11%)	60,91,113	2.09	17 (28%)
39	P3H	2	808	-	49,49,49	1.46	8 (16%)	58,61,61	1.03	4 (6%)
24	BCR	F	4002	-	41,41,41	1.62	4 (9%)	56,56,56	4.55	18 (32%)
21	CLA	B	1210	-	69,73,73	1.41	7 (10%)	82,113,113	1.96	16 (19%)
21	CLA	B	1225	-	69,73,73	1.41	7 (10%)	82,113,113	1.85	17 (20%)
21	CLA	6	601	-	64,68,73	1.40	6 (9%)	76,107,113	1.95	20 (26%)
21	CLA	B	1202	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	21 (25%)
25	LHG	5	801	-	42,42,48	0.45	0	45,48,54	1.18	5 (11%)
21	CLA	2	604	15	69,73,73	1.40	8 (11%)	82,113,113	1.96	18 (21%)
21	CLA	K	1402	-	59,63,73	1.47	6 (10%)	70,101,113	2.06	20 (28%)
27	LMU	A	5005	-	36,36,36	0.40	0	47,47,47	0.85	1 (2%)
21	CLA	1	606	-	54,58,73	1.55	6 (11%)	64,95,113	2.01	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	1231	-	64,68,73	1.46	7 (10%)	76,107,113	2.00	17 (22%)
31	LMG	4	803	-	39,39,55	0.80	2 (5%)	47,47,63	1.00	2 (4%)
36	CHL	1	609	14	60,74,74	1.54	8 (13%)	58,114,114	1.65	12 (20%)
24	BCR	4	503	-	41,41,41	1.64	4 (9%)	56,56,56	4.52	17 (30%)
21	CLA	A	1114	-	59,63,73	1.46	6 (10%)	70,101,113	2.05	18 (25%)
21	CLA	4	603	-	69,73,73	1.37	8 (11%)	82,113,113	1.87	17 (20%)
21	CLA	5	602	-	50,54,73	1.67	8 (16%)	59,90,113	2.06	18 (30%)
21	CLA	2	605	-	69,73,73	1.39	7 (10%)	82,113,113	1.91	22 (26%)
21	CLA	6	603	-	59,63,73	1.45	7 (11%)	70,101,113	2.00	18 (25%)
25	LHG	1	801	-	48,48,48	0.39	0	51,54,54	1.22	3 (5%)
21	CLA	B	1219	-	69,73,73	1.36	7 (10%)	82,113,113	1.87	17 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LHG	A	5001	21	-	23/53/53/53	-
24	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
33	PTY	6	804	-	-	7/26/26/53	-
21	CLA	A	1129	-	1/1/13/20	10/27/103/115	-
21	CLA	B	1221	-	1/1/15/20	12/39/115/115	-
24	BCR	I	4001	-	-	12/29/63/63	0/2/2/2
38	LMK	4	805	-	-	7/41/41/60	-
21	CLA	A	1104	-	1/1/15/20	16/39/115/115	-
21	CLA	4	608	-	1/1/11/20	9/17/93/115	-
31	LMG	3	802	-	-	7/26/46/70	0/1/1/1
34	LUT	5	503	-	-	8/29/67/67	0/2/2/2
21	CLA	A	1102	-	1/1/15/20	17/39/115/115	-
22	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
21	CLA	H	1701	-	1/1/14/20	13/33/109/115	-
21	CLA	6	609	-	1/1/11/20	9/17/93/115	-
25	LHG	6	801	-	-	17/29/29/53	-
32	4RF	L	5002	-	-	17/41/41/59	-
34	LUT	3	501	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	L	4002	-	-	8/29/63/63	0/2/2/2
21	CLA	A	1141	25	1/1/14/20	14/33/109/115	-
36	CHL	2	610	-	4/4/18/26	0/27/125/137	-
34	LUT	6	501	-	1/1/12/27	4/29/67/67	0/2/2/2
21	CLA	3	602	-	1/1/12/20	11/24/100/115	-
21	CLA	B	1021	-	1/1/15/20	14/39/115/115	-
21	CLA	1	607	-	1/1/11/20	8/17/93/115	-
21	CLA	3	613	-	1/1/11/20	9/17/93/115	-
21	CLA	A	1113	-	1/1/15/20	18/39/115/115	-
21	CLA	L	1503	-	1/1/12/20	3/21/97/115	-
21	CLA	A	1126	-	1/1/15/20	18/39/115/115	-
21	CLA	5	603	-	1/1/14/20	15/33/109/115	-
21	CLA	A	1136	-	1/1/15/20	13/39/115/115	-
21	CLA	F	1301	-	1/1/11/20	10/18/94/115	-
21	CLA	2	606	-	1/1/12/20	7/21/97/115	-
21	CLA	4	615	17	1/1/12/20	11/23/99/115	-
21	CLA	5	607	-	1/1/14/20	13/33/109/115	-
21	CLA	6	607	-	1/1/14/20	18/33/109/115	-
21	CLA	A	1137	-	1/1/14/20	10/33/109/115	-
21	CLA	2	612	-	1/1/15/20	18/39/115/115	-
21	CLA	B	1216	-	1/1/15/20	11/39/115/115	-
21	CLA	B	1212	-	1/1/13/20	12/27/103/115	-
21	CLA	B	1230	-	1/1/15/20	16/39/115/115	-
21	CLA	1	615	-	1/1/14/20	16/33/109/115	-
21	CLA	B	1238	-	1/1/15/20	15/39/115/115	-
28	DGD	3	804	-	-	11/28/68/95	0/2/2/2
34	LUT	4	501	-	1/1/12/27	6/29/67/67	0/2/2/2
36	CHL	1	610	-	3/3/16/26	1/17/115/137	-
21	CLA	5	614	-	1/1/15/20	20/39/115/115	-
24	BCR	A	4007	-	-	10/29/63/63	0/2/2/2
28	DGD	3	805	-	-	11/34/74/95	0/2/2/2
24	BCR	A	4003	-	-	6/29/63/63	0/2/2/2
21	CLA	A	1108	-	1/1/13/20	14/27/103/115	-
21	CLA	A	1122	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1213	-	1/1/14/20	15/33/109/115	-
21	CLA	4	602	-	1/1/12/20	9/21/97/115	-
24	BCR	B	4005	-	-	12/29/63/63	0/2/2/2
21	CLA	A	1128	-	1/1/15/20	12/39/115/115	-
21	CLA	5	605	-	1/1/15/20	18/39/115/115	-
24	BCR	J	4002	-	-	14/29/63/63	0/2/2/2
33	PTY	5	803	-	-	25/39/39/53	-
35	XAT	6	504	-	1/1/12/26	6/31/93/93	0/4/4/4
21	CLA	B	1236	-	1/1/13/20	10/27/103/115	-
25	LHG	2	803	-	-	23/40/40/53	-
21	CLA	1	612	-	1/1/14/20	13/33/109/115	-
21	CLA	B	1214	-	1/1/15/20	17/39/115/115	-
34	LUT	2	501	-	-	2/29/67/67	0/2/2/2
31	LMG	4	802	-	-	16/41/61/70	0/1/1/1
21	CLA	5	601	-	1/1/11/20	7/15/91/115	-
21	CLA	A	1103	-	1/1/15/20	15/39/115/115	-
21	CLA	B	1204	-	1/1/15/20	14/39/115/115	-
20	CL0	A	1011	-	3/3/20/25	13/37/135/135	-
21	CLA	2	602	-	1/1/12/20	8/24/100/115	-
21	CLA	1	611	-	1/1/15/20	18/39/115/115	-
21	CLA	A	1105	-	1/1/14/20	13/33/109/115	-
24	BCR	I	4002	-	-	12/29/63/63	0/2/2/2
24	BCR	B	4003	-	-	14/29/63/63	0/2/2/2
33	PTY	1	806	-	-	5/19/19/53	-
21	CLA	6	612	-	1/1/15/20	15/39/115/115	-
21	CLA	A	1116	-	1/1/13/20	15/29/105/115	-
21	CLA	A	1123	-	1/1/15/20	14/39/115/115	-
36	CHL	4	613	-	4/4/19/26	5/33/131/137	-
21	CLA	L	1502	-	1/1/15/20	14/39/115/115	-
21	CLA	B	1218	-	1/1/15/20	21/39/115/115	-
34	LUT	5	502	-	-	5/29/67/67	0/2/2/2
21	CLA	B	1240	-	1/1/15/20	13/39/115/115	-
35	XAT	4	502	-	2/2/12/26	0/31/93/93	0/4/4/4
31	LMG	2	804	-	-	16/45/65/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1226	-	1/1/15/20	13/39/115/115	-
21	CLA	A	1120	-	1/1/14/20	18/33/109/115	-
25	LHG	5	802	-	-	15/27/27/53	-
33	PTY	O	5002	-	-	9/24/24/53	-
24	BCR	G	4001	-	-	12/29/63/63	0/2/2/2
39	P3H	5	806	-	-	10/27/51/68	0/1/1/1
21	CLA	K	1401	-	1/1/11/20	12/15/91/115	-
21	CLA	B	1234	-	1/1/13/20	9/27/103/115	-
21	CLA	J	1901	-	1/1/11/20	8/20/96/115	-
35	XAT	2	502	-	2/2/12/26	2/31/93/93	0/4/4/4
36	CHL	4	610	-	3/3/16/26	1/17/115/137	-
33	PTY	3	808	-	-	12/22/22/53	-
36	CHL	4	611	-	3/3/17/26	0/21/119/137	-
32	4RF	5	805	-	-	16/34/34/59	-
35	XAT	6	502	-	2/2/12/26	0/31/93/93	0/4/4/4
21	CLA	4	612	-	1/1/15/20	14/39/115/115	-
21	CLA	A	1121	-	1/1/14/20	16/33/109/115	-
25	LHG	1	802	-	-	16/30/30/53	-
21	CLA	5	604	18	1/1/15/20	15/39/115/115	-
29	3PH	5	807	-	-	12/30/30/49	-
23	SF4	C	3002	3	-	-	0/6/5/5
21	CLA	6	608	-	1/1/11/20	8/17/93/115	-
21	CLA	1	605	-	1/1/15/20	14/39/115/115	-
21	CLA	3	603	-	1/1/15/20	15/39/115/115	-
23	SF4	C	3003	3	-	-	0/6/5/5
21	CLA	A	1132	-	1/1/15/20	17/39/115/115	-
27	LMU	6	805	-	-	12/21/61/61	0/2/2/2
24	BCR	A	4005	-	-	7/29/63/63	0/2/2/2
36	CHL	6	610	-	3/3/16/26	5/17/115/137	-
33	PTY	1	805	-	-	18/43/43/53	-
22	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
36	CHL	2	611	-	3/3/16/26	2/18/116/137	-
37	SQD	3	806	-	-	12/30/50/69	0/1/1/1
21	CLA	A	1138	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1228	-	1/1/14/20	13/33/109/115	-
25	LHG	F	5001	-	-	32/53/53/53	-
21	CLA	1	608	-	1/1/13/20	11/27/103/115	-
21	CLA	1	604	-	1/1/15/20	19/39/115/115	-
21	CLA	5	608	-	1/1/13/20	10/27/103/115	-
31	LMG	1	804	-	-	9/27/47/70	0/1/1/1
28	DGD	B	5002	-	-	16/50/90/95	0/2/2/2
21	CLA	B	1222	-	1/1/15/20	11/39/115/115	-
36	CHL	3	604	-	4/4/20/26	9/39/137/137	-
21	CLA	5	606	-	1/1/12/20	7/21/97/115	-
35	XAT	3	502	-	2/2/12/26	4/31/93/93	0/4/4/4
25	LHG	3	801	-	-	12/19/19/53	-
33	PTY	4	804	-	-	23/38/38/53	-
21	CLA	A	1112	-	1/1/15/20	17/39/115/115	-
21	CLA	6	606	-	1/1/12/20	10/21/97/115	-
21	CLA	B	1239	-	1/1/15/20	14/39/115/115	-
23	SF4	A	3001	2,1	-	-	0/6/5/5
31	LMG	6	802	-	-	11/32/52/70	0/1/1/1
21	CLA	A	1110	-	1/1/13/20	8/27/103/115	-
24	BCR	F	4001	-	-	9/29/63/63	0/2/2/2
26	OCD	A	5003	-	-	2/16/16/16	-
21	CLA	B	1207	-	1/1/15/20	19/39/115/115	-
21	CLA	3	601	-	1/1/14/20	15/33/109/115	-
21	CLA	A	1124	-	1/1/14/20	13/33/109/115	-
29	3PH	F	5003	-	-	22/35/35/49	-
36	CHL	5	610	-	4/4/16/26	3/17/115/137	-
21	CLA	A	1119	-	1/1/15/20	16/39/115/115	-
21	CLA	B	1217	-	1/1/15/20	14/39/115/115	-
21	CLA	K	1404	-	1/1/11/20	7/15/91/115	-
27	LMU	A	5004	-	-	10/21/61/61	0/2/2/2
21	CLA	A	1117	-	1/1/15/20	19/39/115/115	-
21	CLA	B	1223	-	1/1/15/20	11/39/115/115	-
21	CLA	A	1135	-	1/1/12/20	8/23/99/115	-
25	LHG	4	801	-	-	17/33/33/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	613	-	1/1/11/20	7/15/91/115	-
21	CLA	B	1227	-	1/1/15/20	20/39/115/115	-
21	CLA	A	1127	-	1/1/15/20	14/39/115/115	-
21	CLA	B	1215	-	1/1/15/20	13/39/115/115	-
21	CLA	B	1022	-	1/1/15/20	11/39/115/115	-
21	CLA	O	1803	-	1/1/14/20	15/33/109/115	-
21	CLA	3	606	-	1/1/13/20	7/27/103/115	-
21	CLA	4	607	-	1/1/14/20	15/33/109/115	-
36	CHL	2	609	15	4/4/20/26	3/39/137/137	-
21	CLA	A	1106	-	1/1/15/20	13/39/115/115	-
21	CLA	A	1012	-	1/1/15/20	16/39/115/115	-
21	CLA	L	1504	-	1/1/12/20	10/21/97/115	-
21	CLA	1	613	-	1/1/11/20	5/15/91/115	-
24	BCR	K	4001	-	-	13/29/63/63	0/2/2/2
21	CLA	4	601	-	1/1/14/20	18/33/109/115	-
24	BCR	A	4001	-	-	13/29/63/63	0/2/2/2
21	CLA	2	608	-	1/1/12/20	9/21/97/115	-
21	CLA	A	1107	-	1/1/15/20	16/39/115/115	-
21	CLA	1	603	-	1/1/14/20	19/33/109/115	-
21	CLA	3	615	-	1/1/13/20	8/29/105/115	-
21	CLA	B	1220	-	1/1/13/20	14/27/103/115	-
21	CLA	2	607	25	1/1/14/20	10/33/109/115	-
21	CLA	B	1206	2	1/1/15/20	16/39/115/115	-
21	CLA	A	1125	-	1/1/15/20	17/39/115/115	-
21	CLA	B	1023	-	1/1/15/20	20/39/115/115	-
21	CLA	O	1802	-	1/1/10/20	2/4/80/115	-
27	LMU	B	5004	-	-	14/21/61/61	0/2/2/2
34	LUT	5	501	-	1/1/12/27	3/29/67/67	0/2/2/2
37	SQD	6	803	-	-	4/27/47/69	0/1/1/1
21	CLA	5	613	-	1/1/11/20	8/15/91/115	-
21	CLA	B	1211	-	1/1/15/20	15/39/115/115	-
24	BCR	B	4002	-	-	14/29/63/63	0/2/2/2
21	CLA	4	609	17	1/1/14/20	21/33/109/115	-
35	XAT	1	502	-	2/2/12/26	5/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LMK	2	807	-	-	7/37/37/60	-
21	CLA	3	614	-	1/1/10/20	4/12/88/115	-
24	BCR	B	4001	-	-	10/29/63/63	0/2/2/2
31	LMG	F	5002	-	-	17/45/65/70	0/1/1/1
24	BCR	3	504	-	-	12/29/63/63	0/2/2/2
21	CLA	G	1602	-	1/1/11/20	8/17/93/115	-
21	CLA	3	612	-	1/1/15/20	17/39/115/115	-
37	SQD	2	805	-	-	17/34/54/69	0/1/1/1
21	CLA	3	610	16	1/1/12/20	8/21/97/115	-
21	CLA	A	1109	-	1/1/15/20	17/39/115/115	-
25	LHG	1	803	-	-	13/35/35/53	-
34	LUT	1	501	-	-	4/29/67/67	0/2/2/2
21	CLA	A	1131	-	1/1/15/20	12/39/115/115	-
21	CLA	6	605	-	1/1/15/20	20/39/115/115	-
21	CLA	F	1302	-	1/1/11/20	8/20/96/115	-
21	CLA	1	601	-	1/1/15/20	12/39/115/115	-
24	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
21	CLA	1	602	-	1/1/11/20	9/17/93/115	-
24	BCR	O	4001	-	-	13/29/63/63	0/2/2/2
21	CLA	A	1111	-	1/1/15/20	10/39/115/115	-
21	CLA	2	615	-	1/1/15/20	19/39/115/115	-
21	CLA	A	1118	-	1/1/12/20	8/21/97/115	-
34	LUT	5	504	-	1/1/12/27	7/29/67/67	0/2/2/2
24	BCR	L	4001	-	-	11/29/63/63	0/2/2/2
21	CLA	3	607	-	1/1/14/20	13/33/109/115	-
29	3PH	5	804	-	-	12/29/29/49	-
21	CLA	2	603	-	1/1/15/20	16/39/115/115	-
21	CLA	3	611	-	1/1/15/20	12/39/115/115	-
21	CLA	4	605	-	1/1/15/20	15/39/115/115	-
24	BCR	2	503	-	-	15/29/63/63	0/2/2/2
25	LHG	A	5002	-	-	36/53/53/53	-
21	CLA	G	1603	-	1/1/11/20	5/15/91/115	-
21	CLA	6	604	-	1/1/14/20	14/33/109/115	-
21	CLA	A	1130	-	1/1/13/20	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	H	1702	-	1/1/11/20	11/17/93/115	-
31	LMG	3	803	-	-	19/45/65/70	0/1/1/1
21	CLA	K	1403	-	1/1/11/20	9/19/95/115	-
21	CLA	B	1208	-	1/1/14/20	13/33/109/115	-
25	LHG	2	801	21	-	24/39/39/53	-
36	CHL	2	613	-	3/3/16/26	1/15/113/137	-
21	CLA	A	1133	-	1/1/15/20	16/39/115/115	-
21	CLA	A	1013	-	1/1/15/20	13/39/115/115	-
21	CLA	3	605	-	1/1/15/20	16/39/115/115	-
21	CLA	A	1101	-	1/1/15/20	20/39/115/115	-
21	CLA	A	1139	-	1/1/15/20	14/39/115/115	-
21	CLA	O	1801	-	1/1/9/20	5/6/78/115	-
21	CLA	B	1205	-	1/1/15/20	13/39/115/115	-
21	CLA	B	1224	-	1/1/15/20	17/39/115/115	-
21	CLA	2	601	-	1/1/15/20	20/39/115/115	-
24	BCR	3	503	-	-	12/29/63/63	0/2/2/2
21	CLA	B	1209	-	1/1/11/20	6/17/93/115	-
21	CLA	B	1229	-	1/1/15/20	13/39/115/115	-
33	PTY	L	5003	-	-	7/22/22/53	-
24	BCR	1	504	-	-	12/29/63/63	0/2/2/2
21	CLA	B	1237	-	1/1/15/20	18/39/115/115	-
21	CLA	4	606	-	1/1/12/20	10/21/97/115	-
21	CLA	L	1501	-	1/1/15/20	18/39/115/115	-
24	BCR	B	4006	-	-	7/29/63/63	0/2/2/2
21	CLA	B	1232	-	1/1/13/20	12/27/103/115	-
21	CLA	A	1134	1	1/1/13/20	13/27/103/115	-
33	PTY	3	807	-	-	8/29/29/53	-
24	BCR	H	4001	-	-	19/29/63/63	0/2/2/2
24	BCR	J	4001	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1140	-	1/1/14/20	15/35/111/115	-
21	CLA	3	608	-	1/1/15/20	16/39/115/115	-
21	CLA	A	1115	-	1/1/14/20	14/33/109/115	-
21	CLA	B	1203	-	1/1/15/20	16/39/115/115	-
21	CLA	B	1235	-	1/1/14/20	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	6	602	-	1/1/12/20	8/21/97/115	-
24	BCR	A	4002	-	-	17/29/63/63	0/2/2/2
25	LHG	B	5001	-	-	34/46/46/53	-
25	LHG	2	802	-	-	26/47/47/53	-
21	CLA	B	1201	-	1/1/11/20	11/19/95/115	-
21	CLA	4	604	-	1/1/14/20	12/33/109/115	-
24	BCR	A	4006	-	-	19/29/63/63	0/2/2/2
28	DGD	2	806	-	-	12/28/68/95	0/2/2/2
21	CLA	5	612	18	1/1/11/20	11/17/93/115	-
24	BCR	3	506	-	-	9/29/63/63	0/2/2/2
29	3PH	B	5003	-	-	24/32/32/49	-
36	CHL	5	609	-	4/4/20/26	4/39/137/137	-
21	CLA	G	1601	-	1/1/11/20	10/18/94/115	-
39	P3H	2	808	-	-	19/44/68/68	0/1/1/1
24	BCR	F	4002	-	-	13/29/63/63	0/2/2/2
21	CLA	B	1210	-	1/1/15/20	22/39/115/115	-
21	CLA	B	1225	-	1/1/15/20	16/39/115/115	-
21	CLA	6	601	-	1/1/14/20	16/33/109/115	-
21	CLA	B	1202	-	1/1/15/20	18/39/115/115	-
25	LHG	5	801	-	-	22/47/47/53	-
21	CLA	2	604	15	1/1/15/20	19/39/115/115	-
21	CLA	K	1402	-	1/1/13/20	13/27/103/115	-
27	LMU	A	5005	-	-	11/21/61/61	0/2/2/2
21	CLA	1	606	-	1/1/12/20	8/21/97/115	-
21	CLA	B	1231	-	1/1/14/20	14/33/109/115	-
36	CHL	1	609	14	4/4/20/26	6/39/137/137	-
31	LMG	4	803	-	-	11/34/54/70	0/1/1/1
24	BCR	4	503	-	-	11/29/63/63	0/2/2/2
21	CLA	A	1114	-	1/1/13/20	8/27/103/115	-
21	CLA	4	603	-	1/1/15/20	11/39/115/115	-
21	CLA	5	602	-	1/1/11/20	8/17/93/115	-
21	CLA	2	605	-	1/1/15/20	16/39/115/115	-
21	CLA	6	603	-	1/1/13/20	6/27/103/115	-
25	LHG	1	801	-	-	31/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B	1219	-	1/1/15/20	16/39/115/115	-

The worst 5 of 1611 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	5	501	LUT	C24-C25	16.44	1.52	1.33
34	5	504	LUT	C24-C25	15.96	1.52	1.33
34	5	503	LUT	C24-C25	15.44	1.51	1.33
34	5	502	LUT	C24-C25	15.37	1.51	1.33
34	6	501	LUT	C24-C25	15.22	1.51	1.33

The worst 5 of 4340 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	6	504	XAT	C20-C13-C14	-27.29	78.60	122.82
35	6	504	XAT	C20-C13-C12	-25.51	79.12	118.09
35	6	504	XAT	C12-C13-C14	24.61	157.72	119.01
34	5	501	LUT	C37-C21-C36	-19.82	79.03	107.87
34	5	504	LUT	C37-C21-C36	-19.68	79.24	107.87

5 of 236 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	1011	CL0	NC
20	A	1011	CL0	NA
20	A	1011	CL0	ND
21	A	1012	CLA	ND
21	A	1013	CLA	ND

5 of 3569 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1011	CL0	C2-C1-O2A-CGA
21	A	1101	CLA	C1A-C2A-CAA-CBA
21	A	1102	CLA	C3A-C2A-CAA-CBA
21	A	1102	CLA	CHA-CBD-CGD-O1D
21	A	1102	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

248 monomers are involved in 1116 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	A	5001	LHG	3	0
24	B	4004	BCR	3	0
33	6	804	PTY	1	0
21	A	1129	CLA	1	0
21	B	1221	CLA	2	0
24	I	4001	BCR	9	0
21	A	1104	CLA	4	0
31	3	802	LMG	2	0
34	5	503	LUT	7	0
21	A	1102	CLA	5	0
22	A	2001	PQN	3	0
21	H	1701	CLA	4	0
21	6	609	CLA	1	0
32	L	5002	4RF	2	0
34	3	501	LUT	9	0
24	L	4002	BCR	2	0
21	A	1141	CLA	4	0
36	2	610	CHL	2	0
34	6	501	LUT	22	0
21	3	602	CLA	1	0
21	B	1021	CLA	3	0
21	1	607	CLA	1	0
21	3	613	CLA	1	0
21	A	1113	CLA	14	0
21	L	1503	CLA	5	0
21	A	1126	CLA	8	0
21	5	603	CLA	6	0
21	A	1136	CLA	3	0
21	F	1301	CLA	2	0
21	4	615	CLA	1	0
21	5	607	CLA	2	0
21	6	607	CLA	4	0
21	A	1137	CLA	2	0
21	2	612	CLA	3	0
21	B	1216	CLA	2	0
21	B	1212	CLA	17	0
21	B	1230	CLA	5	0
21	B	1238	CLA	3	0
28	3	804	DGD	1	0
34	4	501	LUT	4	0
36	1	610	CHL	4	0
21	5	614	CLA	8	0
24	A	4007	BCR	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	3	805	DGD	5	0
24	A	4003	BCR	7	0
21	A	1108	CLA	3	0
21	A	1122	CLA	2	0
21	B	1213	CLA	3	0
21	4	602	CLA	3	0
24	B	4005	BCR	2	0
21	A	1128	CLA	5	0
21	5	605	CLA	15	0
24	J	4002	BCR	4	0
33	5	803	PTY	10	0
36	2	609	CHL	3	0
35	6	504	XAT	9	0
21	B	1236	CLA	2	0
25	2	803	LHG	2	0
21	1	612	CLA	3	0
21	B	1214	CLA	3	0
34	2	501	LUT	6	0
31	4	802	LMG	2	0
21	5	601	CLA	4	0
21	A	1103	CLA	3	0
21	B	1204	CLA	2	0
20	A	1011	CL0	10	0
21	1	611	CLA	13	0
21	A	1105	CLA	4	0
24	I	4002	BCR	10	0
24	B	4003	BCR	6	0
21	6	612	CLA	7	0
21	A	1116	CLA	10	0
21	A	1123	CLA	1	0
21	L	1502	CLA	13	0
21	B	1218	CLA	2	0
34	5	502	LUT	13	0
21	B	1240	CLA	4	0
35	4	502	XAT	3	0
21	B	1226	CLA	5	0
21	A	1120	CLA	10	0
33	O	5002	PTY	5	0
24	G	4001	BCR	20	0
39	5	806	P3H	1	0
21	K	1401	CLA	6	0
21	B	1234	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	J	1901	CLA	3	0
35	2	502	XAT	3	0
36	4	611	CHL	1	0
32	5	805	4RF	1	0
35	6	502	XAT	5	0
21	A	1121	CLA	31	0
21	5	604	CLA	28	0
29	5	807	3PH	2	0
21	6	608	CLA	2	0
21	1	605	CLA	2	0
21	3	603	CLA	8	0
21	A	1132	CLA	20	0
27	6	805	LMU	1	0
24	A	4005	BCR	2	0
36	6	610	CHL	7	0
22	B	2002	PQN	7	0
36	2	611	CHL	3	0
37	3	806	SQD	2	0
21	A	1138	CLA	5	0
21	B	1228	CLA	2	0
25	F	5001	LHG	2	0
21	1	608	CLA	1	0
21	1	604	CLA	6	0
21	5	608	CLA	12	0
31	1	804	LMG	1	0
28	B	5002	DGD	5	0
21	B	1222	CLA	3	0
36	3	604	CHL	3	0
21	5	606	CLA	24	0
35	3	502	XAT	7	0
21	A	1112	CLA	14	0
21	6	606	CLA	13	0
21	B	1239	CLA	8	0
31	6	802	LMG	12	0
21	A	1110	CLA	1	0
24	F	4001	BCR	19	0
21	B	1207	CLA	16	0
21	3	601	CLA	2	0
21	A	1124	CLA	3	0
36	5	610	CHL	7	0
21	A	1119	CLA	8	0
21	B	1217	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	K	1404	CLA	9	0
27	A	5004	LMU	1	0
21	B	1223	CLA	6	0
21	A	1135	CLA	6	0
21	6	613	CLA	8	0
21	B	1227	CLA	5	0
21	A	1127	CLA	1	0
21	B	1215	CLA	6	0
21	B	1022	CLA	10	0
21	O	1803	CLA	1	0
21	3	606	CLA	3	0
21	4	607	CLA	4	0
24	K	4001	BCR	8	0
21	A	1106	CLA	3	0
21	A	1012	CLA	9	0
21	L	1504	CLA	8	0
21	4	601	CLA	3	0
24	A	4001	BCR	9	0
21	A	1107	CLA	3	0
21	1	603	CLA	1	0
21	B	1220	CLA	2	0
21	B	1206	CLA	11	0
21	A	1125	CLA	4	0
21	B	1023	CLA	25	0
27	B	5004	LMU	2	0
34	5	501	LUT	5	0
37	6	803	SQD	1	0
21	5	613	CLA	7	0
21	B	1211	CLA	1	0
24	B	4002	BCR	4	0
21	4	609	CLA	3	0
35	1	502	XAT	2	0
24	B	4001	BCR	19	0
31	F	5002	LMG	3	0
24	3	504	BCR	10	0
21	G	1602	CLA	7	0
21	3	612	CLA	6	0
37	2	805	SQD	2	0
21	3	610	CLA	19	0
21	A	1109	CLA	3	0
25	1	803	LHG	1	0
34	1	501	LUT	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	1131	CLA	3	0
21	6	605	CLA	9	0
21	1	601	CLA	25	0
24	A	4004	BCR	8	0
21	1	602	CLA	4	0
24	O	4001	BCR	7	0
21	A	1111	CLA	2	0
21	A	1118	CLA	1	0
34	5	504	LUT	16	0
24	L	4001	BCR	3	0
29	5	804	3PH	3	0
21	2	603	CLA	2	0
21	4	605	CLA	1	0
24	2	503	BCR	1	0
25	A	5002	LHG	3	0
21	G	1603	CLA	1	0
21	6	604	CLA	4	0
21	A	1130	CLA	2	0
31	3	803	LMG	17	0
21	K	1403	CLA	6	0
21	B	1208	CLA	19	0
25	2	801	LHG	3	0
21	A	1133	CLA	3	0
21	A	1013	CLA	8	0
21	3	605	CLA	5	0
21	A	1101	CLA	4	0
21	A	1139	CLA	5	0
21	O	1801	CLA	2	0
21	B	1205	CLA	3	0
21	B	1224	CLA	2	0
21	2	601	CLA	2	0
24	3	503	BCR	2	0
21	B	1209	CLA	4	0
21	B	1229	CLA	3	0
24	1	504	BCR	5	0
21	B	1237	CLA	2	0
21	L	1501	CLA	3	0
24	B	4006	BCR	4	0
21	B	1232	CLA	2	0
21	A	1134	CLA	6	0
24	H	4001	BCR	5	0
24	J	4001	BCR	3	0

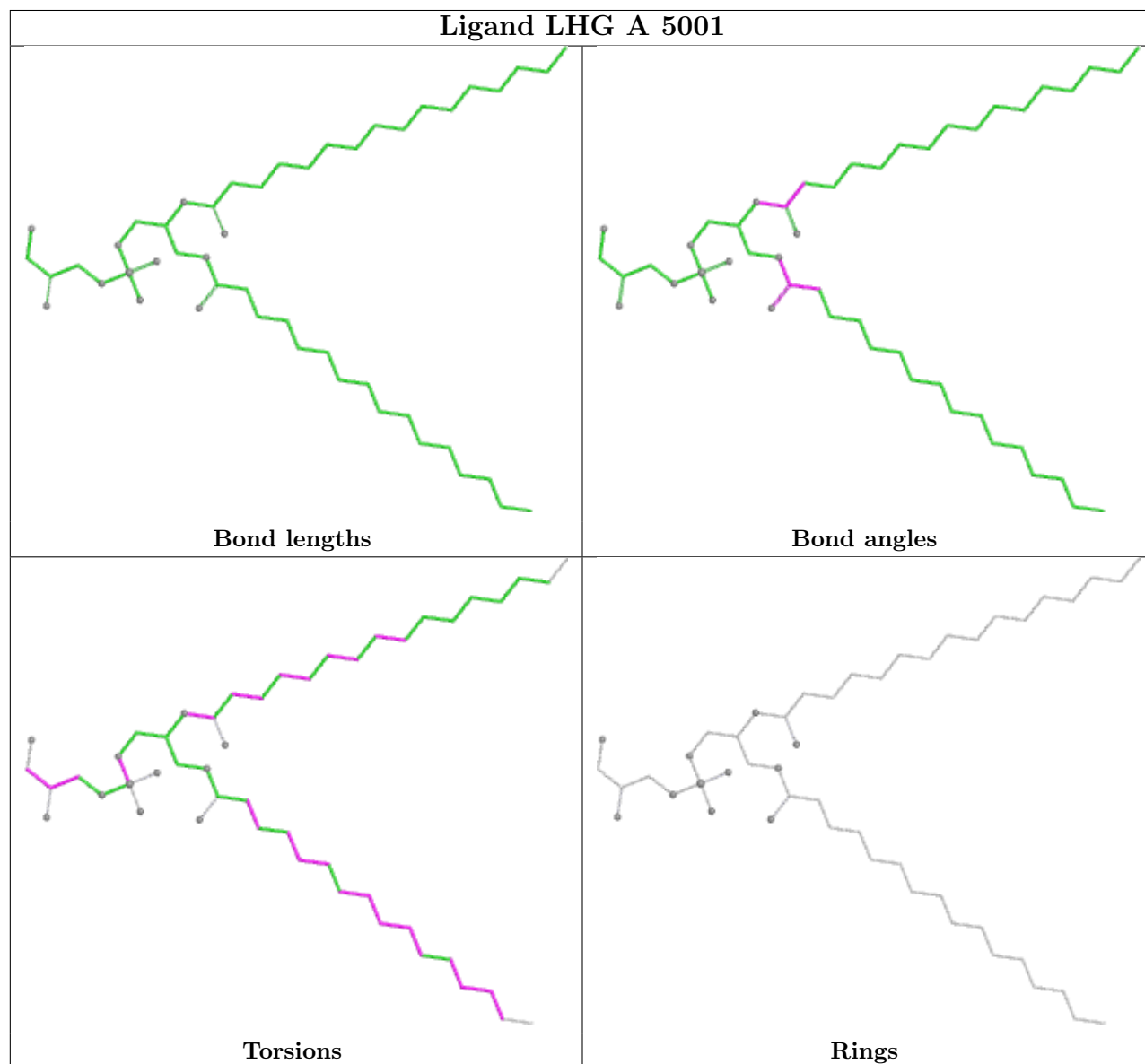
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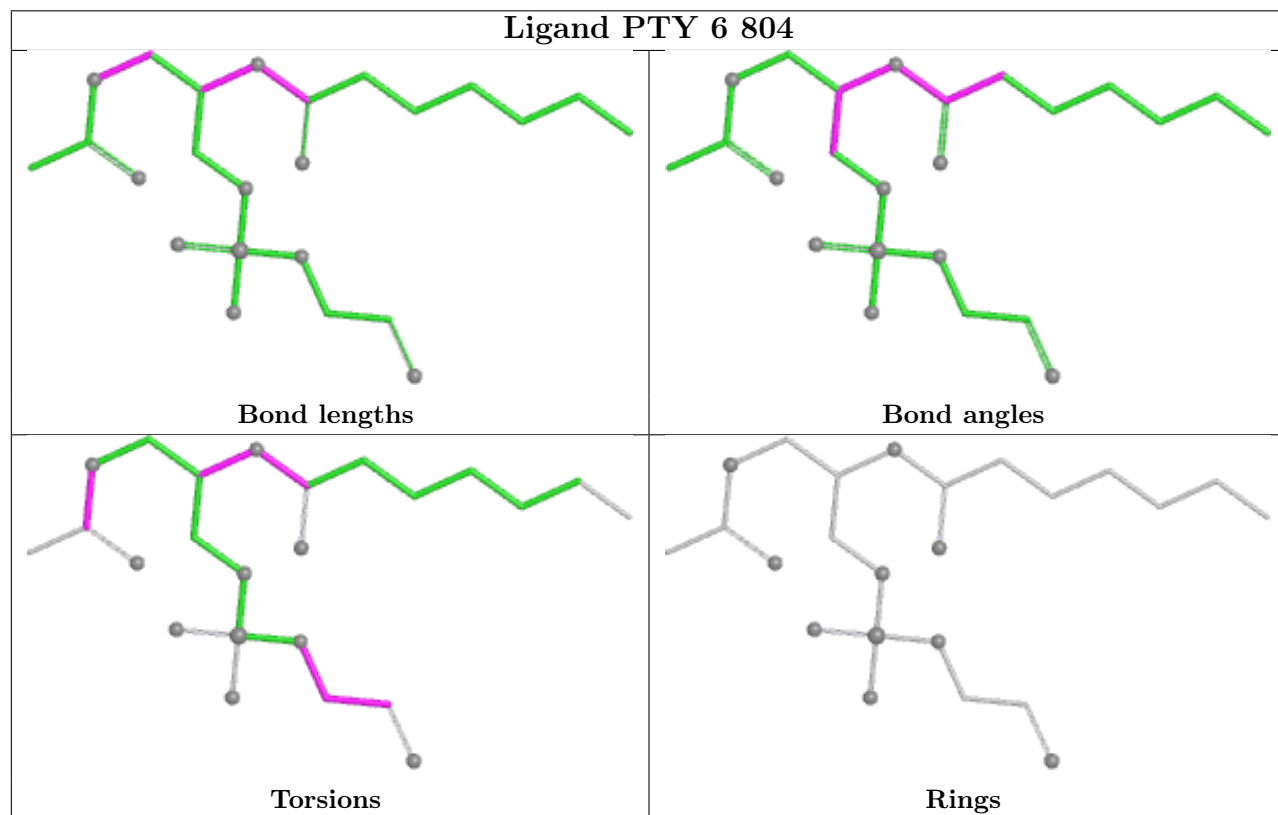
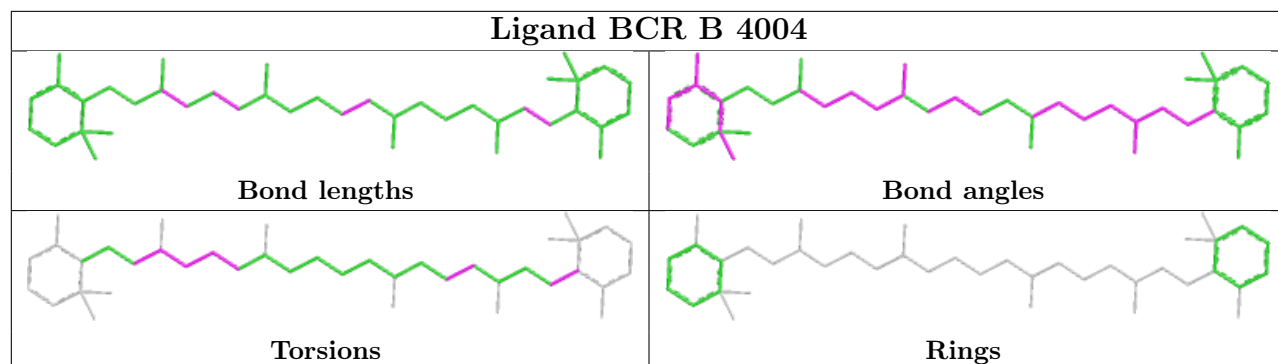
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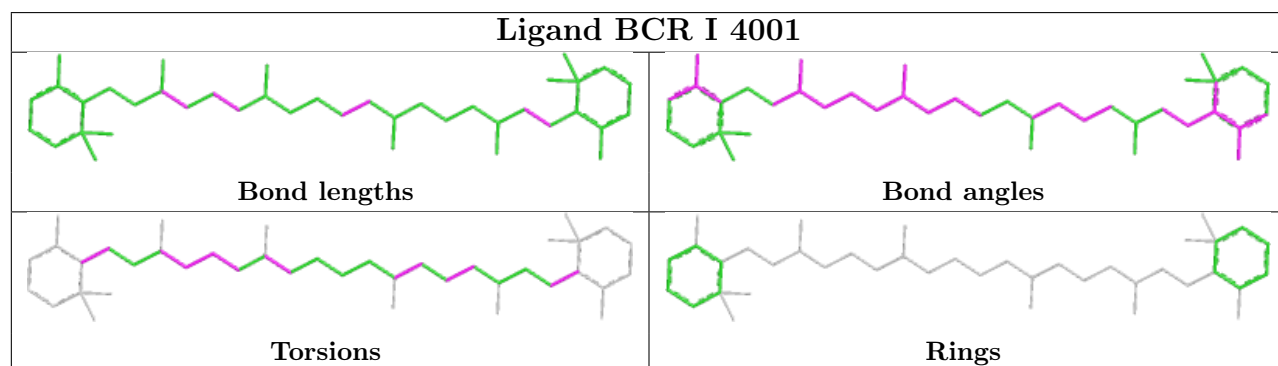
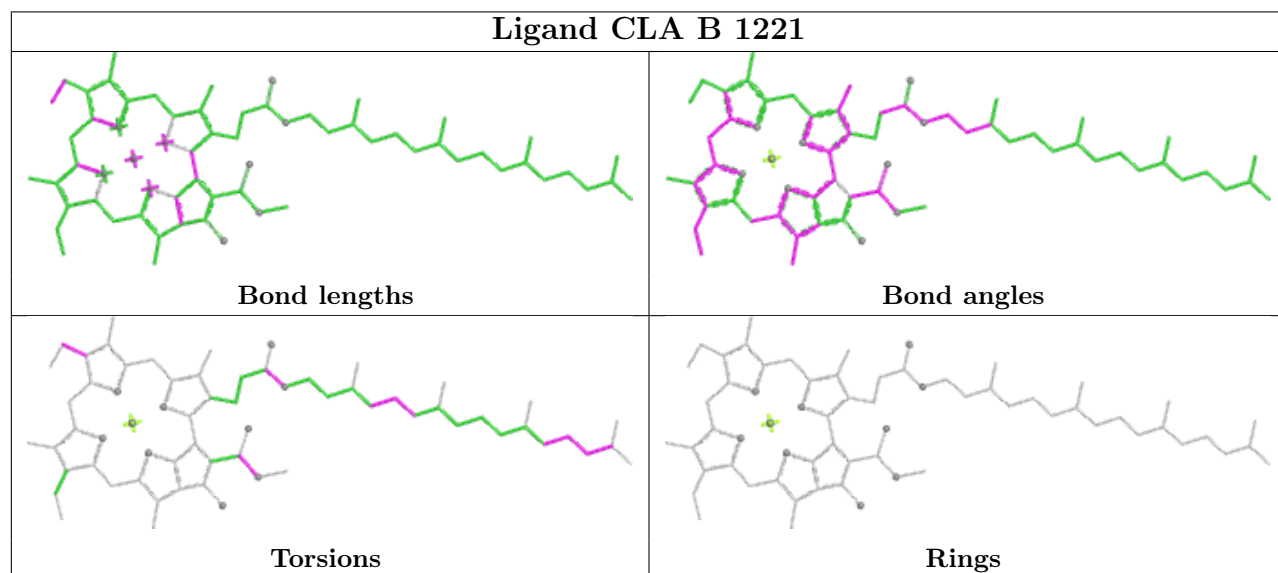
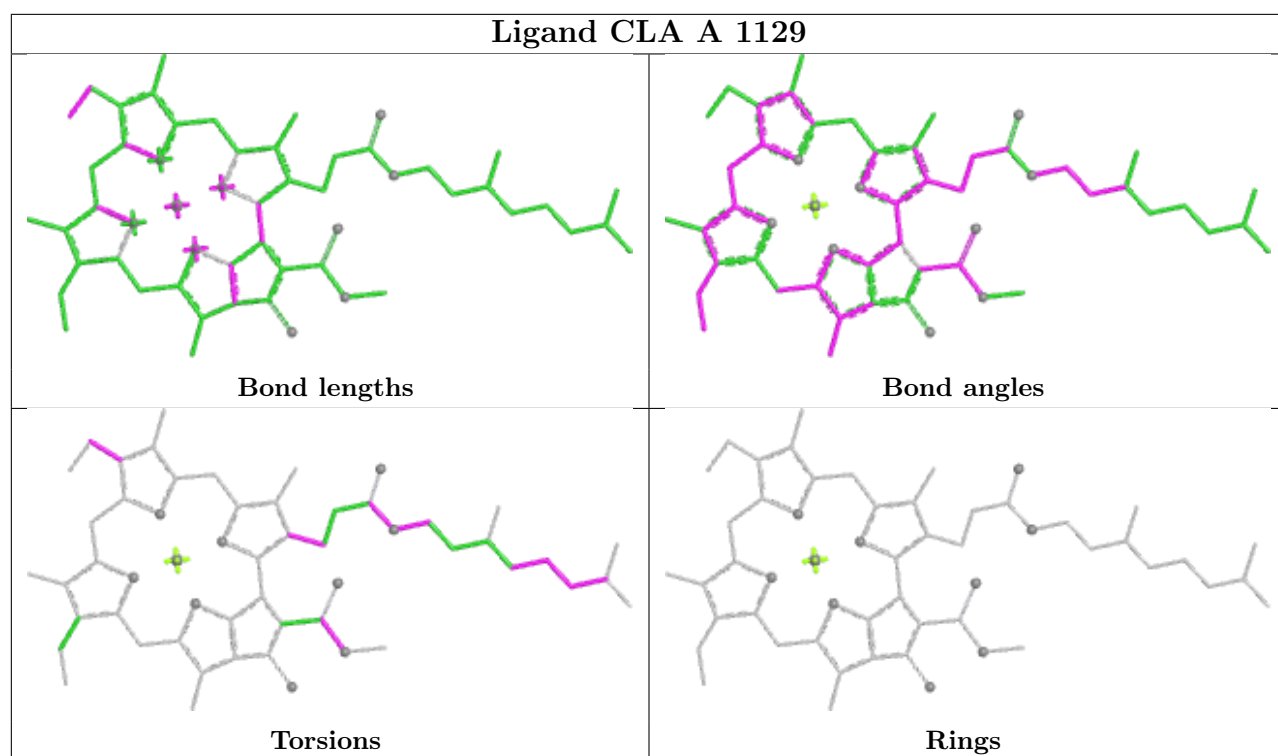
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	3	608	CLA	4	0
21	A	1115	CLA	12	0
21	B	1203	CLA	5	0
21	B	1235	CLA	5	0
21	6	602	CLA	10	0
24	A	4002	BCR	6	0
25	B	5001	LHG	3	0
25	2	802	LHG	3	0
21	4	604	CLA	13	0
24	A	4006	BCR	2	0
28	2	806	DGD	2	0
21	5	612	CLA	4	0
24	3	506	BCR	3	0
29	B	5003	3PH	2	0
36	5	609	CHL	33	0
21	G	1601	CLA	10	0
24	F	4002	BCR	5	0
21	B	1210	CLA	4	0
21	B	1225	CLA	5	0
21	6	601	CLA	25	0
21	B	1202	CLA	1	0
25	5	801	LHG	11	0
21	2	604	CLA	5	0
21	K	1402	CLA	14	0
27	A	5005	LMU	1	0
21	1	606	CLA	2	0
21	B	1231	CLA	5	0
36	1	609	CHL	3	0
24	4	503	BCR	1	0
21	A	1114	CLA	16	0
21	4	603	CLA	3	0
21	5	602	CLA	1	0
21	2	605	CLA	1	0
21	6	603	CLA	20	0
25	1	801	LHG	4	0
21	B	1219	CLA	5	0

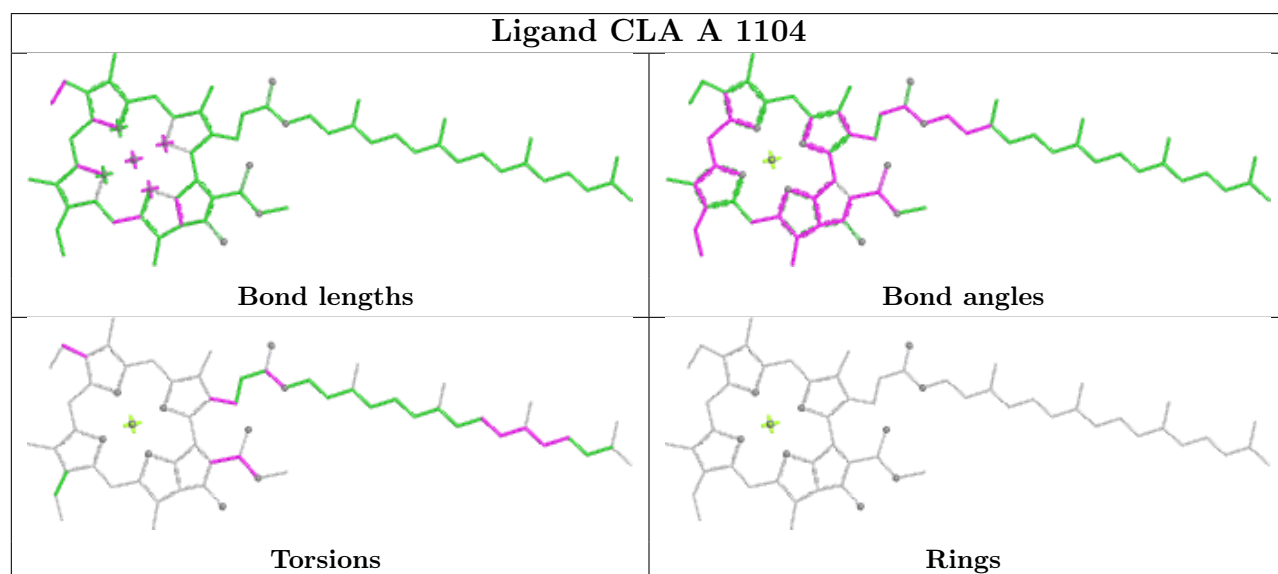
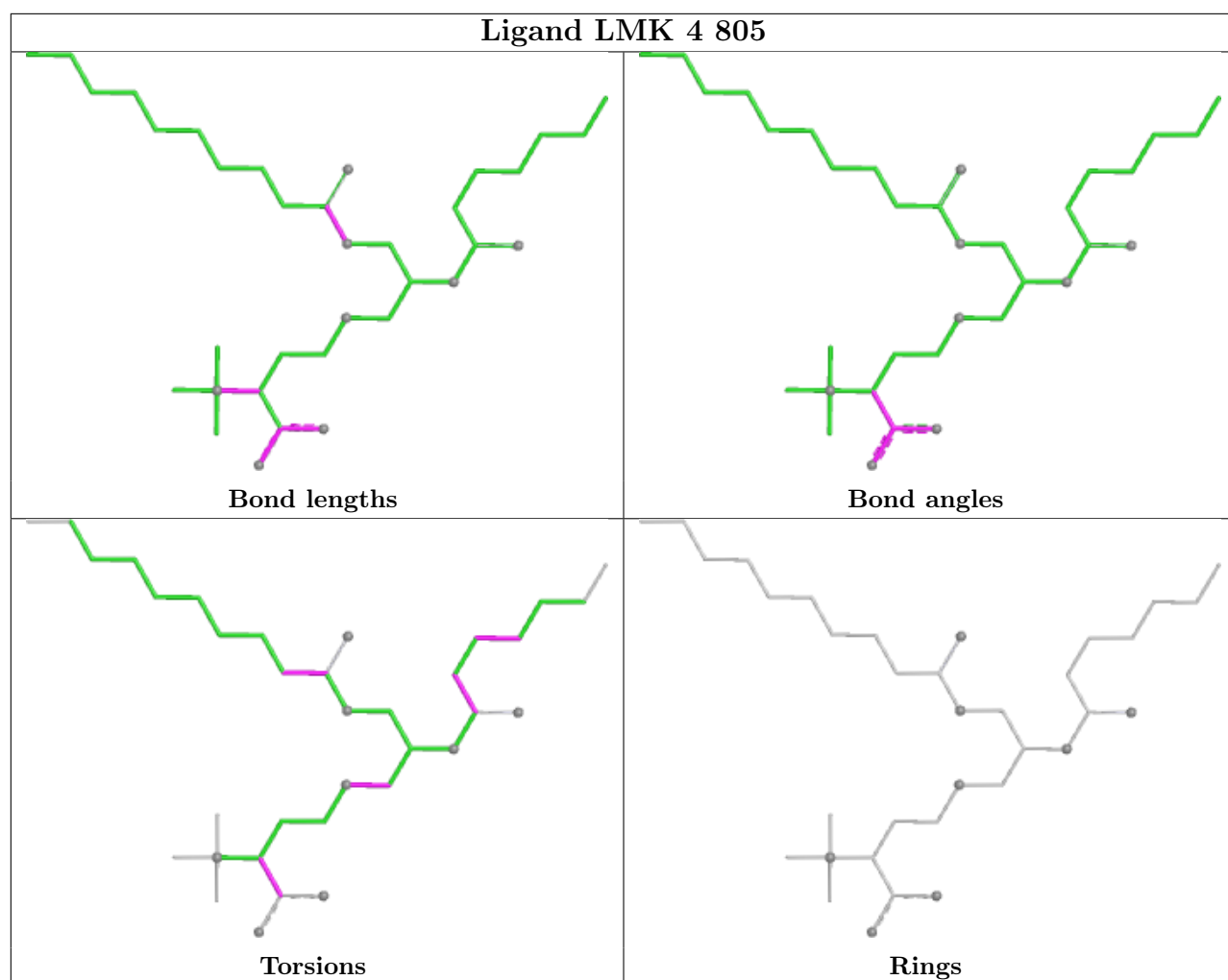
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

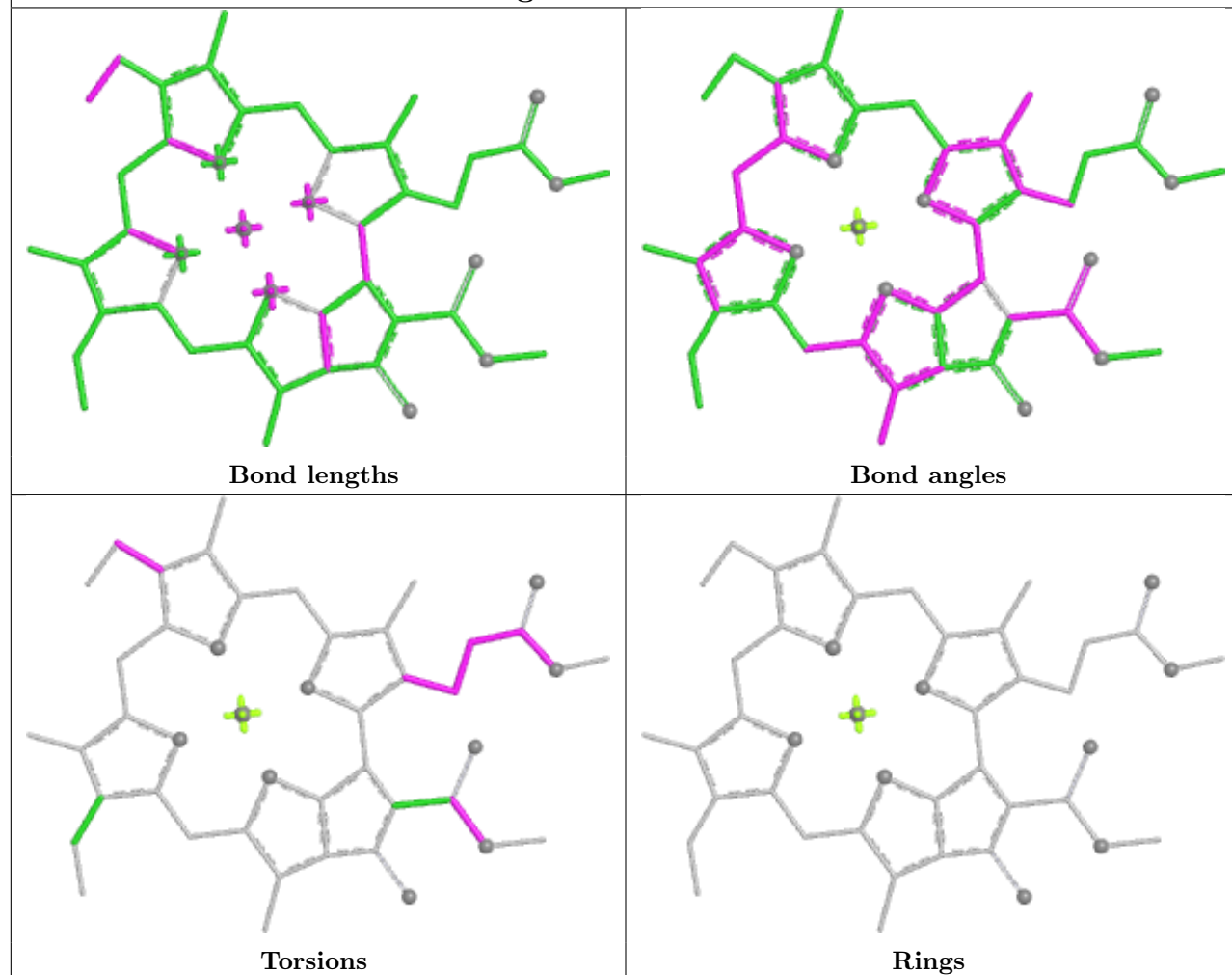




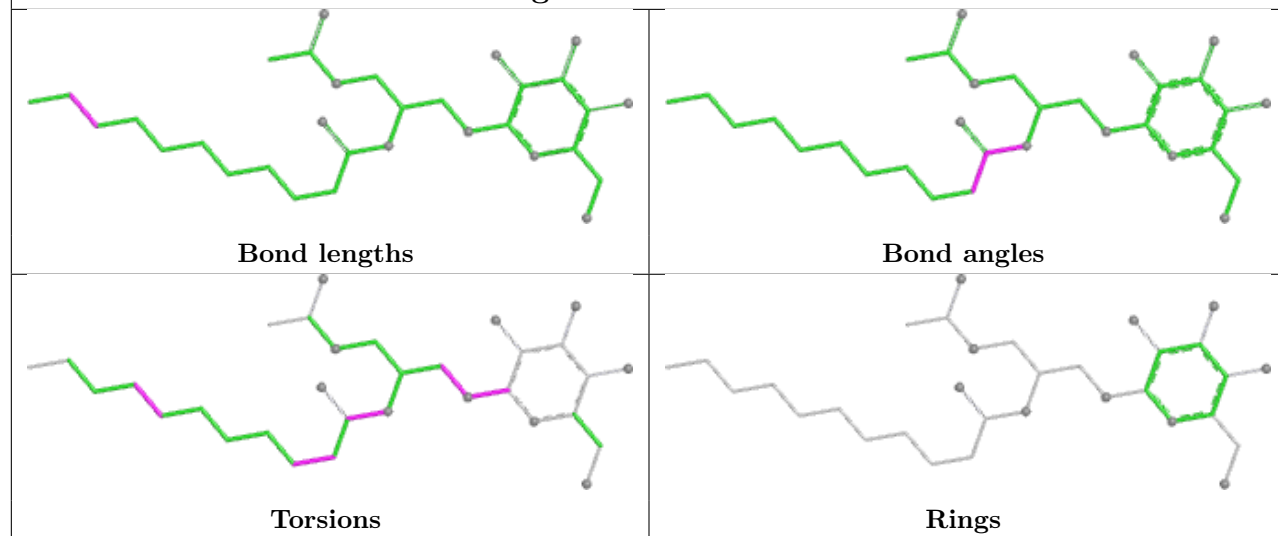


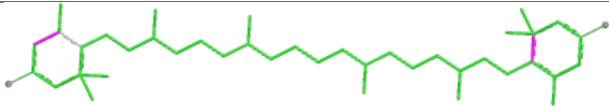
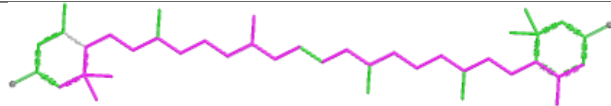
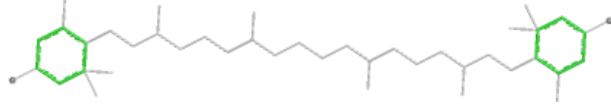


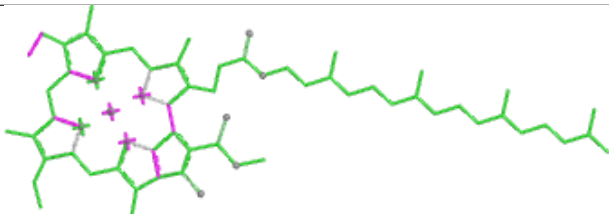
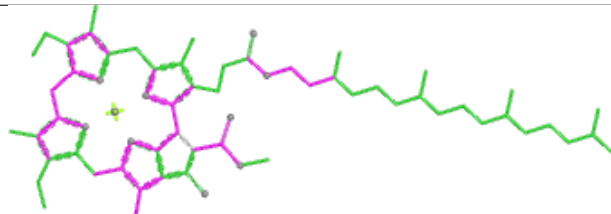
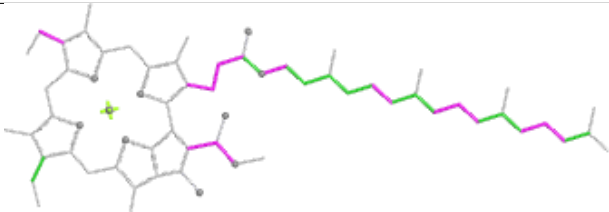
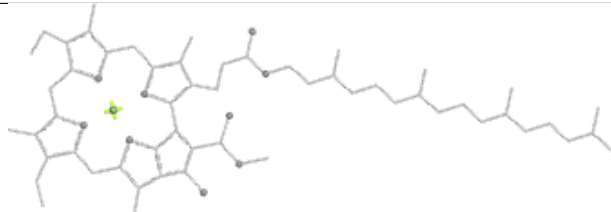
Ligand CLA 4 608

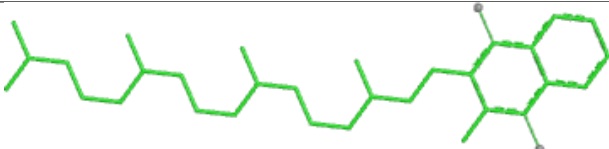
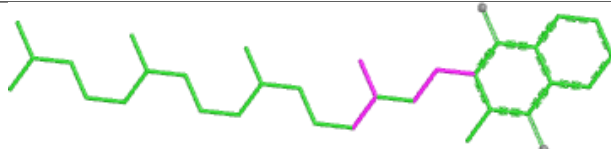
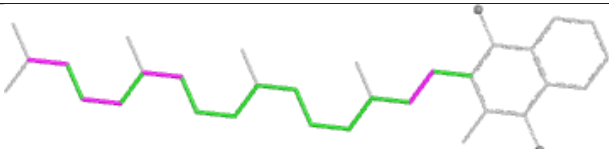
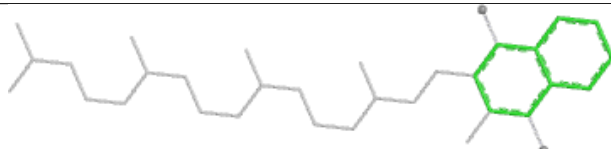


Ligand LMG 3 802

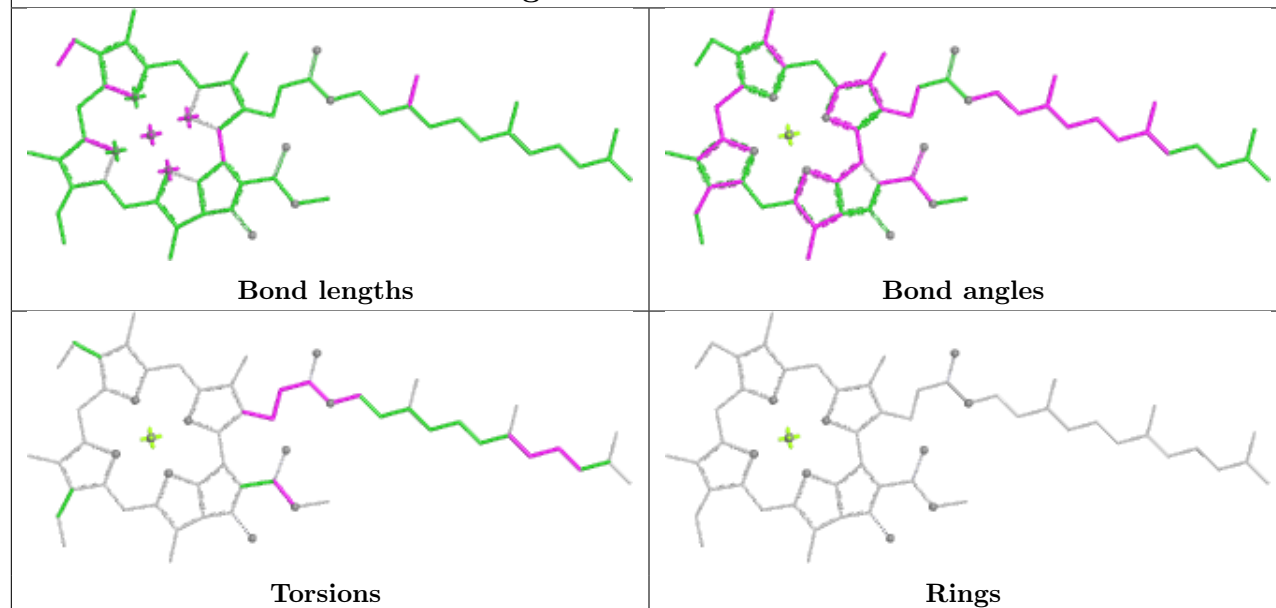


Ligand LUT 5 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

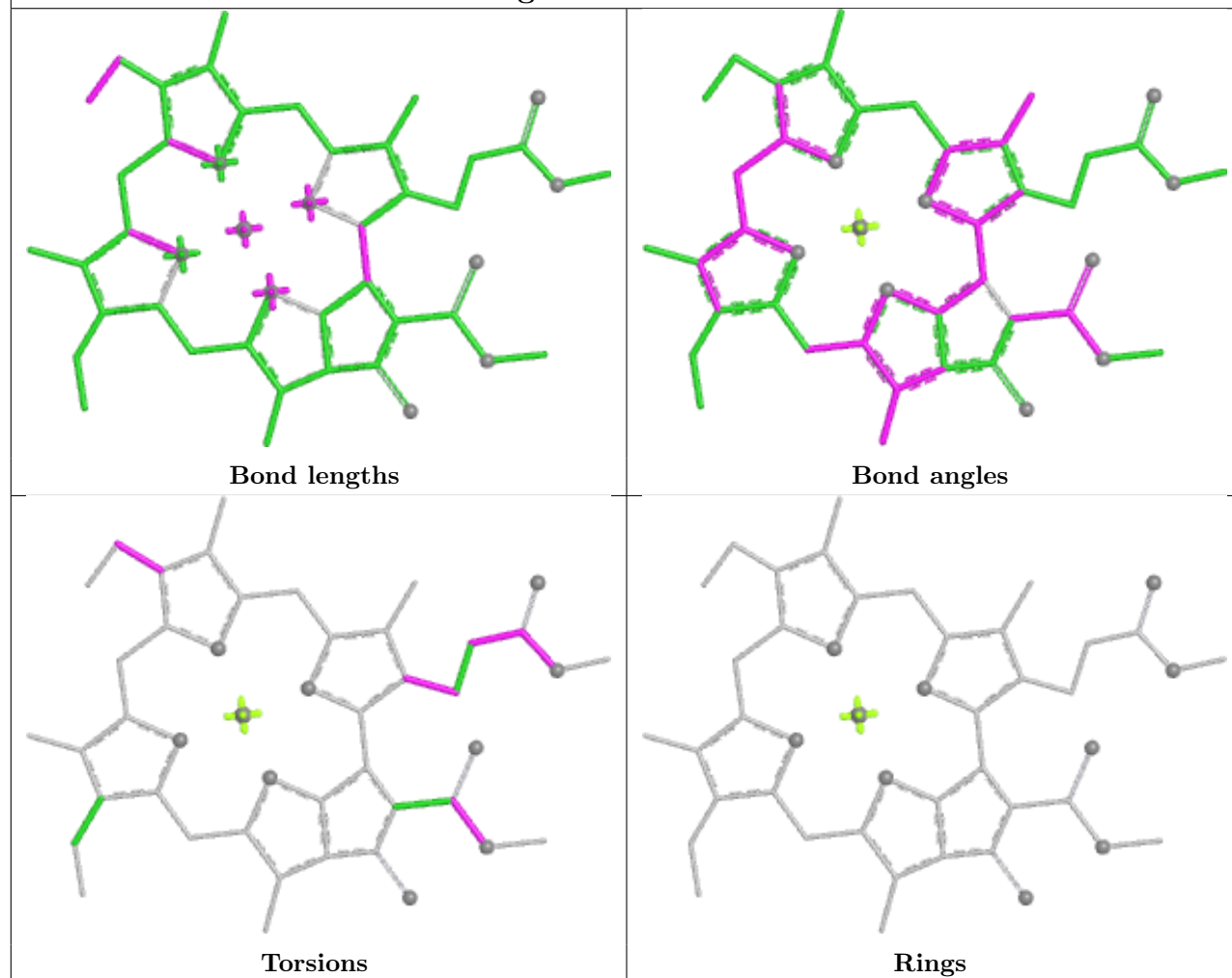
Ligand CLA A 1102	
	
Bond lengths	Bond angles
	
Torsions	Rings

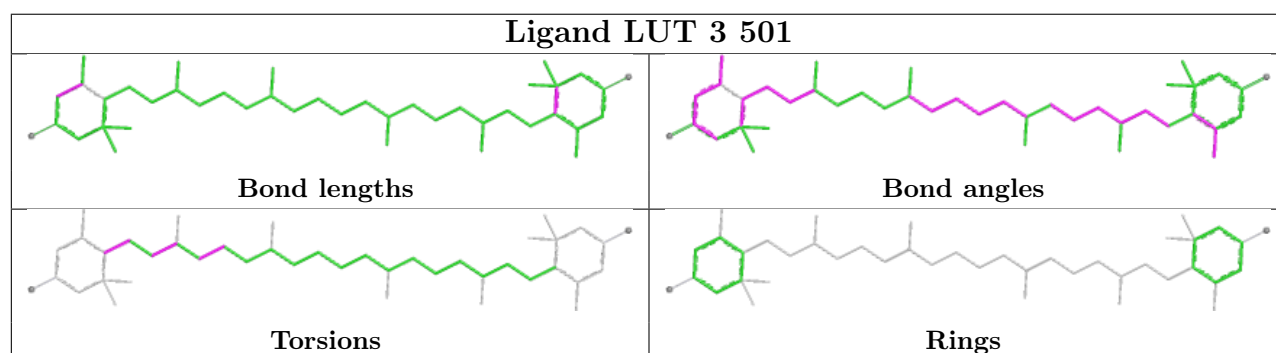
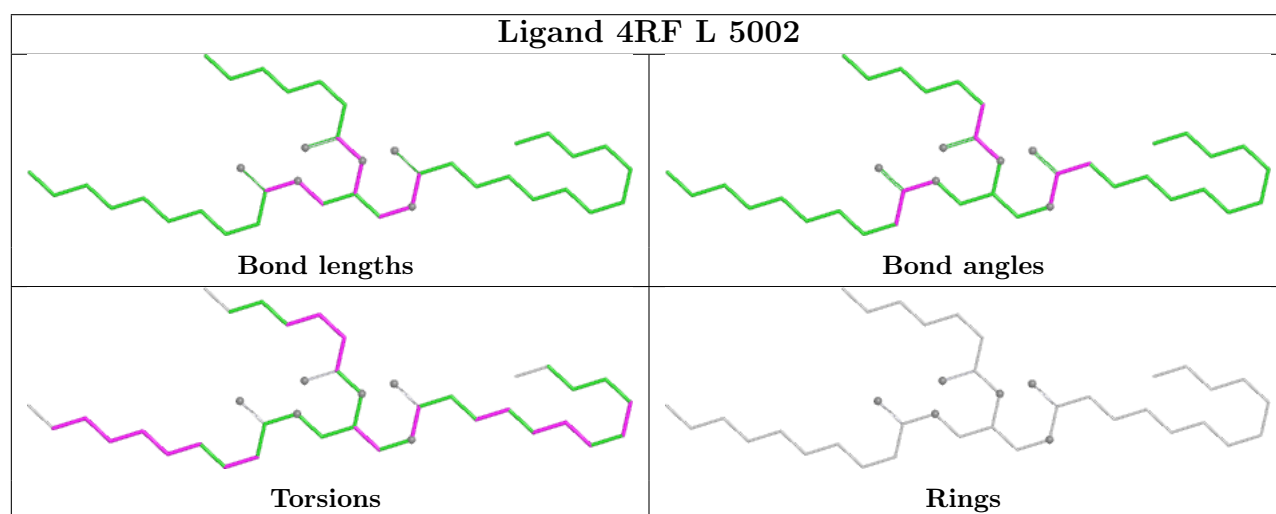
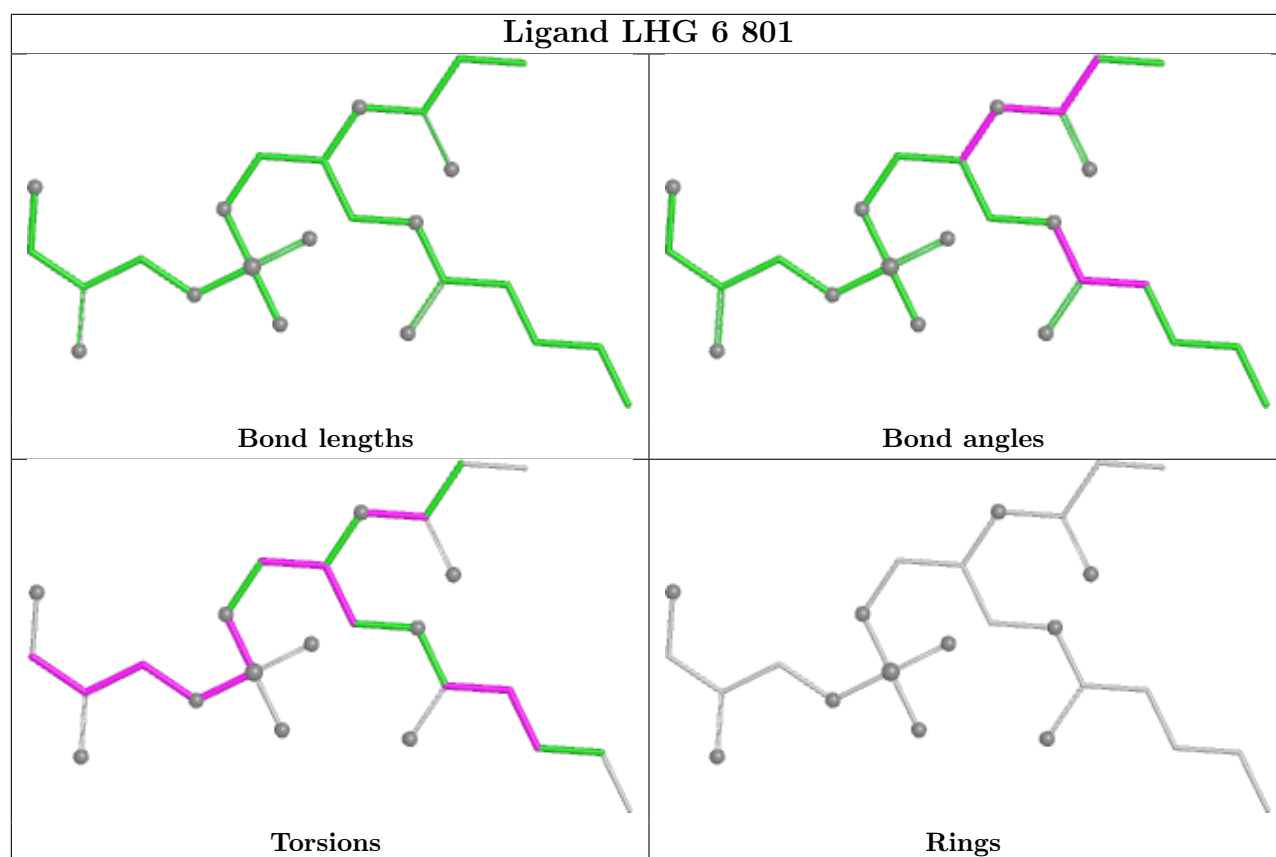
Ligand PQN A 2001	
	
Bond lengths	Bond angles
	
Torsions	Rings

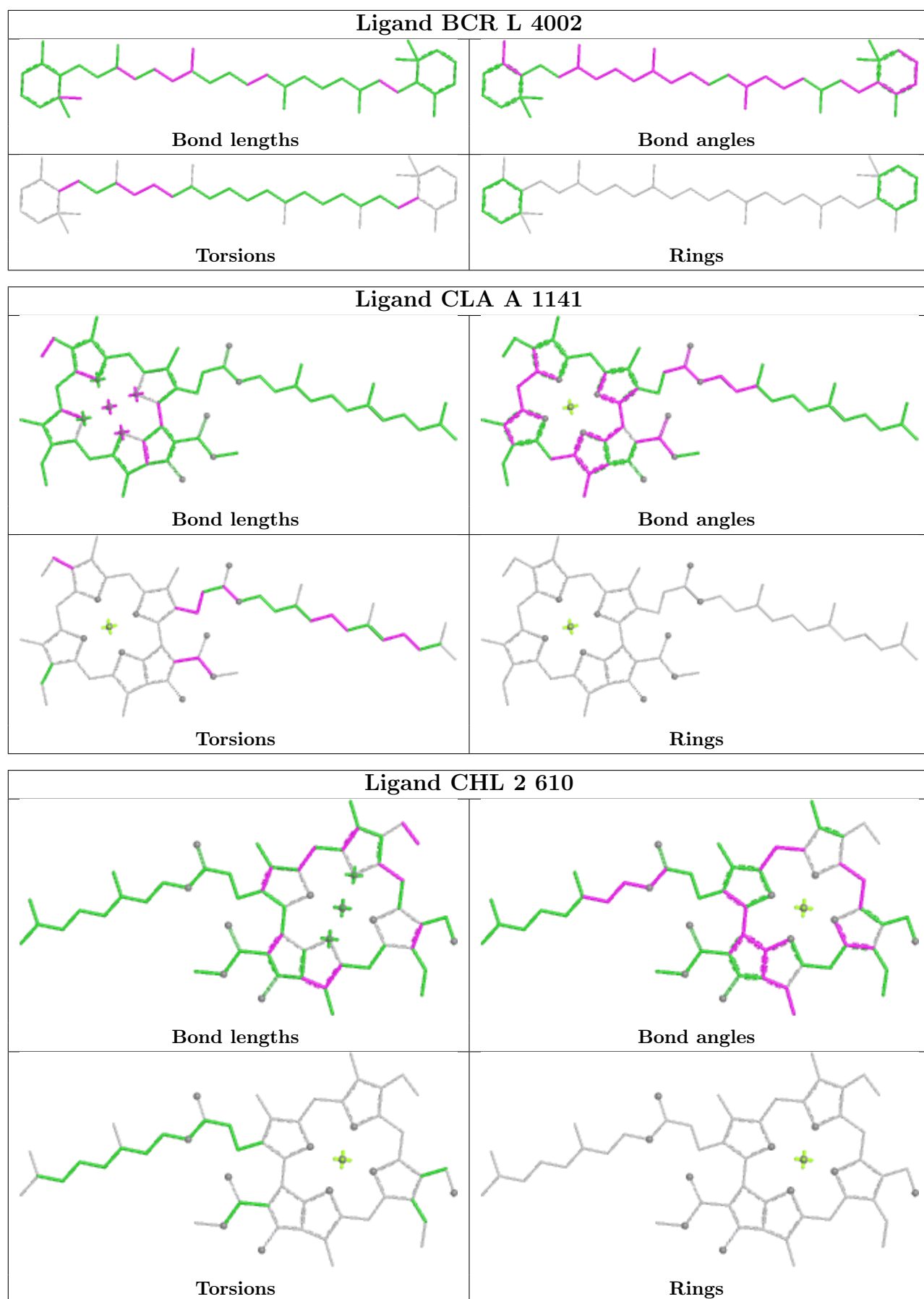
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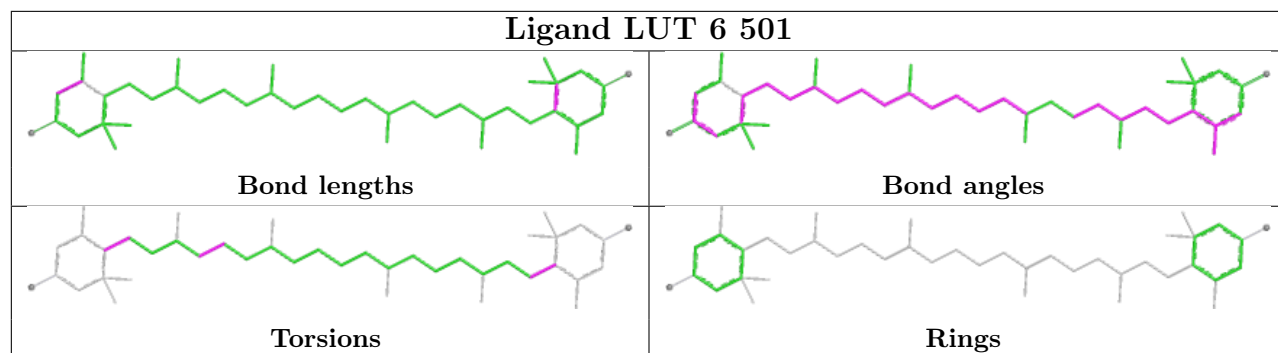
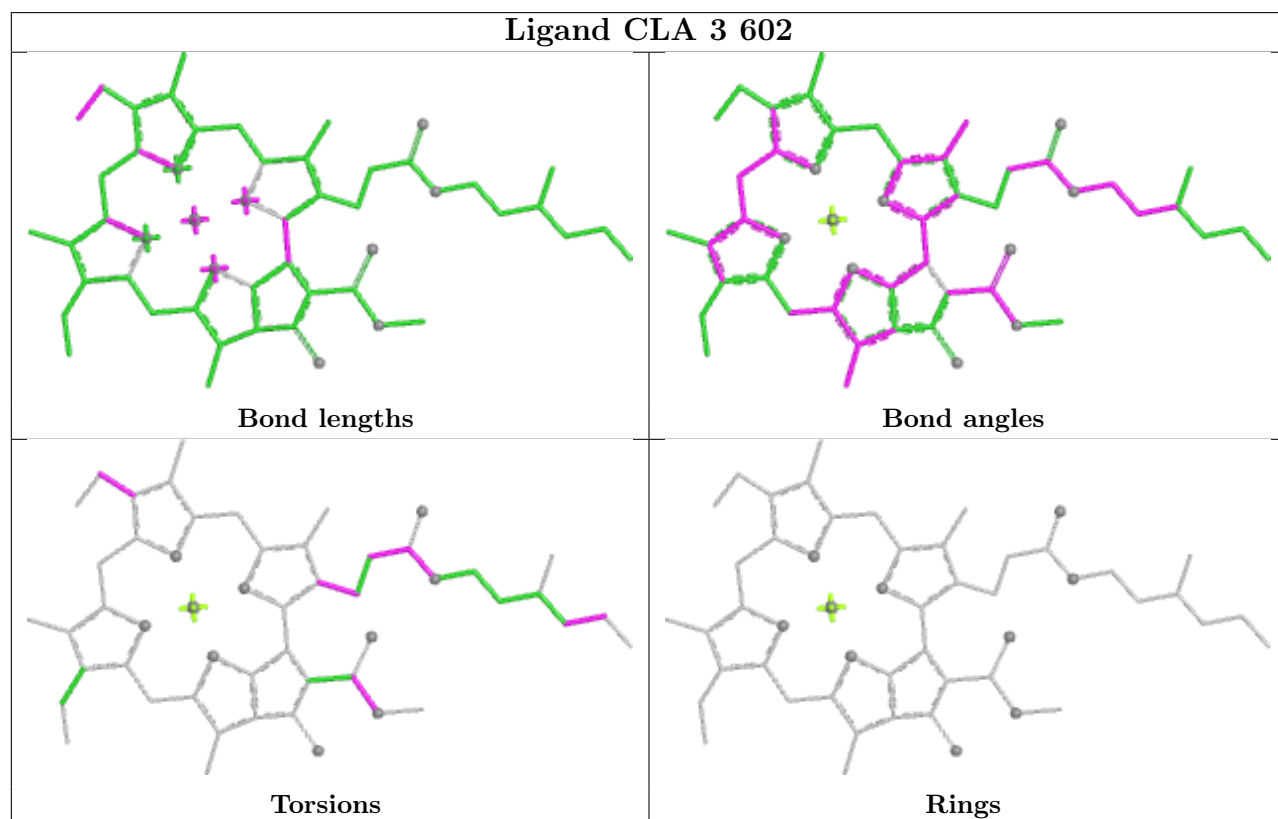
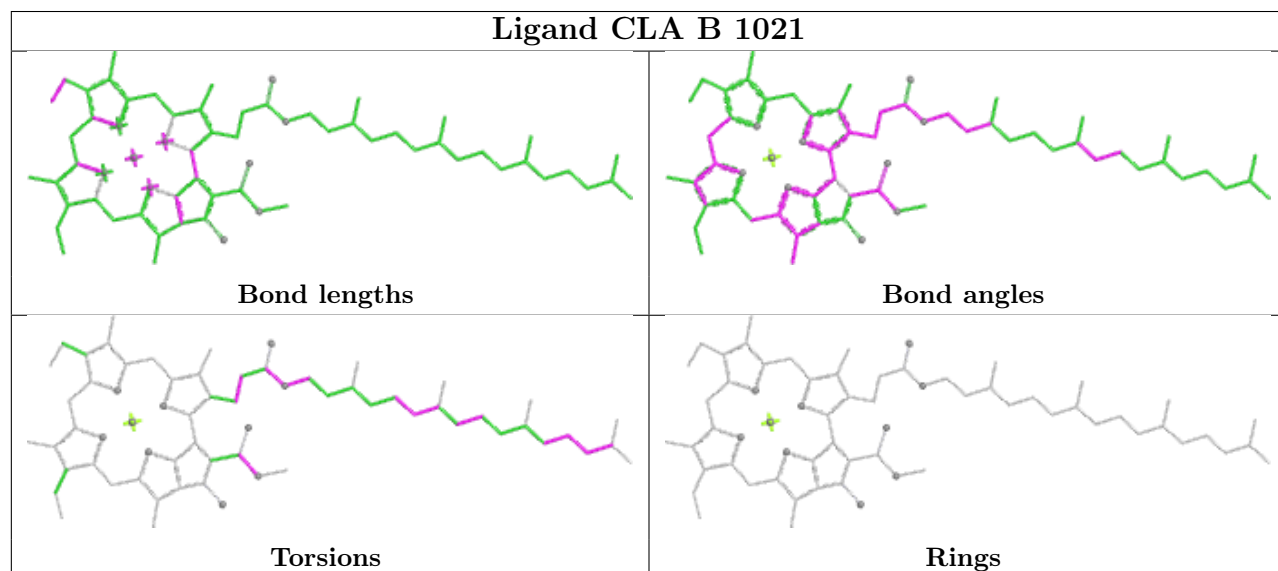


Ligand CLA 6 609

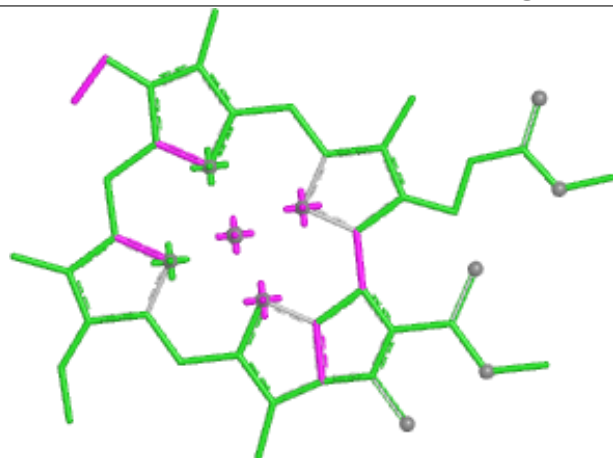




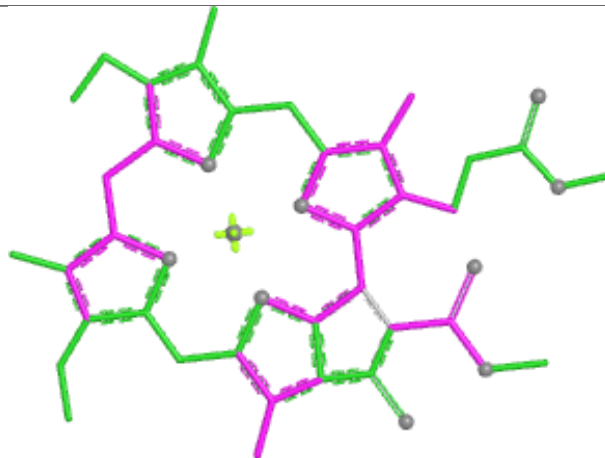


Ligand LUT 6 501**Ligand CLA 3 602****Ligand CLA B 1021**

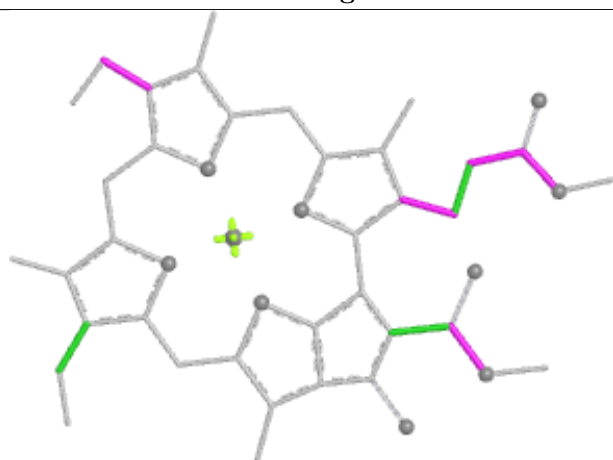
Ligand CLA 1 607



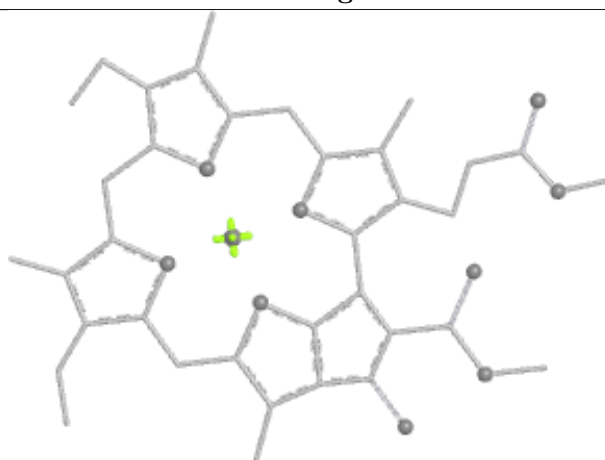
Bond lengths



Bond angles

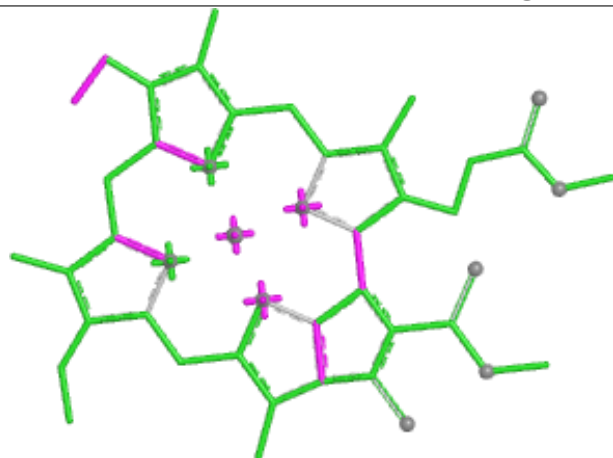


Torsions

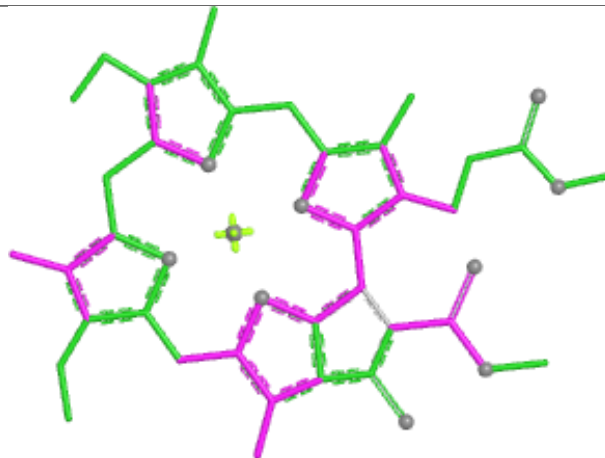


Rings

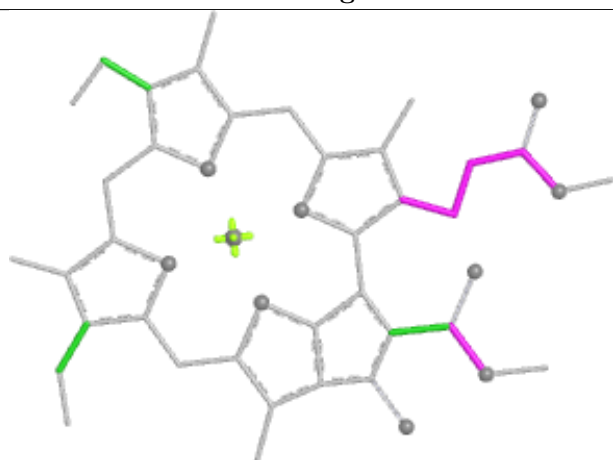
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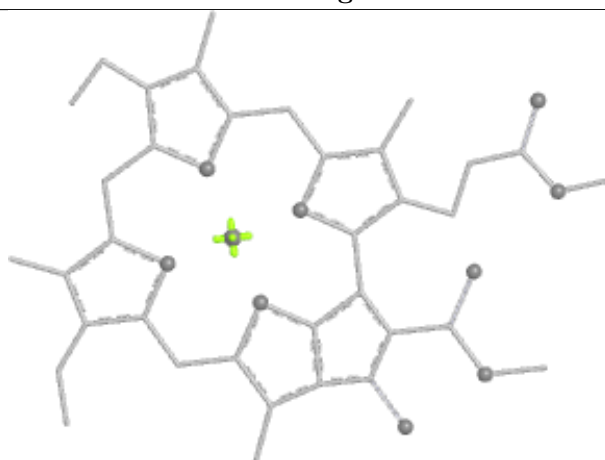
Bond lengths



Bond angles

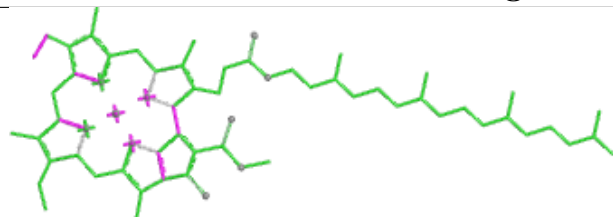


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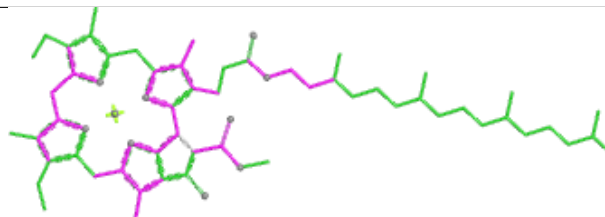


Rings

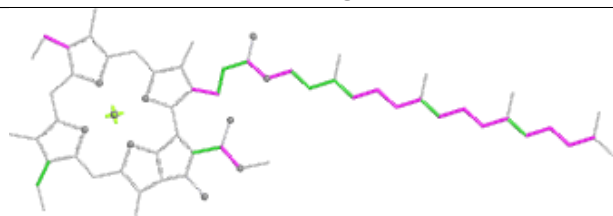
Ligand CLA A 1113



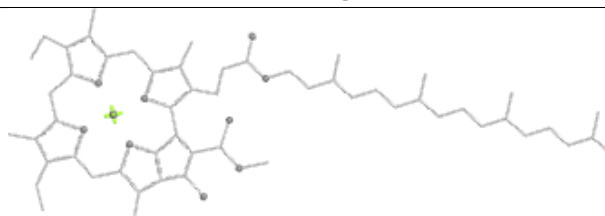
Bond lengths



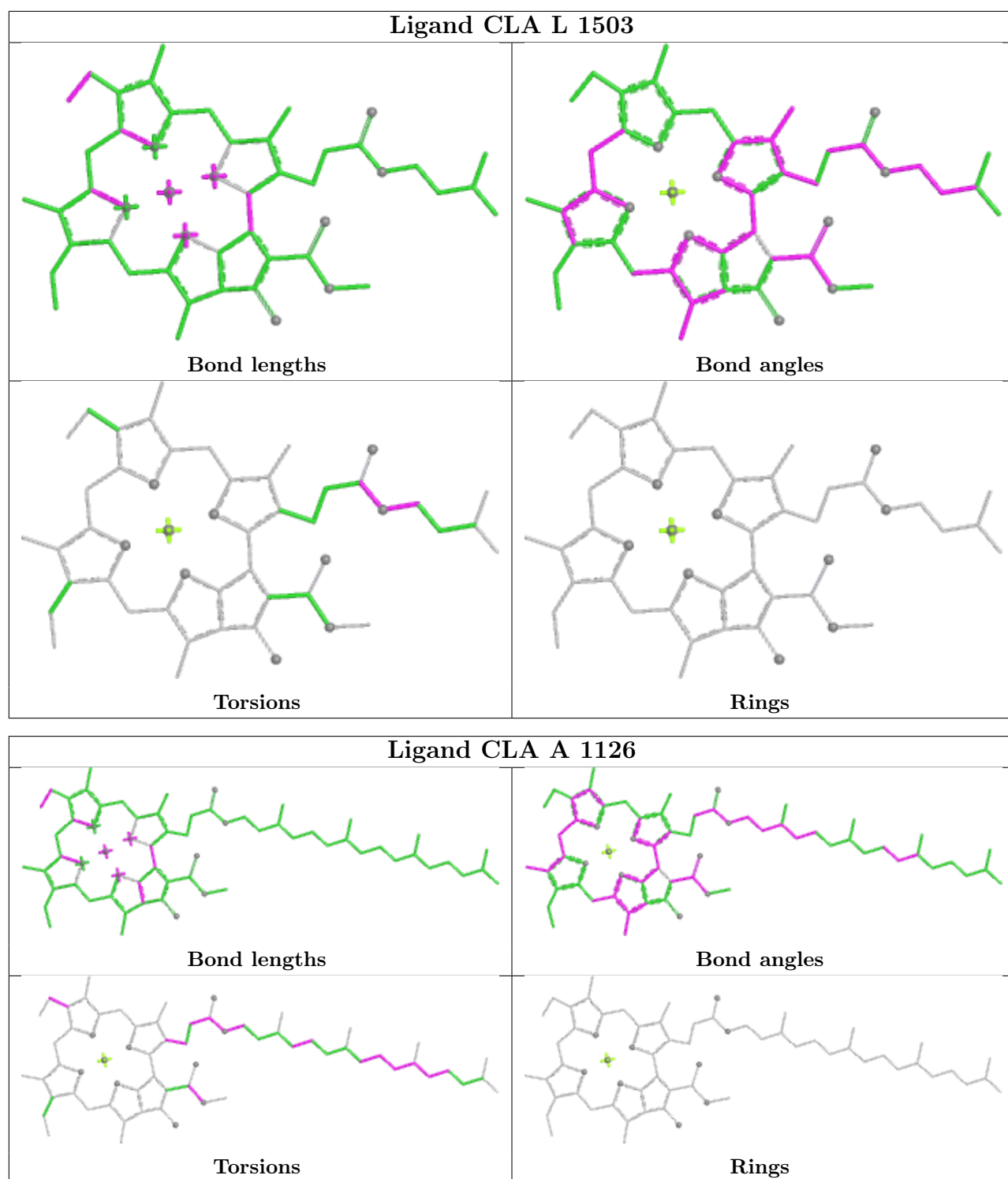
Bond angles

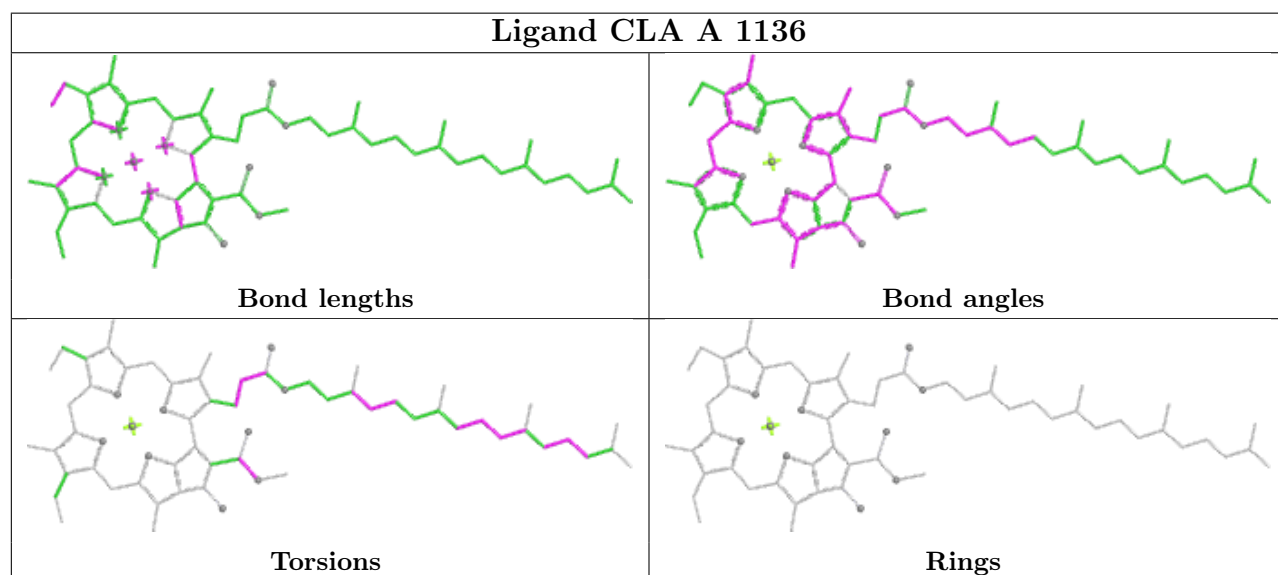
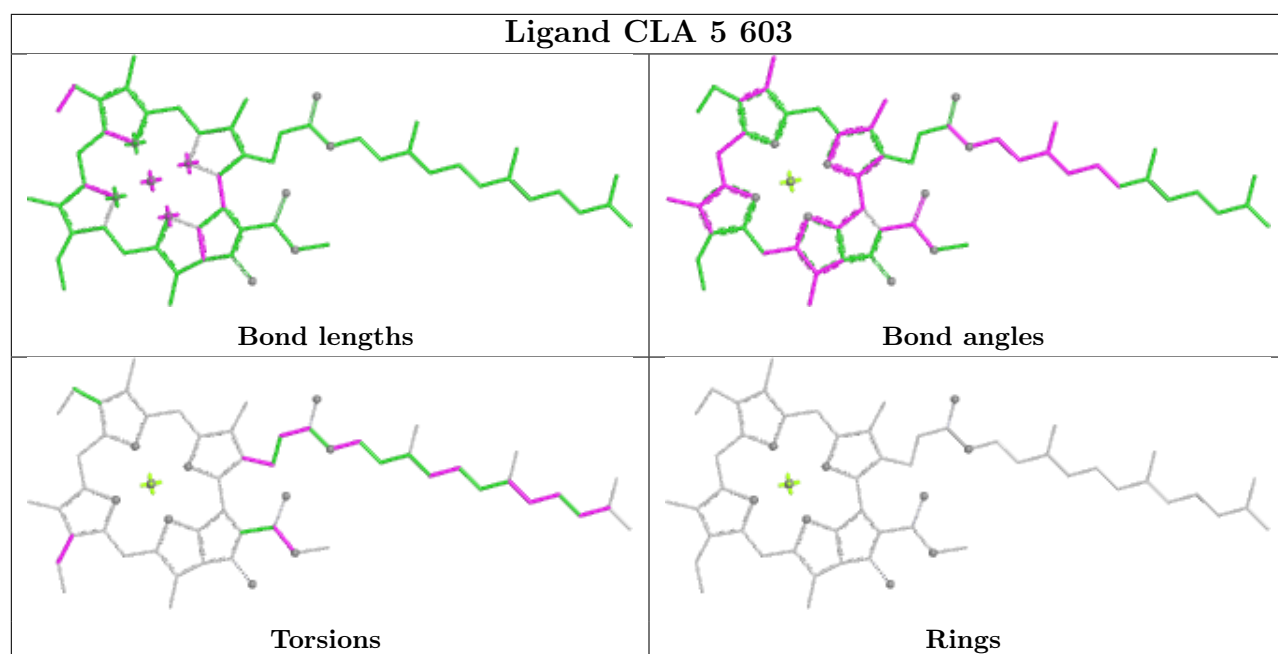


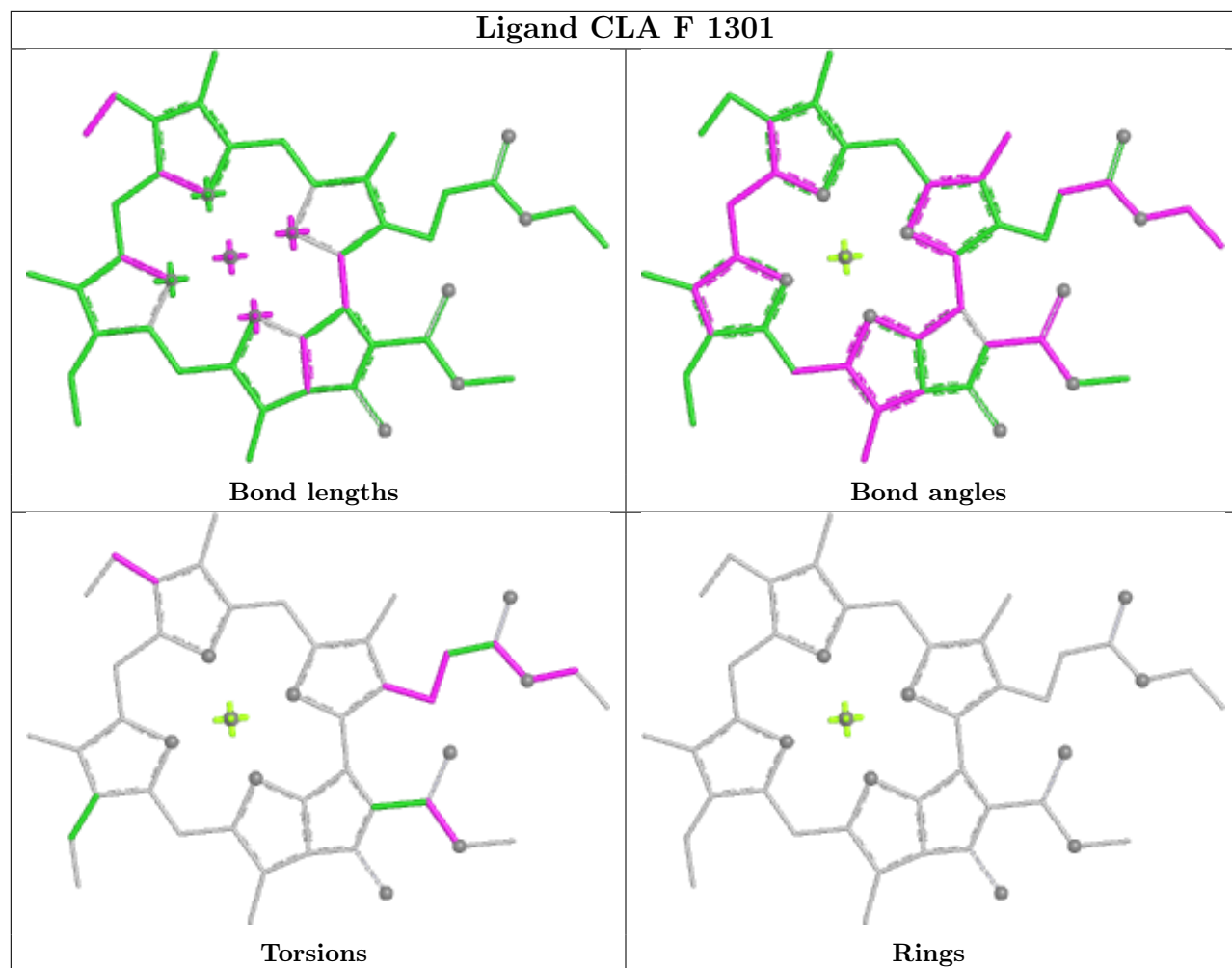
Torsions



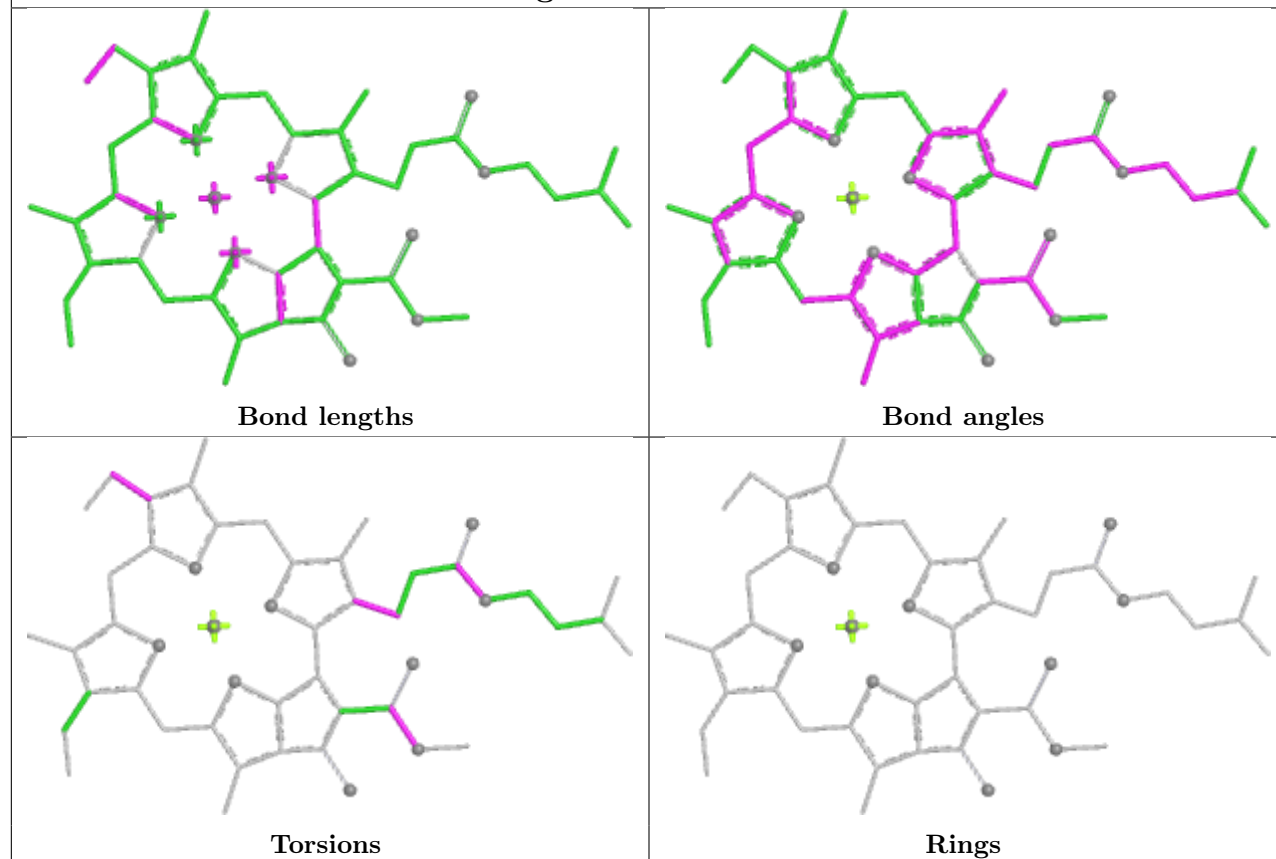
Rings



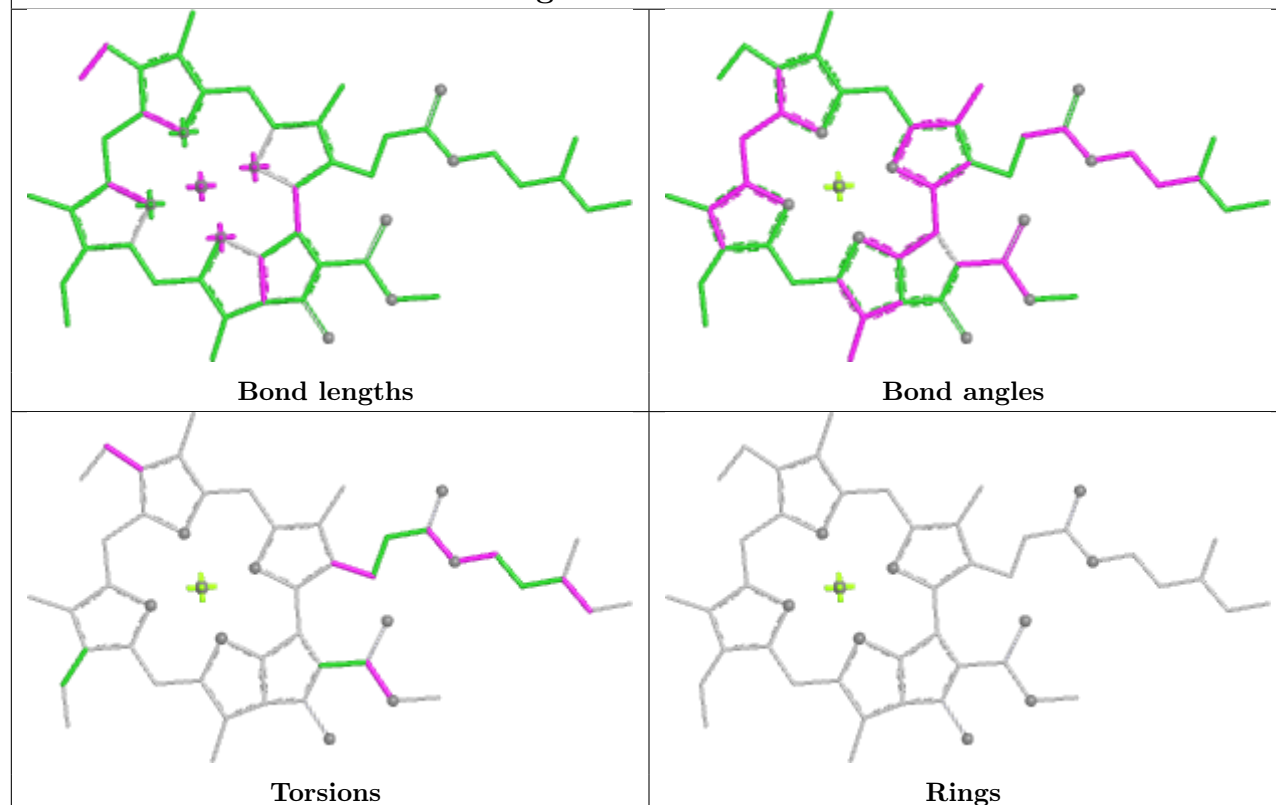


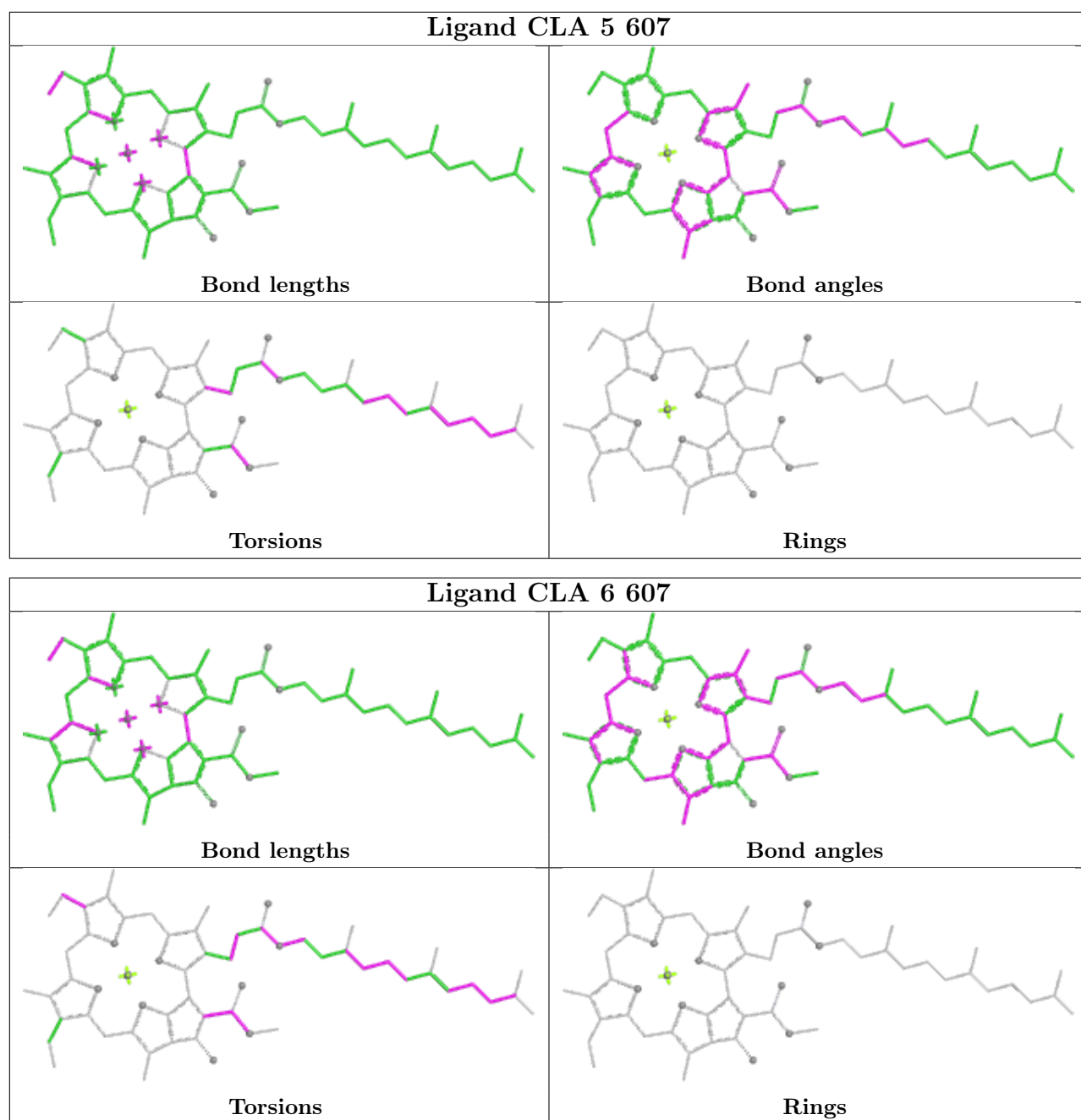


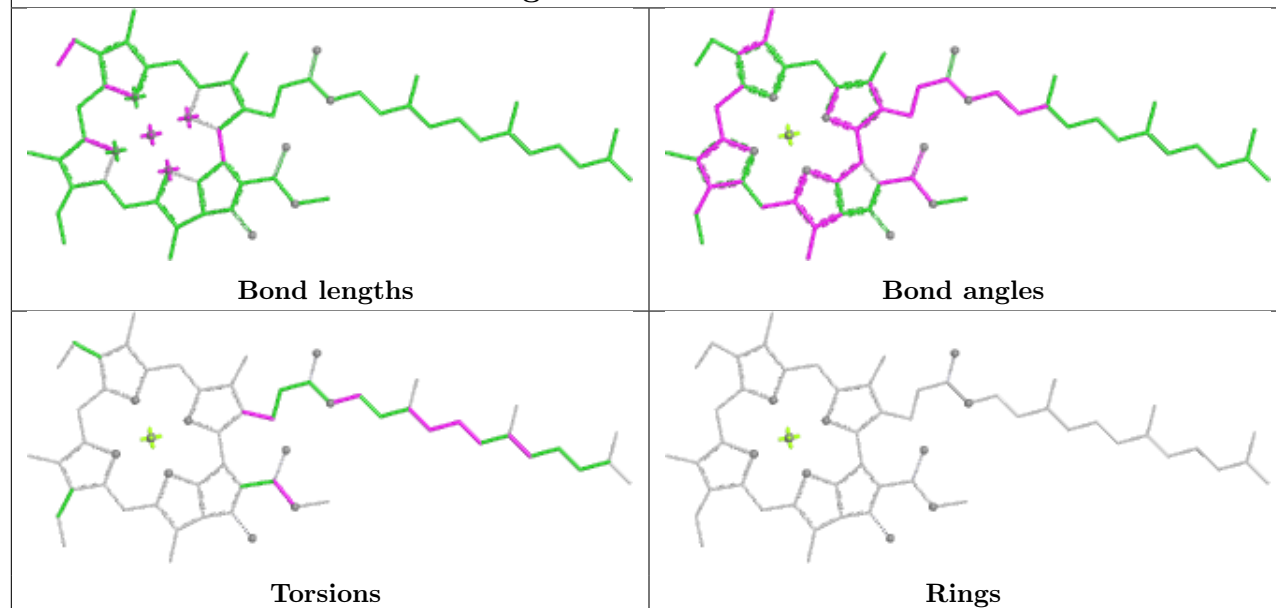
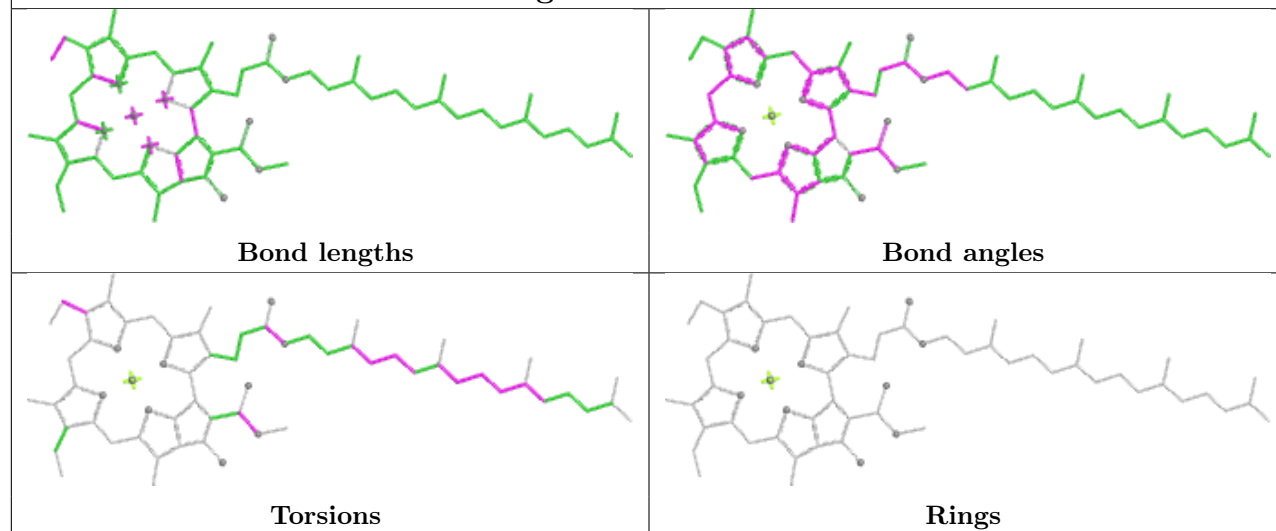
Ligand CLA 2 606

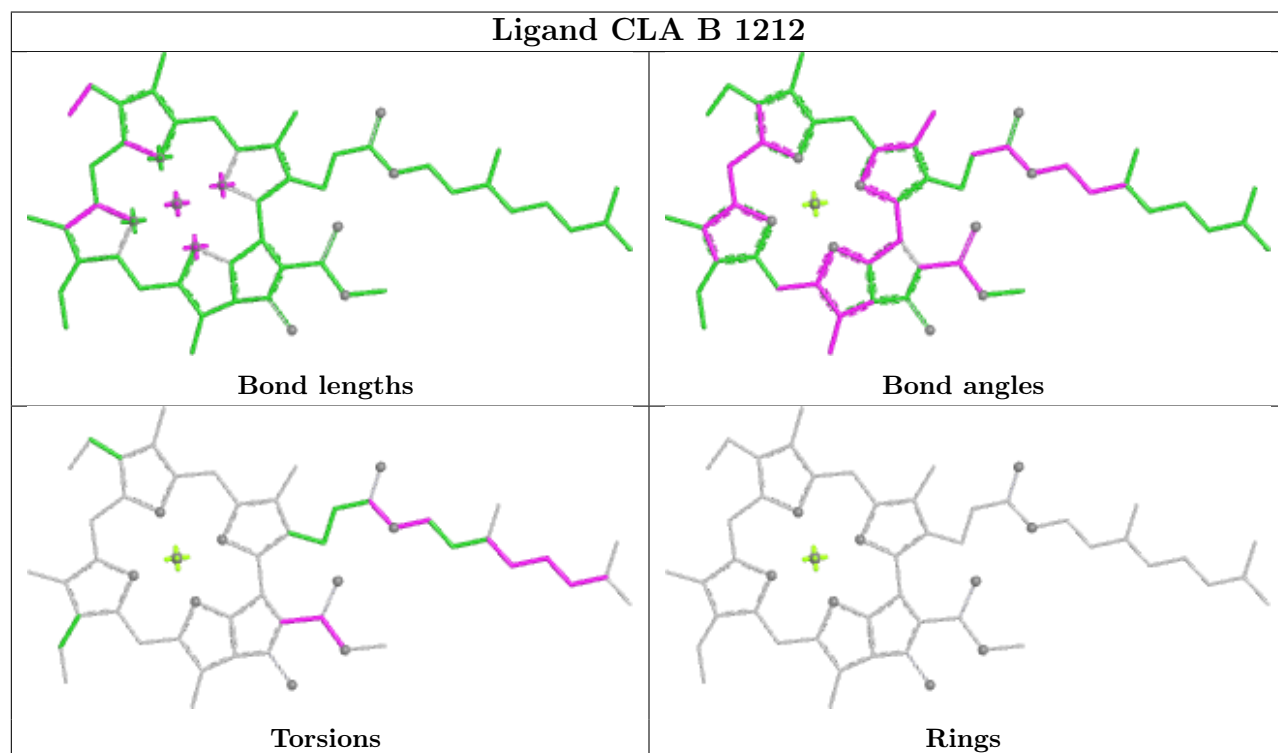
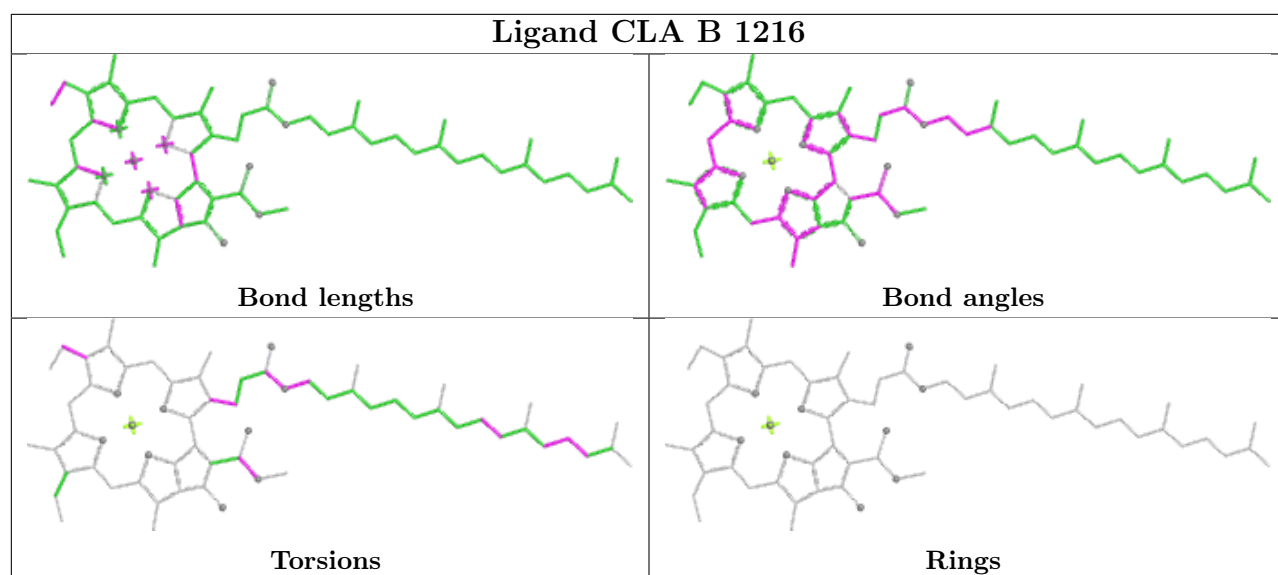


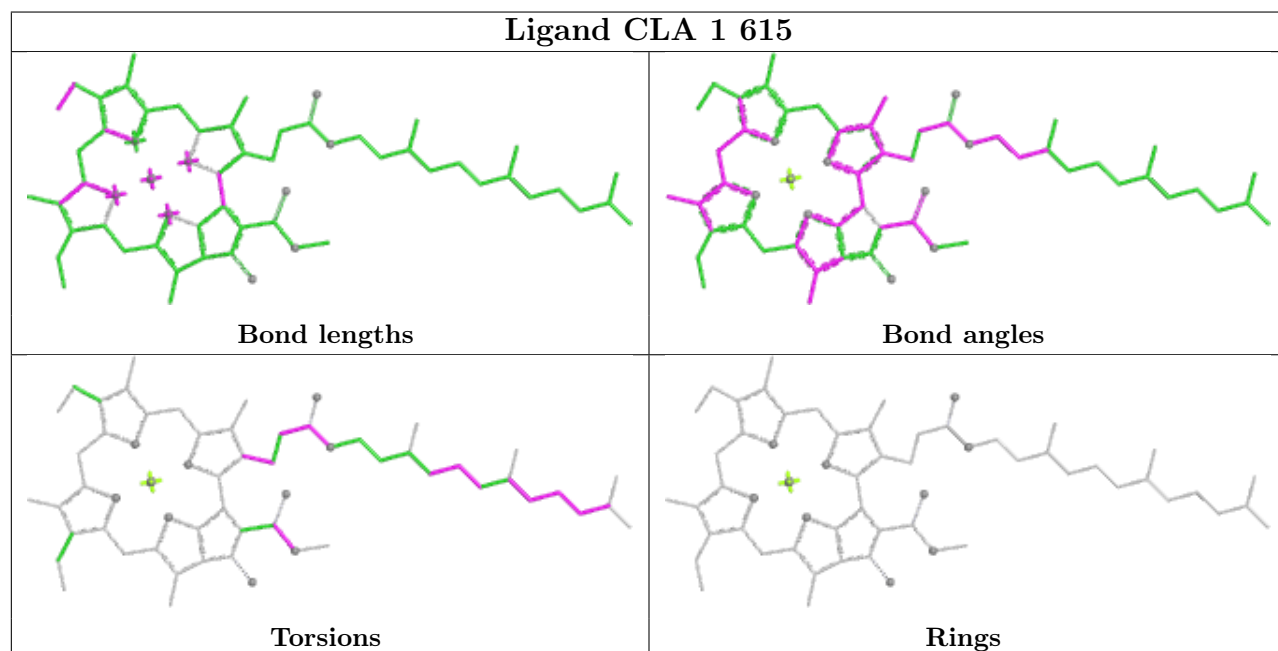
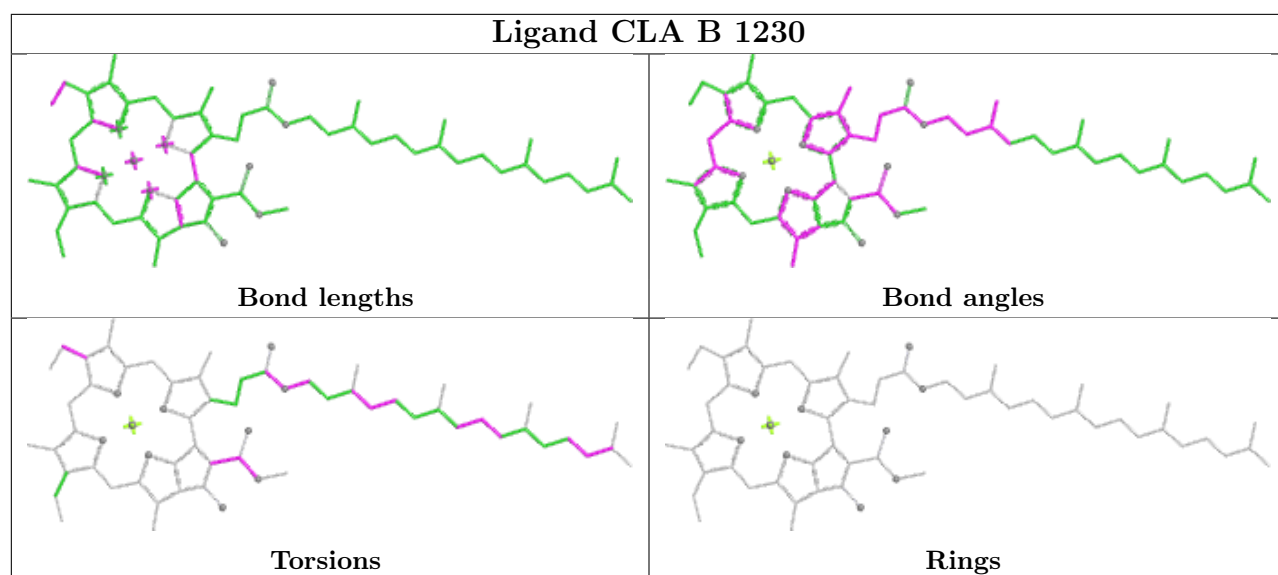
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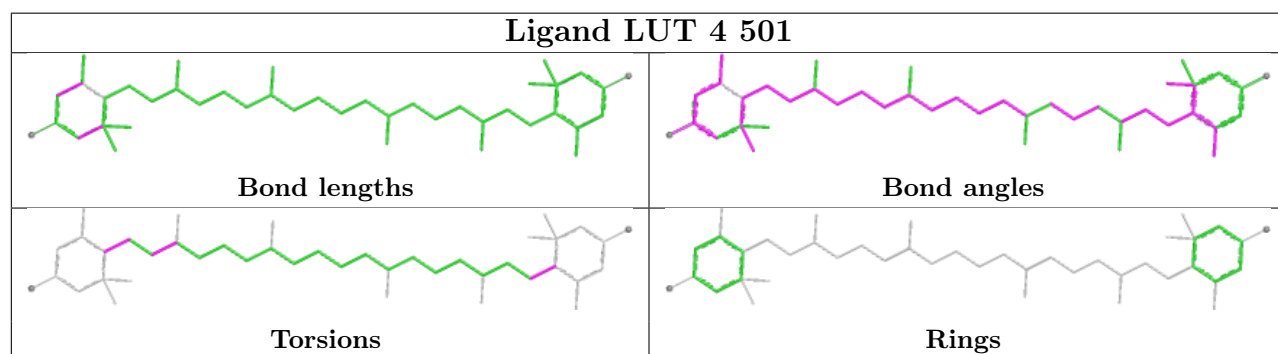
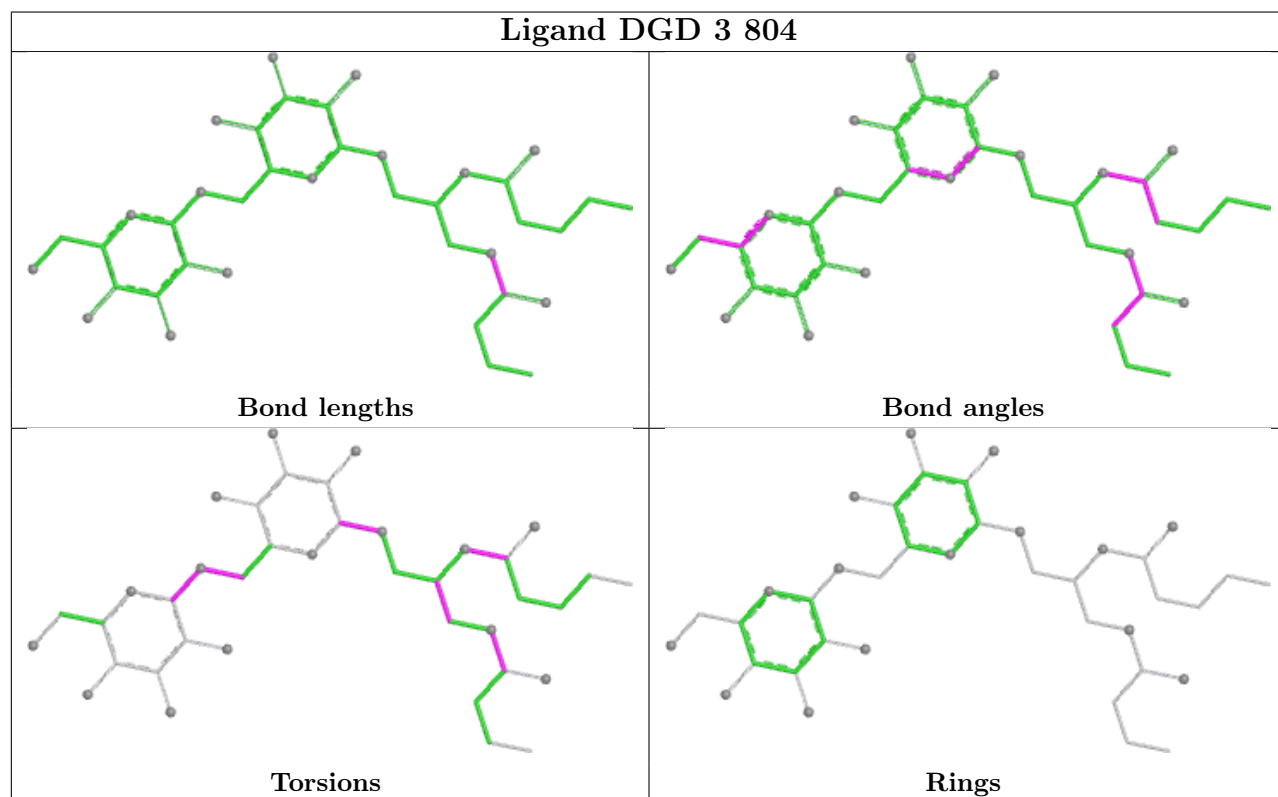
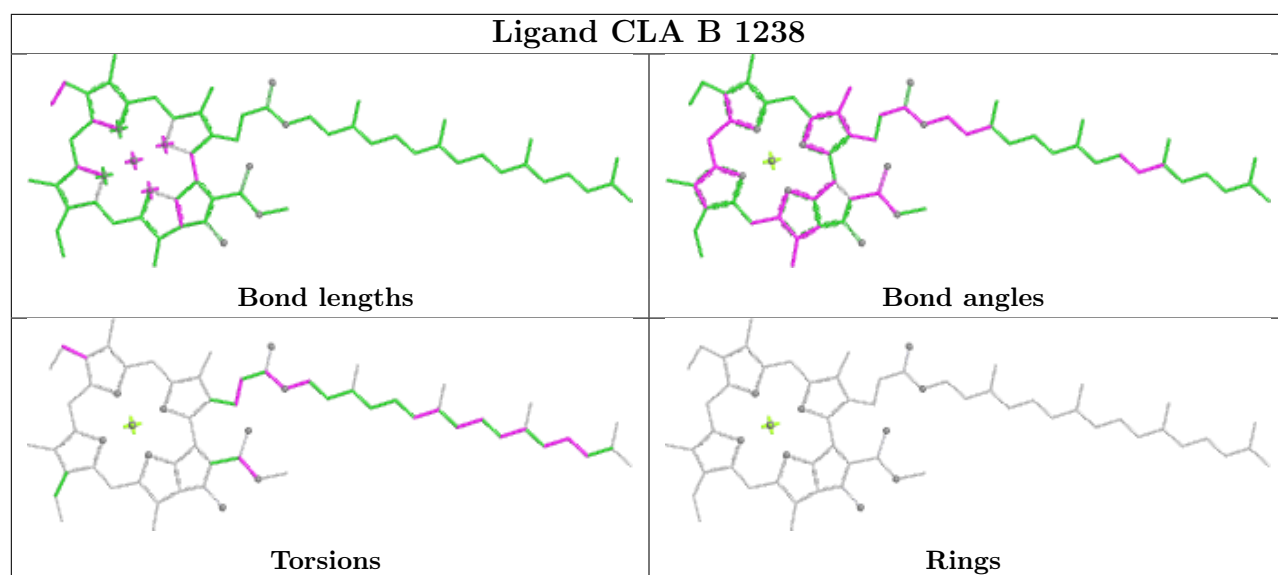




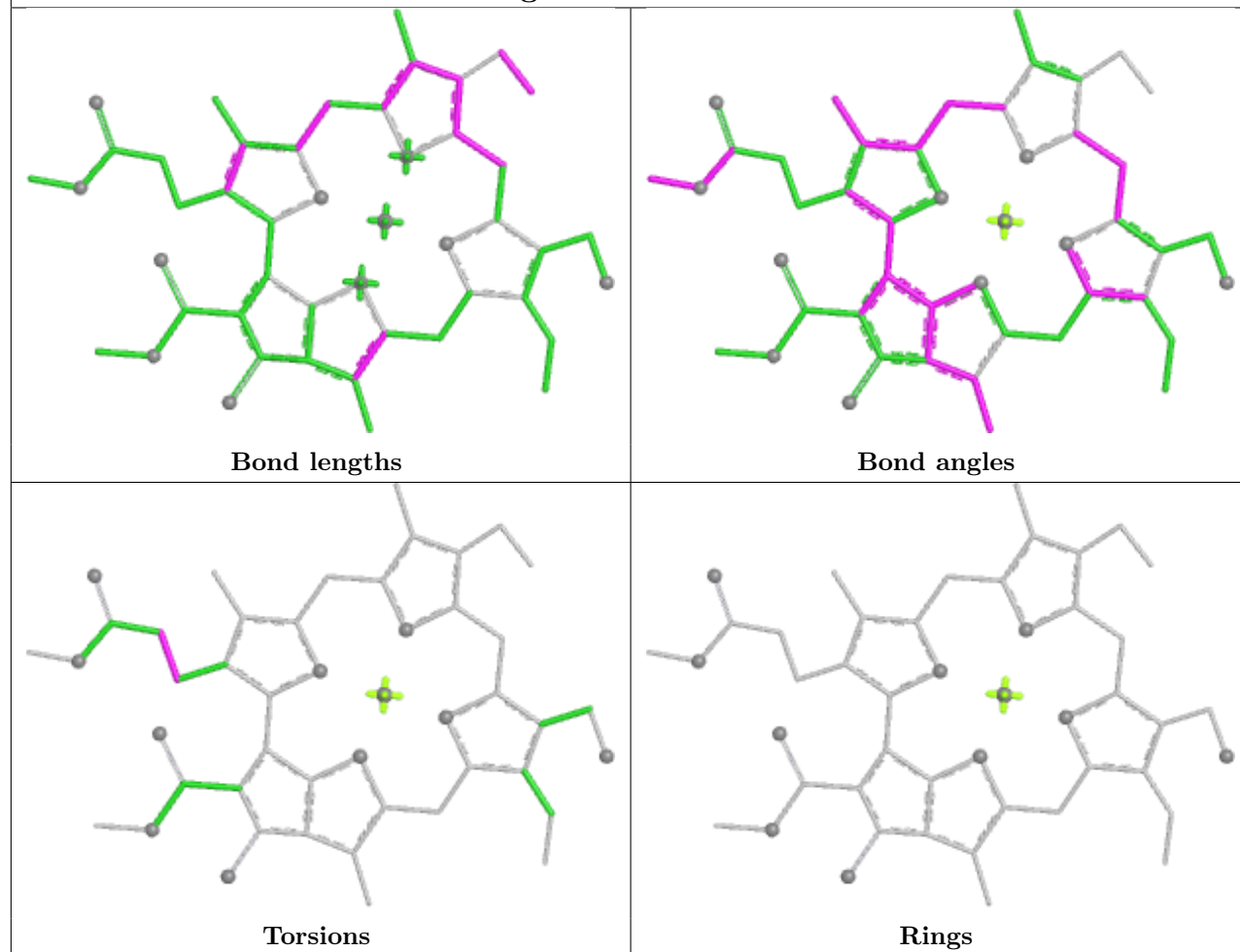
Ligand CLA A 1137**Ligand CLA 2 612**



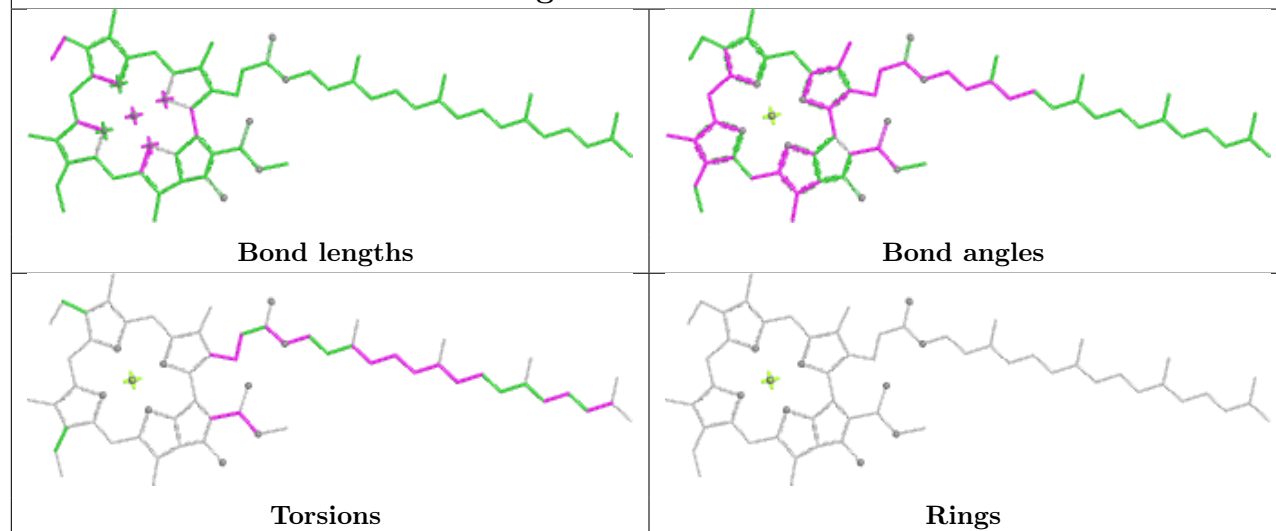


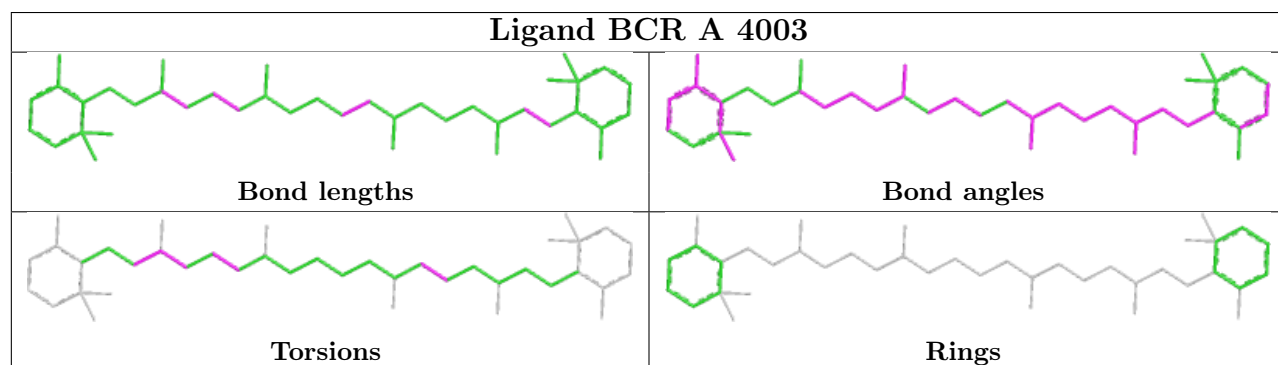
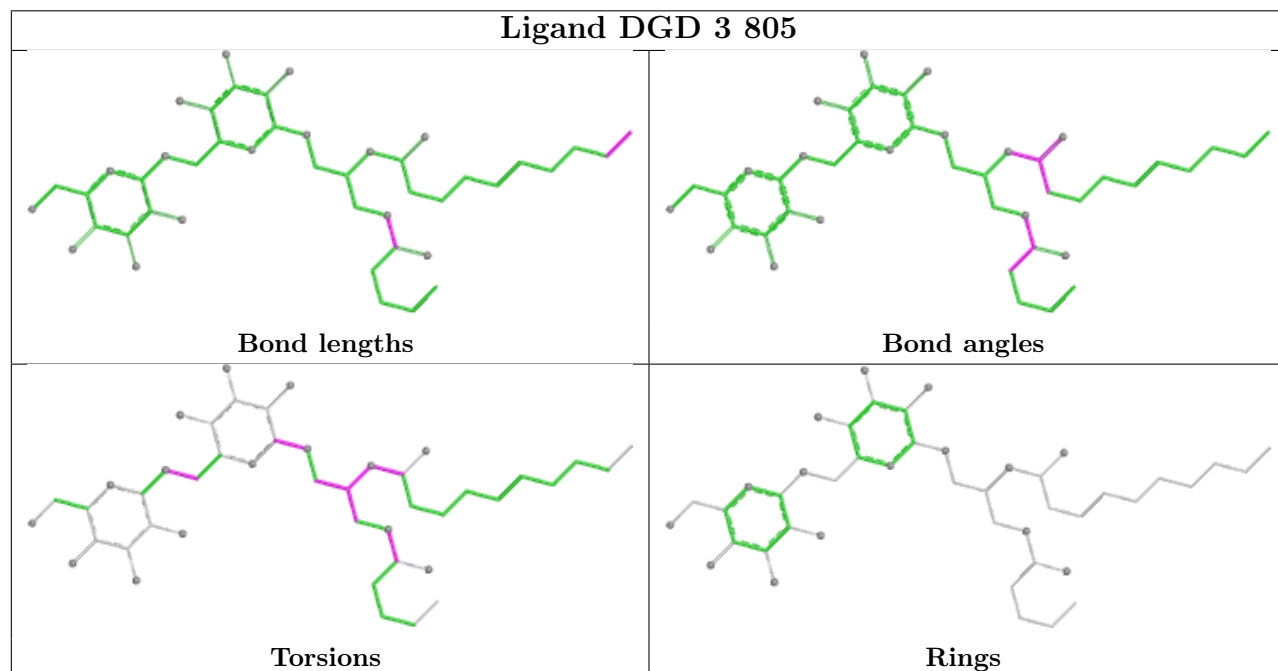
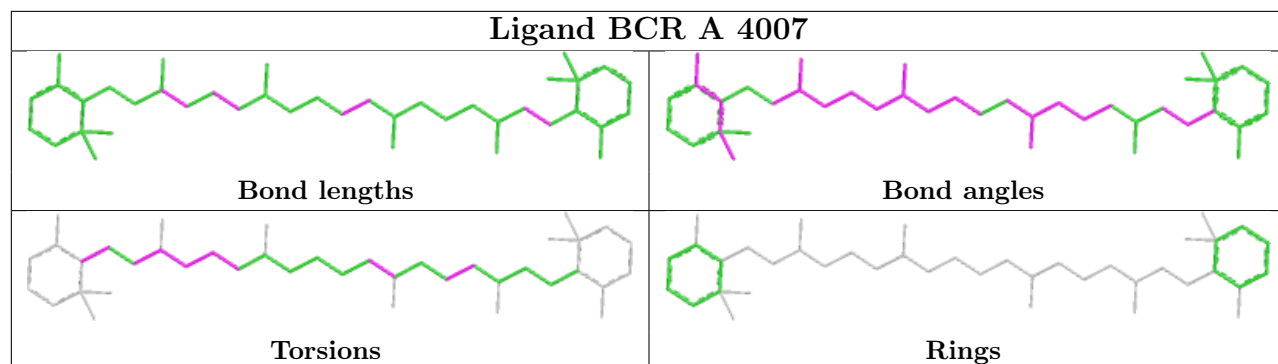


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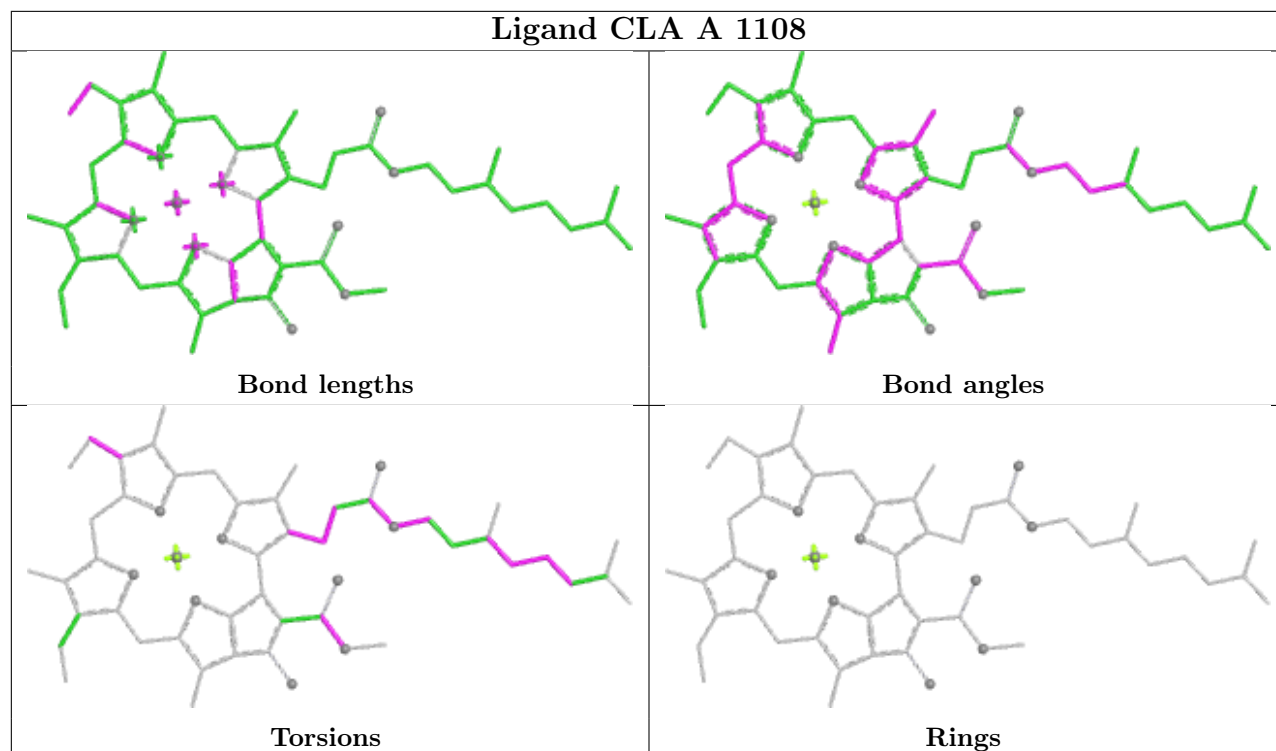


Ligand CLA 5 614

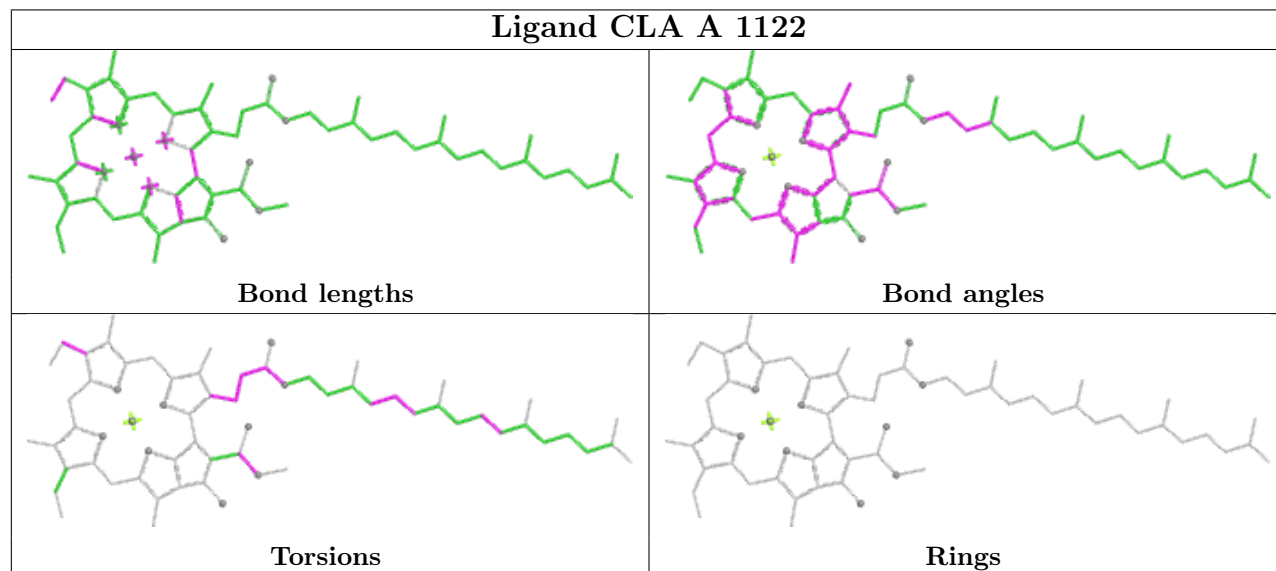


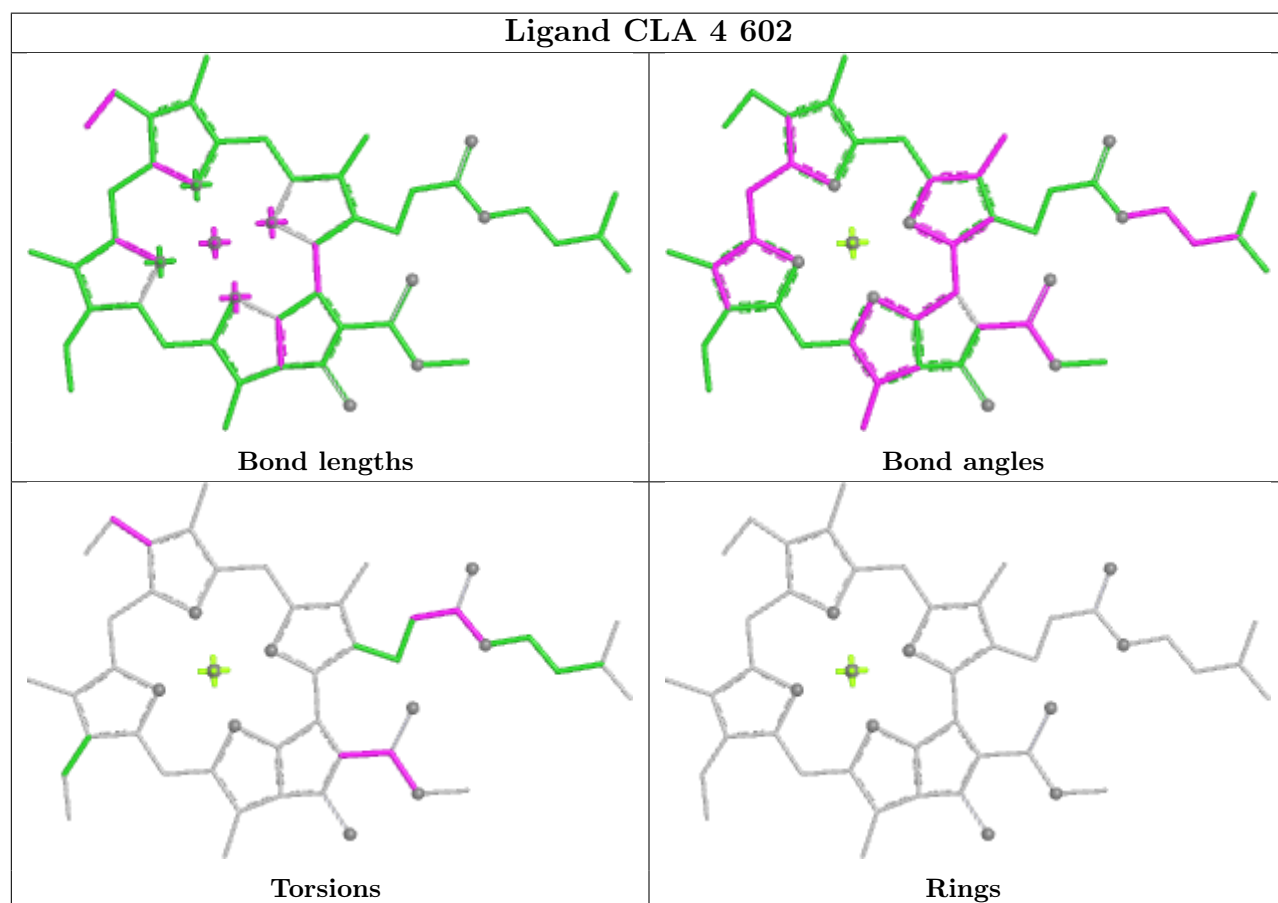
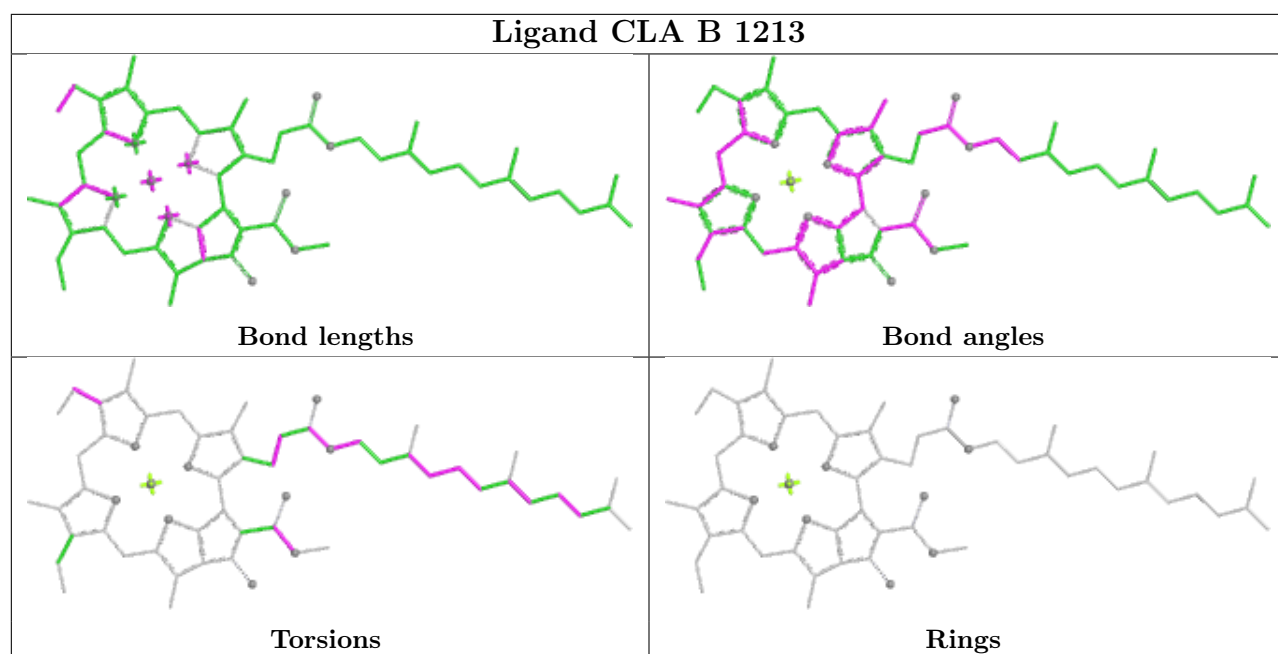


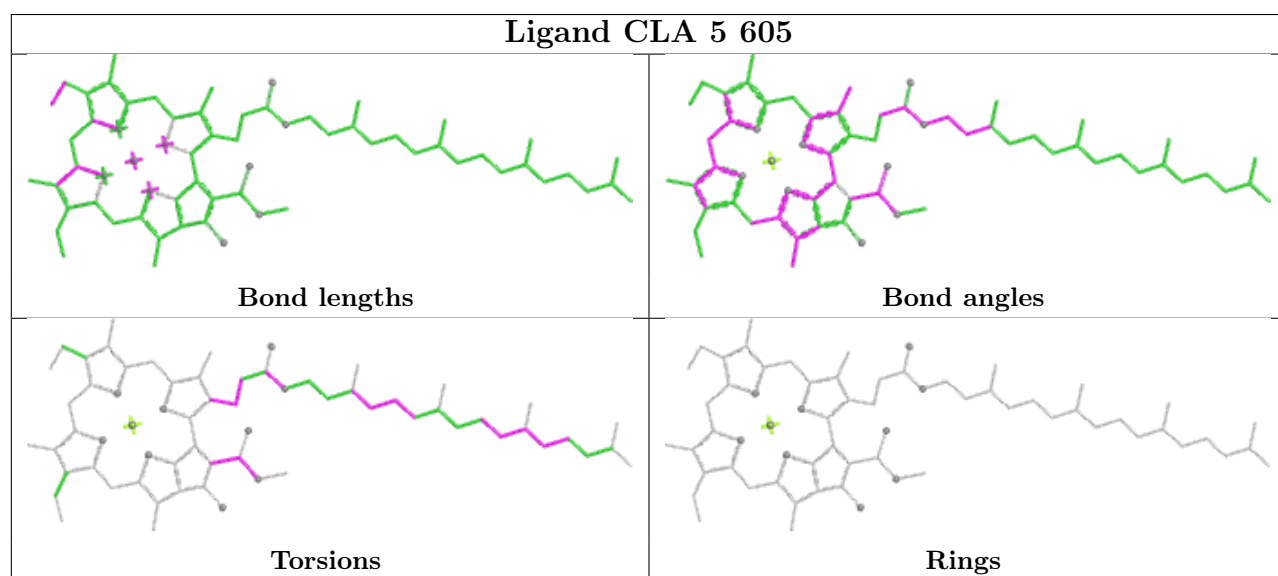
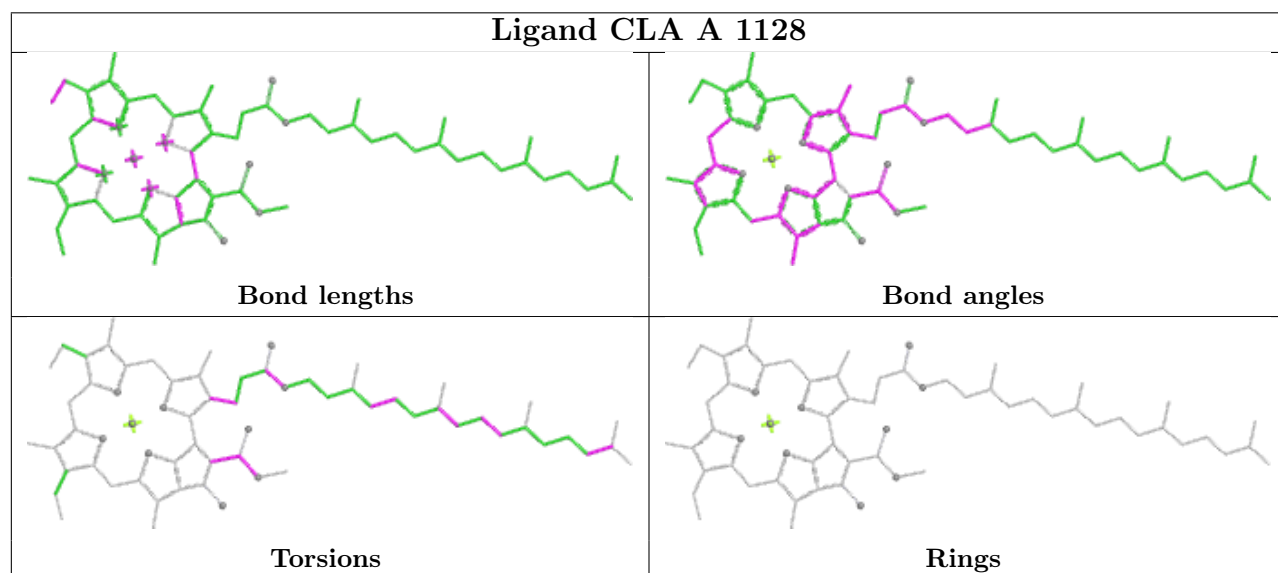
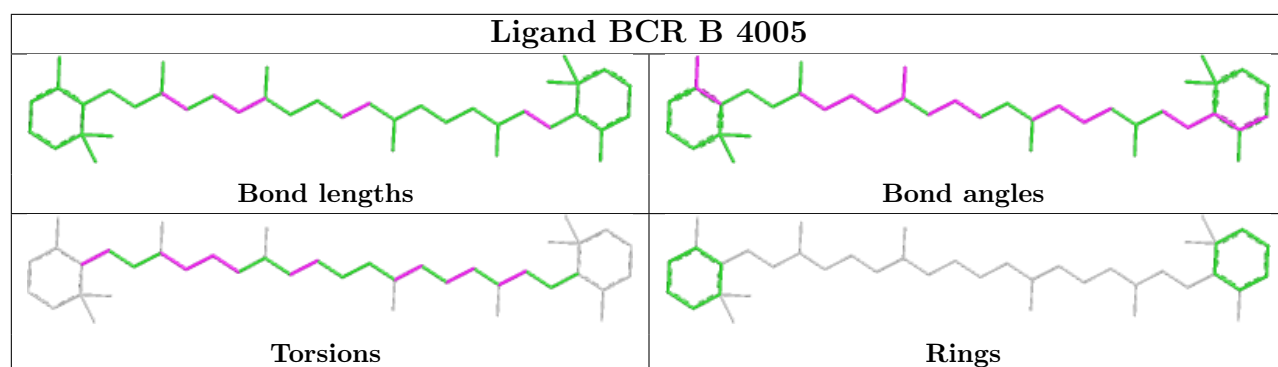
Ligand CLA A 1108

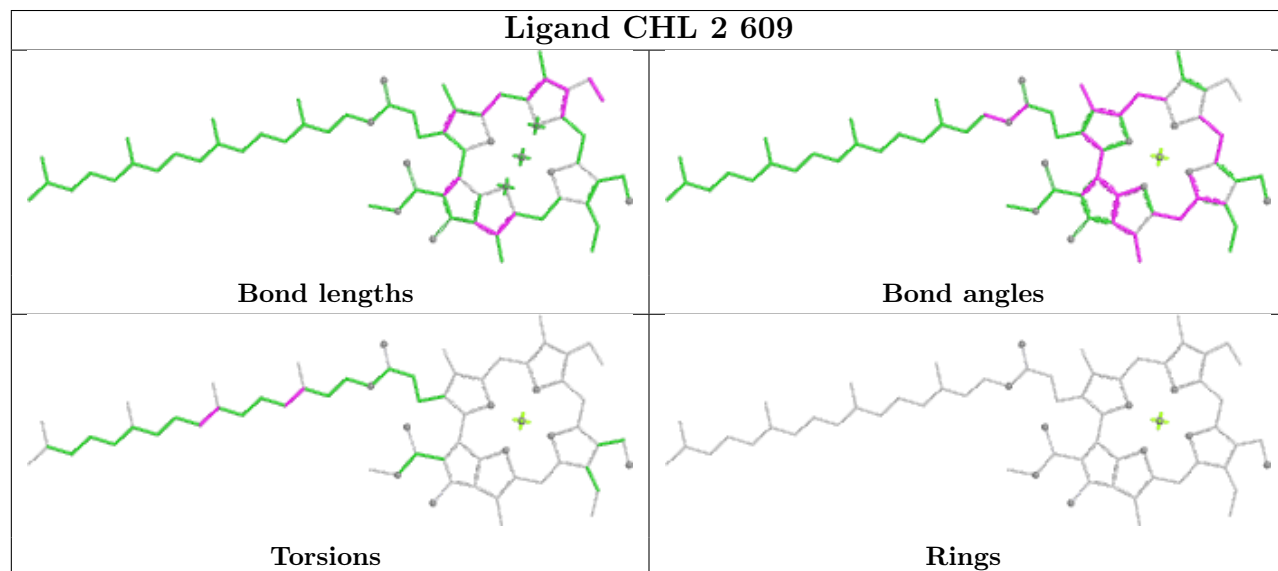
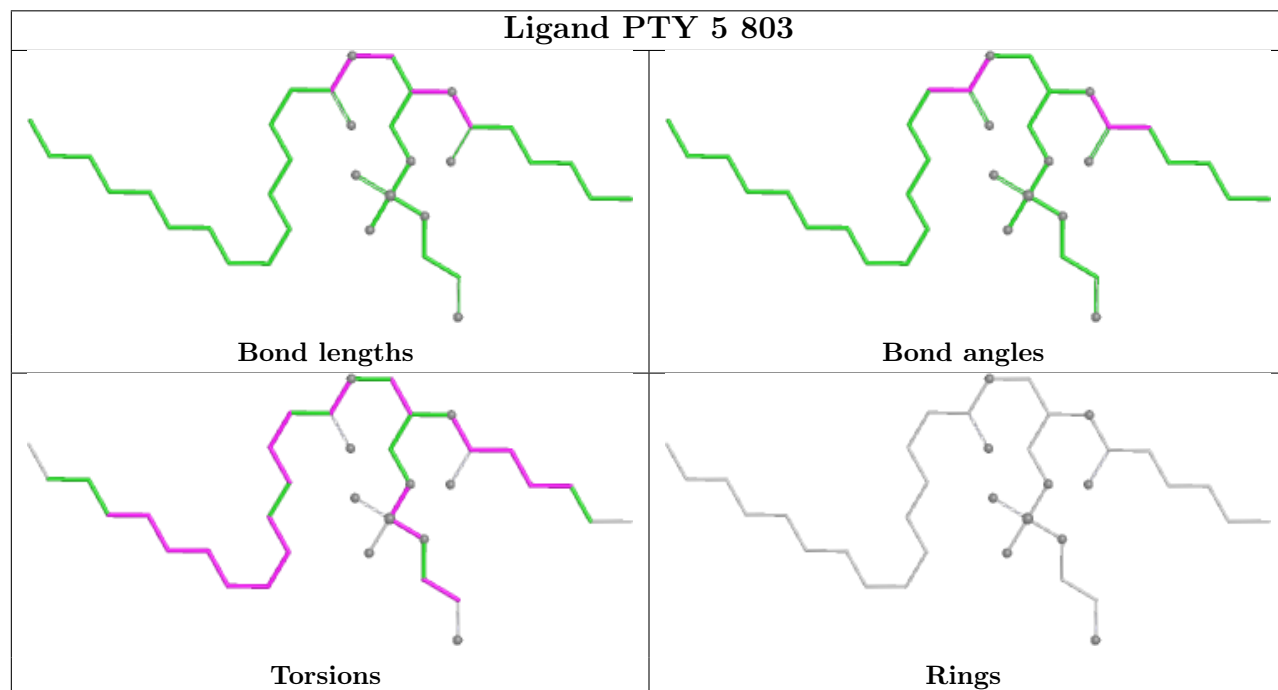
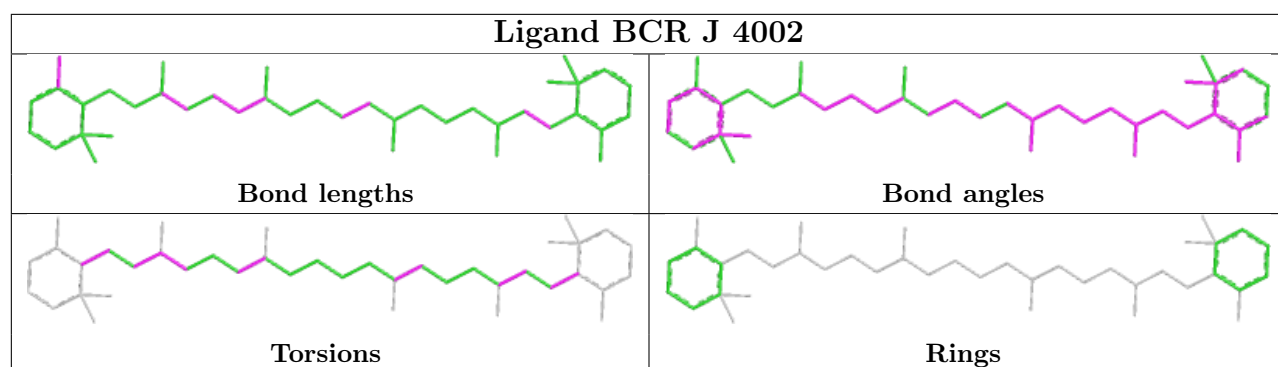


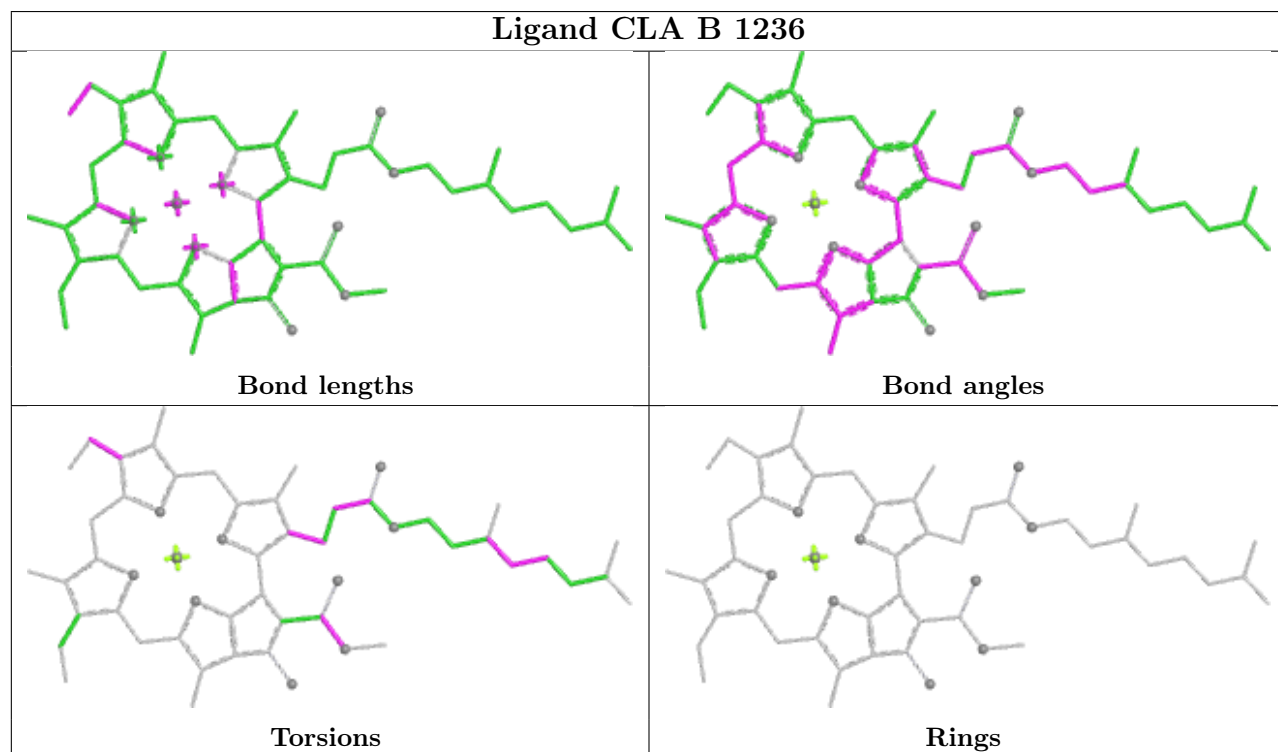
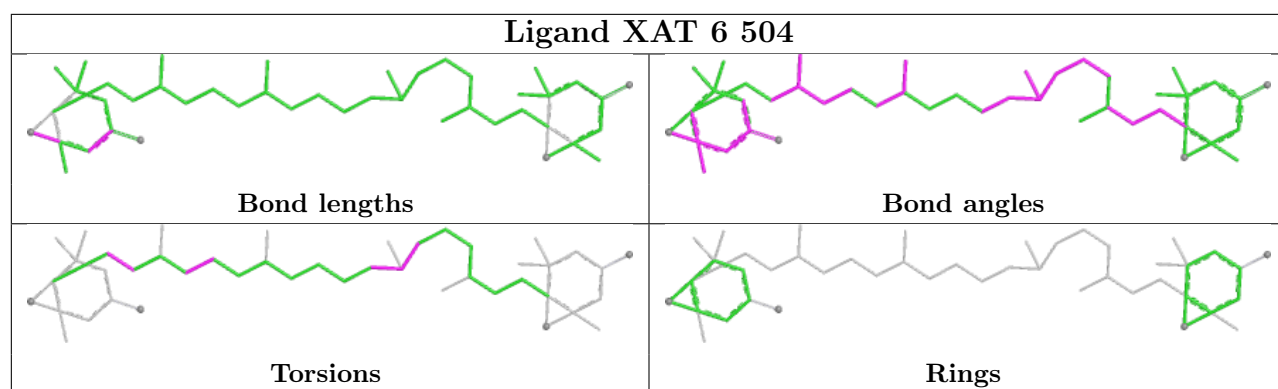
Ligand CLA A 1122

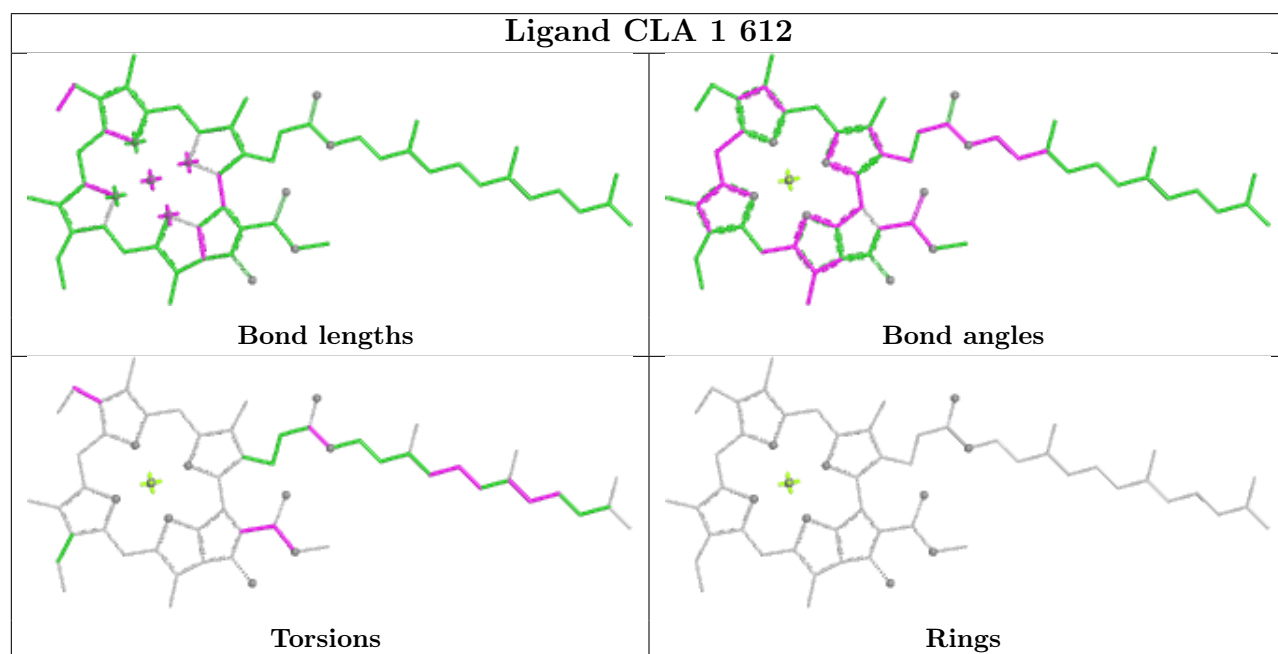
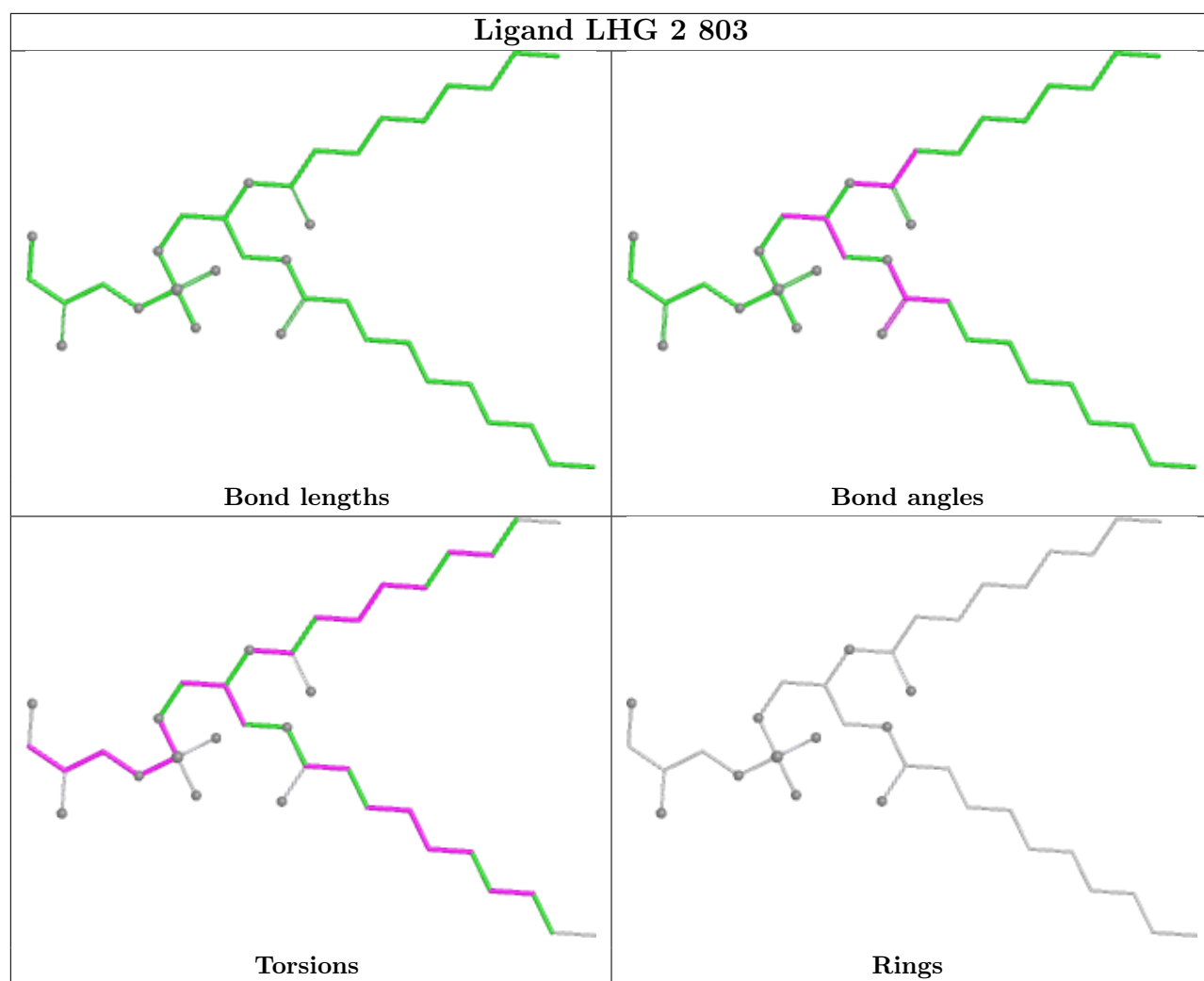


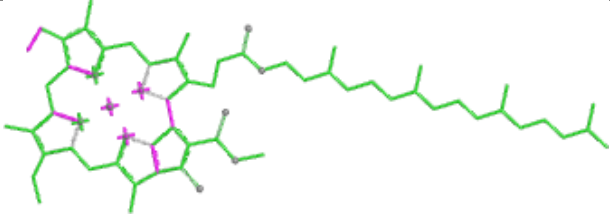
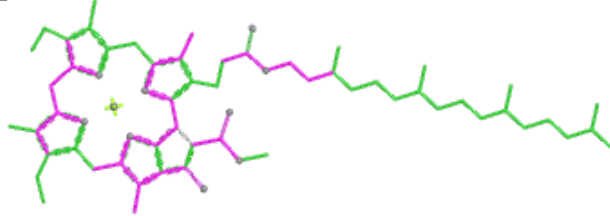
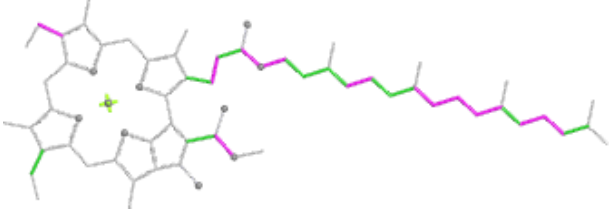
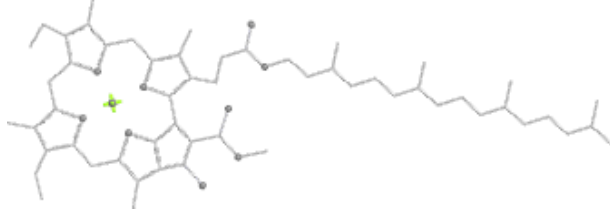
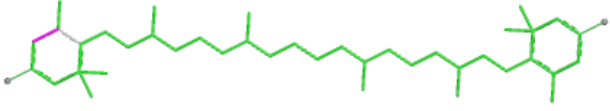
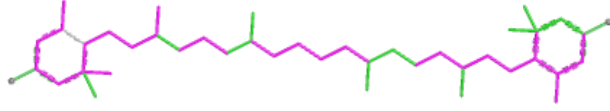
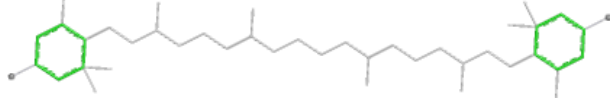
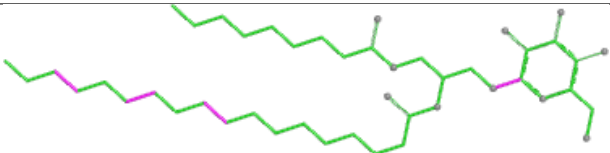
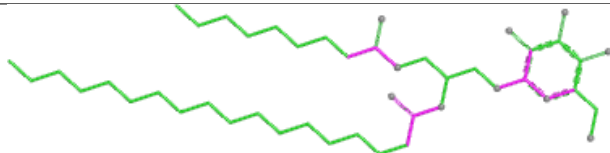
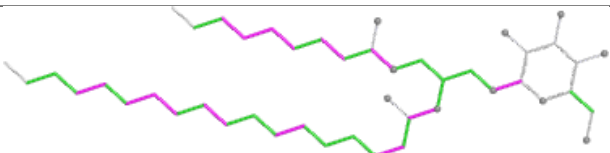




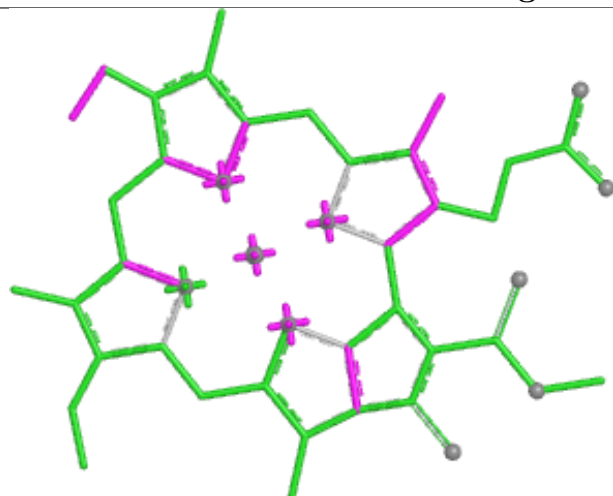




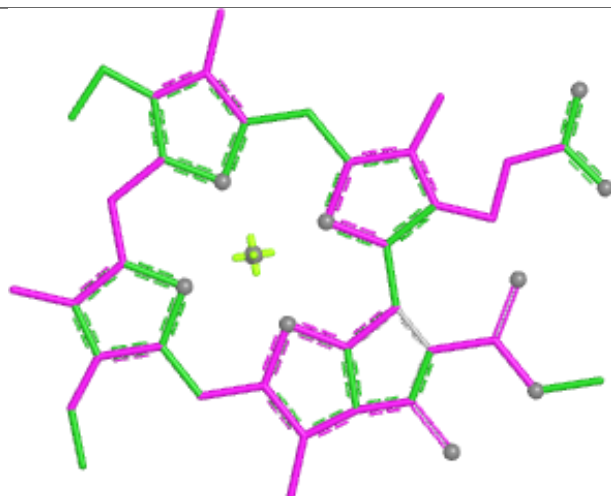


Ligand CLA B 1214	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 2 501	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 4 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

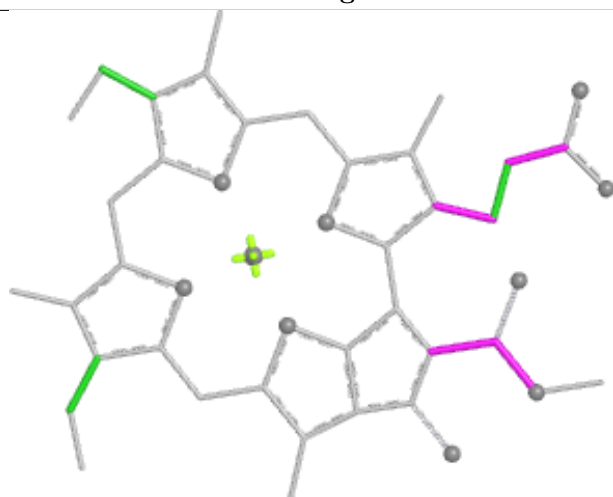
Ligand CLA 5 601



Bond lengths



Bond angles

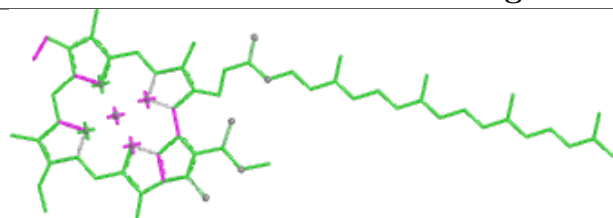


Torsions

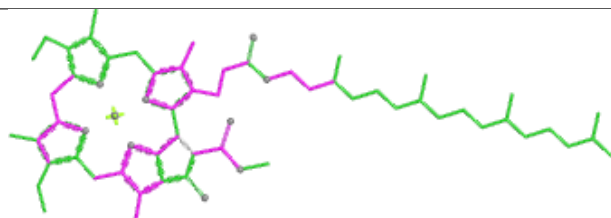


Rings

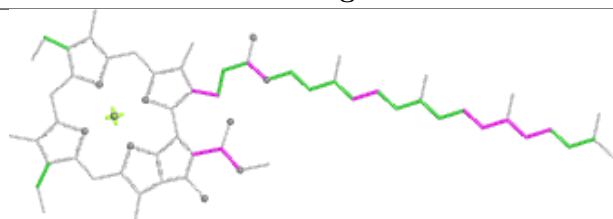
Ligand CLA A 1103



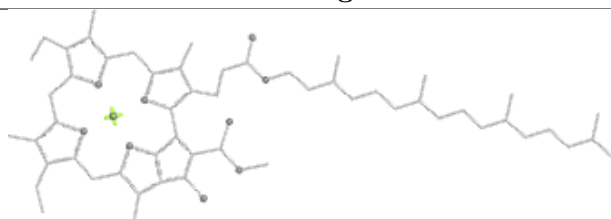
Bond lengths



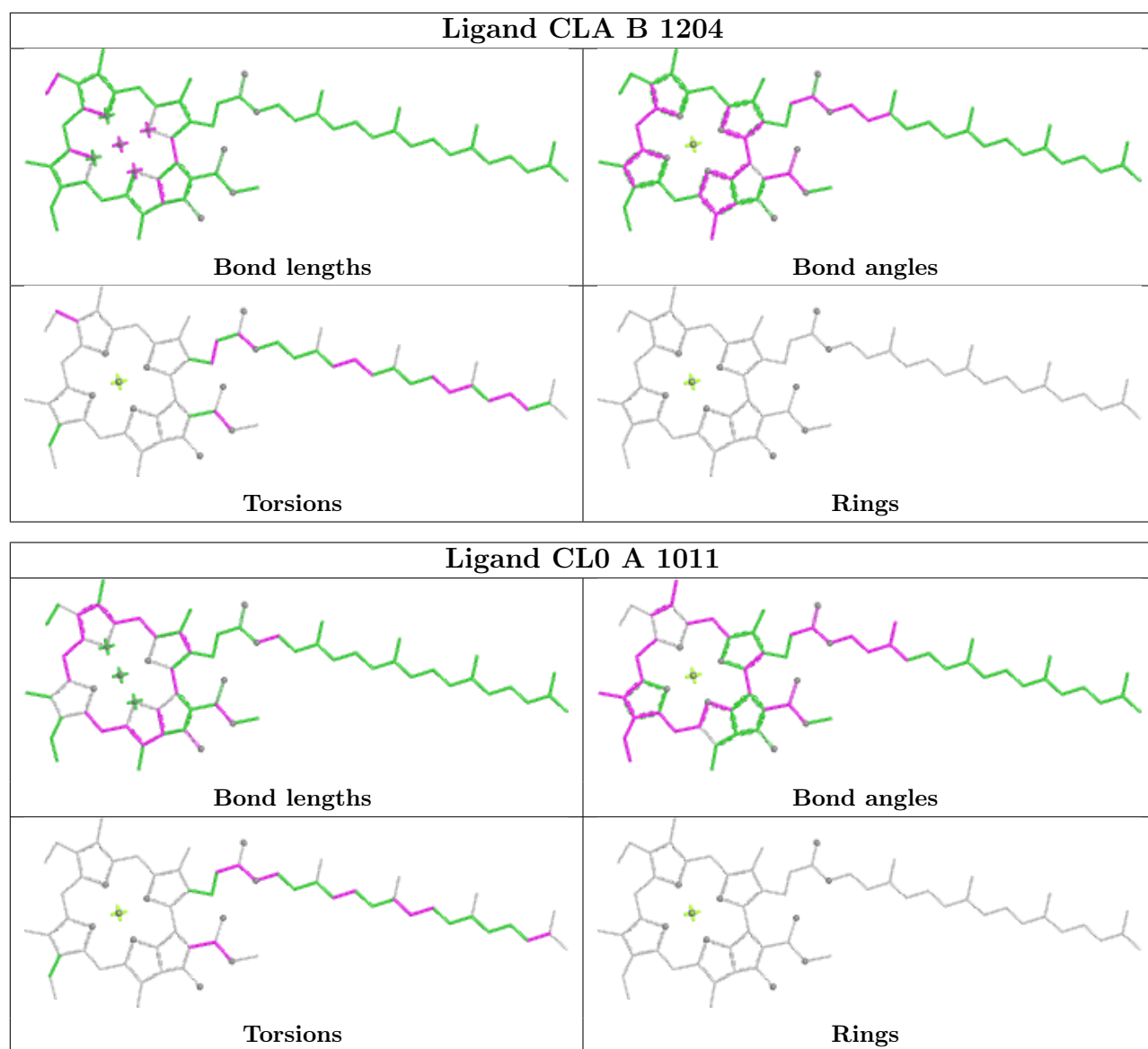
Bond angles

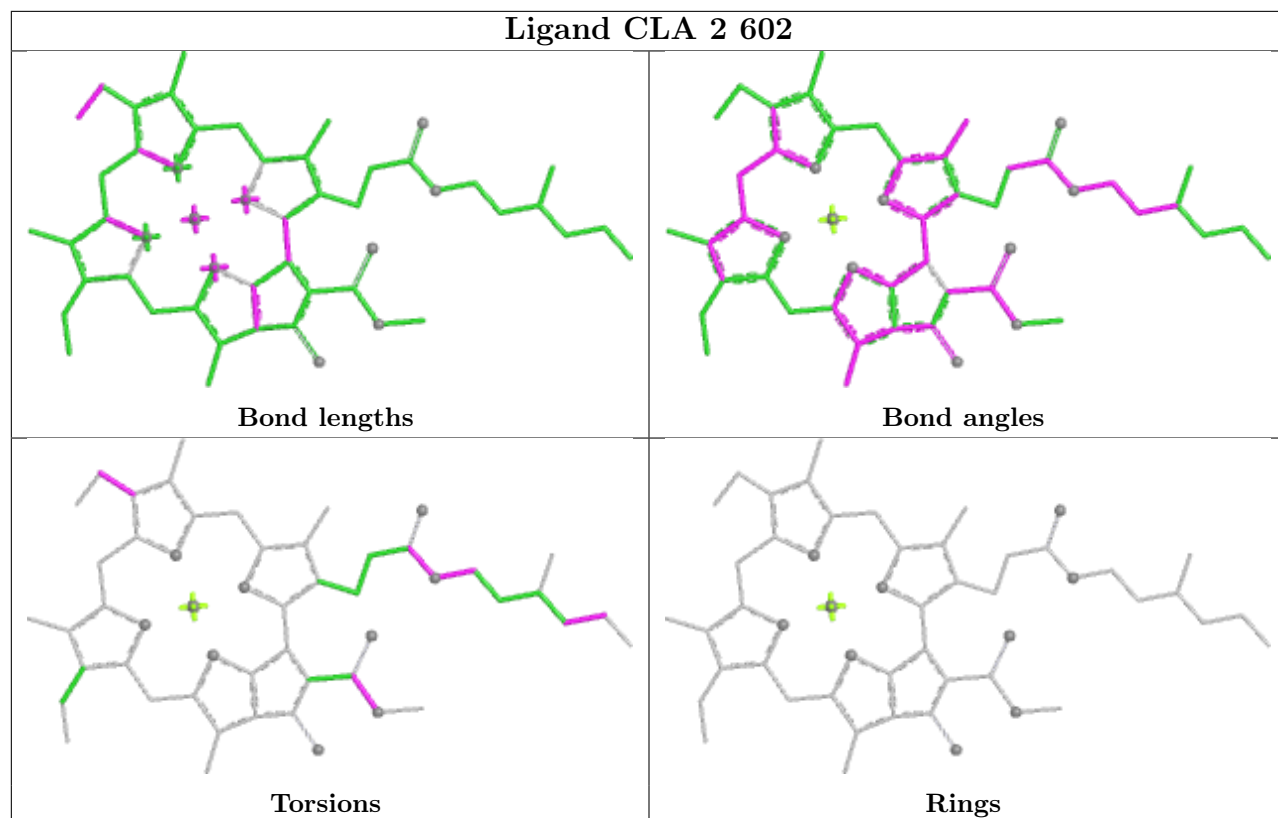
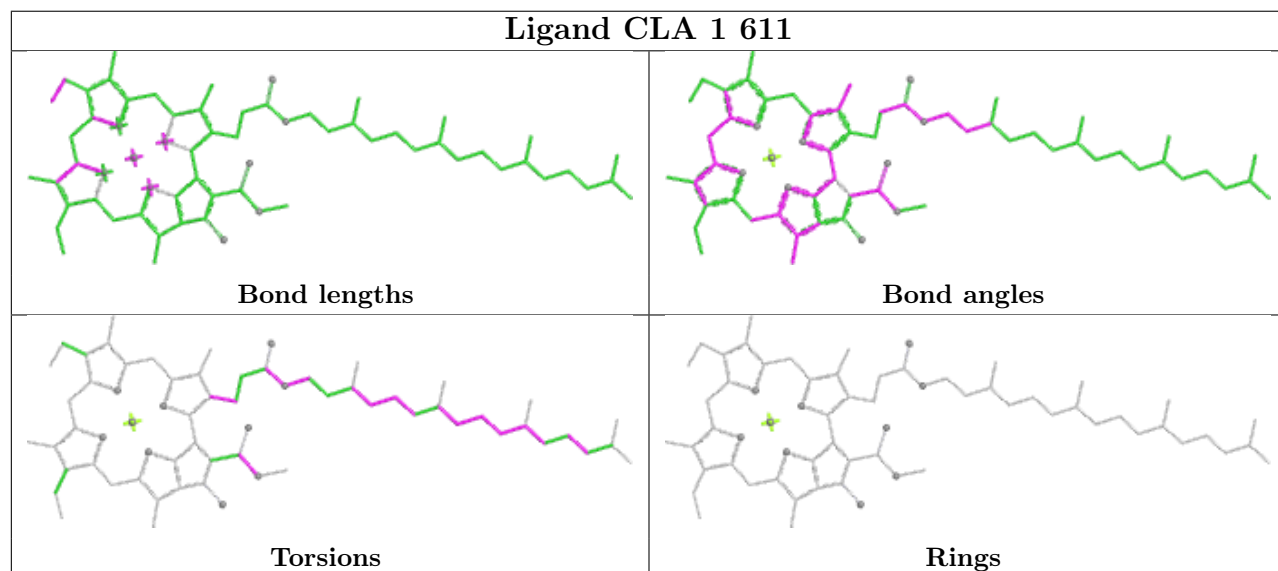


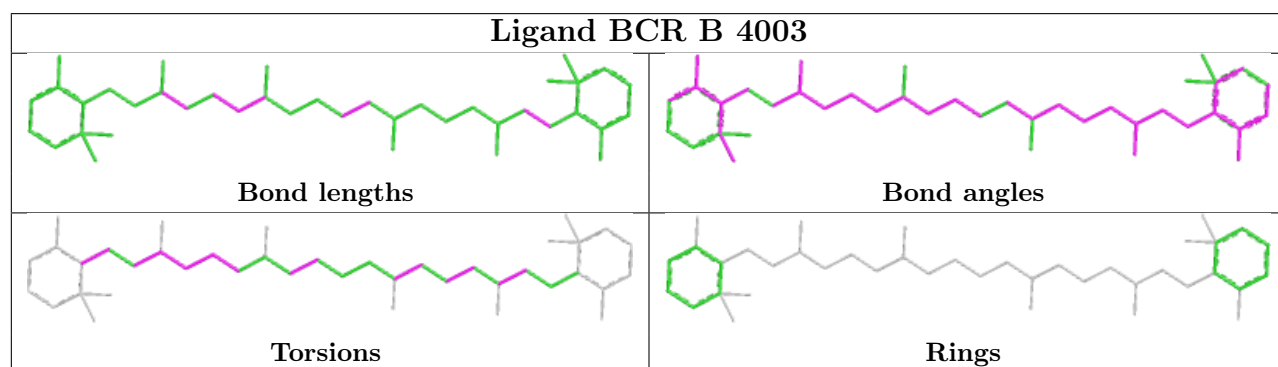
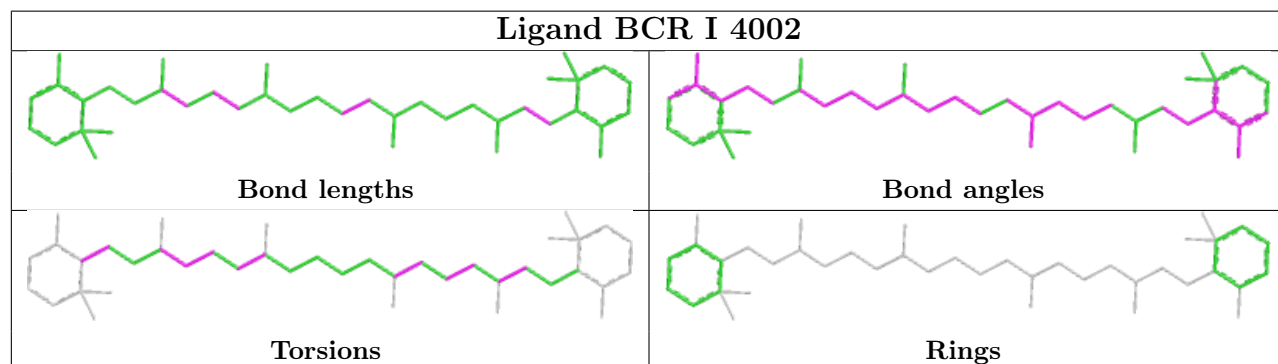
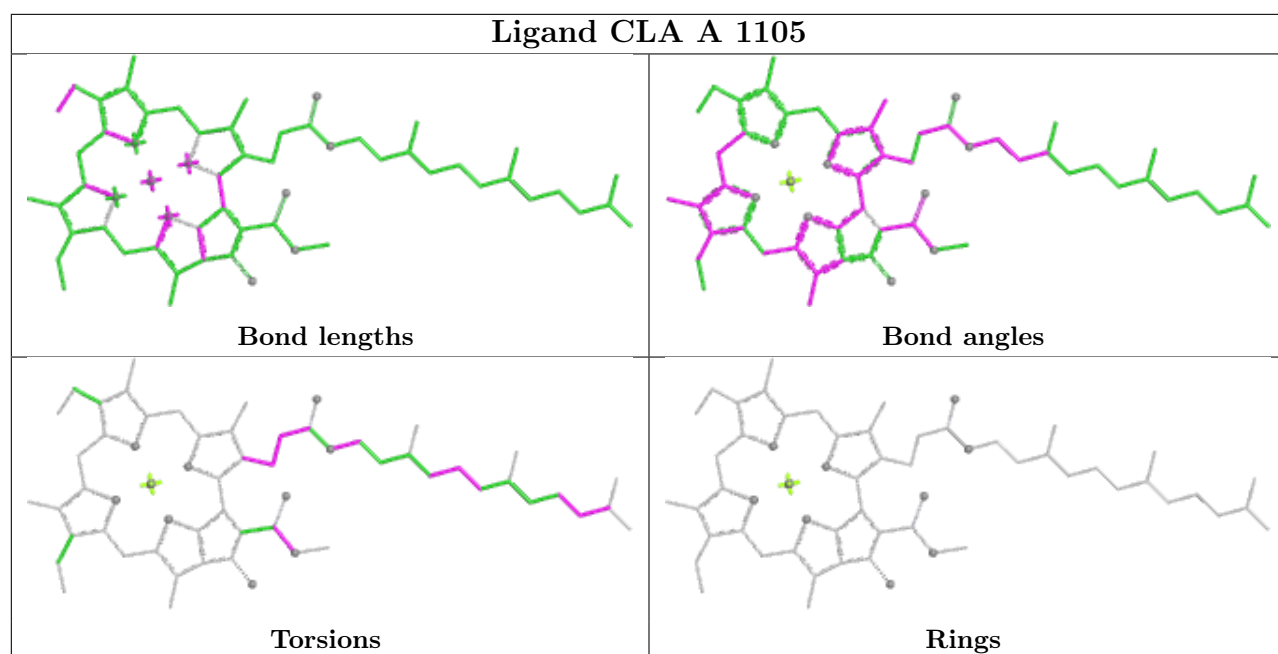
Torsions



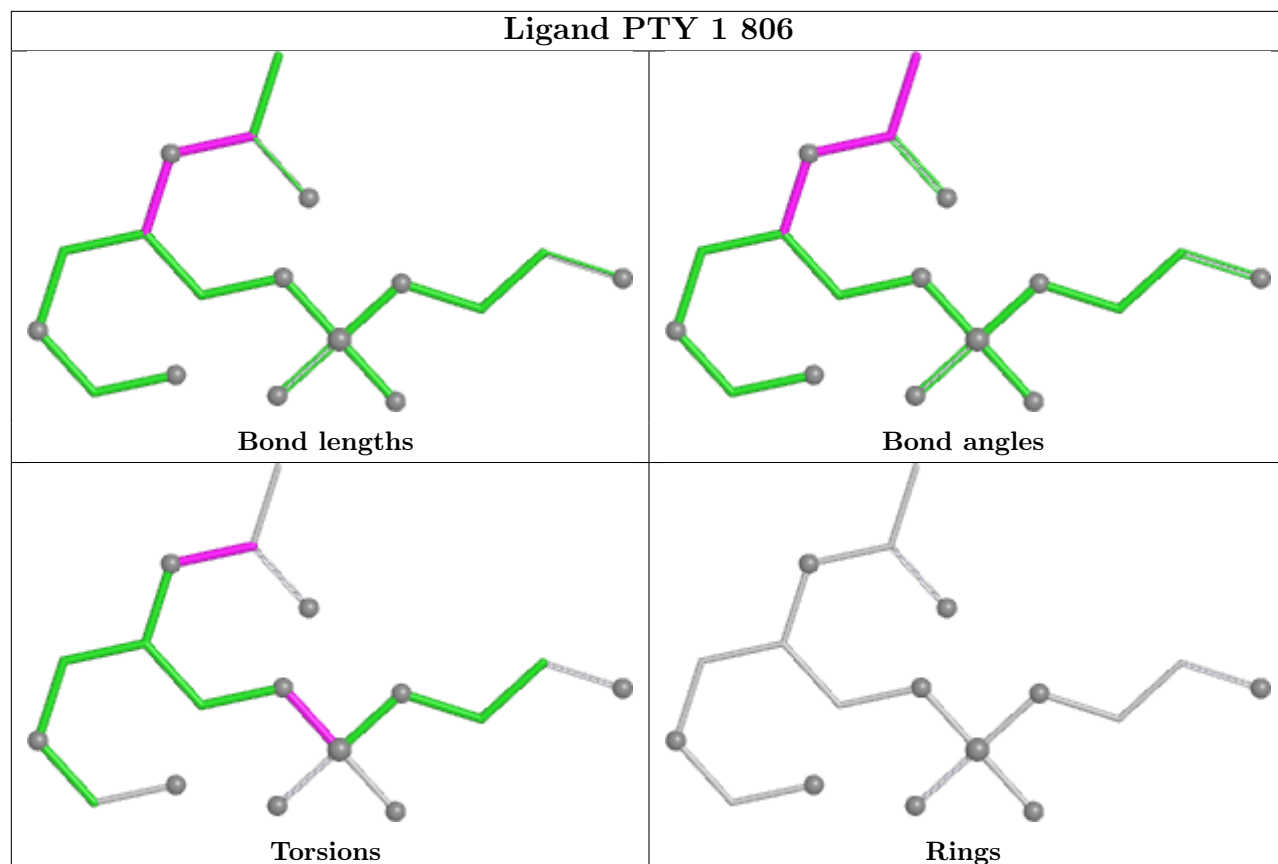
Rings



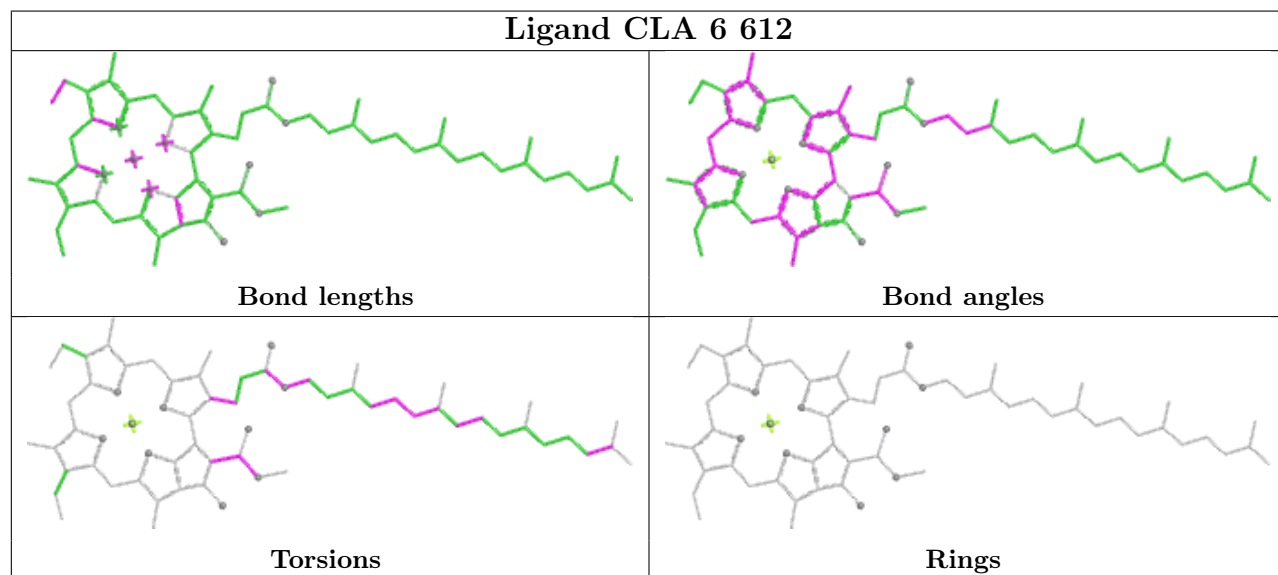
Ligand CLA 2 602**Ligand CLA 1 611**

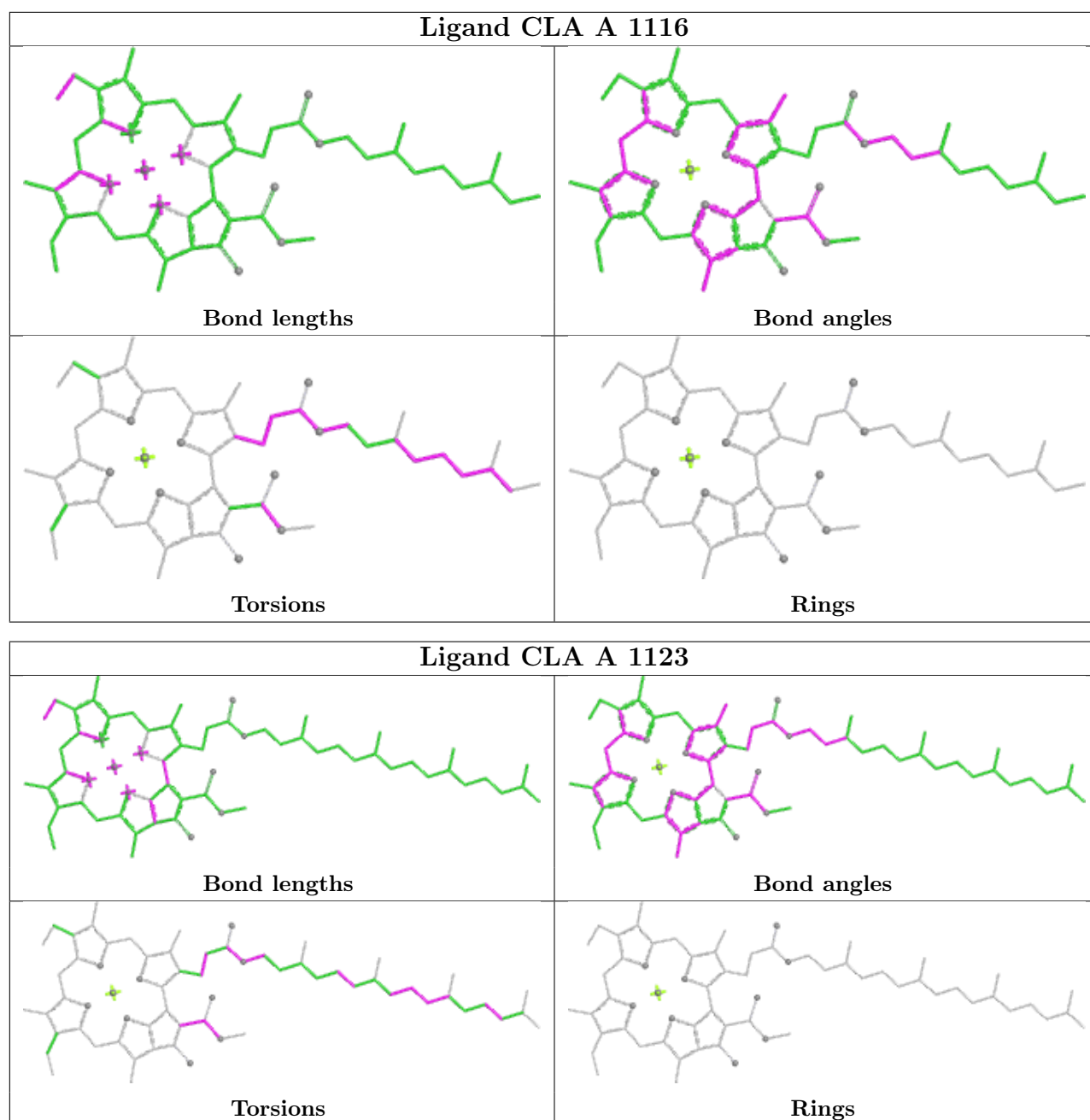


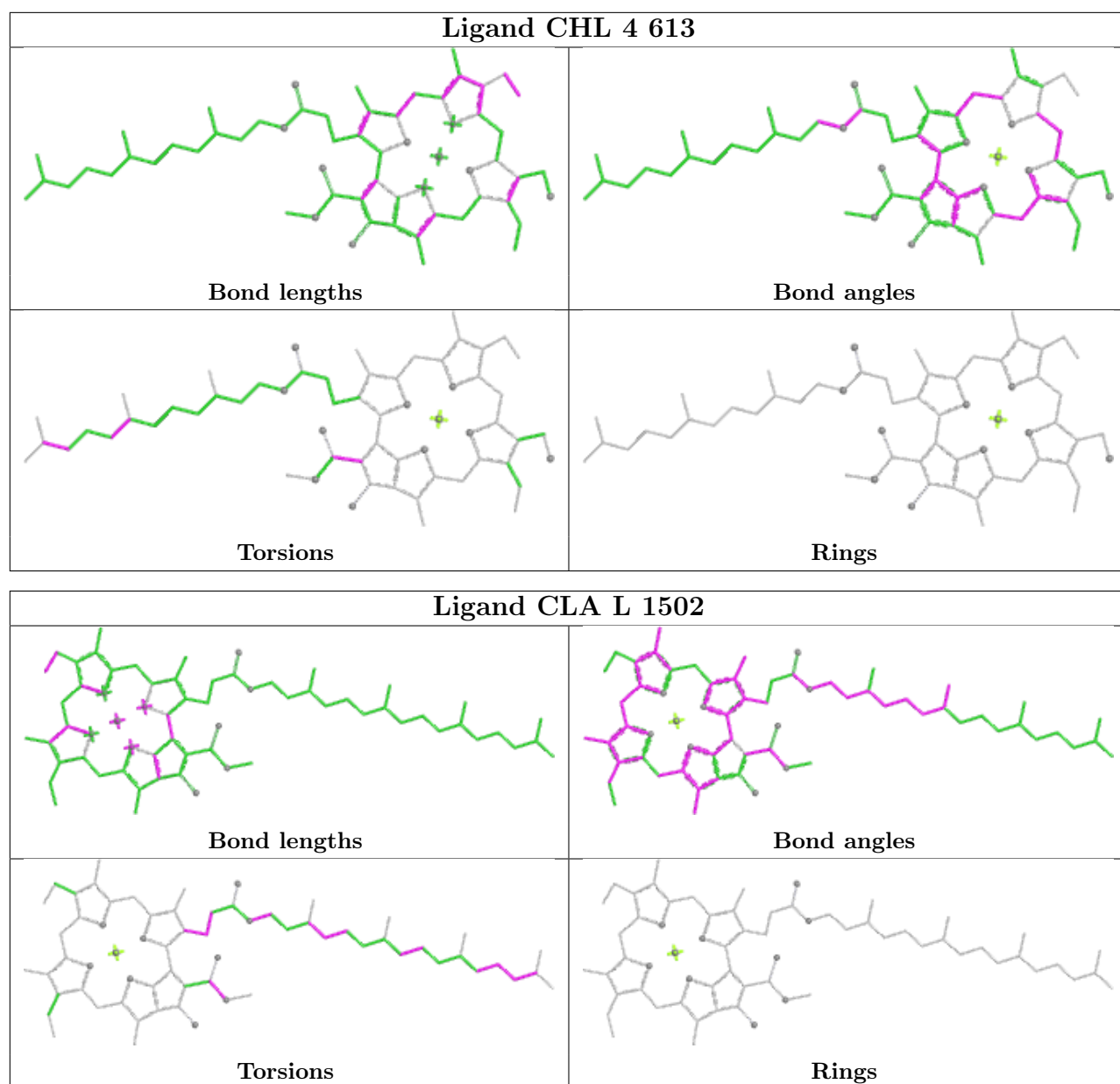
Ligand PTY 1 806

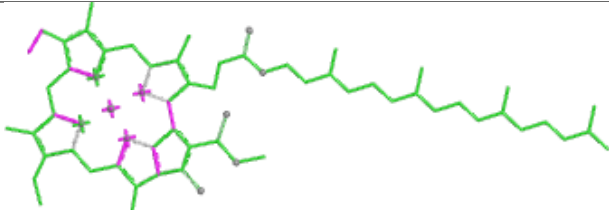
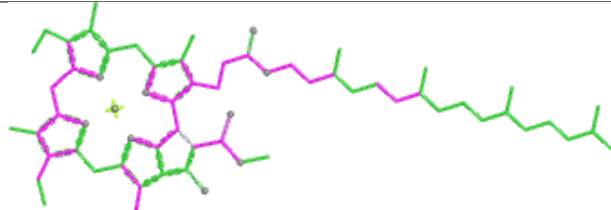
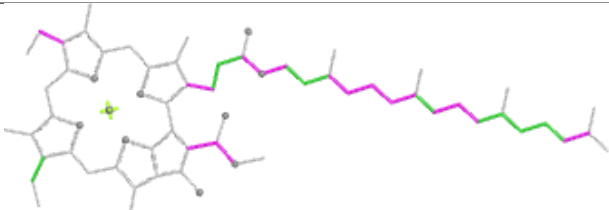
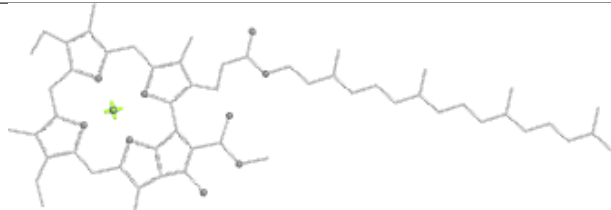


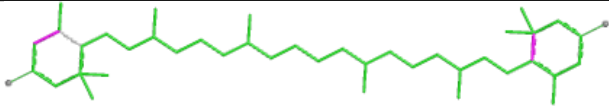
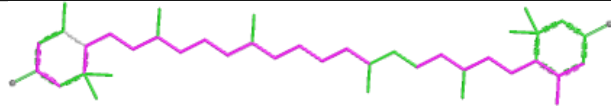
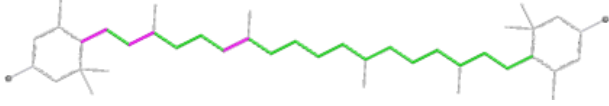
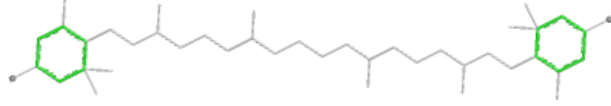
Ligand CLA 6 612

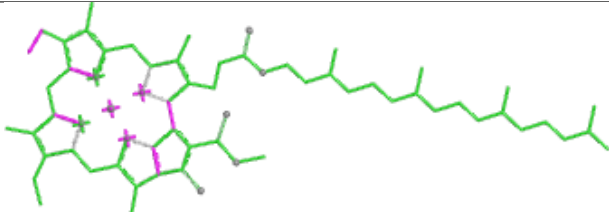
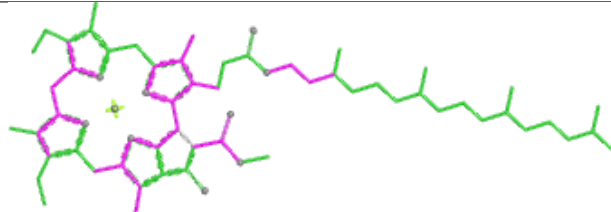
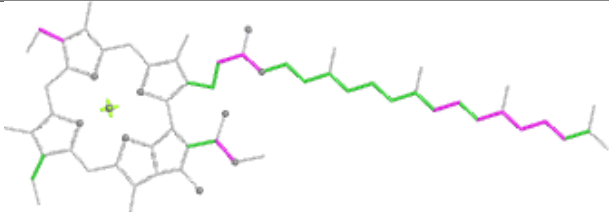
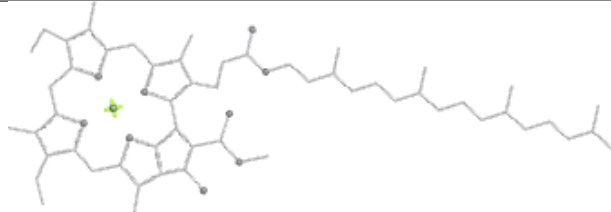


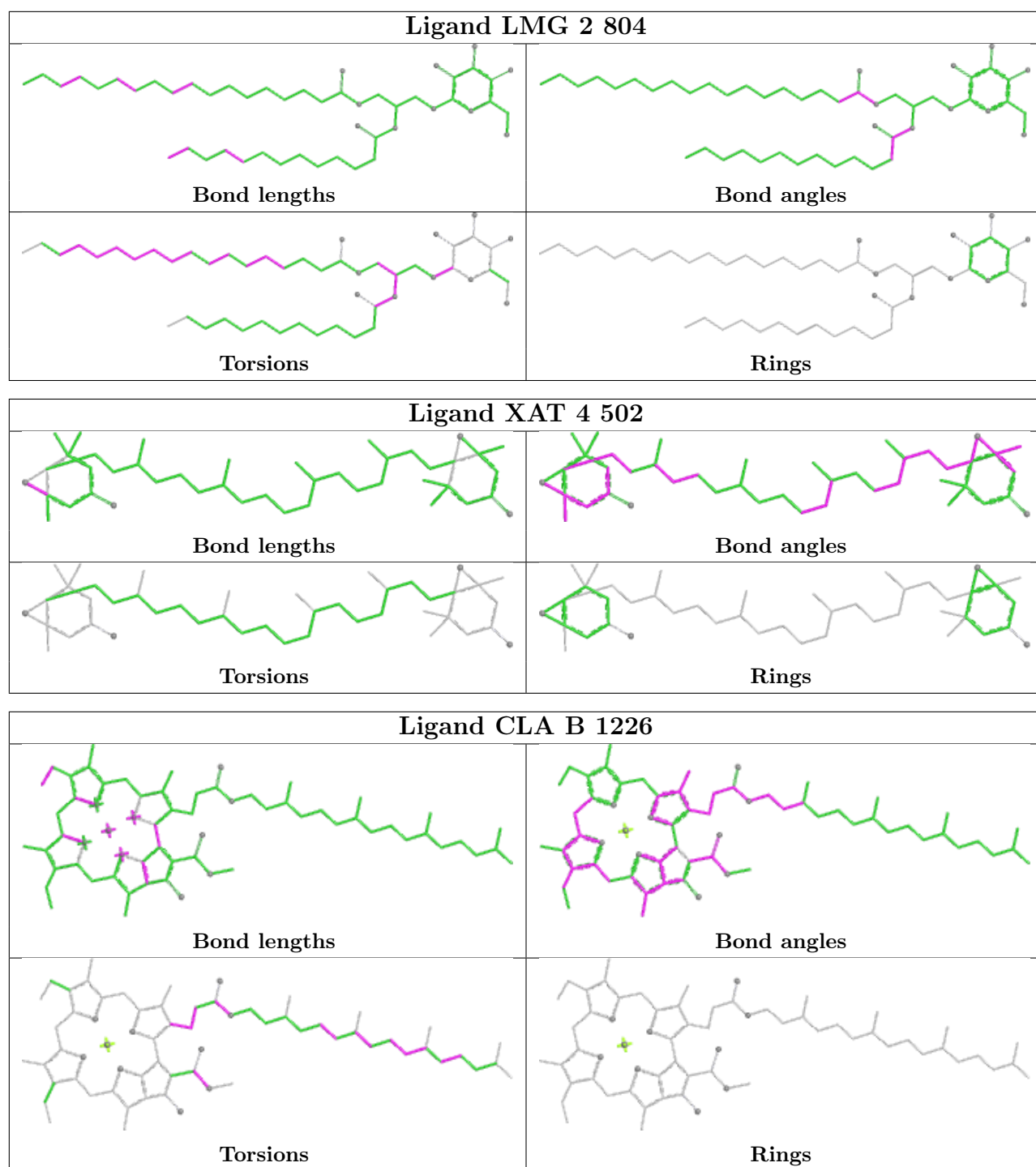


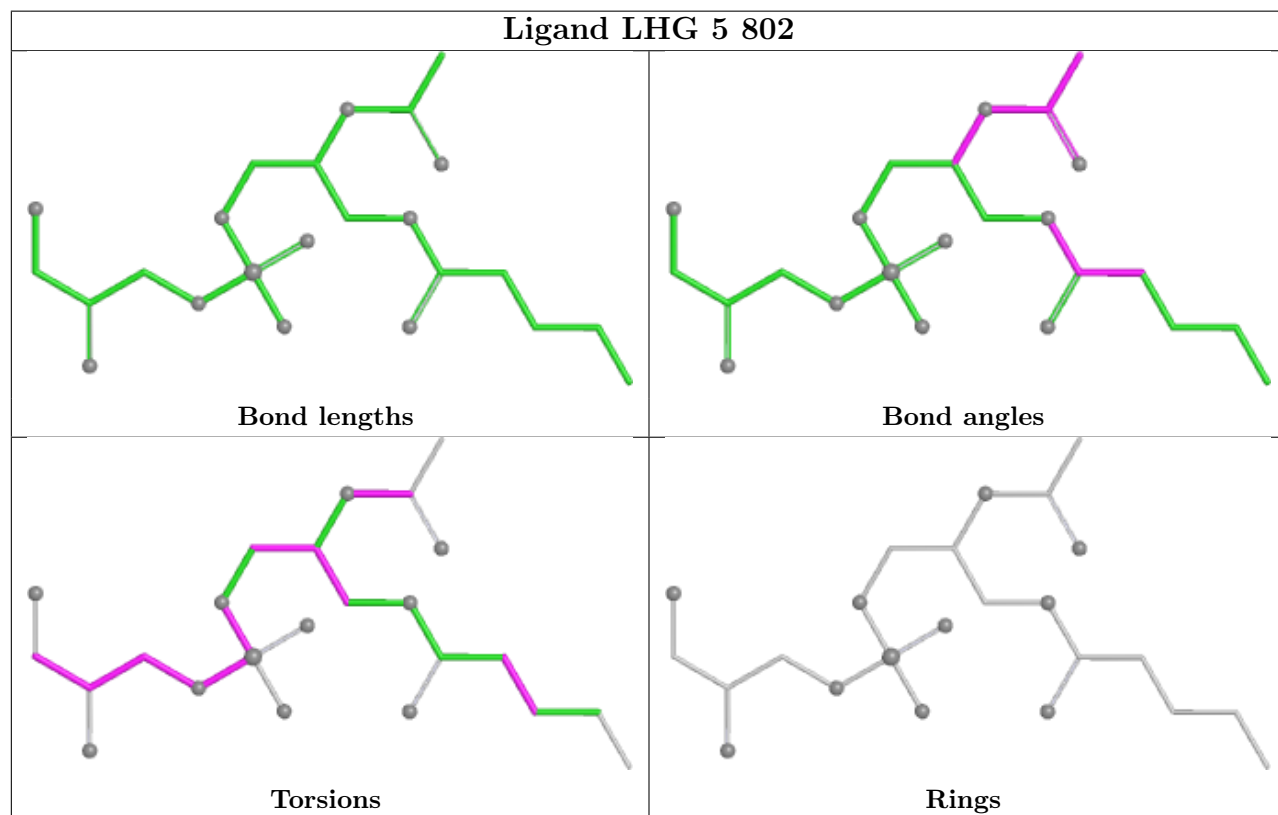
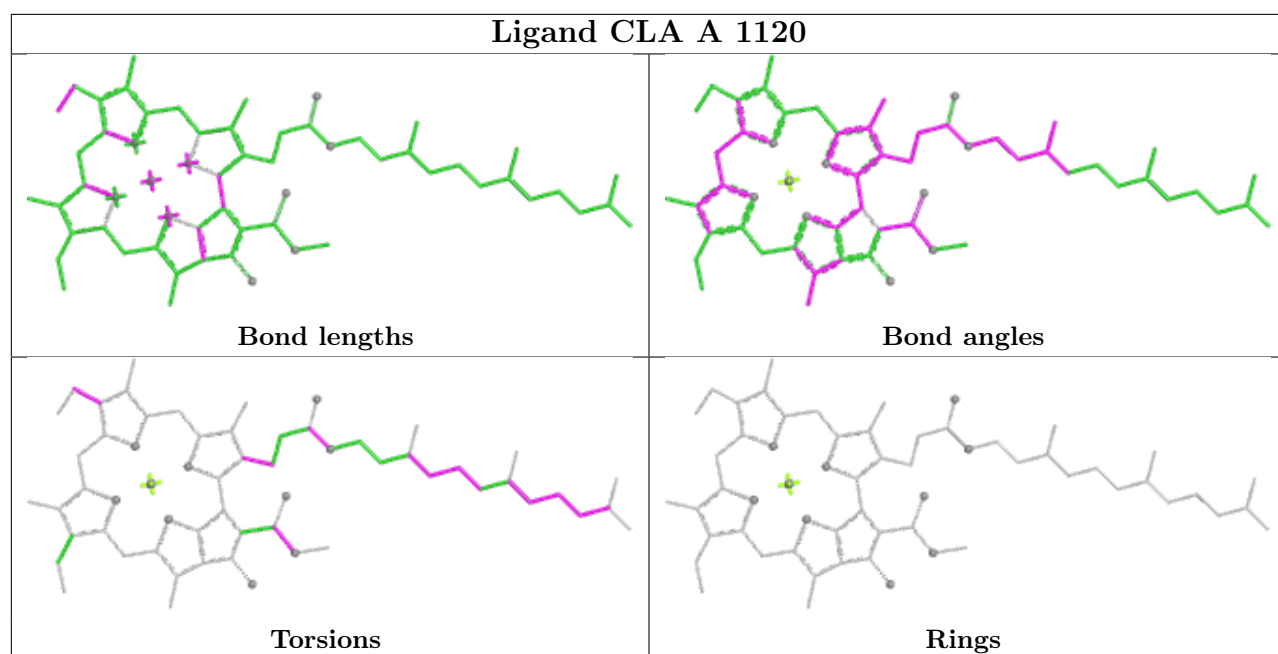


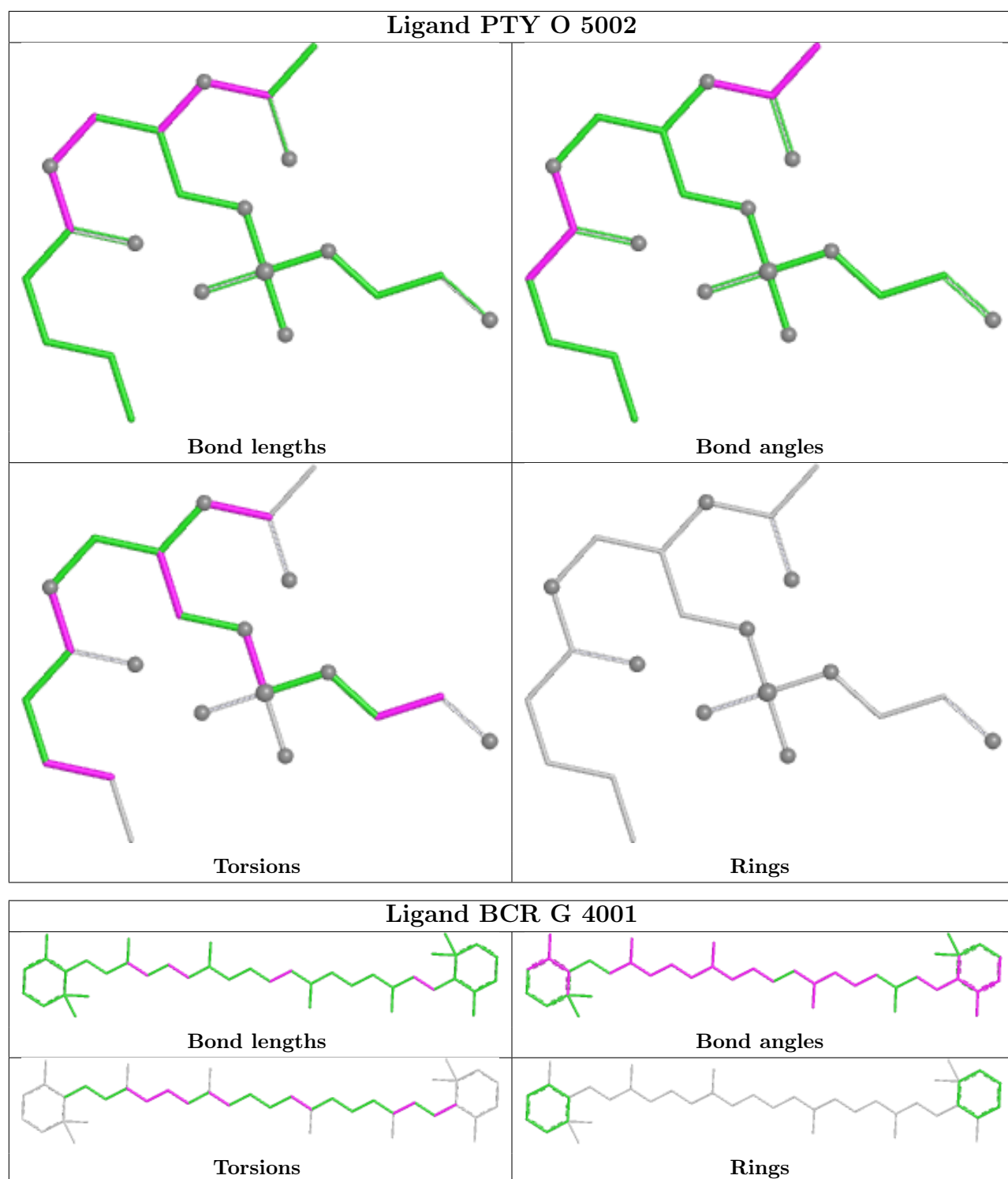
Ligand CLA B 1218	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 5 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

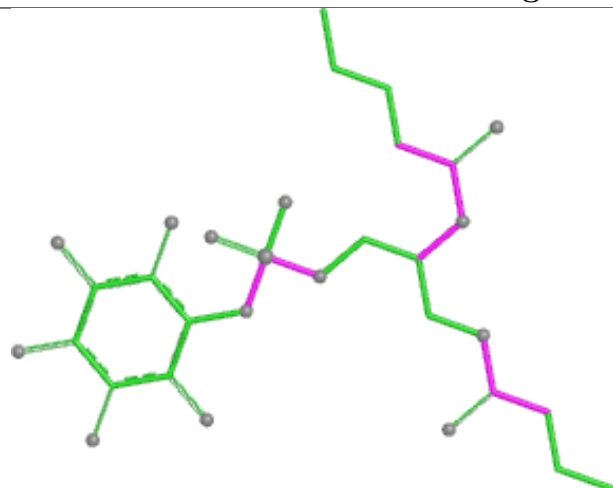
Ligand CLA B 1240	
	
Bond lengths	Bond angles
	
Torsions	Rings



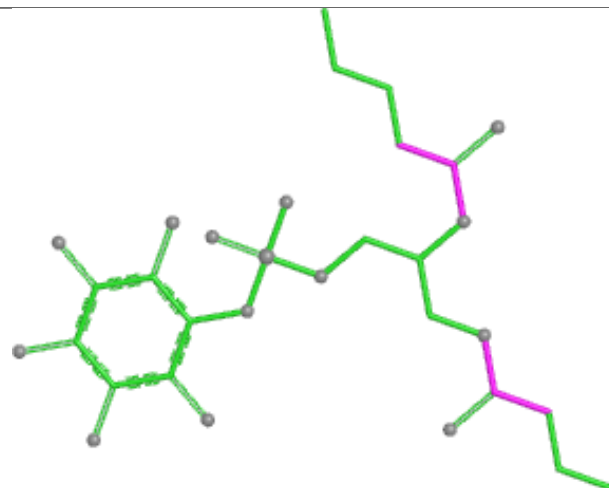




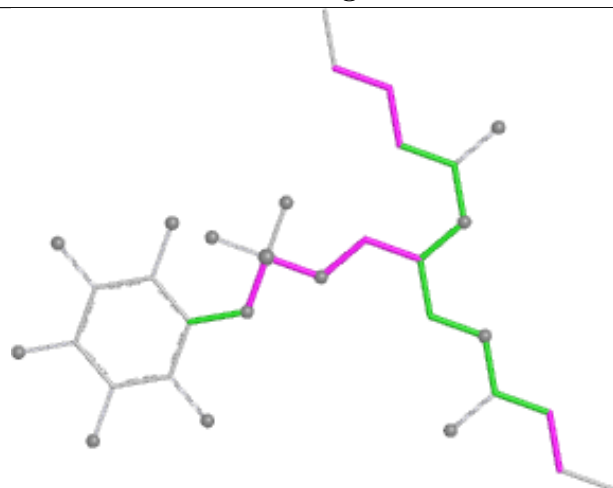
Ligand P3H 5 806



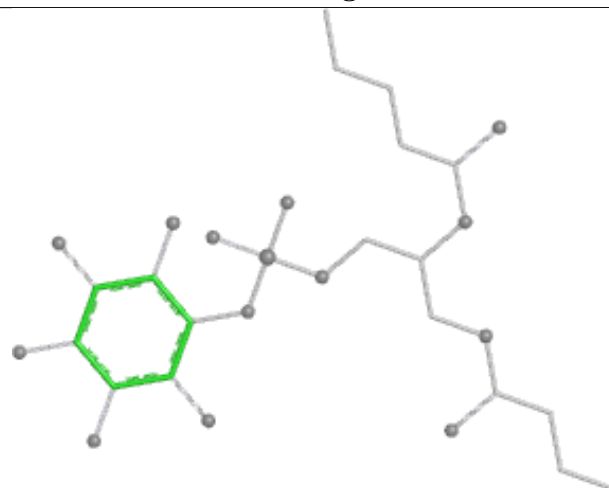
Bond lengths



Bond angles

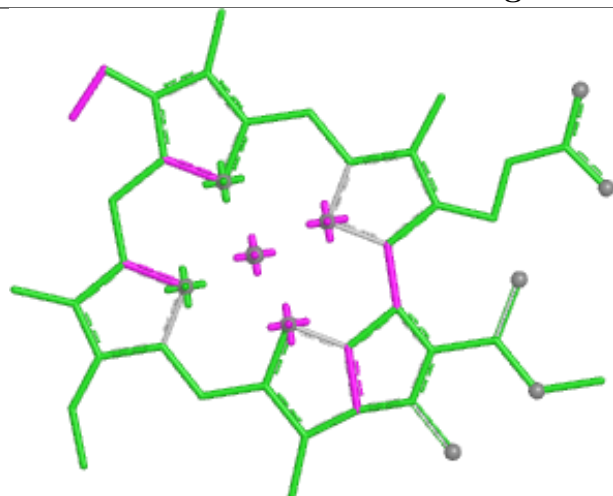


Torsions

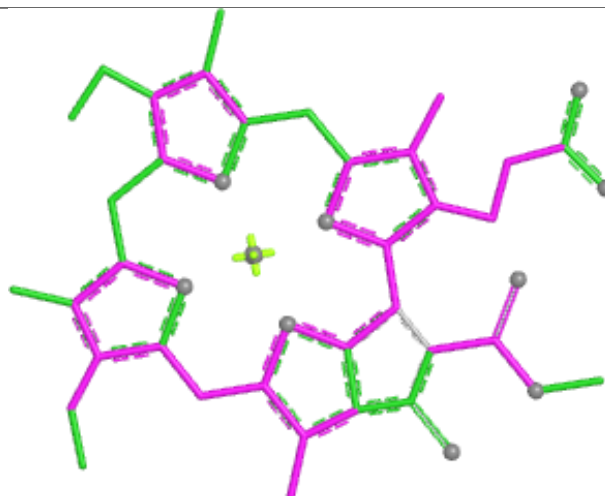


Rings

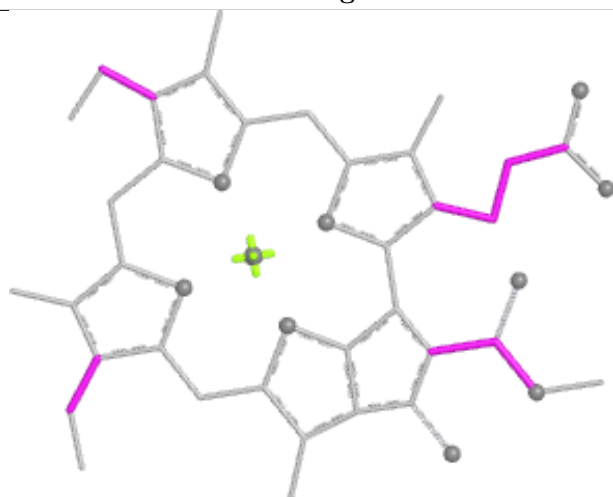
Ligand CLA K 1401



Bond lengths



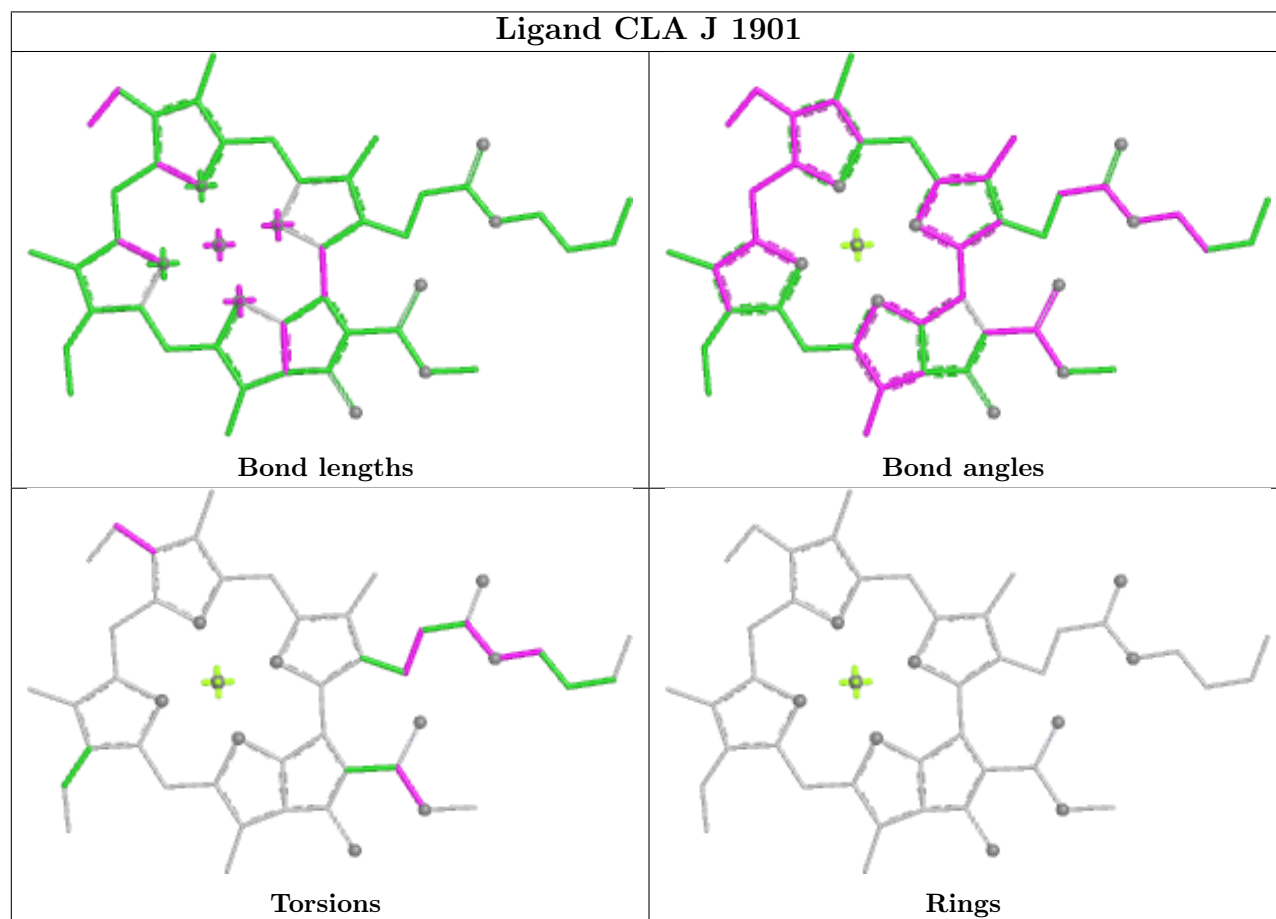
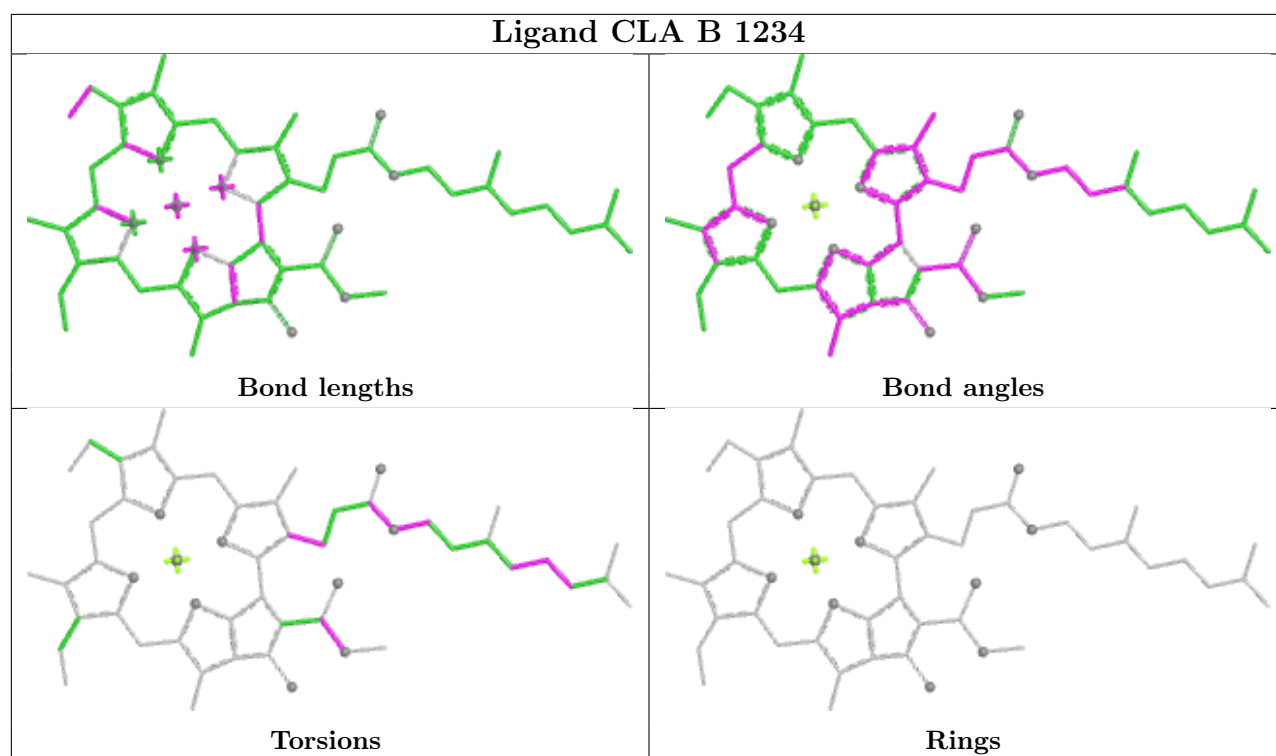
Bond angles

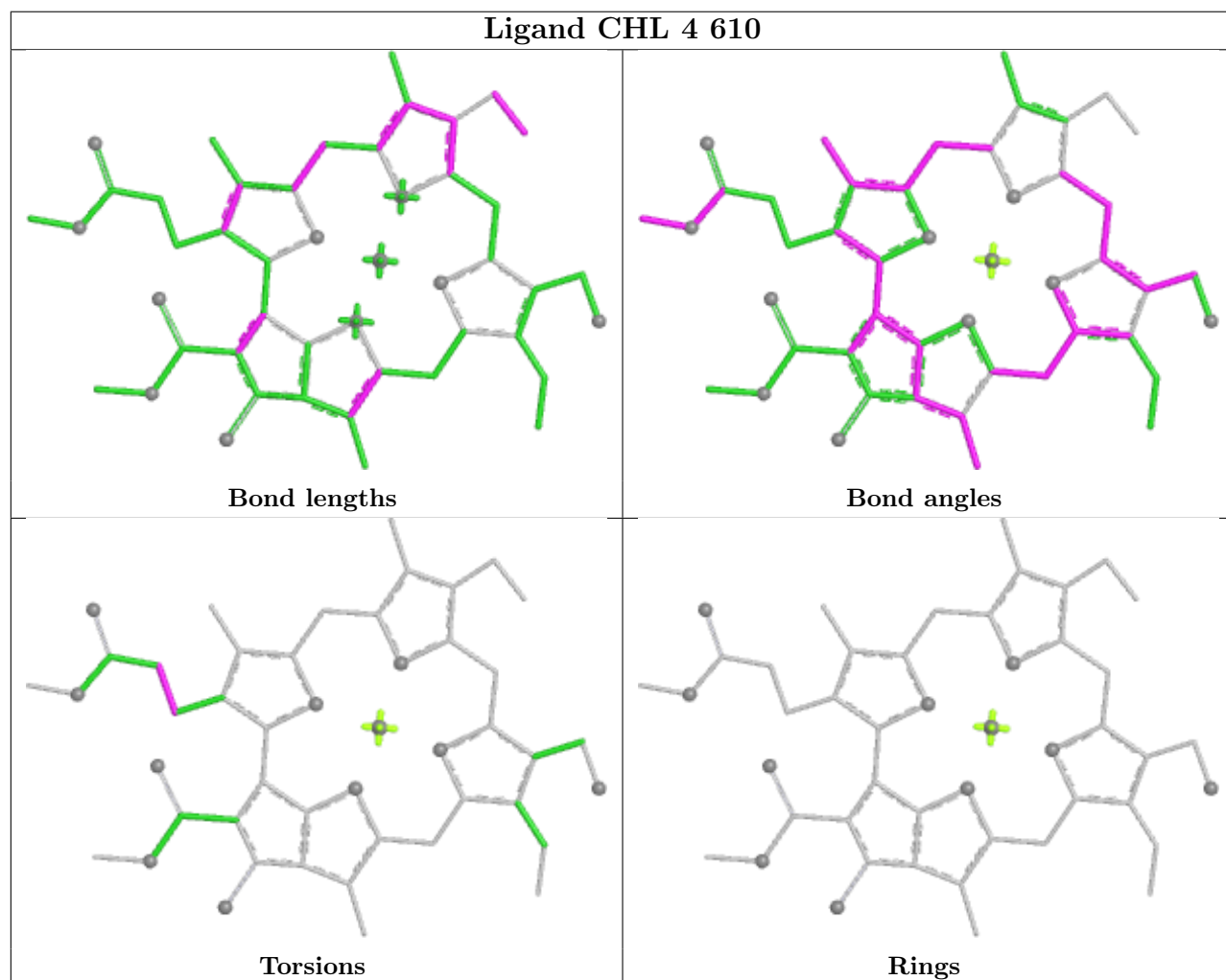
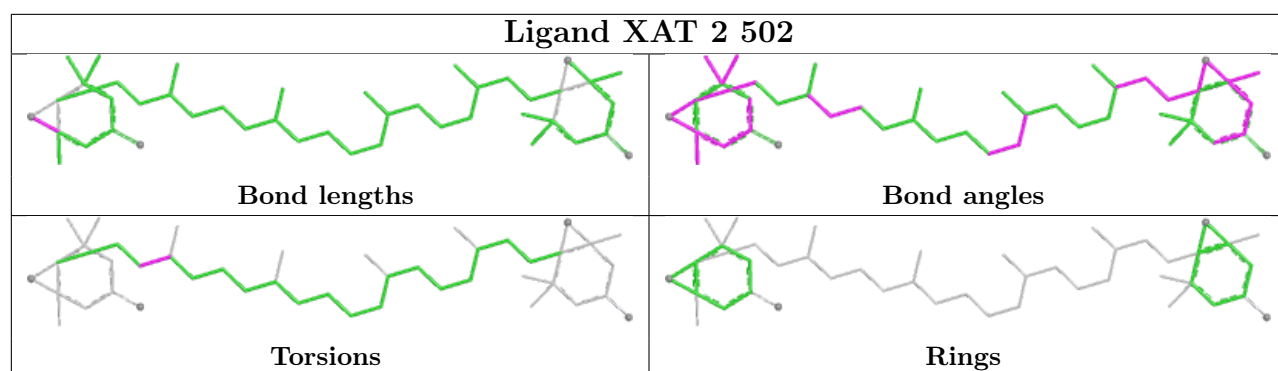


Torsions

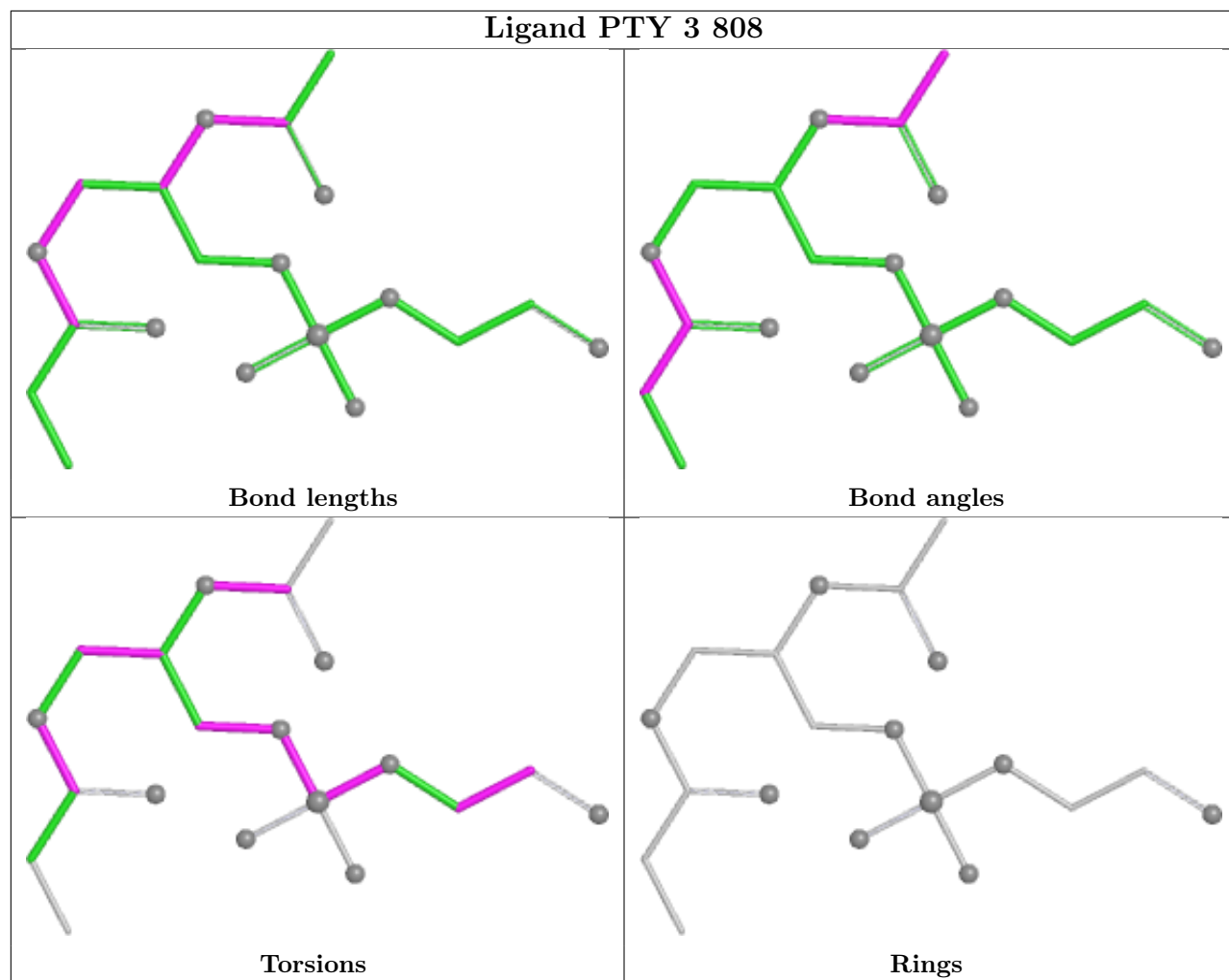


Rings

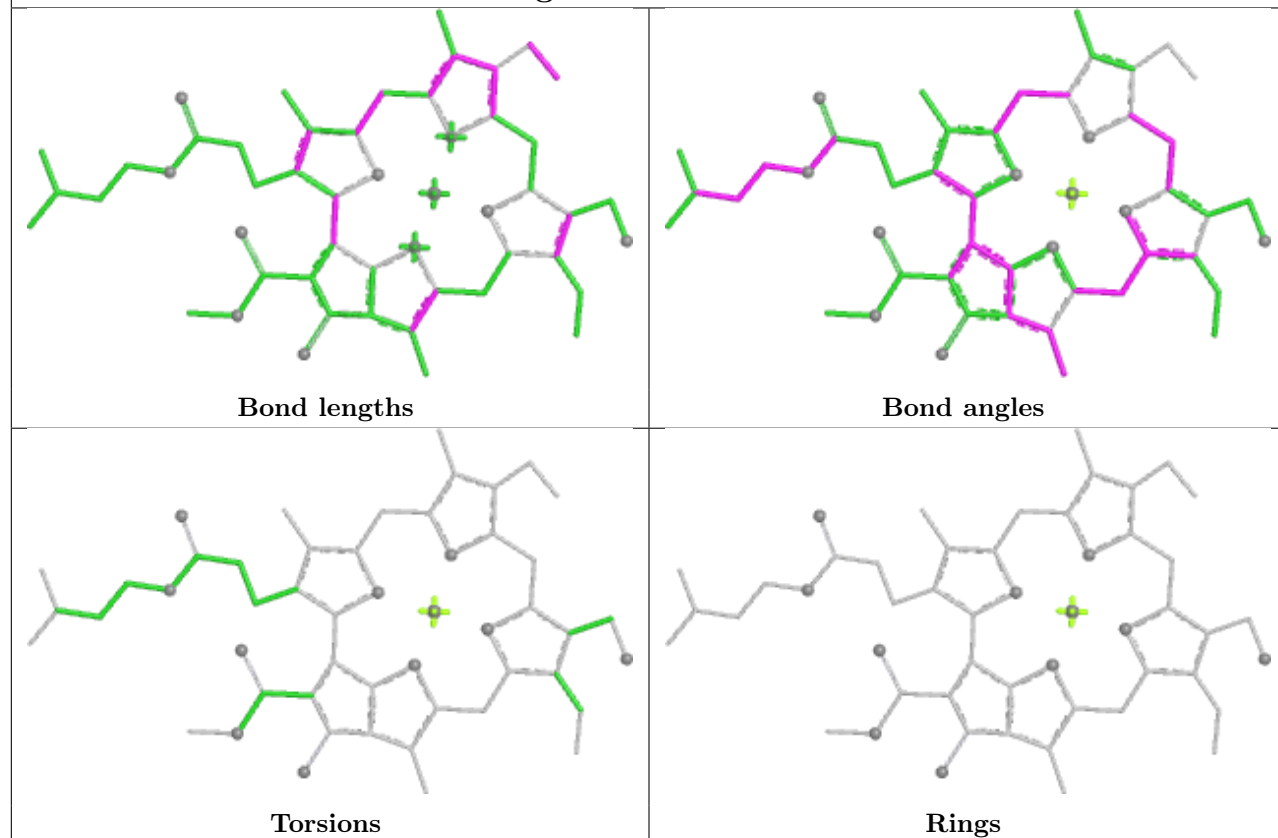




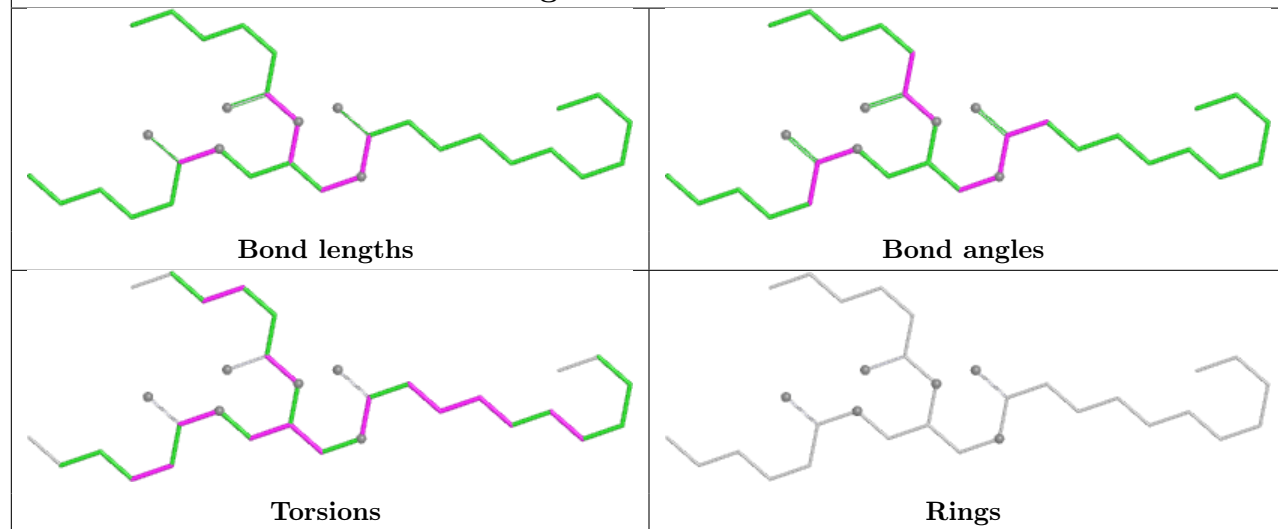
Ligand PTY 3 808

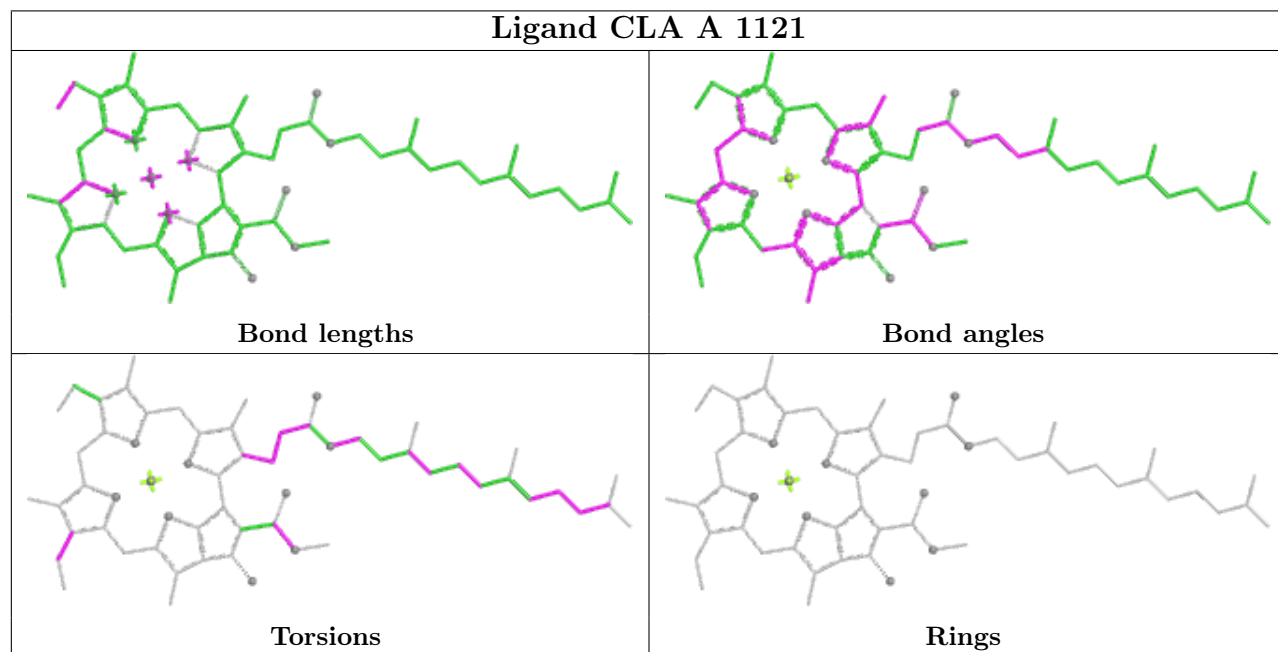
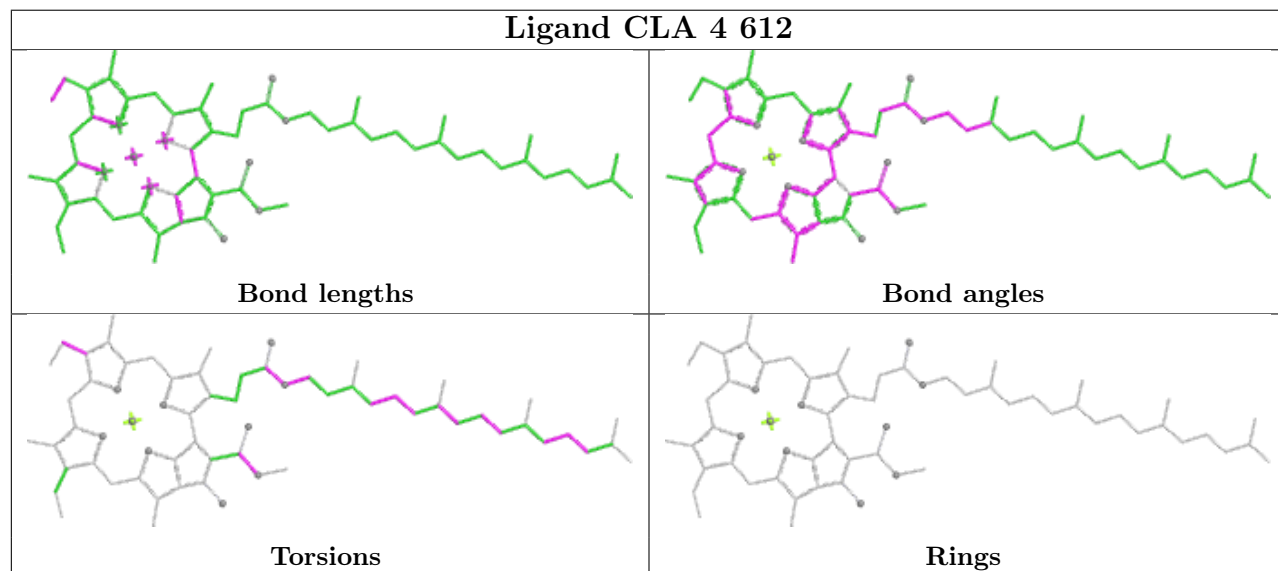
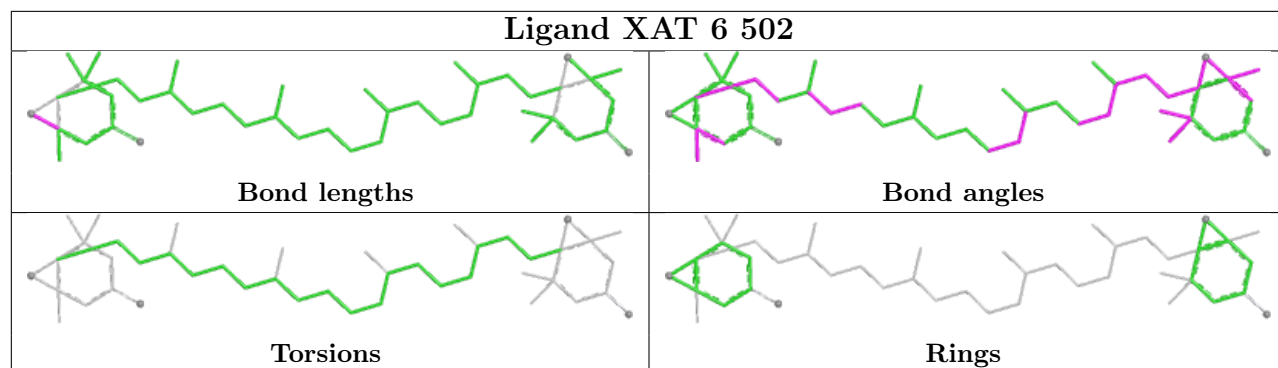


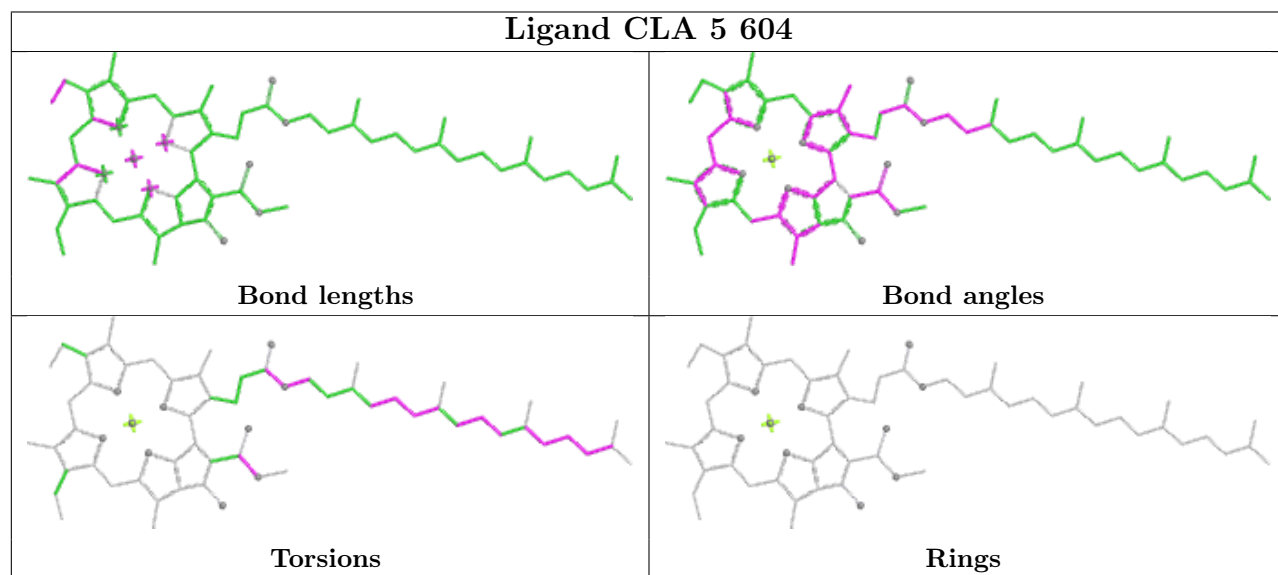
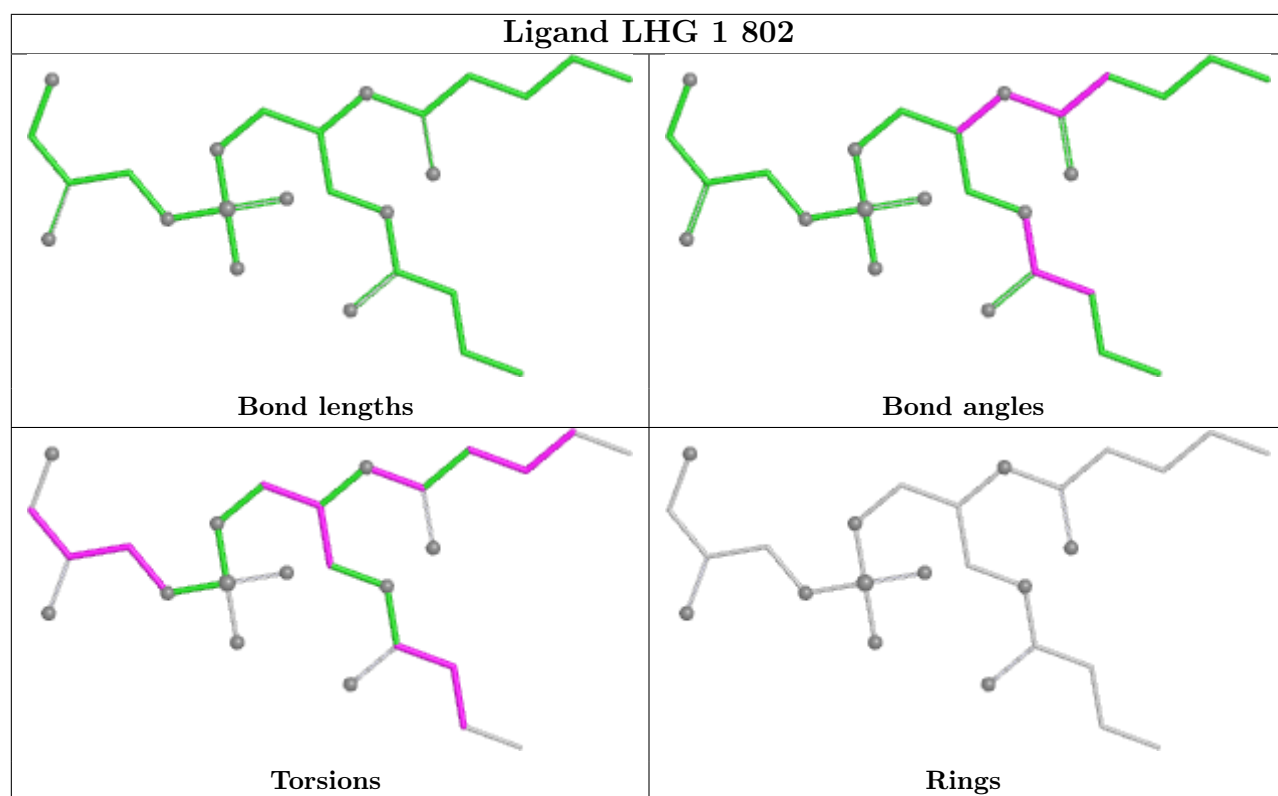
Ligand CHL 4 611



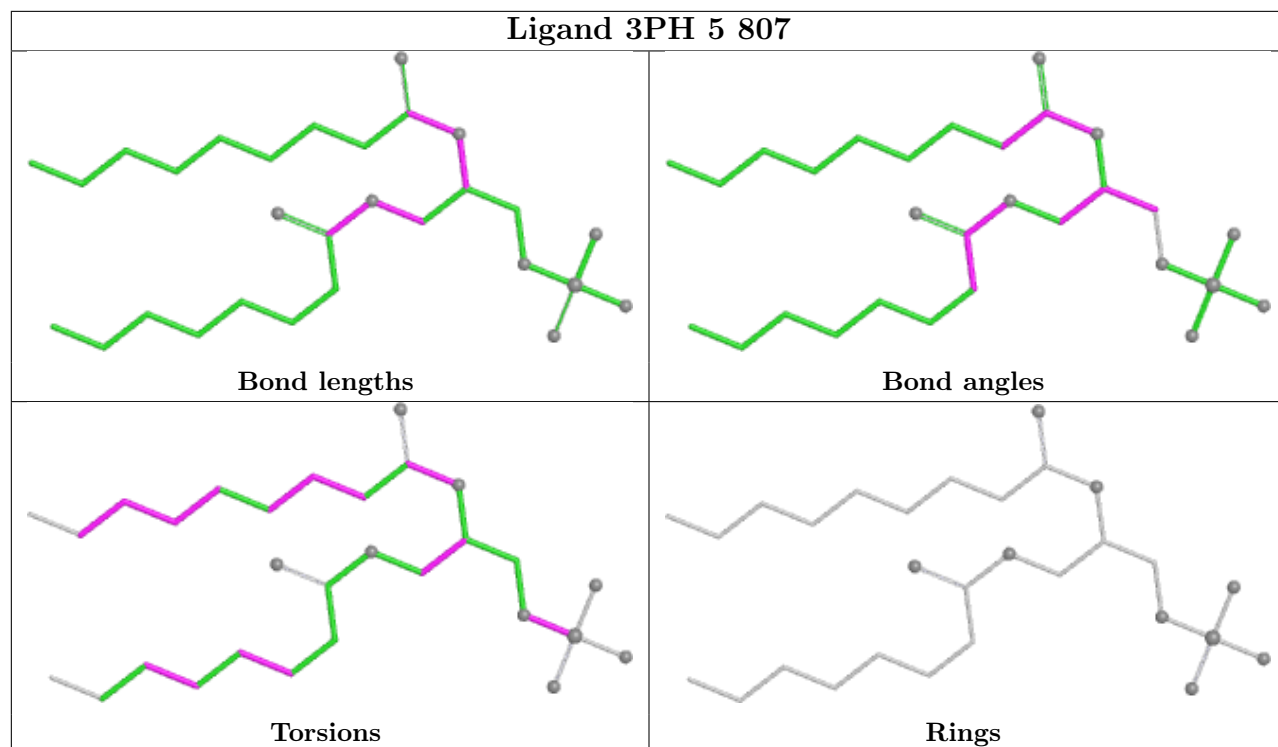
Ligand 4RF 5 805



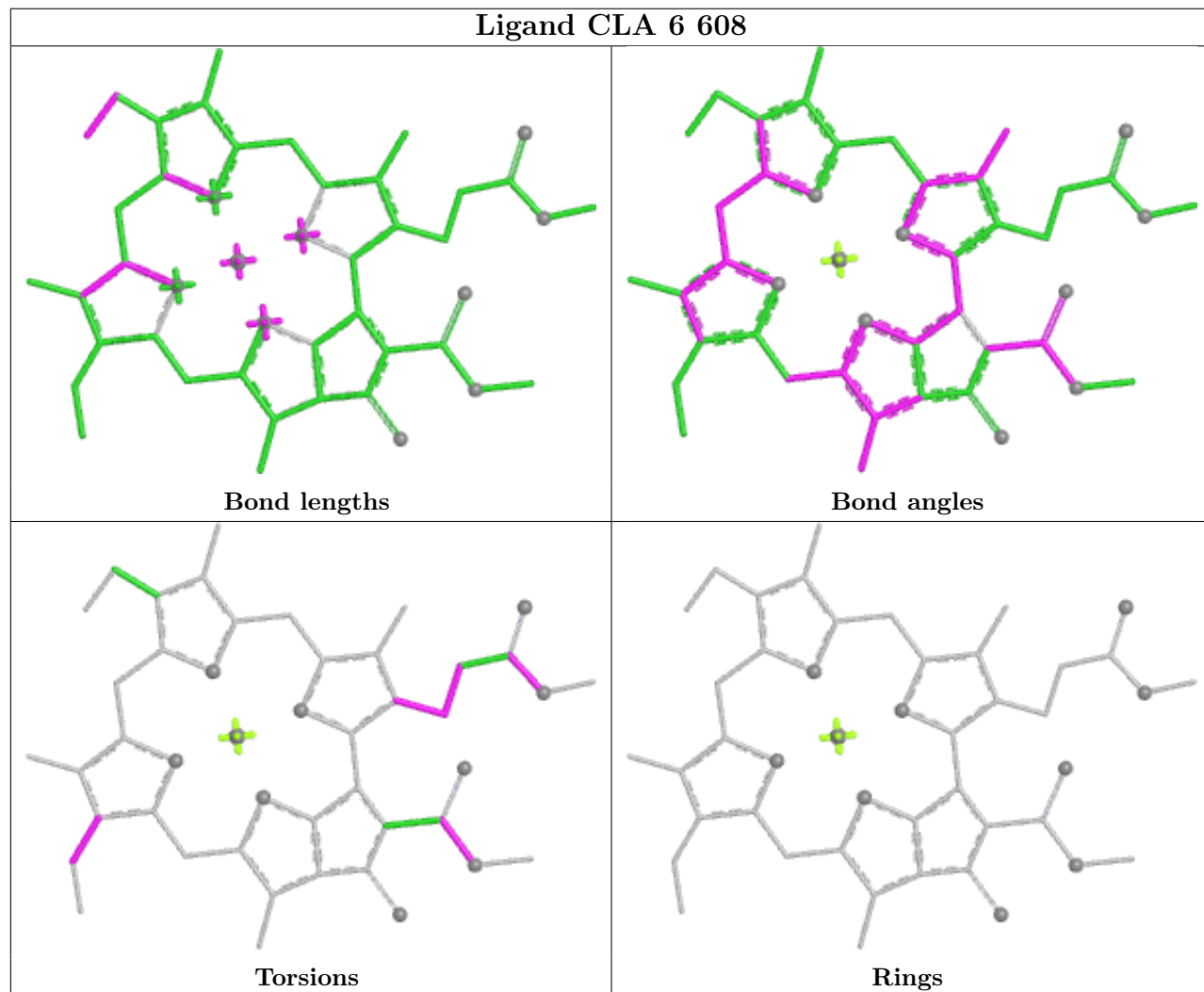


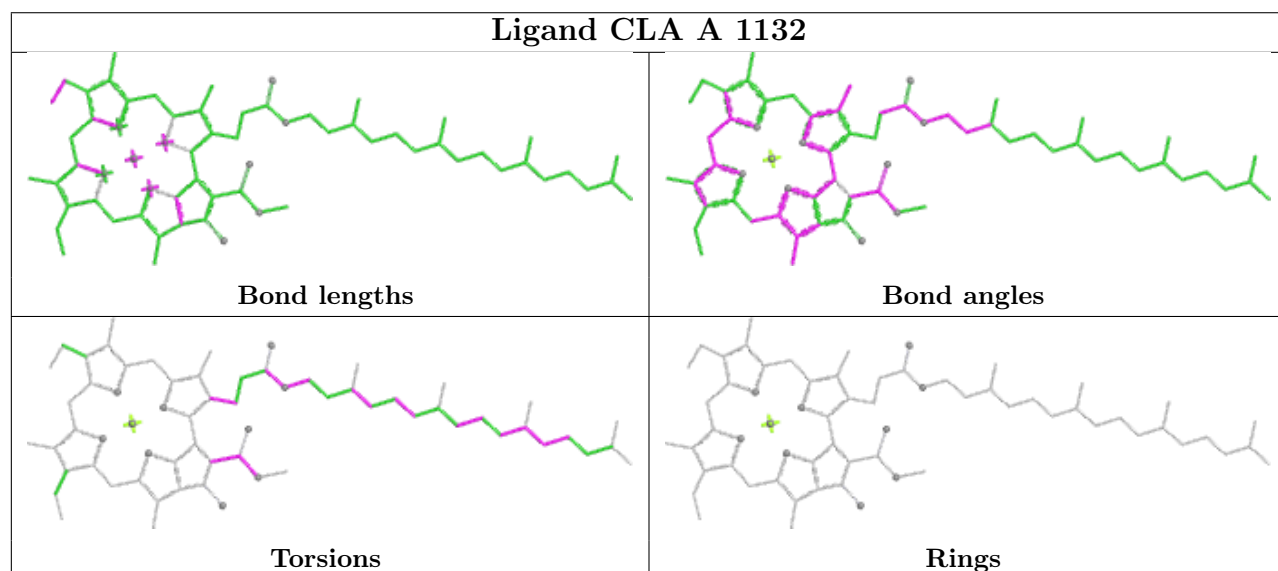
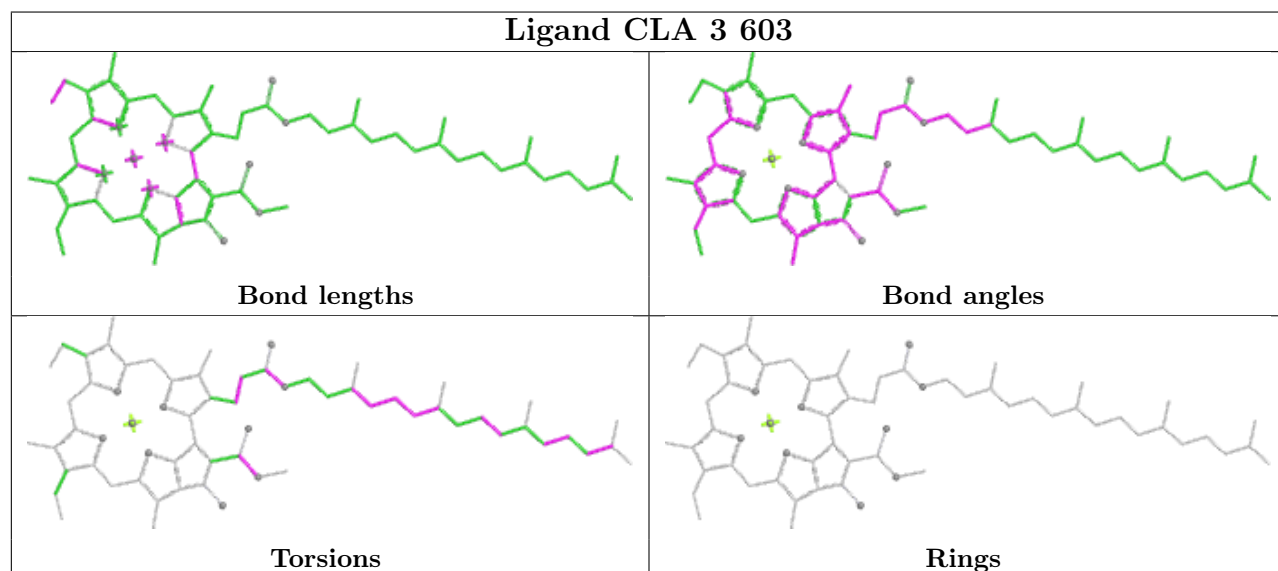
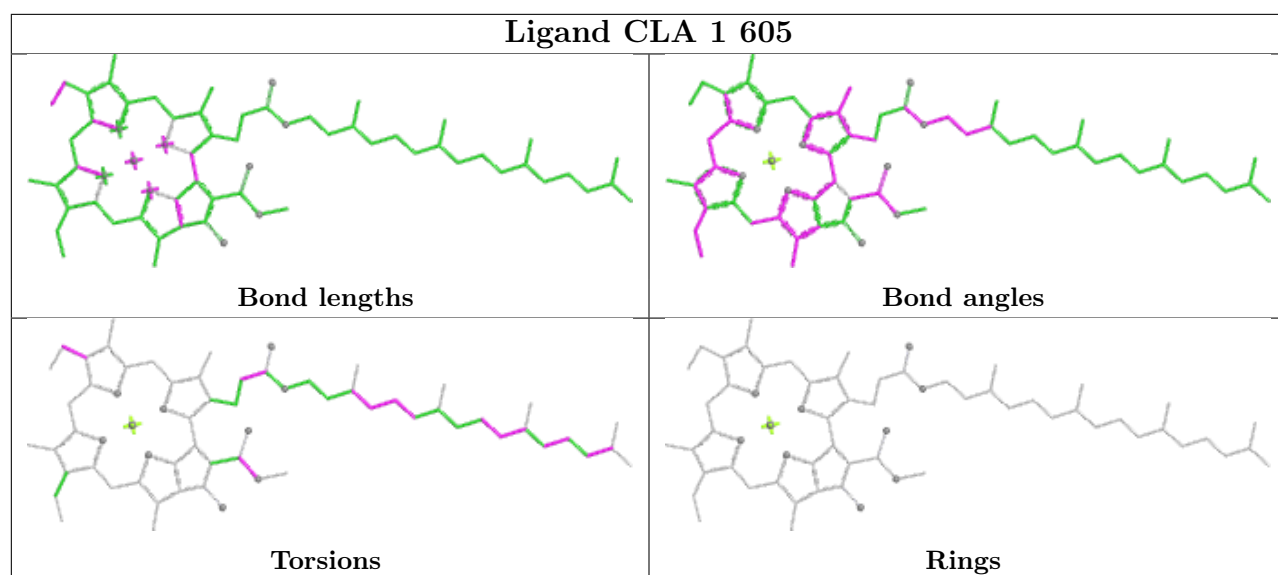


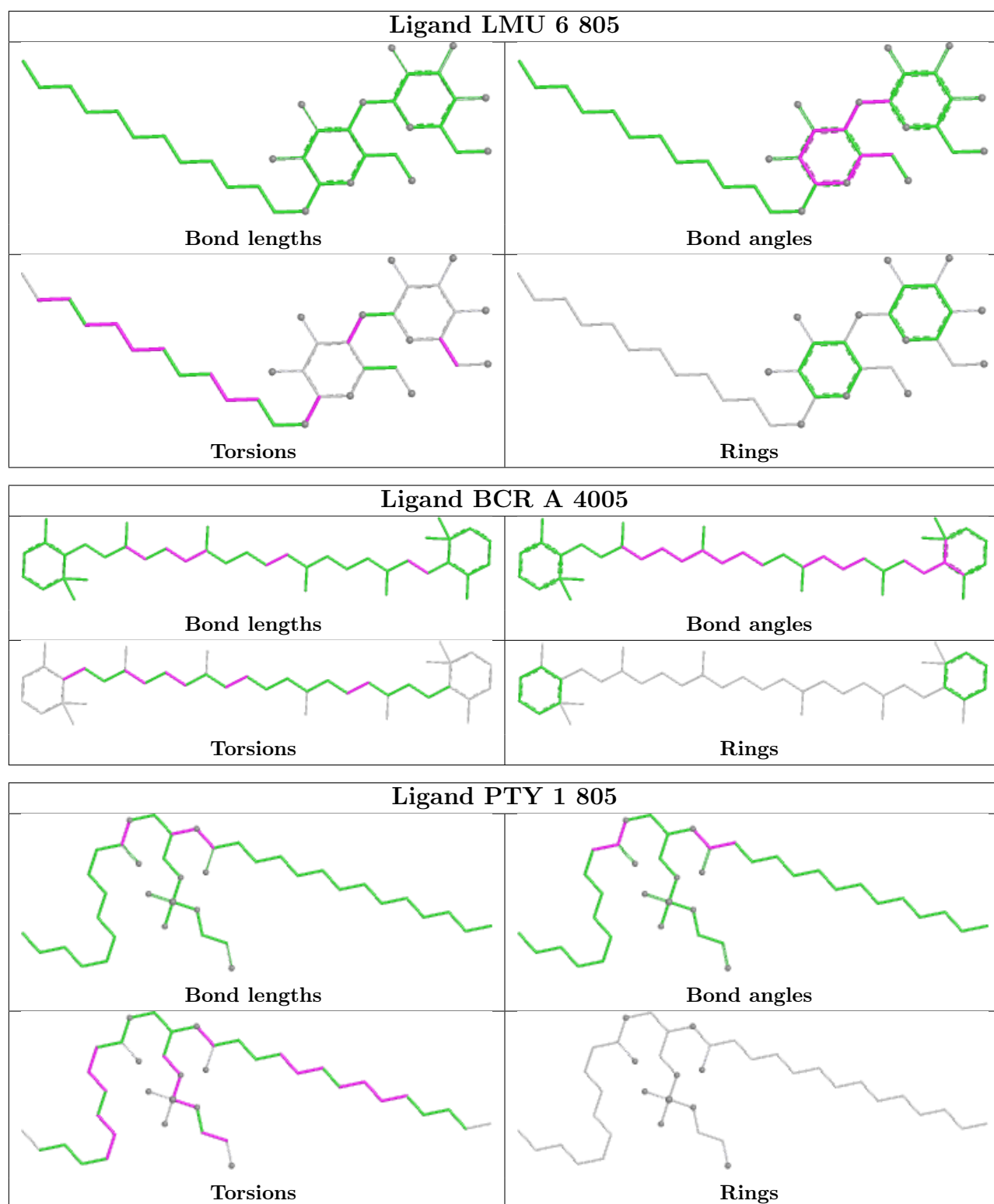
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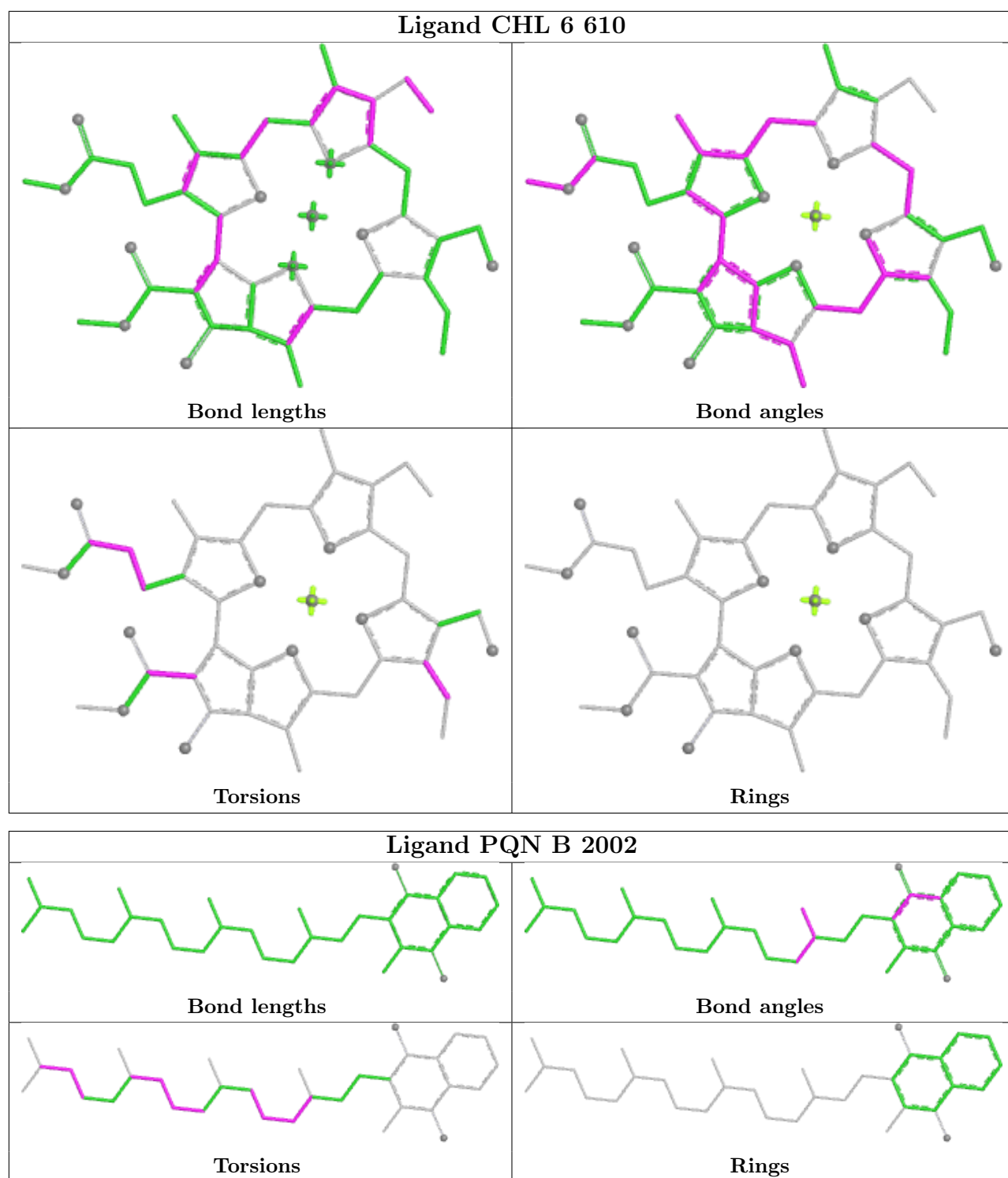


Ligand CLA 6 608

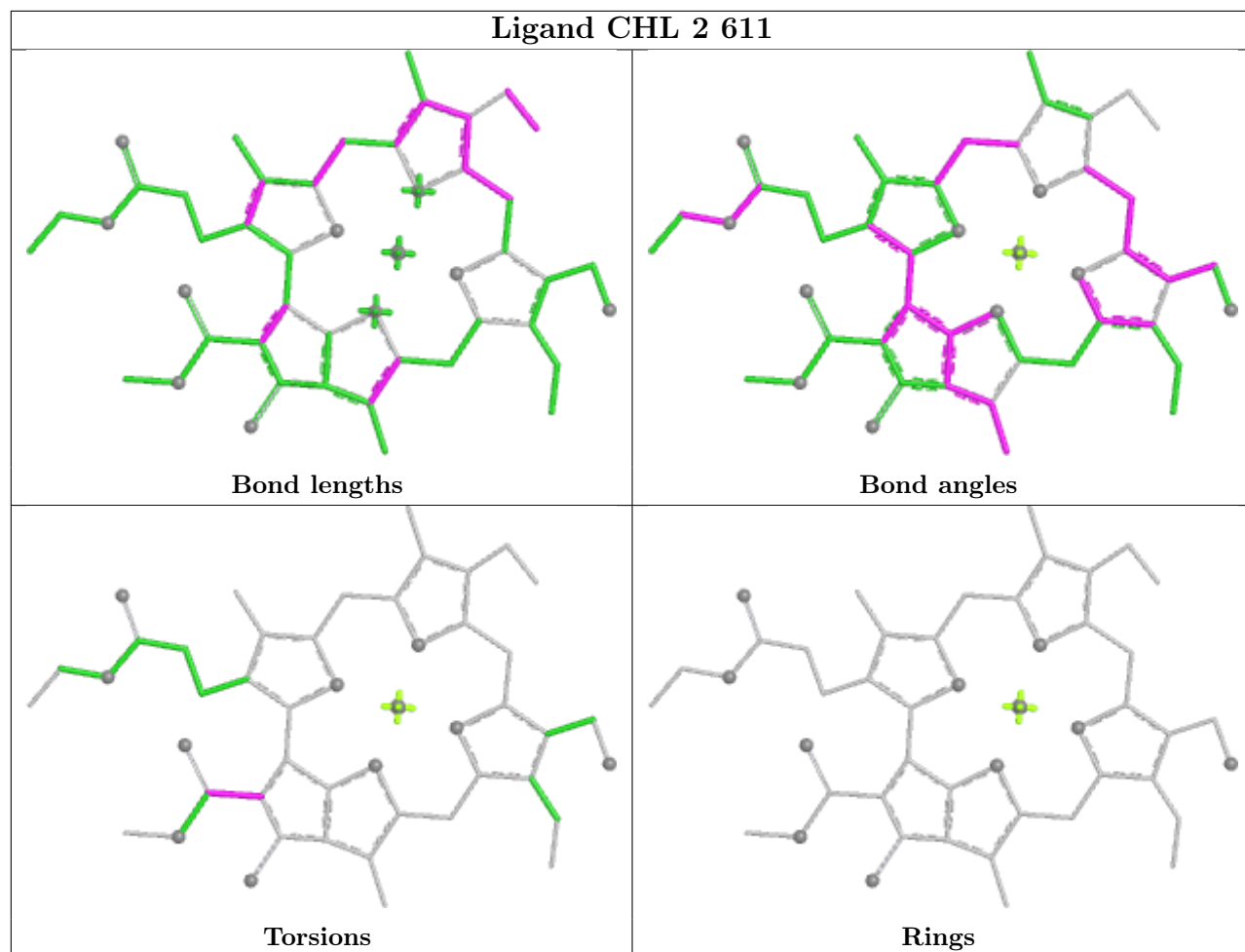




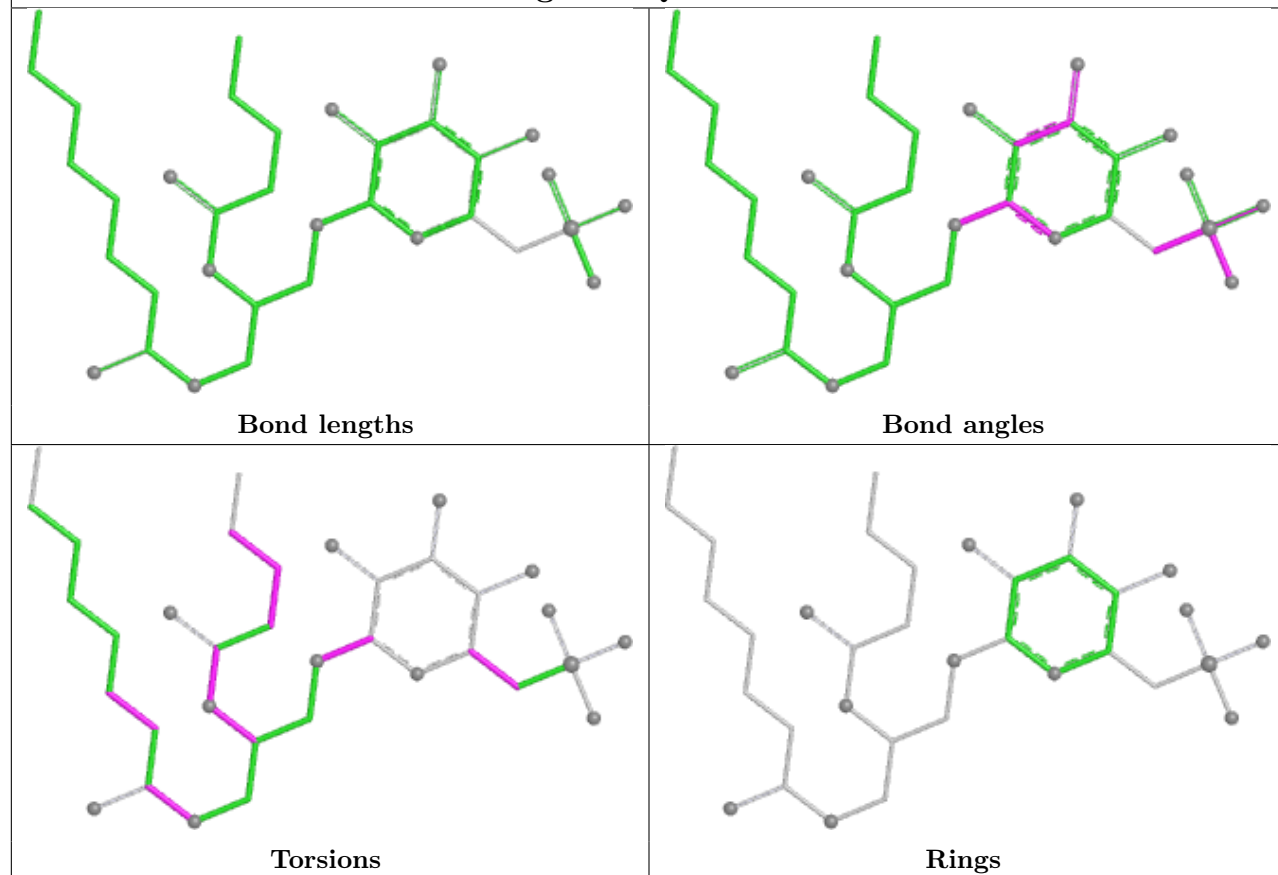




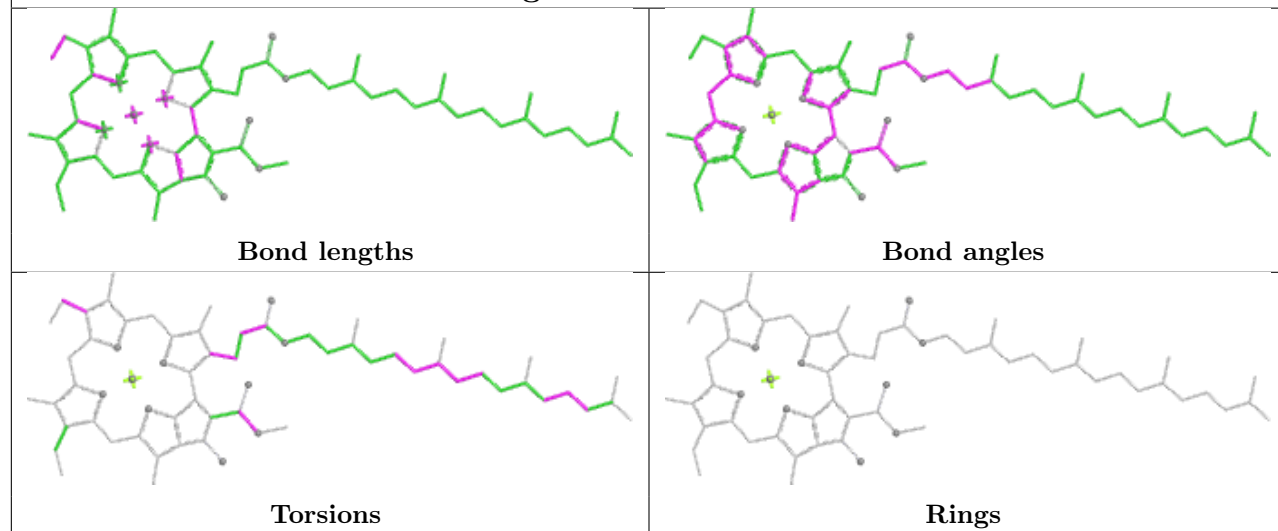
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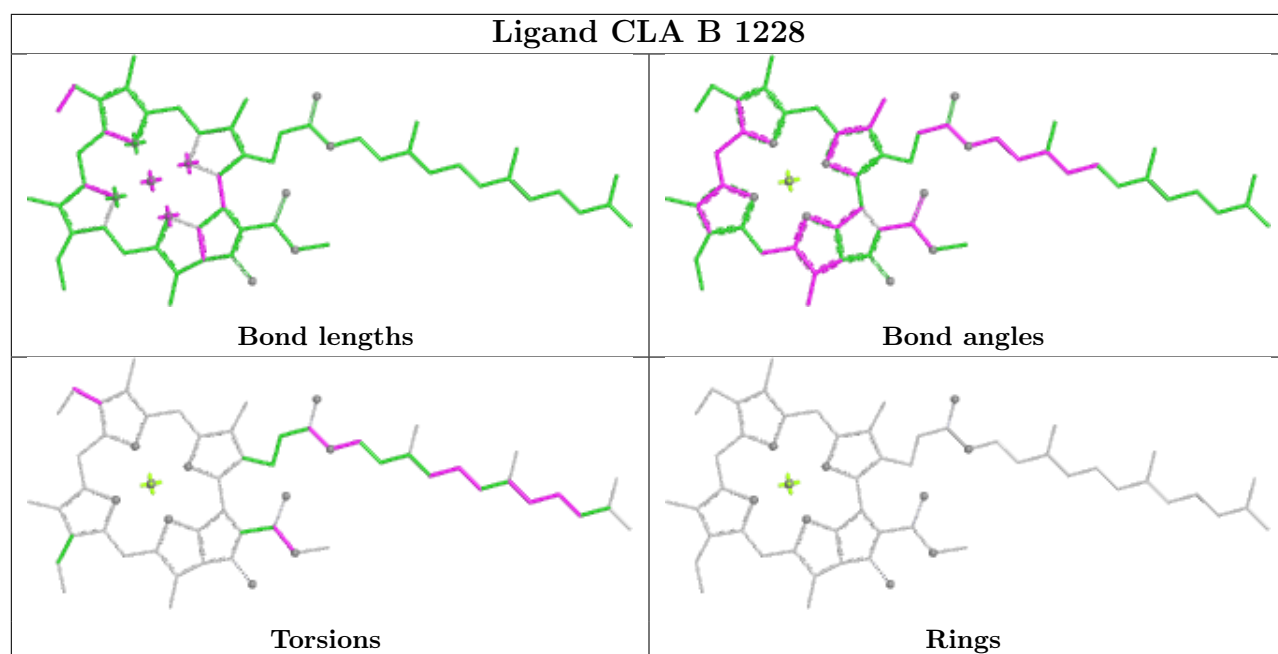


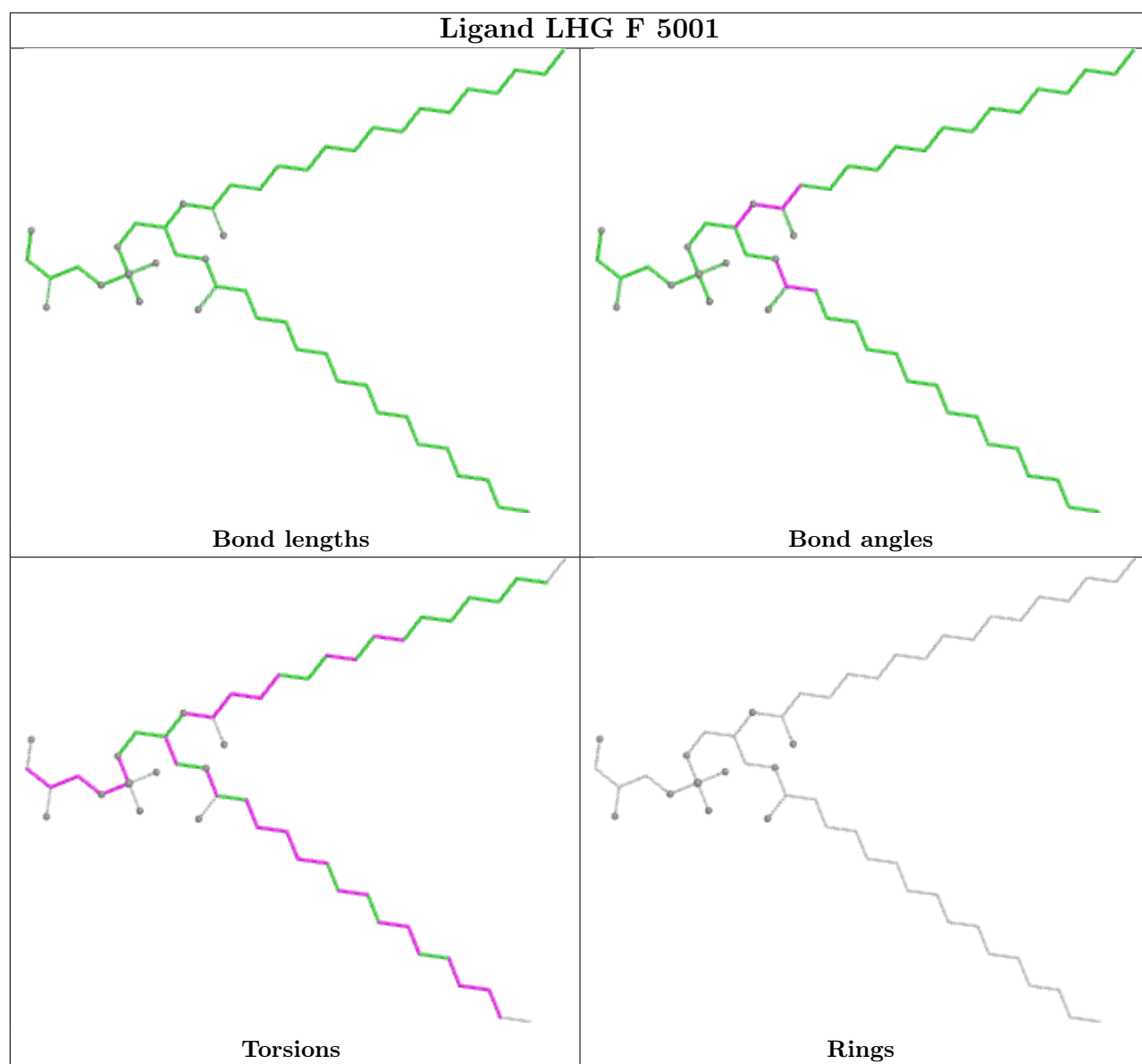
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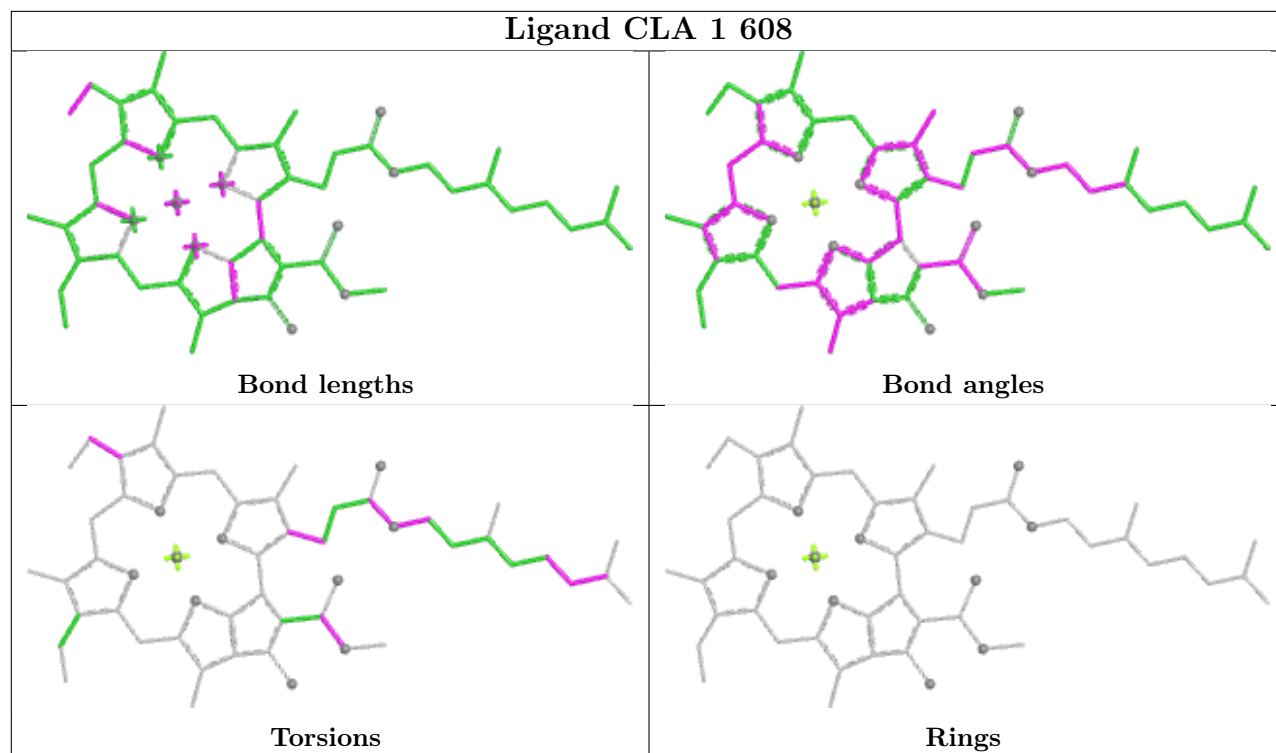
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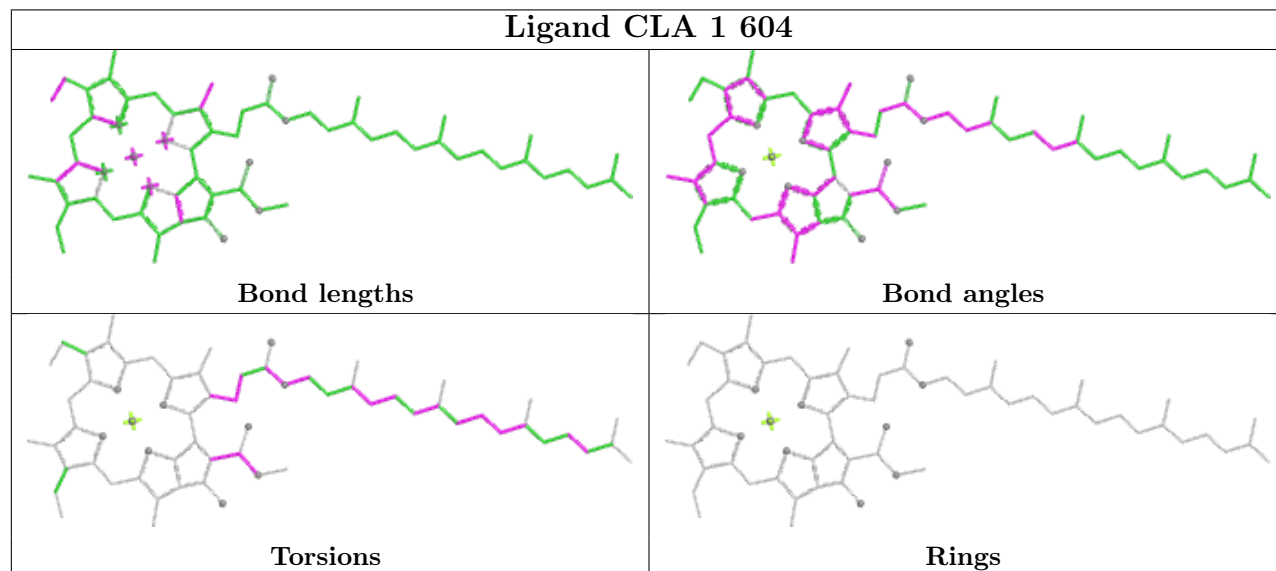


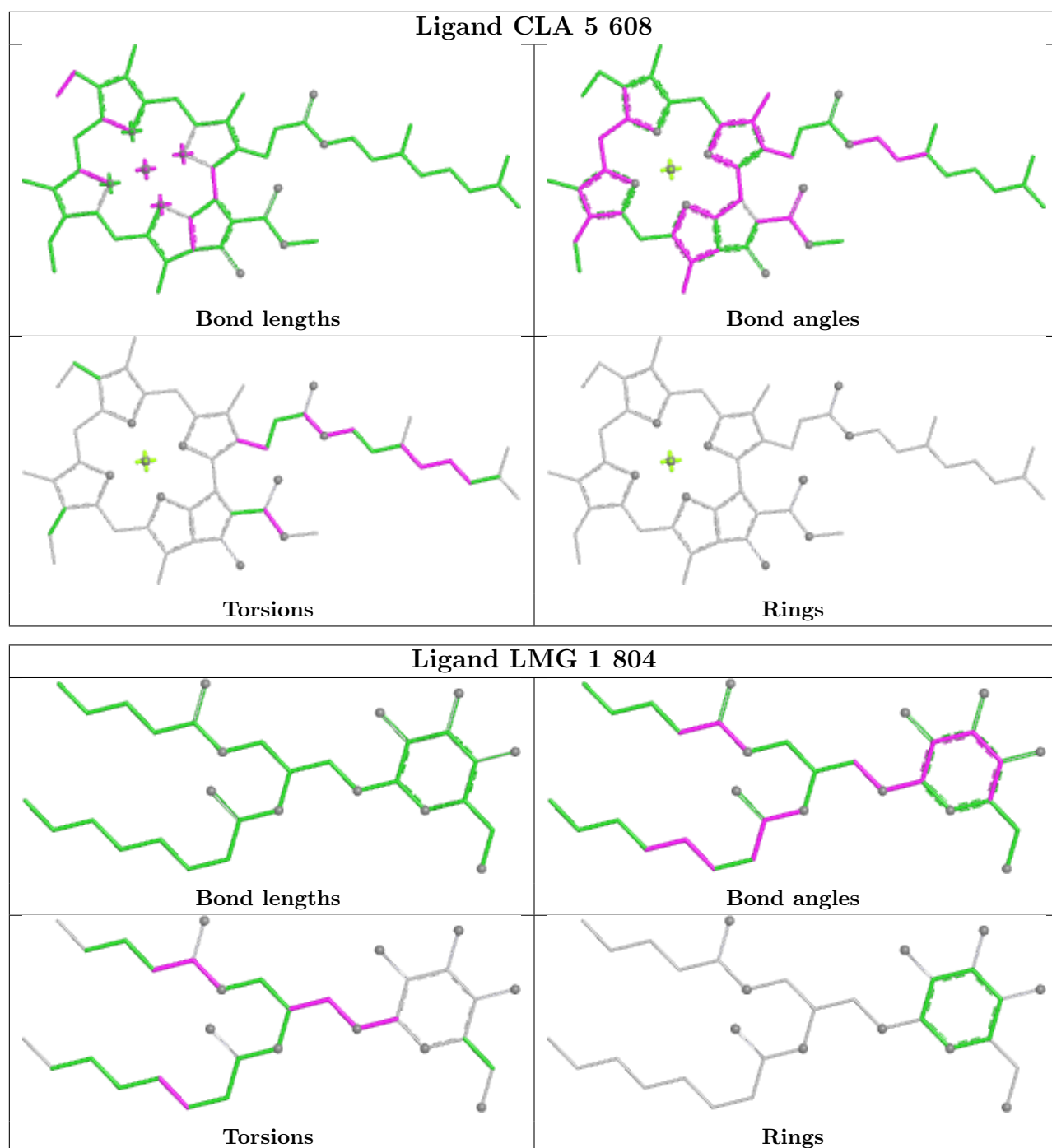


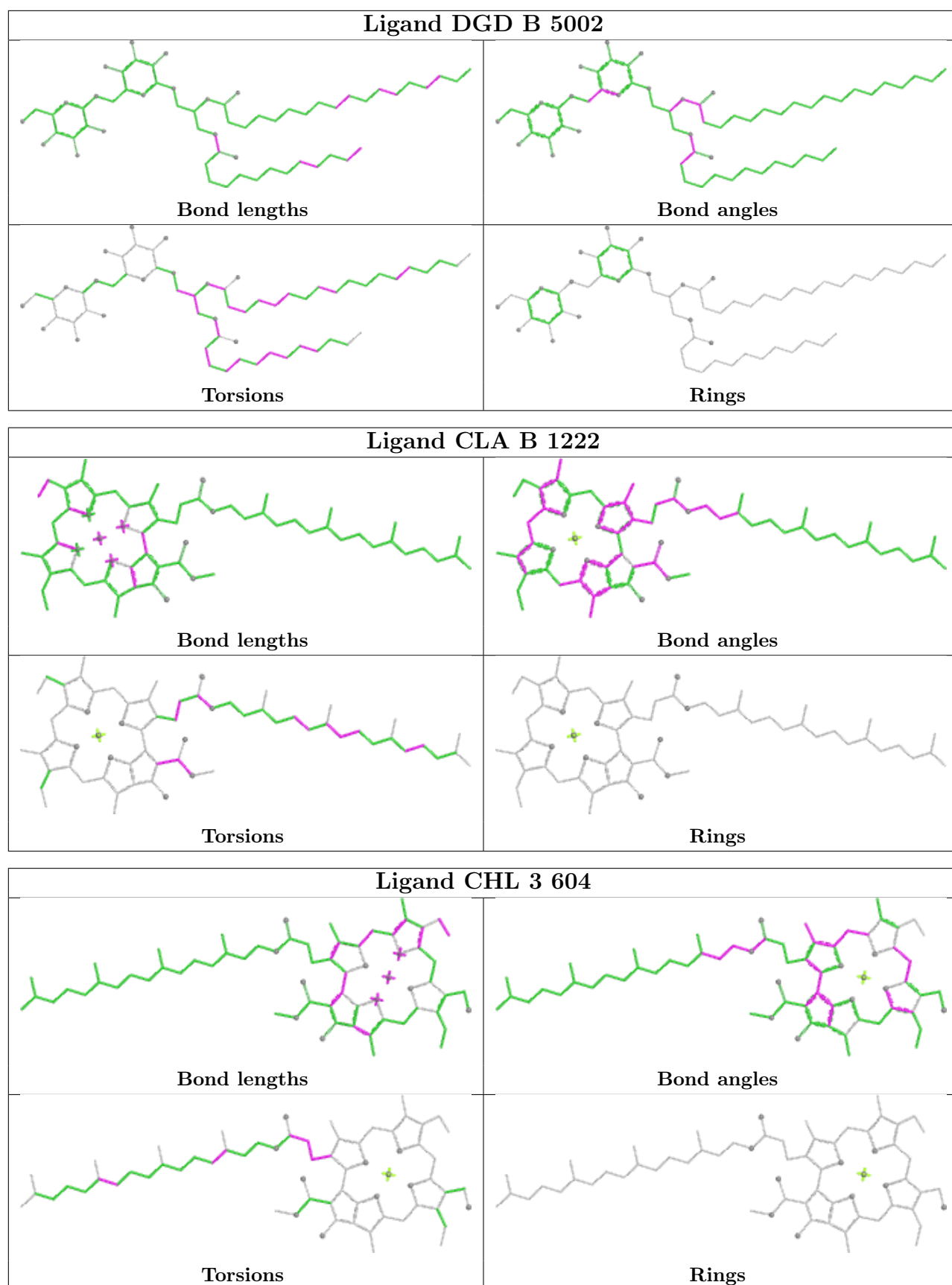
Ligand CLA 1 608



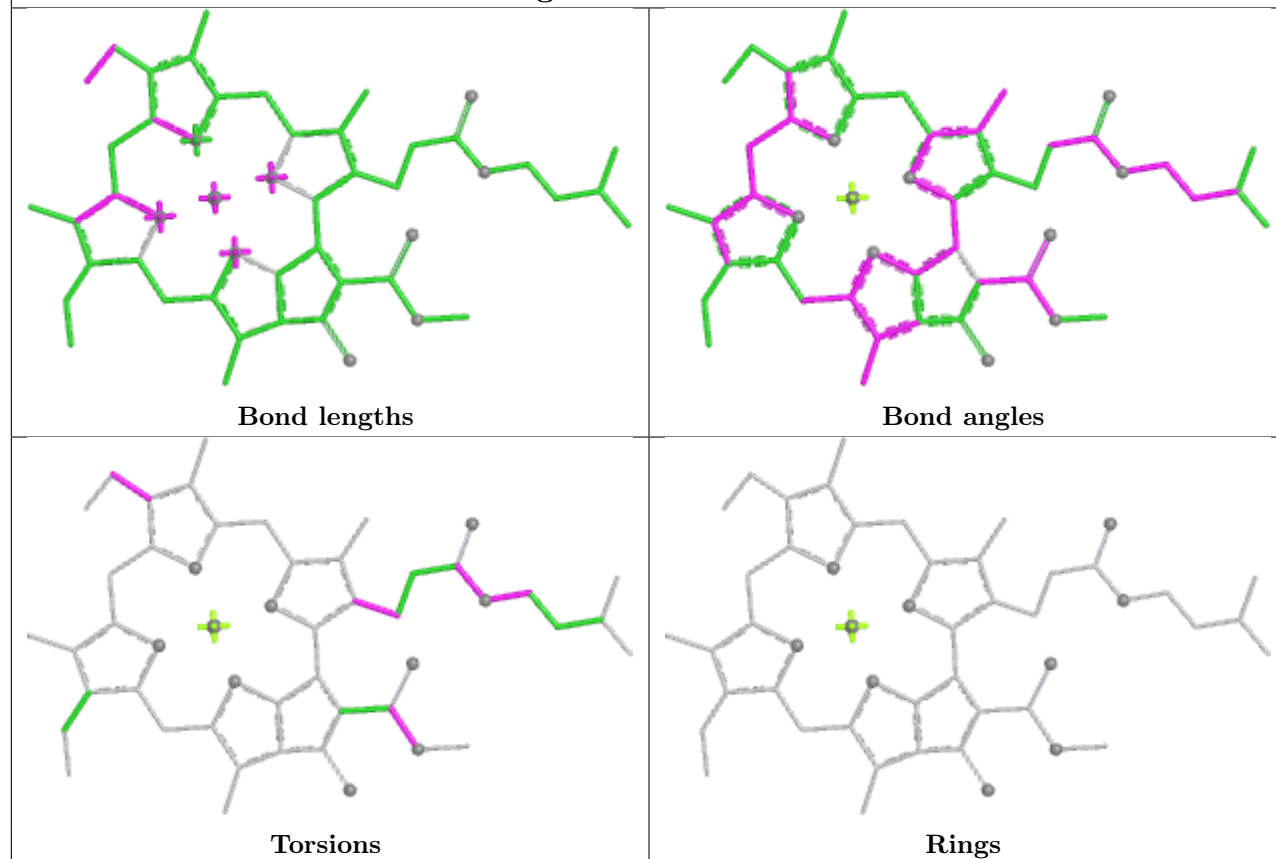
Ligand CLA 1 604



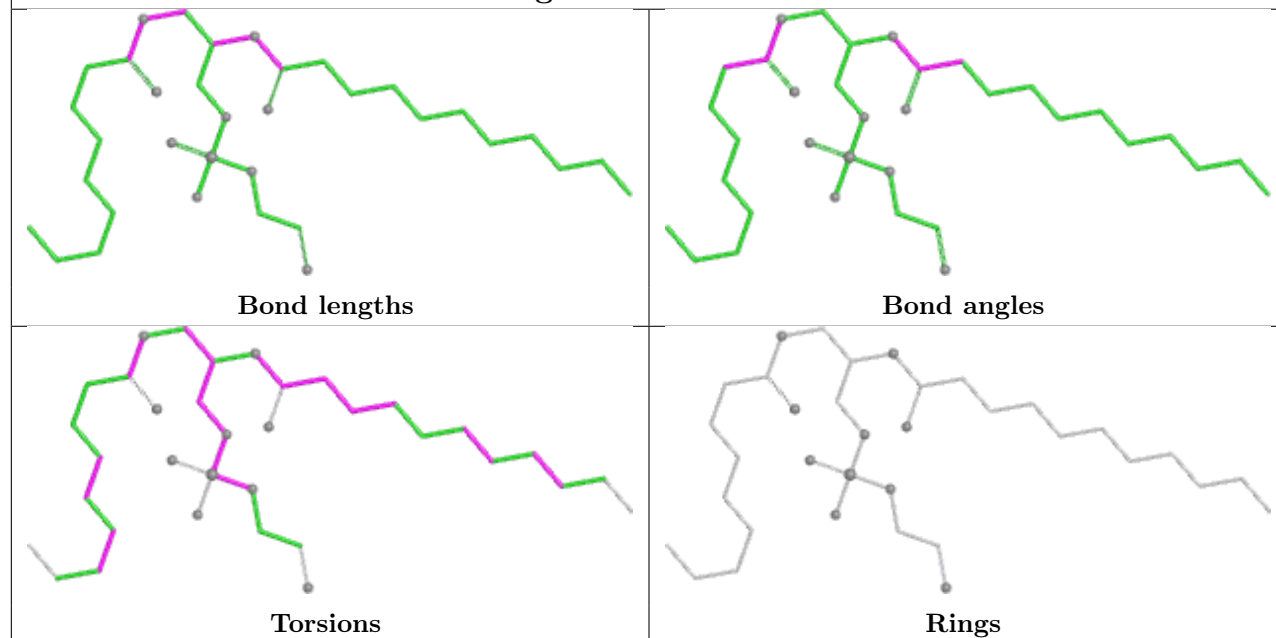


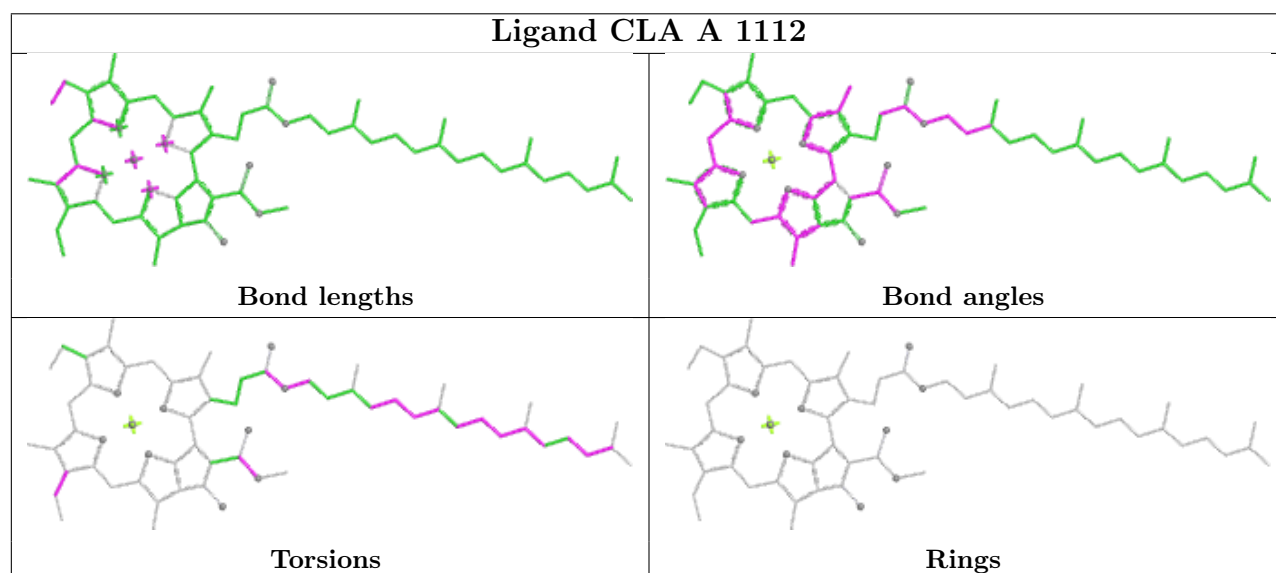
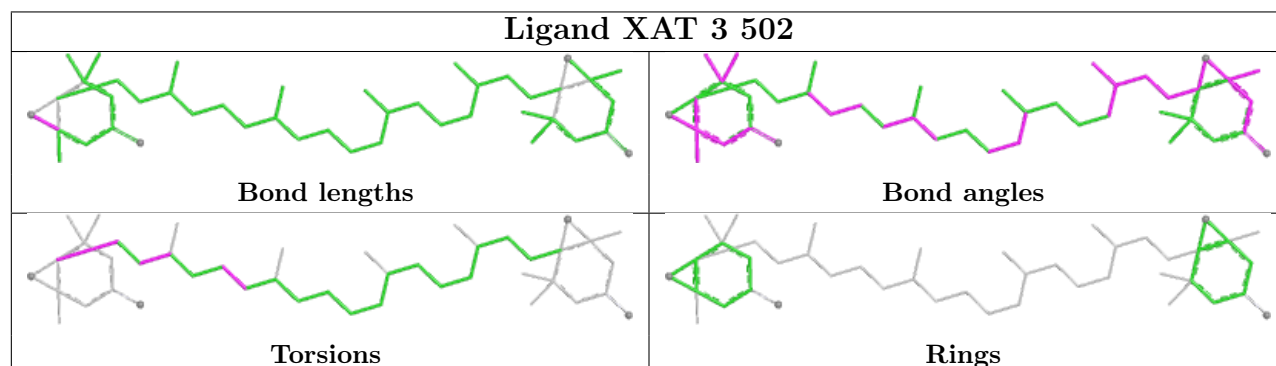
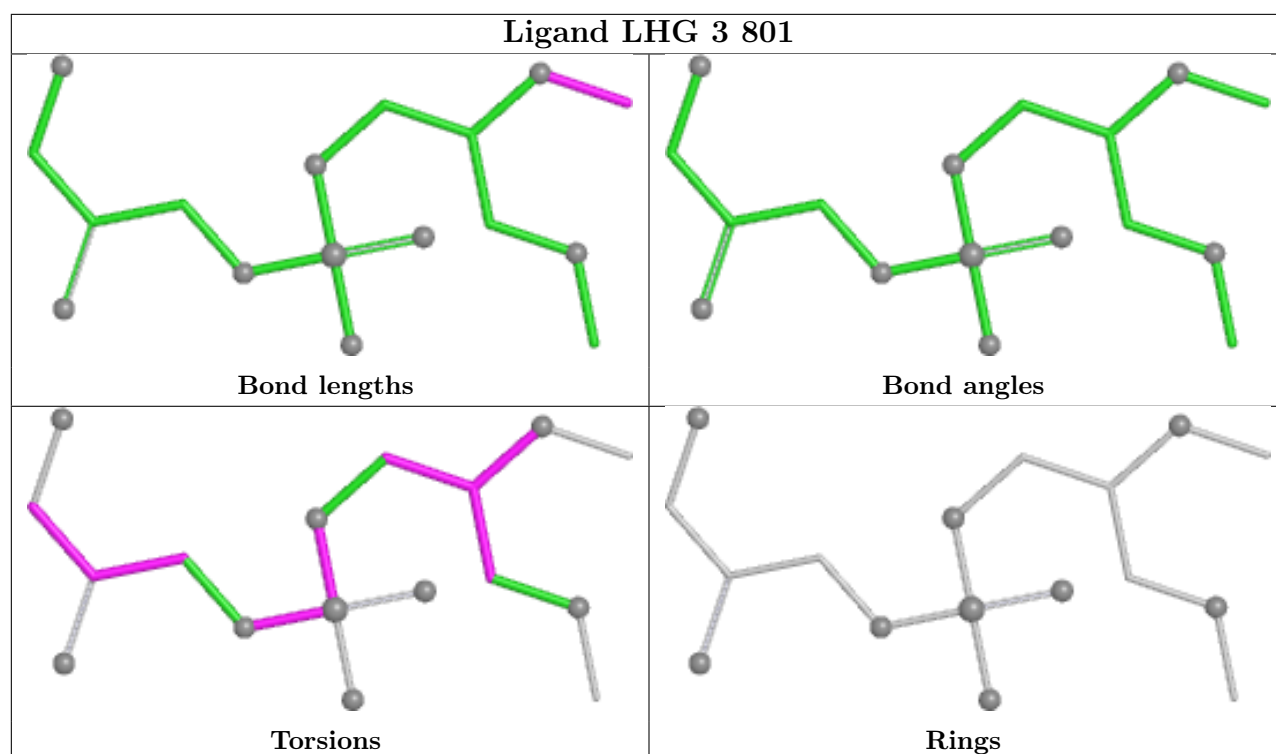


Ligand CLA 5 606

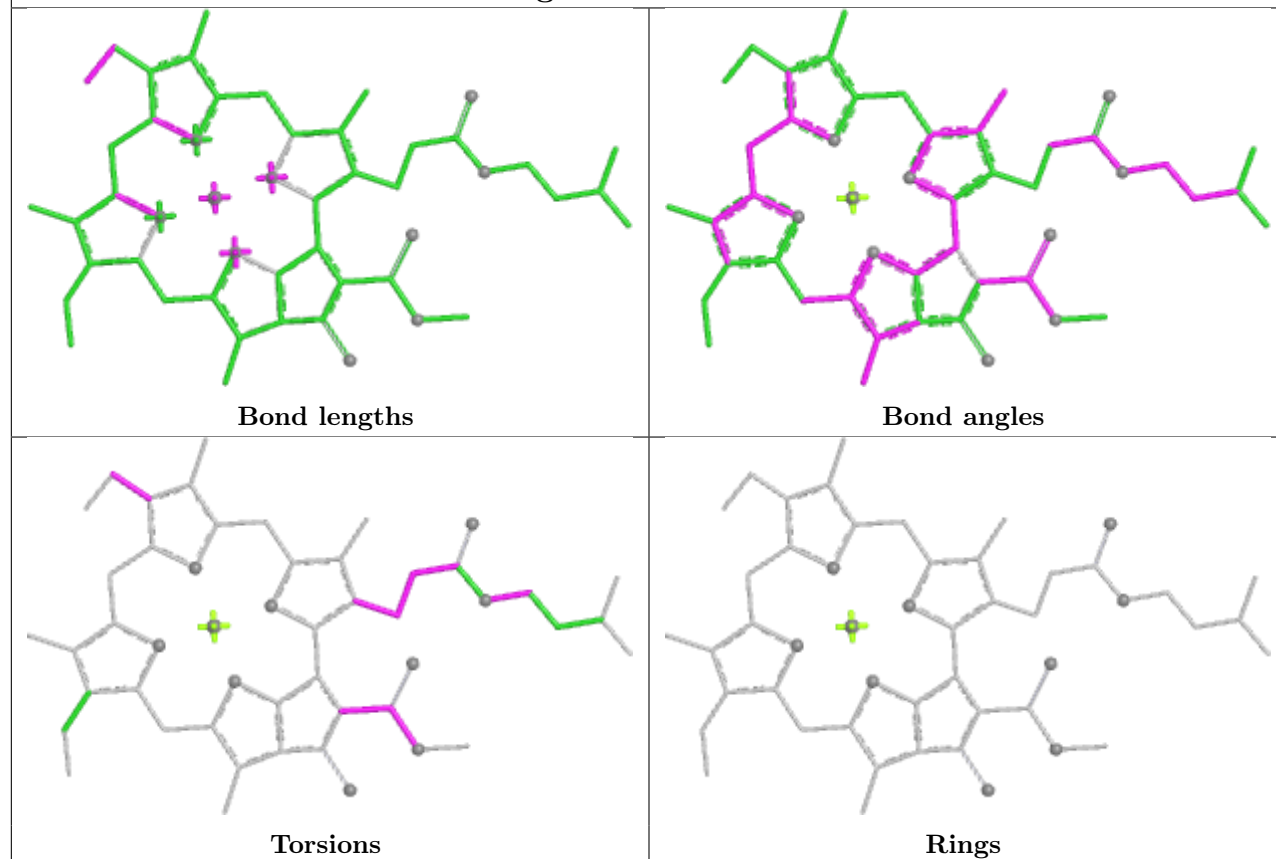


Ligand PTY 4 804

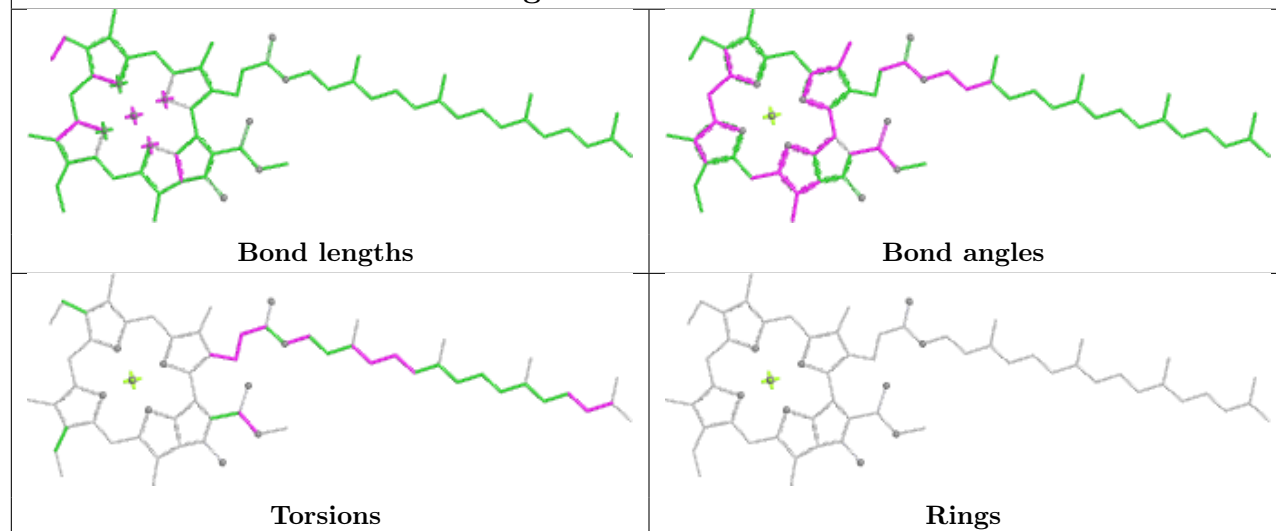


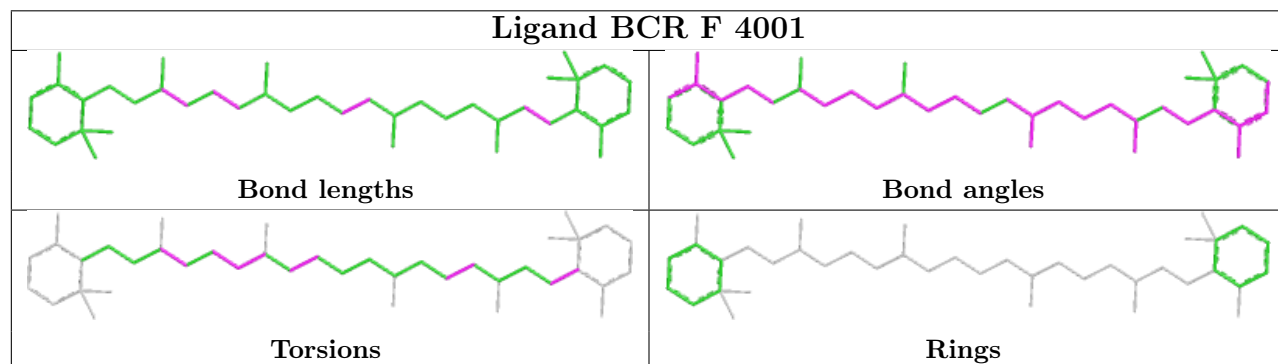
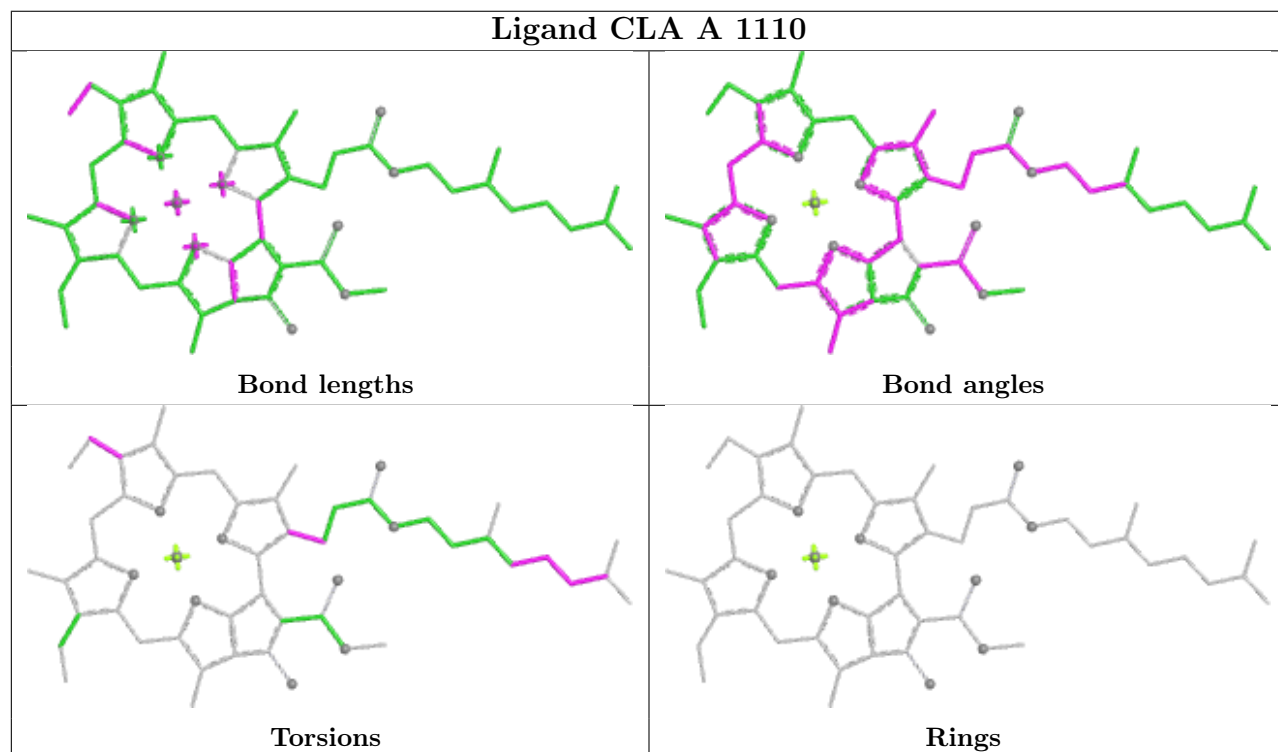
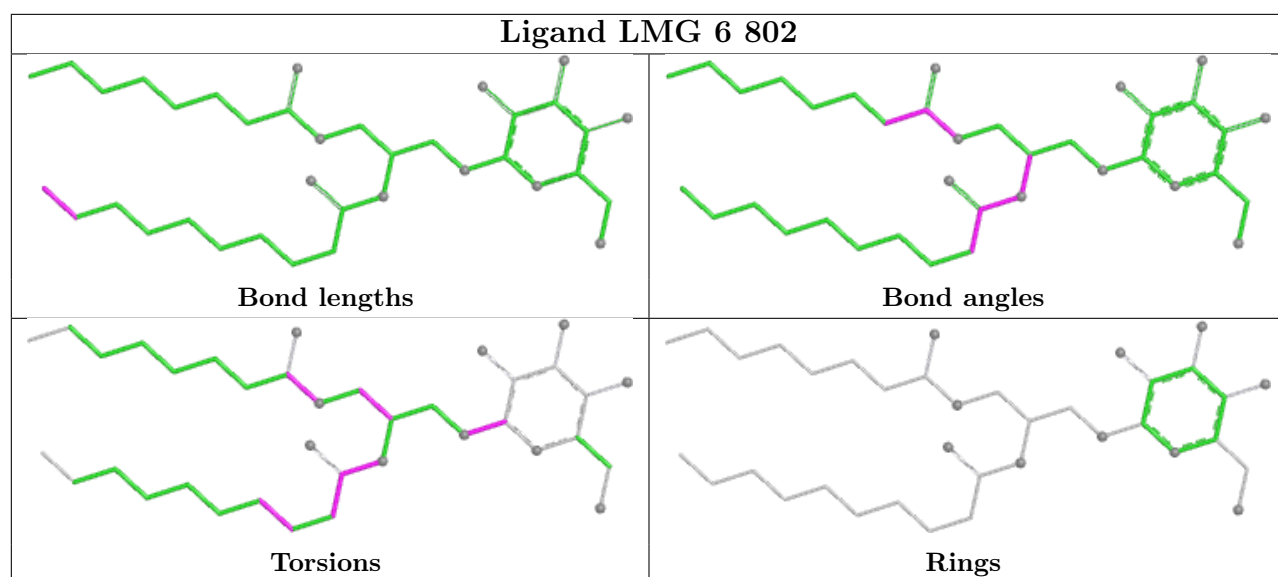


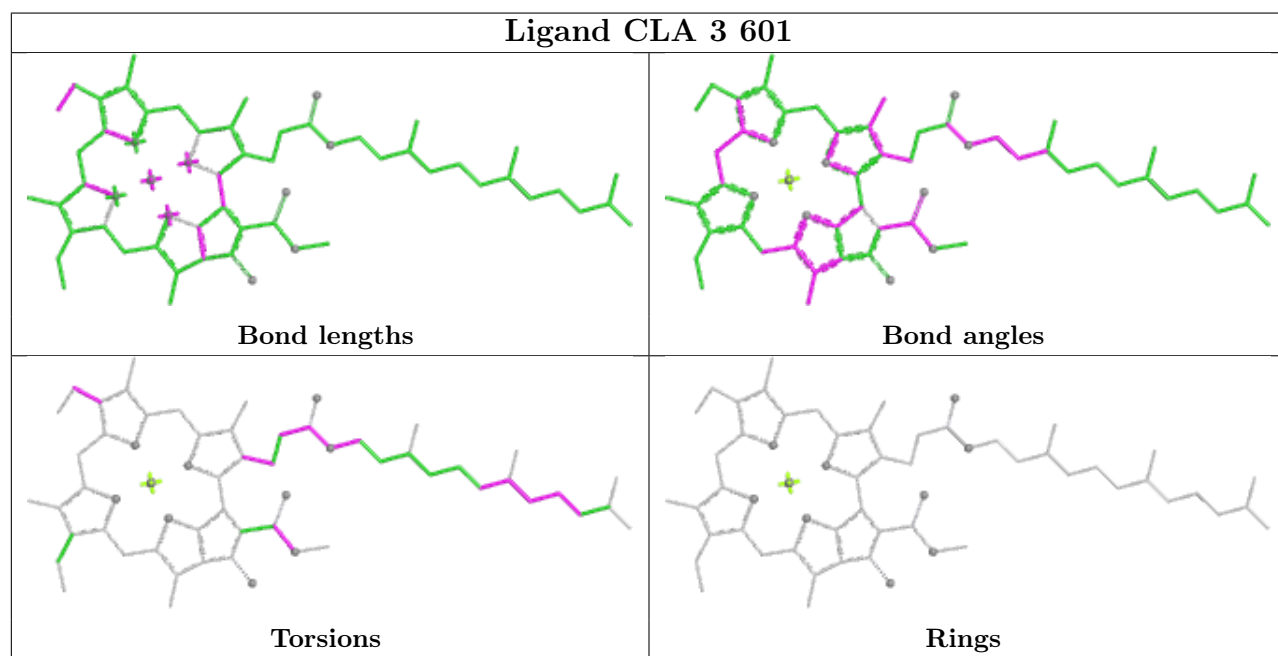
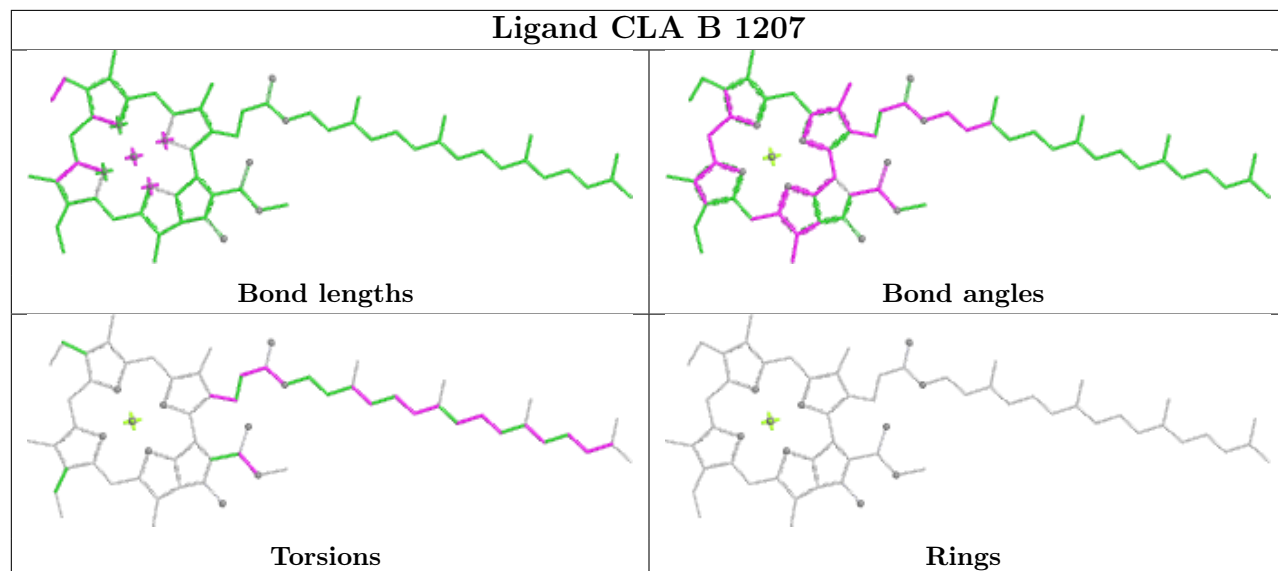
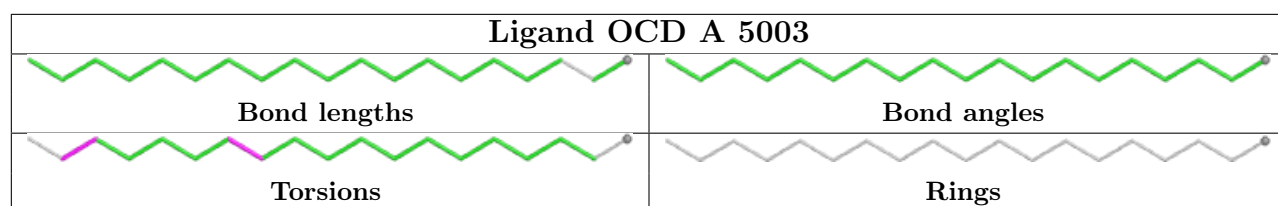
Ligand CLA 6 606

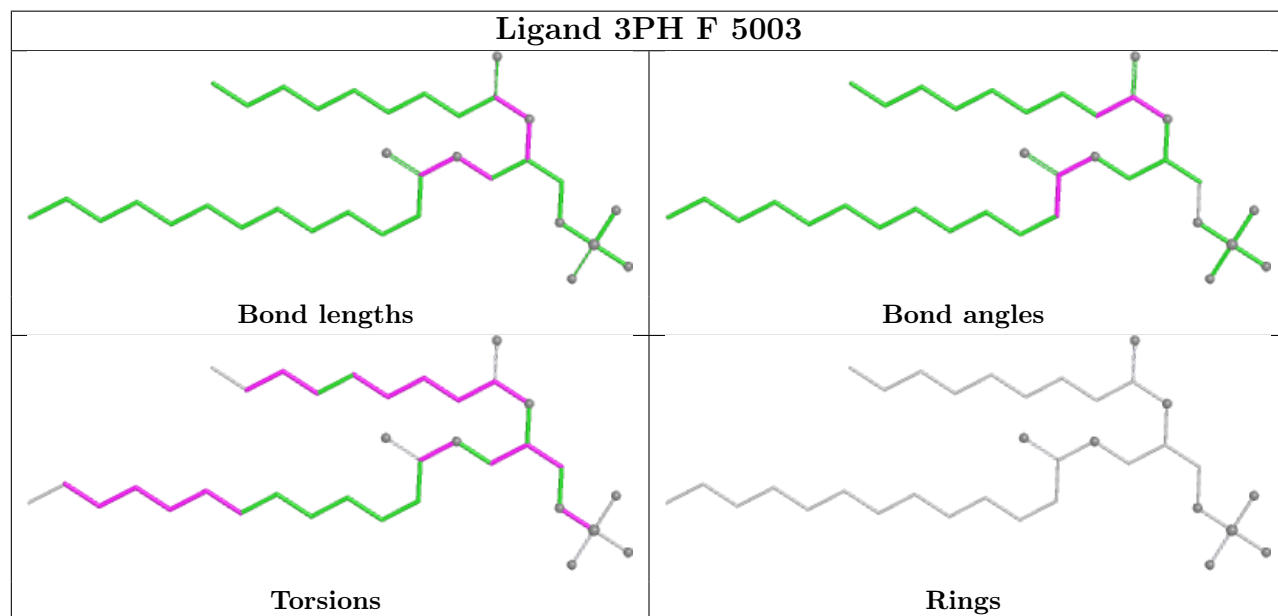
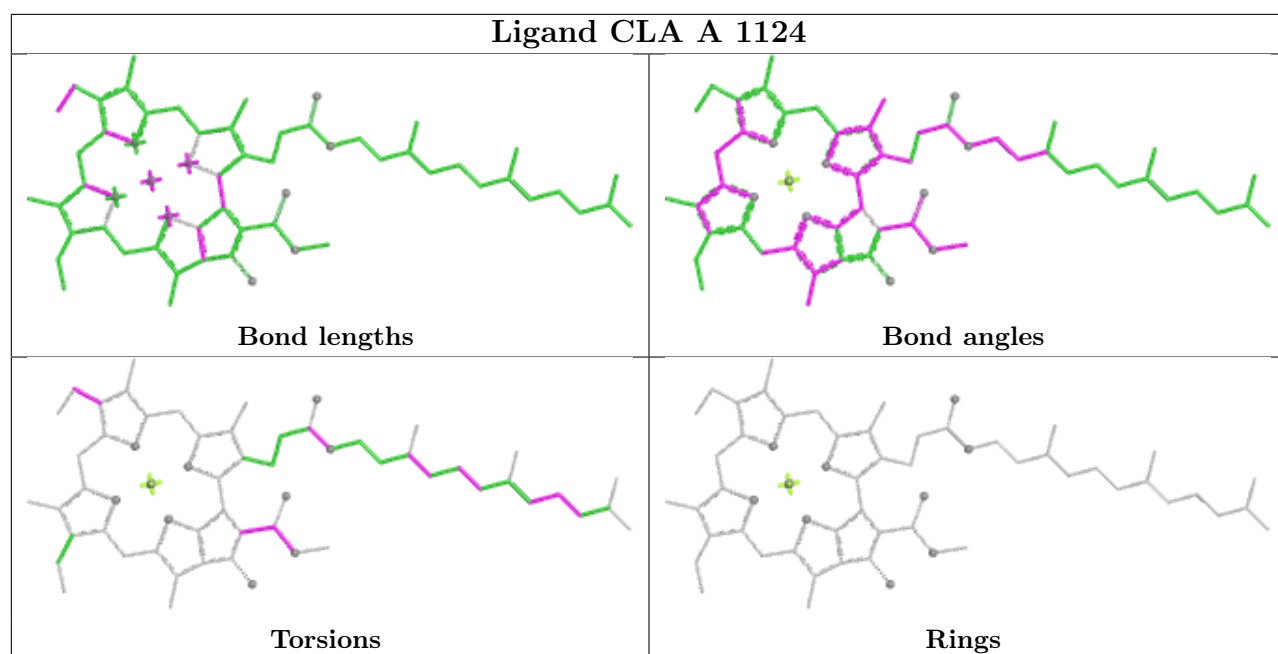


Ligand CLA B 1239

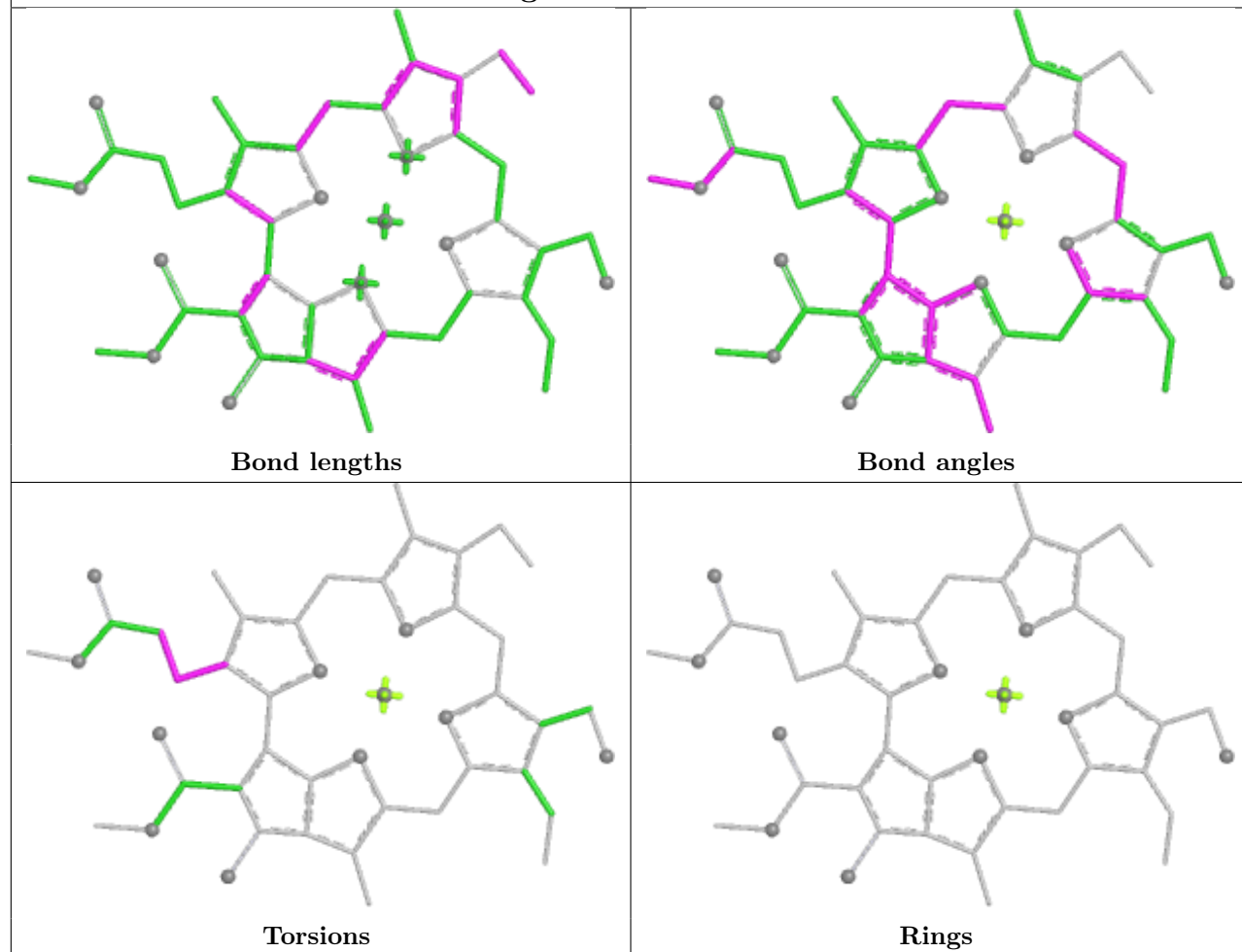




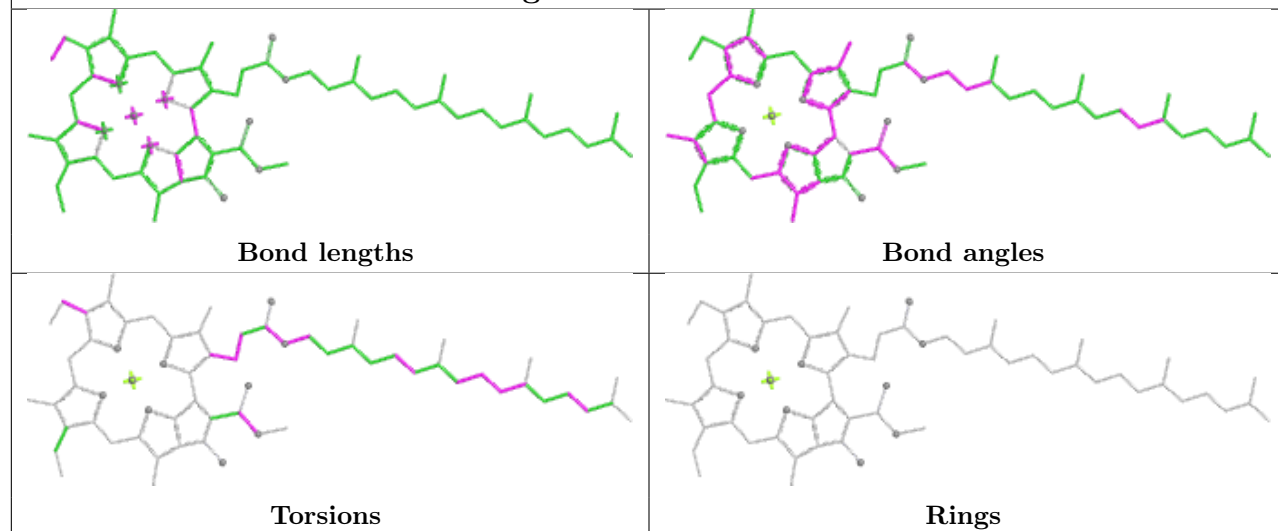


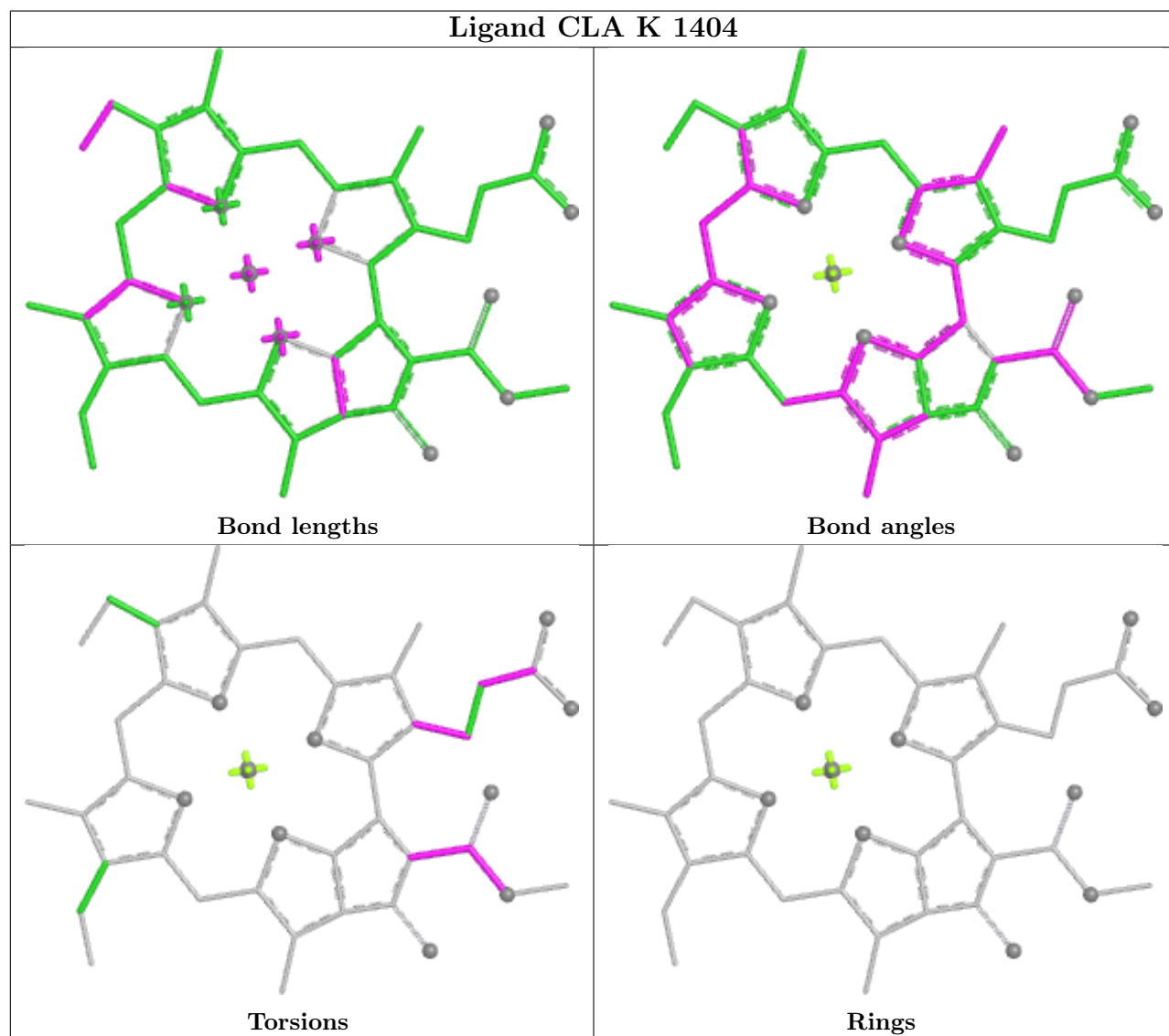
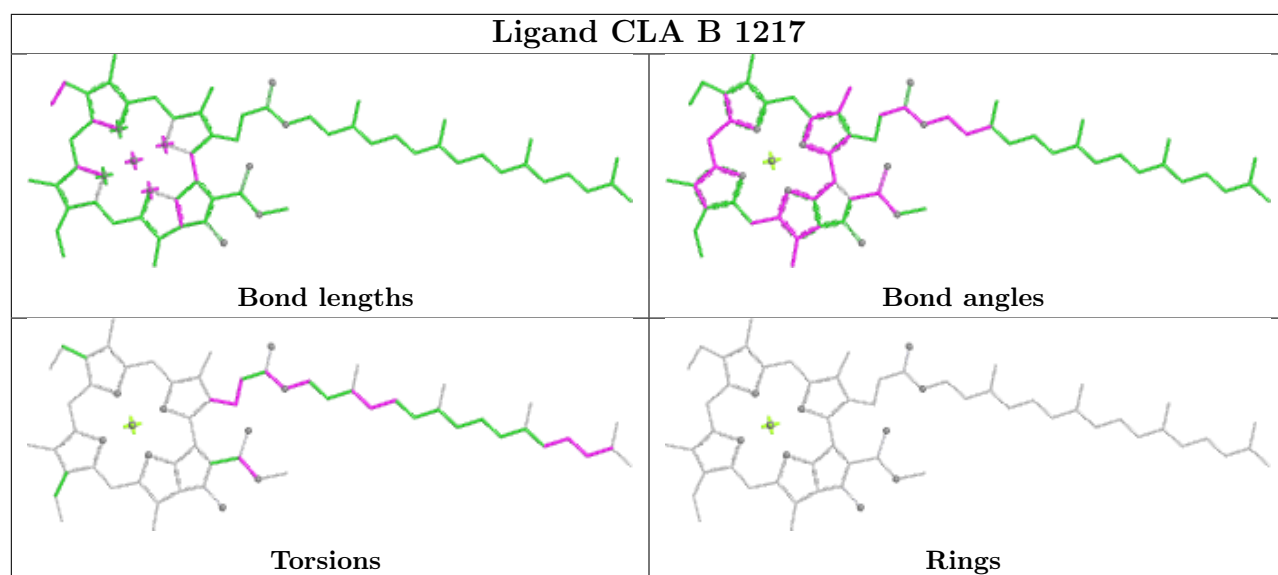


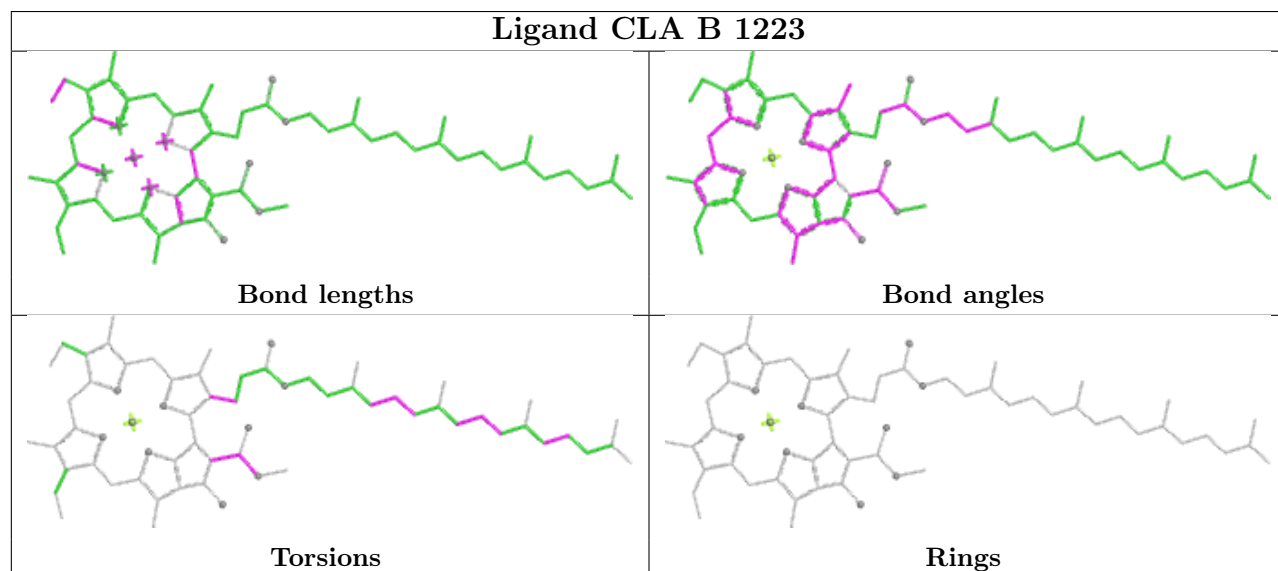
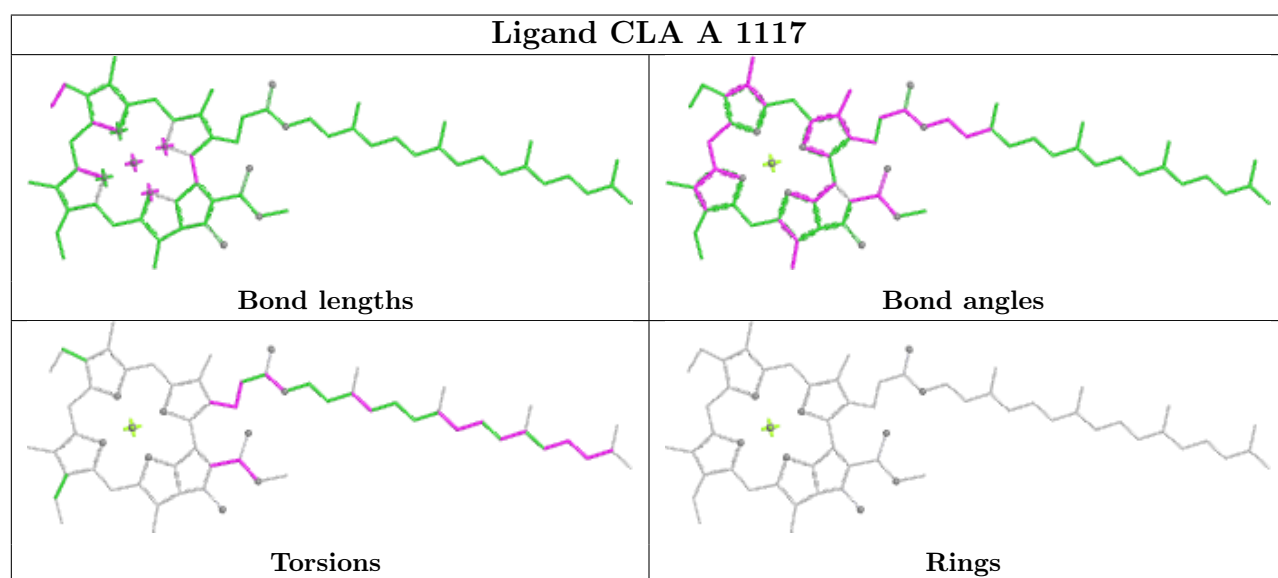
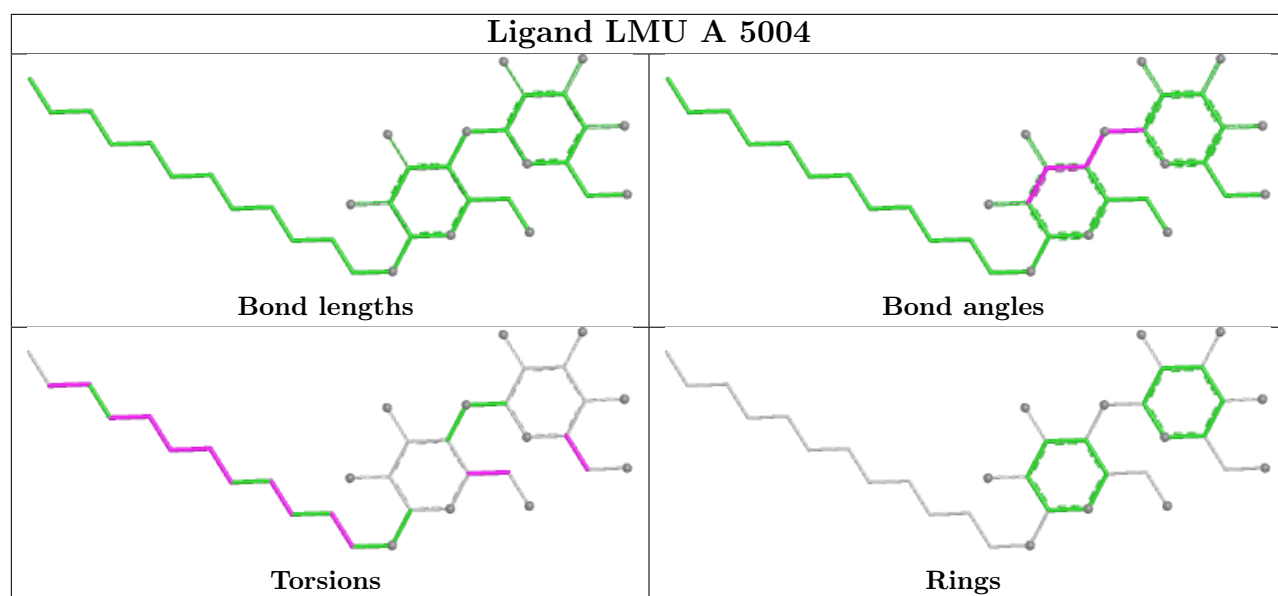
Ligand CHL 5 610

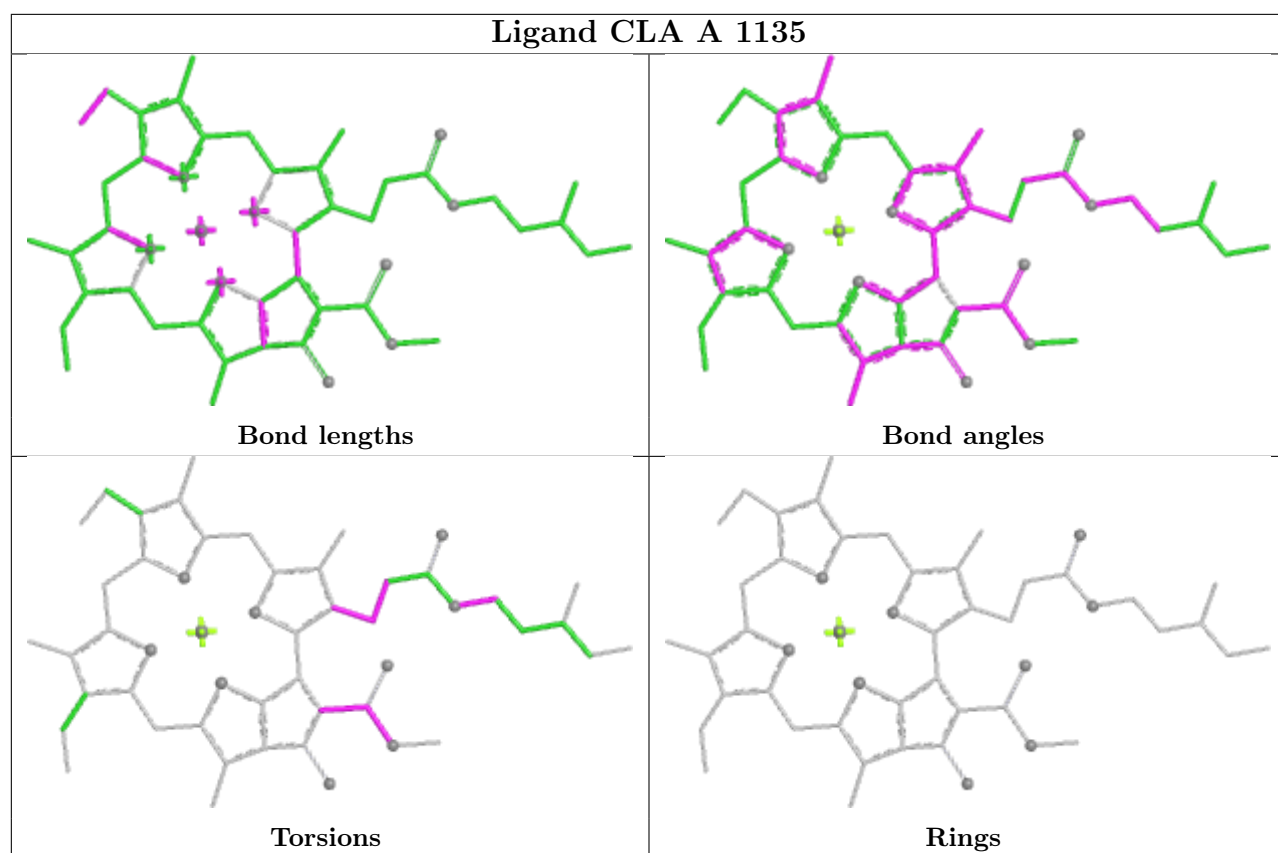


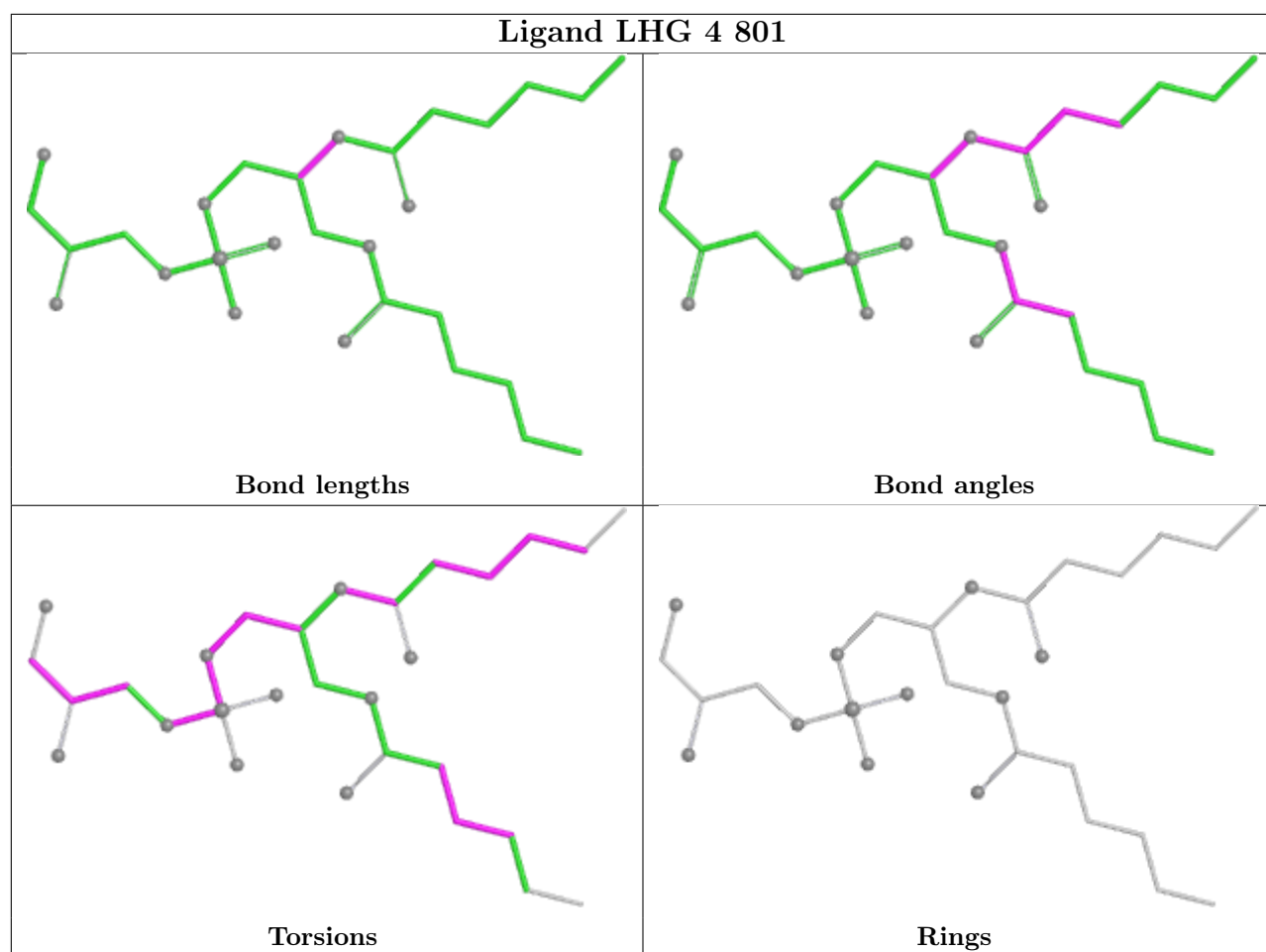
Ligand CLA A 1119



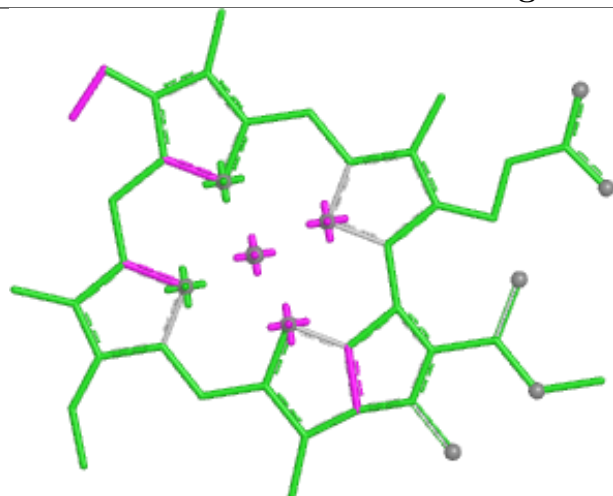




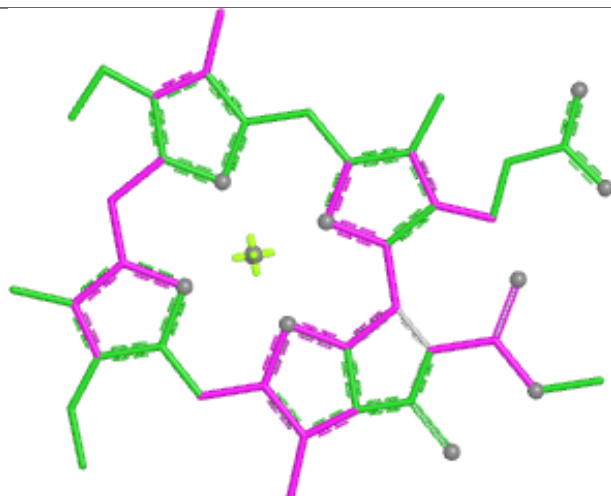




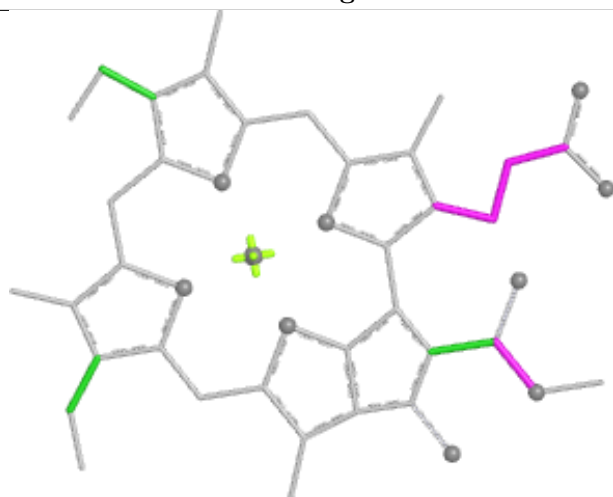
Ligand CLA 6 613



Bond lengths



Bond angles

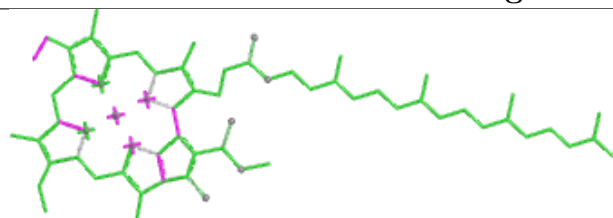


Torsions

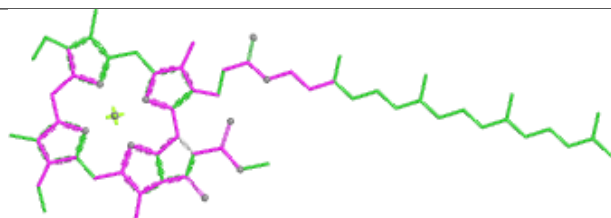


Rings

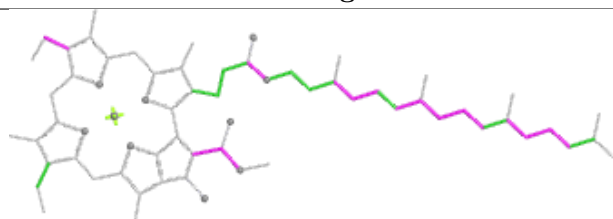
Ligand CLA B 1227



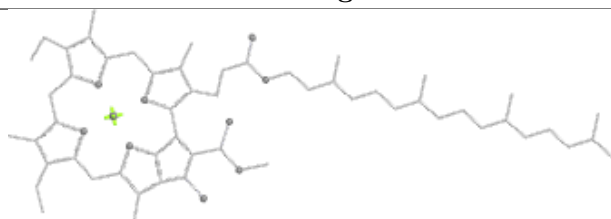
Bond lengths



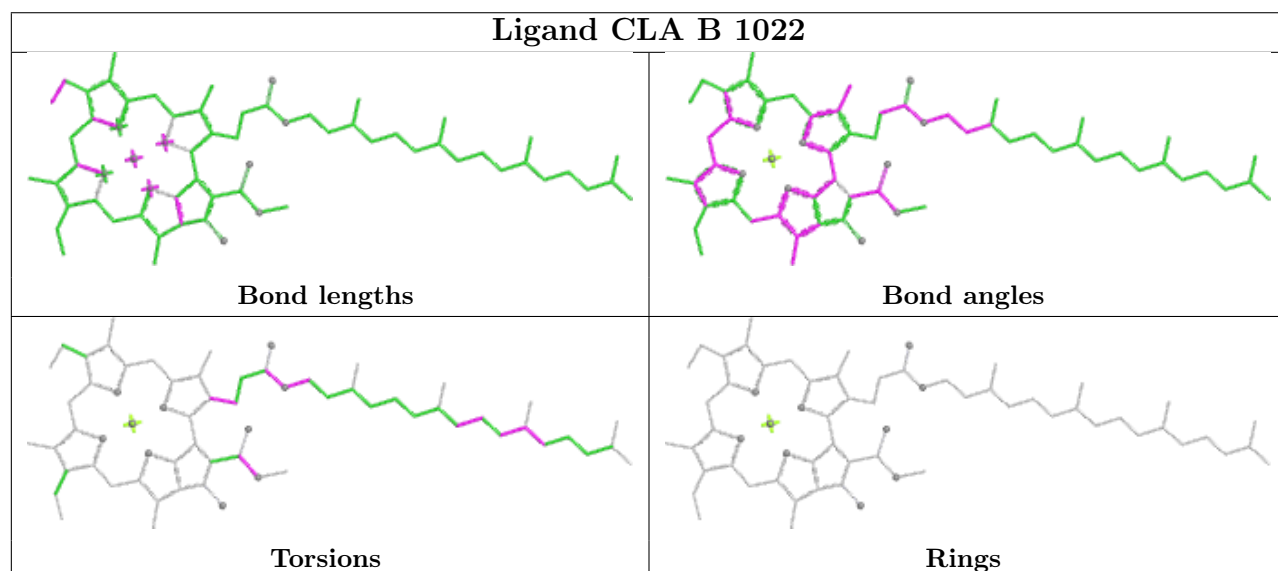
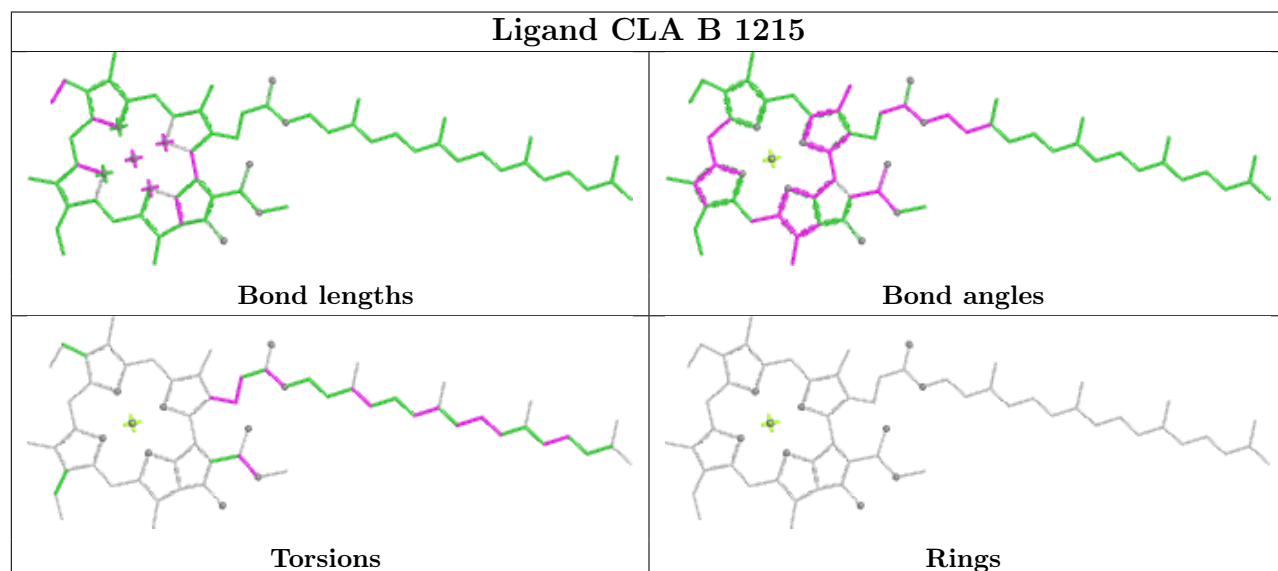
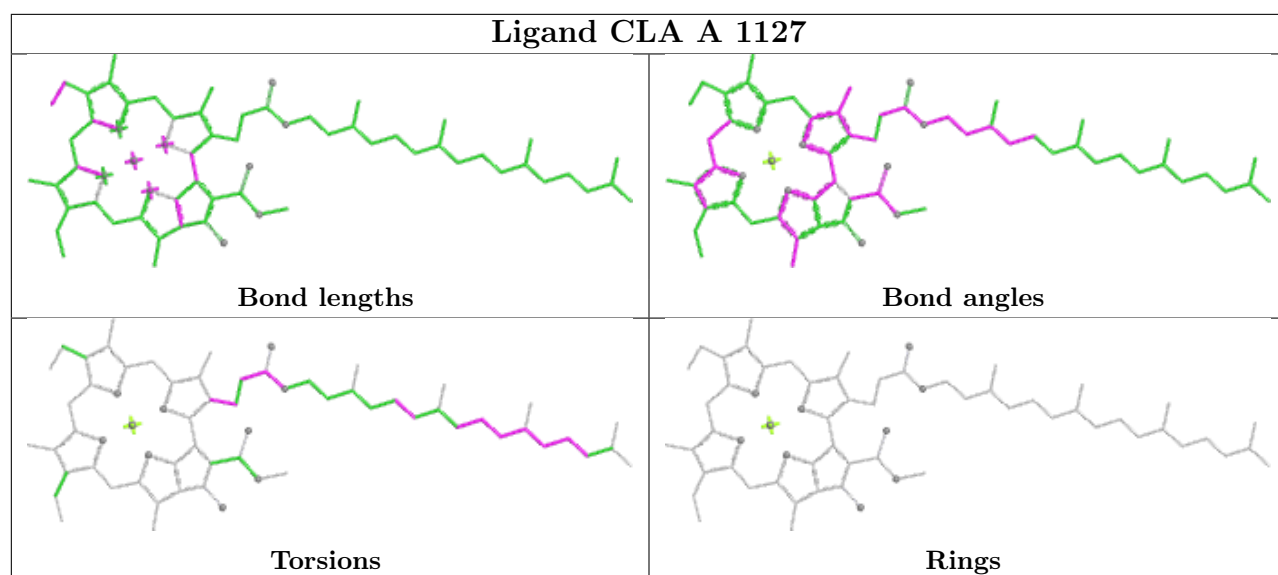
Bond angles

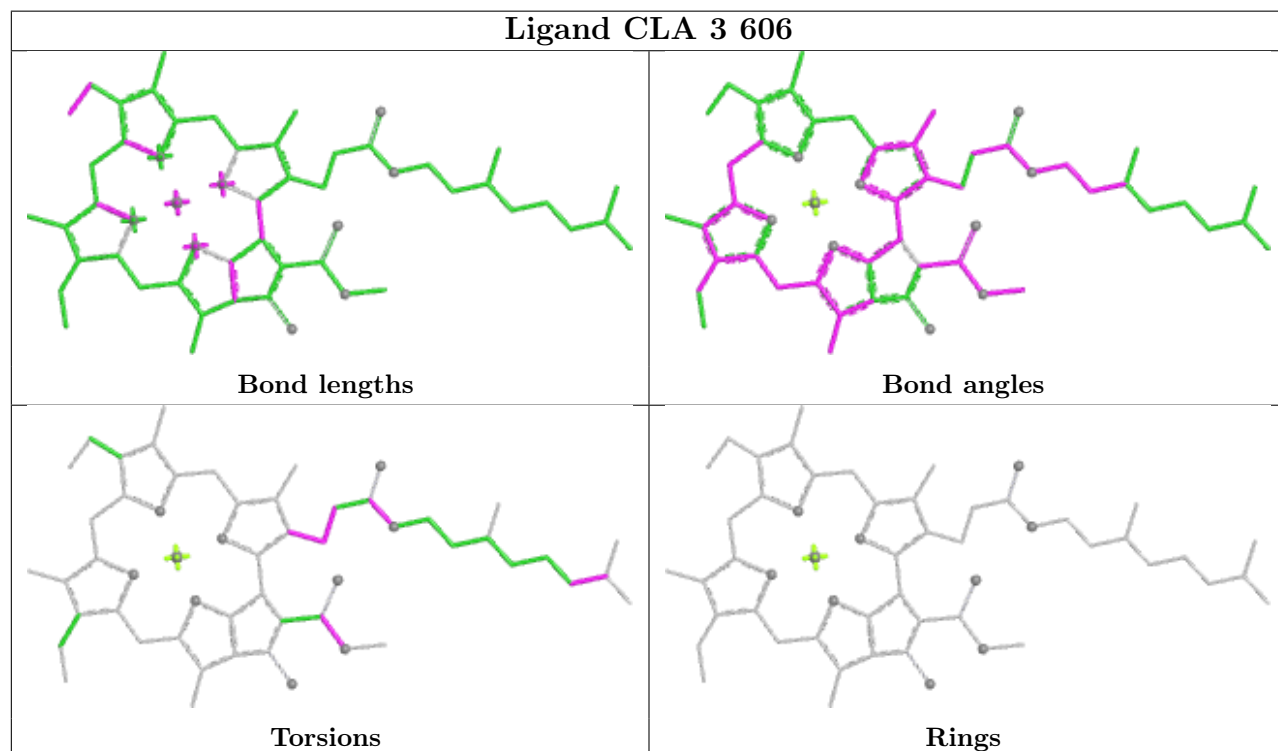
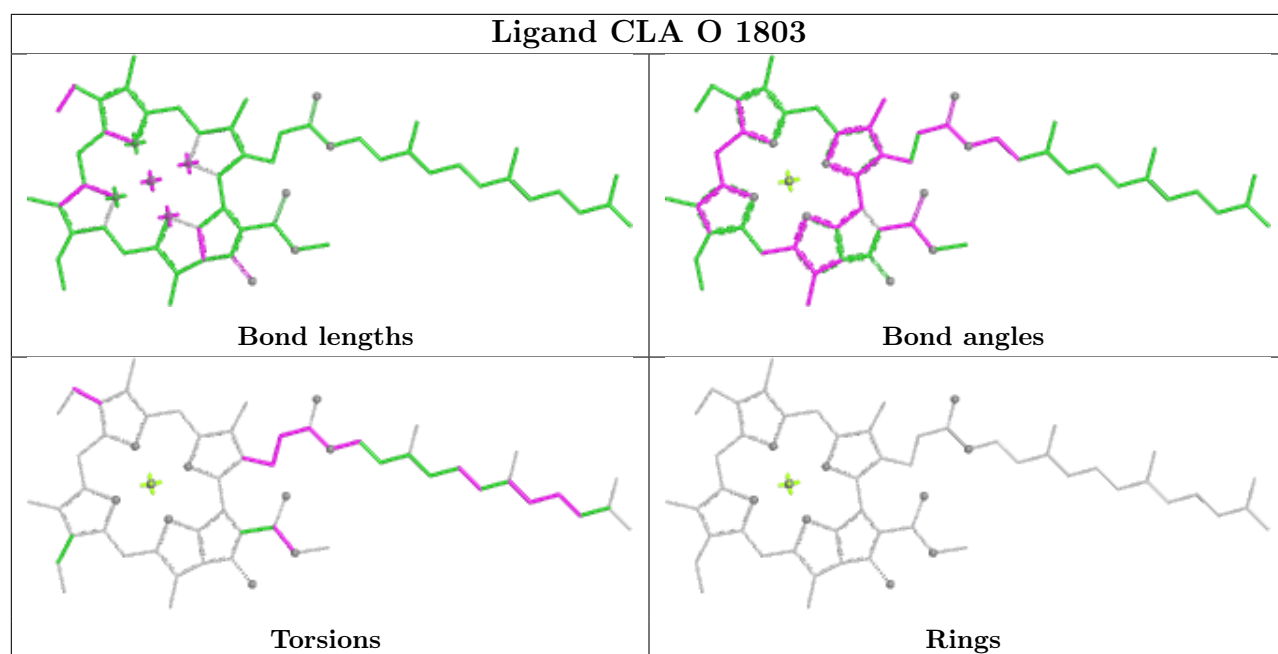


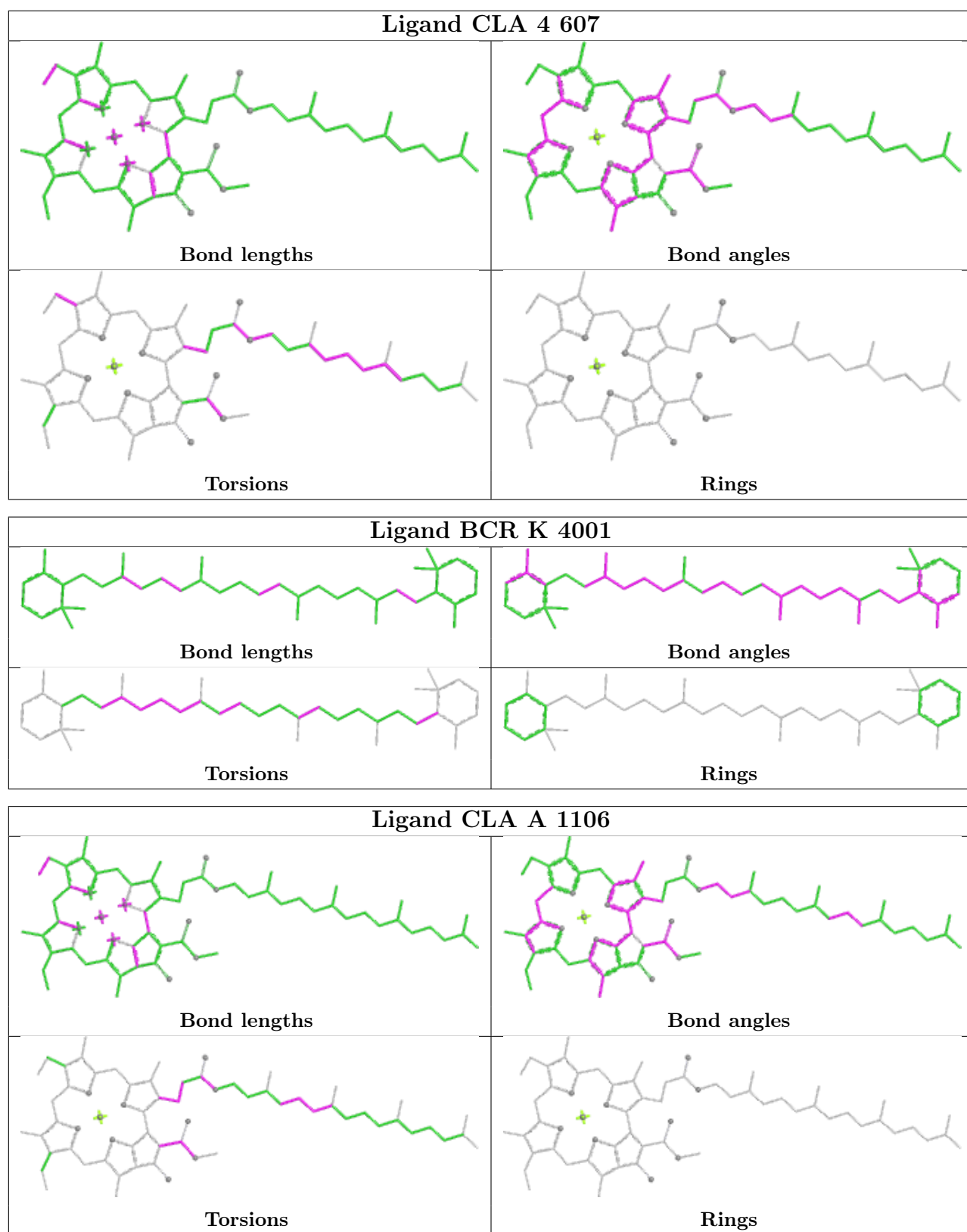
Torsions

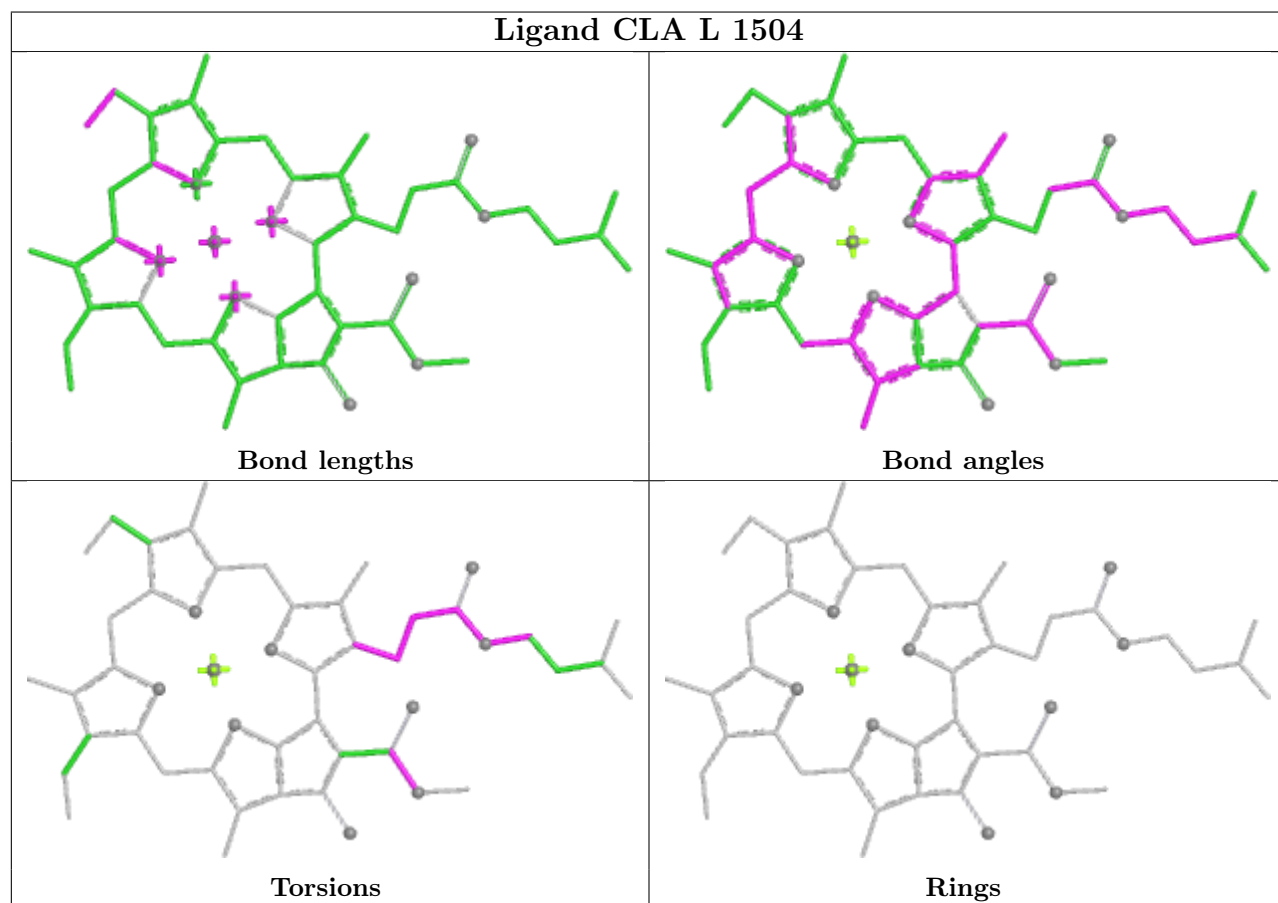
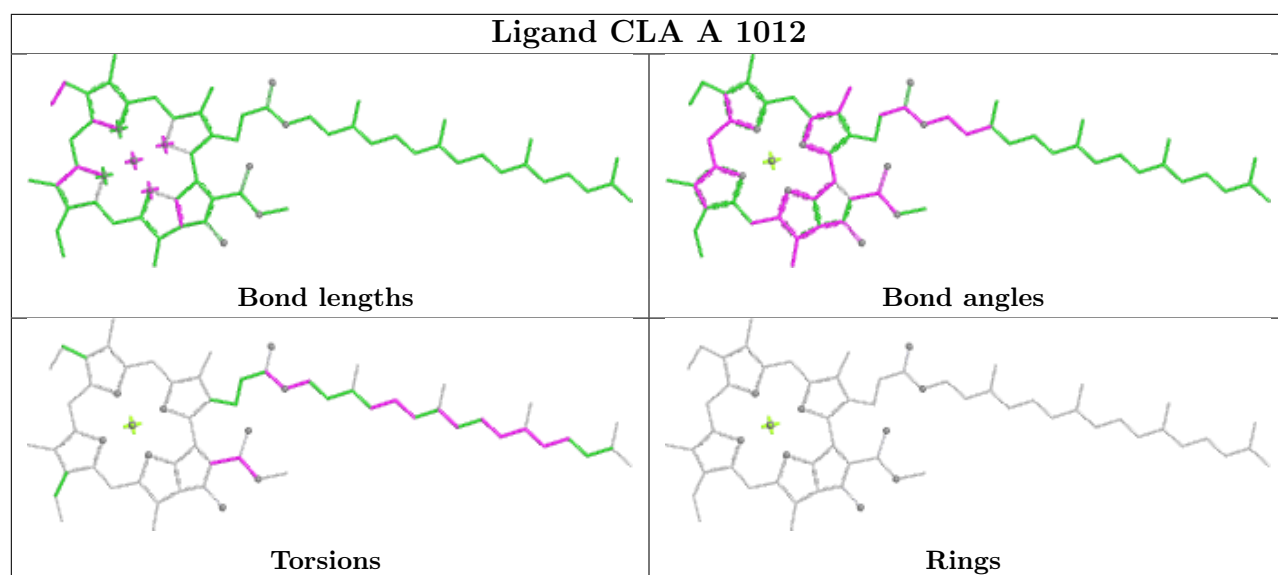


Rings

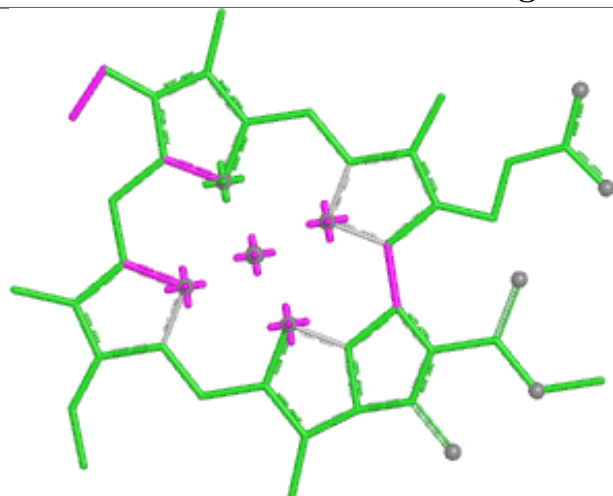




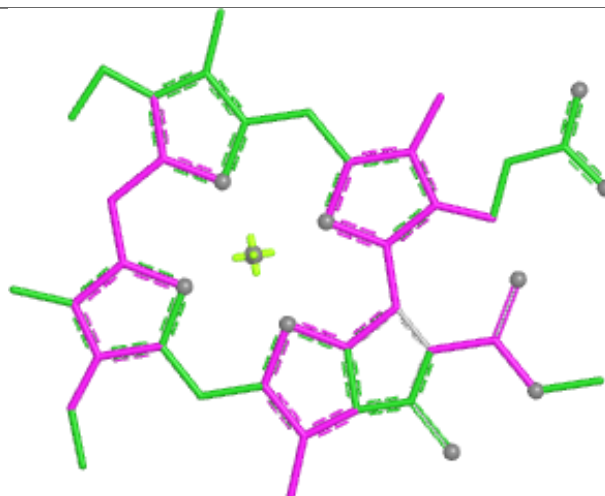




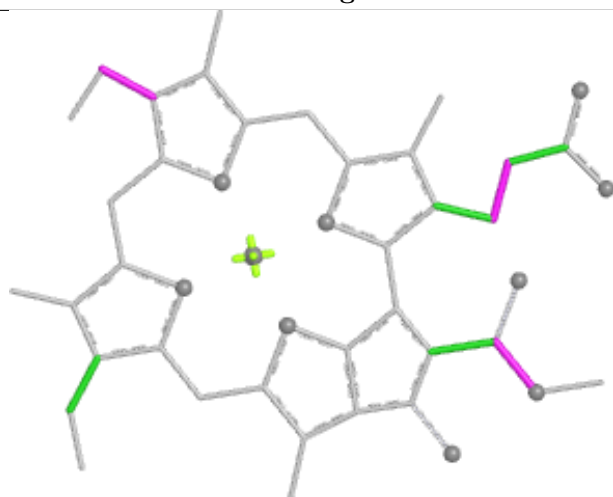
Ligand CLA 1 613



Bond lengths



Bond angles

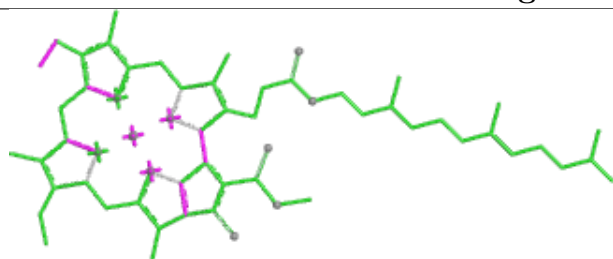


Torsions

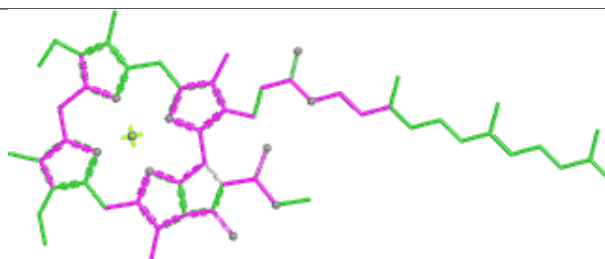


Rings

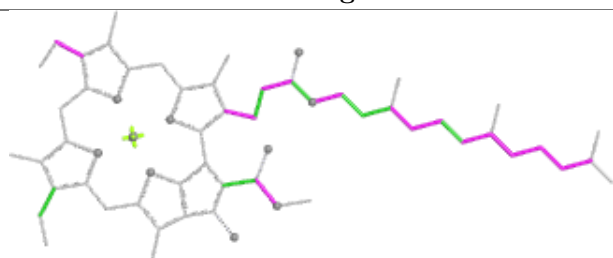
Ligand CLA 4 601



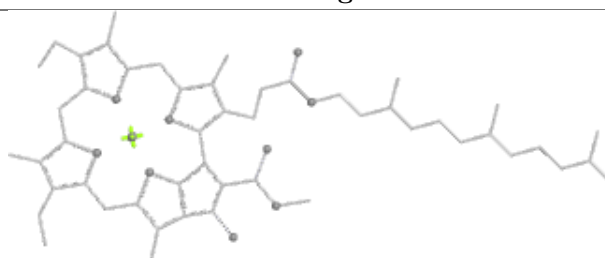
Bond lengths



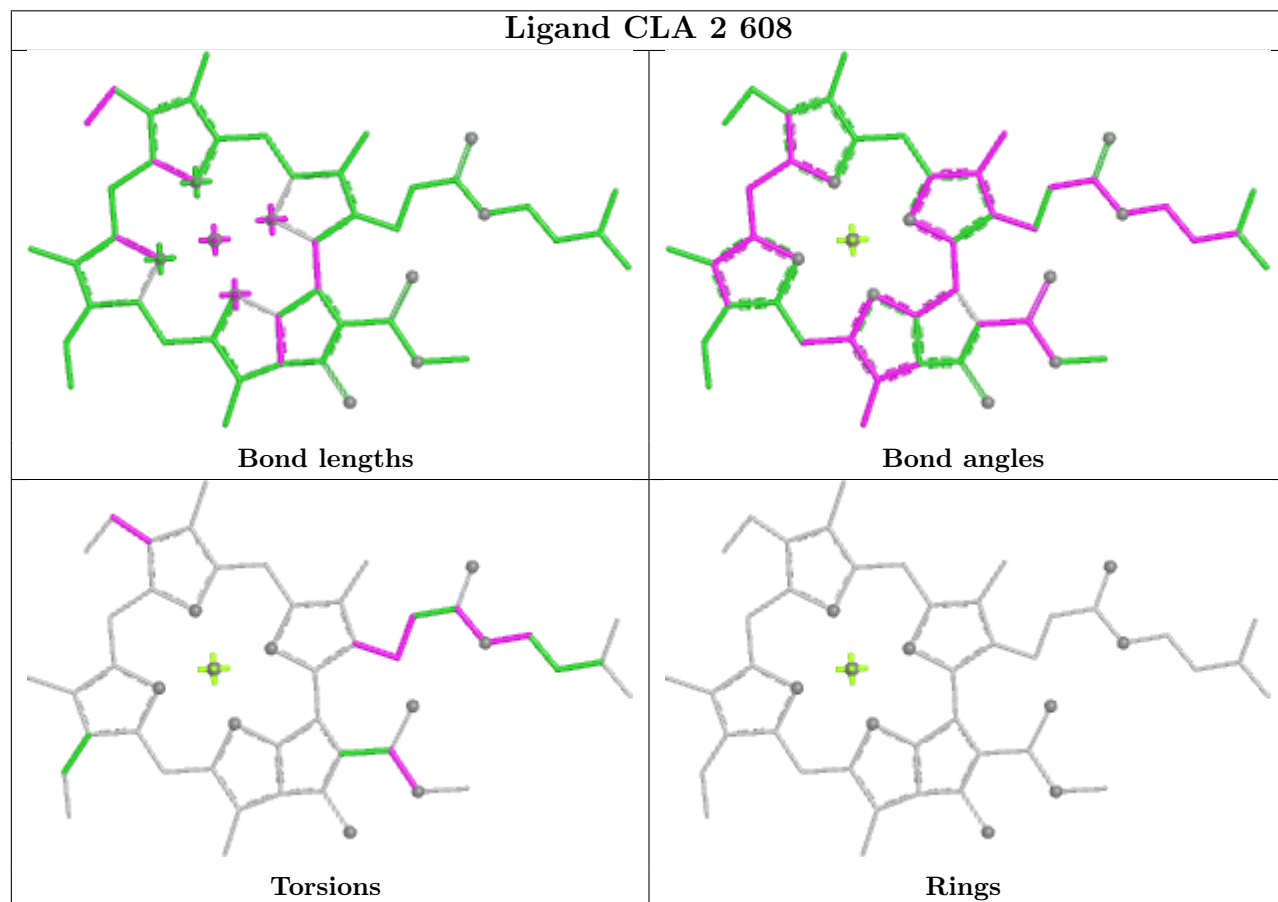
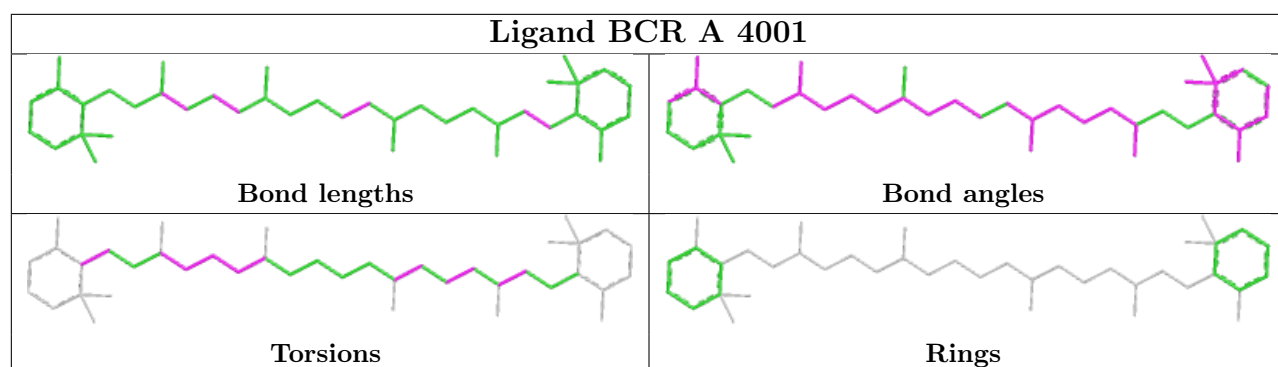
Bond angles

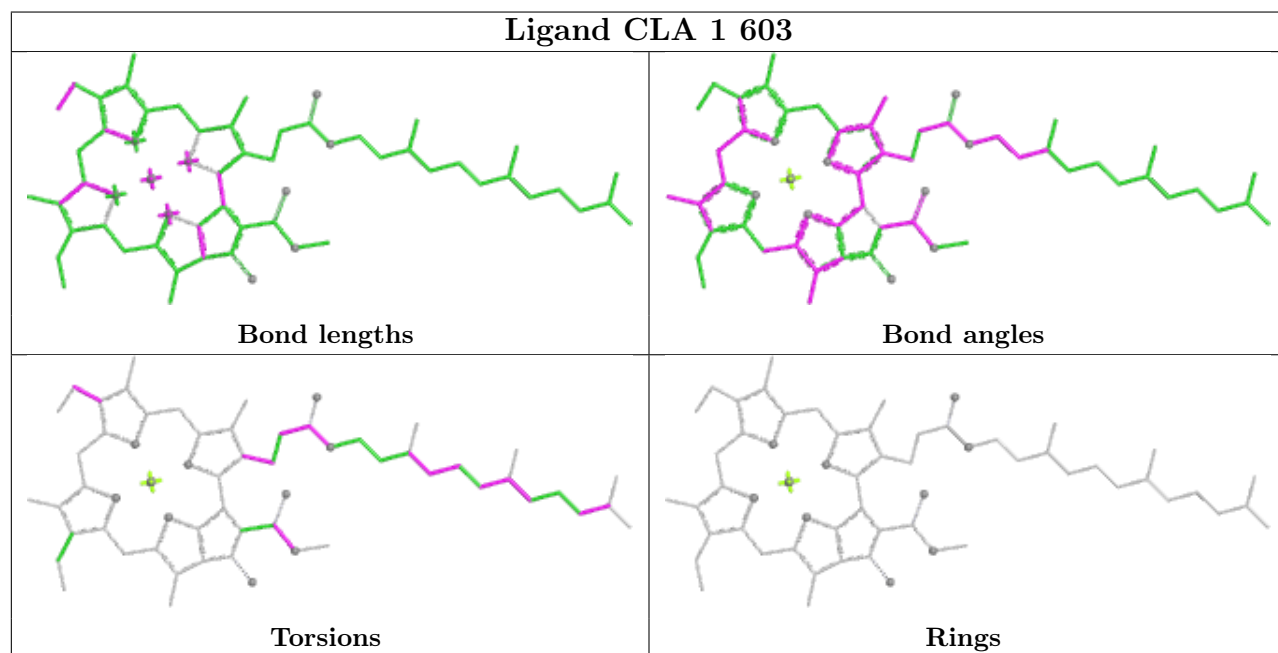
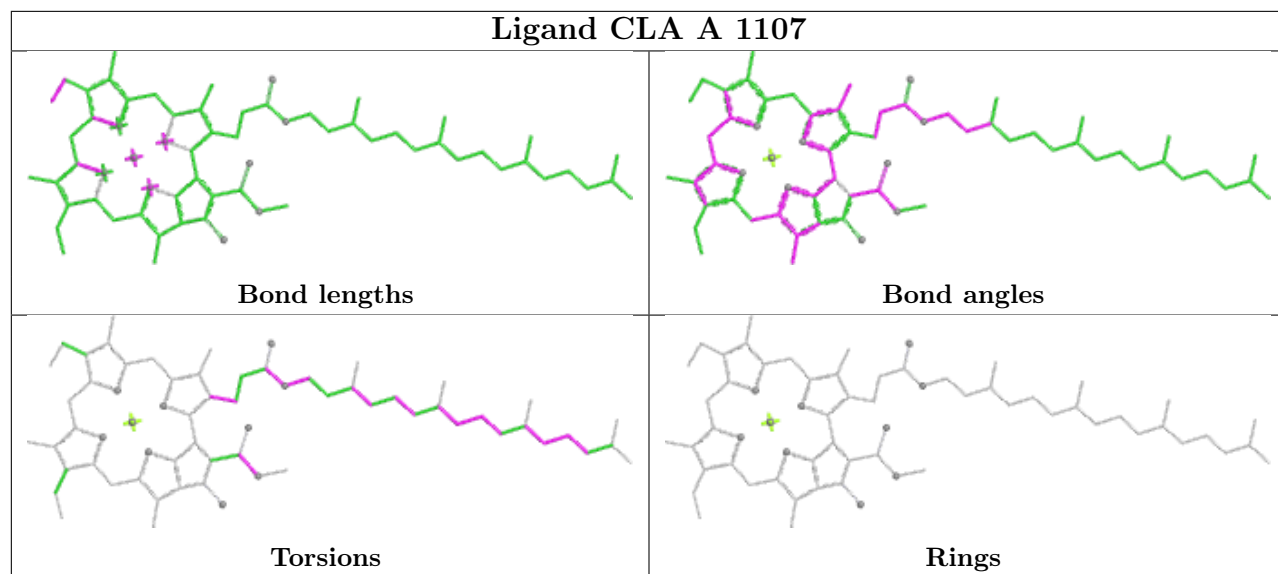


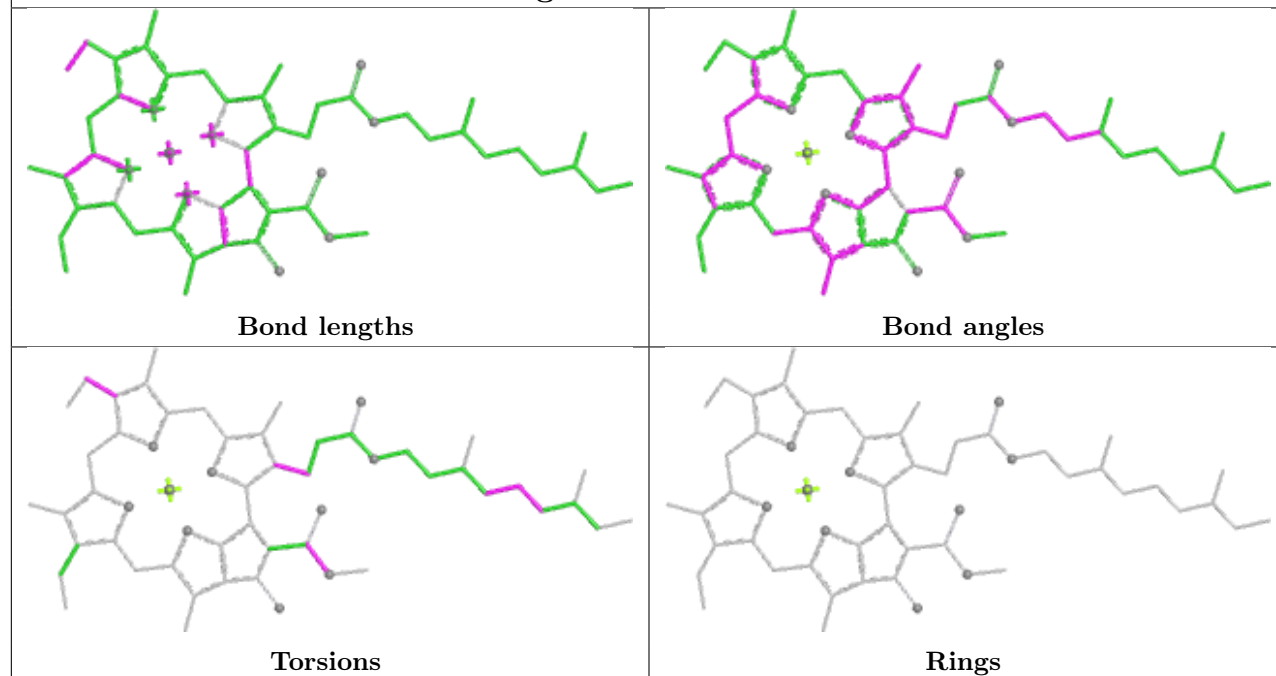
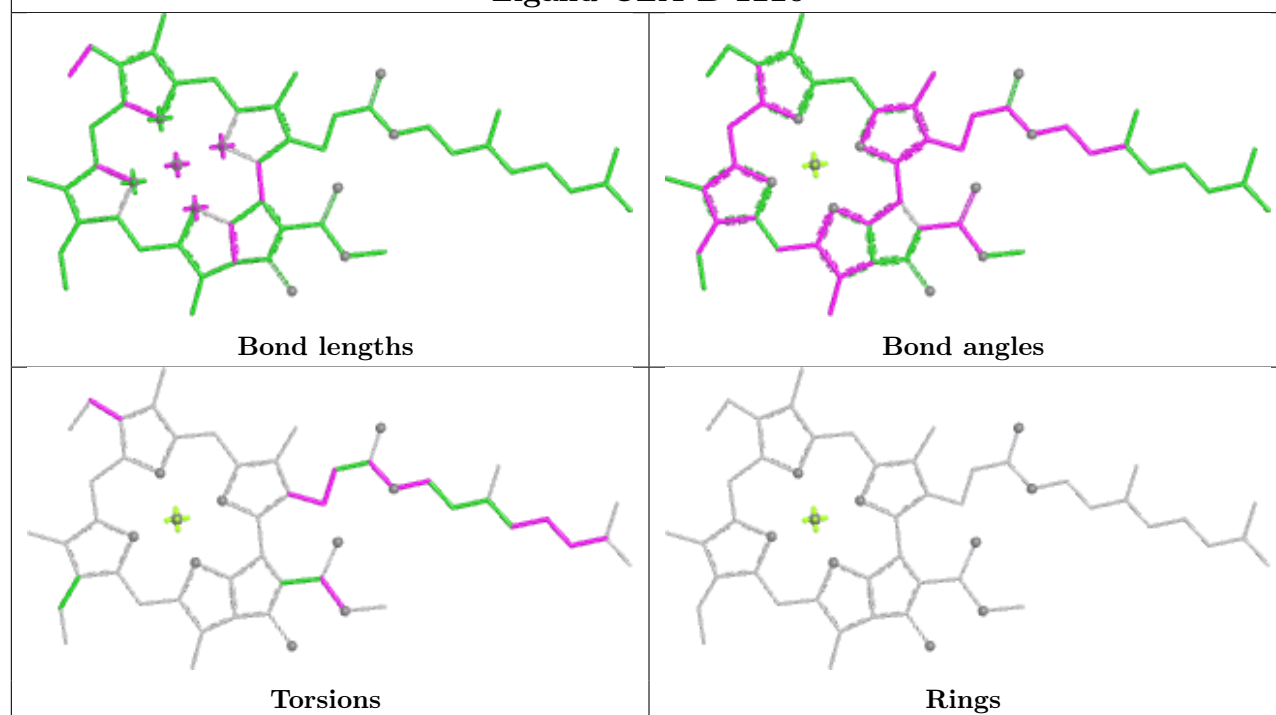
Torsions

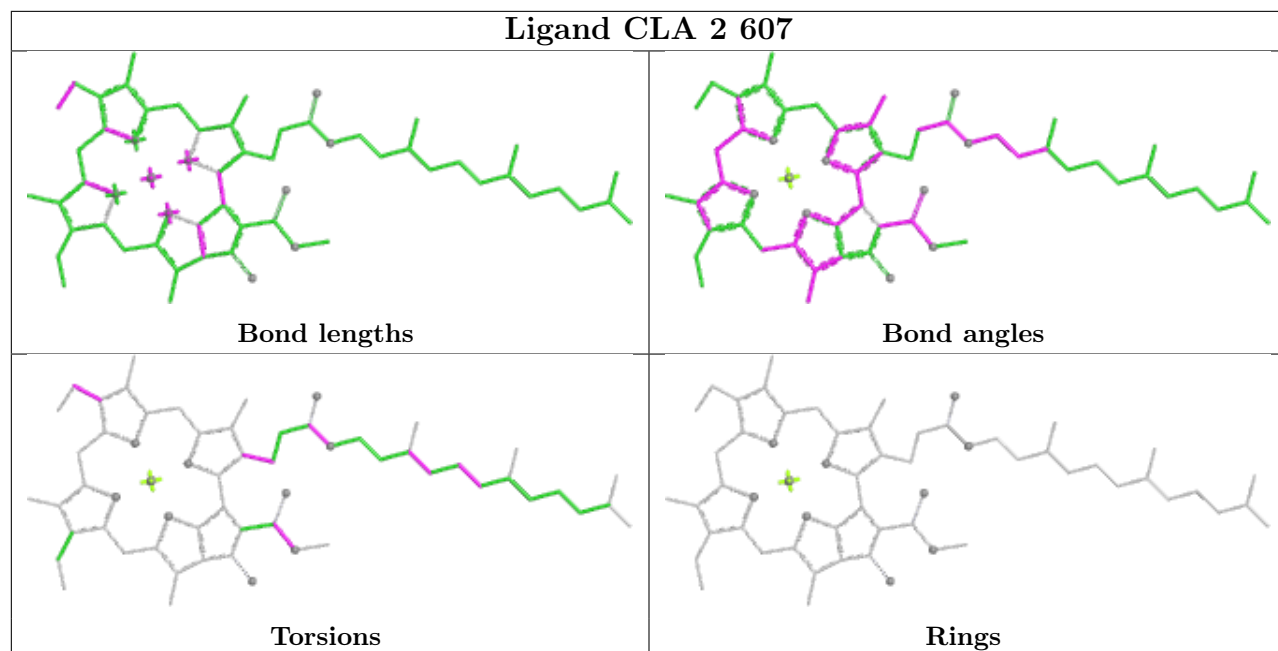
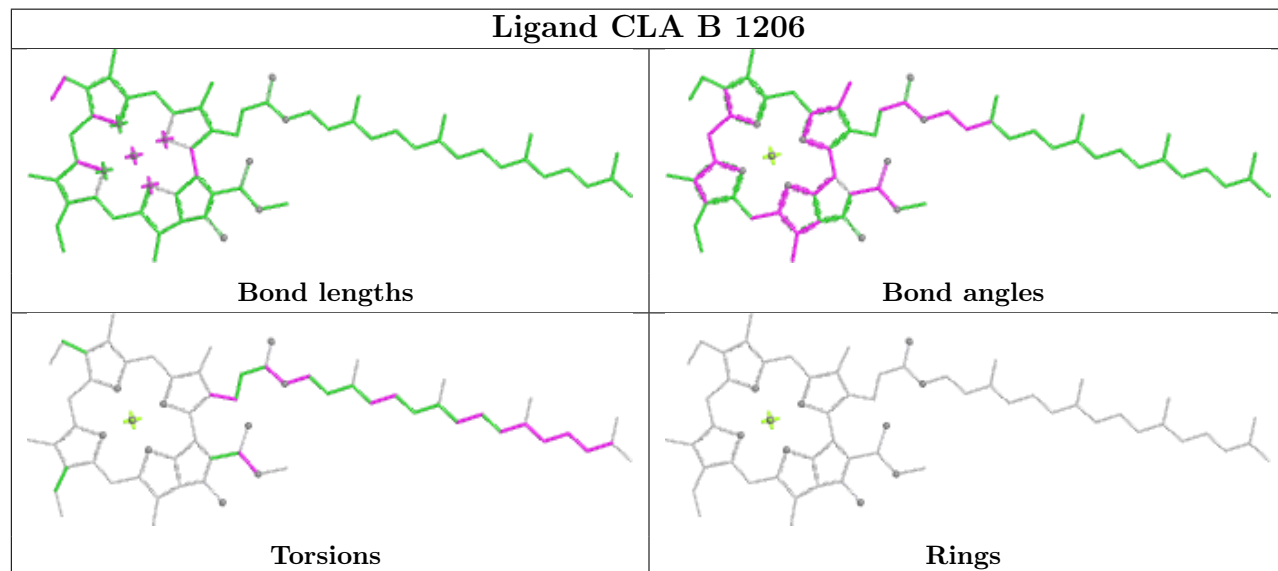


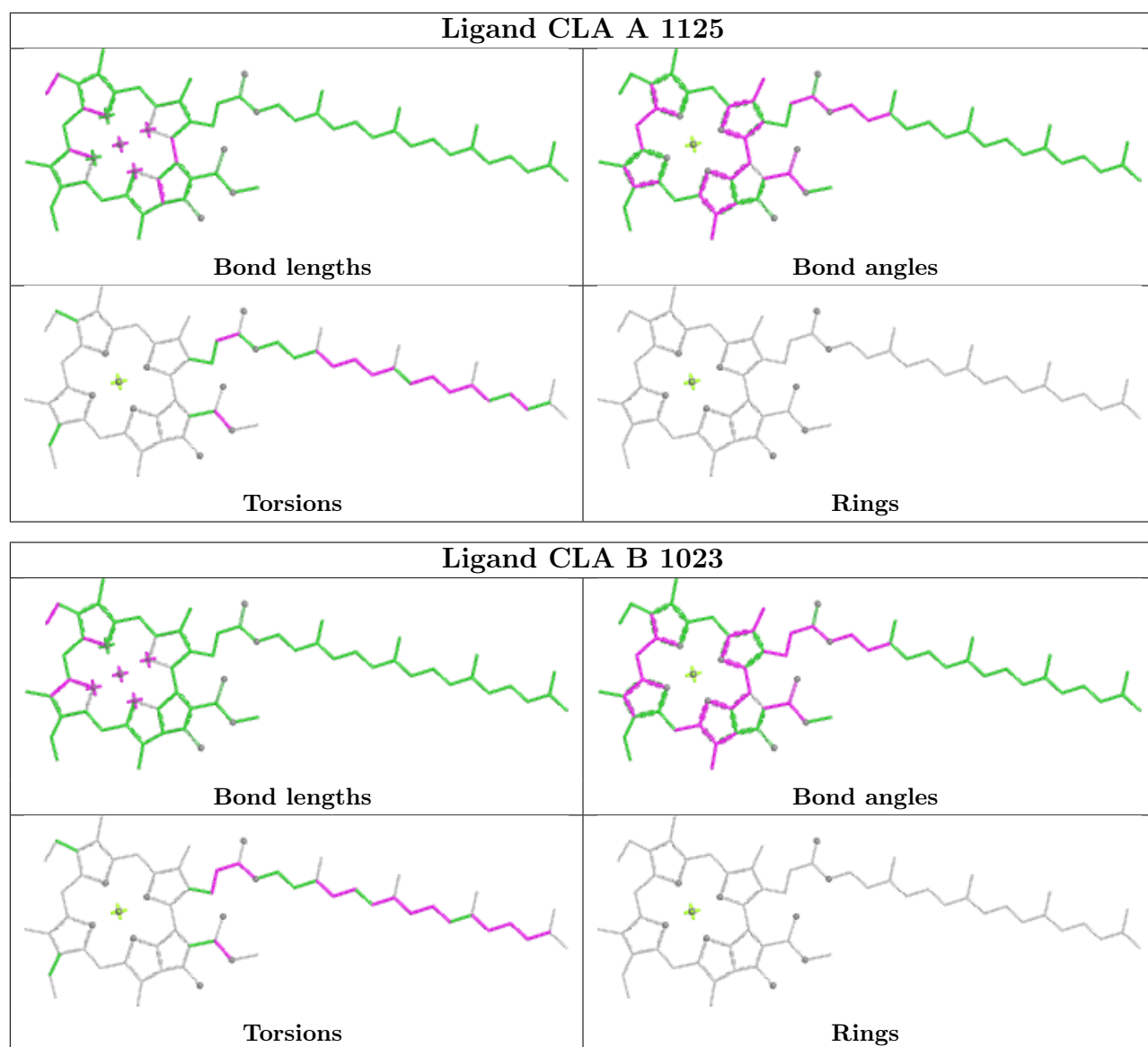
Rings



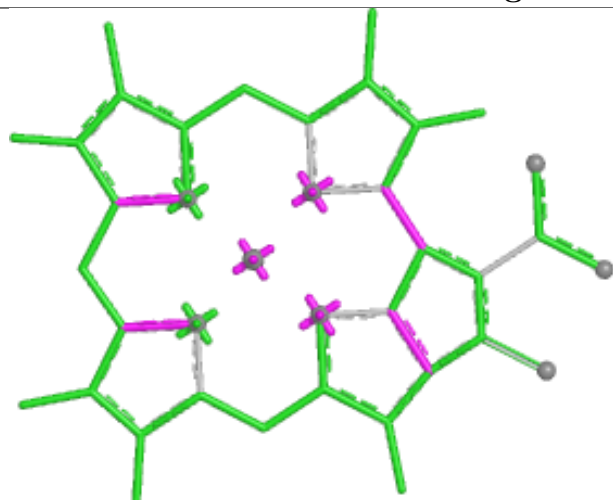


Ligand CLA 3 615**Ligand CLA B 1220**

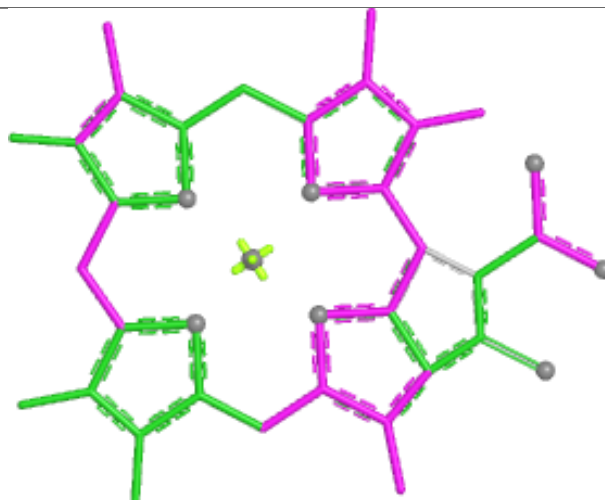
Ligand CLA 2 607**Ligand CLA B 1206**



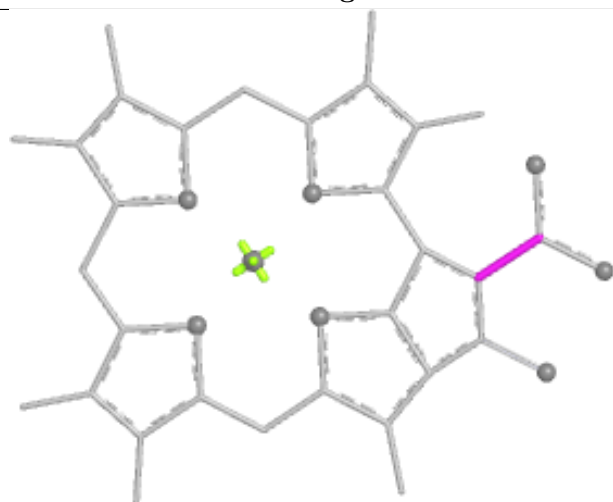
Ligand CLA O 1802



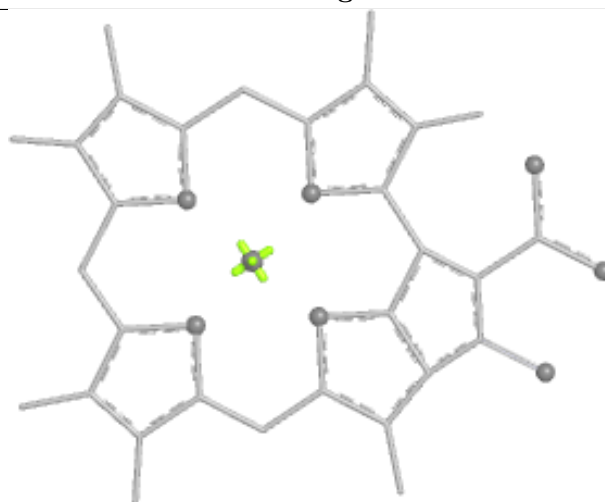
Bond lengths



Bond angles

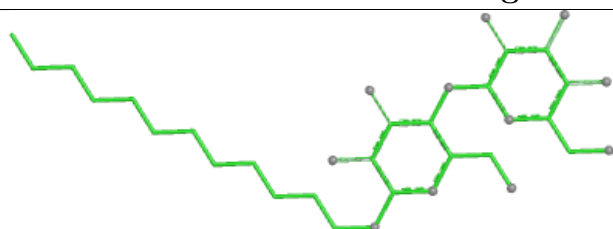


Torsions

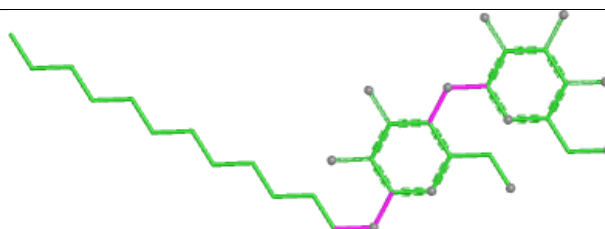


Rings

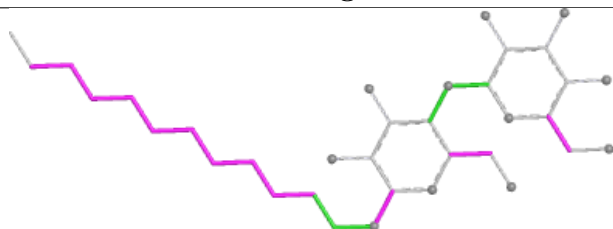
Ligand LMU B 5004



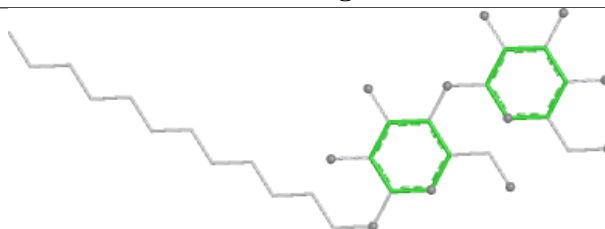
Bond lengths



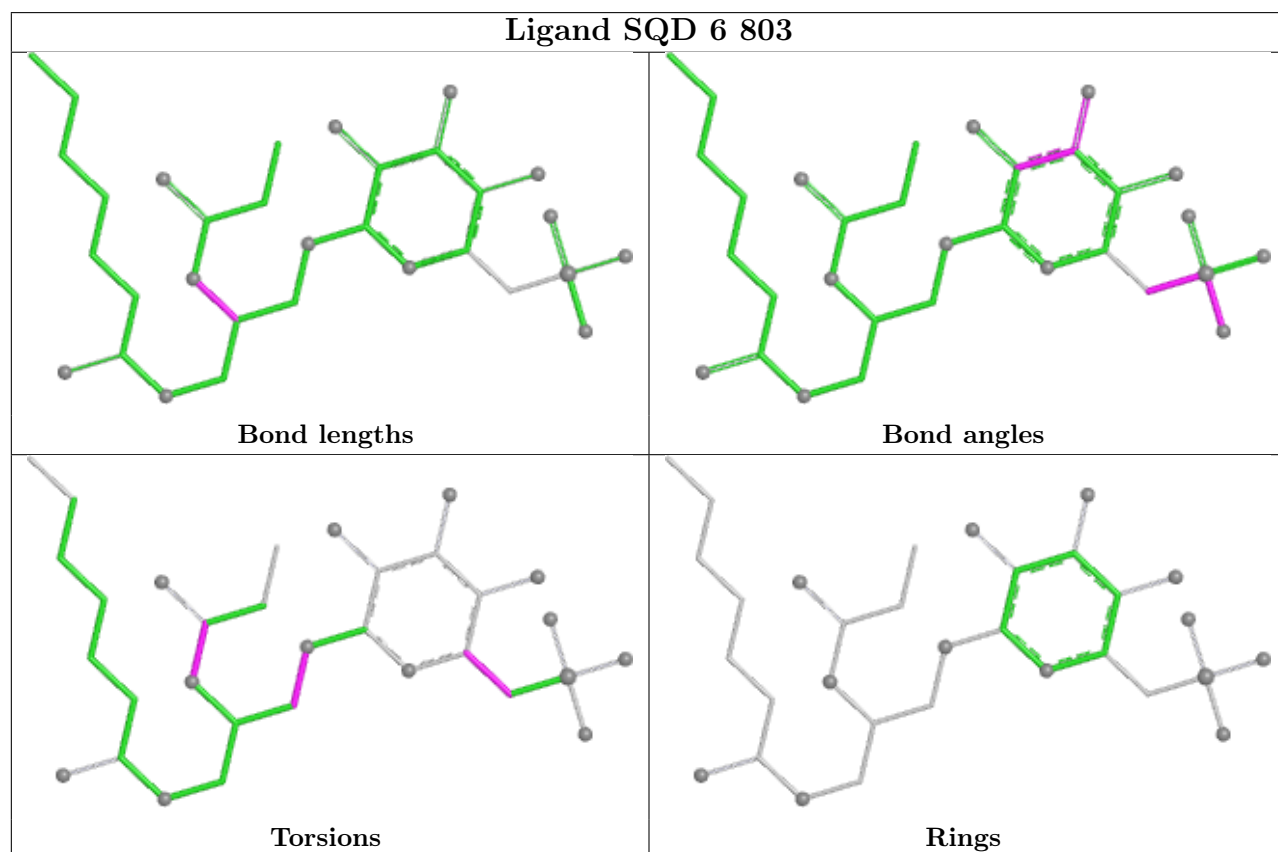
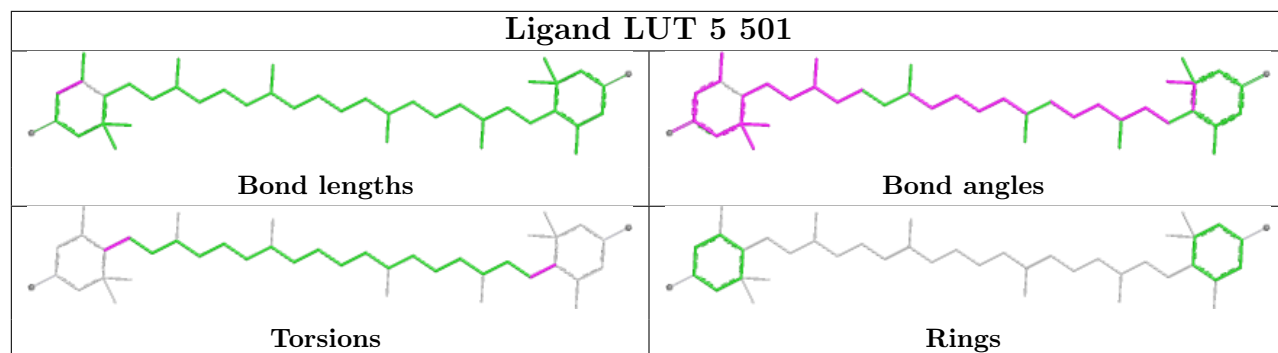
Bond angles



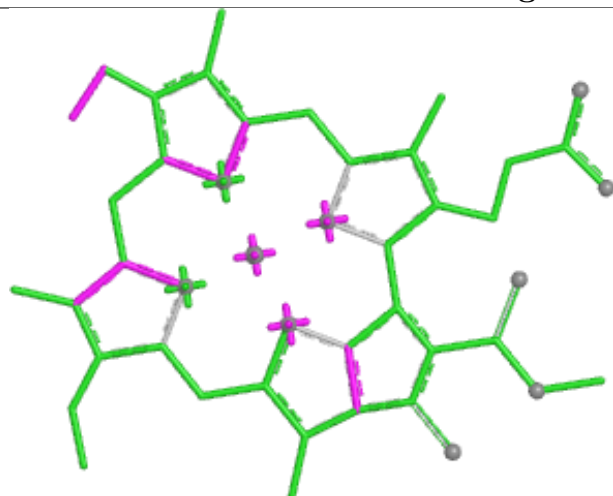
Torsions



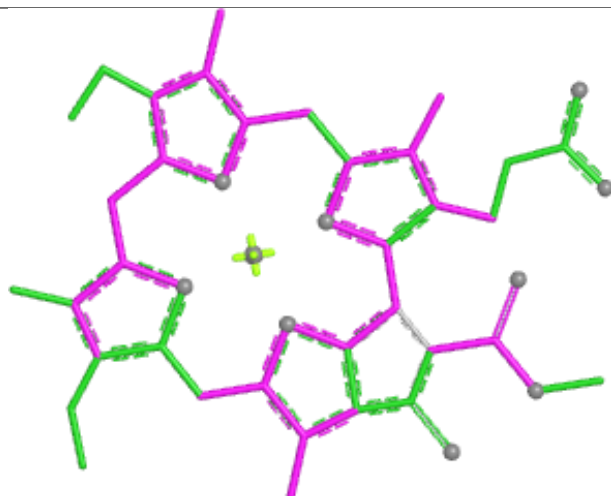
Rings



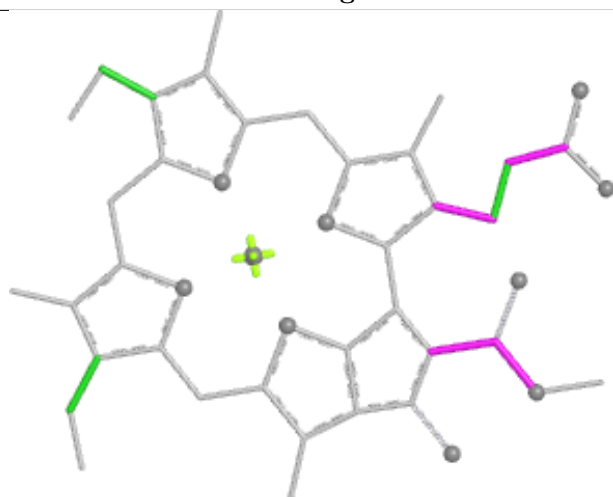
Ligand CLA 5 613



Bond lengths



Bond angles

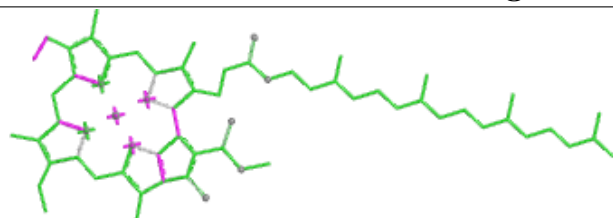


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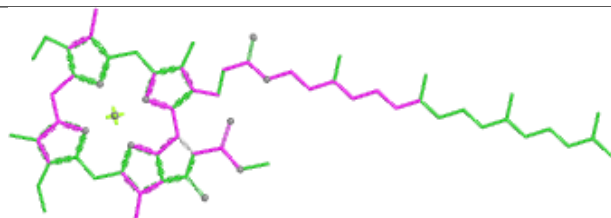


Rings

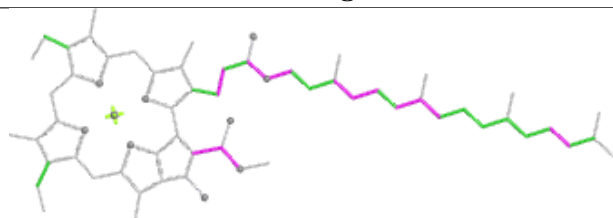
Ligand CLA B 1211



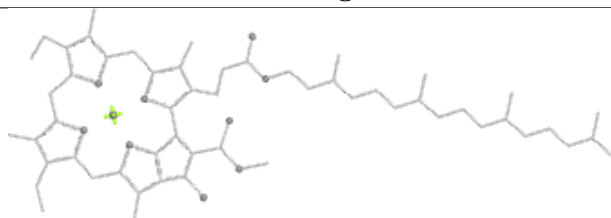
Bond lengths



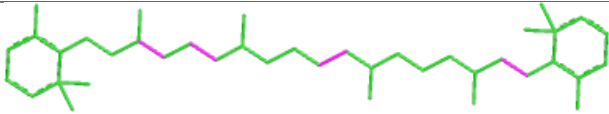
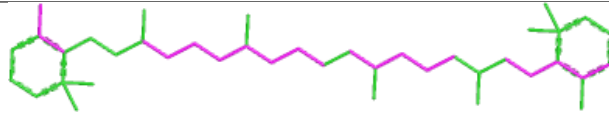
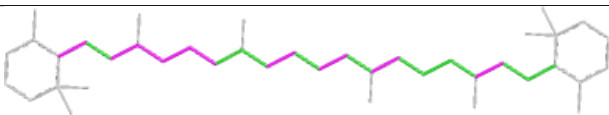
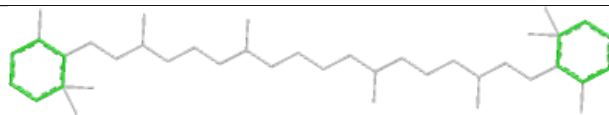
Bond angles

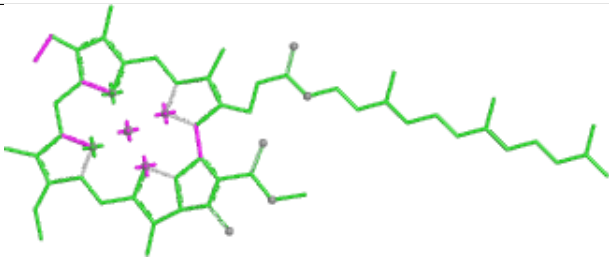
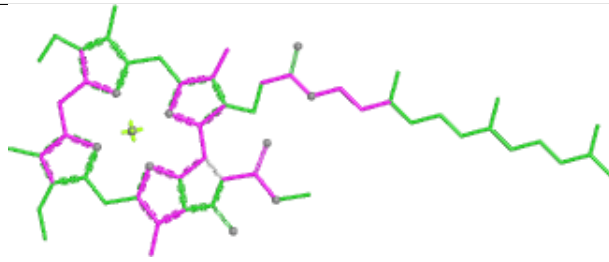
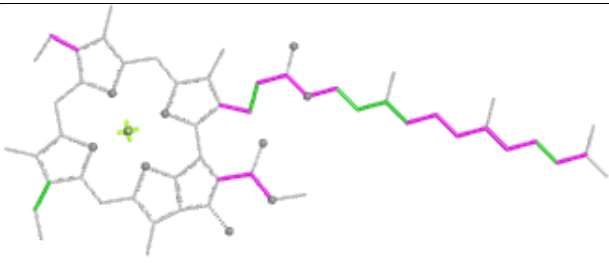
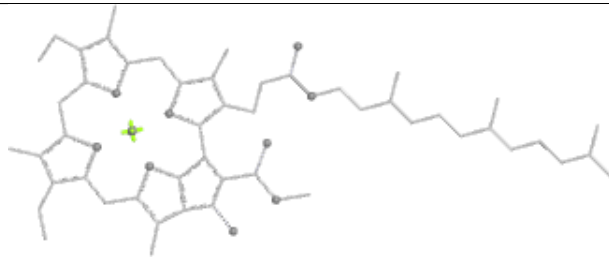


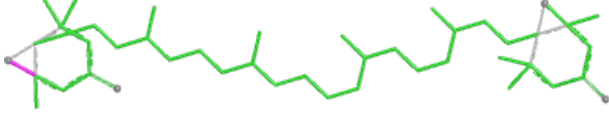
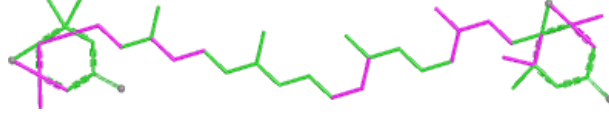
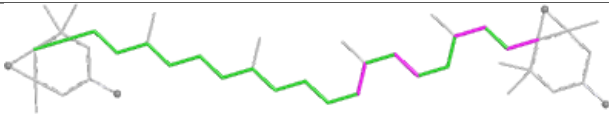
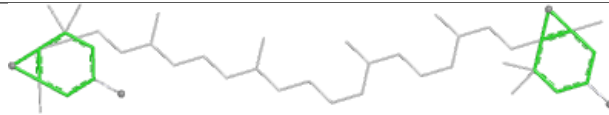
Torsions

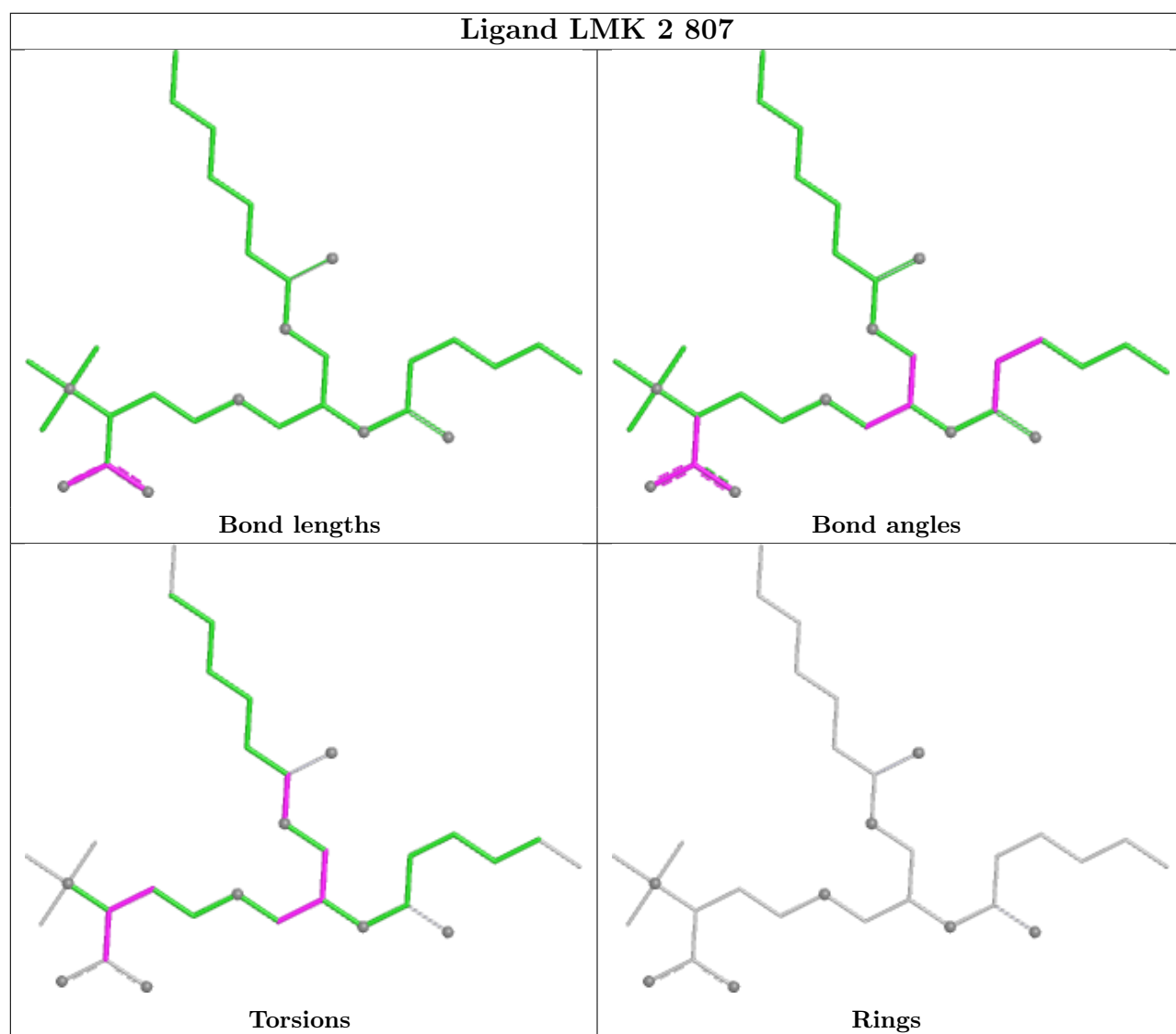


Rings

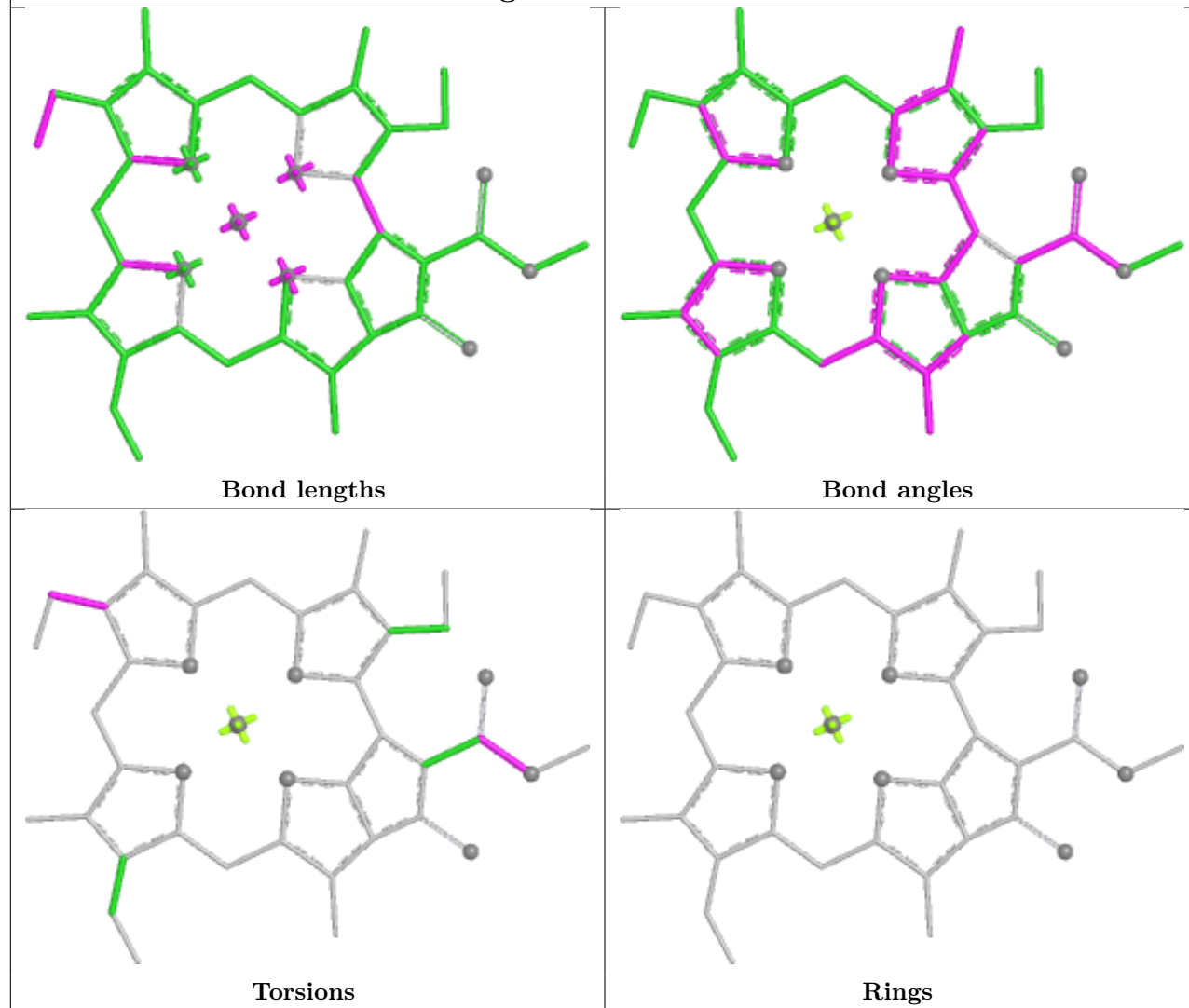
Ligand BCR B 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 4 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

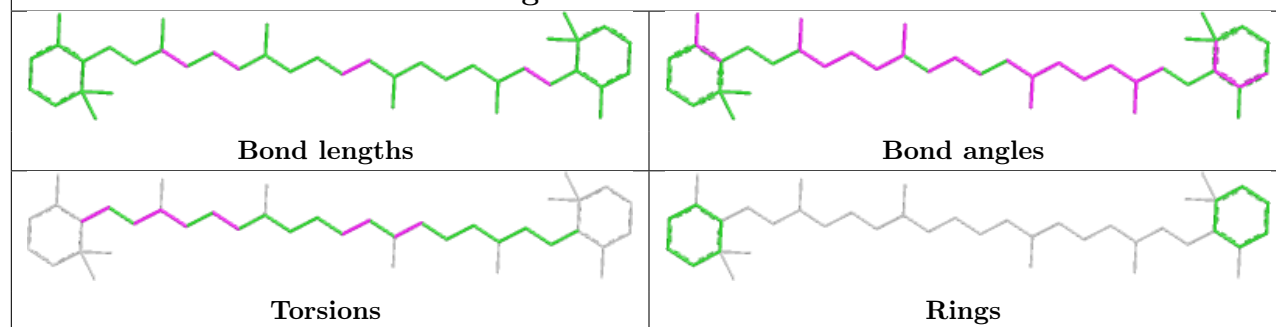
Ligand XAT 1 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

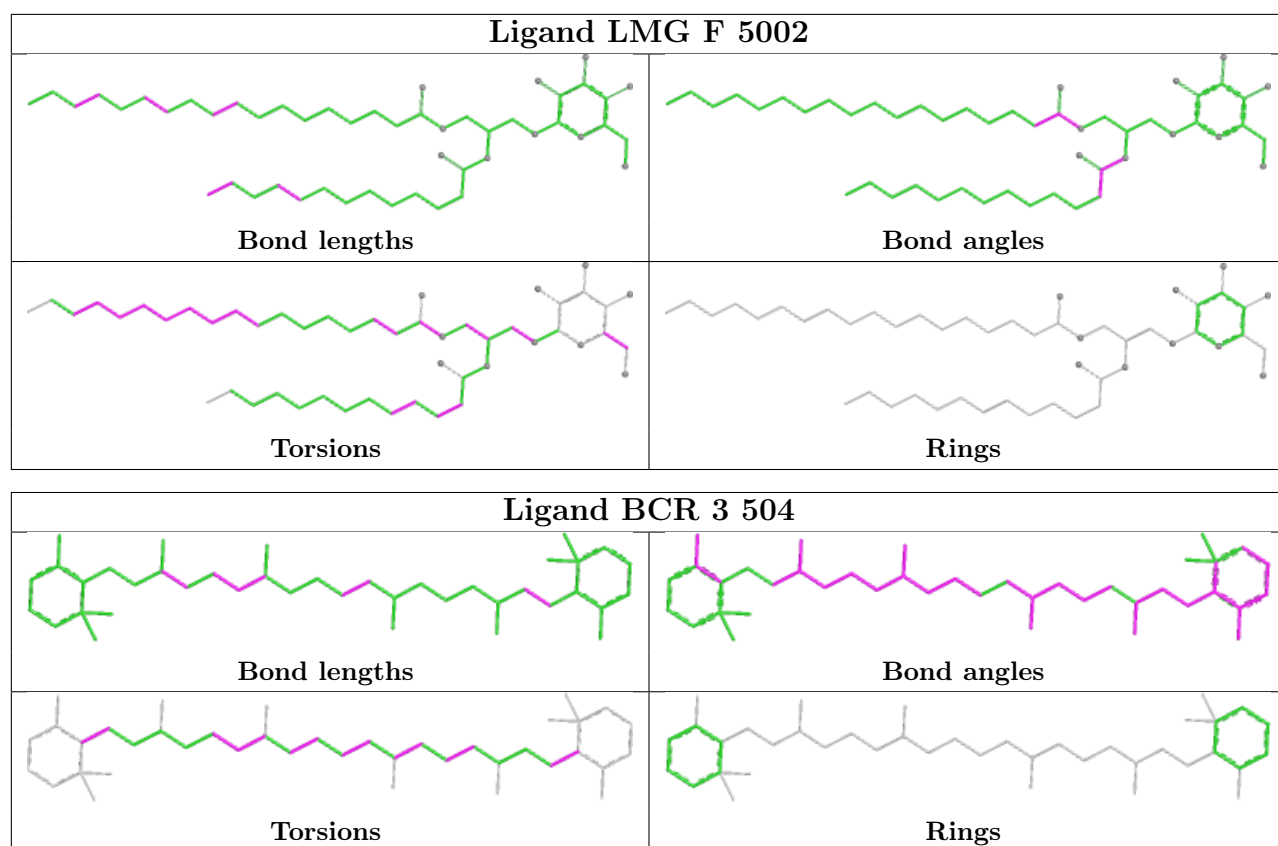


Ligand CLA 3 614

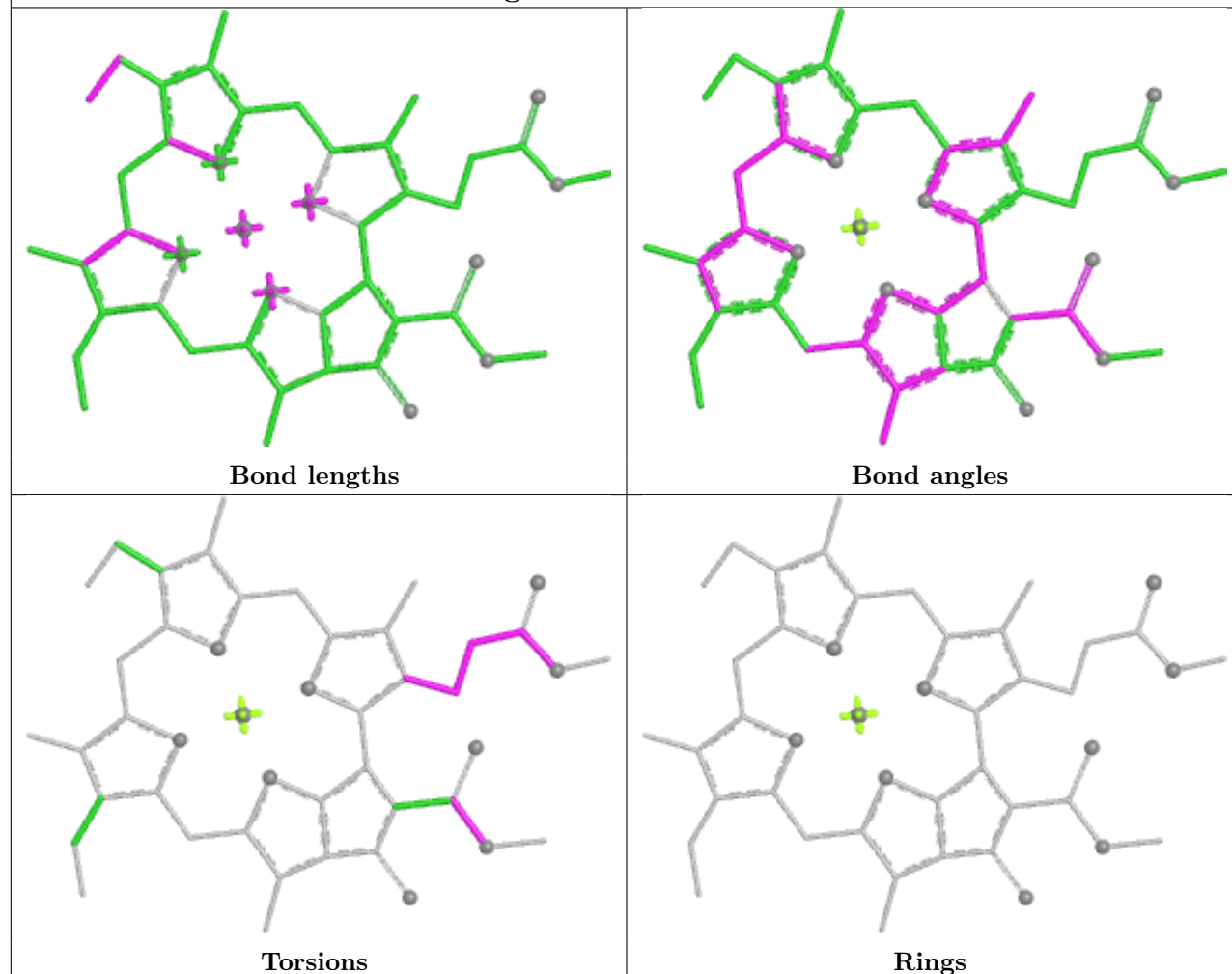


Ligand BCR B 4001

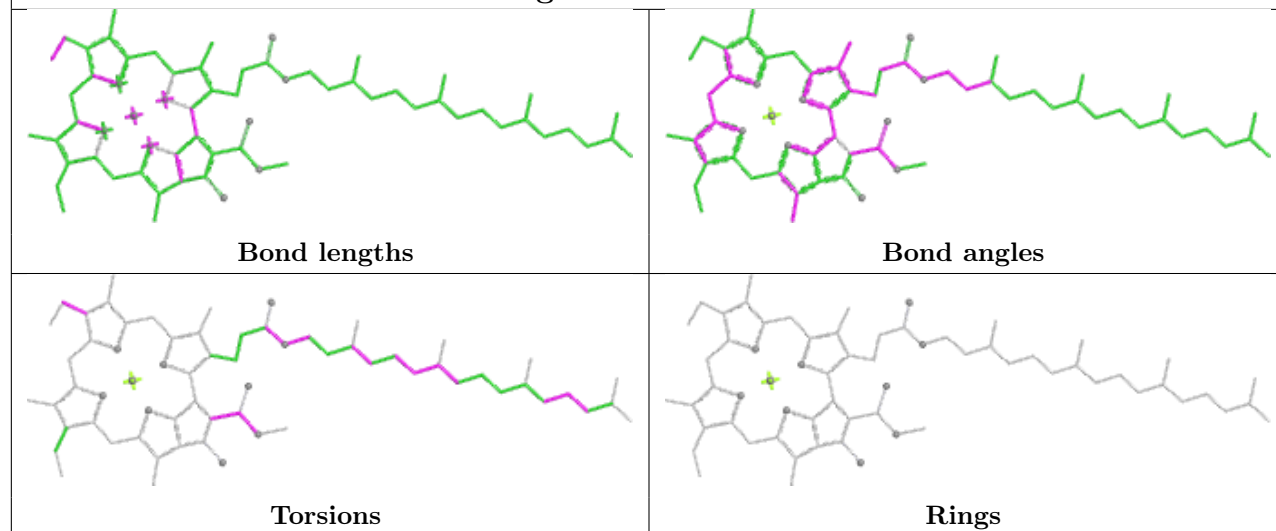


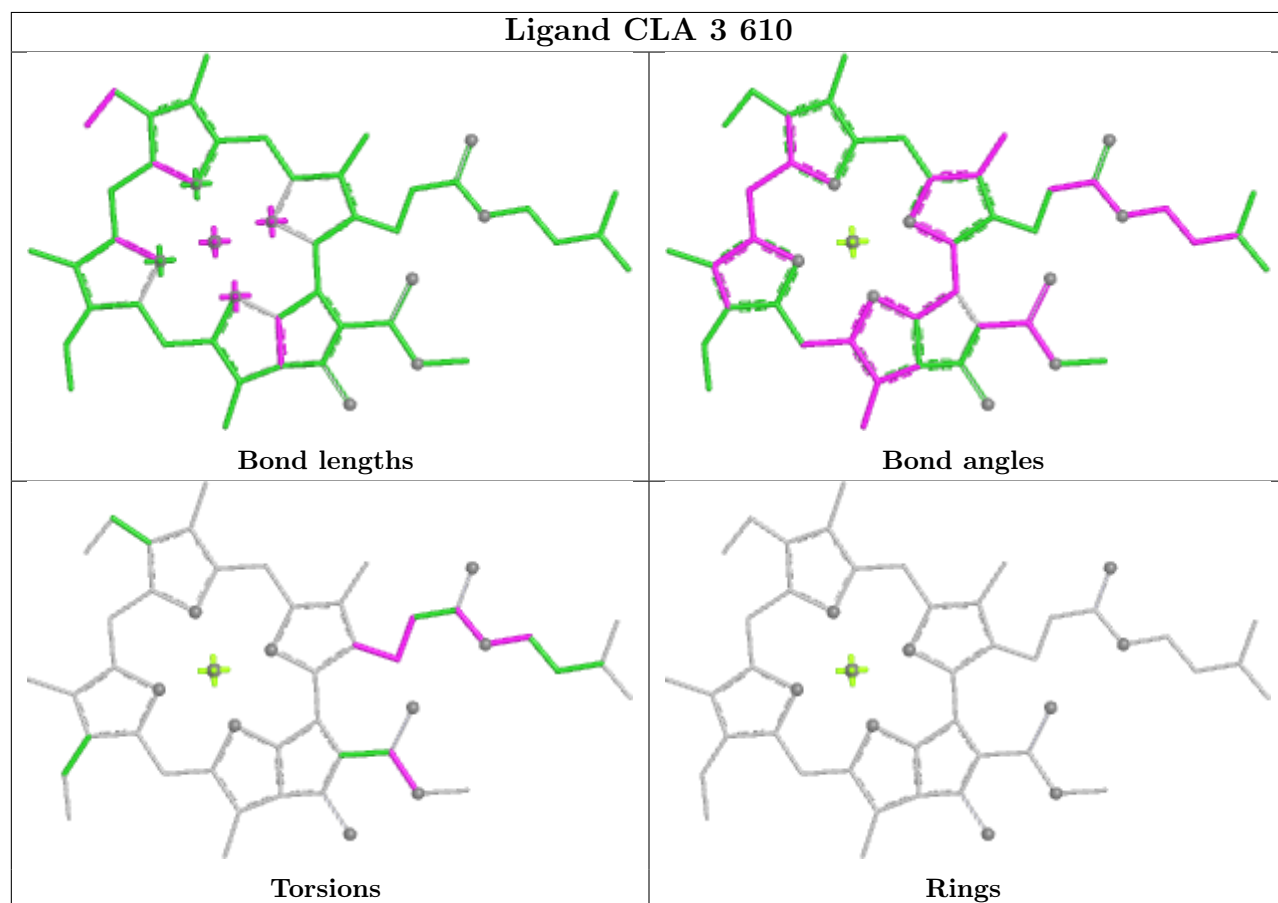
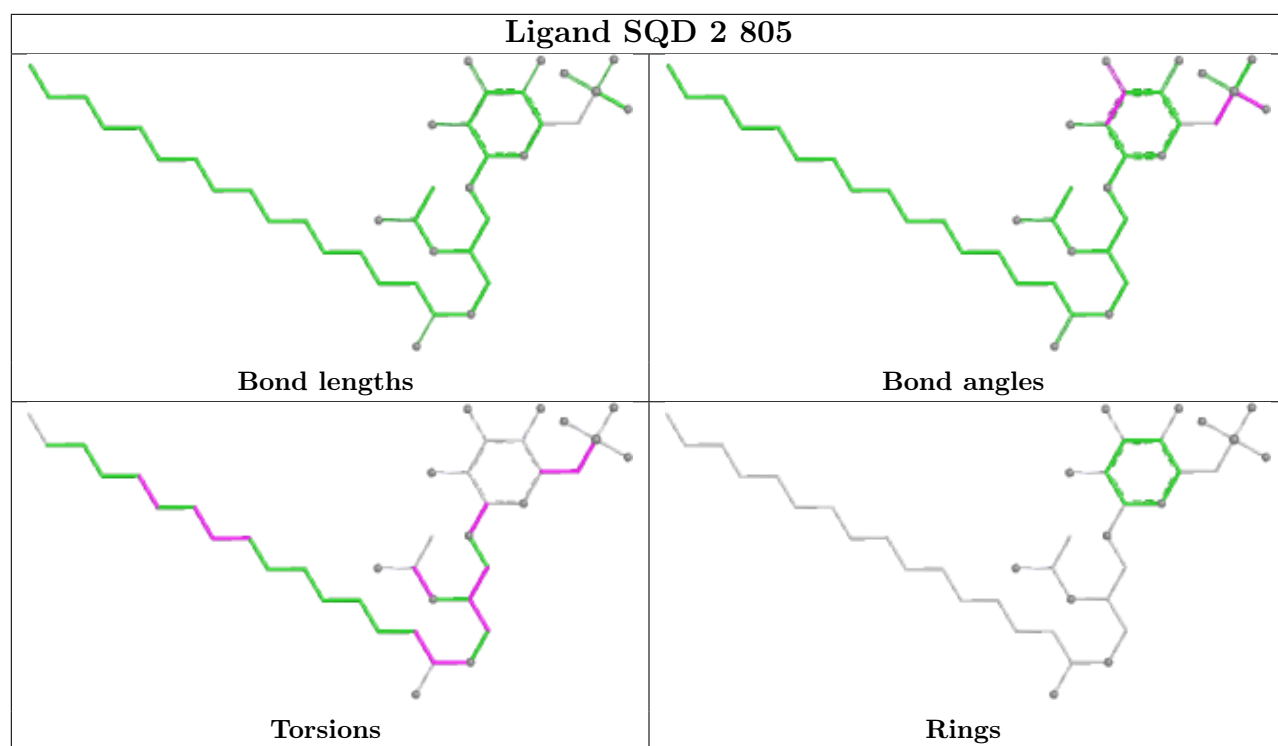


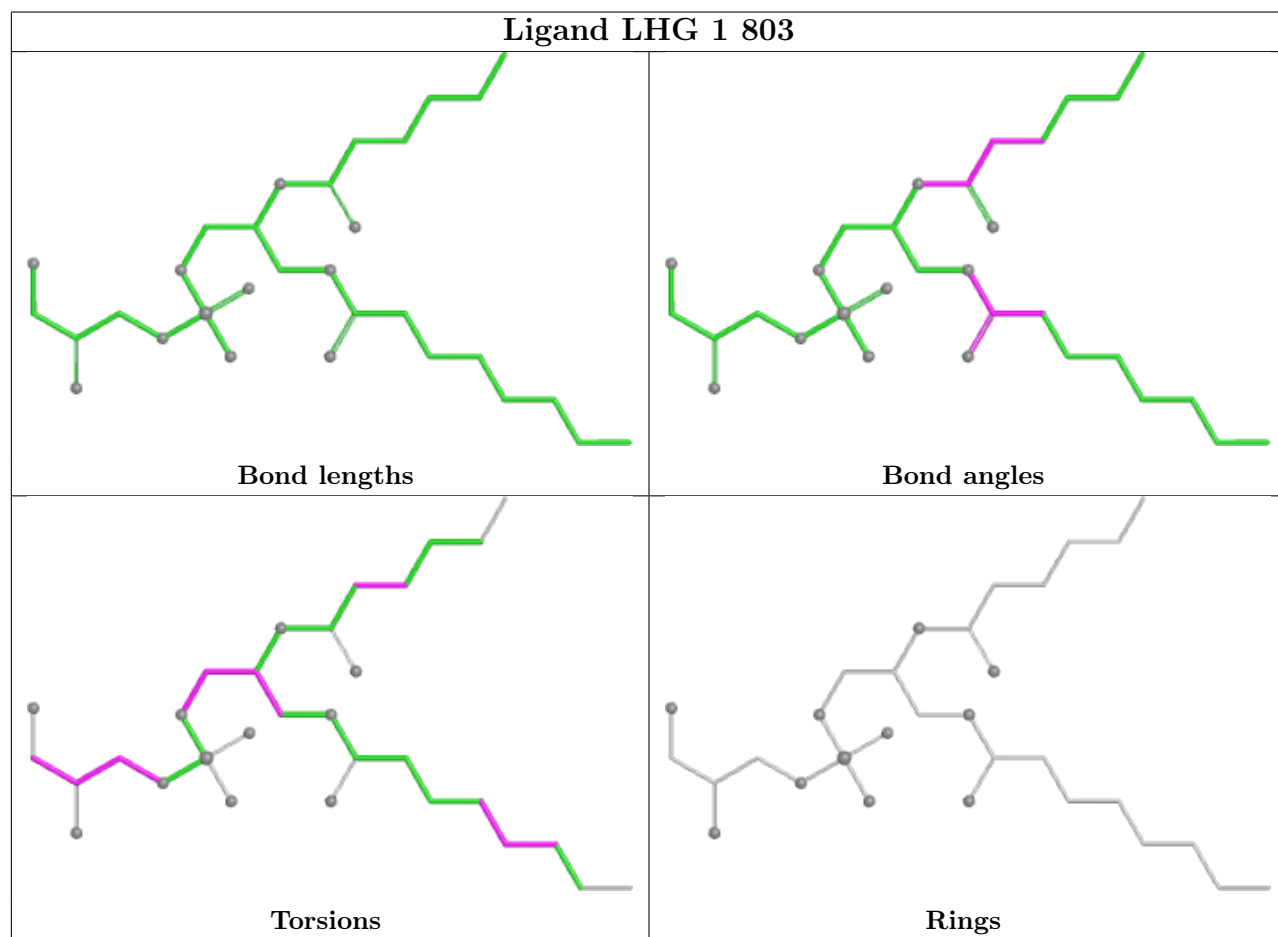
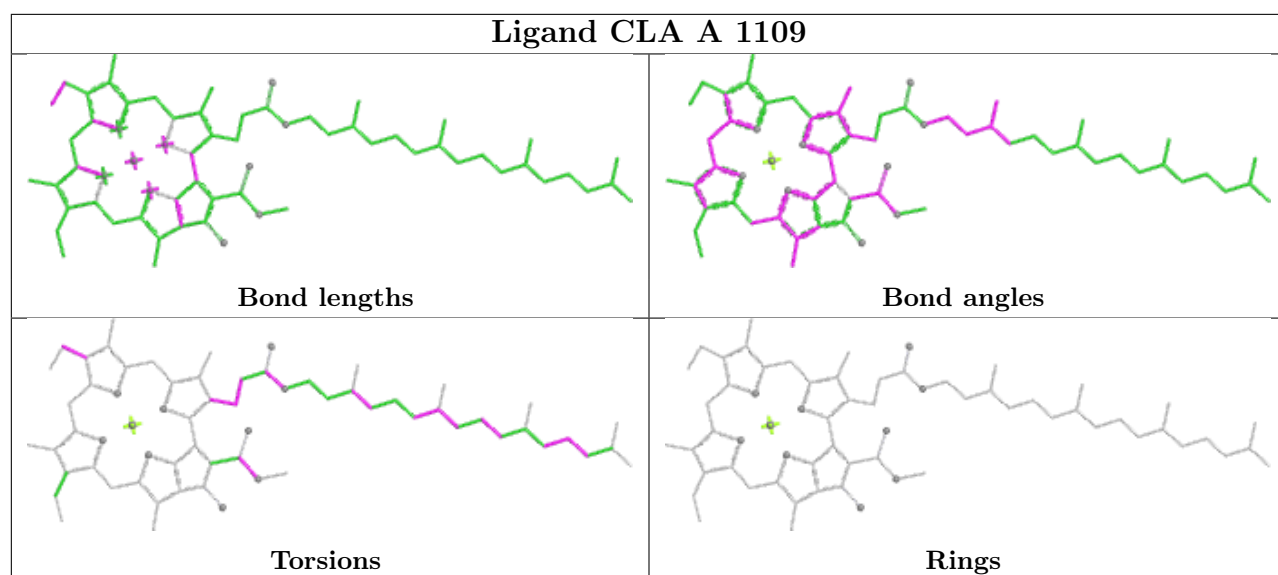
Ligand CLA G 1602

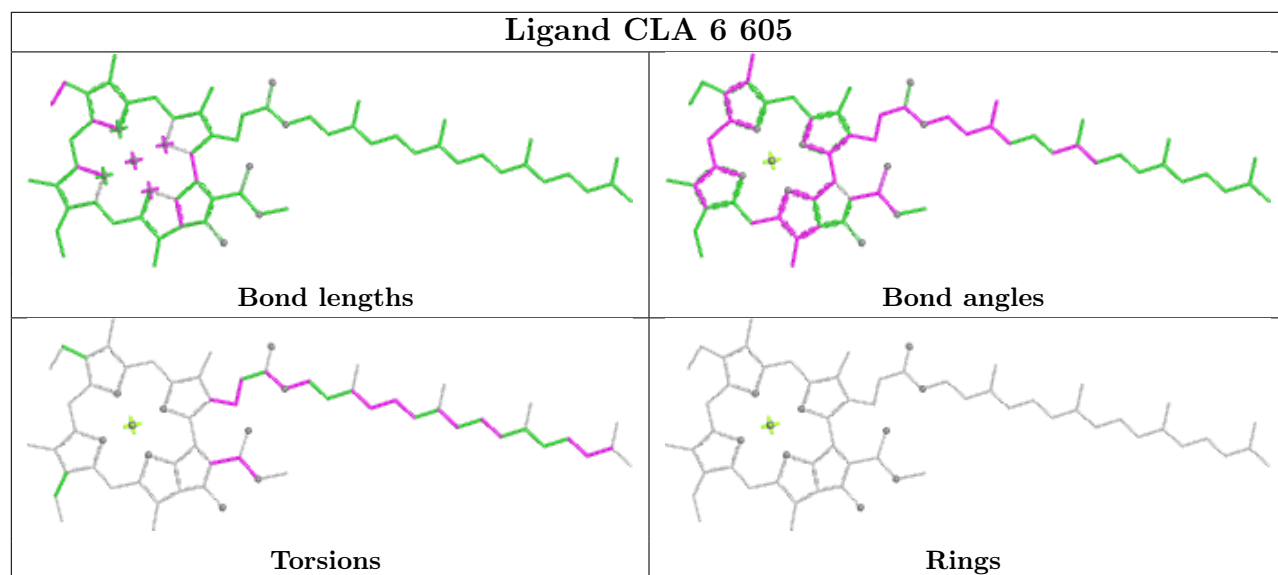
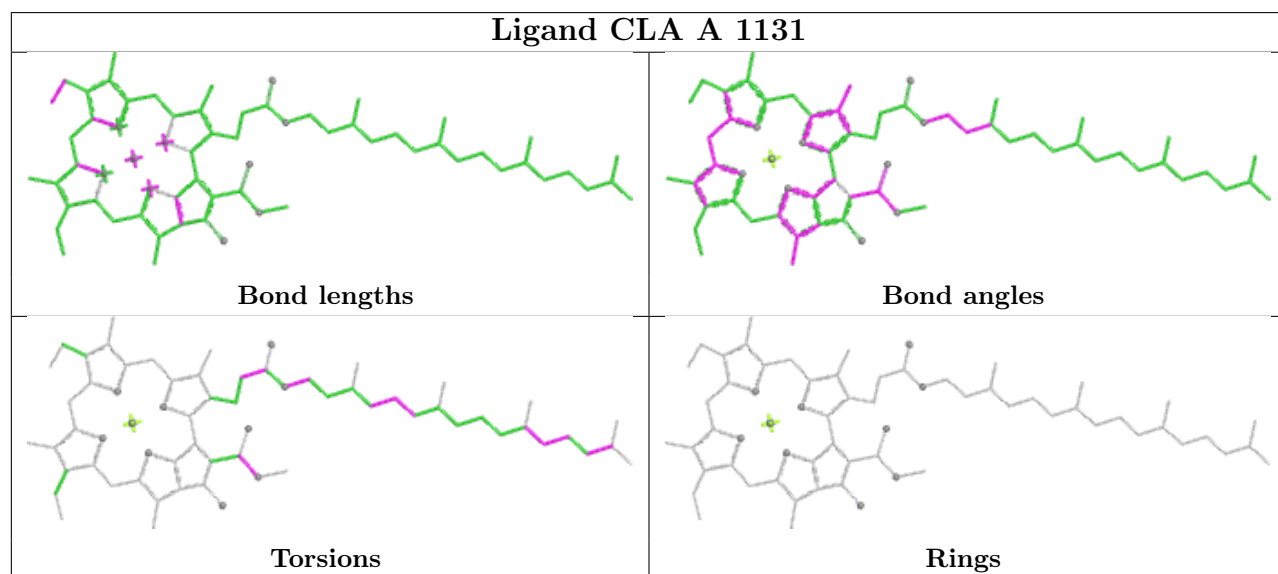
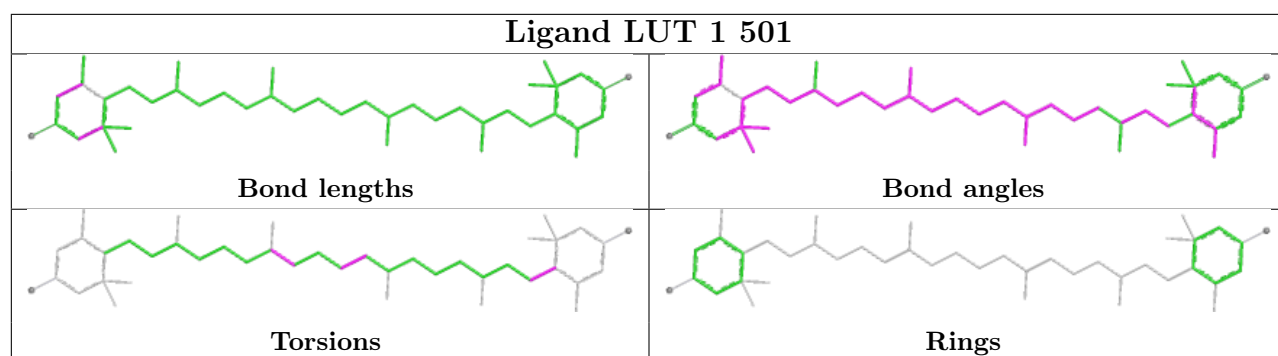


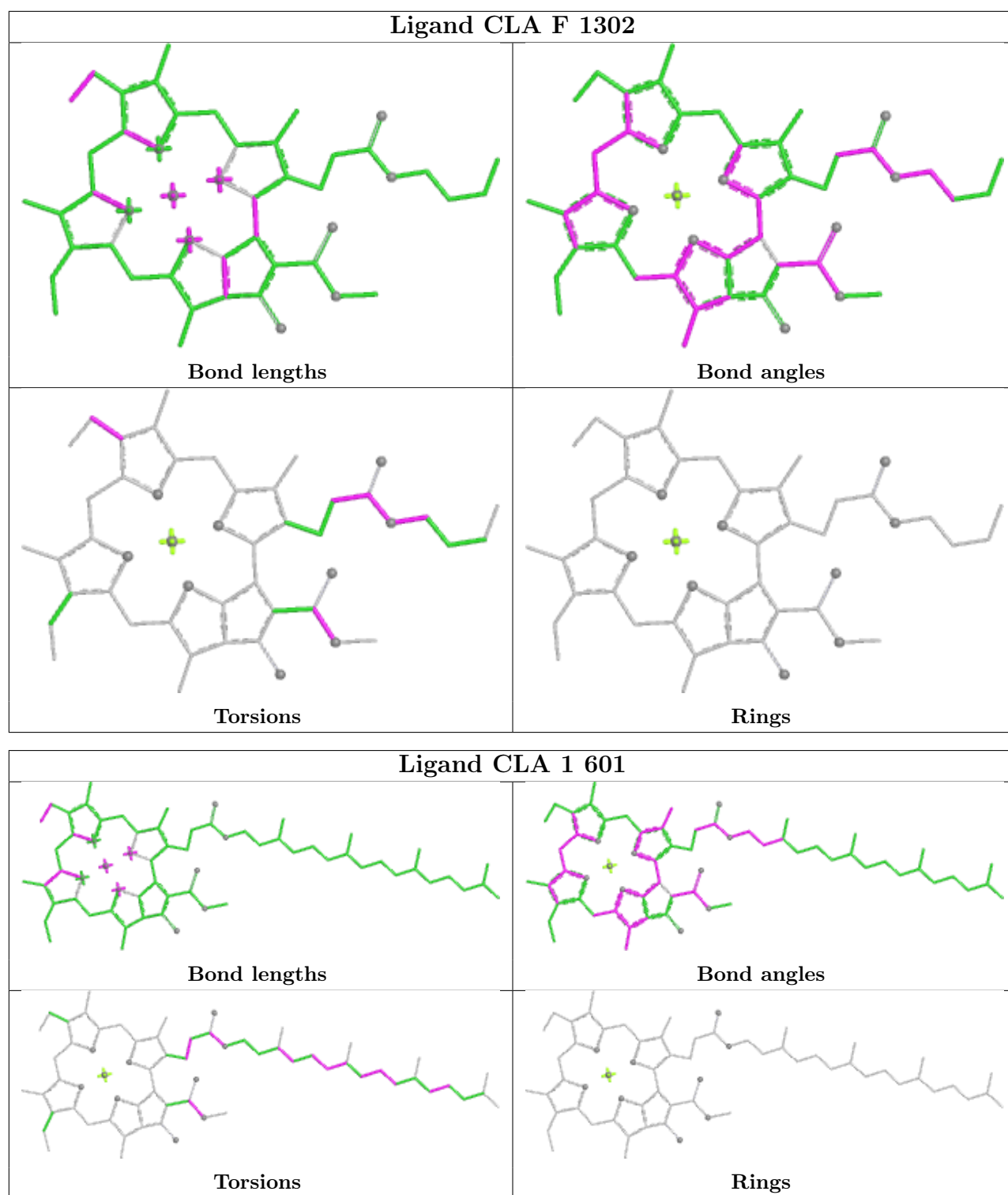
Ligand CLA 3 612

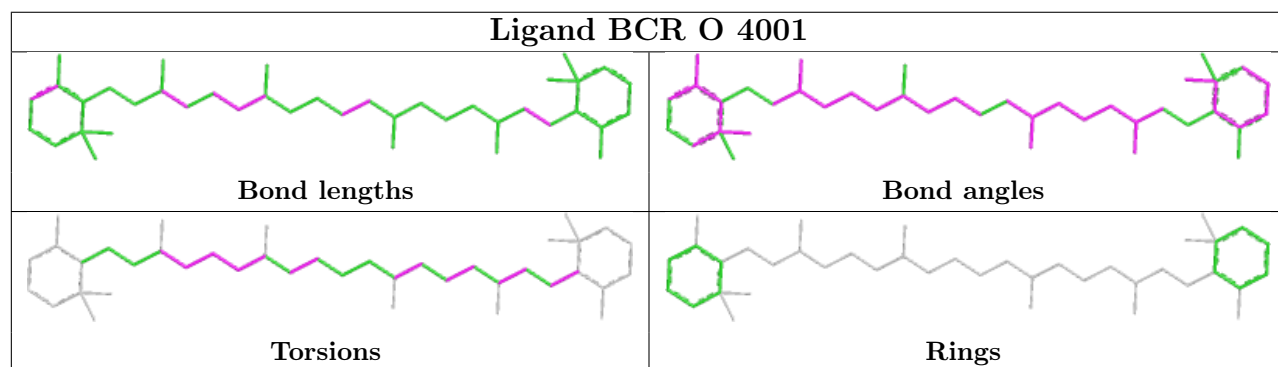
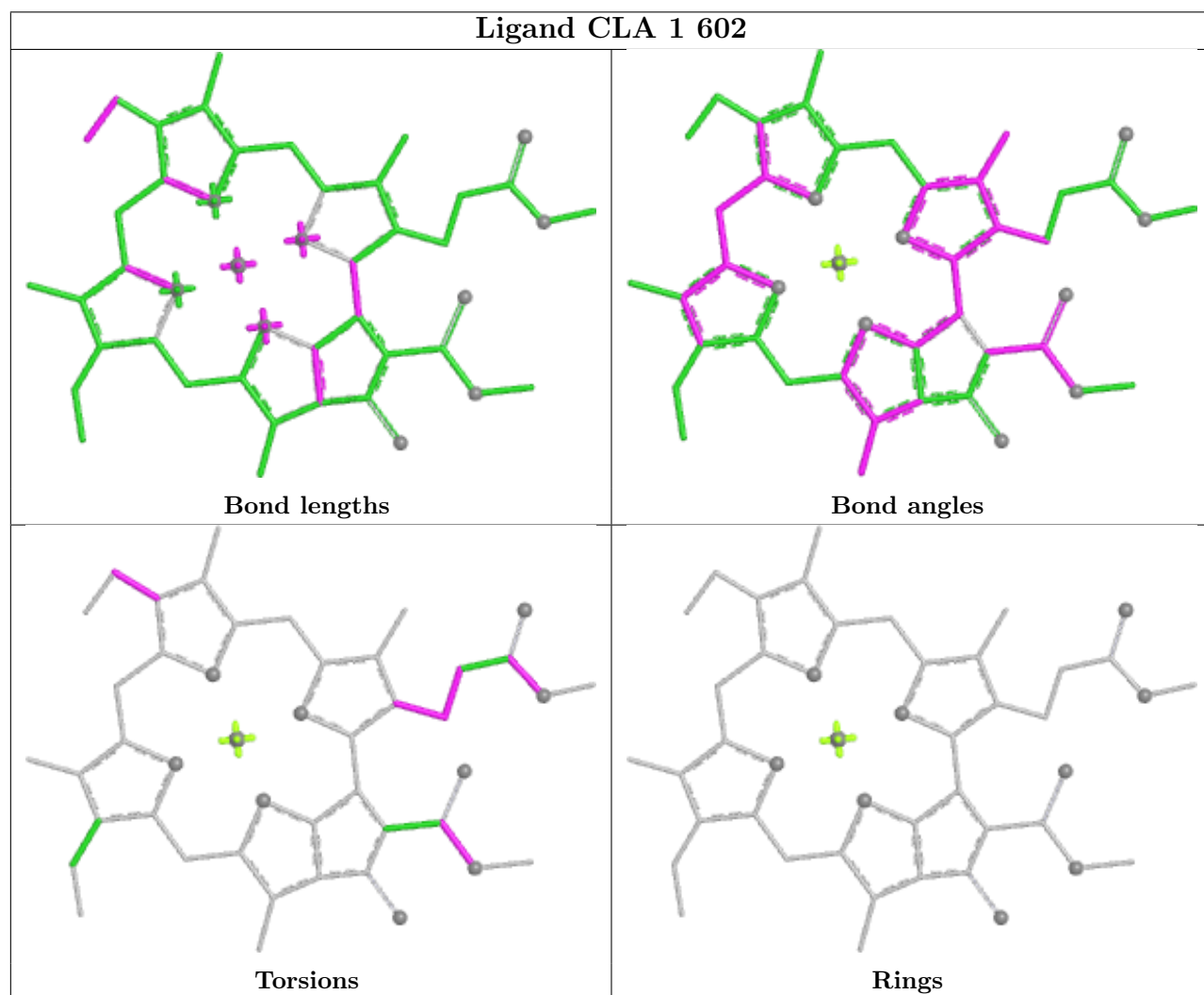
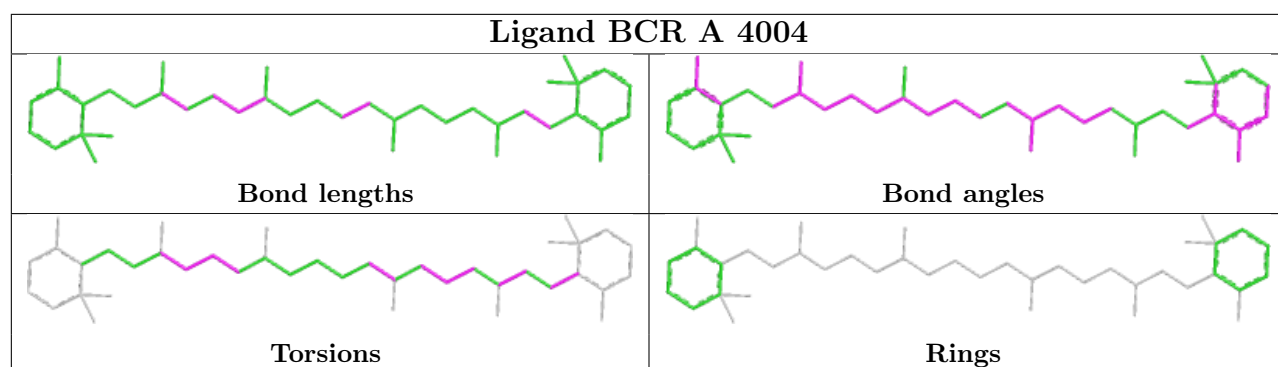


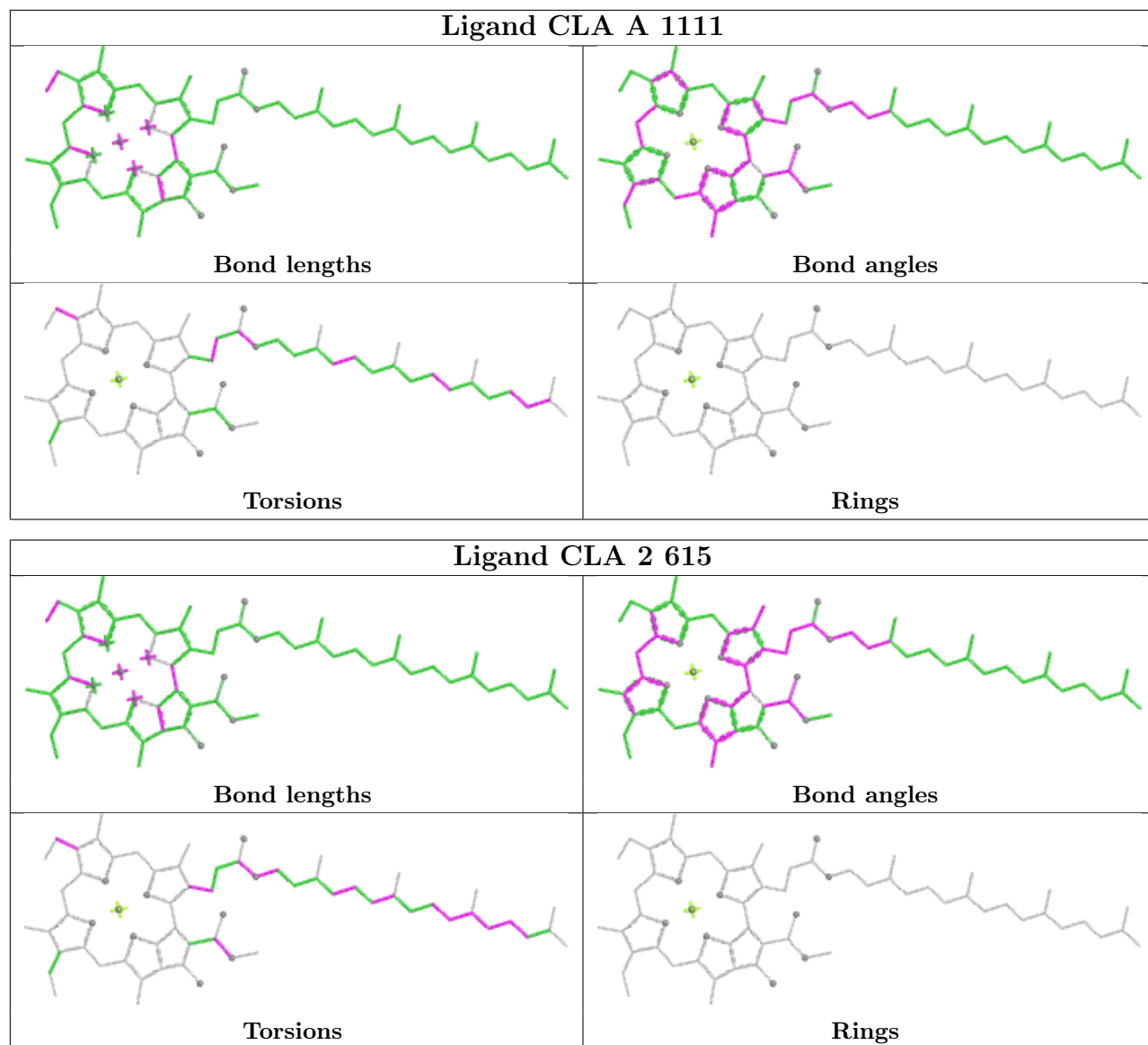


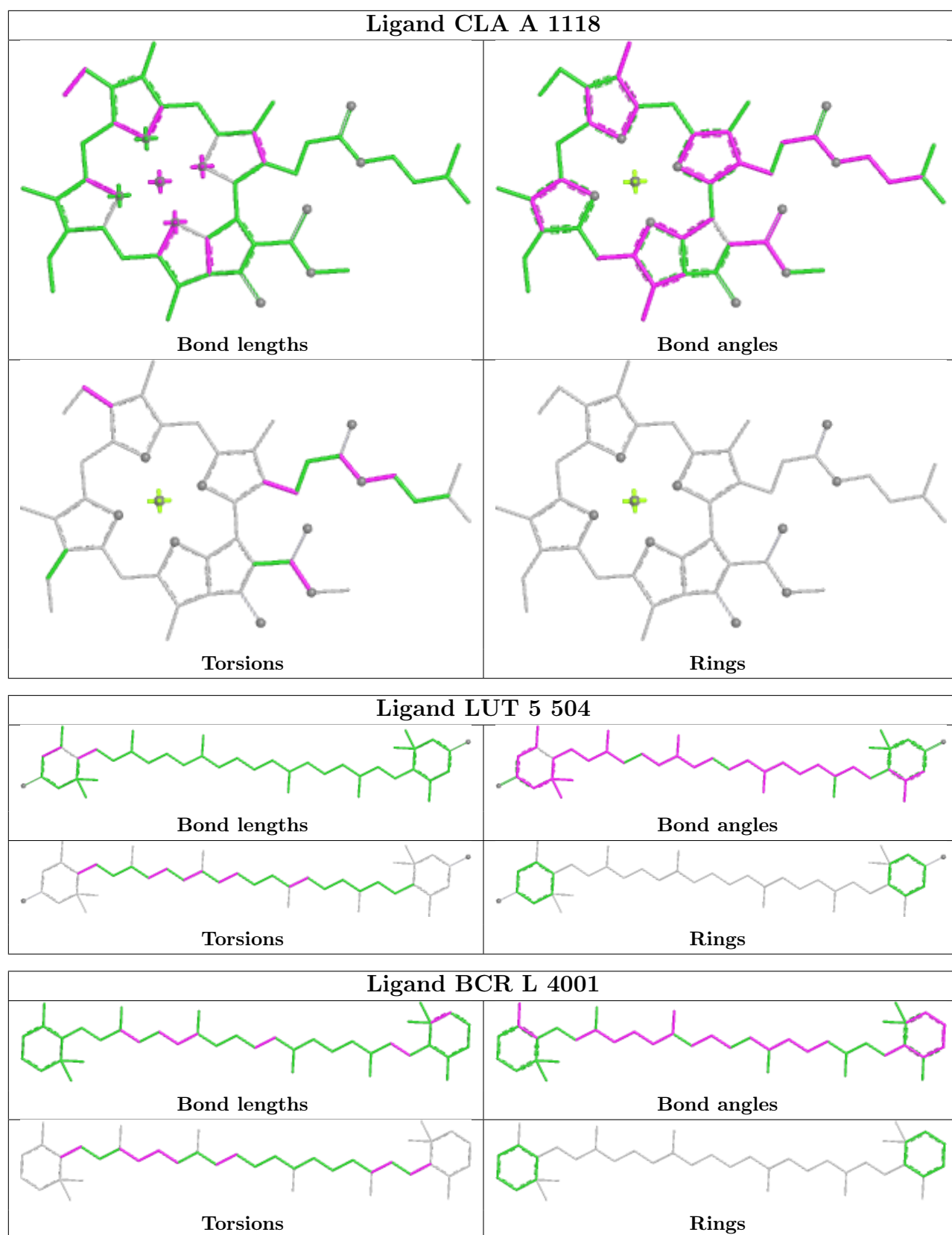


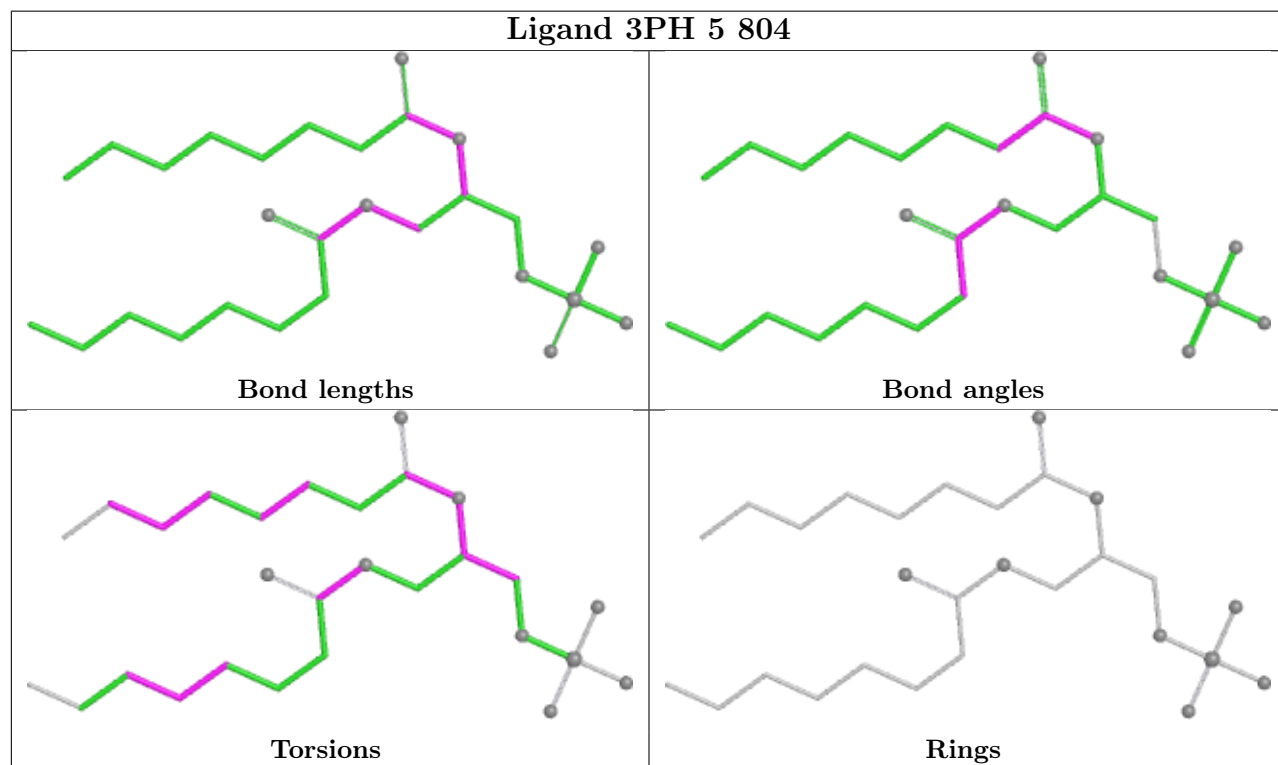
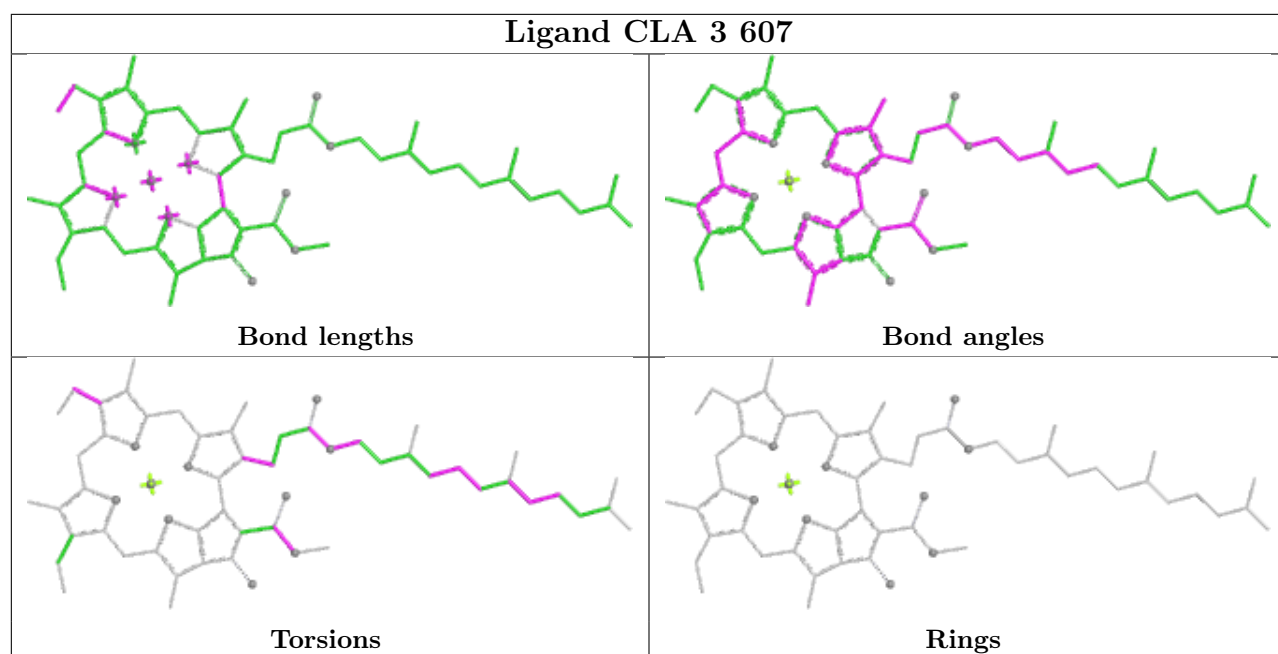


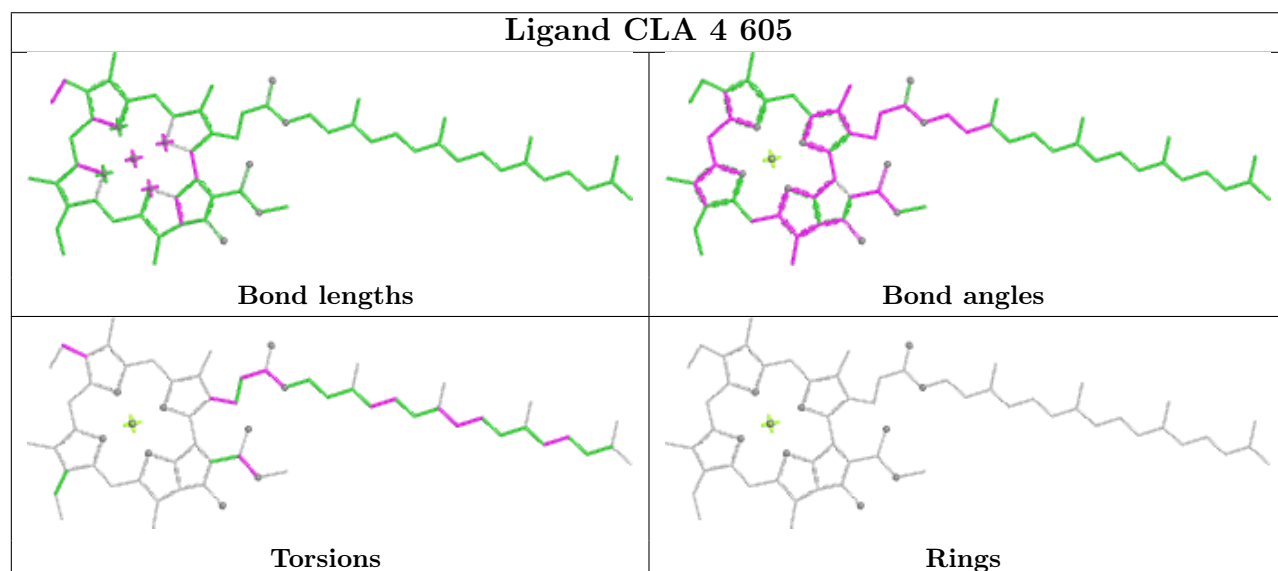
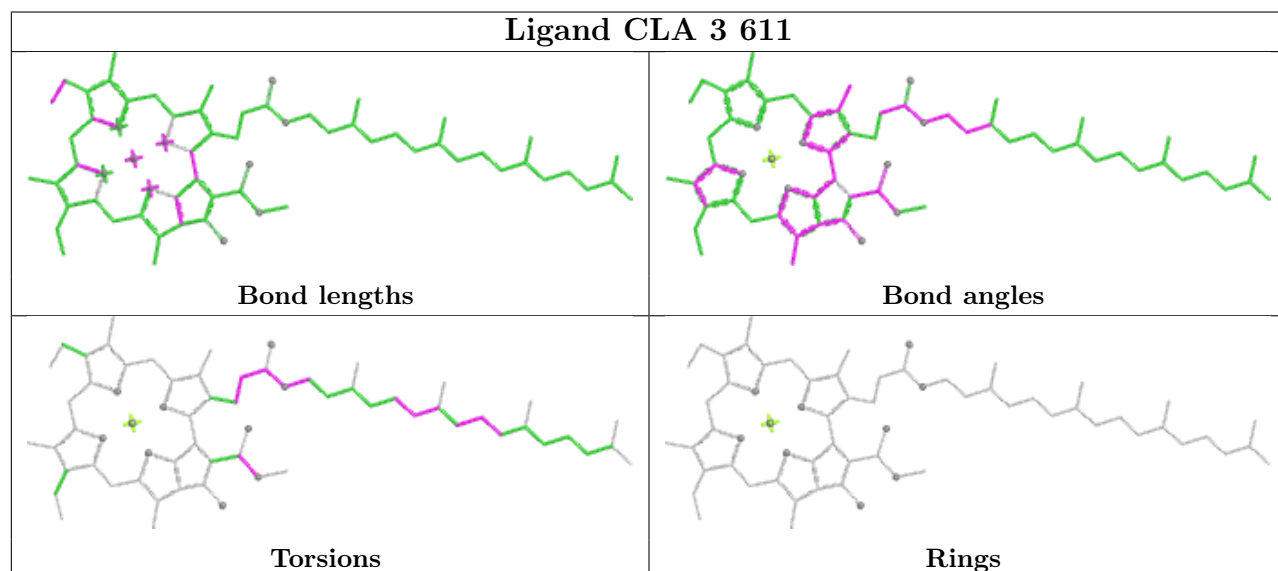
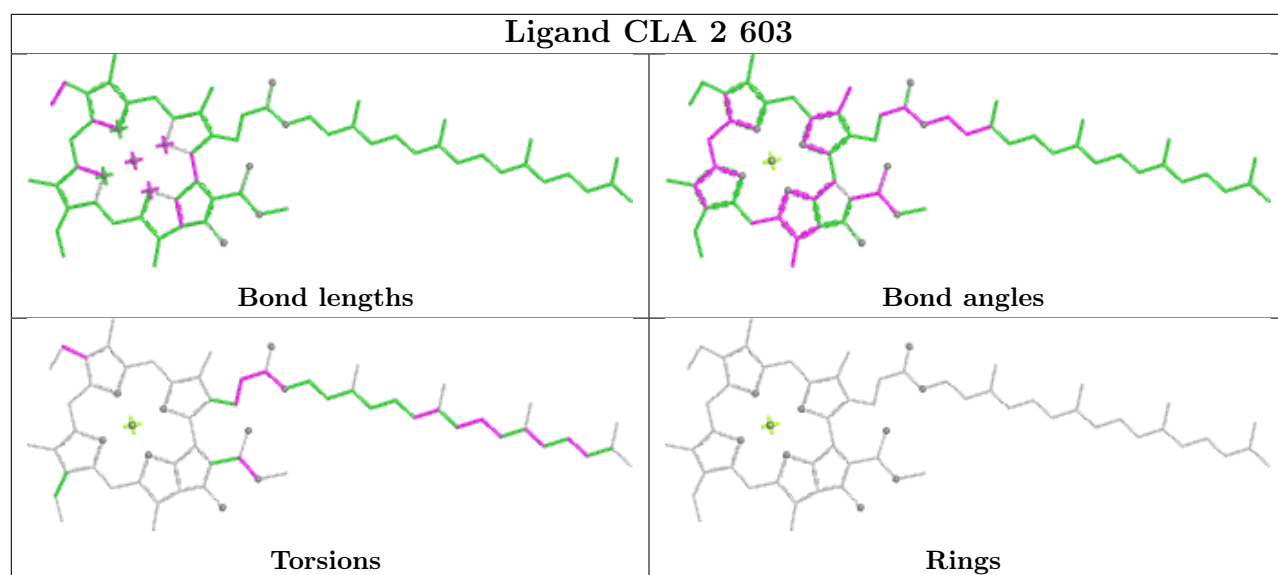


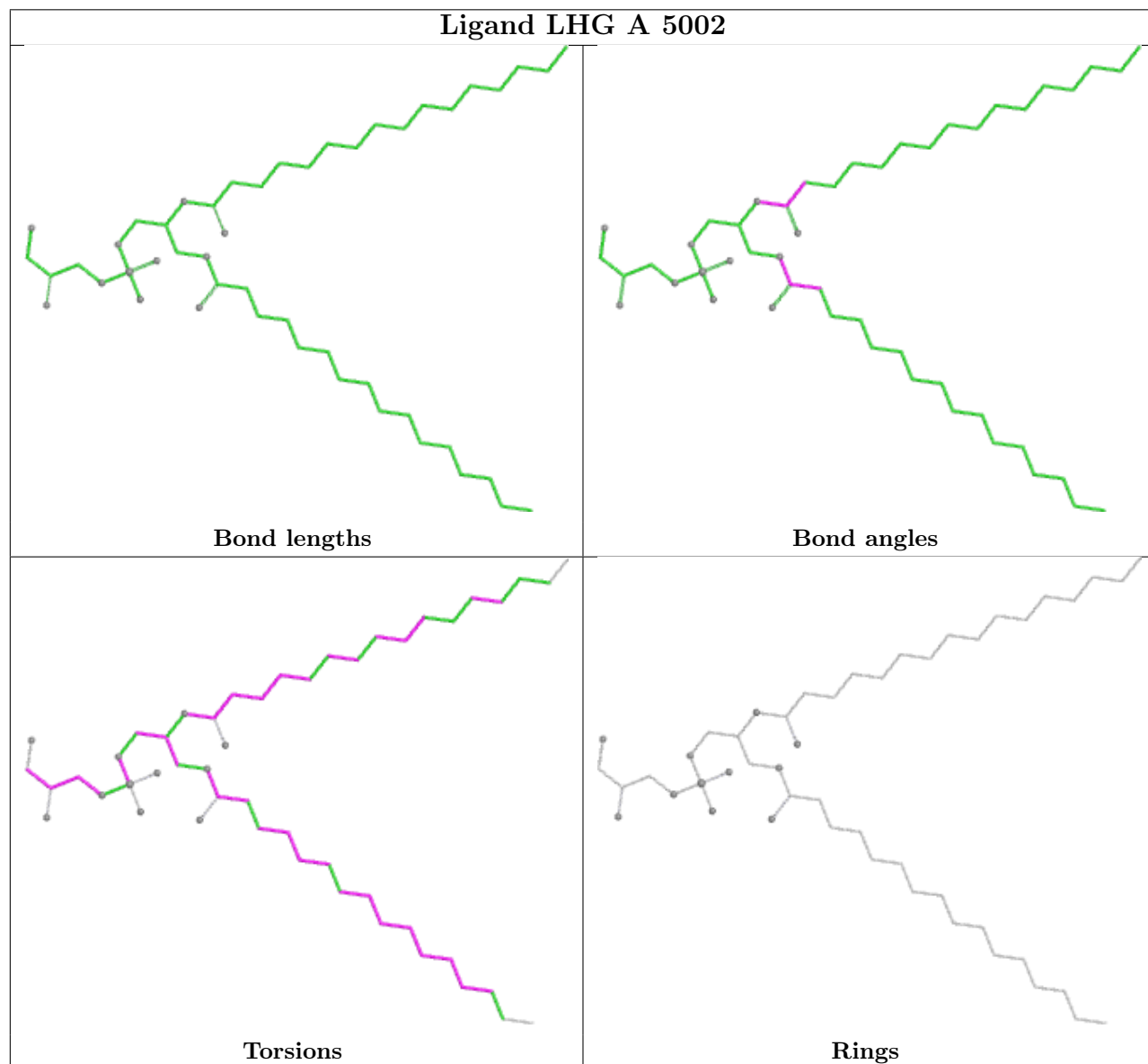
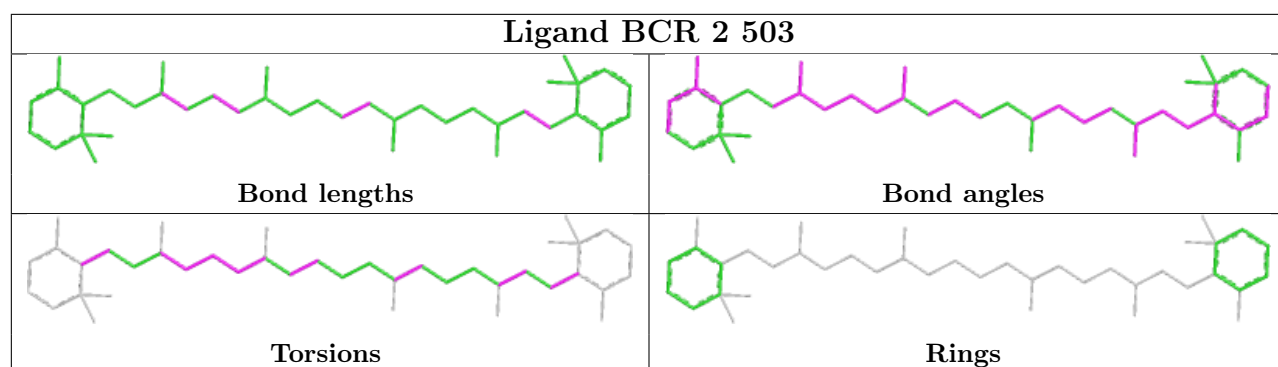




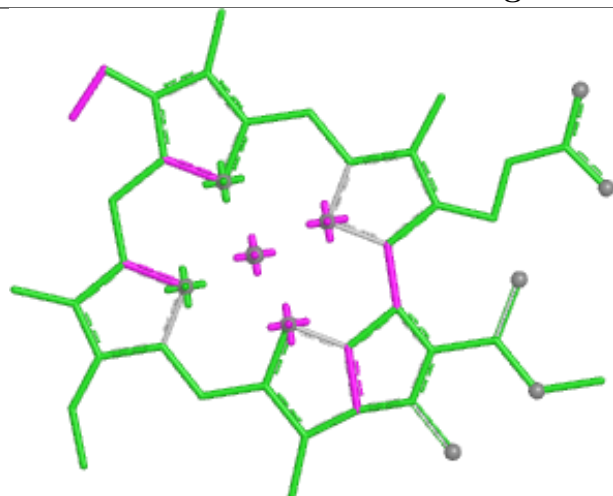




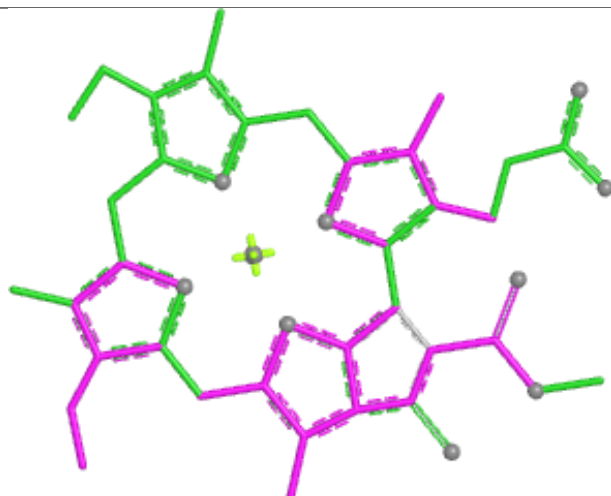




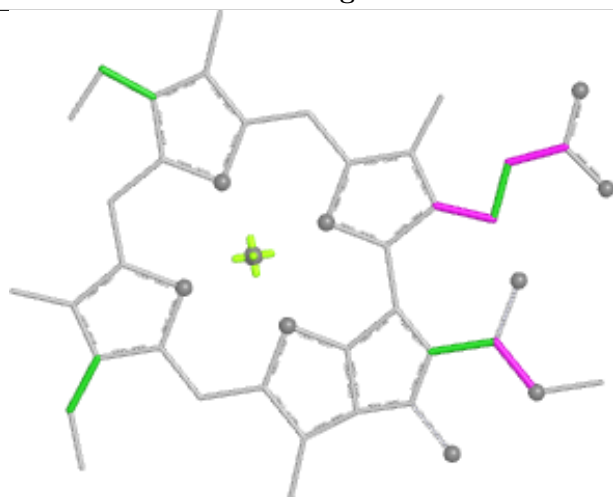
Ligand CLA G 1603



Bond lengths



Bond angles

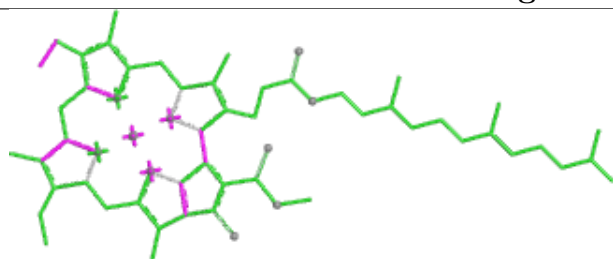


Torsions

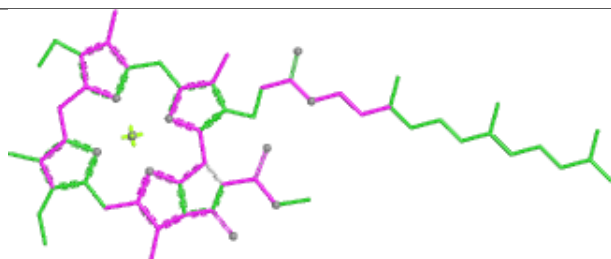


Rings

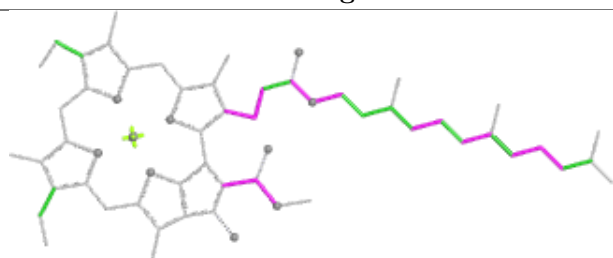
Ligand CLA 6 604



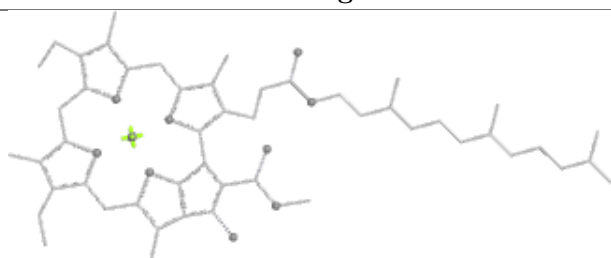
Bond lengths



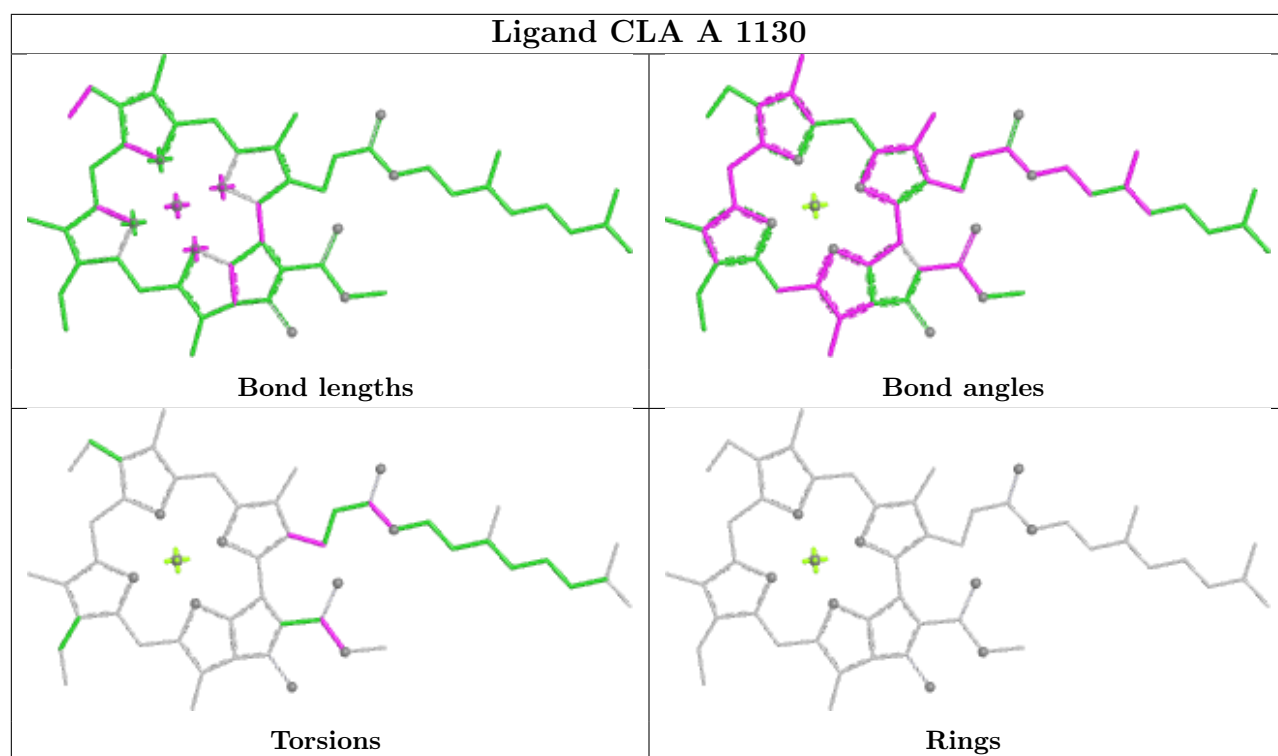
Bond angles

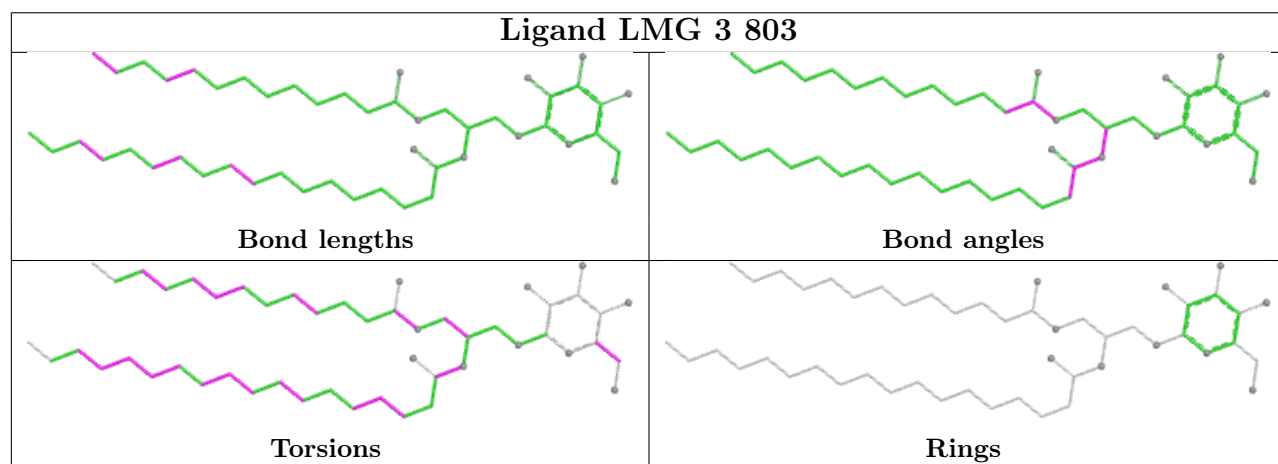
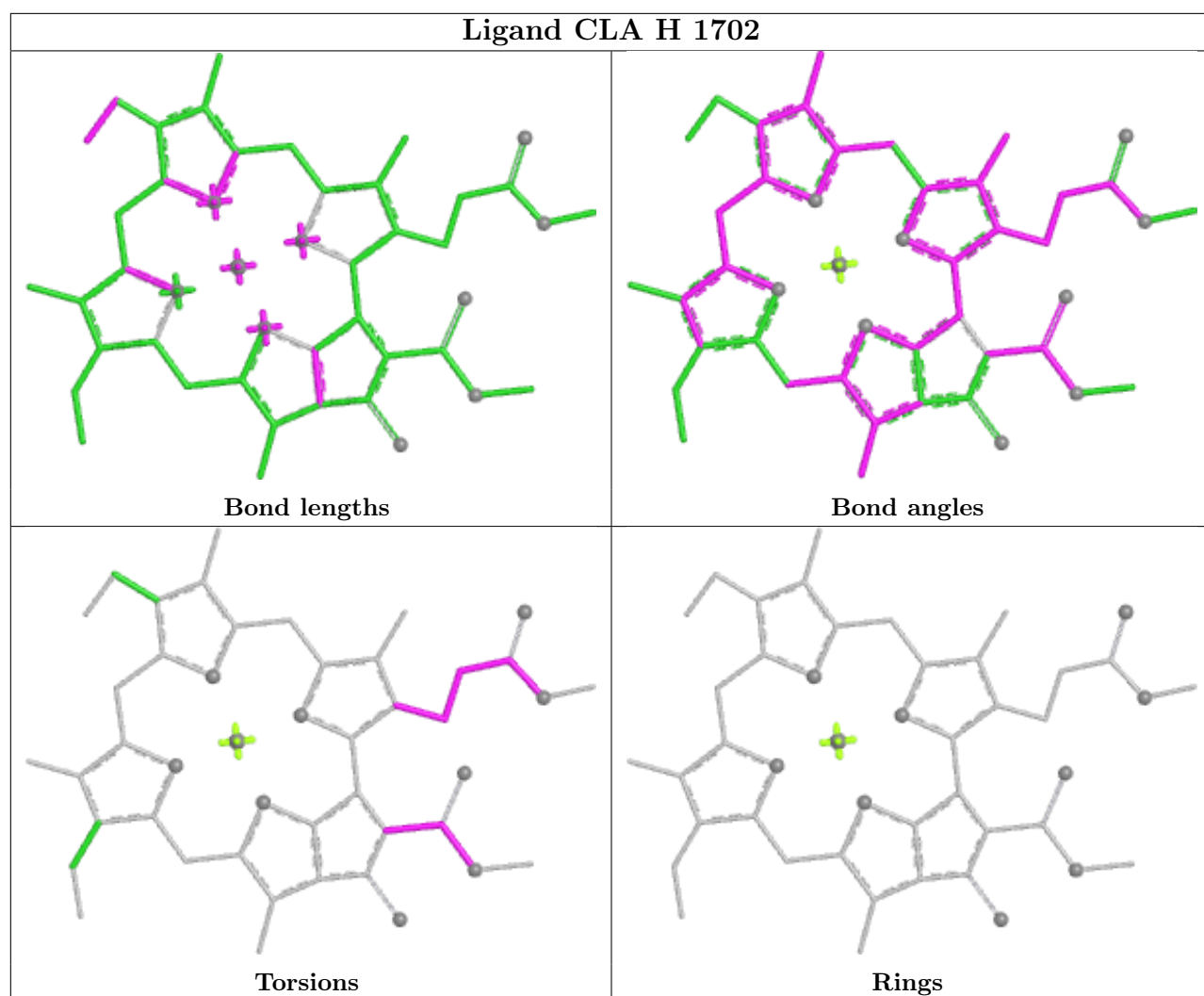


Torsions

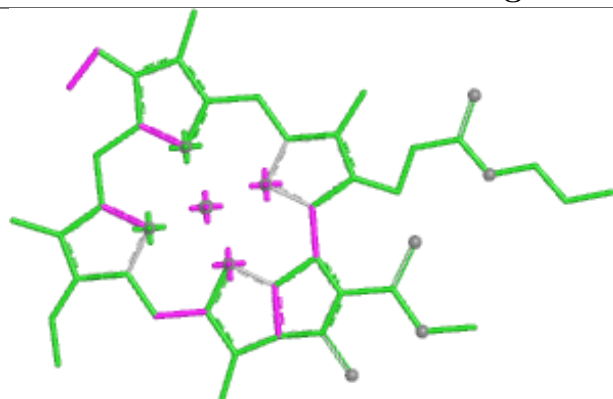


Rings

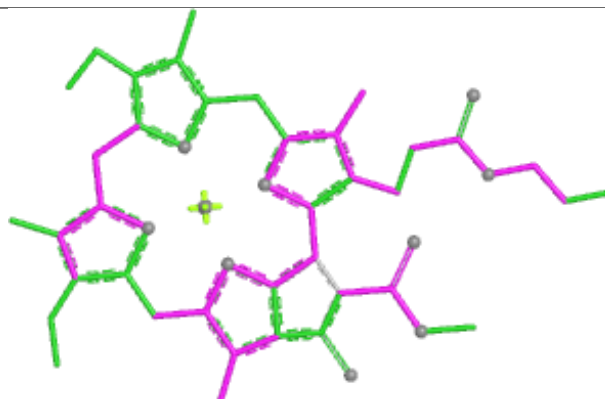




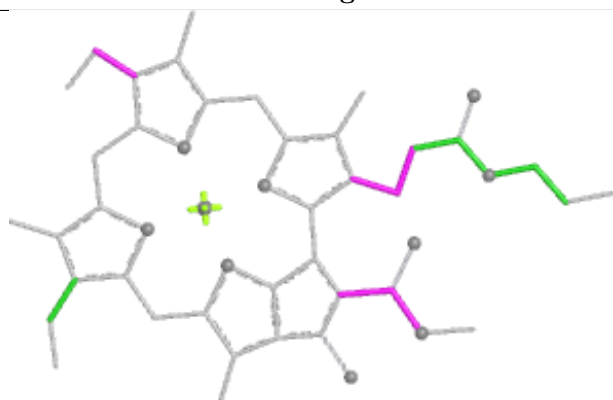
Ligand CLA K 1403



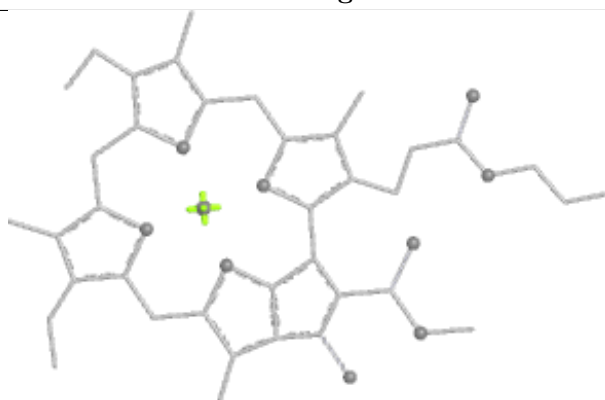
Bond lengths



Bond angles

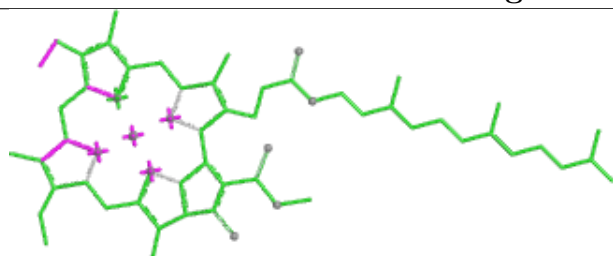


Torsions

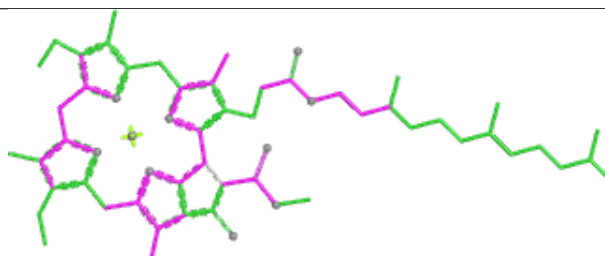


Rings

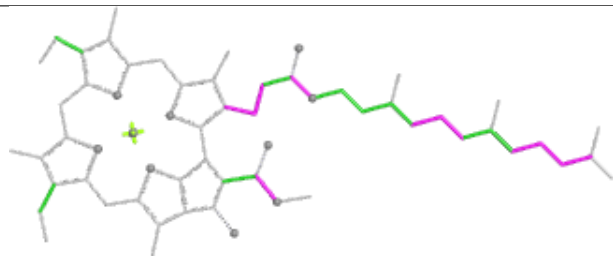
Ligand CLA B 1208



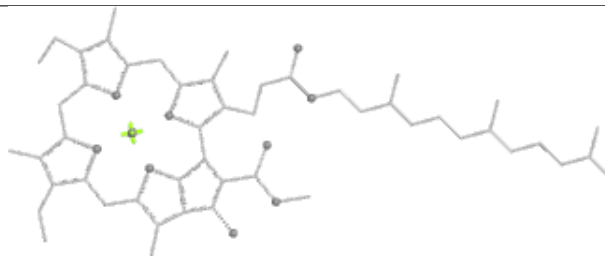
Bond lengths



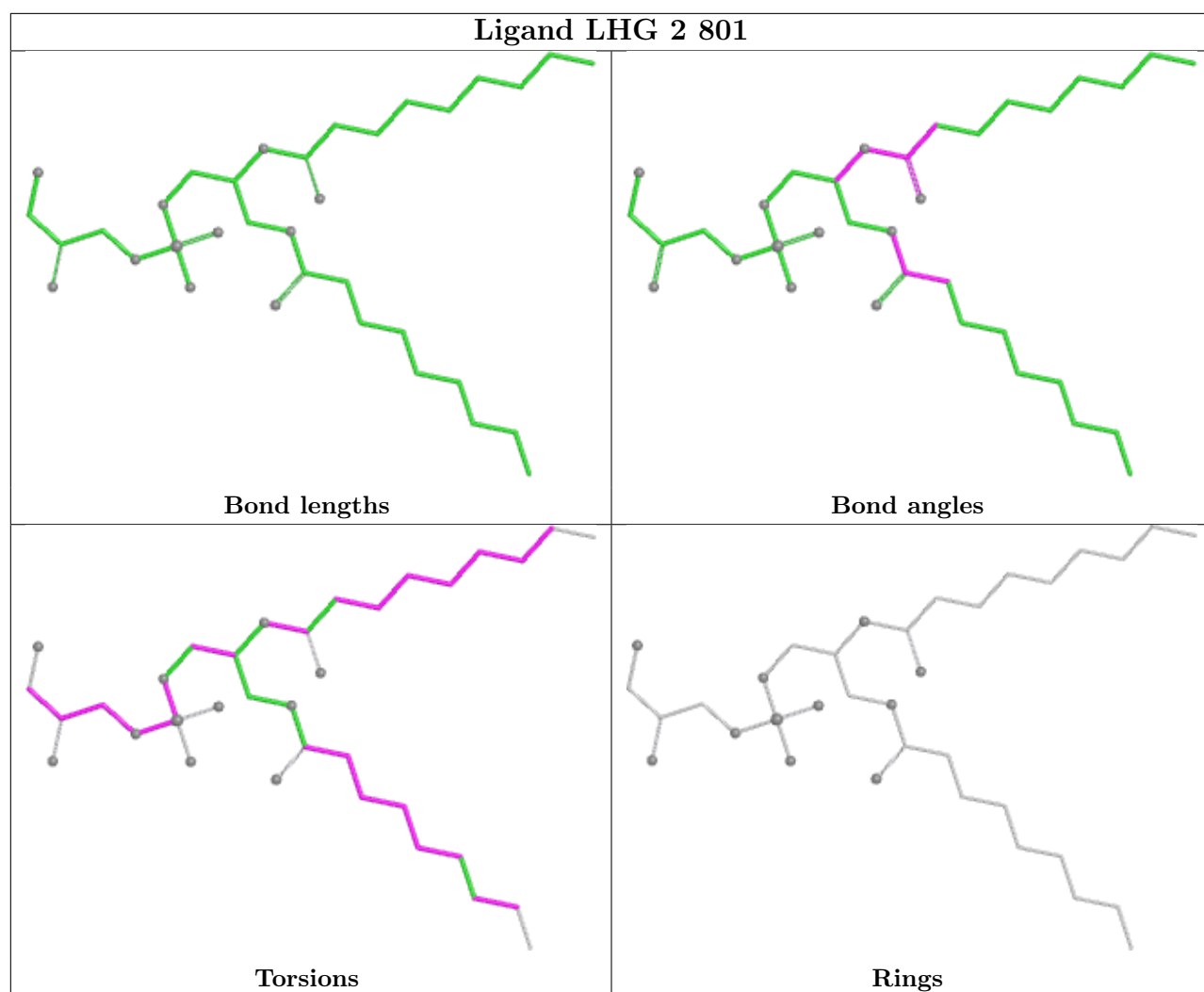
Bond angles



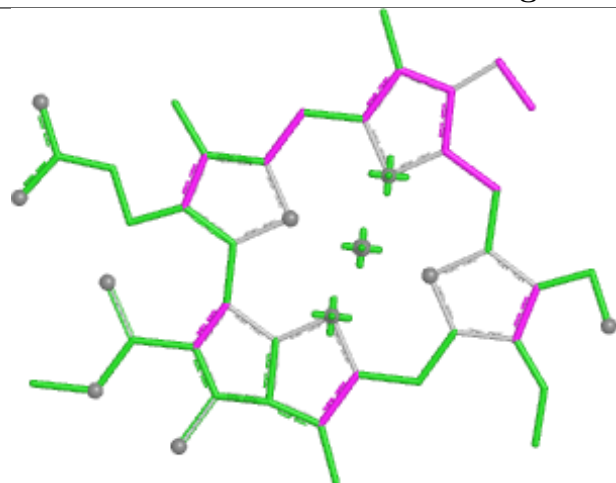
Torsions



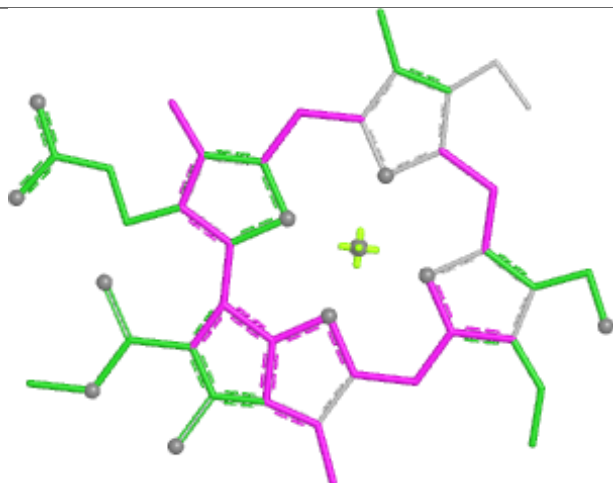
Rings



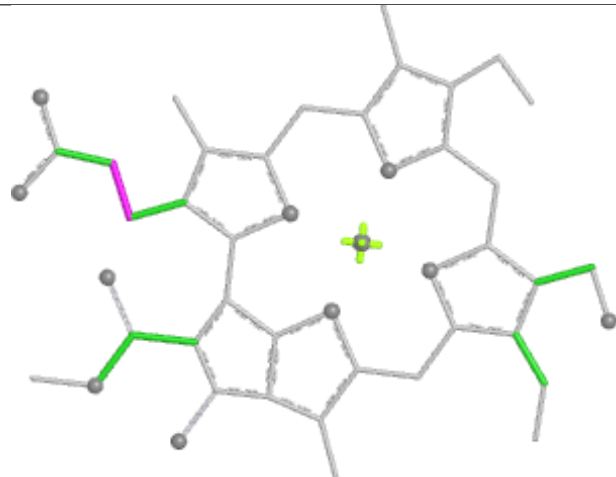
Ligand CHL 2 613



Bond lengths



Bond angles

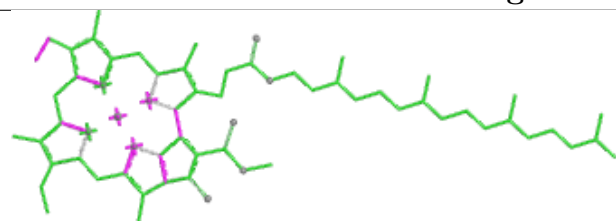


Torsions

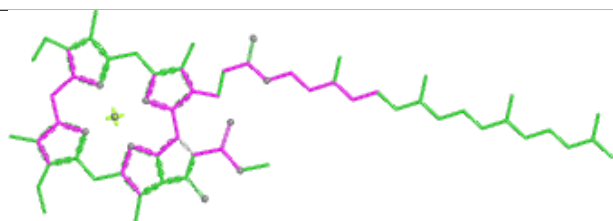


Rings

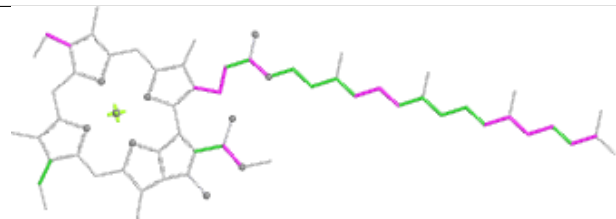
Ligand CLA A 1133



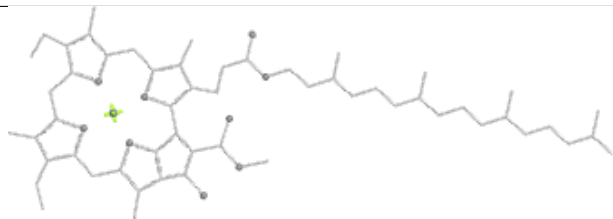
Bond lengths



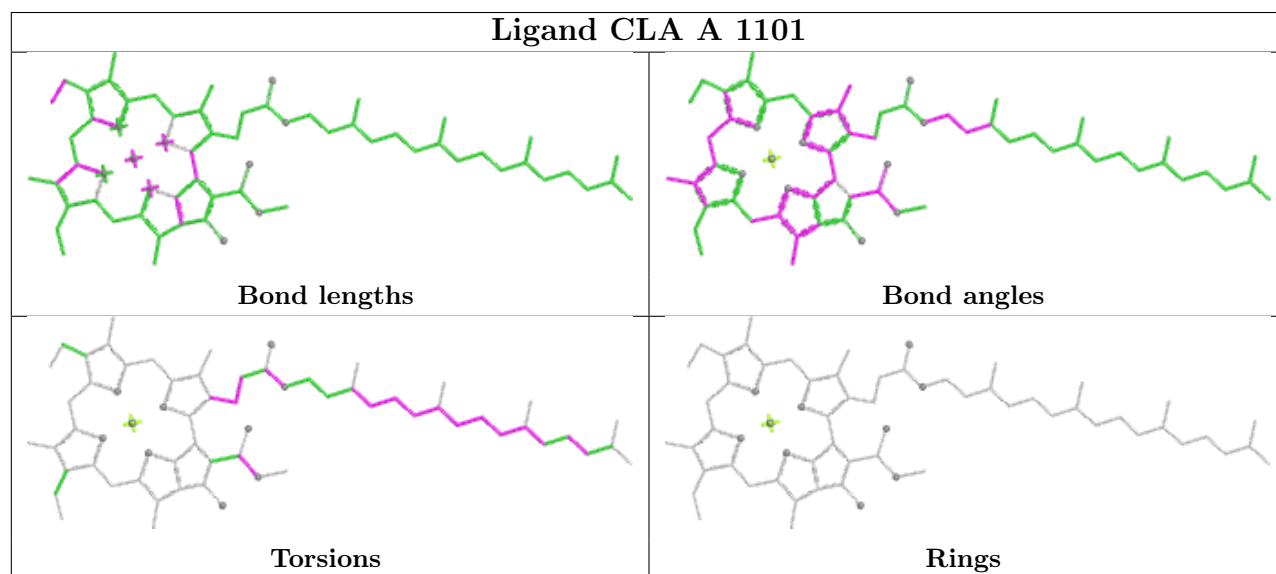
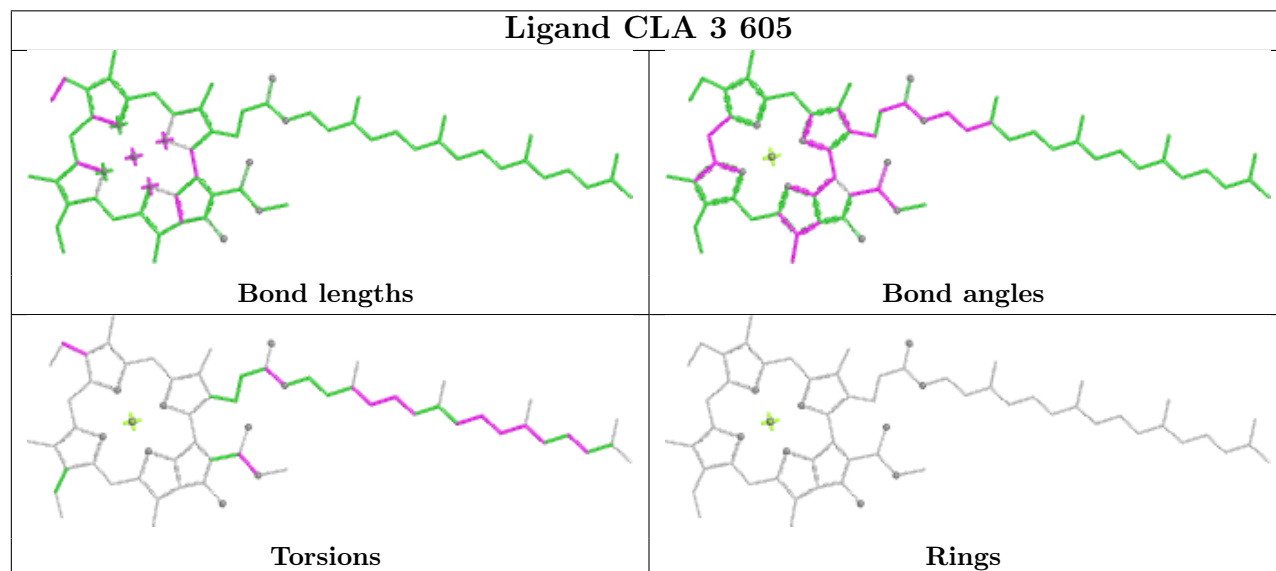
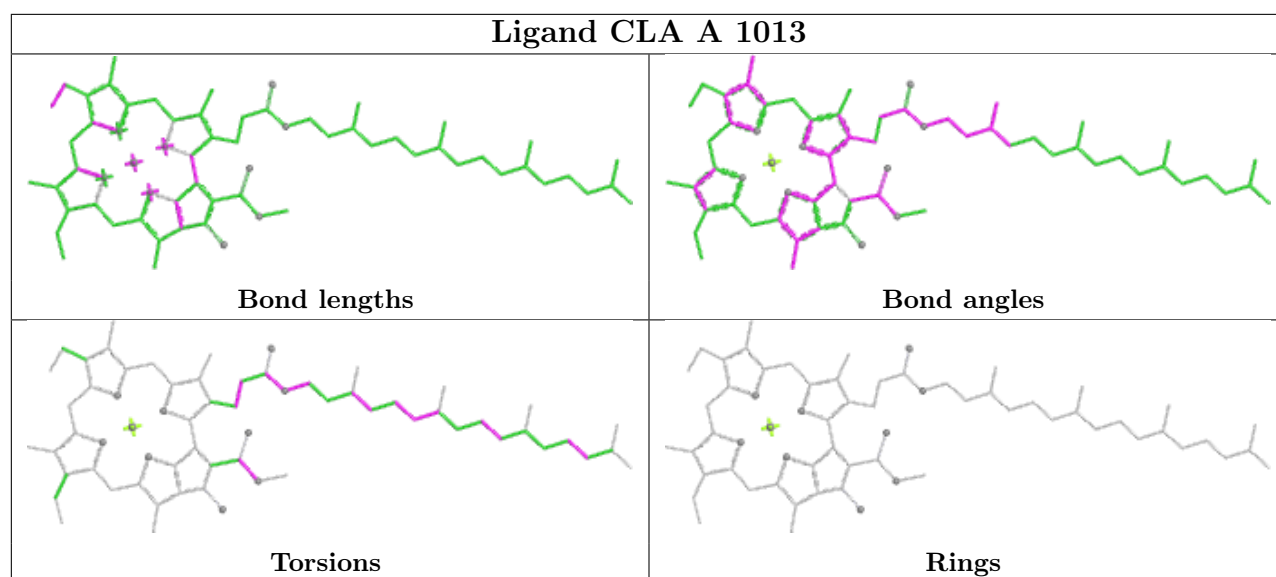
Bond angles



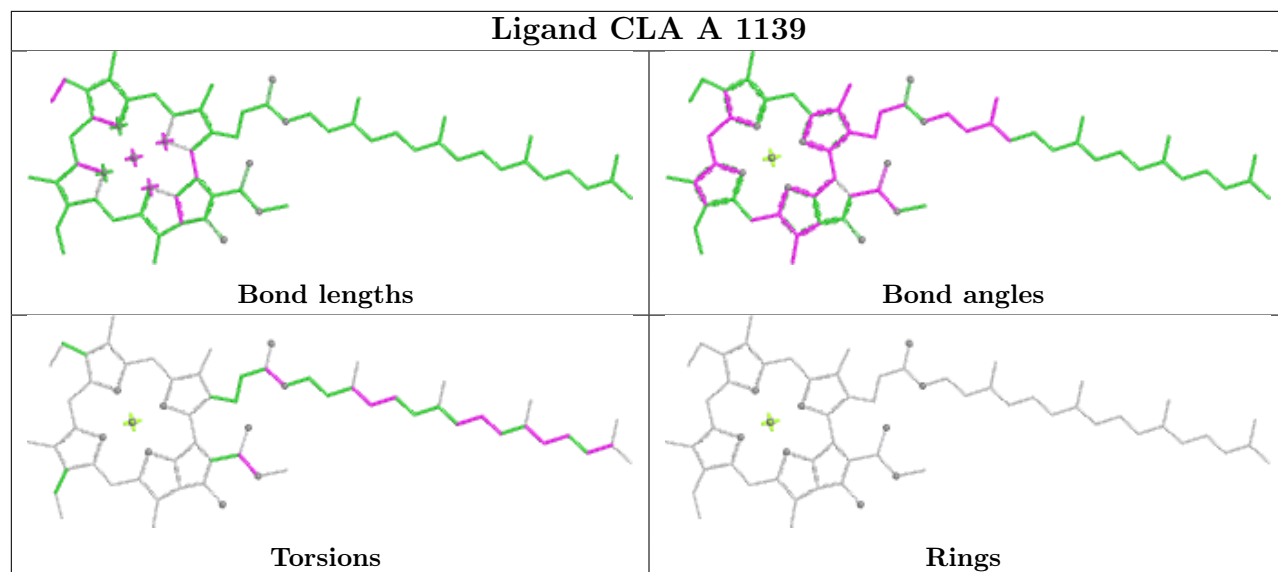
Torsions



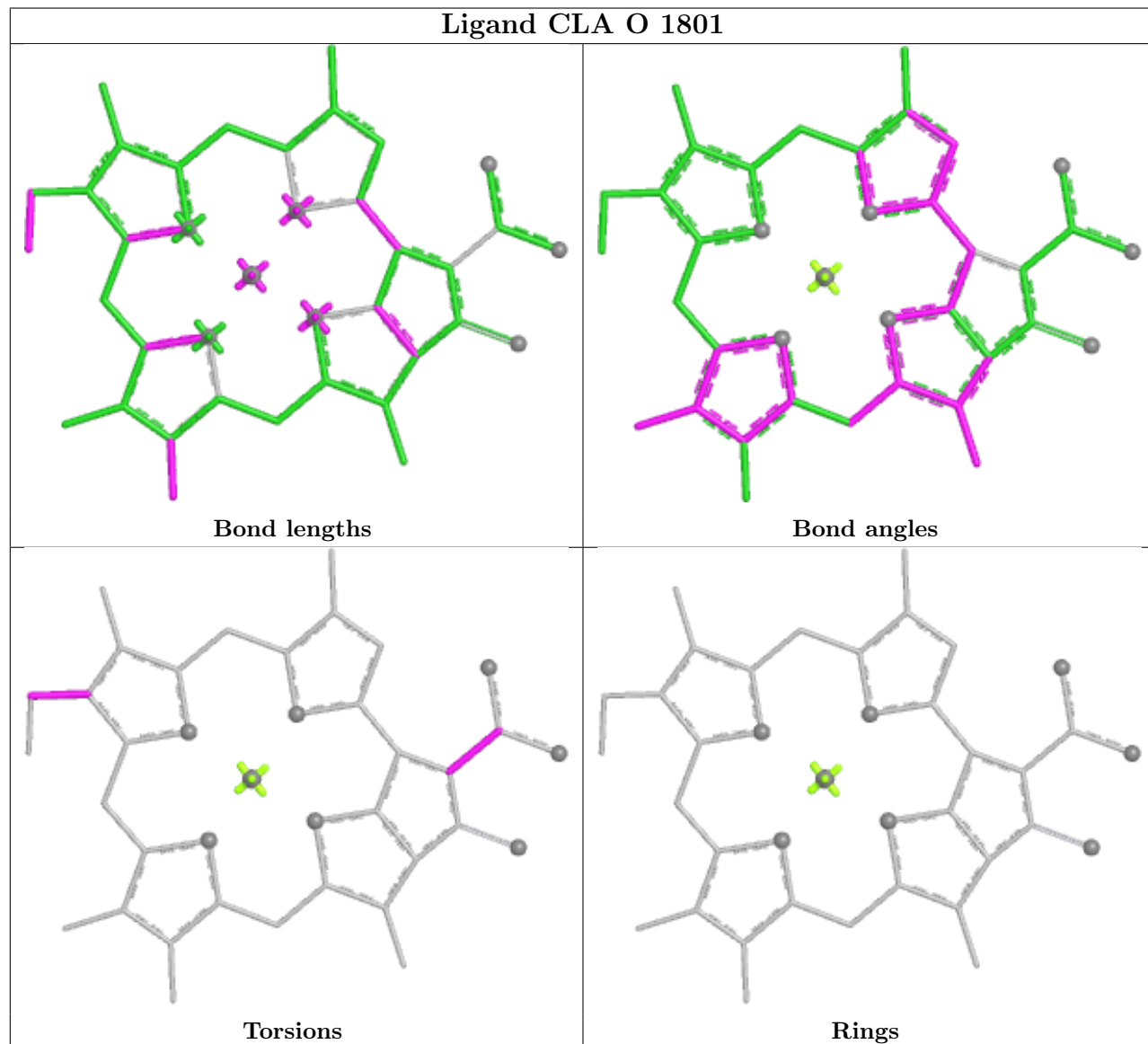
Rings

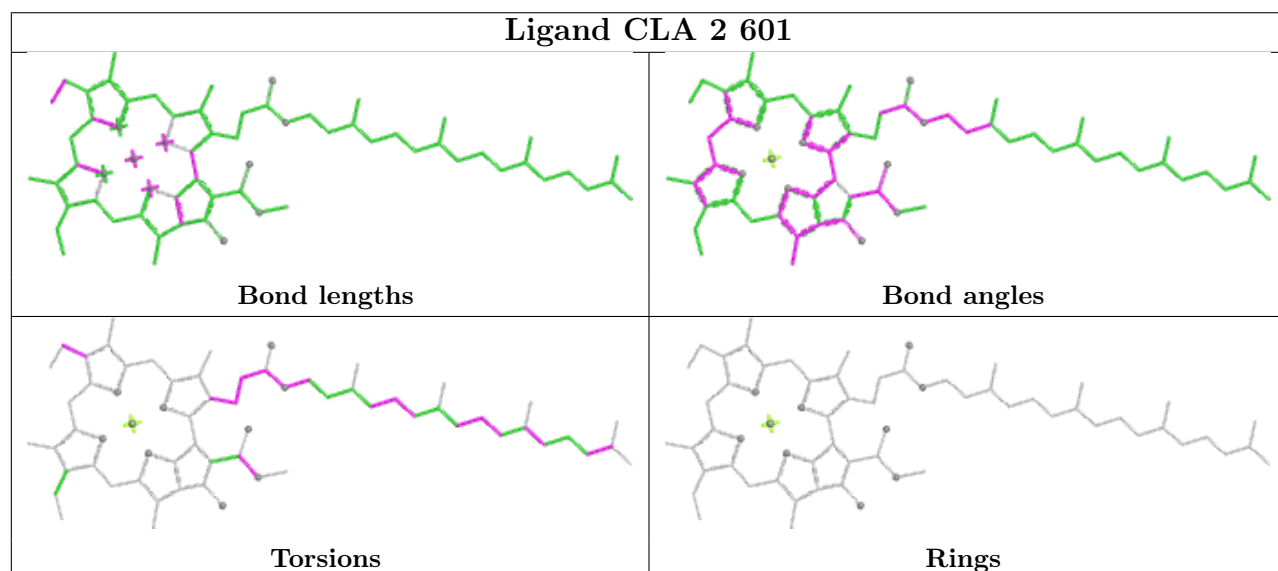
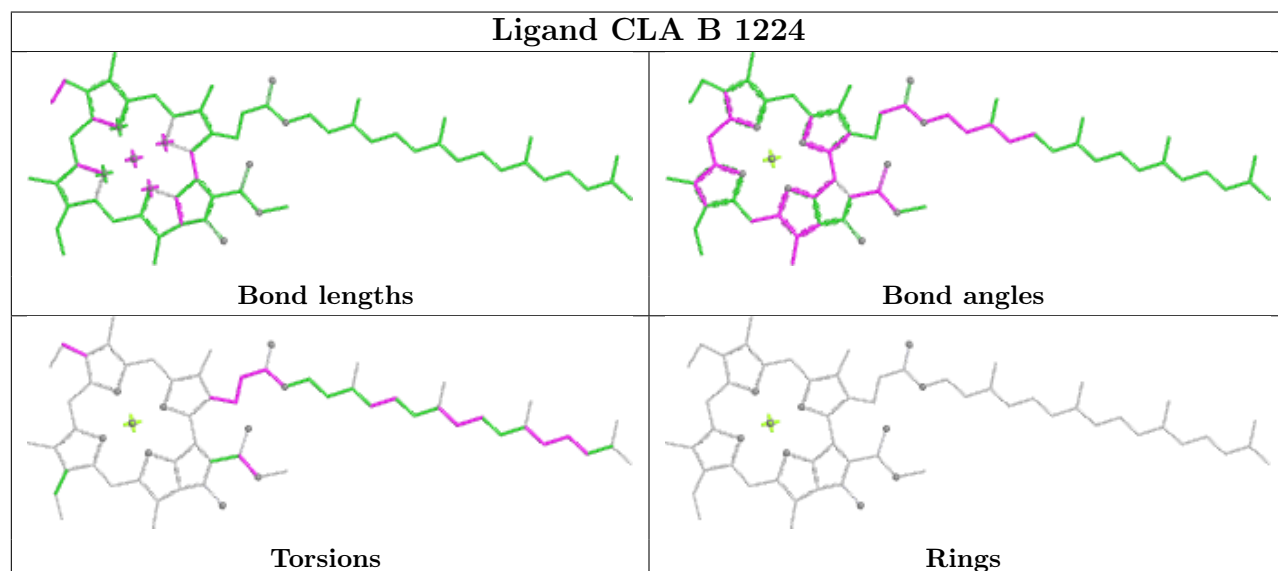
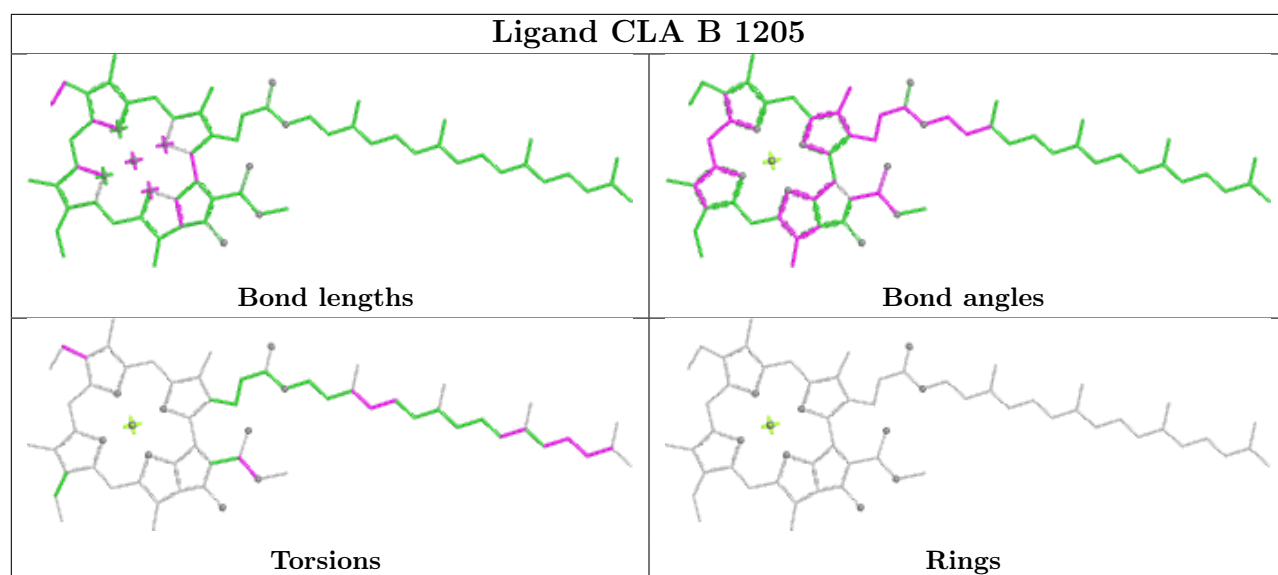


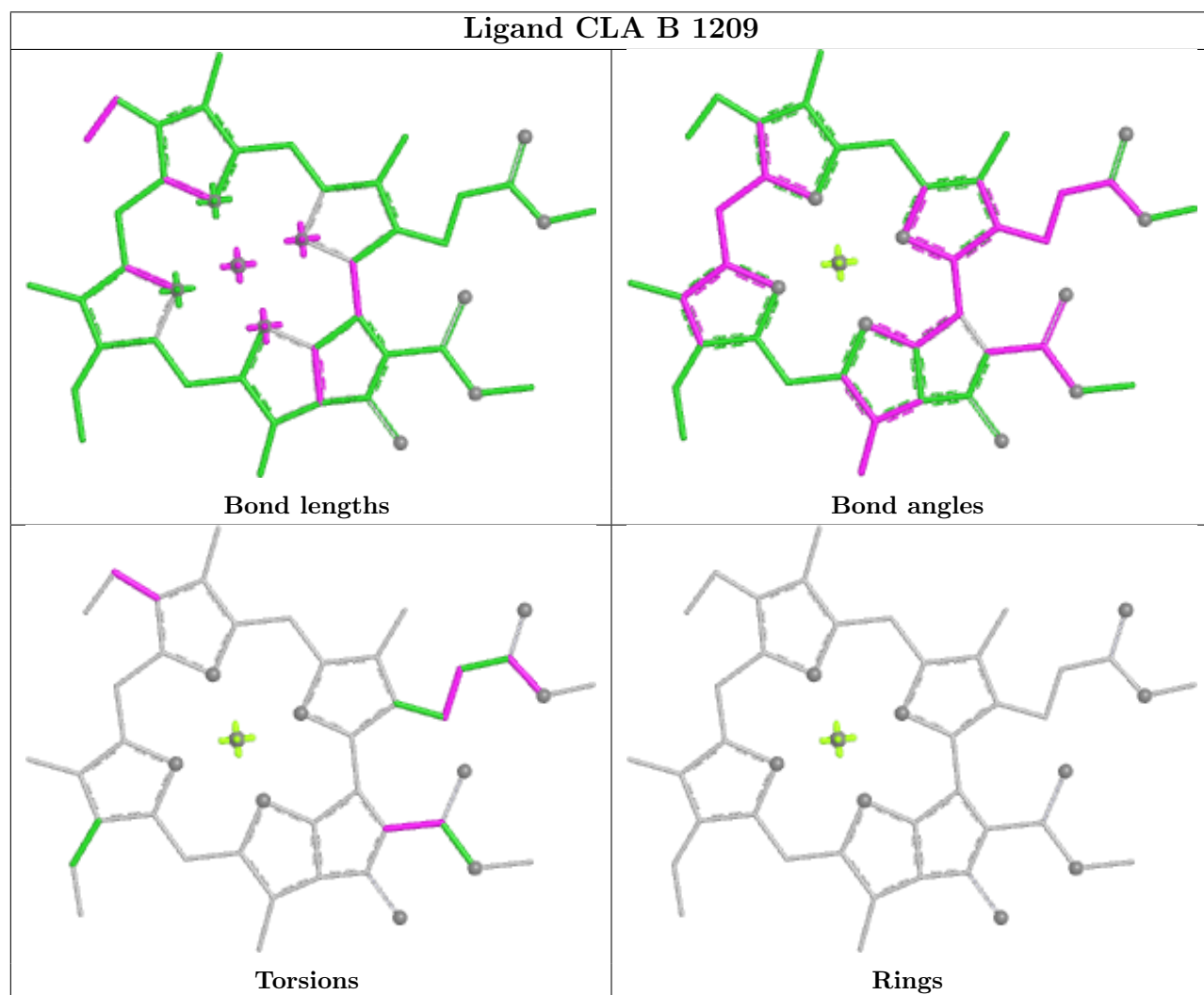
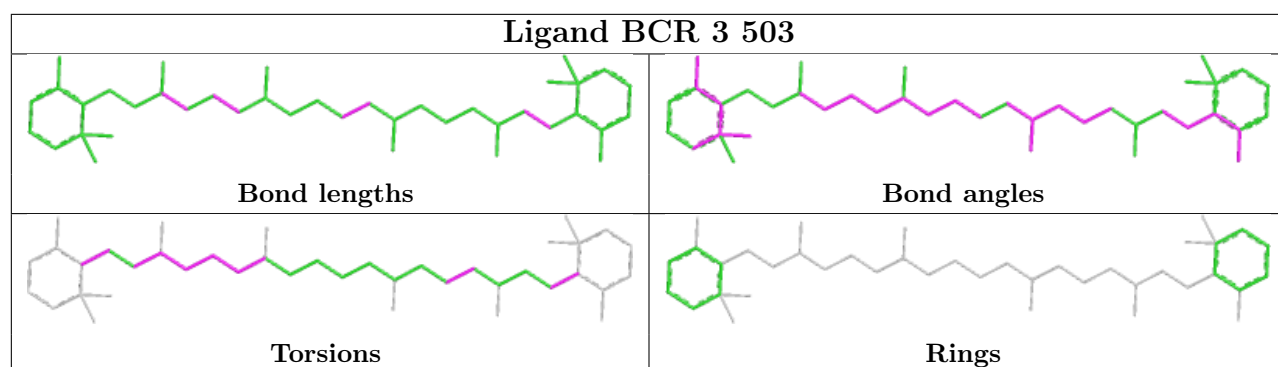
Ligand CLA A 1139

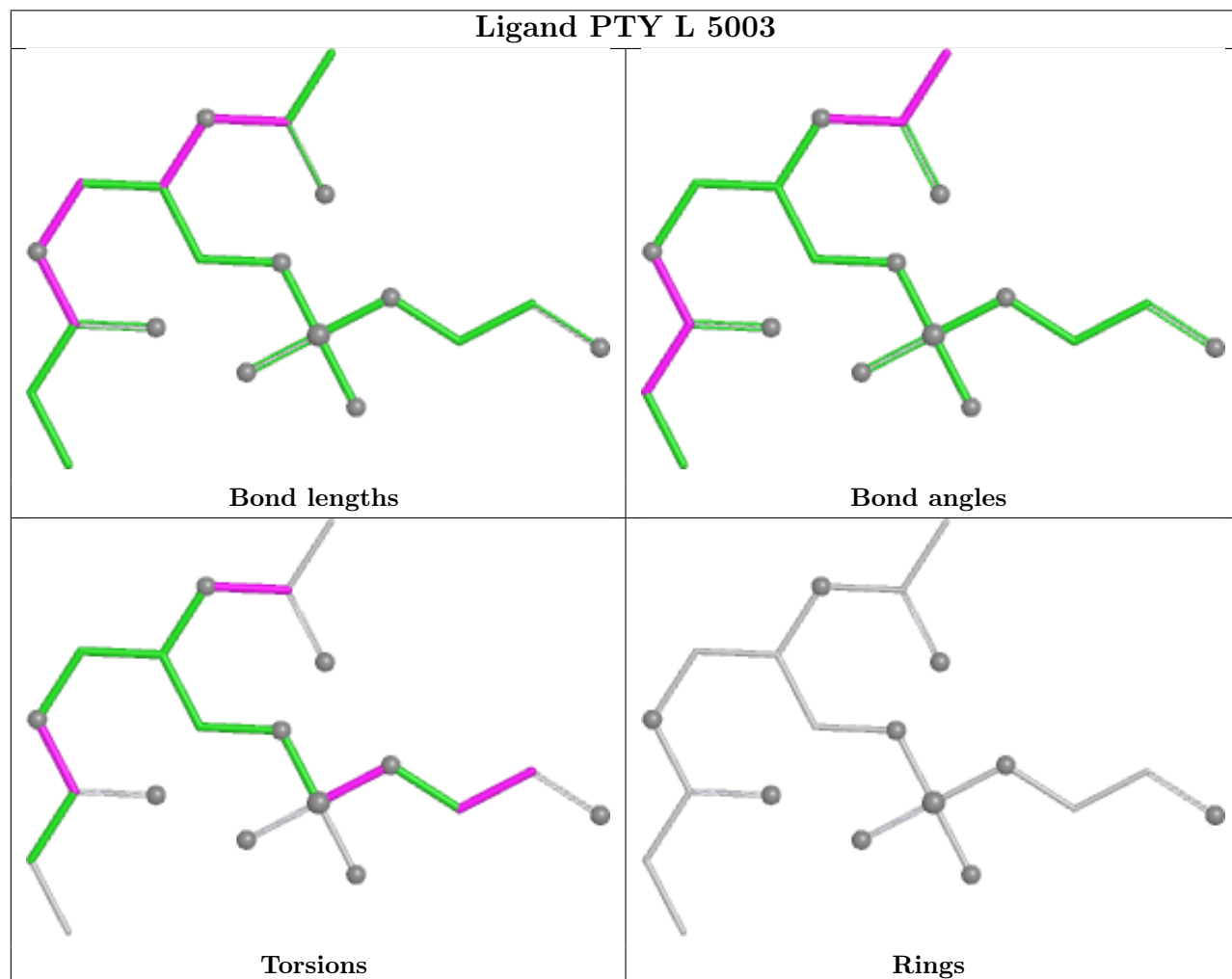
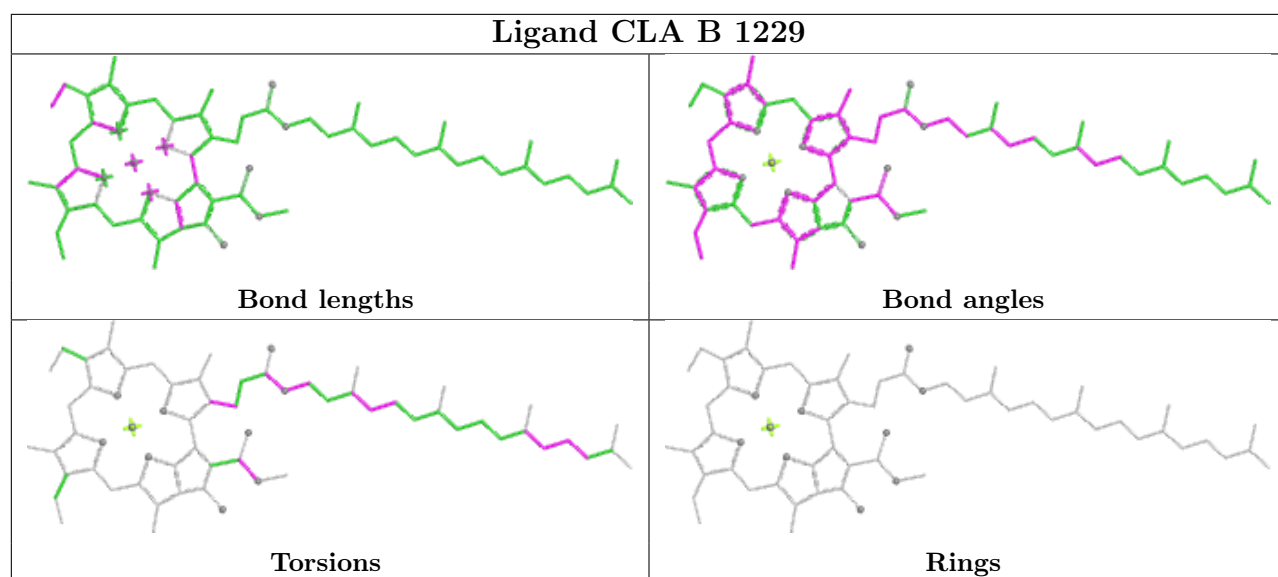


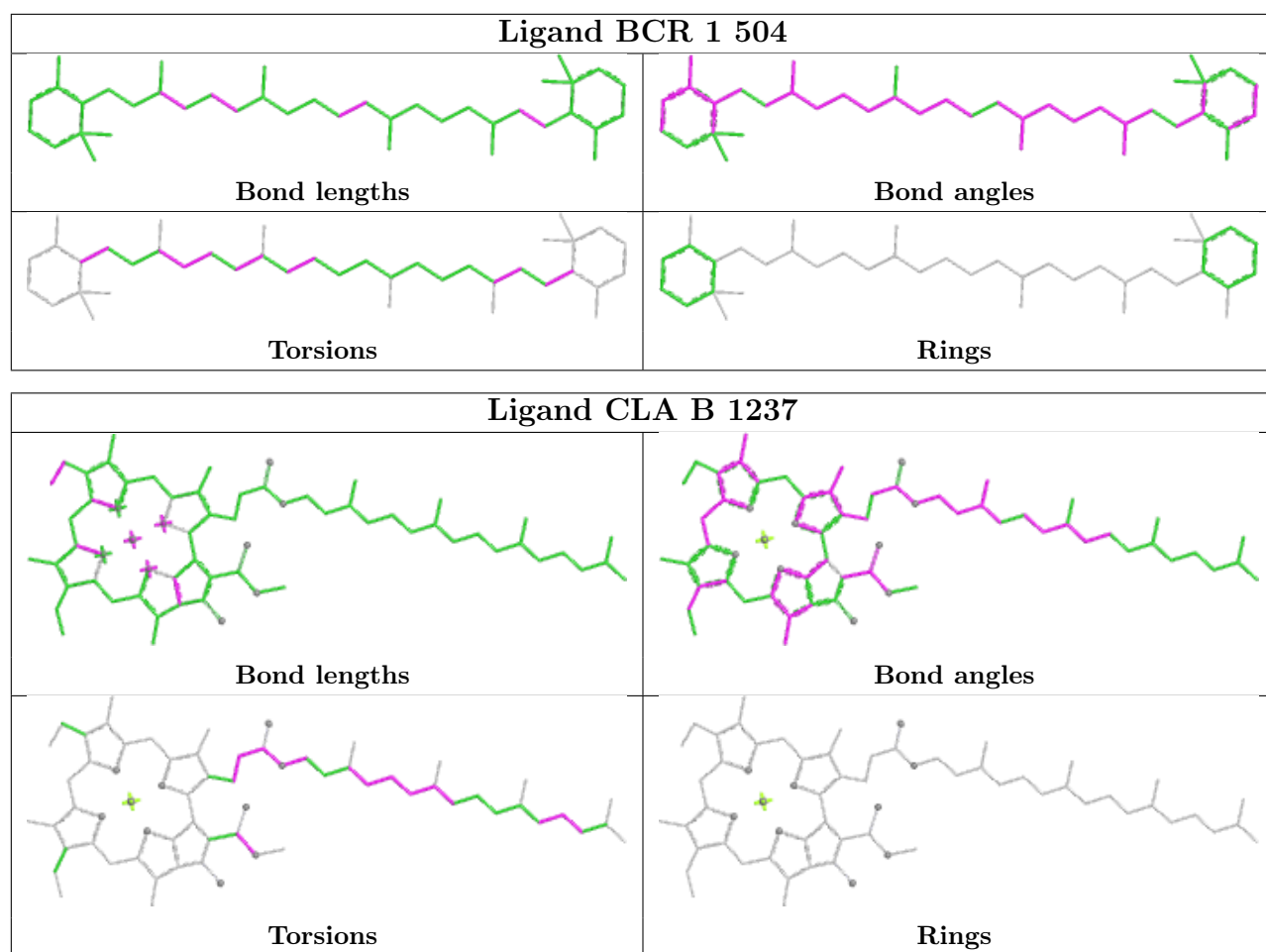
Ligand CLA O 1801



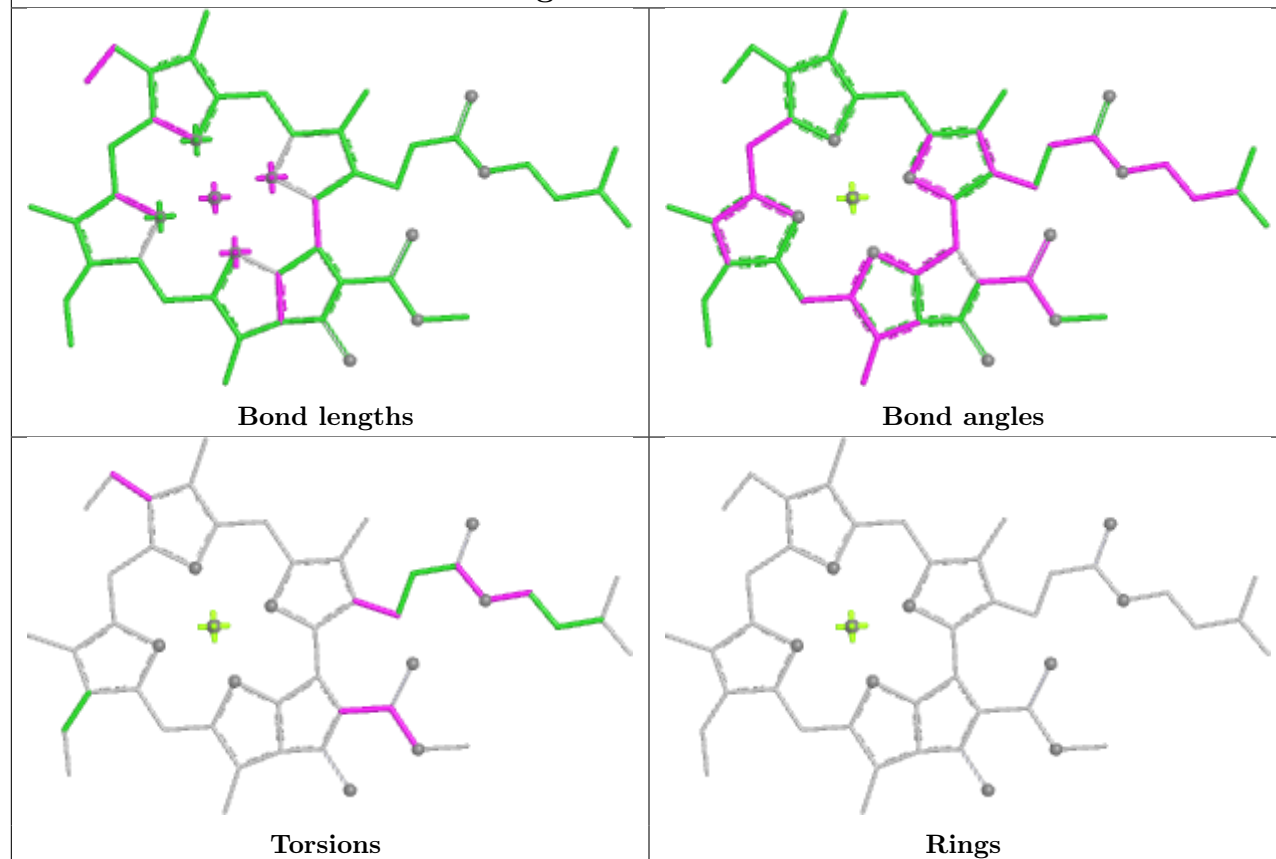




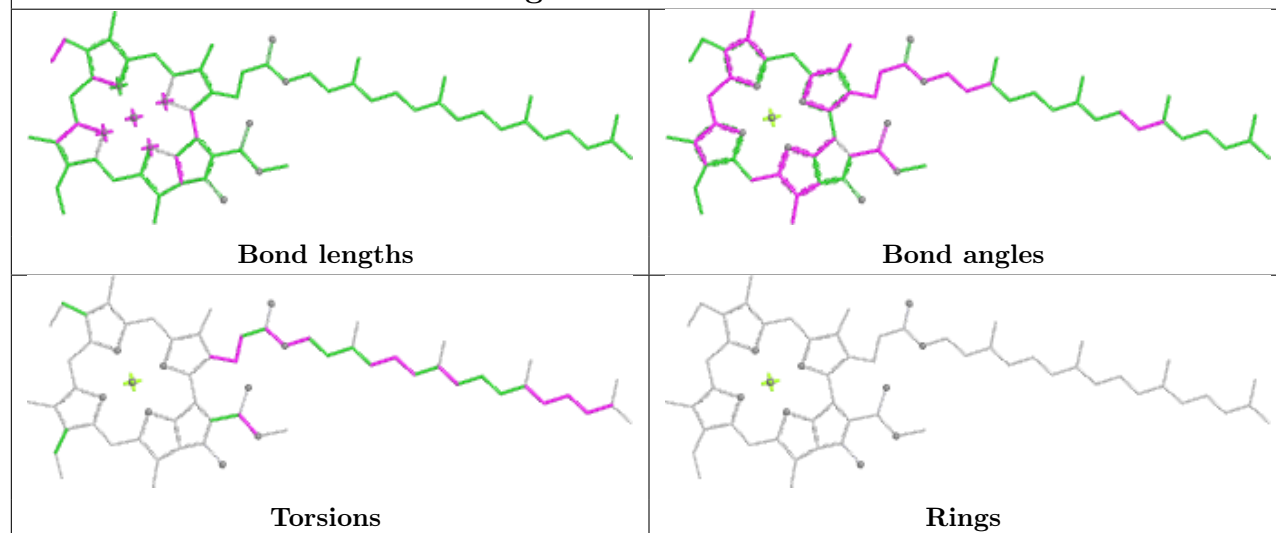


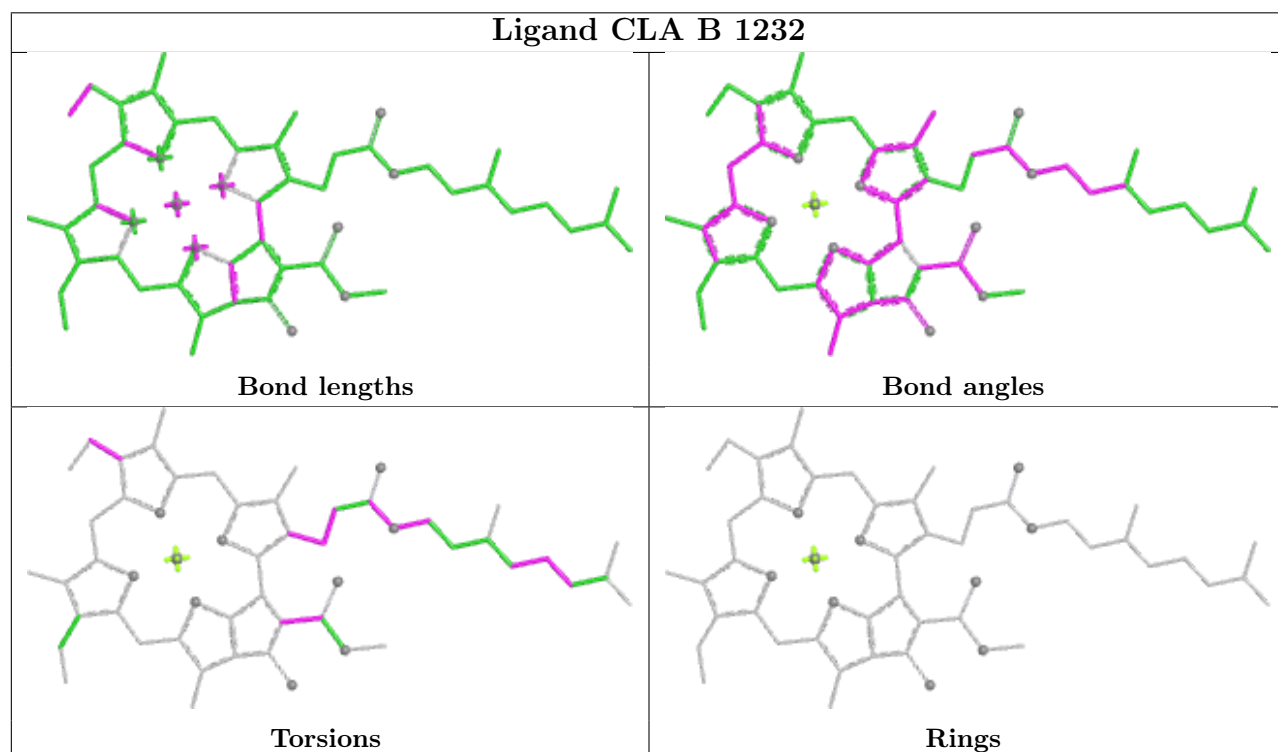
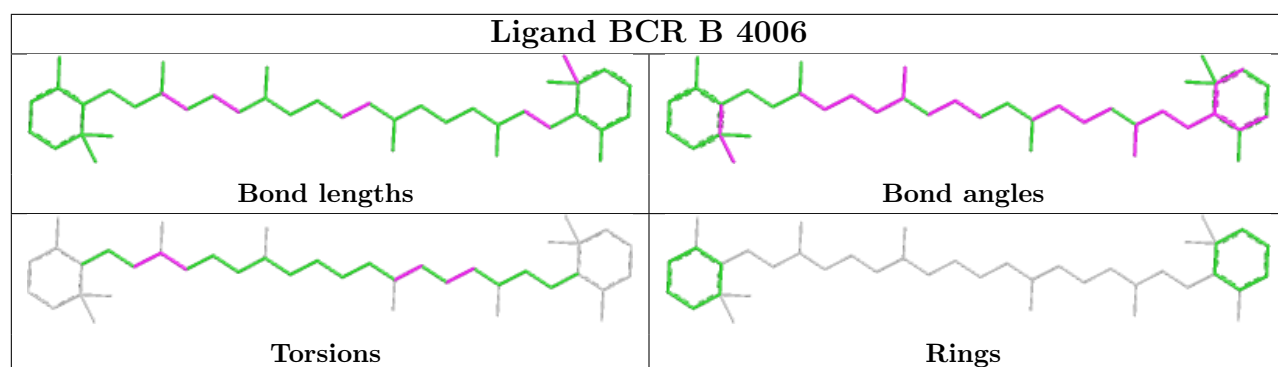


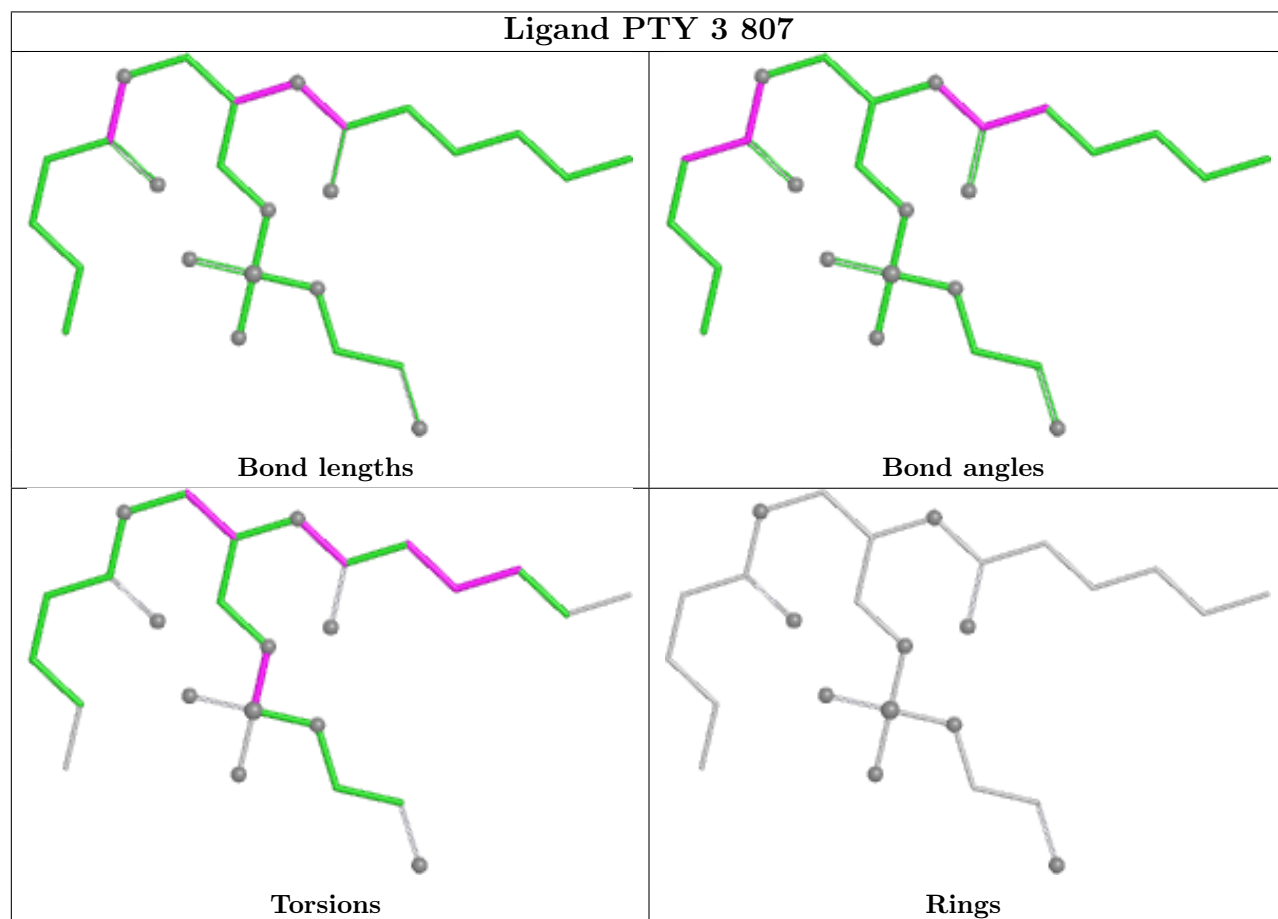
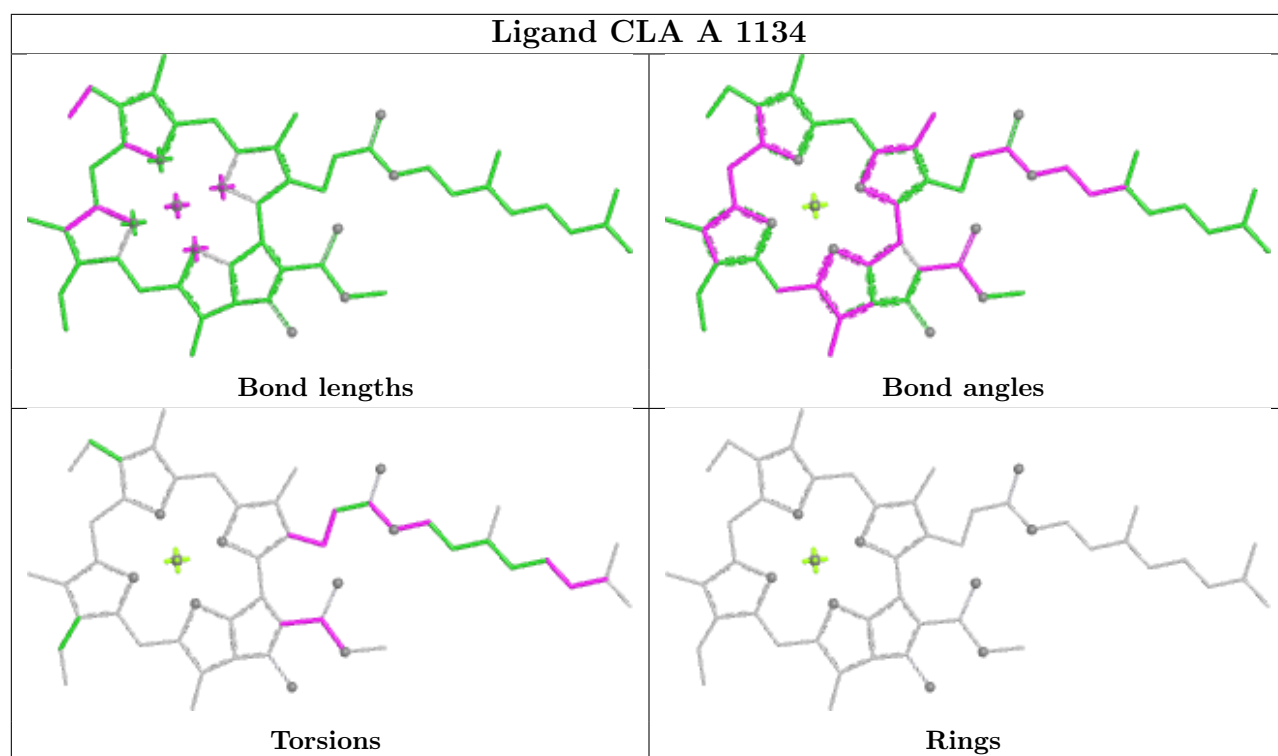
Ligand CLA 4 606

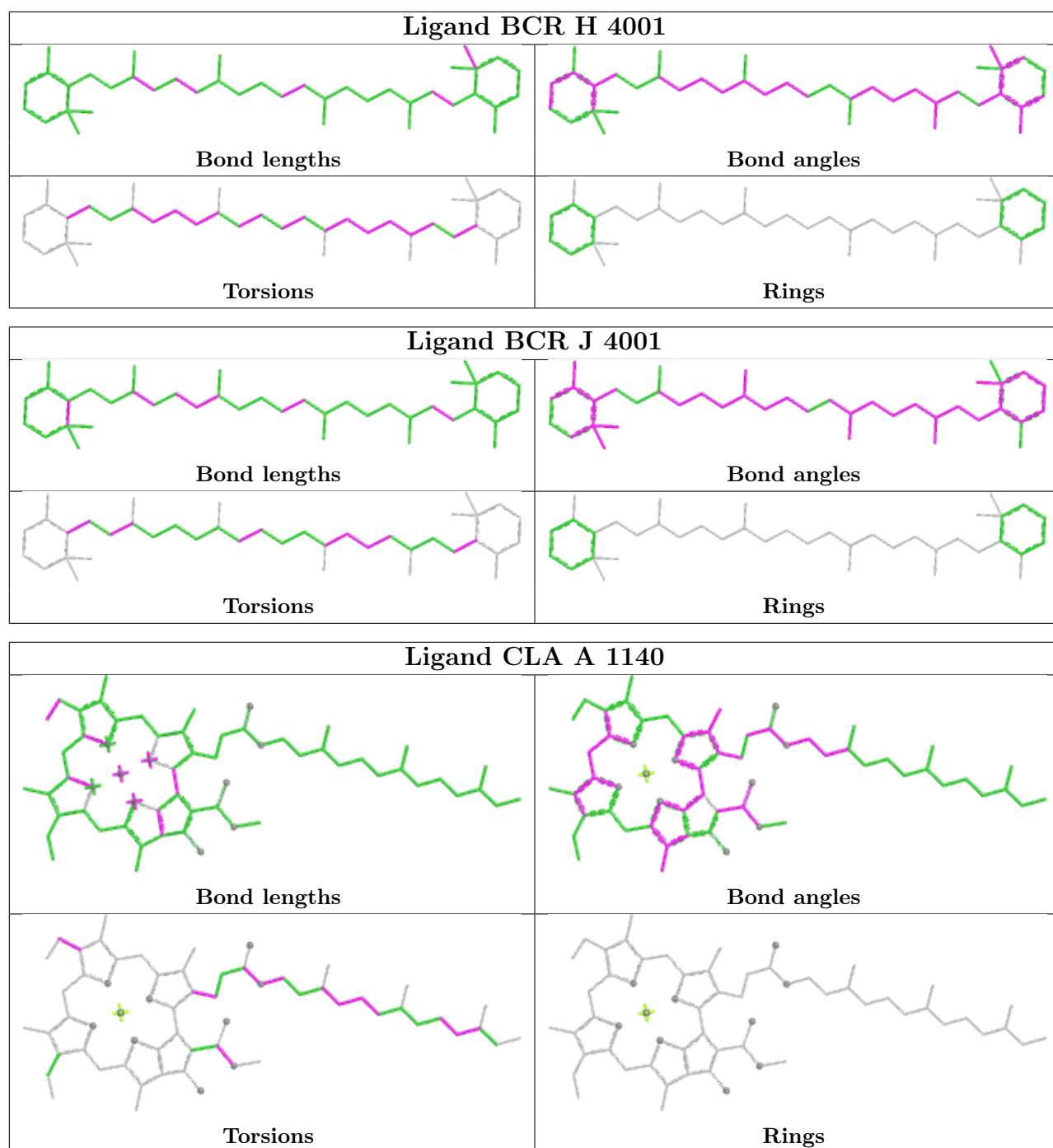


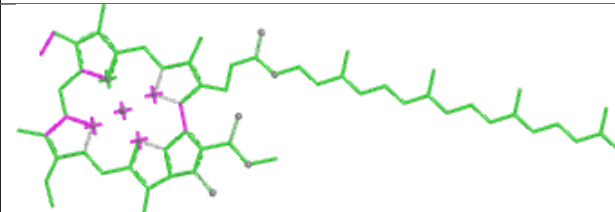
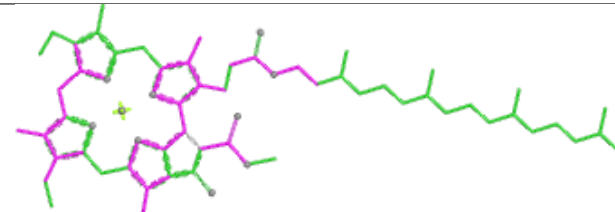
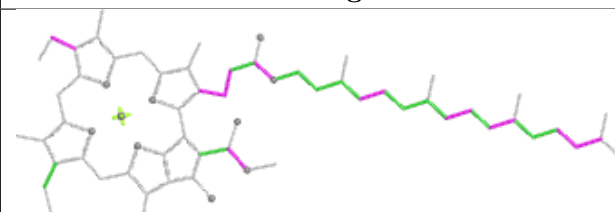
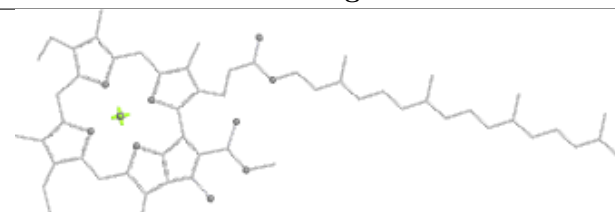
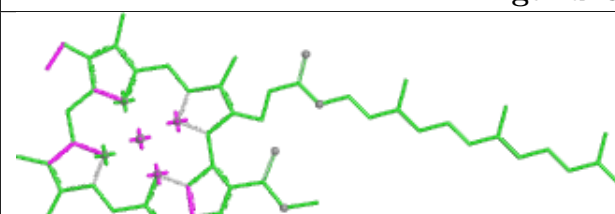
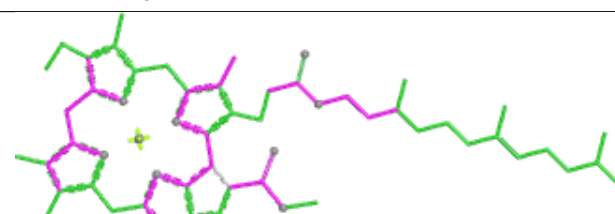
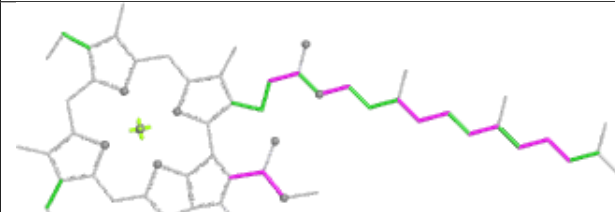
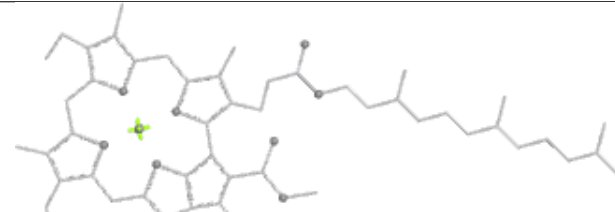
Ligand CLA L 1501

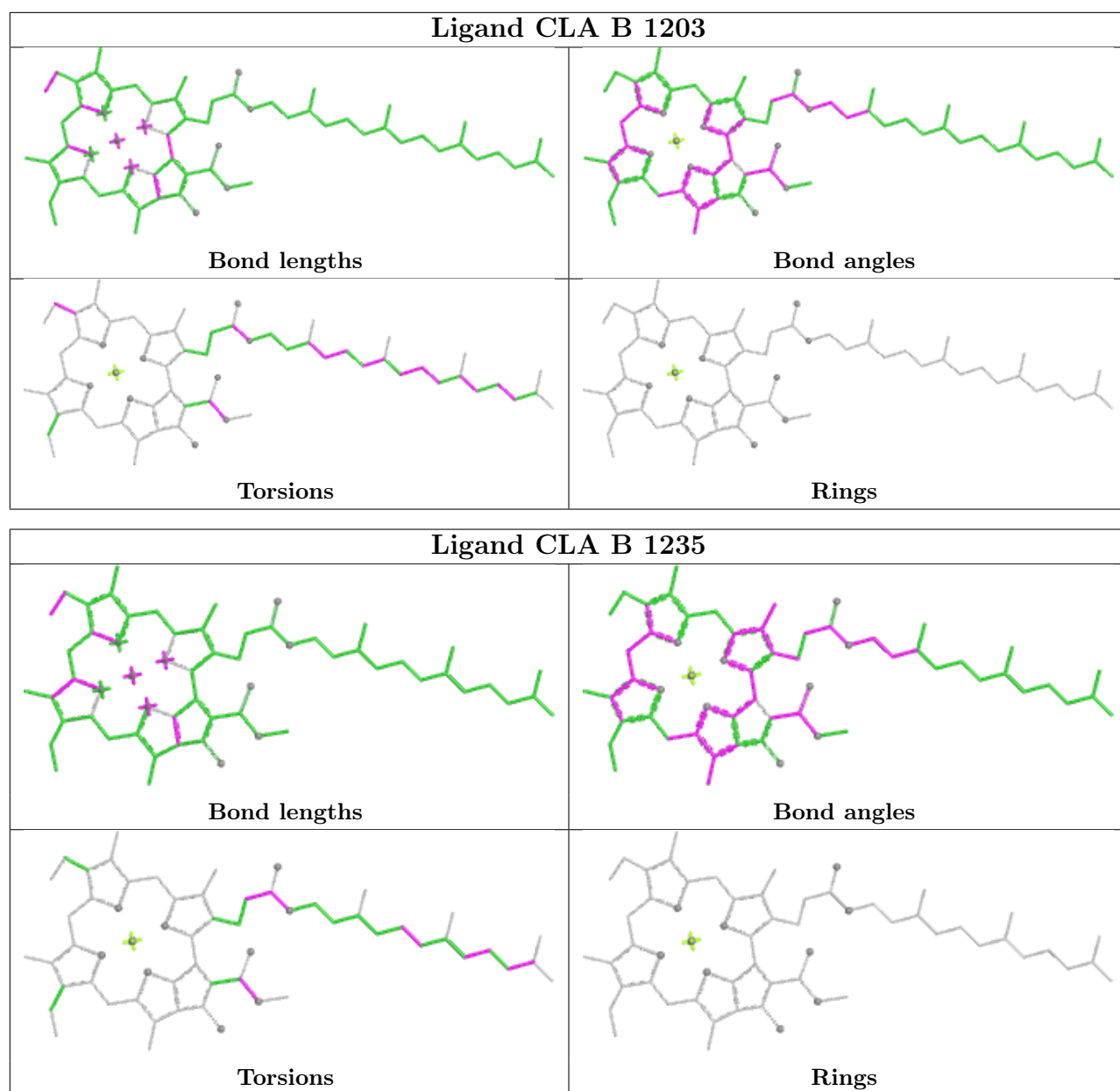


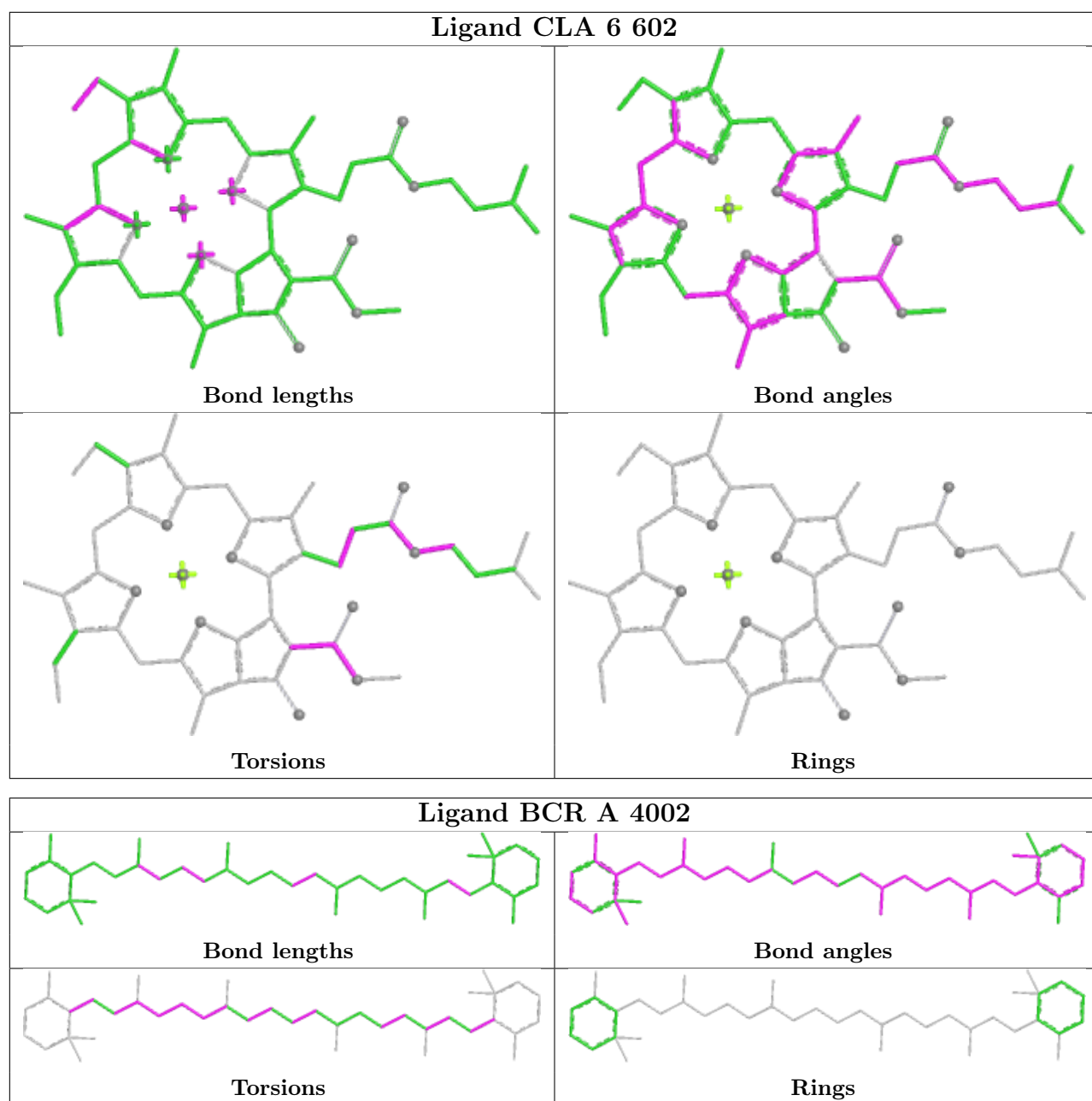


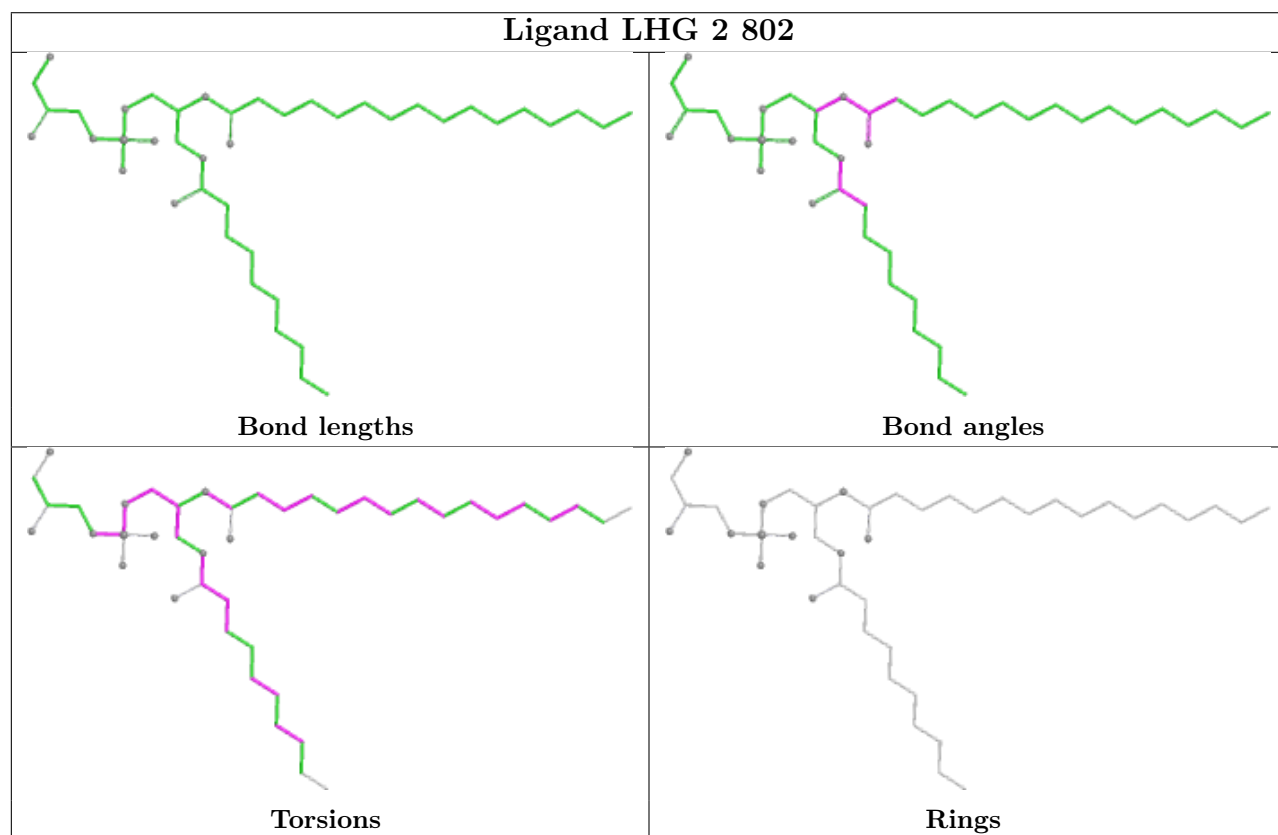
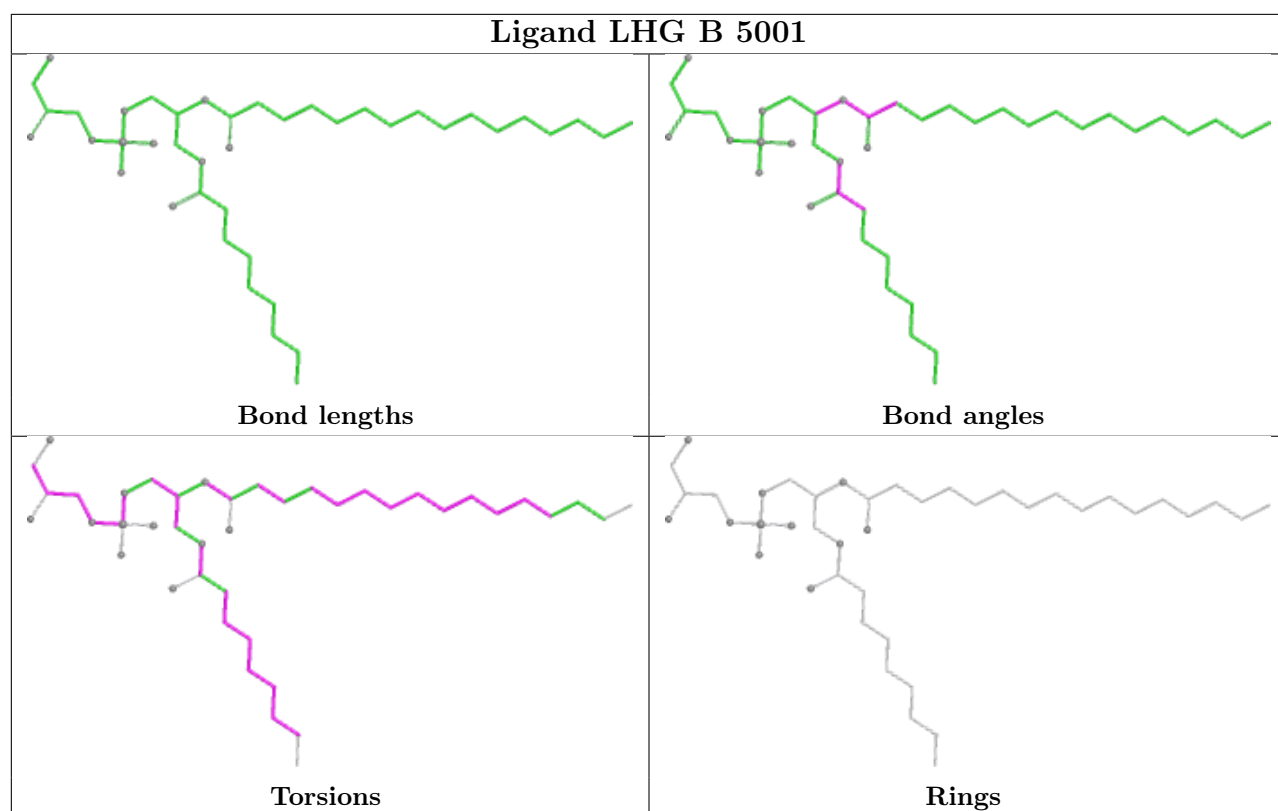




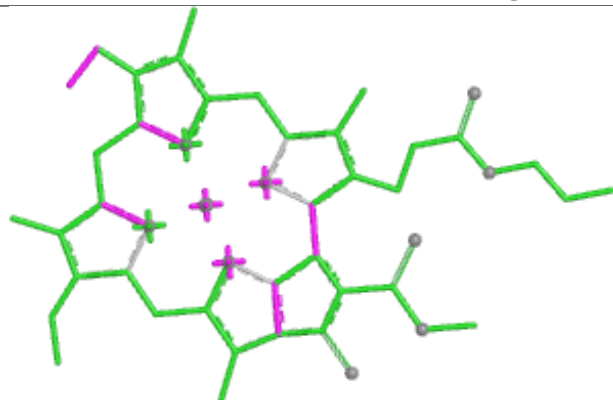
Ligand CLA 3 608	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 1115	
 Bond lengths	 Bond angles
 Torsions	 Rings



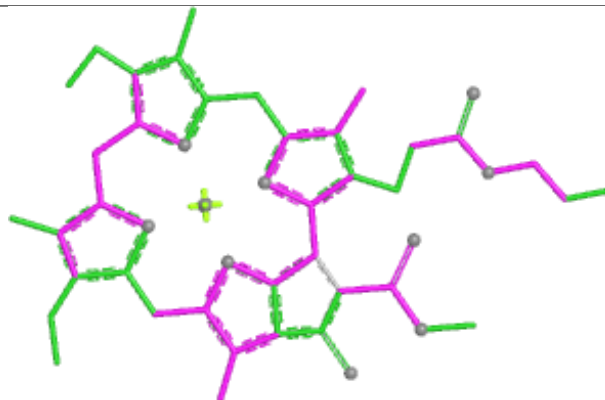




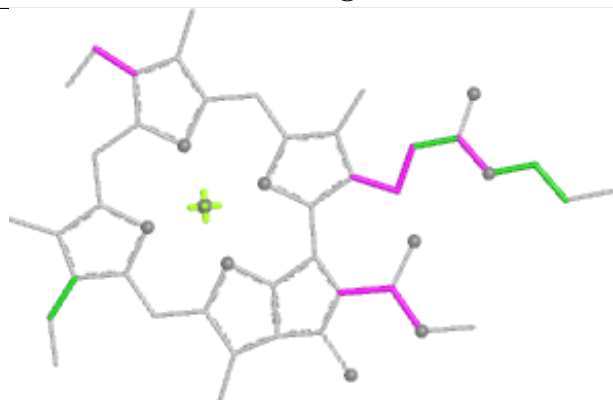
Ligand CLA B 1201



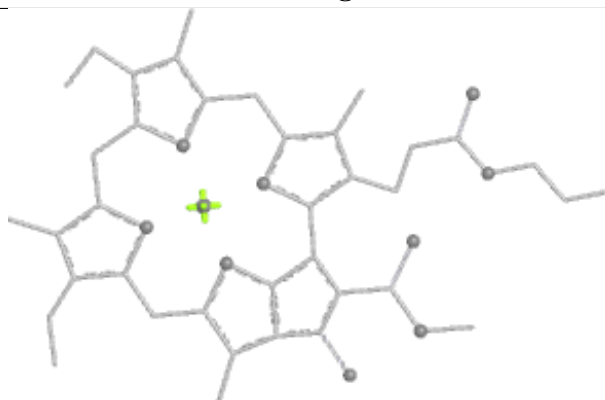
Bond lengths



Bond angles

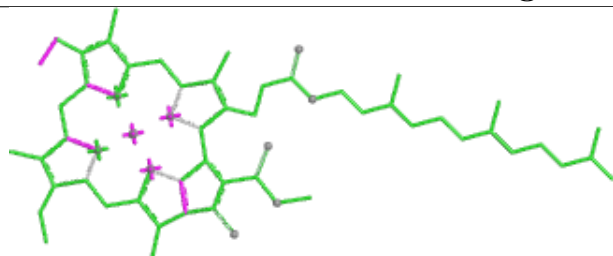


Torsions

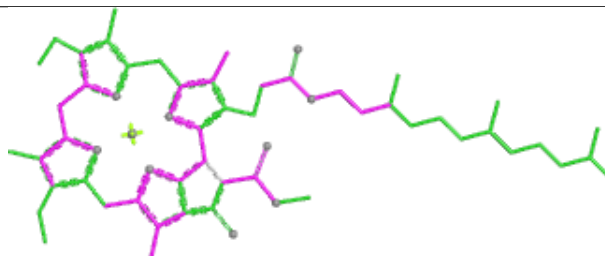


Rings

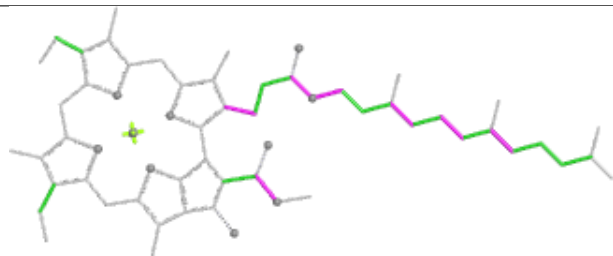
Ligand CLA 4 604



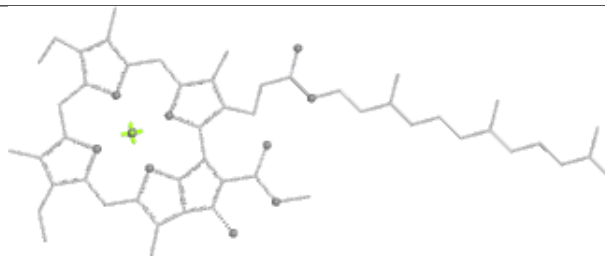
Bond lengths



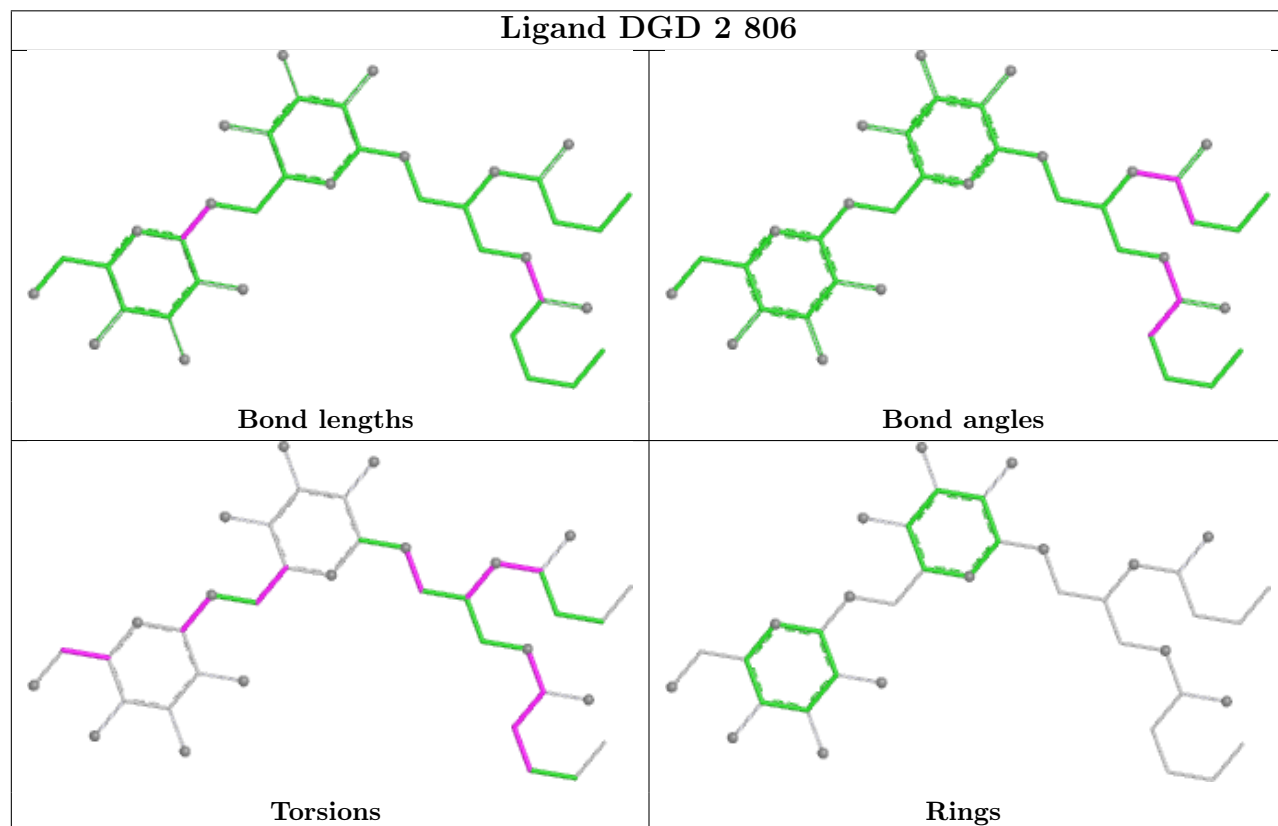
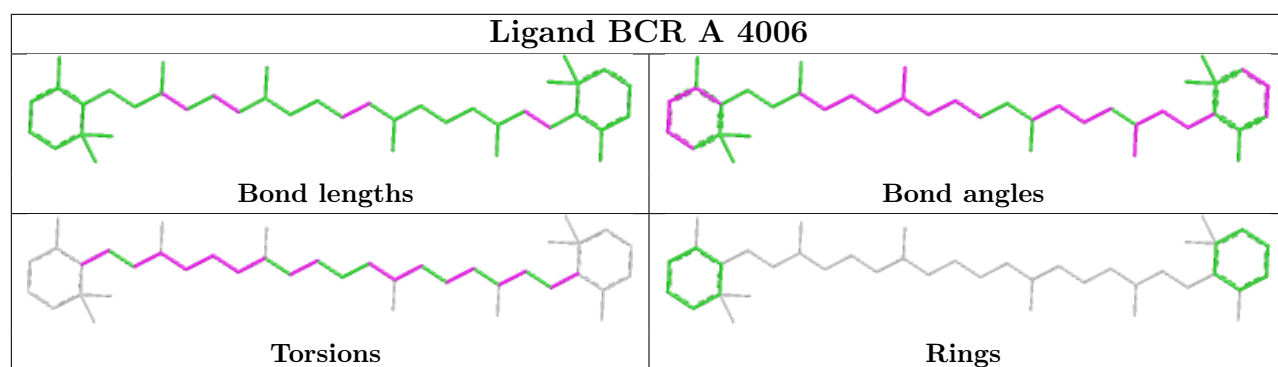
Bond angles



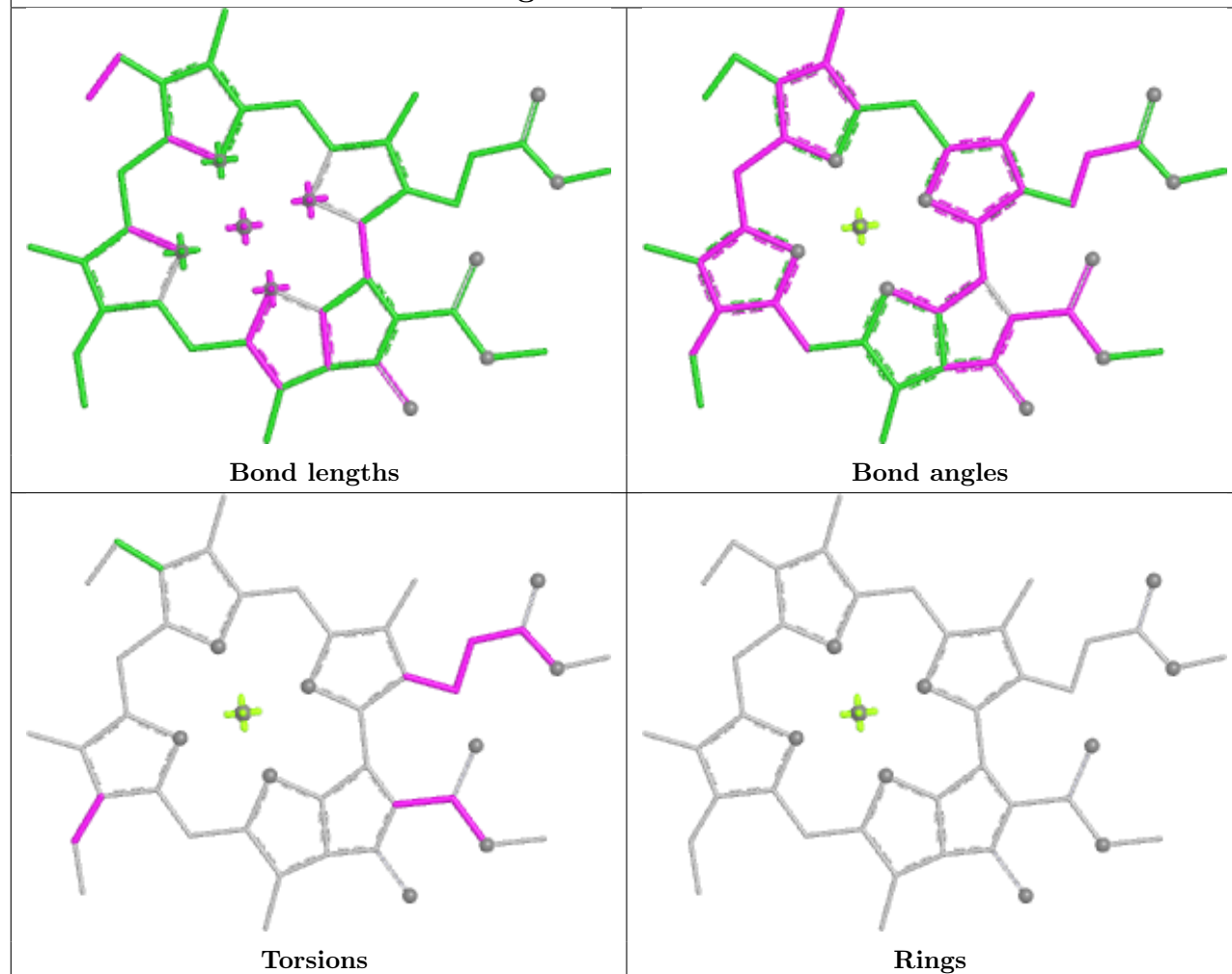
Torsions



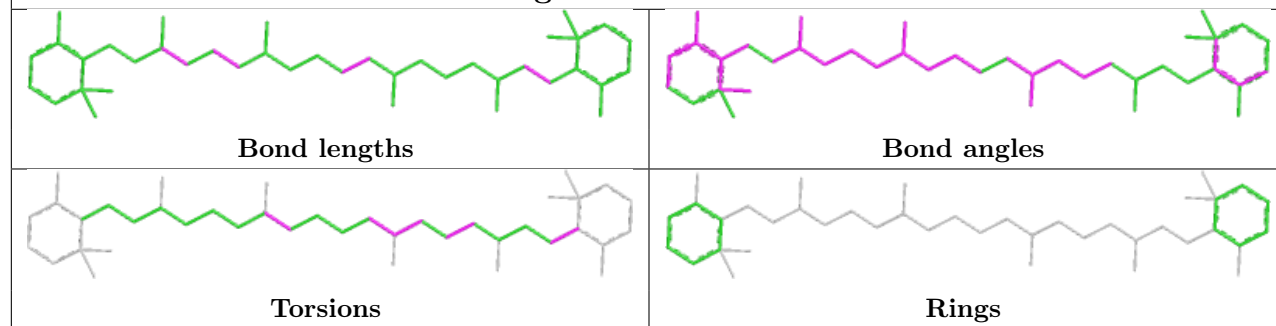
Rings

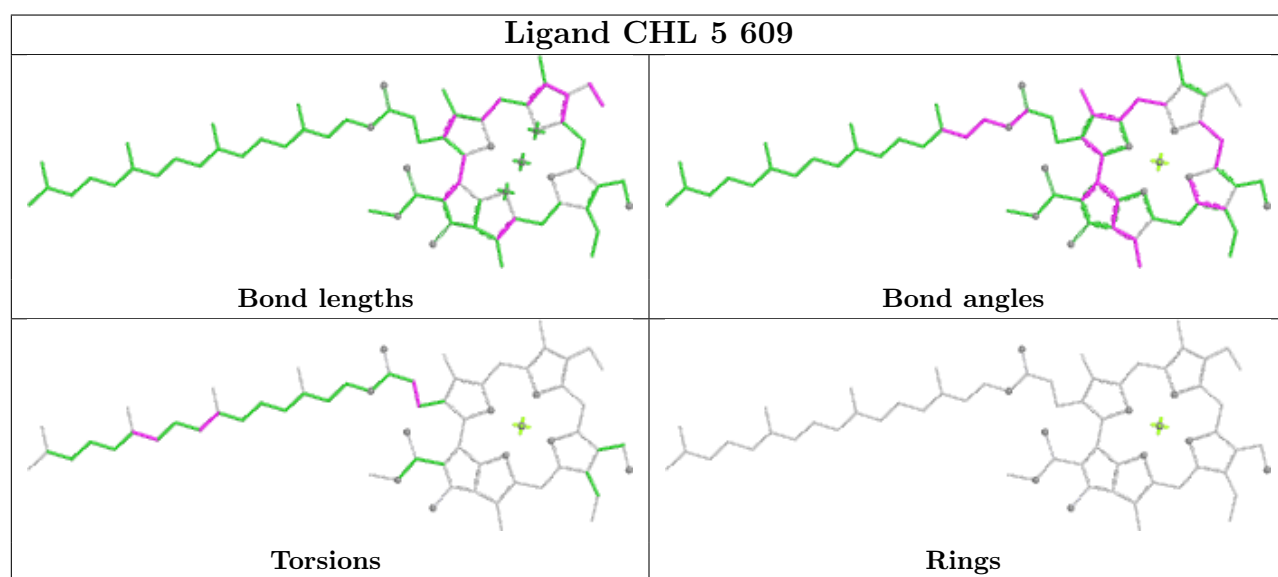
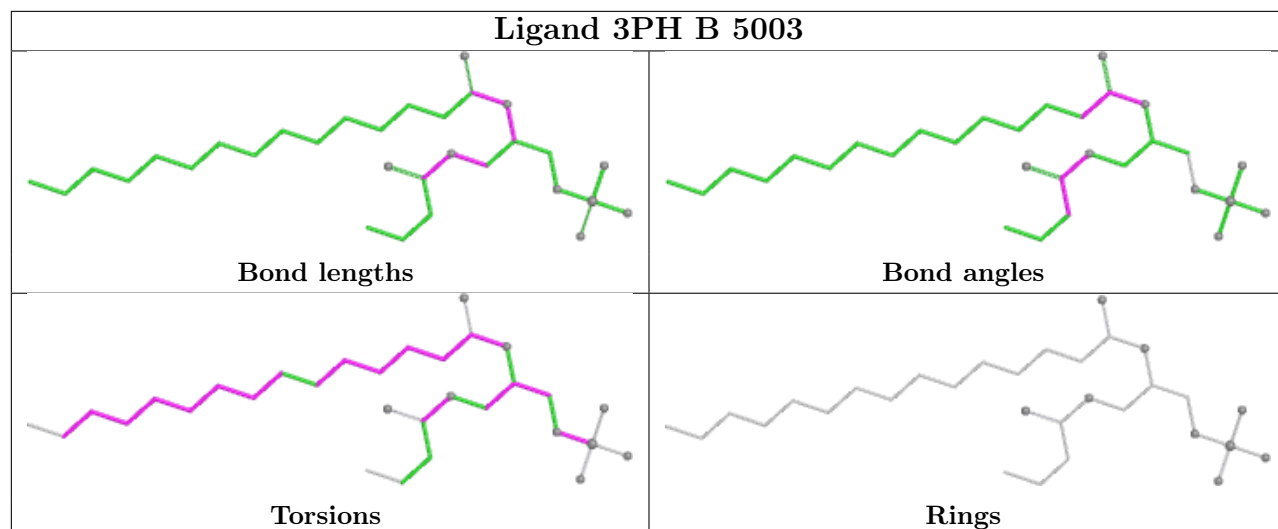


Ligand CLA 5 612

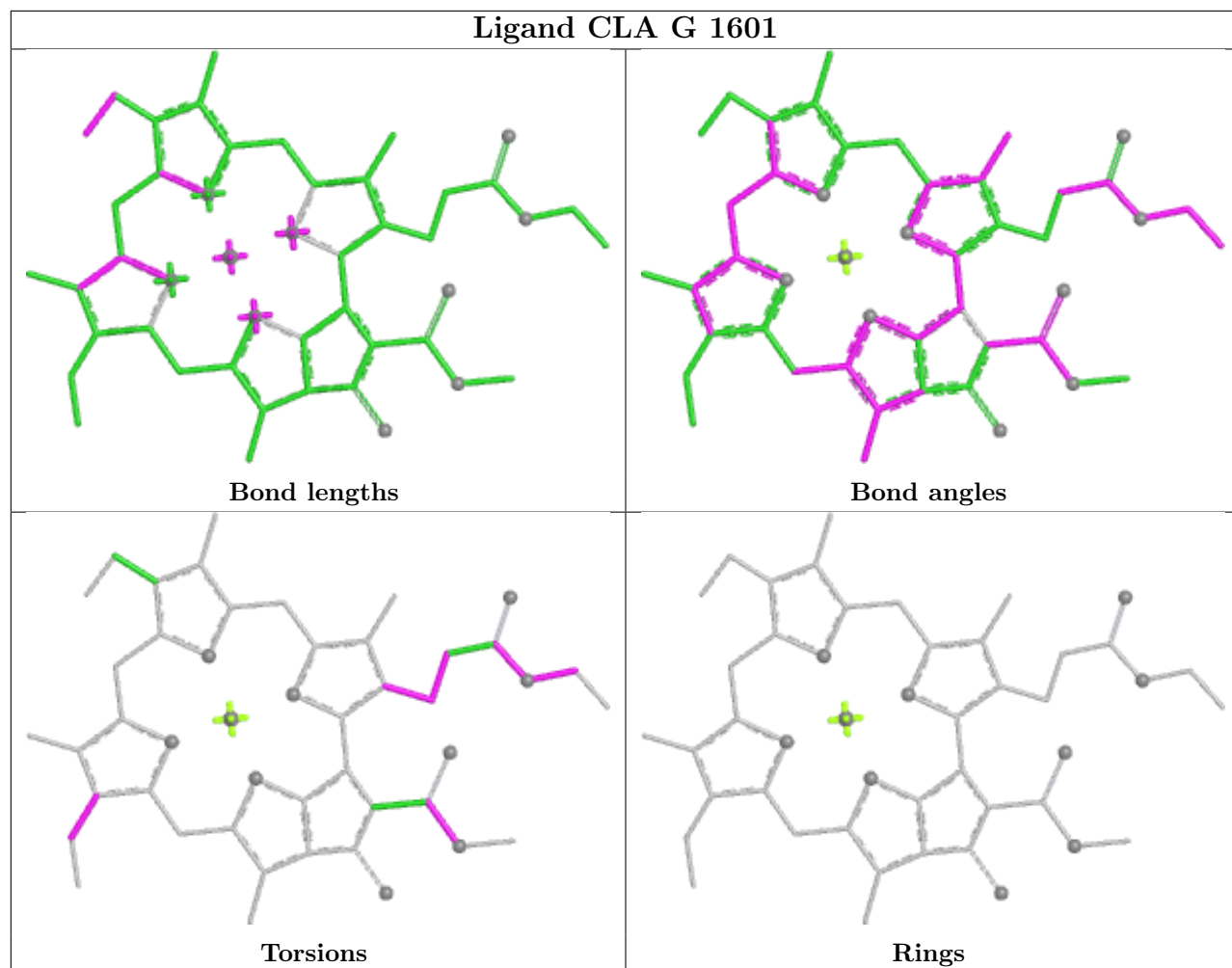


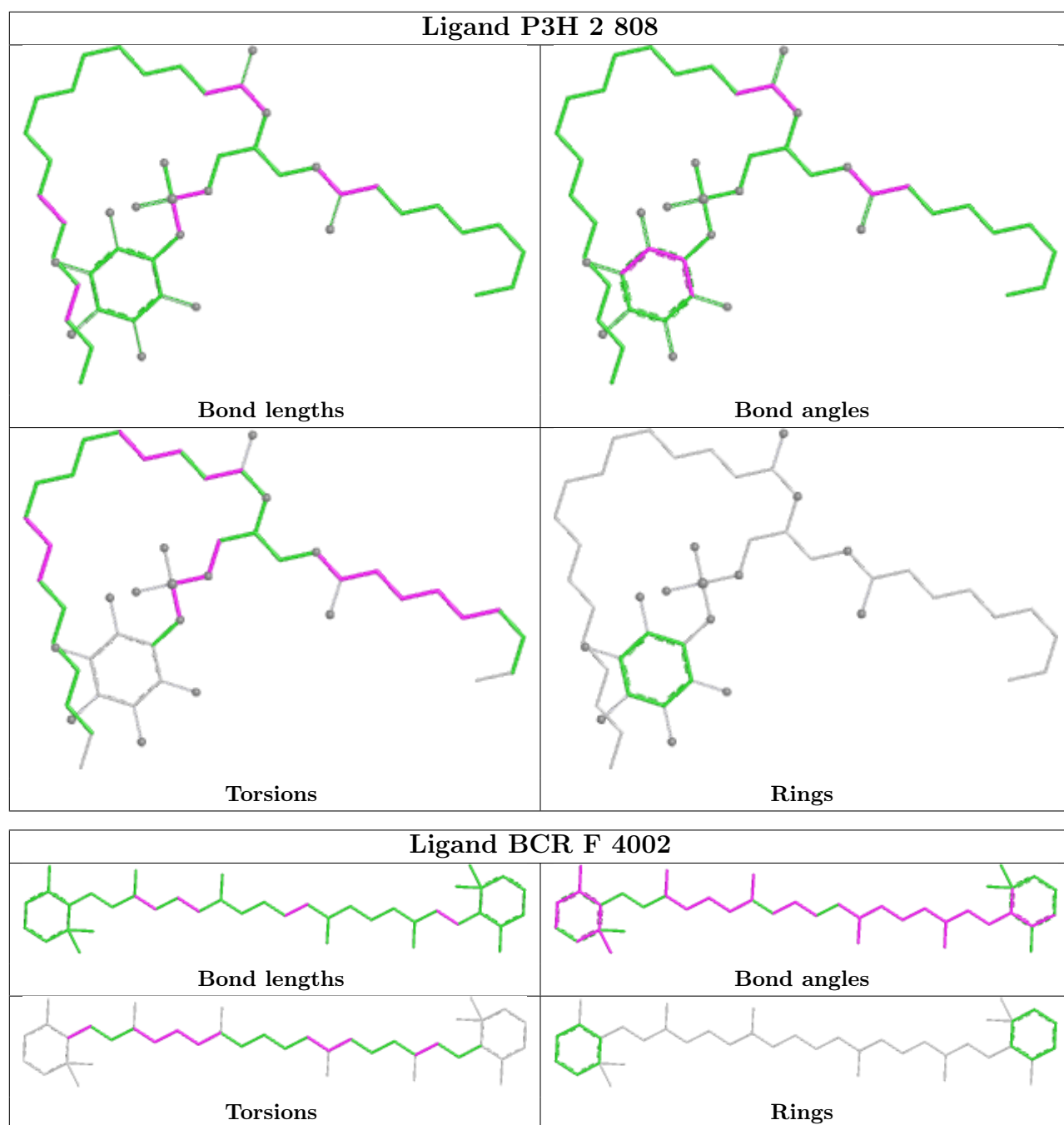
Ligand BCR 3 506

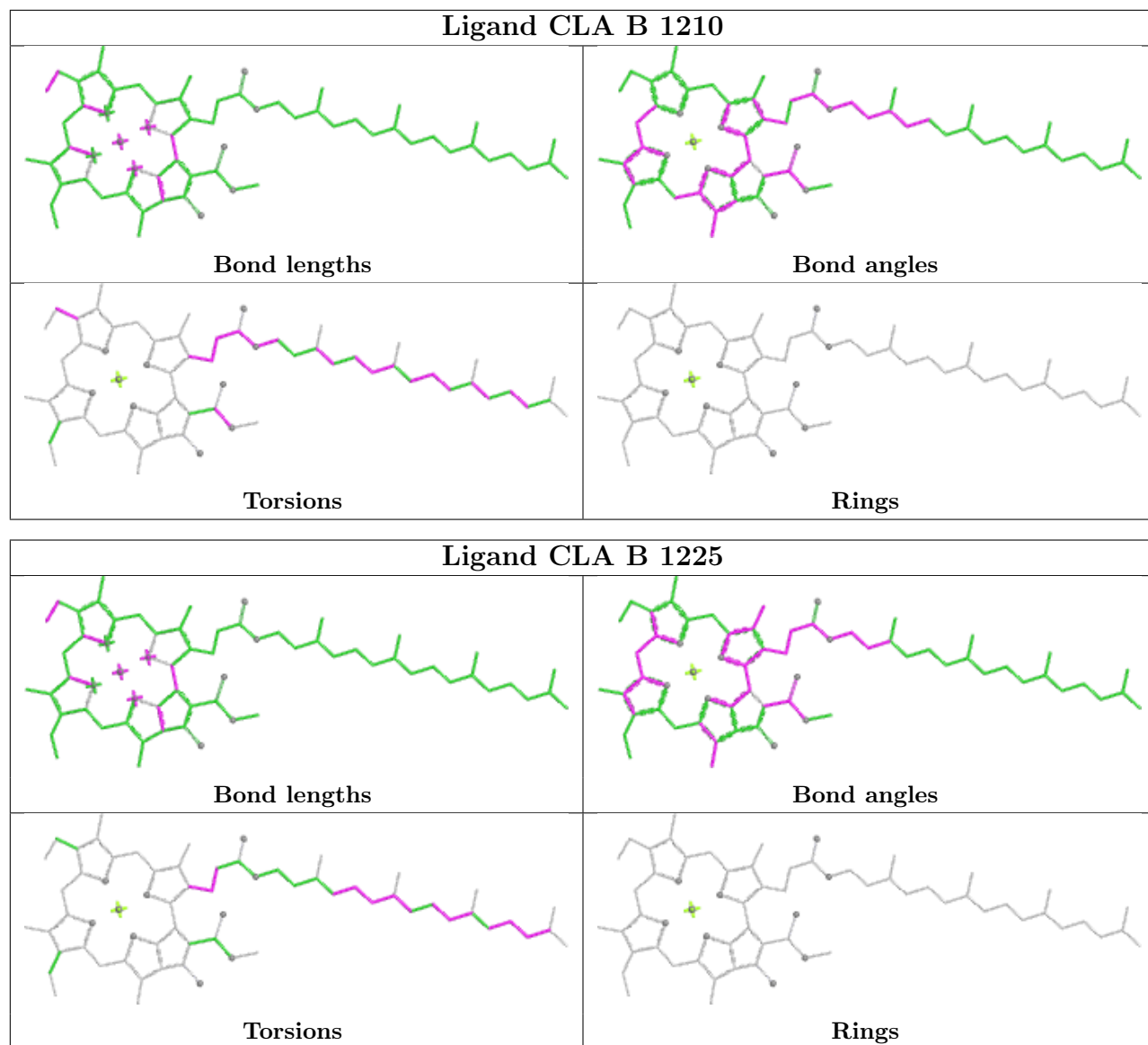


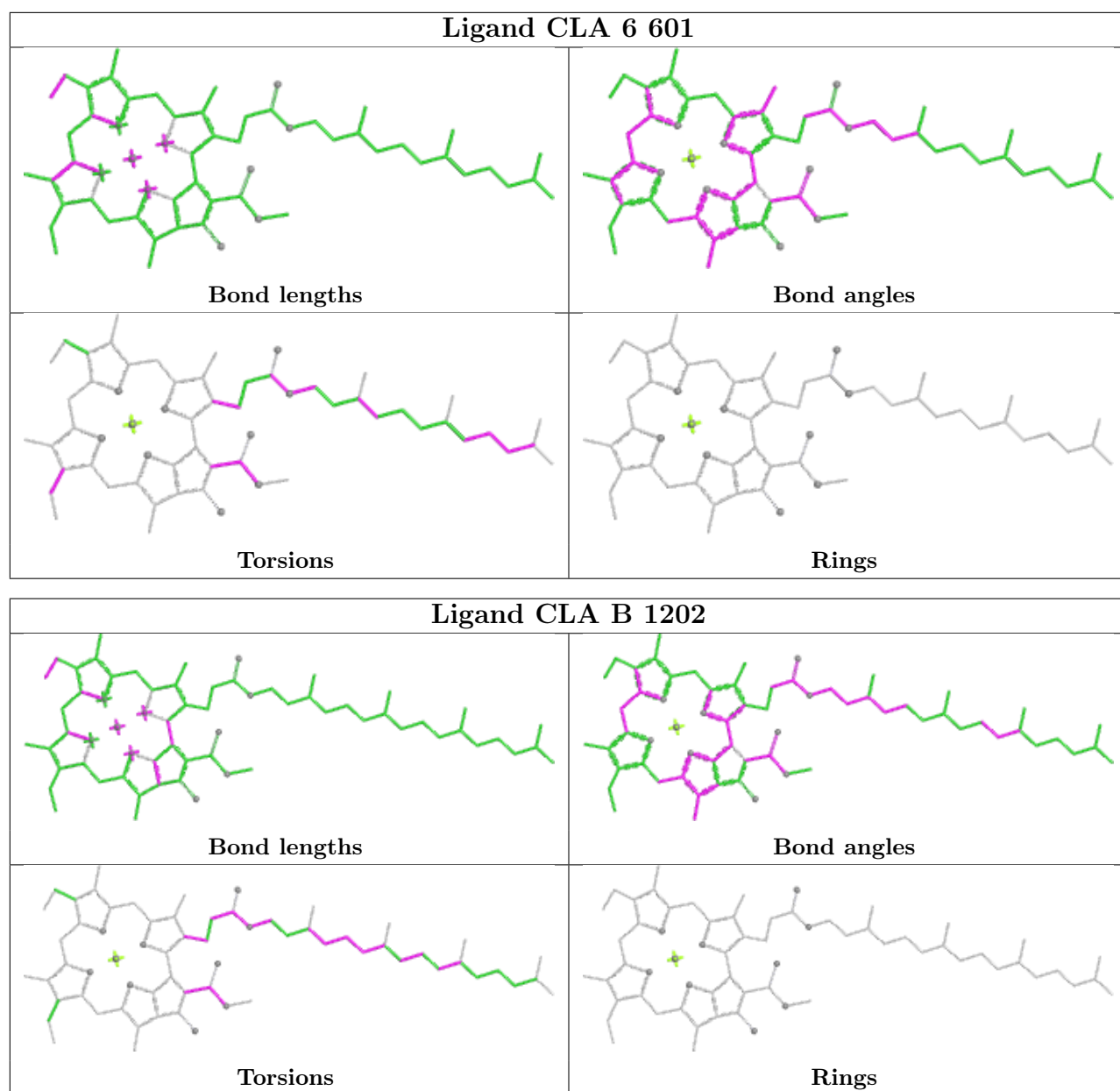


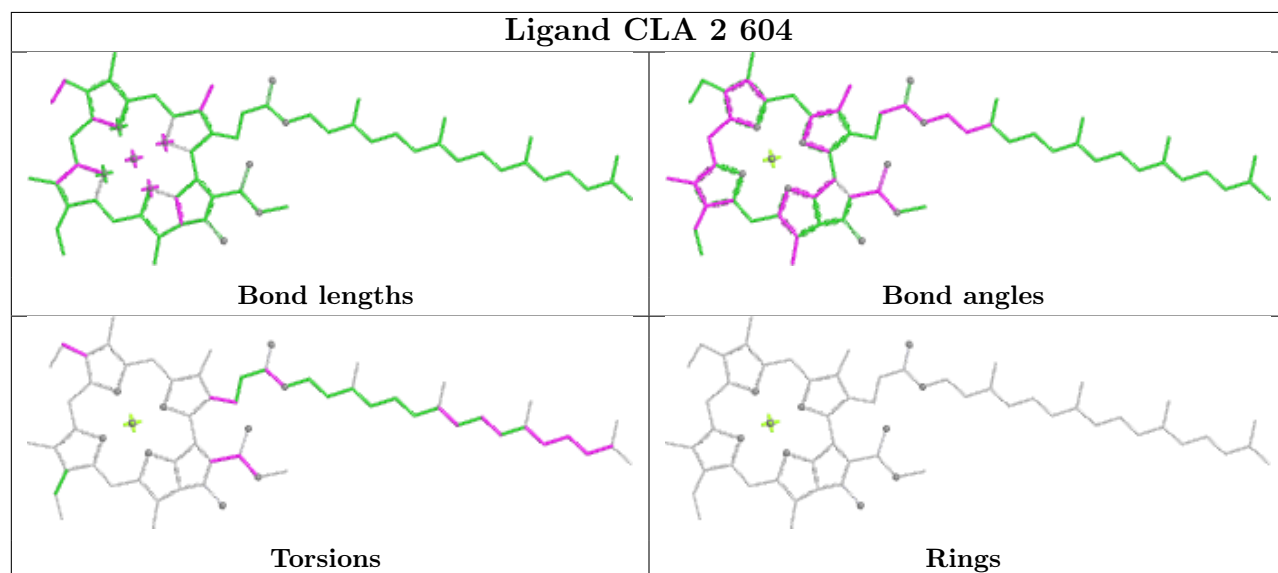
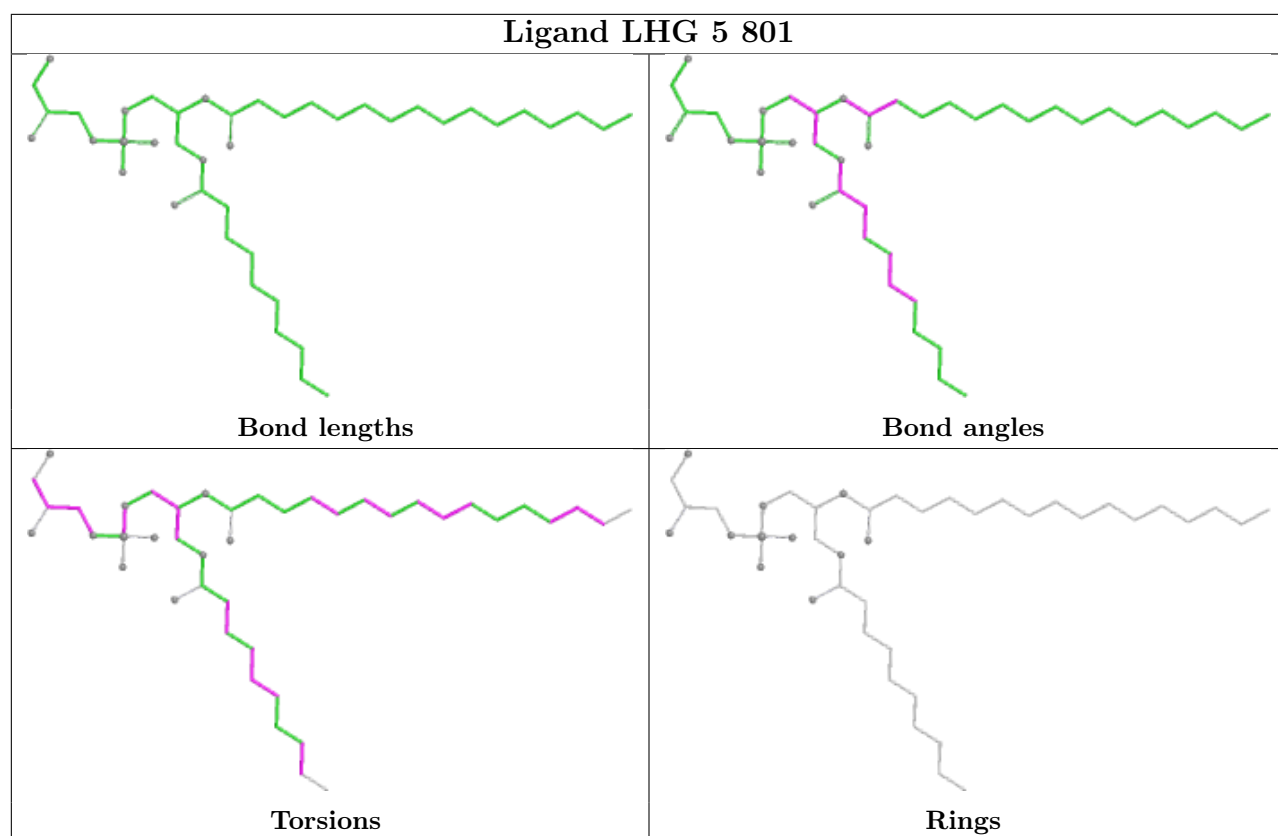
Ligand CLA G 1601

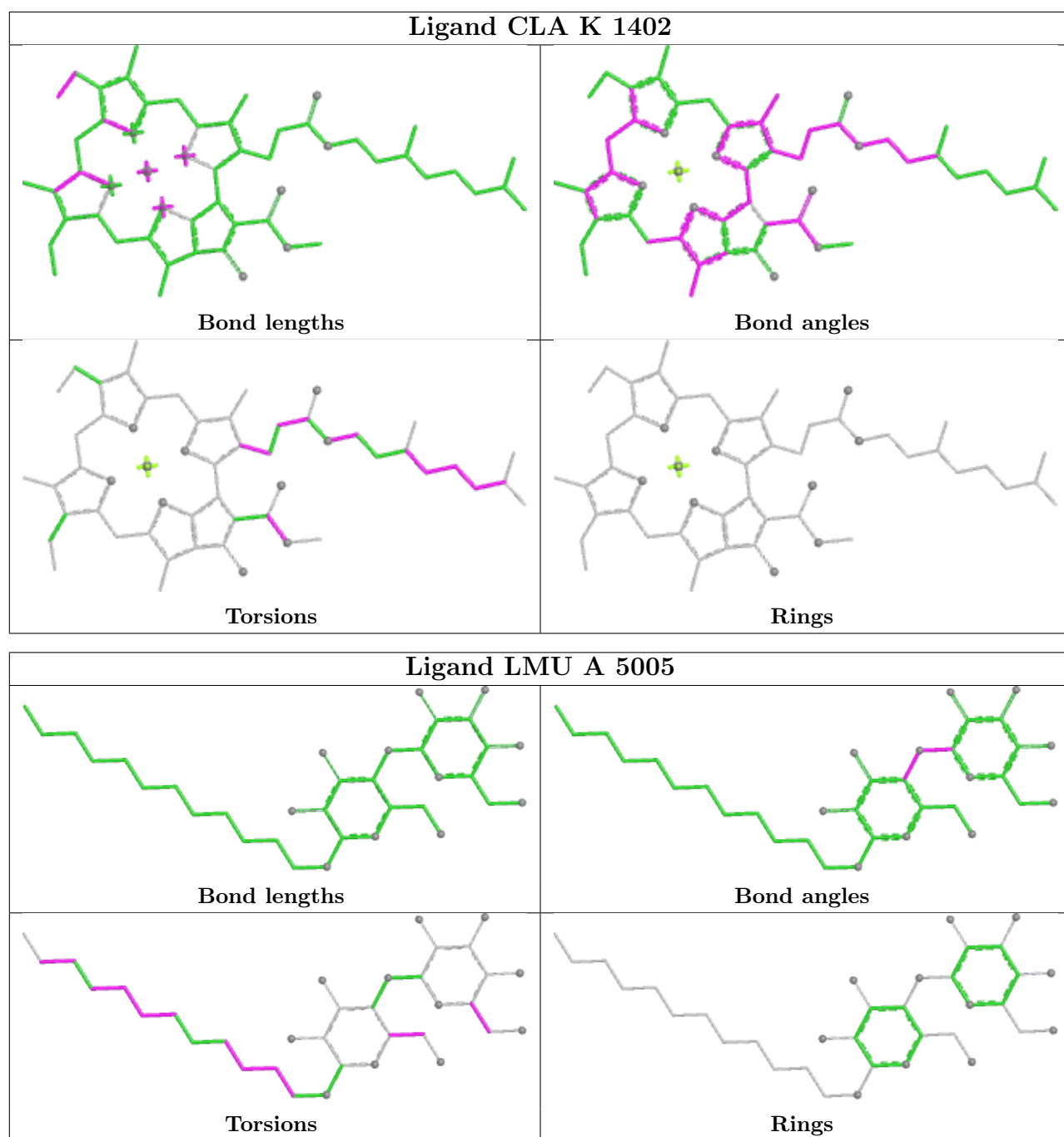




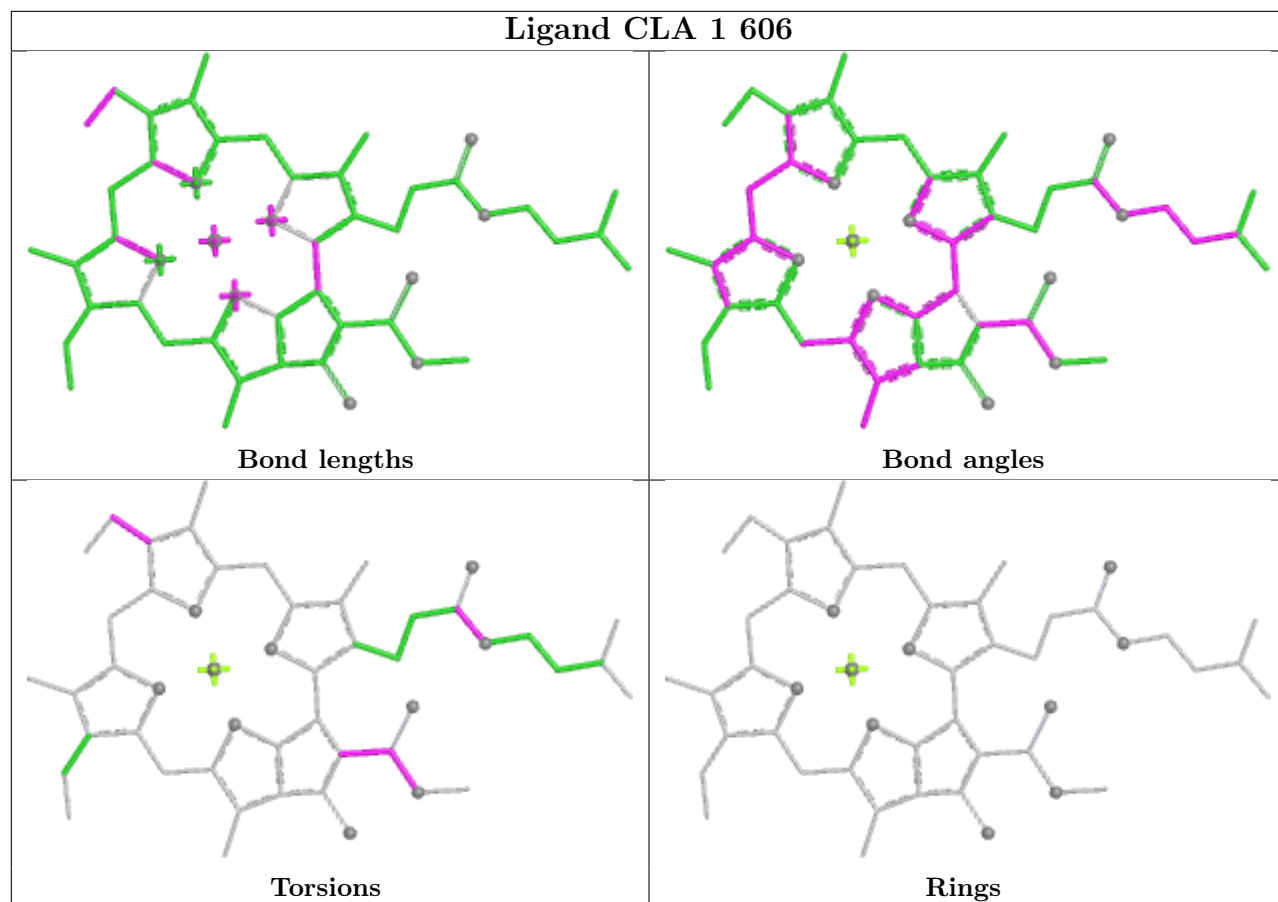




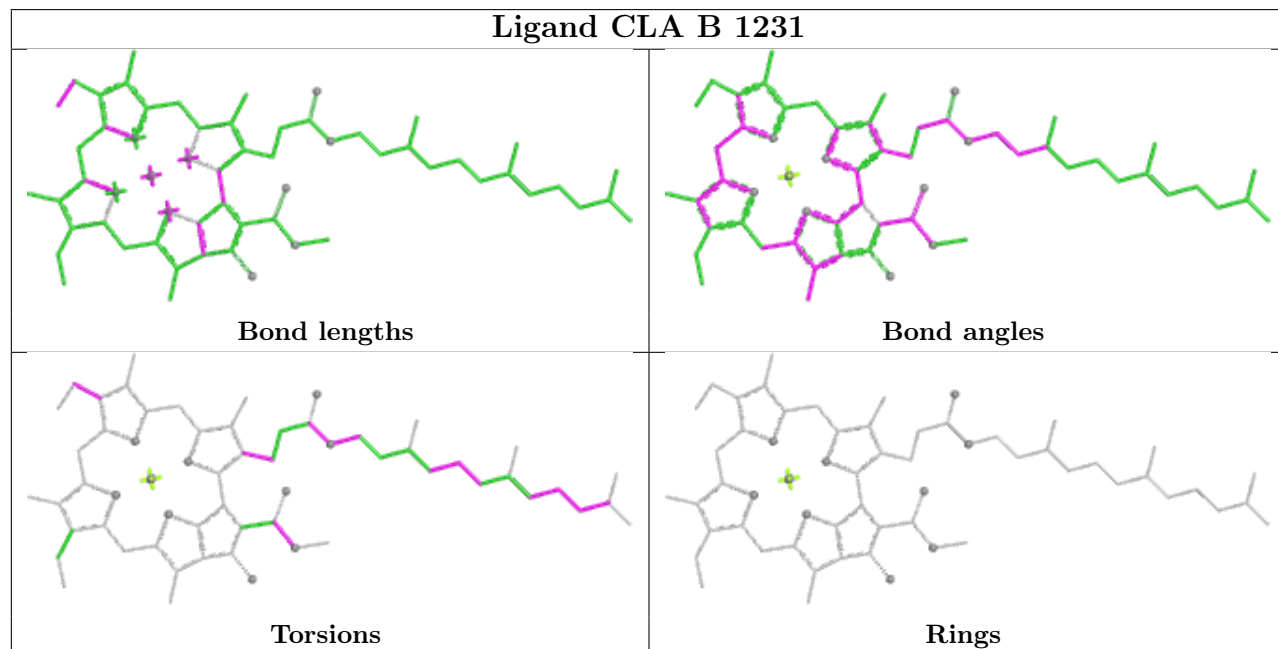


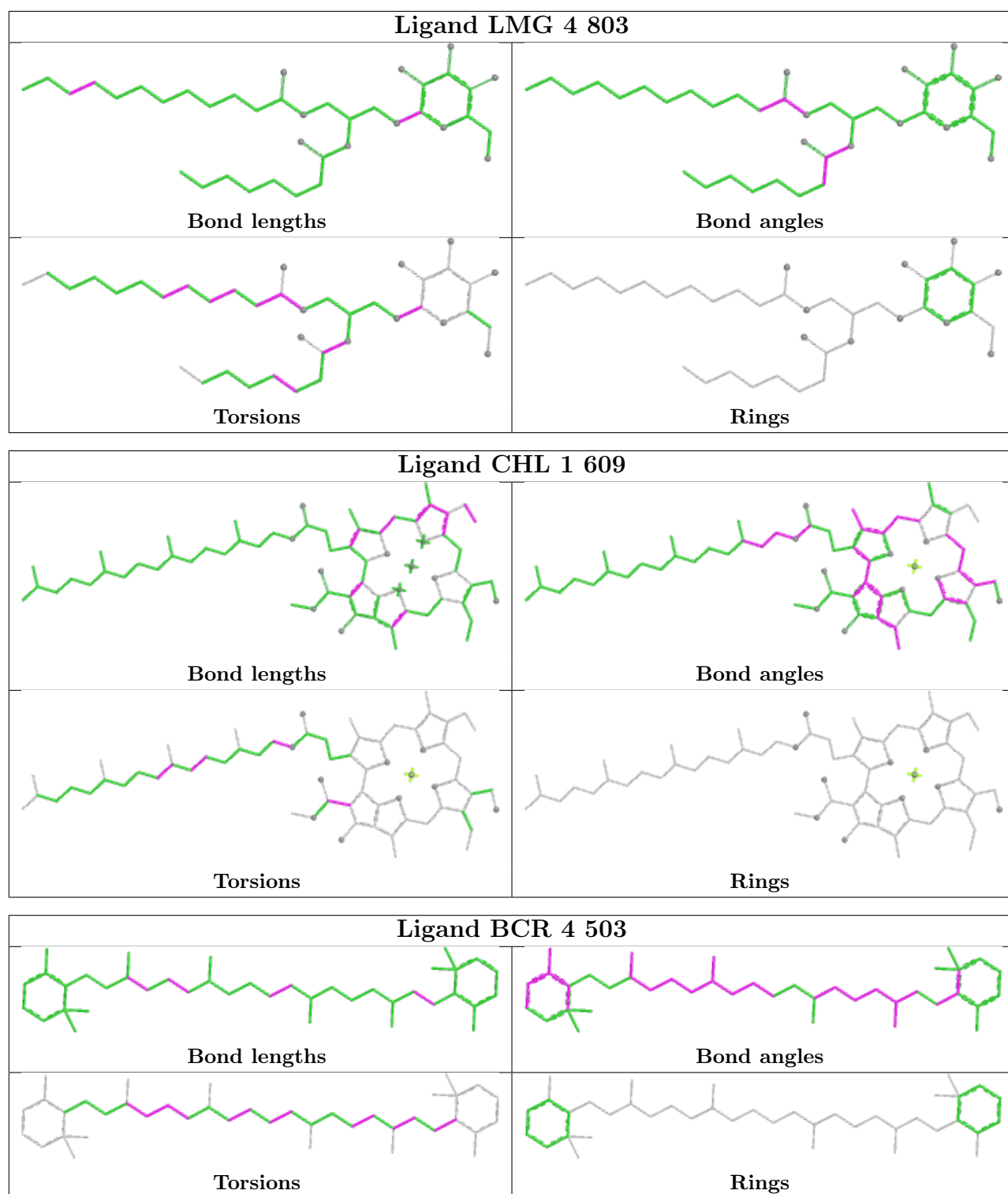


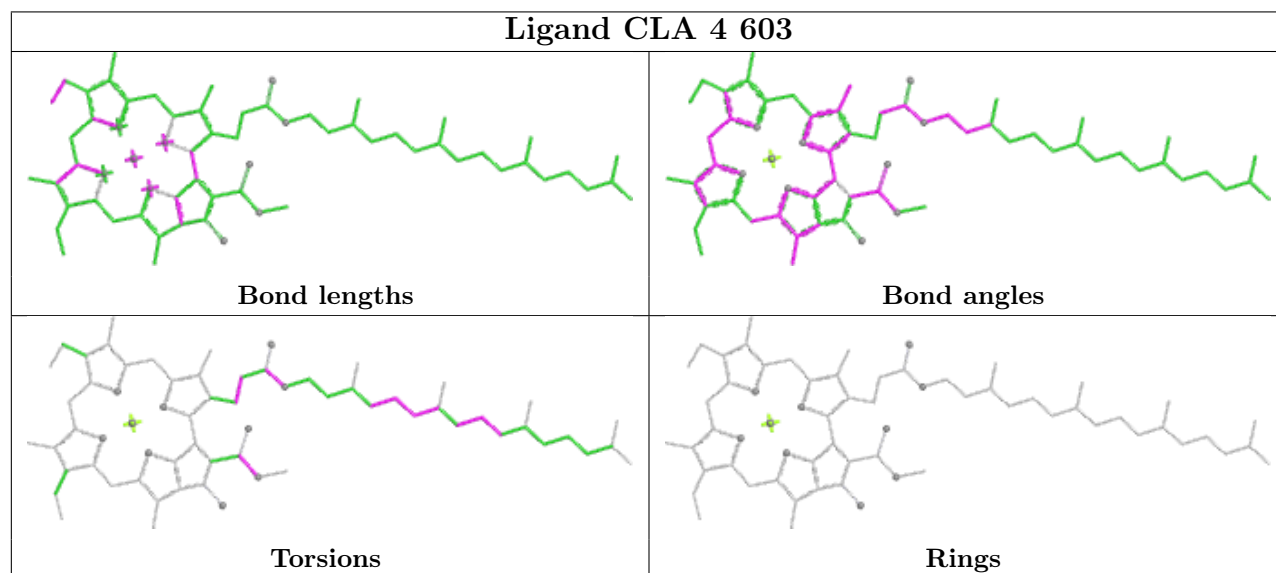
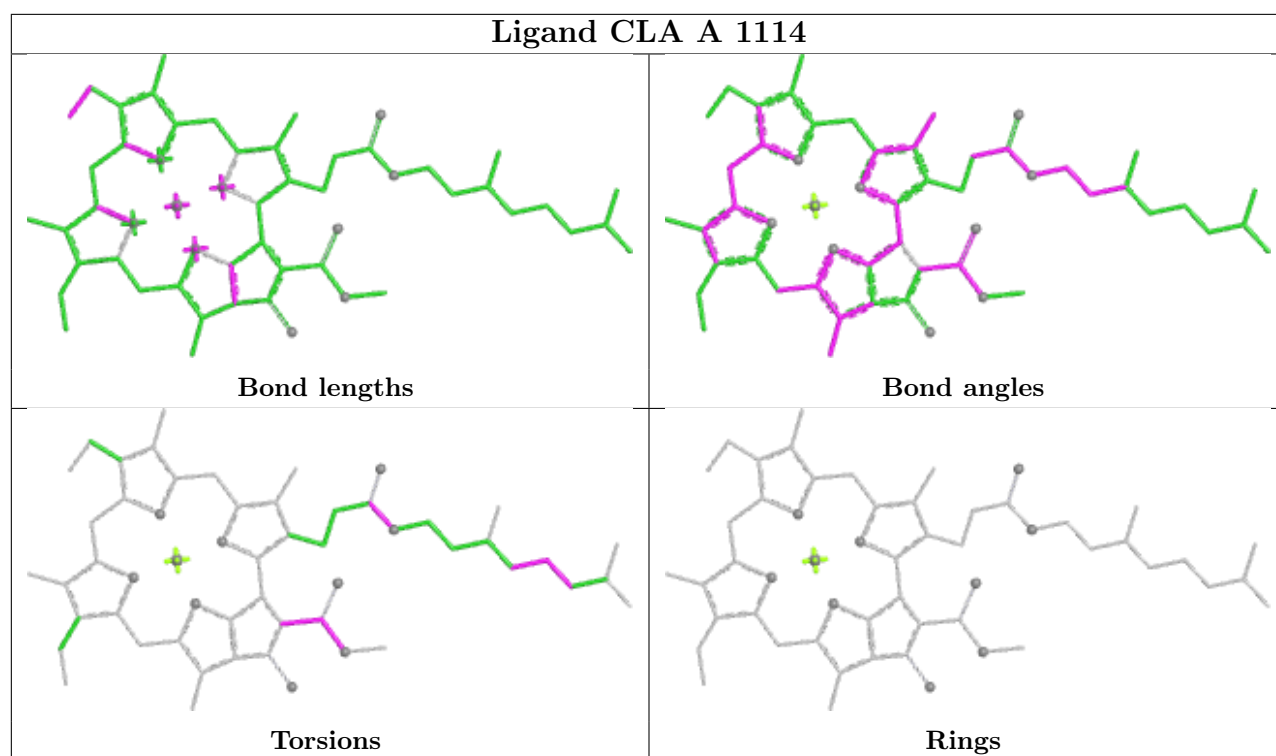
Ligand CLA 1 606



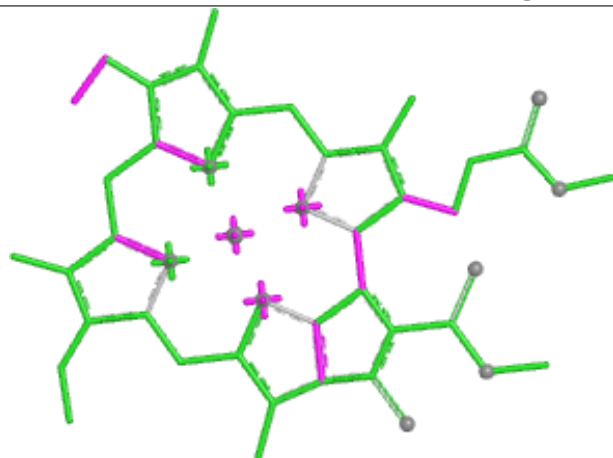
Ligand CLA B 1231



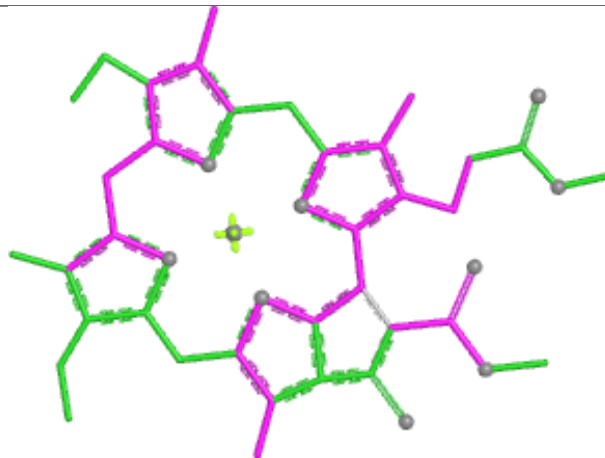




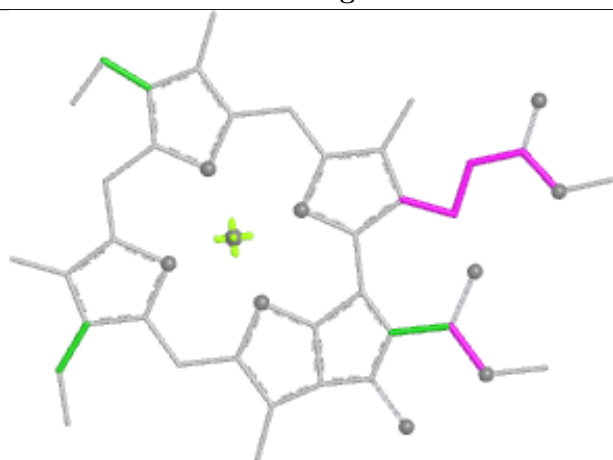
Ligand CLA 5 602



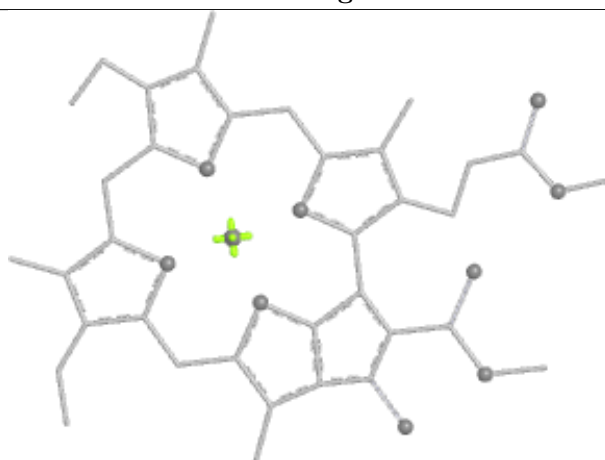
Bond lengths



Bond angles

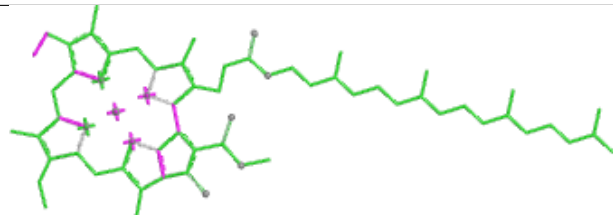


Torsions

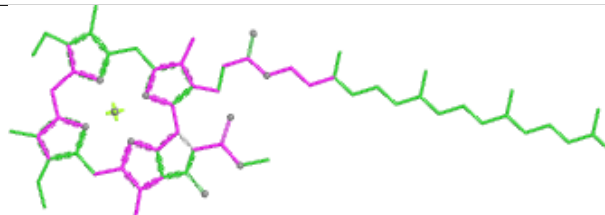


Rings

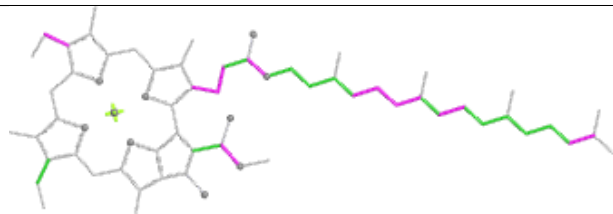
Ligand CLA 2 605



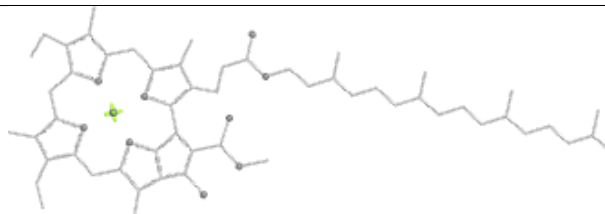
Bond lengths



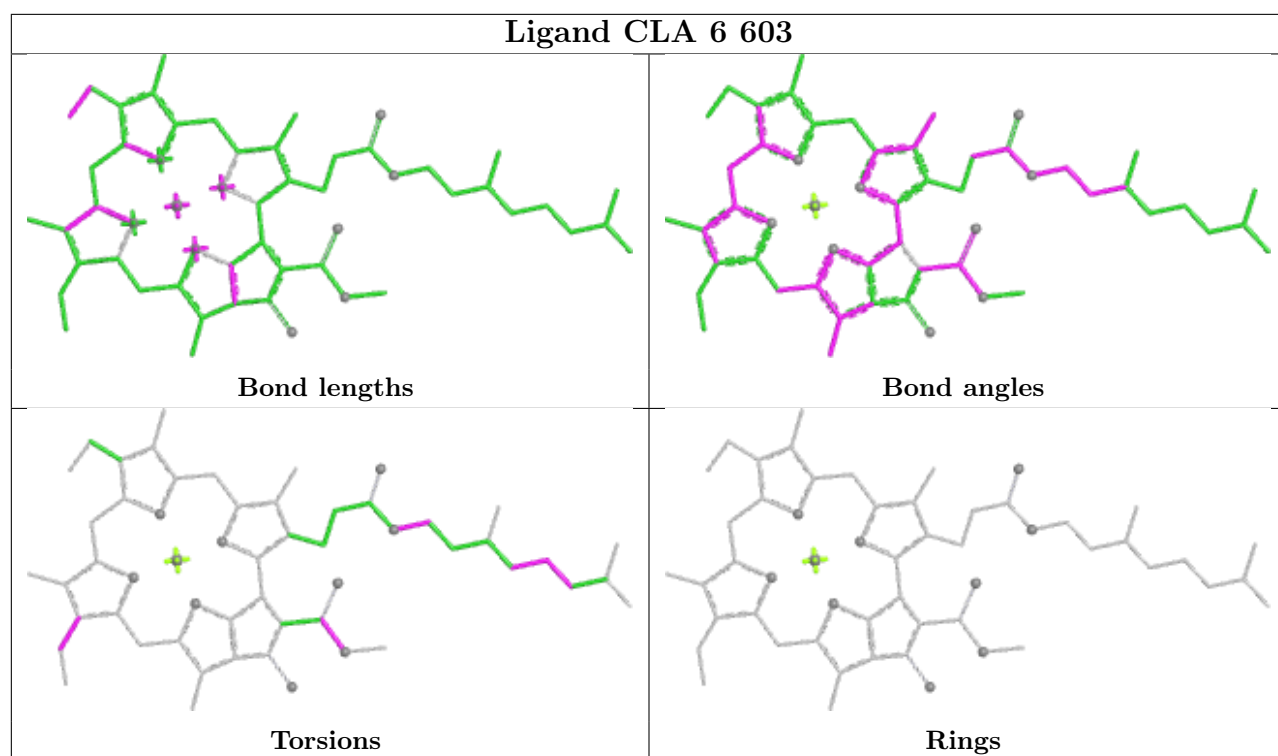
Bond angles

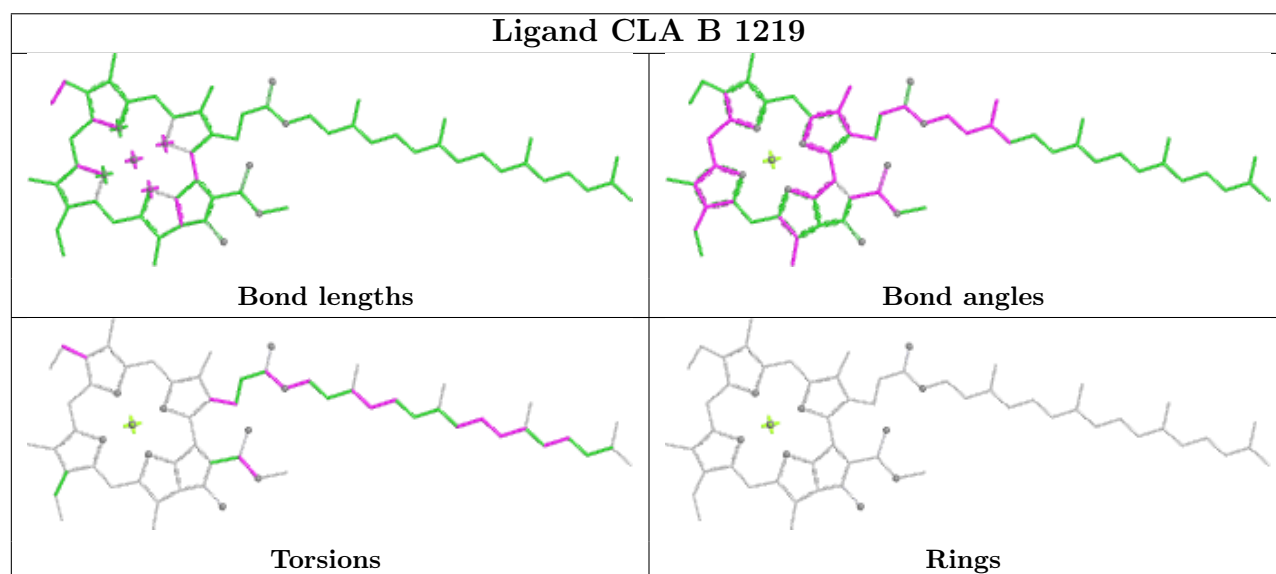
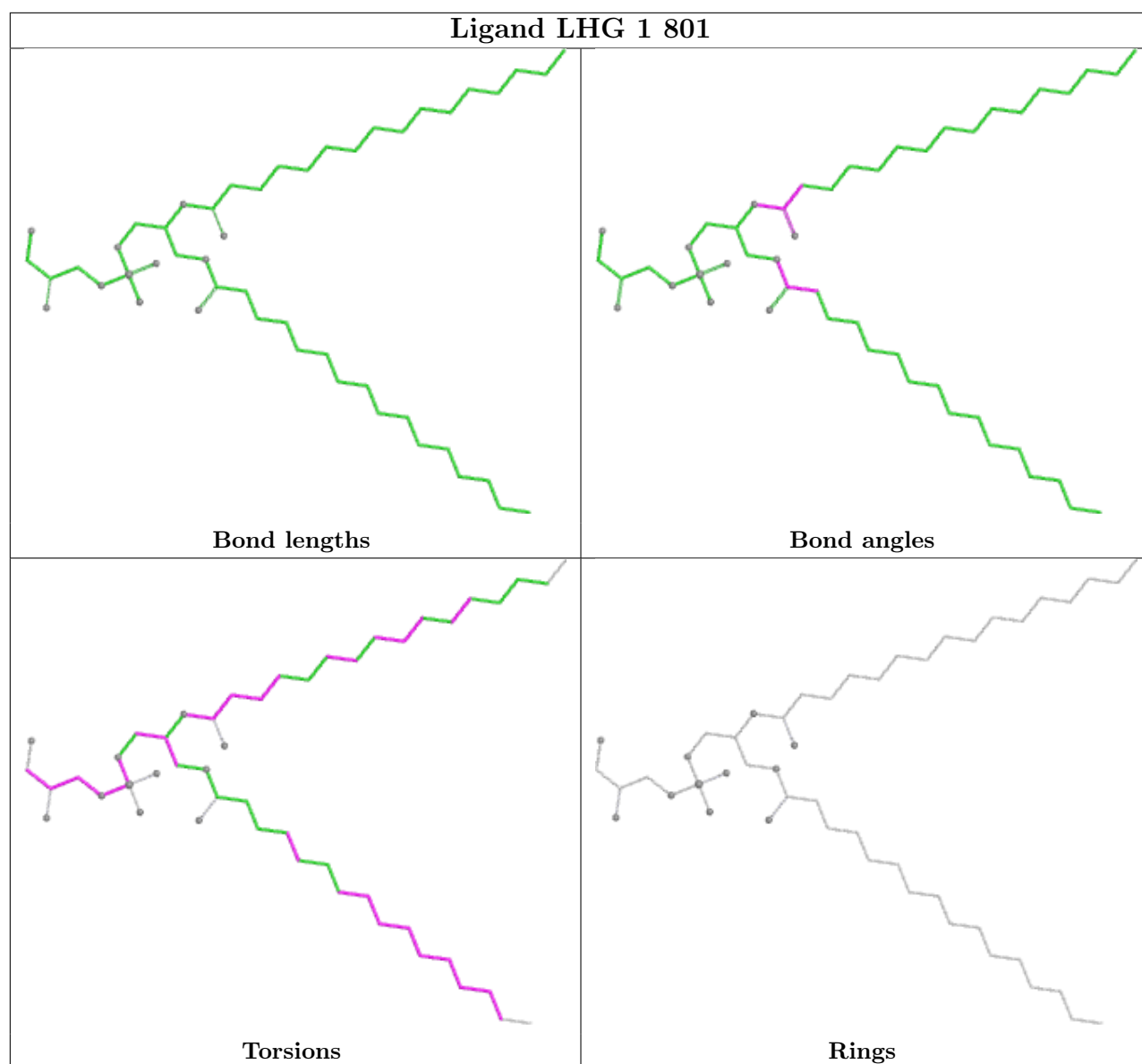


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

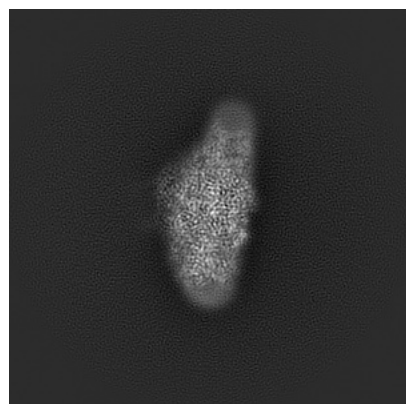
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10236. These allow visual inspection of the internal detail of the map and identification of artifacts.

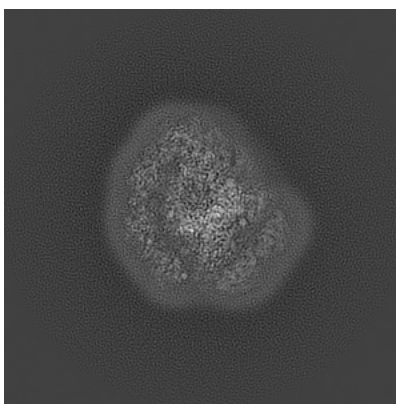
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

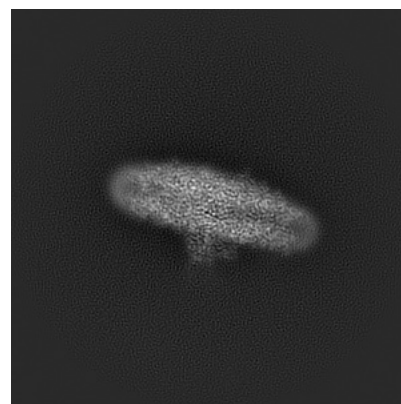
6.1.1 Primary map



X

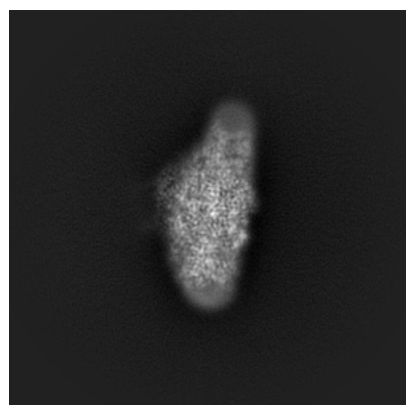


Y

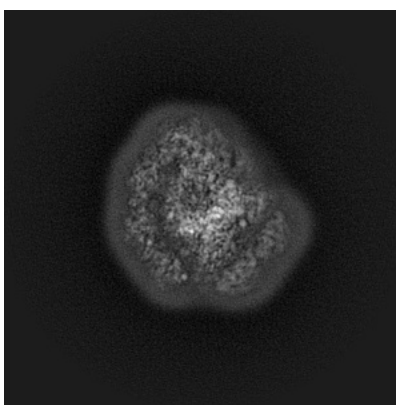


Z

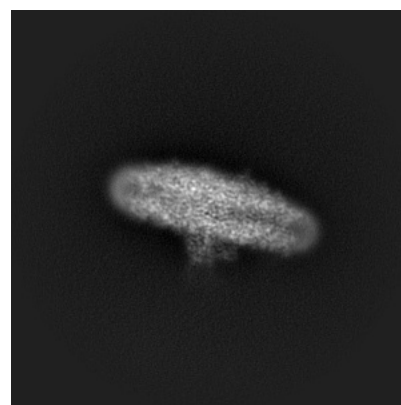
6.1.2 Raw map



X



Y

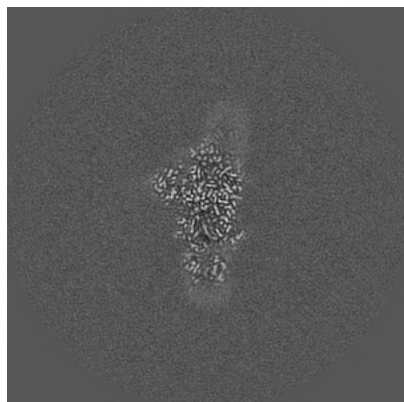


Z

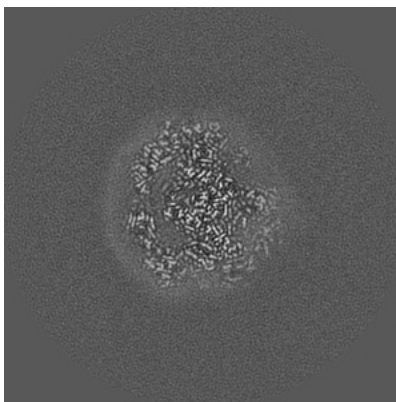
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

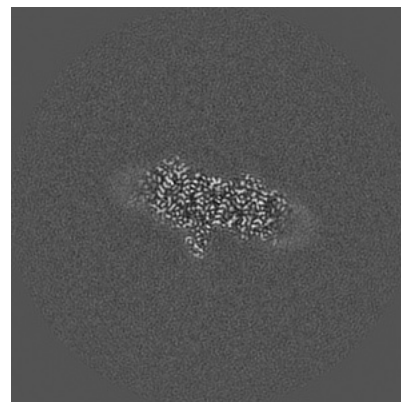
6.2.1 Primary map



X Index: 180

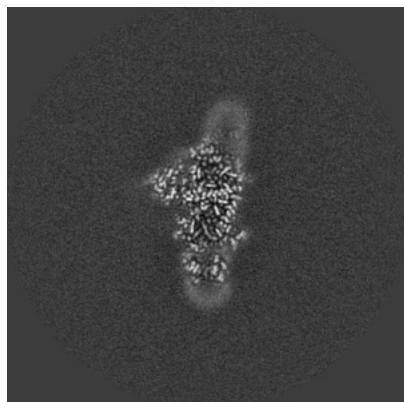


Y Index: 180

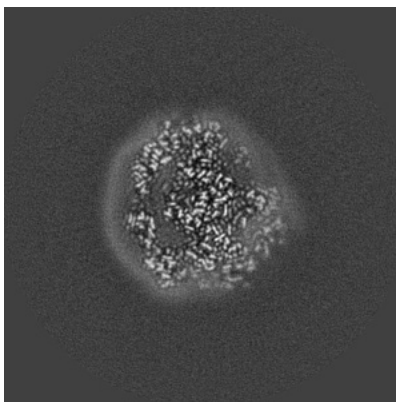


Z Index: 180

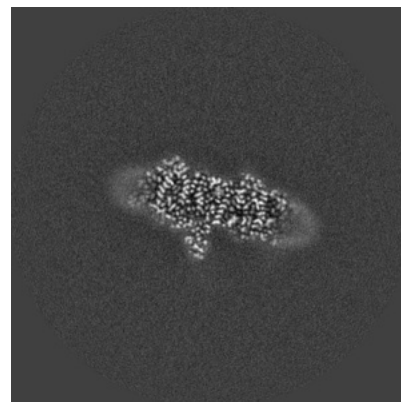
6.2.2 Raw map



X Index: 180



Y Index: 180

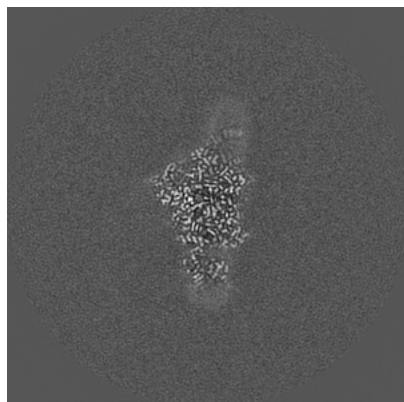


Z Index: 180

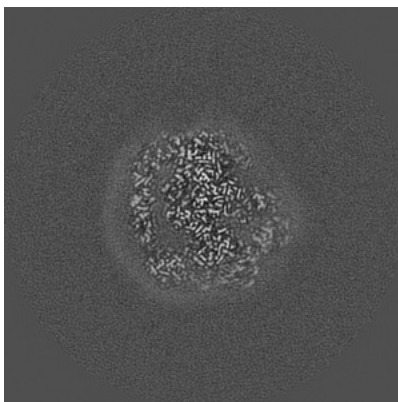
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

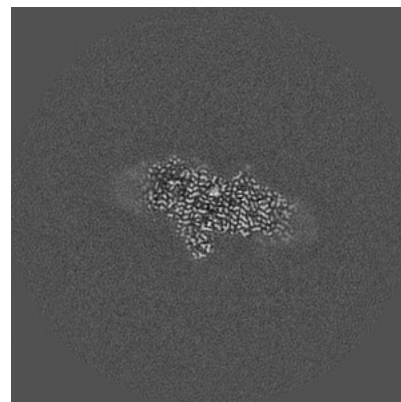
6.3.1 Primary map



X Index: 177

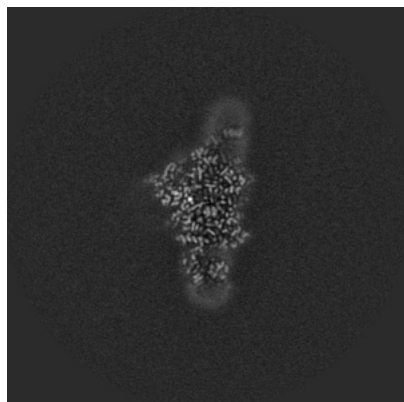


Y Index: 184

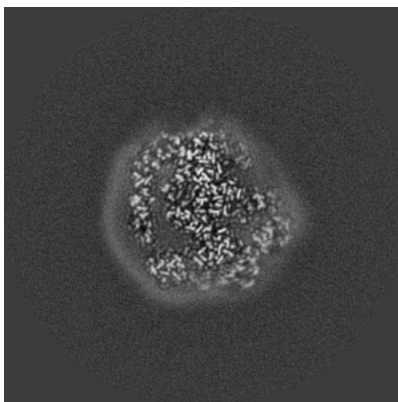


Z Index: 185

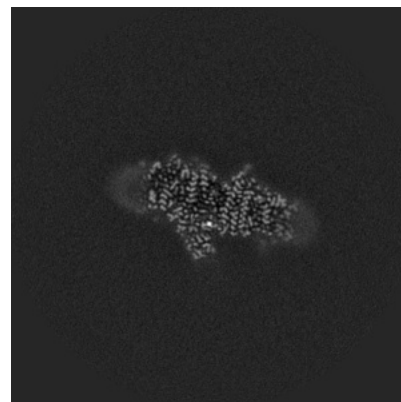
6.3.2 Raw map



X Index: 177



Y Index: 184

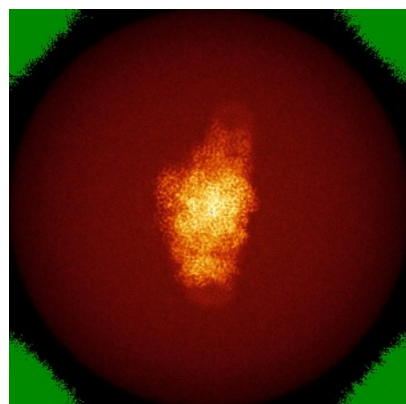


Z Index: 186

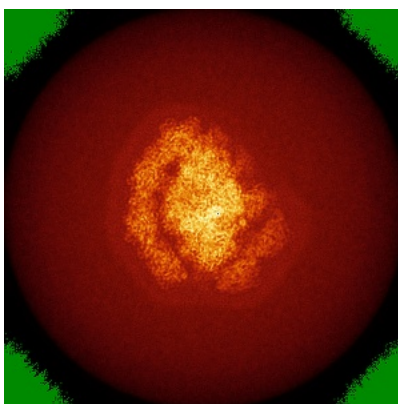
The images above show the largest variance slices of the map in three orthogonal directions.

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

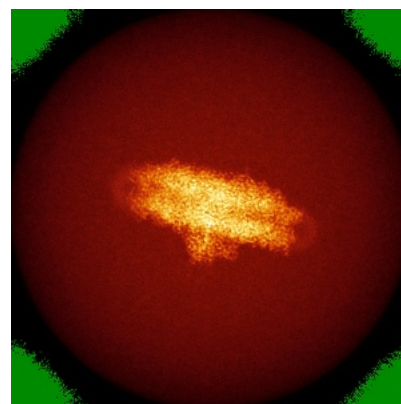
6.4.1 Primary map



X

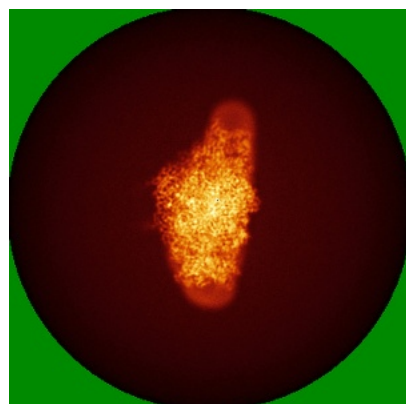


Y

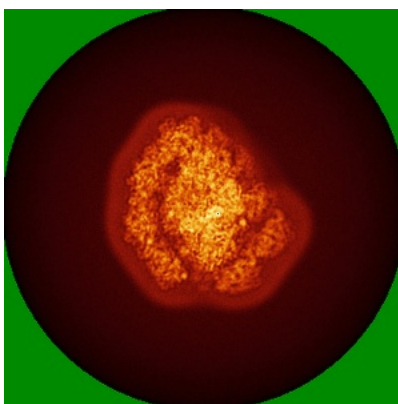


Z

6.4.2 Raw map



X



Y

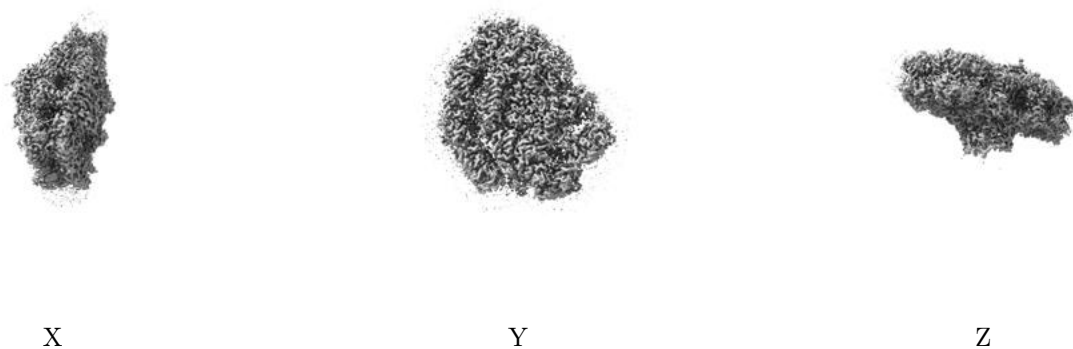


Z

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

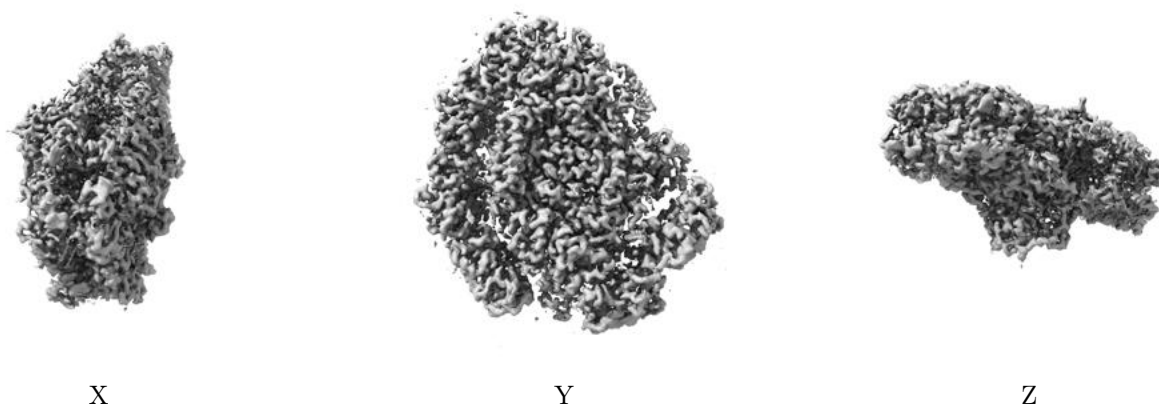
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0247. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

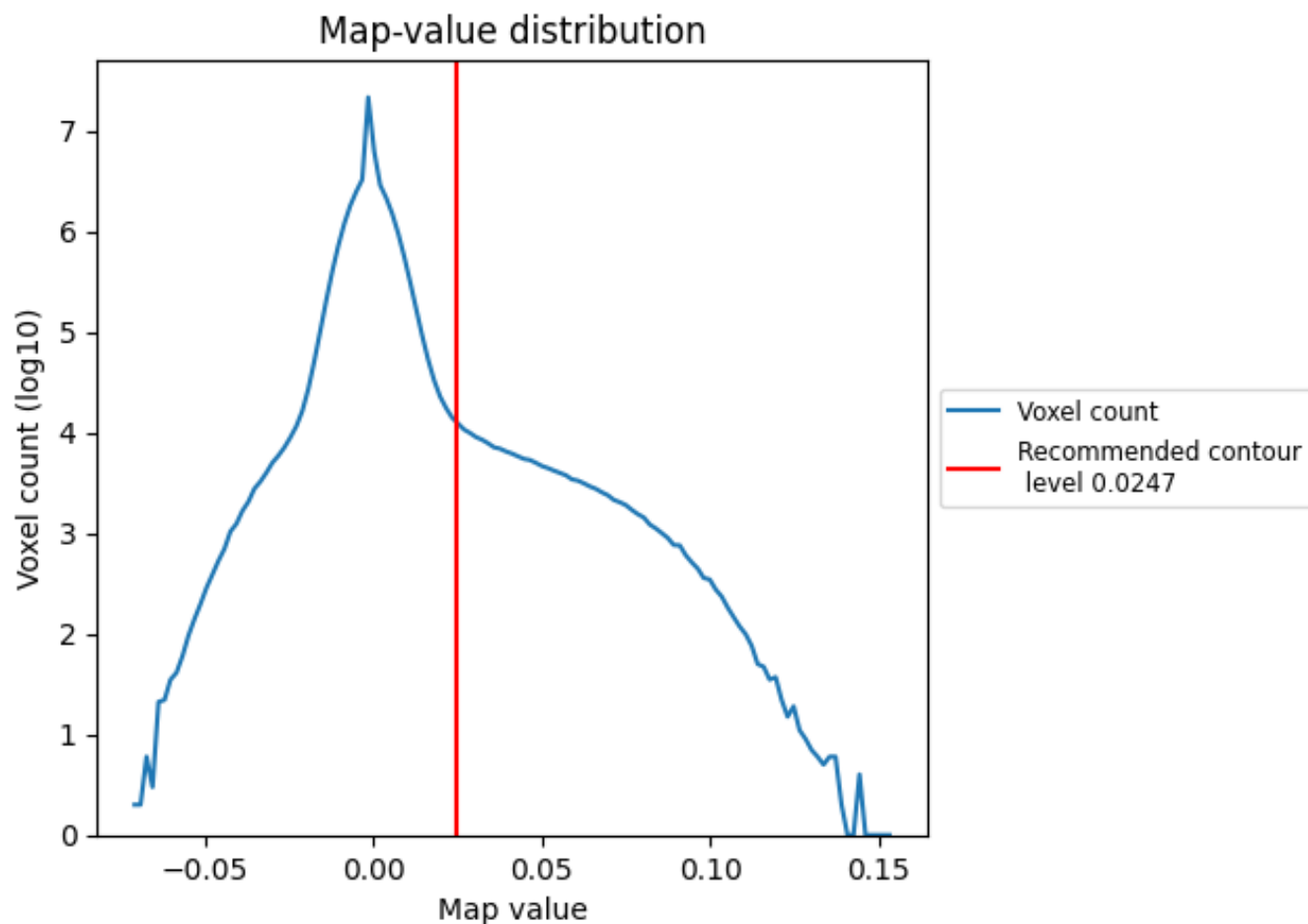
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

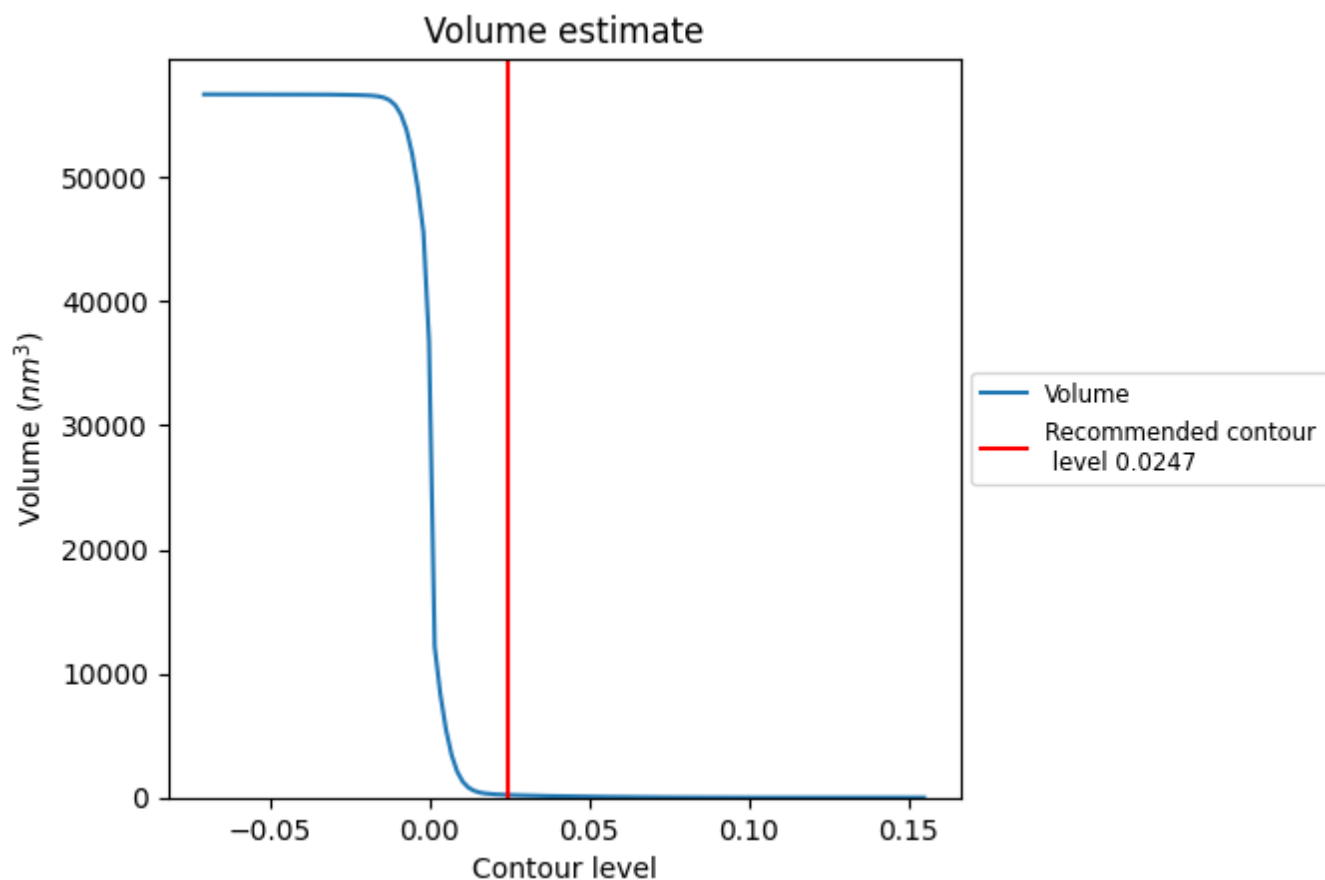
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

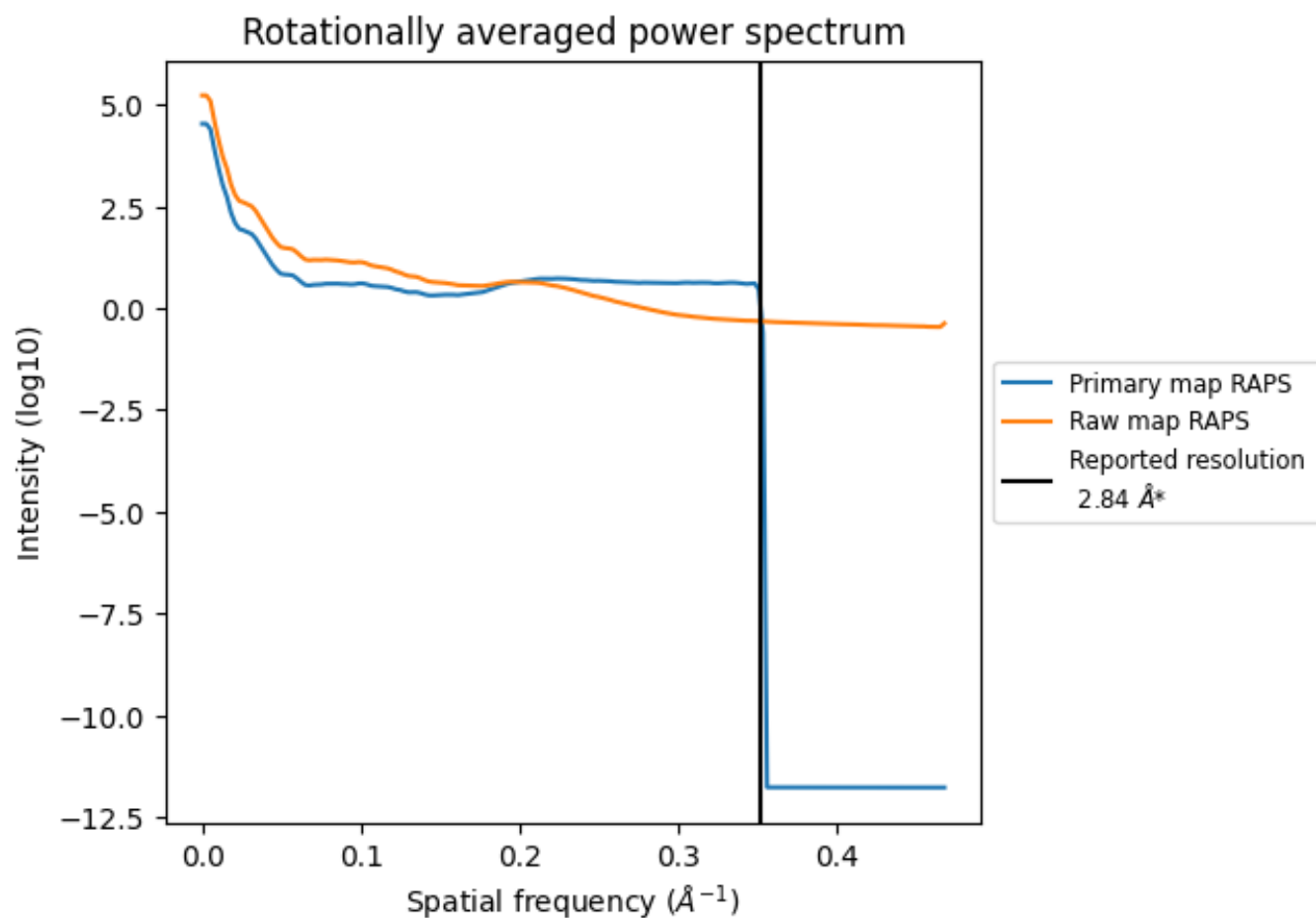
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 209 nm³; this corresponds to an approximate mass of 188 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

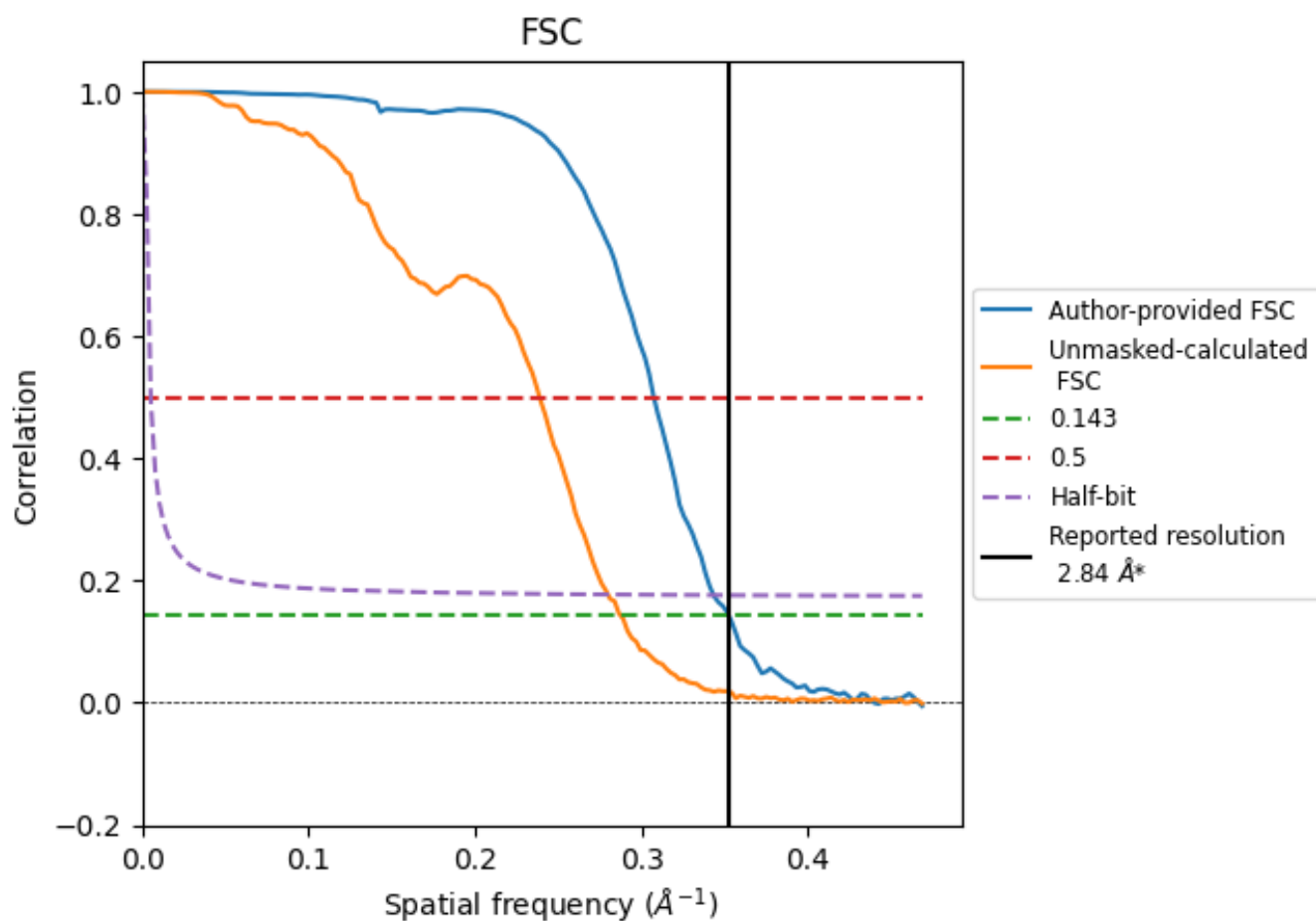


*Reported resolution corresponds to spatial frequency of 0.352 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.352 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

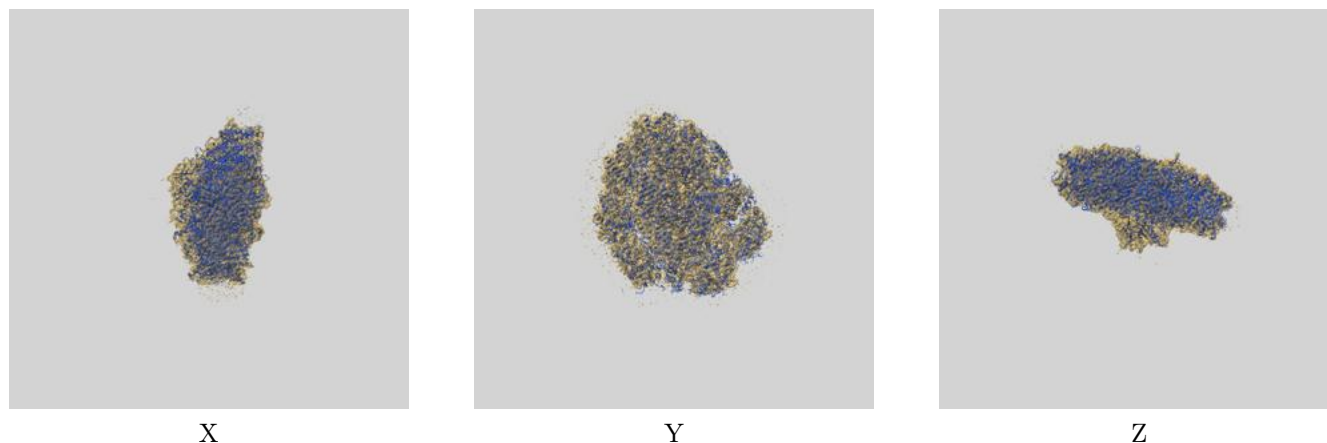
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.84	-	-
Author-provided FSC curve	2.84	3.25	2.91
Unmasked-calculated*	3.48	4.19	3.57

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.48 differs from the reported value 2.84 by more than 10 %

9 Map-model fit [i](#)

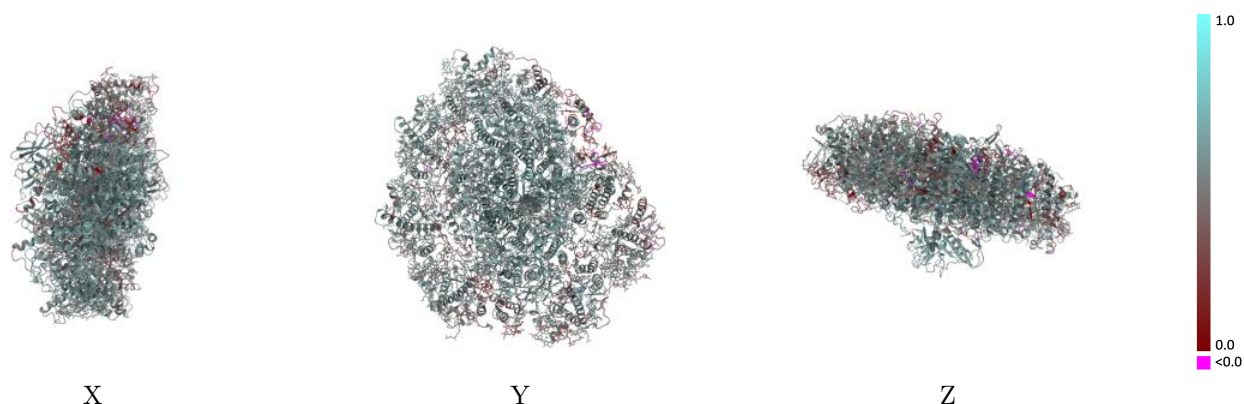
This section contains information regarding the fit between EMDB map EMD-10236 and PDB model 6SL5. Per-residue inclusion information can be found in [section 3](#) on [page 37](#).

9.1 Map-model overlay [i](#)



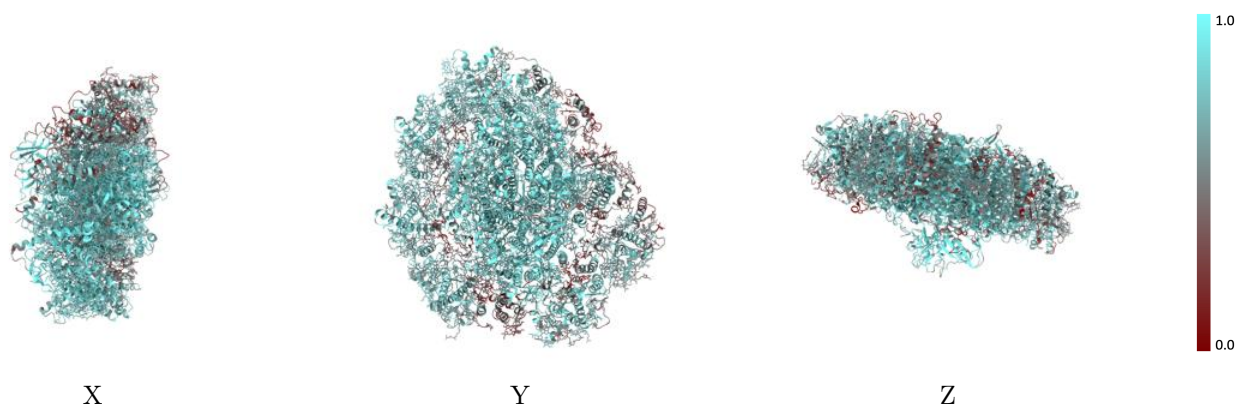
The images above show the 3D surface view of the map at the recommended contour level 0.0247 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



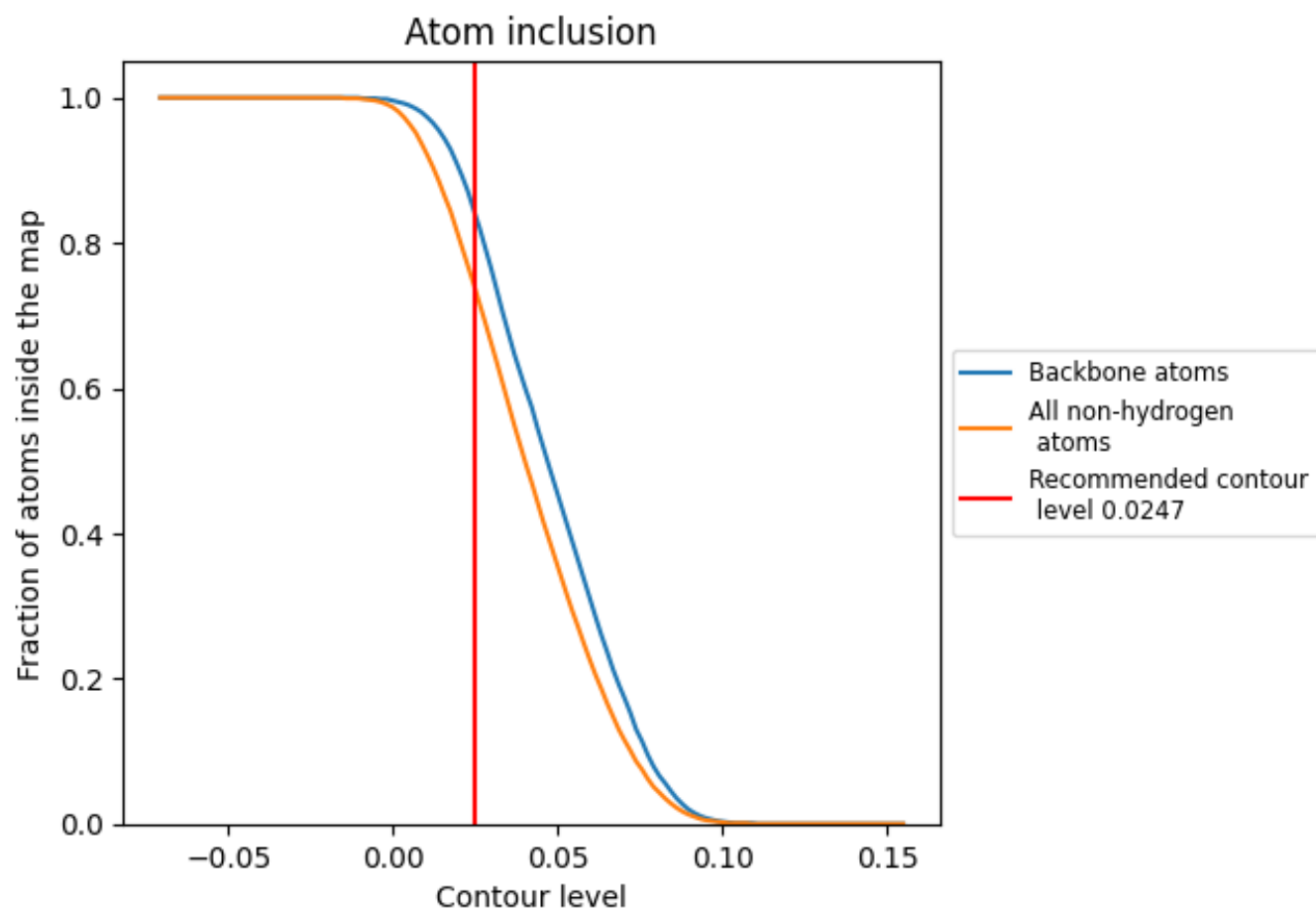
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0247).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.0247) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.5300
1	0.6550	0.4930
2	0.7430	0.5330
3	0.7530	0.5240
4	0.7140	0.4980
5	0.5470	0.4550
6	0.6290	0.4660
A	0.8750	0.5960
B	0.8640	0.5930
C	0.9150	0.6030
D	0.8050	0.5410
E	0.8020	0.5550
F	0.7420	0.5350
G	0.2700	0.3280
H	0.3330	0.3910
I	0.7370	0.5120
J	0.7720	0.5060
K	0.5120	0.4340
L	0.5980	0.4500
O	0.3310	0.3300

1.0

0.0

<0.0