



wwPDB EM Validation Summary Report ⓘ

Nov 2, 2024 – 08:17 pm GMT

PDB ID : 7BGI
EMDB ID : EMD-12180
Title : Photosystem I of a temperature sensitive mutant *Chlamydomonas reinhardtii*
Authors : Caspy, I.; Nelson, N.
Deposited on : 2021-01-07
Resolution : 2.54 Å(reported)
Based on initial model : 6JO5

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

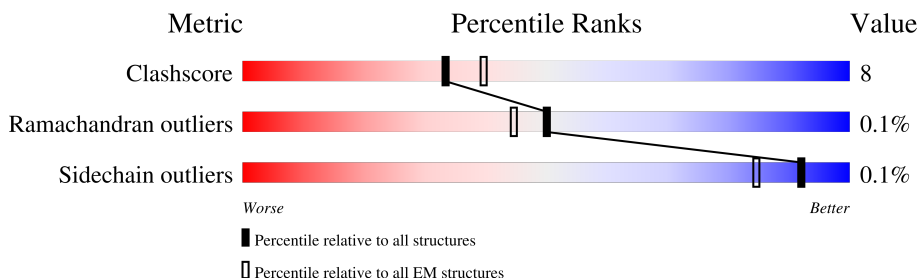
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.54 Å.

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














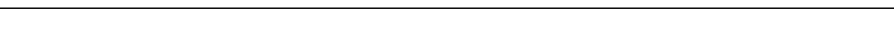
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	741	 88% 12%
2	B	733	 86% 14%
3	C	80	 95% 5%
4	D	144	 90% 10%
5	E	63	 97% .
6	F	165	 93% 7%
7	G	91	 77% . 19%
8	I	37	 86% 14%

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Mol	Chain	Length	Quality of chain
9	J	39	
10	K	84	
11	L	138	
12	1	194	
12	Z	194	
13	3	219	
14	7	213	
15	8	217	
16	4	210	
17	5	227	
18	6	229	
19	2	198	
20	9	183	

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
21	CL0	A	1011	X	-	-	-
22	CLA	1	601	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-
22	CLA	1	604	X	-	-	-
22	CLA	1	605	X	-	-	-
22	CLA	1	606	X	-	-	-
22	CLA	1	607	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	615	X	-	-	-
22	CLA	2	601	X	-	-	-
22	CLA	2	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	2	603	X	-	-	-
22	CLA	2	604	X	-	-	-
22	CLA	2	605	X	-	-	-
22	CLA	2	606	X	-	-	-
22	CLA	2	607	X	-	-	-
22	CLA	2	608	X	-	-	-
22	CLA	2	612	X	-	-	-
22	CLA	2	615	X	-	-	-
22	CLA	3	601	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	605	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	608	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	613	X	-	-	-
22	CLA	3	616	X	-	-	-
22	CLA	3	618	X	-	-	-
22	CLA	4	601	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	605	X	-	-	-
22	CLA	4	606	X	-	-	-
22	CLA	4	607	X	-	-	-
22	CLA	4	608	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	615	X	-	-	-
22	CLA	5	601	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	605	X	-	-	-
22	CLA	5	606	X	-	-	-
22	CLA	5	607	X	-	-	-
22	CLA	5	608	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	613	X	-	-	-
22	CLA	5	615	X	-	-	-
22	CLA	5	618	X	-	-	-
22	CLA	5	622	X	-	-	-
22	CLA	6	601	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	605	X	-	-	-
22	CLA	6	606	X	-	-	-
22	CLA	6	607	X	-	-	-
22	CLA	6	608	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	615	X	-	-	-
22	CLA	6	618	X	-	-	-
22	CLA	6	619	X	-	-	-
22	CLA	7	601	X	-	-	-
22	CLA	7	602	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	605	X	-	-	-
22	CLA	7	606	X	-	-	-
22	CLA	7	607	X	-	-	-
22	CLA	7	608	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	613	X	-	-	-
22	CLA	7	615	X	-	-	-
22	CLA	7	616	X	-	-	-
22	CLA	8	601	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	605	X	-	-	-
22	CLA	8	606	X	-	-	-
22	CLA	8	607	X	-	-	-
22	CLA	8	608	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	8	615	X	-	-	-
22	CLA	9	601	X	-	-	-
22	CLA	9	602	X	-	-	-
22	CLA	9	603	X	-	-	-
22	CLA	9	604	X	-	-	-
22	CLA	9	606	X	-	-	-
22	CLA	9	607	X	-	-	-
22	CLA	9	608	X	-	-	-
22	CLA	9	609	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	A	1012	X	-	-	-
22	CLA	A	1013	X	-	-	-
22	CLA	A	1101	X	-	-	-
22	CLA	A	1102	X	-	-	-
22	CLA	A	1103	X	-	-	-
22	CLA	A	1104	X	-	-	-
22	CLA	A	1105	X	-	-	-
22	CLA	A	1106	X	-	-	-
22	CLA	A	1107	X	-	-	-
22	CLA	A	1108	X	-	-	-
22	CLA	A	1109	X	-	-	-
22	CLA	A	1110	X	-	-	-
22	CLA	A	1111	X	-	-	-
22	CLA	A	1112	X	-	-	-
22	CLA	A	1113	X	-	-	-
22	CLA	A	1114	X	-	-	-
22	CLA	A	1115	X	-	-	-
22	CLA	A	1116	X	-	-	-
22	CLA	A	1117	X	-	-	-
22	CLA	A	1118	X	-	-	-
22	CLA	A	1119	X	-	-	-
22	CLA	A	1120	X	-	-	-
22	CLA	A	1121	X	-	-	-
22	CLA	A	1122	X	-	-	-
22	CLA	A	1123	X	-	-	-
22	CLA	A	1124	X	-	-	-
22	CLA	A	1125	X	-	-	-
22	CLA	A	1126	X	-	-	-
22	CLA	A	1127	X	-	-	-
22	CLA	A	1128	X	-	-	-
22	CLA	A	1129	X	-	-	-
22	CLA	A	1130	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	1131	X	-	-	-
22	CLA	A	1132	X	-	-	-
22	CLA	A	1133	X	-	-	-
22	CLA	A	1134	X	-	-	-
22	CLA	A	1135	X	-	-	-
22	CLA	A	1136	X	-	-	-
22	CLA	A	1137	X	-	-	-
22	CLA	A	1138	X	-	-	-
22	CLA	A	1139	X	-	-	-
22	CLA	A	1140	X	-	-	-
22	CLA	A	1141	X	-	-	-
22	CLA	B	1021	X	-	-	-
22	CLA	B	1022	X	-	-	-
22	CLA	B	1023	X	-	-	-
22	CLA	B	1201	X	-	-	-
22	CLA	B	1202	X	-	-	-
22	CLA	B	1203	X	-	-	-
22	CLA	B	1204	X	-	-	-
22	CLA	B	1205	X	-	-	-
22	CLA	B	1206	X	-	-	-
22	CLA	B	1207	X	-	-	-
22	CLA	B	1208	X	-	-	-
22	CLA	B	1209	X	-	-	-
22	CLA	B	1210	X	-	-	-
22	CLA	B	1211	X	-	-	-
22	CLA	B	1212	X	-	-	-
22	CLA	B	1213	X	-	-	-
22	CLA	B	1214	X	-	-	-
22	CLA	B	1215	X	-	-	-
22	CLA	B	1216	X	-	-	-
22	CLA	B	1217	X	-	-	-
22	CLA	B	1218	X	-	-	-
22	CLA	B	1219	X	-	-	-
22	CLA	B	1220	X	-	-	-
22	CLA	B	1221	X	-	-	-
22	CLA	B	1222	X	-	-	-
22	CLA	B	1223	X	-	-	-
22	CLA	B	1224	X	-	-	-
22	CLA	B	1225	X	-	-	-
22	CLA	B	1226	X	-	-	-
22	CLA	B	1227	X	-	-	-
22	CLA	B	1228	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	1229	X	-	-	-
22	CLA	B	1230	X	-	-	-
22	CLA	B	1231	X	-	-	-
22	CLA	B	1232	X	-	-	-
22	CLA	B	1234	X	-	-	-
22	CLA	B	1235	X	-	-	-
22	CLA	B	1236	X	-	-	-
22	CLA	B	1237	X	-	-	-
22	CLA	B	1238	X	-	-	-
22	CLA	B	1239	X	-	-	-
22	CLA	B	1240	X	-	-	-
22	CLA	B	1241	X	-	-	-
22	CLA	F	1301	X	-	-	-
22	CLA	F	1302	X	-	-	-
22	CLA	G	1601	X	-	-	-
22	CLA	G	1602	X	-	-	-
22	CLA	J	1901	X	-	-	-
22	CLA	K	1401	X	-	-	-
22	CLA	K	1402	X	-	-	-
22	CLA	K	1403	X	-	-	-
22	CLA	K	1404	X	-	-	-
22	CLA	L	1502	X	-	-	-
22	CLA	L	1503	X	-	-	-
22	CLA	Z	601	X	-	-	-
22	CLA	Z	602	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	605	X	-	-	-
22	CLA	Z	606	X	-	-	-
22	CLA	Z	607	X	-	-	-
22	CLA	Z	608	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-
22	CLA	Z	615	X	-	-	-
36	RRX	F	4001	X	-	-	-
37	C7Z	1	503	X	-	-	-
37	C7Z	5	505	X	-	-	-
37	C7Z	J	4002	X	-	-	-
39	LUT	2	501	X	-	-	-
39	LUT	2	503	X	-	-	-
40	CHL	1	609	X	-	-	-
40	CHL	1	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
40	CHL	2	609	X	-	-	-
40	CHL	2	610	X	-	-	-
40	CHL	2	613	X	-	-	-
40	CHL	3	611	X	-	-	-
40	CHL	4	610	X	-	-	-
40	CHL	4	611	X	-	-	-
40	CHL	4	613	X	-	-	-
40	CHL	4	617	X	-	-	-
40	CHL	5	610	X	-	-	-
40	CHL	5	611	X	-	-	-
40	CHL	5	617	X	-	-	-
40	CHL	6	610	X	-	-	-
40	CHL	6	611	X	-	-	-
40	CHL	6	613	X	-	-	-
40	CHL	6	617	X	-	-	-
40	CHL	7	610	X	-	-	-
40	CHL	8	610	X	-	-	-
40	CHL	8	613	X	-	-	-
40	CHL	9	610	X	-	-	-
40	CHL	9	613	X	-	-	-
40	CHL	Z	609	X	-	-	-
40	CHL	Z	610	X	-	-	-
40	CHL	Z	613	X	-	-	-
42	QTB	Z	504	X	-	-	-

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 52213 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	741	Total	C	N	O	S	0	0
			5820	3805	993	1000	22		

- 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
			5825	3825	977	1005	18		

- 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
			601	369	103	117	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1135	725	201	202	7		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			497	316	87	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	74	Total	C	N	O	0	0
			550	354	94	102		

- Molecule 8 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			282	195	39	47	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			321	219	45	56	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			571	362	98	109	2		

- Molecule 11 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	126	Total	C	N	O	S	0	0
			914	595	148	168	3		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
12	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	219	Total	C	N	O	S	0	0
			1674	1092	270	304	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	213	Total	C	N	O	S	0	0
			1650	1072	274	298	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1650	1073	280	293	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	210	Total	C	N	O	S	0	0
			1628	1068	262	293	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	227	Total	C	N	O	S	0	0
			1775	1154	297	316	8		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1766	1164	292	304	6		

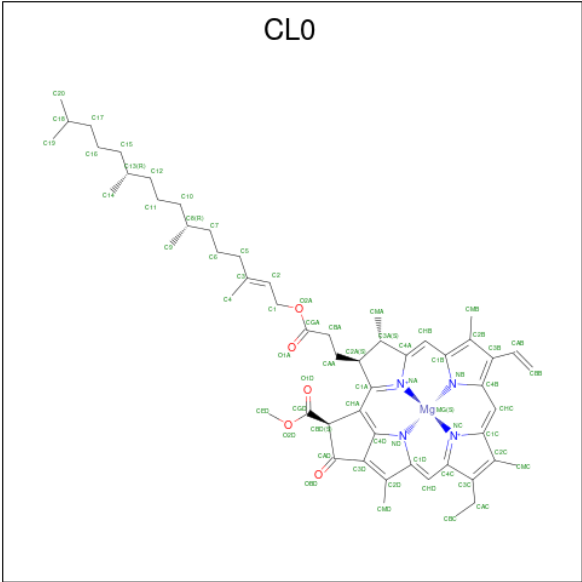
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	2	198	Total	C	N	O	S	0	0
			1518	983	249	276	10		

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

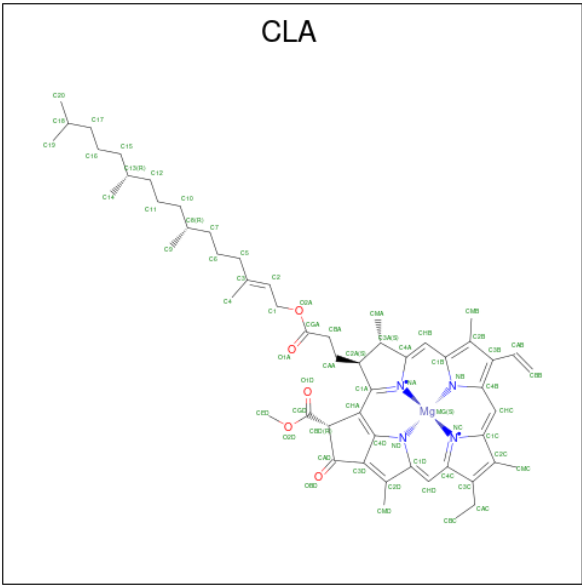
Mol	Chain	Residues	Atoms					AltConf	Trace
20	9	183	Total	C	N	O	S	0	0
			1406	910	235	254	7		

- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 22 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 59	C 49	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	F	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	K	1	Total 49	C 39	Mg 1	N 4	O 5	0
22	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	1	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
22	Z	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	7	1	Total 58	C 48	Mg 1	N 4	O 5	0
22	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	8	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	8	1	Total 62	C 52	Mg 1	N 4	O 5	0
22	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	4	1	Total 41	C 33	Mg 1	N 4	O 3	0
22	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	5	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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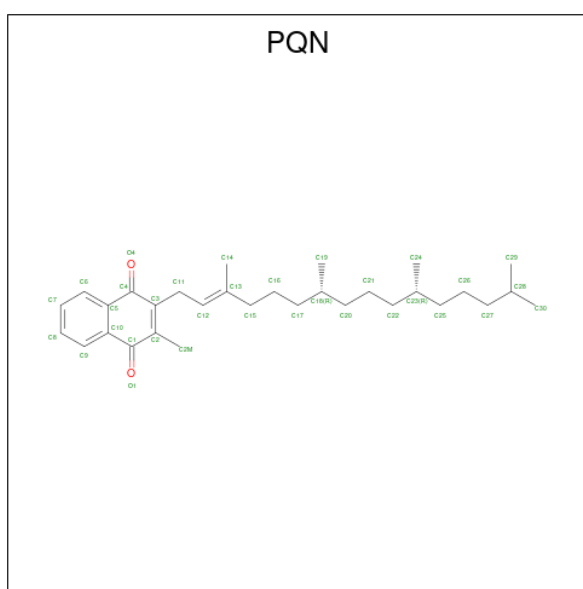
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	6	1	Total 61	C 51	Mg 1	N 4	O 5	0
22	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	2	1	Total 56	C 46	Mg 1	N 4	O 5	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
22	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
22	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	9	1	Total 45	C 35	Mg 1	N 4	O 5	0
22	9	1	Total 60	C 50	Mg 1	N 4	O 5	0
22	9	1	Total 65	C 55	Mg 1	N 4	O 5	0
22	9	1	Total 55	C 45	Mg 1	N 4	O 5	0
22	9	1	Total 50	C 40	Mg 1	N 4	O 5	0

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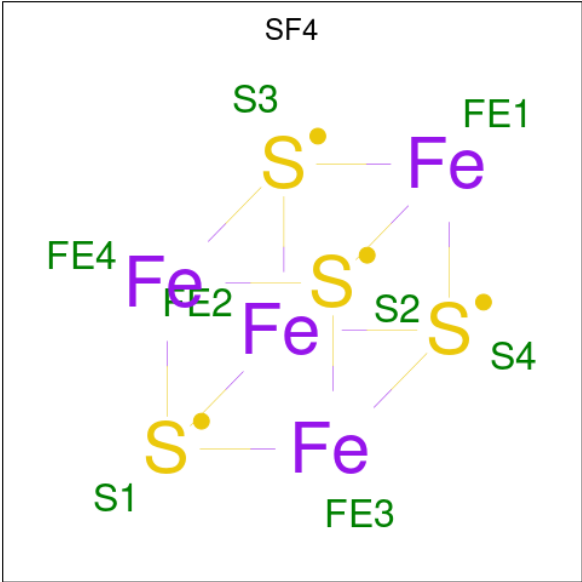
Mol	Chain	Residues	Atoms					AltConf
22	9	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
22	9	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 23 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



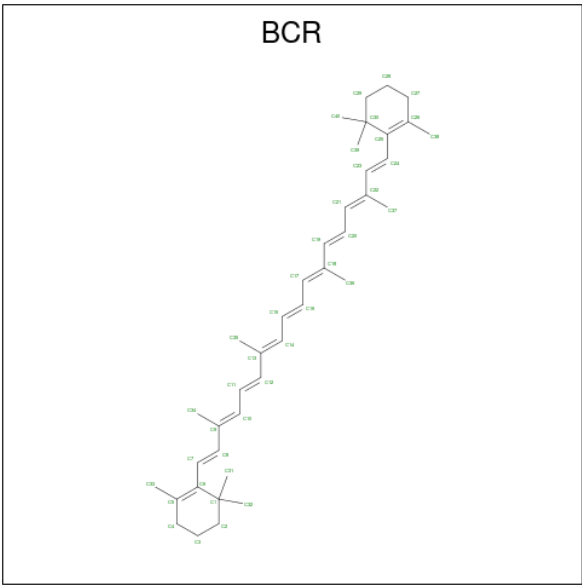
Mol	Chain	Residues	Atoms			AltConf
23	A	1	Total	C	O	0
			33	31	2	
23	B	1	Total	C	O	0
			33	31	2	

- Molecule 24 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



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

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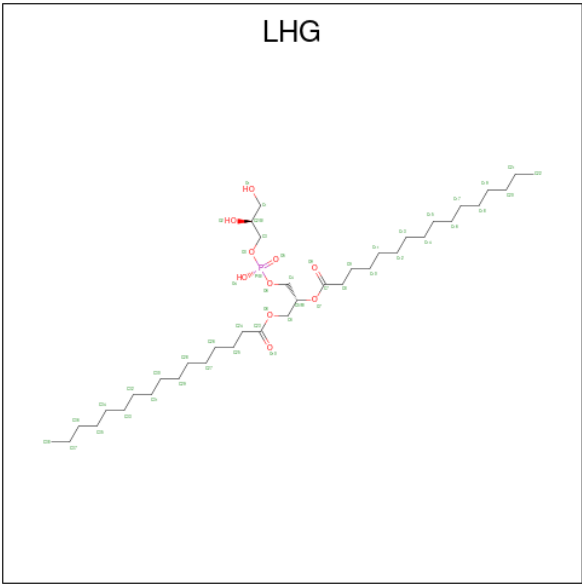
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	G	1	Total C 40 40	0
25	I	1	Total C 40 40	0
25	J	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	K	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	L	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0
25	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
25	3	1	Total	C	0
			40	40	
25	7	1	Total	C	0
			40	40	
25	7	1	Total	C	0
			40	40	
25	8	1	Total	C	0
			40	40	
25	4	1	Total	C	0
			40	40	
25	5	1	Total	C	0
			40	40	
25	5	1	Total	C	0
			40	40	
25	6	1	Total	C	0
			40	40	
25	6	1	Total	C	0
			40	40	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	P	0
			35	24	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
26	B	1	Total	C	O	P	0
			23	12	10	1	
26	B	1	Total	C	O	P	0
			20	9	10	1	
26	B	1	Total	C	O	P	0
			33	22	10	1	
26	1	1	Total	C	O	P	0
			43	32	10	1	
26	Z	1	Total	C	O	P	0
			43	32	10	1	
26	3	1	Total	C	O	P	0
			20	9	10	1	
26	7	1	Total	C	O	P	0
			37	26	10	1	
26	8	1	Total	C	O	P	0
			38	27	10	1	
26	4	1	Total	C	O	P	0
			49	38	10	1	
26	4	1	Total	C	O	P	0
			32	21	10	1	
26	5	1	Total	C	O	P	0
			37	26	10	1	
26	6	1	Total	C	O	P	0
			49	38	10	1	
26	2	1	Total	C	O	P	0
			34	23	10	1	
26	9	1	Total	C	O	P	0
			33	22	10	1	

- Molecule 27 is (2R)-2-hydroxy-3-(phosphonoxy)propyl (9E)-octadec-9-enoate (three-letter code: NKP) (formula: C₂₁H₄₁O₇P).

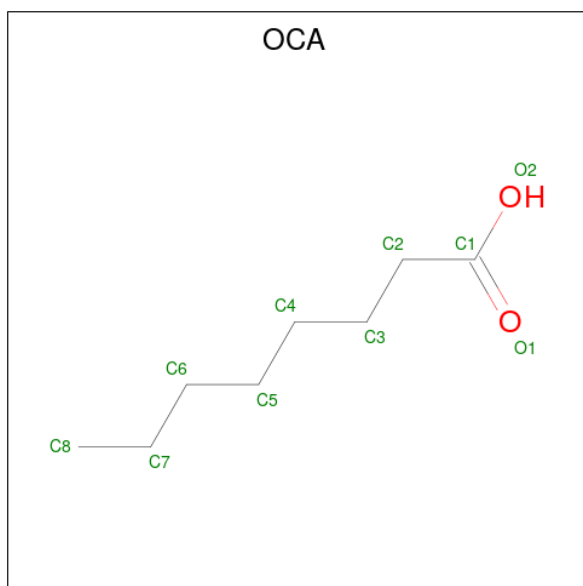


- Molecule 28 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



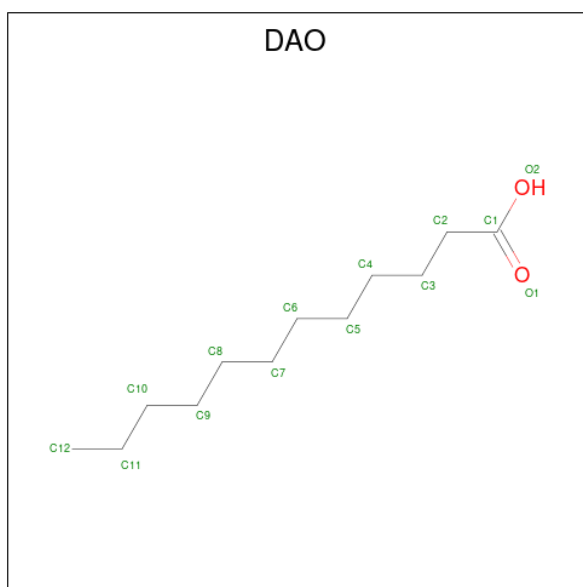
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			35	24	11	
28	B	1	Total	C	O	0
			35	24	11	
28	B	1	Total	C	O	0
			35	24	11	
28	F	1	Total	C	O	0
			35	24	11	
28	1	1	Total	C	O	0
			35	24	11	
28	8	1	Total	C	O	0
			35	24	11	
28	4	1	Total	C	O	0
			35	24	11	
28	9	1	Total	C	O	0
			35	24	11	

- Molecule 29 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula: $C_8H_{16}O_2$).



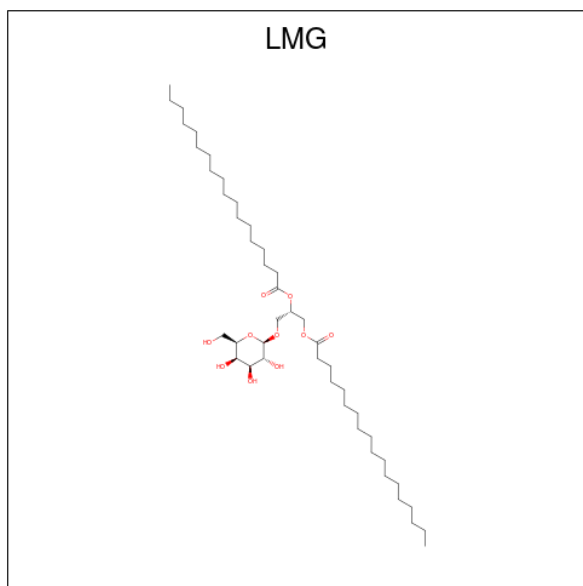
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			10	8	2	

- Molecule 30 is LAURIC ACID (three-letter code: DAO) (formula: $C_{12}H_{24}O_2$).



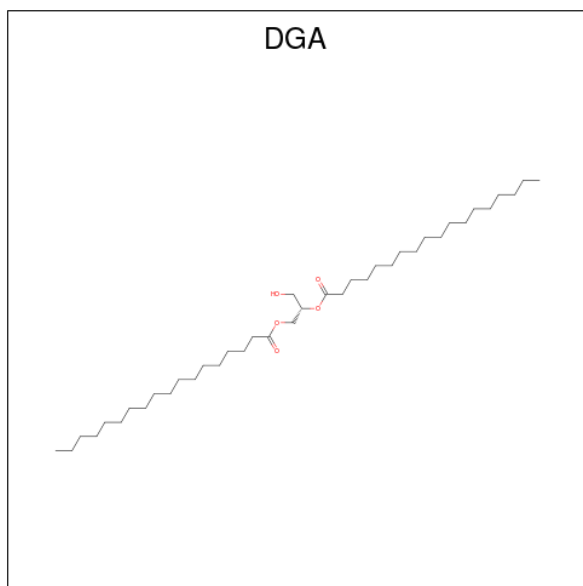
Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			14	12	2	

- Molecule 31 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



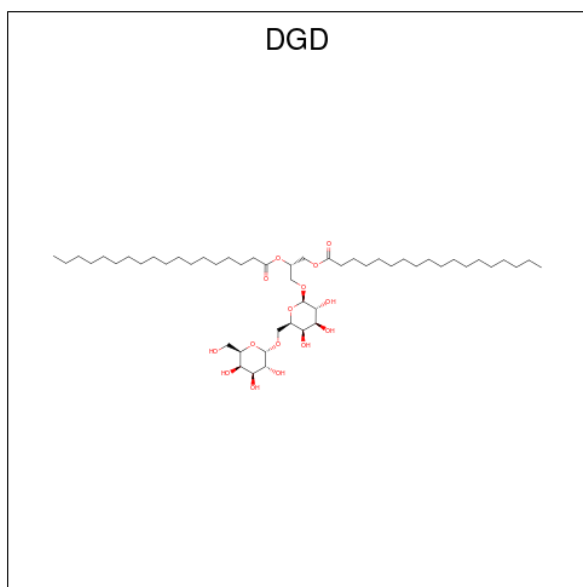
Mol	Chain	Residues	Atoms			AltConf
31	A	1	Total	C	O	0
			29	19	10	
31	J	1	Total	C	O	0
			35	25	10	

- Molecule 32 is DIACYL GLYCEROL (three-letter code: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
32	A	1	Total	C	O	0
			44	39	5	
32	9	1	Total	C	O	0
			39	34	5	

- Molecule 33 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

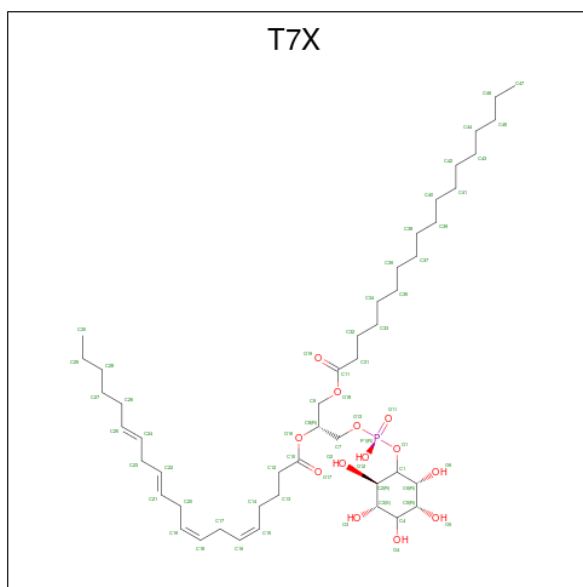


Mol	Chain	Residues	Atoms			AltConf
33	B	1	Total	C	O	0
			66	51	15	

- Molecule 34 is CALCIUM ION (three-letter code: CA) (formula: Ca).

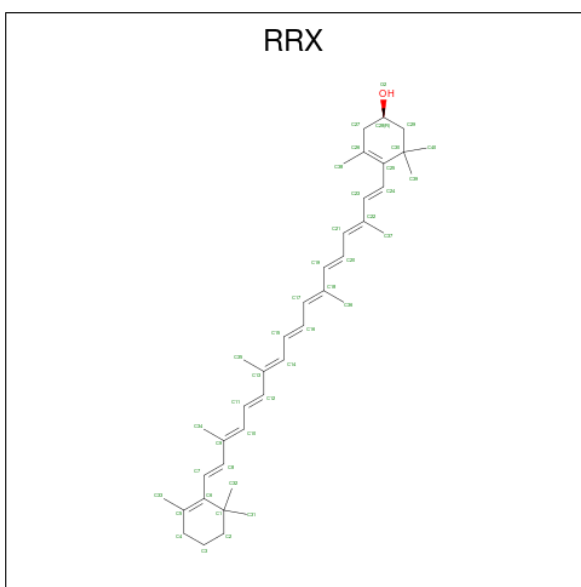
Mol	Chain	Residues	Atoms			AltConf
34	B	1	Total	Ca		0
			1	1		

- Molecule 35 is Phosphatidylinositol (three-letter code: T7X) (formula: C₄₇H₈₃O₁₃P).



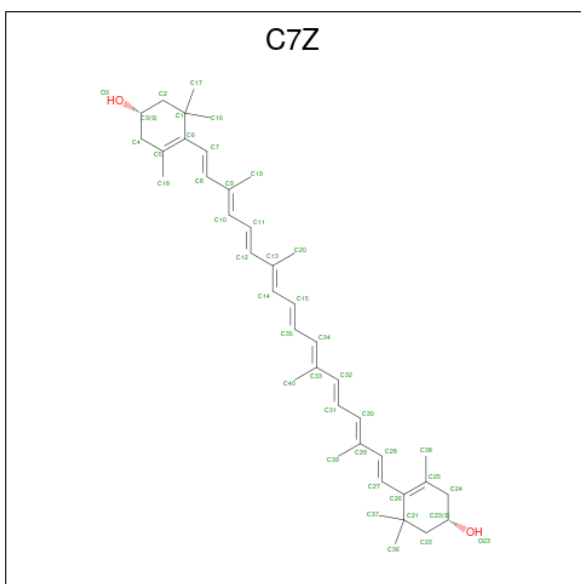
Mol	Chain	Residues	Atoms				AltConf
35	B	1	Total	C	O	P	0
			49	35	13	1	

- Molecule 36 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C₄₀H₅₆O).



Mol	Chain	Residues	Atoms			AltConf
36	F	1	Total	C	O	0
			41	40	1	

- Molecule 37 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: C₄₀H₅₆O₂).



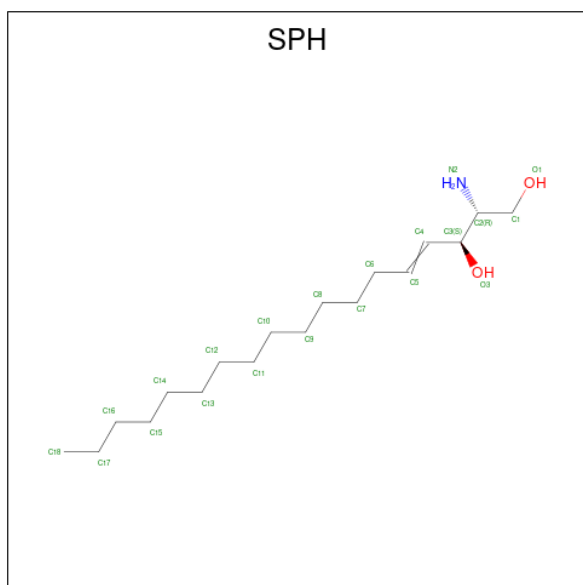
Mol	Chain	Residues	Atoms			AltConf
37	J	1	Total	C	O	0
			42	40	2	

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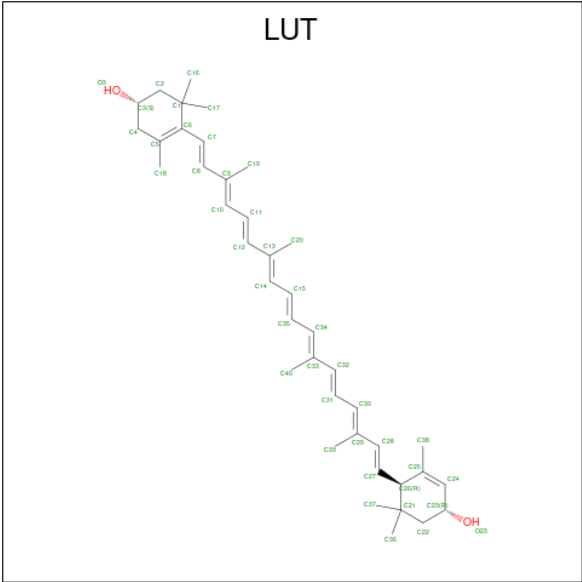
Mol	Chain	Residues	Atoms			AltConf
37	1	1	Total	C	O	0
			42	40	2	
37	5	1	Total	C	O	0
			42	40	2	

- Molecule 38 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
38	K	1	Total	C	N	O	0
			21	18	1	2	
38	7	1	Total	C	N	O	0
			21	18	1	2	
38	7	1	Total	C	N	O	0
			21	18	1	2	

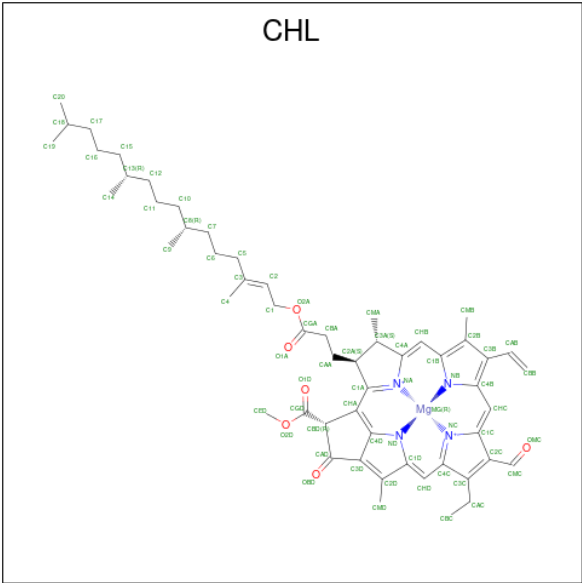
- Molecule 39 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



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Mol	Chain	Residues	Atoms			AltConf
39	5	1	Total	C	O	0
			42	40	2	
39	6	1	Total	C	O	0
			42	40	2	
39	6	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	2	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	
39	9	1	Total	C	O	0
			42	40	2	

- Molecule 40 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
40	1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
40	1	1	Total	C	Mg	N	O	0
			58	47	1	4	6	
40	Z	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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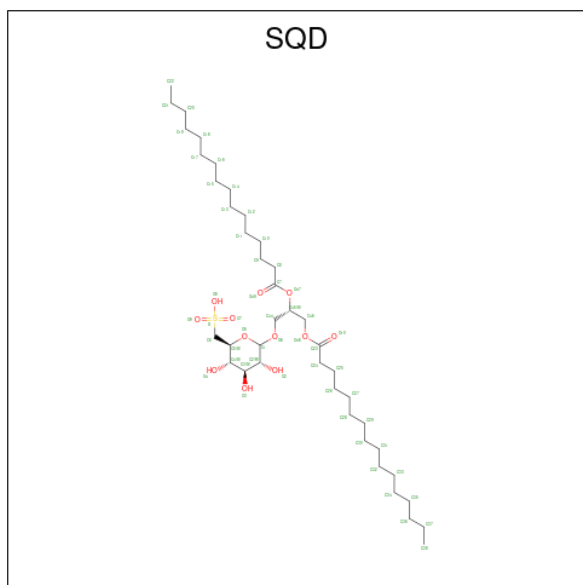
Mol	Chain	Residues	Atoms					AltConf
40	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
40	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
40	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
40	7	1	Total 54	C 43	Mg 1	N 4	O 6	0
40	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
40	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
40	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
40	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
40	4	1	Total 56	C 45	Mg 1	N 4	O 6	0
40	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
40	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
40	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
40	5	1	Total 43	C 34	Mg 1	N 4	O 4	0
40	6	1	Total 56	C 45	Mg 1	N 4	O 6	0
40	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
40	6	1	Total 56	C 45	Mg 1	N 4	O 6	0
40	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
40	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
40	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
40	2	1	Total 51	C 40	Mg 1	N 4	O 6	0
40	9	1	Total 66	C 55	Mg 1	N 4	O 6	0

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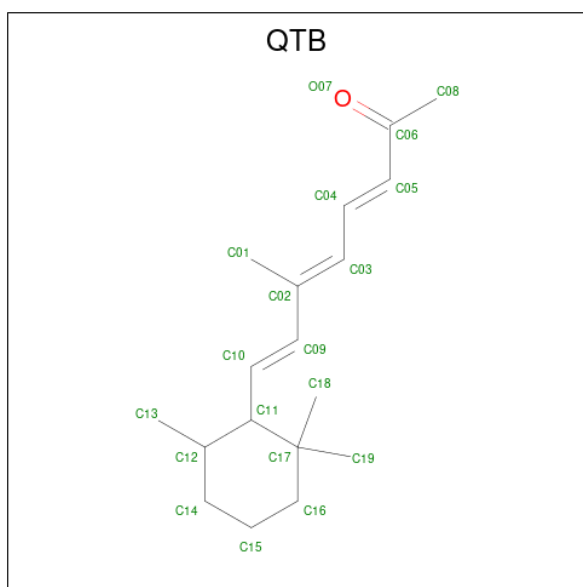
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
40	9	1	42	33	1	4	4	0

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



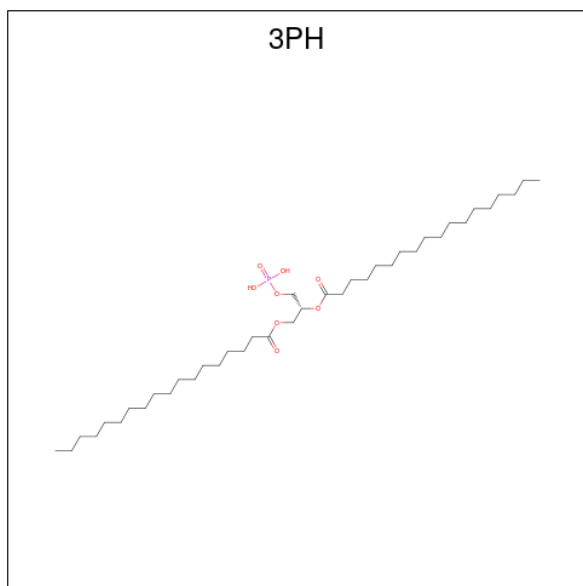
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
41	1	1	48	35	12	1	0
41	2	1	43	30	12	1	0

- Molecule 42 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (three-letter code: QTB) (formula: $C_{18}H_{28}O$).



Mol	Chain	Residues	Atoms			AltConf
42	Z	1	Total	C	O	0
			19	18	1	

- Molecule 43 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



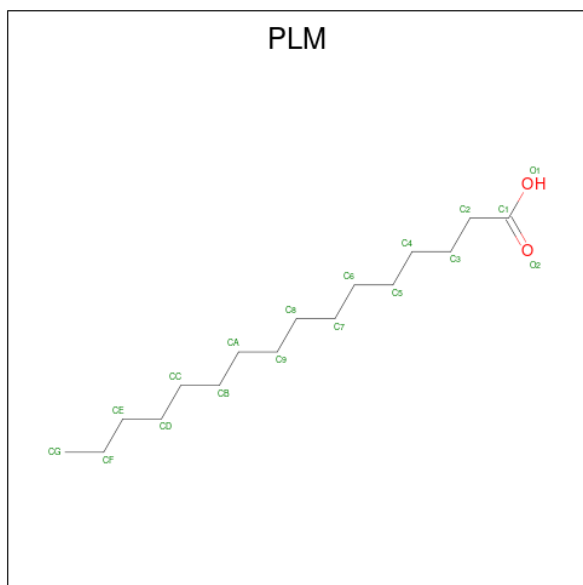
Mol	Chain	Residues	Atoms				AltConf
43	7	1	Total	C	O	P	0
			39	30	8	1	
43	8	1	Total	C	O	P	0
			30	21	8	1	

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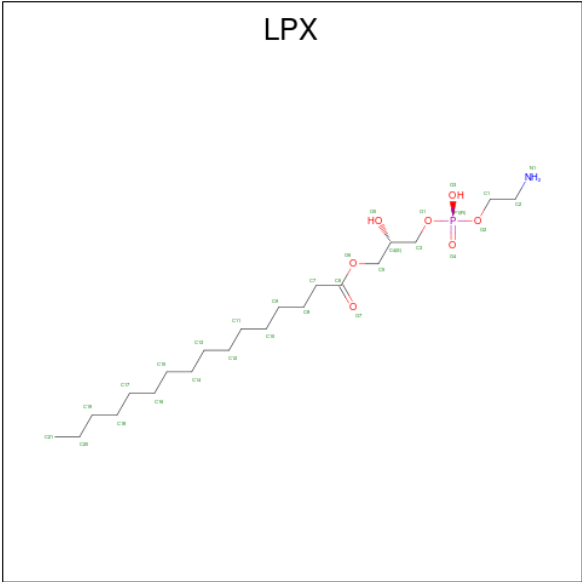
Mol	Chain	Residues	Atoms				AltConf
43	5	1	Total	C	O	P	0
			23	14	8	1	
43	6	1	Total	C	O	P	0
			29	20	8	1	
43	2	1	Total	C	O	P	0
			27	18	8	1	

- Molecule 44 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			AltConf
44	7	1	Total	C	O	0
			18	16	2	

- Molecule 45 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
45	8	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 46 is water.

Mol	Chain	Residues	Atoms		AltConf
46	A	2	Total	O	0
			2	2	
46	A	15	Total	O	0
			15	15	
46	A	2	Total	O	0
			2	2	
46	A	6	Total	O	0
			6	6	
46	A	9	Total	O	0
			9	9	
46	A	2	Total	O	0
			2	2	
46	A	7	Total	O	0
			7	7	
46	A	18	Total	O	0
			18	18	
46	A	8	Total	O	0
			8	8	
46	A	14	Total	O	0
			14	14	
46	A	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	A	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	1	Total O 1 1	0
46	B	2	Total O 2 2	0
46	B	12	Total O 12 12	0
46	B	10	Total O 10 10	0
46	B	16	Total O 16 16	0
46	B	2	Total O 2 2	0
46	B	2	Total O 2 2	0
46	B	1	Total O 1 1	0
46	B	28	Total O 28 28	0
46	B	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
46	C	1	Total 1	O 1	0
46	C	1	Total 1	O 1	0
46	C	1	Total 1	O 1	0
46	C	1	Total 1	O 1	0
46	C	1	Total 1	O 1	0
46	C	12	Total 12	O 12	0
46	C	1	Total 1	O 1	0
46	C	1	Total 1	O 1	0
46	D	1	Total 1	O 1	0
46	D	1	Total 1	O 1	0
46	D	1	Total 1	O 1	0
46	D	2	Total 2	O 2	0
46	D	1	Total 1	O 1	0
46	D	2	Total 2	O 2	0
46	D	1	Total 1	O 1	0
46	D	2	Total 2	O 2	0
46	D	1	Total 1	O 1	0
46	E	1	Total 1	O 1	0
46	E	4	Total 4	O 4	0
46	E	1	Total 1	O 1	0
46	E	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms	AltConf
46	F	1	Total O 1 1	0
46	F	1	Total O 1 1	0
46	F	2	Total O 2 2	0
46	F	8	Total O 8 8	0
46	F	1	Total O 1 1	0
46	F	1	Total O 1 1	0
46	J	2	Total O 2 2	0
46	J	1	Total O 1 1	0
46	K	2	Total O 2 2	0
46	L	1	Total O 1 1	0
46	L	1	Total O 1 1	0
46	L	1	Total O 1 1	0
46	L	2	Total O 2 2	0
46	1	16	Total O 16 16	0
46	Z	1	Total O 1 1	0
46	Z	7	Total O 7 7	0
46	3	17	Total O 17 17	0
46	7	18	Total O 18 18	0
46	8	1	Total O 1 1	0
46	8	15	Total O 15 15	0
46	4	7	Total O 7 7	0

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Mol	Chain	Residues	Atoms		AltConf
46	5	9	Total 9	O 9	0
46	6	8	Total 8	O 8	0
46	2	4	Total 4	O 4	0
46	9	2	Total 2	O 2	0

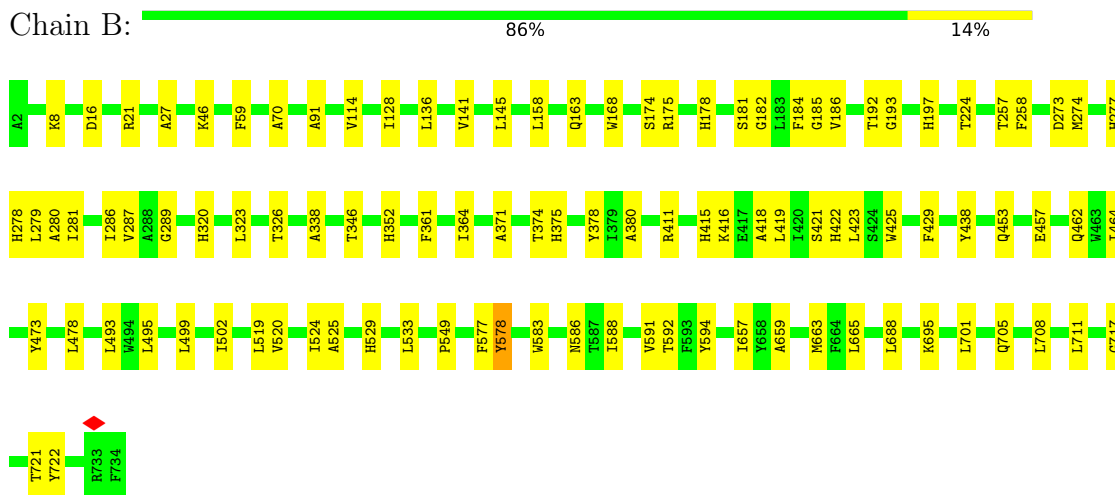
3 Residue-property plots

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

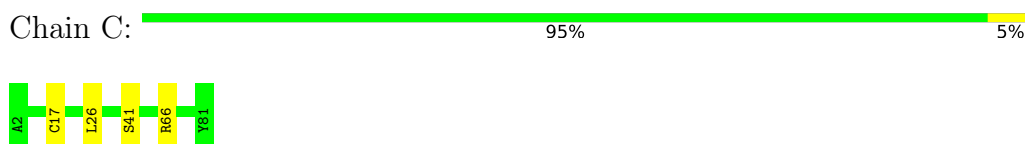
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



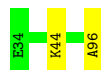
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:  90% 10%



- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

Chain E:  97% .




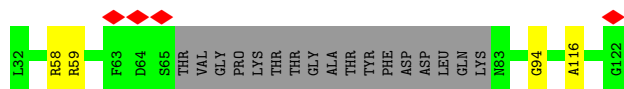
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain F:  93% 7%




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

Chain G:  77% . 19%




- Molecule 8: Photosystem I reaction center subunit VIII

Chain I:  86% 14%




- Molecule 9: Photosystem I reaction center subunit IX

Chain J:  90% 10%




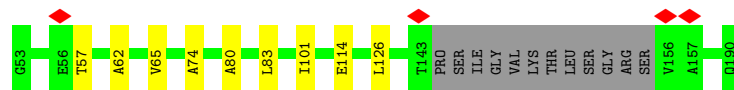
- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  85% 15%




- Molecule 11: PSI subunit V

Chain L:  85% 7% 9%

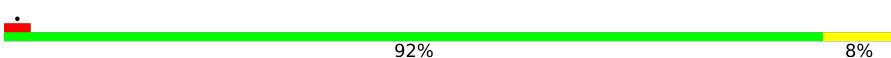


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:  88% 12%



- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:  92% 8%




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

Chain 3:  91% 9%




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

Chain 7:  90% 10%




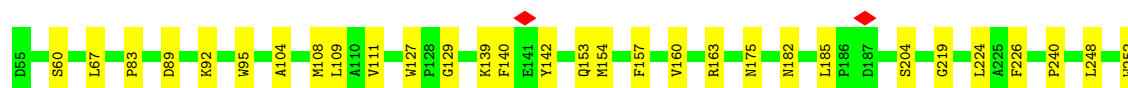
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

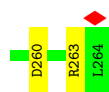
Chain 8:  88% 12%



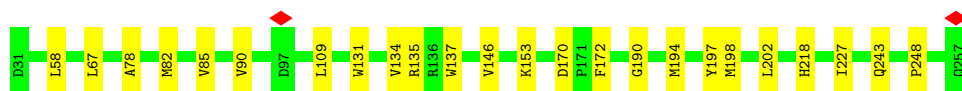
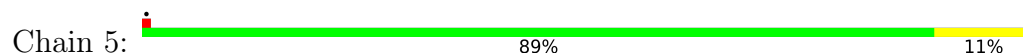
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

Chain 4:  85% 15%





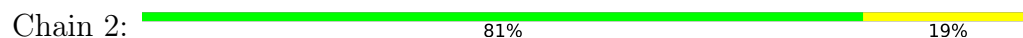
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	103082	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 ($e^-/\text{\AA}^2$)	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.125	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	264.64, 264.64, 264.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.827, 0.827, 0.827	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCA, BCR, T7X, LMG, SPH, PQN, C7Z, DGD, QTB, RRX, PLM, CLA, DGA, SQD, CL0, LUT, 3PH, LMT, CA, SF4, DAO, NKP, LPX, SNC, LHG, CHL

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	0.31	0/6016	0.51	0/8201
2	B	0.33	1/6037 (0.0%)	0.53	0/8242
3	C	0.26	0/611	0.56	0/826
4	D	0.28	0/1154	0.56	0/1556
5	E	0.28	0/507	0.50	0/689
6	F	0.29	0/1292	0.51	0/1747
7	G	0.28	0/561	0.47	0/760
8	I	0.32	0/294	0.55	0/406
9	J	0.29	0/332	0.46	0/454
10	K	0.26	0/576	0.46	0/779
11	L	0.29	0/935	0.50	0/1277
12	1	0.28	0/1491	0.45	0/2028
12	Z	0.27	0/1491	0.44	0/2028
13	3	0.31	0/1722	0.51	0/2336
14	7	0.29	0/1702	0.49	0/2310
15	8	0.28	0/1701	0.45	0/2315
16	4	0.28	0/1683	0.47	0/2296
17	5	0.28	0/1830	0.47	0/2492
18	6	0.27	0/1828	0.48	0/2497
19	2	0.28	0/1556	0.52	0/2109
20	9	0.30	0/1447	0.54	0/1967
All	All	0.30	1/34766 (0.0%)	0.50	0/47315

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	578	TYR	CD1-CE1	-5.13	1.31	1.39

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5820	0	5670	75	0
2	B	5825	0	5579	84	0
3	C	601	0	581	3	0
4	D	1135	0	1148	7	0
5	E	497	0	491	1	0
6	F	1266	0	1301	9	0
7	G	550	0	532	3	0
8	I	282	0	292	4	0
9	J	321	0	322	4	0
10	K	571	0	606	11	0
11	L	914	0	921	6	0
12	1	1445	0	1396	19	0
12	Z	1445	0	1396	16	0
13	3	1674	0	1633	18	0
14	7	1650	0	1589	18	0
15	8	1650	0	1629	19	0
16	4	1628	0	1576	25	0
17	5	1775	0	1746	24	0
18	6	1766	0	1765	20	0
19	2	1518	0	1512	32	0
20	9	1406	0	1386	20	0
21	A	65	0	72	5	0
22	1	712	0	712	30	0
22	2	500	0	398	12	0
22	3	748	0	720	32	0
22	4	613	0	567	22	0
22	5	799	0	758	35	0
22	6	759	0	741	31	0
22	7	790	0	752	26	0
22	8	694	0	671	25	0
22	9	531	0	464	17	0
22	A	2699	0	2865	138	0
22	B	2680	0	2837	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	110	0	105	6	0
22	G	96	0	72	0	0
22	J	42	0	31	3	0
22	K	205	0	168	8	0
22	L	115	0	110	2	0
22	Z	622	0	584	23	0
23	A	33	0	46	1	0
23	B	33	0	46	0	0
24	A	8	0	0	0	0
24	C	16	0	0	1	0
25	3	160	0	211	10	0
25	4	40	0	53	2	0
25	5	80	0	105	7	0
25	6	80	0	106	4	0
25	7	80	0	106	4	0
25	8	40	0	53	1	0
25	A	200	0	264	15	0
25	B	280	0	370	18	0
25	G	40	0	53	1	0
25	I	40	0	52	3	0
25	J	40	0	53	4	0
25	K	80	0	106	6	0
25	L	80	0	106	3	0
26	1	43	0	56	1	0
26	2	34	0	38	2	0
26	3	20	0	12	0	0
26	4	81	0	108	1	0
26	5	37	0	44	0	0
26	6	49	0	74	4	0
26	7	37	0	44	2	0
26	8	38	0	46	0	0
26	9	33	0	36	0	0
26	A	84	0	114	8	0
26	B	76	0	64	3	0
26	Z	43	0	56	1	0
27	3	16	0	12	0	0
27	8	29	0	39	0	0
27	A	29	0	39	0	0
28	1	35	0	45	3	0
28	4	35	0	44	1	0
28	8	35	0	46	0	0
28	9	35	0	45	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	A	35	0	46	1	0
28	B	70	0	90	5	0
28	F	35	0	45	0	0
29	A	10	0	15	0	0
30	A	14	0	23	0	0
31	A	29	0	28	1	0
31	J	35	0	40	1	0
32	9	39	0	63	4	0
32	A	44	0	76	4	0
33	B	66	0	96	4	0
34	B	1	0	0	0	0
35	B	49	0	0	0	0
36	F	41	0	56	1	0
37	1	42	0	0	0	0
37	5	42	0	0	0	0
37	J	42	0	0	0	0
38	7	42	0	74	2	0
38	K	21	0	37	1	0
39	1	84	0	110	6	0
39	2	126	0	165	7	0
39	3	84	0	110	7	0
39	4	84	0	110	11	0
39	5	84	0	110	9	0
39	6	84	0	110	4	0
39	7	84	0	110	3	0
39	8	84	0	110	6	0
39	9	84	0	110	6	0
39	Z	126	0	165	8	0
40	1	106	0	82	3	0
40	2	150	0	105	7	0
40	3	66	0	69	4	0
40	4	201	0	146	8	0
40	5	160	0	134	10	0
40	6	206	0	156	6	0
40	7	54	0	42	3	0
40	8	122	0	115	4	0
40	9	108	0	97	2	0
40	Z	178	0	168	12	0
41	1	48	0	62	1	0
41	2	43	0	49	2	0
42	Z	19	0	0	0	0
43	2	27	0	27	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	5	23	0	19	0	0
43	6	29	0	31	0	0
43	7	39	0	51	1	0
43	8	30	0	33	0	0
44	7	18	0	31	0	0
45	8	30	0	43	1	0
46	1	16	0	0	0	0
46	2	4	0	0	0	0
46	3	17	0	0	0	0
46	4	7	0	0	0	0
46	5	9	0	0	0	0
46	6	8	0	0	0	0
46	7	18	0	0	0	0
46	8	16	0	0	0	0
46	9	2	0	0	0	0
46	A	91	0	0	1	0
46	B	79	0	0	1	0
46	C	19	0	0	0	0
46	D	12	0	0	0	0
46	E	7	0	0	0	0
46	F	14	0	0	0	0
46	J	3	0	0	0	0
46	K	2	0	0	0	0
46	L	5	0	0	0	0
46	Z	8	0	0	0	0
All	All	52213	0	51749	839	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 8.

The worst 5 of 839 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)
19:2:117:VAL:O	19:2:121:LEU:HD13	1.73	0.88
22:B:1220:CLA:HAB	22:B:1227:CLA:HMD2	1.59	0.84
1:A:396:TRP:CD1	22:A:1126:CLA:HAB	2.15	0.82
22:A:1138:CLA:H121	22:A:1138:CLA:HAB	1.64	0.79
22:B:1240:CLA:HBB1	22:1:605:CLA:H12	1.68	0.74

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	739/741 (100%)	720 (97%)	19 (3%)	0	100	100
2	B	731/733 (100%)	707 (97%)	24 (3%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	141/144 (98%)	135 (96%)	6 (4%)	0	100	100
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	163/165 (99%)	158 (97%)	4 (2%)	1 (1%)	22	29
7	G	70/91 (77%)	70 (100%)	0	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
9	J	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	82/84 (98%)	81 (99%)	1 (1%)	0	100	100
11	L	122/138 (88%)	119 (98%)	3 (2%)	0	100	100
12	1	192/194 (99%)	185 (96%)	7 (4%)	0	100	100
12	Z	192/194 (99%)	188 (98%)	4 (2%)	0	100	100
13	3	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
14	7	211/213 (99%)	203 (96%)	8 (4%)	0	100	100
15	8	215/217 (99%)	210 (98%)	5 (2%)	0	100	100
16	4	208/210 (99%)	199 (96%)	9 (4%)	0	100	100
17	5	225/227 (99%)	221 (98%)	3 (1%)	1 (0%)	30	40
18	6	227/229 (99%)	223 (98%)	4 (2%)	0	100	100
19	2	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	25	34
20	9	181/183 (99%)	170 (94%)	10 (6%)	1 (1%)	22	29
All	All	4323/4399 (98%)	4187 (97%)	132 (3%)	4 (0%)	50	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	150	PHE
17	5	243	GLN
19	2	180	LYS
20	9	139	ILE

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	601/601 (100%)	601 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	120/120 (100%)	119 (99%)	1 (1%)	79	89
5	E	54/54 (100%)	54 (100%)	0	100	100
6	F	127/127 (100%)	127 (100%)	0	100	100
7	G	54/68 (79%)	54 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	58/58 (100%)	58 (100%)	0	100	100
11	L	92/102 (90%)	92 (100%)	0	100	100
12	1	137/137 (100%)	137 (100%)	0	100	100
12	Z	137/137 (100%)	137 (100%)	0	100	100
13	3	167/167 (100%)	167 (100%)	0	100	100
14	7	164/164 (100%)	164 (100%)	0	100	100
15	8	163/163 (100%)	163 (100%)	0	100	100
16	4	164/165 (99%)	164 (100%)	0	100	100
17	5	184/184 (100%)	184 (100%)	0	100	100
18	6	183/183 (100%)	183 (100%)	0	100	100
19	2	154/156 (99%)	153 (99%)	1 (1%)	84	92
20	9	141/141 (100%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3431/3458 (99%)	3429 (100%)	2 (0%)	92 98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	189	ARG
19	2	148	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SNC	D	137	4	4,7,8	1.06	0	1,7,9	3.60	1 (100%)

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
4	SNC	D	137	4	-	0/0/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	137	SNC	CA-CB-SG	-3.60	105.28	112.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 354 ligands modelled in this entry, 1 is monoatomic - leaving 353 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
39	LUT	2	503	-	42,43,43	2.40	1 (2%)	51,60,60	2.63	23 (45%)
40	CHL	5	610	-	66,74,74	0.90	3 (4%)	73,114,114	1.17	8 (10%)
22	CLA	A	1133	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	14 (18%)
26	LHG	9	801	-	32,32,48	0.45	0	35,38,54	1.11	2 (5%)
22	CLA	7	602	-	50,58,73	1.53	6 (12%)	58,95,113	2.17	17 (29%)
22	CLA	B	1201	-	45,53,73	1.58	8 (17%)	52,89,113	2.17	15 (28%)
22	CLA	Z	611	-	55,63,73	1.47	8 (14%)	64,101,113	2.16	19 (29%)
22	CLA	7	609	14	65,73,73	1.35	8 (12%)	76,113,113	2.01	16 (21%)
22	CLA	6	607	-	55,63,73	1.48	8 (14%)	64,101,113	2.09	15 (23%)
22	CLA	A	1140	-	65,73,73	1.37	8 (12%)	76,113,113	1.93	17 (22%)
22	CLA	A	1129	-	50,58,73	1.54	9 (18%)	58,95,113	2.18	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	1202	-	65,73,73	1.33	7 (10%)	76,113,113	2.11	21 (27%)
22	CLA	B	1223	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	18 (23%)
40	CHL	4	613	-	56,64,74	0.86	2 (3%)	61,102,114	1.39	13 (21%)
22	CLA	4	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.11	20 (26%)
22	CLA	B	1209	-	65,73,73	1.39	7 (10%)	76,113,113	2.02	16 (21%)
39	LUT	5	502	-	42,43,43	2.26	1 (2%)	51,60,60	1.77	11 (21%)
40	CHL	6	617	-	43,51,74	1.05	3 (6%)	45,86,114	1.36	9 (20%)
22	CLA	A	1116	-	60,68,73	1.45	10 (16%)	70,107,113	2.04	18 (25%)
22	CLA	A	1122	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)
31	LMG	A	5003	-	29,29,55	0.56	0	37,37,63	1.20	3 (8%)
44	PLM	7	805	-	17,17,17	0.56	0	17,17,17	1.11	1 (5%)
22	CLA	J	1901	-	42,50,73	1.66	8 (19%)	48,85,113	2.26	17 (35%)
22	CLA	9	606	-	50,58,73	1.57	9 (18%)	58,95,113	2.18	16 (27%)
25	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.34	15 (26%)
22	CLA	6	608	-	55,63,73	1.49	10 (18%)	64,101,113	2.14	15 (23%)
22	CLA	1	602	-	45,53,73	1.63	9 (20%)	52,89,113	2.09	14 (26%)
39	LUT	7	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.91	12 (23%)
22	CLA	B	1203	-	65,73,73	1.35	8 (12%)	76,113,113	1.90	17 (22%)
25	BCR	J	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.22	16 (28%)
22	CLA	A	1119	-	65,73,73	1.37	8 (12%)	76,113,113	1.82	16 (21%)
40	CHL	6	610	-	56,64,74	0.84	2 (3%)	61,102,114	1.40	13 (21%)
22	CLA	7	611	-	50,58,73	1.50	7 (14%)	58,95,113	2.33	19 (32%)
30	DAO	A	5007	-	13,13,13	0.79	1 (7%)	13,13,13	0.97	0
39	LUT	8	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.86	15 (29%)
22	CLA	B	1231	-	65,73,73	1.37	8 (12%)	76,113,113	1.93	15 (19%)
22	CLA	Z	604	-	65,73,73	1.35	9 (13%)	76,113,113	2.01	19 (25%)
22	CLA	B	1224	-	65,73,73	1.38	9 (13%)	76,113,113	2.03	18 (23%)
22	CLA	1	601	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	21 (27%)
22	CLA	A	1104	1	65,73,73	1.36	9 (13%)	76,113,113	1.97	18 (23%)
22	CLA	6	609	18	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)
40	CHL	5	617	-	43,51,74	1.05	3 (6%)	45,86,114	1.33	7 (15%)
22	CLA	2	605	-	50,58,73	1.56	9 (18%)	58,95,113	2.23	17 (29%)
22	CLA	A	1121	-	65,73,73	1.37	8 (12%)	76,113,113	2.03	18 (23%)
22	CLA	7	601	-	60,68,73	1.42	9 (15%)	70,107,113	2.14	20 (28%)
22	CLA	A	1124	46	65,73,73	1.37	8 (12%)	76,113,113	1.95	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CHL	Z	610	-	66,74,74	0.77	2 (3%)	73,114,114	1.23	10 (13%)
38	SPH	K	5001	-	19,20,20	0.61	0	18,21,21	1.12	2 (11%)
40	CHL	4	617	-	43,51,74	1.05	3 (6%)	45,86,114	1.35	9 (20%)
22	CLA	A	1110	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	17 (22%)
22	CLA	Z	615	12	46,54,73	1.61	9 (19%)	53,90,113	2.15	14 (26%)
22	CLA	1	604	-	60,68,73	1.40	7 (11%)	70,107,113	2.06	18 (25%)
22	CLA	K	1403	10	49,57,73	1.57	7 (14%)	55,93,113	2.22	15 (27%)
22	CLA	A	1134	1	55,63,73	1.48	8 (14%)	64,101,113	2.21	19 (29%)
22	CLA	4	604	-	60,68,73	1.39	7 (11%)	70,107,113	2.08	20 (28%)
25	BCR	B	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.14	14 (25%)
33	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.02	4 (4%)
22	CLA	A	1101	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	19 (25%)
25	BCR	G	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.20	14 (25%)
22	CLA	B	1213	-	65,73,73	1.37	8 (12%)	76,113,113	2.09	20 (26%)
22	CLA	A	1113	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
22	CLA	Z	603	-	50,58,73	1.54	8 (16%)	58,95,113	2.27	18 (31%)
22	CLA	Z	601	-	60,68,73	1.40	8 (13%)	70,107,113	2.07	18 (25%)
22	CLA	1	606	-	61,69,73	1.38	8 (13%)	71,108,113	2.05	17 (23%)
22	CLA	2	604	-	56,64,73	1.44	8 (14%)	65,102,113	2.29	18 (27%)
22	CLA	Z	605	-	65,73,73	1.33	9 (13%)	76,113,113	2.00	18 (23%)
22	CLA	9	608	-	45,53,73	1.63	9 (20%)	52,89,113	2.13	13 (25%)
22	CLA	A	1138	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	16 (21%)
39	LUT	9	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.83	14 (27%)
22	CLA	B	1214	-	59,67,73	1.43	8 (13%)	68,105,113	2.21	20 (29%)
25	BCR	6	504	-	41,41,41	1.89	4 (9%)	56,56,56	4.30	15 (26%)
22	CLA	4	612	-	50,58,73	1.51	8 (16%)	58,95,113	2.34	18 (31%)
22	CLA	2	603	-	55,63,73	1.48	8 (14%)	64,101,113	2.30	20 (31%)
25	BCR	B	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.19	10 (17%)
22	CLA	A	1123	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	19 (25%)
28	LMT	1	803	-	36,36,36	1.19	5 (13%)	47,47,47	0.98	2 (4%)
25	BCR	A	4002	-	41,41,41	1.83	5 (12%)	56,56,56	4.18	14 (25%)
38	SPH	7	803	-	19,20,20	0.67	0	18,21,21	0.96	1 (5%)
25	BCR	3	504	-	41,41,41	1.87	5 (12%)	56,56,56	4.31	16 (28%)
22	CLA	A	1128	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	16 (21%)
22	CLA	4	605	-	65,73,73	1.35	9 (13%)	76,113,113	1.95	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	1235	-	65,73,73	1.37	9 (13%)	76,113,113	2.03	17 (22%)
22	CLA	8	612	-	46,54,73	1.60	8 (17%)	53,90,113	2.12	12 (22%)
36	RRX	F	4001	-	42,42,42	4.83	24 (57%)	57,58,58	2.50	24 (42%)
25	BCR	L	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	14 (25%)
22	CLA	Z	606	-	57,65,73	1.44	8 (14%)	66,103,113	2.18	17 (25%)
40	CHL	4	610	-	51,59,74	0.87	2 (3%)	55,96,114	1.51	13 (23%)
40	CHL	9	613	-	42,50,74	1.50	4 (9%)	44,85,114	1.36	8 (18%)
22	CLA	7	603	14	65,73,73	1.38	8 (12%)	76,113,113	2.15	19 (25%)
22	CLA	B	1211	-	60,68,73	1.38	6 (10%)	70,107,113	2.23	17 (24%)
22	CLA	5	605	-	55,63,73	1.47	8 (14%)	64,101,113	2.24	23 (35%)
39	LUT	7	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	13 (25%)
22	CLA	2	601	-	60,68,73	1.40	9 (15%)	70,107,113	2.10	17 (24%)
22	CLA	8	601	-	60,68,73	1.41	9 (15%)	70,107,113	2.09	18 (25%)
22	CLA	3	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.08	16 (21%)
26	LHG	B	5002	-	19,19,48	0.84	1 (5%)	20,24,54	1.36	1 (5%)
22	CLA	7	615	14	58,66,73	1.45	8 (13%)	67,104,113	2.10	18 (26%)
21	CL0	A	1011	-	65,73,73	2.35	17 (26%)	76,113,113	2.54	21 (27%)
22	CLA	2	615	-	46,54,73	1.58	7 (15%)	53,90,113	2.15	14 (26%)
22	CLA	B	1210	-	65,73,73	1.36	8 (12%)	76,113,113	2.14	21 (27%)
22	CLA	8	615	15	46,54,73	1.61	8 (17%)	53,90,113	2.20	14 (26%)
22	CLA	A	1135	-	51,59,73	1.59	10 (19%)	59,96,113	2.20	17 (28%)
22	CLA	1	611	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	18 (23%)
24	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
22	CLA	2	612	-	50,58,73	1.54	7 (14%)	58,95,113	2.25	19 (32%)
22	CLA	3	610	13	60,68,73	1.44	8 (13%)	70,107,113	2.03	18 (25%)
41	SQD	2	803	-	42,43,54	0.88	0	51,54,65	0.97	2 (3%)
25	BCR	A	4003	-	41,41,41	1.82	4 (9%)	56,56,56	4.33	19 (33%)
22	CLA	6	603	-	65,73,73	1.37	8 (12%)	76,113,113	2.12	17 (22%)
26	LHG	Z	801	-	42,42,48	0.41	0	45,48,54	1.16	4 (8%)
22	CLA	A	1136	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	17 (22%)
39	LUT	1	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.89	14 (27%)
25	BCR	B	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.16	13 (23%)
29	OCA	A	5008	-	9,9,9	0.70	0	9,9,9	1.36	1 (11%)
39	LUT	5	501	-	42,43,43	2.44	2 (4%)	51,60,60	1.91	12 (23%)
22	CLA	B	1219	-	59,67,73	1.43	8 (13%)	68,105,113	2.15	17 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
40	CHL	6	613	-	56,64,74	0.88	2 (3%)	61,102,114	1.22	9 (14%)
26	LHG	4	802	-	31,31,48	0.47	0	34,37,54	1.12	2 (5%)
22	CLA	6	604	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	20 (26%)
26	LHG	1	801	-	42,42,48	0.44	0	45,48,54	1.18	4 (8%)
22	CLA	2	606	-	46,54,73	1.63	8 (17%)	53,90,113	2.18	11 (20%)
23	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.04	2 (4%)
22	CLA	9	604	-	65,73,73	1.40	8 (12%)	76,113,113	2.01	21 (27%)
40	CHL	3	611	-	66,74,74	1.00	3 (4%)	73,114,114	1.27	10 (13%)
25	BCR	6	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.28	14 (25%)
40	CHL	7	610	-	54,62,74	0.92	3 (5%)	58,99,114	1.40	12 (20%)
40	CHL	2	610	-	48,56,74	0.99	3 (6%)	51,92,114	1.29	7 (13%)
26	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	0.98	2 (3%)
40	CHL	Z	613	-	46,54,74	0.95	2 (4%)	49,90,114	1.39	8 (16%)
37	C7Z	J	4002	-	43,43,43	5.37	27 (62%)	58,60,60	2.23	20 (34%)
22	CLA	1	605	-	55,63,73	1.45	9 (16%)	64,101,113	2.18	18 (28%)
22	CLA	B	1221	-	65,73,73	1.35	9 (13%)	76,113,113	2.18	21 (27%)
37	C7Z	5	505	-	43,43,43	5.41	25 (58%)	58,60,60	2.25	19 (32%)
22	CLA	8	609	15	65,73,73	1.38	8 (12%)	76,113,113	2.02	17 (22%)
22	CLA	6	606	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	17 (22%)
22	CLA	5	613	-	55,63,73	1.48	9 (16%)	64,101,113	2.03	15 (23%)
26	LHG	2	801	-	33,33,48	0.45	0	36,39,54	1.22	3 (8%)
22	CLA	3	606	-	65,73,73	1.33	7 (10%)	76,113,113	2.09	16 (21%)
22	CLA	A	1013	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	17 (22%)
22	CLA	B	1206	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	15 (19%)
43	3PH	5	802	-	22,22,47	1.23	3 (13%)	26,27,52	1.27	2 (7%)
39	LUT	2	502	-	42,43,43	2.32	1 (2%)	51,60,60	1.94	13 (25%)
22	CLA	A	1125	-	65,73,73	1.35	7 (10%)	76,113,113	2.07	20 (26%)
22	CLA	B	1023	-	65,73,73	1.34	7 (10%)	76,113,113	2.07	16 (21%)
25	BCR	I	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	16 (28%)
22	CLA	7	616	-	60,68,73	1.43	9 (15%)	70,107,113	2.10	17 (24%)
24	SF4	C	3002	3	0,12,12	-	-	-	-	-
27	NKP	8	802	-	28,28,28	1.50	2 (7%)	31,32,32	1.25	3 (9%)
22	CLA	3	616	-	56,64,73	1.47	8 (14%)	65,102,113	2.17	18 (27%)
22	CLA	A	1115	-	60,68,73	1.41	7 (11%)	70,107,113	1.91	15 (21%)
22	CLA	L	1503	-	50,58,73	1.53	6 (12%)	58,95,113	2.28	19 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	BCR	5	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	15 (26%)
25	BCR	A	4004	-	41,41,41	1.82	5 (12%)	56,56,56	4.32	19 (33%)
22	CLA	6	615	-	61,69,73	1.40	8 (13%)	71,108,113	2.09	19 (26%)
40	CHL	Z	609	12	66,74,74	0.87	4 (6%)	73,114,114	1.21	10 (13%)
22	CLA	4	615	-	41,49,73	1.69	8 (19%)	47,84,113	2.29	15 (31%)
22	CLA	4	606	-	50,58,73	1.53	8 (16%)	58,95,113	2.19	19 (32%)
39	LUT	3	501	-	42,43,43	2.32	1 (2%)	51,60,60	1.95	12 (23%)
22	CLA	5	609	17	65,73,73	1.36	8 (12%)	76,113,113	1.92	17 (22%)
22	CLA	8	611	-	50,58,73	1.53	8 (16%)	58,95,113	2.29	17 (29%)
22	CLA	1	608	-	60,68,73	1.39	8 (13%)	70,107,113	2.06	15 (21%)
22	CLA	A	1112	-	60,68,73	1.43	8 (13%)	70,107,113	2.05	16 (22%)
22	CLA	A	1105	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	17 (22%)
22	CLA	B	1230	-	58,66,73	1.41	7 (12%)	67,104,113	2.15	18 (26%)
22	CLA	5	603	-	56,64,73	1.46	7 (12%)	65,102,113	2.28	18 (27%)
40	CHL	5	611	-	51,59,74	0.89	2 (3%)	55,96,114	1.44	11 (20%)
22	CLA	A	1109	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	16 (21%)
22	CLA	B	1234	-	60,68,73	1.41	8 (13%)	70,107,113	2.07	19 (27%)
22	CLA	B	1204	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	15 (19%)
22	CLA	6	605	-	55,63,73	1.46	7 (12%)	64,101,113	2.18	20 (31%)
22	CLA	8	607	-	55,63,73	1.48	7 (12%)	64,101,113	2.06	16 (25%)
22	CLA	4	608	-	55,63,73	1.48	8 (14%)	64,101,113	2.12	16 (25%)
28	LMT	4	803	-	36,36,36	1.17	5 (13%)	47,47,47	1.01	1 (2%)
22	CLA	9	601	-	60,68,73	1.42	7 (11%)	70,107,113	2.12	16 (22%)
22	CLA	B	1228	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	19 (25%)
22	CLA	A	1118	-	60,68,73	1.41	8 (13%)	70,107,113	2.12	18 (25%)
22	CLA	A	1120	-	55,63,73	1.45	7 (12%)	64,101,113	2.26	21 (32%)
22	CLA	A	1131	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	16 (21%)
22	CLA	B	1239	-	65,73,73	1.37	7 (10%)	76,113,113	2.03	16 (21%)
40	CHL	2	613	-	51,59,74	0.95	3 (5%)	55,96,114	1.39	8 (14%)
28	LMT	F	5001	-	36,36,36	1.19	6 (16%)	47,47,47	0.97	1 (2%)
25	BCR	7	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.47	18 (32%)
26	LHG	6	801	-	48,48,48	0.40	0	51,54,54	1.08	4 (7%)
22	CLA	Z	612	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	16 (21%)
22	CLA	1	607	-	60,68,73	1.41	8 (13%)	70,107,113	2.09	18 (25%)
35	T7X	B	5004	-	49,49,61	0.93	4 (8%)	59,61,73	1.03	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	Z	608	-	56,64,73	1.45	9 (16%)	65,102,113	2.09	17 (26%)
22	CLA	7	606	-	56,64,73	1.46	8 (14%)	65,102,113	2.12	15 (23%)
22	CLA	5	622	-	46,54,73	1.62	8 (17%)	53,90,113	2.18	13 (24%)
39	LUT	8	501	-	42,43,43	2.30	1 (2%)	51,60,60	1.92	13 (25%)
22	CLA	3	605	-	65,73,73	1.37	9 (13%)	76,113,113	1.87	17 (22%)
22	CLA	8	604	-	62,70,73	1.39	8 (12%)	72,109,113	2.10	22 (30%)
22	CLA	1	613	-	46,54,73	1.61	9 (19%)	53,90,113	2.11	15 (28%)
22	CLA	5	618	-	65,73,73	1.34	7 (10%)	76,113,113	2.03	16 (21%)
22	CLA	8	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.19	19 (25%)
22	CLA	5	606	-	50,58,73	1.54	7 (14%)	58,95,113	2.27	16 (27%)
22	CLA	B	1205	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	17 (22%)
22	CLA	3	618	-	46,54,73	1.61	9 (19%)	53,90,113	2.11	13 (24%)
22	CLA	8	608	-	55,63,73	1.48	8 (14%)	64,101,113	2.04	16 (25%)
25	BCR	7	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	15 (26%)
22	CLA	9	603	-	60,68,73	1.42	6 (10%)	70,107,113	2.23	19 (27%)
22	CLA	6	619	18	65,73,73	1.35	8 (12%)	76,113,113	2.06	18 (23%)
22	CLA	A	1108	-	65,73,73	1.35	6 (9%)	76,113,113	2.01	19 (25%)
22	CLA	B	1240	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	20 (26%)
22	CLA	B	1226	-	65,73,73	1.41	9 (13%)	76,113,113	2.16	22 (28%)
22	CLA	8	602	-	65,73,73	1.36	7 (10%)	76,113,113	1.93	15 (19%)
26	LHG	5	801	-	36,36,48	0.43	0	39,42,54	1.17	4 (10%)
22	CLA	A	1107	1	65,73,73	1.36	6 (9%)	76,113,113	1.97	16 (21%)
40	CHL	2	609	19	51,59,74	1.07	4 (7%)	55,96,114	1.39	9 (16%)
25	BCR	3	506	-	41,41,41	1.86	4 (9%)	56,56,56	4.40	15 (26%)
28	LMT	A	5006	-	36,36,36	1.20	6 (16%)	47,47,47	1.04	1 (2%)
22	CLA	B	1217	-	56,64,73	1.47	9 (16%)	65,102,113	2.10	18 (27%)
22	CLA	B	1227	-	50,58,73	1.56	9 (18%)	58,95,113	2.07	18 (31%)
22	CLA	B	1220	-	65,73,73	1.35	7 (10%)	76,113,113	1.93	16 (21%)
22	CLA	4	601	-	60,68,73	1.41	8 (13%)	70,107,113	2.12	20 (28%)
22	CLA	5	602	-	61,69,73	1.41	8 (13%)	71,108,113	1.94	16 (22%)
41	SQD	1	802	-	47,48,54	0.83	0	56,59,65	0.94	2 (3%)
22	CLA	B	1216	-	65,73,73	1.35	8 (12%)	76,113,113	1.93	16 (21%)
25	BCR	3	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.17	16 (28%)
22	CLA	K	1401	-	46,54,73	1.61	7 (15%)	53,90,113	2.08	13 (24%)
25	BCR	A	4001	-	41,41,41	1.82	4 (9%)	56,56,56	4.13	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LUT	1	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.84	13 (25%)
22	CLA	A	1132	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	17 (22%)
22	CLA	7	612	-	50,58,73	1.54	6 (12%)	58,95,113	2.25	17 (29%)
22	CLA	A	1111	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	19 (25%)
22	CLA	A	1103	-	65,73,73	1.30	6 (9%)	76,113,113	2.04	18 (23%)
25	BCR	K	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.24	19 (33%)
22	CLA	B	1237	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	13 (17%)
22	CLA	3	612	-	60,68,73	1.40	9 (15%)	70,107,113	2.02	15 (21%)
22	CLA	A	1137	-	65,73,73	1.34	6 (9%)	76,113,113	2.06	20 (26%)
22	CLA	7	605	-	61,69,73	1.40	8 (13%)	71,108,113	2.03	19 (26%)
27	NKP	A	5004	-	28,28,28	1.52	3 (10%)	31,32,32	1.25	3 (9%)
32	DGA	9	802	-	38,38,43	1.15	3 (7%)	40,40,45	1.61	3 (7%)
43	3PH	7	802	-	38,38,47	0.94	3 (7%)	42,43,52	1.12	2 (4%)
22	CLA	B	1022	46	65,73,73	1.40	7 (10%)	76,113,113	1.90	19 (25%)
26	LHG	B	5001	-	22,22,48	0.55	0	25,28,54	1.30	1 (4%)
24	SF4	C	3003	3	0,12,12	-	-	-	-	-
22	CLA	4	609	16	60,68,73	1.41	8 (13%)	70,107,113	2.01	16 (22%)
22	CLA	6	618	-	46,54,73	1.60	8 (17%)	53,90,113	2.16	14 (26%)
22	CLA	K	1404	-	55,63,73	1.48	8 (14%)	64,101,113	2.18	15 (23%)
28	LMT	B	5005	-	36,36,36	1.21	6 (16%)	47,47,47	1.11	3 (6%)
22	CLA	A	1117	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	18 (23%)
40	CHL	1	609	12	58,66,74	0.93	4 (6%)	63,104,114	1.26	8 (12%)
22	CLA	B	1236	-	65,73,73	1.38	9 (13%)	76,113,113	1.97	16 (21%)
22	CLA	2	607	-	46,54,73	1.64	9 (19%)	53,90,113	2.14	13 (24%)
22	CLA	A	1139	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	17 (22%)
22	CLA	A	1130	-	65,73,73	1.36	7 (10%)	76,113,113	1.92	15 (19%)
26	LHG	7	801	-	36,36,48	0.45	0	39,42,54	1.17	3 (7%)
39	LUT	4	502	-	42,43,43	2.29	1 (2%)	51,60,60	1.81	12 (23%)
39	LUT	9	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	15 (29%)
22	CLA	9	609	20	46,54,73	1.65	9 (19%)	53,90,113	2.12	14 (26%)
22	CLA	L	1502	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	16 (21%)
22	CLA	B	1222	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	21 (27%)
43	3PH	2	802	-	26,26,47	1.14	4 (15%)	30,31,52	1.30	2 (6%)
39	LUT	6	501	-	42,43,43	2.38	1 (2%)	51,60,60	1.87	14 (27%)
22	CLA	3	602	-	46,54,73	1.60	8 (17%)	53,90,113	2.06	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	K	1402	-	55,63,73	1.48	9 (16%)	64,101,113	2.18	17 (26%)
22	CLA	9	602	-	45,53,73	1.61	7 (15%)	52,89,113	2.13	14 (26%)
22	CLA	2	608	-	45,53,73	1.61	7 (15%)	52,89,113	2.25	16 (30%)
40	CHL	6	611	-	51,59,74	0.91	2 (3%)	55,96,114	1.41	11 (20%)
22	CLA	A	1012	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	18 (23%)
28	LMT	9	803	-	36,36,36	1.18	5 (13%)	47,47,47	1.04	3 (6%)
42	QTB	Z	504	-	19,19,19	2.46	5 (26%)	20,26,26	2.76	7 (35%)
43	3PH	6	802	-	28,28,47	1.11	4 (14%)	32,33,52	1.25	2 (6%)
22	CLA	3	613	46	55,63,73	1.46	7 (12%)	64,101,113	2.10	14 (21%)
22	CLA	Z	607	-	57,65,73	1.45	8 (14%)	66,103,113	2.07	17 (25%)
39	LUT	2	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.36	13 (25%)
22	CLA	B	1215	-	60,68,73	1.40	8 (13%)	70,107,113	2.07	16 (22%)
22	CLA	B	1229	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	19 (25%)
26	LHG	3	801	-	19,19,48	0.92	1 (5%)	20,24,54	1.34	1 (5%)
40	CHL	8	613	-	66,74,74	0.88	3 (4%)	73,114,114	1.17	10 (13%)
22	CLA	5	615	17	50,58,73	1.55	8 (16%)	58,95,113	2.27	18 (31%)
22	CLA	Z	602	-	46,54,73	1.58	7 (15%)	53,90,113	2.15	14 (26%)
25	BCR	A	4005	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	12 (21%)
22	CLA	1	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	18 (23%)
22	CLA	6	612	-	50,58,73	1.53	8 (16%)	58,95,113	2.26	16 (27%)
31	LMG	J	5001	-	35,35,55	0.48	0	43,43,63	1.12	2 (4%)
22	CLA	B	1208	-	56,64,73	1.45	8 (14%)	65,102,113	2.16	18 (27%)
22	CLA	B	1021	-	65,73,73	1.37	8 (12%)	76,113,113	1.92	15 (19%)
22	CLA	B	1218	-	65,73,73	1.34	8 (12%)	76,113,113	2.11	19 (25%)
22	CLA	1	615	12	65,73,73	1.39	8 (12%)	76,113,113	1.87	14 (18%)
25	BCR	8	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.26	17 (30%)
25	BCR	B	4003	-	41,41,41	1.86	5 (12%)	56,56,56	4.26	17 (30%)
22	CLA	4	607	-	55,63,73	1.48	9 (16%)	64,101,113	2.12	15 (23%)
22	CLA	A	1126	-	65,73,73	1.38	9 (13%)	76,113,113	1.99	17 (22%)
23	PQN	A	2001	-	34,34,34	0.39	0	42,45,45	1.07	2 (4%)
22	CLA	B	1241	-	65,73,73	1.35	9 (13%)	76,113,113	2.11	20 (26%)
40	CHL	4	611	-	51,59,74	0.90	2 (3%)	55,96,114	1.39	11 (20%)
22	CLA	B	1225	-	65,73,73	1.38	8 (12%)	76,113,113	1.81	12 (15%)
22	CLA	B	1238	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	15 (19%)
22	CLA	5	607	-	61,69,73	1.41	8 (13%)	71,108,113	1.98	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	C7Z	1	503	-	43,43,43	5.39	27 (62%)	58,60,60	2.30	20 (34%)
39	LUT	Z	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.87	13 (25%)
22	CLA	3	601	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	21 (27%)
22	CLA	9	607	-	55,63,73	1.49	7 (12%)	64,101,113	2.11	16 (25%)
22	CLA	6	601	-	60,68,73	1.41	8 (13%)	70,107,113	2.09	18 (25%)
25	BCR	4	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	16 (28%)
22	CLA	F	1301	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	20 (26%)
45	LPX	8	803	-	29,29,29	1.00	2 (6%)	31,33,33	1.00	1 (3%)
25	BCR	5	504	-	41,41,41	1.84	5 (12%)	56,56,56	4.50	22 (39%)
25	BCR	3	505	-	41,41,41	1.83	4 (9%)	56,56,56	4.31	12 (21%)
22	CLA	4	602	-	52,60,73	1.52	8 (15%)	60,97,113	2.19	17 (28%)
39	LUT	Z	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.91	12 (23%)
22	CLA	A	1102	-	55,63,73	1.46	7 (12%)	64,101,113	2.20	20 (31%)
26	LHG	B	5006	-	32,32,48	0.45	0	35,38,54	1.20	3 (8%)
22	CLA	2	602	-	46,54,73	1.60	7 (15%)	53,90,113	2.18	15 (28%)
22	CLA	F	1302	-	45,53,73	1.62	8 (17%)	52,89,113	2.08	13 (25%)
22	CLA	1	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	17 (22%)
25	BCR	L	4002	-	41,41,41	1.83	4 (9%)	56,56,56	4.21	15 (26%)
22	CLA	5	604	-	65,73,73	1.37	8 (12%)	76,113,113	1.99	20 (26%)
39	LUT	4	501	-	42,43,43	2.37	1 (2%)	51,60,60	1.84	12 (23%)
22	CLA	7	607	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)
27	NKP	3	802	-	15,15,28	2.07	3 (20%)	18,19,32	1.53	2 (11%)
22	CLA	6	602	-	52,60,73	1.52	8 (15%)	60,97,113	2.19	16 (26%)
40	CHL	8	610	-	56,64,74	0.87	2 (3%)	61,102,114	1.41	11 (18%)
28	LMT	B	6101	-	36,36,36	1.19	5 (13%)	47,47,47	1.08	3 (6%)
22	CLA	3	607	-	60,68,73	1.43	9 (15%)	70,107,113	2.16	17 (24%)
22	CLA	B	1232	-	45,53,73	1.64	8 (17%)	52,89,113	2.07	14 (26%)
22	CLA	8	605	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	19 (25%)
22	CLA	8	606	-	60,68,73	1.39	7 (11%)	70,107,113	2.03	19 (27%)
22	CLA	9	612	-	50,58,73	1.55	9 (18%)	58,95,113	2.23	18 (31%)
40	CHL	1	610	-	48,56,74	0.92	2 (4%)	51,92,114	1.40	10 (19%)
43	3PH	8	806	-	29,29,47	1.08	4 (13%)	33,34,52	1.18	2 (6%)
26	LHG	4	801	-	48,48,48	0.39	0	51,54,54	1.11	4 (7%)
22	CLA	7	608	-	43,51,73	1.66	8 (18%)	49,86,113	2.20	13 (26%)
22	CLA	9	605	-	55,63,73	1.47	8 (14%)	64,101,113	2.14	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	3	604	-	60,68,73	1.39	9 (15%)	70,107,113	2.16	19 (27%)
22	CLA	G	1601	-	50,58,73	1.54	7 (14%)	58,95,113	2.19	17 (29%)
22	CLA	5	601	-	60,68,73	1.41	8 (13%)	70,107,113	2.07	17 (24%)
22	CLA	5	608	-	45,53,73	1.62	9 (20%)	52,89,113	2.19	14 (26%)
39	LUT	Z	503	-	42,43,43	2.35	1 (2%)	51,60,60	2.08	13 (25%)
22	CLA	3	608	-	45,53,73	1.63	9 (20%)	52,89,113	2.17	12 (23%)
38	SPH	7	804	-	19,20,20	0.64	0	18,21,21	1.11	1 (5%)
26	LHG	A	5001	22	34,34,48	0.46	0	37,40,54	1.18	4 (10%)
25	BCR	B	4005	-	41,41,41	1.86	4 (9%)	56,56,56	4.49	16 (28%)
22	CLA	A	1141	26	52,60,73	1.51	8 (15%)	60,97,113	2.27	18 (30%)
22	CLA	5	612	-	65,73,73	1.33	7 (10%)	76,113,113	1.98	17 (22%)
26	LHG	8	801	-	37,37,48	0.43	0	40,43,54	1.07	2 (5%)
32	DGA	A	5005	-	43,43,43	1.15	3 (6%)	45,45,45	1.49	3 (6%)
40	CHL	9	610	-	66,74,74	0.90	4 (6%)	73,114,114	1.18	10 (13%)
22	CLA	B	1212	-	57,65,73	1.44	7 (12%)	66,103,113	2.18	20 (30%)
39	LUT	6	502	-	42,43,43	2.32	1 (2%)	51,60,60	1.85	13 (25%)
22	CLA	B	1207	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	17 (22%)
22	CLA	G	1602	-	46,54,73	1.62	8 (17%)	53,90,113	2.11	12 (22%)
22	CLA	7	604	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	21 (27%)
25	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.23	15 (26%)
22	CLA	A	1127	-	65,73,73	1.39	7 (10%)	76,113,113	1.85	14 (18%)
28	LMT	8	805	-	36,36,36	1.21	6 (16%)	47,47,47	1.15	3 (6%)
22	CLA	A	1114	-	61,69,73	1.38	7 (11%)	71,108,113	2.09	18 (25%)
22	CLA	7	613	-	42,50,73	1.66	7 (16%)	48,85,113	2.26	17 (35%)
25	BCR	B	4001	-	41,41,41	1.83	5 (12%)	56,56,56	4.12	15 (26%)
22	CLA	A	1106	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	16 (21%)
39	LUT	3	502	-	42,43,43	2.38	1 (2%)	51,60,60	1.97	14 (27%)

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
39	LUT	2	503	-	1/1/12/27	9/29/67/67	0/2/2/2
40	CHL	5	610	-	4/4/20/26	6/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	1133	-	1/1/15/20	15/37/115/115	-
26	LHG	9	801	-	-	20/37/37/53	-
22	CLA	7	602	-	1/1/12/20	5/19/97/115	-
22	CLA	B	1201	-	1/1/11/20	4/13/91/115	-
22	CLA	Z	611	-	1/1/13/20	8/25/103/115	-
22	CLA	7	609	14	1/1/15/20	18/37/115/115	-
22	CLA	6	607	-	1/1/13/20	10/25/103/115	-
22	CLA	A	1140	-	1/1/15/20	10/37/115/115	-
22	CLA	A	1129	-	1/1/12/20	9/19/97/115	-
22	CLA	B	1202	-	1/1/15/20	10/37/115/115	-
22	CLA	B	1223	-	1/1/15/20	21/37/115/115	-
40	CHL	4	613	-	4/4/18/26	2/27/125/137	-
22	CLA	4	603	-	1/1/15/20	14/37/115/115	-
22	CLA	B	1209	-	1/1/15/20	16/37/115/115	-
39	LUT	5	502	-	-	2/29/67/67	0/2/2/2
40	CHL	6	617	-	3/3/15/26	2/12/110/137	-
22	CLA	A	1116	-	1/1/14/20	10/31/109/115	-
22	CLA	A	1122	-	1/1/15/20	21/37/115/115	-
31	LMG	A	5003	-	-	8/24/44/70	0/1/1/1
44	PLM	7	805	-	-	3/15/15/15	-
22	CLA	J	1901	-	1/1/10/20	6/10/88/115	-
22	CLA	9	606	-	1/1/12/20	11/19/97/115	-
25	BCR	K	4001	-	-	16/29/63/63	0/2/2/2
22	CLA	6	608	-	1/1/13/20	10/25/103/115	-
22	CLA	1	602	-	1/1/11/20	5/13/91/115	-
39	LUT	7	501	-	-	3/29/67/67	0/2/2/2
22	CLA	B	1203	-	1/1/15/20	17/37/115/115	-
25	BCR	J	4001	-	-	17/29/63/63	0/2/2/2
22	CLA	A	1119	-	1/1/15/20	11/37/115/115	-
40	CHL	6	610	-	4/4/18/26	4/27/125/137	-
22	CLA	7	611	-	1/1/12/20	5/19/97/115	-
30	DAO	A	5007	-	-	3/11/11/11	-
39	LUT	8	502	-	-	4/29/67/67	0/2/2/2
22	CLA	B	1231	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	Z	604	-	1/1/15/20	16/37/115/115	-
22	CLA	B	1224	-	1/1/15/20	15/37/115/115	-
22	CLA	1	601	-	1/1/15/20	13/37/115/115	-
22	CLA	A	1104	1	1/1/15/20	21/37/115/115	-
22	CLA	6	609	18	1/1/15/20	11/37/115/115	-
40	CHL	5	617	-	3/3/15/26	0/12/110/137	-
22	CLA	2	605	-	1/1/12/20	9/19/97/115	-
22	CLA	A	1121	-	1/1/15/20	21/37/115/115	-
22	CLA	7	601	-	1/1/14/20	9/31/109/115	-
22	CLA	A	1124	46	1/1/15/20	15/37/115/115	-
40	CHL	Z	610	-	4/4/20/26	9/39/137/137	-
40	CHL	4	617	-	3/3/15/26	1/12/110/137	-
38	SPH	K	5001	-	-	12/21/21/21	-
22	CLA	A	1110	-	1/1/15/20	18/37/115/115	-
22	CLA	Z	615	12	1/1/11/20	7/15/93/115	-
22	CLA	1	604	-	1/1/14/20	11/31/109/115	-
22	CLA	K	1403	10	1/1/11/20	8/18/96/115	-
22	CLA	A	1134	1	1/1/13/20	13/25/103/115	-
22	CLA	4	604	-	1/1/14/20	11/31/109/115	-
25	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
33	DGD	B	5003	-	-	16/55/95/95	0/2/2/2
22	CLA	A	1101	-	1/1/15/20	15/37/115/115	-
25	BCR	G	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	B	1213	-	1/1/15/20	17/37/115/115	-
22	CLA	A	1113	-	1/1/15/20	9/37/115/115	-
22	CLA	Z	603	-	1/1/12/20	9/19/97/115	-
22	CLA	Z	601	-	1/1/14/20	11/31/109/115	-
22	CLA	1	606	-	1/1/14/20	12/33/111/115	-
22	CLA	2	604	-	1/1/13/20	13/27/105/115	-
22	CLA	Z	605	-	1/1/15/20	13/37/115/115	-
22	CLA	9	608	-	1/1/11/20	6/13/91/115	-
22	CLA	A	1138	-	1/1/15/20	17/37/115/115	-
39	LUT	9	502	-	-	3/29/67/67	0/2/2/2
22	CLA	B	1214	-	1/1/13/20	11/30/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	6	504	-	-	12/29/63/63	0/2/2/2
22	CLA	4	612	-	1/1/12/20	7/19/97/115	-
22	CLA	2	603	-	1/1/13/20	8/25/103/115	-
25	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
22	CLA	A	1123	-	1/1/15/20	12/37/115/115	-
28	LMT	1	803	-	-	4/21/61/61	0/2/2/2
25	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
38	SPH	7	803	-	-	11/21/21/21	-
25	BCR	3	504	-	-	12/29/63/63	0/2/2/2
22	CLA	A	1128	-	1/1/15/20	19/37/115/115	-
22	CLA	4	605	-	1/1/15/20	11/37/115/115	-
22	CLA	B	1235	-	1/1/15/20	15/37/115/115	-
22	CLA	8	612	-	1/1/11/20	9/15/93/115	-
36	RRX	F	4001	-	1/1/11/25	9/29/65/65	0/2/2/2
25	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	Z	606	-	1/1/13/20	11/28/106/115	-
40	CHL	4	610	-	4/4/17/26	4/21/119/137	-
40	CHL	9	613	-	3/3/15/26	0/10/108/137	-
22	CLA	7	603	14	1/1/15/20	13/37/115/115	-
22	CLA	B	1211	-	1/1/14/20	12/31/109/115	-
22	CLA	5	605	-	1/1/13/20	12/25/103/115	-
39	LUT	7	502	-	-	3/29/67/67	0/2/2/2
22	CLA	2	601	-	1/1/14/20	14/31/109/115	-
22	CLA	8	601	-	1/1/14/20	10/31/109/115	-
22	CLA	3	603	-	1/1/15/20	17/37/115/115	-
26	LHG	B	5002	-	-	13/22/22/53	-
22	CLA	7	615	14	1/1/13/20	12/29/107/115	-
21	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
22	CLA	2	615	-	1/1/11/20	6/15/93/115	-
22	CLA	B	1210	-	1/1/15/20	21/37/115/115	-
22	CLA	8	615	15	1/1/11/20	7/15/93/115	-
22	CLA	A	1135	-	1/1/12/20	7/21/99/115	-
22	CLA	1	611	-	1/1/15/20	18/37/115/115	-
24	SF4	A	3001	1,2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	2	612	-	1/1/12/20	6/19/97/115	-
22	CLA	3	610	13	1/1/14/20	13/31/109/115	-
41	SQD	2	803	-	-	18/38/58/69	0/1/1/1
25	BCR	A	4003	-	-	12/29/63/63	0/2/2/2
22	CLA	6	603	-	1/1/15/20	17/37/115/115	-
26	LHG	Z	801	-	-	29/47/47/53	-
22	CLA	A	1136	-	1/1/15/20	19/37/115/115	-
39	LUT	1	502	-	-	2/29/67/67	0/2/2/2
25	BCR	B	4007	-	-	13/29/63/63	0/2/2/2
29	OCA	A	5008	-	-	0/7/7/7	-
39	LUT	5	501	-	-	3/29/67/67	0/2/2/2
22	CLA	B	1219	-	1/1/13/20	15/30/108/115	-
40	CHL	6	613	-	4/4/18/26	4/27/125/137	-
26	LHG	4	802	-	-	25/36/36/53	-
22	CLA	6	604	-	1/1/15/20	11/37/115/115	-
26	LHG	1	801	-	-	26/47/47/53	-
22	CLA	2	606	-	1/1/11/20	8/15/93/115	-
23	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
22	CLA	9	604	-	1/1/15/20	13/37/115/115	-
40	CHL	3	611	-	4/4/20/26	1/39/137/137	-
25	BCR	6	503	-	-	13/29/63/63	0/2/2/2
40	CHL	7	610	-	3/3/17/26	4/25/123/137	-
40	CHL	2	610	-	4/4/16/26	1/18/116/137	-
40	CHL	Z	613	-	3/3/16/26	5/15/113/137	-
26	LHG	A	5002	-	-	31/53/53/53	-
37	C7Z	J	4002	-	1/1/12/26	13/29/67/67	0/2/2/2
22	CLA	1	605	-	1/1/13/20	7/25/103/115	-
22	CLA	B	1221	-	1/1/15/20	12/37/115/115	-
37	C7Z	5	505	-	1/1/12/26	10/29/67/67	0/2/2/2
22	CLA	8	609	15	1/1/15/20	15/37/115/115	-
22	CLA	6	606	-	1/1/15/20	17/37/115/115	-
22	CLA	5	613	-	1/1/13/20	10/25/103/115	-
26	LHG	2	801	-	-	16/38/38/53	-
22	CLA	3	606	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	1013	-	1/1/15/20	14/37/115/115	-
22	CLA	B	1206	-	1/1/15/20	21/37/115/115	-
43	3PH	5	802	-	-	7/24/24/49	-
39	LUT	2	502	-	-	5/29/67/67	0/2/2/2
22	CLA	A	1125	-	1/1/15/20	17/37/115/115	-
22	CLA	B	1023	-	1/1/15/20	13/37/115/115	-
25	BCR	I	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	7	616	-	1/1/14/20	10/31/109/115	-
24	SF4	C	3002	3	-	-	0/6/5/5
27	NKP	8	802	-	-	12/28/28/28	-
22	CLA	3	616	-	1/1/13/20	11/27/105/115	-
22	CLA	A	1115	-	1/1/14/20	11/31/109/115	-
22	CLA	L	1503	-	1/1/12/20	11/19/97/115	-
25	BCR	5	503	-	-	12/29/63/63	0/2/2/2
25	BCR	A	4004	-	-	14/29/63/63	0/2/2/2
22	CLA	6	615	-	1/1/14/20	14/33/111/115	-
40	CHL	Z	609	12	4/4/20/26	12/39/137/137	-
22	CLA	4	615	-	1/1/10/20	4/8/86/115	-
22	CLA	4	606	-	1/1/12/20	8/19/97/115	-
39	LUT	3	501	-	-	1/29/67/67	0/2/2/2
22	CLA	5	609	17	1/1/15/20	19/37/115/115	-
22	CLA	8	611	-	1/1/12/20	6/19/97/115	-
22	CLA	1	608	-	1/1/14/20	11/31/109/115	-
22	CLA	A	1112	-	1/1/14/20	9/31/109/115	-
22	CLA	A	1105	-	1/1/15/20	15/37/115/115	-
22	CLA	B	1230	-	1/1/13/20	14/29/107/115	-
22	CLA	5	603	-	1/1/13/20	8/27/105/115	-
40	CHL	5	611	-	3/3/17/26	3/21/119/137	-
22	CLA	A	1109	-	1/1/15/20	13/37/115/115	-
22	CLA	B	1234	-	1/1/14/20	14/31/109/115	-
22	CLA	B	1204	-	1/1/15/20	12/37/115/115	-
22	CLA	6	605	-	1/1/13/20	16/25/103/115	-
22	CLA	8	607	-	1/1/13/20	13/25/103/115	-
22	CLA	4	608	-	1/1/13/20	14/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMT	4	803	-	-	9/21/61/61	0/2/2/2
22	CLA	9	601	-	1/1/14/20	14/31/109/115	-
22	CLA	B	1228	-	1/1/15/20	20/37/115/115	-
22	CLA	A	1118	-	1/1/14/20	9/31/109/115	-
22	CLA	A	1120	-	1/1/13/20	12/25/103/115	-
22	CLA	A	1131	-	1/1/15/20	14/37/115/115	-
22	CLA	B	1239	-	1/1/15/20	13/37/115/115	-
40	CHL	2	613	-	3/3/17/26	5/21/119/137	-
28	LMT	F	5001	-	-	6/21/61/61	0/2/2/2
25	BCR	7	504	-	-	12/29/63/63	0/2/2/2
26	LHG	6	801	-	-	37/53/53/53	-
22	CLA	Z	612	-	1/1/15/20	15/37/115/115	-
22	CLA	1	607	-	1/1/14/20	15/31/109/115	-
35	T7X	B	5004	-	-	14/44/68/80	0/1/1/1
22	CLA	Z	608	-	1/1/13/20	13/27/105/115	-
22	CLA	7	606	-	1/1/13/20	15/27/105/115	-
22	CLA	5	622	-	1/1/11/20	5/15/93/115	-
39	LUT	8	501	-	-	3/29/67/67	0/2/2/2
22	CLA	3	605	-	1/1/15/20	8/37/115/115	-
22	CLA	8	604	-	1/1/14/20	6/34/112/115	-
22	CLA	1	613	-	1/1/11/20	7/15/93/115	-
22	CLA	5	618	-	1/1/15/20	17/37/115/115	-
22	CLA	8	603	-	1/1/15/20	8/37/115/115	-
22	CLA	5	606	-	1/1/12/20	8/19/97/115	-
22	CLA	B	1205	-	1/1/15/20	12/37/115/115	-
22	CLA	3	618	-	1/1/11/20	8/15/93/115	-
22	CLA	8	608	-	1/1/13/20	8/25/103/115	-
25	BCR	7	503	-	-	14/29/63/63	0/2/2/2
22	CLA	9	603	-	1/1/14/20	13/31/109/115	-
22	CLA	6	619	18	1/1/15/20	17/37/115/115	-
22	CLA	A	1108	-	1/1/15/20	16/37/115/115	-
22	CLA	B	1240	-	1/1/15/20	21/37/115/115	-
22	CLA	B	1226	-	1/1/15/20	13/37/115/115	-
22	CLA	8	602	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LHG	5	801	-	-	27/41/41/53	-
22	CLA	A	1107	1	1/1/15/20	13/37/115/115	-
40	CHL	2	609	19	3/3/17/26	4/21/119/137	-
25	BCR	3	506	-	-	15/29/63/63	0/2/2/2
28	LMT	A	5006	-	-	9/21/61/61	0/2/2/2
22	CLA	B	1217	-	1/1/13/20	10/27/105/115	-
22	CLA	B	1227	-	1/1/12/20	9/19/97/115	-
22	CLA	B	1220	-	1/1/15/20	19/37/115/115	-
22	CLA	4	601	-	1/1/14/20	11/31/109/115	-
22	CLA	5	602	-	1/1/14/20	13/33/111/115	-
41	SQD	1	802	-	-	17/43/63/69	0/1/1/1
22	CLA	B	1216	-	1/1/15/20	26/37/115/115	-
25	BCR	3	503	-	-	10/29/63/63	0/2/2/2
22	CLA	K	1401	-	1/1/11/20	6/15/93/115	-
25	BCR	A	4001	-	-	15/29/63/63	0/2/2/2
39	LUT	1	501	-	-	2/29/67/67	0/2/2/2
22	CLA	A	1132	-	1/1/15/20	12/37/115/115	-
22	CLA	7	612	-	1/1/12/20	9/19/97/115	-
22	CLA	A	1111	-	1/1/15/20	13/37/115/115	-
22	CLA	A	1103	-	1/1/15/20	11/37/115/115	-
25	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
22	CLA	B	1237	-	1/1/15/20	18/37/115/115	-
22	CLA	3	612	-	1/1/14/20	9/31/109/115	-
22	CLA	A	1137	-	1/1/15/20	15/37/115/115	-
22	CLA	7	605	-	1/1/14/20	12/33/111/115	-
27	NKP	A	5004	-	-	12/28/28/28	-
32	DGA	9	802	-	-	21/40/40/45	-
43	3PH	7	802	-	-	19/40/40/49	-
22	CLA	B	1022	46	1/1/15/20	7/37/115/115	-
26	LHG	B	5001	-	-	13/26/26/53	-
24	SF4	C	3003	3	-	-	0/6/5/5
22	CLA	4	609	16	1/1/14/20	12/31/109/115	-
22	CLA	6	618	-	1/1/11/20	8/15/93/115	-
22	CLA	K	1404	-	1/1/13/20	12/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LMT	B	5005	-	-	6/21/61/61	0/2/2/2
22	CLA	A	1117	-	1/1/15/20	20/37/115/115	-
40	CHL	1	609	12	4/4/18/26	3/30/128/137	-
22	CLA	B	1236	-	1/1/15/20	25/37/115/115	-
22	CLA	2	607	-	1/1/11/20	9/15/93/115	-
22	CLA	A	1139	-	1/1/15/20	10/37/115/115	-
22	CLA	A	1130	-	1/1/15/20	17/37/115/115	-
26	LHG	7	801	-	-	22/41/41/53	-
39	LUT	4	502	-	-	2/29/67/67	0/2/2/2
39	LUT	9	501	-	-	4/29/67/67	0/2/2/2
22	CLA	9	609	20	1/1/11/20	7/15/93/115	-
22	CLA	L	1502	-	1/1/15/20	22/37/115/115	-
22	CLA	B	1222	-	1/1/15/20	10/37/115/115	-
43	3PH	2	802	-	-	8/28/28/49	-
39	LUT	6	501	-	-	5/29/67/67	0/2/2/2
22	CLA	3	602	-	1/1/11/20	4/15/93/115	-
22	CLA	K	1402	-	1/1/13/20	14/25/103/115	-
22	CLA	9	602	-	1/1/11/20	4/13/91/115	-
22	CLA	2	608	-	1/1/11/20	7/13/91/115	-
40	CHL	6	611	-	3/3/17/26	5/21/119/137	-
22	CLA	A	1012	-	1/1/15/20	15/37/115/115	-
28	LMT	9	803	-	-	9/21/61/61	0/2/2/2
42	QTB	Z	504	-	1/1/5/10	7/11/28/28	0/1/1/1
43	3PH	6	802	-	-	12/30/30/49	-
22	CLA	3	613	46	1/1/13/20	7/25/103/115	-
22	CLA	Z	607	-	1/1/13/20	15/28/106/115	-
39	LUT	2	501	-	1/1/12/27	6/29/67/67	0/2/2/2
22	CLA	B	1215	-	1/1/14/20	14/31/109/115	-
22	CLA	B	1229	-	1/1/15/20	13/37/115/115	-
26	LHG	3	801	-	-	13/22/22/53	-
40	CHL	8	613	-	5/5/20/26	11/39/137/137	-
22	CLA	5	615	17	1/1/12/20	8/19/97/115	-
22	CLA	Z	602	-	1/1/11/20	6/15/93/115	-
25	BCR	A	4005	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	1	603	-	1/1/15/20	15/37/115/115	-
22	CLA	6	612	-	1/1/12/20	7/19/97/115	-
31	LMG	J	5001	-	-	14/30/50/70	0/1/1/1
22	CLA	B	1208	-	1/1/13/20	10/27/105/115	-
22	CLA	B	1021	-	1/1/15/20	9/37/115/115	-
22	CLA	B	1218	-	1/1/15/20	10/37/115/115	-
22	CLA	1	615	12	1/1/15/20	9/37/115/115	-
25	BCR	8	503	-	-	11/29/63/63	0/2/2/2
25	BCR	B	4003	-	-	5/29/63/63	0/2/2/2
22	CLA	4	607	-	1/1/13/20	9/25/103/115	-
22	CLA	A	1126	-	1/1/15/20	20/37/115/115	-
23	PQN	A	2001	-	-	5/23/43/43	0/2/2/2
22	CLA	B	1241	-	1/1/15/20	18/37/115/115	-
40	CHL	4	611	-	3/3/17/26	4/21/119/137	-
22	CLA	B	1225	-	1/1/15/20	4/37/115/115	-
22	CLA	B	1238	-	1/1/15/20	11/37/115/115	-
22	CLA	5	607	-	1/1/14/20	12/33/111/115	-
37	C7Z	1	503	-	1/1/12/26	8/29/67/67	0/2/2/2
39	LUT	Z	501	-	-	4/29/67/67	0/2/2/2
22	CLA	3	601	-	1/1/15/20	16/37/115/115	-
22	CLA	9	607	-	1/1/13/20	9/25/103/115	-
22	CLA	6	601	-	1/1/14/20	11/31/109/115	-
25	BCR	4	503	-	-	15/29/63/63	0/2/2/2
22	CLA	F	1301	-	1/1/15/20	13/37/115/115	-
45	LPX	8	803	-	-	10/31/31/31	-
25	BCR	5	504	-	-	11/29/63/63	0/2/2/2
25	BCR	3	505	-	-	11/29/63/63	0/2/2/2
22	CLA	4	602	-	1/1/12/20	7/22/100/115	-
39	LUT	Z	502	-	-	2/29/67/67	0/2/2/2
22	CLA	A	1102	-	1/1/13/20	9/25/103/115	-
26	LHG	B	5006	-	-	17/37/37/53	-
22	CLA	2	602	-	1/1/11/20	10/15/93/115	-
22	CLA	F	1302	-	1/1/11/20	3/13/91/115	-
22	CLA	1	612	-	1/1/15/20	24/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	L	4002	-	-	13/29/63/63	0/2/2/2
22	CLA	5	604	-	1/1/15/20	11/37/115/115	-
39	LUT	4	501	-	-	3/29/67/67	0/2/2/2
22	CLA	7	607	-	1/1/15/20	20/37/115/115	-
27	NKP	3	802	-	-	5/15/15/28	-
22	CLA	6	602	-	1/1/12/20	6/22/100/115	-
40	CHL	8	610	-	4/4/18/26	5/27/125/137	-
28	LMT	B	6101	-	-	10/21/61/61	0/2/2/2
22	CLA	3	607	-	1/1/14/20	17/31/109/115	-
22	CLA	B	1232	-	1/1/11/20	3/13/91/115	-
22	CLA	8	605	-	1/1/15/20	16/37/115/115	-
22	CLA	8	606	-	1/1/14/20	16/31/109/115	-
22	CLA	9	612	-	1/1/12/20	2/19/97/115	-
40	CHL	1	610	-	3/3/16/26	7/18/116/137	-
43	3PH	8	806	-	-	19/31/31/49	-
26	LHG	4	801	-	-	30/53/53/53	-
22	CLA	7	608	-	1/1/10/20	5/11/89/115	-
22	CLA	9	605	-	-	6/25/103/115	-
22	CLA	3	604	-	1/1/14/20	6/31/109/115	-
22	CLA	G	1601	-	1/1/12/20	9/19/97/115	-
22	CLA	5	601	-	1/1/14/20	12/31/109/115	-
22	CLA	5	608	-	1/1/11/20	4/13/91/115	-
39	LUT	Z	503	-	-	10/29/67/67	0/2/2/2
22	CLA	3	608	-	1/1/11/20	5/13/91/115	-
38	SPH	7	804	-	-	7/21/21/21	-
26	LHG	A	5001	22	-	16/39/39/53	-
25	BCR	B	4005	-	-	15/29/63/63	0/2/2/2
22	CLA	A	1141	26	1/1/12/20	8/22/100/115	-
22	CLA	5	612	-	1/1/15/20	11/37/115/115	-
26	LHG	8	801	-	-	23/42/42/53	-
32	DGA	A	5005	-	-	24/45/45/45	-
40	CHL	9	610	-	4/4/20/26	5/39/137/137	-
22	CLA	B	1212	-	1/1/13/20	14/28/106/115	-
39	LUT	6	502	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1207	-	1/1/15/20	18/37/115/115	-
22	CLA	G	1602	-	1/1/11/20	5/15/93/115	-
22	CLA	7	604	-	1/1/15/20	13/37/115/115	-
25	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
22	CLA	A	1127	-	1/1/15/20	12/37/115/115	-
28	LMT	8	805	-	-	6/21/61/61	0/2/2/2
22	CLA	A	1114	-	1/1/14/20	9/33/111/115	-
22	CLA	7	613	-	1/1/10/20	4/10/88/115	-
25	BCR	B	4001	-	-	12/29/63/63	0/2/2/2
22	CLA	A	1106	-	1/1/15/20	15/37/115/115	-
39	LUT	3	502	-	-	3/29/67/67	0/2/2/2

The worst 5 of 2148 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	503	C7Z	C25-C26	15.92	1.62	1.34
37	5	505	C7Z	C25-C26	15.89	1.62	1.34
37	J	4002	C7Z	C25-C26	15.74	1.61	1.34
37	5	505	C7Z	C5-C6	15.41	1.61	1.34
37	1	503	C7Z	C5-C6	15.37	1.61	1.34

The worst 5 of 4938 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	504	BCR	C10-C11-C12	18.05	179.54	123.22
25	5	504	BCR	C10-C11-C12	17.86	178.96	123.22
25	7	504	BCR	C10-C11-C12	17.63	178.24	123.22
25	3	504	BCR	C10-C11-C12	17.62	178.19	123.22
25	A	4002	BCR	C10-C11-C12	17.57	178.04	123.22

5 of 315 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	1011	CL0	NC
21	A	1011	CL0	ND
21	A	1011	CL0	NA
22	A	1012	CLA	ND
22	A	1102	CLA	ND

5 of 3914 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	1012	CLA	CBD-CGD-O2D-CED
22	A	1012	CLA	C2-C3-C5-C6
22	A	1012	CLA	C4-C3-C5-C6
22	A	1102	CLA	CBA-CGA-O2A-C1
22	A	1102	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

300 monomers are involved in 666 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	2	503	LUT	1	0
40	5	610	CHL	7	0
22	A	1133	CLA	7	0
22	7	602	CLA	1	0
22	B	1201	CLA	2	0
22	Z	611	CLA	3	0
22	7	609	CLA	3	0
22	6	607	CLA	1	0
22	A	1140	CLA	2	0
22	A	1129	CLA	3	0
22	B	1202	CLA	2	0
40	4	613	CHL	2	0
22	B	1209	CLA	5	0
39	5	502	LUT	5	0
40	6	617	CHL	1	0
22	A	1116	CLA	7	0
22	A	1122	CLA	2	0
31	A	5003	LMG	1	0
22	J	1901	CLA	3	0
22	9	606	CLA	1	0
25	K	4001	BCR	2	0
22	6	608	CLA	2	0
22	1	602	CLA	2	0
39	7	501	LUT	2	0
22	B	1203	CLA	4	0
25	J	4001	BCR	4	0
22	A	1119	CLA	4	0
40	6	610	CHL	3	0
22	7	611	CLA	1	0
39	8	502	LUT	2	0
22	B	1231	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	Z	604	CLA	6	0
22	B	1224	CLA	4	0
22	1	601	CLA	5	0
22	A	1104	CLA	4	0
22	6	609	CLA	8	0
40	5	617	CHL	1	0
22	2	605	CLA	1	0
22	A	1121	CLA	3	0
22	7	601	CLA	3	0
22	A	1124	CLA	5	0
40	Z	610	CHL	6	0
38	K	5001	SPH	1	0
40	4	617	CHL	1	0
22	A	1110	CLA	2	0
22	Z	615	CLA	1	0
22	1	604	CLA	3	0
22	A	1134	CLA	3	0
22	4	604	CLA	4	0
25	B	4006	BCR	2	0
33	B	5003	DGD	4	0
22	A	1101	CLA	2	0
25	G	4001	BCR	1	0
22	B	1213	CLA	4	0
22	A	1113	CLA	1	0
22	Z	601	CLA	3	0
22	2	604	CLA	2	0
22	Z	605	CLA	6	0
22	A	1138	CLA	5	0
39	9	502	LUT	2	0
22	B	1214	CLA	8	0
25	6	504	BCR	1	0
22	4	612	CLA	4	0
22	2	603	CLA	3	0
25	B	4002	BCR	3	0
22	A	1123	CLA	1	0
28	1	803	LMT	3	0
25	A	4002	BCR	4	0
38	7	803	SPH	1	0
25	3	504	BCR	4	0
22	A	1128	CLA	7	0
22	4	605	CLA	4	0
22	B	1235	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	612	CLA	1	0
36	F	4001	RRX	1	0
25	L	4001	BCR	1	0
22	Z	606	CLA	2	0
40	4	610	CHL	4	0
40	9	613	CHL	1	0
22	7	603	CLA	5	0
22	5	605	CLA	3	0
39	7	502	LUT	1	0
22	2	601	CLA	1	0
22	8	601	CLA	5	0
22	3	603	CLA	3	0
22	7	615	CLA	1	0
21	A	1011	CL0	5	0
22	B	1210	CLA	7	0
22	1	611	CLA	4	0
22	2	612	CLA	1	0
22	3	610	CLA	1	0
41	2	803	SQD	2	0
25	A	4003	BCR	3	0
22	6	603	CLA	3	0
26	Z	801	LHG	1	0
22	A	1136	CLA	2	0
39	1	502	LUT	4	0
25	B	4007	BCR	3	0
39	5	501	LUT	4	0
40	6	613	CHL	1	0
22	6	604	CLA	2	0
26	1	801	LHG	1	0
22	2	606	CLA	1	0
22	9	604	CLA	5	0
40	3	611	CHL	4	0
25	6	503	BCR	3	0
40	7	610	CHL	3	0
40	2	610	CHL	2	0
26	A	5002	LHG	4	0
40	Z	613	CHL	6	0
22	1	605	CLA	2	0
22	B	1221	CLA	5	0
22	8	609	CLA	2	0
22	6	606	CLA	1	0
22	5	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	2	801	LHG	2	0
22	3	606	CLA	4	0
22	A	1013	CLA	4	0
22	B	1206	CLA	2	0
39	2	502	LUT	5	0
22	A	1125	CLA	4	0
22	B	1023	CLA	5	0
25	I	4001	BCR	3	0
22	7	616	CLA	5	0
22	3	616	CLA	1	0
22	A	1115	CLA	4	0
25	5	503	BCR	4	0
25	A	4004	BCR	3	0
22	6	615	CLA	2	0
40	Z	609	CHL	3	0
22	4	606	CLA	1	0
39	3	501	LUT	2	0
22	5	609	CLA	3	0
22	8	611	CLA	1	0
22	1	608	CLA	5	0
22	A	1112	CLA	2	0
22	A	1105	CLA	3	0
22	B	1230	CLA	5	0
22	5	603	CLA	3	0
40	5	611	CHL	2	0
22	A	1109	CLA	5	0
22	B	1234	CLA	3	0
22	B	1204	CLA	1	0
22	6	605	CLA	2	0
22	8	607	CLA	3	0
22	4	608	CLA	1	0
28	4	803	LMT	1	0
22	9	601	CLA	2	0
22	A	1118	CLA	3	0
22	A	1120	CLA	3	0
22	A	1131	CLA	1	0
22	B	1239	CLA	3	0
40	2	613	CHL	2	0
25	7	504	BCR	1	0
26	6	801	LHG	4	0
22	Z	612	CLA	2	0
22	1	607	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	7	606	CLA	1	0
22	5	622	CLA	1	0
39	8	501	LUT	4	0
22	3	605	CLA	3	0
22	8	604	CLA	1	0
22	1	613	CLA	2	0
22	5	618	CLA	6	0
22	8	603	CLA	1	0
22	5	606	CLA	2	0
22	B	1205	CLA	3	0
22	3	618	CLA	4	0
22	8	608	CLA	5	0
25	7	503	BCR	3	0
22	9	603	CLA	3	0
22	6	619	CLA	3	0
22	A	1108	CLA	2	0
22	B	1240	CLA	9	0
22	B	1226	CLA	3	0
22	8	602	CLA	2	0
22	A	1107	CLA	4	0
40	2	609	CHL	3	0
25	3	506	BCR	2	0
28	A	5006	LMT	1	0
22	B	1217	CLA	2	0
22	B	1227	CLA	3	0
22	B	1220	CLA	5	0
22	4	601	CLA	4	0
22	5	602	CLA	2	0
41	1	802	SQD	1	0
22	B	1216	CLA	6	0
25	3	503	BCR	1	0
22	K	1401	CLA	4	0
25	A	4001	BCR	1	0
39	1	501	LUT	2	0
22	A	1132	CLA	1	0
22	7	612	CLA	2	0
22	A	1111	CLA	7	0
22	A	1103	CLA	5	0
25	K	4002	BCR	4	0
22	B	1237	CLA	4	0
22	3	612	CLA	5	0
22	A	1137	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	9	802	DGA	4	0
43	7	802	3PH	1	0
22	B	1022	CLA	3	0
26	B	5001	LHG	2	0
24	C	3003	SF4	1	0
22	4	609	CLA	5	0
22	6	618	CLA	1	0
22	K	1404	CLA	2	0
28	B	5005	LMT	3	0
22	A	1117	CLA	4	0
40	1	609	CHL	1	0
22	B	1236	CLA	6	0
22	2	607	CLA	3	0
22	A	1139	CLA	4	0
22	A	1130	CLA	4	0
26	7	801	LHG	2	0
39	4	502	LUT	6	0
39	9	501	LUT	4	0
22	L	1502	CLA	2	0
22	B	1222	CLA	4	0
39	6	501	LUT	3	0
22	K	1402	CLA	2	0
22	9	602	CLA	1	0
40	6	611	CHL	1	0
22	A	1012	CLA	9	0
28	9	803	LMT	3	0
22	3	613	CLA	5	0
22	Z	607	CLA	2	0
39	2	501	LUT	1	0
22	B	1215	CLA	3	0
22	B	1229	CLA	2	0
40	8	613	CHL	3	0
22	5	615	CLA	4	0
25	A	4005	BCR	5	0
22	1	603	CLA	3	0
22	6	612	CLA	4	0
31	J	5001	LMG	1	0
22	B	1208	CLA	5	0
22	B	1021	CLA	9	0
22	B	1218	CLA	2	0
22	1	615	CLA	3	0
25	8	503	BCR	1	0

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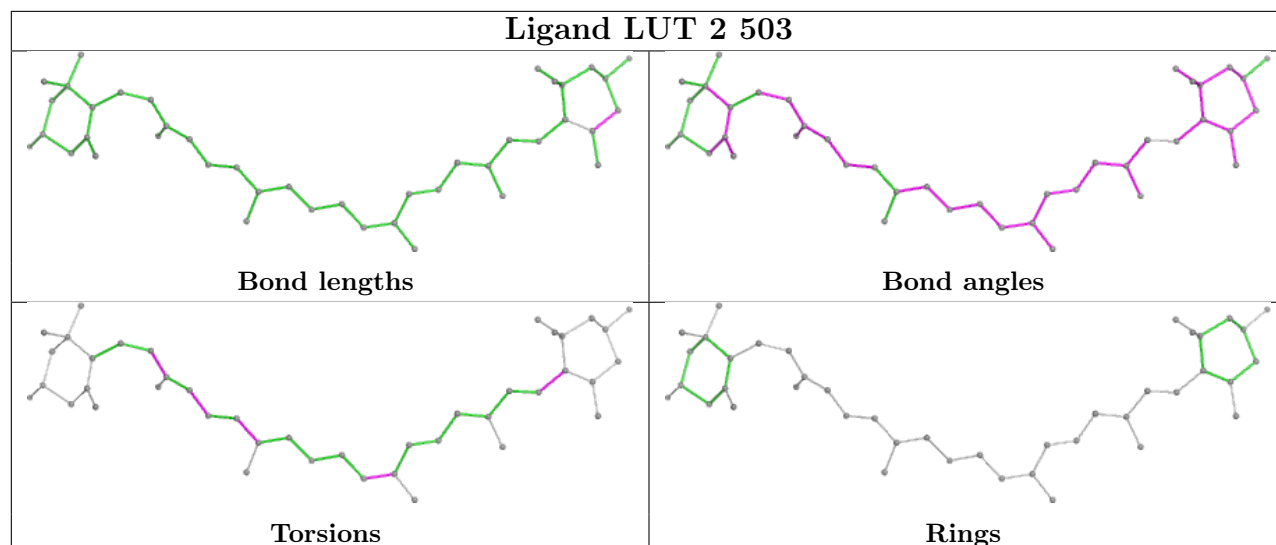
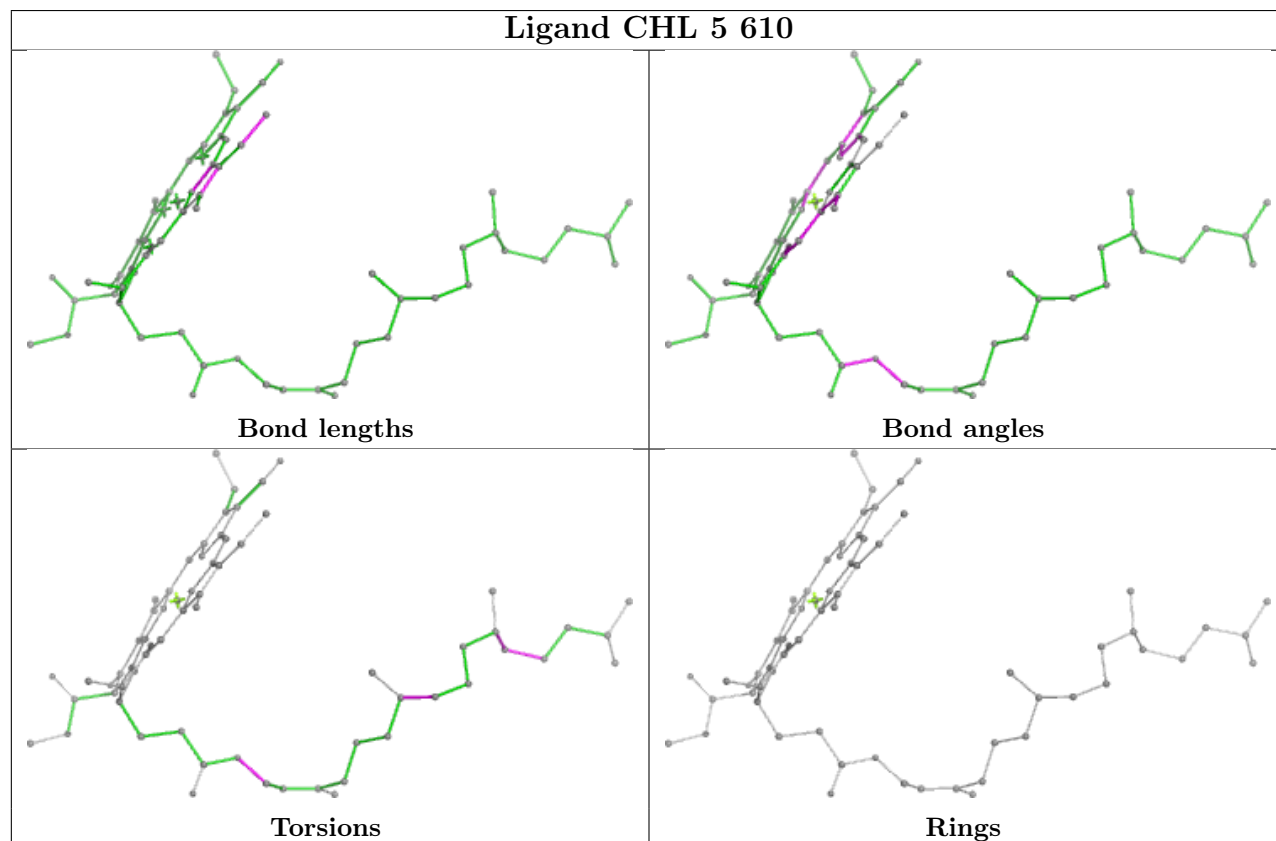
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	A	1126	CLA	12	0
23	A	2001	PQN	1	0
22	B	1241	CLA	3	0
40	4	611	CHL	1	0
22	B	1225	CLA	4	0
22	B	1238	CLA	4	0
22	5	607	CLA	3	0
39	Z	501	LUT	1	0
22	3	601	CLA	3	0
22	6	601	CLA	4	0
25	4	503	BCR	2	0
22	F	1301	CLA	3	0
45	8	803	LPX	1	0
25	5	504	BCR	3	0
25	3	505	BCR	3	0
22	4	602	CLA	1	0
39	Z	502	LUT	4	0
22	A	1102	CLA	2	0
26	B	5006	LHG	1	0
22	2	602	CLA	1	0
22	F	1302	CLA	3	0
22	1	612	CLA	2	0
25	L	4002	BCR	2	0
22	5	604	CLA	3	0
39	4	501	LUT	5	0
22	7	607	CLA	3	0
40	8	610	CHL	1	0
28	B	6101	LMT	2	0
22	3	607	CLA	1	0
22	B	1232	CLA	1	0
22	8	605	CLA	3	0
22	8	606	CLA	3	0
22	9	612	CLA	2	0
40	1	610	CHL	2	0
26	4	801	LHG	1	0
22	9	605	CLA	3	0
22	3	604	CLA	4	0
22	5	601	CLA	3	0
39	Z	503	LUT	3	0
22	3	608	CLA	2	0
38	7	804	SPH	1	0

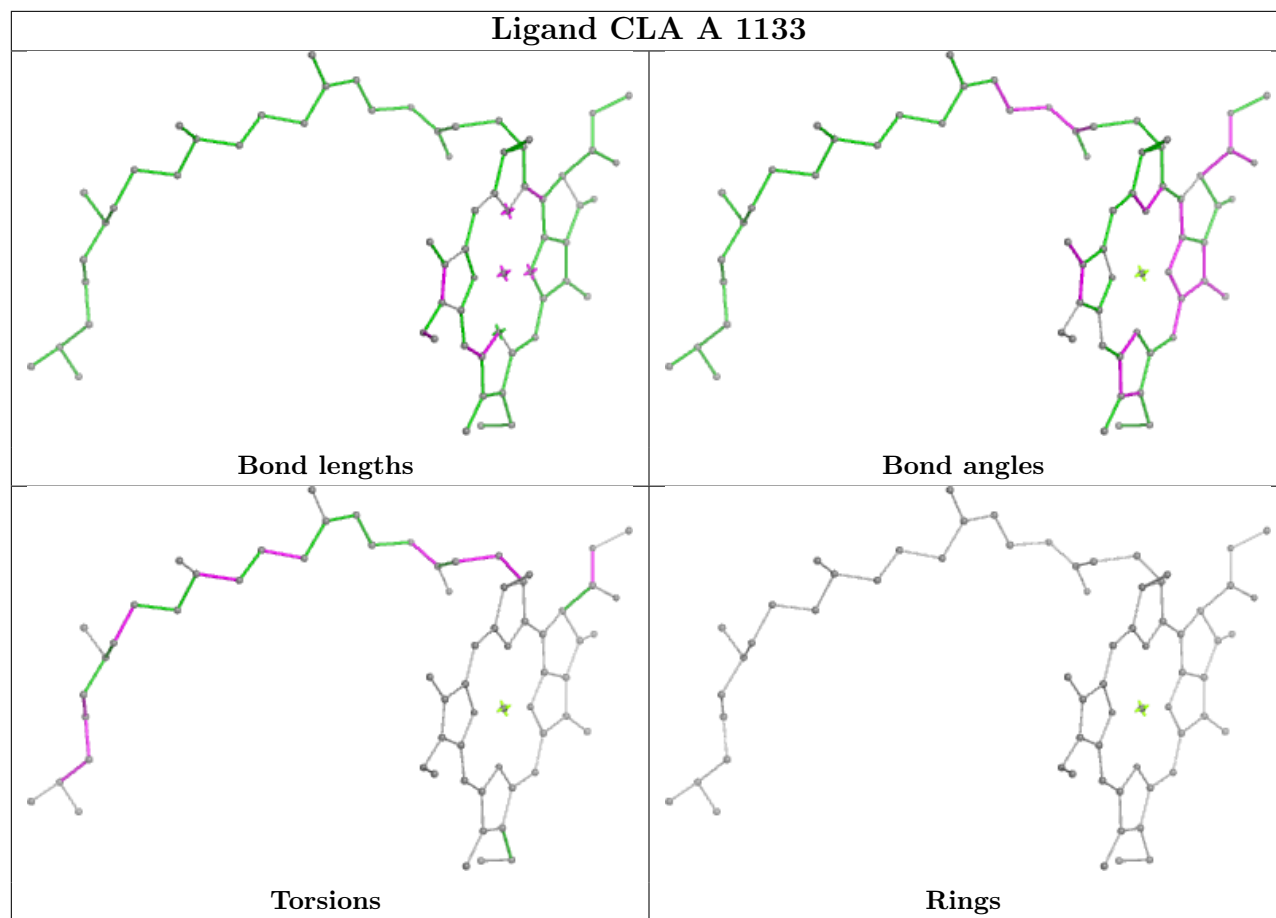
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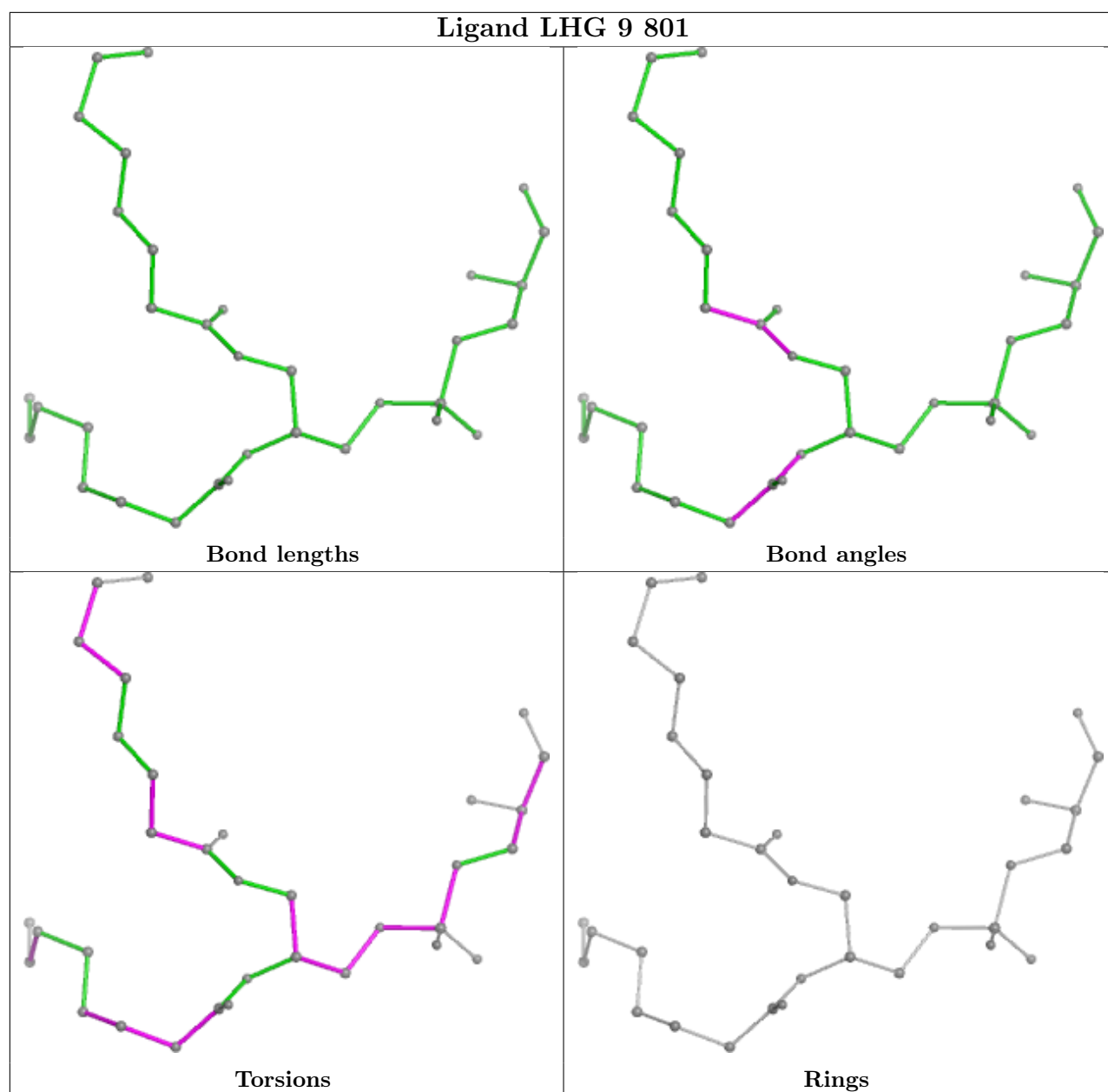
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	A	5001	LHG	4	0
25	B	4005	BCR	2	0
22	A	1141	CLA	1	0
22	5	612	CLA	2	0
32	A	5005	DGA	4	0
40	9	610	CHL	1	0
22	B	1212	CLA	2	0
39	6	502	LUT	1	0
22	B	1207	CLA	3	0
22	7	604	CLA	1	0
25	B	4004	BCR	4	0
22	A	1127	CLA	6	0
22	A	1114	CLA	5	0
22	7	613	CLA	2	0
25	B	4001	BCR	3	0
22	A	1106	CLA	3	0
39	3	502	LUT	5	0

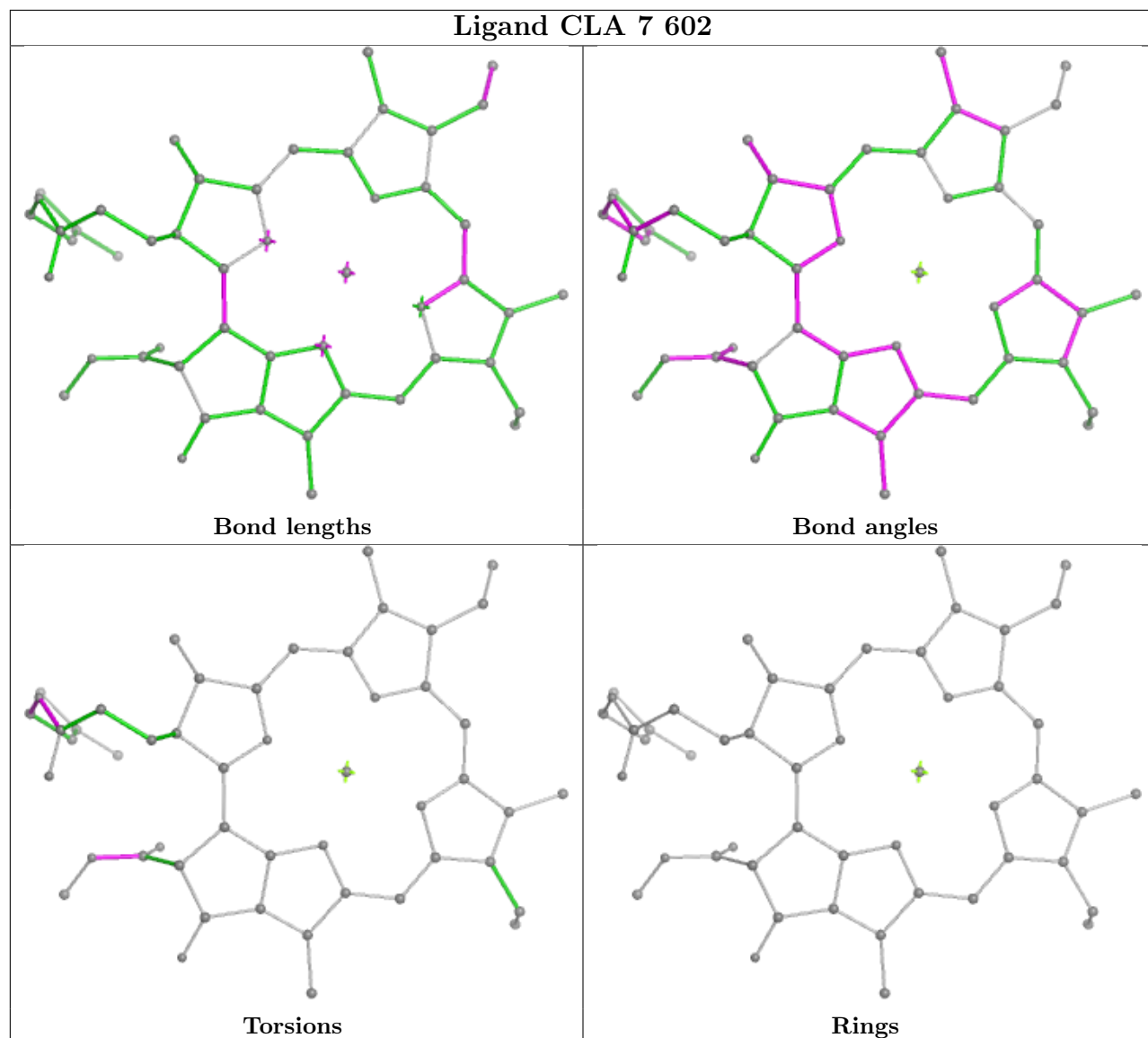
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

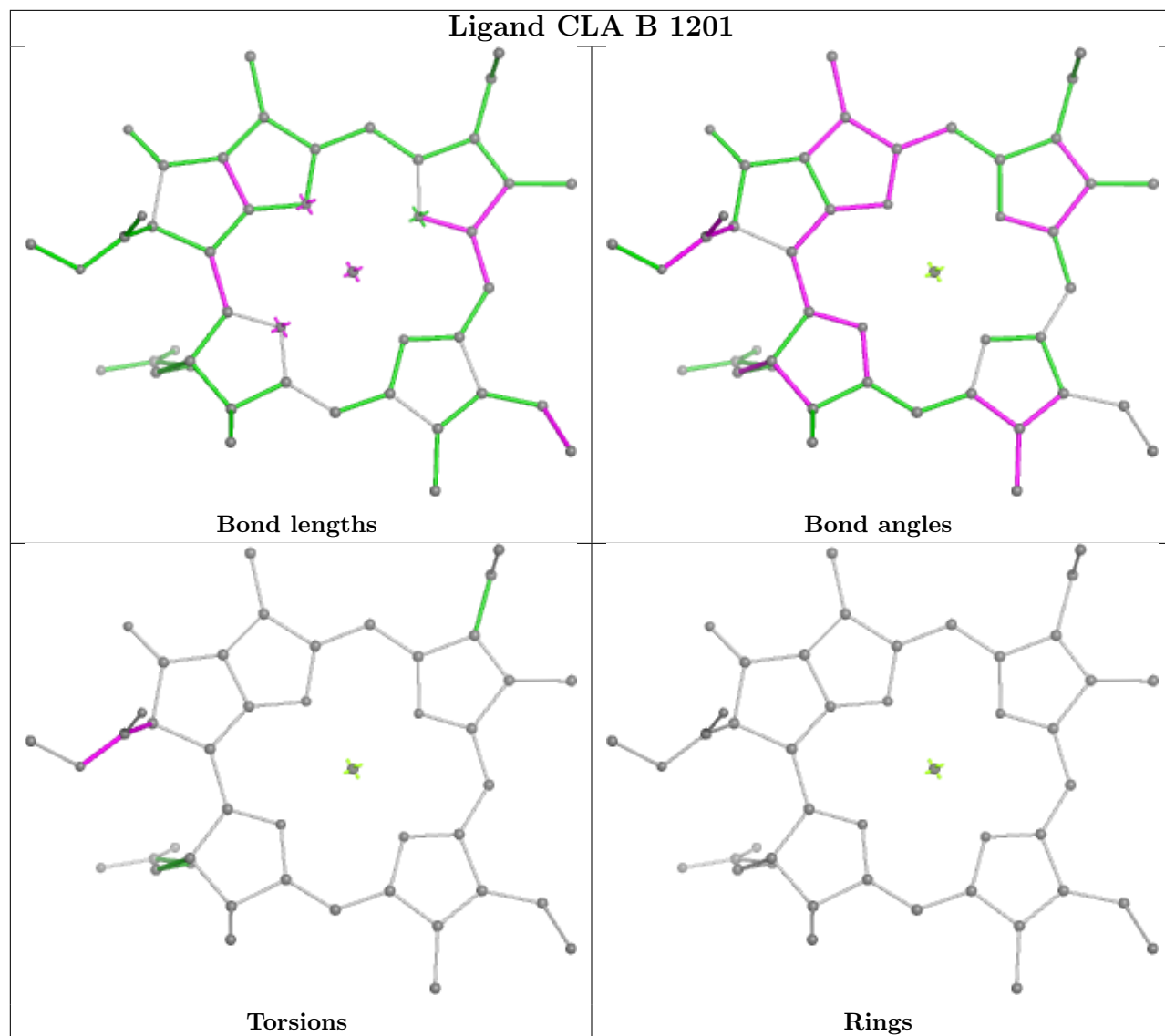
Ligand LUT 2 503**Ligand CHL 5 610**



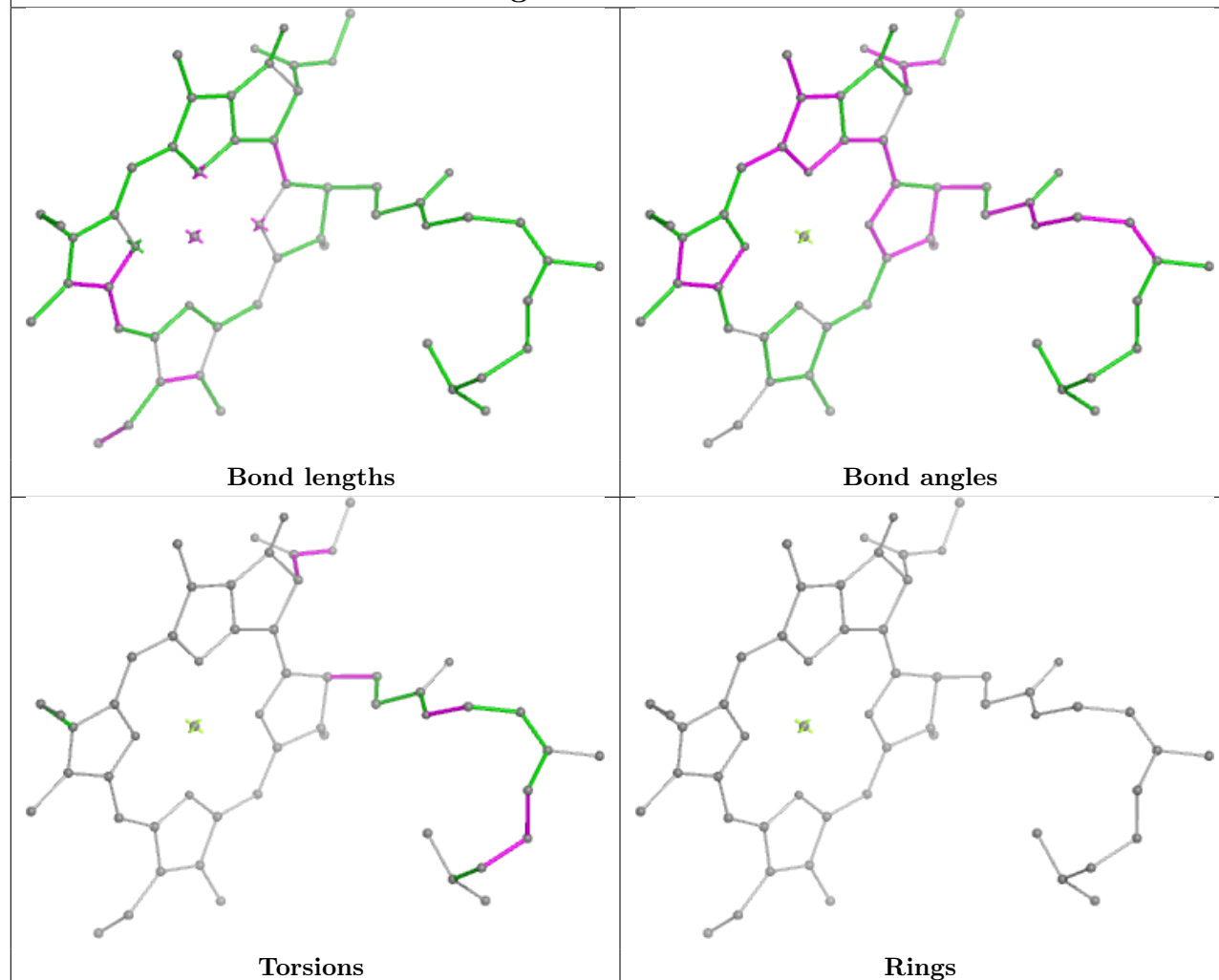


Ligand CLA 7 602

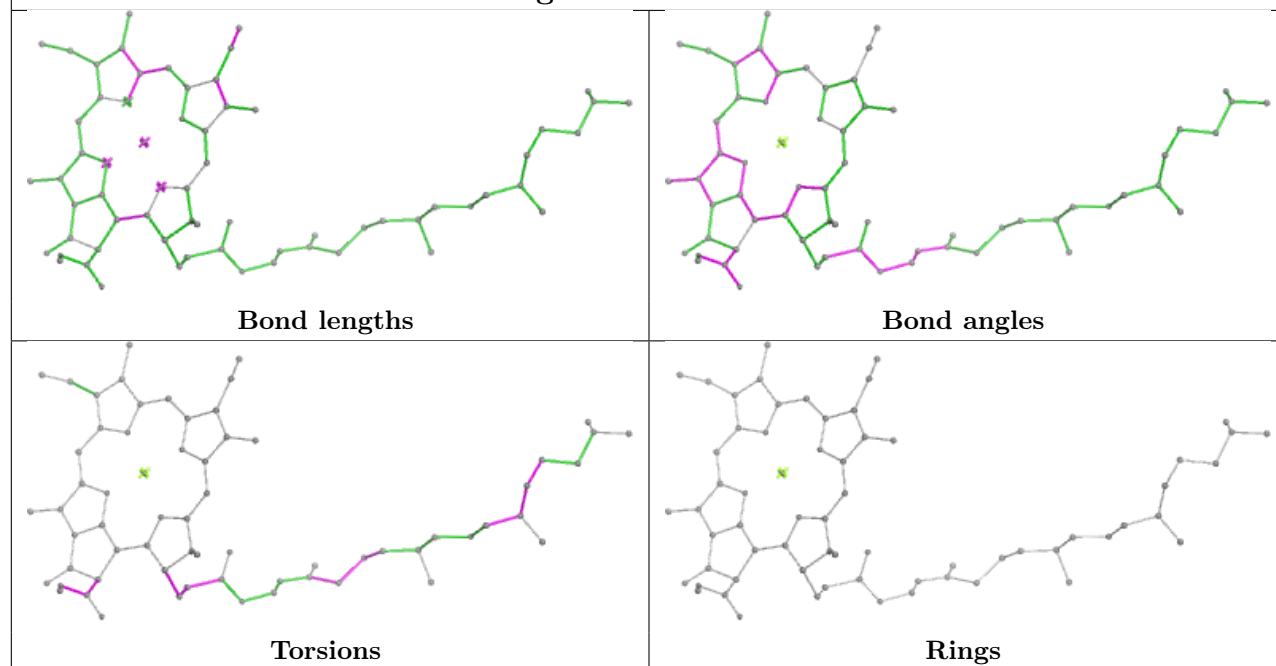




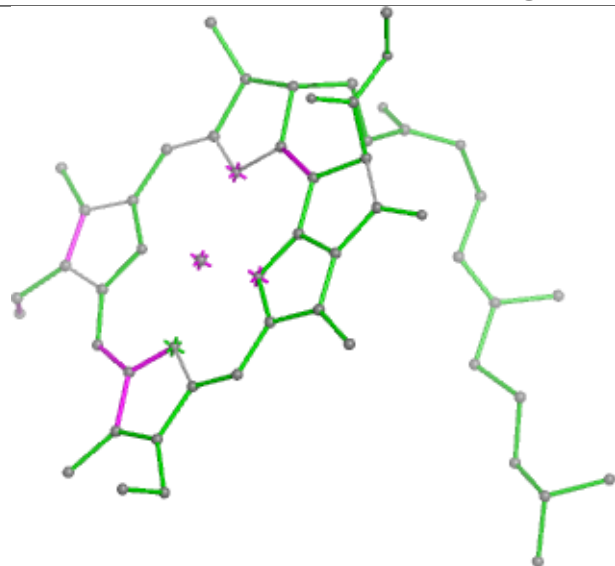
Ligand CLA Z 611



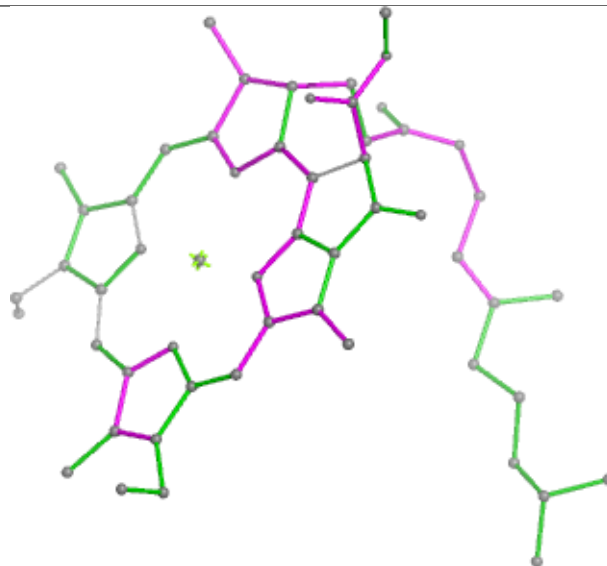
Ligand CLA 7 609



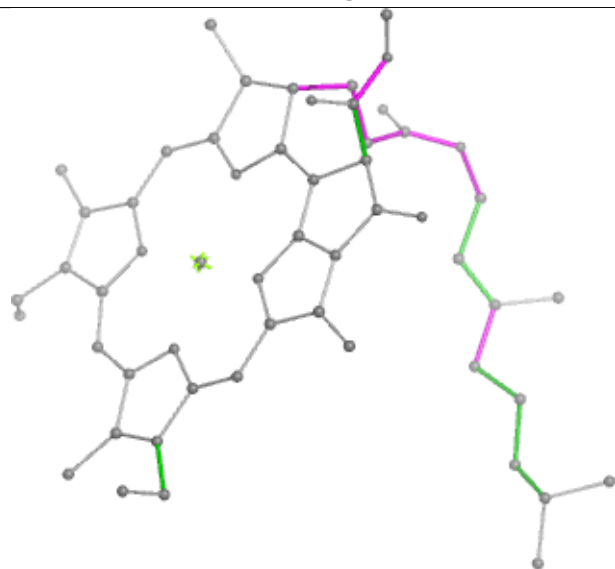
Ligand CLA 6 607



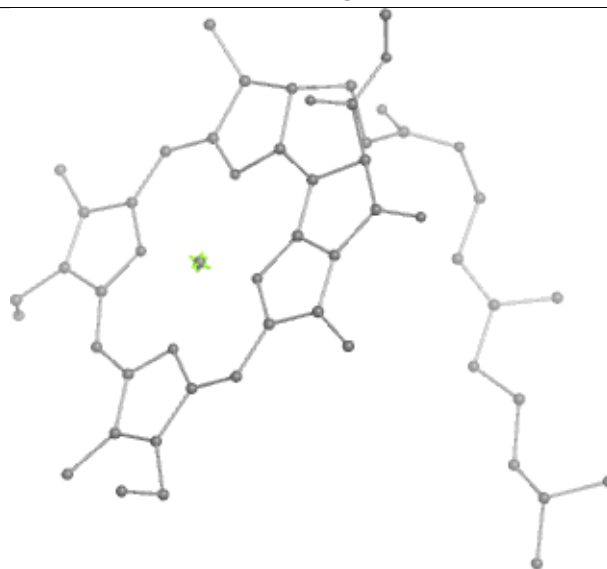
Bond lengths



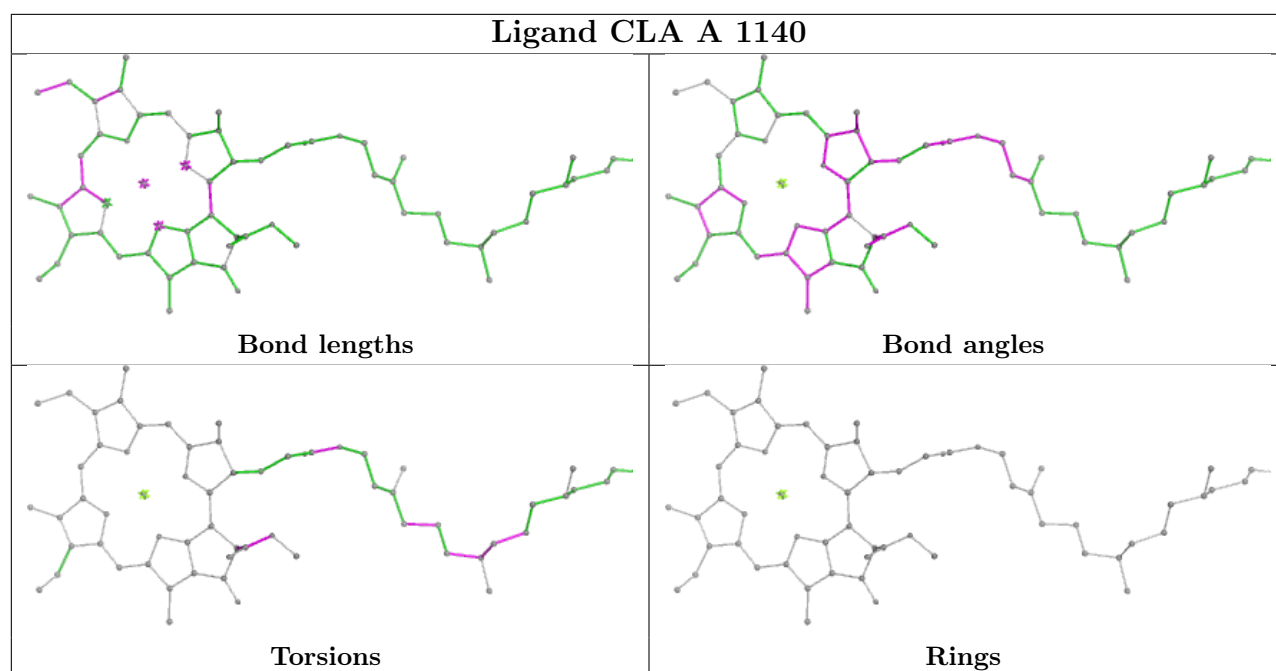
Bond angles

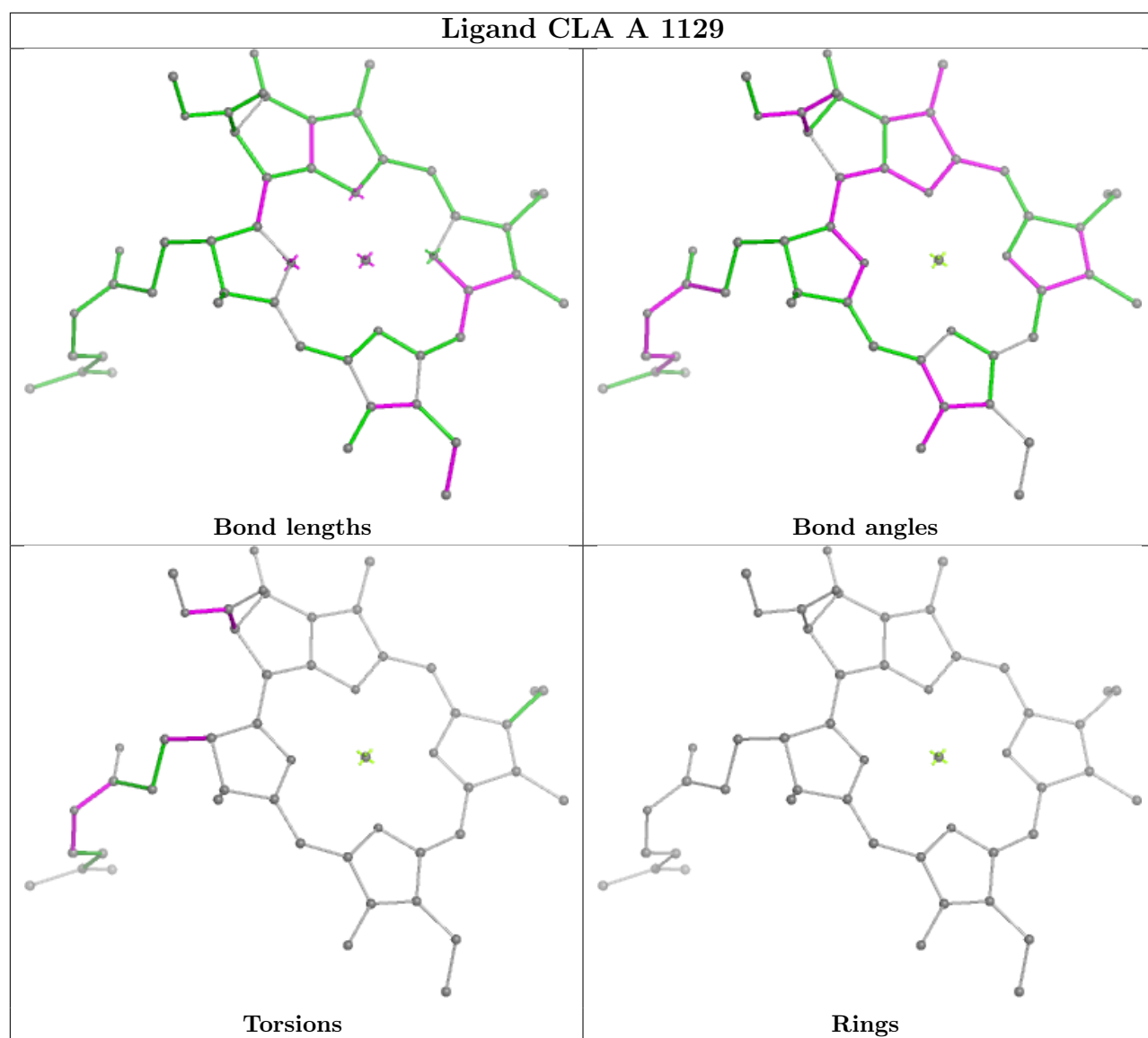


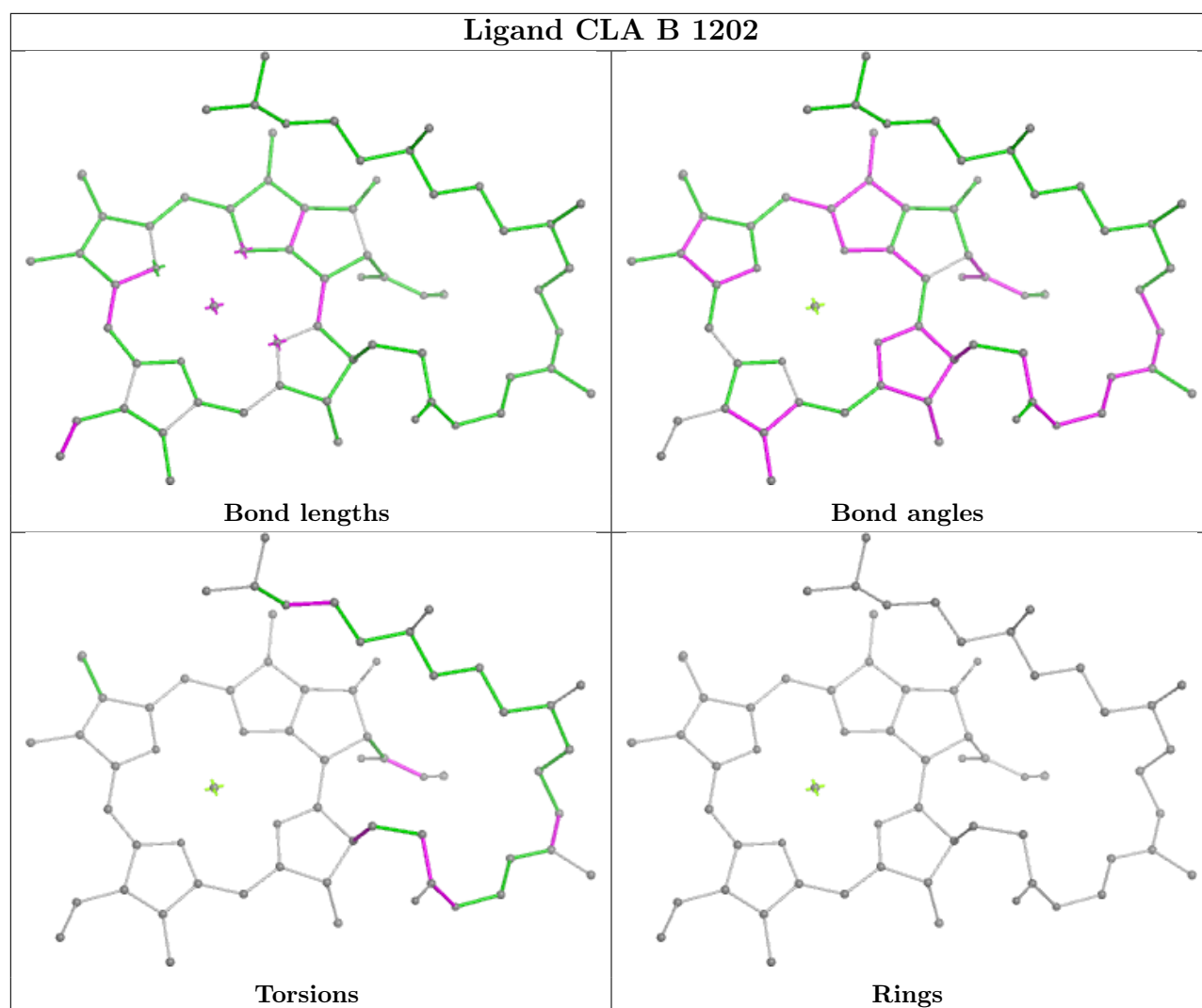
Torsions

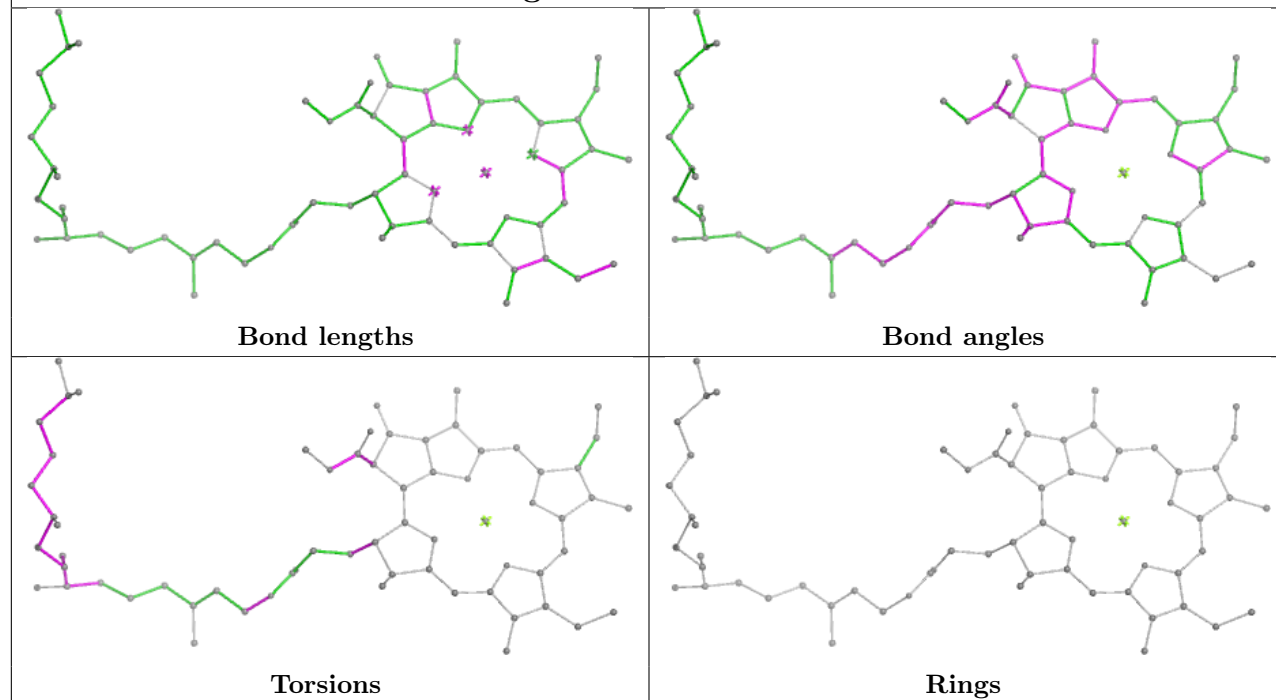
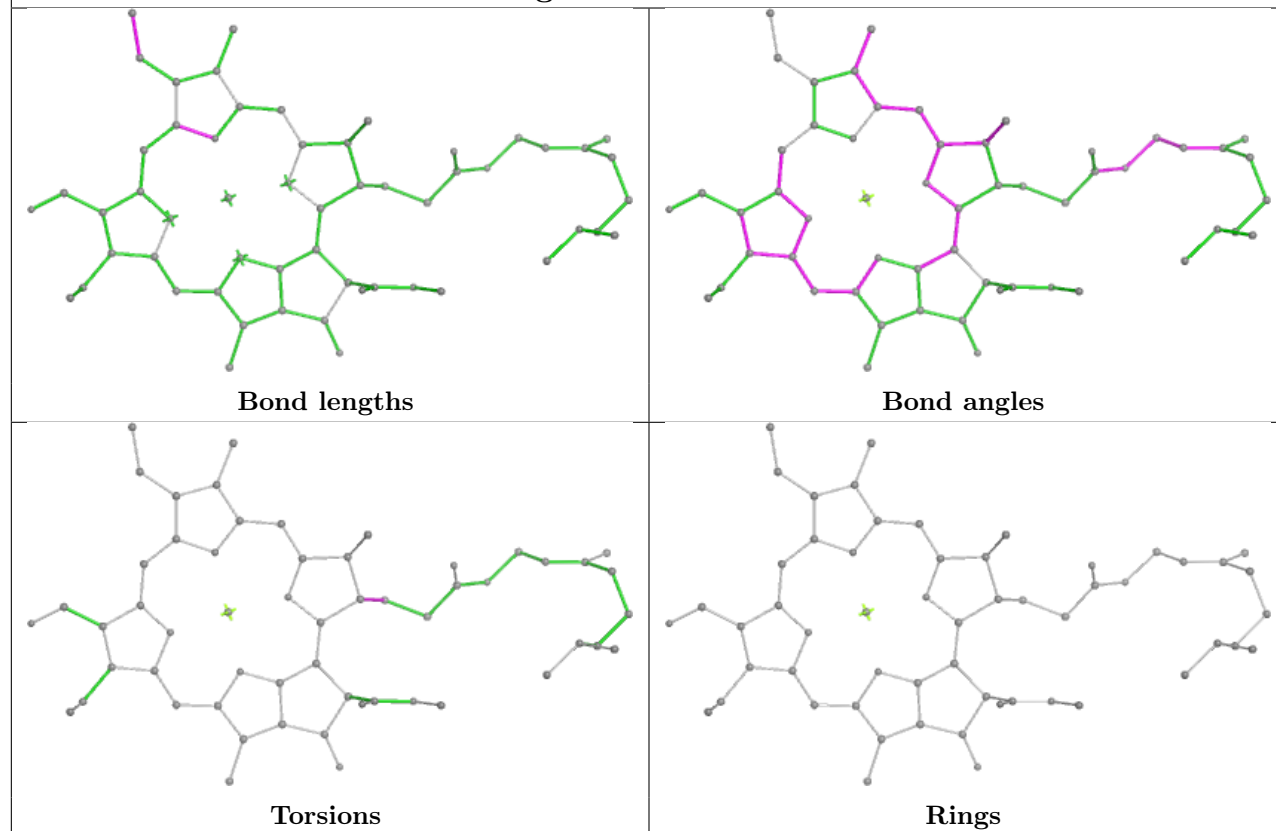


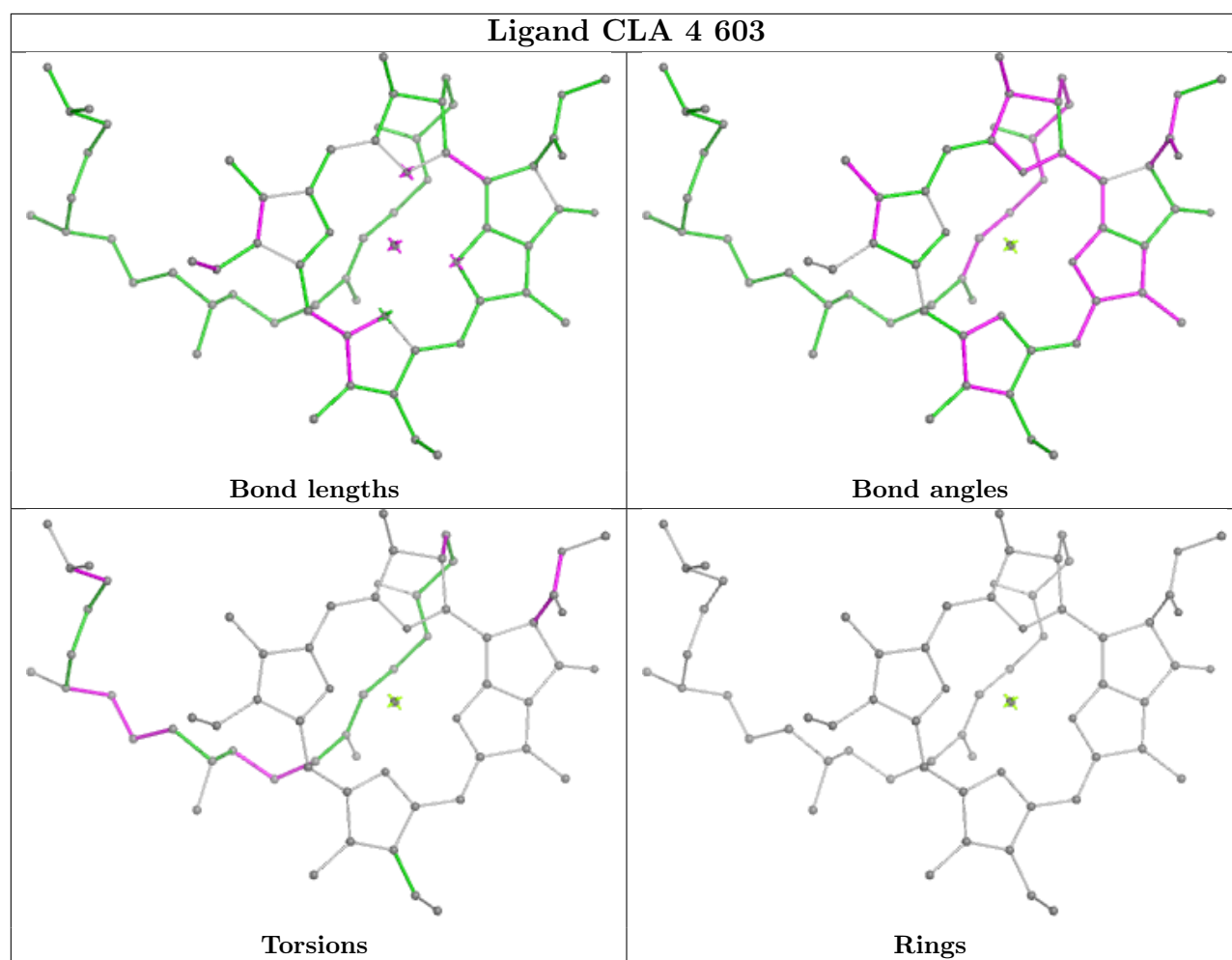
Rings

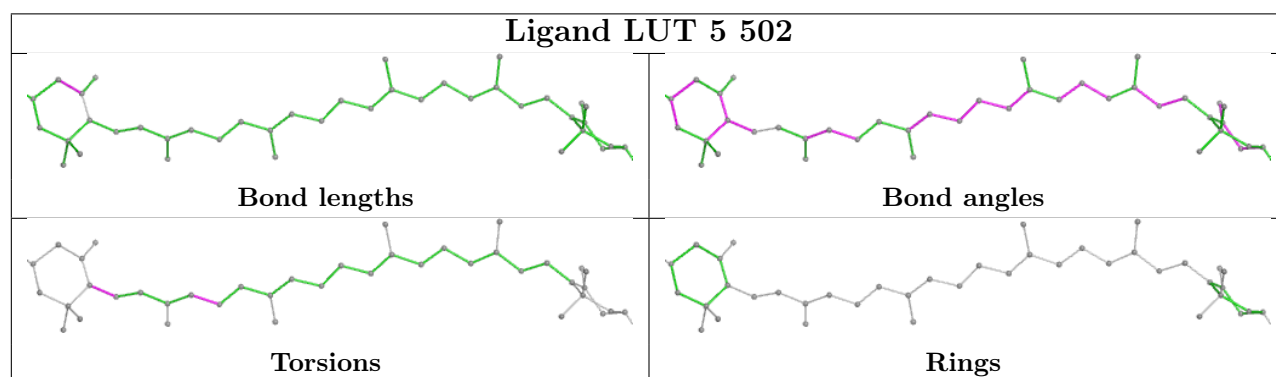
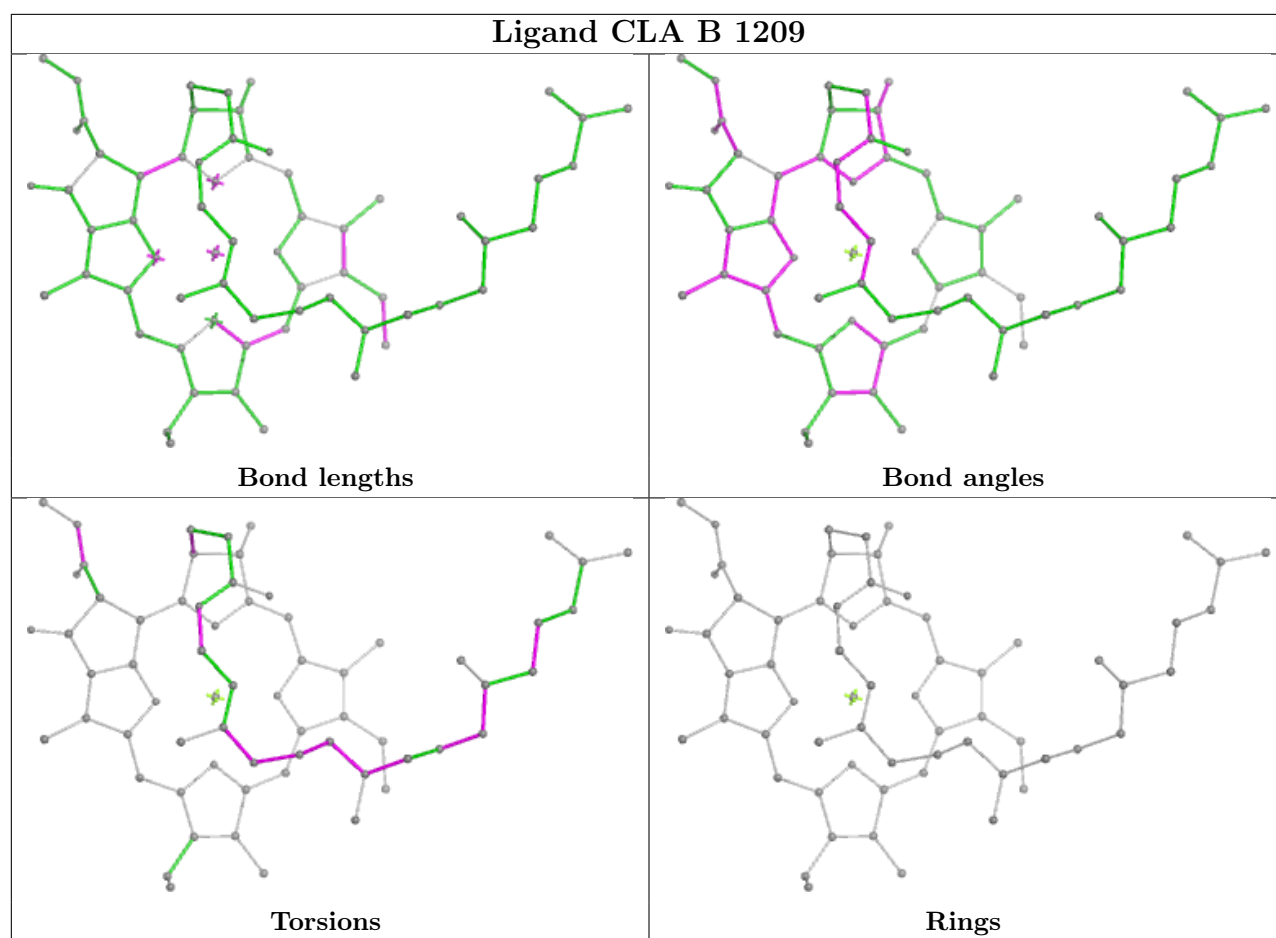




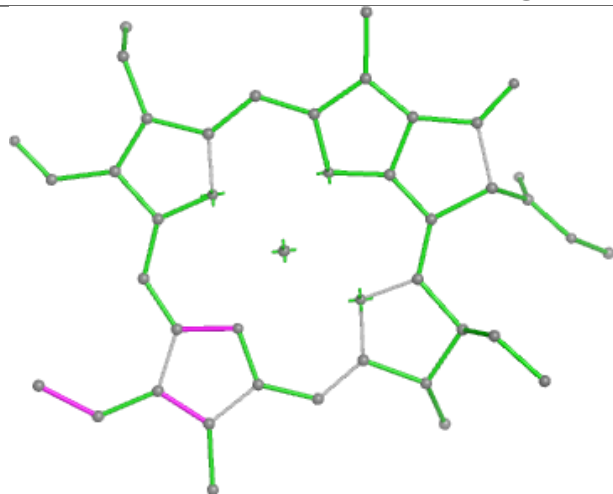


Ligand CLA B 1223**Ligand CHL 4 613**

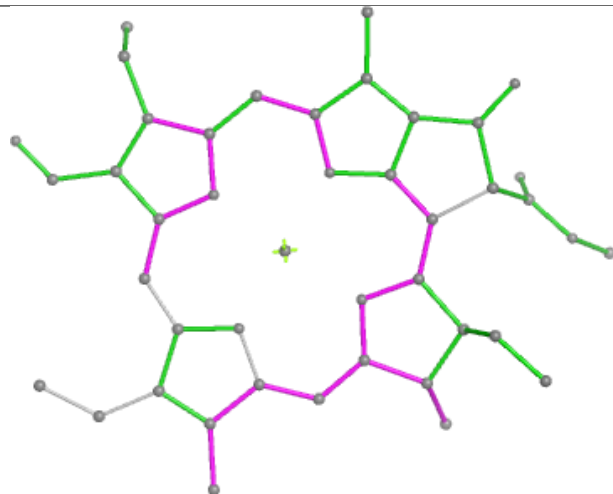




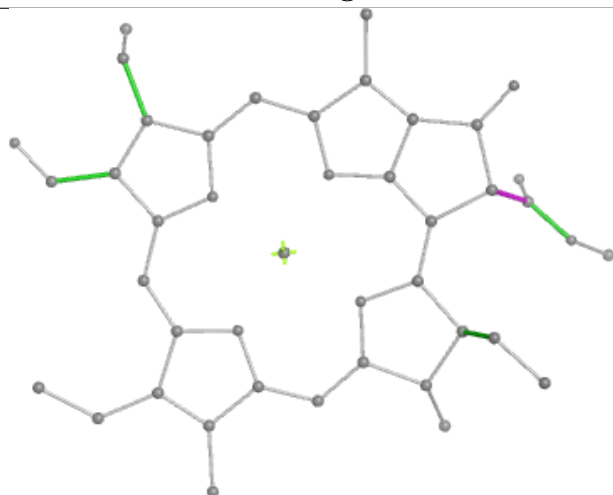
Ligand CHL 6 617



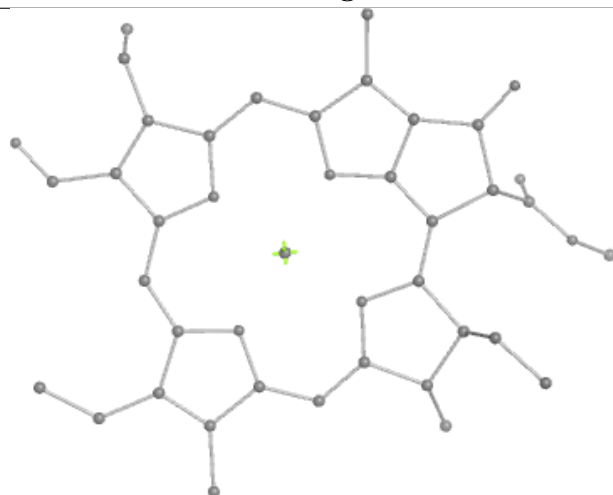
Bond lengths



Bond angles

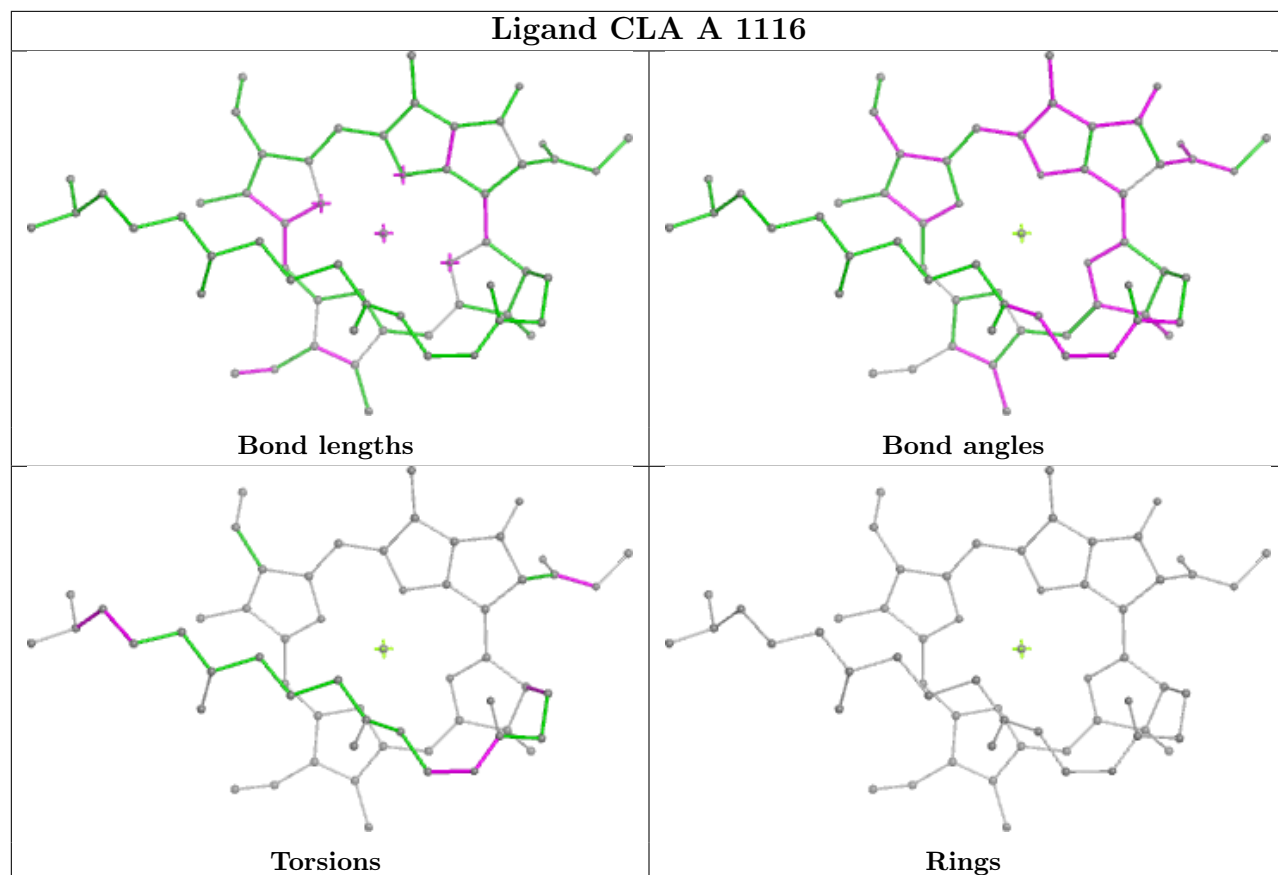


Torsions

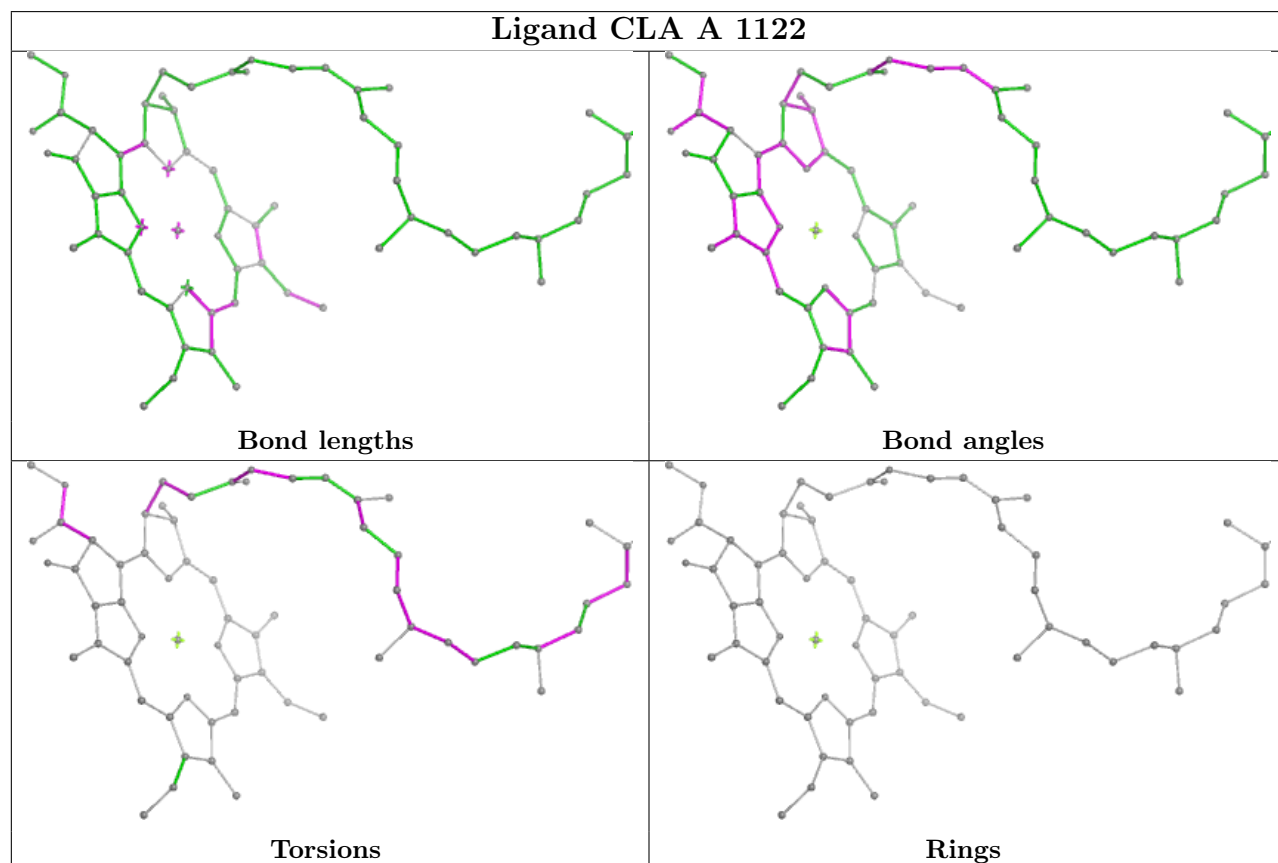


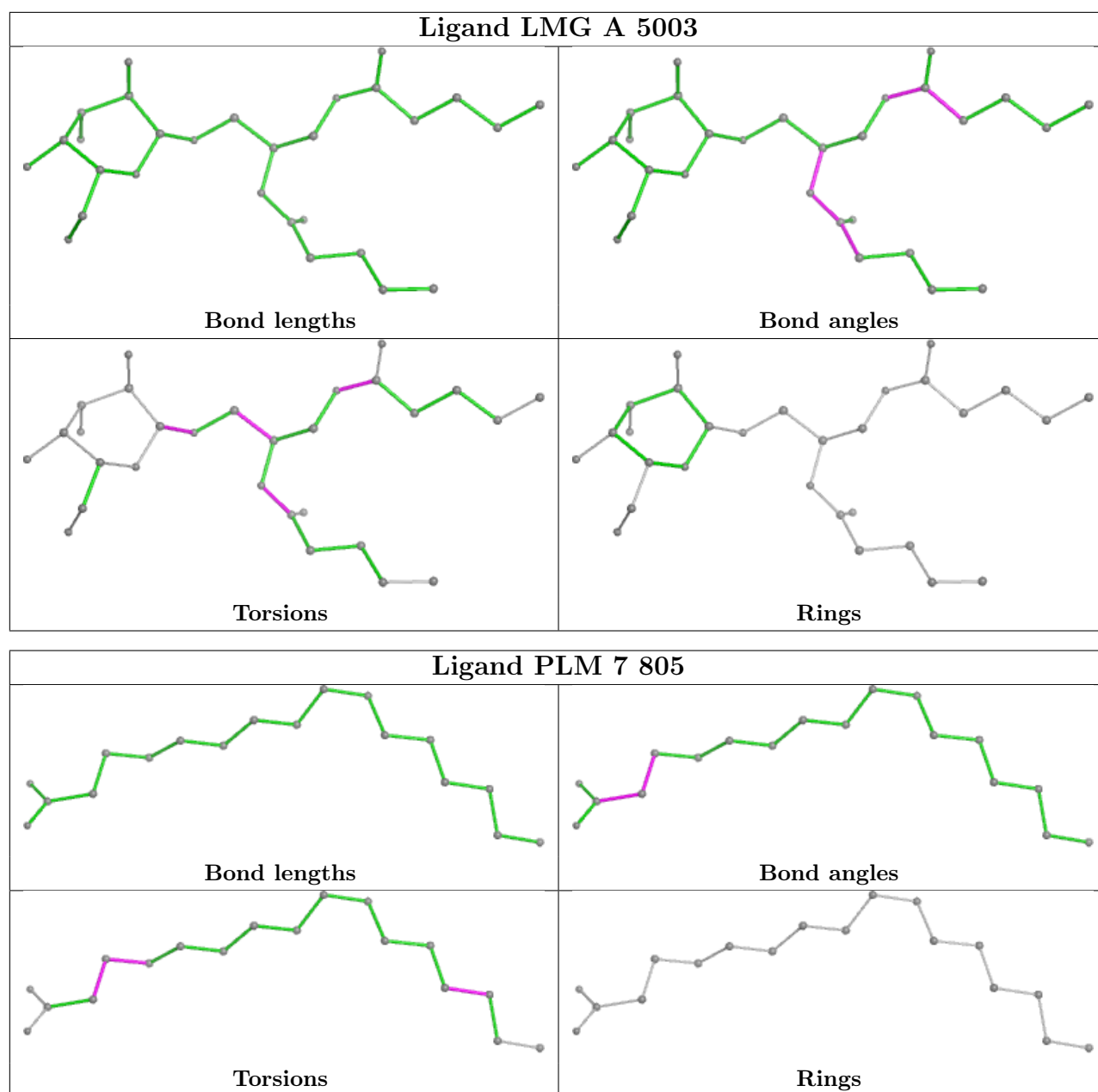
Rings

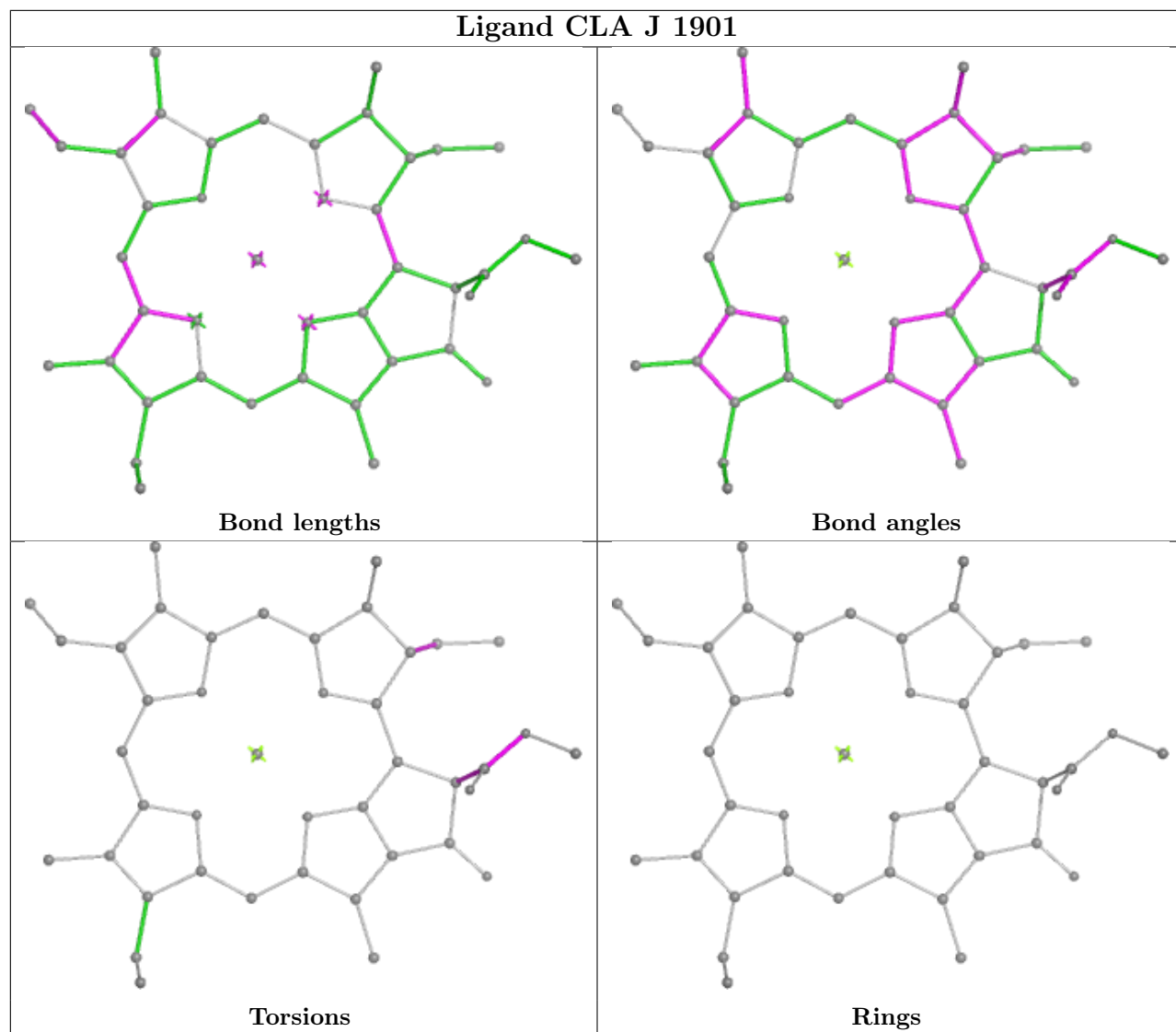
Ligand CLA A 1116



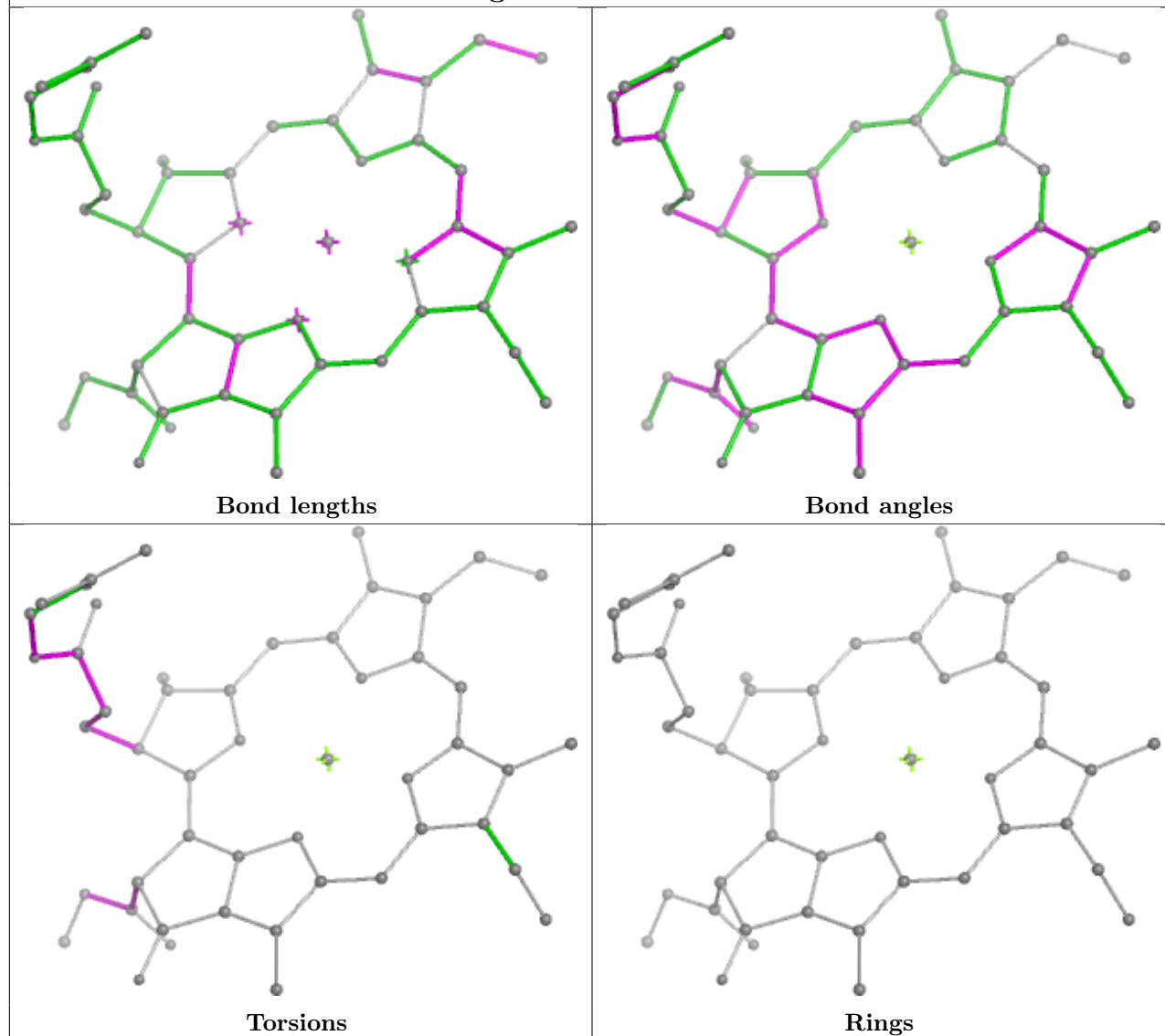
Ligand CLA A 1122



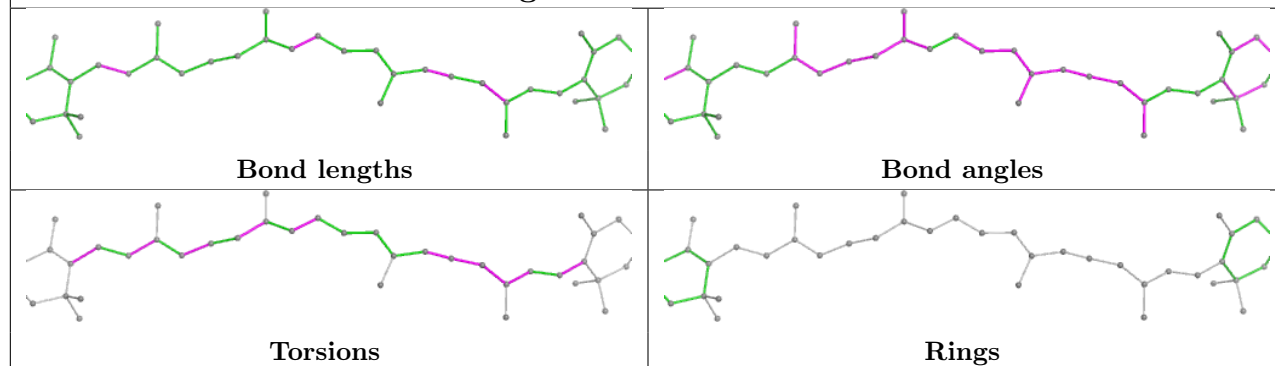


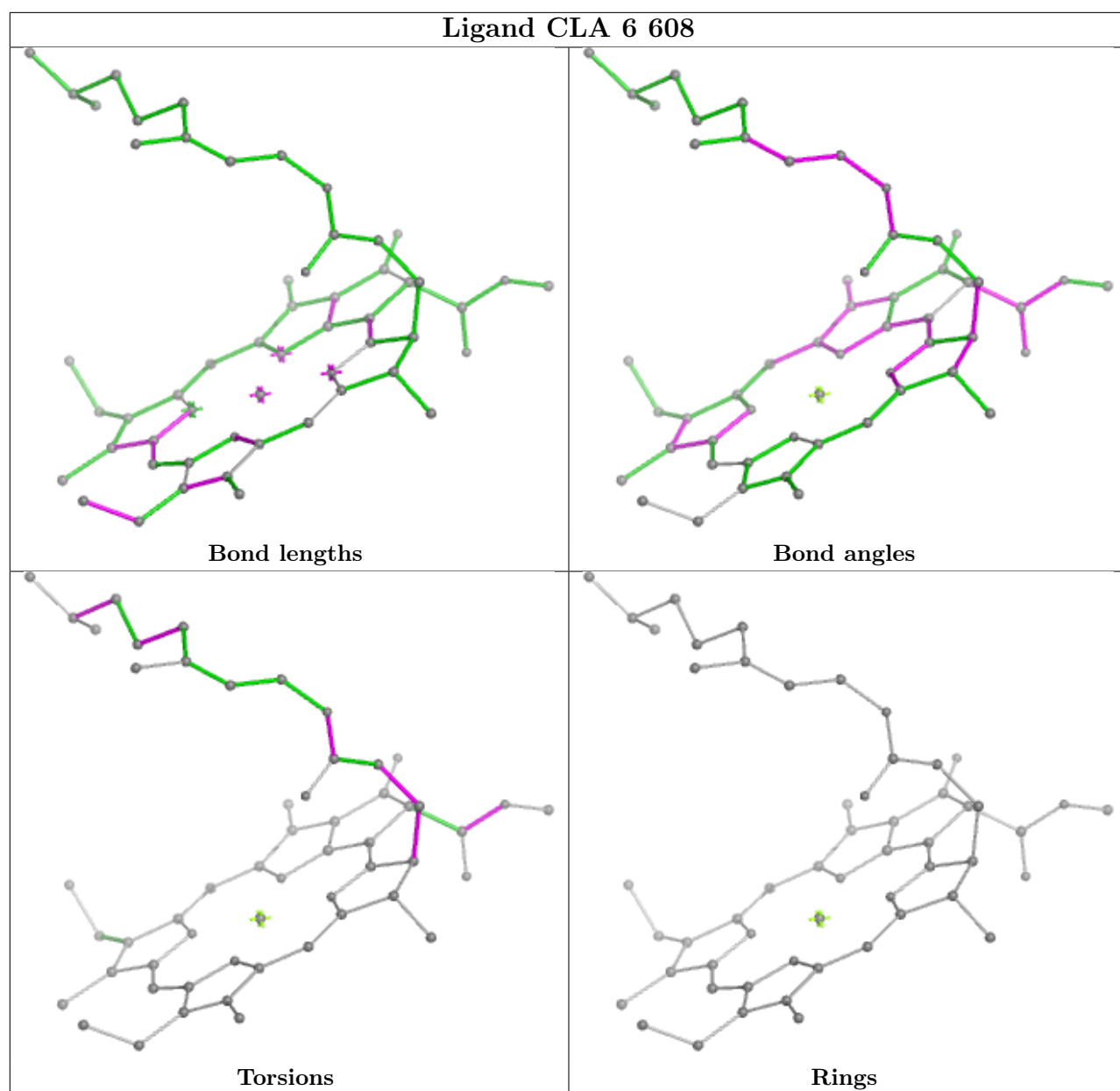


Ligand CLA 9 606

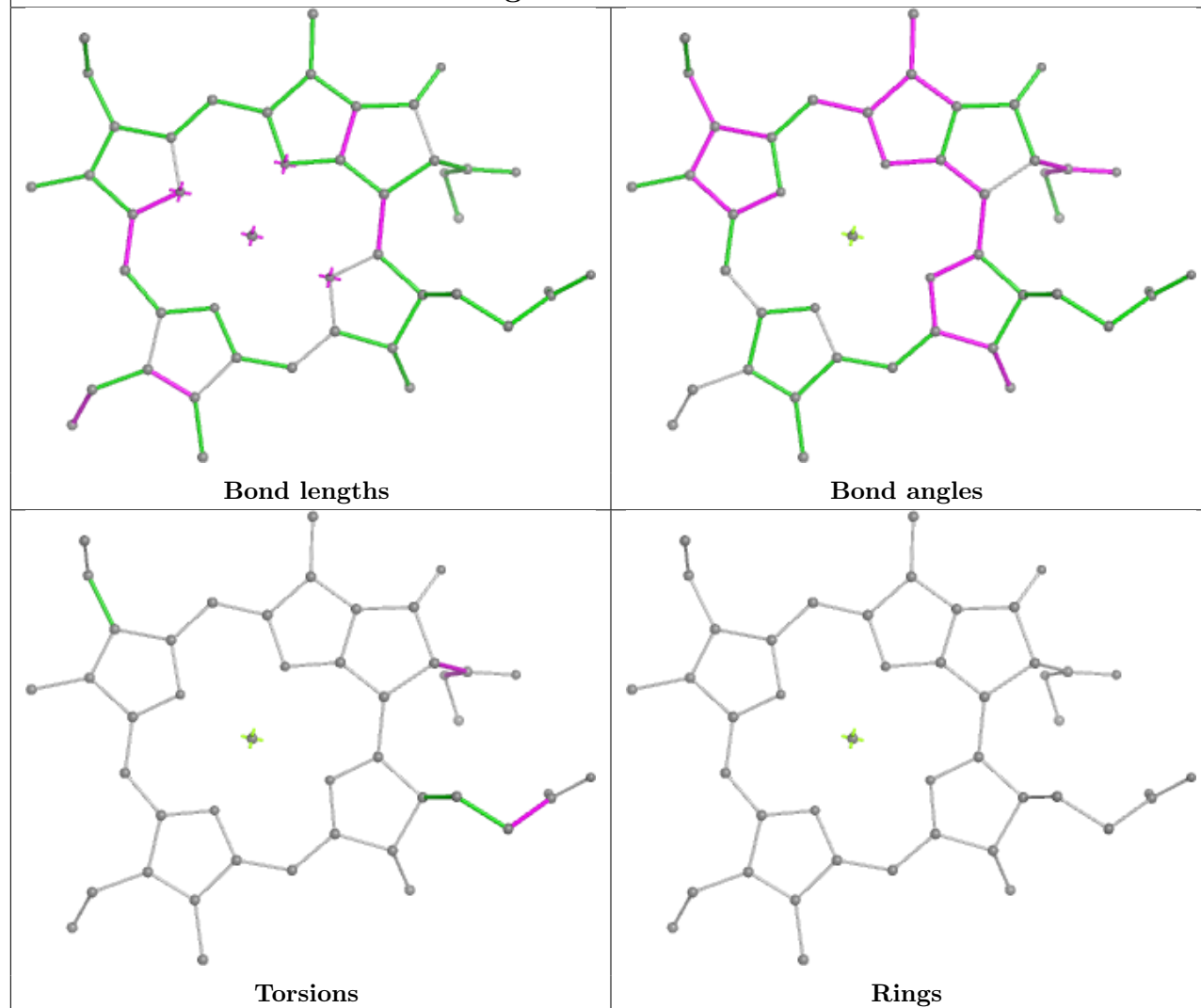


Ligand BCR K 4001

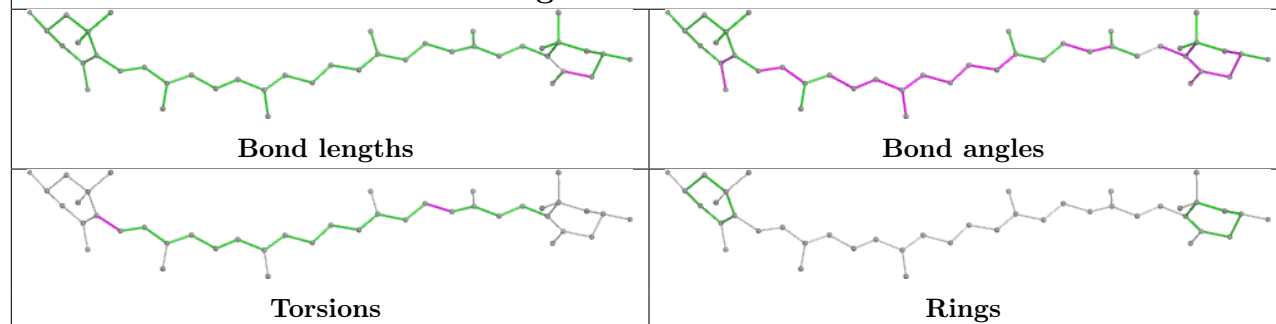


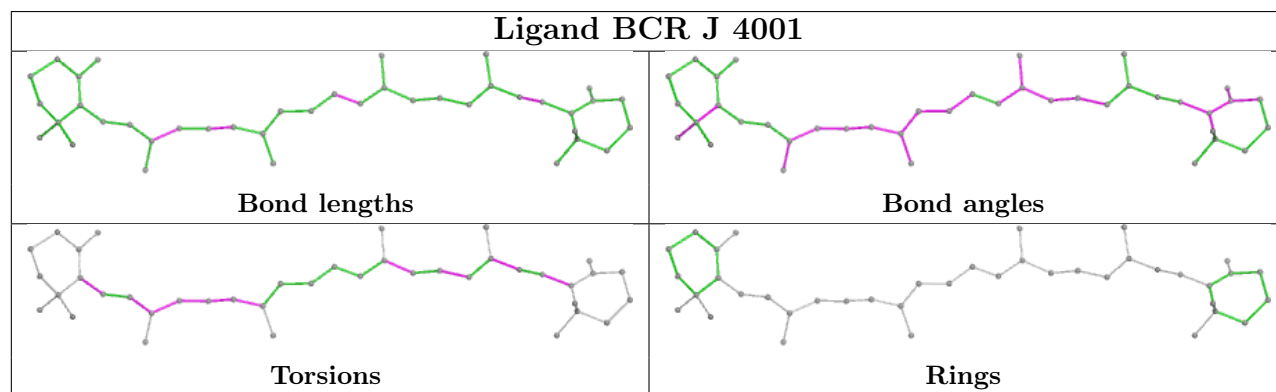
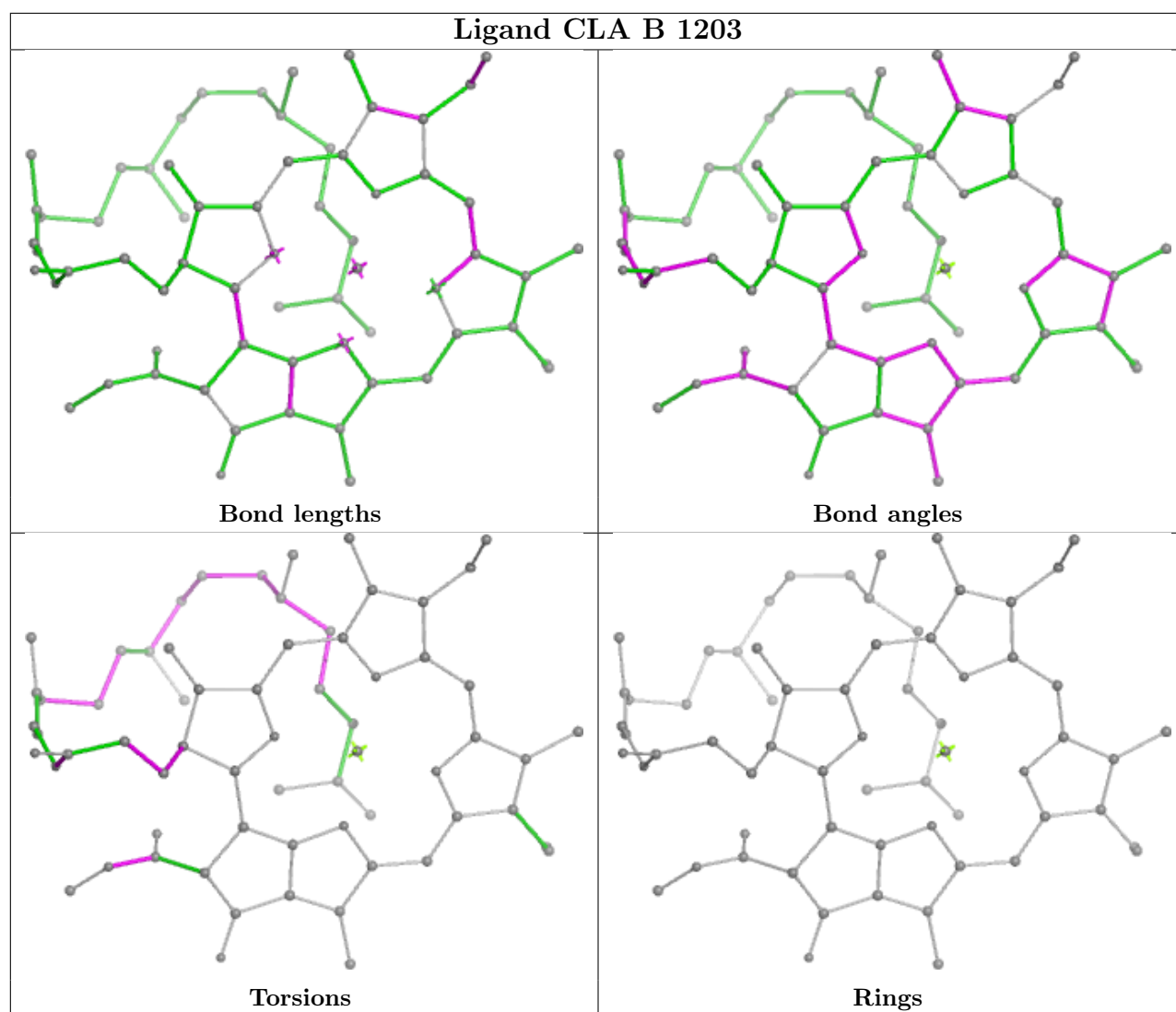


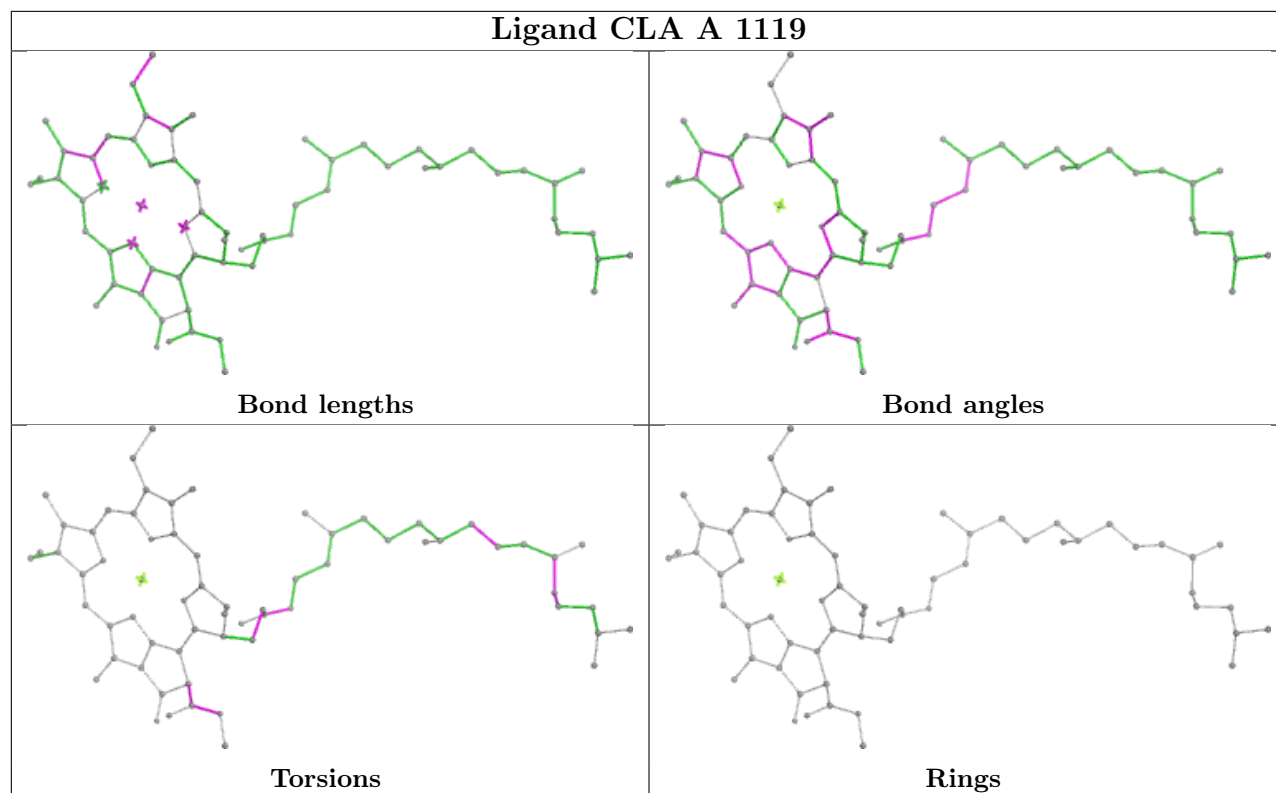
Ligand CLA 1 602



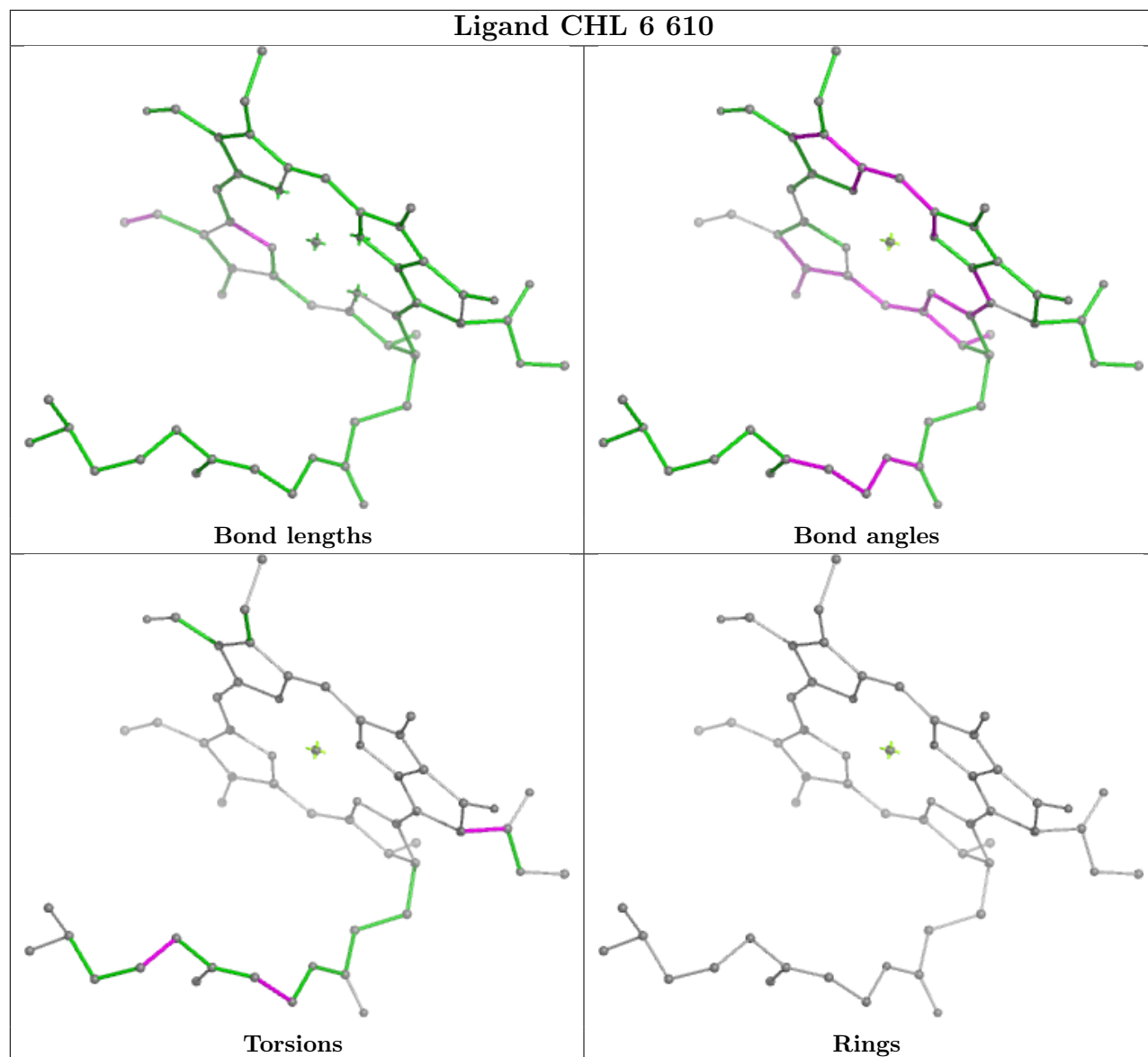
Ligand LUT 7 501

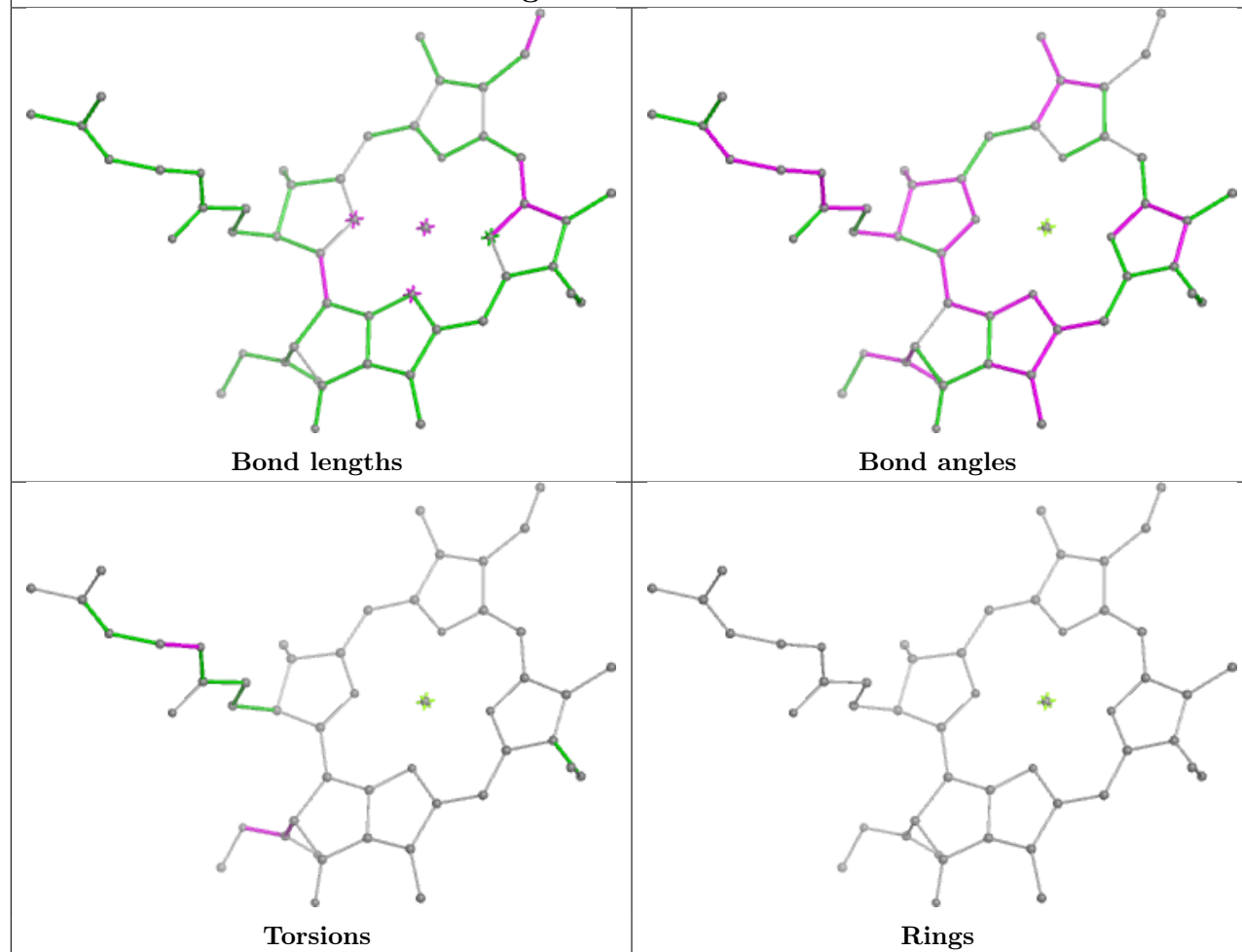
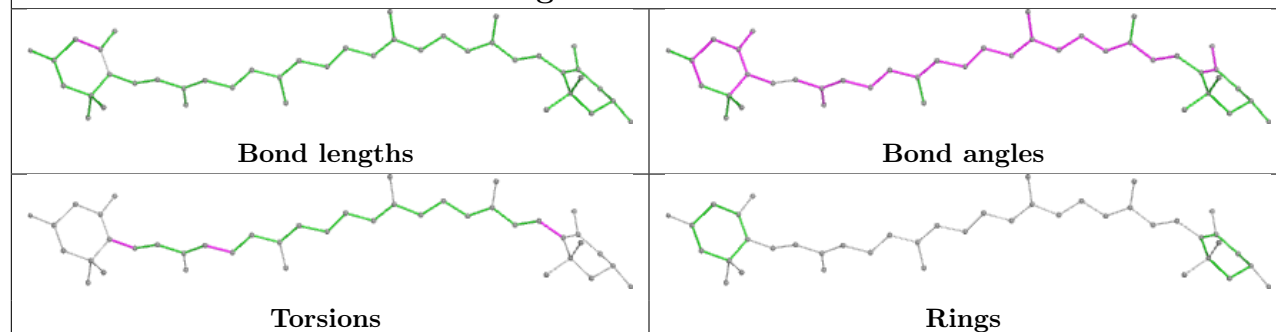


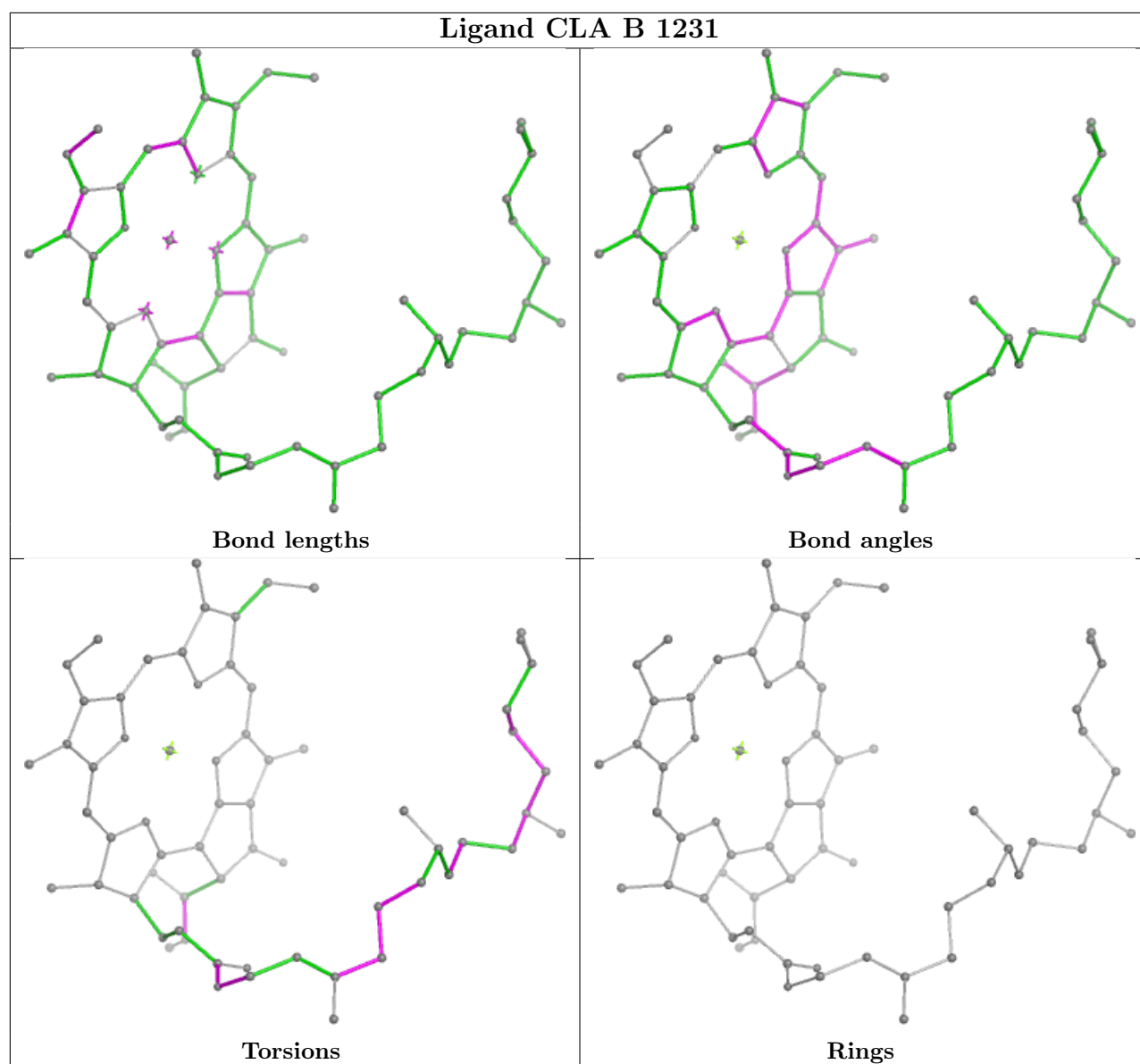


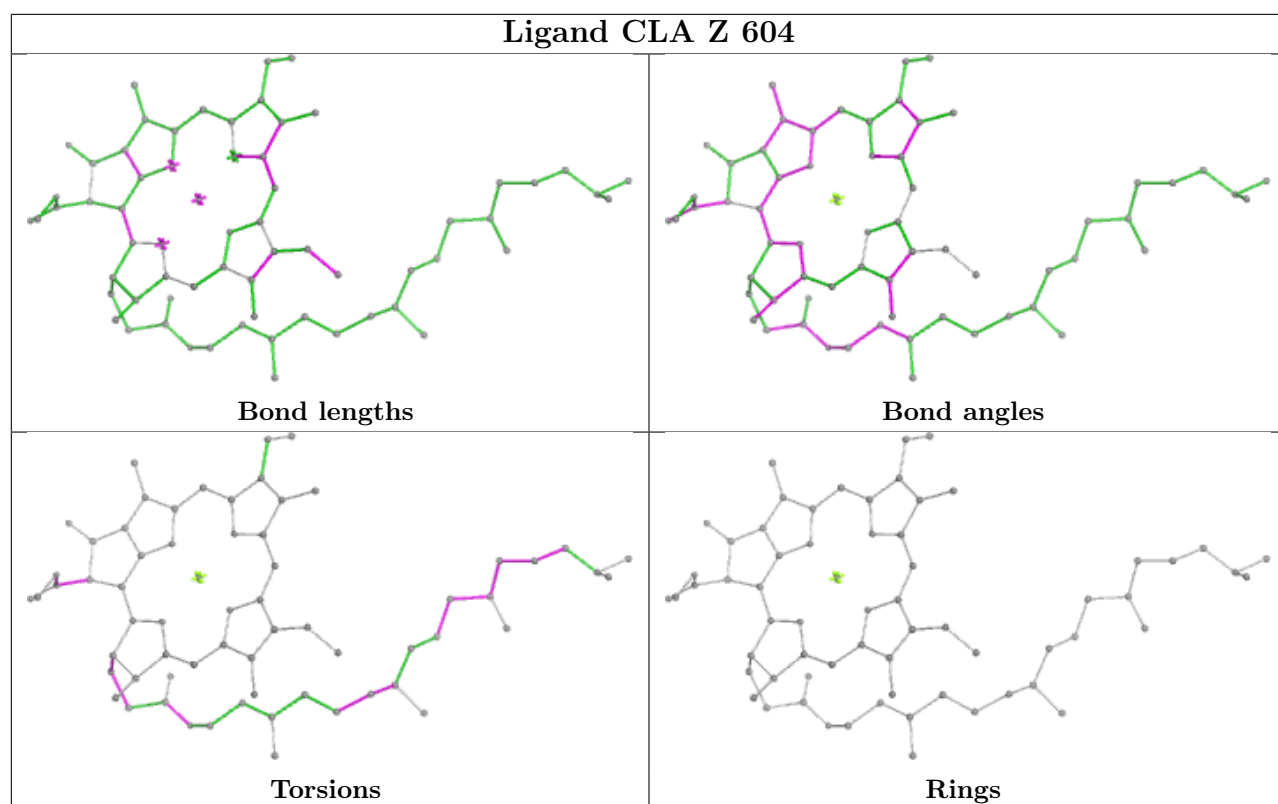


Ligand CHL 6 610

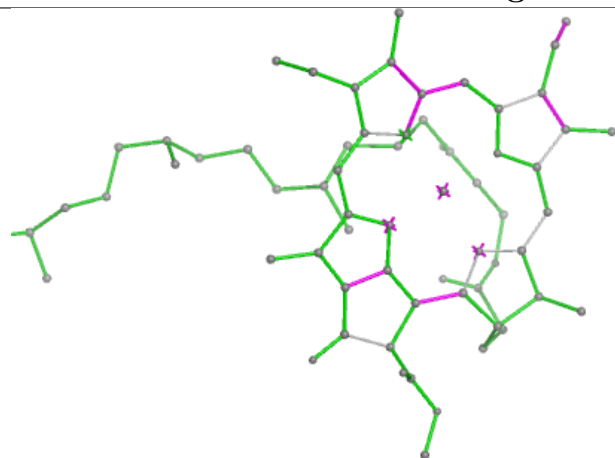


Ligand CLA 7 611**Ligand LUT 8 502**

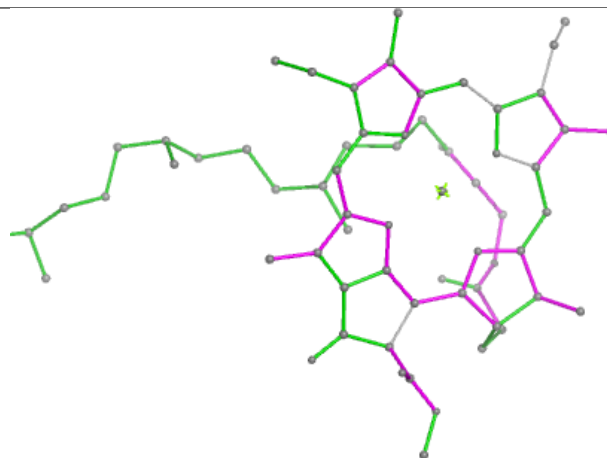




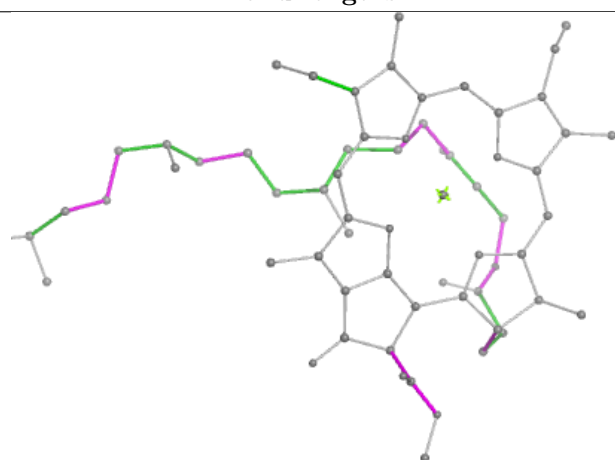
Ligand CLA B 1224



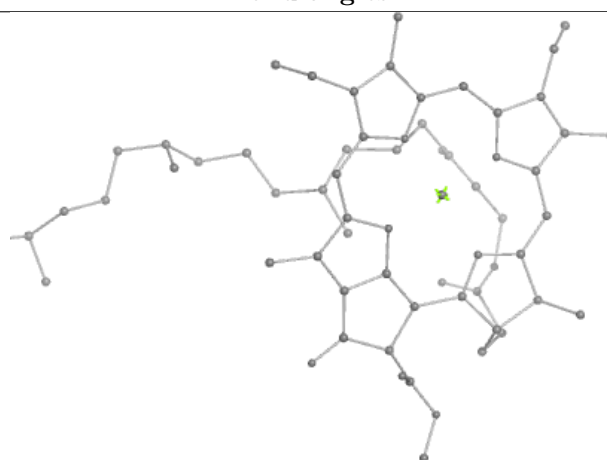
Bond lengths



Bond angles

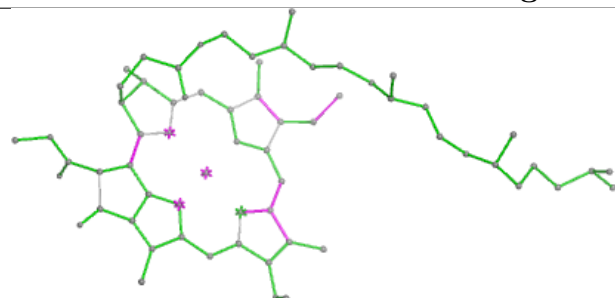


Torsions

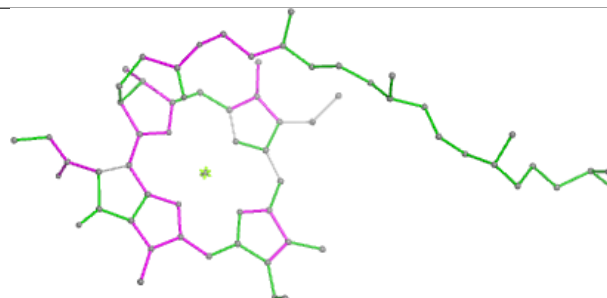


Rings

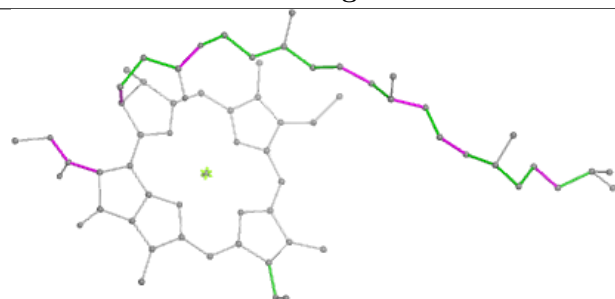
Ligand CLA 1 601



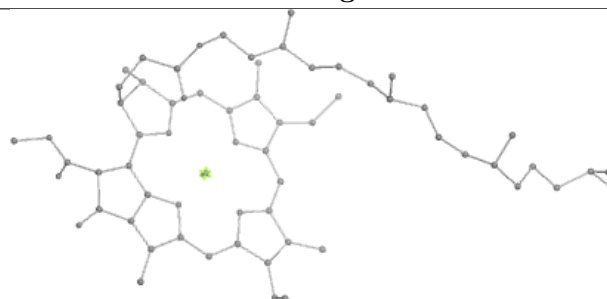
Bond lengths



Bond angles

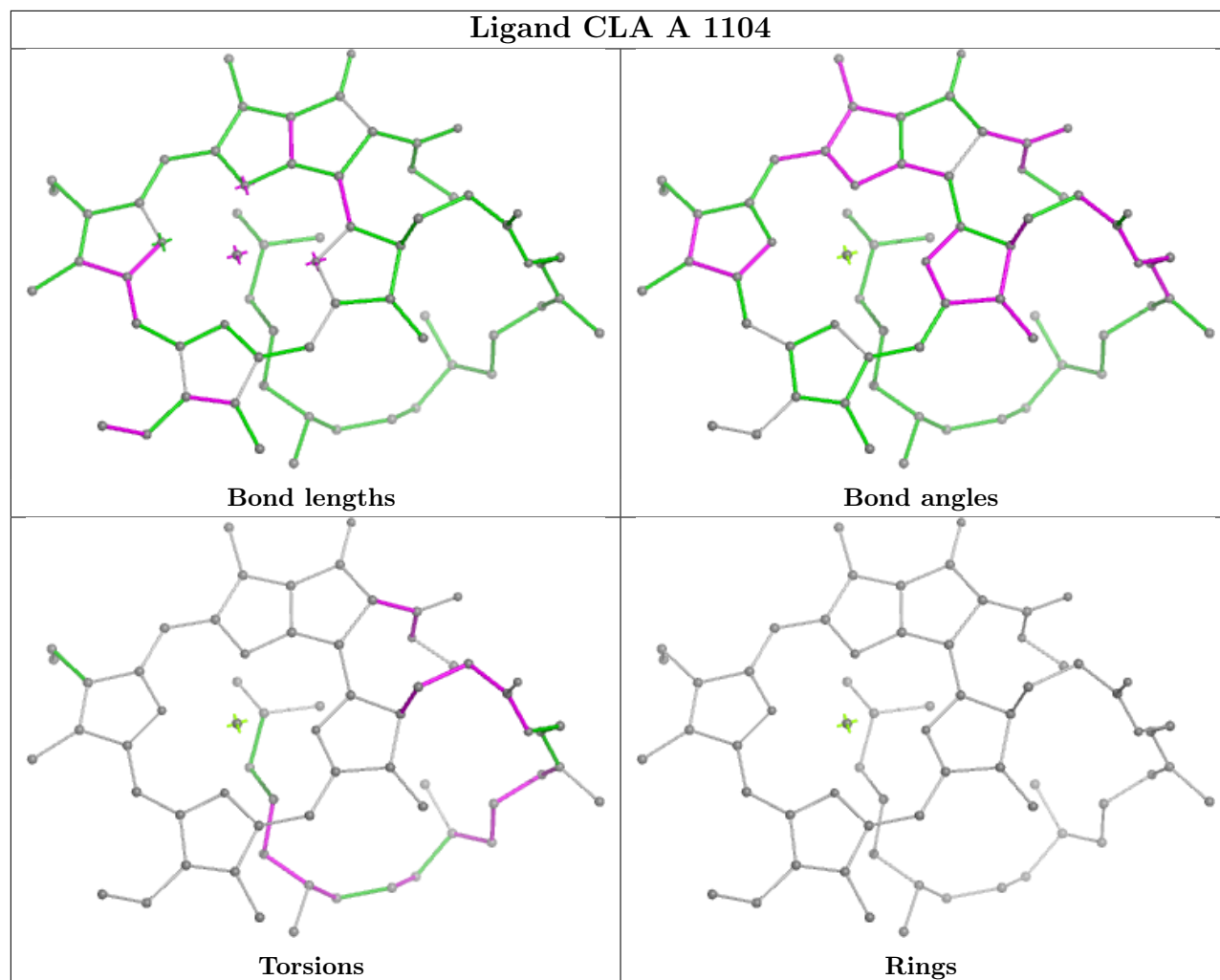


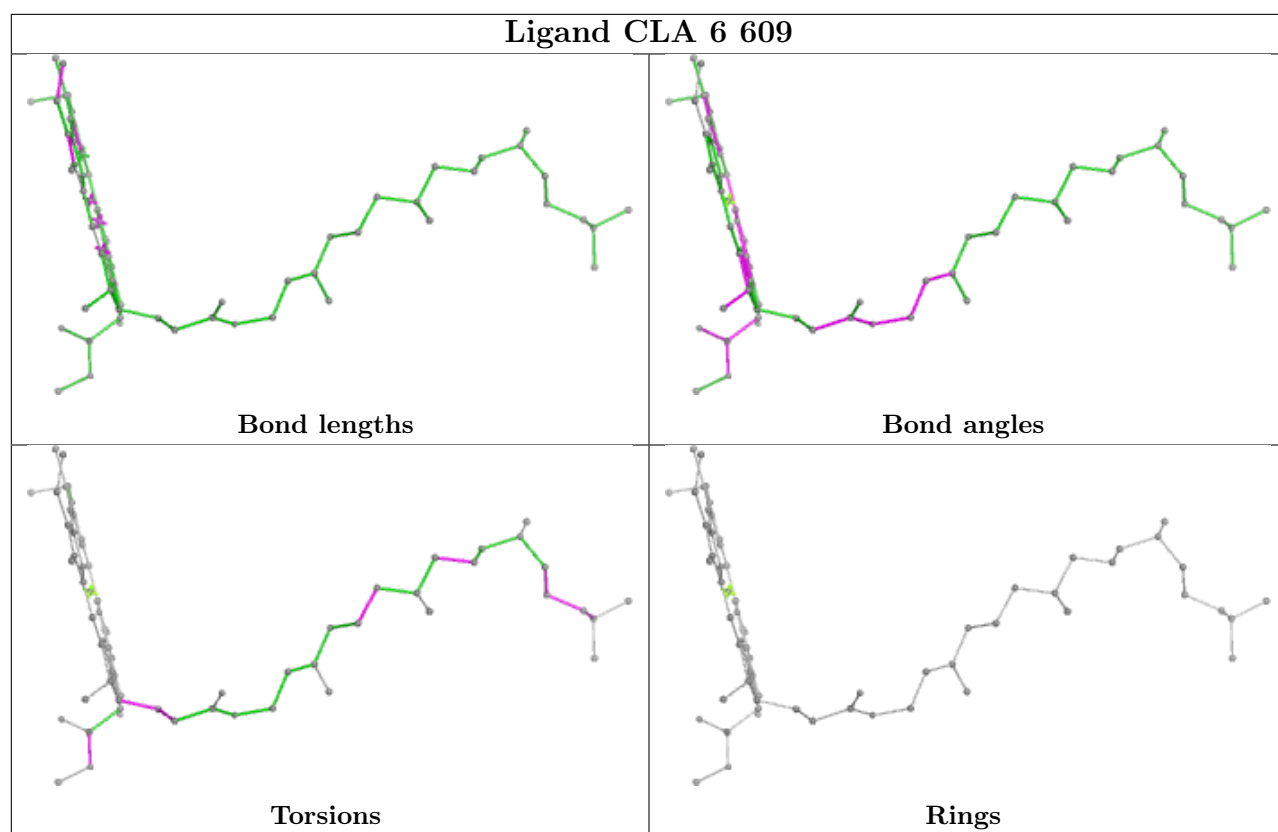
Torsions



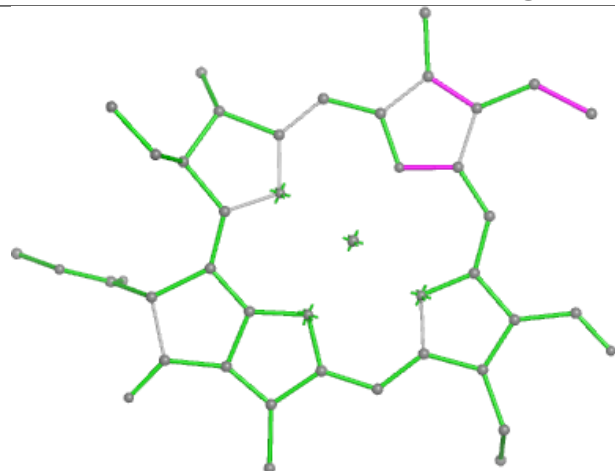
Rings

Ligand CLA A 1104

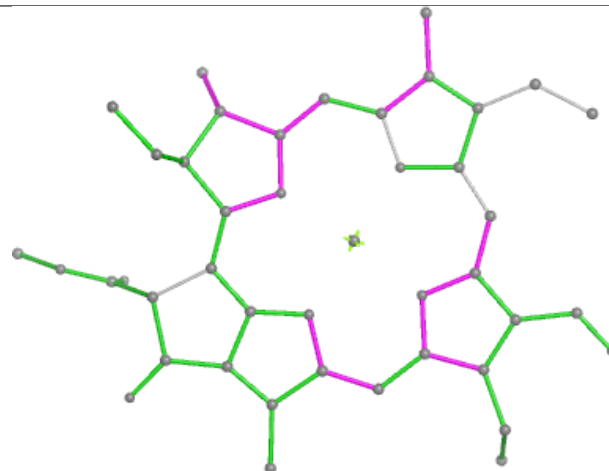




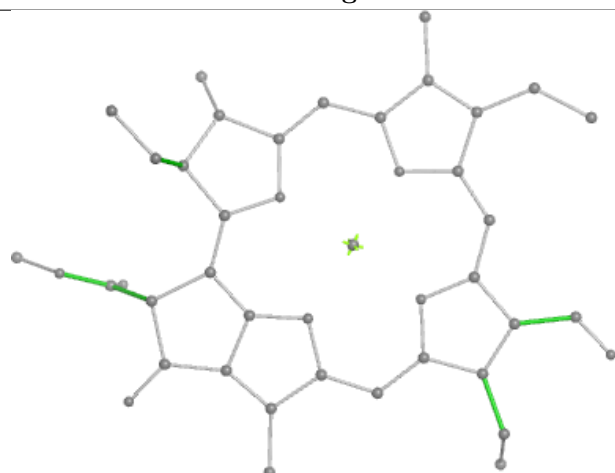
Ligand CHL 5 617



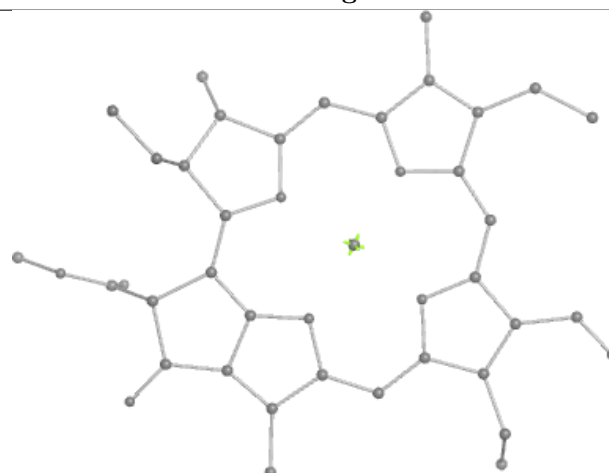
Bond lengths



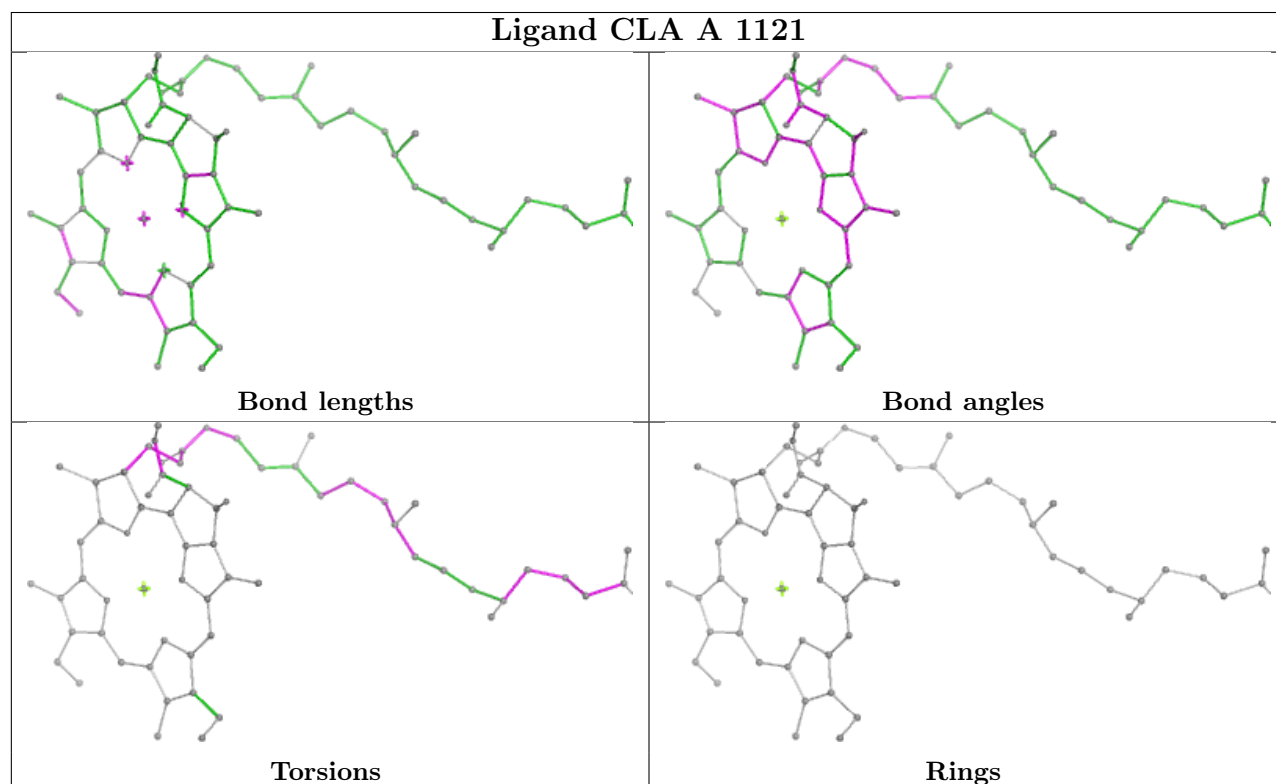
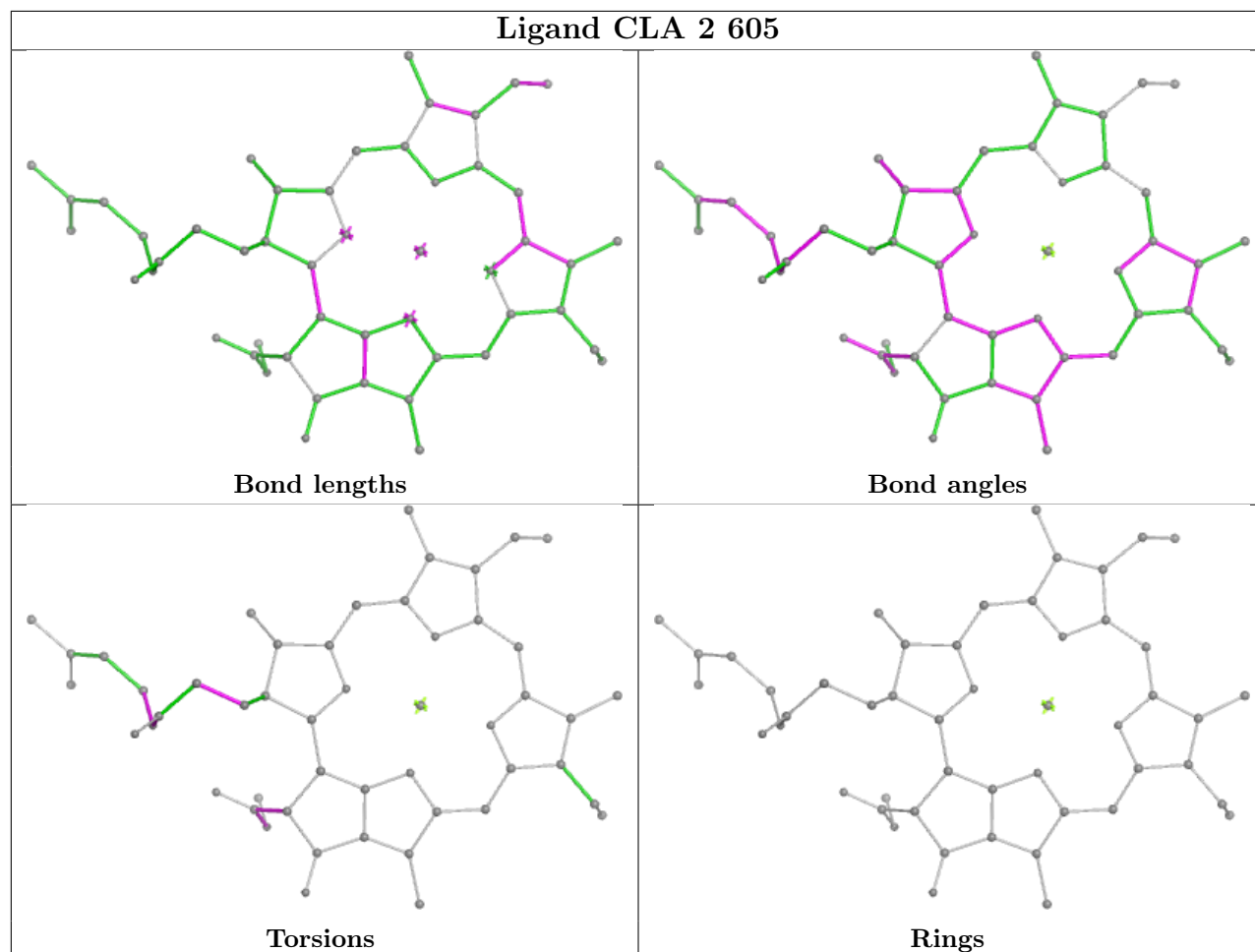
Bond angles



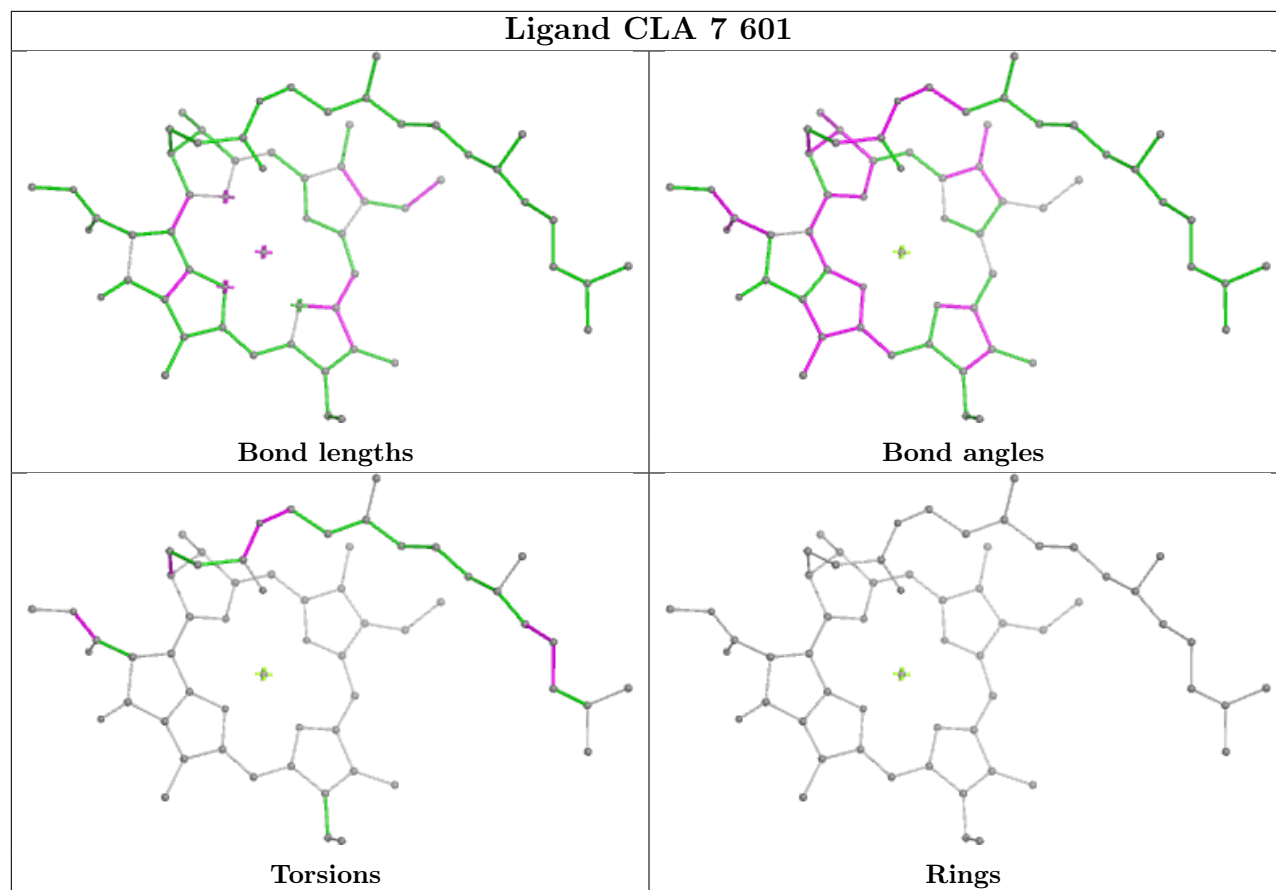
Torsions

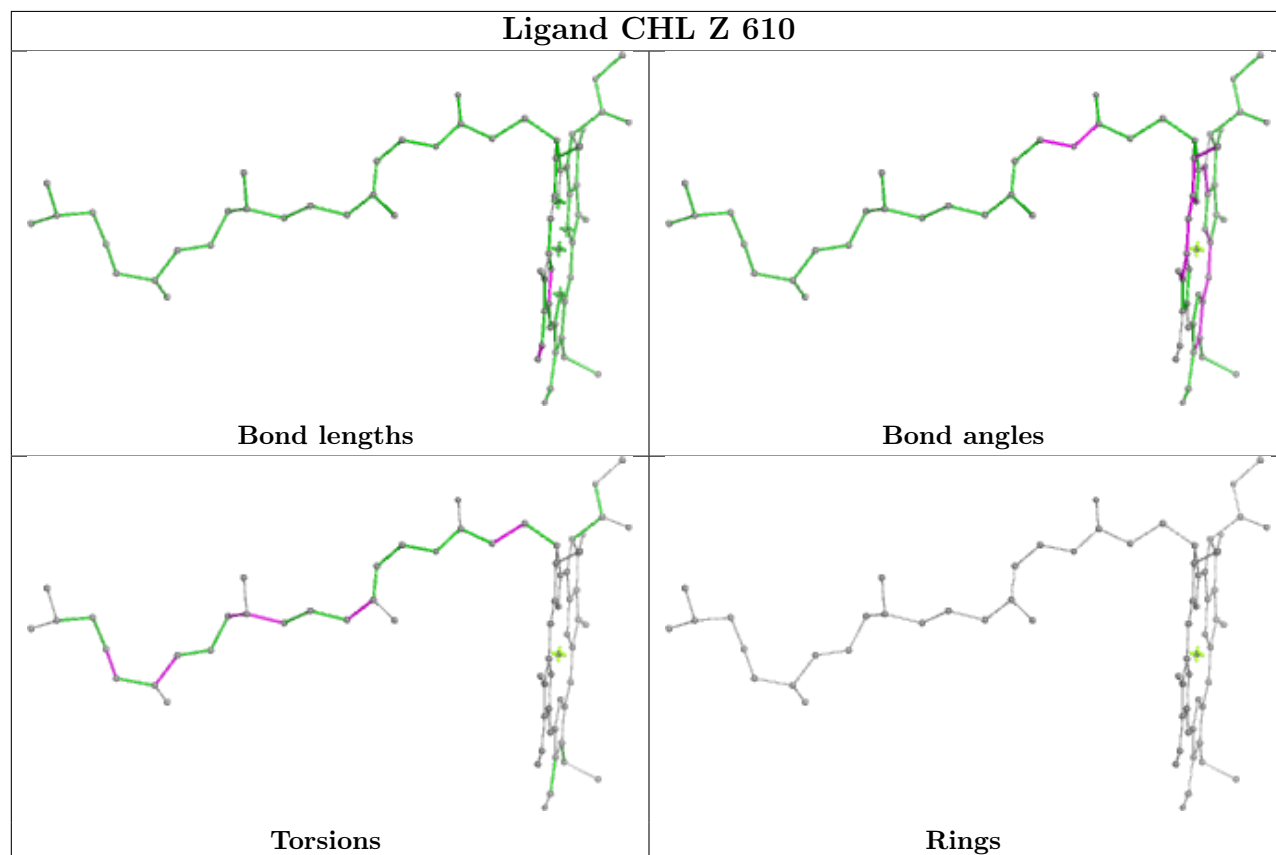
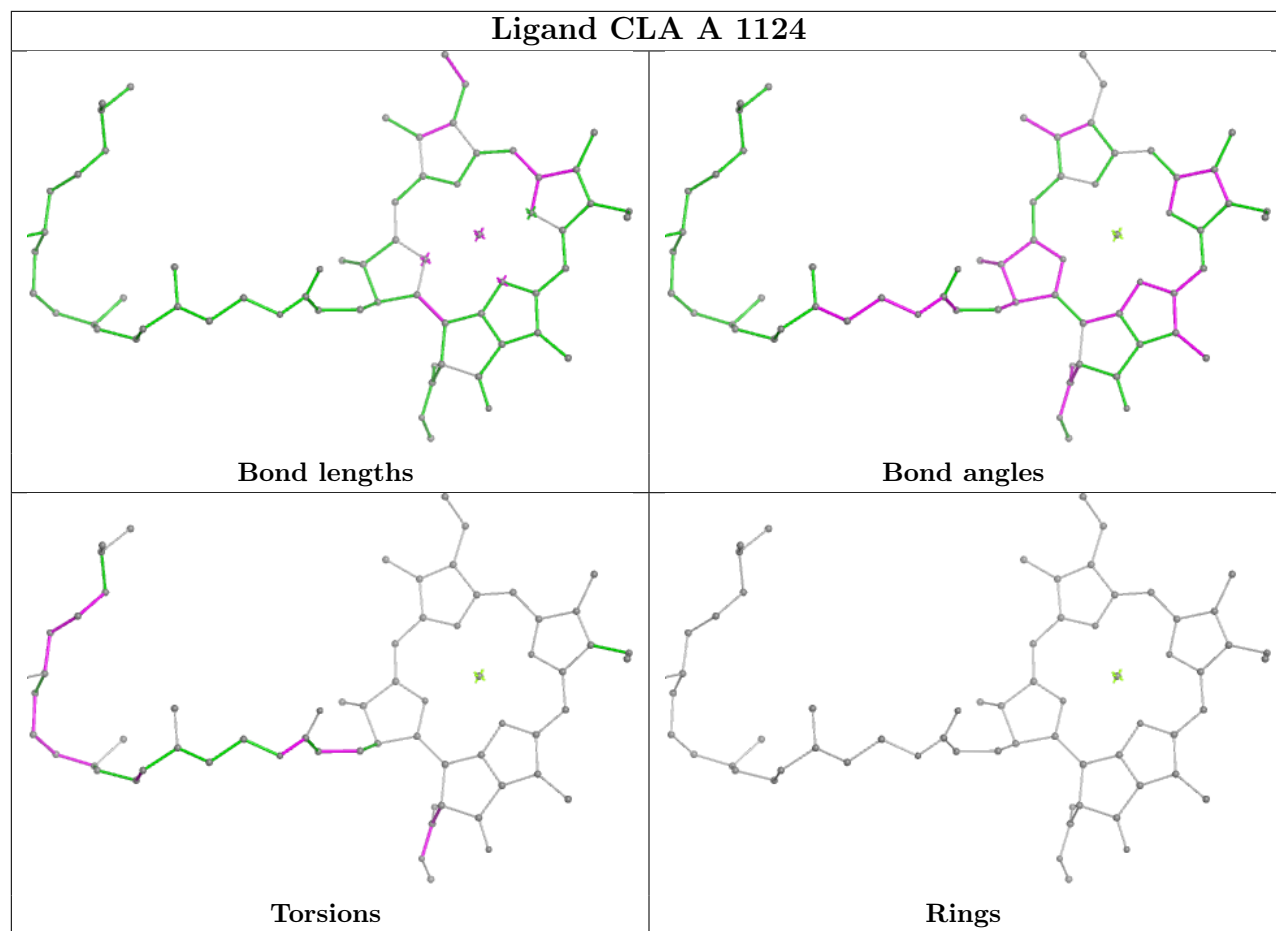


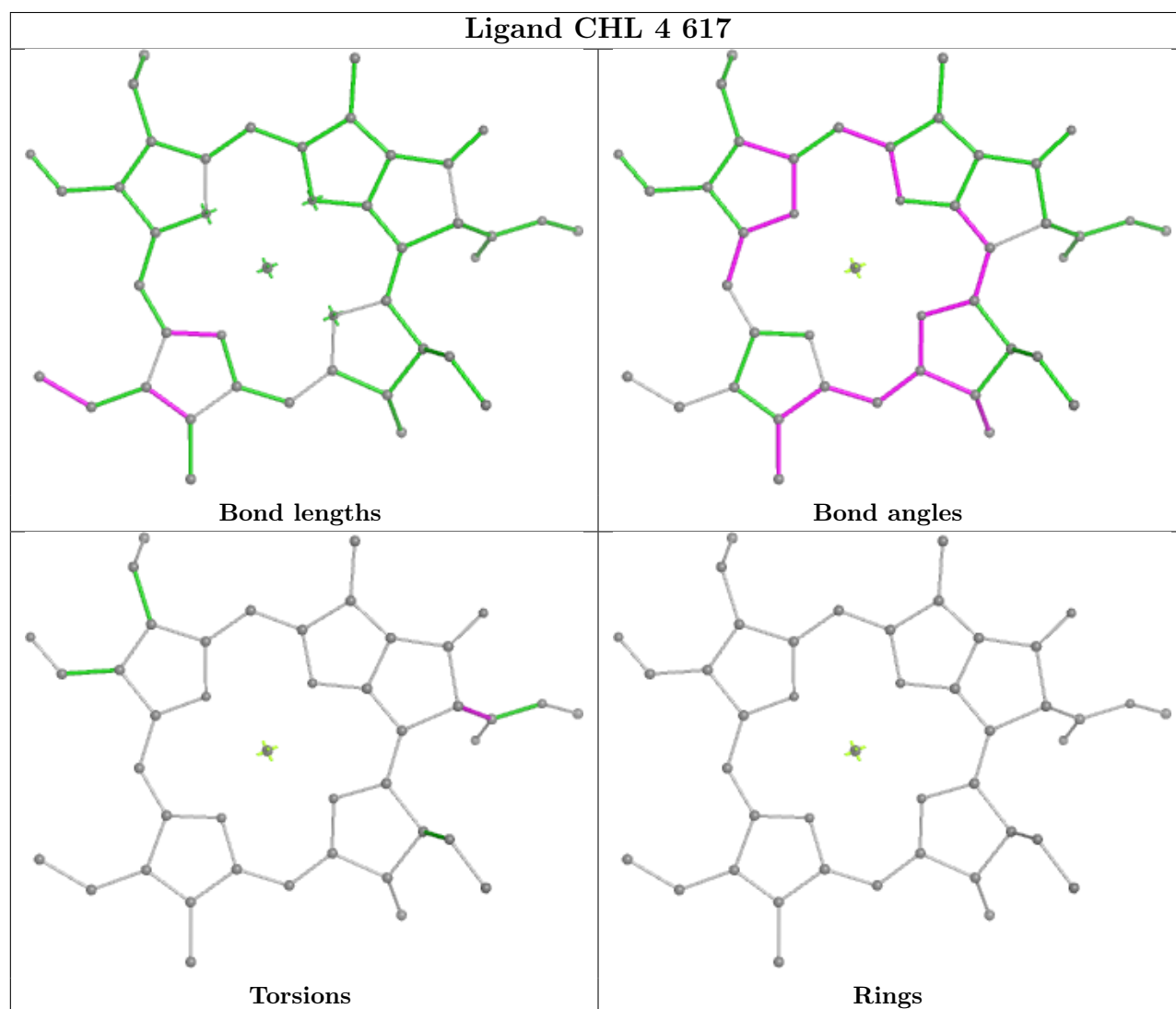
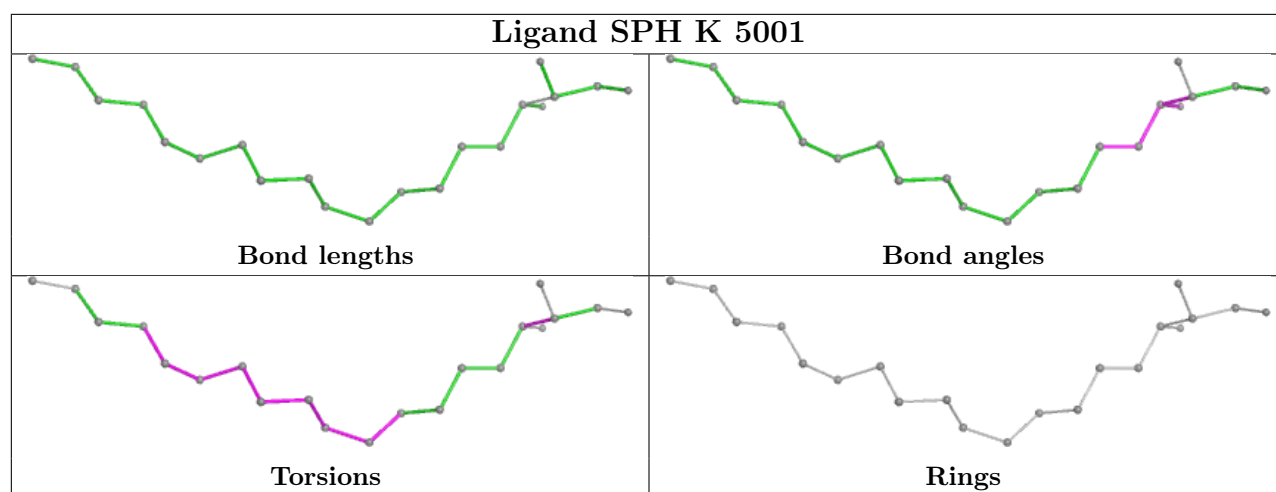
Rings



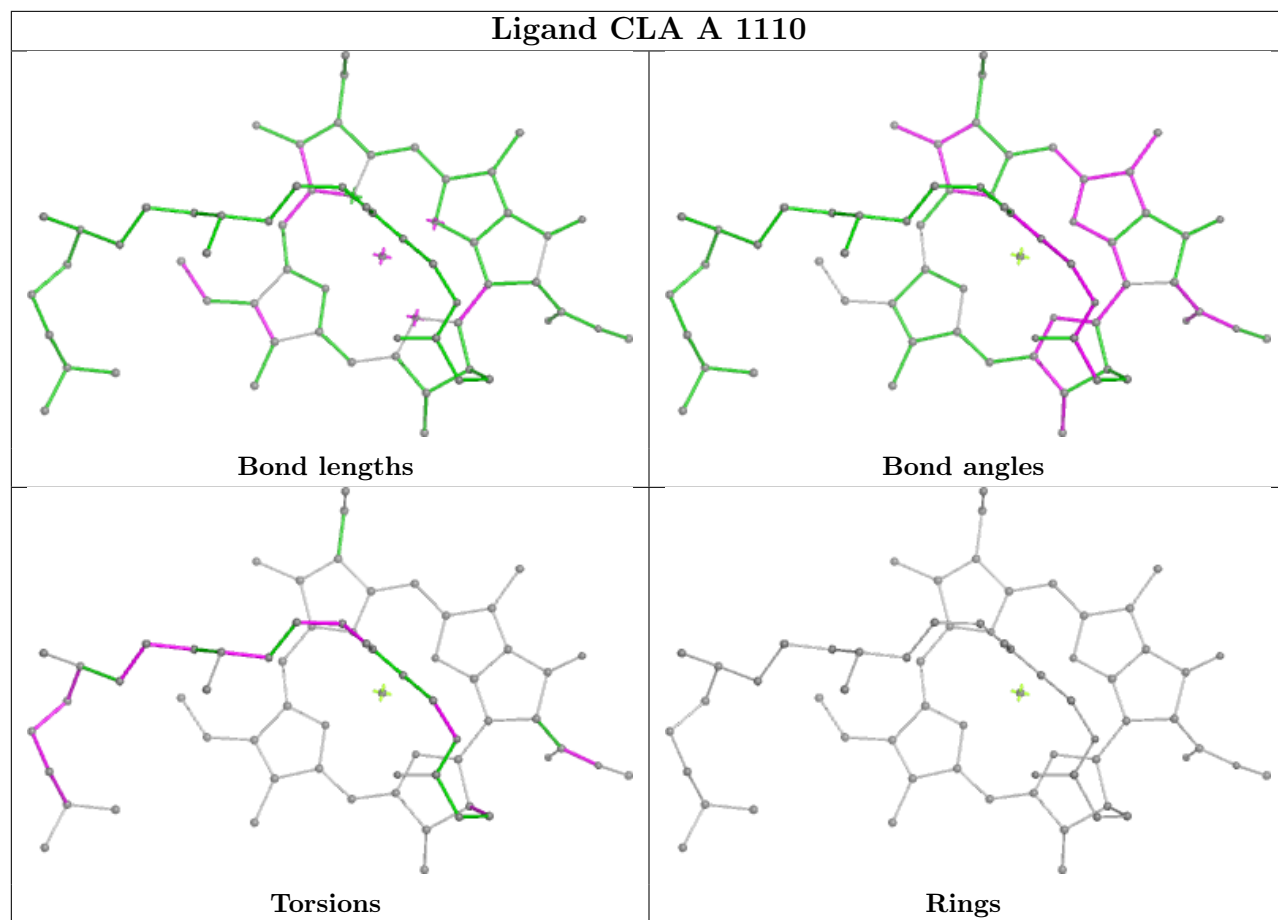
Ligand CLA 7 601



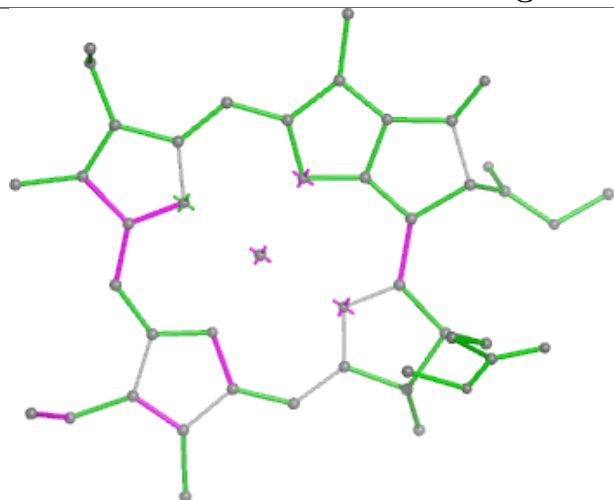




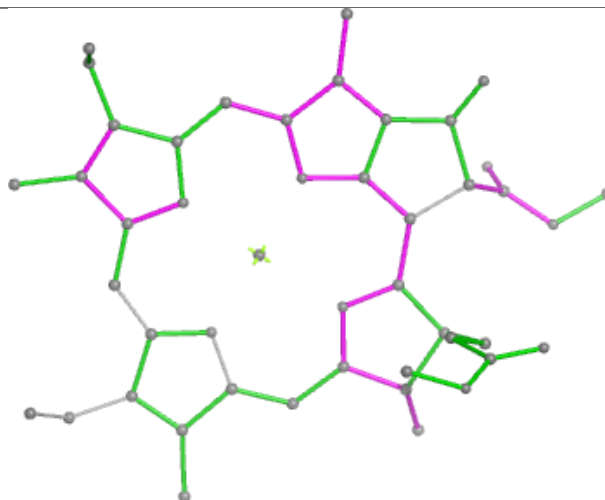
Ligand CLA A 1110



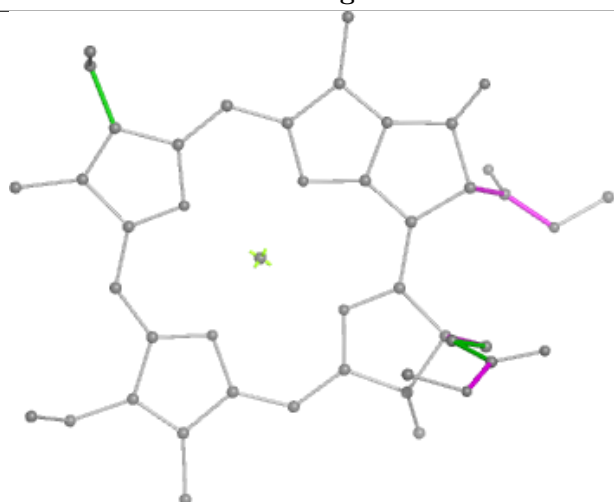
Ligand CLA Z 615



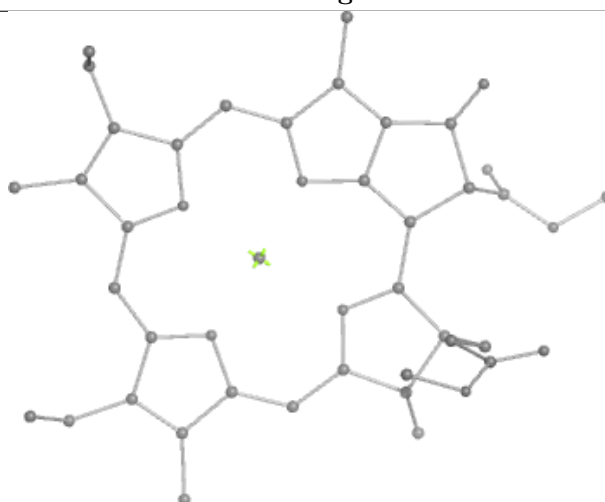
Bond lengths



Bond angles

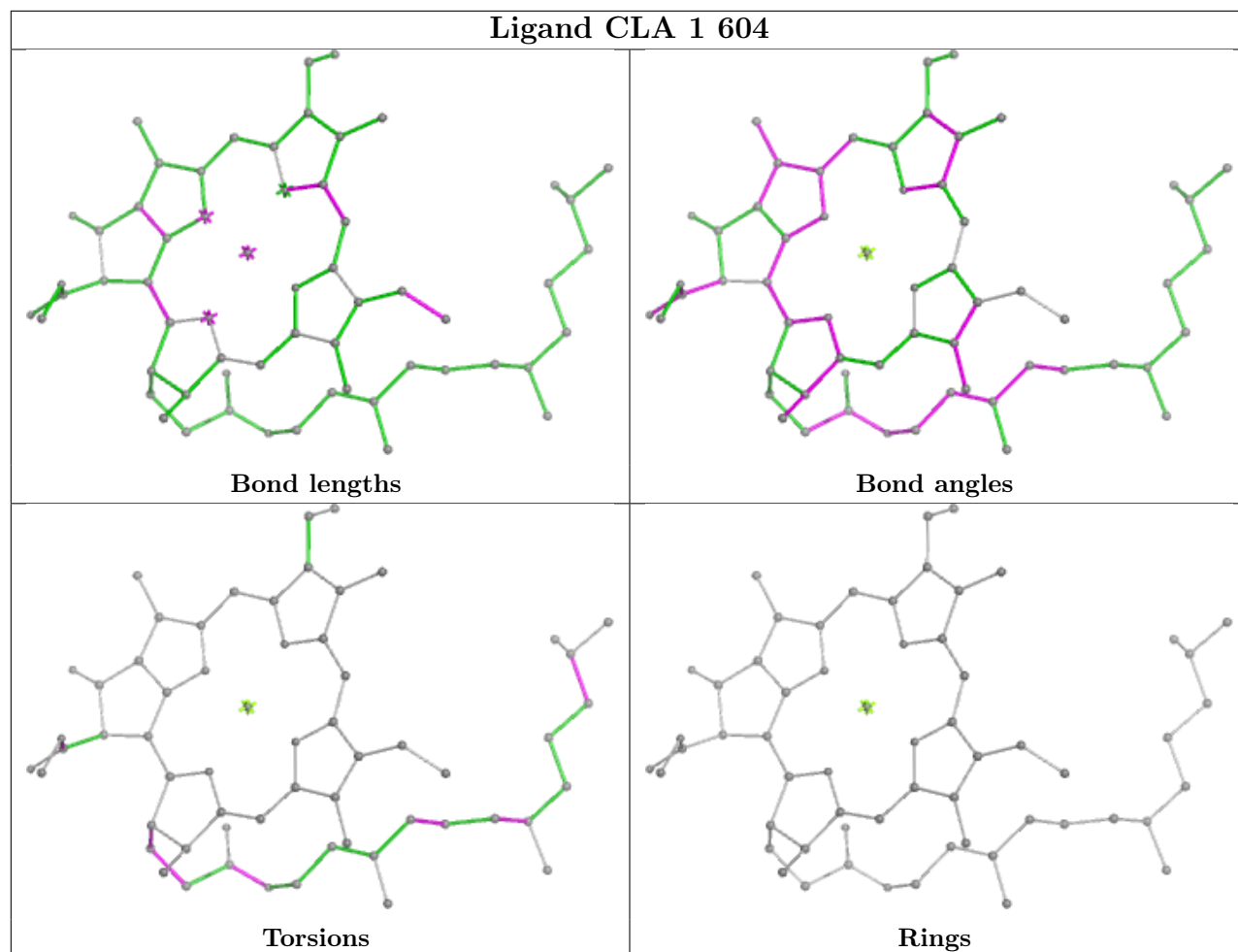


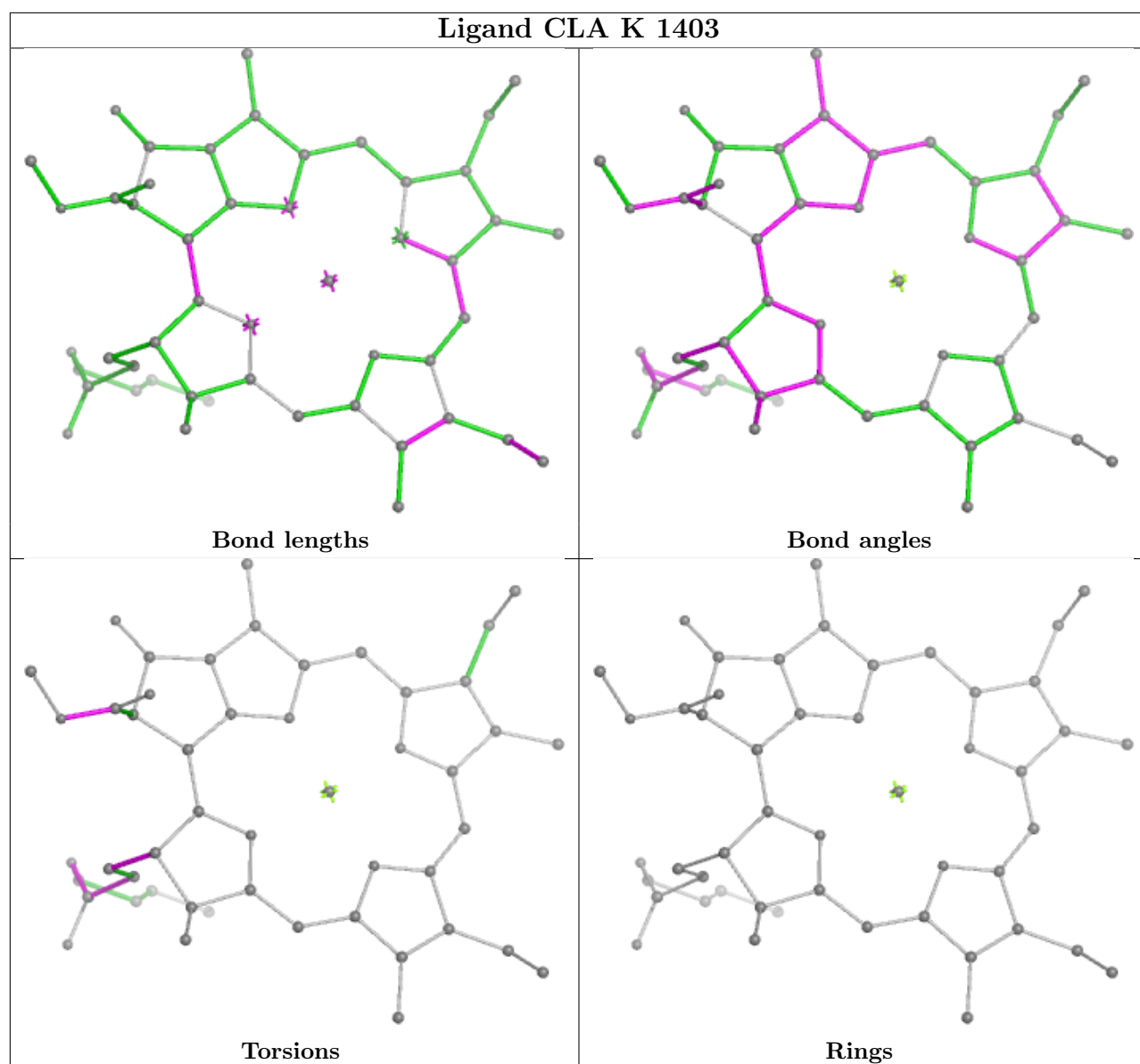
Torsions

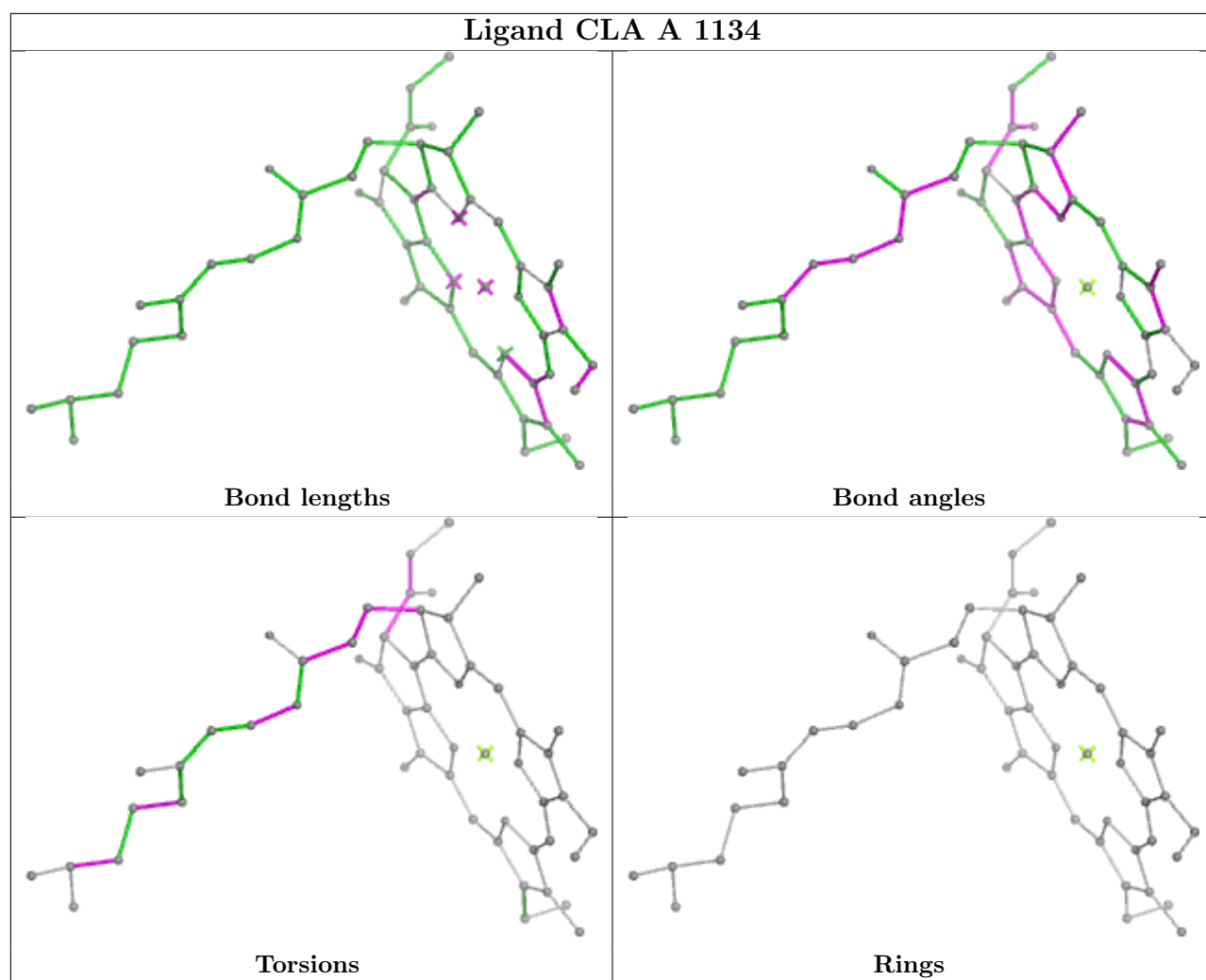


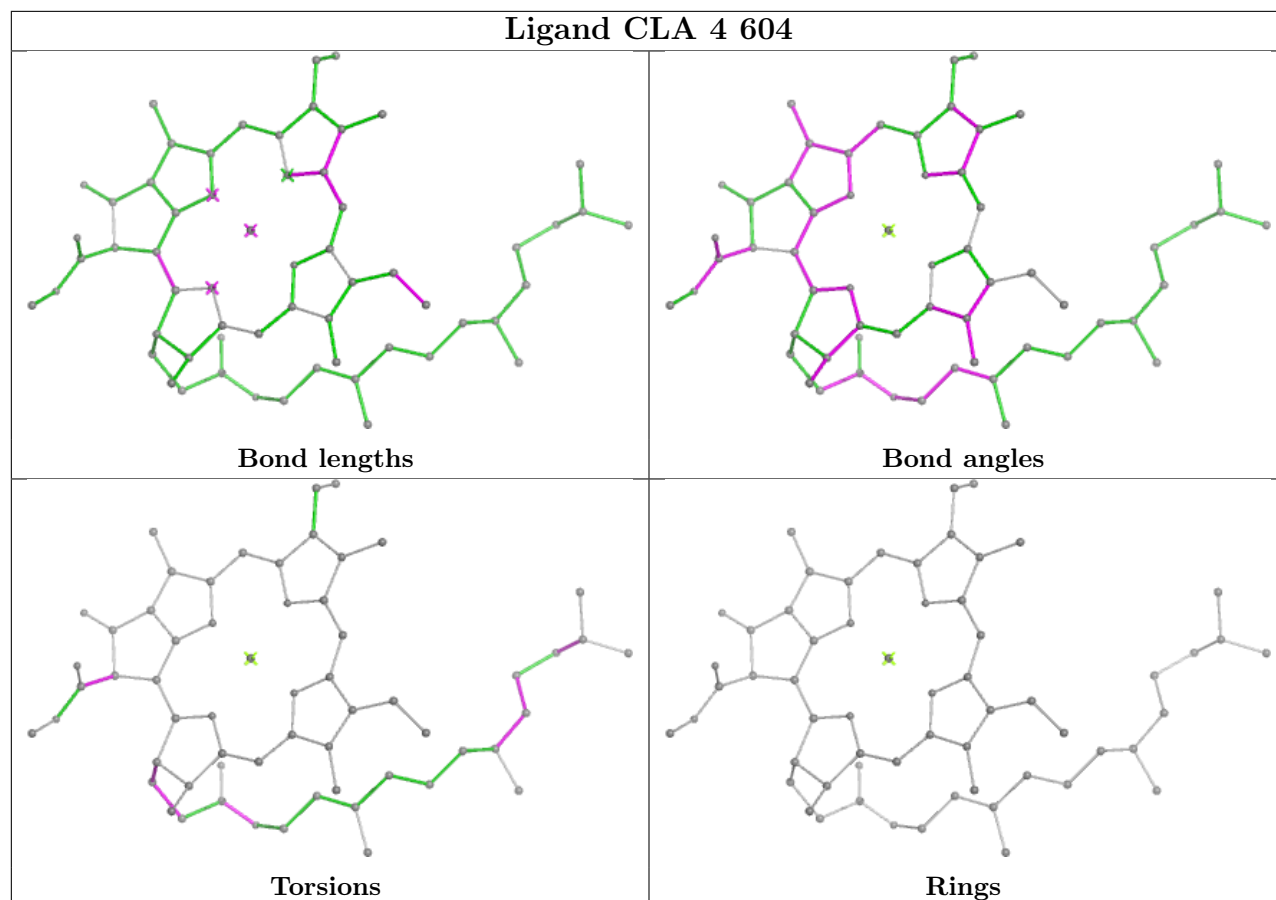
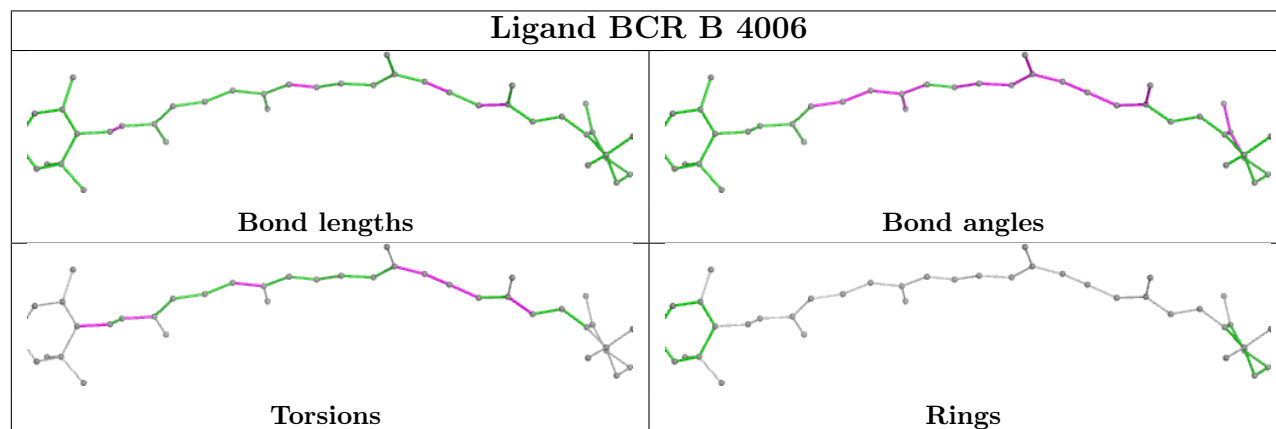
Rings

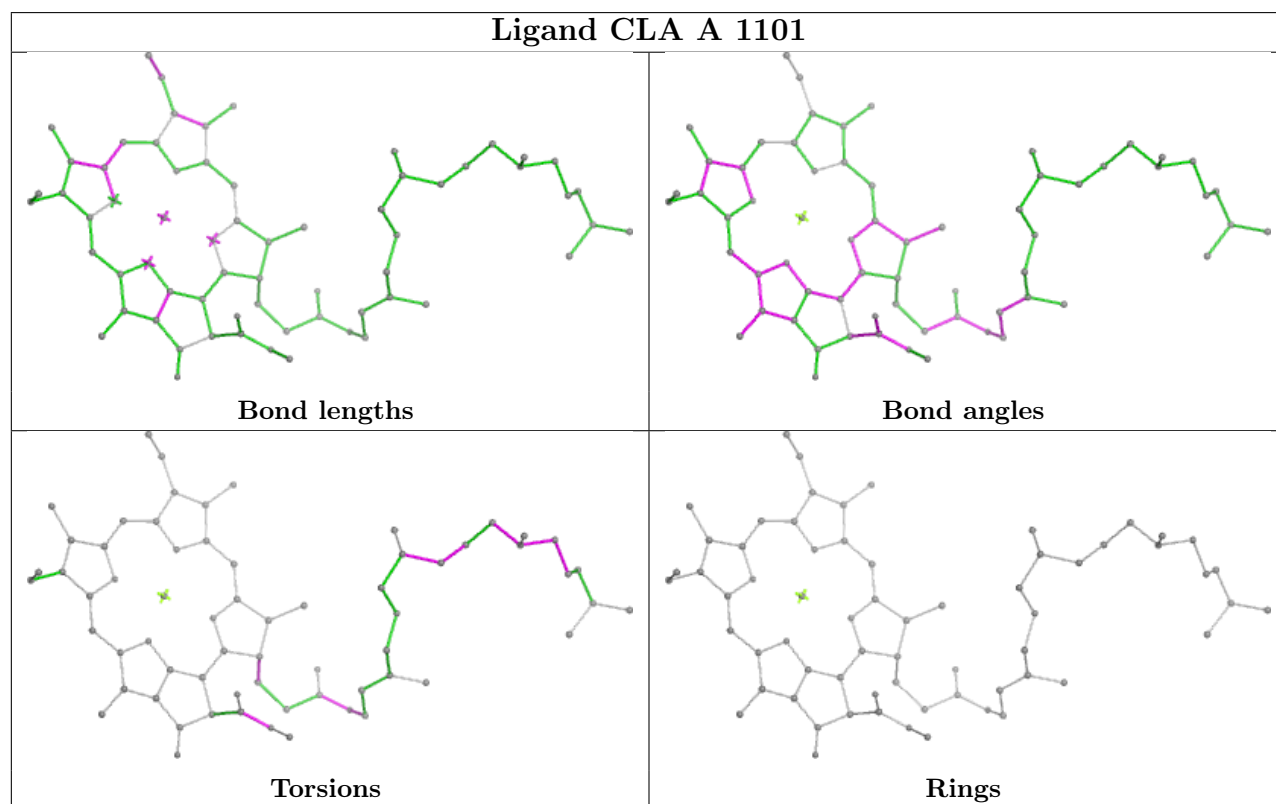
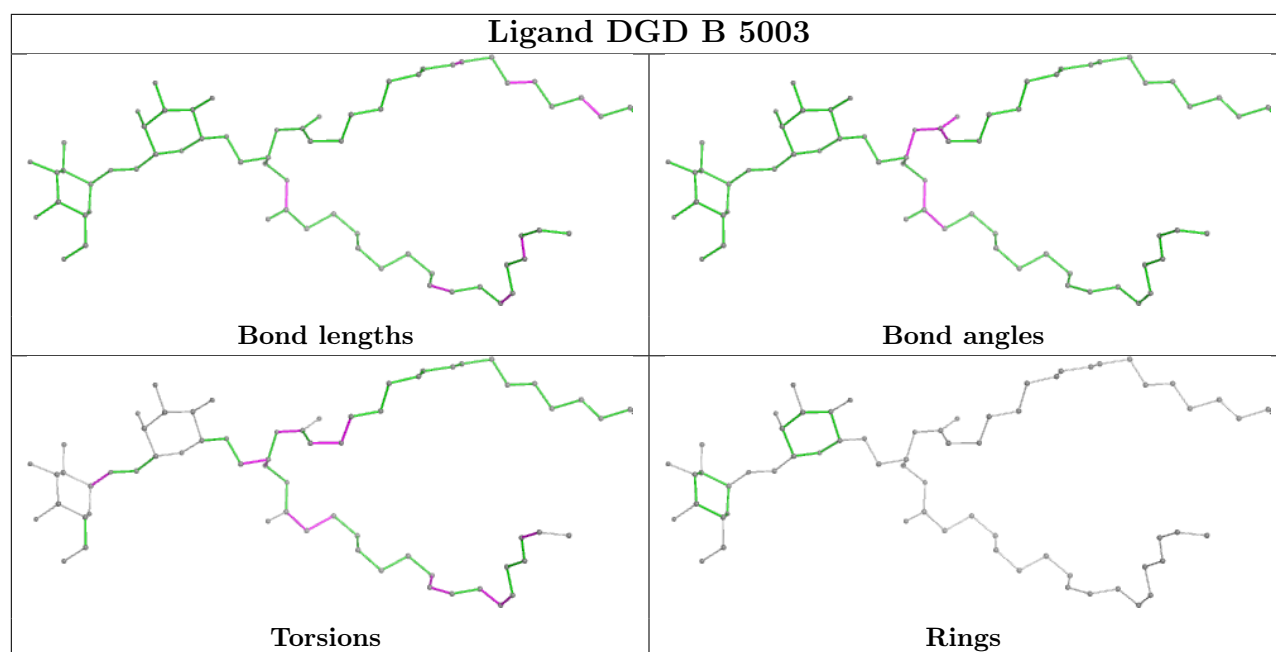
Ligand CLA 1 604

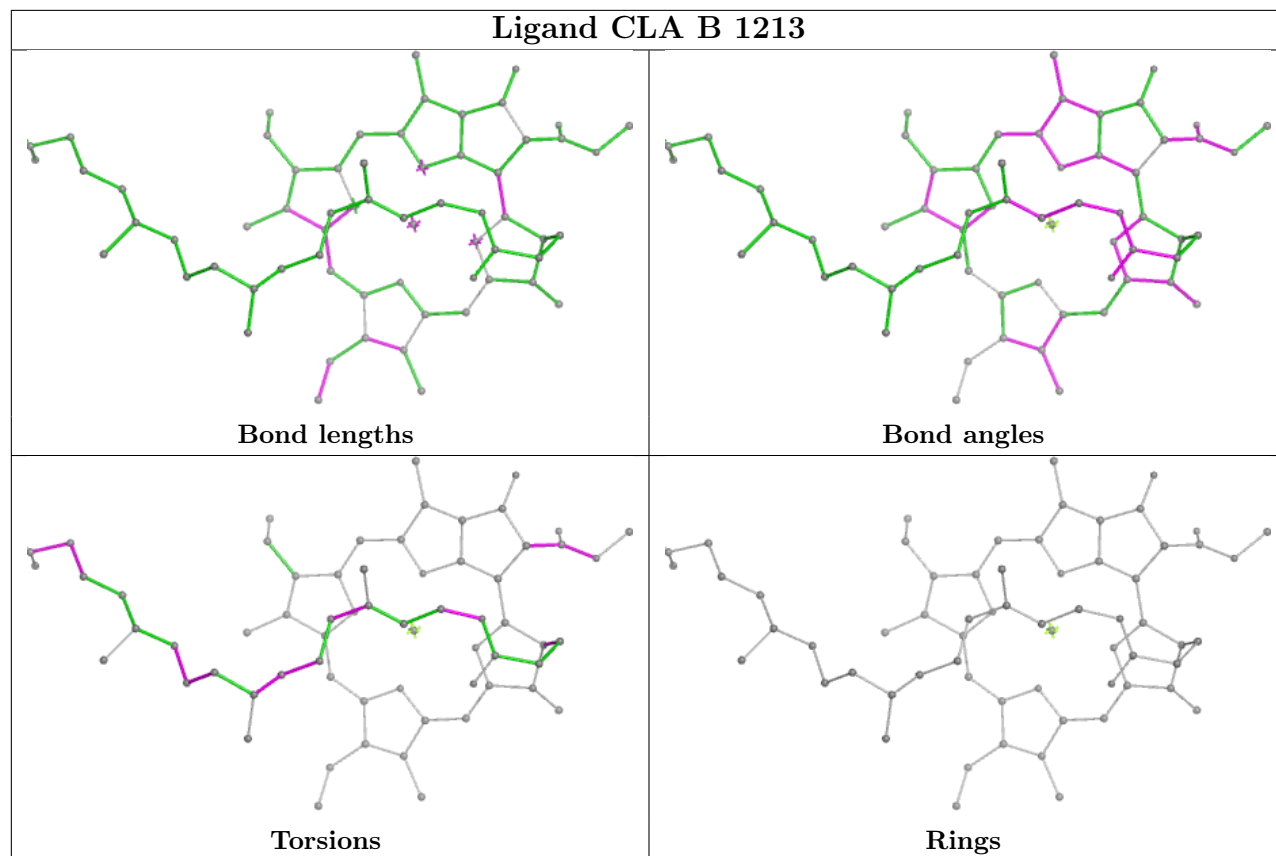
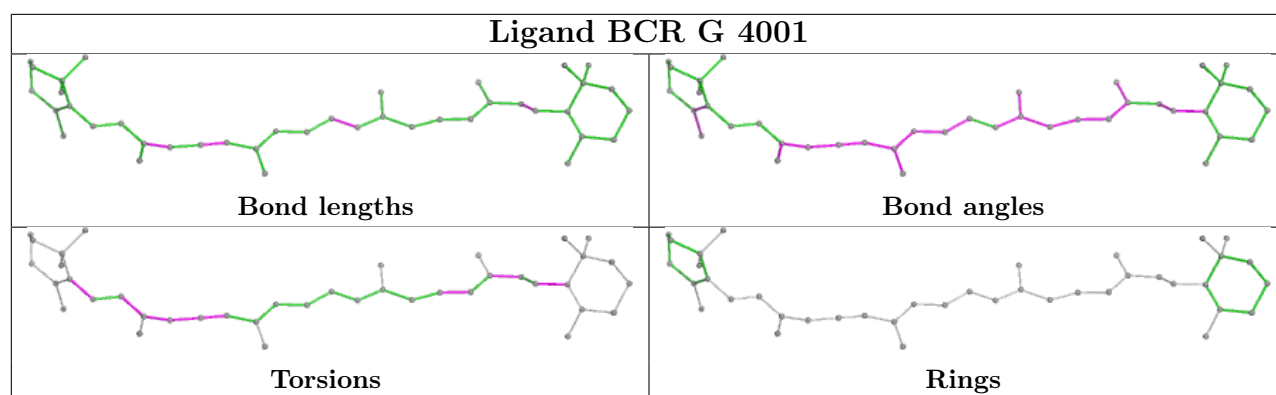


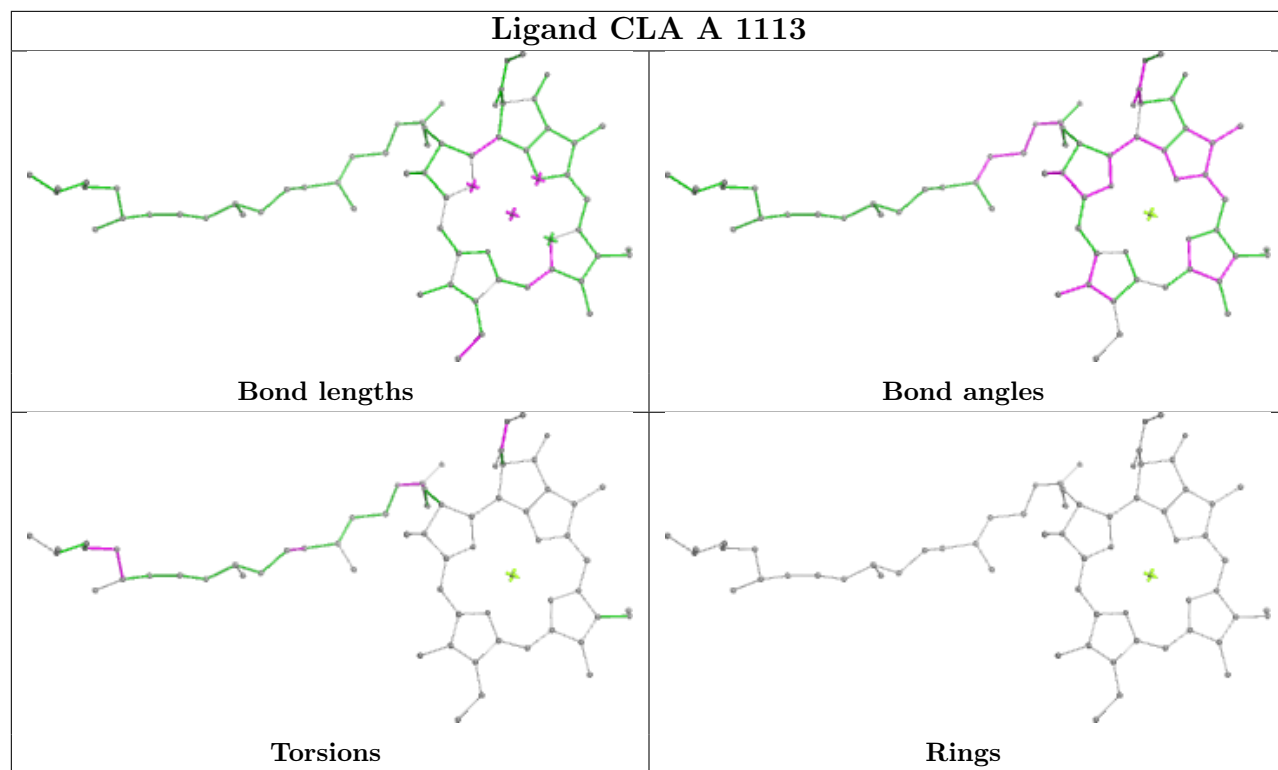




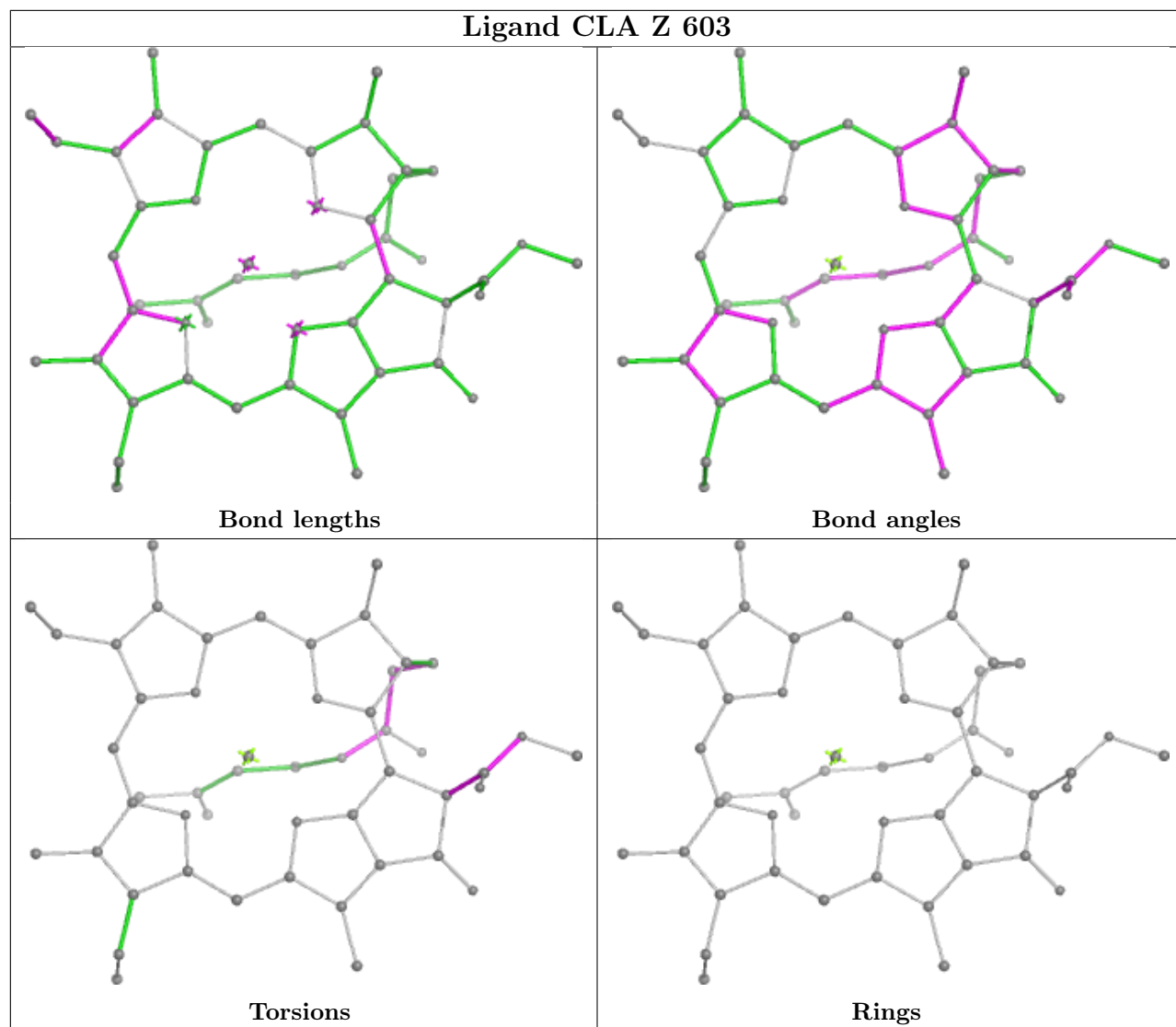
Ligand CLA 4 604**Ligand BCR B 4006**



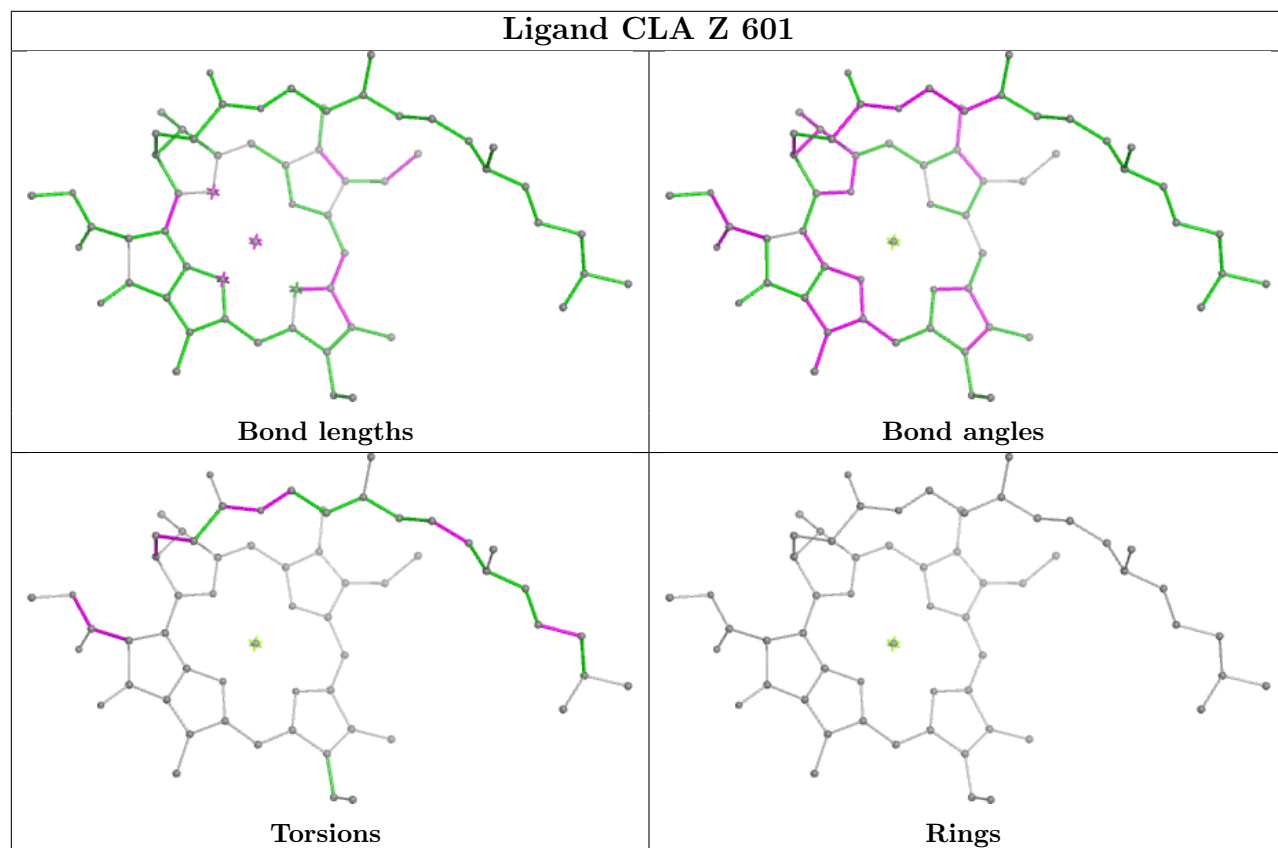




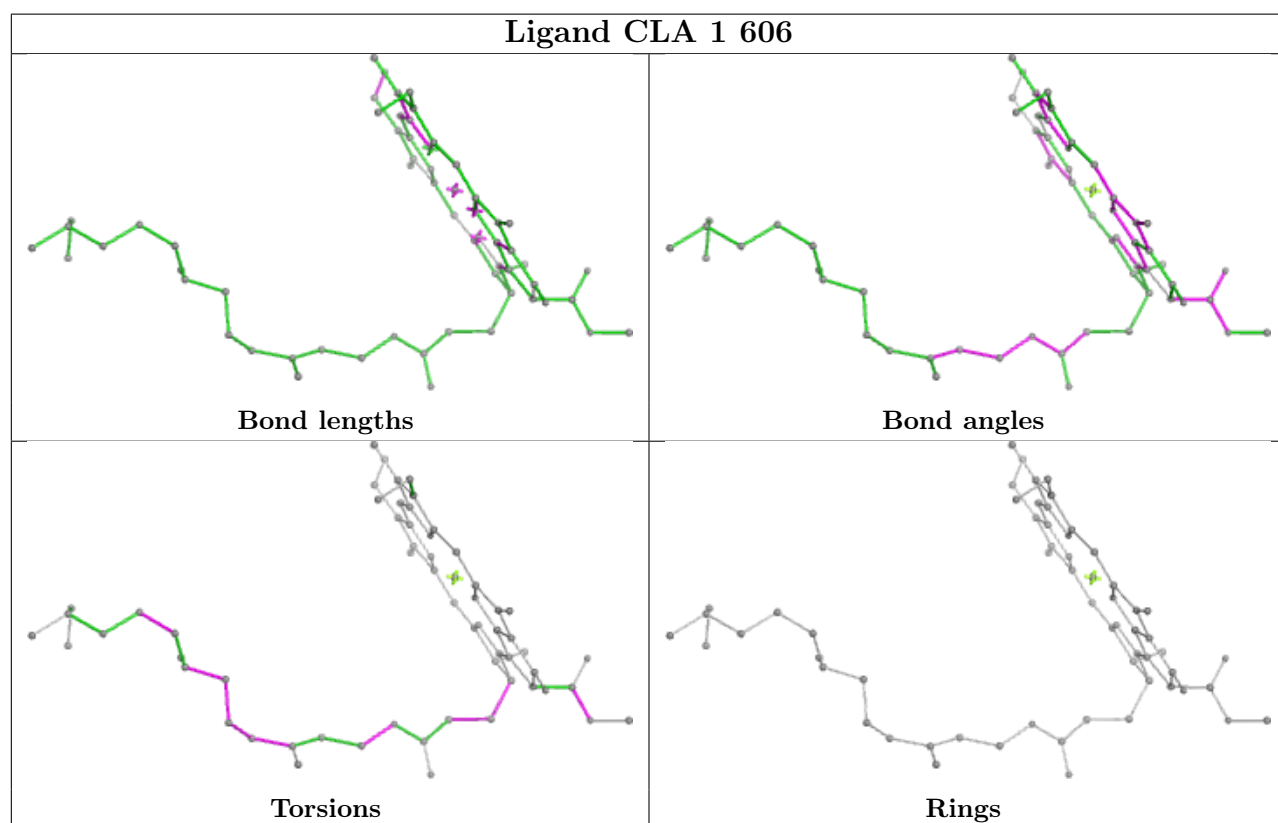
Ligand CLA Z 603



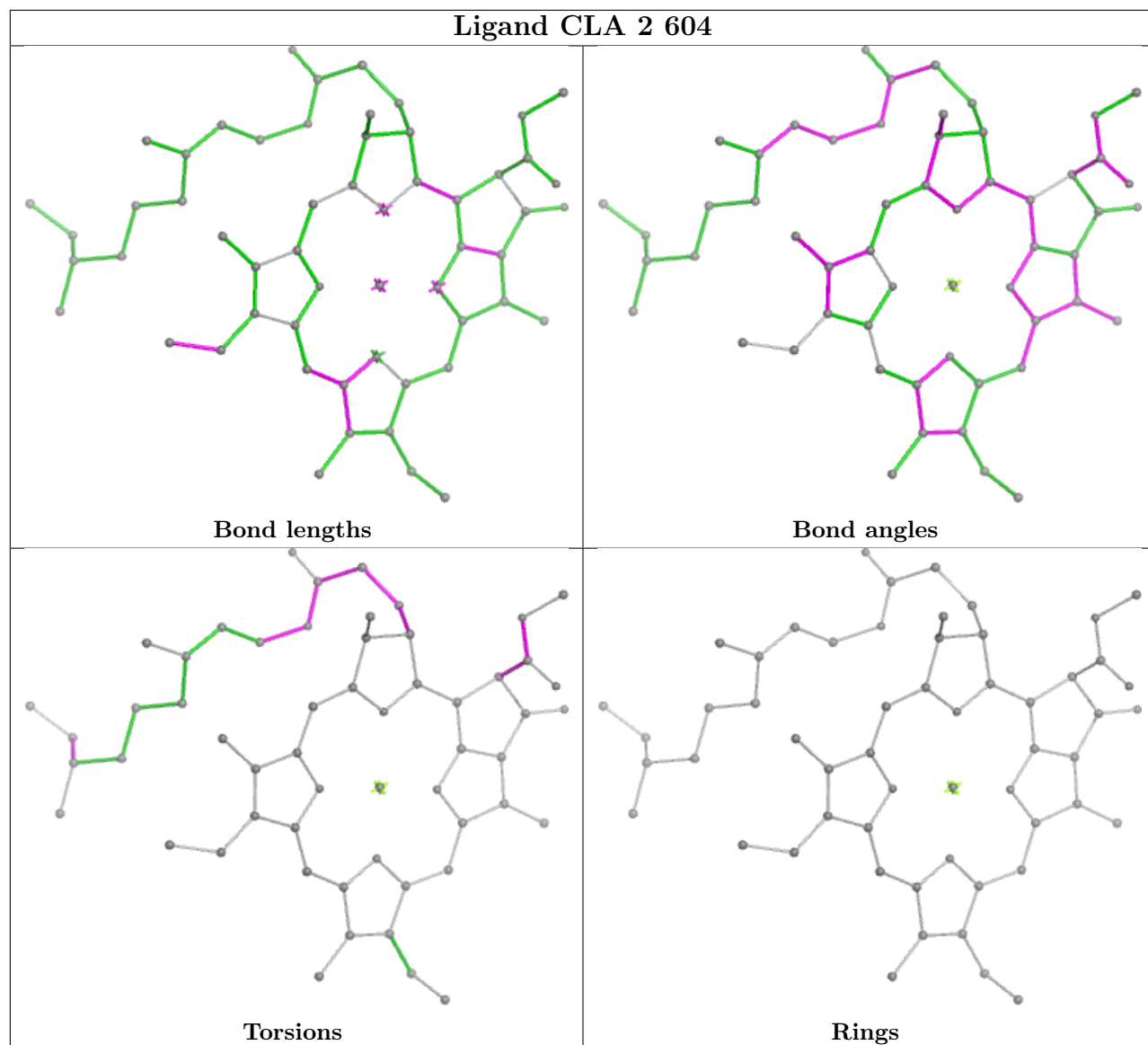
Ligand CLA Z 601

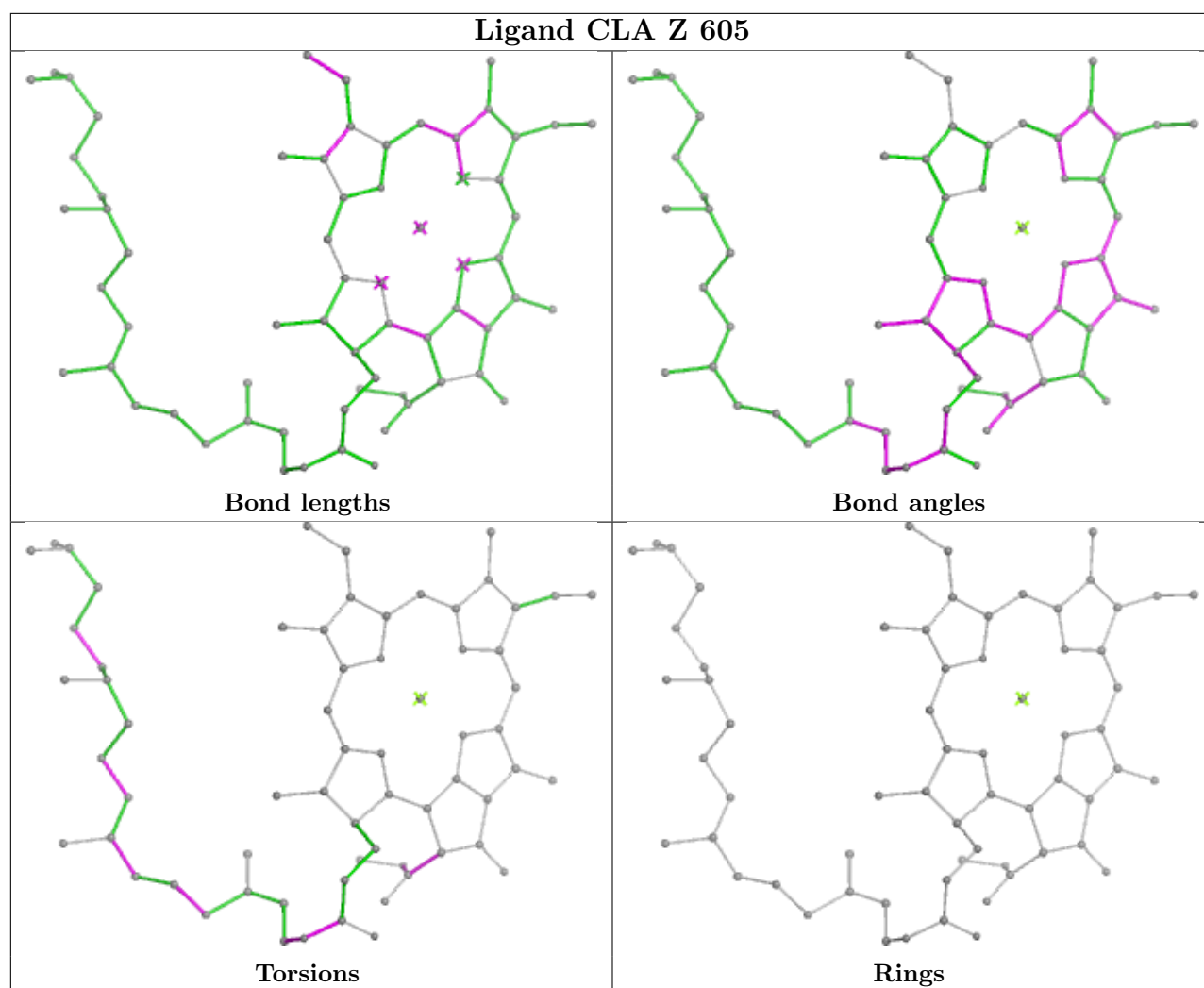


Ligand CLA 1 606

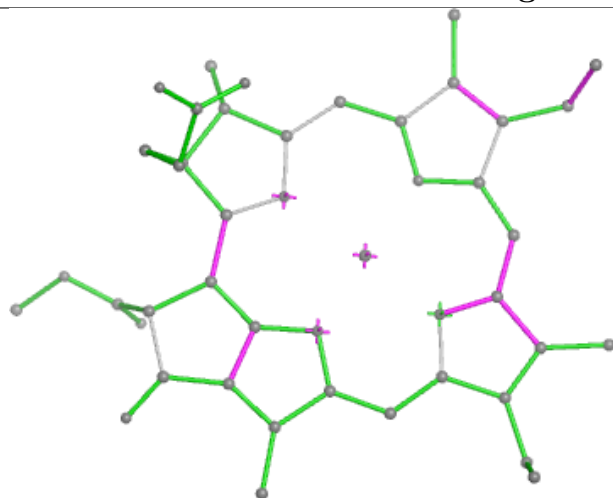


Ligand CLA 2 604

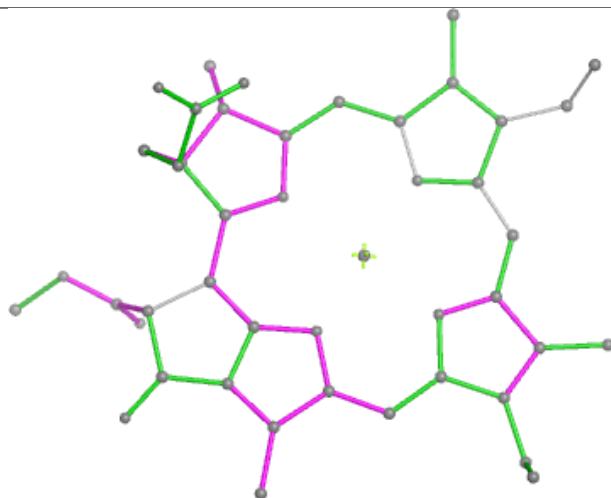




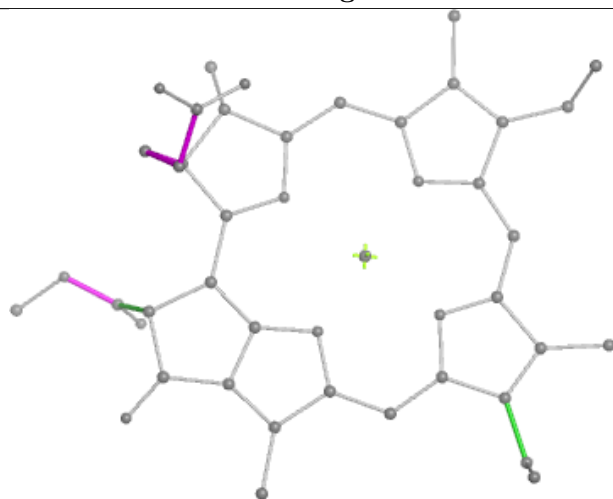
Ligand CLA 9 608



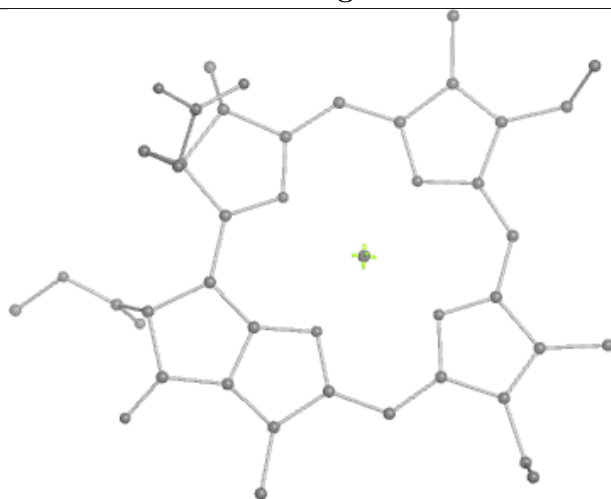
Bond lengths



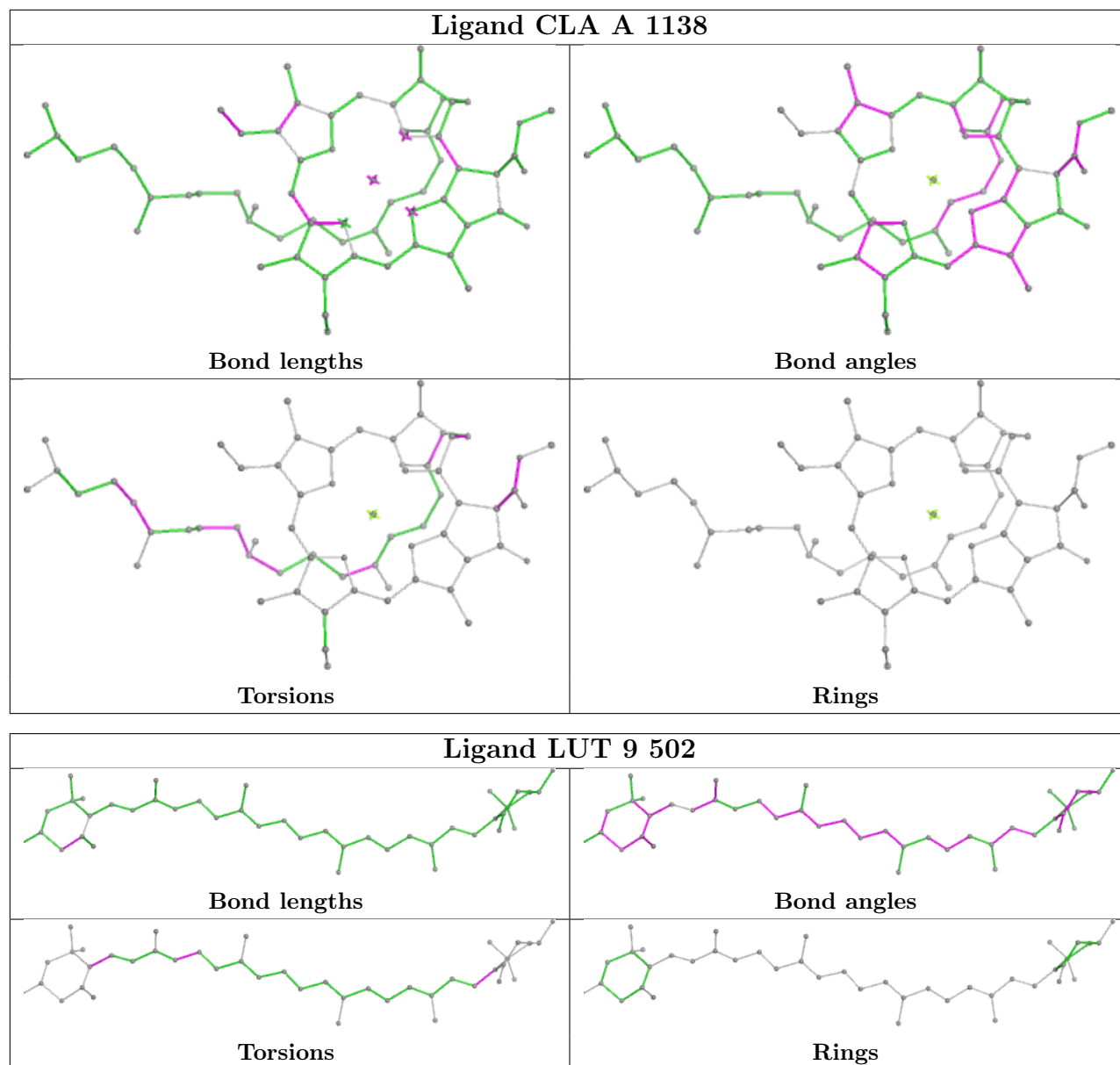
Bond angles

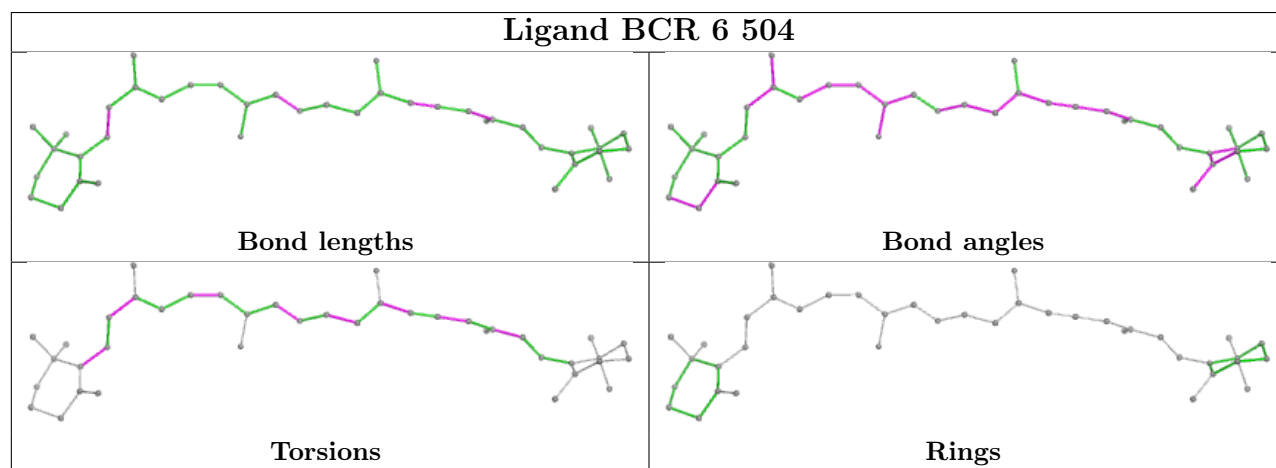
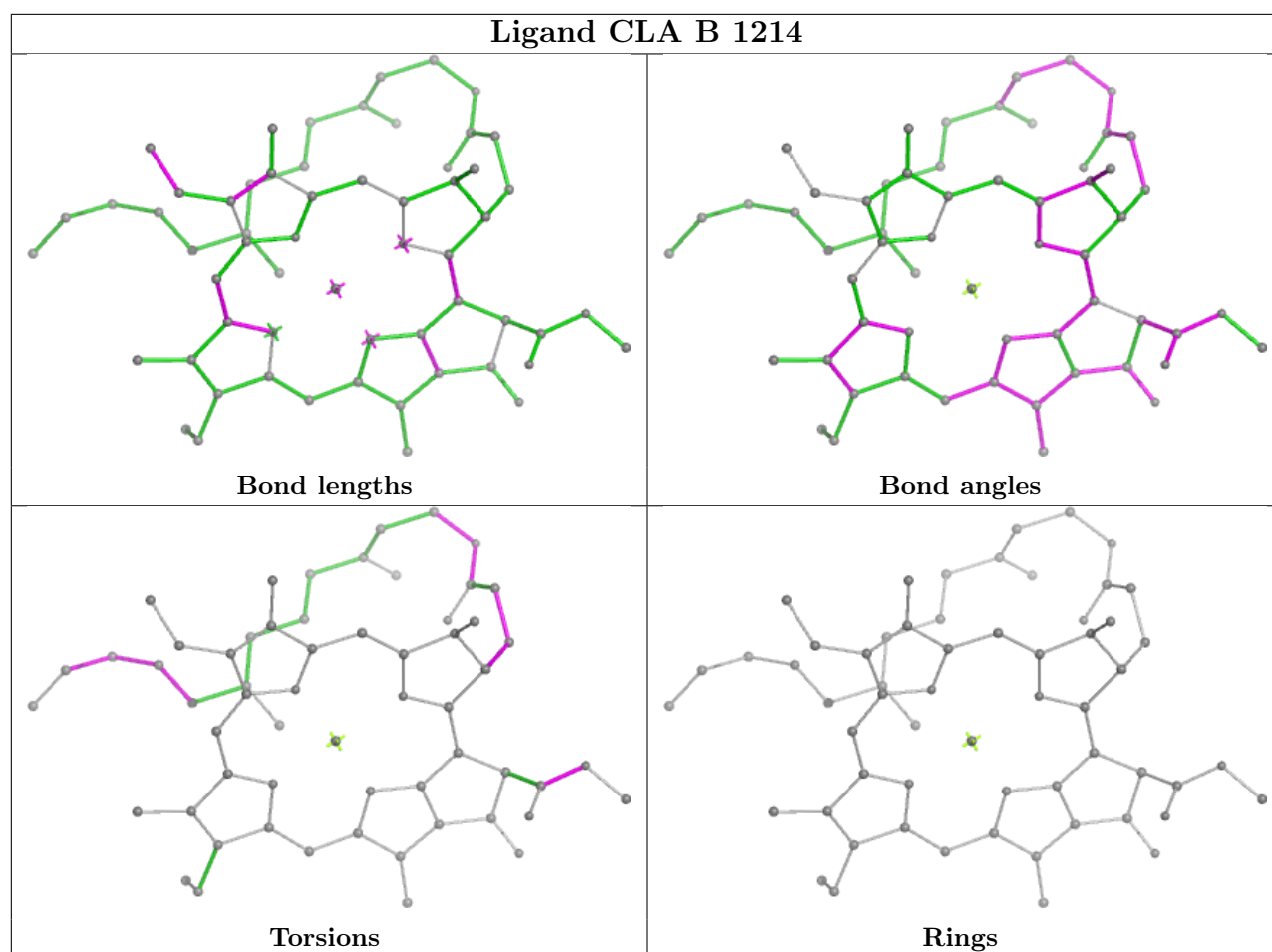


Torsions

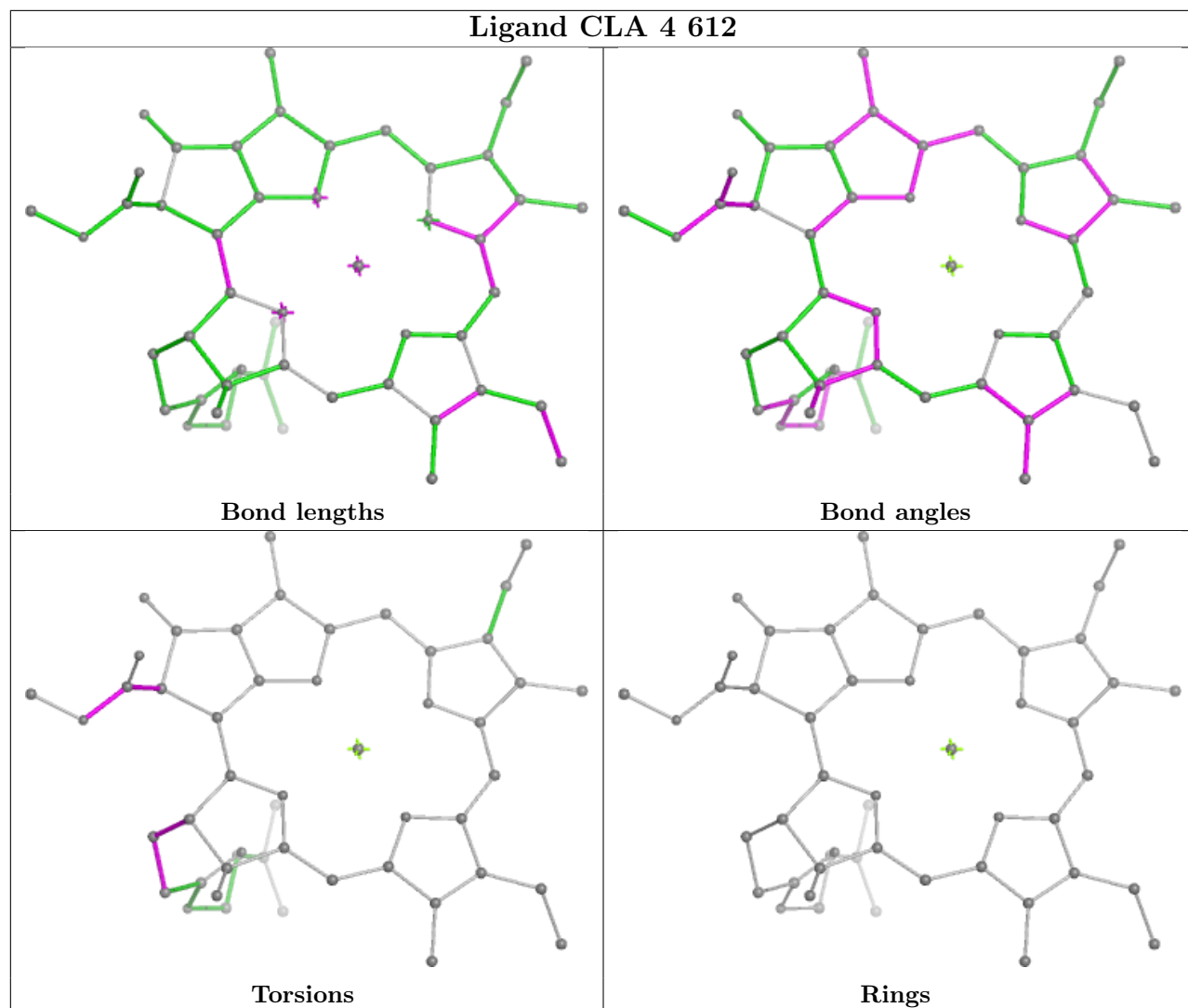


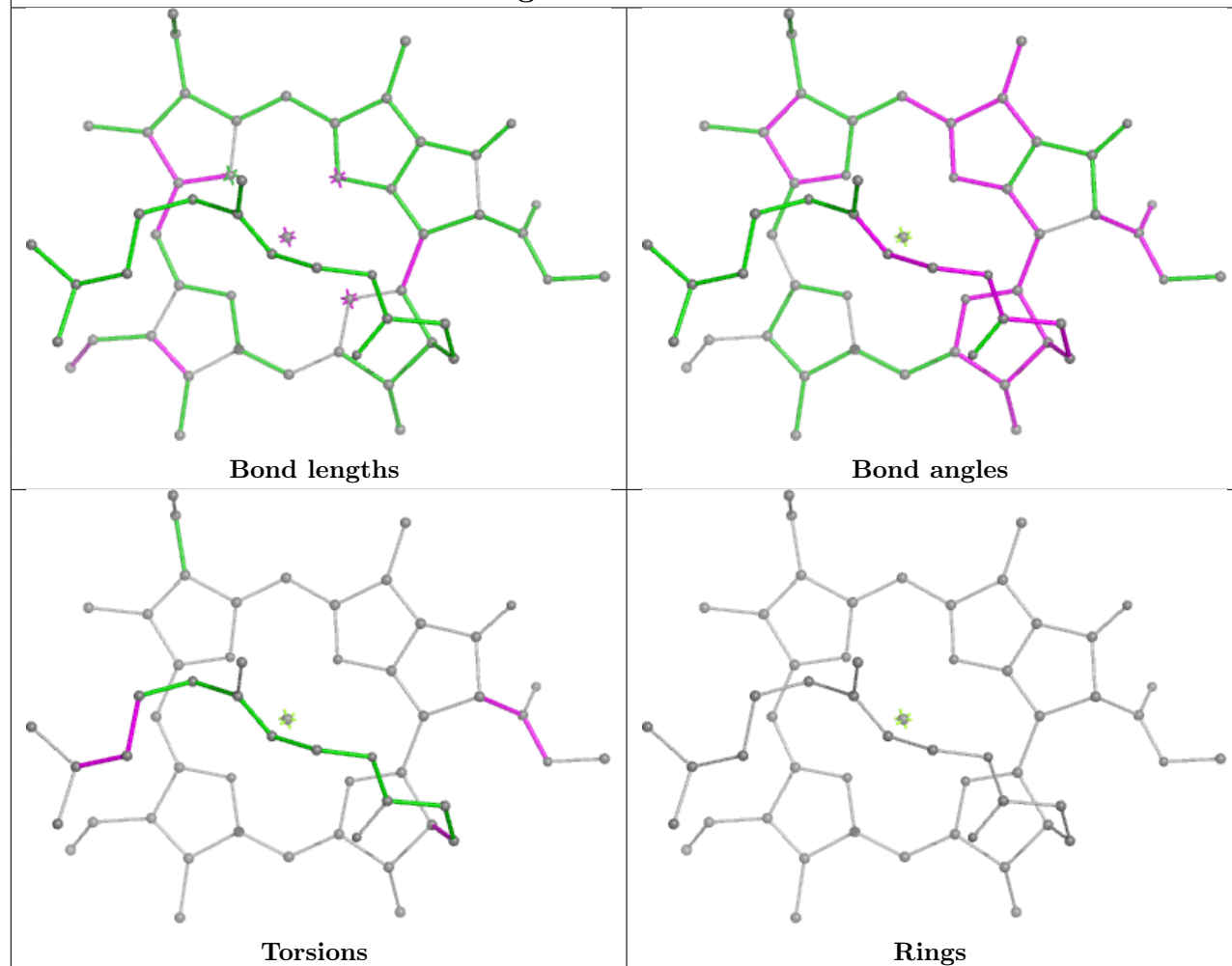
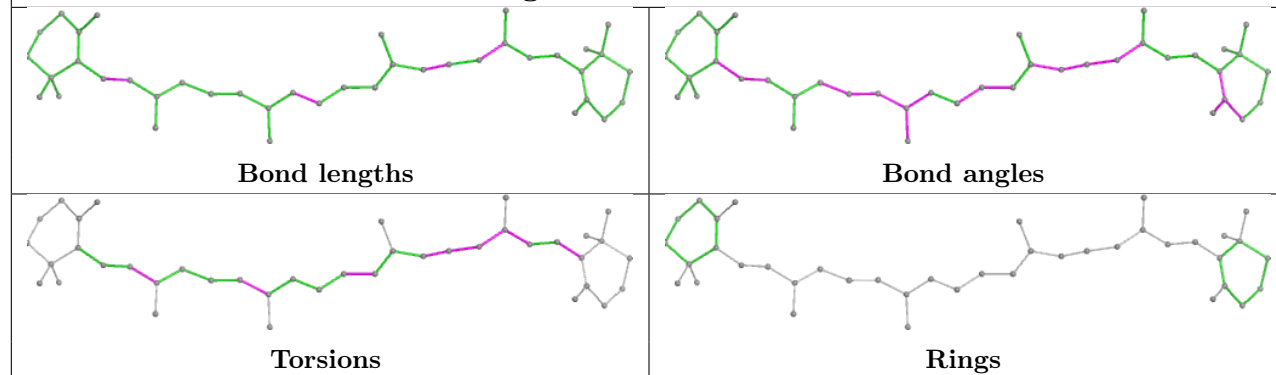
Rings

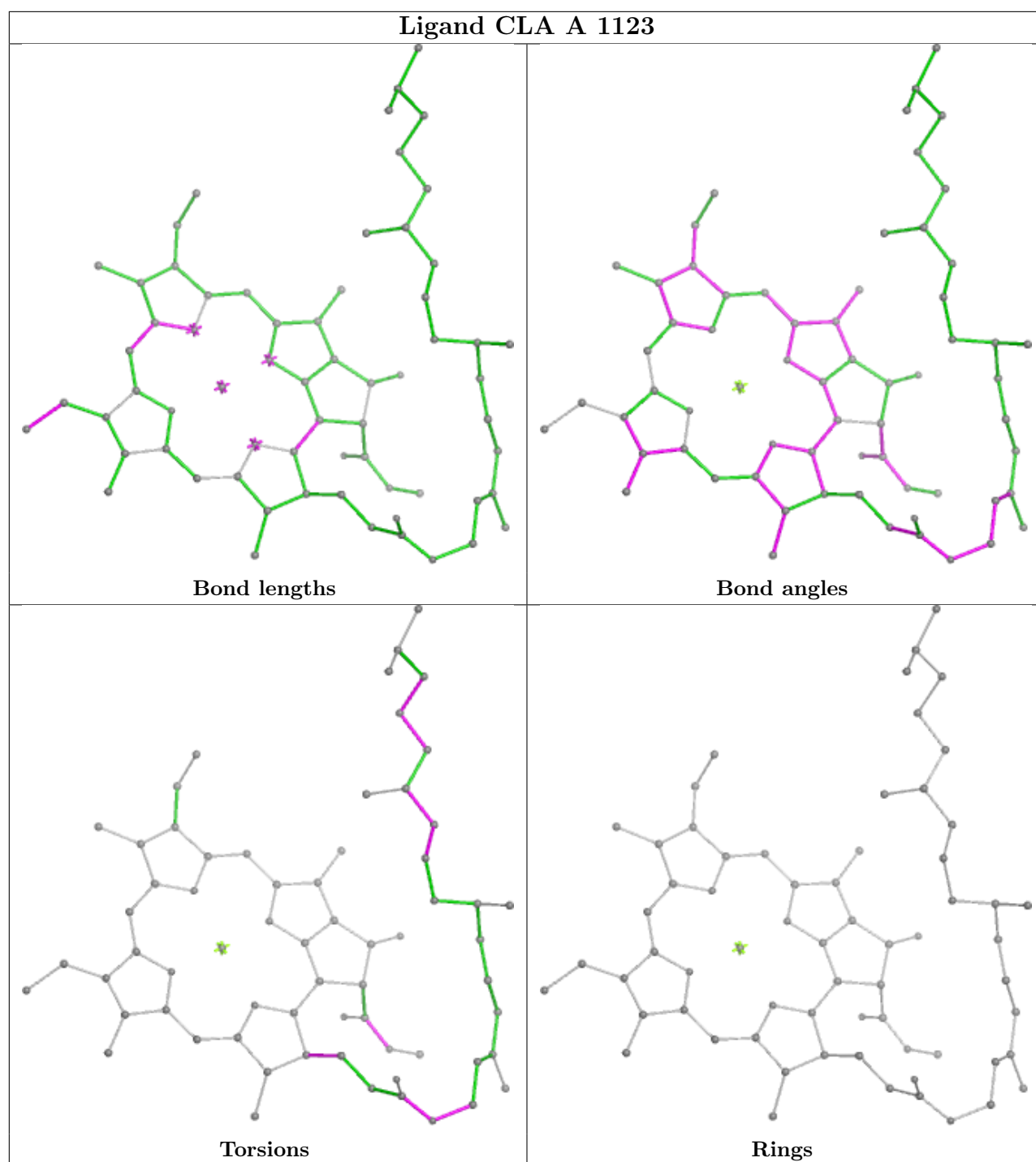


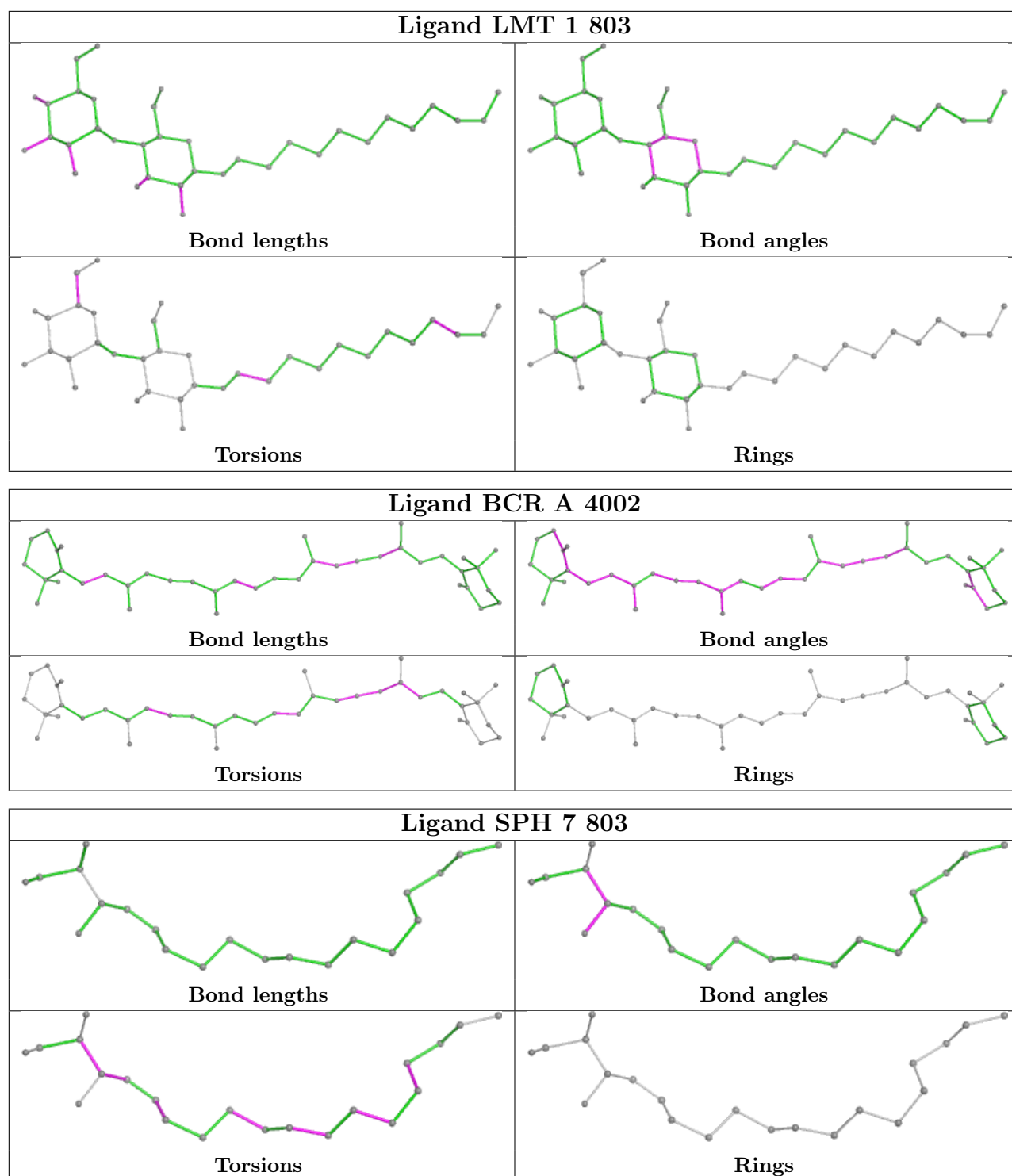


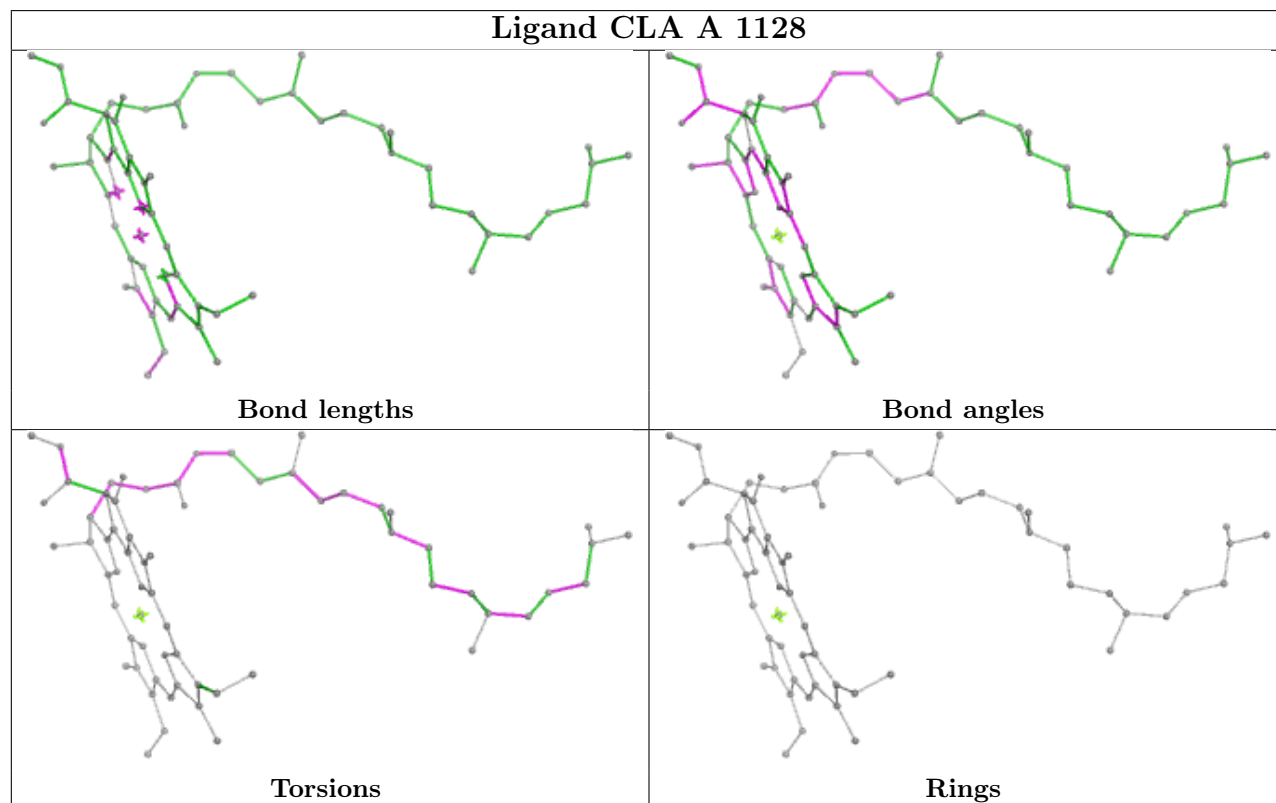
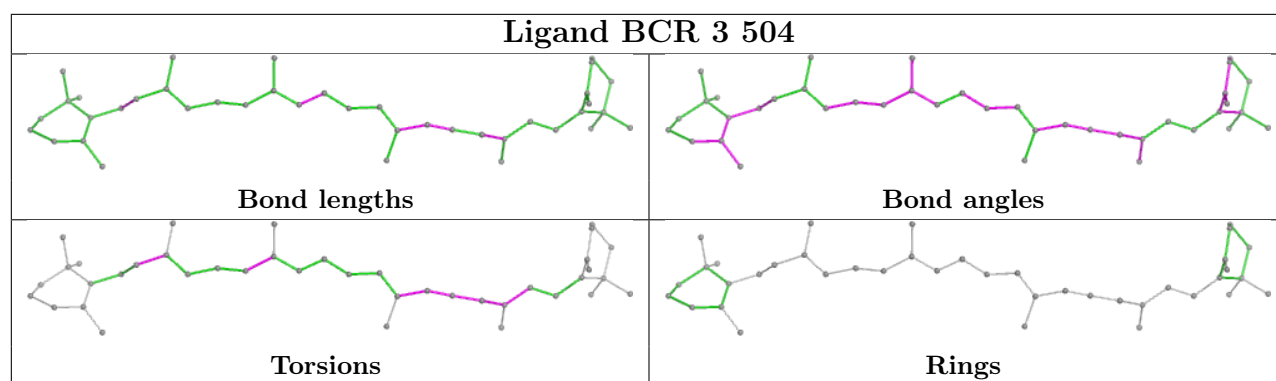
Ligand CLA 4 612

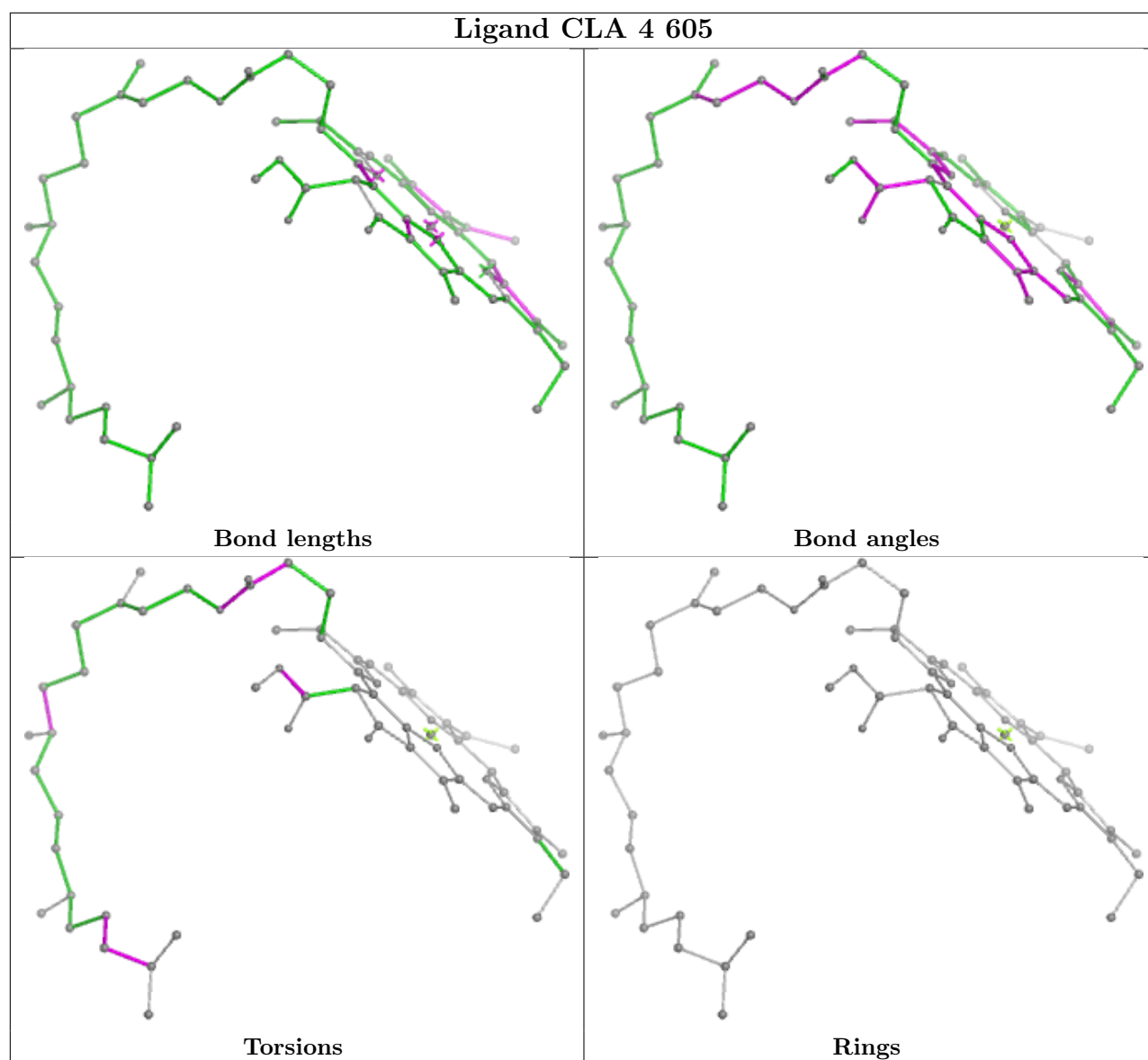


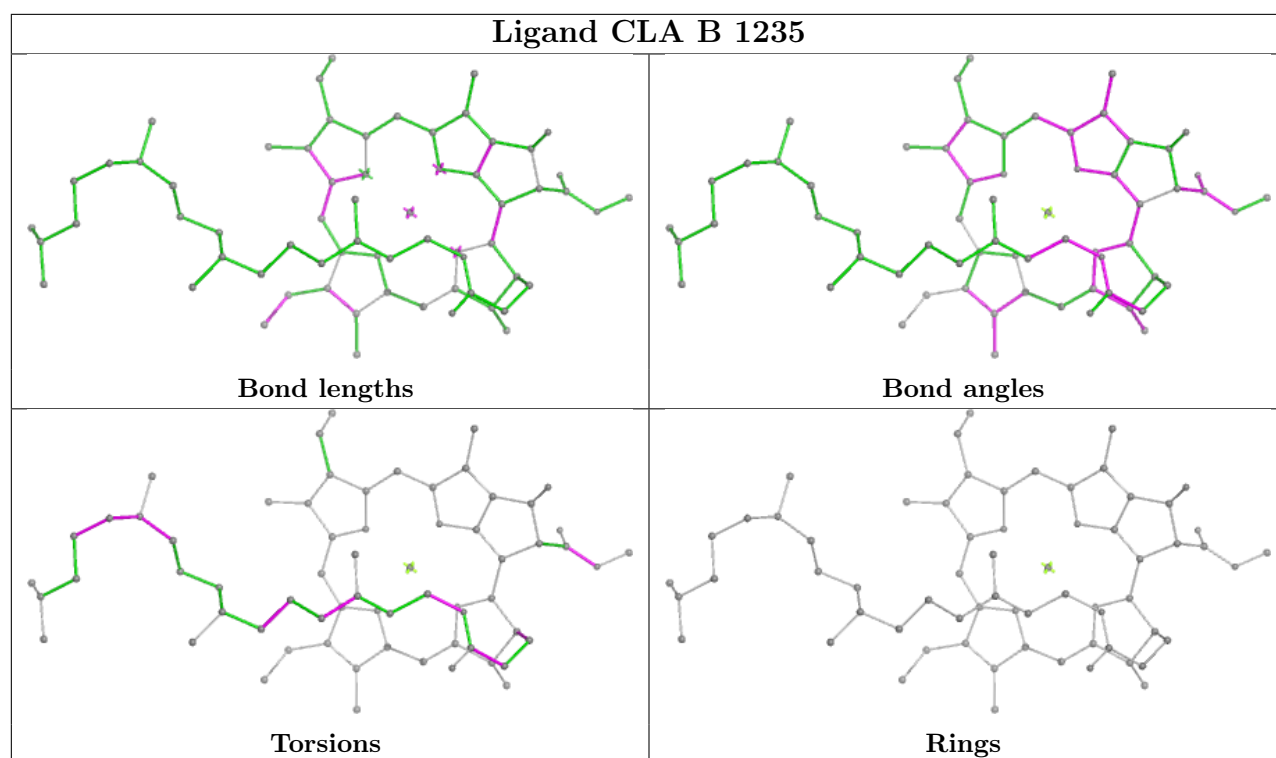
Ligand CLA 2 603**Ligand BCR B 4002**



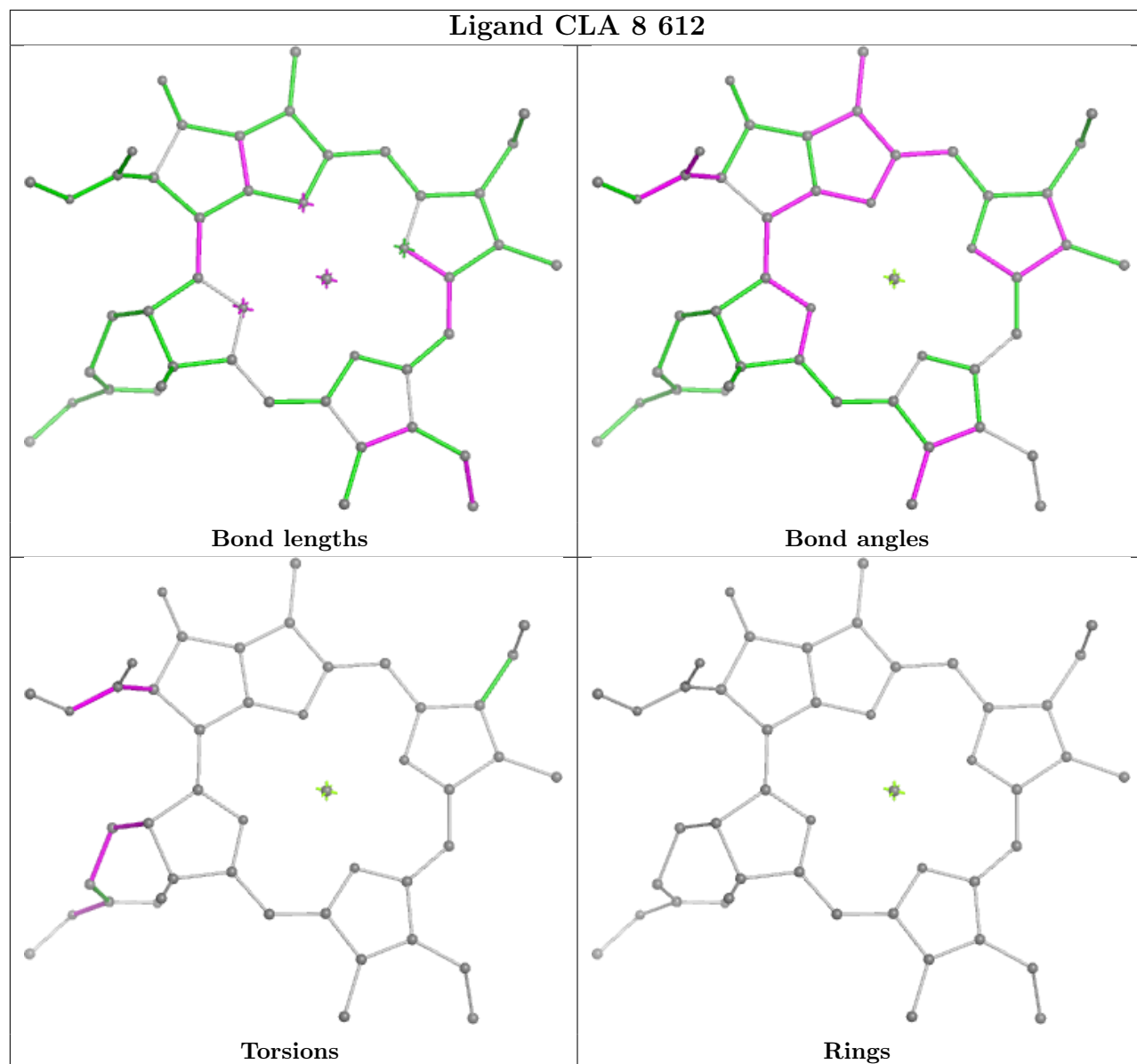


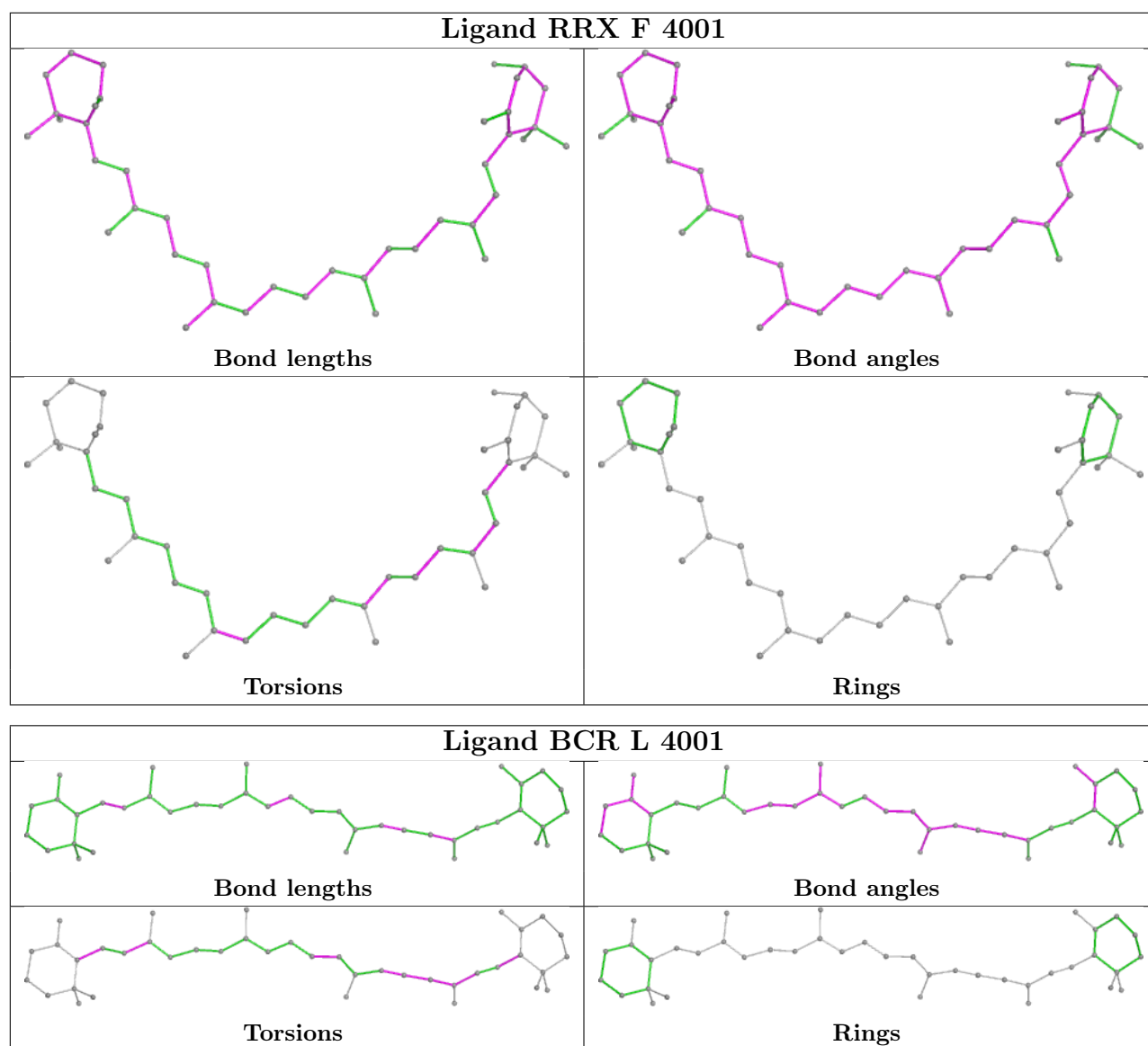


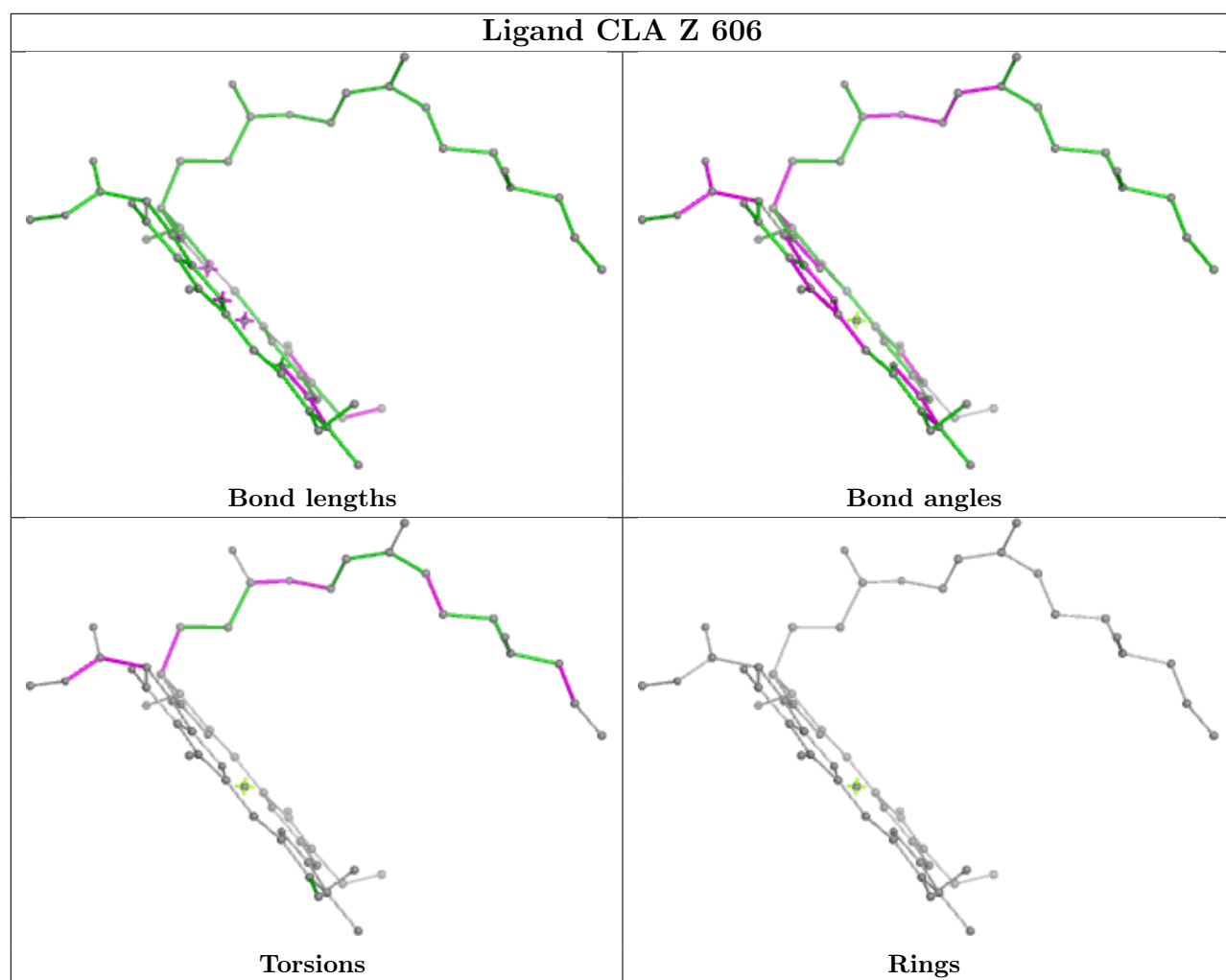




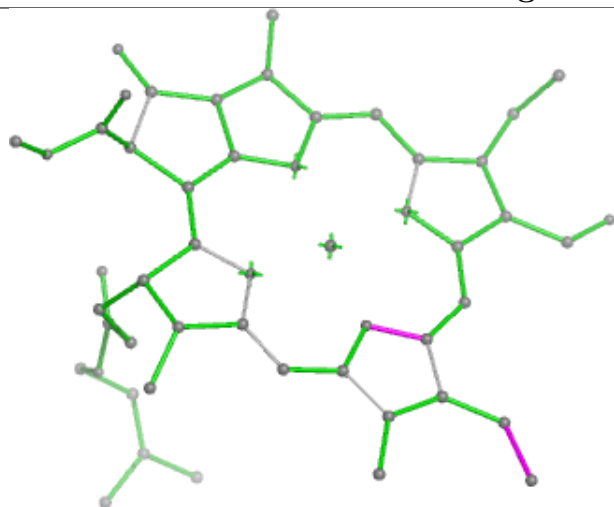
Ligand CLA 8 612



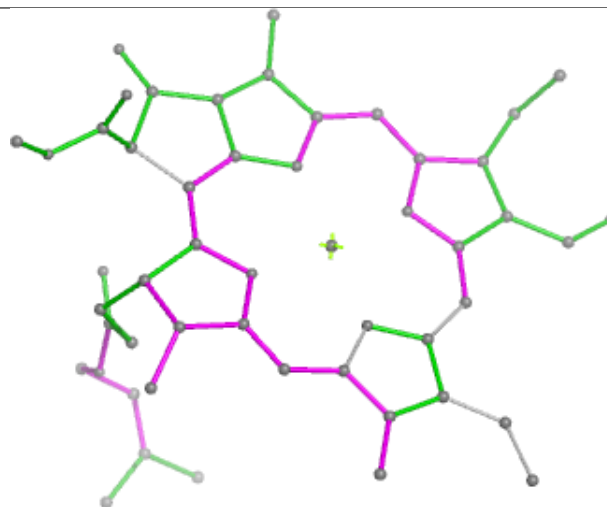




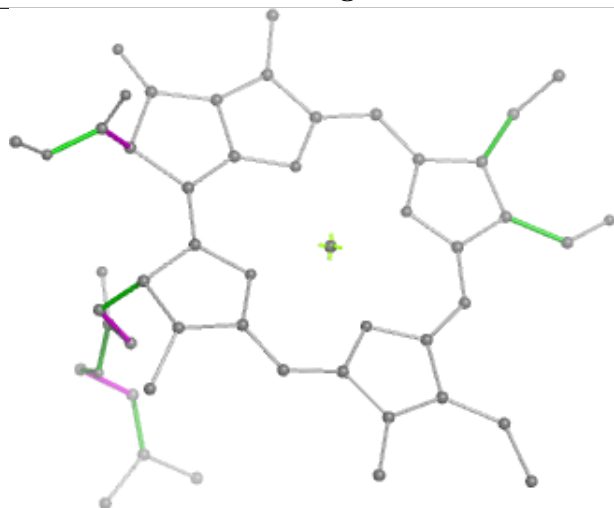
Ligand CHL 4 610



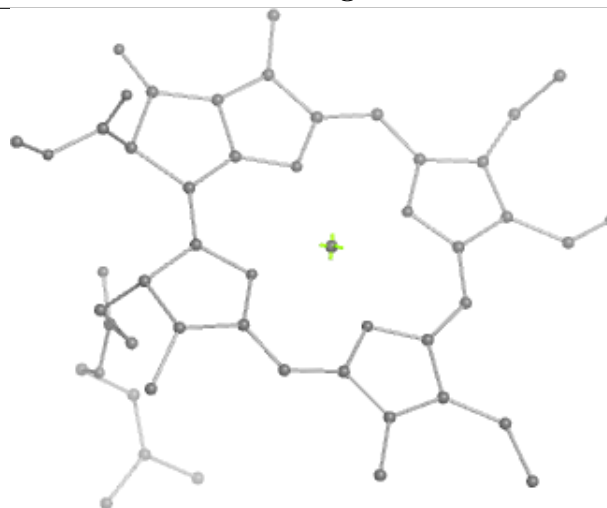
Bond lengths



Bond angles

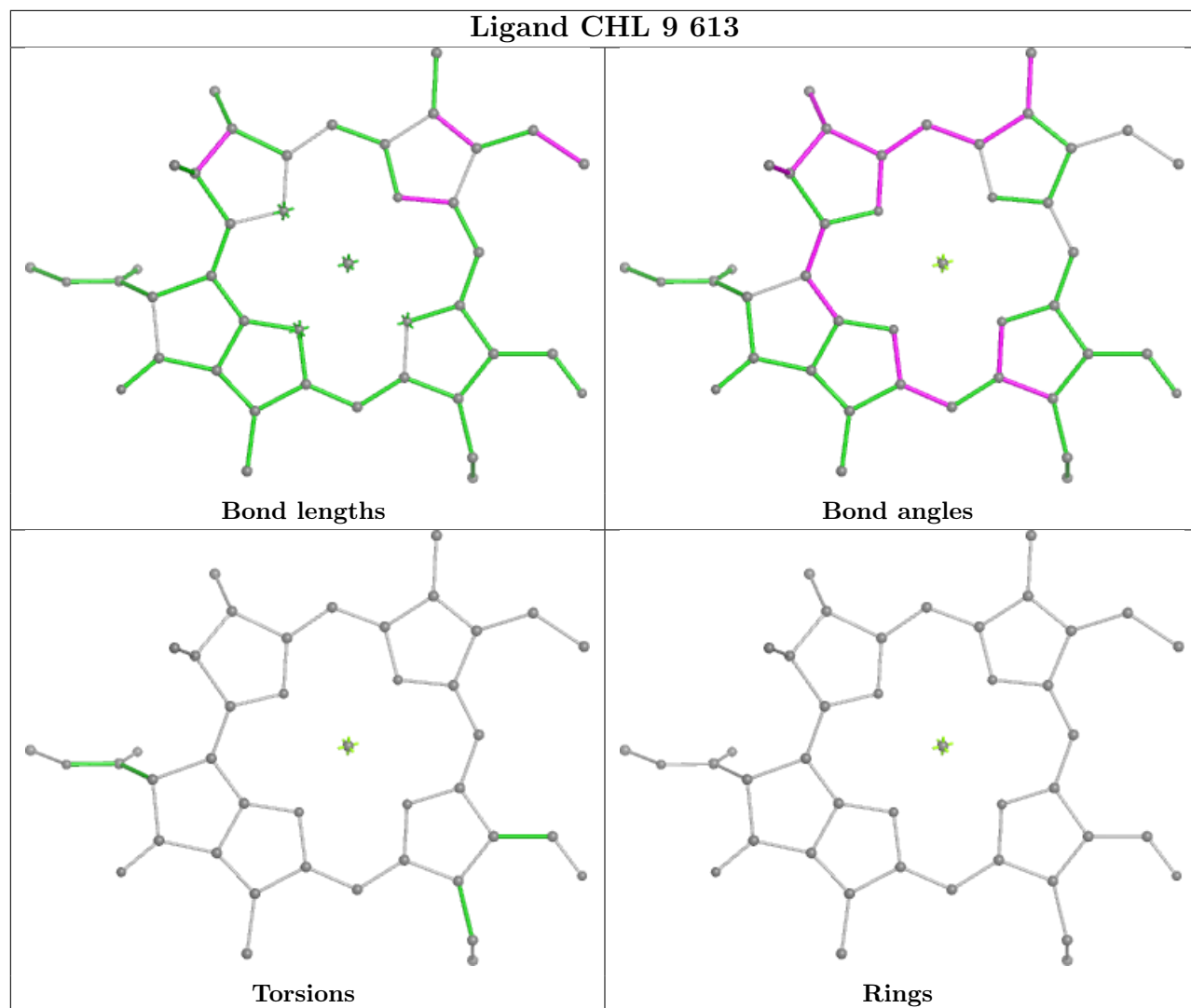


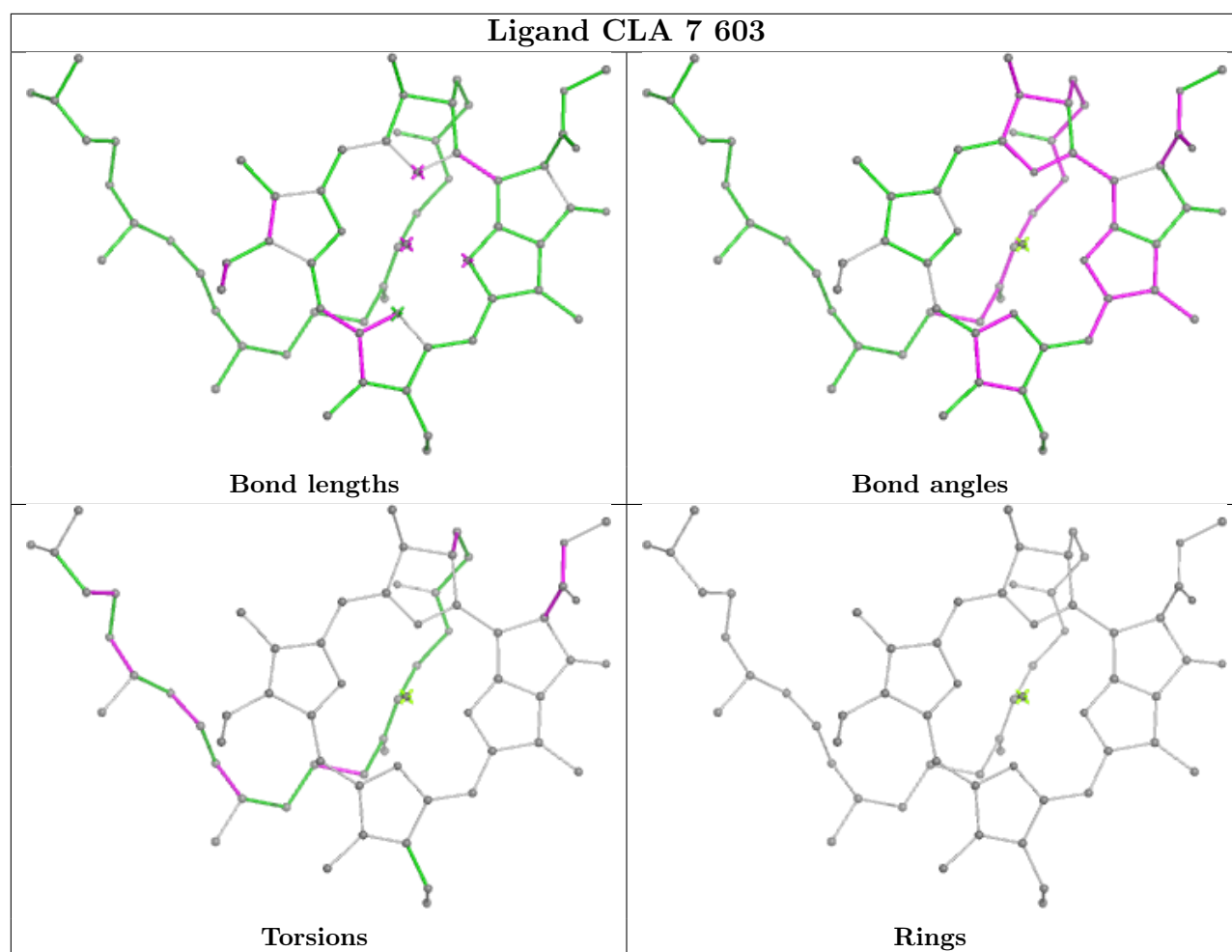
Torsions

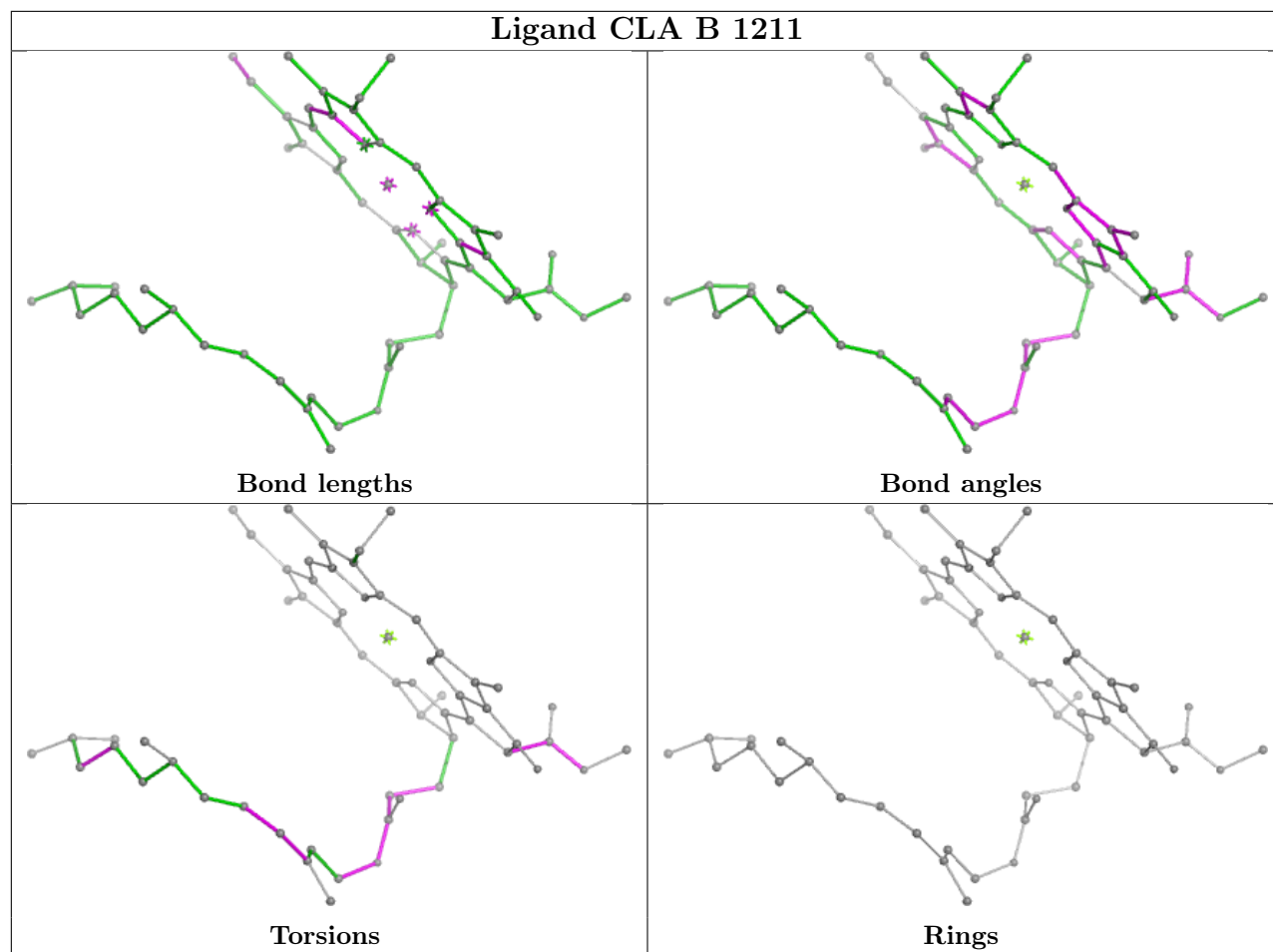


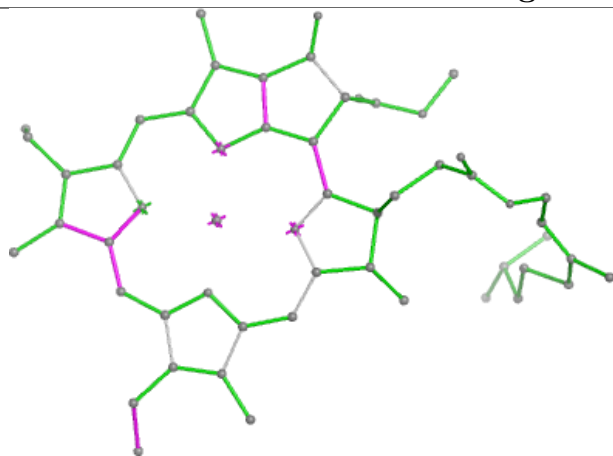
Rings

Ligand CHL 9 613

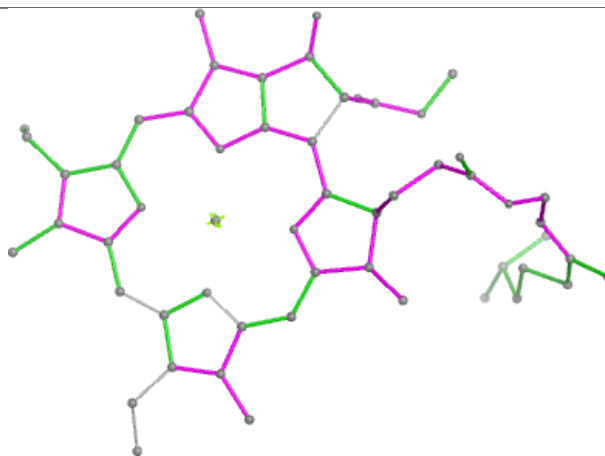




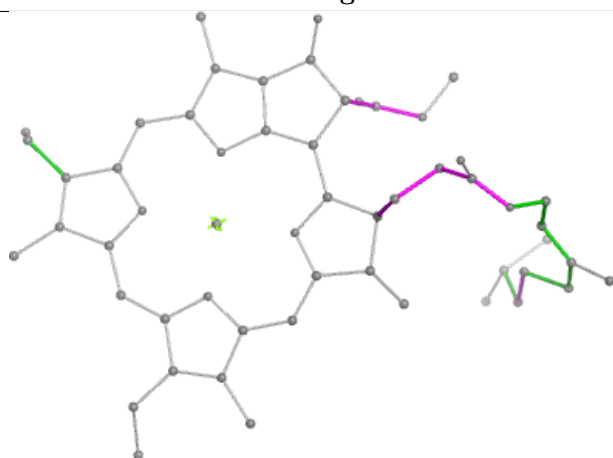


Ligand CLA 5 605

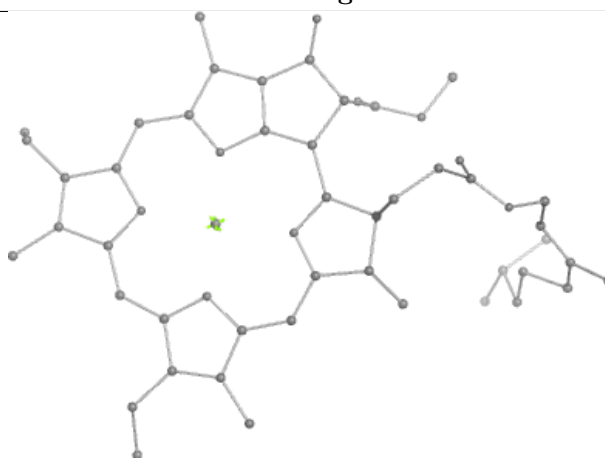
Bond lengths



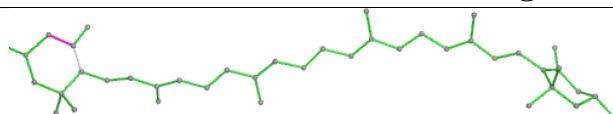
Bond angles



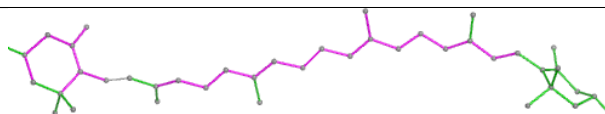
Torsions



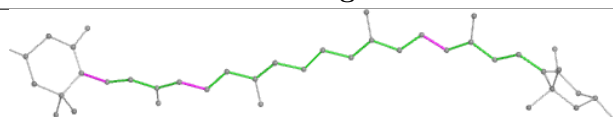
Rings

Ligand LUT 7 502

Bond lengths



Bond angles

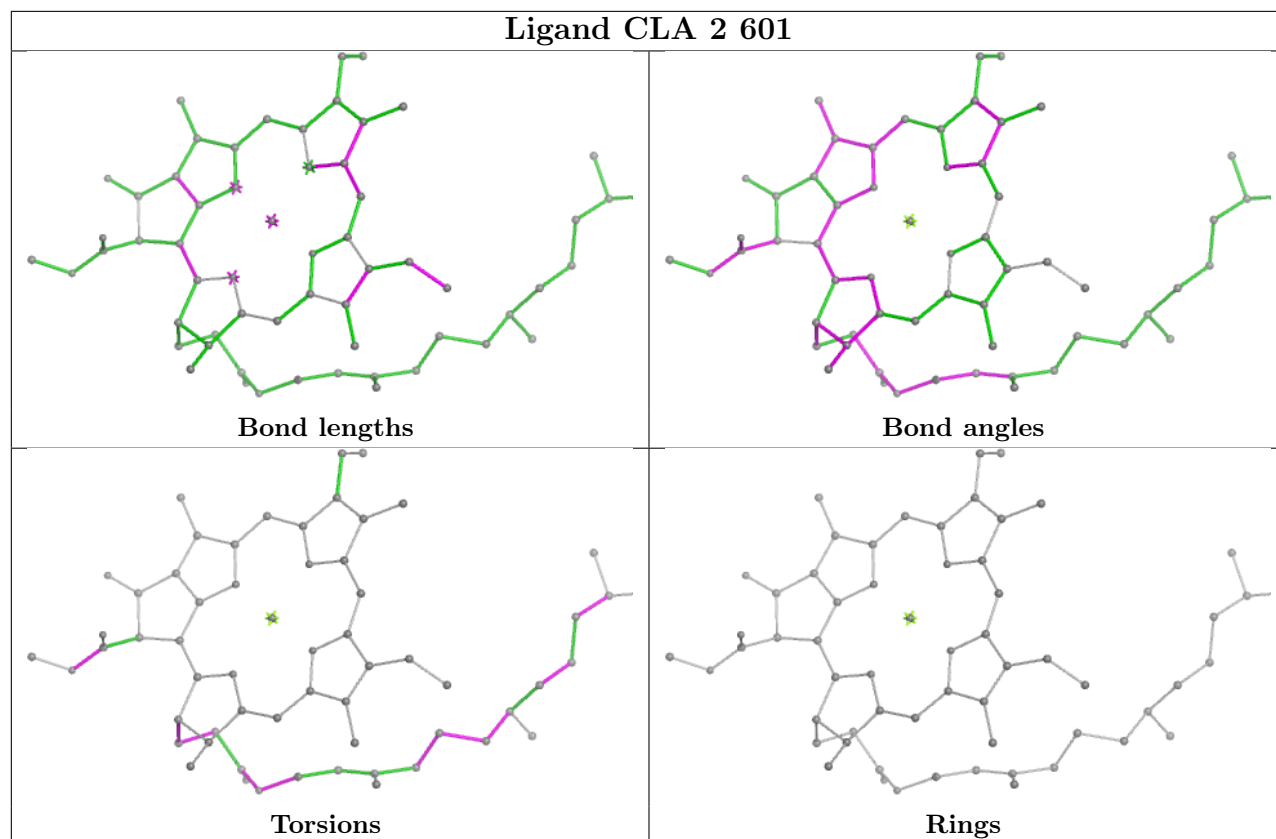


Torsions

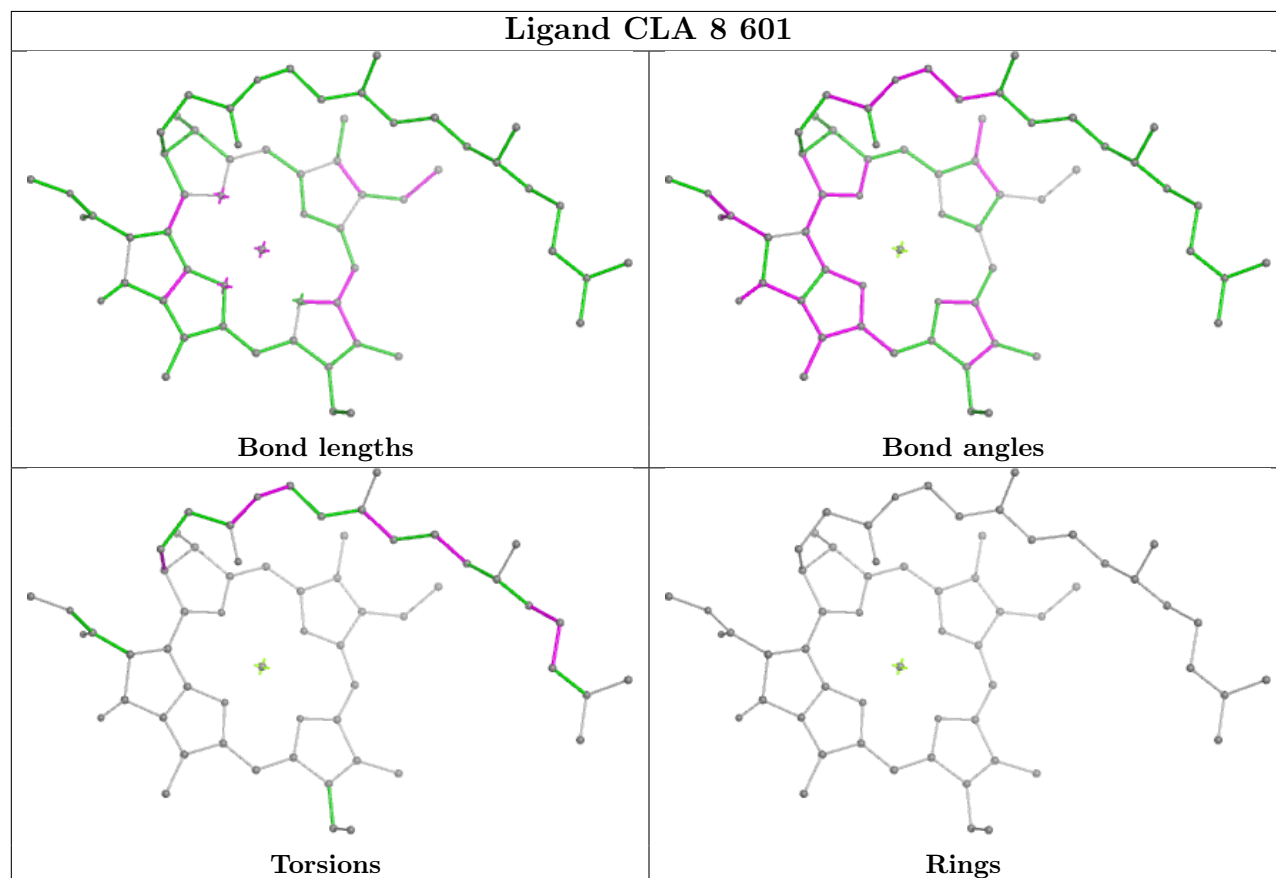


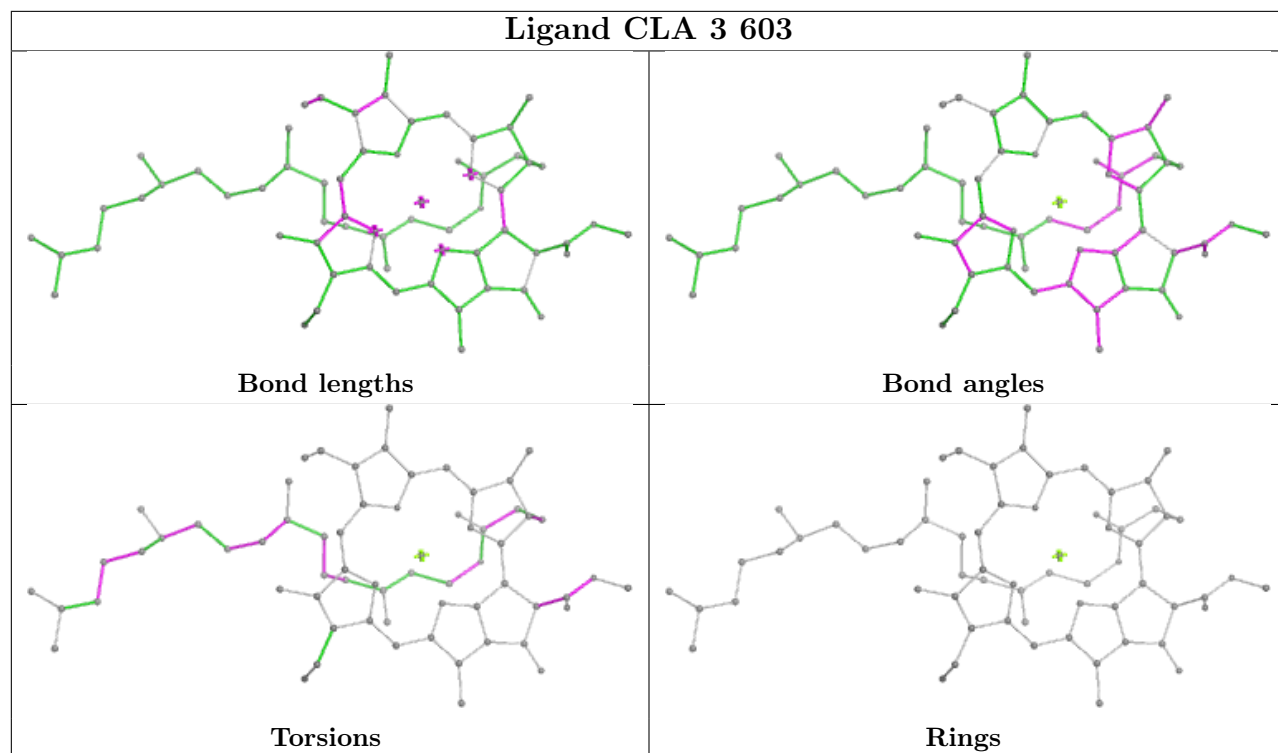
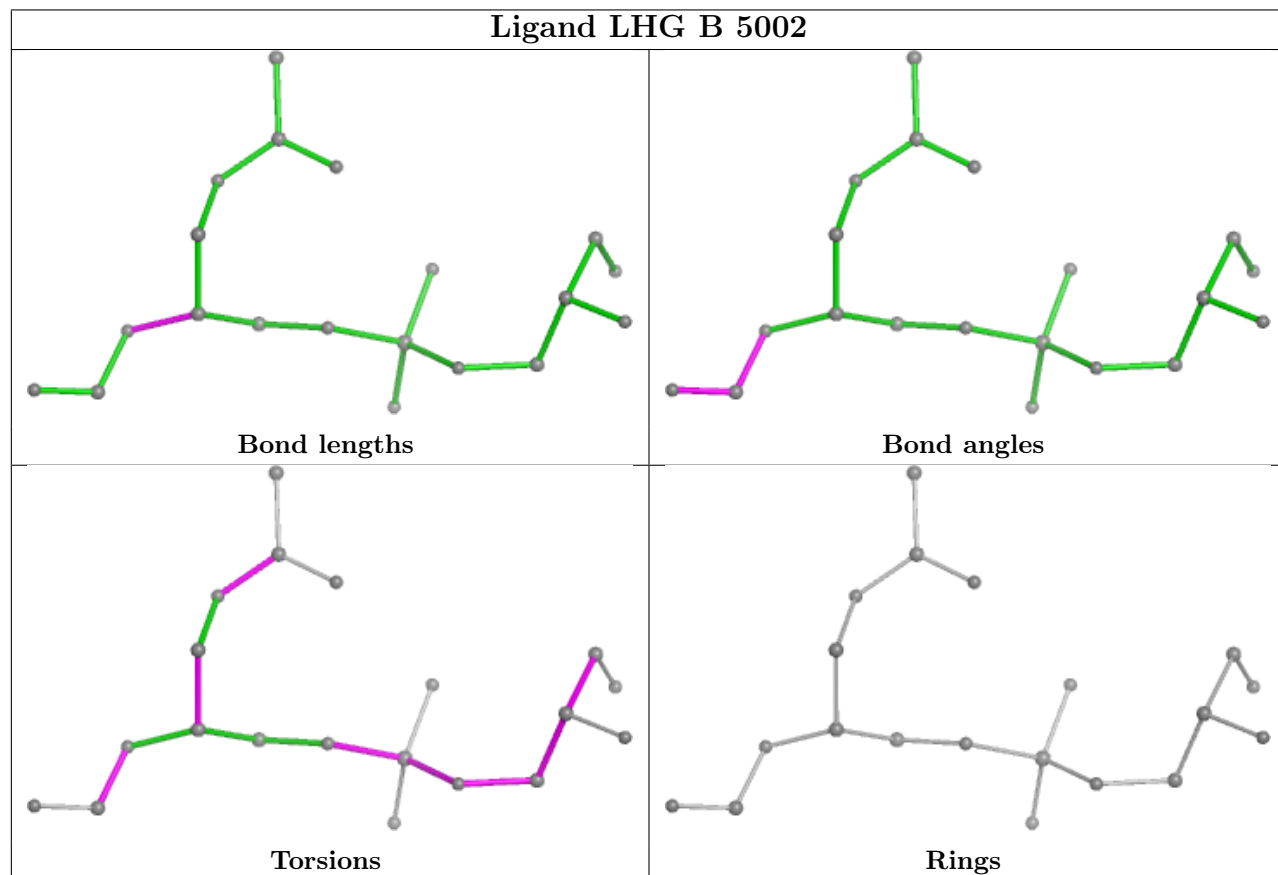
Rings

Ligand CLA 2 601

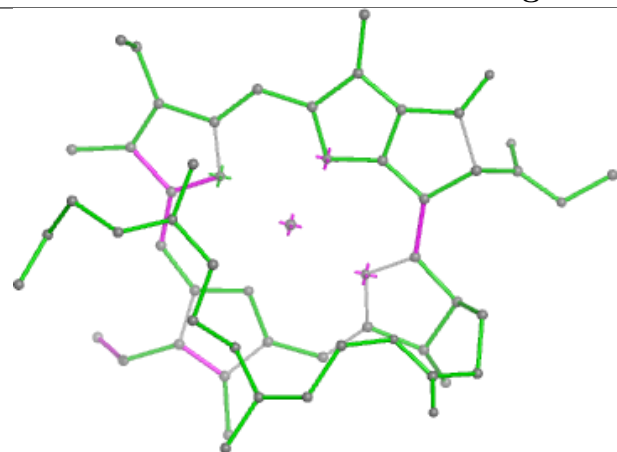


Ligand CLA 8 601

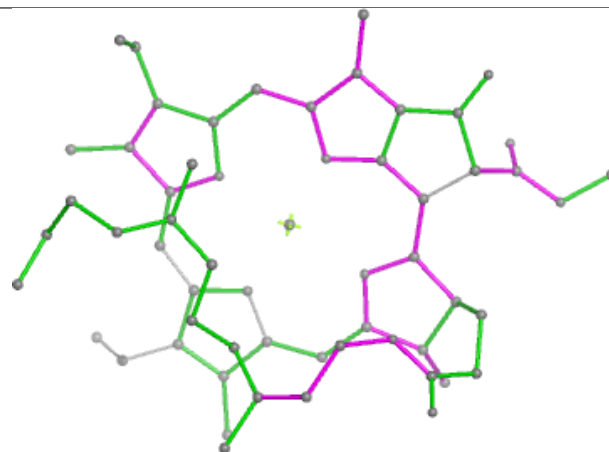


Ligand CLA 3 603**Ligand LHG B 5002**

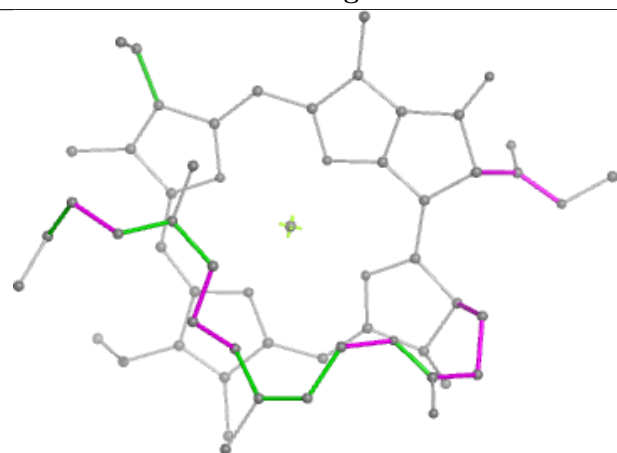
Ligand CLA 7 615



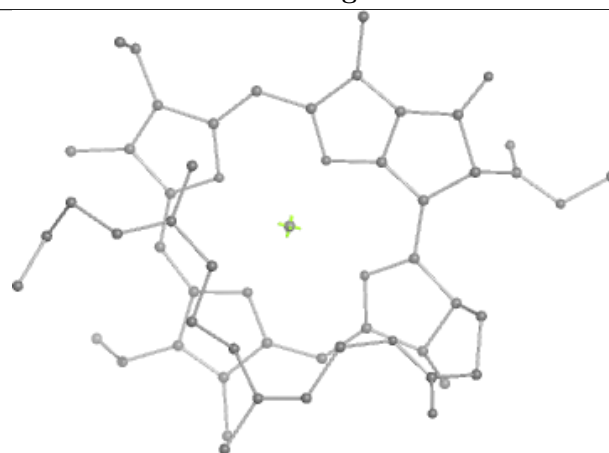
Bond lengths



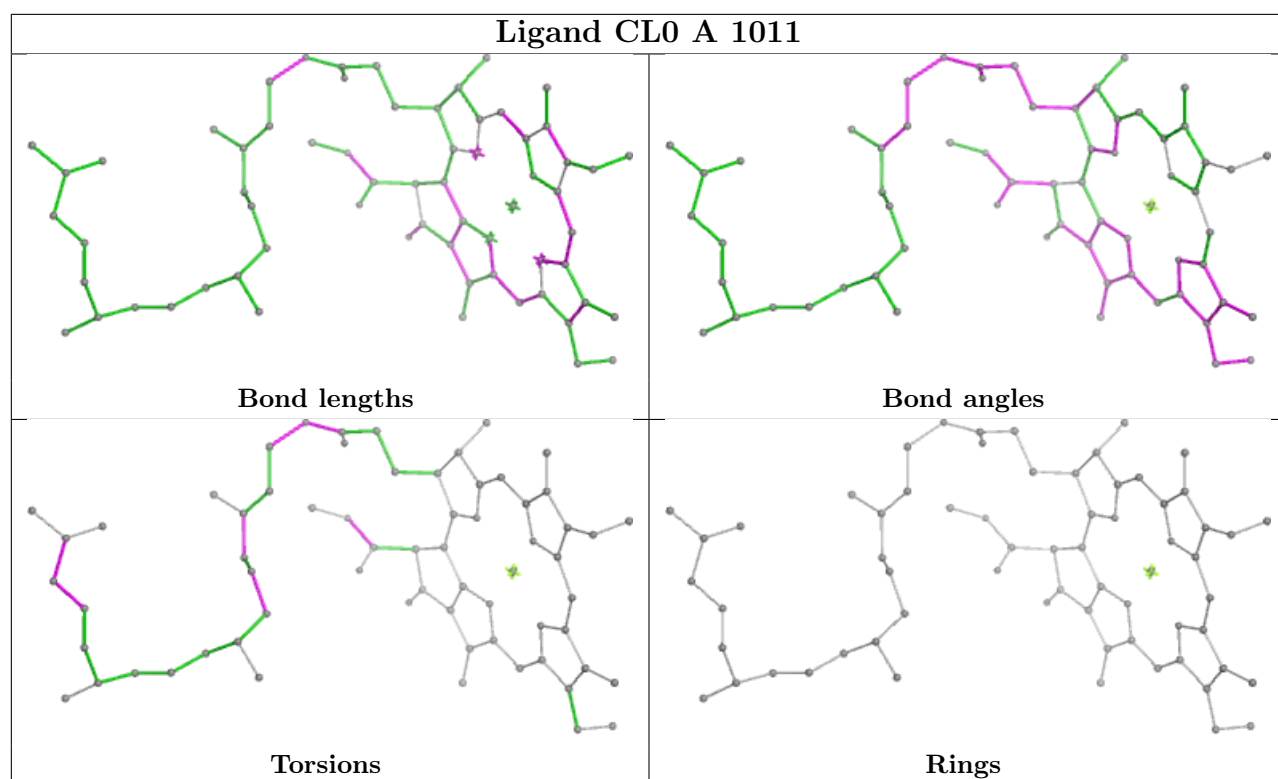
Bond angles



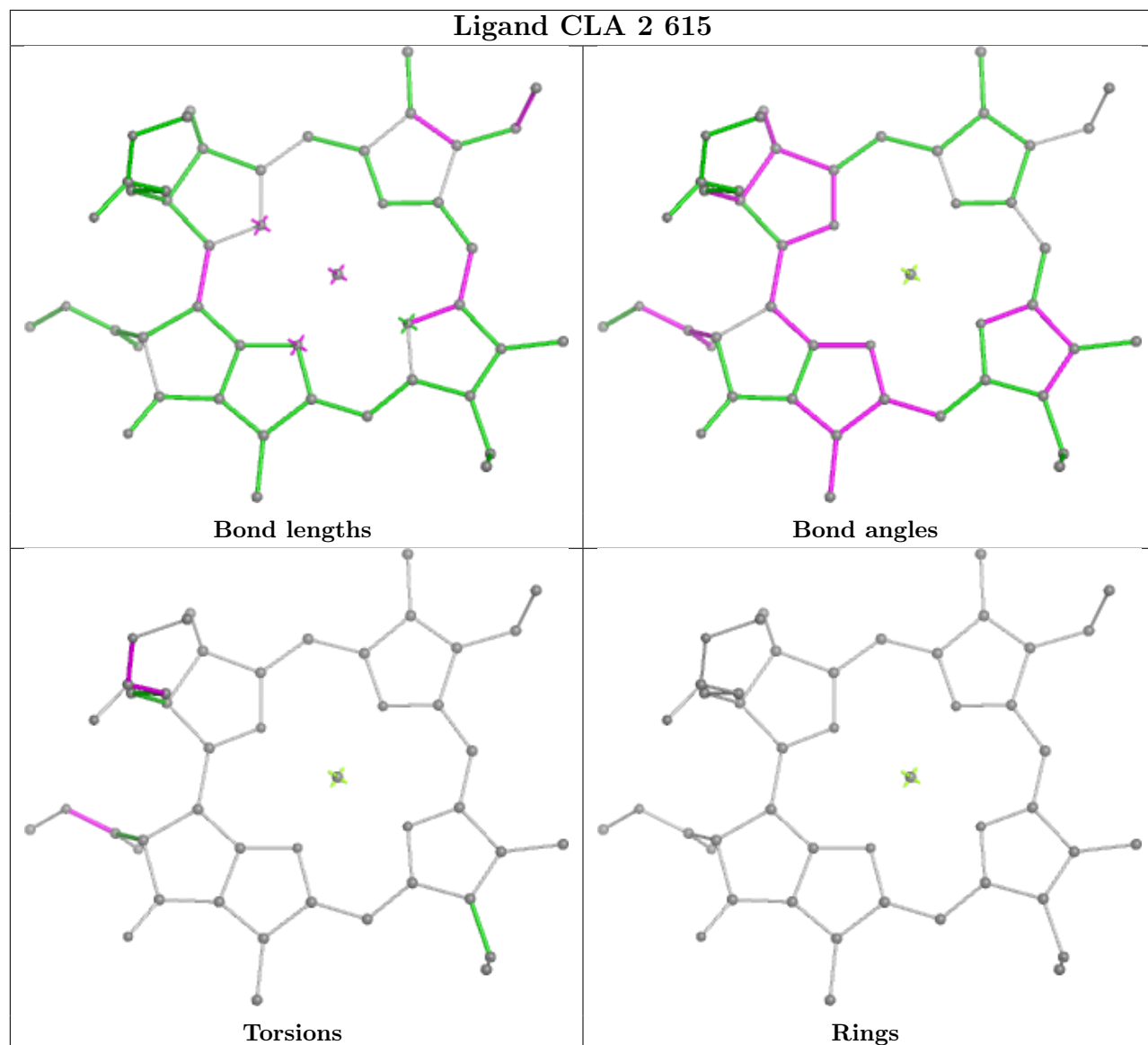
Torsions

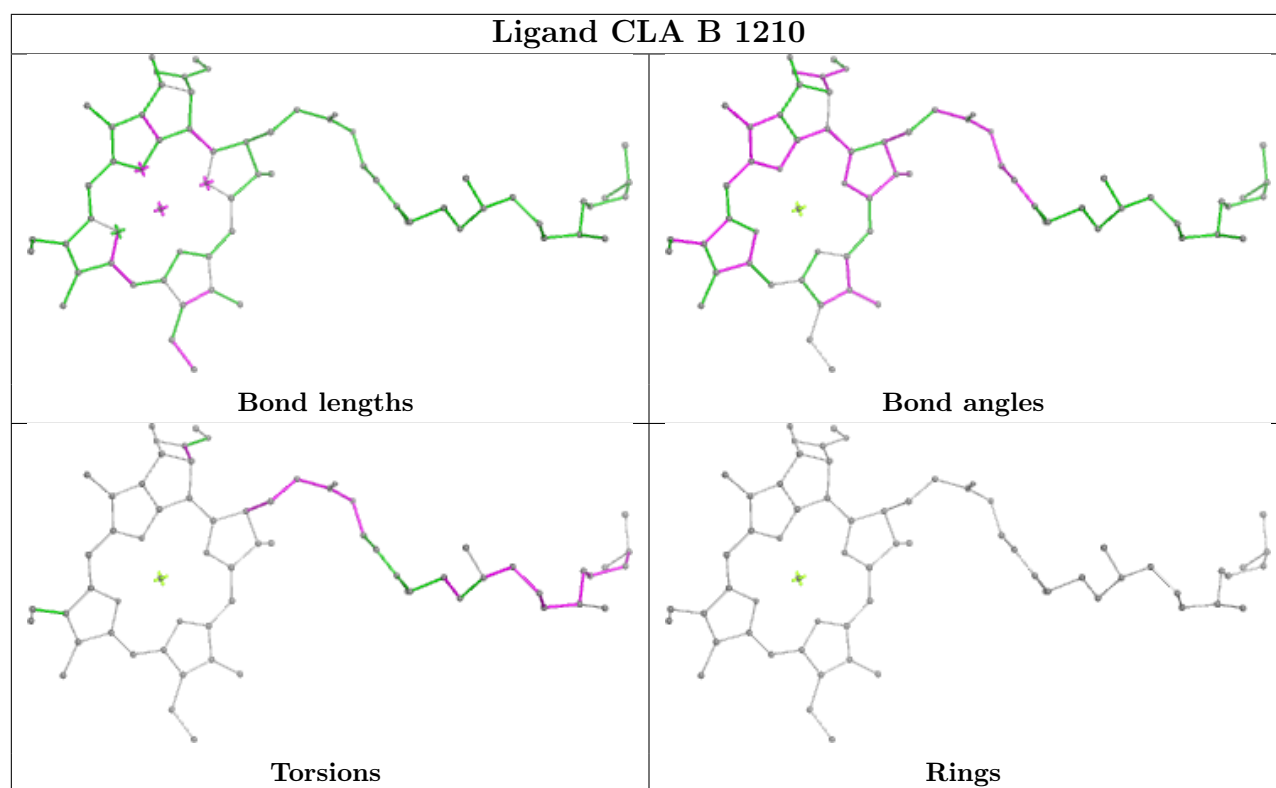


Rings

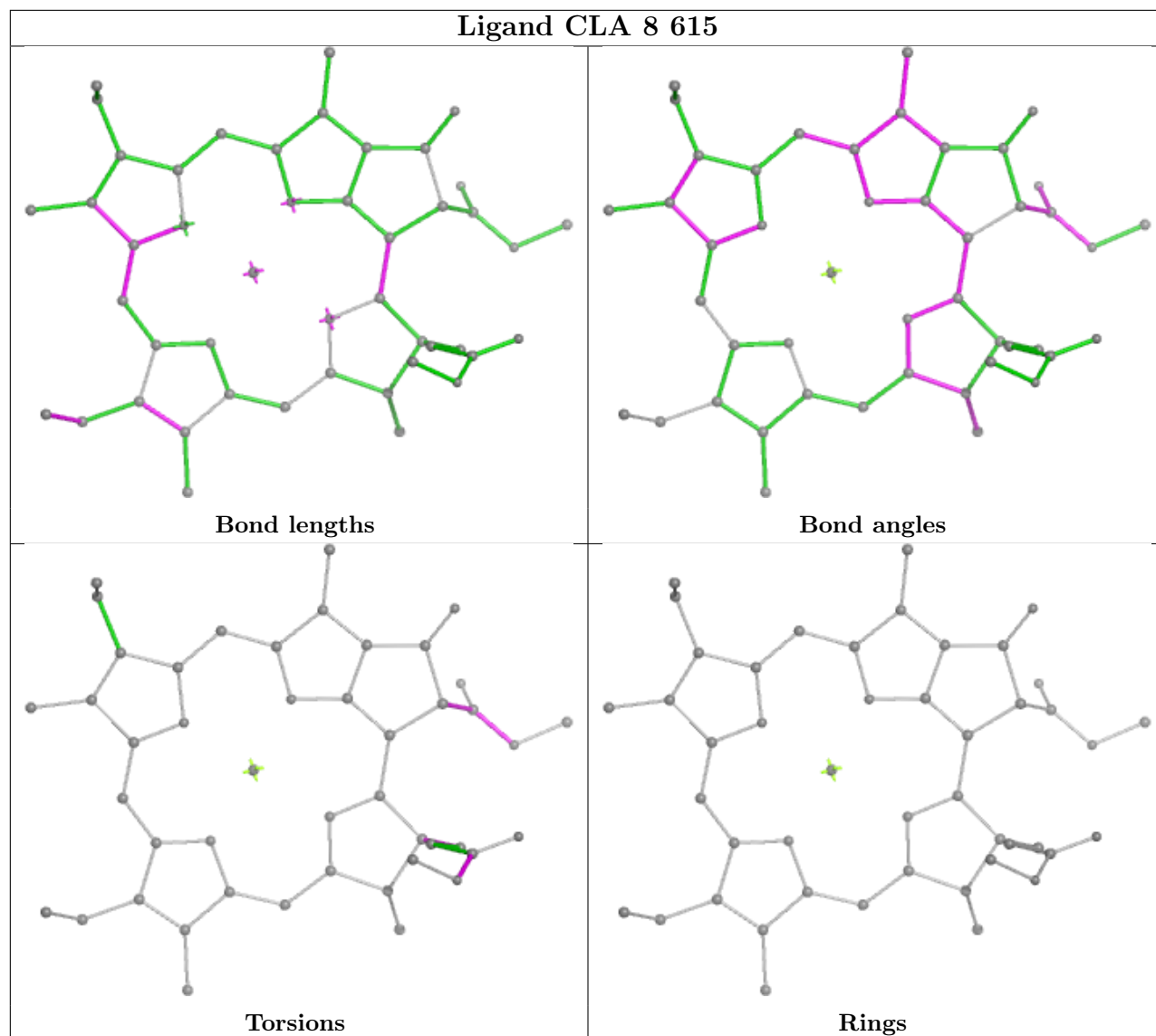


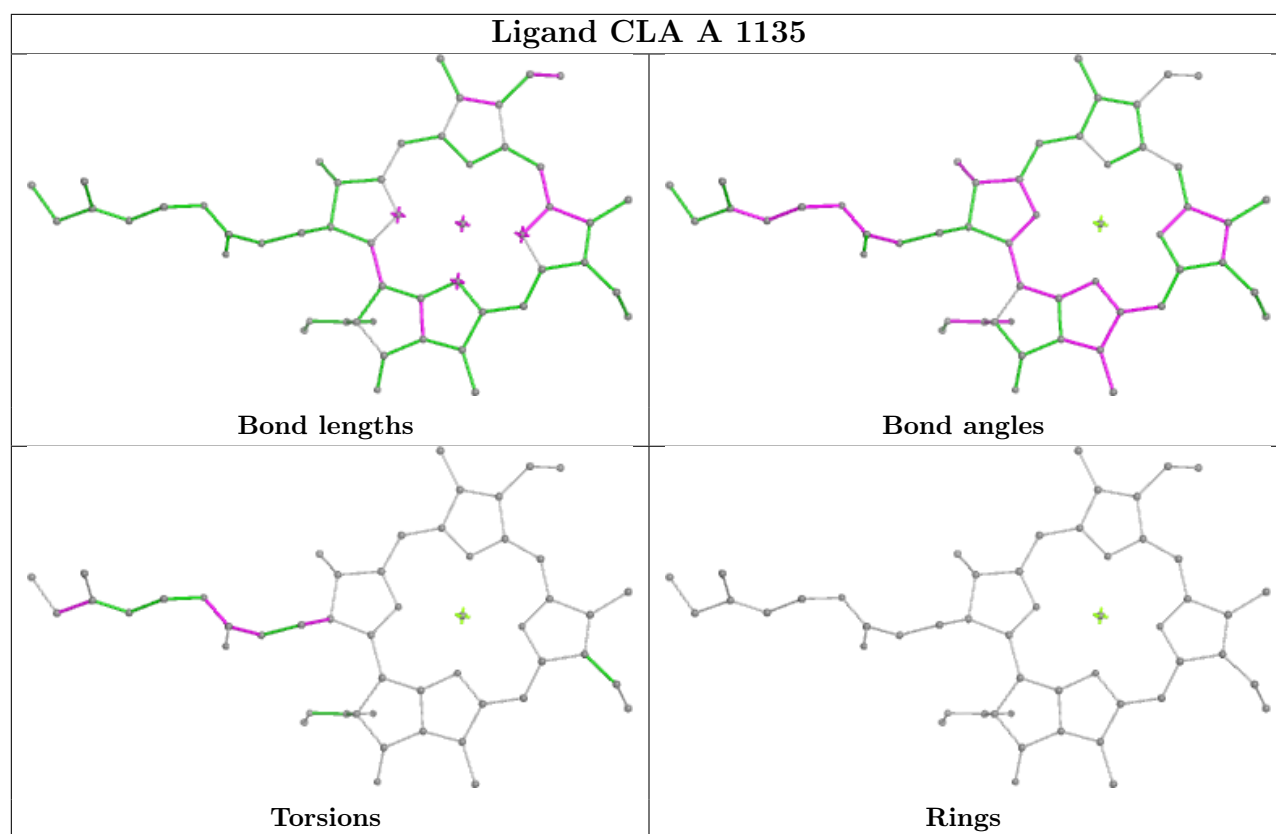
Ligand CLA 2 615



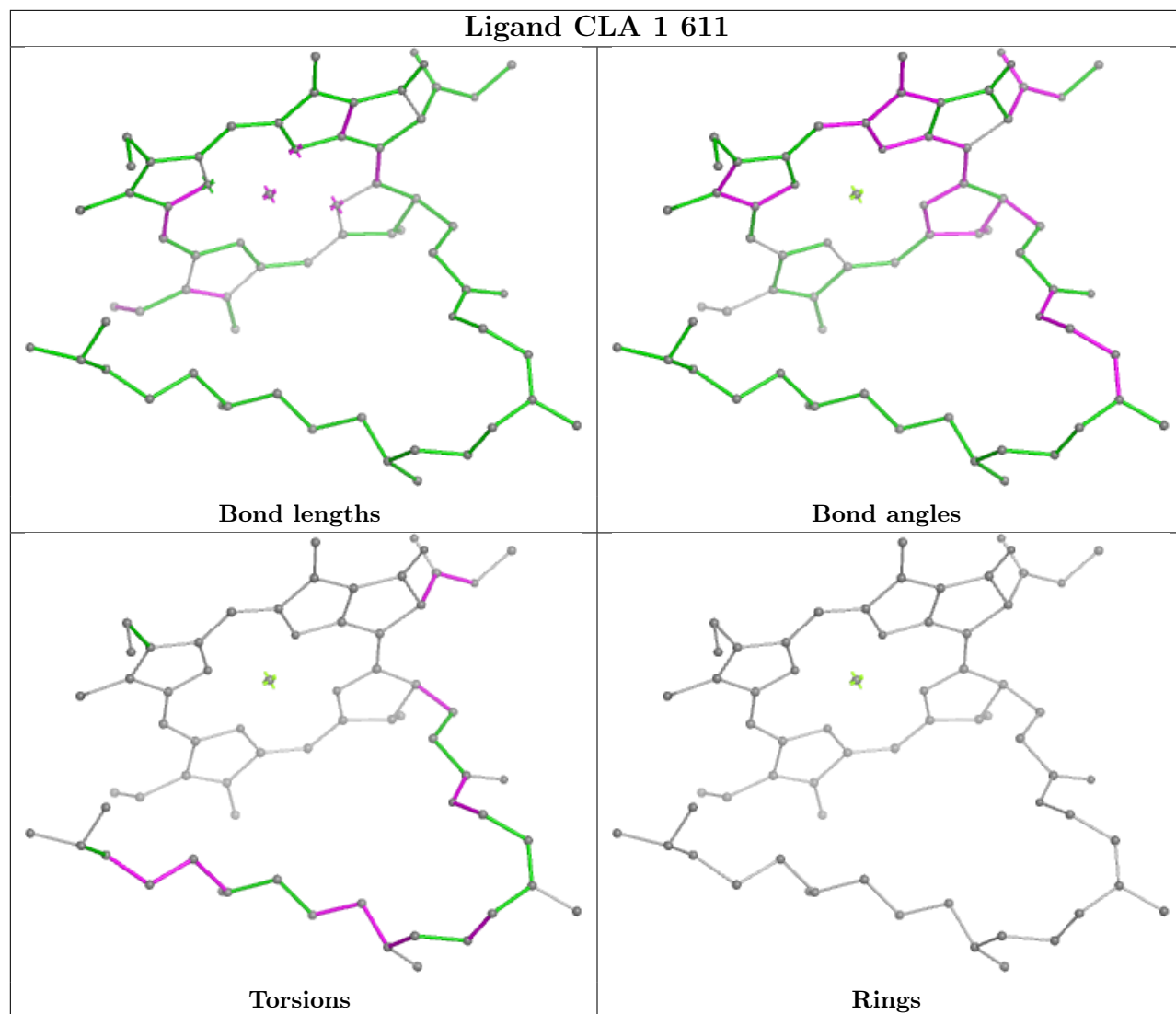


Ligand CLA 8 615

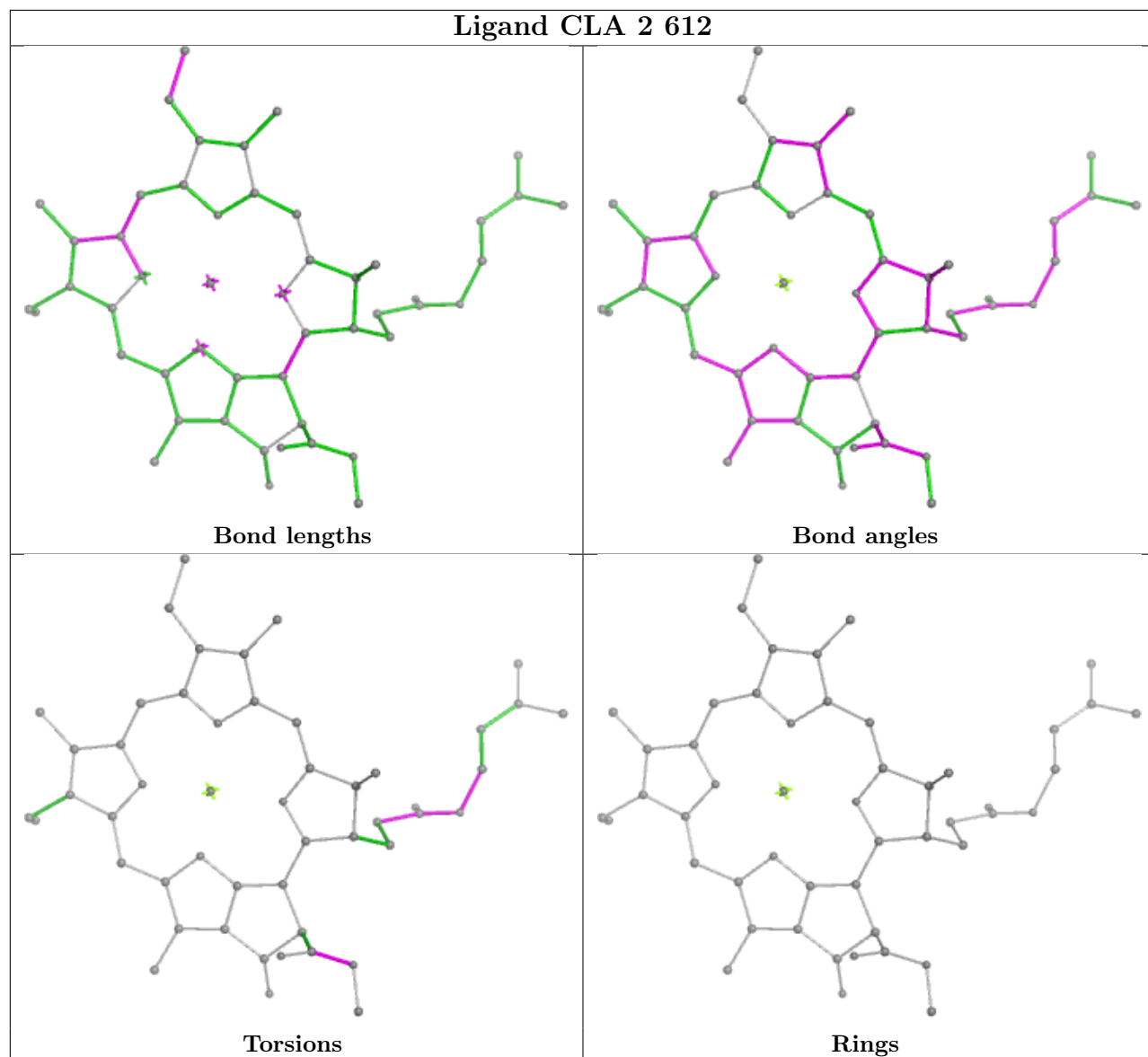


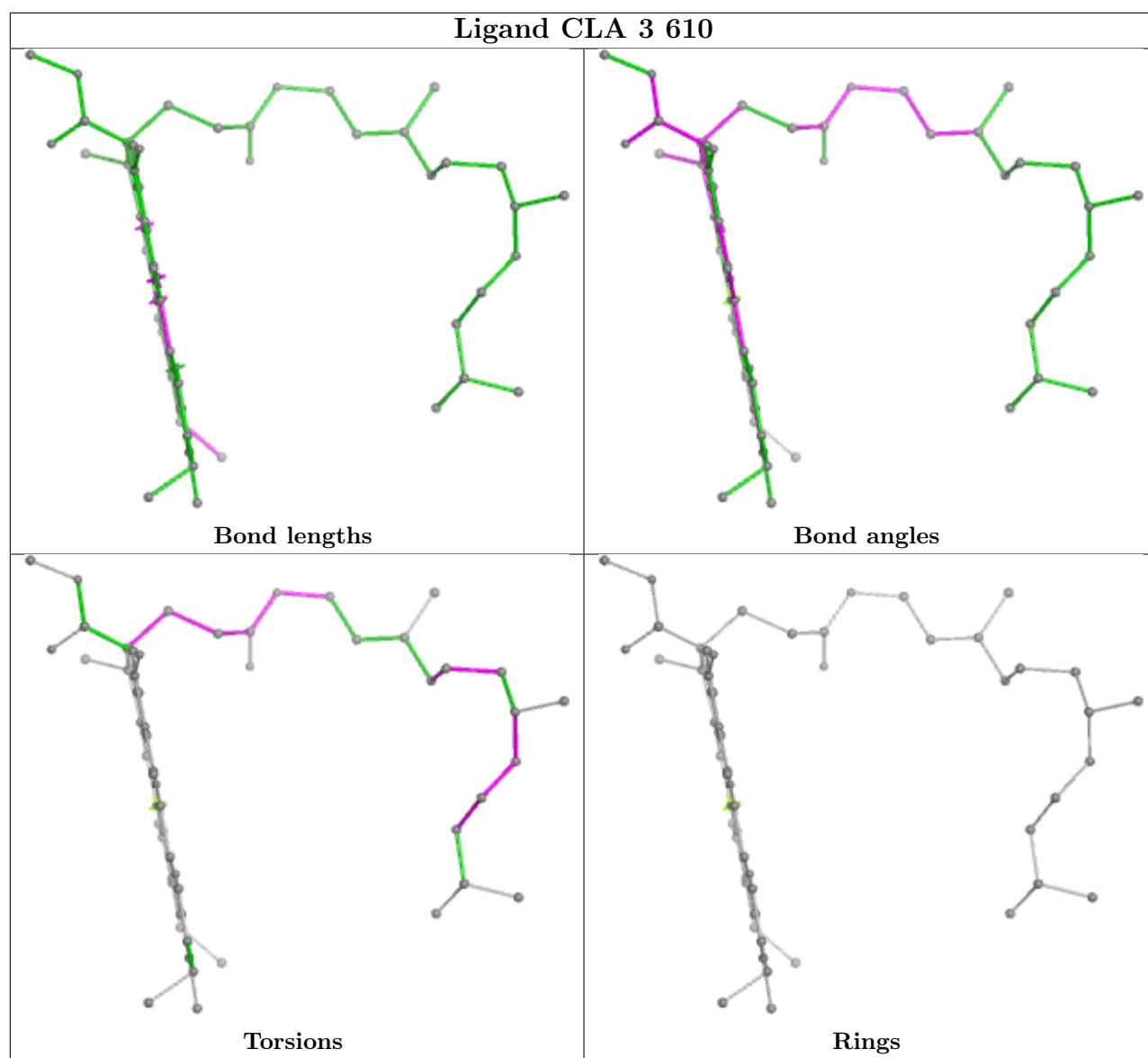


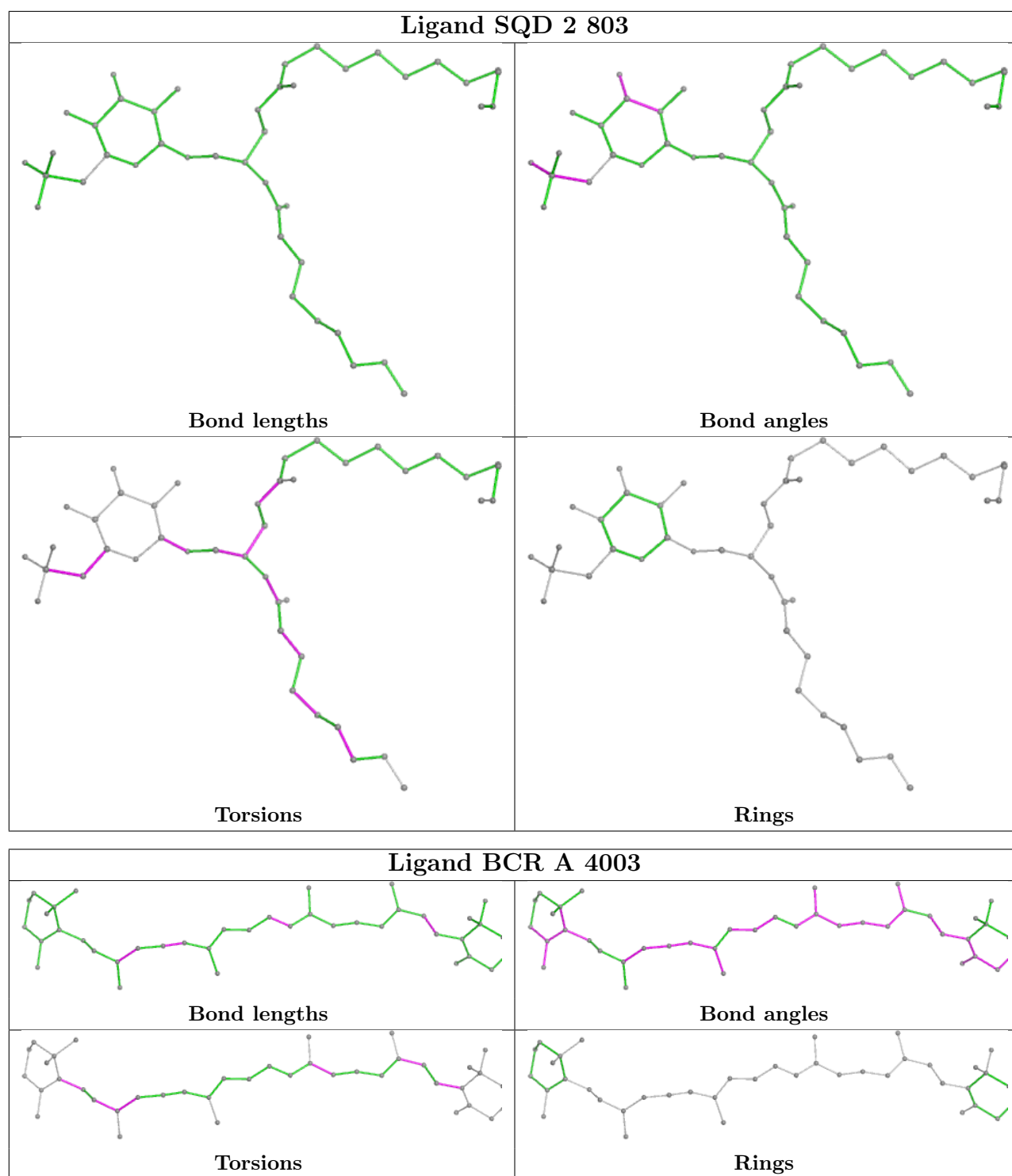
Ligand CLA 1 611



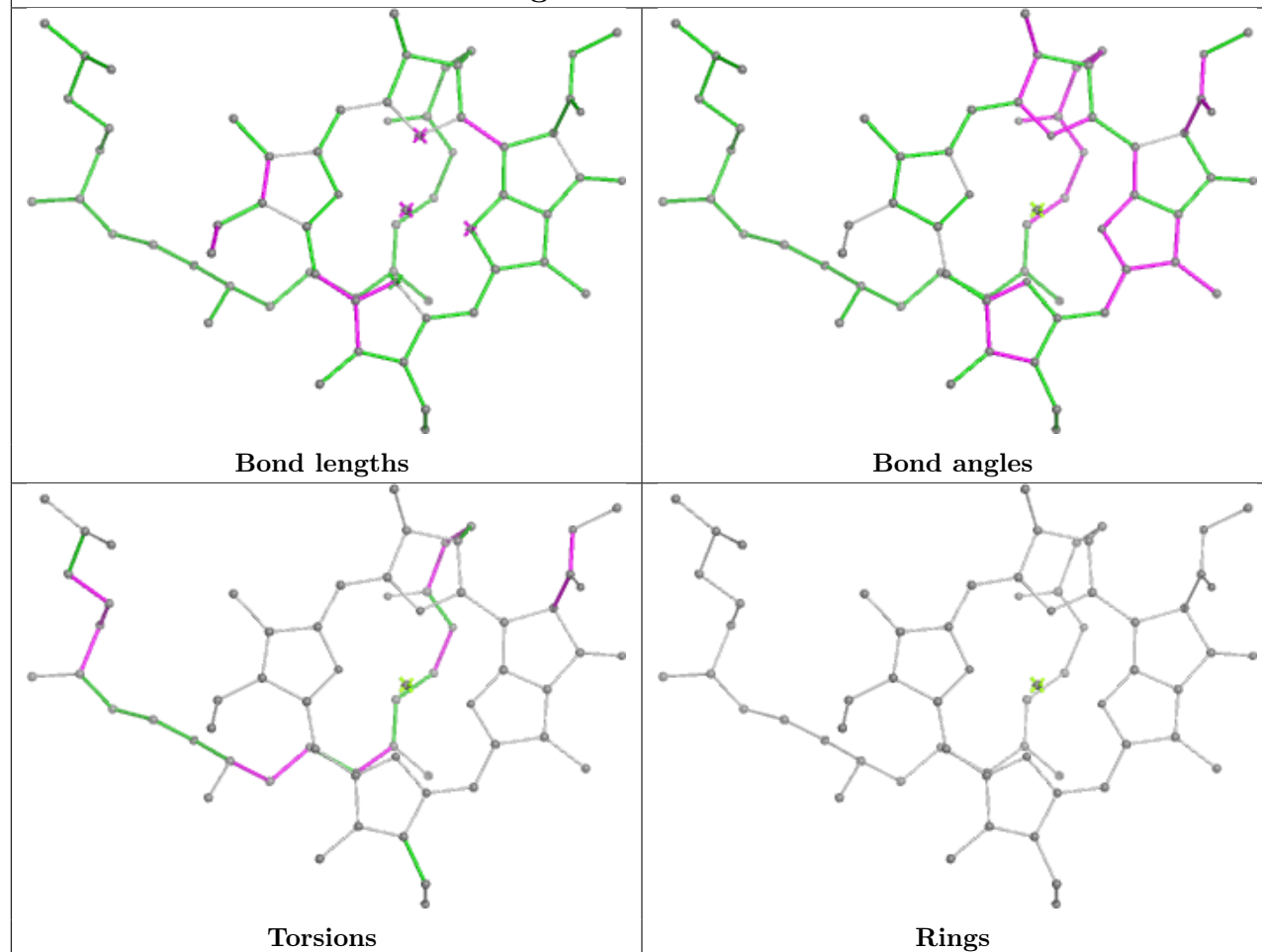
Ligand CLA 2 612



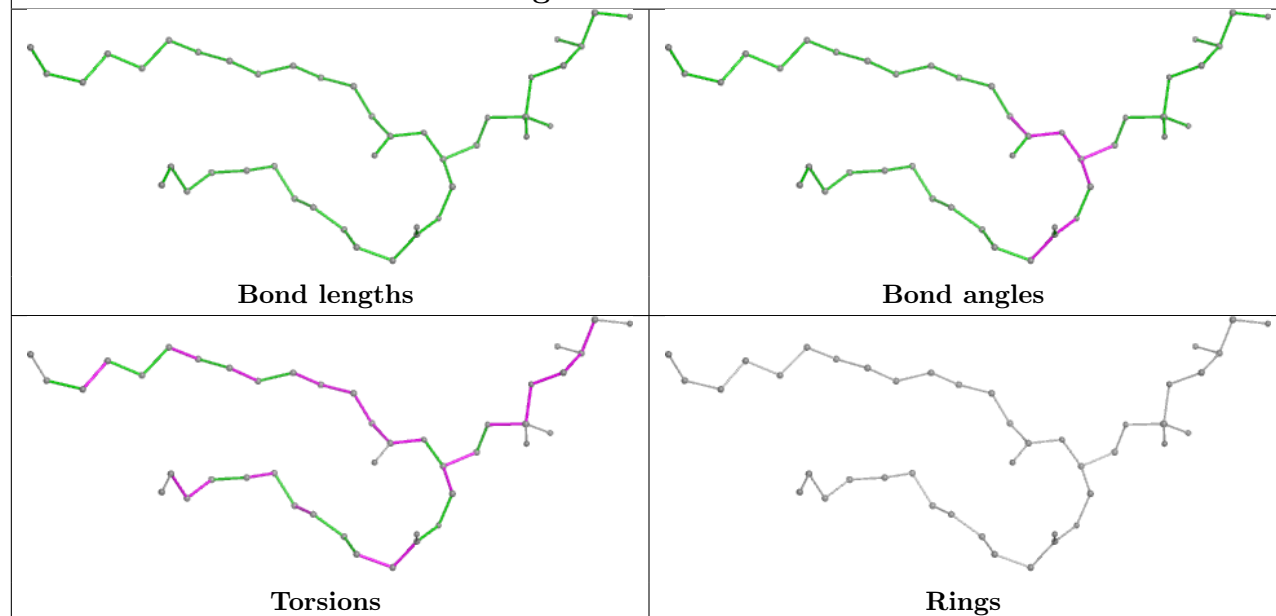


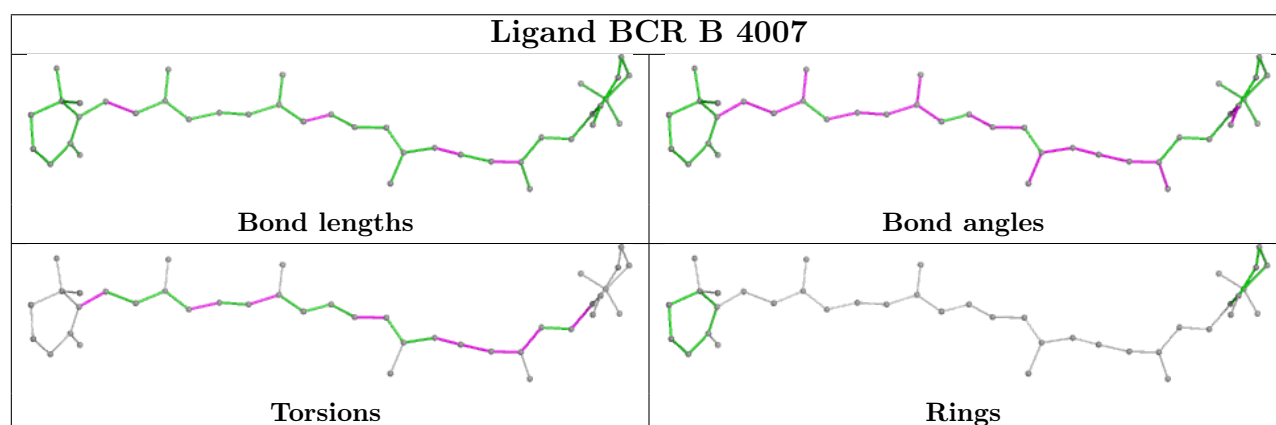
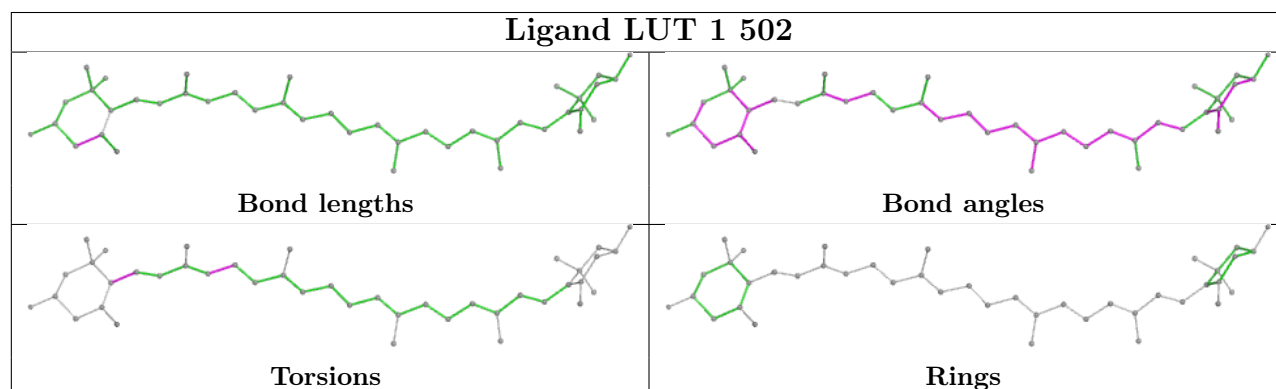
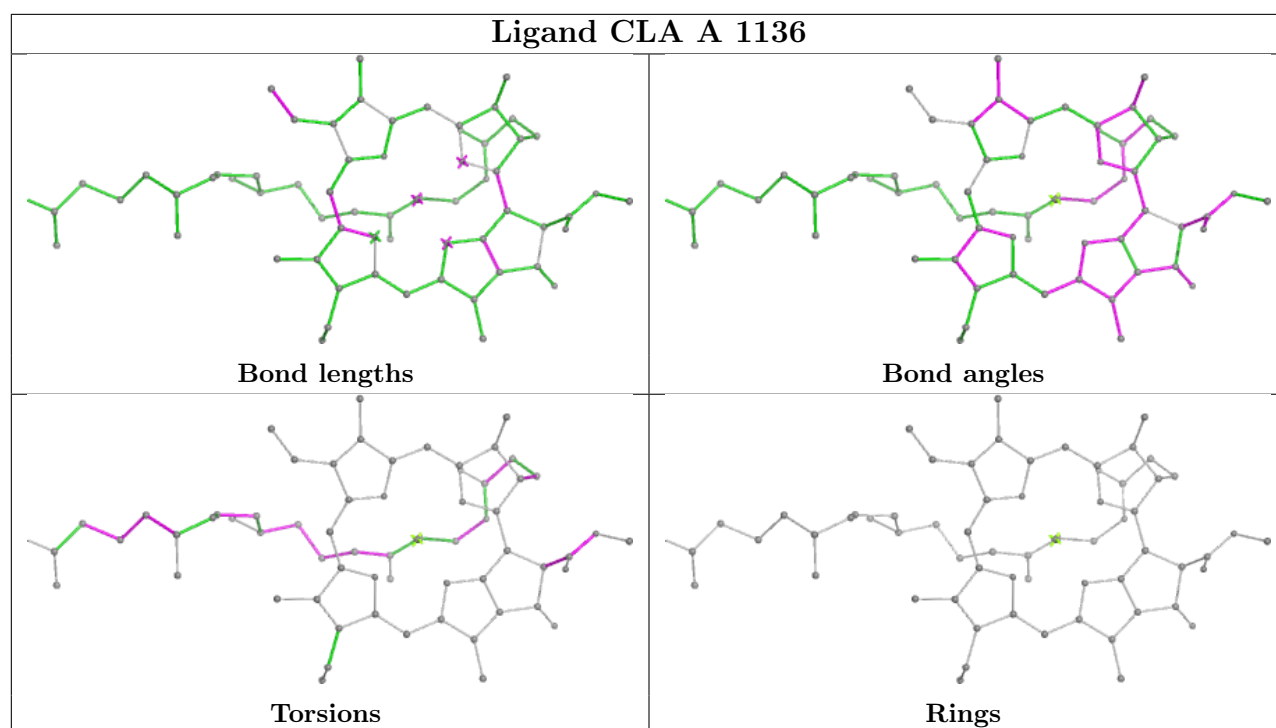


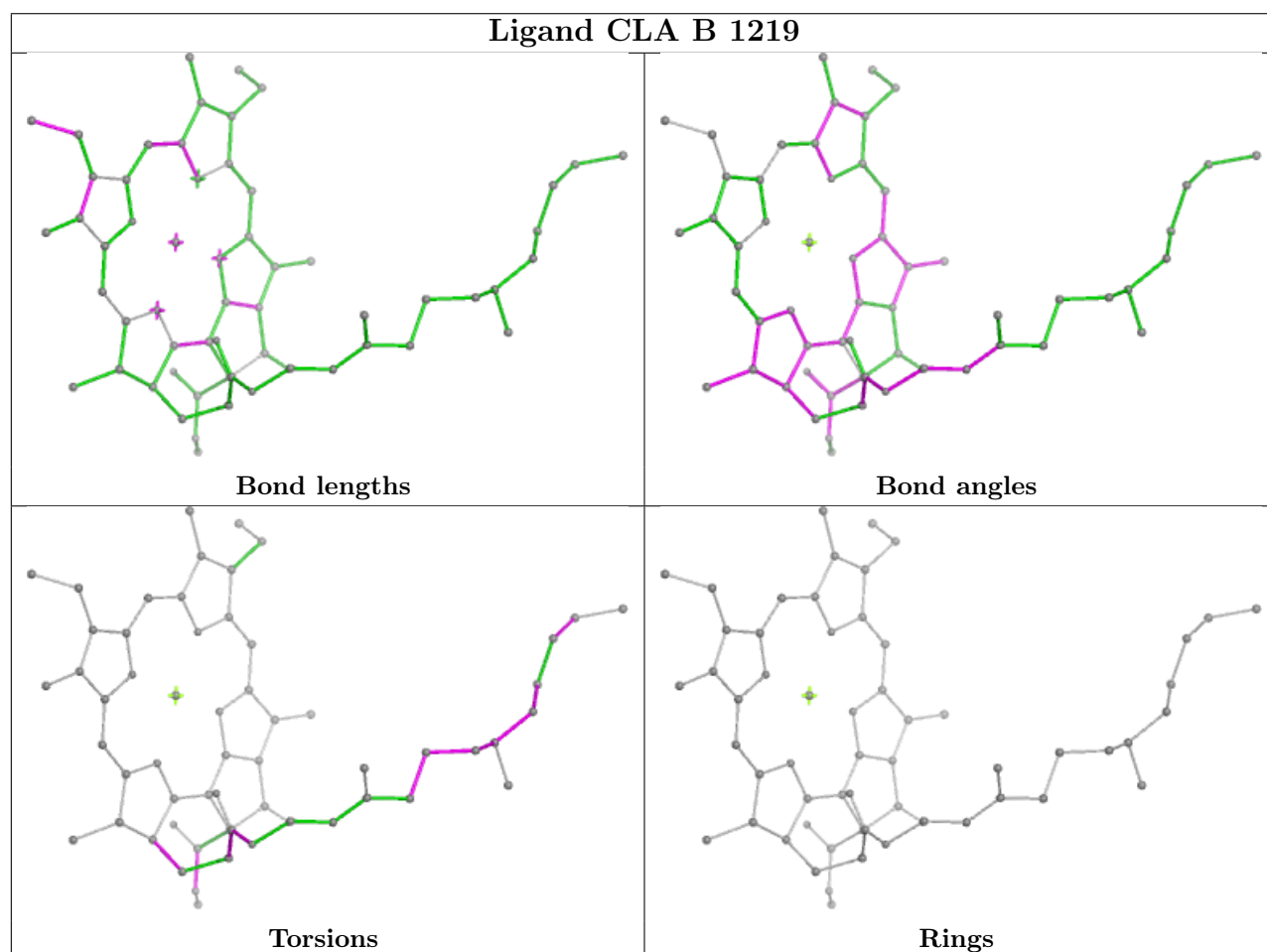
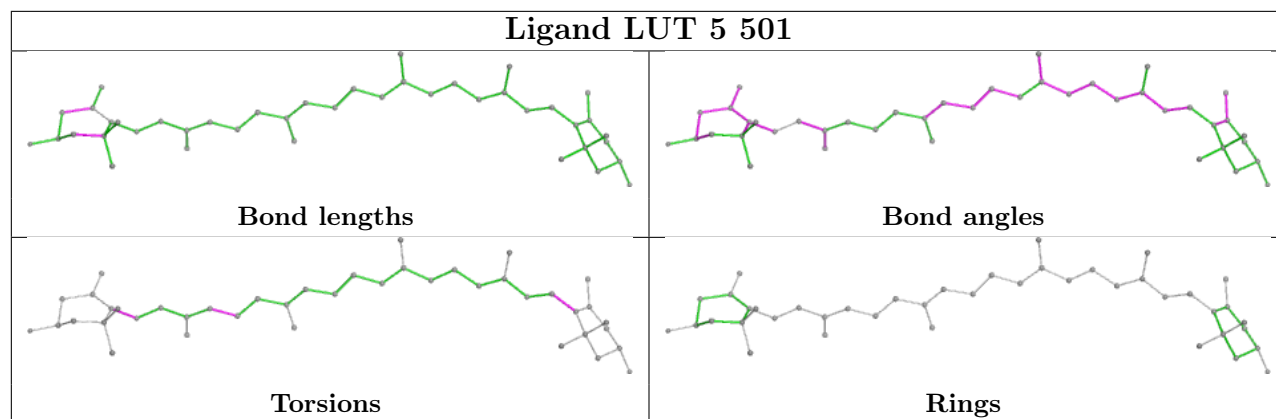
Ligand CLA 6 603



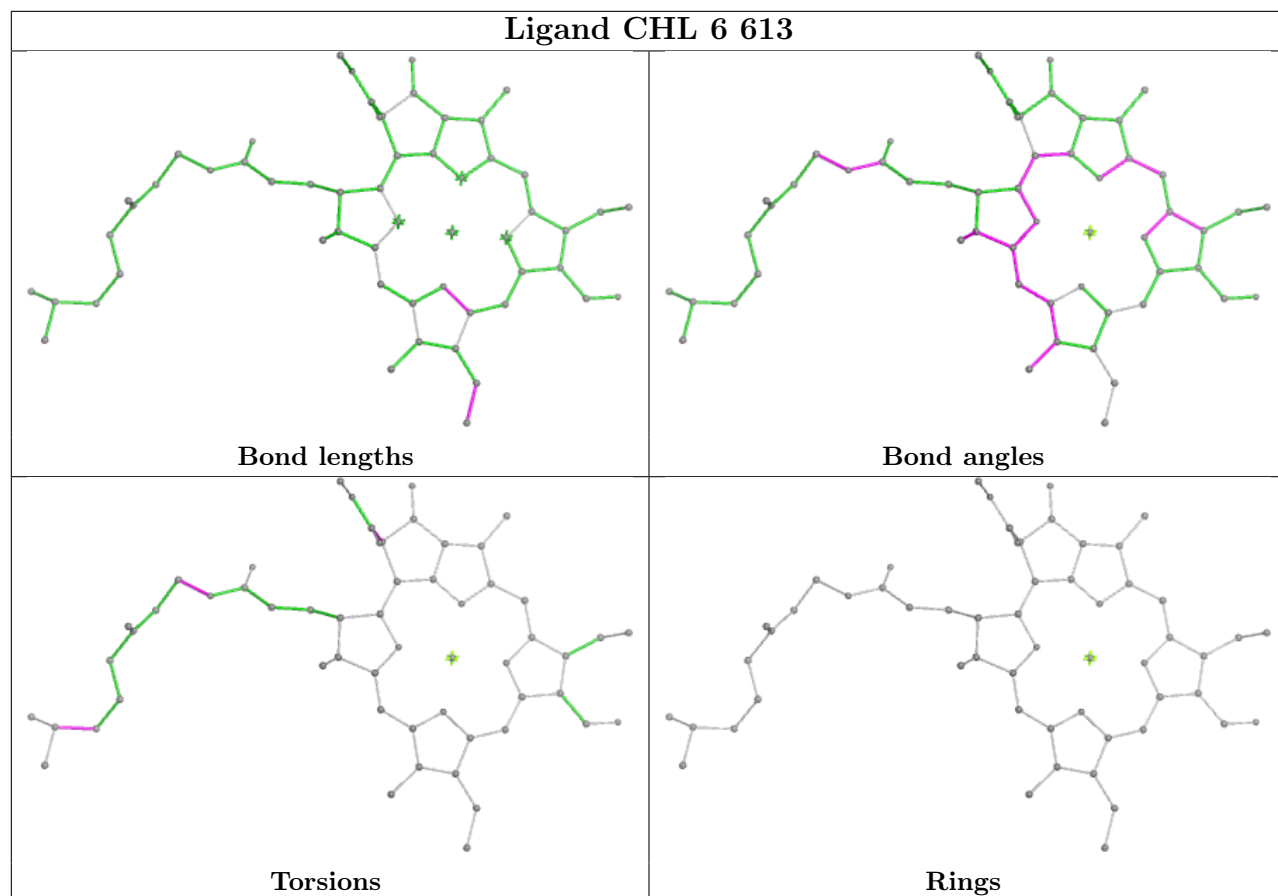
Ligand LHG Z 801



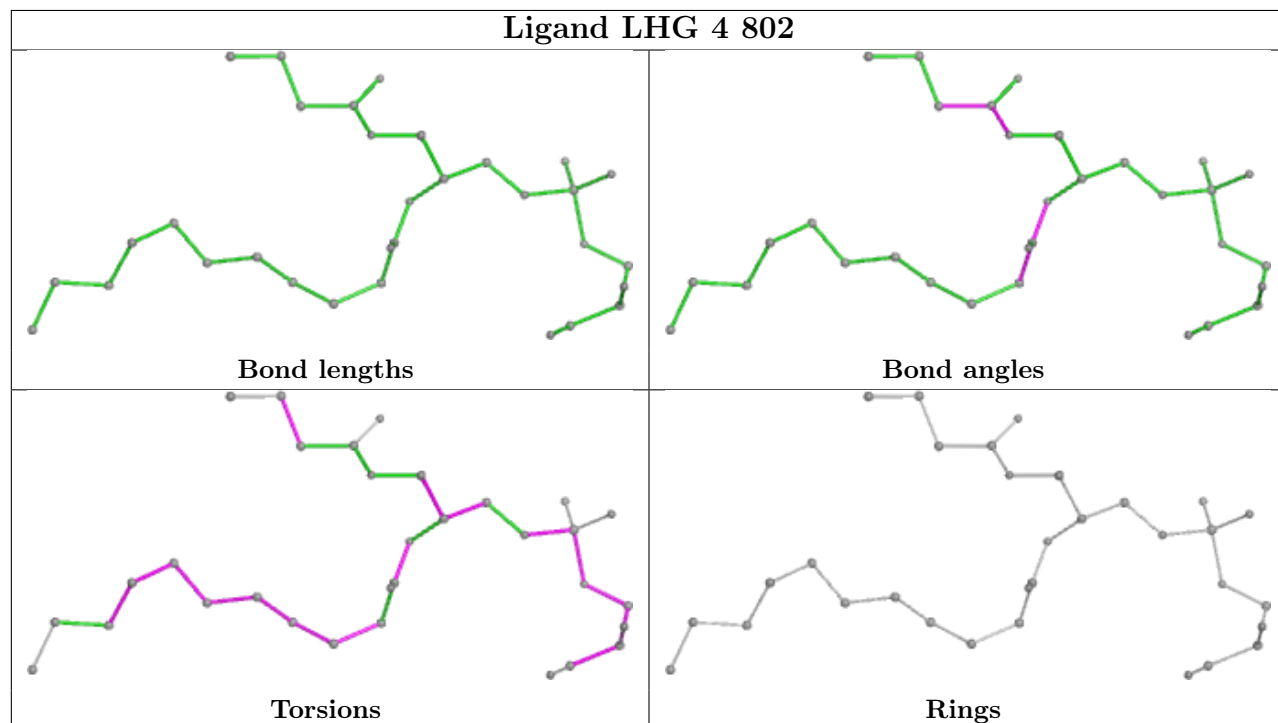




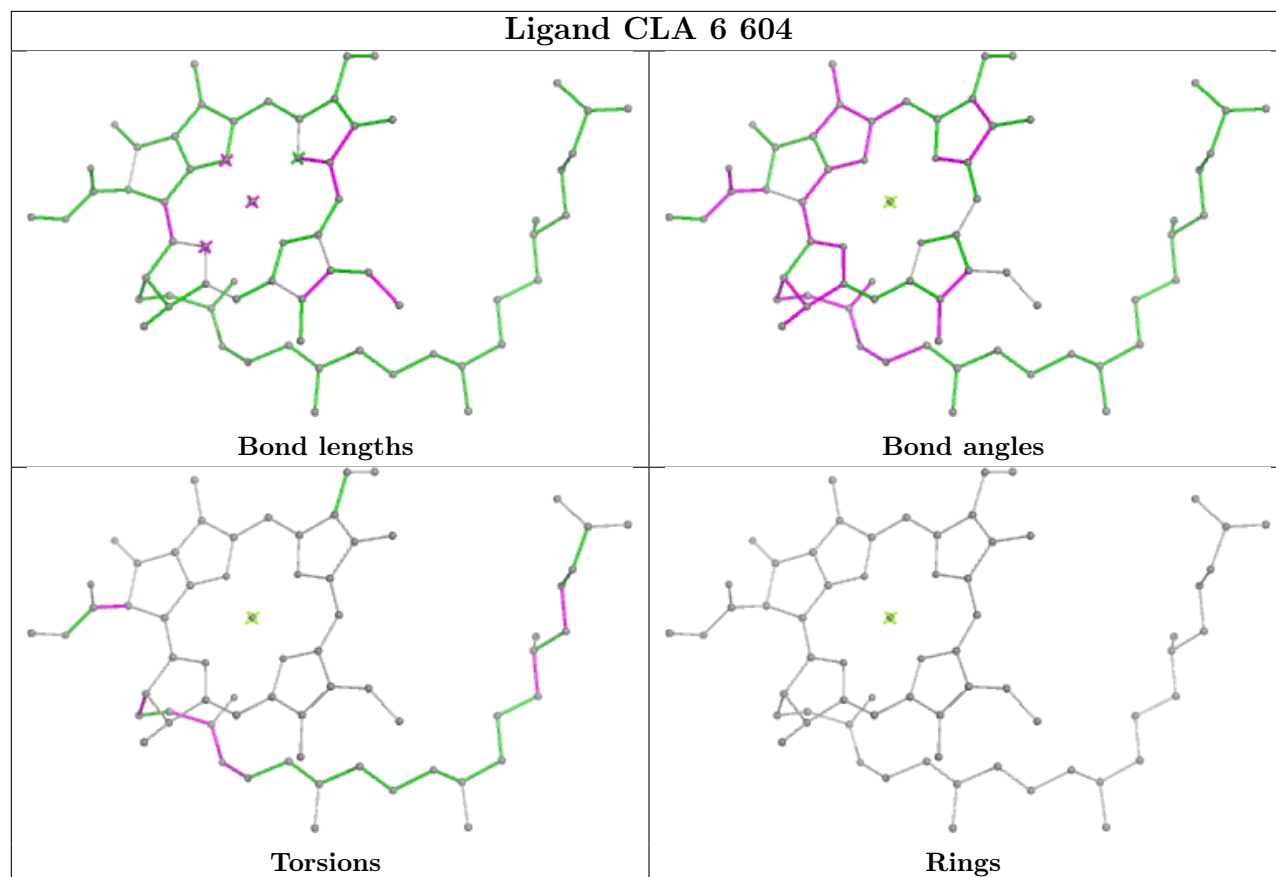
Ligand CHL 6 613



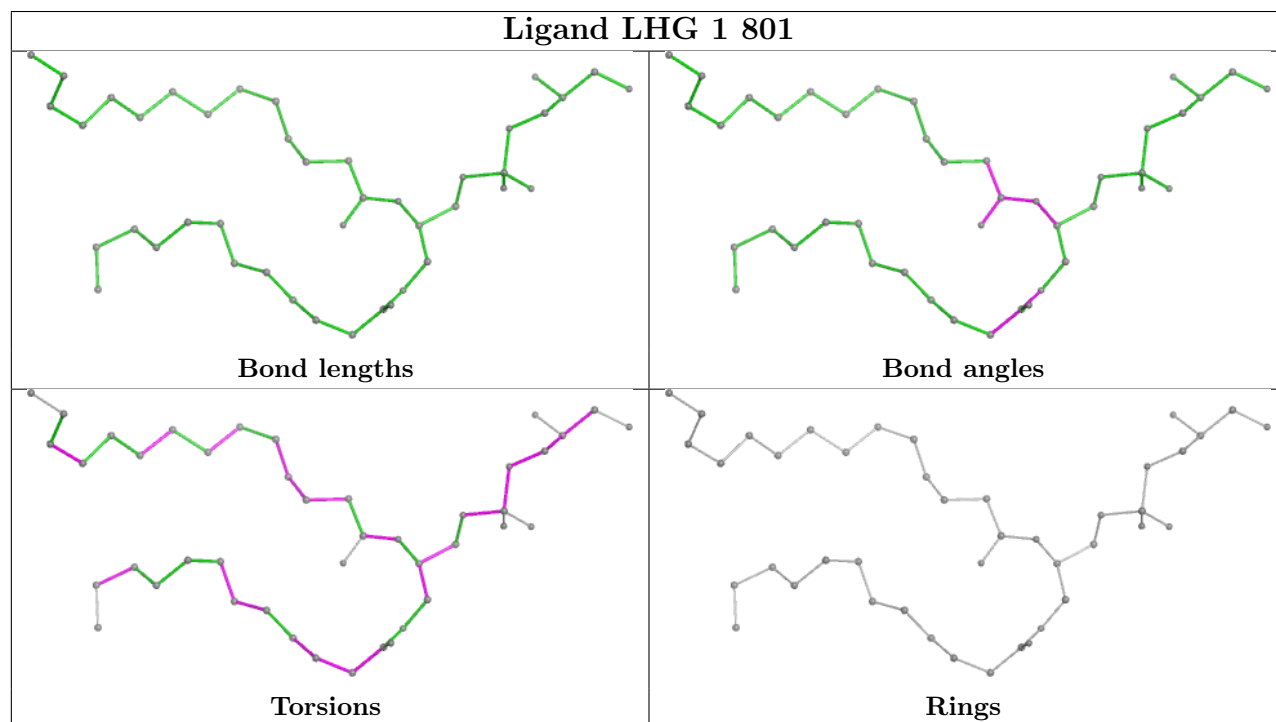
Ligand LHG 4 802



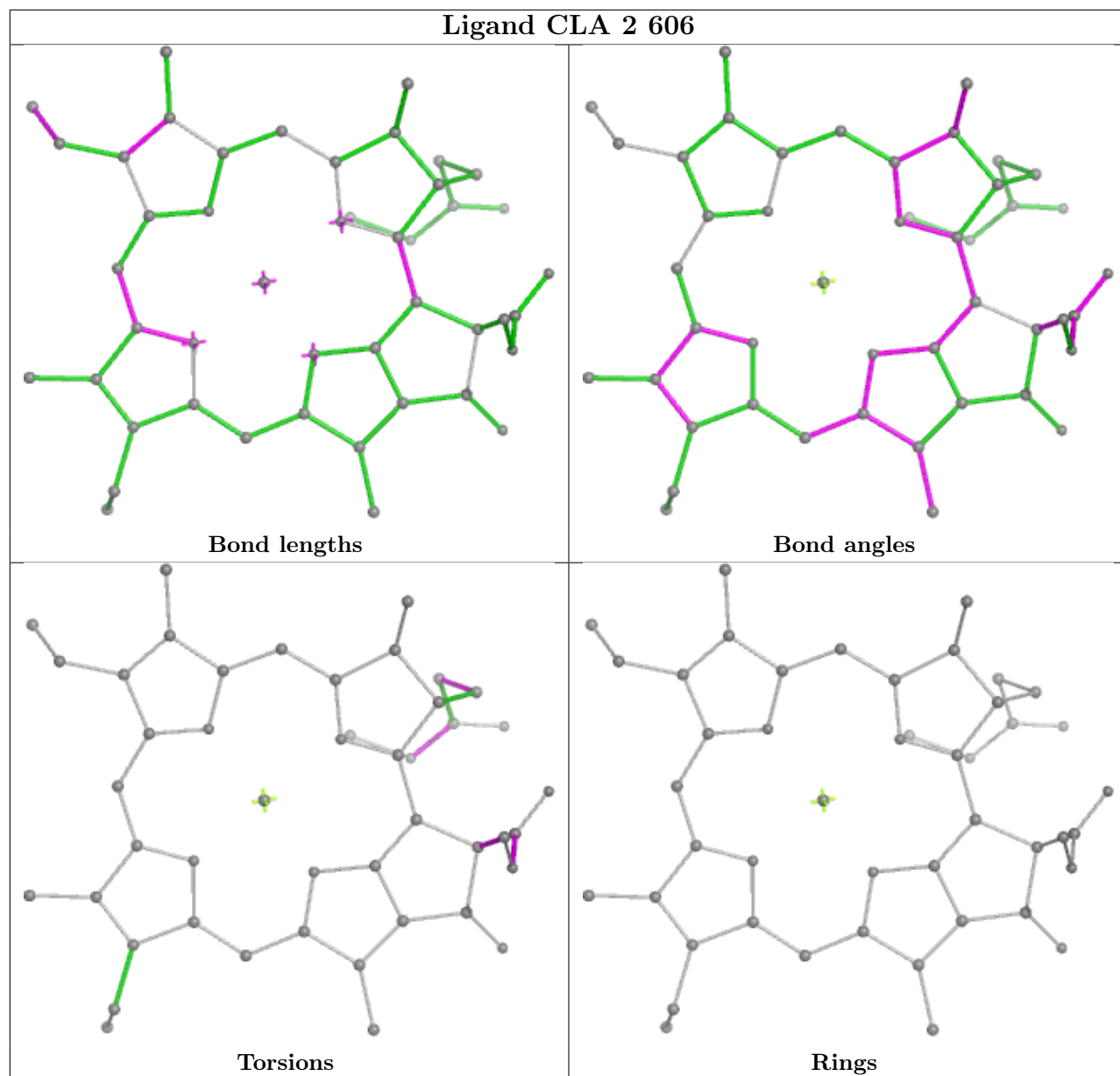
Ligand CLA 6 604

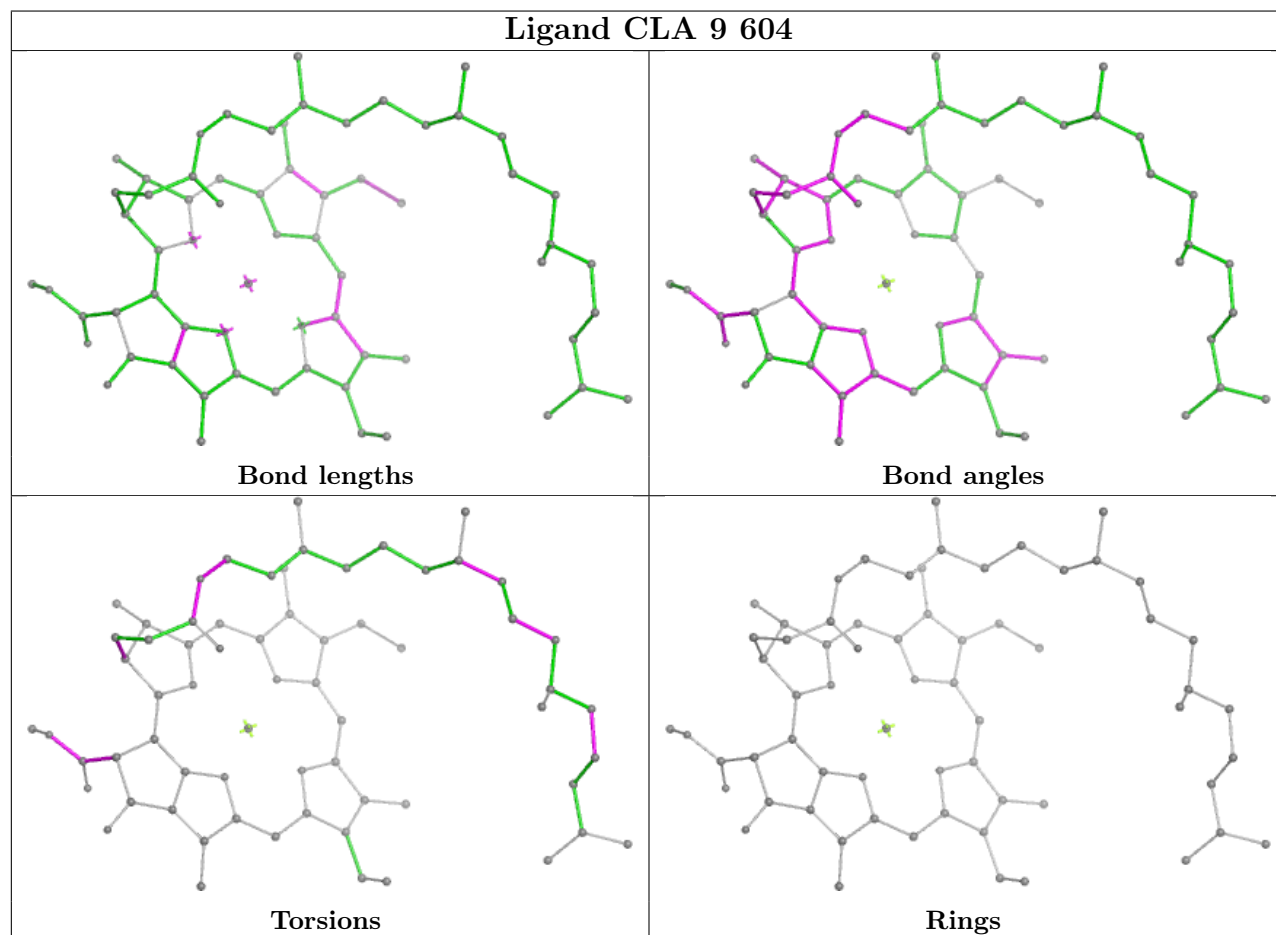
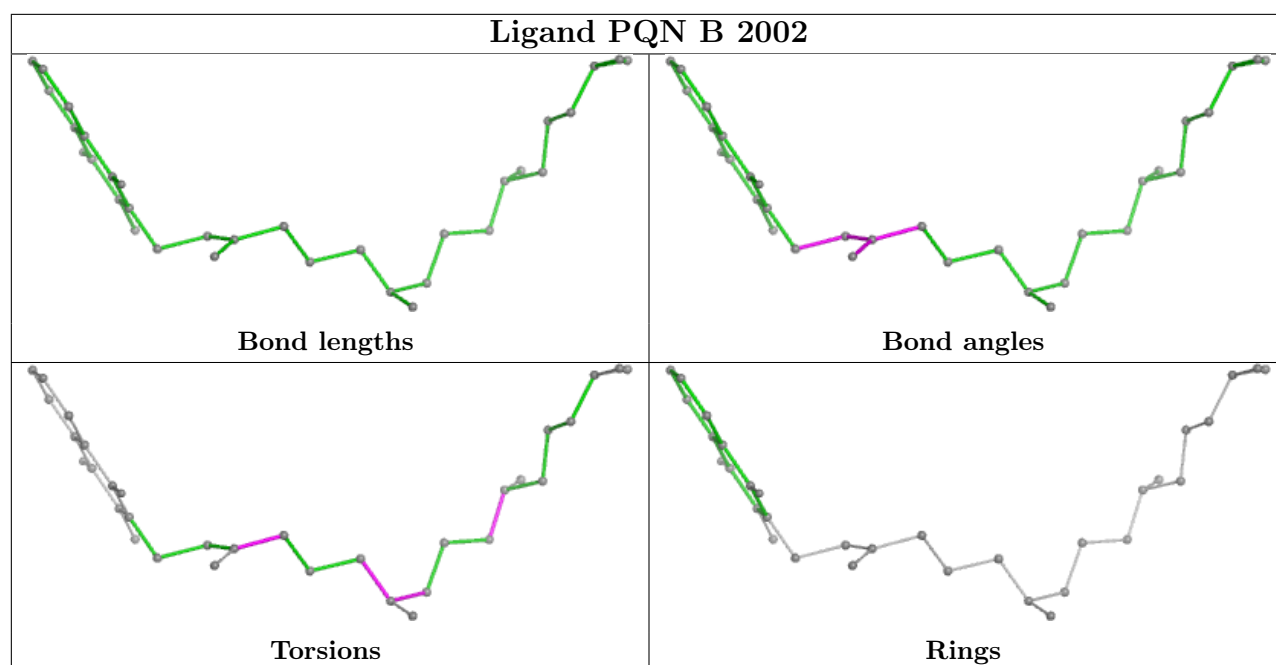


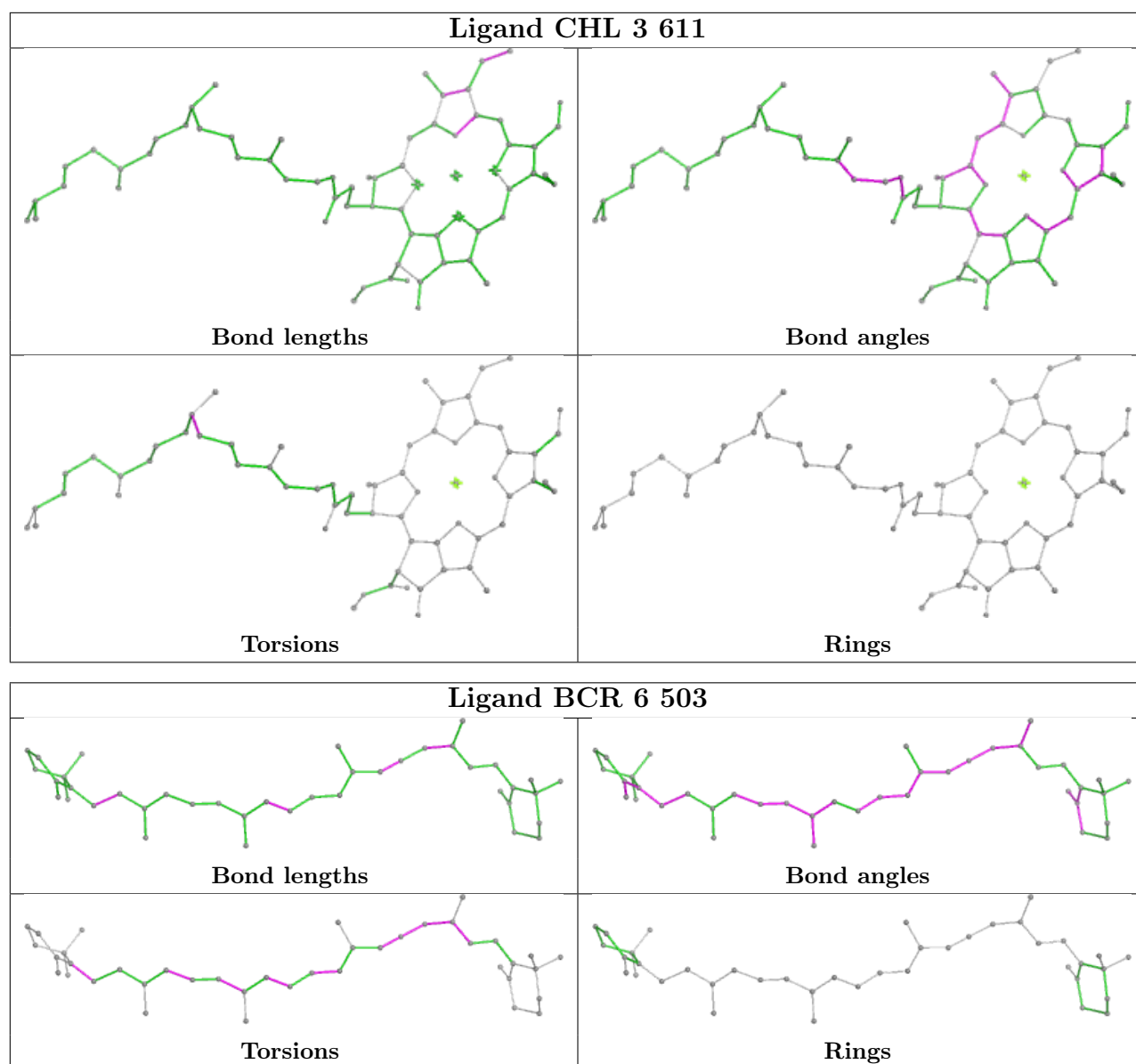
Ligand LHG 1 801



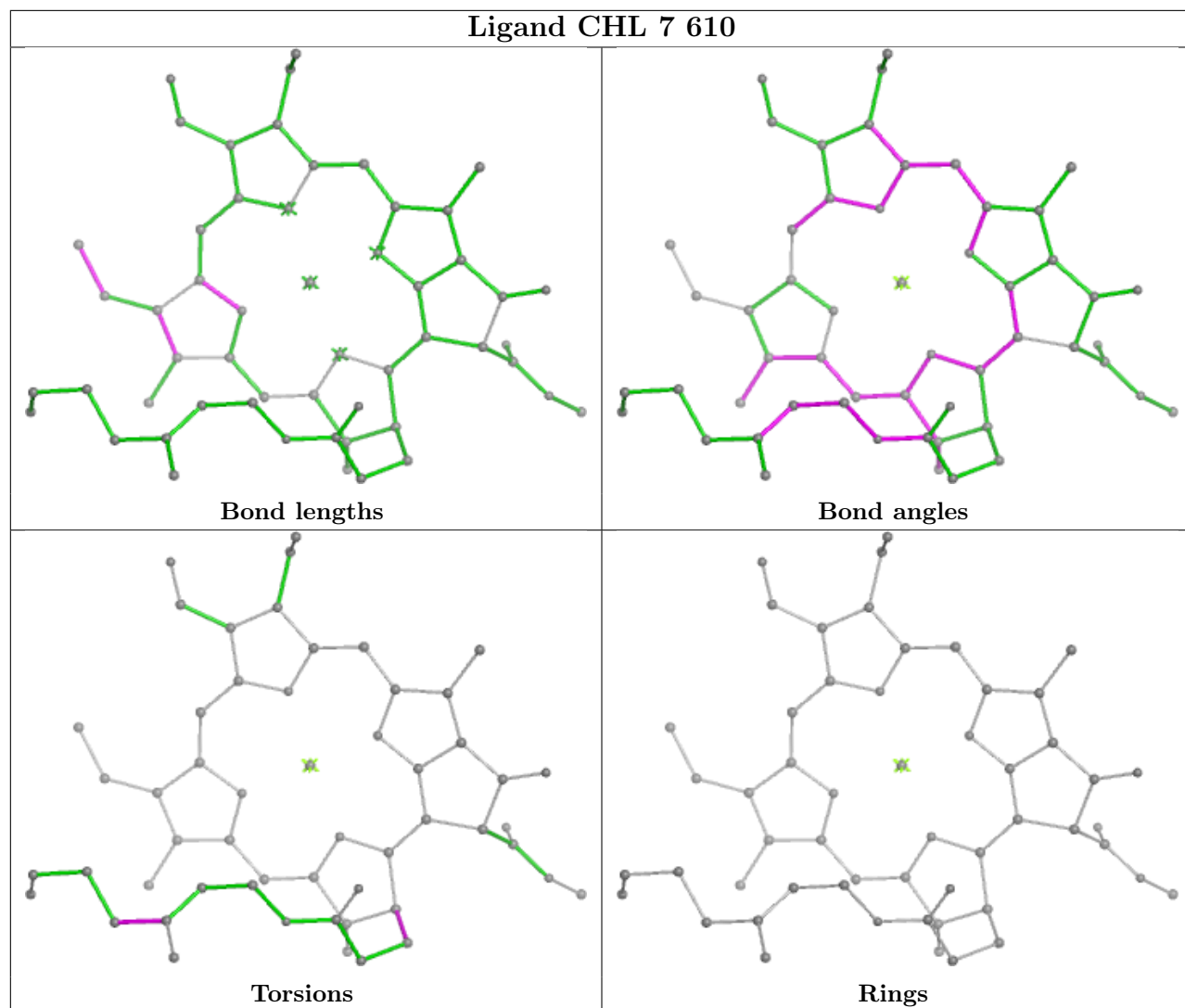
Ligand CLA 2 606



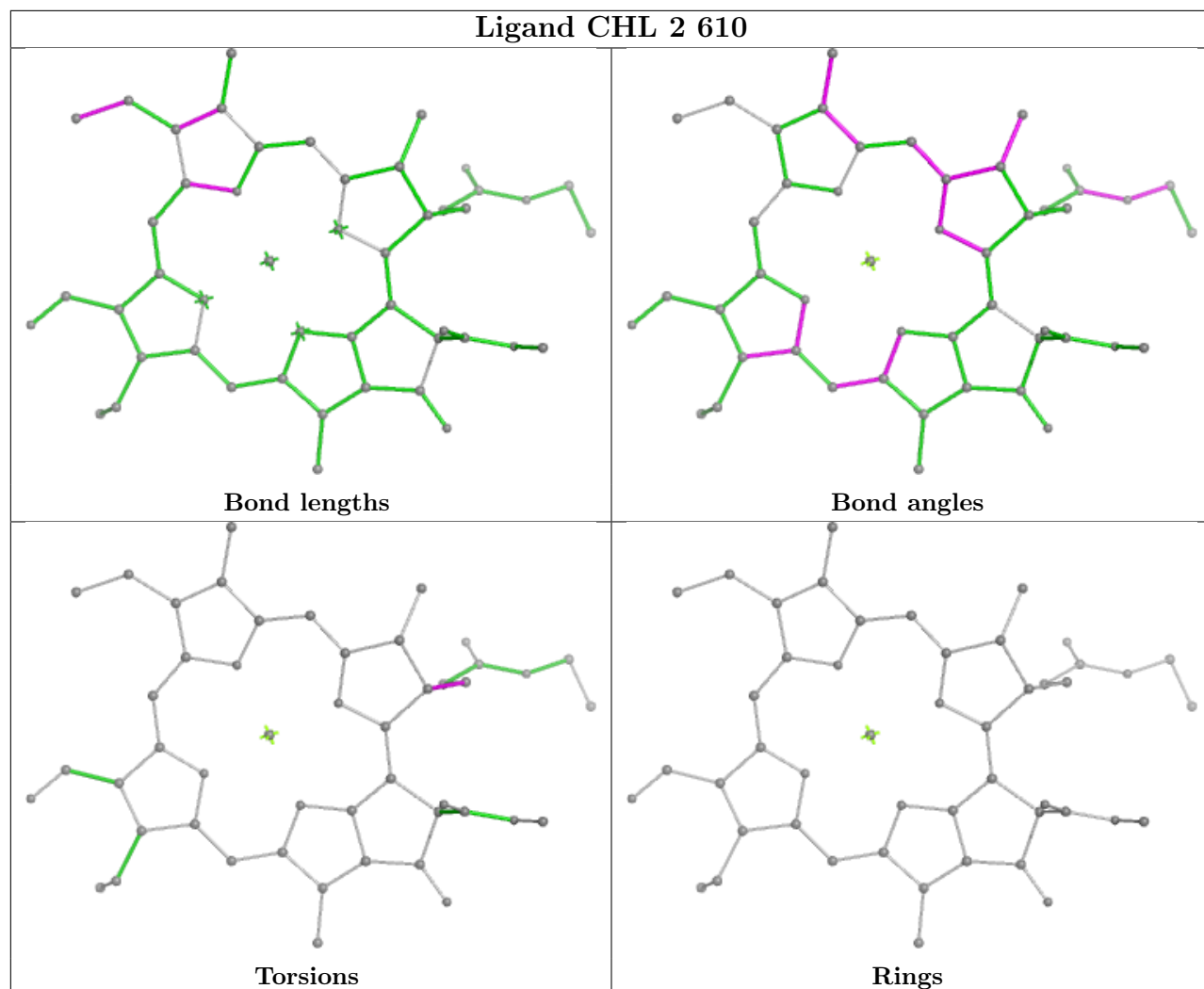


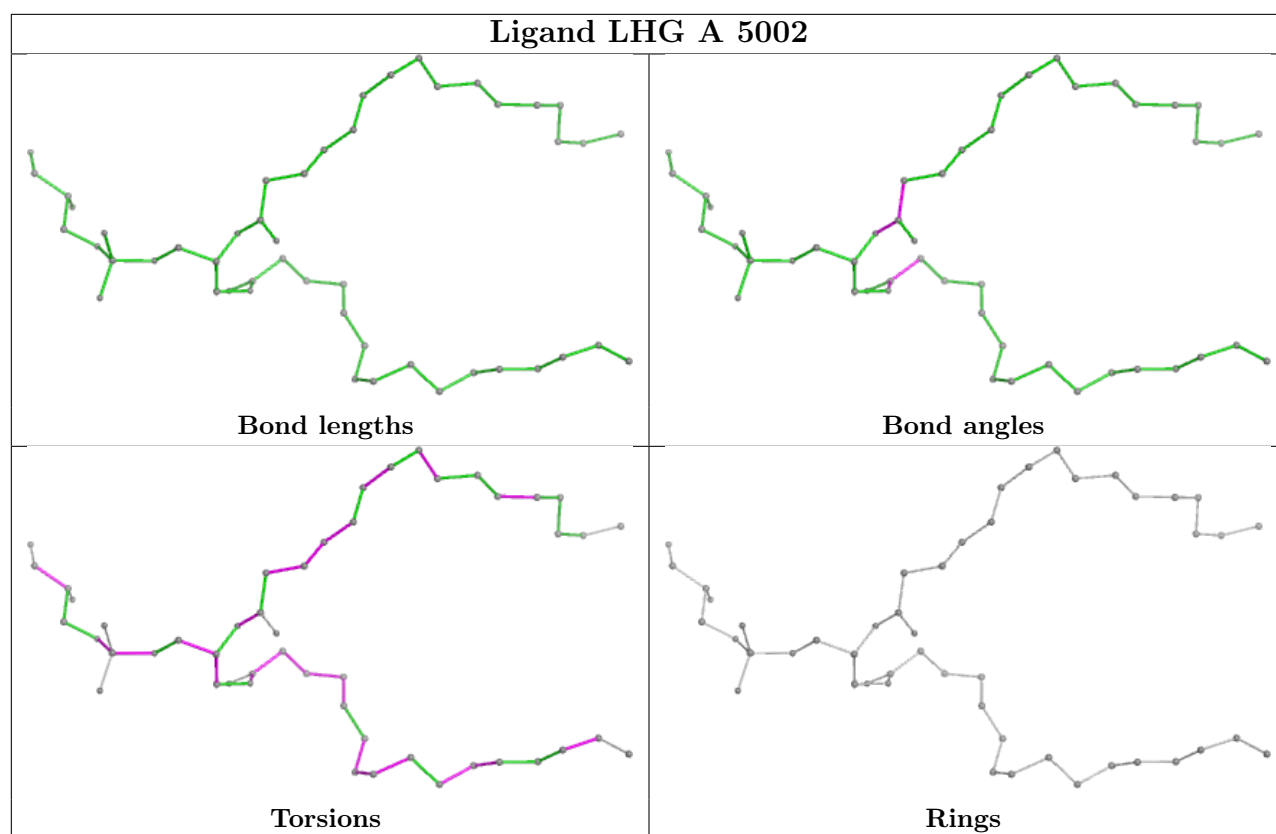


Ligand CHL 7 610

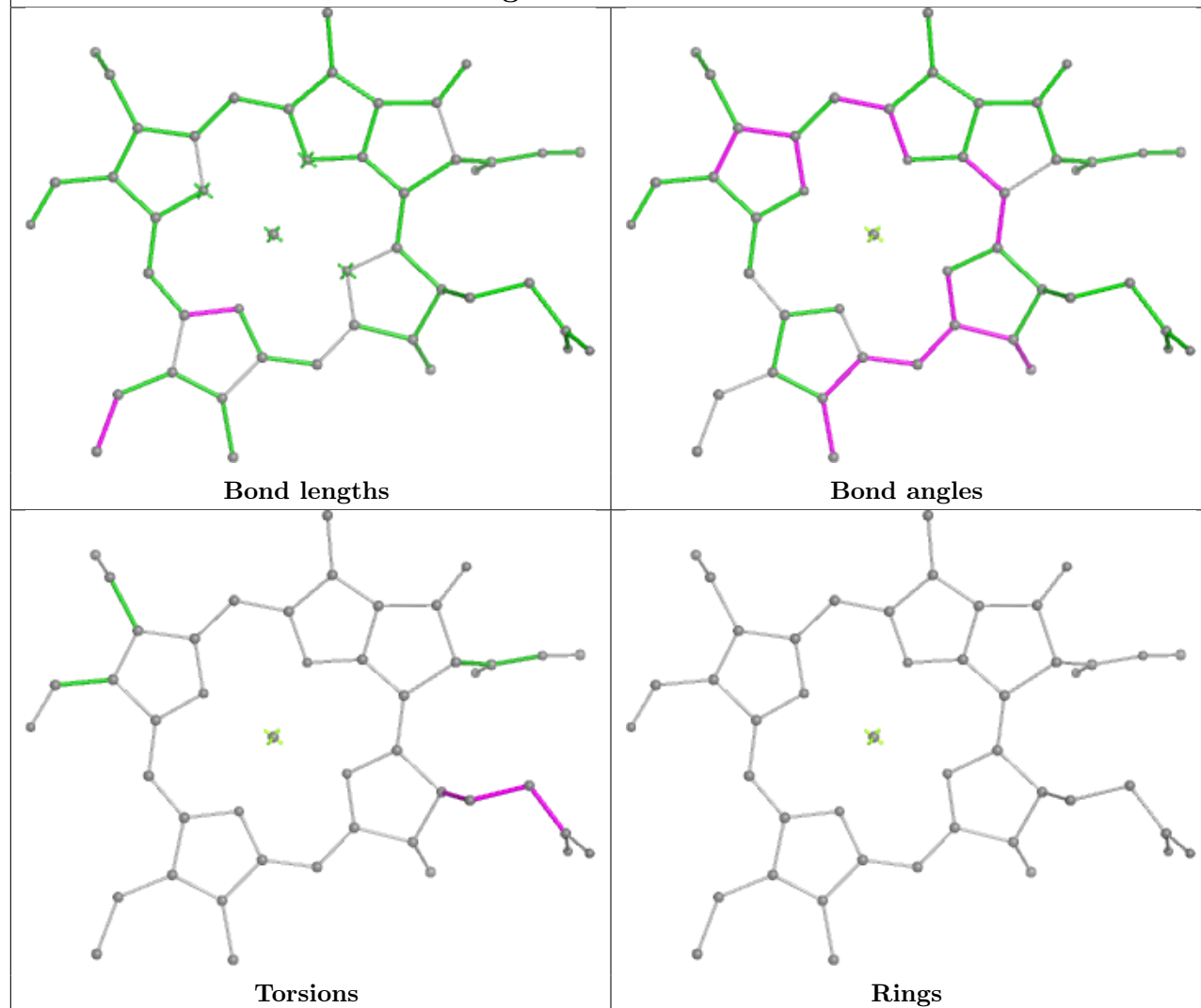


Ligand CHL 2 610

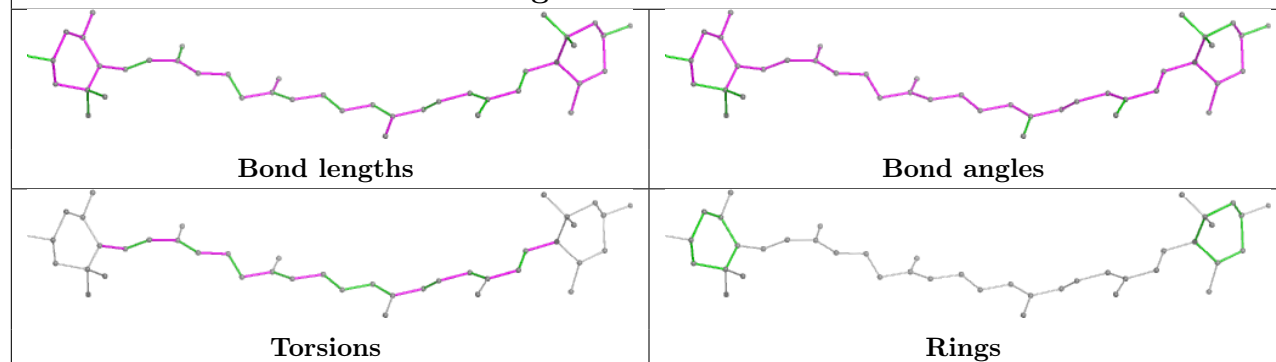




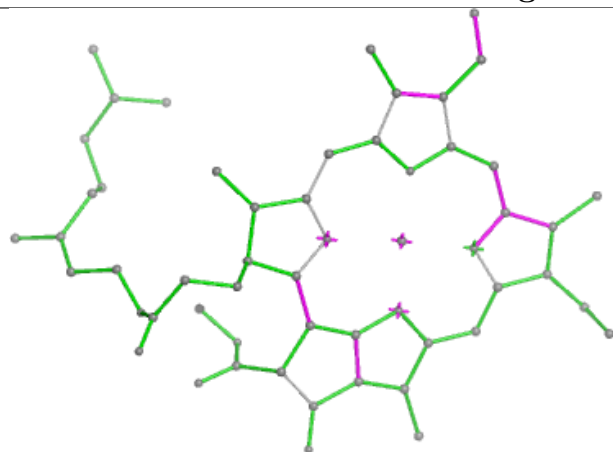
Ligand CHL Z 613



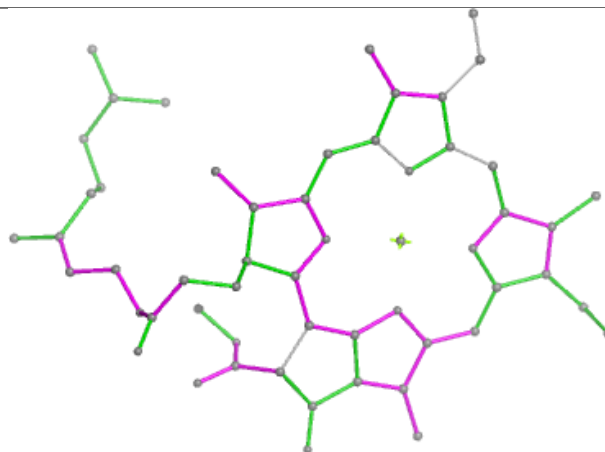
Ligand C7Z J 4002



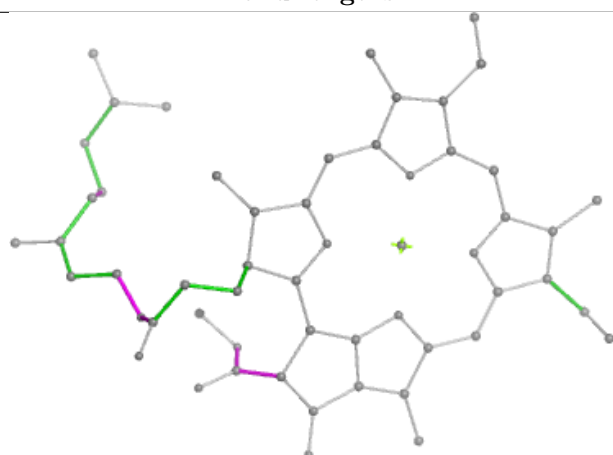
Ligand CLA 1 605



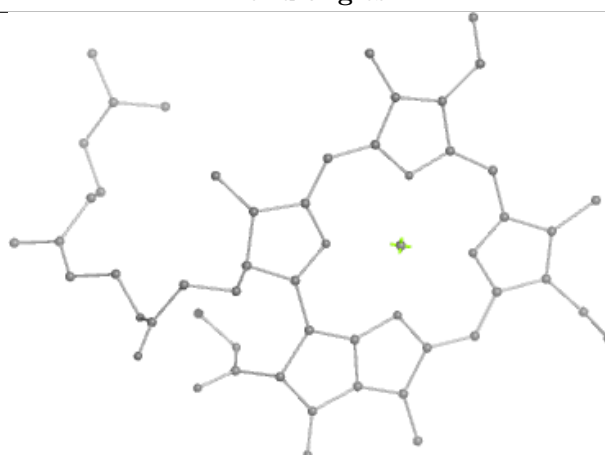
Bond lengths



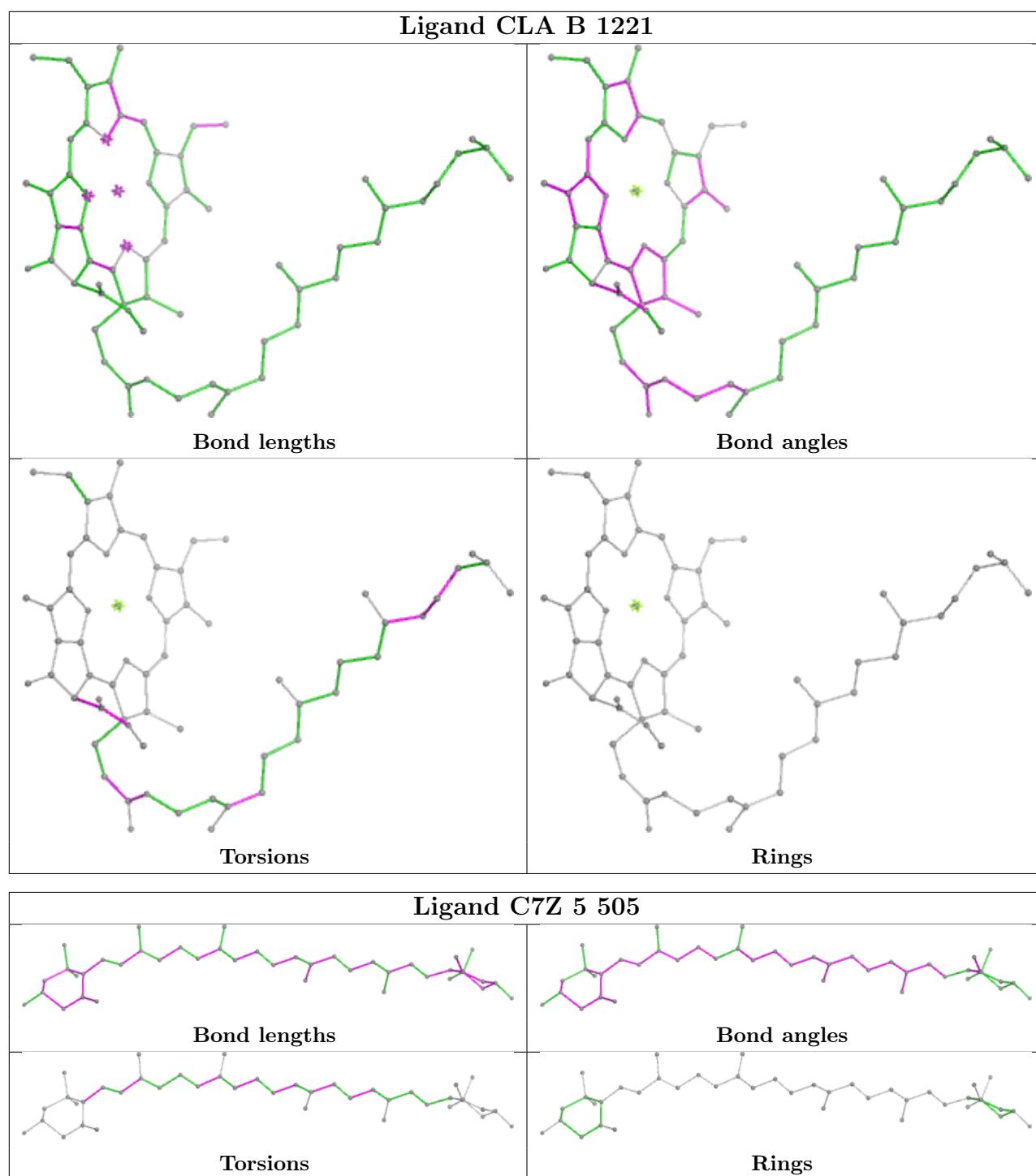
Bond angles

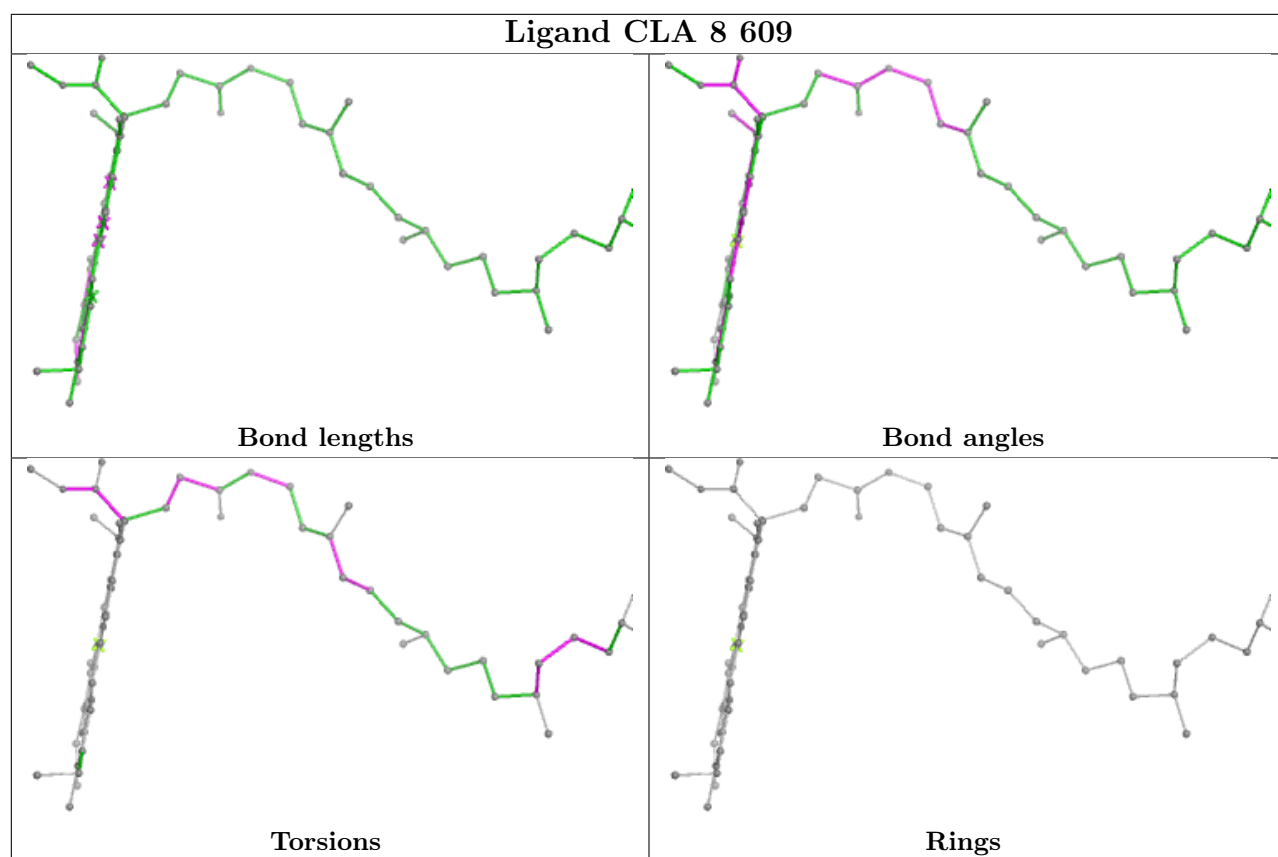


Torsions

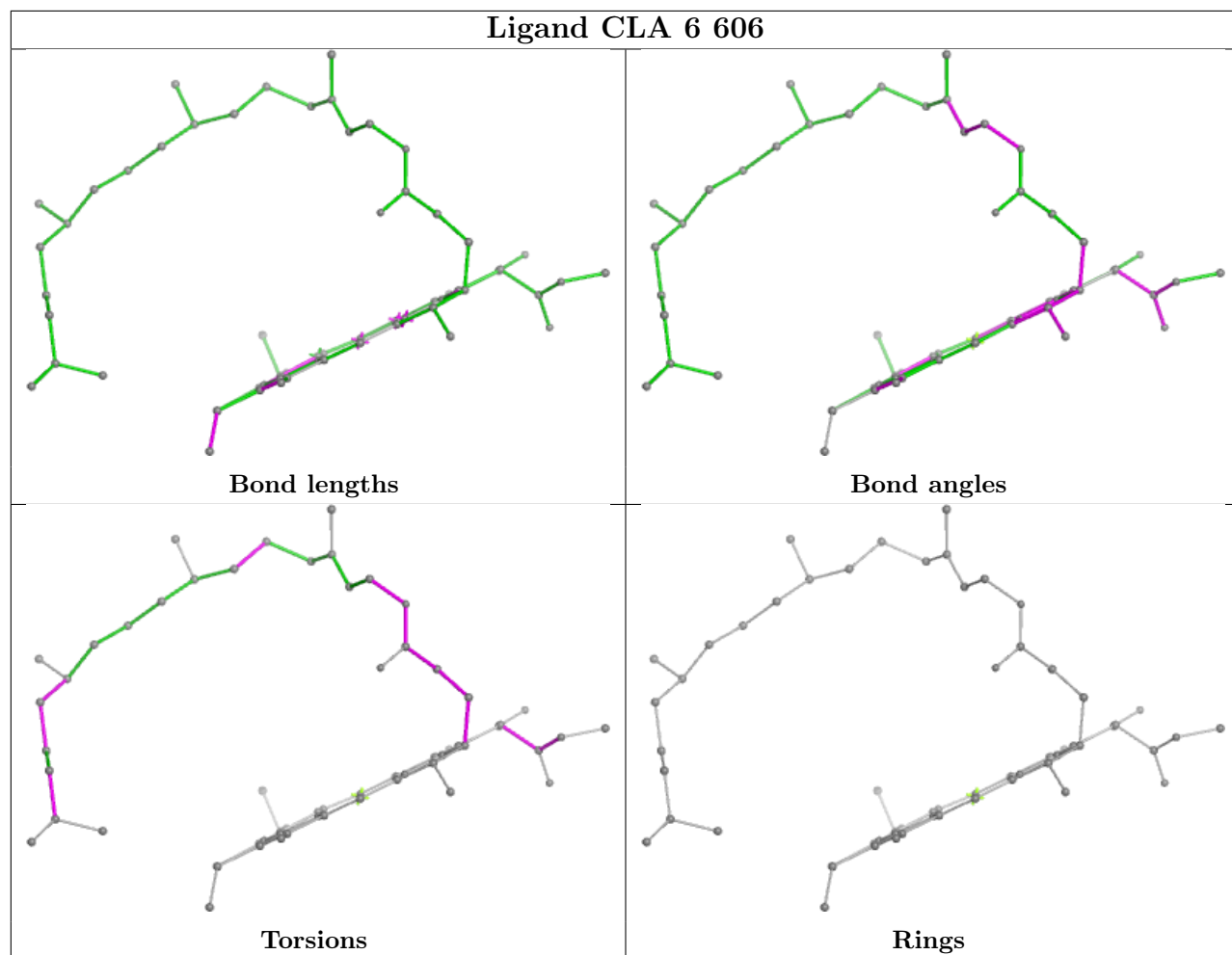


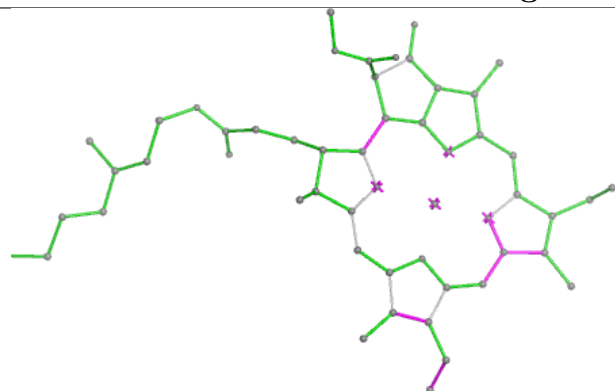
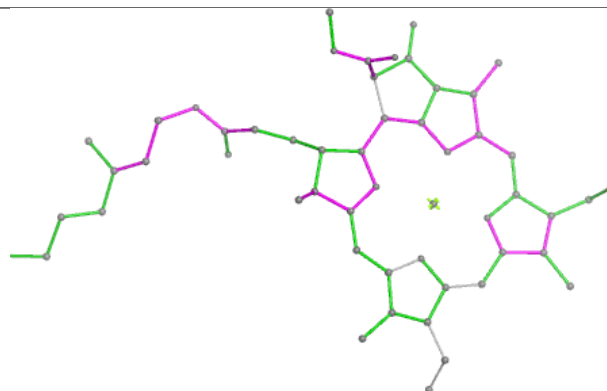
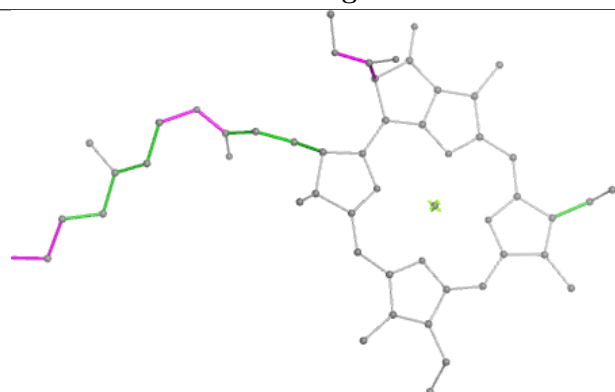
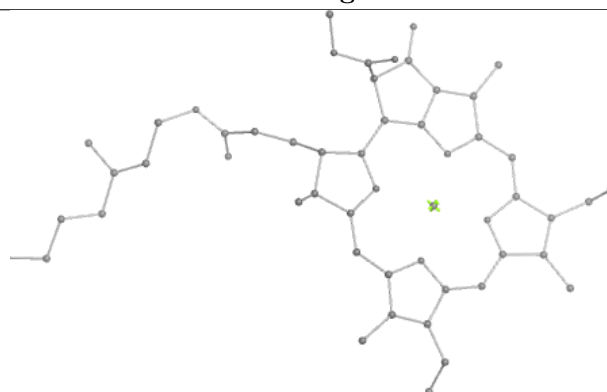
Rings

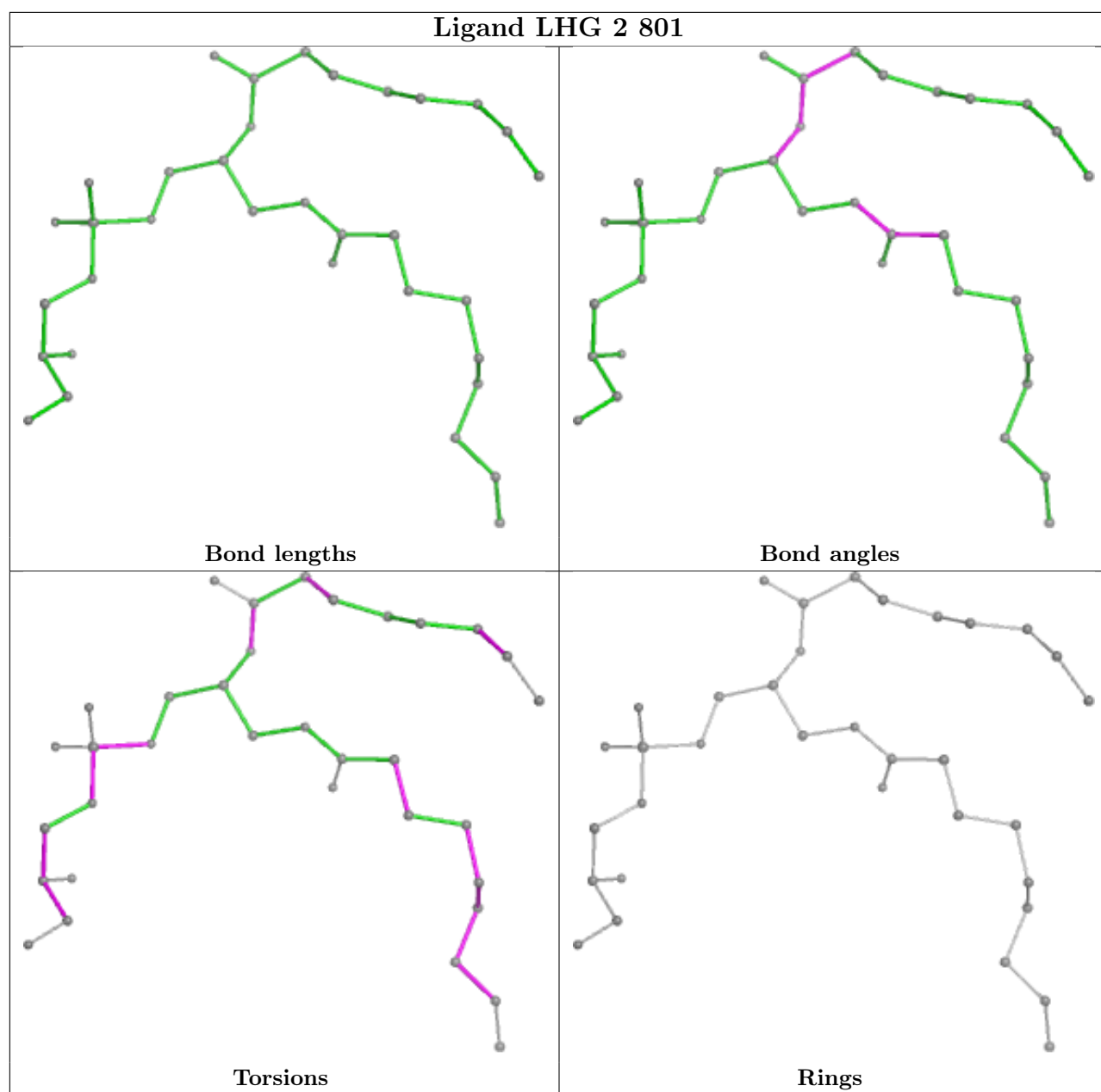


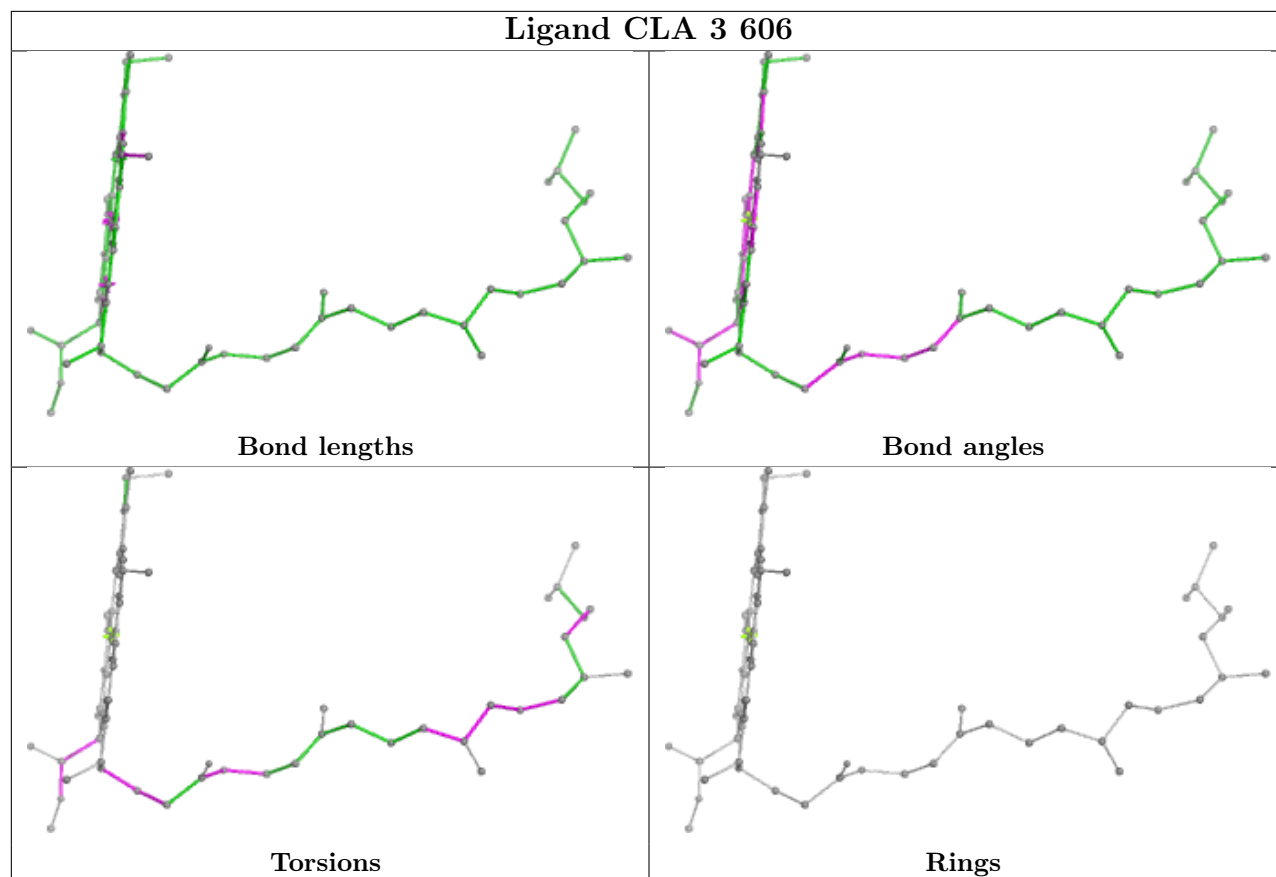
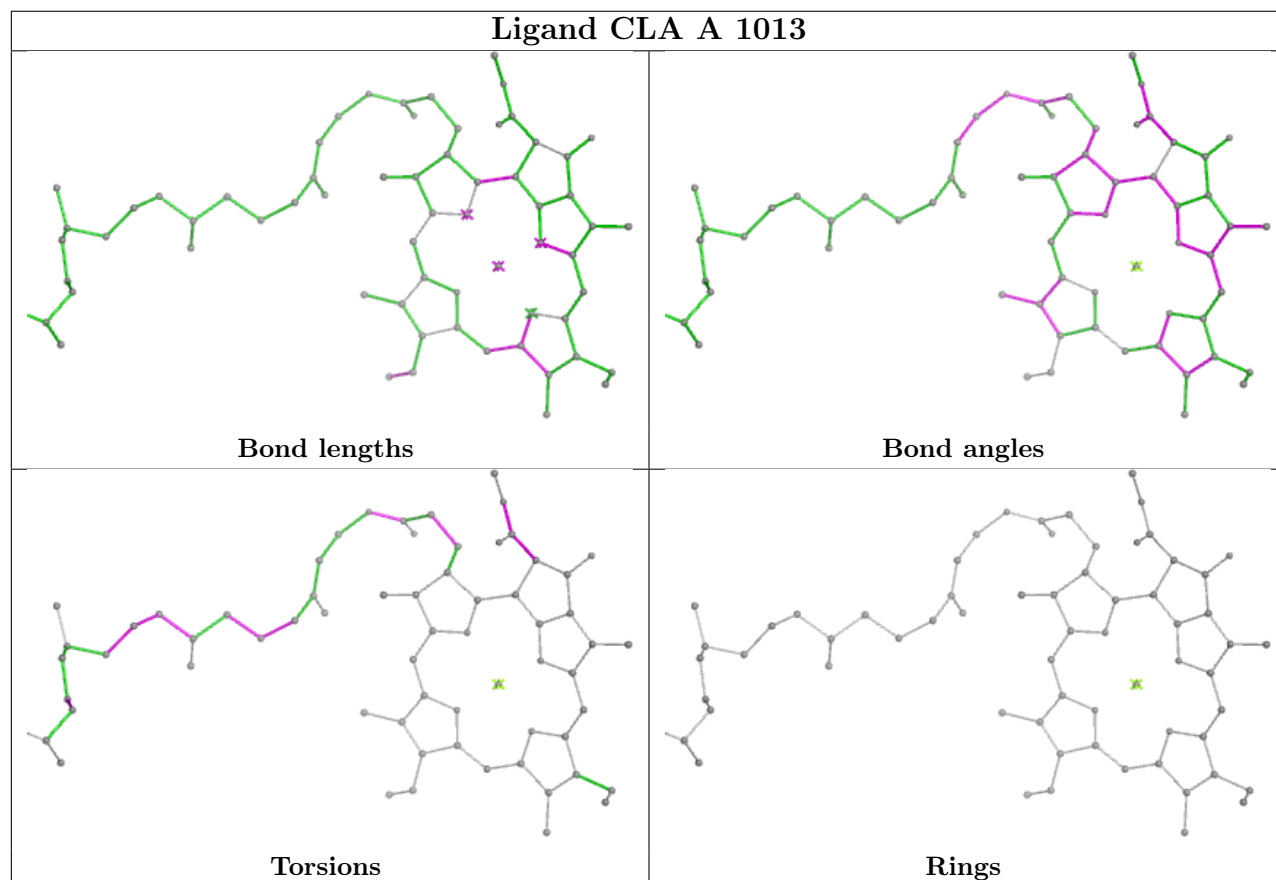


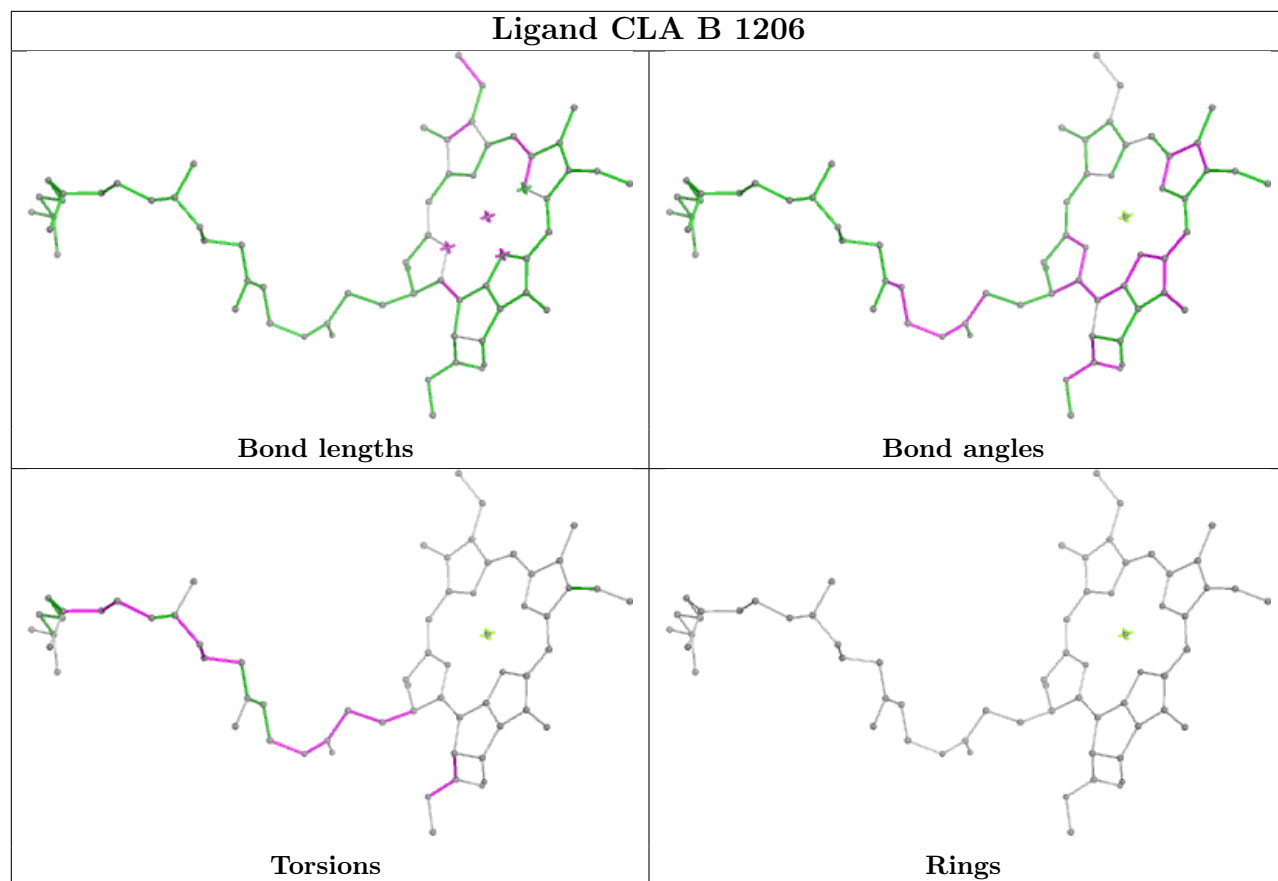
Ligand CLA 6 606

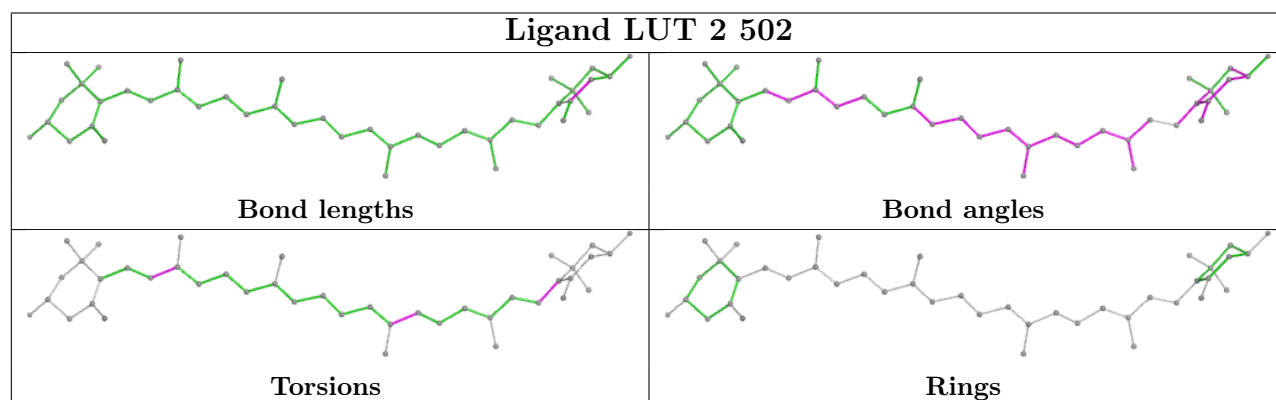
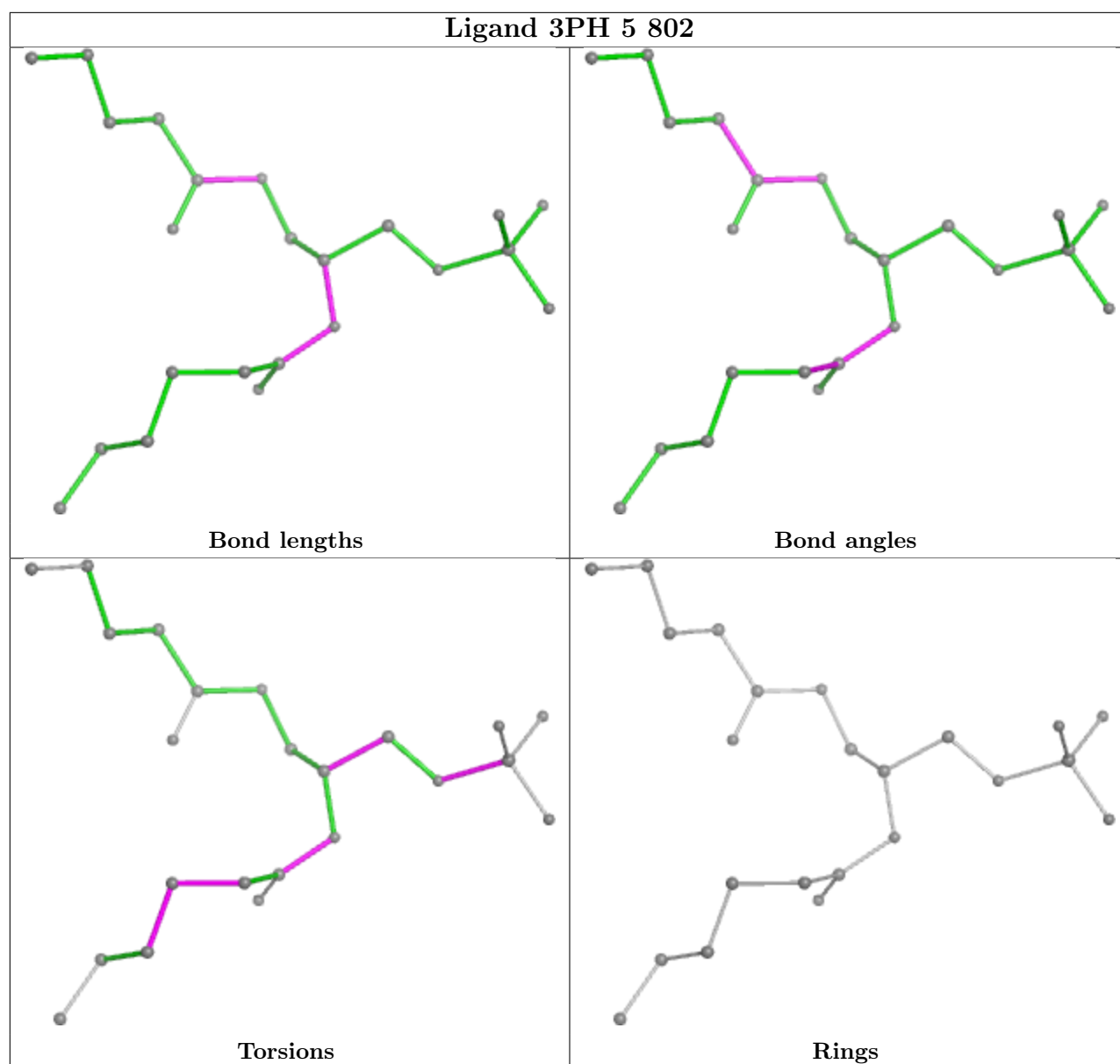


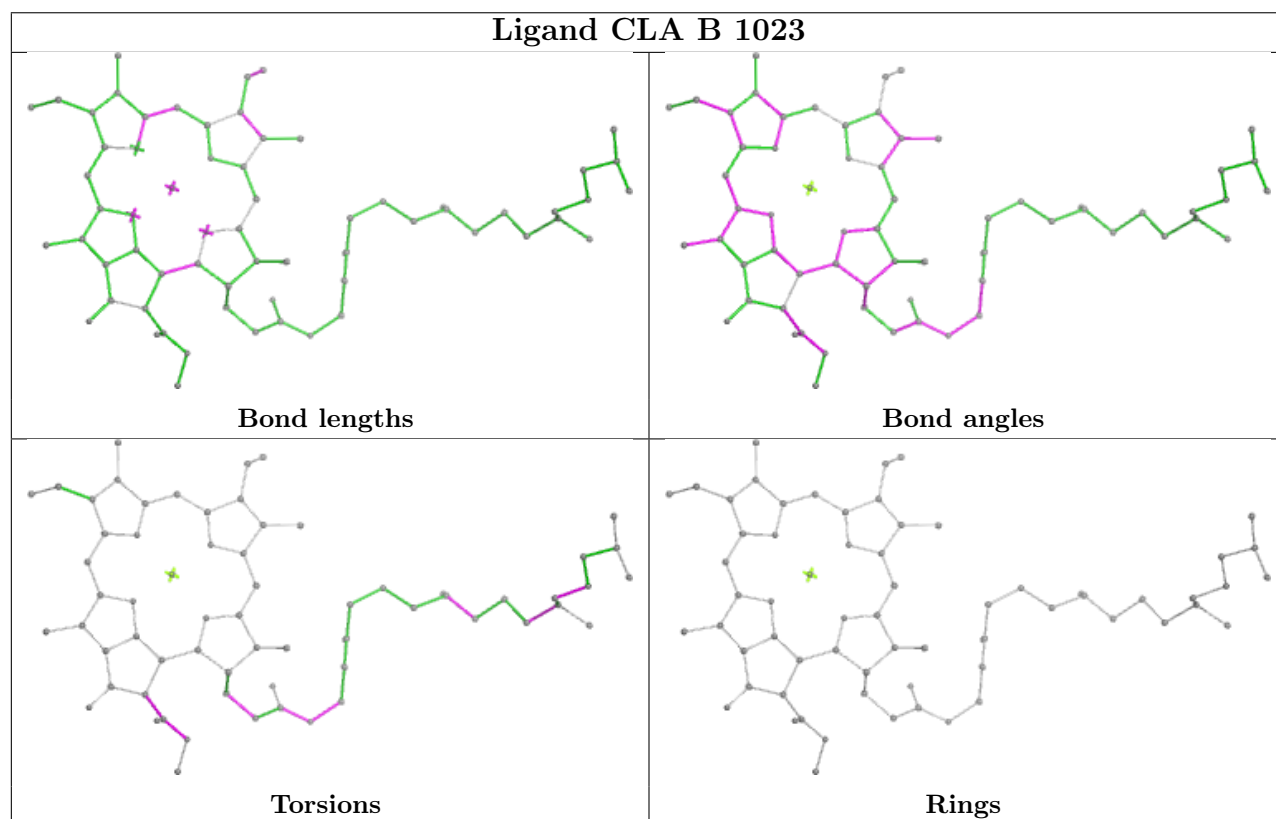
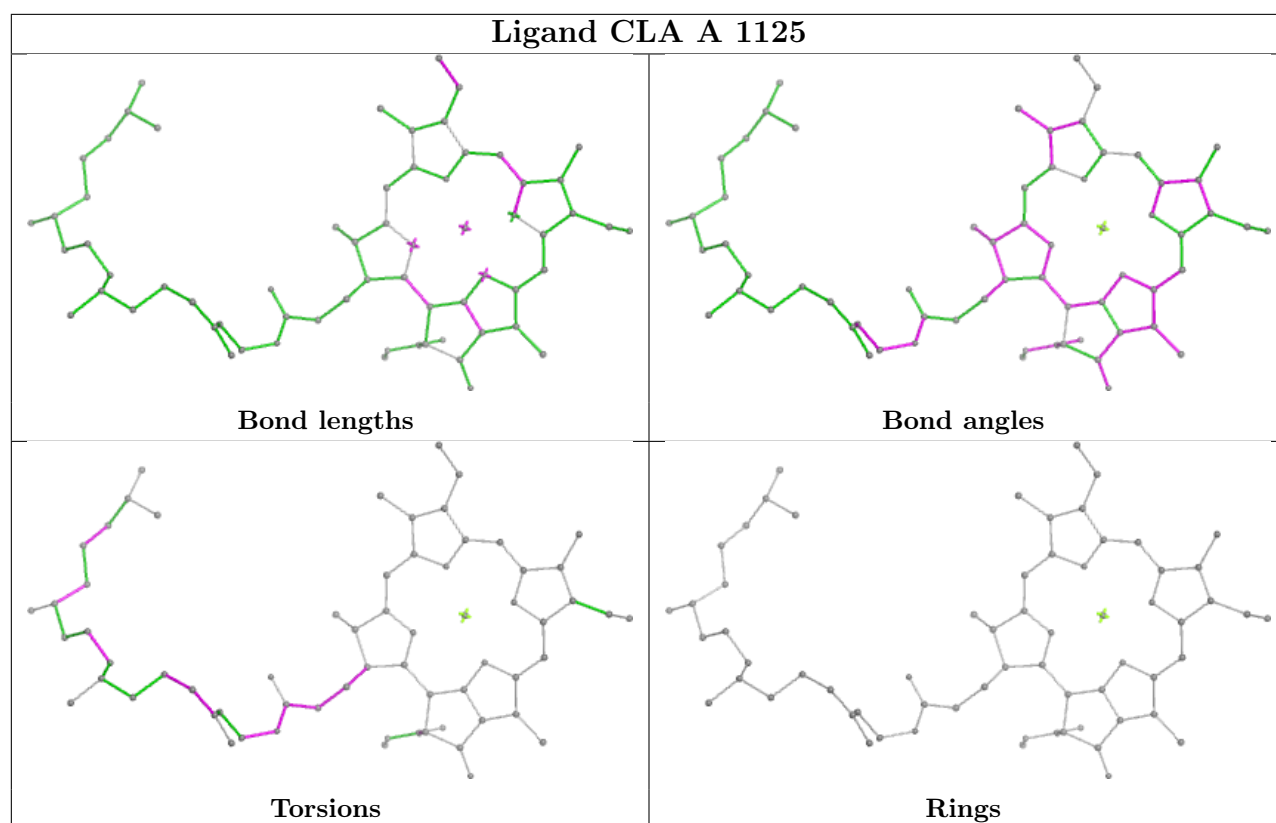
Ligand CLA 5 613**Bond lengths****Bond angles****Torsions****Rings**

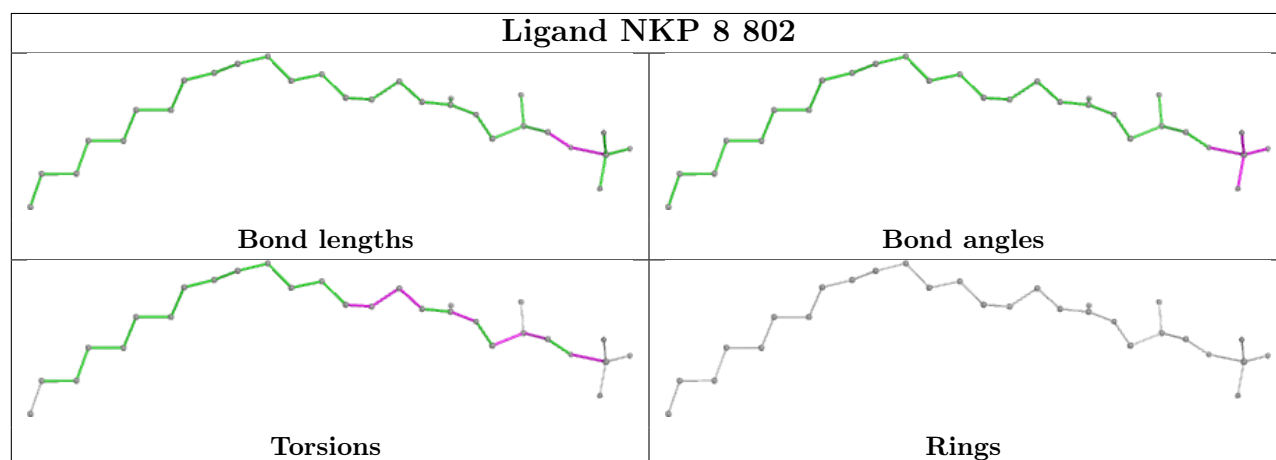
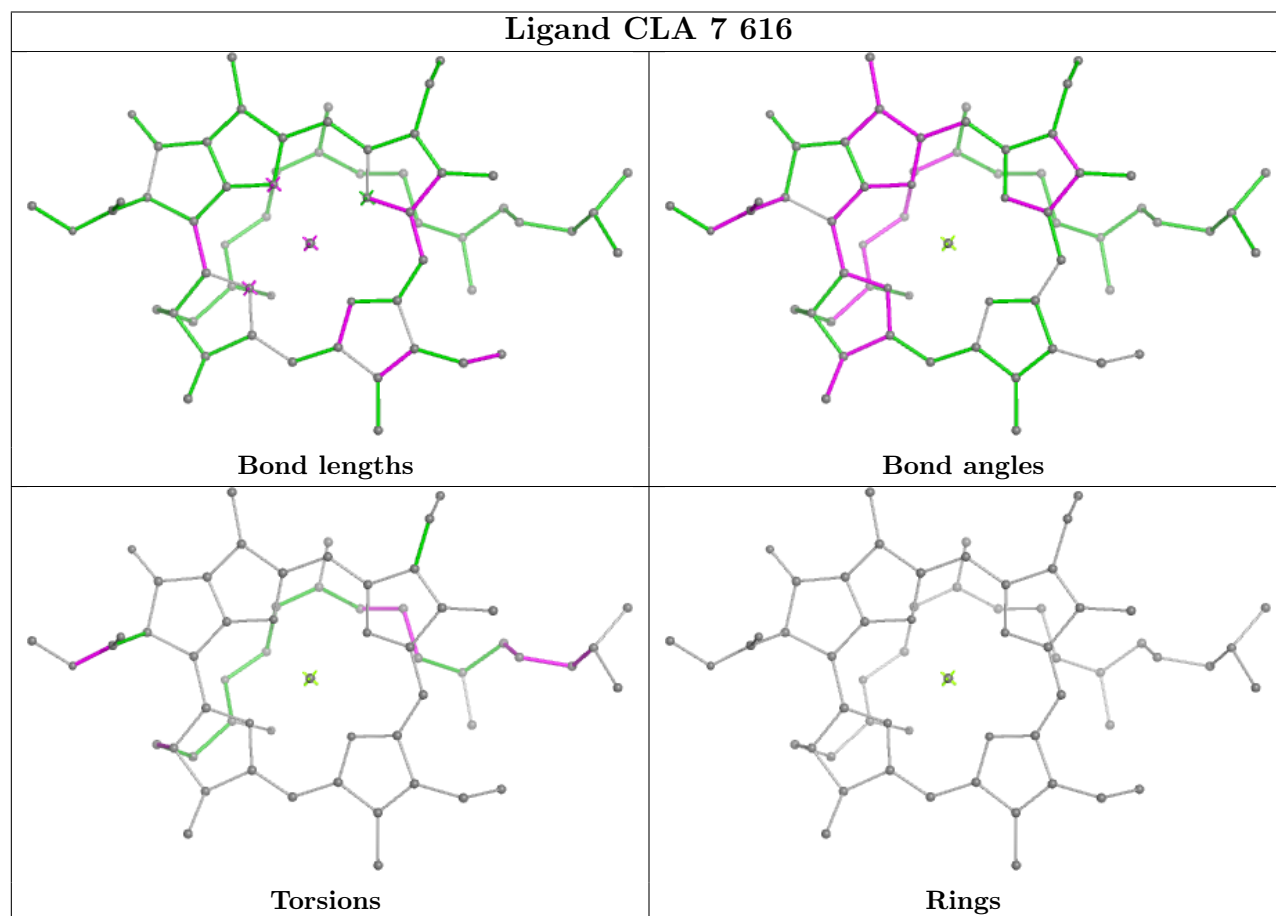
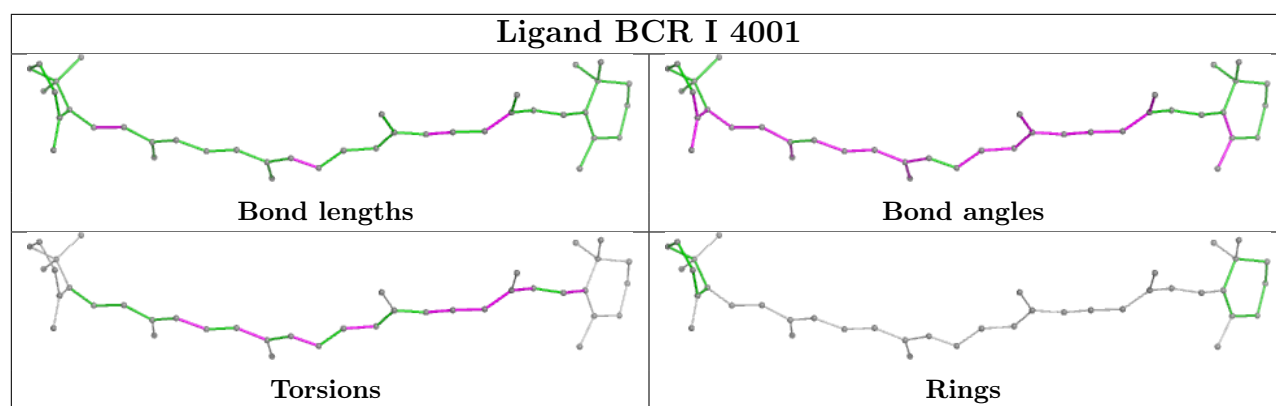


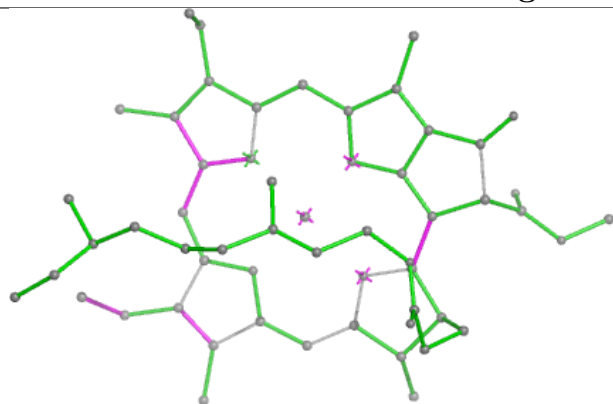
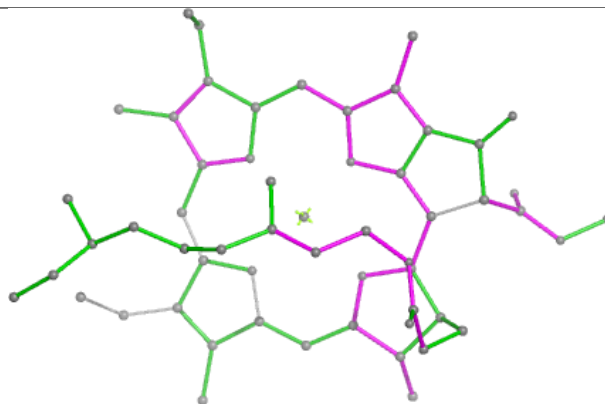
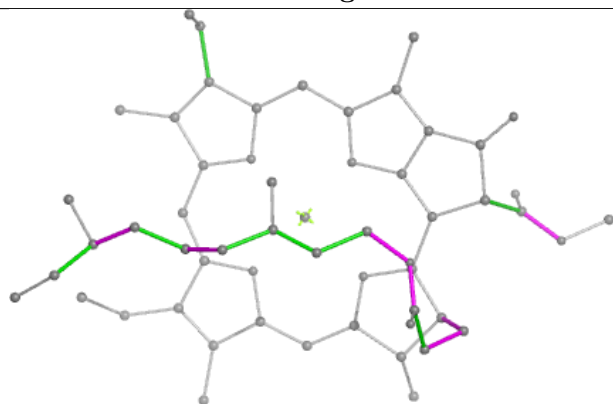
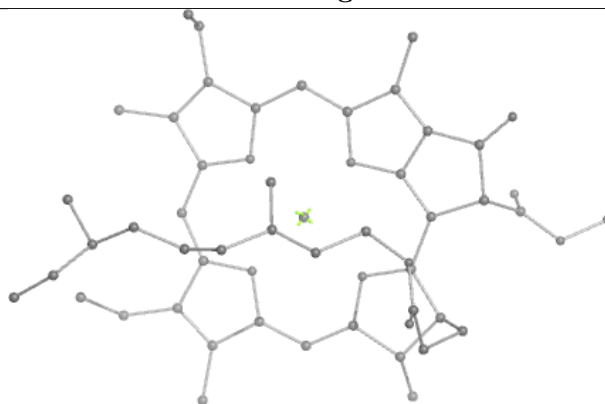
Ligand CLA 3 606**Ligand CLA A 1013**

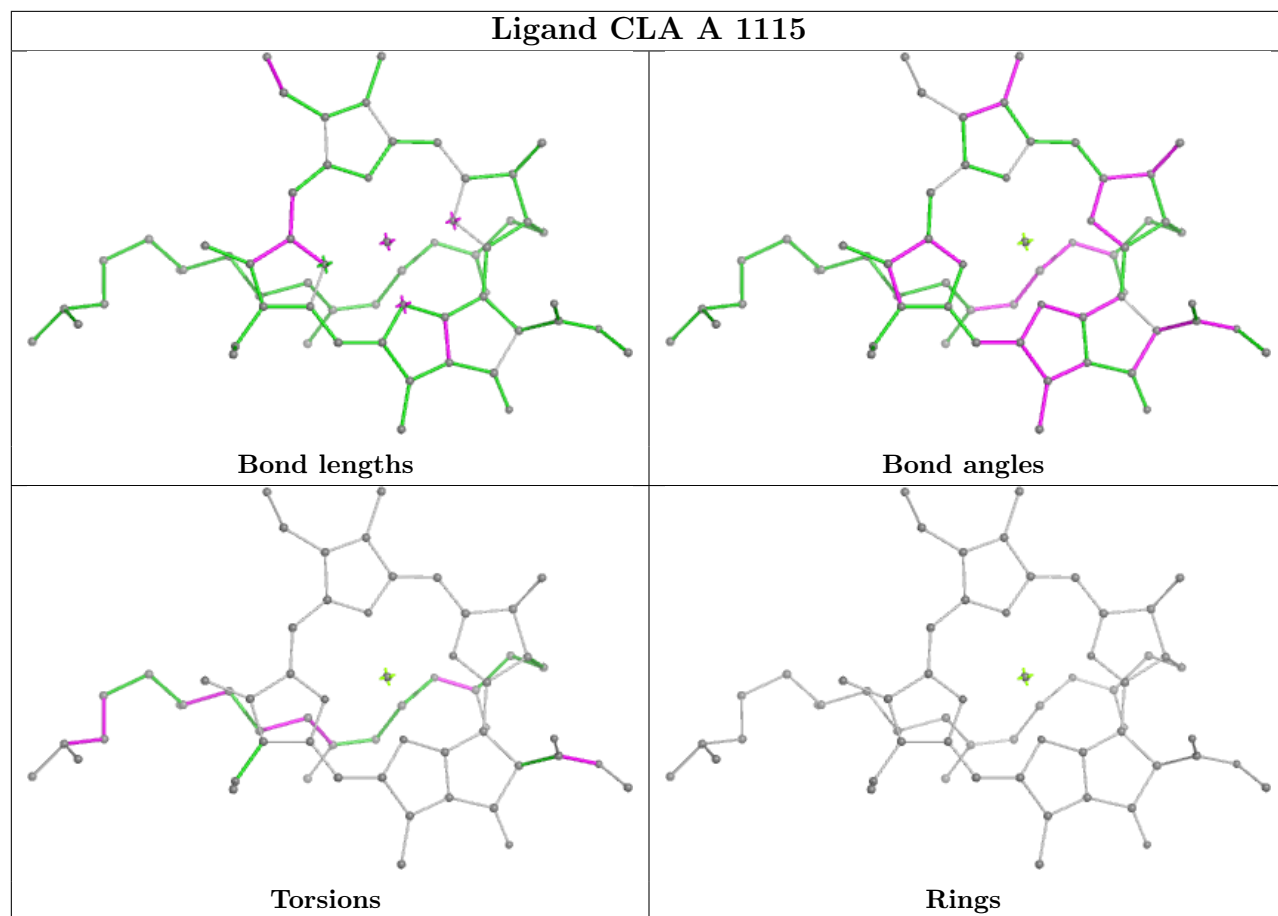


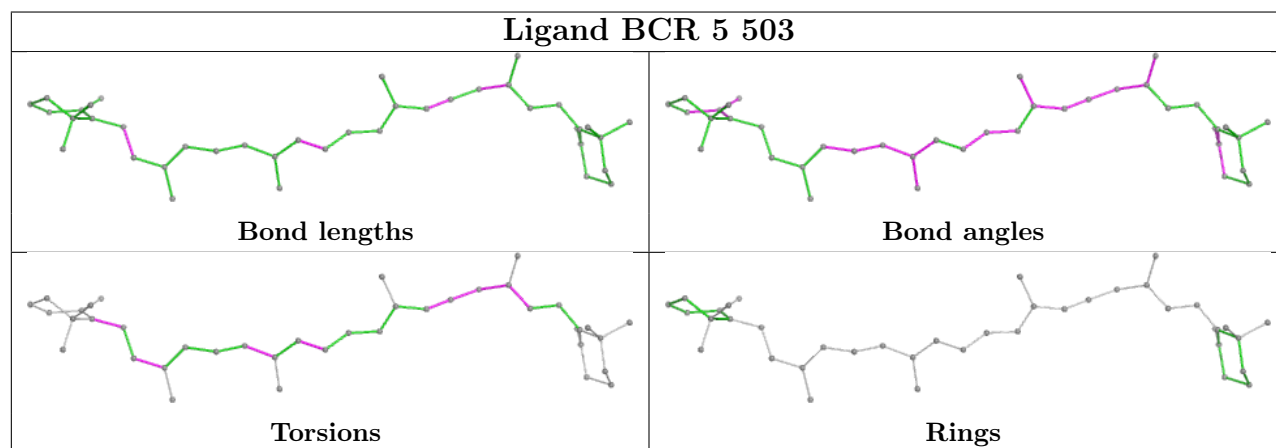
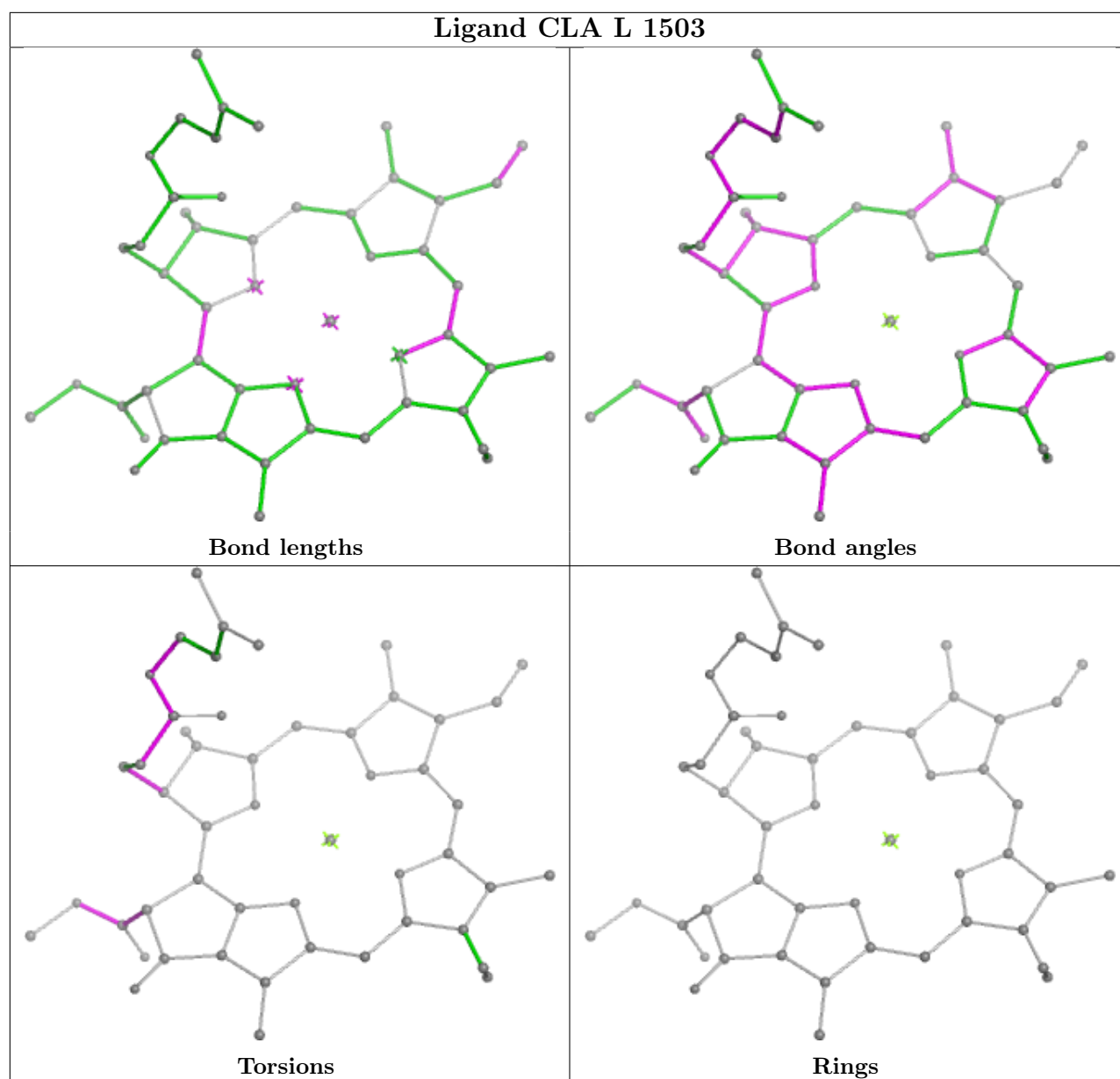


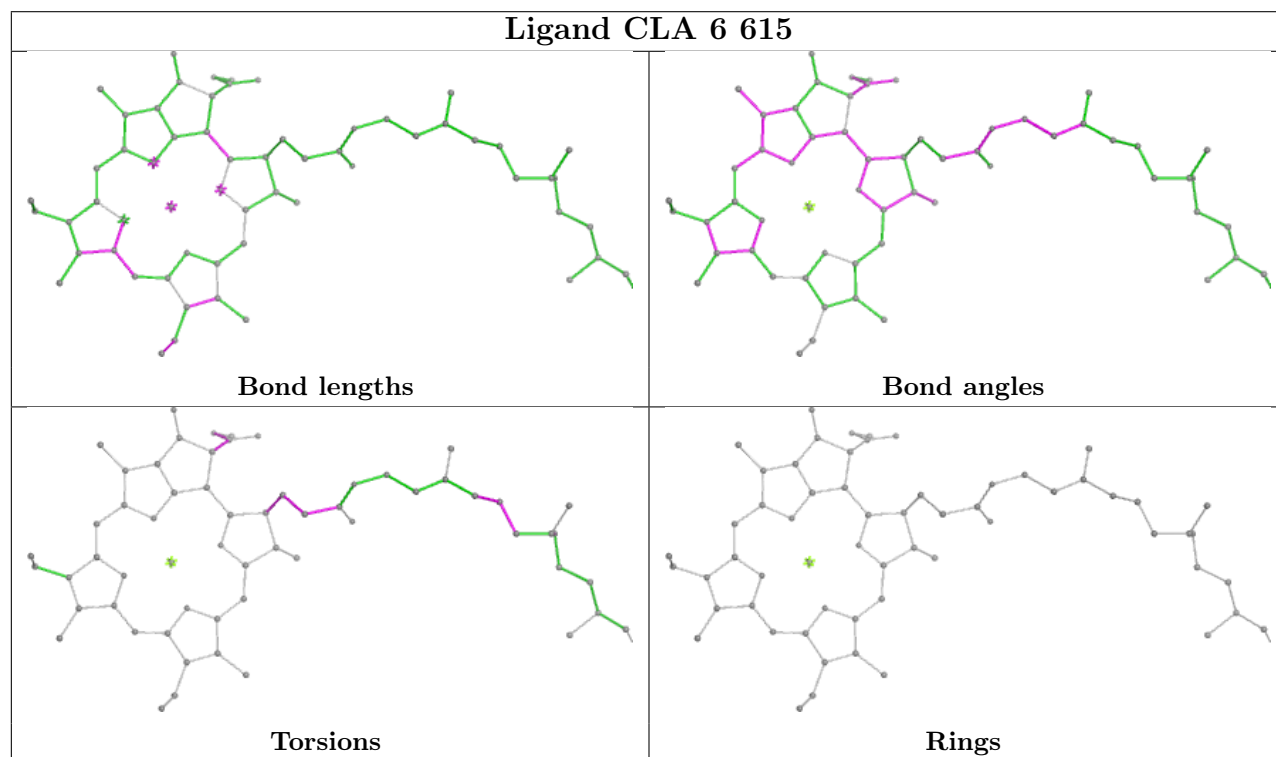
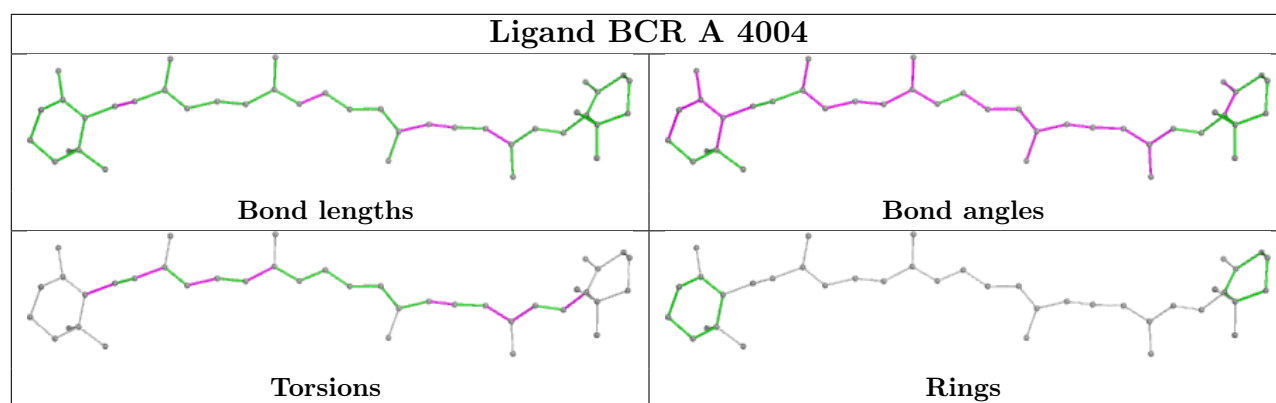


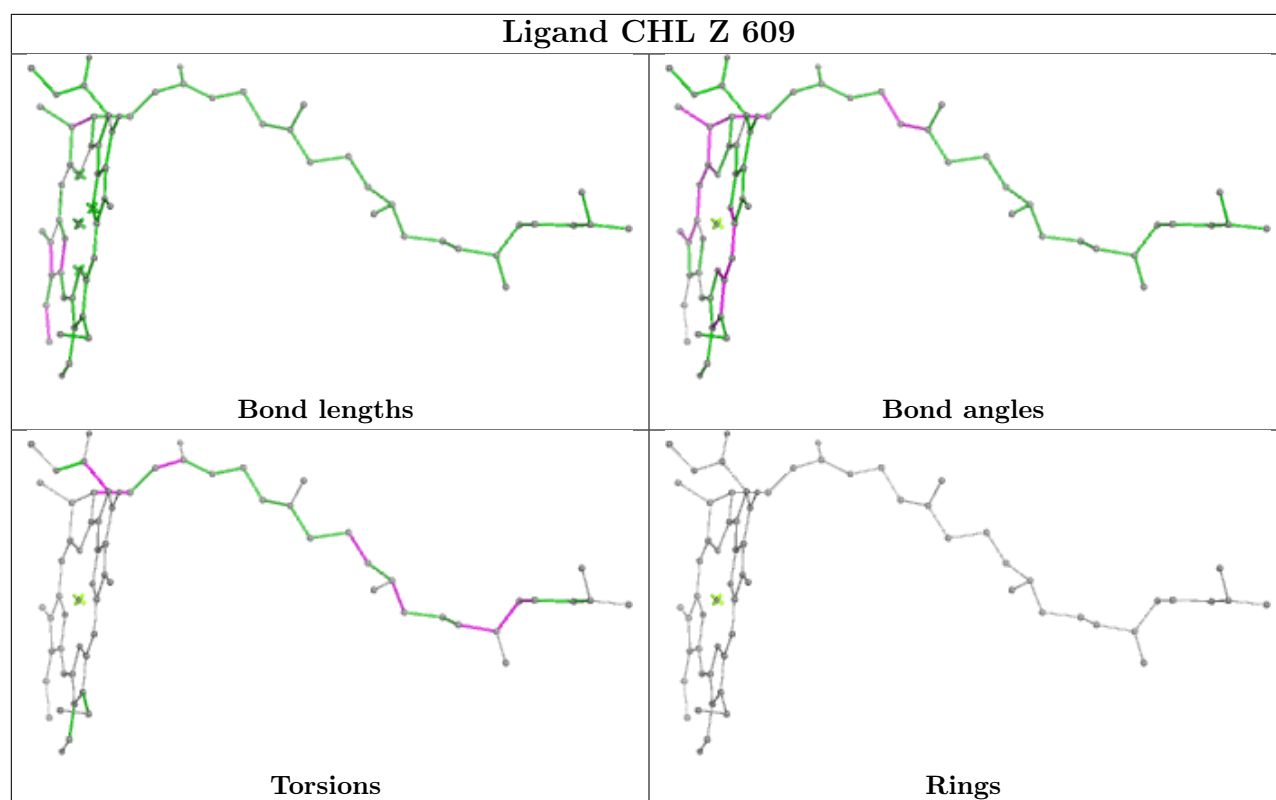


Ligand CLA 3 616**Bond lengths****Bond angles****Torsions****Rings**

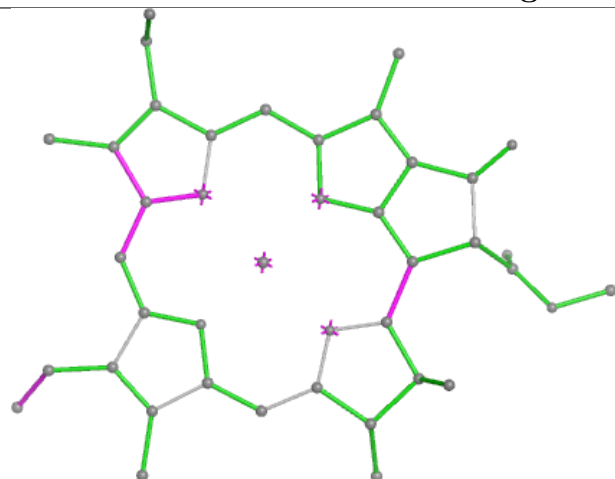




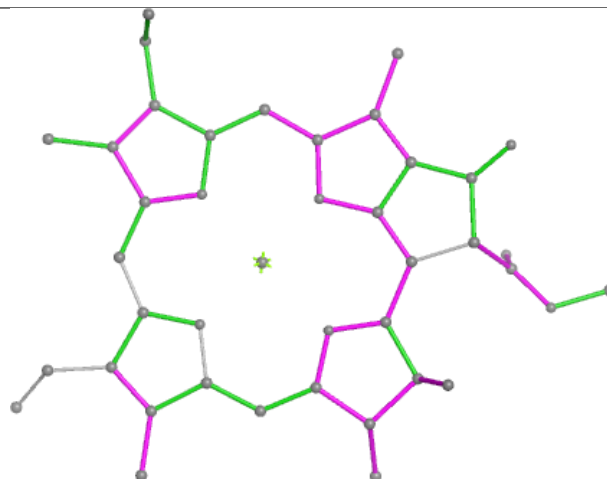




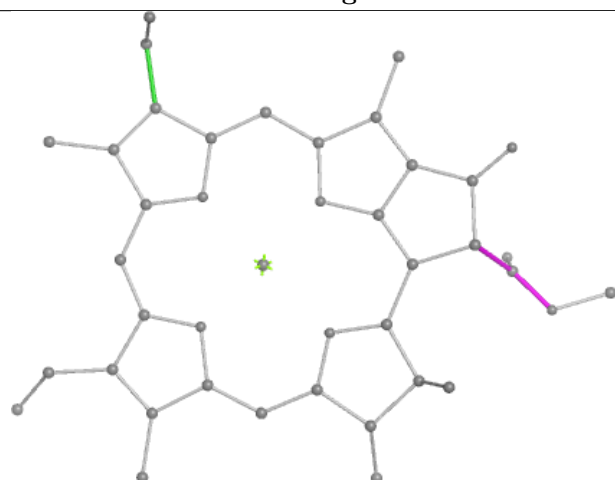
Ligand CLA 4 615



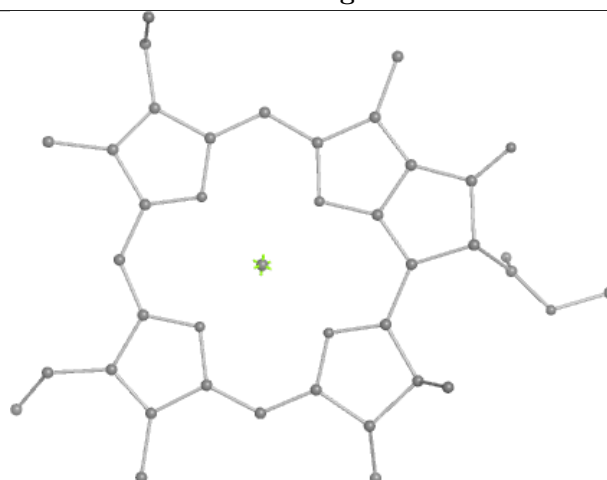
Bond lengths



Bond angles

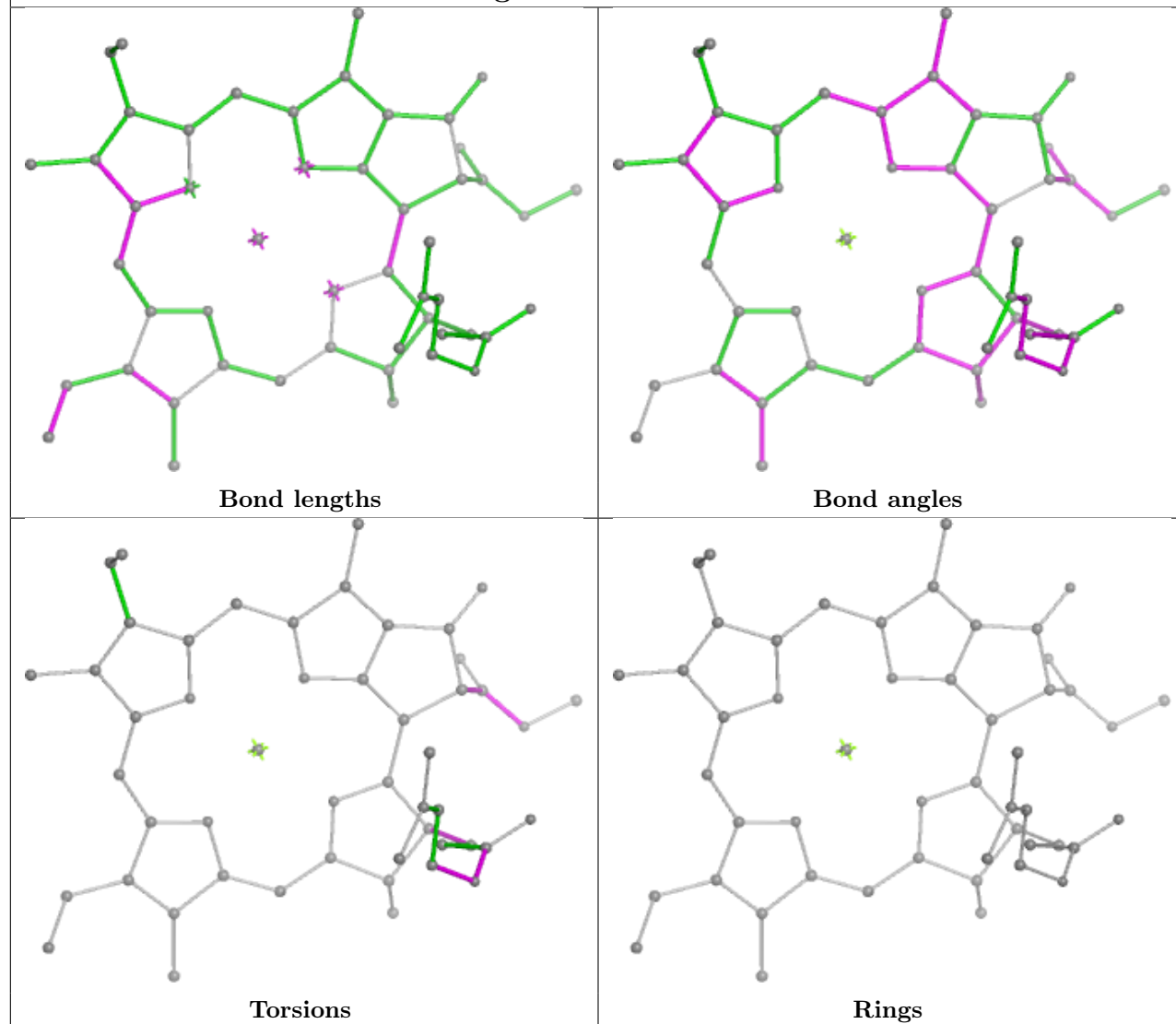


Torsions

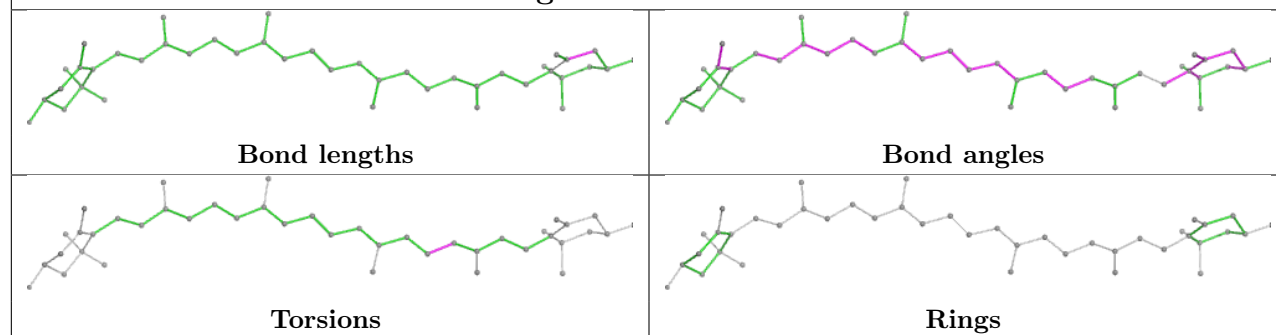


Rings

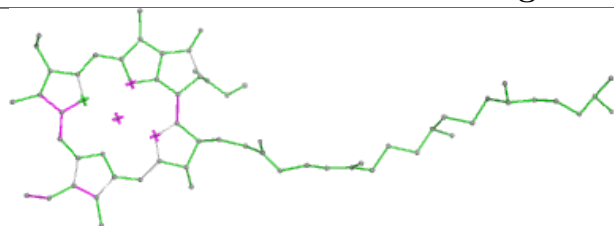
Ligand CLA 4 606



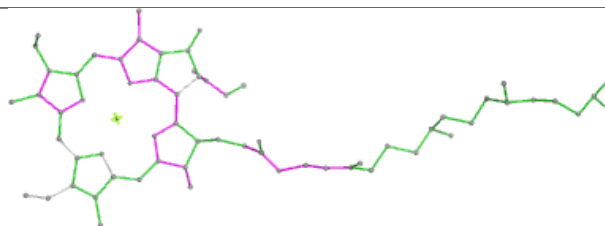
Ligand LUT 3 501



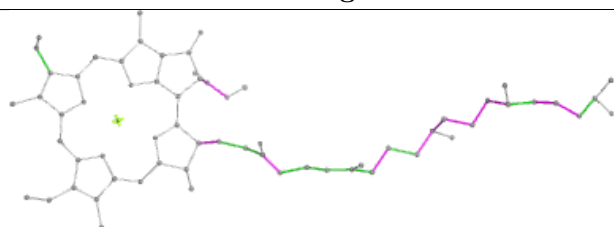
Ligand CLA 5 609



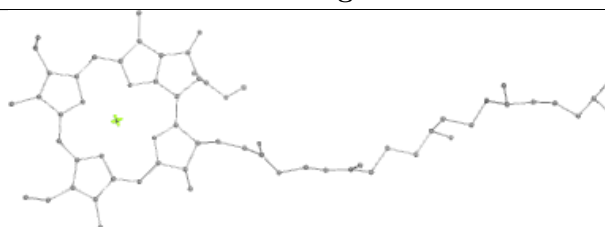
Bond lengths



Bond angles

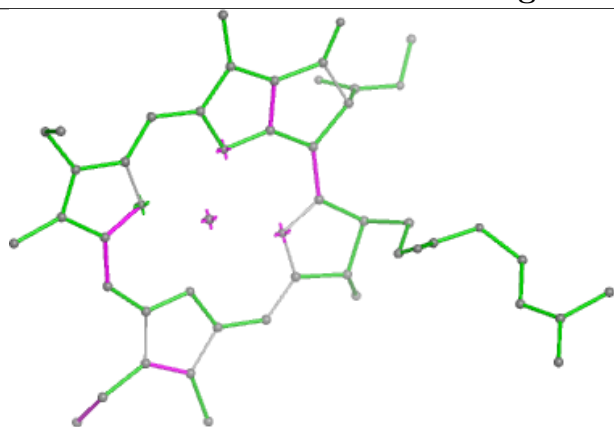


Torsions

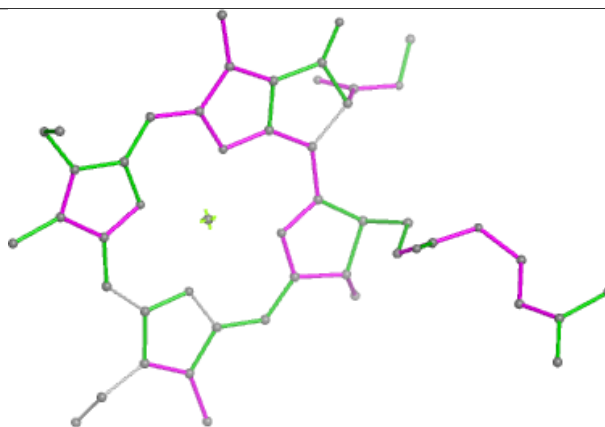


Rings

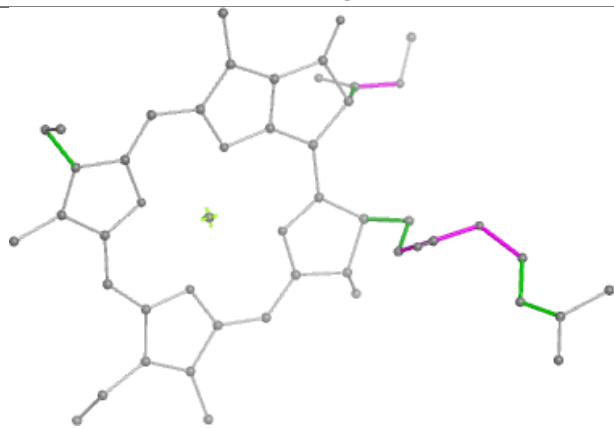
Ligand CLA 8 611



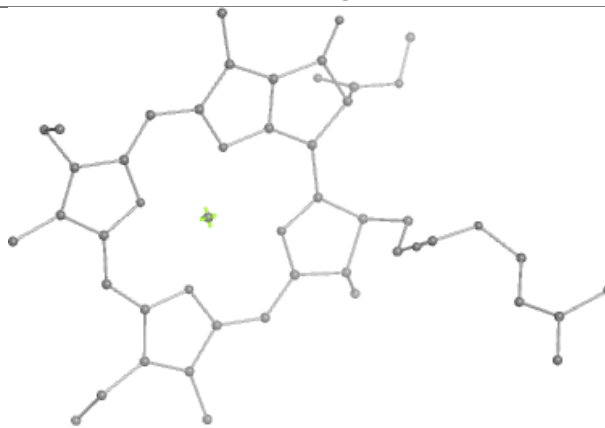
Bond lengths



Bond angles

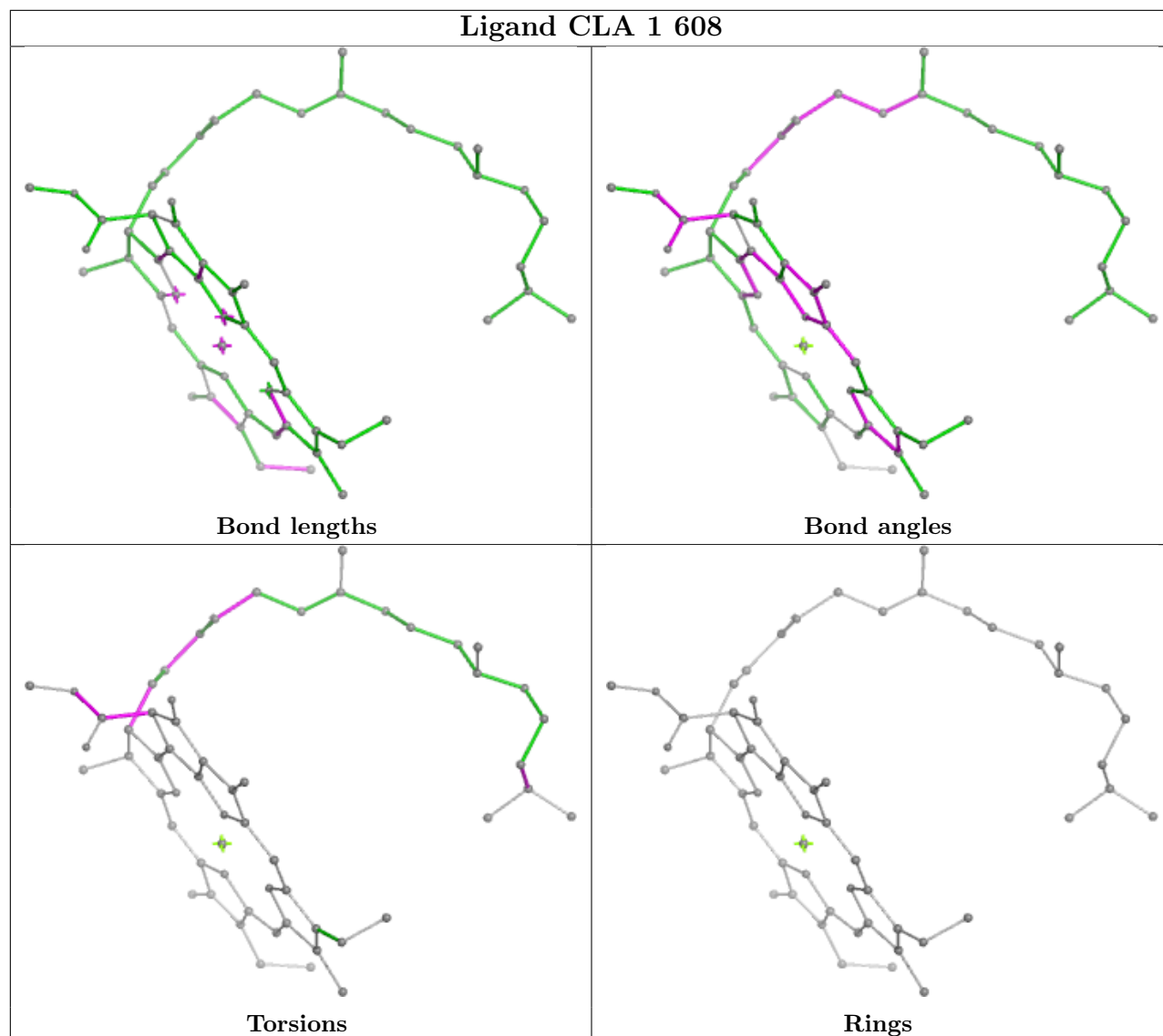


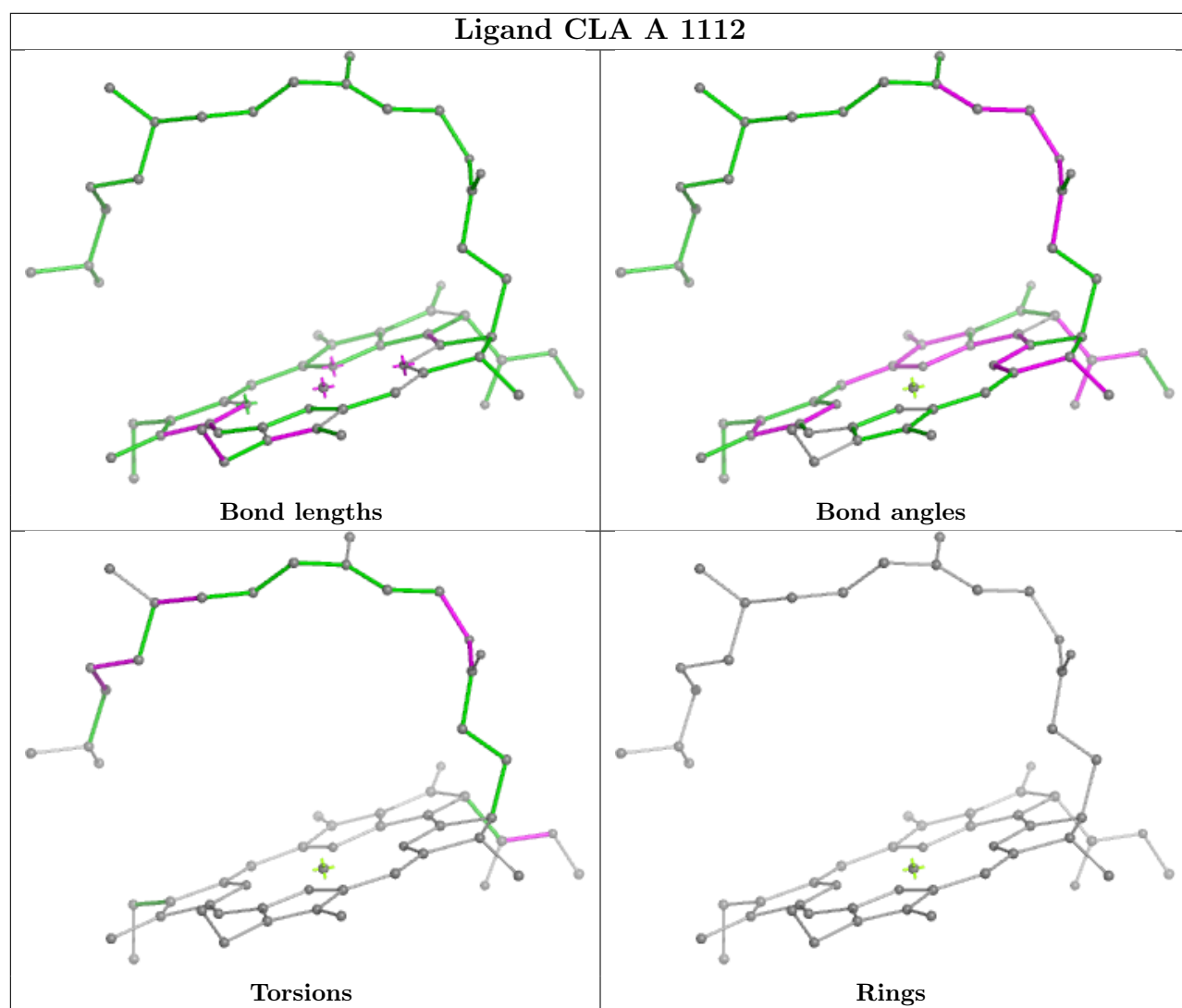
Torsions

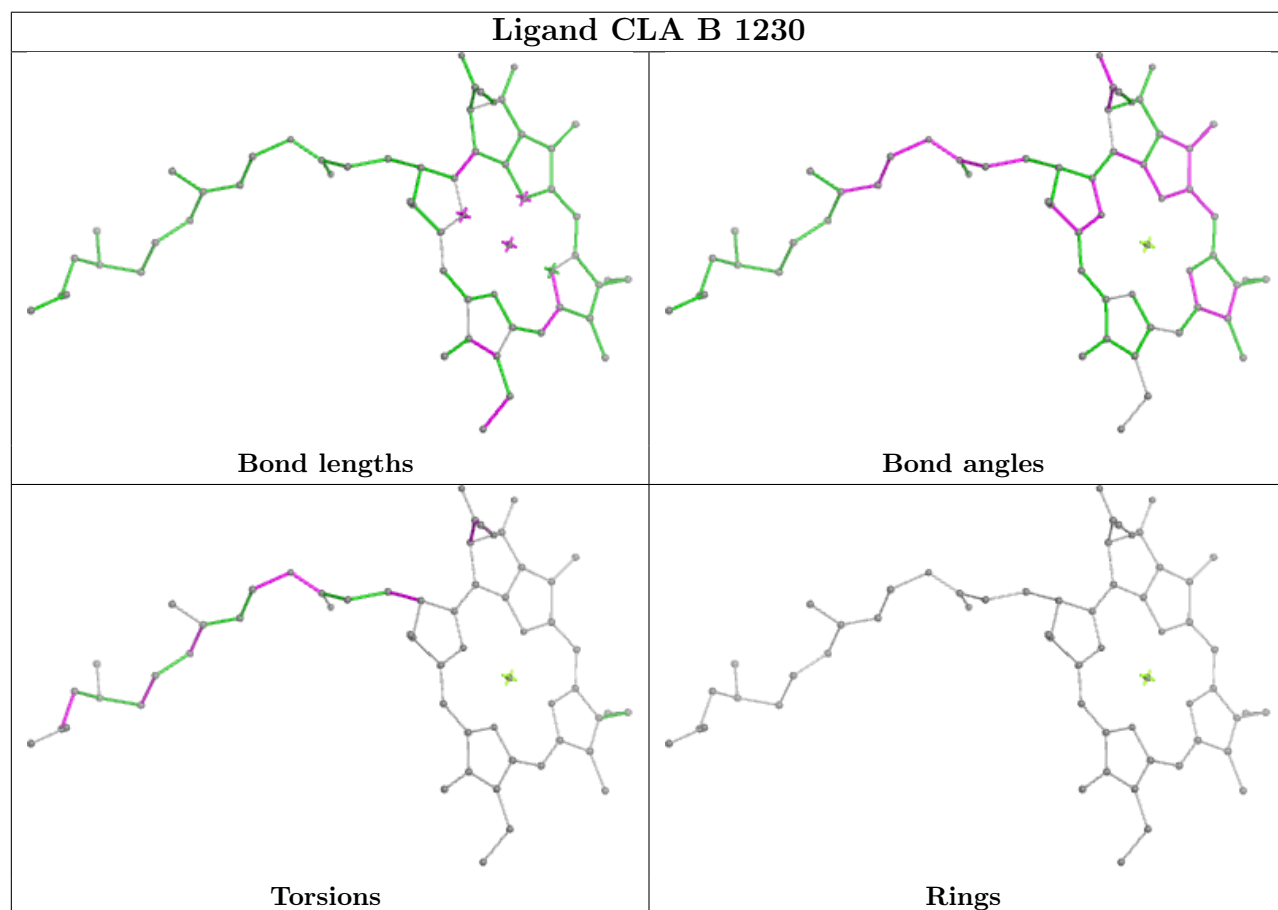
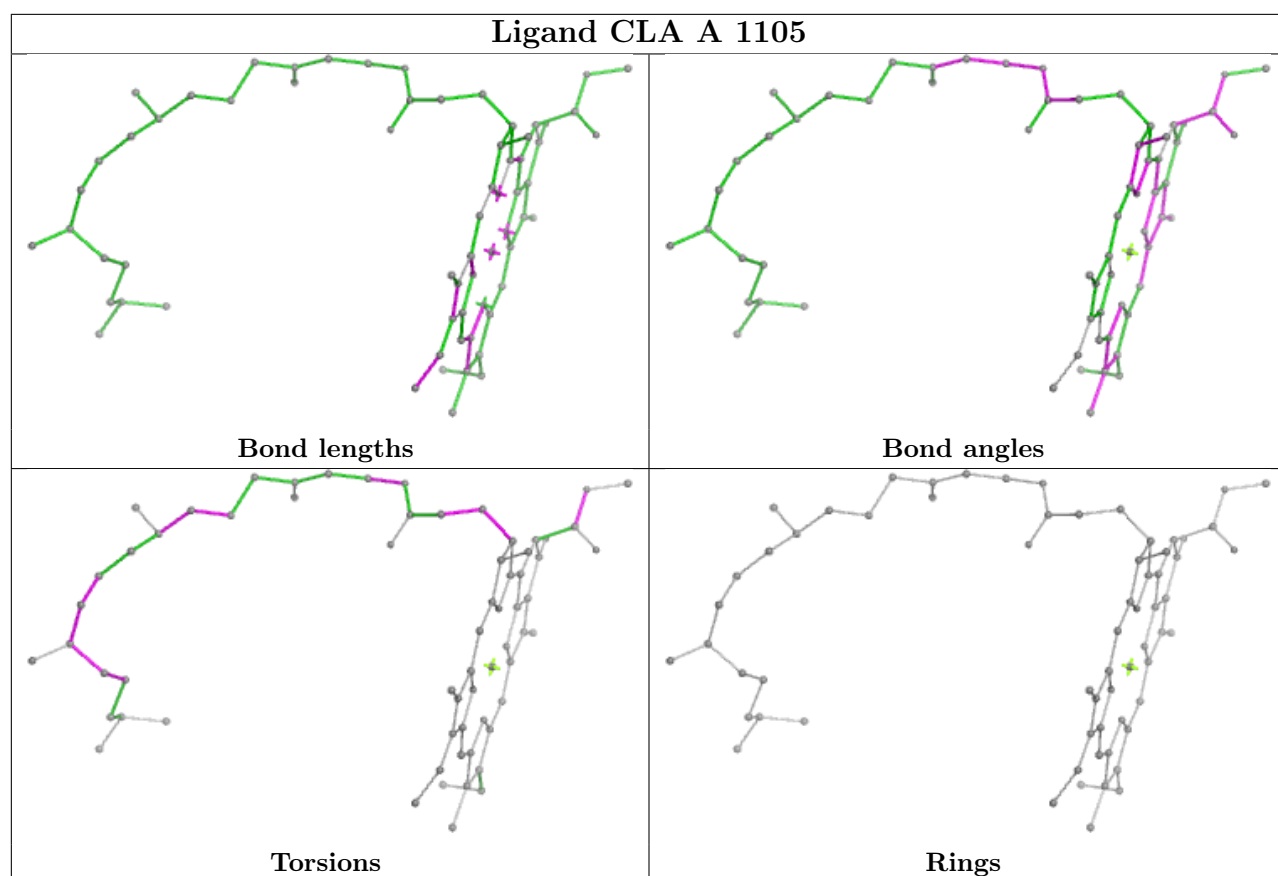


Rings

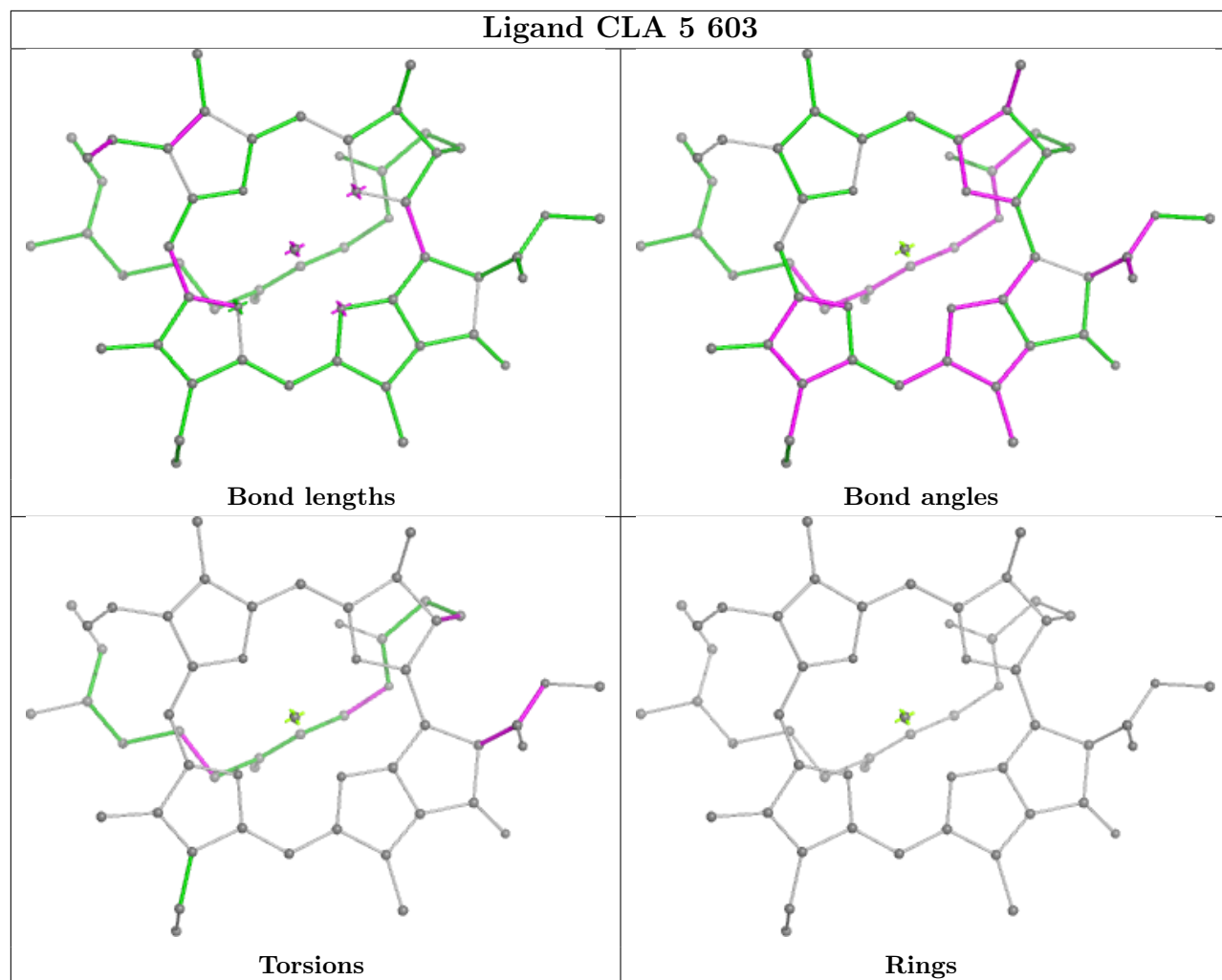
Ligand CLA 1 608



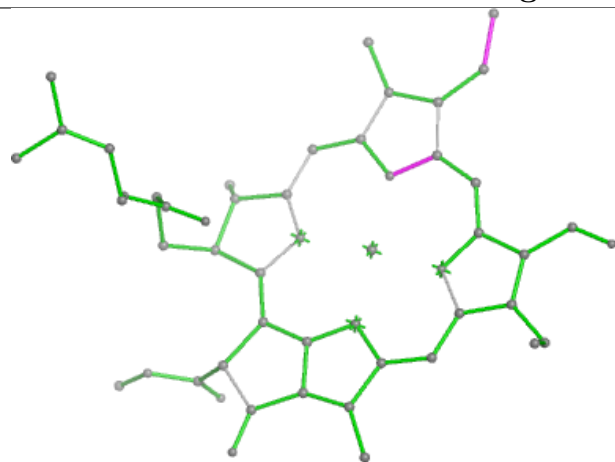




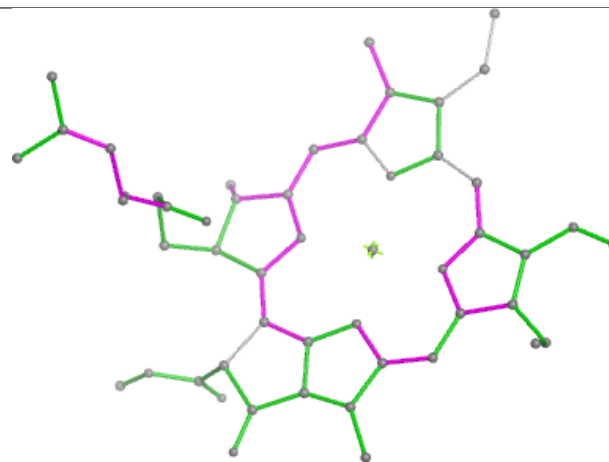
Ligand CLA 5 603



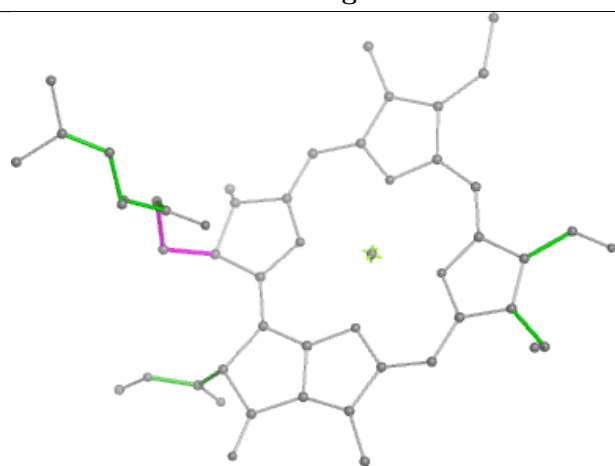
Ligand CHL 5 611



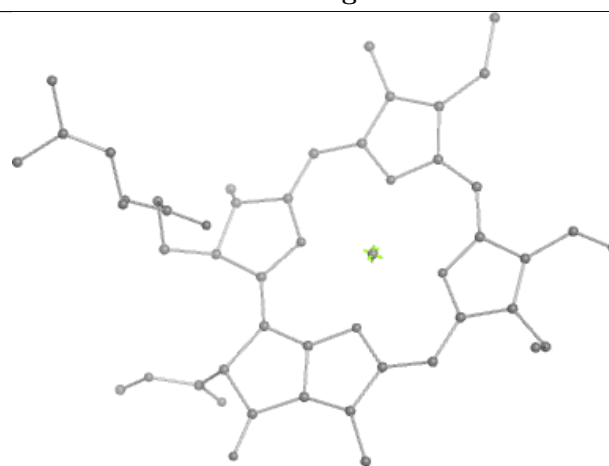
Bond lengths



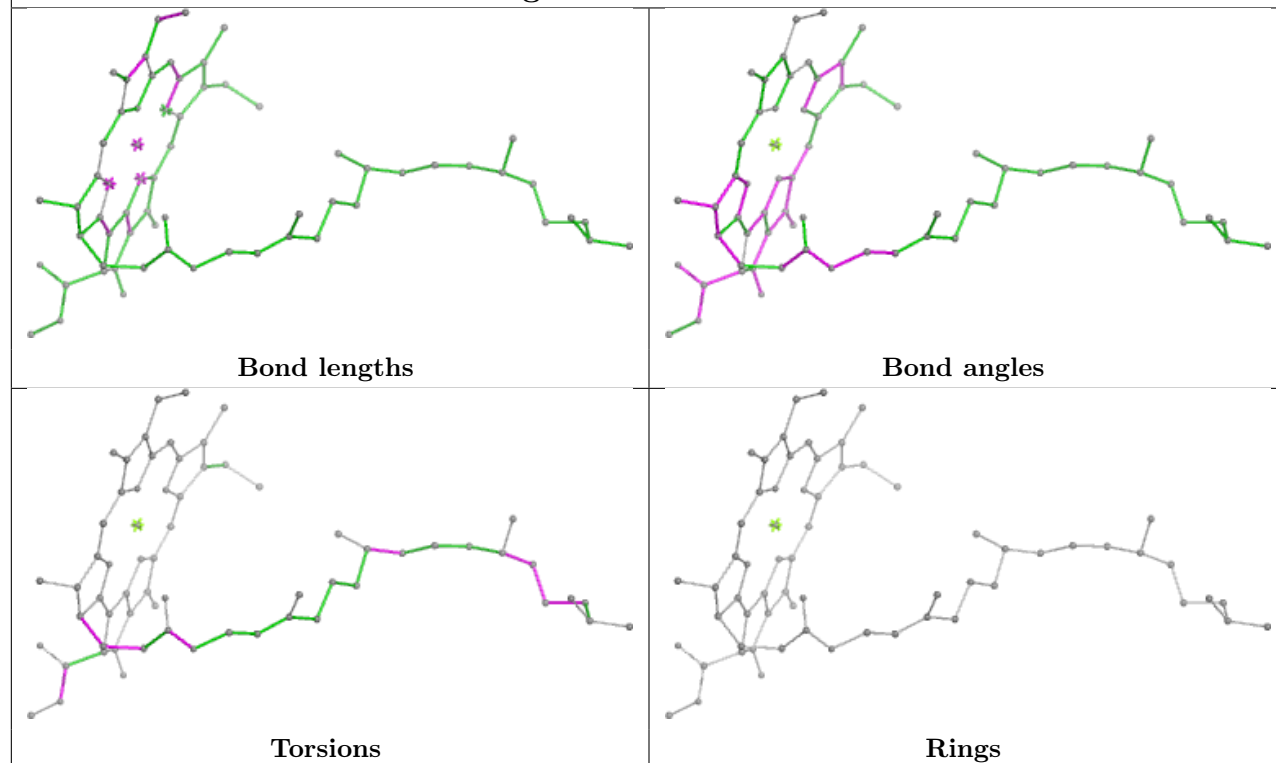
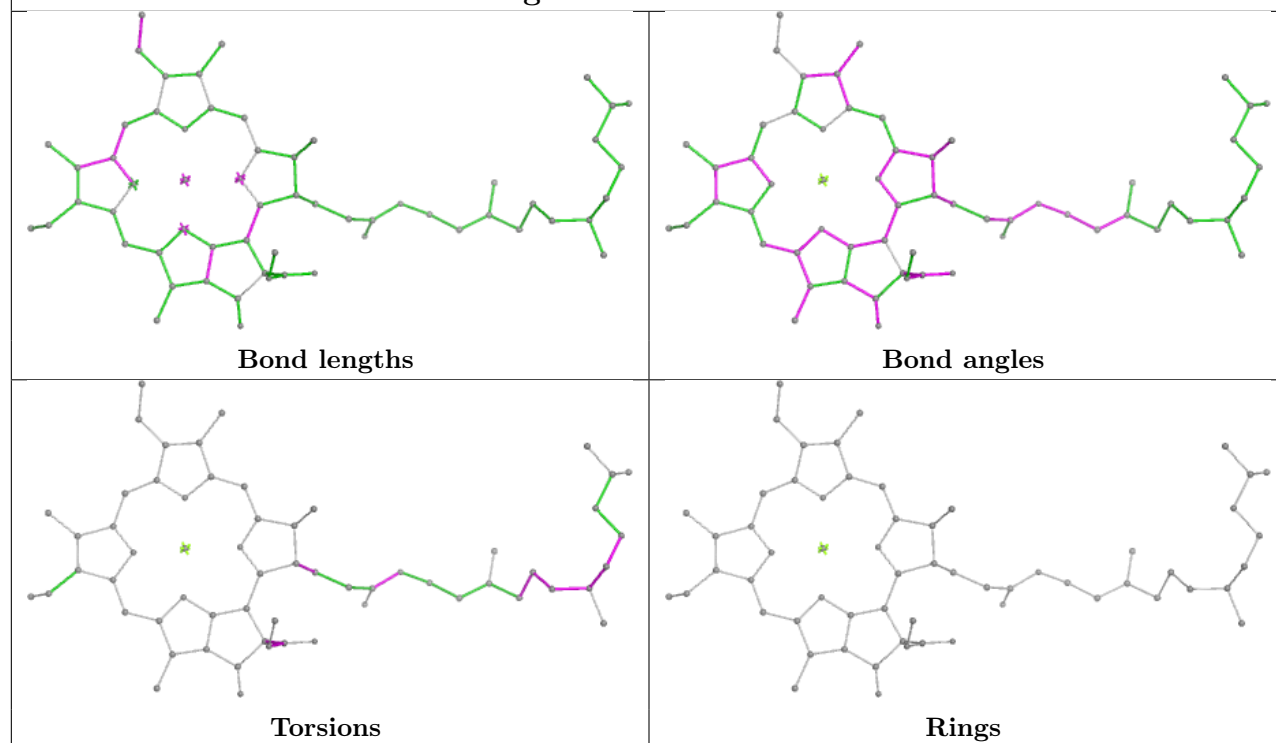
Bond angles

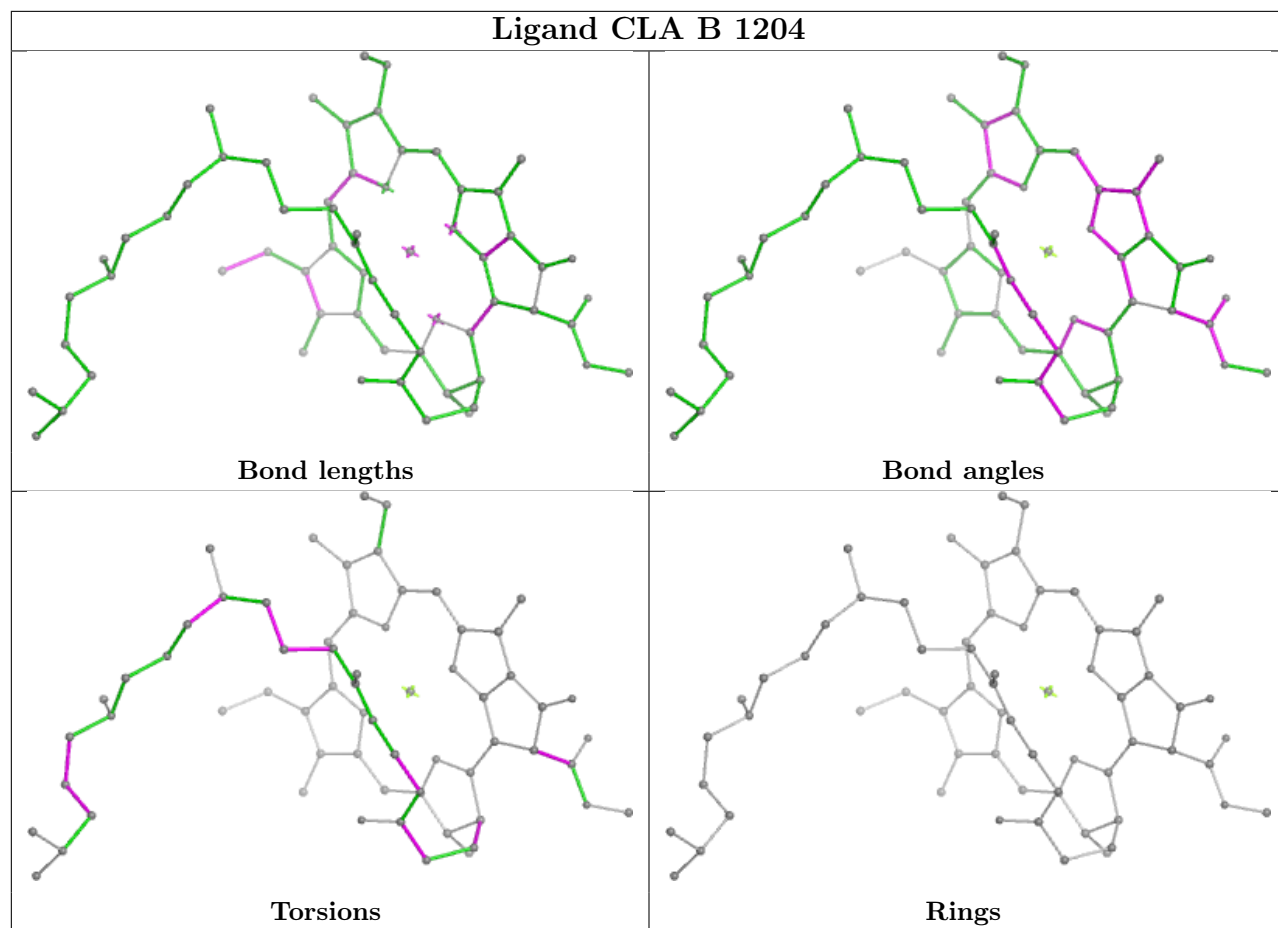


Torsions

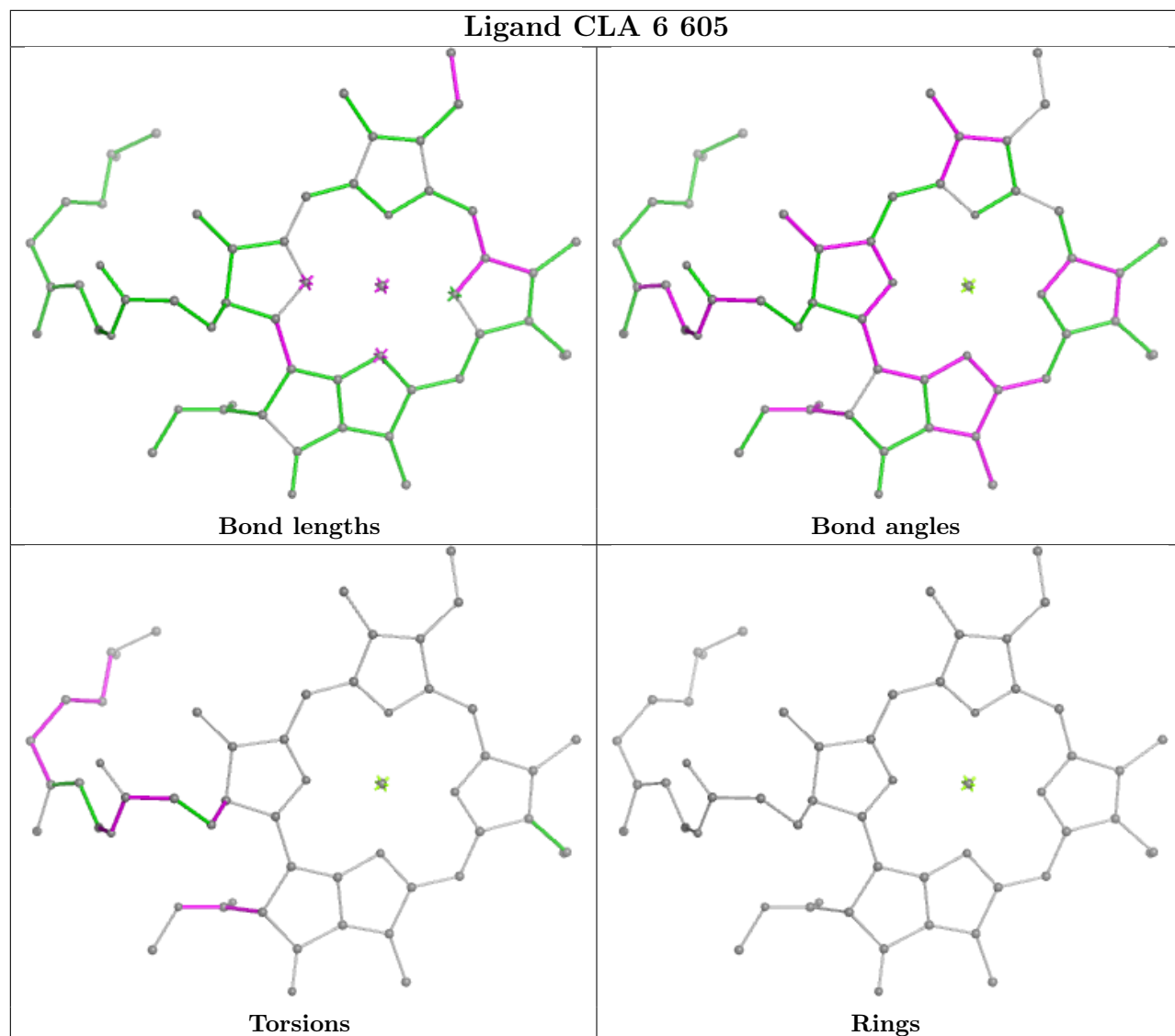


Rings

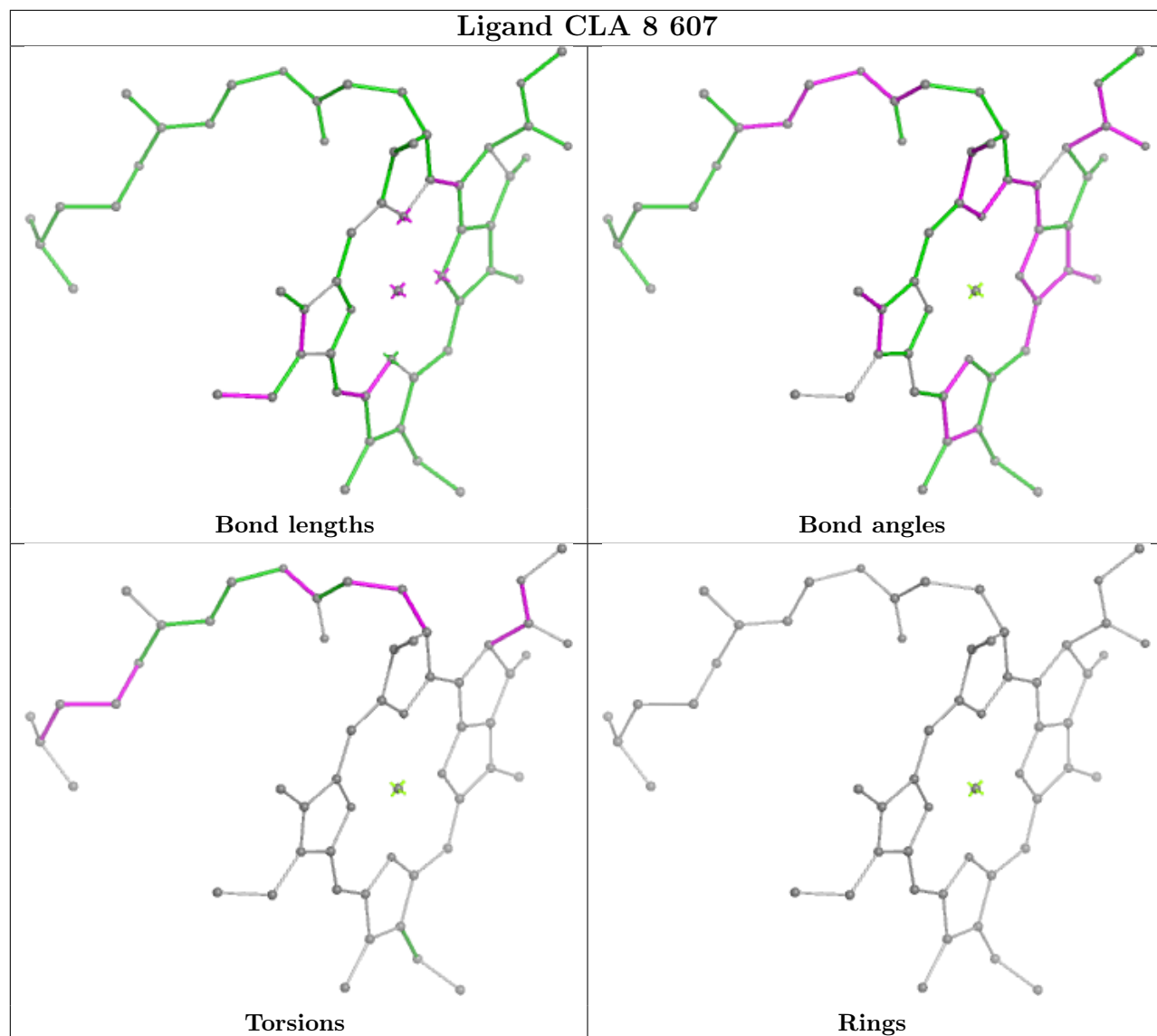
Ligand CLA A 1109**Ligand CLA B 1234**

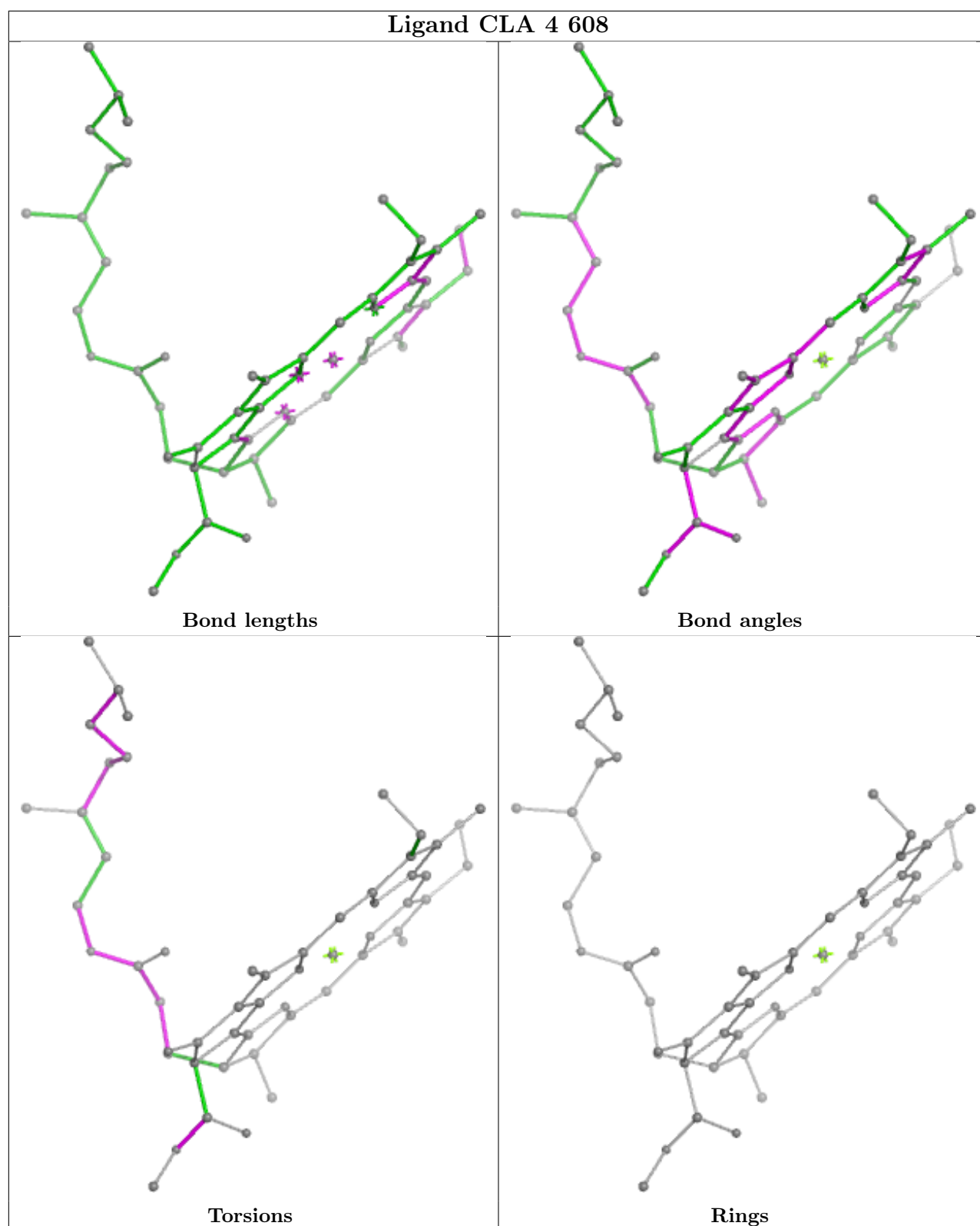


Ligand CLA 6 605

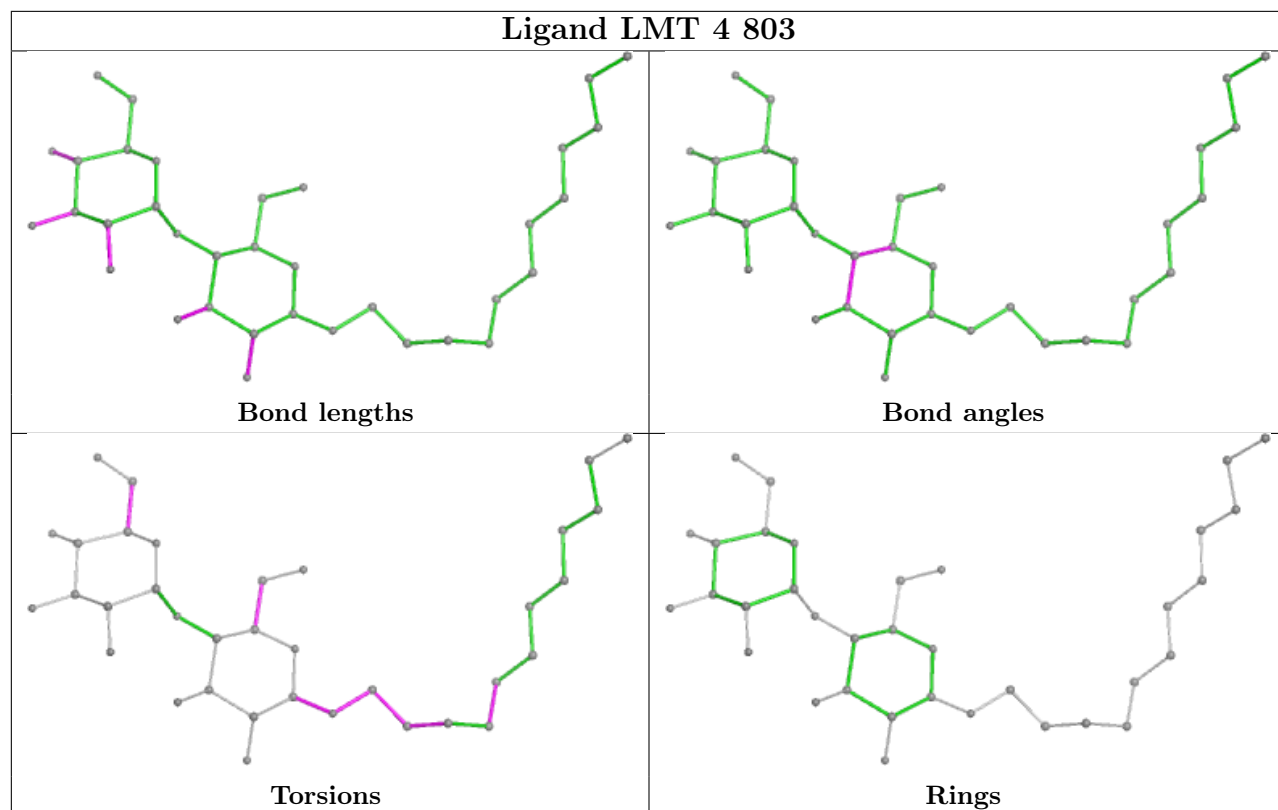


Ligand CLA 8 607

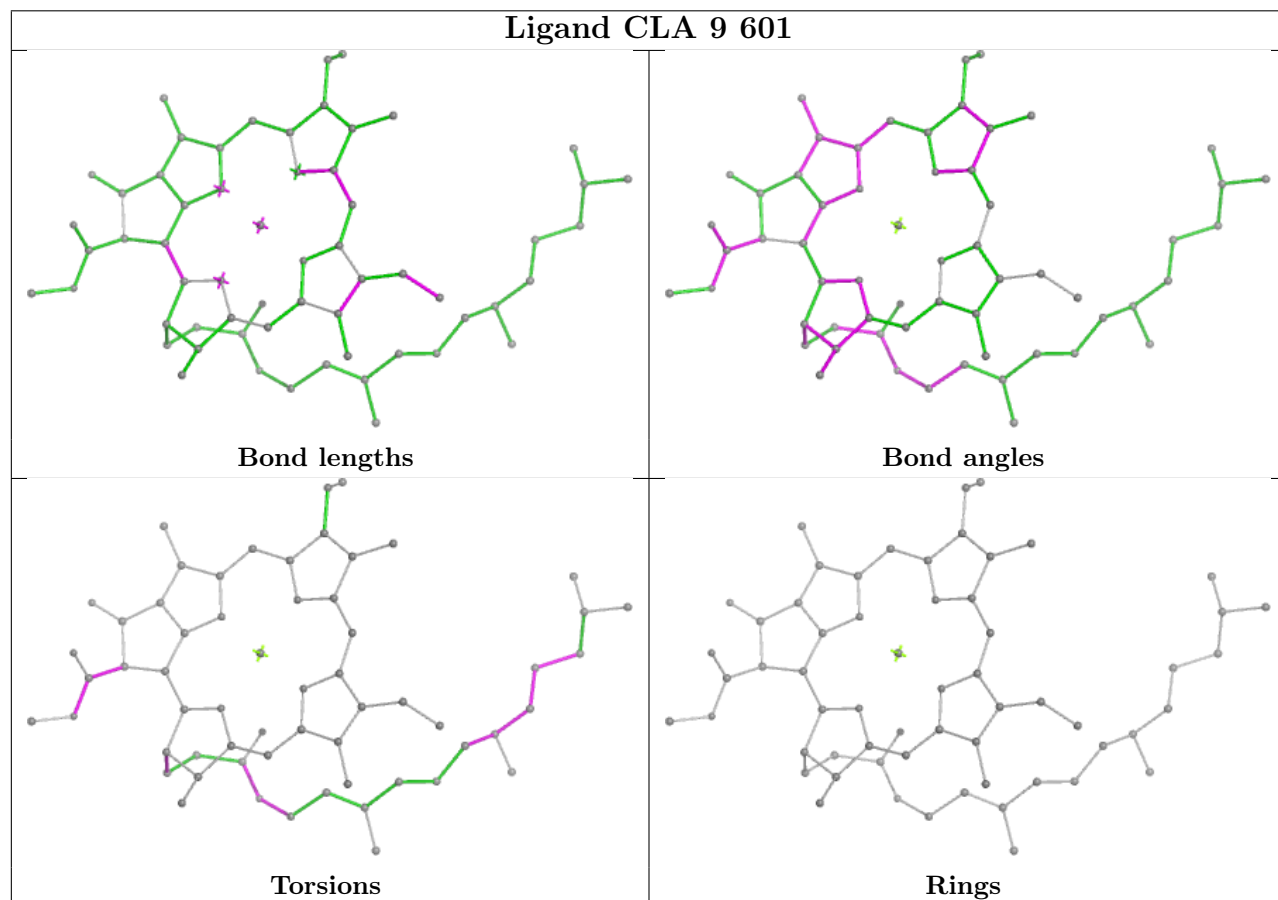


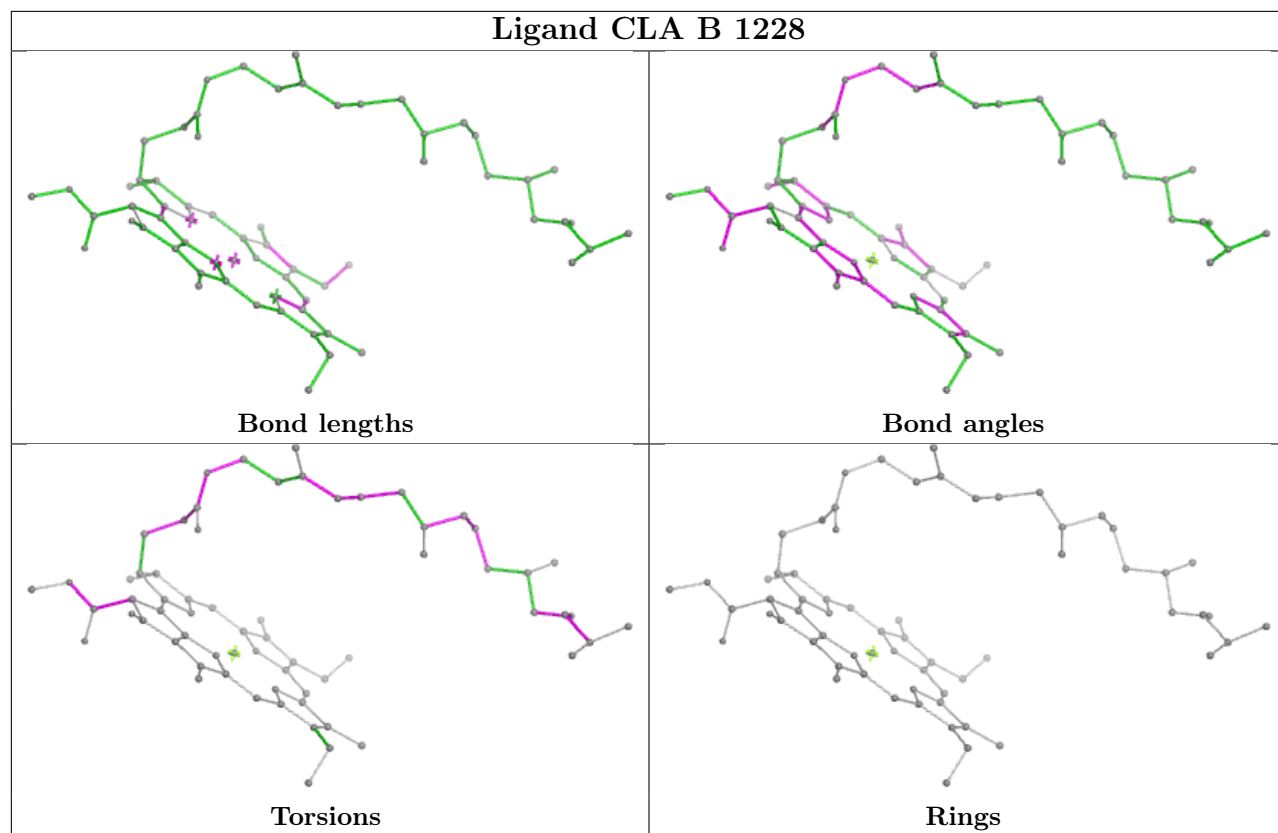


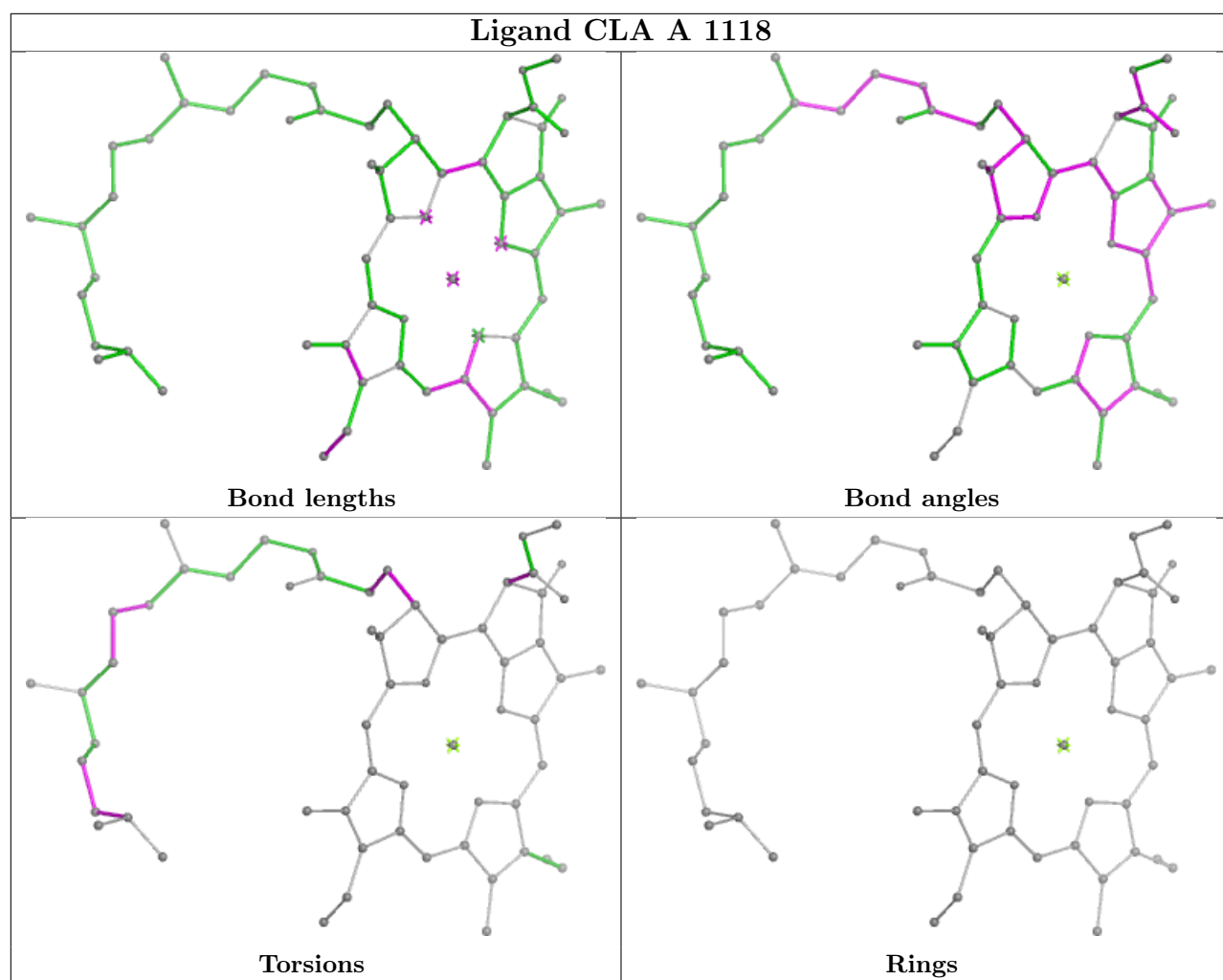
Ligand LMT 4 803

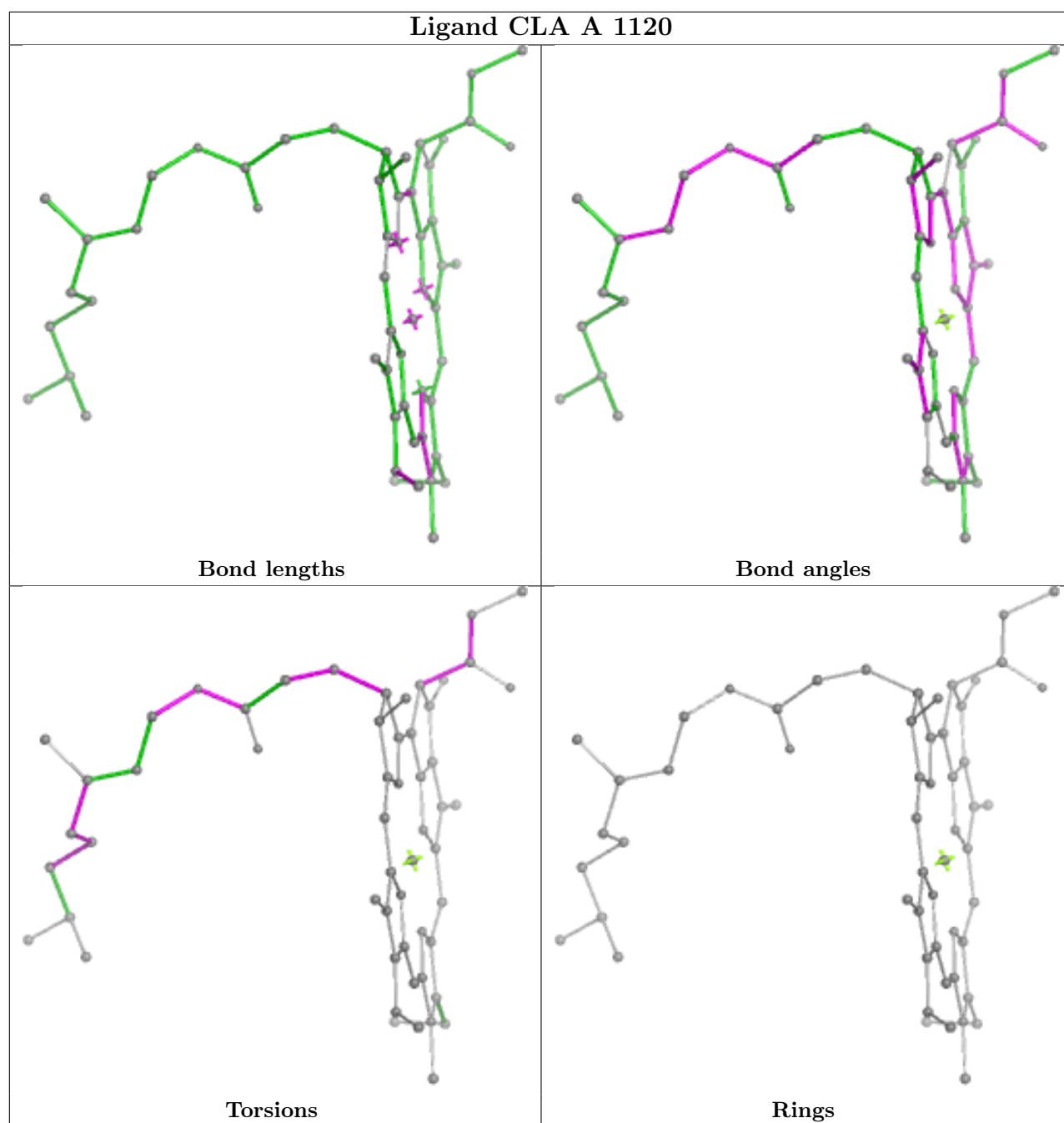


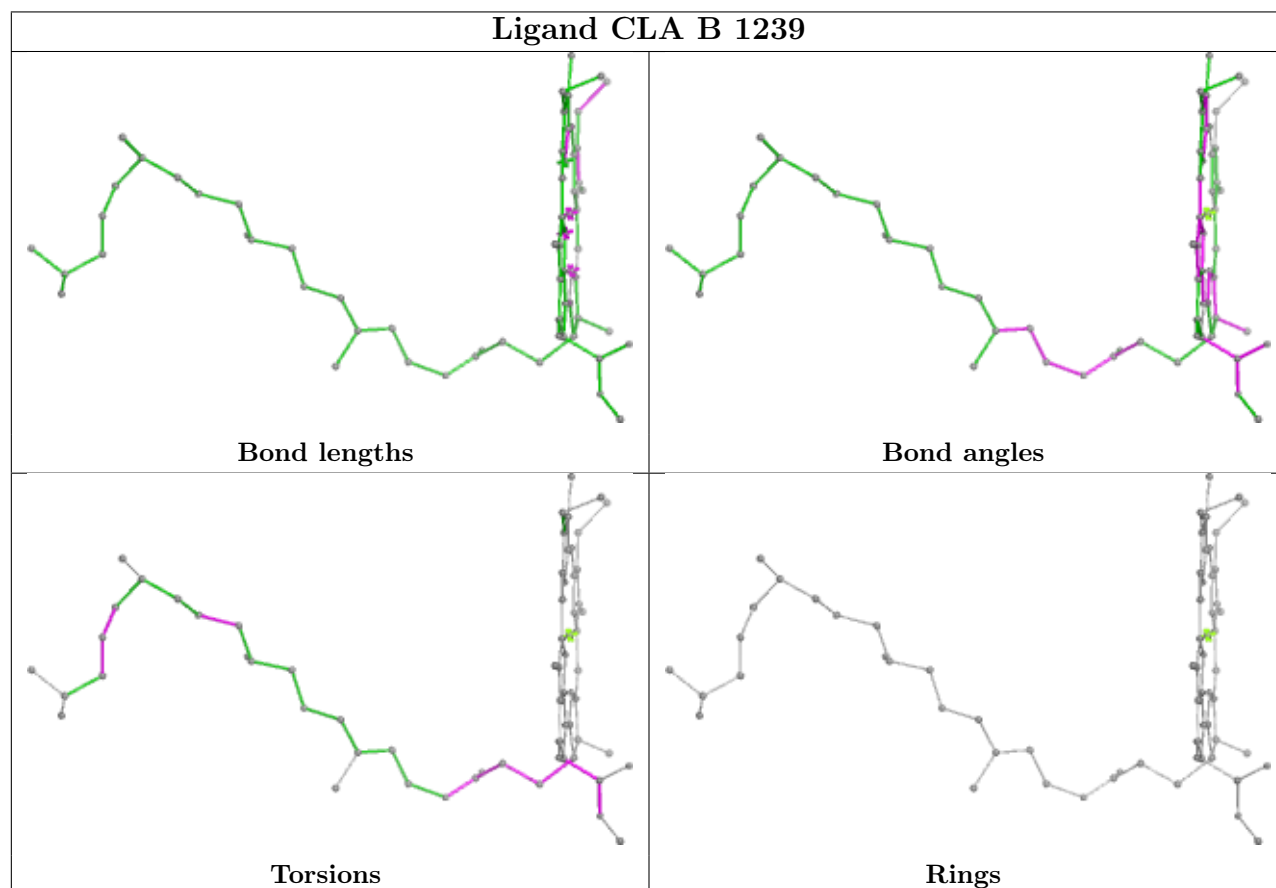
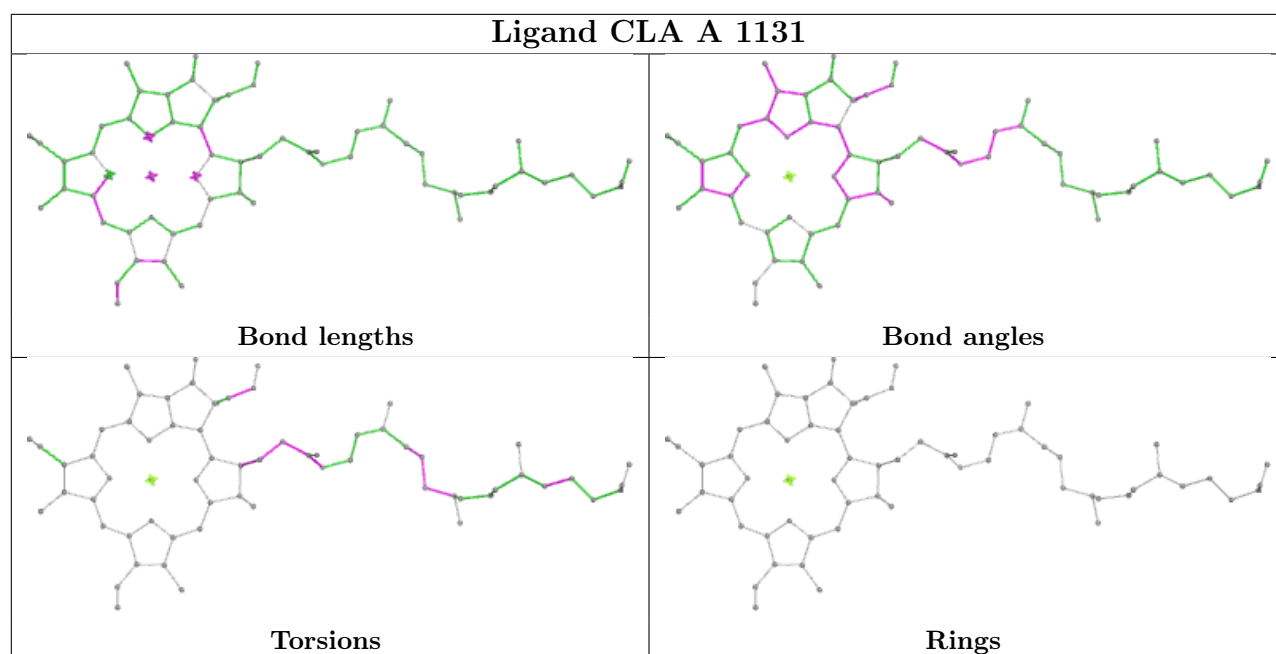
Ligand CLA 9 601



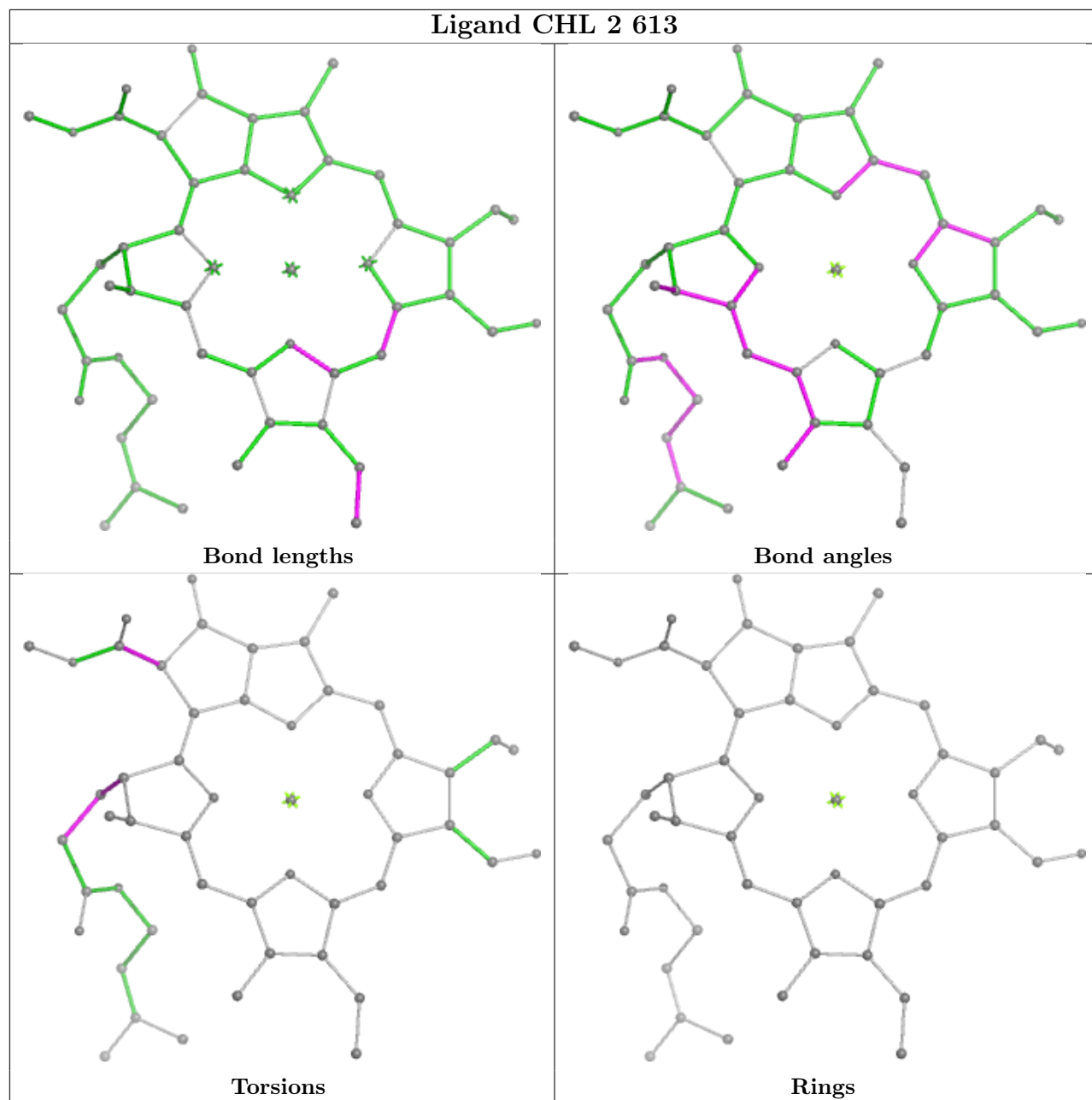


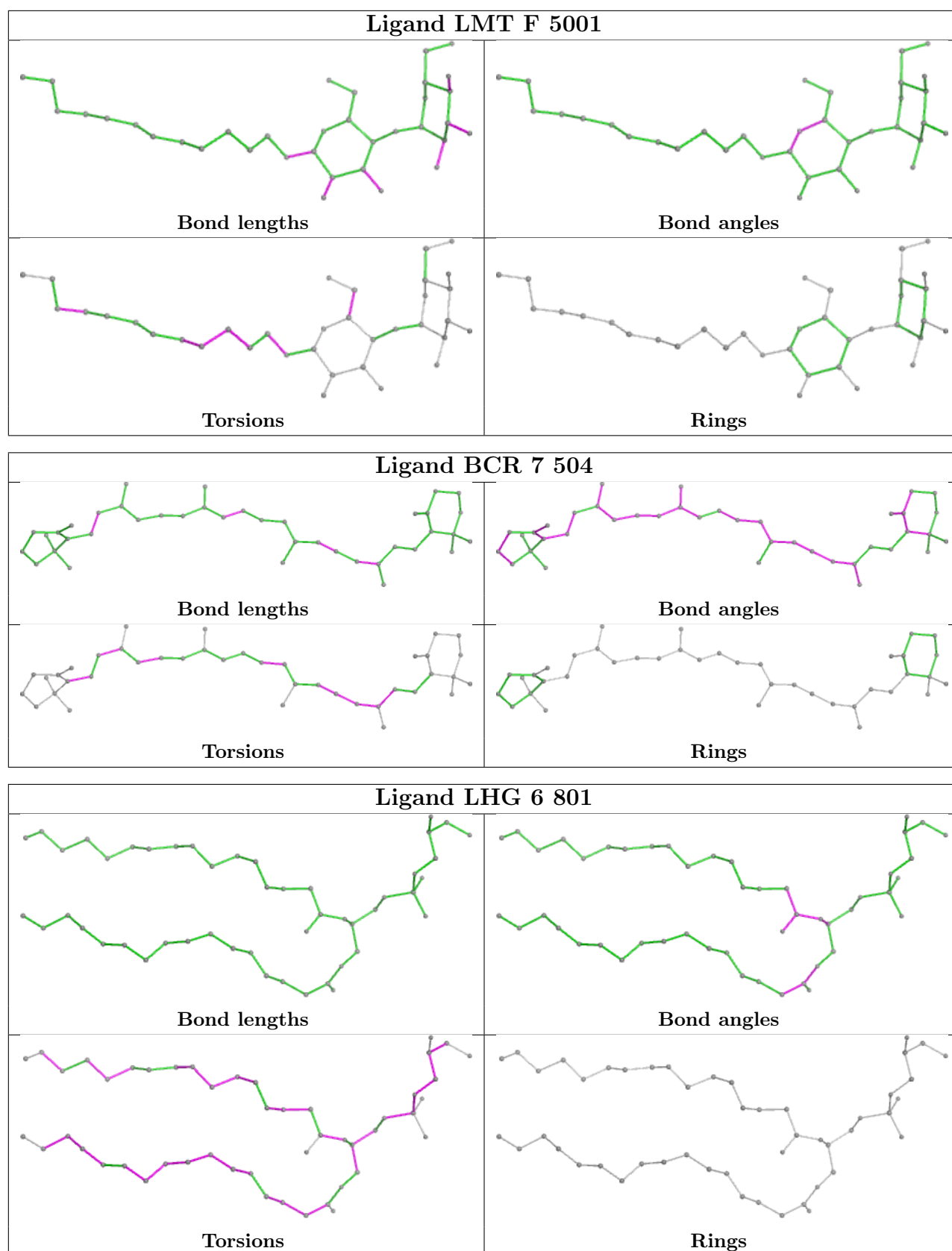




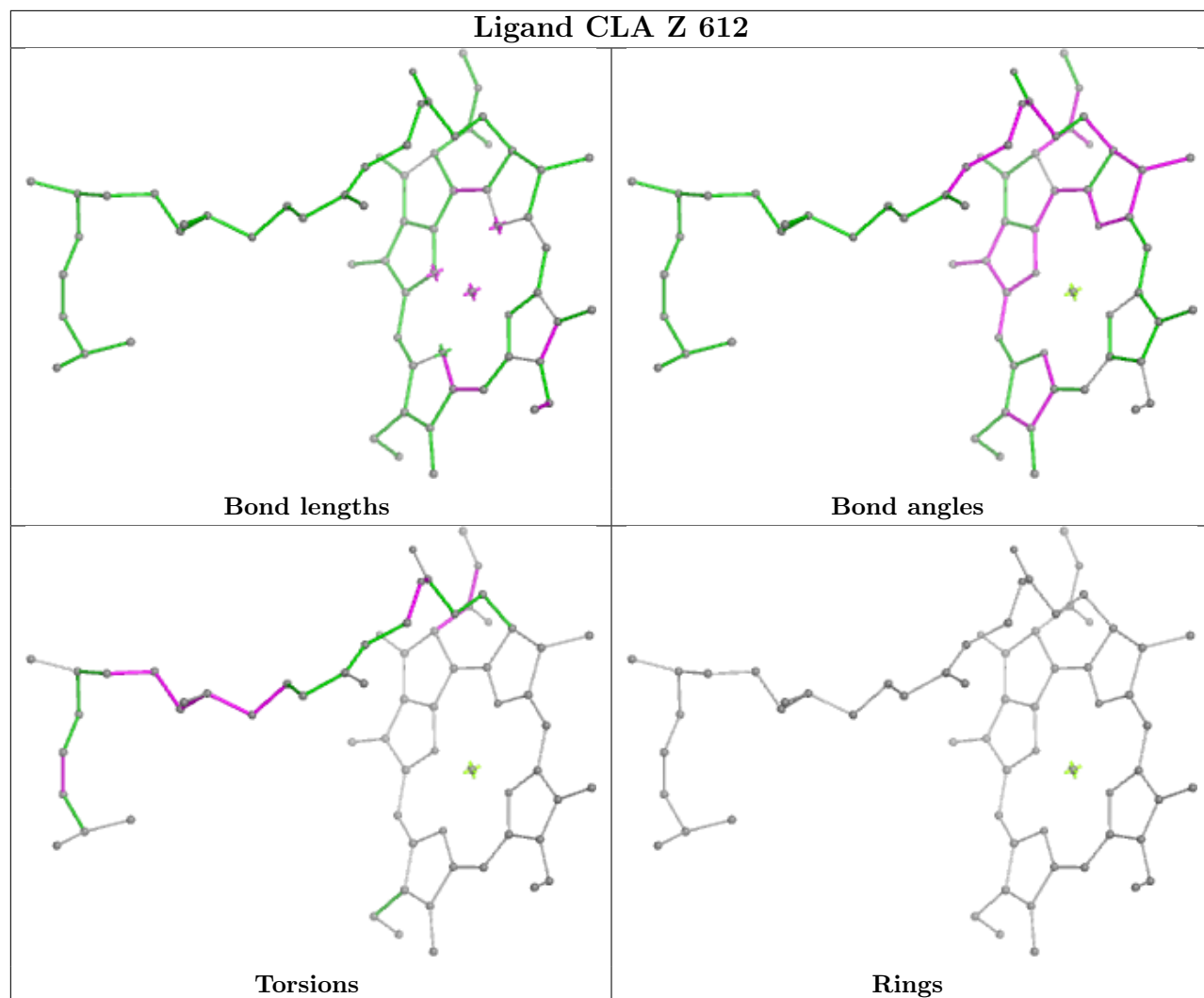


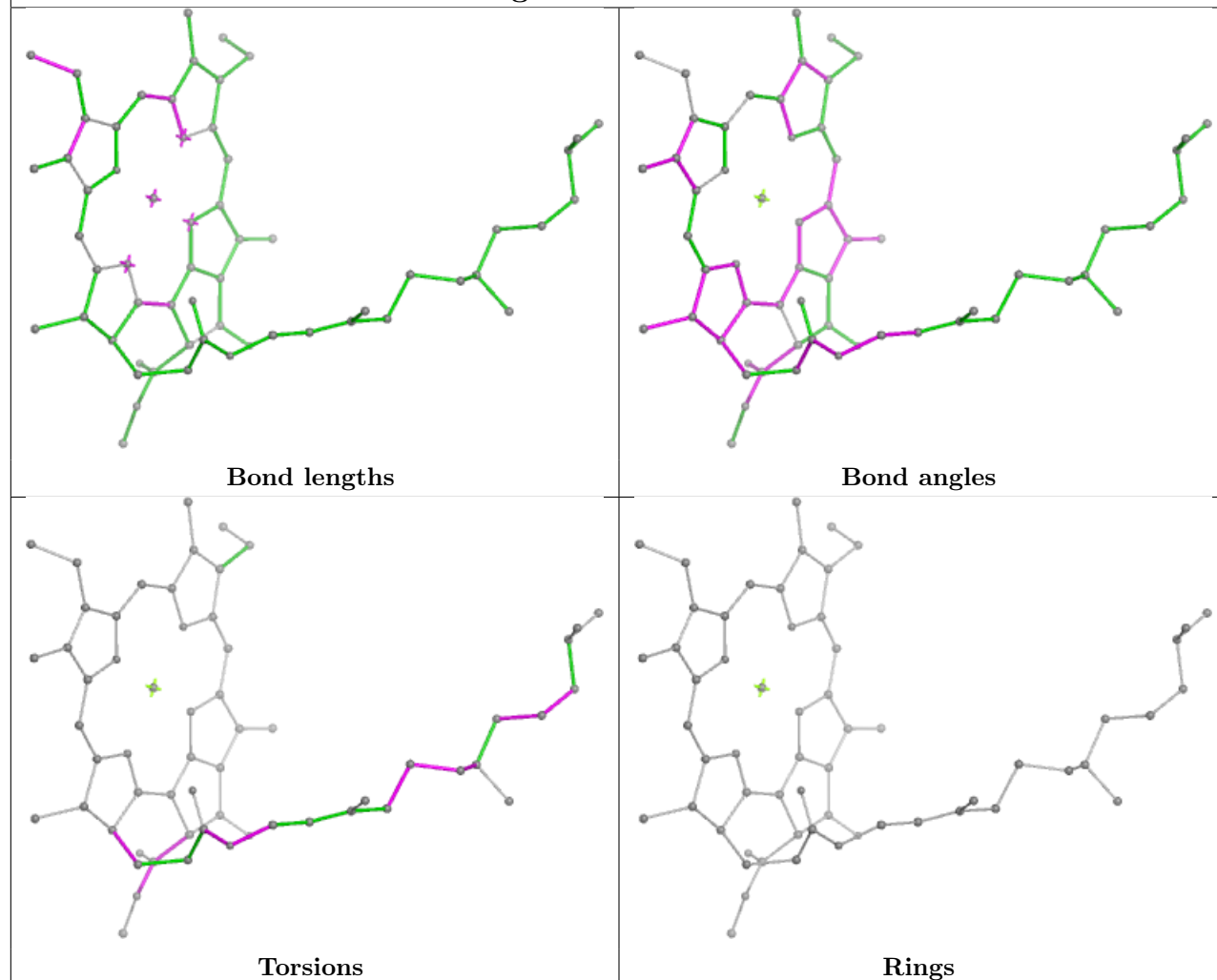
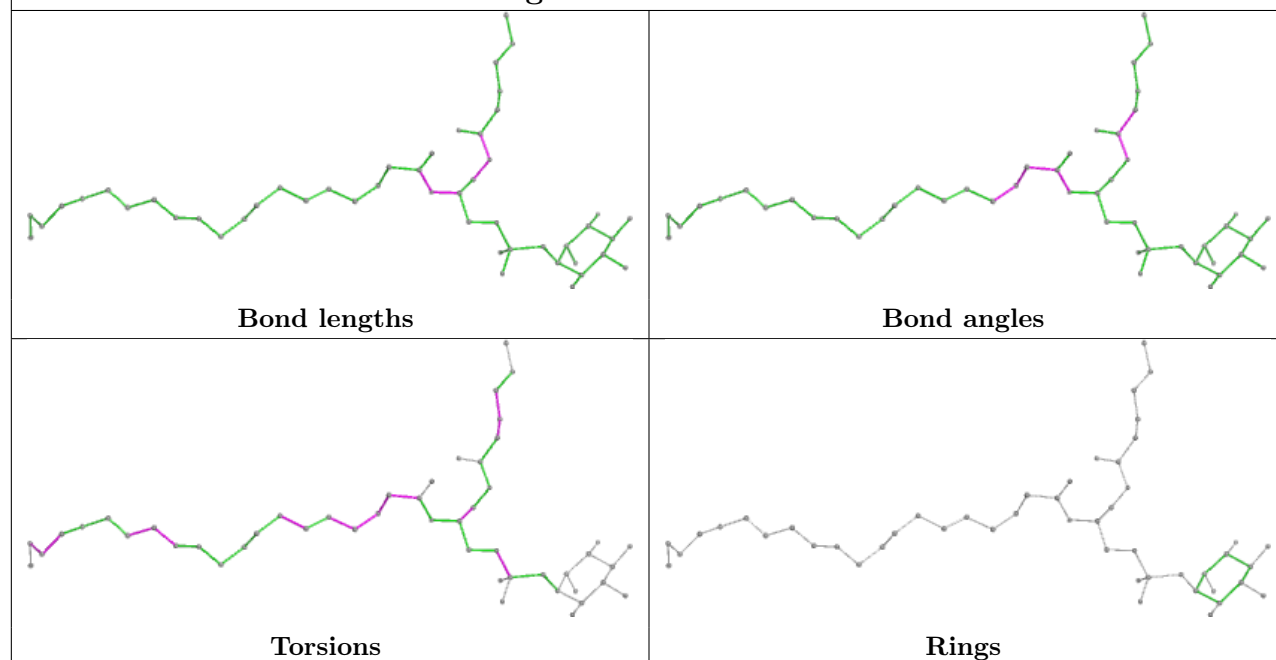
Ligand CHL 2 613



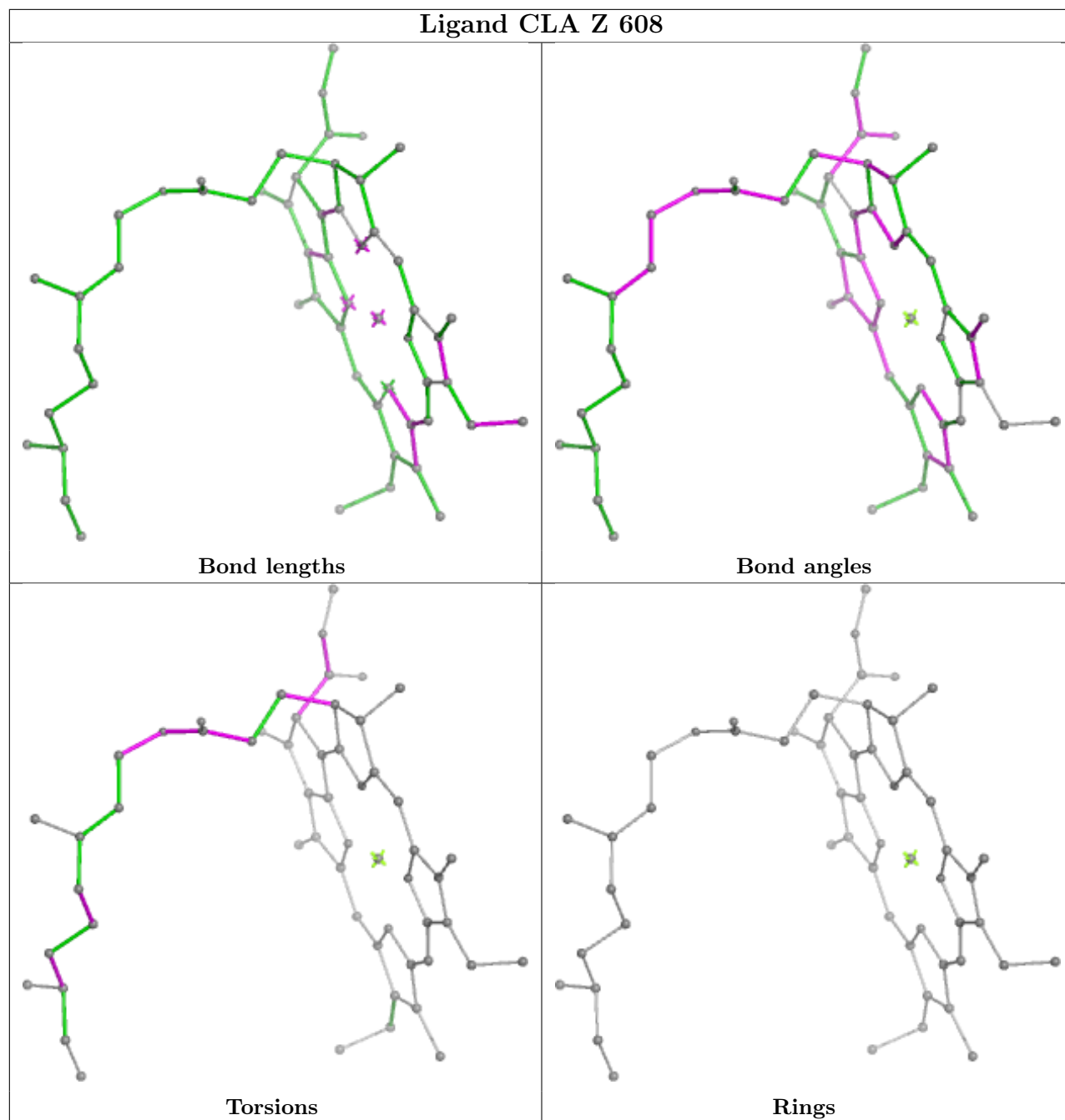


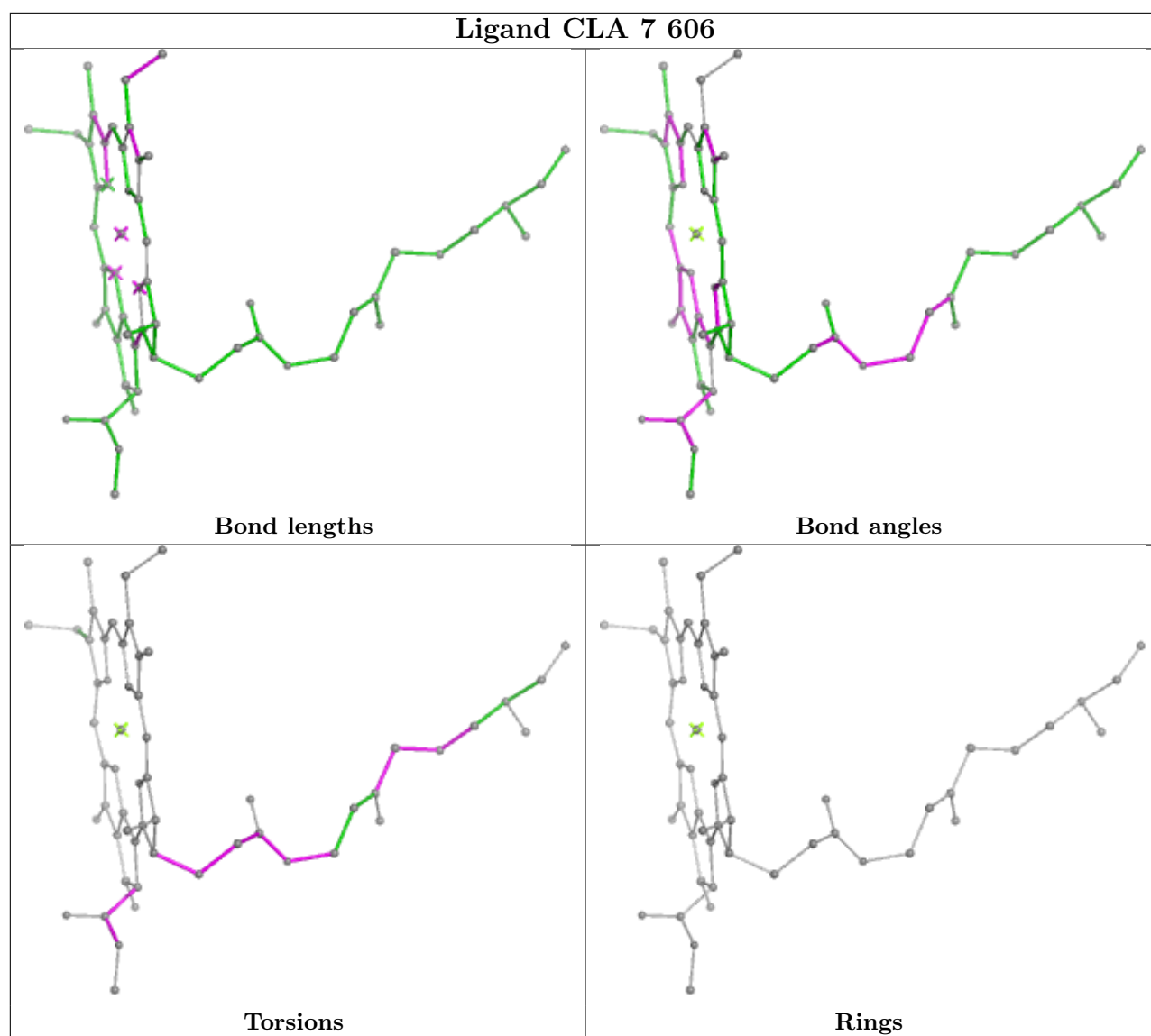
Ligand CLA Z 612



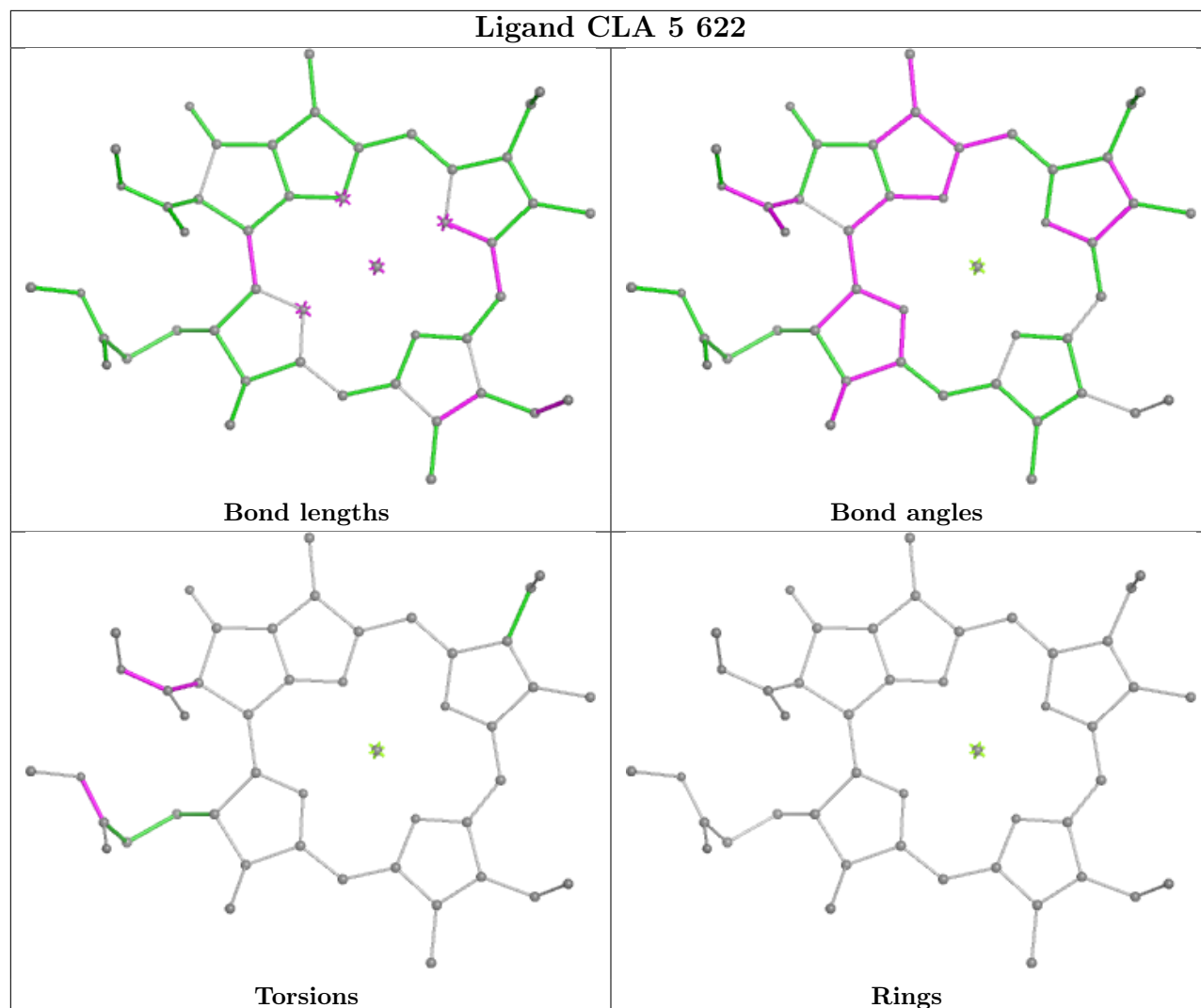
Ligand CLA 1 607**Ligand T7X B 5004**

Ligand CLA Z 608

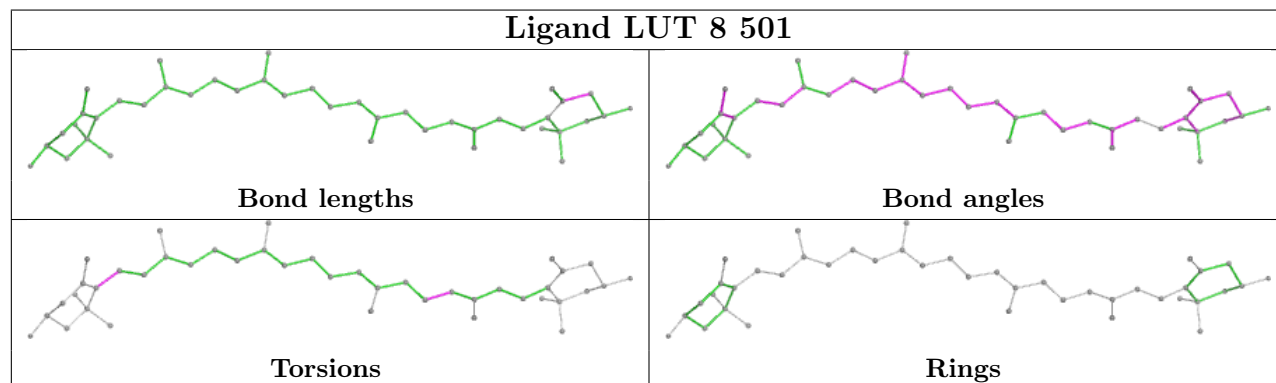


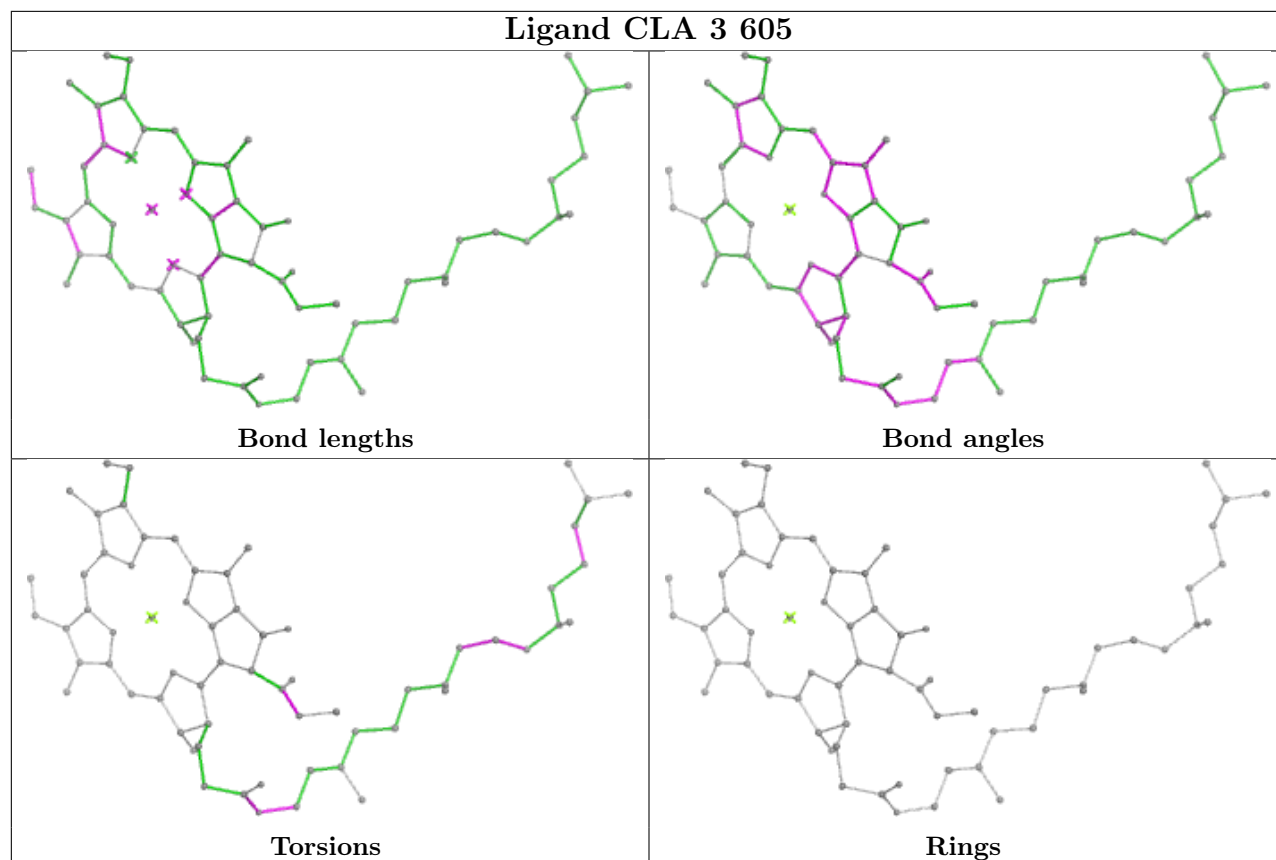
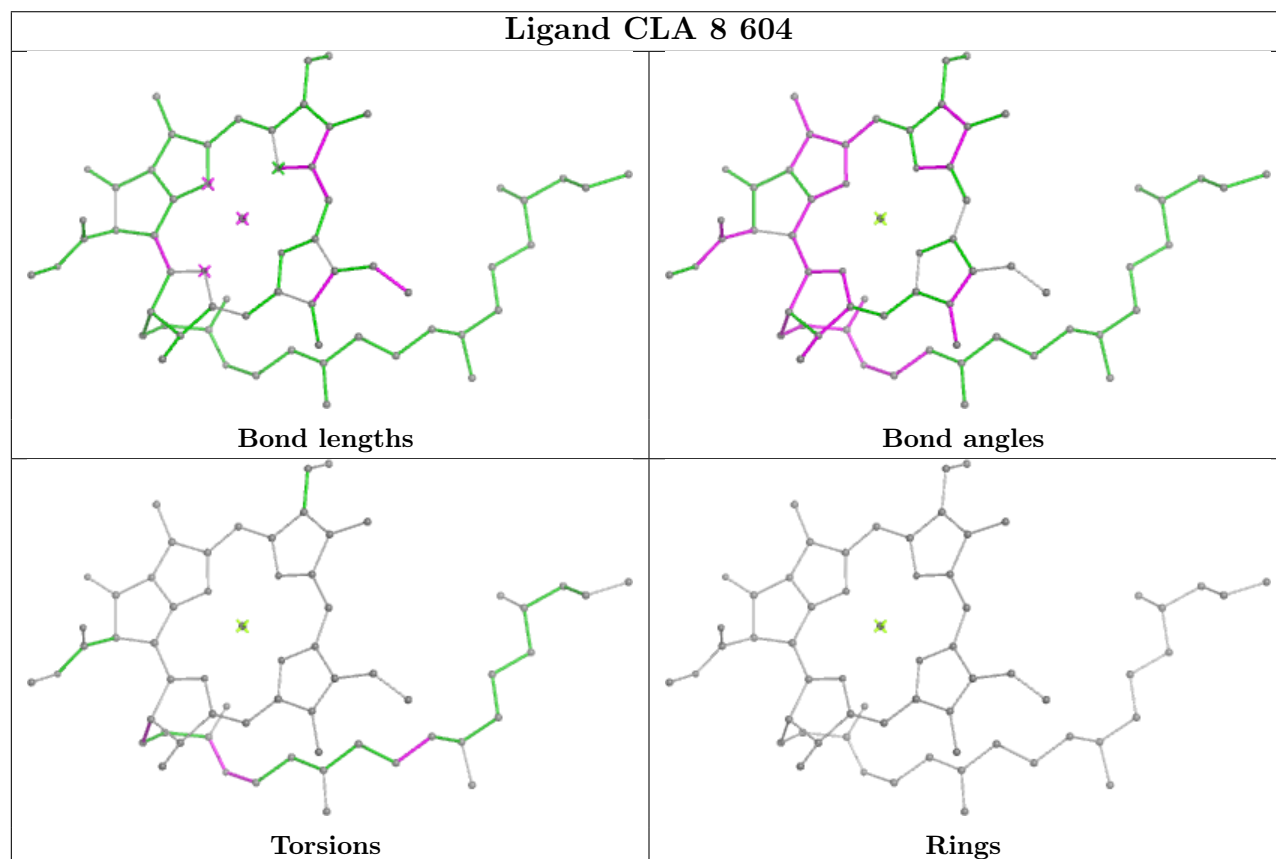


Ligand CLA 5 622

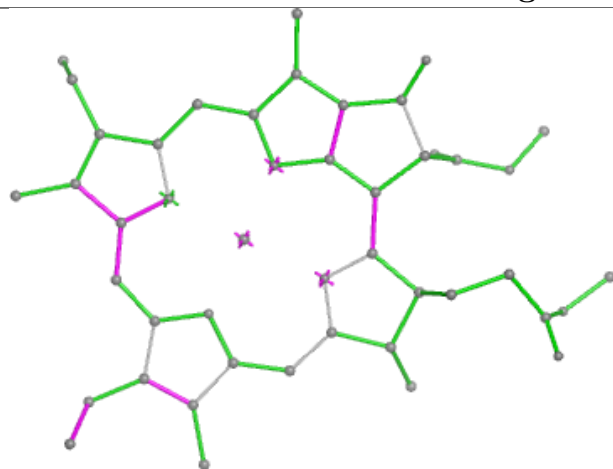


Ligand LUT 8 501

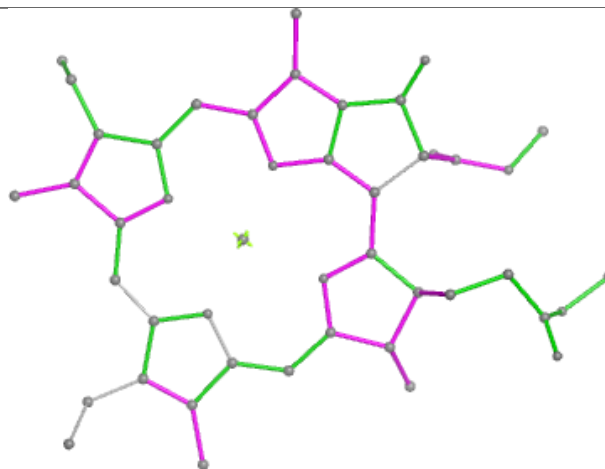


Ligand CLA 3 605**Ligand CLA 8 604**

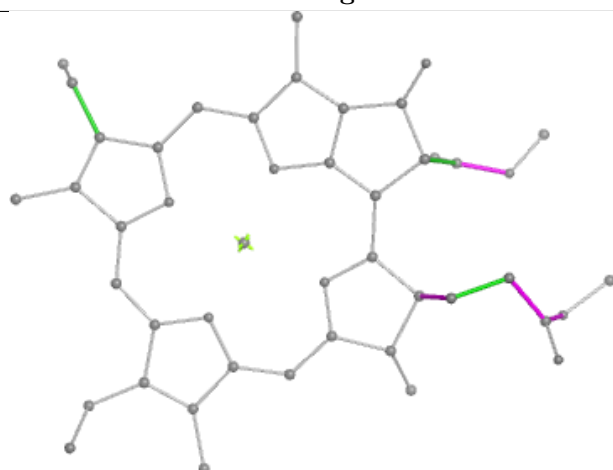
Ligand CLA 1 613



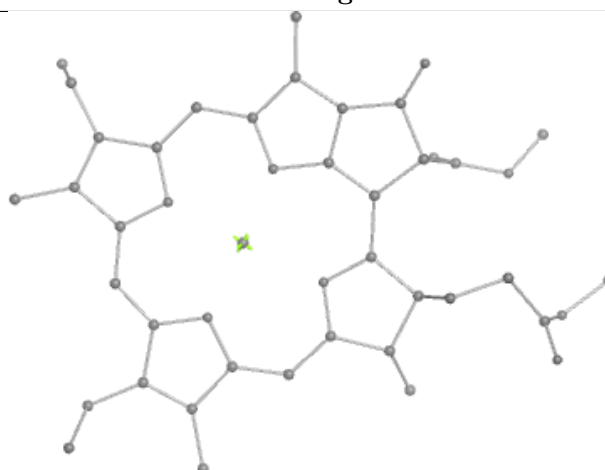
Bond lengths



Bond angles

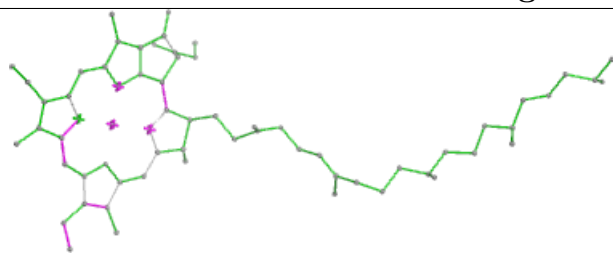


Torsions

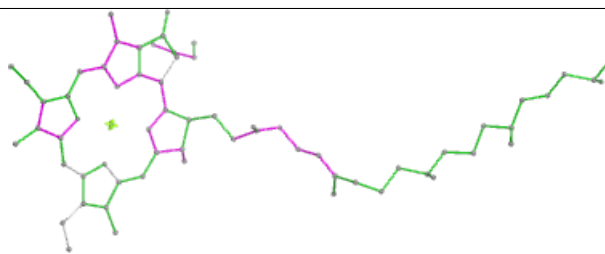


Rings

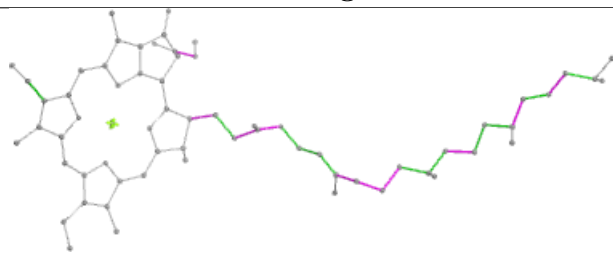
Ligand CLA 5 618



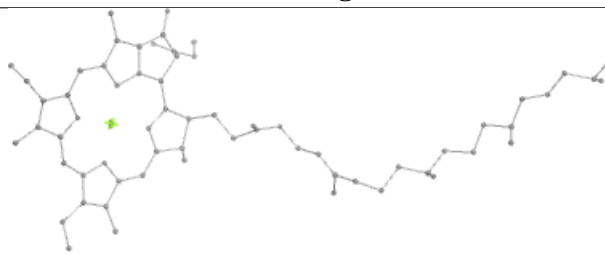
Bond lengths



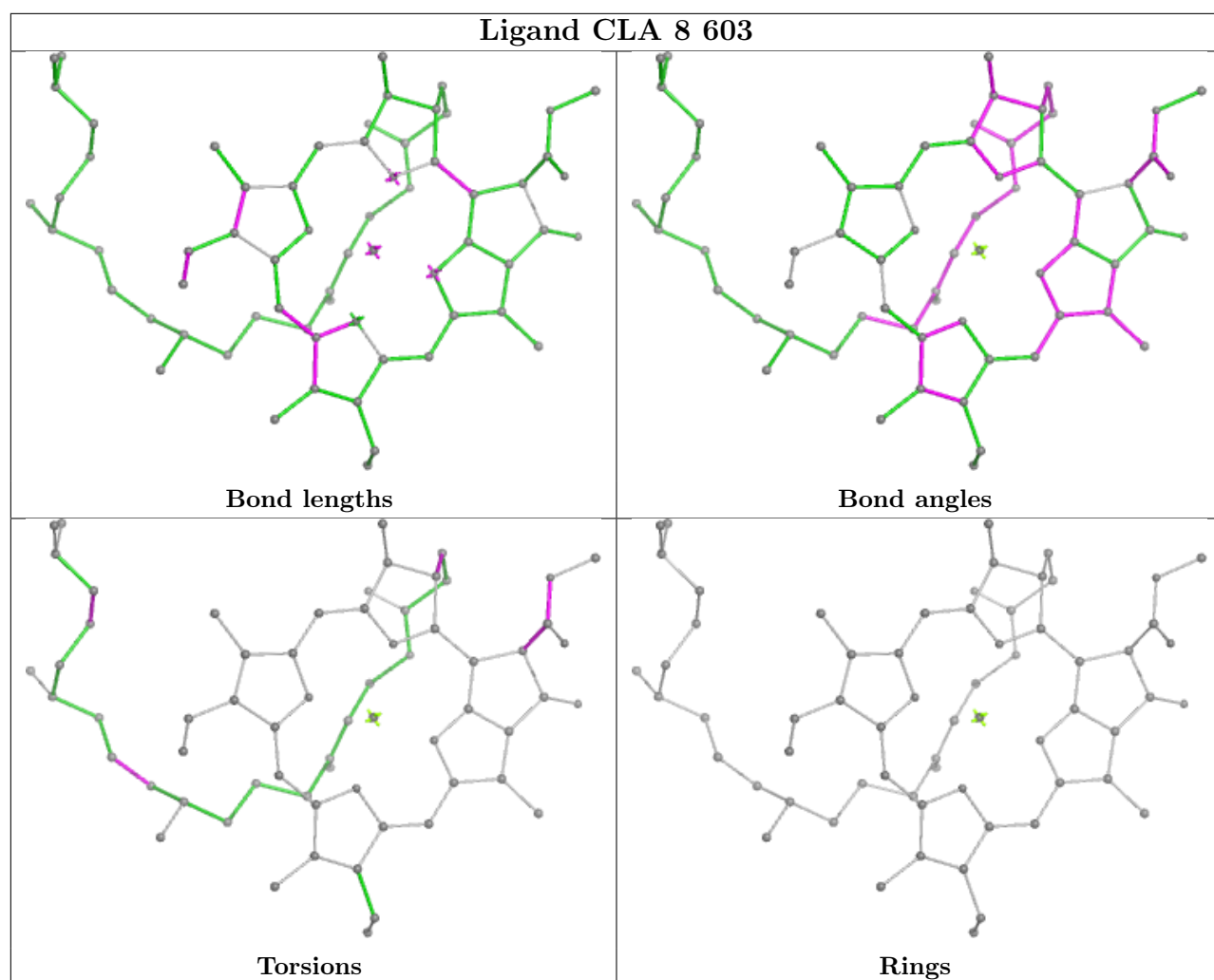
Bond angles



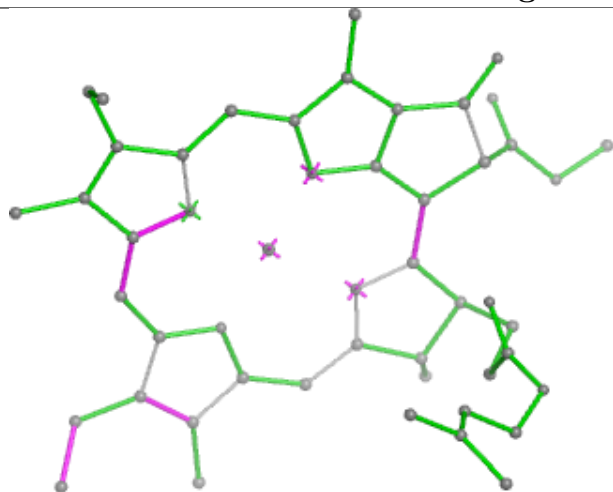
Torsions



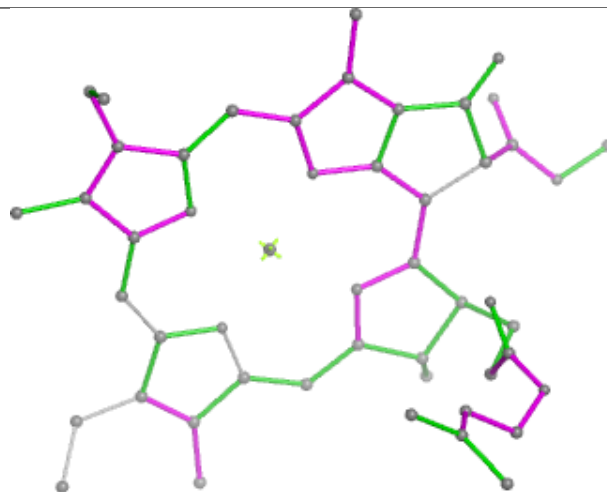
Rings



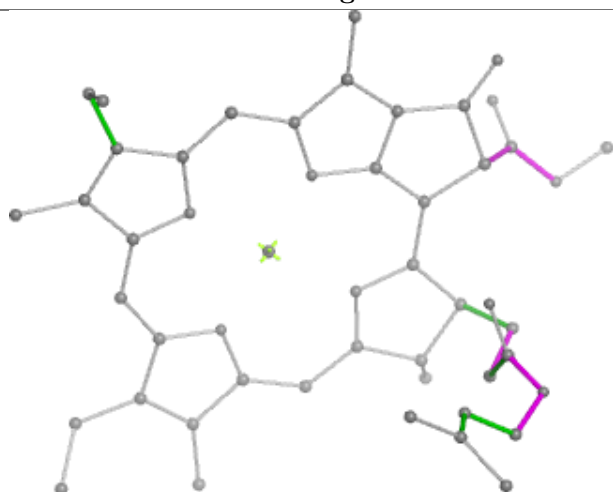
Ligand CLA 5 606



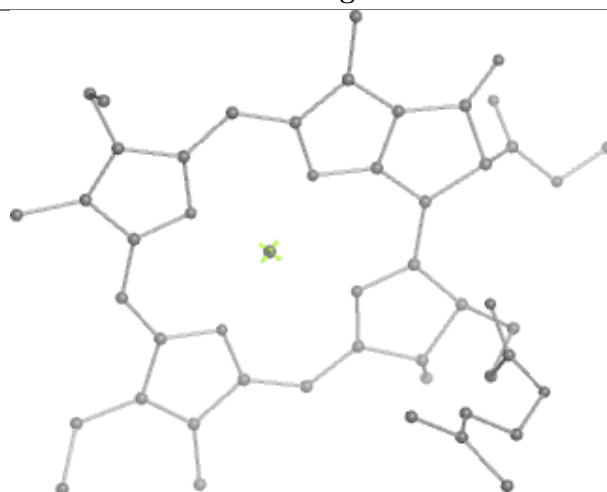
Bond lengths



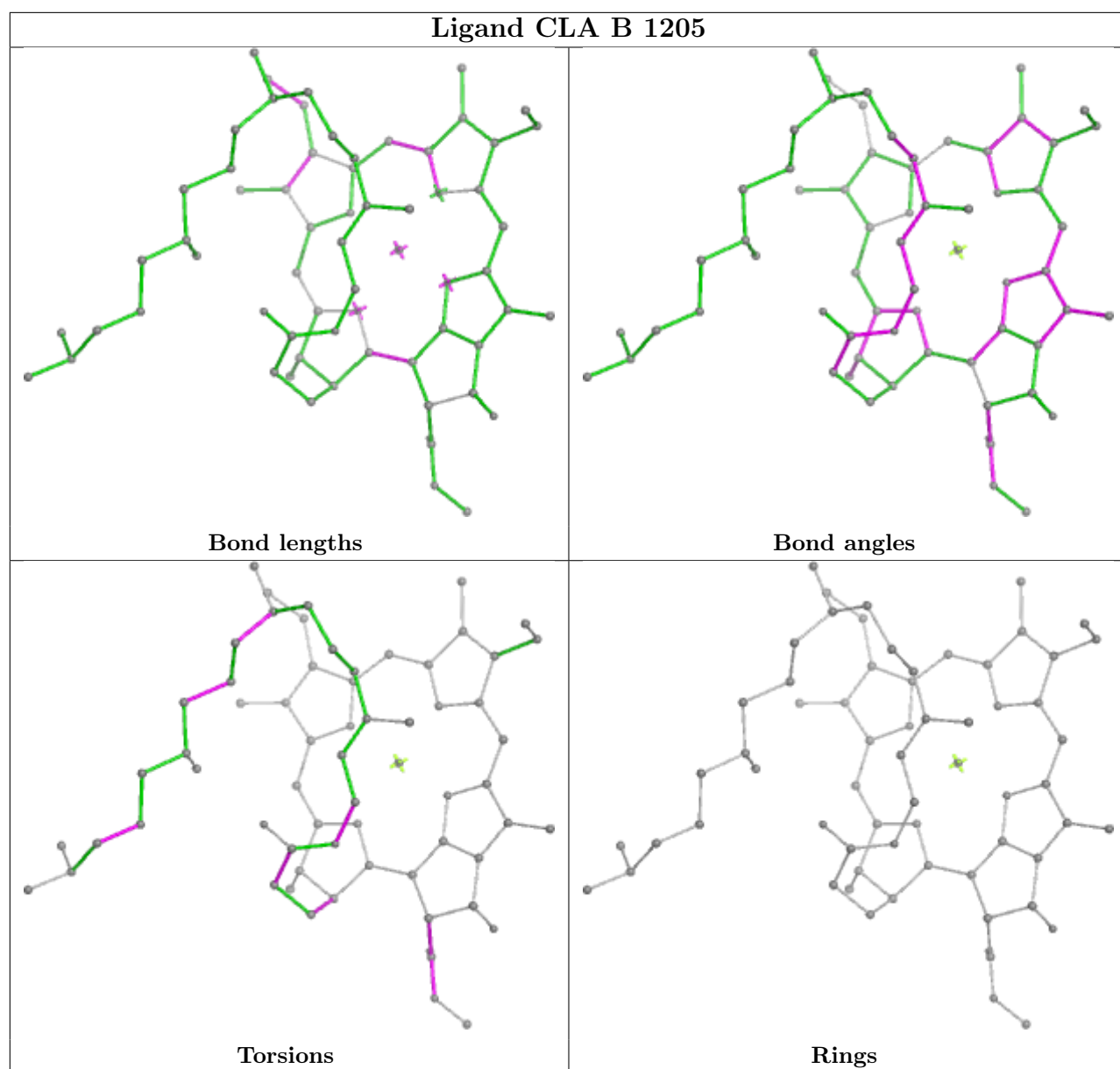
Bond angles



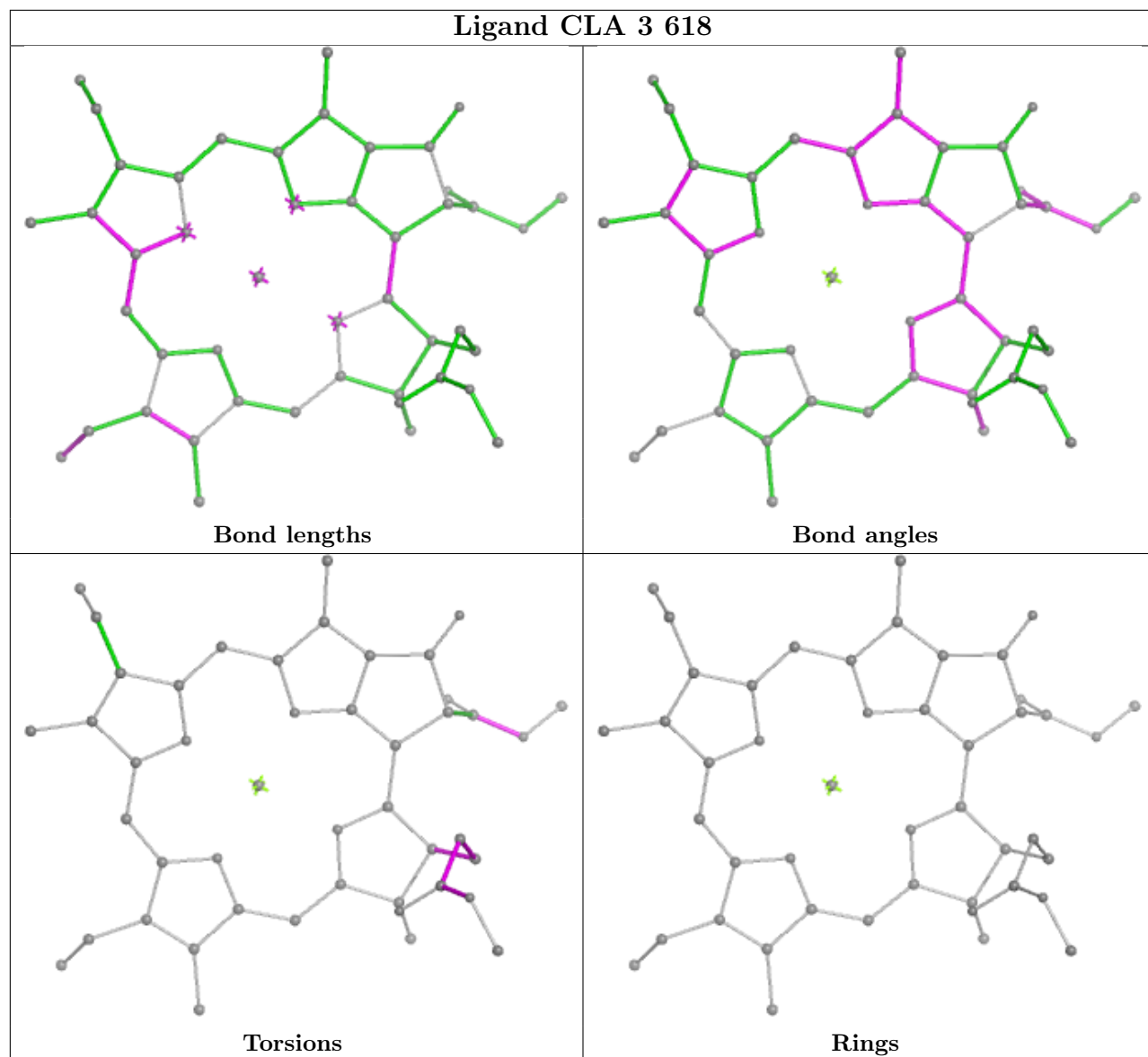
Torsions



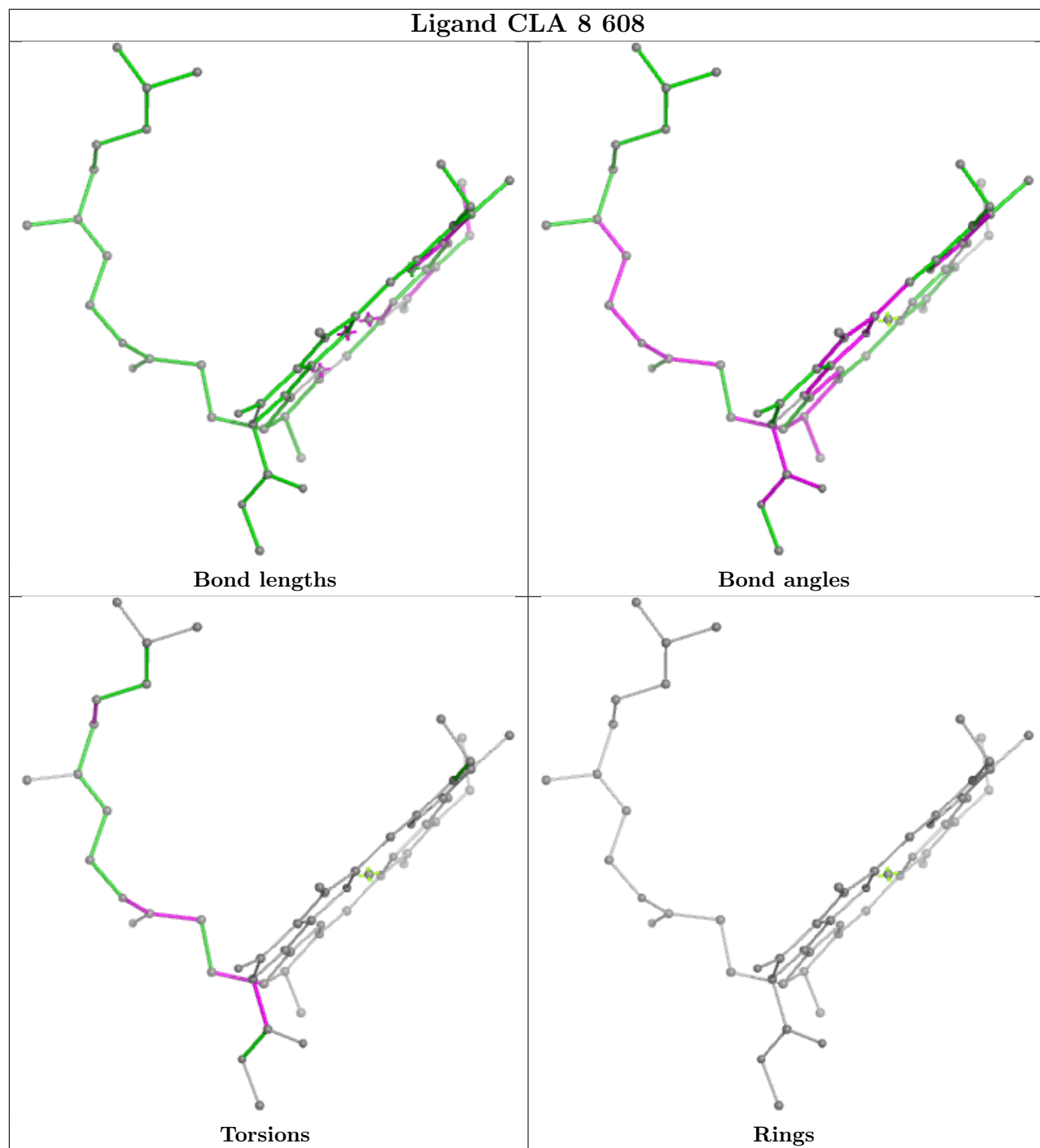
Rings

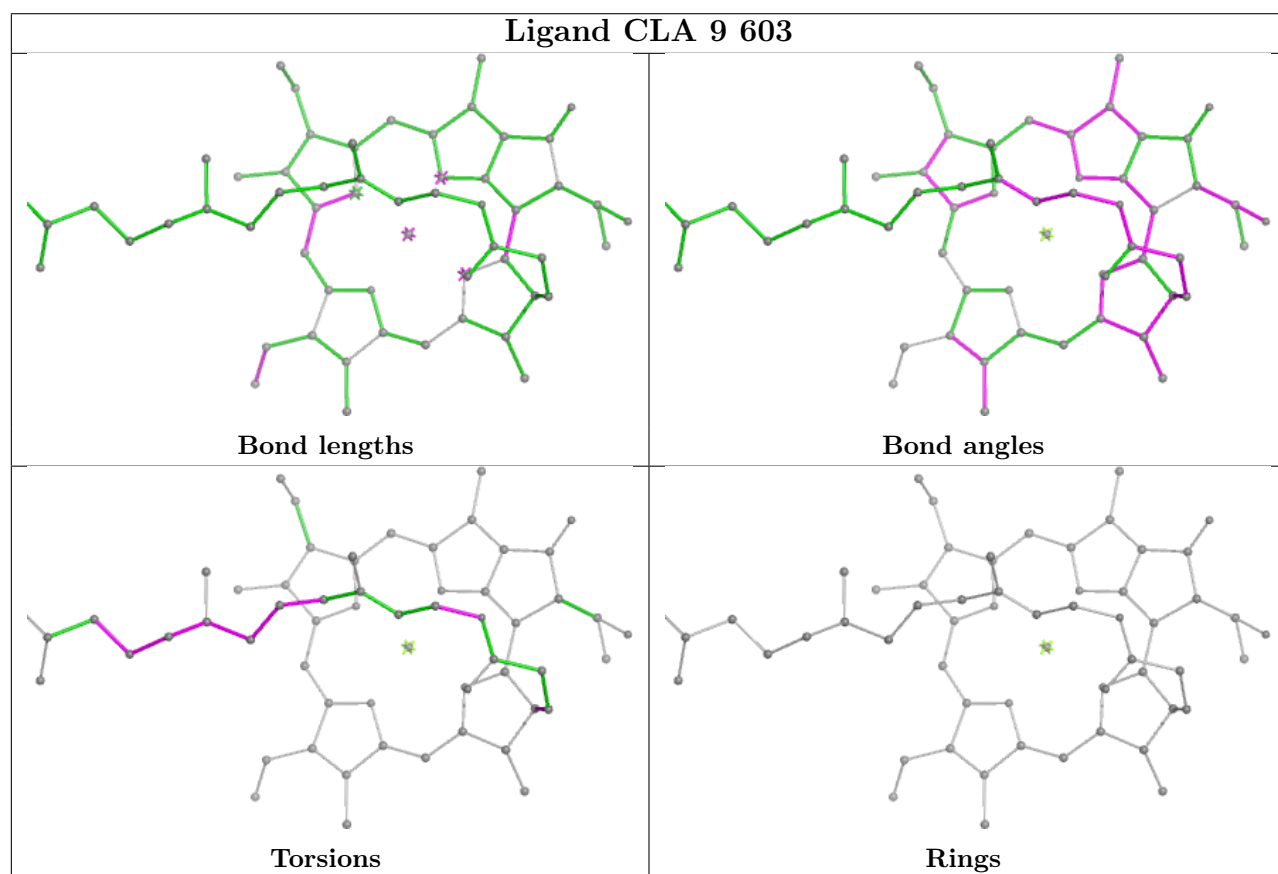
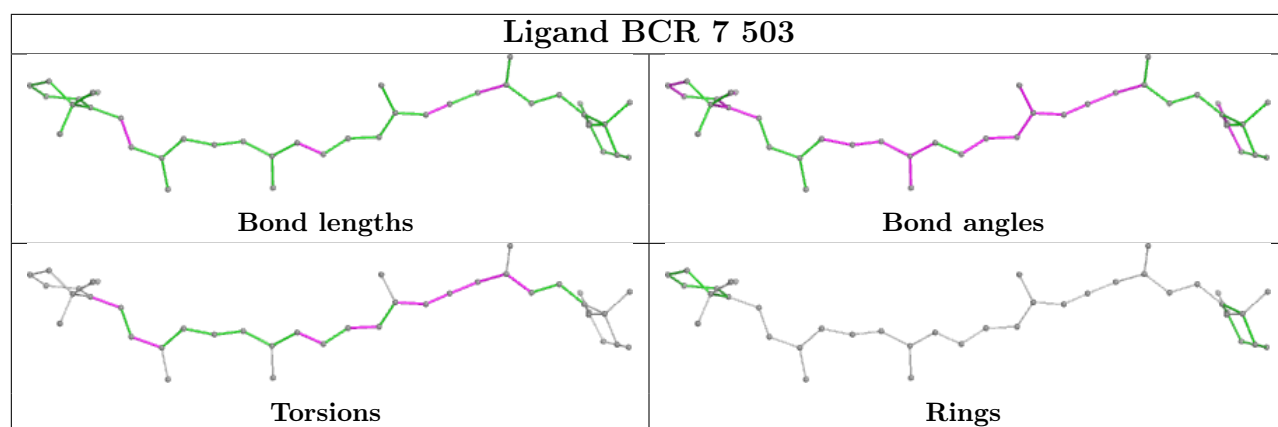


Ligand CLA 3 618

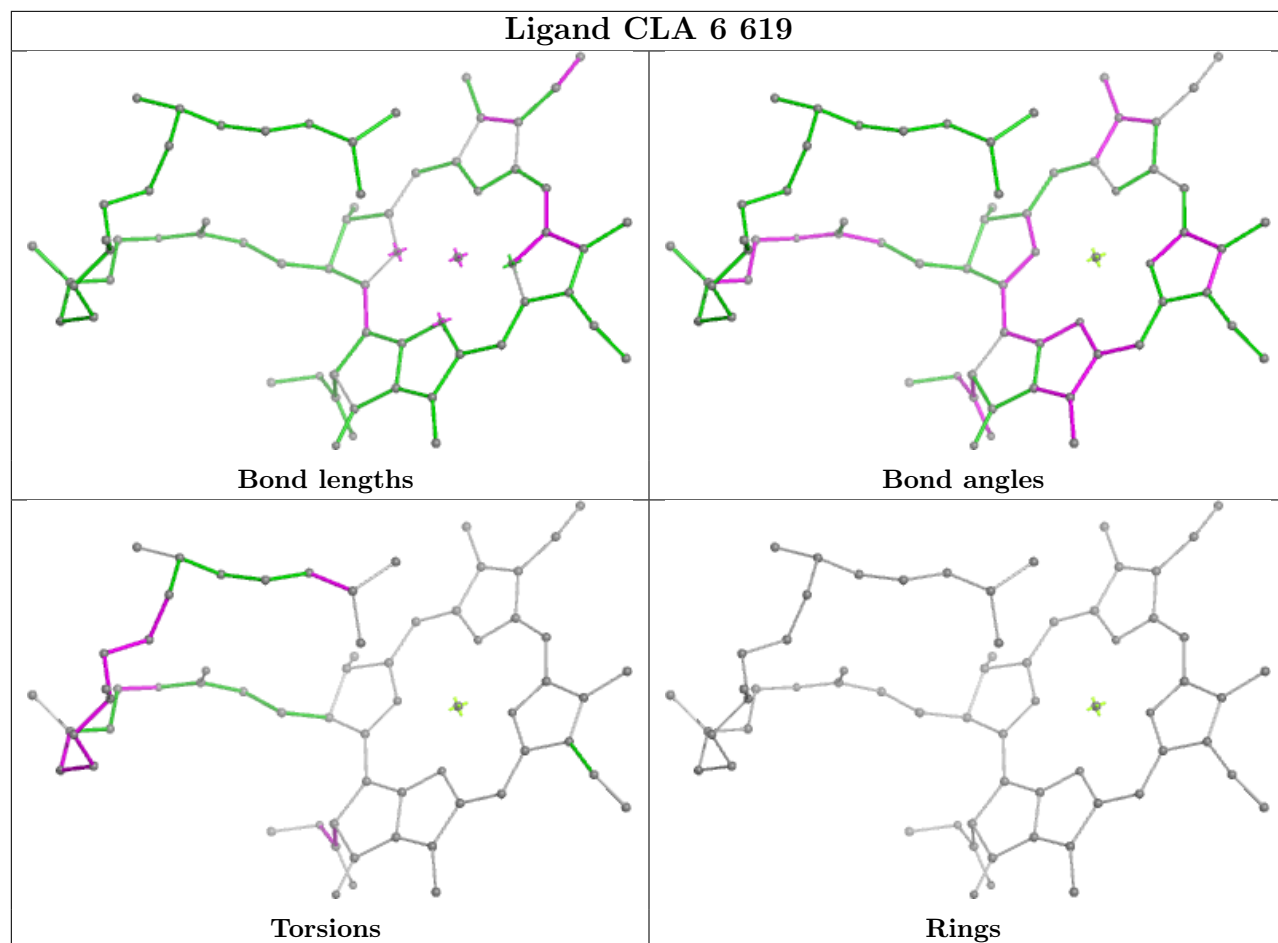


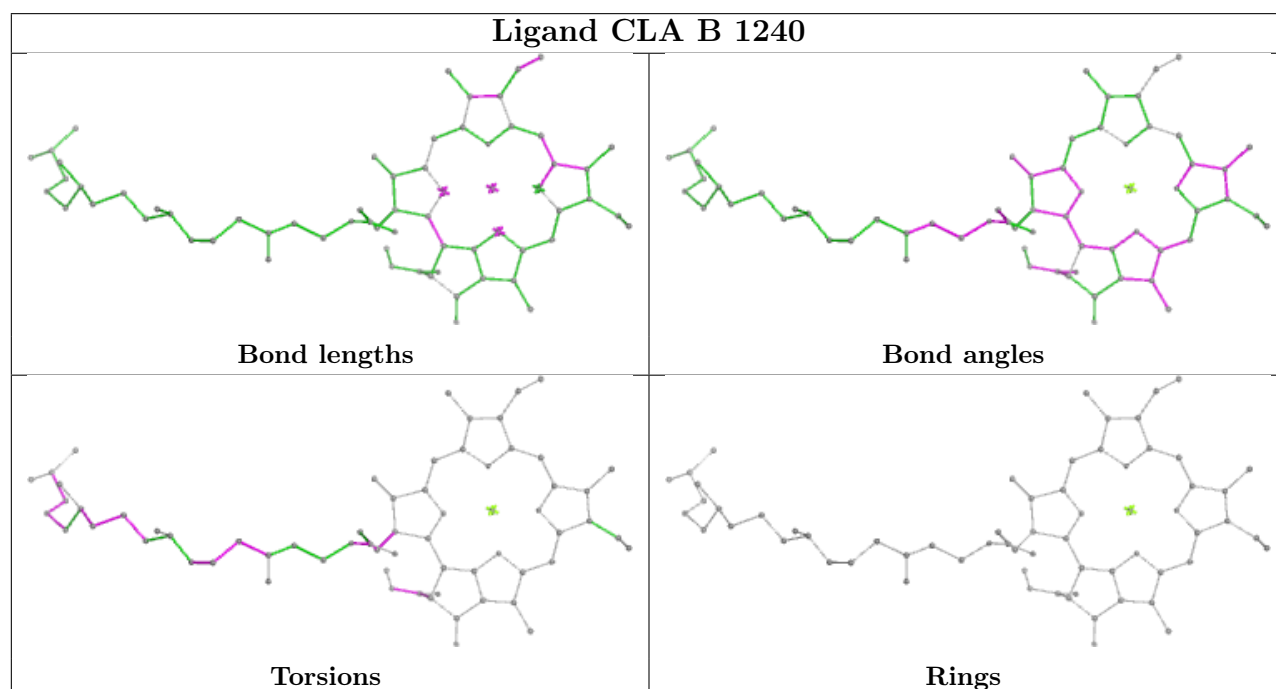
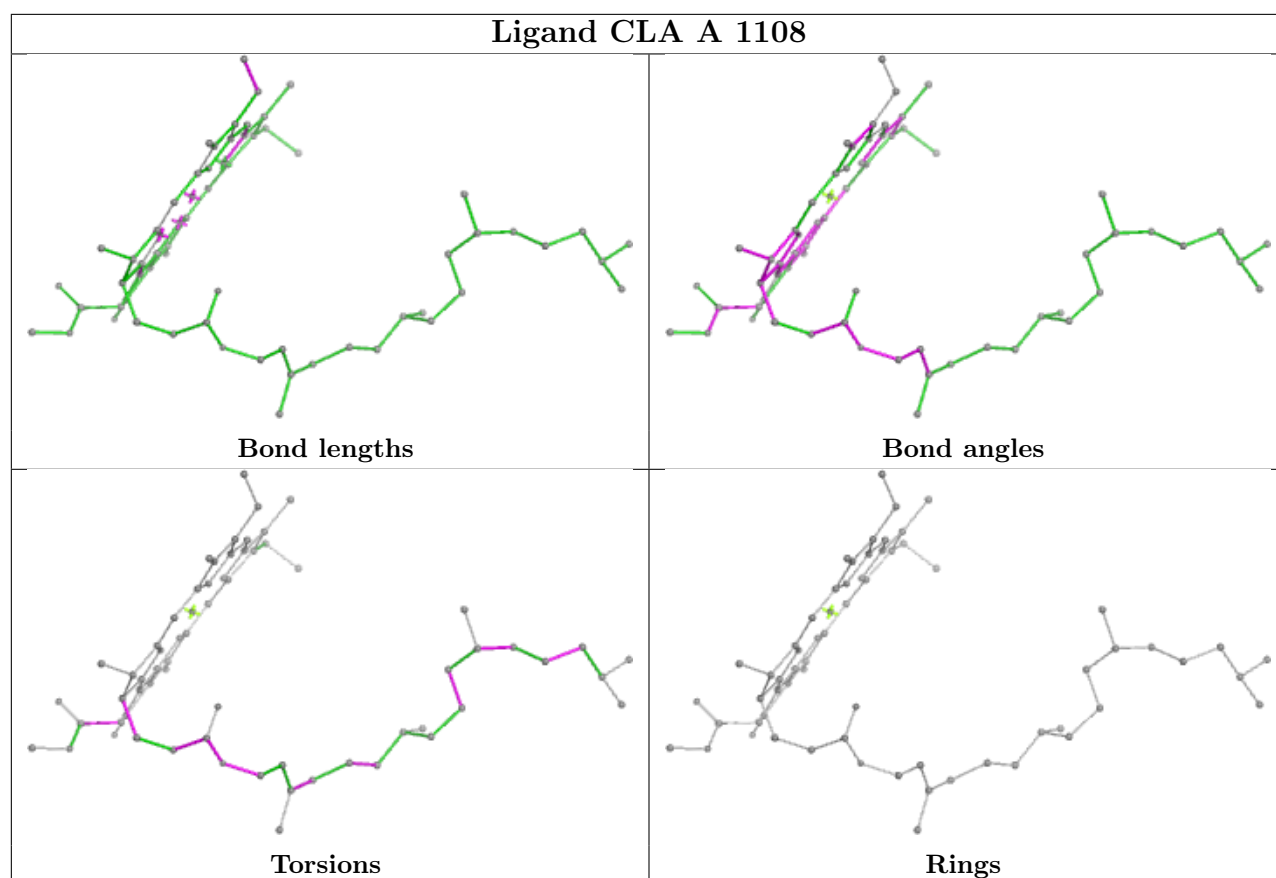
Ligand CLA 8 608

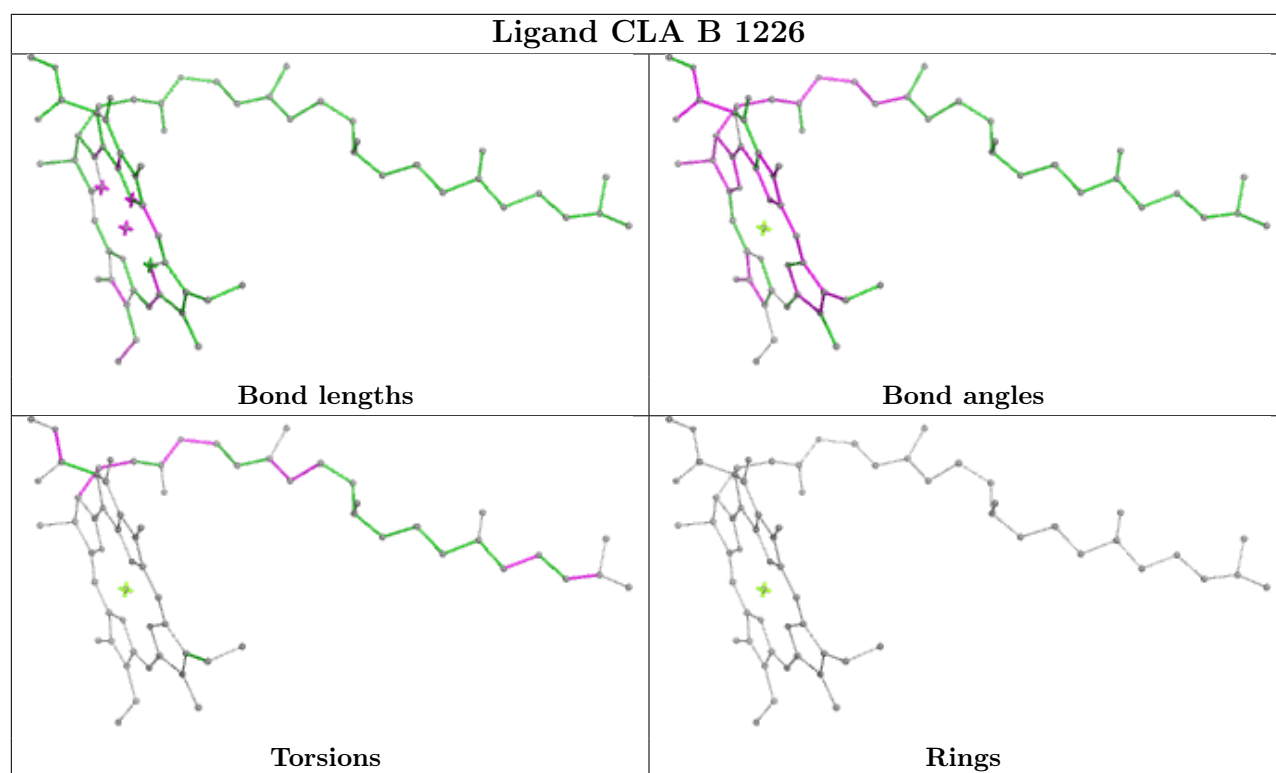


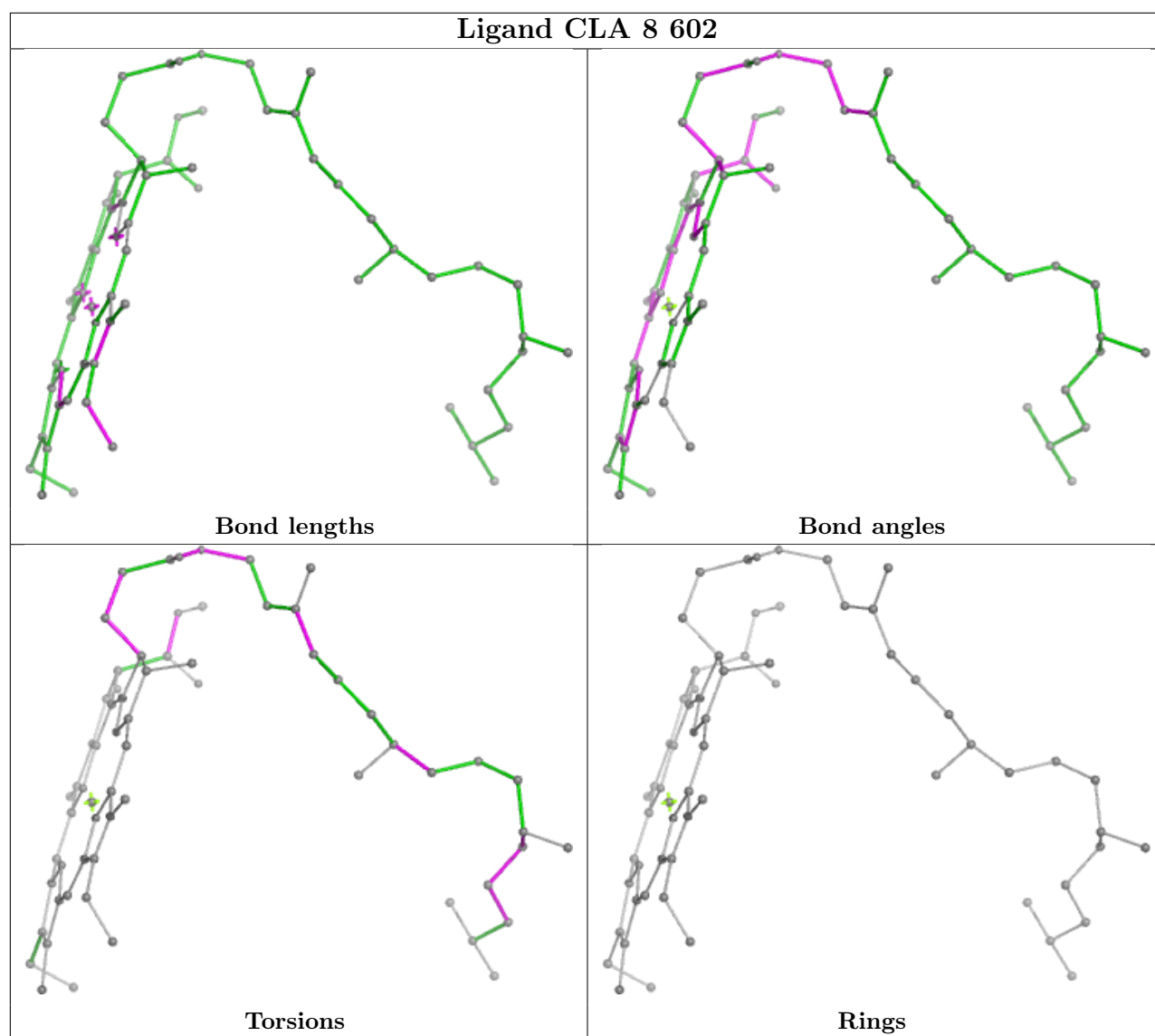


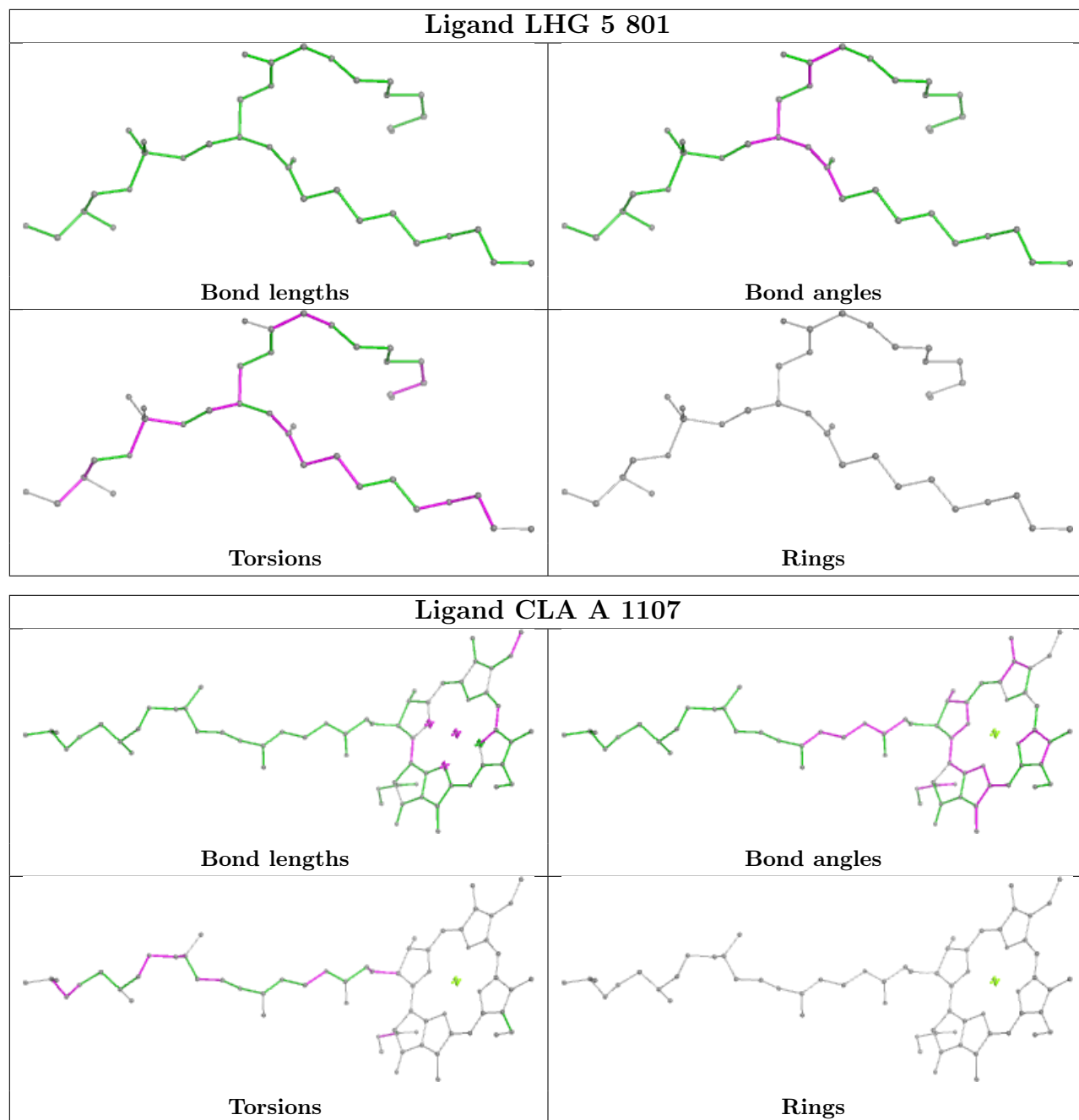
Ligand CLA 6 619



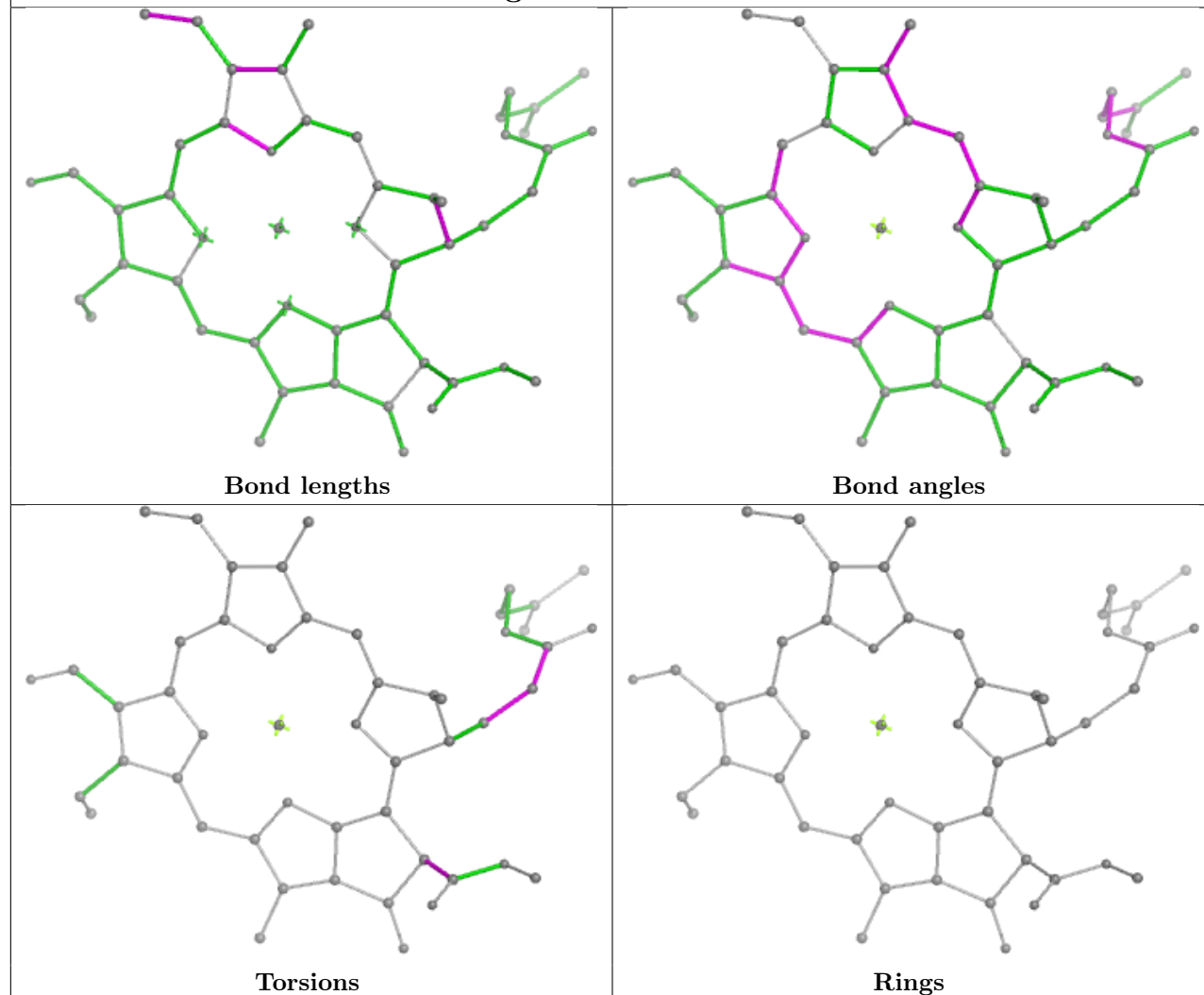




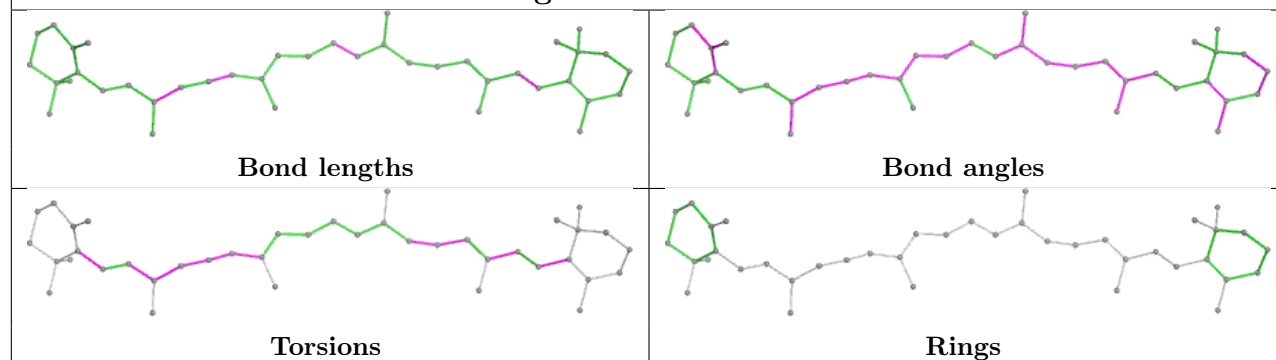


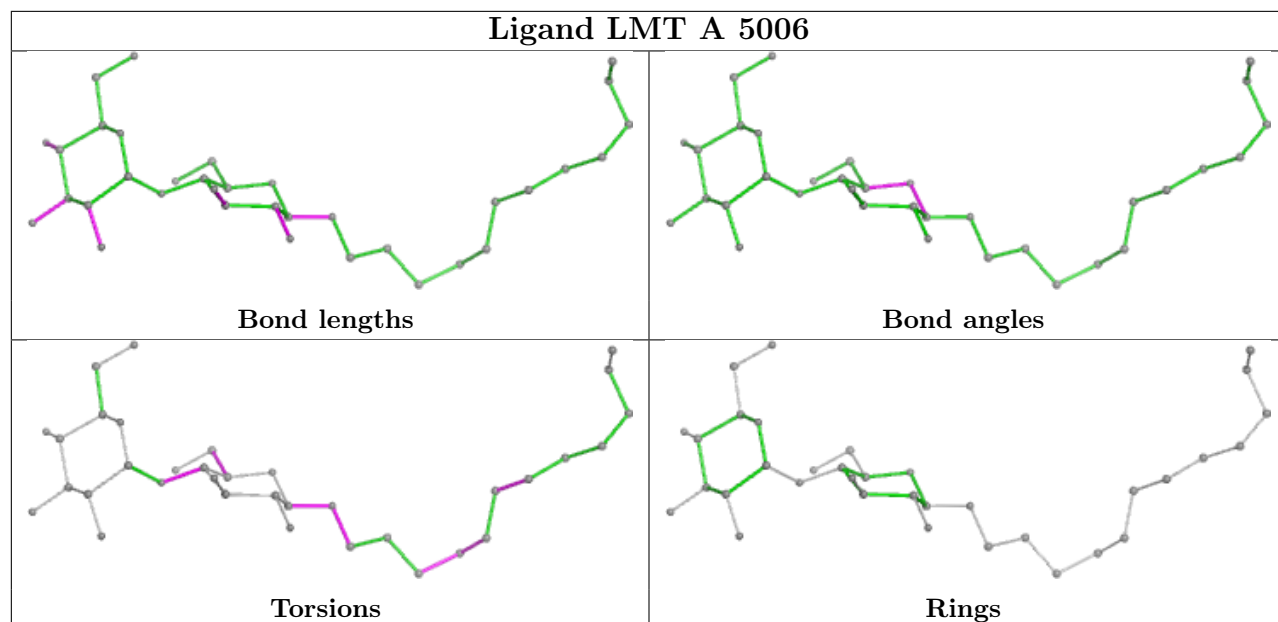
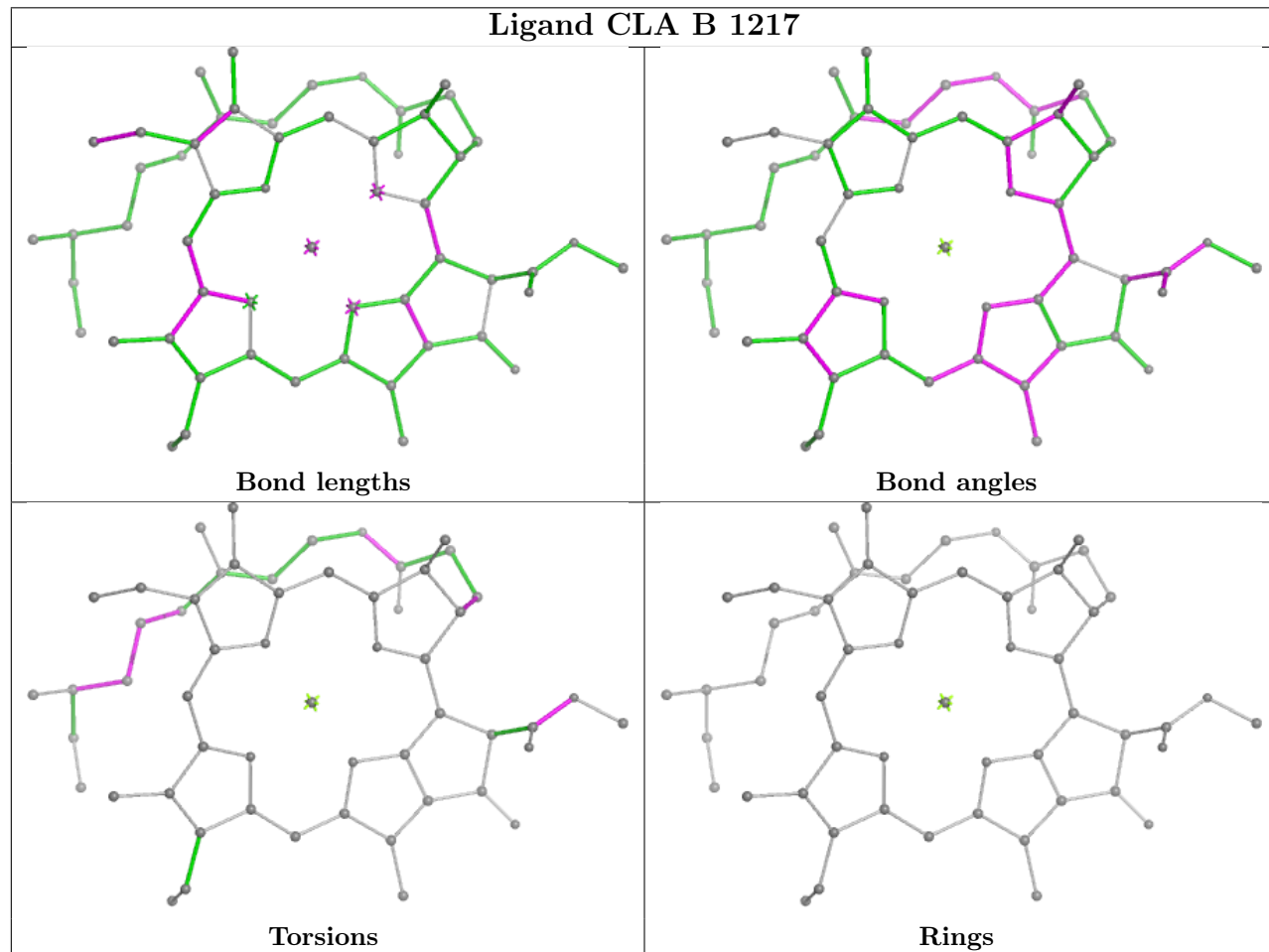


Ligand CHL 2 609

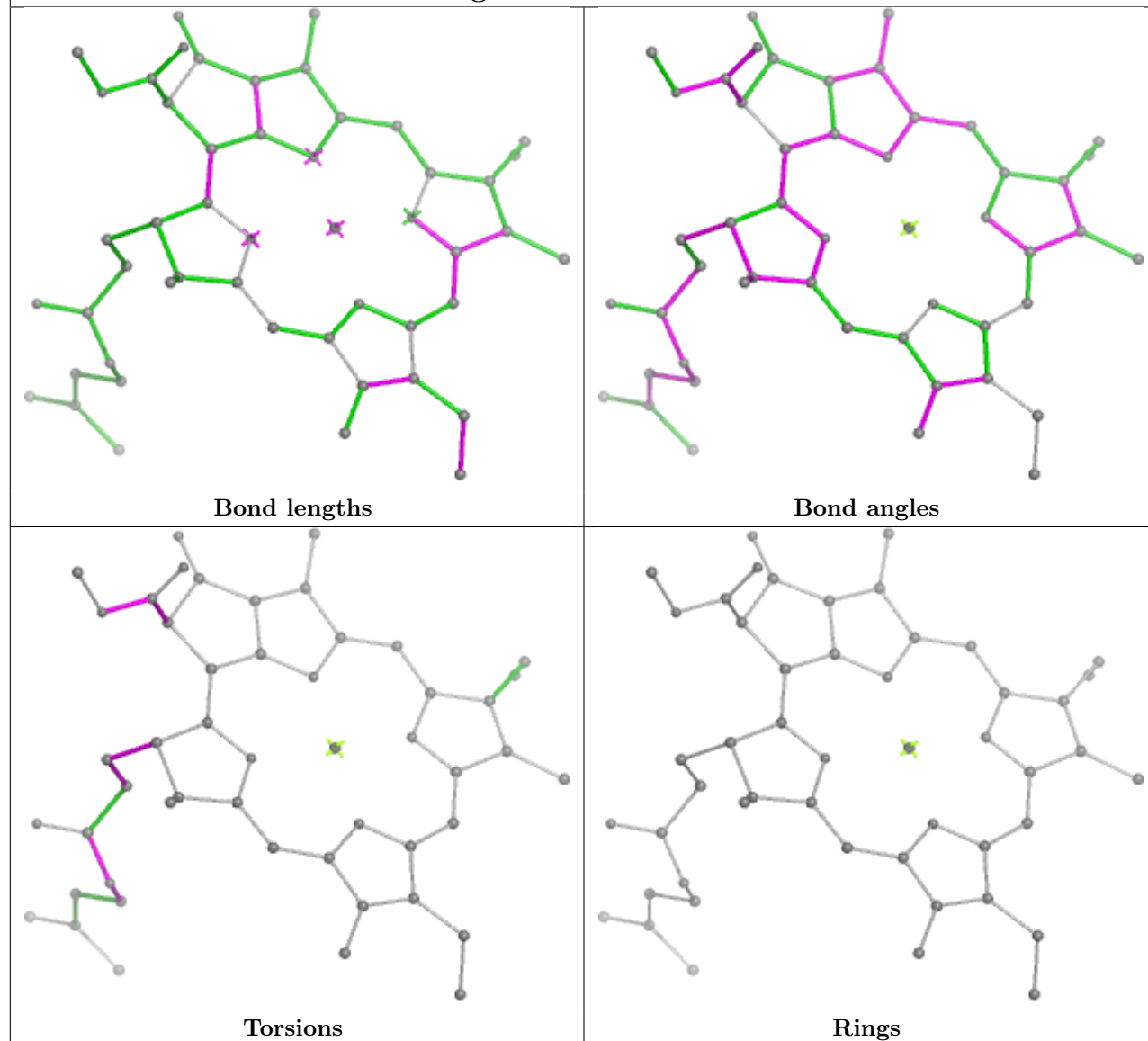


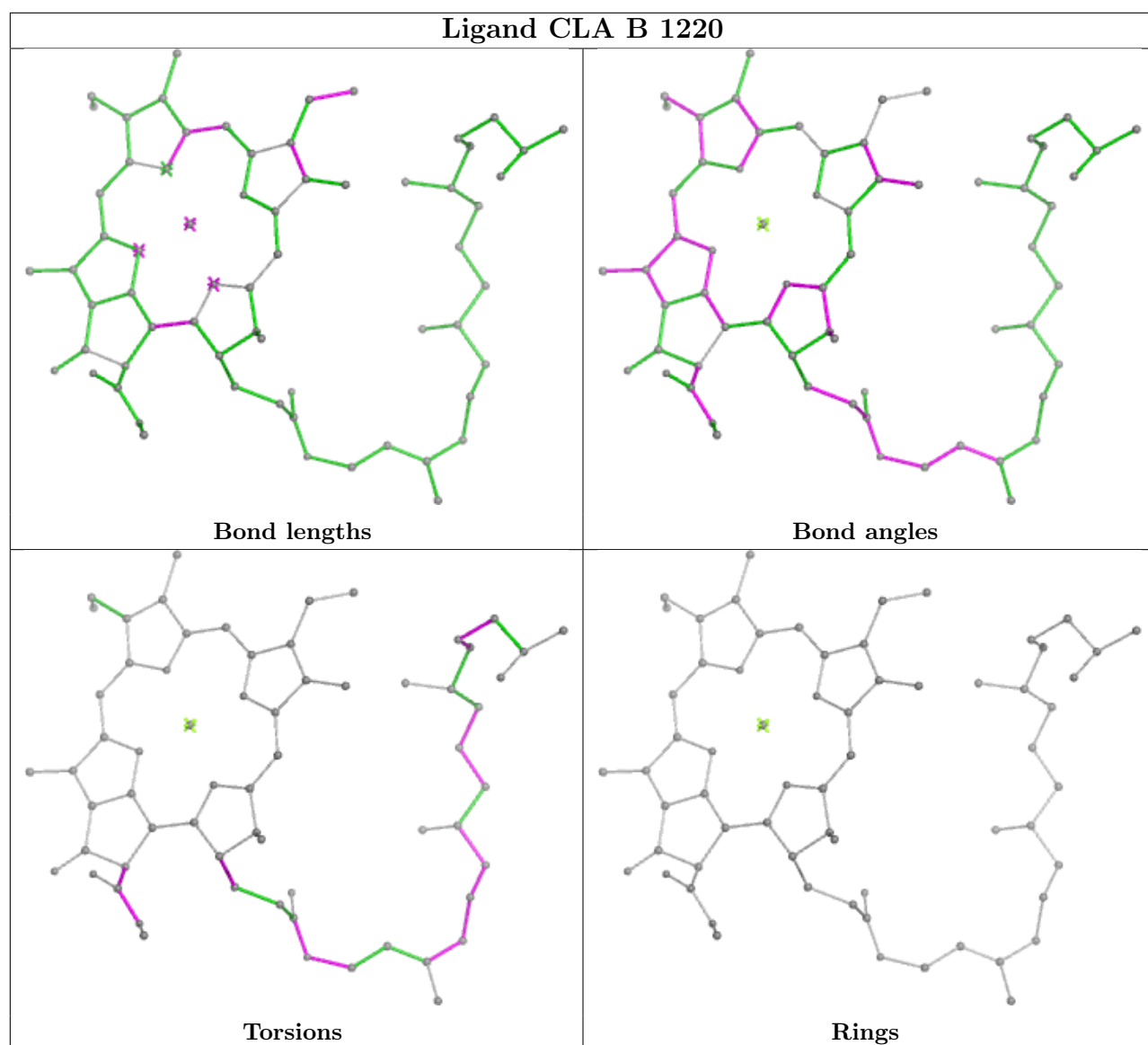
Ligand BCR 3 506

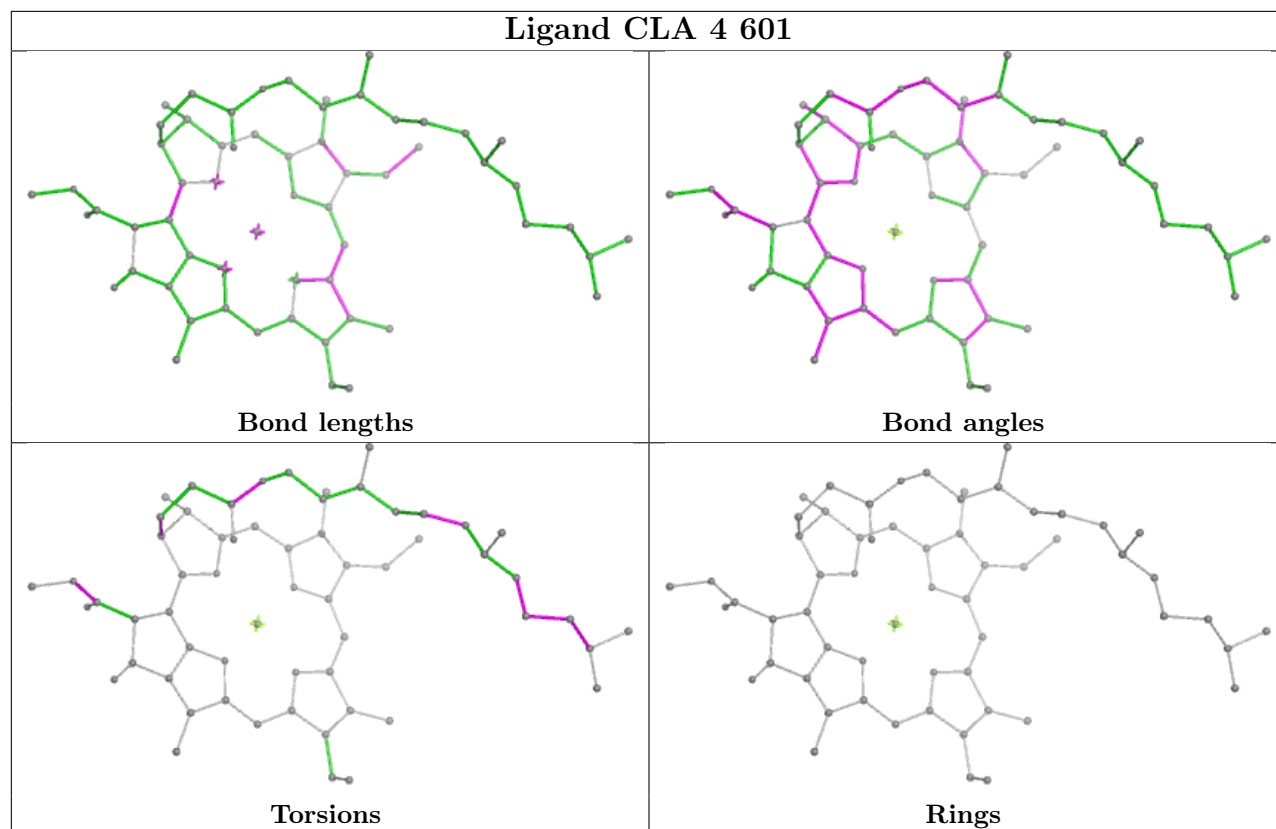


Ligand LMT A 5006**Ligand CLA B 1217**

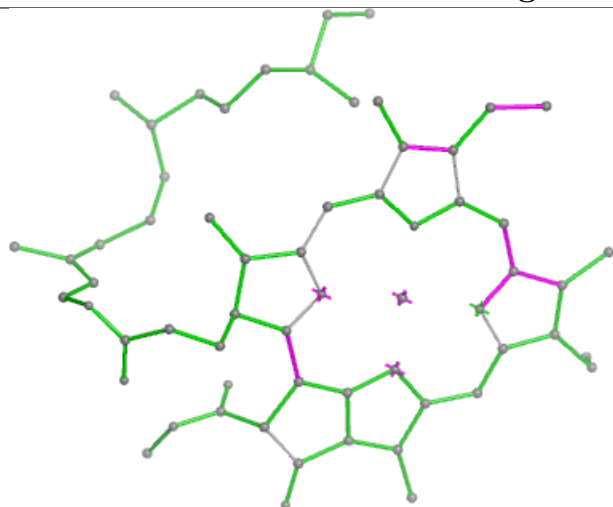
Ligand CLA B 1227



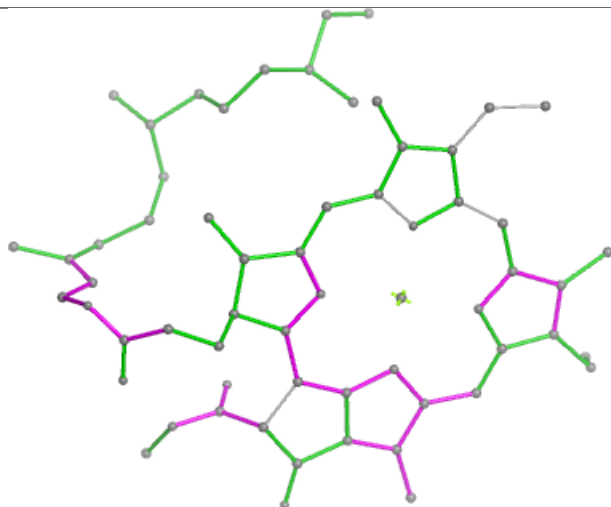




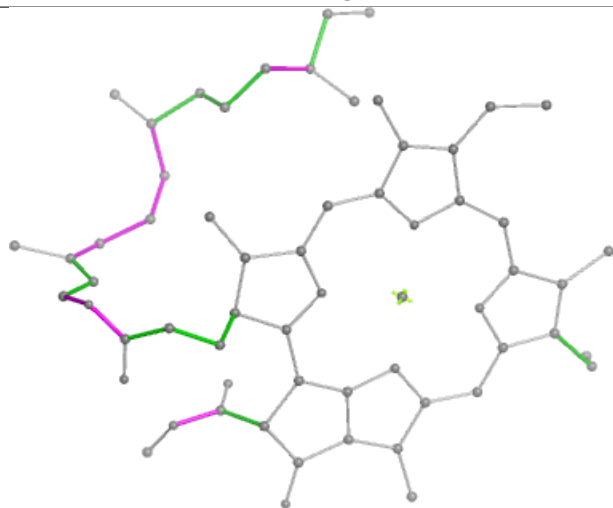
Ligand CLA 5 602



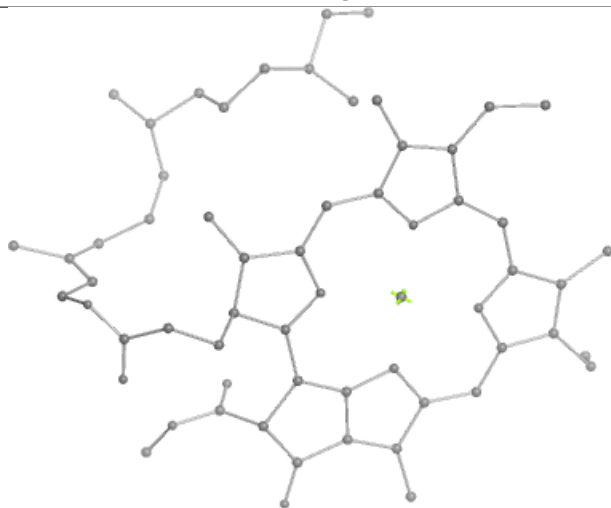
Bond lengths



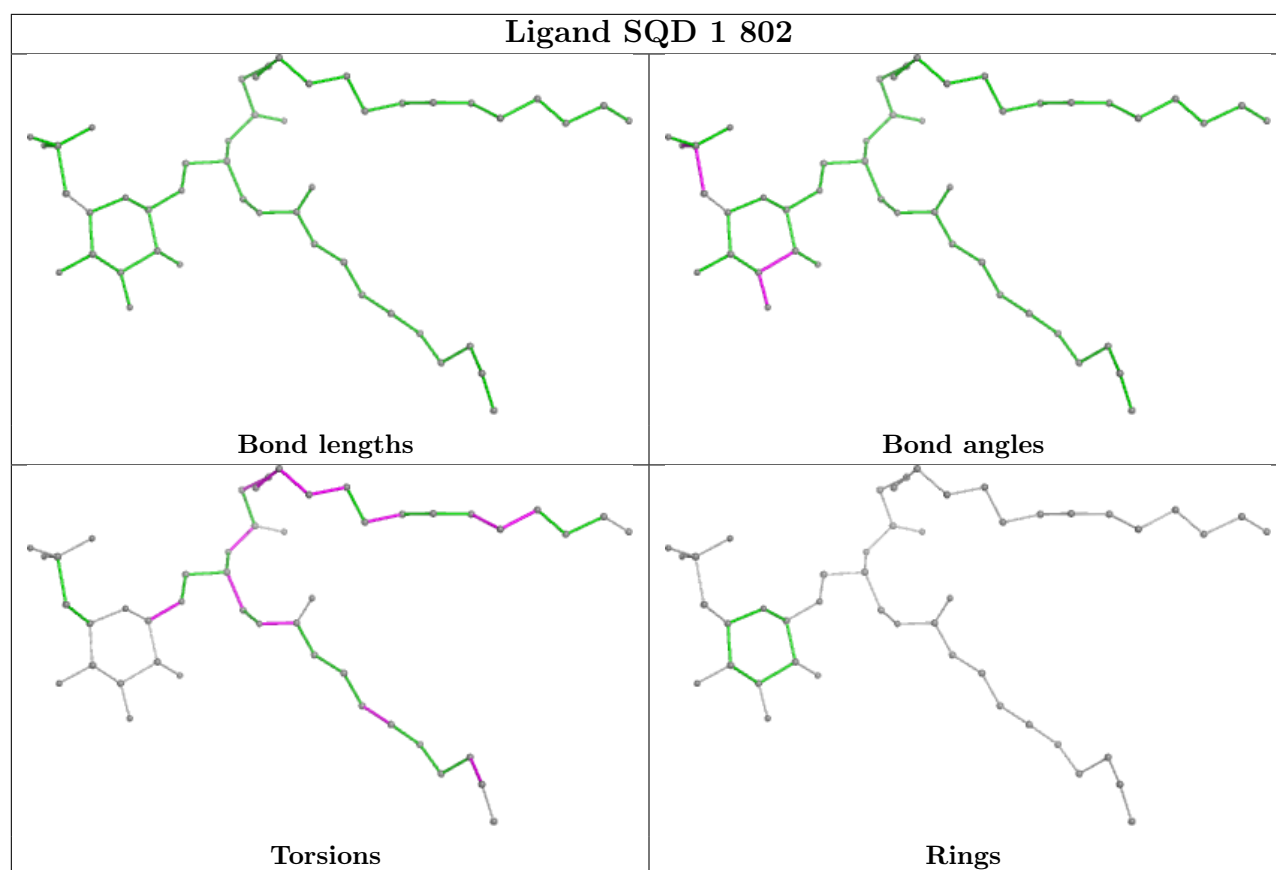
Bond angles

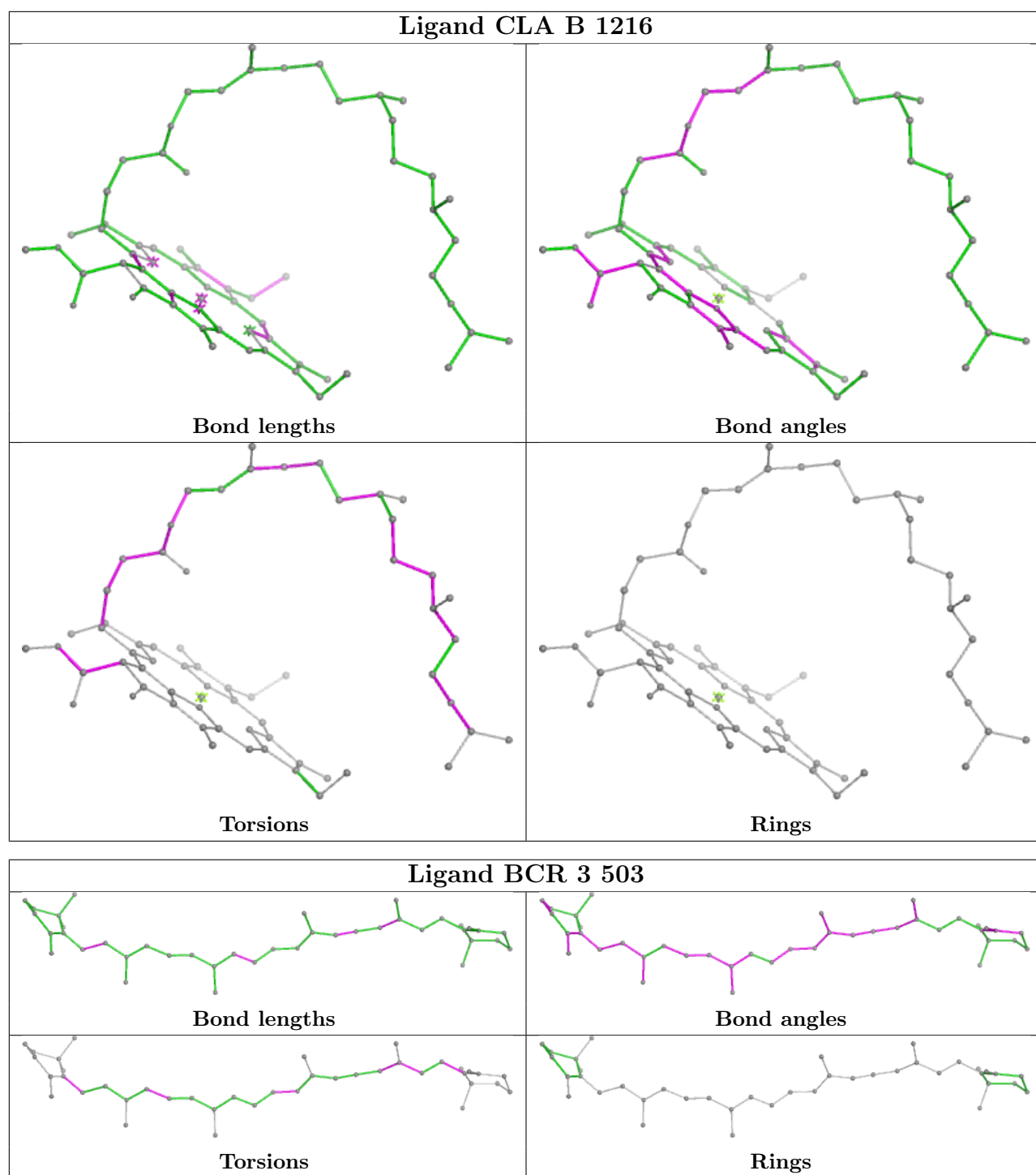


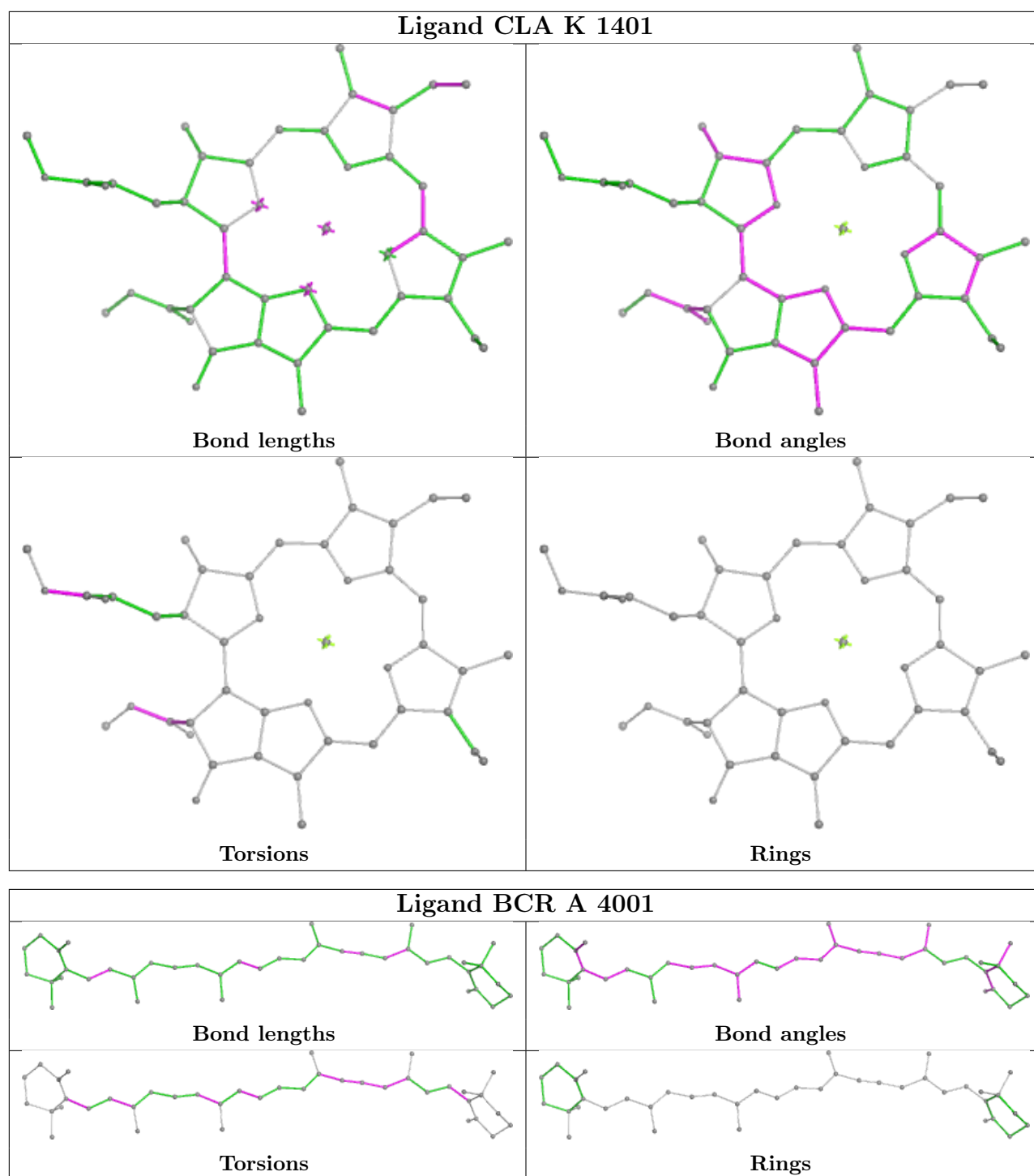
Torsions

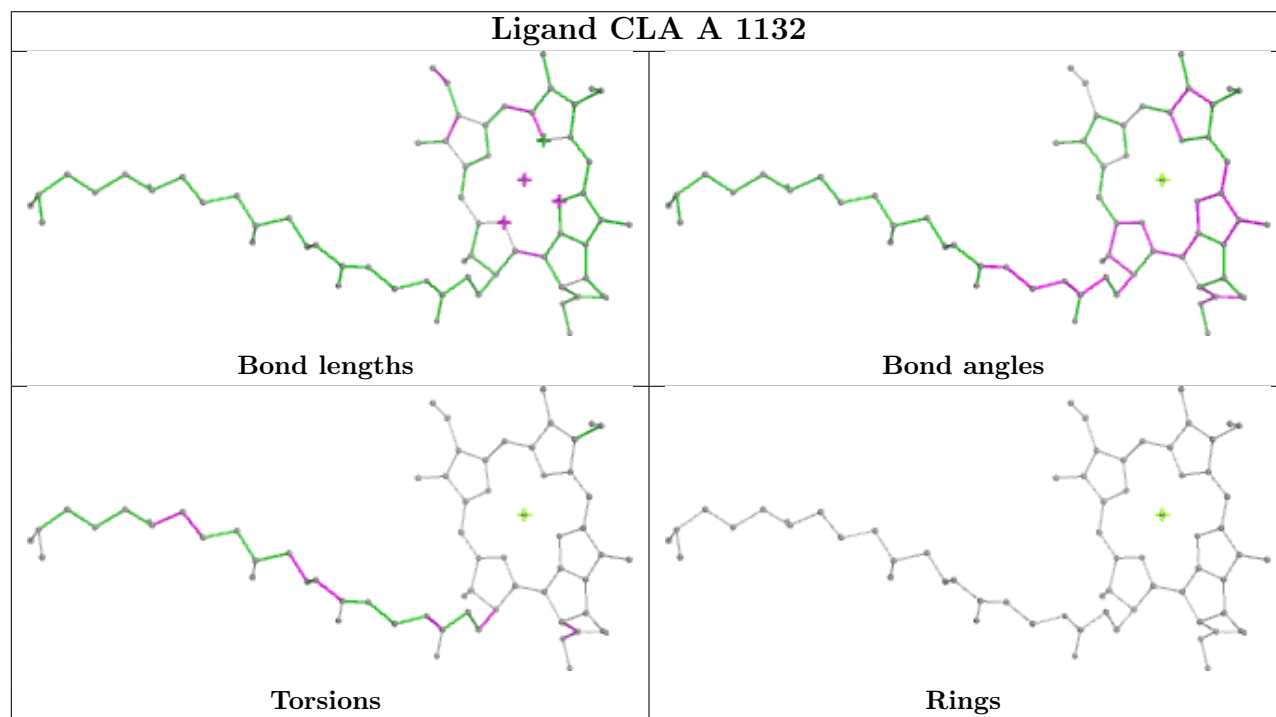
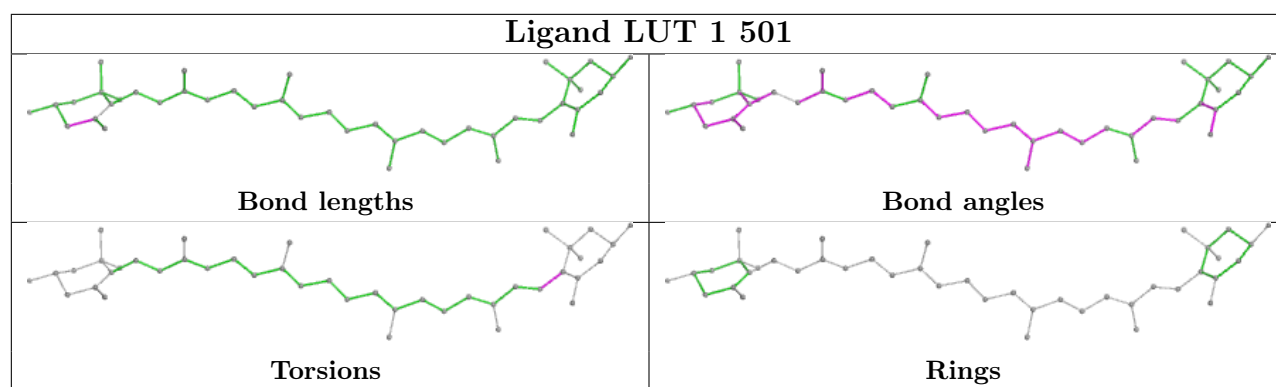


Rings

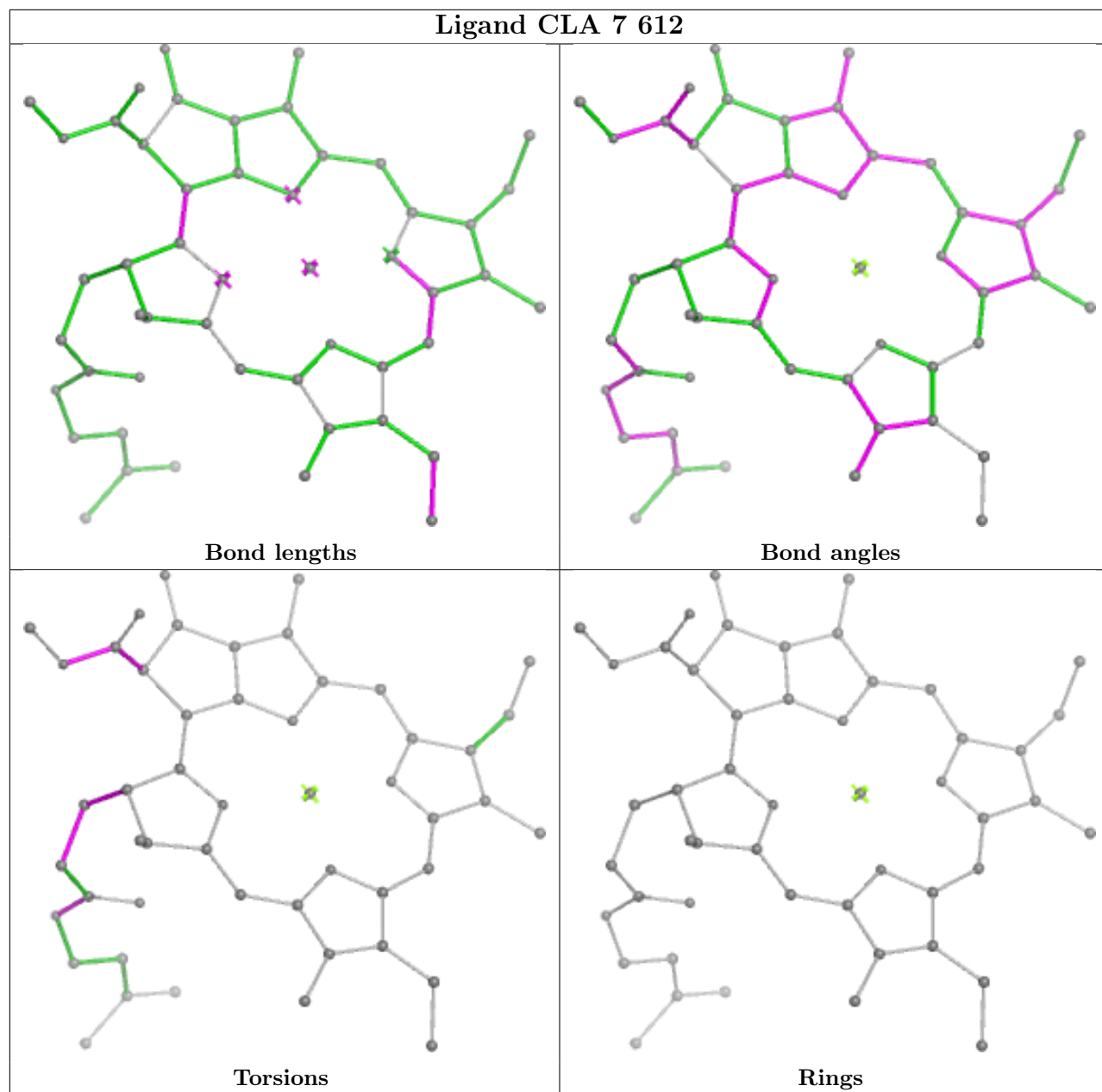


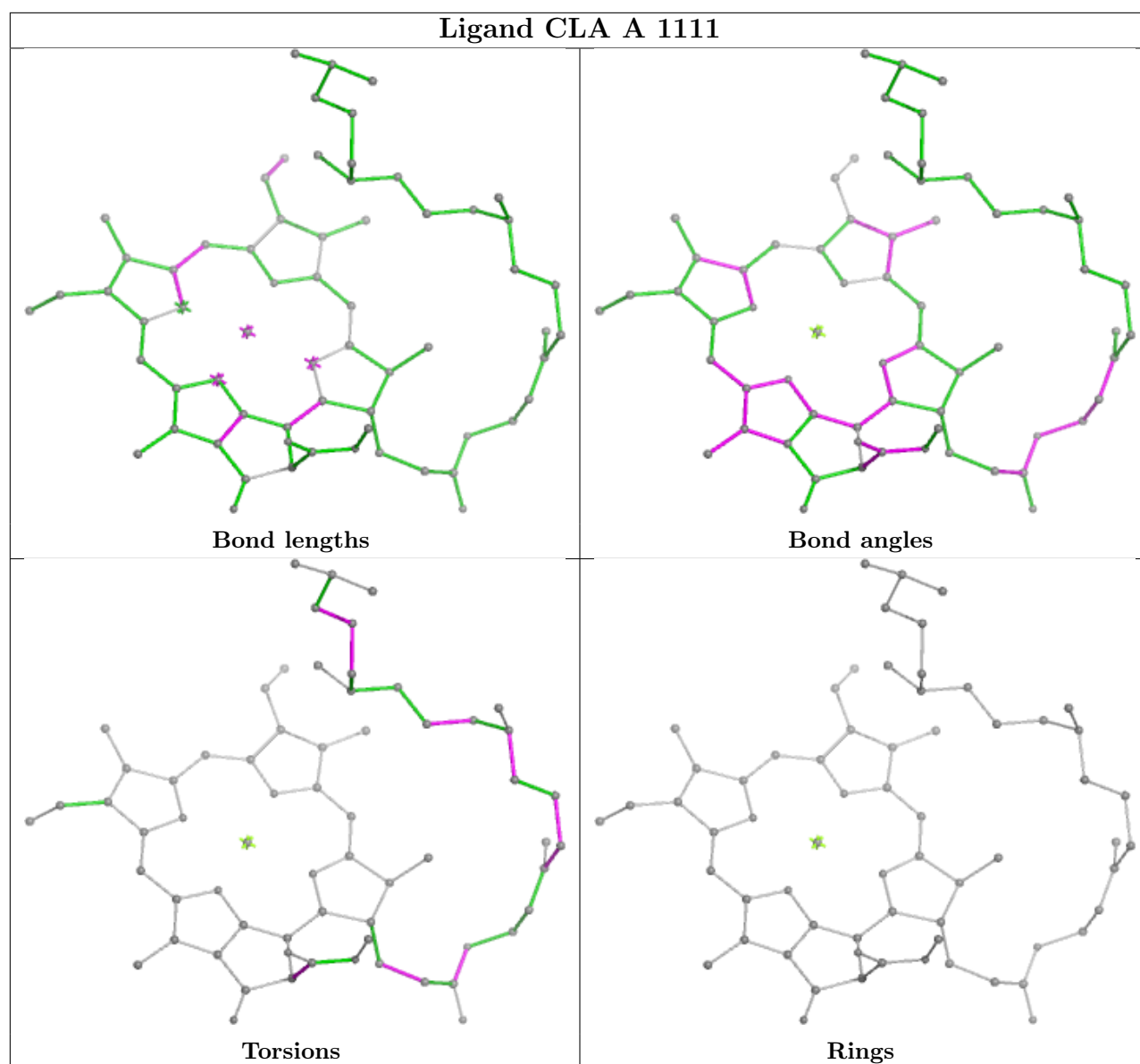


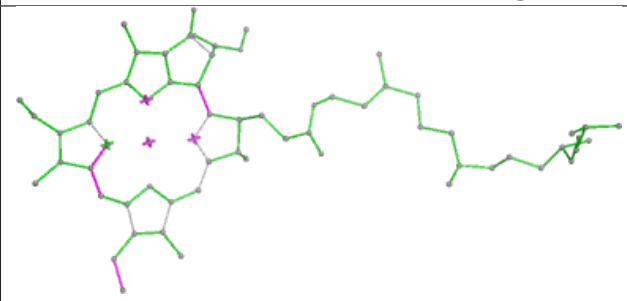
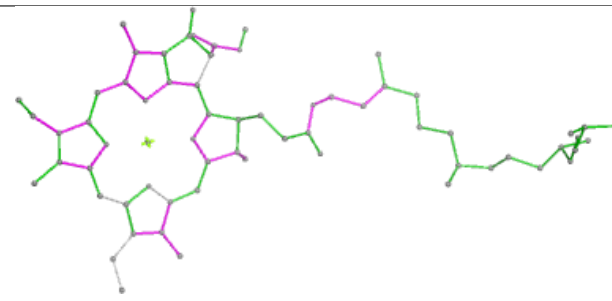
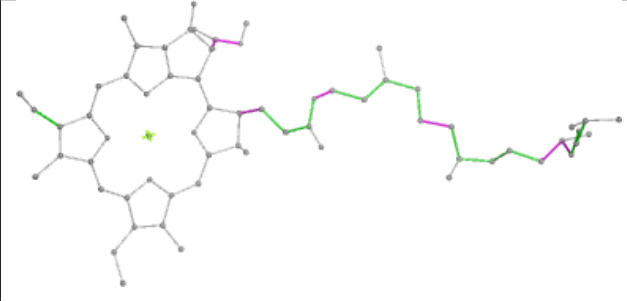
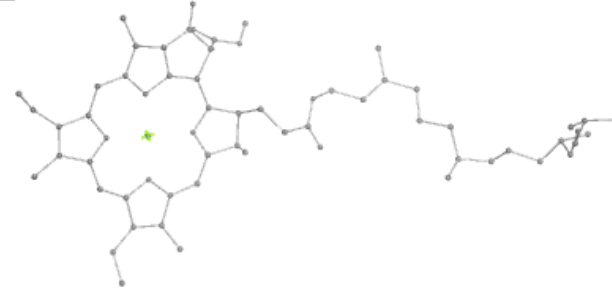


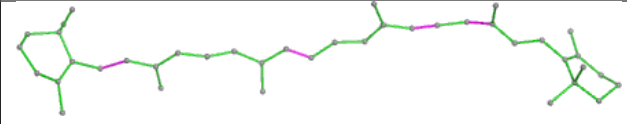
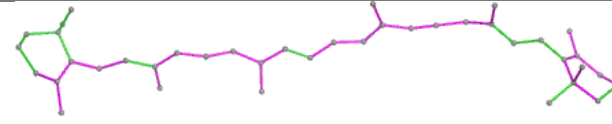
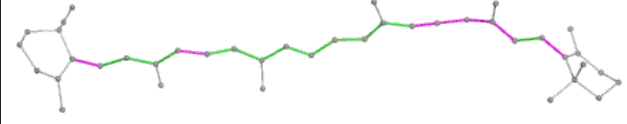
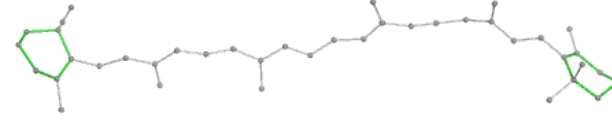


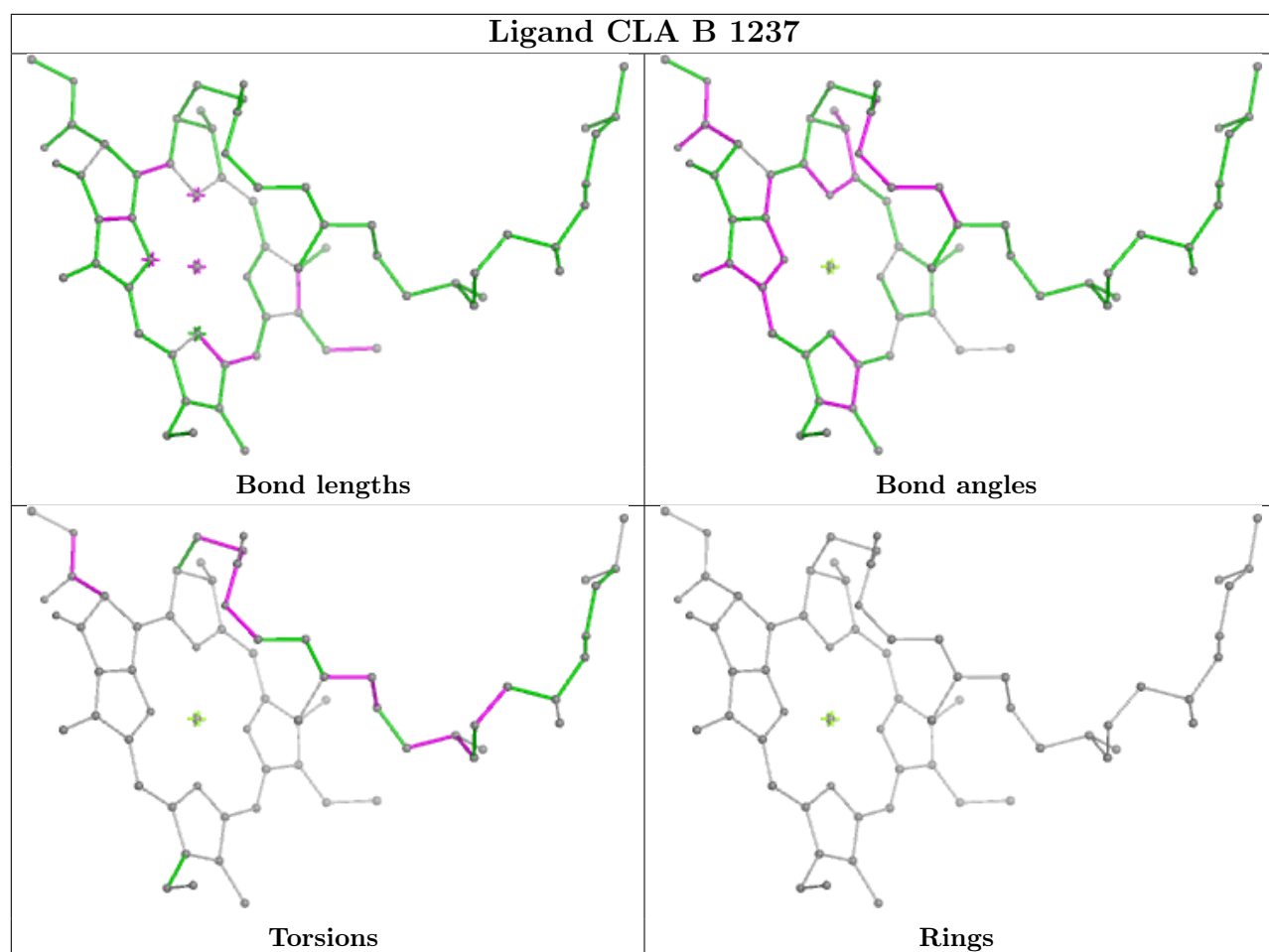
Ligand CLA 7 612



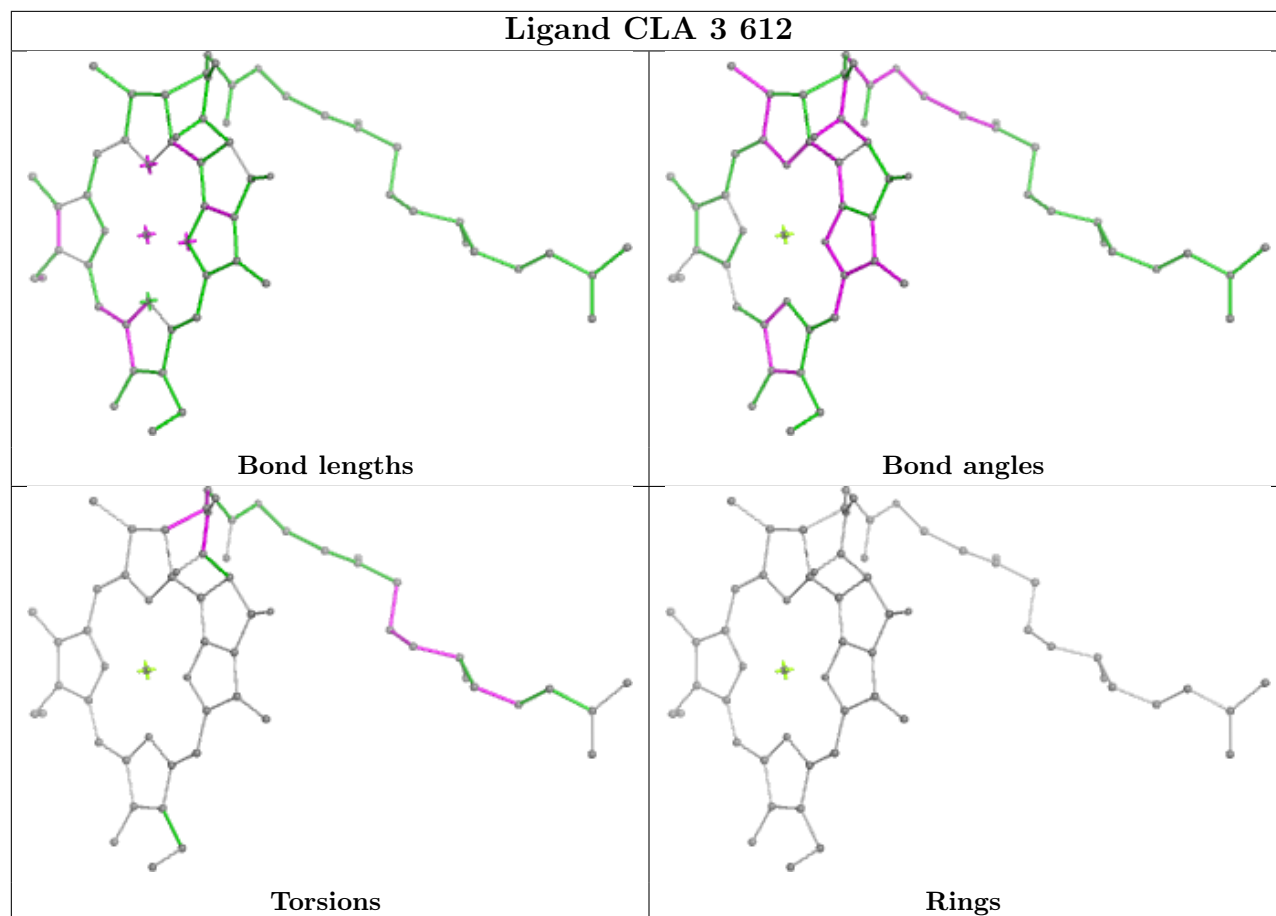


Ligand CLA A 1103	
	
Bond lengths	Bond angles
	
Torsions	Rings

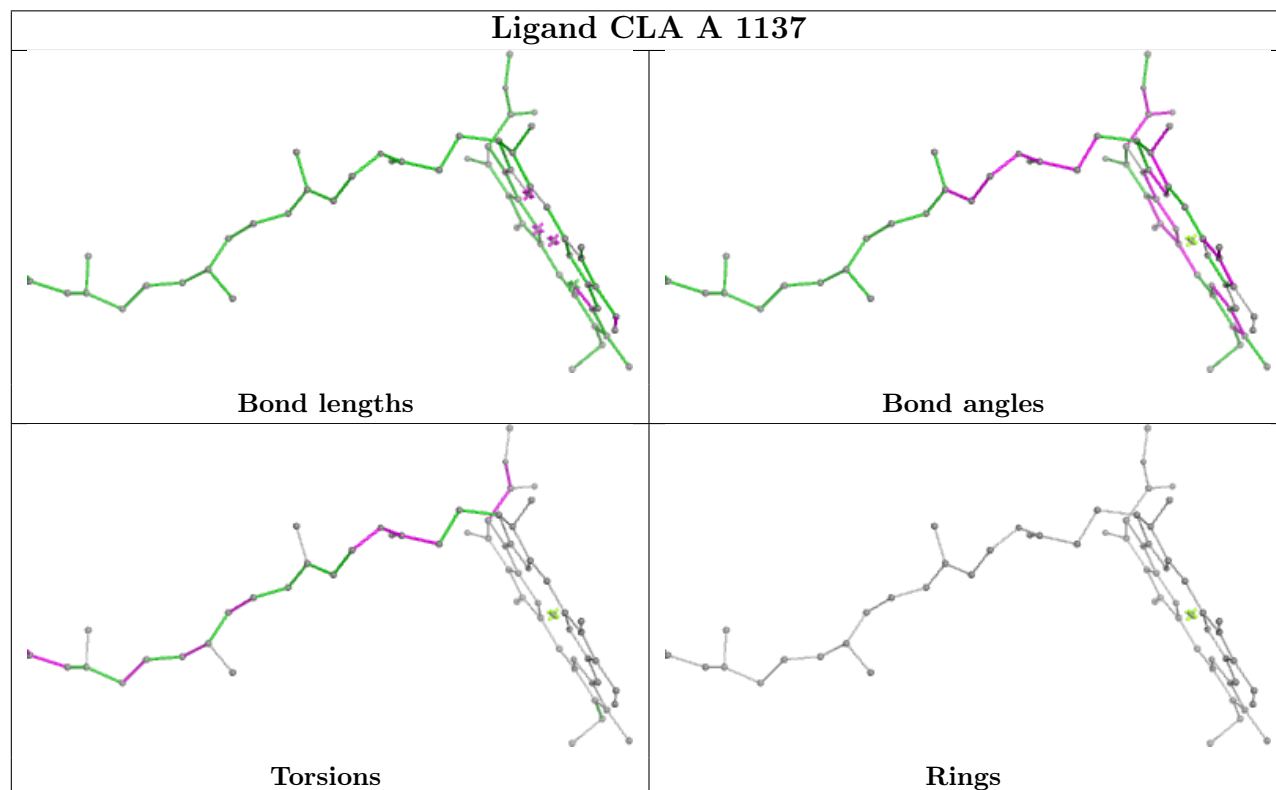
Ligand BCR K 4002	
	
Bond lengths	Bond angles
	
Torsions	Rings

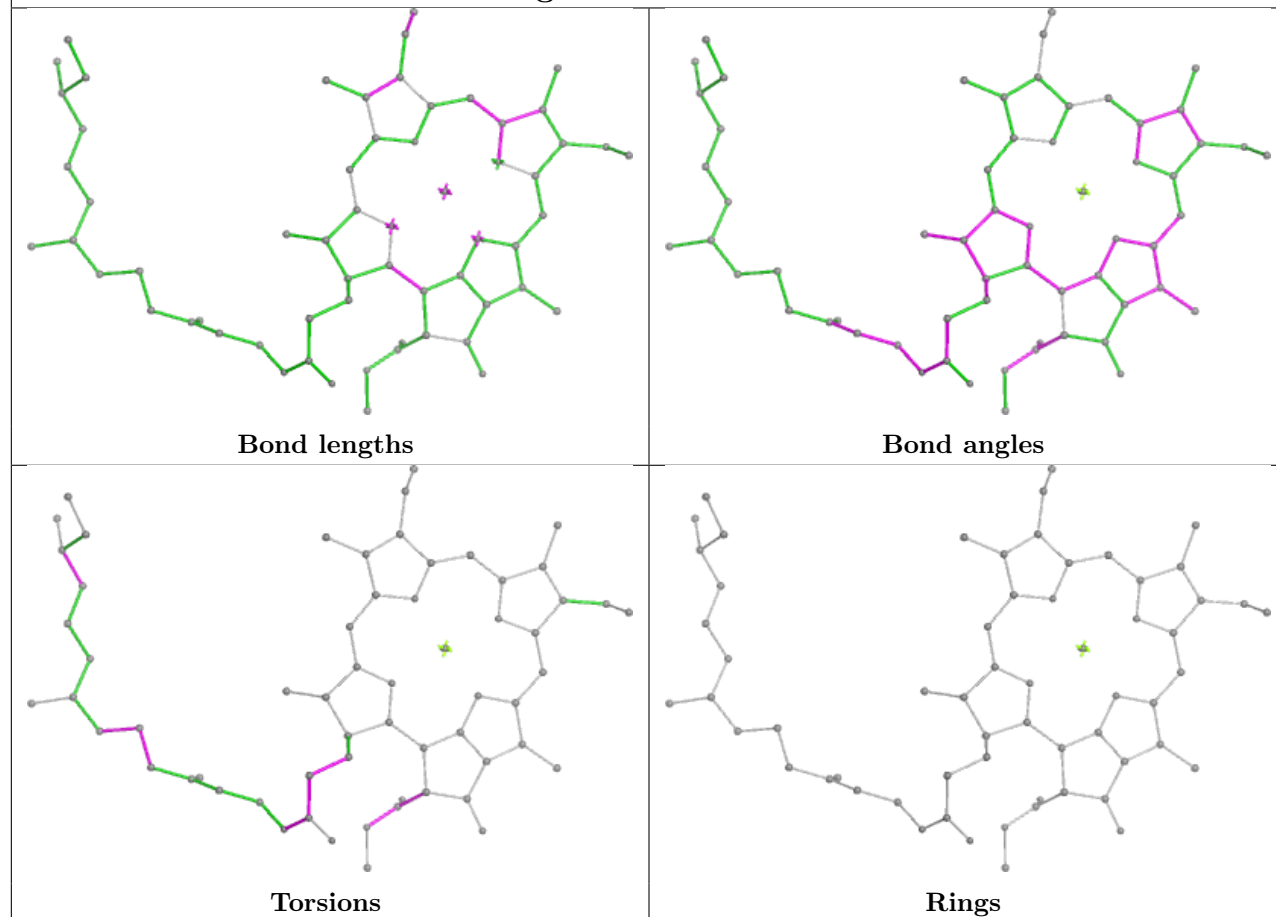
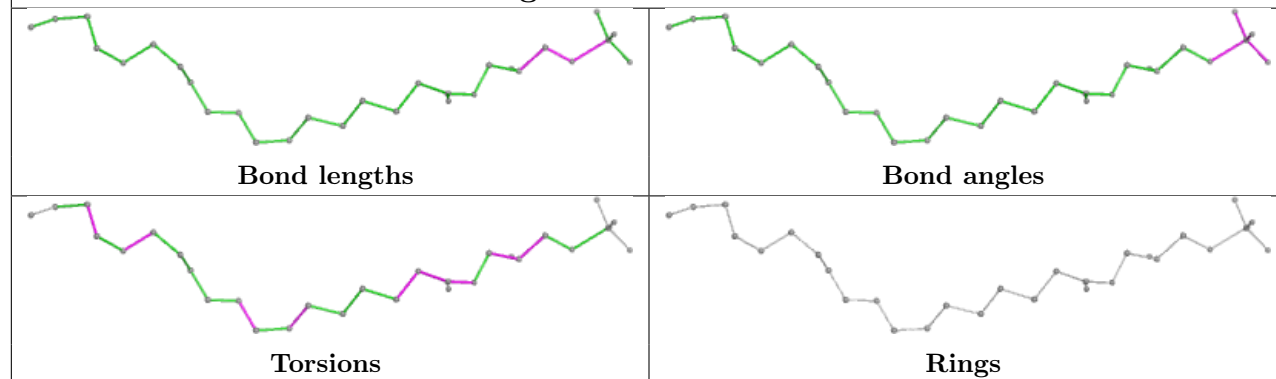


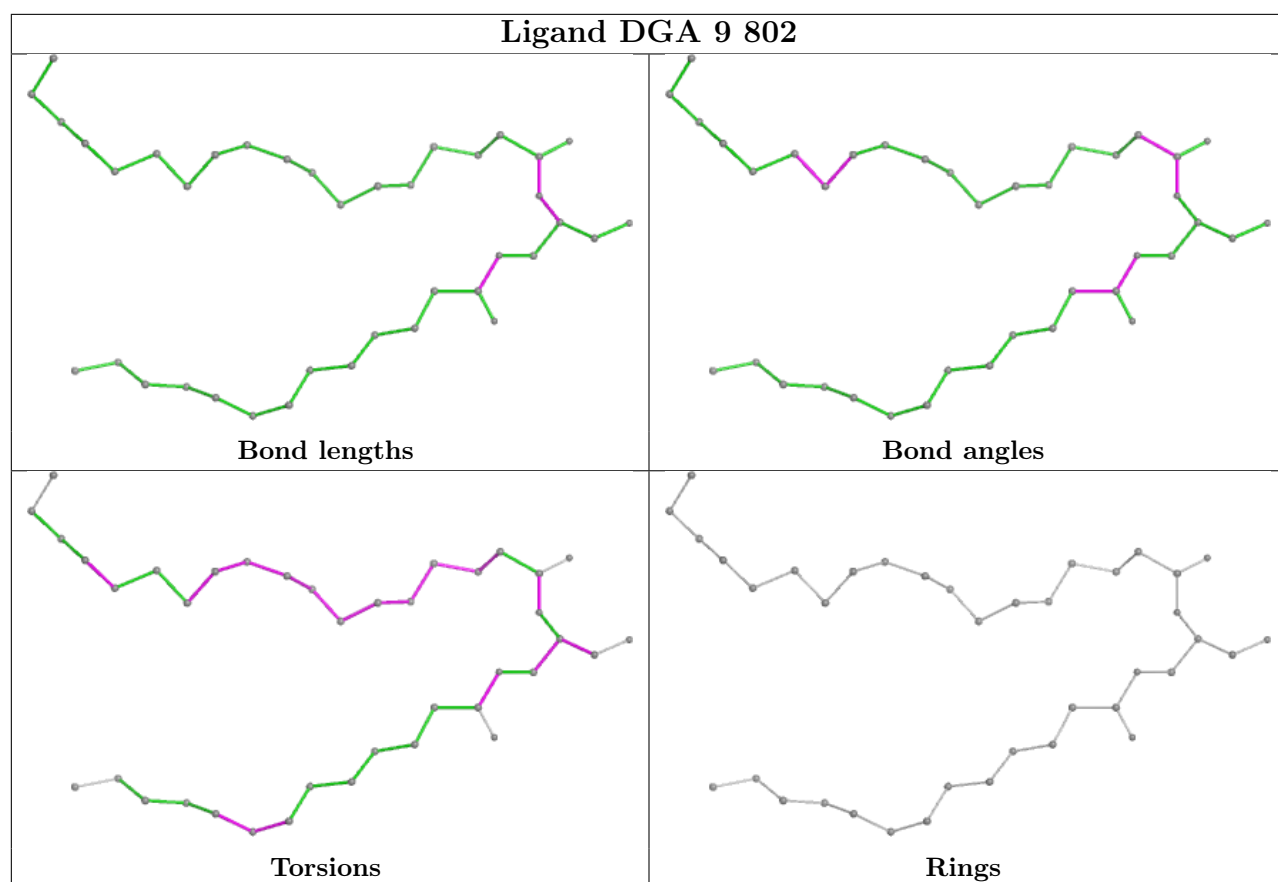
Ligand CLA 3 612

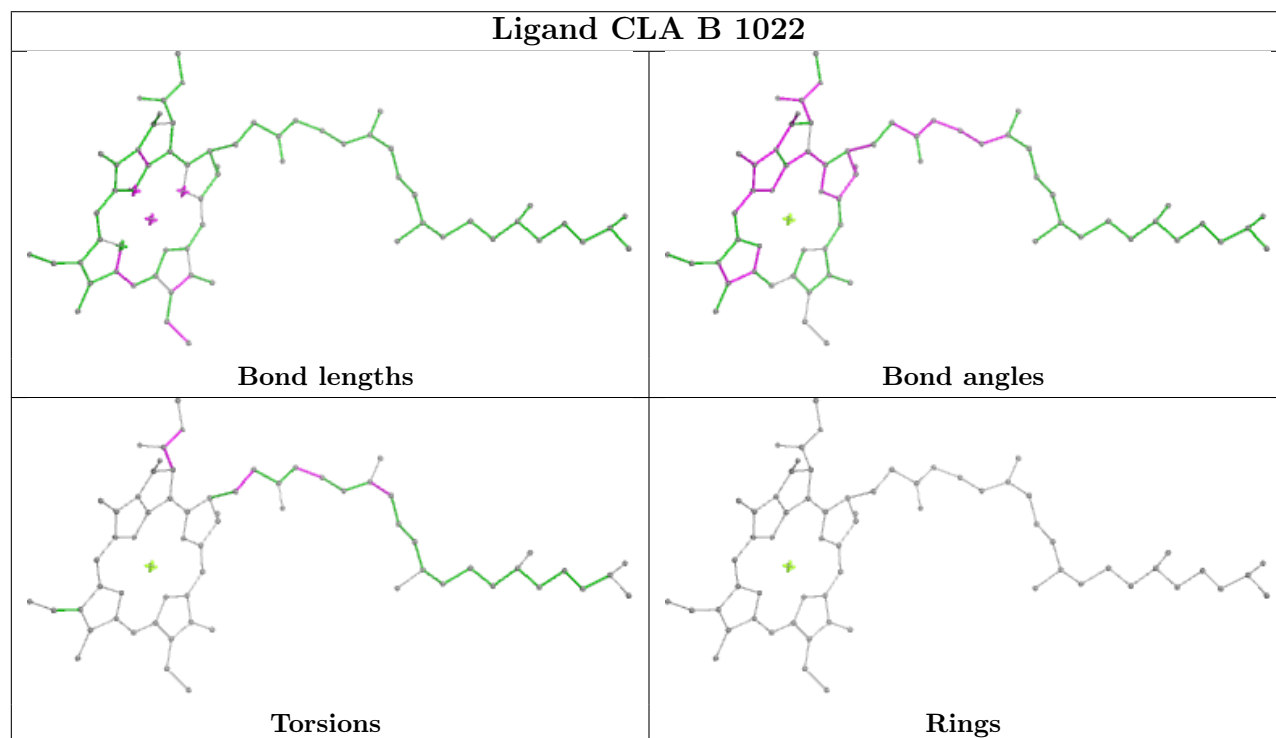
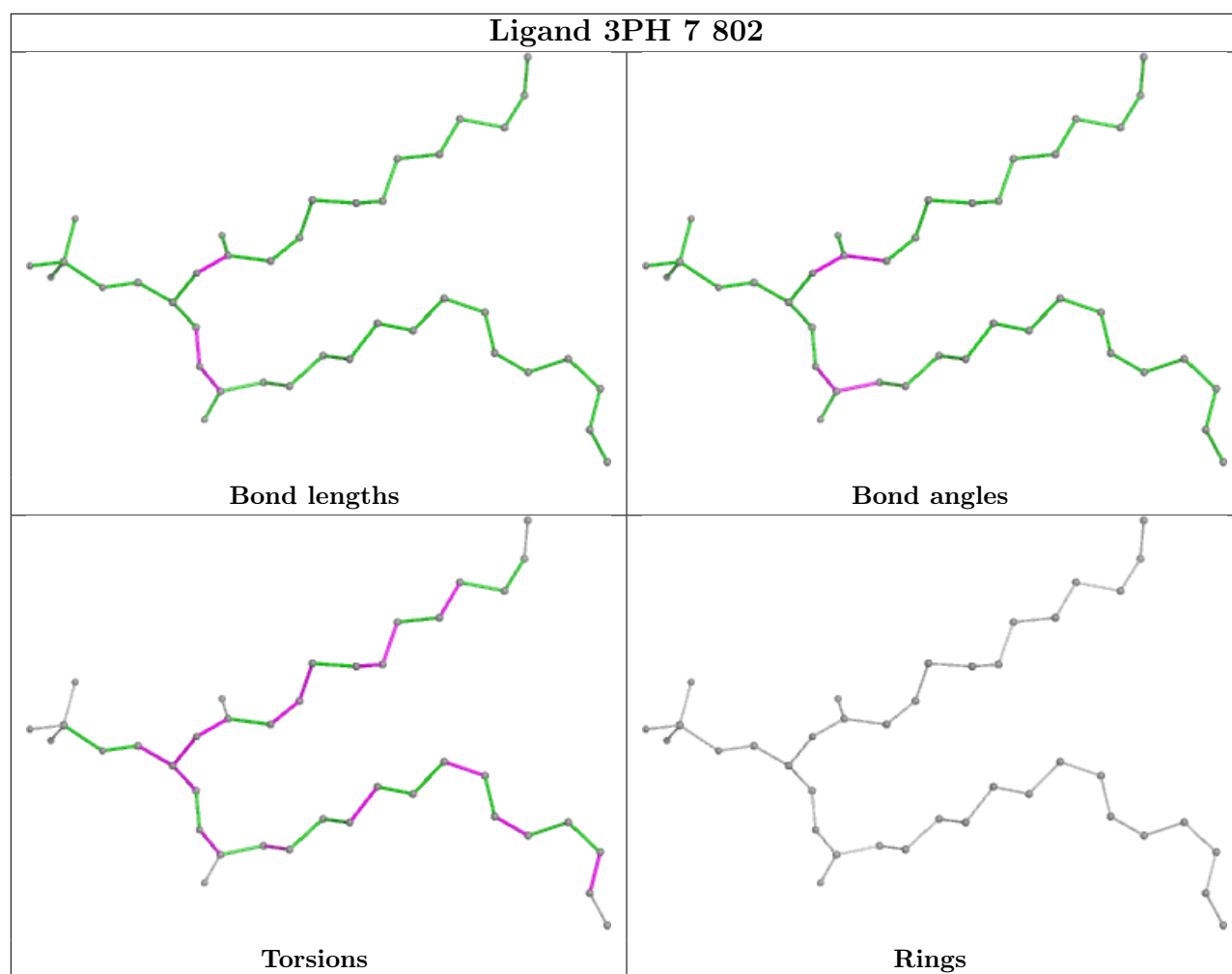


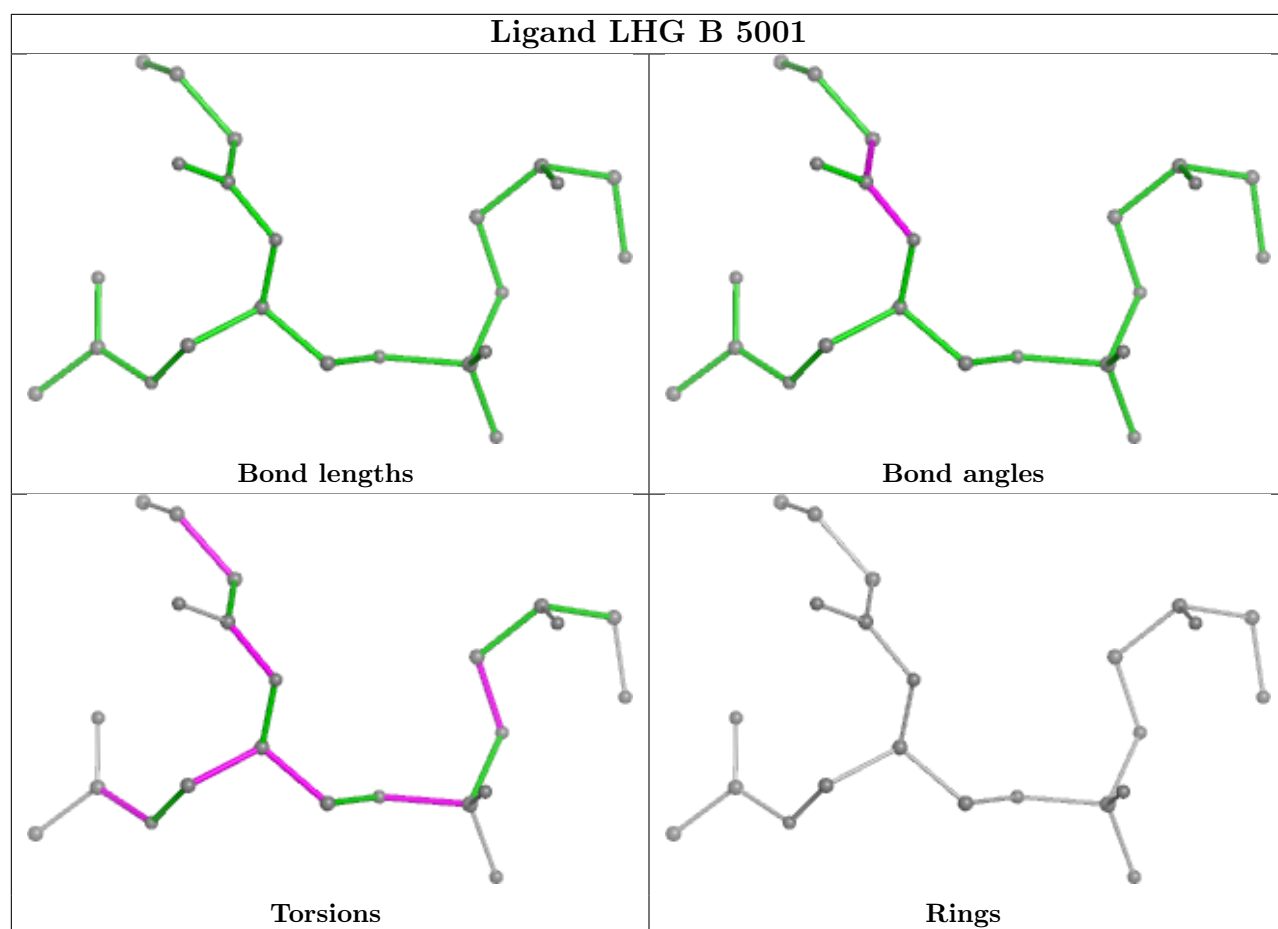
Ligand CLA A 1137

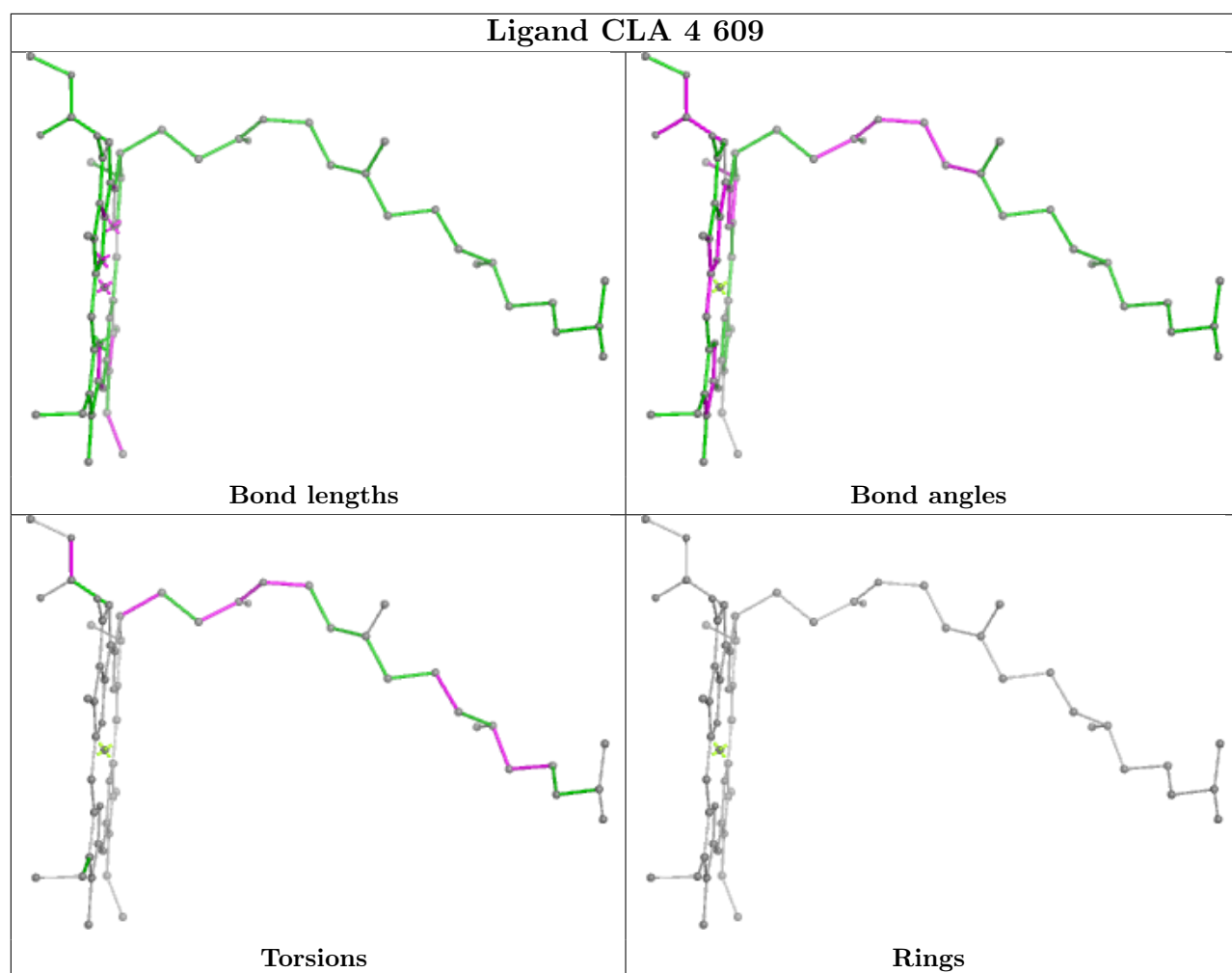


Ligand CLA 7 605**Ligand NKP A 5004**

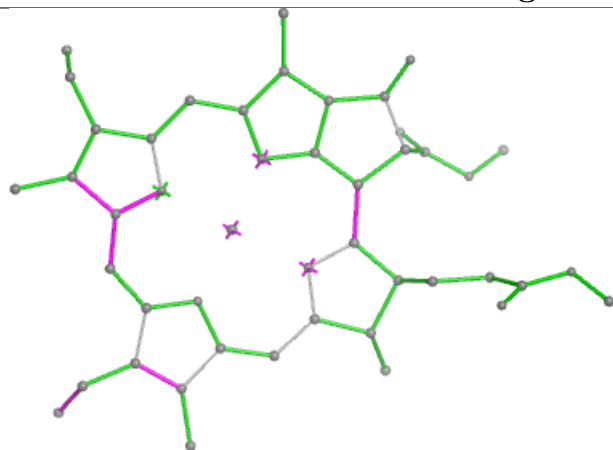




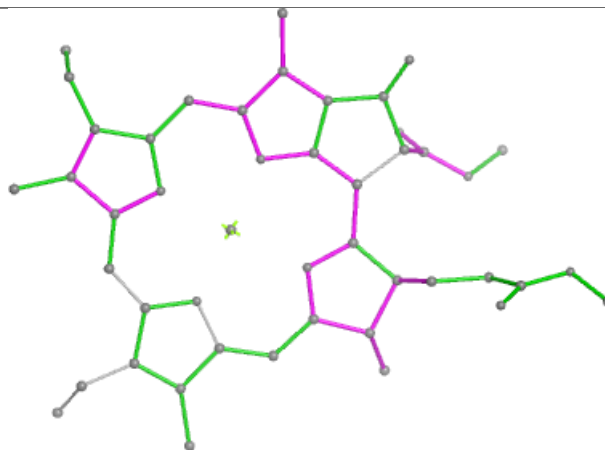




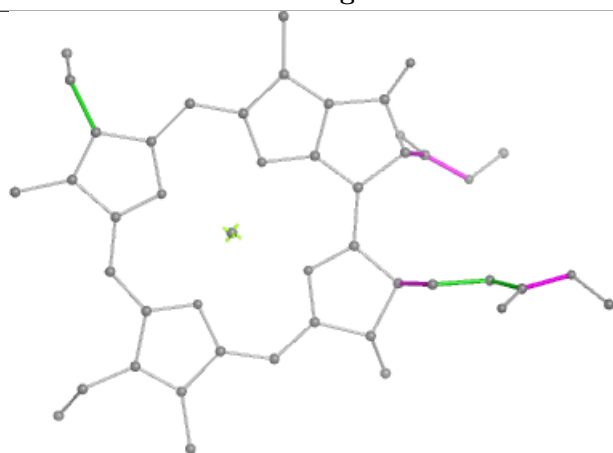
Ligand CLA 6 618



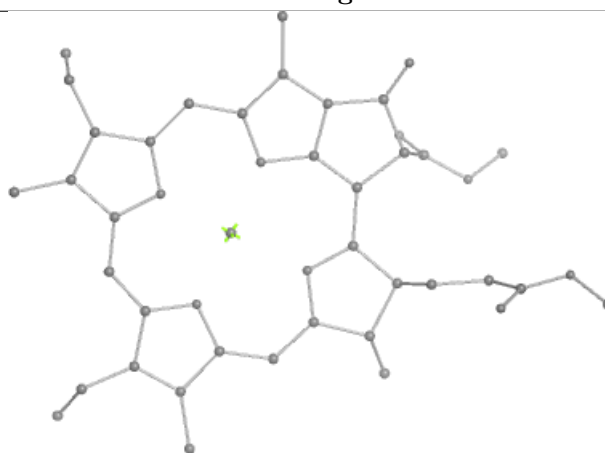
Bond lengths



Bond angles

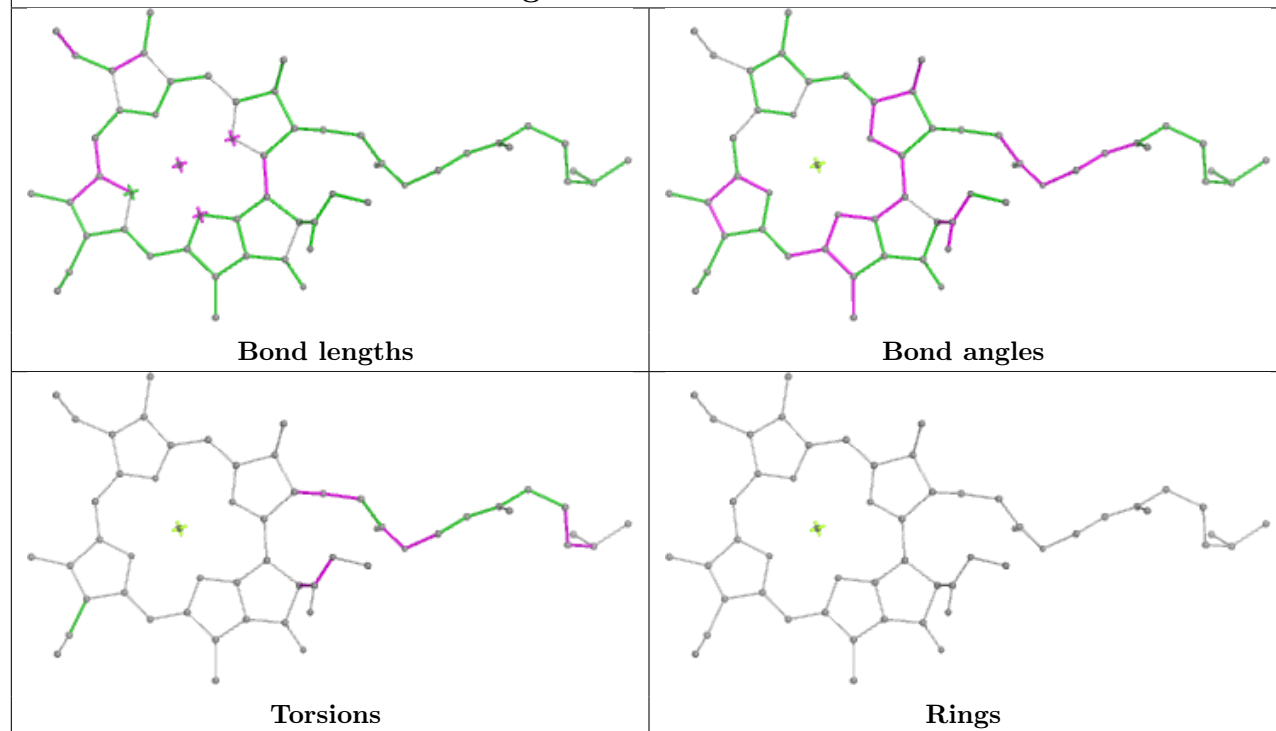


Torsions

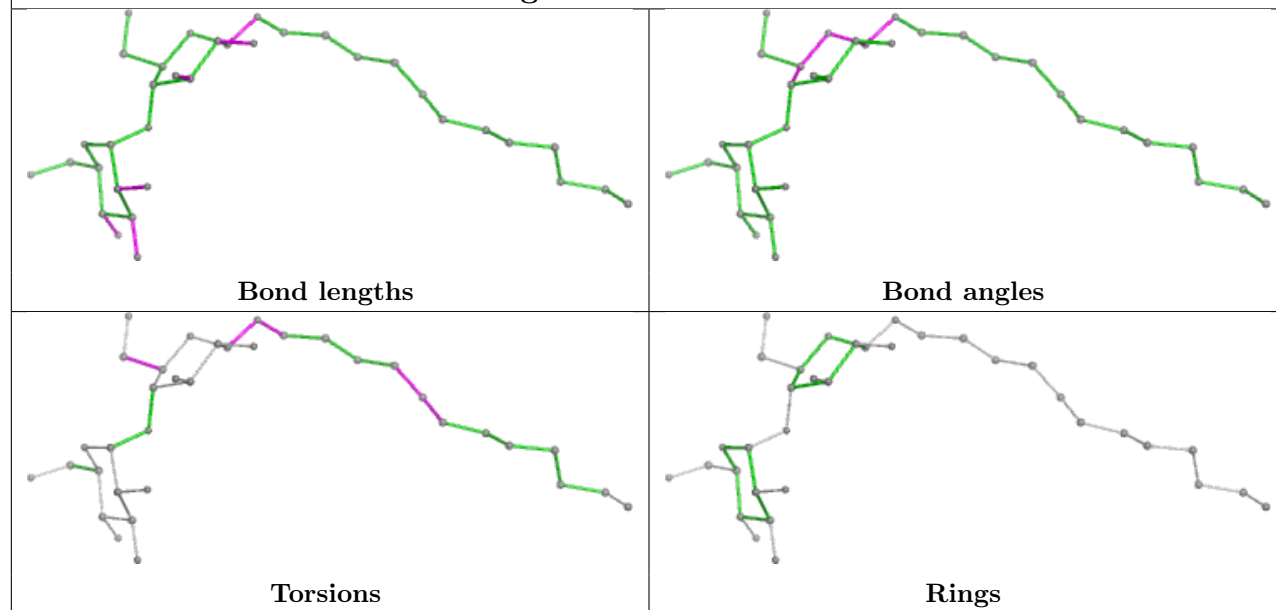


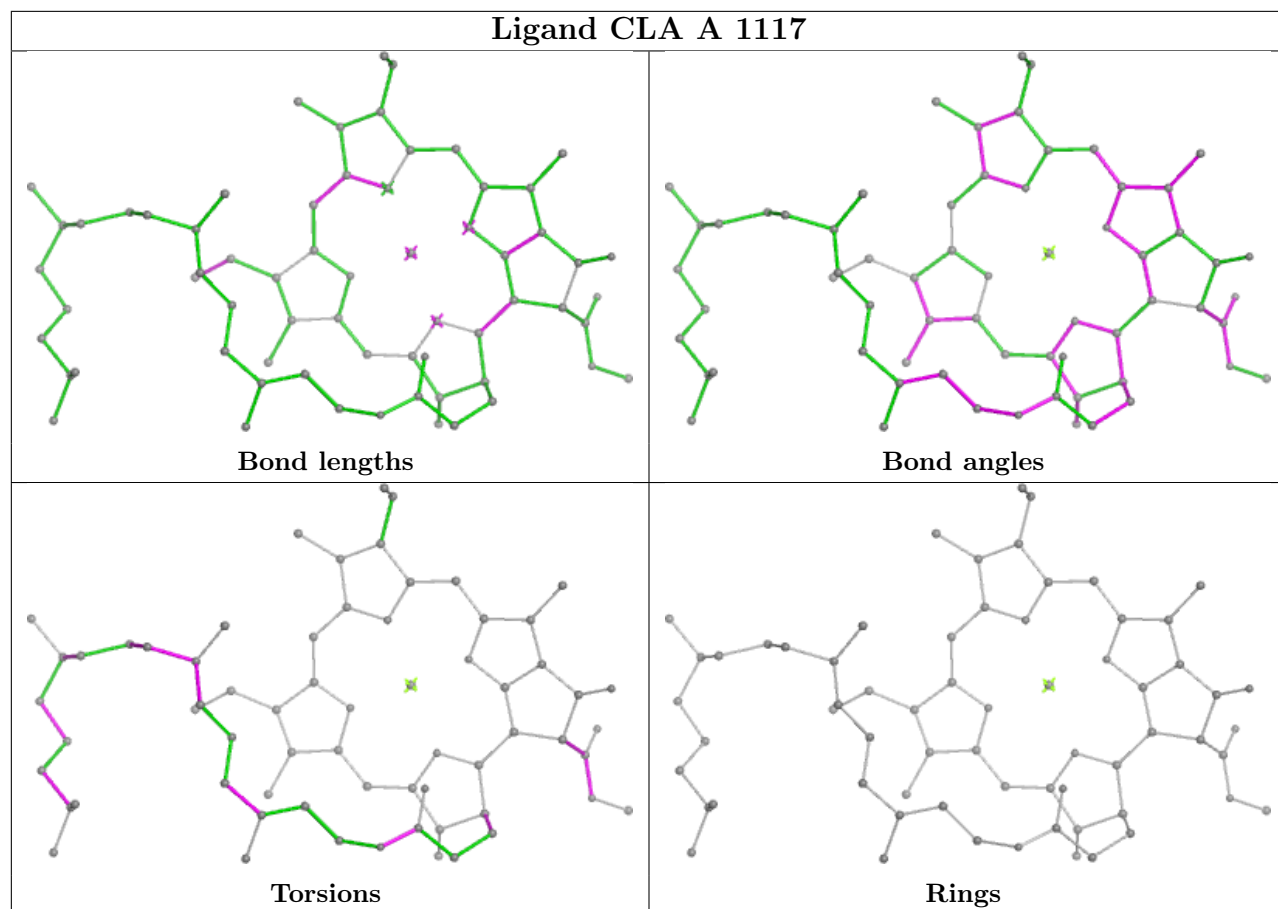
Rings

Ligand CLA K 1404

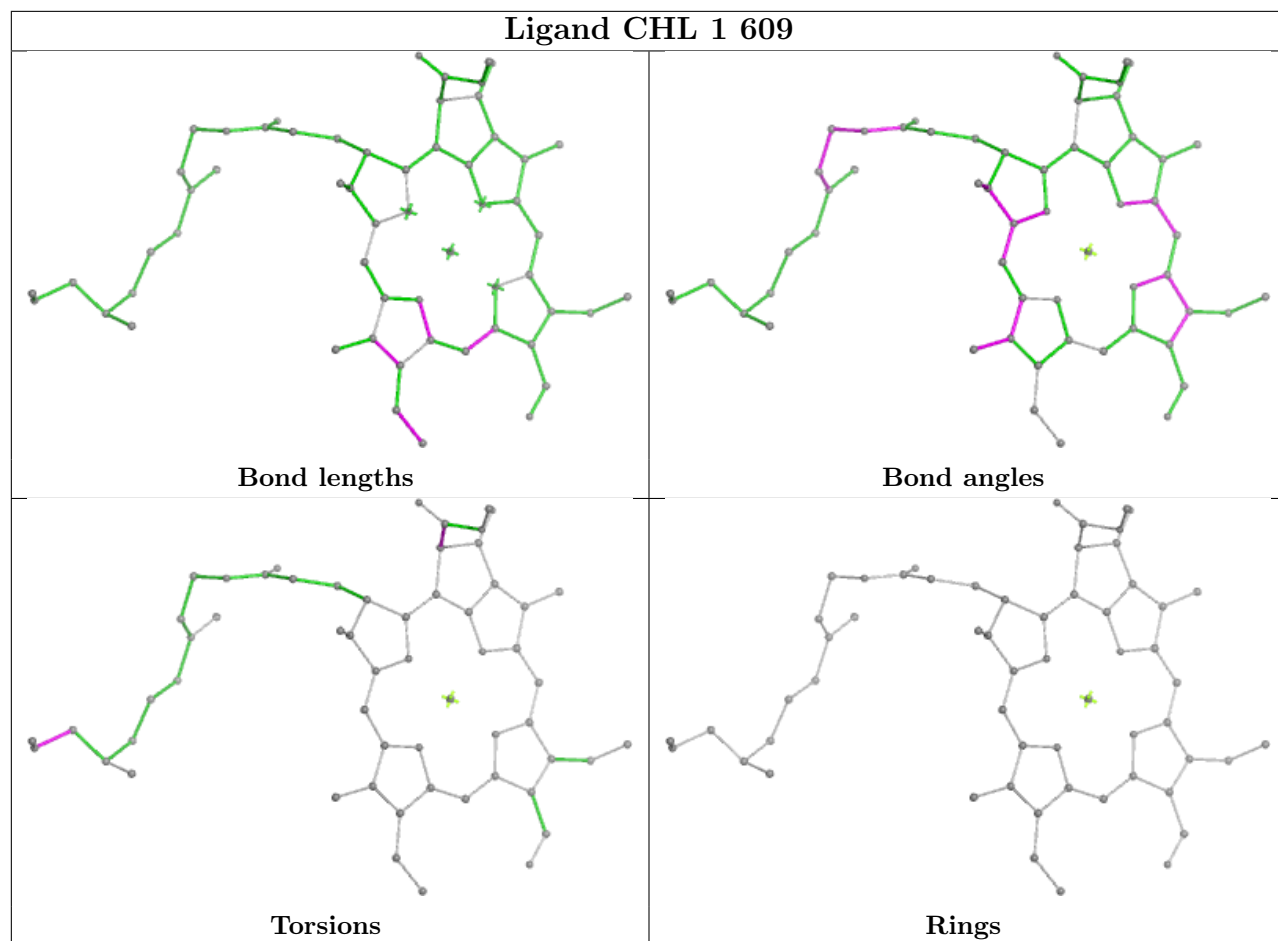


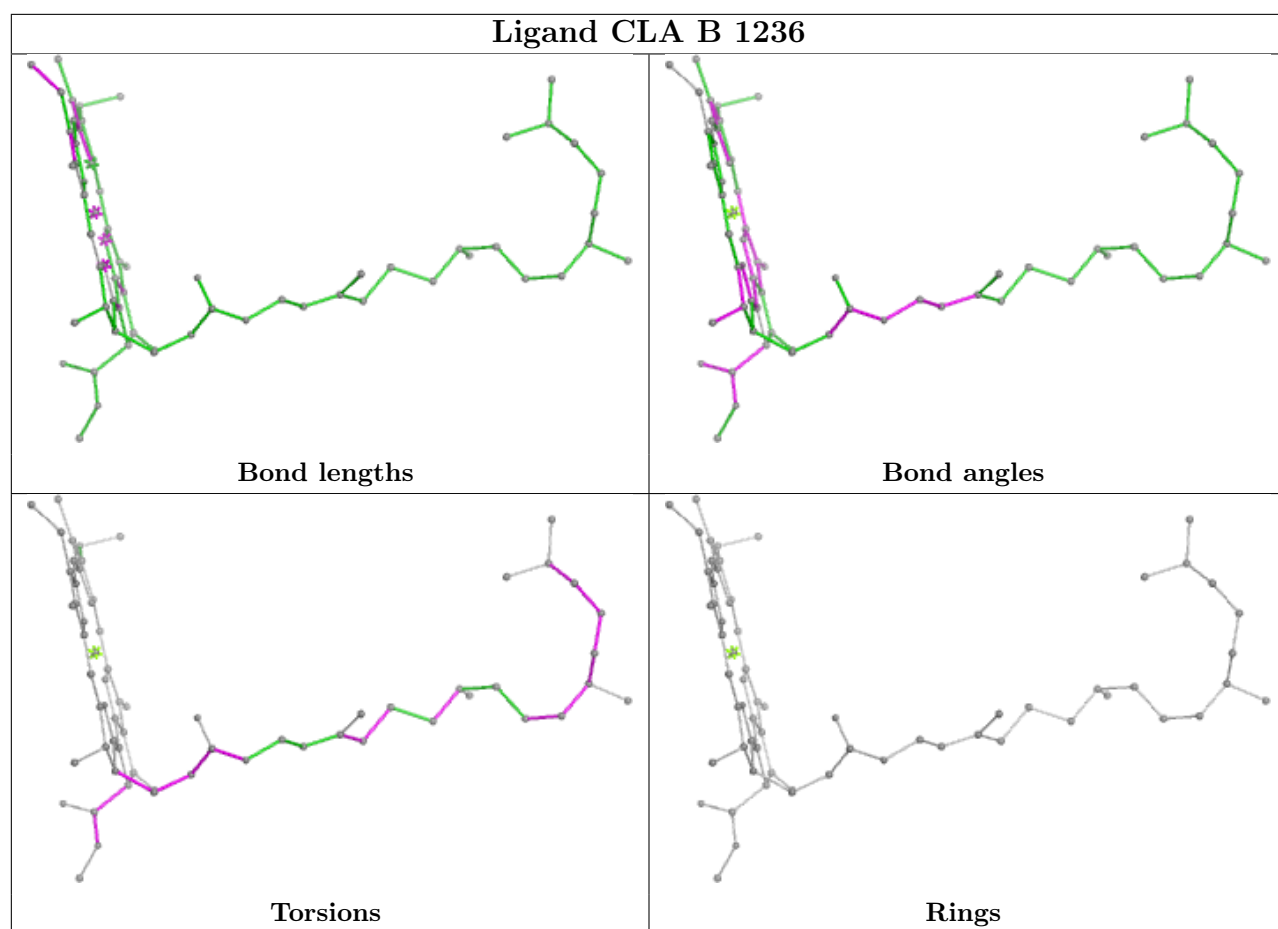
Ligand LMT B 5005



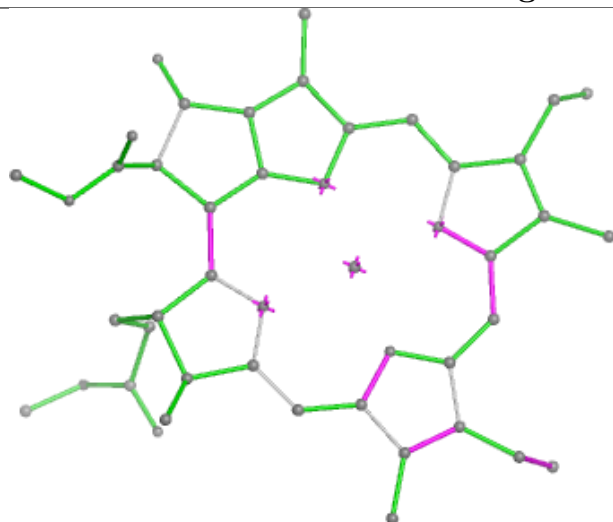
Ligand CLA A 1117

Ligand CHL 1 609

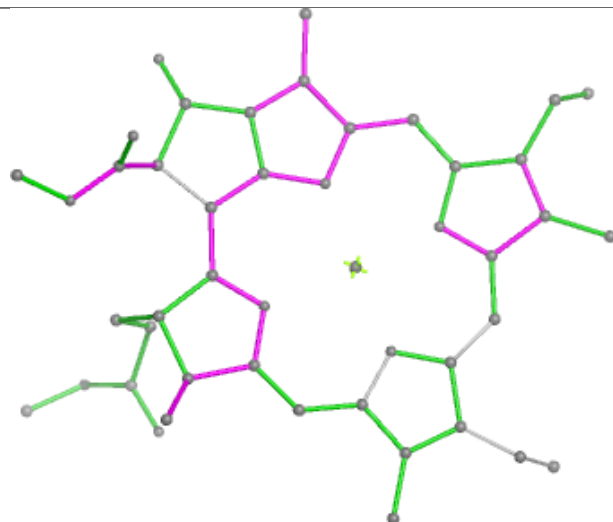




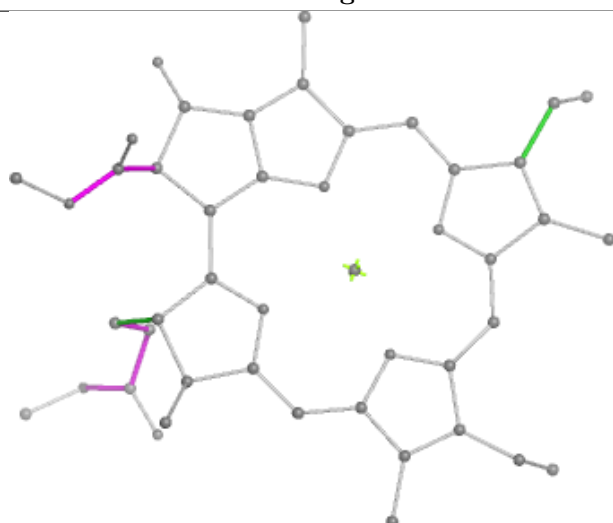
Ligand CLA 2 607



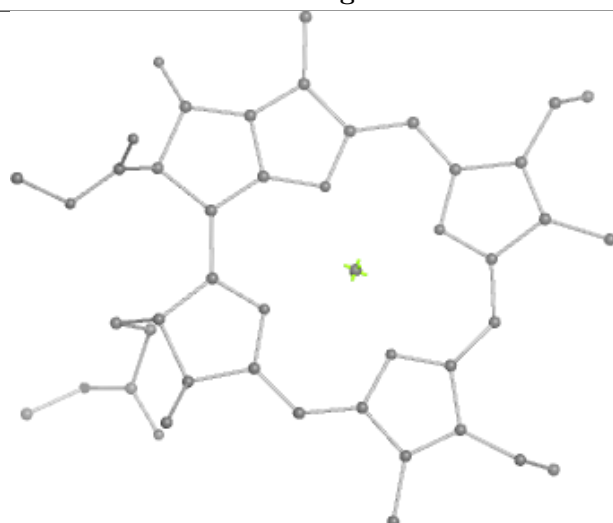
Bond lengths



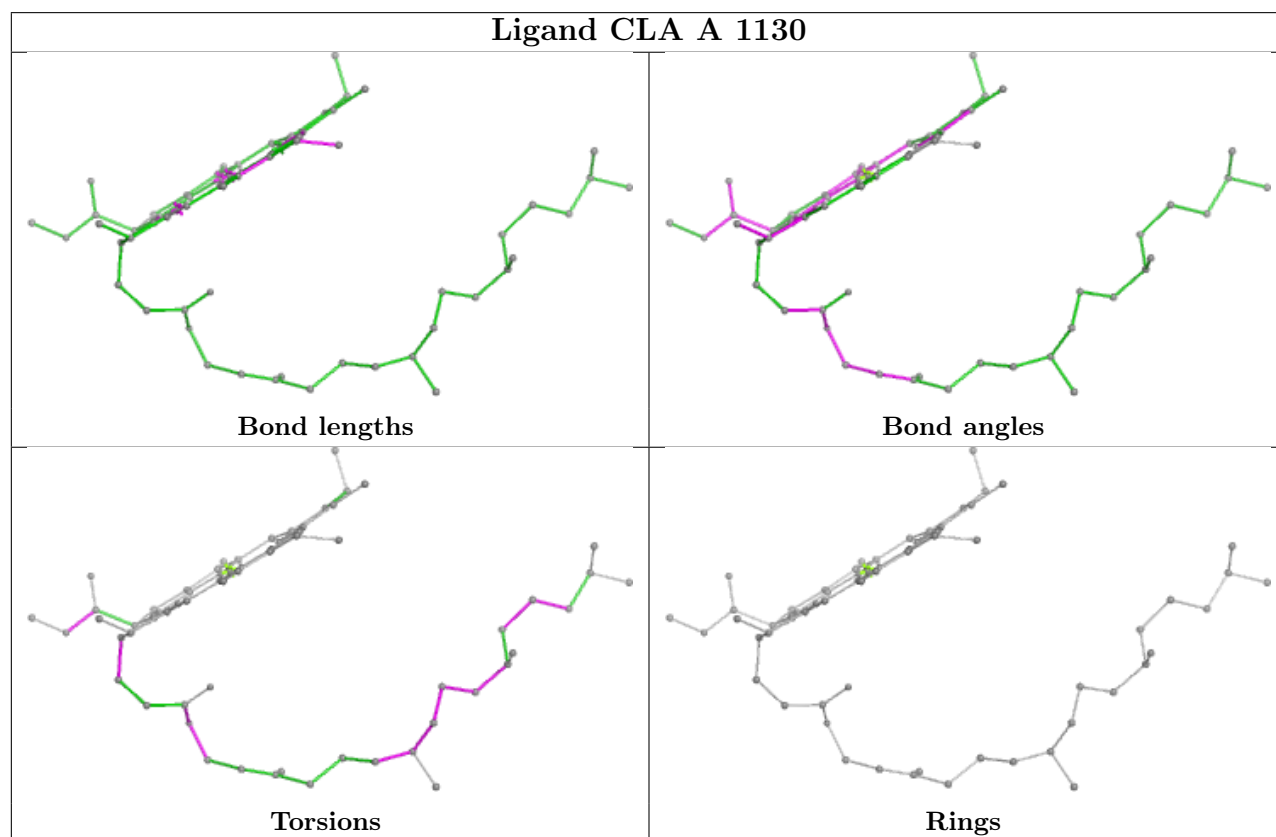
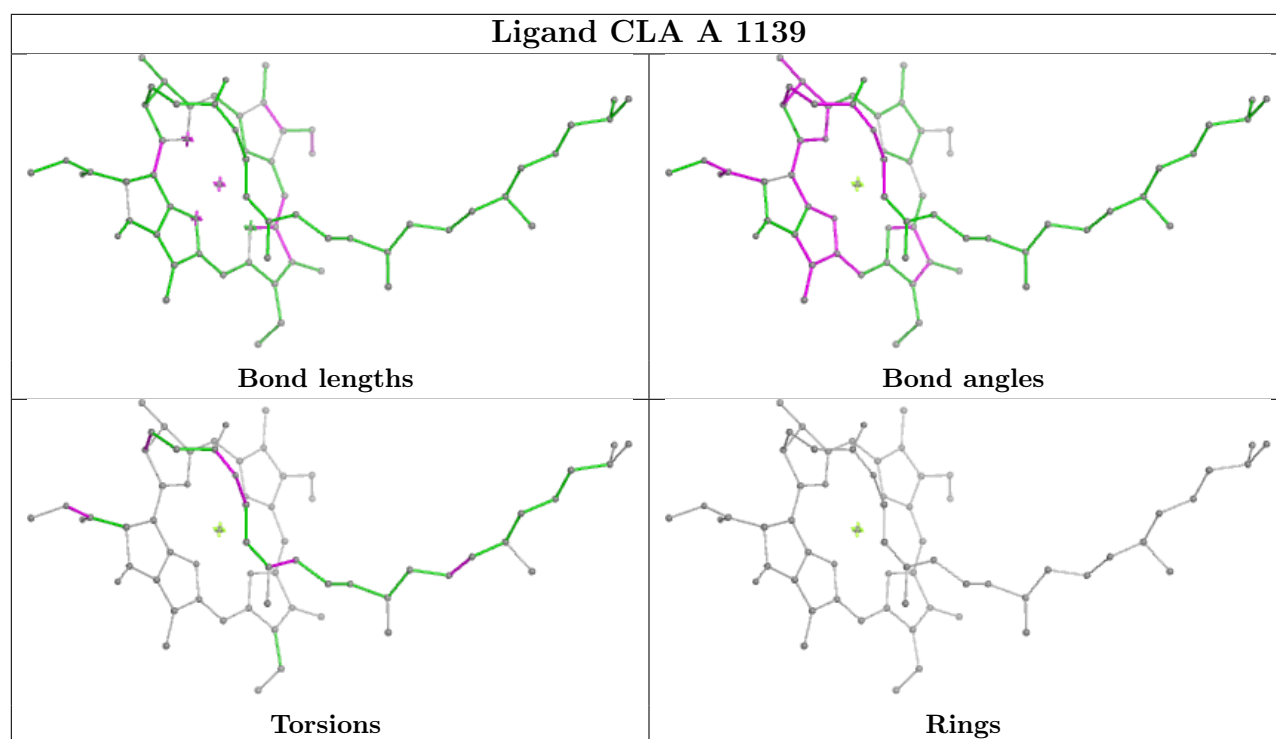
Bond angles

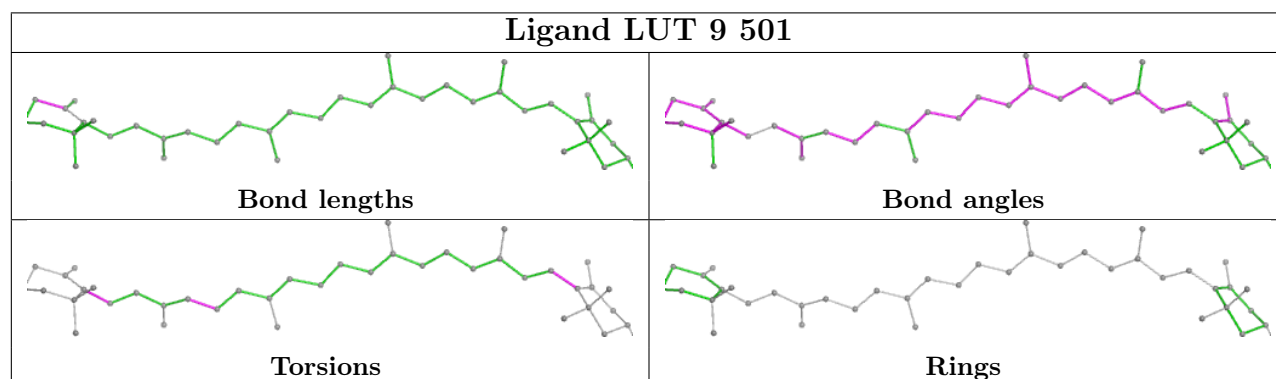
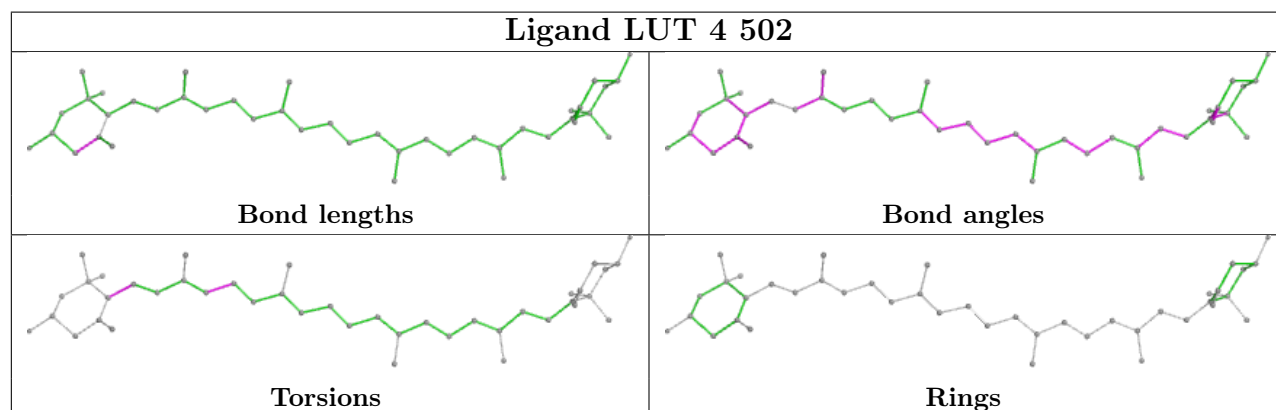
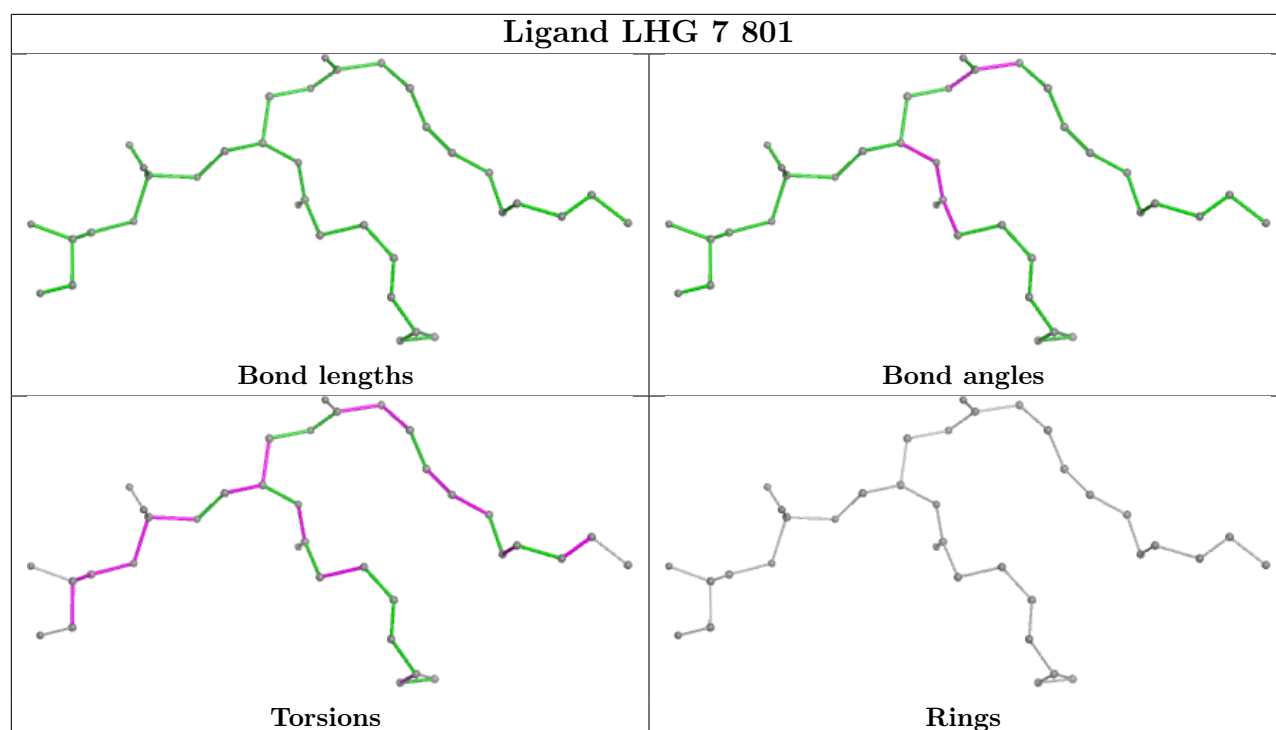


Torsions

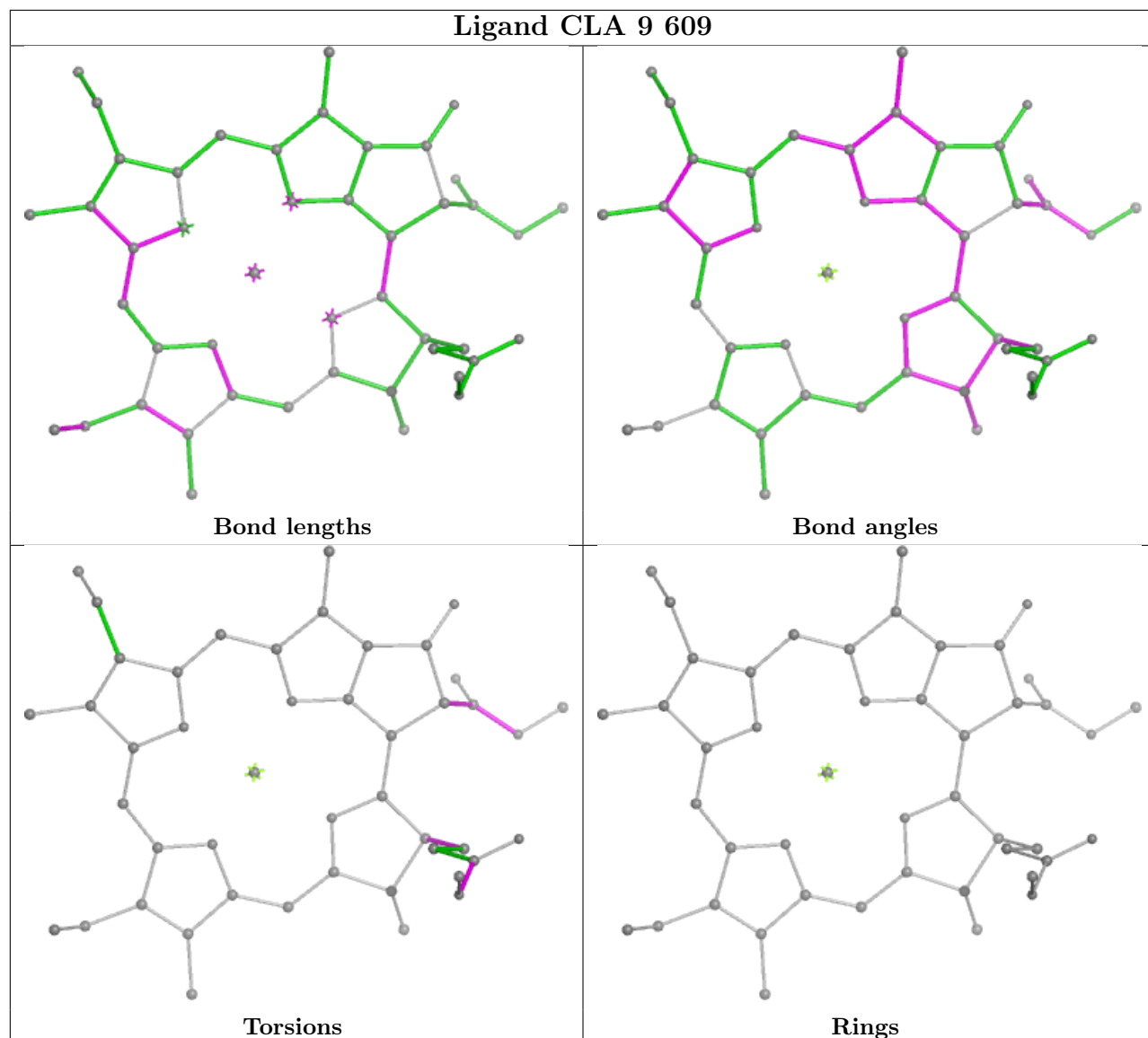


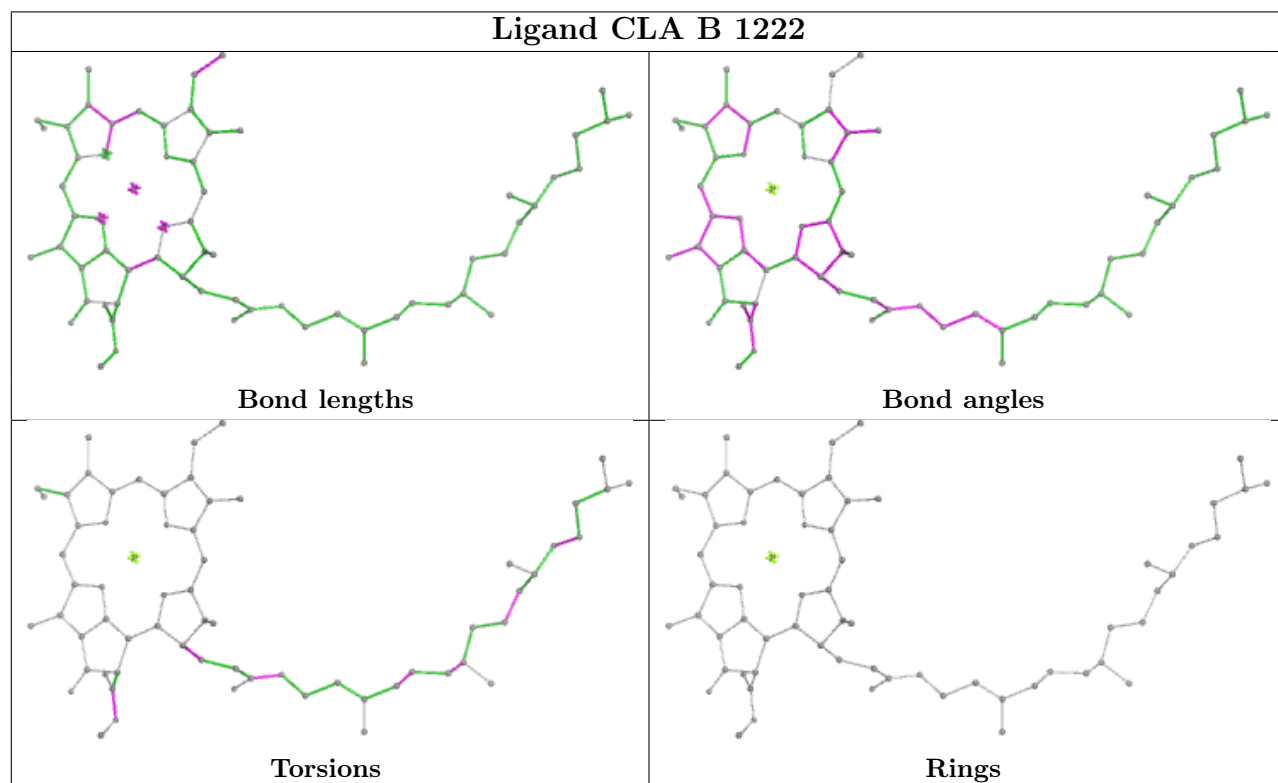
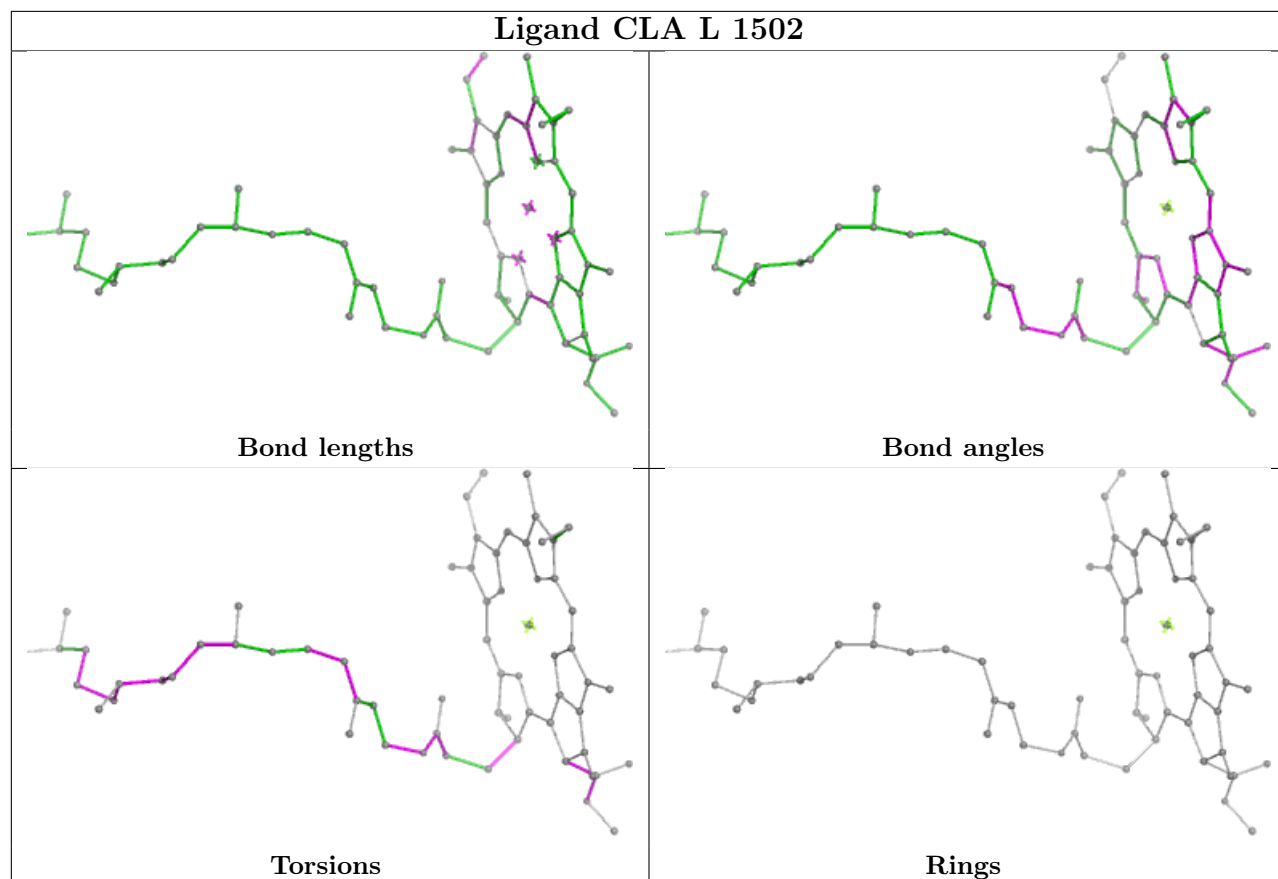
Rings

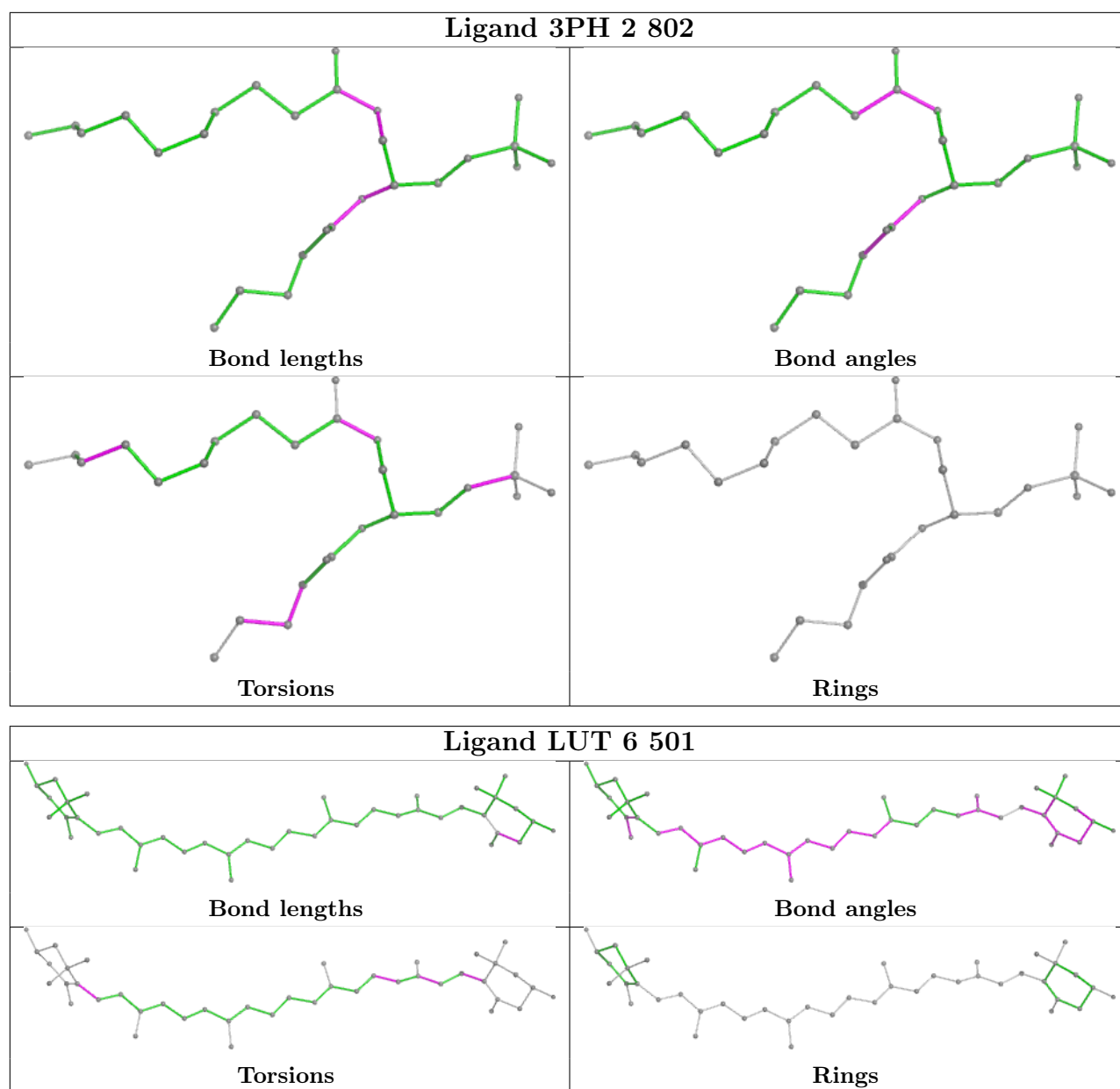




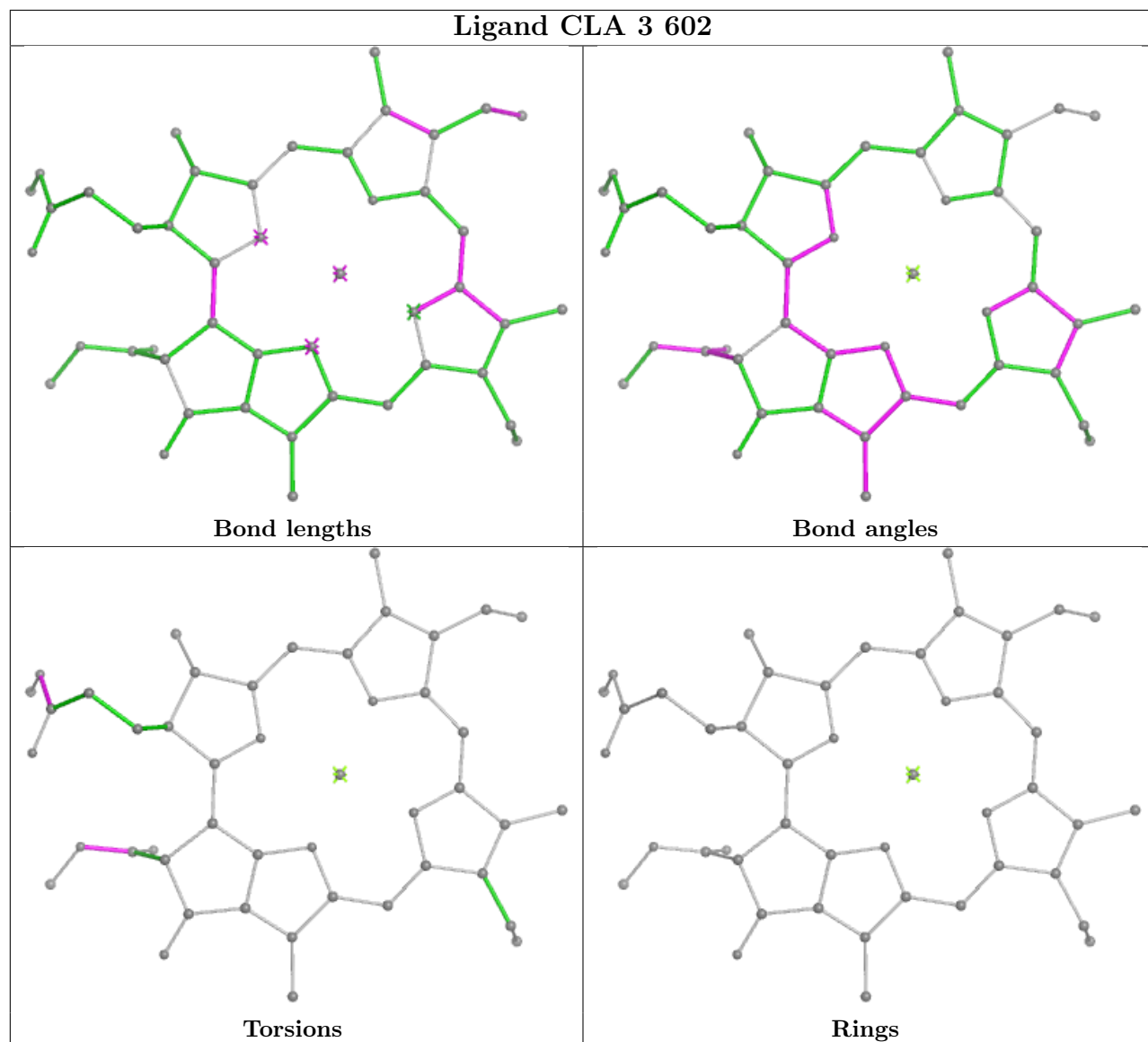
Ligand CLA 9 609



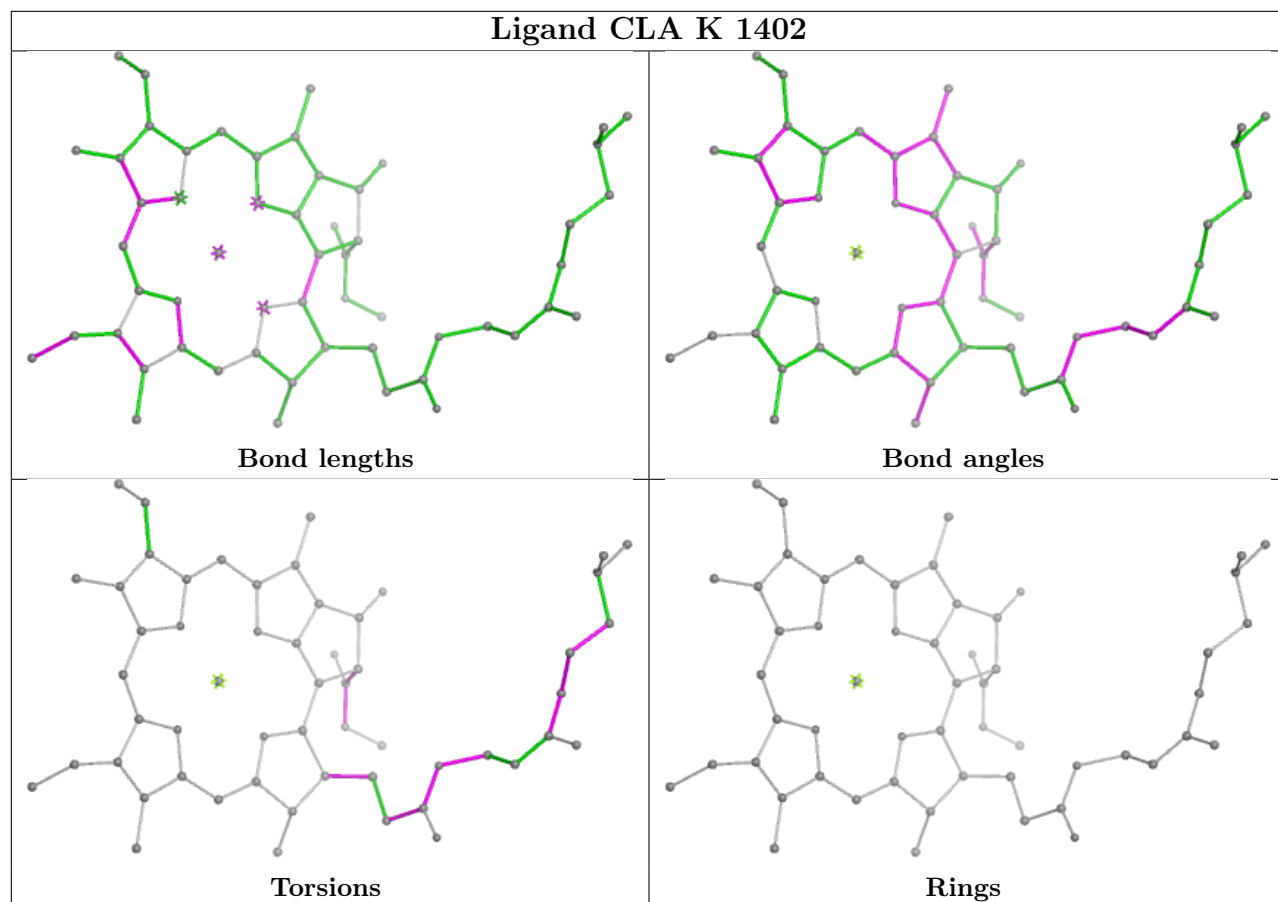




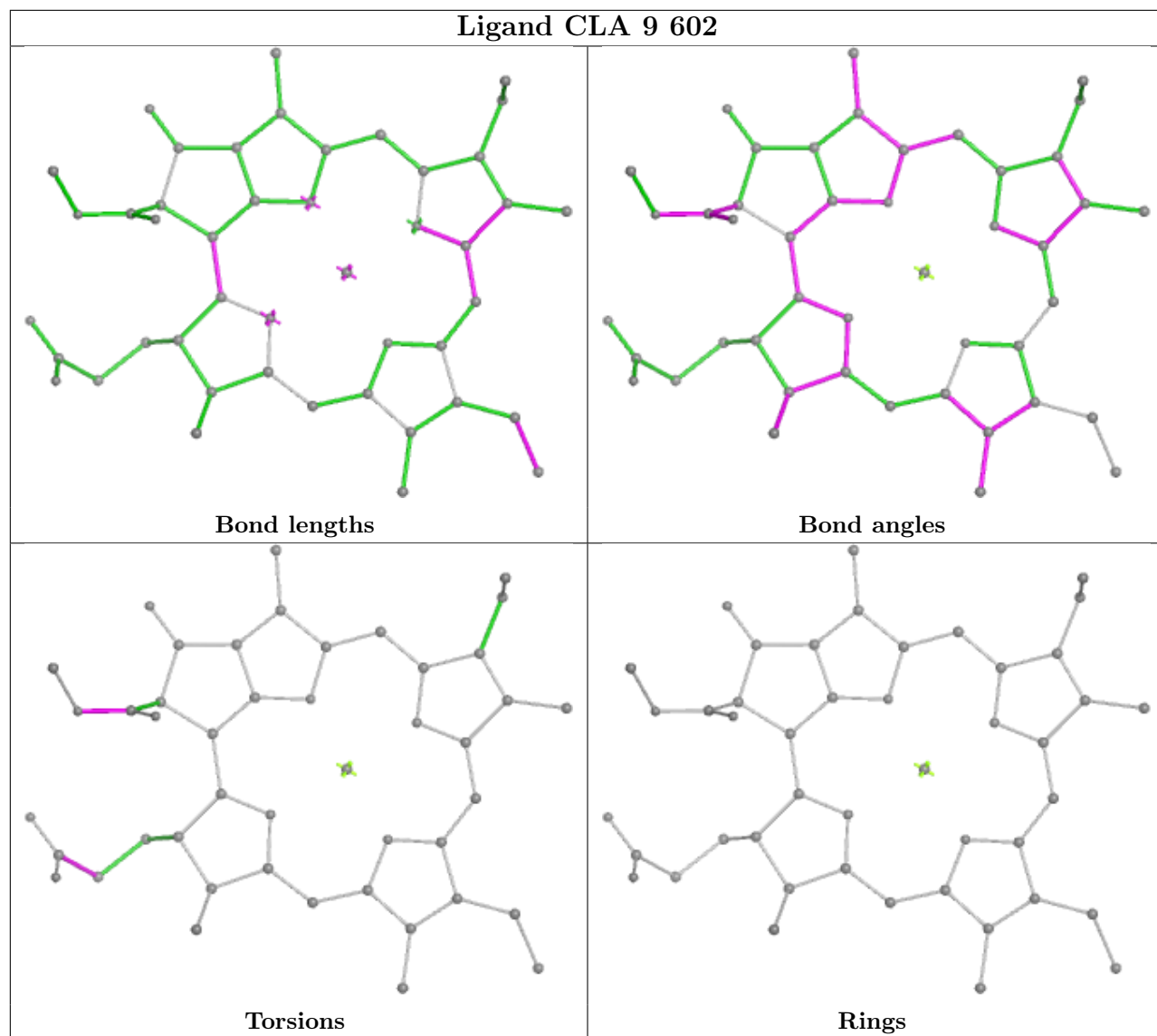
Ligand CLA 3 602



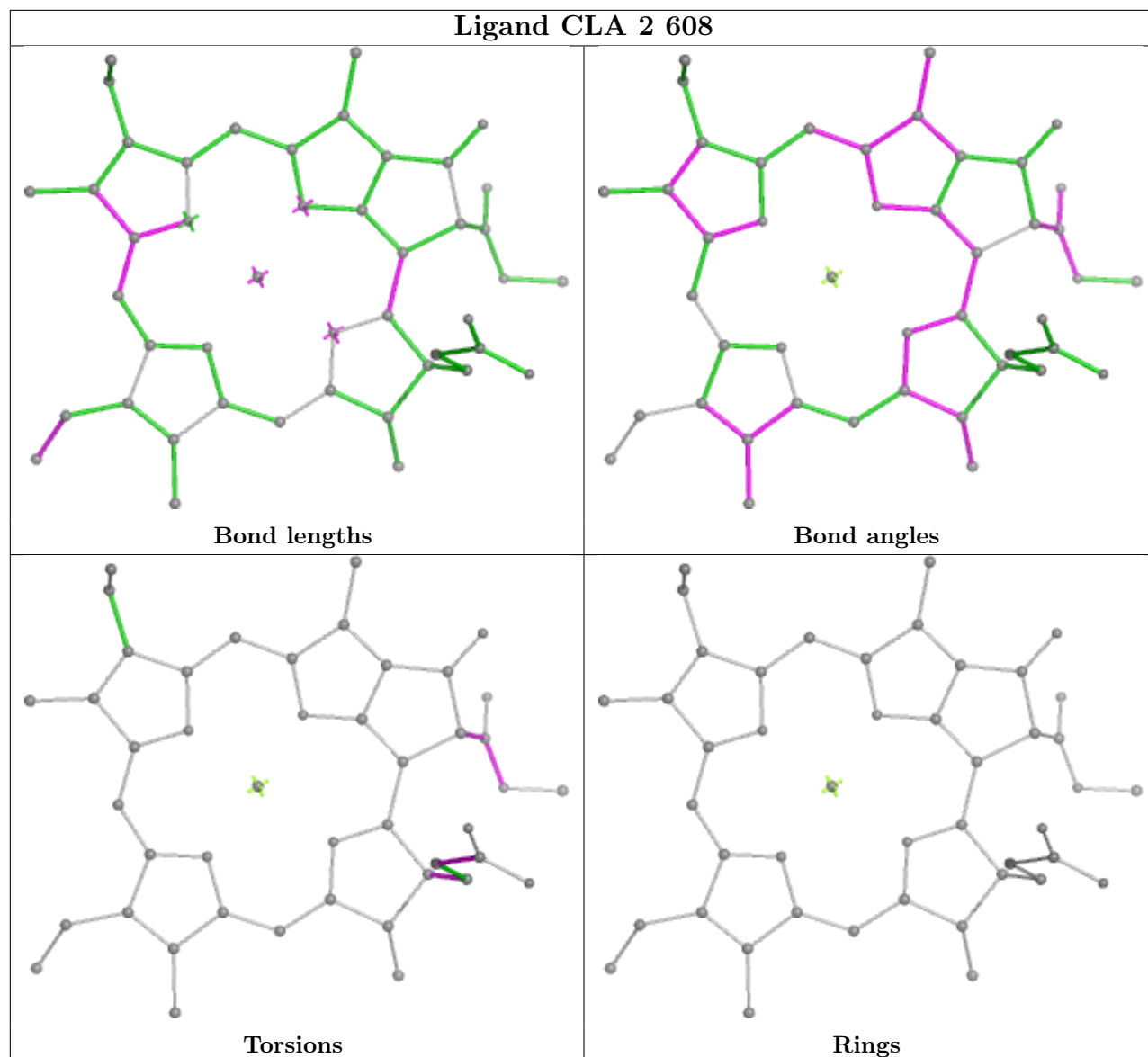
Ligand CLA K 1402



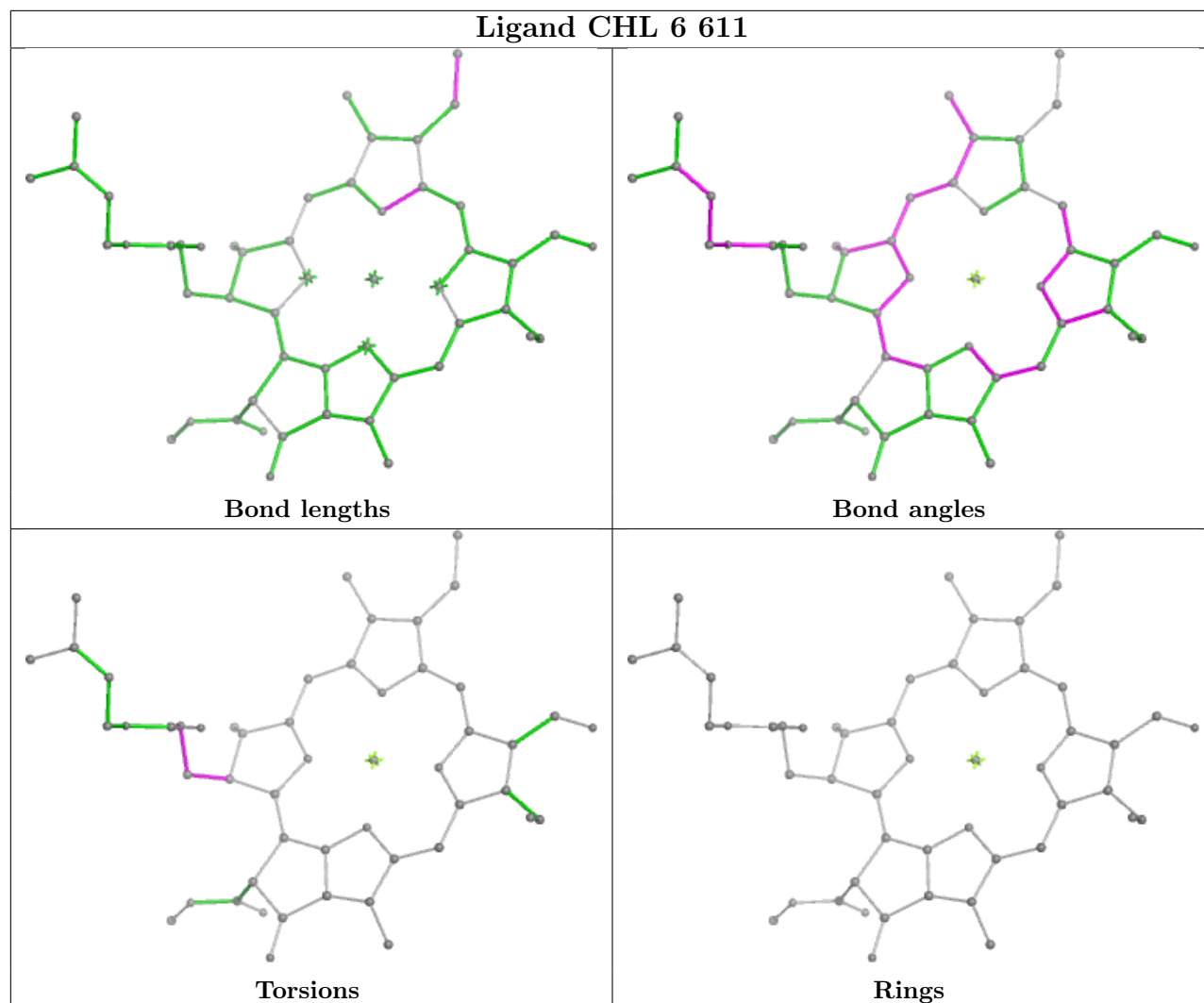
Ligand CLA 9 602

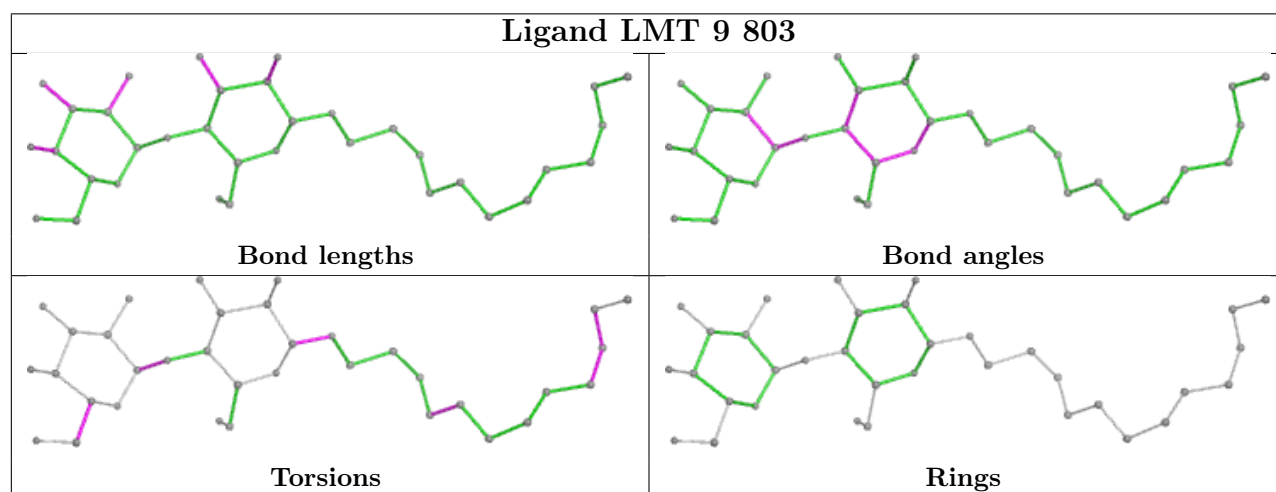
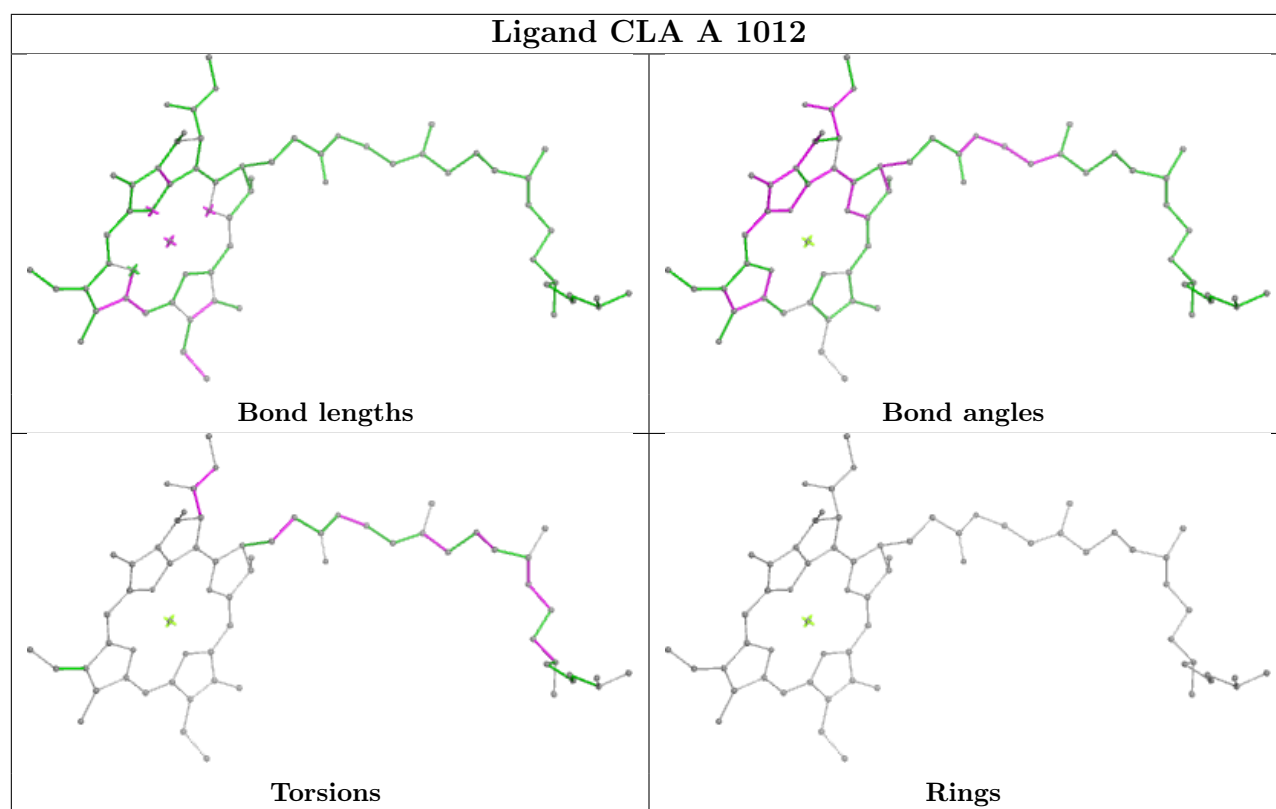


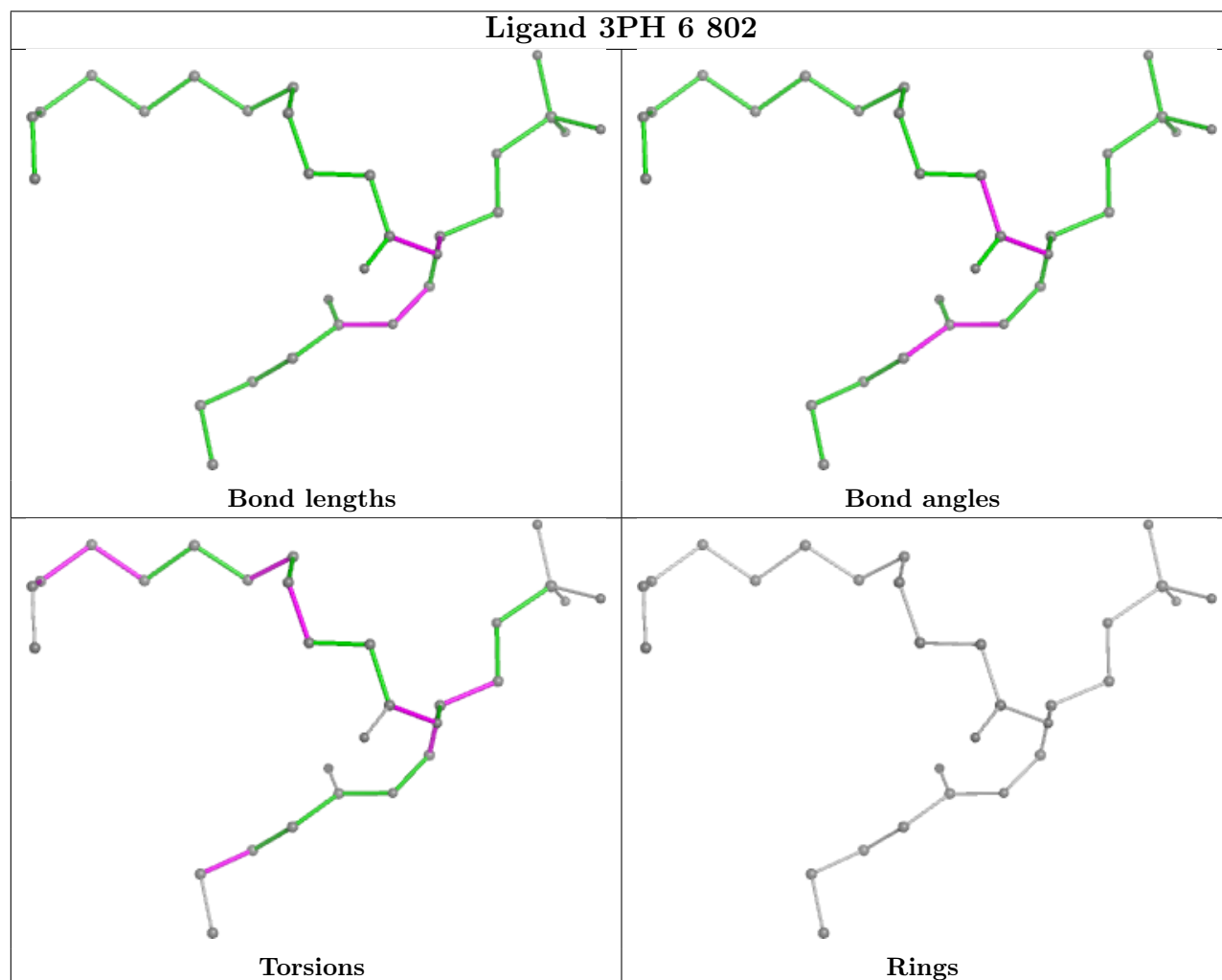
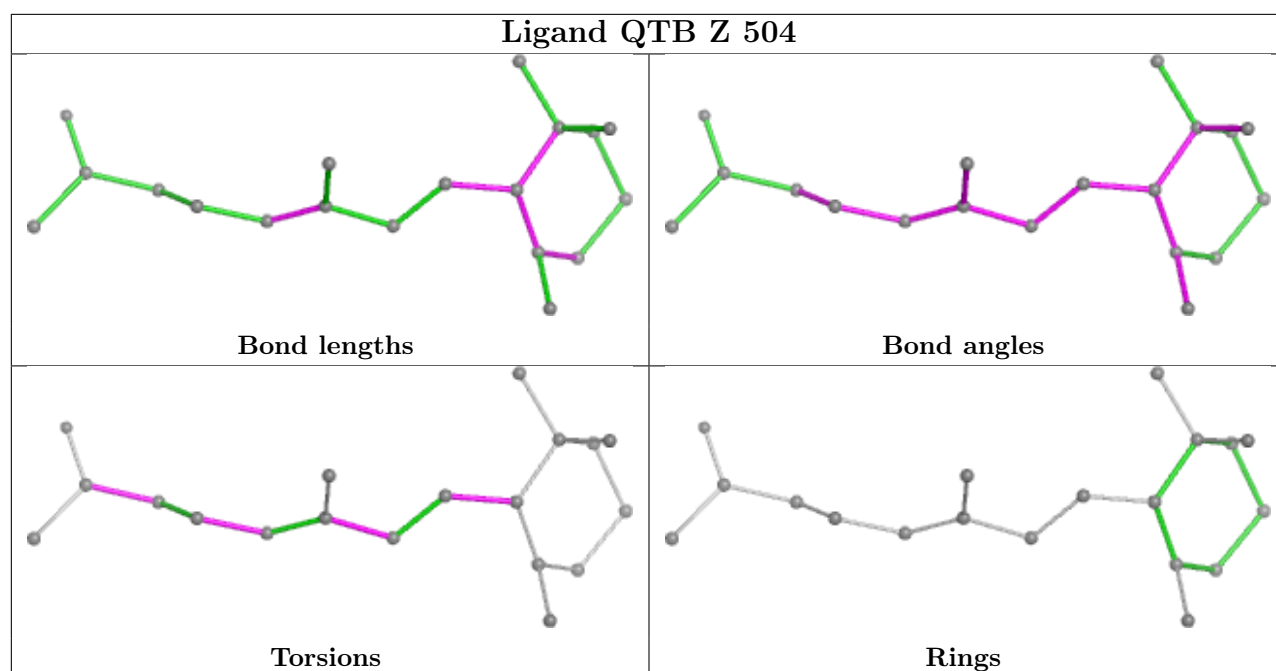
Ligand CLA 2 608



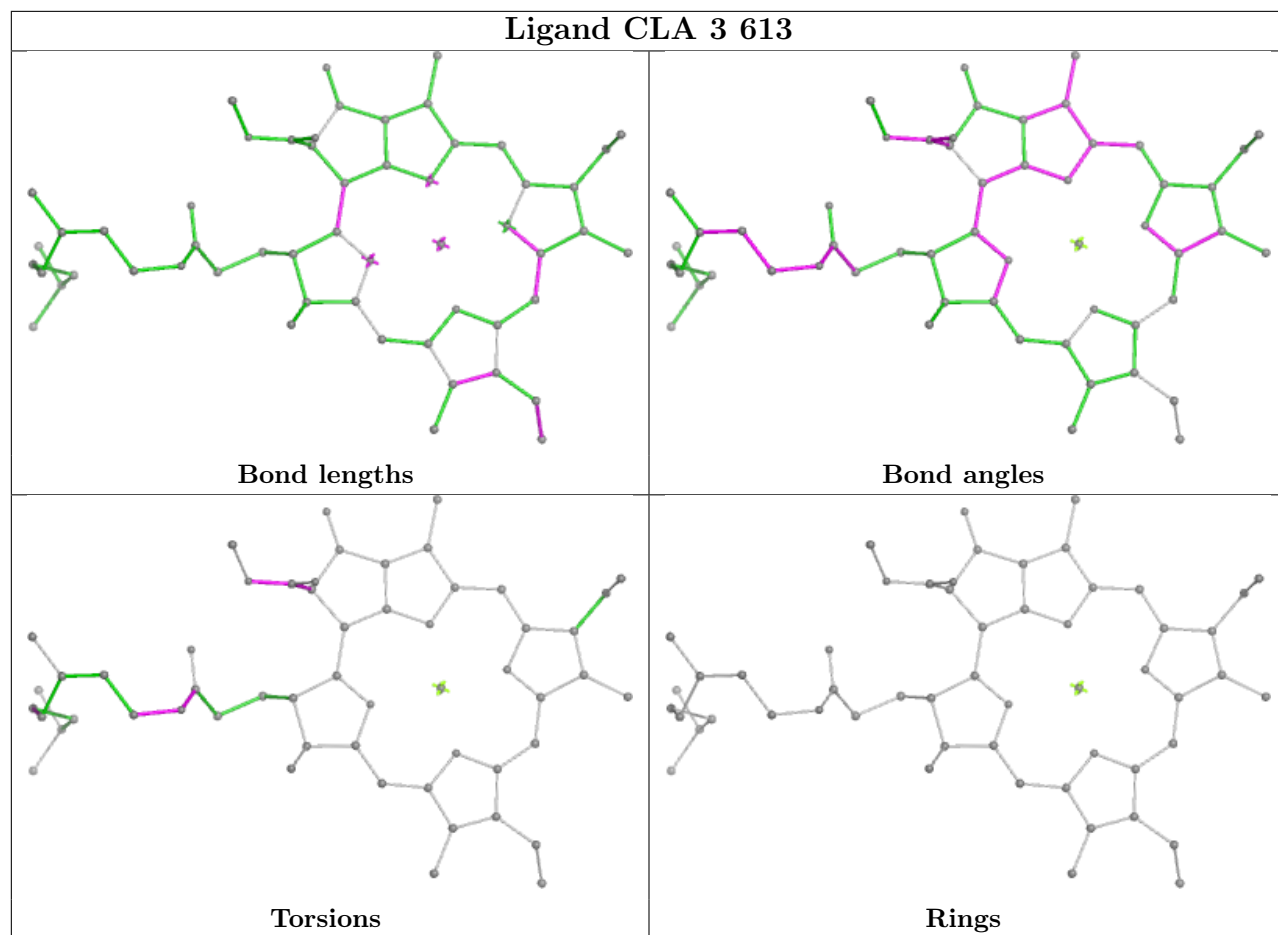
Ligand CHL 6 611



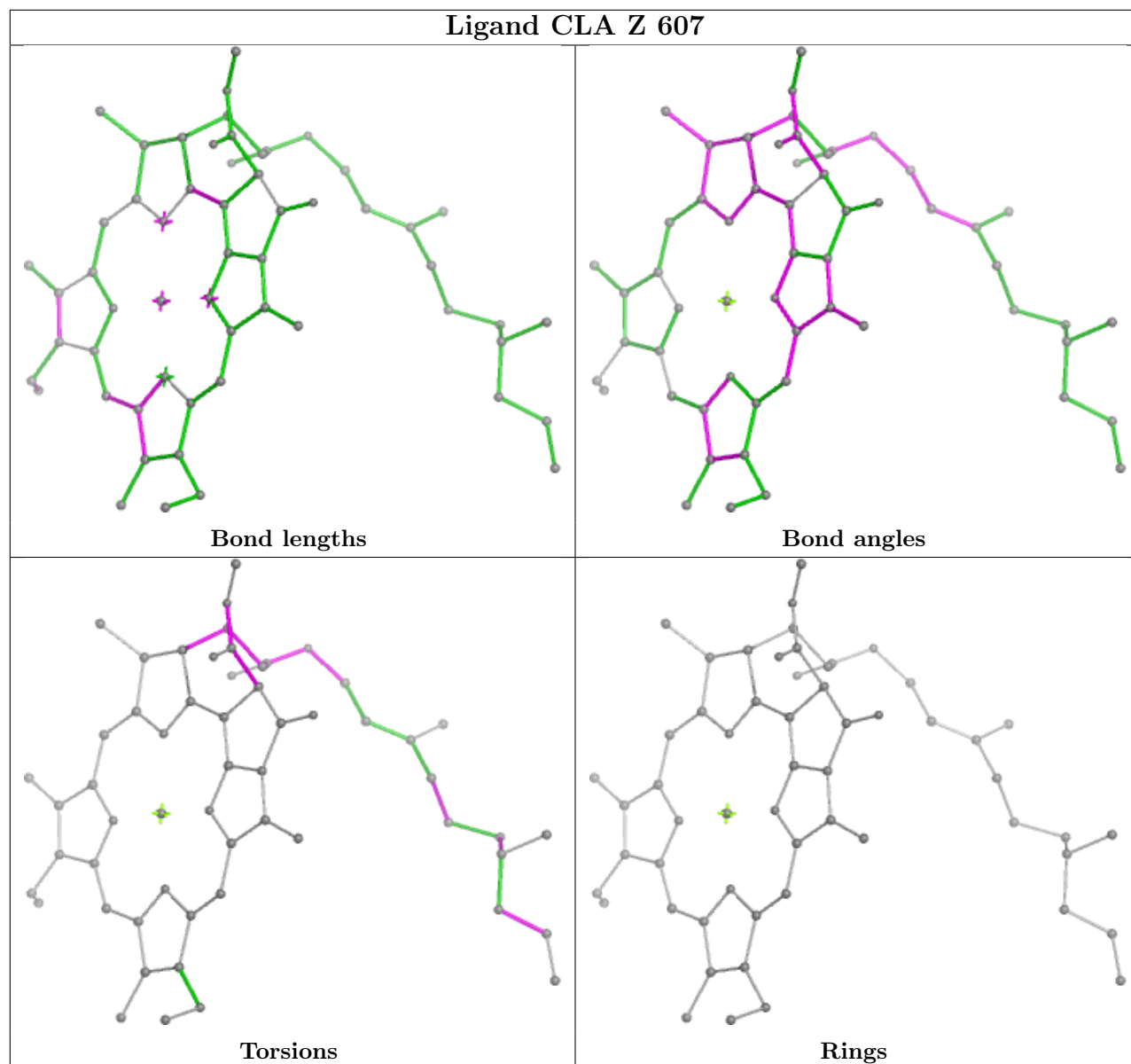




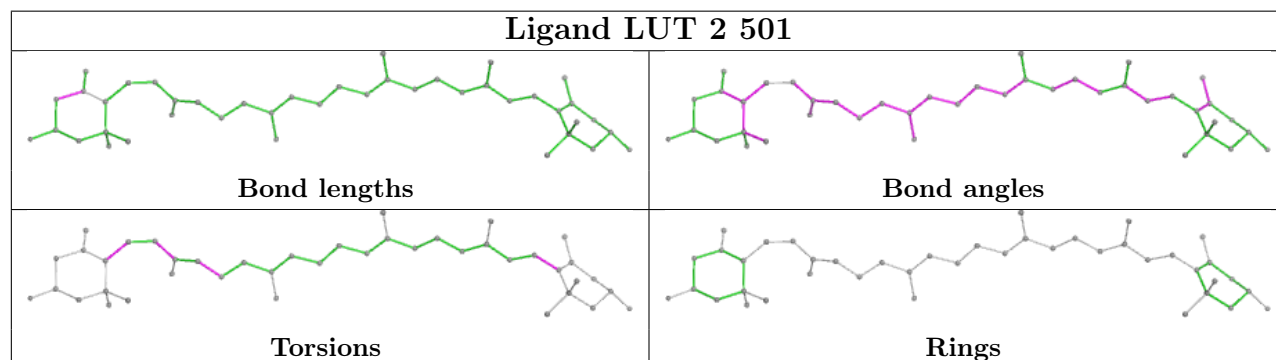
Ligand CLA 3 613

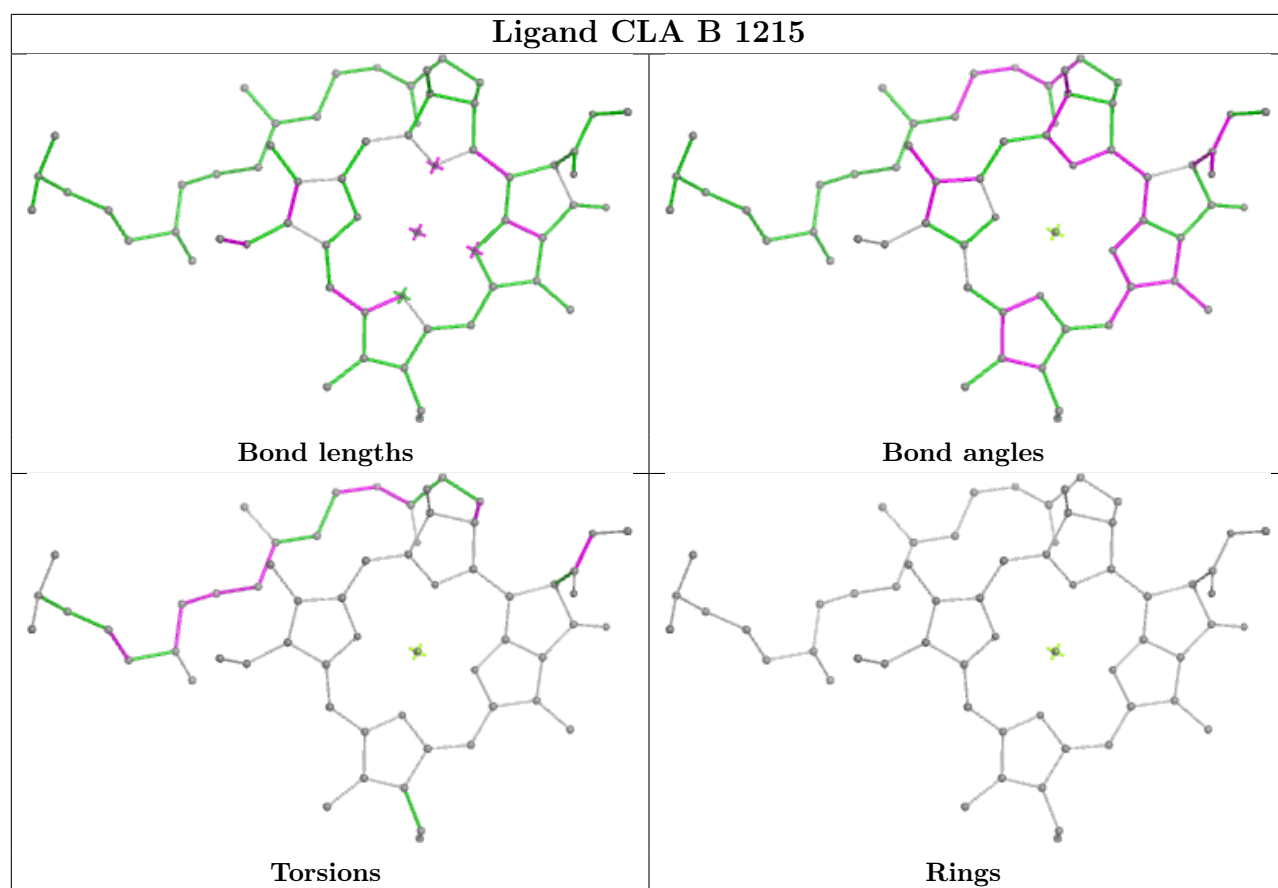


Ligand CLA Z 607

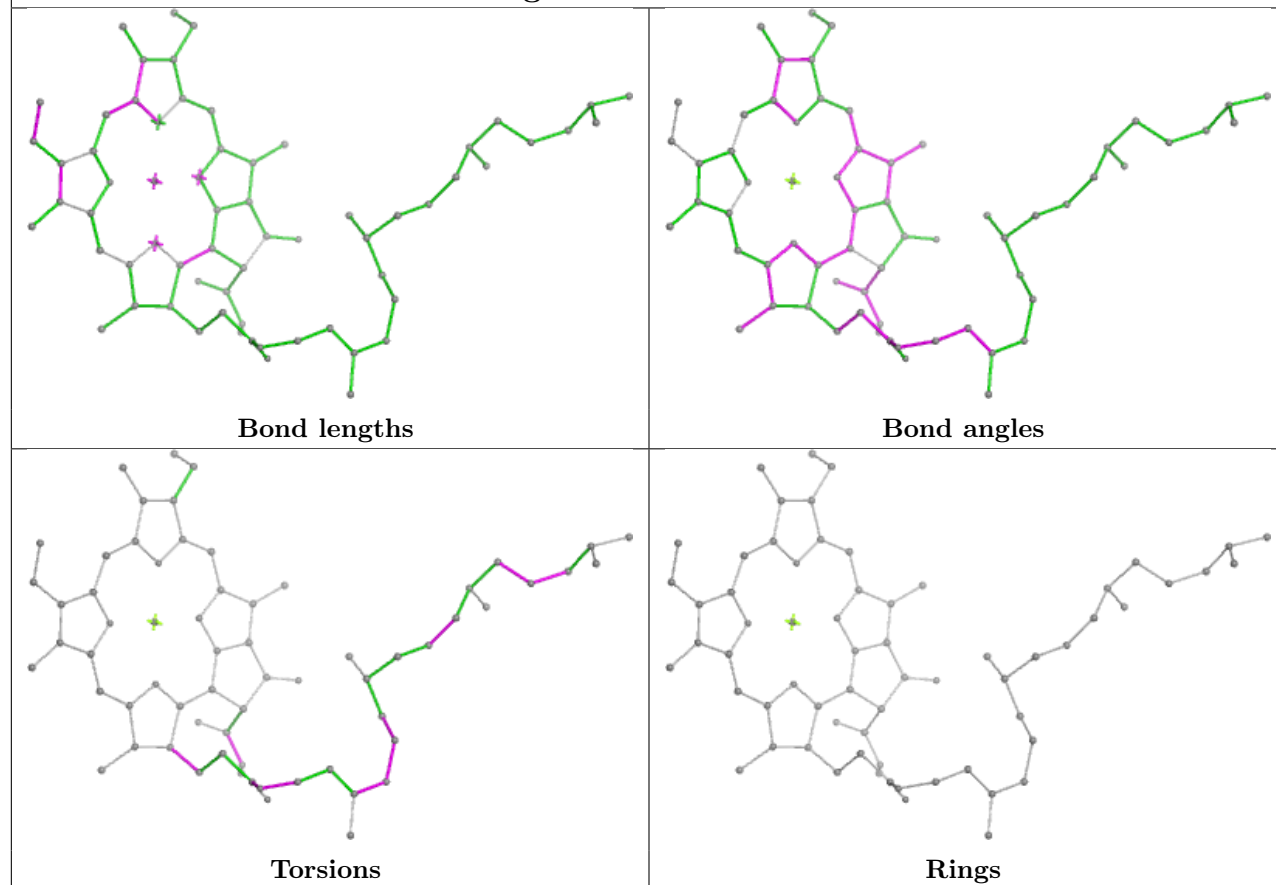


Ligand LUT 2 501

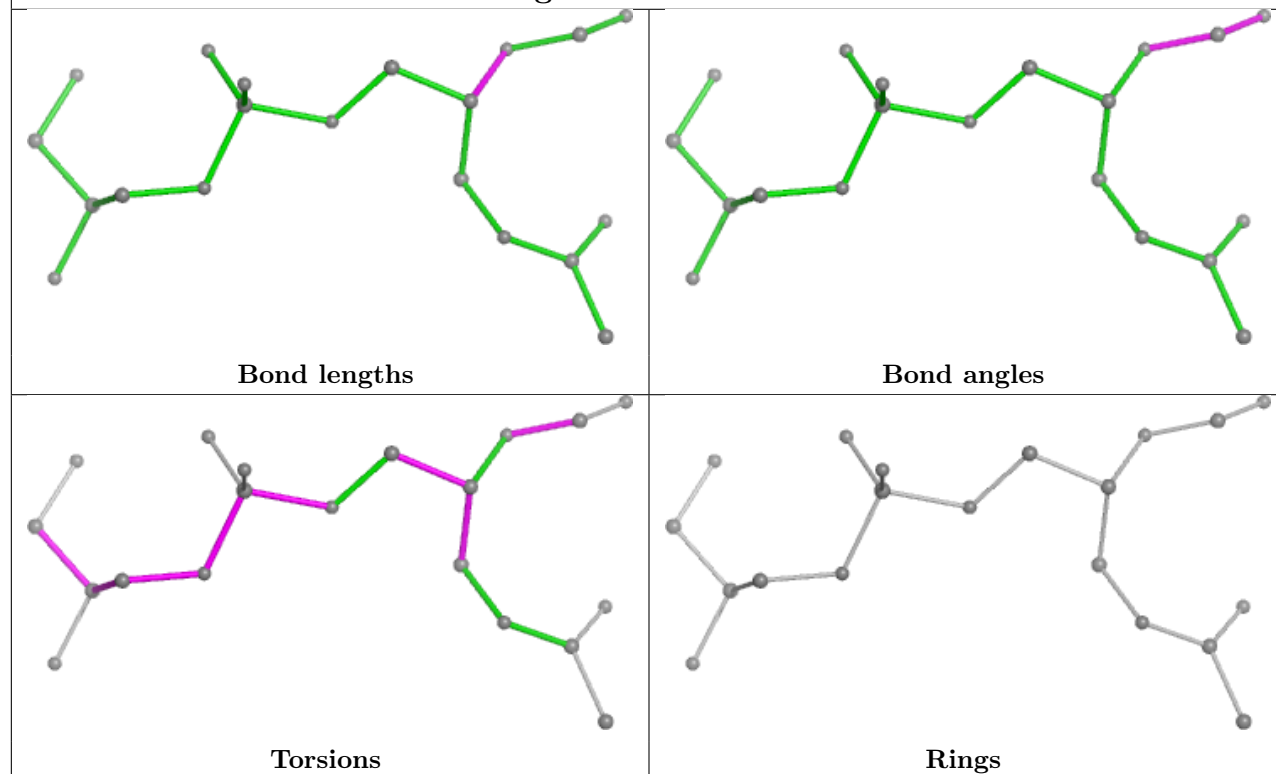




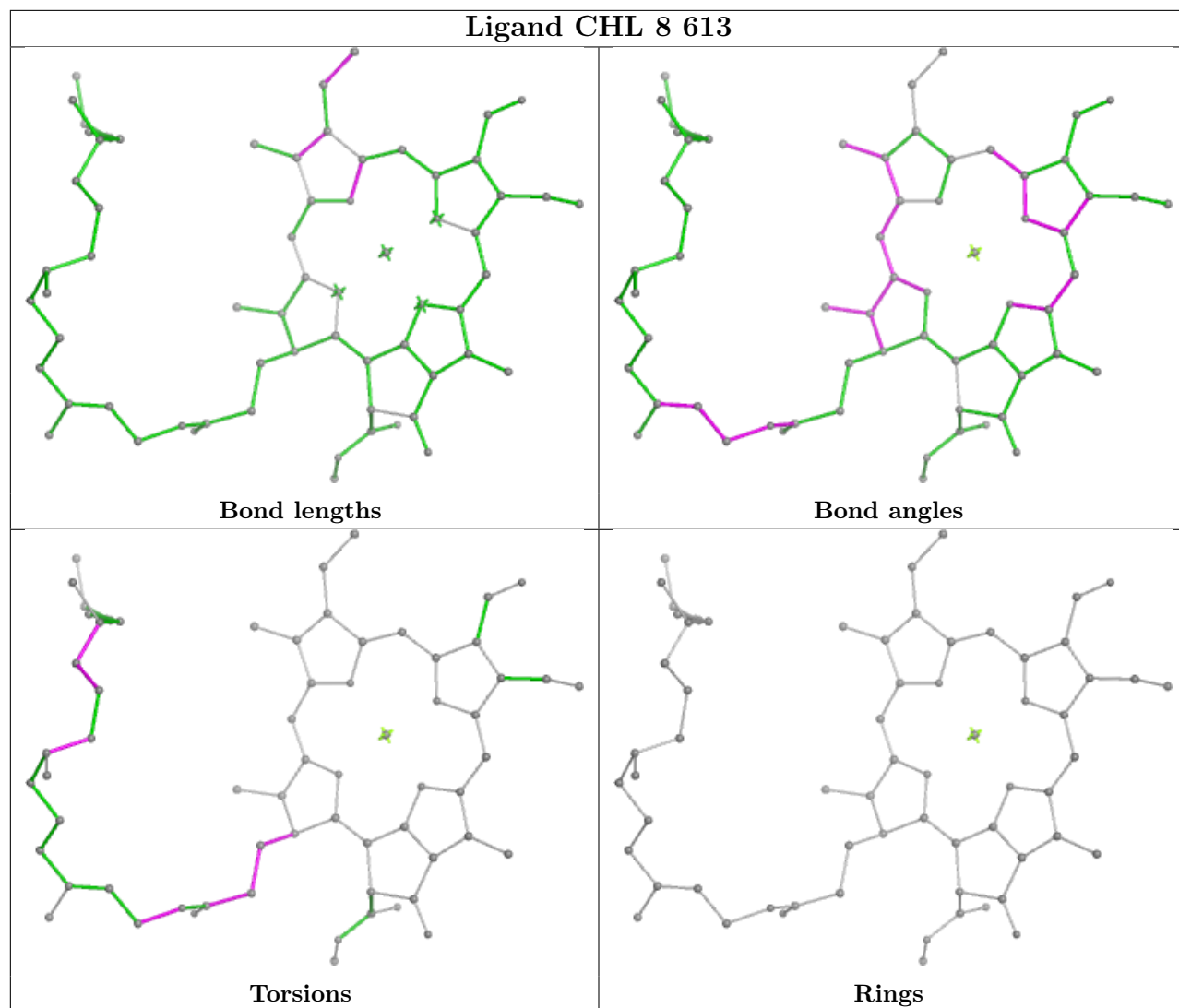
Ligand CLA B 1229



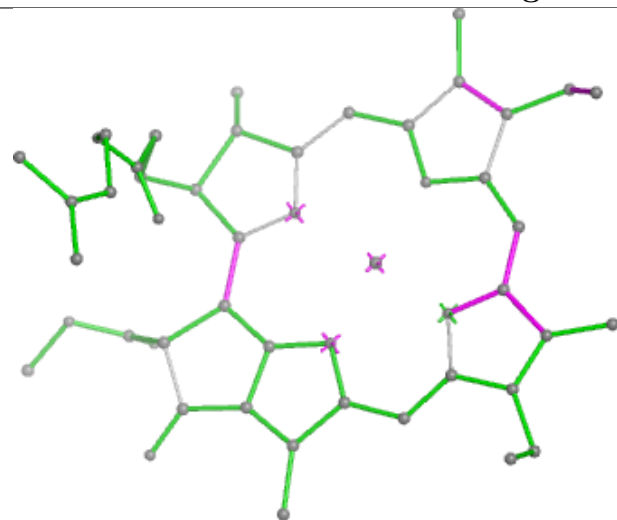
Ligand LHG 3 801



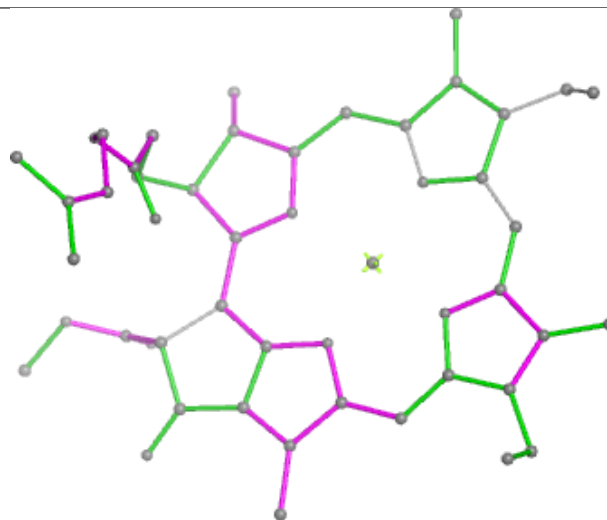
Ligand CHL 8 613



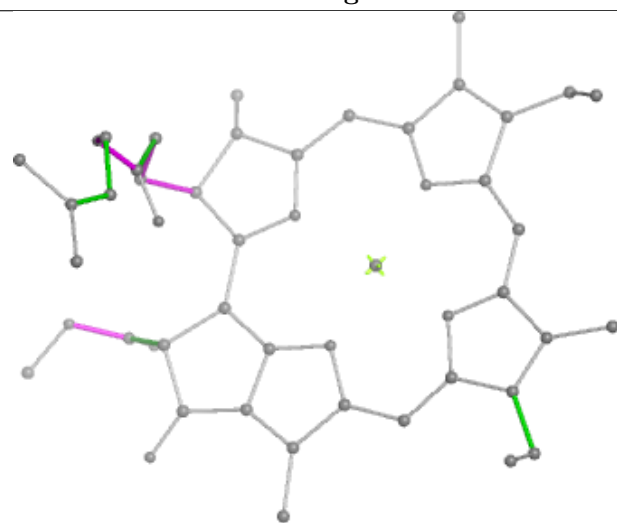
Ligand CLA 5 615



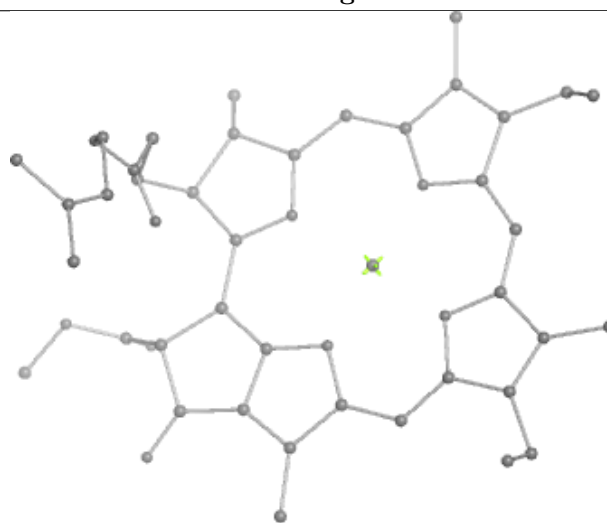
Bond lengths



Bond angles

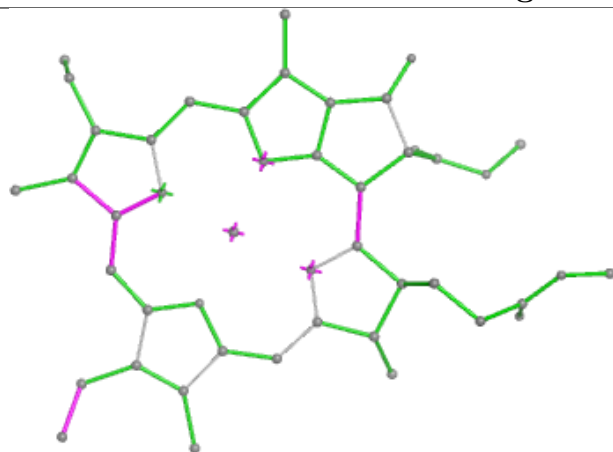


Torsions

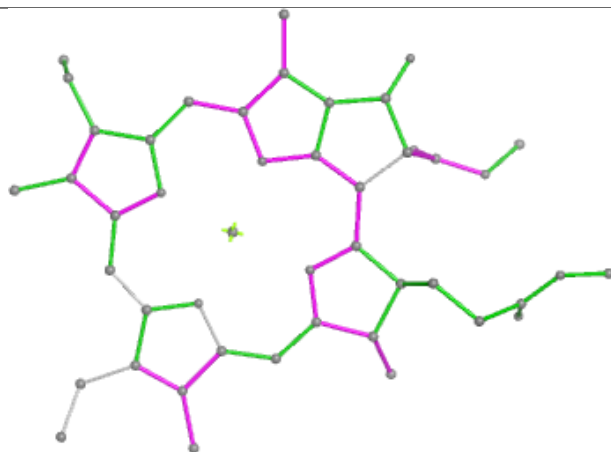


Rings

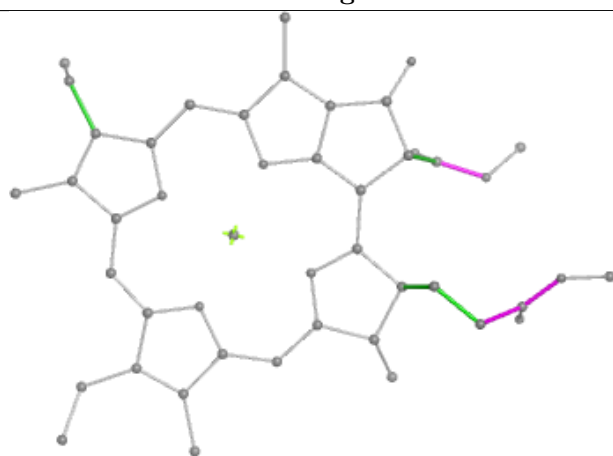
Ligand CLA Z 602



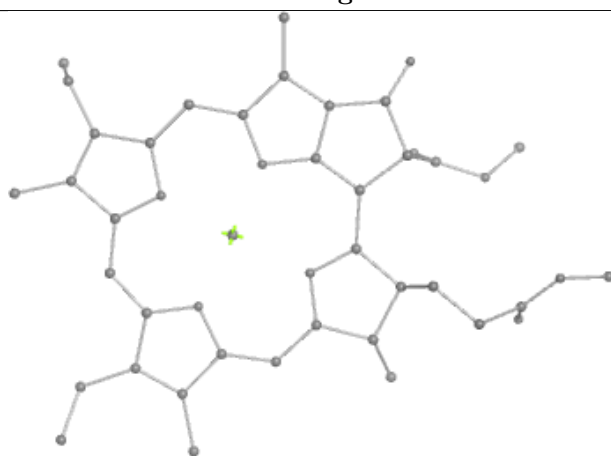
Bond lengths



Bond angles

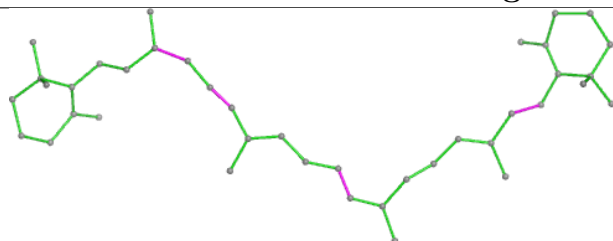


Torsions

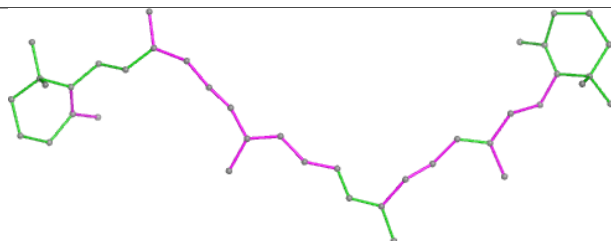


Rings

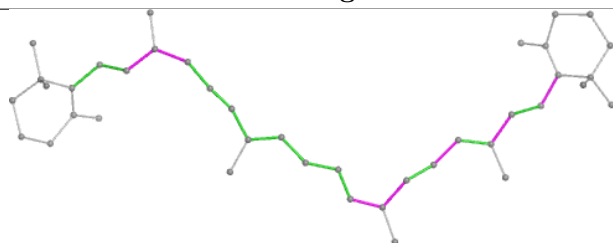
Ligand BCR A 4005



Bond lengths



Bond angles

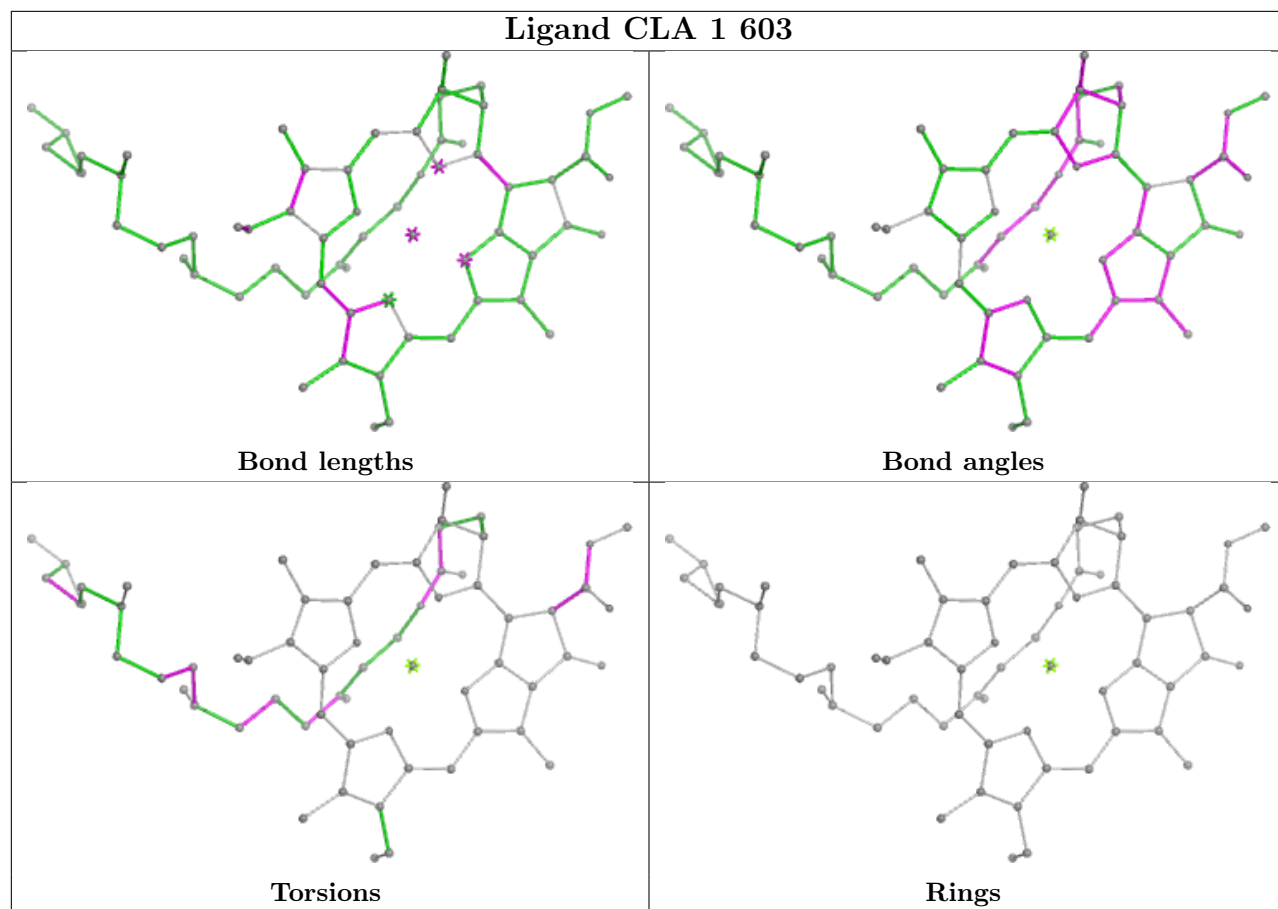


Torsions

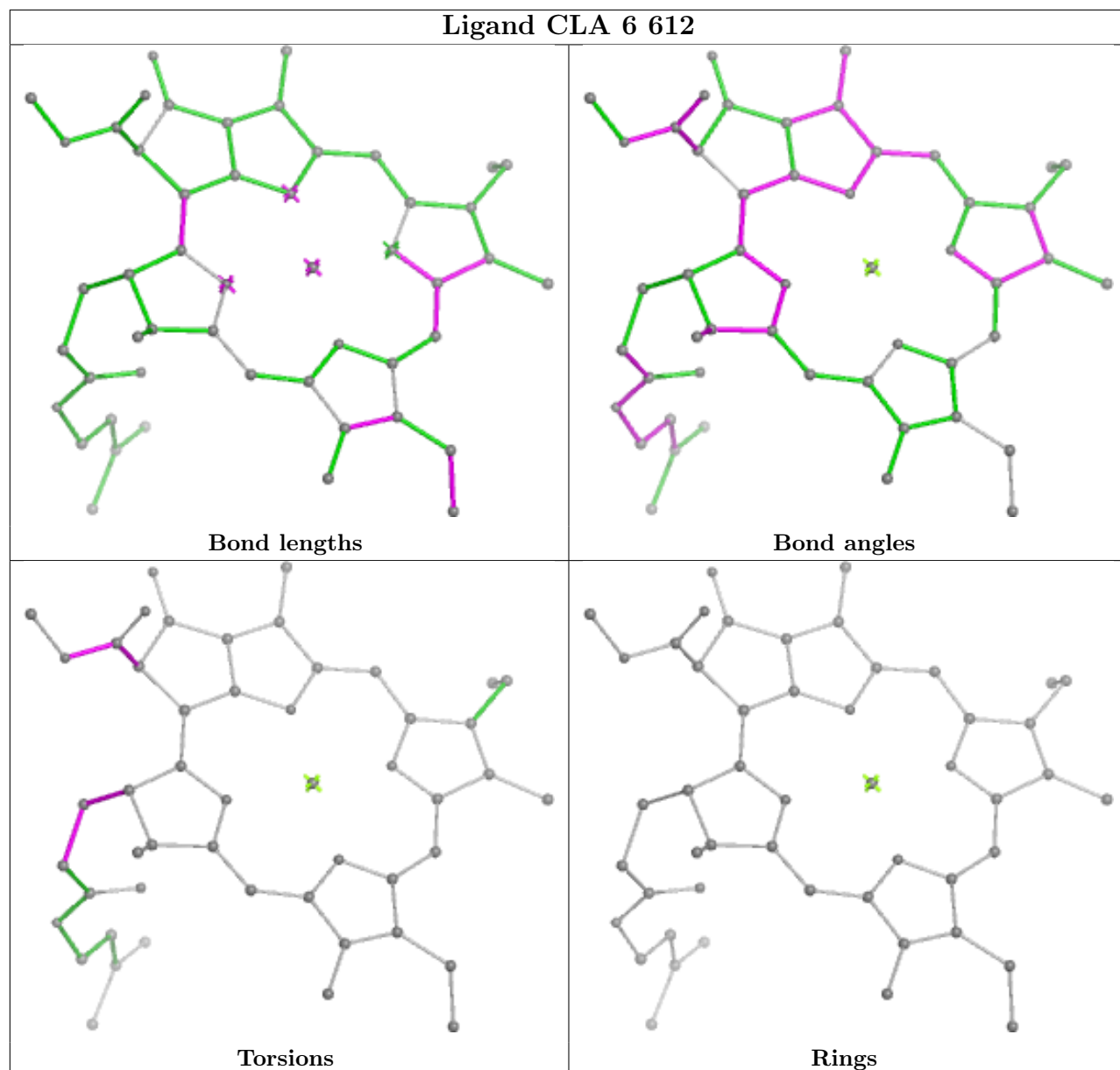


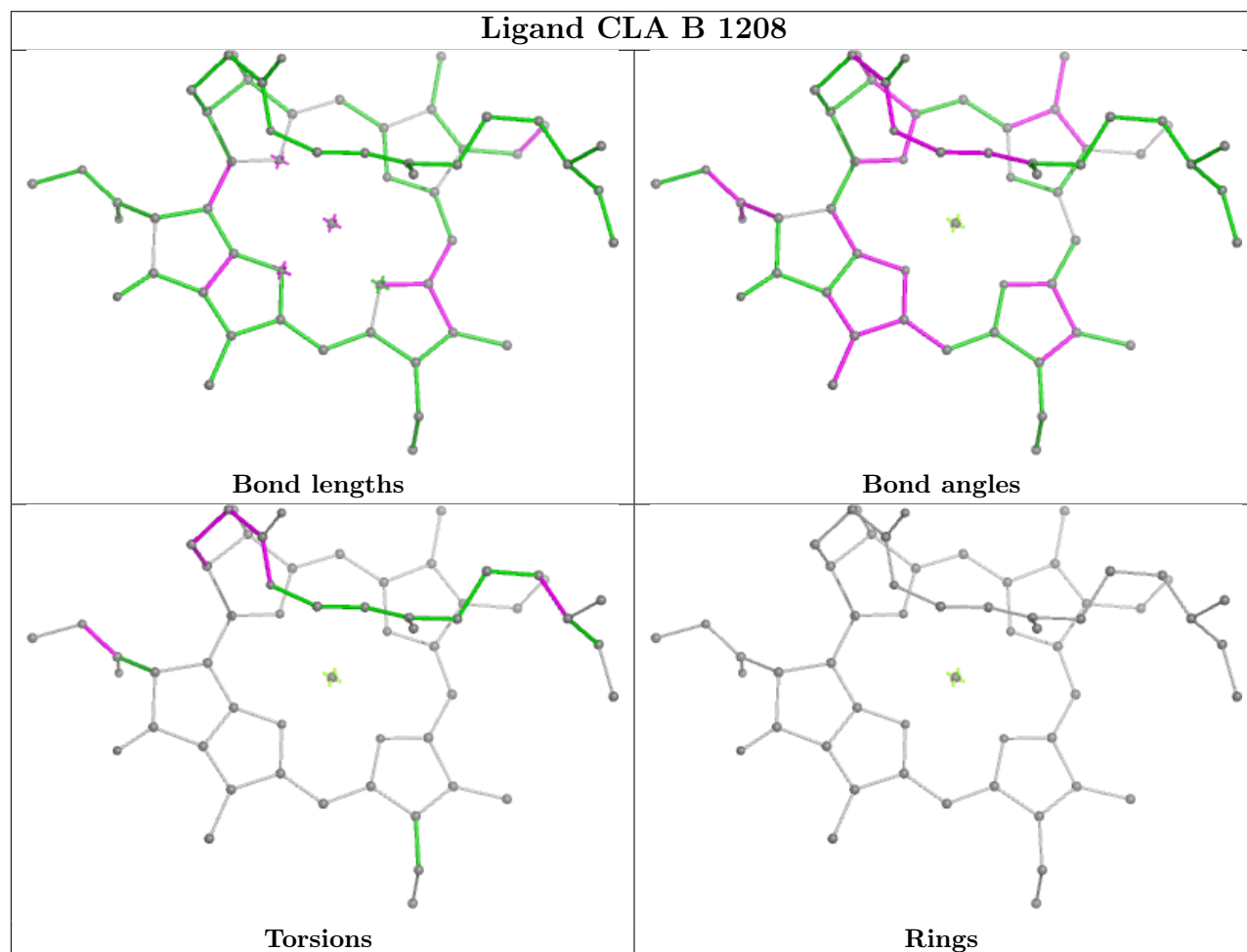
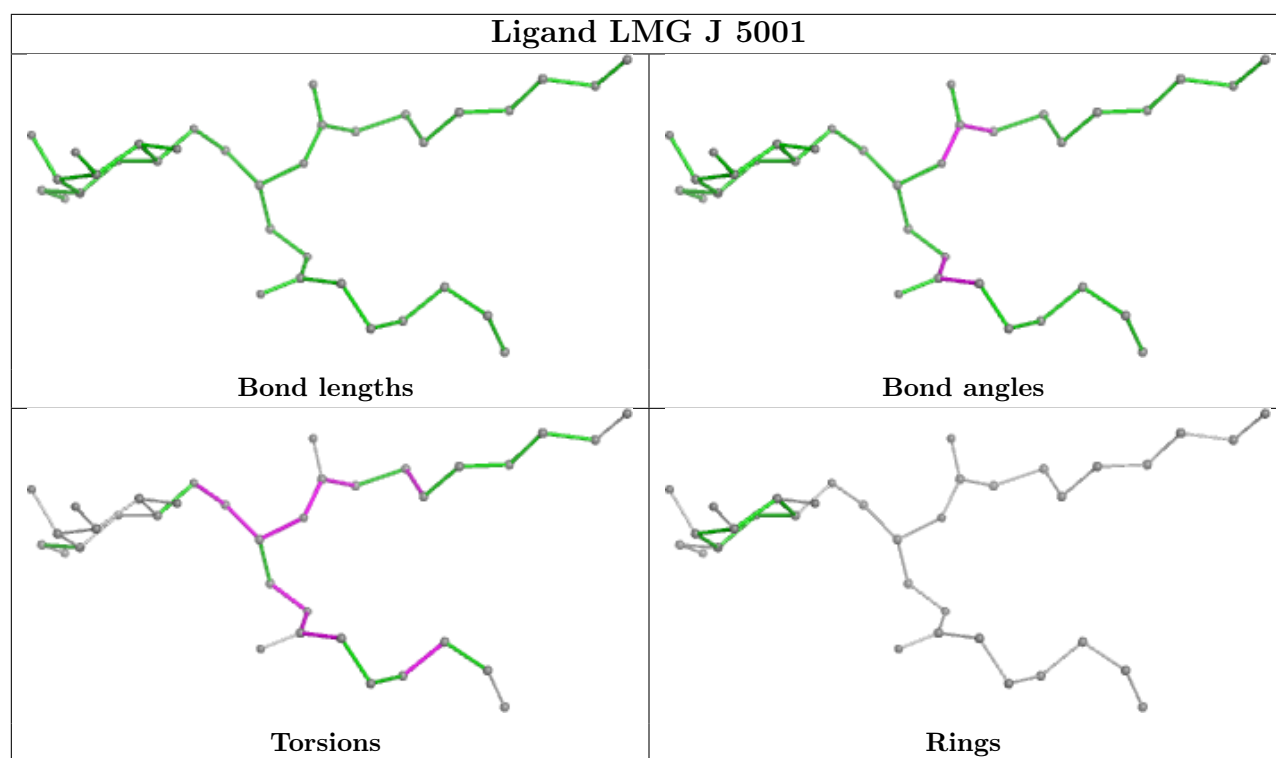
Rings

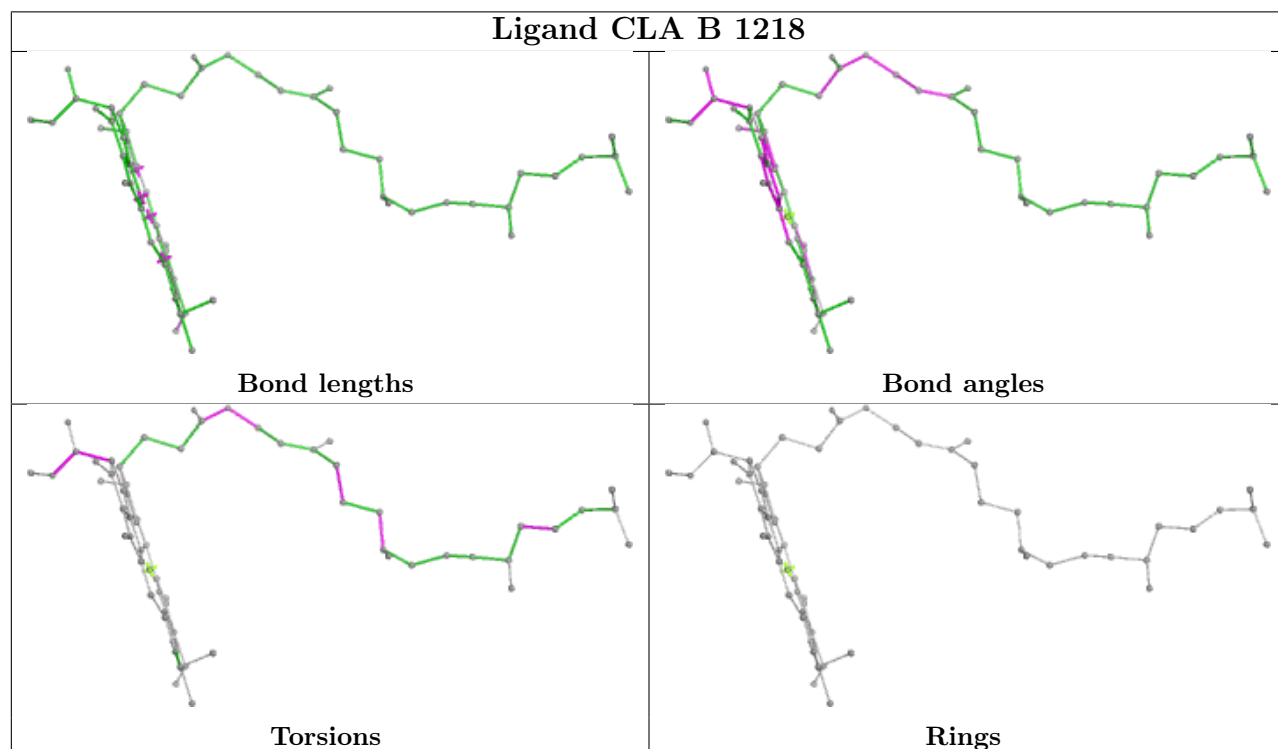
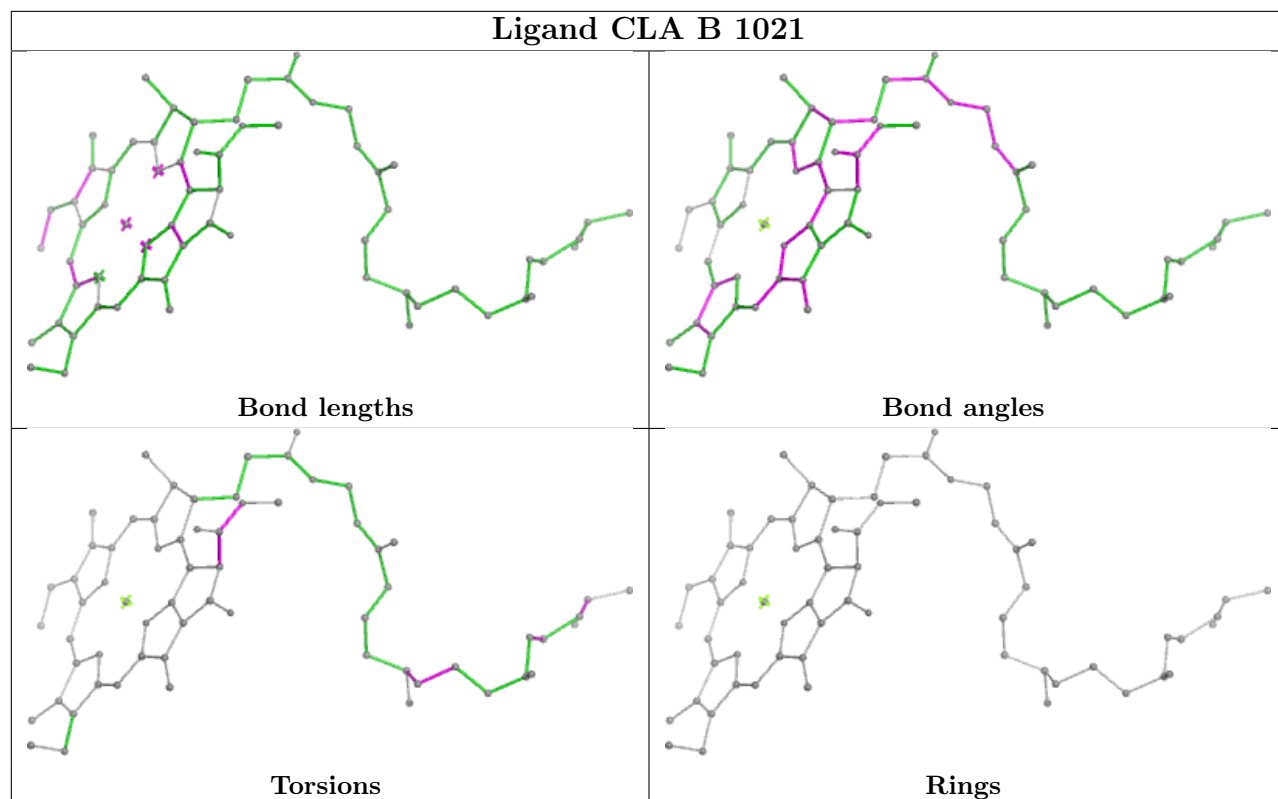
Ligand CLA 1 603



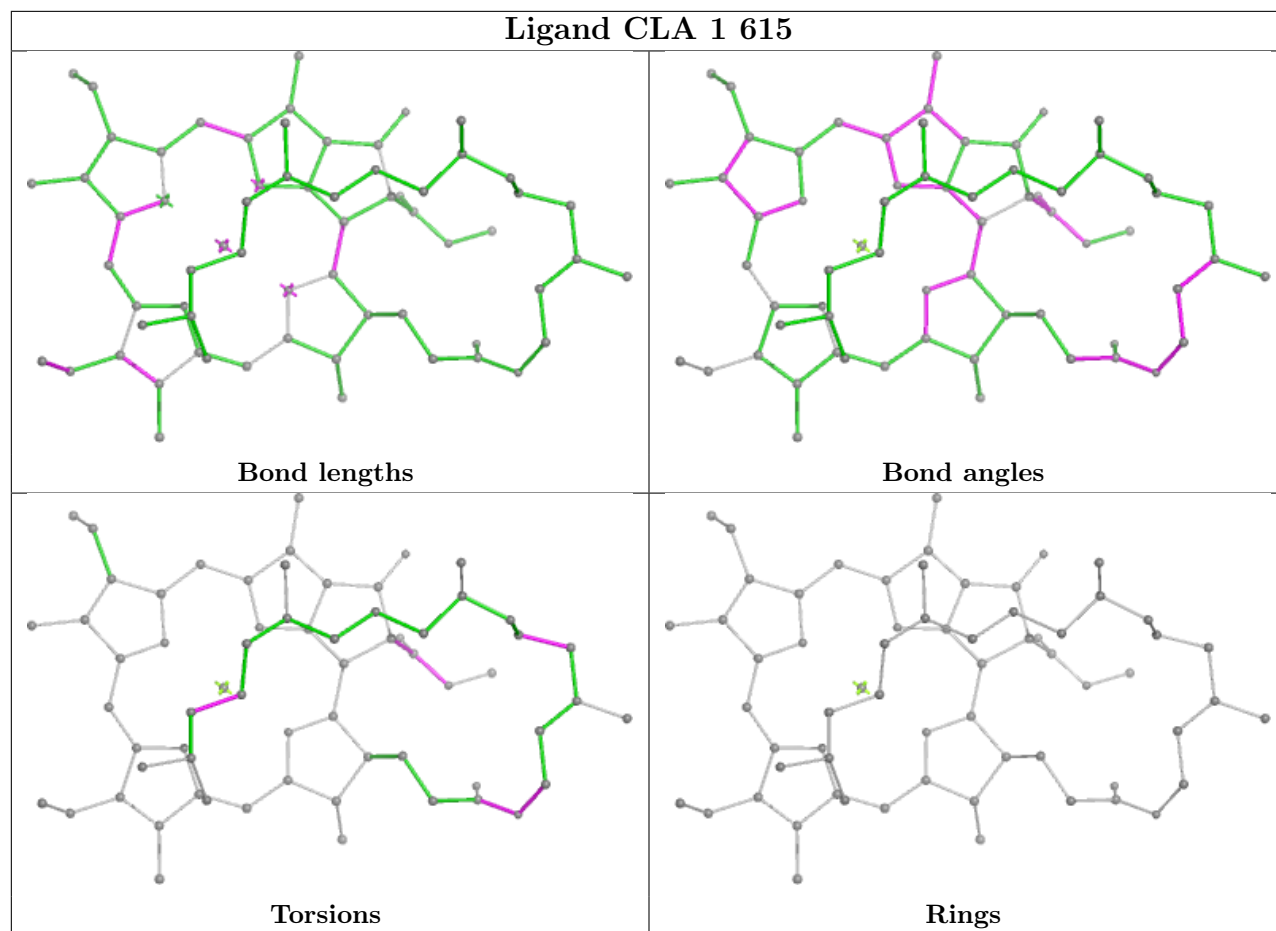
Ligand CLA 6 612



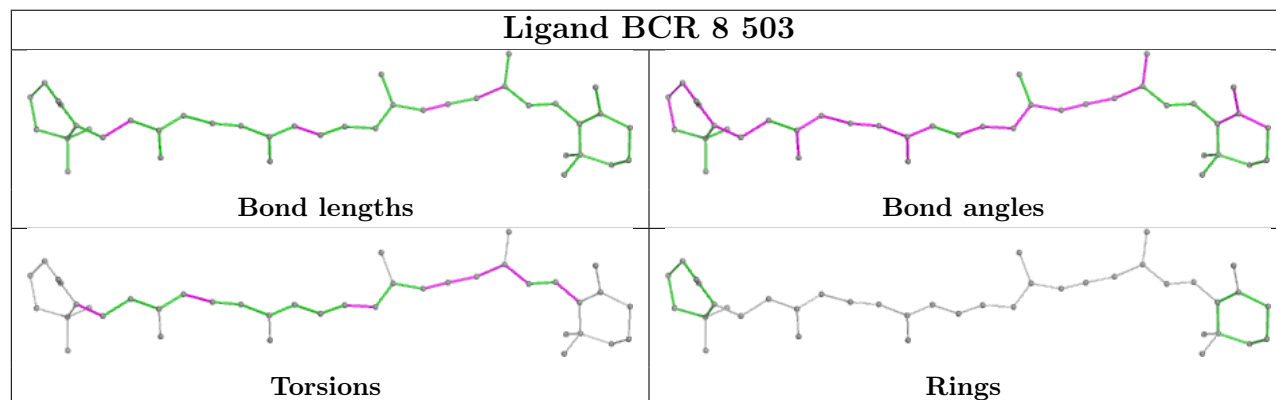


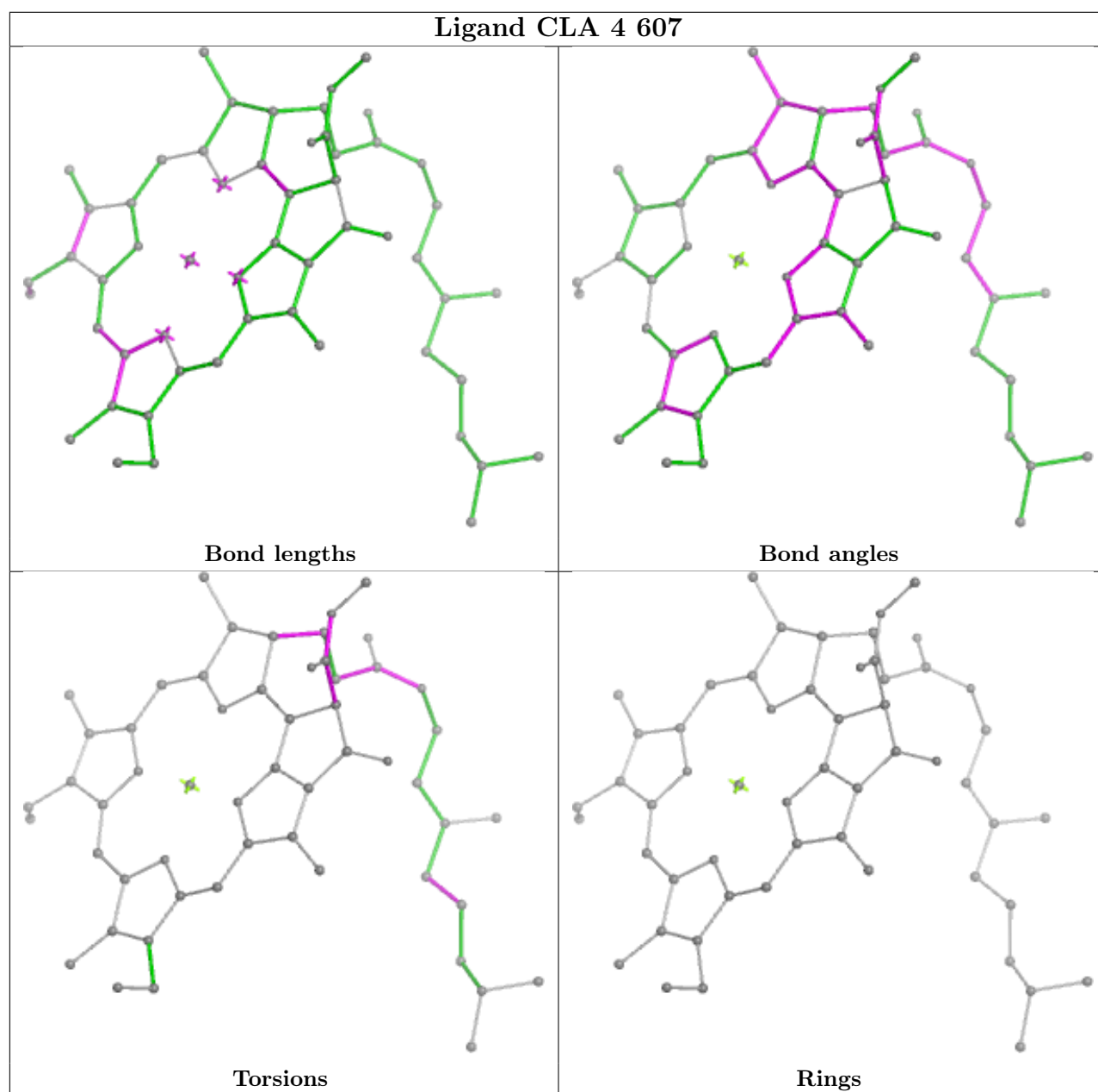
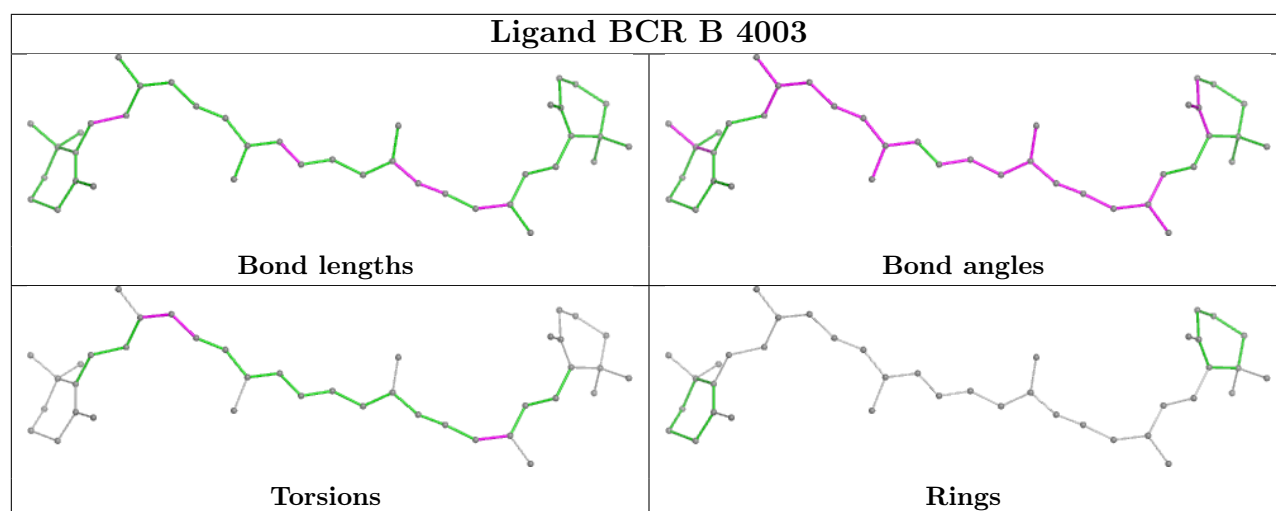


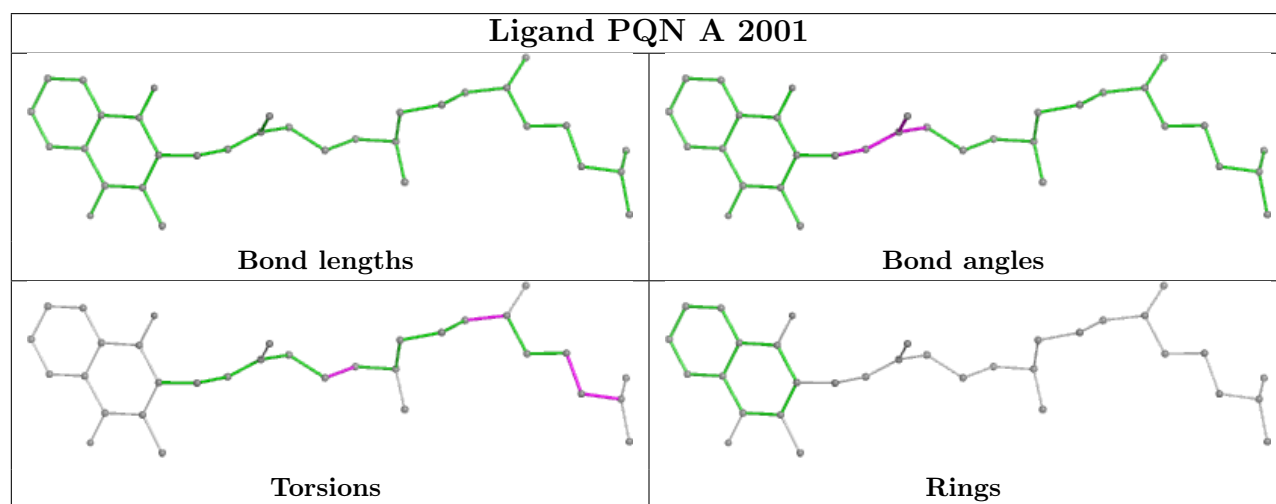
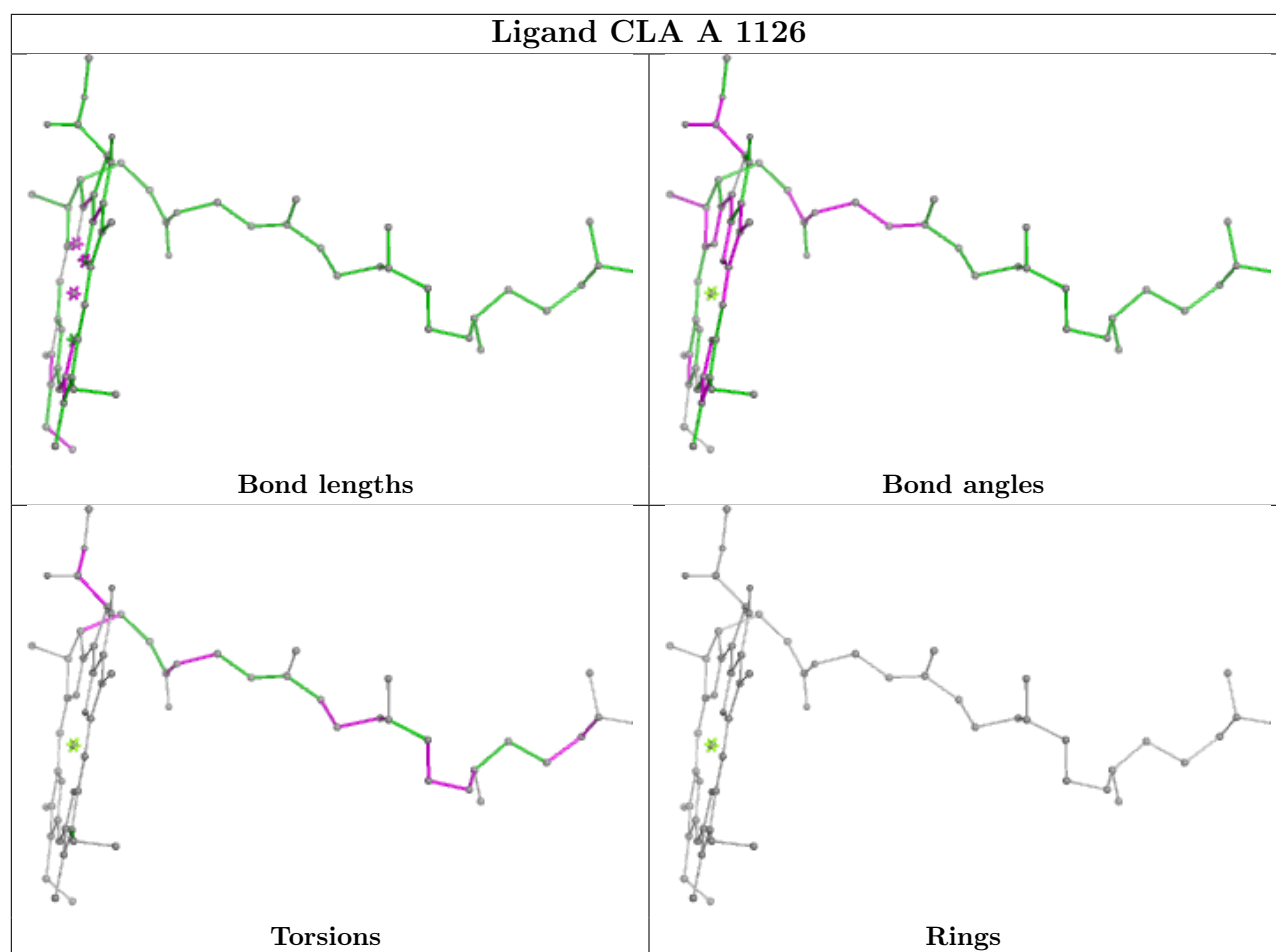
Ligand CLA 1 615

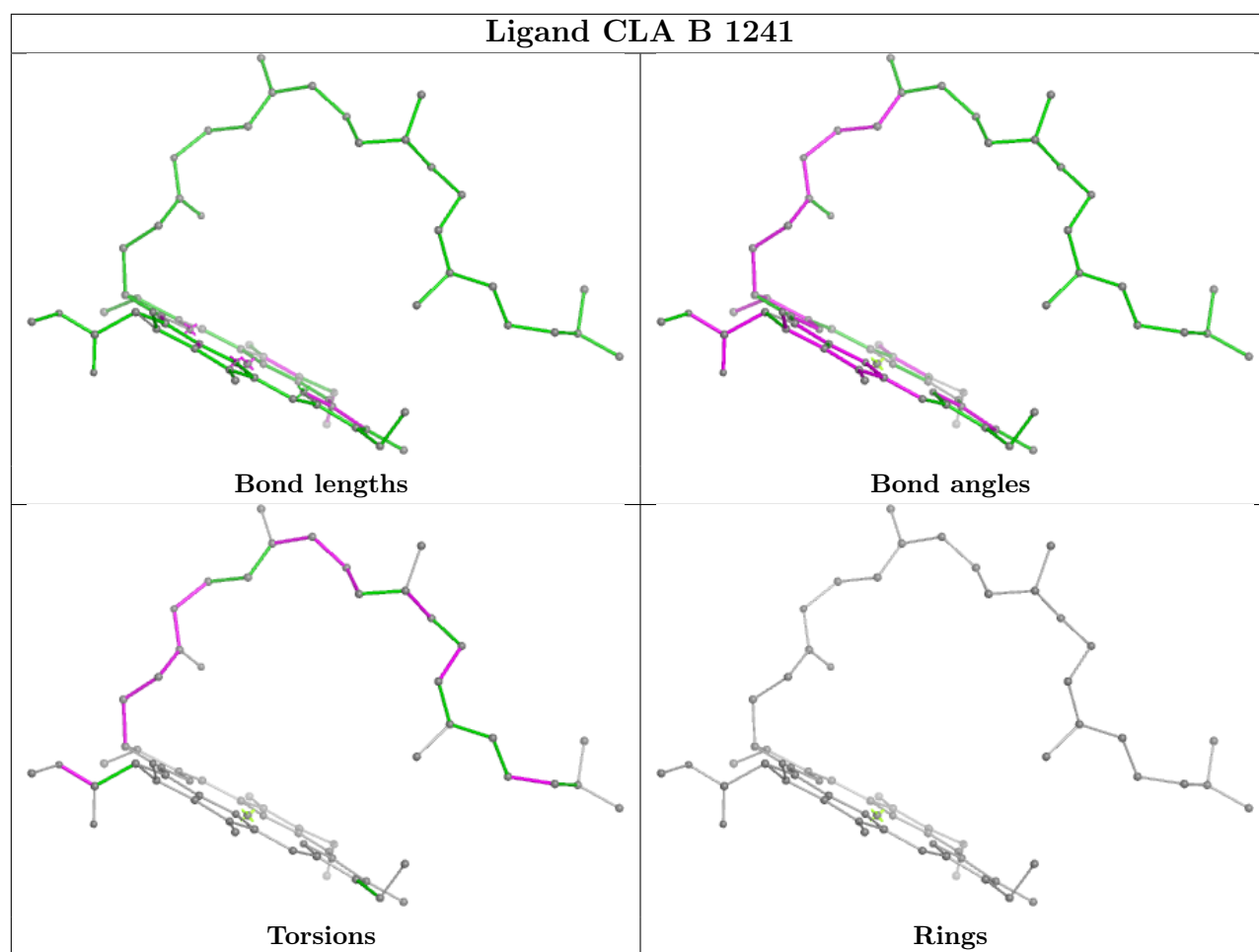


Ligand BCR 8 503

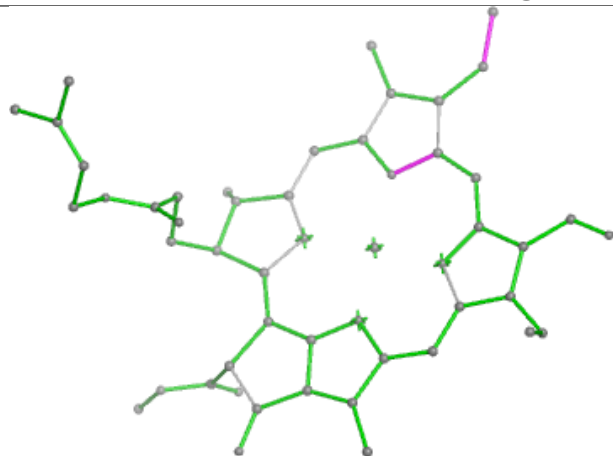




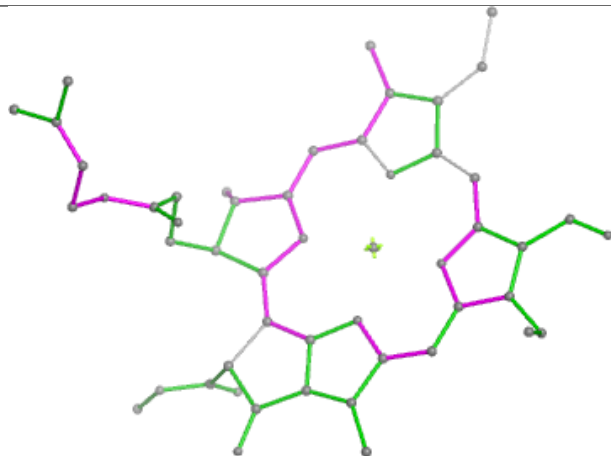




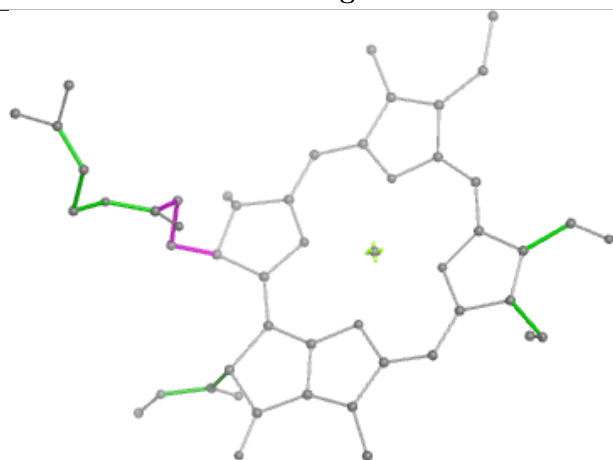
Ligand CHL 4 611



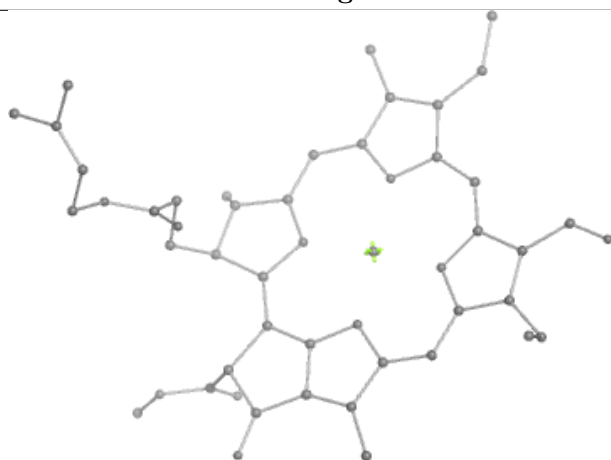
Bond lengths



Bond angles

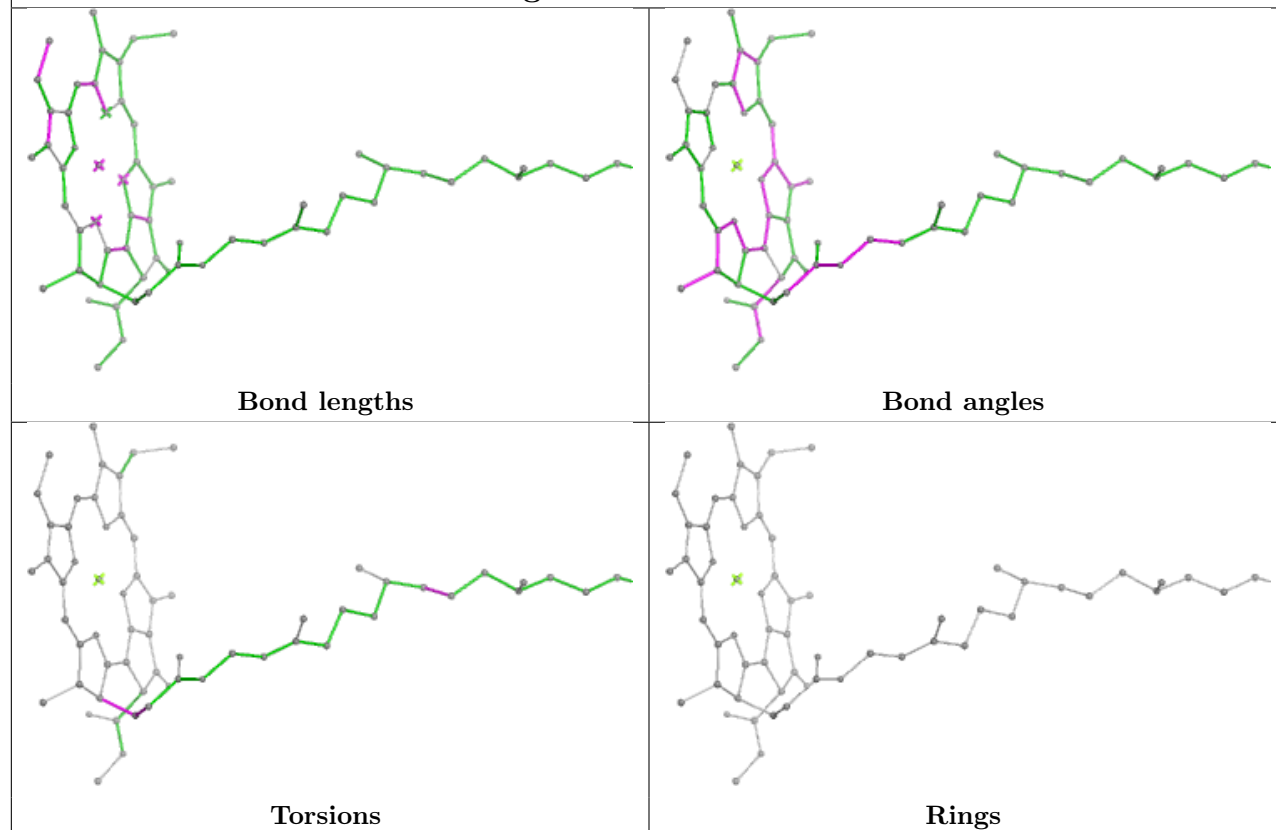


Torsions

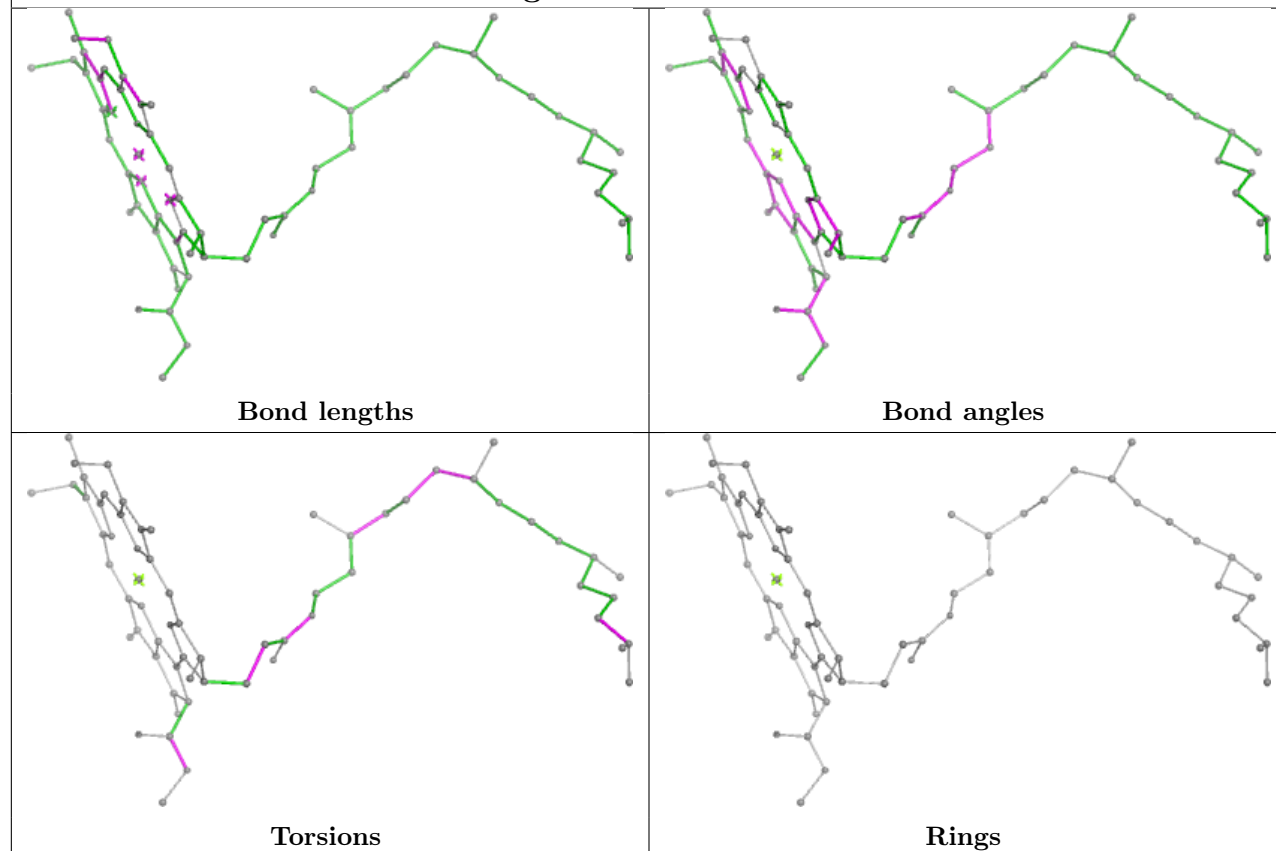


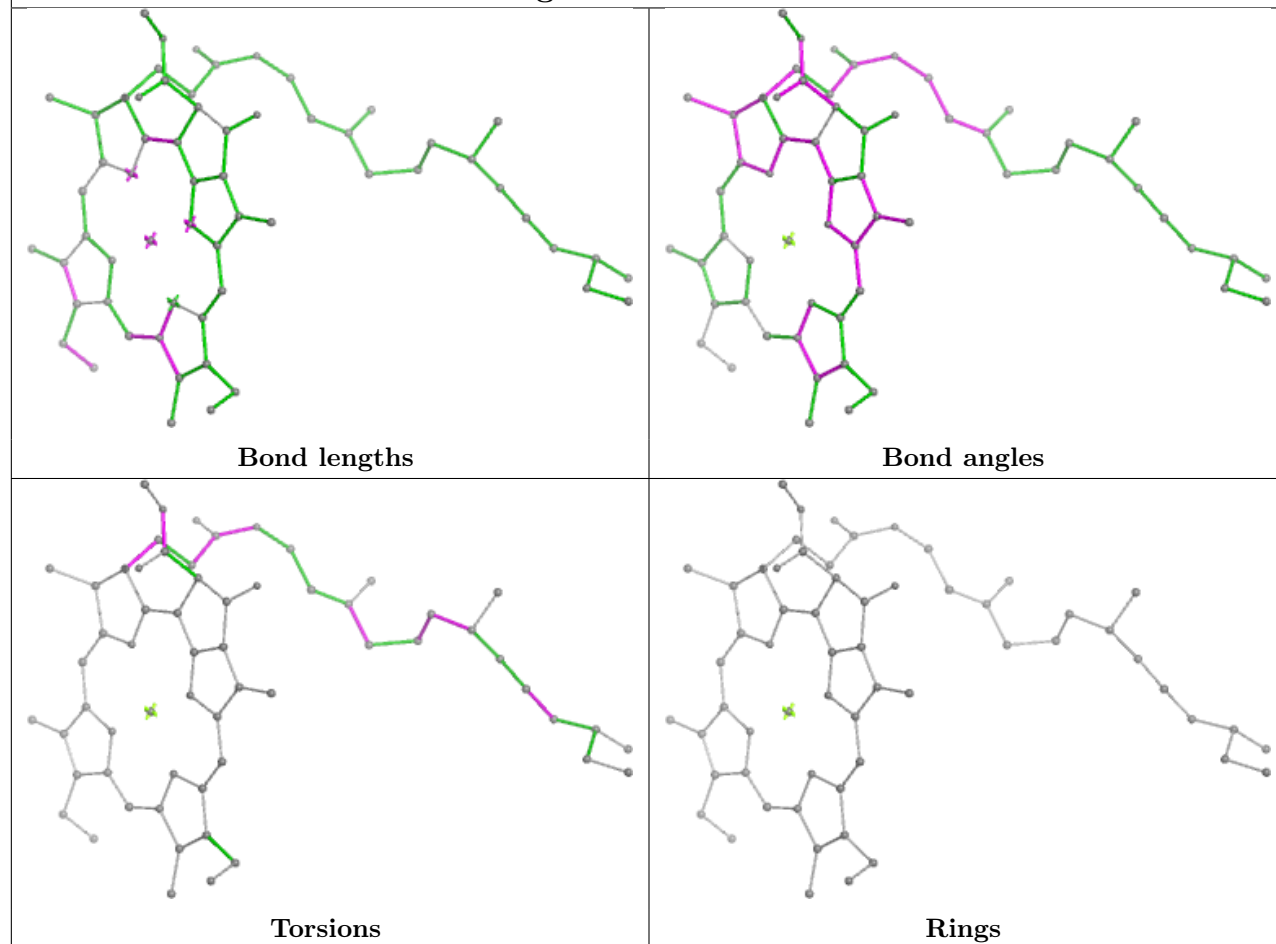
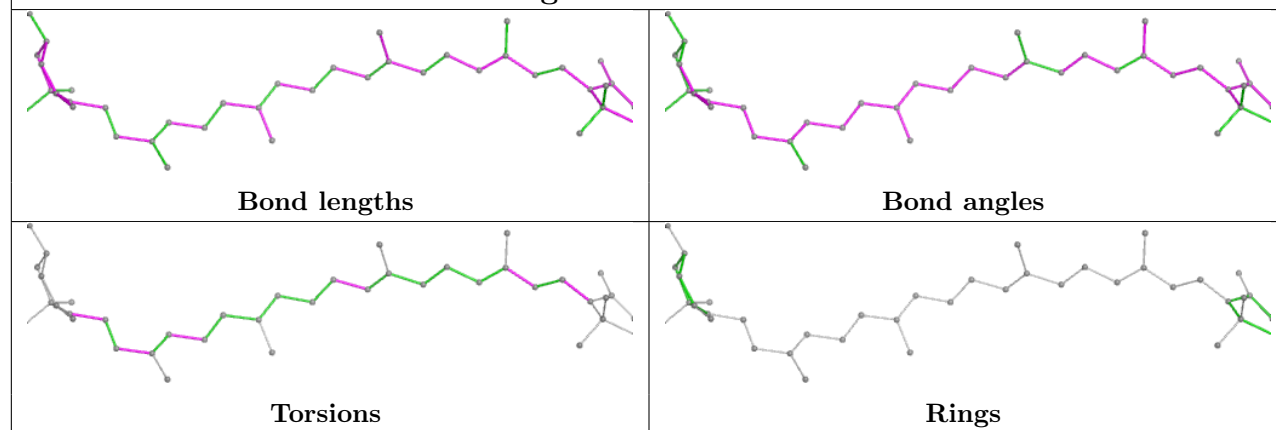
Rings

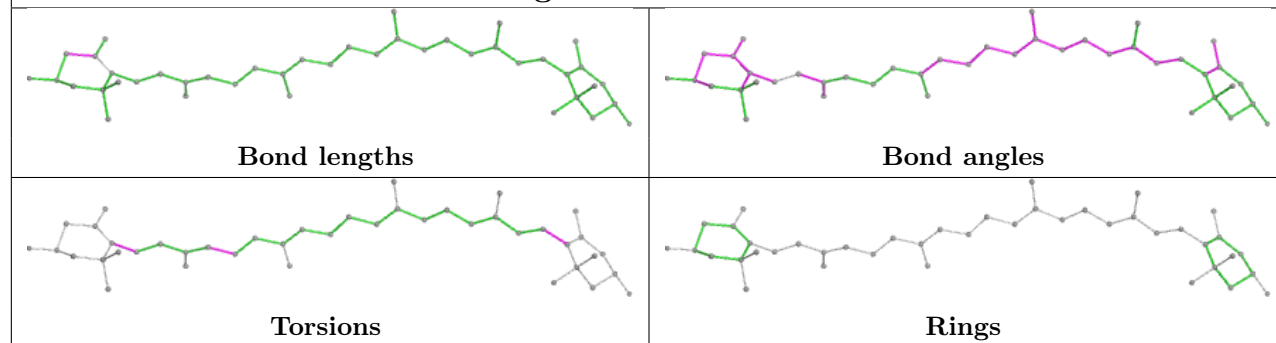
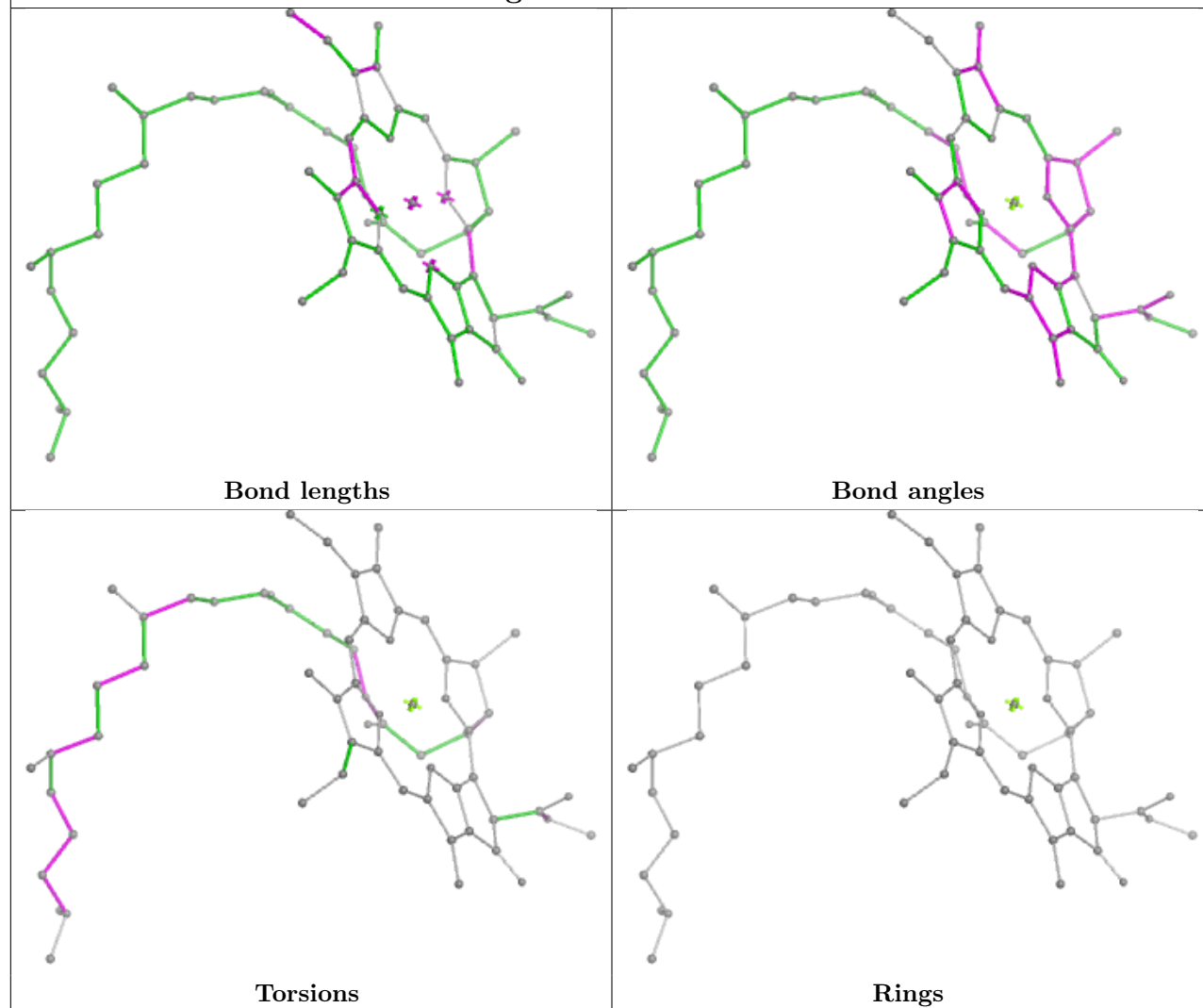
Ligand CLA B 1225



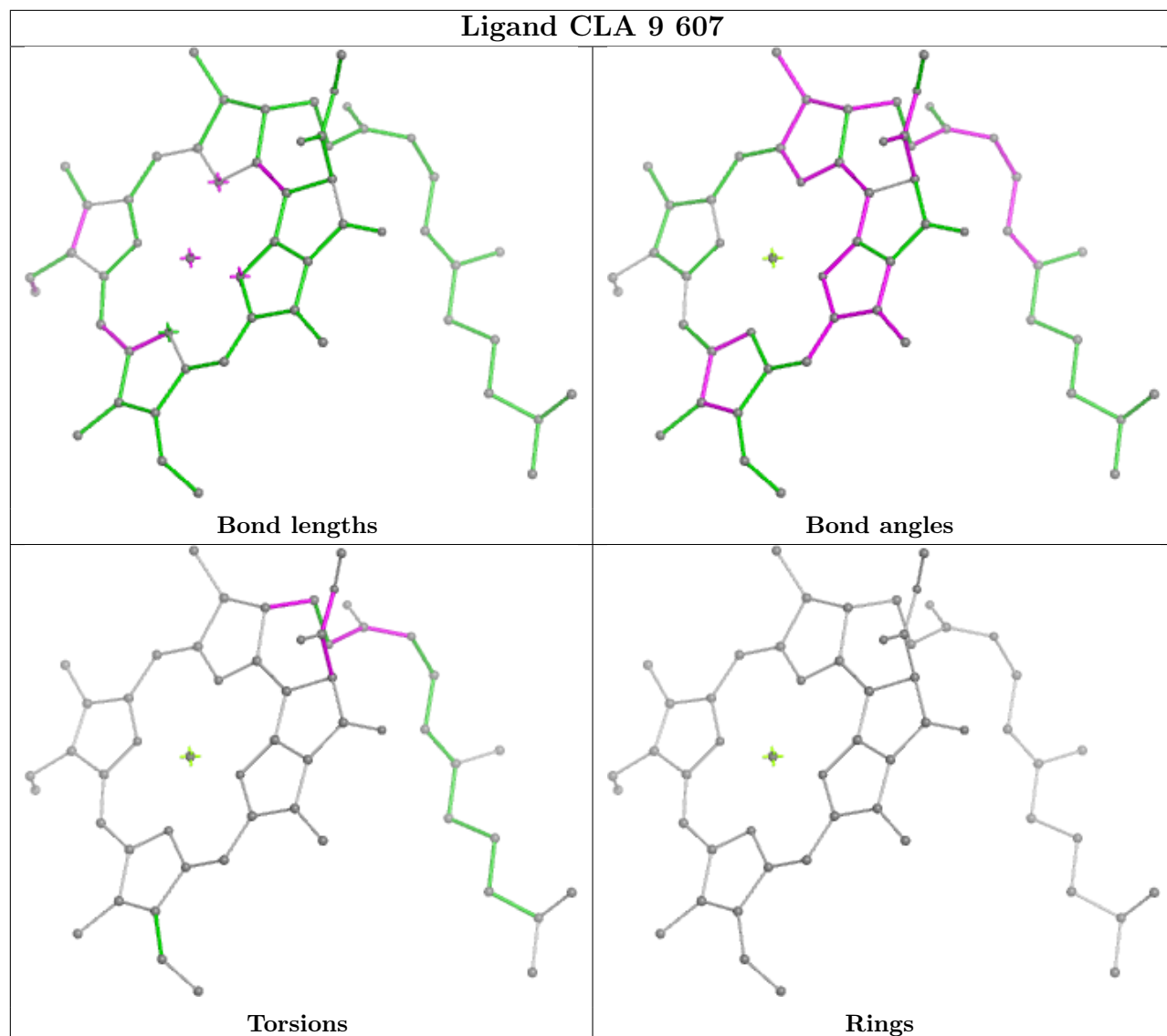
Ligand CLA B 1238

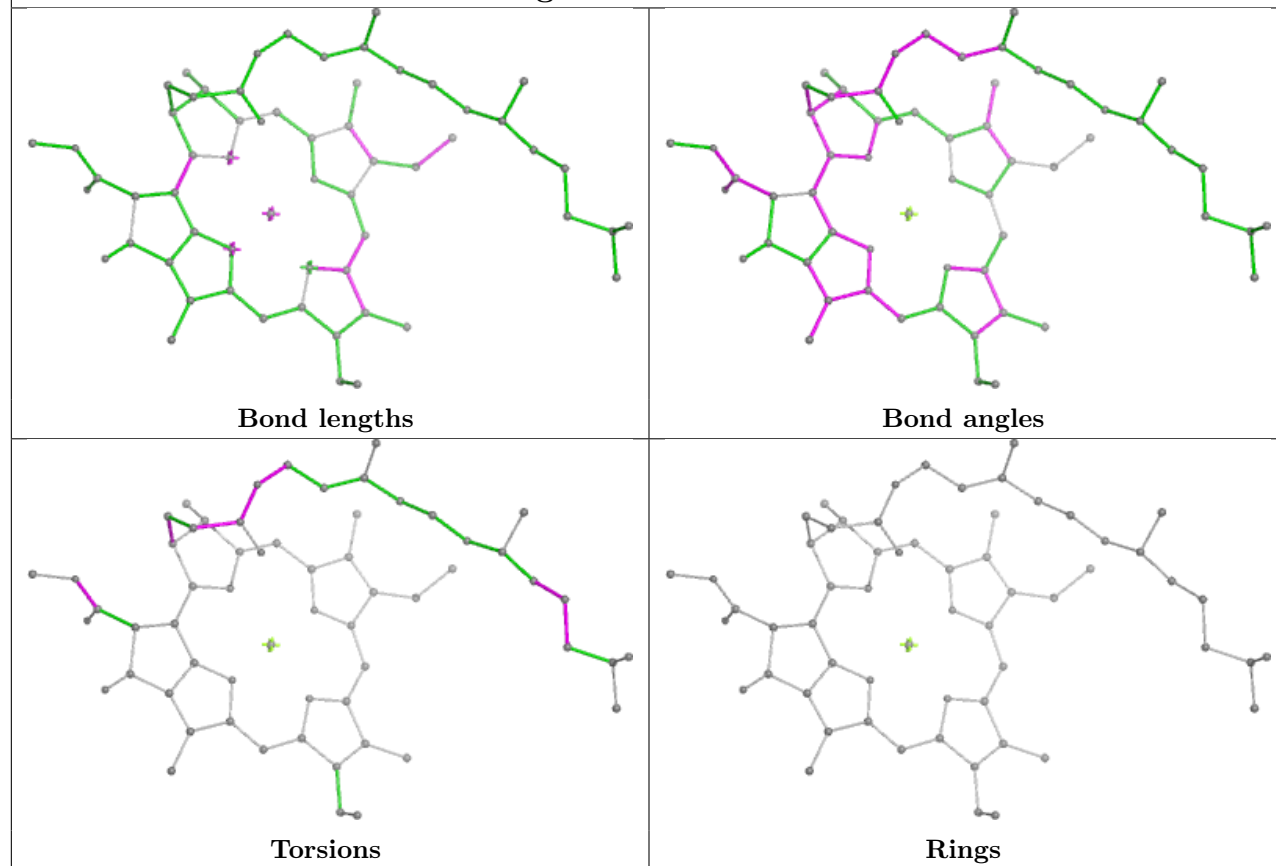
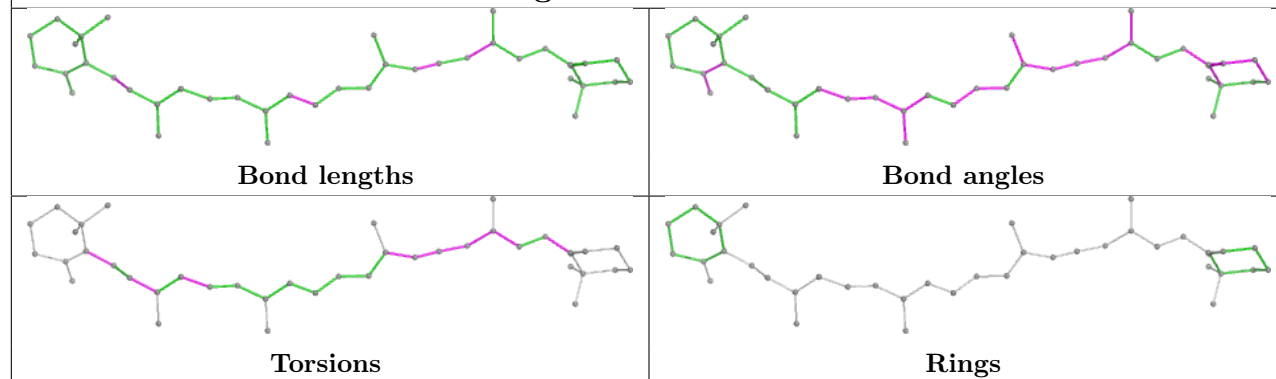


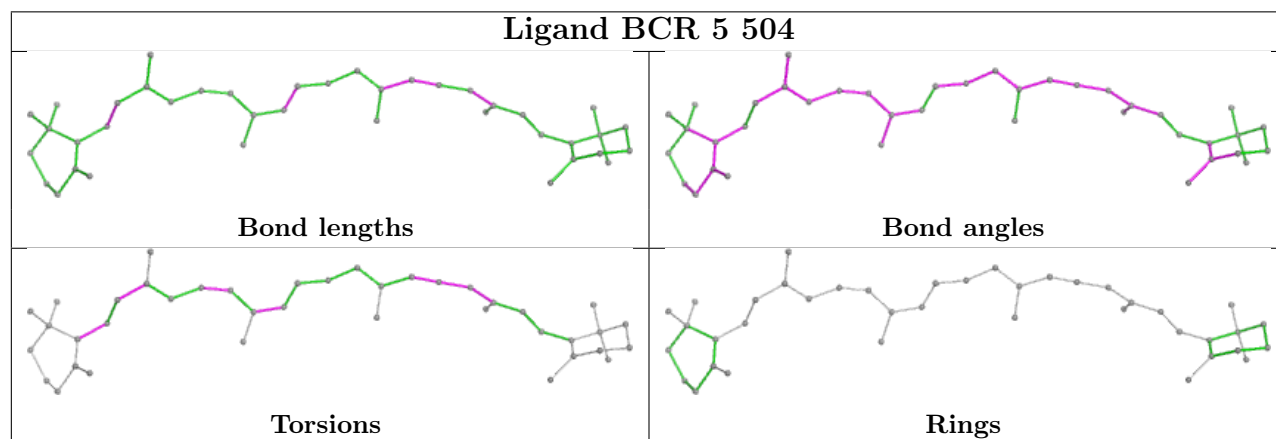
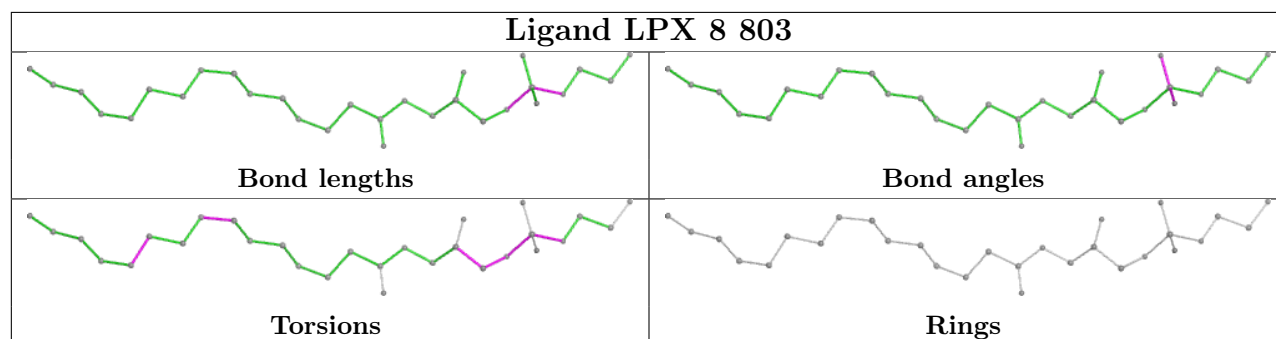
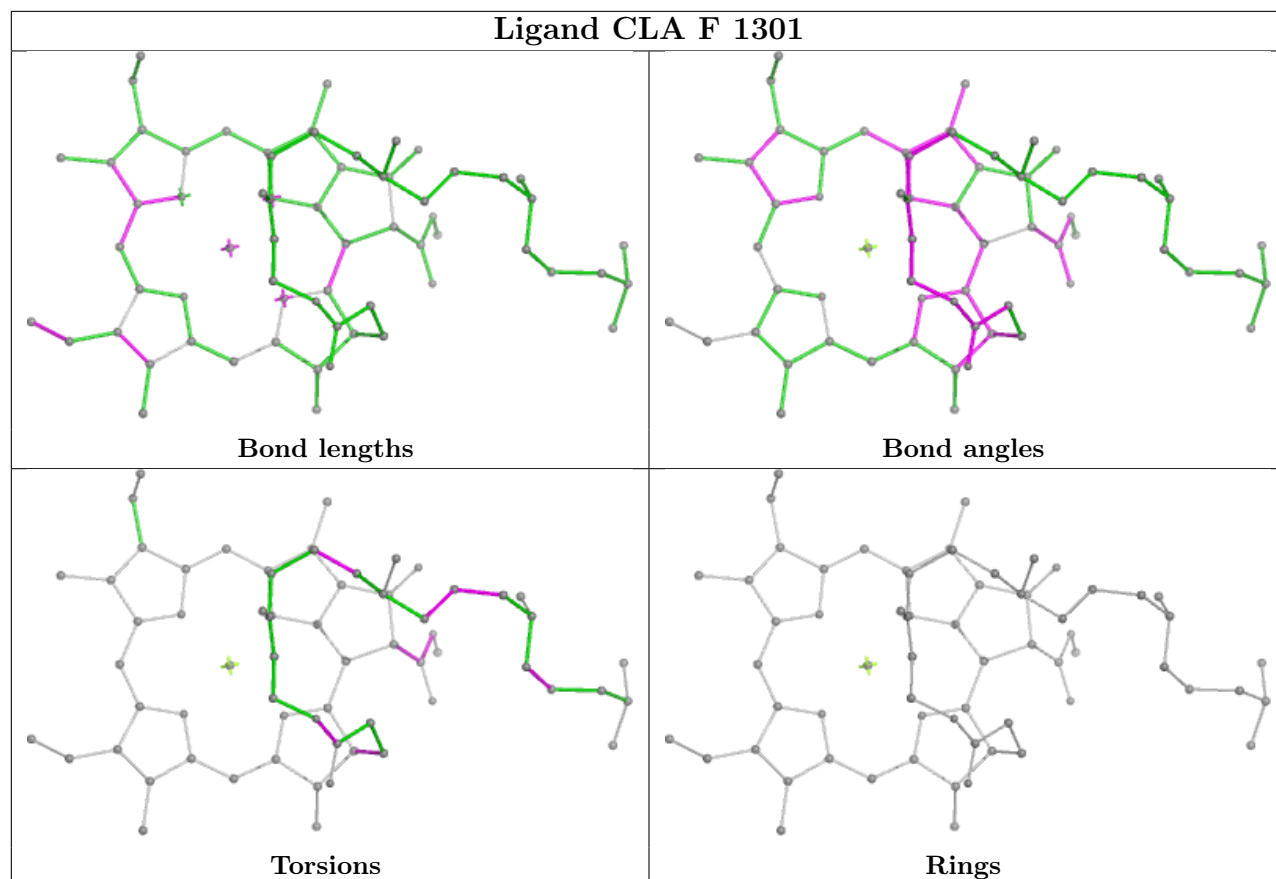
Ligand CLA 5 607**Ligand C7Z 1 503**

Ligand LUT Z 501**Ligand CLA 3 601**

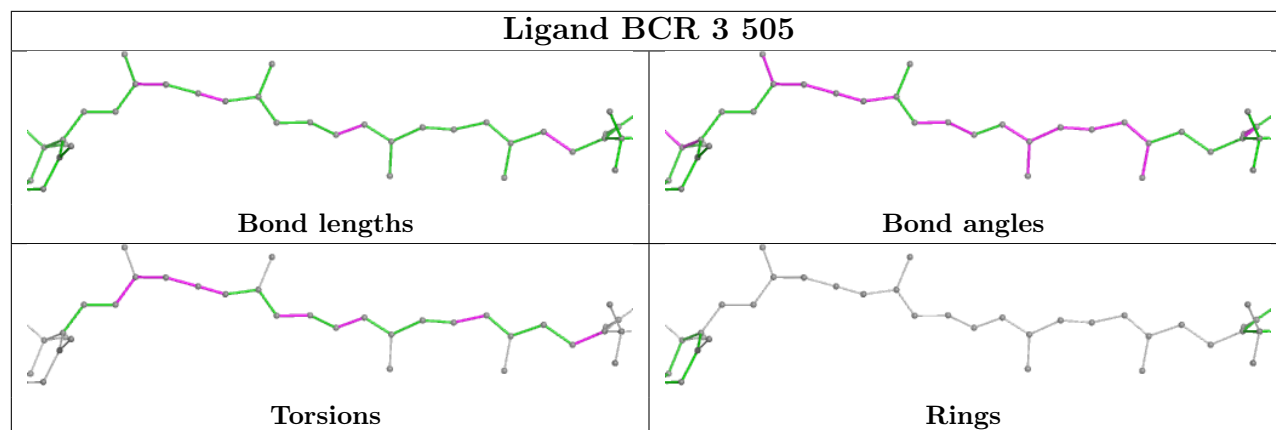
Ligand CLA 9 607



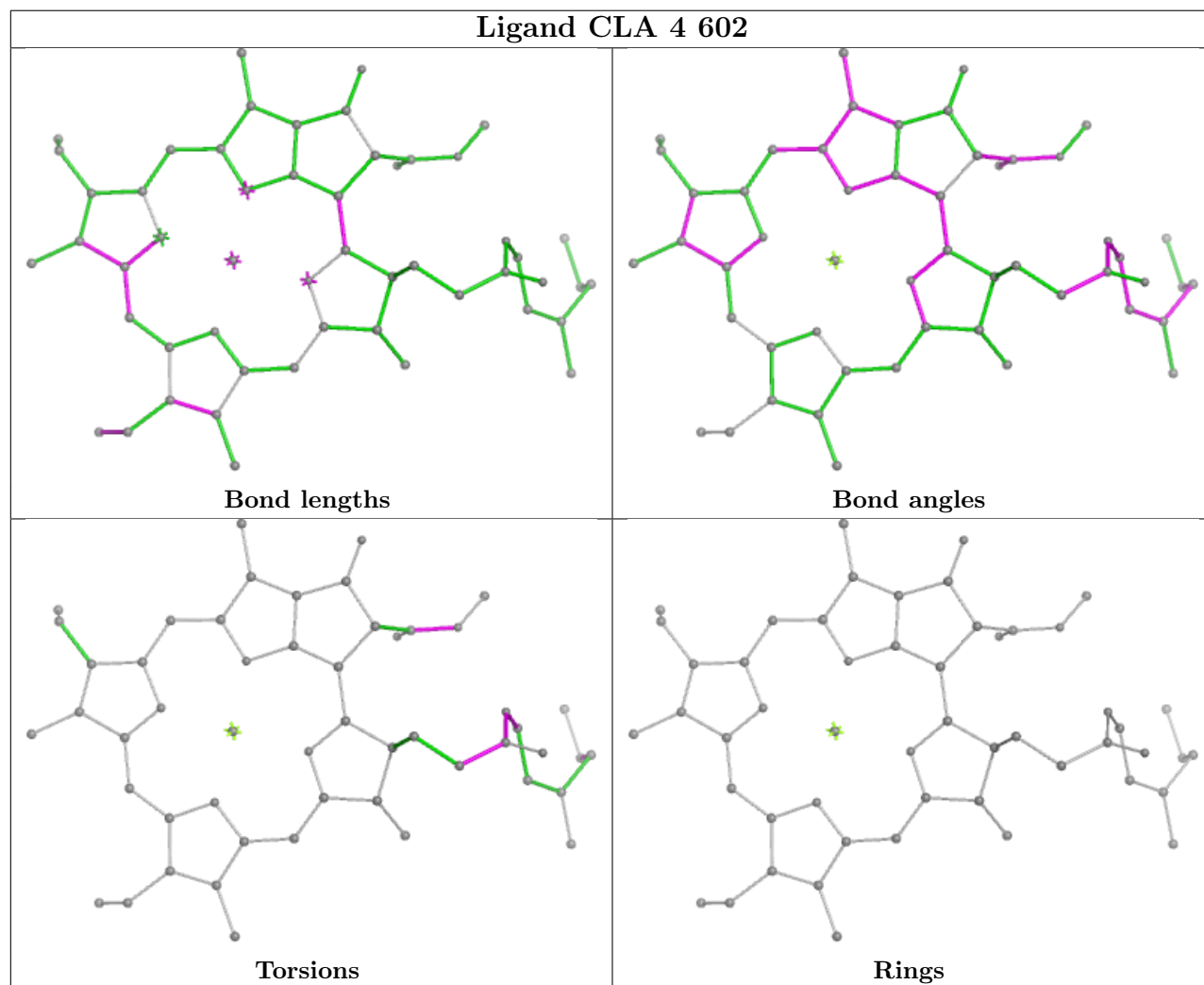
Ligand CLA 6 601**Ligand BCR 4 503**



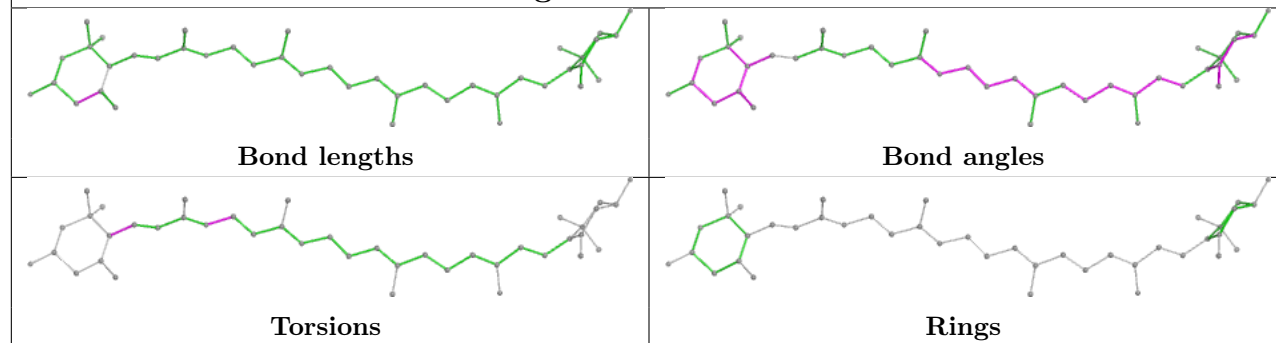
Ligand BCR 3 505



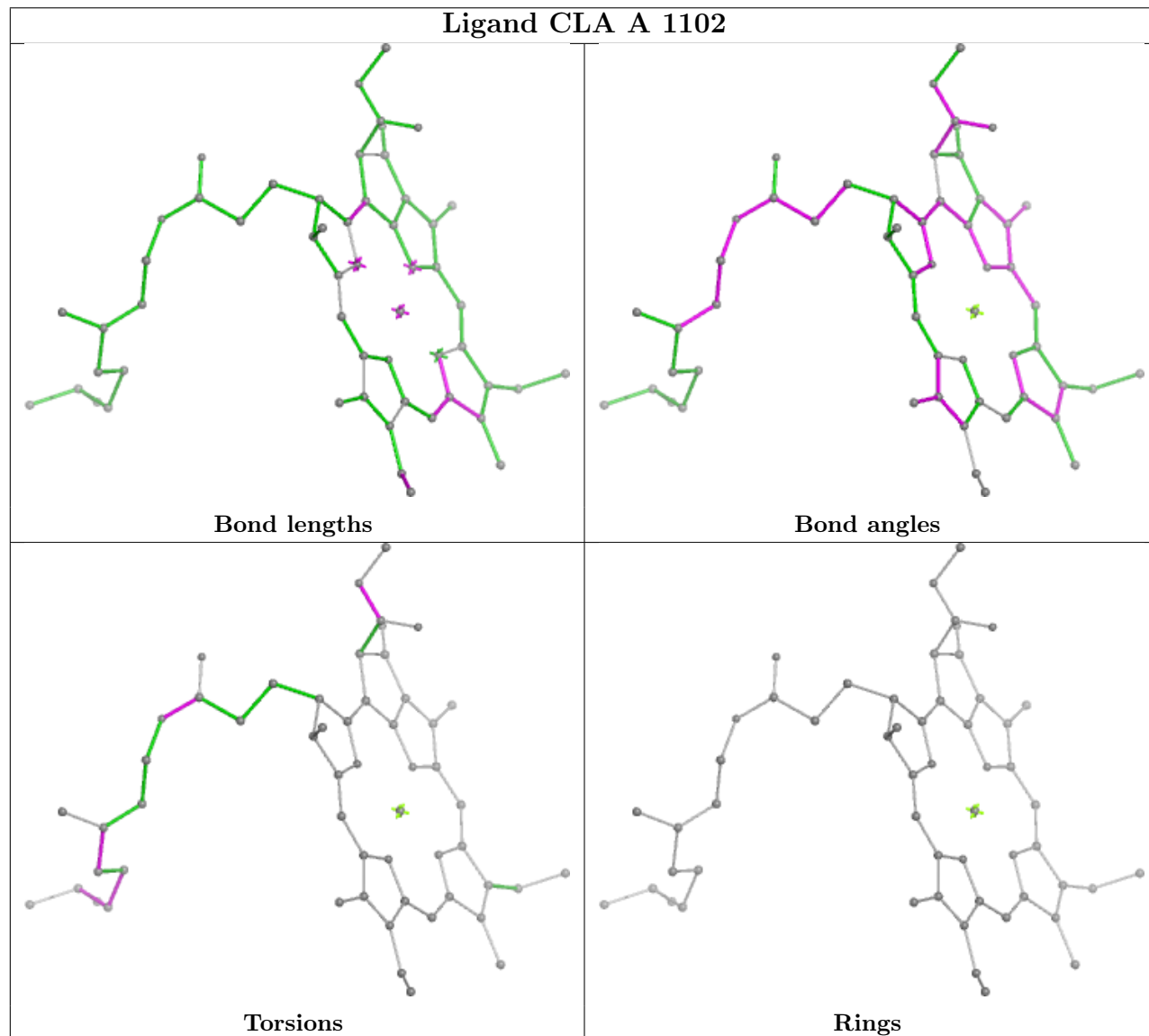
Ligand CLA 4 602

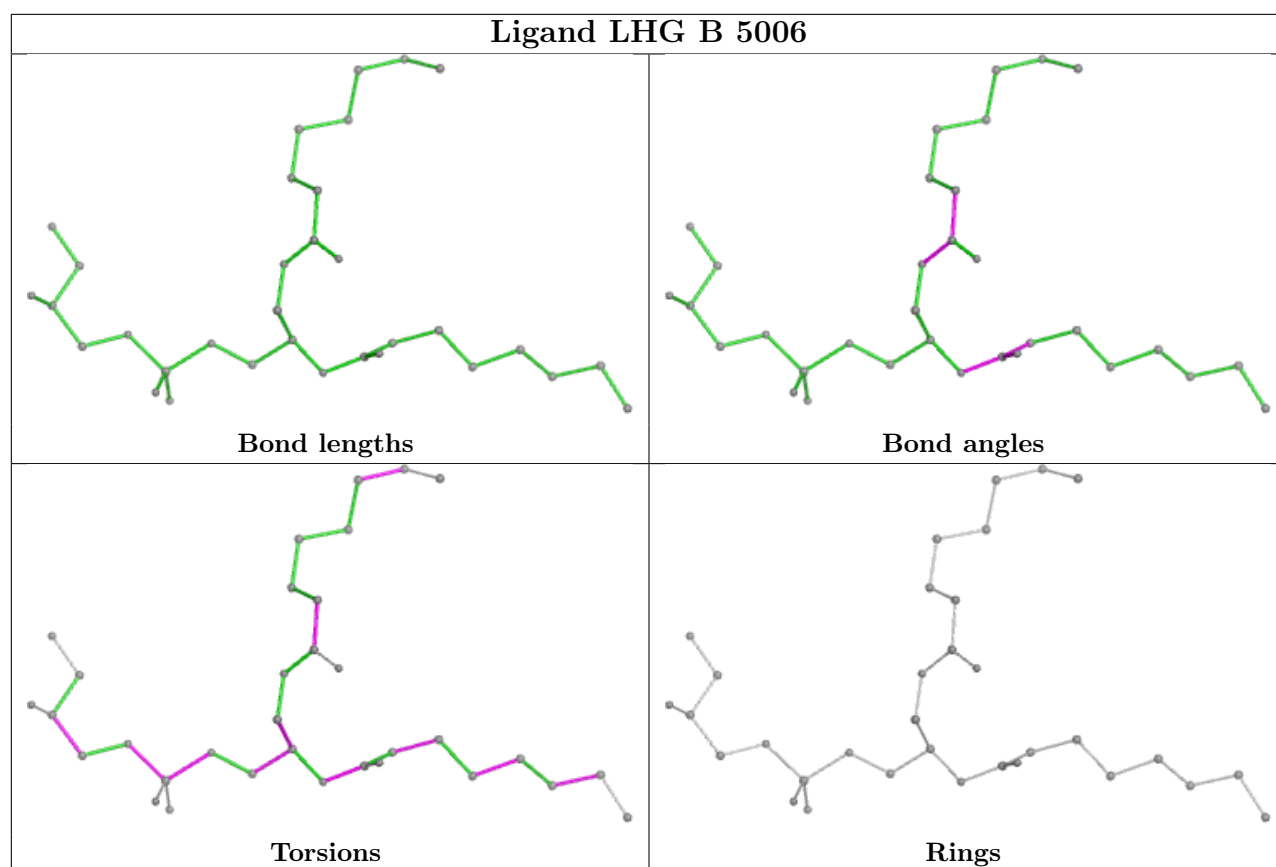


Ligand LUT Z 502

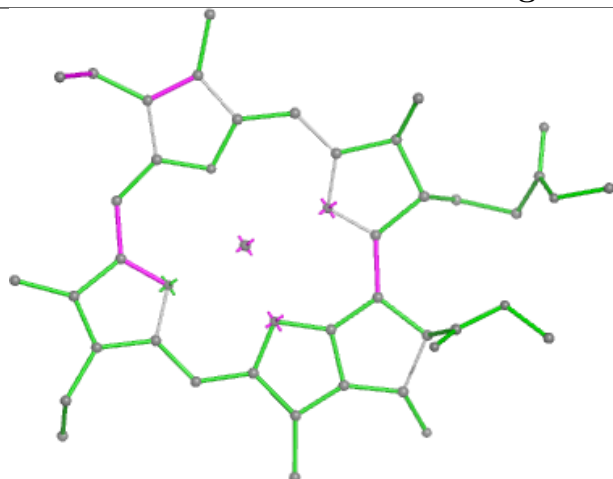


Ligand CLA A 1102

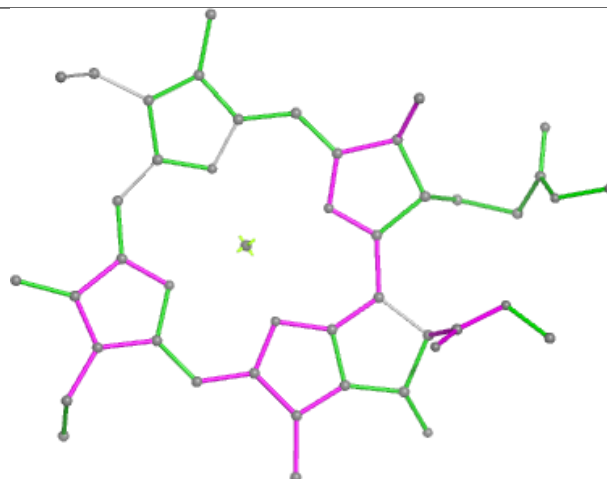




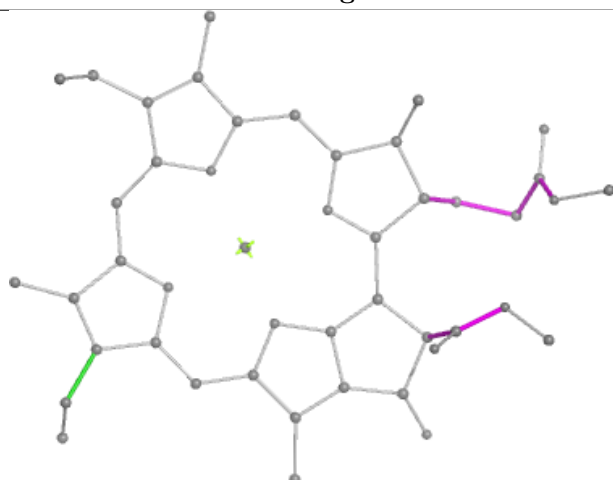
Ligand CLA 2 602



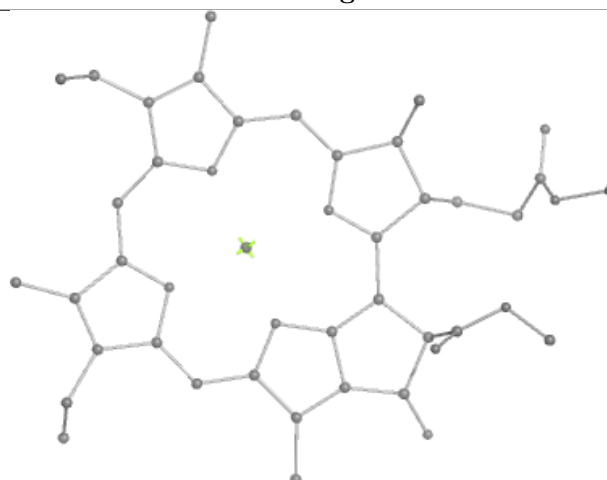
Bond lengths



Bond angles

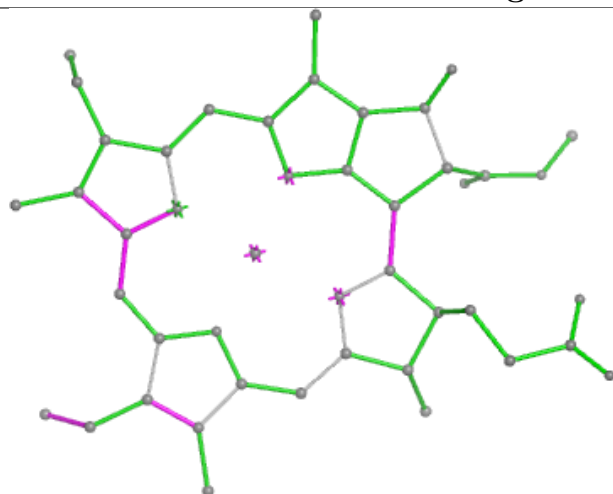


Torsions

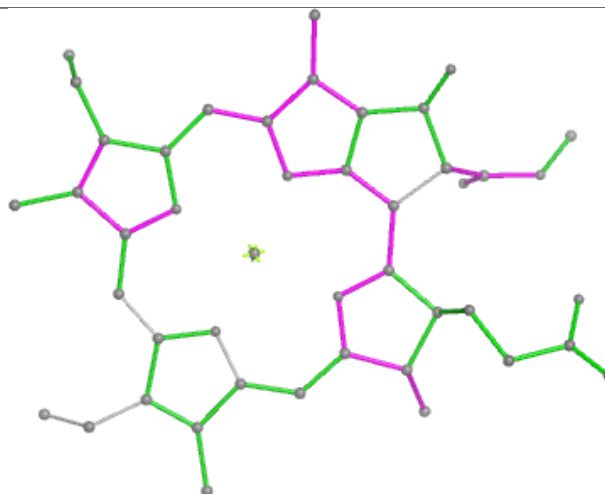


Rings

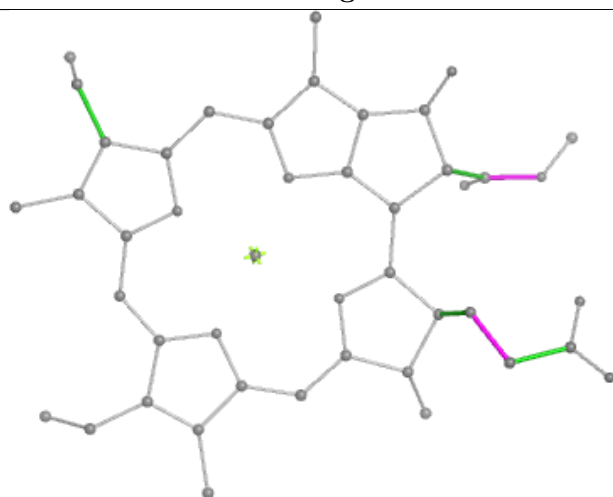
Ligand CLA F 1302



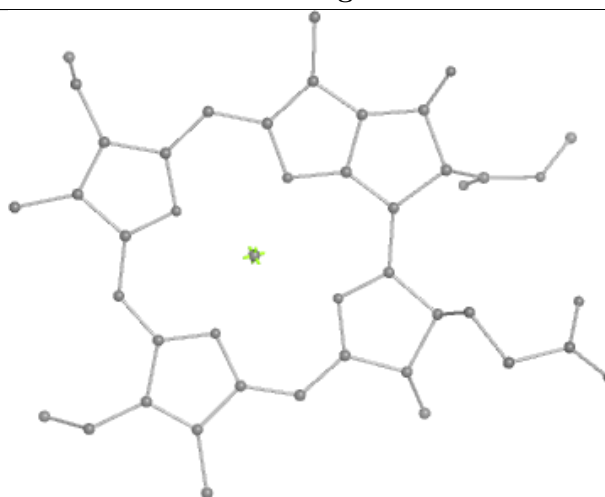
Bond lengths



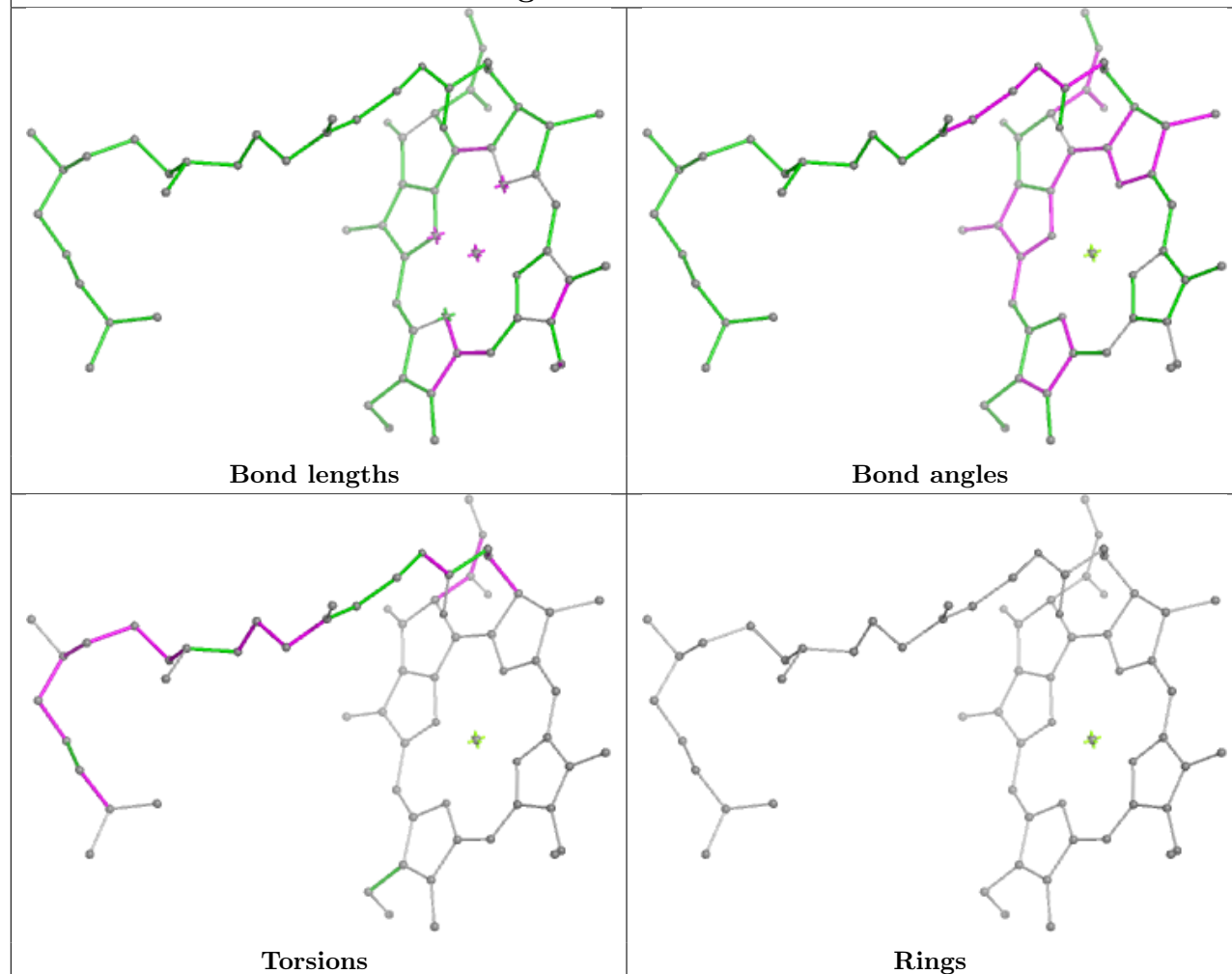
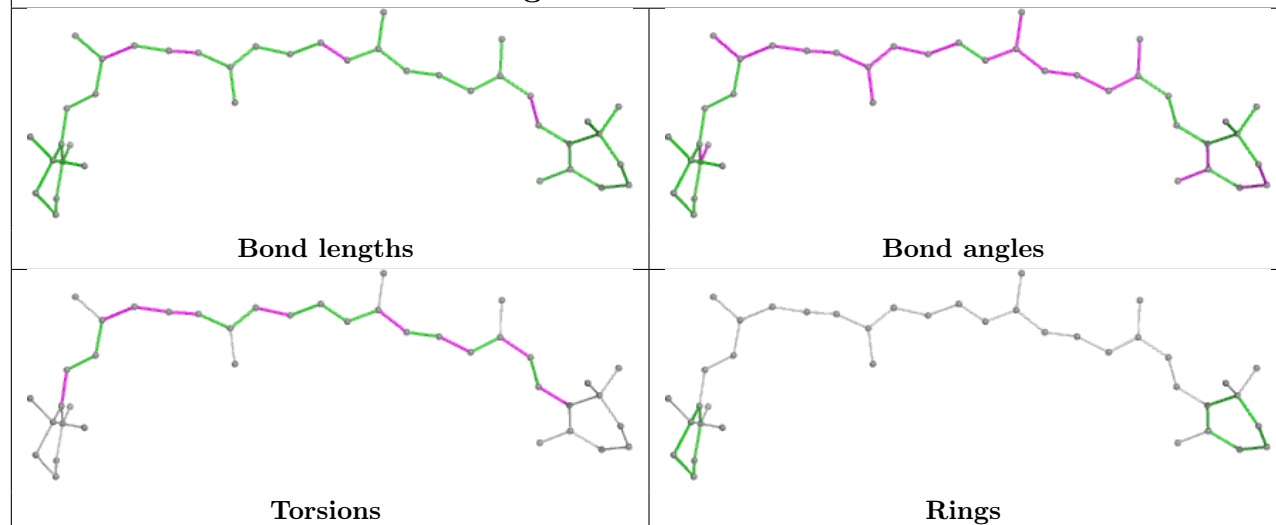
Bond angles

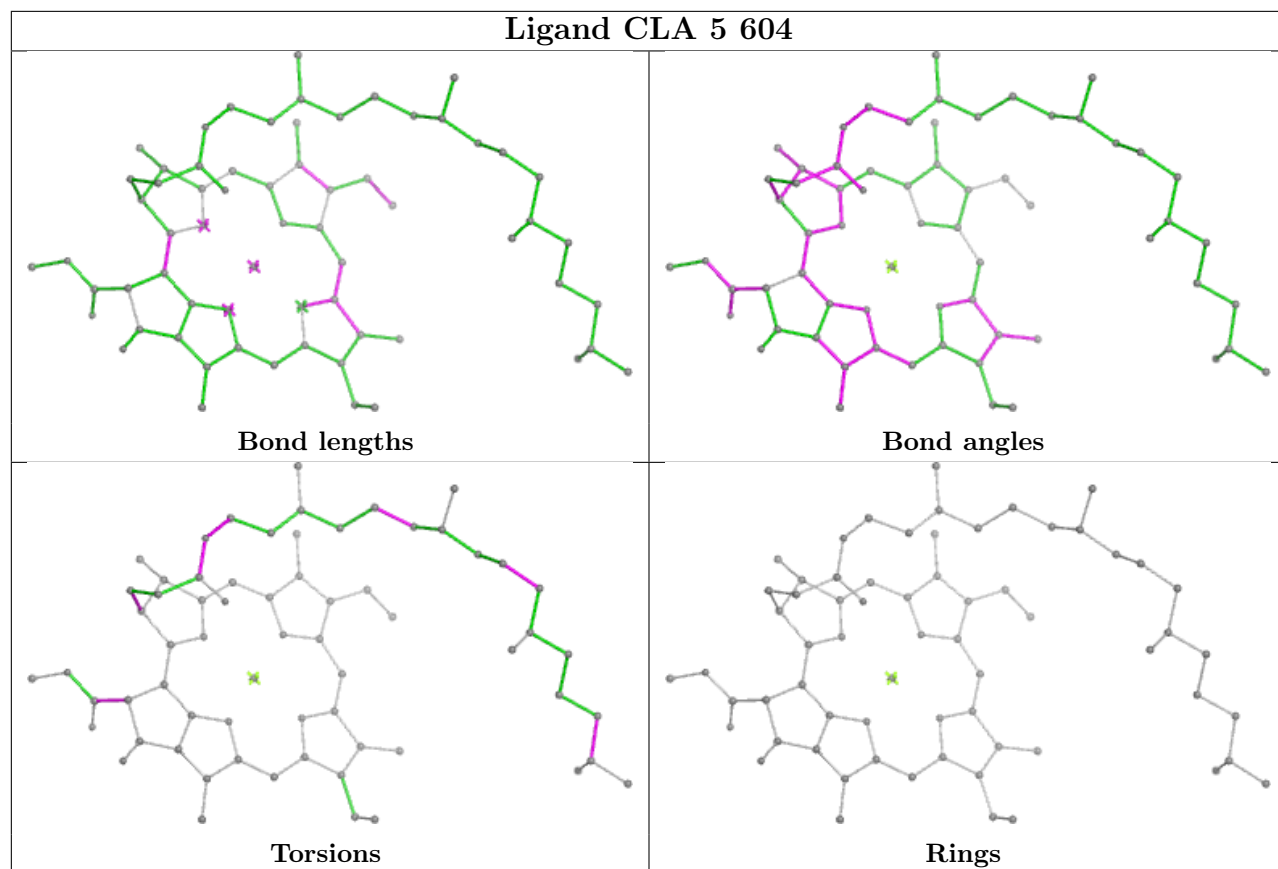
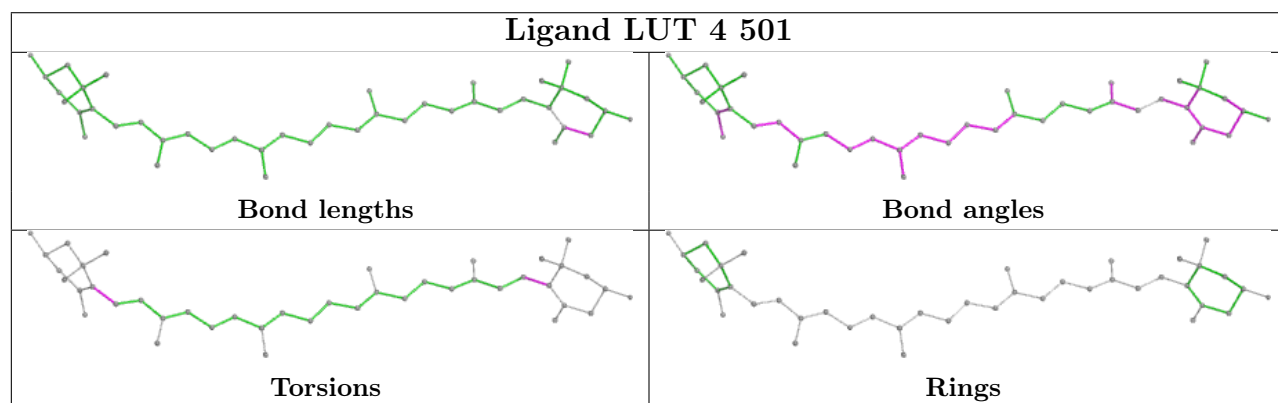


Torsions

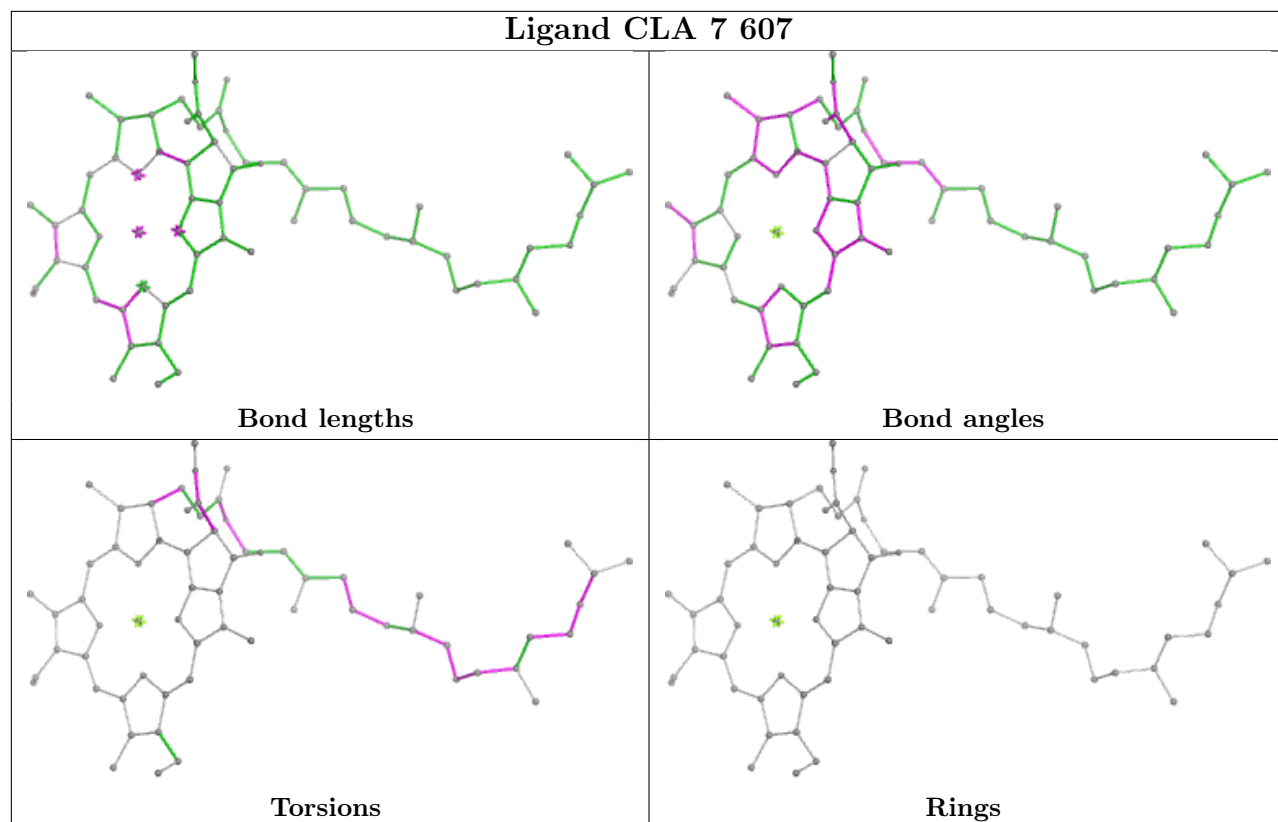


Rings

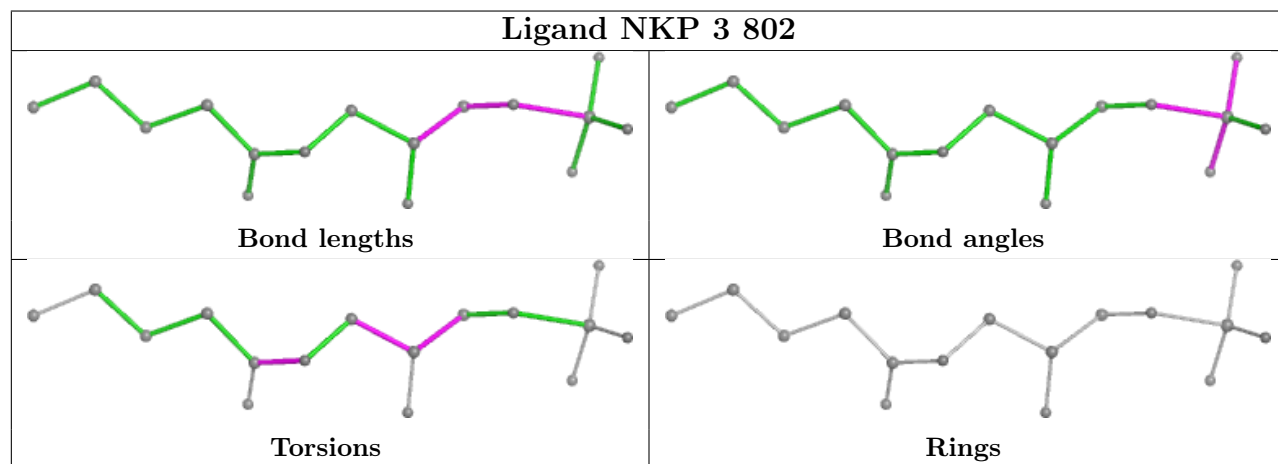
Ligand CLA 1 612**Ligand BCR L 4002**

Ligand CLA 5 604**Ligand LUT 4 501**

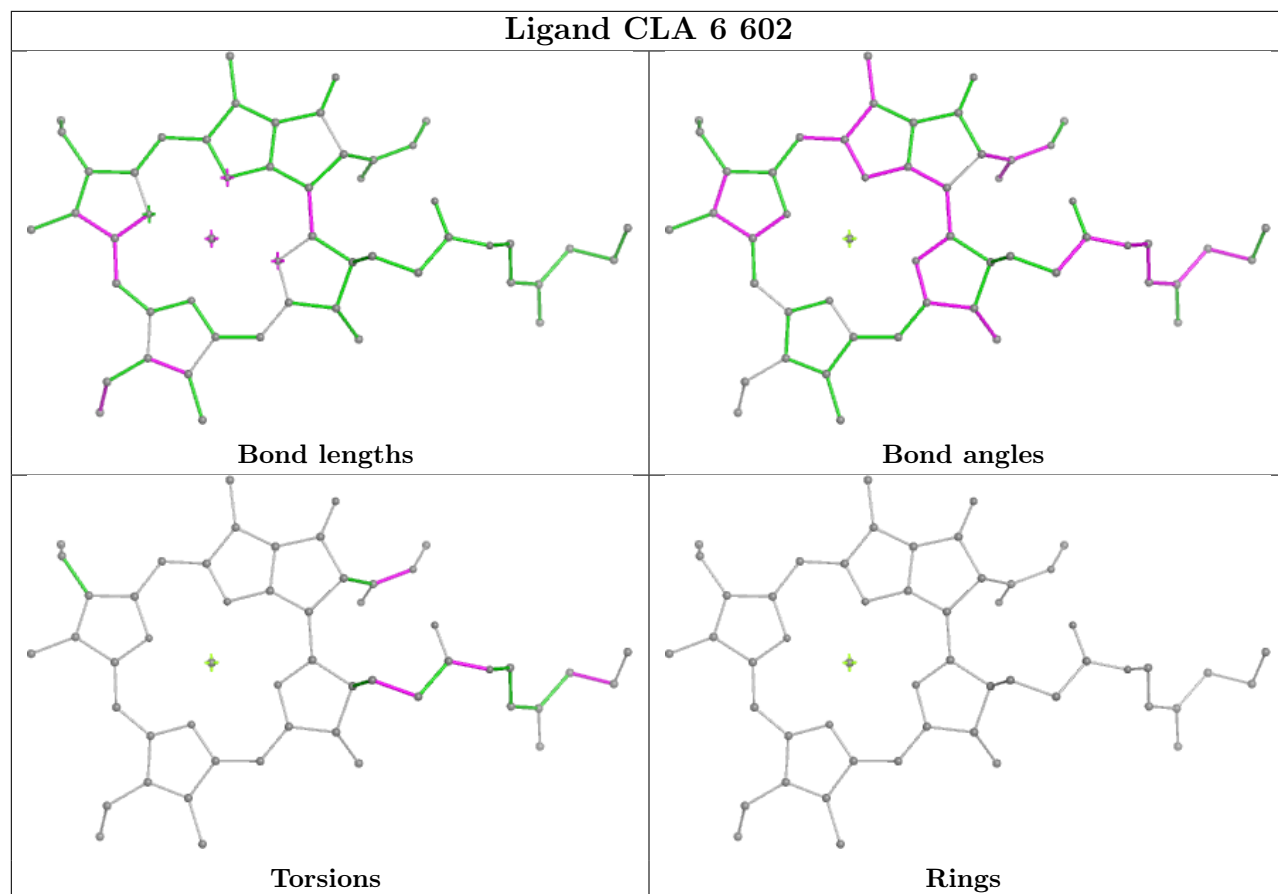
Ligand CLA 7 607



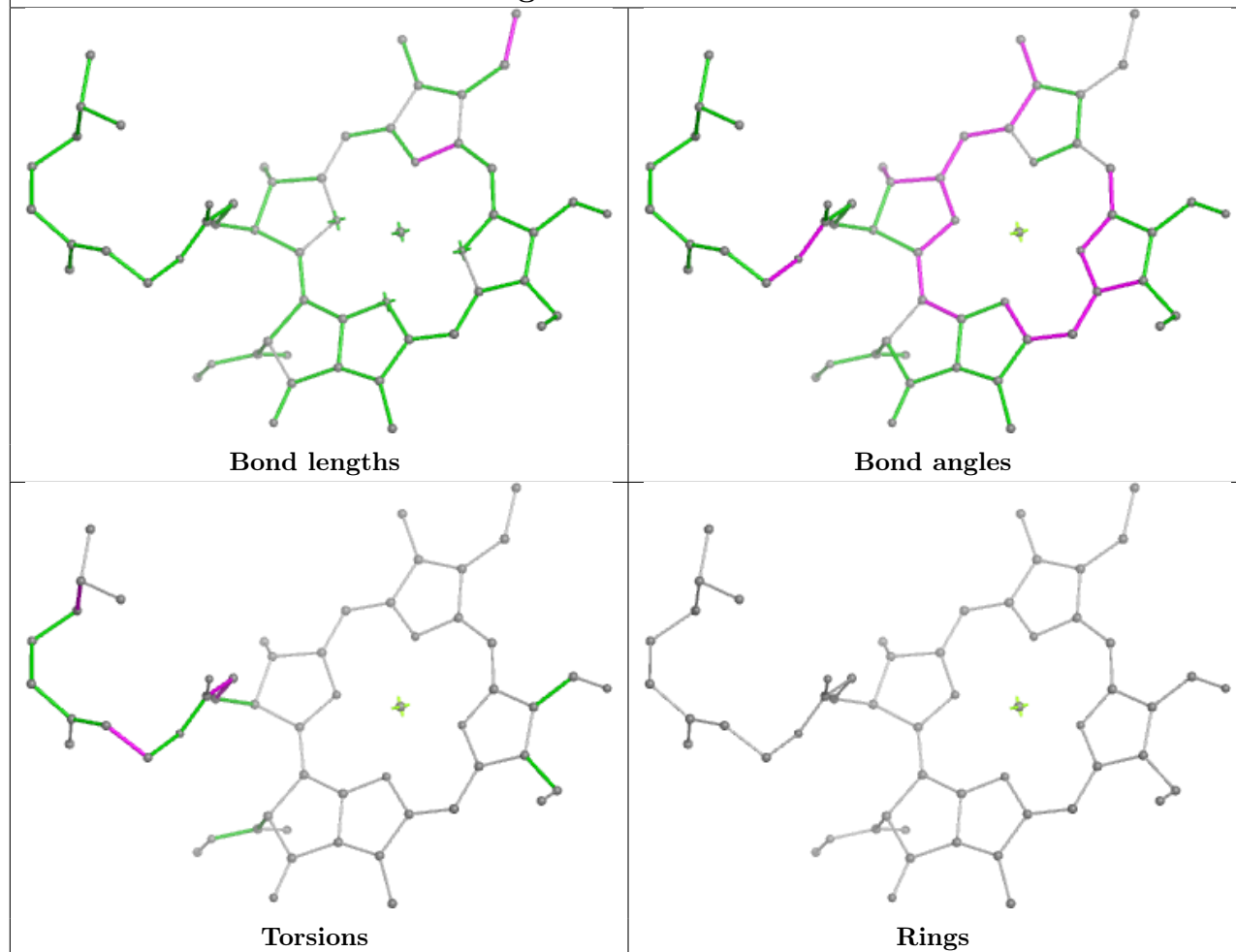
Ligand NKP 3 802



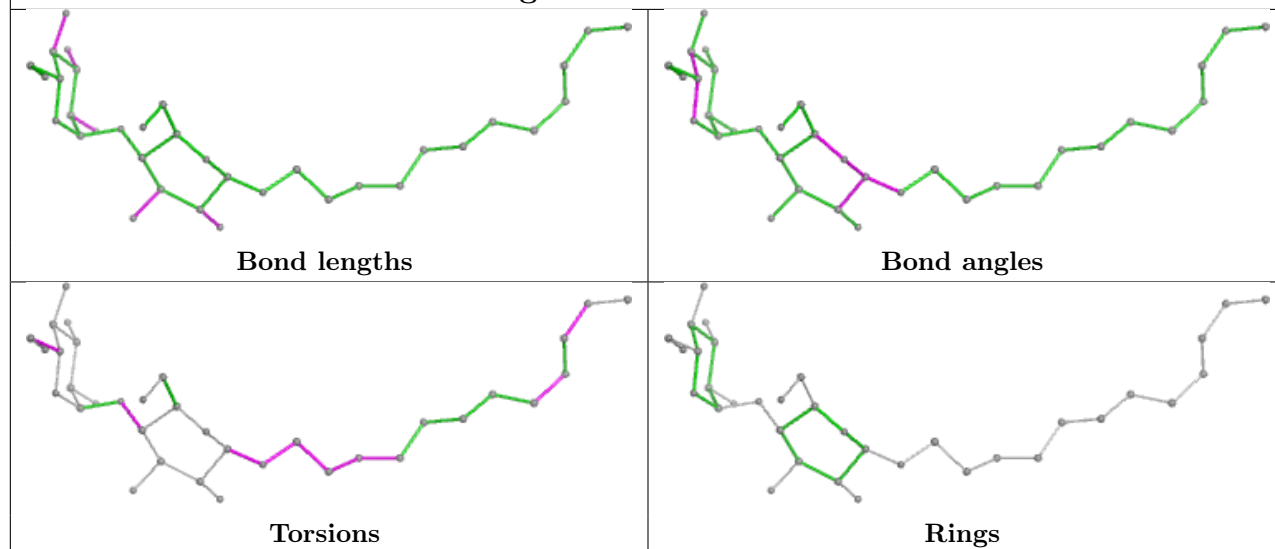
Ligand CLA 6 602



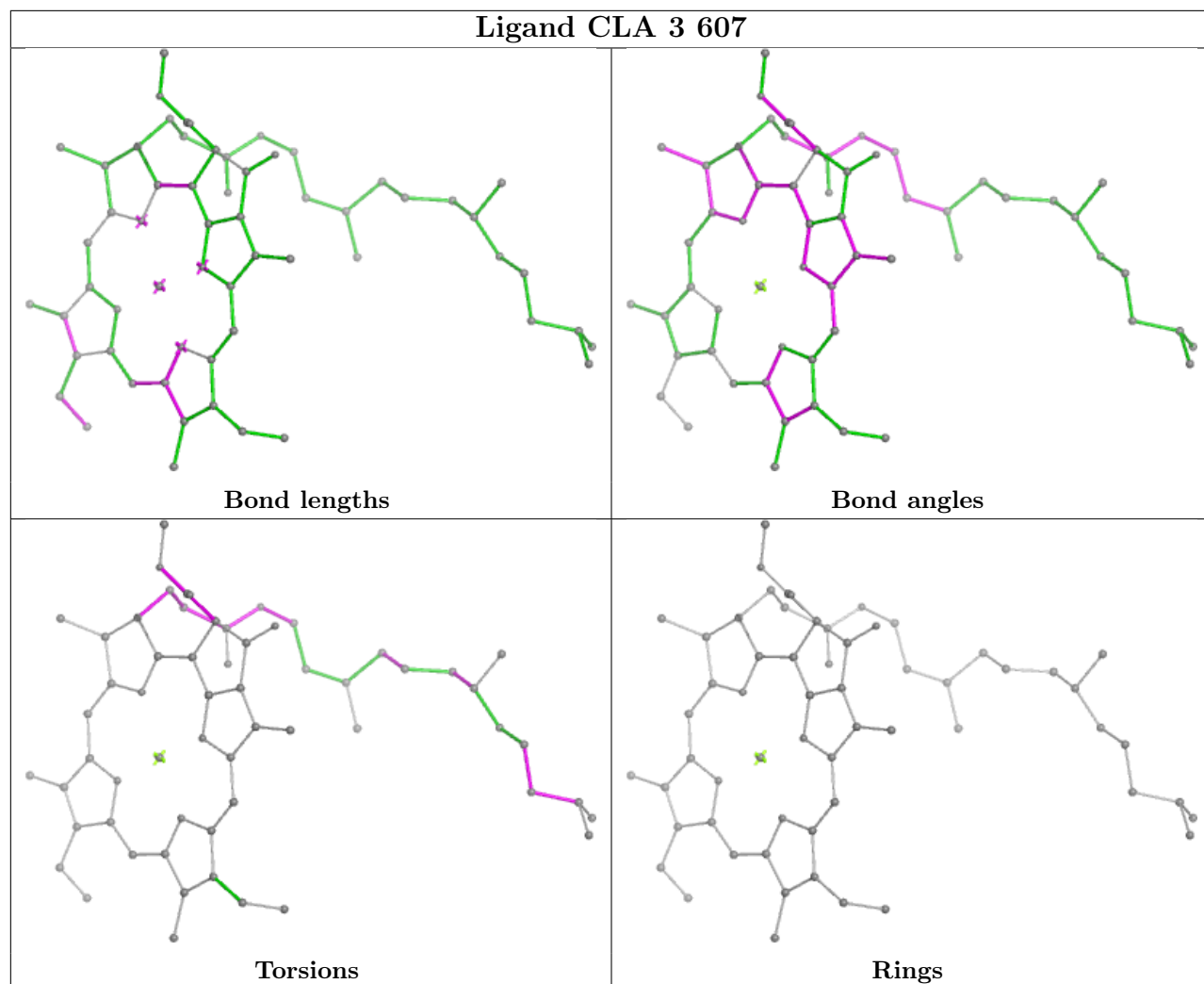
Ligand CHL 8 610

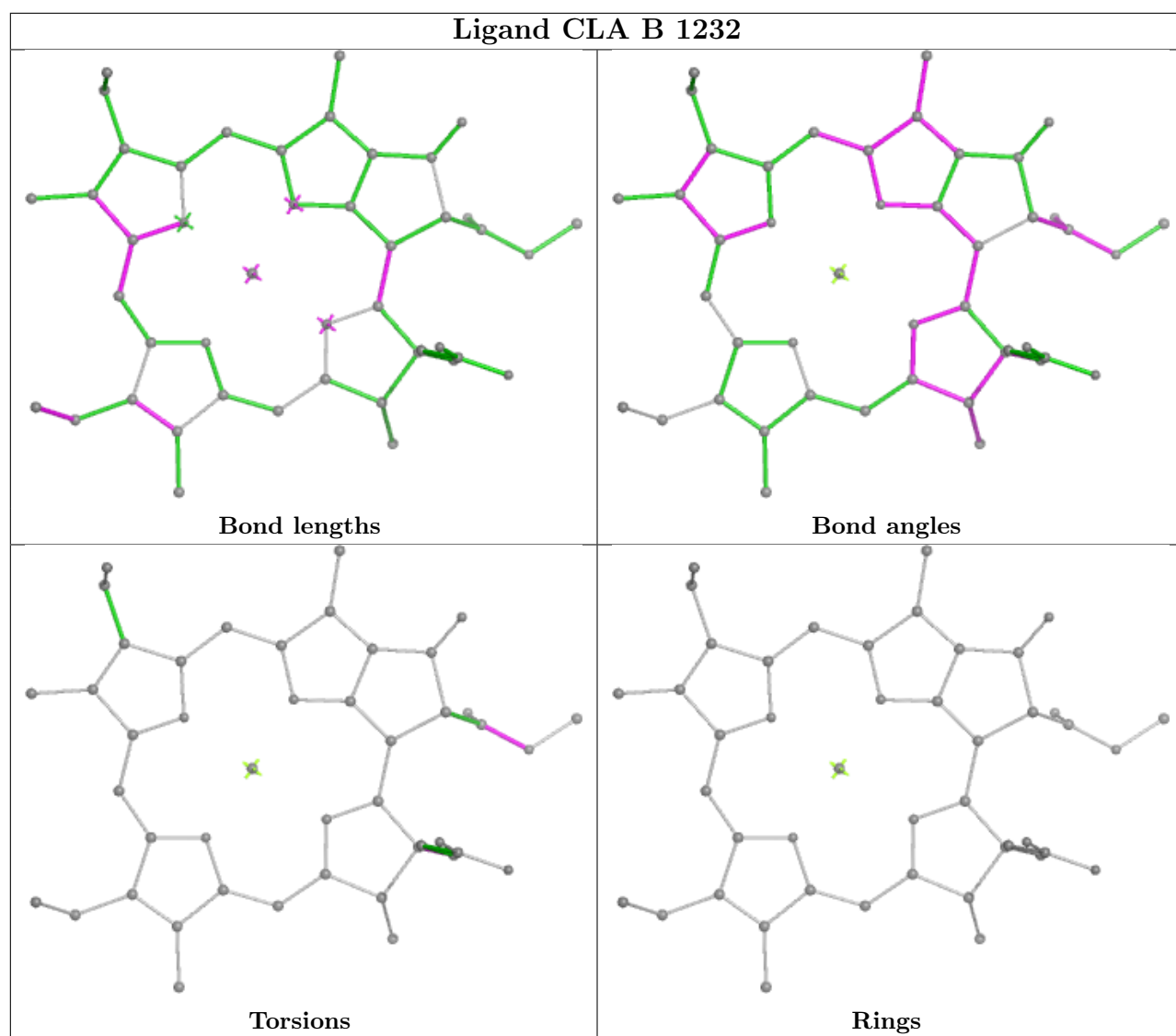


Ligand LMT B 6101

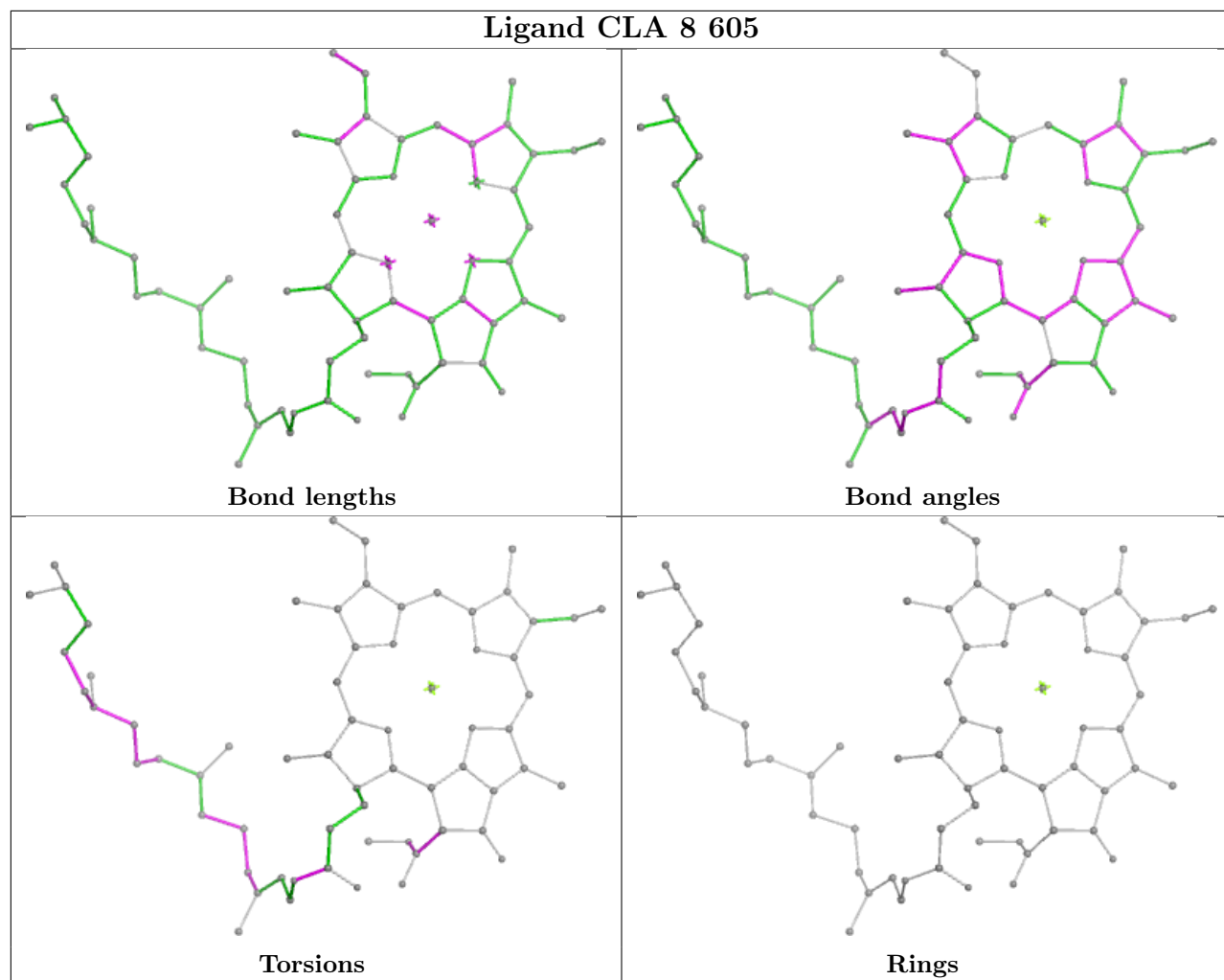


Ligand CLA 3 607

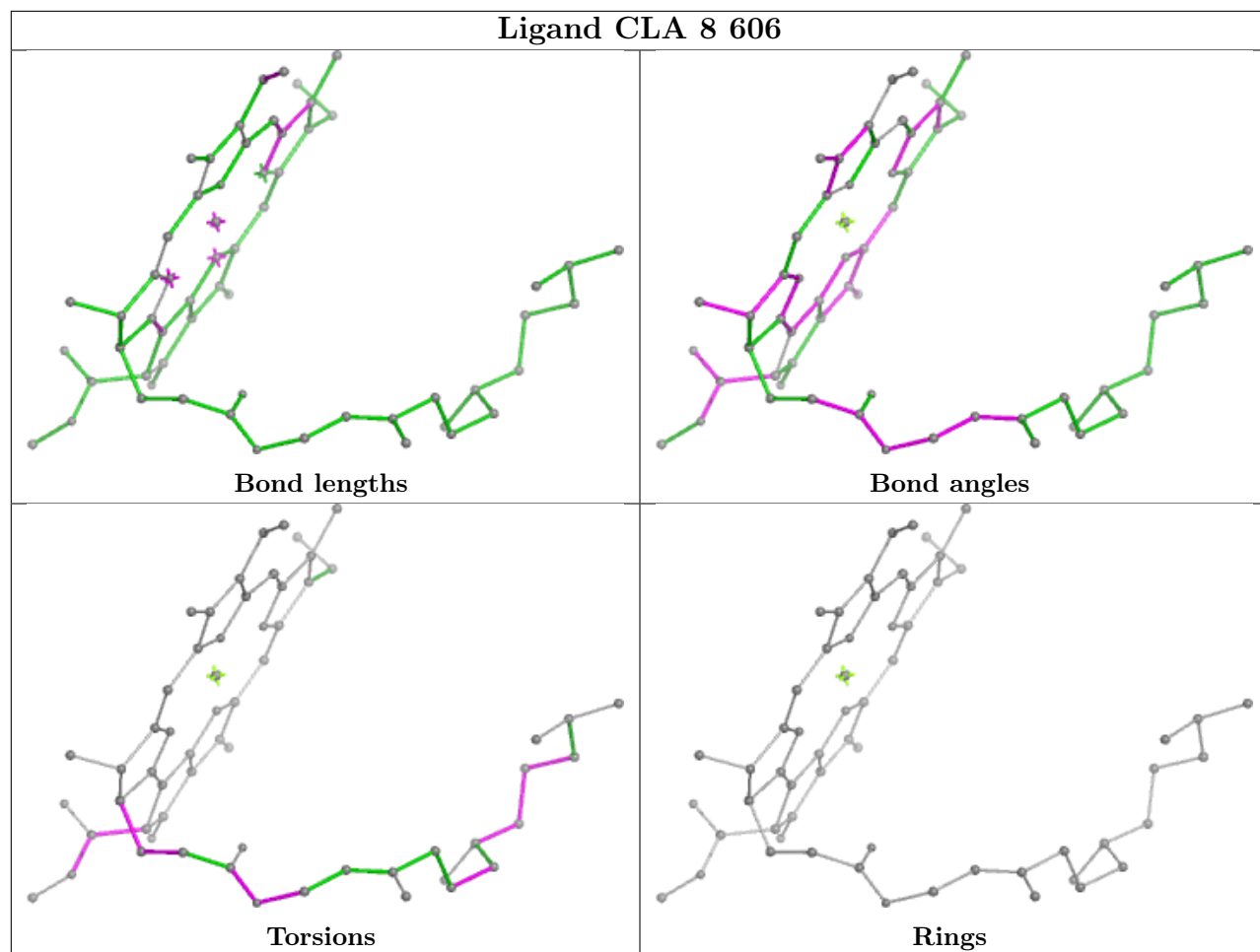




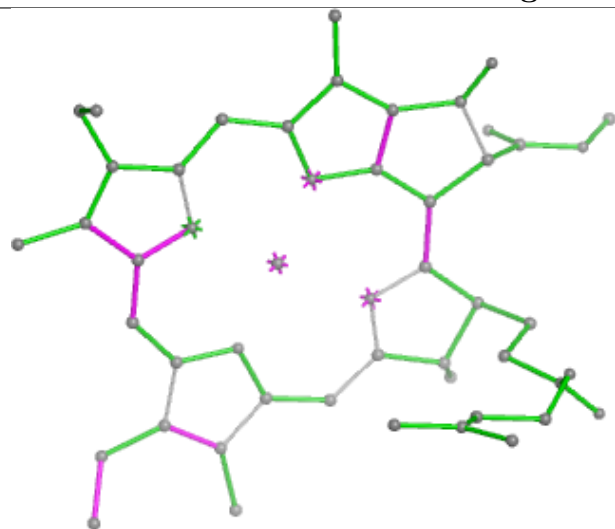
Ligand CLA 8 605



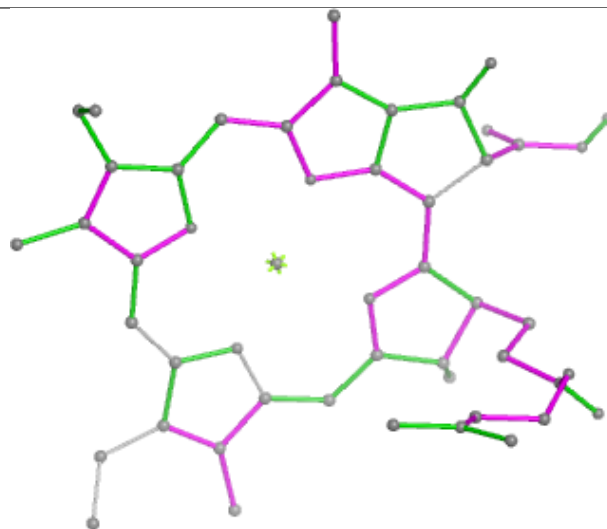
Ligand CLA 8 606



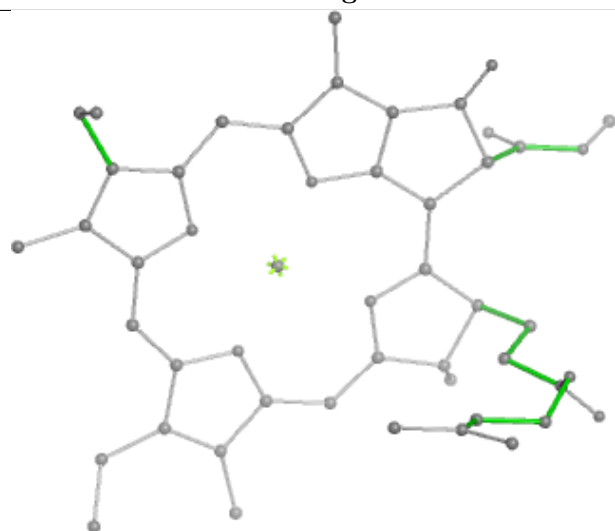
Ligand CLA 9 612



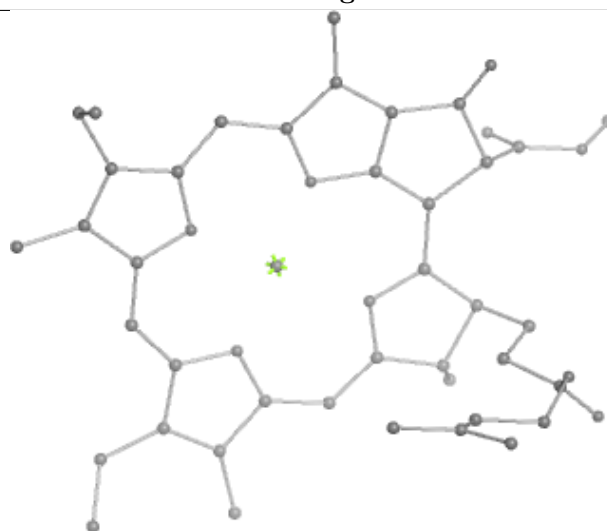
Bond lengths



Bond angles

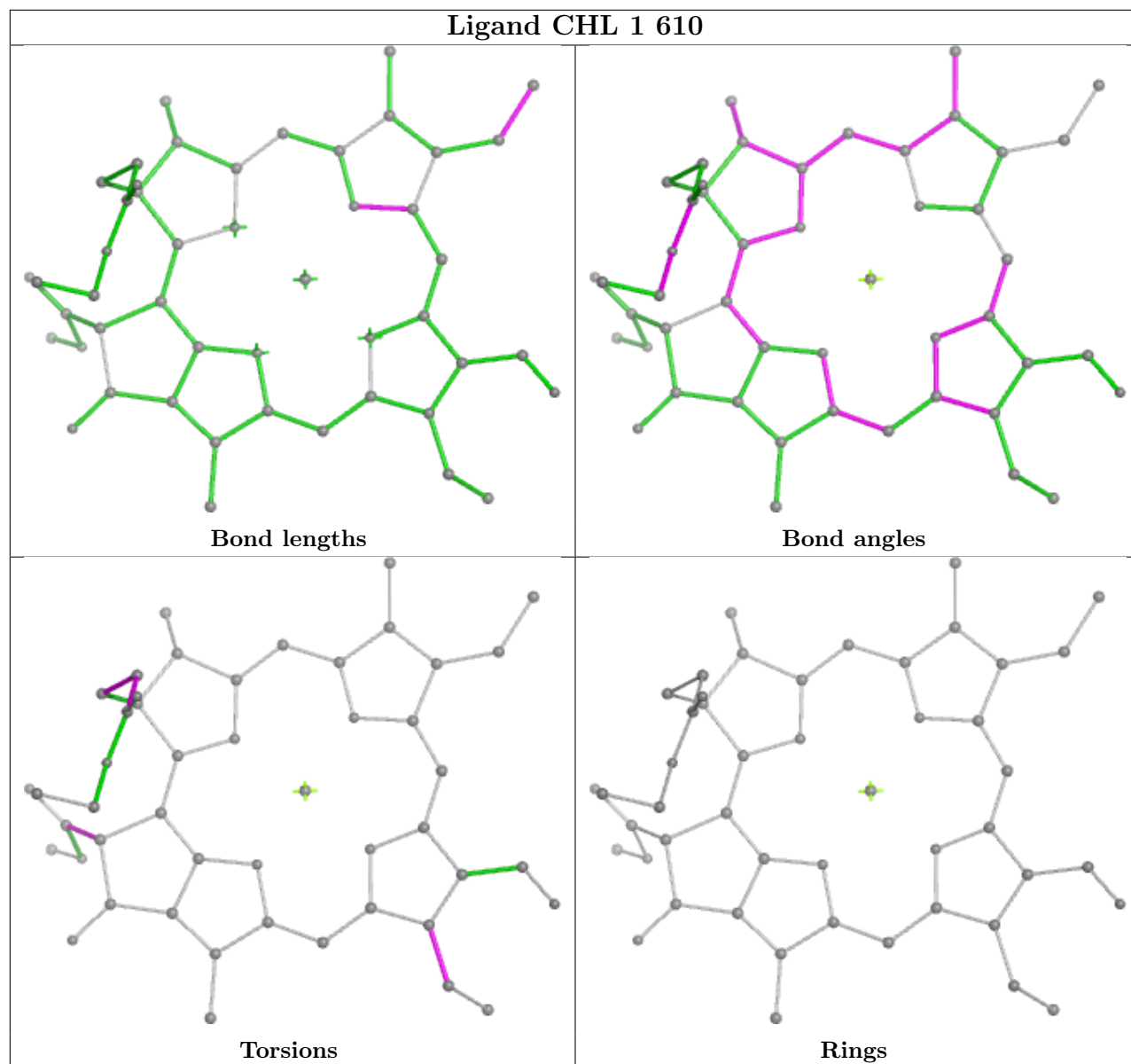


Torsions

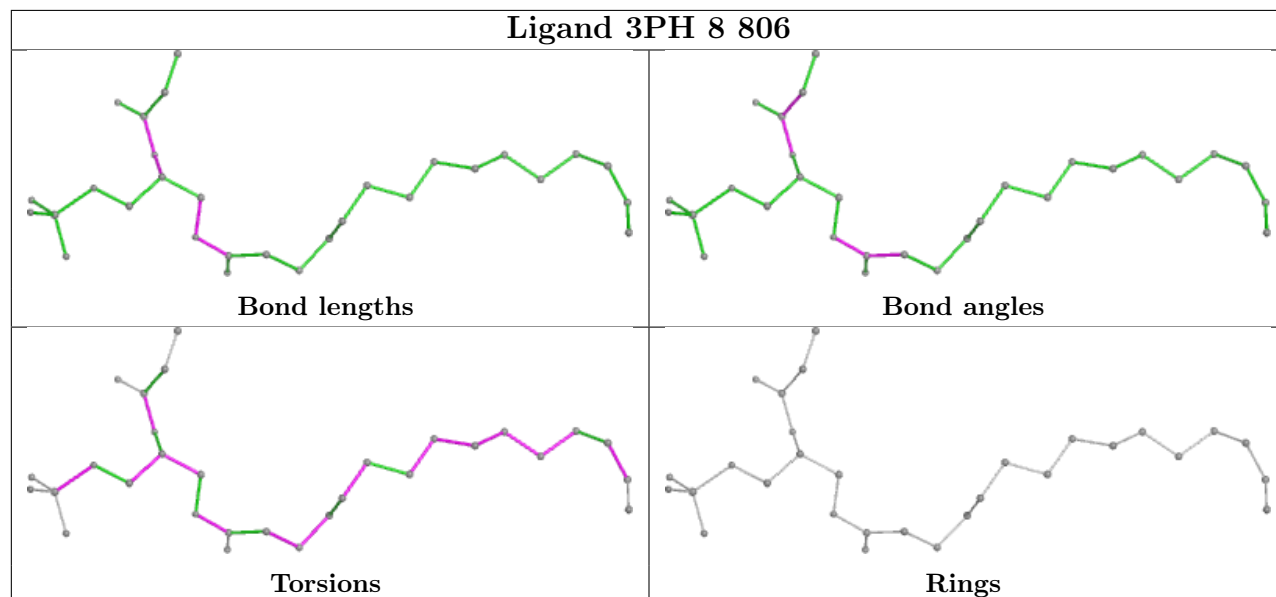


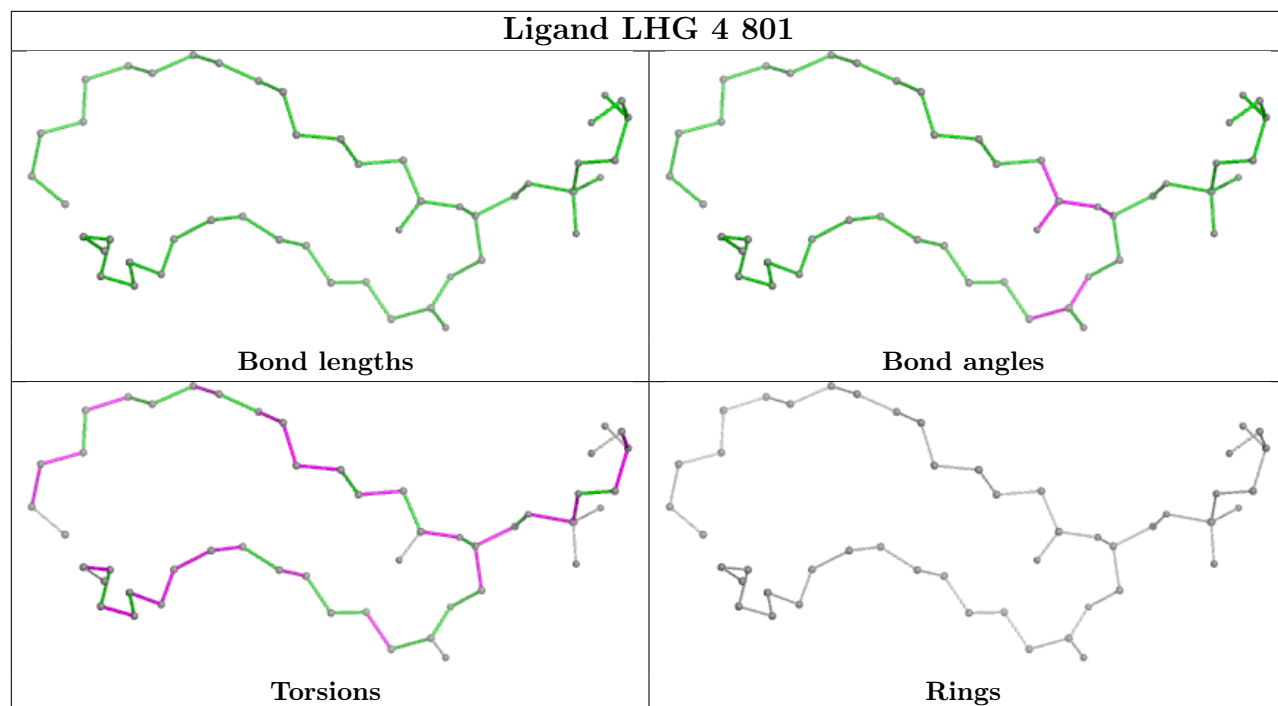
Rings

Ligand CHL 1 610

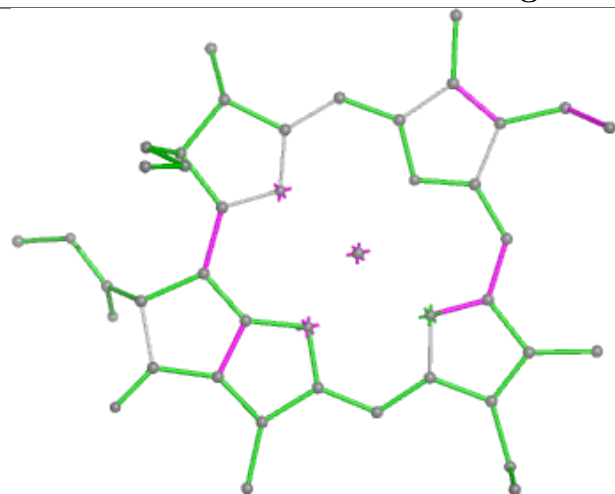


Ligand 3PH 8 806

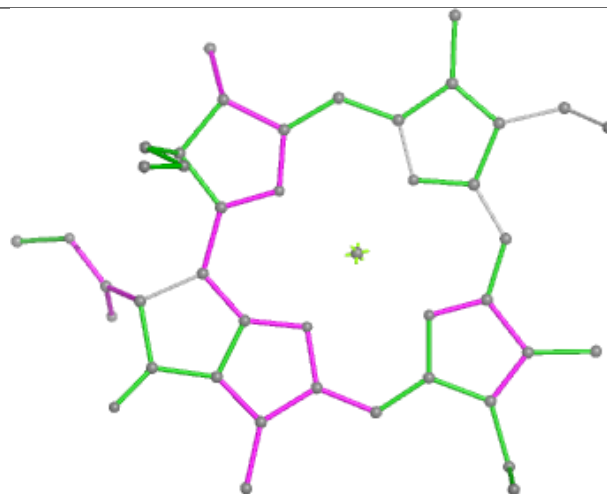




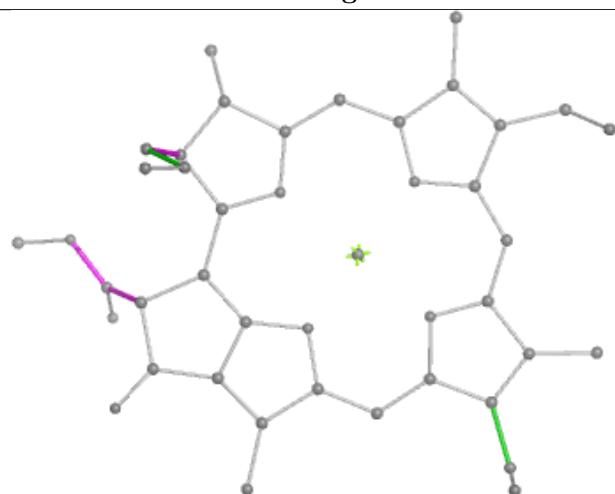
Ligand CLA 7 608



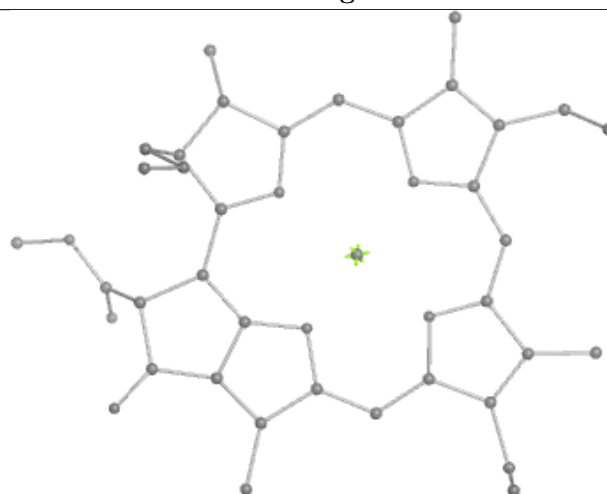
Bond lengths



Bond angles

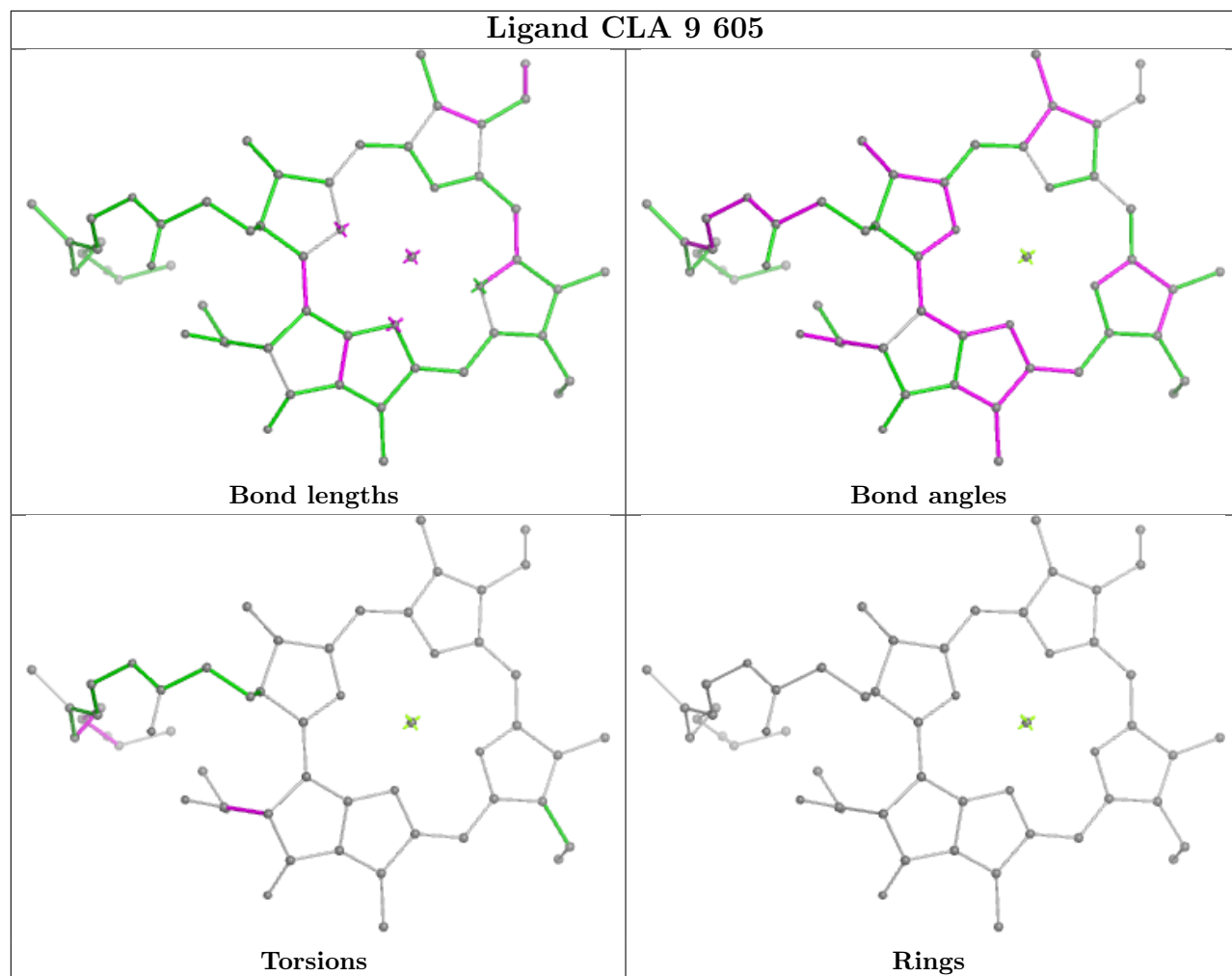


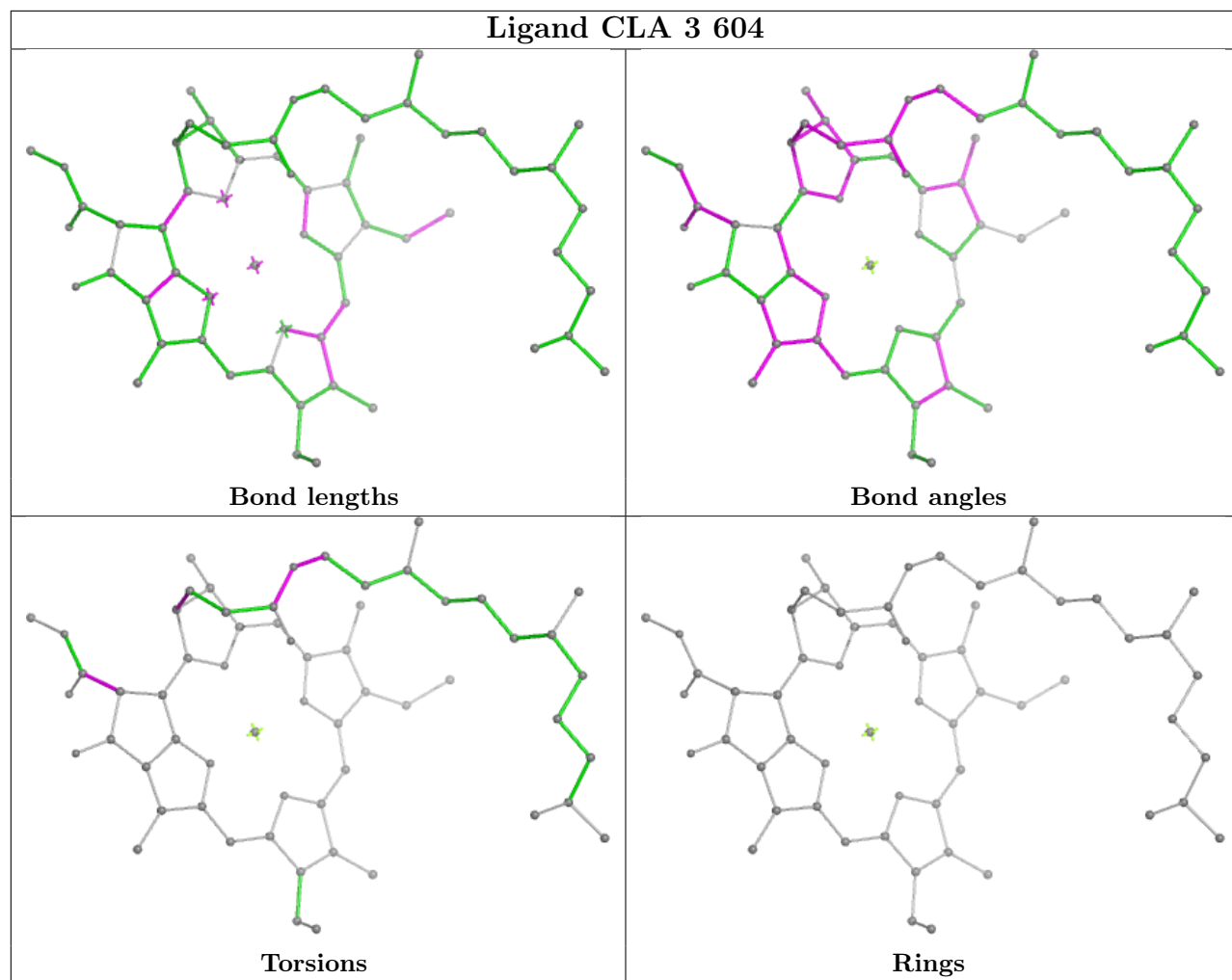
Torsions



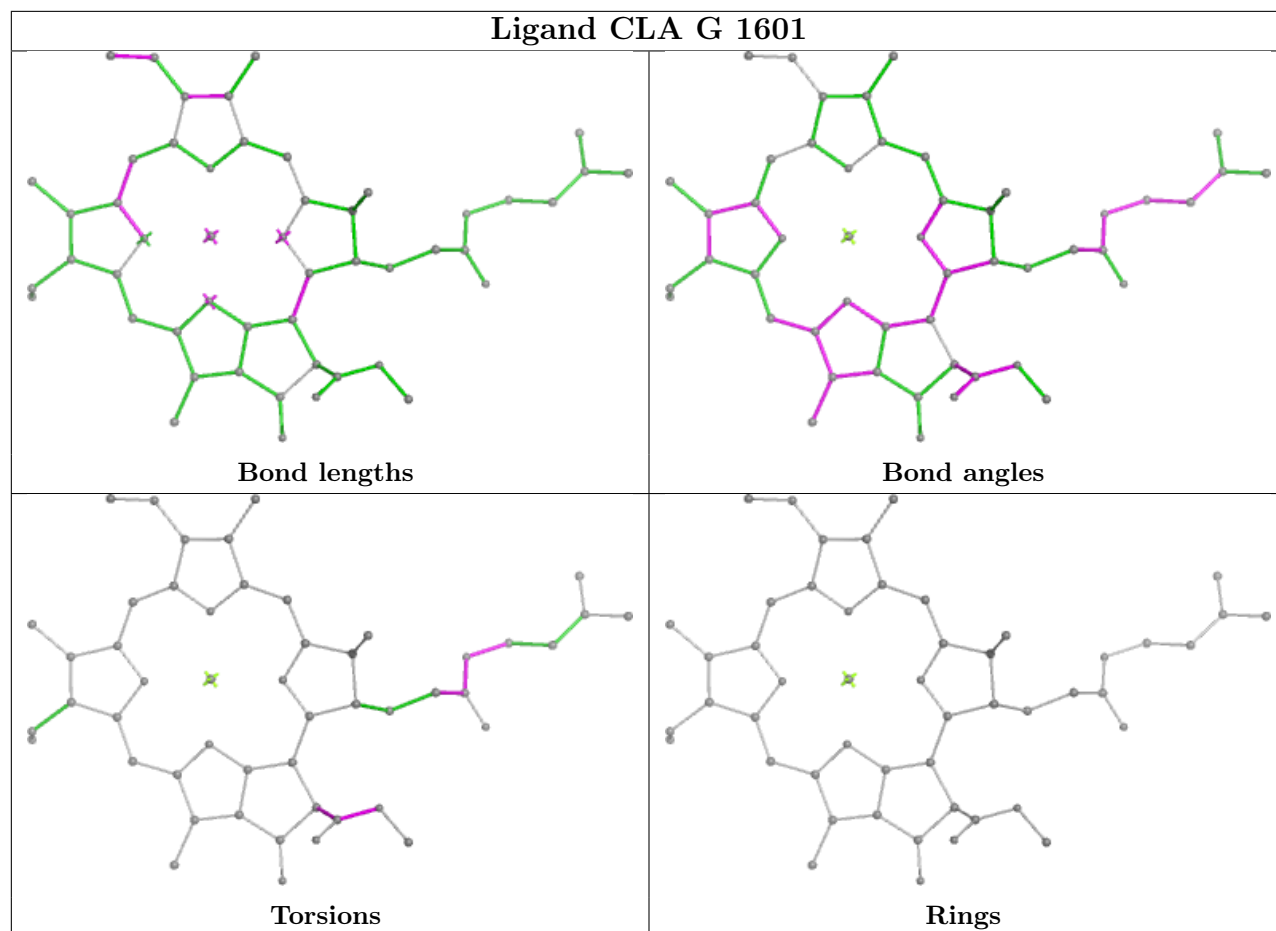
Rings

Ligand CLA 9 605

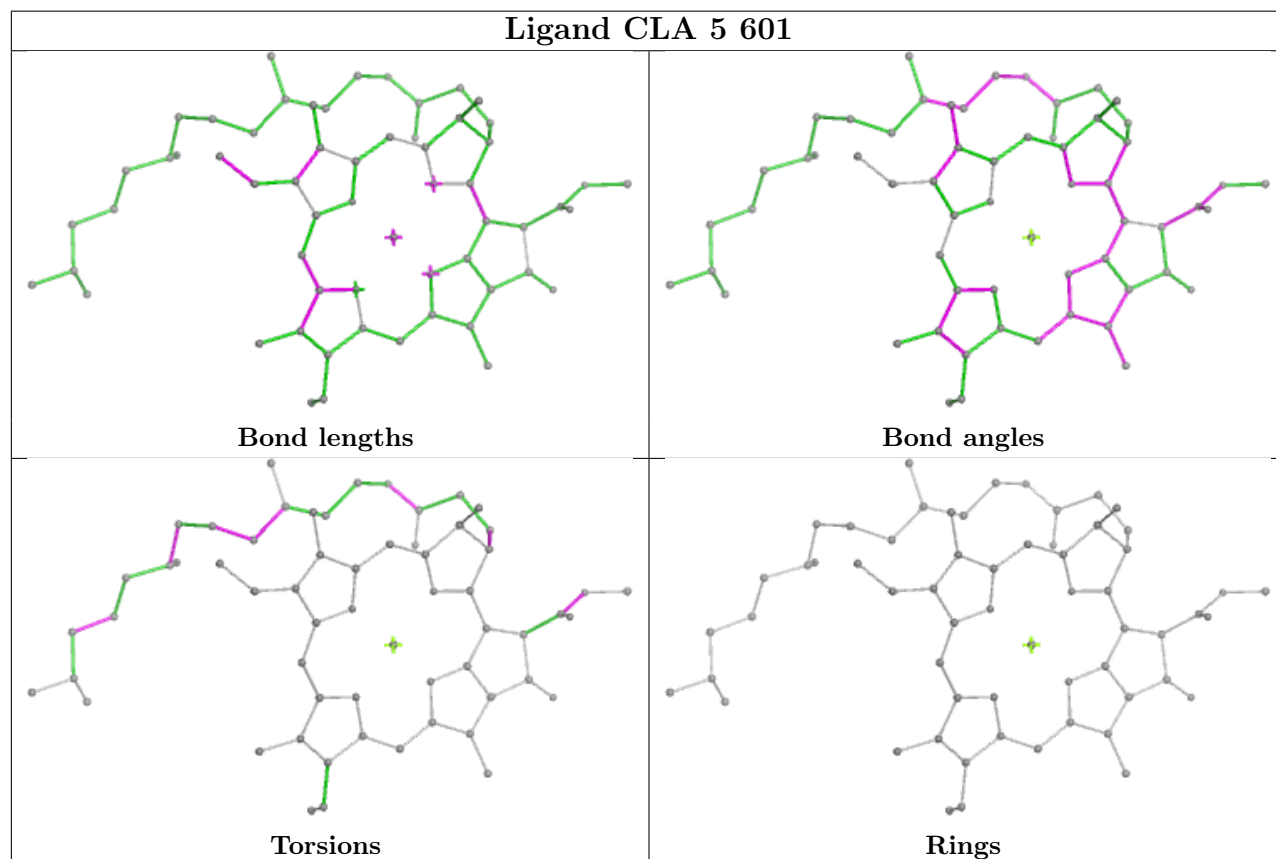




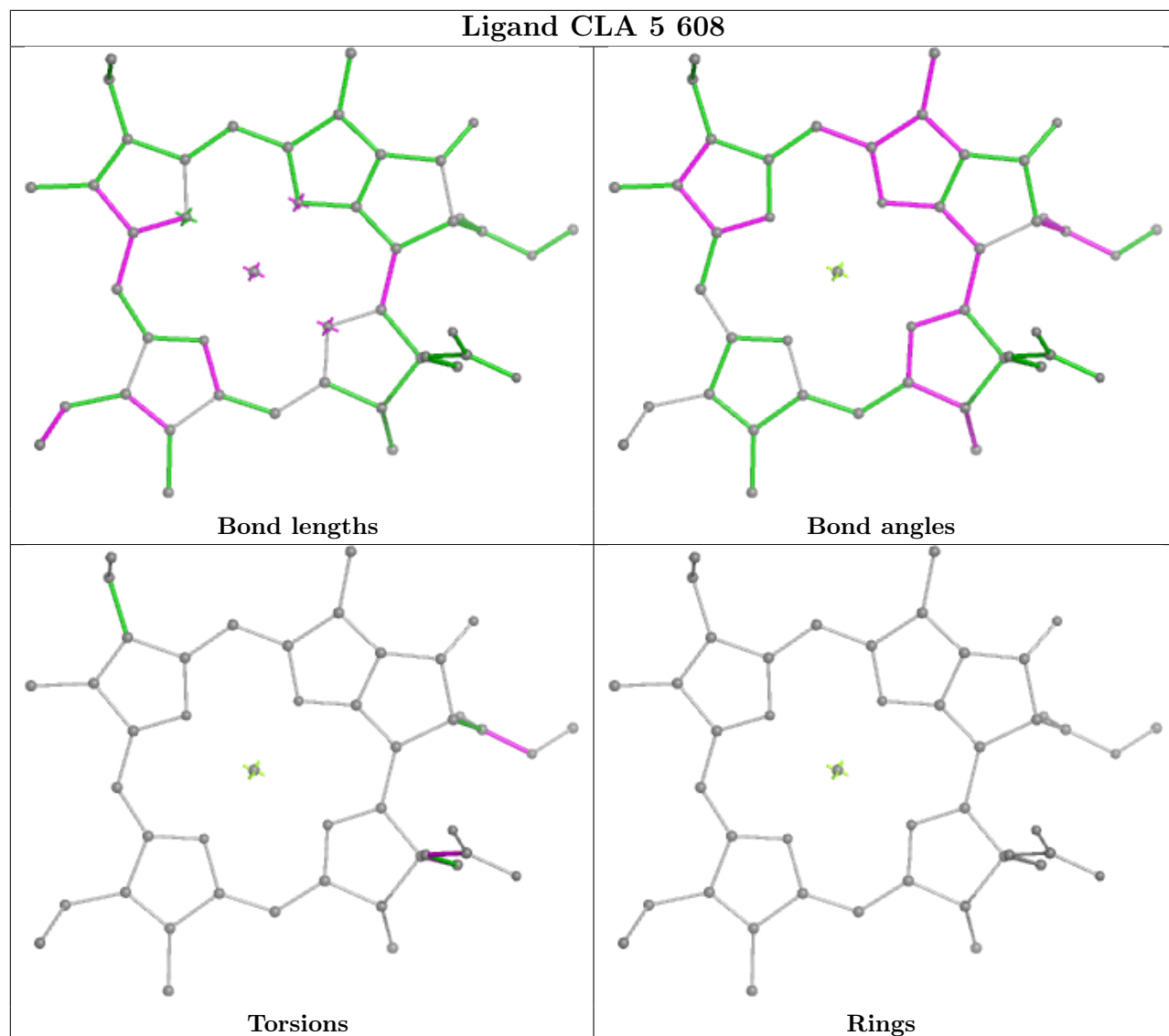
Ligand CLA G 1601



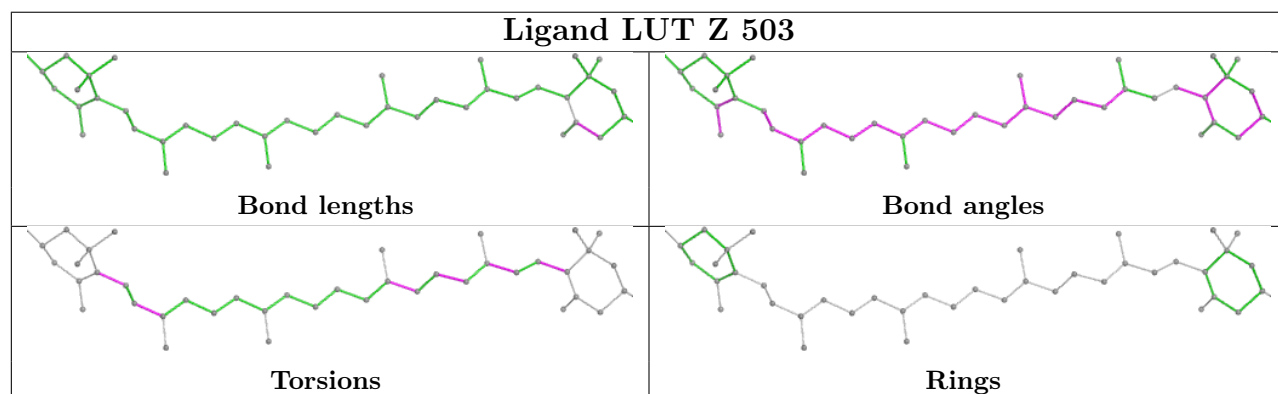
Ligand CLA 5 601



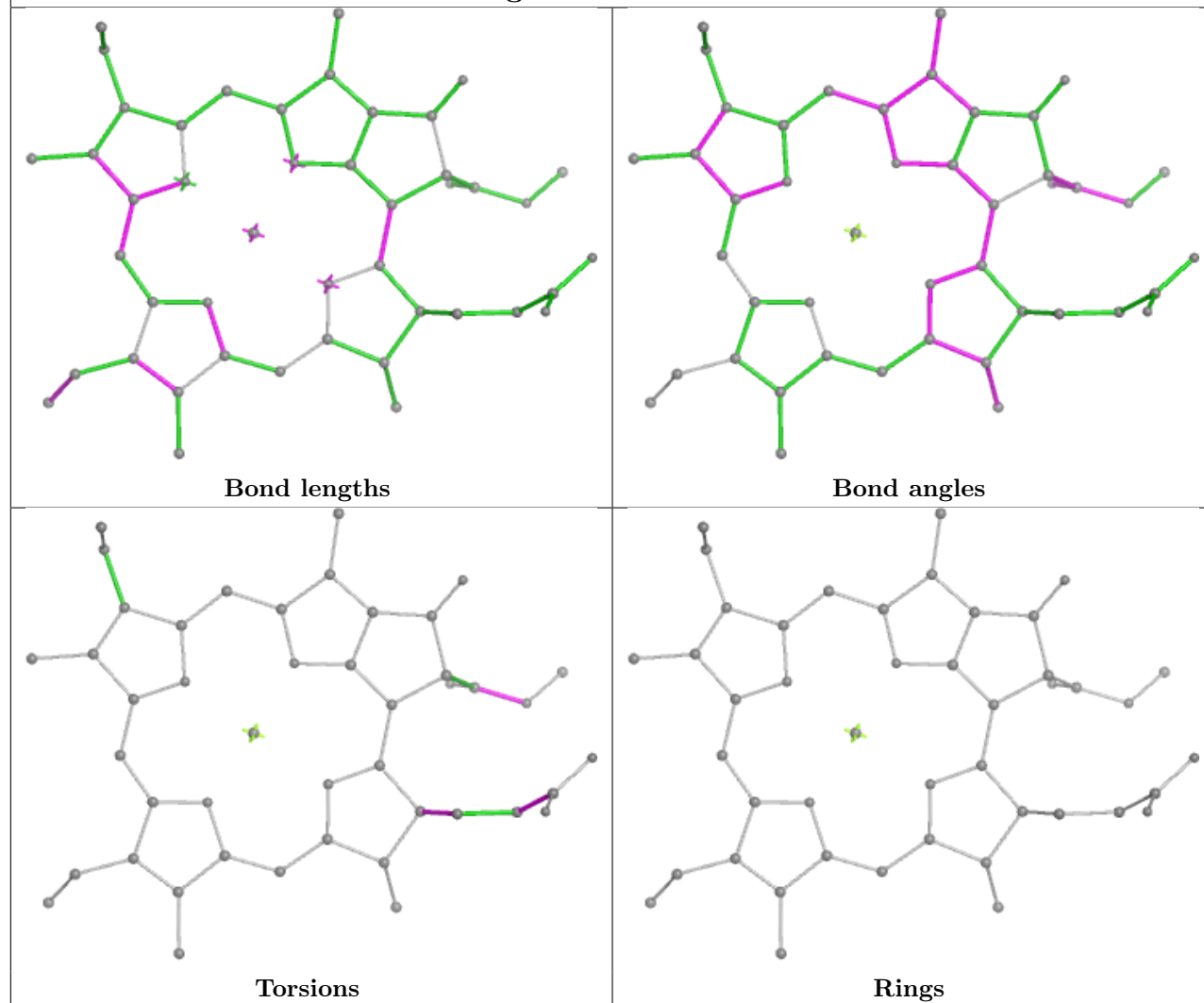
Ligand CLA 5 608



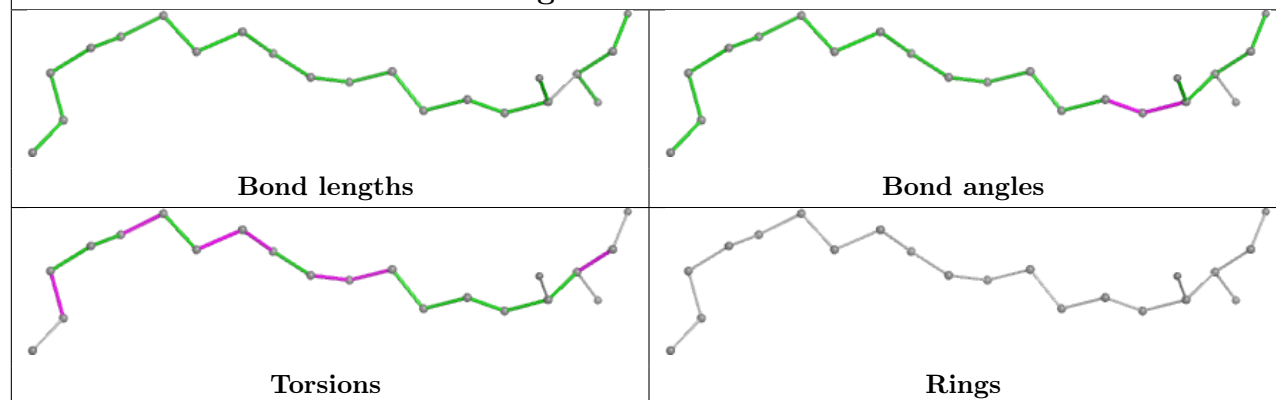
Ligand LUT Z 503

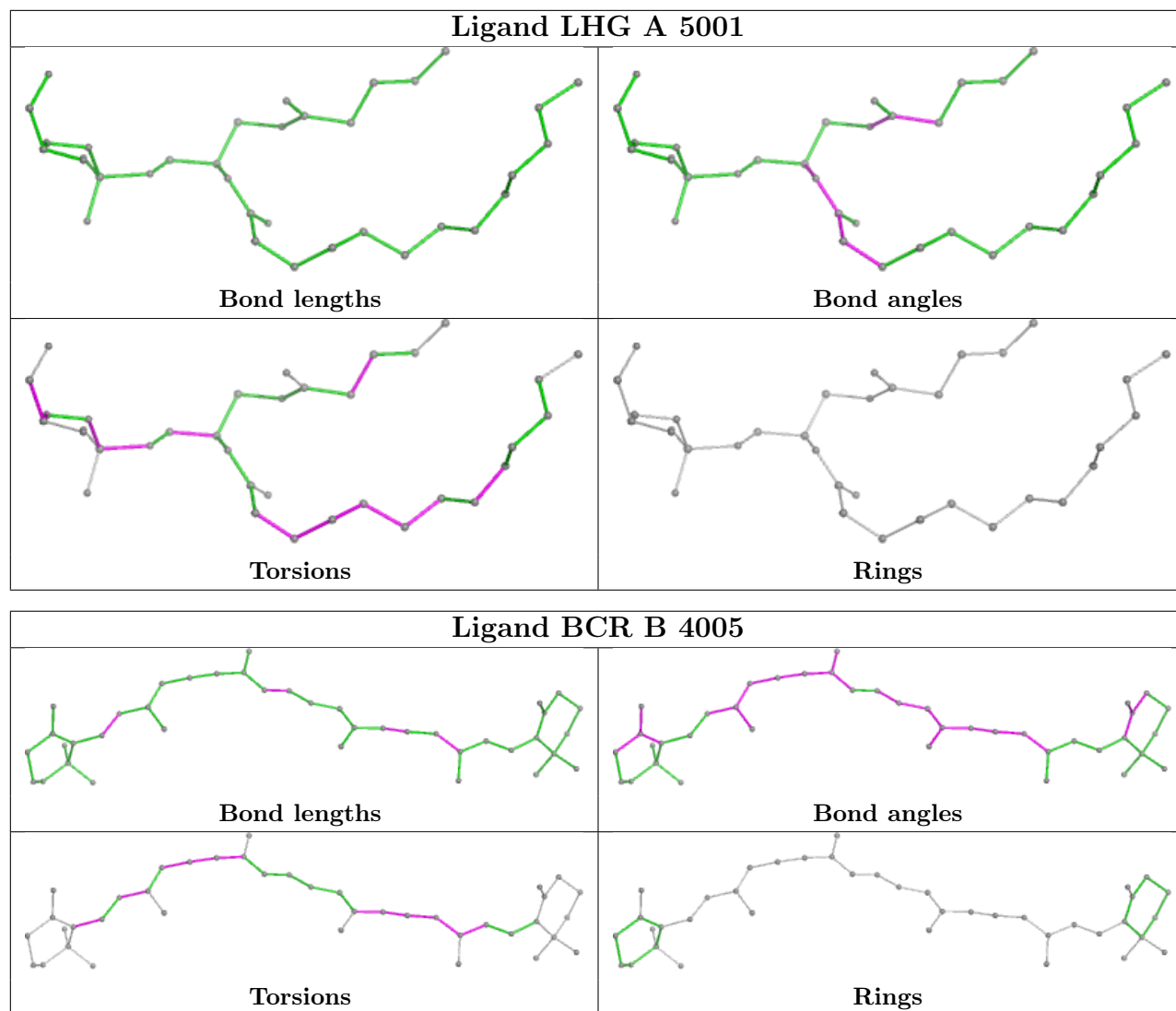


Ligand CLA 3 608

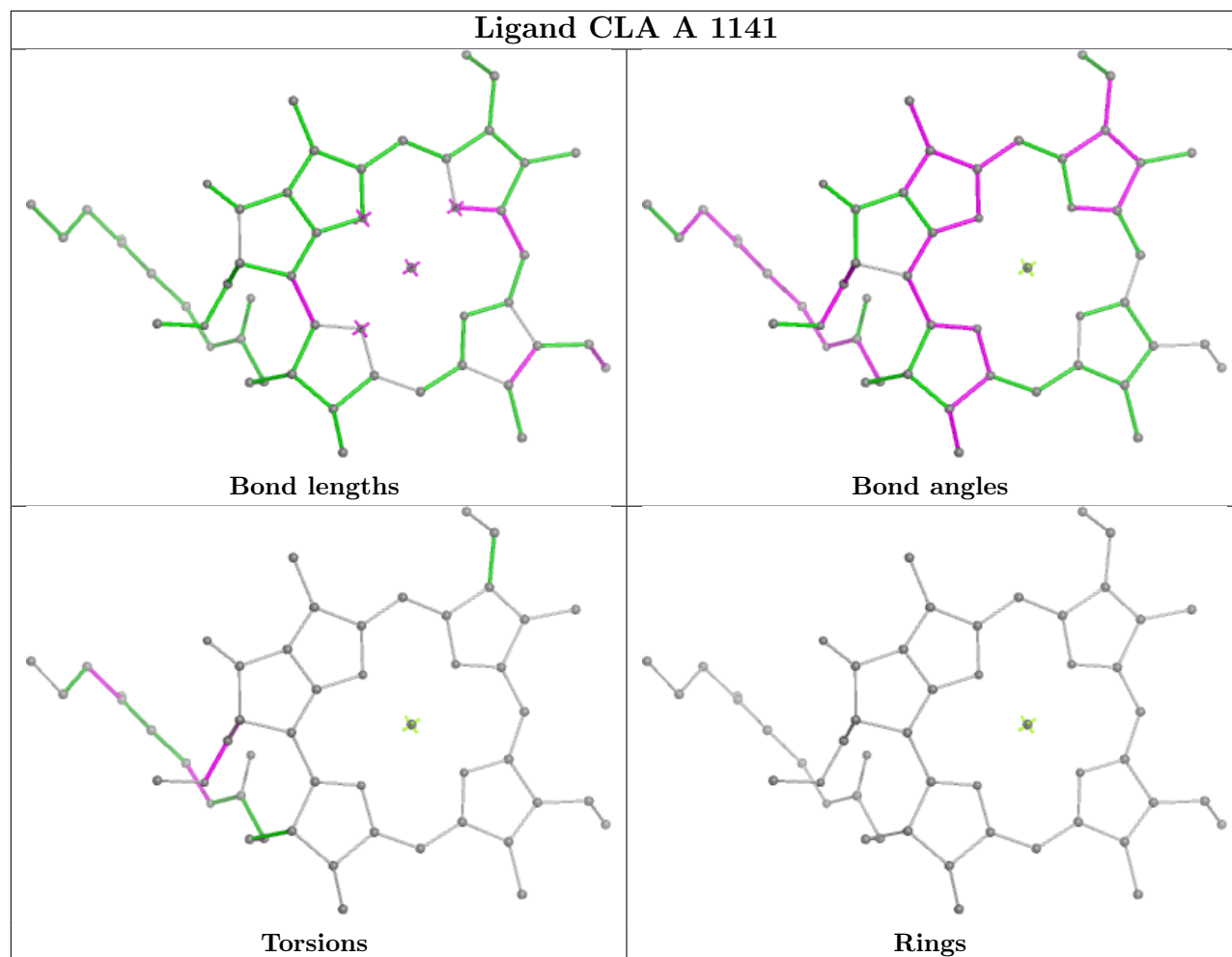


Ligand SPH 7 804

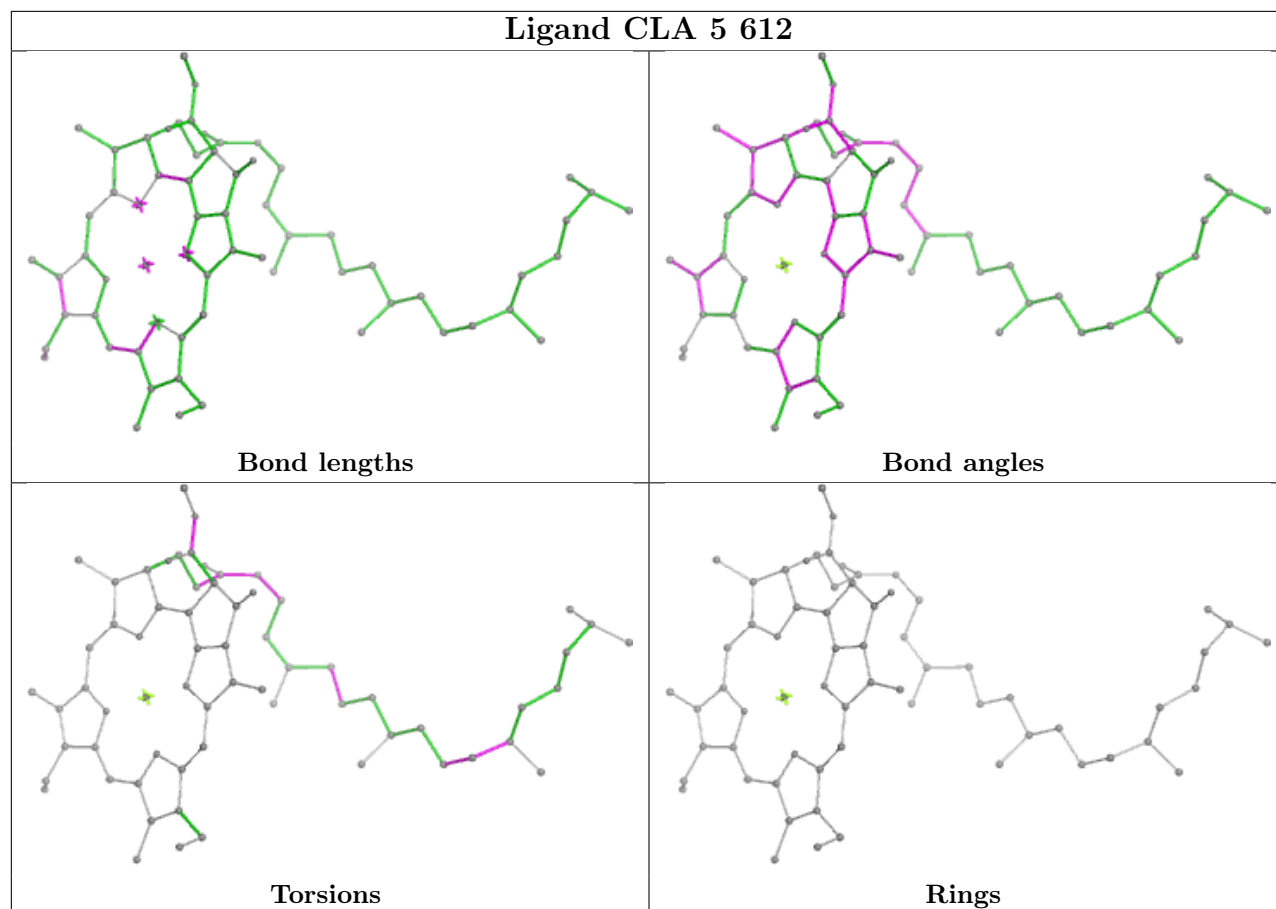




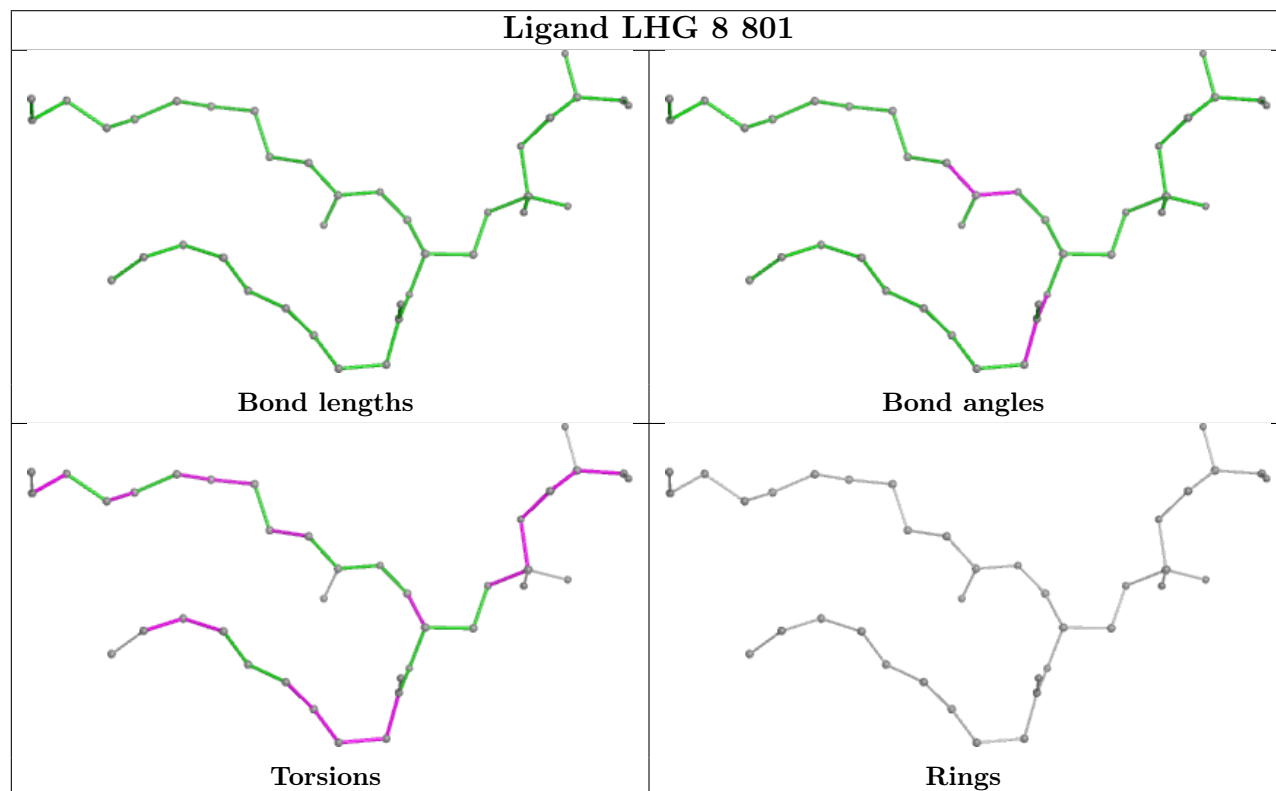
Ligand CLA A 1141

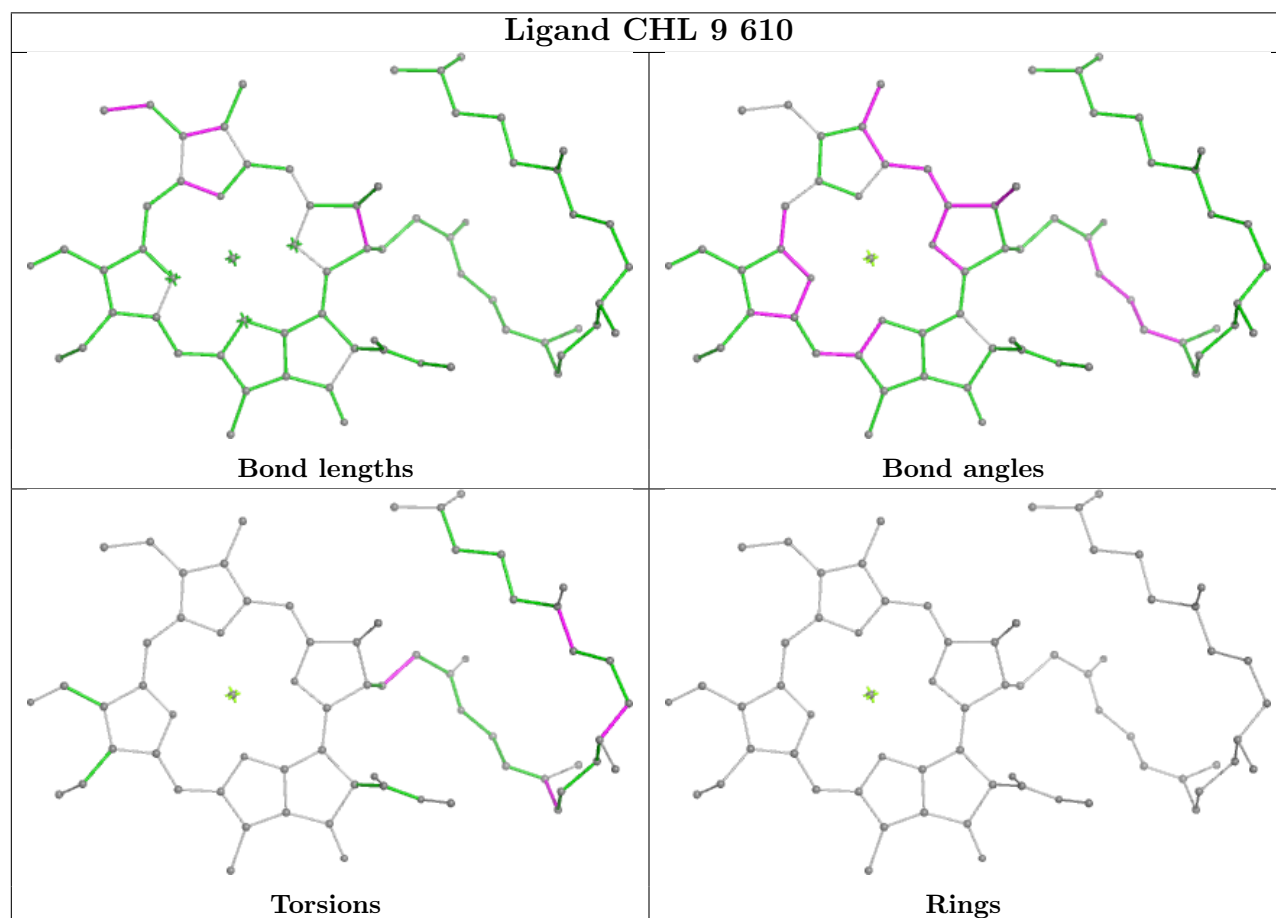
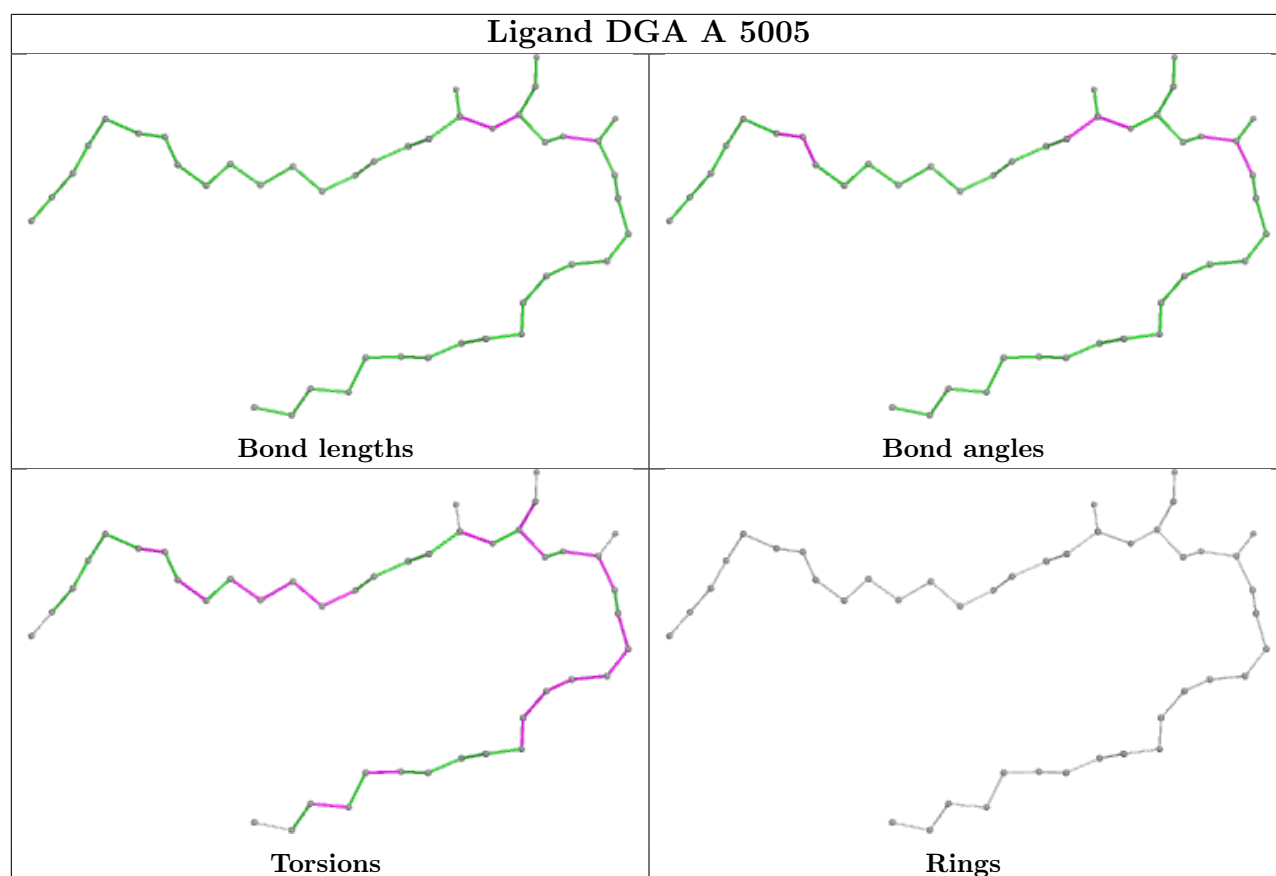


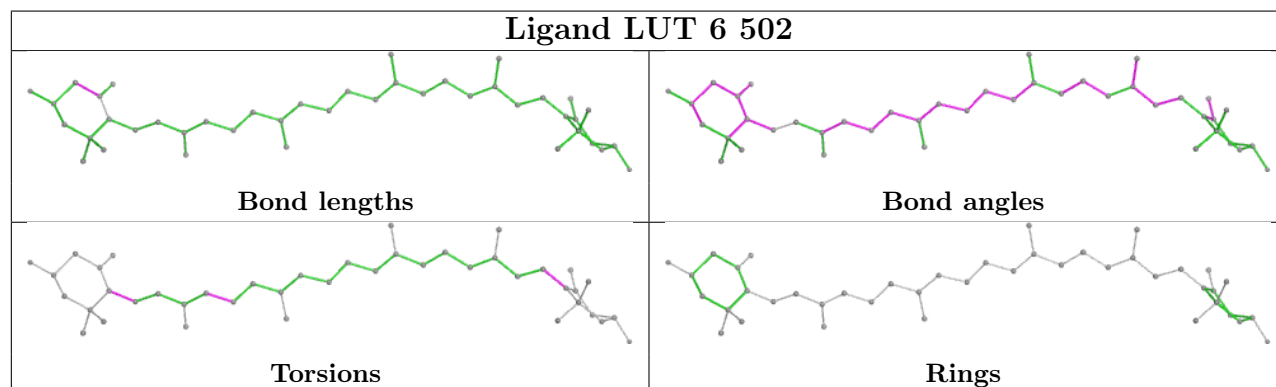
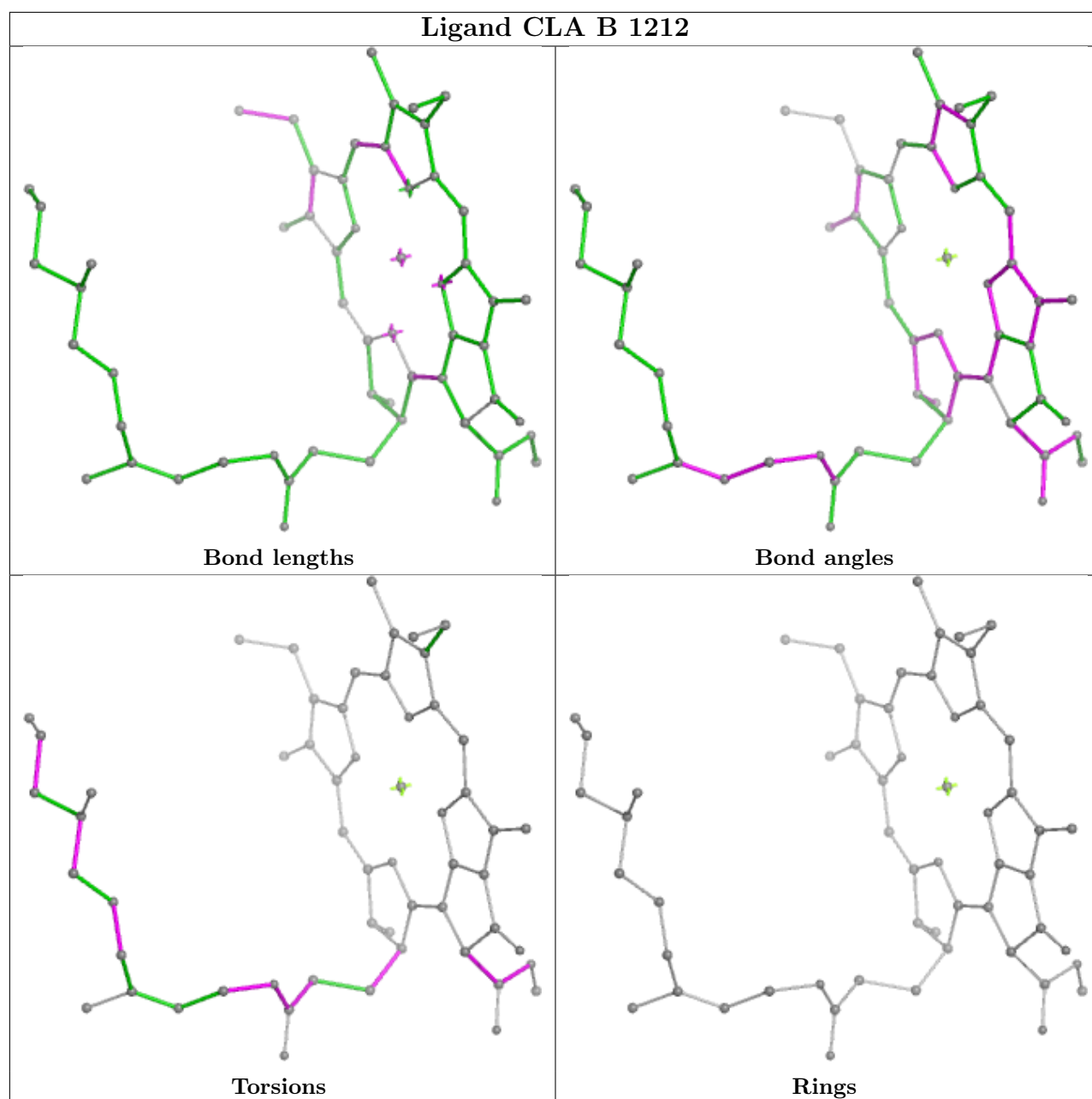
Ligand CLA 5 612

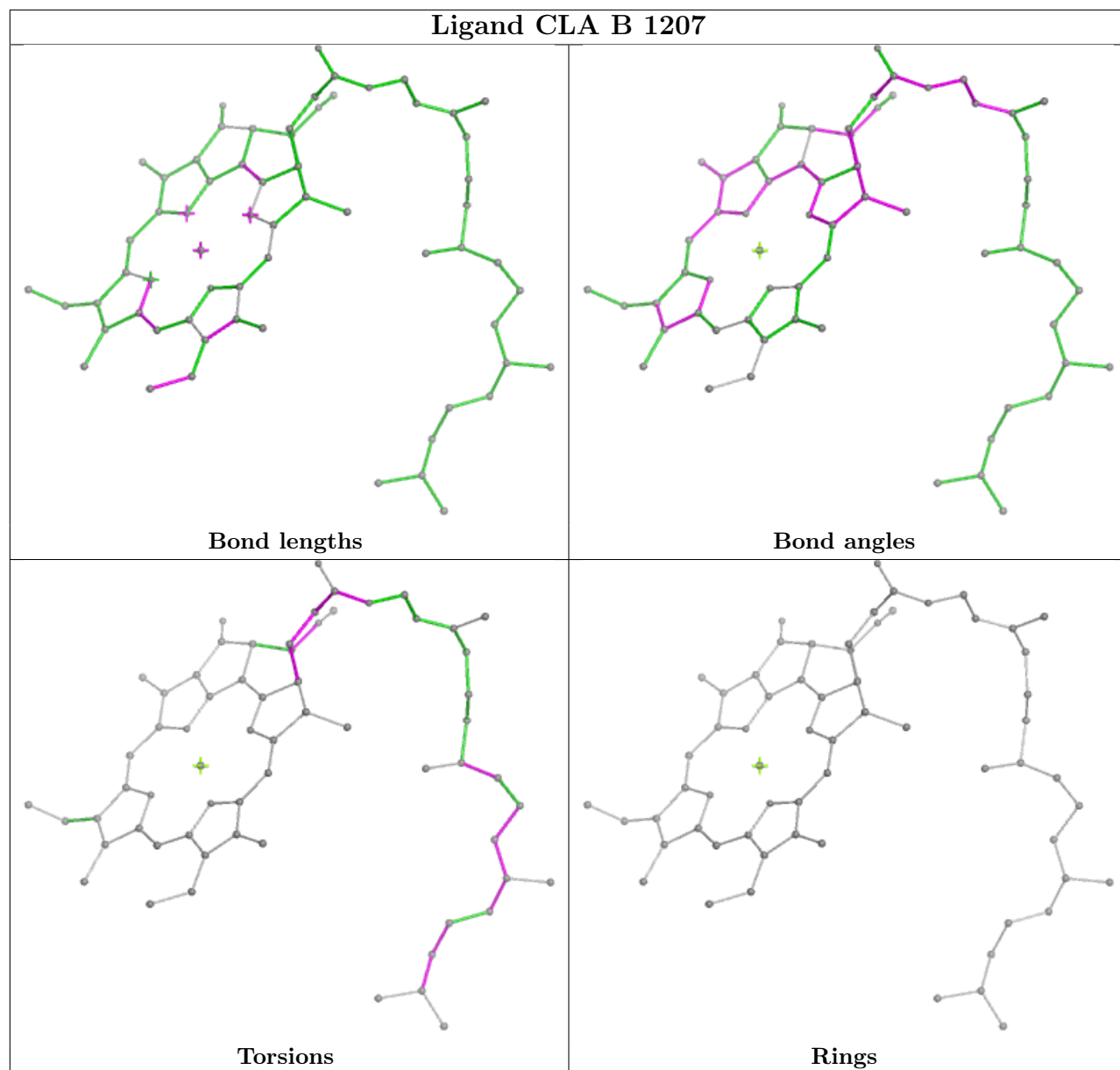


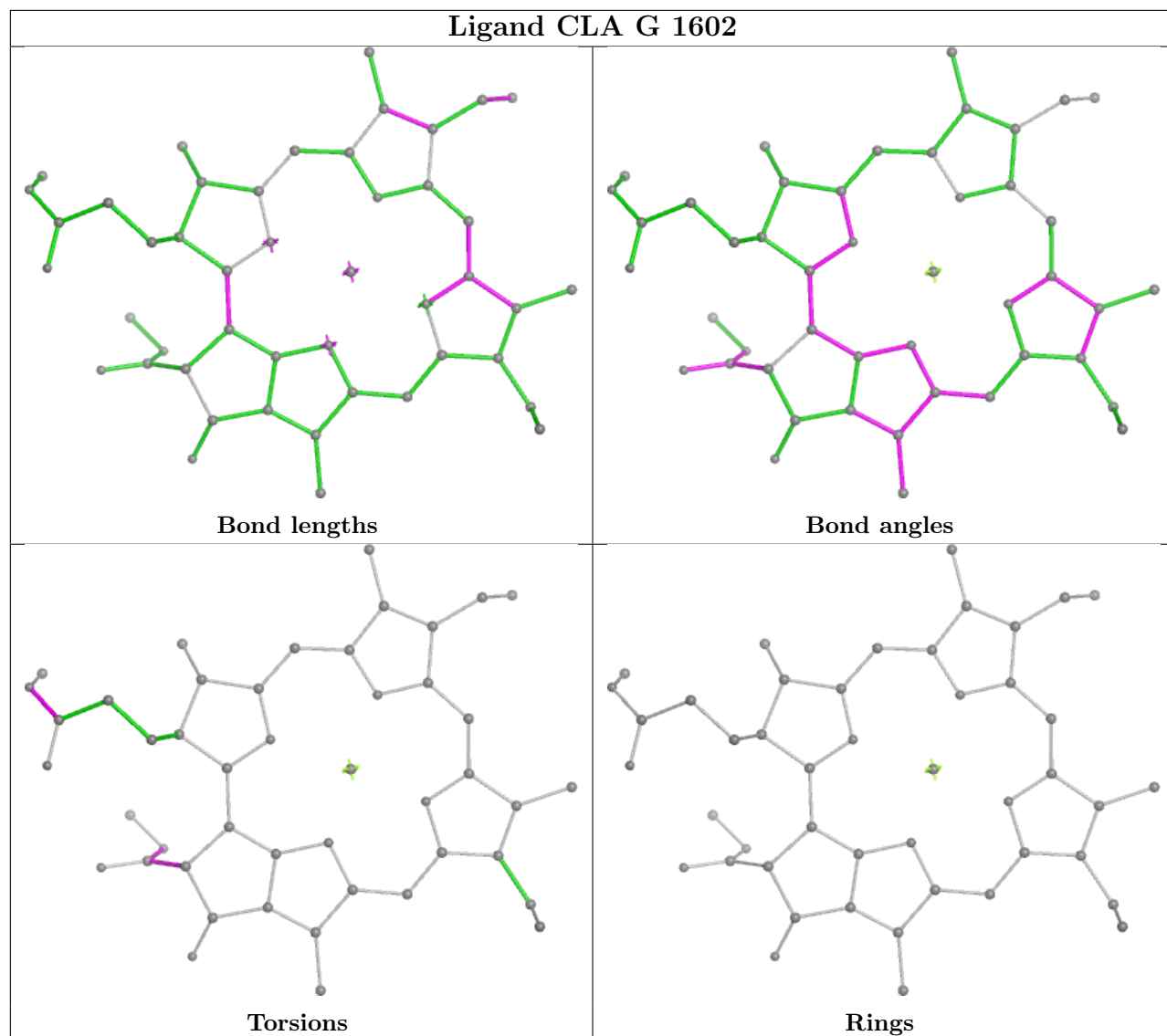
Ligand LHG 8 801

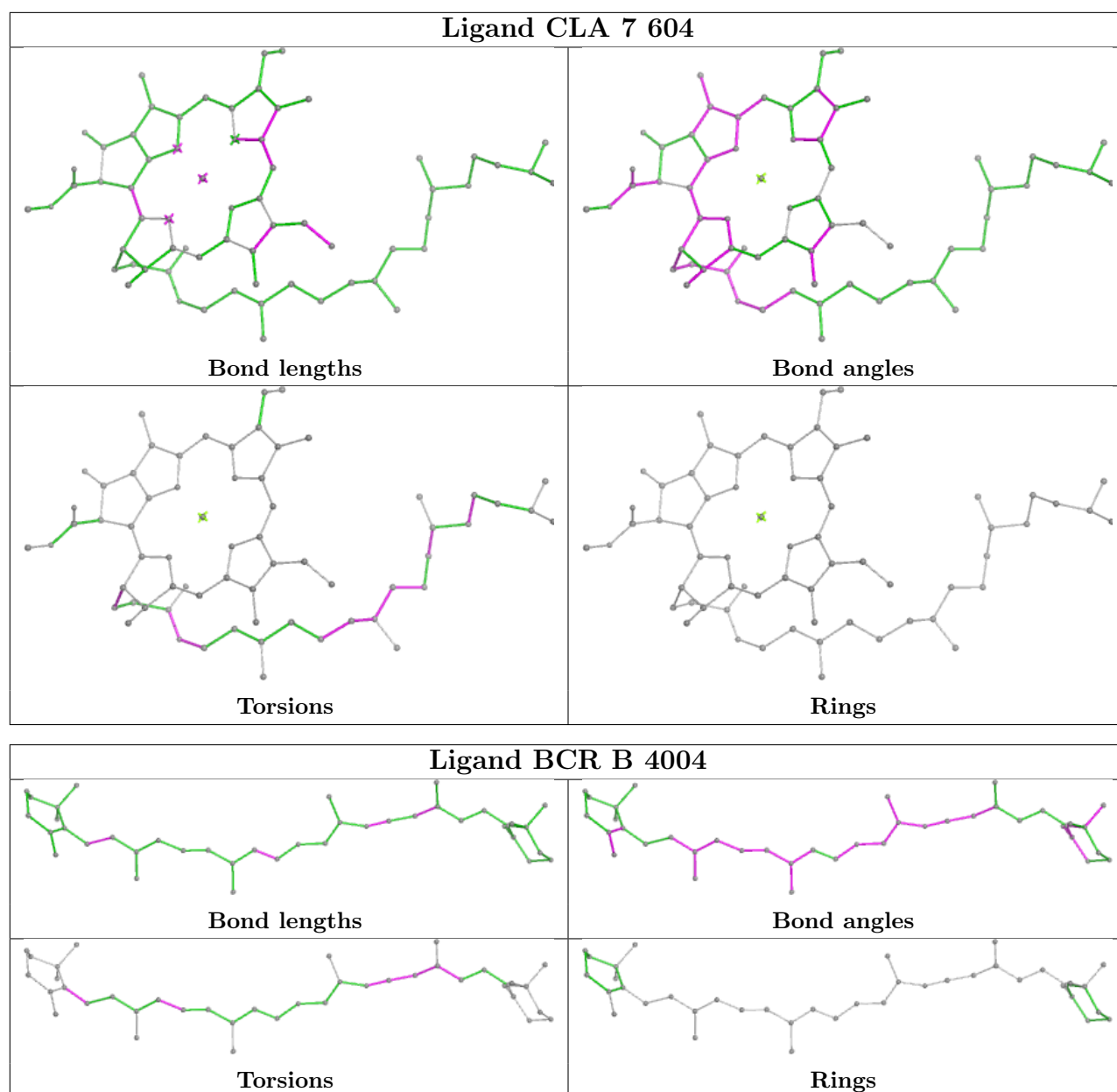


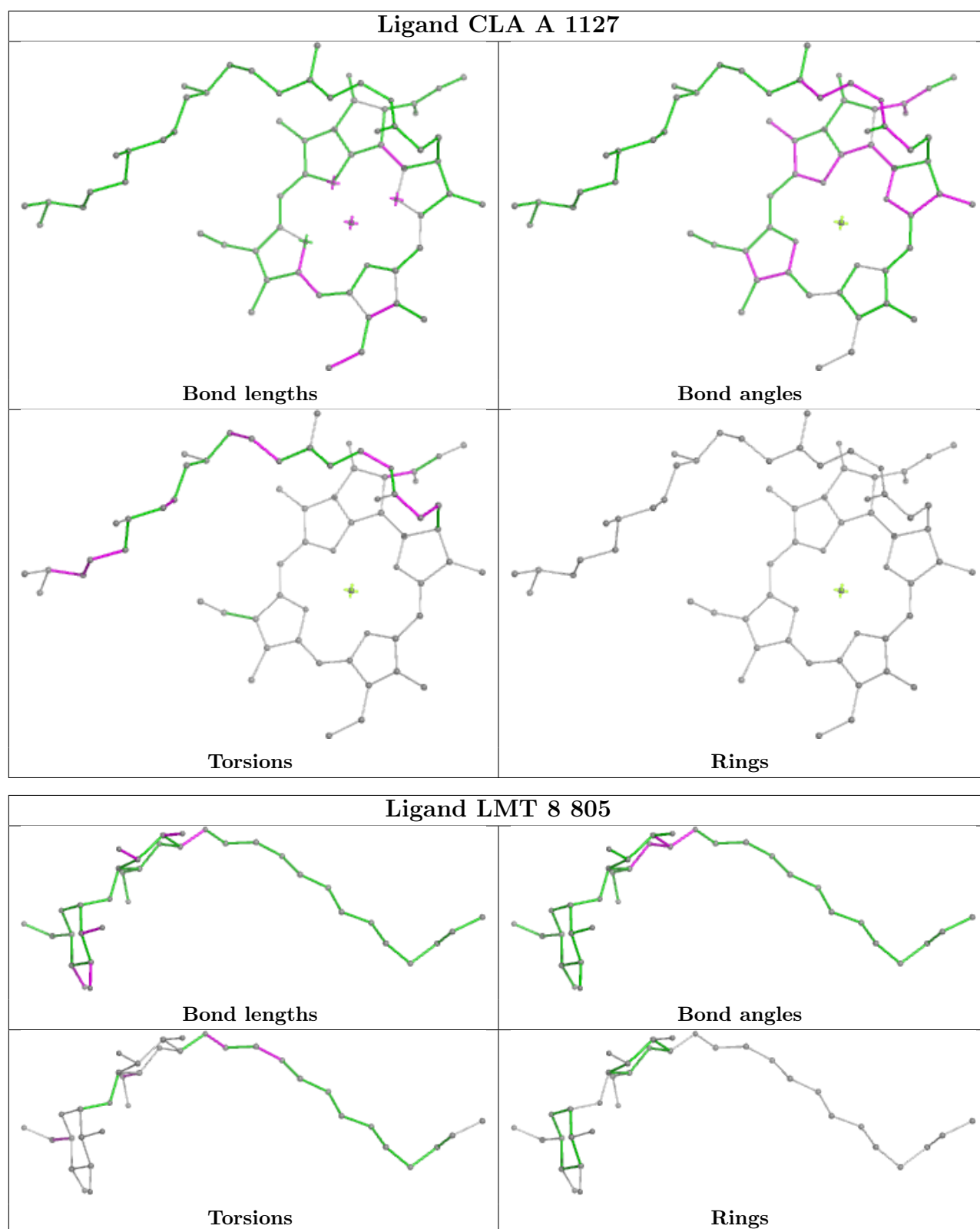


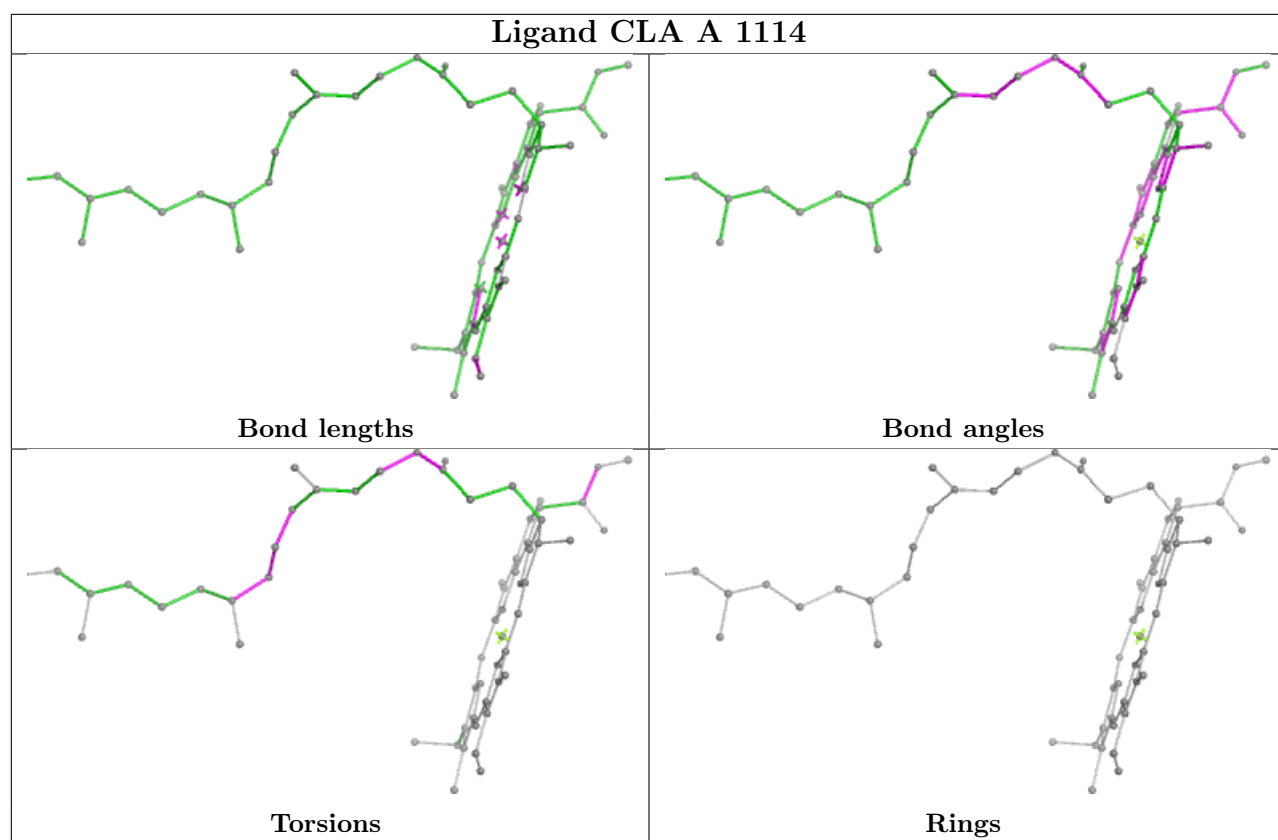




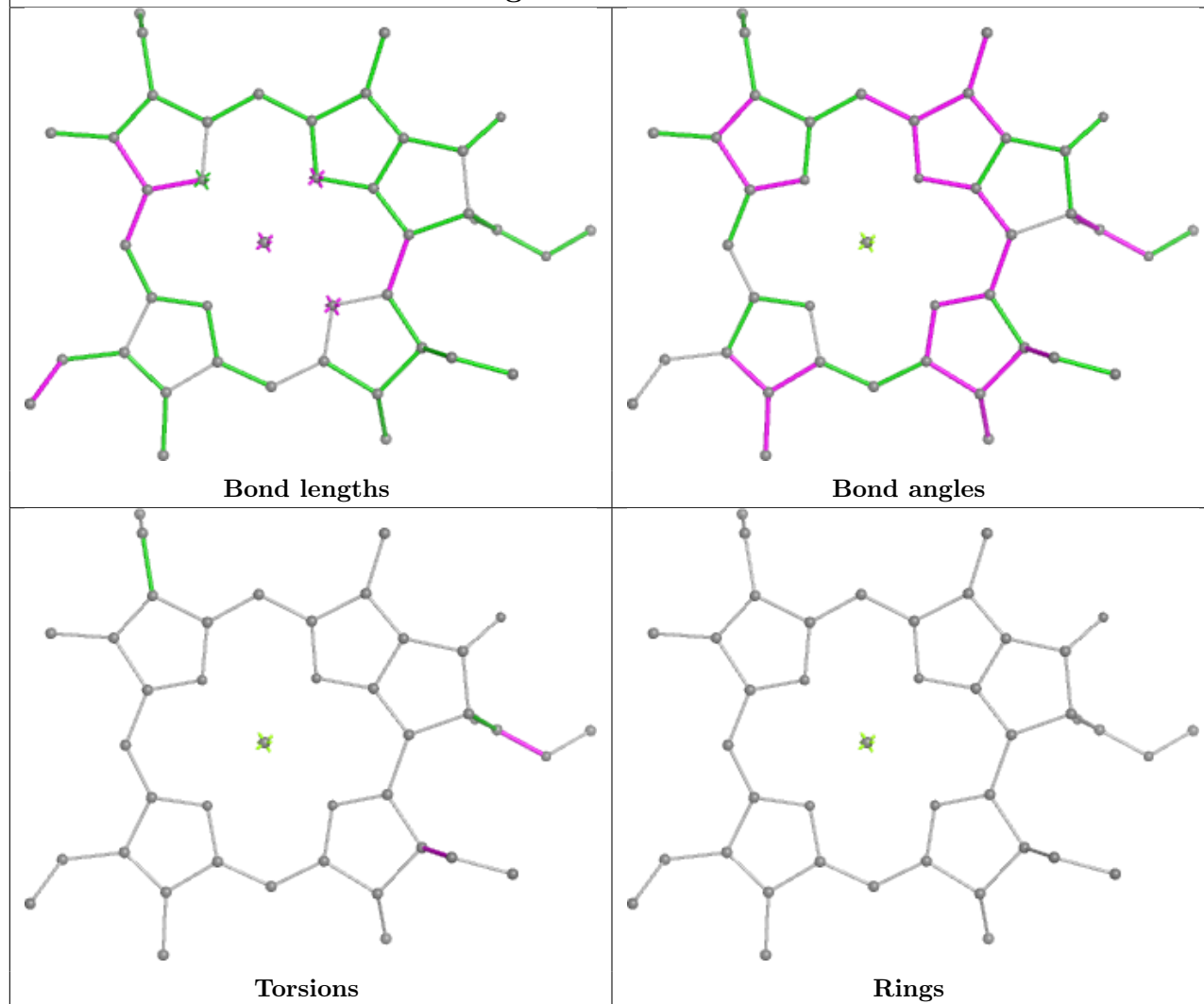




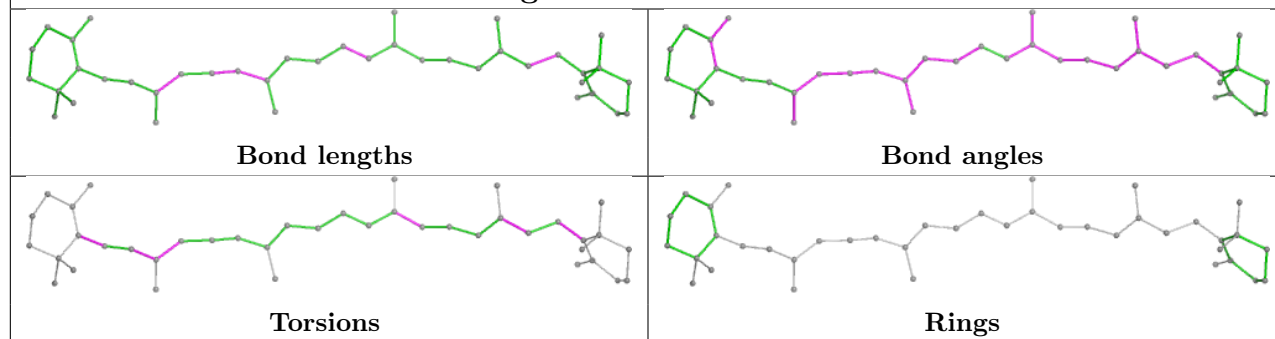


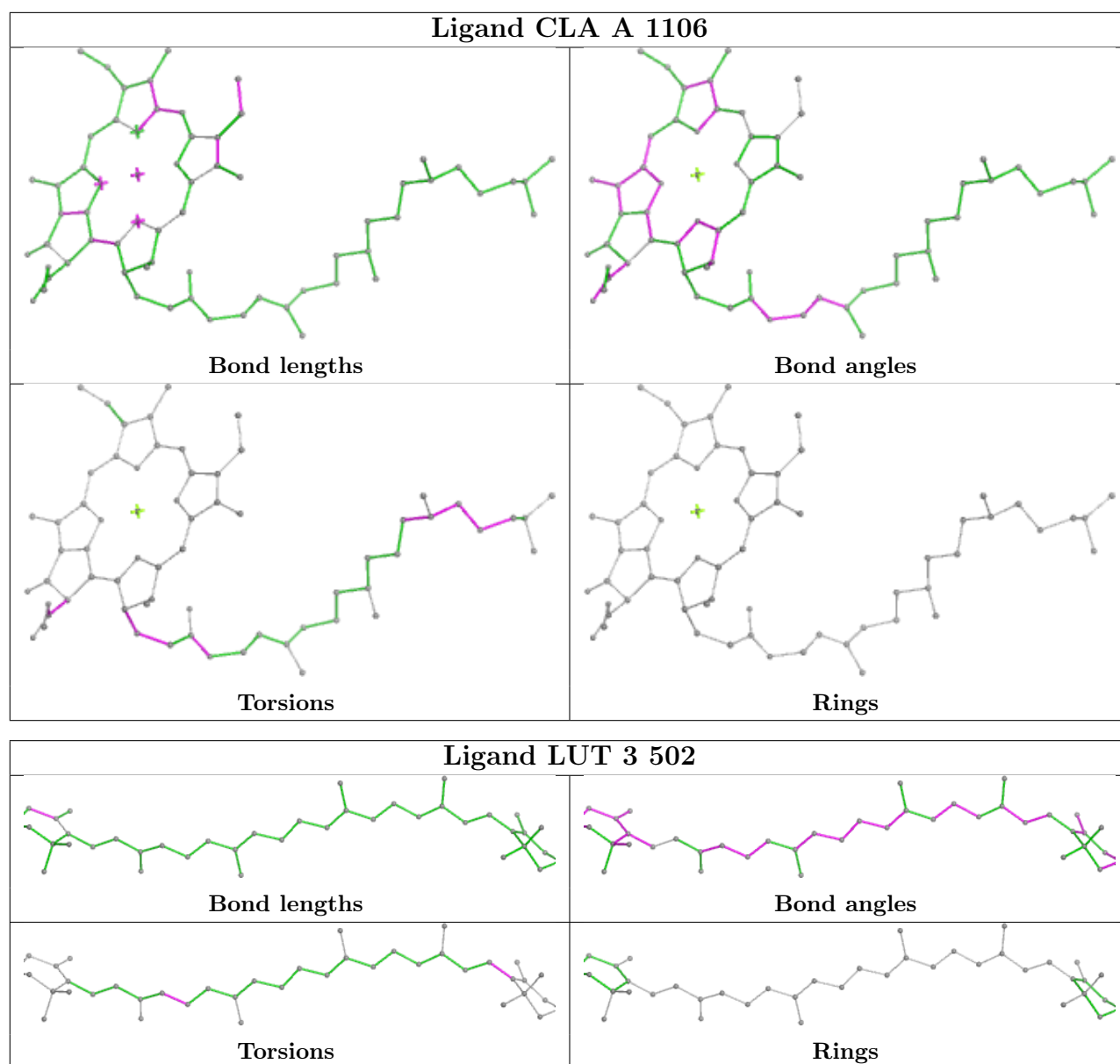


Ligand CLA 7 613



Ligand BCR B 4001





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.

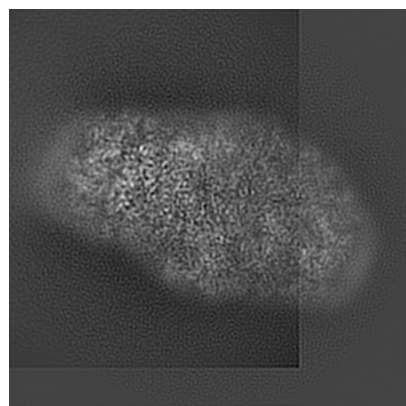
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12180. These allow visual inspection of the internal detail of the map and identification of artifacts.

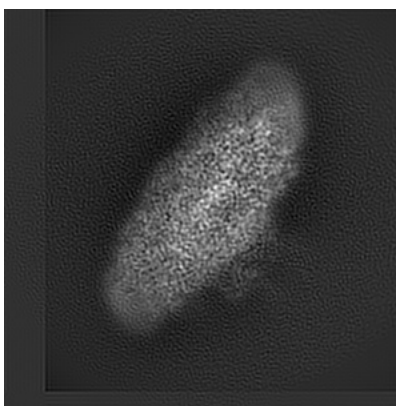
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

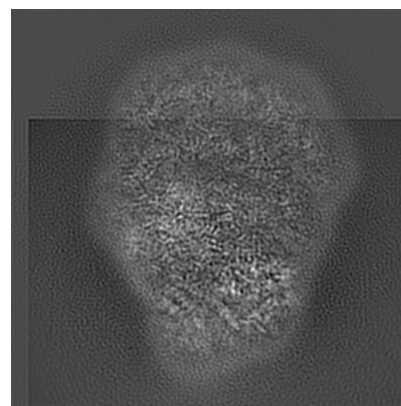
6.1.1 Primary map



X

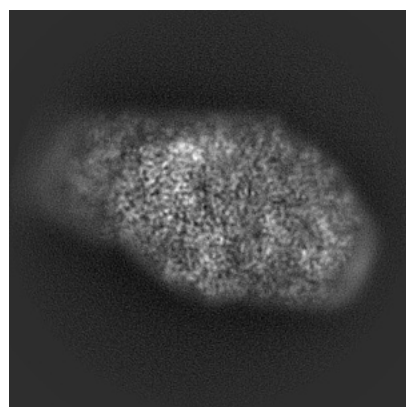


Y

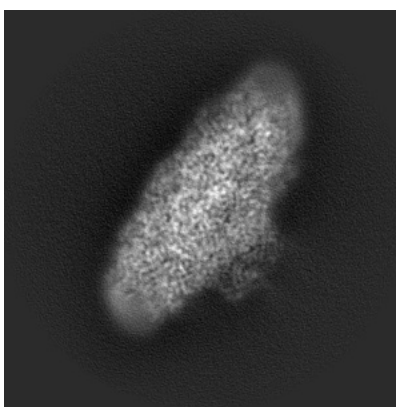


Z

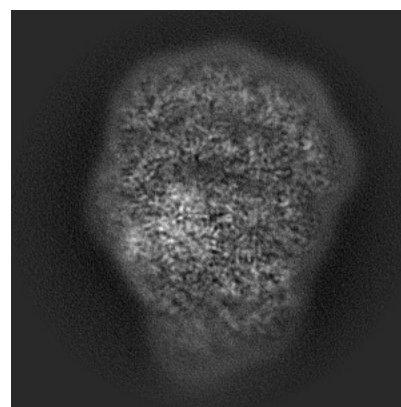
6.1.2 Raw map



X



Y

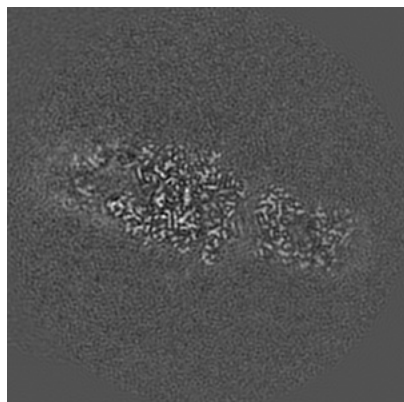


Z

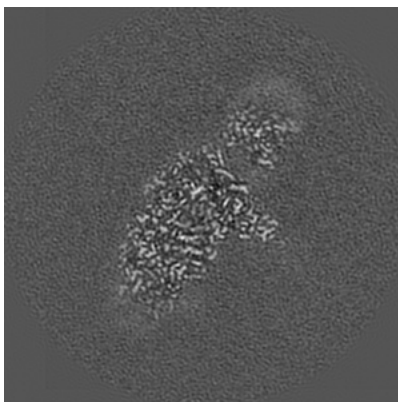
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

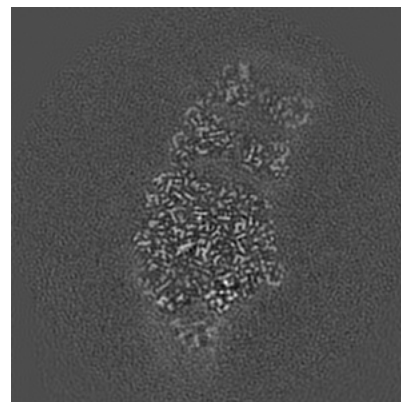
6.2.1 Primary map



X Index: 160

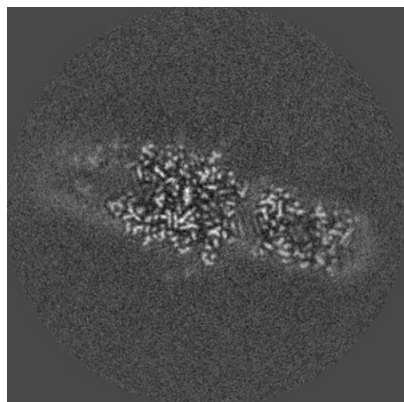


Y Index: 160

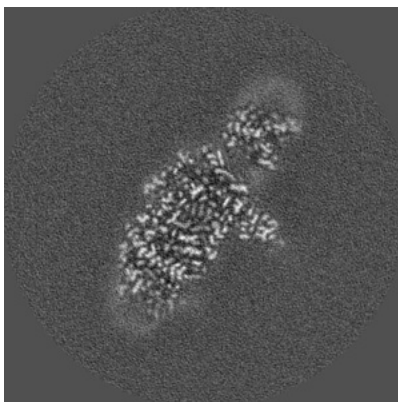


Z Index: 160

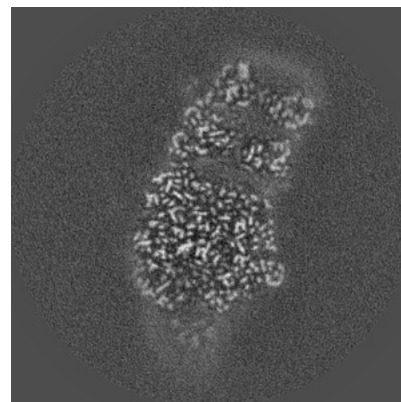
6.2.2 Raw map



X Index: 160



Y Index: 160

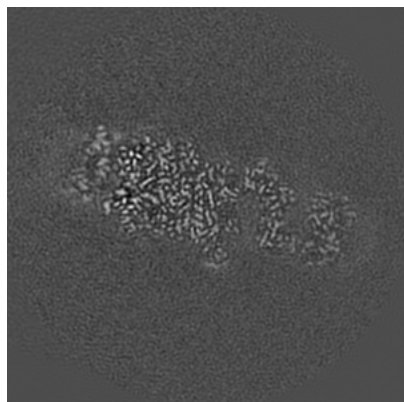


Z Index: 160

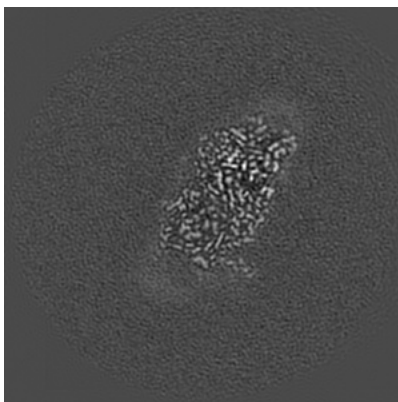
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

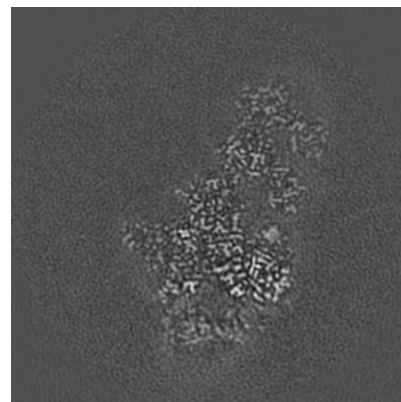
6.3.1 Primary map



X Index: 172

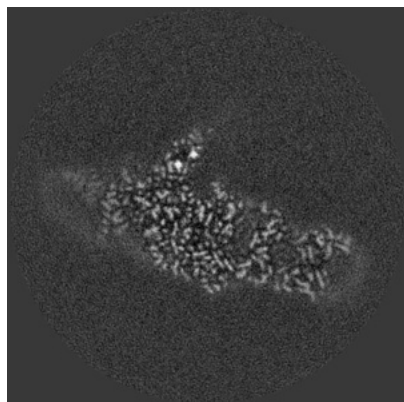


Y Index: 112

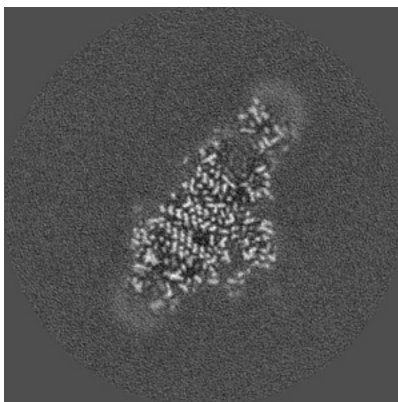


Z Index: 180

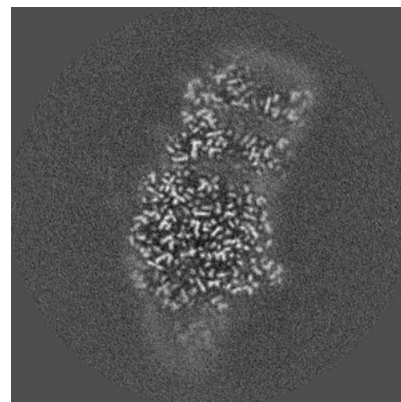
6.3.2 Raw map



X Index: 127



Y Index: 145

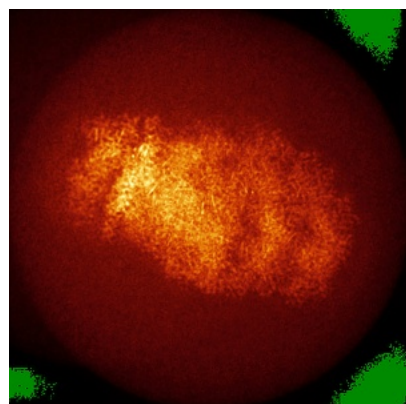


Z Index: 157

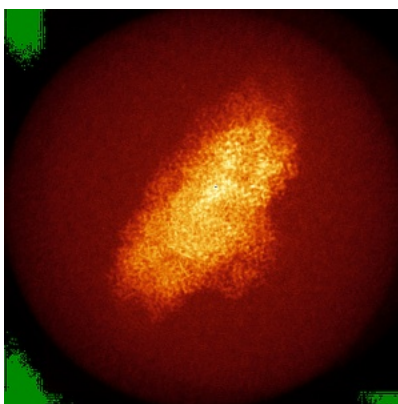
The images above show the largest variance slices of the map in three orthogonal directions.

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

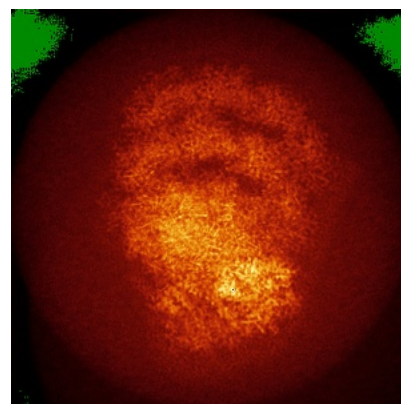
6.4.1 Primary map



X

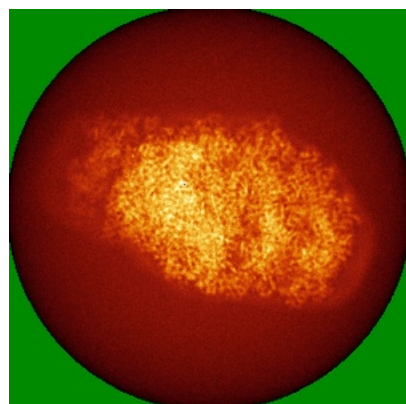


Y

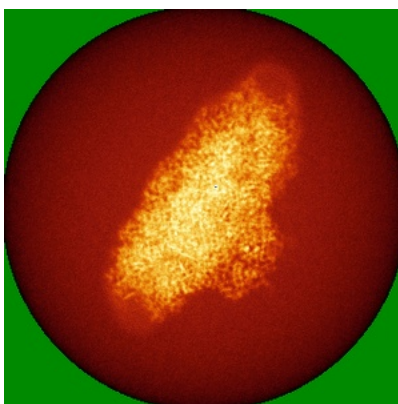


Z

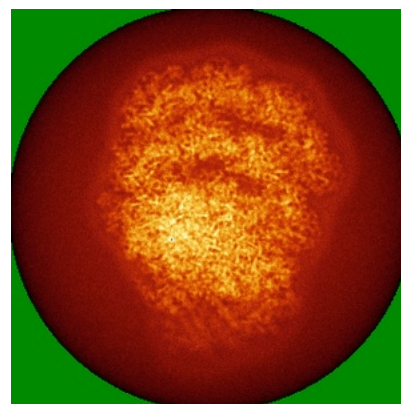
6.4.2 Raw map



X



Y

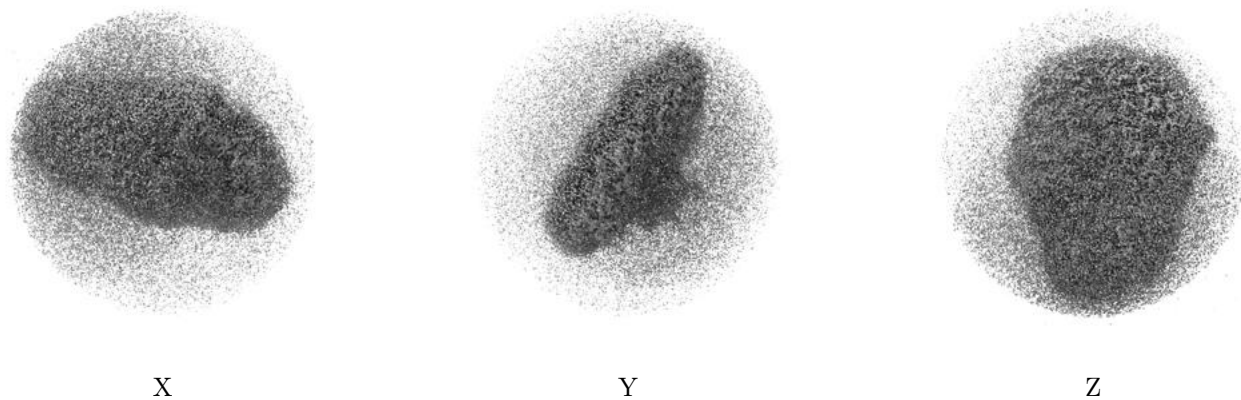


Z

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.

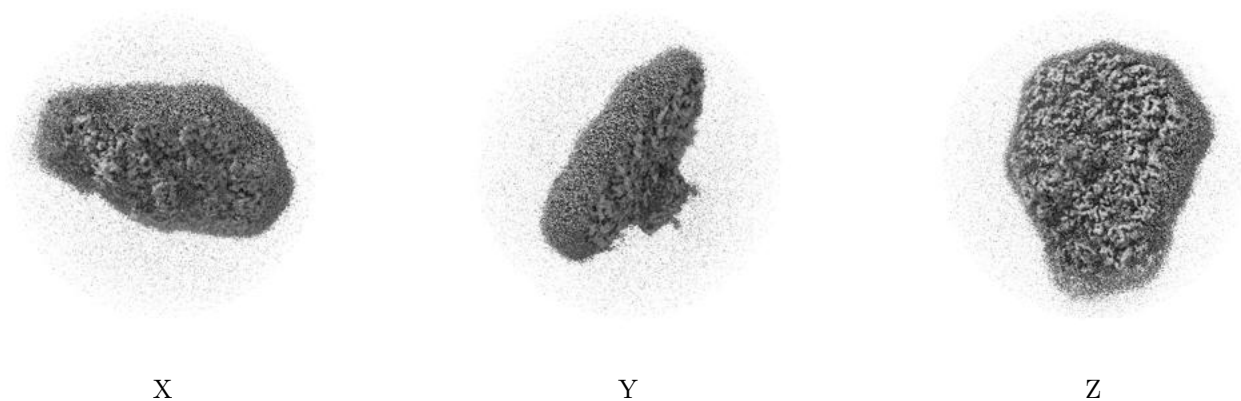
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. 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.

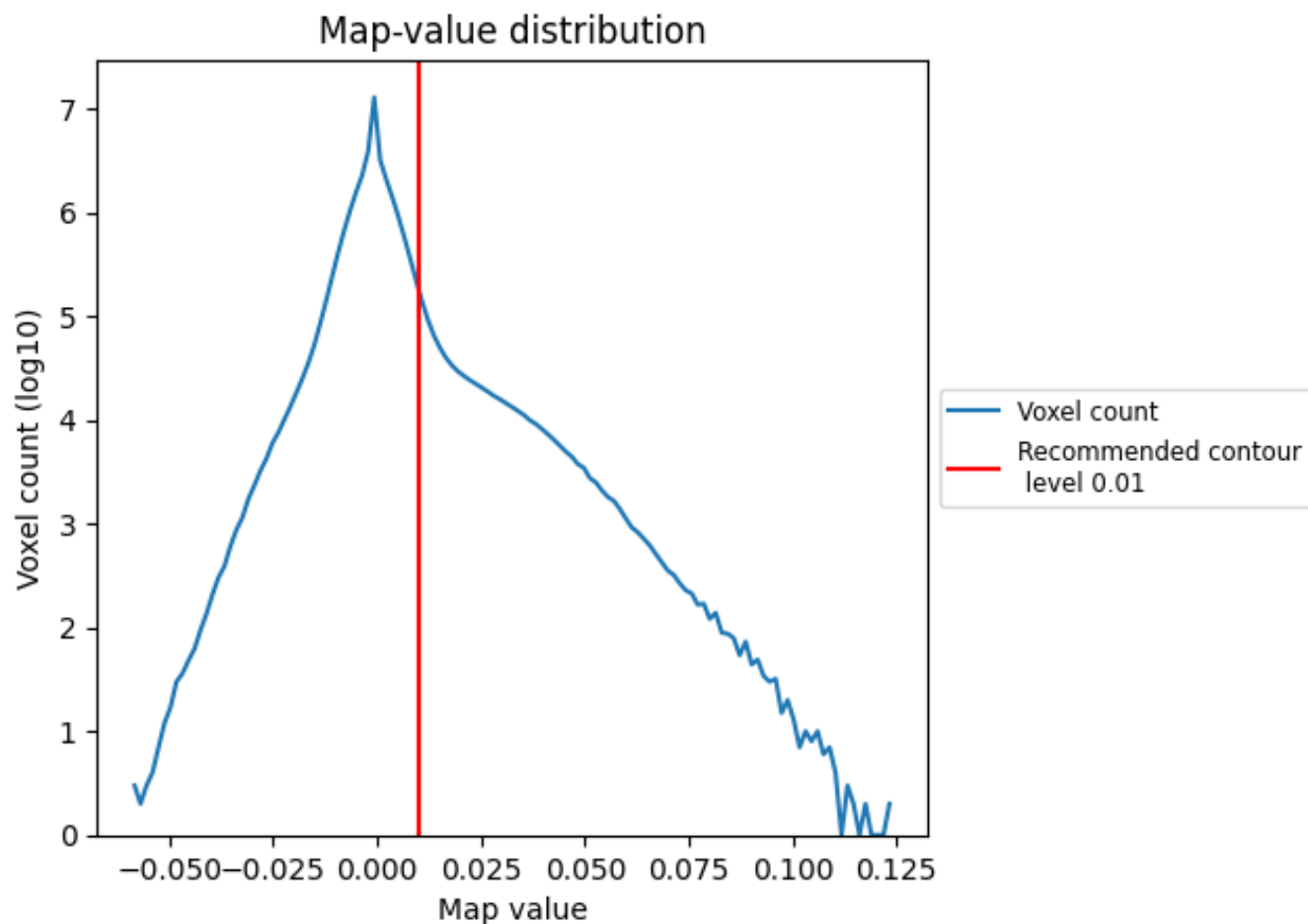
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

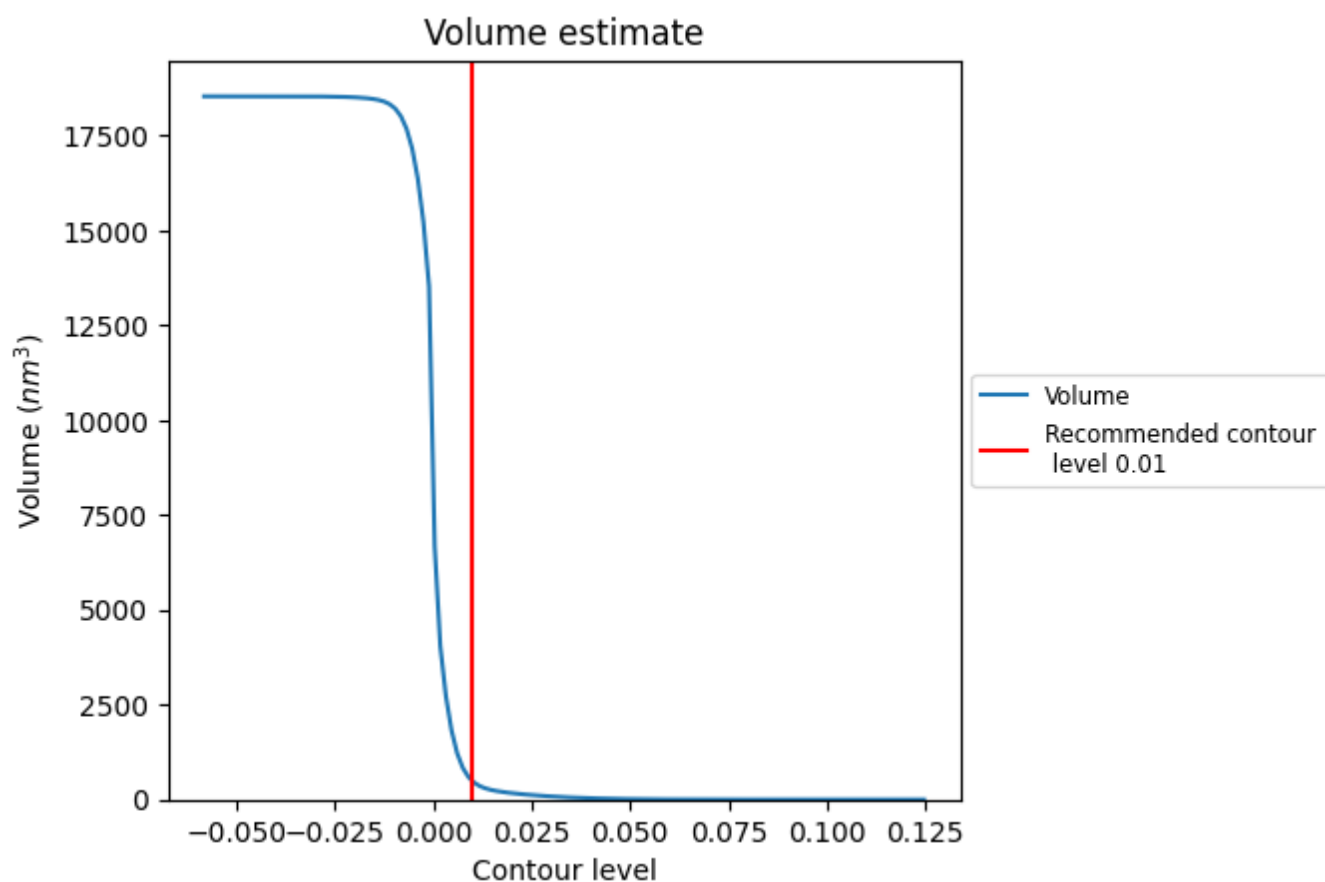
This section contains the results of statistical analysis of the map.

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.

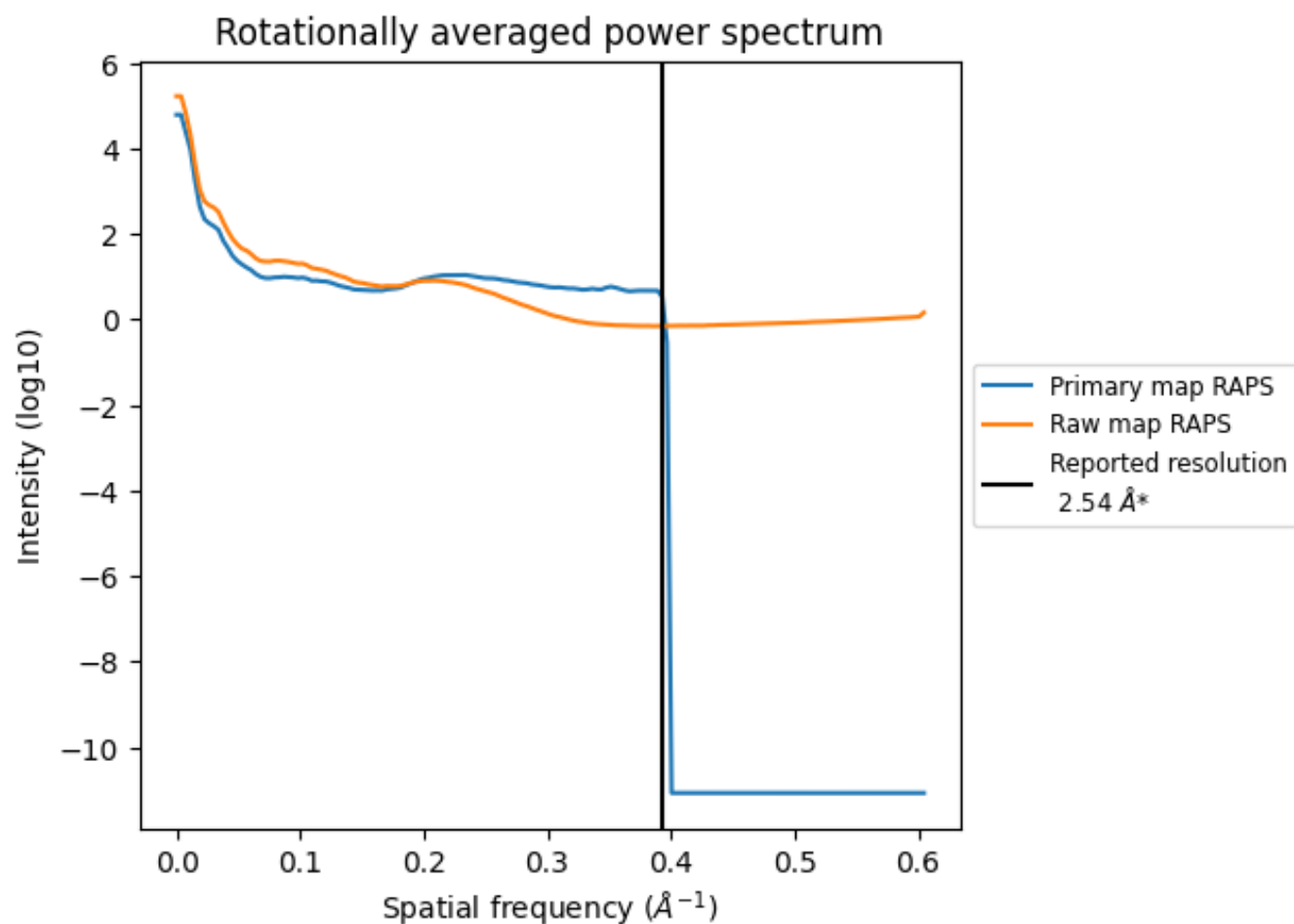
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 483 nm^3 ; this corresponds to an approximate mass of 436 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 ⓘ

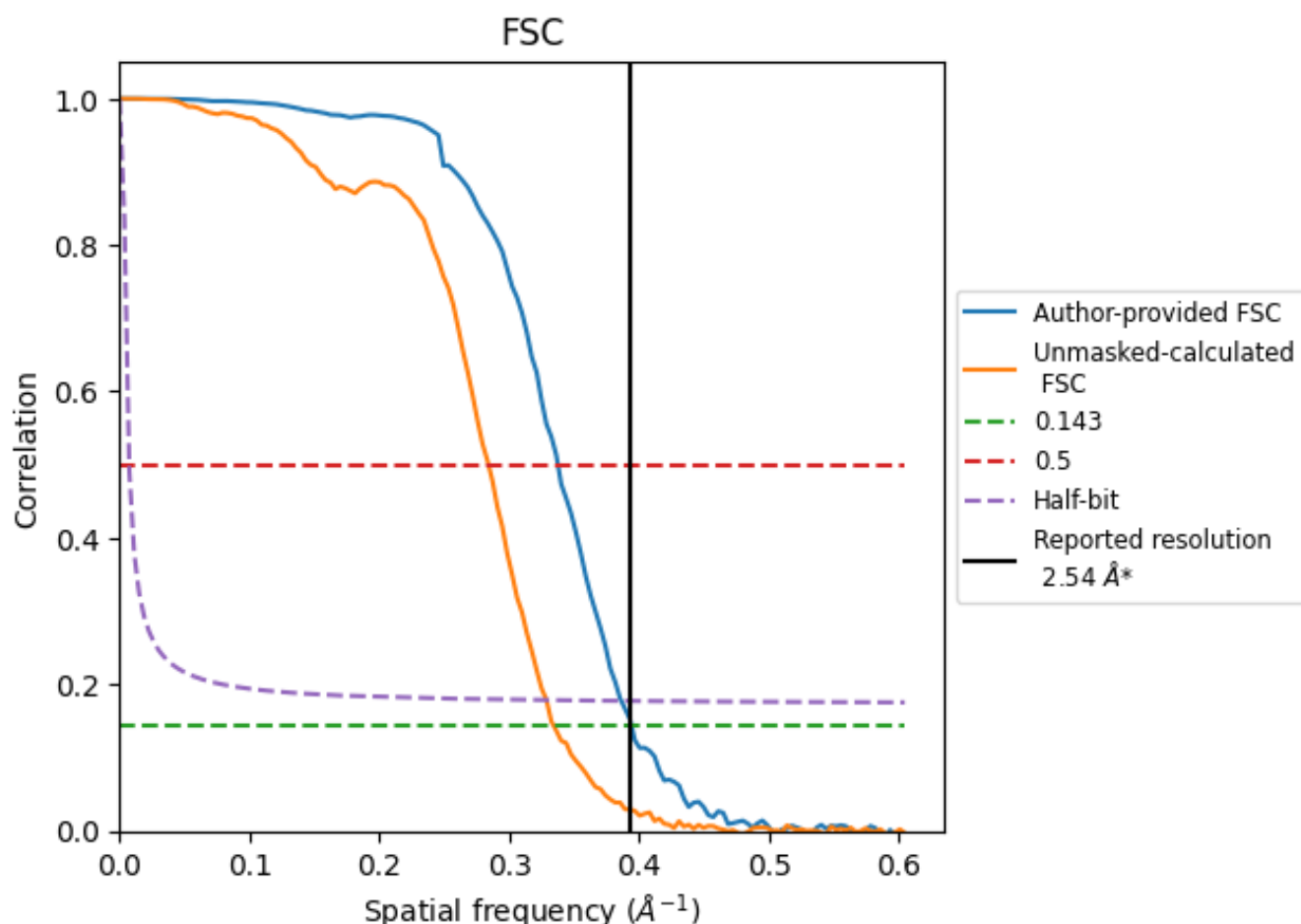


*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.394 Å⁻¹

8.2 Resolution estimates

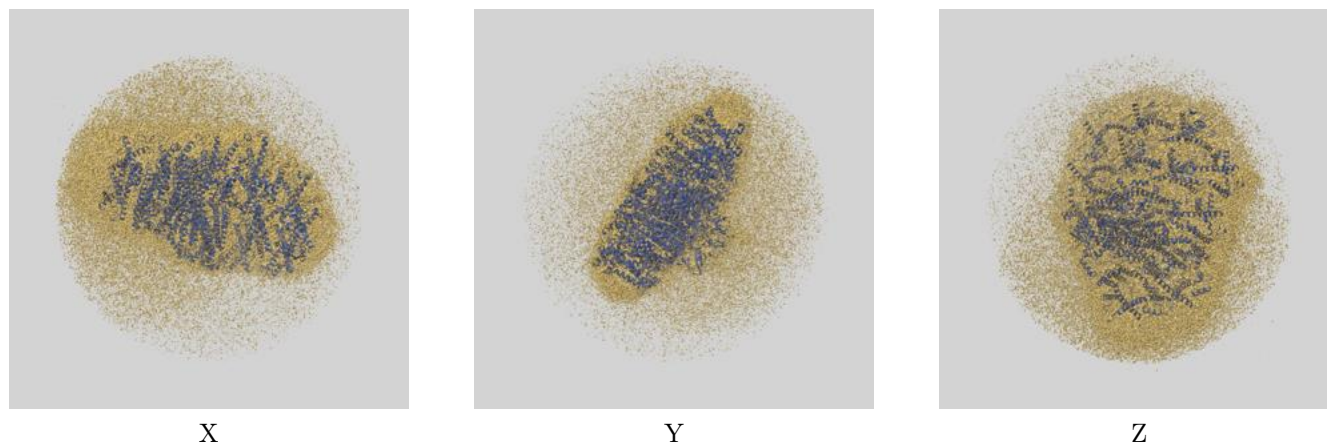
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.54	-	-
Author-provided FSC curve	2.54	2.96	2.59
Unmasked-calculated*	2.99	3.52	3.04

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.99 differs from the reported value 2.54 by more than 10 %

9 Map-model fit [i](#)

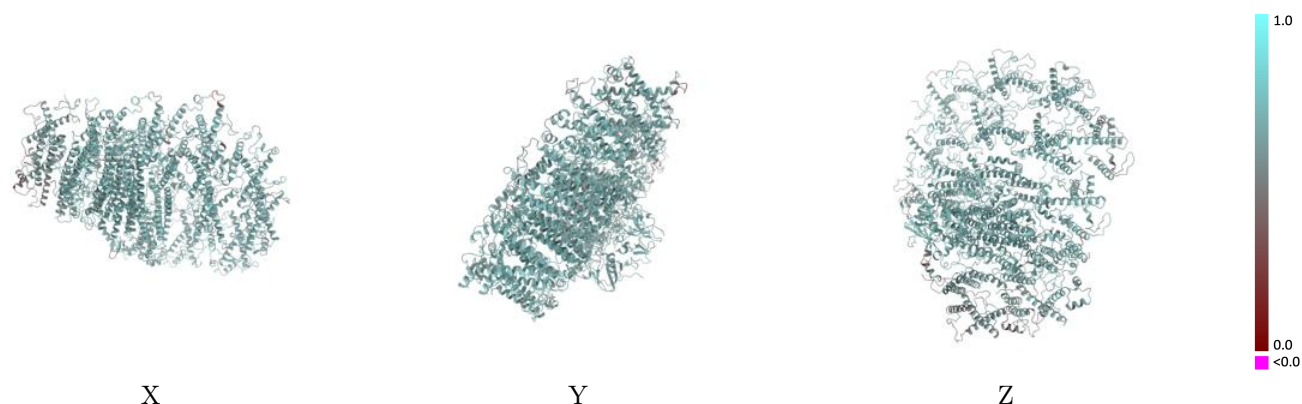
This section contains information regarding the fit between EMDB map EMD-12180 and PDB model 7BGI. Per-residue inclusion information can be found in [section 3](#) on [page 47](#).

9.1 Map-model overlay [i](#)



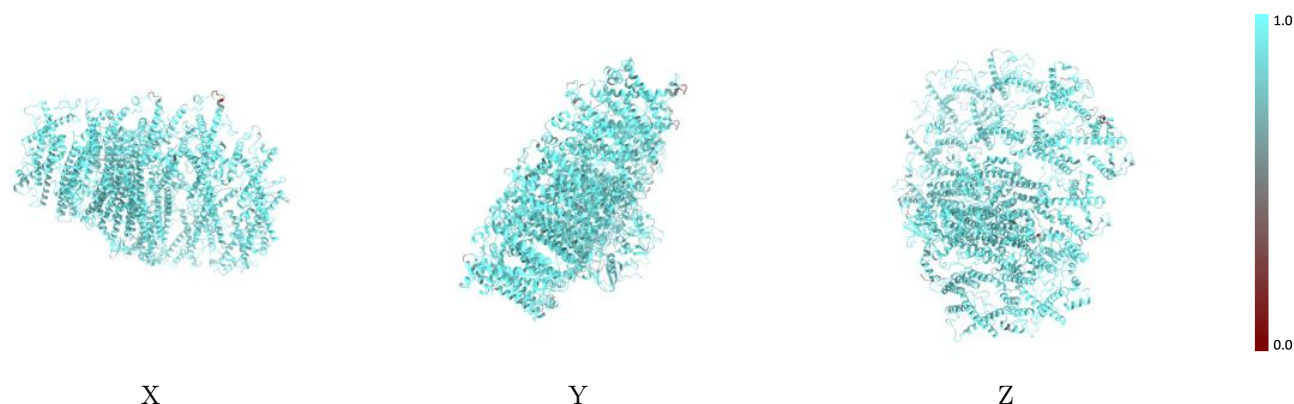
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



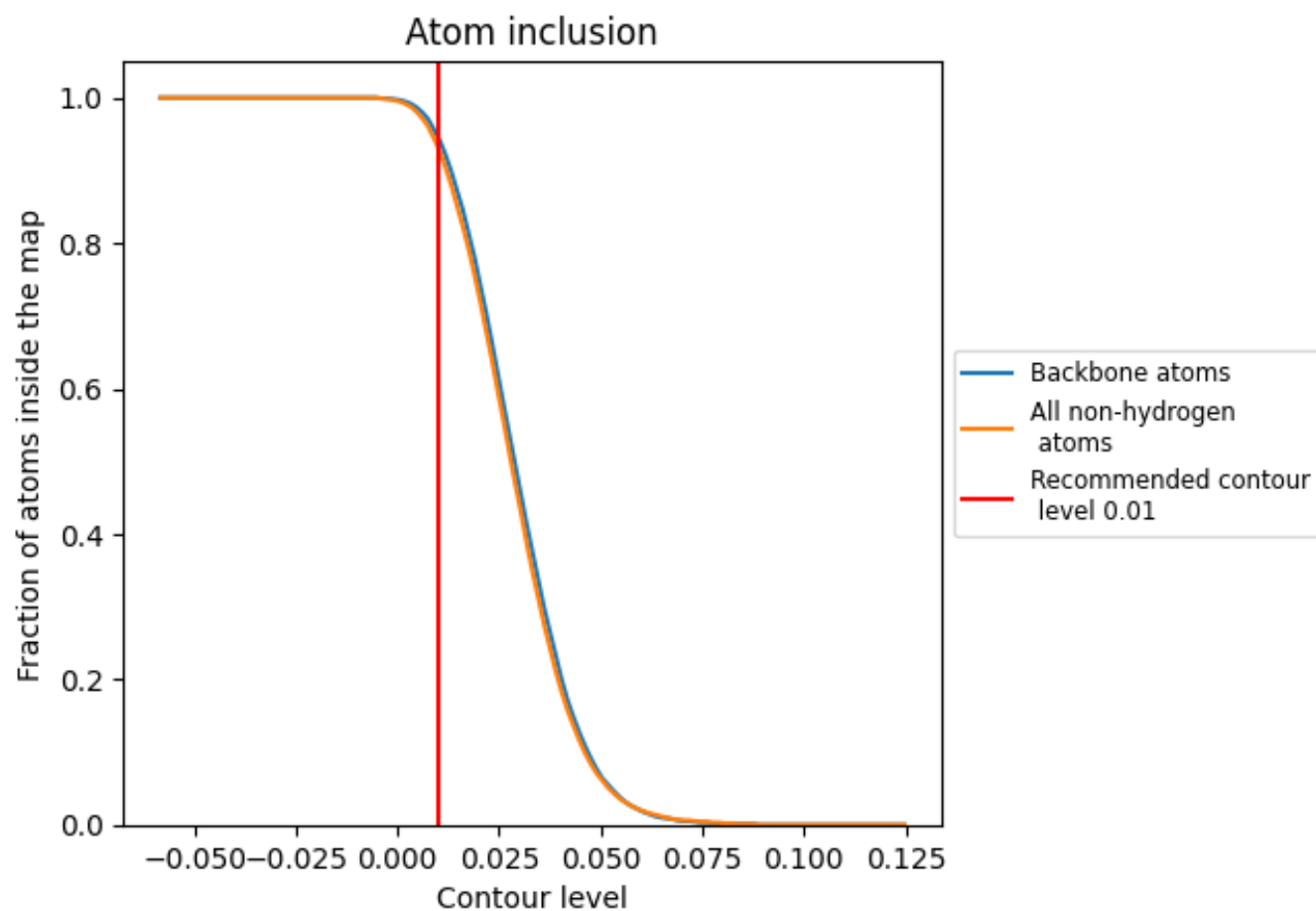
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9320	 0.6290
1	 0.9110	 0.6250
2	 0.8940	 0.5190
3	 0.9240	 0.6360
4	 0.8850	 0.6060
5	 0.8950	 0.6180
6	 0.9010	 0.6180
7	 0.9310	 0.6430
8	 0.9370	 0.6450
9	 0.9380	 0.5690
A	 0.9590	 0.6640
B	 0.9710	 0.6600
C	 0.9700	 0.6640
D	 0.9410	 0.6380
E	 0.9530	 0.6430
F	 0.9410	 0.6430
G	 0.9100	 0.5900
I	 0.9750	 0.6150
J	 0.9600	 0.6600
K	 0.8510	 0.5850
L	 0.9030	 0.5770
Z	 0.8490	 0.5870

