



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 07:24 am GMT

PDB ID : 7A4P
EMDB ID : EMD-11640
Title : Structure of small high-light grown *Chlorella ohadii* photosystem I
Authors : Caspy, I.; Nelson, N.; Nechushtai, R.; Shkolnisky, Y.; Neumann, E.
Deposited on : 2020-08-20
Resolution : 4.20 Å(reported)
Based on initial model : 6IJO

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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

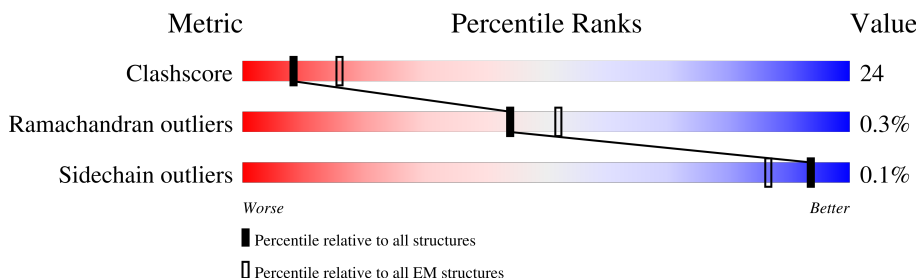
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	<div> <div>55%</div> <div>68%</div> <div>31%</div> <div>.</div> </div>
2	B	731	<div> <div>73%</div> <div>69%</div> <div>31%</div> <div>.</div> </div>
3	C	80	<div> <div>39%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
4	D	143	<div> <div>83%</div> <div>71%</div> <div>29%</div> <div>.</div> </div>
5	E	64	<div> <div>59%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
6	F	165	<div> <div>71%</div> <div>71%</div> <div>28%</div> <div>.</div> </div>
7	G	99	<div> <div>100%</div> <div>59%</div> <div>40%</div> <div>.</div> </div>
8	J	41	<div> <div>59%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
9	K	86	<div> <div>94%</div> <div>70% 30%</div> </div>
10	M	31	<div> <div>100%</div> <div>84% 16%</div> </div>
11	I	35	<div> <div>97%</div> <div>86% 14%</div> </div>
12	L	157	<div> <div>89%</div> <div>55% 34% 11%</div> </div>
13	1	192	<div> <div>89%</div> <div>73% 27%</div> </div>
13	a	192	<div> <div>94%</div> <div>99%</div> </div>
14	3	241	<div> <div>85%</div> <div>63% 36%</div> </div>
15	4	207	<div> <div>89%</div> <div>68% 32%</div> </div>
16	5	227	<div> <div>93%</div> <div>66% 33%</div> </div>
17	6	231	<div> <div>97%</div> <div>54% 46%</div> </div>
18	7	221	<div> <div>67%</div> <div>69% 30%</div> </div>
19	8	219	<div> <div>69%</div> <div>67% 32%</div> </div>

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	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	615	X	-	-	-
22	CLA	3	601	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	3	605	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	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	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	615	X	-	-	-
22	CLA	4	616	X	-	-	-
22	CLA	4	617	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	-	-	-
22	CLA	5	614	X	-	-	-
22	CLA	5	616	X	-	-	-
22	CLA	5	617	X	-	-	-
22	CLA	5	618	X	-	-	-
22	CLA	6	601	X	-	X	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	X	-
22	CLA	6	605	X	-	-	-
22	CLA	6	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	6	607	X	-	-	-
22	CLA	6	608	X	-	-	-
22	CLA	6	609	X	-	X	-
22	CLA	6	612	X	-	-	-
22	CLA	6	615	X	-	-	-
22	CLA	6	617	X	-	-	-
22	CLA	6	618	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	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	615	X	-	-	-
22	CLA	7	617	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	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	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	615	X	-	-	-
22	CLA	8	618	X	-	-	-
22	CLA	8	620	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	F	1301	X	-	-	-
22	CLA	F	1302	X	-	-	-
22	CLA	G	1601	X	-	-	-
22	CLA	G	1602	X	-	-	-
22	CLA	G	1603	X	-	-	-
22	CLA	J	1901	X	-	-	-
22	CLA	K	1401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	K	1402	X	-	-	-
22	CLA	K	1403	X	-	X	-
22	CLA	K	1404	X	-	-	-
22	CLA	L	1501	X	-	-	-
22	CLA	L	1502	X	-	-	-
22	CLA	L	1503	X	-	-	-
22	CLA	a	601	X	-	-	-
22	CLA	a	602	X	-	-	-
22	CLA	a	603	X	-	-	-
22	CLA	a	604	X	-	-	-
22	CLA	a	605	X	-	-	-
22	CLA	a	607	X	-	-	-
22	CLA	a	608	X	-	-	-
22	CLA	a	611	X	-	-	-
22	CLA	a	612	X	-	-	-
22	CLA	a	615	X	-	-	-
34	ERG	G	5002	X	-	-	-
35	RRX	J	4002	X	-	-	-
38	LUT	1	503	X	-	-	-
38	LUT	5	505	X	-	-	-
38	LUT	6	501	X	-	-	-
38	LUT	6	502	X	-	-	-
38	LUT	7	501	X	-	-	-
38	LUT	a	502	X	-	-	-
39	CHL	1	609	X	-	-	-
39	CHL	1	613	X	-	-	-
39	CHL	3	608	X	-	-	-
39	CHL	3	611	X	-	-	-
39	CHL	4	609	X	-	-	-
39	CHL	4	613	X	-	-	-
39	CHL	4	618	X	-	-	-
39	CHL	5	610	X	-	-	-
39	CHL	5	611	X	-	-	-
39	CHL	5	613	X	-	-	-
39	CHL	6	610	X	-	-	-
39	CHL	6	611	X	-	X	-
39	CHL	6	613	X	-	-	-
39	CHL	6	619	X	-	-	-
39	CHL	7	613	X	-	-	-
39	CHL	8	601	X	-	-	-
39	CHL	8	604	X	-	-	-
39	CHL	8	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
39	CHL	a	606	X	-	-	-
39	CHL	a	609	X	-	-	-
39	CHL	a	610	X	-	-	-
39	CHL	a	613	X	-	-	-
41	QTB	3	506	X	-	-	-
46	XAT	7	502	X	-	-	-
48	C7Z	7	504	X	-	-	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 48636 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
			5824	3815	988	1001	20		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	ALA	SER	variant	UNP W8SY74
A	437	ILE	MET	variant	UNP W8SY74

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	731	Total	C	N	O	S	0	0
			5796	3807	980	994	15		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	LYS	THR	conflict	UNP W8SUA3
B	5	LEU	LYS	conflict	UNP W8SUA3
B	241	ALA	VAL	conflict	UNP W8SUA3
B	402	ALA	GLU	conflict	UNP W8SUA3
B	403	GLN	ALA	conflict	UNP W8SUA3

- 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	367	104	119	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	716	196	208	4		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	188	ALA	VAL	variant	UNP A0A2P6TKF8
D	320	ILE	VAL	variant	UNP A0A2P6TKF8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			509	323	91	95			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	44	GLN	THR	variant	UNP A0A2P6U4S6
E	48	LEU	MET	variant	UNP A0A2P6U4S6
E	96	VAL	GLU	variant	UNP A0A2P6U4S6
E	97	ALA	GLU	variant	UNP A0A2P6U4S6
E	98	ALA	VAL	variant	UNP A0A2P6U4S6

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1277	830	216	228	3		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	346	LEU	MET	variant	UNP A0A2P6TPV8
F	348	ASN	LYS	variant	UNP A0A2P6TPV8
F	351	ALA	GLU	variant	UNP A0A2P6TPV8
F	352	ASP	GLY	variant	UNP A0A2P6TPV8
F	360	LYS	GLN	variant	UNP A0A2P6TPV8
F	364	ALA	ASP	variant	UNP A0A2P6TPV8
F	367	GLU	ASN	variant	UNP A0A2P6TPV8
F	430	ALA	SER	variant	UNP A0A2P6TPV8
F	431	ALA	SER	variant	UNP A0A2P6TPV8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	432	THR	MET	variant	UNP A0A2P6TPV8
F	433	ALA	THR	variant	UNP A0A2P6TPV8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	99	Total	C	N	O	S	0	0
			727	466	127	130	4		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1229	ALA	SER	variant	UNP A0A2P6TZI8
G	1272	LEU	MET	variant	UNP A0A2P6TZI8
G	1285	ILE	VAL	variant	UNP A0A2P6TZI8
G	1313	ILE	LEU	variant	UNP A0A2P6TZI8
G	1317	SER	HIS	variant	UNP A0A2P6TZI8
G	1320	GLY	GLN	variant	UNP A0A2P6TZI8
G	1321	LEU	VAL	variant	UNP A0A2P6TZI8
G	1324	ASN	VAL	variant	UNP A0A2P6TZI8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			316	212	46	57	1		

- Molecule 9 is a protein called PSI-K.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	86	Total	C	N	O	S	0	0
			613	390	106	115	2		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	74	ALA	GLU	variant	UNP A0A2P6U0J1
K	103	LEU	ILE	variant	UNP A0A2P6U0J1
K	105	CYS	VAL	variant	UNP A0A2P6U0J1
K	107	ILE	VAL	variant	UNP A0A2P6U0J1
K	108	VAL	ILE	variant	UNP A0A2P6U0J1

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Chain	Residue	Modelled	Actual	Comment	Reference
K	112	LYS	ARG	variant	UNP A0A2P6U0J1
K	113	SER	GLY	variant	UNP A0A2P6U0J1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	31	Total	C	N	O	S	0	0
			239	163	36	39	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	35	Total	C	N	O	S	0	0
			270	183	37	47	3		

- Molecule 12 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	140	Total	C	N	O	S	0	0
			1041	682	167	188	4		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	350	TYR	PHE	conflict	UNP A0A2P6TC44
L	364	ASP	ASN	conflict	UNP A0A2P6TC44
L	?	-	ALA	deletion	UNP A0A2P6TC44
L	421	ASP	GLU	conflict	UNP A0A2P6TC44
L	443	LEU	ILE	conflict	UNP A0A2P6TC44

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		
13	a	192	Total	C	N	O	S	0	0
			1405	900	237	261	7		

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	166	SER	LEU	conflict	UNP A0A2P6TT36
1	167	LYS	GLU	conflict	UNP A0A2P6TT36
1	171	THR	VAL	conflict	UNP A0A2P6TT36
1	194	THR	ASN	conflict	UNP A0A2P6TT36
1	196	ALA	GLN	conflict	UNP A0A2P6TT36
1	204	SER	ALA	conflict	UNP A0A2P6TT36
1	210	MET	LEU	conflict	UNP A0A2P6TT36
a	166	SER	LEU	conflict	UNP A0A2P6TT36
a	167	LYS	GLU	conflict	UNP A0A2P6TT36
a	171	THR	VAL	conflict	UNP A0A2P6TT36
a	194	THR	ASN	conflict	UNP A0A2P6TT36
a	196	ALA	GLN	conflict	UNP A0A2P6TT36
a	204	SER	ALA	conflict	UNP A0A2P6TT36
a	210	MET	LEU	conflict	UNP A0A2P6TT36

- Molecule 14 is a protein called Glutathione reductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	3	241	Total	C	N	O	S	0	0
			1844	1194	302	337	11		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	314	CYS	GLY	conflict	UNP A0A2P6TMT4
3	329	ILE	VAL	conflict	UNP A0A2P6TMT4
3	339	THR	SER	conflict	UNP A0A2P6TMT4
3	359	LYS	ASN	conflict	UNP A0A2P6TMT4
3	405	GLY	ALA	conflict	UNP A0A2P6TMT4
3	429	GLU	ALA	conflict	UNP A0A2P6TMT4
3	484	THR	ARG	conflict	UNP A0A2P6TMT4
3	485	ILE	ARG	conflict	UNP A0A2P6TMT4
3	486	LEU	ARG	conflict	UNP A0A2P6TMT4
3	487	LYS	ALA	conflict	UNP A0A2P6TMT4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	4	207	Total	C	N	O	S	0	0
			1631	1056	277	294	4		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	37	GLU	ASP	conflict	UNP A0A2P6TQ14
4	109	ASP	ASN	conflict	UNP A0A2P6TQ14
4	112	ASN	ASP	conflict	UNP A0A2P6TQ14
4	213	GLY	SER	conflict	UNP A0A2P6TQ14
4	218	ASN	ASP	conflict	UNP A0A2P6TQ14
4	?	-	LEU	deletion	UNP A0A2P6TQ14
4	236	ASN	ARG	conflict	UNP A0A2P6TQ14

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	5	227	Total	C	N	O	S	0	0
			1769	1136	307	314	12		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	32	LYS	ASP	conflict	UNP A0A2P6U4K1
5	38	VAL	ALA	conflict	UNP A0A2P6U4K1
5	40	ALA	SER	conflict	UNP A0A2P6U4K1
5	42	GLY	ALA	conflict	UNP A0A2P6U4K1
5	113	SER	GLY	conflict	UNP A0A2P6U4K1
5	127	ILE	LEU	conflict	UNP A0A2P6U4K1
5	195	VAL	ILE	conflict	UNP A0A2P6U4K1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	6	231	Total	C	N	O	S	0	0
			1787	1168	295	314	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	83	CYS	ALA	conflict	UNP A0A2P6TPR7
6	94	LEU	MET	conflict	UNP A0A2P6TPR7
6	196	ILE	VAL	conflict	UNP A0A2P6TPR7
6	201	ALA	GLY	conflict	UNP A0A2P6TPR7
6	250	GLN	ASN	conflict	UNP A0A2P6TPR7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	7	221	Total	C	N	O	S	0	0
			1698	1090	294	308	6		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	6	VAL	ASP	conflict	UNP A0A2P6TS63
7	8	GLU	PRO	conflict	UNP A0A2P6TS63
7	17	VAL	ALA	conflict	UNP A0A2P6TS63
7	82	PHE	TYR	conflict	UNP A0A2P6TS63
7	96	ASP	SER	conflict	UNP A0A2P6TS63
7	107	MET	LEU	conflict	UNP A0A2P6TS63
7	154	TYR	PHE	conflict	UNP A0A2P6TS63
7	205	VAL	ILE	conflict	UNP A0A2P6TS63
7	209	ALA	SER	conflict	UNP A0A2P6TS63
7	218	HIS	TYR	conflict	UNP A0A2P6TS63

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	8	219	Total	C	N	O	S	0	0
			1669	1073	285	305	6		

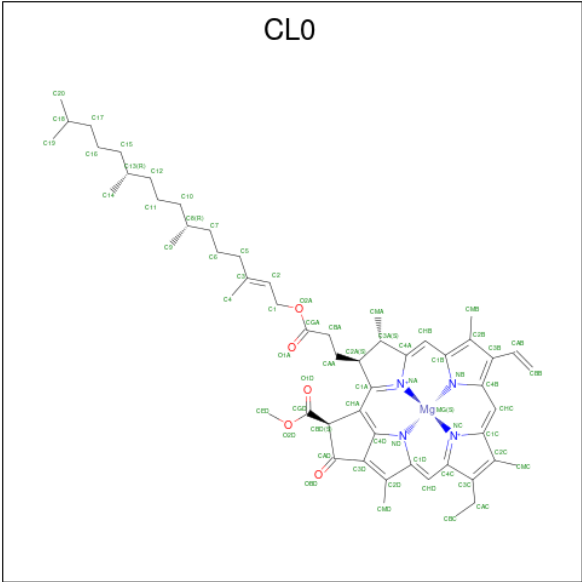
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	103	GLU	ASP	conflict	UNP A0A2P6TZ50

- Molecule 20 is a protein called Photosystem I reaction center subunit VI-chloroplastic-like.

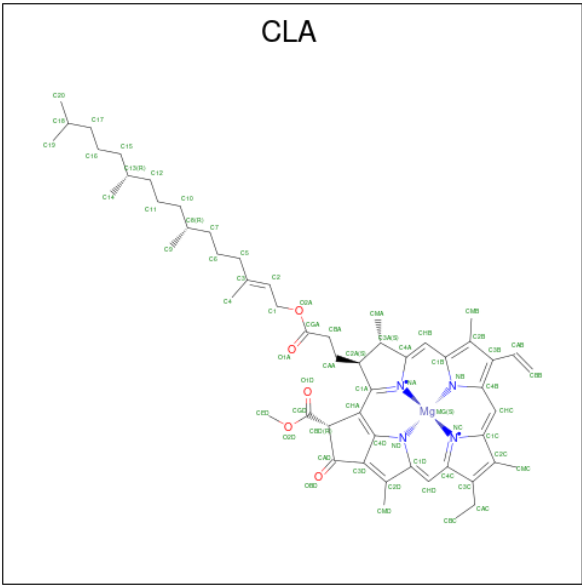
Mol	Chain	Residues	Atoms	AltConf	Trace
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- Molecule 21 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	
22	A	1	Total	C	Mg	N	O	0
			2621	2191	43	172	215	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	A	1	Total 2621	C 2191	Mg 43	N 172	O 215	0
22	B	1	Total 2583	C 2163	Mg 42	N 168	O 210	0
22	B	1	Total 2583	C 2163	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	

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Mol	Chain	Residues	Atoms					AltConf
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	B	1	Total	C	Mg	N	O	0
			2583	2163	42	168	210	
22	F	1	Total	C	Mg	N	O	0
			105	85	2	8	10	
22	F	1	Total	C	Mg	N	O	0
			105	85	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
22	G	1	Total 141	C 111	Mg 3	N 12	O 15	0
22	G	1	Total 141	C 111	Mg 3	N 12	O 15	0
22	G	1	Total 141	C 111	Mg 3	N 12	O 15	0
22	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
22	K	1	Total 204	C 164	Mg 4	N 16	O 20	0
22	K	1	Total 204	C 164	Mg 4	N 16	O 20	0
22	K	1	Total 204	C 164	Mg 4	N 16	O 20	0
22	K	1	Total 204	C 164	Mg 4	N 16	O 20	0
22	L	1	Total 155	C 125	Mg 3	N 12	O 15	0
22	L	1	Total 155	C 125	Mg 3	N 12	O 15	0
22	L	1	Total 155	C 125	Mg 3	N 12	O 15	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0
22	1	1	Total 693	C 573	Mg 12	N 48	O 60	0

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Mol	Chain	Residues	Atoms					AltConf
22	1	1	Total	C	Mg	N	O	0
			693	573	12	48	60	
22	1	1	Total	C	Mg	N	O	0
			693	573	12	48	60	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	a	1	Total	C	Mg	N	O	0
			571	471	10	40	50	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	

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Mol	Chain	Residues	Atoms					AltConf
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	3	1	Total	C	Mg	N	O	0
			719	599	12	48	60	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	4	1	Total	C	Mg	N	O	0
			768	628	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	

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Mol	Chain	Residues	Atoms					AltConf
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	5	1	Total	C	Mg	N	O	0
			739	599	14	56	70	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	

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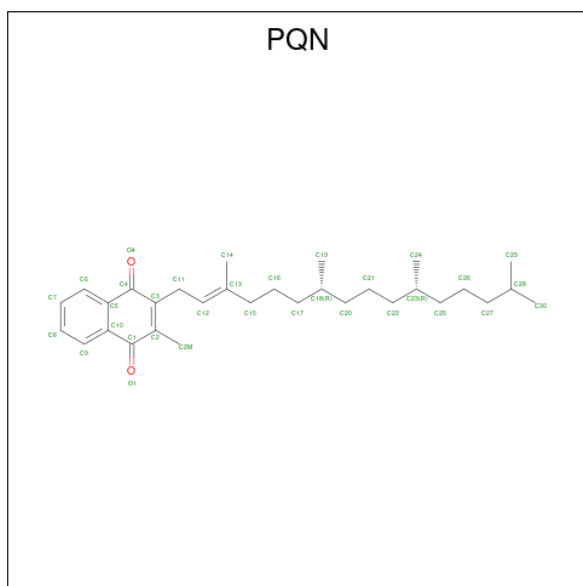
Mol	Chain	Residues	Atoms					AltConf
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	6	1	Total	C	Mg	N	O	0
			711	581	13	52	65	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	7	1	Total	C	Mg	N	O	0
			778	641	14	56	67	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	

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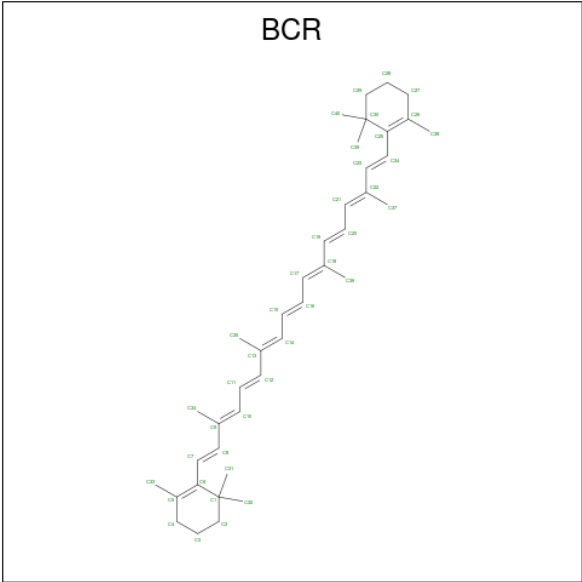
Mol	Chain	Residues	Atoms					AltConf
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	
22	8	1	Total	C	Mg	N	O	0
			699	569	13	52	65	

- 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 BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



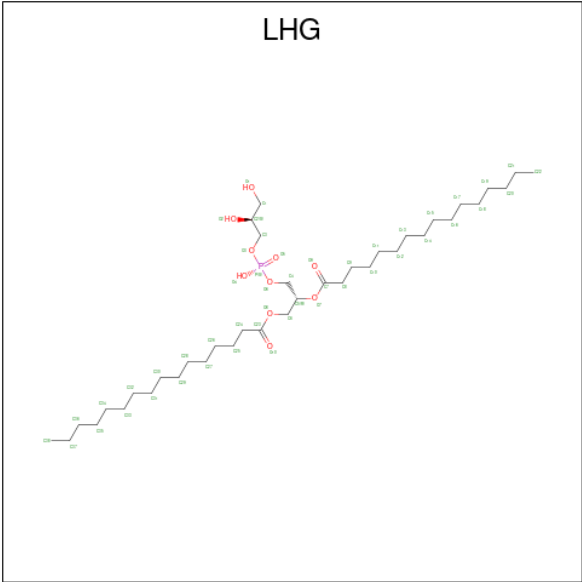
Mol	Chain	Residues	Atoms		AltConf
24	A	1	Total	C	0
			200	200	
24	A	1	Total	C	0
			200	200	
24	A	1	Total	C	0
			200	200	
24	A	1	Total	C	0
			200	200	
24	A	1	Total	C	0
			200	200	
24	B	1	Total	C	0
			280	280	
24	B	1	Total	C	0
			280	280	
24	B	1	Total	C	0
			280	280	
24	B	1	Total	C	0
			280	280	
24	B	1	Total	C	0
			280	280	
24	B	1	Total	C	0
			280	280	
24	F	1	Total	C	0
			40	40	
24	G	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
24	J	1	Total C 40 40	0
24	K	1	Total C 80 80	0
24	K	1	Total C 80 80	0
24	I	1	Total C 40 40	0
24	L	1	Total C 120 120	0
24	L	1	Total C 120 120	0
24	L	1	Total C 120 120	0
24	3	1	Total C 120 120	0
24	3	1	Total C 120 120	0
24	3	1	Total C 120 120	0
24	4	1	Total C 40 40	0
24	5	1	Total C 80 80	0
24	5	1	Total C 80 80	0
24	6	1	Total C 80 80	0
24	6	1	Total C 80 80	0
24	7	1	Total C 40 40	0
24	8	1	Total C 40 40	0

- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



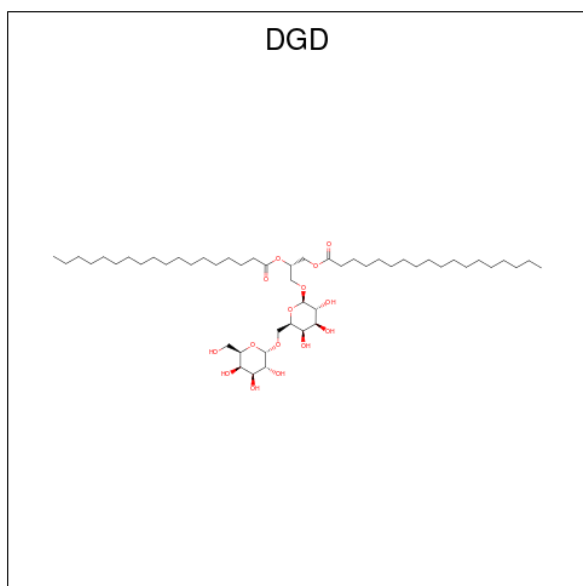
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			120	87	30	3	
25	A	1	Total	C	O	P	0
			120	87	30	3	
25	A	1	Total	C	O	P	0
			120	87	30	3	
25	B	1	Total	C	O	P	0
			95	73	20	2	
25	B	1	Total	C	O	P	0
			95	73	20	2	
25	F	1	Total	C	O	P	0
			79	57	20	2	
25	F	1	Total	C	O	P	0
			79	57	20	2	
25	1	1	Total	C	O	P	0
			77	55	20	2	
25	1	1	Total	C	O	P	0
			77	55	20	2	
25	a	1	Total	C	O	P	0
			35	24	10	1	
25	3	1	Total	C	O	P	0
			49	38	10	1	
25	4	1	Total	C	O	P	0
			81	59	20	2	
25	4	1	Total	C	O	P	0
			81	59	20	2	
25	5	1	Total	C	O	P	0
			49	38	10	1	

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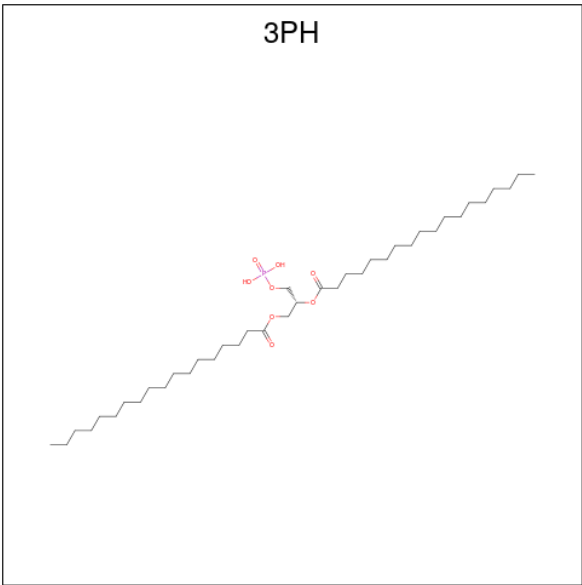
Mol	Chain	Residues	Atoms				AltConf
25	6	1	Total	C	O	P	0
			86	64	20	2	
25	6	1	Total	C	O	P	0
			86	64	20	2	
25	7	1	Total	C	O	P	0
			128	95	30	3	
25	7	1	Total	C	O	P	0
			128	95	30	3	
25	7	1	Total	C	O	P	0
			128	95	30	3	
25	8	1	Total	C	O	P	0
			37	26	10	1	

- Molecule 26 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



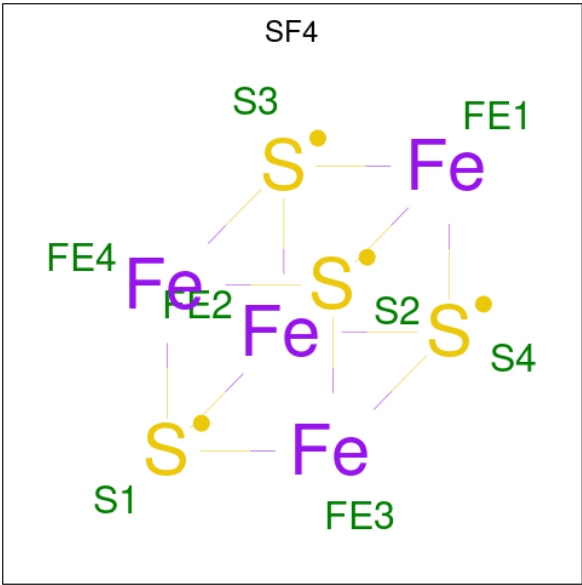
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			51	36	15	
26	B	1	Total	C	O	0
			66	51	15	
26	8	1	Total	C	O	0
			66	51	15	

- Molecule 27 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: $C_{39}H_{77}O_8P$).



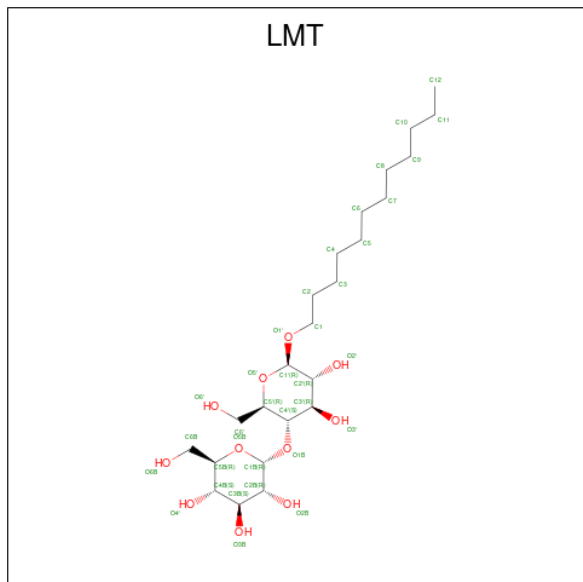
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
27	A	1	33	24	8	1	0

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



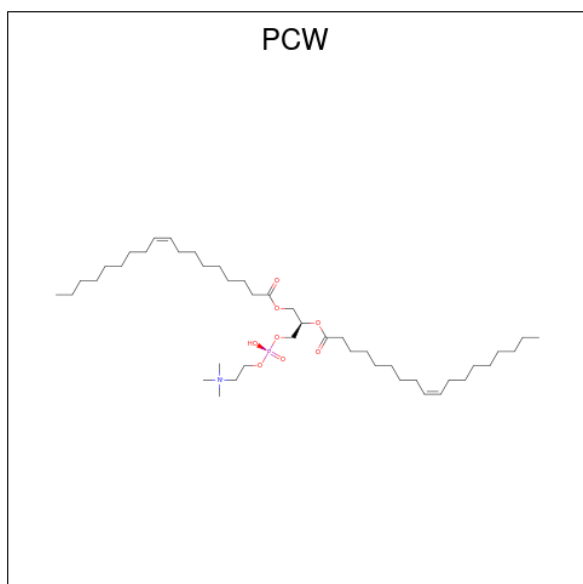
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	A	1	8	4	4	0
28	C	1	16	8	8	0
28	C	1	16	8	8	0

- Molecule 29 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



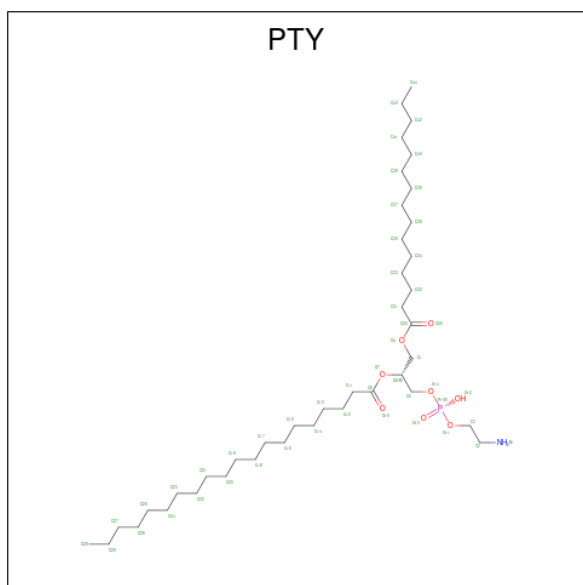
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			35	24	11	
29	B	1	Total	C	O	0
			35	24	11	
29	1	1	Total	C	O	0
			35	24	11	

- Molecule 30 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: $C_{44}H_{85}NO_8P$).



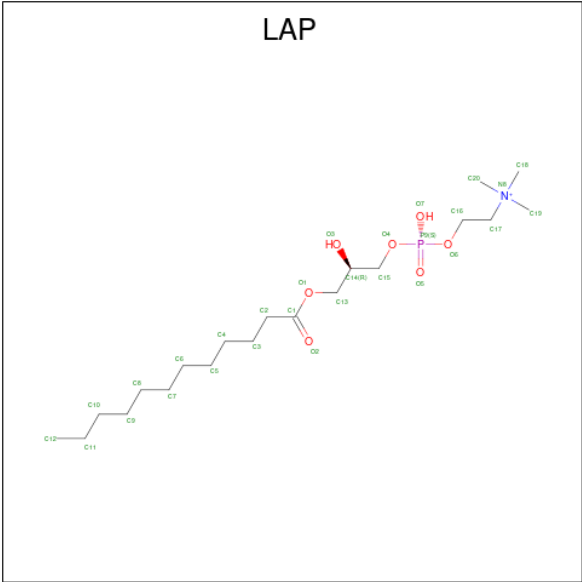
Mol	Chain	Residues	Atoms					AltConf
30	B	1	Total	C	N	O	P	0
			30	20	1	8	1	
30	6	1	Total	C	N	O	P	0
			36	26	1	8	1	

- Molecule 31 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: $C_{40}H_{80}NO_8P$).



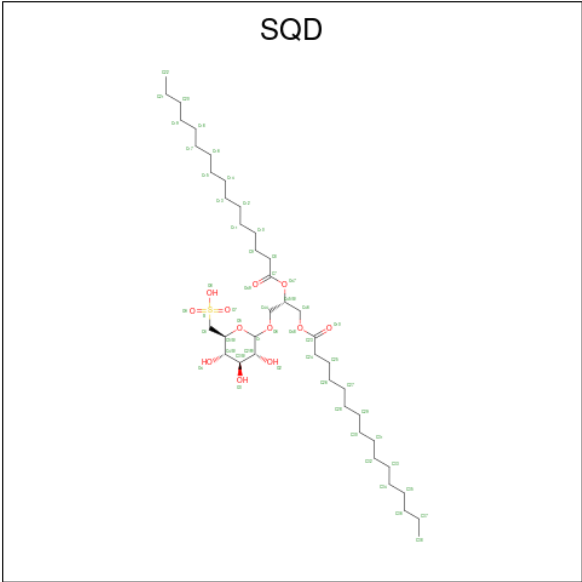
Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	N	O	P	0
			41	31	1	8	1	
31	3	1	Total	C	N	O	P	0
			38	28	1	8	1	
31	5	1	Total	C	N	O	P	0
			38	28	1	8	1	
31	7	1	Total	C	N	O	P	0
			33	23	1	8	1	
31	8	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 32 is [2-((1-OXODODECANOXY-(2-HYDROXY-3-PROPANYL))-PHOSPHONATE-OXY)-ETHYL]-TRIMETHYLAMMONIUM (three-letter code: LAP) (formula: $C_{20}H_{43}NO_7P$).



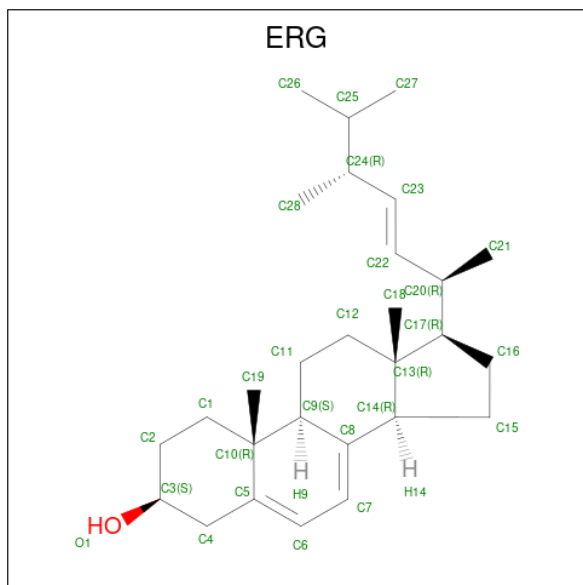
Mol	Chain	Residues	Atoms					AltConf
32	B	1	Total	C	N	O	P	0
			29	20	1	7	1	
32	F	1	Total	C	N	O	P	0
			29	20	1	7	1	
32	K	1	Total	C	N	O	P	0
			29	20	1	7	1	

- Molecule 33 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



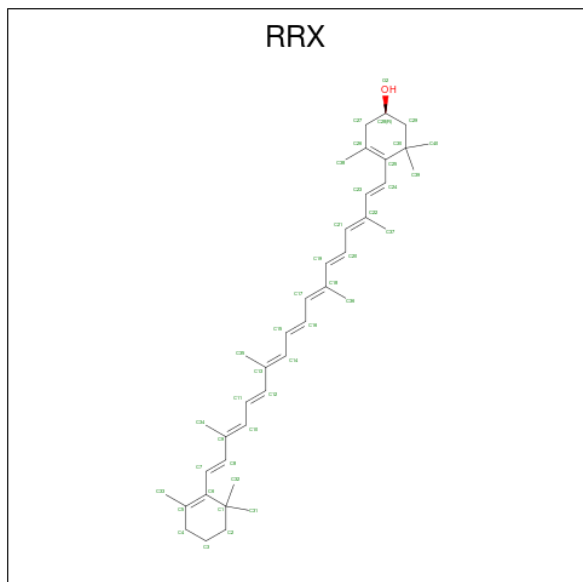
Mol	Chain	Residues	Atoms				AltConf
33	G	1	Total	C	O	S	0
			46	33	12	1	
33	7	1	Total	C	O	S	0
			39	26	12	1	

- Molecule 34 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$).



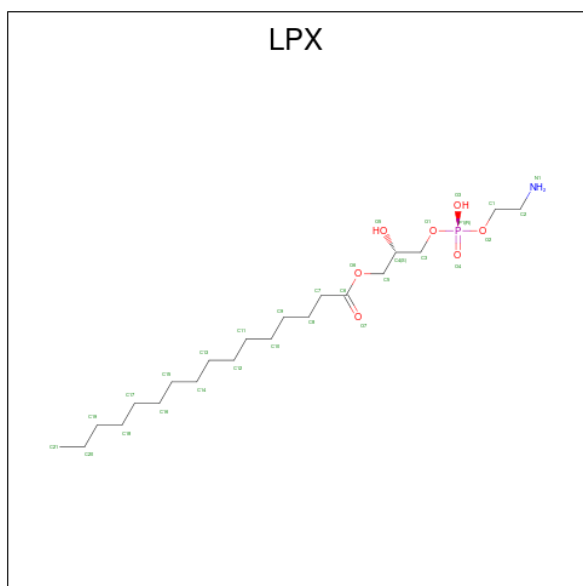
Mol	Chain	Residues	Atoms				AltConf
34	G	1	Total	C	O		0
			29	28	1		

- Molecule 35 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: $C_{40}H_{56}O$).



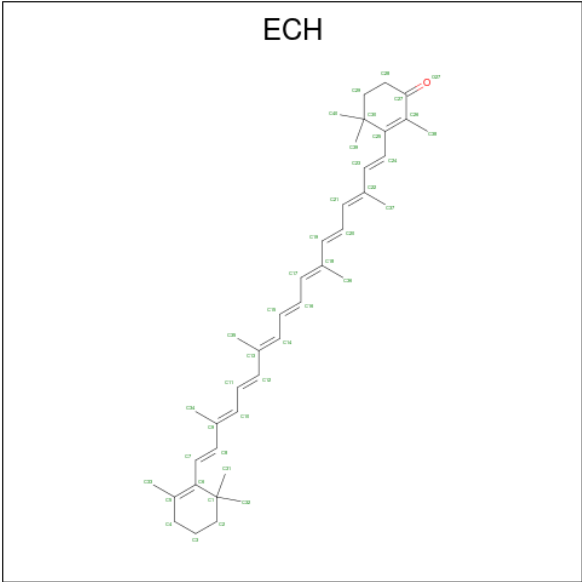
Mol	Chain	Residues	Atoms			AltConf
35	J	1	Total	C	O	0
			41	40	1	

- Molecule 36 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C₂₁H₄₄NO₇P).



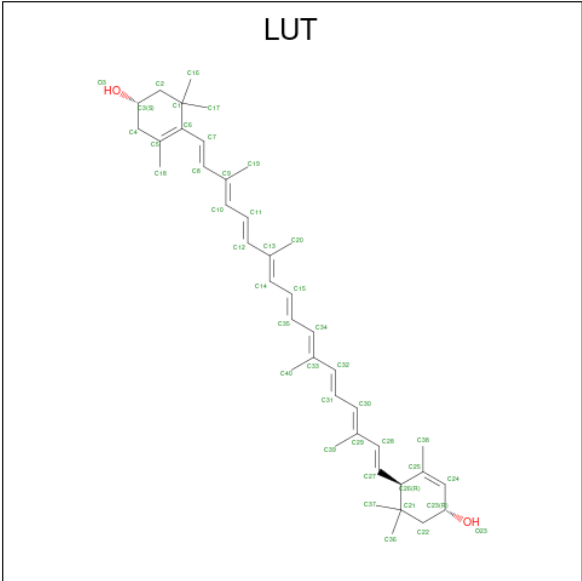
Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total	C	N	O	P	0
			17	8	1	7	1	
36	a	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 37 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: C₄₀H₅₄O).



Mol	Chain	Residues	Atoms			AltConf
37	M	1	Total	C	O	0
			41	40	1	

- Molecule 38 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



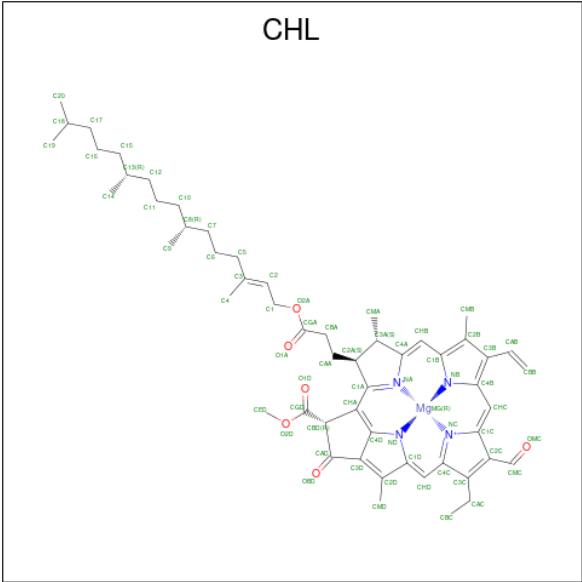
Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	C	O	0
			126	120	6	
38	1	1	Total	C	O	0
			126	120	6	

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Mol	Chain	Residues	Atoms			AltConf
38	1	1	Total	C	O	0
			126	120	6	
38	a	1	Total	C	O	0
			126	120	6	
38	a	1	Total	C	O	0
			126	120	6	
38	a	1	Total	C	O	0
			126	120	6	
38	3	1	Total	C	O	0
			84	80	4	
38	3	1	Total	C	O	0
			84	80	4	
38	4	1	Total	C	O	0
			84	80	4	
38	4	1	Total	C	O	0
			84	80	4	
38	5	1	Total	C	O	0
			126	120	6	
38	5	1	Total	C	O	0
			126	120	6	
38	5	1	Total	C	O	0
			126	120	6	
38	6	1	Total	C	O	0
			84	80	4	
38	6	1	Total	C	O	0
			84	80	4	
38	7	1	Total	C	O	0
			42	40	2	
38	8	1	Total	C	O	0
			84	80	4	
38	8	1	Total	C	O	0
			84	80	4	

- Molecule 39 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



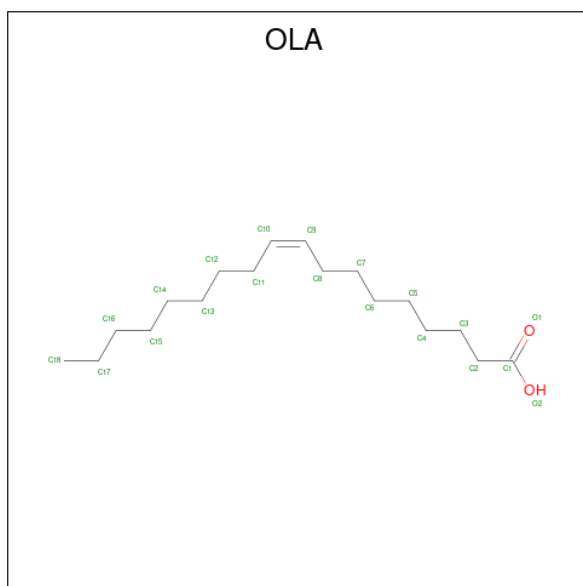
Mol	Chain	Residues	Atoms					AltConf
39	1	1	Total	C	Mg	N	O	0
			114	92	2	8	12	
39	1	1	Total	C	Mg	N	O	0
			114	92	2	8	12	
39	a	1	Total	C	Mg	N	O	0
			203	159	4	16	24	
39	a	1	Total	C	Mg	N	O	0
			203	159	4	16	24	
39	a	1	Total	C	Mg	N	O	0
			203	159	4	16	24	
39	a	1	Total	C	Mg	N	O	0
			203	159	4	16	24	
39	3	1	Total	C	Mg	N	O	0
			98	78	2	8	10	
39	3	1	Total	C	Mg	N	O	0
			98	78	2	8	10	
39	4	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	4	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	4	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	5	1	Total	C	Mg	N	O	0
			173	140	3	12	18	
39	5	1	Total	C	Mg	N	O	0
			173	140	3	12	18	
39	5	1	Total	C	Mg	N	O	0
			173	140	3	12	18	

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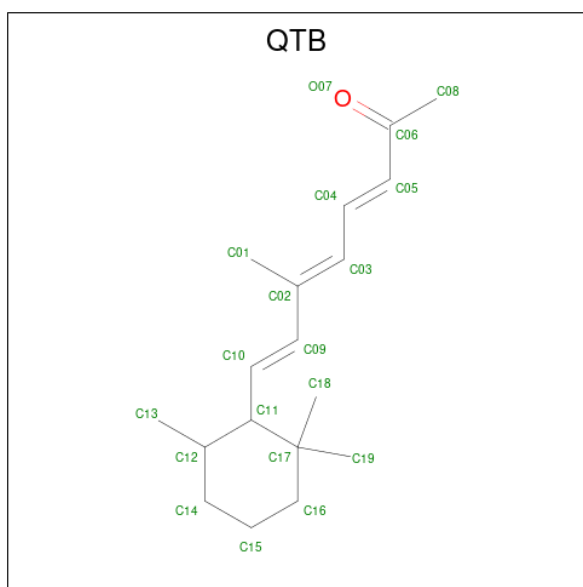
Mol	Chain	Residues	Atoms					AltConf
39	6	1	Total	C	Mg	N	O	0
			224	180	4	16	24	
39	6	1	Total	C	Mg	N	O	0
			224	180	4	16	24	
39	6	1	Total	C	Mg	N	O	0
			224	180	4	16	24	
39	6	1	Total	C	Mg	N	O	0
			224	180	4	16	24	
39	7	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
39	8	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	8	1	Total	C	Mg	N	O	0
			174	141	3	12	18	
39	8	1	Total	C	Mg	N	O	0
			174	141	3	12	18	

- Molecule 40 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).



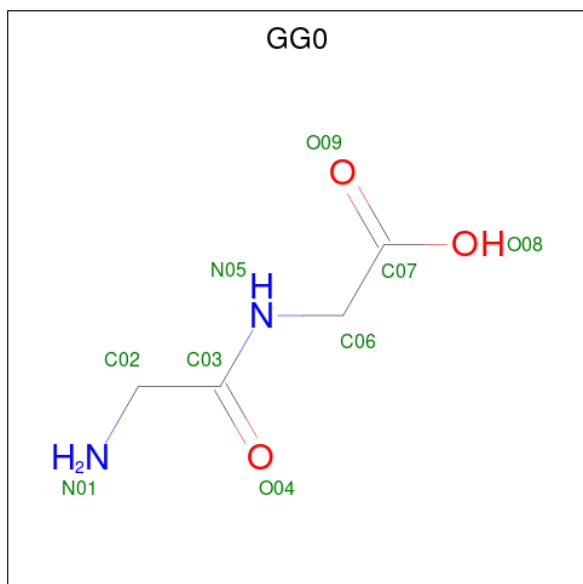
Mol	Chain	Residues	Atoms			AltConf
40	1	1	Total	C	O	0
			20	18	2	
40	8	1	Total	C	O	0
			20	18	2	

- Molecule 41 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: $C_{18}H_{28}O$).



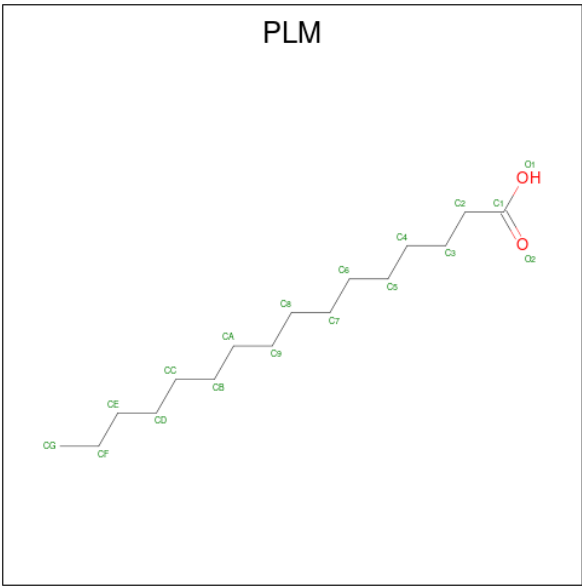
Mol	Chain	Residues	Atoms			AltConf
41	a	1	Total	C	O	0
			19	18	1	
41	3	1	Total	C	O	0
			19	18	1	

- Molecule 42 is 2-(2-azanylethanoylamino)ethanoic acid (three-letter code: GG0) (formula: $C_4H_8N_2O_3$).



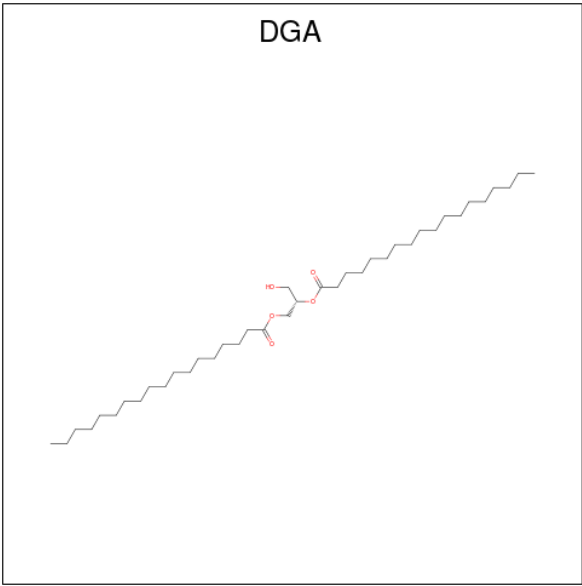
Mol	Chain	Residues	Atoms				AltConf
42	a	1	Total	C	N	O	0
			9	4	2	3	

- Molecule 43 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			AltConf
43	4	1	Total	C	O	0
			17	16	1	
43	6	1	Total	C	O	0
			18	16	2	

- Molecule 44 is DIACYL GLYCEROL (three-letter code: DGA) (formula: C₃₉H₇₆O₅).



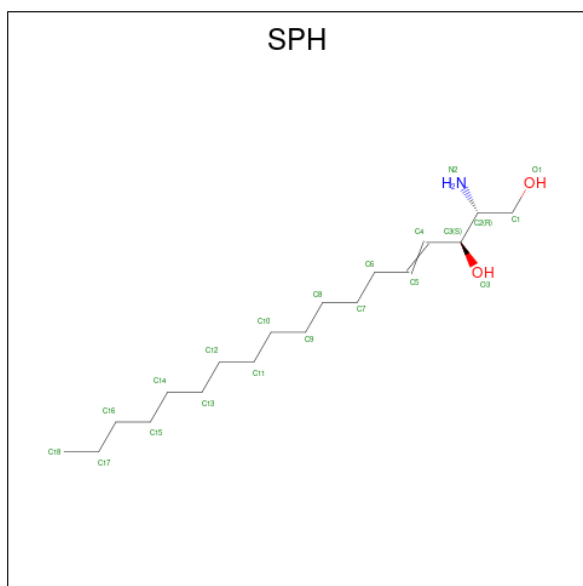
Mol	Chain	Residues	Atoms			AltConf
44	5	1	Total	C	O	0
			23	18	5	

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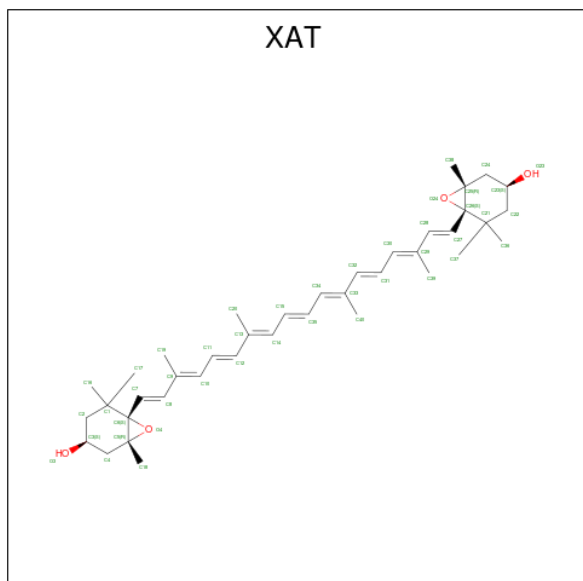
Mol	Chain	Residues	Atoms			AltConf
44	8	1	Total	C	O	0
			30	25	5	

- Molecule 45 is SPHINGOSINE (three-letter code: SPH) (formula: $C_{18}H_{37}NO_2$).



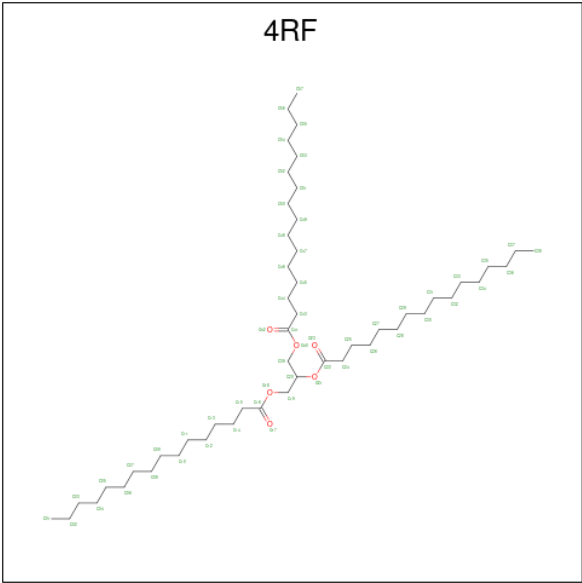
Mol	Chain	Residues	Atoms				AltConf
45	6	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 46 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: $C_{40}H_{56}O_4$).



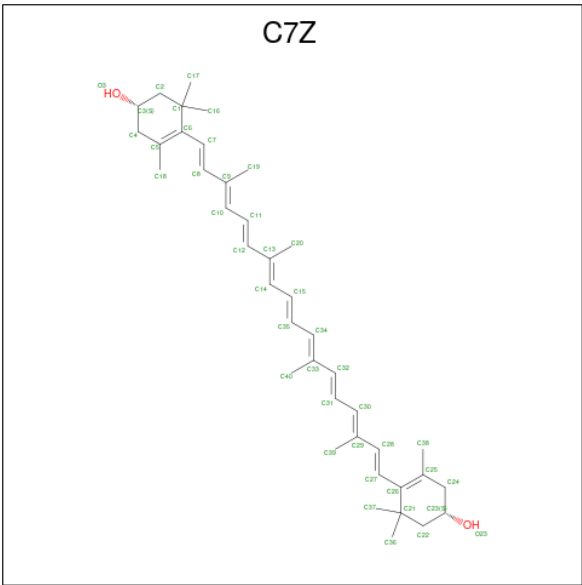
Mol	Chain	Residues	Atoms			AltConf
46	7	1	Total	C	O	0
			44	40	4	

- Molecule 47 is Tripalmitoylglycerol (three-letter code: 4RF) (formula: C₅₁H₉₈O₆).



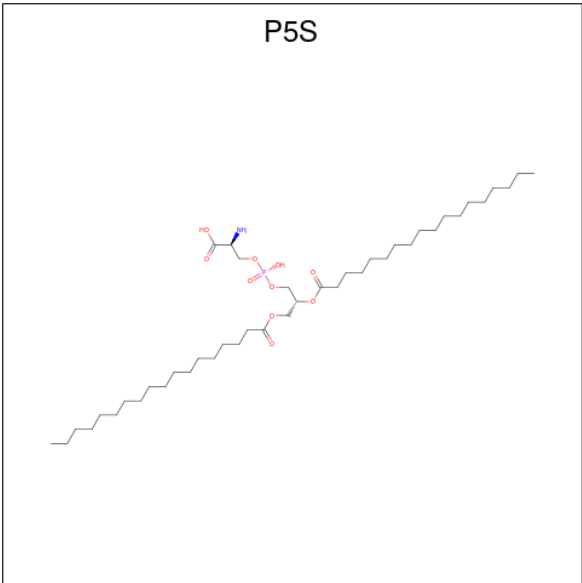
Mol	Chain	Residues	Atoms			AltConf
47	7	1	Total	C	O	0
			32	26	6	
47	8	1	Total	C	O	0
			96	84	12	
47	8	1	Total	C	O	0
			96	84	12	

- Molecule 48 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
48	7	1	Total	C	O	0
			42	40	2	

- Molecule 49 is O-[(R)-{[(2R)-2,3-bis(octadecanoyloxy)propyl]oxy}(hydroxy)phosphoryl]-L-serine (three-letter code: P5S) (formula: C₄₂H₈₂NO₁₀P).



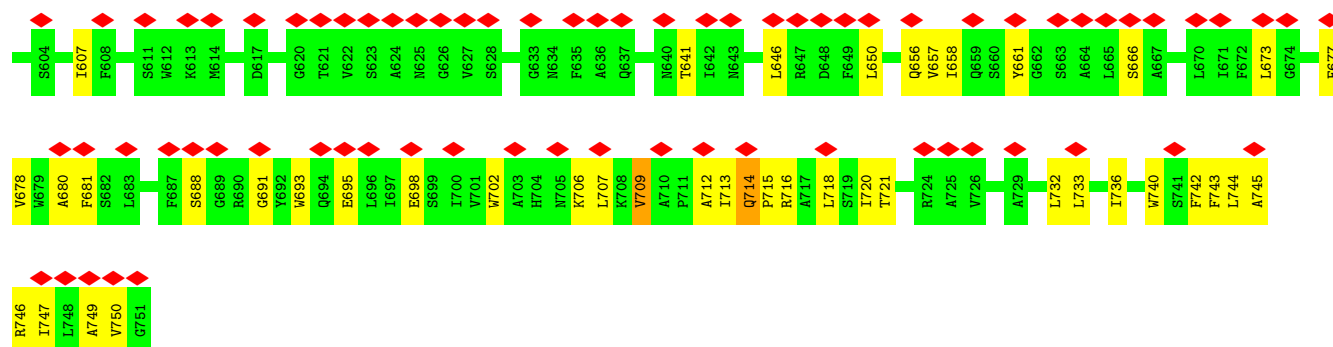
Mol	Chain	Residues	Atoms					AltConf
49	8	1	Total	C	N	O	P	0
			37	25	1	10	1	

3 Residue-property plots

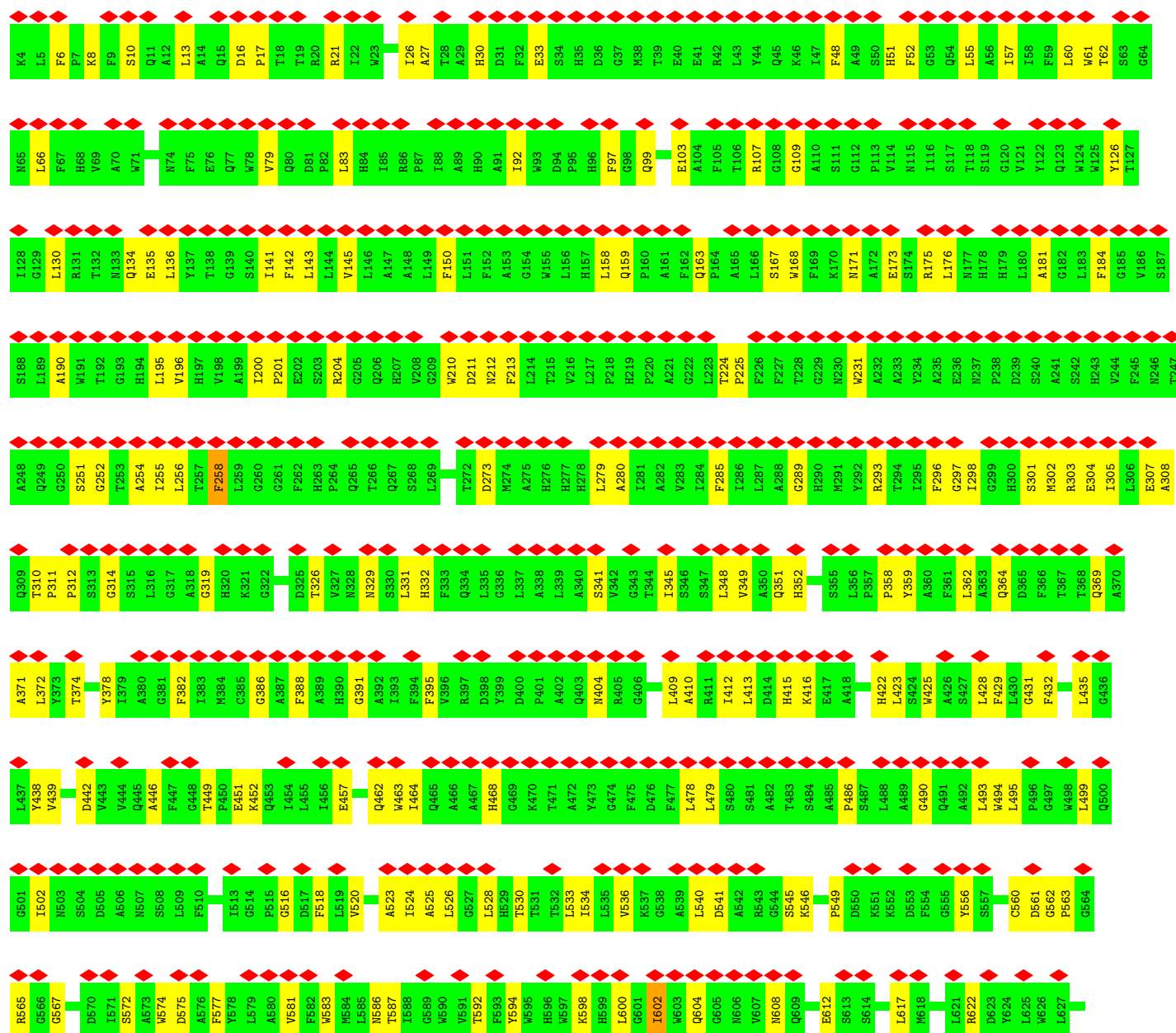
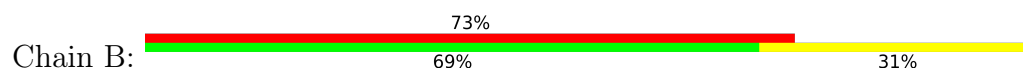
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

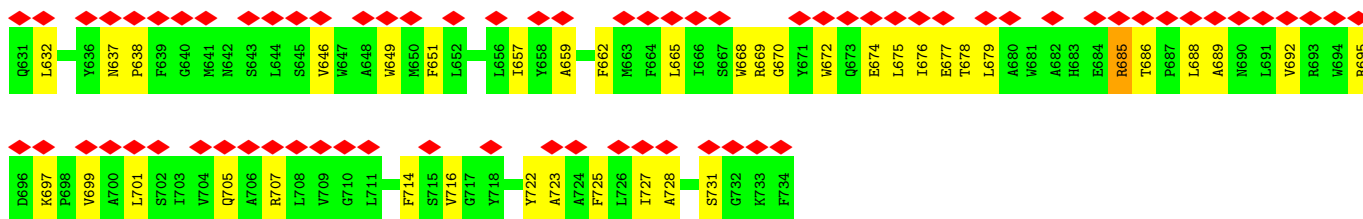
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



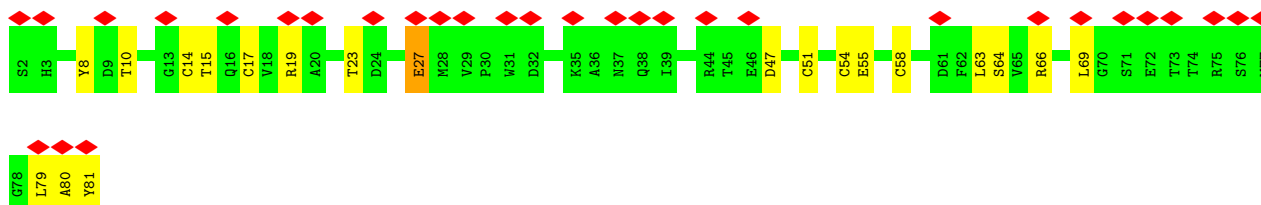
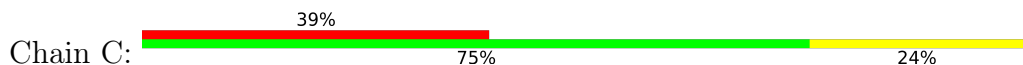


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

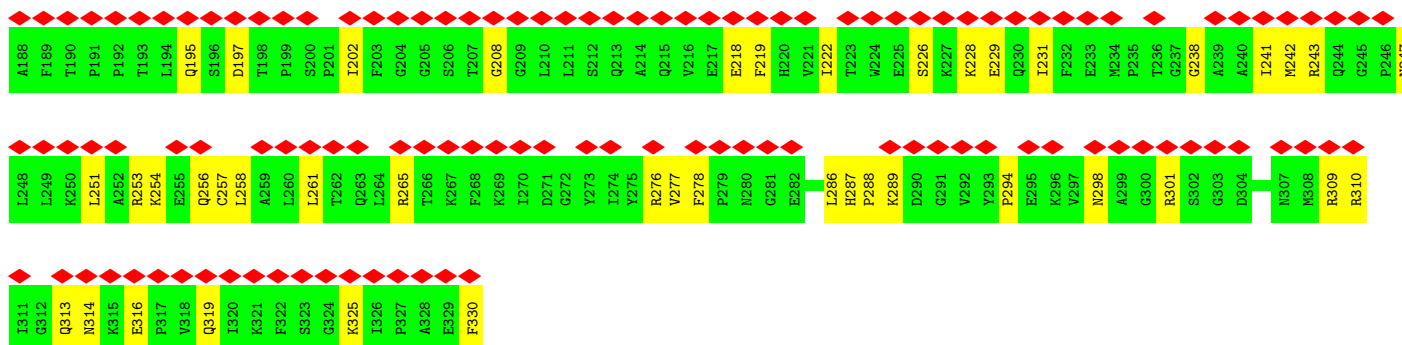
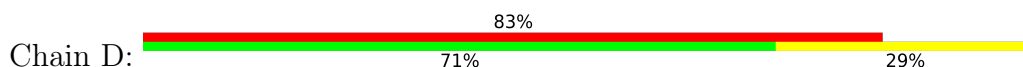




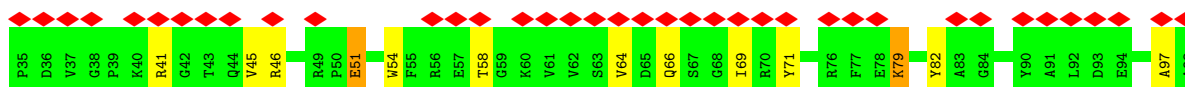
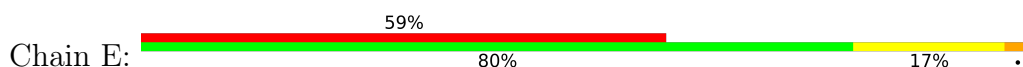
• Molecule 3: Photosystem I iron-sulfur center



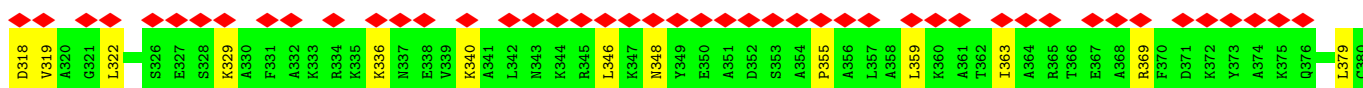
• Molecule 4: Photosystem I reaction center subunit chloroplastic

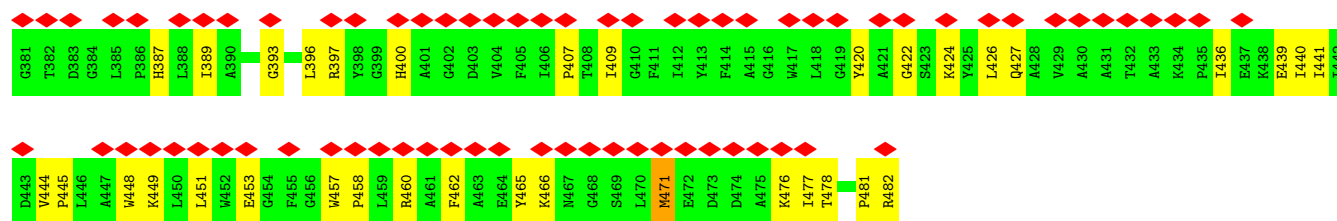


• Molecule 5: Photosystem I reaction center subunit IV

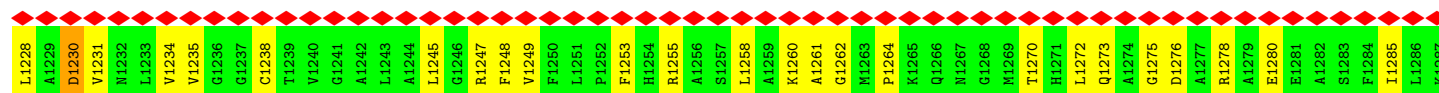


• Molecule 6: PSI-F

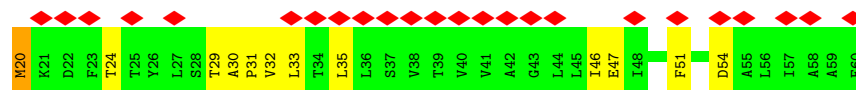




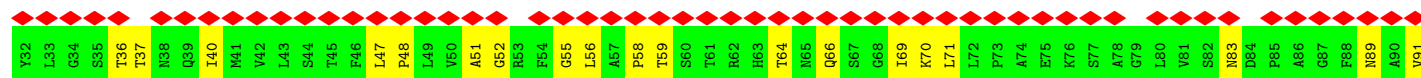
• Molecule 7: Photosystem I reaction center subunit chloroplastic



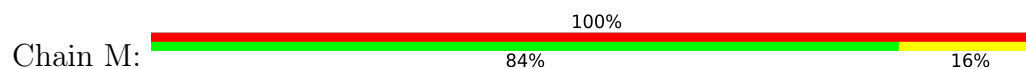
• Molecule 8: Photosystem I reaction center subunit IX



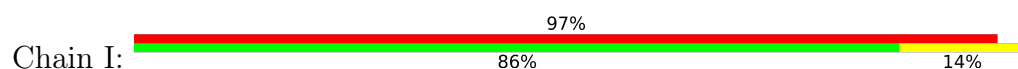
• Molecule 9: PSI-K

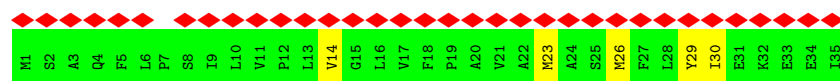


• Molecule 10: Photosystem I reaction center subunit XII

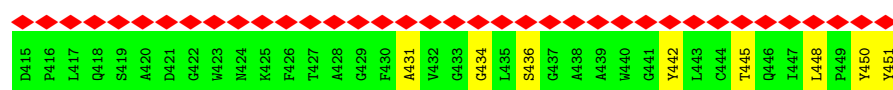
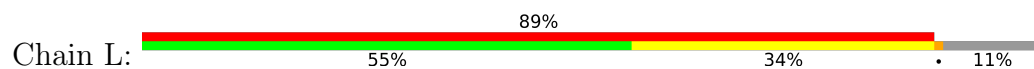


• Molecule 11: Photosystem I reaction center subunit VIII

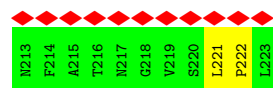
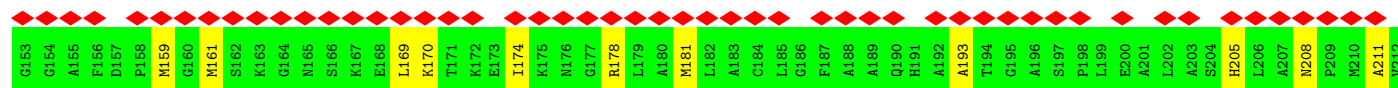
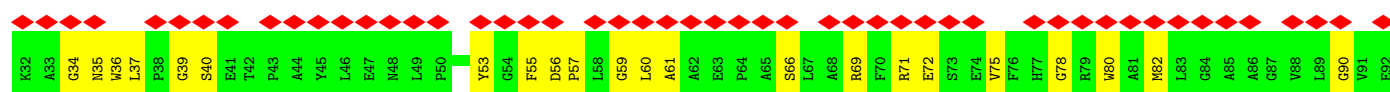
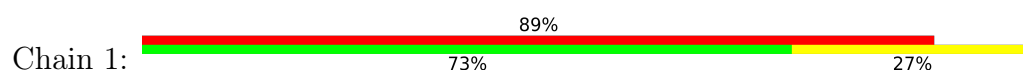




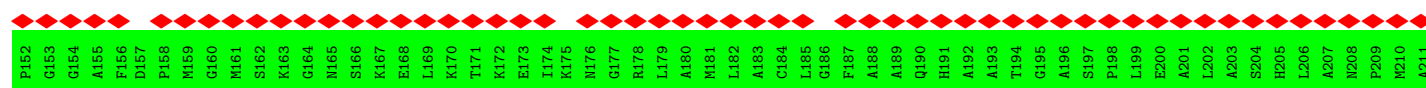
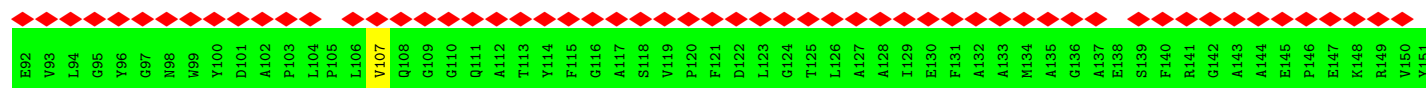
• Molecule 12: PSI subunit V

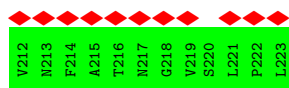


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

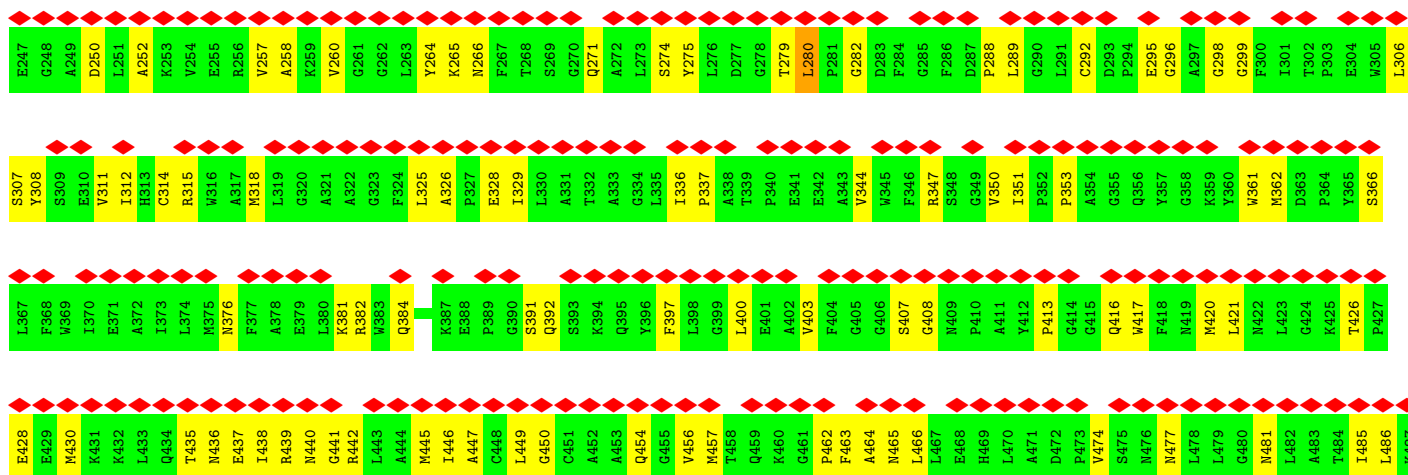
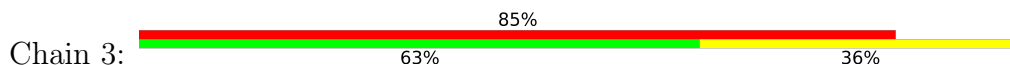


• Molecule 13: Chlorophyll a-b binding protein, chloroplastic

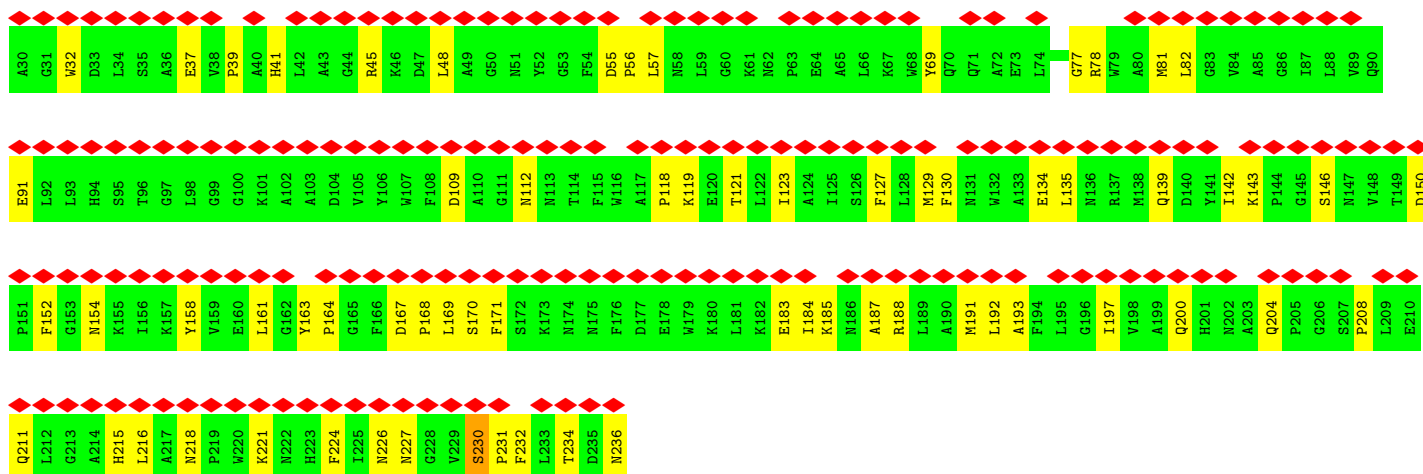
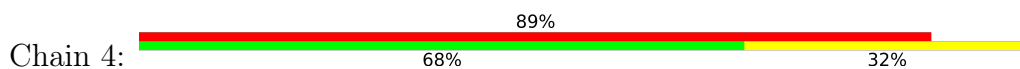




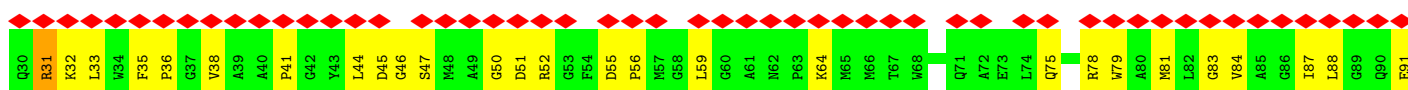
• Molecule 14: Glutathione reductase

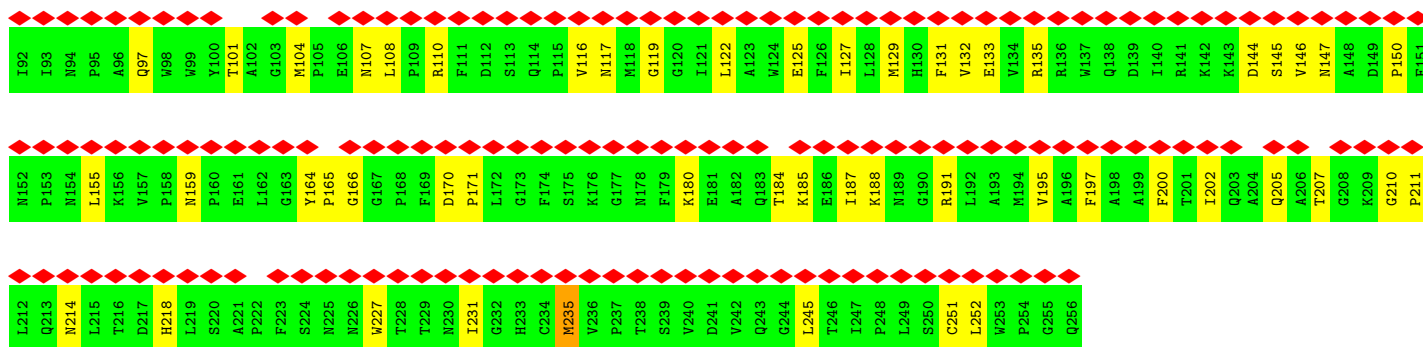


• Molecule 15: Chlorophyll a-b binding protein, chloroplastic

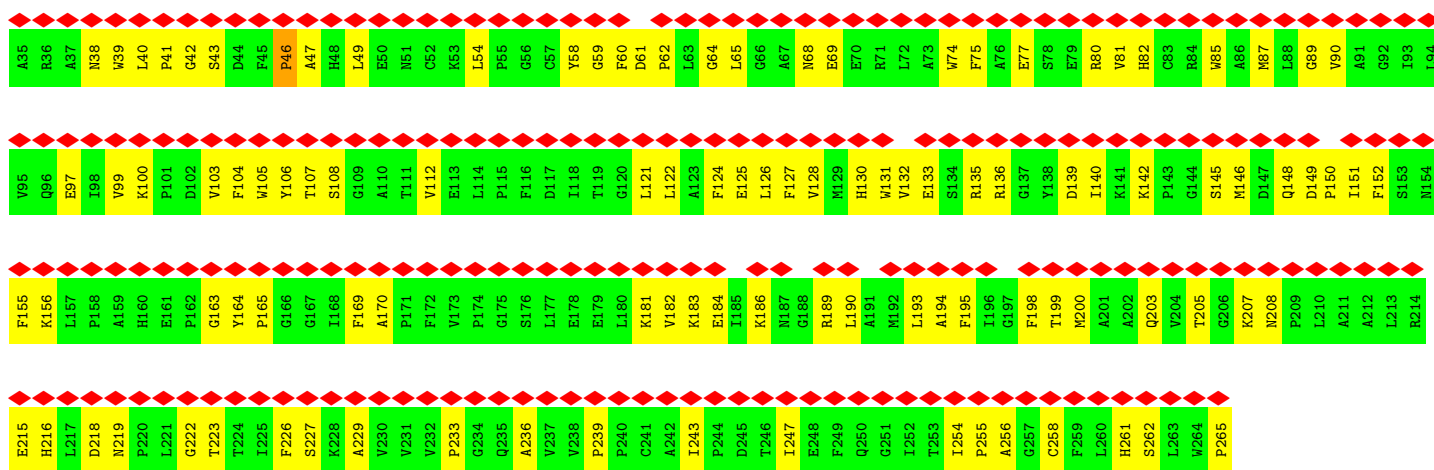


• Molecule 16: Chlorophyll a-b binding protein, chloroplastic

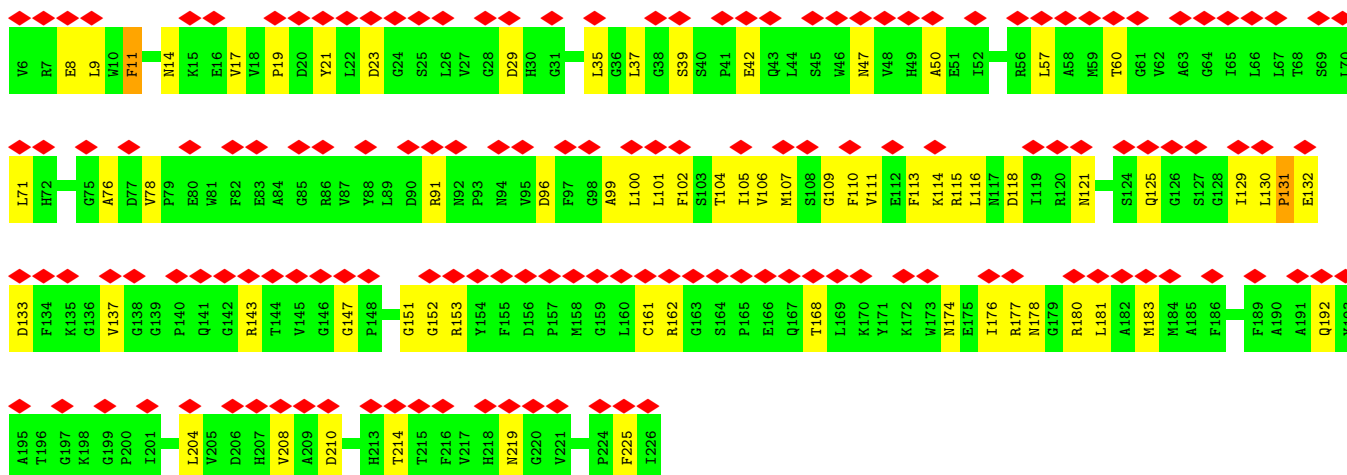




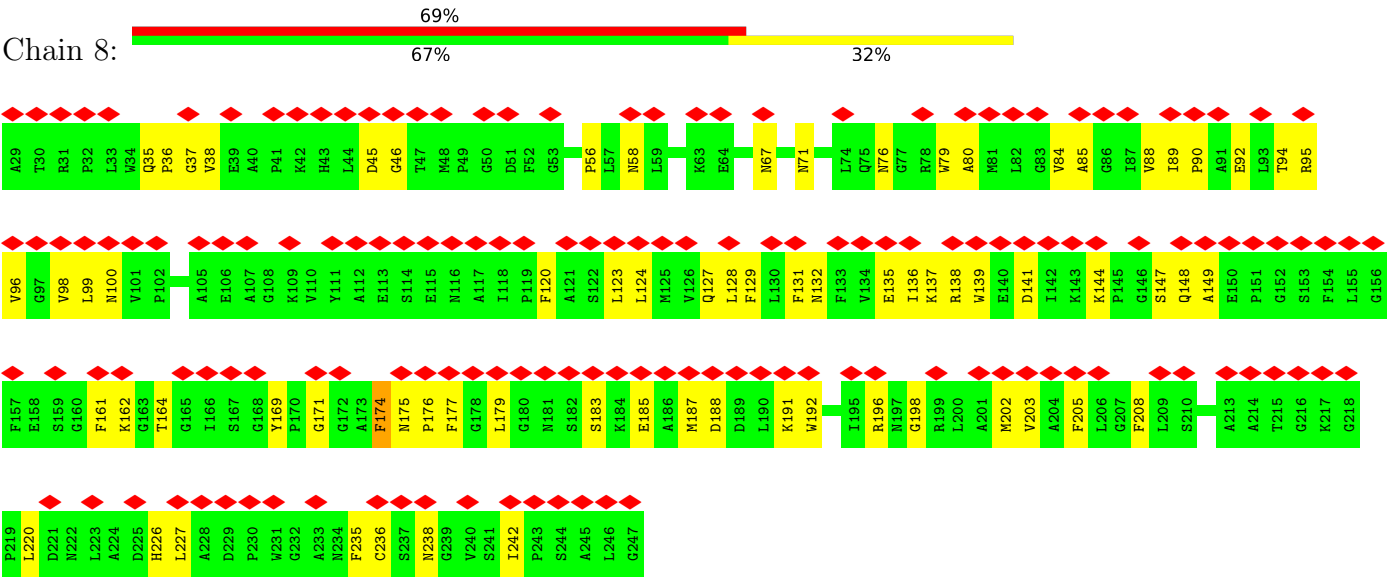
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



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



- Molecule 19: 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	25248	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 ($e^-/\text{\AA}^2$)	46.04	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.034	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	414.72, 414.72, 414.72	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.81, 0.81, 0.81	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, BCR, QTB, DGA, GG0, LUT, 4RF, SF4, ERG, PTY, SPH, SQD, XAT, CL0, PLM, CHL, OLA, LPX, DGD, LAP, P5S, LHG, 3PH, RRX, PQN, ECH, C7Z, CLA, PCW

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	0.41	0/6022	0.54	4/8215 (0.0%)
2	B	0.42	3/6006 (0.0%)	0.51	1/8205 (0.0%)
3	C	0.48	0/611	0.67	2/828 (0.2%)
4	D	0.44	0/1150	0.57	0/1551
5	E	1.09	4/520 (0.8%)	0.76	1/705 (0.1%)
6	F	0.39	1/1309 (0.1%)	0.76	2/1771 (0.1%)
7	G	0.35	0/743	0.55	0/1007
8	J	0.43	0/322	0.72	1/439 (0.2%)
9	K	0.31	0/622	0.51	0/844
10	M	0.36	0/244	0.46	0/330
11	I	0.36	0/276	0.51	0/373
12	L	0.36	0/1068	0.66	2/1462 (0.1%)
13	1	0.36	0/1443	0.57	1/1960 (0.1%)
13	a	0.38	0/1443	0.59	0/1960
14	3	0.37	0/1896	0.53	0/2573
15	4	0.35	0/1681	0.52	0/2285
16	5	0.34	0/1825	0.55	1/2483 (0.0%)
17	6	0.38	0/1845	0.58	1/2515 (0.0%)
18	7	0.42	0/1748	0.54	2/2372 (0.1%)
19	8	0.42	0/1717	0.53	1/2330 (0.0%)
All	All	0.42	8/32491 (0.0%)	0.56	19/44208 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	E	0	1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	79	LYS	CE-NZ	17.65	1.93	1.49
5	E	51	GLU	CB-CG	-9.11	1.34	1.52
5	E	79	LYS	CB-CG	-8.41	1.29	1.52
2	B	258	PHE	CE1-CZ	-5.74	1.26	1.37
6	F	471	MET	CB-CG	-5.46	1.33	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	471	MET	CB-CG-SD	-18.05	58.27	112.40
13	1	221	LEU	CB-CG-CD1	-10.38	93.35	111.00
6	F	471	MET	CG-SD-CE	-9.62	84.81	100.20
1	A	374	MET	CG-SD-CE	-9.00	85.80	100.20
17	6	200	MET	CA-CB-CG	-8.72	98.47	113.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	51	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5824	0	5675	240	0
2	B	5796	0	5576	242	0
3	C	601	0	576	23	0
4	D	1124	0	1129	44	0
5	E	509	0	507	11	0
6	F	1277	0	1296	58	0
7	G	727	0	724	55	0
8	J	316	0	332	18	0
9	K	613	0	639	48	0
10	M	239	0	255	9	0
11	I	270	0	287	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	1041	0	1047	51	0
13	1	1405	0	1370	52	0
13	a	1405	0	1370	0	0
14	3	1844	0	1805	91	0
15	4	1631	0	1575	61	0
16	5	1769	0	1719	98	0
17	6	1787	0	1762	187	0
18	7	1698	0	1640	80	0
19	8	1669	0	1619	70	0
21	A	65	0	72	3	0
22	1	693	0	678	75	0
22	3	719	0	726	66	0
22	4	768	0	686	52	0
22	5	739	0	638	64	0
22	6	711	0	649	117	0
22	7	778	0	720	69	0
22	8	699	0	617	65	0
22	A	2621	0	2695	265	0
22	B	2583	0	2678	288	0
22	F	105	0	87	13	0
22	G	141	0	105	11	0
22	J	42	0	31	1	0
22	K	204	0	167	41	0
22	L	155	0	130	23	0
22	a	571	0	540	0	0
23	A	33	0	46	6	0
23	B	33	0	46	8	0
24	3	120	0	159	14	0
24	4	40	0	53	3	0
24	5	80	0	104	10	0
24	6	80	0	105	16	0
24	7	40	0	52	9	0
24	8	40	0	53	5	0
24	A	200	0	264	22	0
24	B	280	0	369	35	0
24	F	40	0	53	5	0
24	G	40	0	53	3	0
24	I	40	0	52	8	0
24	J	40	0	53	3	0
24	K	80	0	106	7	0
24	L	120	0	159	23	0
25	1	77	0	97	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	3	49	0	74	5	0
25	4	81	0	108	20	0
25	5	49	0	74	9	0
25	6	86	0	118	19	0
25	7	128	0	175	12	0
25	8	37	0	44	5	0
25	A	120	0	159	16	0
25	B	95	0	139	9	0
25	F	79	0	101	8	0
25	a	35	0	40	0	0
26	8	66	0	96	13	0
26	A	51	0	60	3	0
26	B	66	0	96	10	0
27	A	33	0	39	1	0
28	A	8	0	0	0	0
28	C	16	0	0	2	0
29	1	35	0	45	8	0
29	A	35	0	46	4	0
29	B	35	0	44	2	0
30	6	36	0	44	3	0
30	B	30	0	34	6	0
31	3	38	0	49	5	0
31	5	38	0	49	2	0
31	7	33	0	39	3	0
31	8	35	0	43	6	0
31	B	41	0	55	6	0
32	B	29	0	42	3	0
32	F	29	0	42	6	0
32	K	29	0	42	3	0
33	7	39	0	41	1	0
33	G	46	0	55	4	0
34	G	29	0	38	16	0
35	J	41	0	56	10	0
36	J	17	0	14	3	0
36	a	30	0	43	0	0
37	M	41	0	54	6	0
38	1	126	0	165	16	0
38	3	84	0	110	10	0
38	4	84	0	110	9	0
38	5	126	0	165	20	0
38	6	84	0	110	29	0
38	7	42	0	55	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	8	84	0	110	17	0
38	a	126	0	165	0	0
39	1	114	0	102	16	0
39	3	98	0	73	11	0
39	4	174	0	154	18	0
39	5	173	0	153	22	0
39	6	224	0	188	56	0
39	7	66	0	70	6	0
39	8	174	0	153	20	0
39	a	203	0	148	0	0
40	1	20	0	33	2	0
40	8	20	0	33	4	0
41	3	19	0	0	0	0
41	a	19	0	0	0	0
42	a	9	0	0	0	0
43	4	17	0	31	0	0
43	6	18	0	31	1	0
44	5	23	0	28	3	0
44	8	30	0	42	5	0
45	6	21	0	37	7	0
46	7	44	0	56	5	0
47	7	32	0	39	6	0
47	8	96	0	142	16	0
48	7	42	0	0	4	0
49	8	37	0	40	0	0
All	All	48636	0	48687	2217	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 24.

The worst 5 of 2217 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)
34:G:5002:ERG:O1	34:G:5002:ERG:C3	1.70	1.40
5:E:79:LYS:NZ	5:E:79:LYS:CE	1.93	1.29
22:B:1201:CLA:H72	11:I:29:TYR:CE2	1.77	1.17
17:6:135:ARG:NE	39:6:611:CHL:OMC	1.78	1.14
7:G:1317:SER:HA	34:G:5002:ERG:H7	1.13	1.11

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%)	702 (95%)	36 (5%)	1 (0%)	51	85
2	B	729/731 (100%)	682 (94%)	47 (6%)	0	100	100
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	D	141/143 (99%)	131 (93%)	10 (7%)	0	100	100
5	E	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
6	F	163/165 (99%)	150 (92%)	13 (8%)	0	100	100
7	G	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	15	54
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	K	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
10	M	29/31 (94%)	29 (100%)	0	0	100	100
11	I	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
12	L	136/157 (87%)	129 (95%)	7 (5%)	0	100	100
13	1	190/192 (99%)	167 (88%)	22 (12%)	1 (0%)	29	68
13	a	190/192 (99%)	164 (86%)	25 (13%)	1 (0%)	29	68
14	3	239/241 (99%)	219 (92%)	19 (8%)	1 (0%)	34	72
15	4	205/207 (99%)	188 (92%)	16 (8%)	1 (0%)	29	68
16	5	225/227 (99%)	201 (89%)	23 (10%)	1 (0%)	34	72
17	6	229/231 (99%)	208 (91%)	19 (8%)	2 (1%)	17	56
18	7	219/221 (99%)	198 (90%)	20 (9%)	1 (0%)	29	68
19	8	217/219 (99%)	194 (89%)	21 (10%)	2 (1%)	17	56
All	All	4044/4103 (99%)	3732 (92%)	300 (7%)	12 (0%)	44	76

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	1	36	TRP

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Mol	Chain	Res	Type
17	6	46	PRO
18	7	131	PRO
19	8	45	ASP
13	a	107	VAL

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	600/600 (100%)	598 (100%)	2 (0%)	92	95
2	B	588/588 (100%)	588 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	121/121 (100%)	121 (100%)	0	100	100
5	E	55/55 (100%)	55 (100%)	0	100	100
6	F	126/126 (100%)	126 (100%)	0	100	100
7	G	71/71 (100%)	70 (99%)	1 (1%)	67	80
8	J	35/35 (100%)	35 (100%)	0	100	100
9	K	66/66 (100%)	66 (100%)	0	100	100
10	M	23/23 (100%)	23 (100%)	0	100	100
11	I	30/30 (100%)	30 (100%)	0	100	100
12	L	108/122 (88%)	108 (100%)	0	100	100
13	1	134/134 (100%)	134 (100%)	0	100	100
13	a	134/134 (100%)	133 (99%)	1 (1%)	84	90
14	3	186/186 (100%)	186 (100%)	0	100	100
15	4	165/165 (100%)	165 (100%)	0	100	100
16	5	183/183 (100%)	183 (100%)	0	100	100
17	6	187/187 (100%)	187 (100%)	0	100	100
18	7	176/176 (100%)	176 (100%)	0	100	100
19	8	168/168 (100%)	168 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3225/3239 (100%)	3221 (100%)	4 (0%)	93 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	421	ASN
7	G	1307	HIS
13	a	35	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
16	5	107	ASN
16	5	117	ASN
19	8	76	ASN
16	5	205	GLN
12	L	396	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

337 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	4	613	-	52,60,74	1.07	3 (5%)	56,97,114	1.59	12 (21%)
39	CHL	5	613	-	56,64,74	0.90	2 (3%)	61,102,114	1.39	10 (16%)
22	CLA	a	608	-	55,63,73	1.47	8 (14%)	64,101,113	2.03	15 (23%)
24	BCR	A	4005	-	41,41,41	1.85	6 (14%)	56,56,56	4.26	15 (26%)
22	CLA	5	608	-	45,53,73	1.62	8 (17%)	52,89,113	2.19	15 (28%)
22	CLA	B	1216	-	61,69,73	1.41	7 (11%)	71,108,113	1.97	17 (23%)
22	CLA	A	1119	-	65,73,73	1.37	7 (10%)	76,113,113	1.82	16 (21%)
25	LHG	4	801	22	48,48,48	0.40	0	51,54,54	1.07	3 (5%)
22	CLA	B	1211	-	55,63,73	1.49	7 (12%)	64,101,113	2.13	18 (28%)
22	CLA	K	1402	-	60,68,73	1.41	8 (13%)	70,107,113	2.08	18 (25%)
22	CLA	8	607	25	46,54,73	1.60	7 (15%)	53,90,113	2.11	11 (20%)
22	CLA	4	603	15	56,64,73	1.46	7 (12%)	65,102,113	2.15	17 (26%)
22	CLA	B	1234	-	56,64,73	1.50	7 (12%)	65,102,113	2.26	17 (26%)
22	CLA	5	616	-	46,54,73	1.62	8 (17%)	53,90,113	2.11	13 (24%)
22	CLA	6	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.04	16 (21%)
22	CLA	a	612	13	57,65,73	1.47	6 (10%)	66,103,113	2.02	18 (27%)
22	CLA	1	603	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	17 (22%)
39	CHL	3	608	-	43,51,74	1.07	3 (6%)	45,86,114	1.47	9 (20%)
22	CLA	F	1301	6	50,58,73	1.53	7 (14%)	58,95,113	2.29	17 (29%)
23	PQN	A	2001	-	34,34,34	0.34	0	42,45,45	1.27	4 (9%)
22	CLA	B	1203	-	65,73,73	1.37	7 (10%)	76,113,113	1.96	15 (19%)
25	LHG	7	801	22	48,48,48	0.37	0	51,54,54	1.23	4 (7%)
48	C7Z	7	504	-	43,43,43	5.33	27 (62%)	58,60,60	2.76	26 (44%)
22	CLA	B	1229	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	18 (23%)
22	CLA	8	612	19	46,54,73	1.63	7 (15%)	53,90,113	2.08	12 (22%)
22	CLA	5	612	16	65,73,73	1.36	7 (10%)	76,113,113	1.93	13 (17%)
24	BCR	F	4001	-	41,41,41	1.89	5 (12%)	56,56,56	3.99	16 (28%)
22	CLA	1	601	13	60,68,73	1.41	8 (13%)	70,107,113	2.03	17 (24%)
40	OLA	8	809	-	19,19,19	0.56	0	19,19,19	1.07	0
31	PTY	3	802	-	37,37,49	1.00	4 (10%)	40,42,54	1.09	2 (5%)
22	CLA	6	615	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	18 (23%)
22	CLA	K	1401	-	46,54,73	1.62	8 (17%)	53,90,113	2.05	12 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	3	801	22	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
22	CLA	B	1201	-	65,73,73	1.35	8 (12%)	76,113,113	2.08	23 (30%)
22	CLA	4	605	-	46,54,73	1.60	7 (15%)	53,90,113	2.25	17 (32%)
22	CLA	6	606	-	52,60,73	1.52	7 (13%)	60,97,113	2.15	17 (28%)
22	CLA	3	603	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	14 (18%)
22	CLA	A	1103	-	65,73,73	1.35	7 (10%)	76,113,113	2.07	18 (23%)
22	CLA	A	1137	-	60,68,73	1.40	7 (11%)	70,107,113	2.06	20 (28%)
22	CLA	8	618	-	60,68,73	1.42	7 (11%)	70,107,113	2.08	17 (24%)
30	PCW	6	803	-	35,35,53	1.28	4 (11%)	41,43,61	1.13	2 (4%)
38	LUT	1	501	-	42,43,43	2.40	1 (2%)	51,60,60	2.02	17 (33%)
22	CLA	A	1129	-	50,58,73	1.57	7 (14%)	58,95,113	2.27	17 (29%)
22	CLA	B	1232	-	45,53,73	1.66	8 (17%)	52,89,113	2.07	11 (21%)
22	CLA	A	1104	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	18 (23%)
29	LMT	1	804	-	36,36,36	1.18	6 (16%)	47,47,47	1.05	1 (2%)
24	BCR	4	503	-	41,41,41	1.86	5 (12%)	56,56,56	4.38	12 (21%)
24	BCR	L	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.26	18 (32%)
22	CLA	1	602	-	45,53,73	1.59	7 (15%)	52,89,113	2.10	12 (23%)
25	LHG	a	801	-	34,34,48	0.47	0	37,40,54	1.31	5 (13%)
22	CLA	1	605	-	65,73,73	1.34	7 (10%)	76,113,113	2.11	20 (26%)
43	PLM	6	804	-	17,17,17	0.56	0	17,17,17	1.12	0
22	CLA	A	1126	-	65,73,73	1.40	8 (12%)	76,113,113	2.00	15 (19%)
22	CLA	8	606	-	57,65,73	1.46	7 (12%)	66,103,113	2.20	18 (27%)
45	SPH	6	806	-	19,20,20	0.61	0	18,21,21	1.13	1 (5%)
36	LPX	J	5001	-	16,16,29	1.32	2 (12%)	18,20,33	1.06	2 (11%)
22	CLA	6	607	25	55,63,73	1.49	8 (14%)	64,101,113	2.07	16 (25%)
25	LHG	F	5002	-	35,35,48	0.45	0	38,41,54	1.22	4 (10%)
22	CLA	A	1138	-	65,73,73	1.37	8 (12%)	76,113,113	2.10	18 (23%)
22	CLA	1	607	-	65,73,73	1.35	7 (10%)	76,113,113	1.94	16 (21%)
22	CLA	K	1403	9	46,54,73	1.63	8 (17%)	53,90,113	2.12	11 (20%)
22	CLA	7	612	-	60,68,73	1.49	8 (13%)	70,107,113	2.03	17 (24%)
22	CLA	A	1125	-	65,73,73	1.43	8 (12%)	76,113,113	2.26	19 (25%)
22	CLA	5	617	-	50,58,73	1.55	7 (14%)	58,95,113	2.31	17 (29%)
22	CLA	7	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	22 (28%)
22	CLA	B	1022	-	65,73,73	1.42	7 (10%)	76,113,113	1.90	16 (21%)
22	CLA	4	611	-	56,64,73	1.46	7 (12%)	65,102,113	2.09	17 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	CHL	4	618	15	56,64,74	1.07	4 (7%)	61,102,114	1.36	11 (18%)
22	CLA	A	1114	-	65,73,73	1.40	7 (10%)	76,113,113	2.03	20 (26%)
33	SQD	7	805	-	38,39,54	0.90	0	47,50,65	1.01	3 (6%)
33	SQD	G	5001	-	45,46,54	0.82	0	54,57,65	0.95	2 (3%)
22	CLA	B	1231	-	65,73,73	1.38	7 (10%)	76,113,113	2.00	16 (21%)
44	DGA	5	803	-	22,22,43	1.43	3 (13%)	24,24,45	1.38	2 (8%)
22	CLA	4	602	15	52,60,73	1.51	7 (13%)	60,97,113	2.20	18 (30%)
31	PTY	8	810	-	34,34,49	1.02	3 (8%)	37,39,54	1.33	3 (8%)
24	BCR	B	4005	-	41,41,41	1.89	6 (14%)	56,56,56	4.28	20 (35%)
22	CLA	a	605	-	65,73,73	1.33	7 (10%)	76,113,113	2.00	20 (26%)
22	CLA	B	1222	-	58,66,73	1.45	7 (12%)	67,104,113	2.10	15 (22%)
22	CLA	1	604	-	65,73,73	1.40	8 (12%)	76,113,113	1.98	18 (23%)
22	CLA	A	1105	-	57,65,73	1.46	8 (14%)	66,103,113	2.12	19 (28%)
27	3PH	A	5007	-	32,32,47	1.01	4 (12%)	36,37,52	1.20	2 (5%)
22	CLA	A	1121	-	57,65,73	1.47	8 (14%)	66,103,113	2.25	18 (27%)
26	DGD	A	5005	-	52,52,67	0.92	4 (7%)	66,66,81	1.13	5 (7%)
22	CLA	A	1113	-	52,60,73	1.52	7 (13%)	60,97,113	2.26	19 (31%)
39	CHL	3	611	-	55,63,74	1.15	4 (7%)	59,100,114	1.44	11 (18%)
22	CLA	B	1226	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	14 (18%)
24	BCR	B	4003	-	41,41,41	1.84	5 (12%)	56,56,56	4.49	18 (32%)
22	CLA	a	615	13	46,54,73	1.59	7 (15%)	53,90,113	2.12	16 (30%)
22	CLA	5	614	-	46,54,73	1.59	8 (17%)	53,90,113	2.15	12 (22%)
46	XAT	7	502	-	39,47,47	0.78	1 (2%)	54,74,74	1.98	12 (22%)
22	CLA	7	610	-	55,63,73	1.48	7 (12%)	64,101,113	2.06	18 (28%)
22	CLA	8	610	-	55,63,73	1.48	7 (12%)	64,101,113	2.14	19 (29%)
25	LHG	B	5002	-	48,48,48	0.41	0	51,54,54	0.96	3 (5%)
24	BCR	6	504	-	41,41,41	1.86	6 (14%)	56,56,56	4.27	20 (35%)
31	PTY	B	5005	-	40,40,49	0.94	4 (10%)	43,45,54	1.17	2 (4%)
22	CLA	A	1136	-	65,73,73	1.37	7 (10%)	76,113,113	1.97	15 (19%)
22	CLA	A	1108	-	65,73,73	1.38	7 (10%)	76,113,113	2.10	15 (19%)
22	CLA	B	1209	-	65,73,73	1.37	8 (12%)	76,113,113	2.08	19 (25%)
22	CLA	3	602	14	46,54,73	1.58	7 (15%)	53,90,113	2.22	17 (32%)
31	PTY	7	804	-	32,32,49	1.06	4 (12%)	35,37,54	1.20	2 (5%)
22	CLA	3	604	-	60,68,73	1.42	7 (11%)	70,107,113	2.13	20 (28%)
22	CLA	8	611	-	50,58,73	1.51	7 (14%)	58,95,113	2.32	17 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	1135	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	18 (23%)
35	RRX	J	4002	-	42,42,42	4.86	24 (57%)	57,58,58	2.45	20 (35%)
22	CLA	7	603	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	15 (19%)
22	CLA	6	602	17	52,60,73	1.51	8 (15%)	60,97,113	2.21	17 (28%)
24	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.36	20 (35%)
22	CLA	A	1139	-	55,63,73	1.53	7 (12%)	64,101,113	2.08	17 (26%)
22	CLA	6	604	-	65,73,73	1.33	7 (10%)	76,113,113	2.16	23 (30%)
22	CLA	7	608	-	42,50,73	1.69	7 (16%)	48,85,113	2.28	12 (25%)
22	CLA	5	606	-	50,58,73	1.56	7 (14%)	58,95,113	2.22	18 (31%)
22	CLA	A	1123	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	19 (25%)
24	BCR	L	4002	-	41,41,41	1.81	4 (9%)	56,56,56	4.41	17 (30%)
32	LAP	K	5001	-	28,28,28	1.26	3 (10%)	33,35,35	1.06	2 (6%)
32	LAP	B	5007	-	28,28,28	1.21	3 (10%)	33,35,35	0.96	1 (3%)
21	CL0	A	1011	-	65,73,73	2.31	17 (26%)	76,113,113	2.54	24 (31%)
40	OLA	1	803	-	19,19,19	0.56	0	19,19,19	1.06	1 (5%)
22	CLA	4	612	15	62,70,73	1.39	9 (14%)	72,109,113	2.13	19 (26%)
22	CLA	G	1602	-	46,54,73	1.61	8 (17%)	53,90,113	2.10	15 (28%)
22	CLA	1	606	-	57,65,73	1.45	8 (14%)	66,103,113	2.14	18 (27%)
22	CLA	6	612	-	50,58,73	1.52	7 (14%)	58,95,113	2.30	17 (29%)
26	DGD	8	802	-	67,67,67	1.18	7 (10%)	81,81,81	1.11	5 (6%)
22	CLA	A	1117	-	65,73,73	1.36	7 (10%)	76,113,113	2.00	16 (21%)
22	CLA	B	1206	2	55,63,73	1.51	8 (14%)	64,101,113	2.20	18 (28%)
22	CLA	A	1128	-	65,73,73	1.41	7 (10%)	76,113,113	2.08	18 (23%)
39	CHL	4	609	15	66,74,74	0.90	3 (4%)	73,114,114	1.42	13 (17%)
22	CLA	4	616	-	50,58,73	1.57	8 (16%)	58,95,113	2.22	16 (27%)
24	BCR	A	4003	-	41,41,41	1.85	5 (12%)	56,56,56	4.32	16 (28%)
24	BCR	A	4004	-	41,41,41	1.93	6 (14%)	56,56,56	4.50	15 (26%)
22	CLA	5	602	-	52,60,73	1.54	7 (13%)	60,97,113	2.20	17 (28%)
41	QTB	3	506	-	19,19,19	2.67	6 (31%)	20,26,26	2.78	8 (40%)
26	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.08	4 (4%)
22	CLA	B	1214	-	62,70,73	1.41	7 (11%)	72,109,113	1.98	18 (25%)
22	CLA	B	1215	-	60,68,73	1.42	7 (11%)	70,107,113	1.94	16 (22%)
22	CLA	A	1130	-	56,64,73	1.46	7 (12%)	65,102,113	2.08	16 (24%)
38	LUT	8	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.91	14 (27%)
22	CLA	5	604	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
38	LUT	1	503	-	42,43,43	2.41	1 (2%)	51,60,60	2.31	13 (25%)
39	CHL	8	601	19	61,69,74	1.08	6 (9%)	67,108,114	1.30	8 (11%)
39	CHL	8	613	-	51,59,74	1.11	4 (7%)	55,96,114	1.43	8 (14%)
22	CLA	B	1223	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	17 (22%)
22	CLA	B	1213	-	60,68,73	1.46	8 (13%)	70,107,113	2.06	18 (25%)
24	BCR	G	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.29	19 (33%)
25	LHG	A	5003	-	41,41,48	0.43	0	44,47,54	1.16	3 (6%)
24	BCR	5	504	-	41,41,41	1.85	6 (14%)	56,56,56	4.18	18 (32%)
22	CLA	6	618	-	46,54,73	1.57	7 (15%)	53,90,113	2.20	13 (24%)
24	BCR	B	4006	-	41,41,41	1.81	5 (12%)	56,56,56	4.34	15 (26%)
39	CHL	5	611	-	51,59,74	1.13	5 (9%)	55,96,114	1.43	11 (20%)
22	CLA	3	606	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	16 (21%)
24	BCR	6	503	-	41,41,41	1.89	5 (12%)	56,56,56	4.32	15 (26%)
24	BCR	K	4002	-	41,41,41	1.88	5 (12%)	56,56,56	4.14	15 (26%)
22	CLA	B	1023	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	18 (23%)
22	CLA	B	1230	-	58,66,73	1.43	7 (12%)	67,104,113	2.19	19 (28%)
22	CLA	4	615	15	60,68,73	1.42	7 (11%)	70,107,113	2.06	19 (27%)
38	LUT	5	505	-	42,43,43	2.42	2 (4%)	51,60,60	2.72	19 (37%)
22	CLA	A	1109	22	65,73,73	1.33	8 (12%)	76,113,113	2.14	19 (25%)
47	4RF	8	808	-	53,53,56	0.90	5 (9%)	56,56,59	1.04	3 (5%)
22	CLA	A	1116	-	60,68,73	1.45	7 (11%)	70,107,113	2.13	19 (27%)
22	CLA	1	610	-	45,53,73	1.63	7 (15%)	52,89,113	2.16	14 (26%)
24	BCR	A	4001	-	41,41,41	1.79	5 (12%)	56,56,56	4.02	18 (32%)
39	CHL	a	609	13	53,61,74	1.03	4 (7%)	57,98,114	1.42	11 (19%)
25	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
22	CLA	B	1237	-	65,73,73	1.39	7 (10%)	76,113,113	1.98	18 (23%)
22	CLA	B	1212	-	65,73,73	1.39	8 (12%)	76,113,113	2.07	19 (25%)
22	CLA	8	608	-	52,60,73	1.53	7 (13%)	60,97,113	2.37	19 (31%)
38	LUT	4	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.92	12 (23%)
22	CLA	5	603	-	56,64,73	1.45	8 (14%)	65,102,113	2.18	17 (26%)
38	LUT	4	501	-	42,43,43	2.28	1 (2%)	51,60,60	1.94	15 (29%)
22	CLA	A	1122	-	65,73,73	1.38	8 (12%)	76,113,113	1.93	14 (18%)
22	CLA	8	620	19	65,73,73	1.34	7 (10%)	76,113,113	1.99	19 (25%)
25	LHG	4	802	-	31,31,48	0.45	0	34,37,54	1.16	2 (5%)
42	GG0	a	805	-	7,8,8	1.37	2 (28%)	6,9,9	0.80	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LHG	B	5001	22	45,45,48	0.41	0	48,51,54	1.05	3 (6%)
28	SF4	A	3001	1,2	0,12,12	-	-	-		
38	LUT	6	502	-	42,43,43	2.32	2 (4%)	51,60,60	2.29	13 (25%)
22	CLA	1	608	-	60,68,73	1.43	8 (13%)	70,107,113	2.02	16 (22%)
22	CLA	1	611	-	55,63,73	1.49	8 (14%)	64,101,113	2.07	18 (28%)
25	LHG	6	802	-	36,36,48	0.43	0	39,42,54	1.17	3 (7%)
39	CHL	6	613	-	51,59,74	0.91	2 (3%)	55,96,114	1.45	11 (20%)
39	CHL	6	610	-	56,64,74	0.92	3 (5%)	61,102,114	1.42	11 (18%)
38	LUT	3	501	-	42,43,43	2.35	1 (2%)	51,60,60	2.08	15 (29%)
22	CLA	3	601	-	65,73,73	1.35	7 (10%)	76,113,113	2.04	18 (23%)
22	CLA	3	613	-	61,69,73	1.41	7 (11%)	71,108,113	2.00	15 (21%)
25	LHG	F	5001	22	42,42,48	0.42	0	45,48,54	1.13	3 (6%)
39	CHL	8	604	19	62,70,74	1.06	5 (8%)	68,109,114	1.32	9 (13%)
22	CLA	B	1218	-	55,63,73	1.47	8 (14%)	64,101,113	2.24	19 (29%)
22	CLA	a	601	13	60,68,73	1.40	7 (11%)	70,107,113	2.07	19 (27%)
24	BCR	J	4001	-	41,41,41	1.84	5 (12%)	56,56,56	4.37	16 (28%)
47	4RF	8	807	-	41,41,56	1.00	6 (14%)	44,44,59	1.08	3 (6%)
22	CLA	3	610	14	60,68,73	1.41	7 (11%)	70,107,113	2.05	17 (24%)
36	LPX	a	804	-	29,29,29	1.01	2 (6%)	31,33,33	0.92	1 (3%)
22	CLA	4	607	25	55,63,73	1.49	8 (14%)	64,101,113	2.10	15 (23%)
38	LUT	a	503	-	42,43,43	2.38	1 (2%)	51,60,60	2.19	15 (29%)
24	BCR	7	503	-	41,41,41	1.83	5 (12%)	56,56,56	4.31	13 (23%)
24	BCR	8	503	-	41,41,41	1.88	4 (9%)	56,56,56	4.25	17 (30%)
22	CLA	B	1227	-	50,58,73	1.52	8 (16%)	58,95,113	2.24	19 (32%)
22	CLA	a	603	-	65,73,73	1.38	7 (10%)	76,113,113	2.03	18 (23%)
22	CLA	A	1133	-	65,73,73	1.37	7 (10%)	76,113,113	1.95	16 (21%)
22	CLA	A	1102	22	65,73,73	1.36	8 (12%)	76,113,113	2.28	18 (23%)
38	LUT	7	501	-	42,43,43	2.37	2 (4%)	51,60,60	1.97	15 (29%)
38	LUT	a	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.24	16 (31%)
22	CLA	B	1208	-	60,68,73	1.41	7 (11%)	70,107,113	2.14	21 (30%)
38	LUT	5	502	-	42,43,43	2.35	2 (4%)	51,60,60	2.05	13 (25%)
22	CLA	A	1134	1	60,68,73	1.41	7 (11%)	70,107,113	2.07	17 (24%)
22	CLA	8	602	19	52,60,73	1.54	7 (13%)	60,97,113	2.13	16 (26%)
32	LAP	F	5003	-	28,28,28	1.24	3 (10%)	33,35,35	0.93	1 (3%)
22	CLA	A	1112	-	55,63,73	1.49	9 (16%)	64,101,113	2.24	19 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	1131	-	65,73,73	1.40	7 (10%)	76,113,113	1.96	16 (21%)
22	CLA	6	608	-	45,53,73	1.62	7 (15%)	52,89,113	2.19	15 (28%)
22	CLA	7	607	25	59,67,73	1.45	7 (11%)	68,105,113	2.03	14 (20%)
22	CLA	7	601	-	60,68,73	1.42	8 (13%)	70,107,113	2.05	20 (28%)
22	CLA	B	1219	-	59,67,73	1.44	7 (11%)	68,105,113	2.09	16 (23%)
22	CLA	B	1202	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	15 (19%)
22	CLA	A	1124	-	55,63,73	1.51	7 (12%)	64,101,113	2.07	16 (25%)
22	CLA	B	1240	25	65,73,73	1.39	7 (10%)	76,113,113	1.99	16 (21%)
24	BCR	3	505	-	41,41,41	1.89	4 (9%)	56,56,56	4.12	17 (30%)
22	CLA	6	601	-	60,68,73	1.42	7 (11%)	70,107,113	2.13	17 (24%)
22	CLA	3	607	25	65,73,73	1.33	6 (9%)	76,113,113	2.04	17 (22%)
22	CLA	A	1132	-	65,73,73	1.37	7 (10%)	76,113,113	2.05	18 (23%)
22	CLA	B	1210	-	65,73,73	1.38	8 (12%)	76,113,113	2.18	18 (23%)
38	LUT	3	502	-	42,43,43	2.36	1 (2%)	51,60,60	2.01	12 (23%)
39	CHL	6	619	17	66,74,74	0.89	3 (4%)	73,114,114	1.29	11 (15%)
22	CLA	B	1221	-	65,73,73	1.36	8 (12%)	76,113,113	2.07	17 (22%)
41	QTB	a	504	-	19,19,19	2.62	5 (26%)	20,26,26	2.82	10 (50%)
22	CLA	1	615	13	46,54,73	1.60	7 (15%)	53,90,113	2.12	13 (24%)
22	CLA	B	1236	-	53,61,73	1.52	7 (13%)	61,98,113	2.35	18 (29%)
24	BCR	B	4007	-	41,41,41	1.84	5 (12%)	56,56,56	4.14	16 (28%)
22	CLA	a	604	13	65,73,73	1.36	8 (12%)	76,113,113	2.05	19 (25%)
22	CLA	7	605	-	43,52,73	1.68	8 (18%)	49,88,113	2.13	12 (24%)
22	CLA	5	601	16	60,68,73	1.40	7 (11%)	70,107,113	2.10	21 (30%)
23	PQN	B	2002	-	34,34,34	0.41	0	42,45,45	1.28	4 (9%)
22	CLA	B	1239	-	65,73,73	1.39	7 (10%)	76,113,113	1.95	16 (21%)
22	CLA	B	1217	-	56,64,73	1.45	7 (12%)	65,102,113	2.11	15 (23%)
28	SF4	C	3002	3	0,12,12	-	-	-	-	-
29	LMT	A	5008	-	36,36,36	1.12	5 (13%)	47,47,47	1.04	3 (6%)
22	CLA	A	1140	-	55,63,73	1.50	9 (16%)	64,101,113	2.07	14 (21%)
39	CHL	a	613	-	46,54,74	1.01	3 (6%)	49,90,114	1.52	10 (20%)
22	CLA	5	607	25	55,63,73	1.49	7 (12%)	64,101,113	2.02	15 (23%)
29	LMT	B	5006	-	36,36,36	1.18	5 (13%)	47,47,47	1.01	2 (4%)
22	CLA	A	1101	-	65,73,73	1.36	7 (10%)	76,113,113	2.05	17 (22%)
25	LHG	1	802	-	41,41,48	0.42	0	44,47,54	1.07	4 (9%)
34	ERG	G	5002	-	31,32,32	8.20	18 (58%)	47,50,50	3.19	21 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
49	P5S	8	806	-	35,36,53	1.17	3 (8%)	39,43,60	1.18	3 (7%)
39	CHL	1	613	-	48,56,74	1.00	3 (6%)	51,92,114	1.36	9 (17%)
22	CLA	8	605	-	45,53,73	1.66	7 (15%)	52,89,113	2.09	13 (25%)
22	CLA	A	1127	-	65,73,73	1.40	7 (10%)	76,113,113	1.89	14 (18%)
22	CLA	A	1107	1	55,63,73	1.46	8 (14%)	64,101,113	2.18	18 (28%)
24	BCR	A	4002	-	41,41,41	1.85	6 (14%)	56,56,56	4.31	16 (28%)
22	CLA	L	1502	-	60,68,73	1.41	8 (13%)	70,107,113	2.16	17 (24%)
25	LHG	A	5001	22	28,28,48	0.51	0	31,34,54	1.34	3 (9%)
39	CHL	a	606	-	56,64,74	1.00	3 (5%)	61,102,114	1.32	11 (18%)
25	LHG	6	801	22	48,48,48	0.40	0	51,54,54	1.12	3 (5%)
22	CLA	A	1111	-	65,73,73	1.37	7 (10%)	76,113,113	2.01	20 (26%)
22	CLA	J	1901	8	42,50,73	1.62	7 (16%)	48,85,113	2.23	13 (27%)
22	CLA	a	607	-	58,66,73	1.44	8 (13%)	67,104,113	2.18	16 (23%)
22	CLA	F	1302	25	55,63,73	1.47	6 (10%)	64,101,113	2.27	20 (31%)
22	CLA	B	1204	-	65,73,73	1.39	7 (10%)	76,113,113	2.01	17 (22%)
22	CLA	A	1110	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	16 (22%)
22	CLA	B	1205	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	16 (21%)
22	CLA	7	609	-	60,68,73	1.41	7 (11%)	70,107,113	2.10	18 (25%)
25	LHG	7	802	-	35,35,48	0.45	0	38,41,54	1.15	3 (7%)
22	CLA	A	1120	-	49,57,73	1.56	8 (16%)	55,93,113	2.35	17 (30%)
22	CLA	4	617	-	45,53,73	1.62	7 (15%)	52,89,113	2.19	15 (28%)
22	CLA	A	1118	-	55,63,73	1.48	7 (12%)	64,101,113	2.16	15 (23%)
39	CHL	7	613	-	66,74,74	0.95	3 (4%)	73,114,114	1.31	13 (17%)
22	CLA	7	602	-	44,52,73	1.66	7 (15%)	49,87,113	2.20	15 (30%)
24	BCR	3	503	-	41,41,41	1.88	6 (14%)	56,56,56	4.07	18 (32%)
22	CLA	B	1220	-	60,68,73	1.45	7 (11%)	70,107,113	2.10	15 (21%)
22	CLA	4	610	-	65,73,73	1.37	8 (12%)	76,113,113	2.02	17 (22%)
22	CLA	3	605	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	17 (22%)
47	4RF	7	807	-	31,31,56	1.16	6 (19%)	34,34,59	1.17	3 (8%)
25	LHG	1	801	-	34,34,48	0.45	0	37,40,54	1.25	4 (10%)
25	LHG	5	801	22	48,48,48	0.39	0	51,54,54	1.04	3 (5%)
22	CLA	6	605	-	46,54,73	1.59	8 (17%)	53,90,113	2.19	14 (26%)
22	CLA	6	617	17	45,53,73	1.60	7 (15%)	52,89,113	2.14	15 (28%)
22	CLA	B	1235	-	65,73,73	1.38	8 (12%)	76,113,113	2.05	16 (21%)
22	CLA	B	1228	-	65,73,73	1.41	10 (15%)	76,113,113	2.89	24 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	4	606	-	50,58,73	1.53	7 (14%)	58,95,113	2.23	17 (29%)
22	CLA	B	1225	-	65,73,73	1.40	7 (10%)	76,113,113	1.90	14 (18%)
24	BCR	K	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.34	17 (30%)
38	LUT	6	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.26	15 (29%)
22	CLA	5	618	16	52,60,73	1.53	8 (15%)	60,97,113	2.13	19 (31%)
37	ECH	M	4001	-	42,42,42	1.19	3 (7%)	55,58,58	2.03	15 (27%)
22	CLA	B	1021	-	65,73,73	1.41	7 (10%)	76,113,113	1.95	16 (21%)
22	CLA	G	1603	-	45,53,73	1.61	8 (17%)	52,89,113	2.06	12 (23%)
22	CLA	4	601	-	60,68,73	1.42	6 (10%)	70,107,113	2.09	18 (25%)
22	CLA	3	616	-	56,64,73	1.48	7 (12%)	65,102,113	2.05	17 (26%)
31	PTY	5	802	-	37,37,49	0.98	4 (10%)	40,42,54	1.18	2 (5%)
43	PLM	4	803	-	16,16,17	0.44	0	15,15,17	0.69	0
22	CLA	5	605	-	46,54,73	1.63	7 (15%)	53,90,113	2.13	15 (28%)
39	CHL	1	609	13	66,74,74	0.97	6 (9%)	73,114,114	1.33	12 (16%)
22	CLA	8	615	-	46,54,73	1.59	7 (15%)	53,90,113	2.13	15 (28%)
22	CLA	7	611	-	60,68,73	1.37	8 (13%)	70,107,113	2.21	22 (31%)
22	CLA	L	1501	-	50,58,73	1.56	8 (16%)	58,95,113	2.38	18 (31%)
22	CLA	A	1115	-	60,68,73	1.44	8 (13%)	70,107,113	2.06	17 (24%)
22	CLA	L	1503	-	45,53,73	1.65	9 (20%)	52,89,113	2.32	20 (38%)
38	LUT	8	501	-	42,43,43	2.37	2 (4%)	51,60,60	1.83	14 (27%)
22	CLA	1	612	13	65,73,73	1.36	7 (10%)	76,113,113	1.95	15 (19%)
22	CLA	6	609	17	65,73,73	1.34	8 (12%)	76,113,113	1.99	16 (21%)
24	BCR	5	503	-	41,41,41	1.85	5 (12%)	56,56,56	4.32	18 (32%)
25	LHG	8	801	22	36,36,48	0.46	0	39,42,54	1.22	4 (10%)
38	LUT	5	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.03	15 (29%)
22	CLA	B	1224	-	65,73,73	1.38	8 (12%)	76,113,113	1.98	17 (22%)
22	CLA	3	618	-	46,54,73	1.64	8 (17%)	53,90,113	2.12	12 (22%)
22	CLA	8	603	19	65,73,73	1.36	8 (12%)	76,113,113	2.14	19 (25%)
24	BCR	L	4003	-	41,41,41	1.88	4 (9%)	56,56,56	4.35	15 (26%)
28	SF4	C	3003	3	0,12,12	-	-	-	-	-
25	LHG	7	803	-	42,42,48	0.39	0	45,48,54	1.07	2 (4%)
24	BCR	3	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.26	15 (26%)
22	CLA	A	1141	25	45,53,73	1.62	8 (17%)	52,89,113	2.17	12 (23%)
22	CLA	8	609	19	60,68,73	1.42	7 (11%)	70,107,113	2.06	15 (21%)
39	CHL	6	611	-	51,59,74	1.07	3 (5%)	55,96,114	1.46	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	1106	1	65,73,73	1.34	7 (10%)	76,113,113	2.04	15 (19%)
22	CLA	a	611	-	50,58,73	1.56	7 (14%)	58,95,113	2.18	17 (29%)
22	CLA	5	609	16	51,59,73	1.54	8 (15%)	59,96,113	2.24	17 (28%)
38	LUT	a	502	-	42,43,43	2.37	2 (4%)	51,60,60	1.99	14 (27%)
22	CLA	A	1012	-	65,73,73	1.39	7 (10%)	76,113,113	1.92	14 (18%)
22	CLA	B	1207	-	60,68,73	1.43	7 (11%)	70,107,113	2.02	17 (24%)
44	DGA	8	803	-	29,29,43	1.25	2 (6%)	31,31,45	1.16	2 (6%)
22	CLA	a	602	-	50,58,73	1.56	8 (16%)	58,95,113	2.19	16 (27%)
22	CLA	3	612	-	65,73,73	1.37	7 (10%)	76,113,113	1.94	15 (19%)
38	LUT	1	502	-	42,43,43	2.28	1 (2%)	51,60,60	2.05	16 (31%)
22	CLA	4	608	-	51,59,73	1.54	8 (15%)	59,96,113	2.26	18 (30%)
39	CHL	a	610	-	48,56,74	1.00	3 (6%)	51,92,114	1.45	11 (21%)
22	CLA	K	1404	9	52,60,73	1.53	9 (17%)	60,97,113	2.22	18 (30%)
39	CHL	5	610	-	66,74,74	0.89	3 (4%)	73,114,114	1.28	12 (16%)
22	CLA	G	1601	-	50,58,73	1.56	7 (14%)	58,95,113	2.23	17 (29%)
22	CLA	B	1238	-	65,73,73	1.36	7 (10%)	76,113,113	1.98	16 (21%)
30	PCW	B	5004	-	29,29,53	1.32	3 (10%)	35,37,61	0.95	1 (2%)
24	BCR	B	4002	-	41,41,41	1.86	4 (9%)	56,56,56	4.35	13 (23%)
22	CLA	A	1013	-	65,73,73	1.36	7 (10%)	76,113,113	2.00	20 (26%)
24	BCR	I	4001	-	41,41,41	1.84	4 (9%)	56,56,56	4.21	17 (30%)
22	CLA	7	606	-	55,63,73	1.45	7 (12%)	64,101,113	2.10	19 (29%)
22	CLA	4	604	15	60,68,73	1.44	9 (15%)	70,107,113	2.01	17 (24%)
24	BCR	B	4001	-	41,41,41	1.85	5 (12%)	56,56,56	4.28	16 (28%)
22	CLA	7	617	18	54,62,73	1.49	7 (12%)	63,100,113	2.16	16 (25%)
22	CLA	7	615	18	55,63,73	1.47	7 (12%)	64,101,113	2.02	15 (23%)

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	CHL	4	613	-	3/3/17/26	7/23/121/137	-
39	CHL	5	613	-	4/4/18/26	5/27/125/137	-
22	CLA	a	608	-	1/1/13/20	13/25/103/115	-
24	BCR	A	4005	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	608	-	1/1/11/20	6/13/91/115	-
22	CLA	B	1216	-	1/1/14/20	21/33/111/115	-
22	CLA	A	1119	-	1/1/15/20	17/37/115/115	-
25	LHG	4	801	22	-	37/53/53/53	-
22	CLA	B	1211	-	1/1/13/20	12/25/103/115	-
22	CLA	K	1402	-	1/1/14/20	13/31/109/115	-
22	CLA	8	607	25	1/1/11/20	6/15/93/115	-
22	CLA	4	603	15	1/1/13/20	14/27/105/115	-
22	CLA	B	1234	-	1/1/13/20	13/27/105/115	-
22	CLA	5	616	-	1/1/11/20	7/15/93/115	-
22	CLA	6	603	-	1/1/15/20	19/37/115/115	-
22	CLA	a	612	13	1/1/13/20	10/28/106/115	-
22	CLA	1	603	-	1/1/15/20	22/37/115/115	-
39	CHL	3	608	-	4/4/15/26	3/12/110/137	-
22	CLA	F	1301	6	1/1/12/20	6/19/97/115	-
23	PQN	A	2001	-	-	9/23/43/43	0/2/2/2
22	CLA	B	1203	-	1/1/15/20	17/37/115/115	-
25	LHG	7	801	22	-	27/53/53/53	-
48	C7Z	7	504	-	1/1/12/26	8/29/67/67	0/2/2/2
22	CLA	B	1229	-	1/1/15/20	11/37/115/115	-
22	CLA	8	612	19	1/1/11/20	8/15/93/115	-
22	CLA	5	612	16	1/1/15/20	20/37/115/115	-
24	BCR	F	4001	-	-	9/29/63/63	0/2/2/2
22	CLA	1	601	13	1/1/14/20	9/31/109/115	-
40	OLA	8	809	-	-	8/17/17/17	-
31	PTY	3	802	-	-	24/41/41/53	-
22	CLA	6	615	-	1/1/15/20	22/37/115/115	-
22	CLA	K	1401	-	1/1/11/20	7/15/93/115	-
25	LHG	3	801	22	-	33/53/53/53	-
22	CLA	B	1201	-	1/1/15/20	17/37/115/115	-
22	CLA	4	605	-	1/1/11/20	6/15/93/115	-
22	CLA	6	606	-	1/1/12/20	12/22/100/115	-
22	CLA	3	603	-	1/1/15/20	19/37/115/115	-
22	CLA	A	1103	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	A	1137	-	1/1/14/20	12/31/109/115	-
22	CLA	8	618	-	1/1/14/20	15/31/109/115	-
30	PCW	6	803	-	-	19/39/39/57	-
38	LUT	1	501	-	-	3/29/67/67	0/2/2/2
22	CLA	A	1129	-	1/1/12/20	12/19/97/115	-
22	CLA	B	1232	-	1/1/11/20	5/13/91/115	-
22	CLA	A	1104	-	1/1/15/20	19/37/115/115	-
29	LMT	1	804	-	-	10/21/61/61	0/2/2/2
24	BCR	4	503	-	-	15/29/63/63	0/2/2/2
24	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
22	CLA	1	602	-	1/1/11/20	7/13/91/115	-
25	LHG	a	801	-	-	25/39/39/53	-
22	CLA	1	605	-	1/1/15/20	16/37/115/115	-
43	PLM	6	804	-	-	6/15/15/15	-
22	CLA	A	1126	-	1/1/15/20	24/37/115/115	-
22	CLA	8	606	-	1/1/13/20	14/28/106/115	-
45	SPH	6	806	-	-	13/21/21/21	-
36	LPX	J	5001	-	-	11/18/18/31	-
22	CLA	6	607	25	1/1/13/20	9/25/103/115	-
25	LHG	F	5002	-	-	28/40/40/53	-
22	CLA	A	1138	-	1/1/15/20	16/37/115/115	-
22	CLA	1	607	-	1/1/15/20	14/37/115/115	-
22	CLA	K	1403	9	1/1/11/20	8/15/93/115	-
22	CLA	7	612	-	1/1/14/20	19/31/109/115	-
22	CLA	A	1125	-	1/1/15/20	22/37/115/115	-
22	CLA	5	617	-	1/1/12/20	11/19/97/115	-
22	CLA	7	604	-	1/1/15/20	18/37/115/115	-
22	CLA	B	1022	-	1/1/15/20	13/37/115/115	-
22	CLA	4	611	-	1/1/13/20	9/27/105/115	-
39	CHL	4	618	15	4/4/18/26	7/27/125/137	-
22	CLA	A	1114	-	1/1/15/20	17/37/115/115	-
33	SQD	7	805	-	-	14/34/54/69	0/1/1/1
33	SQD	G	5001	-	-	21/41/61/69	0/1/1/1
22	CLA	B	1231	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	DGA	5	803	-	-	13/24/24/45	-
22	CLA	4	602	15	1/1/12/20	5/22/100/115	-
31	PTY	8	810	-	-	19/38/38/53	-
24	BCR	B	4005	-	-	12/29/63/63	0/2/2/2
22	CLA	a	605	-	1/1/15/20	10/37/115/115	-
22	CLA	B	1222	-	1/1/13/20	5/29/107/115	-
22	CLA	1	604	-	1/1/15/20	20/37/115/115	-
22	CLA	A	1105	-	1/1/13/20	8/28/106/115	-
27	3PH	A	5007	-	-	10/34/34/49	-
22	CLA	A	1121	-	1/1/13/20	14/28/106/115	-
26	DGD	A	5005	-	-	20/40/80/95	0/2/2/2
22	CLA	A	1113	-	1/1/12/20	11/22/100/115	-
39	CHL	3	611	-	3/3/17/26	4/26/124/137	-
22	CLA	B	1226	-	1/1/15/20	14/37/115/115	-
24	BCR	B	4003	-	-	7/29/63/63	0/2/2/2
22	CLA	a	615	13	1/1/11/20	5/15/93/115	-
22	CLA	5	614	-	1/1/11/20	4/15/93/115	-
46	XAT	7	502	-	3/3/12/26	1/31/93/93	0/4/4/4
22	CLA	7	610	-	1/1/13/20	10/25/103/115	-
22	CLA	8	610	-	1/1/13/20	15/25/103/115	-
25	LHG	B	5002	-	-	37/53/53/53	-
24	BCR	6	504	-	-	9/29/63/63	0/2/2/2
31	PTY	B	5005	-	-	22/44/44/53	-
22	CLA	A	1136	-	1/1/15/20	18/37/115/115	-
22	CLA	A	1108	-	1/1/15/20	17/37/115/115	-
22	CLA	B	1209	-	1/1/15/20	18/37/115/115	-
22	CLA	3	602	14	1/1/11/20	8/15/93/115	-
31	PTY	7	804	-	-	17/36/36/53	-
22	CLA	3	604	-	1/1/14/20	13/31/109/115	-
22	CLA	8	611	-	1/1/12/20	7/19/97/115	-
22	CLA	A	1135	-	1/1/15/20	20/37/115/115	-
35	RRX	J	4002	-	1/1/11/25	12/29/65/65	0/2/2/2
22	CLA	7	603	-	1/1/15/20	21/37/115/115	-
22	CLA	6	602	17	1/1/12/20	4/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
22	CLA	A	1139	-	1/1/13/20	15/25/103/115	-
22	CLA	6	604	-	1/1/15/20	21/37/115/115	-
22	CLA	7	608	-	1/1/10/20	7/10/88/115	-
22	CLA	5	606	-	1/1/12/20	7/19/97/115	-
22	CLA	A	1123	-	1/1/15/20	15/37/115/115	-
24	BCR	L	4002	-	-	8/29/63/63	0/2/2/2
32	LAP	K	5001	-	-	19/30/30/30	-
32	LAP	B	5007	-	-	19/30/30/30	-
21	CL0	A	1011	-	3/3/20/25	13/37/135/135	-
40	OLA	1	803	-	-	8/17/17/17	-
22	CLA	4	612	15	1/1/14/20	16/34/112/115	-
22	CLA	G	1602	-	1/1/11/20	7/15/93/115	-
22	CLA	1	606	-	1/1/13/20	13/28/106/115	-
22	CLA	6	612	-	1/1/12/20	12/19/97/115	-
26	DGD	8	802	-	-	26/55/95/95	0/2/2/2
22	CLA	A	1117	-	1/1/15/20	21/37/115/115	-
22	CLA	B	1206	2	1/1/13/20	13/25/103/115	-
22	CLA	A	1128	-	1/1/15/20	15/37/115/115	-
39	CHL	4	609	15	4/4/20/26	19/39/137/137	-
22	CLA	4	616	-	1/1/12/20	8/19/97/115	-
24	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
24	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
22	CLA	5	602	-	1/1/12/20	8/22/100/115	-
41	QTB	3	506	-	2/2/5/10	3/11/28/28	0/1/1/1
26	DGD	B	5003	-	-	19/55/95/95	0/2/2/2
22	CLA	B	1214	-	1/1/14/20	19/34/112/115	-
22	CLA	B	1215	-	1/1/14/20	20/31/109/115	-
22	CLA	A	1130	-	1/1/13/20	11/27/105/115	-
38	LUT	8	502	-	-	3/29/67/67	0/2/2/2
22	CLA	5	604	-	1/1/15/20	12/37/115/115	-
38	LUT	1	503	-	1/1/12/27	8/29/67/67	0/2/2/2
39	CHL	8	601	19	4/4/19/26	10/33/131/137	-
39	CHL	8	613	-	3/3/17/26	2/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1223	-	1/1/15/20	14/37/115/115	-
22	CLA	B	1213	-	1/1/14/20	17/31/109/115	-
24	BCR	G	4001	-	-	10/29/63/63	0/2/2/2
25	LHG	A	5003	-	-	31/46/46/53	-
24	BCR	5	504	-	-	9/29/63/63	0/2/2/2
22	CLA	6	618	-	1/1/11/20	9/15/93/115	-
24	BCR	B	4006	-	-	13/29/63/63	0/2/2/2
39	CHL	5	611	-	3/3/17/26	6/21/119/137	-
22	CLA	3	606	-	1/1/15/20	12/37/115/115	-
24	BCR	6	503	-	-	14/29/63/63	0/2/2/2
24	BCR	K	4002	-	-	12/29/63/63	0/2/2/2
22	CLA	B	1023	-	1/1/15/20	19/37/115/115	-
22	CLA	B	1230	-	1/1/13/20	13/29/107/115	-
22	CLA	4	615	15	1/1/14/20	14/31/109/115	-
38	LUT	5	505	-	1/1/12/27	9/29/67/67	0/2/2/2
22	CLA	A	1109	22	1/1/15/20	23/37/115/115	-
47	4RF	8	808	-	-	25/56/56/59	-
22	CLA	A	1116	-	1/1/14/20	16/31/109/115	-
22	CLA	1	610	-	1/1/11/20	4/13/91/115	-
24	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
39	CHL	a	609	13	3/3/17/26	4/24/122/137	-
25	LHG	A	5002	-	-	34/53/53/53	-
22	CLA	B	1237	-	1/1/15/20	17/37/115/115	-
22	CLA	B	1212	-	1/1/15/20	21/37/115/115	-
22	CLA	8	608	-	1/1/12/20	12/22/100/115	-
38	LUT	4	502	-	-	3/29/67/67	0/2/2/2
22	CLA	5	603	-	1/1/13/20	16/27/105/115	-
38	LUT	4	501	-	-	2/29/67/67	0/2/2/2
22	CLA	A	1122	-	1/1/15/20	19/37/115/115	-
22	CLA	8	620	19	1/1/15/20	17/37/115/115	-
25	LHG	4	802	-	-	19/36/36/53	-
42	GG0	a	805	-	-	2/7/7/7	-
25	LHG	B	5001	22	-	29/50/50/53	-
28	SF4	A	3001	1,2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	LUT	6	502	-	1/1/12/27	8/29/67/67	0/2/2/2
22	CLA	1	608	-	1/1/14/20	14/31/109/115	-
22	CLA	1	611	-	1/1/13/20	11/25/103/115	-
25	LHG	6	802	-	-	27/41/41/53	-
39	CHL	6	613	-	3/3/17/26	2/21/119/137	-
39	CHL	6	610	-	4/4/18/26	6/27/125/137	-
38	LUT	3	501	-	-	2/29/67/67	0/2/2/2
22	CLA	3	601	-	1/1/15/20	13/37/115/115	-
22	CLA	3	613	-	1/1/14/20	14/33/111/115	-
25	LHG	F	5001	22	-	31/47/47/53	-
39	CHL	8	604	19	4/4/19/26	13/35/133/137	-
22	CLA	B	1218	-	1/1/13/20	10/25/103/115	-
22	CLA	a	601	13	1/1/14/20	8/31/109/115	-
24	BCR	J	4001	-	-	13/29/63/63	0/2/2/2
47	4RF	8	807	-	-	23/44/44/59	-
22	CLA	3	610	14	1/1/14/20	15/31/109/115	-
22	CLA	4	607	25	1/1/13/20	11/25/103/115	-
36	LPX	a	804	-	-	14/31/31/31	-
38	LUT	a	503	-	-	4/29/67/67	0/2/2/2
24	BCR	7	503	-	-	16/29/63/63	0/2/2/2
24	BCR	8	503	-	-	10/29/63/63	0/2/2/2
22	CLA	B	1227	-	1/1/12/20	8/19/97/115	-
22	CLA	a	603	-	1/1/15/20	14/37/115/115	-
22	CLA	A	1133	-	1/1/15/20	19/37/115/115	-
22	CLA	A	1102	22	1/1/15/20	18/37/115/115	-
38	LUT	7	501	-	1/1/12/27	6/29/67/67	0/2/2/2
38	LUT	a	501	-	-	7/29/67/67	0/2/2/2
22	CLA	B	1208	-	1/1/14/20	11/31/109/115	-
38	LUT	5	502	-	-	1/29/67/67	0/2/2/2
22	CLA	A	1134	1	1/1/14/20	20/31/109/115	-
22	CLA	8	602	19	1/1/12/20	8/22/100/115	-
32	LAP	F	5003	-	-	20/30/30/30	-
22	CLA	A	1112	-	1/1/13/20	9/25/103/115	-
22	CLA	A	1131	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	6	608	-	1/1/11/20	4/13/91/115	-
22	CLA	7	607	25	1/1/13/20	12/29/107/115	-
22	CLA	7	601	-	1/1/14/20	17/31/109/115	-
22	CLA	B	1219	-	1/1/13/20	10/30/108/115	-
22	CLA	B	1202	-	1/1/15/20	14/37/115/115	-
22	CLA	A	1124	-	1/1/13/20	9/25/103/115	-
22	CLA	B	1240	25	1/1/15/20	9/37/115/115	-
24	BCR	3	505	-	-	13/29/63/63	0/2/2/2
22	CLA	6	601	-	1/1/14/20	14/31/109/115	-
22	CLA	3	607	25	1/1/15/20	10/37/115/115	-
22	CLA	A	1132	-	1/1/15/20	17/37/115/115	-
22	CLA	B	1210	-	1/1/15/20	22/37/115/115	-
39	CHL	6	619	17	5/5/20/26	17/39/137/137	-
38	LUT	3	502	-	-	2/29/67/67	0/2/2/2
22	CLA	B	1221	-	1/1/15/20	13/37/115/115	-
41	QTB	a	504	-	-	6/11/28/28	0/1/1/1
22	CLA	1	615	13	1/1/11/20	8/15/93/115	-
22	CLA	B	1236	-	1/1/12/20	13/23/101/115	-
24	BCR	B	4007	-	-	10/29/63/63	0/2/2/2
22	CLA	a	604	13	1/1/15/20	18/37/115/115	-
22	CLA	7	605	-	1/1/11/20	8/11/89/115	-
22	CLA	5	601	16	1/1/14/20	13/31/109/115	-
23	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
22	CLA	B	1239	-	1/1/15/20	18/37/115/115	-
22	CLA	B	1217	-	1/1/13/20	15/27/105/115	-
28	SF4	C	3002	3	-	-	0/6/5/5
29	LMT	A	5008	-	-	7/21/61/61	0/2/2/2
22	CLA	A	1140	-	1/1/13/20	16/25/103/115	-
39	CHL	a	613	-	3/3/16/26	6/15/113/137	-
22	CLA	5	607	25	1/1/13/20	12/25/103/115	-
29	LMT	B	5006	-	-	10/21/61/61	0/2/2/2
22	CLA	A	1101	-	1/1/15/20	23/37/115/115	-
25	LHG	1	802	-	-	29/46/46/53	-
34	ERG	G	5002	-	4/4/11/15	10/13/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	P5S	8	806	-	-	31/42/42/59	-
39	CHL	1	613	-	3/3/16/26	1/18/116/137	-
22	CLA	8	605	-	1/1/11/20	6/13/91/115	-
22	CLA	A	1127	-	1/1/15/20	13/37/115/115	-
22	CLA	A	1107	1	1/1/13/20	8/25/103/115	-
24	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
22	CLA	L	1502	-	1/1/14/20	13/31/109/115	-
25	LHG	A	5001	22	-	20/33/33/53	-
39	CHL	a	606	-	4/4/18/26	8/27/125/137	-
25	LHG	6	801	22	-	29/53/53/53	-
22	CLA	A	1111	-	1/1/15/20	25/37/115/115	-
22	CLA	J	1901	8	1/1/10/20	5/10/88/115	-
22	CLA	a	607	-	1/1/13/20	10/29/107/115	-
22	CLA	F	1302	25	1/1/13/20	12/25/103/115	-
22	CLA	B	1204	-	1/1/15/20	25/37/115/115	-
22	CLA	A	1110	-	1/1/14/20	15/31/109/115	-
22	CLA	B	1205	-	1/1/15/20	14/37/115/115	-
22	CLA	7	609	-	1/1/14/20	14/31/109/115	-
25	LHG	7	802	-	-	23/40/40/53	-
22	CLA	A	1120	-	1/1/11/20	9/18/96/115	-
22	CLA	4	617	-	1/1/11/20	5/13/91/115	-
22	CLA	A	1118	-	1/1/13/20	15/25/103/115	-
39	CHL	7	613	-	4/4/20/26	10/39/137/137	-
22	CLA	7	602	-	1/1/10/20	7/11/90/115	-
24	BCR	3	503	-	-	9/29/63/63	0/2/2/2
22	CLA	B	1220	-	1/1/14/20	17/31/109/115	-
22	CLA	4	610	-	1/1/15/20	19/37/115/115	-
22	CLA	3	605	-	1/1/15/20	14/37/115/115	-
47	4RF	7	807	-	-	20/34/34/59	-
25	LHG	1	801	-	-	26/39/39/53	-
25	LHG	5	801	22	-	30/53/53/53	-
22	CLA	6	605	-	1/1/11/20	5/15/93/115	-
22	CLA	6	617	17	1/1/11/20	4/13/91/115	-
22	CLA	B	1235	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	1228	-	1/1/15/20	18/37/115/115	-
22	CLA	4	606	-	1/1/12/20	5/19/97/115	-
22	CLA	B	1225	-	1/1/15/20	12/37/115/115	-
24	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
38	LUT	6	501	-	1/1/12/27	7/29/67/67	0/2/2/2
22	CLA	5	618	16	1/1/12/20	4/22/100/115	-
37	ECH	M	4001	-	-	9/29/66/66	0/2/2/2
22	CLA	B	1021	-	1/1/15/20	25/37/115/115	-
22	CLA	G	1603	-	1/1/11/20	6/13/91/115	-
22	CLA	4	601	-	1/1/14/20	8/31/109/115	-
22	CLA	3	616	-	1/1/13/20	17/27/105/115	-
31	PTY	5	802	-	-	19/41/41/53	-
43	PLM	4	803	-	-	8/13/14/15	-
22	CLA	5	605	-	1/1/11/20	6/15/93/115	-
39	CHL	1	609	13	4/4/20/26	14/39/137/137	-
22	CLA	8	615	-	1/1/11/20	6/15/93/115	-
22	CLA	7	611	-	1/1/14/20	10/31/109/115	-
22	CLA	L	1501	-	1/1/12/20	8/19/97/115	-
22	CLA	A	1115	-	1/1/14/20	10/31/109/115	-
22	CLA	L	1503	-	1/1/11/20	8/13/91/115	-
38	LUT	8	501	-	-	2/29/67/67	0/2/2/2
22	CLA	1	612	13	1/1/15/20	16/37/115/115	-
22	CLA	6	609	17	1/1/15/20	22/37/115/115	-
24	BCR	5	503	-	-	16/29/63/63	0/2/2/2
25	LHG	8	801	22	-	27/41/41/53	-
38	LUT	5	501	-	-	1/29/67/67	0/2/2/2
22	CLA	B	1224	-	1/1/15/20	25/37/115/115	-
22	CLA	3	618	-	1/1/11/20	6/15/93/115	-
22	CLA	8	603	19	1/1/15/20	22/37/115/115	-
24	BCR	L	4003	-	-	9/29/63/63	0/2/2/2
28	SF4	C	3003	3	-	-	0/6/5/5
25	LHG	7	803	-	-	28/47/47/53	-
24	BCR	3	504	-	-	12/29/63/63	0/2/2/2
22	CLA	A	1141	25	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	8	609	19	1/1/14/20	22/31/109/115	-
39	CHL	6	611	-	3/3/17/26	3/21/119/137	-
22	CLA	A	1106	1	1/1/15/20	20/37/115/115	-
22	CLA	a	611	-	1/1/12/20	8/19/97/115	-
22	CLA	5	609	16	1/1/12/20	9/21/99/115	-
38	LUT	a	502	-	1/1/12/27	11/29/67/67	0/2/2/2
22	CLA	A	1012	-	1/1/15/20	12/37/115/115	-
22	CLA	B	1207	-	1/1/14/20	21/31/109/115	-
44	DGA	8	803	-	-	12/31/31/45	-
22	CLA	a	602	-	1/1/12/20	6/19/97/115	-
22	CLA	3	612	-	1/1/15/20	15/37/115/115	-
38	LUT	1	502	-	-	2/29/67/67	0/2/2/2
22	CLA	4	608	-	1/1/12/20	9/21/99/115	-
39	CHL	a	610	-	3/3/16/26	6/18/116/137	-
22	CLA	K	1404	9	1/1/12/20	9/22/100/115	-
39	CHL	5	610	-	4/4/20/26	9/39/137/137	-
22	CLA	G	1601	-	1/1/12/20	12/19/97/115	-
22	CLA	B	1238	-	1/1/15/20	11/37/115/115	-
30	PCW	B	5004	-	-	15/33/33/57	-
24	BCR	B	4002	-	-	13/29/63/63	0/2/2/2
22	CLA	A	1013	-	1/1/15/20	15/37/115/115	-
24	BCR	I	4001	-	-	10/29/63/63	0/2/2/2
22	CLA	7	606	-	1/1/13/20	9/25/103/115	-
22	CLA	4	604	15	1/1/14/20	13/31/109/115	-
24	BCR	B	4001	-	-	15/29/63/63	0/2/2/2
22	CLA	7	617	18	1/1/13/20	13/23/101/115	-
22	CLA	7	615	18	1/1/13/20	13/25/103/115	-

The worst 5 of 1936 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	G	5002	ERG	C1-C10	-24.25	1.08	1.54
34	G	5002	ERG	C10-C9	-22.01	1.26	1.55
48	7	504	C7Z	C25-C26	15.87	1.61	1.34
34	G	5002	ERG	C10-C5	-15.71	1.21	1.52
35	J	4002	RRX	C26-C25	15.66	1.61	1.34

The worst 5 of 4631 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	4001	BCR	C10-C11-C12	18.04	179.50	123.22
24	A	4004	BCR	C10-C11-C12	17.82	178.83	123.22
24	A	4002	BCR	C10-C11-C12	17.72	178.51	123.22
24	4	503	BCR	C10-C11-C12	17.70	178.47	123.22
24	F	4001	BCR	C10-C11-C12	17.67	178.36	123.22

5 of 299 chirality outliers are listed below:

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

5 of 4397 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	1011	CL0	C2-C1-O2A-CGA
22	A	1013	CLA	CHA-CBD-CGD-O1D
22	A	1013	CLA	CHA-CBD-CGD-O2D
22	A	1013	CLA	CBD-CGD-O2D-CED
22	A	1102	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

307 monomers are involved in 1582 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	4	613	CHL	3	0
39	5	613	CHL	4	0
24	A	4005	BCR	3	0
22	5	608	CLA	3	0
22	B	1216	CLA	5	0
22	A	1119	CLA	6	0
25	4	801	LHG	15	0
22	B	1211	CLA	4	0
22	K	1402	CLA	6	0
22	8	607	CLA	2	0
22	4	603	CLA	4	0
22	B	1234	CLA	10	0
22	5	616	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	6	603	CLA	6	0
22	1	603	CLA	8	0
39	3	608	CHL	2	0
22	F	1301	CLA	5	0
23	A	2001	PQN	6	0
22	B	1203	CLA	7	0
25	7	801	LHG	6	0
48	7	504	C7Z	4	0
22	B	1229	CLA	5	0
22	8	612	CLA	6	0
22	5	612	CLA	11	0
24	F	4001	BCR	5	0
22	1	601	CLA	7	0
40	8	809	OLA	4	0
31	3	802	PTY	5	0
22	6	615	CLA	4	0
22	K	1401	CLA	3	0
25	3	801	LHG	5	0
22	B	1201	CLA	19	0
22	4	605	CLA	3	0
22	6	606	CLA	2	0
22	3	603	CLA	9	0
22	A	1103	CLA	11	0
22	A	1137	CLA	7	0
22	8	618	CLA	8	0
30	6	803	PCW	3	0
38	1	501	LUT	5	0
22	A	1129	CLA	2	0
22	B	1232	CLA	6	0
22	A	1104	CLA	6	0
29	1	804	LMT	8	0
24	4	503	BCR	3	0
24	L	4001	BCR	16	0
22	1	602	CLA	6	0
22	1	605	CLA	10	0
43	6	804	PLM	1	0
22	A	1126	CLA	12	0
22	8	606	CLA	4	0
45	6	806	SPH	7	0
36	J	5001	LPX	3	0
22	6	607	CLA	11	0
25	F	5002	LHG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	1138	CLA	8	0
22	1	607	CLA	8	0
22	K	1403	CLA	30	0
22	7	612	CLA	10	0
22	A	1125	CLA	8	0
22	5	617	CLA	6	0
22	7	604	CLA	9	0
22	B	1022	CLA	7	0
22	4	611	CLA	1	0
39	4	618	CHL	6	0
22	A	1114	CLA	8	0
33	7	805	SQD	1	0
33	G	5001	SQD	4	0
22	B	1231	CLA	8	0
44	5	803	DGA	3	0
22	4	602	CLA	1	0
31	8	810	PTY	6	0
24	B	4005	BCR	6	0
22	B	1222	CLA	6	0
22	1	604	CLA	12	0
22	A	1105	CLA	4	0
27	A	5007	3PH	1	0
22	A	1121	CLA	7	0
26	A	5005	DGD	3	0
22	A	1113	CLA	4	0
39	3	611	CHL	9	0
22	B	1226	CLA	9	0
24	B	4003	BCR	5	0
46	7	502	XAT	5	0
22	7	610	CLA	4	0
22	8	610	CLA	8	0
25	B	5002	LHG	2	0
24	6	504	BCR	5	0
31	B	5005	PTY	6	0
22	A	1136	CLA	11	0
22	A	1108	CLA	12	0
22	B	1209	CLA	15	0
22	3	602	CLA	4	0
31	7	804	PTY	3	0
22	3	604	CLA	3	0
22	8	611	CLA	3	0
22	A	1135	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	J	4002	RRX	10	0
22	7	603	CLA	5	0
22	6	602	CLA	4	0
24	B	4004	BCR	9	0
22	A	1139	CLA	5	0
22	6	604	CLA	23	0
22	7	608	CLA	5	0
22	5	606	CLA	2	0
22	A	1123	CLA	8	0
24	L	4002	BCR	5	0
32	K	5001	LAP	3	0
32	B	5007	LAP	3	0
21	A	1011	CL0	3	0
40	1	803	OLA	2	0
22	4	612	CLA	5	0
22	G	1602	CLA	4	0
22	1	606	CLA	4	0
22	6	612	CLA	3	0
26	8	802	DGD	13	0
22	A	1117	CLA	6	0
22	B	1206	CLA	7	0
22	A	1128	CLA	4	0
39	4	609	CHL	9	0
22	4	616	CLA	2	0
24	A	4003	BCR	5	0
24	A	4004	BCR	7	0
22	5	602	CLA	2	0
26	B	5003	DGD	10	0
22	B	1214	CLA	7	0
22	B	1215	CLA	6	0
22	A	1130	CLA	8	0
38	8	502	LUT	5	0
22	5	604	CLA	10	0
38	1	503	LUT	8	0
39	8	601	CHL	9	0
39	8	613	CHL	3	0
22	B	1223	CLA	5	0
22	B	1213	CLA	6	0
24	G	4001	BCR	3	0
25	A	5003	LHG	7	0
24	5	504	BCR	5	0
22	6	618	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	B	4006	BCR	1	0
39	5	611	CHL	8	0
22	3	606	CLA	4	0
24	6	503	BCR	11	0
24	K	4002	BCR	1	0
22	B	1023	CLA	14	0
22	B	1230	CLA	5	0
22	4	615	CLA	3	0
38	5	505	LUT	7	0
22	A	1109	CLA	13	0
47	8	808	4RF	13	0
22	A	1116	CLA	8	0
22	1	610	CLA	4	0
24	A	4001	BCR	5	0
25	A	5002	LHG	8	0
22	B	1237	CLA	8	0
22	B	1212	CLA	10	0
22	8	608	CLA	6	0
38	4	502	LUT	4	0
22	5	603	CLA	5	0
38	4	501	LUT	5	0
22	A	1122	CLA	3	0
22	8	620	CLA	6	0
25	4	802	LHG	5	0
25	B	5001	LHG	7	0
38	6	502	LUT	13	0
22	1	608	CLA	4	0
22	1	611	CLA	4	0
25	6	802	LHG	4	0
39	6	613	CHL	19	0
39	6	610	CHL	9	0
38	3	501	LUT	6	0
22	3	601	CLA	13	0
22	3	613	CLA	4	0
25	F	5001	LHG	5	0
39	8	604	CHL	8	0
22	B	1218	CLA	9	0
24	J	4001	BCR	3	0
47	8	807	4RF	3	0
22	3	610	CLA	5	0
22	4	607	CLA	5	0
24	7	503	BCR	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	8	503	BCR	5	0
22	B	1227	CLA	5	0
22	A	1133	CLA	7	0
22	A	1102	CLA	7	0
38	7	501	LUT	4	0
22	B	1208	CLA	8	0
38	5	502	LUT	5	0
22	A	1134	CLA	8	0
22	8	602	CLA	4	0
32	F	5003	LAP	6	0
22	A	1112	CLA	3	0
22	A	1131	CLA	12	0
22	7	601	CLA	6	0
22	B	1219	CLA	5	0
22	B	1202	CLA	6	0
22	A	1124	CLA	4	0
22	B	1240	CLA	7	0
24	3	505	BCR	1	0
22	6	601	CLA	24	0
22	3	607	CLA	8	0
22	A	1132	CLA	4	0
22	B	1210	CLA	10	0
38	3	502	LUT	4	0
39	6	619	CHL	10	0
22	B	1221	CLA	8	0
22	1	615	CLA	4	0
22	B	1236	CLA	7	0
24	B	4007	BCR	3	0
22	7	605	CLA	7	0
22	5	601	CLA	5	0
23	B	2002	PQN	8	0
22	B	1239	CLA	7	0
22	B	1217	CLA	5	0
28	C	3002	SF4	1	0
29	A	5008	LMT	4	0
22	A	1140	CLA	8	0
22	5	607	CLA	3	0
29	B	5006	LMT	2	0
22	A	1101	CLA	7	0
25	1	802	LHG	2	0
34	G	5002	ERG	16	0
39	1	613	CHL	6	0

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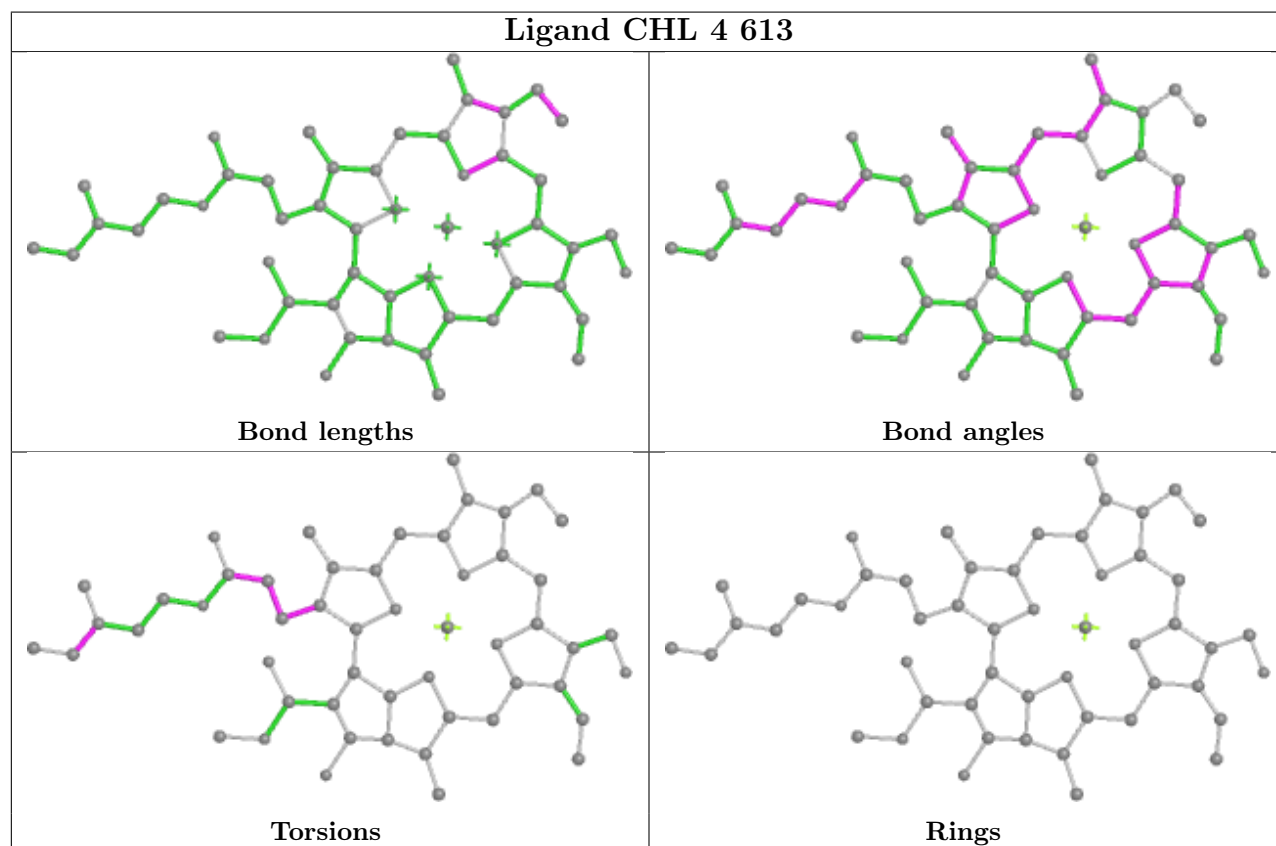
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	8	605	CLA	5	0
22	A	1127	CLA	6	0
22	A	1107	CLA	8	0
24	A	4002	BCR	4	0
22	L	1502	CLA	15	0
25	A	5001	LHG	1	0
25	6	801	LHG	15	0
22	A	1111	CLA	11	0
22	J	1901	CLA	1	0
22	F	1302	CLA	8	0
22	B	1204	CLA	11	0
22	A	1110	CLA	2	0
22	B	1205	CLA	6	0
22	7	609	CLA	5	0
25	7	802	LHG	1	0
22	A	1120	CLA	6	0
22	4	617	CLA	2	0
22	A	1118	CLA	6	0
39	7	613	CHL	6	0
22	7	602	CLA	2	0
24	3	503	BCR	3	0
22	B	1220	CLA	5	0
22	4	610	CLA	8	0
22	3	605	CLA	6	0
47	7	807	4RF	6	0
25	1	801	LHG	3	0
25	5	801	LHG	9	0
22	6	605	CLA	2	0
22	6	617	CLA	14	0
22	B	1235	CLA	10	0
22	B	1228	CLA	9	0
22	4	606	CLA	3	0
22	B	1225	CLA	8	0
24	K	4001	BCR	6	0
38	6	501	LUT	16	0
22	5	618	CLA	9	0
37	M	4001	ECH	6	0
22	B	1021	CLA	13	0
22	G	1603	CLA	7	0
22	4	601	CLA	9	0
22	3	616	CLA	11	0
31	5	802	PTY	2	0

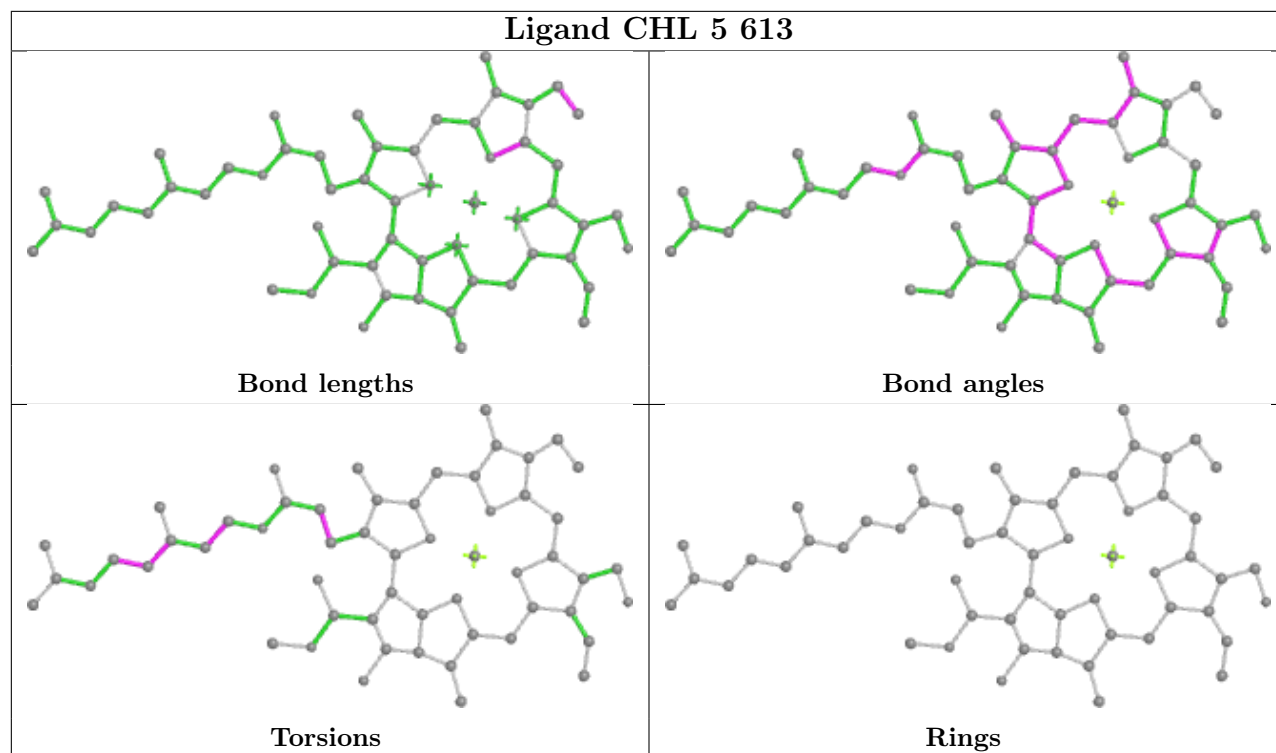
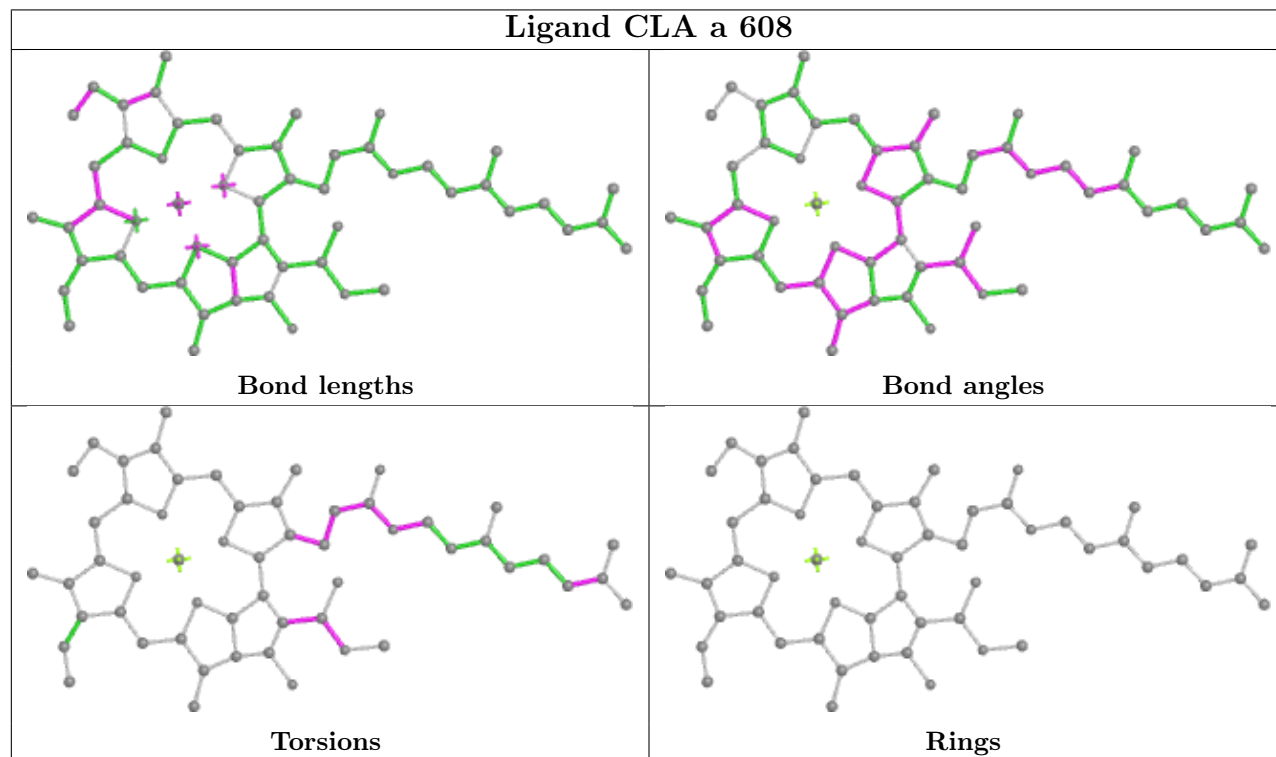
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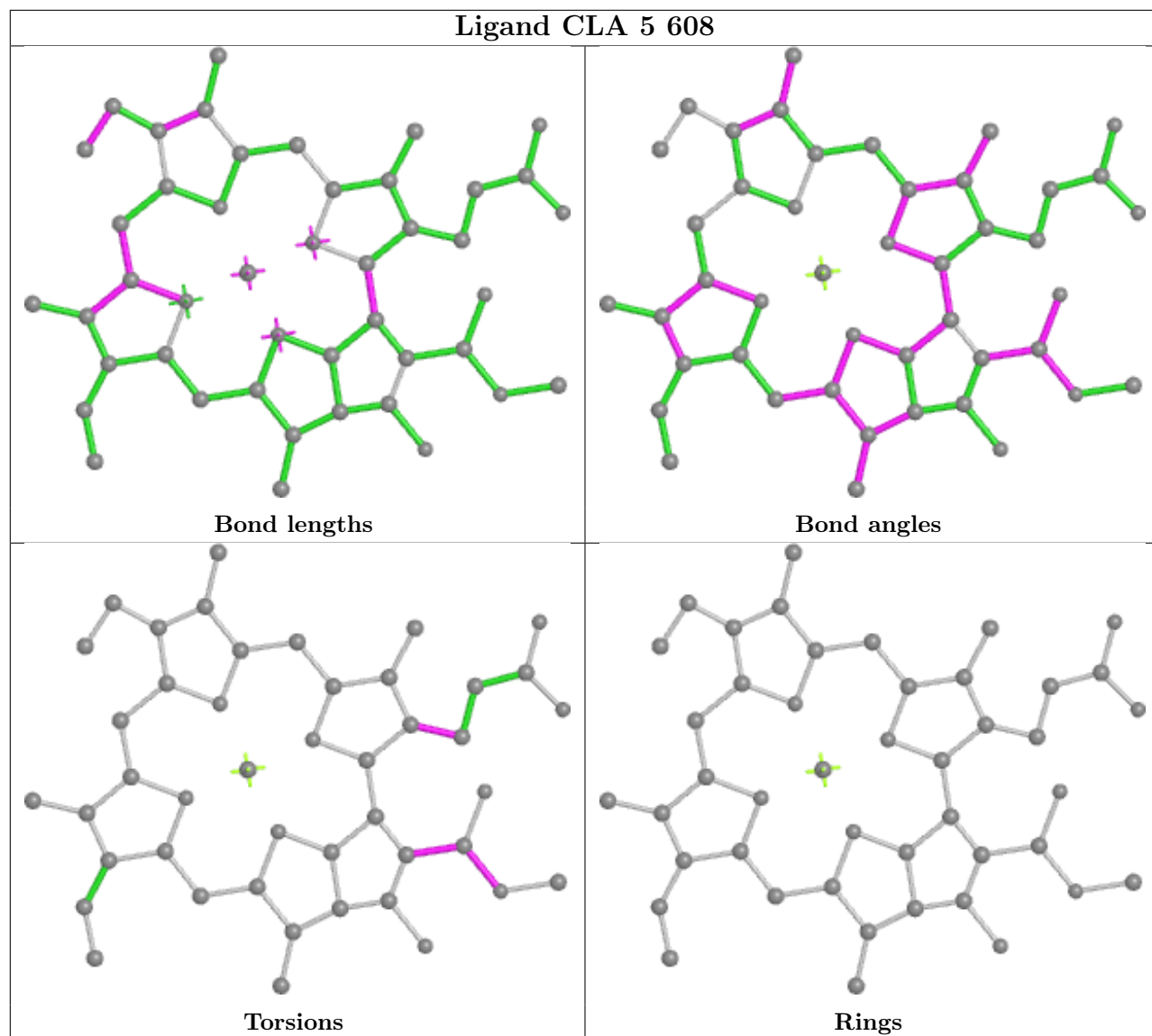
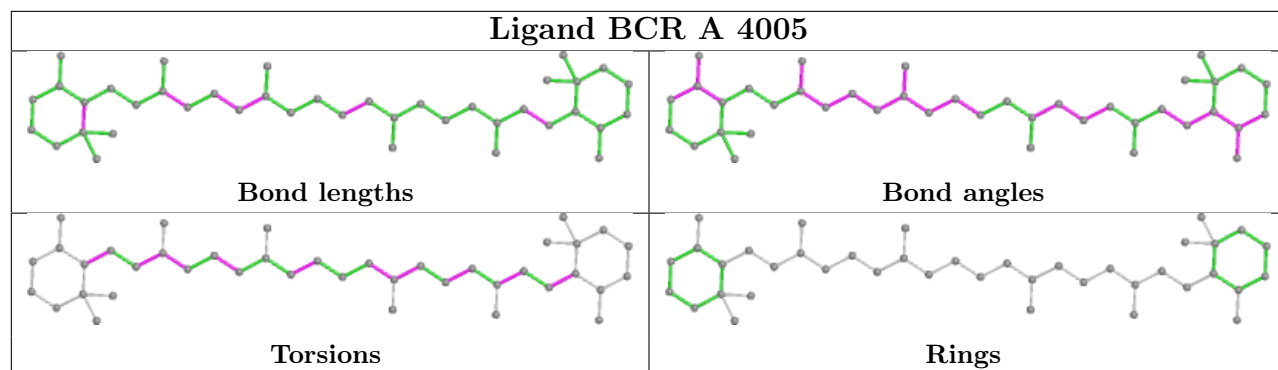
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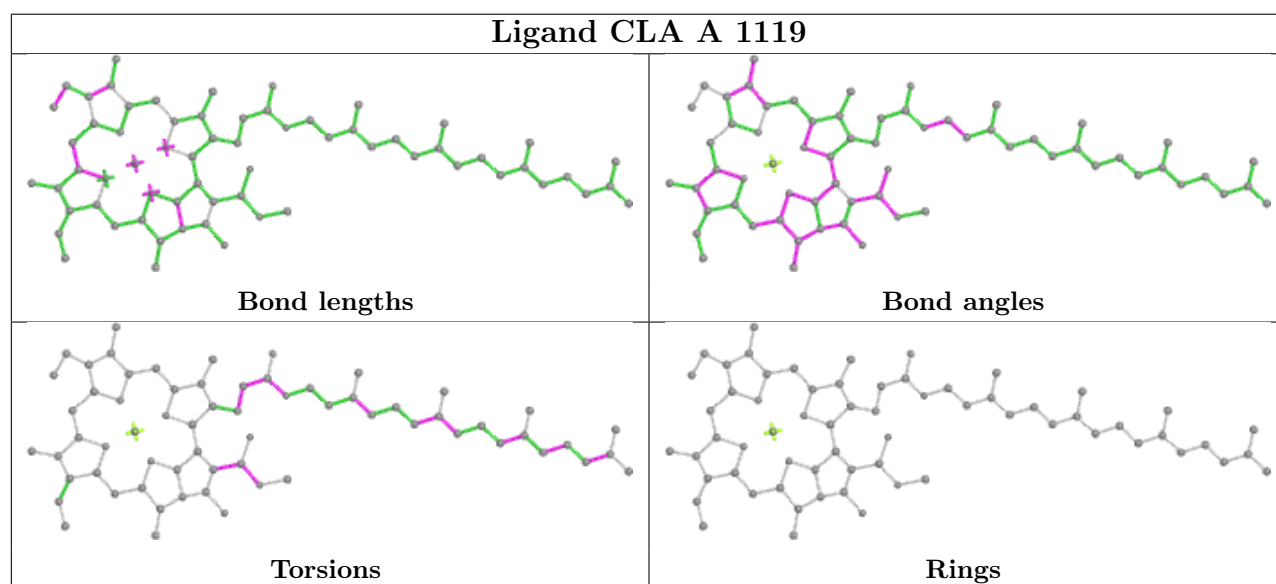
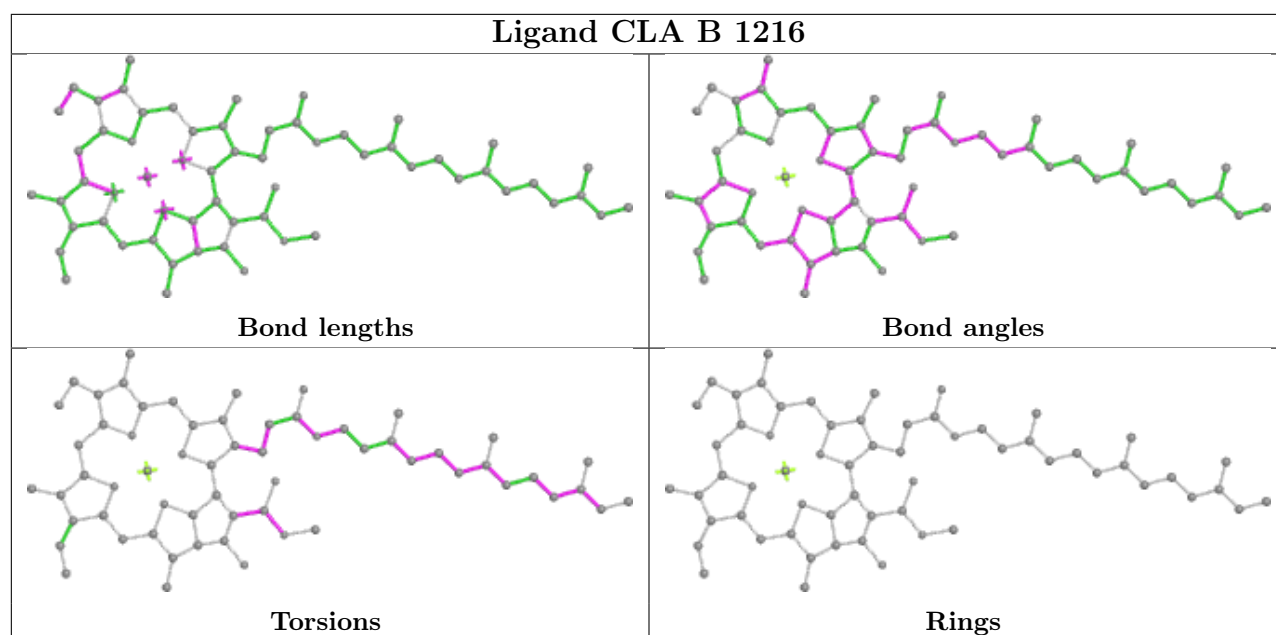
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	5	605	CLA	2	0
39	1	609	CHL	10	0
22	8	615	CLA	3	0
22	7	611	CLA	7	0
22	L	1501	CLA	3	0
22	A	1115	CLA	5	0
22	L	1503	CLA	5	0
38	8	501	LUT	12	0
22	1	612	CLA	10	0
22	6	609	CLA	24	0
24	5	503	BCR	5	0
25	8	801	LHG	5	0
38	5	501	LUT	8	0
22	B	1224	CLA	7	0
22	3	618	CLA	1	0
22	8	603	CLA	4	0
24	L	4003	BCR	2	0
28	C	3003	SF4	1	0
25	7	803	LHG	5	0
24	3	504	BCR	10	0
22	8	609	CLA	8	0
39	6	611	CHL	22	0
22	A	1106	CLA	10	0
22	5	609	CLA	11	0
22	A	1012	CLA	15	0
22	B	1207	CLA	8	0
44	8	803	DGA	5	0
22	3	612	CLA	5	0
38	1	502	LUT	3	0
22	4	608	CLA	5	0
22	K	1404	CLA	2	0
39	5	610	CHL	10	0
22	B	1238	CLA	5	0
30	B	5004	PCW	6	0
24	B	4002	BCR	4	0
22	A	1013	CLA	10	0
24	I	4001	BCR	8	0
22	7	606	CLA	6	0
22	4	604	CLA	8	0
24	B	4001	BCR	7	0
22	7	617	CLA	7	0
22	7	615	CLA	1	0

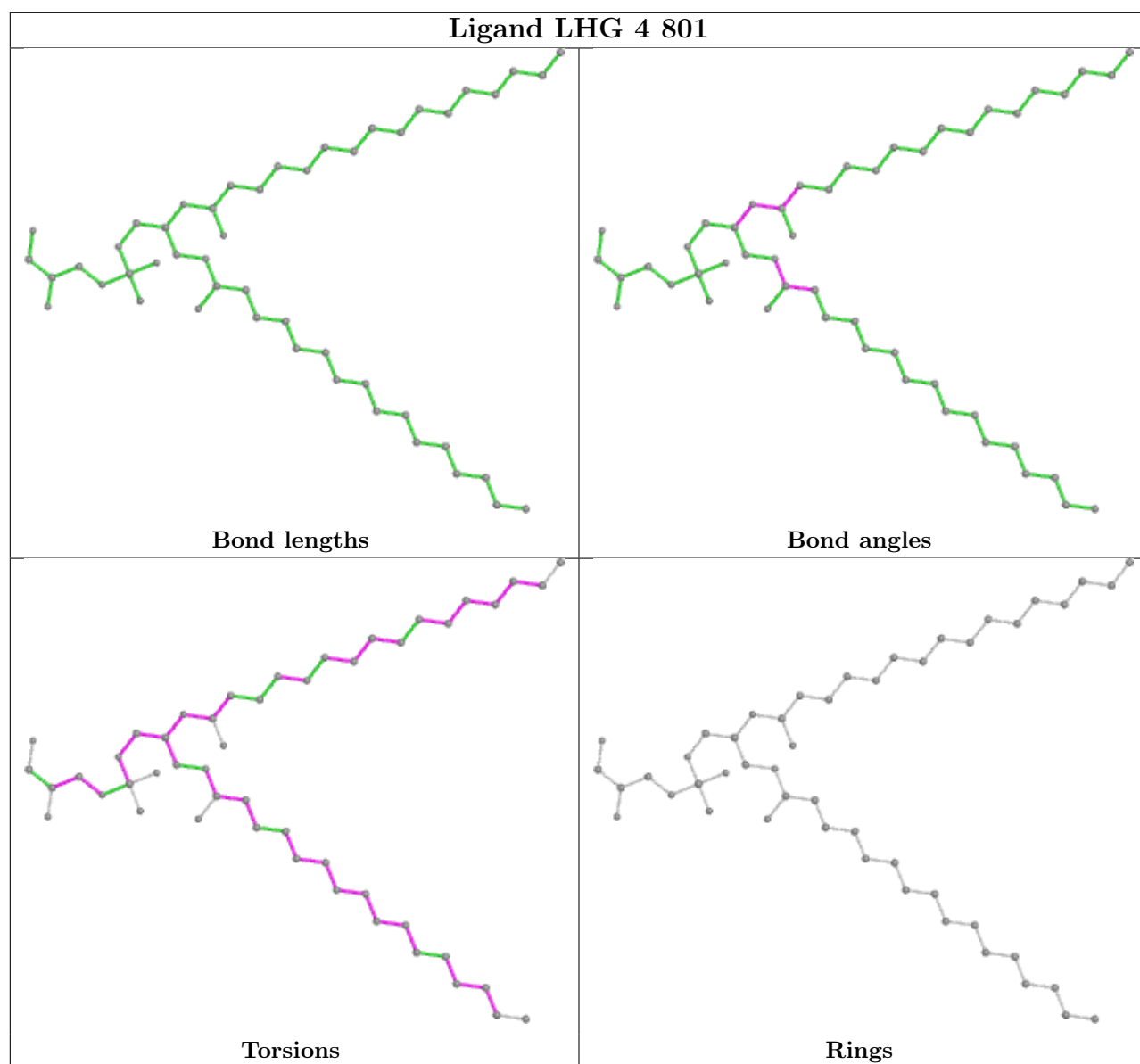
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



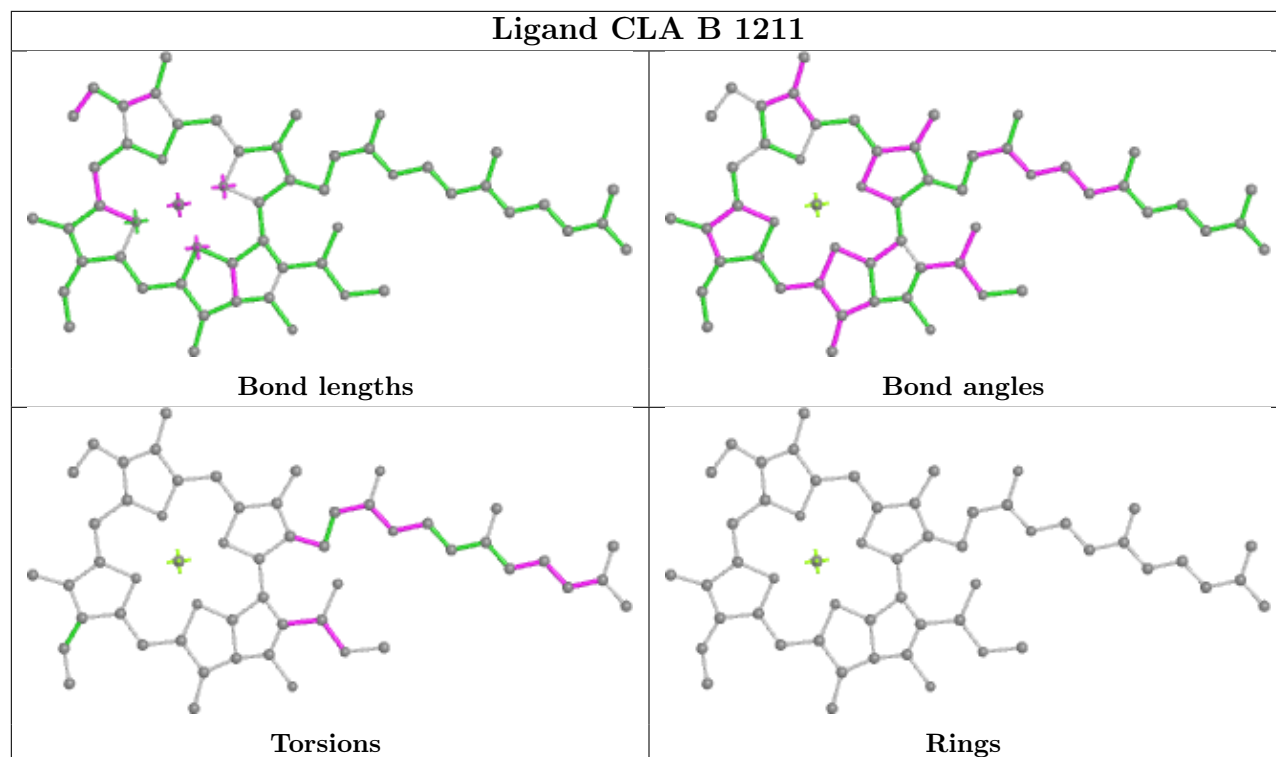
Ligand CHL 5 613**Ligand CLA a 608**



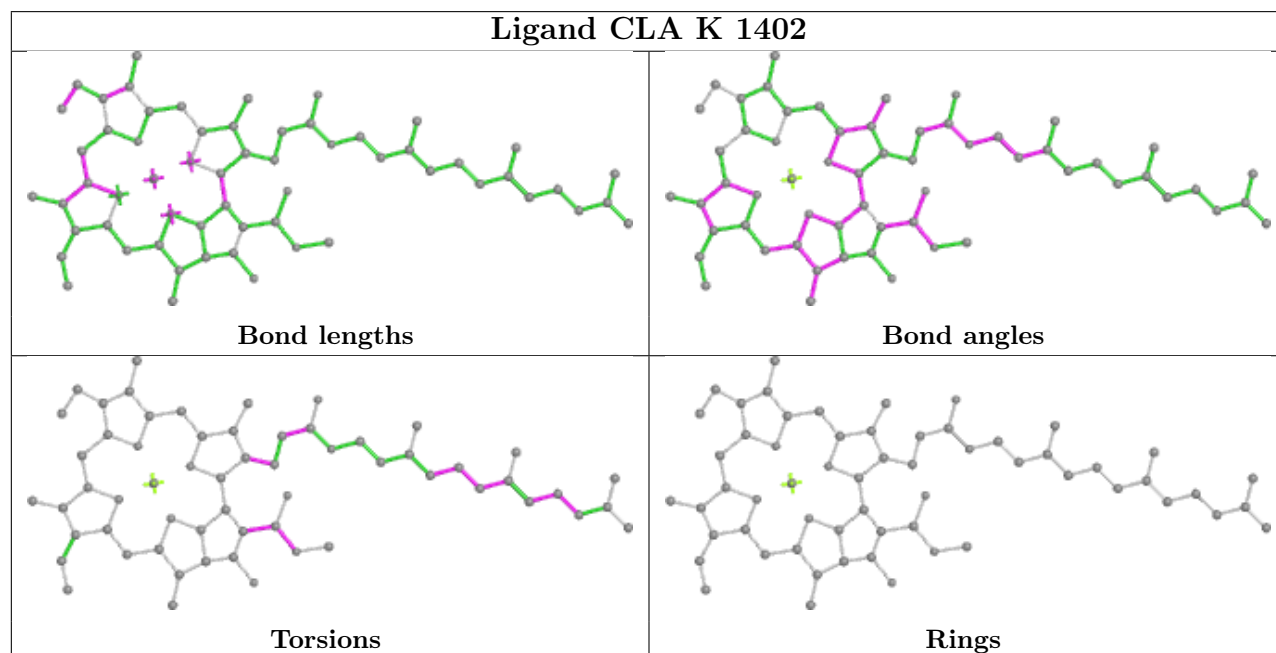




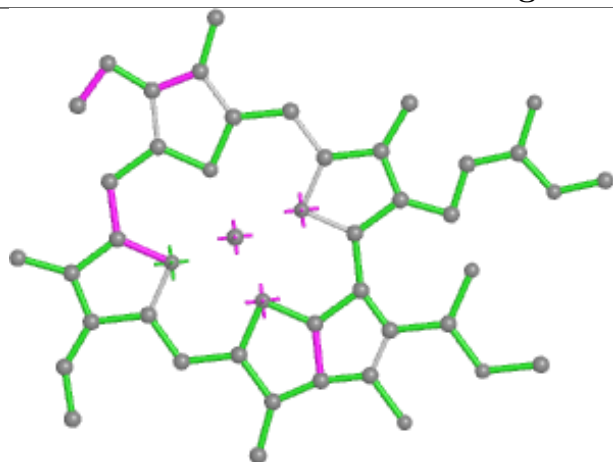
Ligand CLA B 1211



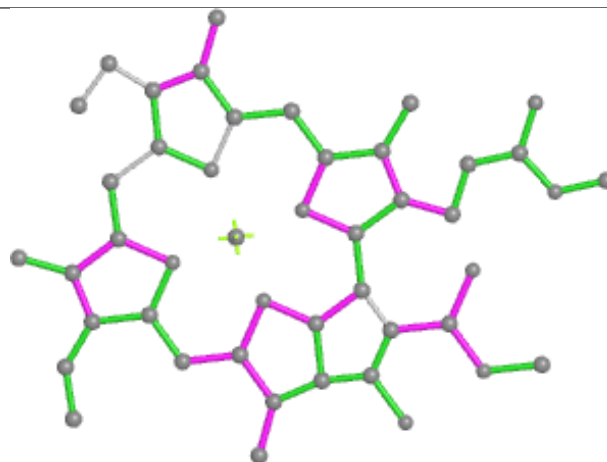
Ligand CLA K 1402



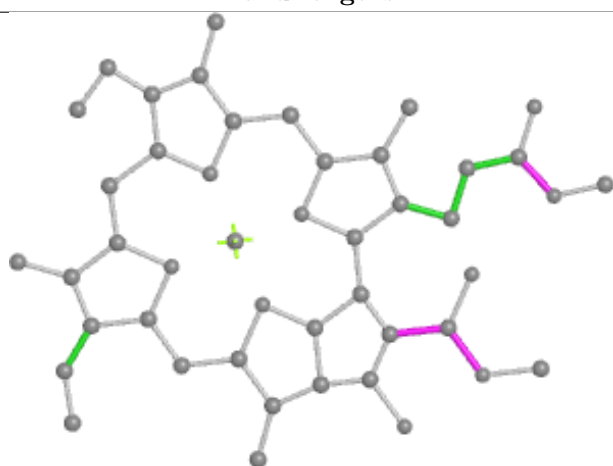
Ligand CLA 8 607



Bond lengths



Bond angles

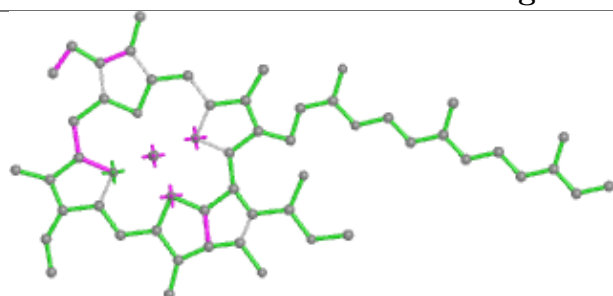


Torsions

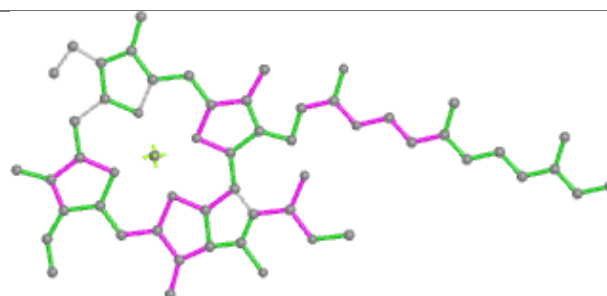


Rings

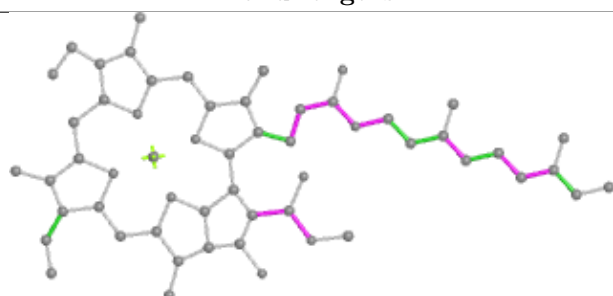
Ligand CLA 4 603



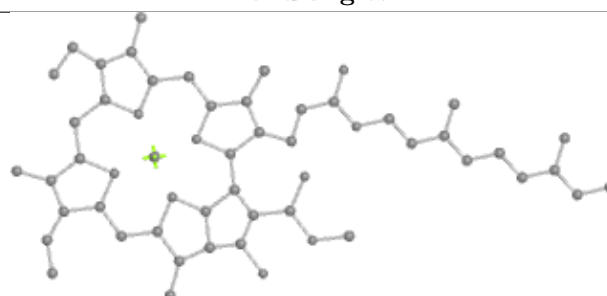
Bond lengths



Bond angles

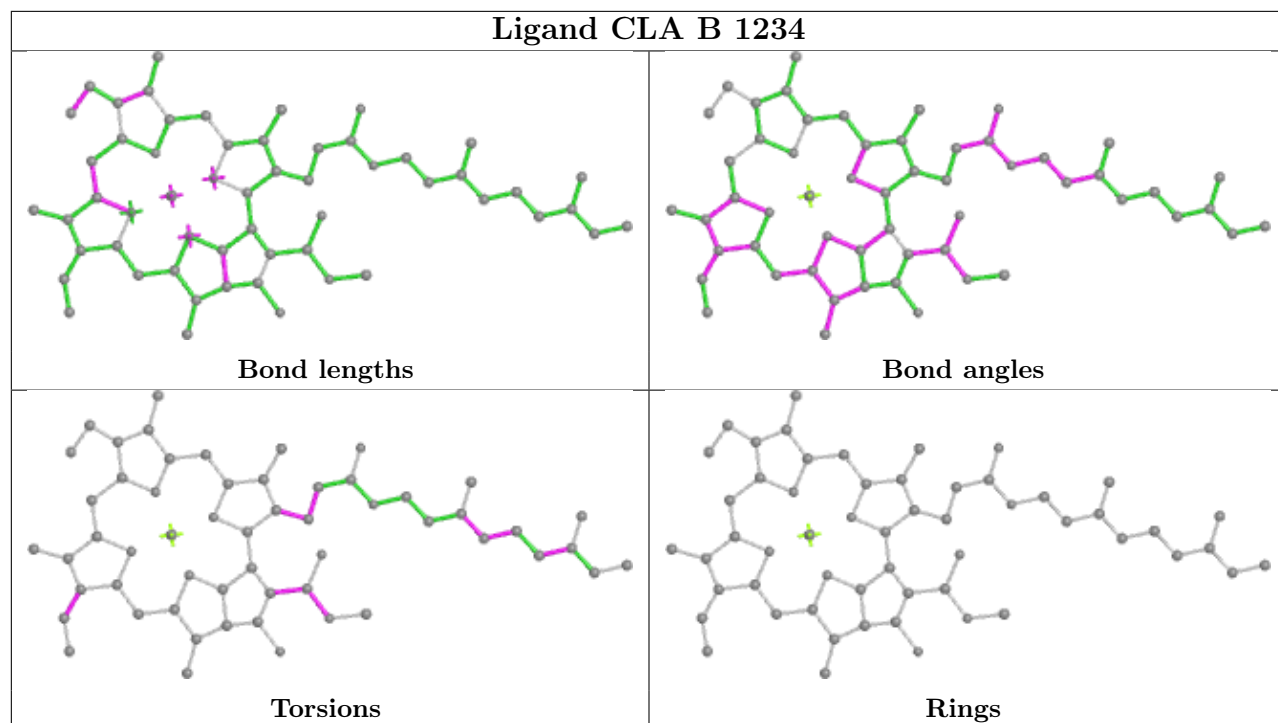


Torsions

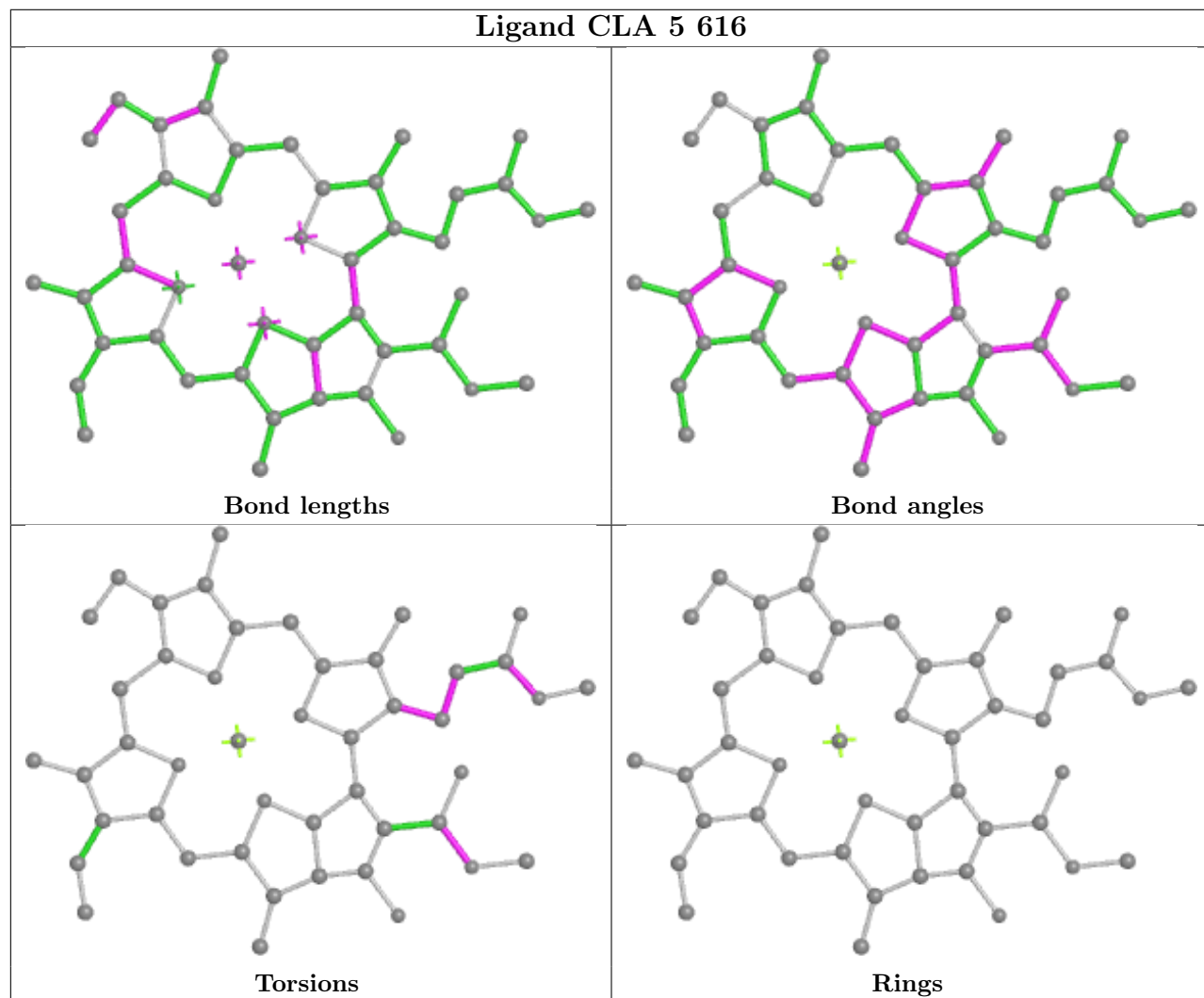


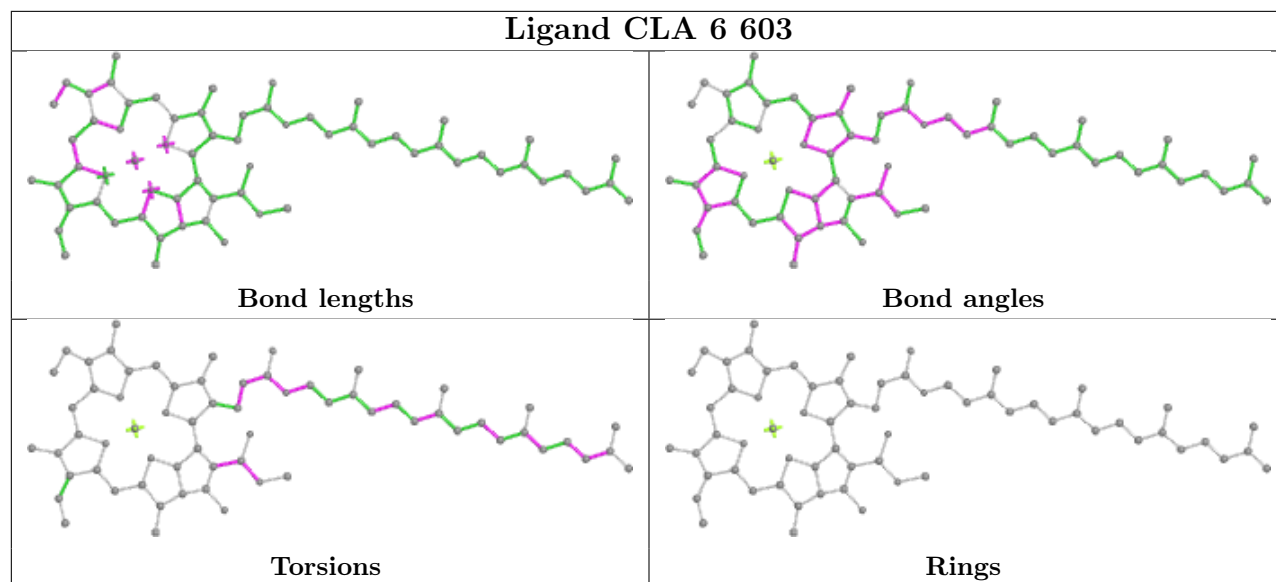
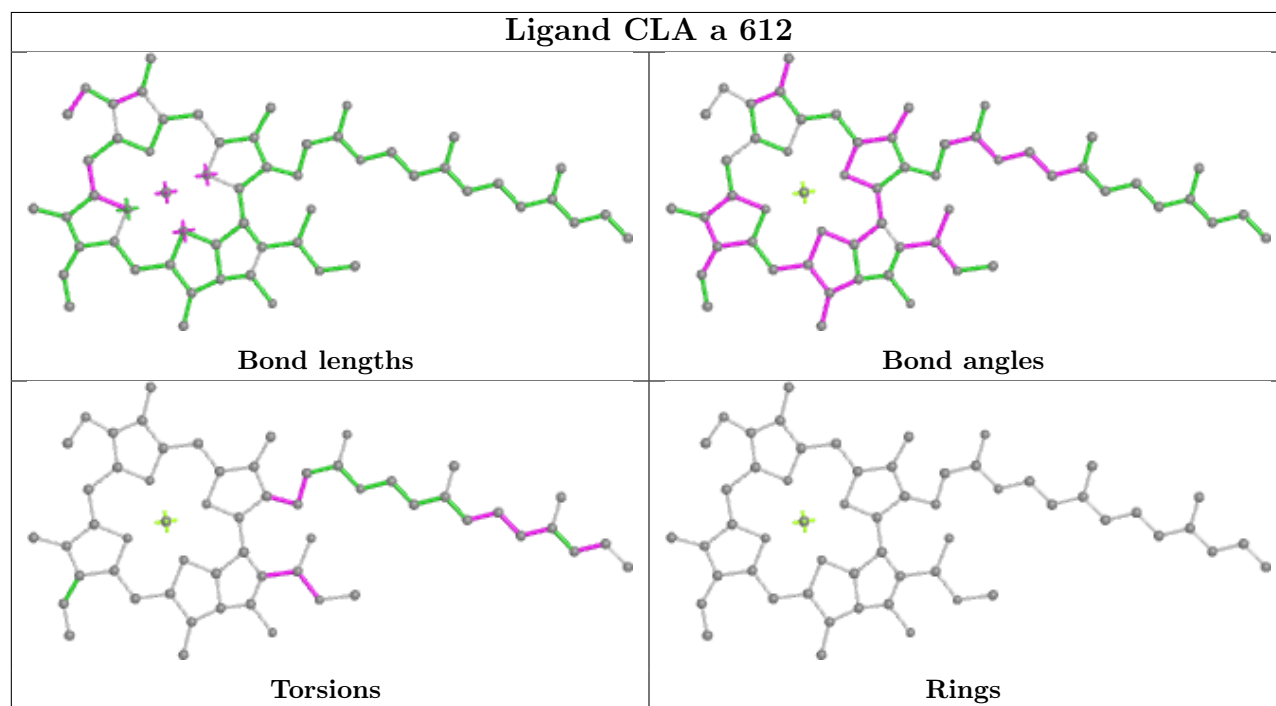
Rings

Ligand CLA B 1234

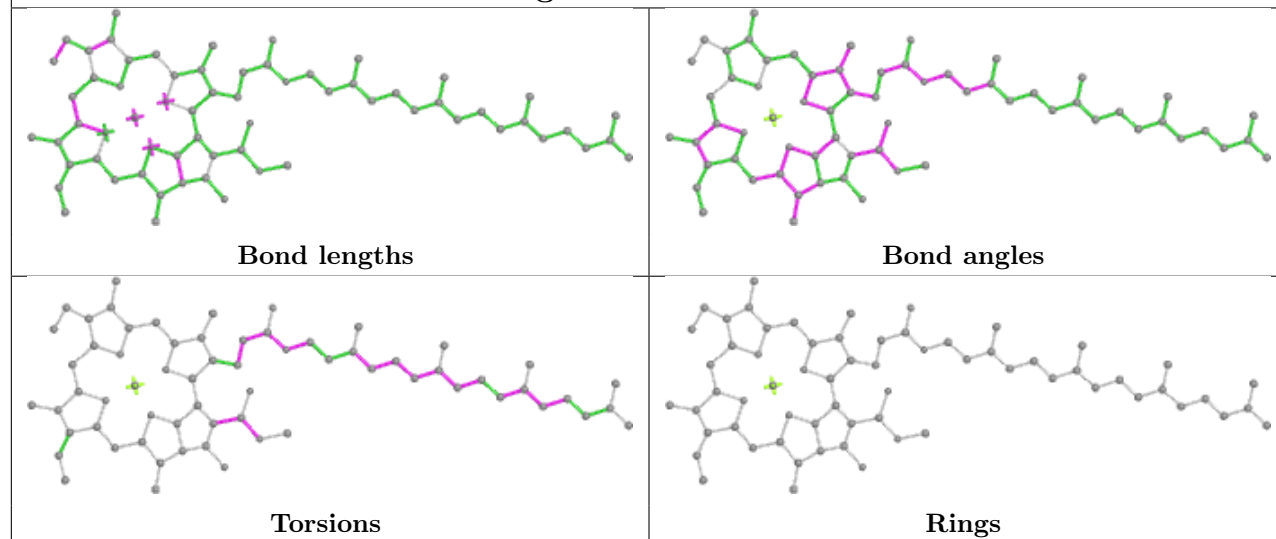


Ligand CLA 5 616

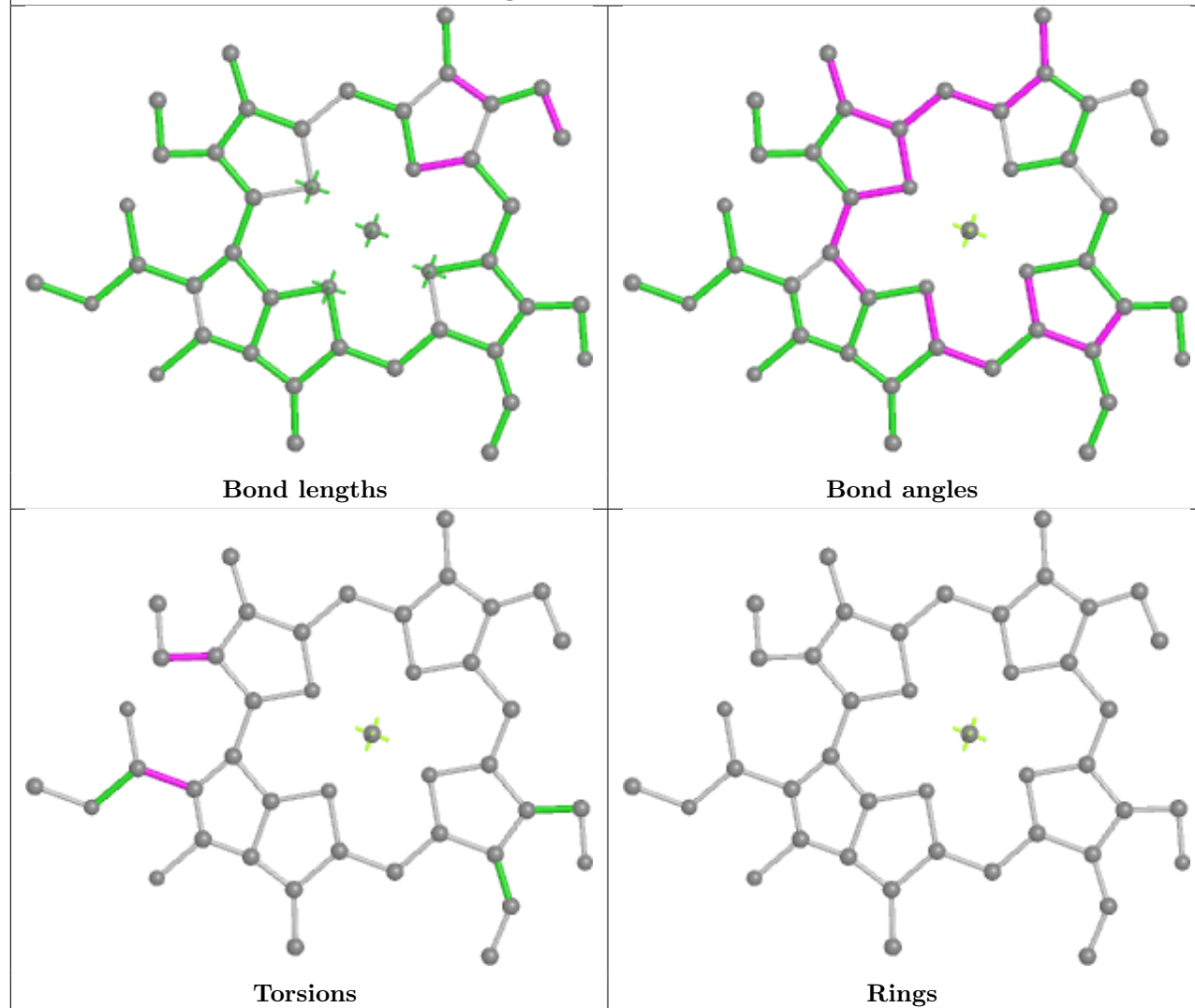


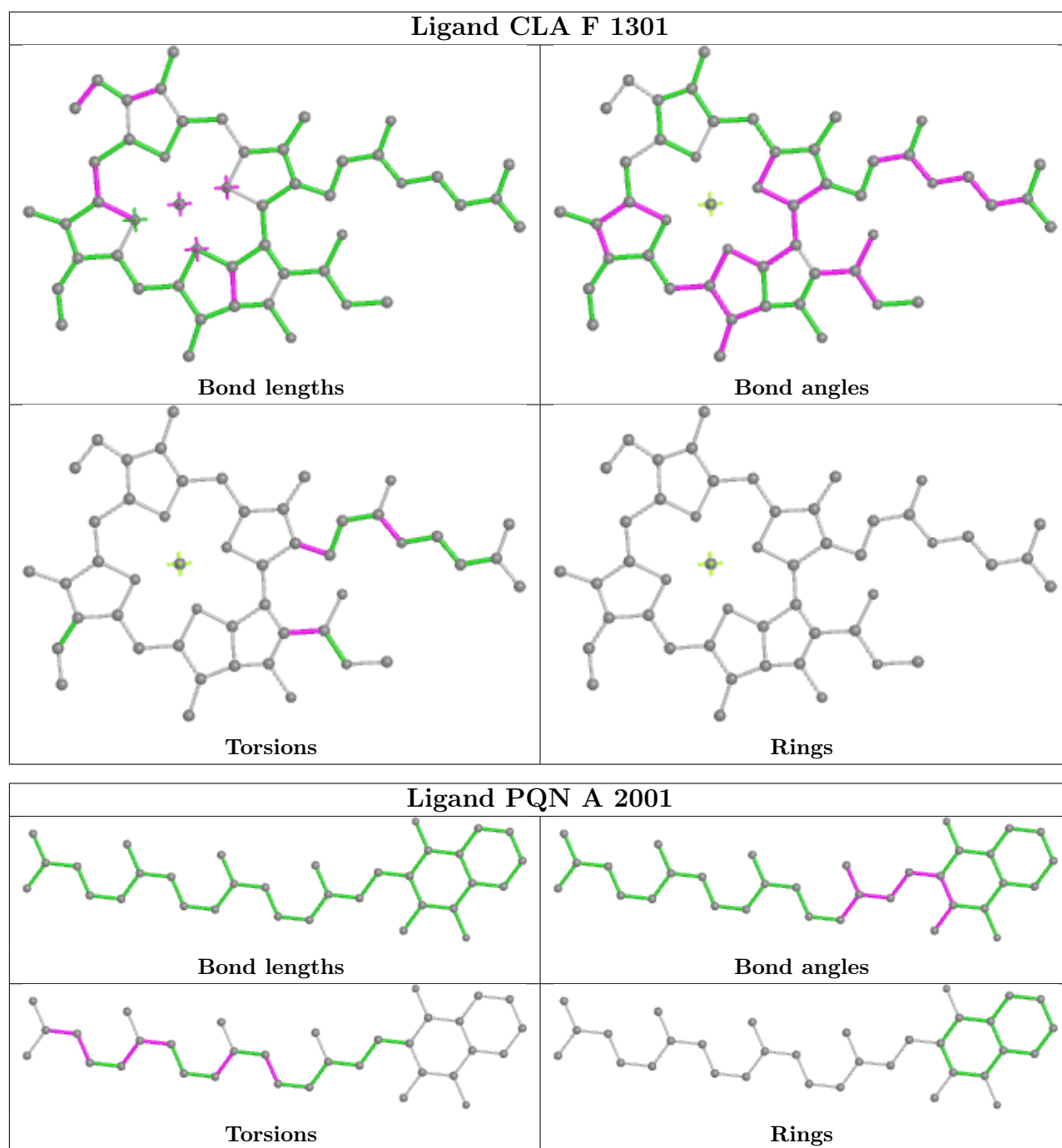
Ligand CLA 6 603**Ligand CLA a 612**

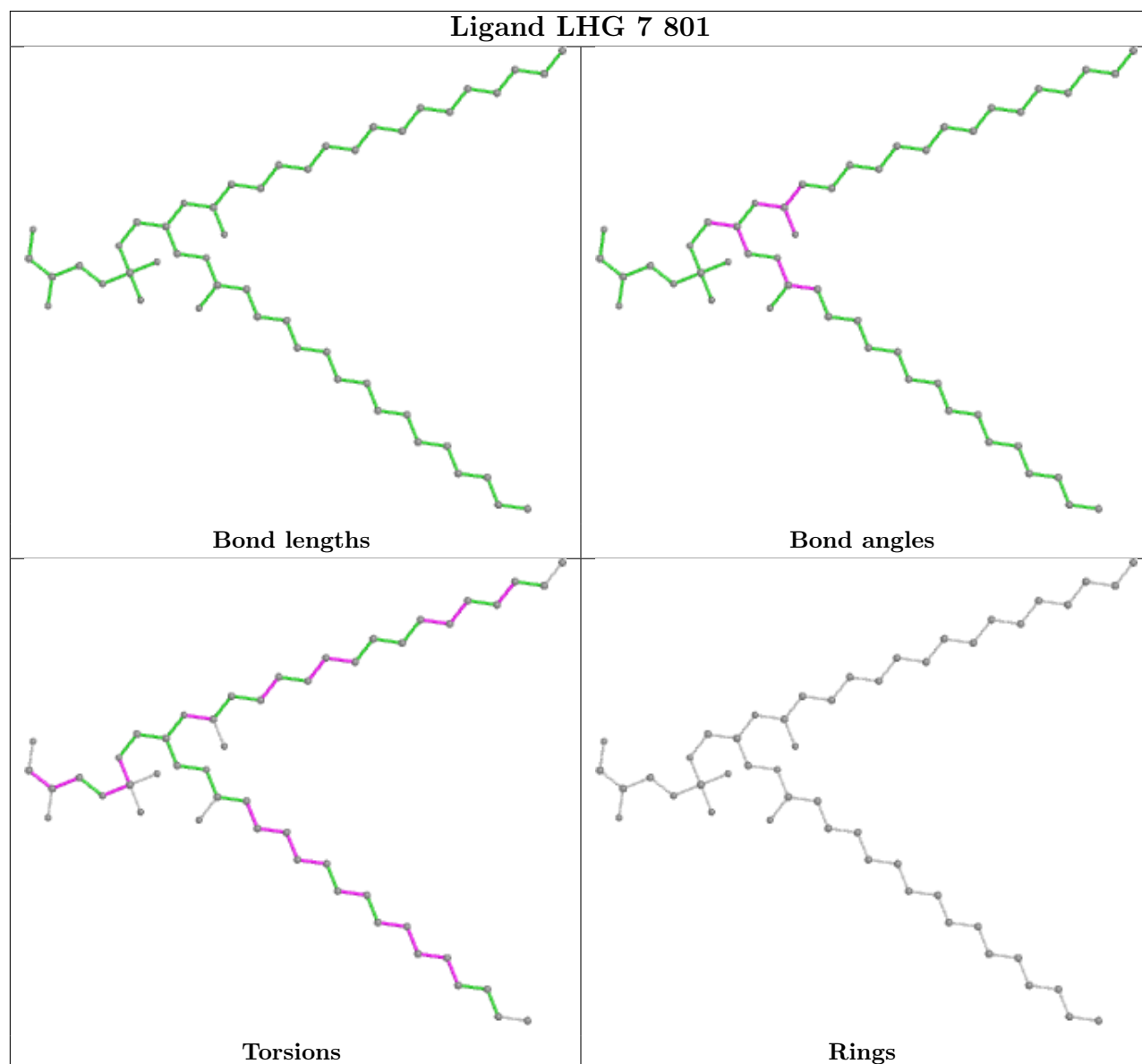
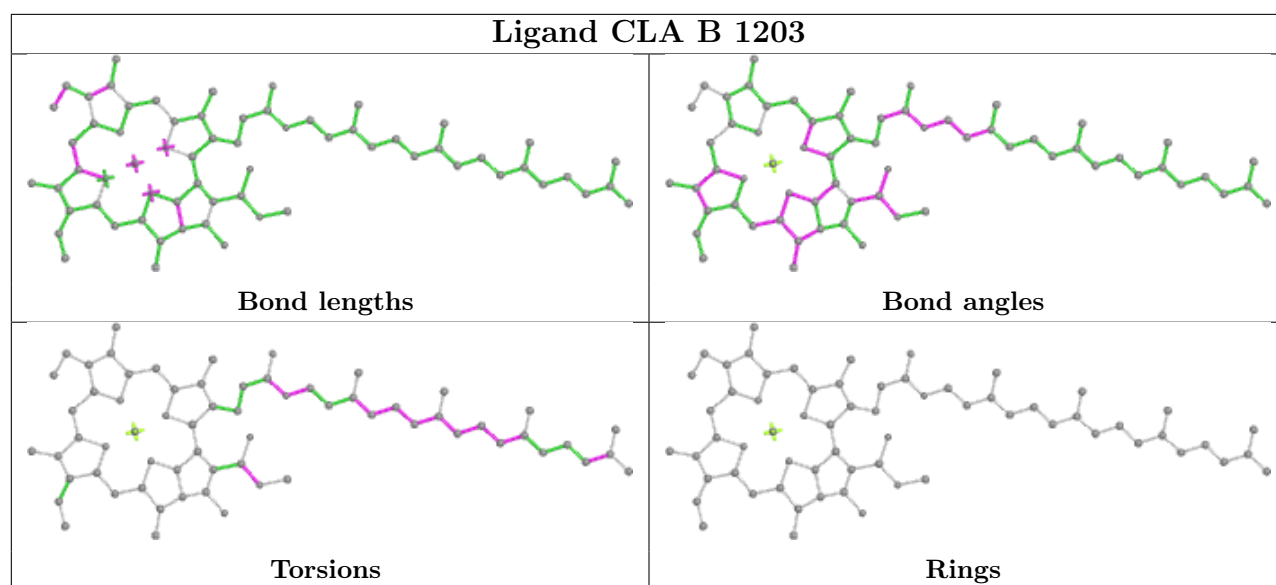
Ligand CLA 1 603

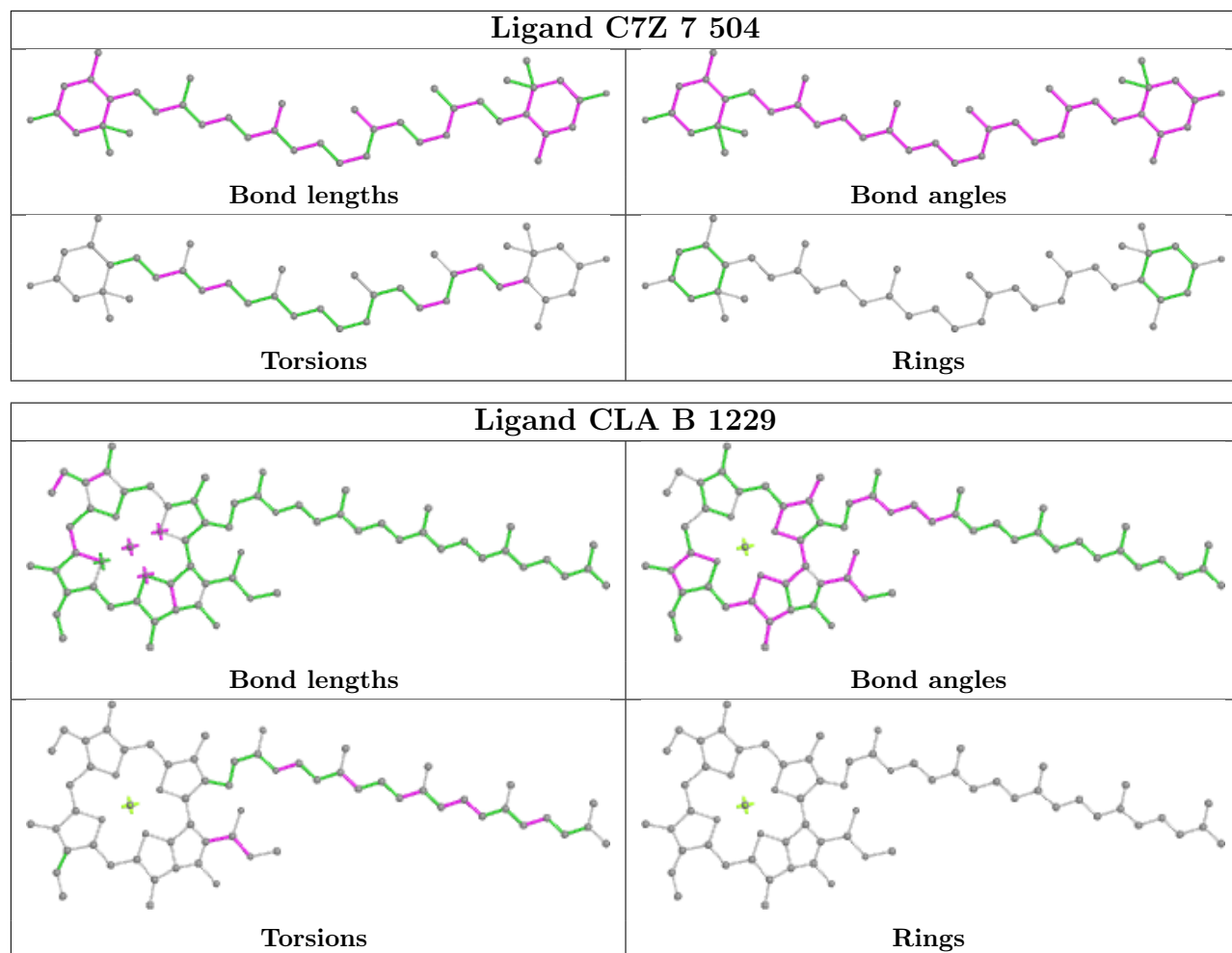


Ligand CHL 3 608

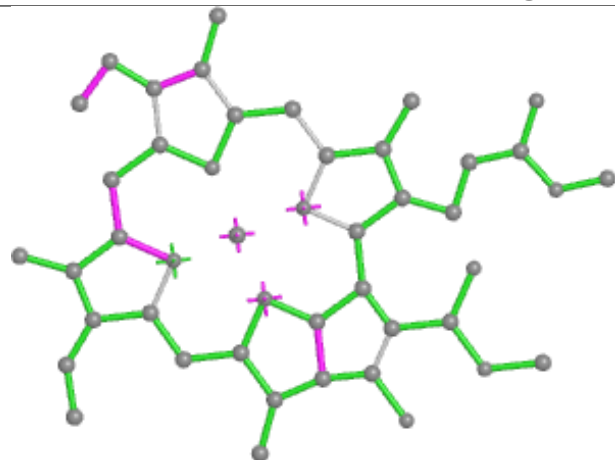




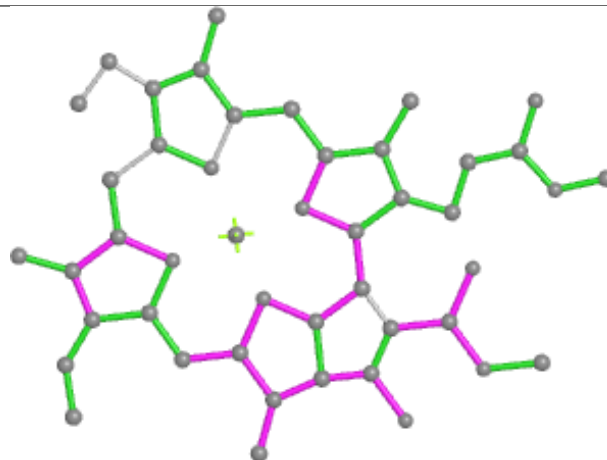




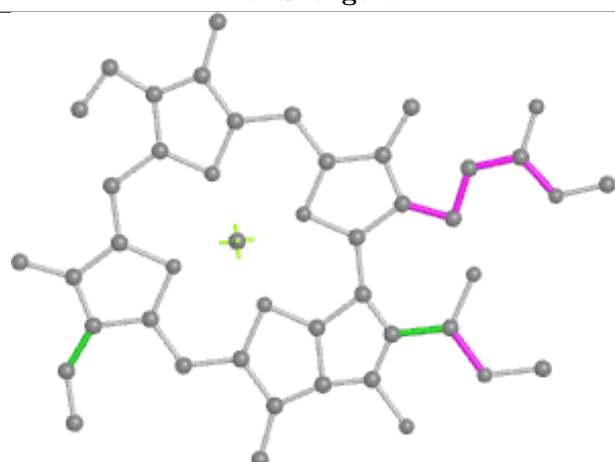
Ligand CLA 8 612



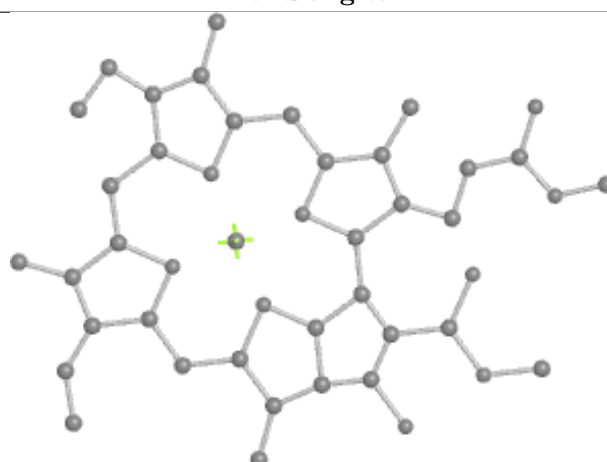
Bond lengths



Bond angles

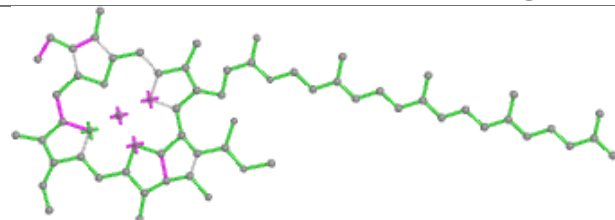


Torsions

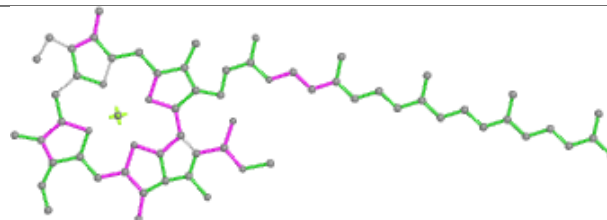


Rings

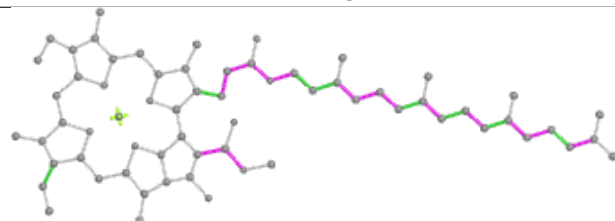
Ligand CLA 5 612



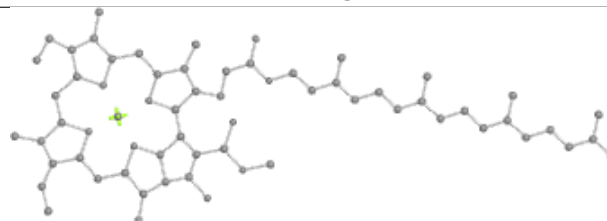
Bond lengths



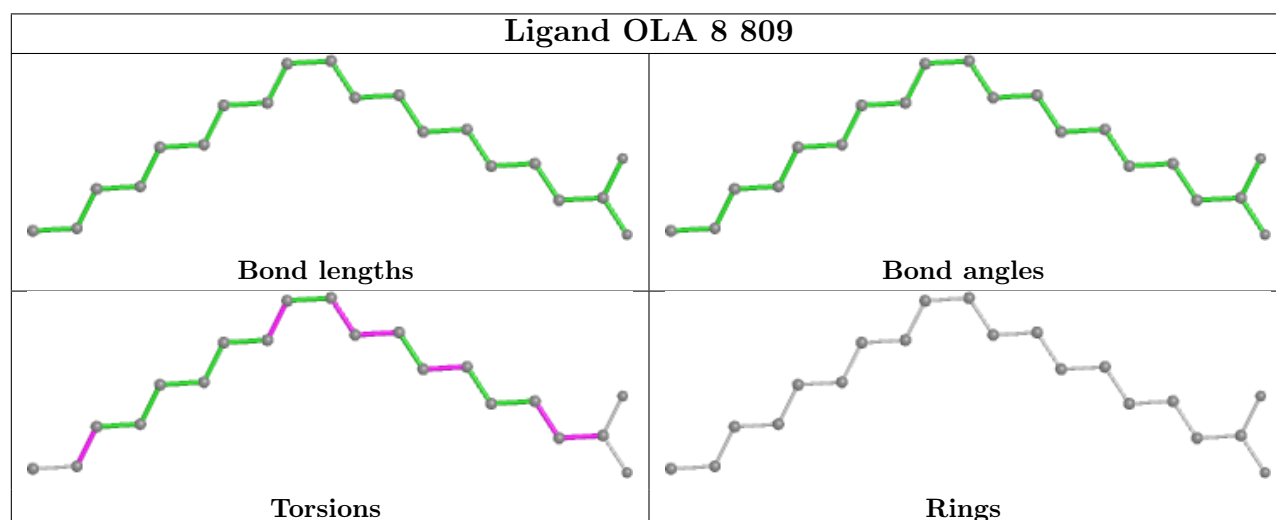
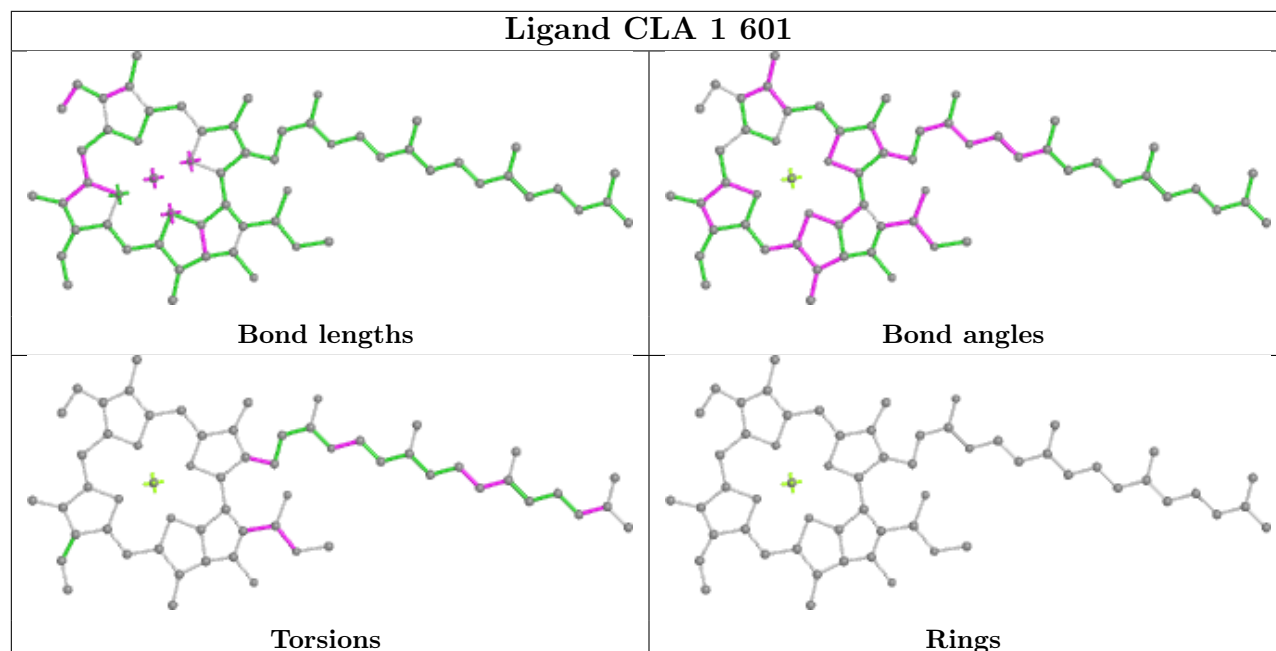
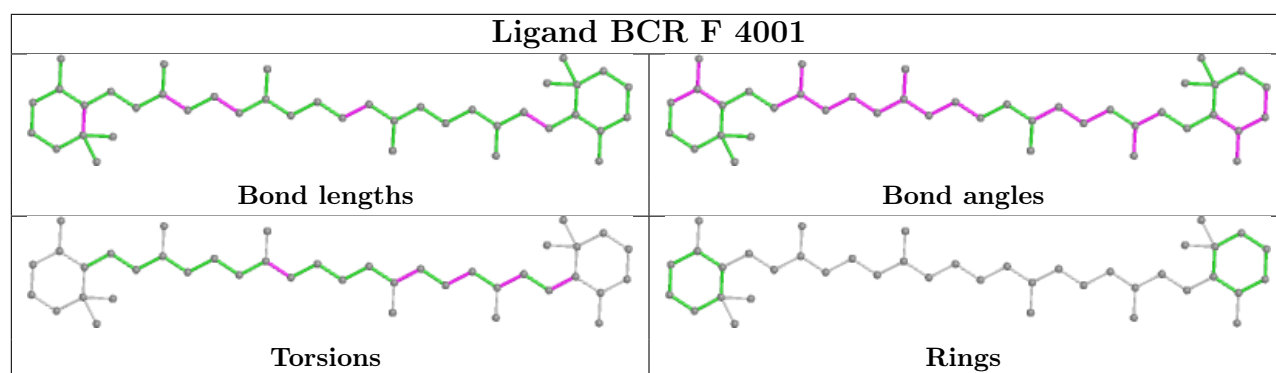
Bond angles

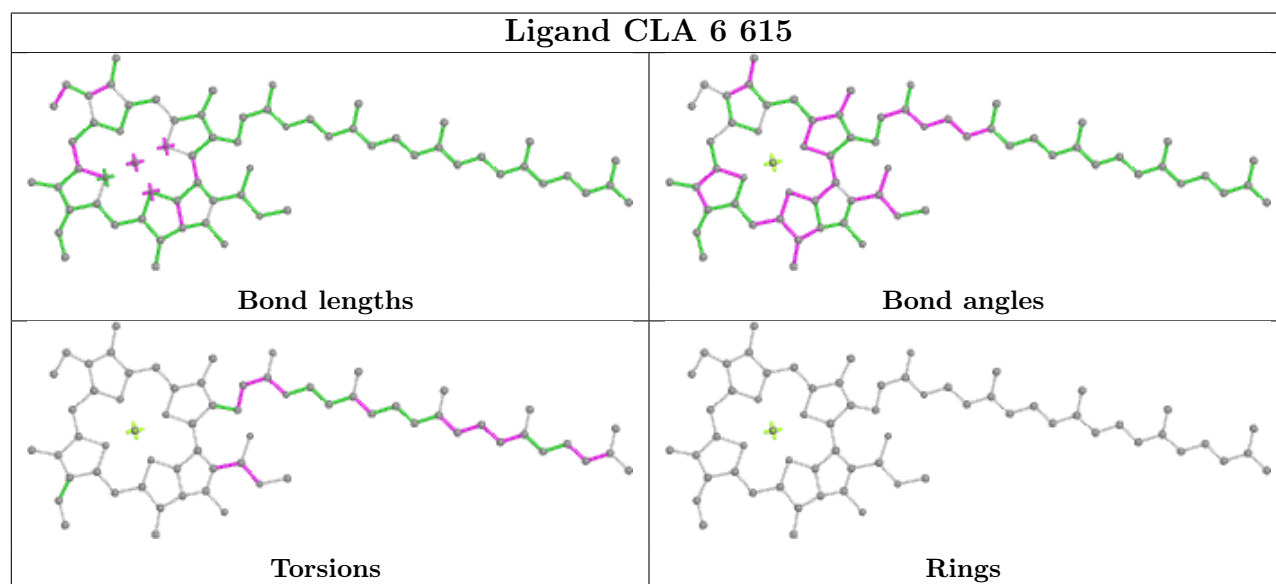
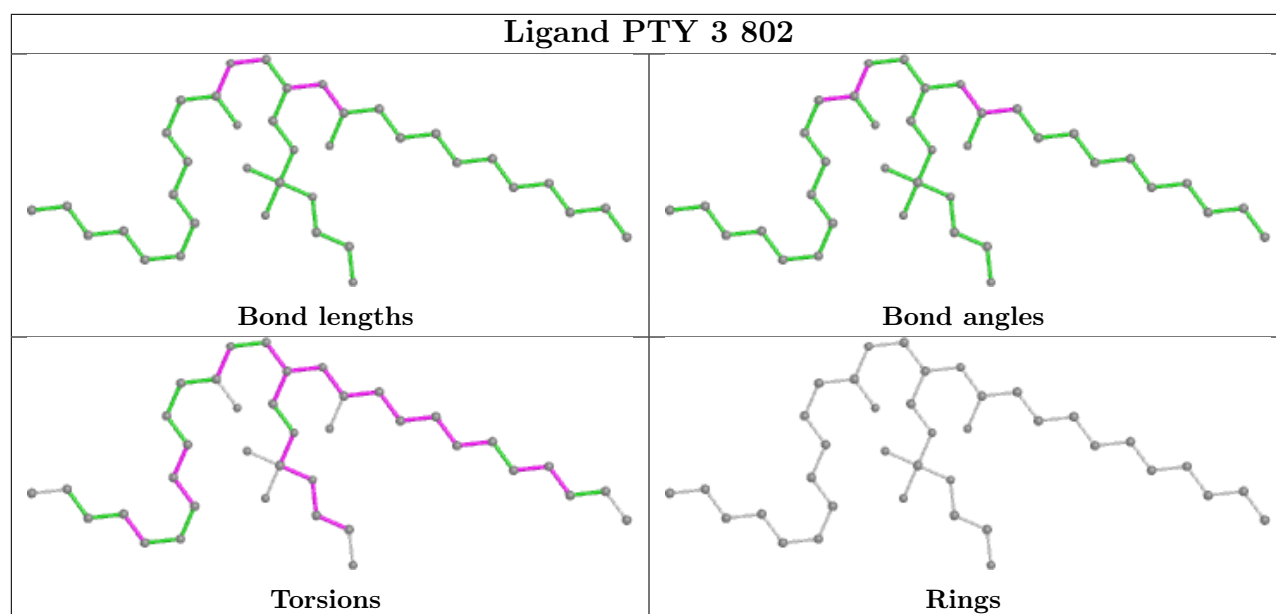


Torsions

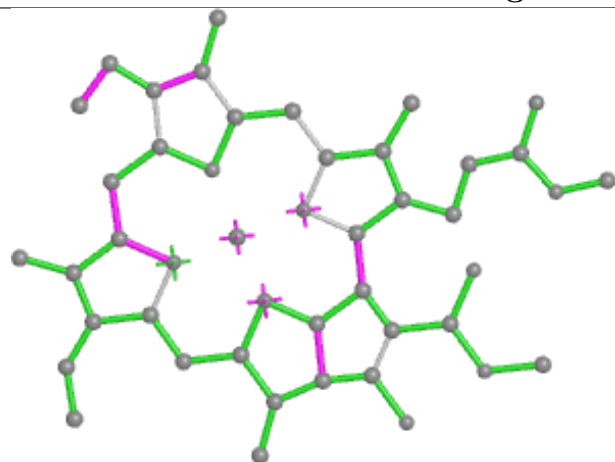


Rings

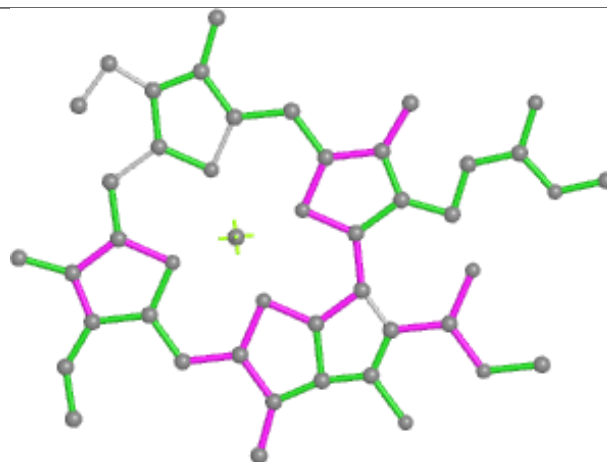




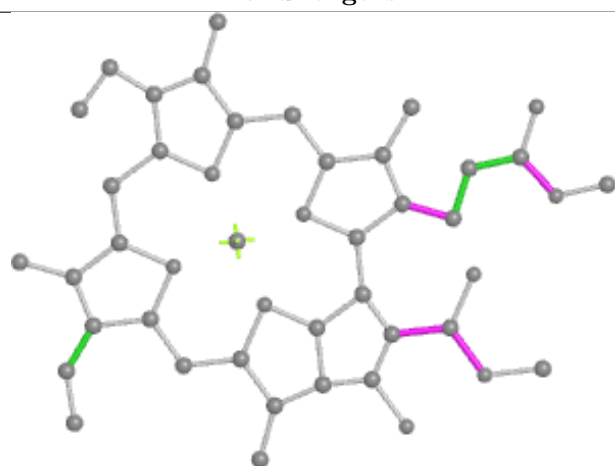
Ligand CLA K 1401



Bond lengths



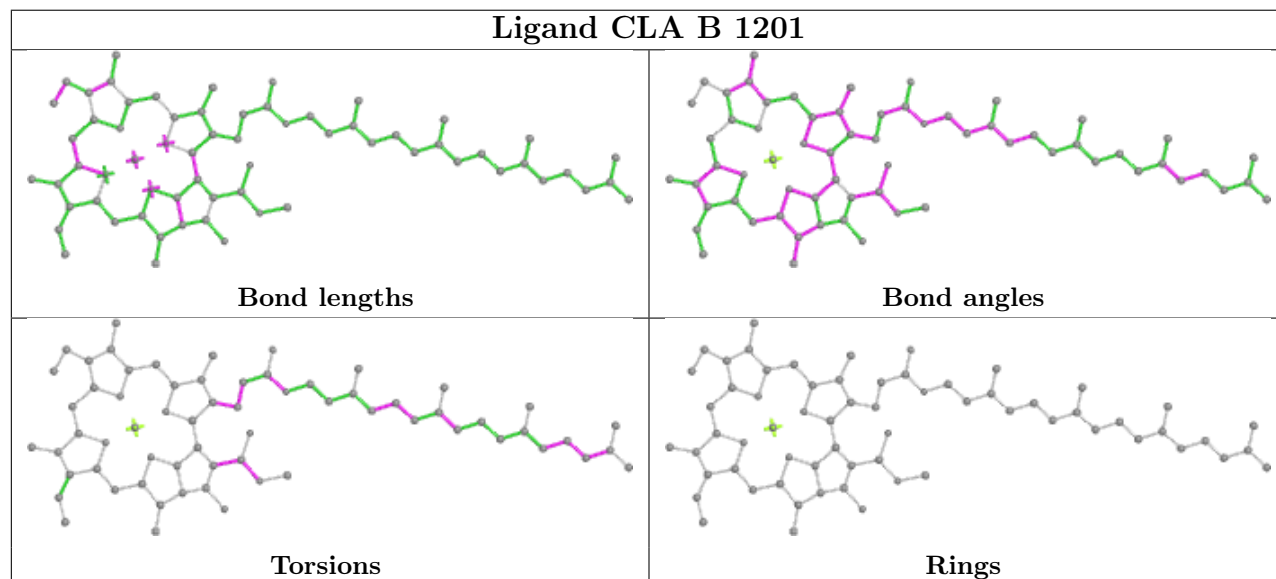
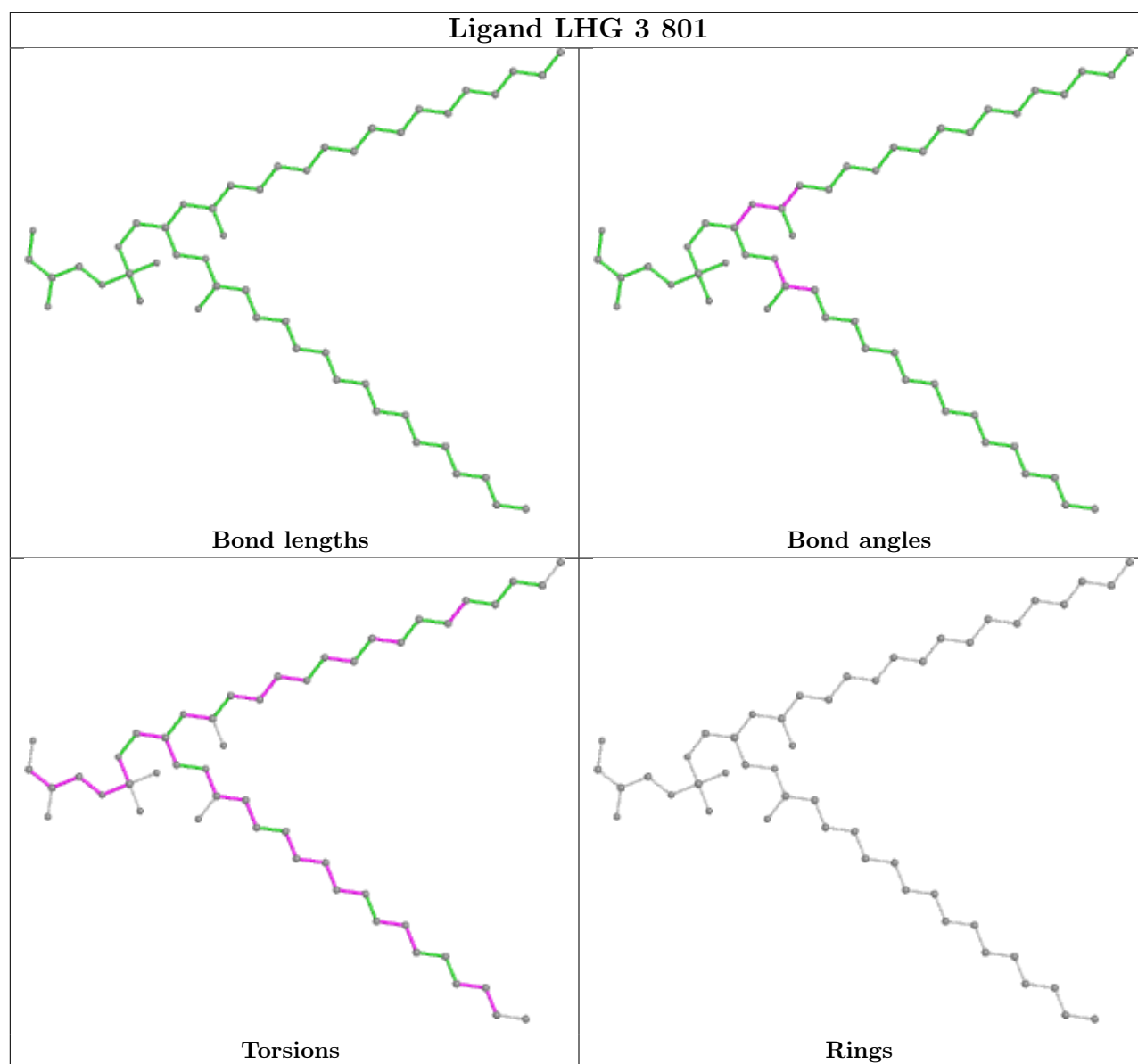
Bond angles



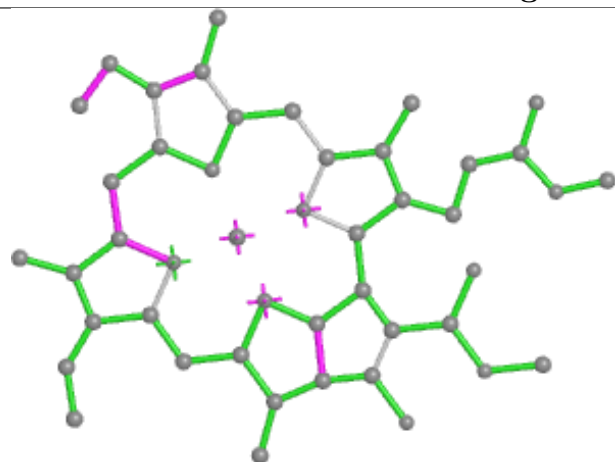
Torsions



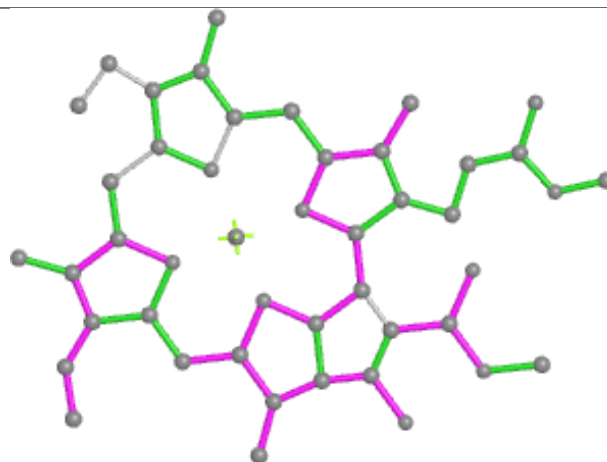
Rings



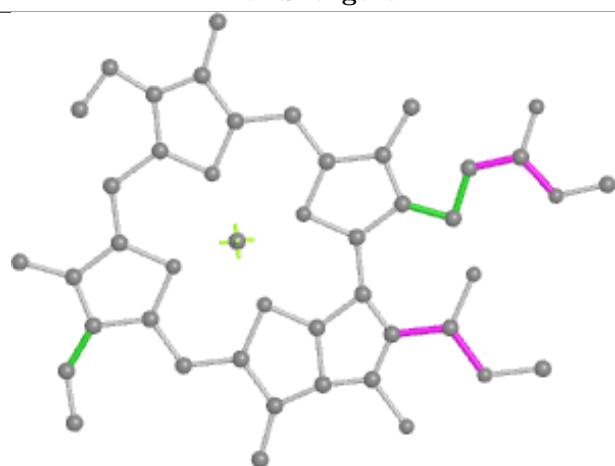
Ligand CLA 4 605



Bond lengths



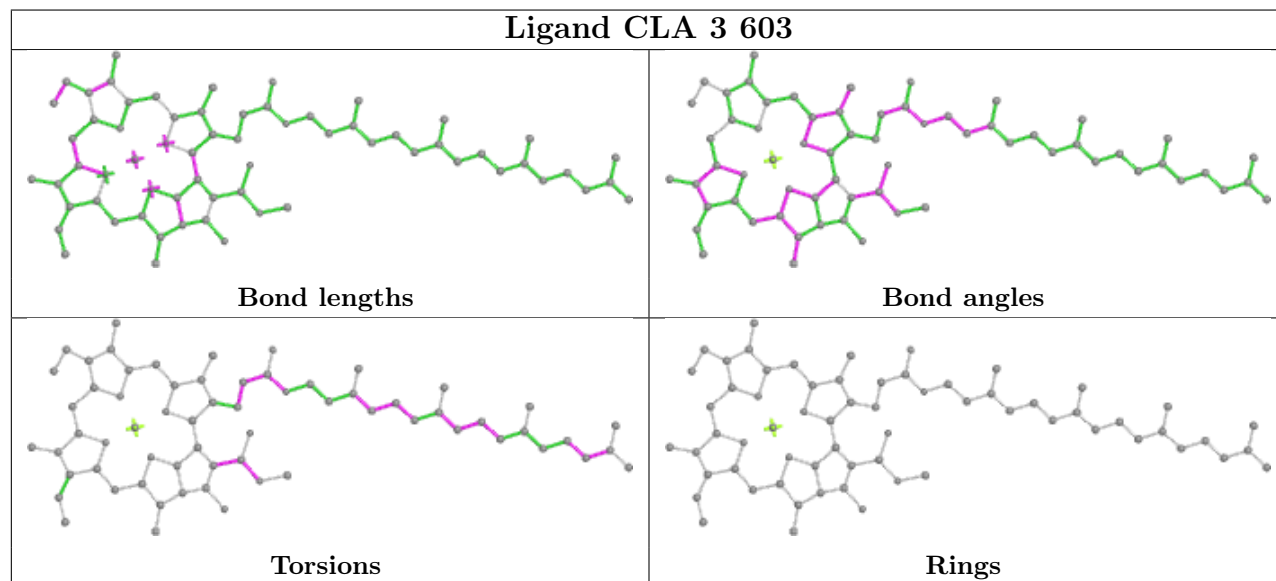
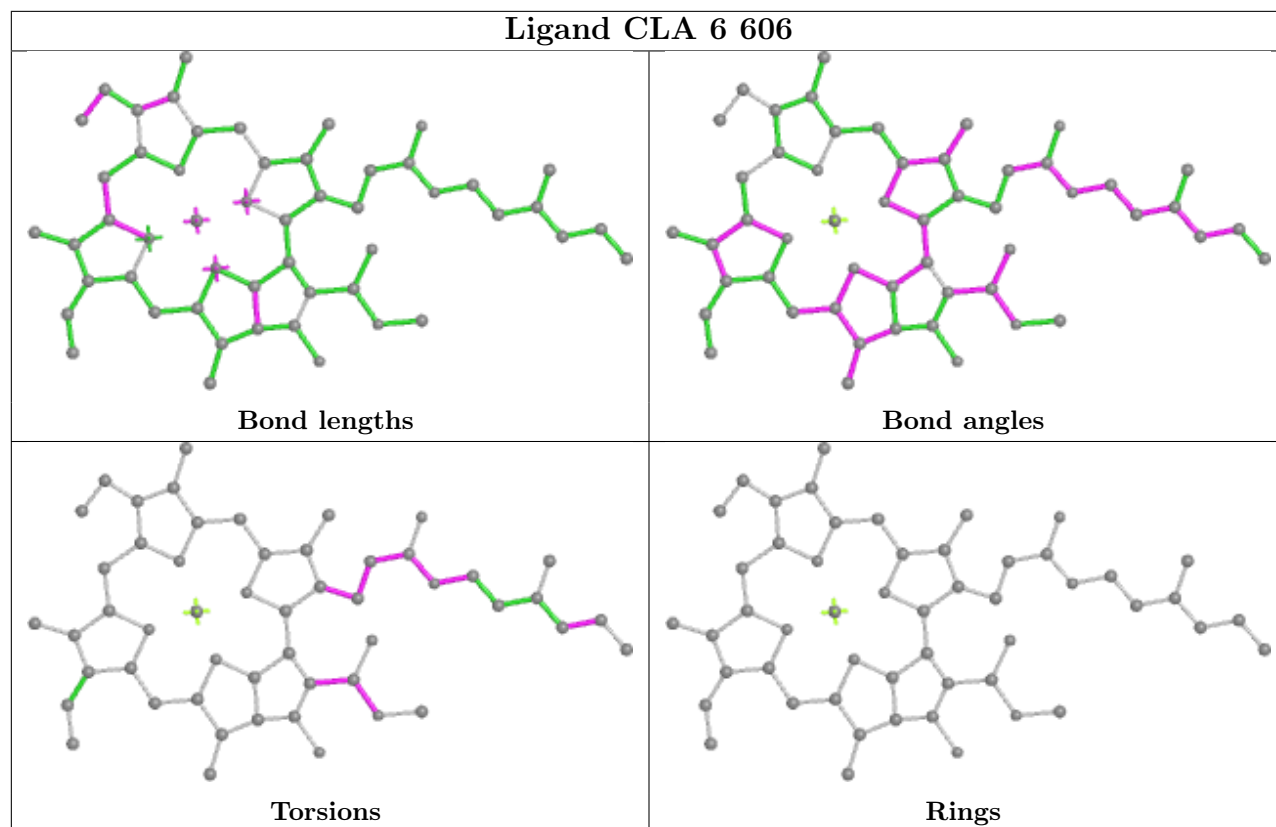
Bond angles

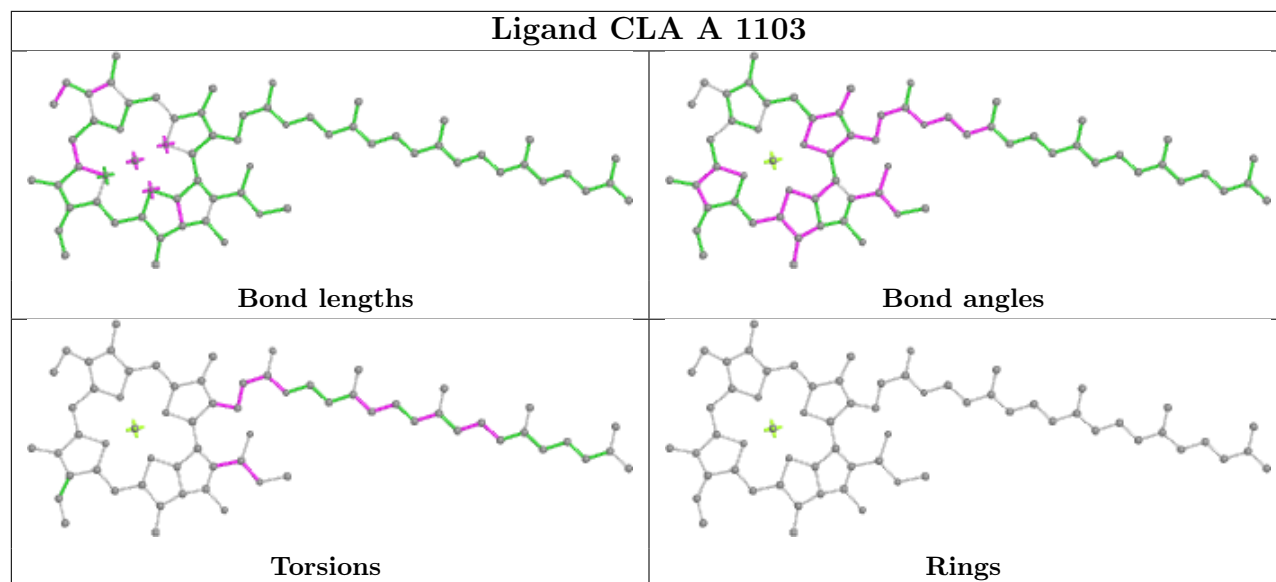
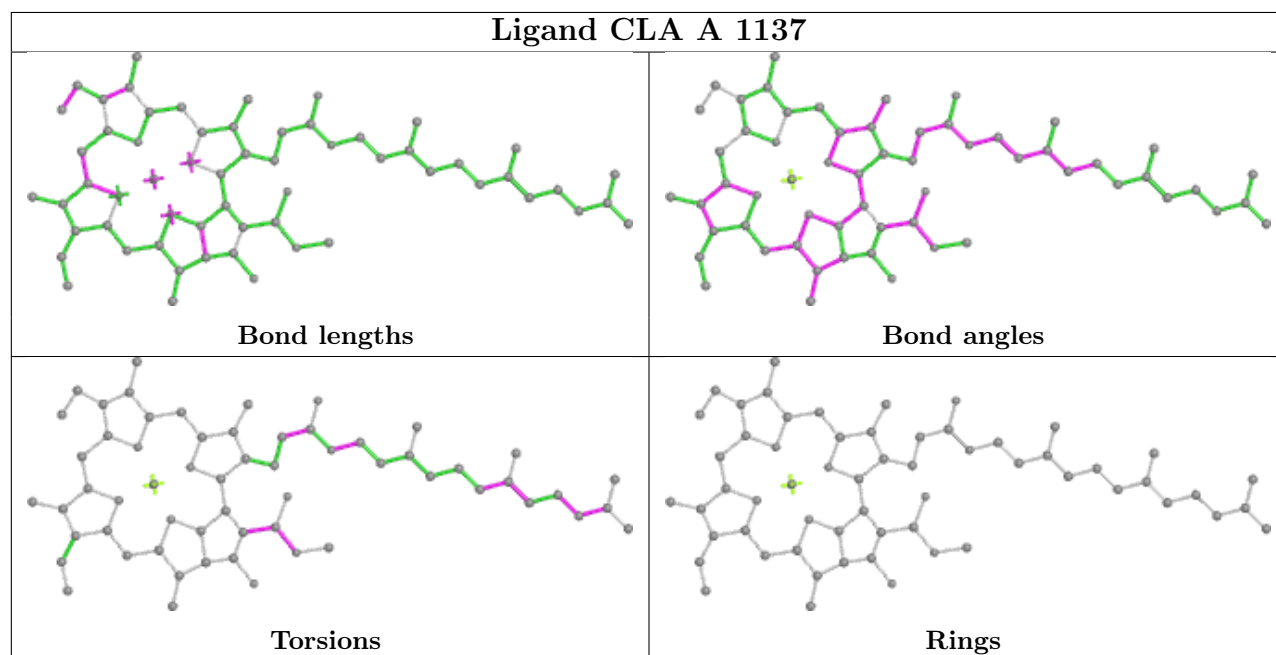


Torsions

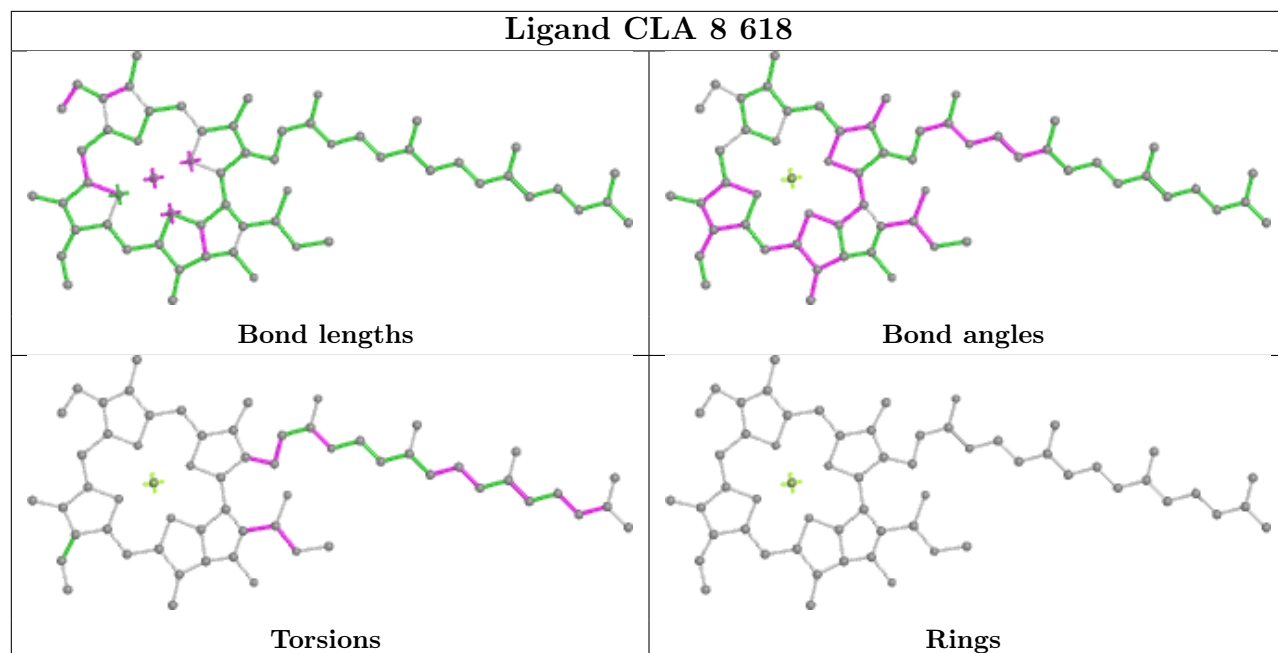


Rings

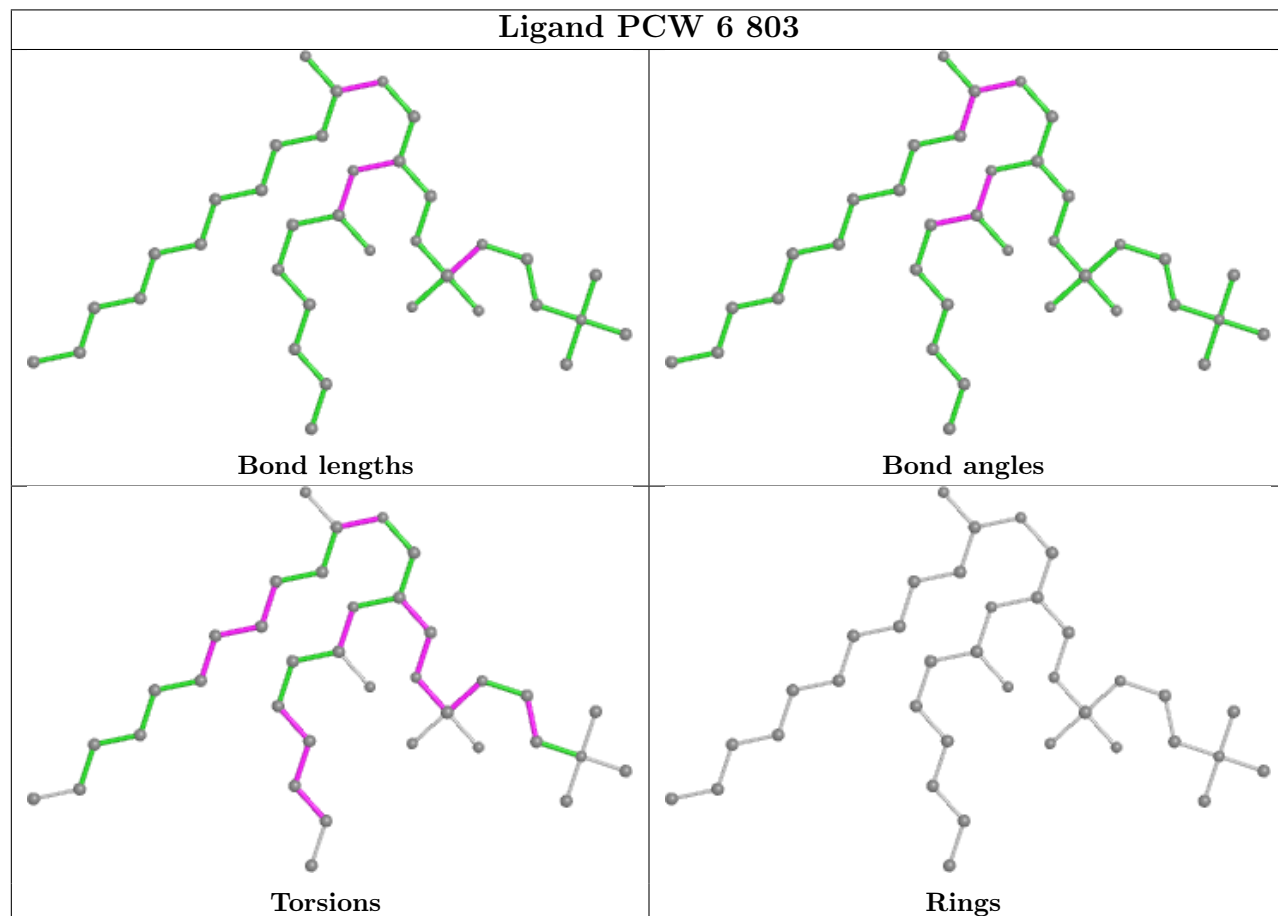


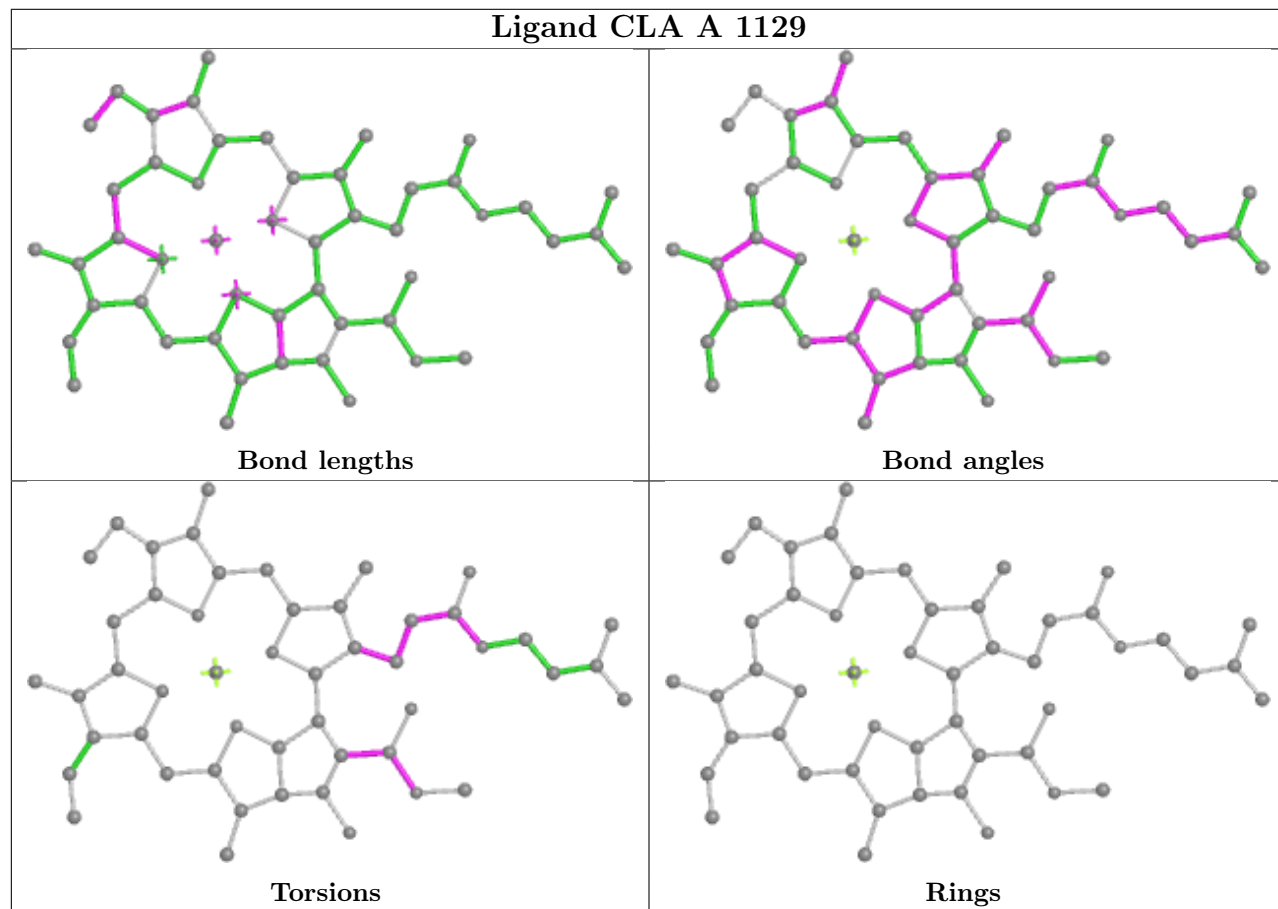
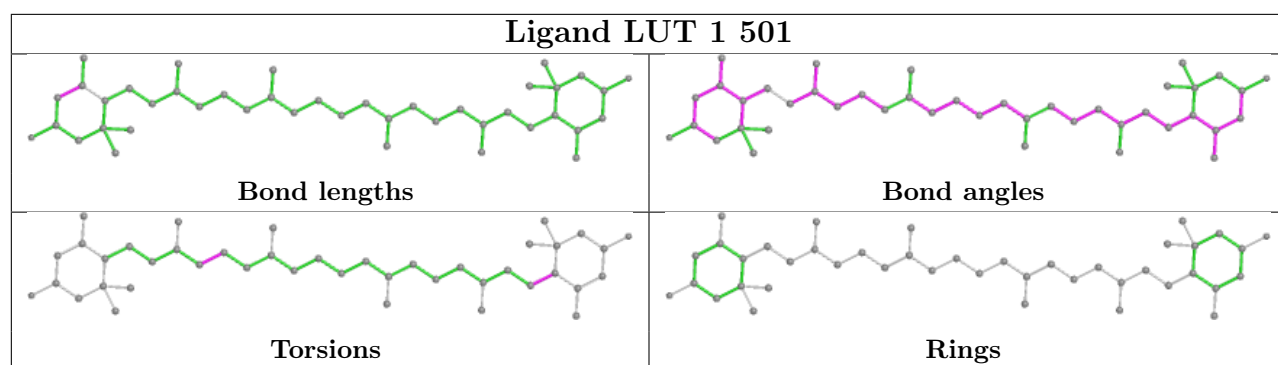
Ligand CLA A 1103**Ligand CLA A 1137**

Ligand CLA 8 618

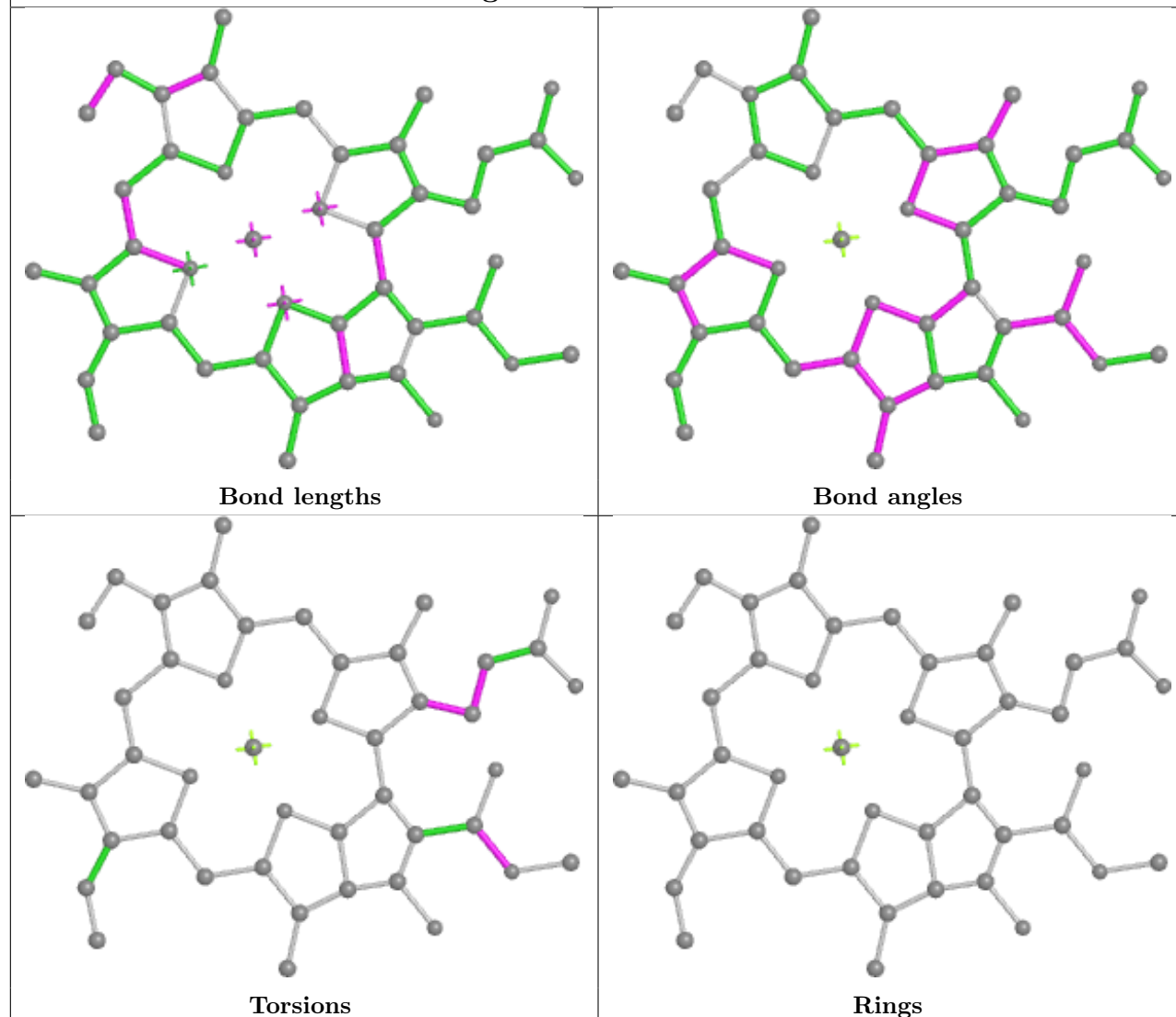


Ligand PCW 6 803

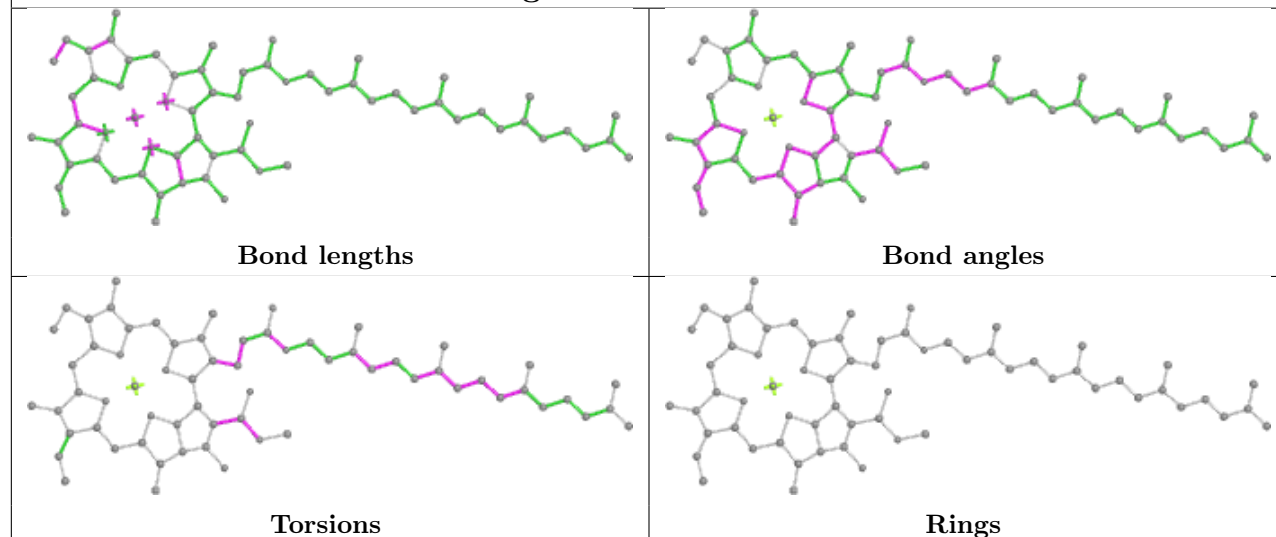


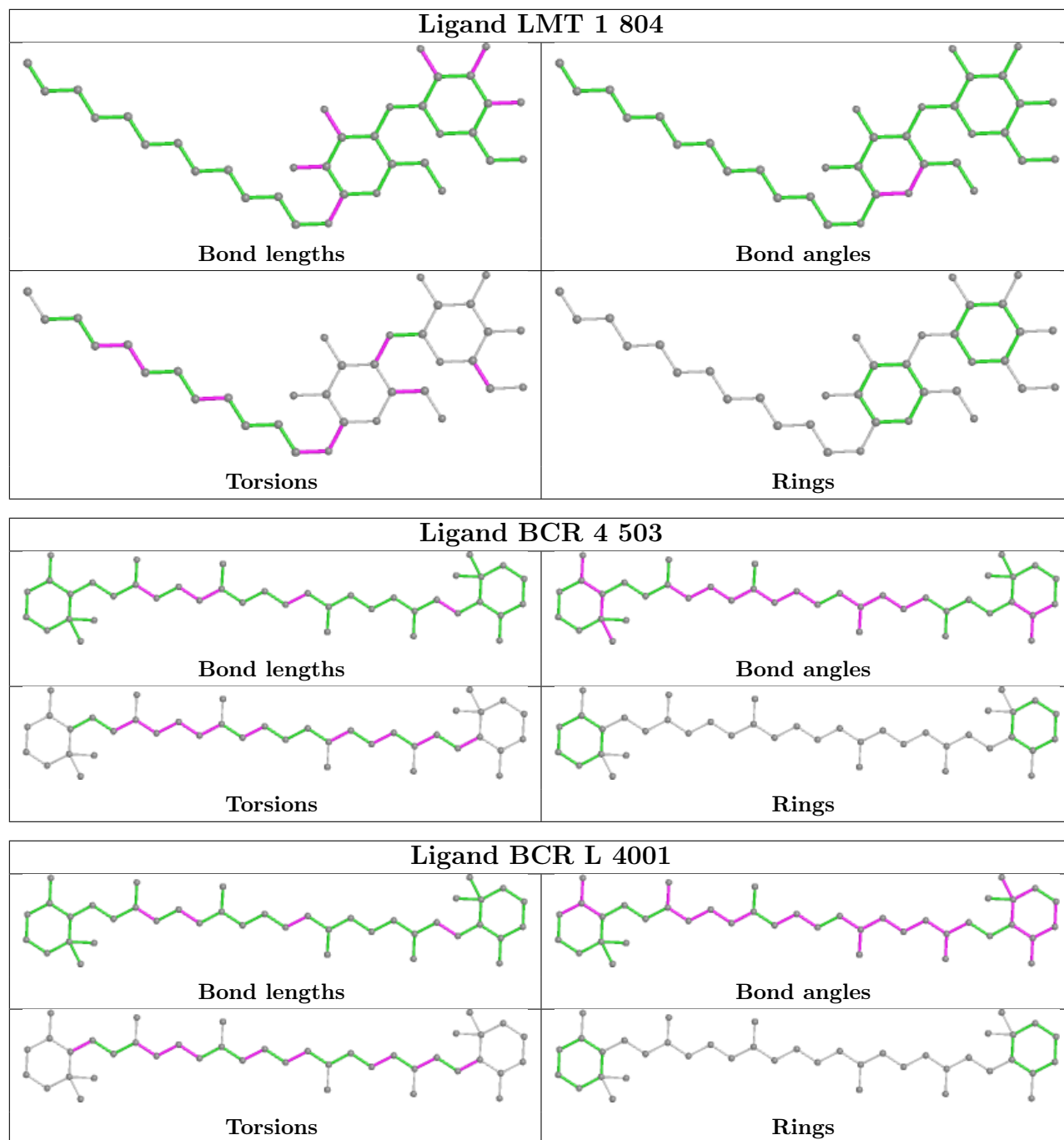


Ligand CLA B 1232

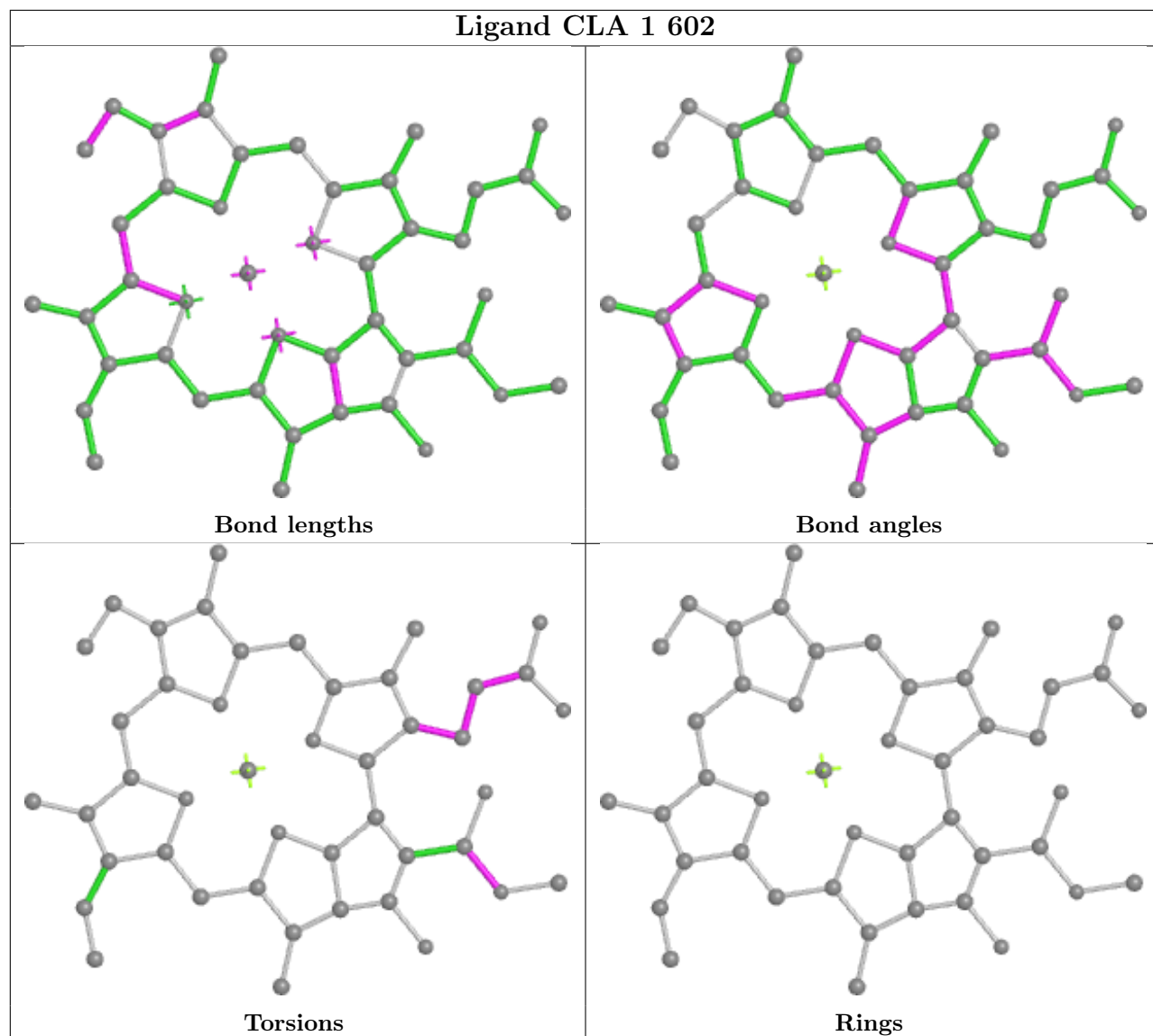


Ligand CLA A 1104

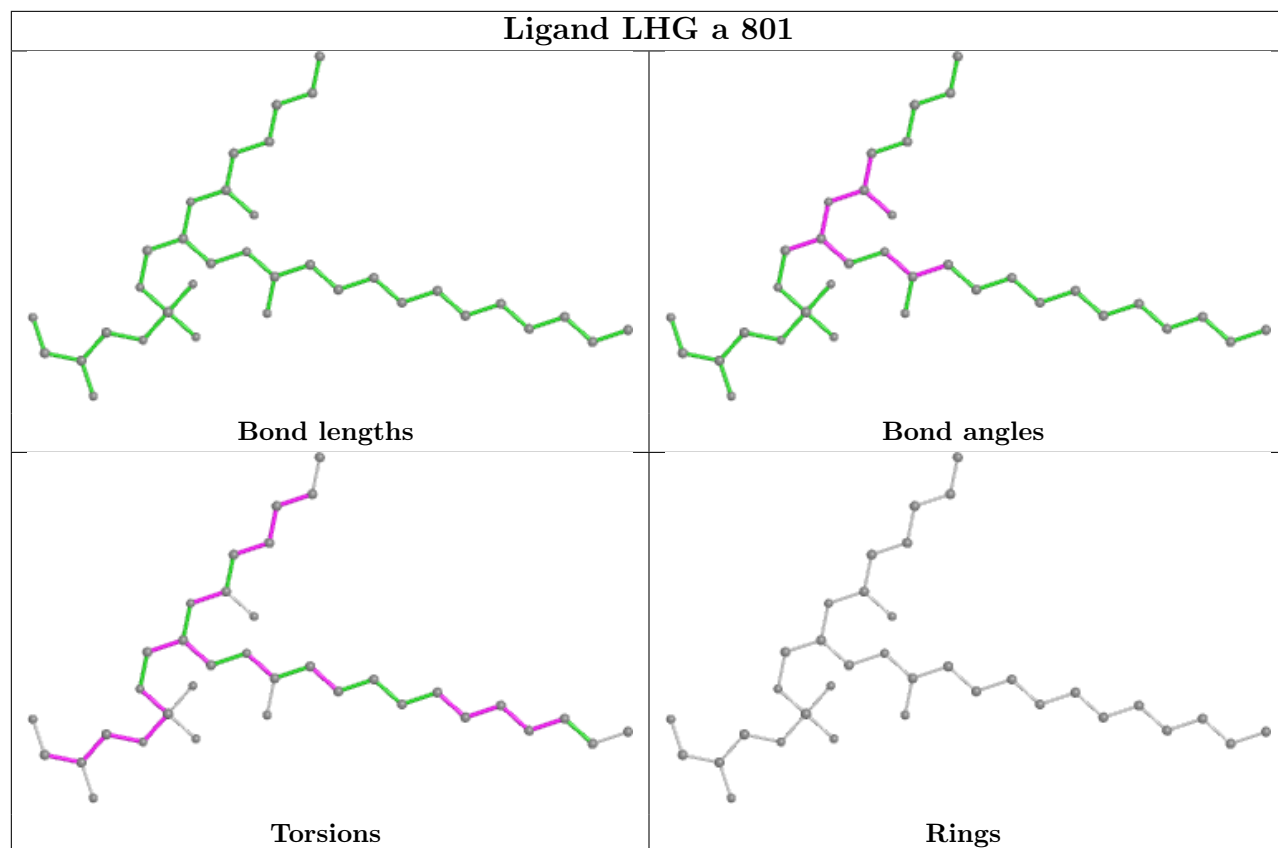




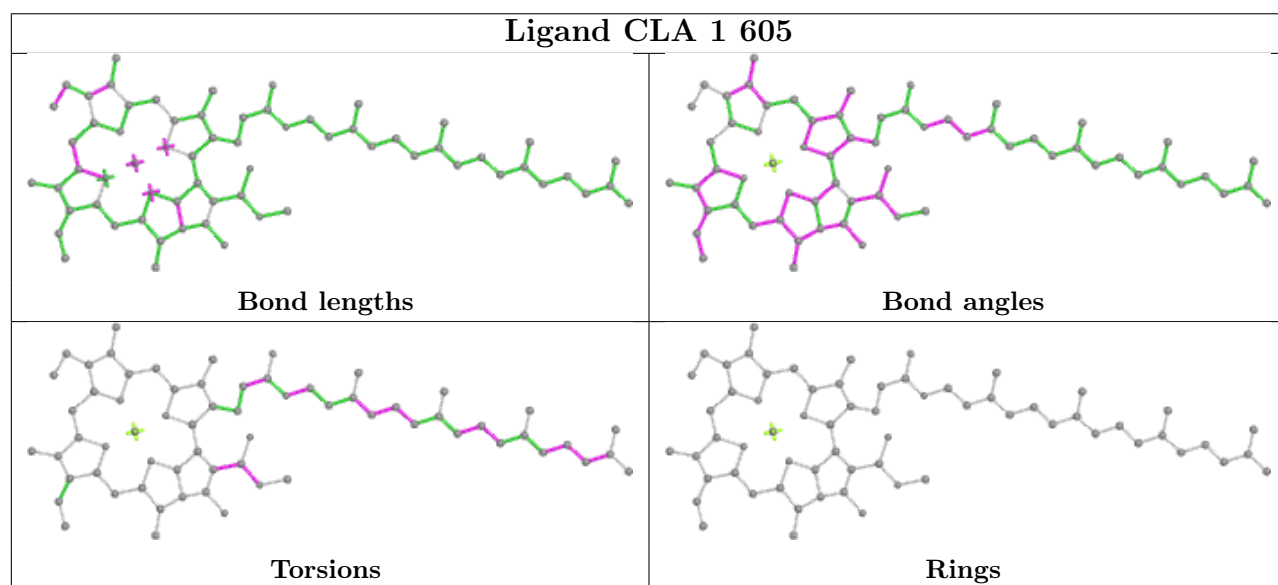
Ligand CLA 1 602

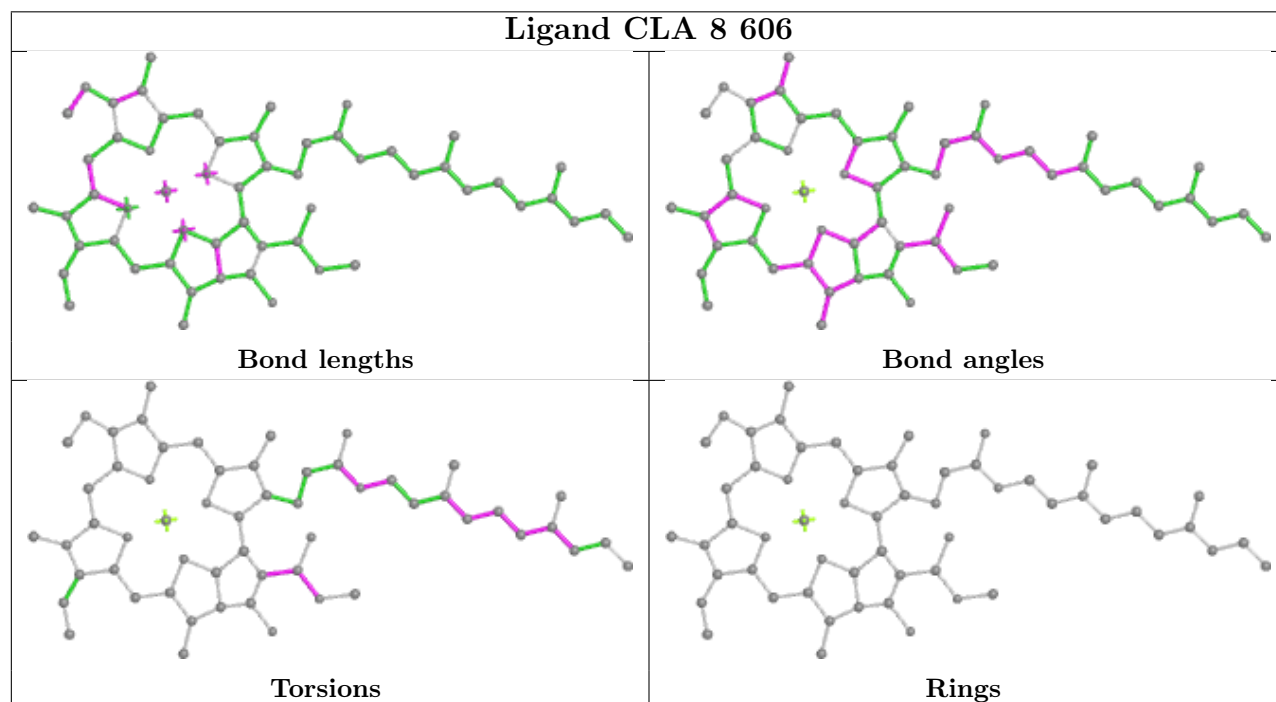
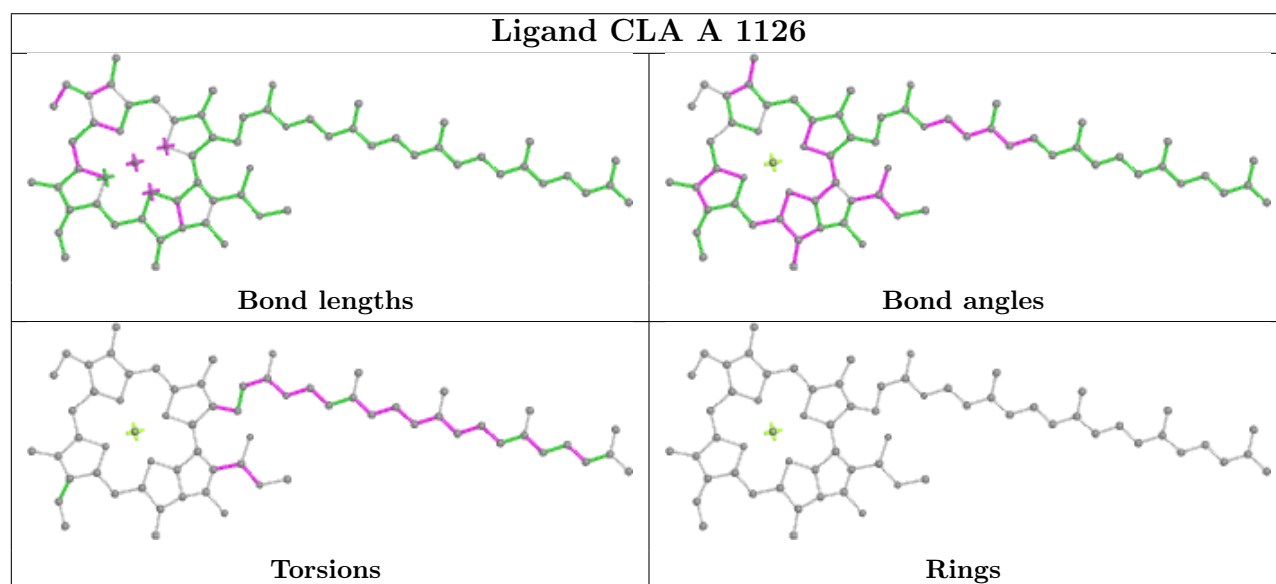
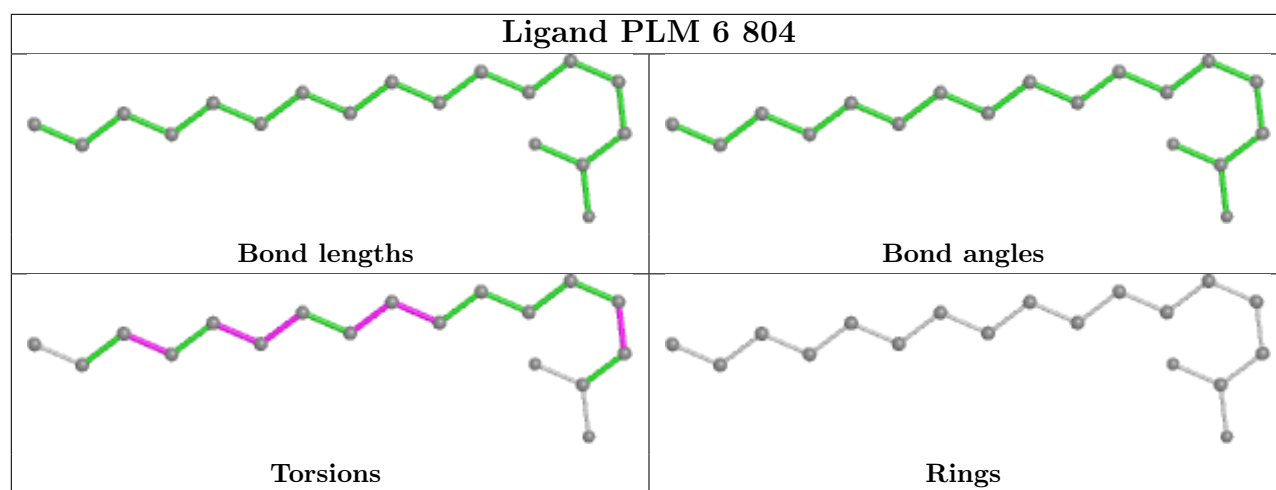


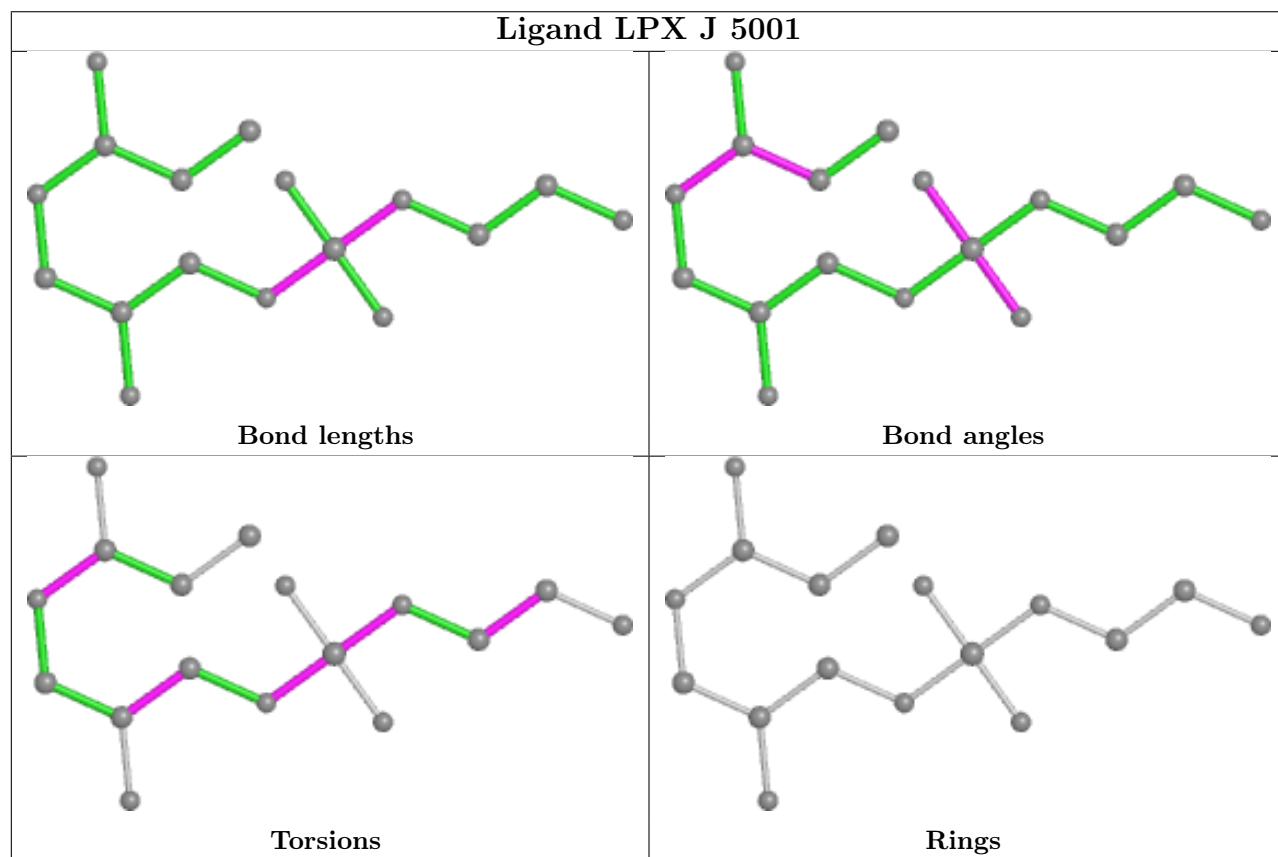
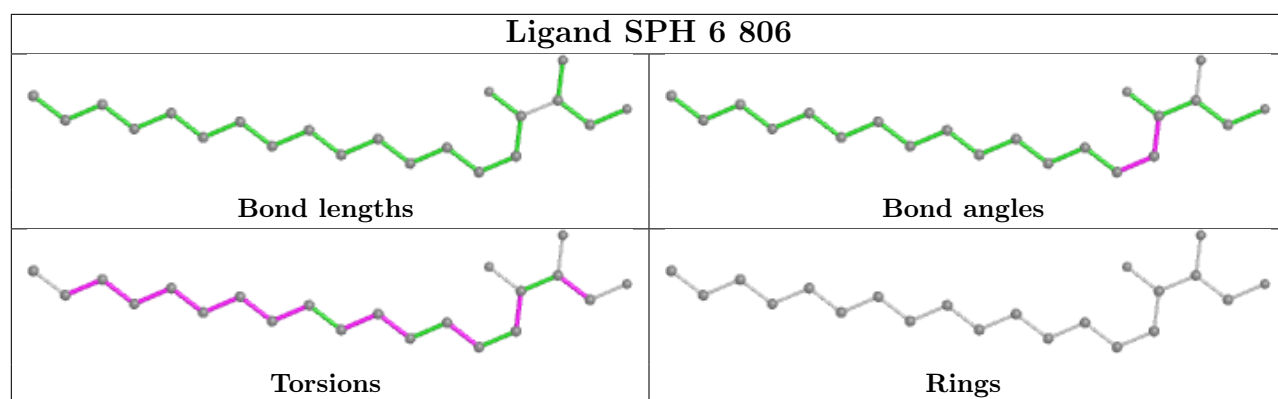
Ligand LHG a 801



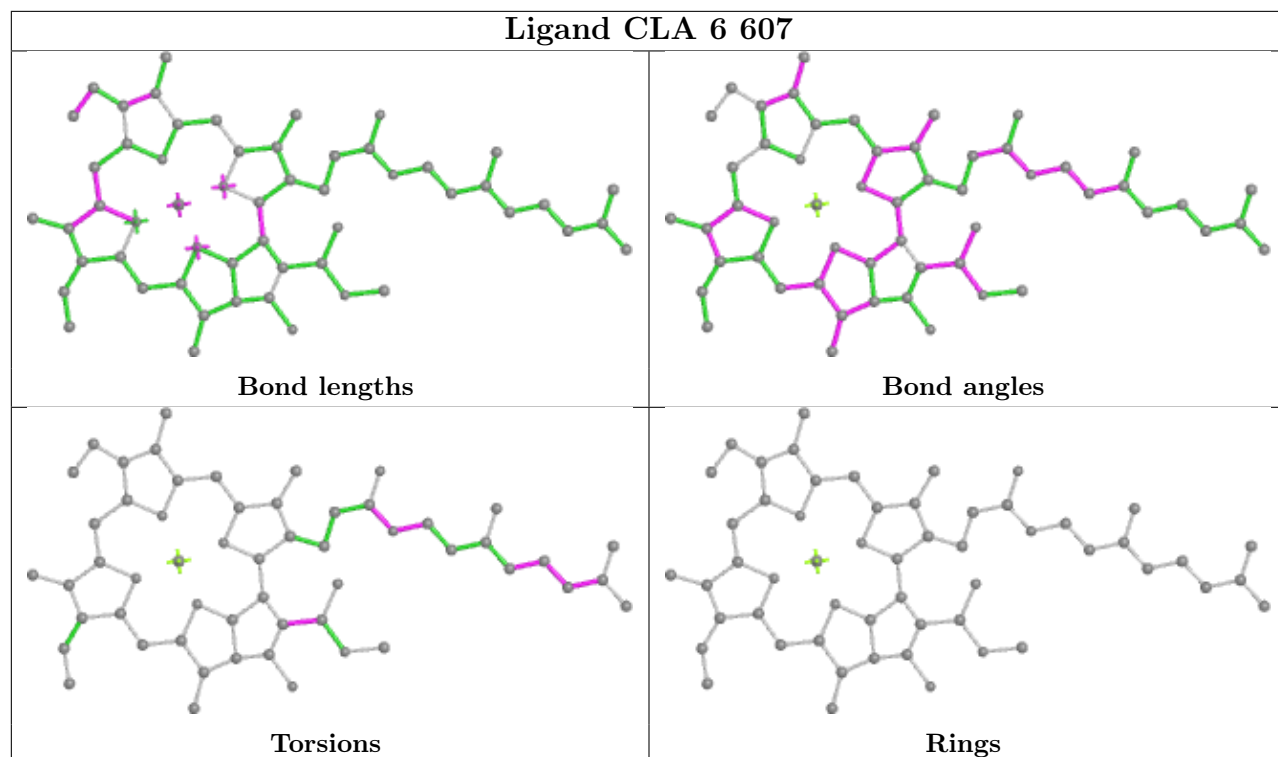
Ligand CLA 1 605



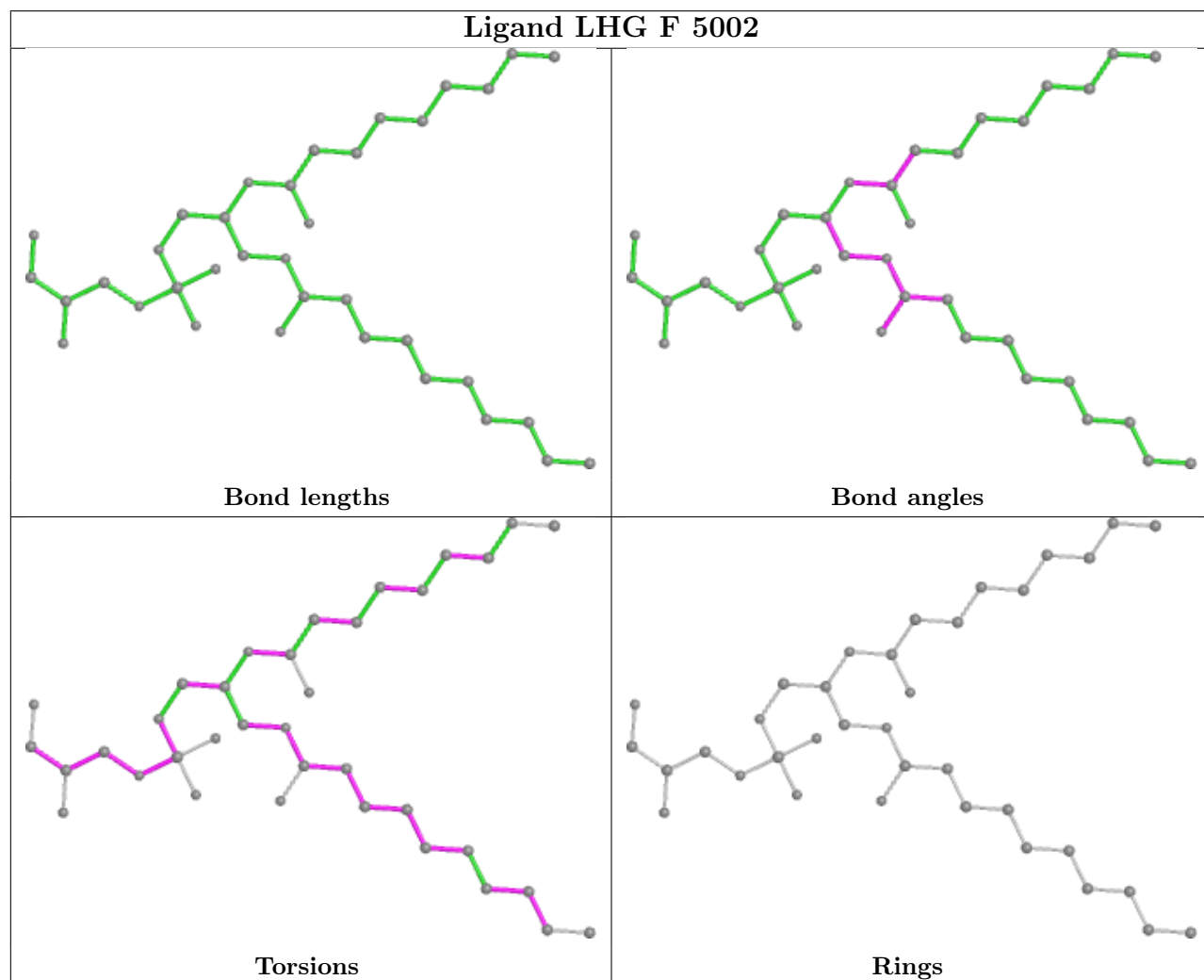


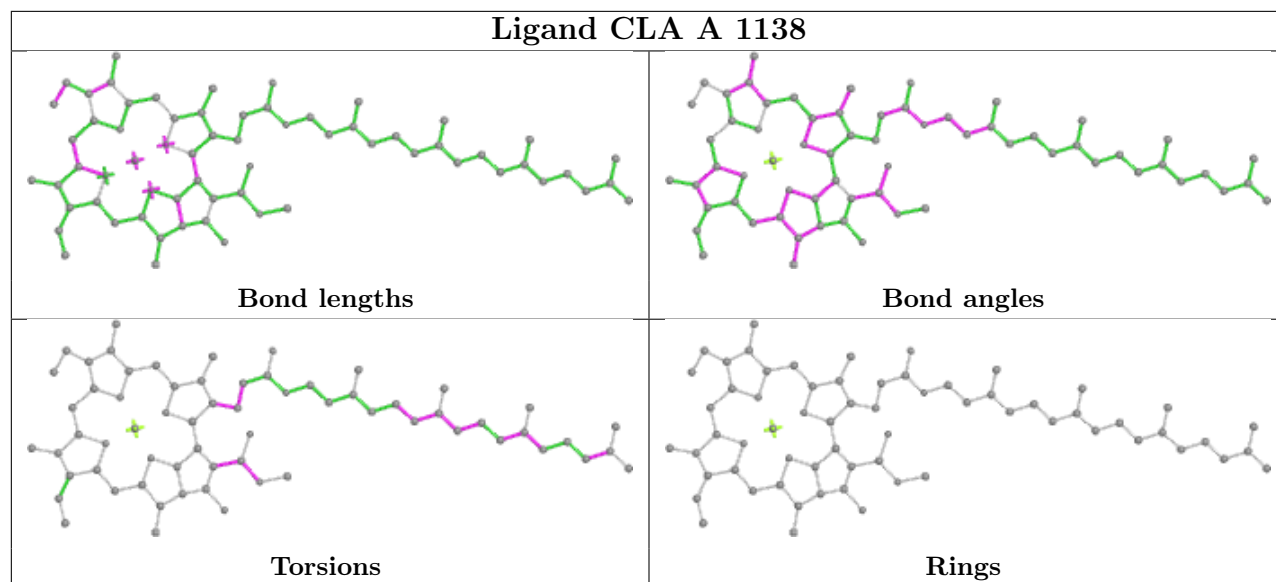
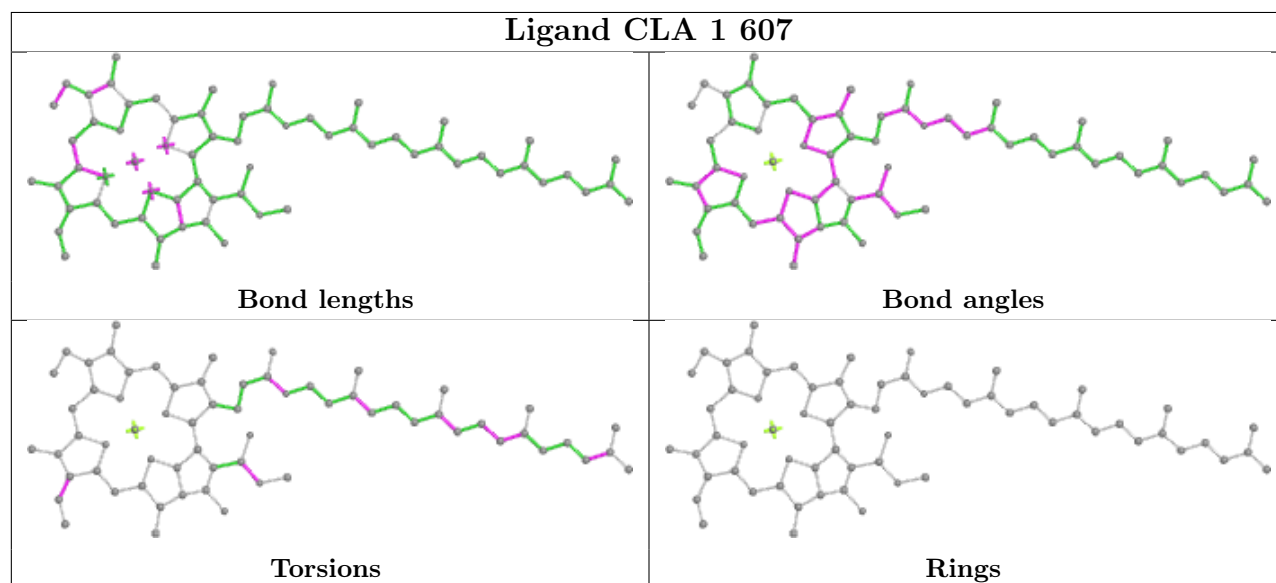


Ligand CLA 6 607

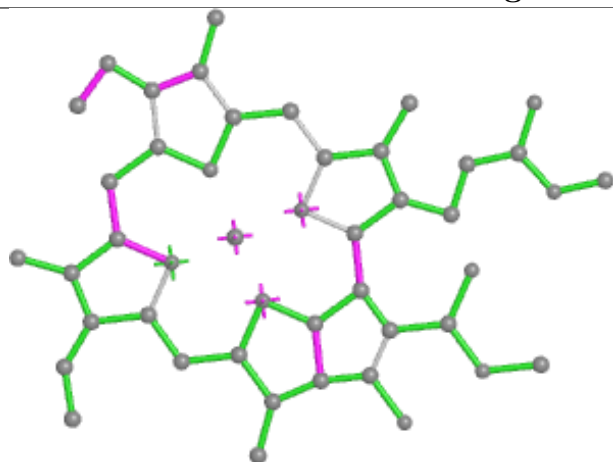


Ligand LHG F 5002

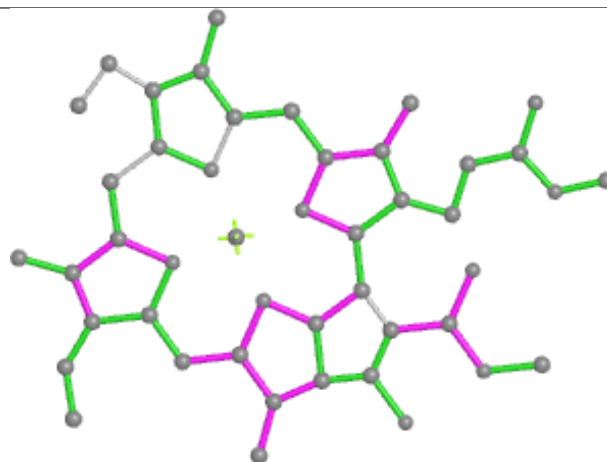


Ligand CLA A 1138**Ligand CLA 1 607**

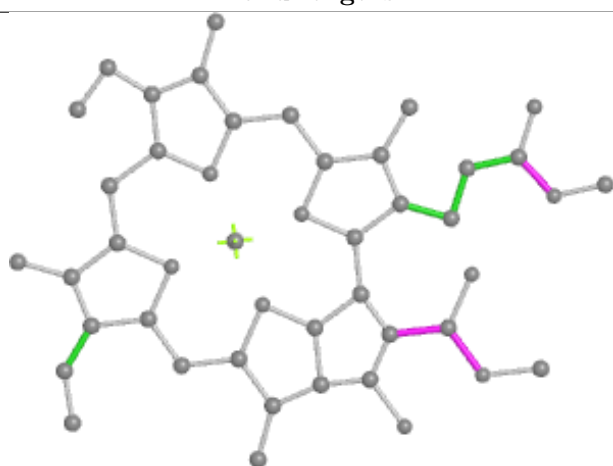
Ligand CLA K 1403



Bond lengths



Bond angles

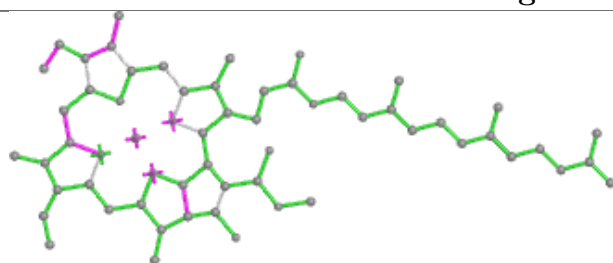


Torsions

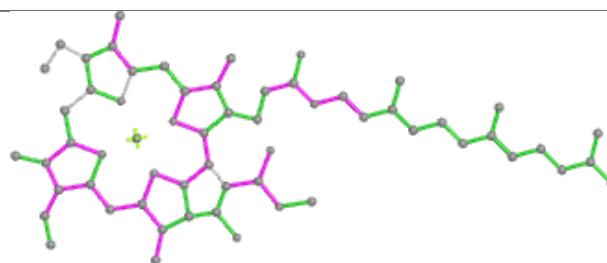


Rings

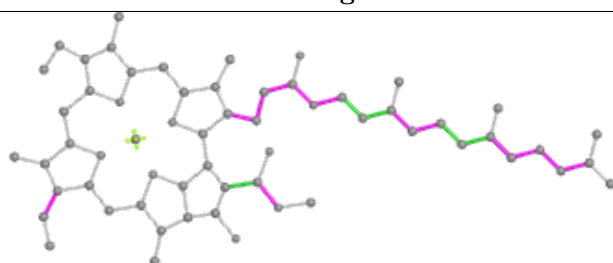
Ligand CLA 7 612



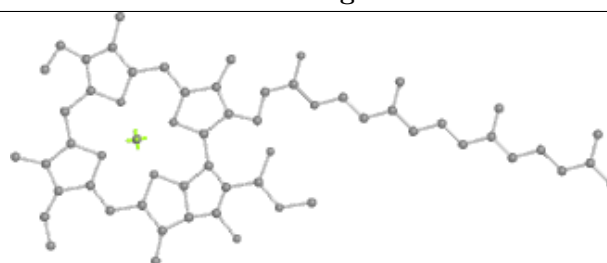
Bond lengths



Bond angles

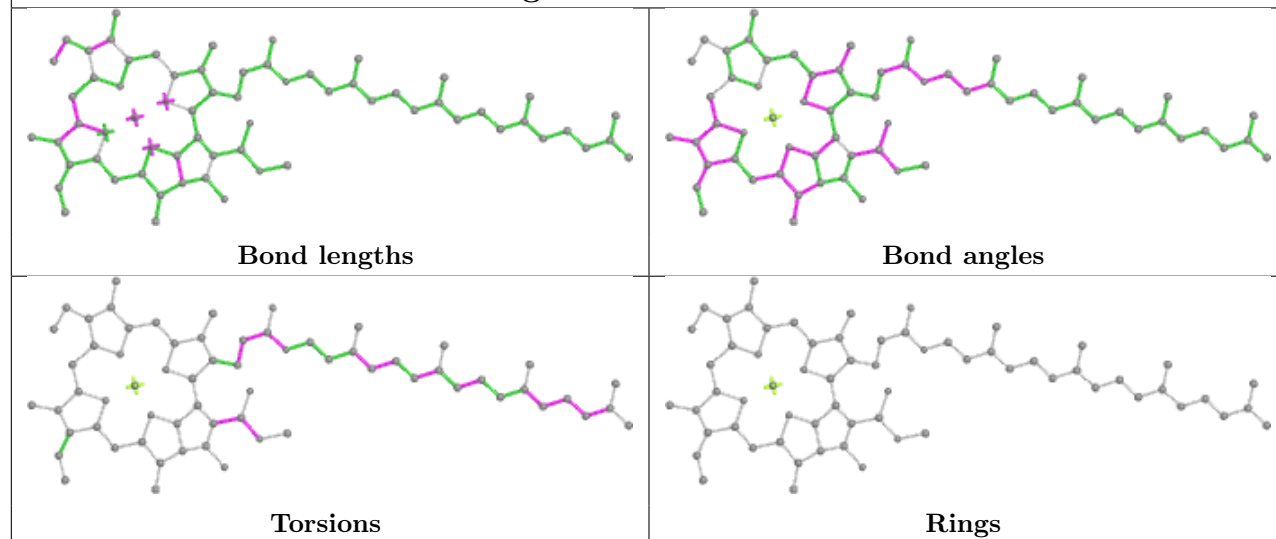


Torsions

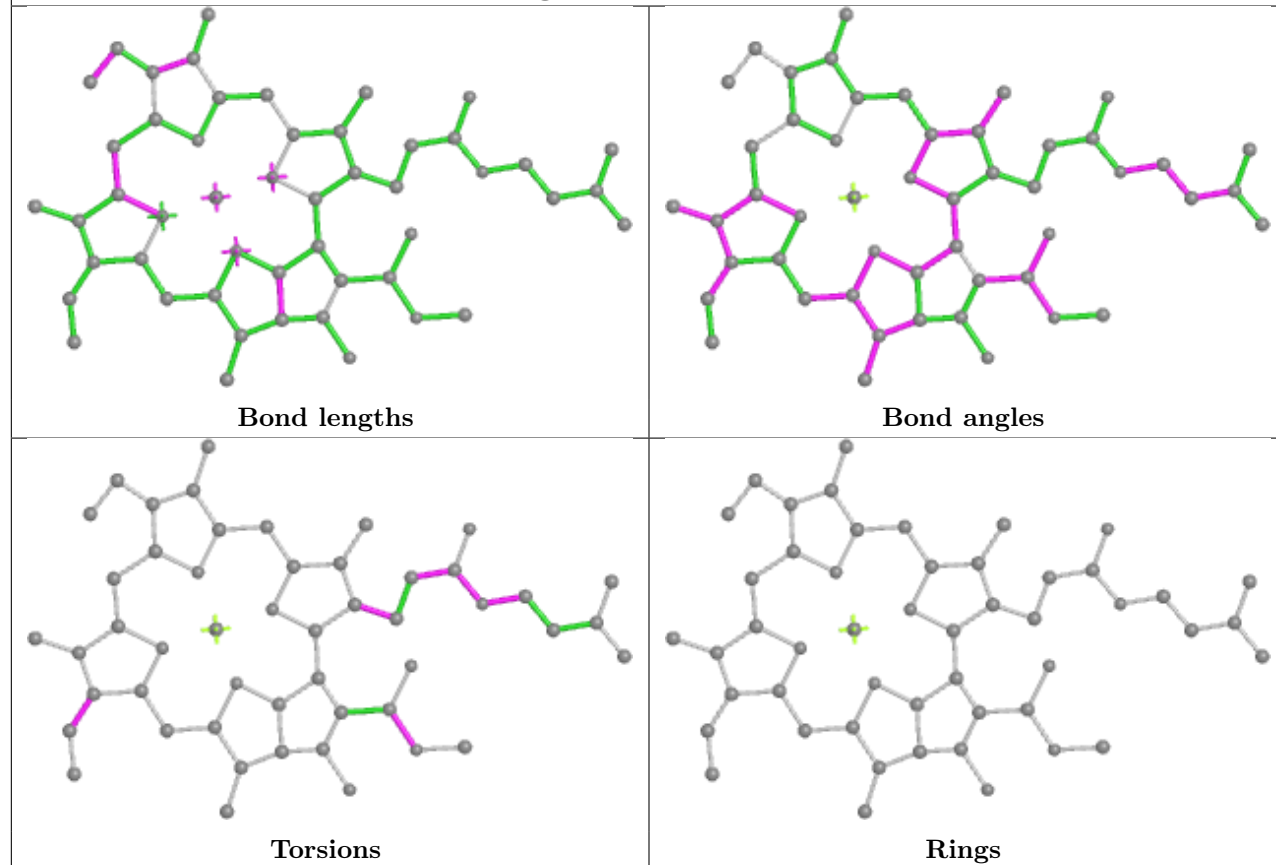


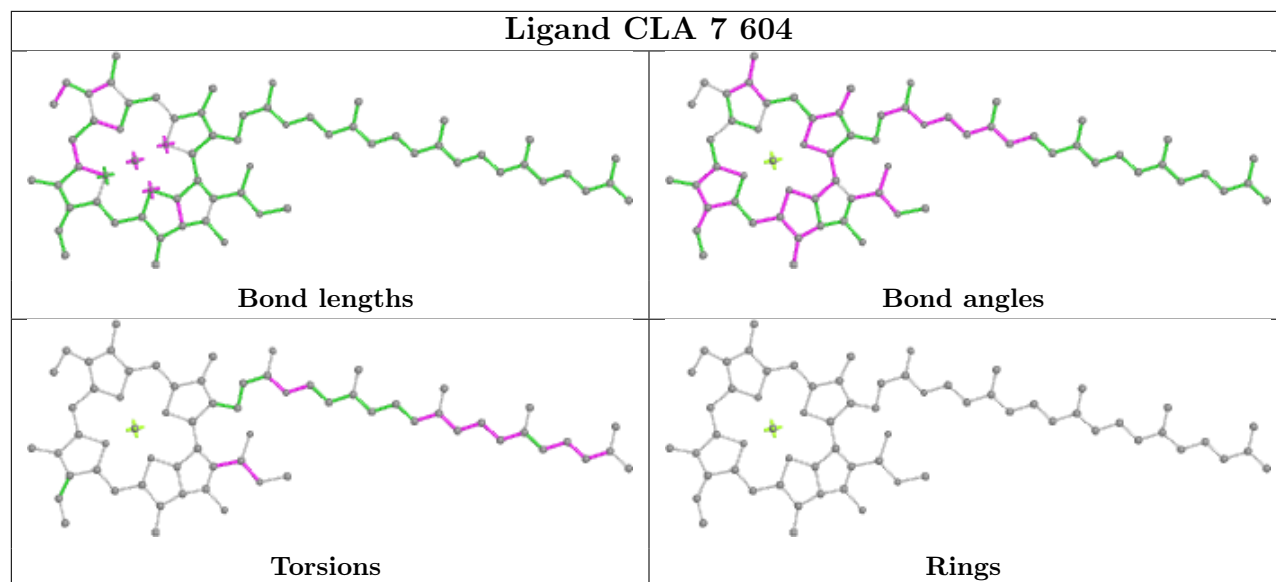
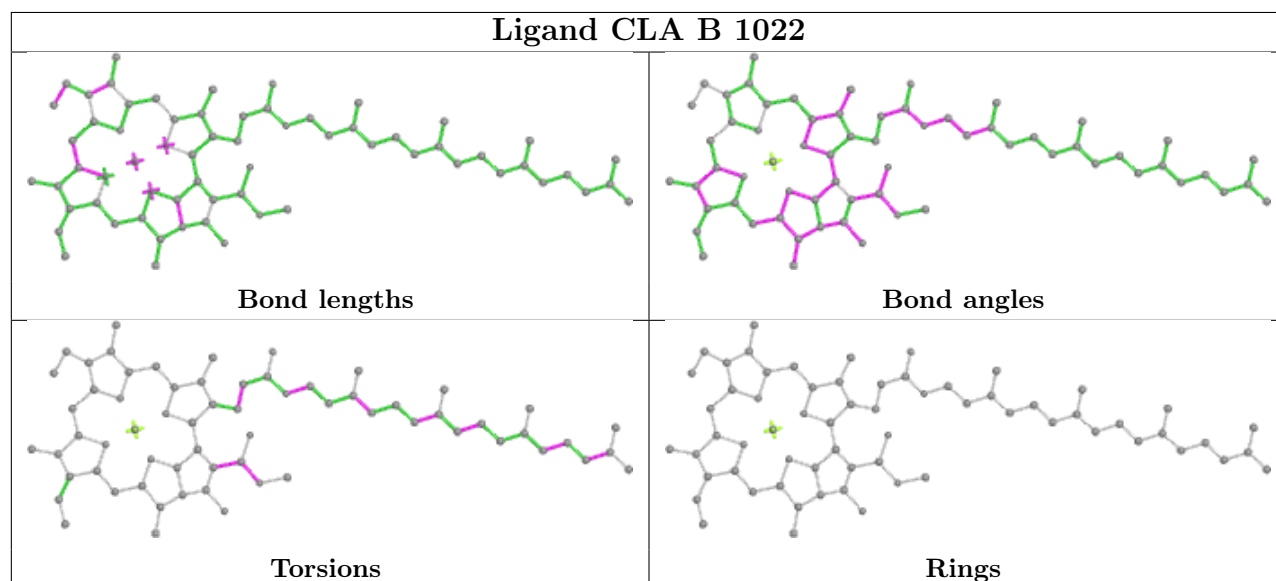
Rings

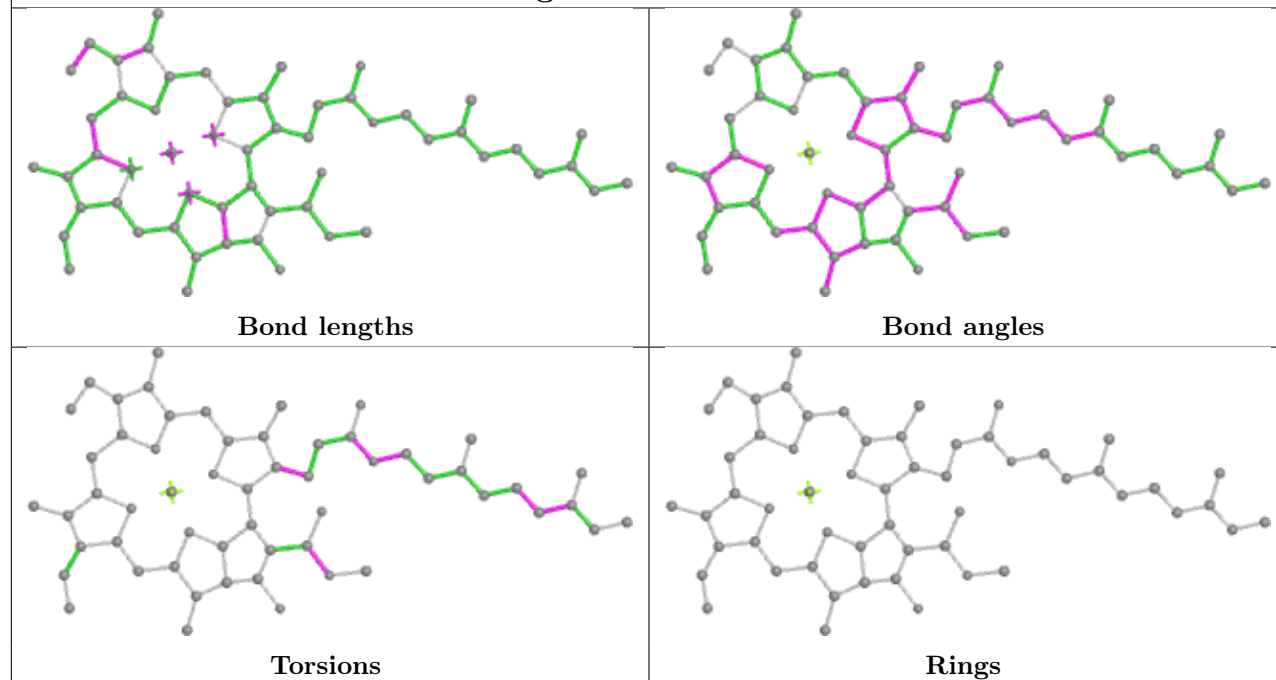
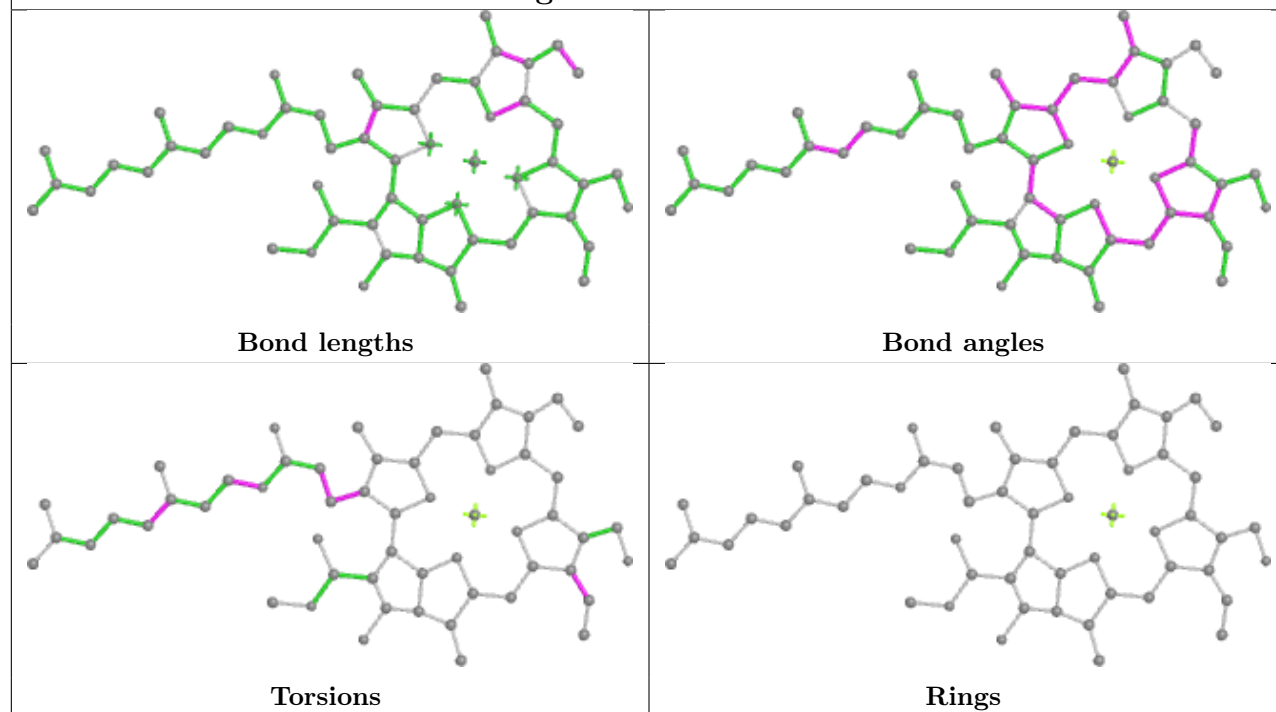
Ligand CLA A 1125



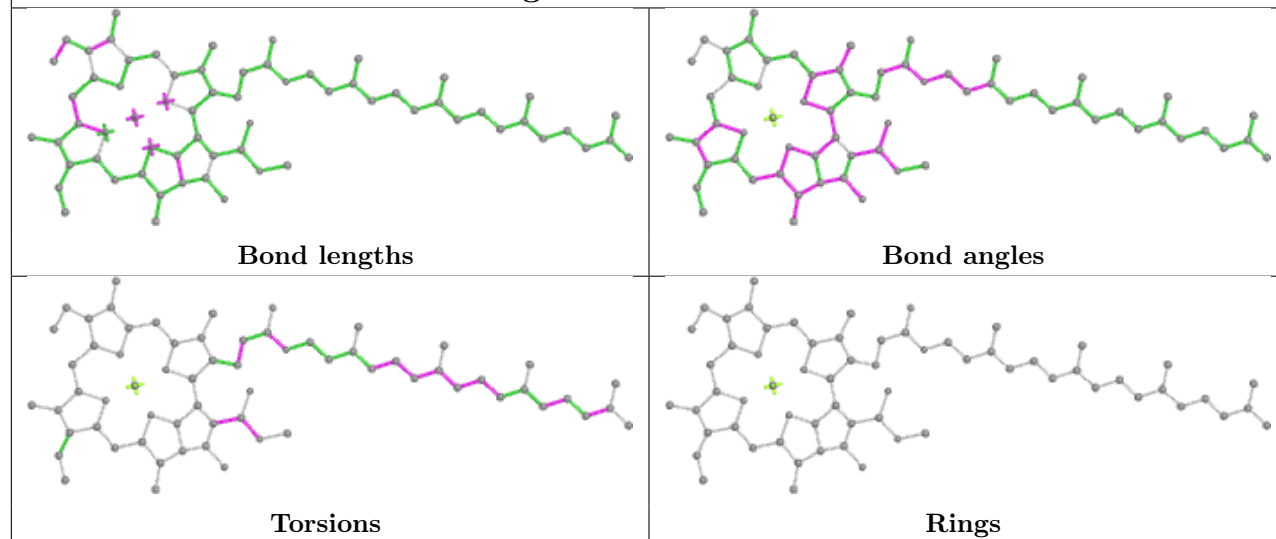
Ligand CLA 5 617



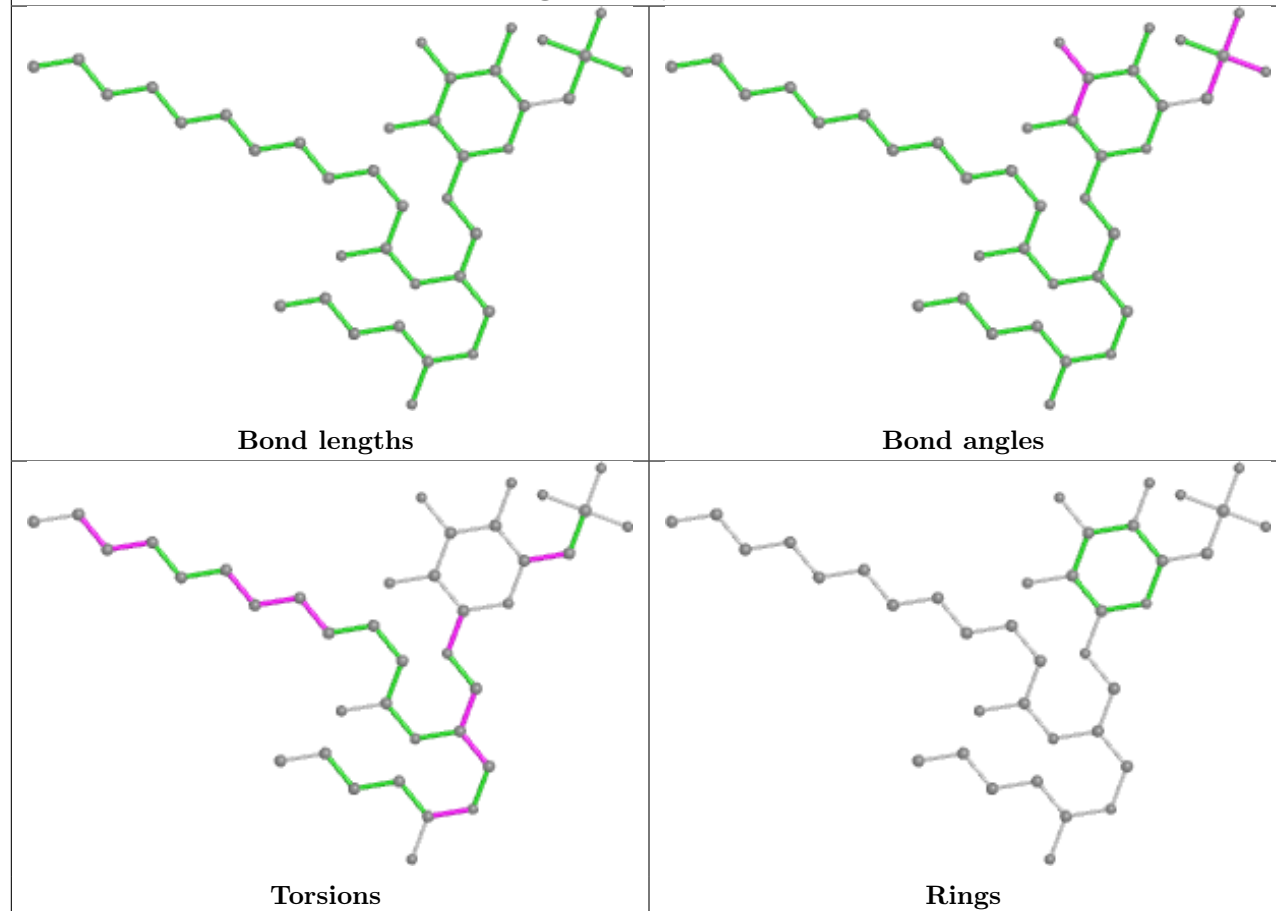
Ligand CLA 7 604**Ligand CLA B 1022**

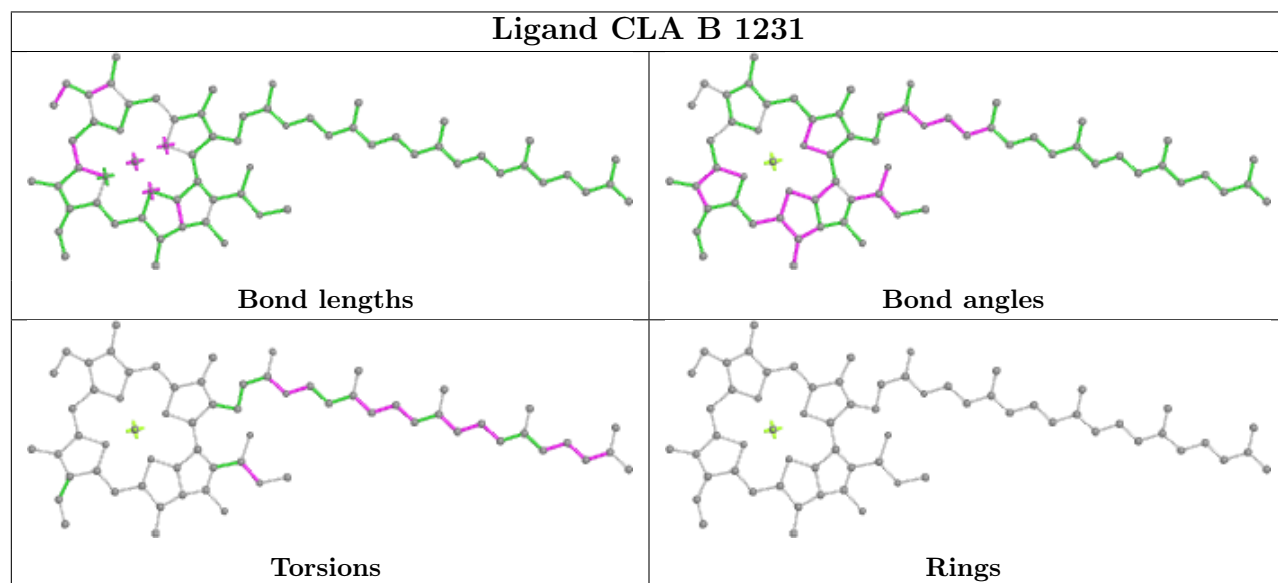
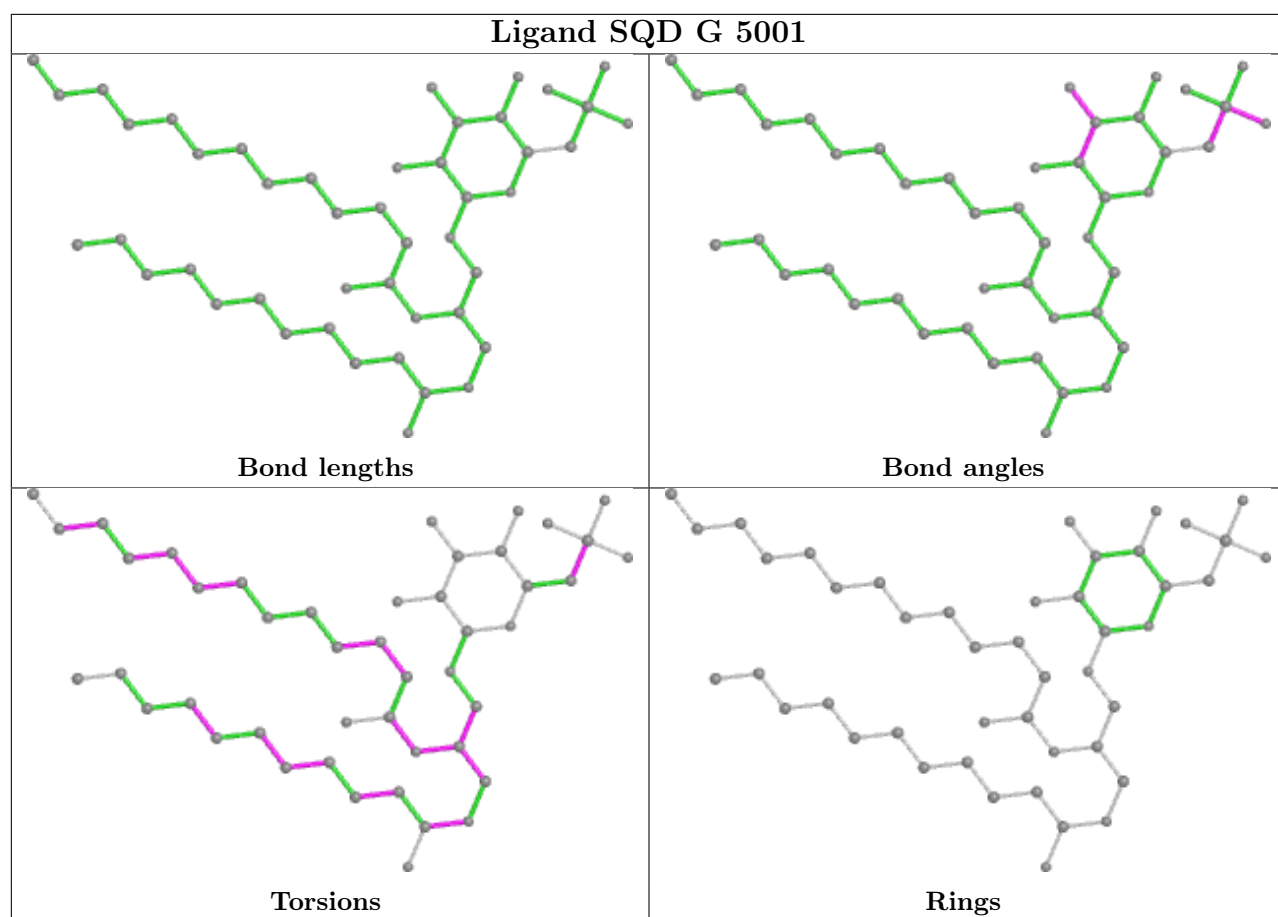
Ligand CLA 4 611**Ligand CHL 4 618**

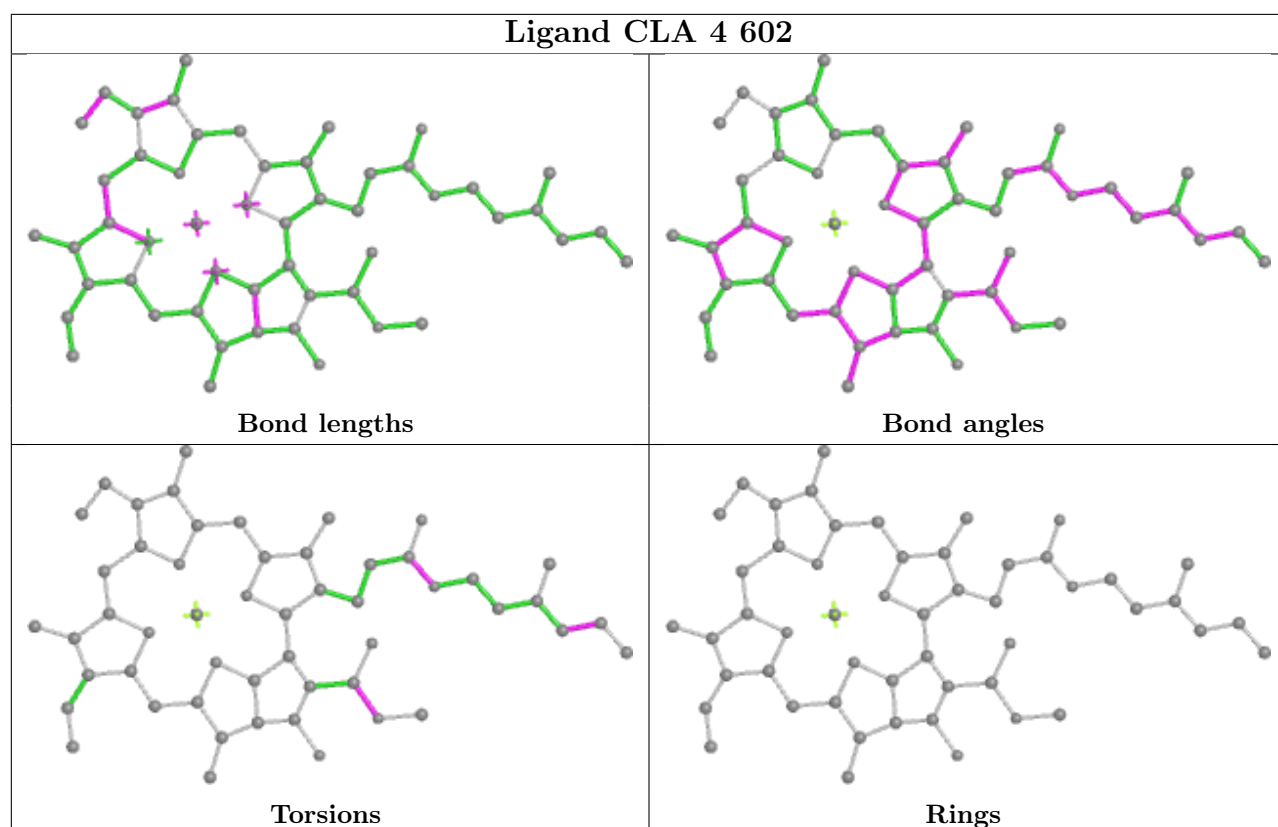
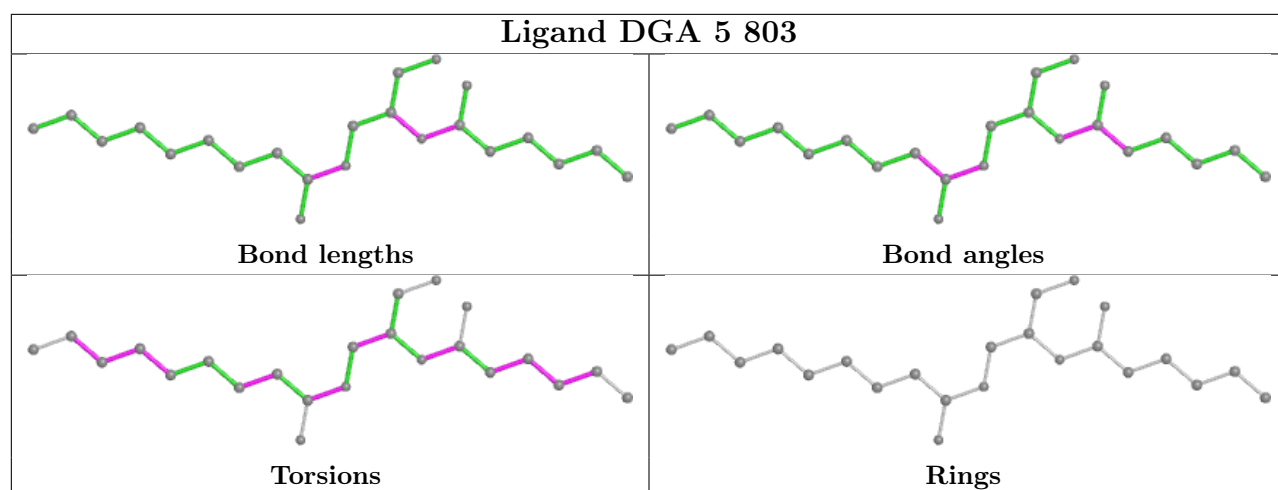
Ligand CLA A 1114

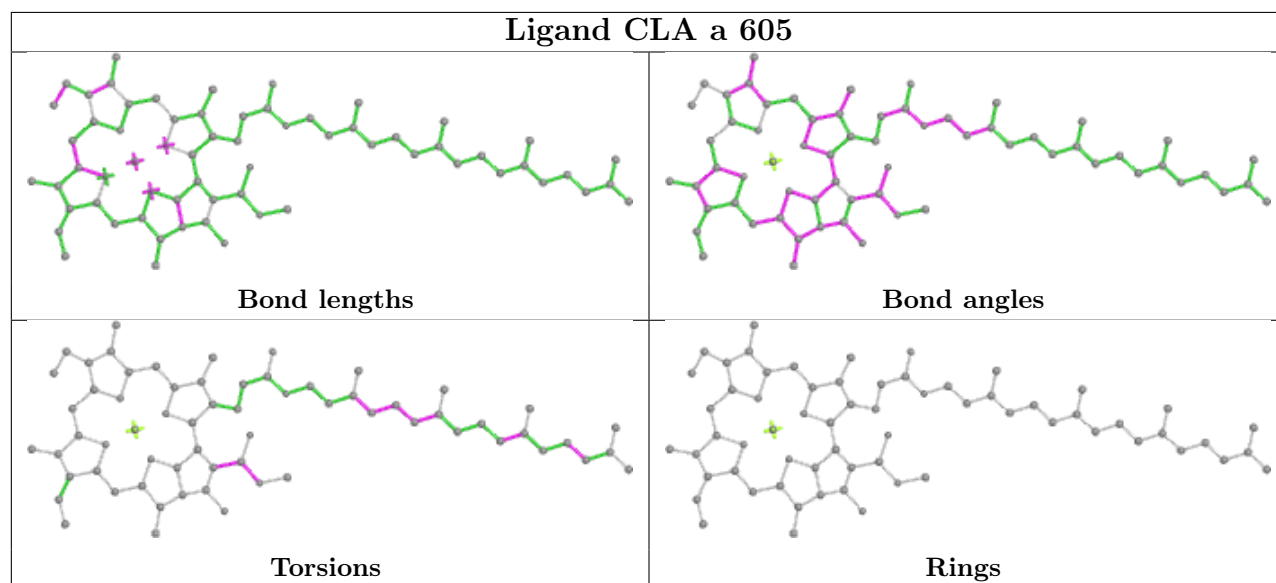
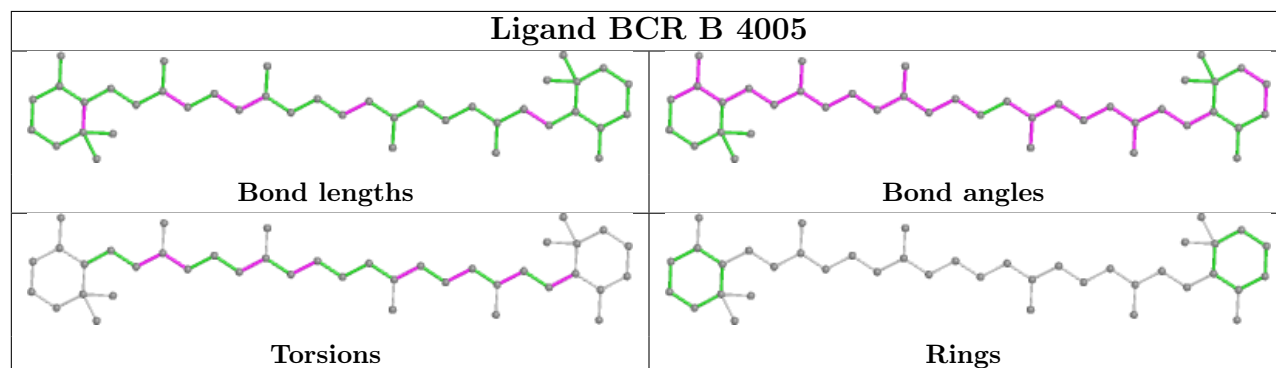
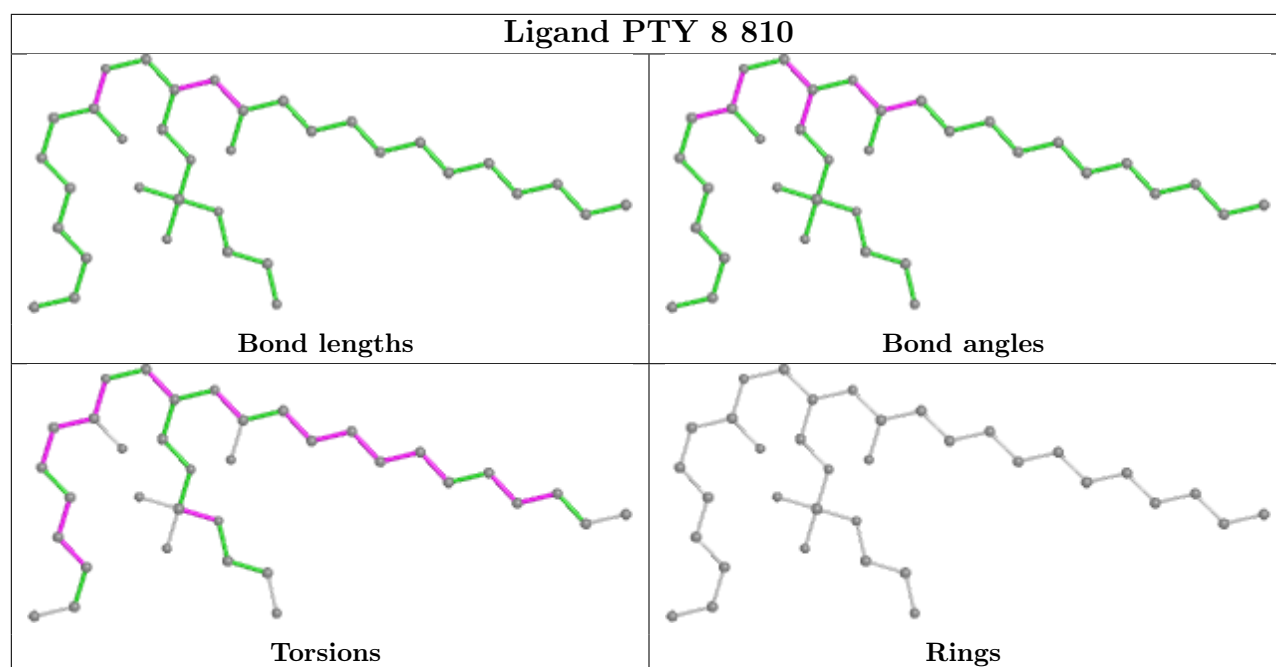


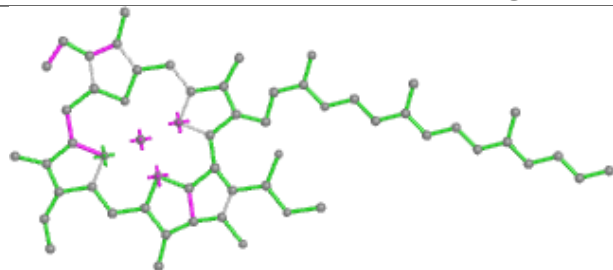
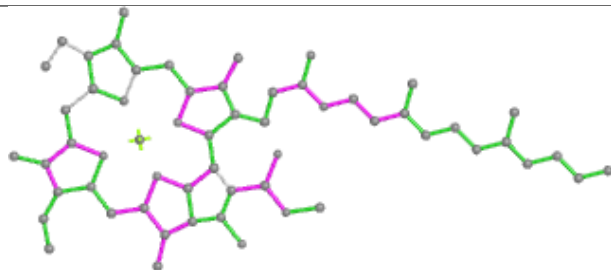
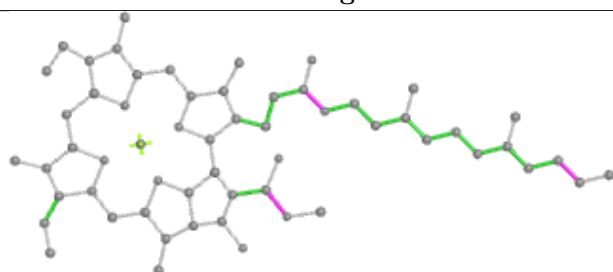
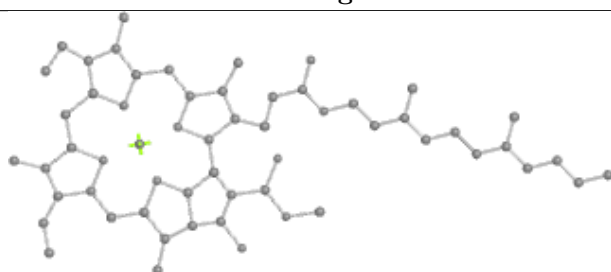
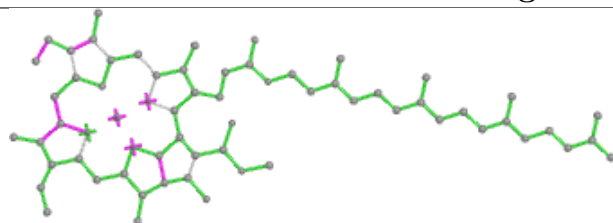
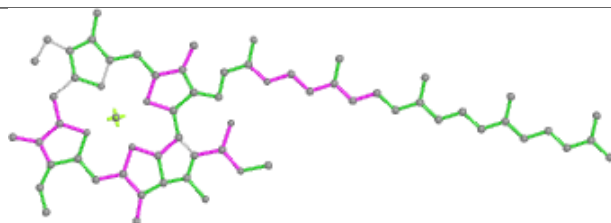
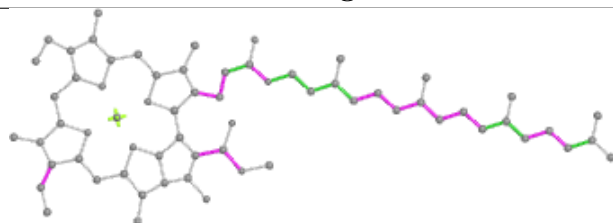
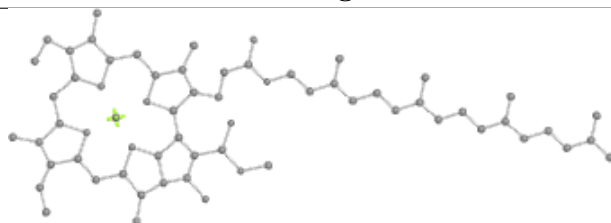
Ligand SQD 7 805



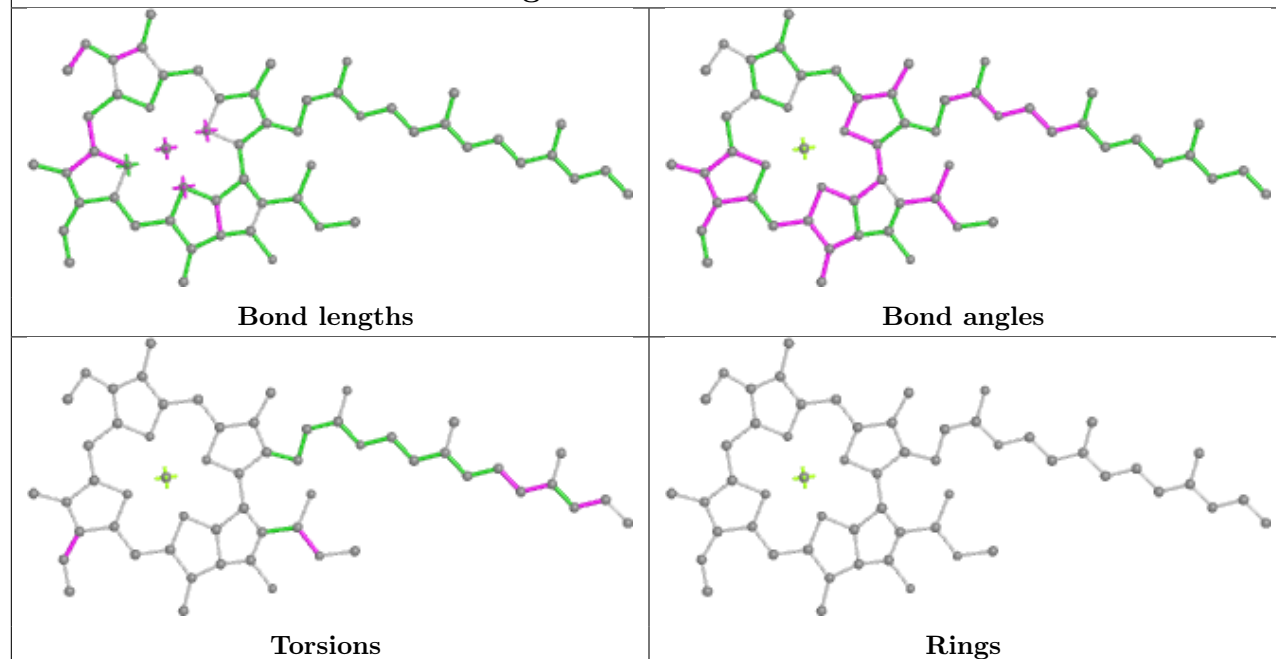




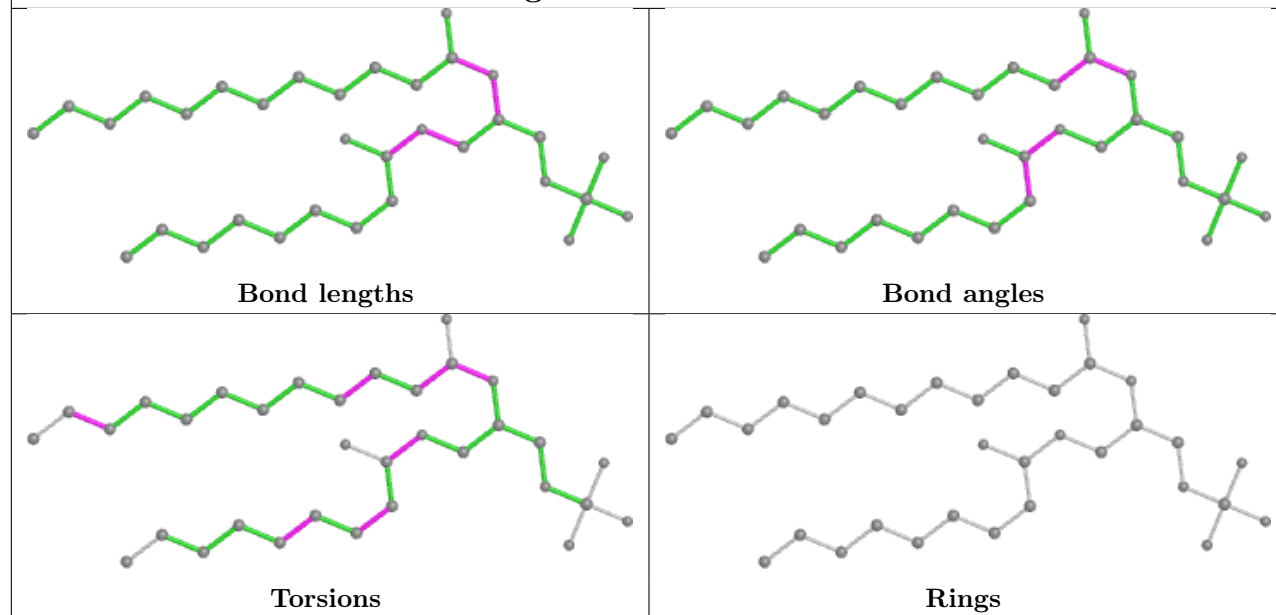


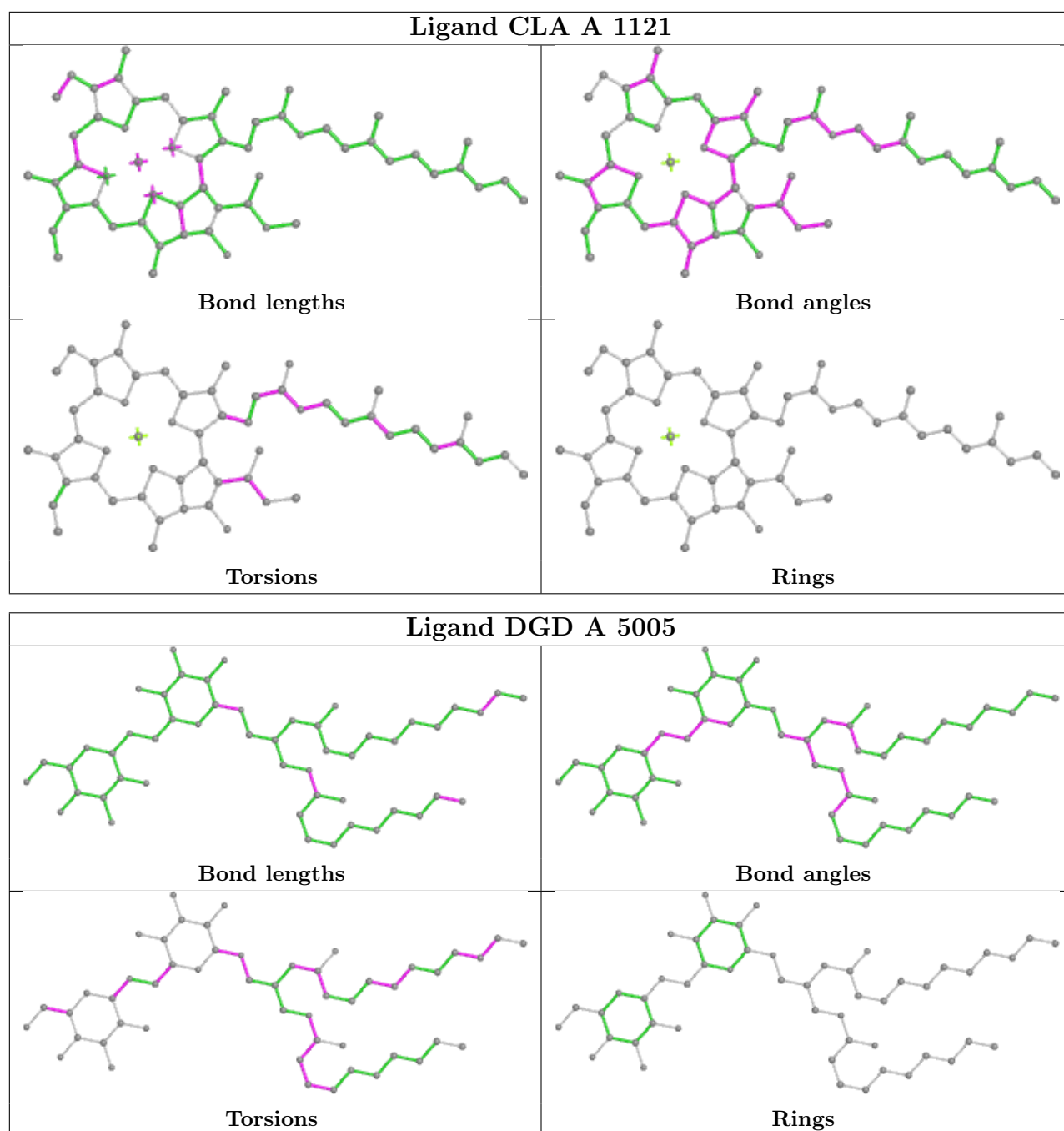
Ligand CLA B 1222**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 1 604****Bond lengths****Bond angles****Torsions****Rings**

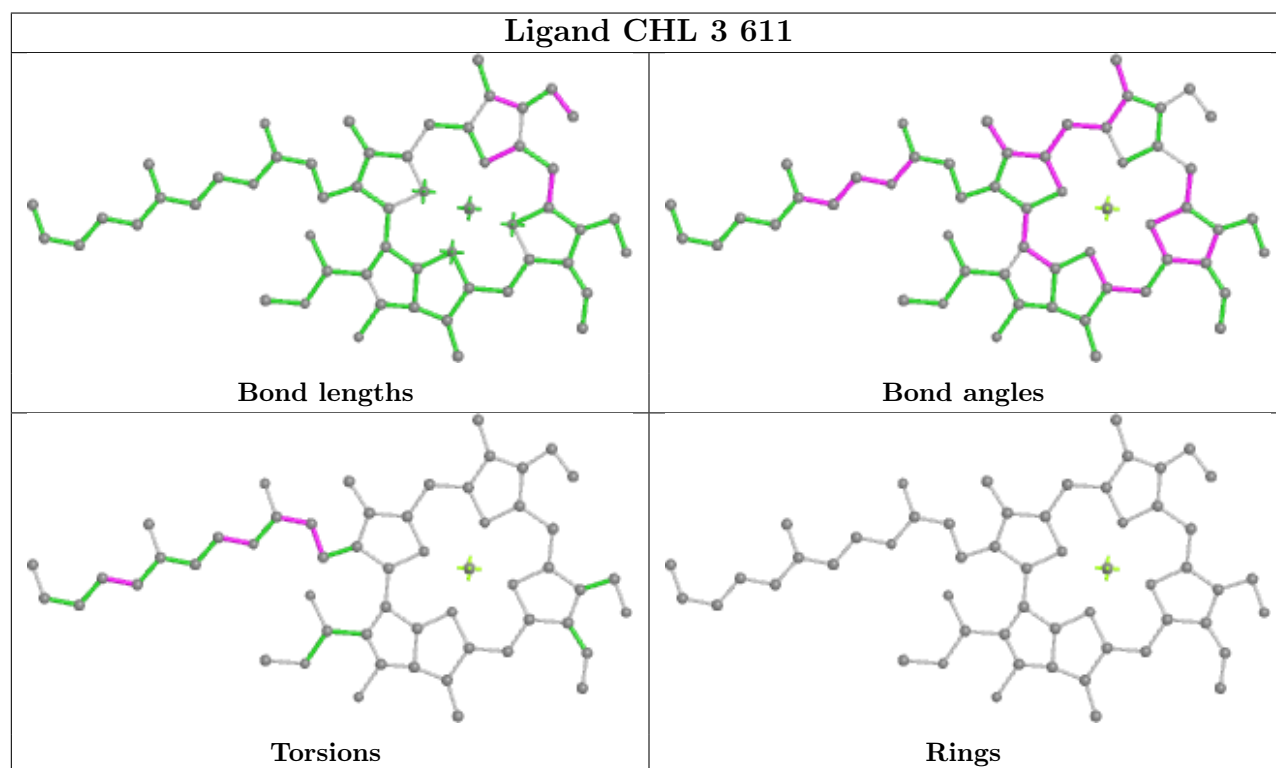
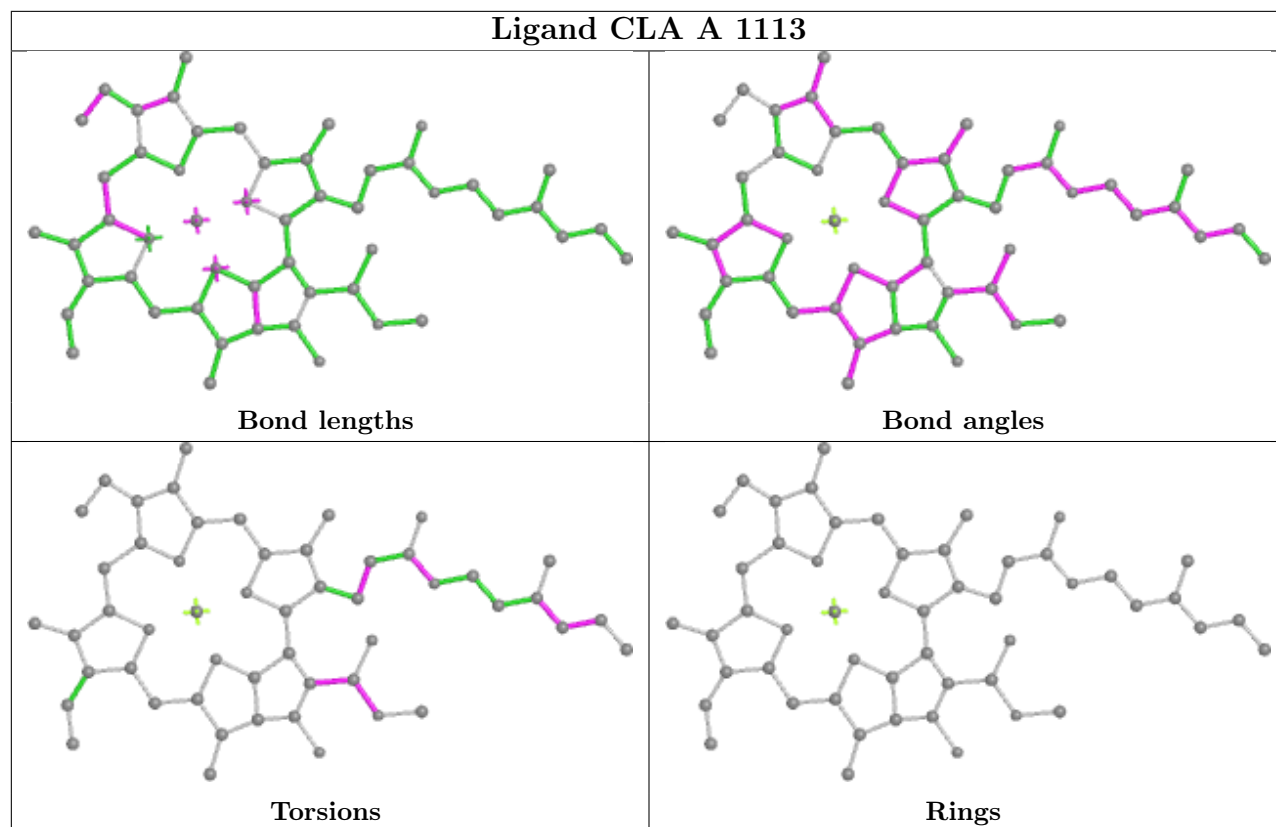
Ligand CLA A 1105

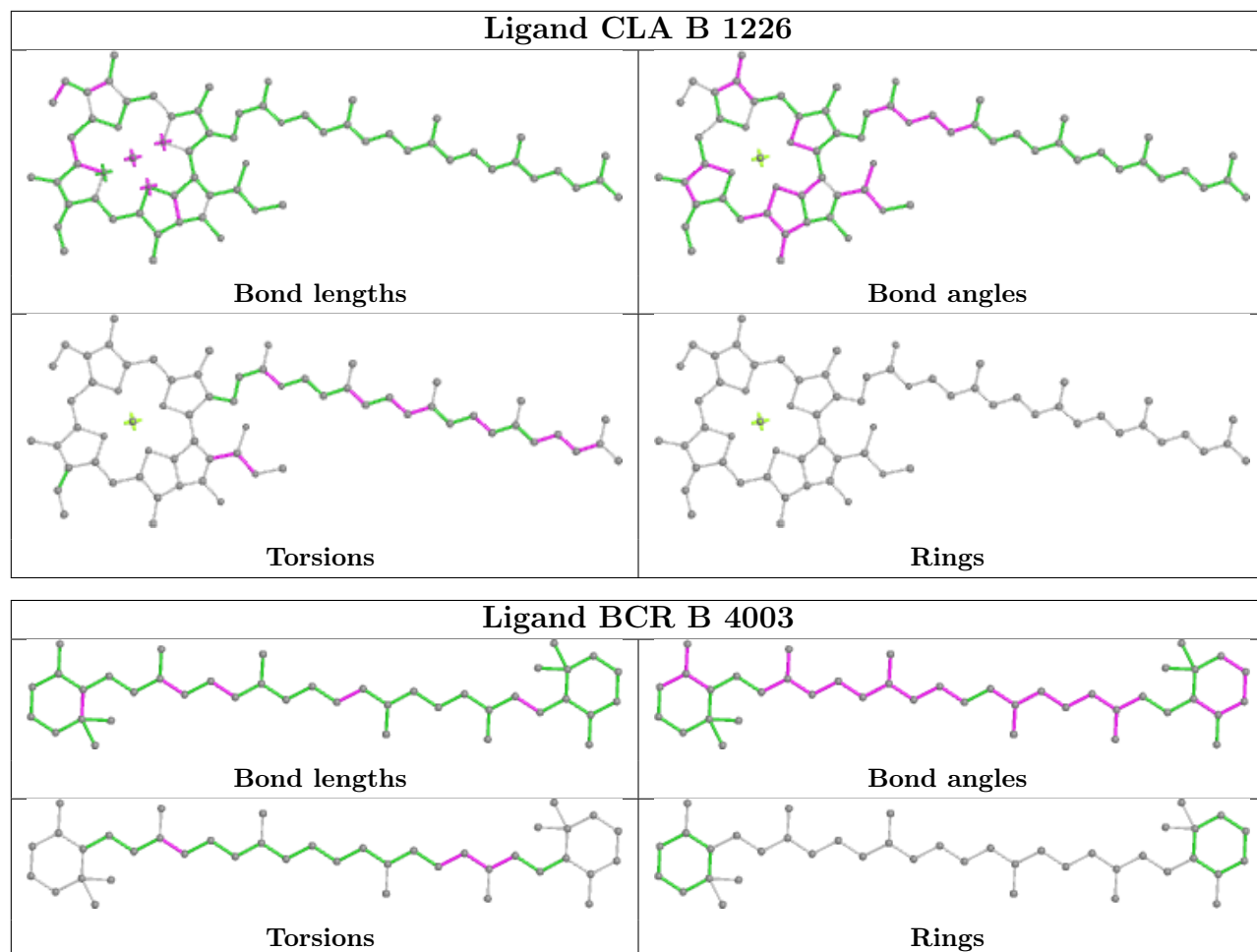


Ligand 3PH A 5007

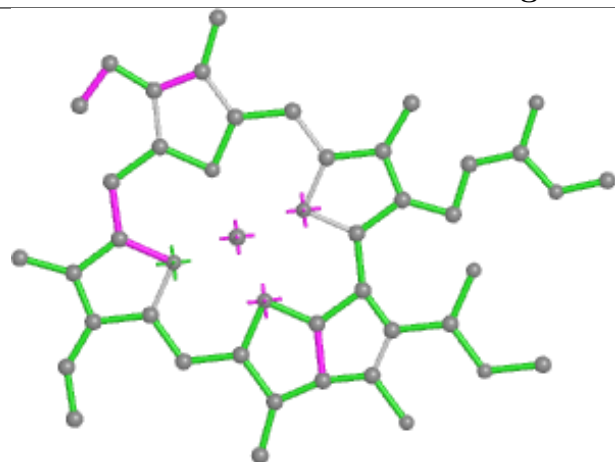




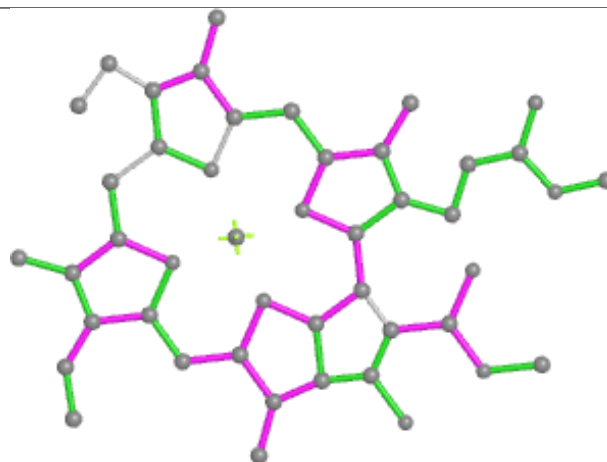




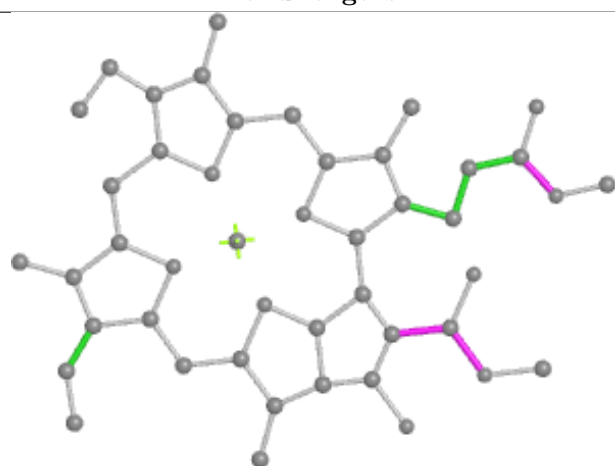
Ligand CLA a 615



Bond lengths



Bond angles

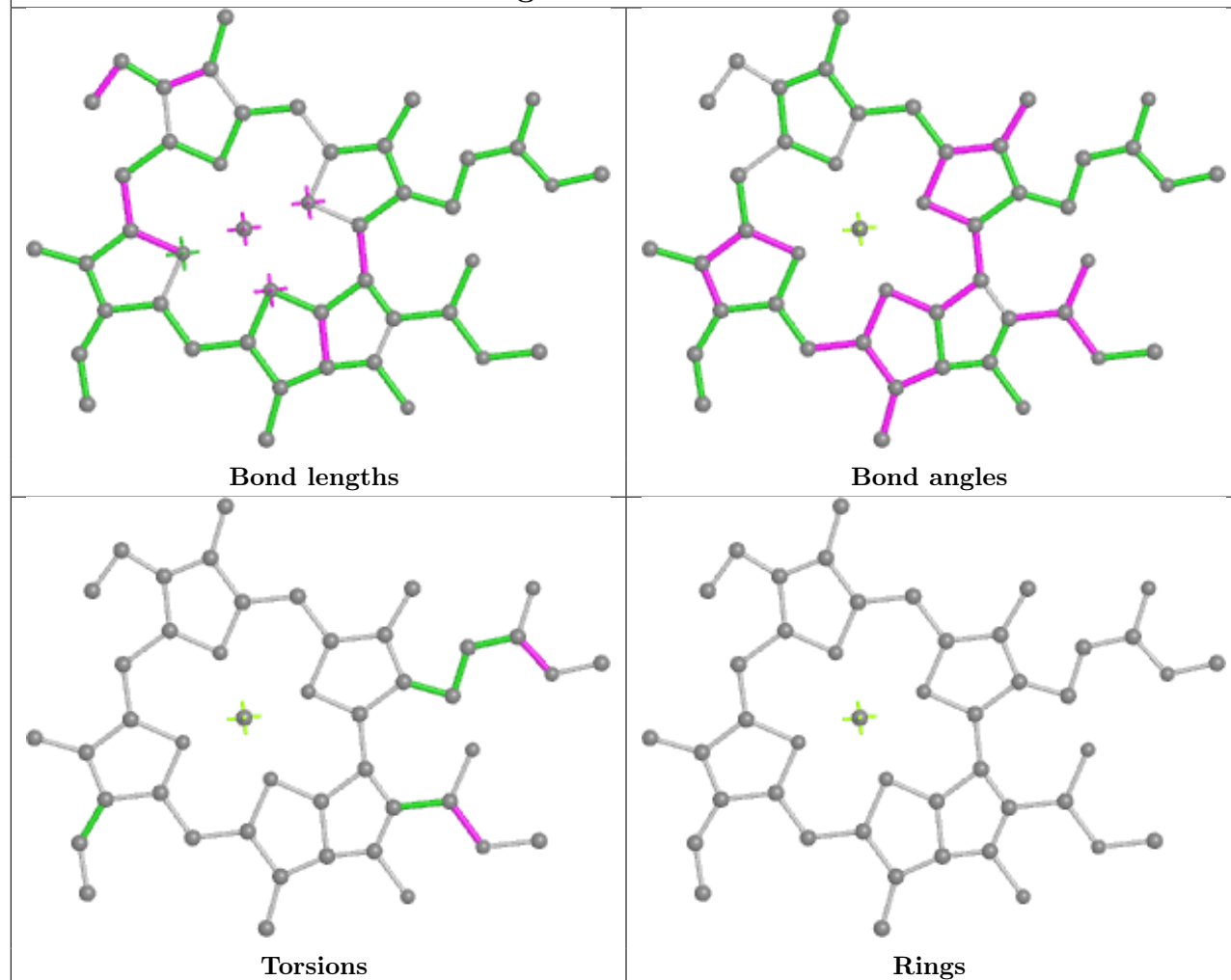


Torsions

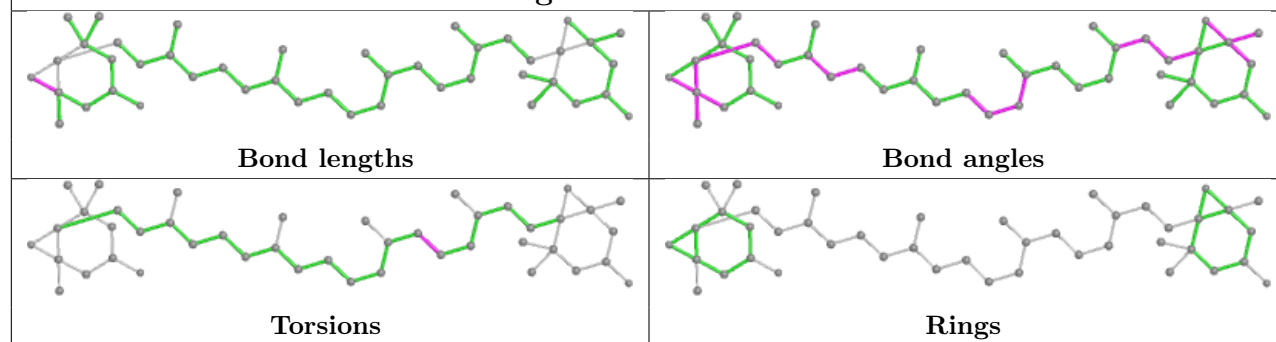


Rings

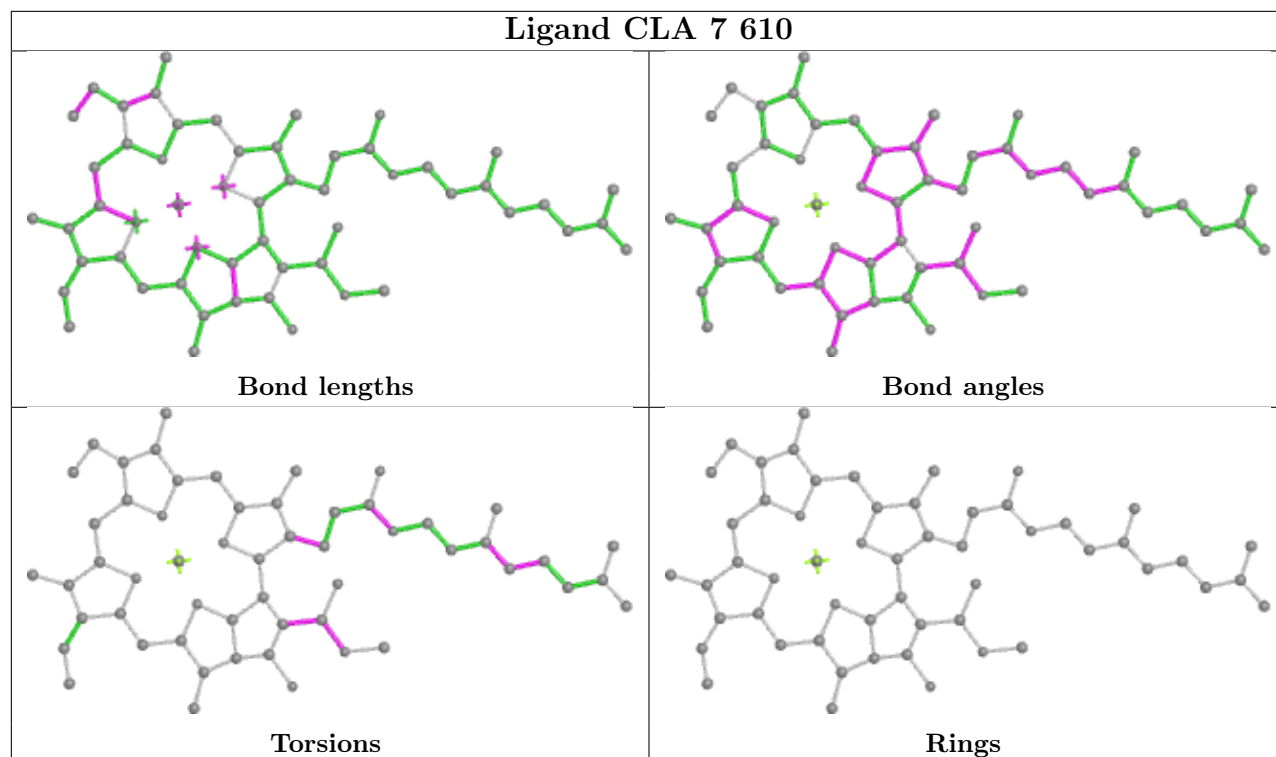
Ligand CLA 5 614



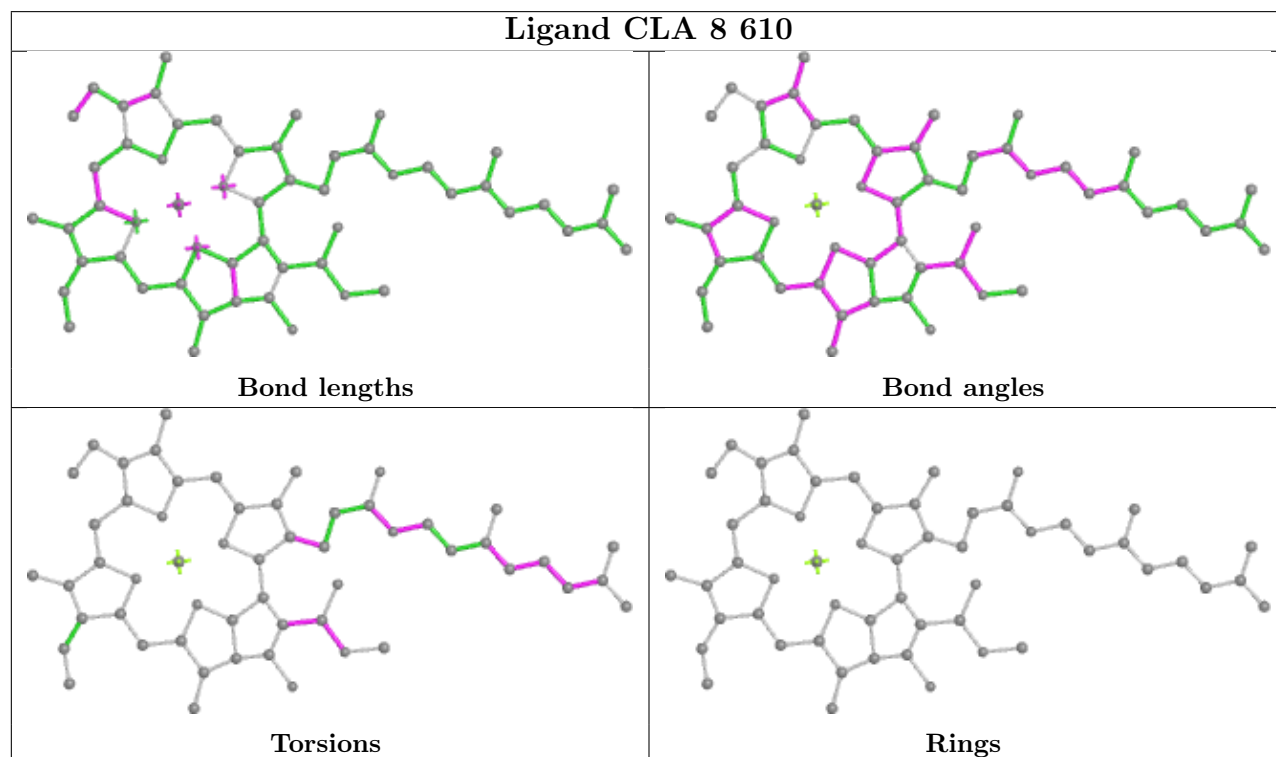
Ligand XAT 7 502

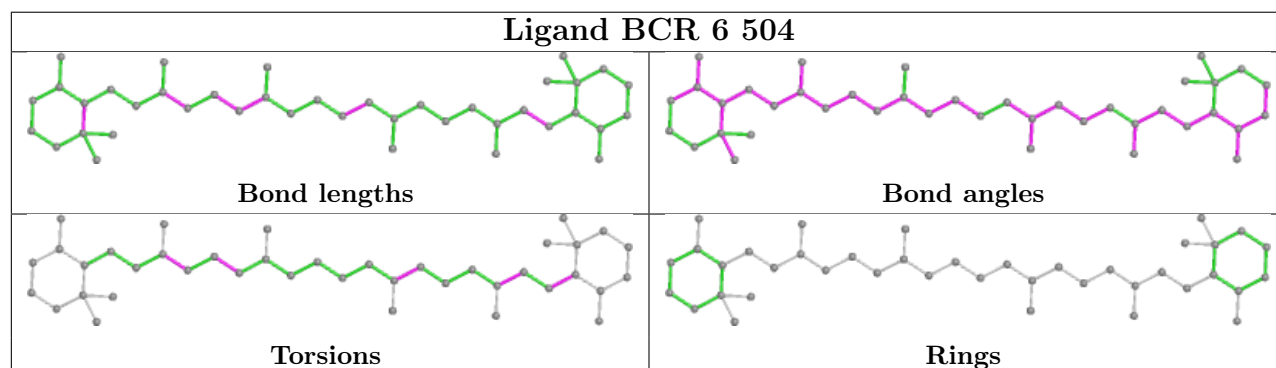
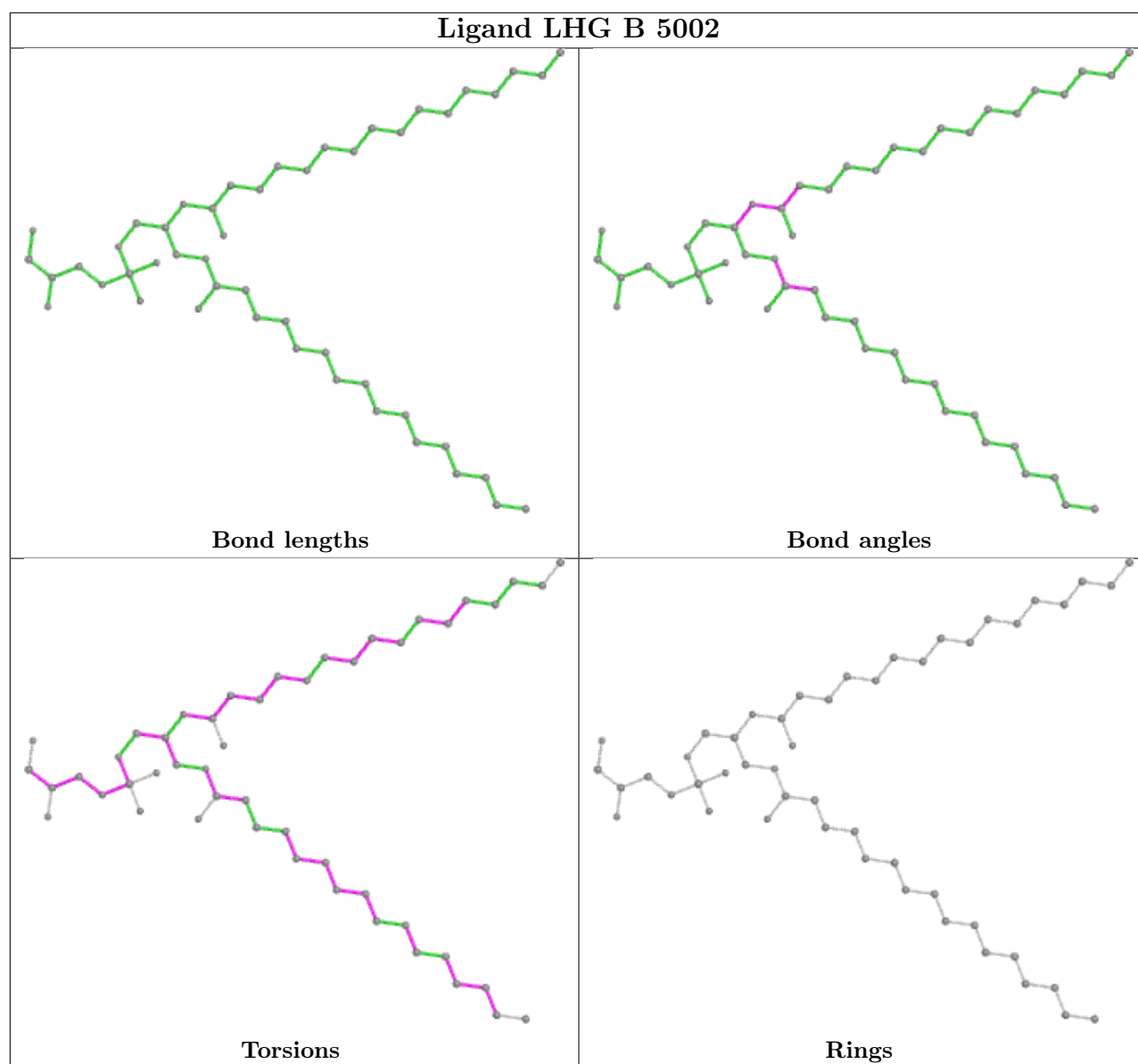


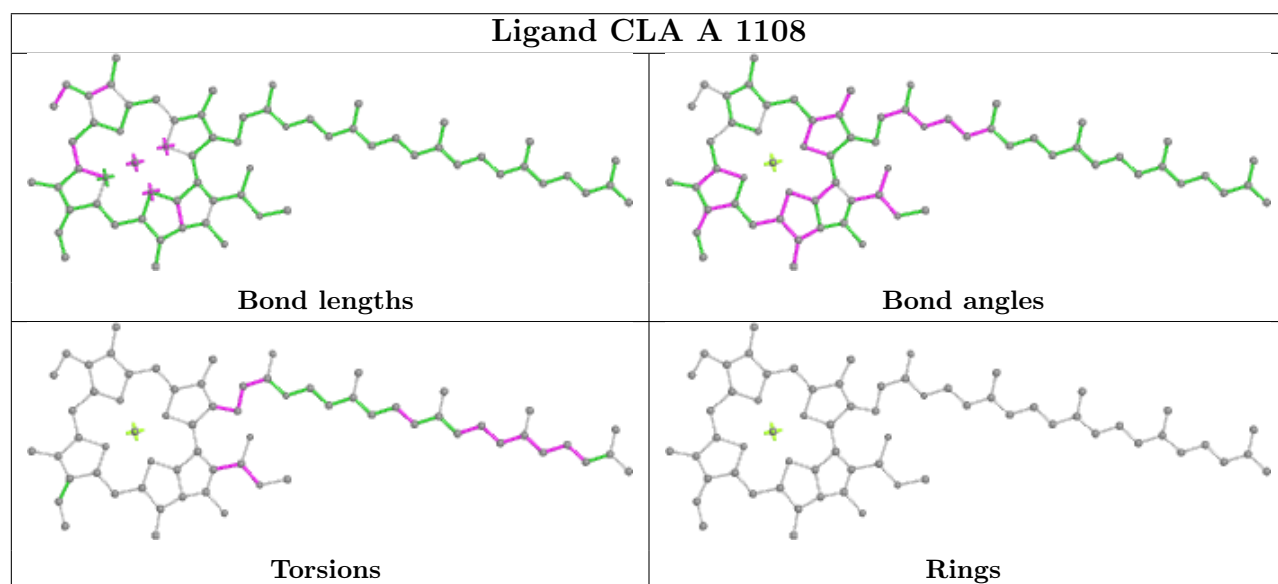
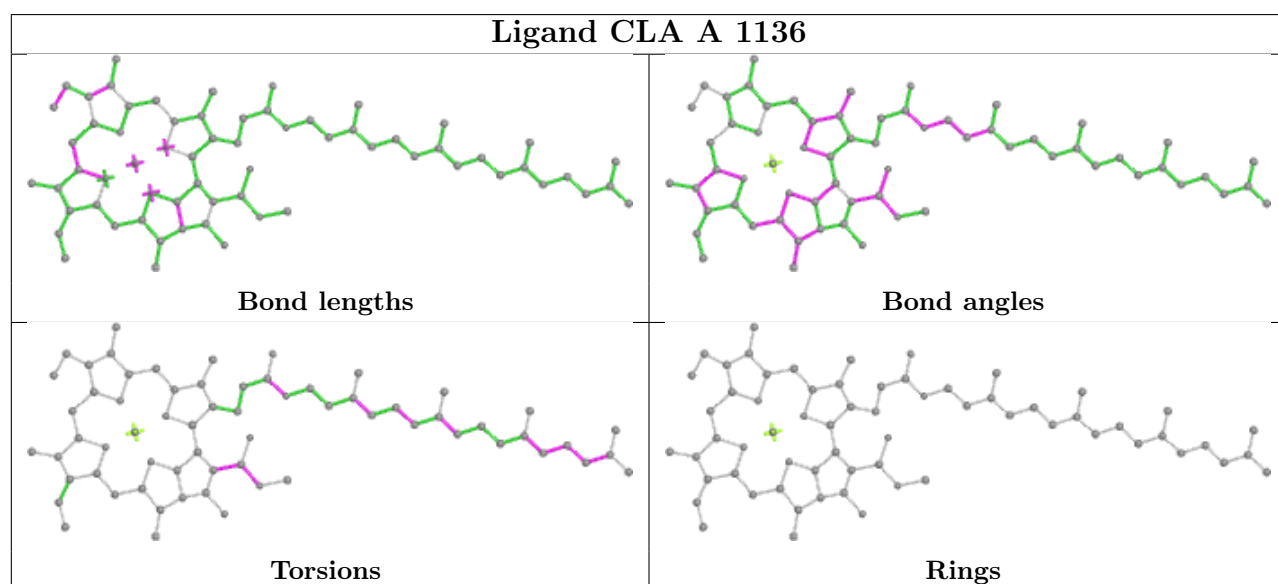
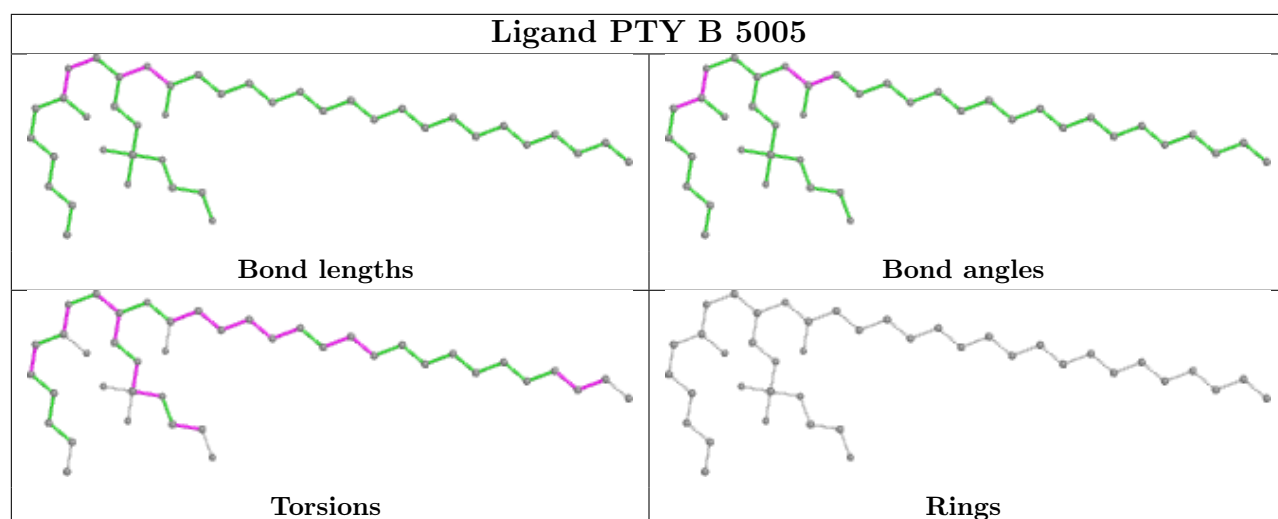
Ligand CLA 7 610



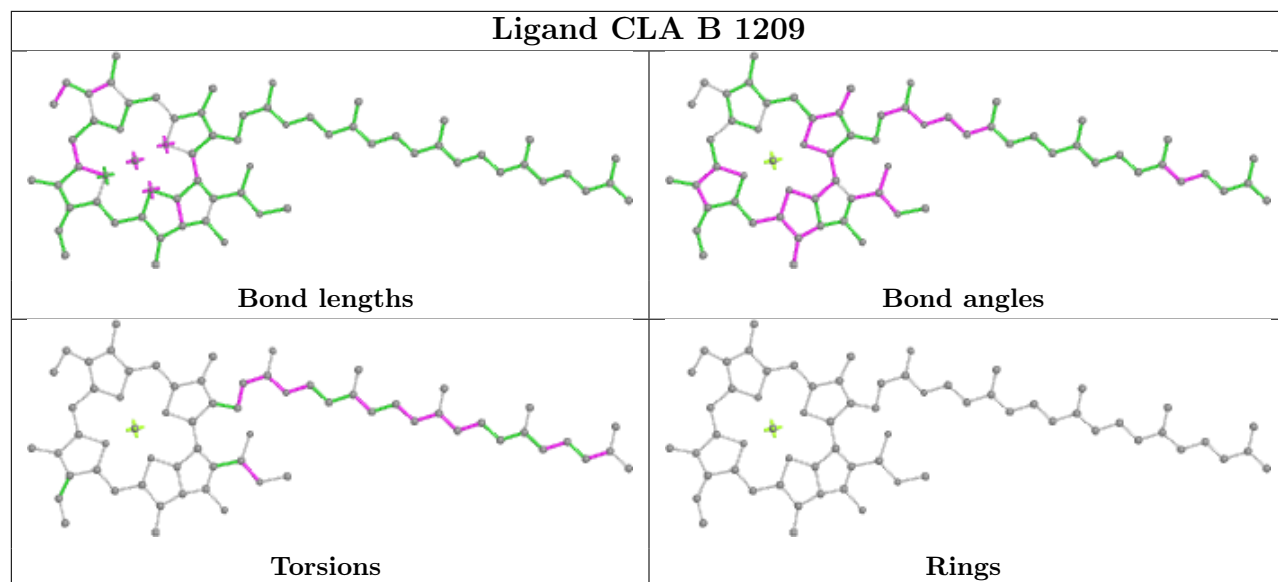
Ligand CLA 8 610



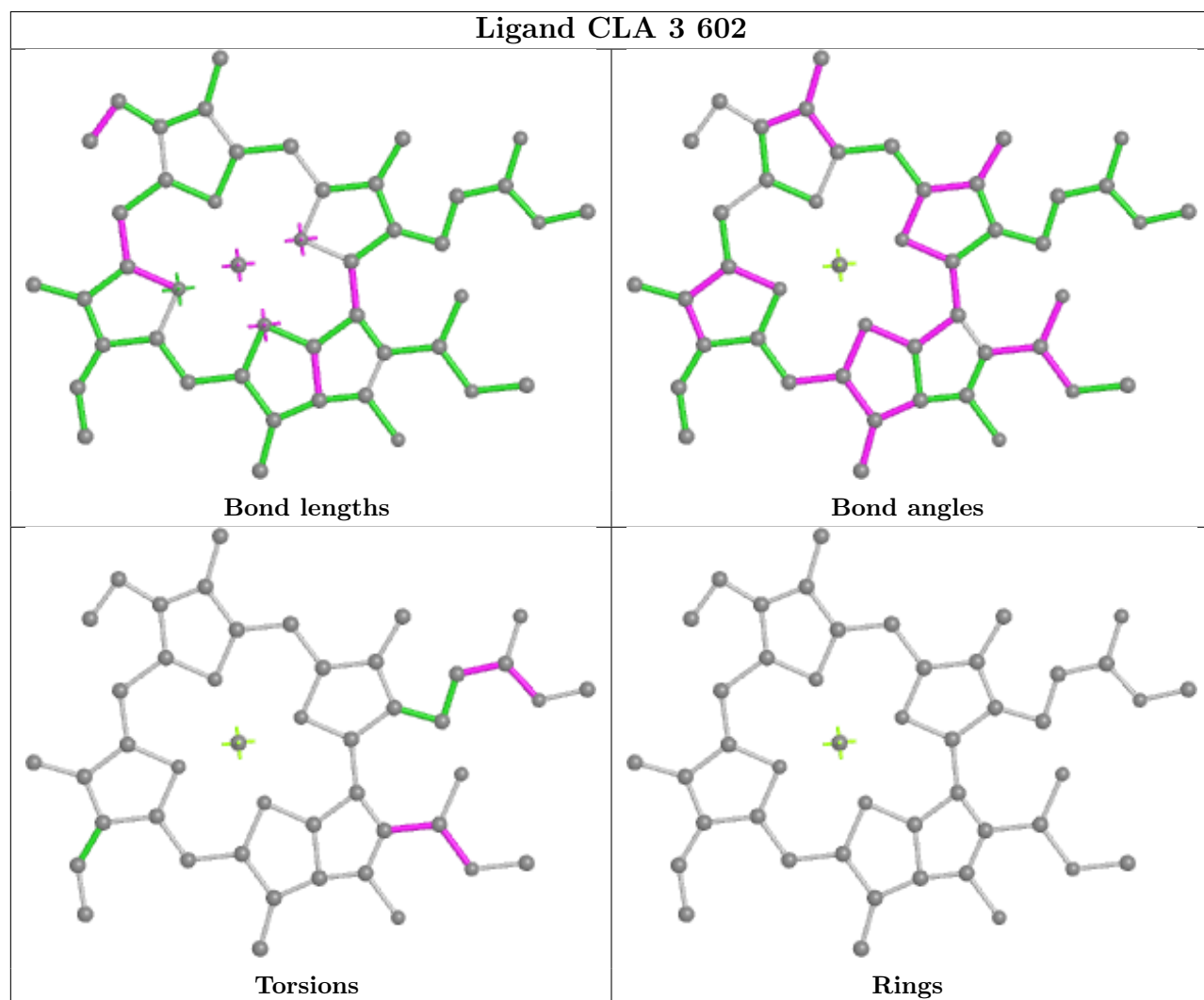


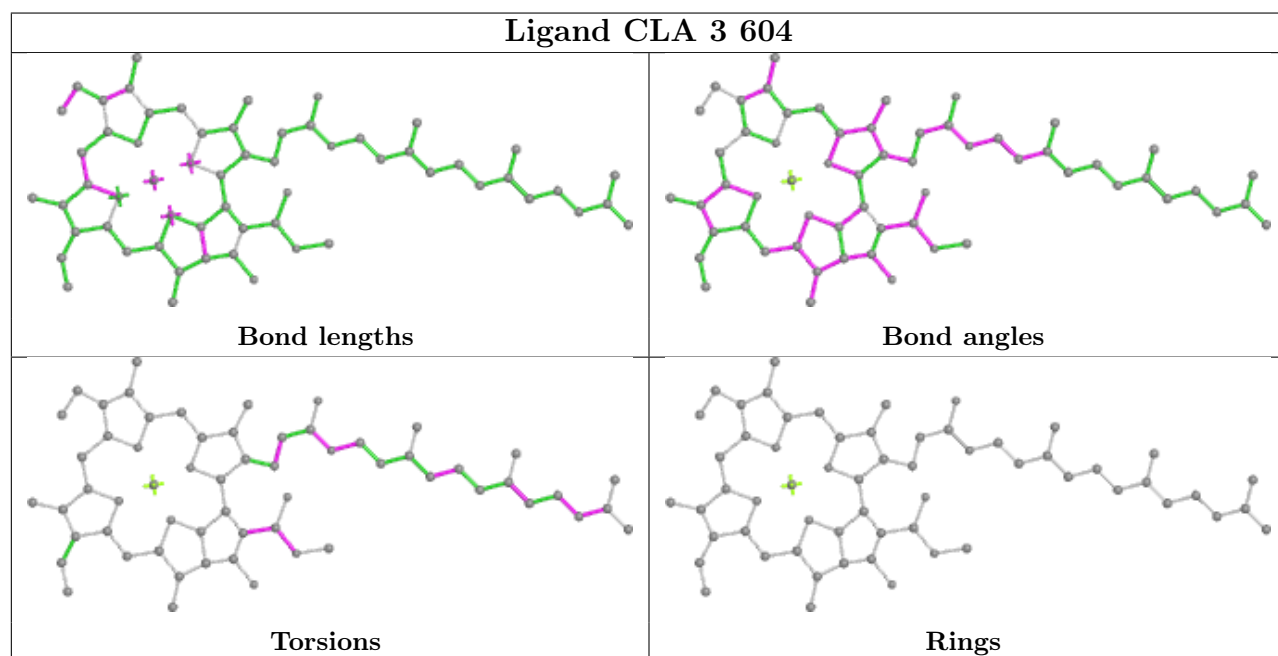
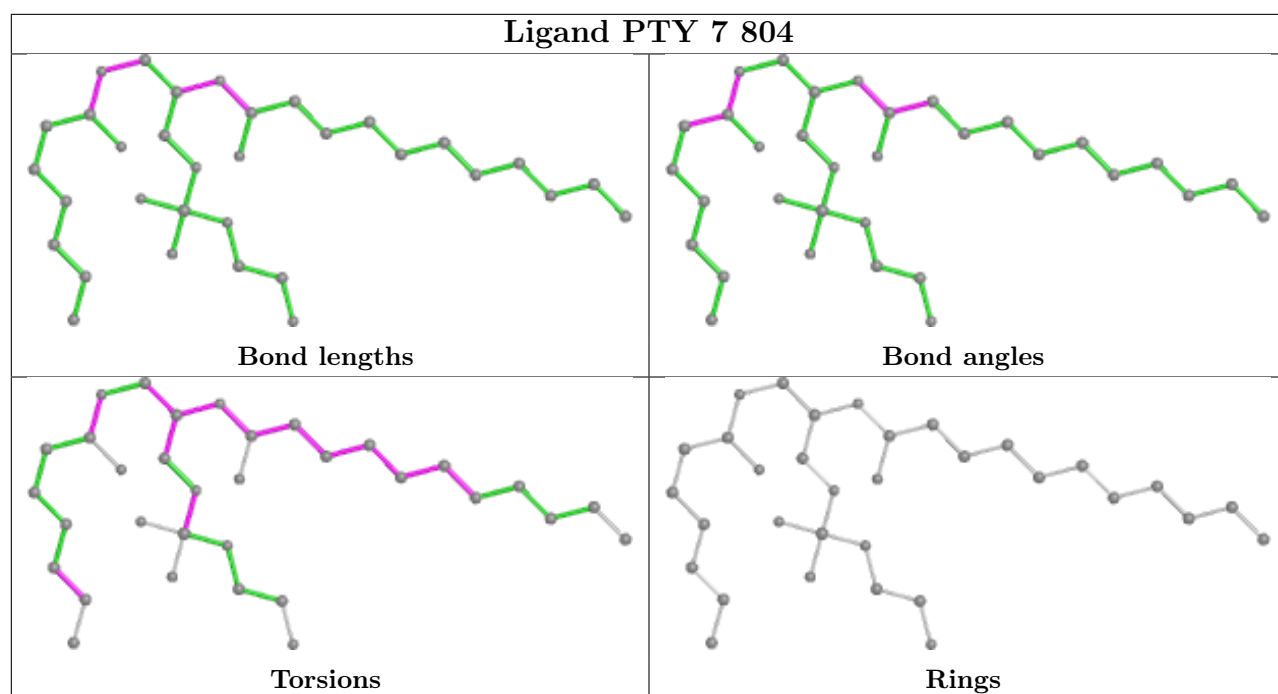


Ligand CLA B 1209

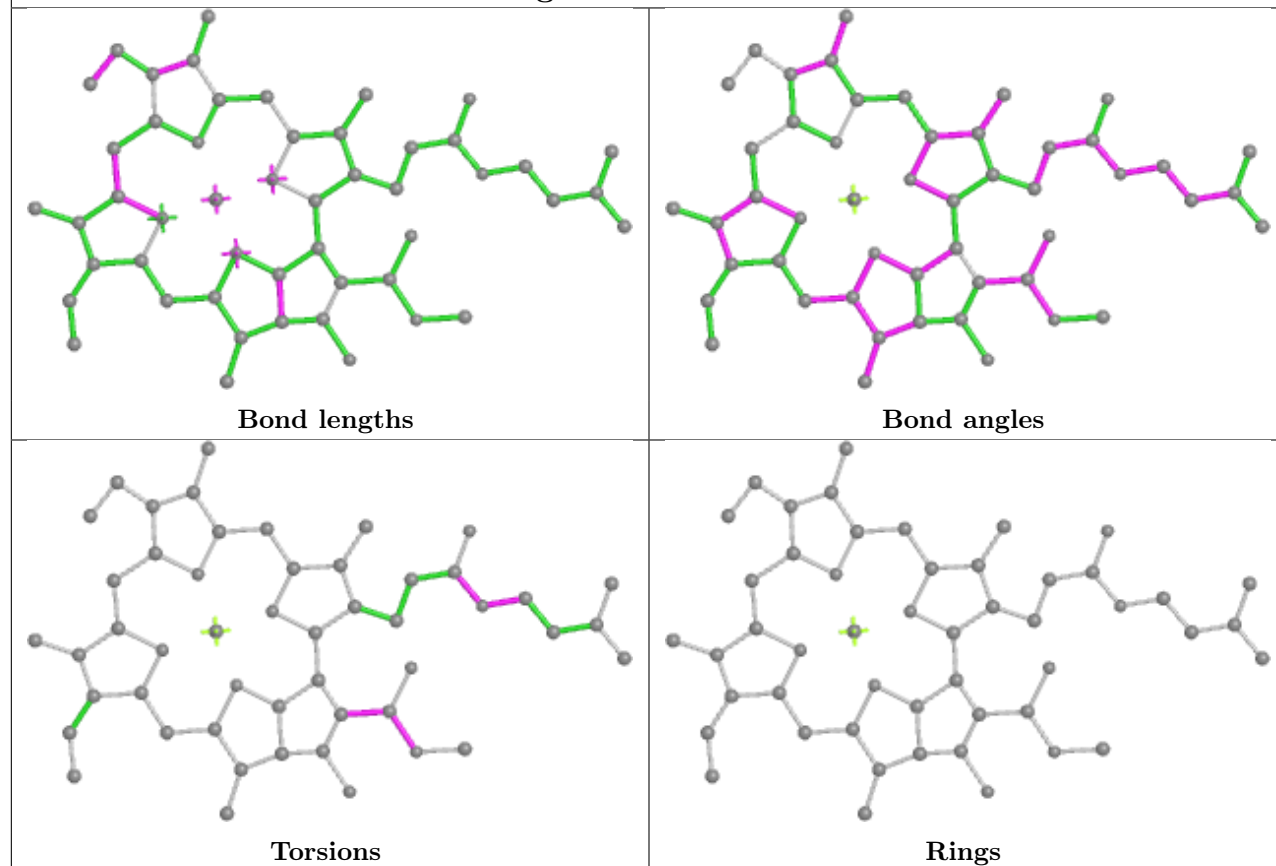


Ligand CLA 3 602

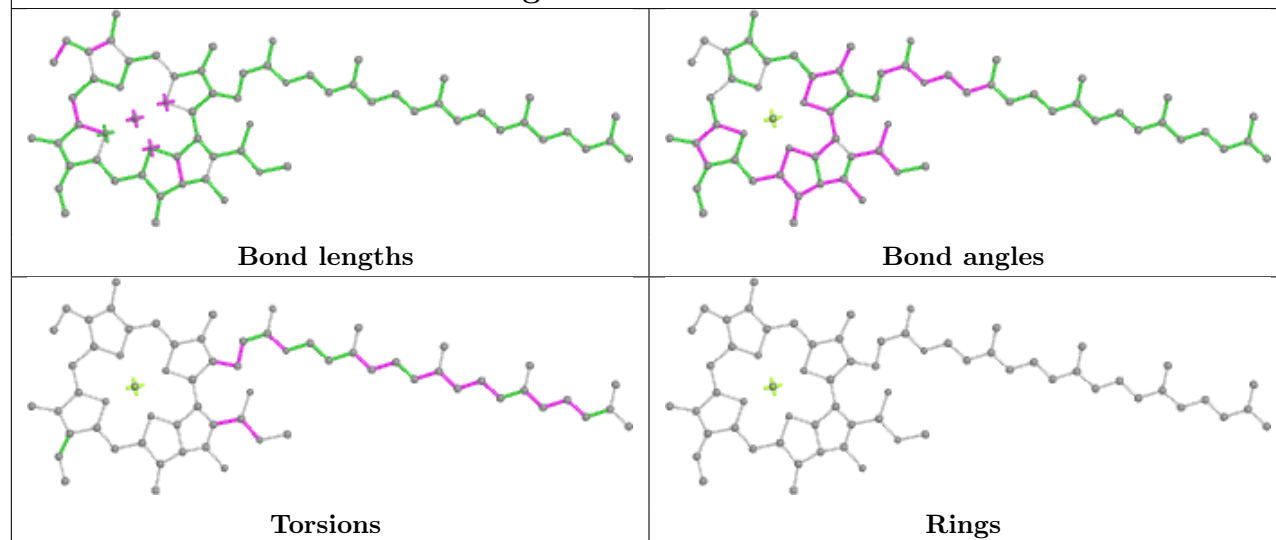


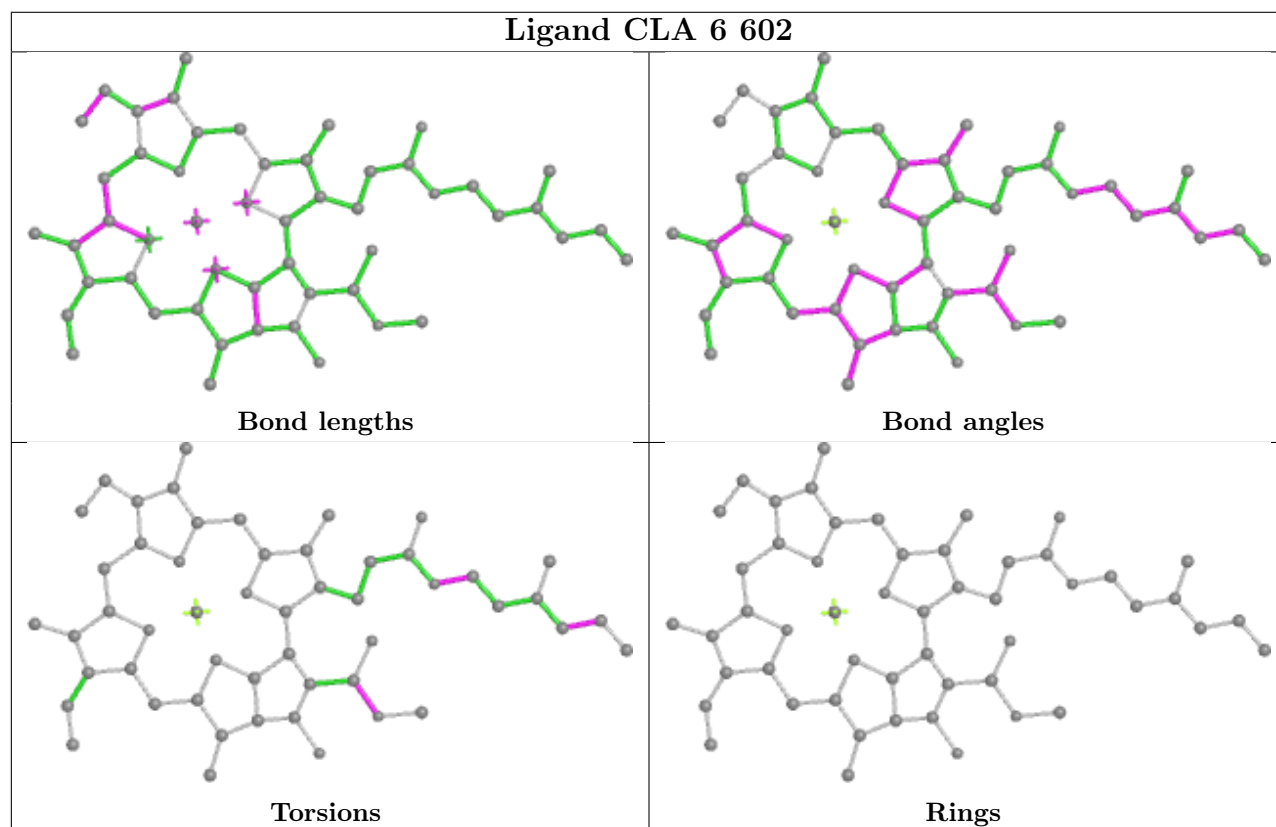
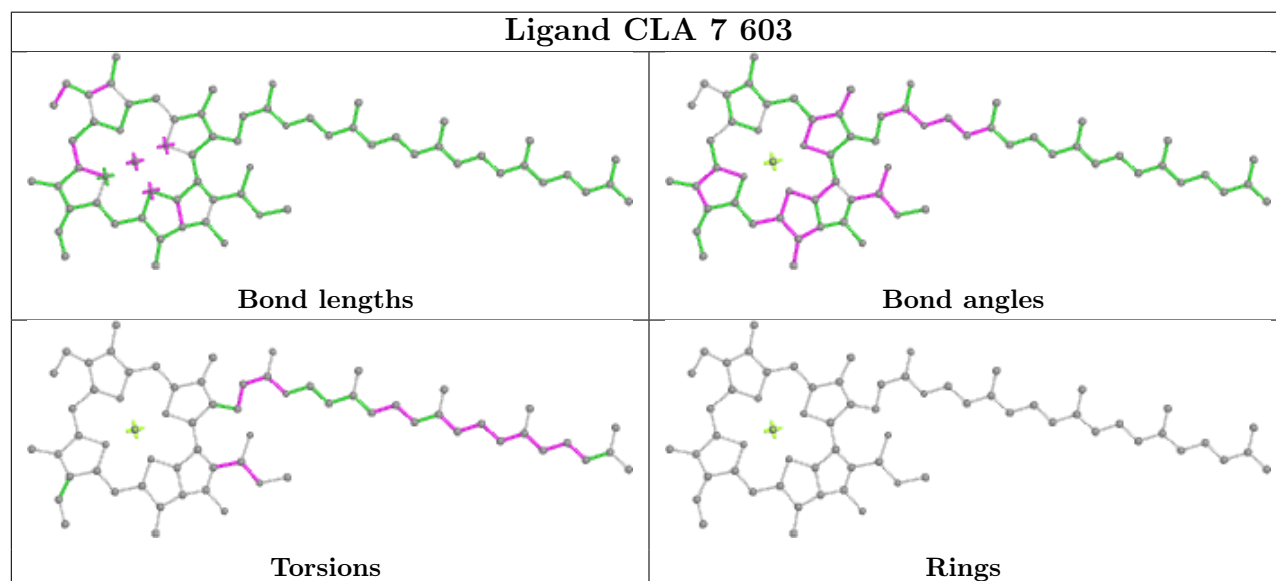
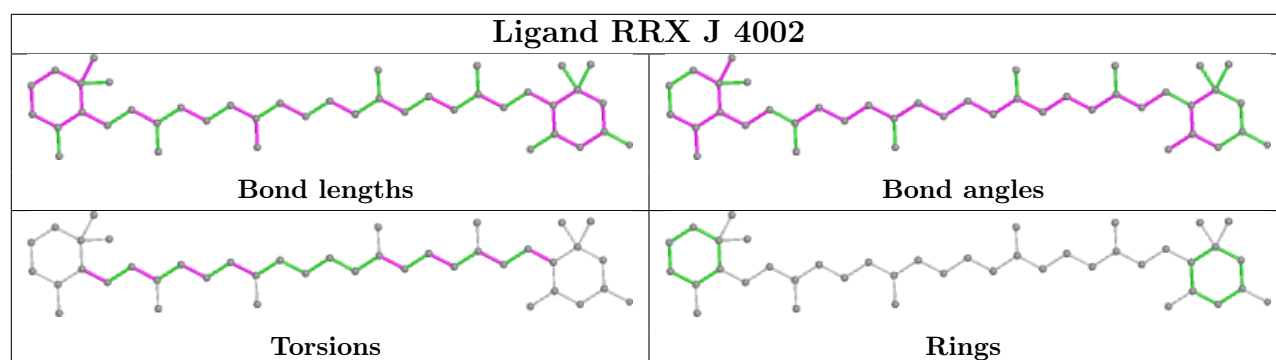


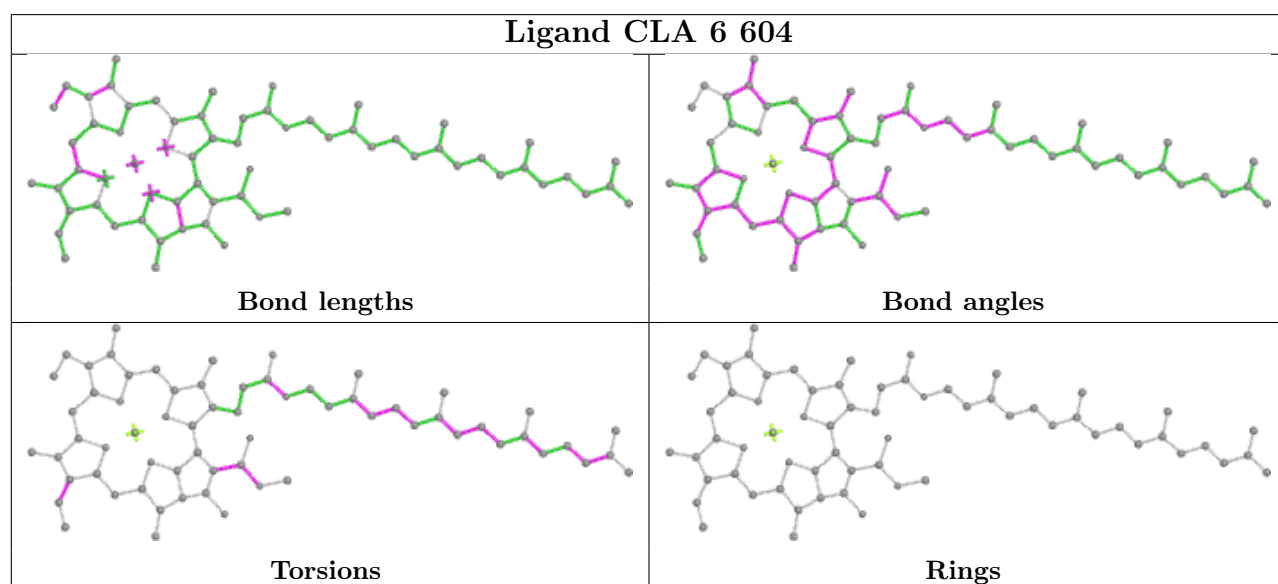
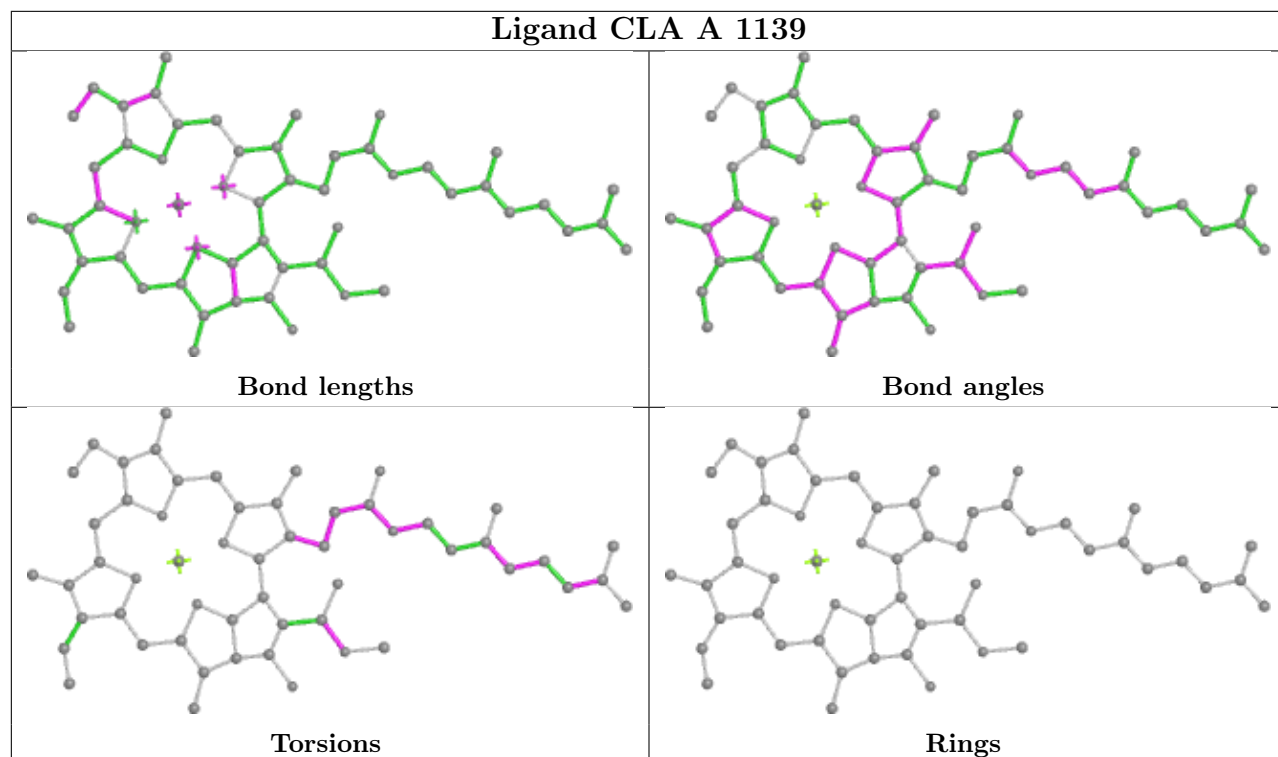
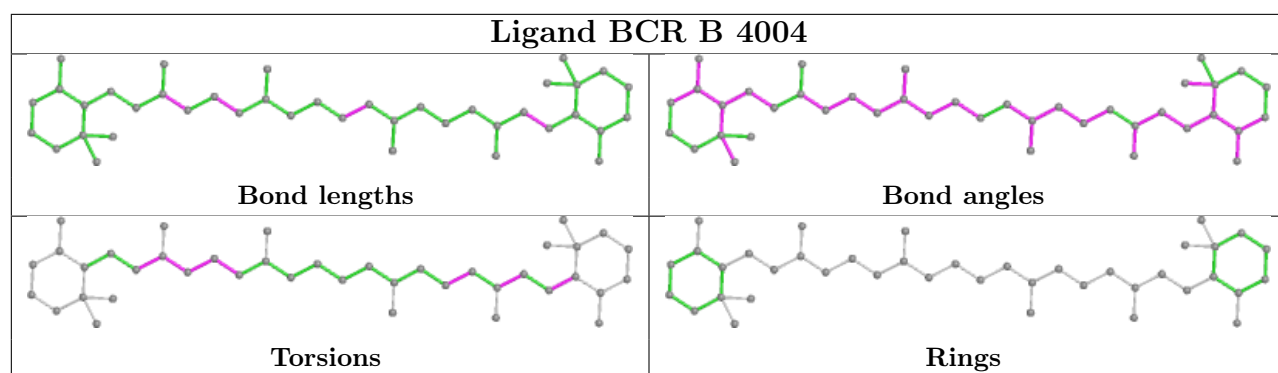
Ligand CLA 8 611



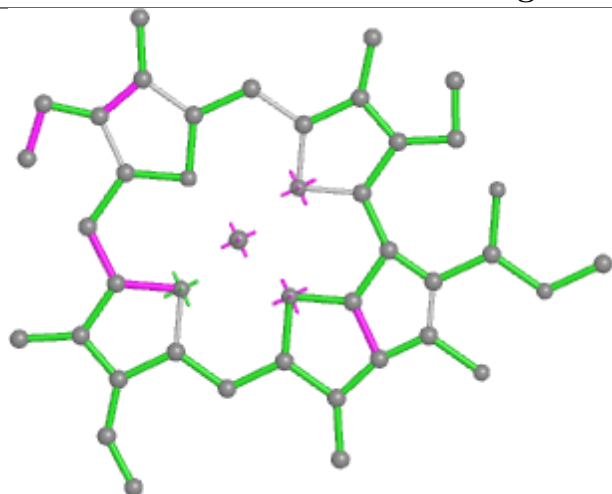
Ligand CLA A 1135



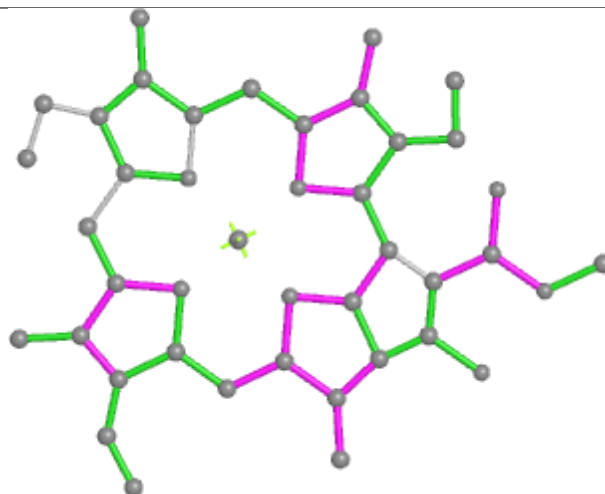




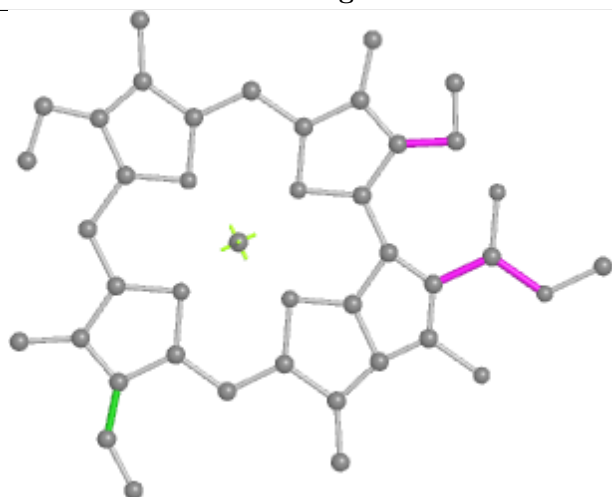
Ligand CLA 7 608



Bond lengths



Bond angles

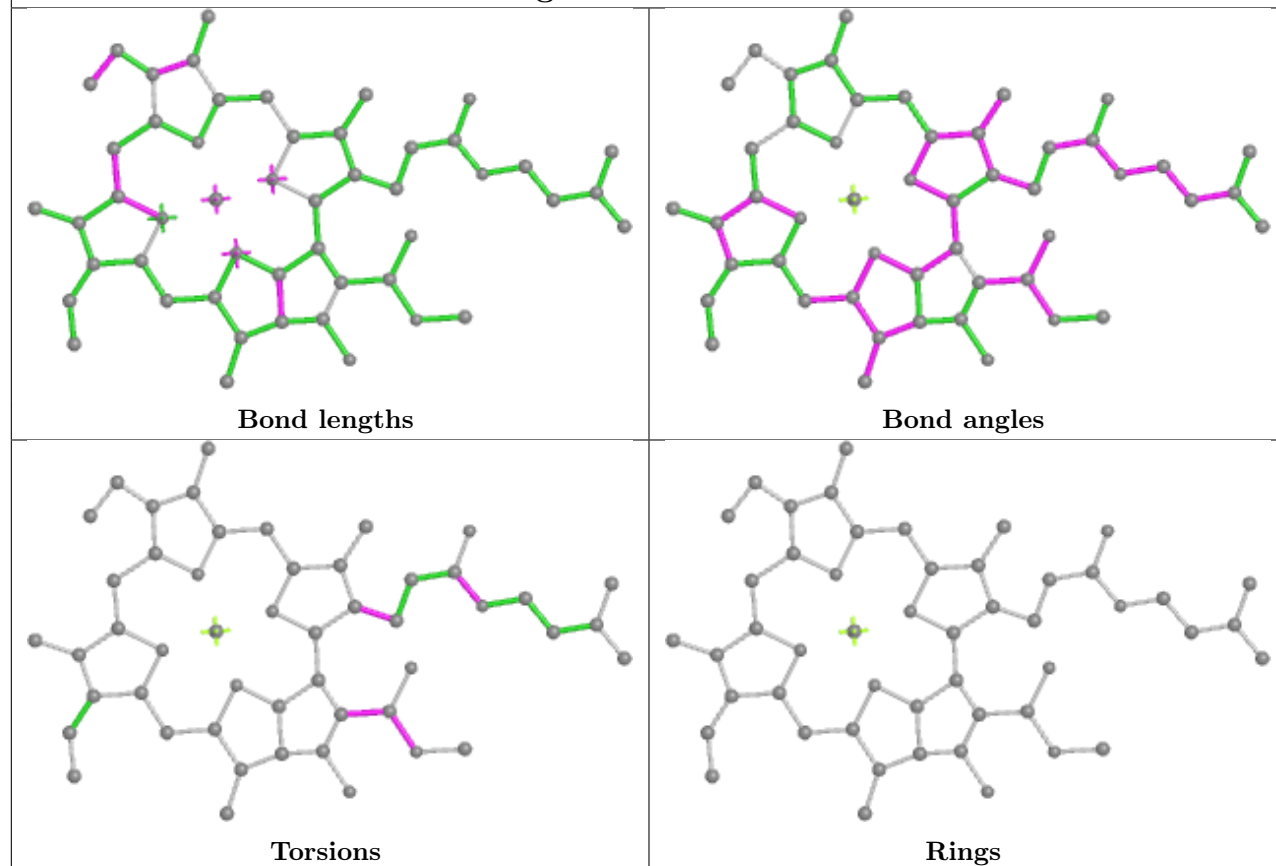


Torsions

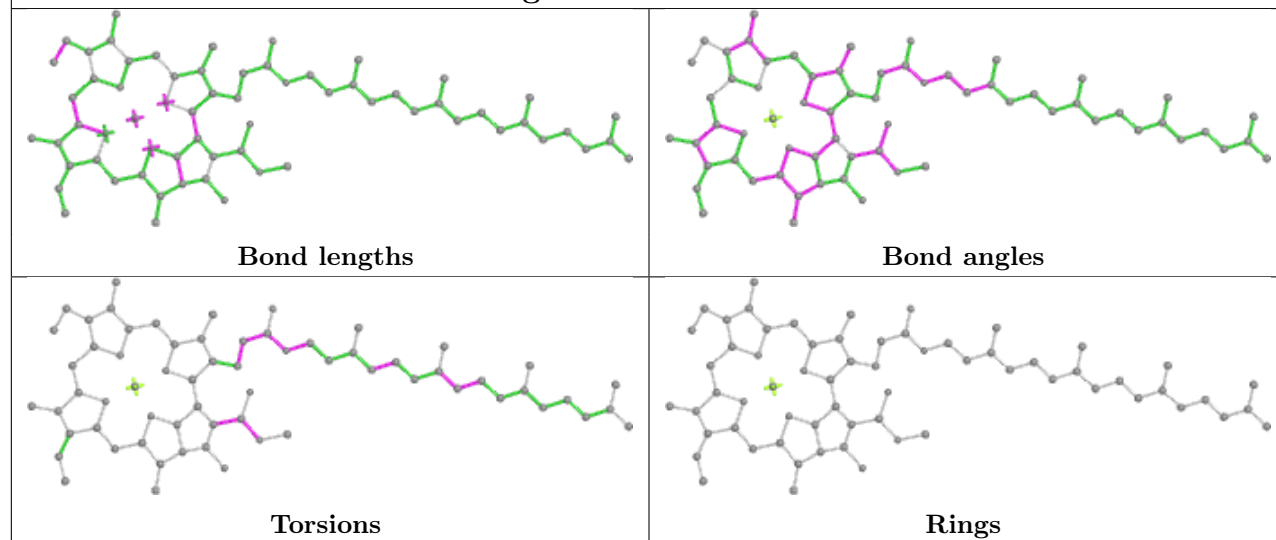


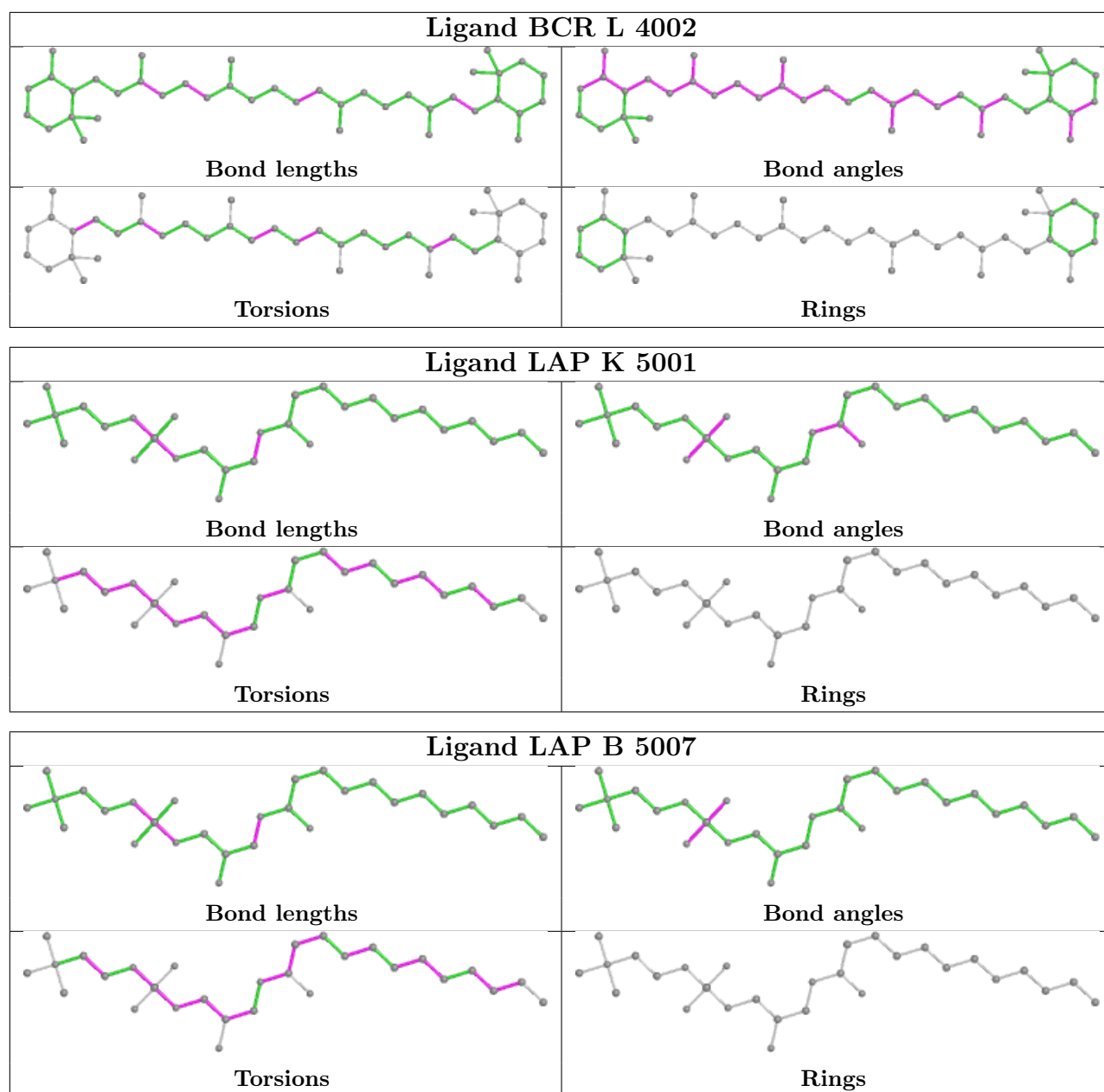
Rings

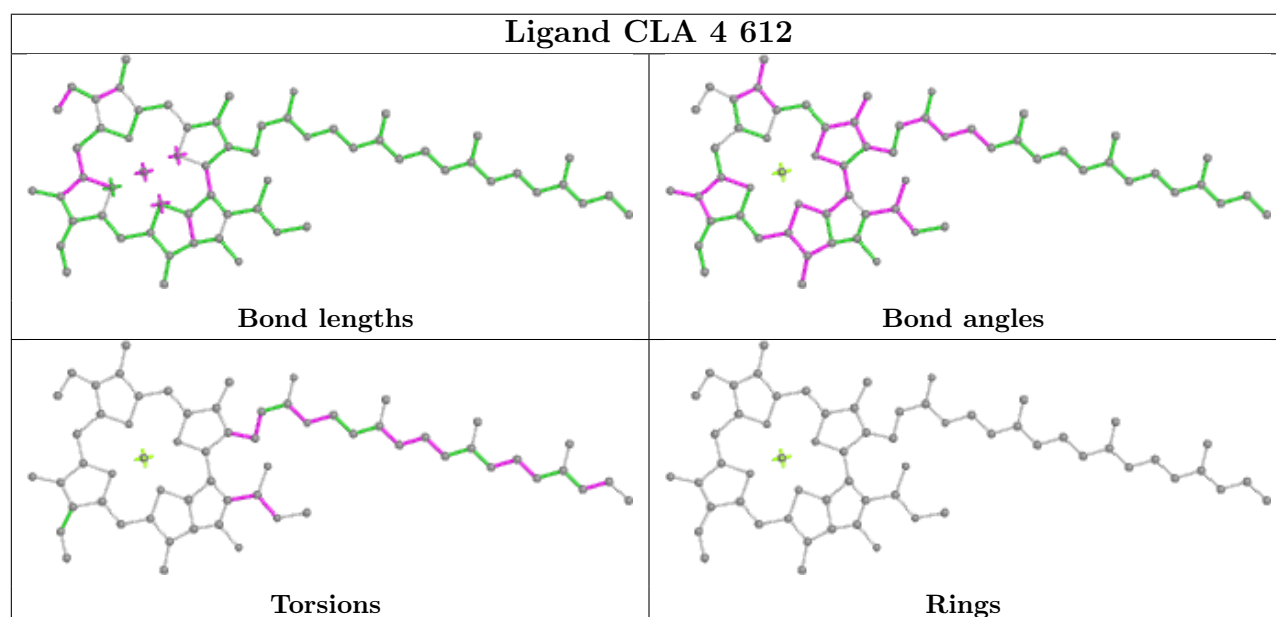
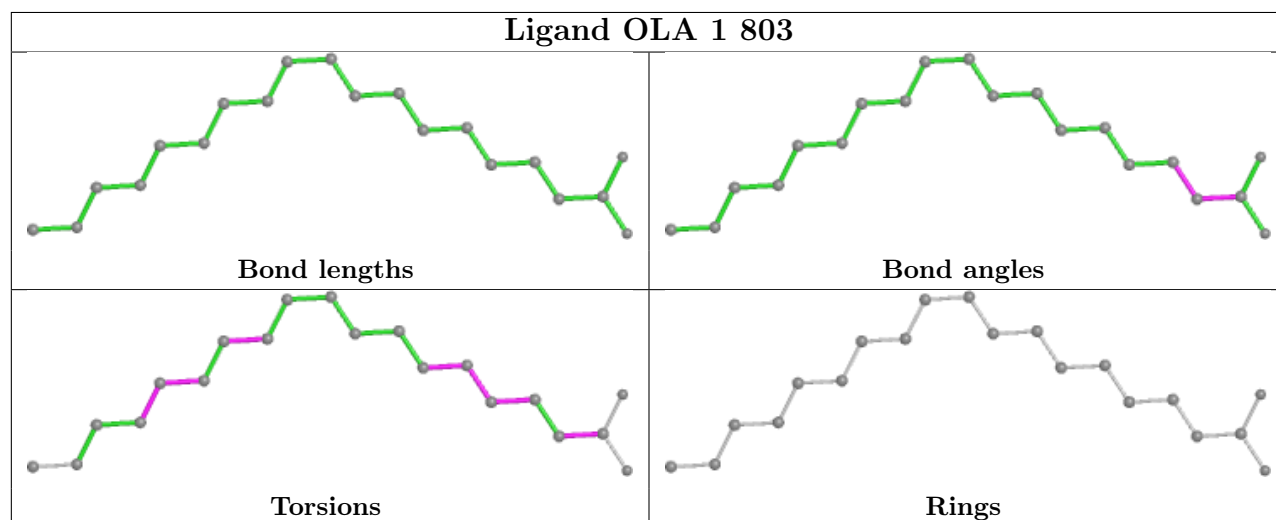
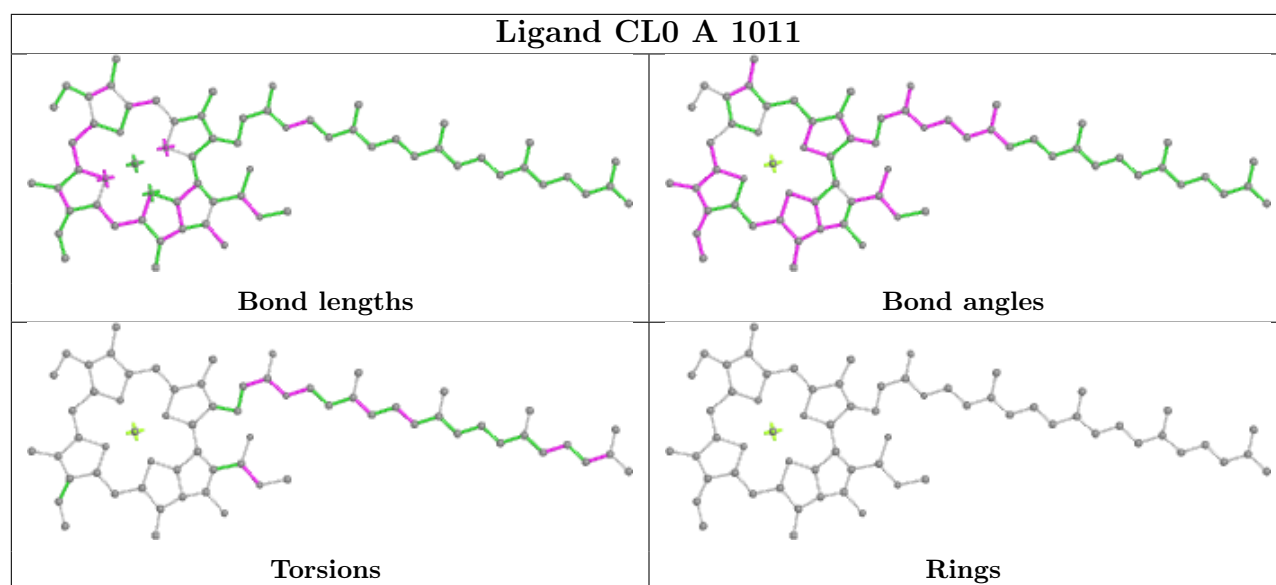
Ligand CLA 5 606



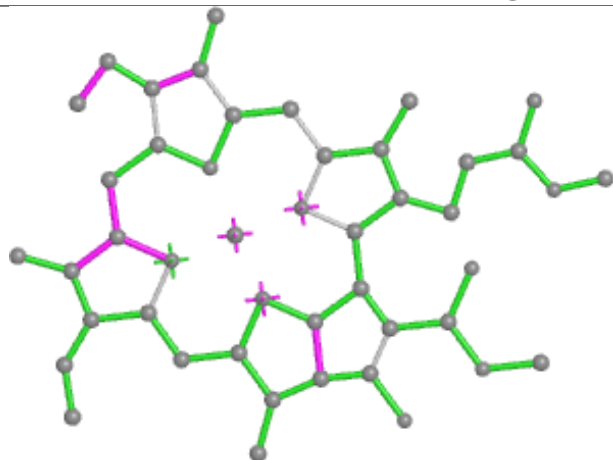
Ligand CLA A 1123



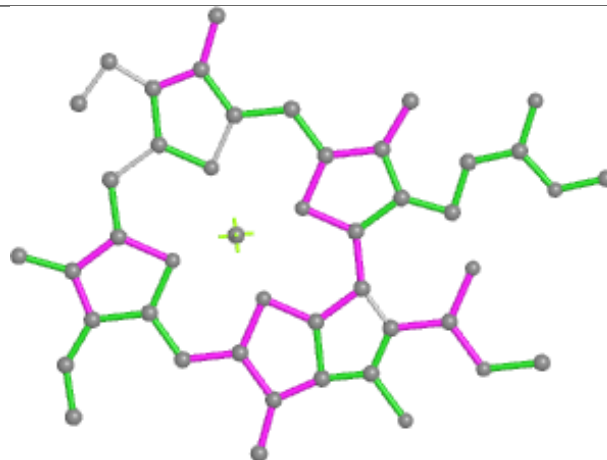




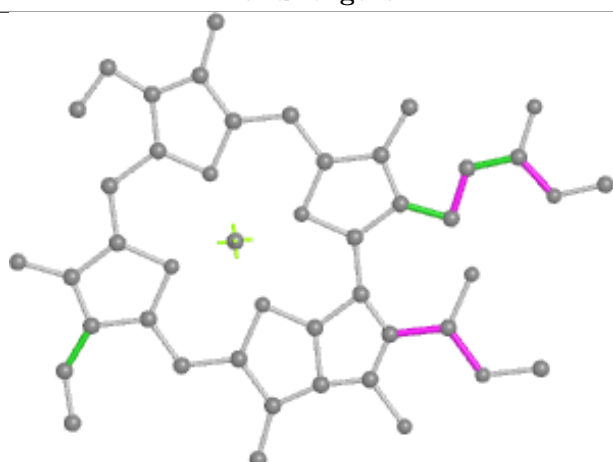
Ligand CLA G 1602



Bond lengths



Bond angles

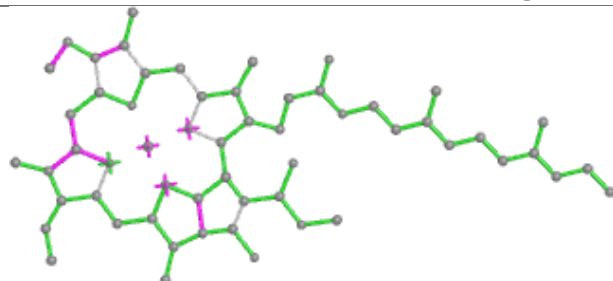


Torsions

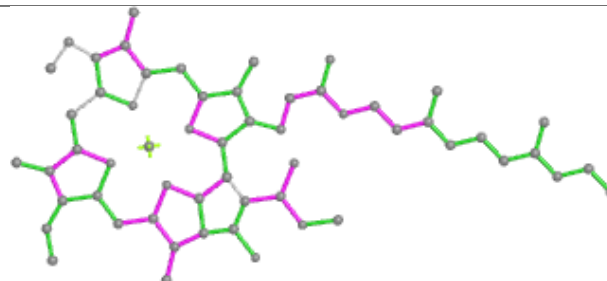


Rings

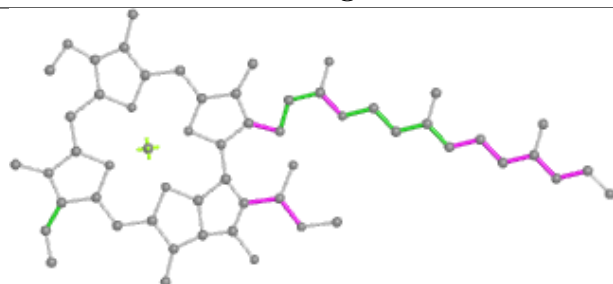
Ligand CLA 1 606



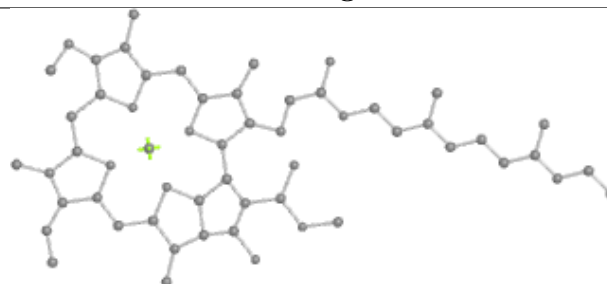
Bond lengths



Bond angles

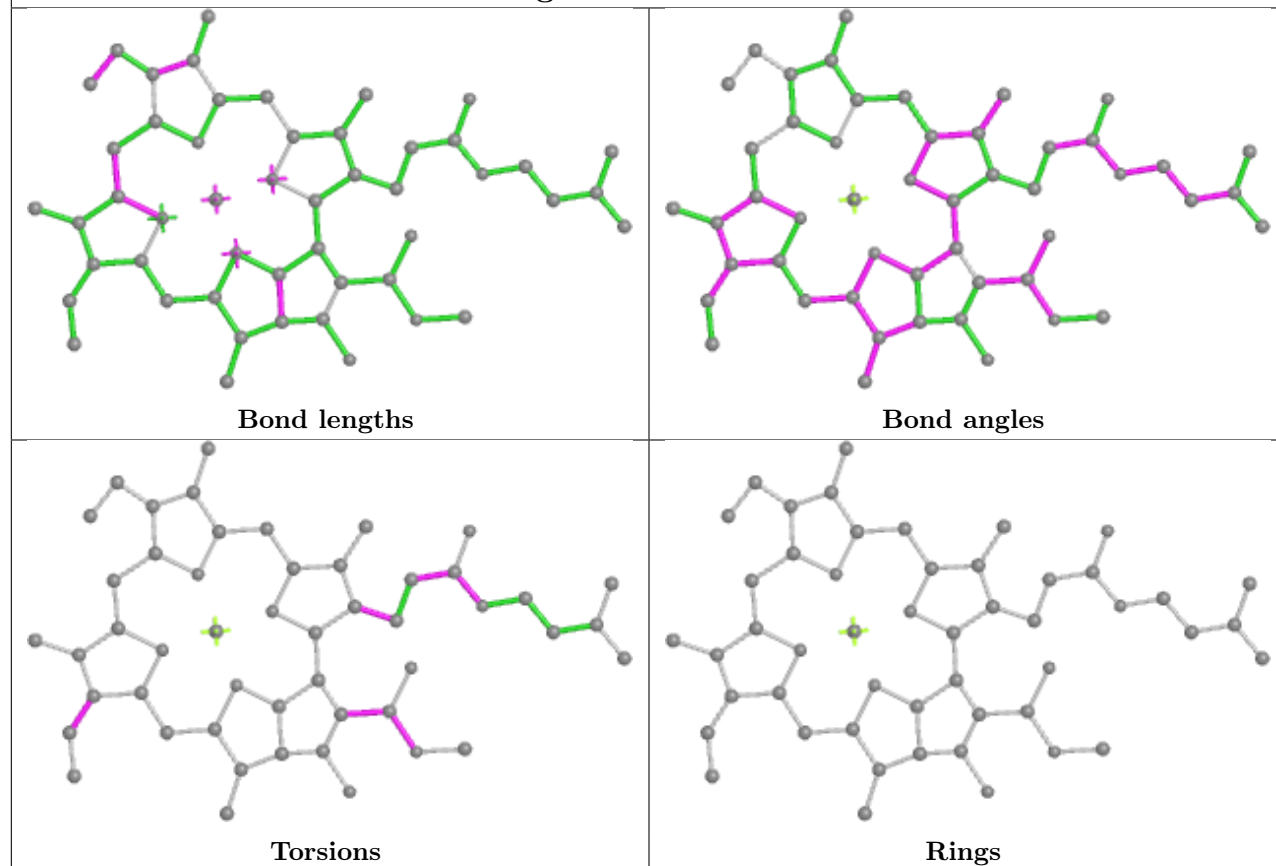


Torsions

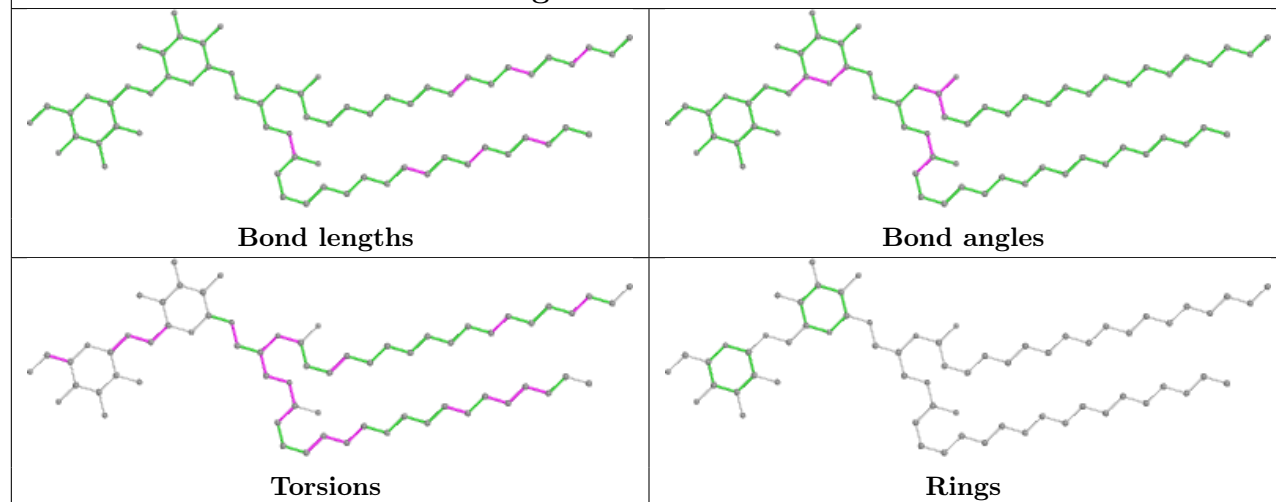


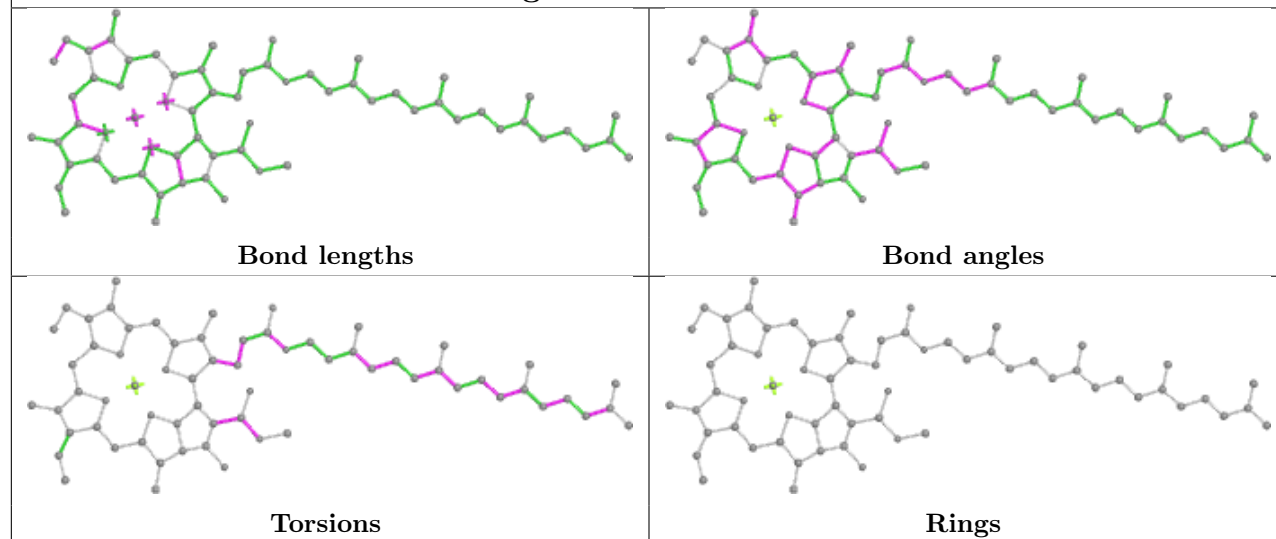
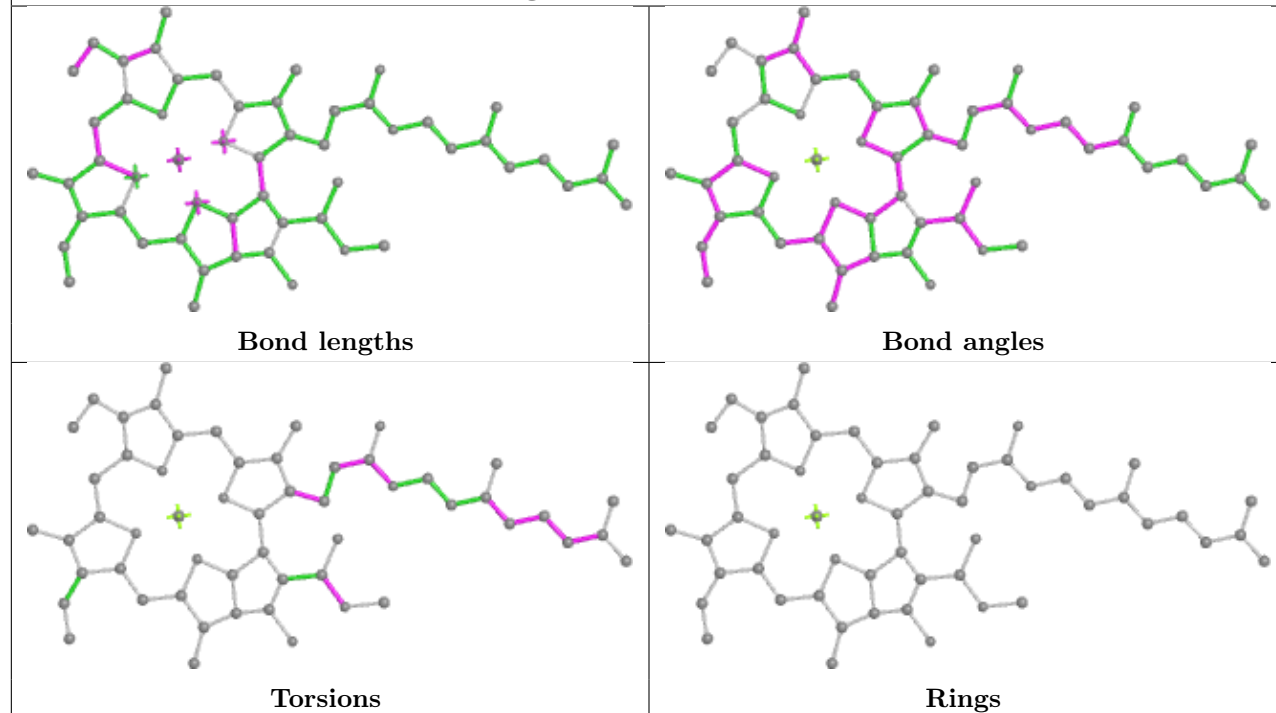
Rings

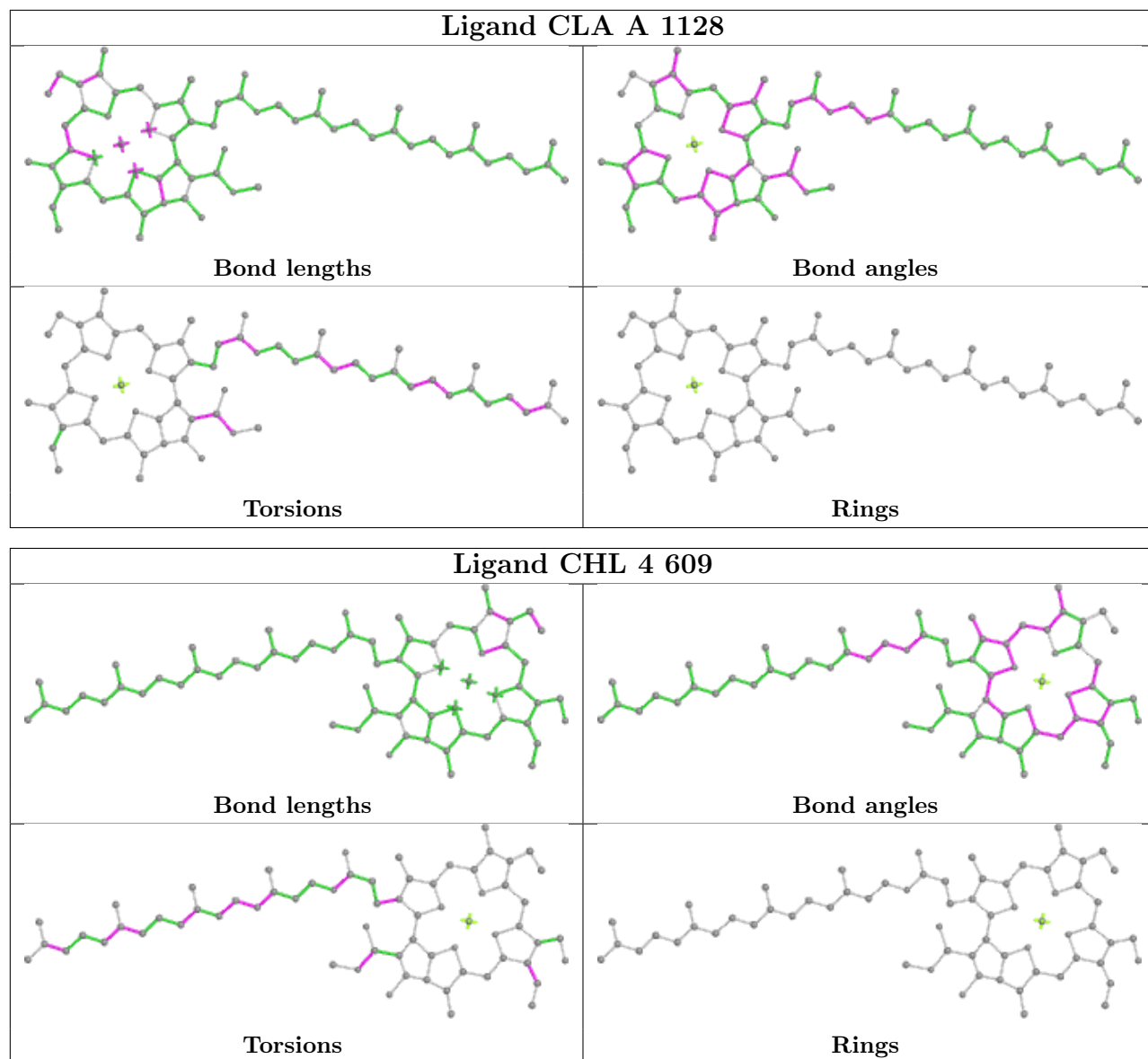
Ligand CLA 6 612

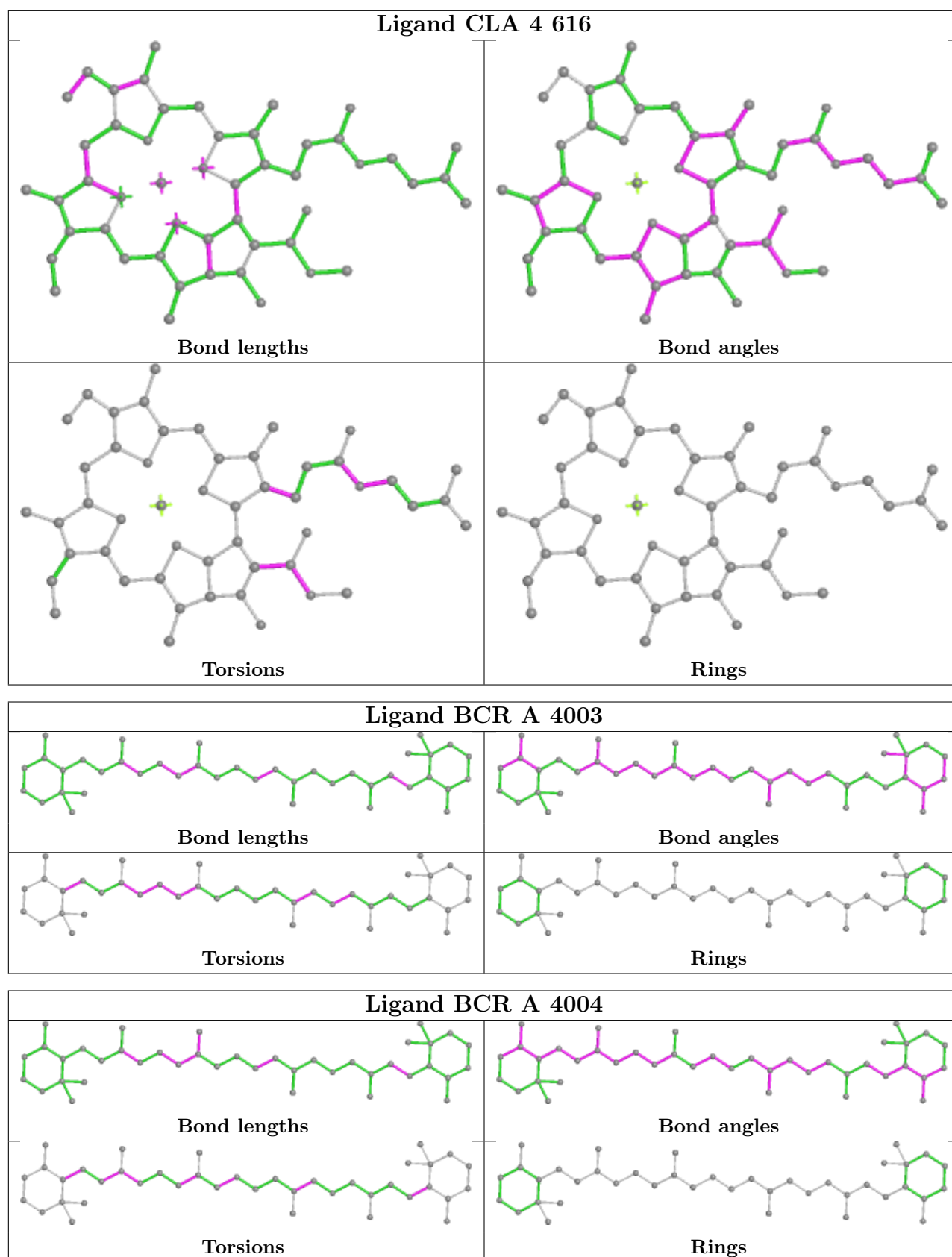


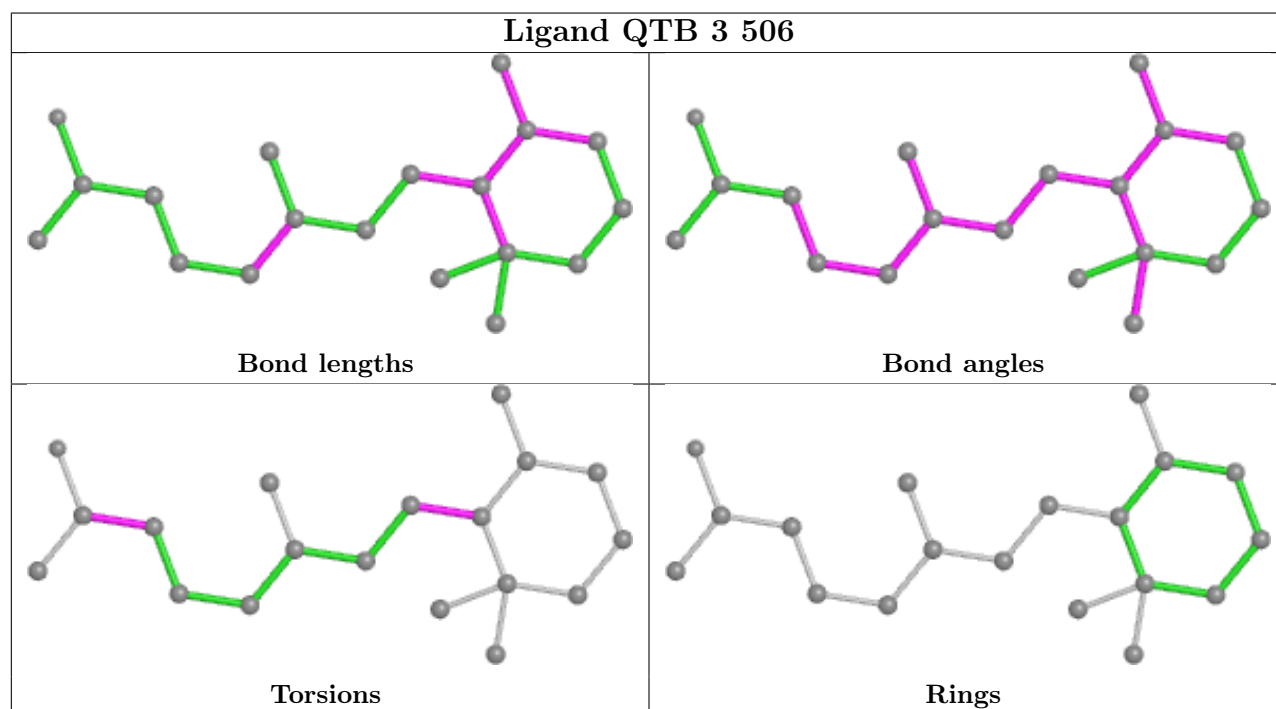
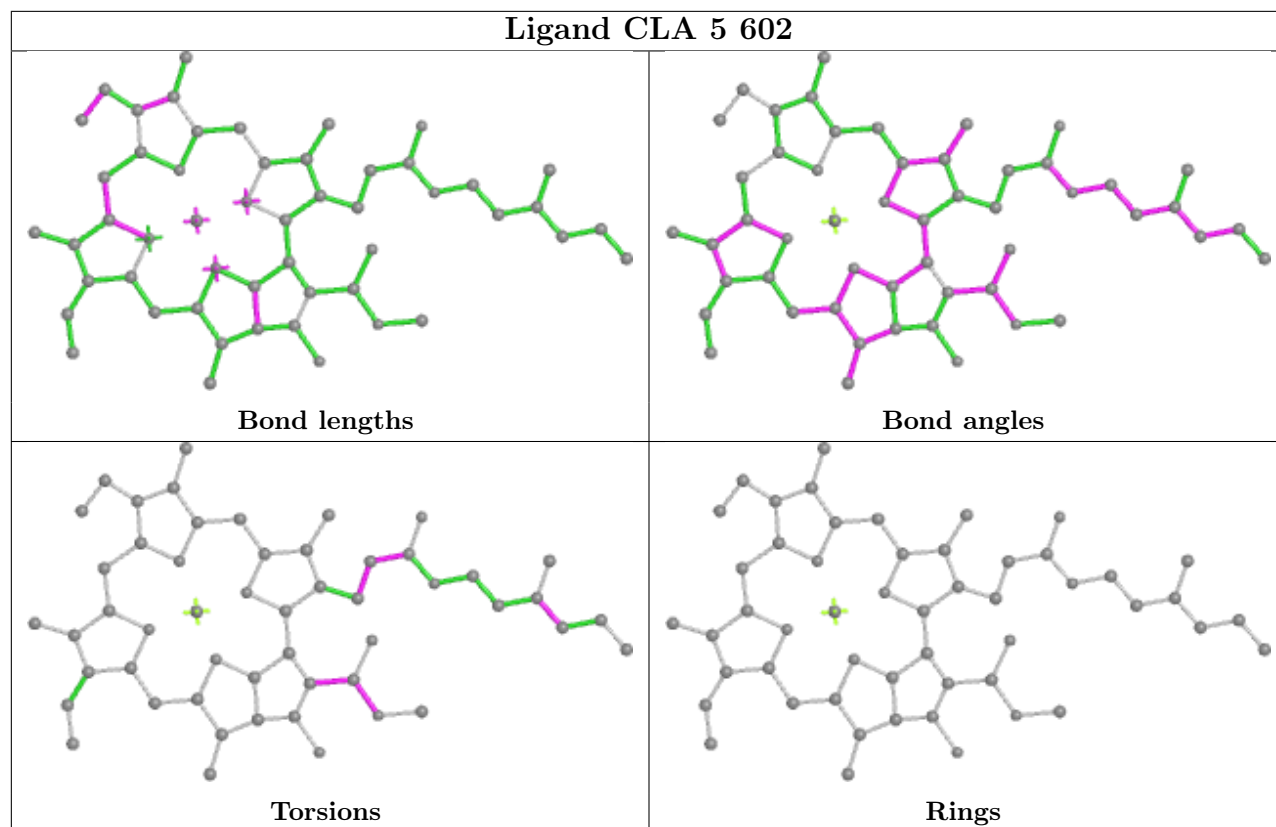
Ligand DGD 8 802

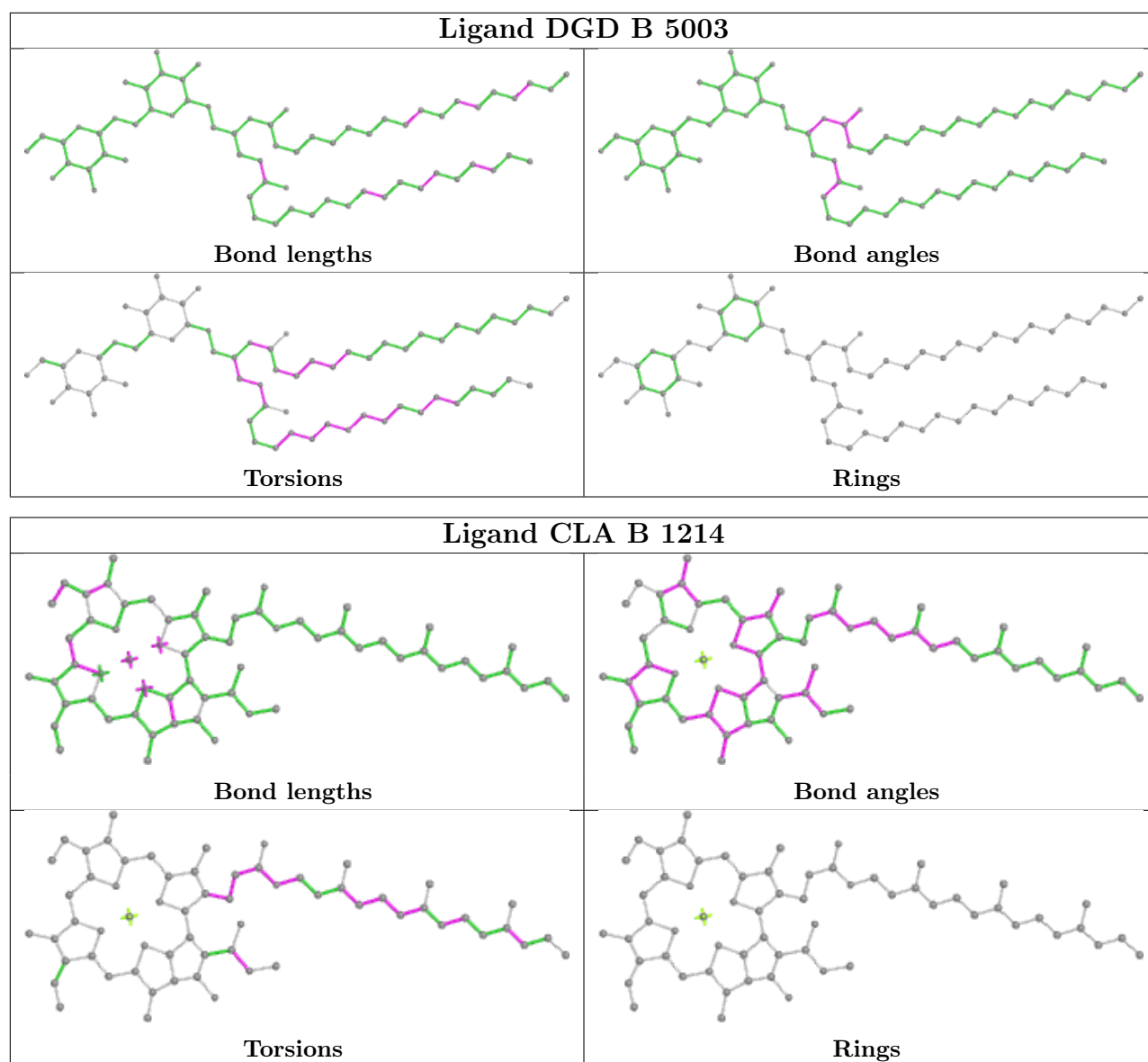


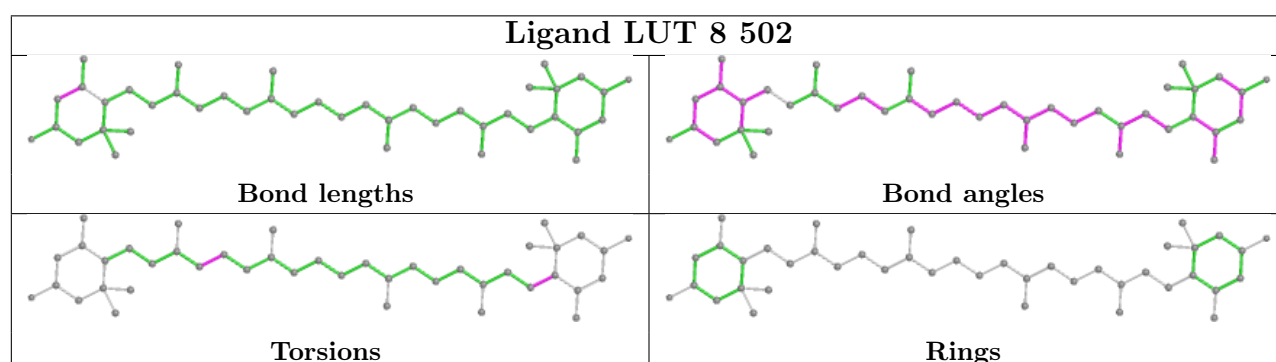
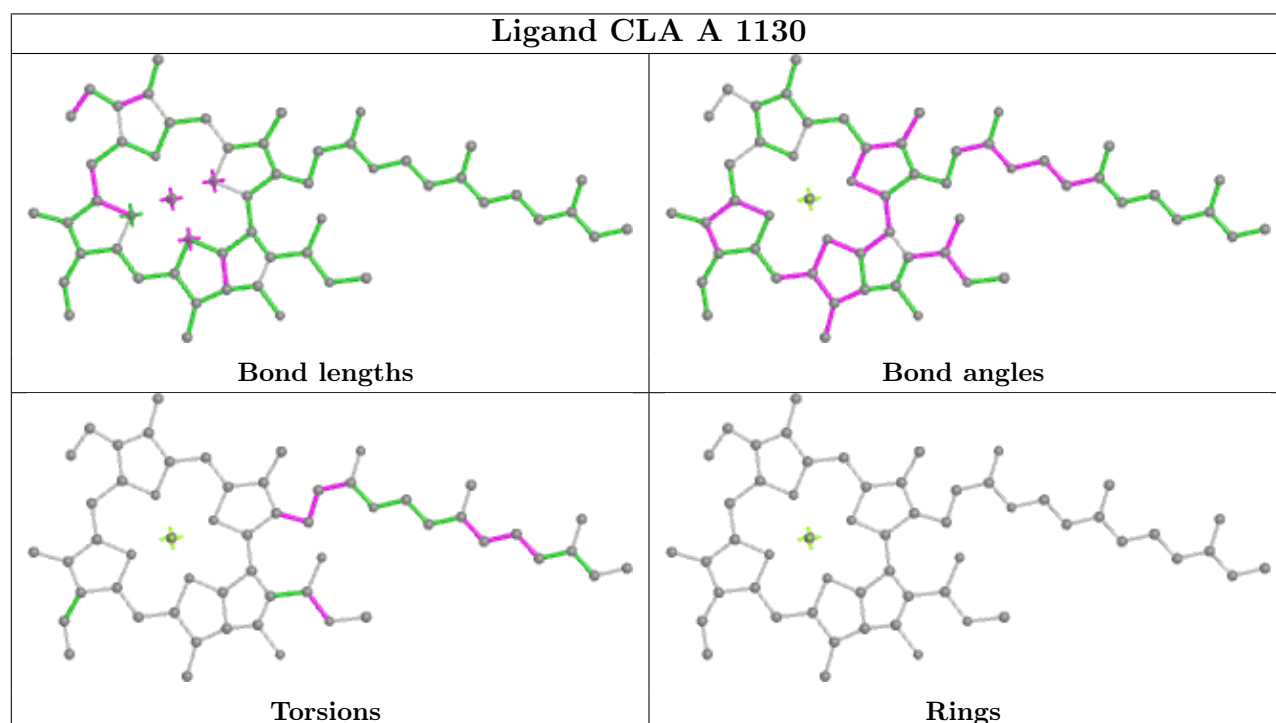
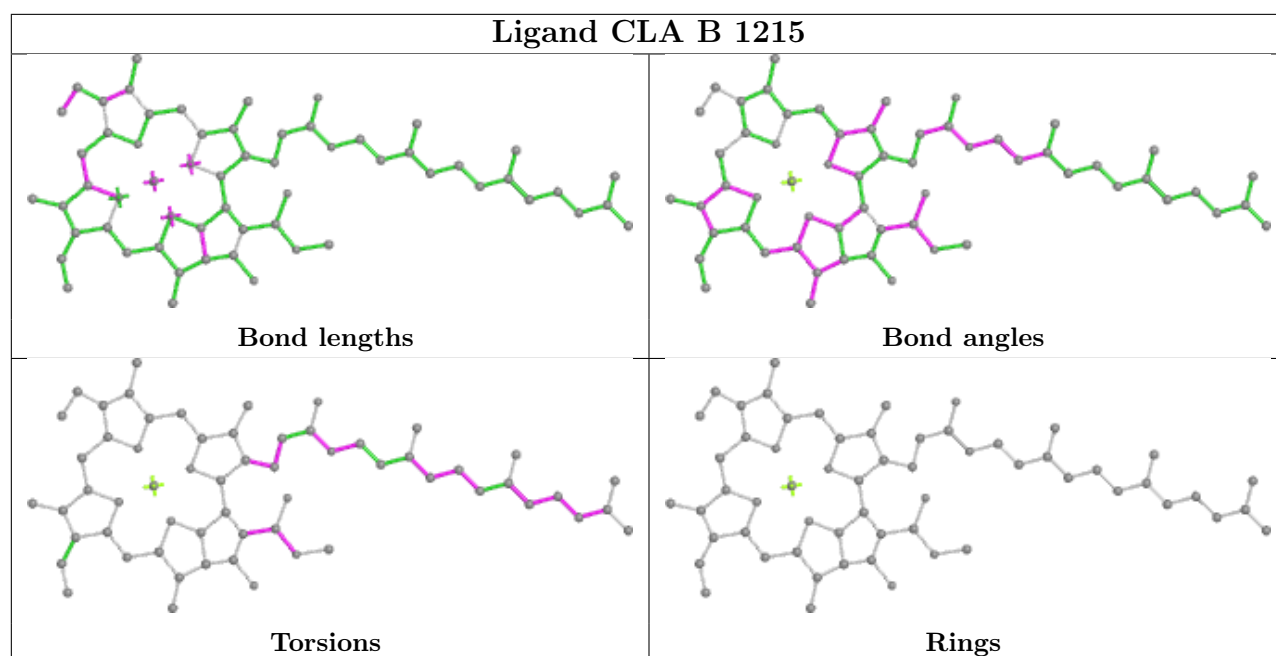
Ligand CLA A 1117**Ligand CLA B 1206**

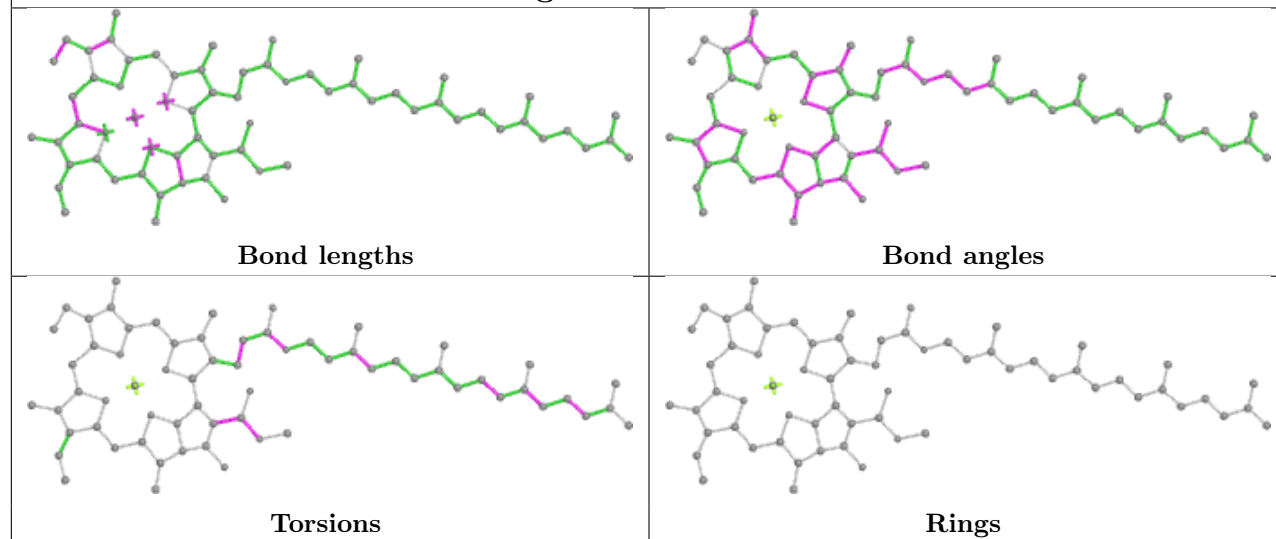
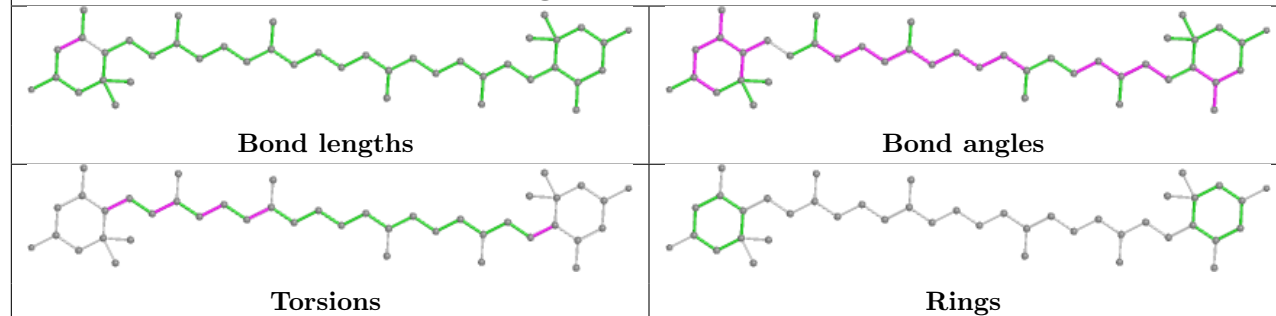
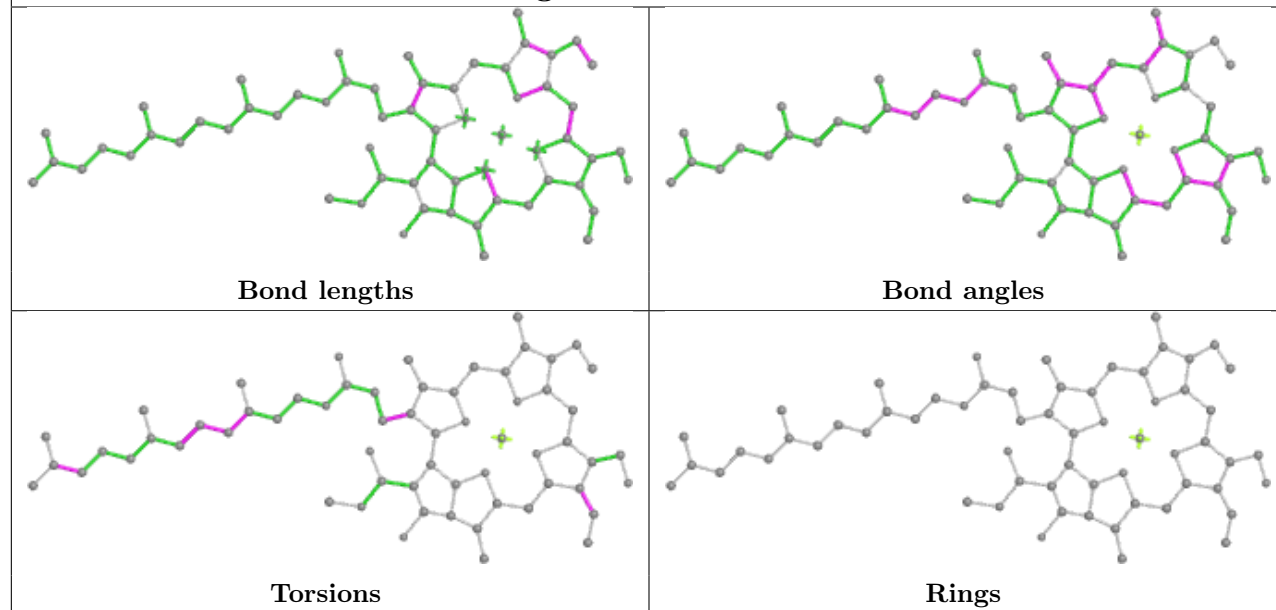




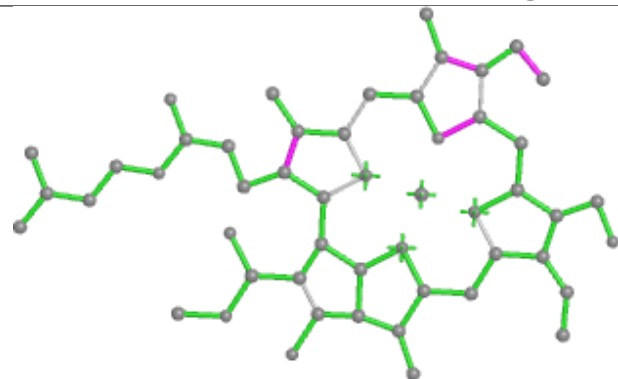




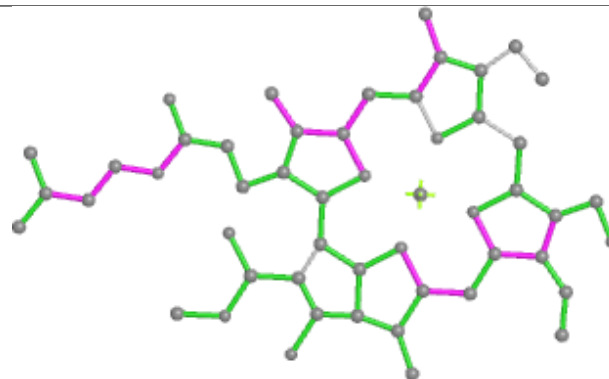


Ligand CLA 5 604**Ligand LUT 1 503****Ligand CHL 8 601**

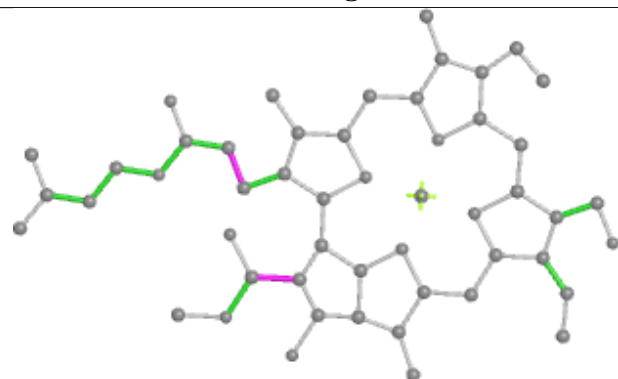
Ligand CHL 8 613



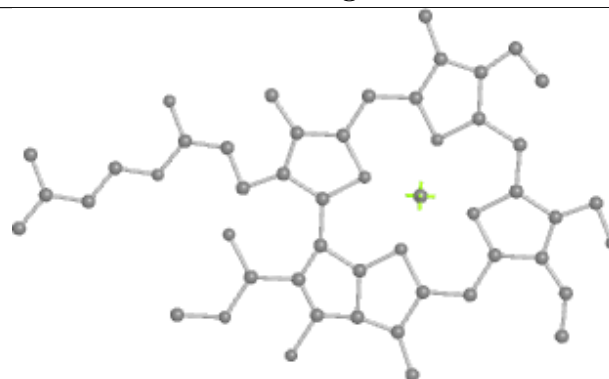
Bond lengths



Bond angles

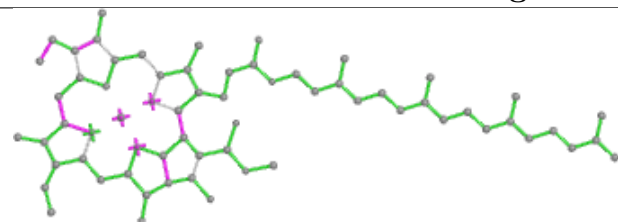


Torsions

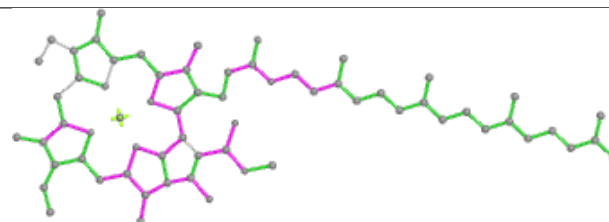


Rings

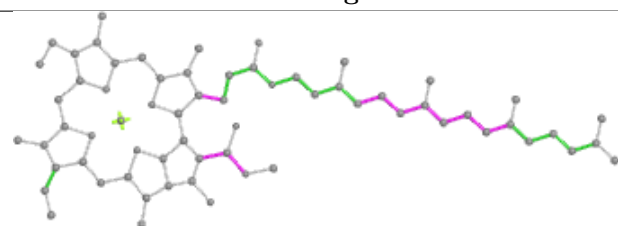
Ligand CLA B 1223



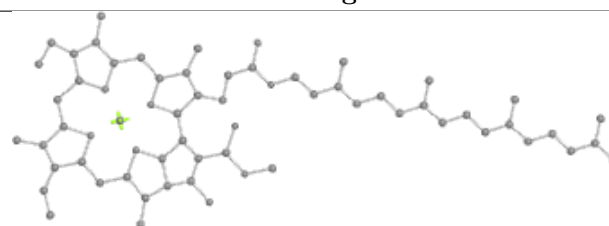
Bond lengths



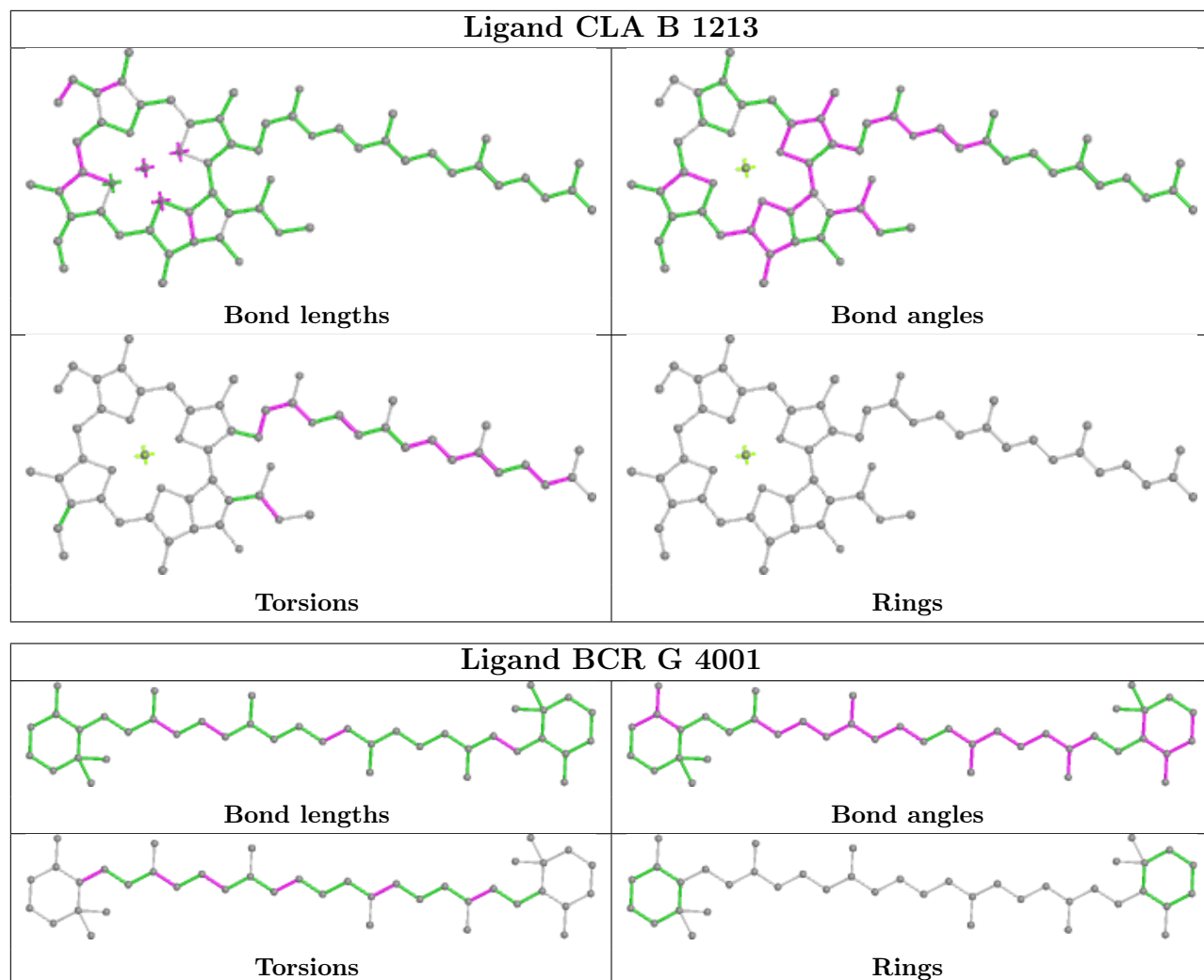
Bond angles

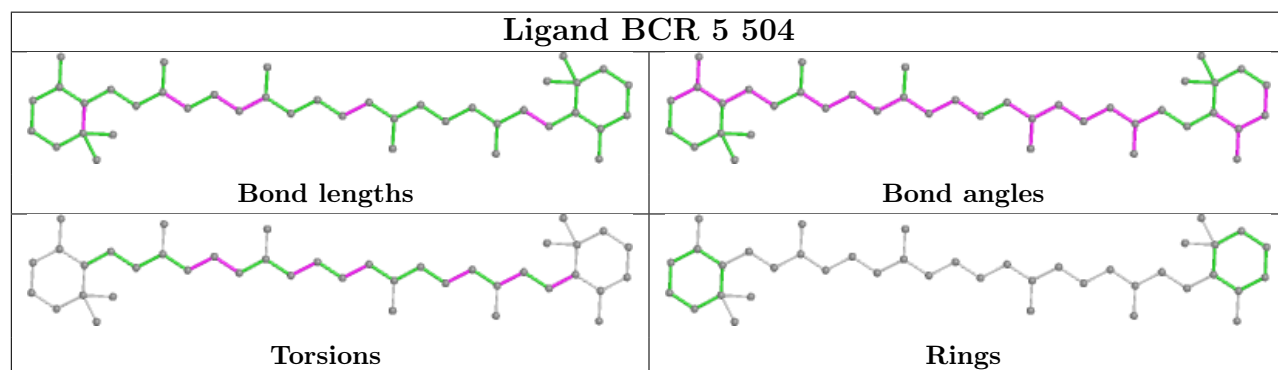
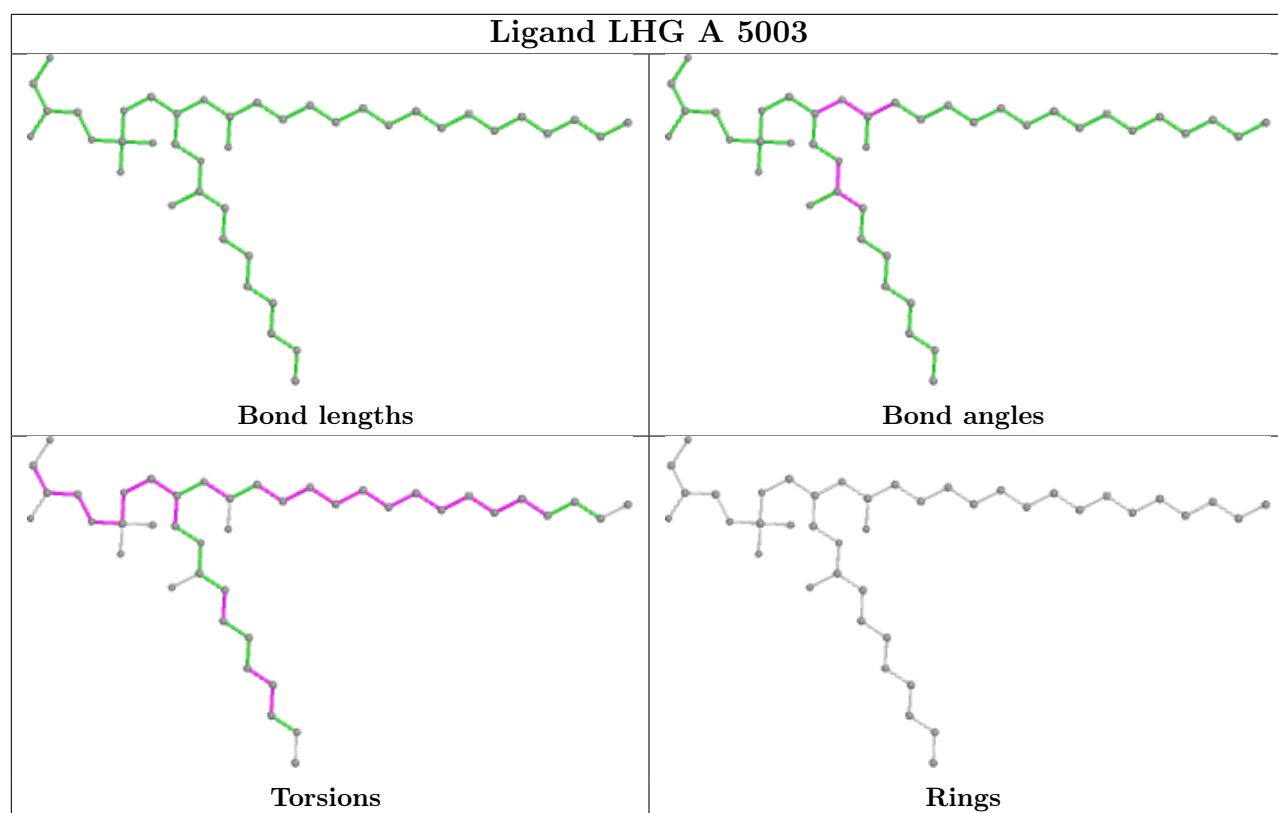


Torsions

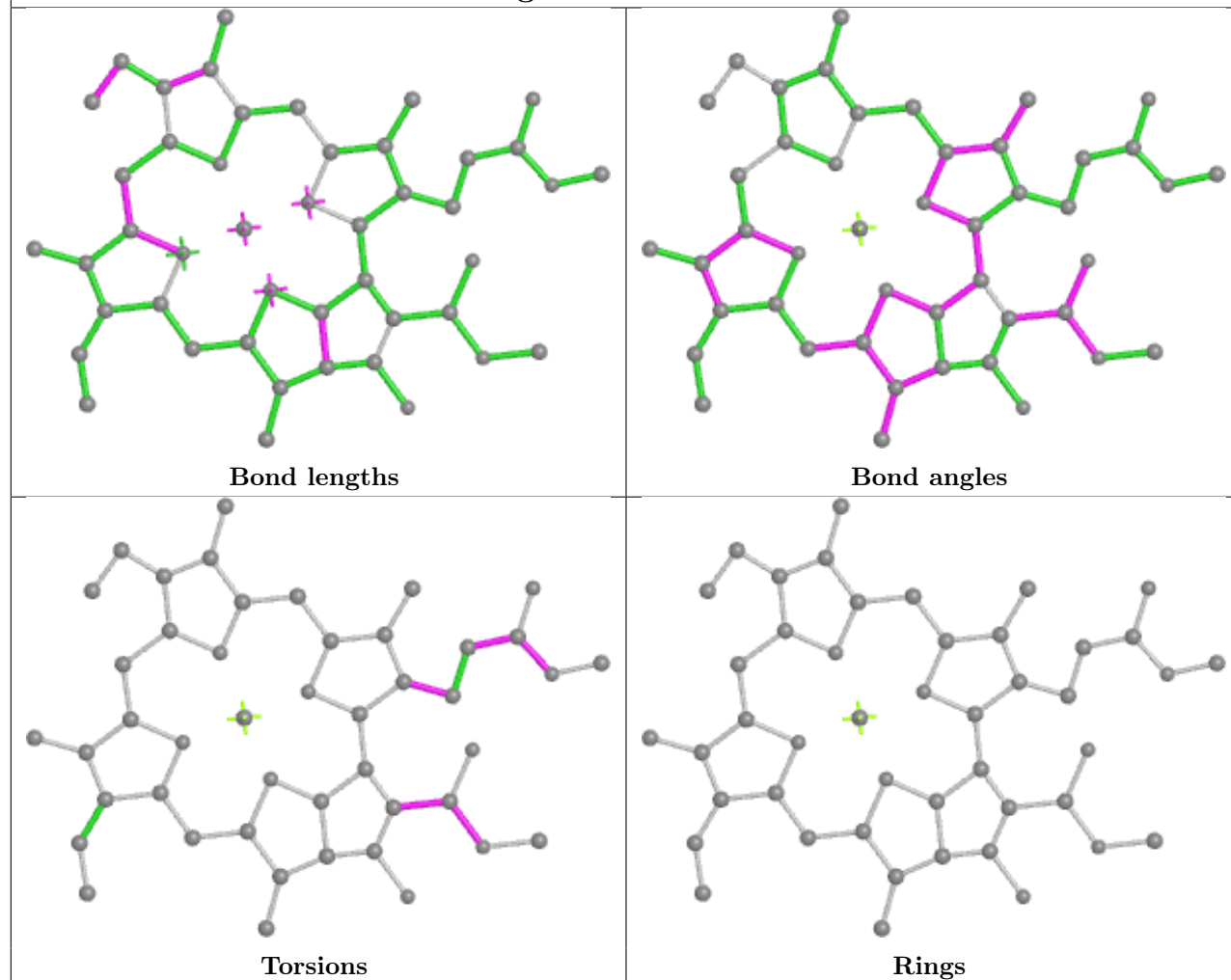


Rings

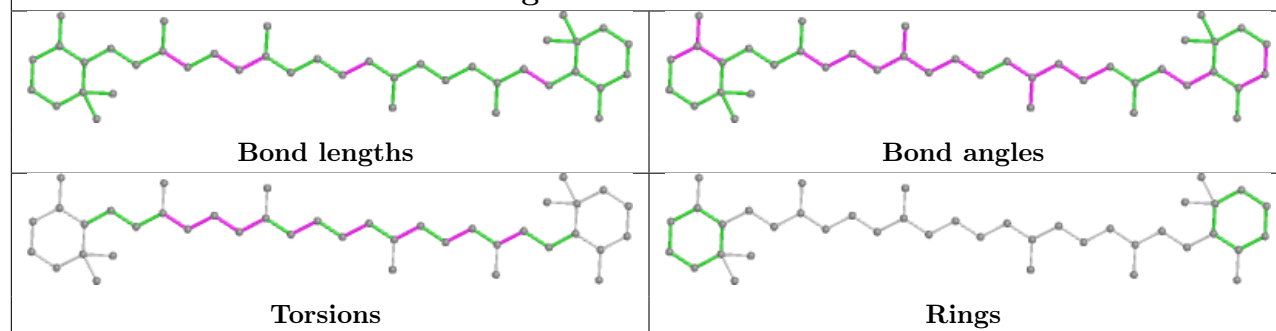




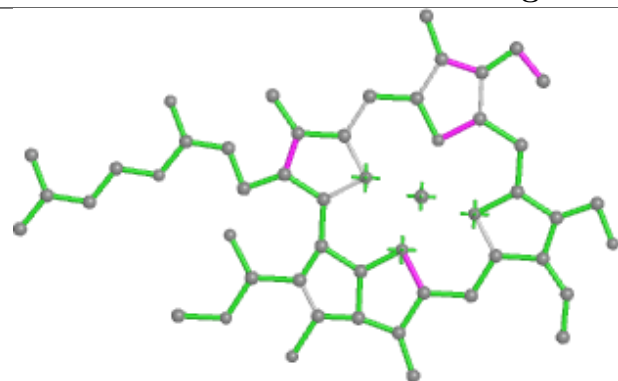
Ligand CLA 6 618



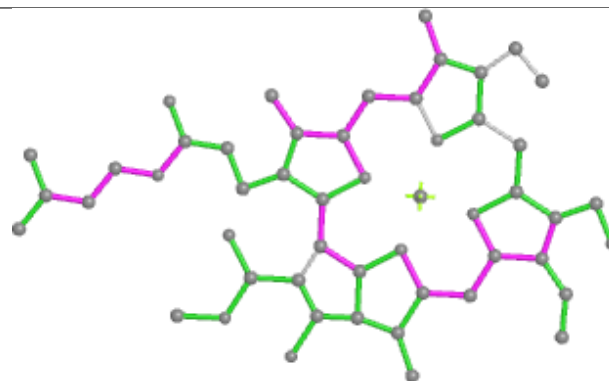
Ligand BCR B 4006



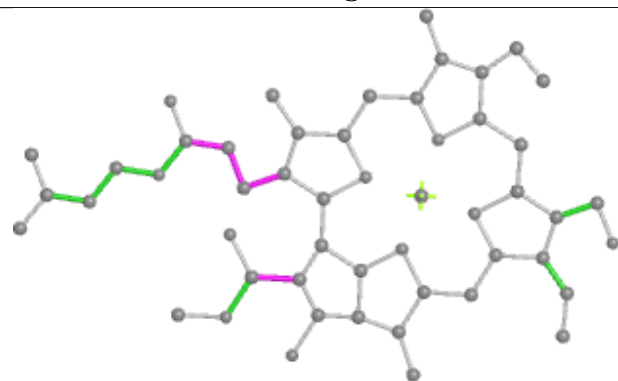
Ligand CHL 5 611



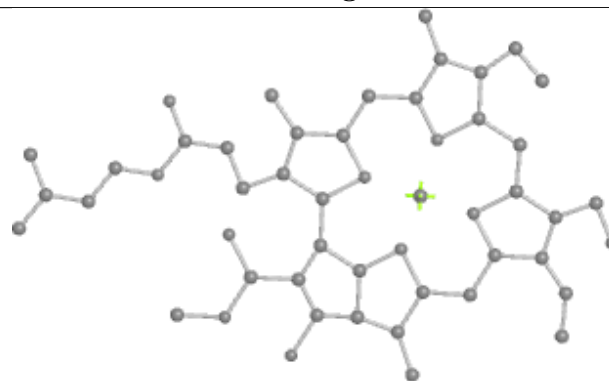
Bond lengths



Bond angles

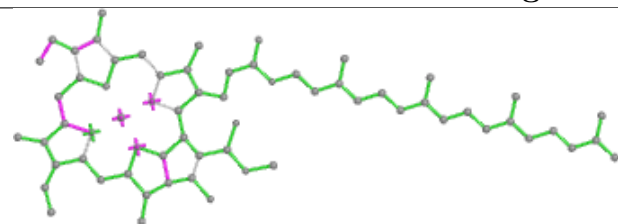


Torsions

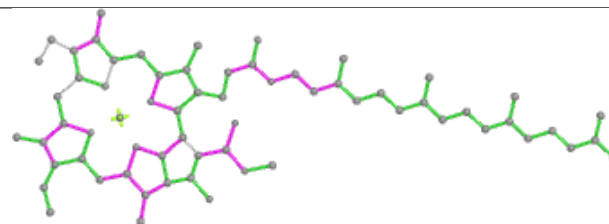


Rings

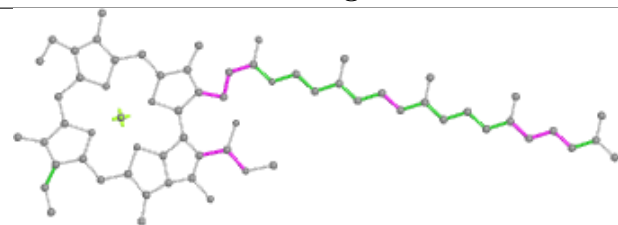
Ligand CLA 3 606



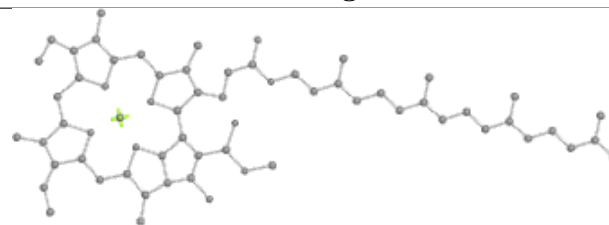
Bond lengths



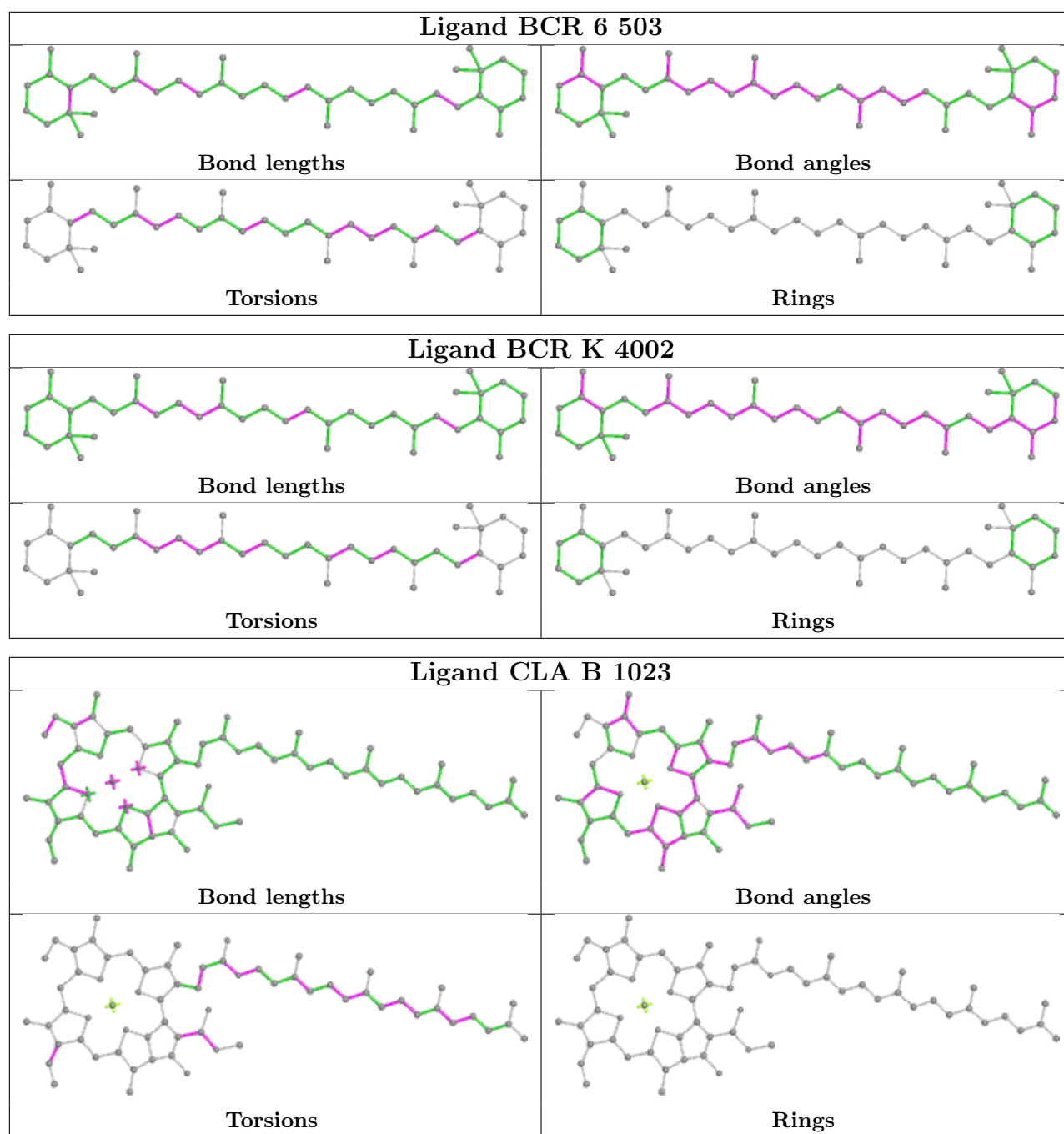
Bond angles

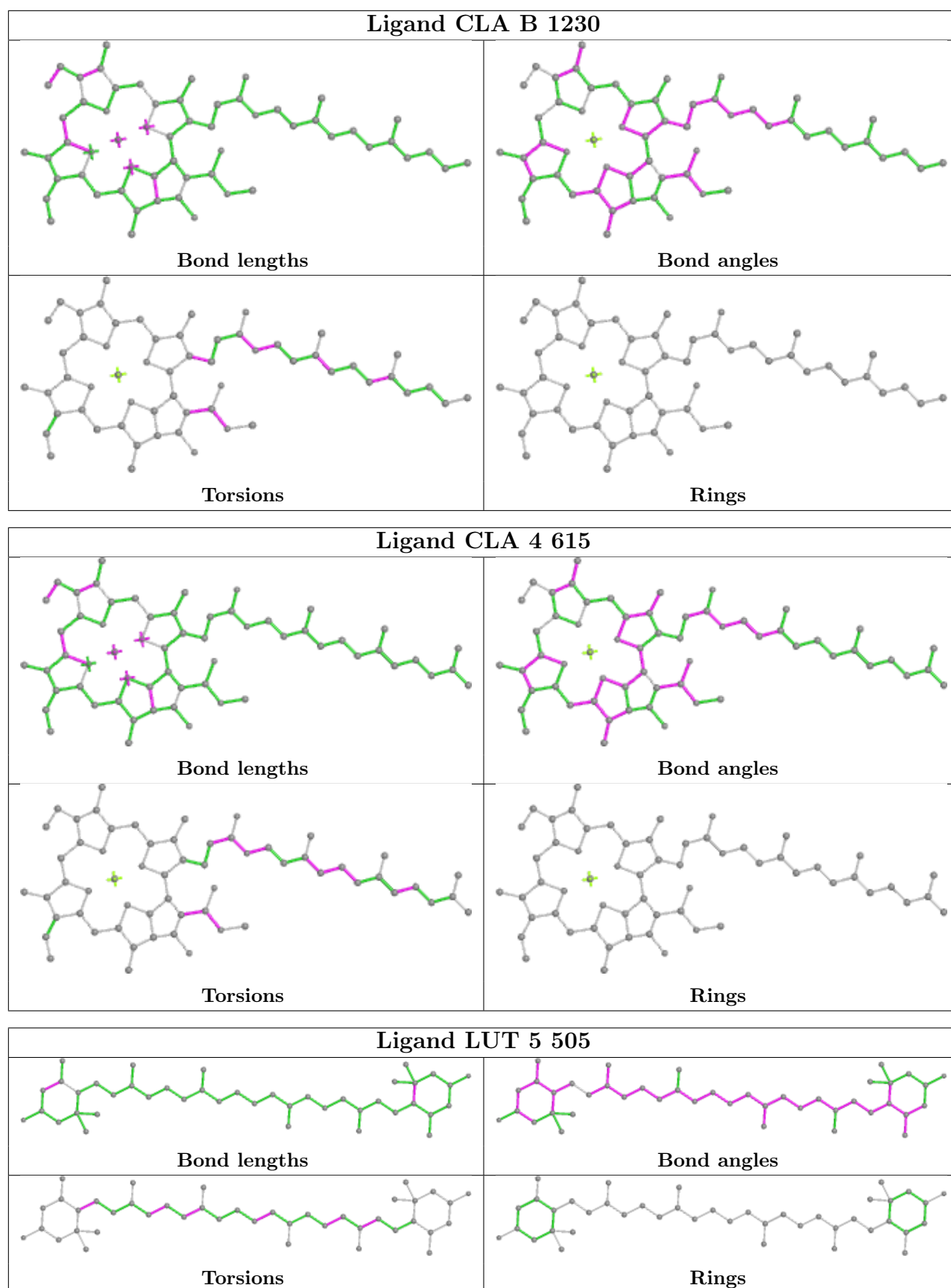


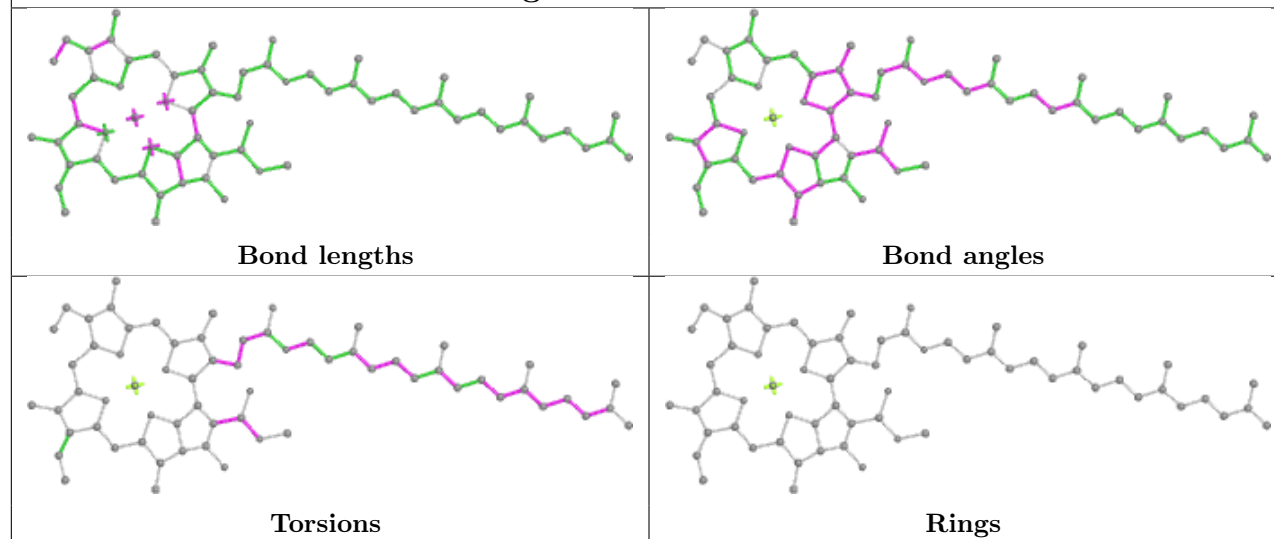
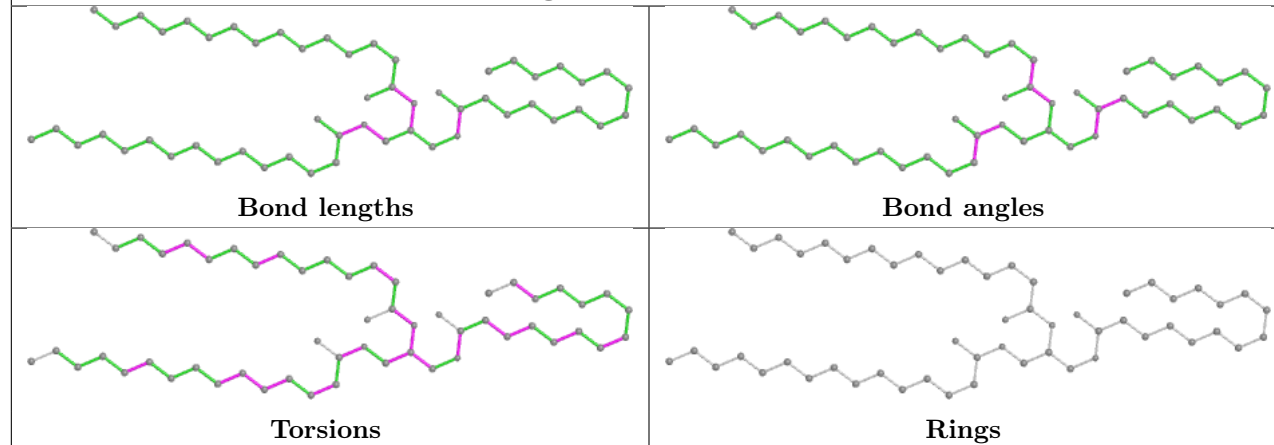
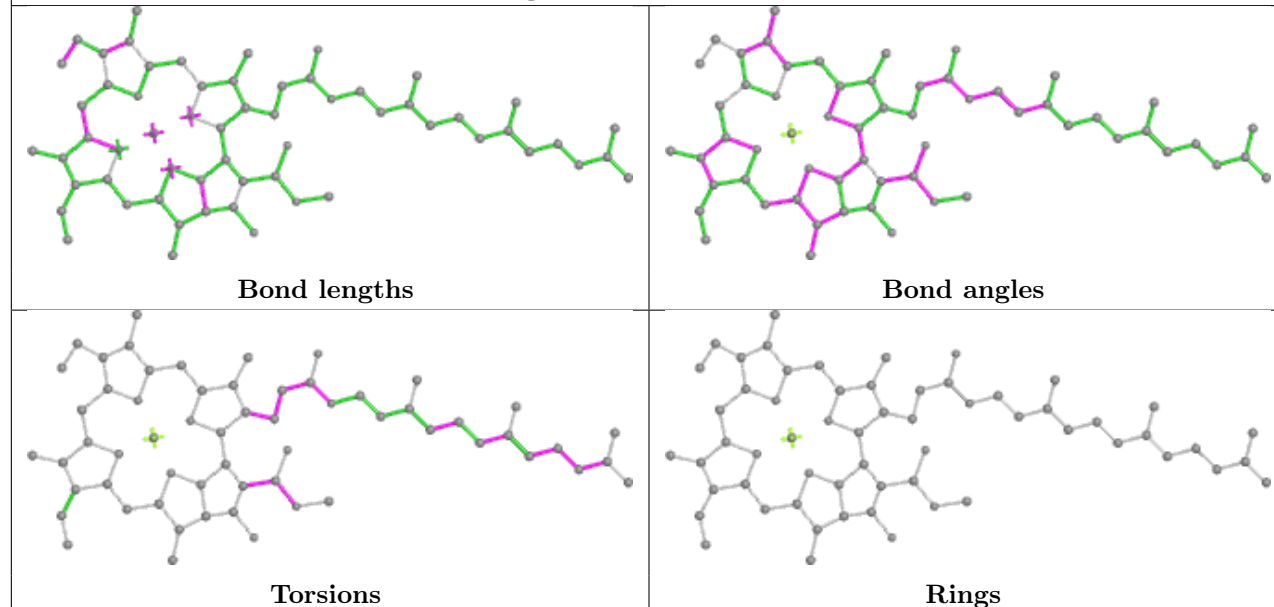
Torsions



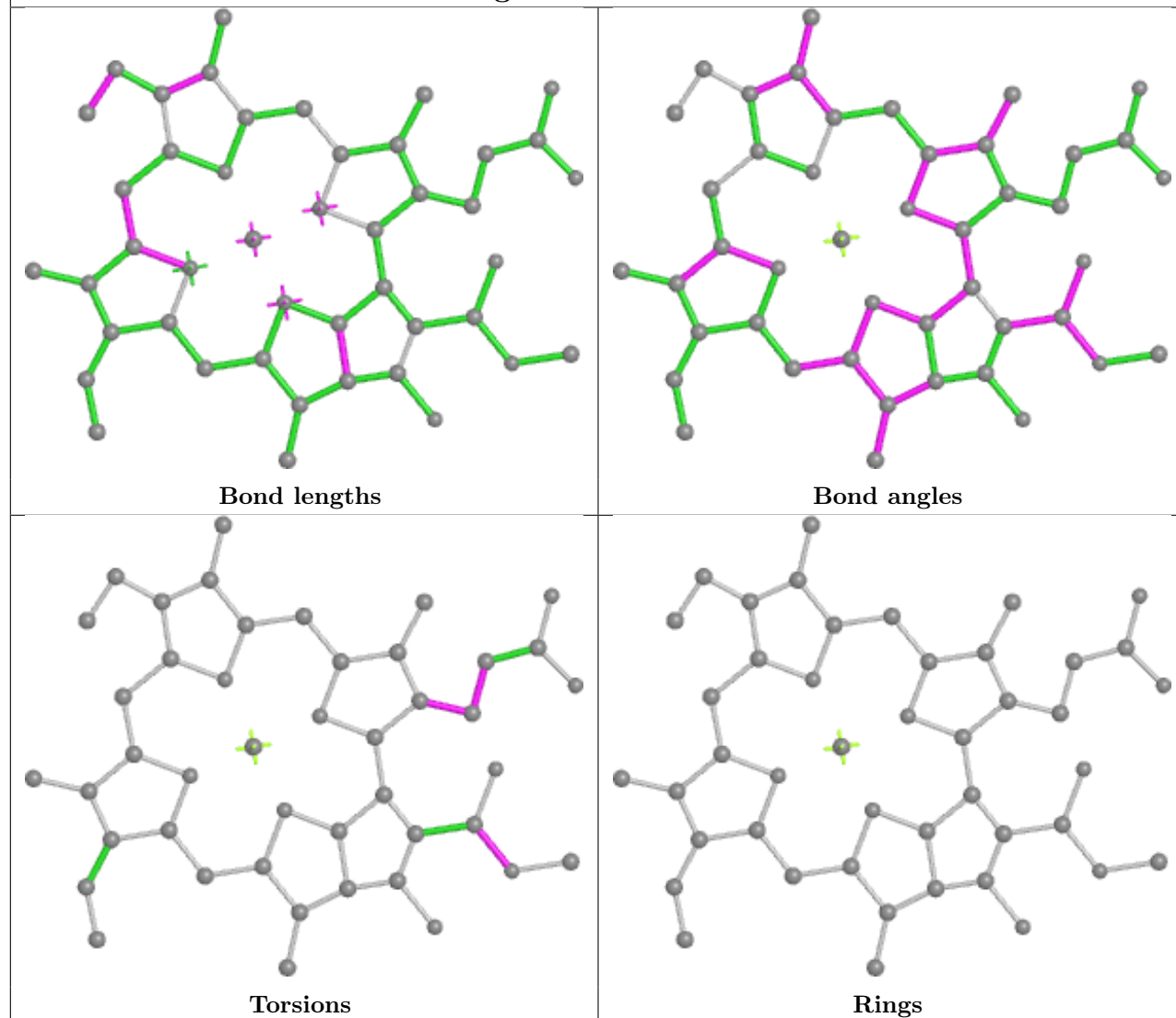
Rings



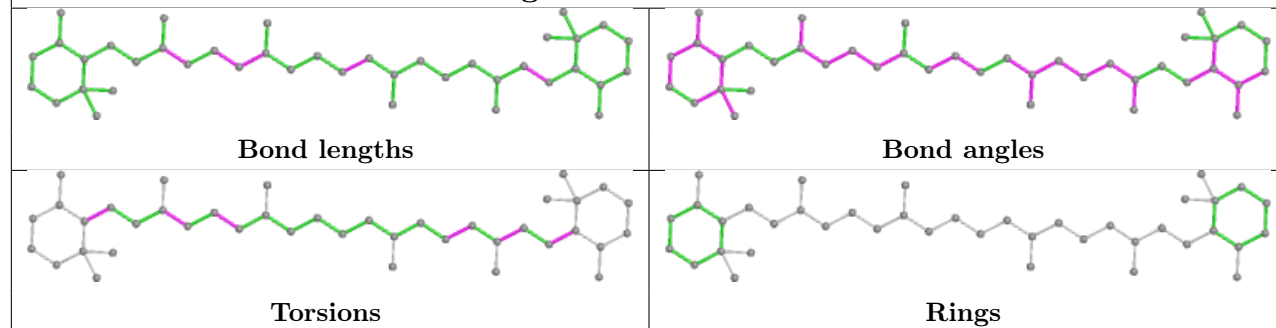


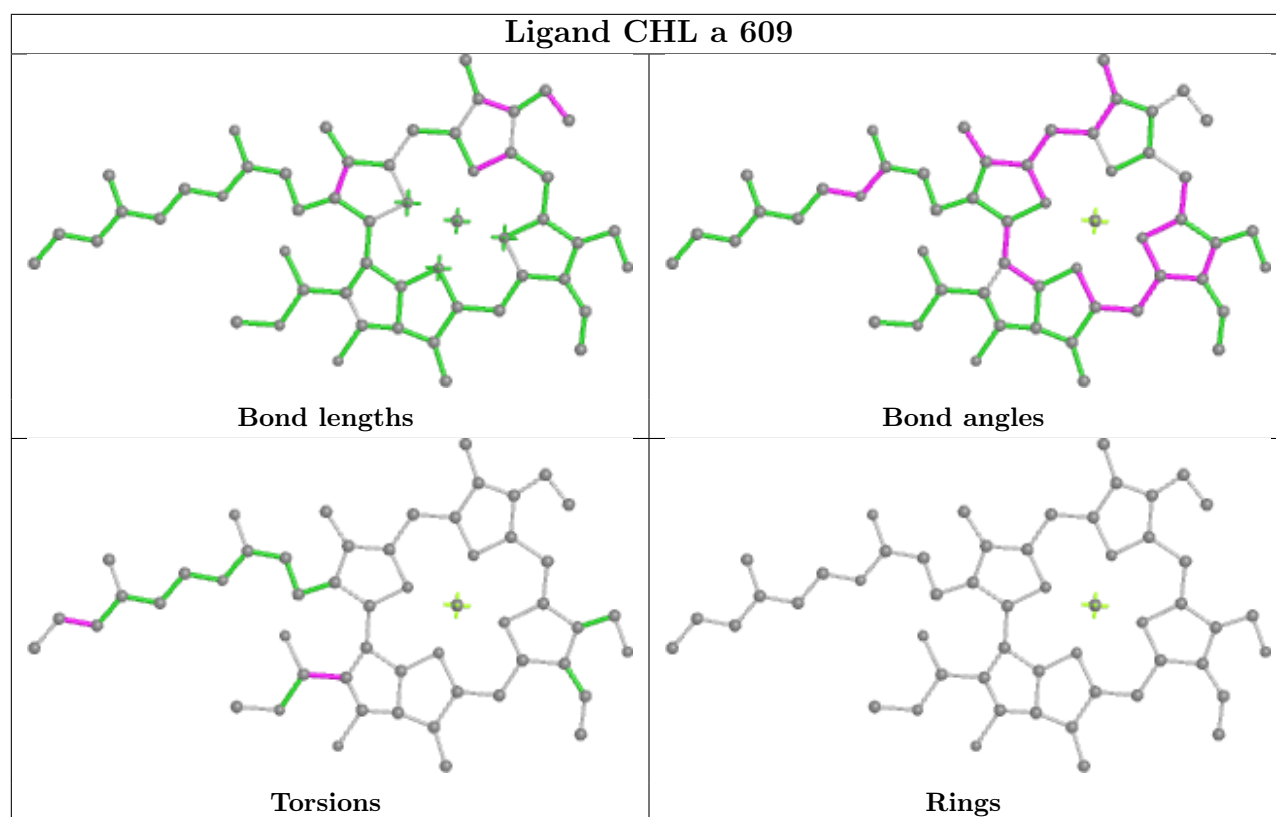
Ligand CLA A 1109**Ligand 4RF 8 808****Ligand CLA A 1116**

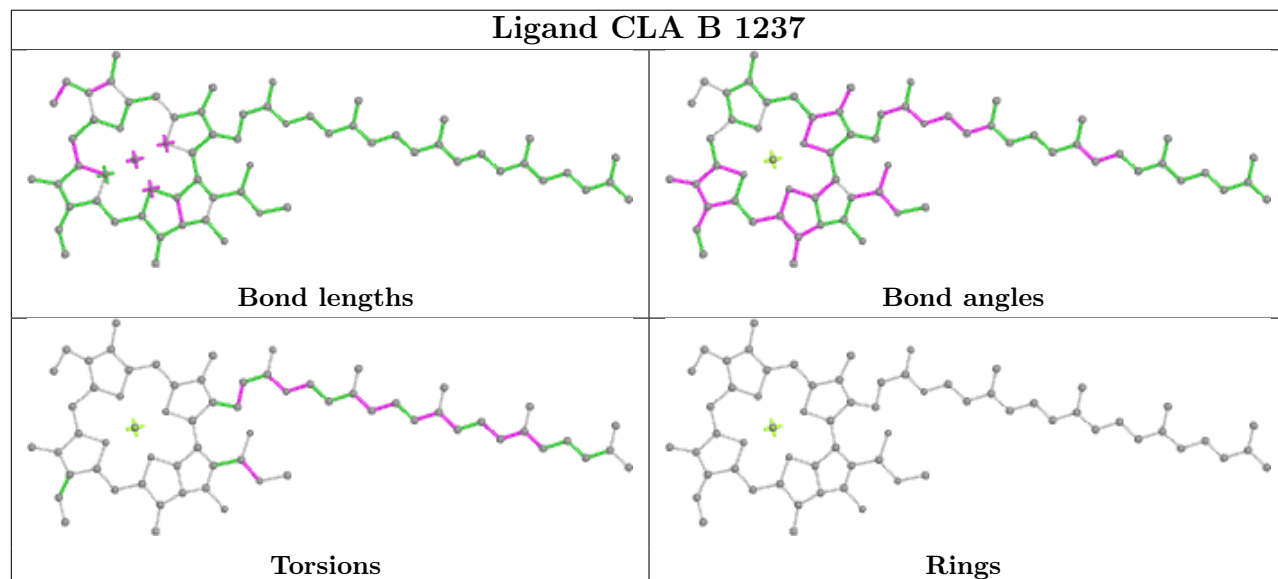
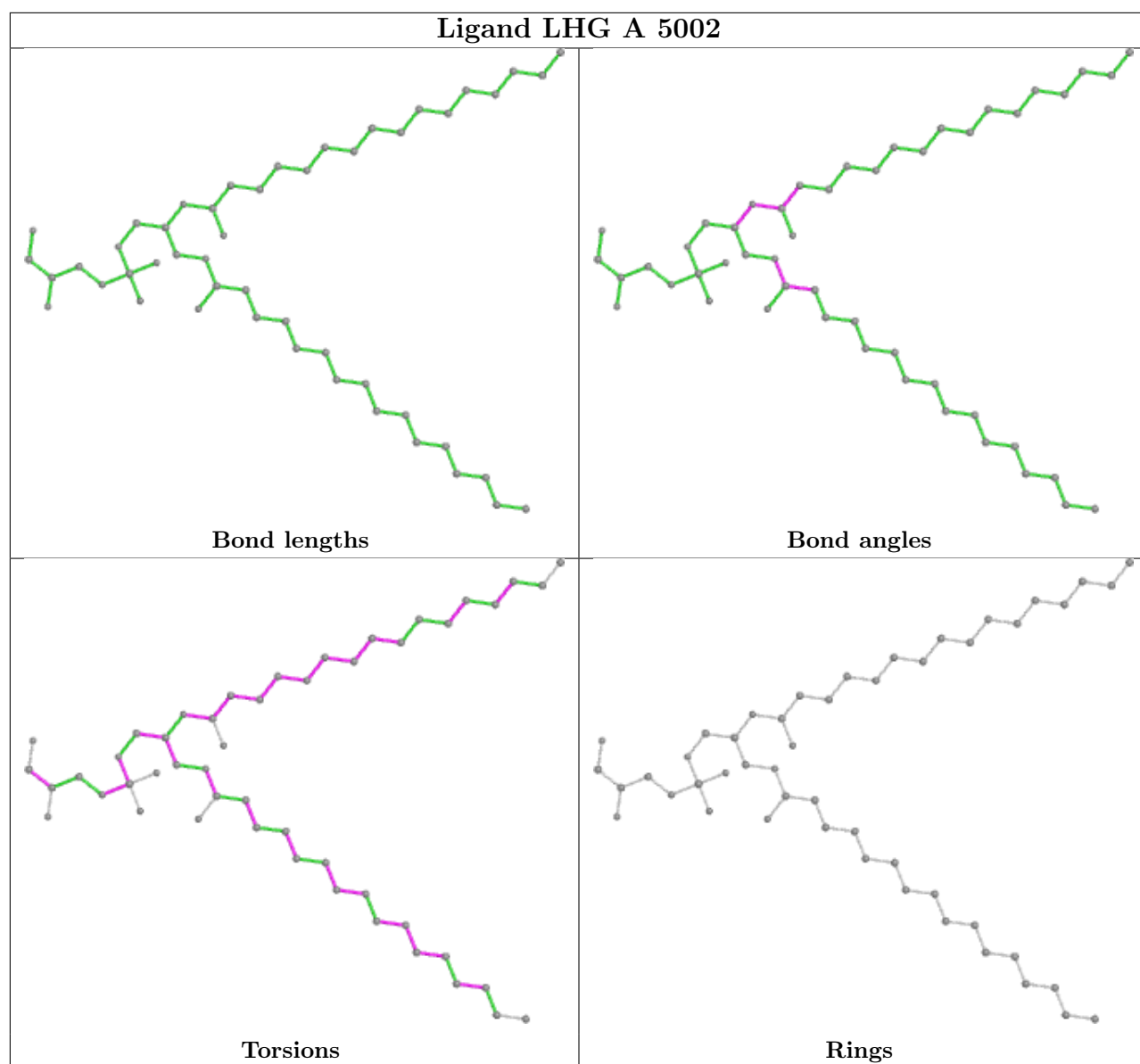
Ligand CLA 1 610



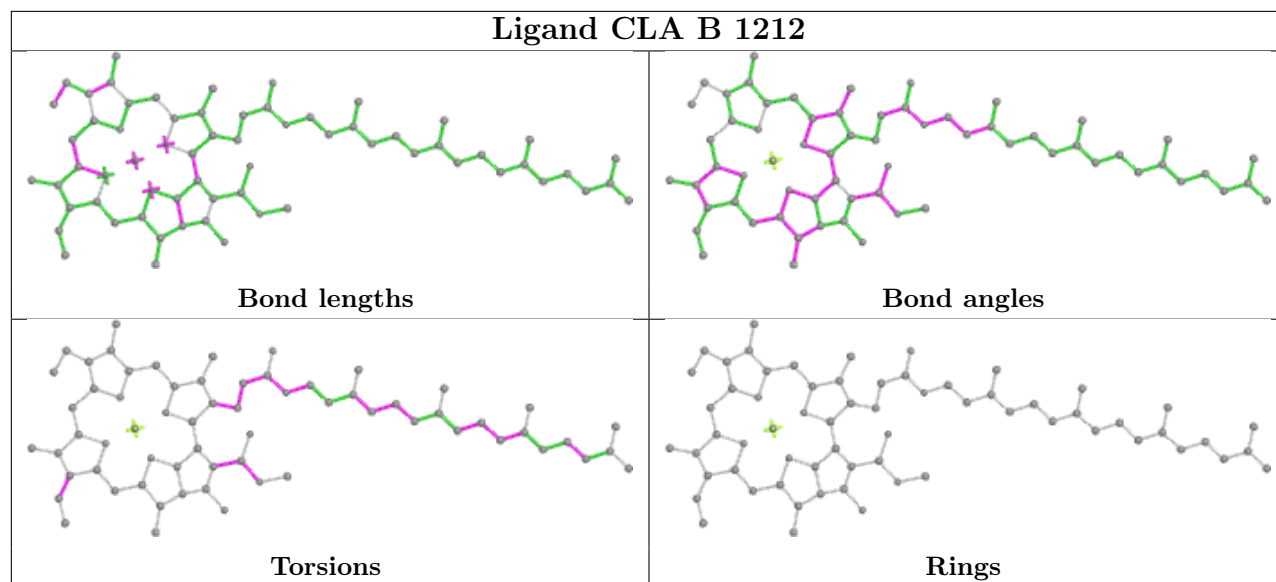
Ligand BCR A 4001



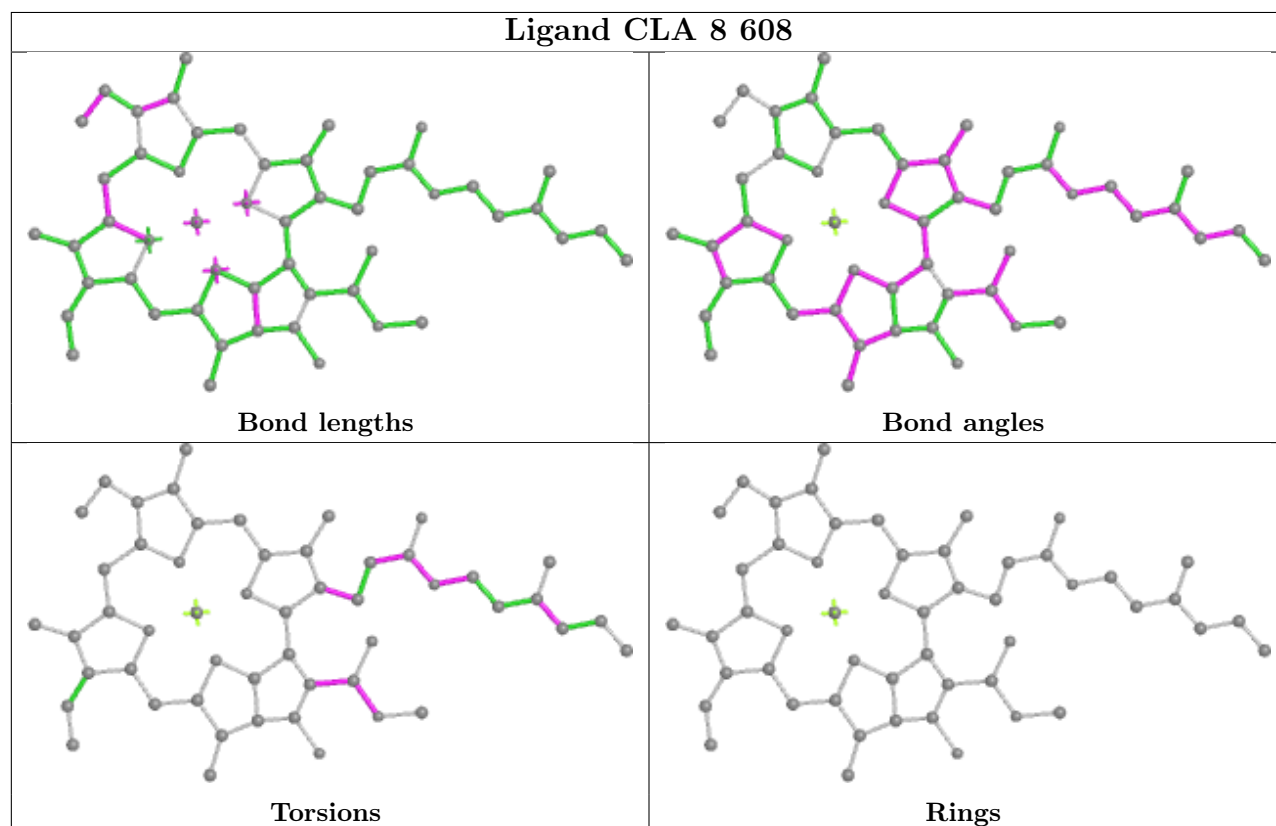




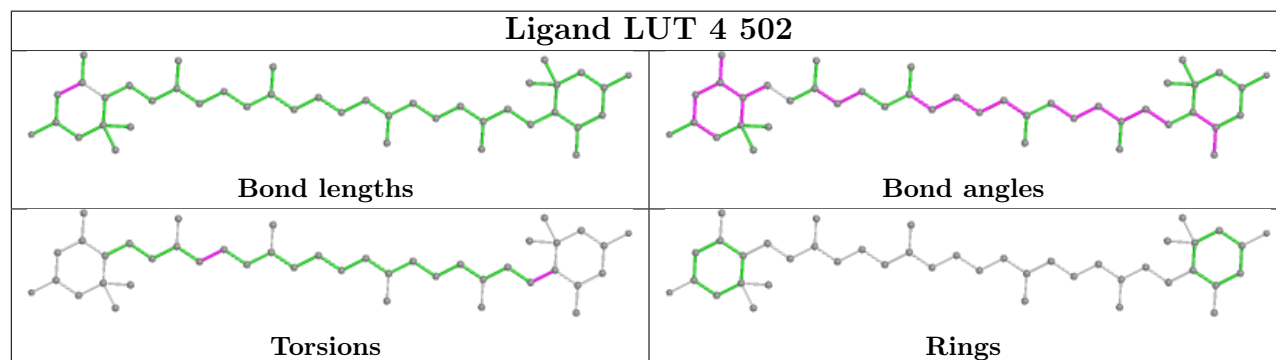
Ligand CLA B 1212

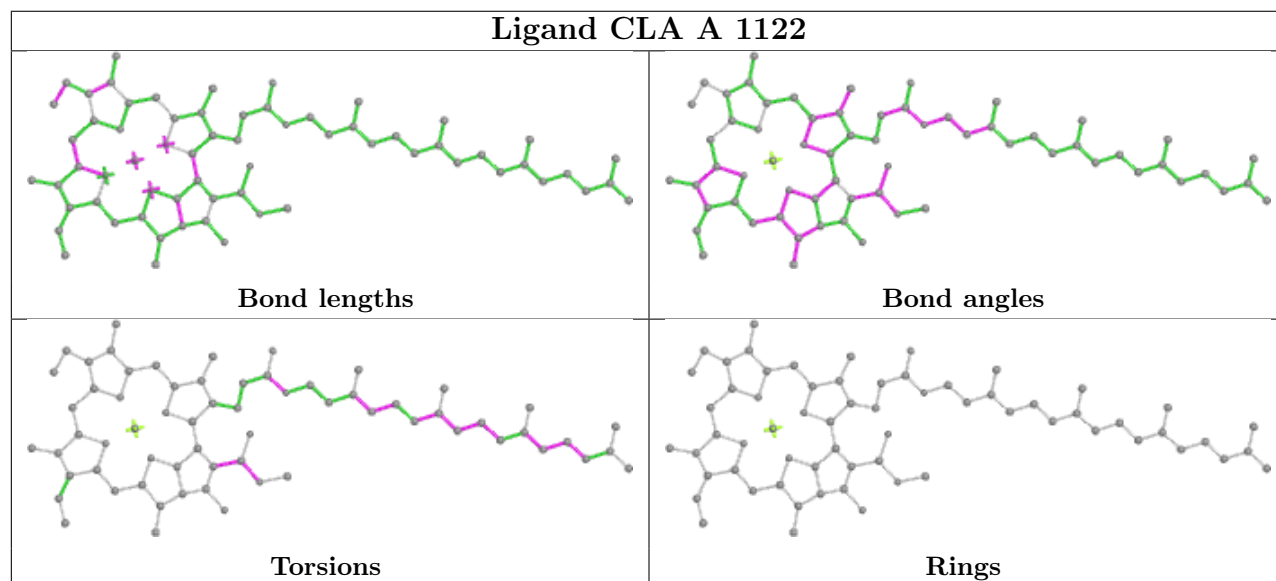
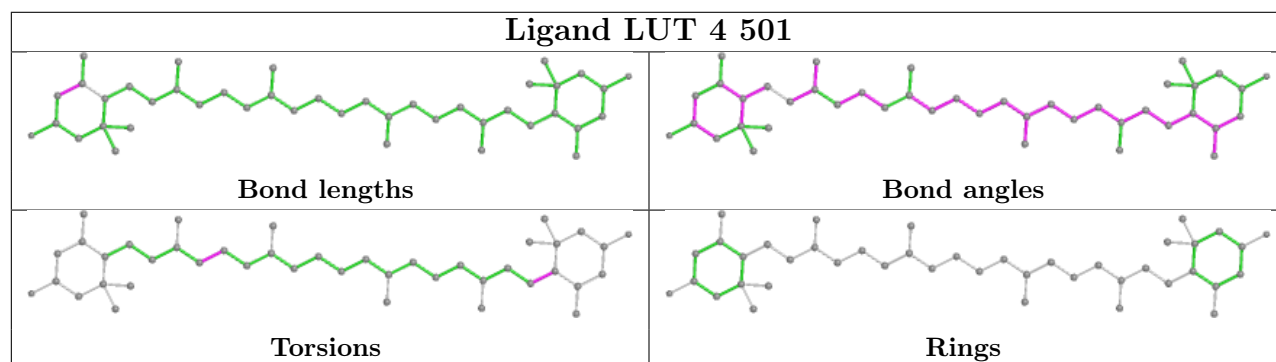
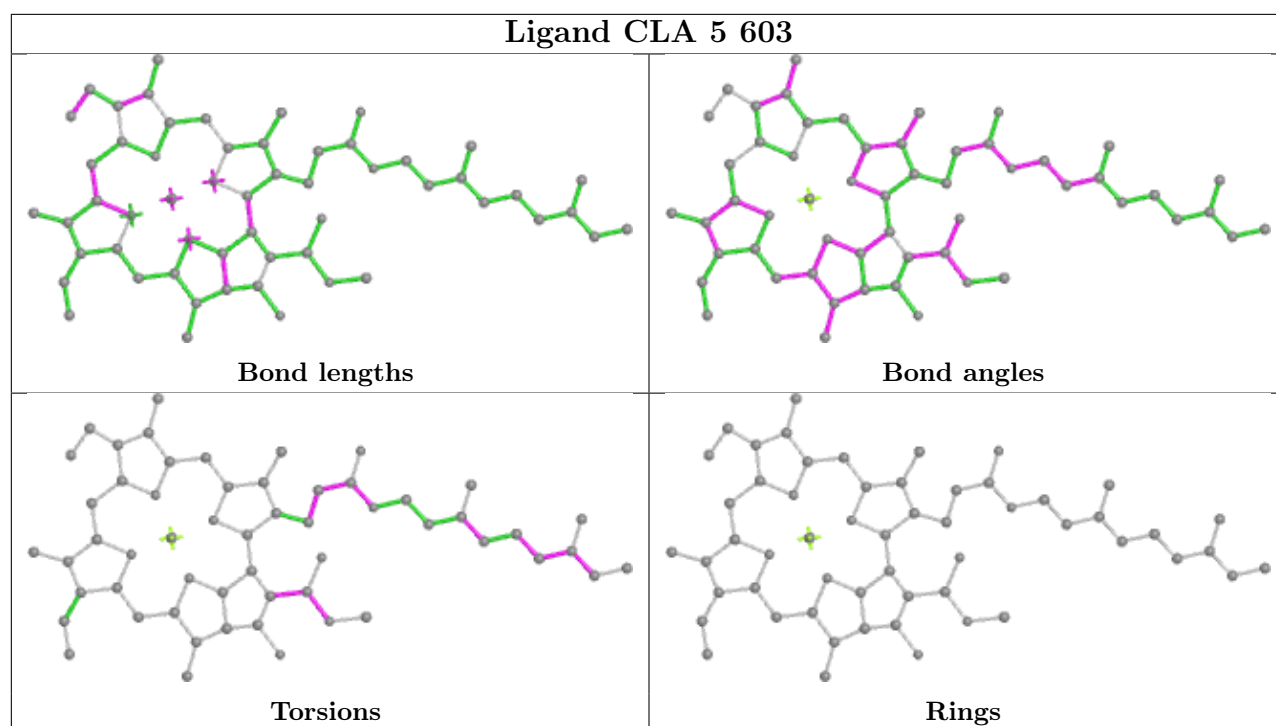


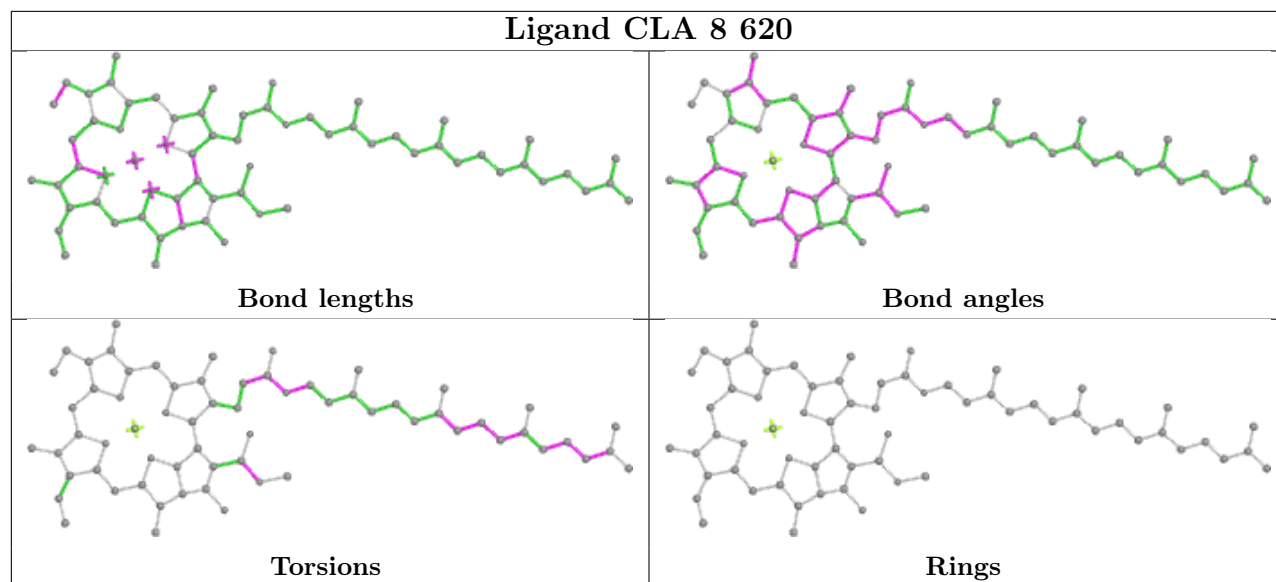
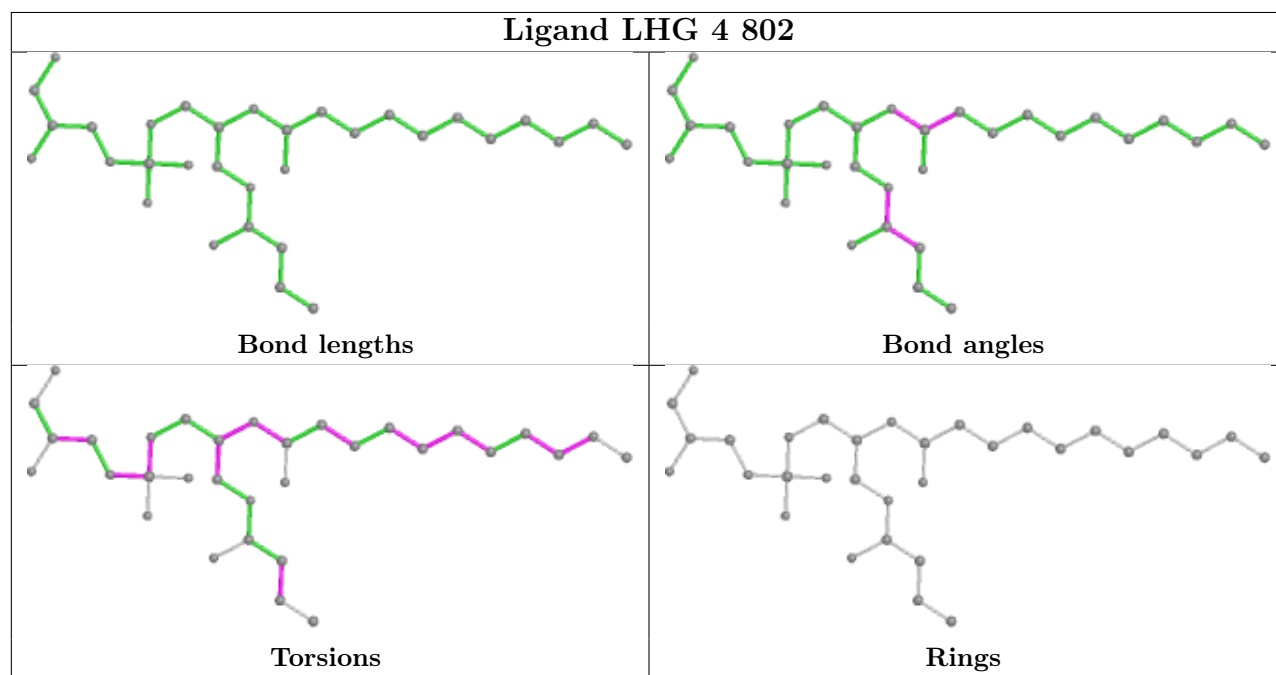
Ligand CLA 8 608

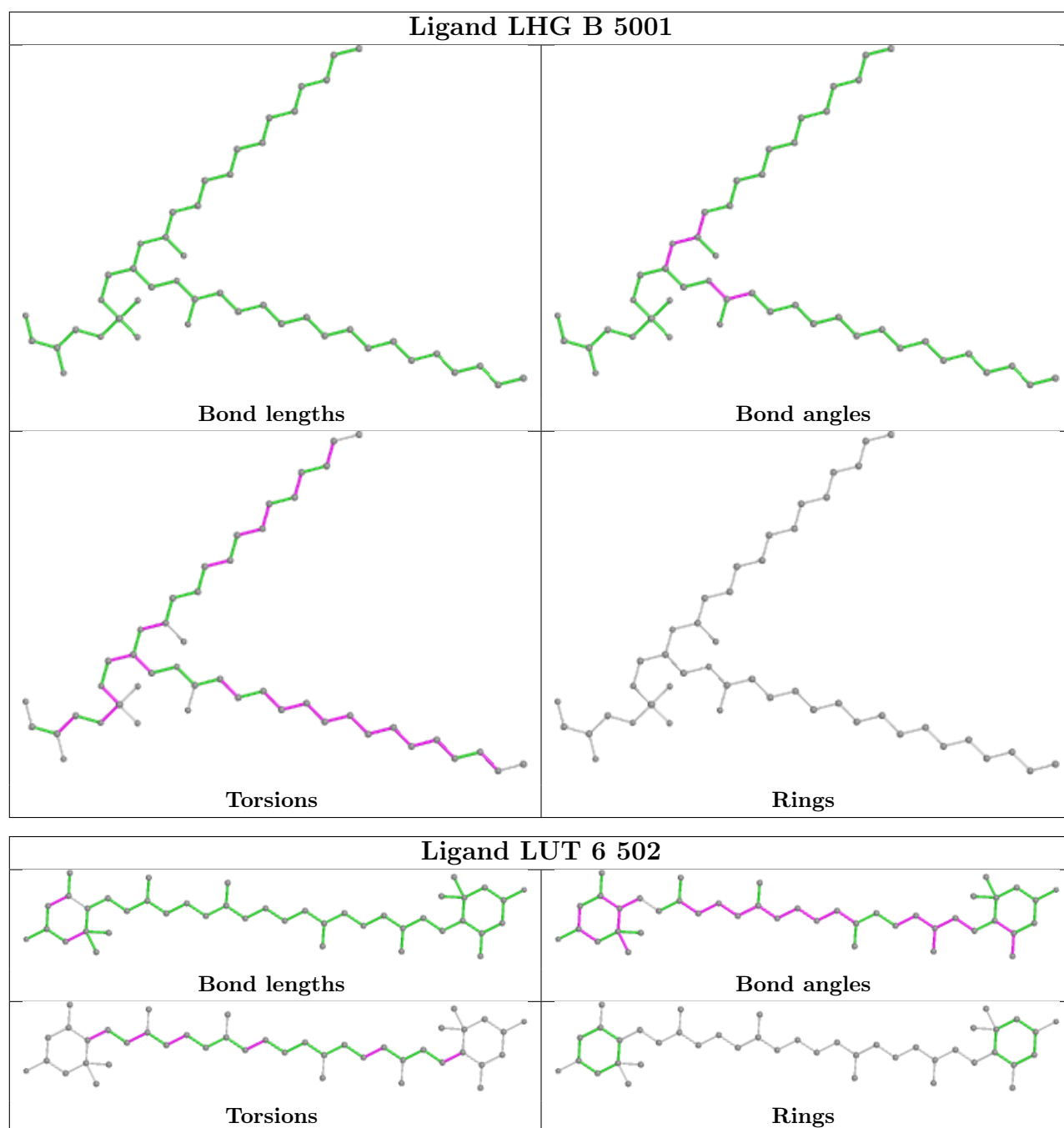


Ligand LUT 4 502

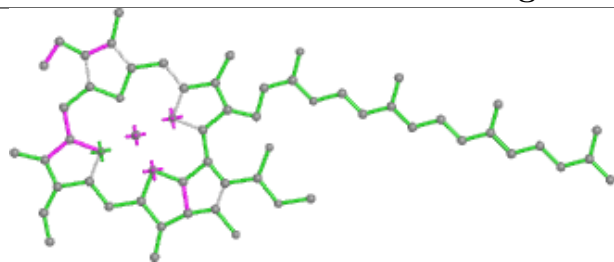




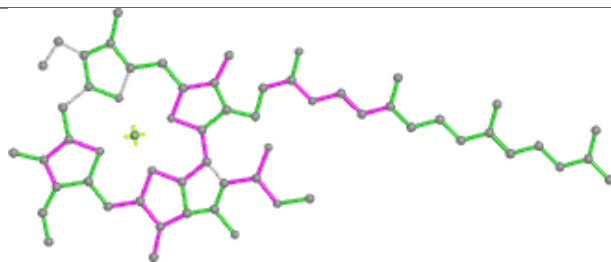
Ligand CLA 8 620**Ligand LHG 4 802**



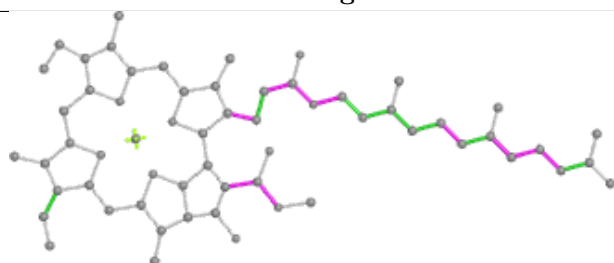
Ligand CLA 1 608



Bond lengths



Bond angles

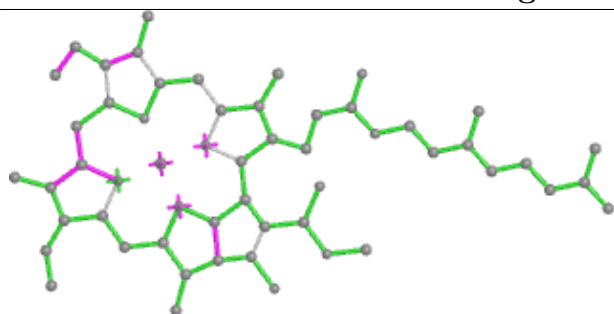


Torsions

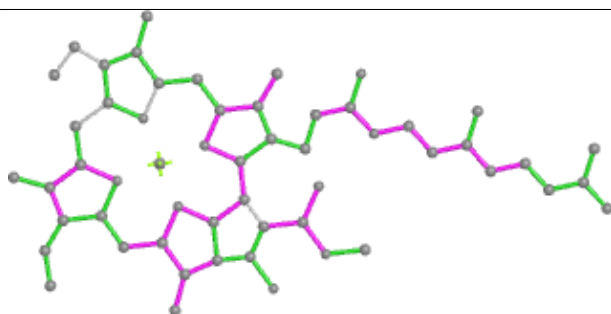


Rings

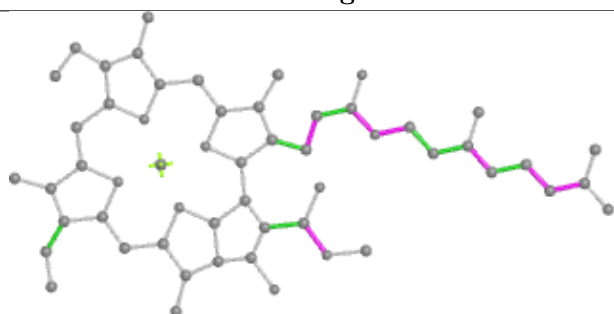
Ligand CLA 1 611



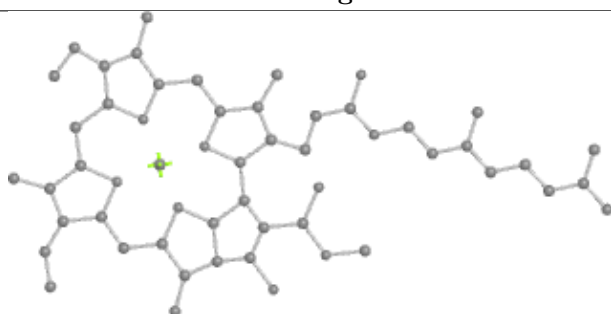
Bond lengths



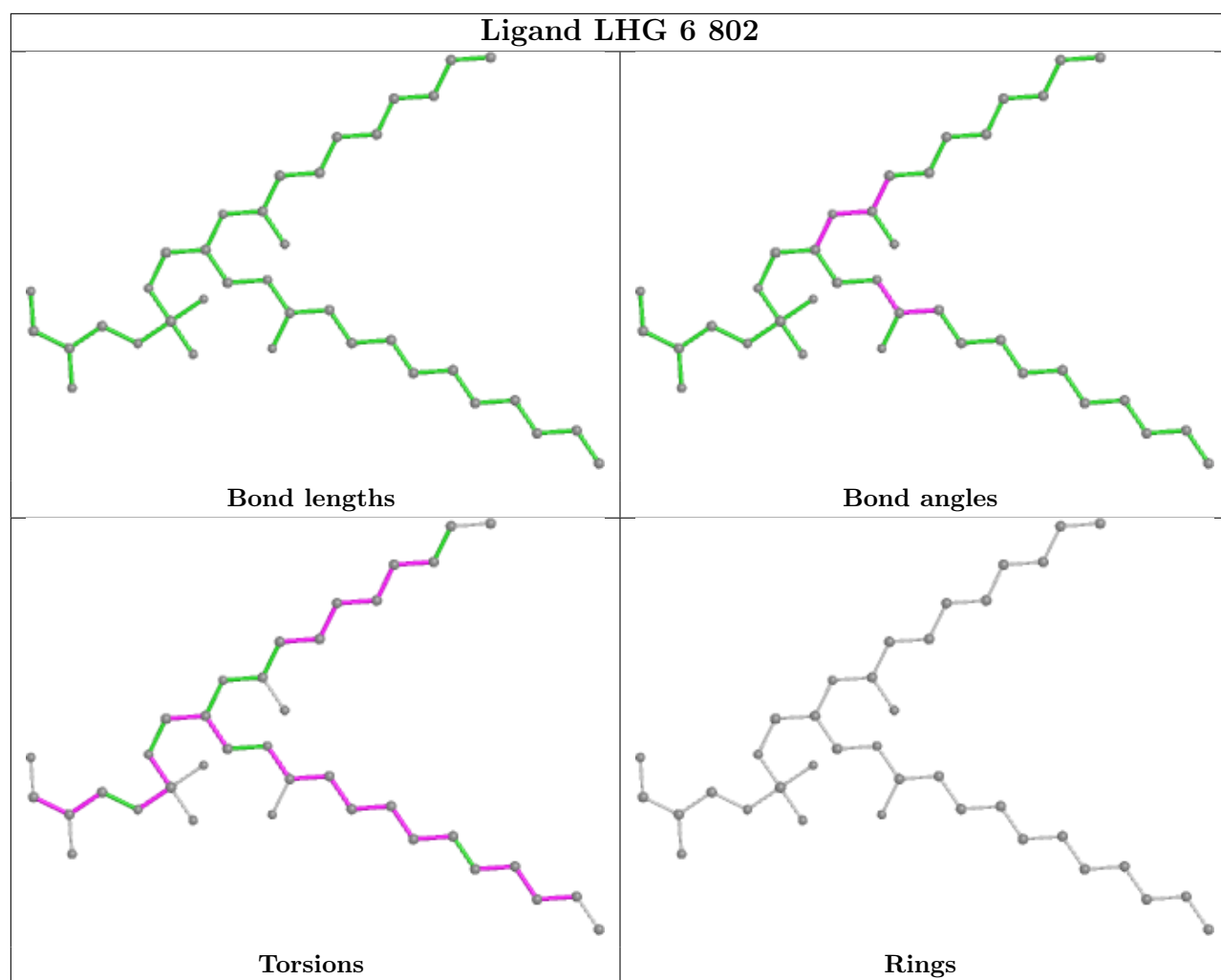
Bond angles



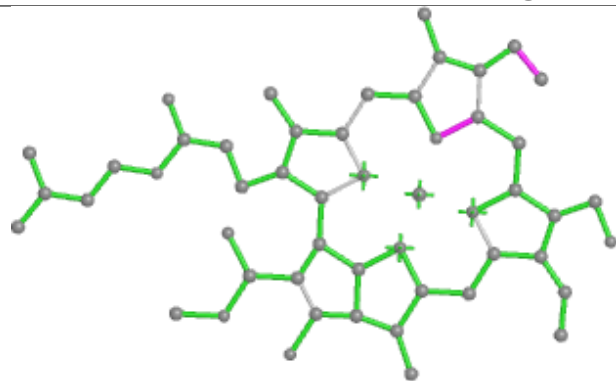
Torsions



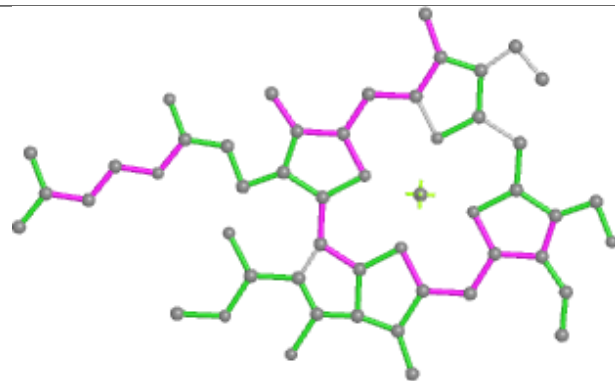
Rings



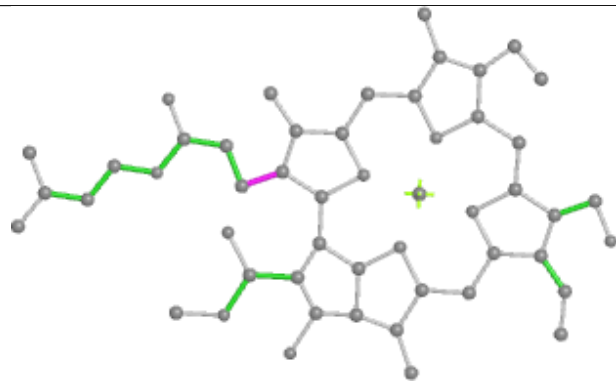
Ligand CHL 6 613



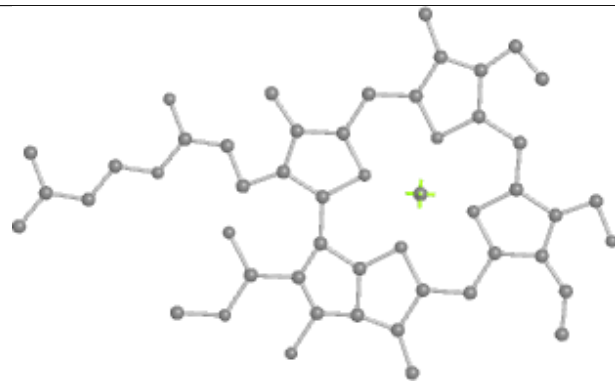
Bond lengths



Bond angles

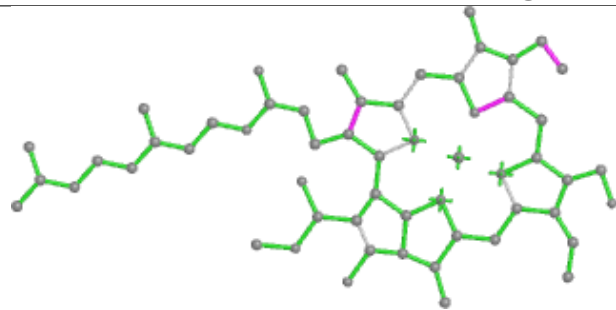


Torsions

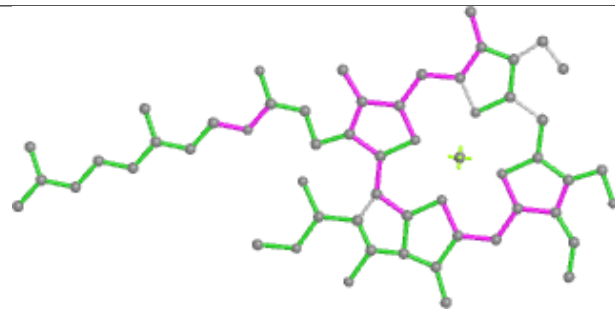


Rings

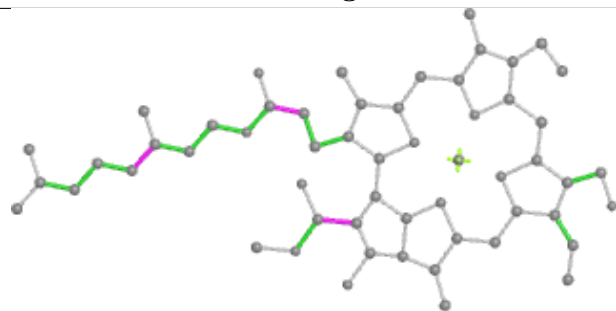
Ligand CHL 6 610



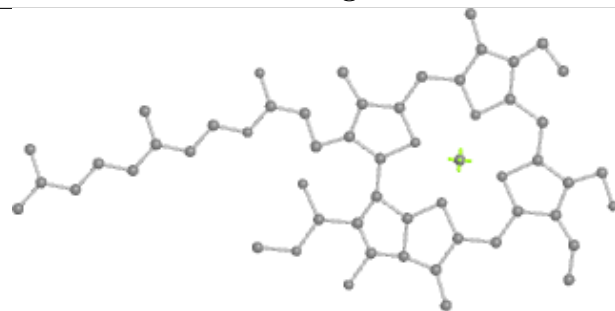
Bond lengths



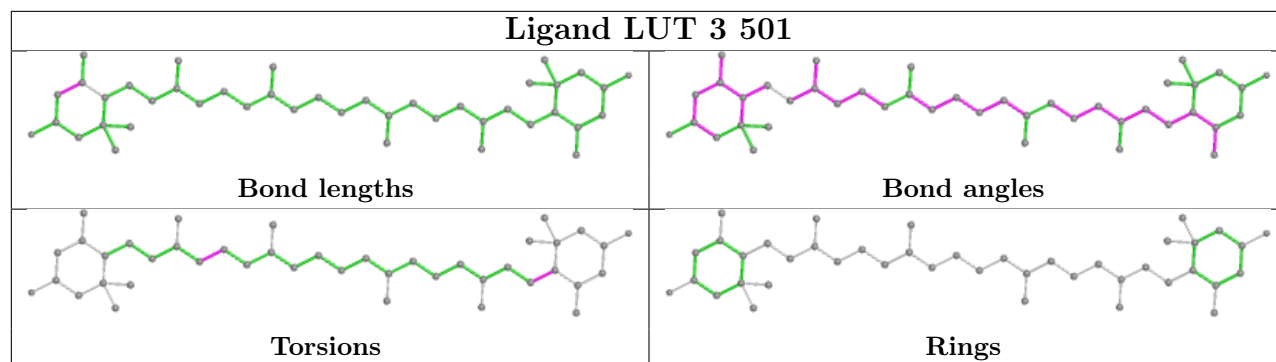
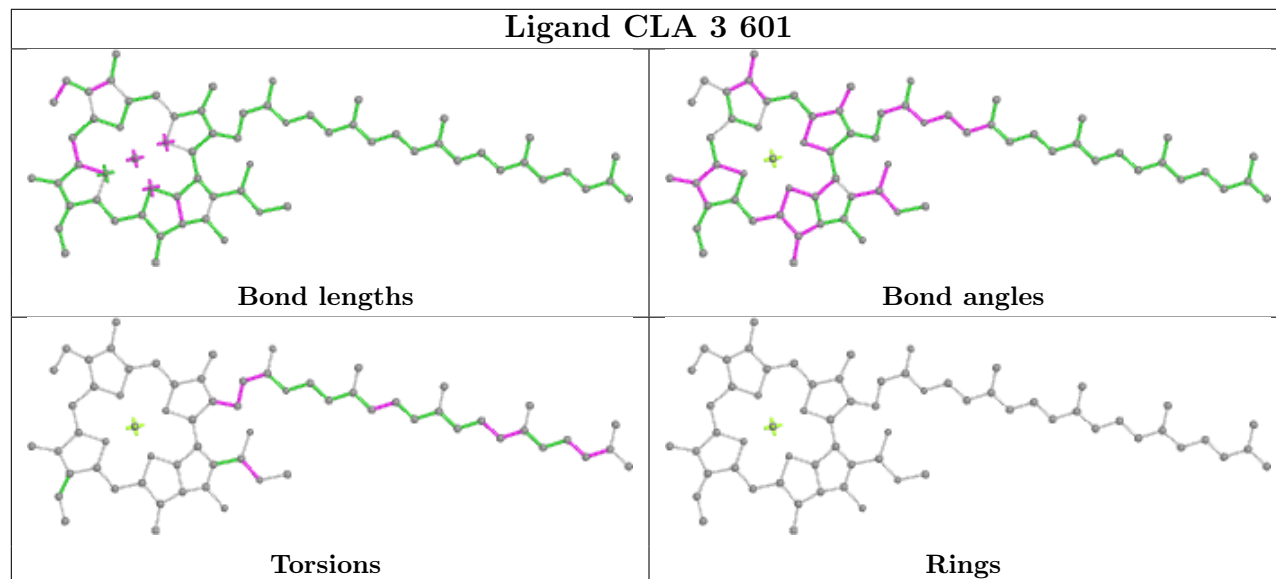
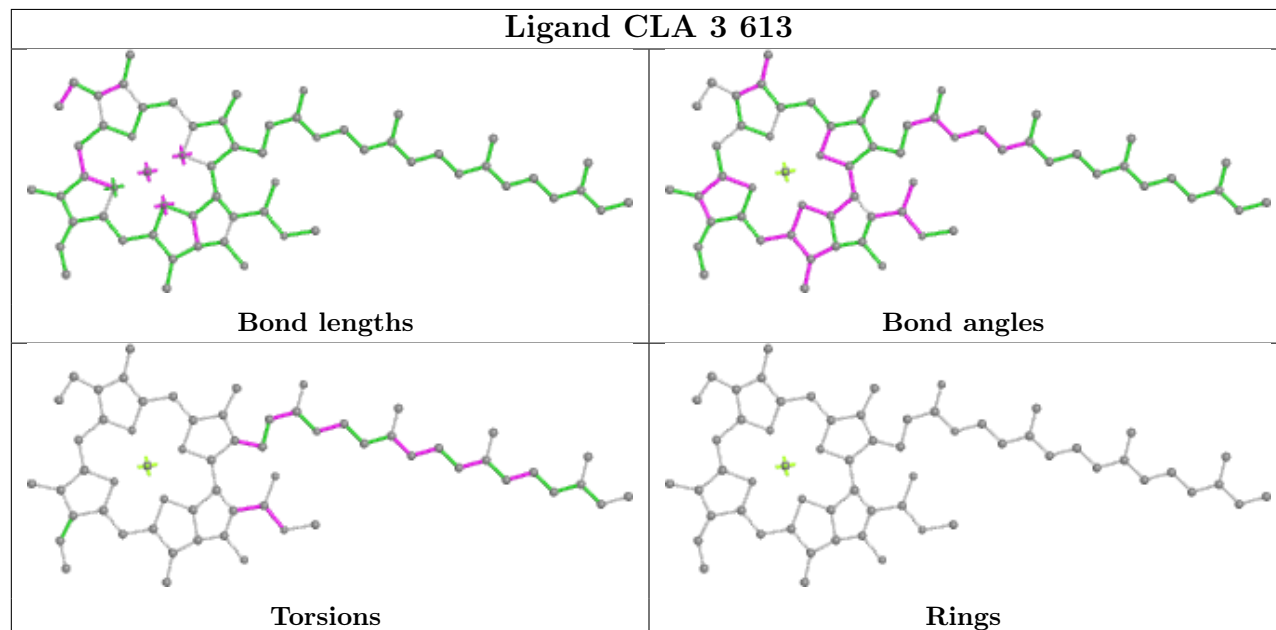
Bond angles

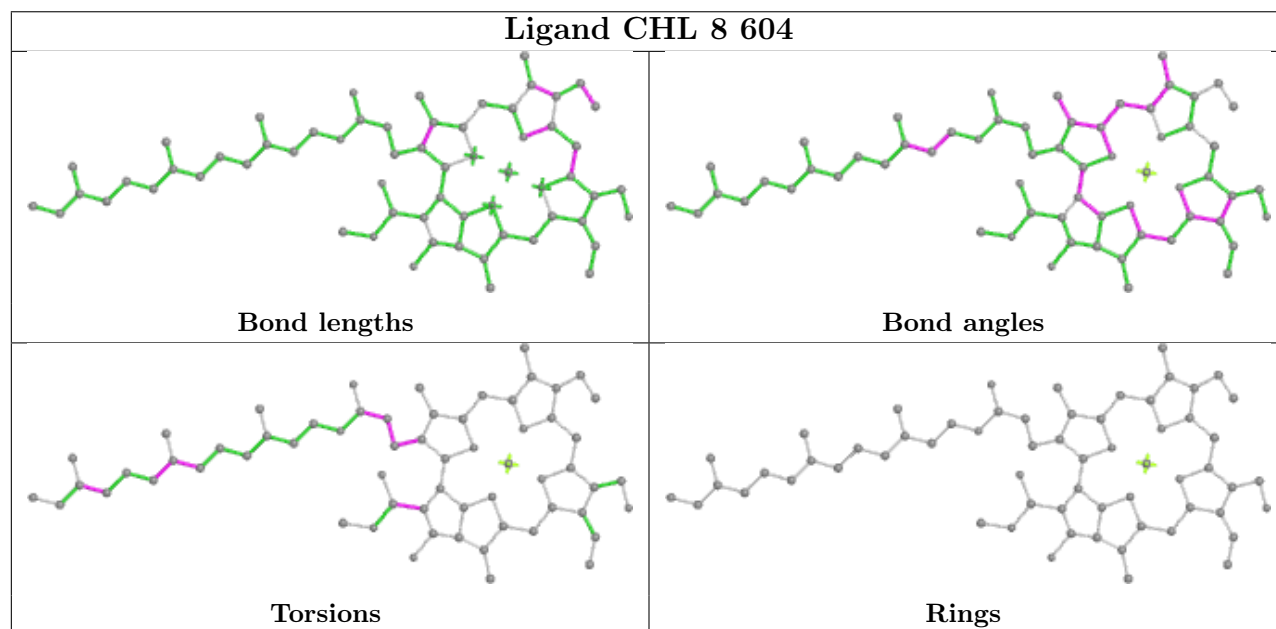
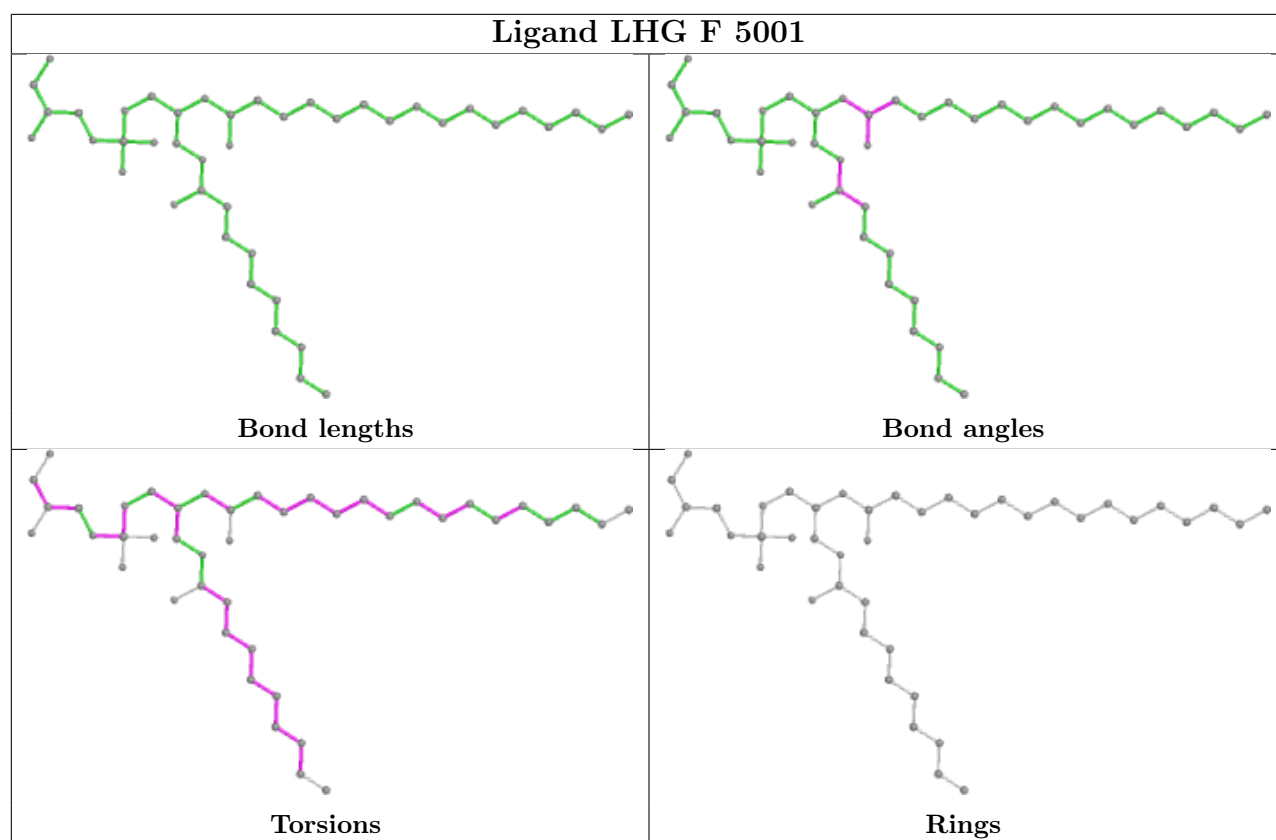


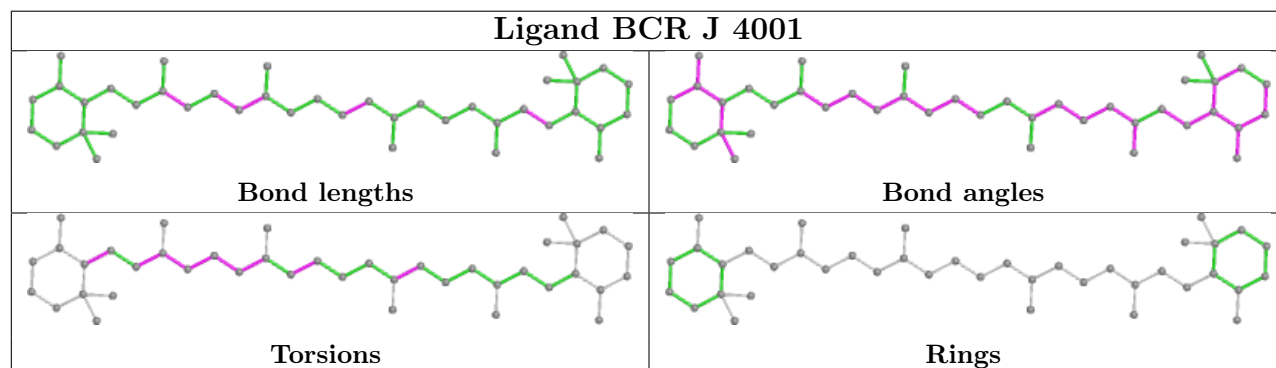
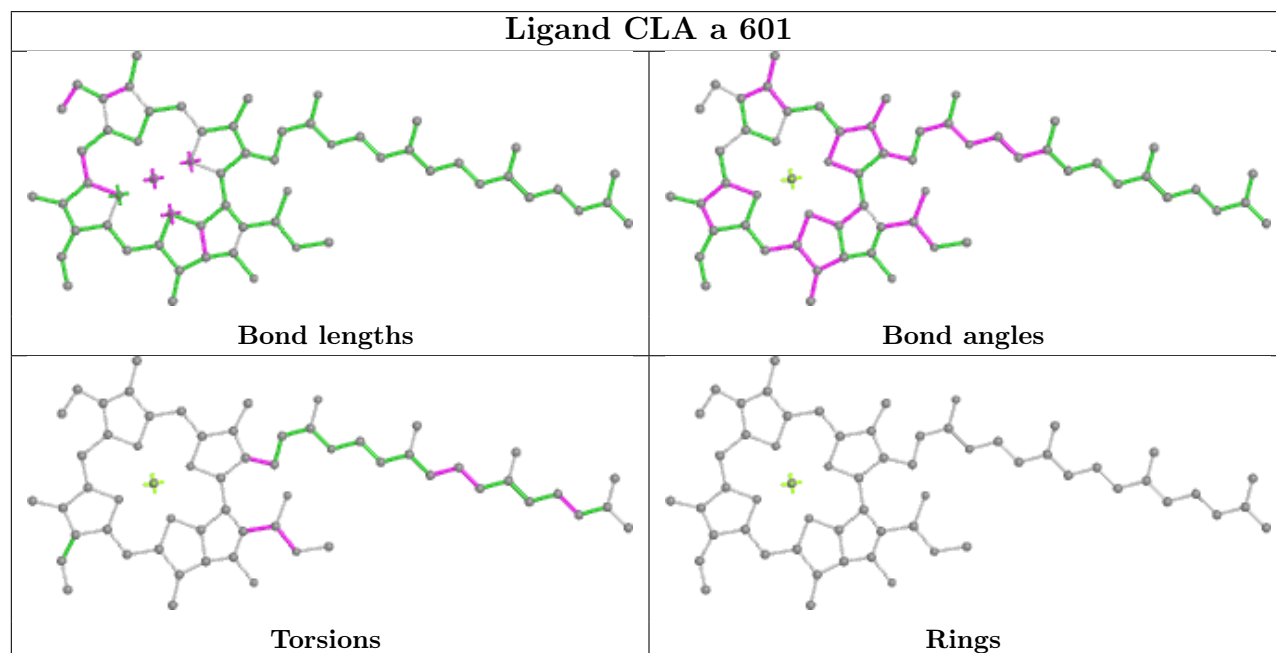
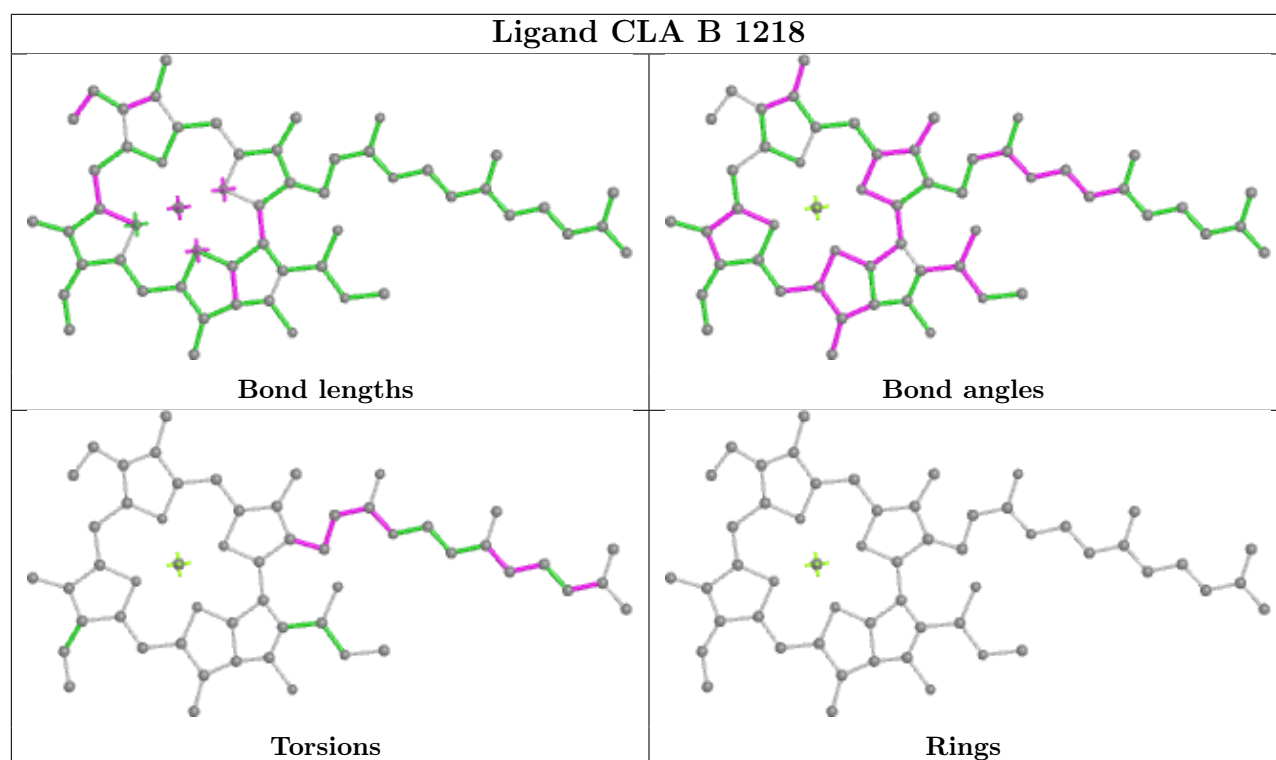
Torsions

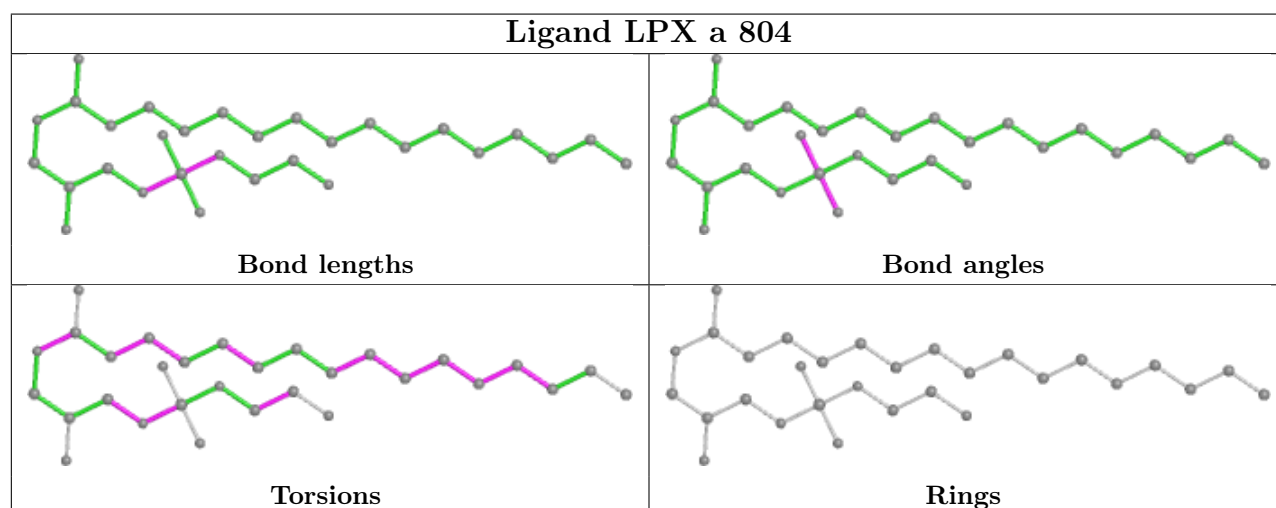
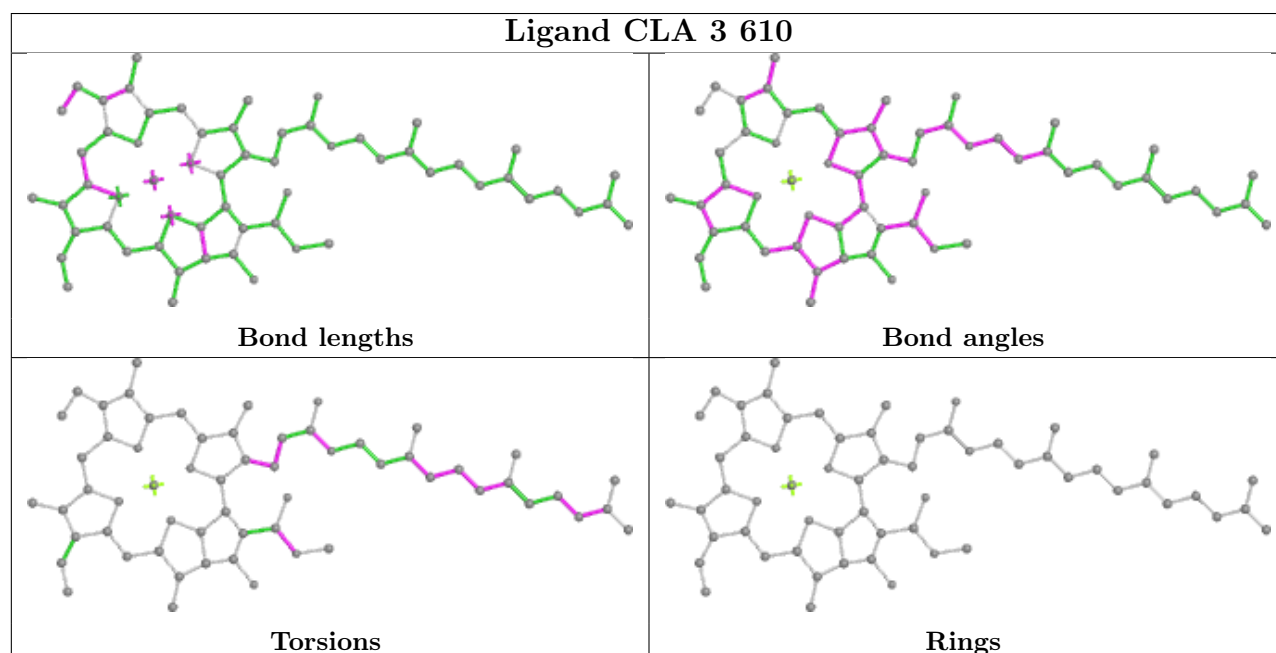
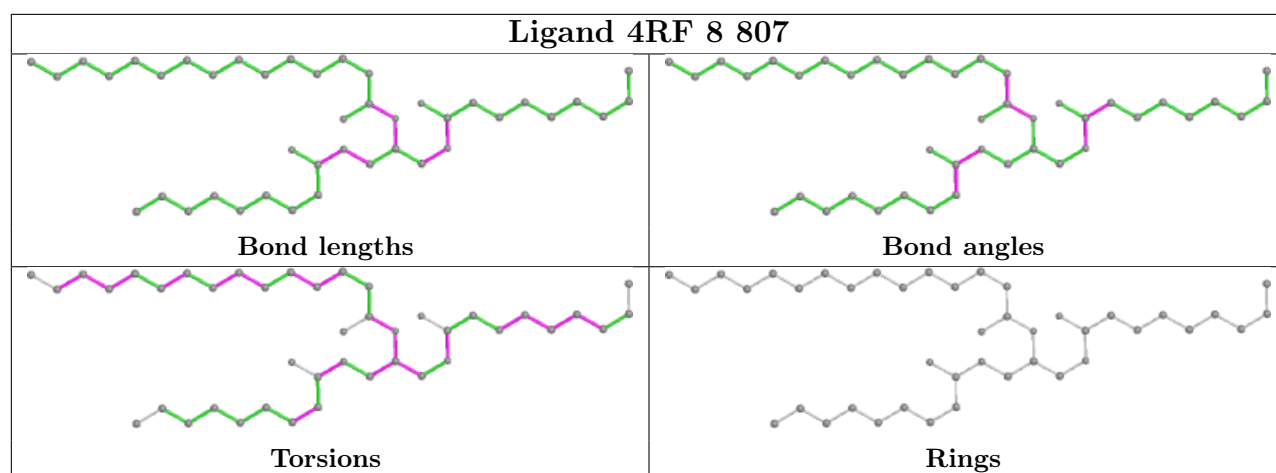


Rings

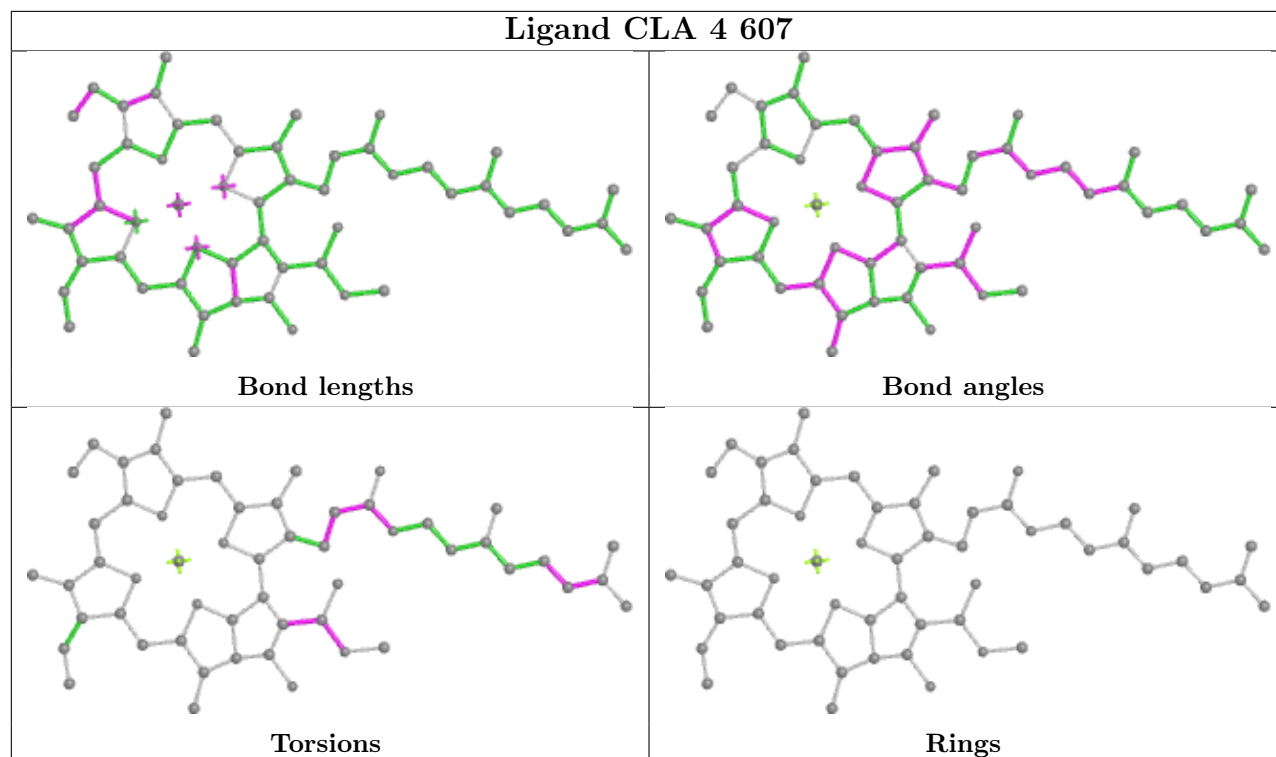
Ligand LUT 3 501**Ligand CLA 3 601****Ligand CLA 3 613**



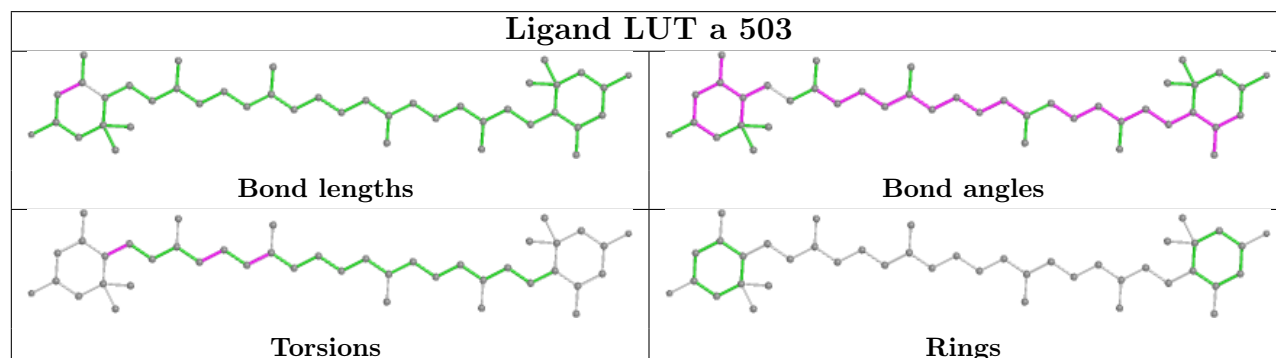




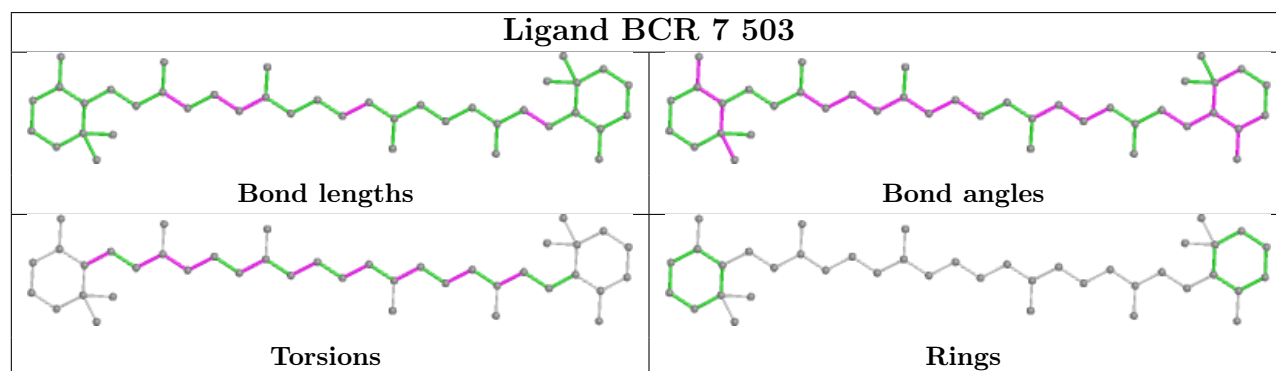
Ligand CLA 4 607

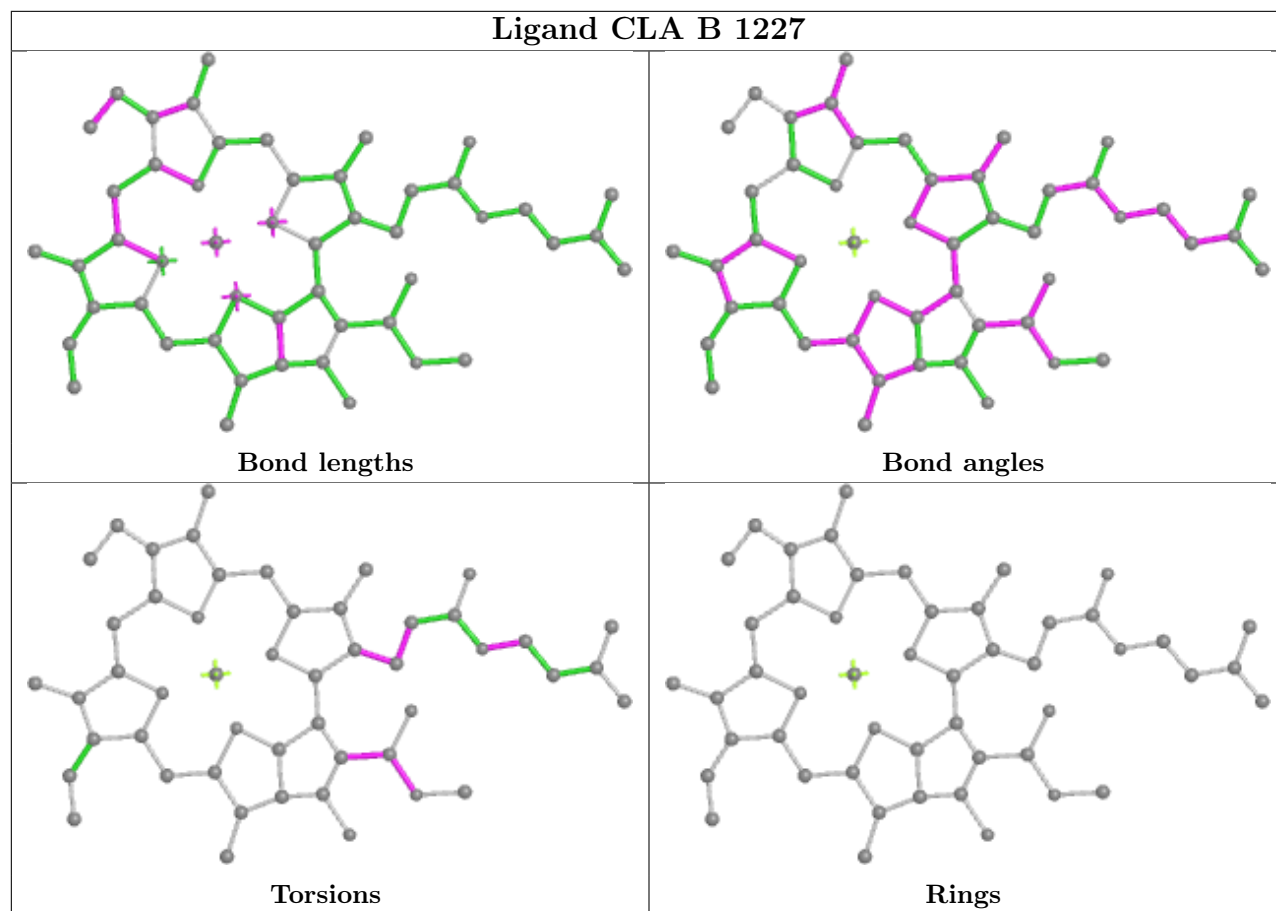
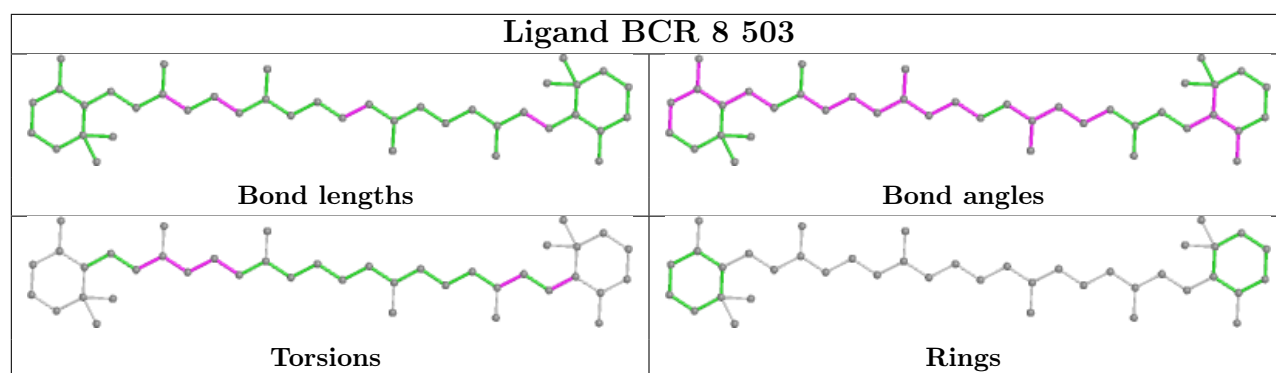


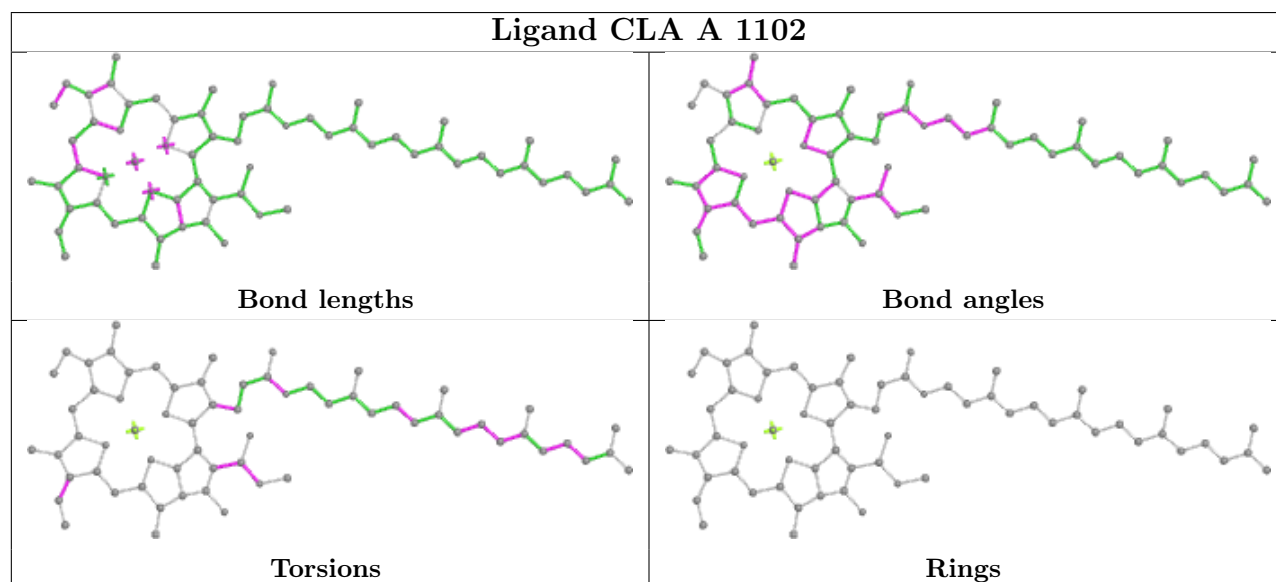
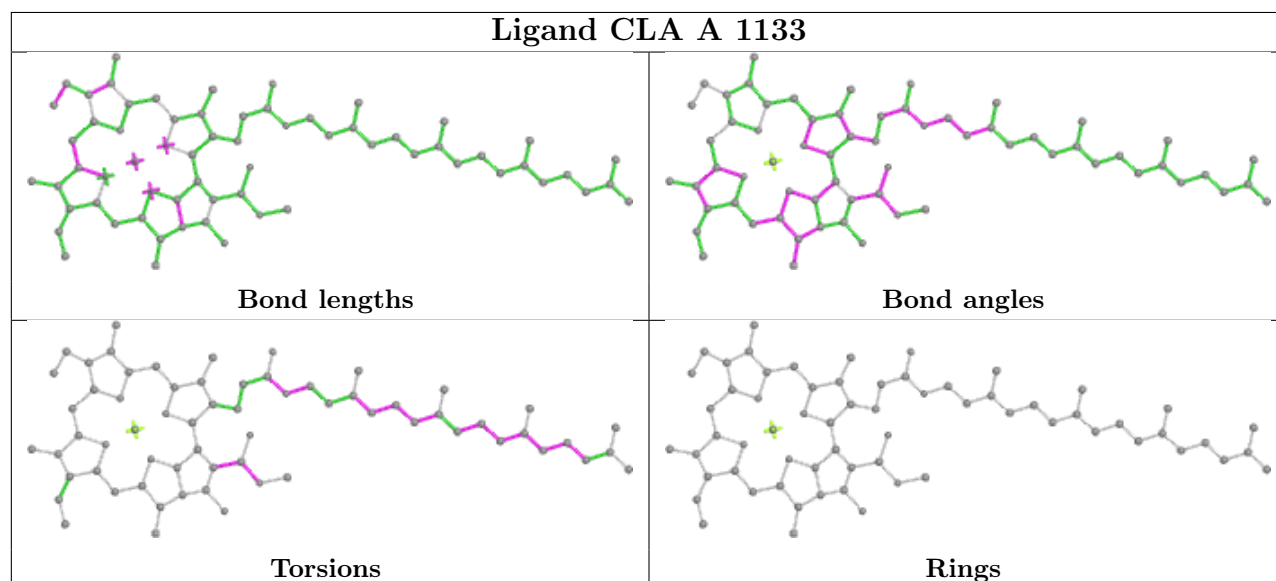
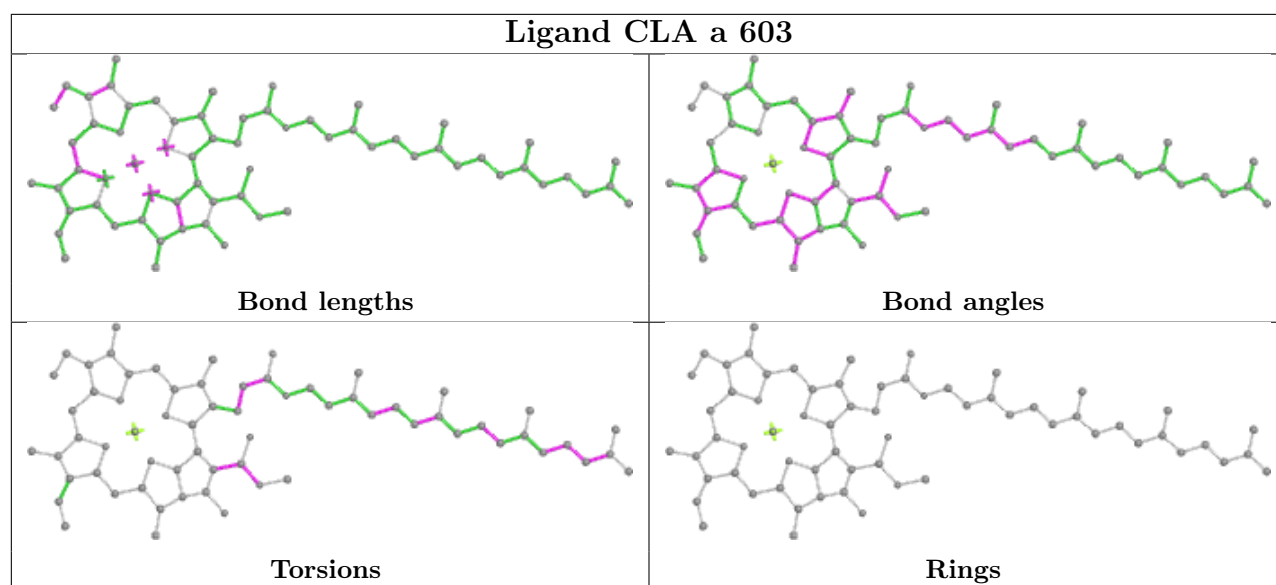
Ligand LUT a 503

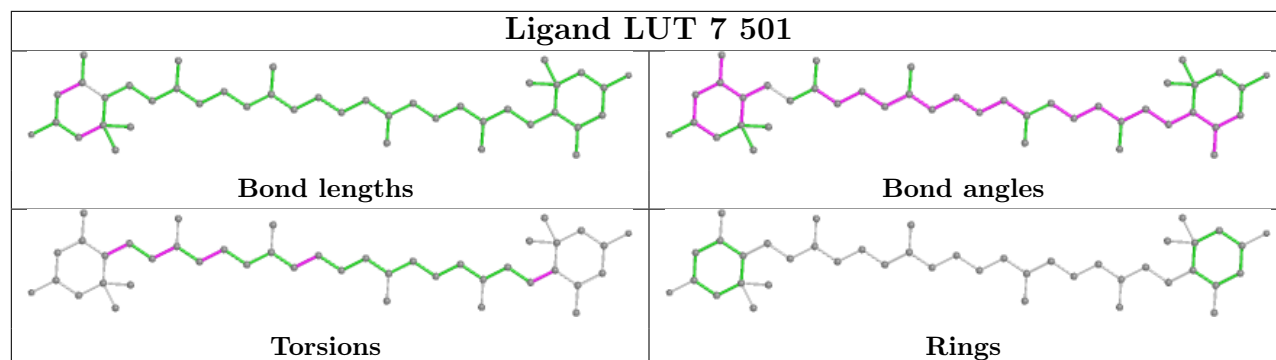
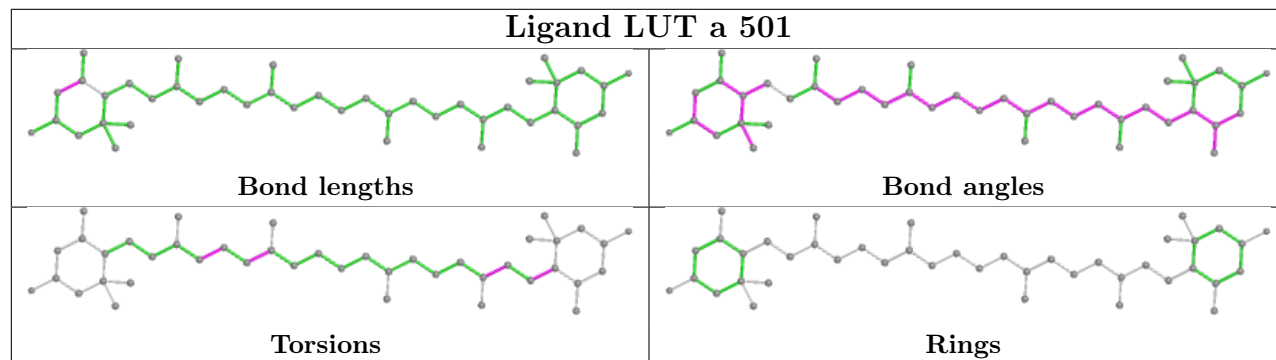
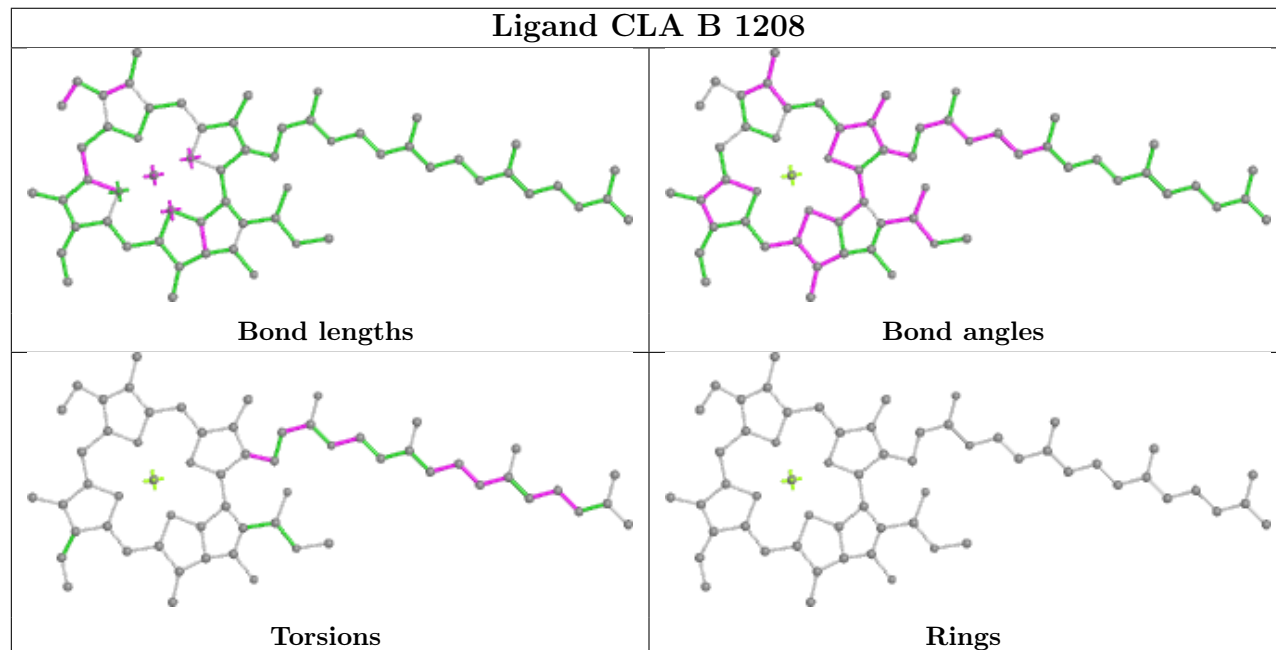
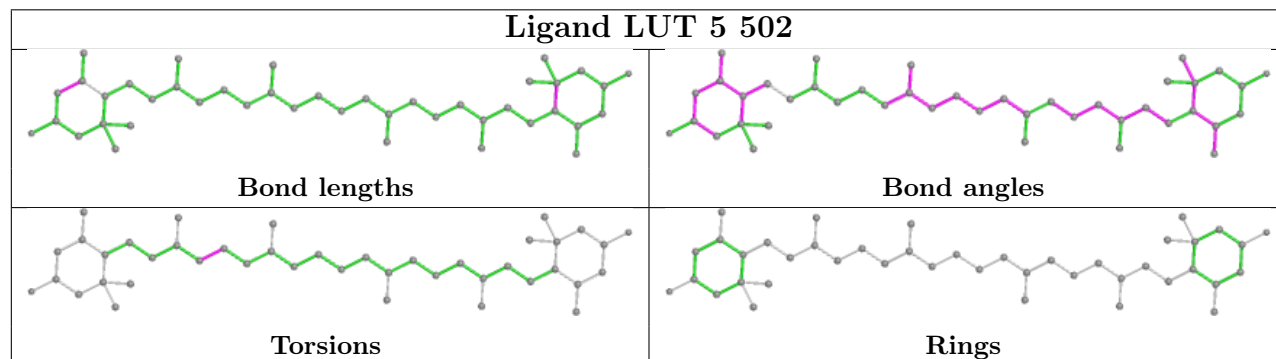


Ligand BCR 7 503

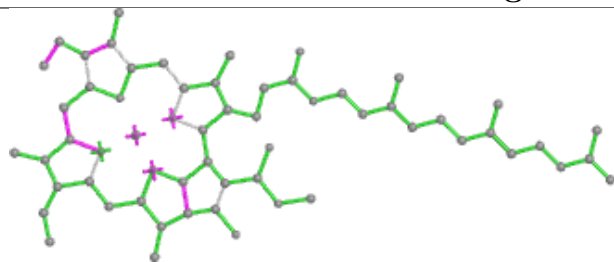




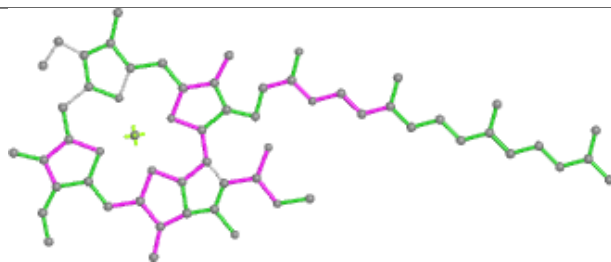


Ligand LUT 7 501**Ligand LUT a 501****Ligand CLA B 1208****Ligand LUT 5 502**

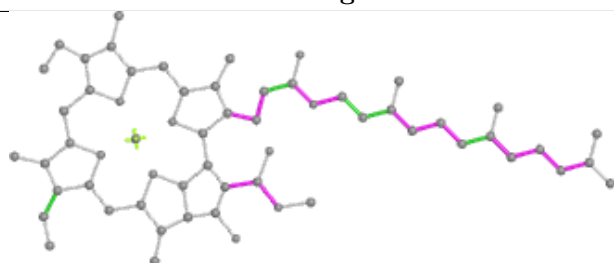
Ligand CLA A 1134



Bond lengths



Bond angles

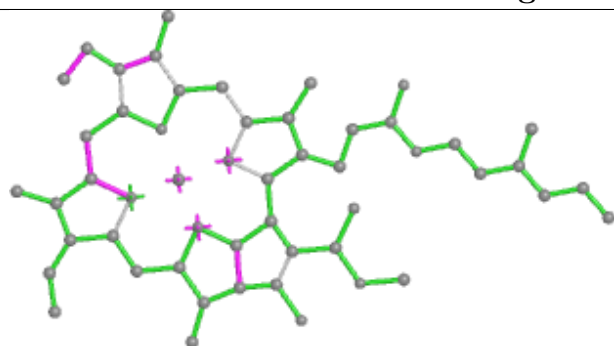


Torsions

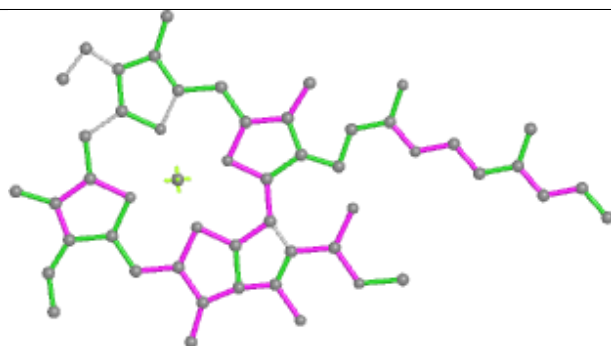


Rings

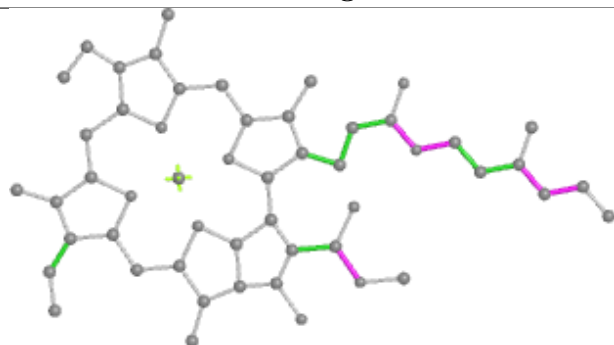
Ligand CLA 8 602



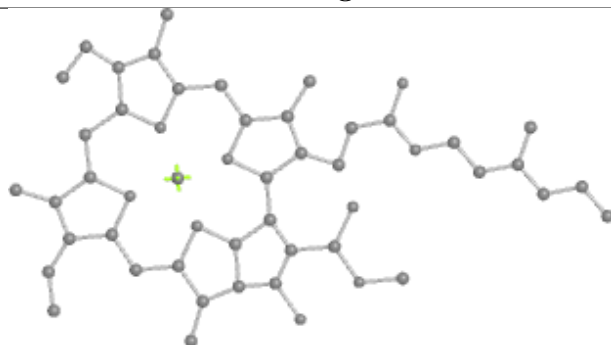
Bond lengths



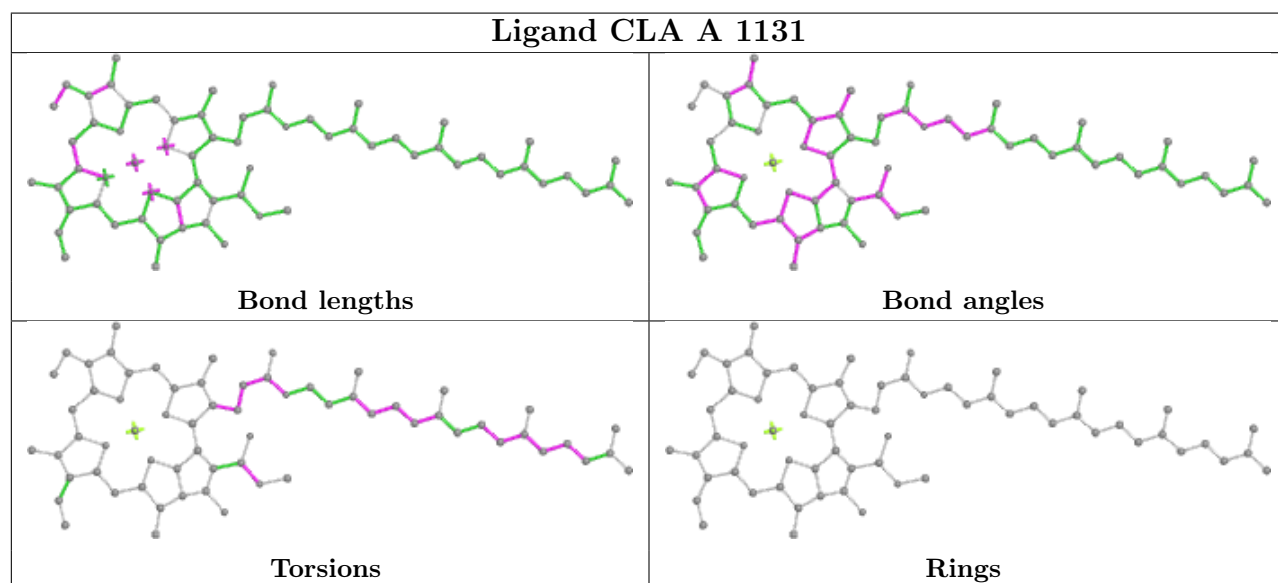
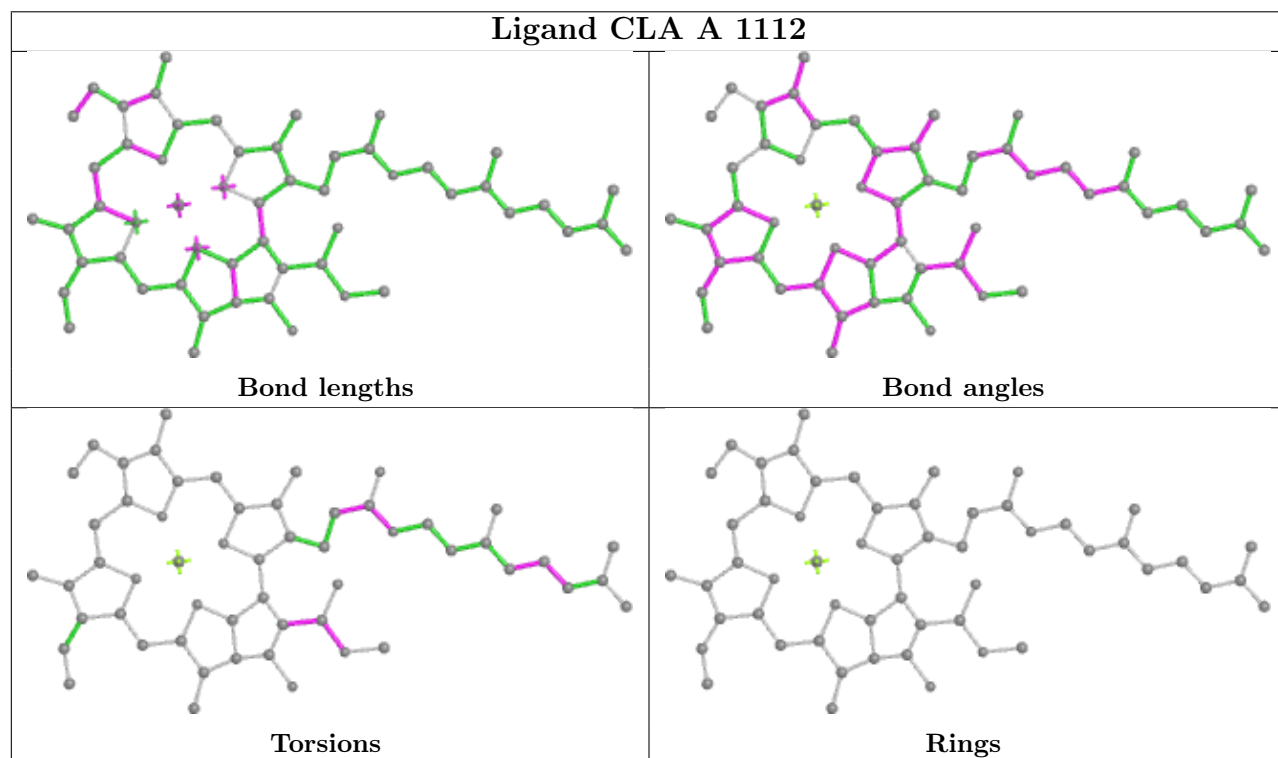
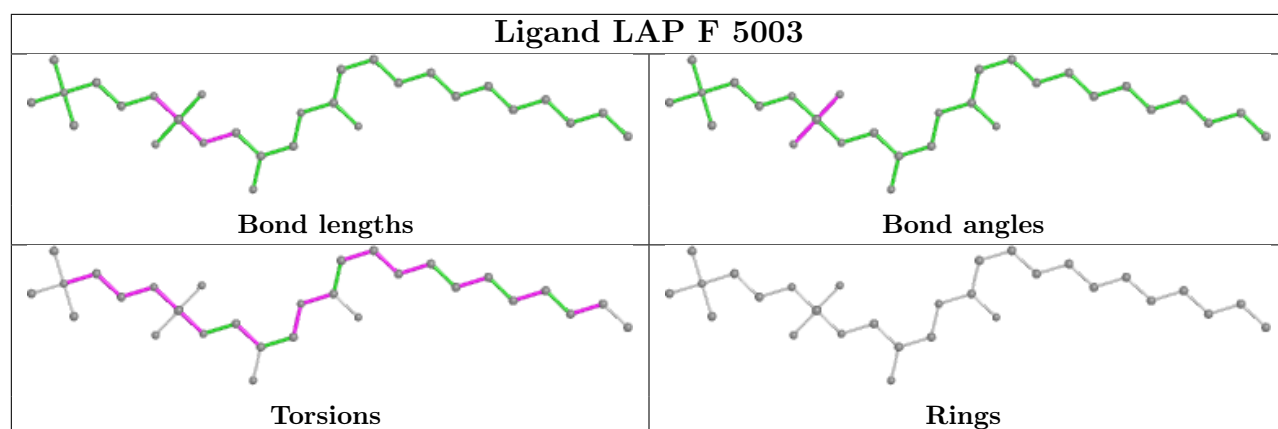
Bond angles



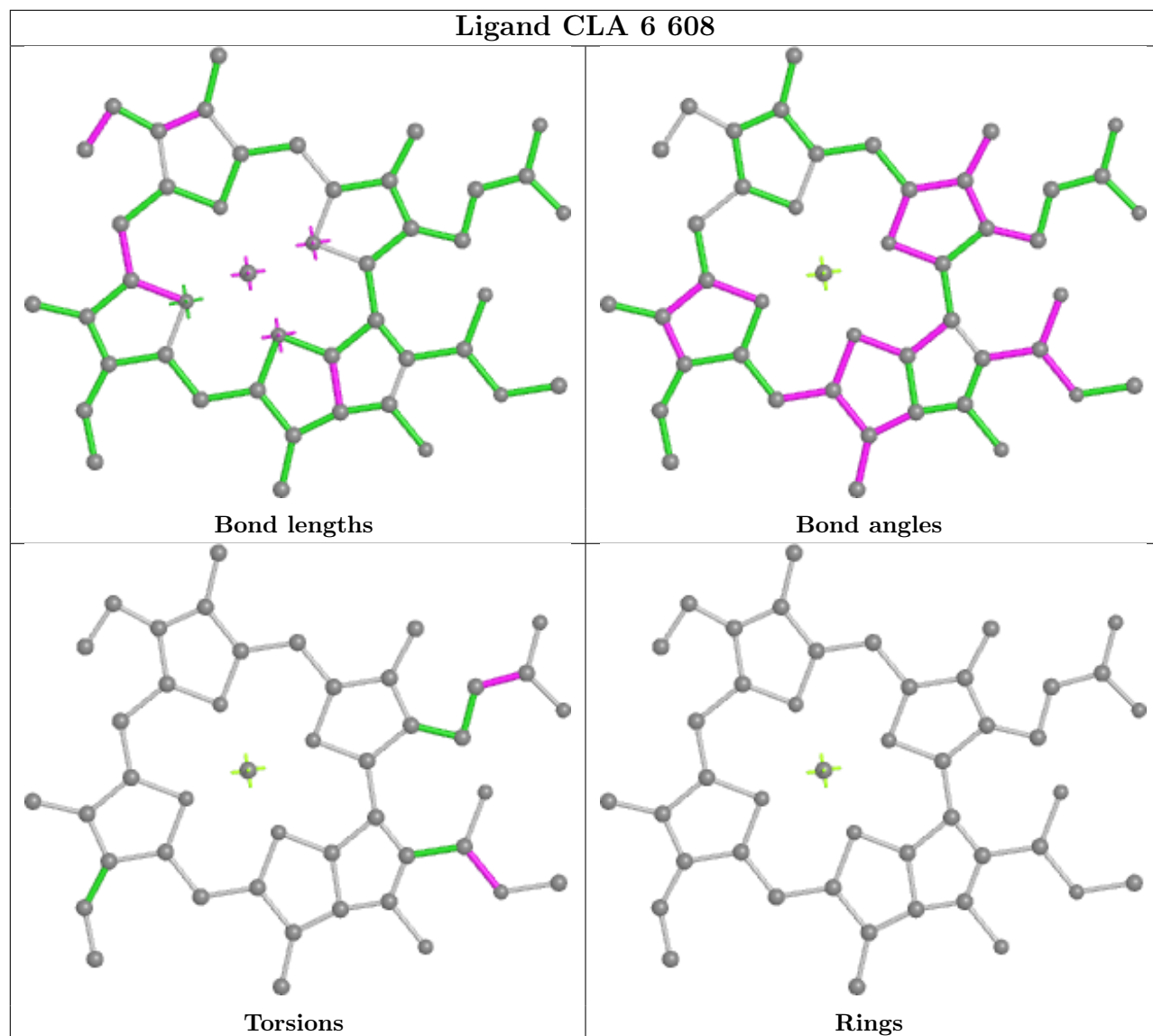
Torsions



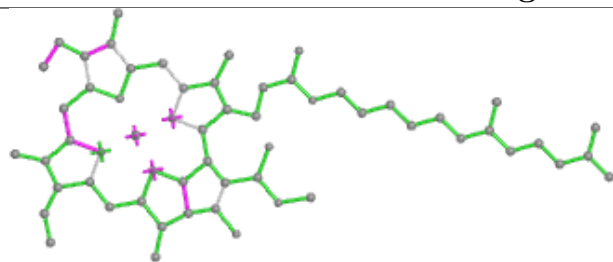
Rings



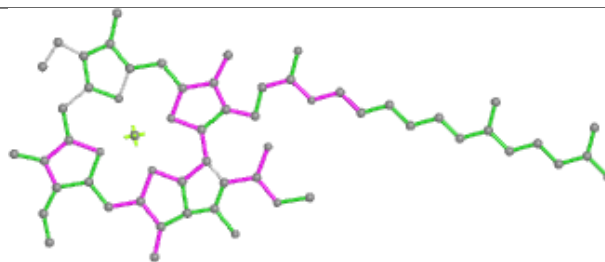
Ligand CLA 6 608



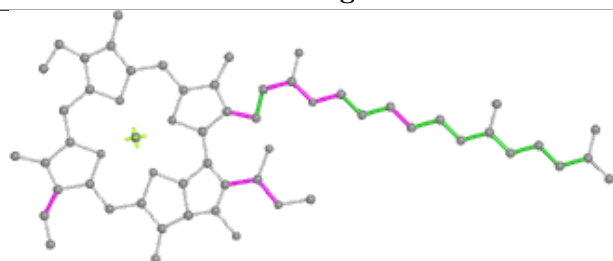
Ligand CLA 7 607



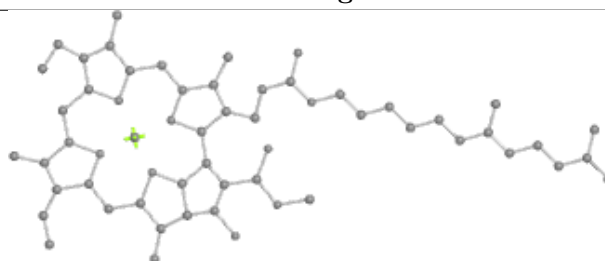
Bond lengths



Bond angles

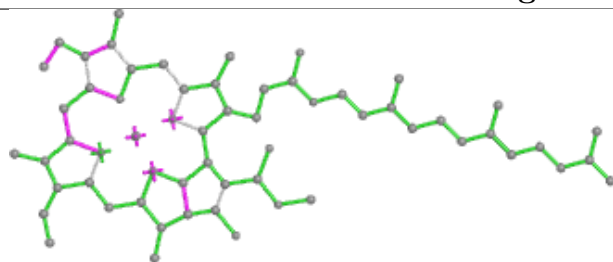


Torsions

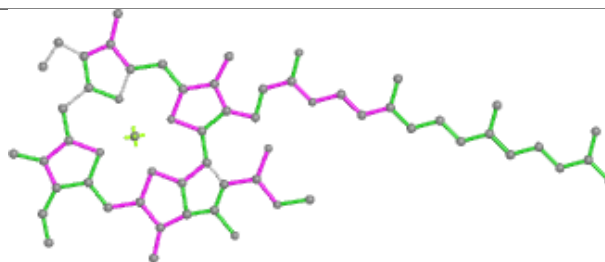


Rings

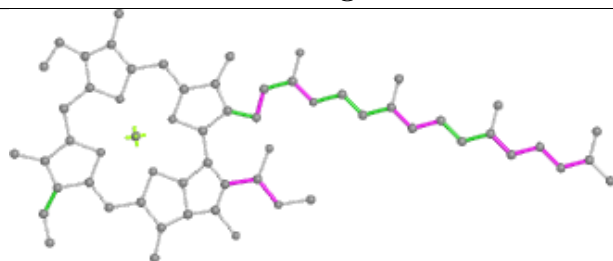
Ligand CLA 7 601



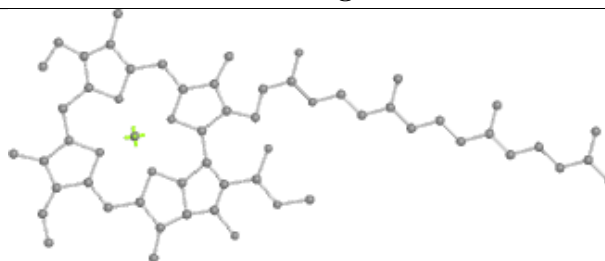
Bond lengths



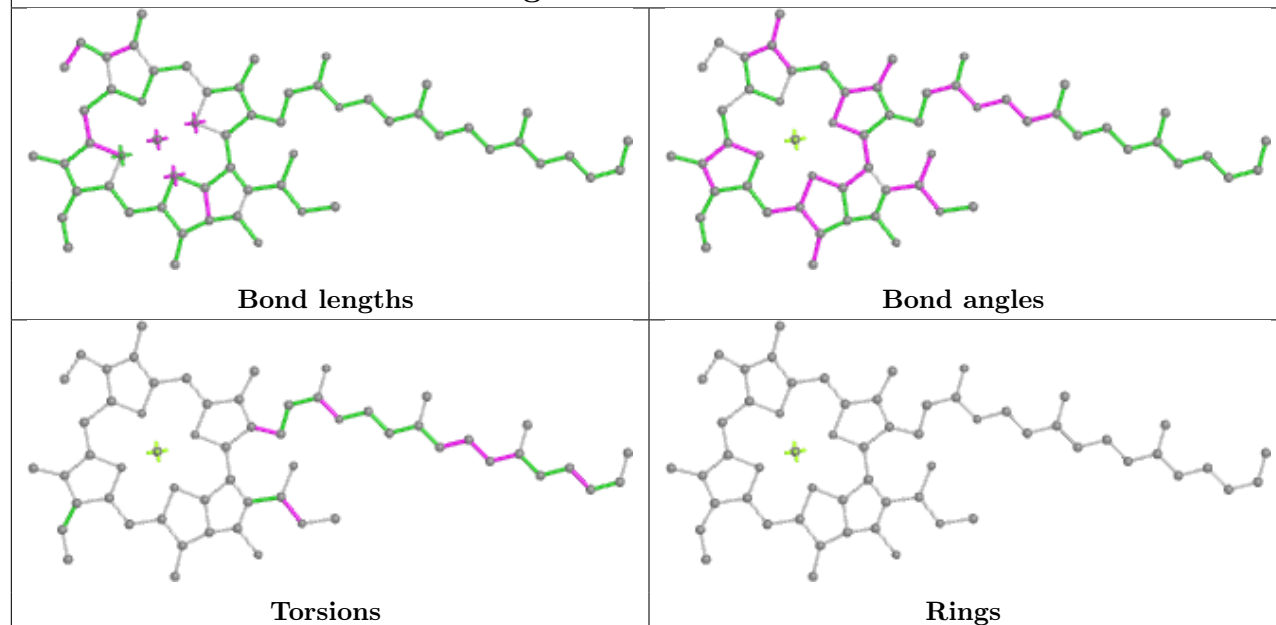
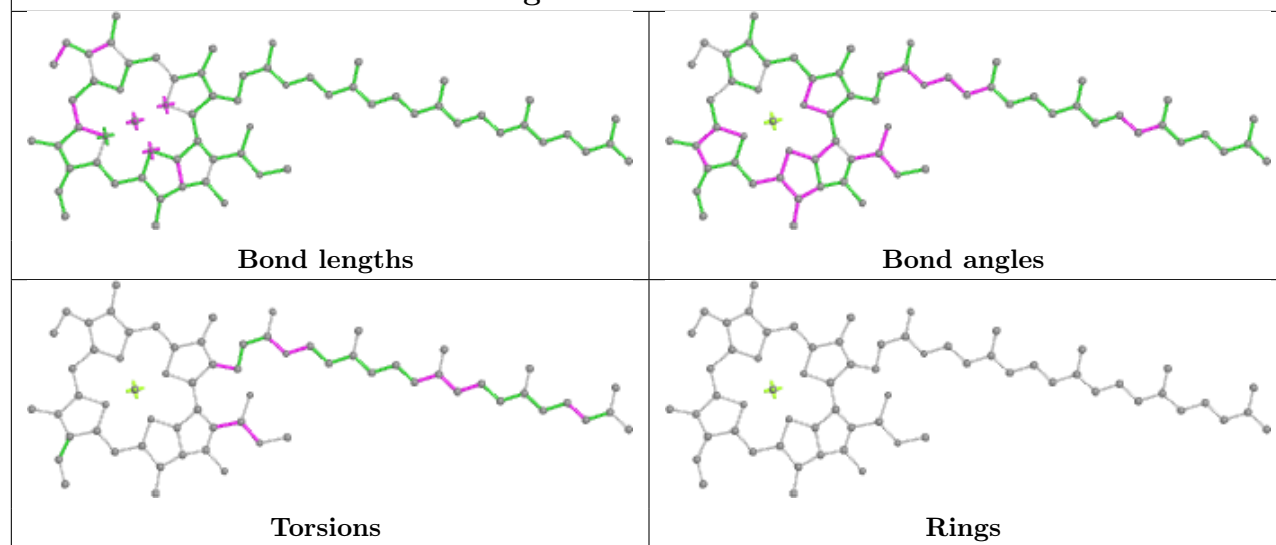
Bond angles

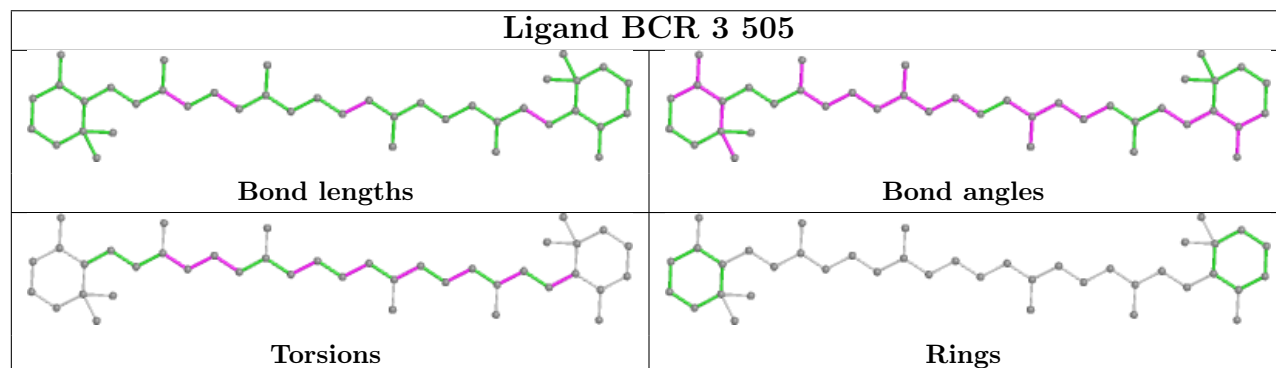
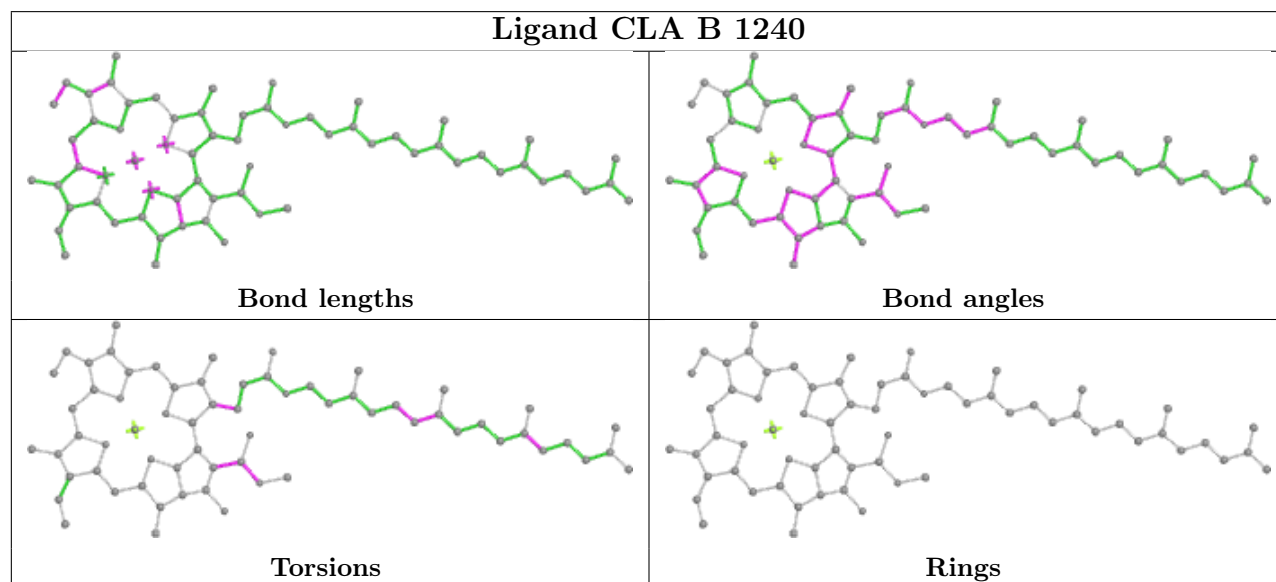
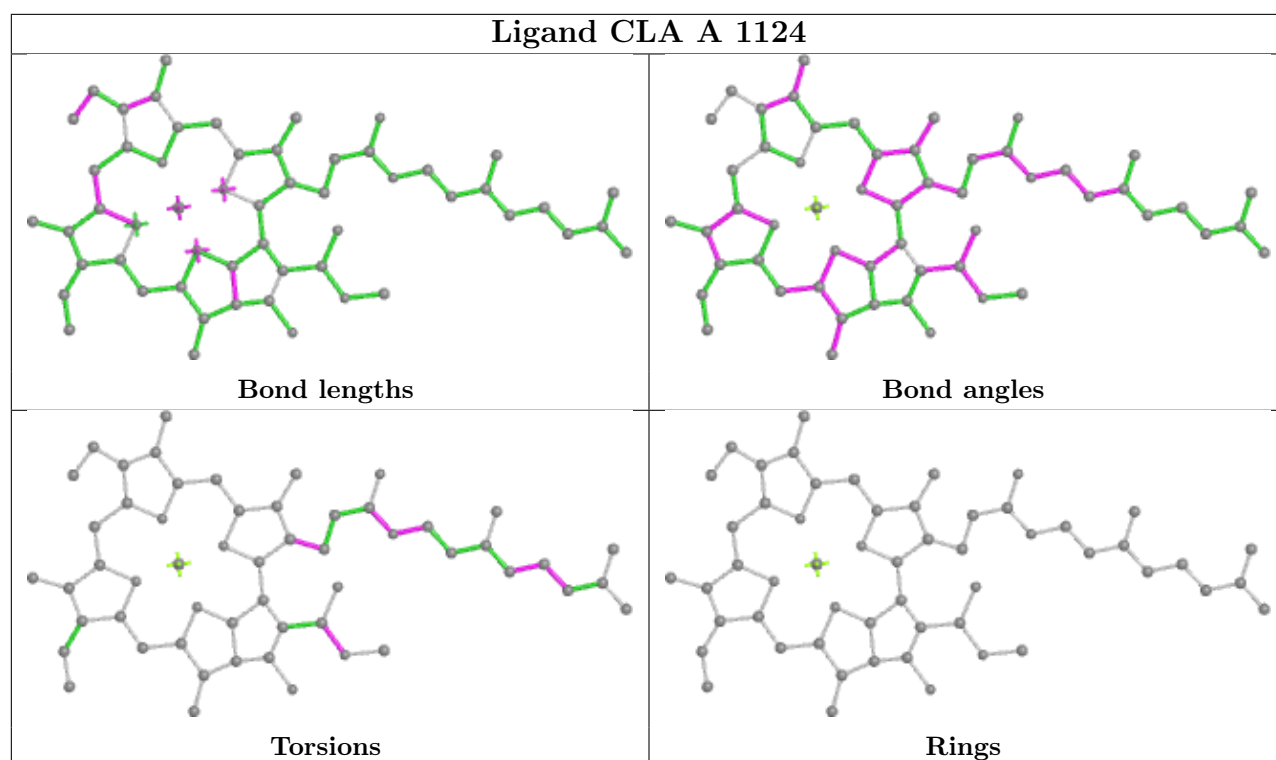


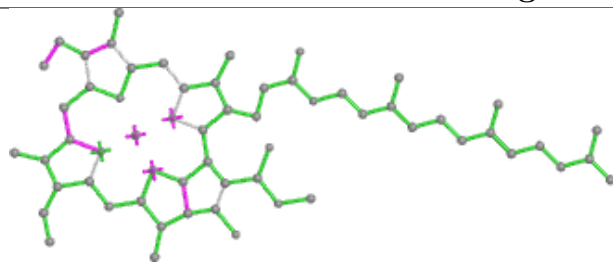
Torsions



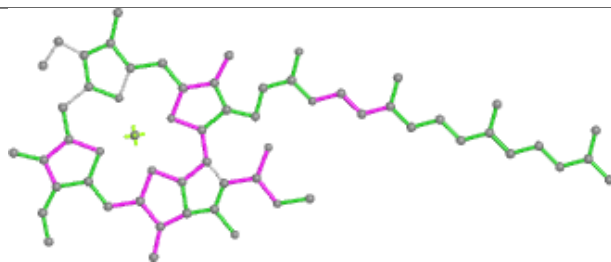
Rings

Ligand CLA B 1219**Ligand CLA B 1202**

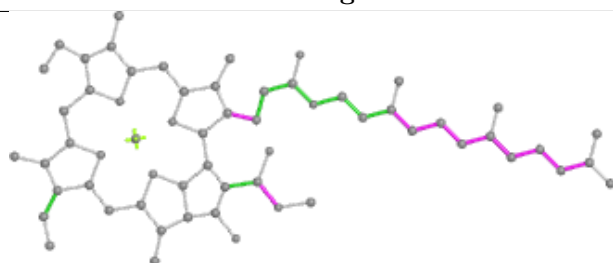


Ligand CLA 6 601

Bond lengths



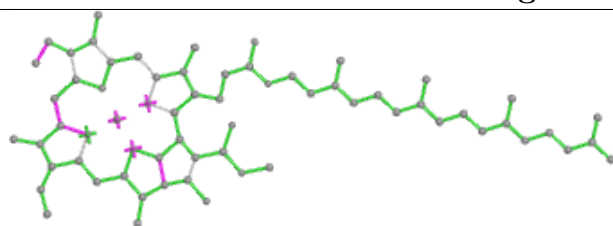
Bond angles



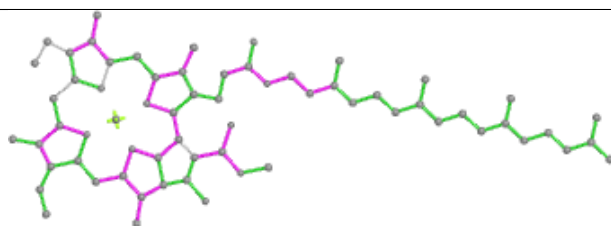
Torsions



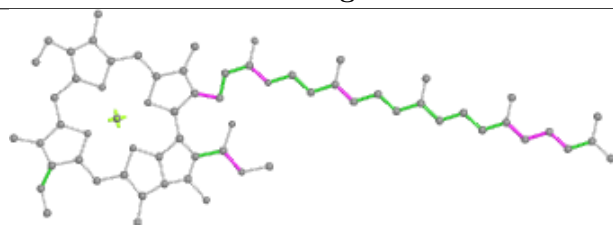
Rings

Ligand CLA 3 607

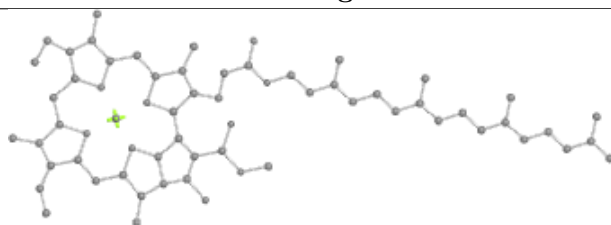
Bond lengths



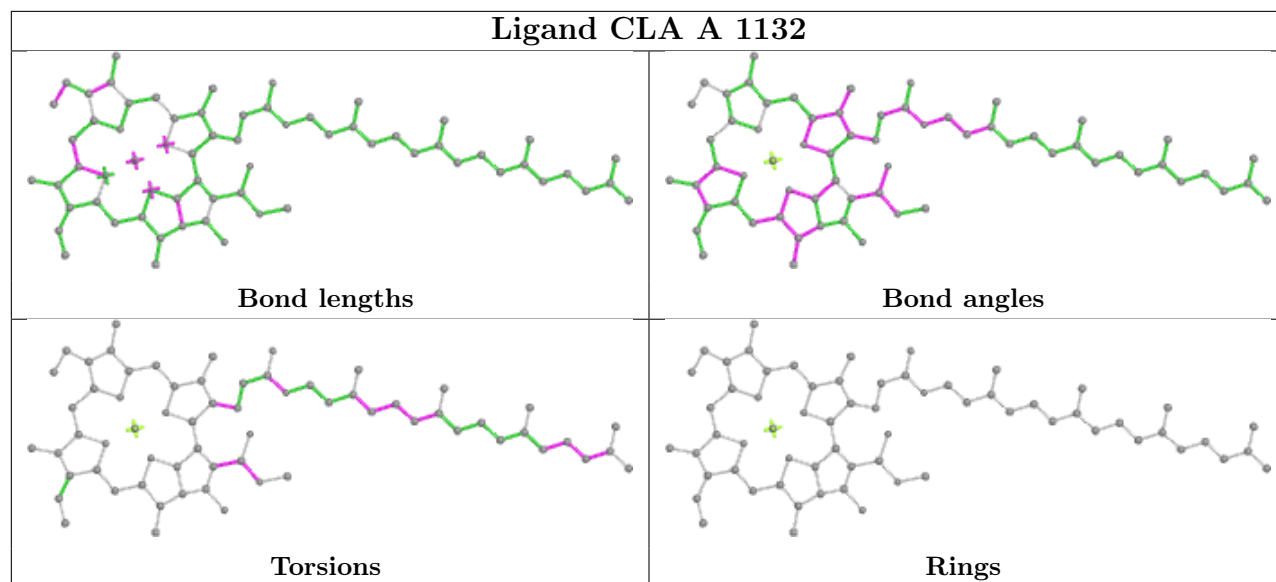
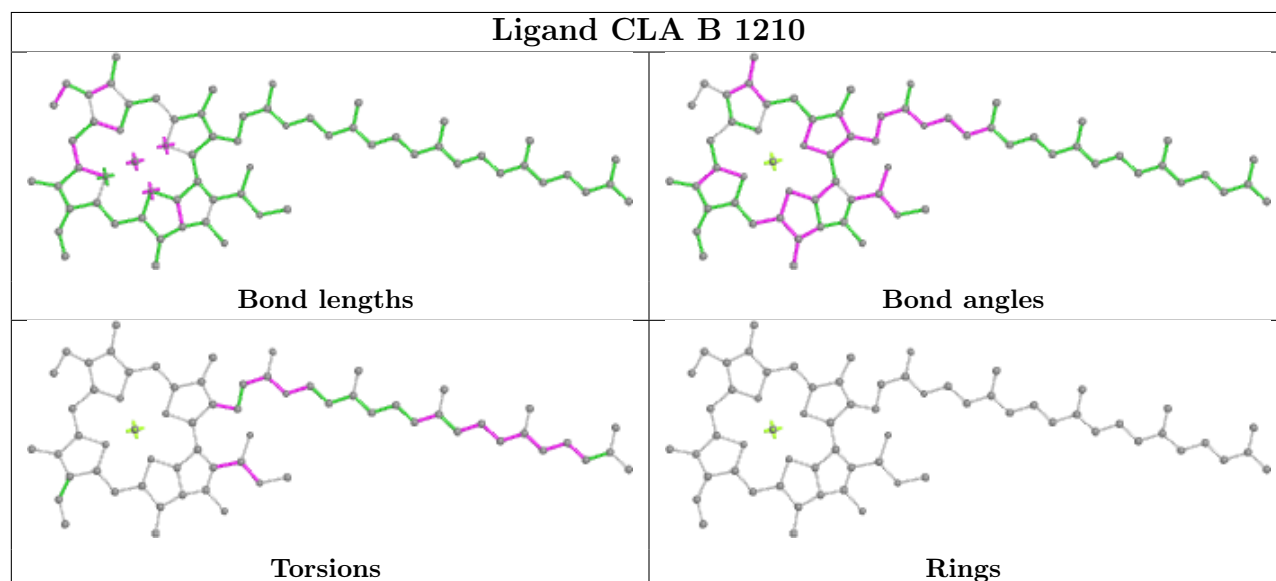
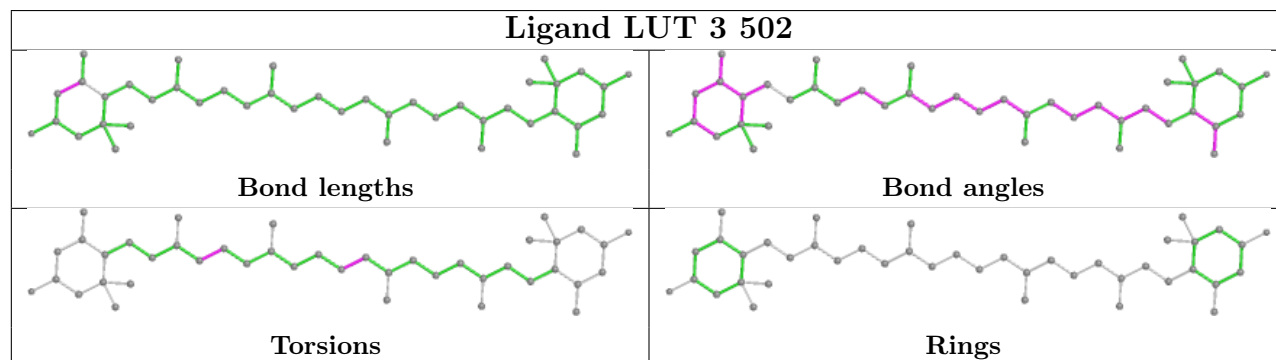
Bond angles

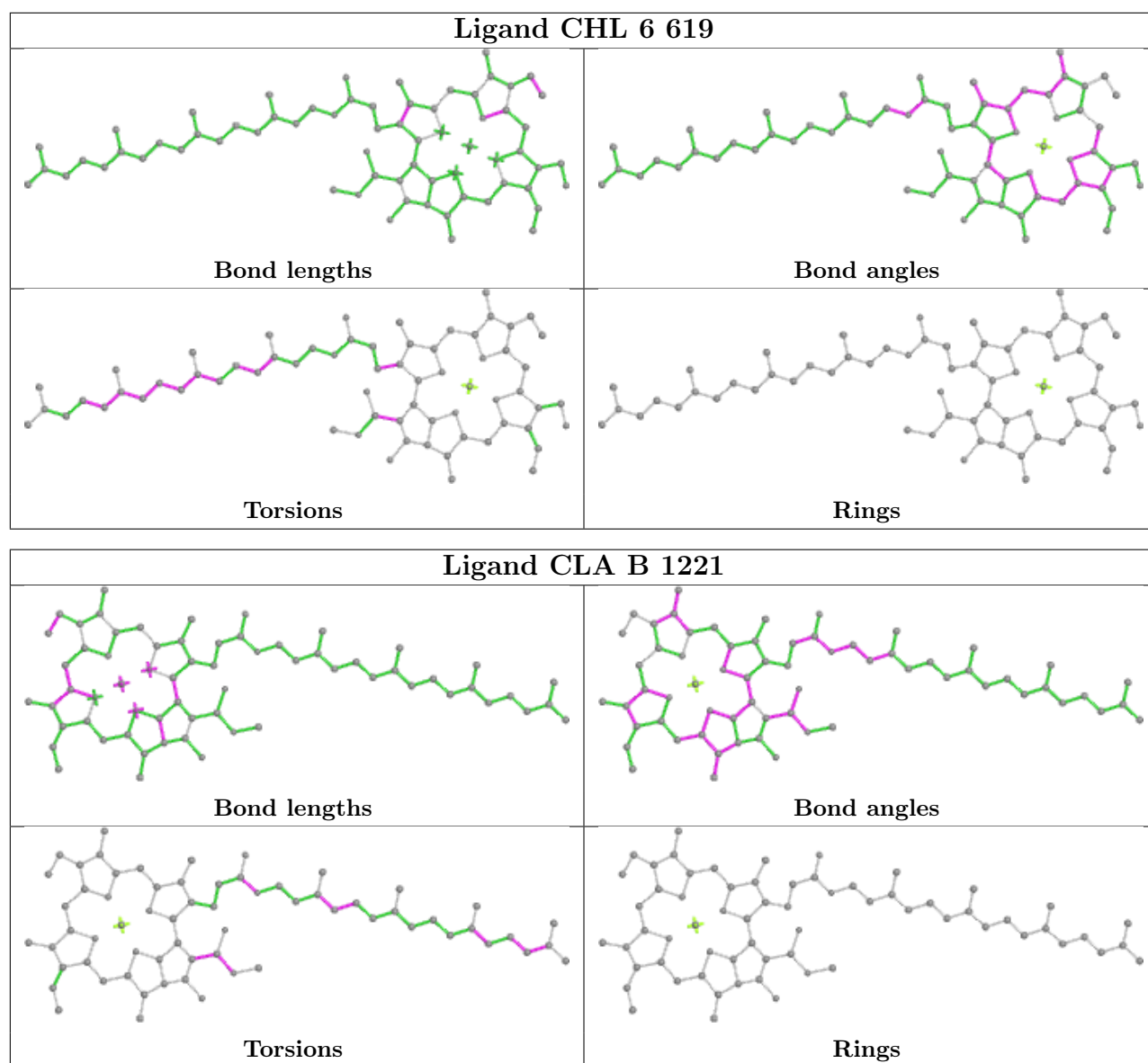


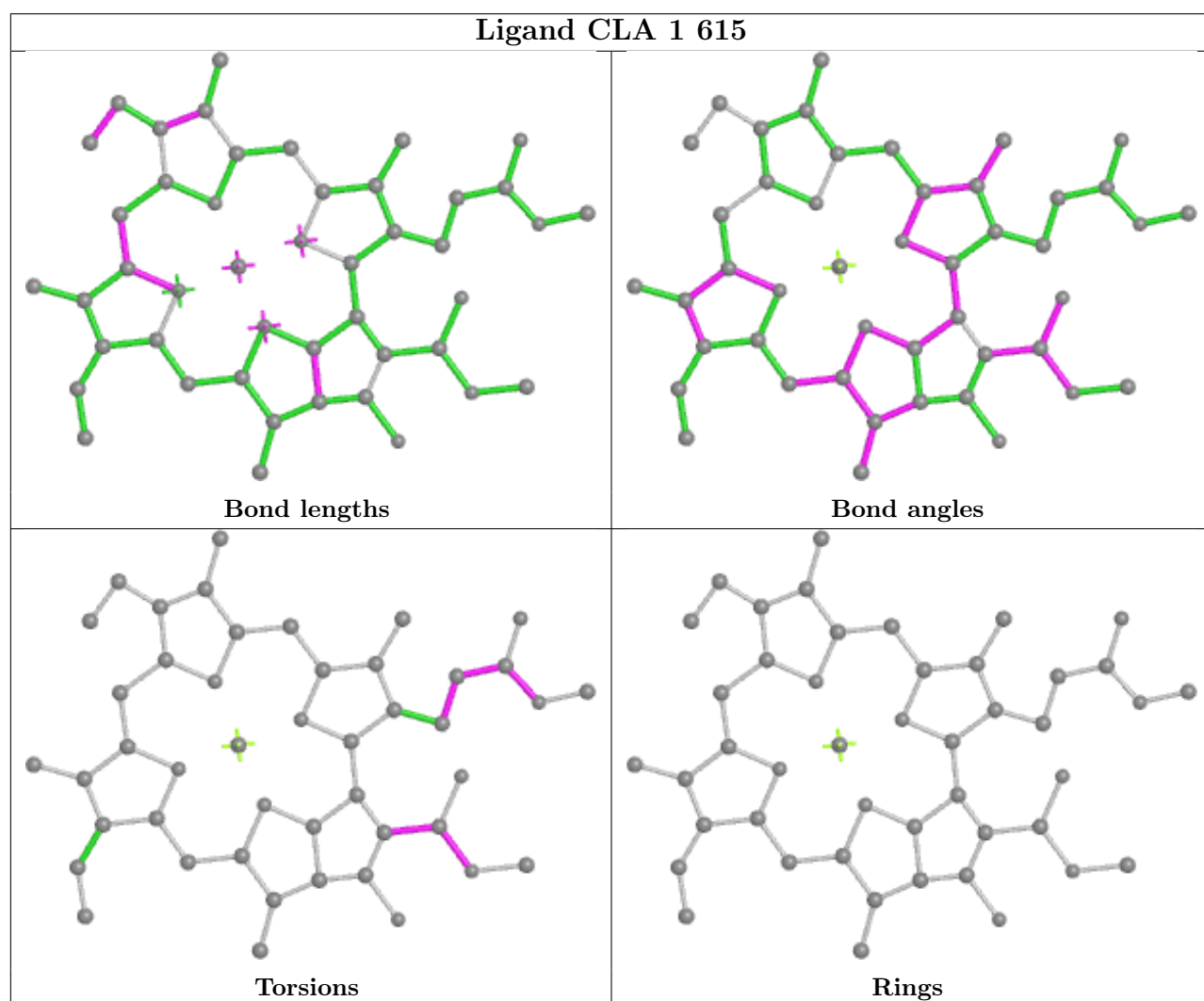
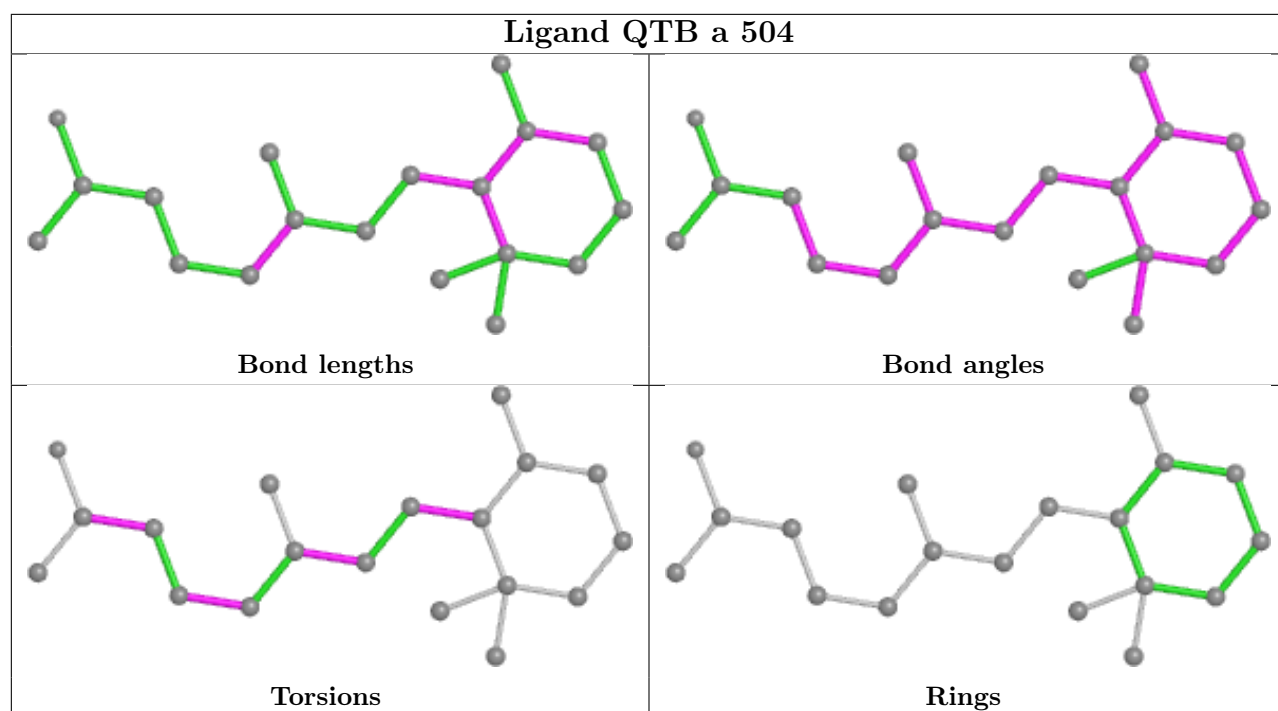
Torsions

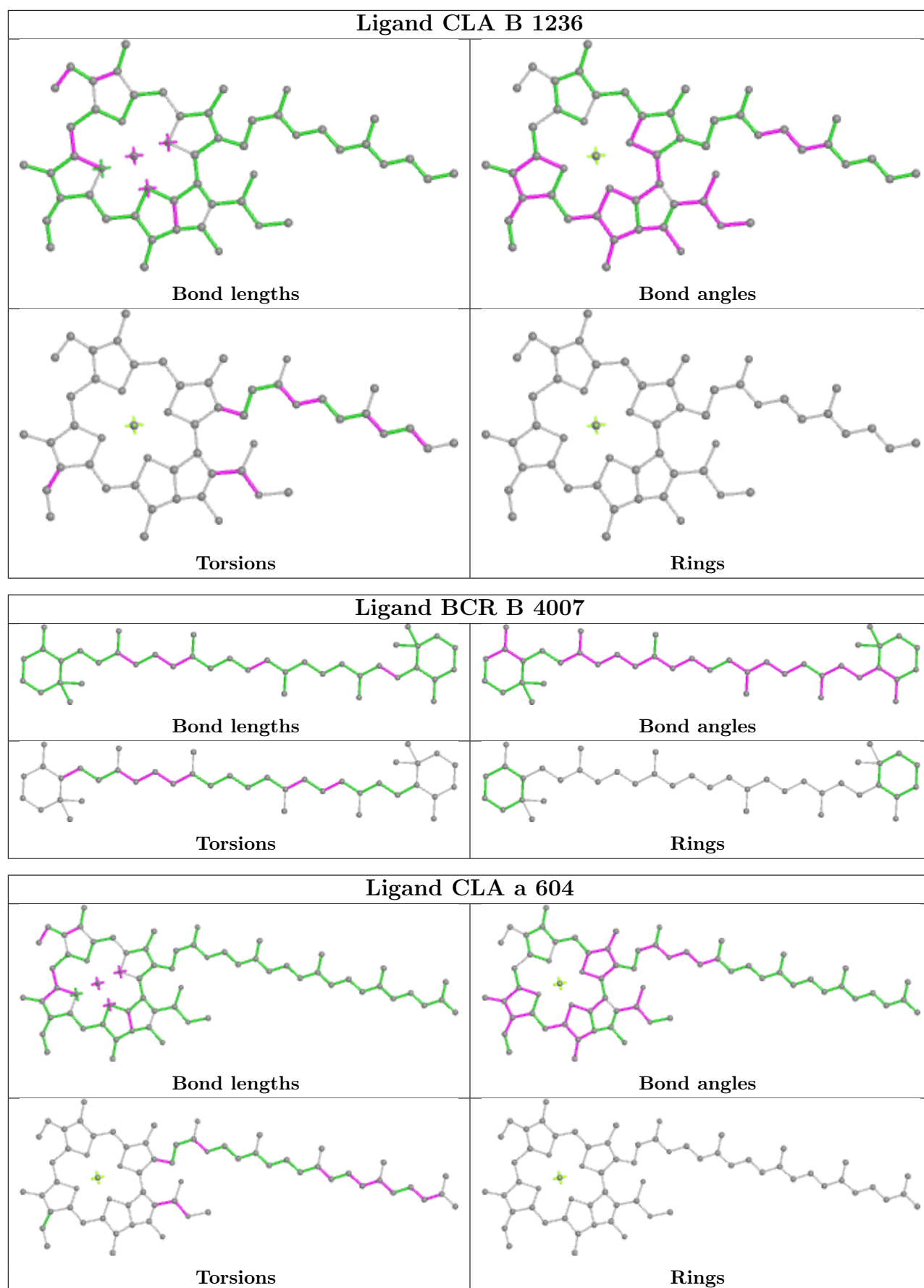


Rings

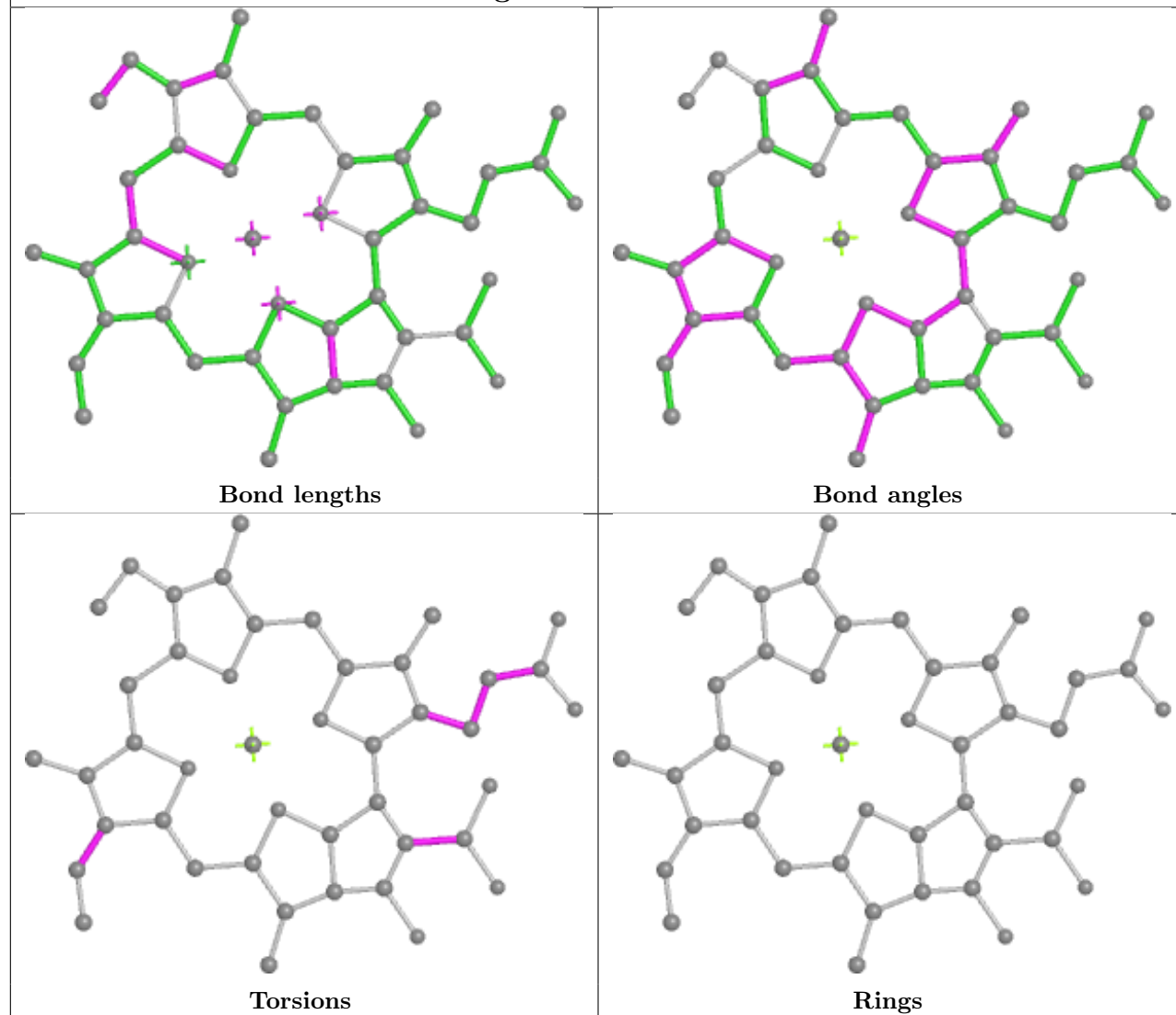
Ligand CLA A 1132**Ligand CLA B 1210****Ligand LUT 3 502**



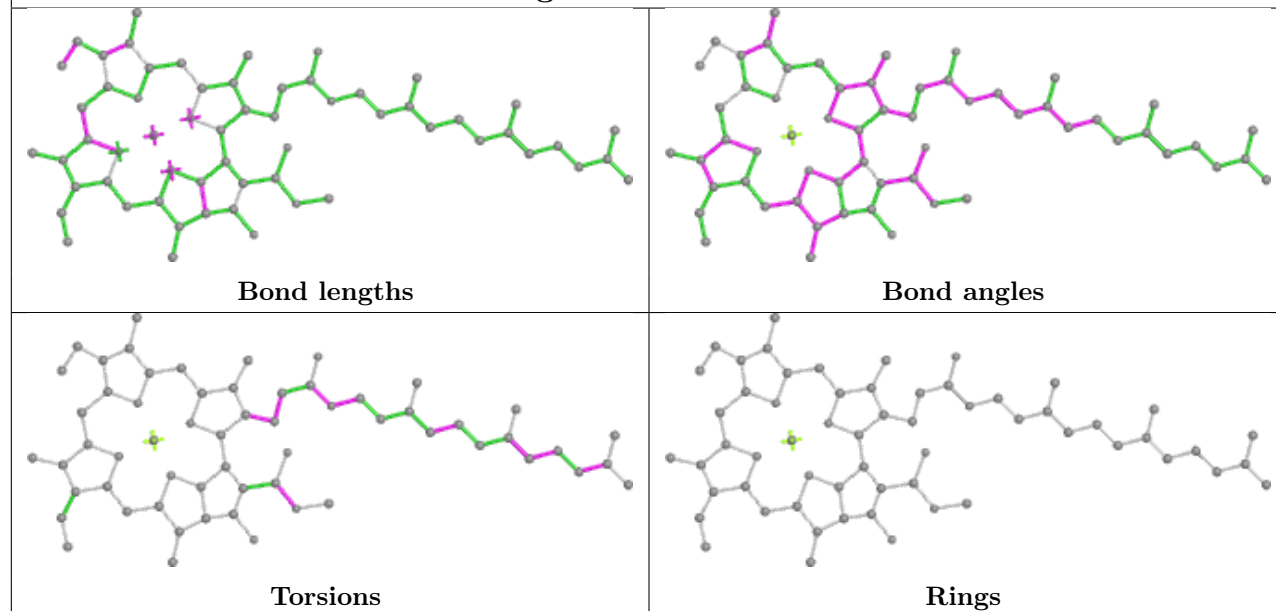


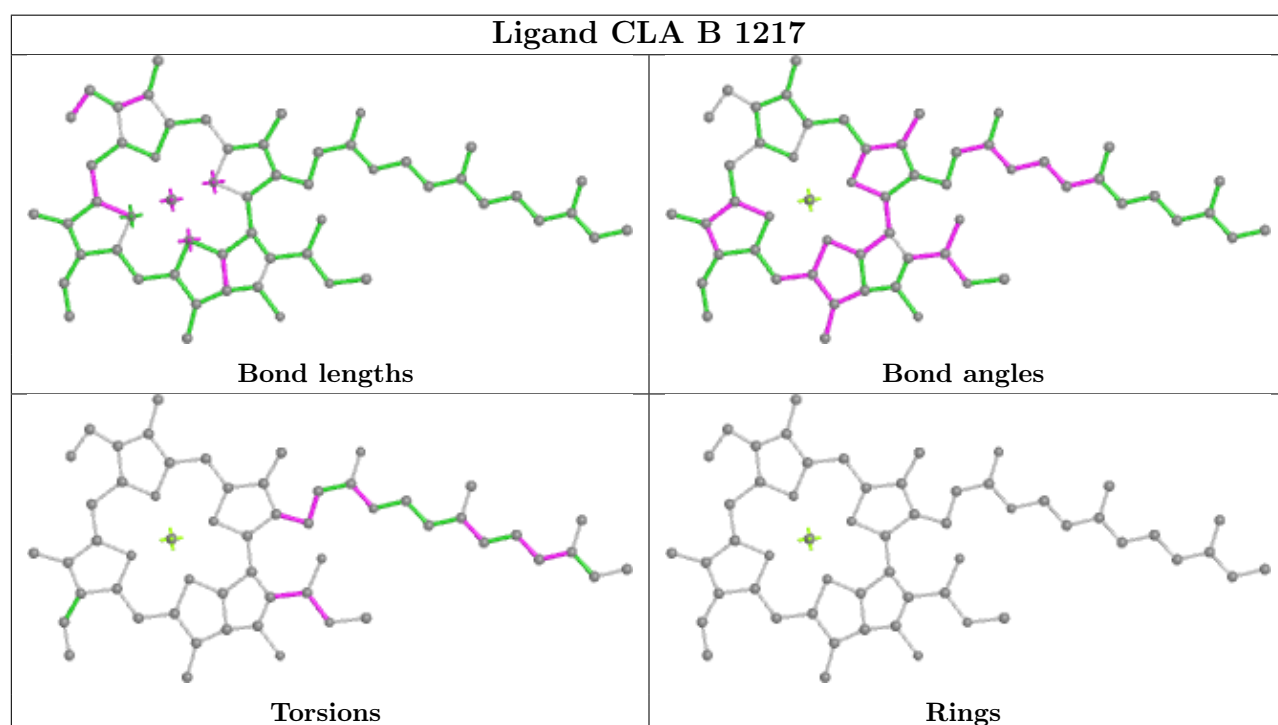
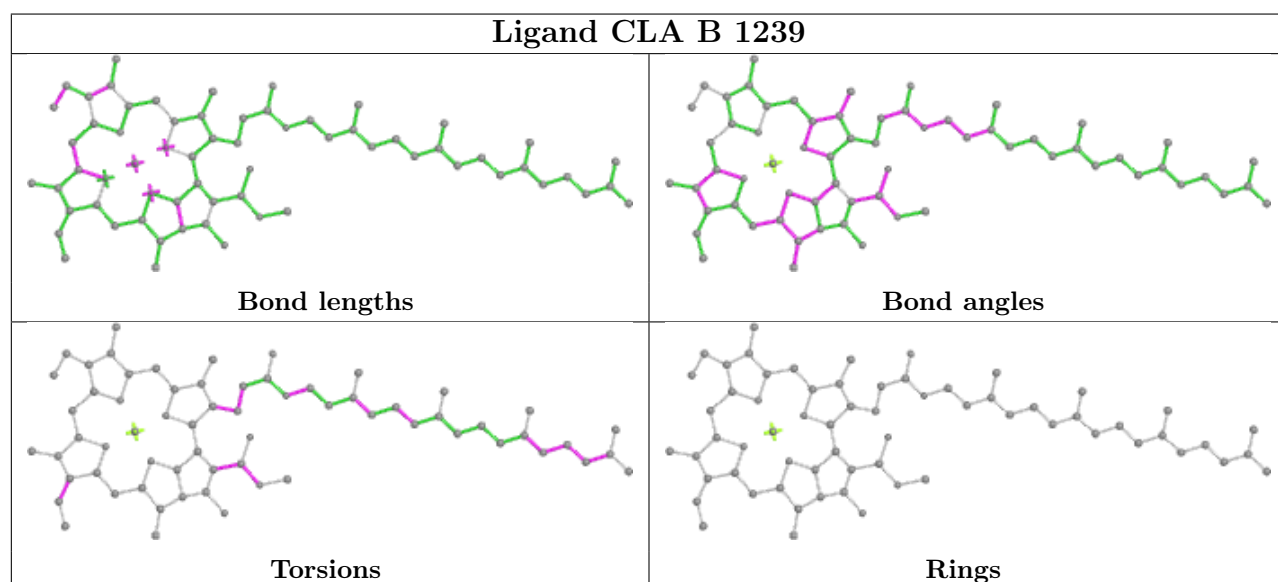
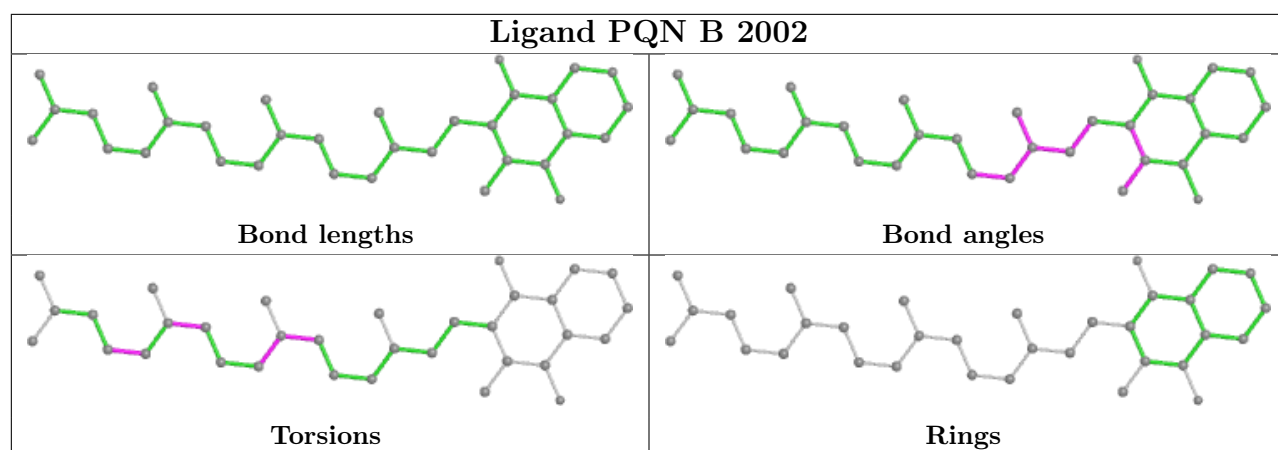


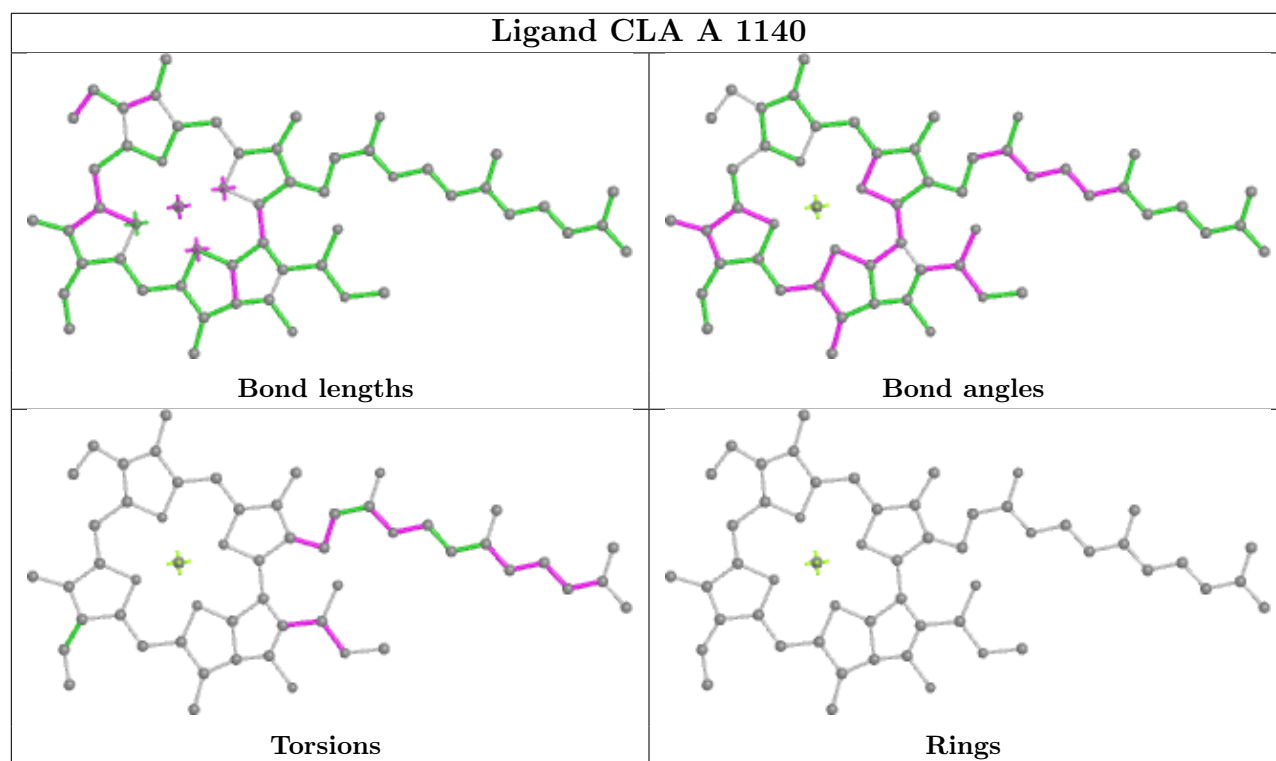
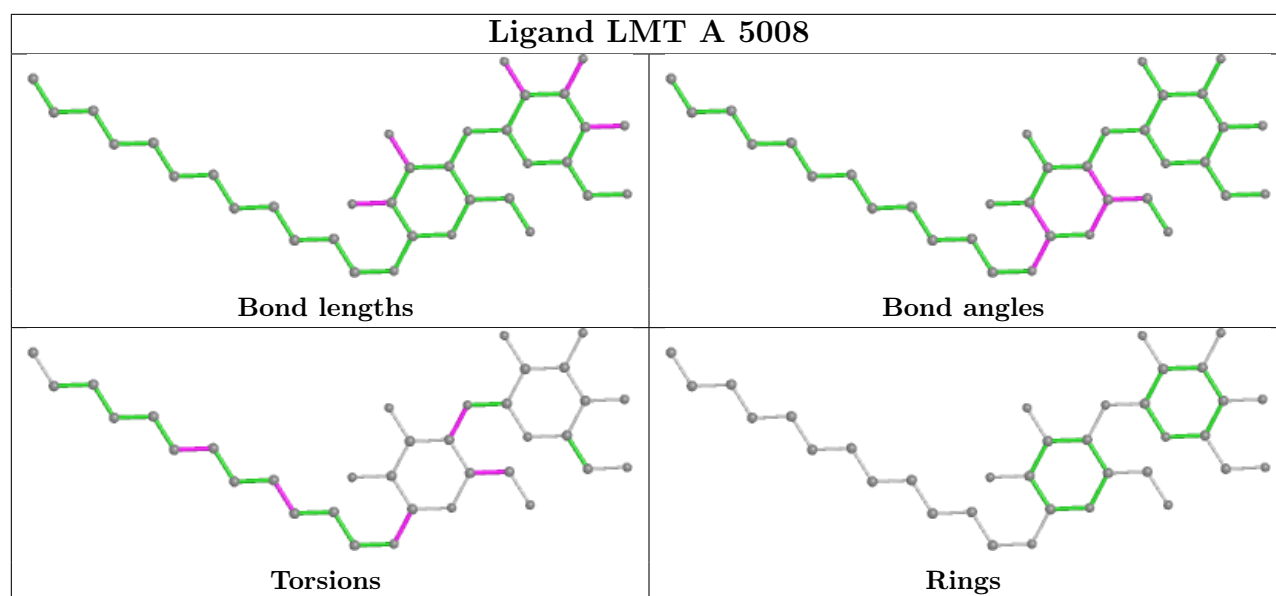
Ligand CLA 7 605



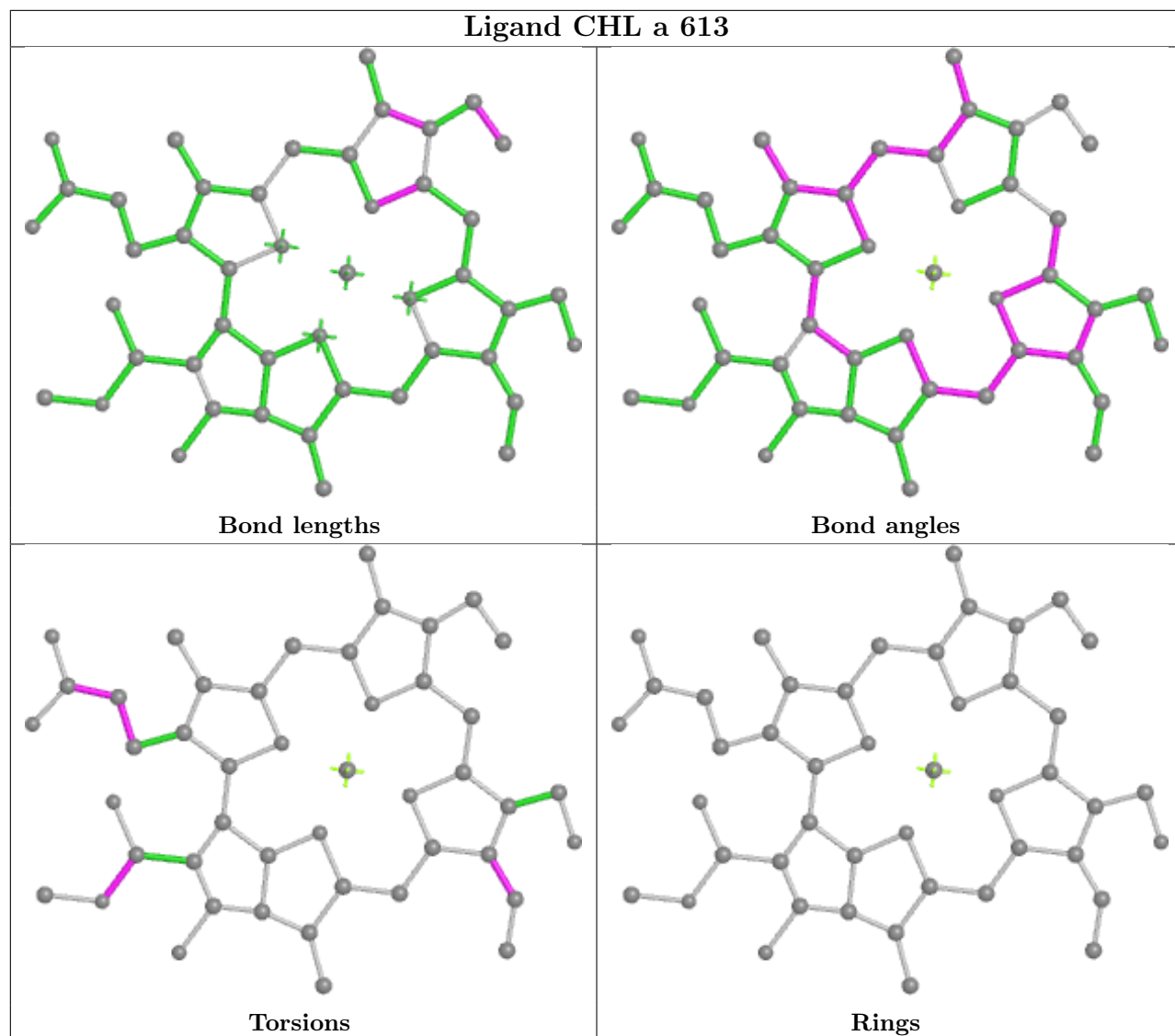
Ligand CLA 5 601

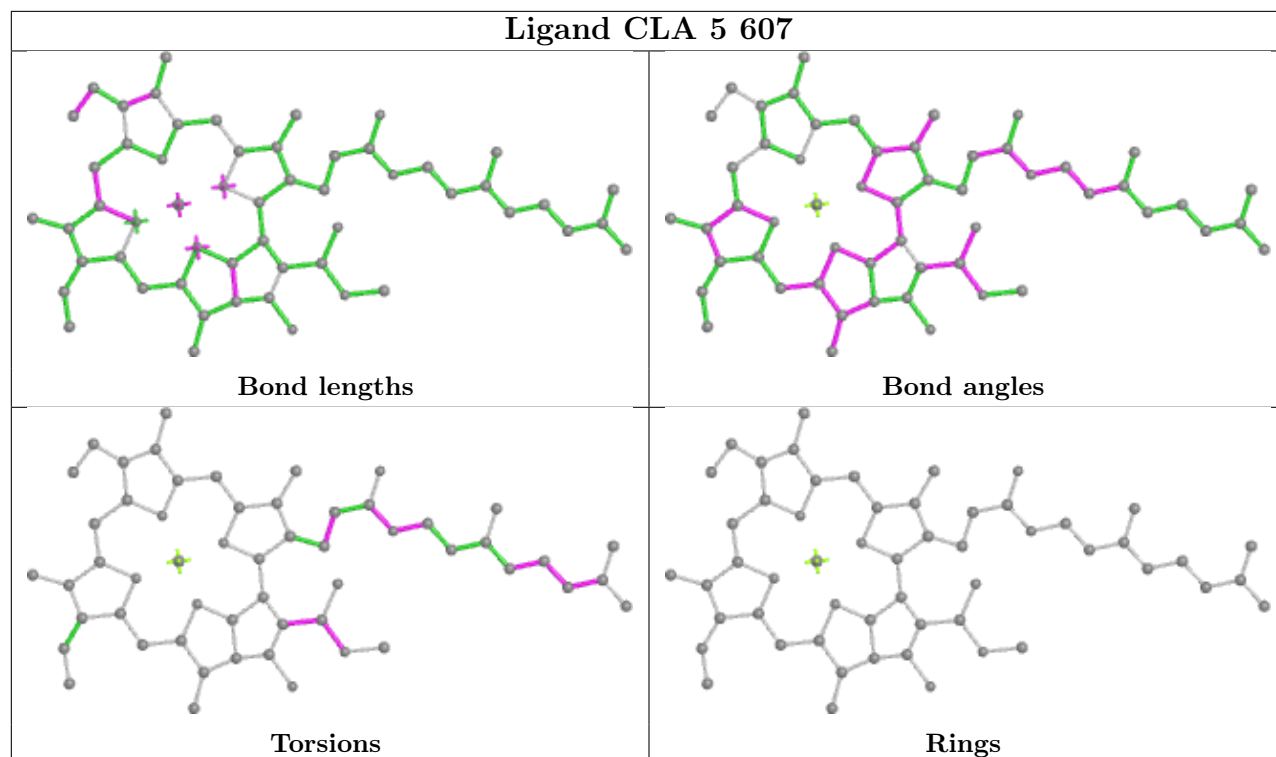
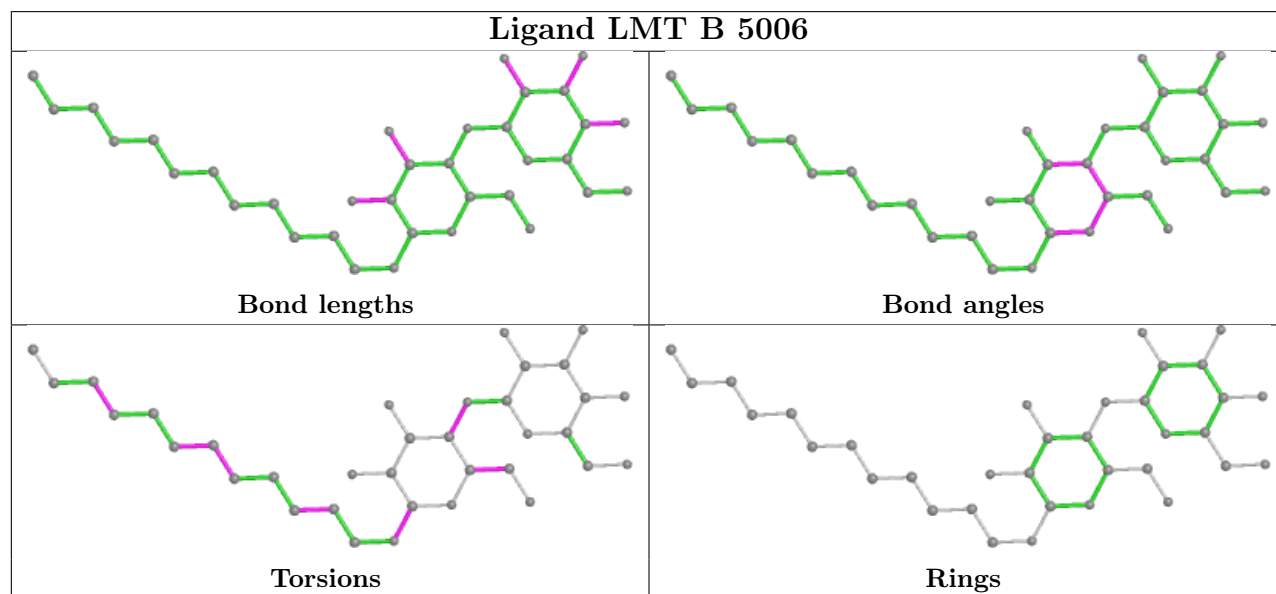


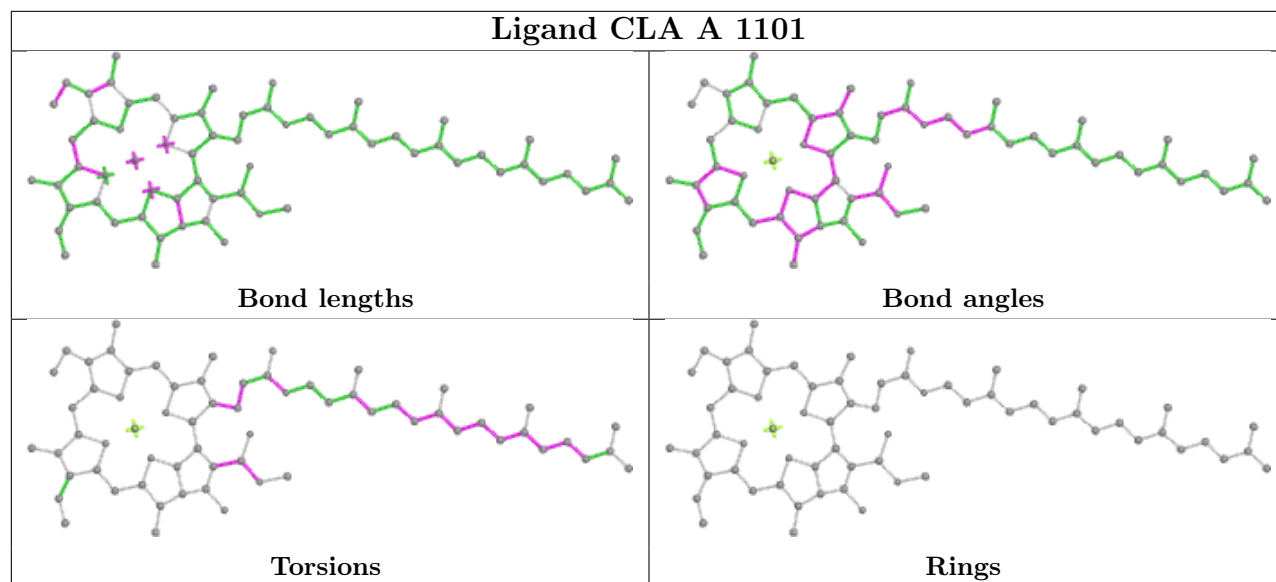
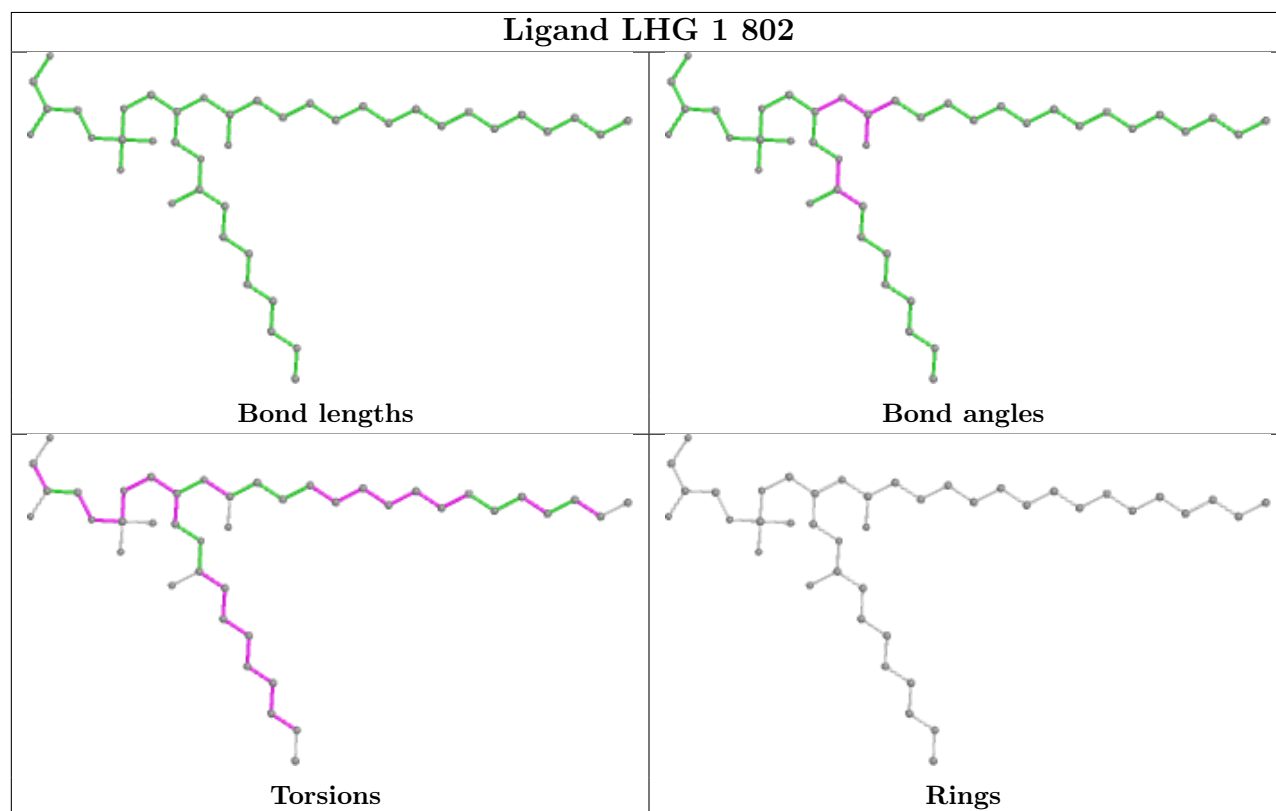


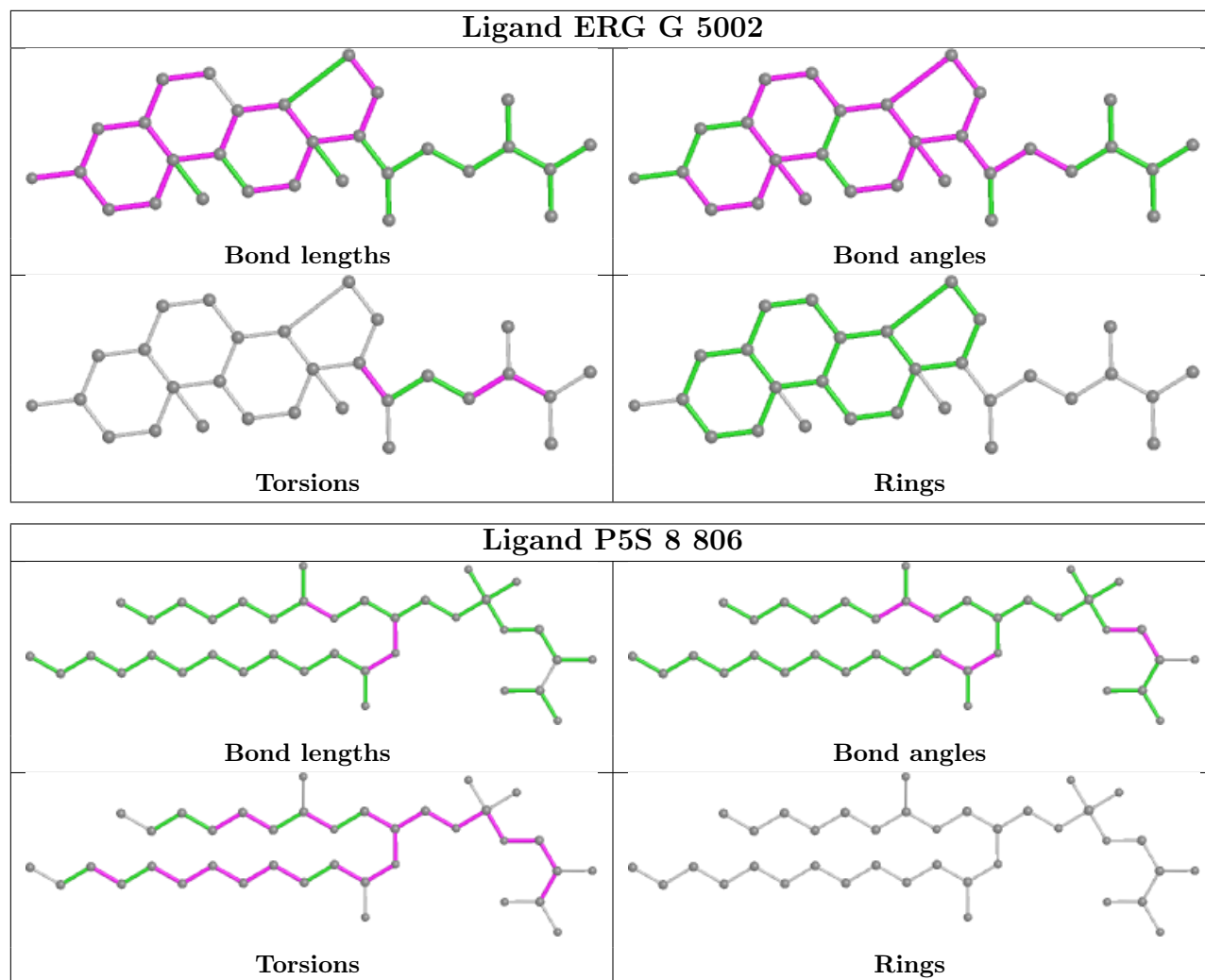


Ligand CHL a 613

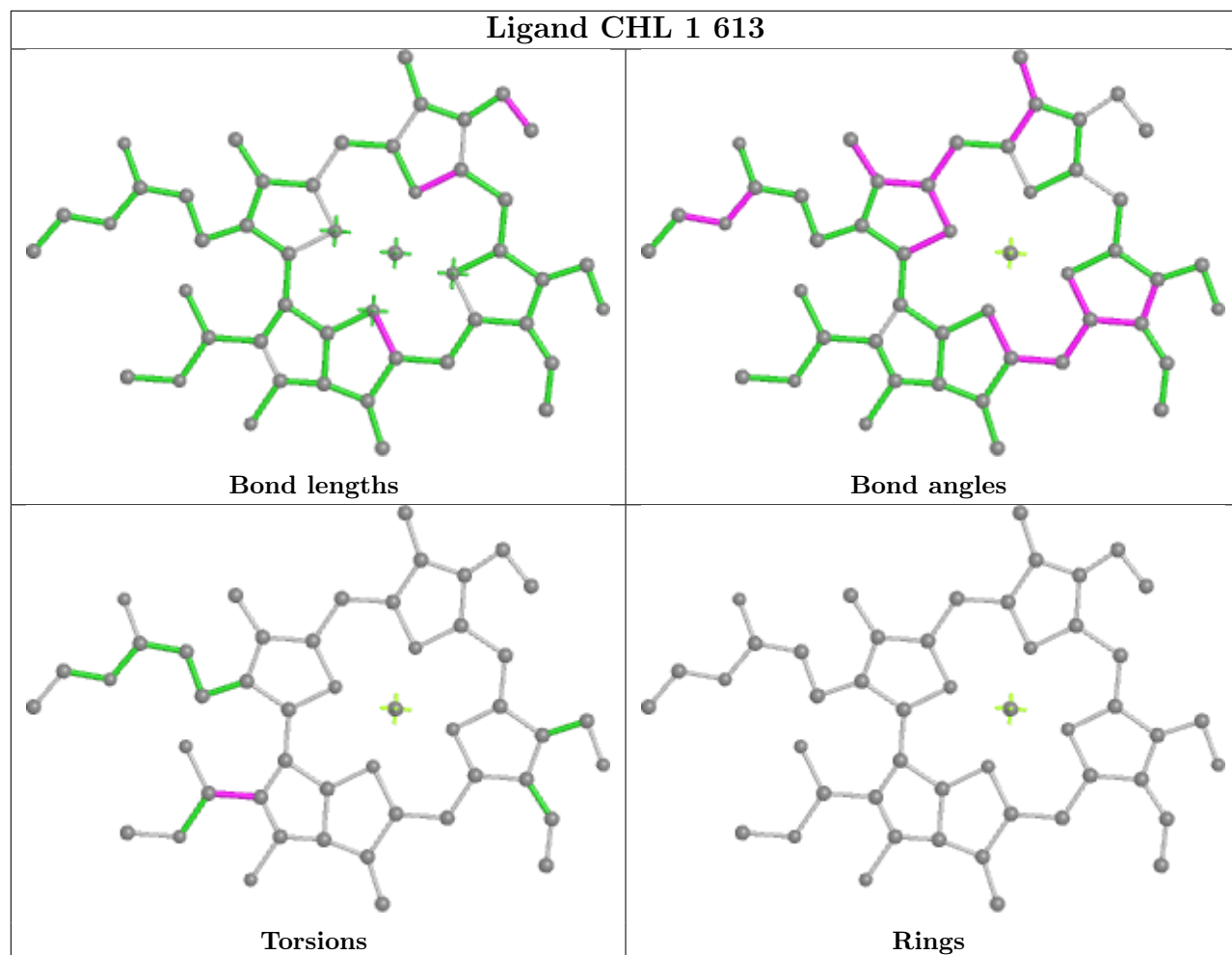


Ligand CLA 5 607**Ligand LMT B 5006**

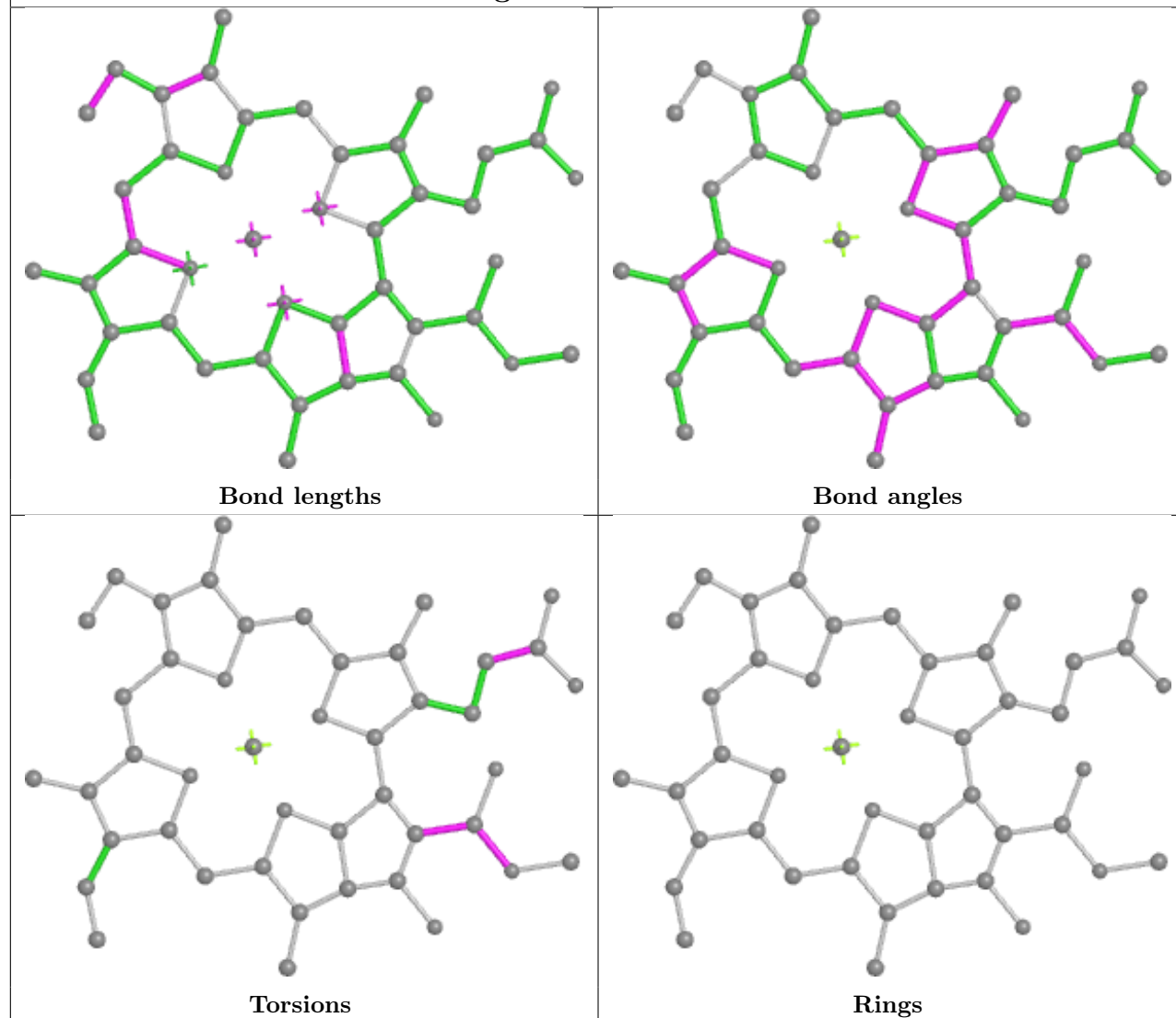
Ligand CLA A 1101**Ligand LHG 1 802**



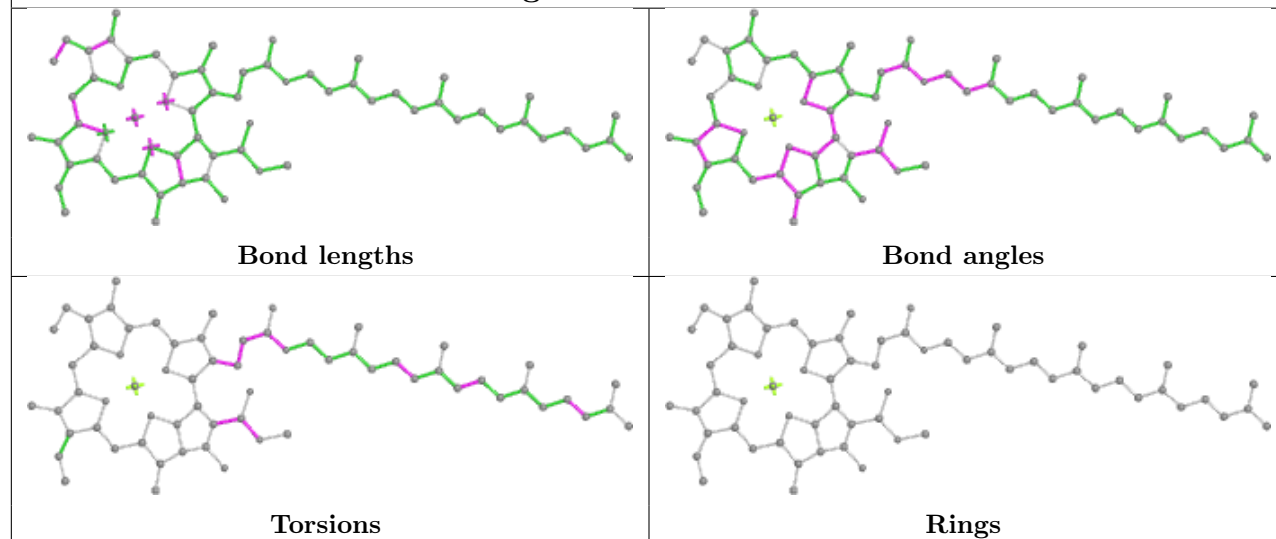
Ligand CHL 1 613

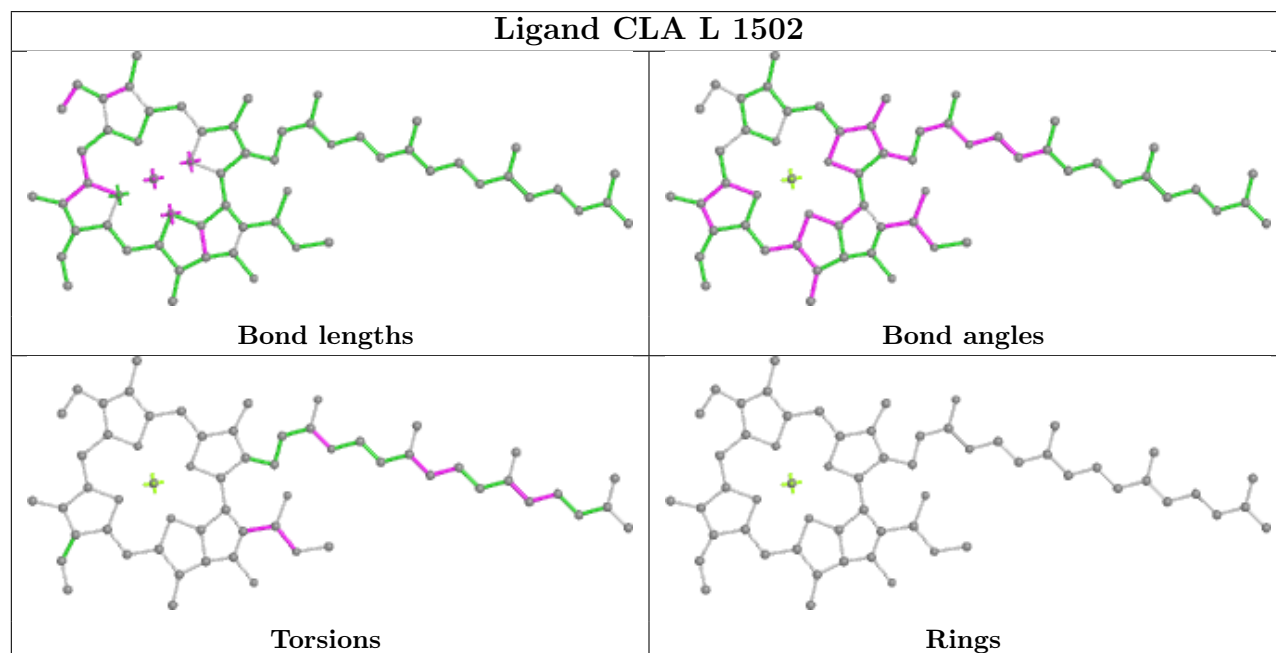
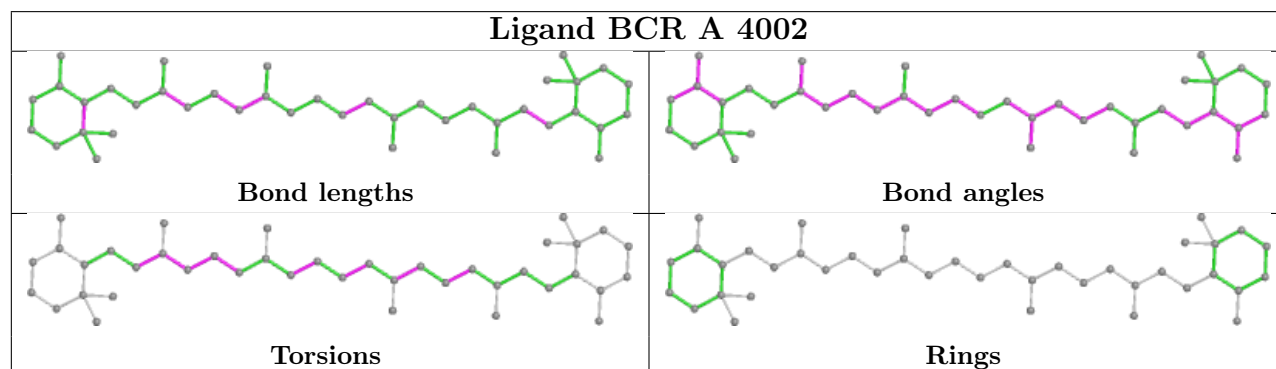
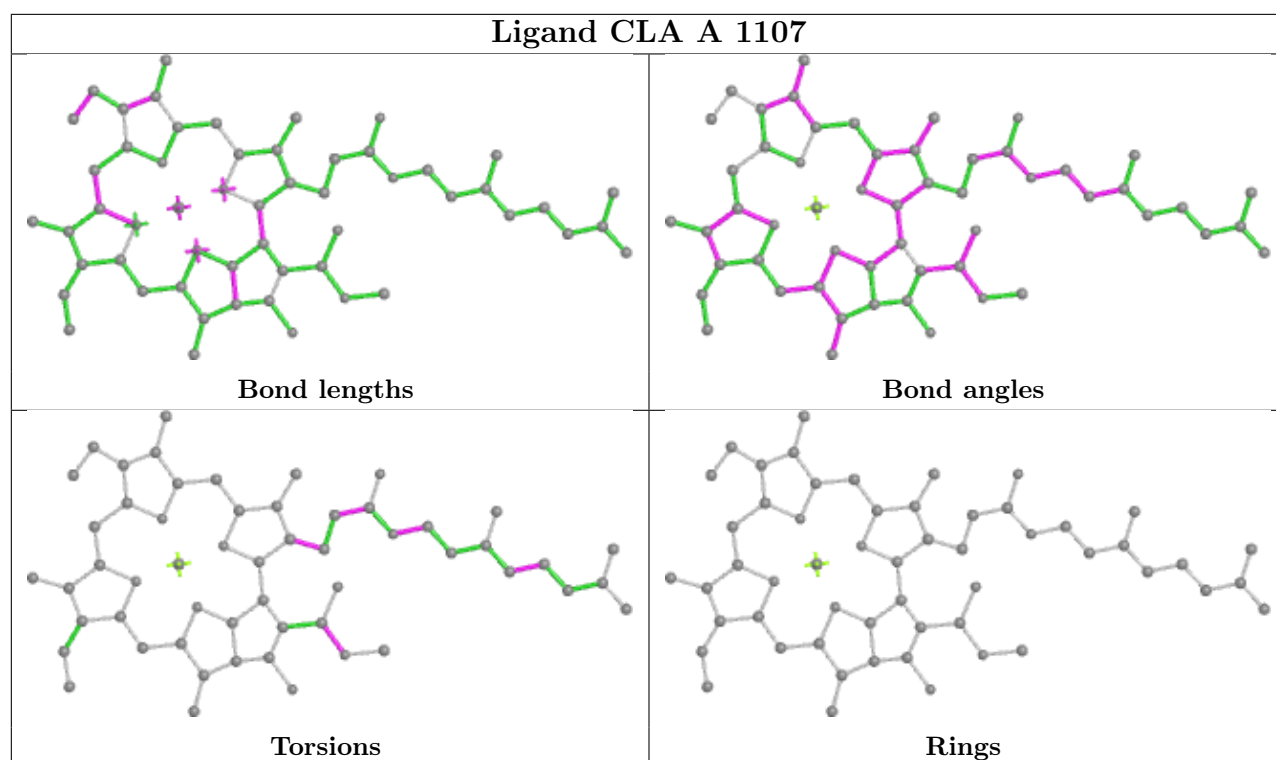


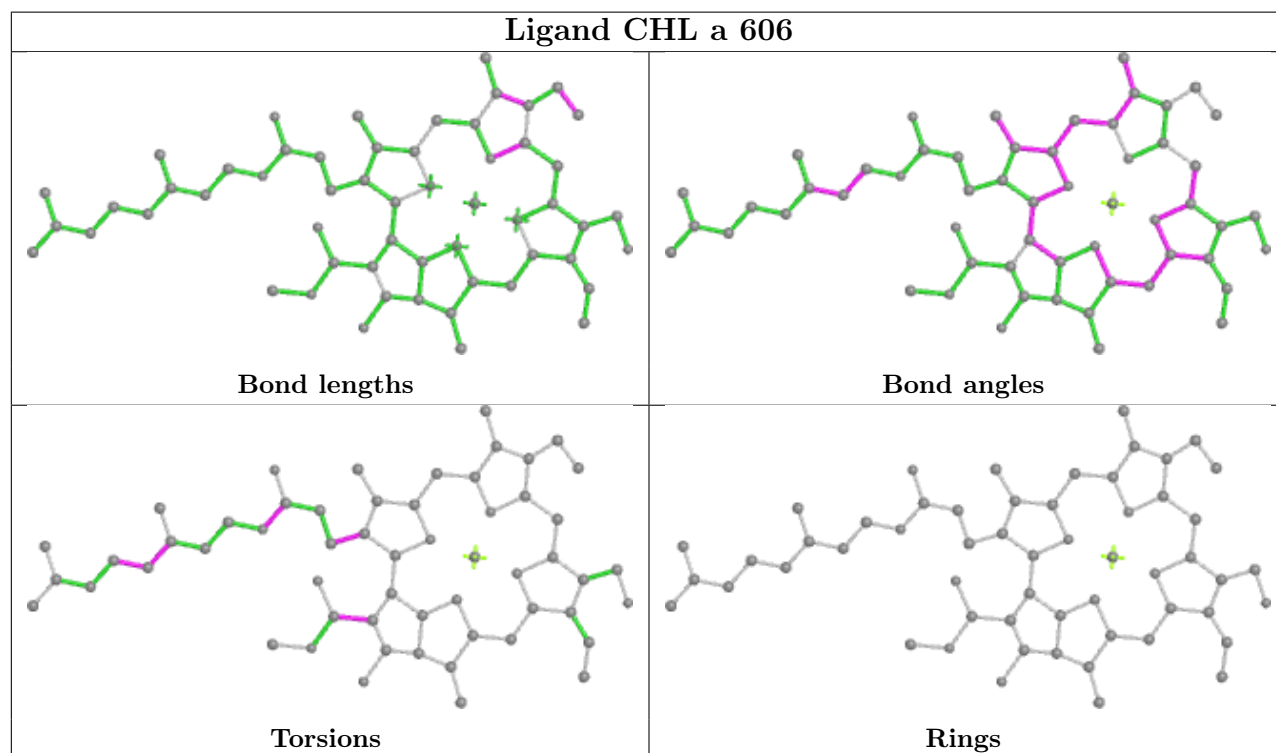
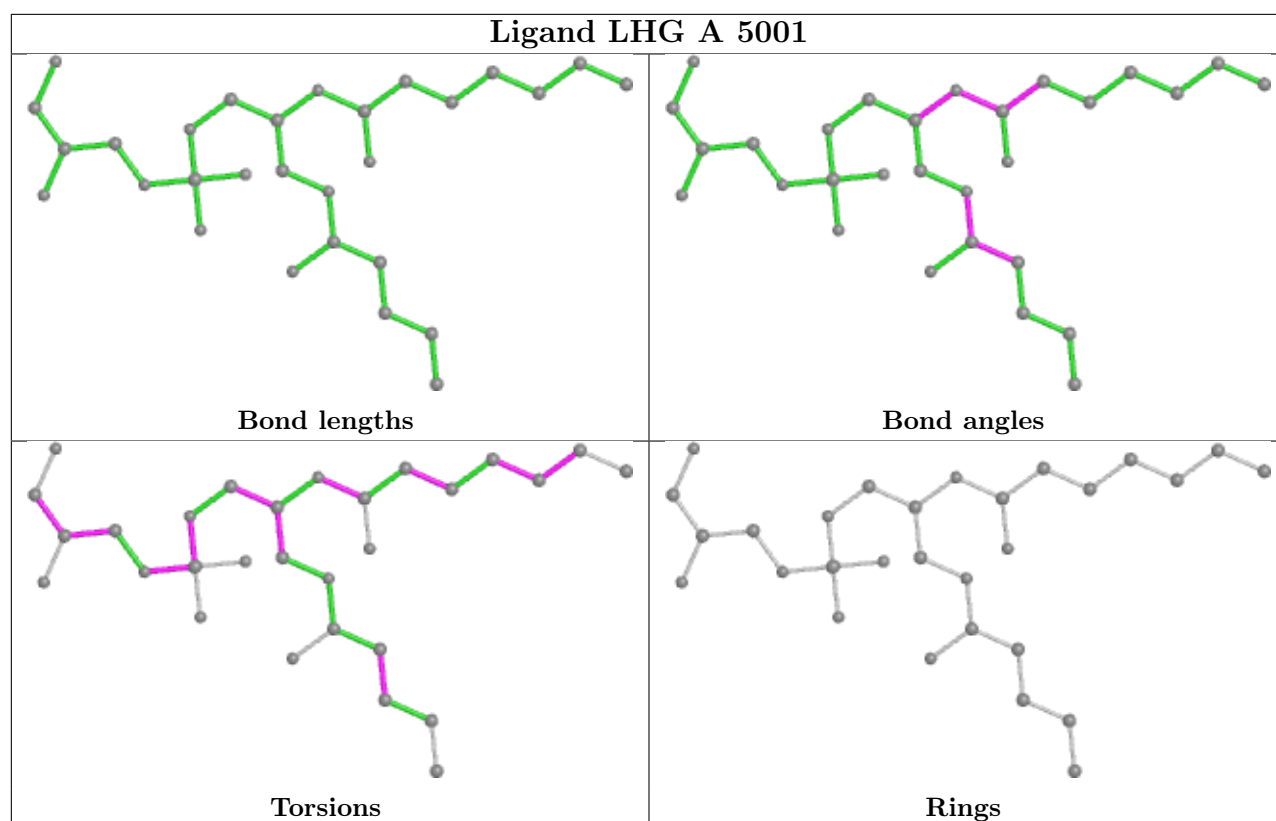
Ligand CLA 8 605

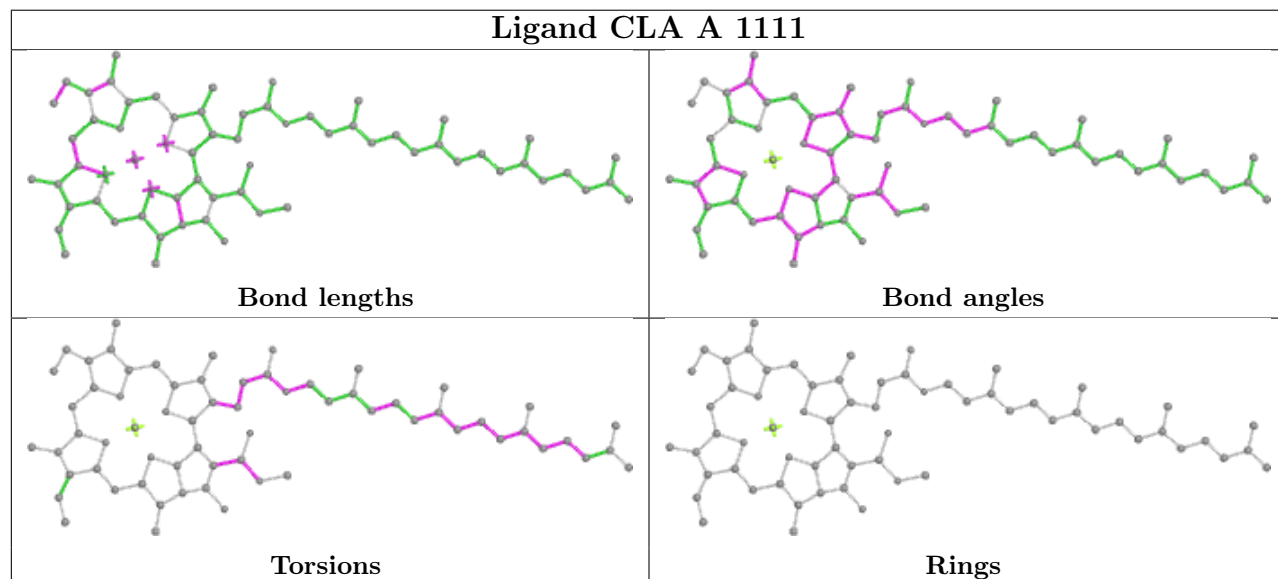
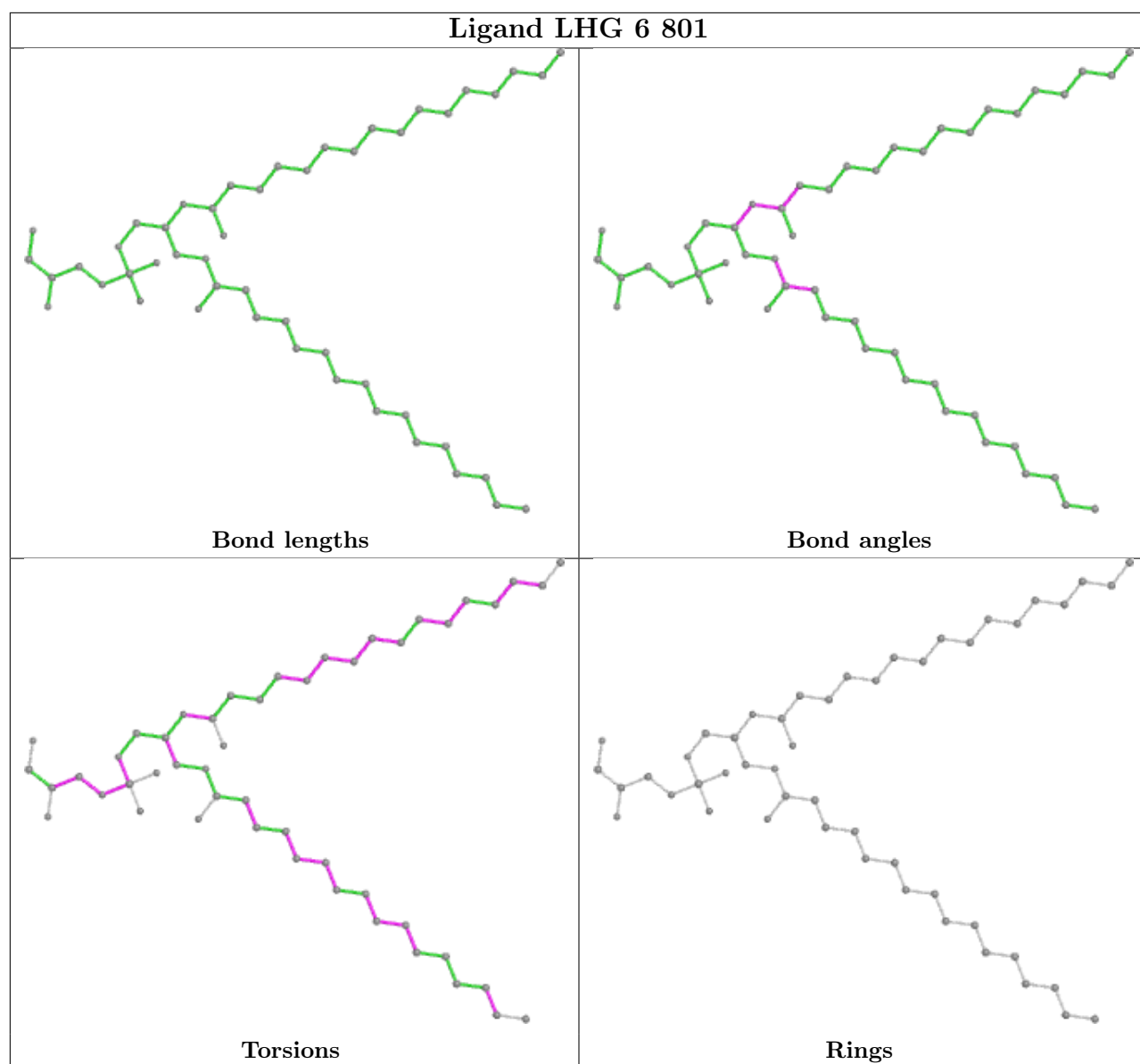


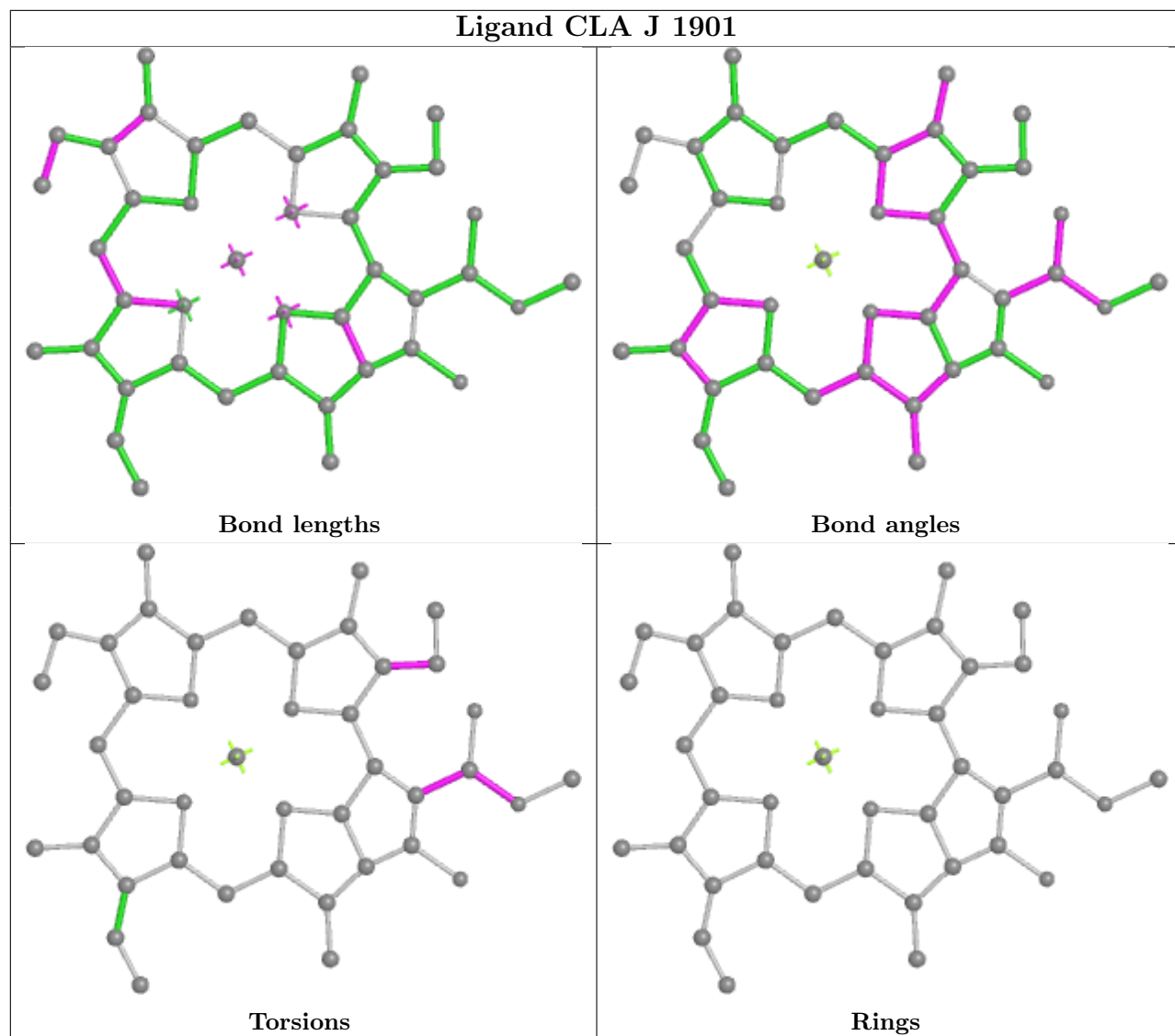
Ligand CLA A 1127



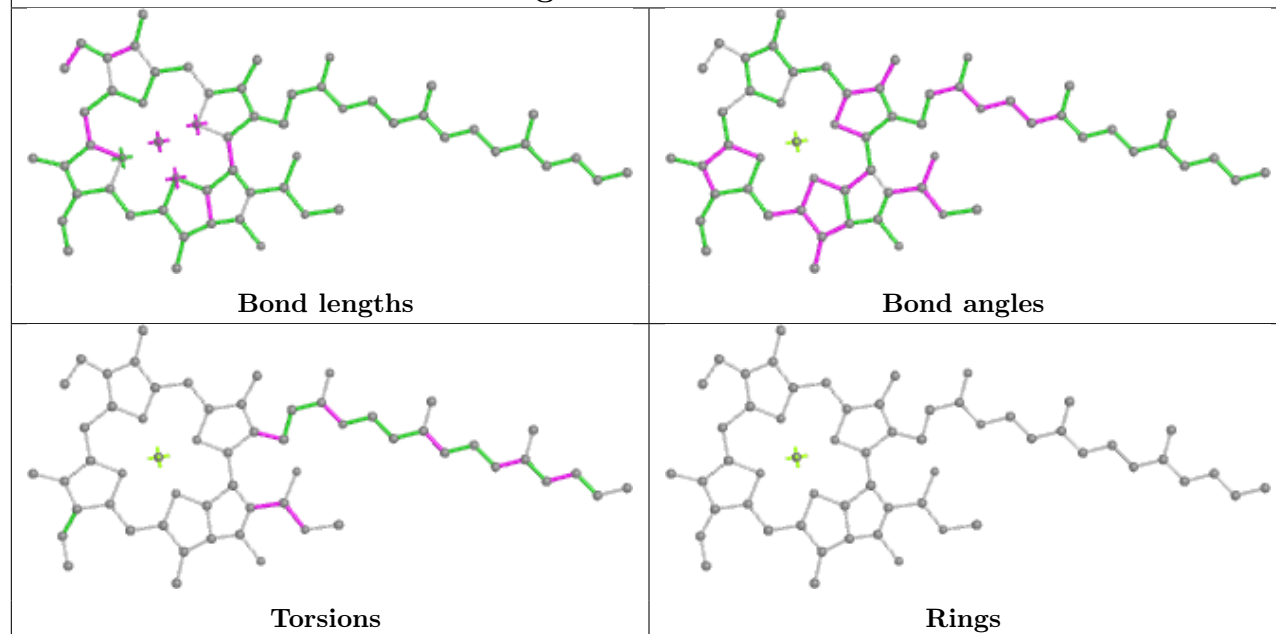




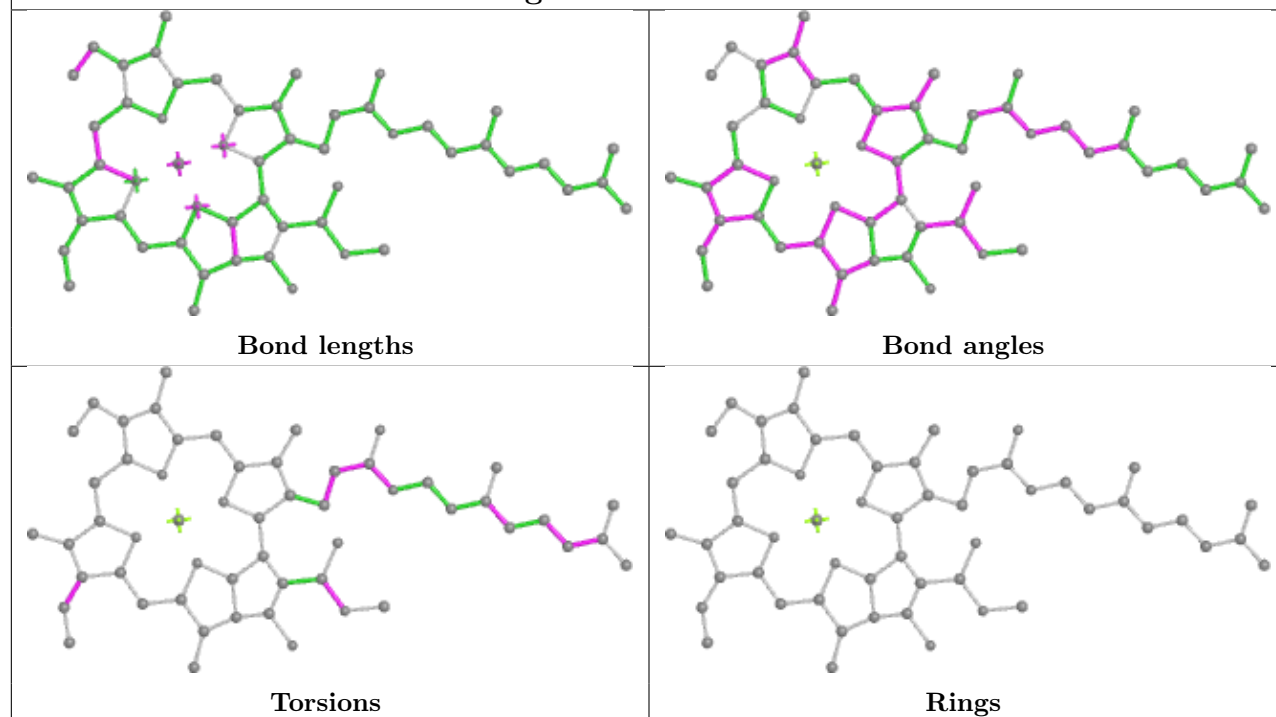


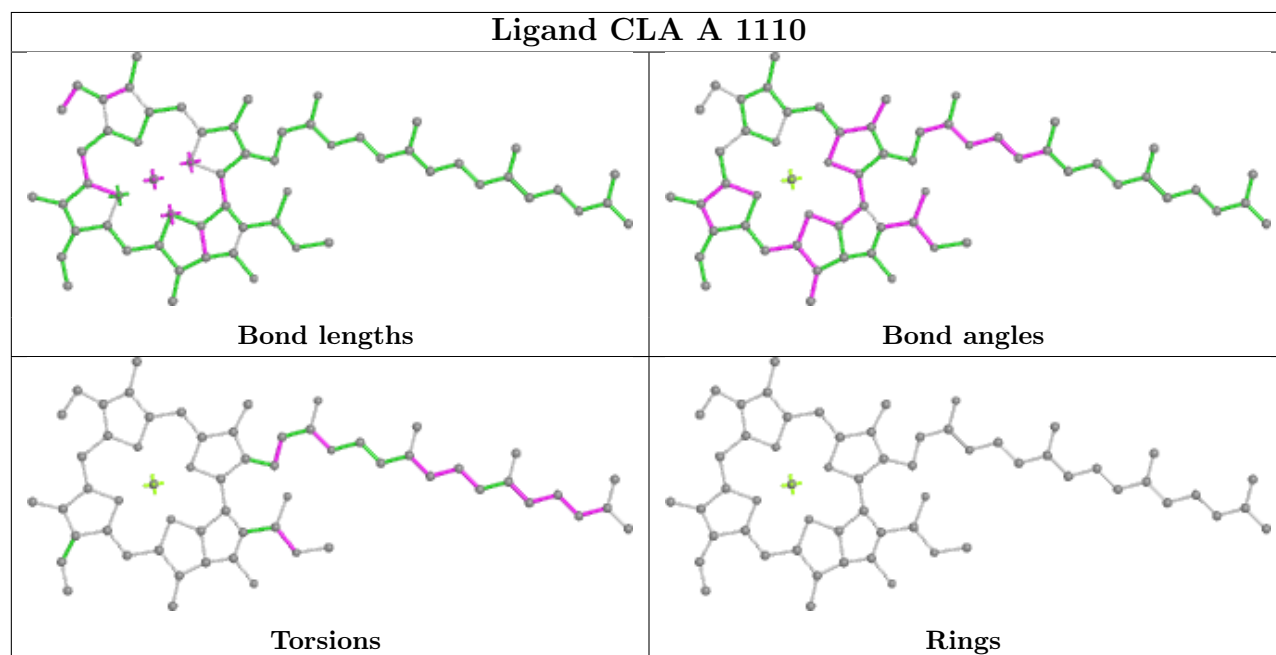
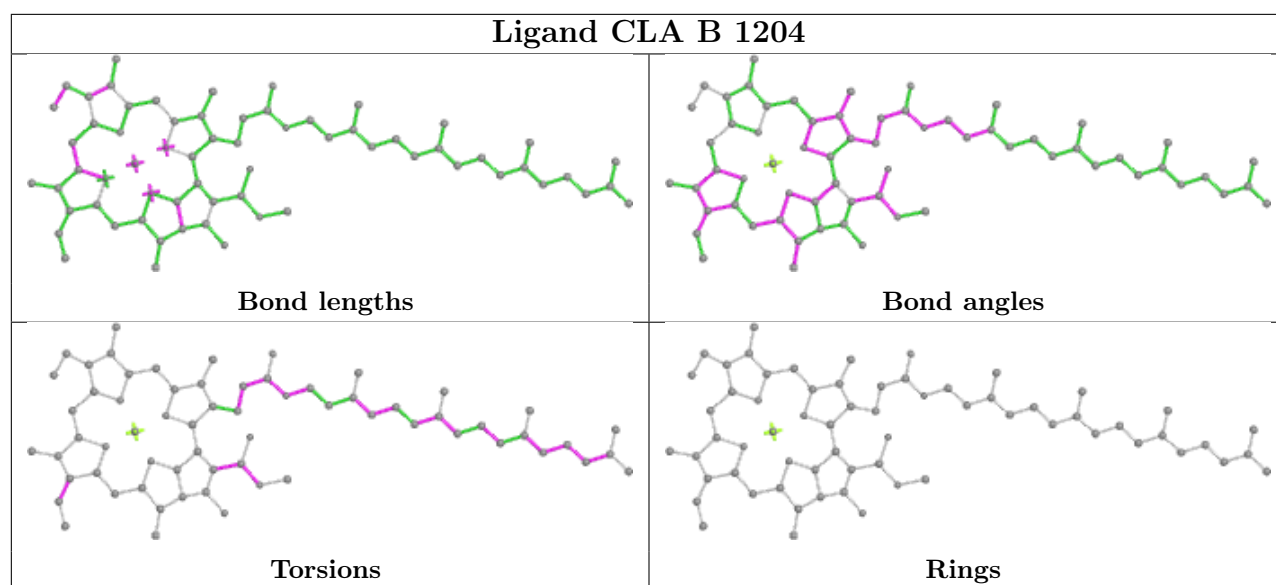


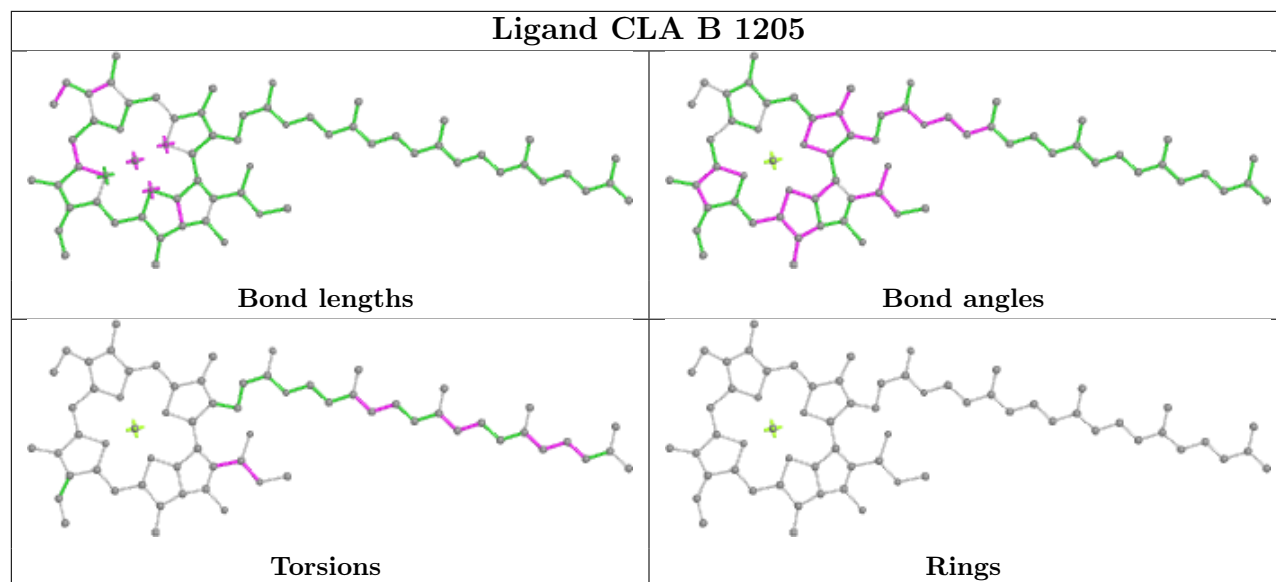
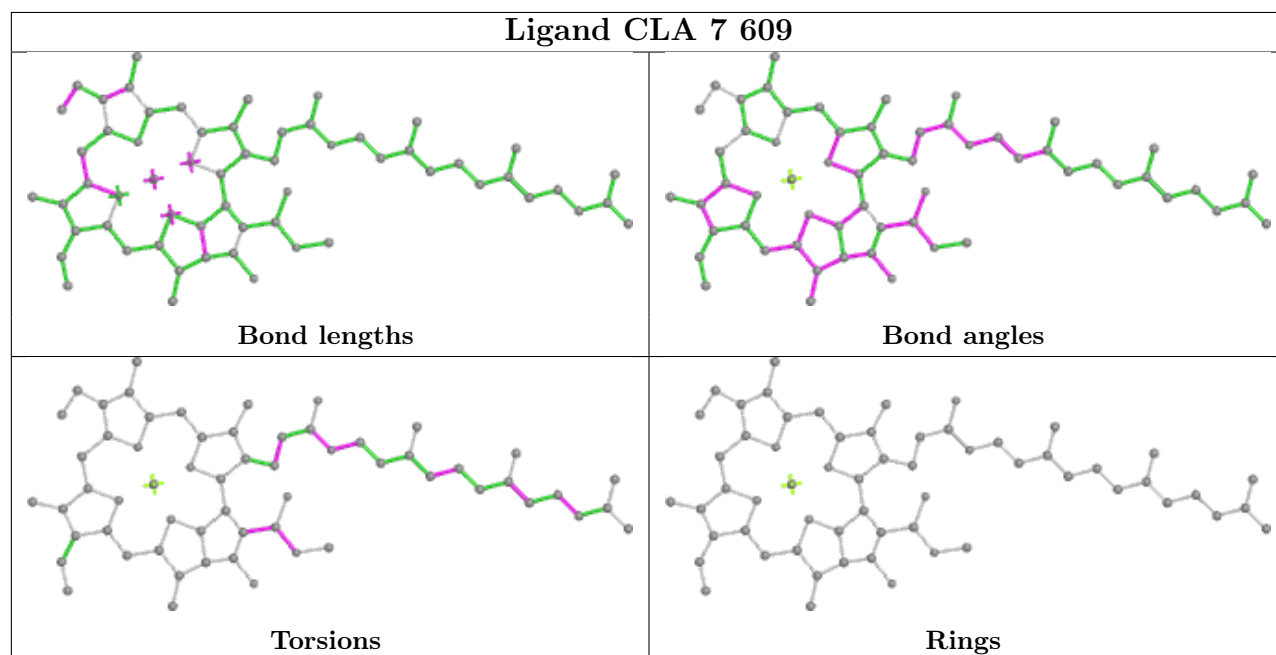
Ligand CLA a 607

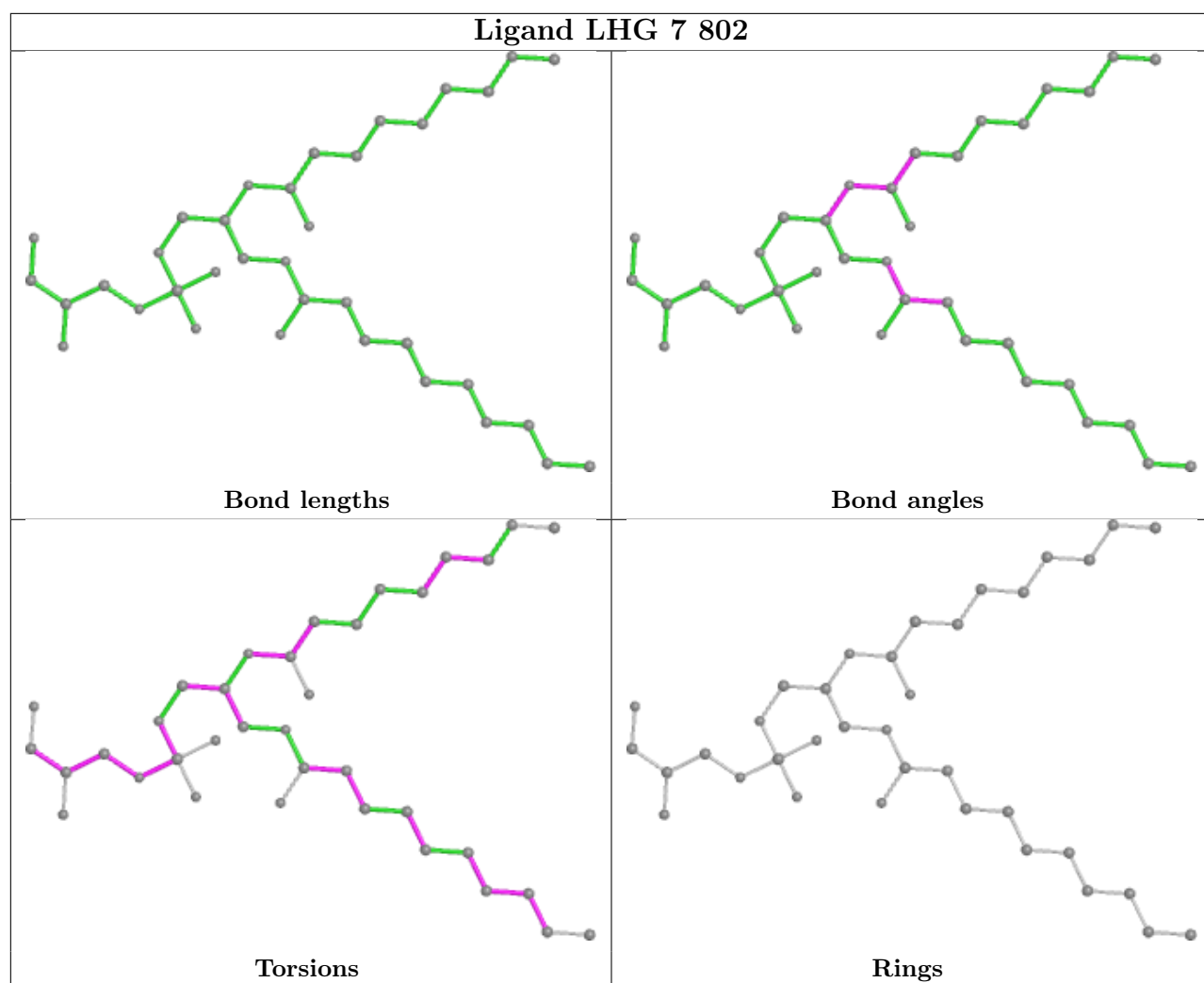


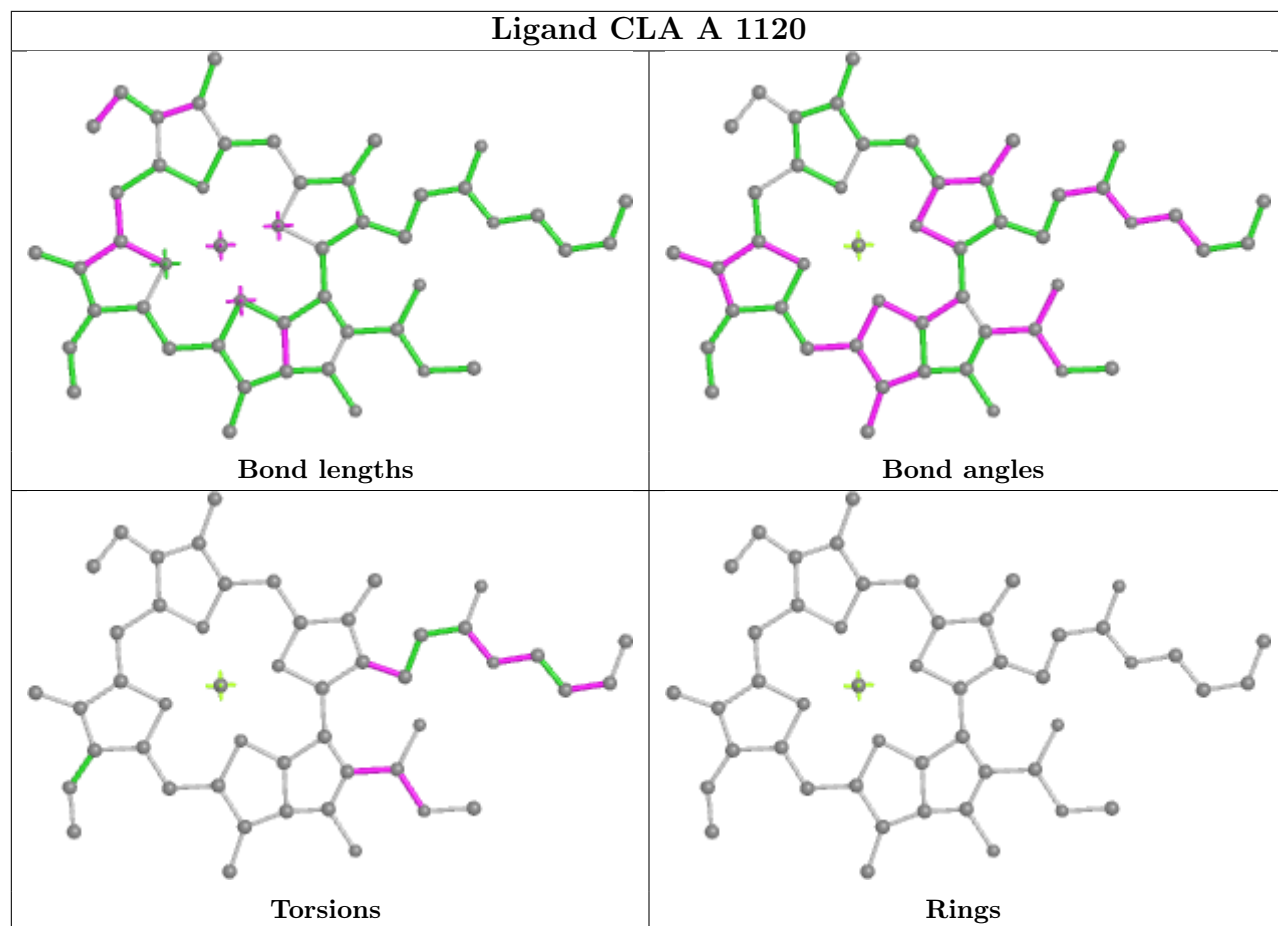
Ligand CLA F 1302



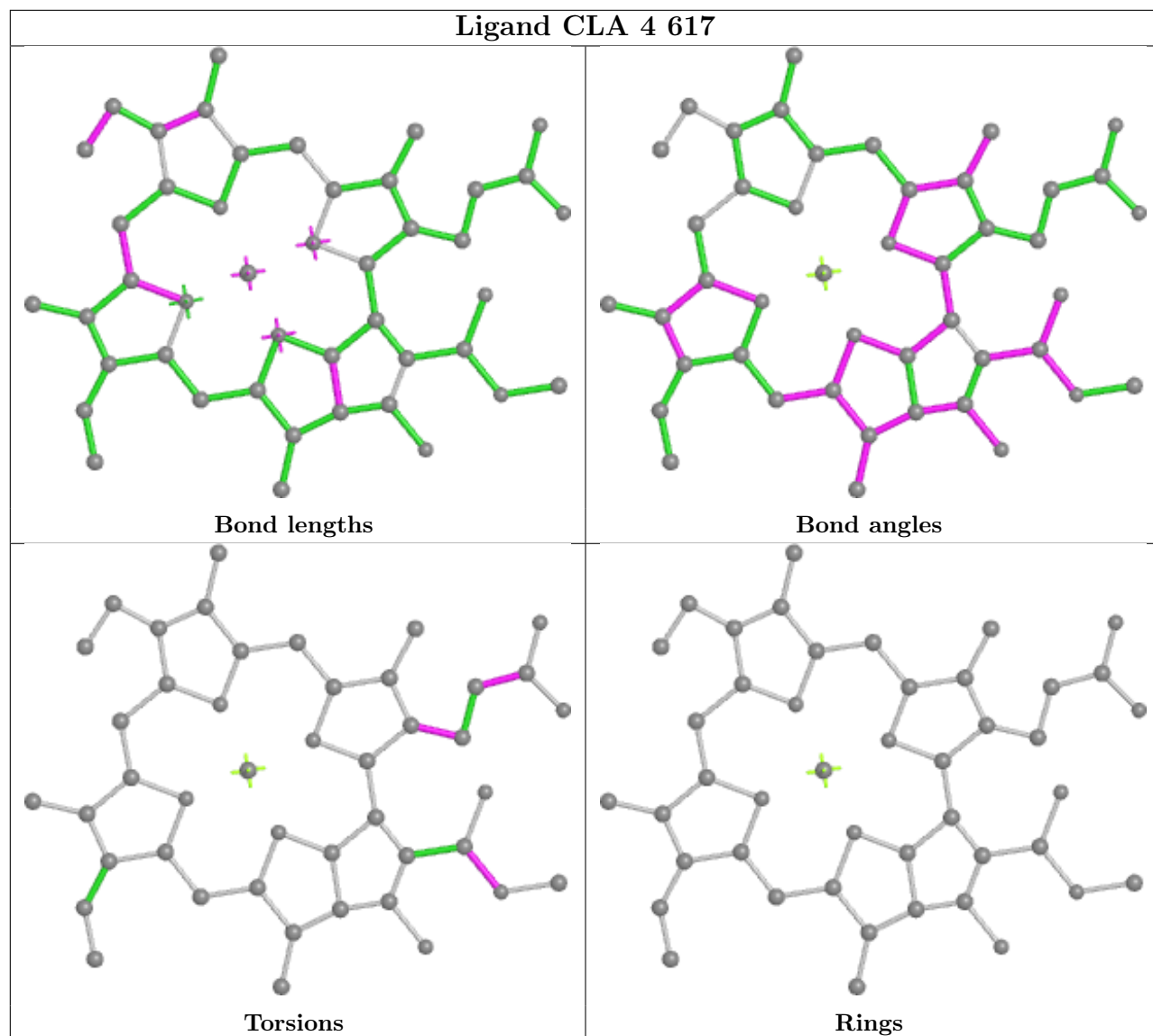


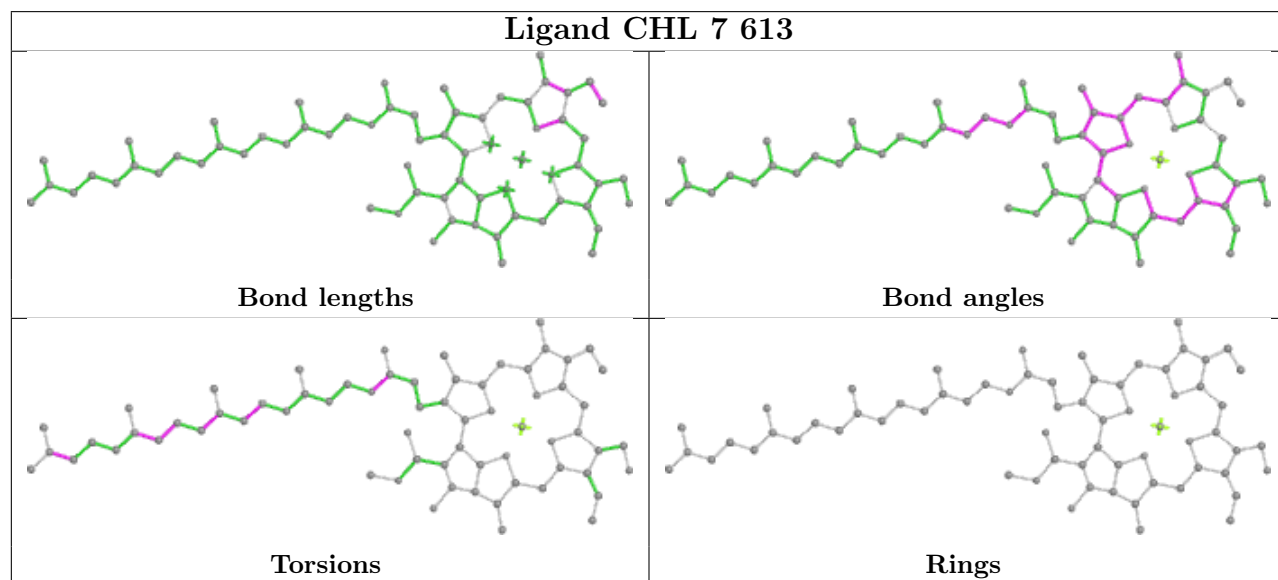
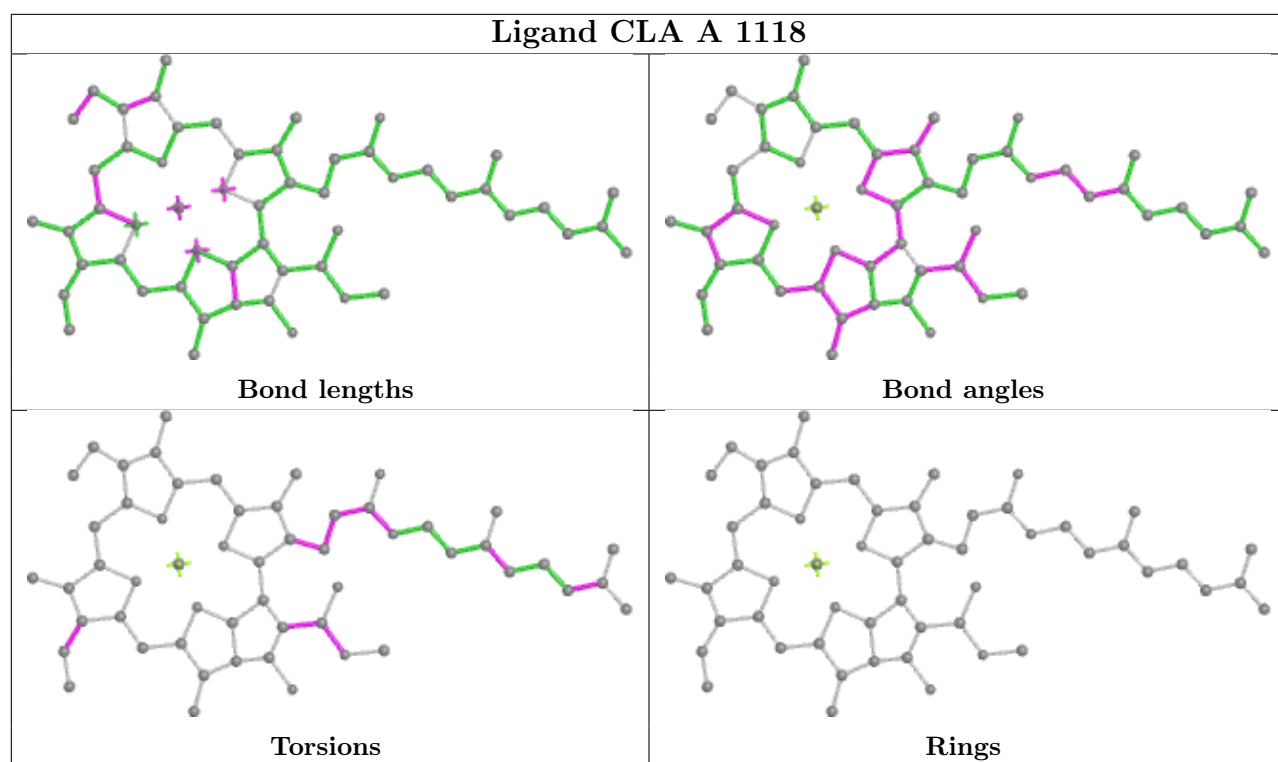
Ligand CLA B 1205**Ligand CLA 7 609**



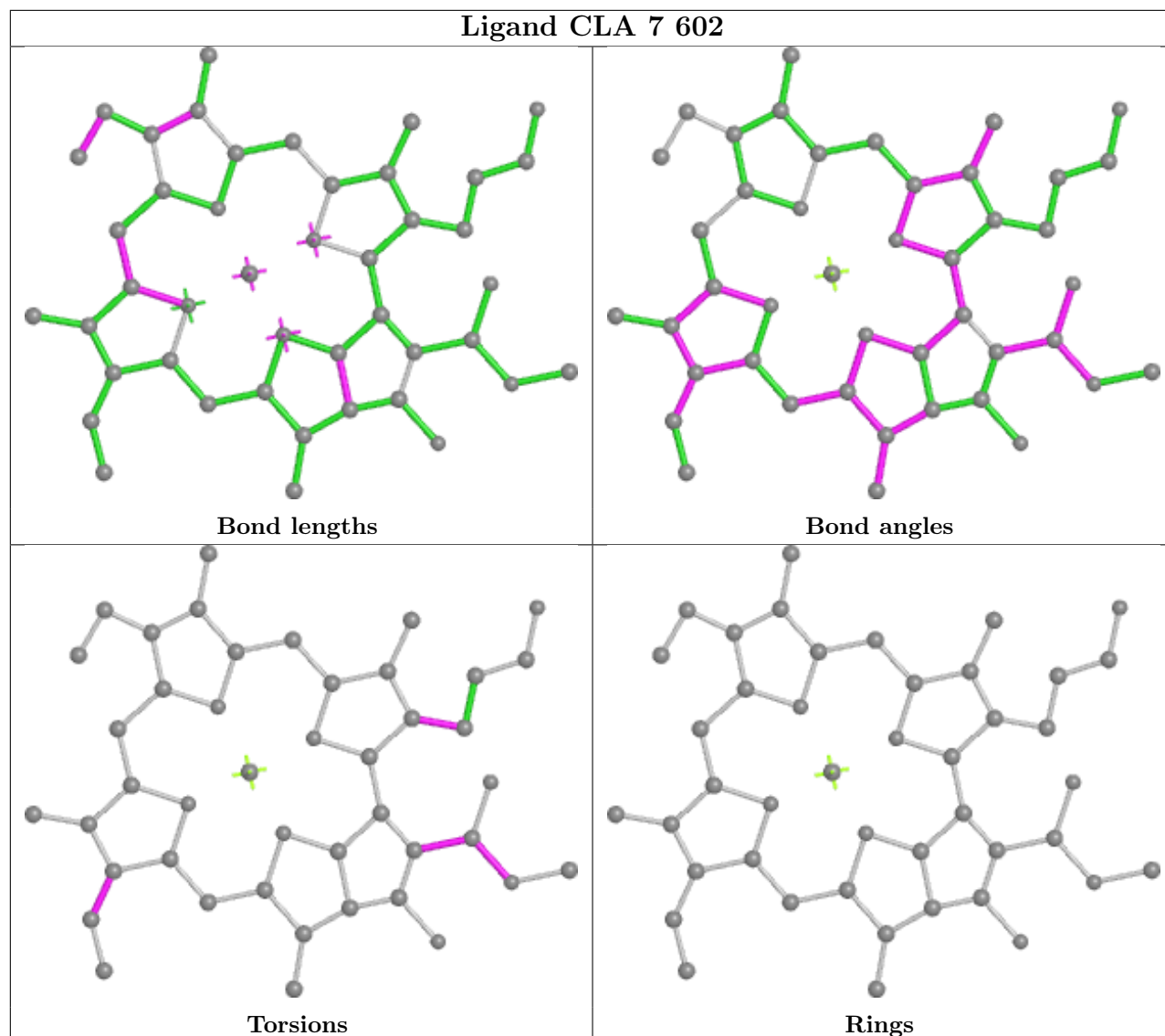


Ligand CLA 4 617

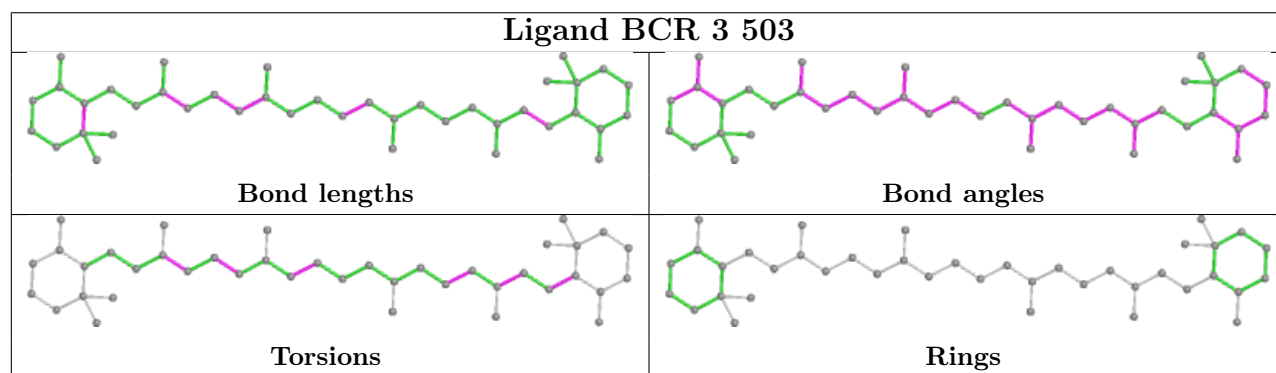


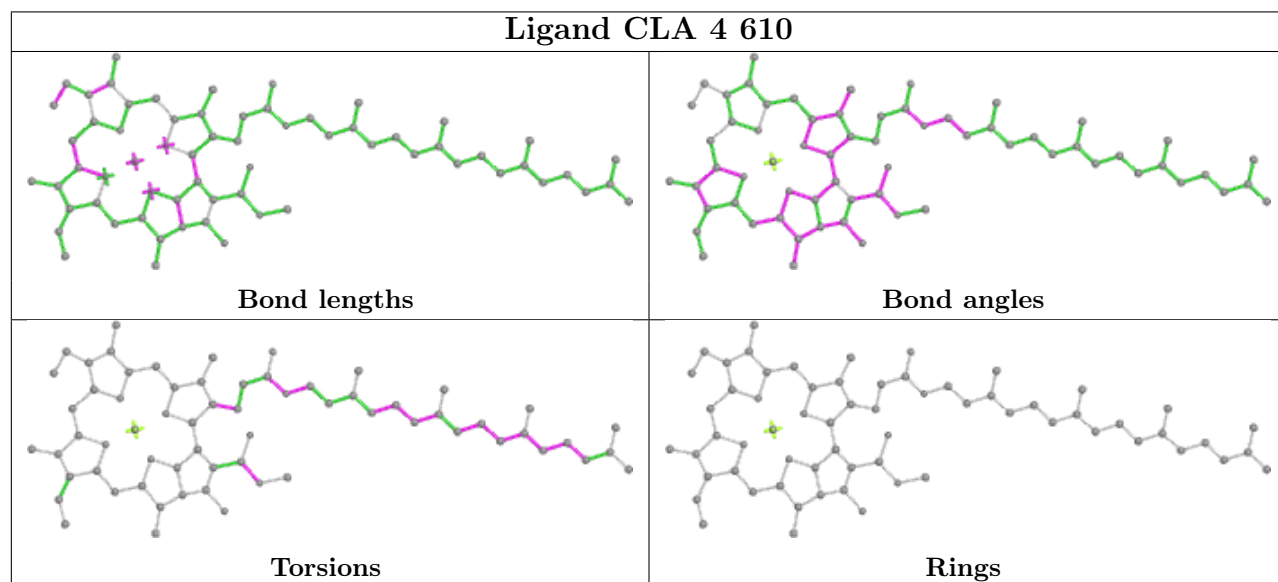
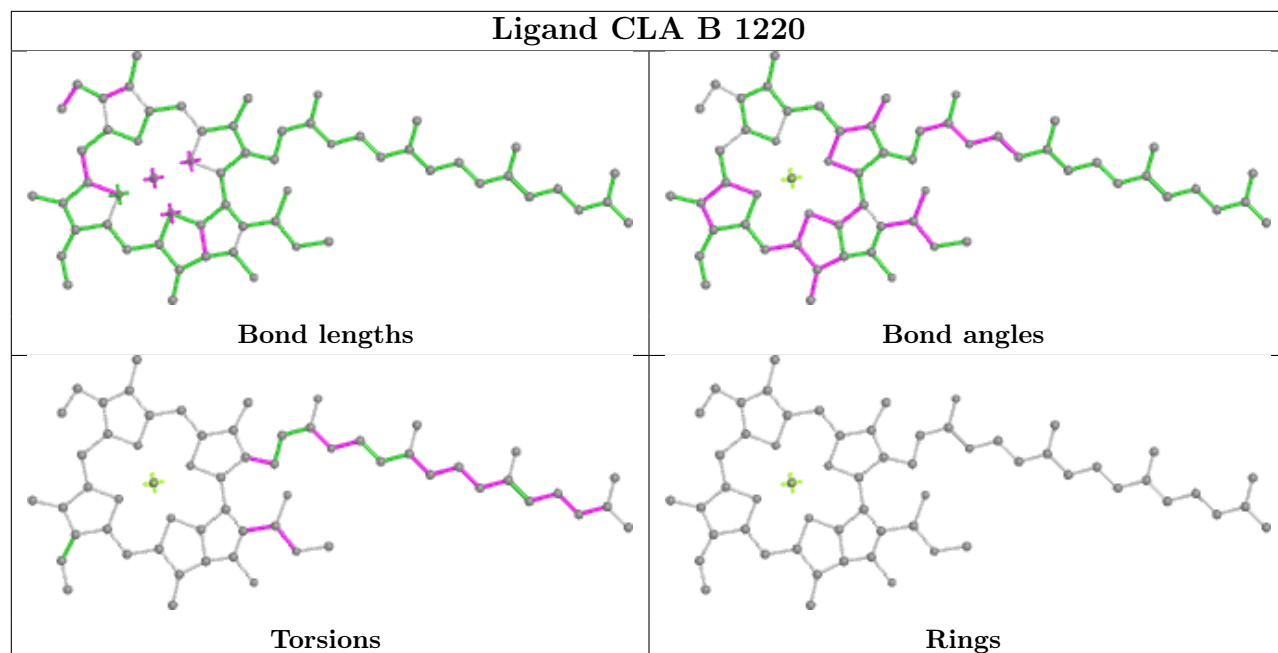


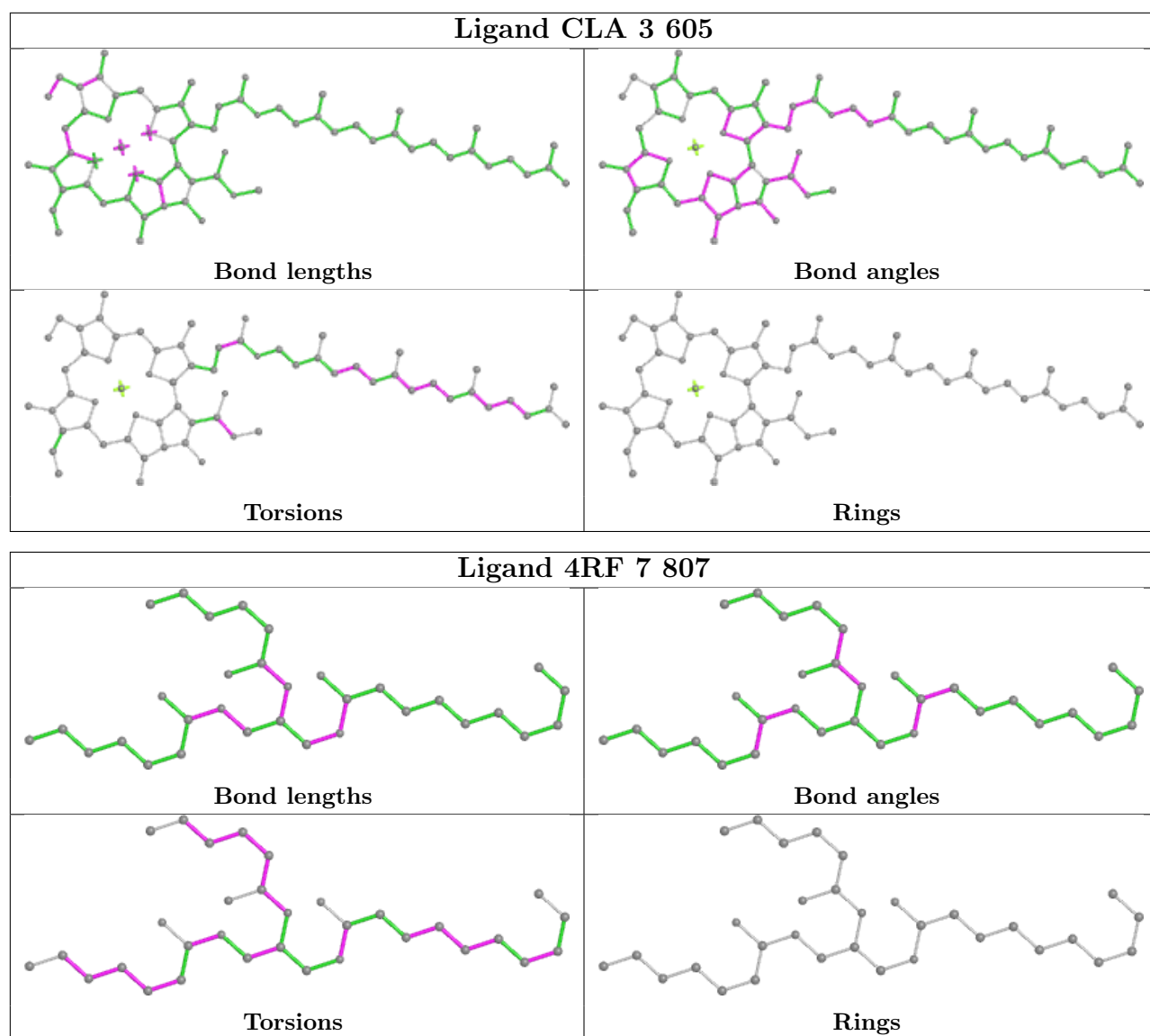
Ligand CLA 7 602

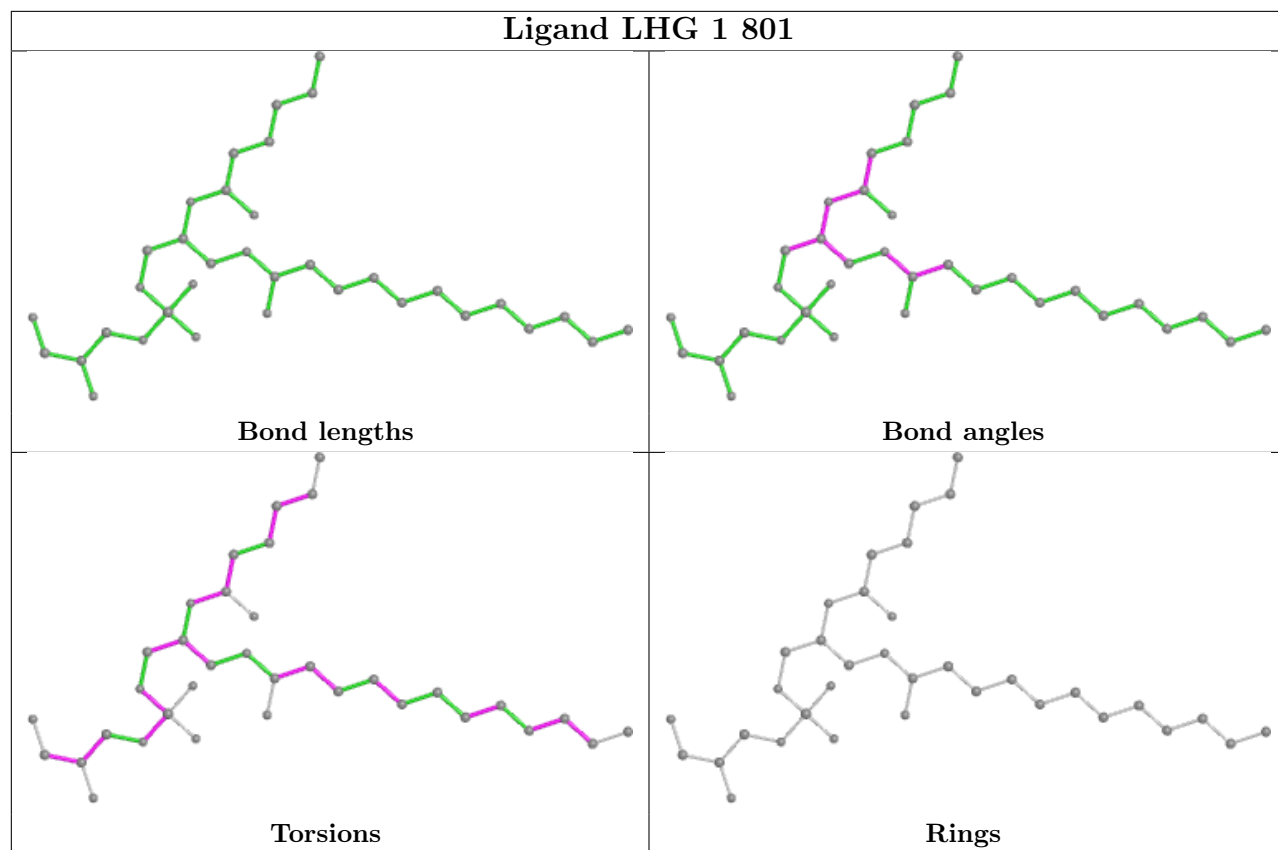


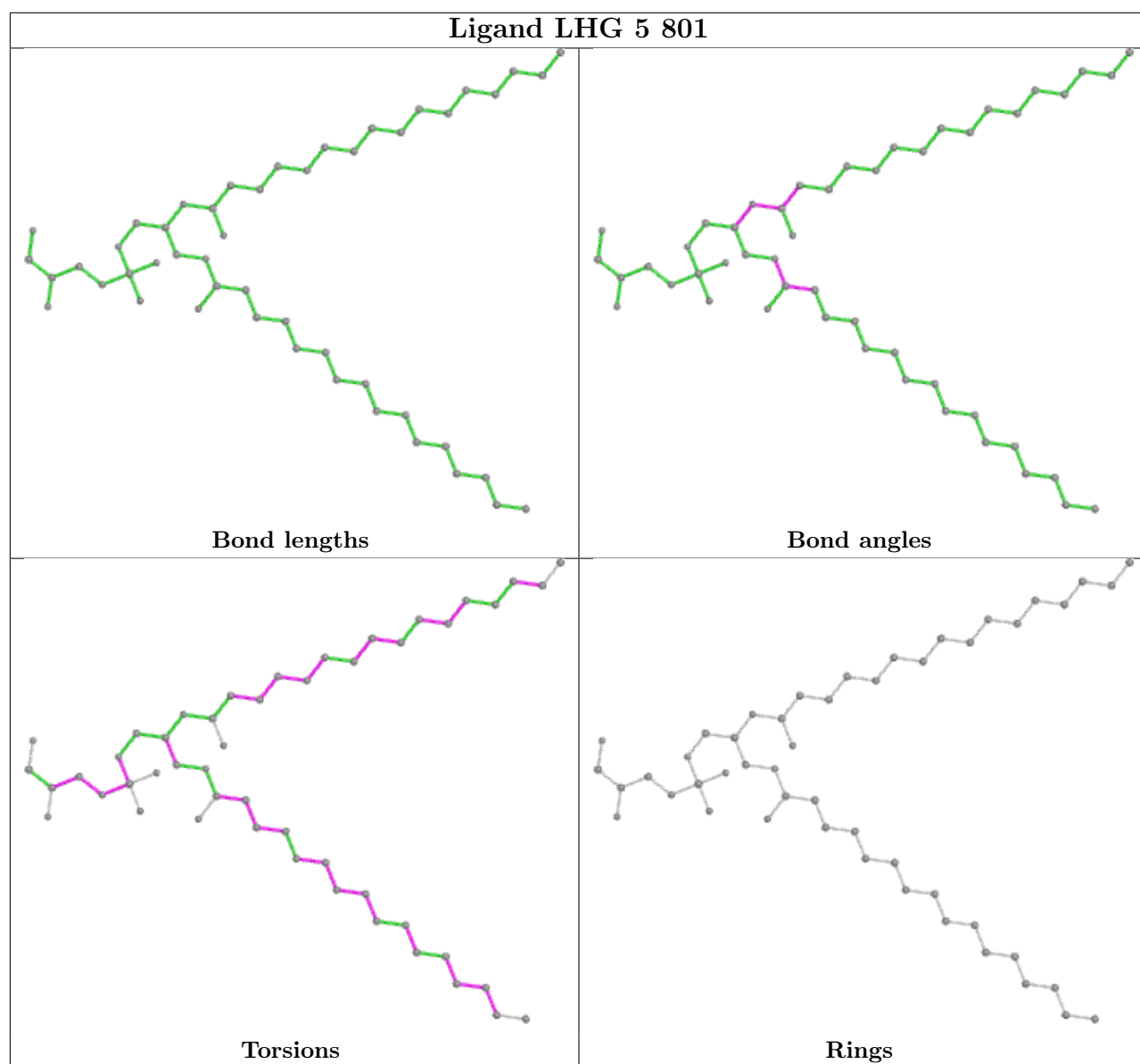
Ligand BCR 3 503



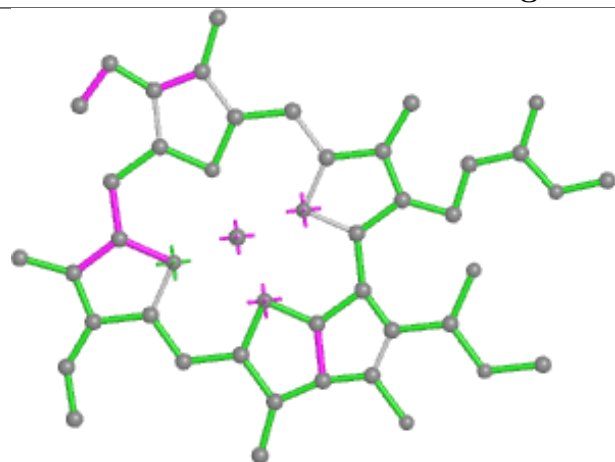




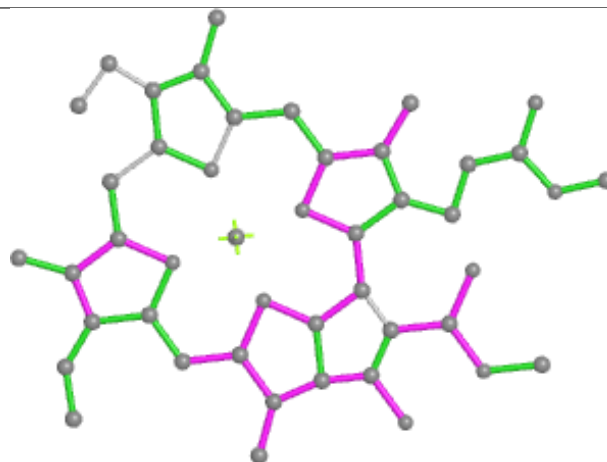




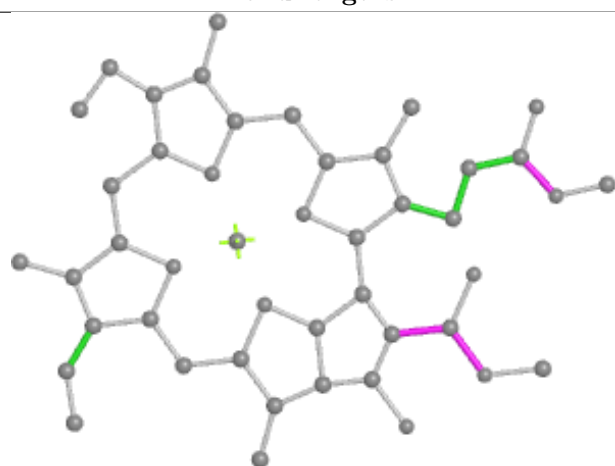
Ligand CLA 6 605



Bond lengths



Bond angles

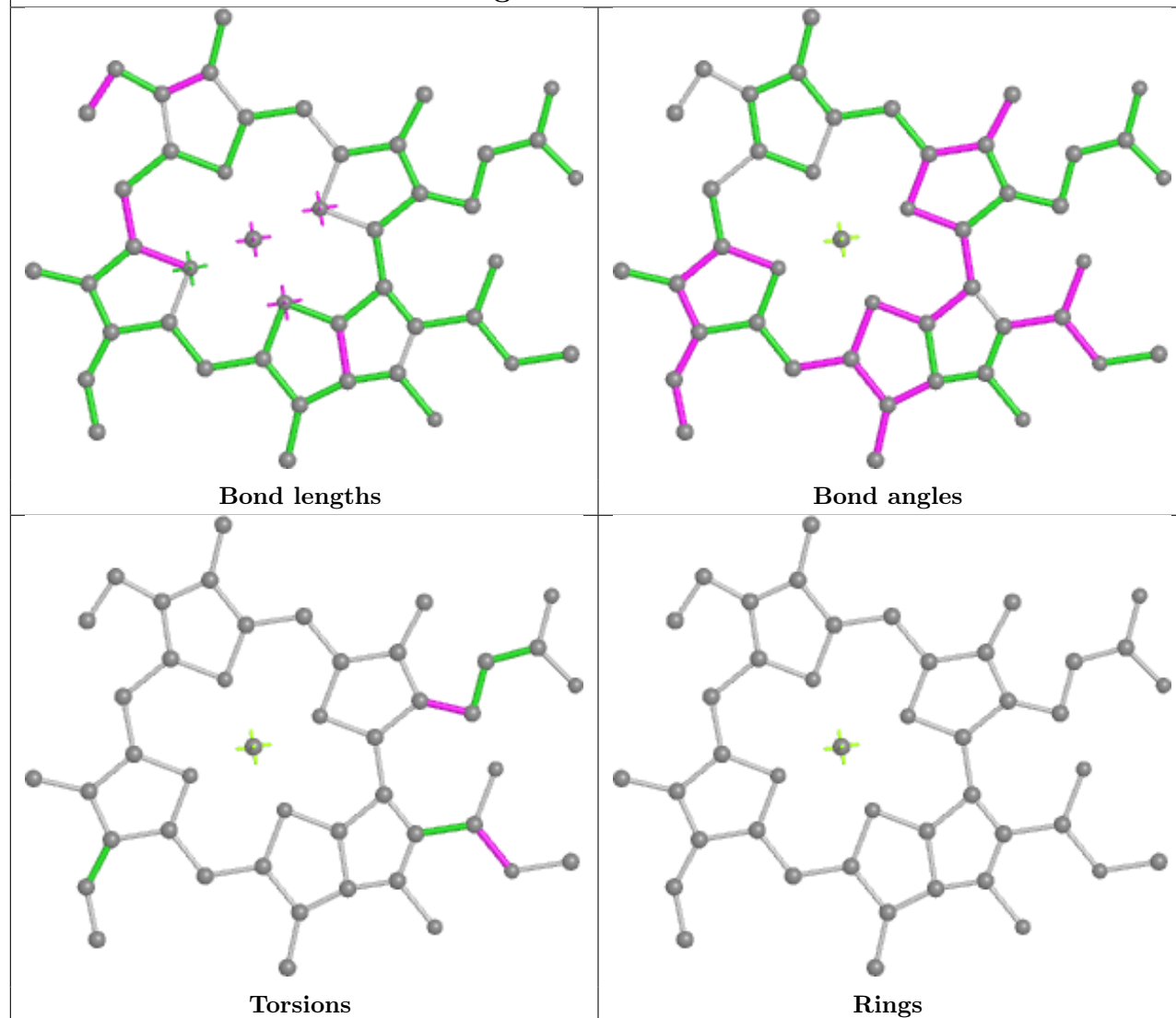


Torsions

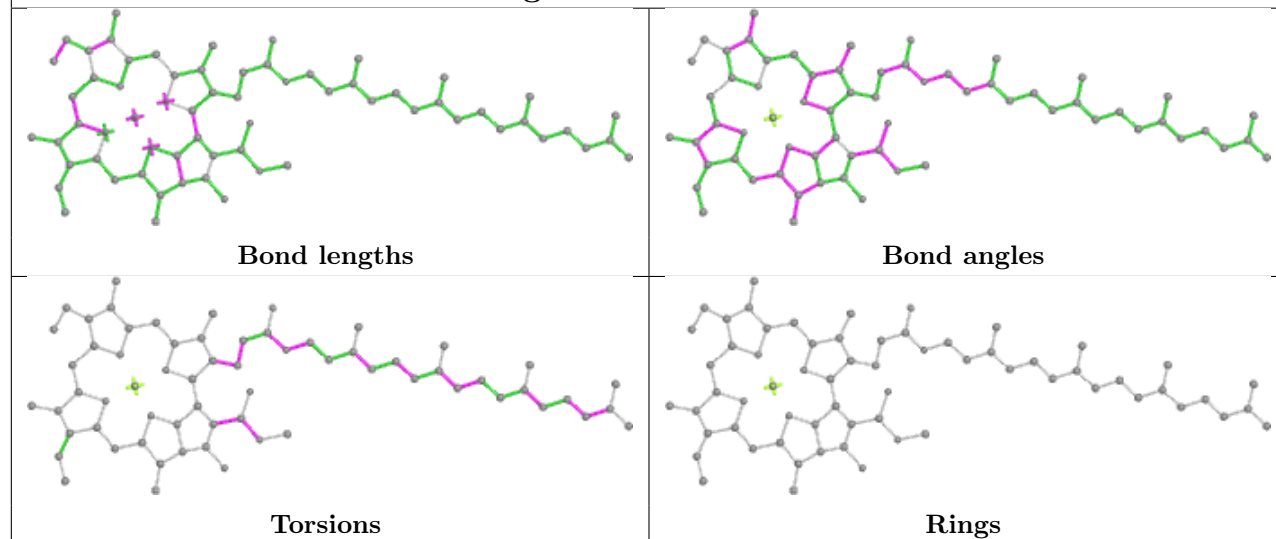


Rings

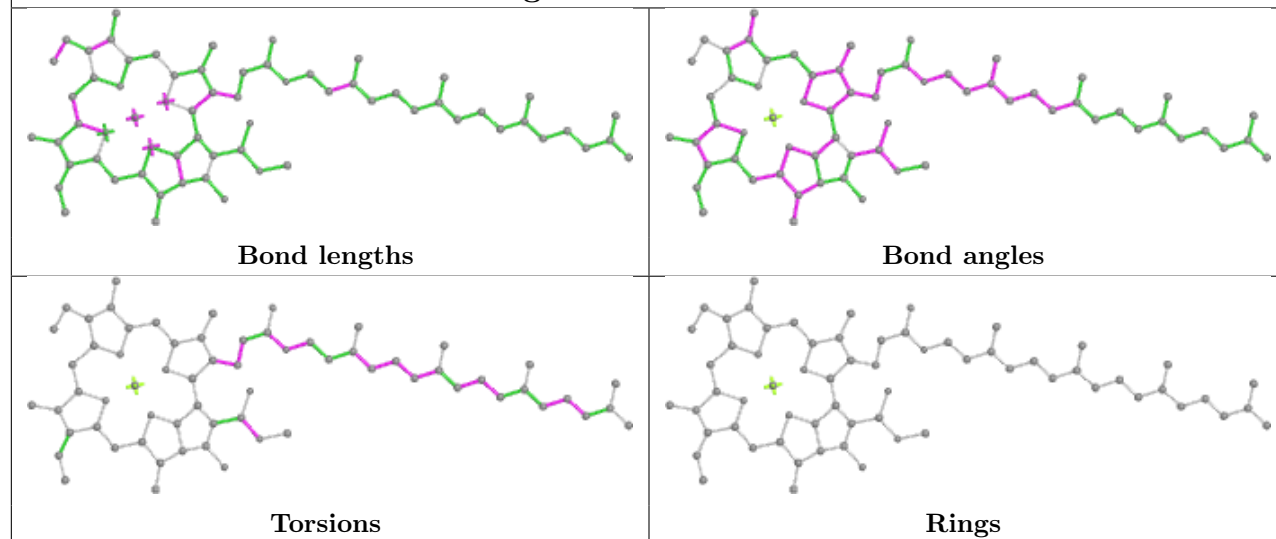
Ligand CLA 6 617



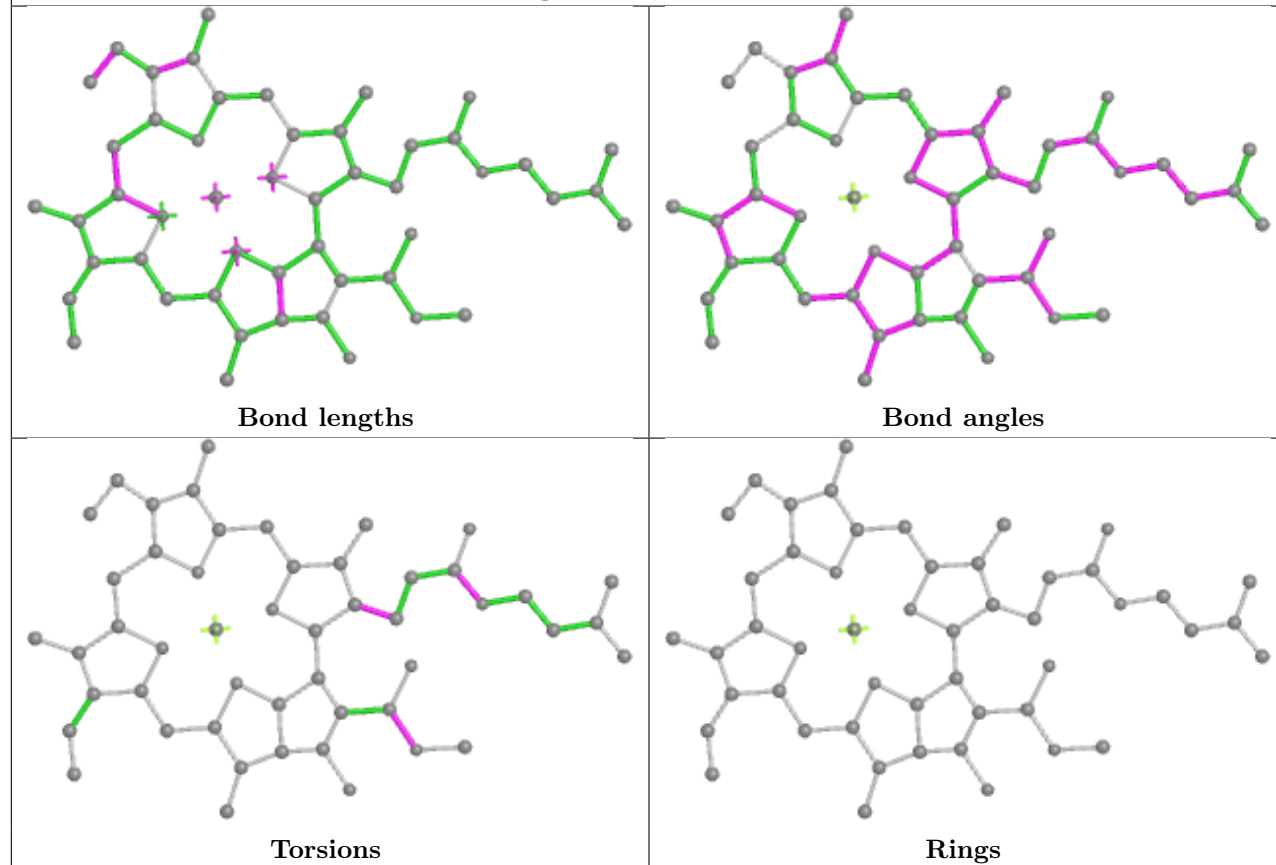
Ligand CLA B 1235

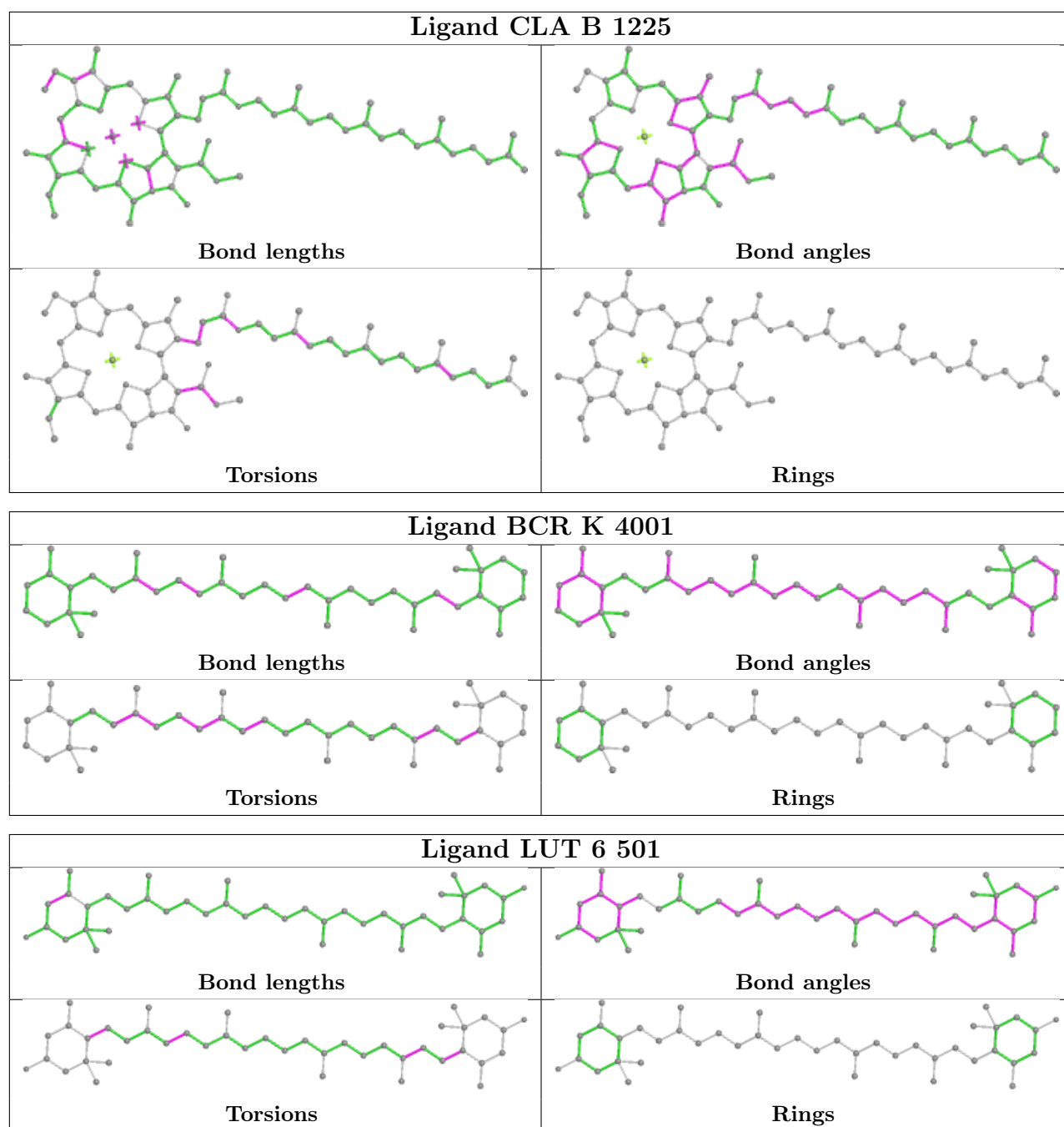


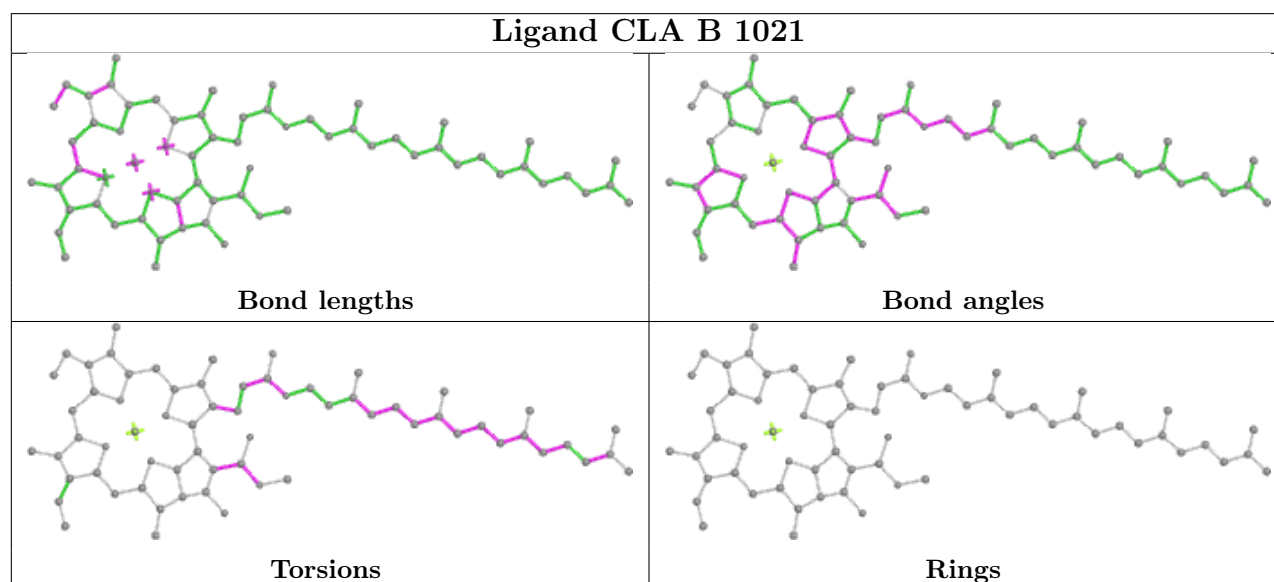
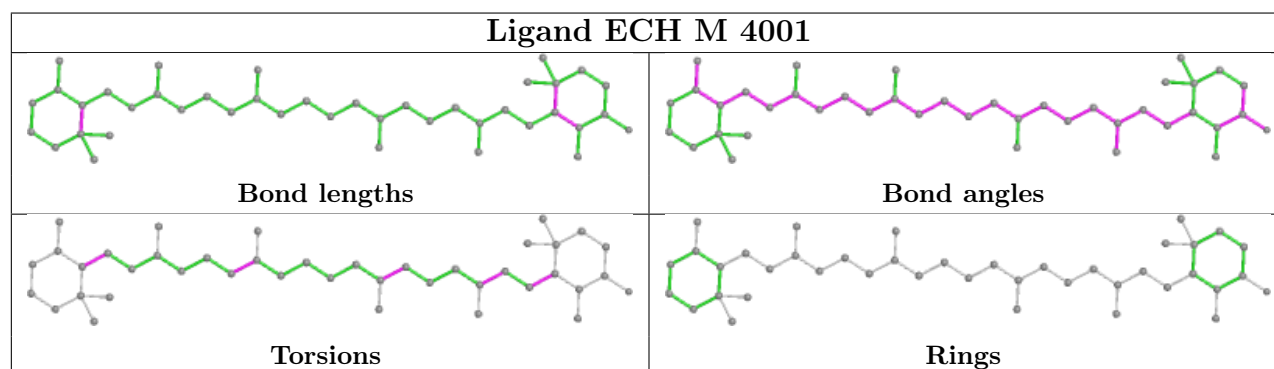
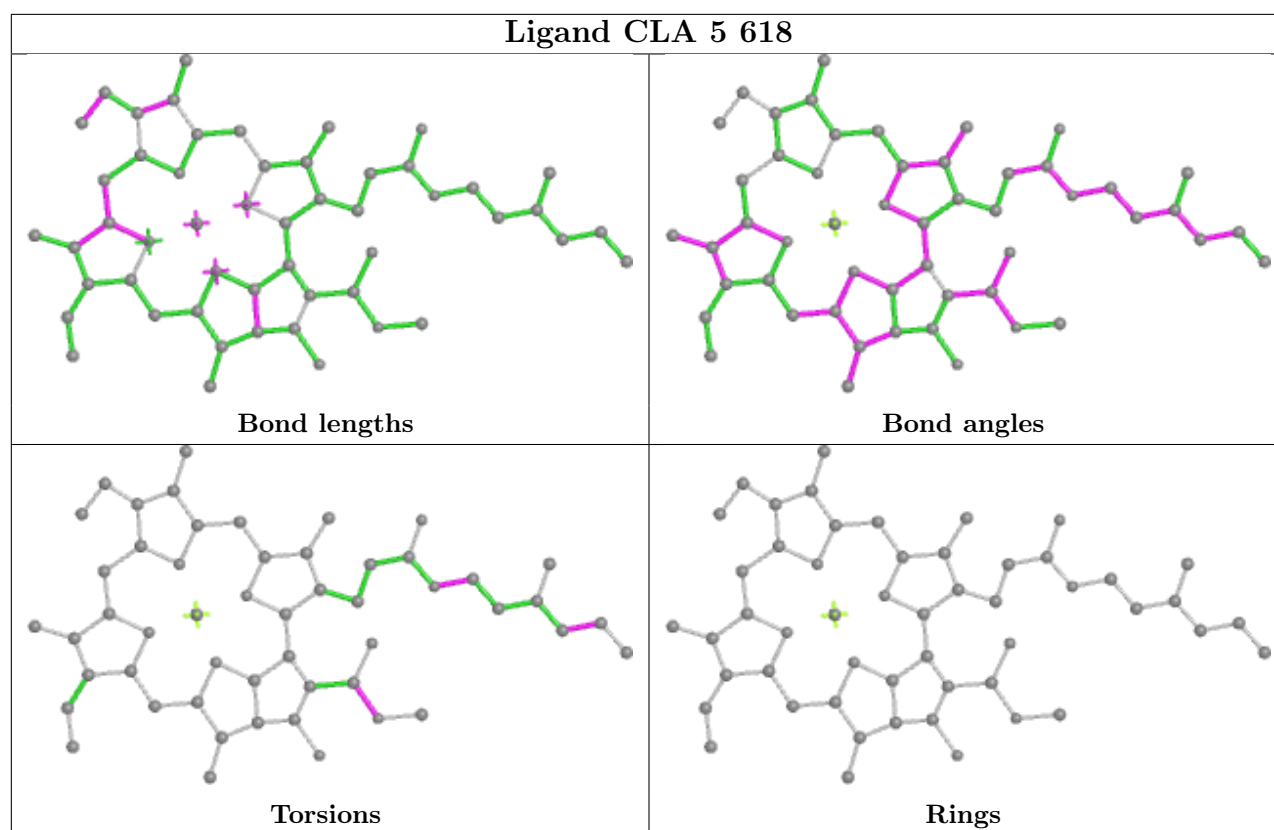
Ligand CLA B 1228



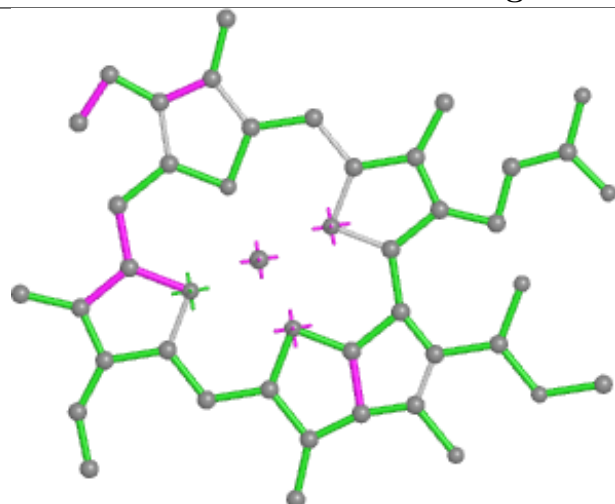
Ligand CLA 4 606



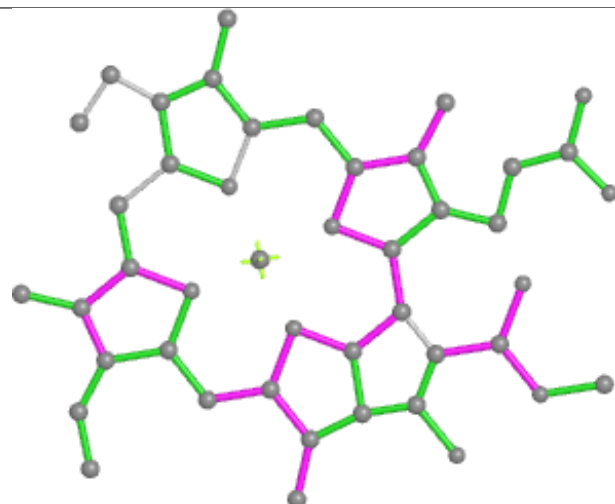




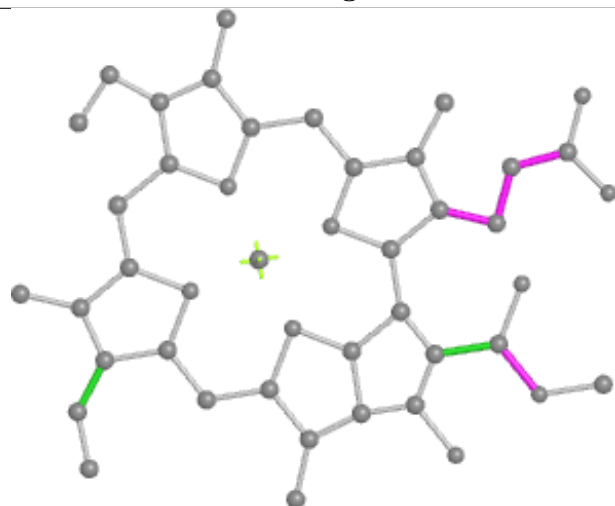
Ligand CLA G 1603



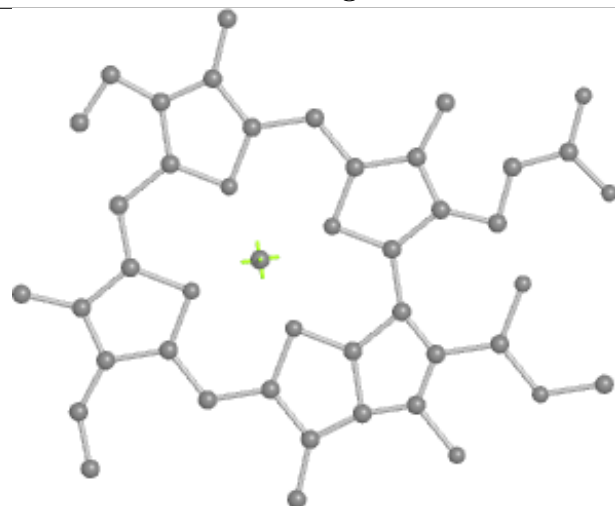
Bond lengths



Bond angles

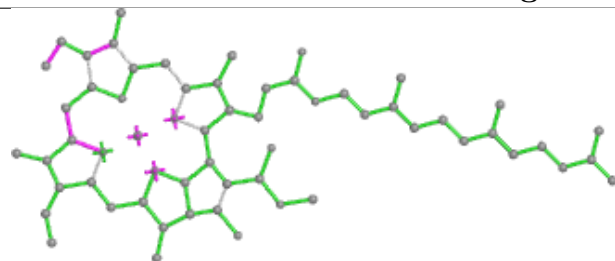


Torsions

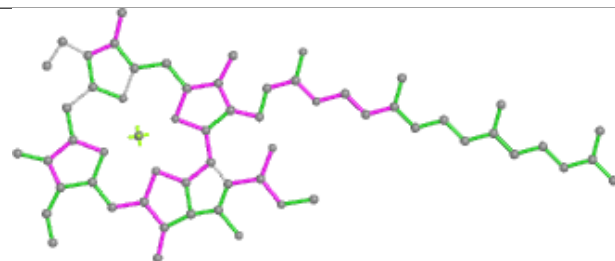


Rings

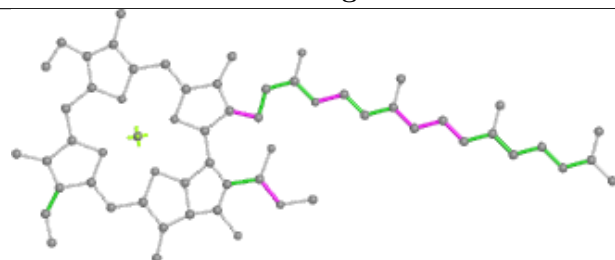
Ligand CLA 4 601



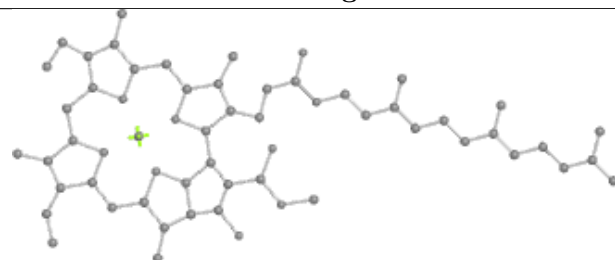
Bond lengths



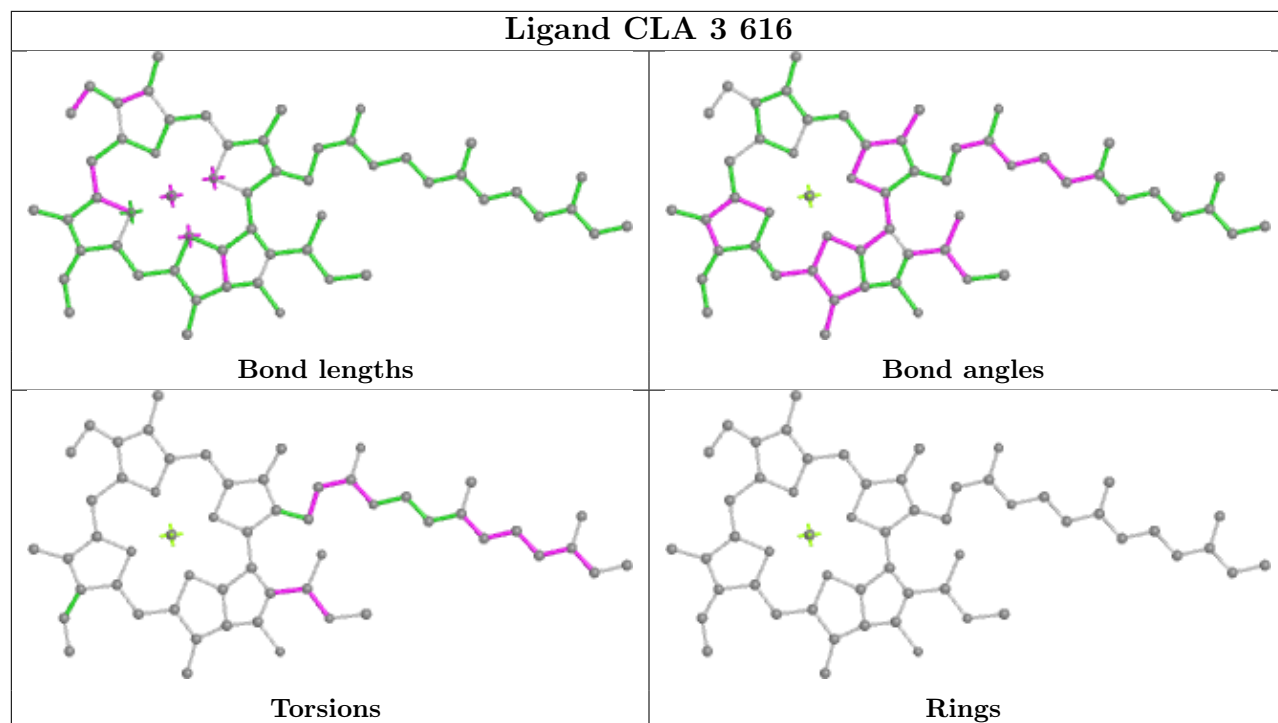
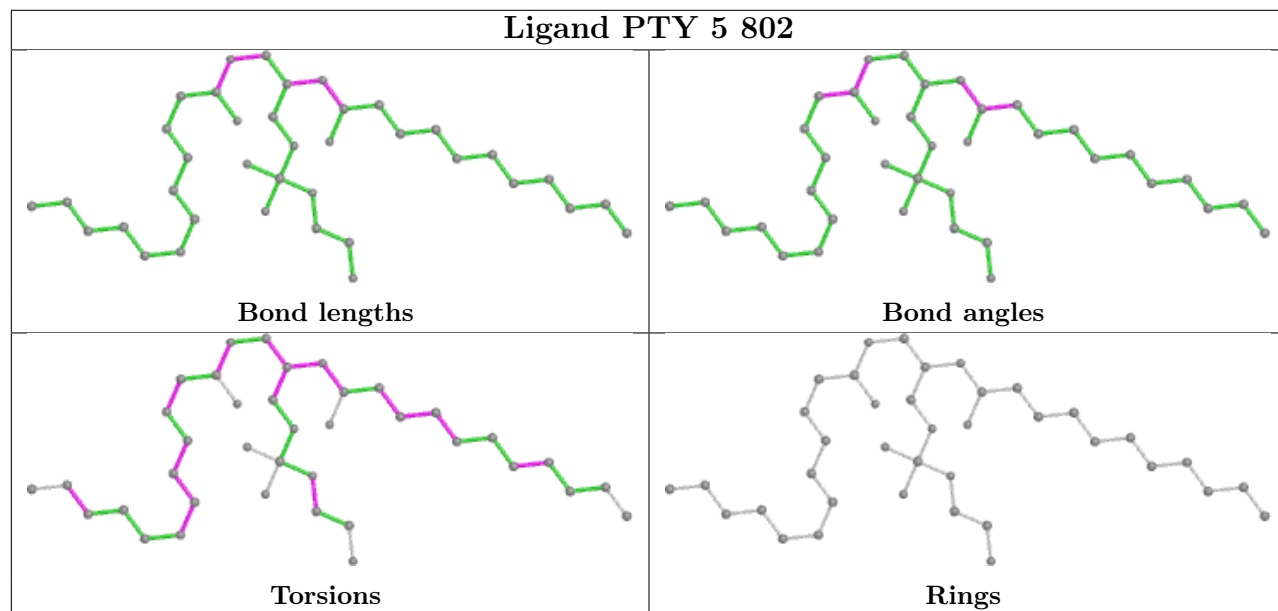
Bond angles

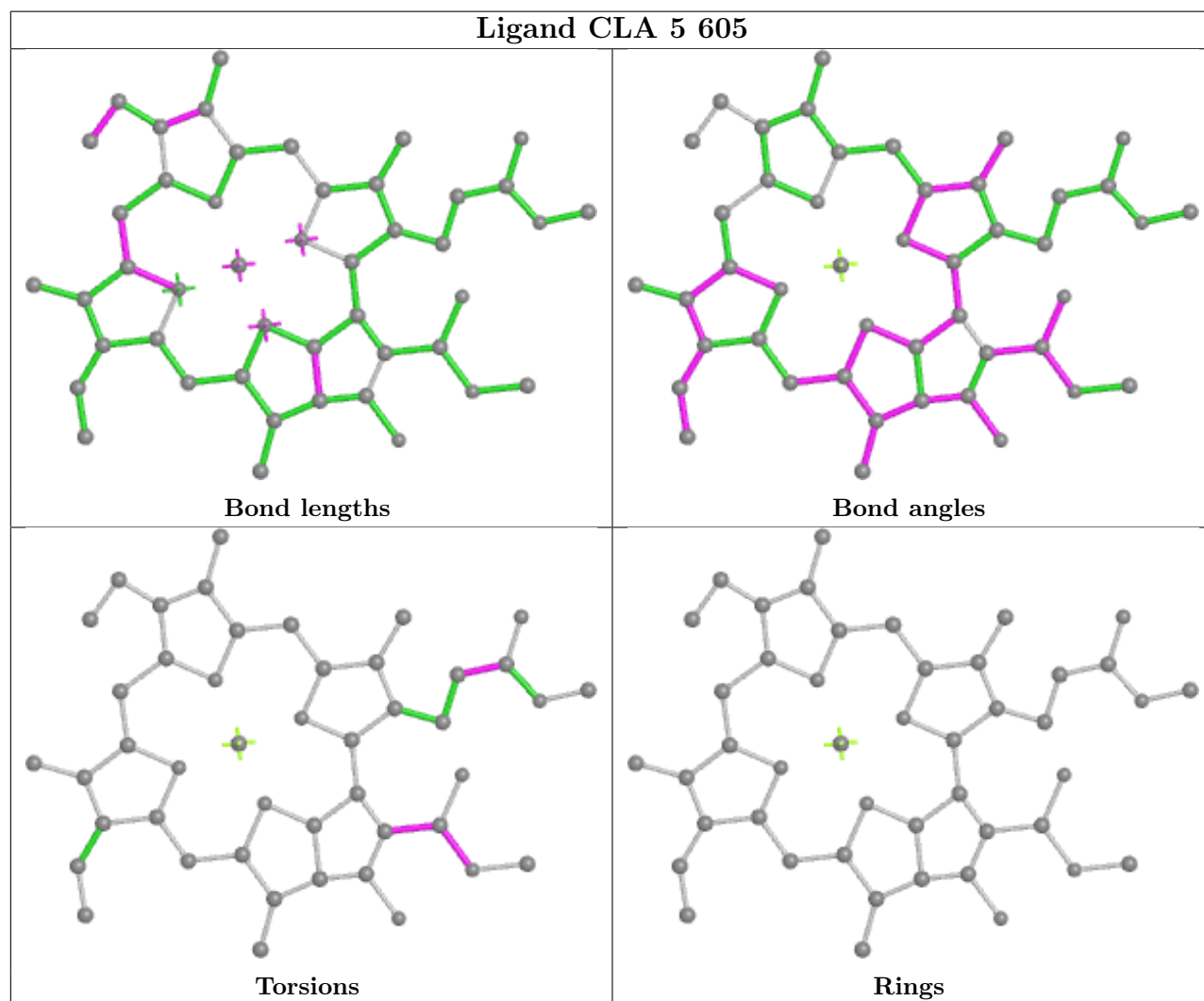
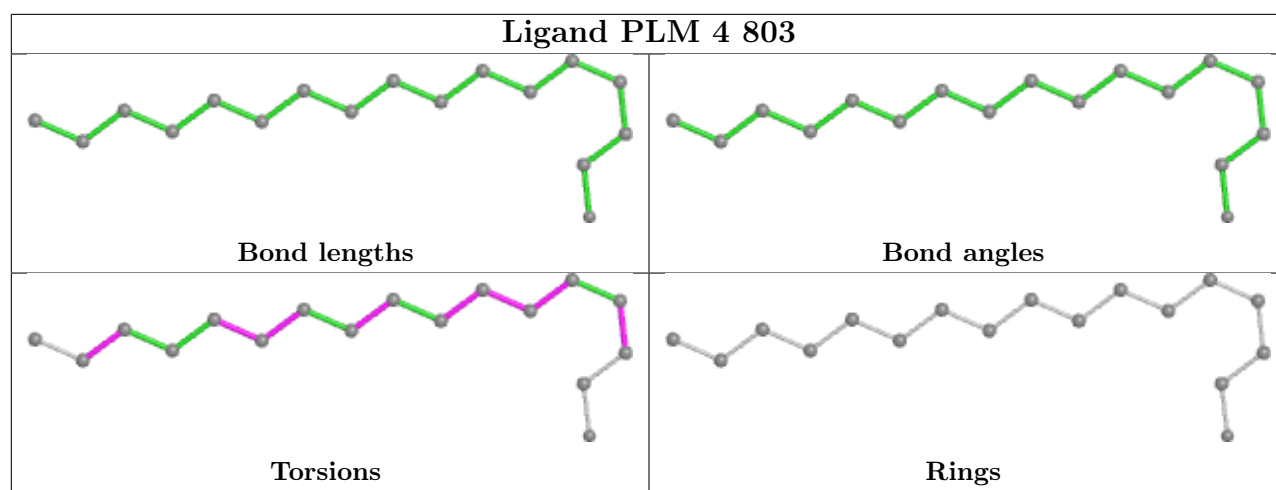


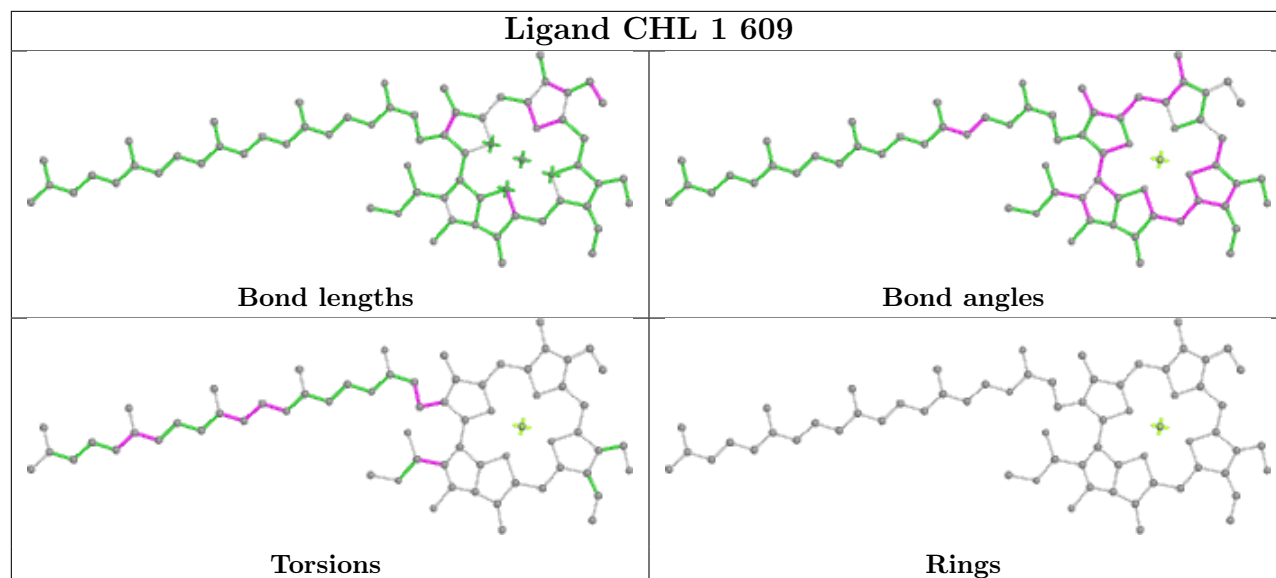
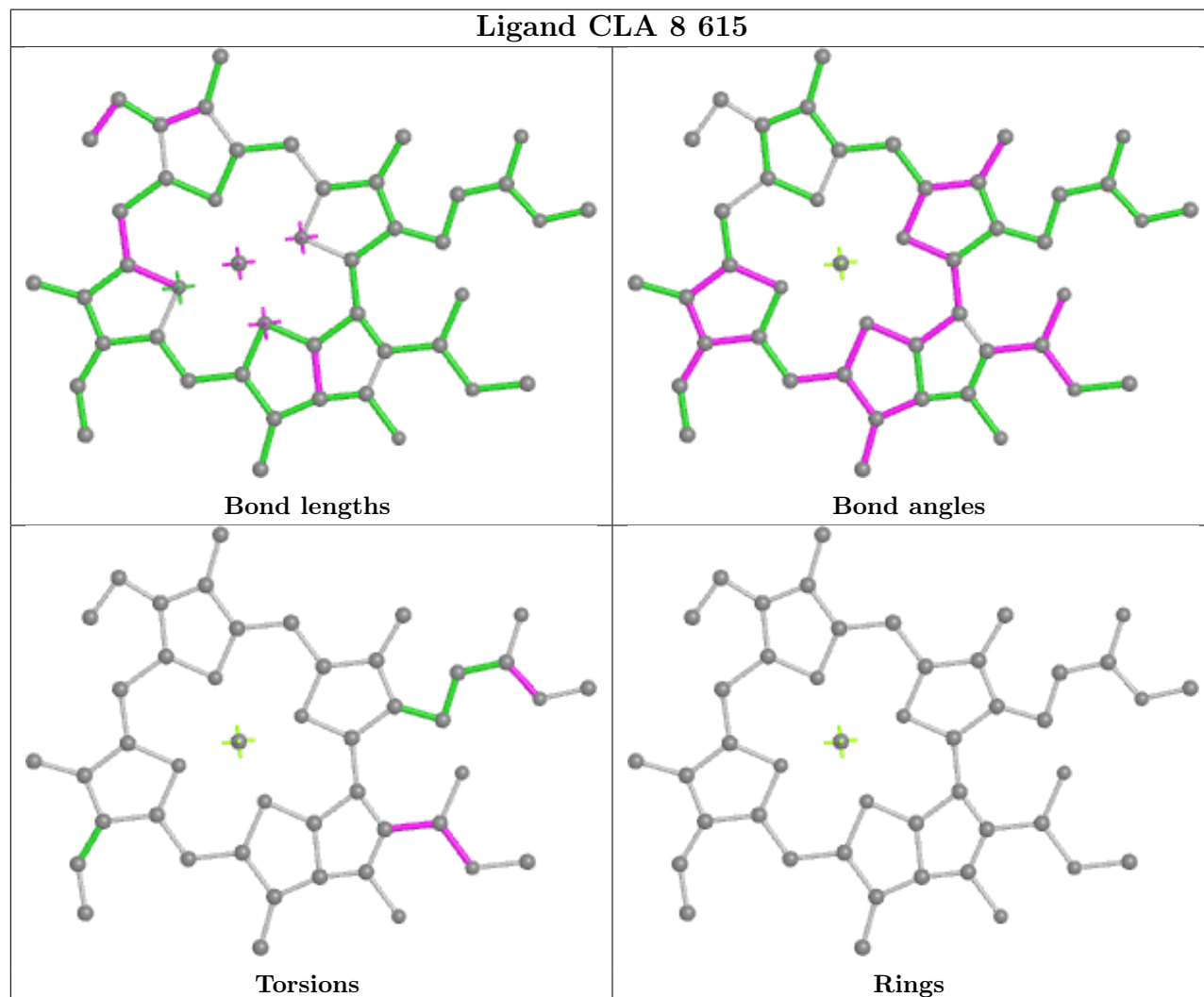
Torsions



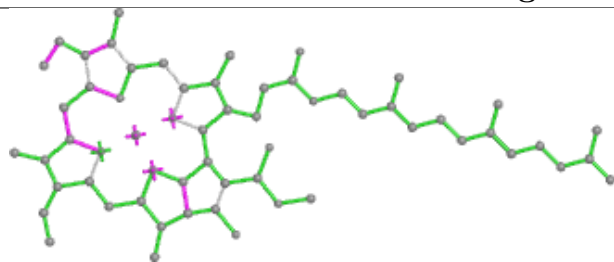
Rings

Ligand CLA 3 616**Ligand PTY 5 802**

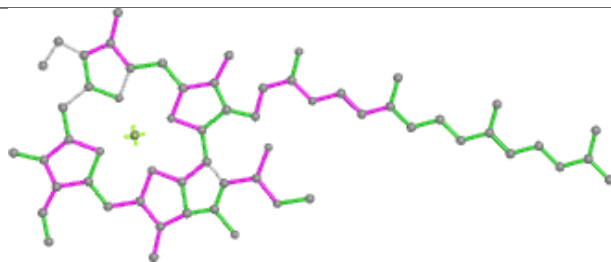


Ligand CHL 1 609**Ligand CLA 8 615**

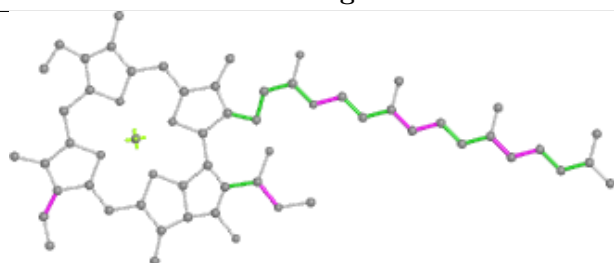
Ligand CLA 7 611



Bond lengths



Bond angles

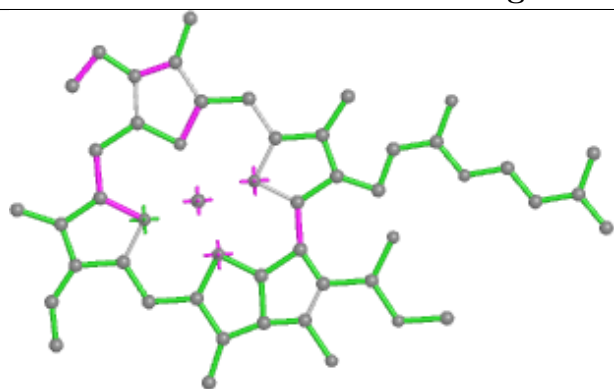


Torsions

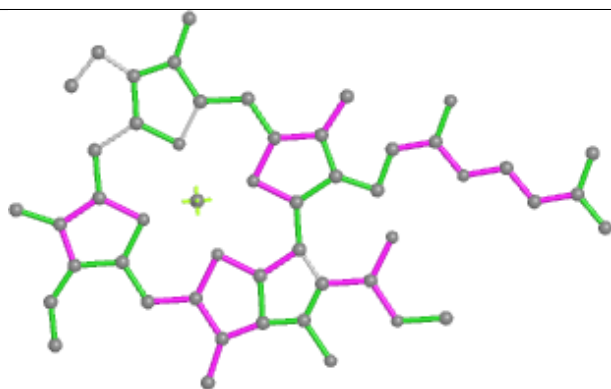


Rings

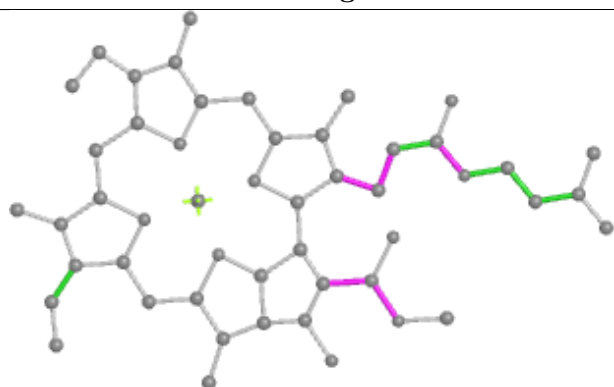
Ligand CLA L 1501



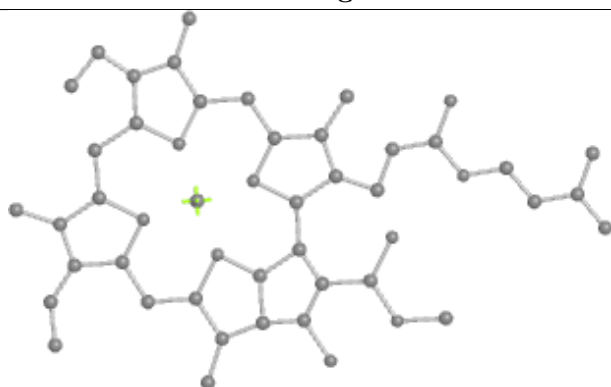
Bond lengths



Bond angles

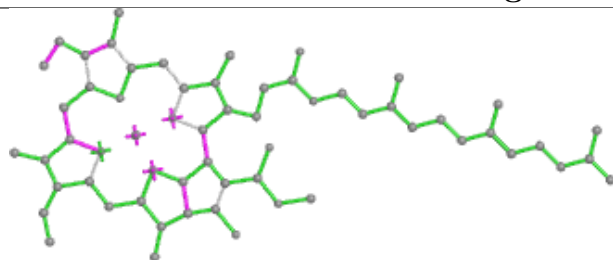


Torsions

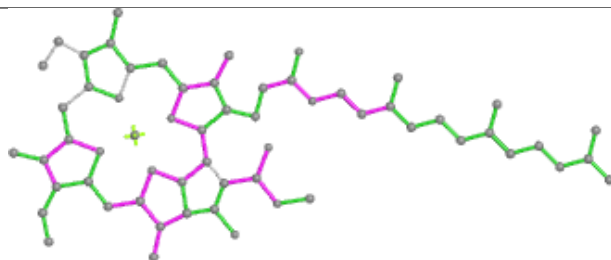


Rings

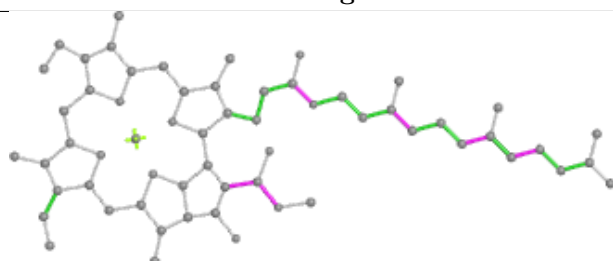
Ligand CLA A 1115



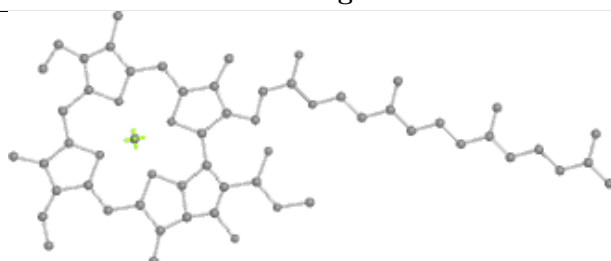
Bond lengths



Bond angles

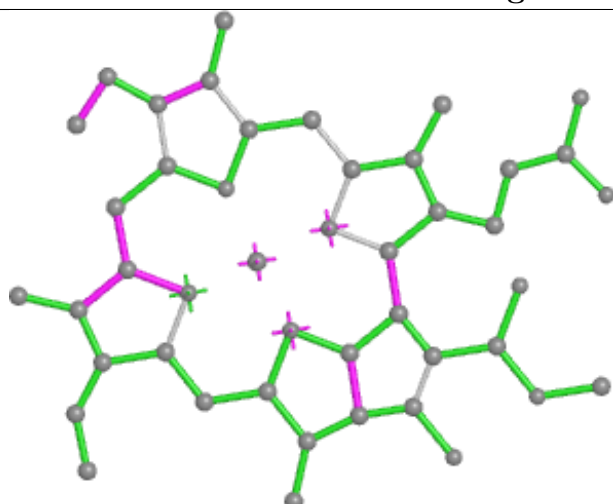


Torsions

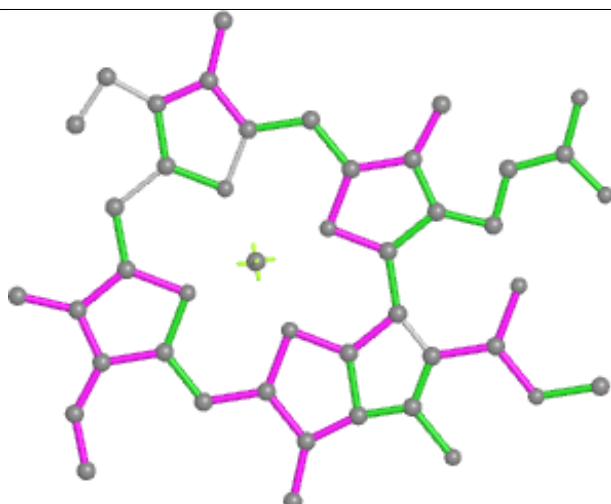


Rings

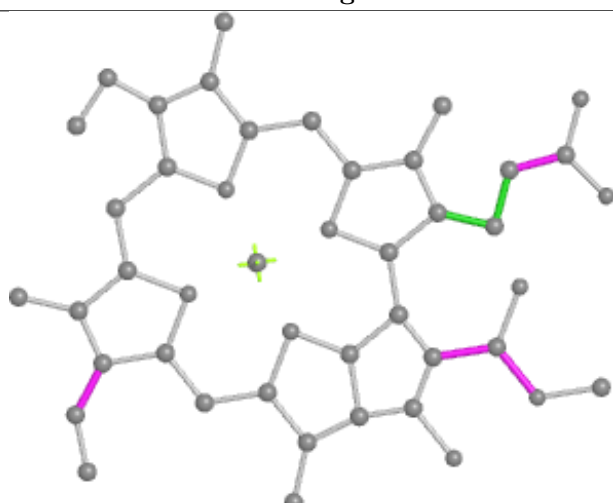
Ligand CLA L 1503



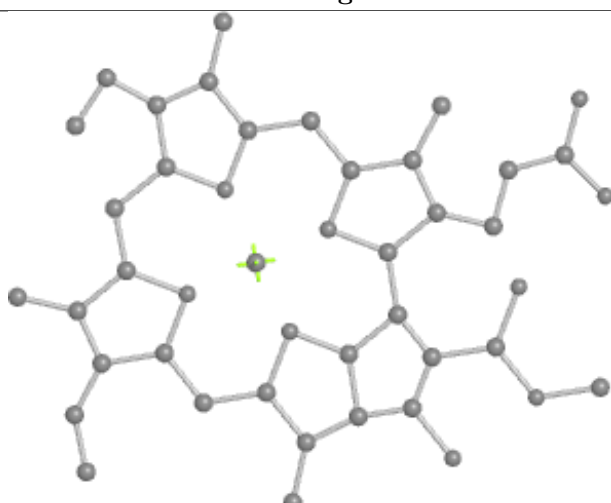
Bond lengths



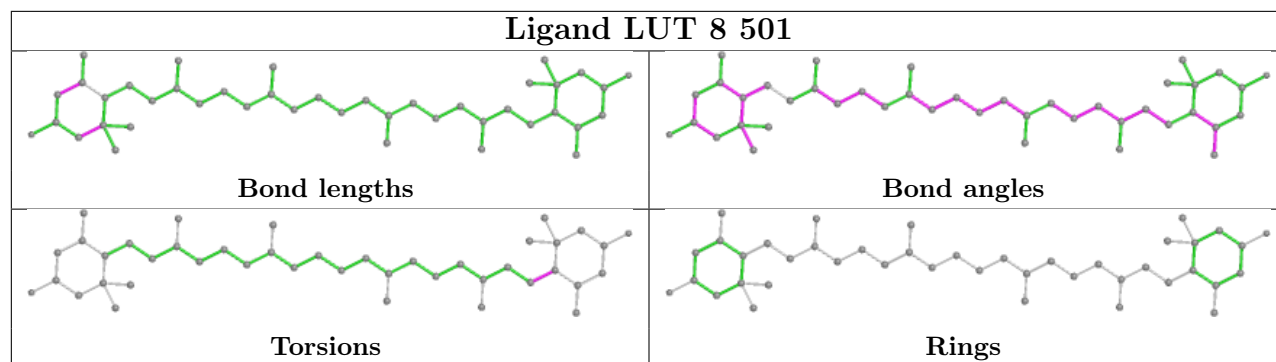
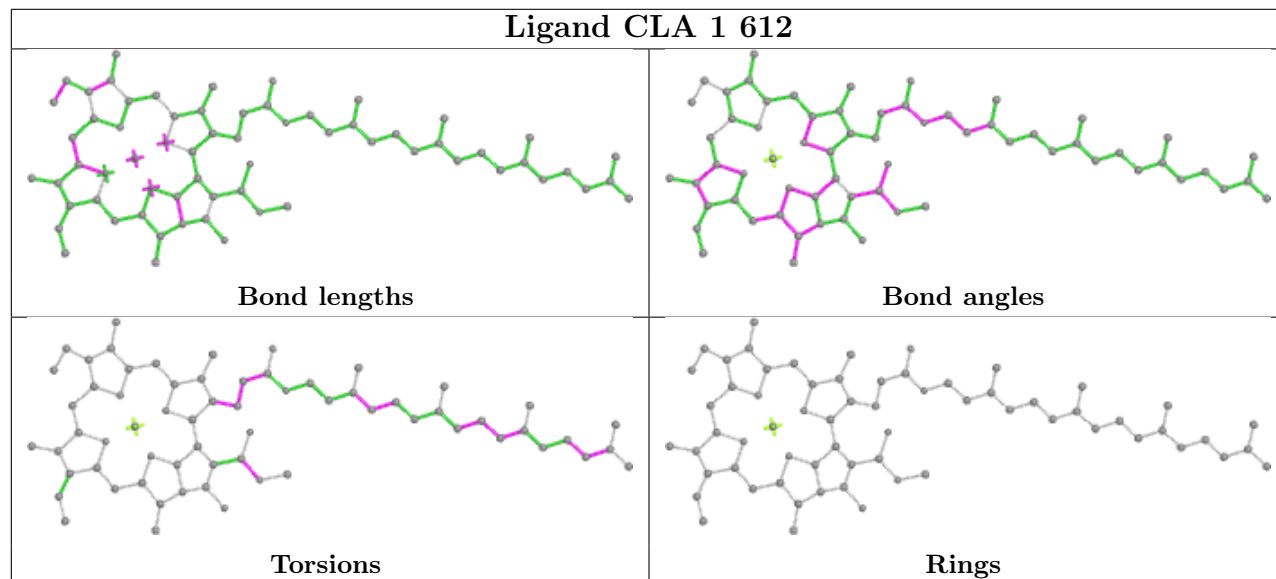
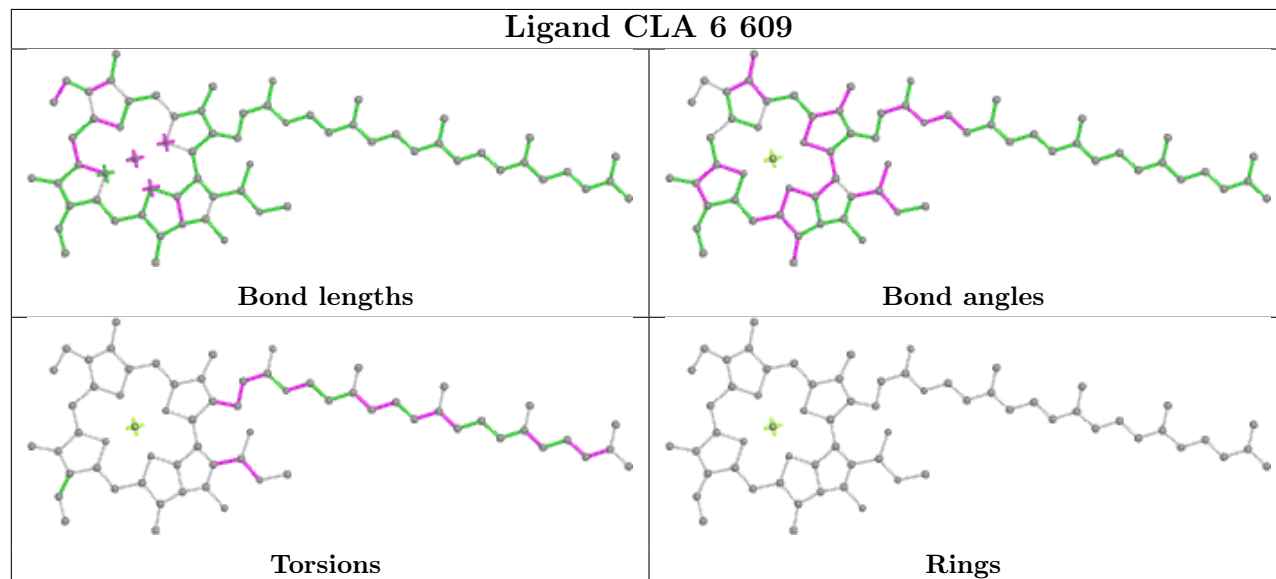
Bond angles

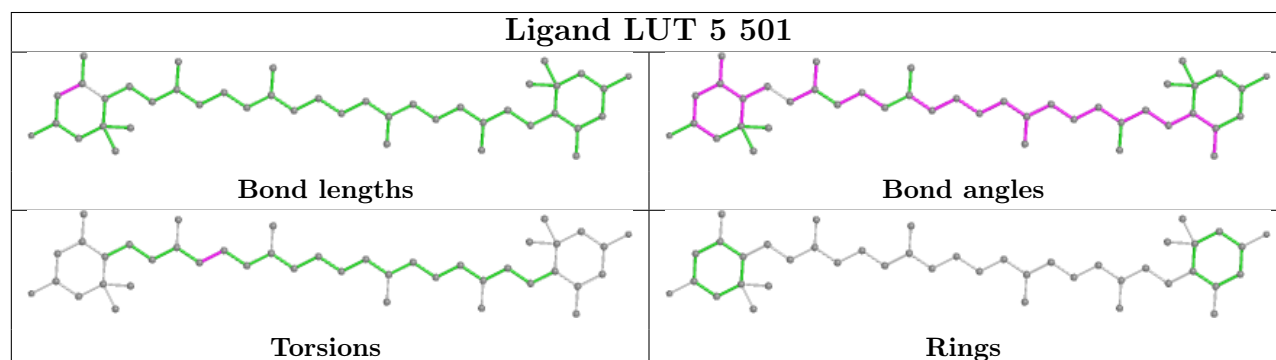
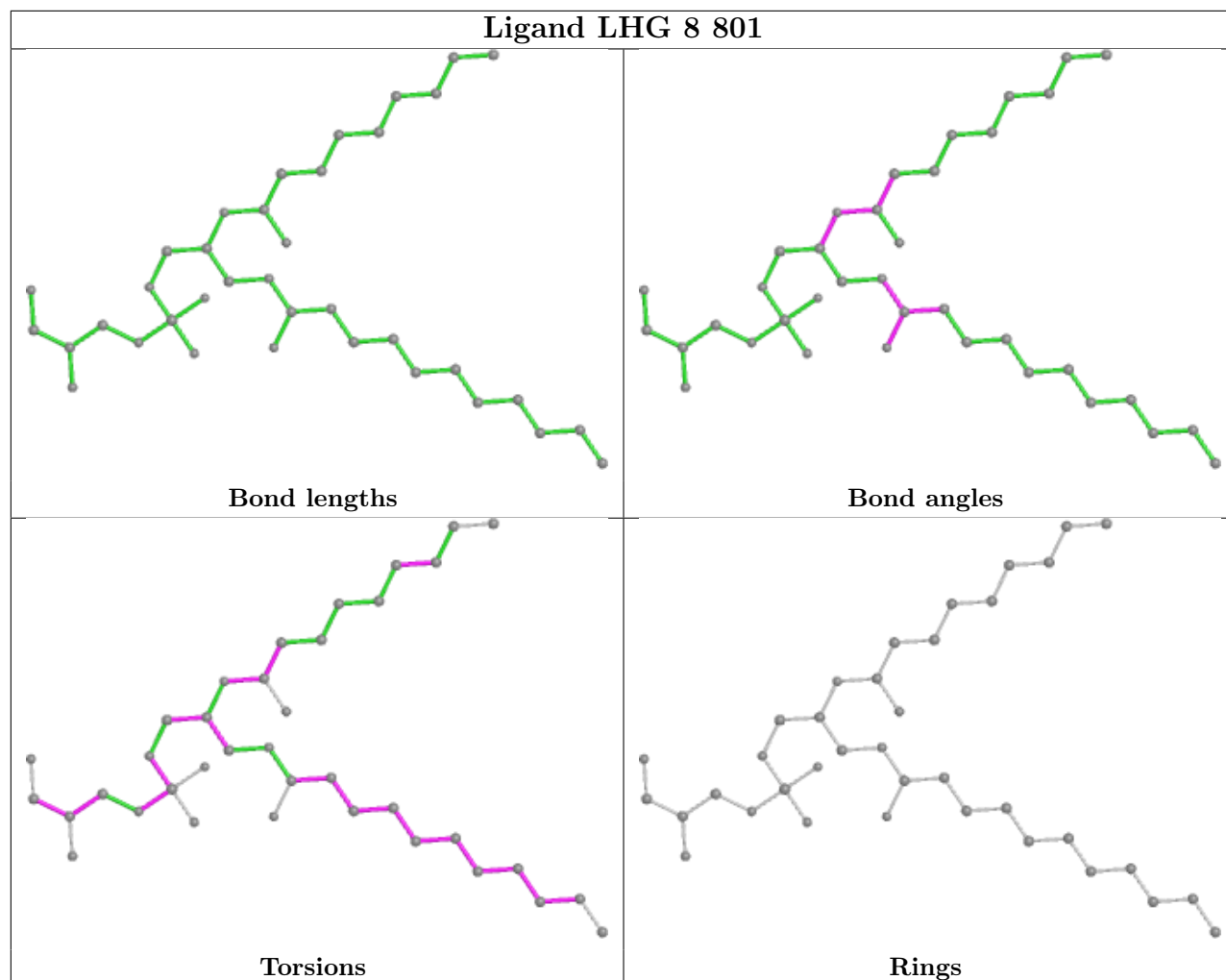
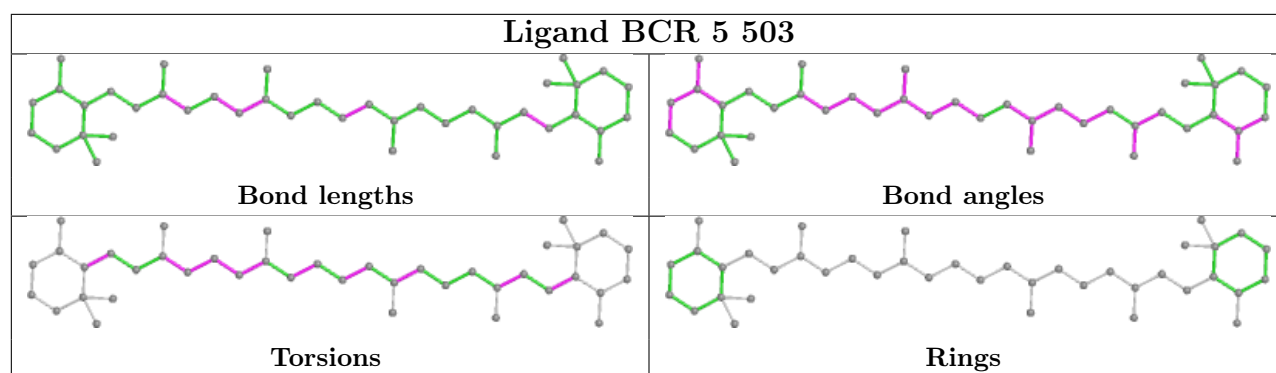


Torsions

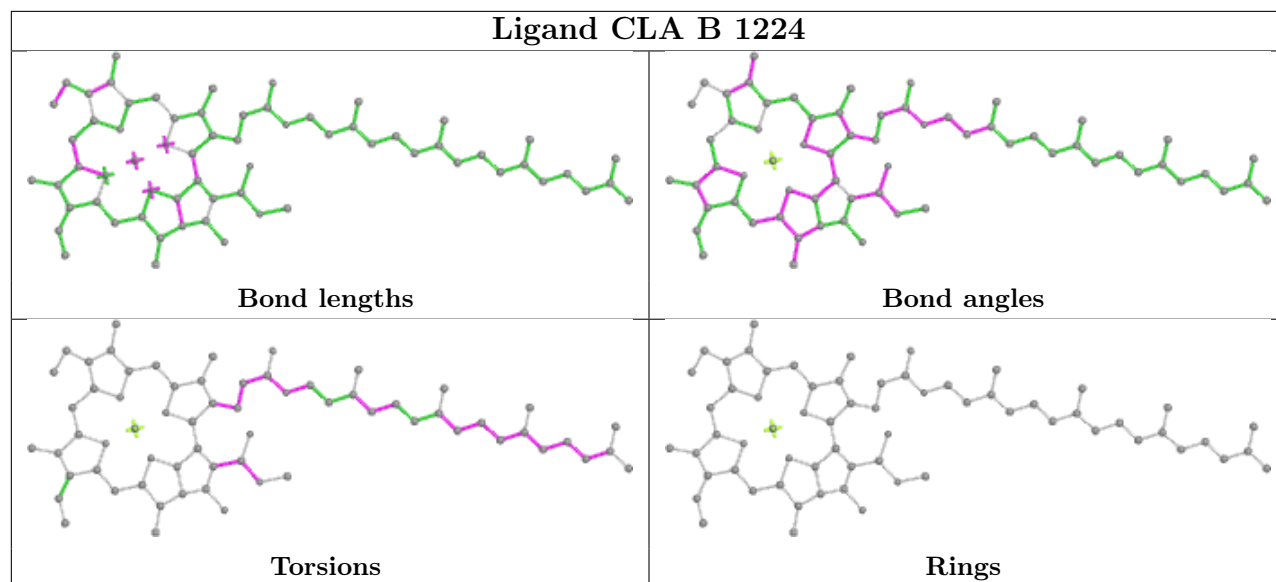


Rings

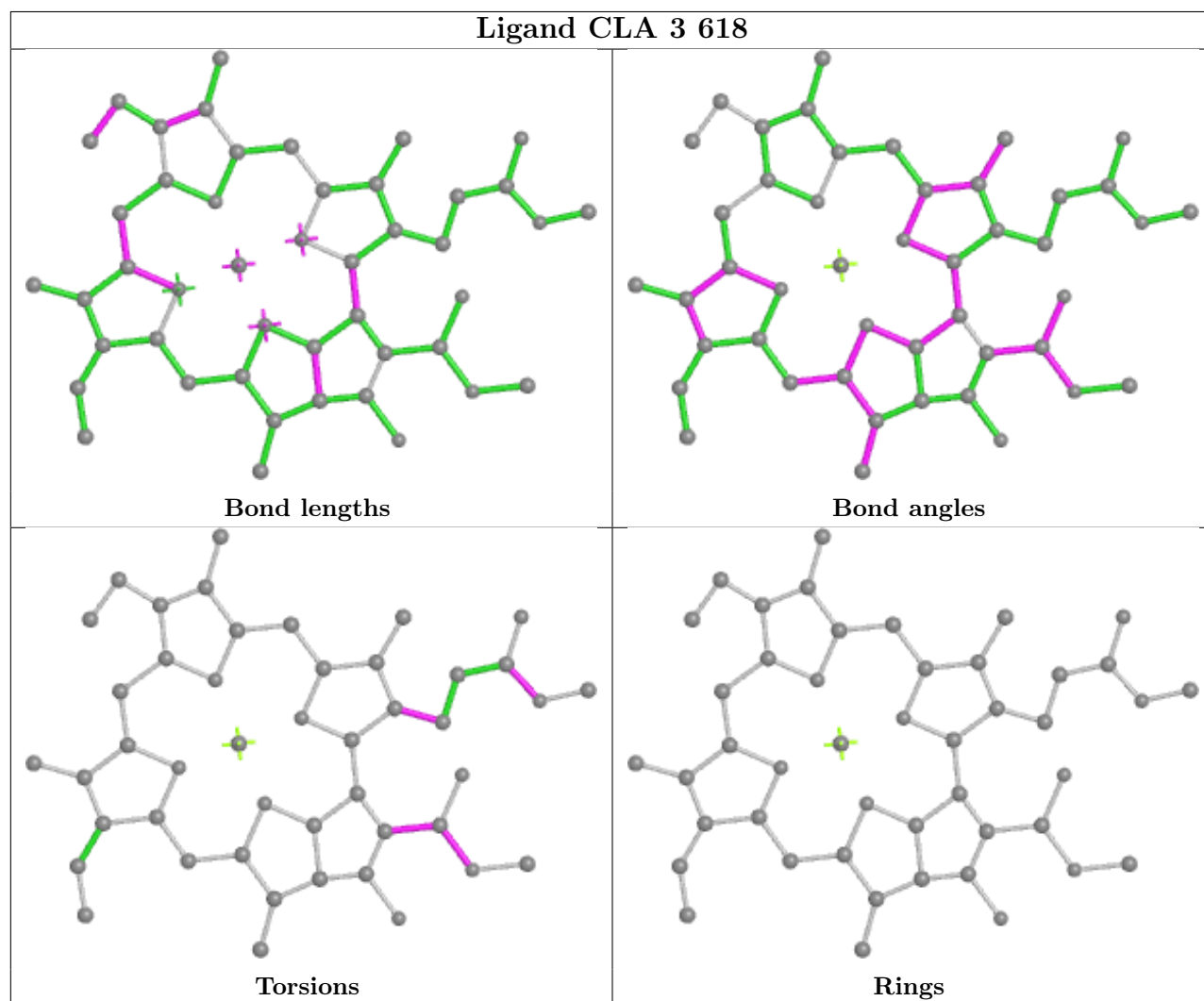
Ligand LUT 8 501**Ligand CLA 1 612****Ligand CLA 6 609**

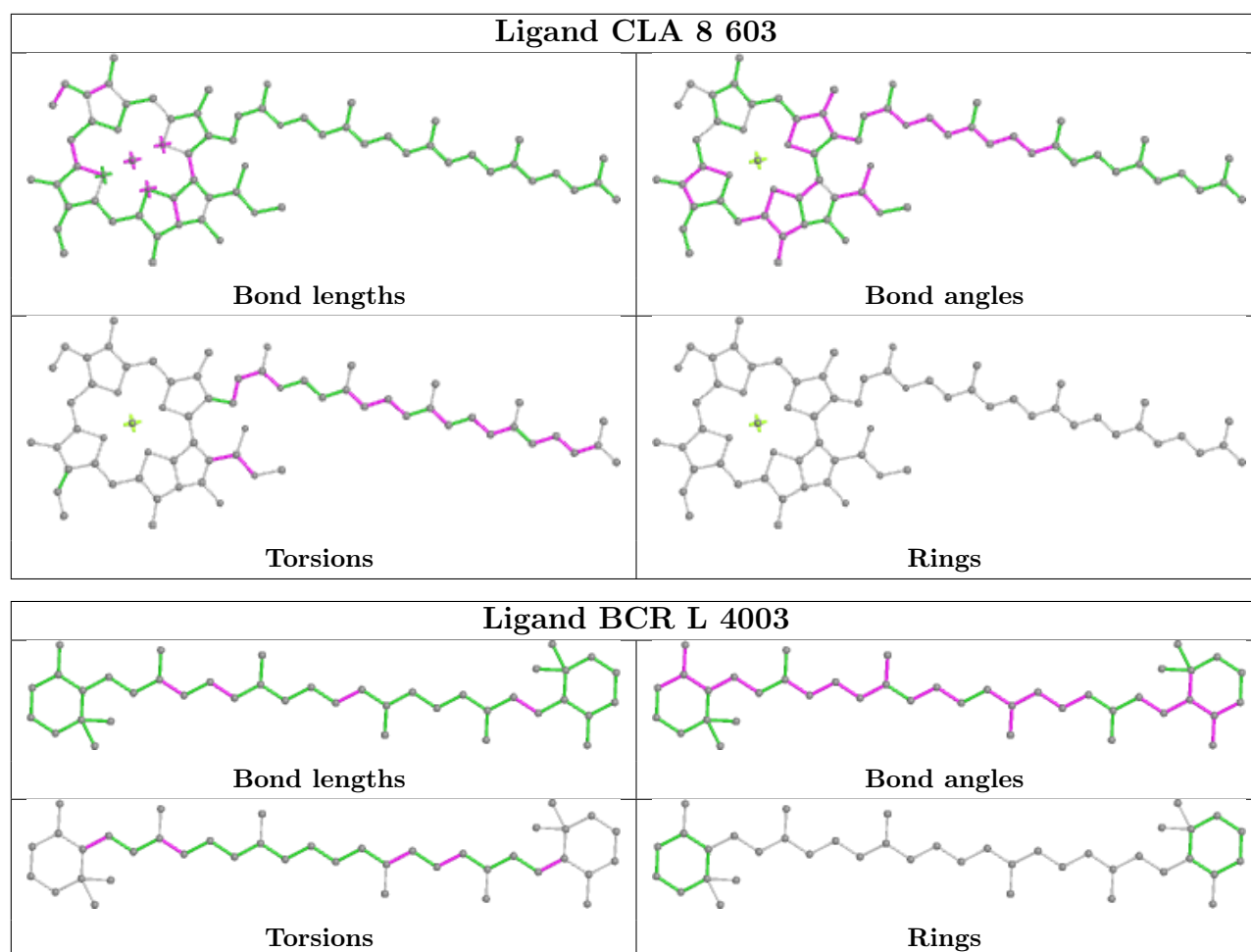


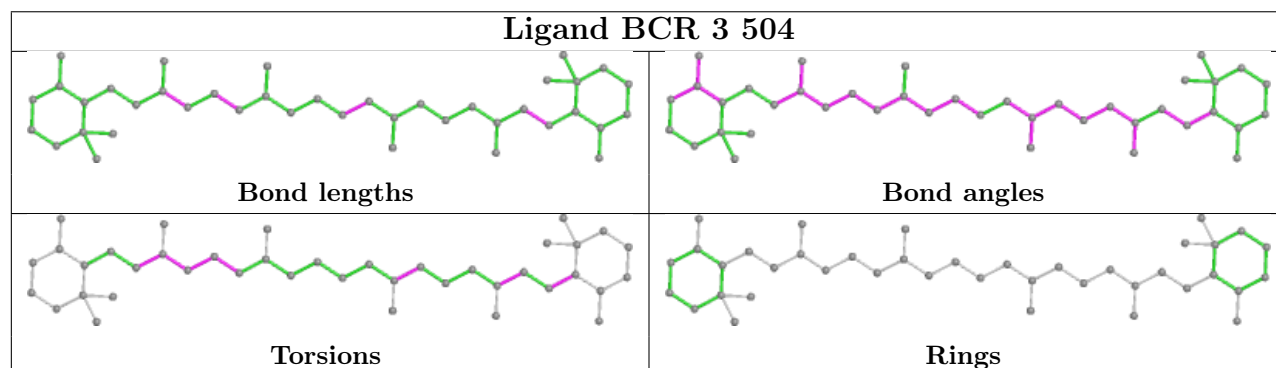
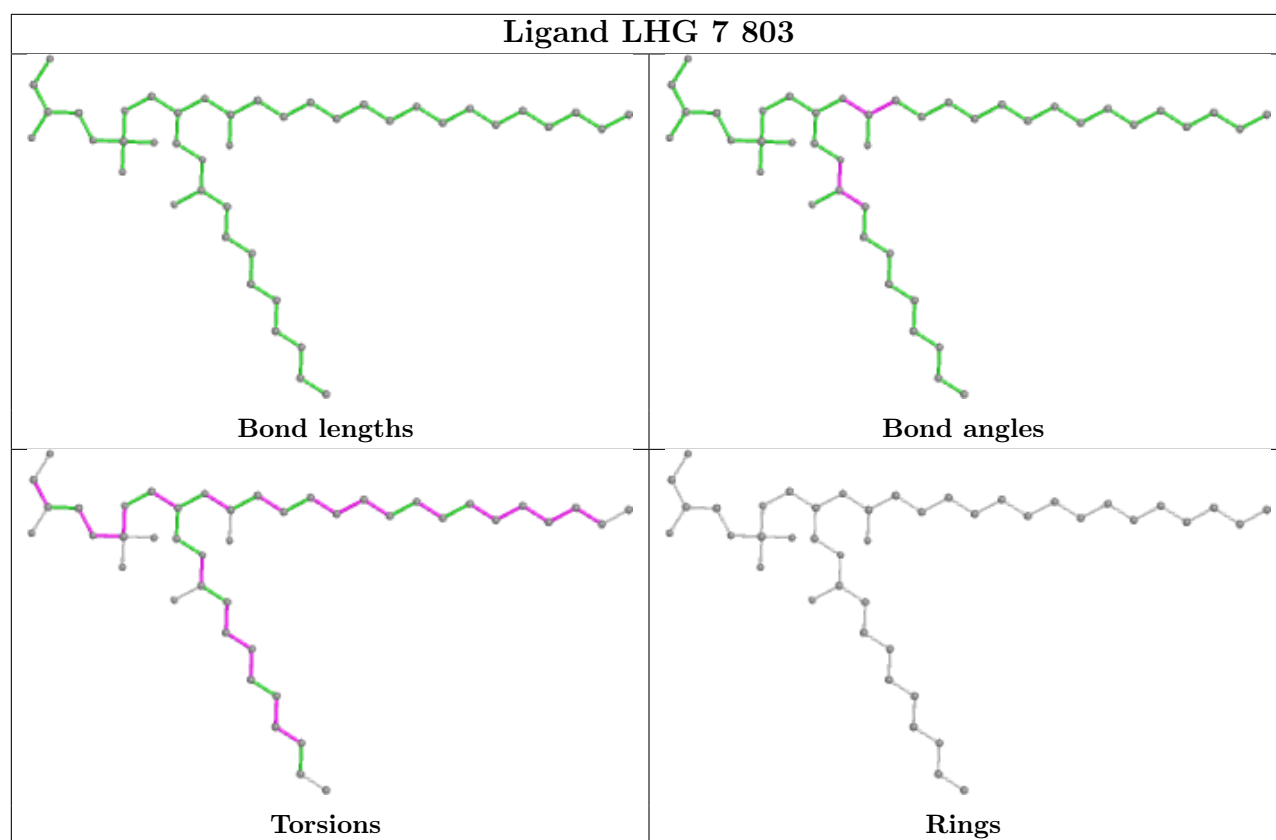
Ligand CLA B 1224



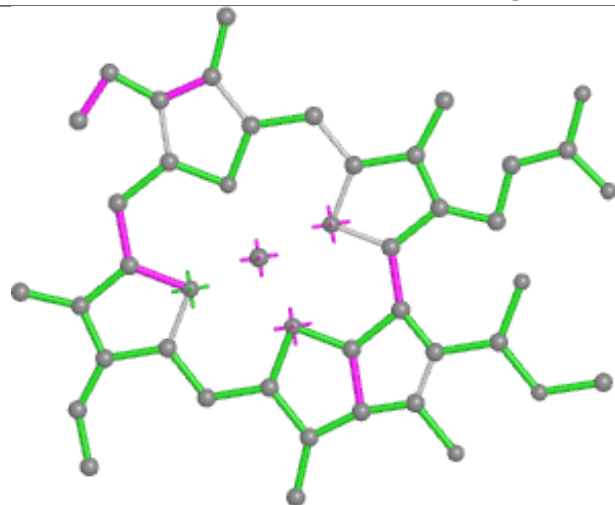
Ligand CLA 3 618



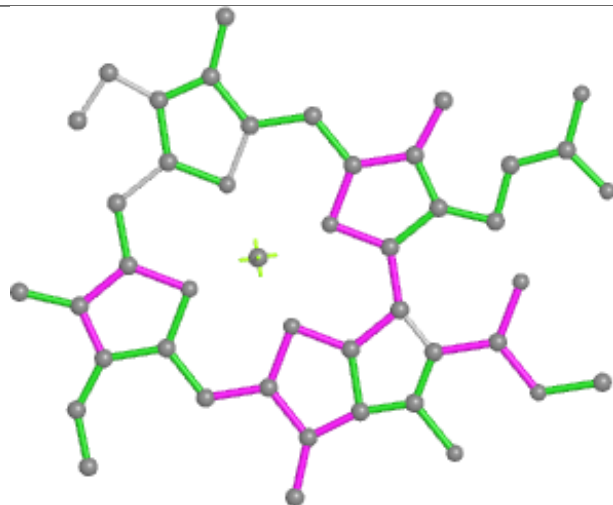




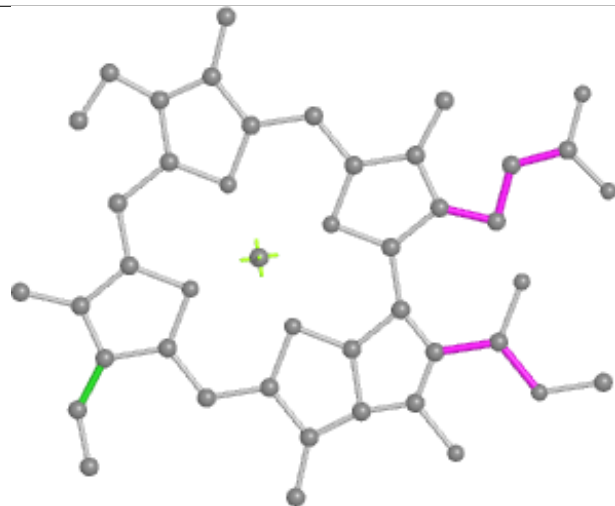
Ligand CLA A 1141



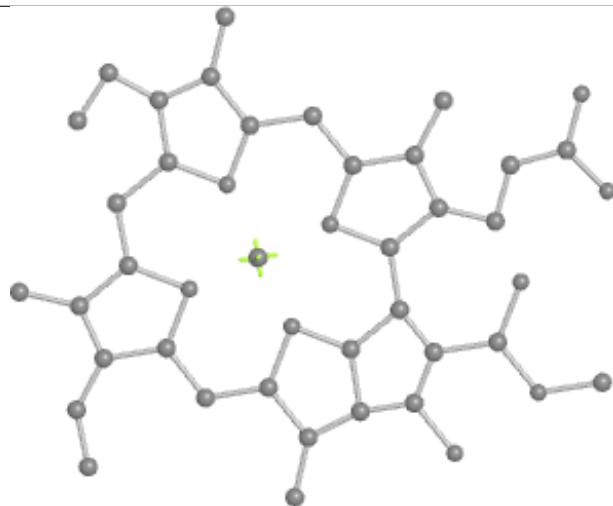
Bond lengths



Bond angles

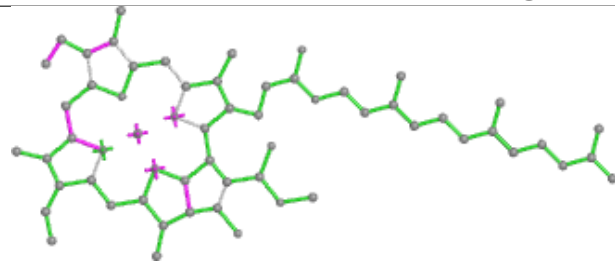


Torsions

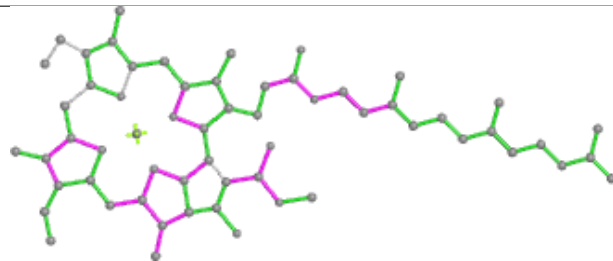


Rings

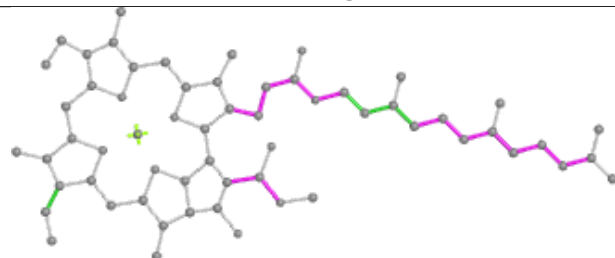
Ligand CLA 8 609



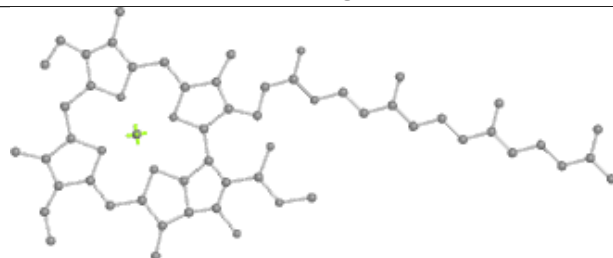
Bond lengths



Bond angles

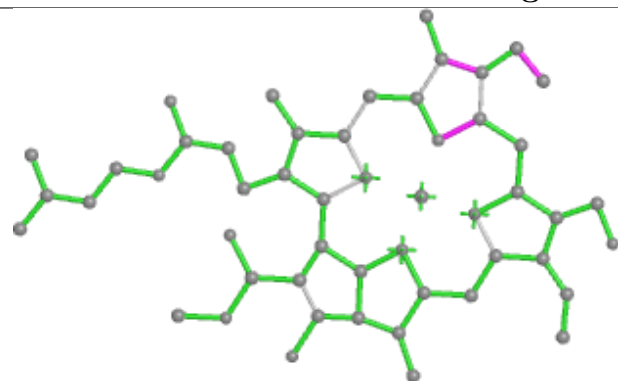


Torsions

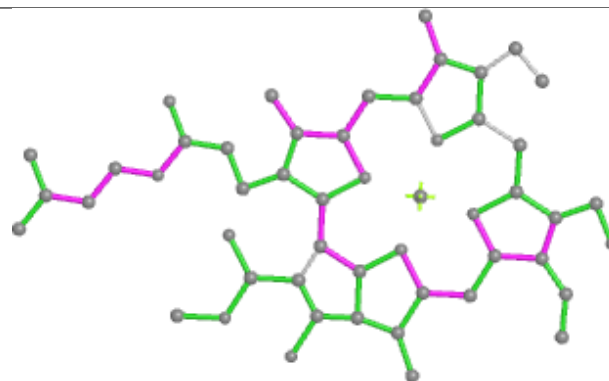


Rings

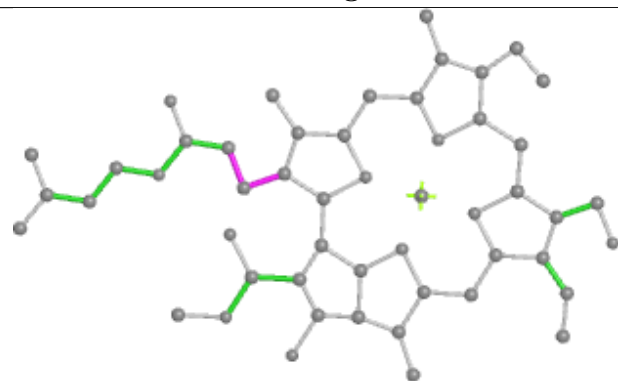
Ligand CHL 6 611



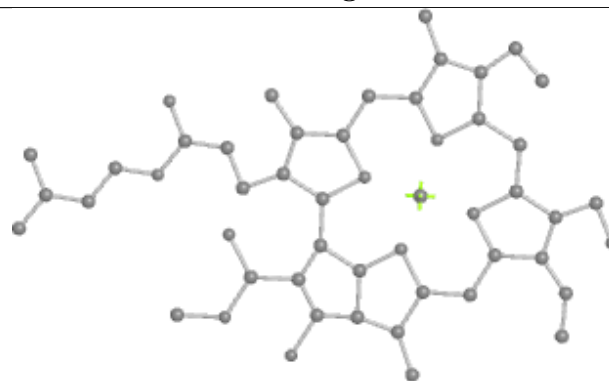
Bond lengths



Bond angles

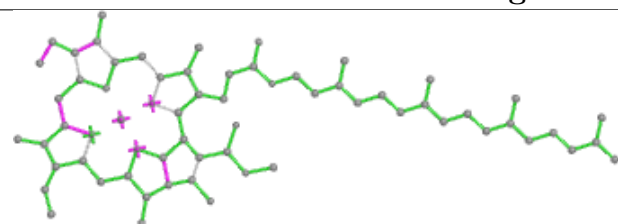


Torsions

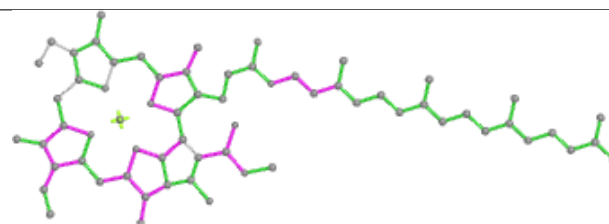


Rings

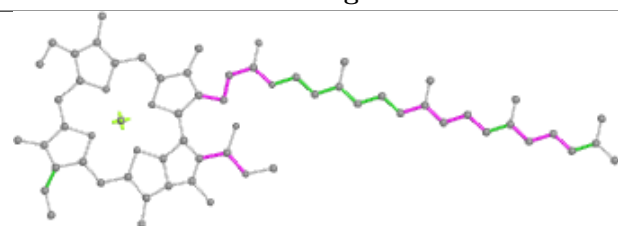
Ligand CLA A 1106



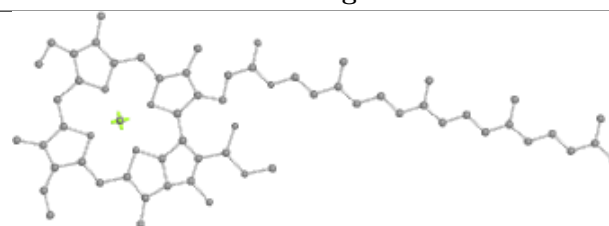
Bond lengths



Bond angles

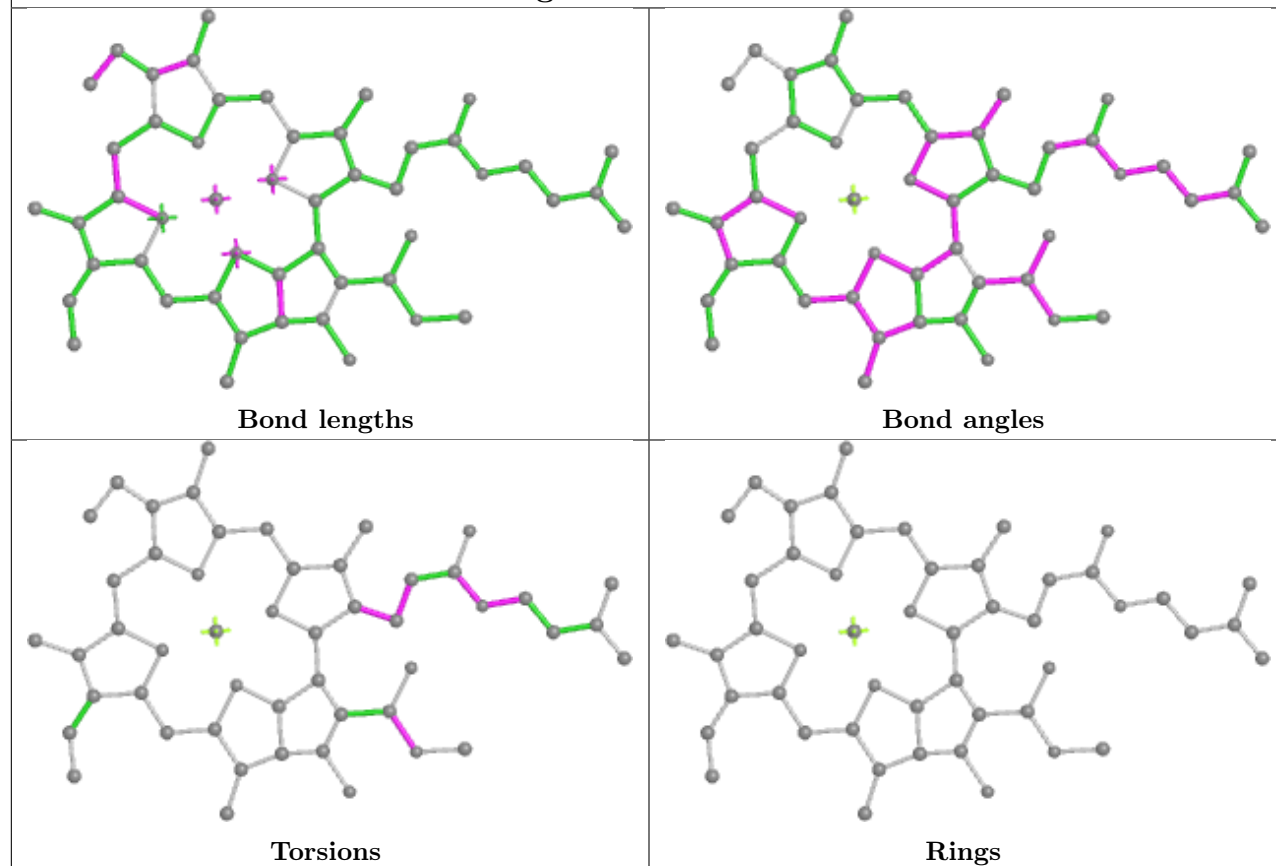


Torsions

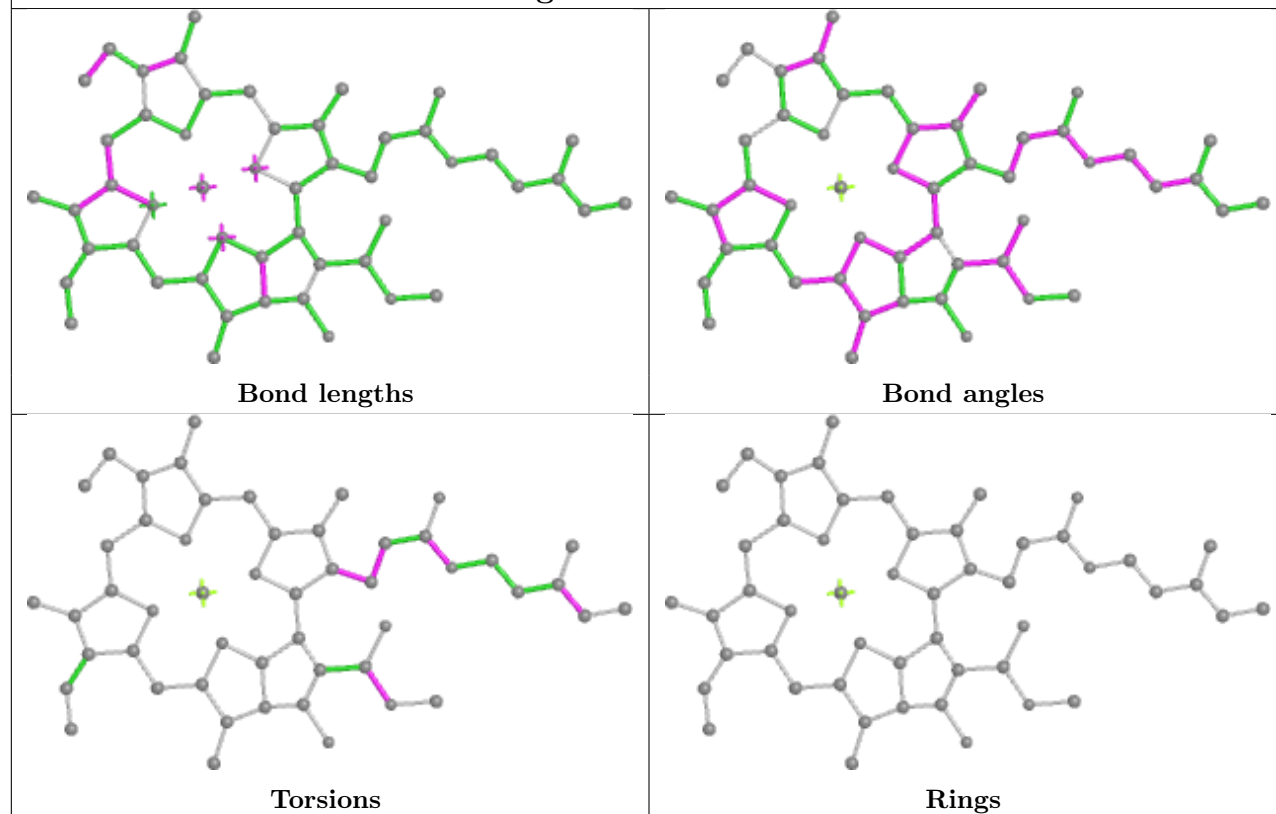


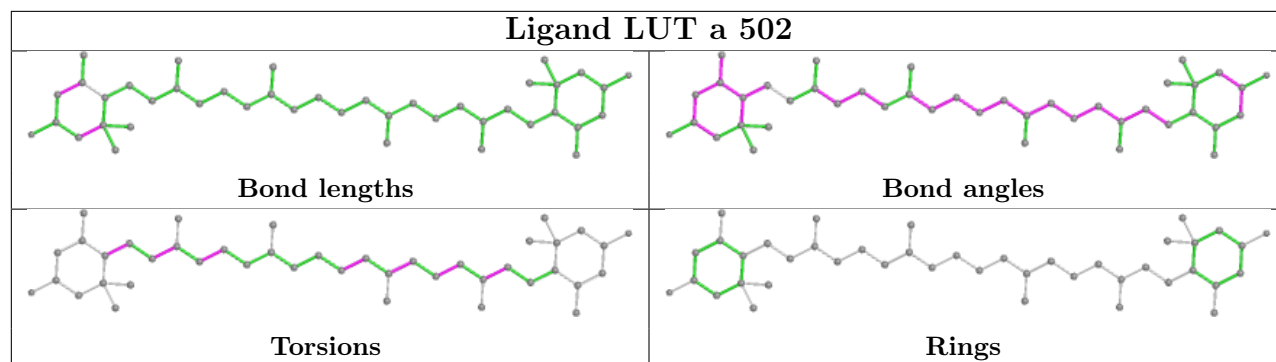
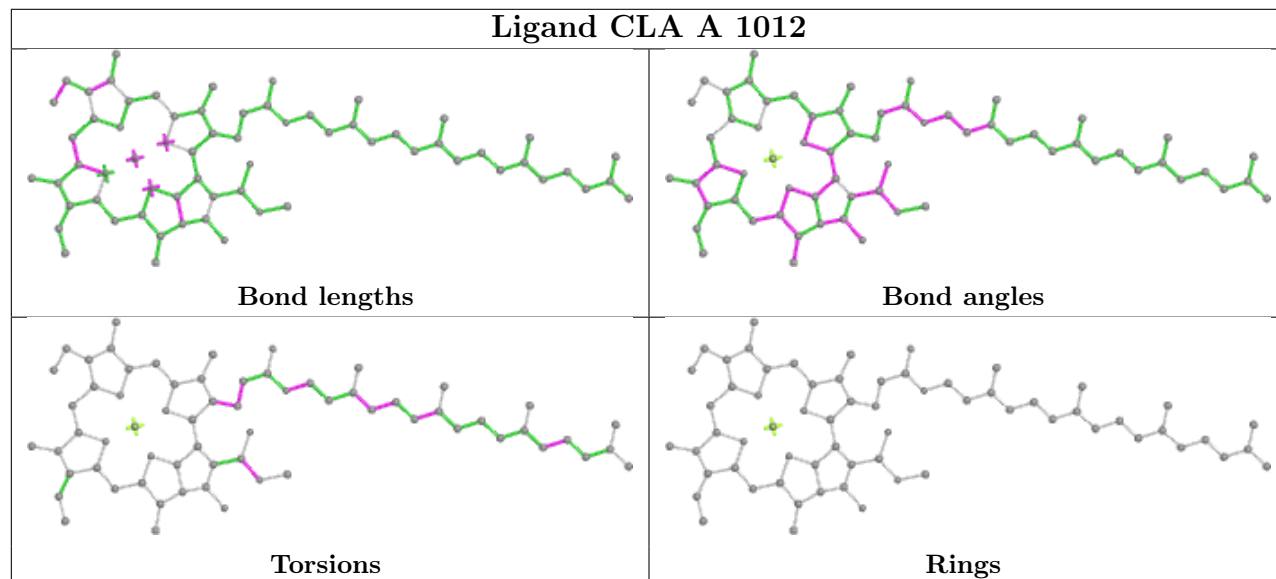
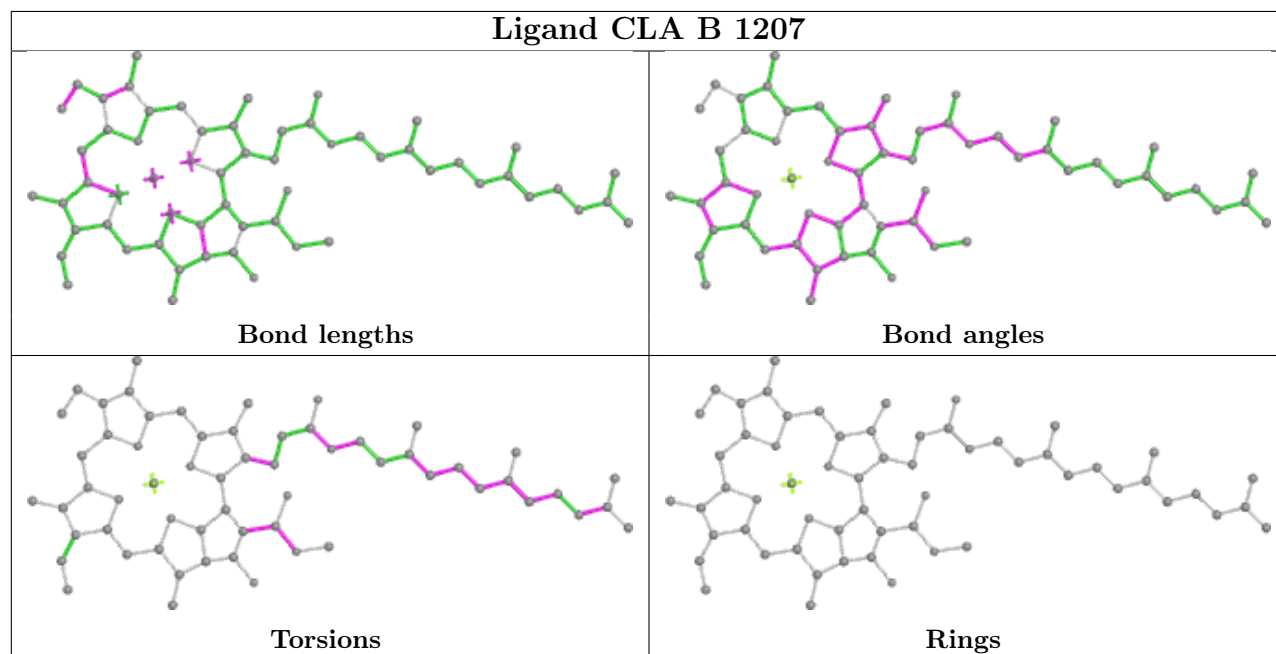
Rings

Ligand CLA a 611

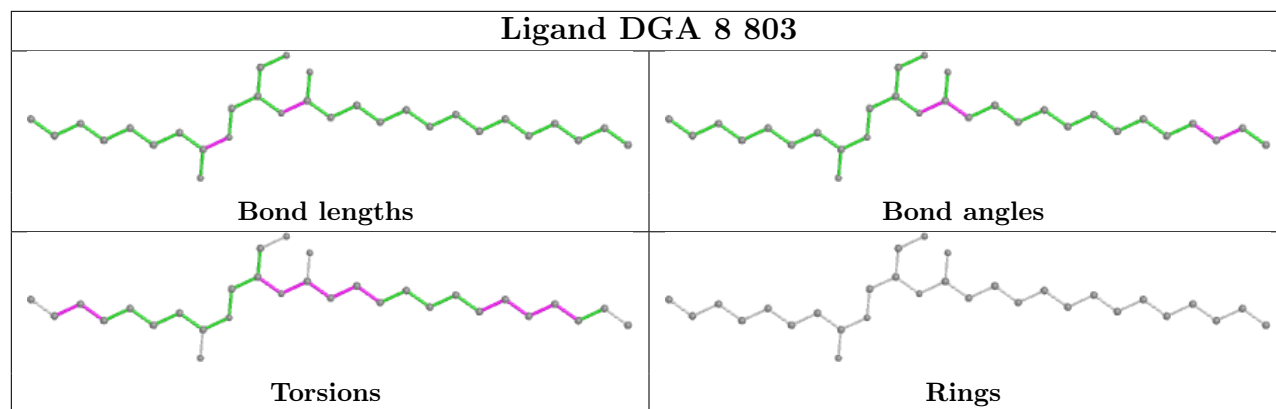


Ligand CLA 5 609

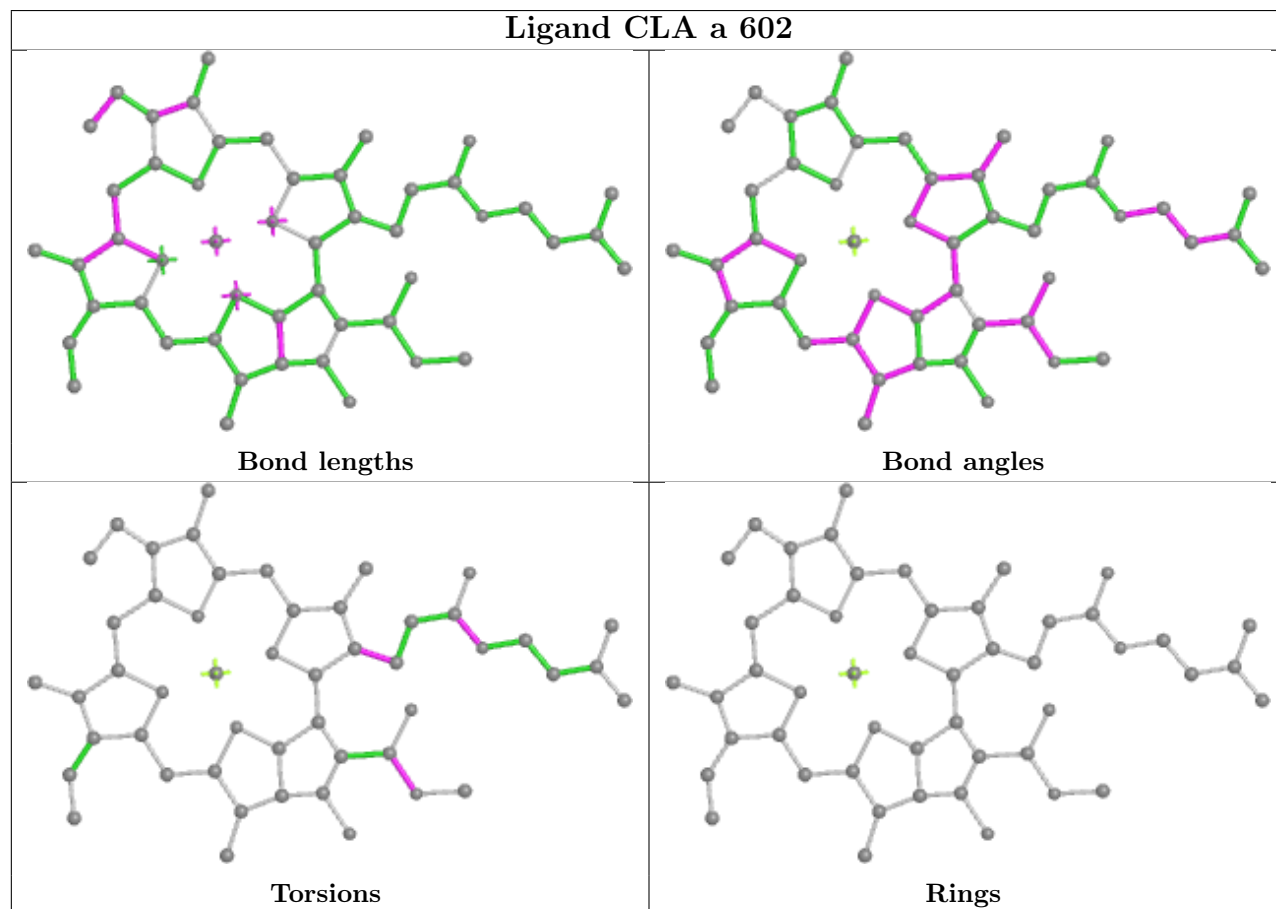


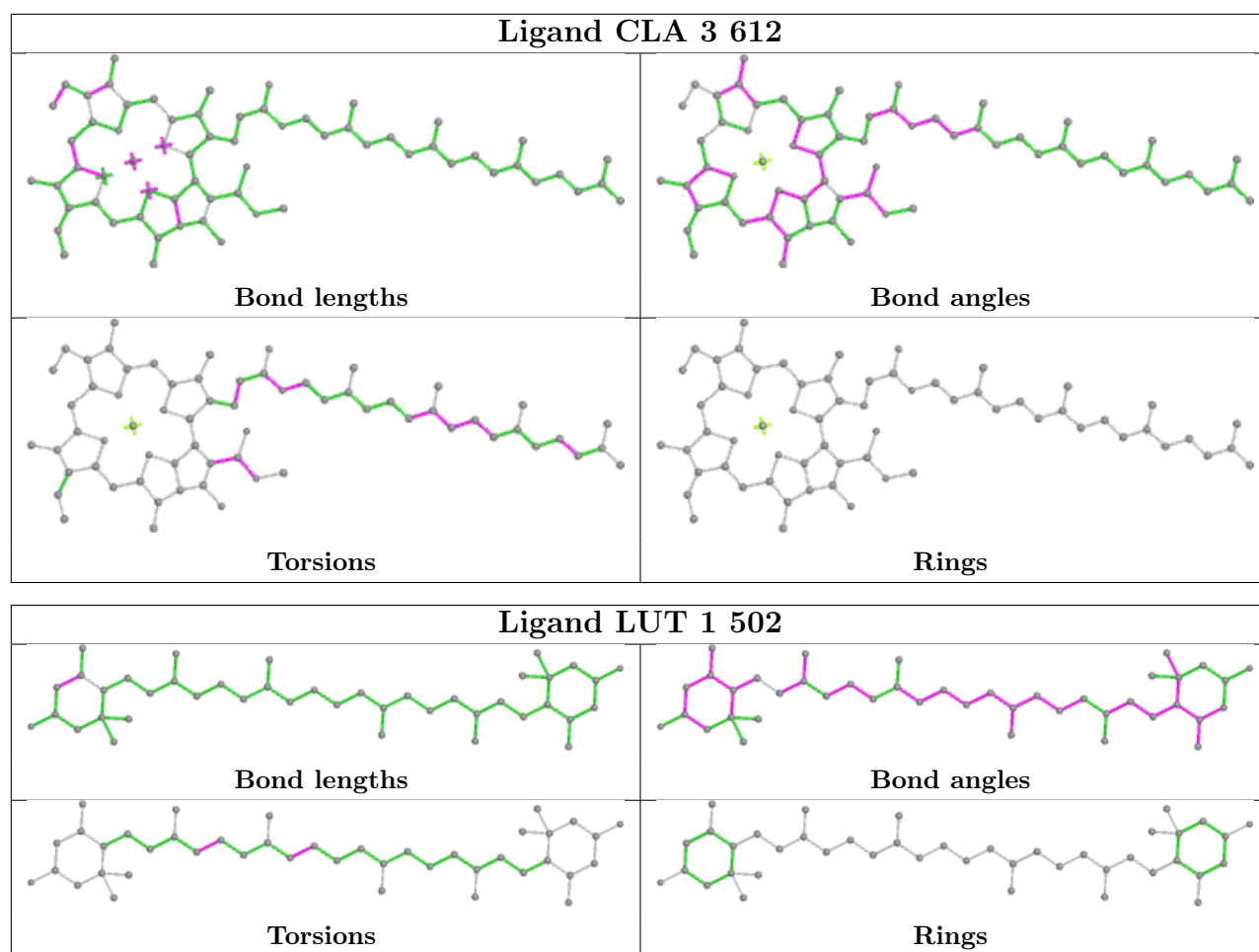
Ligand LUT a 502**Ligand CLA A 1012****Ligand CLA B 1207**

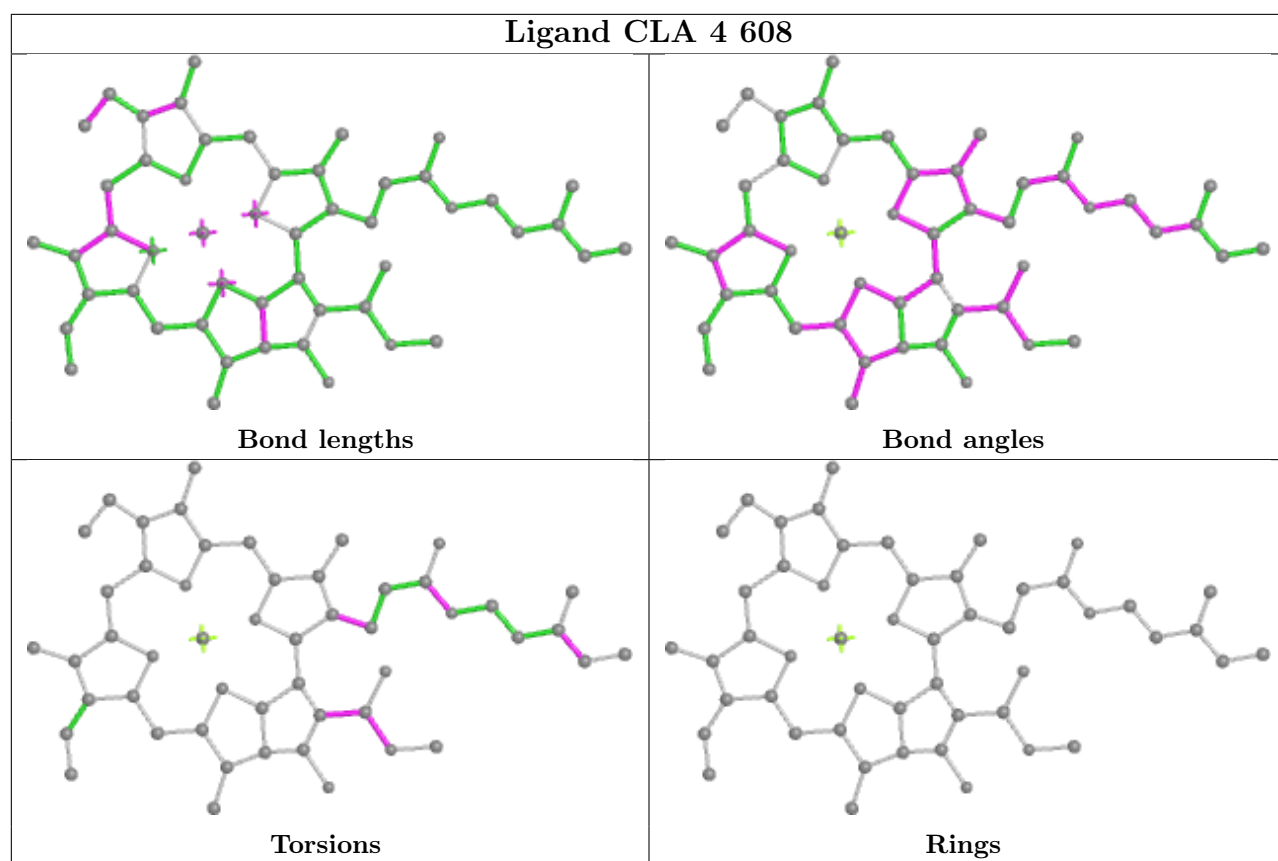
Ligand DGA 8 803



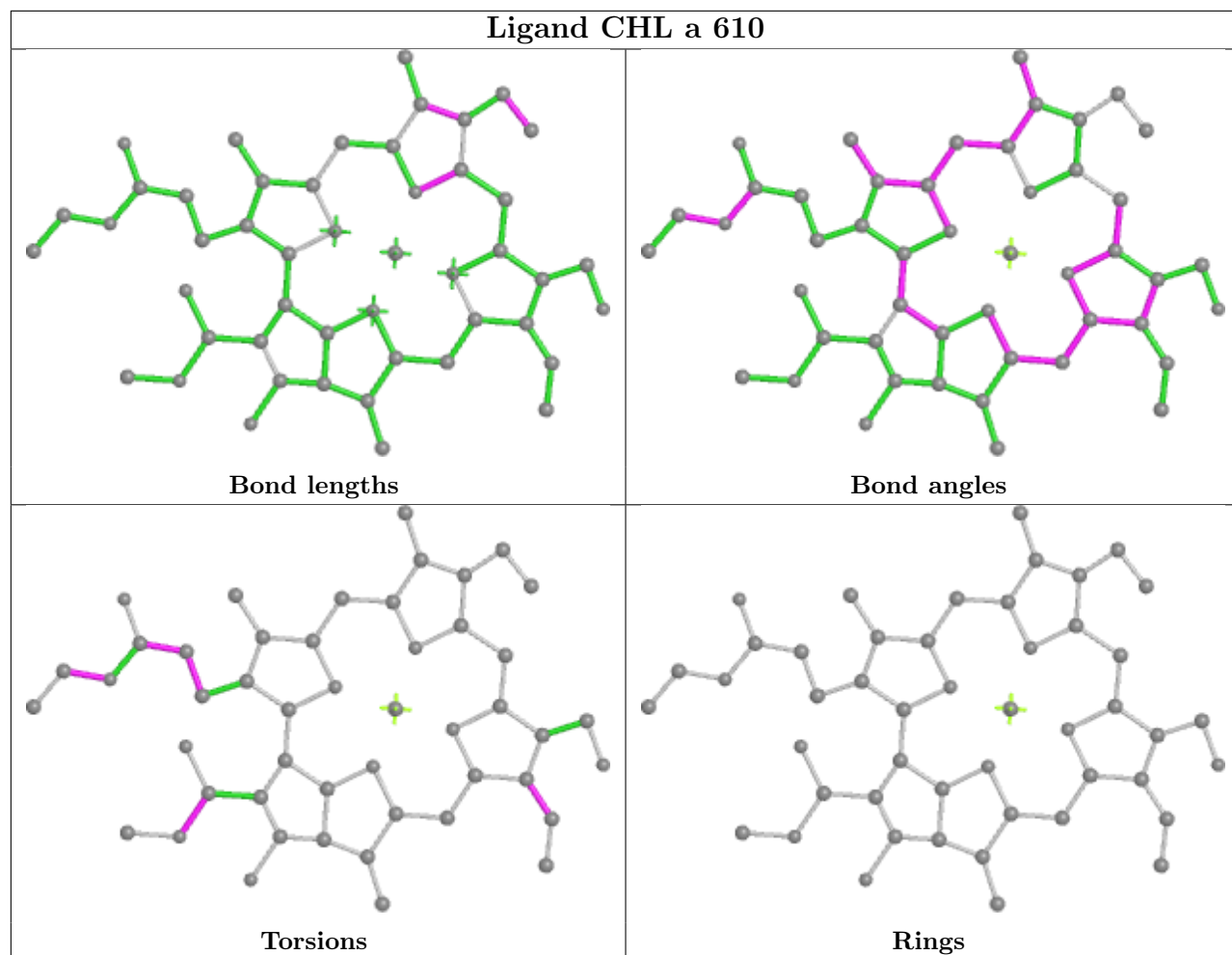
Ligand CLA a 602

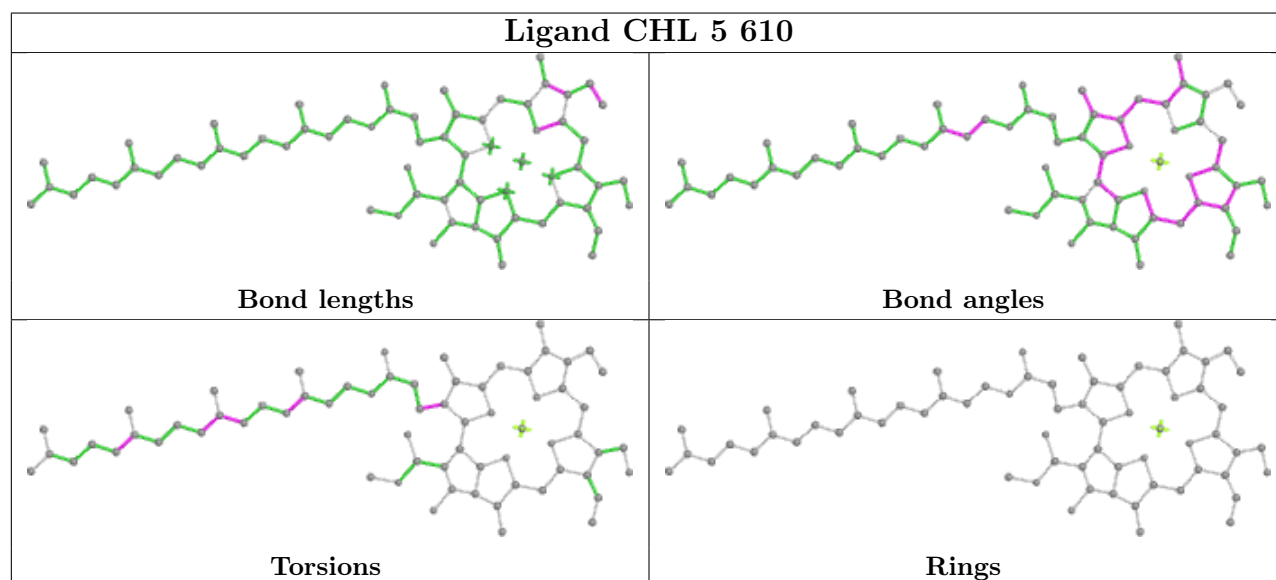
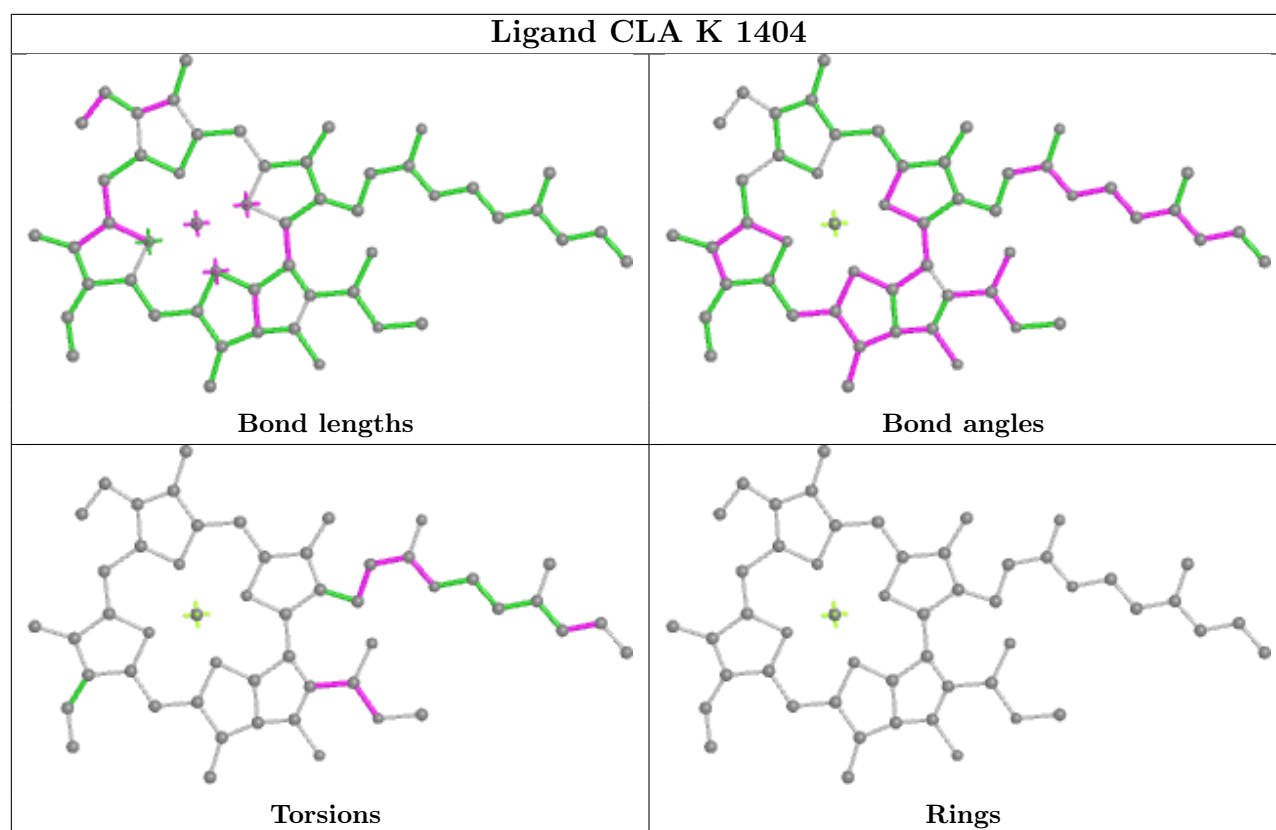




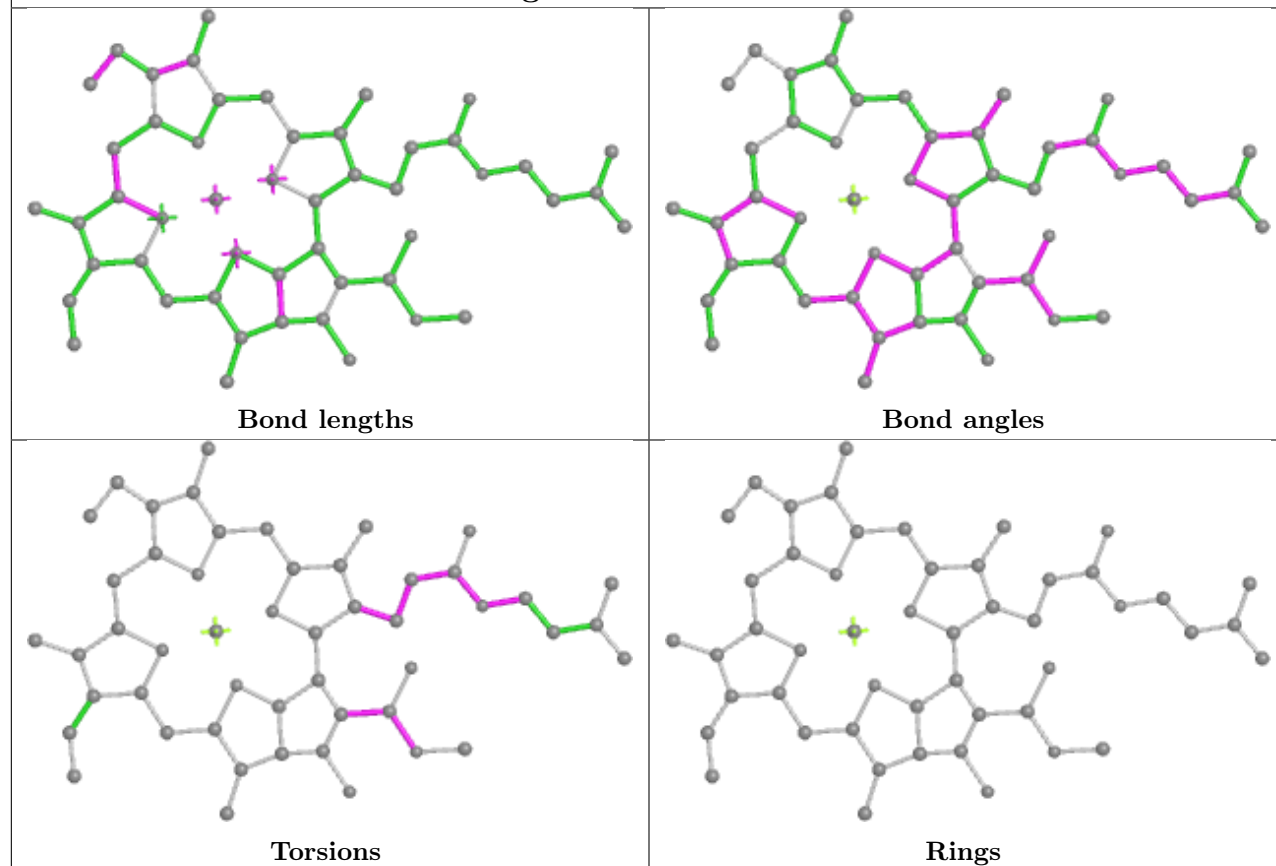


Ligand CHL a 610

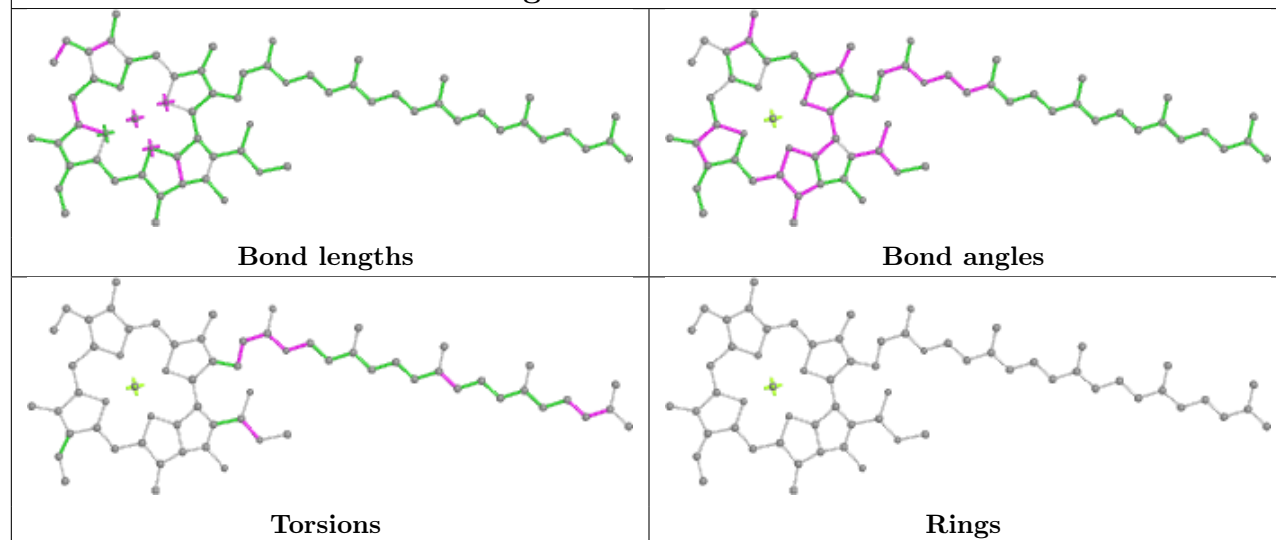


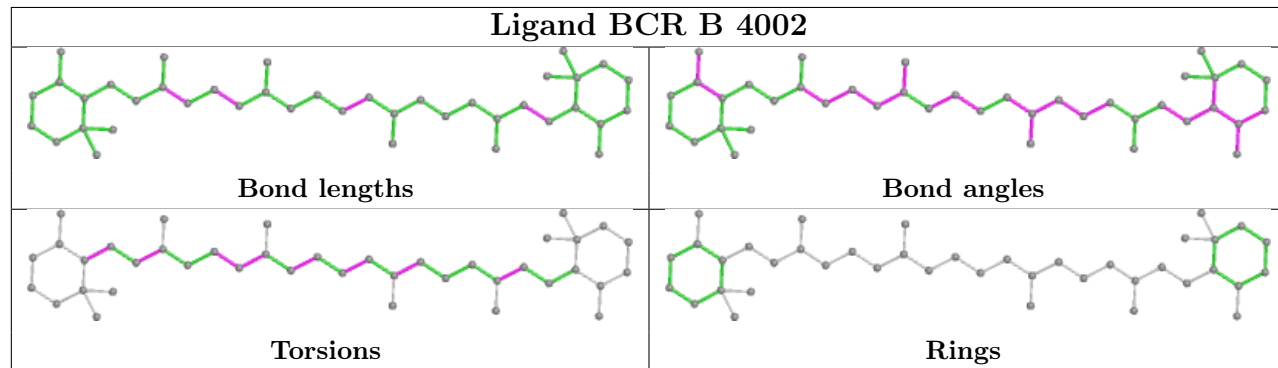
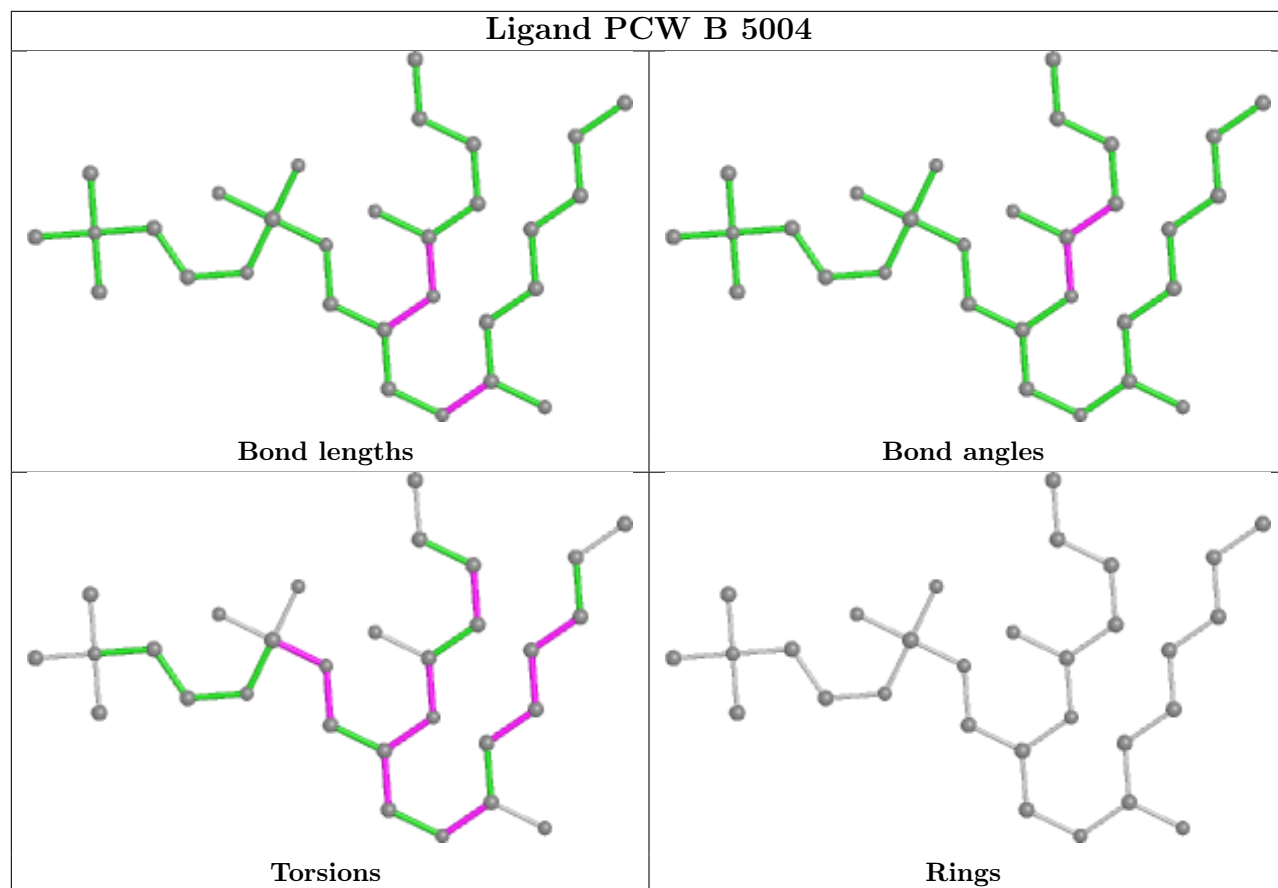


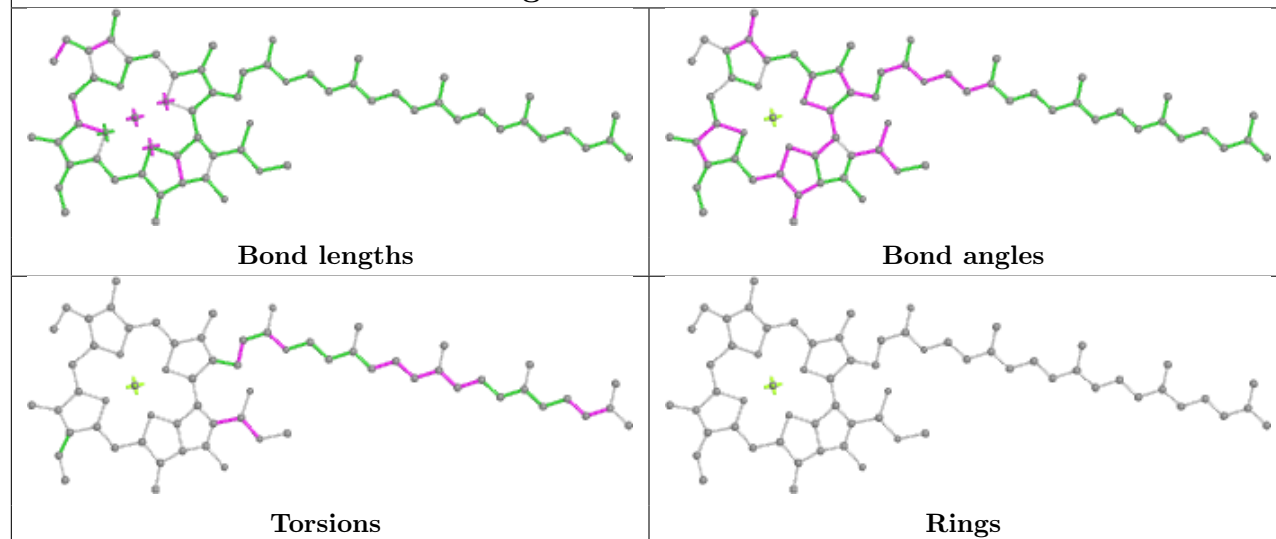
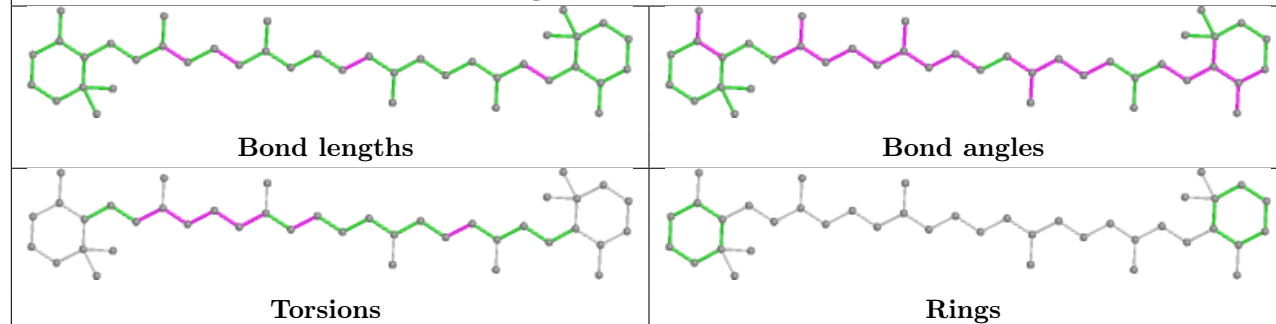
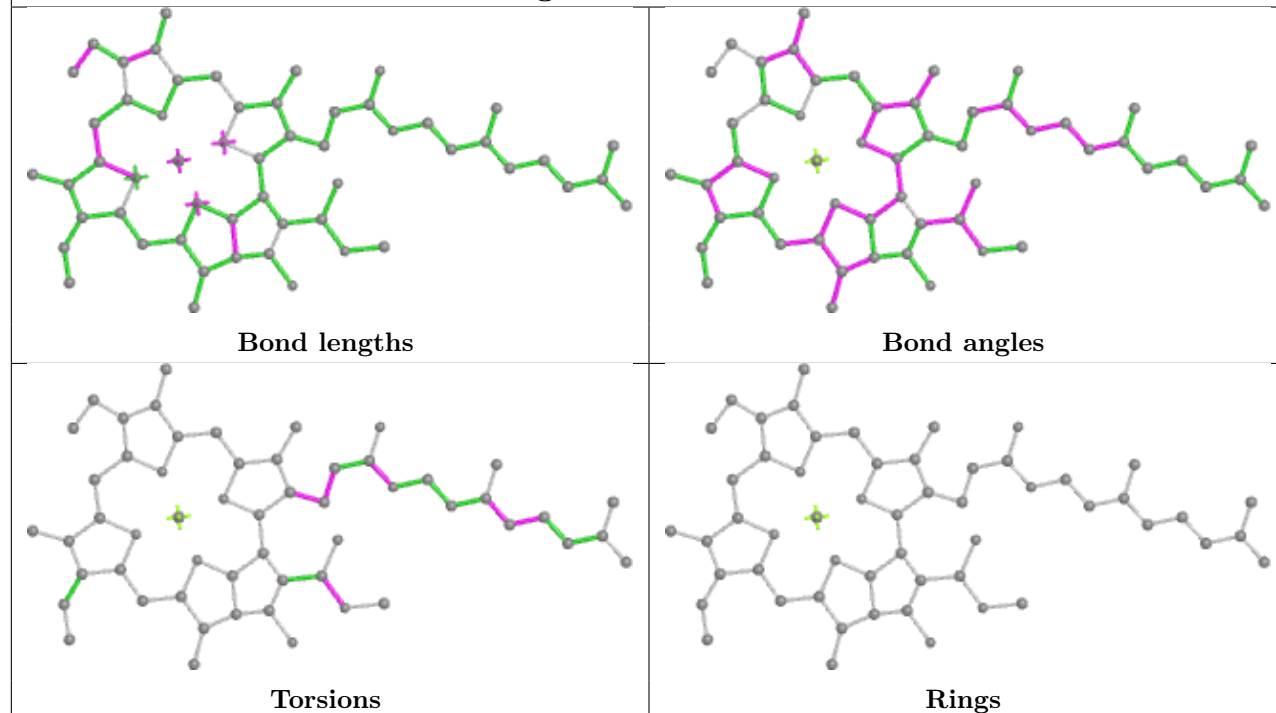
Ligand CLA G 1601



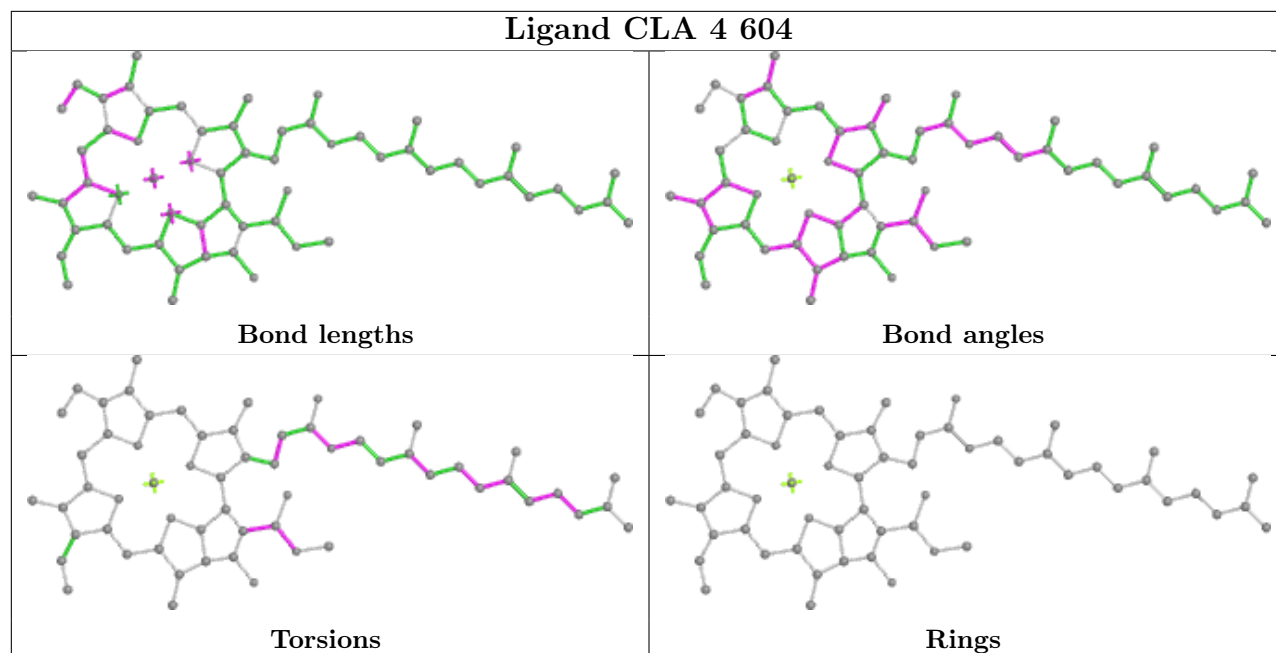
Ligand CLA B 1238



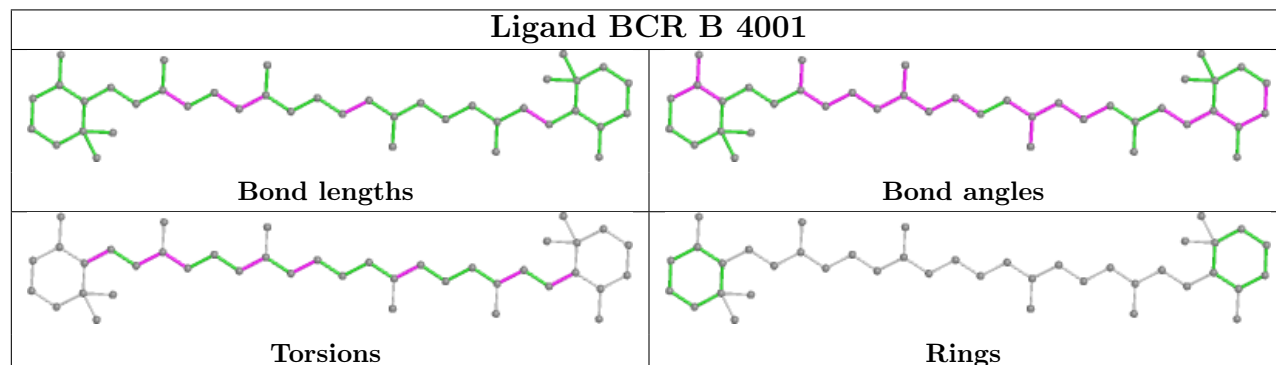


Ligand CLA A 1013**Ligand BCR I 4001****Ligand CLA 7 606**

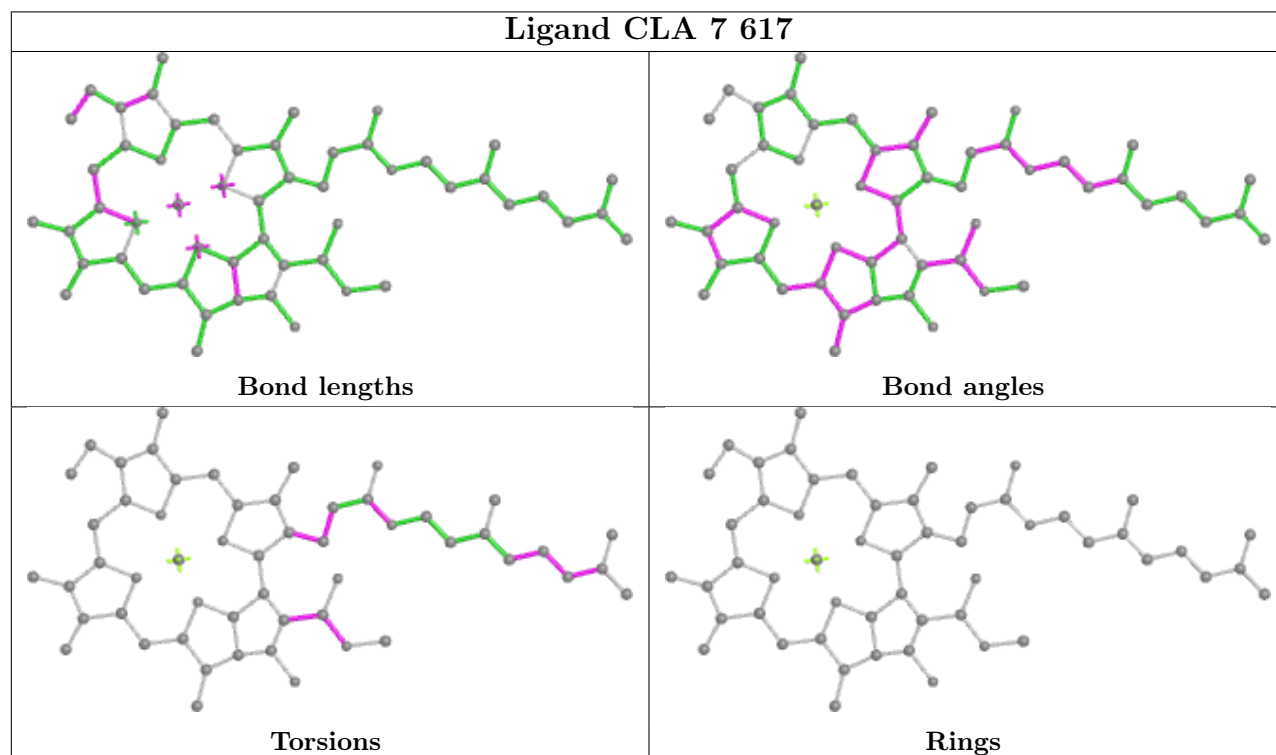
Ligand CLA 4 604

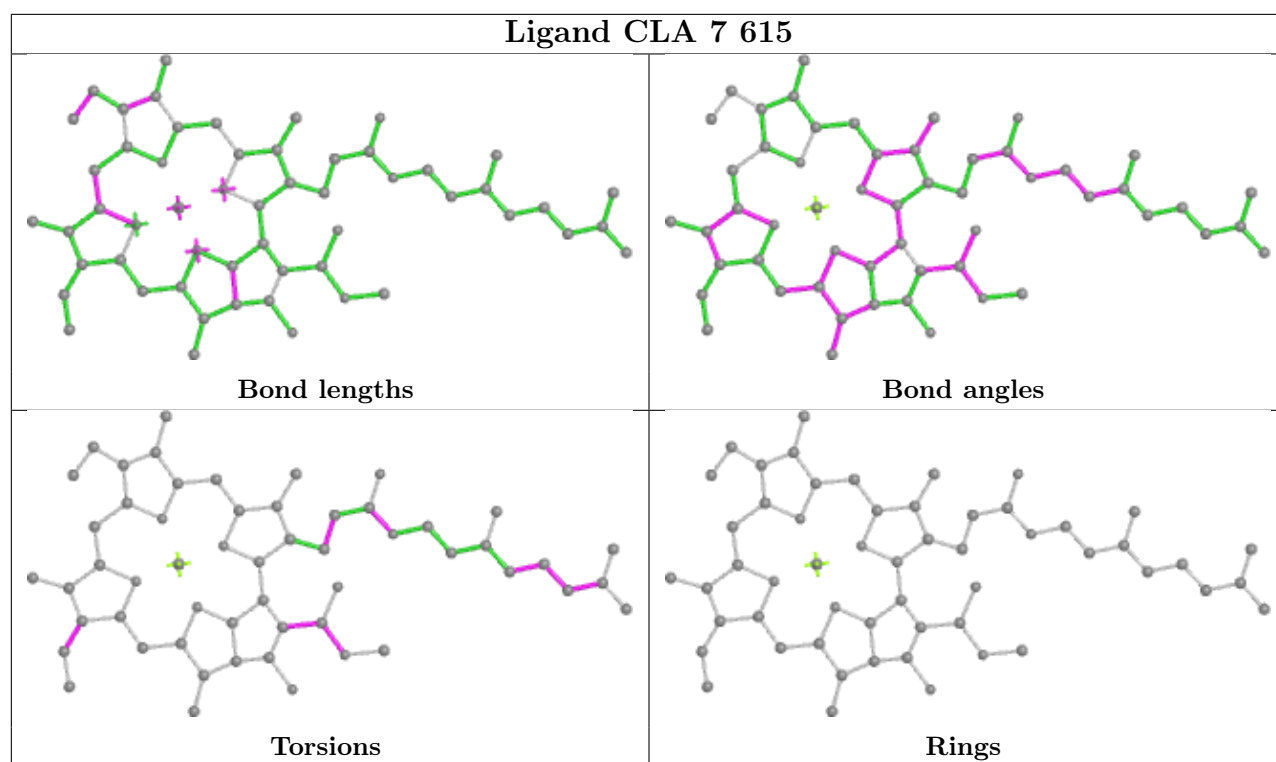


Ligand BCR B 4001



Ligand CLA 7 617





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.

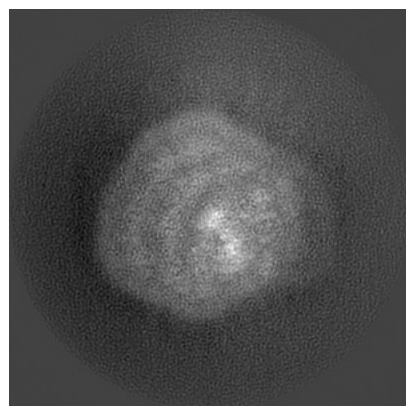
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11640. These allow visual inspection of the internal detail of the map and identification of artifacts.

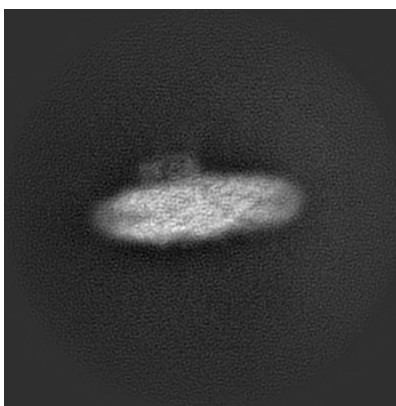
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

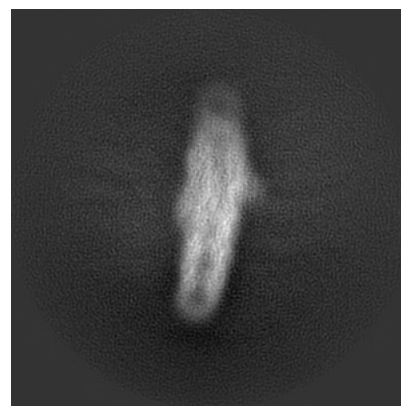
6.1.1 Primary map



X

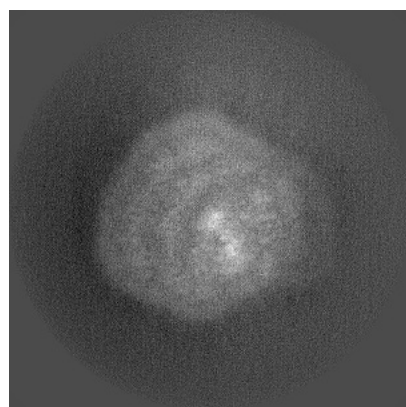


Y

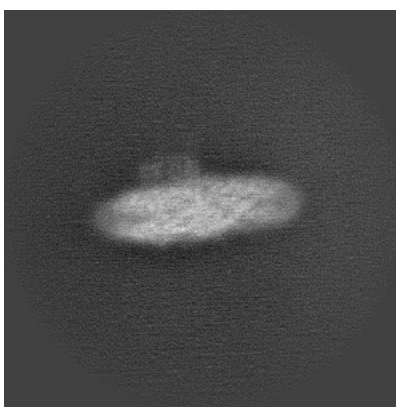


Z

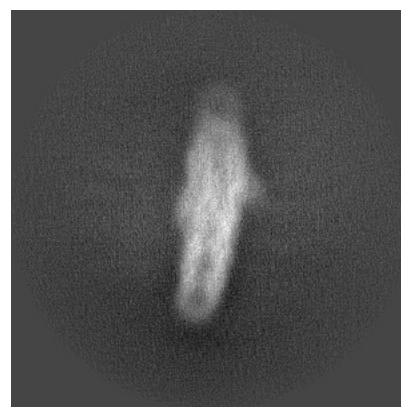
6.1.2 Raw map



X



Y

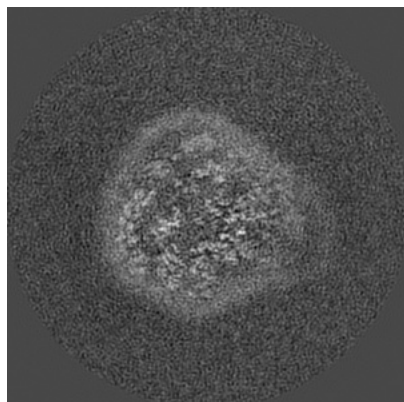


Z

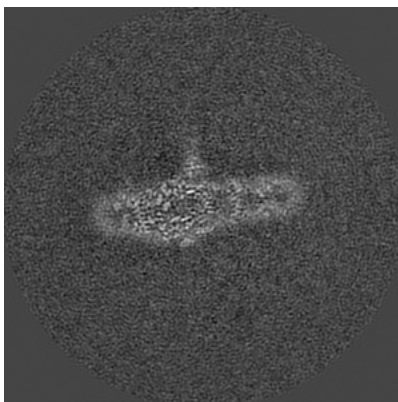
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

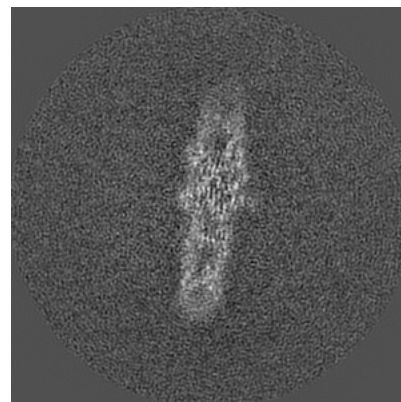
6.2.1 Primary map



X Index: 256

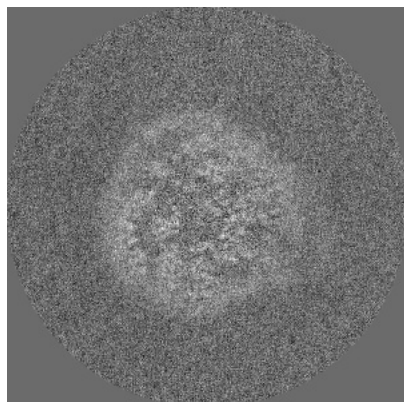


Y Index: 256

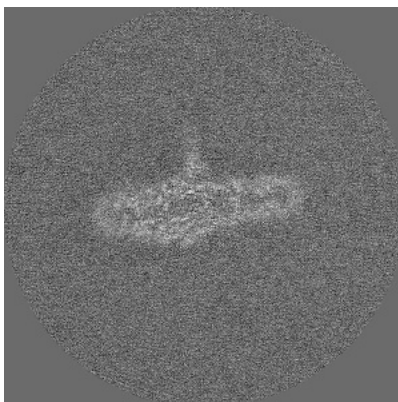


Z Index: 256

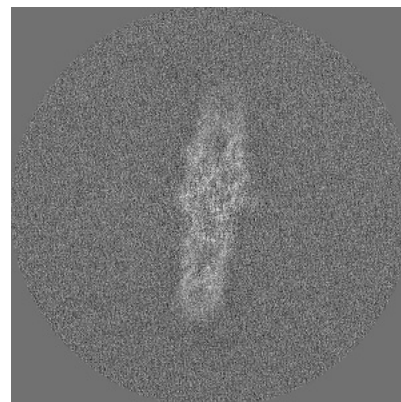
6.2.2 Raw map



X Index: 256



Y Index: 256

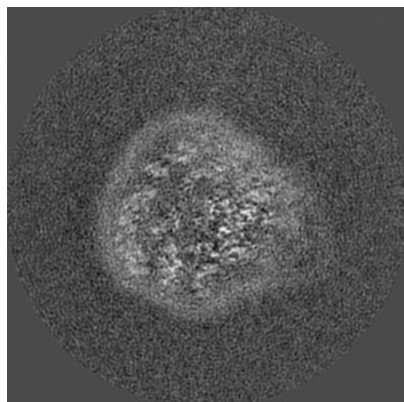


Z Index: 256

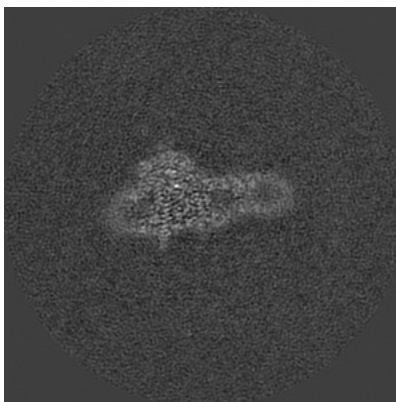
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

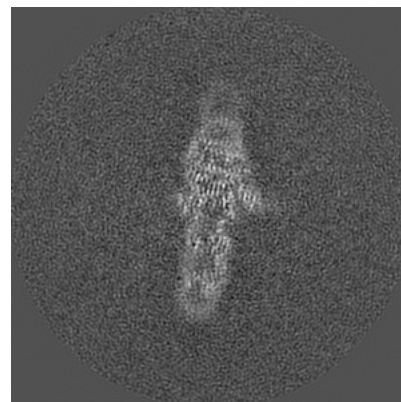
6.3.1 Primary map



X Index: 254

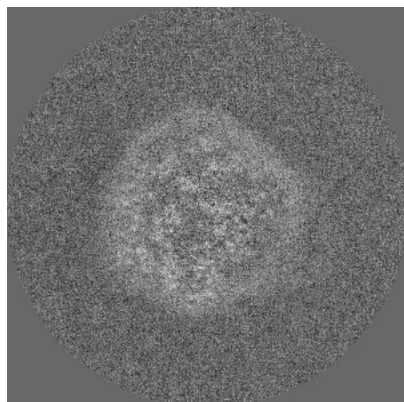


Y Index: 284

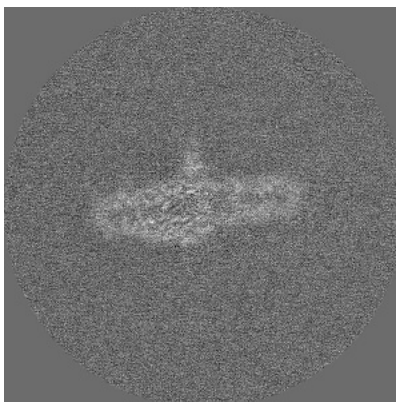


Z Index: 247

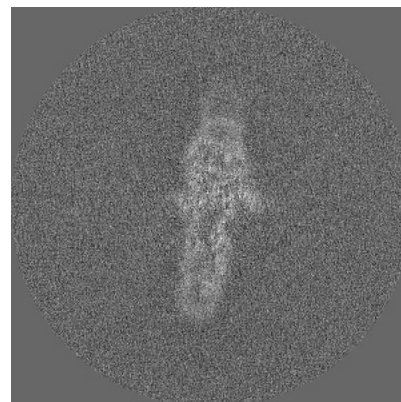
6.3.2 Raw map



X Index: 259



Y Index: 257

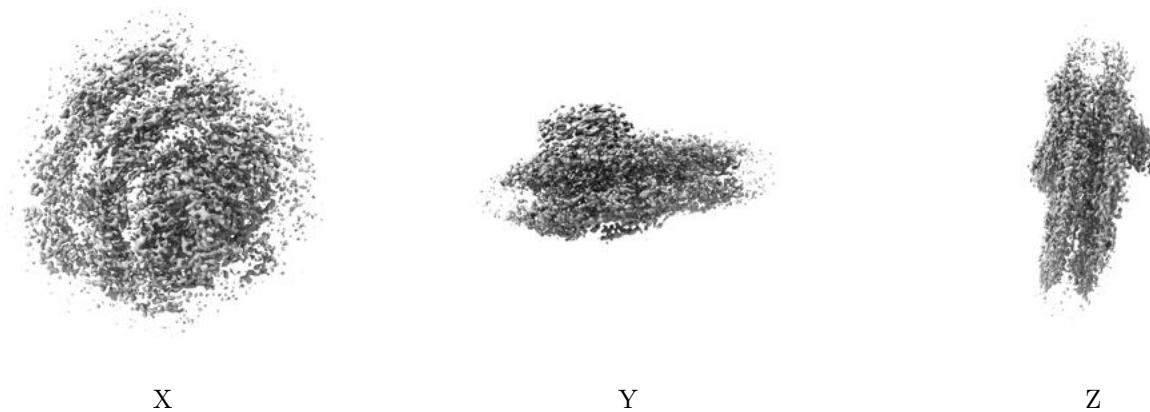


Z Index: 248

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

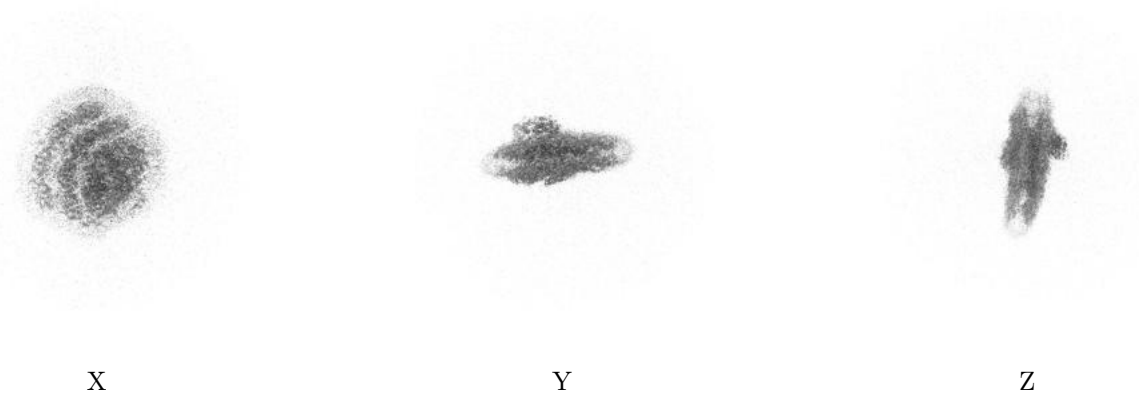
6.4 Orthogonal surface views [i](#)

6.4.1 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.

6.4.2 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.

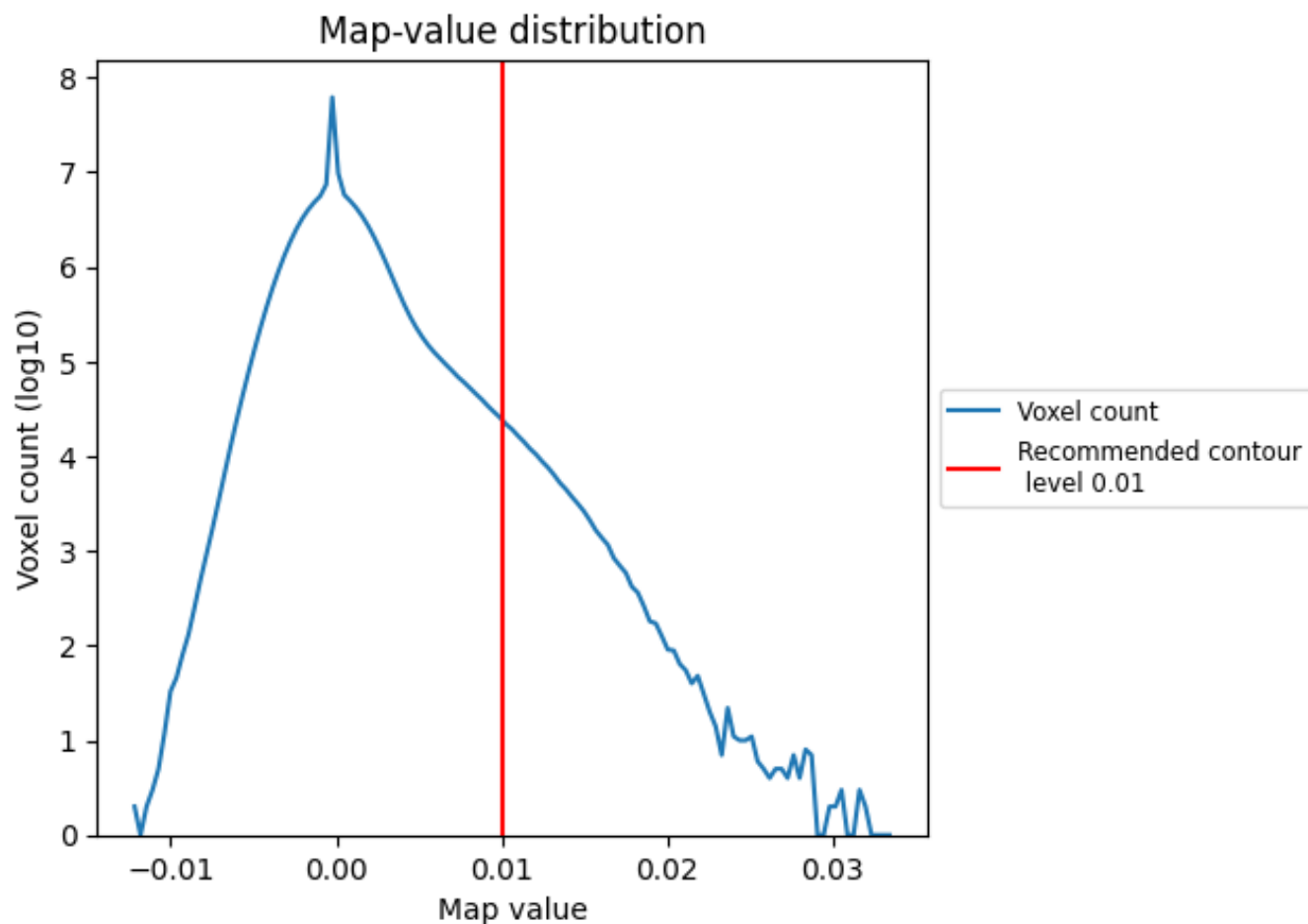
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

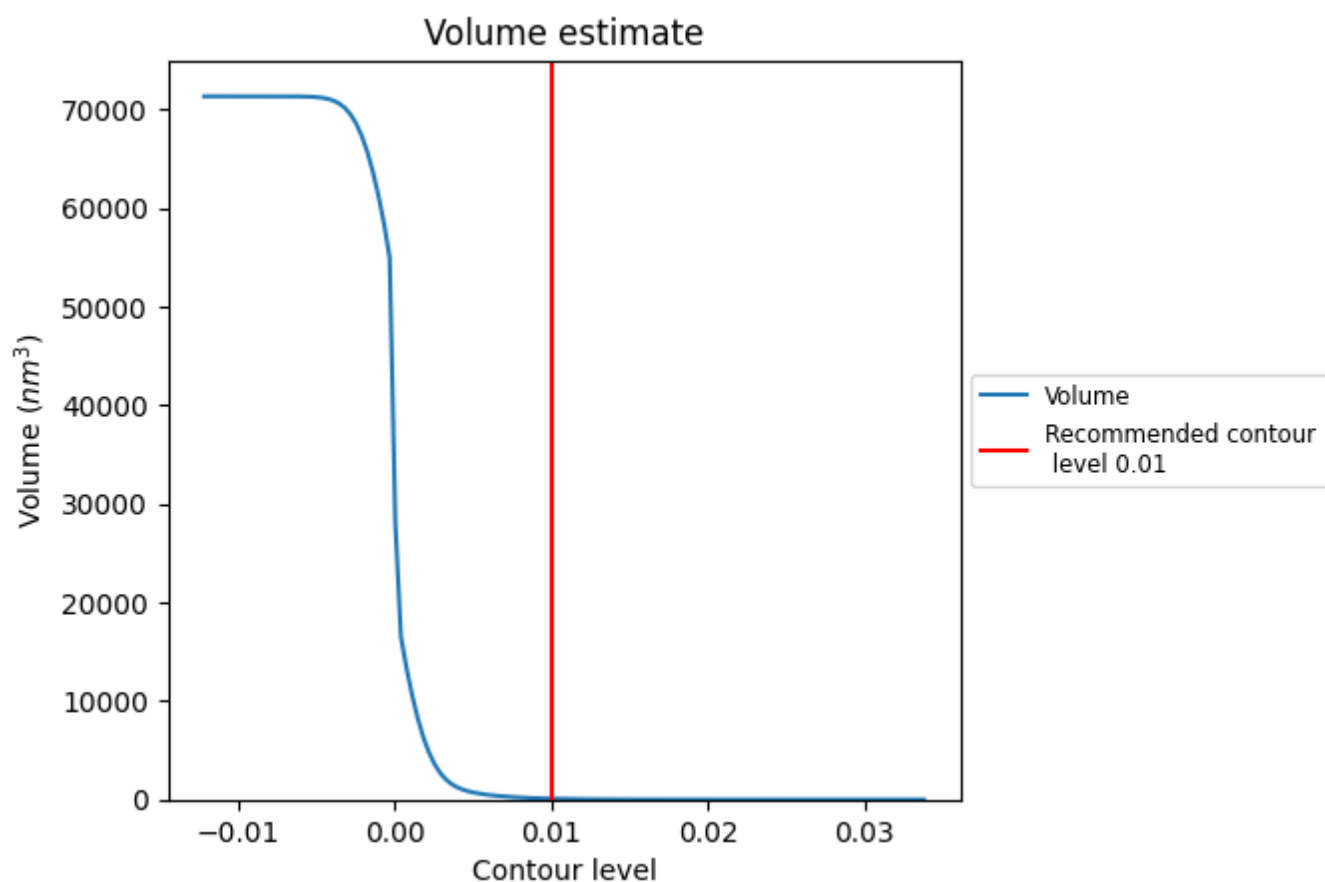
This section contains the results of statistical analysis of the map.

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.

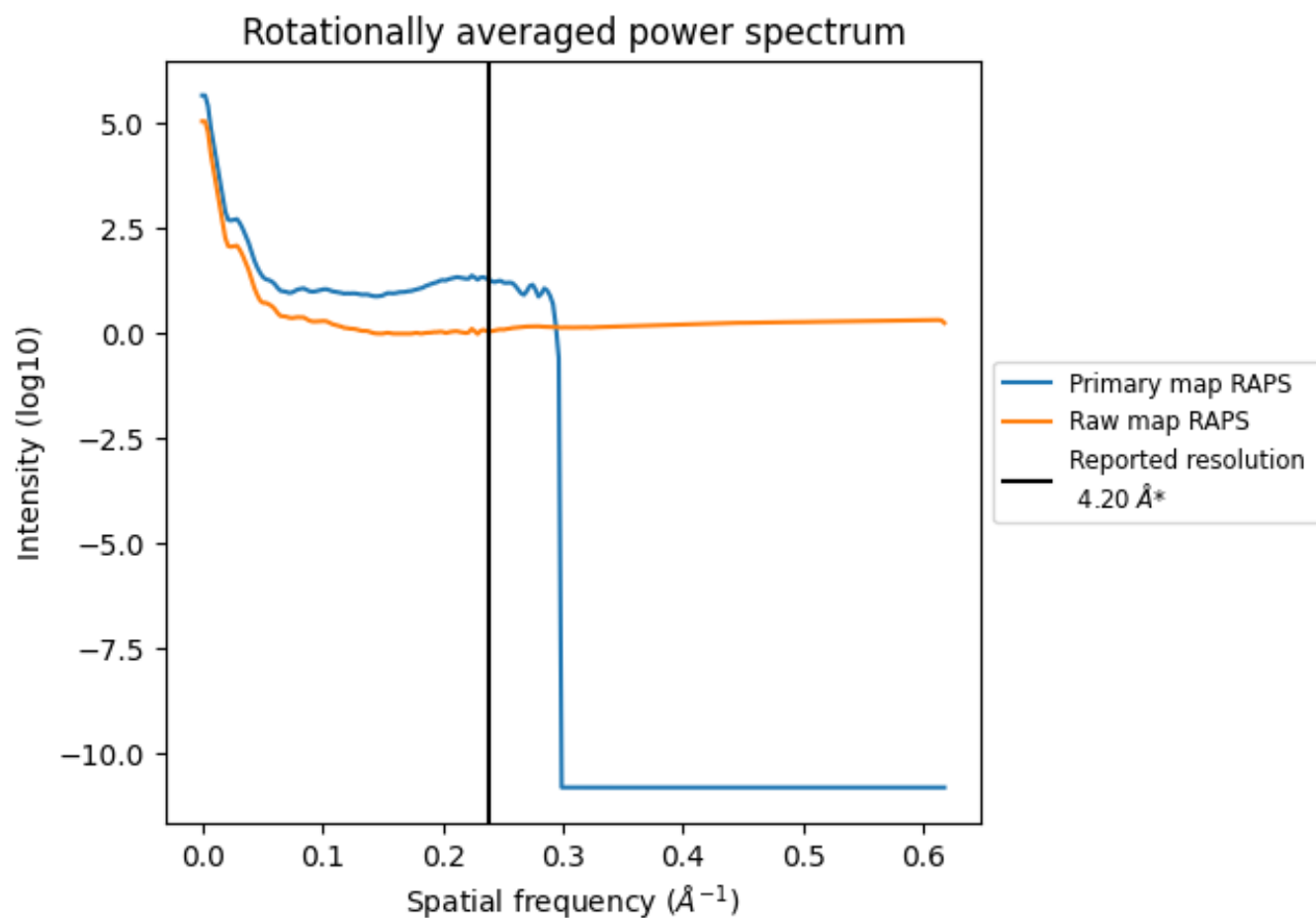
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 88 nm³; this corresponds to an approximate mass of 79 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 ⓘ

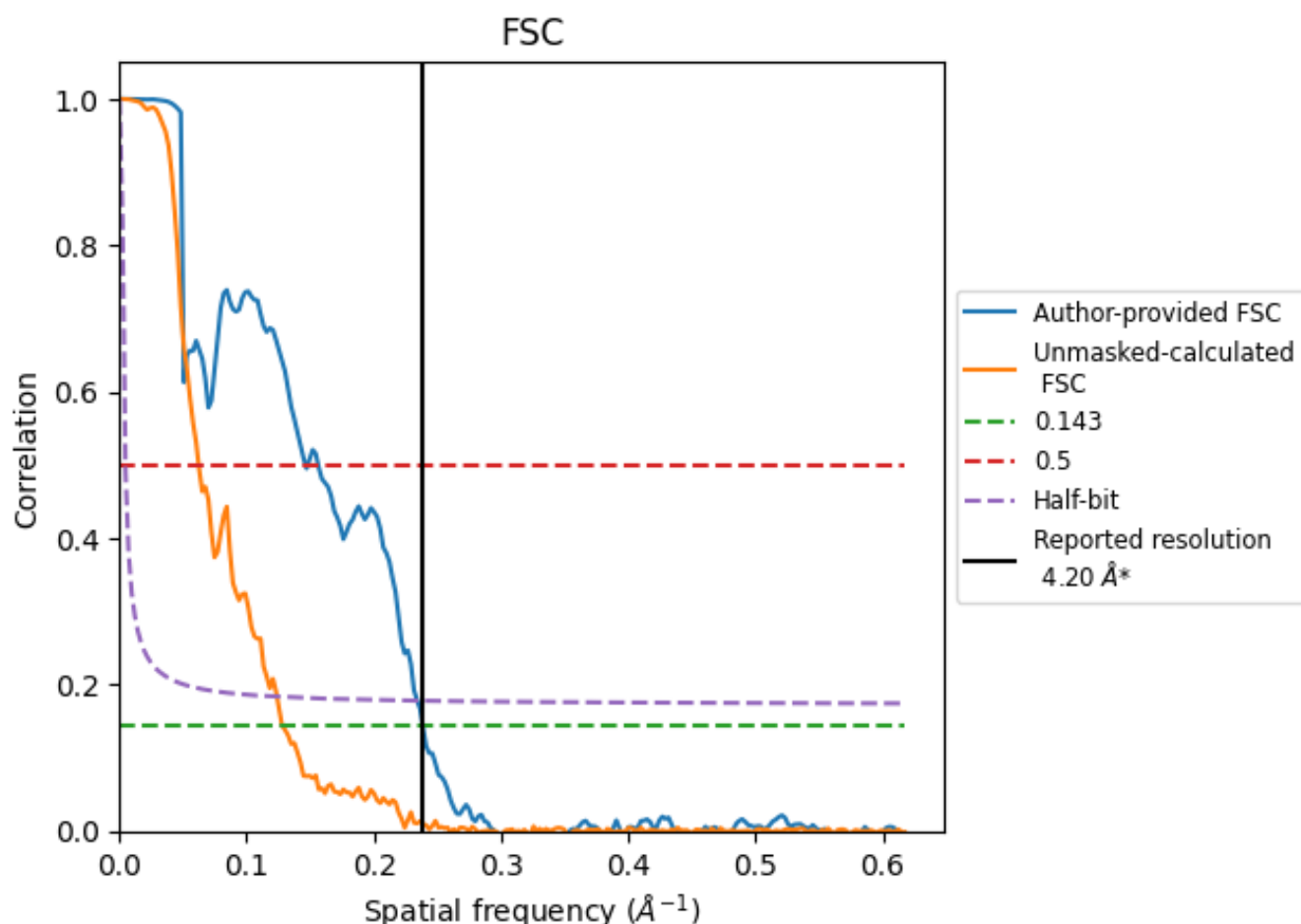


*Reported resolution corresponds to spatial frequency of 0.238 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

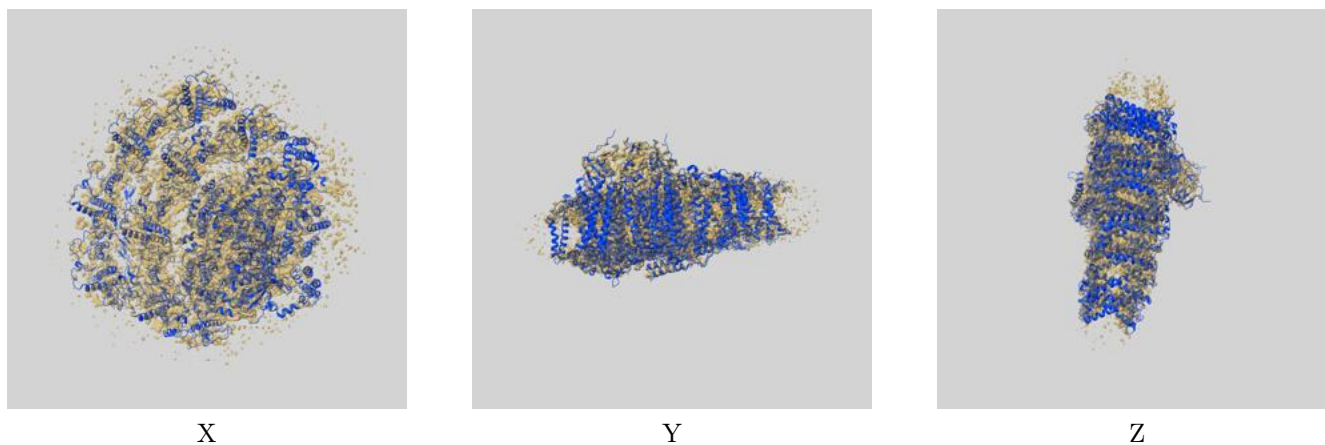
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.19	6.84	4.27
Unmasked-calculated*	7.81	16.08	8.08

*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 7.81 differs from the reported value 4.2 by more than 10 %

9 Map-model fit [i](#)

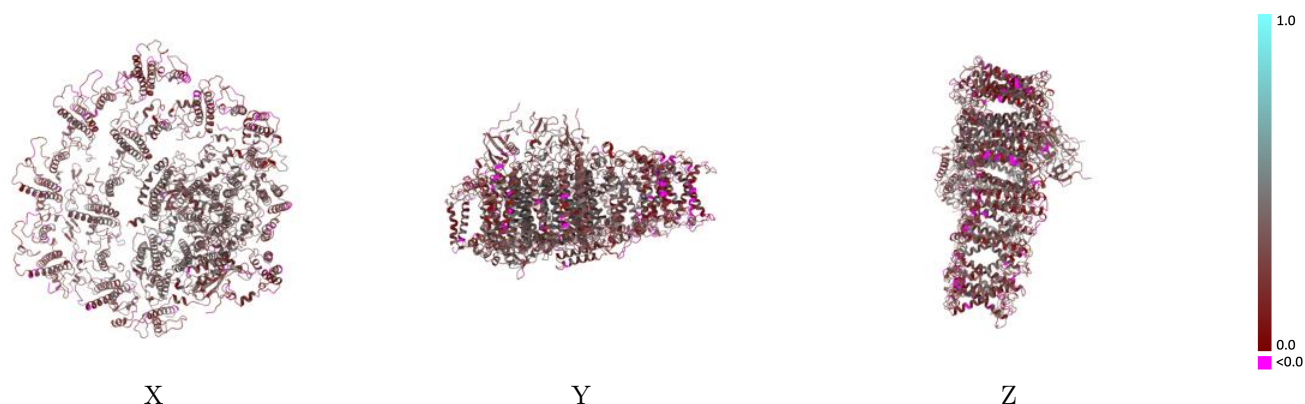
This section contains information regarding the fit between EMDB map EMD-11640 and PDB model 7A4P. Per-residue inclusion information can be found in section [3](#) on page [47](#).

9.1 Map-model overlay [i](#)



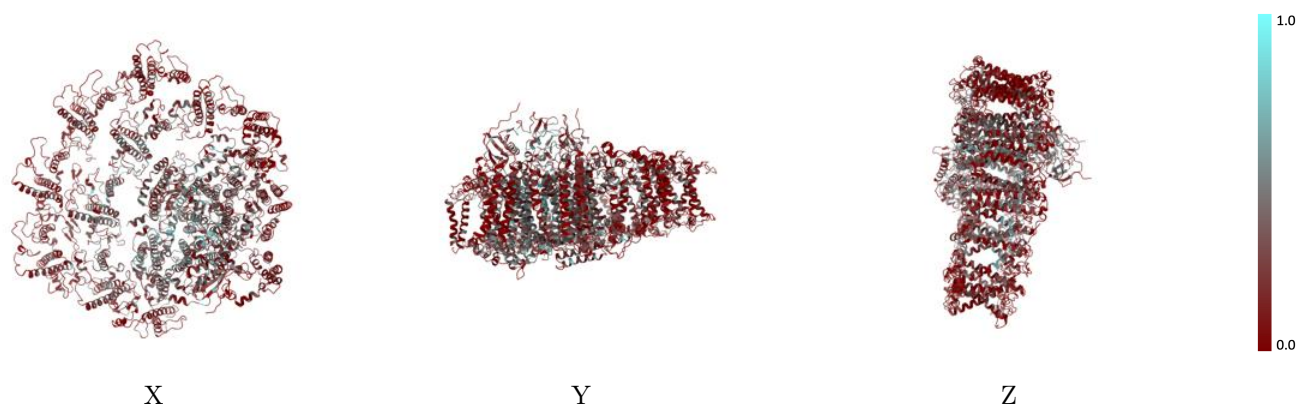
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



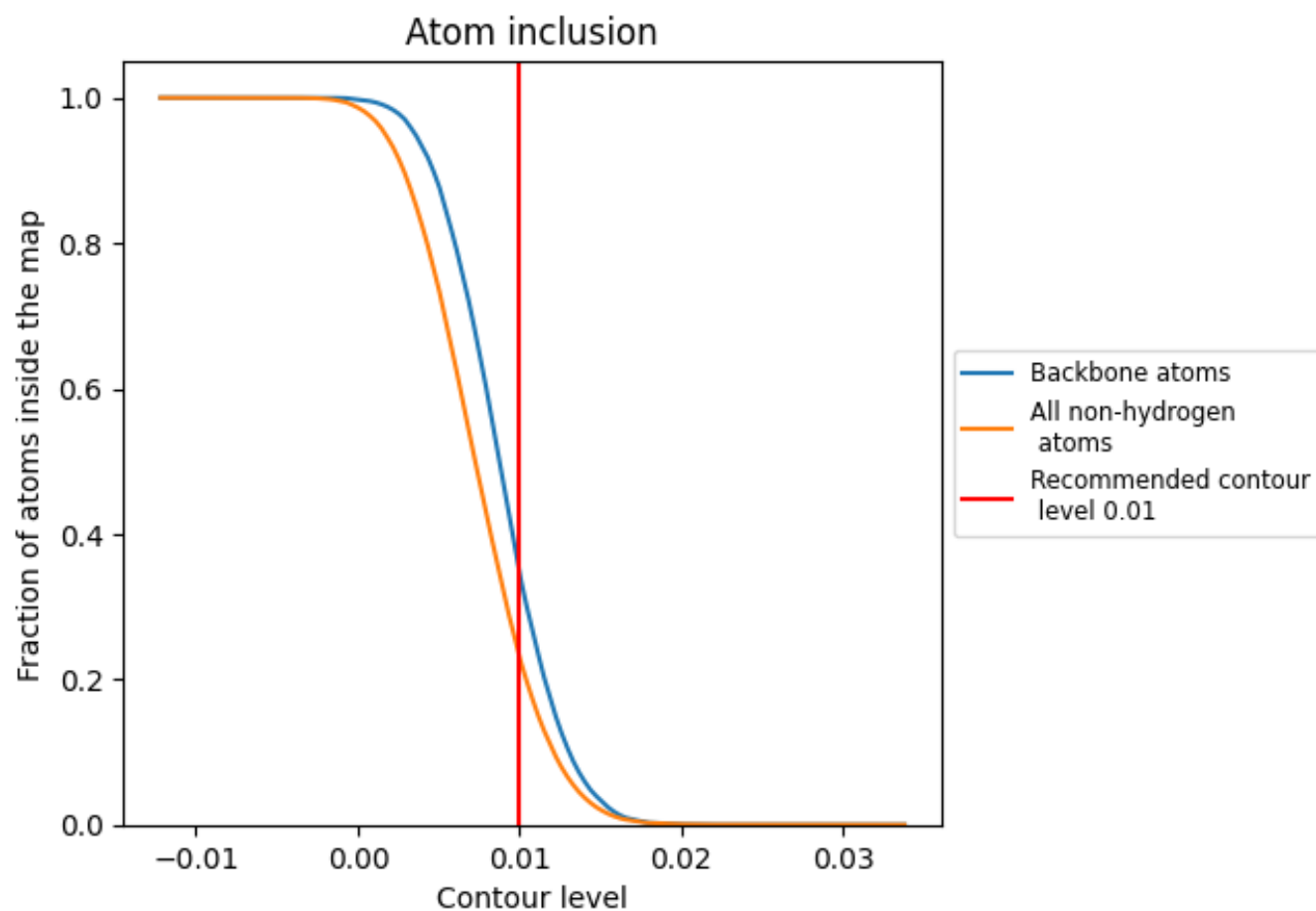
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 35% of all backbone atoms, 23% 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	<div></div> 0.2307	<div></div> 0.2780
1	<div></div> 0.1747	<div></div> 0.2150
3	<div></div> 0.2005	<div></div> 0.2770
4	<div></div> 0.1774	<div></div> 0.2250
5	<div></div> 0.1115	<div></div> 0.2330
6	<div></div> 0.1124	<div></div> 0.2290
7	<div></div> 0.2874	<div></div> 0.2990
8	<div></div> 0.2743	<div></div> 0.2880
A	<div></div> 0.3560	<div></div> 0.3500
B	<div></div> 0.2601	<div></div> 0.3140
C	<div></div> 0.4478	<div></div> 0.3400
D	<div></div> 0.2226	<div></div> 0.2740
E	<div></div> 0.3191	<div></div> 0.2800
F	<div></div> 0.2752	<div></div> 0.2970
G	<div></div> 0.0354	<div></div> 0.1850
I	<div></div> 0.0874	<div></div> 0.2110
J	<div></div> 0.2984	<div></div> 0.3560
K	<div></div> 0.0939	<div></div> 0.2190
L	<div></div> 0.0512	<div></div> 0.1760
M	<div></div> 0.0290	<div></div> 0.1970
a	<div></div> 0.1456	<div></div> 0.1790

1.0

0.0

<0.0