



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:16 PM UTC

PDB ID : 6YAC / pdb_00006yac
EMDB ID : EMD-10746
Title : Plant PSI-ferredoxin supercomplex
Authors : Caspy, I.; Nelson, N.; Shkolnisky, Y.; Klaiman, D.; Sheinker, A.
Deposited on : 2020-03-12
Resolution : 2.50 Å(reported)
Based on initial models : 1A70, 5L8R

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

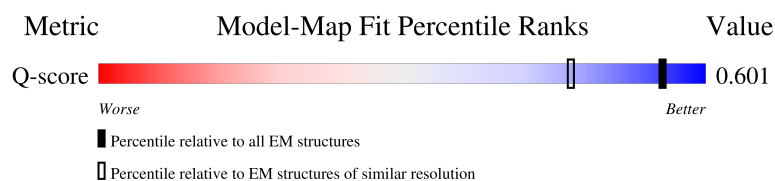
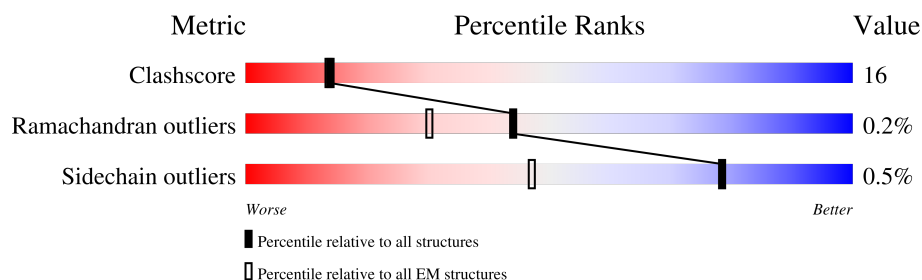
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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



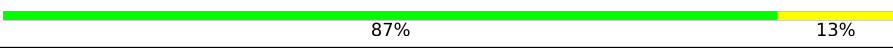
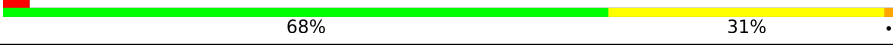
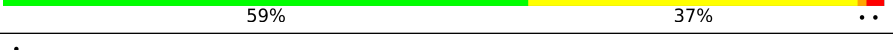
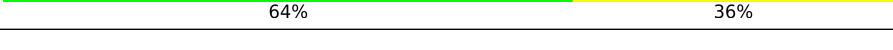
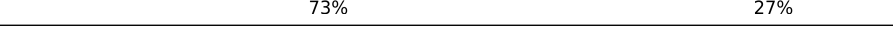
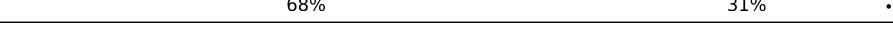
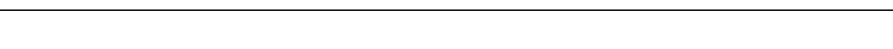
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	743	 84% 16%
2	B	733	 79% 21%
3	C	80	 90% 10%
4	D	143	 78% 22%

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Mol	Chain	Length	Quality of chain
5	E	66	
6	F	154	
7	G	97	
8	H	88	
9	I	31	
10	J	42	
11	K	81	
12	L	157	
13	1	193	
14	2	208	
15	3	221	
16	4	198	
17	N	97	

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
18	CL0	A	1011	X	-	-	-
19	CLA	1	601	X	-	-	-
19	CLA	1	602	X	-	-	-
19	CLA	1	603	X	-	-	-
19	CLA	1	604	X	-	-	-
19	CLA	1	605	X	-	-	-
19	CLA	1	606	X	-	-	-
19	CLA	1	607	X	-	-	-
19	CLA	1	608	X	-	-	-
19	CLA	1	611	X	-	-	-
19	CLA	1	613	X	-	-	-
19	CLA	1	614	X	-	-	-
19	CLA	2	601	X	-	-	-
19	CLA	2	602	X	-	-	-
19	CLA	2	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	2	604	X	-	-	-
19	CLA	2	605	X	-	-	-
19	CLA	2	606	X	-	-	-
19	CLA	2	607	X	-	-	-
19	CLA	2	608	X	-	-	-
19	CLA	2	612	X	-	-	-
19	CLA	3	601	X	-	-	-
19	CLA	3	602	X	-	-	-
19	CLA	3	603	X	-	-	-
19	CLA	3	606	X	-	-	-
19	CLA	3	608	X	-	-	-
19	CLA	3	610	X	-	-	-
19	CLA	3	612	X	-	-	-
19	CLA	3	613	X	-	-	-
19	CLA	3	614	X	-	-	-
19	CLA	3	617	X	-	-	-
19	CLA	4	601	X	-	-	-
19	CLA	4	602	X	-	-	-
19	CLA	4	603	X	-	-	-
19	CLA	4	604	X	-	-	-
19	CLA	4	606	X	-	-	-
19	CLA	4	607	X	-	-	-
19	CLA	4	608	X	-	-	-
19	CLA	4	609	X	-	-	-
19	CLA	4	612	X	-	-	-
19	CLA	4	617	X	-	-	-
19	CLA	A	1012	X	-	-	-
19	CLA	A	1013	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	X	-	-	-
19	CLA	A	1106	X	-	-	-
19	CLA	A	1107	X	-	-	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1111	X	-	-	-
19	CLA	A	1112	X	-	-	-
19	CLA	A	1113	X	-	-	-
19	CLA	A	1114	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1115	X	-	-	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	-	-
19	CLA	A	1118	X	-	-	-
19	CLA	A	1119	X	-	-	-
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	-	-
19	CLA	A	1123	X	-	-	-
19	CLA	A	1124	X	-	-	-
19	CLA	A	1125	X	-	-	-
19	CLA	A	1126	X	-	-	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	-	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1130	X	-	-	-
19	CLA	A	1131	X	-	-	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	-	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	-	-
19	CLA	A	1136	X	-	-	-
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	-	-
19	CLA	A	1139	X	-	-	-
19	CLA	A	1140	X	-	-	-
19	CLA	A	1141	X	-	-	-
19	CLA	B	1021	X	-	-	-
19	CLA	B	1022	X	-	-	-
19	CLA	B	1023	X	-	-	-
19	CLA	B	1201	X	-	-	-
19	CLA	B	1202	X	-	-	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1204	X	-	-	-
19	CLA	B	1205	X	-	-	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1207	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	-	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1213	X	-	-	-
19	CLA	B	1214	X	-	-	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	-	-
19	CLA	B	1221	X	-	-	-
19	CLA	B	1222	X	-	-	-
19	CLA	B	1223	X	-	-	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	-	-
19	CLA	B	1226	X	-	-	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	-	-
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	-	-
19	CLA	B	1236	X	-	-	-
19	CLA	B	1237	X	-	-	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1239	X	-	-	-
19	CLA	B	1240	X	-	-	-
19	CLA	F	1301	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	G	1601	X	-	-	-
19	CLA	G	1602	X	-	-	-
19	CLA	G	1603	X	-	-	-
19	CLA	G	1701	X	-	-	-
19	CLA	J	1901	X	-	-	-
19	CLA	K	1401	X	-	-	-
19	CLA	K	1402	X	-	-	-
19	CLA	K	1403	X	-	-	-
19	CLA	K	1404	X	-	-	-
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	-	-
19	CLA	L	1503	X	-	-	-
28	LUT	2	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	LUT	3	502	X	-	-	-
28	LUT	J	4013	X	-	-	-
29	CHL	1	609	X	-	-	-
29	CHL	1	610	X	-	-	-
29	CHL	1	612	X	-	-	-
29	CHL	2	609	X	-	-	-
29	CHL	2	610	X	-	-	-
29	CHL	2	611	X	-	-	-
29	CHL	2	613	X	-	-	-
29	CHL	2	615	X	-	-	-
29	CHL	3	604	X	-	-	-
29	CHL	3	607	X	-	-	-
29	CHL	3	611	X	-	-	-
29	CHL	4	610	X	-	-	-
29	CHL	4	611	X	-	-	-
29	CHL	4	613	X	-	-	-
29	CHL	4	615	X	-	-	-
30	XAT	2	502	X	-	-	-
30	XAT	4	502	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 38469 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	743	Total	C	N	O	S	0	0
			5858	3839	998	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5857	3848	998	997	14		

- 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
			612	379	107	115	11		

- Molecule 4 is a protein called PsaD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1132	731	194	204	3		

- Molecule 5 is a protein called PsaE.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	66	Total	C	N	O	0	0
			528	336	93	99		

- Molecule 6 is a protein called PsaF.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	154	Total	C	N	O	S	0	0
			1206	782	207	215	2		

- Molecule 7 is a protein called PsaG.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	97	Total	C	N	O	0	0
			757	492	125	140		

- Molecule 8 is a protein called PsaH.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	88	Total	C	N	O	0	0
			673	442	106	125		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	31	Total	C	N	O	S	0	0
			240	165	38	36	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	42	Total	C	N	O	S	0	0
			338	231	51	55	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	PHE	LEU	conflict	UNP D5MAL3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	81	Total	C	N	O	S	0	0
			569	362	99	105	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	86	ALA	VAL	conflict	UNP E1C9L3

- Molecule 12 is a protein called PsaL.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	157	Total	C	N	O	S	0	0
			1174	772	189	212	1		

- Molecule 13 is a protein called Lhca1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1	193	Total	C	N	O	S	0	0
			1508	982	252	269	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	2	208	Total	C	N	O	S	0	0
			1620	1059	265	292	4		

- Molecule 15 is a protein called Chlorophyll a-b binding protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	3	221	Total	C	N	O	S	0	0
			1706	1118	278	305	5		

- Molecule 16 is a protein called Chlorophyll a-b binding protein P4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	198	Total	C	N	O	S	0	0
			1559	1022	253	281	3		

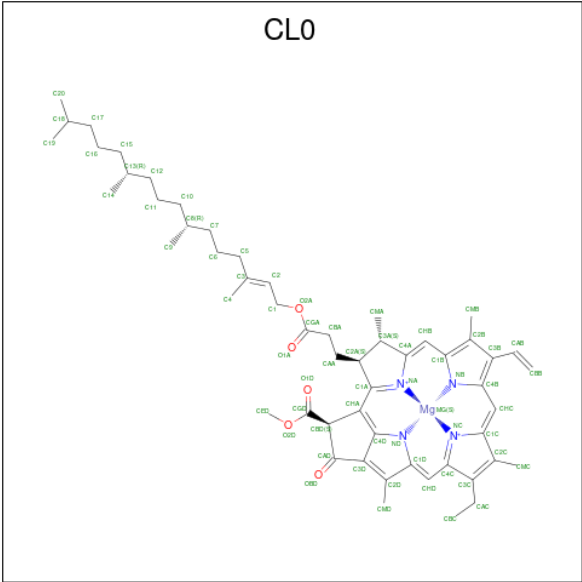
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	89	LYS	ARG	conflict	UNP Q9SQL2
4	128	ASP	ALA	conflict	UNP Q9SQL2
4	149	PHE	SER	conflict	UNP Q9SQL2

- Molecule 17 is a protein called Ferredoxin-1, chloroplastic.

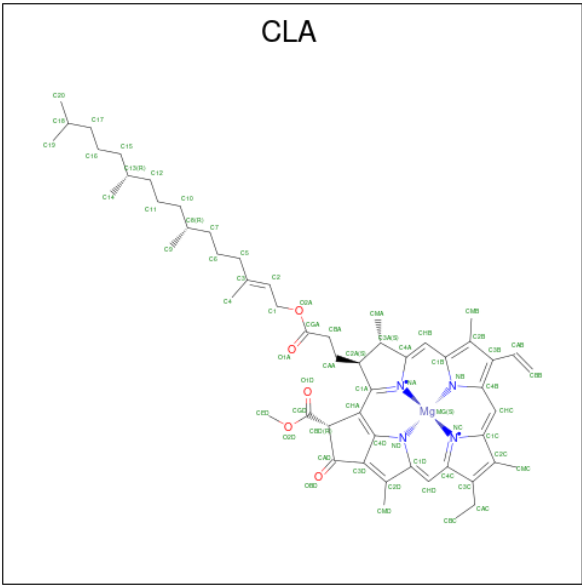
Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	97	Total	C	N	O	S	0	0
			724	448	111	160	5		

- Molecule 18 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
19	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	K	1	Total 48	C 38	Mg 1	N 4	O 5	0
19	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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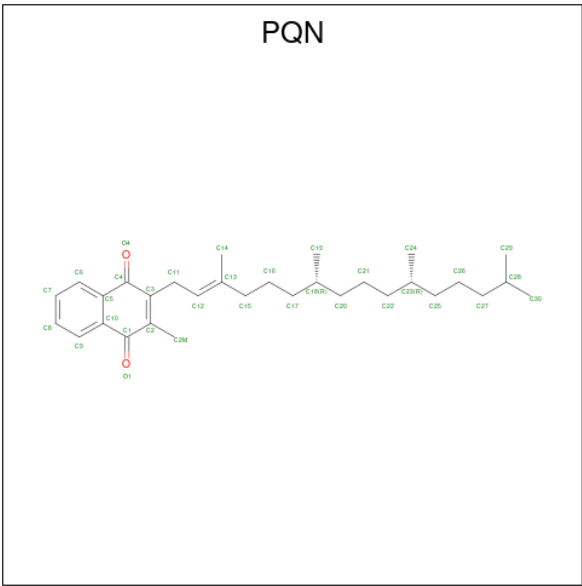
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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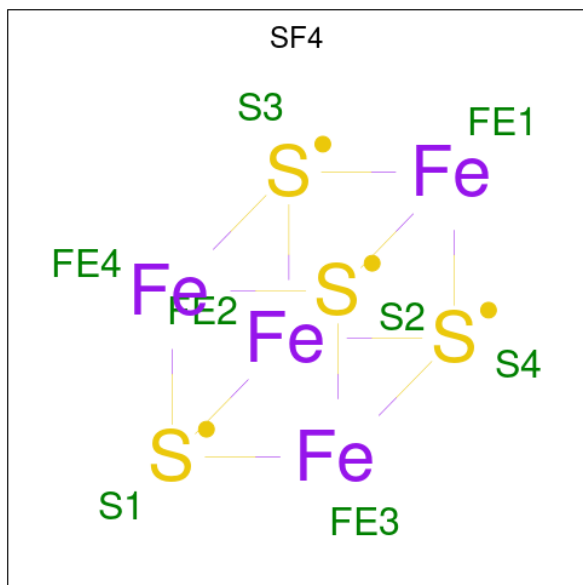
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



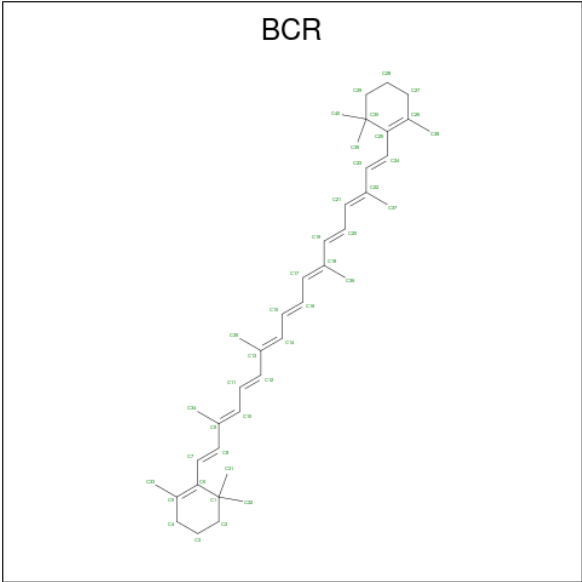
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

- Molecule 21 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



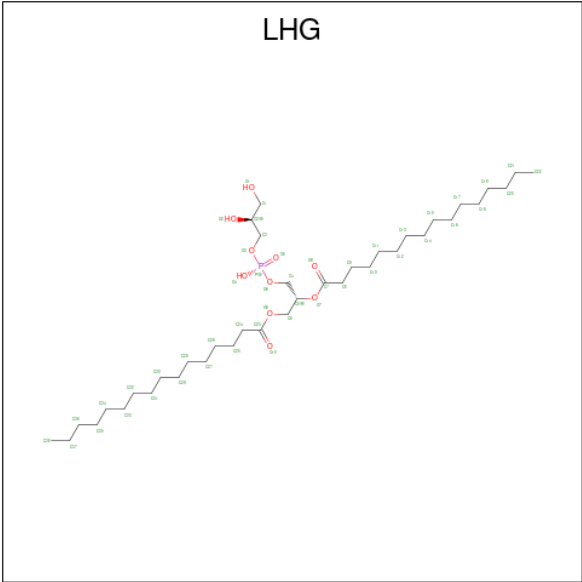
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	F	1	Total	C	0
			40	40	
22	F	1	Total	C	0
			40	40	
22	G	1	Total	C	0
			40	40	

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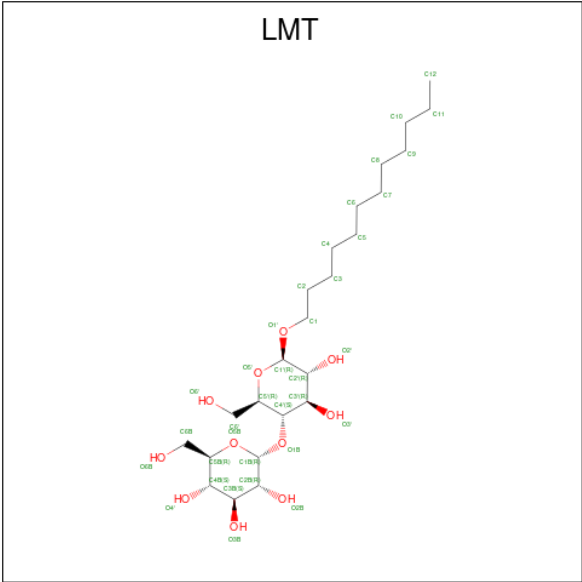
Mol	Chain	Residues	Atoms	AltConf
22	G	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	1	1	Total C 40 40	0
22	1	1	Total C 40 40	0
22	2	1	Total C 40 40	0
22	3	1	Total C 40 40	0
22	3	1	Total C 40 40	0

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



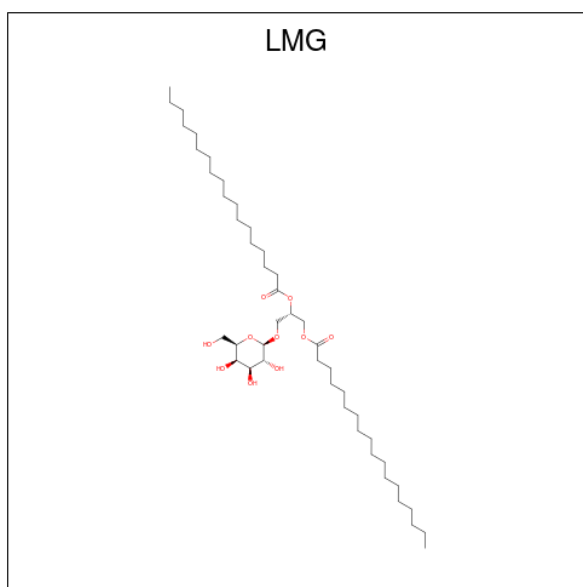
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			21	10	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	2	1	Total	C	O	P	0
			33	22	10	1	
23	3	1	Total	C	O	P	0
			17	8	8	1	

- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			32	21	11	
24	B	1	Total	C	O	0
			31	20	11	
24	G	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			31	20	11	
24	J	1	Total	C	O	0
			25	14	11	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			50	40	10	
25	B	1	Total	C	O	0
			35	25	10	
25	B	1	Total	C	O	0
			33	23	10	
25	B	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			30	20	10	
25	F	1	Total	C	O	0
			47	37	10	
25	F	1	Total	C	O	0
			36	26	10	
25	F	1	Total	C	O	0
			34	24	10	
25	F	1	Total	C	O	0
			13	7	6	
25	G	1	Total	C	O	0
			49	39	10	
25	G	1	Total	C	O	0
			50	40	10	
25	G	1	Total	C	O	0
			25	15	10	
25	1	1	Total	C	O	0
			46	36	10	
25	2	1	Total	C	O	0
			25	15	10	

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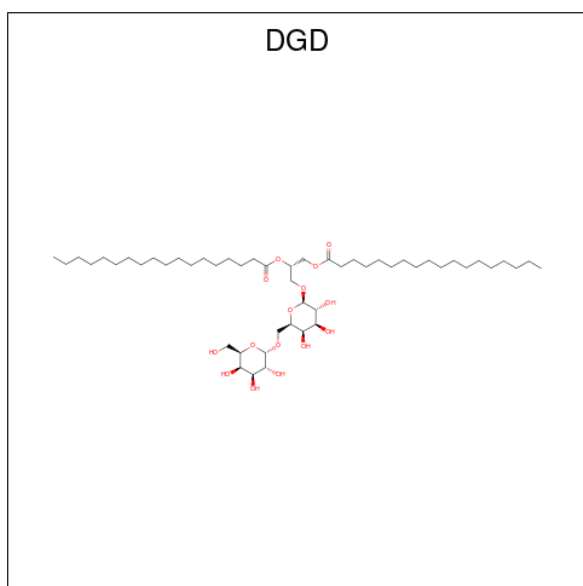
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Mol	Chain	Residues	Atoms			AltConf
25	2	1	Total	C	O	0
			36	26	10	
25	2	1	Total	C	O	0
			30	20	10	
25	2	1	Total	C	O	0
			13	7	6	
25	2	1	Total	C	O	0
			13	7	6	
25	3	1	Total	C	O	0
			30	20	10	

- Molecule 26 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
26	A	1	Total	Ca	0
			1	1	
26	B	1	Total	Ca	0
			1	1	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



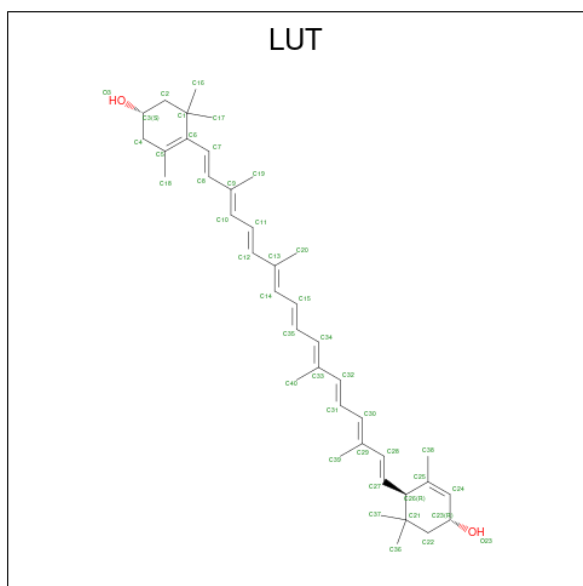
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			61	46	15	
27	F	1	Total	C	O	0
			57	42	15	

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Mol	Chain	Residues	Atoms			AltConf
27	G	1	Total	C	O	0
			47	32	15	
27	J	1	Total	C	O	0
			58	43	15	
27	1	1	Total	C	O	0
			41	26	15	
27	3	1	Total	C	O	0
			51	36	15	
27	4	1	Total	C	O	0
			51	36	15	
27	4	1	Total	C	O	0
			51	36	15	

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂).



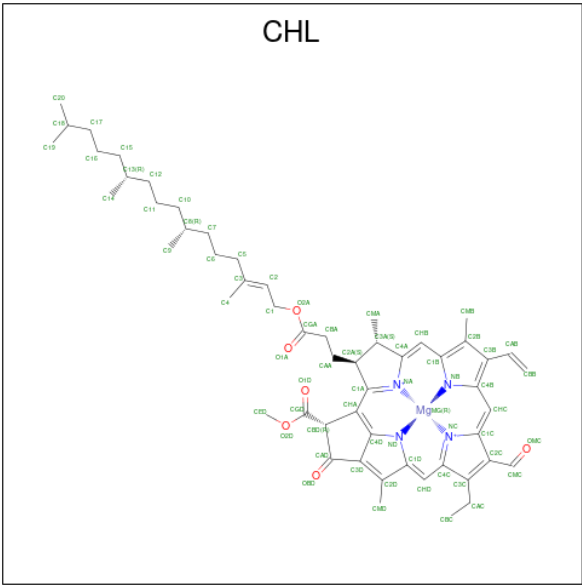
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
28	3	1	Total	C	O	0
			42	40	2	
28	4	1	Total	C	O	0
			42	40	2	

- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



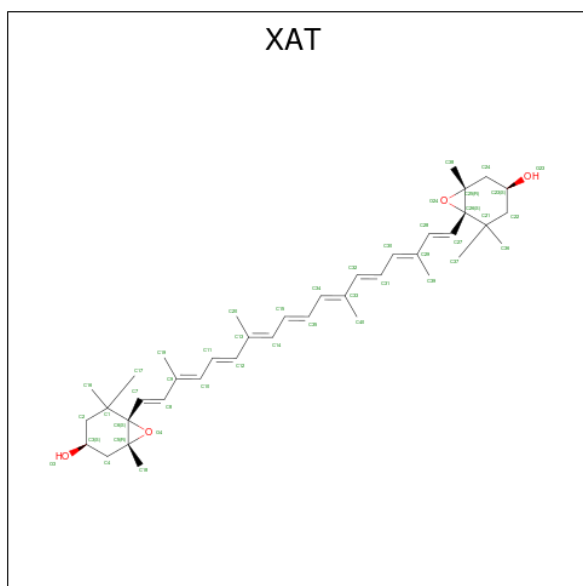
Mol	Chain	Residues	Atoms						AltConf
29	1	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	1	1	Total	C	Mg	N	O	0	
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	
			61	50	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			46	35	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	3	1	Total	C	Mg	N	O	0	
			66	55	1	4	6		

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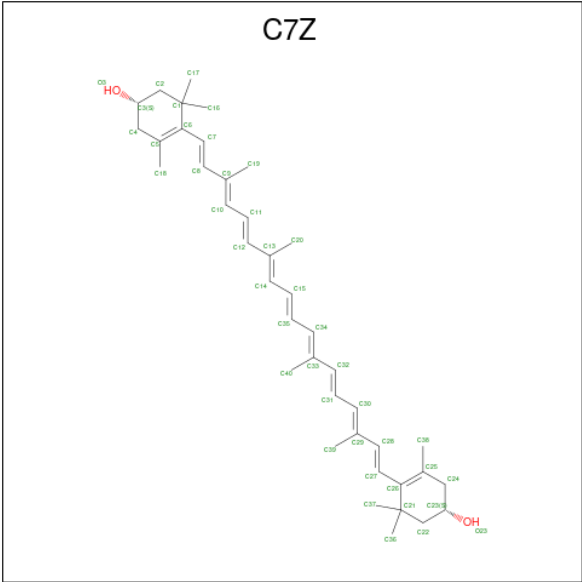
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 30 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



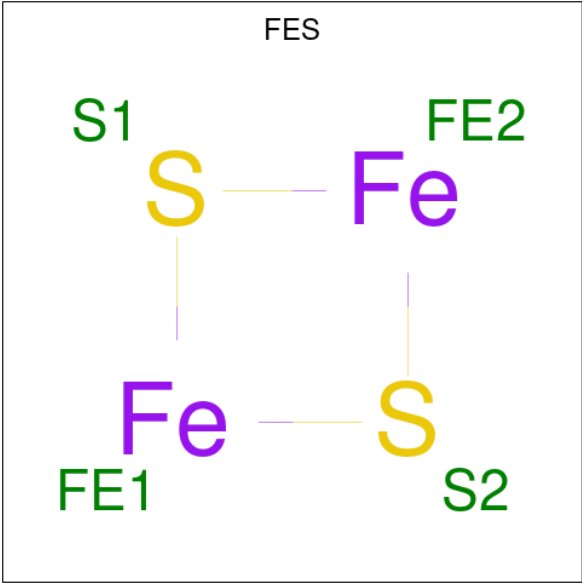
Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	

- Molecule 31 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 (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
31	4	1	Total	C	O	0
			42	40	2	

- Molecule 32 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
32	N	1	Total	Fe	S	0
			4	2	2	

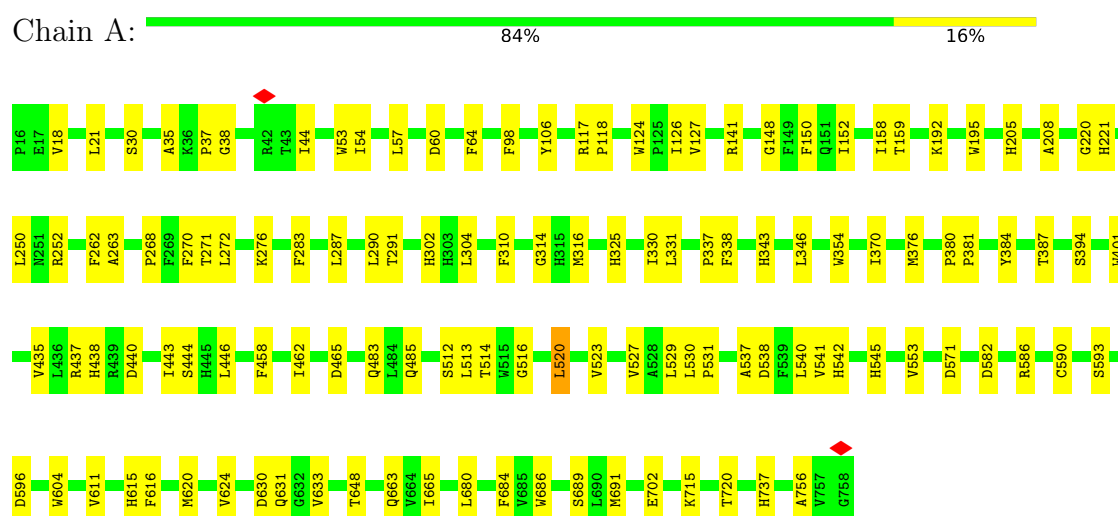
- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	A	13	Total 13	O 13	0
33	B	15	Total 15	O 15	0
33	C	2	Total 2	O 2	0
33	D	1	Total 1	O 1	0
33	F	3	Total 3	O 3	0
33	G	4	Total 4	O 4	0
33	I	1	Total 1	O 1	0
33	J	2	Total 2	O 2	0
33	K	1	Total 1	O 1	0
33	L	3	Total 3	O 3	0
33	1	5	Total 5	O 5	0
33	2	2	Total 2	O 2	0
33	3	3	Total 3	O 3	0
33	4	1	Total 1	O 1	0

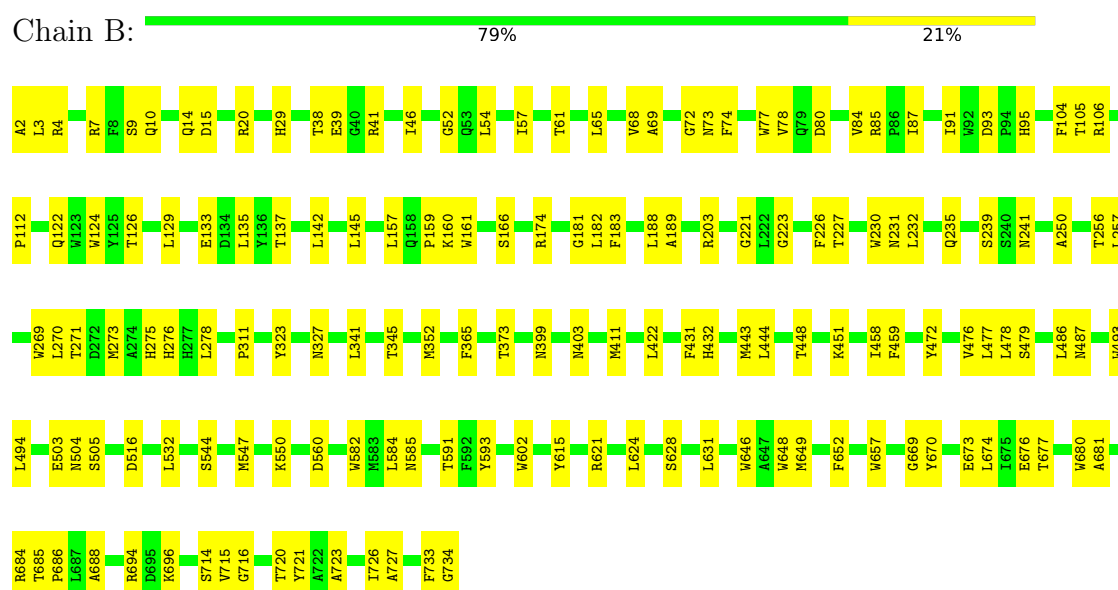
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center

Chain C:  90% 10%



- Molecule 4: PsaD

Chain D:  78% 22%



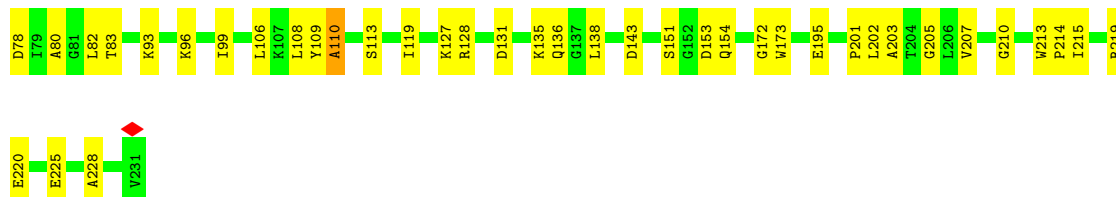
- Molecule 5: PsaE

Chain E:  89% 11%



- Molecule 6: PsaF

Chain F:  75% 25%



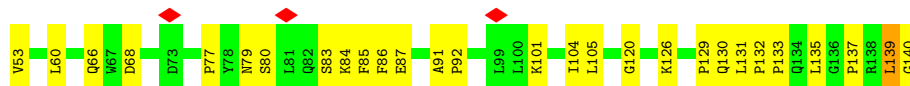
- Molecule 7: PsaG

Chain G:  87% 13%



- Molecule 8: PsaH

Chain H:  68% 31%

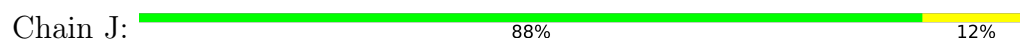


- Molecule 9: Photosystem I reaction center subunit VIII

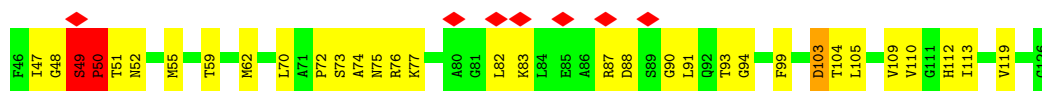
Chain I:  81% 19%



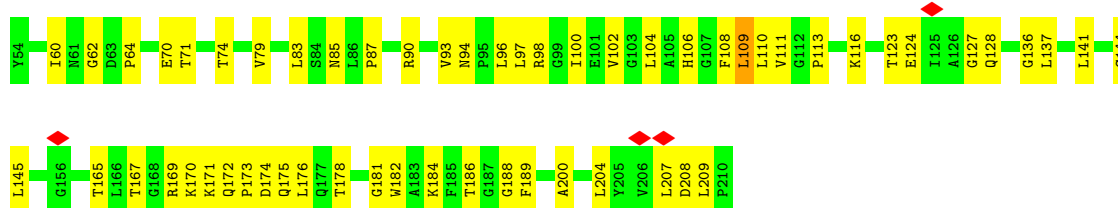
- Molecule 10: Photosystem I reaction center subunit IX



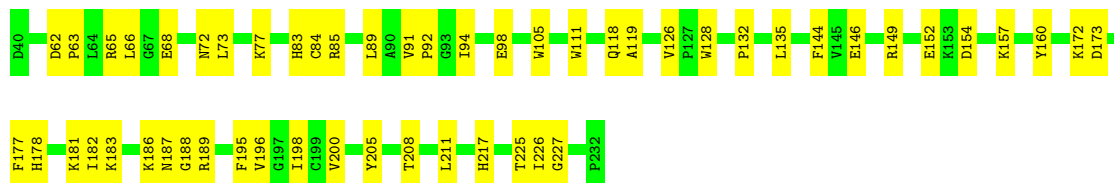
- Molecule 11: Photosystem I reaction center subunit X psaK



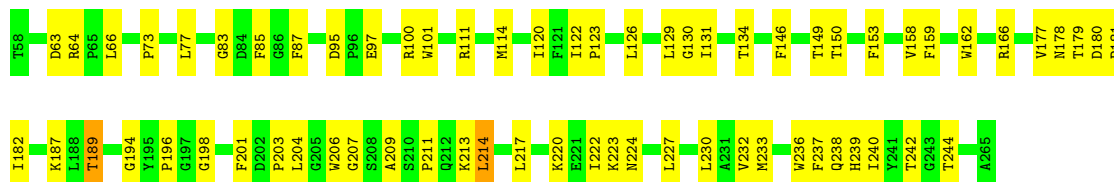
- Molecule 12: PsaL



- Molecule 13: Lhca1

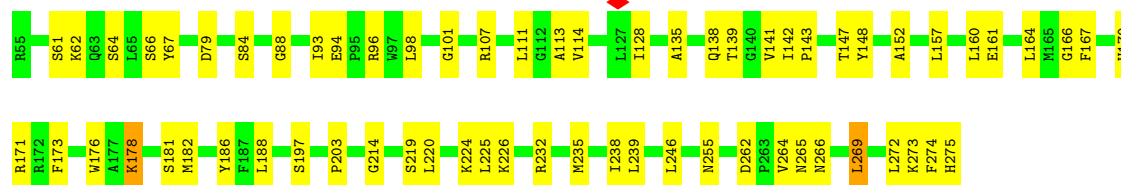


- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



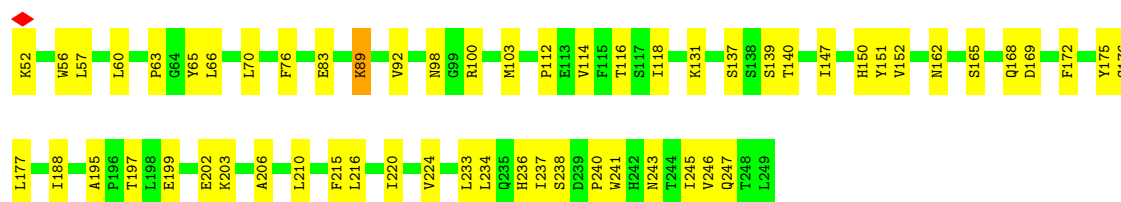
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:  71% 29%



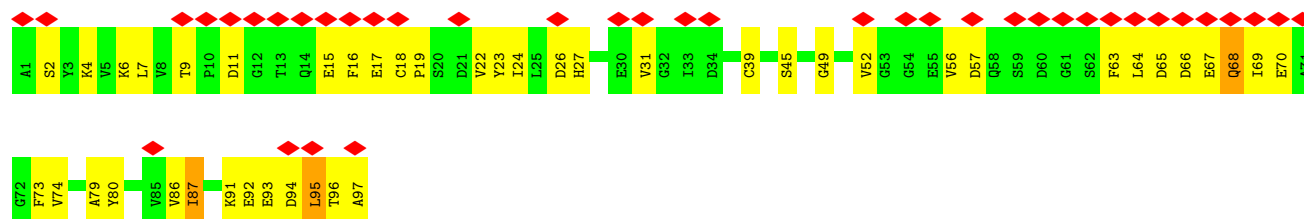
- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:  71% 29%



- Molecule 17: Ferredoxin-1, chloroplastic

Chain N:  40% 55% 42%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269657	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 ($e^-/\text{\AA}^2$)	1.075	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.111	Depositor
Minimum map value	-0.059	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0131	Depositor
Map size ($\text{\AA}$)	358.05002, 358.05002, 358.05002	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.085, 1.085, 1.085	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, LMT, SF4, BCR, CLA, LUT, DGD, CA, CHL, PQN, LMG, FES, CL0, XAT, C7Z

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	0.42	1/6057 (0.0%)	0.55	2/8264 (0.0%)
2	B	0.31	0/6069	0.46	0/8286
3	C	0.27	0/625	0.41	0/846
4	D	0.27	0/1163	0.48	0/1572
5	E	0.25	0/540	0.41	0/734
6	F	0.61	1/1234 (0.1%)	0.88	2/1670 (0.1%)
7	G	0.25	0/776	0.41	0/1054
8	H	0.33	0/693	0.61	2/942 (0.2%)
9	I	0.35	0/246	0.52	0/335
10	J	0.24	0/349	0.37	0/476
11	K	0.86	2/576 (0.3%)	1.00	3/779 (0.4%)
12	L	0.30	0/1207	0.53	0/1651
13	1	0.26	0/1558	0.43	0/2125
14	2	0.41	0/1679	0.65	2/2302 (0.1%)
15	3	0.25	0/1760	0.43	0/2390
16	4	0.28	0/1608	0.48	0/2191
17	N	0.47	0/736	0.75	1/1000 (0.1%)
All	All	0.37	4/26876 (0.0%)	0.55	12/36617 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	50	PRO	N-CA	18.16	1.70	1.47
1	A	117	ARG	C-N	13.23	1.51	1.33
6	F	83	THR	C-N	12.71	1.50	1.33
11	K	49	SER	C-N	5.07	1.45	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	83	THR	CA-C-N	16.03	136.24	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	83	THR	C-N-CA	16.03	136.24	119.89
11	K	49	SER	CA-C-N	15.46	139.17	119.84
11	K	49	SER	C-N-CA	15.46	139.17	119.84
1	A	117	ARG	CA-C-N	13.45	133.60	119.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5858	0	5719	105	0
2	B	5857	0	5653	141	0
3	C	612	0	591	6	0
4	D	1132	0	1141	25	0
5	E	528	0	528	4	0
6	F	1206	0	1231	33	0
7	G	757	0	743	17	0
8	H	673	0	667	27	0
9	I	240	0	264	13	0
10	J	338	0	345	6	0
11	K	569	0	596	40	0
12	L	1174	0	1183	52	0
13	1	1508	0	1489	51	0
14	2	1620	0	1557	72	0
15	3	1706	0	1661	56	0
16	4	1559	0	1527	59	0
17	N	724	0	672	75	0
18	A	65	0	72	5	0
19	1	608	0	565	41	0
19	2	522	0	503	41	0
19	3	578	0	497	27	0
19	4	631	0	600	41	0
19	A	2643	0	2751	161	0
19	B	2610	0	2750	159	0
19	F	130	0	144	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	G	226	0	212	12	0
19	J	50	0	39	0	0
19	K	199	0	158	21	0
19	L	160	0	136	10	0
20	A	33	0	46	0	0
20	B	33	0	46	3	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
22	1	80	0	105	8	0
22	2	40	0	53	9	0
22	3	80	0	105	4	0
22	A	240	0	316	17	0
22	B	200	0	264	14	0
22	F	80	0	104	5	0
22	G	80	0	105	8	0
22	I	80	0	105	6	0
22	J	40	0	53	1	0
22	K	80	0	106	12	0
22	L	80	0	106	7	0
23	1	49	0	74	8	0
23	2	68	0	76	4	0
23	3	17	0	12	0	0
23	A	89	0	127	5	0
23	B	70	0	86	9	0
24	A	35	0	45	3	0
24	B	63	0	69	4	0
24	G	66	0	77	2	0
24	J	25	0	22	0	0
25	1	46	0	65	3	0
25	2	117	0	114	9	0
25	3	30	0	30	0	0
25	A	50	0	73	5	0
25	B	102	0	114	6	0
25	F	160	0	188	13	0
25	G	124	0	161	8	0
26	A	1	0	0	0	0
26	B	1	0	0	0	0
27	1	41	0	40	1	0
27	3	51	0	60	3	0
27	4	102	0	120	6	0
27	B	61	0	83	7	0
27	F	57	0	75	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	G	47	0	52	4	0
27	J	58	0	77	4	0
28	1	84	0	110	16	0
28	2	42	0	55	4	0
28	3	84	0	110	4	0
28	4	42	0	55	6	0
28	J	42	0	55	4	0
29	1	164	0	133	15	0
29	2	272	0	226	22	0
29	3	164	0	137	14	0
29	4	202	0	151	14	0
30	2	44	0	56	9	0
30	4	44	0	56	4	0
31	4	42	0	0	0	0
32	N	4	0	0	1	0
33	1	5	0	0	2	0
33	2	2	0	0	0	0
33	3	3	0	0	0	0
33	4	1	0	0	0	0
33	A	13	0	0	1	0
33	B	15	0	0	0	0
33	C	2	0	0	0	0
33	D	1	0	0	0	0
33	F	3	0	0	0	0
33	G	4	0	0	1	0
33	I	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	L	3	0	0	1	0
All	All	38469	0	38492	1207	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 16.

The worst 5 of 1207 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)
11:K:50:PRO:N	11:K:50:PRO:CA	1.70	1.36
17:N:73:PHE:CG	17:N:95:LEU:HD23	1.75	1.19
17:N:64:LEU:CD2	17:N:69:ILE:HD11	1.80	1.12
11:K:49:SER:H	11:K:50:PRO:CD	1.65	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:4:220:ILE:HG21	19:4:603:CLA:HAC2	1.08	1.07

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/743 (100%)	715 (96%)	26 (4%)	0	100	100
2	B	731/733 (100%)	698 (96%)	33 (4%)	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	64/66 (97%)	61 (95%)	3 (5%)	0	100	100
6	F	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	18	34
7	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
8	H	86/88 (98%)	78 (91%)	8 (9%)	0	100	100
9	I	29/31 (94%)	29 (100%)	0	0	100	100
10	J	40/42 (95%)	40 (100%)	0	0	100	100
11	K	79/81 (98%)	70 (89%)	6 (8%)	3 (4%)	2	3
12	L	155/157 (99%)	143 (92%)	12 (8%)	0	100	100
13	1	191/193 (99%)	175 (92%)	16 (8%)	0	100	100
14	2	206/208 (99%)	178 (86%)	26 (13%)	2 (1%)	12	24
15	3	219/221 (99%)	190 (87%)	29 (13%)	0	100	100
16	4	196/198 (99%)	181 (92%)	15 (8%)	0	100	100
17	N	95/97 (98%)	84 (88%)	9 (10%)	2 (2%)	5	9
All	All	3298/3332 (99%)	3082 (94%)	208 (6%)	8 (0%)	44	63

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	49	SER
11	K	50	PRO
17	N	66	ASP
14	2	149	THR
17	N	68	GLN

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	604/604 (100%)	602 (100%)	2 (0%)	86	94
2	B	598/598 (100%)	598 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	122/122 (100%)	122 (100%)	0	100	100
5	E	58/58 (100%)	58 (100%)	0	100	100
6	F	125/126 (99%)	125 (100%)	0	100	100
7	G	82/82 (100%)	82 (100%)	0	100	100
8	H	71/71 (100%)	70 (99%)	1 (1%)	59	81
9	I	27/27 (100%)	27 (100%)	0	100	100
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	59/59 (100%)	58 (98%)	1 (2%)	53	78
12	L	124/124 (100%)	123 (99%)	1 (1%)	73	88
13	1	158/158 (100%)	158 (100%)	0	100	100
14	2	167/167 (100%)	166 (99%)	1 (1%)	78	91
15	3	171/172 (99%)	168 (98%)	3 (2%)	51	77
16	4	164/164 (100%)	161 (98%)	3 (2%)	51	77
17	N	82/82 (100%)	81 (99%)	1 (1%)	63	83
All	All	2716/2718 (100%)	2703 (100%)	13 (0%)	78	92

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	3	178	LYS
15	3	269	LEU
17	N	87	ILE
16	4	89	LYS
16	4	98	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	111	GLN
8	H	130	GLN
7	G	95	GLN
11	K	75	ASN
2	B	235	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 243 ligands modelled in this entry, 2 are monoatomic - leaving 241 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.93	20 (24%)
19	CLA	B	1235	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	20 (24%)
29	CHL	2	615	-	50,64,74	1.39	9 (18%)	46,102,114	1.85	11 (23%)
22	BCR	B	4006	-	41,41,41	1.65	4 (9%)	56,56,56	4.33	26 (46%)
19	CLA	A	1112	-	69,73,73	1.38	6 (8%)	82,113,113	1.90	19 (23%)
31	C7Z	4	505	-	43,43,43	4.05	18 (41%)	56,60,60	5.32	30 (53%)
28	LUT	1	501	-	42,43,43	2.46	1 (2%)	51,60,60	1.60	10 (19%)
19	CLA	A	1131	-	69,73,73	1.39	6 (8%)	82,113,113	1.90	17 (20%)
19	CLA	G	1602	7	50,54,73	1.60	6 (12%)	59,90,113	2.05	17 (28%)
25	LMG	F	5004	-	34,34,55	0.47	0	42,42,63	1.14	2 (4%)
28	LUT	J	4013	-	42,43,43	2.37	1 (2%)	51,60,60	1.90	9 (17%)
19	CLA	F	1302	6	69,73,73	1.34	6 (8%)	82,113,113	1.91	19 (23%)
19	CLA	4	603	-	69,73,73	1.38	6 (8%)	82,113,113	1.84	18 (21%)
27	DGD	3	803	-	52,52,67	0.91	3 (5%)	66,66,81	1.11	4 (6%)
19	CLA	B	1022	-	69,73,73	1.38	6 (8%)	82,113,113	1.88	20 (24%)
19	CLA	1	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	16 (19%)
19	CLA	A	1129	-	69,73,73	1.38	6 (8%)	82,113,113	1.88	13 (15%)
19	CLA	A	1107	1	69,73,73	1.39	6 (8%)	82,113,113	1.90	19 (23%)
27	DGD	4	801	-	52,52,67	1.00	4 (7%)	66,66,81	1.29	7 (10%)
19	CLA	A	1117	-	69,73,73	1.36	6 (8%)	82,113,113	1.85	14 (17%)
20	PQN	A	2001	-	34,34,34	0.34	0	43,45,45	1.24	4 (9%)
27	DGD	B	5005	-	62,62,67	1.21	6 (9%)	76,76,81	1.11	4 (5%)
22	BCR	K	4001	-	41,41,41	1.62	4 (9%)	56,56,56	4.52	14 (25%)
25	LMG	G	5001	-	49,49,55	1.11	4 (8%)	57,57,63	1.27	4 (7%)
29	CHL	2	613	-	40,54,74	1.69	9 (22%)	34,90,114	2.04	10 (29%)
19	CLA	K	1403	11	52,56,73	1.59	8 (15%)	61,92,113	2.25	18 (29%)
19	CLA	B	1215	-	69,73,73	1.37	6 (8%)	82,113,113	2.02	18 (21%)
25	LMG	2	803	-	36,36,55	0.73	2 (5%)	44,44,63	1.07	3 (6%)
19	CLA	K	1402	-	64,68,73	1.45	8 (12%)	76,107,113	2.02	19 (25%)
19	CLA	4	605	-	64,68,73	1.52	6 (9%)	76,107,113	1.92	20 (26%)
28	LUT	3	502	-	42,43,43	2.43	2 (4%)	51,60,60	1.89	9 (17%)
19	CLA	A	1140	-	69,73,73	1.35	6 (8%)	82,113,113	1.82	18 (21%)
19	CLA	1	606	-	54,58,73	1.52	7 (12%)	64,95,113	2.10	20 (31%)
20	PQN	B	2002	-	34,34,34	0.34	0	43,45,45	1.21	3 (6%)
19	CLA	2	601	-	64,68,73	1.42	7 (10%)	76,107,113	1.90	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DGD	1	803	-	42,42,67	0.88	2 (4%)	56,56,81	1.11	3 (5%)
22	BCR	1	504	-	41,41,41	1.64	4 (9%)	56,56,56	4.79	19 (33%)
19	CLA	B	1206	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	13 (15%)
19	CLA	1	608	-	50,54,73	1.59	6 (12%)	59,90,113	2.22	16 (27%)
19	CLA	A	1125	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	18 (21%)
19	CLA	A	1139	-	69,73,73	1.39	7 (10%)	82,113,113	1.96	21 (25%)
19	CLA	K	1404	-	50,54,73	1.61	8 (16%)	59,90,113	1.99	17 (28%)
19	CLA	A	1130	-	59,63,73	1.48	6 (10%)	70,101,113	1.98	17 (24%)
19	CLA	4	604	-	64,68,73	1.43	6 (9%)	76,107,113	2.05	19 (25%)
25	LMG	B	5007	-	34,34,55	0.50	0	42,42,63	1.19	3 (7%)
22	BCR	I	4018	-	41,41,41	1.61	5 (12%)	56,56,56	4.39	20 (35%)
25	LMG	2	804	-	30,30,55	0.53	0	38,38,63	1.22	3 (7%)
19	CLA	4	607	-	64,68,73	1.41	7 (10%)	76,107,113	1.80	17 (22%)
22	BCR	I	4020	-	41,41,41	1.67	5 (12%)	56,56,56	4.59	16 (28%)
19	CLA	1	601	-	69,73,73	1.38	7 (10%)	82,113,113	1.89	17 (20%)
19	CLA	3	608	-	52,56,73	1.58	8 (15%)	61,92,113	2.14	19 (31%)
23	LHG	3	801	-	16,16,48	0.88	1 (6%)	17,20,54	0.69	0
19	CLA	B	1227	-	69,73,73	1.39	6 (8%)	82,113,113	1.89	18 (21%)
19	CLA	G	1701	-	64,68,73	1.43	7 (10%)	76,107,113	1.94	14 (18%)
19	CLA	B	1202	-	69,73,73	1.35	6 (8%)	82,113,113	1.78	19 (23%)
19	CLA	A	1124	33	59,63,73	1.48	7 (11%)	70,101,113	2.07	19 (27%)
22	BCR	A	4011	-	41,41,41	1.63	4 (9%)	56,56,56	4.45	17 (30%)
19	CLA	B	1219	-	69,73,73	1.39	6 (8%)	82,113,113	1.88	18 (21%)
19	CLA	A	1115	-	69,73,73	1.37	6 (8%)	82,113,113	1.86	16 (19%)
22	BCR	1	503	-	41,41,41	1.60	4 (9%)	56,56,56	4.40	17 (30%)
19	CLA	B	1240	-	69,73,73	1.39	6 (8%)	82,113,113	1.93	17 (20%)
19	CLA	A	1138	-	69,73,73	1.37	7 (10%)	82,113,113	1.78	16 (19%)
19	CLA	2	606	-	54,58,73	1.56	7 (12%)	64,95,113	2.16	16 (25%)
19	CLA	4	608	-	50,54,73	1.59	7 (14%)	59,90,113	1.97	14 (23%)
29	CHL	2	611	-	42,56,74	2.09	9 (21%)	36,92,114	1.97	13 (36%)
19	CLA	B	1224	-	69,73,73	1.39	6 (8%)	82,113,113	1.86	19 (23%)
19	CLA	3	601	15	59,63,73	1.49	6 (10%)	70,101,113	2.00	17 (24%)
19	CLA	B	1229	-	69,73,73	1.38	6 (8%)	82,113,113	1.93	18 (21%)
19	CLA	A	1137	-	69,73,73	1.38	6 (8%)	82,113,113	1.86	17 (20%)
19	CLA	B	1021	-	69,73,73	1.40	6 (8%)	82,113,113	1.91	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1239	-	69,73,73	1.38	7 (10%)	82,113,113	1.91	18 (21%)
21	SF4	A	3001	1,2	0,12,12	-	-	-		
23	LHG	2	807	-	32,32,48	0.45	0	35,38,54	1.24	2 (5%)
29	CHL	4	615	-	37,51,74	1.68	8 (21%)	30,86,114	2.29	10 (33%)
22	BCR	F	4014	-	41,41,41	1.61	4 (9%)	56,56,56	4.44	13 (23%)
19	CLA	A	1121	-	64,68,73	1.43	9 (14%)	76,107,113	1.90	20 (26%)
22	BCR	B	4005	-	41,41,41	1.63	5 (12%)	56,56,56	4.43	16 (28%)
22	BCR	J	4012	-	41,41,41	1.59	4 (9%)	56,56,56	4.40	18 (32%)
29	CHL	1	610	13	41,55,74	1.99	9 (21%)	35,91,114	2.00	9 (25%)
19	CLA	B	1238	-	69,73,73	1.36	6 (8%)	82,113,113	1.94	20 (24%)
22	BCR	A	4008	-	41,41,41	1.63	4 (9%)	56,56,56	4.29	17 (30%)
22	BCR	G	4021	-	41,41,41	1.62	4 (9%)	56,56,56	4.52	17 (30%)
19	CLA	1	605	-	69,73,73	1.39	6 (8%)	82,113,113	1.96	16 (19%)
19	CLA	B	1226	-	69,73,73	1.38	7 (10%)	82,113,113	1.95	15 (18%)
19	CLA	1	603	-	59,63,73	1.49	7 (11%)	70,101,113	2.10	21 (30%)
19	CLA	B	1209	-	50,54,73	1.61	6 (12%)	59,90,113	2.07	14 (23%)
22	BCR	G	4011	-	41,41,41	1.60	4 (9%)	56,56,56	4.69	18 (32%)
19	CLA	B	1236	-	54,58,73	1.55	6 (11%)	64,95,113	2.08	18 (28%)
19	CLA	A	1120	-	64,68,73	1.41	6 (9%)	76,107,113	1.95	16 (21%)
19	CLA	3	613	-	50,54,73	1.63	6 (12%)	59,90,113	2.09	13 (22%)
19	CLA	A	1135	-	55,59,73	1.52	7 (12%)	64,96,113	2.16	20 (31%)
19	CLA	B	1214	-	69,73,73	1.37	6 (8%)	82,113,113	1.92	18 (21%)
19	CLA	G	1601	-	59,63,73	1.51	7 (11%)	70,101,113	1.99	17 (24%)
23	LHG	A	5002	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
29	CHL	2	610	-	50,64,74	1.35	8 (16%)	46,102,114	1.88	13 (28%)
19	CLA	B	1213	-	64,68,73	1.45	6 (9%)	76,107,113	1.93	17 (22%)
19	CLA	3	605	15	59,63,73	1.52	8 (13%)	70,101,113	1.99	20 (28%)
19	CLA	L	1503	33	54,58,73	1.55	7 (12%)	64,95,113	2.10	17 (26%)
22	BCR	3	506	-	41,41,41	1.62	4 (9%)	56,56,56	4.59	15 (26%)
24	LMT	B	5008	-	32,32,36	1.24	6 (18%)	43,43,47	0.97	2 (4%)
29	CHL	4	613	-	55,69,74	1.35	9 (16%)	52,108,114	1.86	11 (21%)
19	CLA	B	1228	-	64,68,73	1.43	6 (9%)	76,107,113	1.92	16 (21%)
19	CLA	A	1111	-	69,73,73	1.36	6 (8%)	82,113,113	1.94	19 (23%)
25	LMG	G	5002	-	50,50,55	1.18	5 (10%)	58,58,63	1.19	4 (6%)
19	CLA	A	1109	-	69,73,73	1.36	6 (8%)	82,113,113	1.88	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	602	-	54,58,73	1.52	7 (12%)	64,95,113	2.18	20 (31%)
19	CLA	B	1212	-	59,63,73	1.50	8 (13%)	70,101,113	2.08	19 (27%)
19	CLA	A	1101	-	69,73,73	1.38	6 (8%)	82,113,113	2.07	18 (21%)
28	LUT	1	502	-	42,43,43	2.32	2 (4%)	51,60,60	1.92	14 (27%)
25	LMG	1	802	-	46,46,55	1.05	3 (6%)	54,54,63	1.11	4 (7%)
19	CLA	A	1118	-	54,58,73	1.56	7 (12%)	64,95,113	2.15	18 (28%)
19	CLA	2	612	-	59,63,73	1.50	6 (10%)	70,101,113	1.99	14 (20%)
19	CLA	B	1210	-	69,73,73	1.35	6 (8%)	82,113,113	2.00	20 (24%)
19	CLA	A	1013	-	69,73,73	1.38	6 (8%)	82,113,113	1.77	16 (19%)
19	CLA	B	1023	-	69,73,73	1.42	6 (8%)	82,113,113	1.88	19 (23%)
19	CLA	A	1126	-	69,73,73	1.40	6 (8%)	82,113,113	1.90	16 (19%)
25	LMG	2	806	-	13,13,55	0.53	0	18,18,63	0.54	0
19	CLA	B	1208	-	64,68,73	1.41	6 (9%)	76,107,113	1.90	18 (23%)
19	CLA	A	1114	-	50,54,73	1.59	7 (14%)	59,90,113	2.11	16 (27%)
19	CLA	A	1102	-	69,73,73	1.33	7 (10%)	82,113,113	1.91	18 (21%)
28	LUT	4	501	-	42,43,43	2.44	2 (4%)	51,60,60	1.90	15 (29%)
25	LMG	2	805	-	13,13,55	0.53	0	18,18,63	0.69	0
19	CLA	A	1122	-	69,73,73	1.37	7 (10%)	82,113,113	1.85	19 (23%)
19	CLA	1	602	13	50,54,73	1.59	6 (12%)	59,90,113	2.07	15 (25%)
19	CLA	3	606	-	54,58,73	1.55	7 (12%)	64,95,113	2.10	18 (28%)
19	CLA	3	617	-	64,68,73	1.40	5 (7%)	76,107,113	1.91	20 (26%)
25	LMG	3	802	-	30,30,55	0.58	1 (3%)	38,38,63	1.18	4 (10%)
19	CLA	1	614	13	64,68,73	1.42	8 (12%)	76,107,113	2.03	21 (27%)
19	CLA	A	1134	1	59,63,73	1.47	7 (11%)	70,101,113	2.07	19 (27%)
19	CLA	B	1223	-	69,73,73	1.42	6 (8%)	82,113,113	1.85	18 (21%)
32	FES	N	101	17	0,4,4	-	-	-	-	-
21	SF4	C	3002	3	0,12,12	-	-	-	-	-
19	CLA	4	606	-	54,58,73	1.57	6 (11%)	64,95,113	2.00	15 (23%)
19	CLA	1	613	-	49,53,73	1.64	7 (14%)	58,89,113	1.98	14 (24%)
19	CLA	B	1237	-	69,73,73	1.36	6 (8%)	82,113,113	1.88	16 (19%)
19	CLA	A	1104	1	69,73,73	1.38	6 (8%)	82,113,113	1.91	19 (23%)
19	CLA	4	617	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	18 (21%)
19	CLA	A	1133	-	69,73,73	1.36	6 (8%)	82,113,113	1.88	18 (21%)
22	BCR	B	4010	-	41,41,41	1.62	4 (9%)	56,56,56	4.34	13 (23%)
19	CLA	B	1217	-	50,54,73	1.63	6 (12%)	59,90,113	2.06	17 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	B	4004	-	41,41,41	1.65	4 (9%)	56,56,56	5.20	21 (37%)
19	CLA	2	602	-	56,60,73	1.54	7 (12%)	65,97,113	1.99	18 (27%)
21	SF4	C	3003	3	0,12,12	-	-	-		
23	LHG	2	801	-	34,34,48	0.50	0	37,40,54	1.20	5 (13%)
19	CLA	A	1127	-	69,73,73	1.38	7 (10%)	82,113,113	1.89	16 (19%)
19	CLA	F	1301	-	69,73,73	1.39	7 (10%)	82,113,113	1.86	16 (19%)
22	BCR	L	4019	-	41,41,41	1.62	4 (9%)	56,56,56	4.44	15 (26%)
22	BCR	2	503	-	41,41,41	1.61	4 (9%)	56,56,56	5.18	24 (42%)
24	LMT	G	5005	-	32,32,36	1.26	6 (18%)	43,43,47	1.14	5 (11%)
23	LHG	B	5001	-	20,20,48	0.63	0	23,26,54	1.65	3 (13%)
19	CLA	L	1501	-	54,58,73	1.53	7 (12%)	64,95,113	2.14	18 (28%)
19	CLA	A	1119	-	69,73,73	1.38	7 (10%)	82,113,113	1.81	16 (19%)
19	CLA	A	1113	-	49,53,73	1.64	7 (14%)	58,89,113	2.07	15 (25%)
24	LMT	J	5003	-	26,26,36	1.30	5 (19%)	37,37,47	1.15	4 (10%)
27	DGD	F	5005	-	58,58,67	1.13	5 (8%)	72,72,81	1.18	4 (5%)
19	CLA	3	603	-	59,63,73	1.46	7 (11%)	70,101,113	2.02	20 (28%)
29	CHL	3	607	-	45,59,74	1.53	9 (20%)	40,96,114	1.90	10 (25%)
29	CHL	3	611	-	41,55,74	1.86	8 (19%)	35,91,114	2.18	9 (25%)
19	CLA	B	1204	-	69,73,73	1.39	6 (8%)	82,113,113	1.79	16 (19%)
19	CLA	4	601	16	64,68,73	1.43	6 (9%)	76,107,113	1.97	18 (23%)
19	CLA	B	1203	2	69,73,73	1.38	6 (8%)	82,113,113	1.76	17 (20%)
19	CLA	A	1106	1	69,73,73	1.37	6 (8%)	82,113,113	1.88	16 (19%)
19	CLA	G	1603	-	69,73,73	1.36	7 (10%)	82,113,113	1.94	16 (19%)
23	LHG	1	801	-	48,48,48	0.40	0	51,54,54	1.15	5 (9%)
25	LMG	A	5006	-	50,50,55	1.19	5 (10%)	58,58,63	1.23	5 (8%)
19	CLA	A	1108	-	54,58,73	1.58	7 (12%)	64,95,113	2.05	19 (29%)
25	LMG	G	5006	-	25,25,55	0.57	0	33,33,63	1.23	2 (6%)
29	CHL	4	610	-	41,55,74	1.72	9 (21%)	35,91,114	2.28	11 (31%)
29	CHL	4	611	-	45,59,74	1.89	9 (20%)	40,96,114	1.98	11 (27%)
19	CLA	A	1012	-	69,73,73	1.41	6 (8%)	82,113,113	2.00	16 (19%)
19	CLA	B	1234	-	59,63,73	1.51	6 (10%)	70,101,113	1.98	19 (27%)
22	BCR	F	4016	-	41,41,41	1.65	5 (12%)	56,56,56	4.37	15 (26%)
19	CLA	3	602	-	56,60,73	1.52	7 (12%)	65,97,113	2.00	19 (29%)
25	LMG	F	5002	-	47,47,55	1.10	4 (8%)	55,55,63	1.23	4 (7%)
22	BCR	L	4020	-	41,41,41	1.63	4 (9%)	56,56,56	4.43	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	1	609	13	50,64,74	1.70	9 (18%)	46,102,114	1.96	13 (28%)
24	LMT	A	5004	-	36,36,36	1.17	6 (16%)	47,47,47	1.22	5 (10%)
25	LMG	2	802	-	25,25,55	0.59	0	33,33,63	1.12	3 (9%)
19	CLA	B	1230	-	62,66,73	1.47	6 (9%)	73,104,113	2.00	18 (24%)
19	CLA	A	1132	-	69,73,73	1.40	7 (10%)	82,113,113	1.95	20 (24%)
27	DGD	4	802	-	52,52,67	0.94	2 (3%)	66,66,81	1.03	2 (3%)
19	CLA	B	1225	-	69,73,73	1.39	6 (8%)	82,113,113	1.78	14 (17%)
25	LMG	B	5004	-	33,33,55	0.55	1 (3%)	41,41,63	1.25	4 (9%)
30	XAT	4	502	-	41,47,47	0.83	1 (2%)	54,74,74	1.77	13 (24%)
27	DGD	J	5001	-	59,59,67	1.14	5 (8%)	73,73,81	1.01	2 (2%)
19	CLA	A	1141	-	64,68,73	1.43	6 (9%)	76,107,113	2.06	19 (25%)
19	CLA	A	1136	-	69,73,73	1.34	7 (10%)	82,113,113	1.94	18 (21%)
19	CLA	K	1401	-	49,53,73	1.59	8 (16%)	58,89,113	2.07	15 (25%)
19	CLA	4	609	16	54,58,73	1.52	7 (12%)	64,95,113	2.15	17 (26%)
23	LHG	B	5002	-	48,48,48	0.40	0	51,54,54	1.09	3 (5%)
19	CLA	A	1116	-	60,64,73	1.49	6 (10%)	71,102,113	1.96	17 (23%)
19	CLA	1	607	-	50,54,73	1.60	6 (12%)	59,90,113	2.01	14 (23%)
19	CLA	3	614	-	46,50,73	1.67	8 (17%)	53,85,113	2.08	16 (30%)
25	LMG	B	5003	-	35,35,55	0.81	1 (2%)	43,43,63	1.18	5 (11%)
19	CLA	3	612	15	54,58,73	1.53	7 (12%)	64,95,113	2.12	16 (25%)
19	CLA	B	1232	-	59,63,73	1.50	7 (11%)	70,101,113	2.08	19 (27%)
25	LMG	F	5003	-	36,36,55	0.78	1 (2%)	44,44,63	1.05	2 (4%)
22	BCR	A	4003	-	41,41,41	1.61	4 (9%)	56,56,56	4.36	15 (26%)
28	LUT	2	501	-	42,43,43	2.48	2 (4%)	51,60,60	2.20	15 (29%)
22	BCR	3	503	-	41,41,41	1.64	4 (9%)	56,56,56	4.55	17 (30%)
19	CLA	L	1502	-	64,68,73	1.43	7 (10%)	76,107,113	1.92	17 (22%)
19	CLA	2	605	-	69,73,73	1.38	6 (8%)	82,113,113	2.02	19 (23%)
19	CLA	A	1128	-	69,73,73	1.39	6 (8%)	82,113,113	1.91	15 (18%)
22	BCR	A	4017	-	41,41,41	1.66	5 (12%)	56,56,56	4.97	18 (32%)
19	CLA	B	1218	-	69,73,73	1.38	8 (11%)	82,113,113	1.96	20 (24%)
18	CL0	A	1011	-	58,73,73	3.01	16 (27%)	60,113,113	2.85	19 (31%)
29	CHL	1	612	-	55,69,74	1.48	9 (16%)	52,108,114	1.78	11 (21%)
19	CLA	4	612	16	69,73,73	1.39	6 (8%)	82,113,113	1.89	19 (23%)
30	XAT	2	502	-	41,47,47	0.80	1 (2%)	54,74,74	2.23	13 (24%)
19	CLA	2	607	-	64,68,73	1.43	6 (9%)	76,107,113	1.95	20 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1231	-	64,68,73	1.43	6 (9%)	76,107,113	1.89	16 (21%)
19	CLA	A	1103	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	19 (23%)
19	CLA	B	1207	-	69,73,73	1.38	7 (10%)	82,113,113	1.92	19 (23%)
19	CLA	B	1221	-	69,73,73	1.38	6 (8%)	82,113,113	1.94	16 (19%)
22	BCR	A	4007	-	41,41,41	1.62	4 (9%)	56,56,56	4.57	19 (33%)
19	CLA	J	1901	33	54,58,73	1.52	8 (14%)	64,95,113	2.00	16 (25%)
24	LMT	B	5006	-	33,33,36	1.20	5 (15%)	44,44,47	1.05	4 (9%)
19	CLA	2	604	-	69,73,73	1.38	7 (10%)	82,113,113	1.92	18 (21%)
25	LMG	F	5001	-	30,30,55	0.55	0	38,38,63	1.14	2 (5%)
19	CLA	1	604	-	69,73,73	1.39	6 (8%)	82,113,113	1.84	19 (23%)
19	CLA	A	1105	-	64,68,73	1.45	7 (10%)	76,107,113	1.96	15 (19%)
19	CLA	B	1201	-	69,73,73	1.37	7 (10%)	82,113,113	1.92	20 (24%)
19	CLA	A	1123	-	69,73,73	1.40	7 (10%)	82,113,113	1.90	16 (19%)
27	DGD	G	5003	-	48,48,67	0.88	2 (4%)	62,62,81	1.14	3 (4%)
19	CLA	B	1216	-	69,73,73	1.36	7 (10%)	82,113,113	1.86	16 (19%)
25	LMG	F	5006	-	13,13,55	0.54	0	18,18,63	0.75	0
22	BCR	K	4002	-	41,41,41	1.63	4 (9%)	56,56,56	4.52	17 (30%)
19	CLA	B	1205	-	69,73,73	1.37	6 (8%)	82,113,113	1.92	17 (20%)
29	CHL	3	604	-	60,74,74	1.43	7 (11%)	58,114,114	1.77	11 (18%)
28	LUT	3	501	-	42,43,43	2.47	1 (2%)	51,60,60	1.90	12 (23%)
19	CLA	B	1220	-	59,63,73	1.49	6 (10%)	70,101,113	1.90	18 (25%)
22	BCR	A	4002	-	41,41,41	1.62	4 (9%)	56,56,56	4.40	21 (37%)
19	CLA	A	1110	-	59,63,73	1.48	7 (11%)	70,101,113	1.98	20 (28%)
19	CLA	B	1222	33	69,73,73	1.38	6 (8%)	82,113,113	1.99	14 (17%)
23	LHG	A	5001	-	39,39,48	0.44	0	42,45,54	1.14	3 (7%)
24	LMT	G	5004	-	36,36,36	1.19	5 (13%)	47,47,47	1.22	4 (8%)
19	CLA	2	608	-	54,58,73	1.54	6 (11%)	64,95,113	2.08	19 (29%)
29	CHL	2	609	14	60,74,74	1.72	9 (15%)	58,114,114	1.64	9 (15%)
19	CLA	B	1211	-	69,73,73	1.37	6 (8%)	82,113,113	1.96	20 (24%)
19	CLA	3	610	15	69,73,73	1.36	7 (10%)	82,113,113	1.86	15 (18%)
22	BCR	B	4009	-	41,41,41	1.62	4 (9%)	56,56,56	4.39	15 (26%)

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
19	CLA	2	603	-	1/1/15/20	14/39/115/115	-
19	CLA	B	1235	-	1/1/15/20	15/39/115/115	-
29	CHL	2	615	-	4/4/18/26	7/27/125/137	-
22	BCR	B	4006	-	-	12/29/63/63	0/2/2/2
19	CLA	A	1112	-	1/1/15/20	22/39/115/115	-
31	C7Z	4	505	-	-	16/29/67/67	0/2/2/2
28	LUT	1	501	-	-	2/29/67/67	0/2/2/2
19	CLA	A	1131	-	1/1/15/20	16/39/115/115	-
19	CLA	G	1602	7	1/1/11/20	6/17/93/115	-
25	LMG	F	5004	-	-	9/29/49/70	0/1/1/1
28	LUT	J	4013	-	1/1/12/27	4/29/67/67	0/2/2/2
19	CLA	F	1302	6	1/1/15/20	19/39/115/115	-
19	CLA	4	603	-	1/1/15/20	15/39/115/115	-
27	DGD	3	803	-	-	11/40/80/95	0/2/2/2
19	CLA	B	1022	-	1/1/15/20	11/39/115/115	-
19	CLA	1	611	-	1/1/15/20	14/39/115/115	-
19	CLA	A	1129	-	1/1/15/20	18/39/115/115	-
19	CLA	A	1107	1	1/1/15/20	19/39/115/115	-
27	DGD	4	801	-	-	17/40/80/95	0/2/2/2
19	CLA	A	1117	-	1/1/15/20	17/39/115/115	-
20	PQN	A	2001	-	-	4/23/43/43	0/2/2/2
27	DGD	B	5005	-	-	25/50/90/95	0/2/2/2
22	BCR	K	4001	-	-	9/29/63/63	0/2/2/2
25	LMG	G	5001	-	-	22/44/64/70	0/1/1/1
29	CHL	2	613	-	3/3/16/26	6/15/113/137	-
19	CLA	K	1403	11	1/1/11/20	10/19/95/115	-
19	CLA	B	1215	-	1/1/15/20	19/39/115/115	-
25	LMG	2	803	-	-	14/31/51/70	0/1/1/1
19	CLA	K	1402	-	1/1/14/20	23/33/109/115	-
19	CLA	4	605	-	-	15/33/109/115	-
28	LUT	3	502	-	1/1/12/27	8/29/67/67	0/2/2/2
19	CLA	A	1140	-	1/1/15/20	9/39/115/115	-
19	CLA	1	606	-	1/1/12/20	7/21/97/115	-
20	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
19	CLA	2	601	-	1/1/14/20	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DGD	1	803	-	-	12/30/70/95	0/2/2/2
22	BCR	1	504	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1206	-	1/1/15/20	18/39/115/115	-
19	CLA	1	608	-	1/1/11/20	9/17/93/115	-
19	CLA	A	1125	-	1/1/15/20	16/39/115/115	-
19	CLA	A	1139	-	1/1/15/20	17/39/115/115	-
19	CLA	K	1404	-	1/1/11/20	7/17/93/115	-
19	CLA	A	1130	-	1/1/13/20	12/27/103/115	-
19	CLA	4	604	-	1/1/14/20	13/33/109/115	-
25	LMG	B	5007	-	-	10/29/49/70	0/1/1/1
22	BCR	I	4018	-	-	13/29/63/63	0/2/2/2
25	LMG	2	804	-	-	9/25/45/70	0/1/1/1
19	CLA	4	607	-	1/1/14/20	18/33/109/115	-
22	BCR	I	4020	-	-	11/29/63/63	0/2/2/2
19	CLA	1	601	-	1/1/15/20	15/39/115/115	-
19	CLA	3	608	-	1/1/11/20	6/19/95/115	-
23	LHG	3	801	-	-	6/19/19/53	-
19	CLA	B	1227	-	1/1/15/20	15/39/115/115	-
19	CLA	G	1701	-	1/1/14/20	9/33/109/115	-
19	CLA	B	1202	-	1/1/15/20	14/39/115/115	-
19	CLA	A	1124	33	1/1/13/20	6/27/103/115	-
22	BCR	A	4011	-	-	11/29/63/63	0/2/2/2
19	CLA	B	1219	-	1/1/15/20	17/39/115/115	-
19	CLA	A	1115	-	1/1/15/20	23/39/115/115	-
22	BCR	1	503	-	-	17/29/63/63	0/2/2/2
19	CLA	B	1240	-	1/1/15/20	14/39/115/115	-
19	CLA	A	1138	-	1/1/15/20	12/39/115/115	-
19	CLA	2	606	-	1/1/12/20	6/21/97/115	-
19	CLA	4	608	-	1/1/11/20	8/17/93/115	-
29	CHL	2	611	-	3/3/16/26	3/18/116/137	-
19	CLA	B	1224	-	1/1/15/20	15/39/115/115	-
19	CLA	3	601	15	1/1/13/20	10/27/103/115	-
19	CLA	B	1229	-	1/1/15/20	13/39/115/115	-
19	CLA	A	1137	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1021	-	1/1/15/20	6/39/115/115	-
19	CLA	B	1239	-	1/1/15/20	18/39/115/115	-
21	SF4	A	3001	1,2	-	-	0/6/5/5
23	LHG	2	807	-	-	18/37/37/53	-
29	CHL	4	615	-	3/3/15/26	0/12/110/137	-
22	BCR	F	4014	-	-	9/29/63/63	0/2/2/2
19	CLA	A	1121	-	1/1/14/20	12/33/109/115	-
29	CHL	1	610	13	3/3/16/26	3/17/115/137	-
22	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
22	BCR	J	4012	-	-	11/29/63/63	0/2/2/2
19	CLA	B	1238	-	1/1/15/20	26/39/115/115	-
22	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
22	BCR	G	4021	-	-	14/29/63/63	0/2/2/2
19	CLA	1	605	-	1/1/15/20	15/39/115/115	-
19	CLA	B	1226	-	1/1/15/20	23/39/115/115	-
19	CLA	1	603	-	1/1/13/20	9/27/103/115	-
19	CLA	B	1209	-	1/1/11/20	6/17/93/115	-
22	BCR	G	4011	-	-	10/29/63/63	0/2/2/2
19	CLA	B	1236	-	1/1/12/20	8/21/97/115	-
19	CLA	A	1120	-	1/1/14/20	11/33/109/115	-
19	CLA	3	613	-	1/1/11/20	6/17/93/115	-
19	CLA	A	1135	-	1/1/12/20	9/23/99/115	-
19	CLA	B	1214	-	1/1/15/20	16/39/115/115	-
19	CLA	G	1601	-	1/1/13/20	8/27/103/115	-
29	CHL	2	610	-	4/4/18/26	5/27/125/137	-
23	LHG	A	5002	-	-	39/53/53/53	-
19	CLA	B	1213	-	1/1/14/20	6/33/109/115	-
19	CLA	3	605	15	-	12/27/103/115	-
19	CLA	L	1503	33	1/1/12/20	6/21/97/115	-
22	BCR	3	506	-	-	14/29/63/63	0/2/2/2
24	LMT	B	5008	-	-	7/17/57/61	0/2/2/2
29	CHL	4	613	-	4/4/19/26	8/33/131/137	-
19	CLA	B	1228	-	1/1/14/20	13/33/109/115	-
19	CLA	A	1111	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	G	5002	-	-	19/45/65/70	0/1/1/1
19	CLA	A	1109	-	1/1/15/20	10/39/115/115	-
19	CLA	4	602	-	1/1/12/20	7/21/97/115	-
19	CLA	B	1212	-	1/1/13/20	12/27/103/115	-
19	CLA	A	1101	-	1/1/15/20	21/39/115/115	-
28	LUT	1	502	-	-	0/29/67/67	0/2/2/2
25	LMG	1	802	-	-	13/41/61/70	0/1/1/1
19	CLA	A	1118	-	1/1/12/20	3/21/97/115	-
19	CLA	2	612	-	1/1/13/20	10/27/103/115	-
19	CLA	B	1210	-	1/1/15/20	15/39/115/115	-
19	CLA	A	1013	-	1/1/15/20	19/39/115/115	-
19	CLA	B	1023	-	1/1/15/20	10/39/115/115	-
19	CLA	A	1126	-	1/1/15/20	21/39/115/115	-
25	LMG	2	806	-	-	1/4/24/70	0/1/1/1
19	CLA	B	1208	-	1/1/14/20	12/33/109/115	-
19	CLA	A	1114	-	1/1/11/20	8/17/93/115	-
19	CLA	A	1102	-	1/1/15/20	27/39/115/115	-
28	LUT	4	501	-	-	4/29/67/67	0/2/2/2
25	LMG	2	805	-	-	2/4/24/70	0/1/1/1
19	CLA	A	1122	-	1/1/15/20	17/39/115/115	-
19	CLA	1	602	13	1/1/11/20	8/17/93/115	-
19	CLA	3	606	-	1/1/12/20	9/21/97/115	-
19	CLA	3	617	-	1/1/14/20	16/33/109/115	-
25	LMG	3	802	-	-	9/25/45/70	0/1/1/1
19	CLA	1	614	13	1/1/14/20	17/33/109/115	-
19	CLA	A	1134	1	1/1/13/20	12/27/103/115	-
19	CLA	B	1223	-	1/1/15/20	15/39/115/115	-
32	FES	N	101	17	-	-	0/1/1/1
21	SF4	C	3002	3	-	-	0/6/5/5
19	CLA	4	606	-	1/1/12/20	6/21/97/115	-
19	CLA	1	613	-	1/1/11/20	4/15/91/115	-
19	CLA	B	1237	-	1/1/15/20	18/39/115/115	-
19	CLA	A	1104	1	1/1/15/20	15/39/115/115	-
19	CLA	4	617	-	1/1/15/20	18/39/115/115	-
19	CLA	A	1133	-	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	B	4010	-	-	11/29/63/63	0/2/2/2
19	CLA	B	1217	-	1/1/11/20	9/17/93/115	-
22	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
19	CLA	2	602	-	1/1/12/20	8/24/100/115	-
21	SF4	C	3003	3	-	-	0/6/5/5
23	LHG	2	801	-	-	19/39/39/53	-
19	CLA	A	1127	-	1/1/15/20	15/39/115/115	-
19	CLA	F	1301	-	1/1/15/20	18/39/115/115	-
22	BCR	L	4019	-	-	12/29/63/63	0/2/2/2
22	BCR	2	503	-	-	13/29/63/63	0/2/2/2
24	LMT	G	5005	-	-	7/17/57/61	0/2/2/2
23	LHG	B	5001	-	-	11/23/23/53	-
19	CLA	L	1501	-	1/1/12/20	4/21/97/115	-
19	CLA	A	1119	-	1/1/15/20	14/39/115/115	-
19	CLA	A	1113	-	1/1/11/20	6/15/91/115	-
24	LMT	J	5003	-	-	6/11/51/61	0/2/2/2
27	DGD	F	5005	-	-	20/46/86/95	0/2/2/2
19	CLA	3	603	-	1/1/13/20	11/27/103/115	-
29	CHL	3	607	-	3/3/17/26	6/21/119/137	-
29	CHL	3	611	-	3/3/16/26	2/17/115/137	-
19	CLA	B	1204	-	1/1/15/20	21/39/115/115	-
19	CLA	4	601	16	1/1/14/20	18/33/109/115	-
19	CLA	B	1203	2	1/1/15/20	15/39/115/115	-
19	CLA	A	1106	1	1/1/15/20	17/39/115/115	-
19	CLA	G	1603	-	1/1/15/20	17/39/115/115	-
23	LHG	1	801	-	-	29/53/53/53	-
25	LMG	A	5006	-	-	16/45/65/70	0/1/1/1
19	CLA	A	1108	-	1/1/12/20	5/21/97/115	-
29	CHL	4	610	-	3/3/16/26	5/17/115/137	-
25	LMG	G	5006	-	-	10/20/40/70	0/1/1/1
29	CHL	4	611	-	3/3/17/26	2/21/119/137	-
19	CLA	A	1012	-	1/1/15/20	18/39/115/115	-
19	CLA	B	1234	-	1/1/13/20	10/27/103/115	-
22	BCR	F	4016	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	602	-	1/1/12/20	11/24/100/115	-
25	LMG	F	5002	-	-	10/42/62/70	0/1/1/1
29	CHL	1	609	13	4/4/18/26	3/27/125/137	-
22	BCR	L	4020	-	-	8/29/63/63	0/2/2/2
24	LMT	A	5004	-	-	7/21/61/61	0/2/2/2
25	LMG	2	802	-	-	8/20/40/70	0/1/1/1
19	CLA	B	1230	-	1/1/13/20	11/31/107/115	-
19	CLA	A	1132	-	1/1/15/20	15/39/115/115	-
27	DGD	4	802	-	-	17/40/80/95	0/2/2/2
19	CLA	B	1225	-	1/1/15/20	15/39/115/115	-
25	LMG	B	5004	-	-	14/28/48/70	0/1/1/1
30	XAT	4	502	-	2/2/12/26	6/31/93/93	0/4/4/4
27	DGD	J	5001	-	-	12/47/87/95	0/2/2/2
19	CLA	A	1141	-	1/1/14/20	11/33/109/115	-
19	CLA	A	1136	-	1/1/15/20	17/39/115/115	-
19	CLA	K	1401	-	1/1/11/20	6/15/91/115	-
19	CLA	4	609	16	1/1/12/20	8/21/97/115	-
23	LHG	B	5002	-	-	28/53/53/53	-
19	CLA	A	1116	-	1/1/13/20	16/29/105/115	-
19	CLA	1	607	-	1/1/11/20	4/17/93/115	-
19	CLA	3	614	-	1/1/10/20	3/12/88/115	-
25	LMG	B	5003	-	-	9/30/50/70	0/1/1/1
19	CLA	3	612	15	1/1/12/20	7/21/97/115	-
19	CLA	B	1232	-	1/1/13/20	14/27/103/115	-
28	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
22	BCR	A	4003	-	-	8/29/63/63	0/2/2/2
25	LMG	F	5003	-	-	15/31/51/70	0/1/1/1
22	BCR	3	503	-	-	11/29/63/63	0/2/2/2
19	CLA	L	1502	-	1/1/14/20	12/33/109/115	-
19	CLA	2	605	-	1/1/15/20	18/39/115/115	-
19	CLA	A	1128	-	1/1/15/20	11/39/115/115	-
22	BCR	A	4017	-	-	6/29/63/63	0/2/2/2
19	CLA	B	1218	-	1/1/15/20	11/39/115/115	-
18	CL0	A	1011	-	3/3/20/25	10/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	1	612	-	4/4/19/26	6/33/131/137	-
19	CLA	4	612	16	1/1/15/20	14/39/115/115	-
30	XAT	2	502	-	1/1/12/26	5/31/93/93	0/4/4/4
19	CLA	2	607	-	1/1/14/20	13/33/109/115	-
19	CLA	B	1231	-	1/1/14/20	11/33/109/115	-
19	CLA	A	1103	-	1/1/15/20	21/39/115/115	-
19	CLA	B	1207	-	1/1/15/20	17/39/115/115	-
19	CLA	B	1221	-	1/1/15/20	19/39/115/115	-
22	BCR	A	4007	-	-	4/29/63/63	0/2/2/2
19	CLA	J	1901	33	1/1/12/20	7/21/97/115	-
24	LMT	B	5006	-	-	10/18/58/61	0/2/2/2
19	CLA	2	604	-	1/1/15/20	15/39/115/115	-
25	LMG	F	5001	-	-	9/25/45/70	0/1/1/1
19	CLA	1	604	-	1/1/15/20	15/39/115/115	-
19	CLA	A	1105	-	1/1/14/20	17/33/109/115	-
19	CLA	B	1201	-	1/1/15/20	16/39/115/115	-
19	CLA	A	1123	-	1/1/15/20	15/39/115/115	-
27	DGD	G	5003	-	-	10/36/76/95	0/2/2/2
19	CLA	B	1216	-	1/1/15/20	16/39/115/115	-
25	LMG	F	5006	-	-	1/4/24/70	0/1/1/1
22	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
19	CLA	B	1205	-	1/1/15/20	12/39/115/115	-
29	CHL	3	604	-	4/4/20/26	12/39/137/137	-
28	LUT	3	501	-	-	3/29/67/67	0/2/2/2
19	CLA	B	1220	-	1/1/13/20	9/27/103/115	-
22	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
19	CLA	A	1110	-	1/1/13/20	6/27/103/115	-
19	CLA	B	1222	33	1/1/15/20	21/39/115/115	-
23	LHG	A	5001	-	-	24/44/44/53	-
24	LMT	G	5004	-	-	11/21/61/61	0/2/2/2
19	CLA	2	608	-	1/1/12/20	9/21/97/115	-
29	CHL	2	609	14	4/4/20/26	7/39/137/137	-
19	CLA	B	1211	-	1/1/15/20	17/39/115/115	-
19	CLA	3	610	15	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	B	4009	-	-	8/29/63/63	0/2/2/2

The worst 5 of 1300 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	3	501	LUT	C24-C25	15.22	1.51	1.33
28	2	501	LUT	C24-C25	15.12	1.51	1.33
28	1	501	LUT	C24-C25	14.86	1.50	1.33
28	4	501	LUT	C24-C25	14.84	1.50	1.33
28	3	502	LUT	C24-C25	14.83	1.50	1.33

The worst 5 of 3393 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4004	BCR	C11-C10-C9	19.73	154.96	127.28
22	1	504	BCR	C10-C11-C12	19.01	178.27	123.20
22	G	4021	BCR	C10-C11-C12	18.85	177.83	123.20
22	I	4018	BCR	C10-C11-C12	18.82	177.72	123.20
22	B	4004	BCR	C10-C11-C12	18.79	177.64	123.20

5 of 200 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	A	1011	CL0	ND
18	A	1011	CL0	NA
18	A	1011	CL0	NC
19	A	1012	CLA	ND
19	A	1013	CLA	ND

5 of 2844 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1013	CLA	C2-C1-O2A-CGA
19	A	1102	CLA	C3A-C2A-CAA-CBA
19	A	1103	CLA	C1A-C2A-CAA-CBA
19	A	1103	CLA	C3A-C2A-CAA-CBA
19	A	1103	CLA	CAD-CBD-CGD-O1D

There are no ring outliers.

218 monomers are involved in 718 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	603	CLA	8	0
19	B	1235	CLA	6	0
29	2	615	CHL	5	0
22	B	4006	BCR	5	0
19	A	1112	CLA	7	0
28	1	501	LUT	9	0
19	A	1131	CLA	3	0
19	G	1602	CLA	1	0
25	F	5004	LMG	2	0
28	J	4013	LUT	4	0
19	F	1302	CLA	4	0
19	4	603	CLA	10	0
27	3	803	DGD	3	0
19	B	1022	CLA	3	0
19	1	611	CLA	4	0
19	A	1129	CLA	2	0
19	A	1107	CLA	3	0
27	4	801	DGD	3	0
19	A	1117	CLA	1	0
27	B	5005	DGD	7	0
22	K	4001	BCR	4	0
25	G	5001	LMG	3	0
29	2	613	CHL	3	0
19	K	1403	CLA	1	0
19	B	1215	CLA	3	0
25	2	803	LMG	6	0
19	K	1402	CLA	2	0
19	4	605	CLA	6	0
28	3	502	LUT	2	0
19	A	1140	CLA	3	0
19	1	606	CLA	1	0
20	B	2002	PQN	3	0
19	2	601	CLA	8	0
27	1	803	DGD	1	0
22	1	504	BCR	2	0
19	B	1206	CLA	5	0
19	A	1125	CLA	5	0
19	A	1139	CLA	2	0
19	K	1404	CLA	4	0
19	A	1130	CLA	2	0
19	4	604	CLA	2	0
25	B	5007	LMG	2	0
22	I	4018	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	607	CLA	6	0
22	I	4020	BCR	3	0
19	1	601	CLA	12	0
19	B	1227	CLA	4	0
19	G	1701	CLA	4	0
19	B	1202	CLA	7	0
19	A	1124	CLA	2	0
22	A	4011	BCR	3	0
19	B	1219	CLA	7	0
19	A	1115	CLA	8	0
22	1	503	BCR	6	0
19	B	1240	CLA	10	0
19	A	1138	CLA	4	0
19	2	606	CLA	5	0
29	2	611	CHL	5	0
19	B	1224	CLA	6	0
19	3	601	CLA	6	0
19	B	1229	CLA	4	0
19	A	1137	CLA	4	0
19	B	1021	CLA	4	0
19	B	1239	CLA	6	0
23	2	807	LHG	2	0
29	4	615	CHL	3	0
19	A	1121	CLA	6	0
22	B	4005	BCR	2	0
22	J	4012	BCR	1	0
29	1	610	CHL	4	0
19	B	1238	CLA	8	0
22	A	4008	BCR	2	0
22	G	4021	BCR	4	0
19	1	605	CLA	4	0
19	B	1226	CLA	6	0
19	1	603	CLA	6	0
22	G	4011	BCR	4	0
19	B	1236	CLA	1	0
19	A	1120	CLA	4	0
19	3	613	CLA	3	0
19	A	1135	CLA	7	0
19	B	1214	CLA	5	0
19	G	1601	CLA	3	0
23	A	5002	LHG	2	0
29	2	610	CHL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1213	CLA	5	0
19	3	605	CLA	3	0
19	L	1503	CLA	3	0
22	3	506	BCR	2	0
24	B	5008	LMT	1	0
29	4	613	CHL	9	0
19	B	1228	CLA	2	0
19	A	1111	CLA	6	0
25	G	5002	LMG	5	0
19	A	1109	CLA	8	0
19	4	602	CLA	2	0
19	B	1212	CLA	1	0
19	A	1101	CLA	4	0
28	1	502	LUT	7	0
25	1	802	LMG	3	0
19	2	612	CLA	2	0
19	B	1210	CLA	5	0
19	A	1013	CLA	9	0
19	B	1023	CLA	5	0
19	A	1126	CLA	6	0
25	2	806	LMG	1	0
19	B	1208	CLA	2	0
19	A	1114	CLA	2	0
19	A	1102	CLA	6	0
28	4	501	LUT	6	0
19	A	1122	CLA	6	0
19	1	602	CLA	3	0
19	3	606	CLA	2	0
19	3	617	CLA	2	0
19	1	614	CLA	3	0
19	A	1134	CLA	3	0
19	B	1223	CLA	5	0
32	N	101	FES	1	0
19	4	606	CLA	3	0
19	1	613	CLA	4	0
19	B	1237	CLA	7	0
19	A	1104	CLA	3	0
19	4	617	CLA	3	0
19	A	1133	CLA	4	0
22	B	4010	BCR	1	0
19	B	1217	CLA	1	0
22	B	4004	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	602	CLA	3	0
23	2	801	LHG	2	0
19	A	1127	CLA	1	0
19	F	1301	CLA	2	0
22	L	4019	BCR	7	0
22	2	503	BCR	9	0
23	B	5001	LHG	4	0
19	L	1501	CLA	3	0
19	A	1119	CLA	7	0
19	A	1113	CLA	5	0
27	F	5005	DGD	7	0
19	3	603	CLA	3	0
29	3	607	CHL	5	0
29	3	611	CHL	2	0
19	B	1204	CLA	4	0
19	4	601	CLA	3	0
19	B	1203	CLA	2	0
19	A	1106	CLA	4	0
19	G	1603	CLA	4	0
23	1	801	LHG	8	0
25	A	5006	LMG	5	0
29	4	610	CHL	3	0
29	4	611	CHL	1	0
19	A	1012	CLA	7	0
19	B	1234	CLA	7	0
22	F	4016	BCR	5	0
19	3	602	CLA	4	0
25	F	5002	LMG	8	0
29	1	609	CHL	5	0
24	A	5004	LMT	3	0
25	2	802	LMG	2	0
19	B	1230	CLA	4	0
19	A	1132	CLA	2	0
27	4	802	DGD	3	0
19	B	1225	CLA	2	0
25	B	5004	LMG	1	0
30	4	502	XAT	4	0
27	J	5001	DGD	4	0
19	A	1141	CLA	4	0
19	A	1136	CLA	9	0
19	K	1401	CLA	14	0
19	4	609	CLA	3	0

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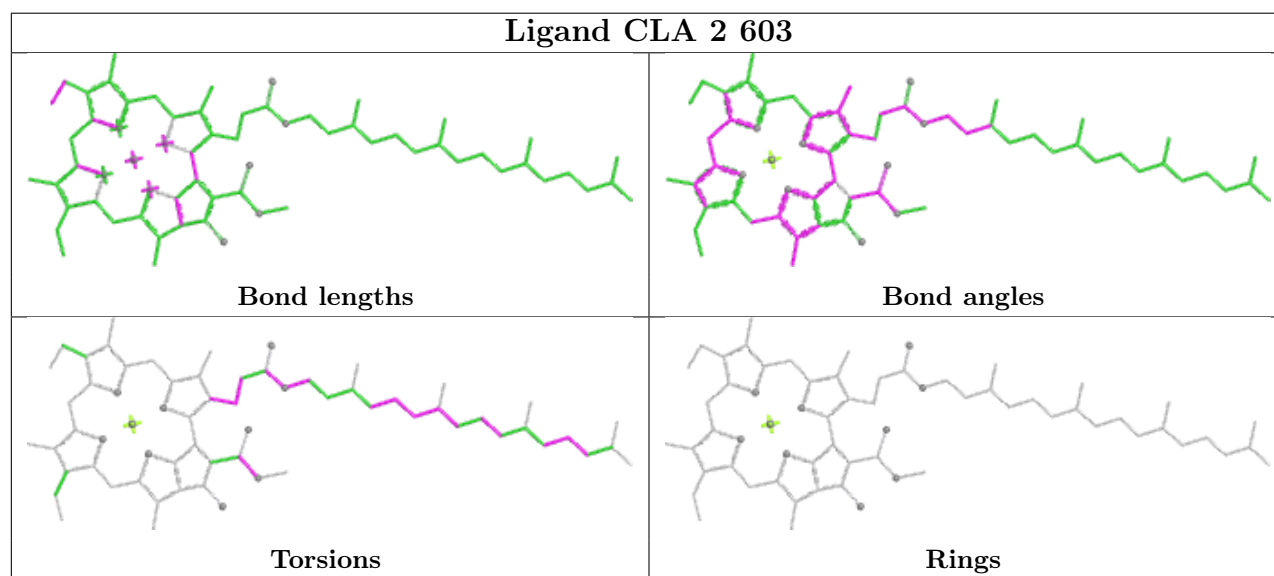
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19	1	607	CLA	1	0
25	B	5003	LMG	3	0
19	3	612	CLA	1	0
19	B	1232	CLA	3	0
25	F	5003	LMG	1	0
22	A	4003	BCR	2	0
28	2	501	LUT	4	0
22	3	503	BCR	2	0
19	L	1502	CLA	4	0
19	2	605	CLA	4	0
22	A	4017	BCR	5	0
19	B	1218	CLA	4	0
18	A	1011	CL0	5	0
29	1	612	CHL	6	0
19	4	612	CLA	4	0
30	2	502	XAT	9	0
19	2	607	CLA	2	0
19	B	1231	CLA	3	0
19	A	1103	CLA	7	0
19	B	1207	CLA	10	0
19	B	1221	CLA	4	0
22	A	4007	BCR	4	0
24	B	5006	LMT	3	0
19	2	604	CLA	11	0
25	F	5001	LMG	1	0
19	1	604	CLA	5	0
19	A	1105	CLA	6	0
19	B	1201	CLA	4	0
19	A	1123	CLA	4	0
27	G	5003	DGD	4	0
19	B	1216	CLA	2	0
25	F	5006	LMG	1	0
22	K	4002	BCR	8	0
19	B	1205	CLA	3	0
29	3	604	CHL	7	0
28	3	501	LUT	2	0
19	B	1220	CLA	4	0
22	A	4002	BCR	3	0
19	A	1110	CLA	5	0
19	B	1222	CLA	9	0

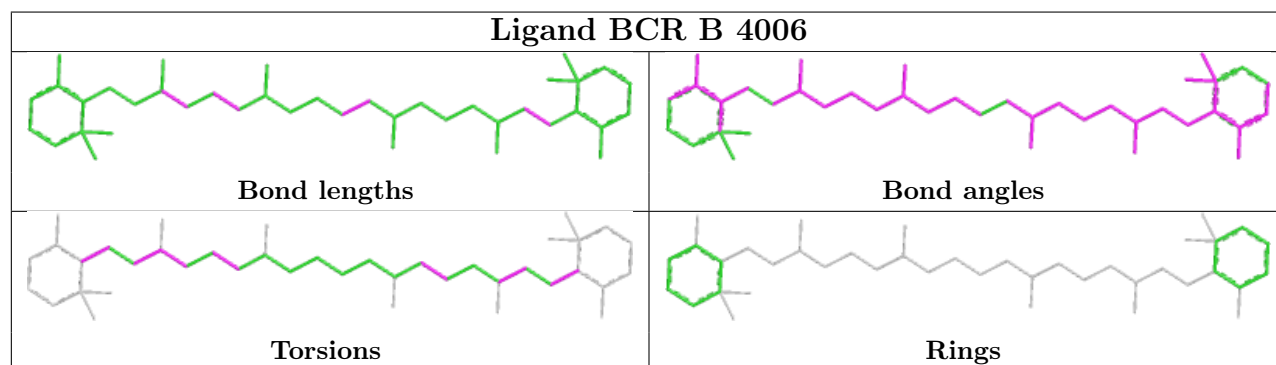
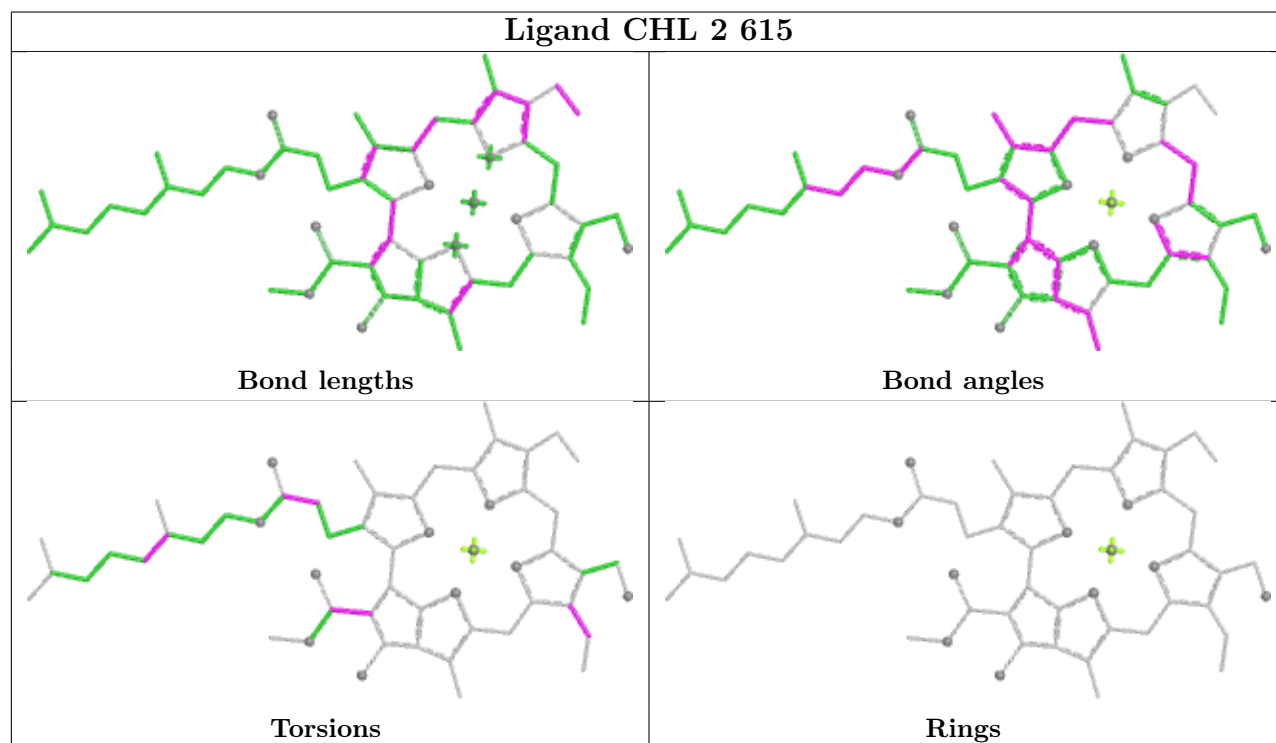
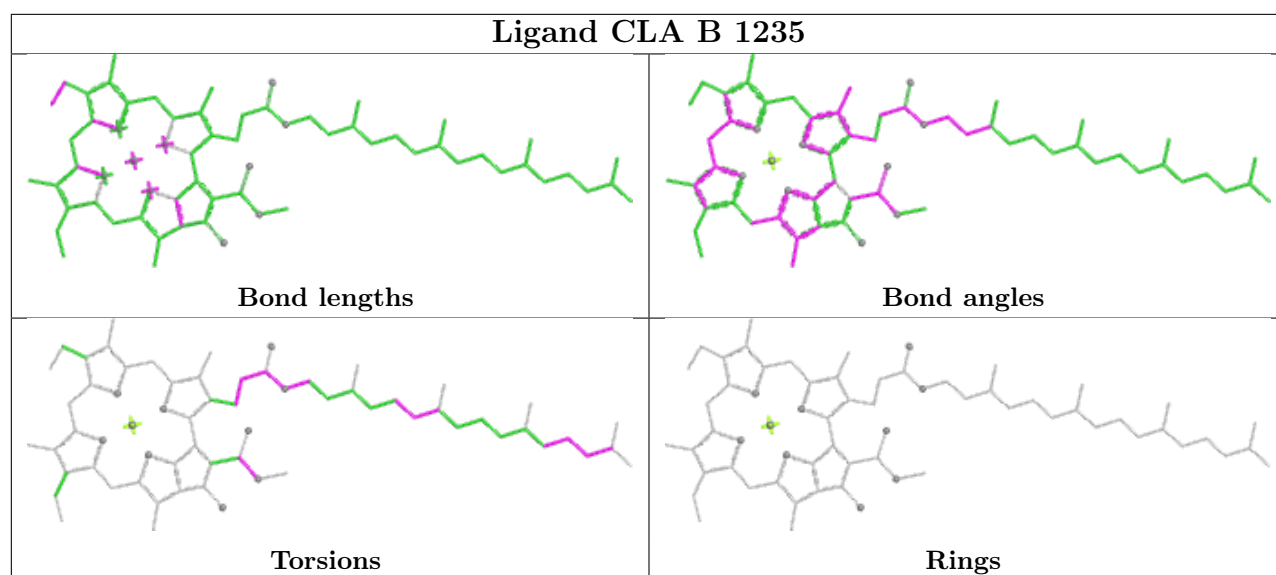
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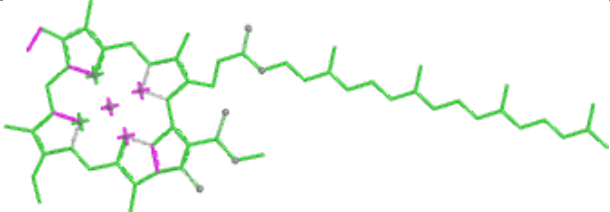
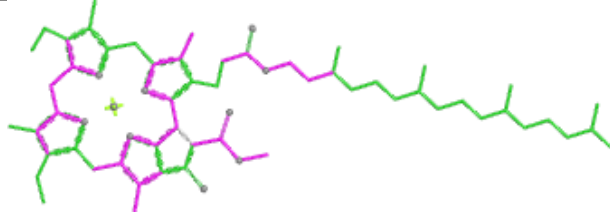
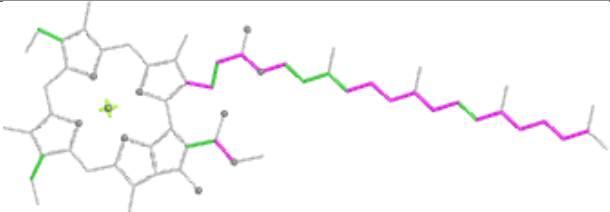
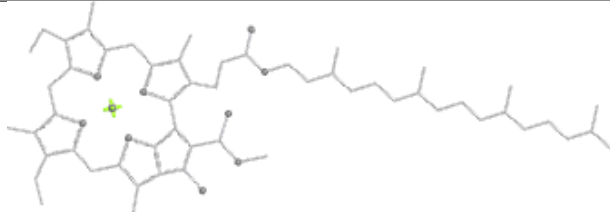
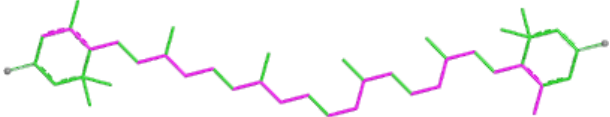
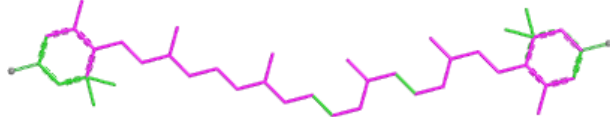
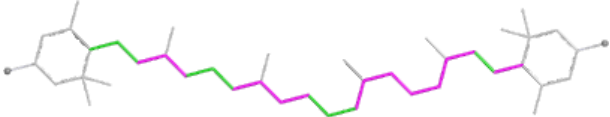
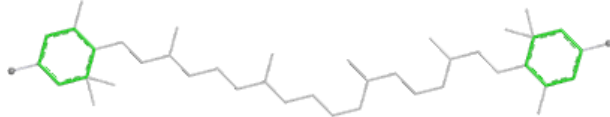
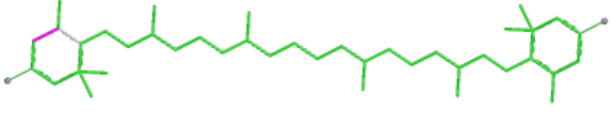
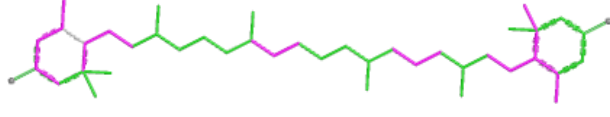
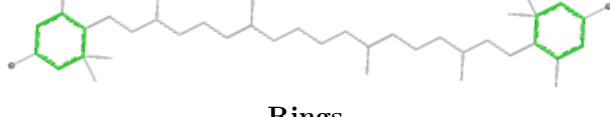
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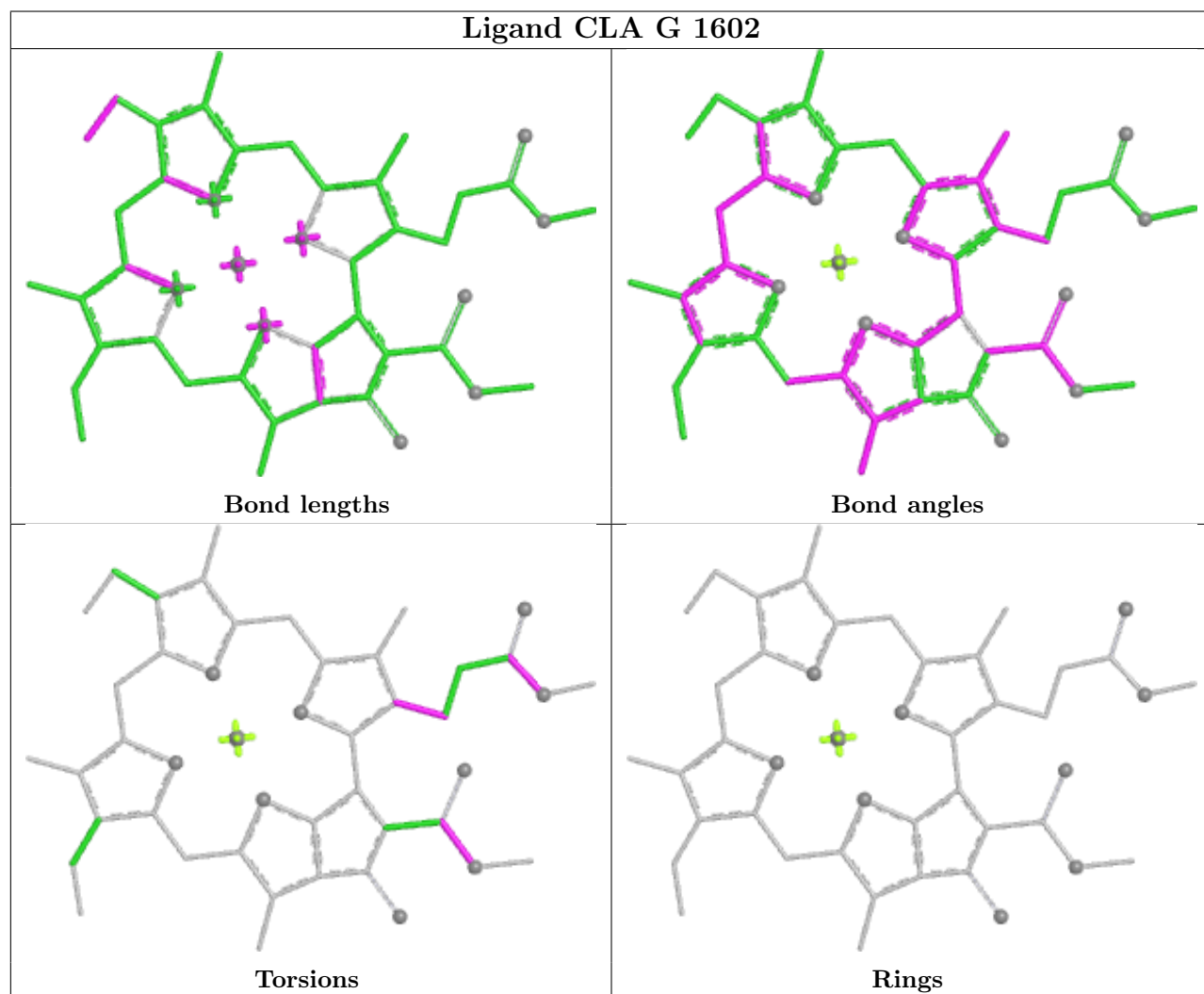
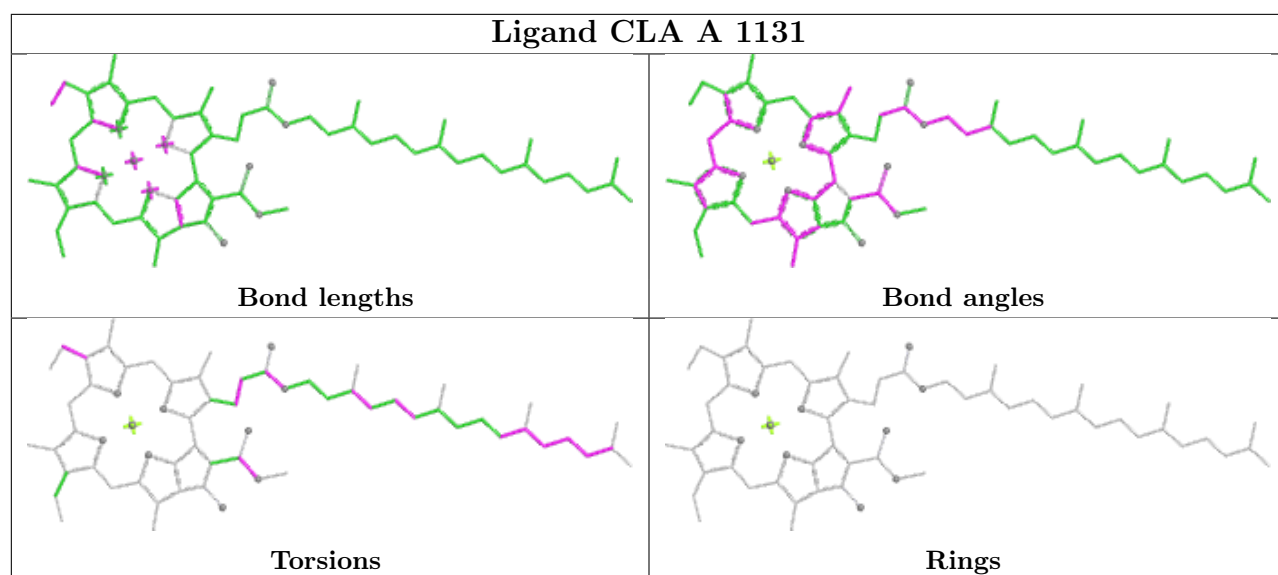
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	5001	LHG	3	0
24	G	5004	LMT	2	0
19	2	608	CLA	2	0
29	2	609	CHL	2	0
19	B	1211	CLA	3	0
19	3	610	CLA	5	0
22	B	4009	BCR	3	0

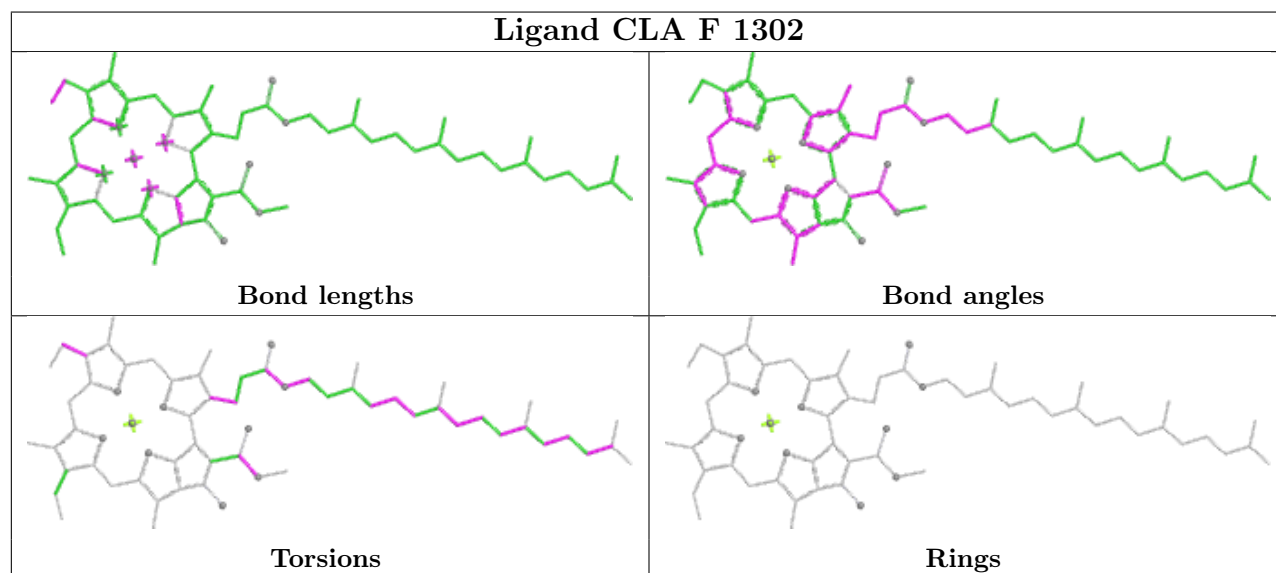
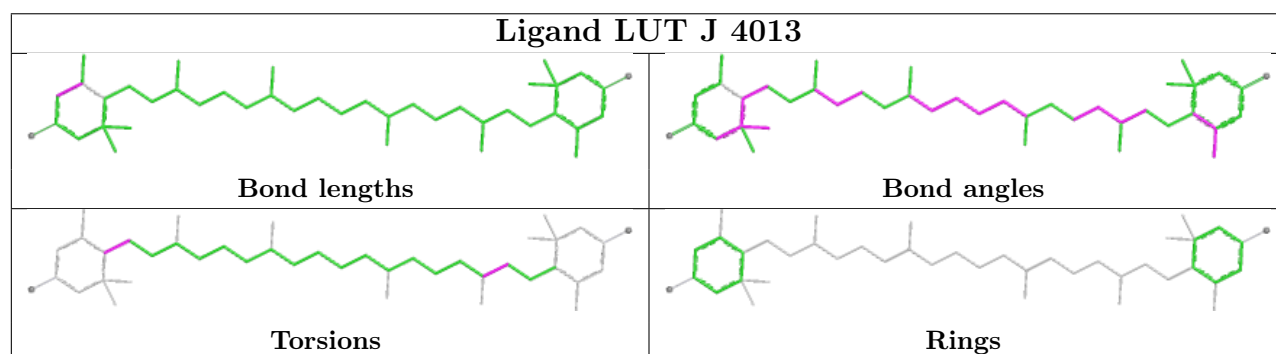
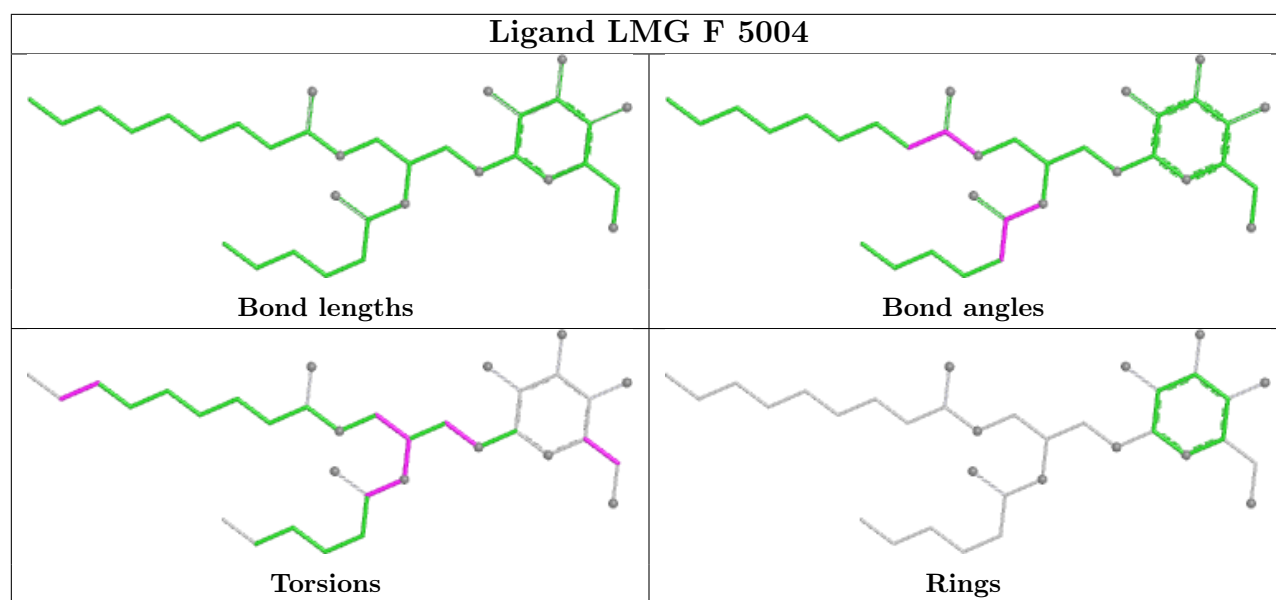
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

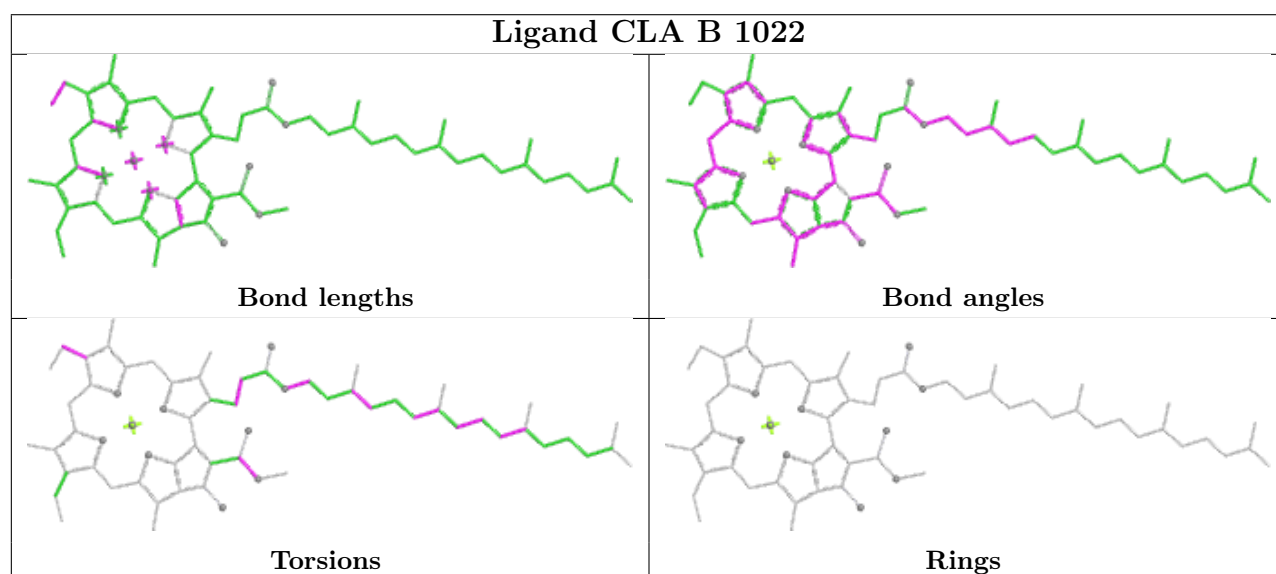
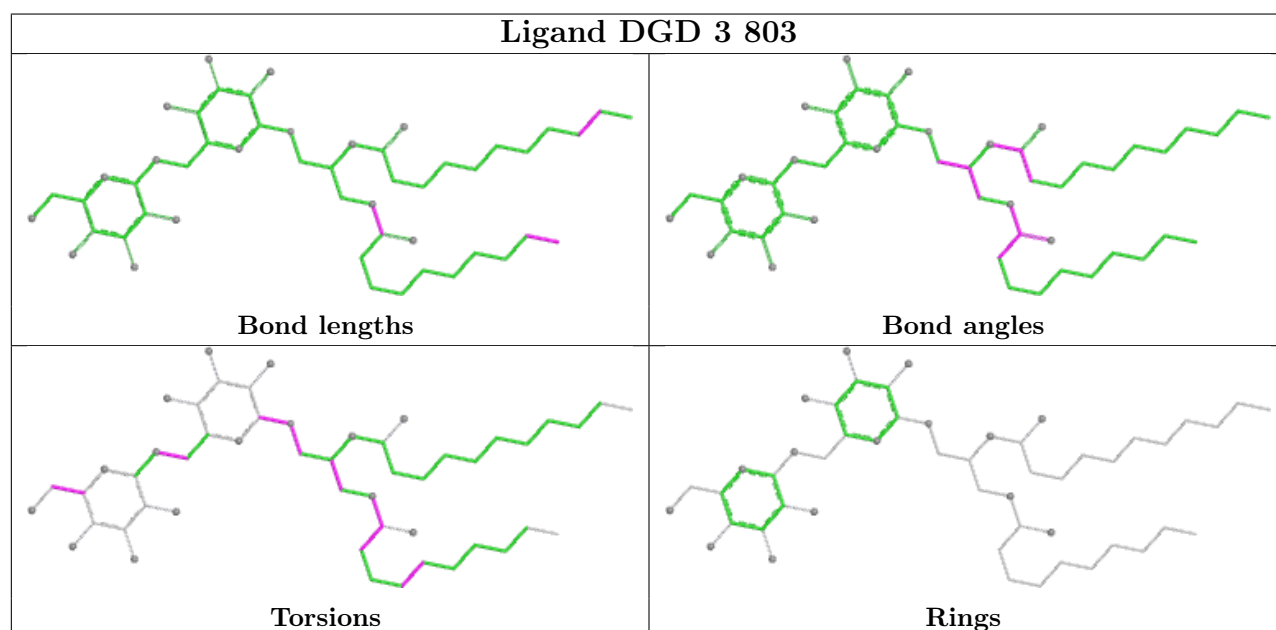
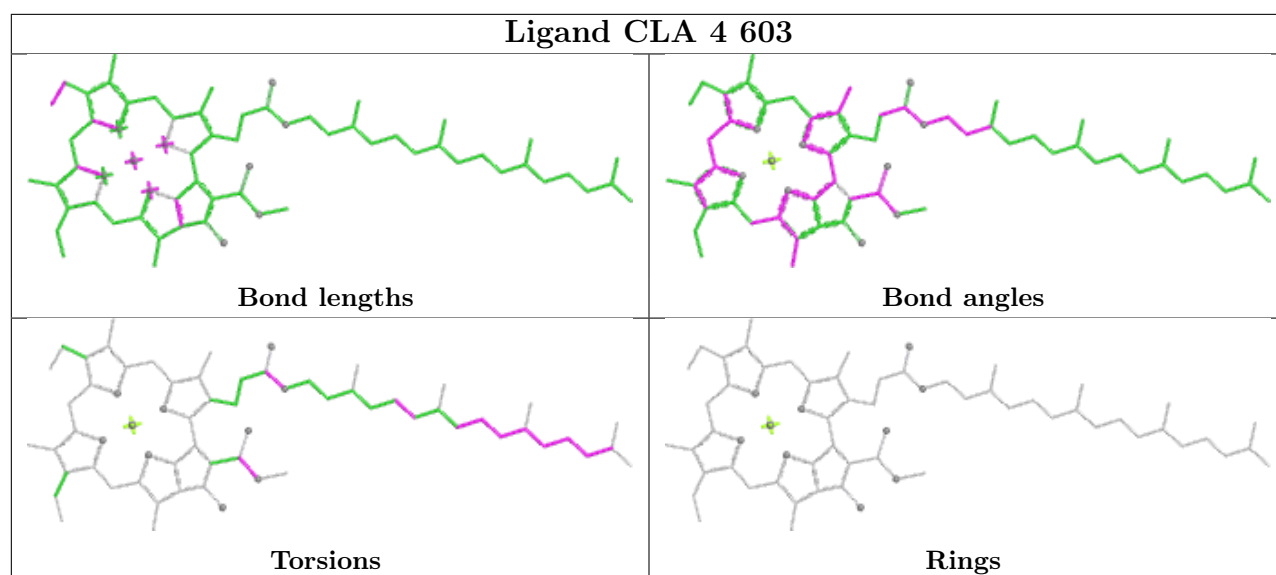


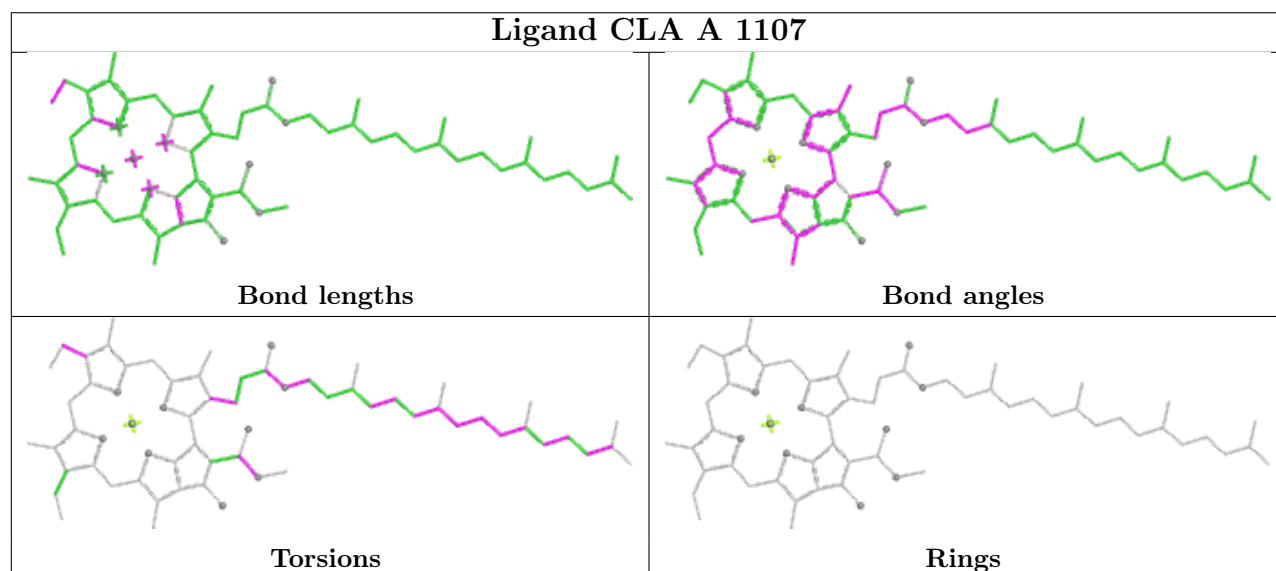
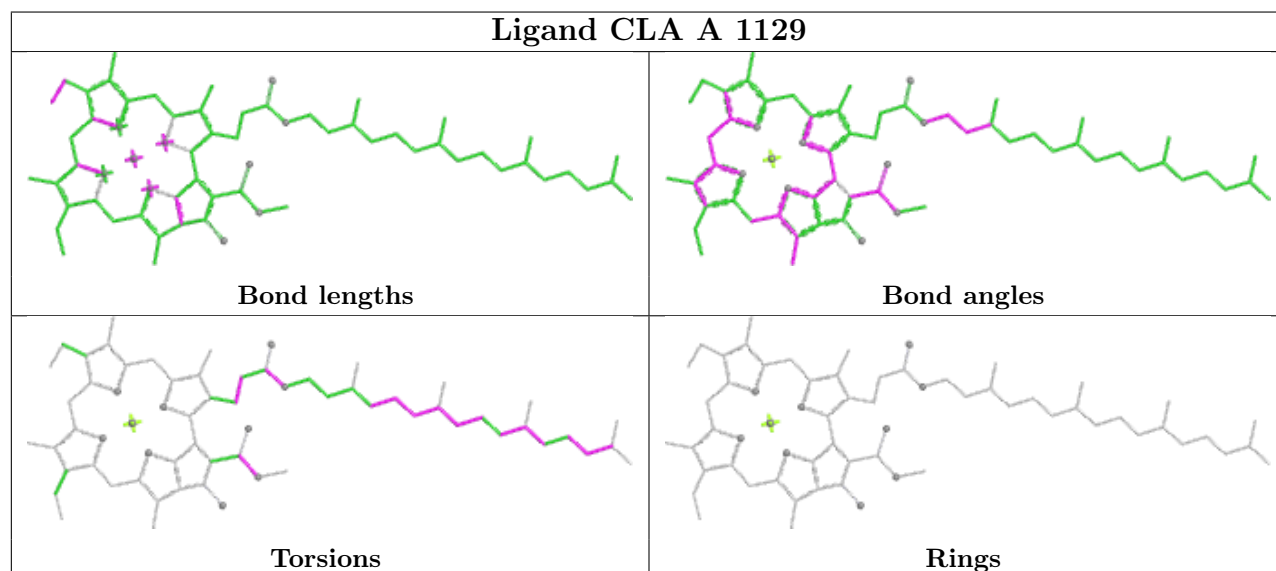
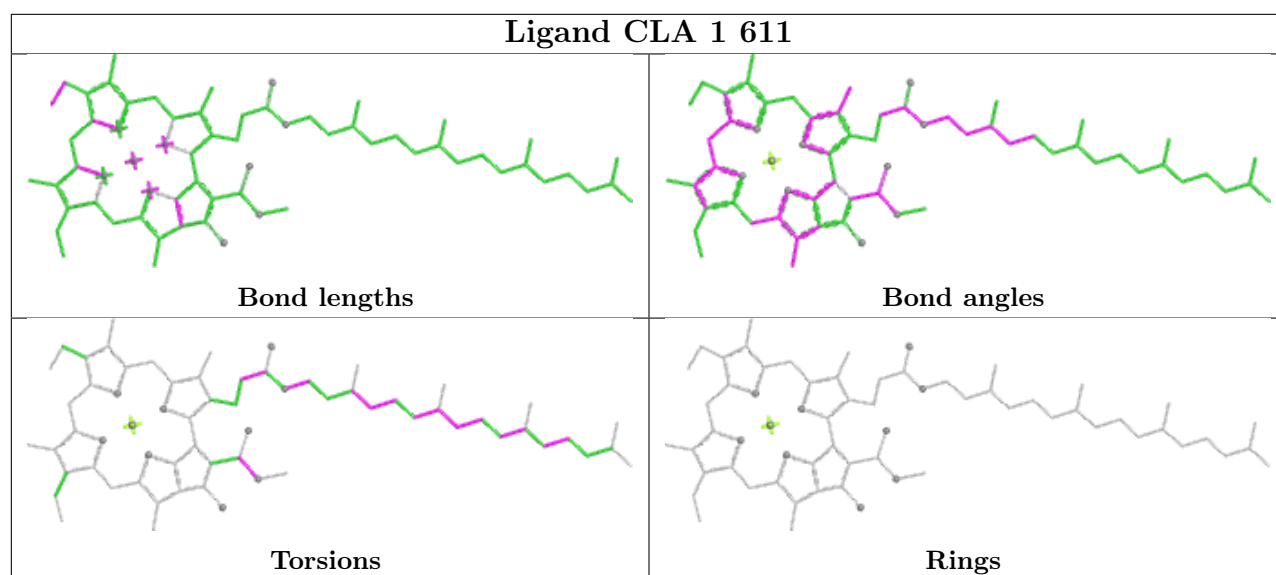


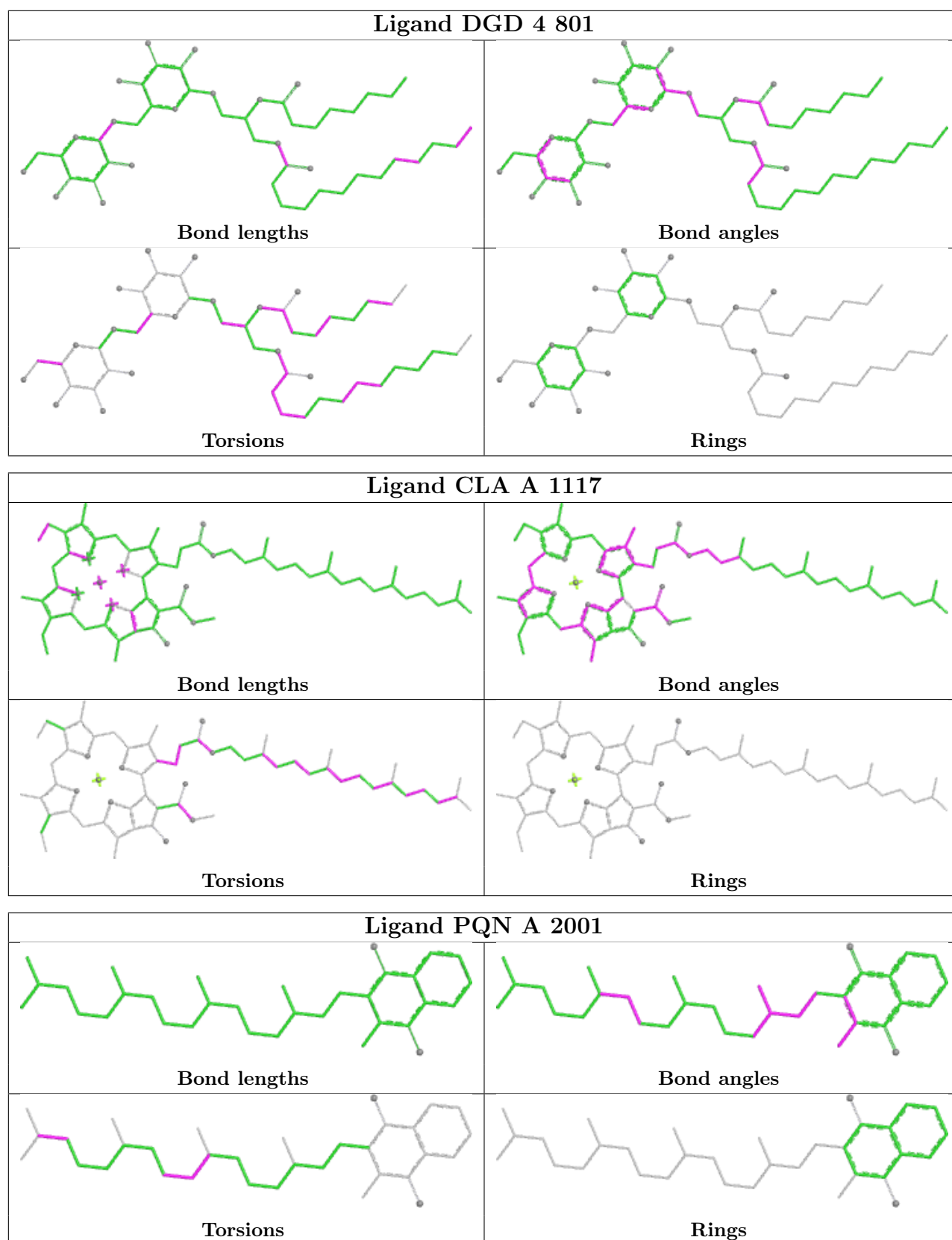
Ligand CLA A 1112	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand C7Z 4 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 1 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

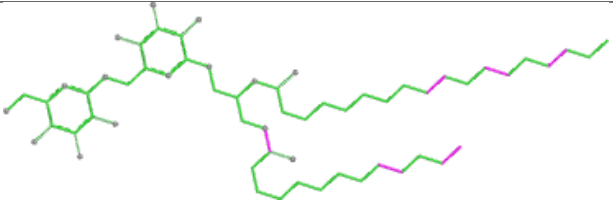
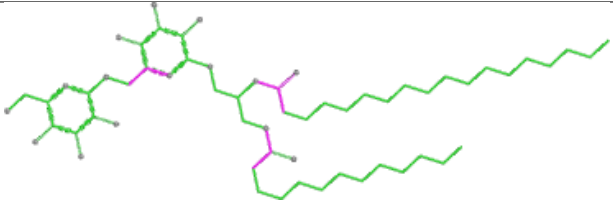
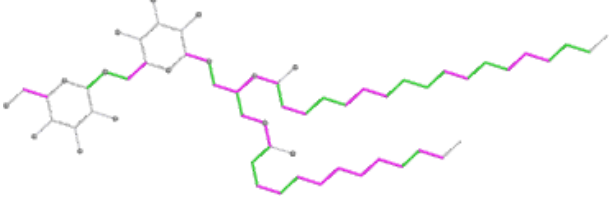
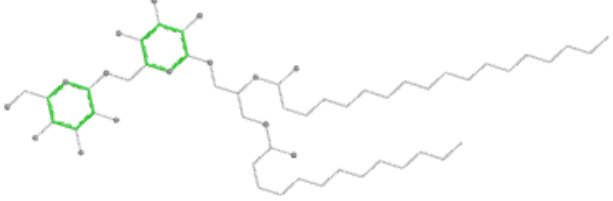
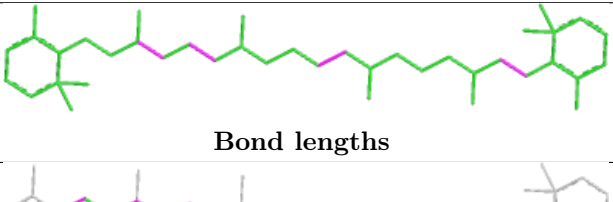
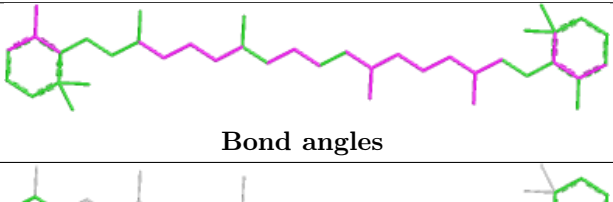
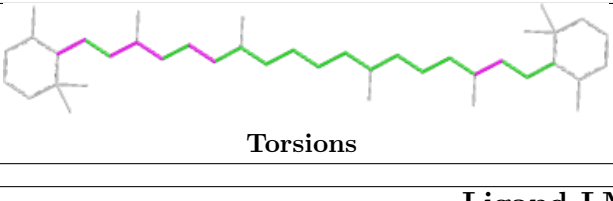
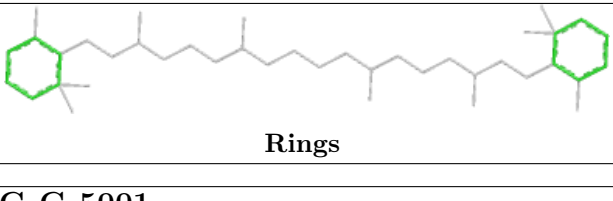
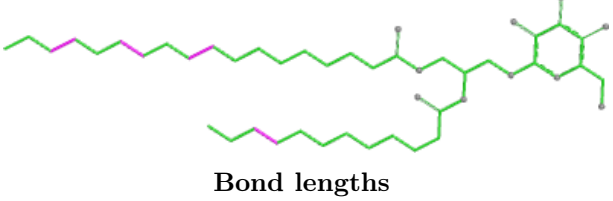
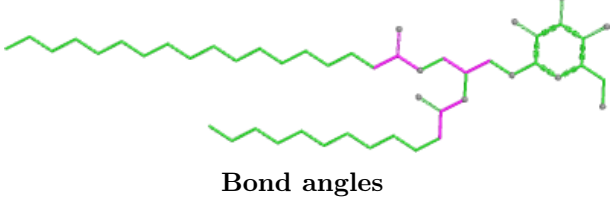
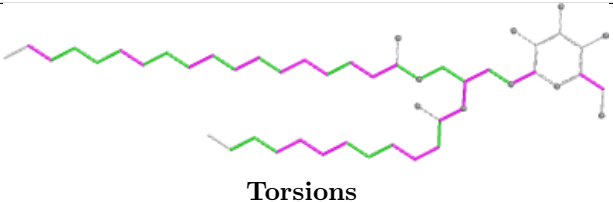
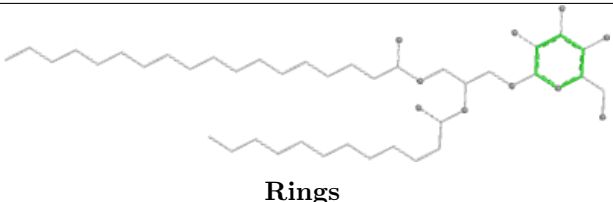




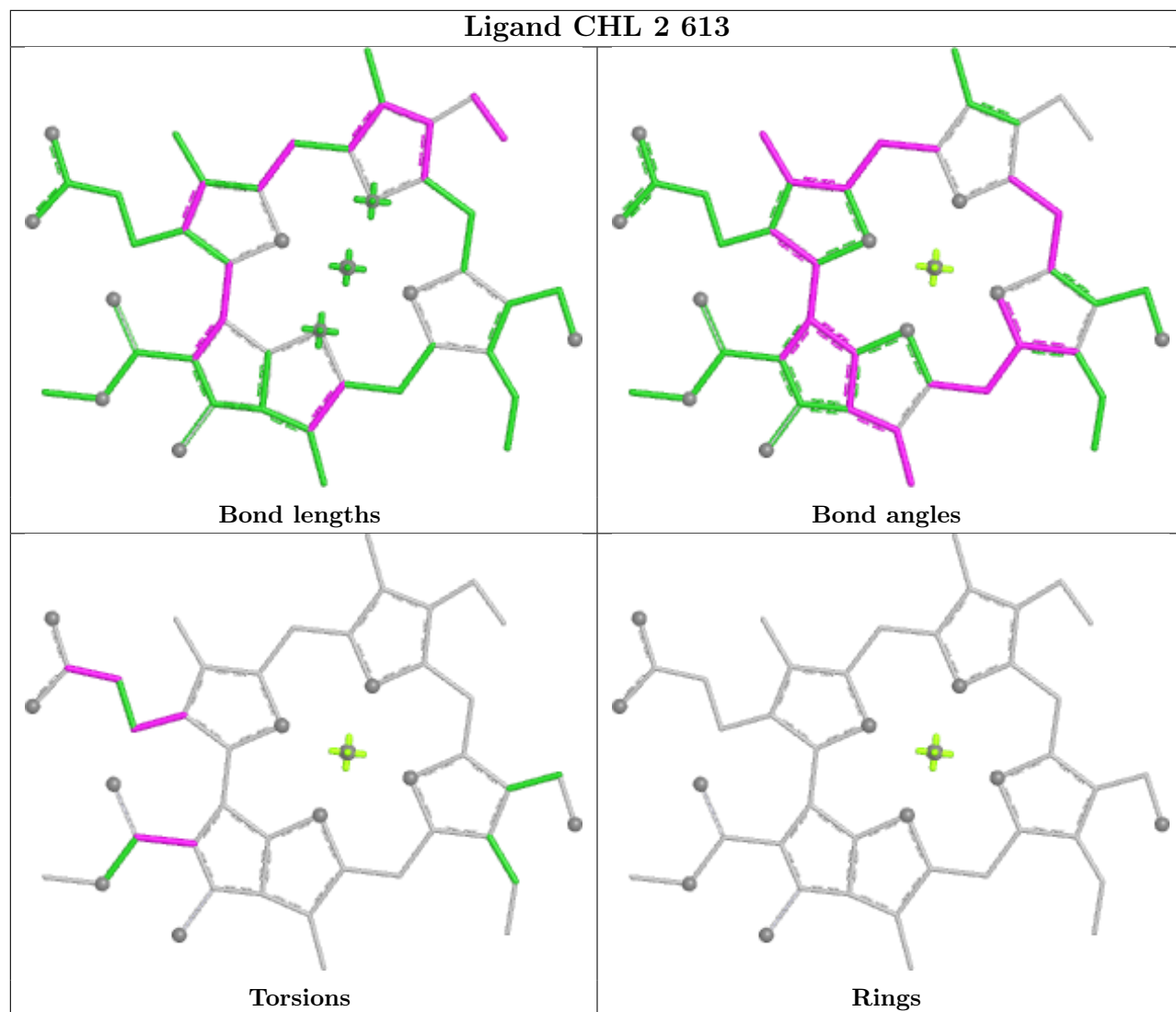


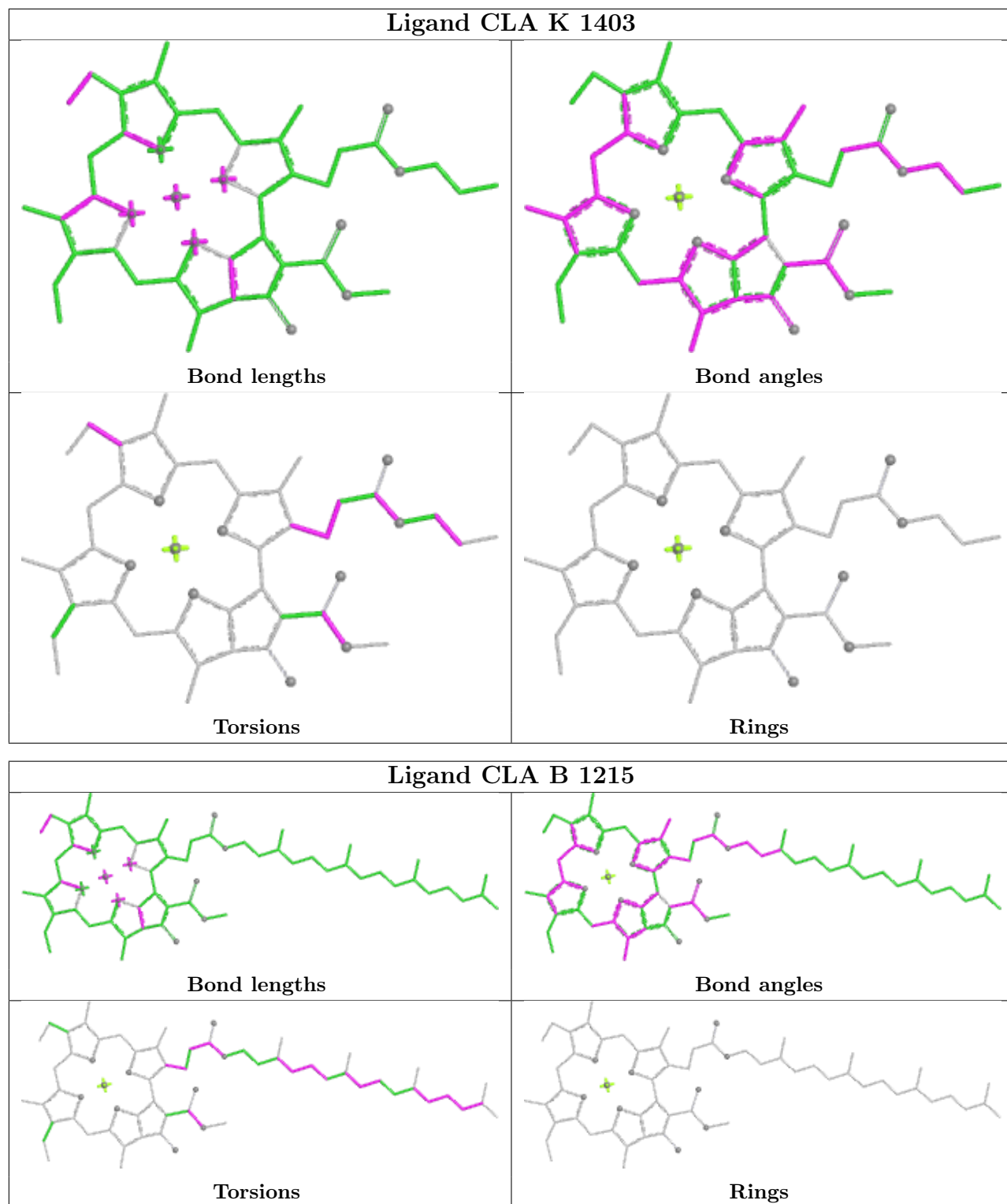


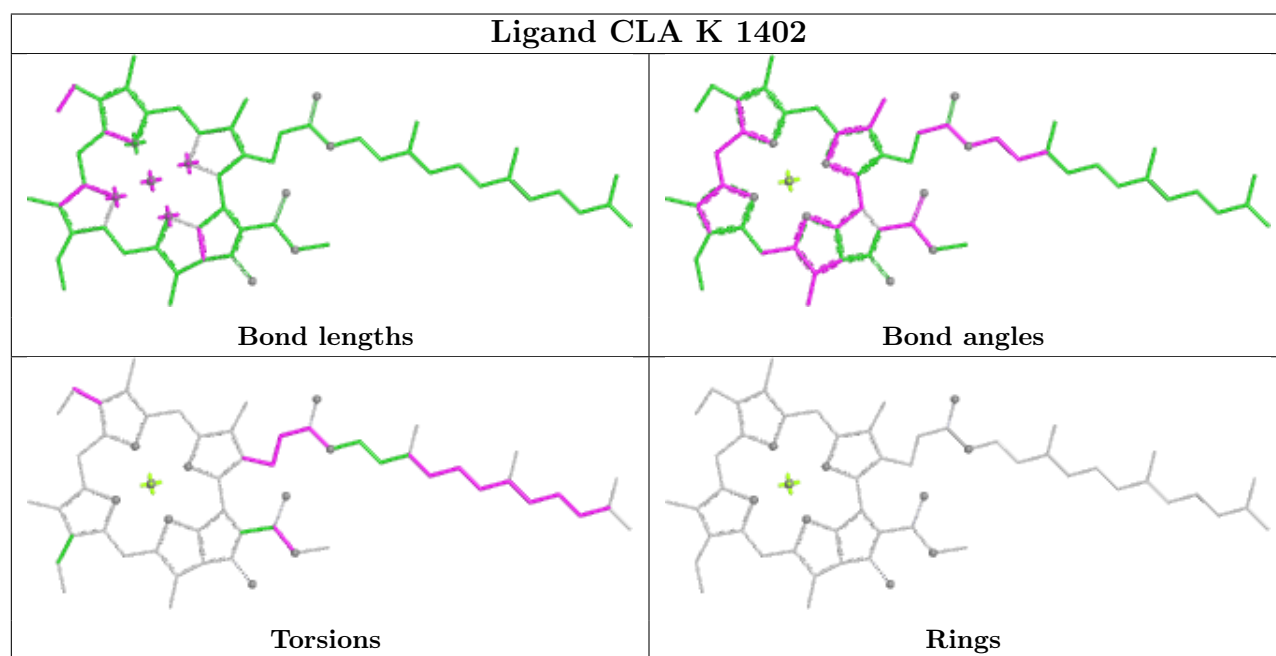
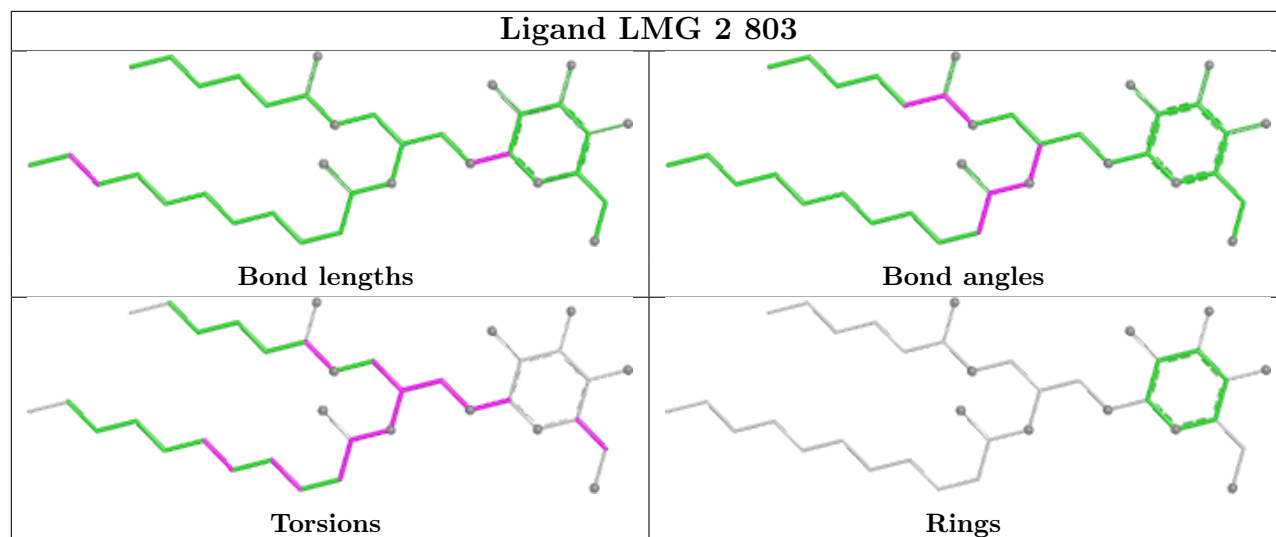


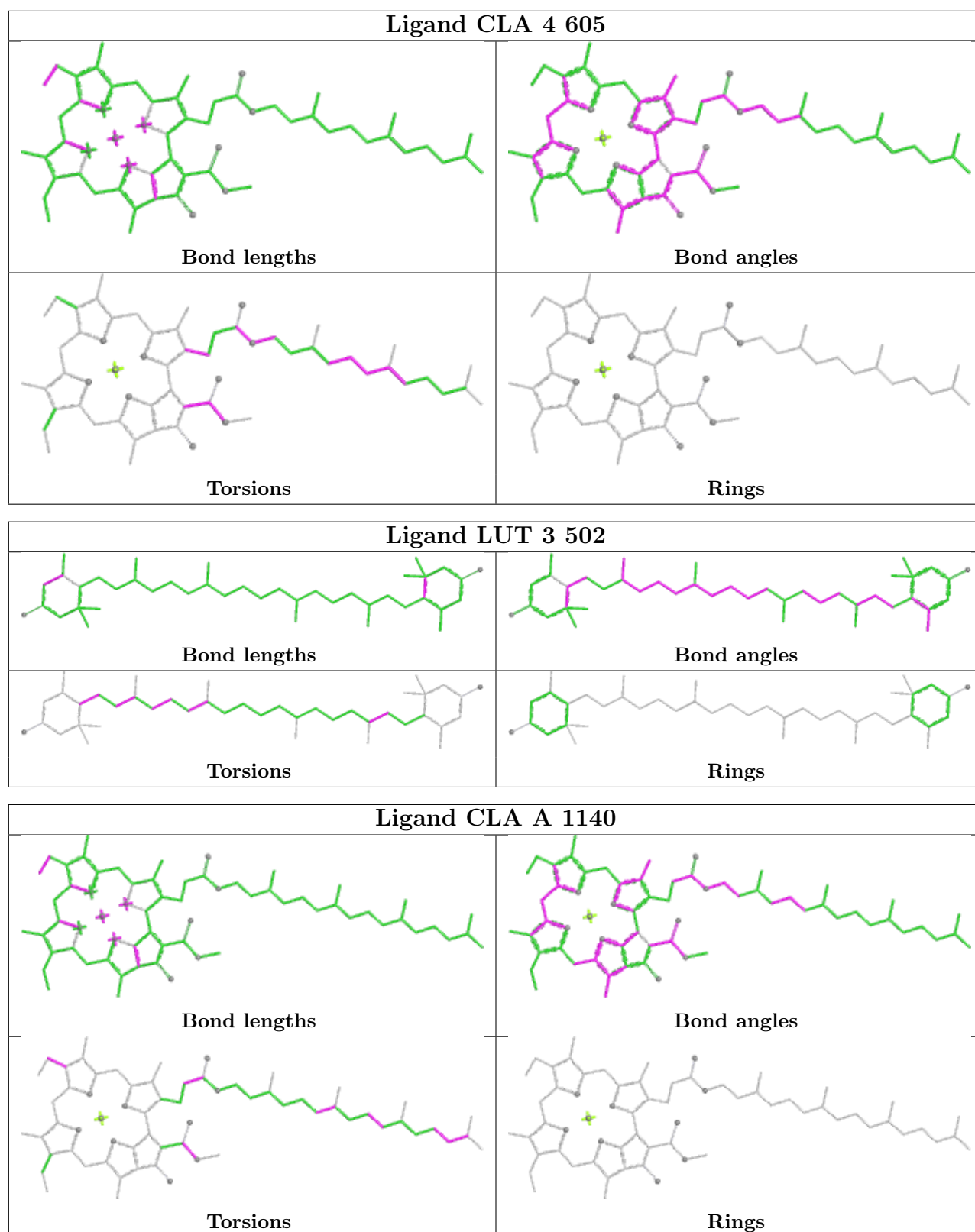
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG G 5001	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL 2 613

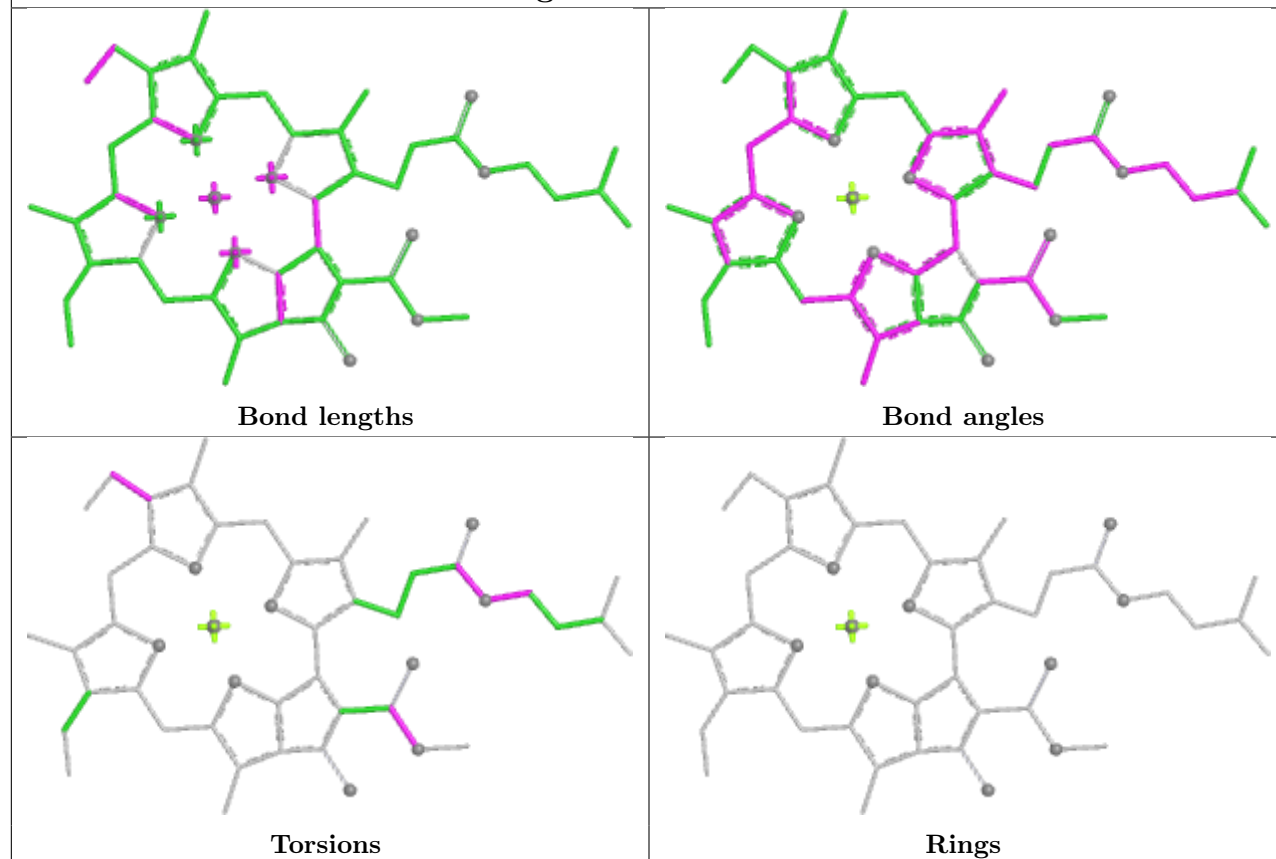




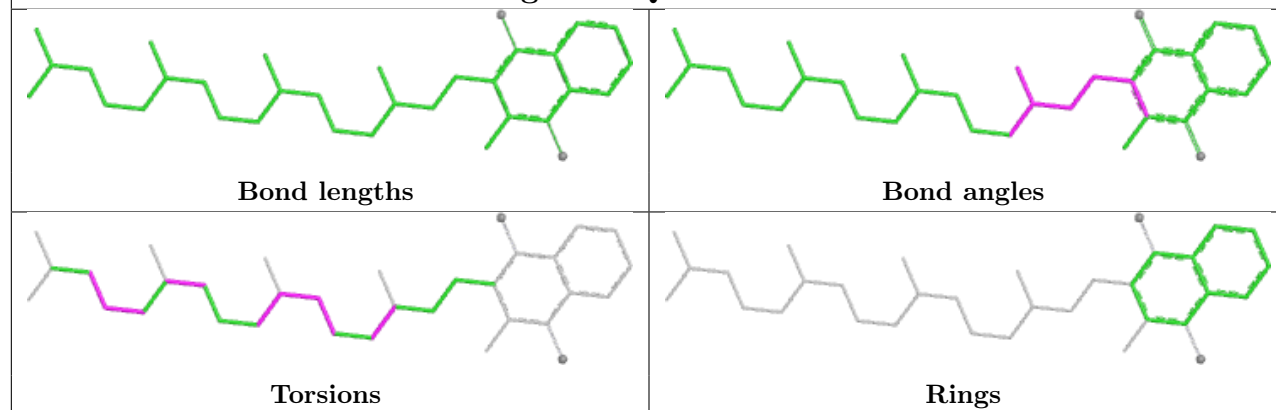


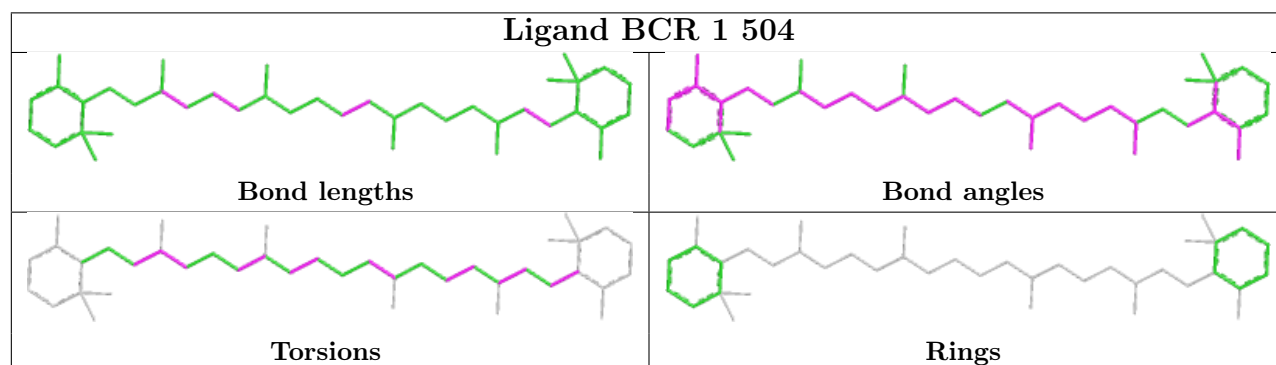
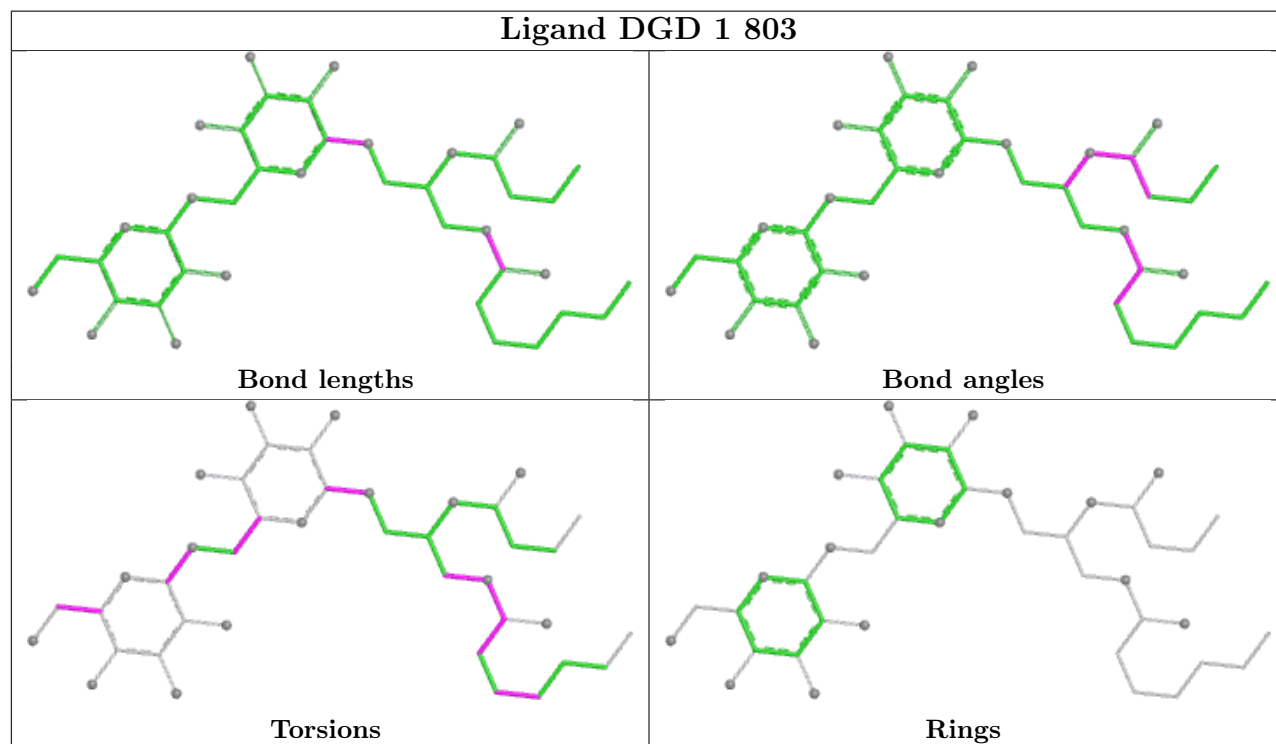
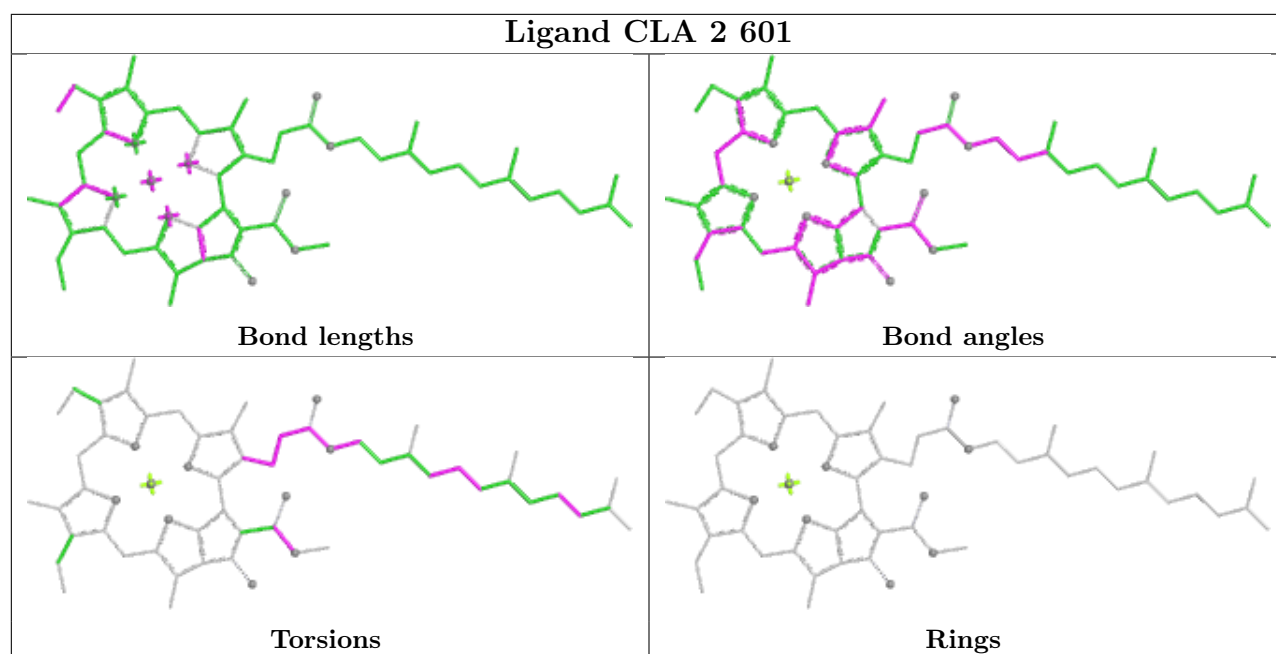


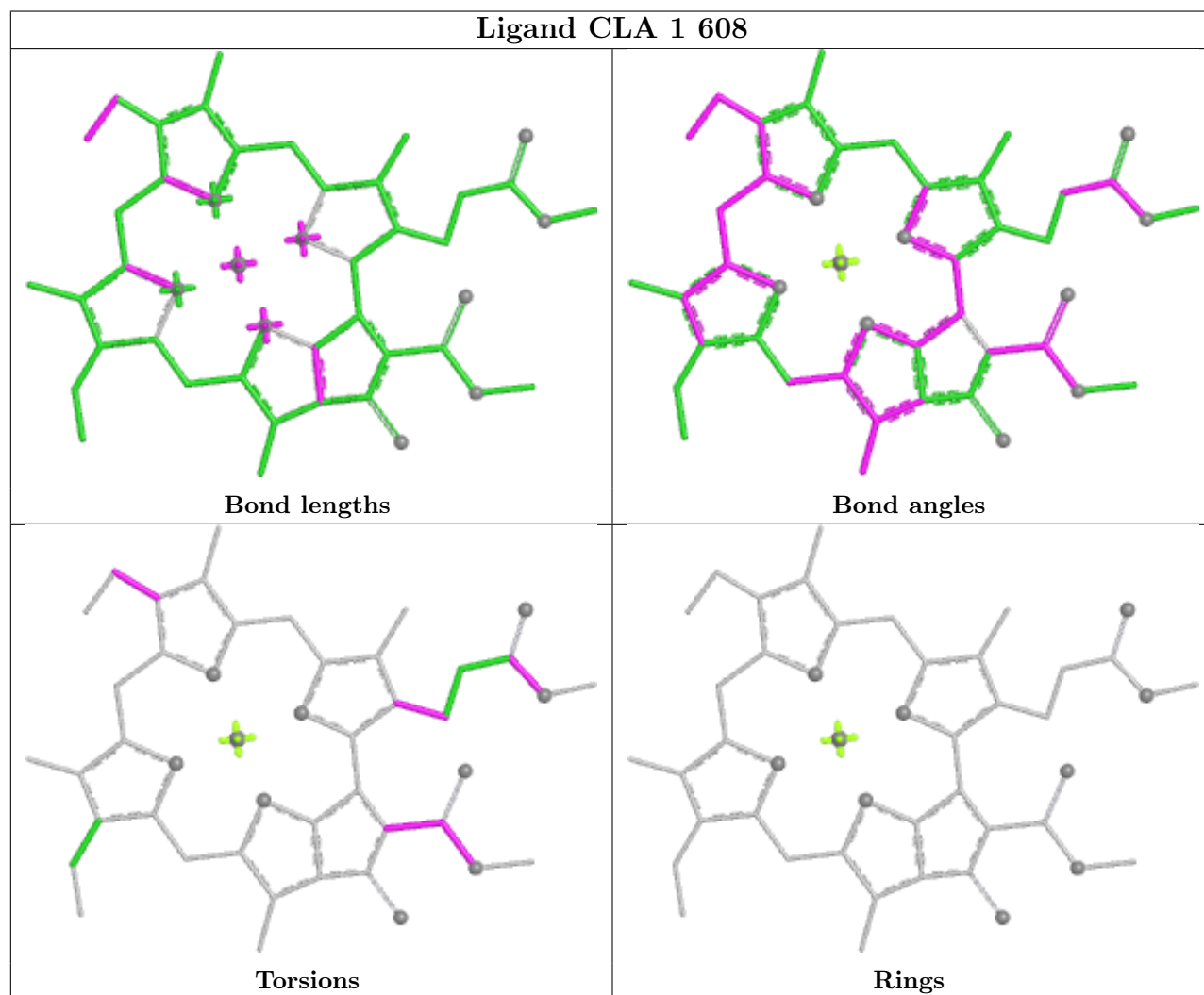
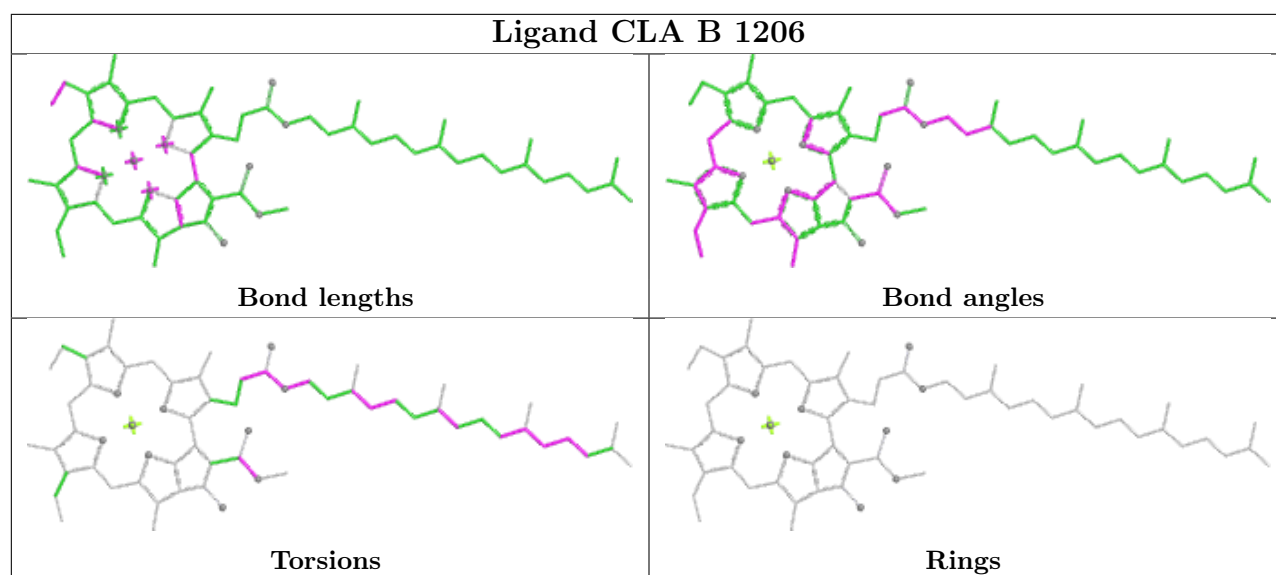
Ligand CLA 1 606

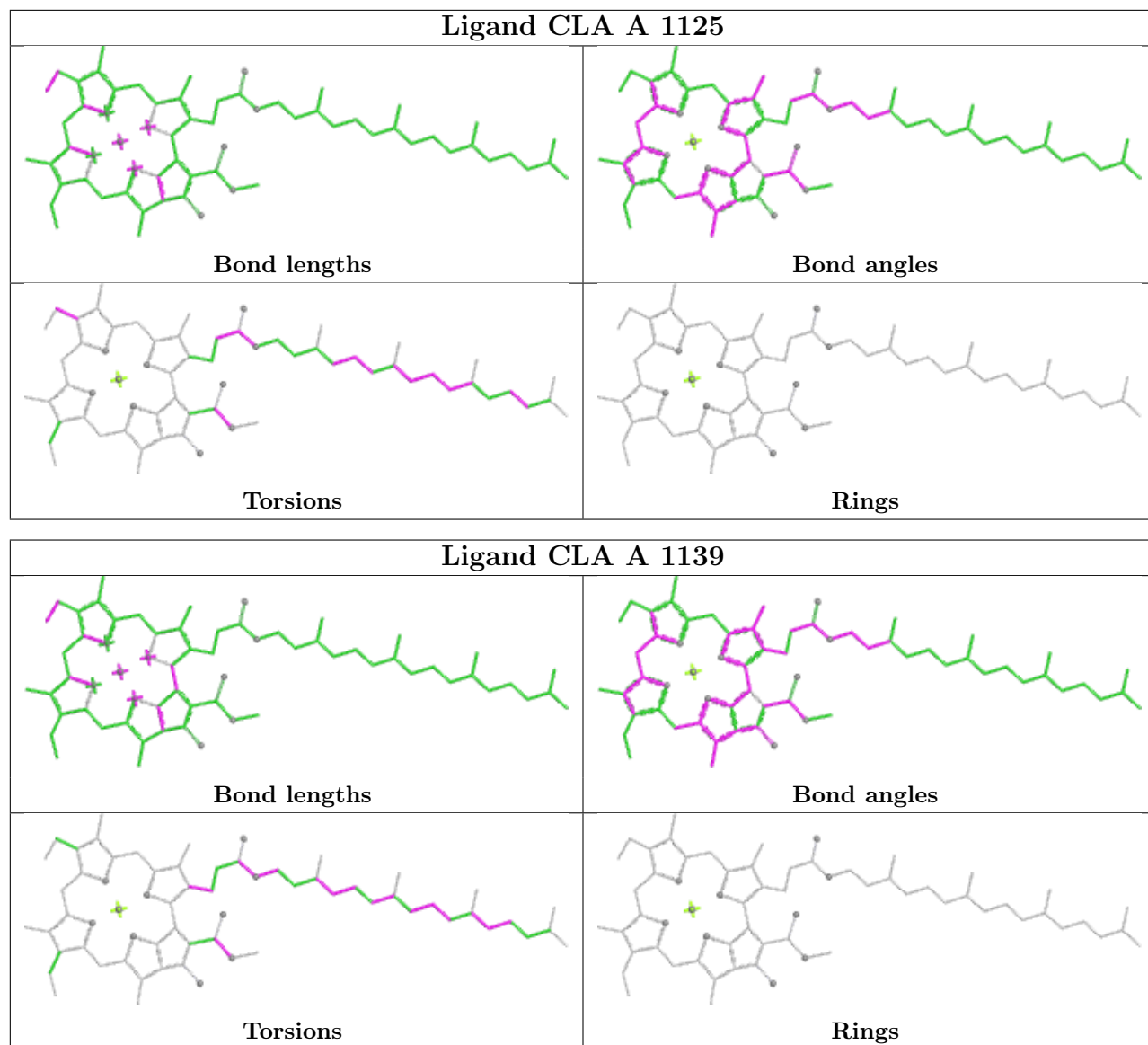


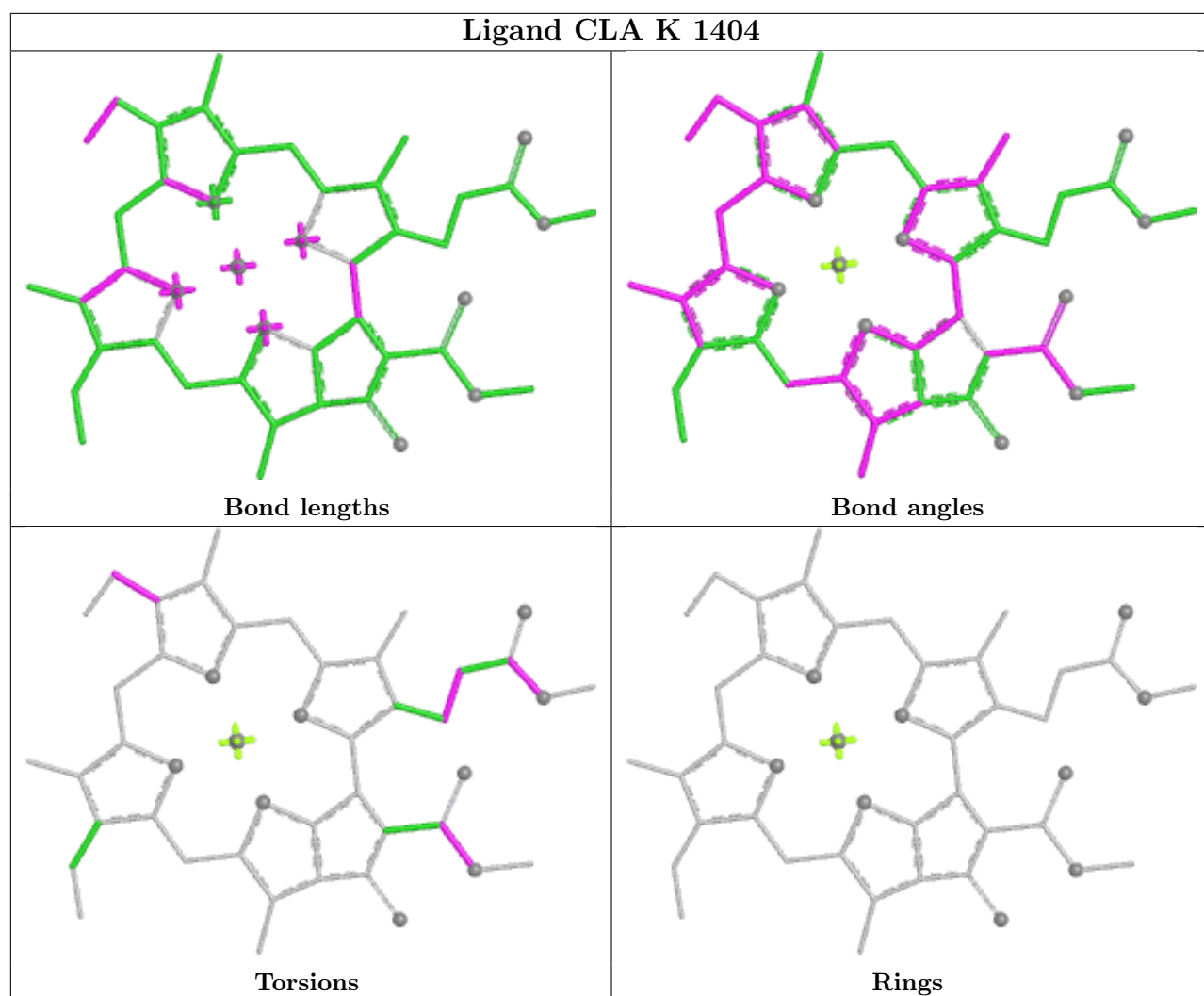
Ligand PQN B 2002



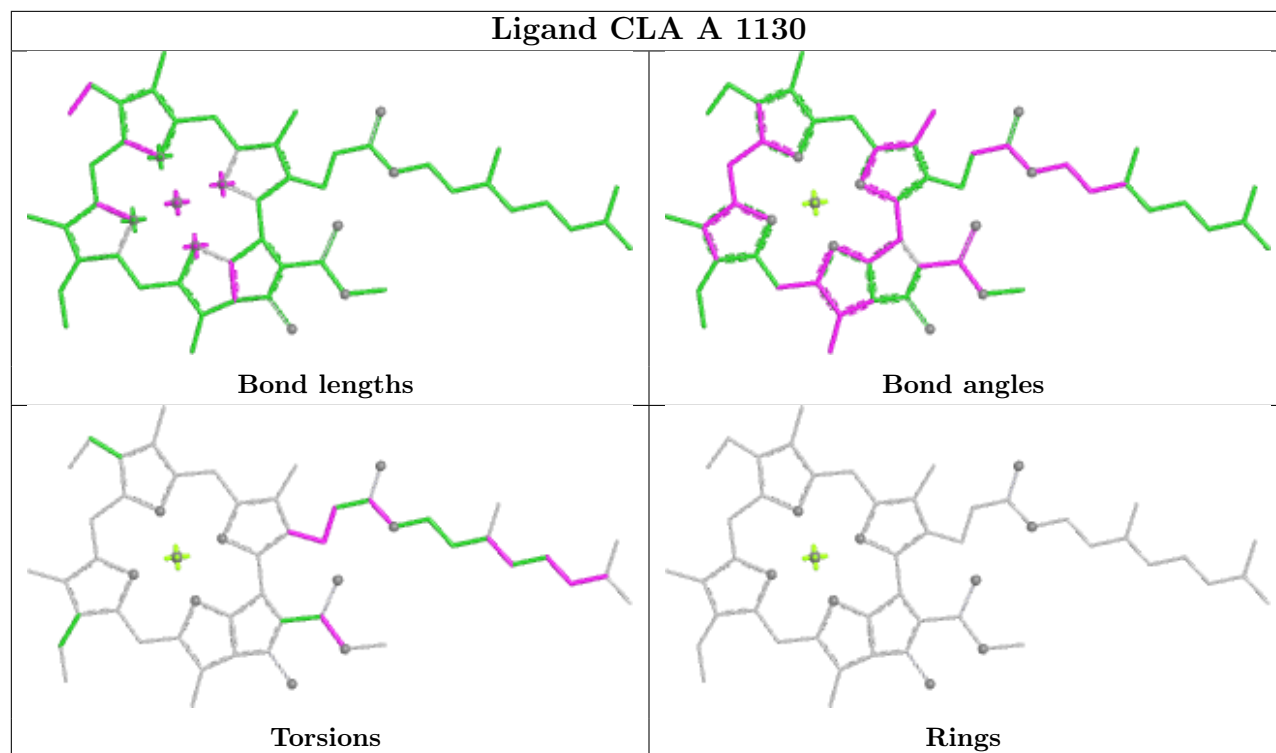




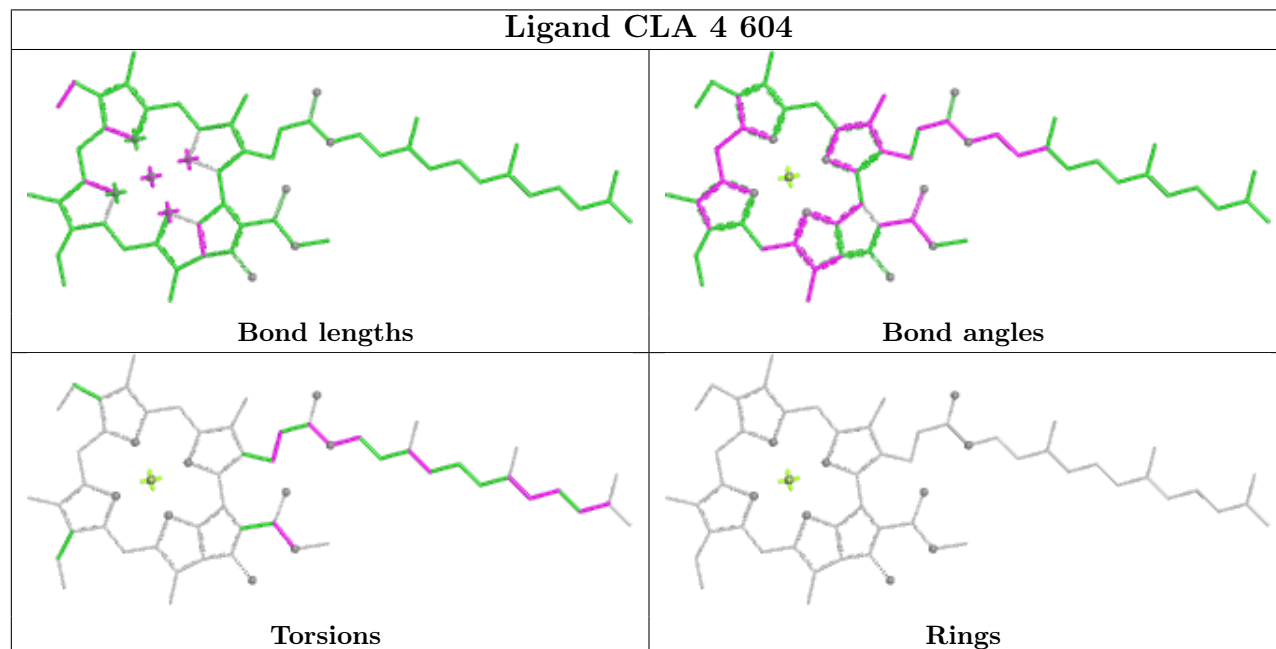


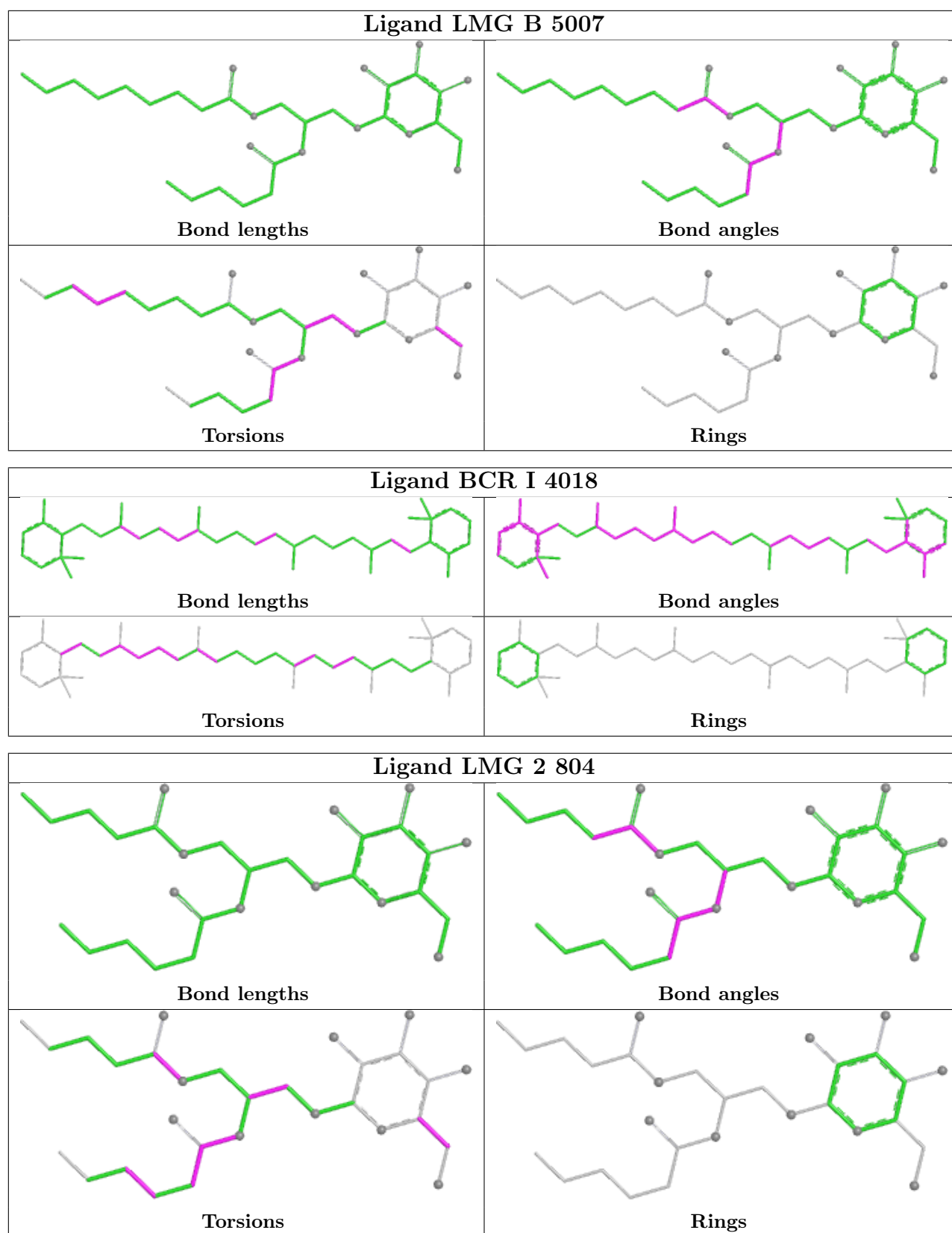


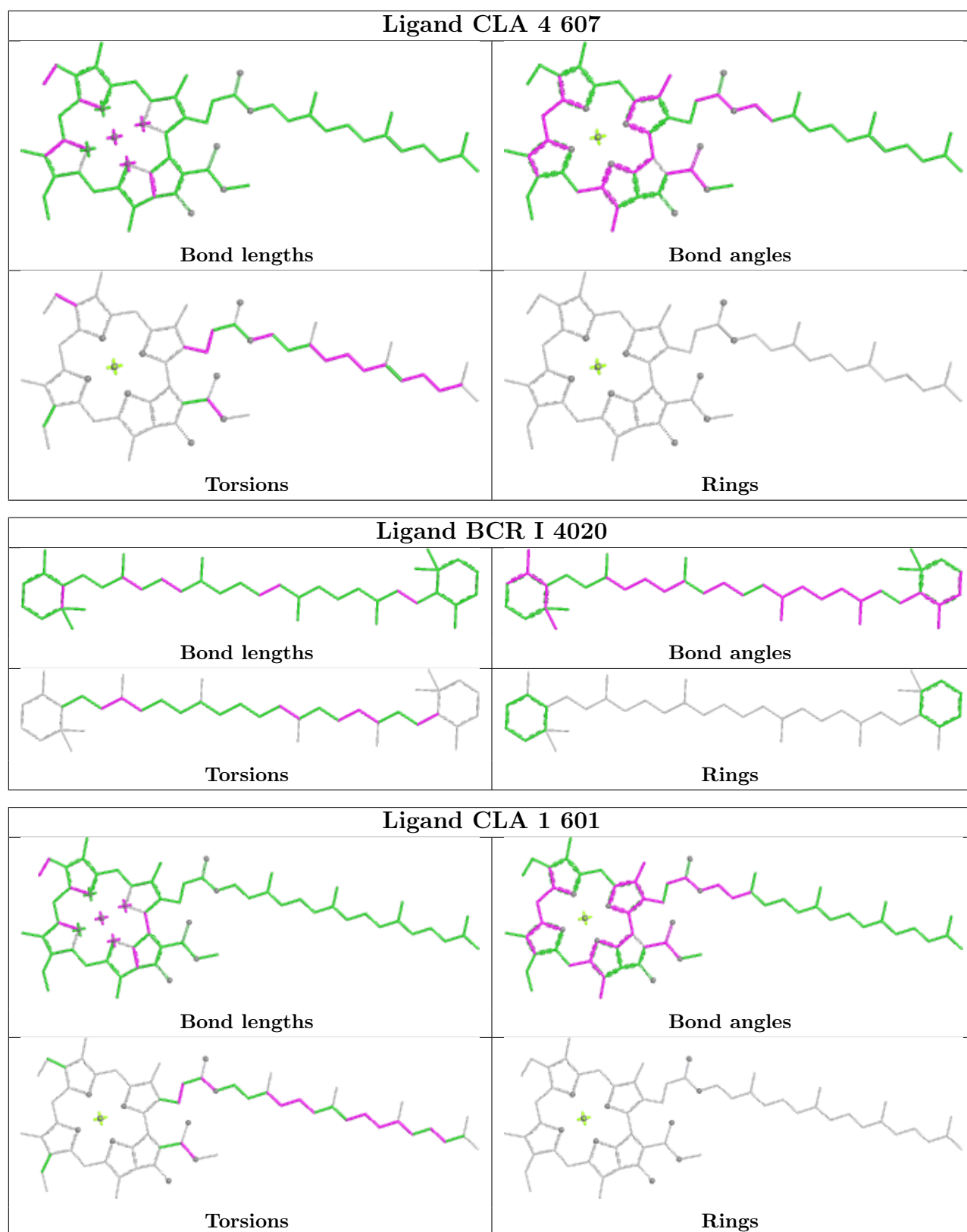
Ligand CLA A 1130



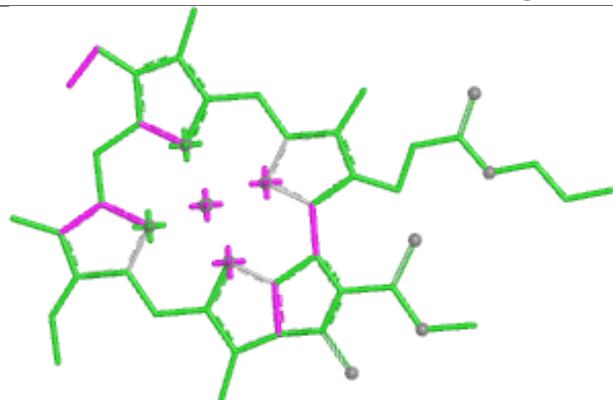
Ligand CLA 4 604



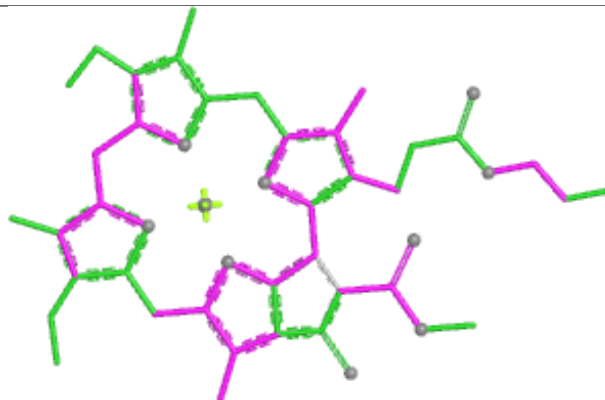




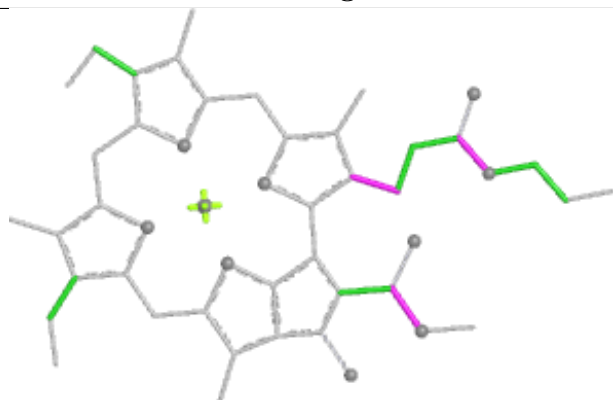
Ligand CLA 3 608



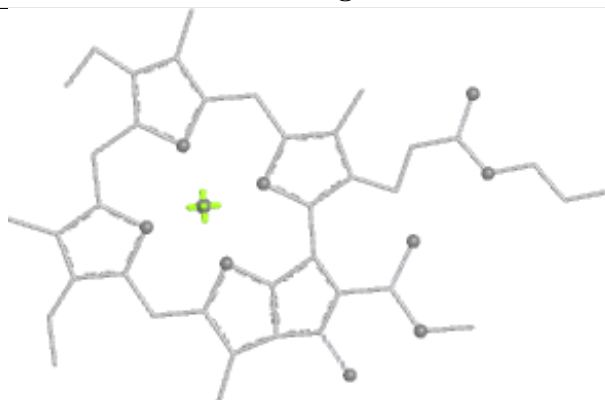
Bond lengths



Bond angles

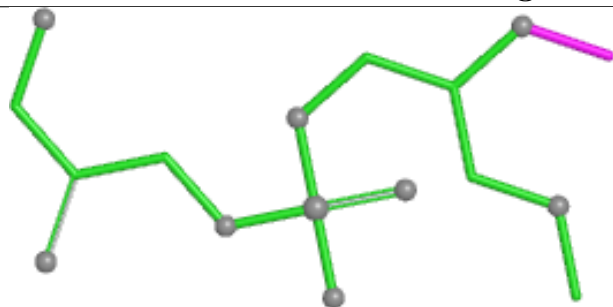


Torsions

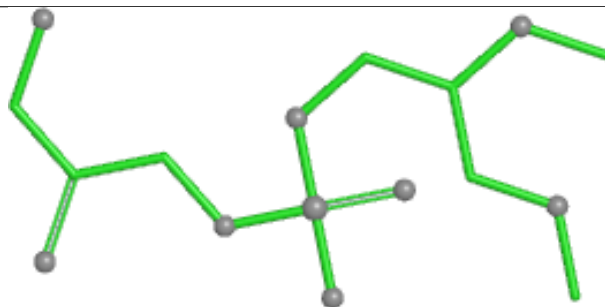


Rings

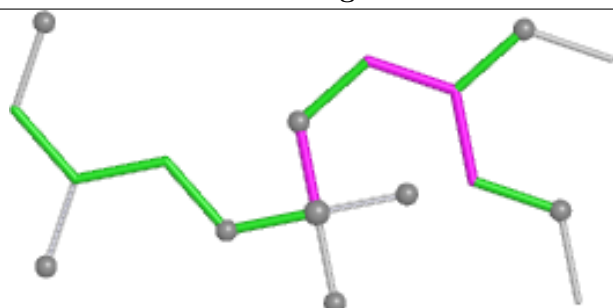
Ligand LHG 3 801



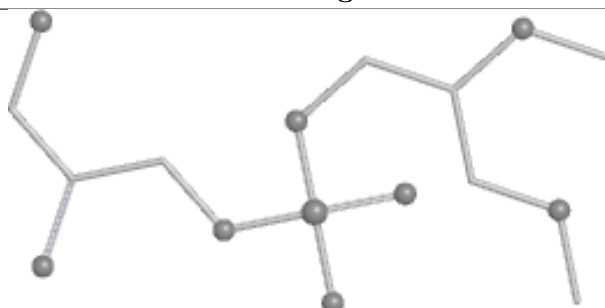
Bond lengths



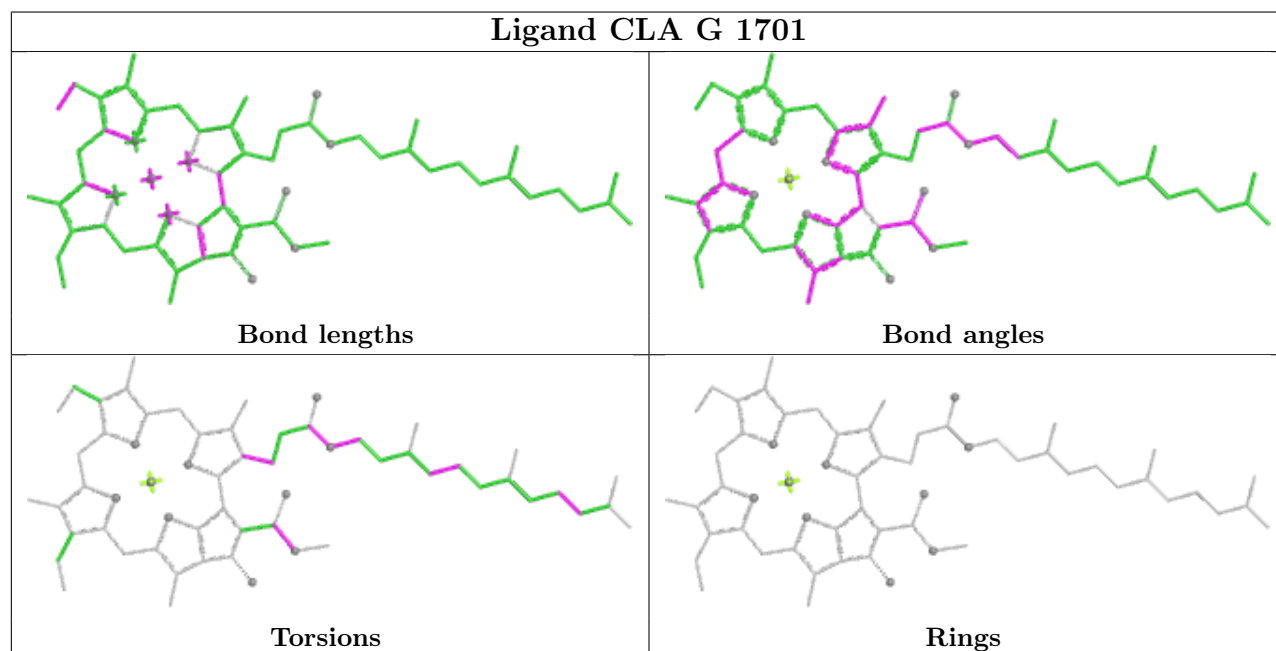
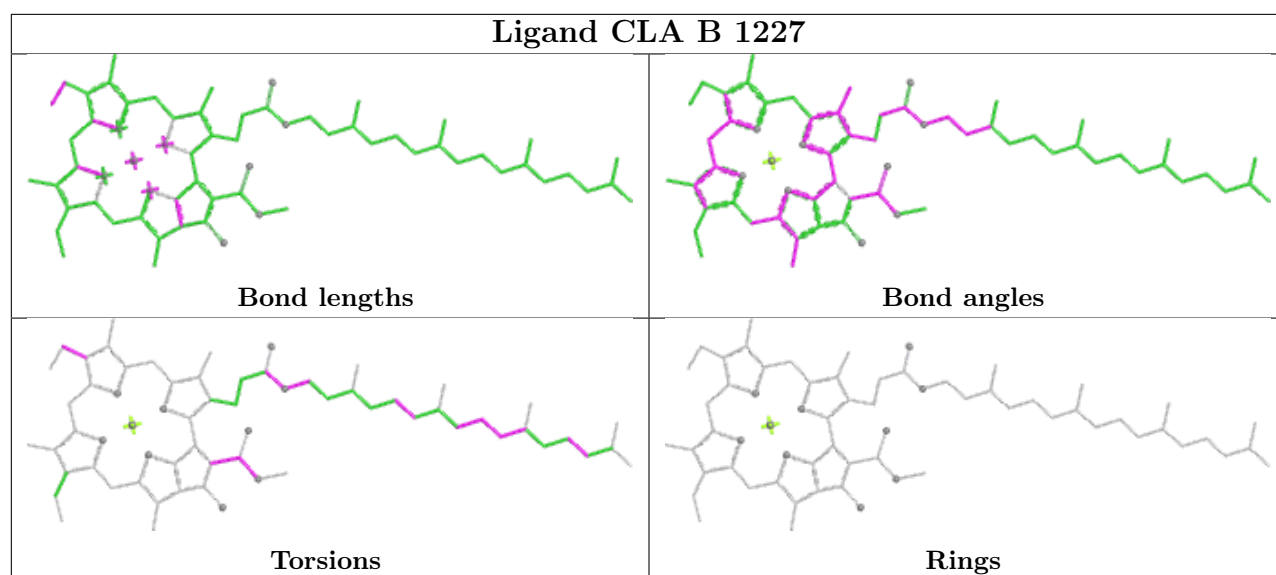
Bond angles

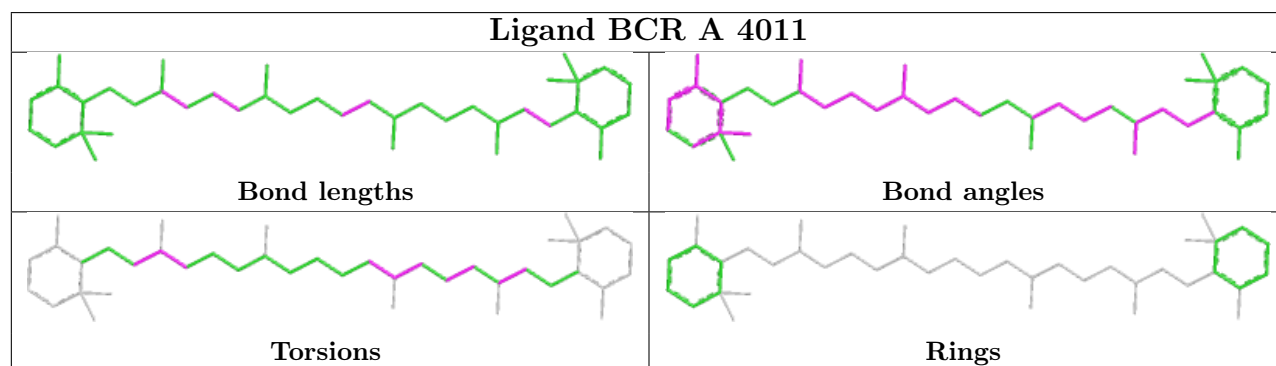
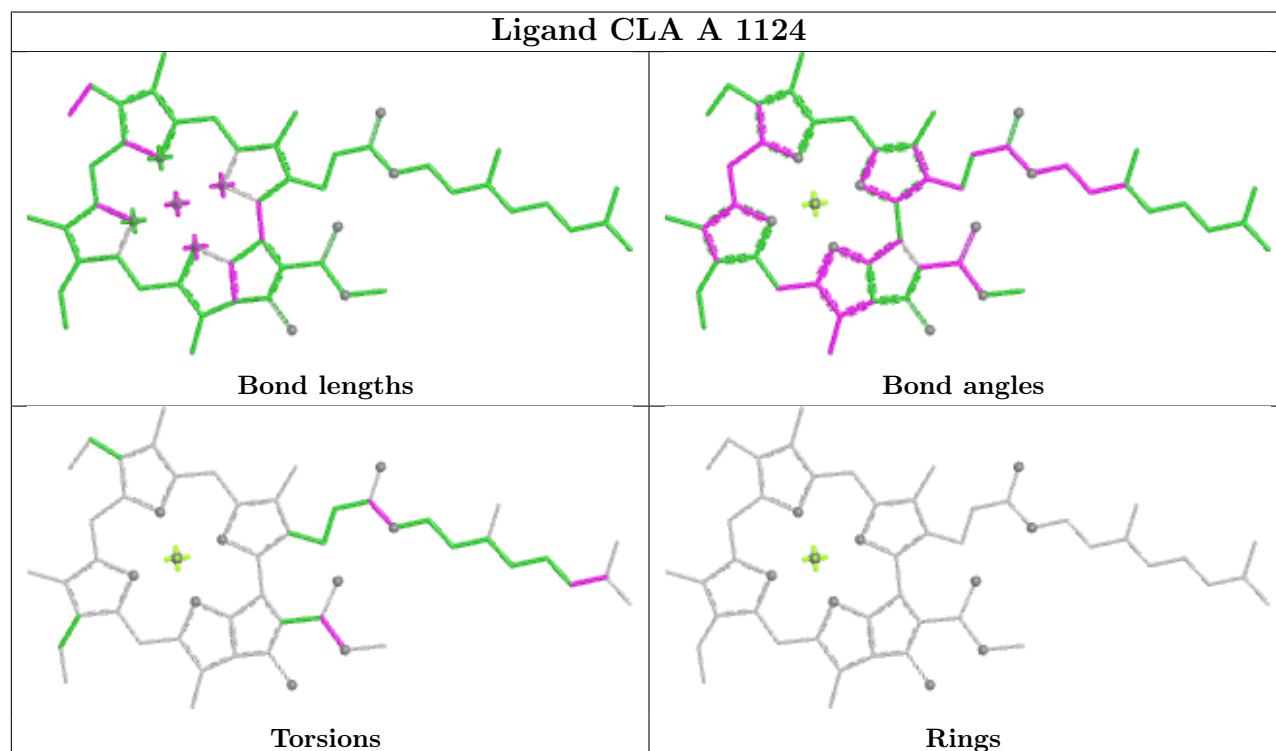
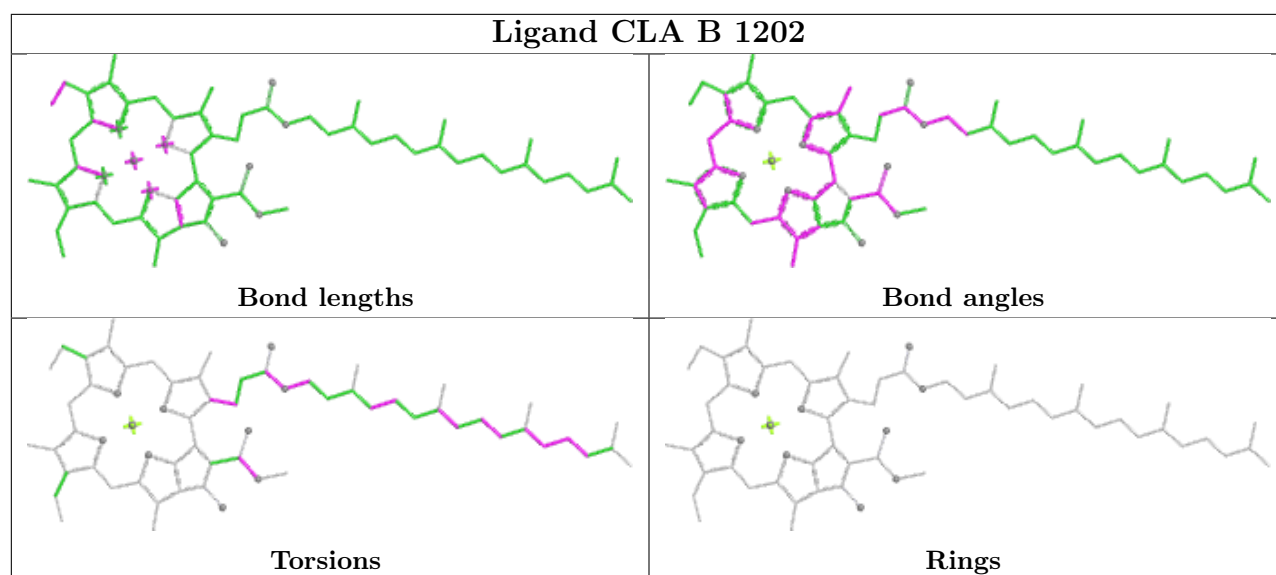


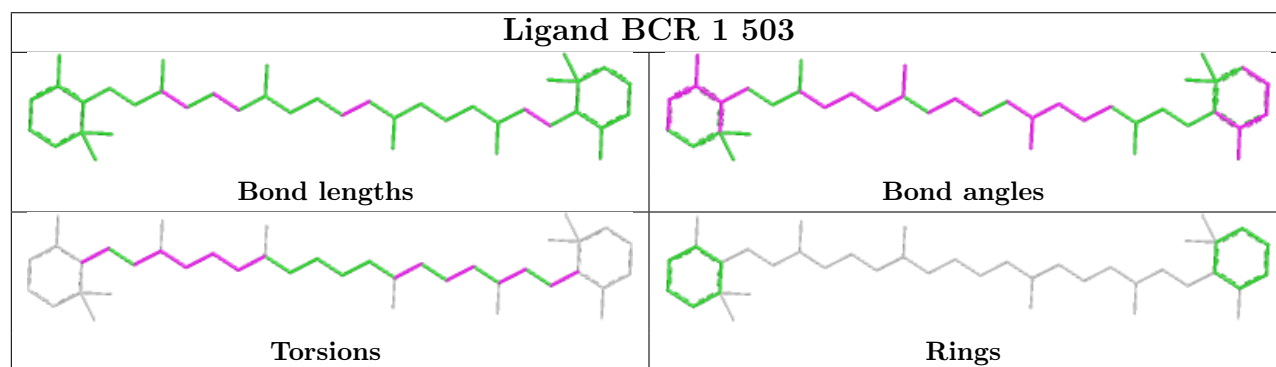
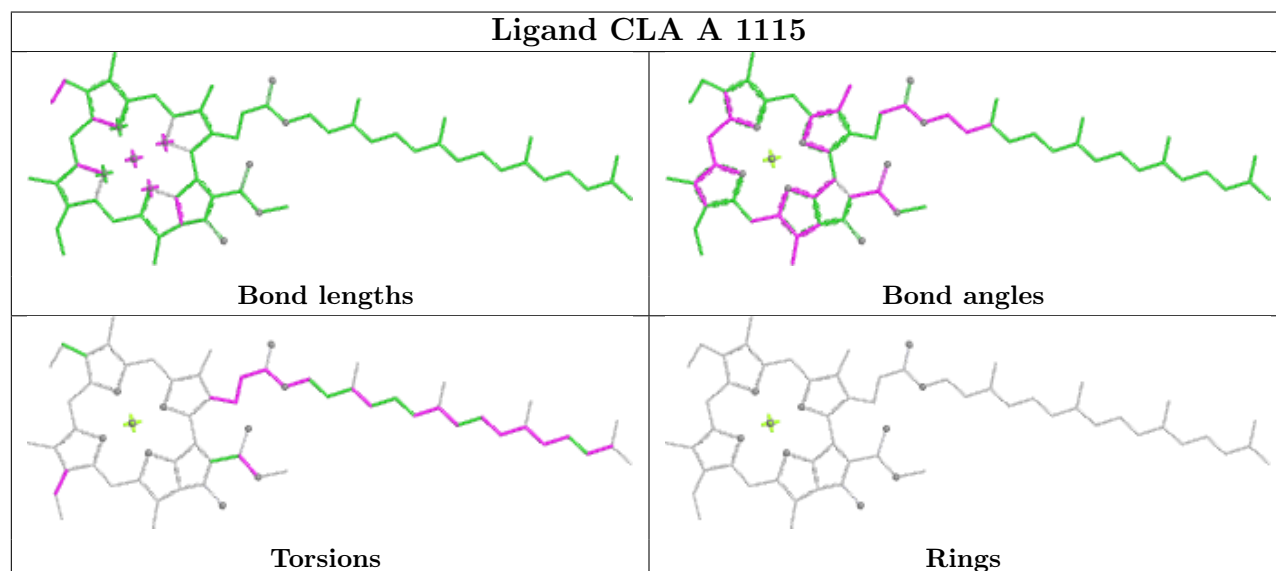
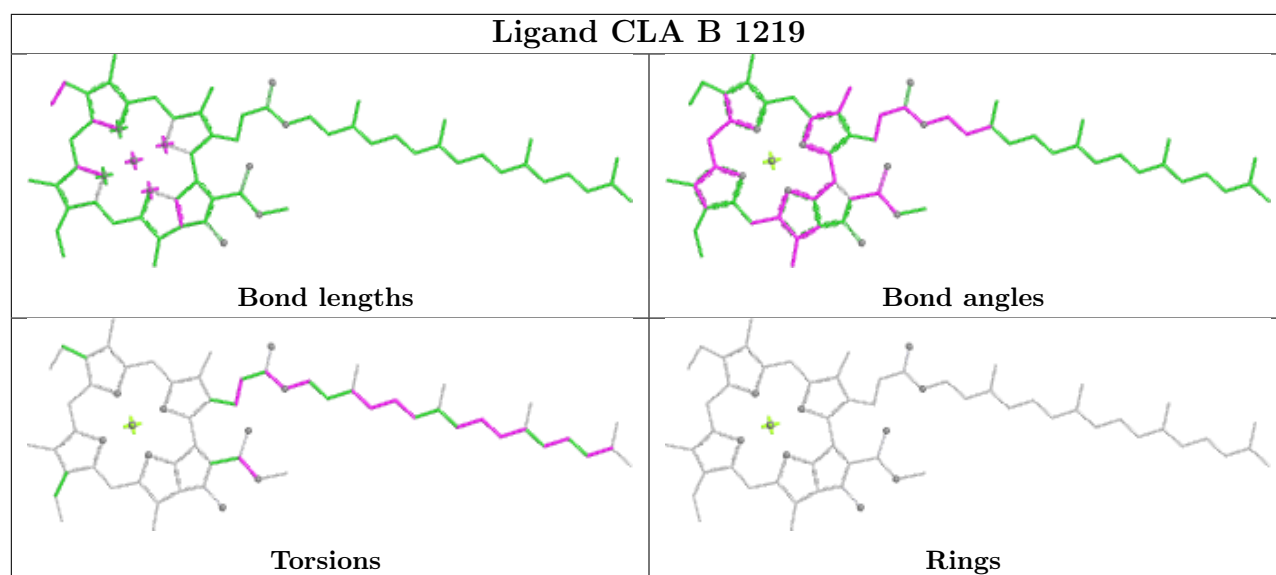
Torsions

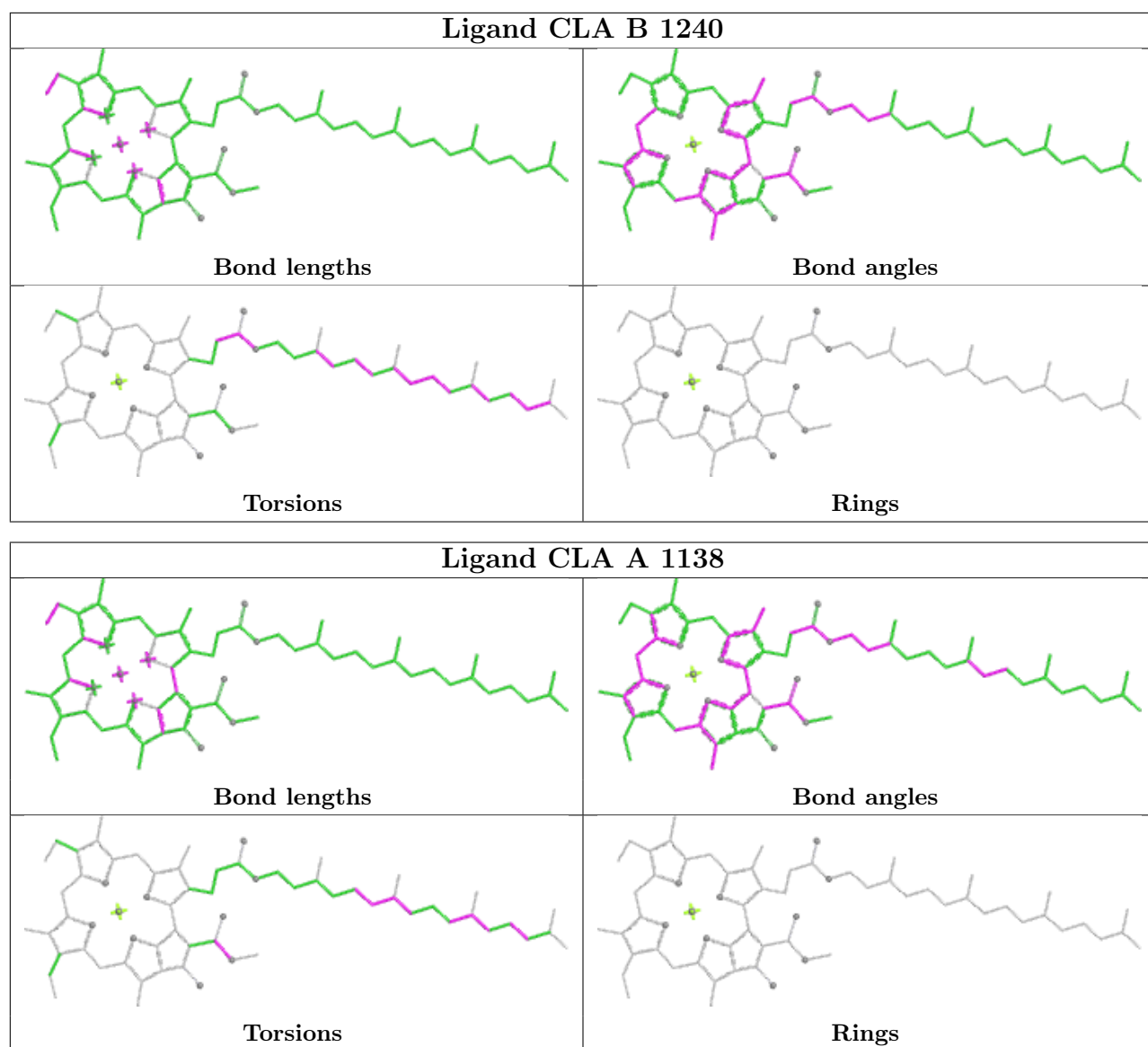


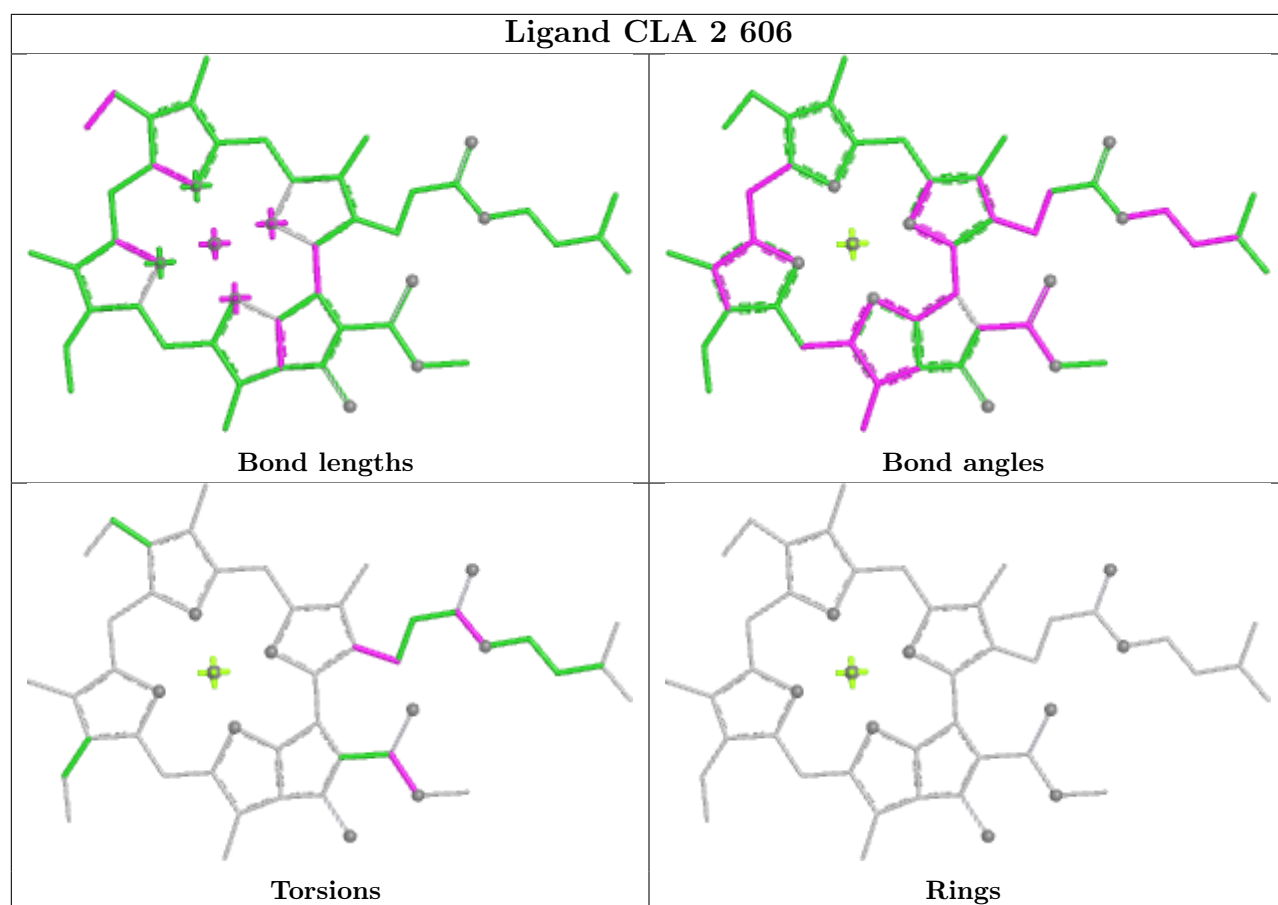
Rings



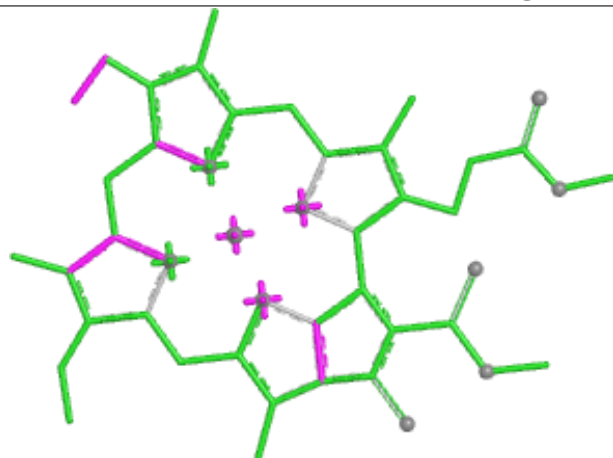




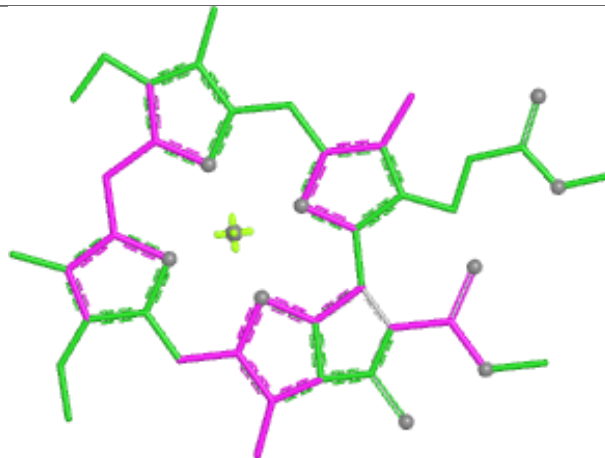




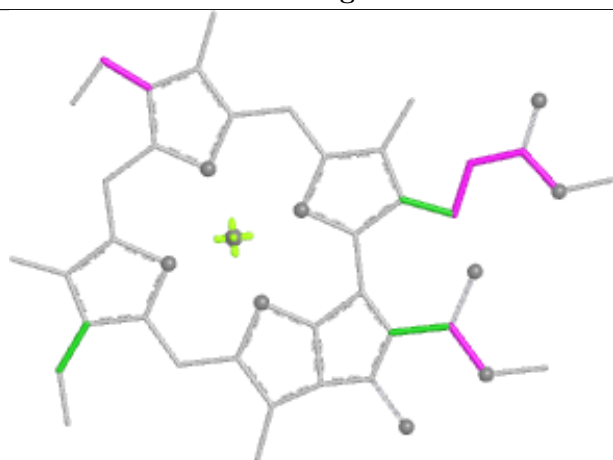
Ligand CLA 4 608



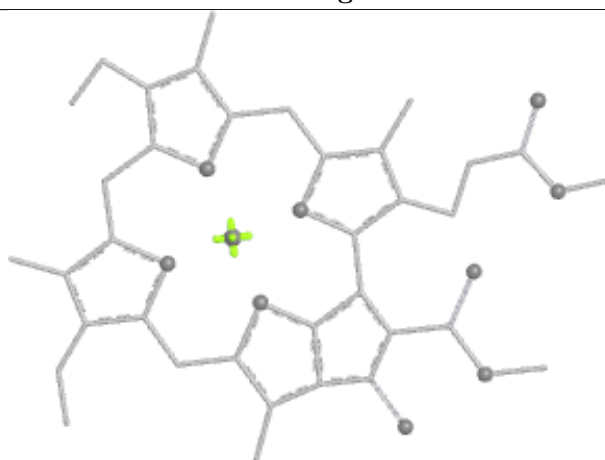
Bond lengths



Bond angles

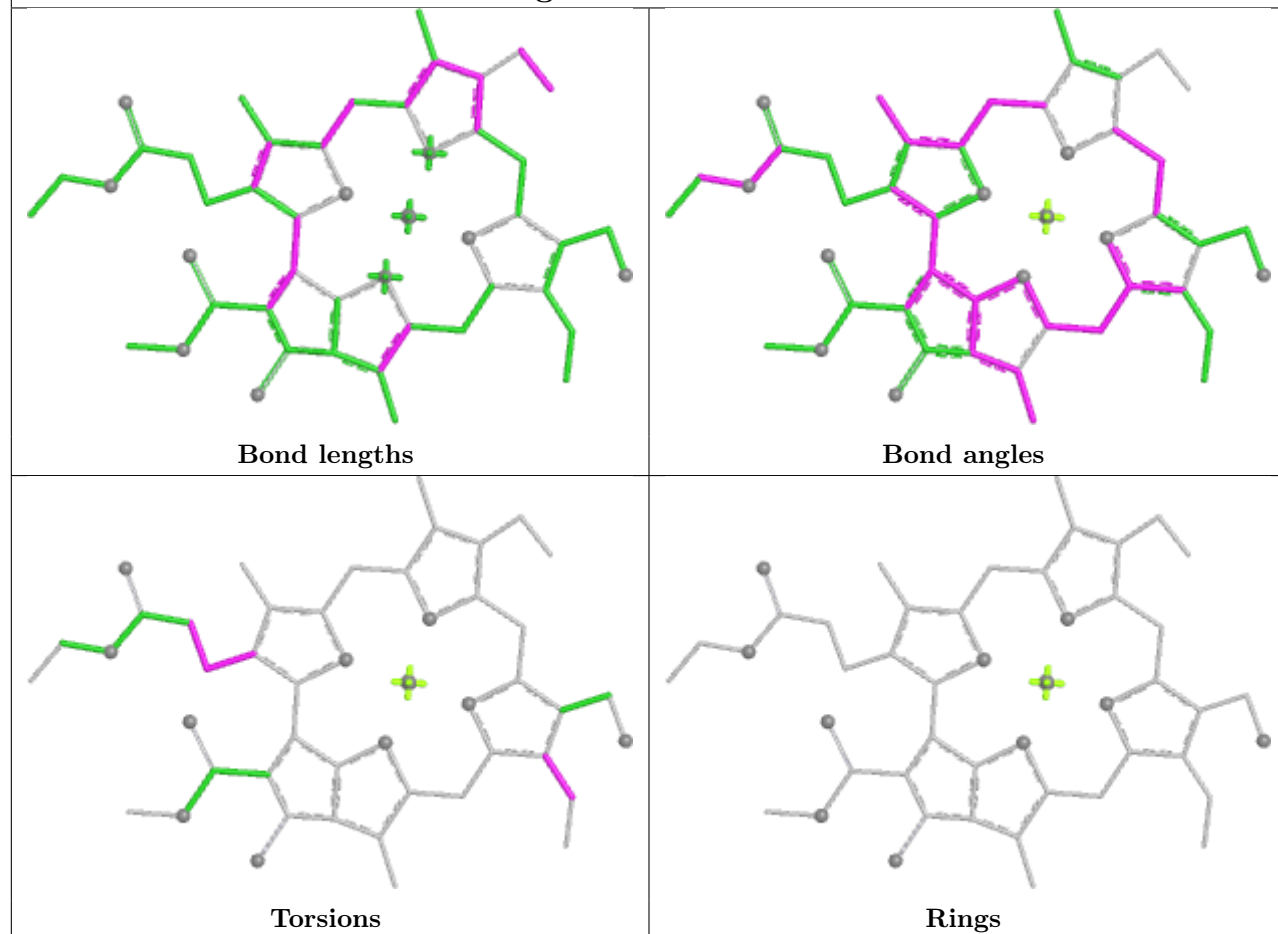


Torsions

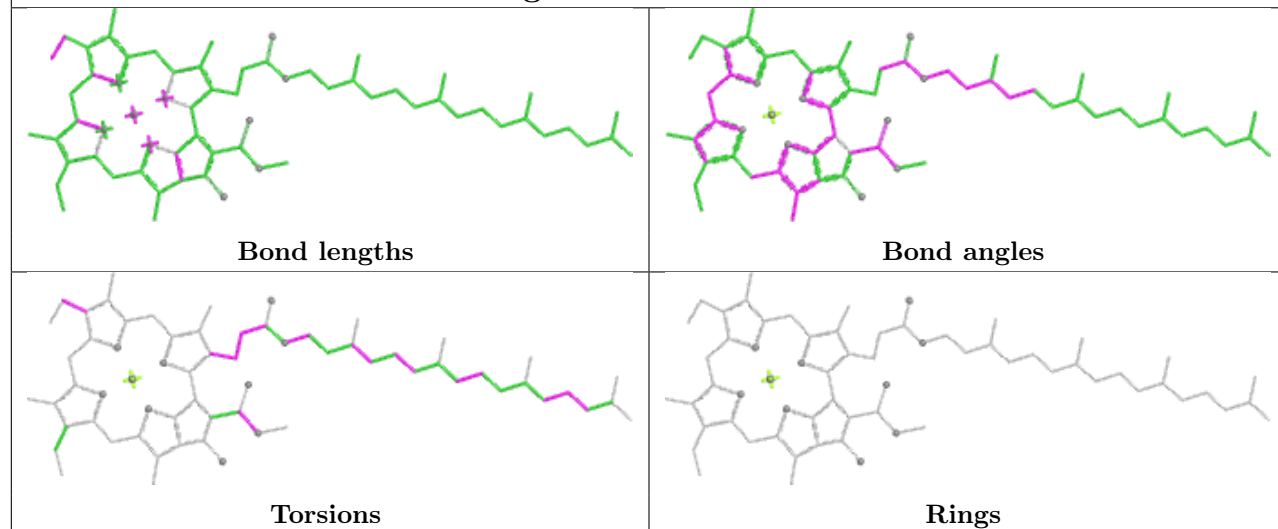


Rings

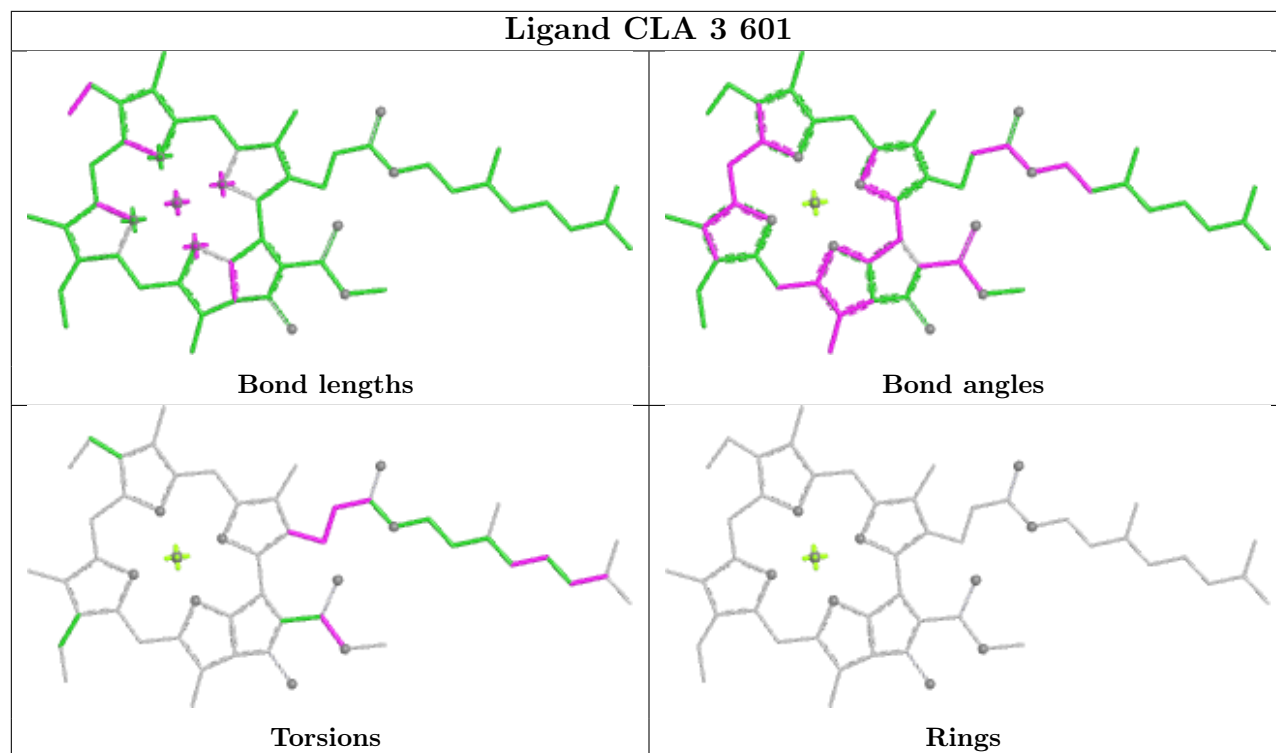
Ligand CHL 2 611



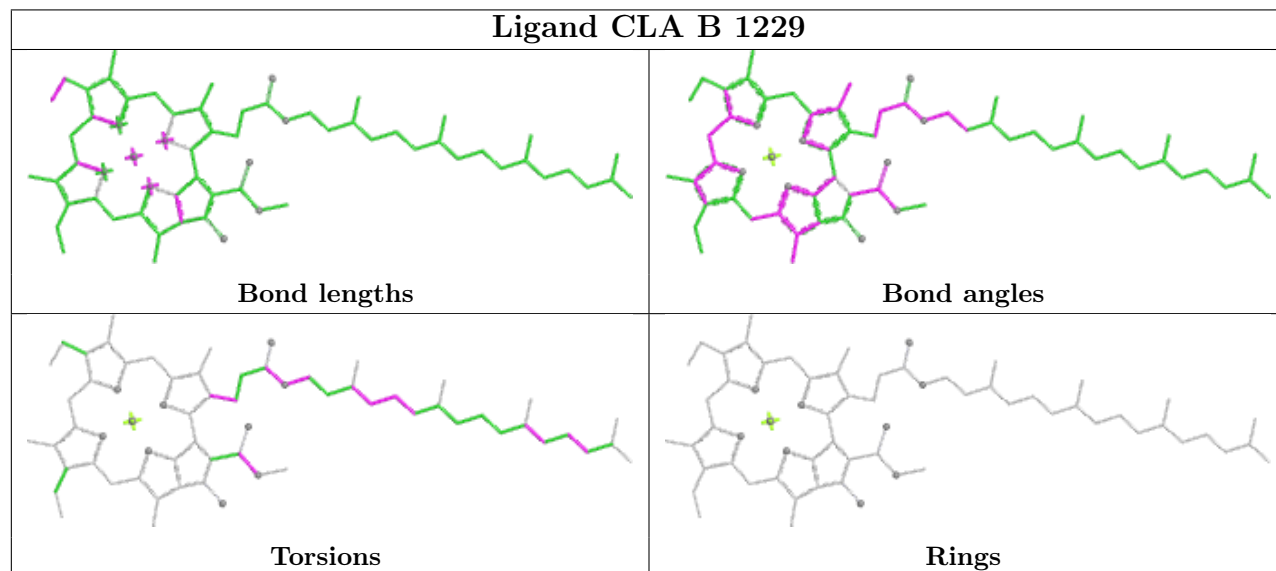
Ligand CLA B 1224

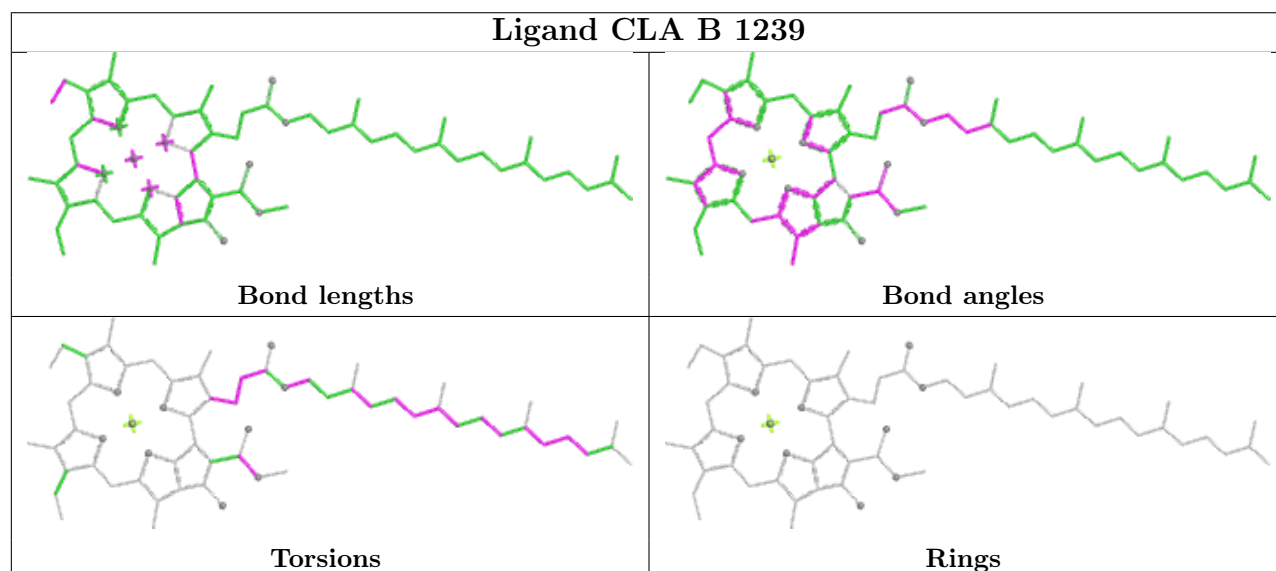
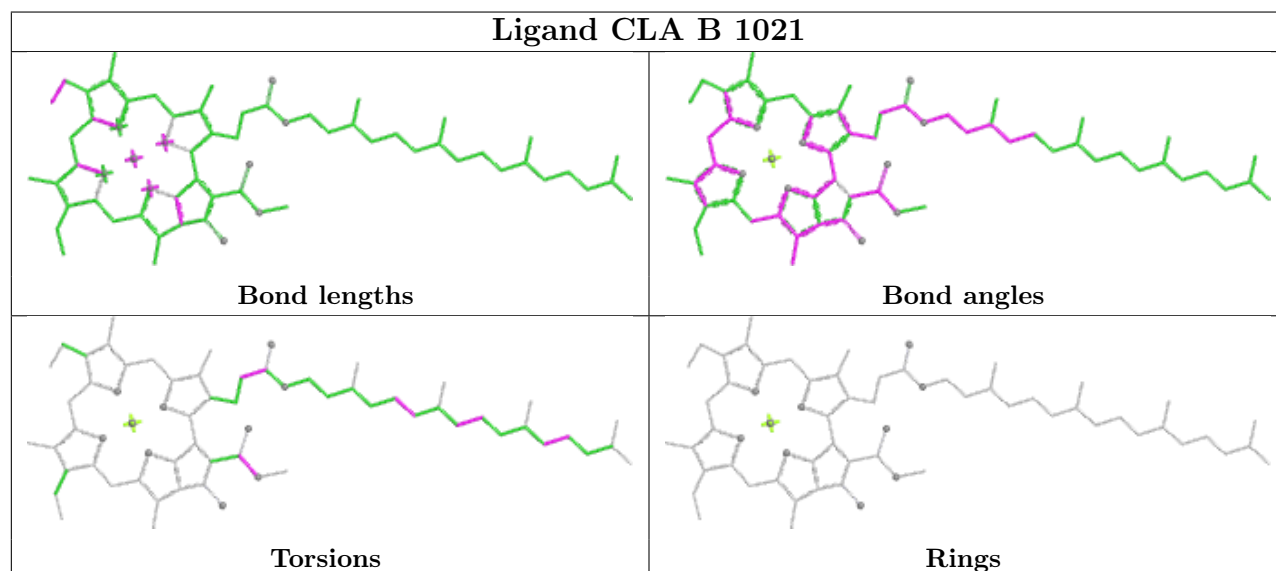
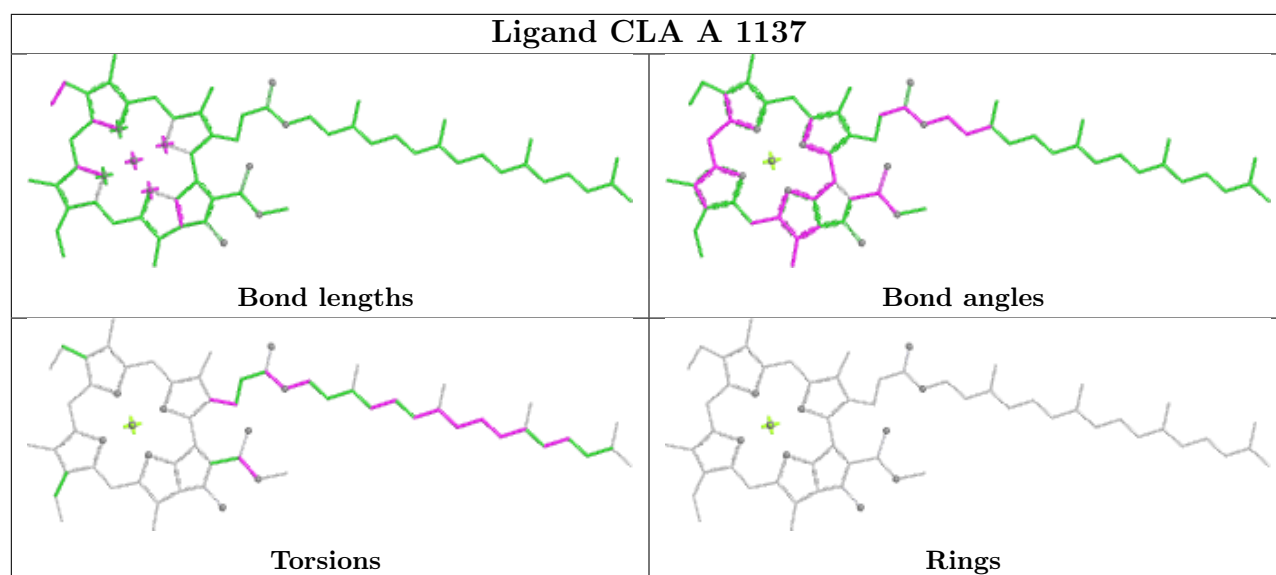


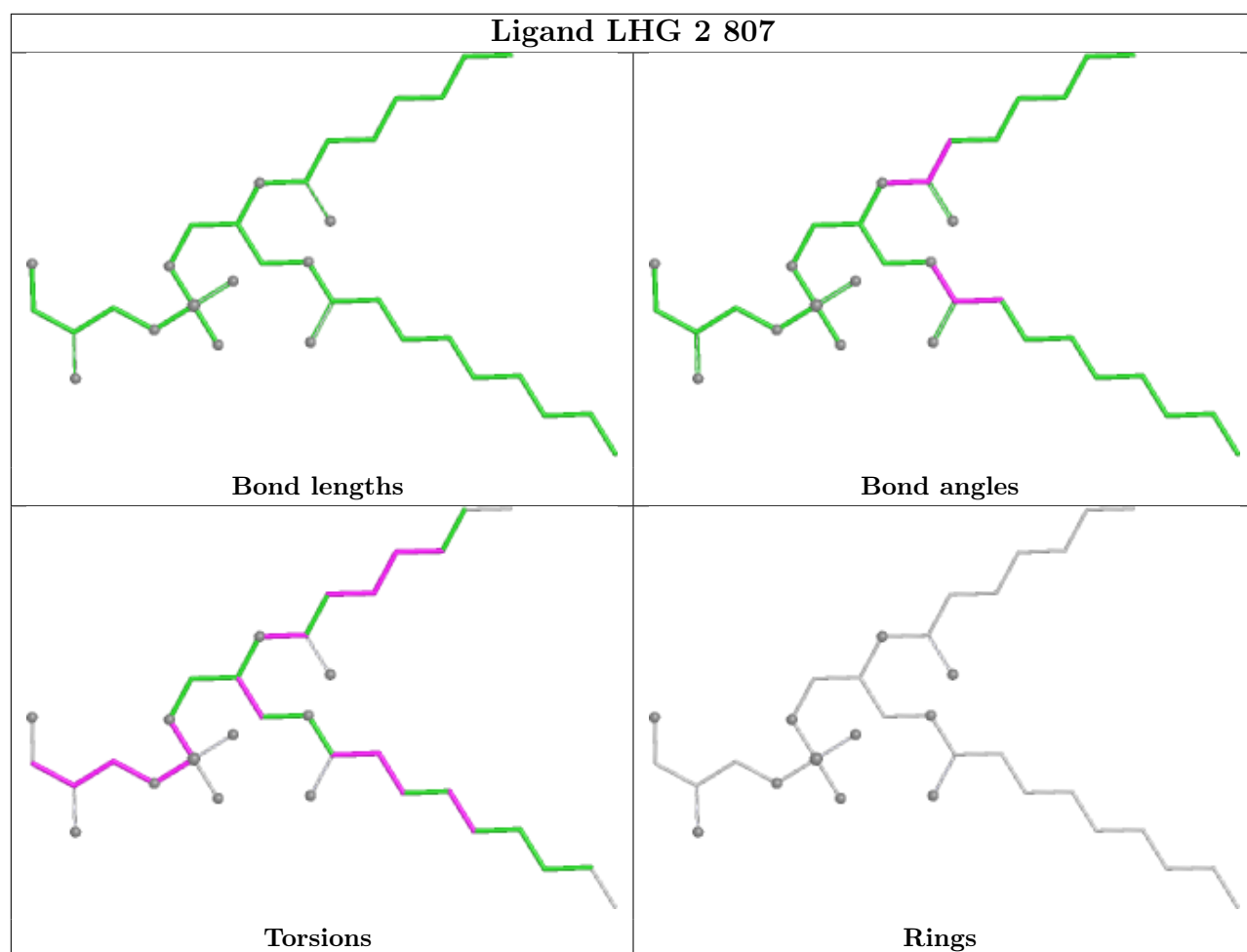
Ligand CLA 3 601



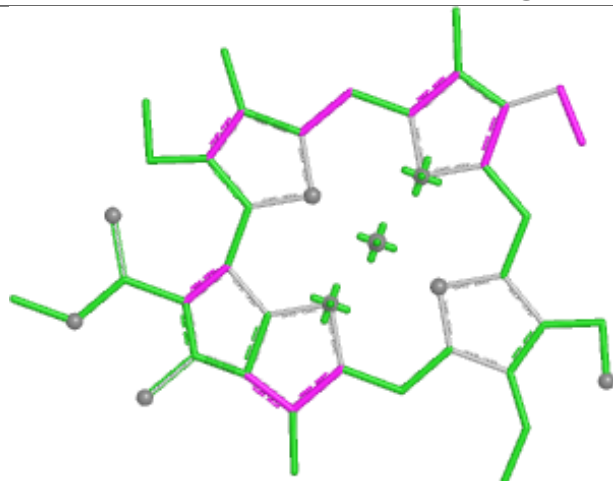
Ligand CLA B 1229



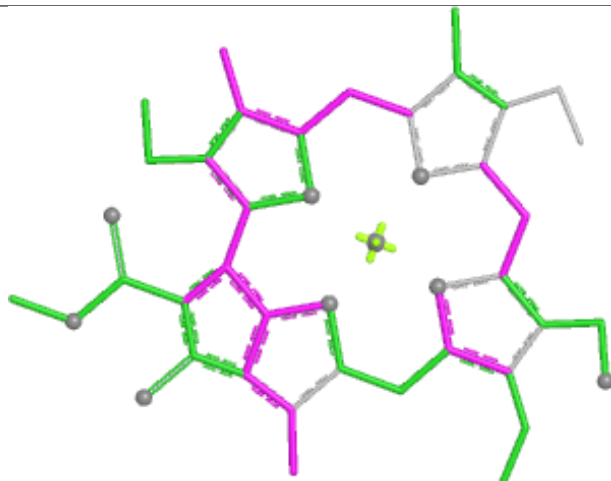




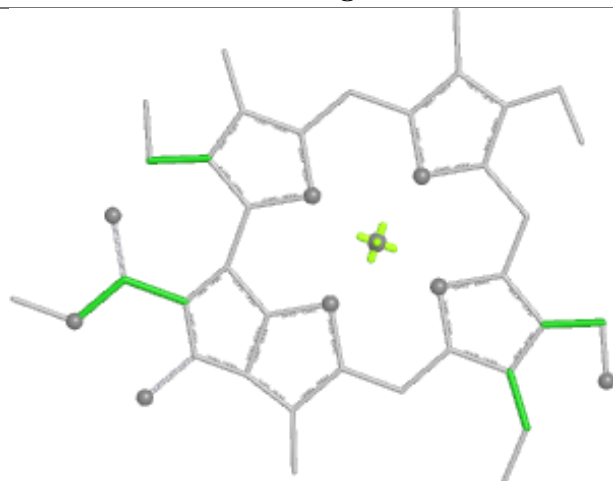
Ligand CHL 4 615



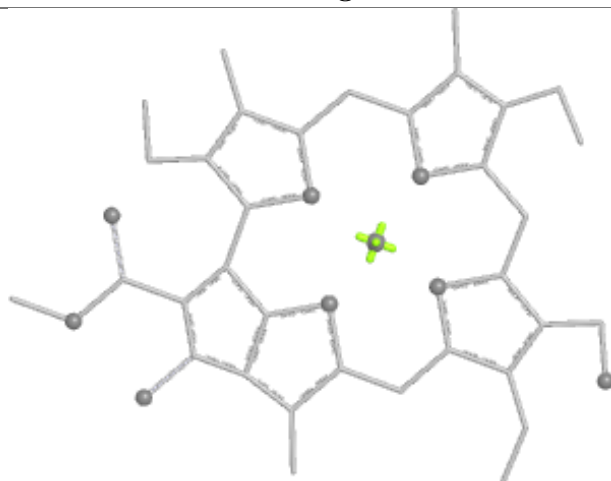
Bond lengths



Bond angles

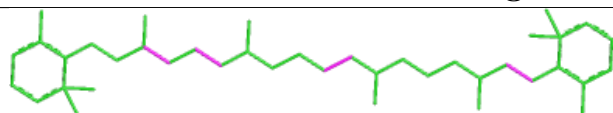


Torsions

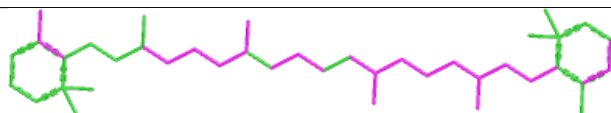


Rings

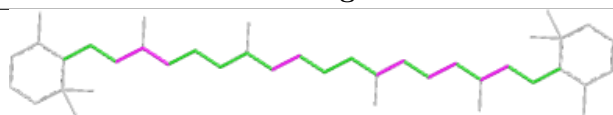
Ligand BCR F 4014



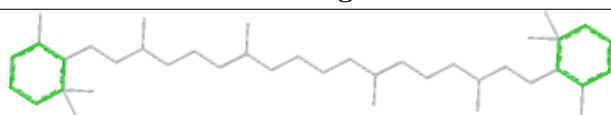
Bond lengths



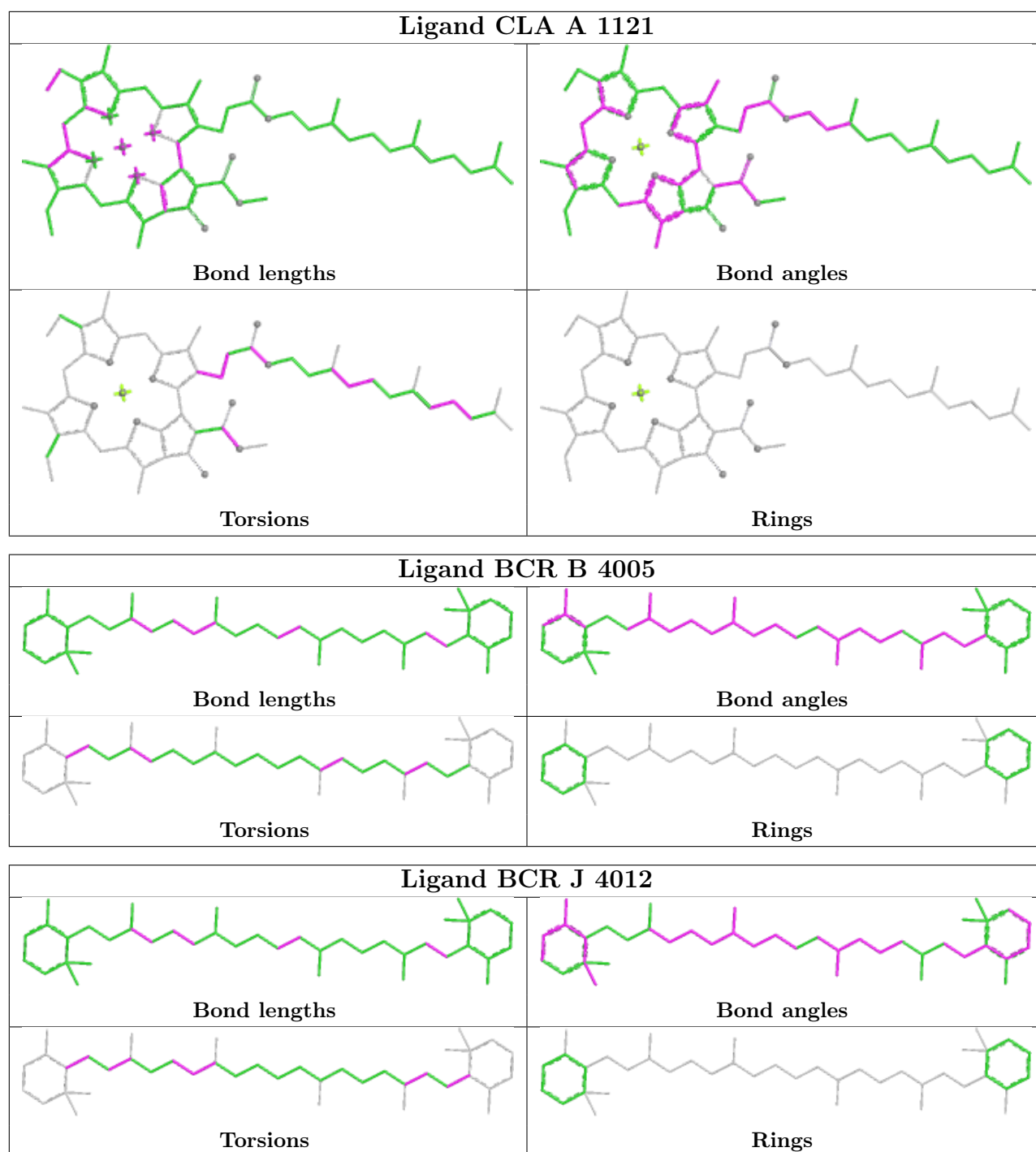
Bond angles



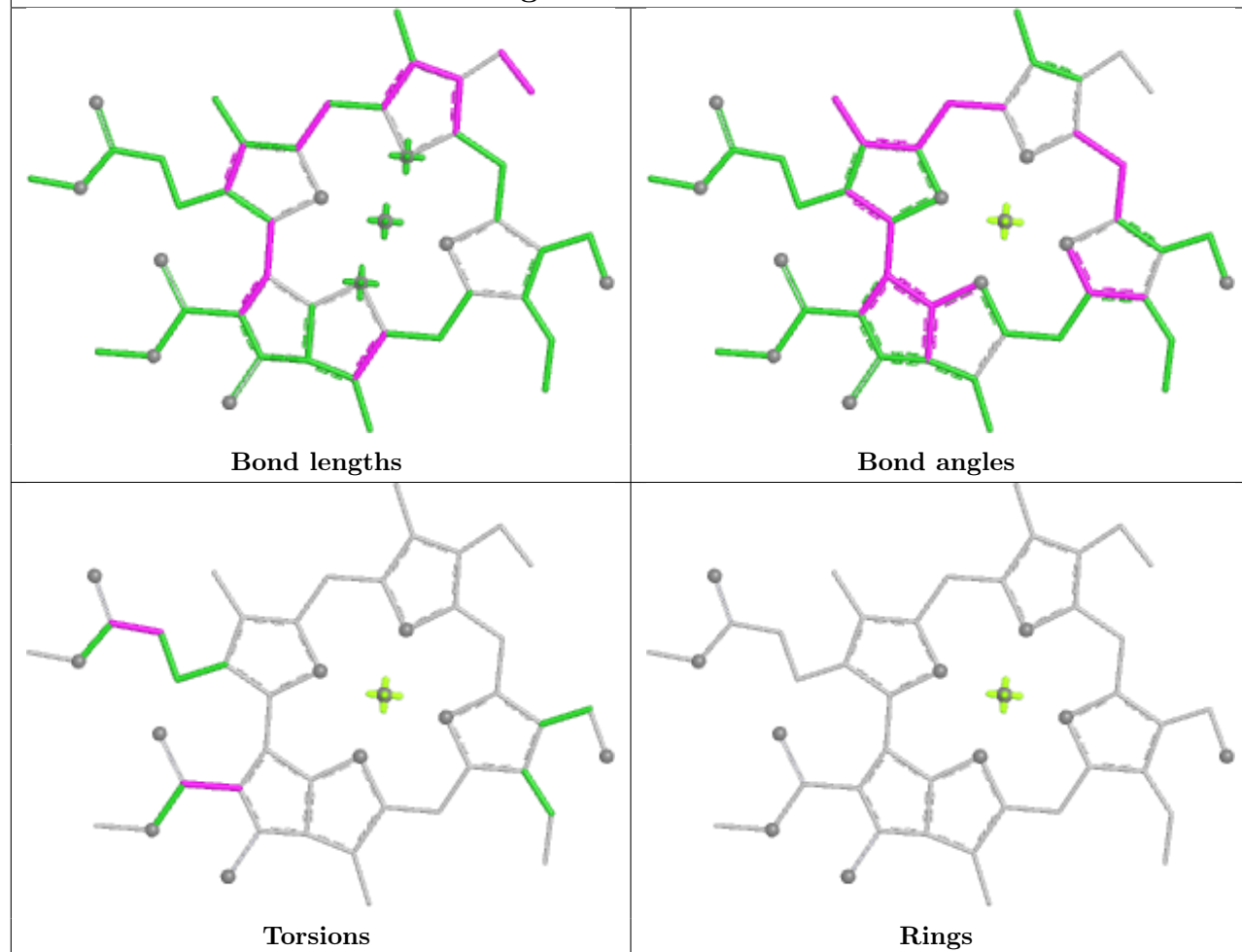
Torsions



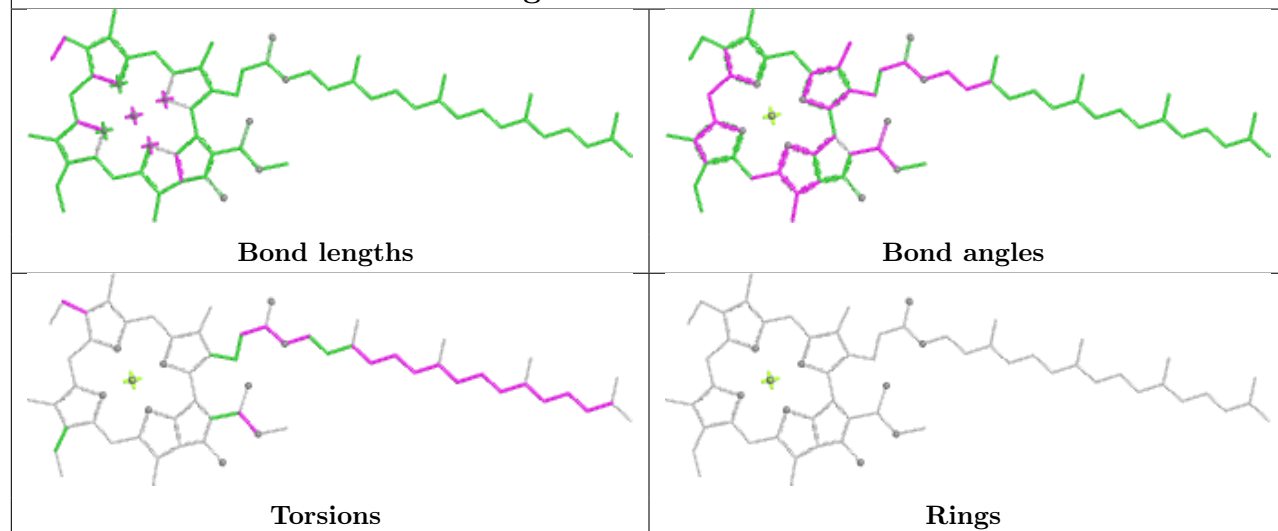
Rings

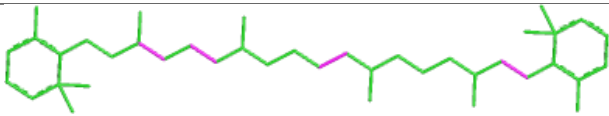
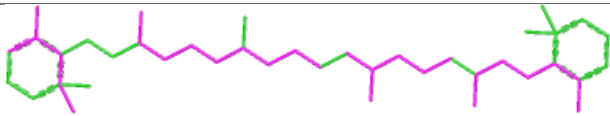
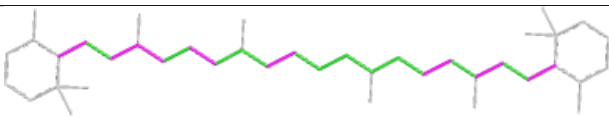
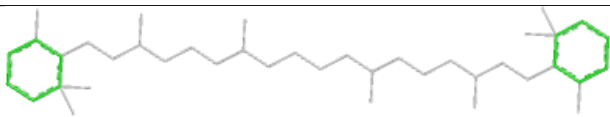


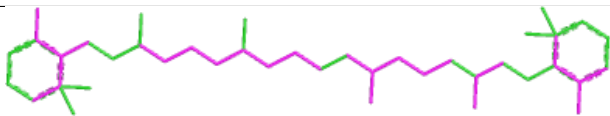
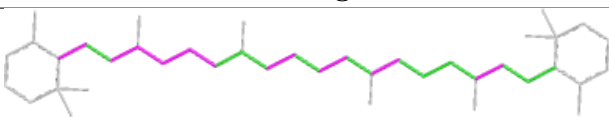
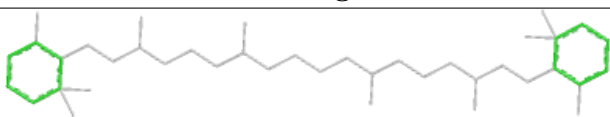
Ligand CHL 1 610

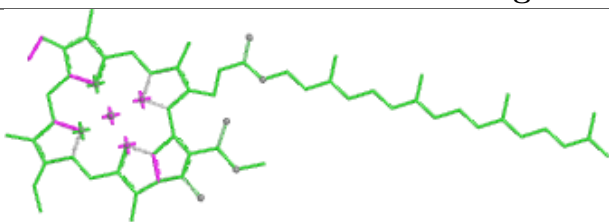
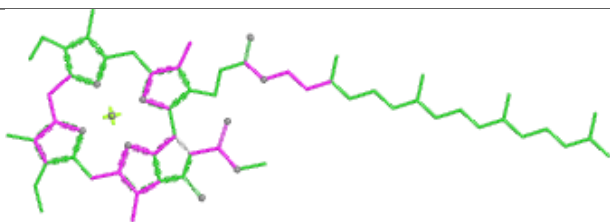
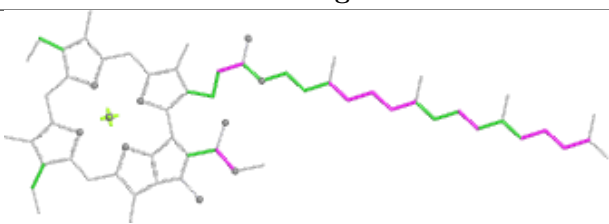
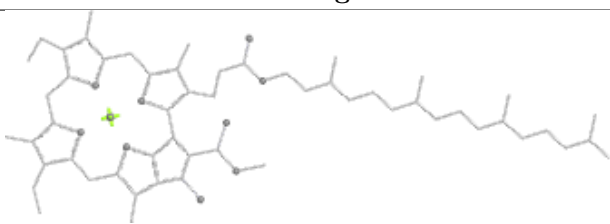


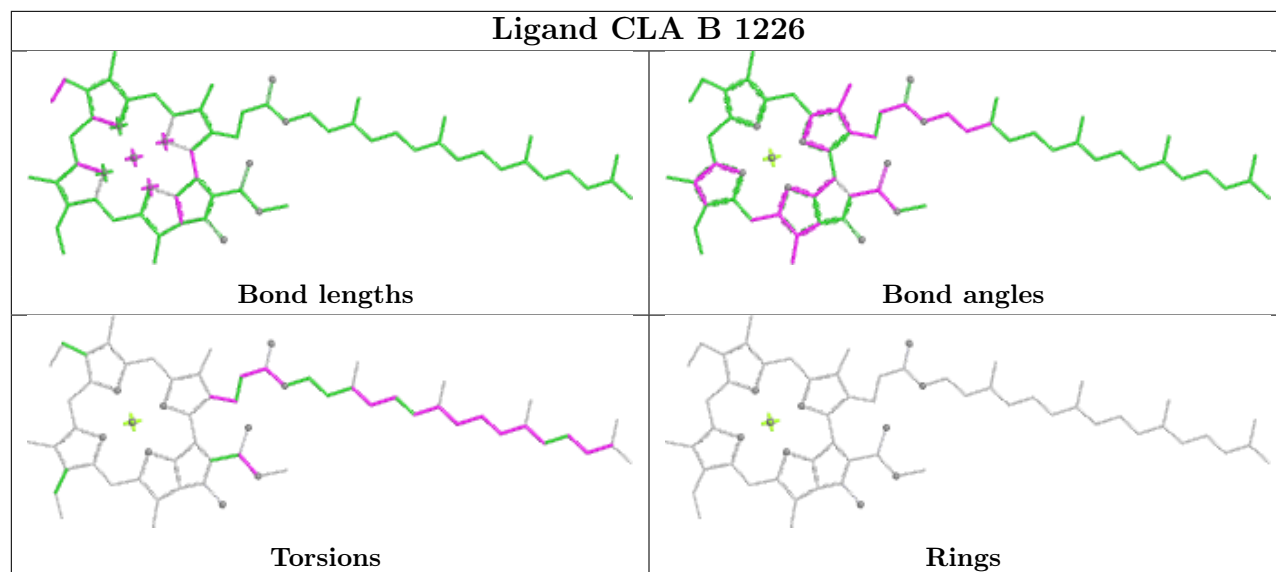
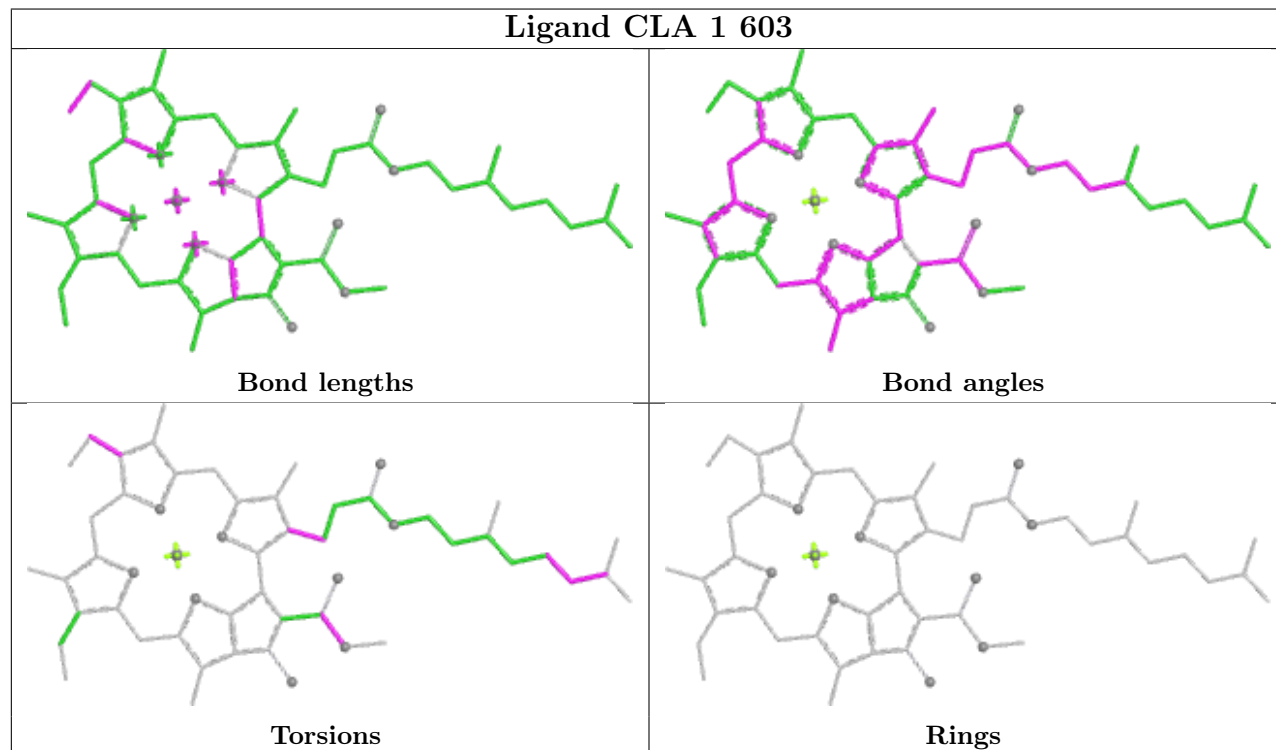
Ligand CLA B 1238

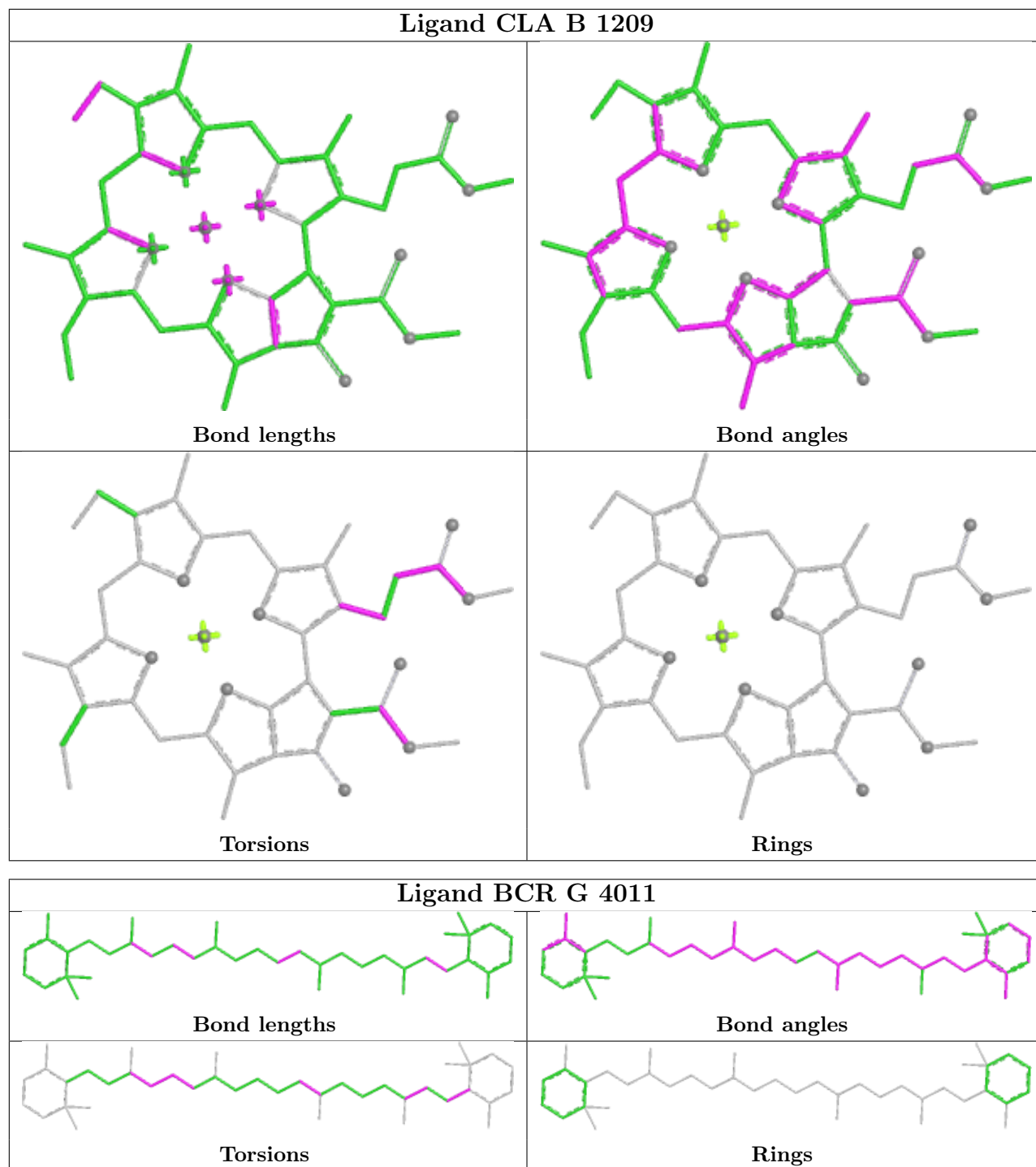


Ligand BCR A 4008	
	
Bond lengths	Bond angles
	
Torsions	Rings

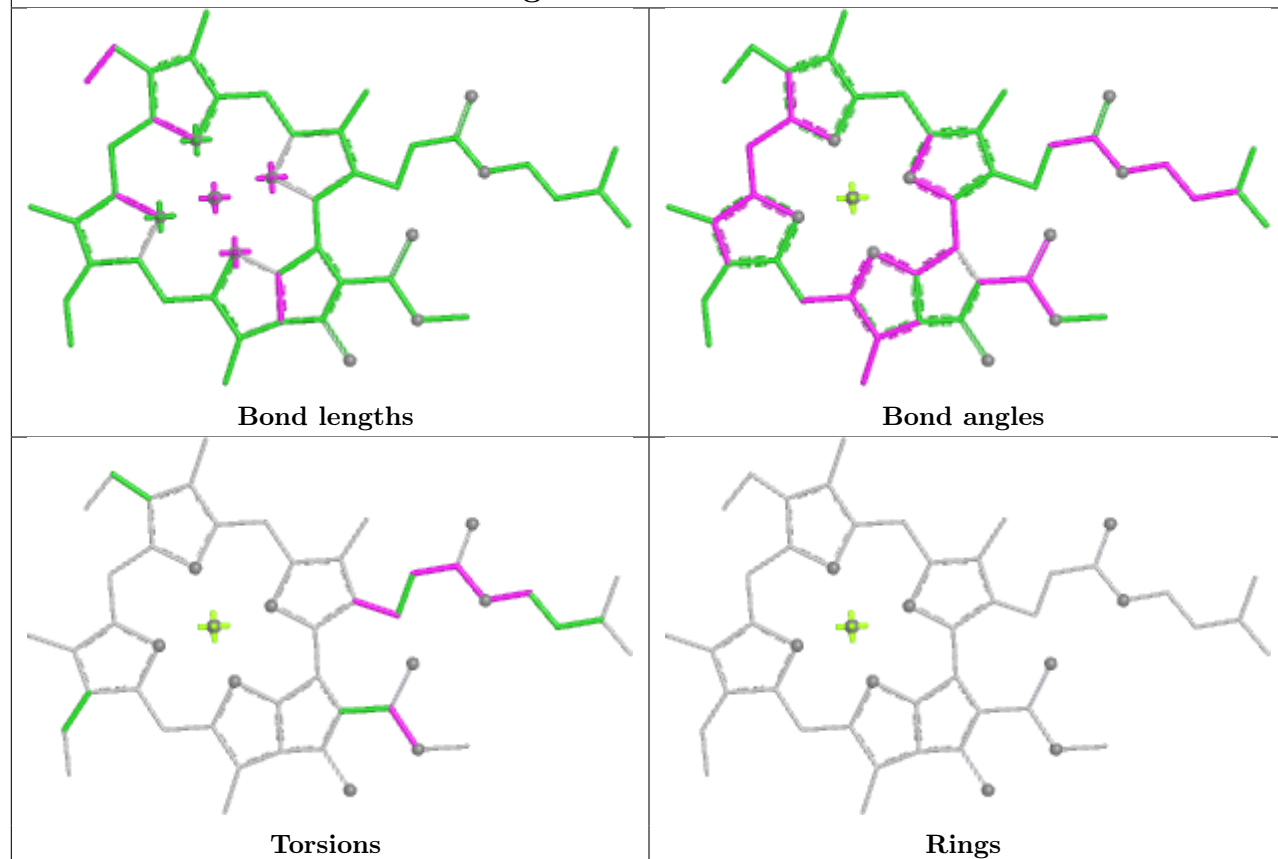
Ligand BCR G 4021	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 1 605	
	
Bond lengths	Bond angles
	
Torsions	Rings

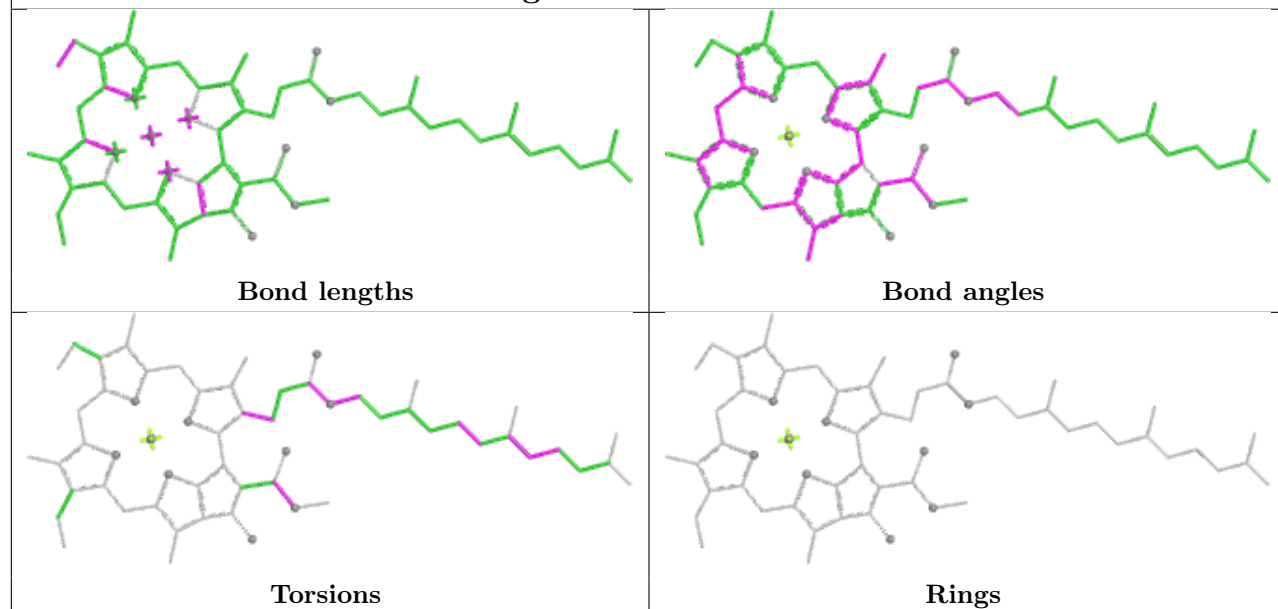
Ligand CLA B 1226**Ligand CLA 1 603**



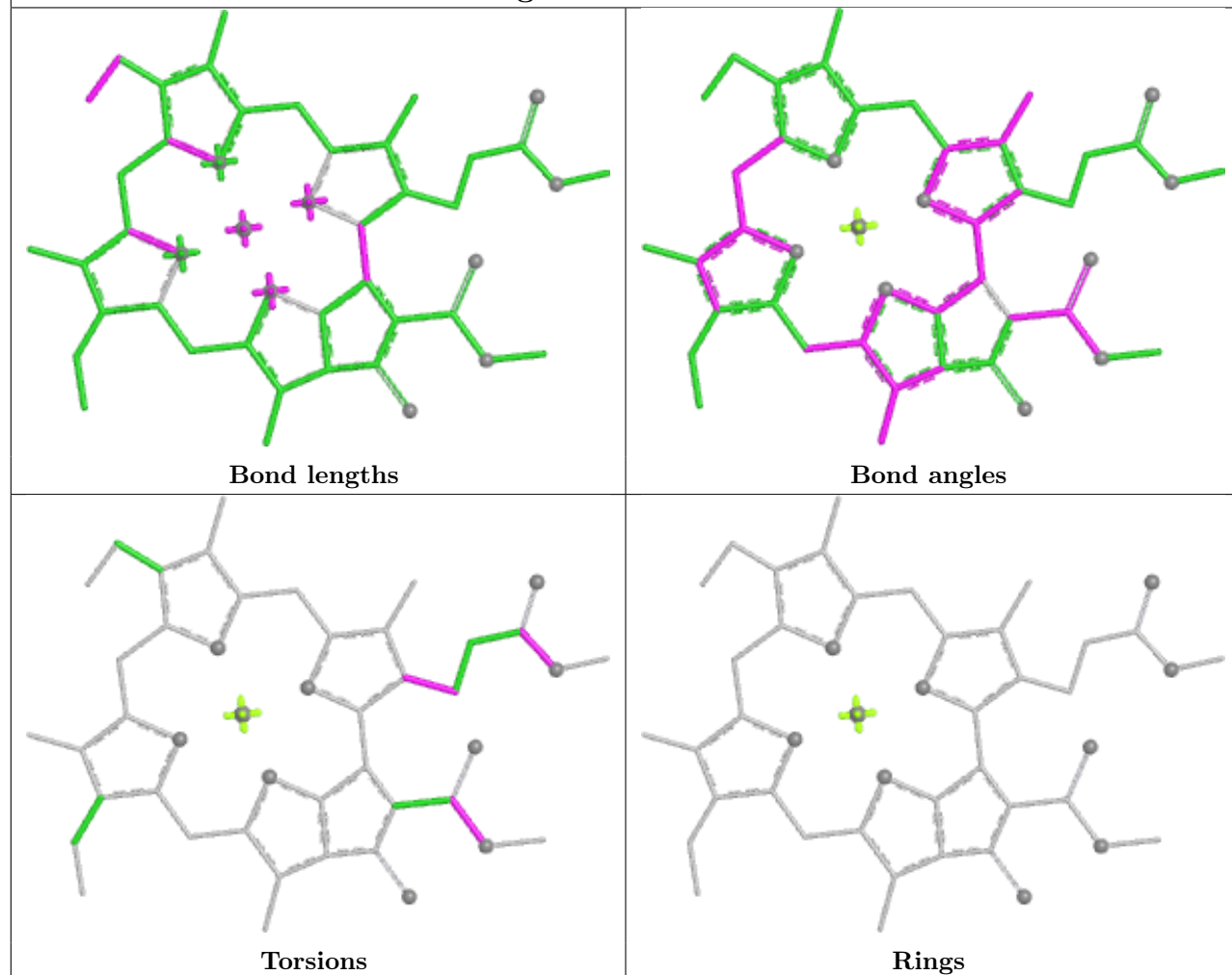
Ligand CLA B 1236



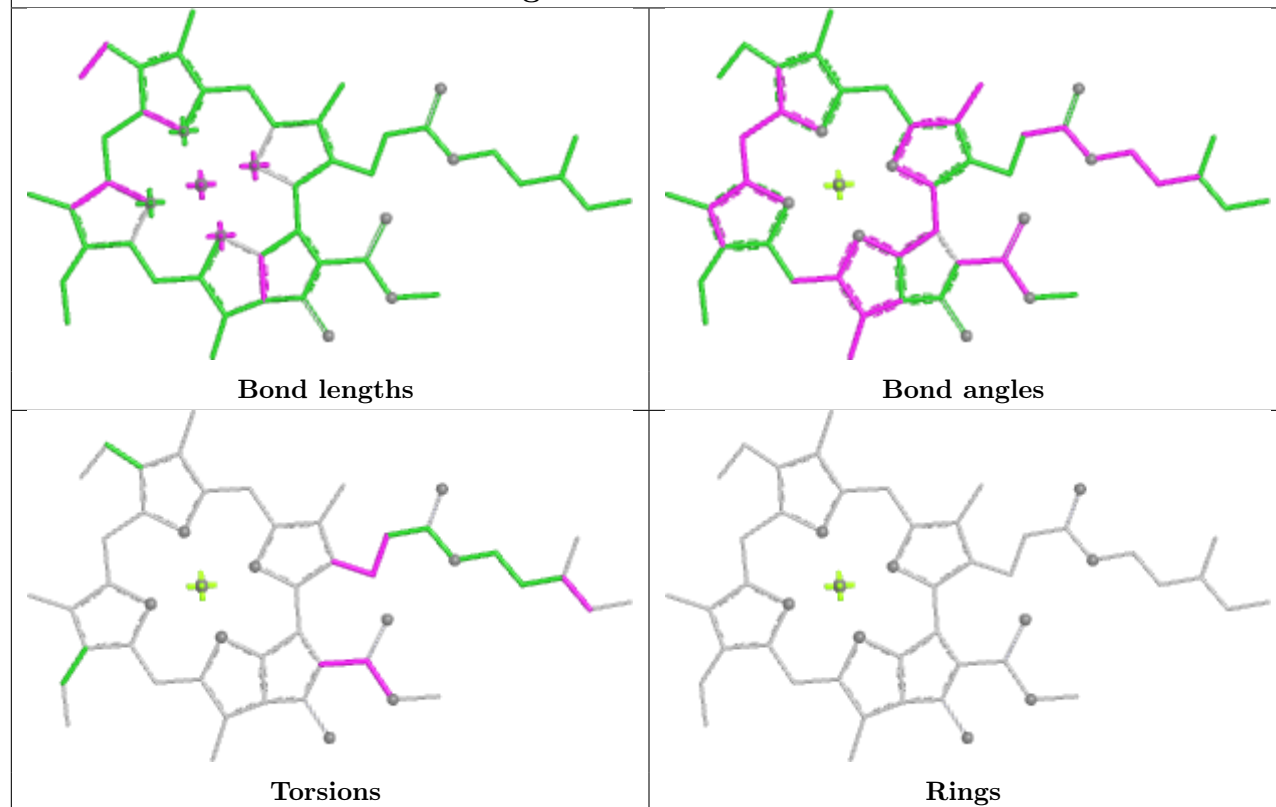
Ligand CLA A 1120



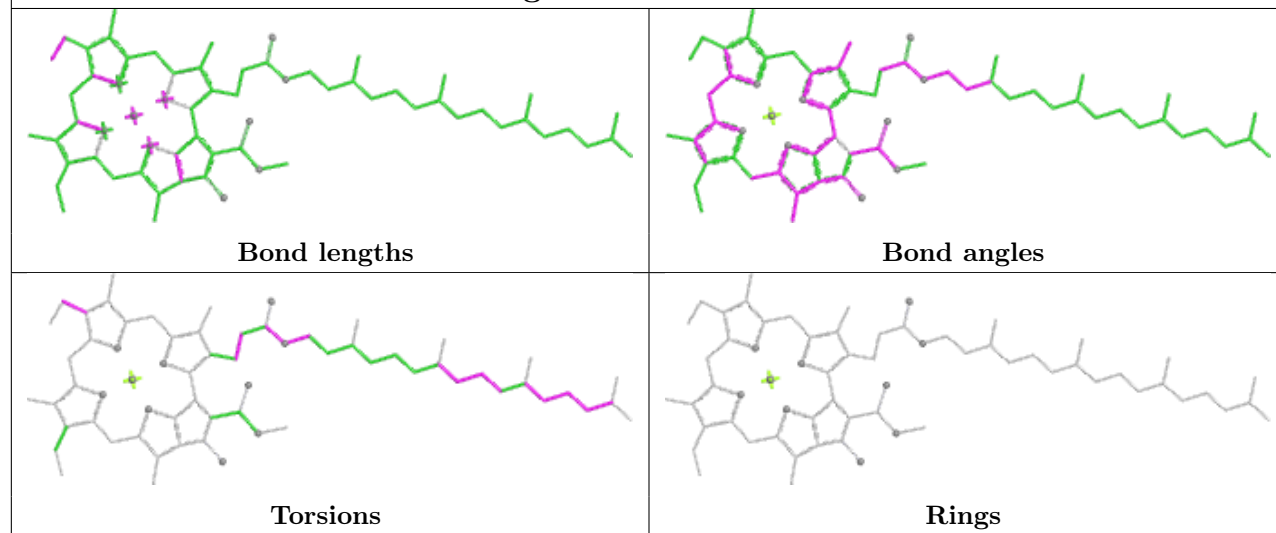
Ligand CLA 3 613

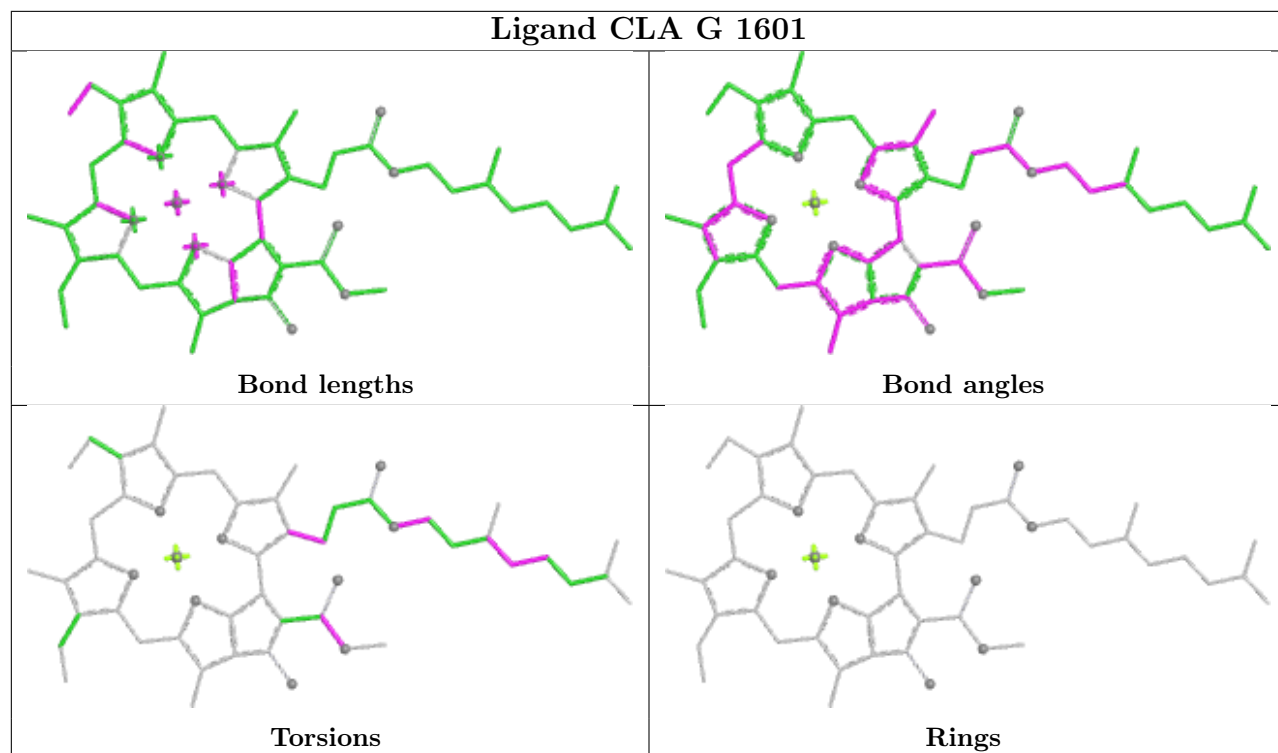


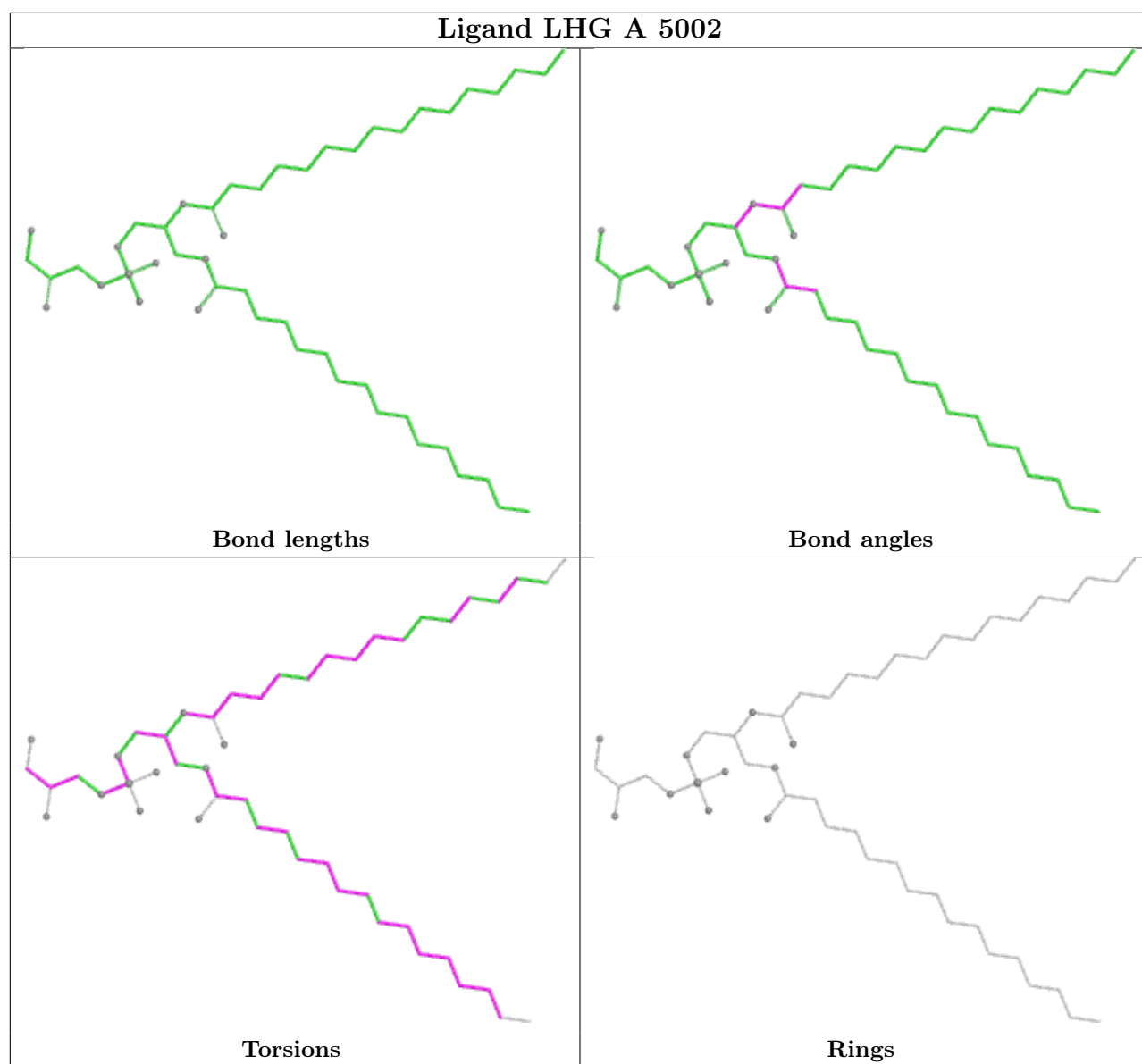
Ligand CLA A 1135

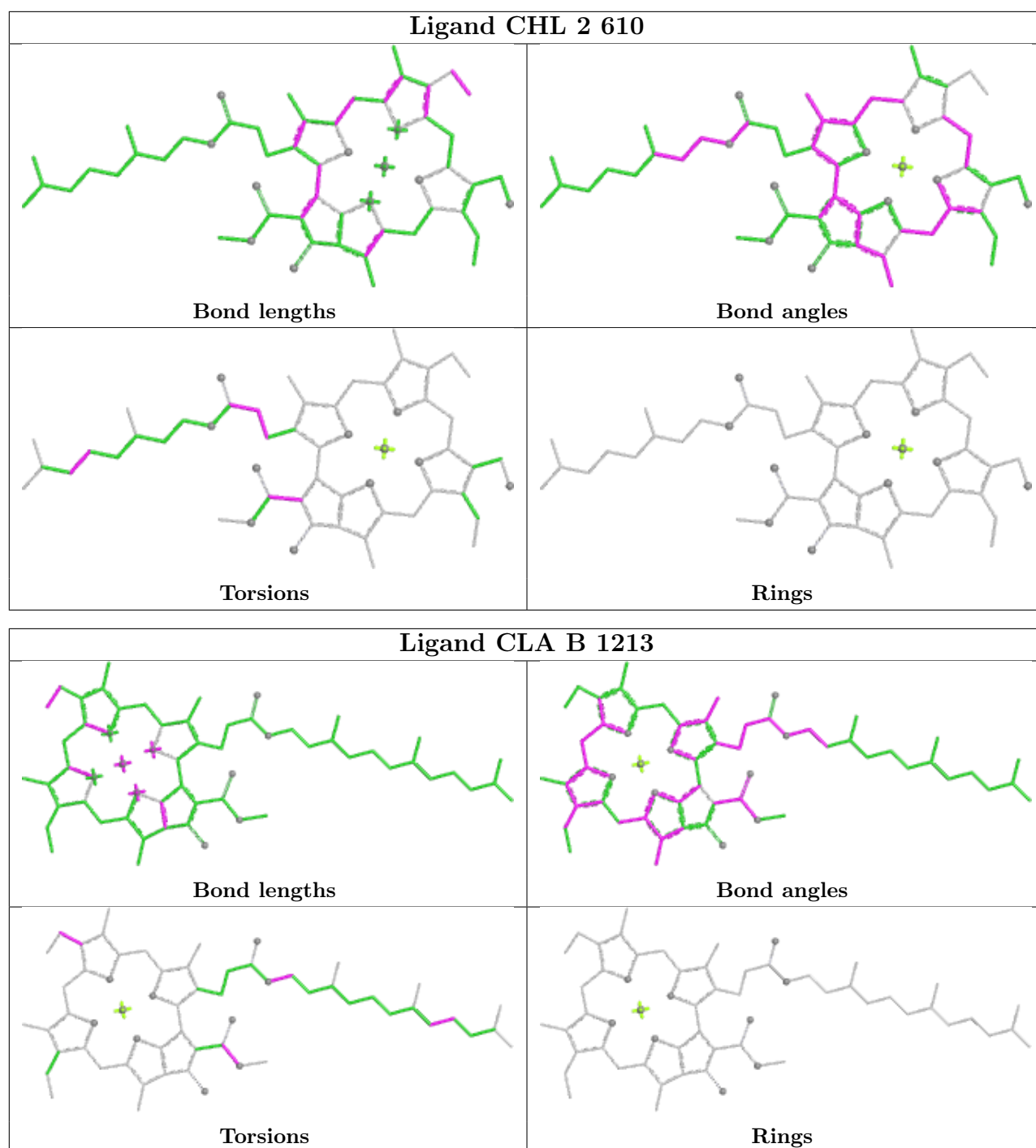


Ligand CLA B 1214

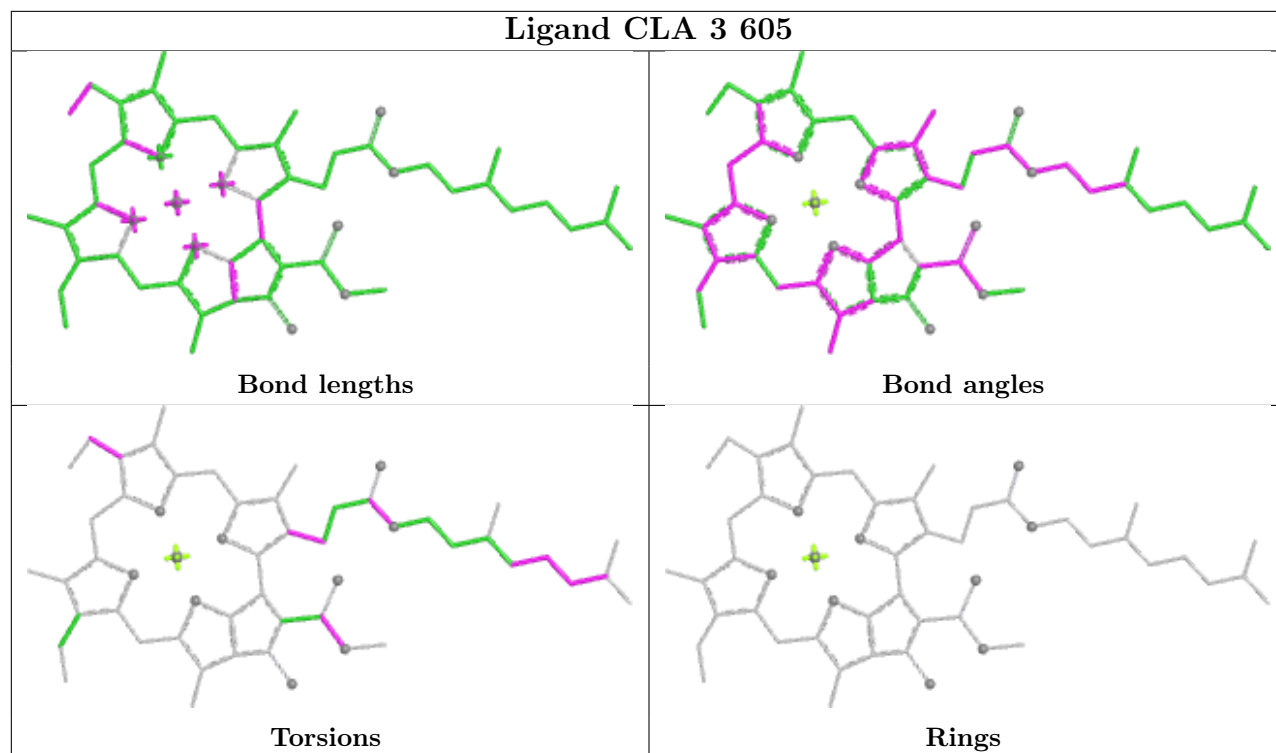




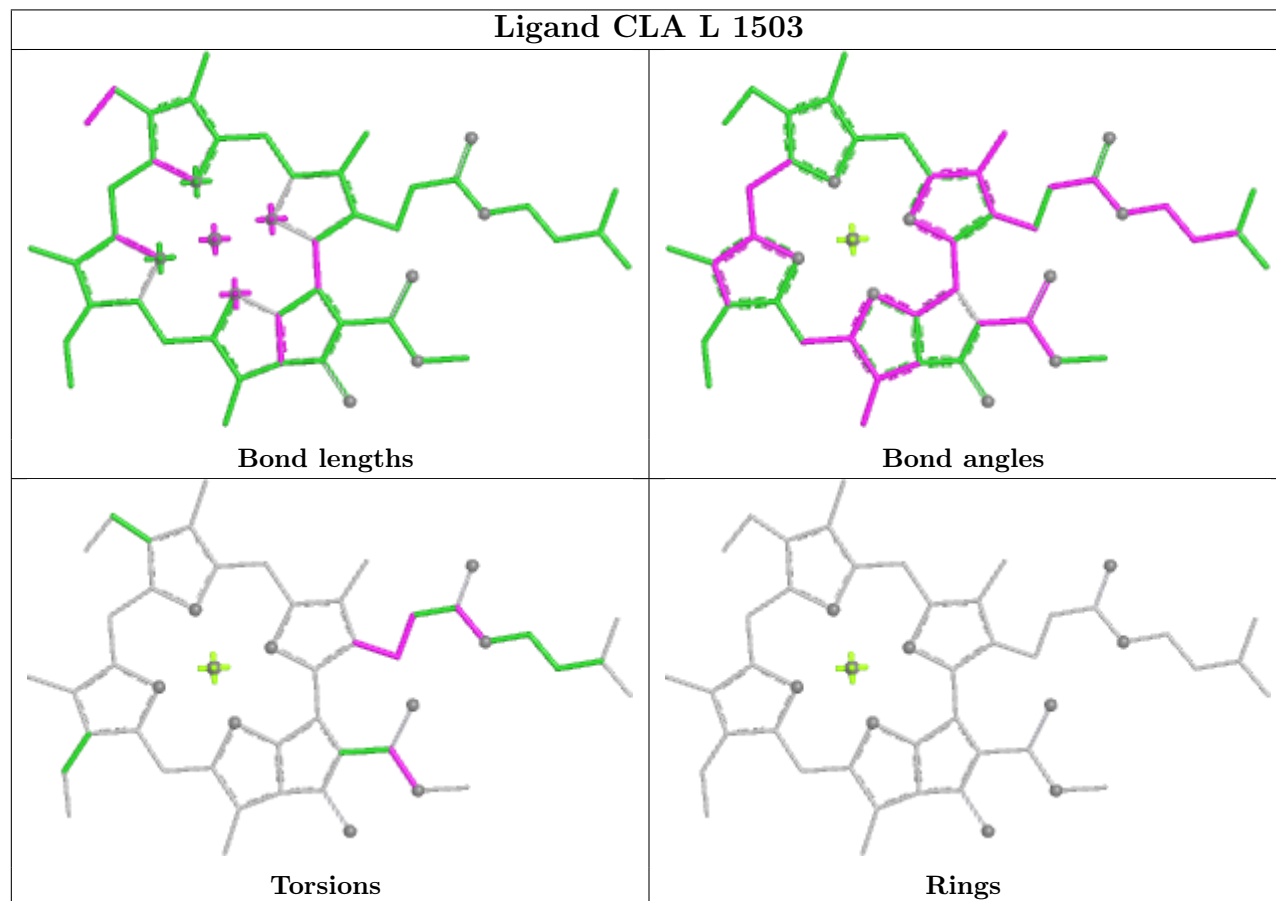


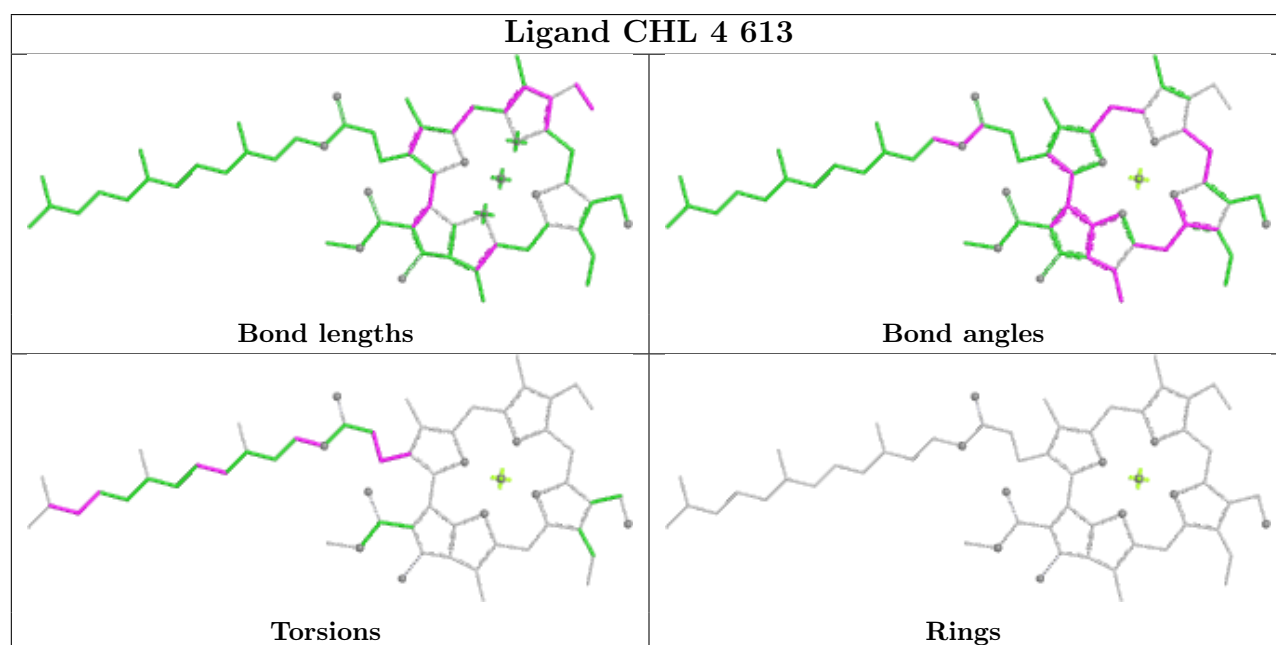
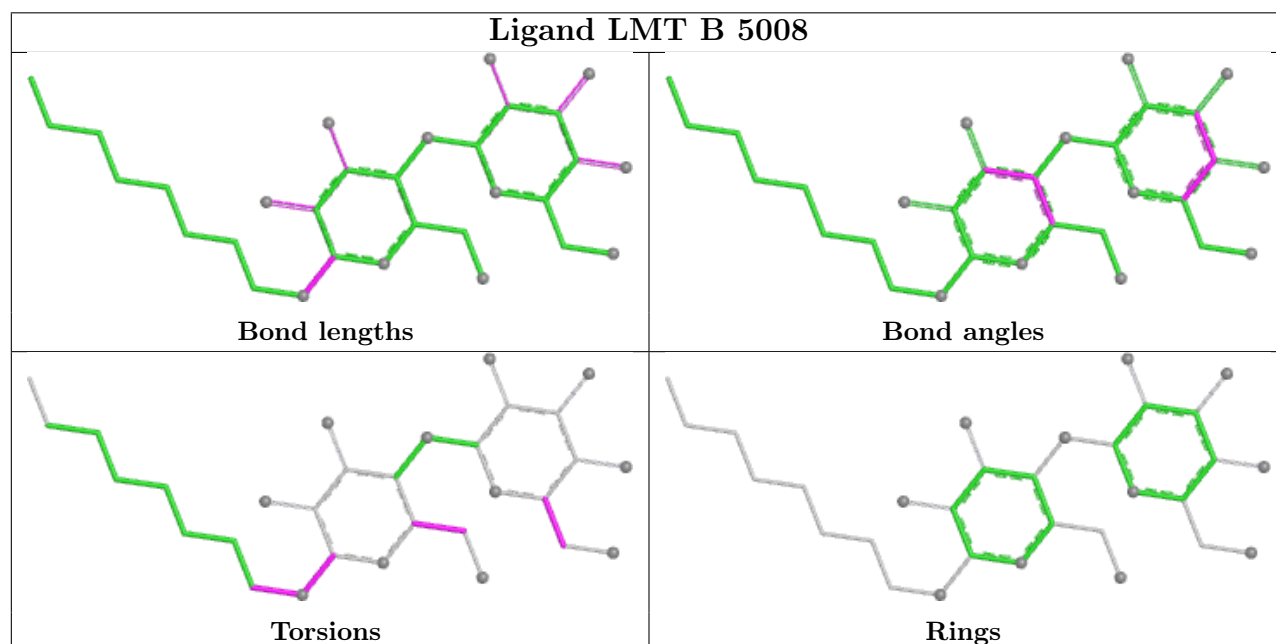
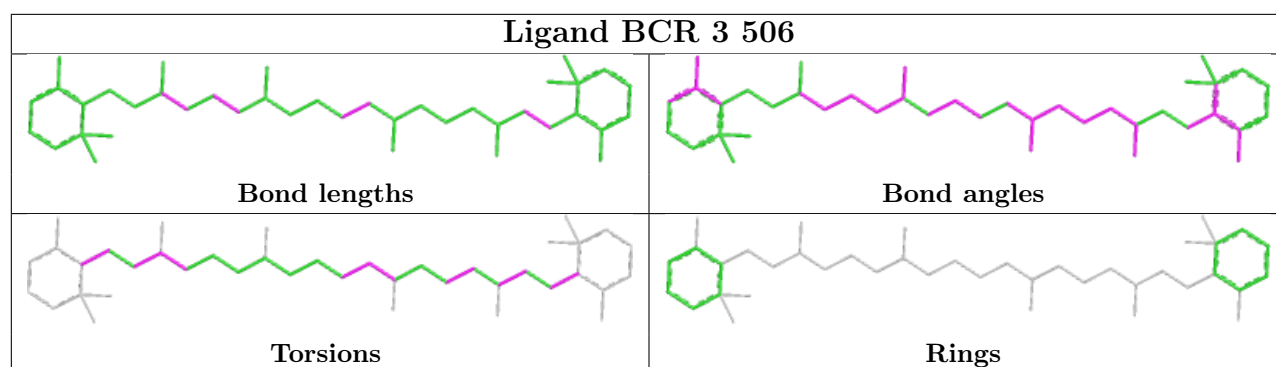


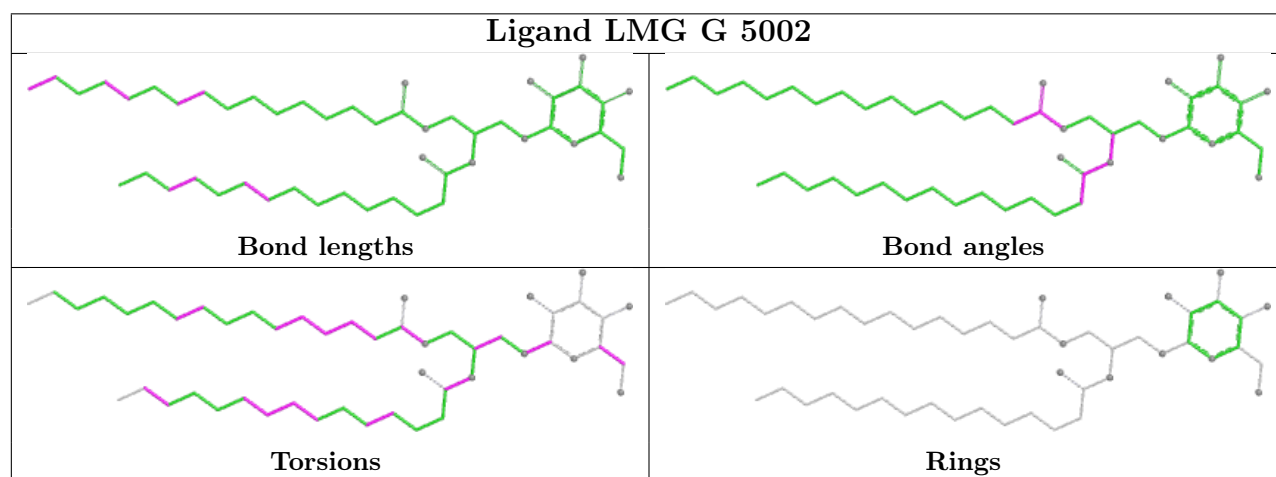
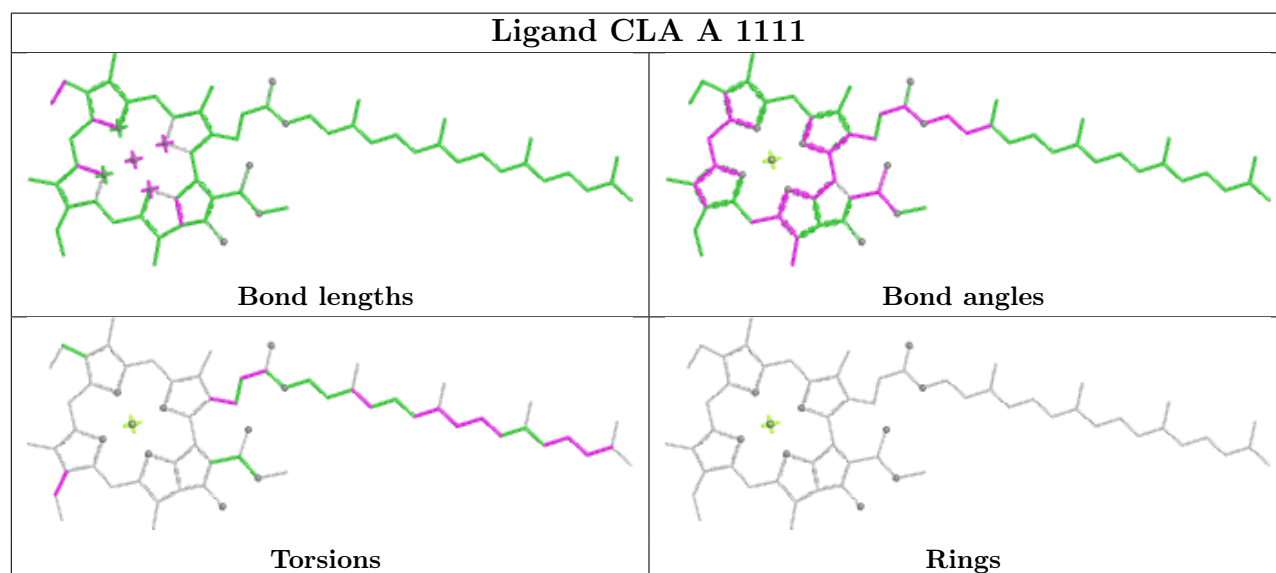
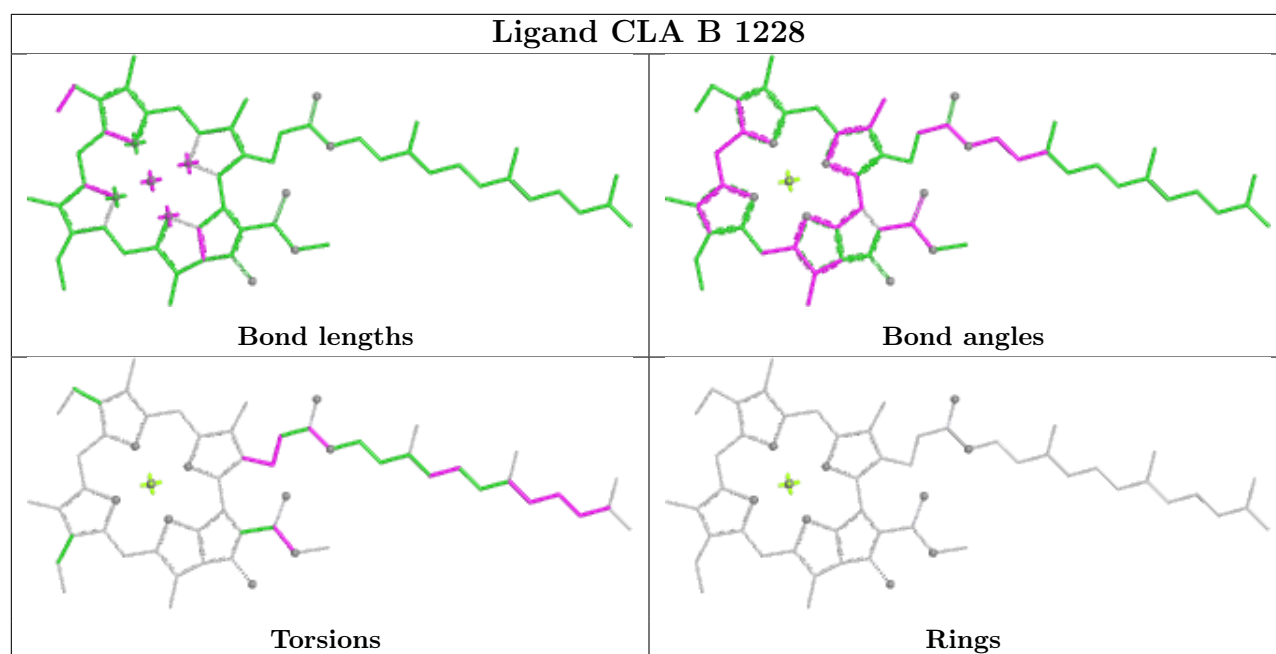
Ligand CLA 3 605



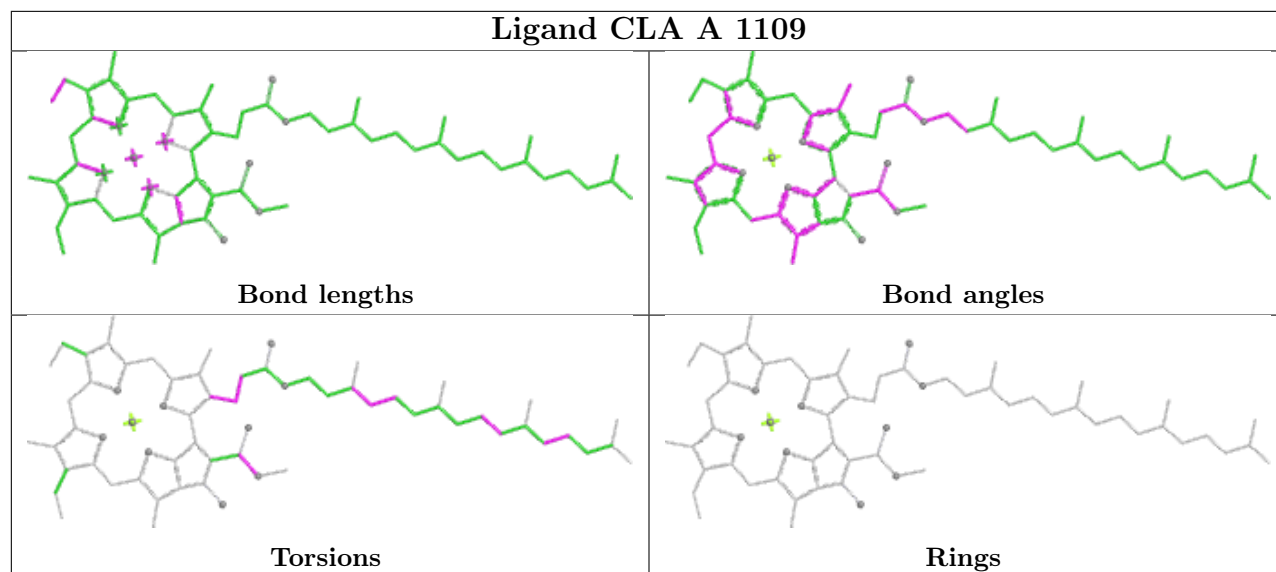
Ligand CLA L 1503



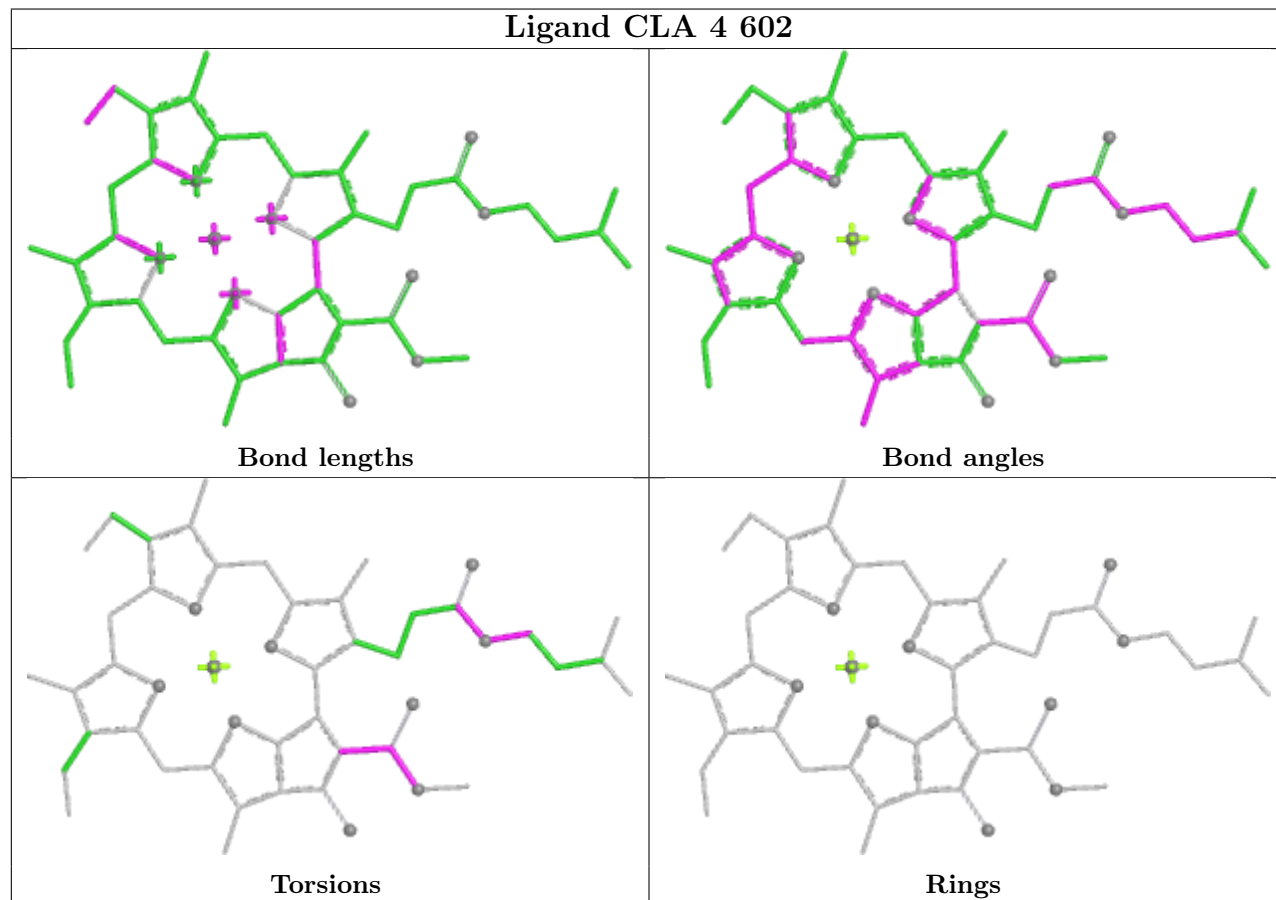


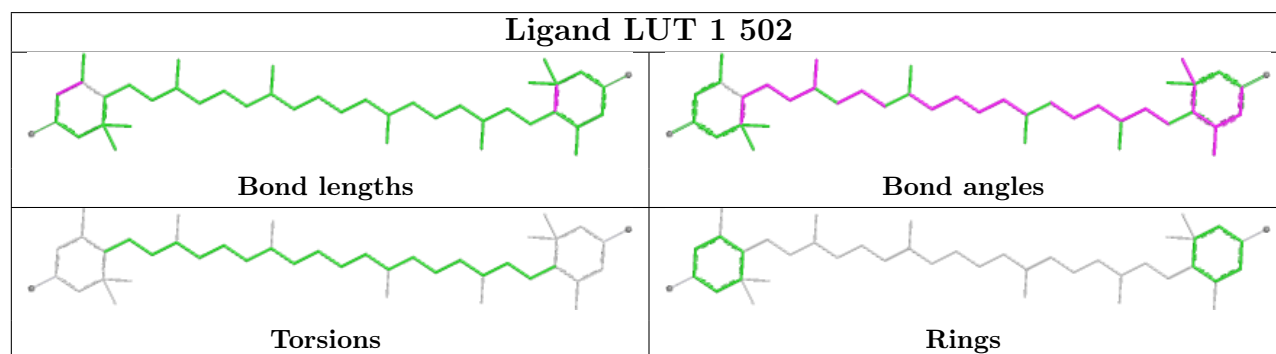
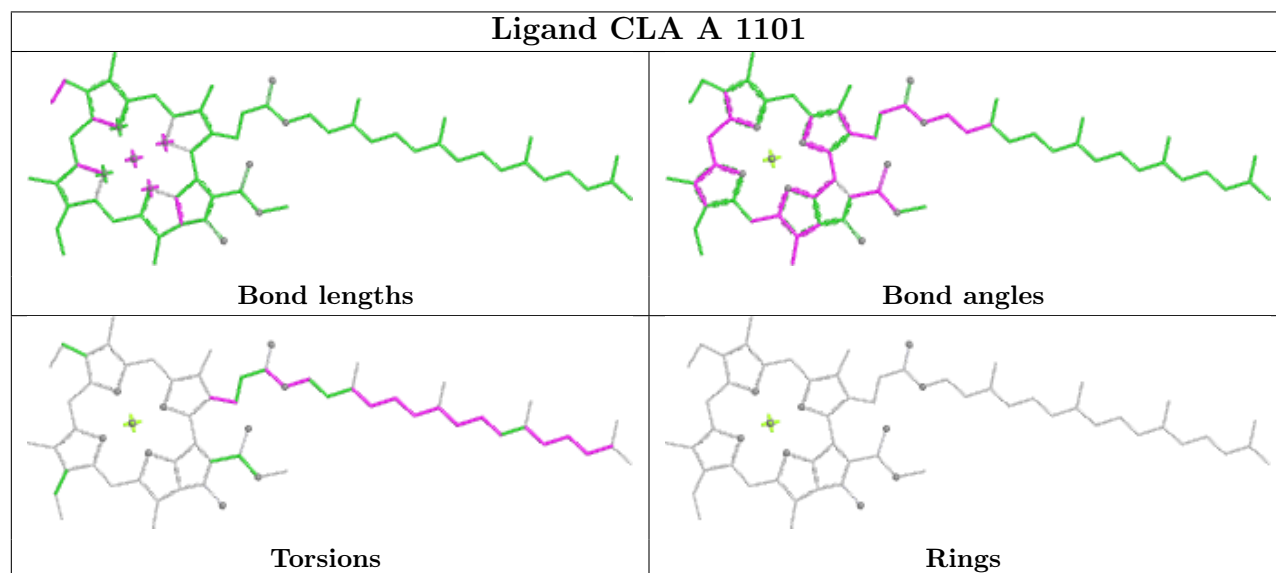
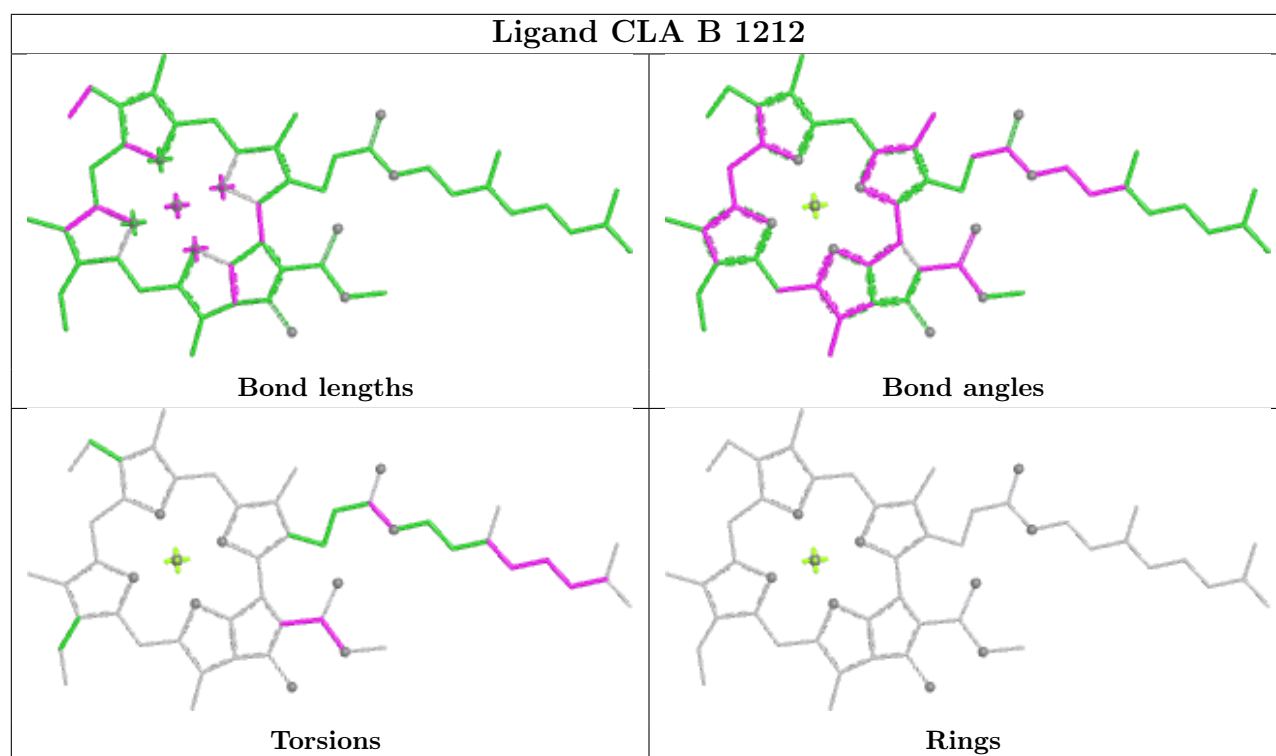


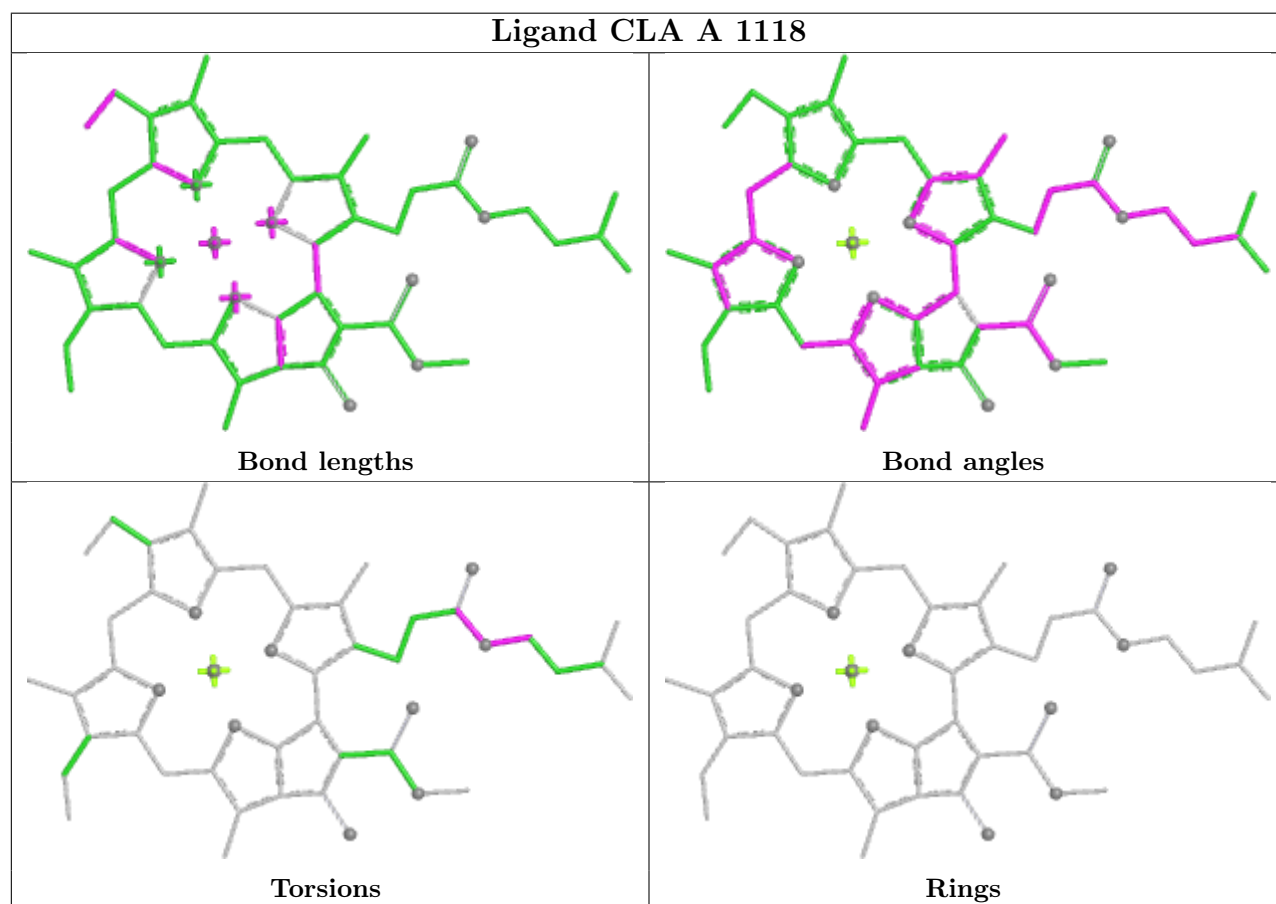
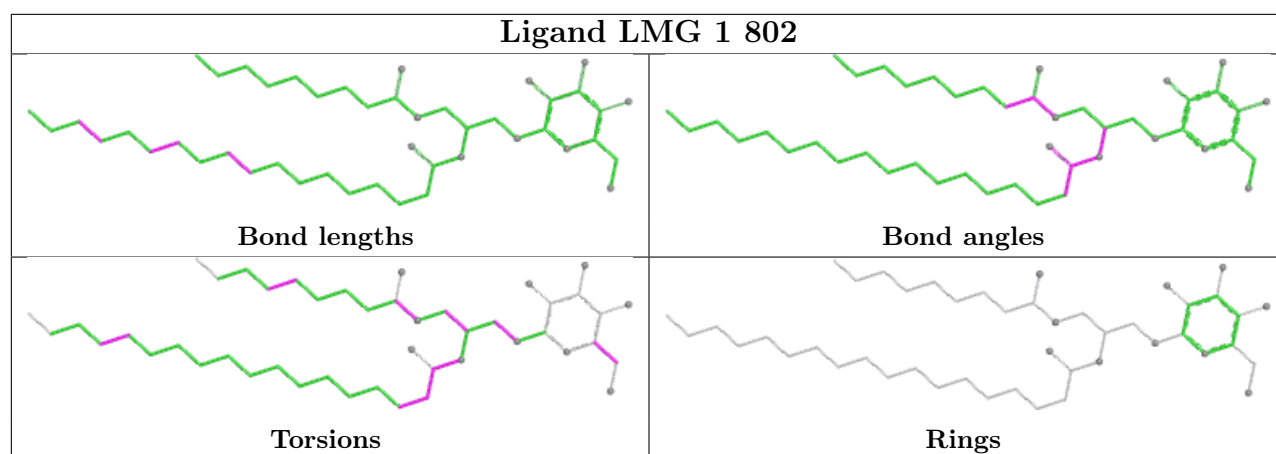
Ligand CLA A 1109

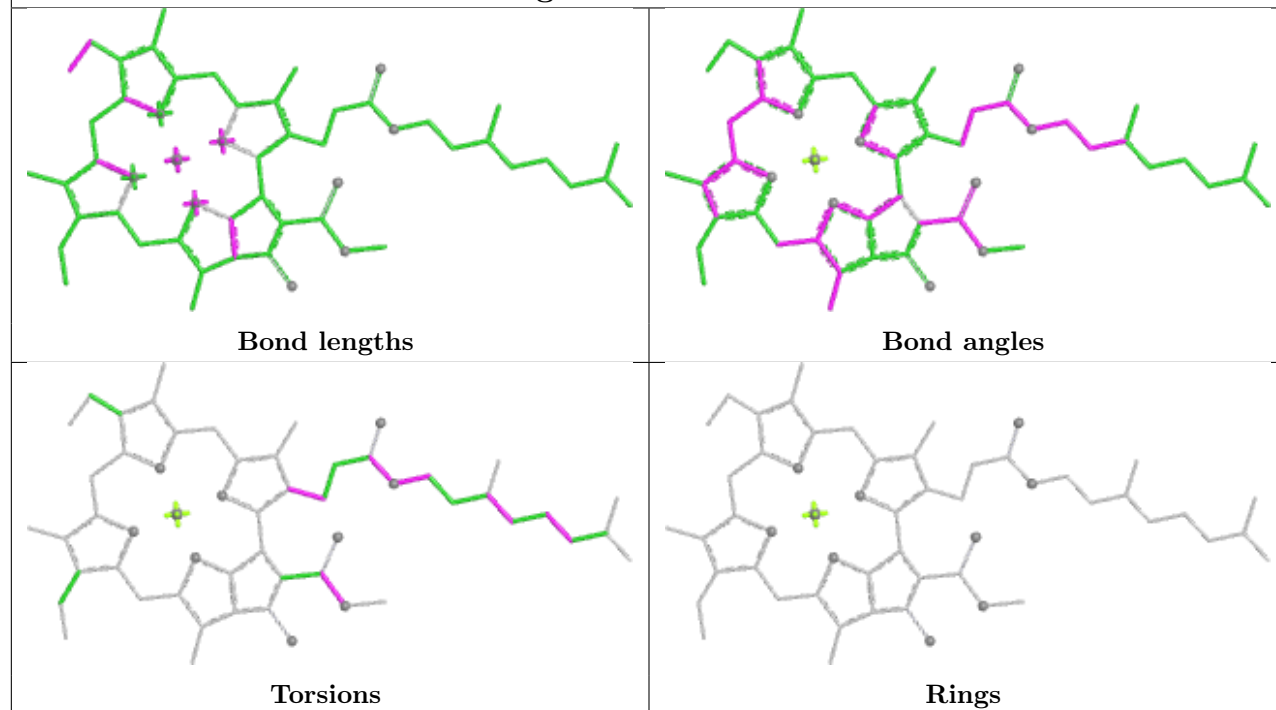
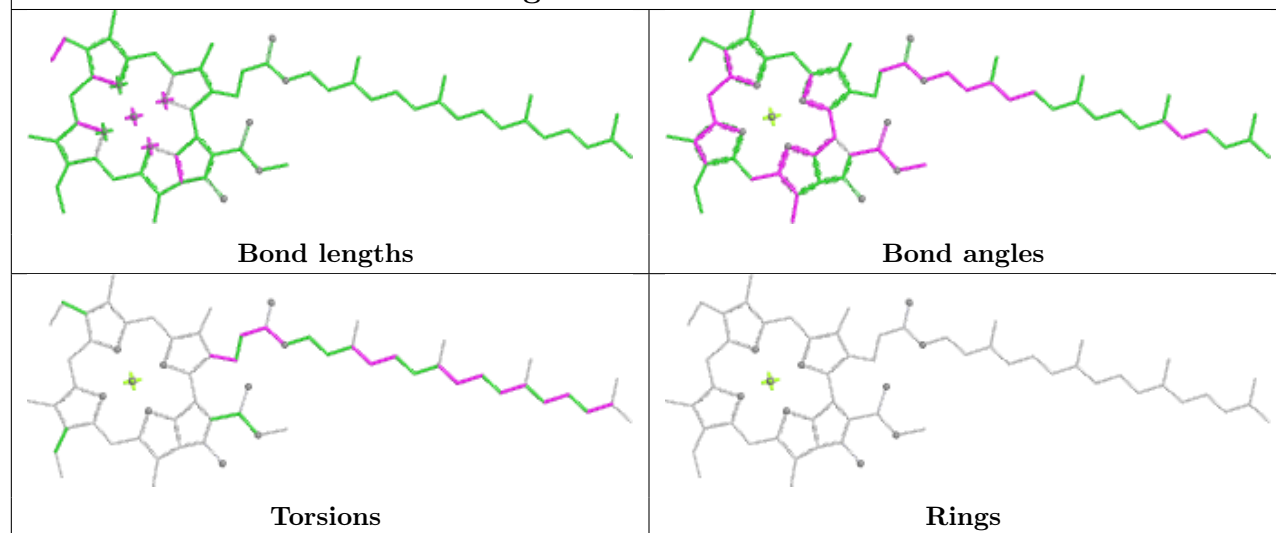


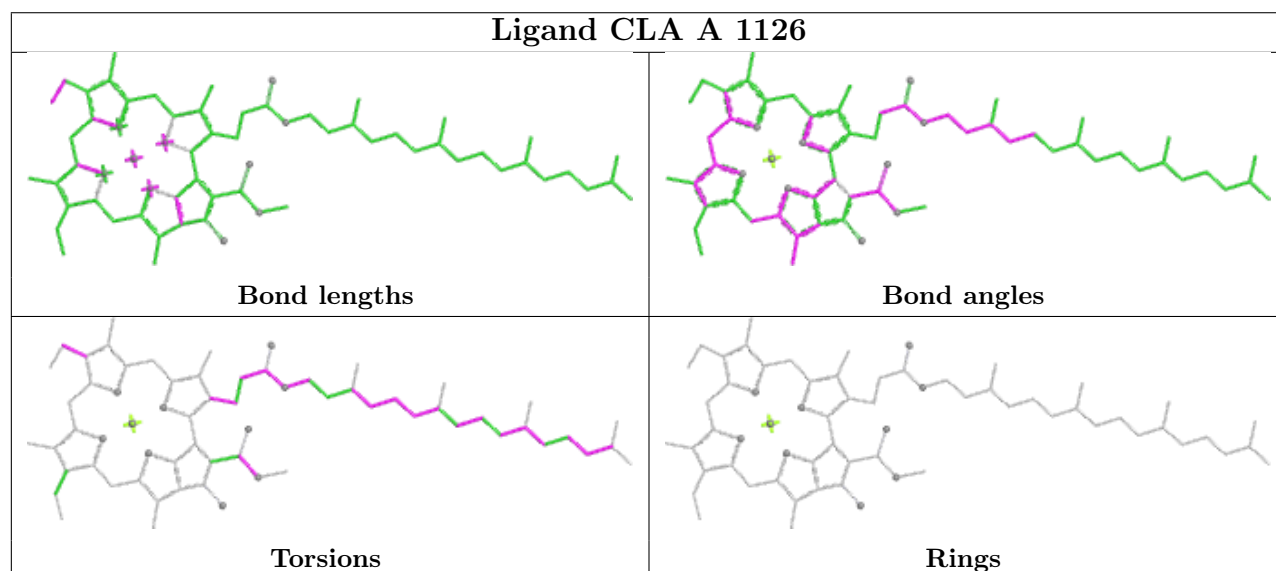
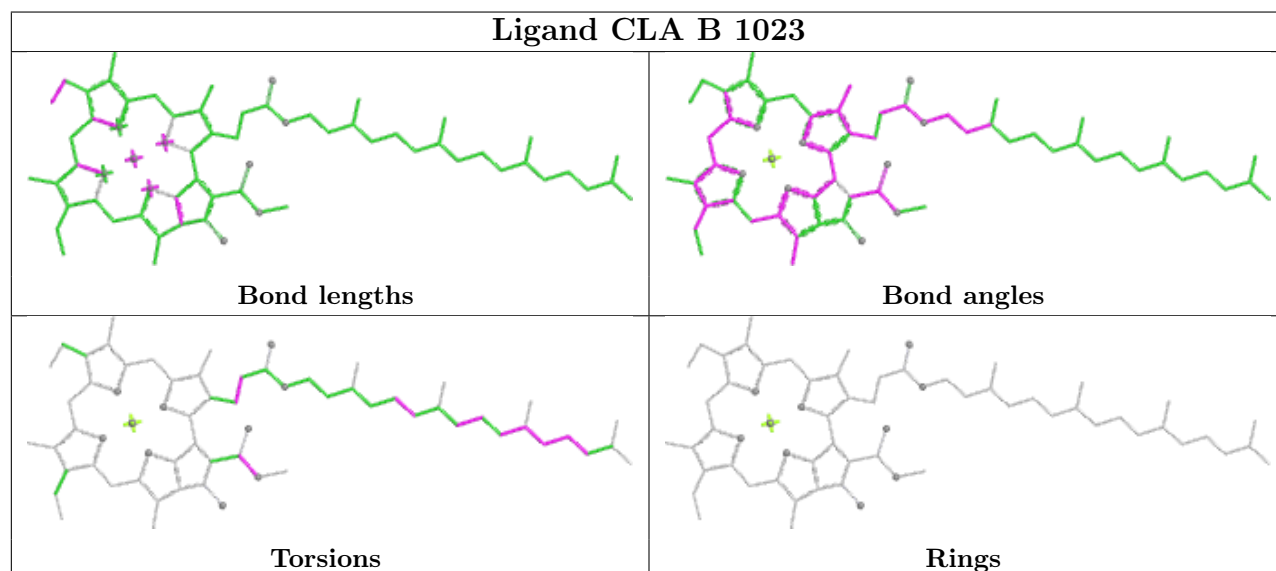
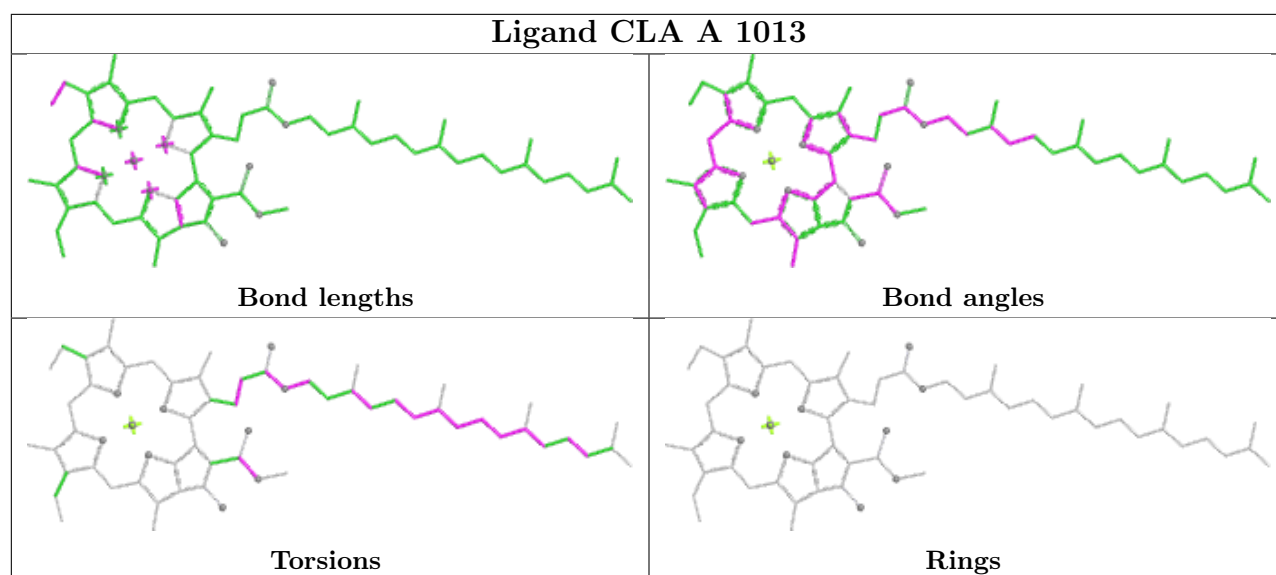
Ligand CLA 4 602



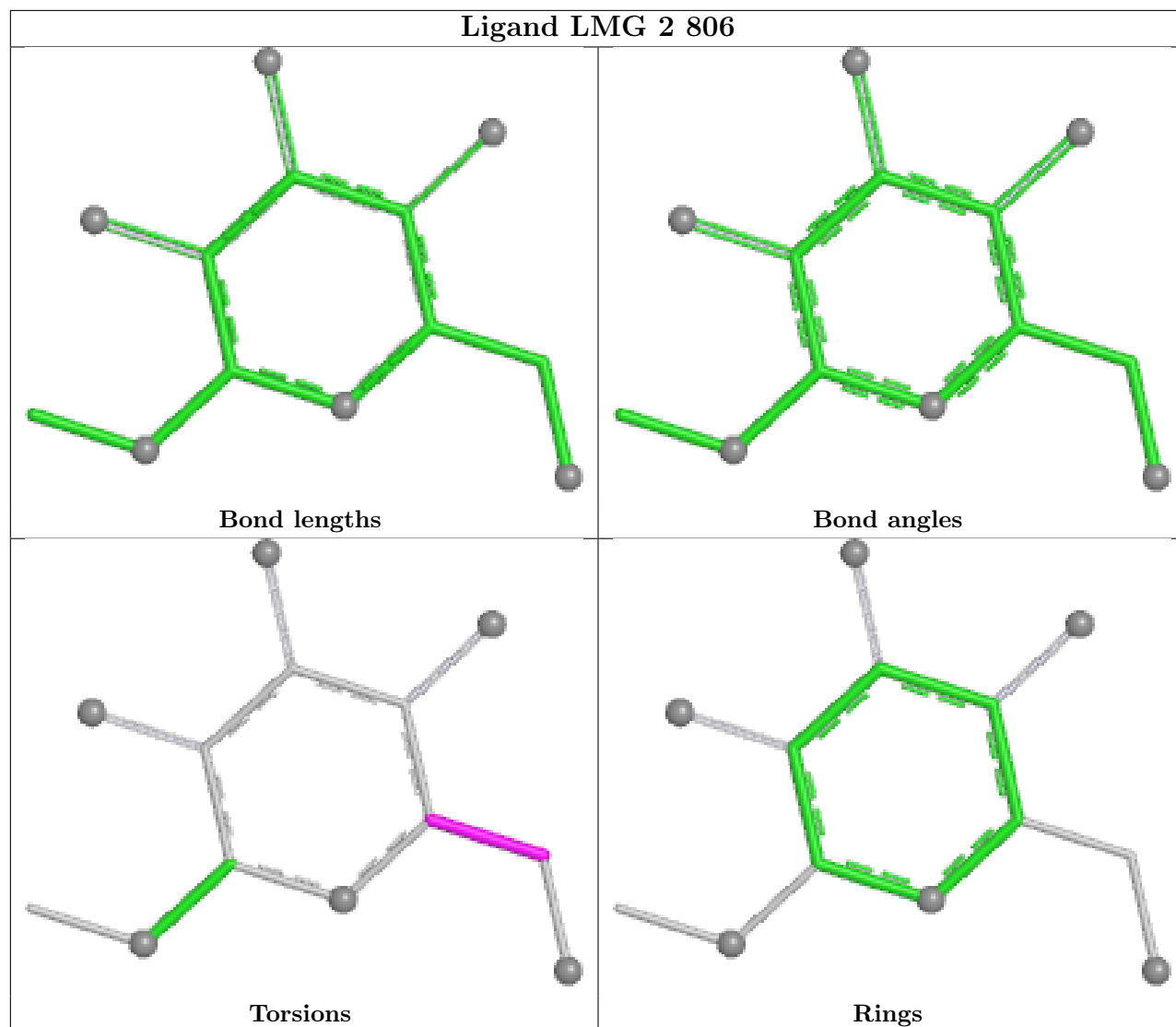




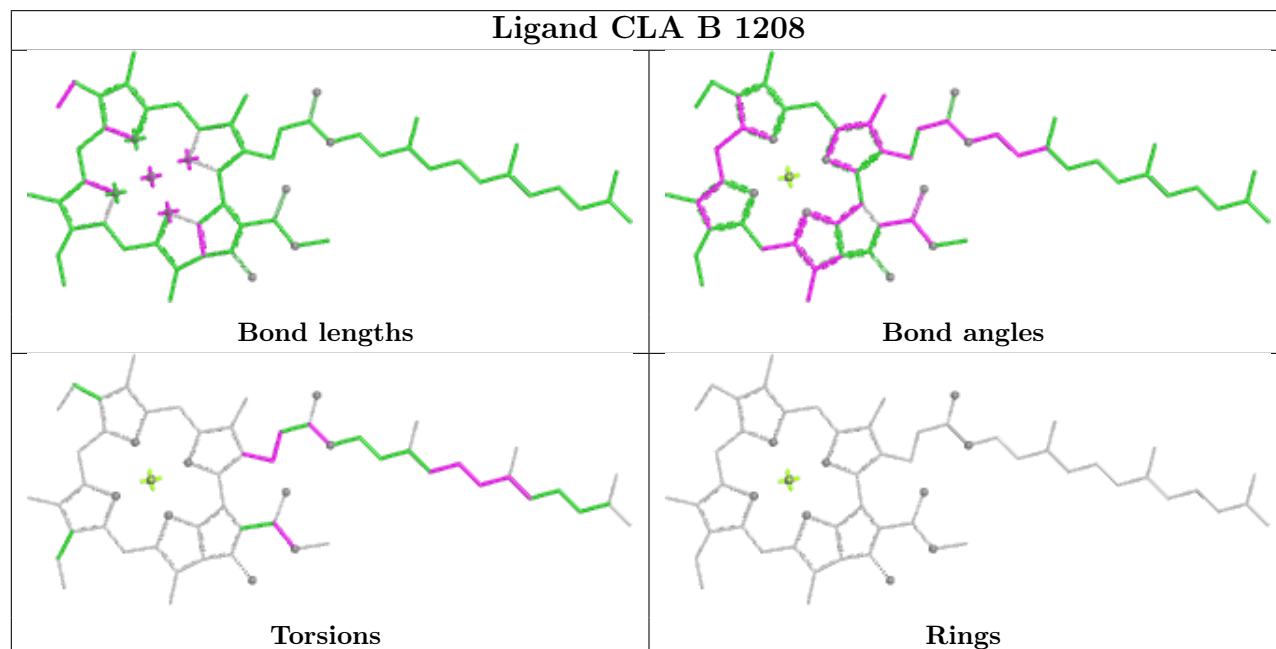
Ligand CLA 2 612**Ligand CLA B 1210**



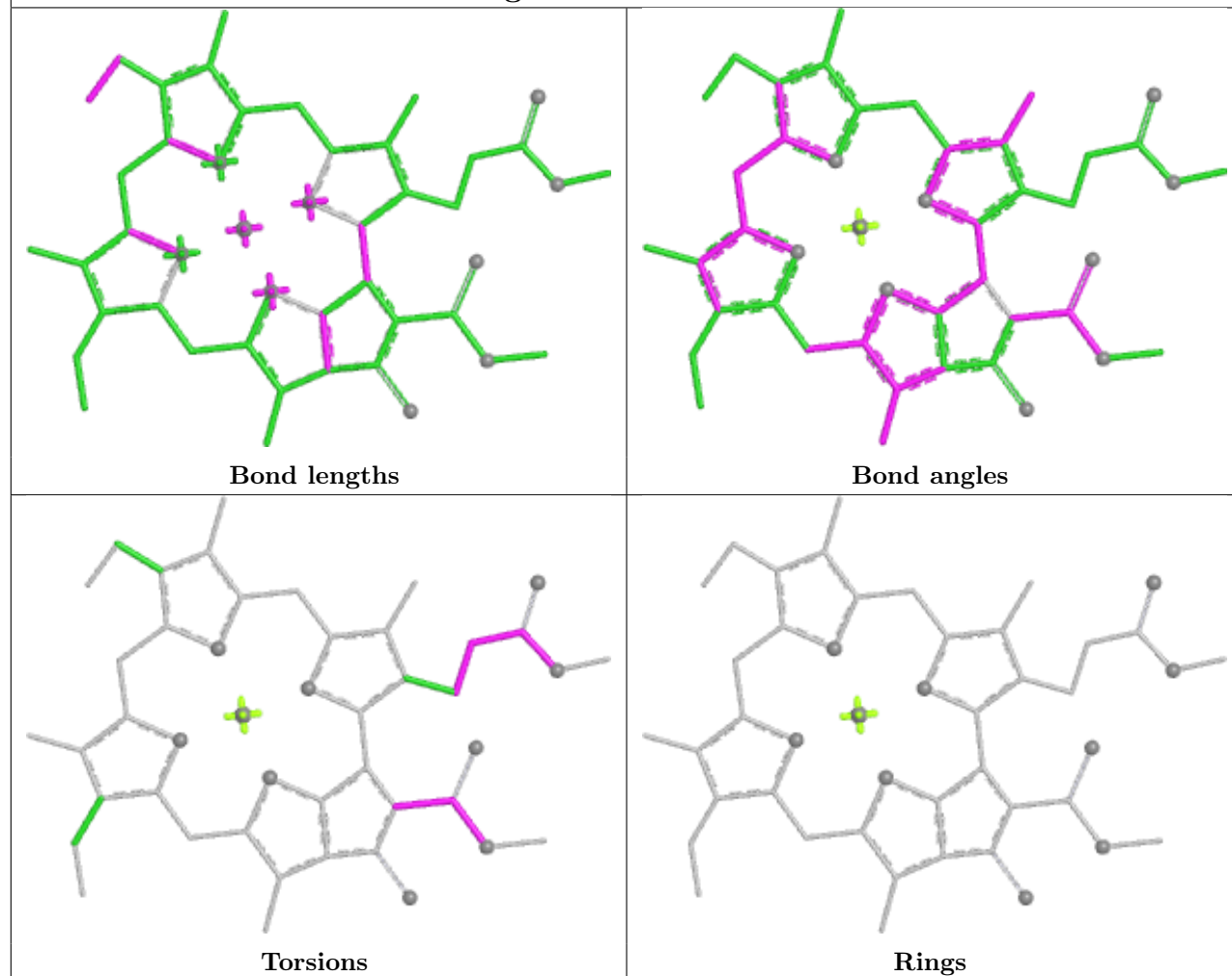
Ligand LMG 2 806



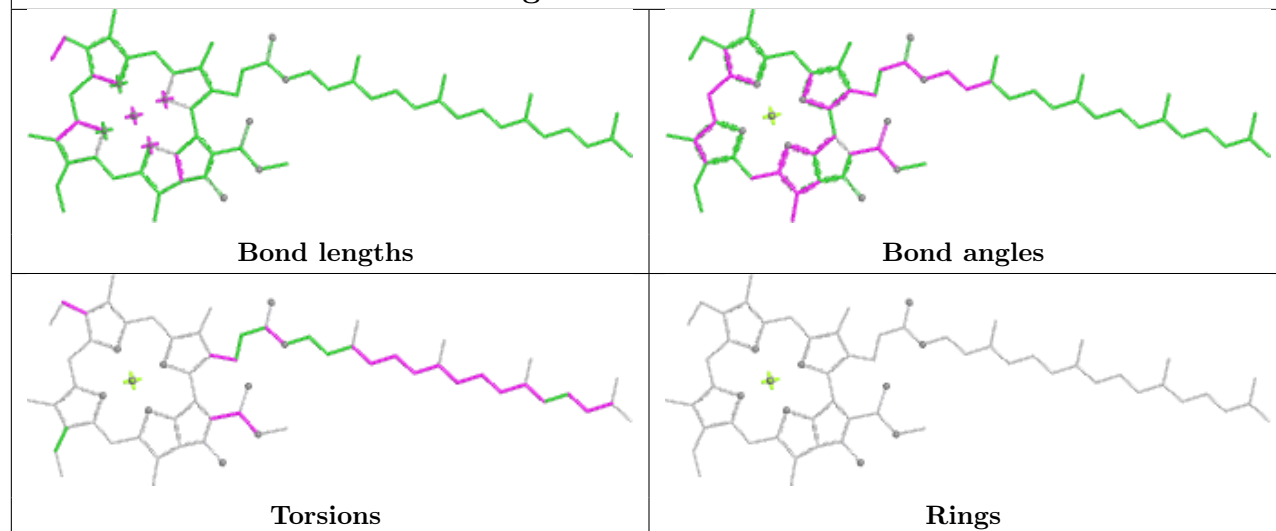
Ligand CLA B 1208

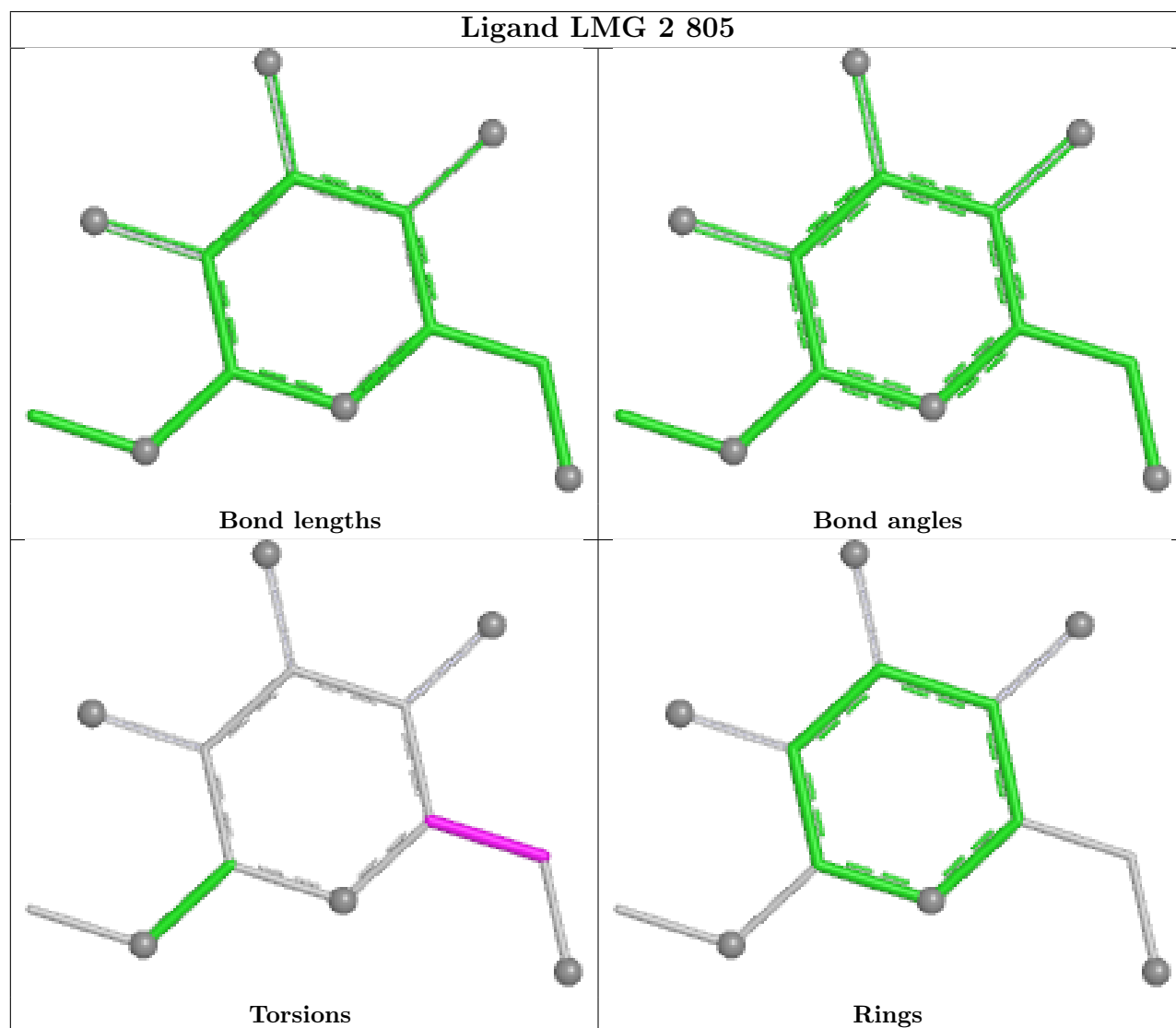
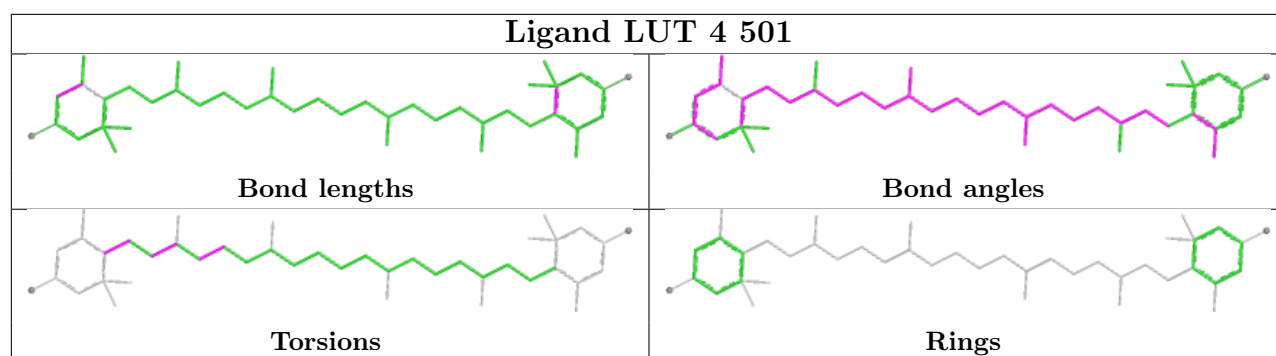


Ligand CLA A 1114

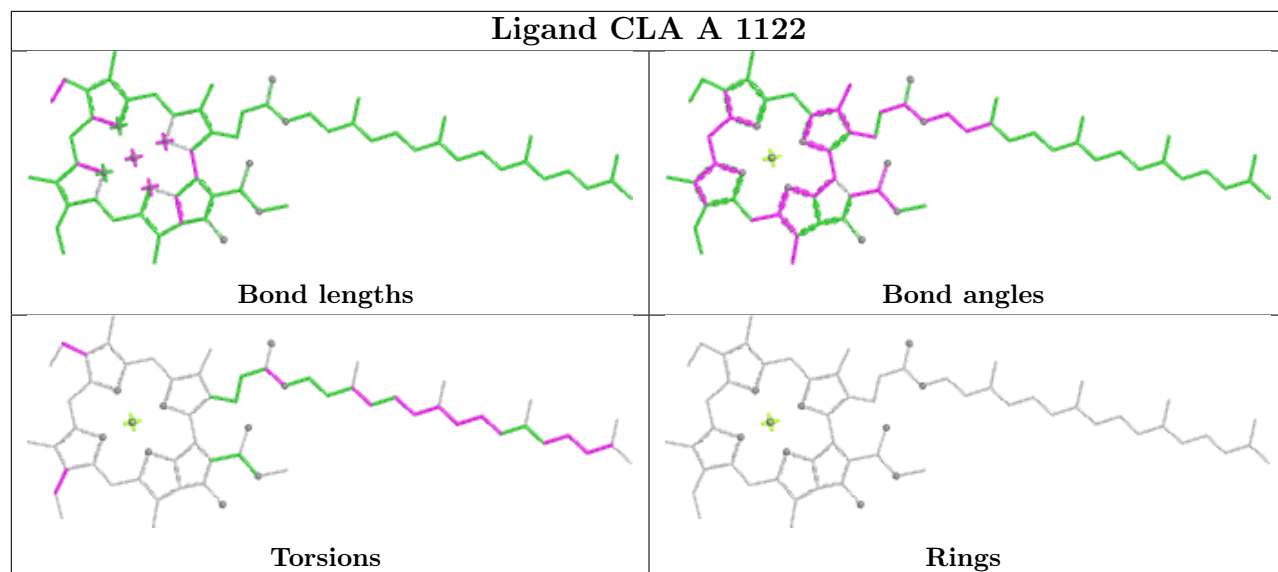


Ligand CLA A 1102

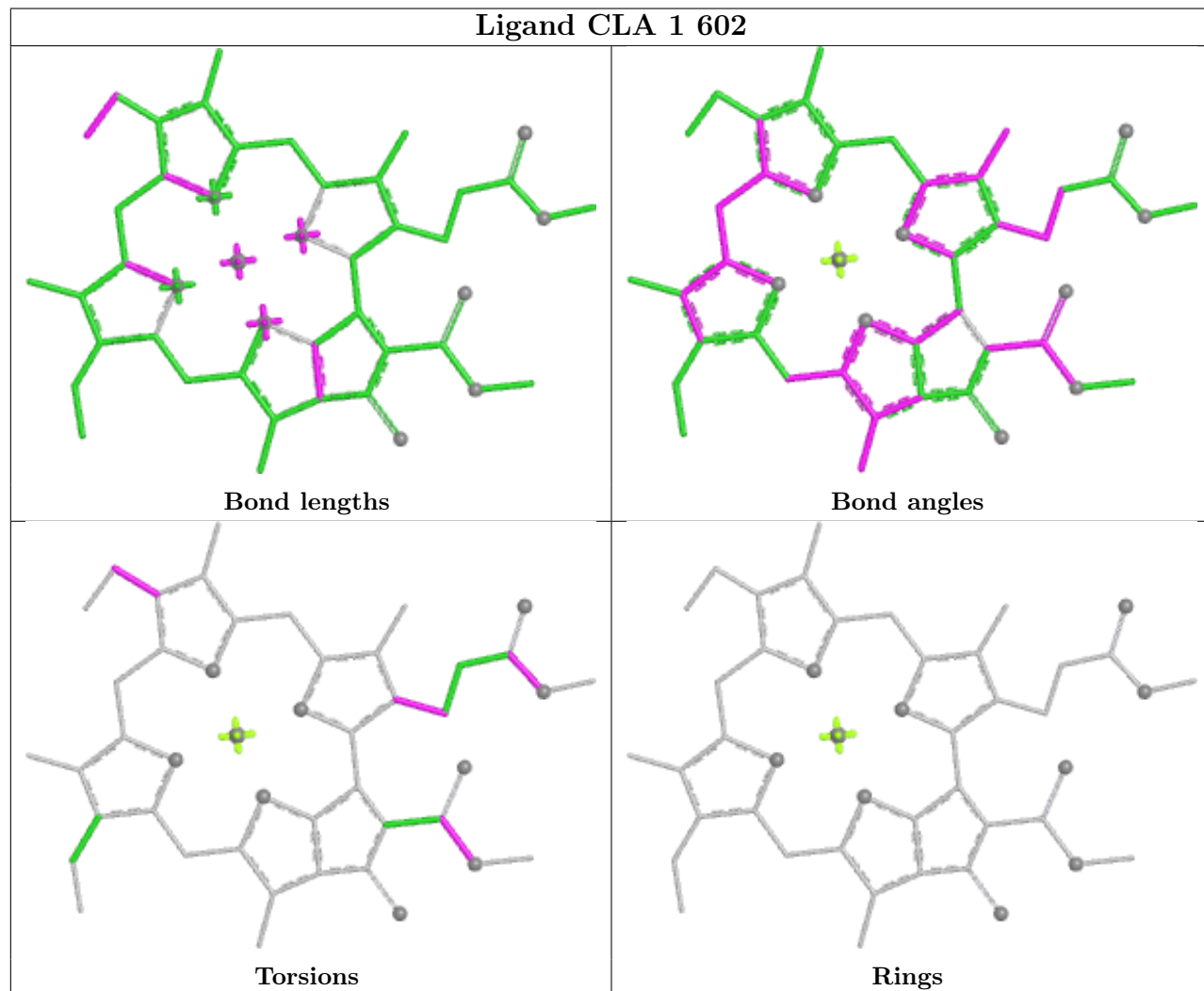




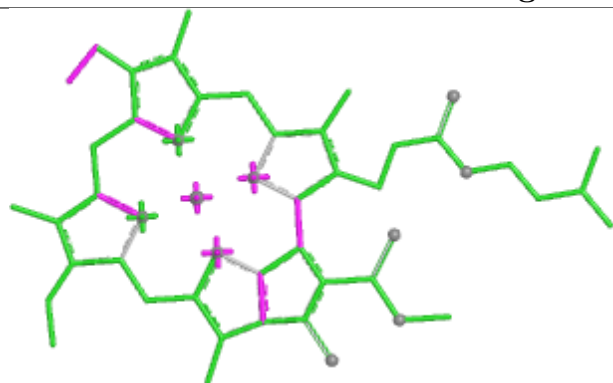
Ligand CLA A 1122



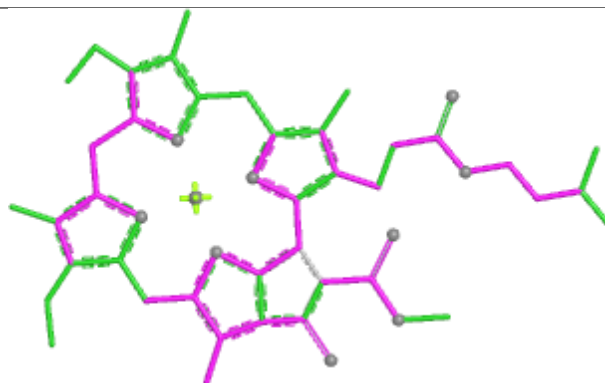
Ligand CLA 1 602



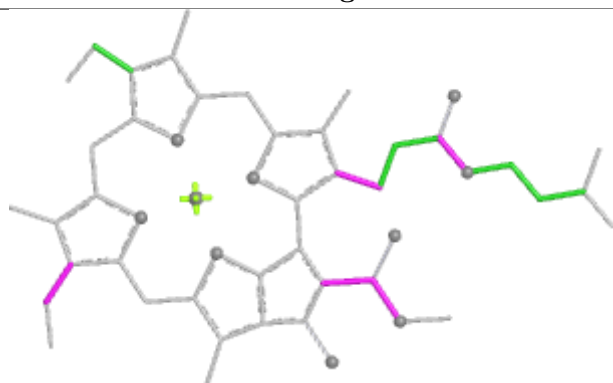
Ligand CLA 3 606



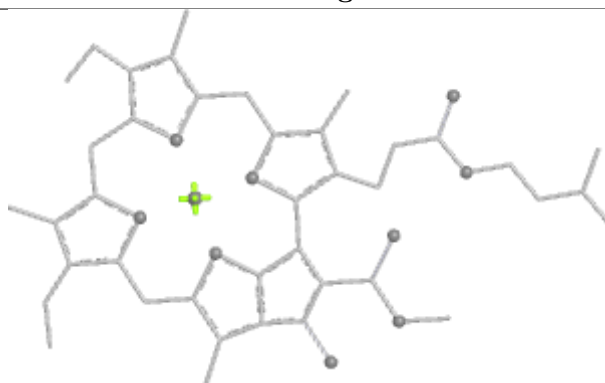
Bond lengths



Bond angles

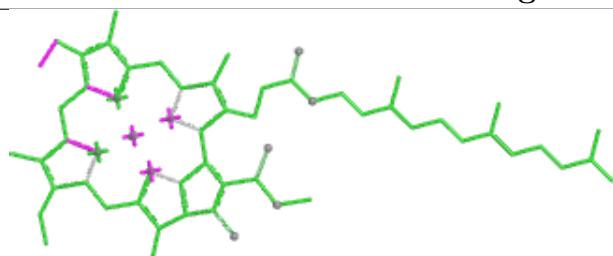


Torsions

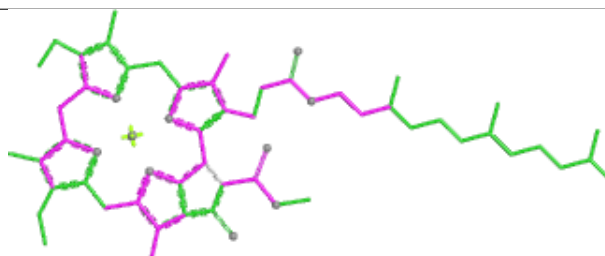


Rings

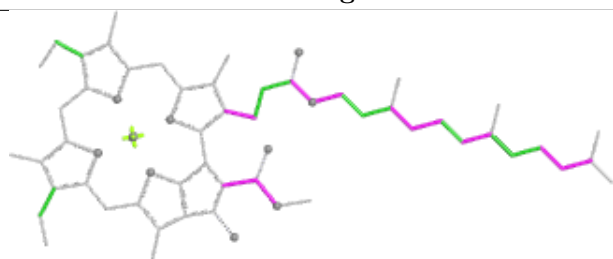
Ligand CLA 3 617



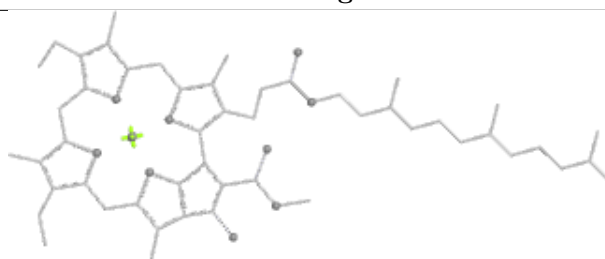
Bond lengths



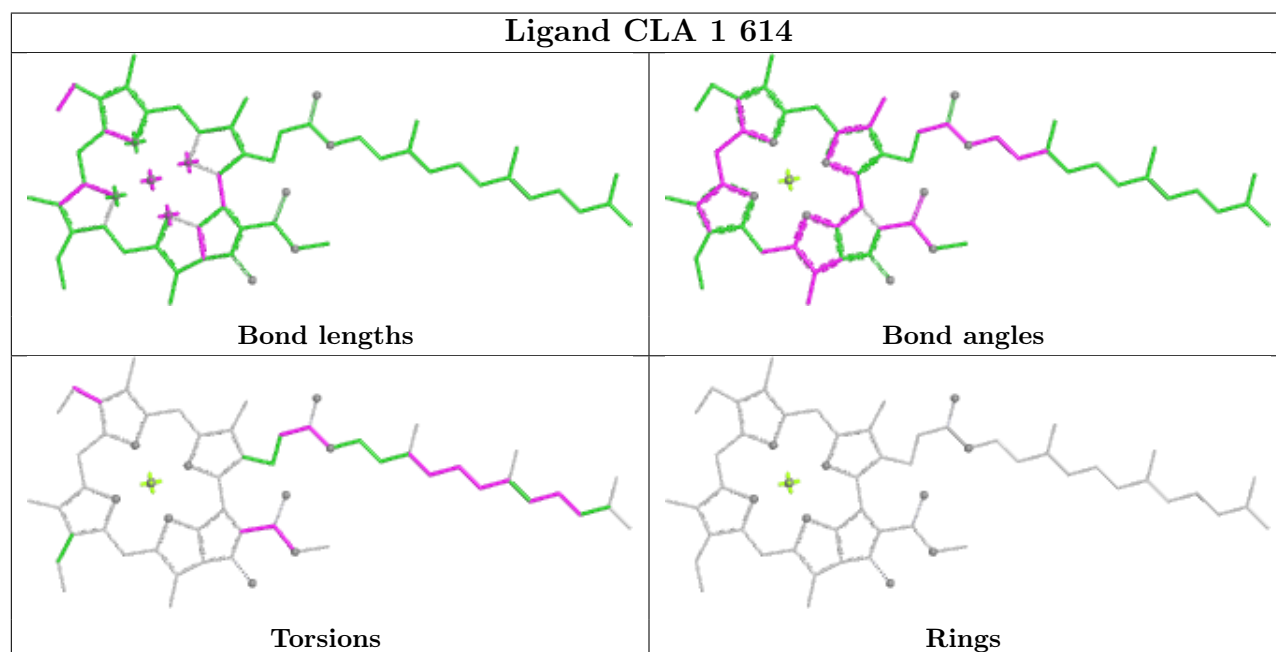
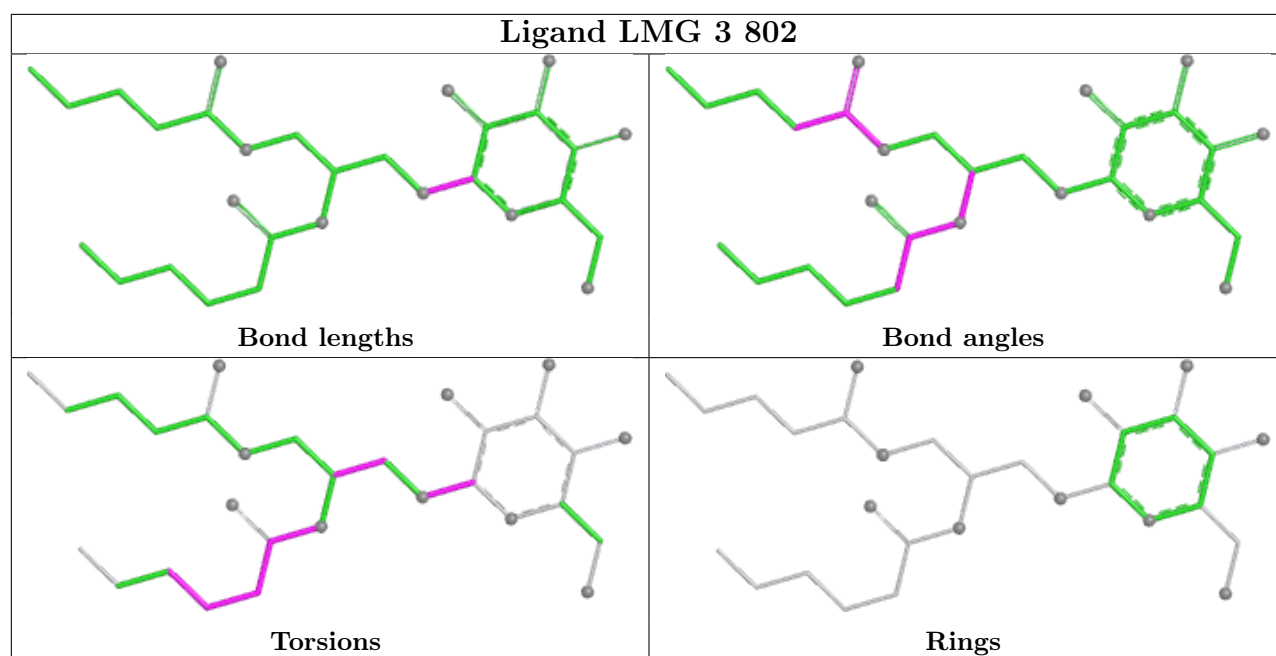
Bond angles



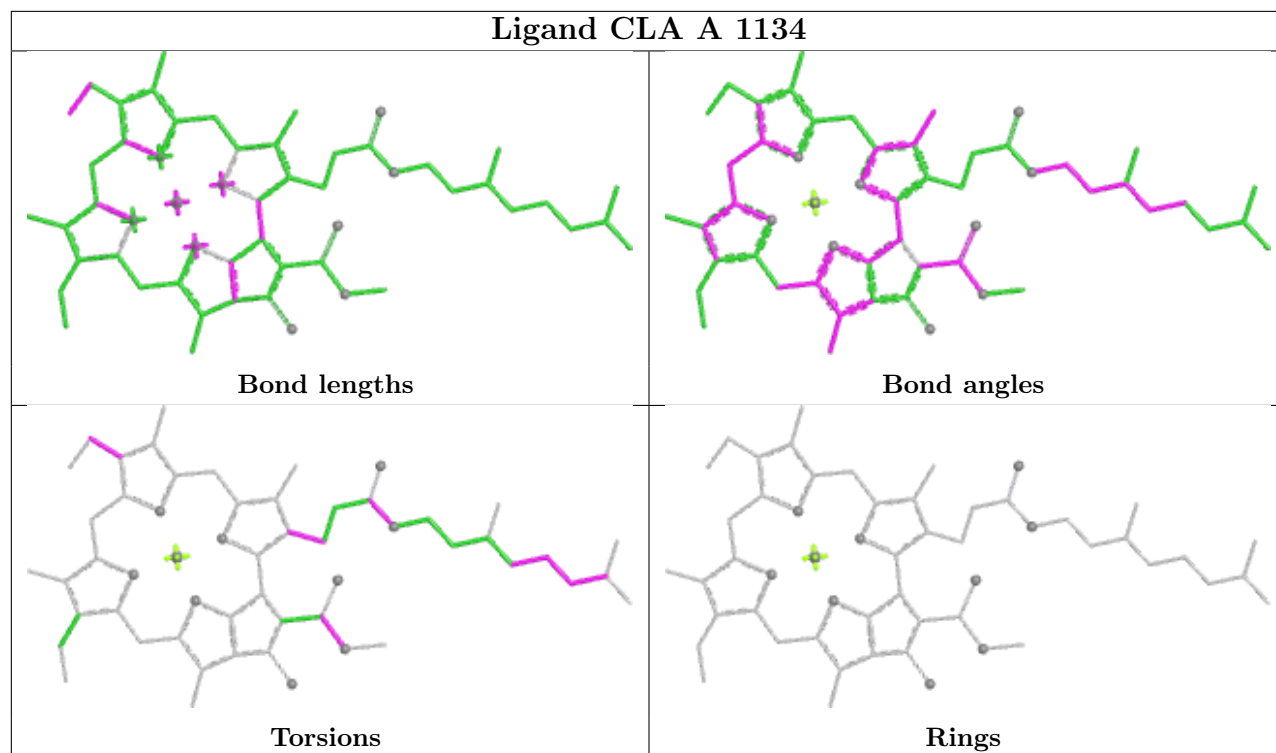
Torsions



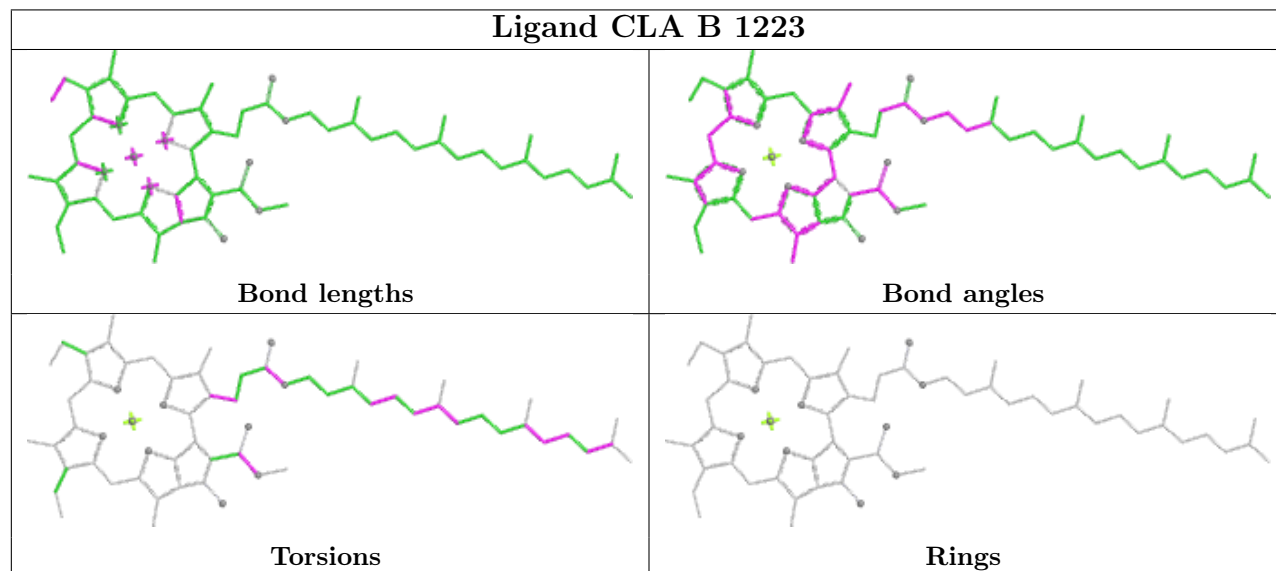
Rings



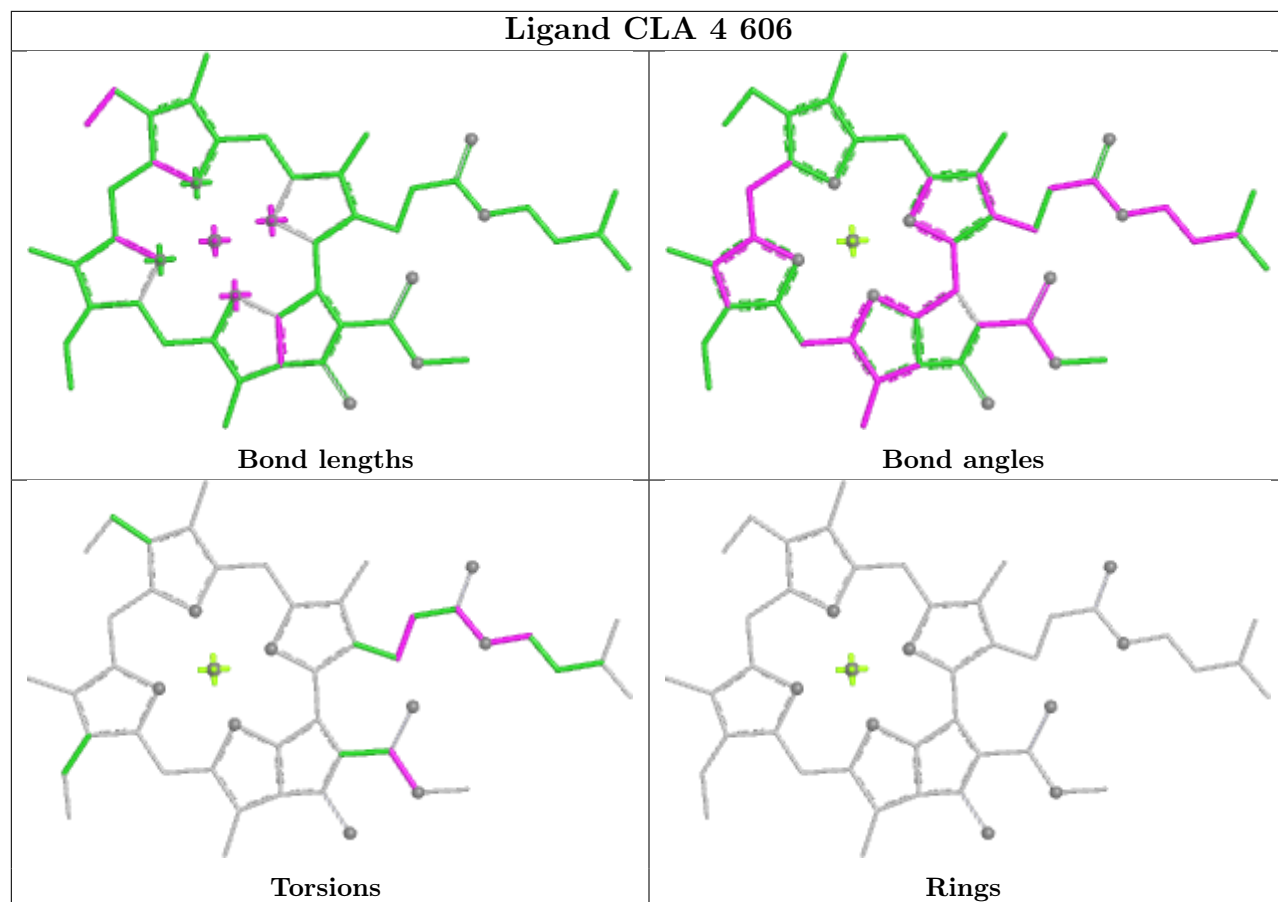
Ligand CLA A 1134



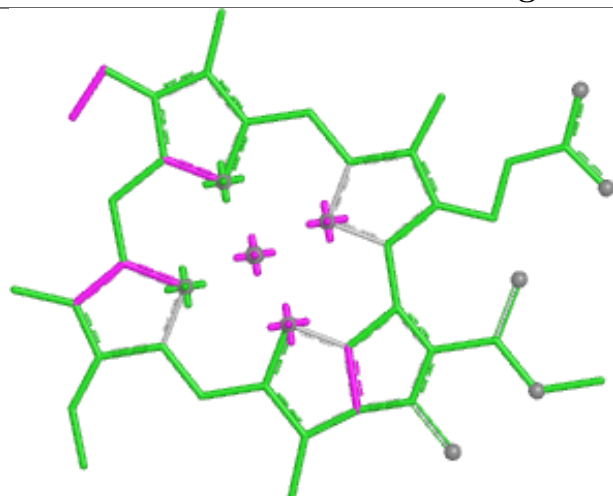
Ligand CLA B 1223



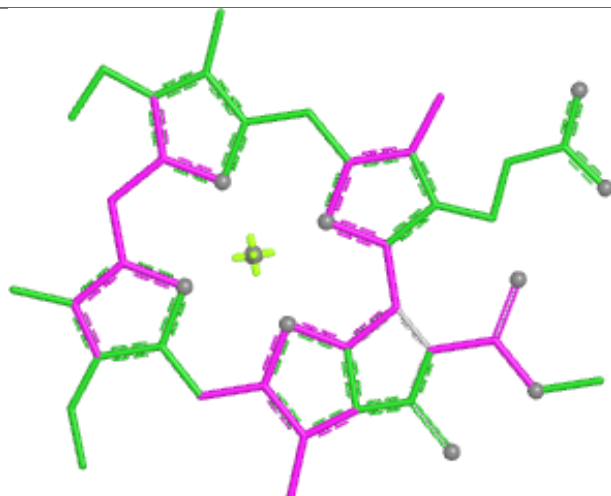
Ligand CLA 4 606



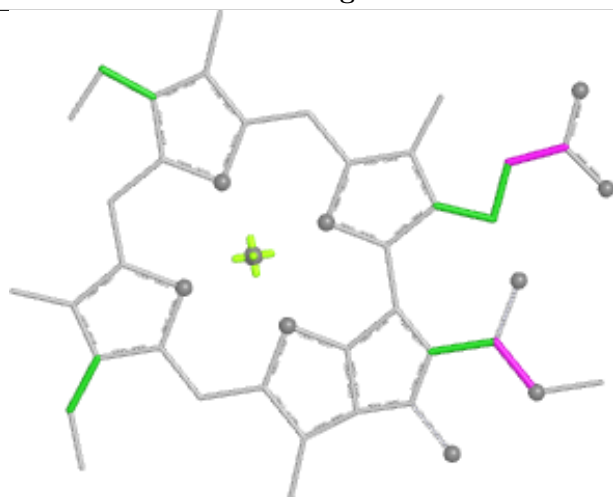
Ligand CLA 1 613



Bond lengths



Bond angles

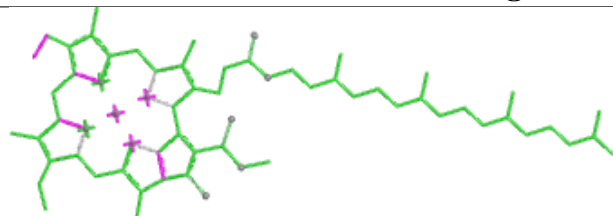


Torsions

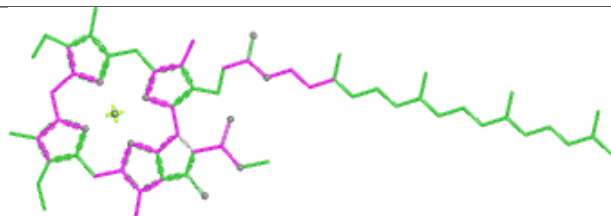


Rings

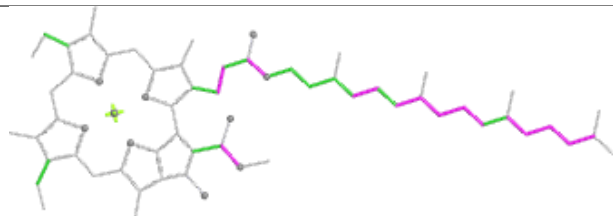
Ligand CLA B 1237



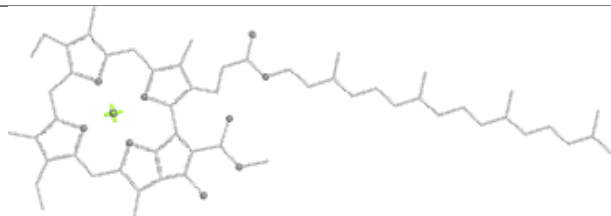
Bond lengths



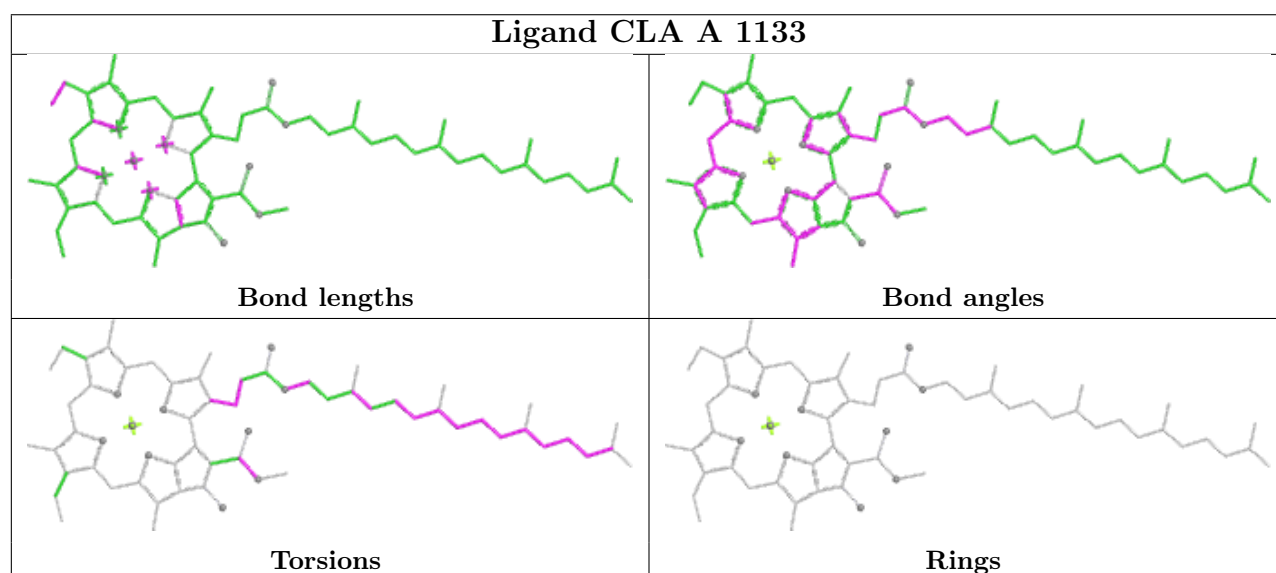
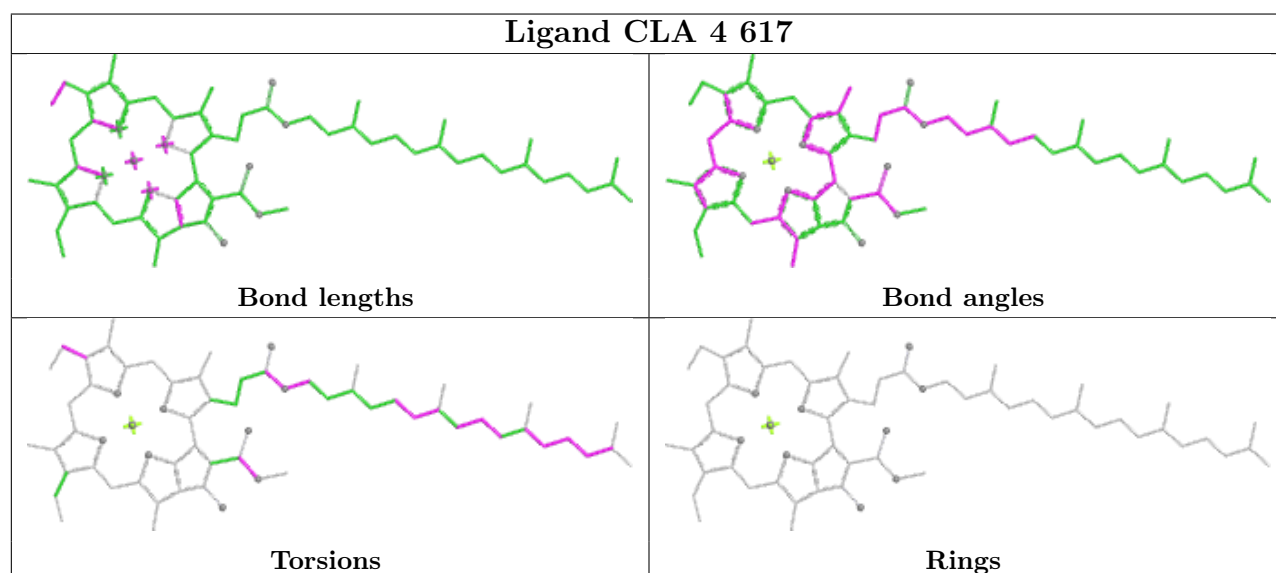
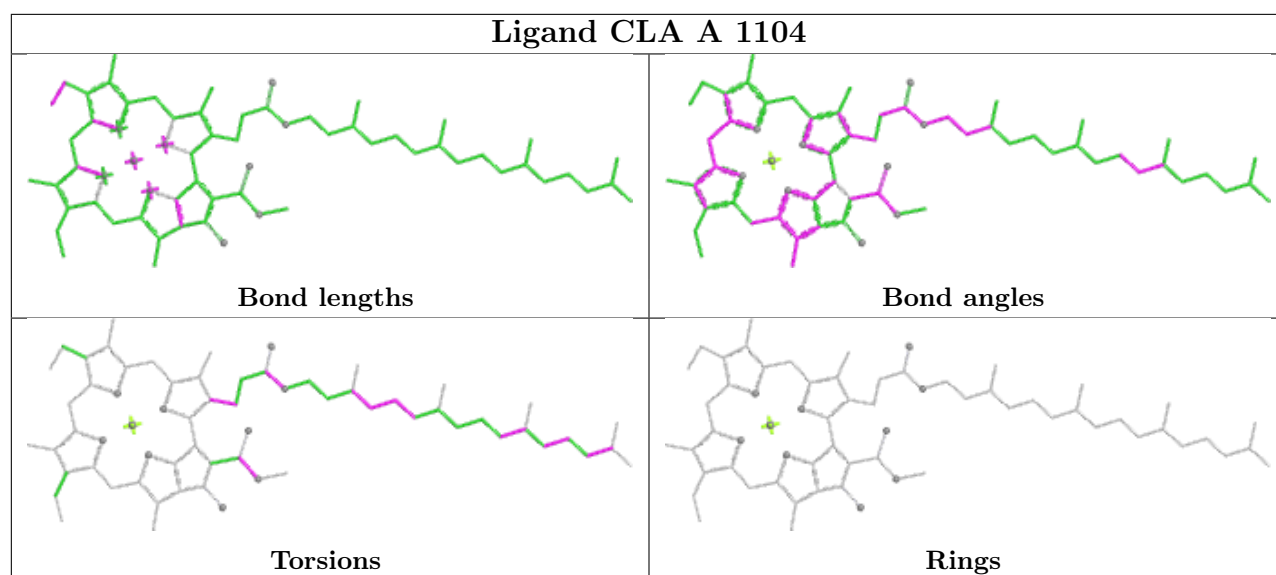
Bond angles

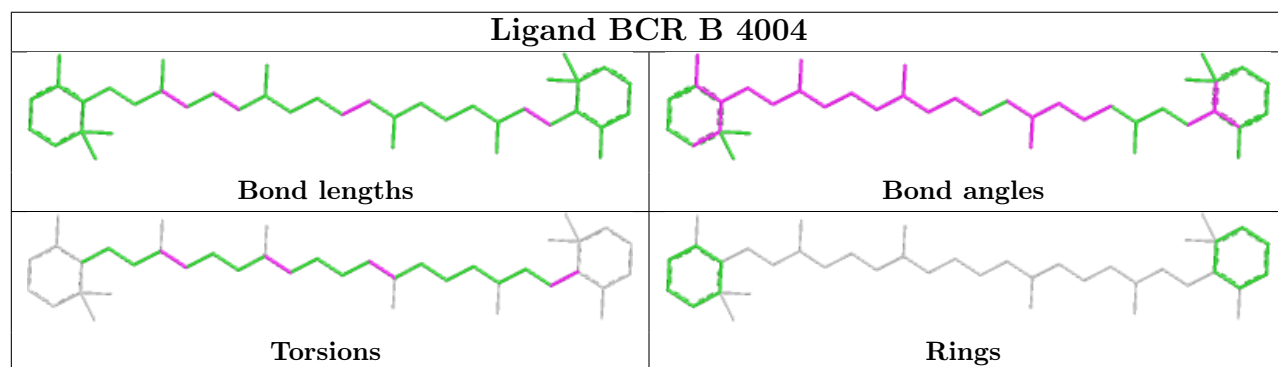
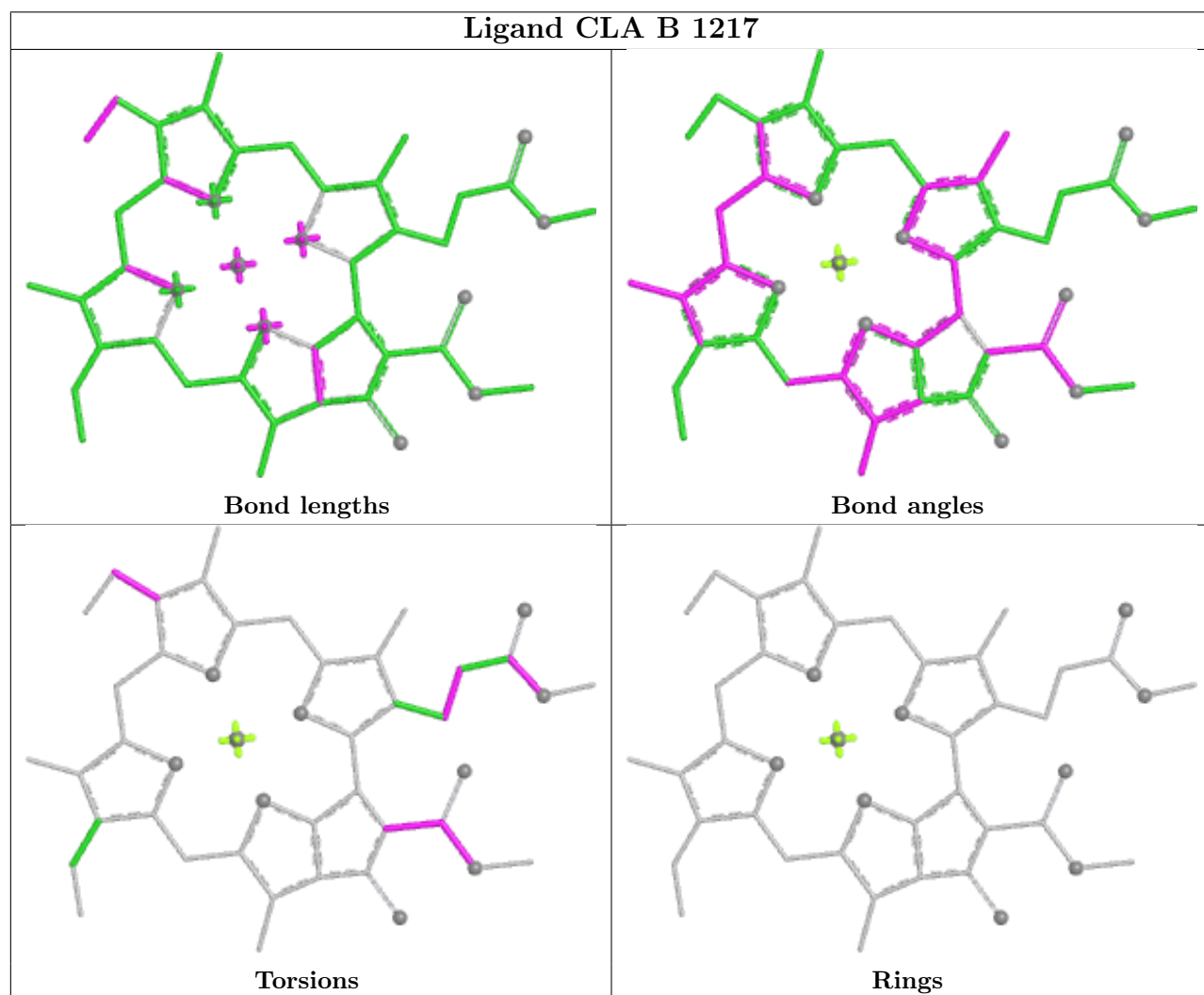
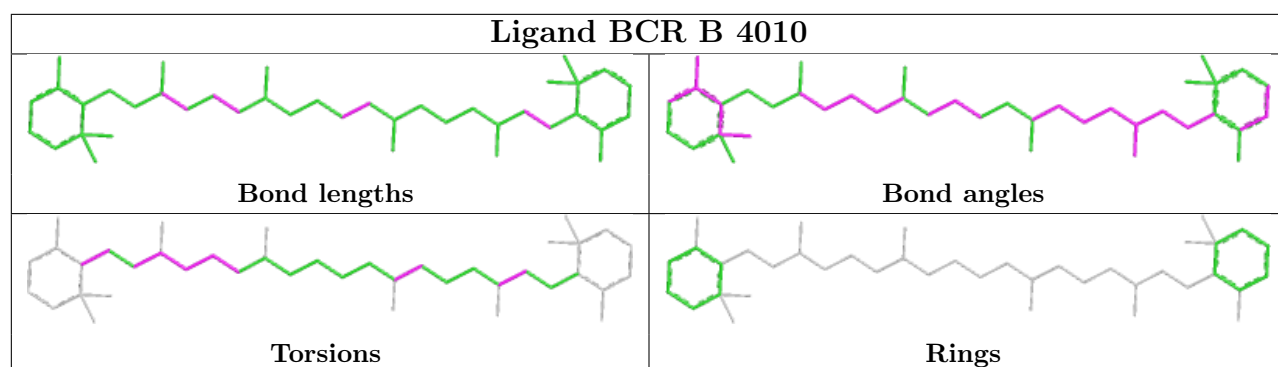


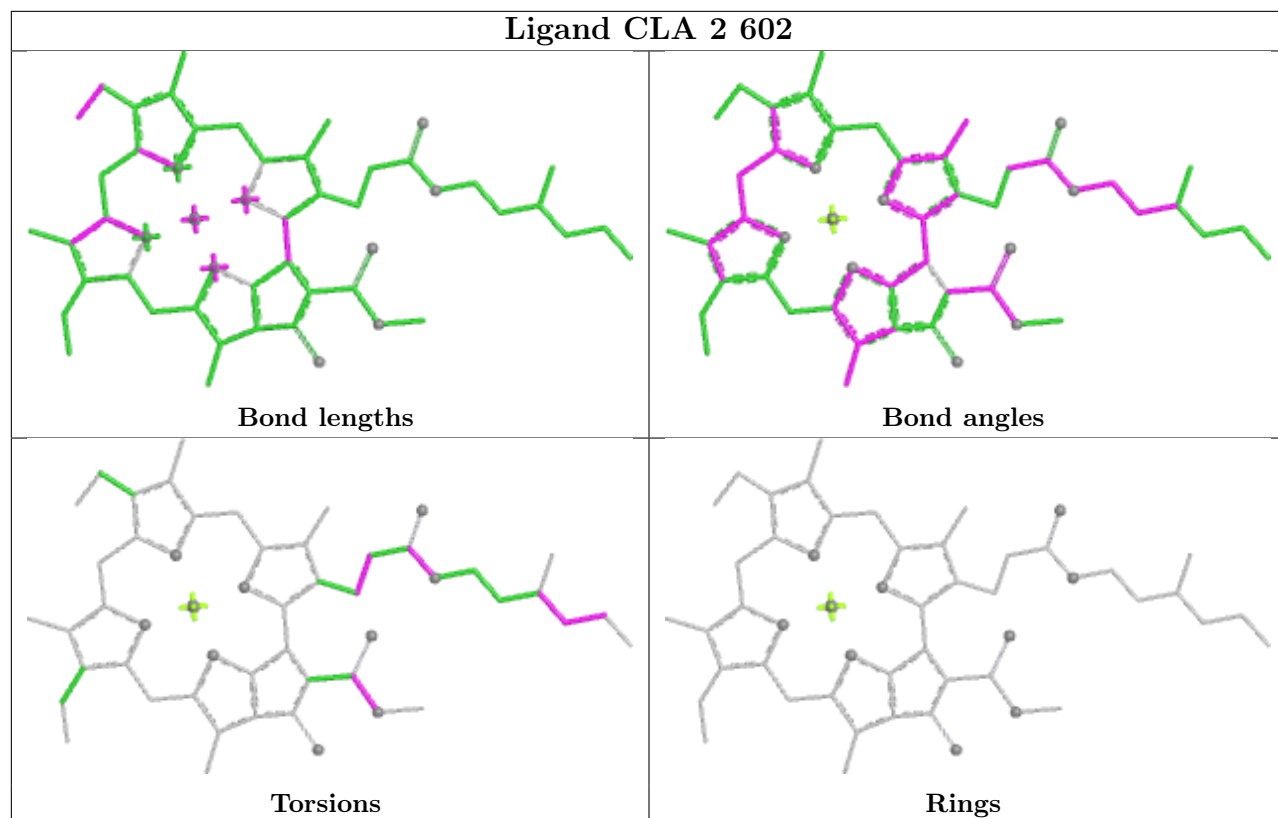
Torsions

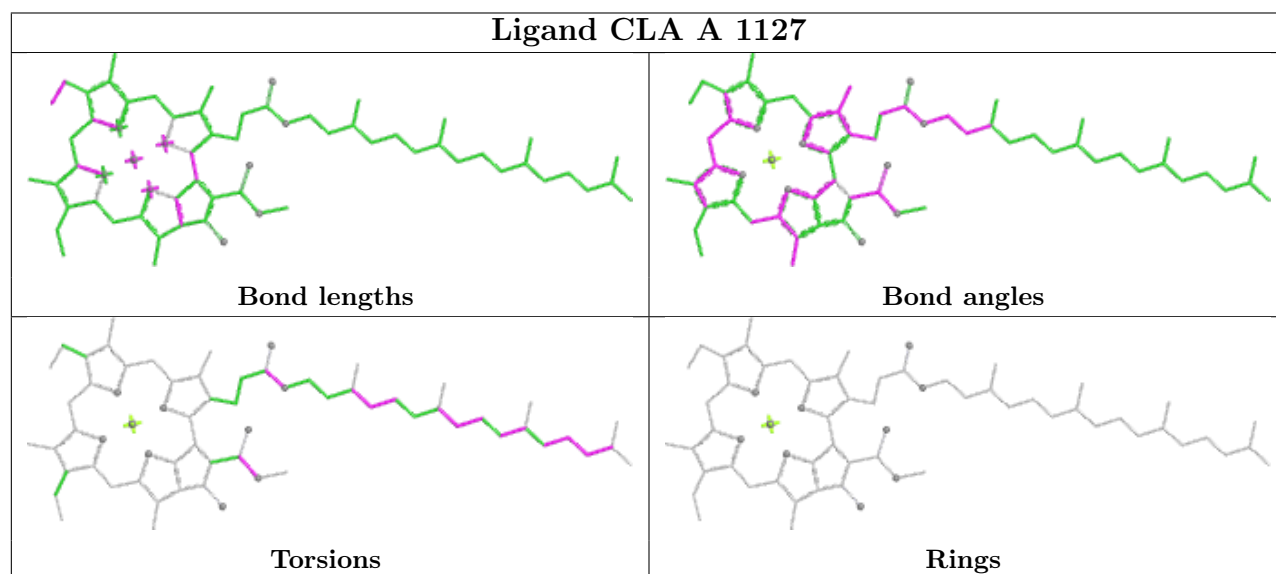
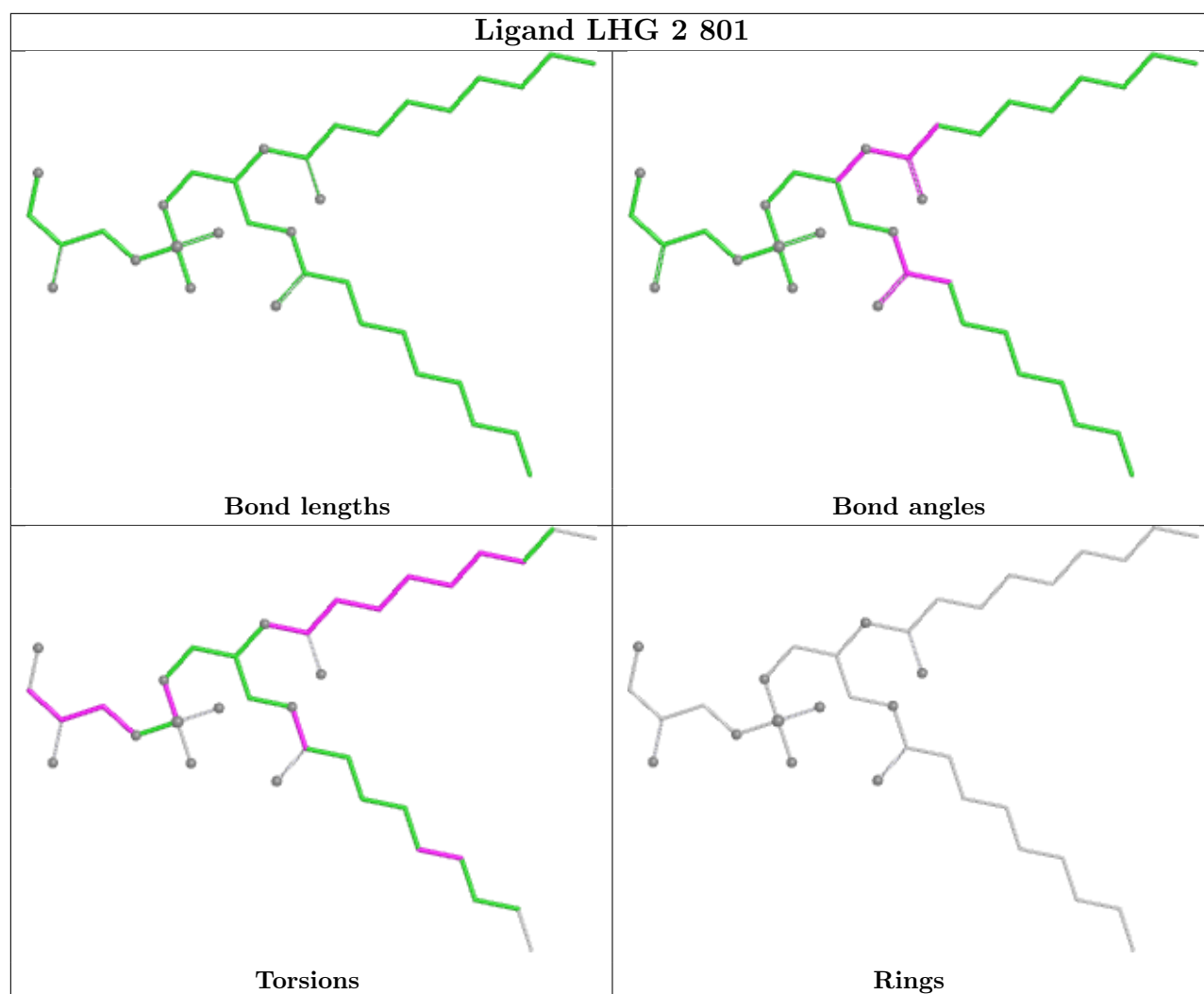


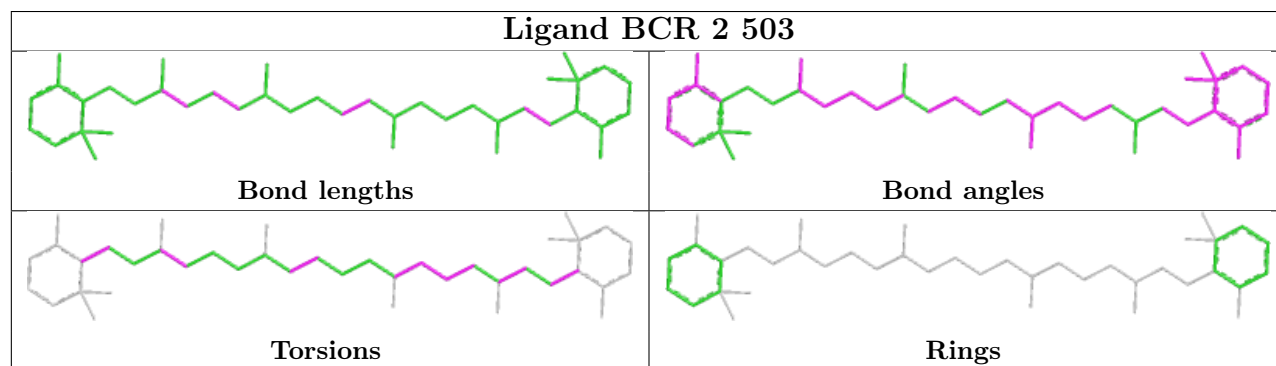
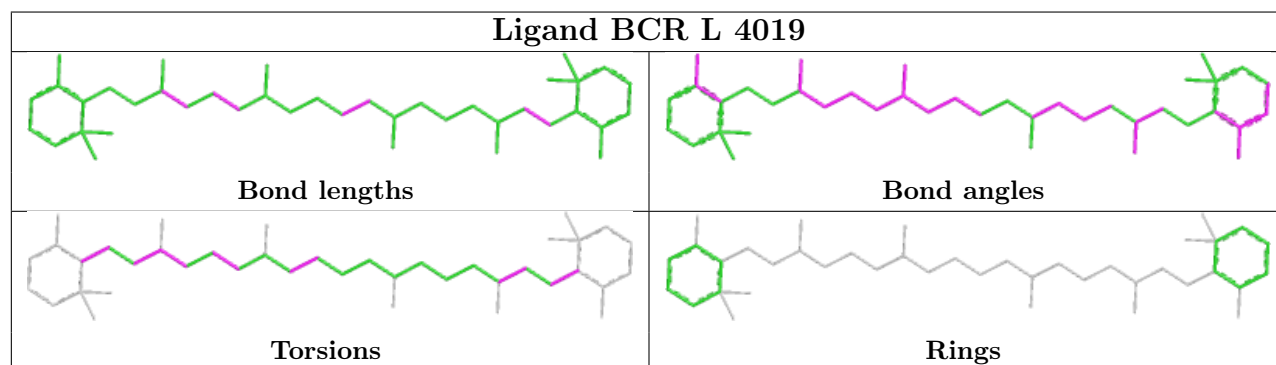
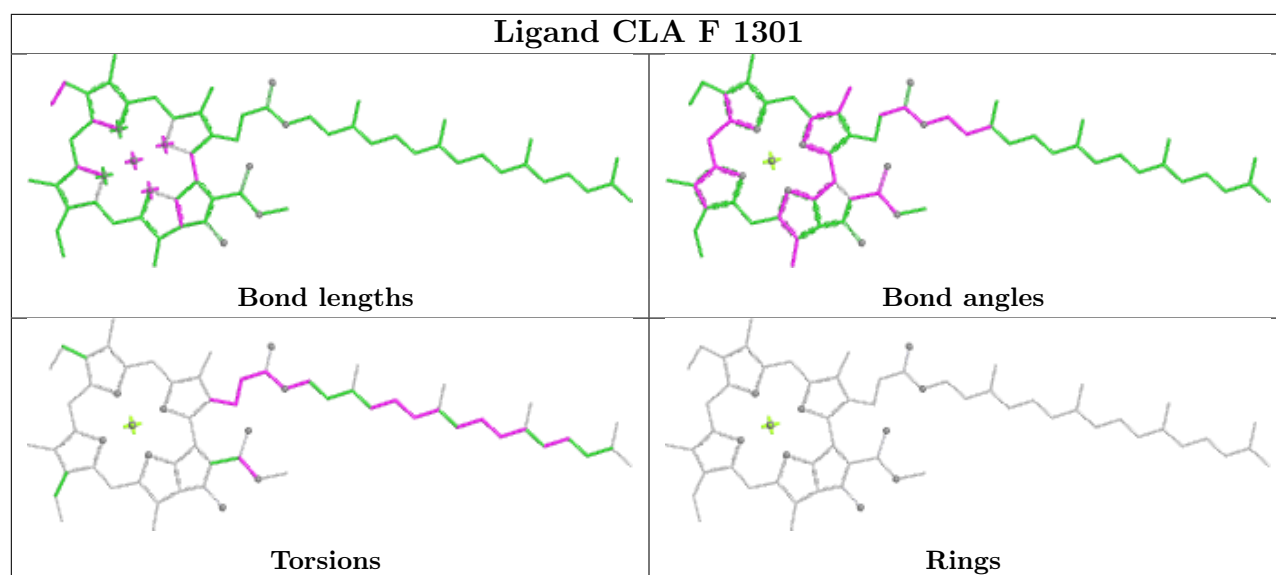
Rings

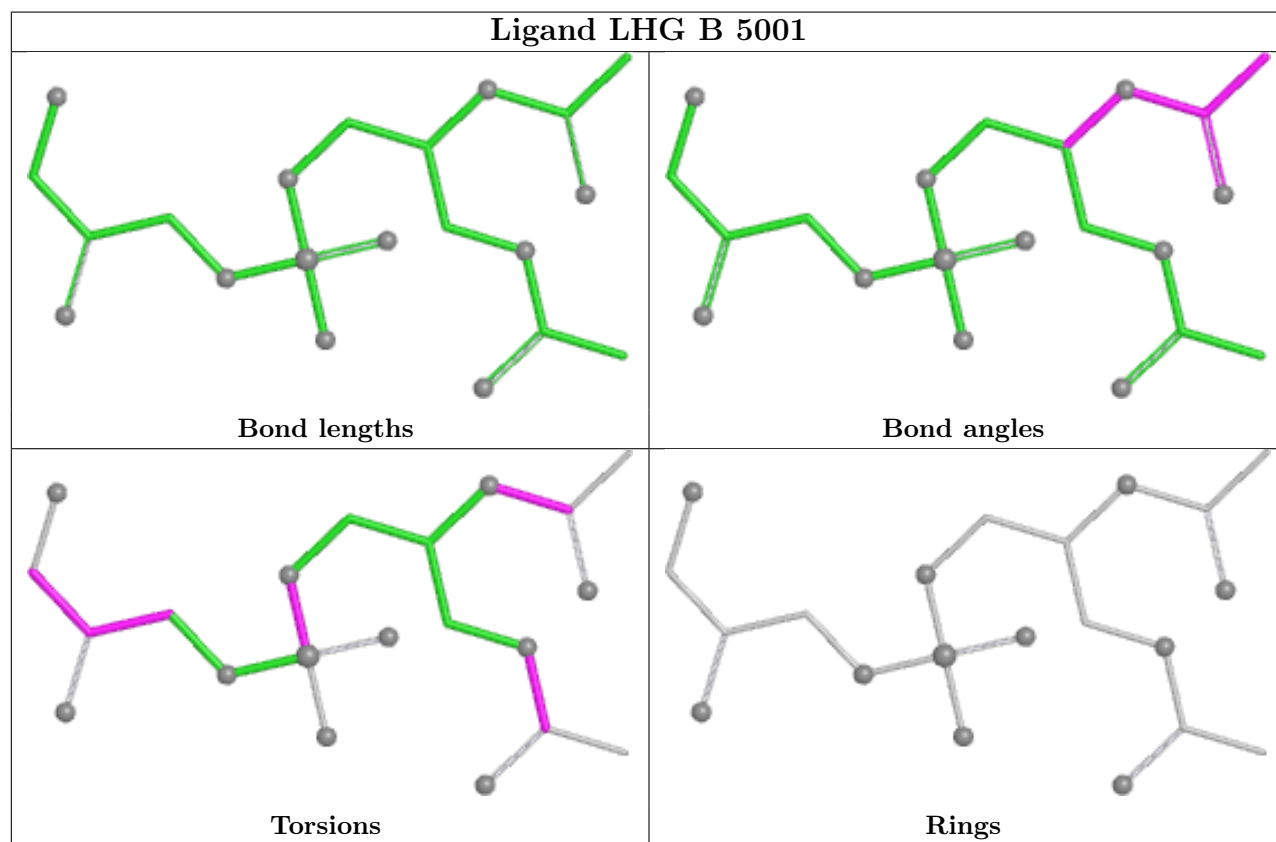
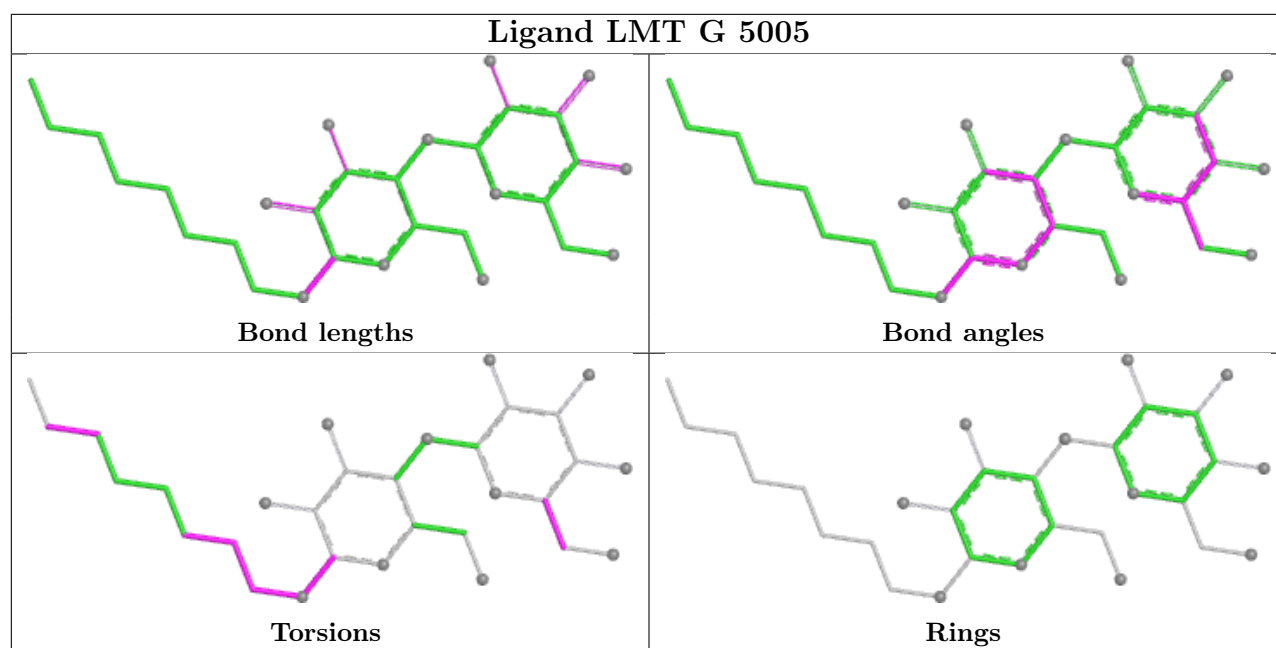


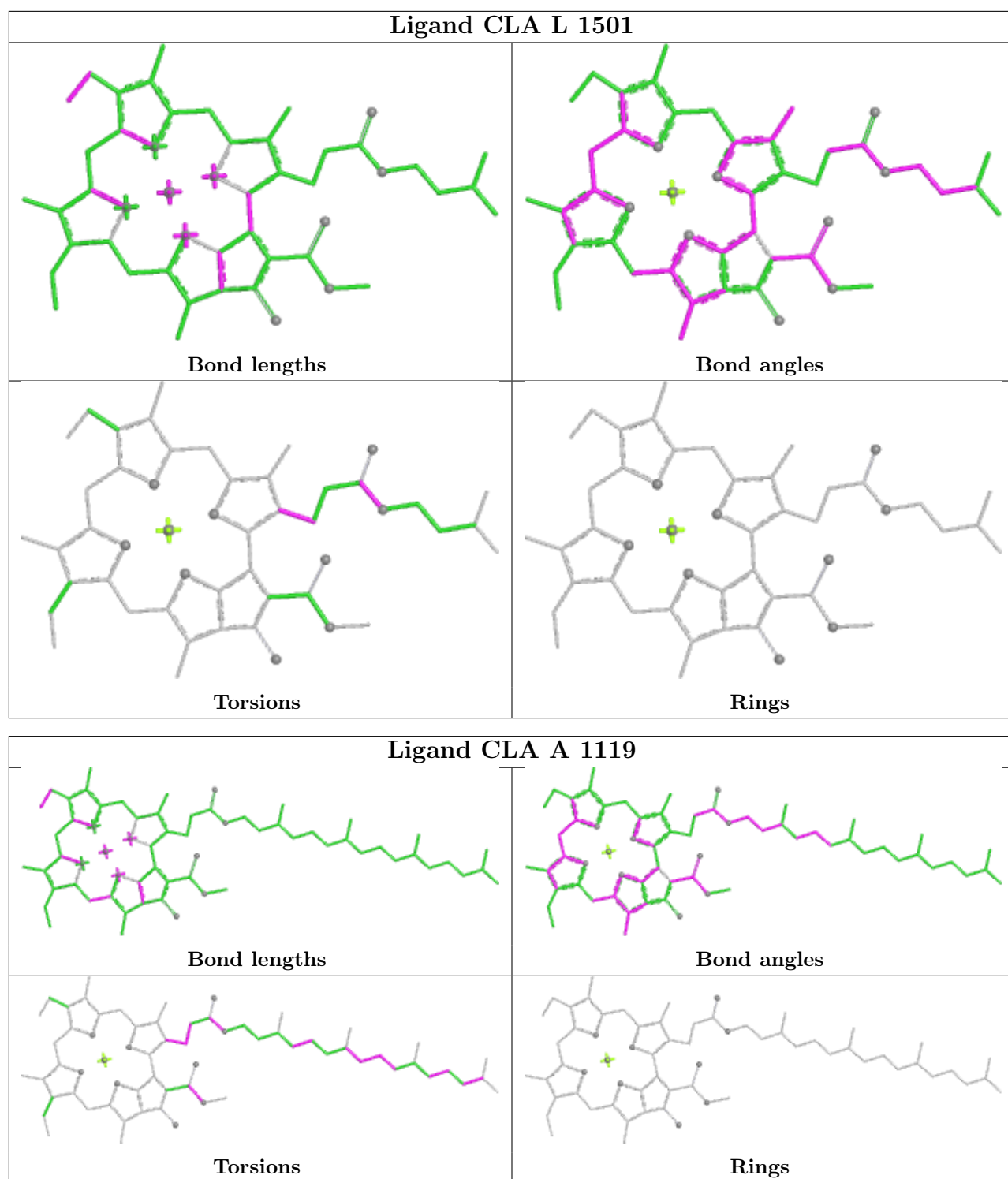




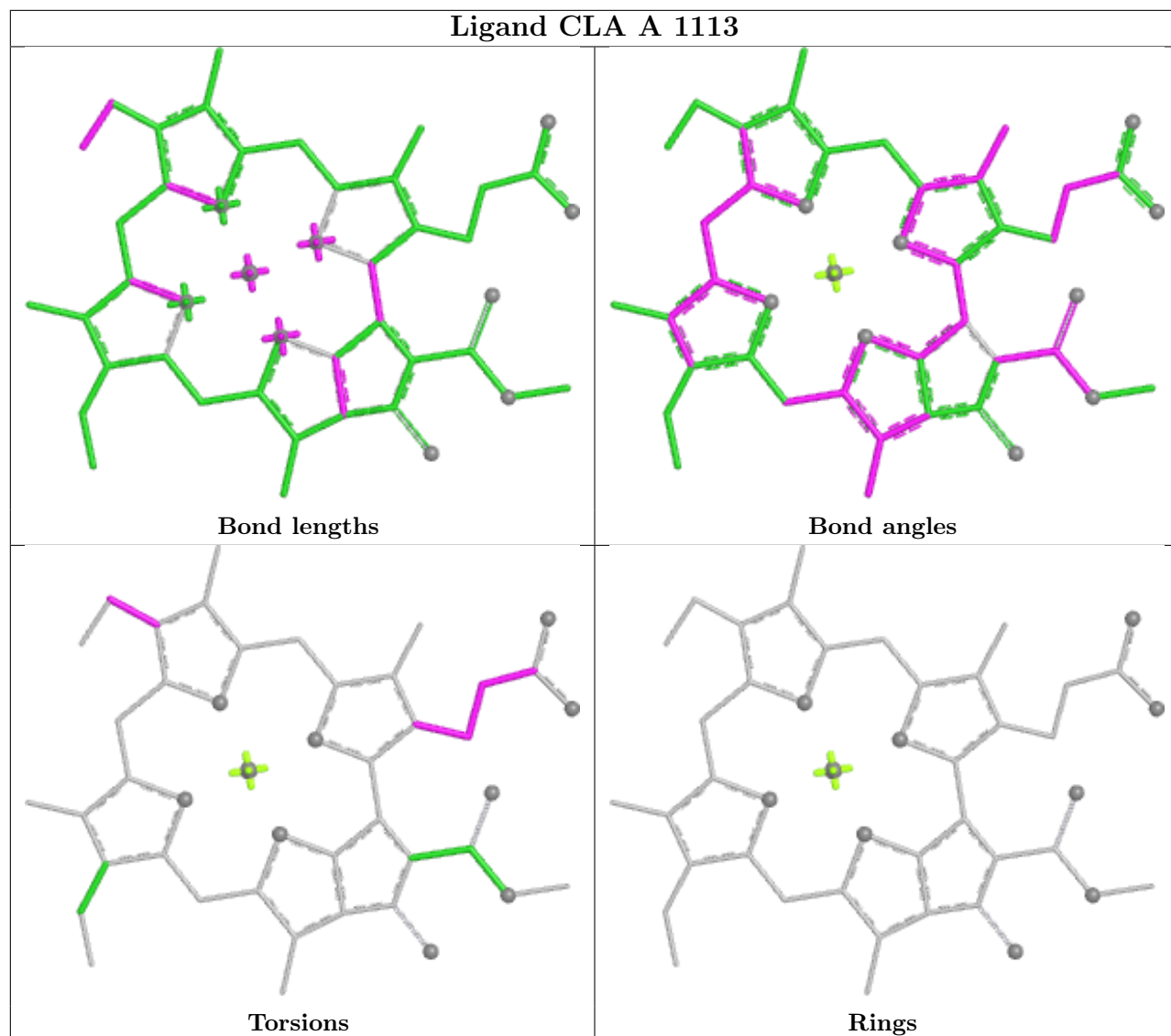


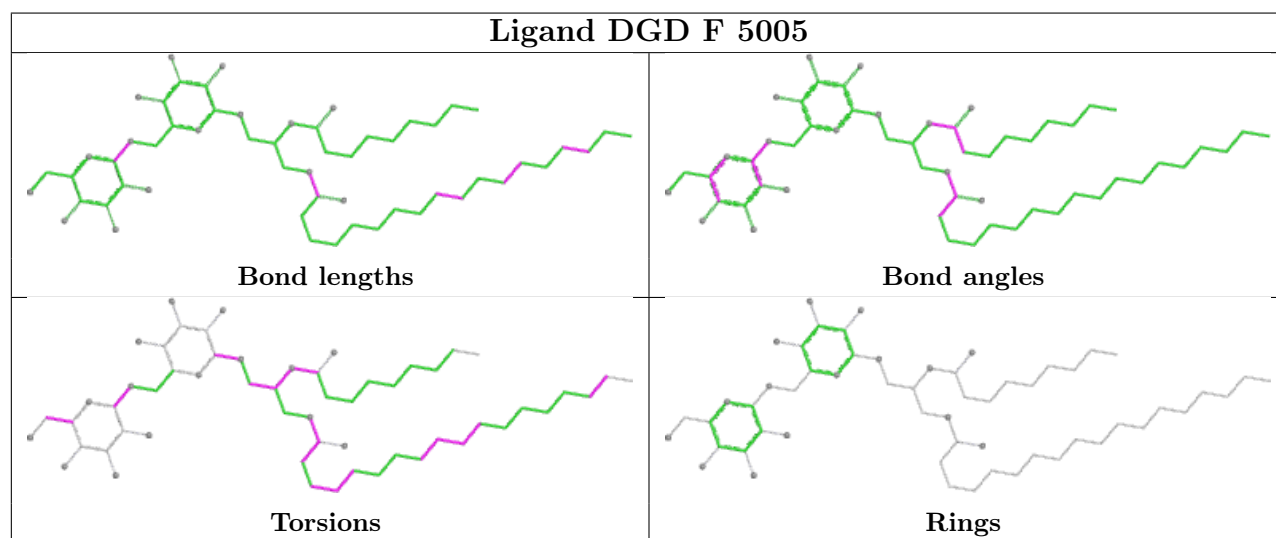
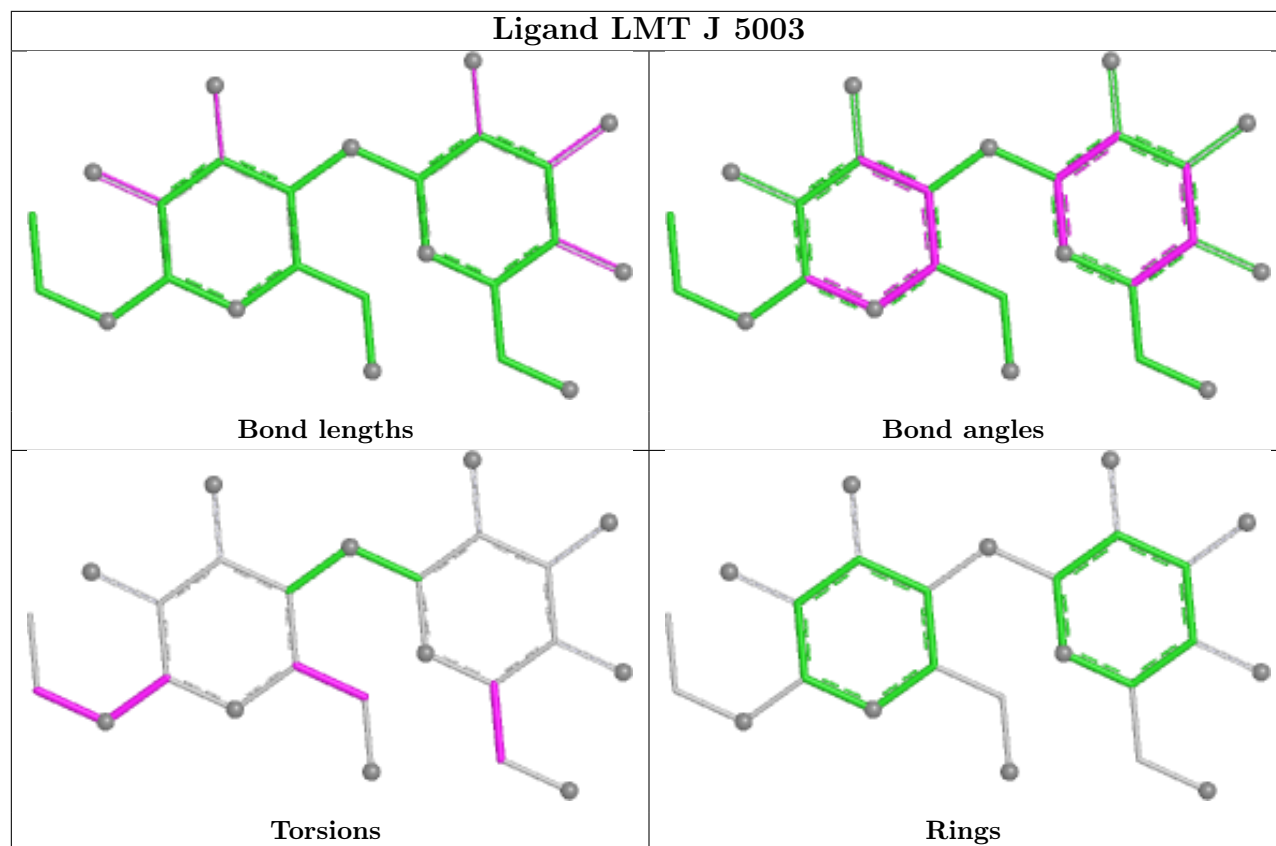




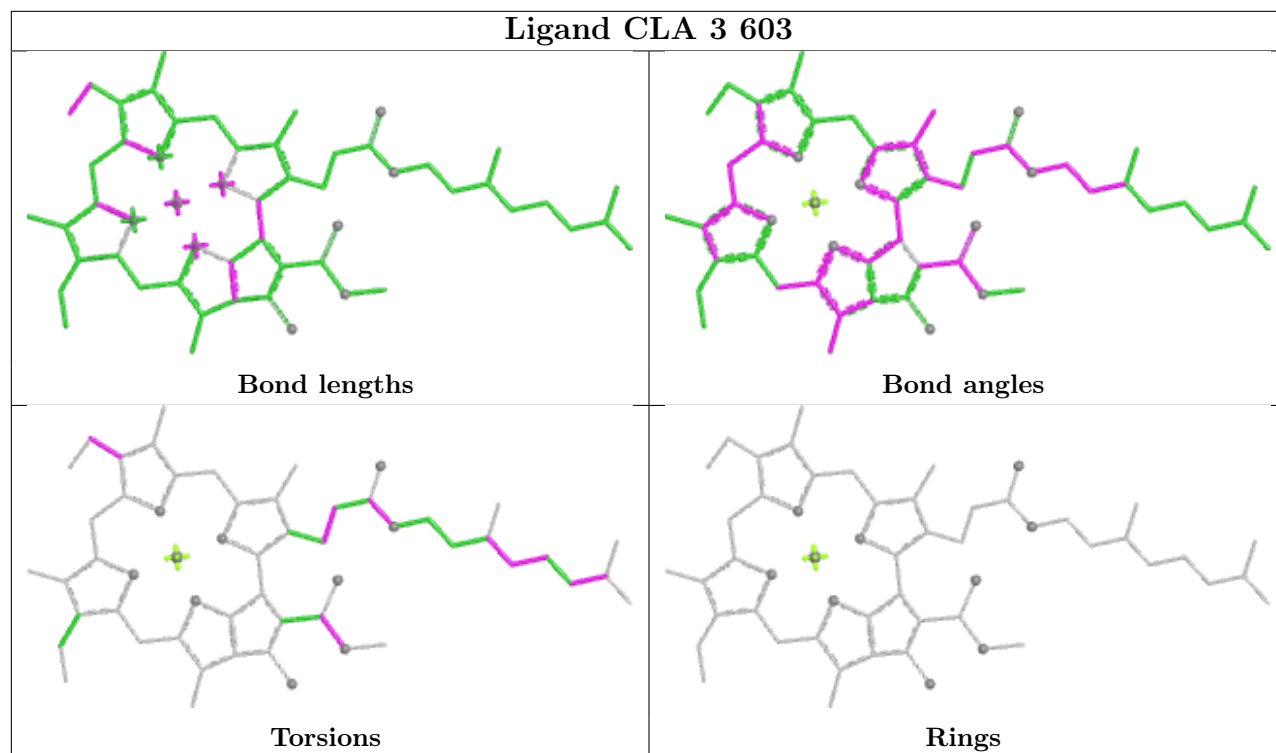


Ligand CLA A 1113

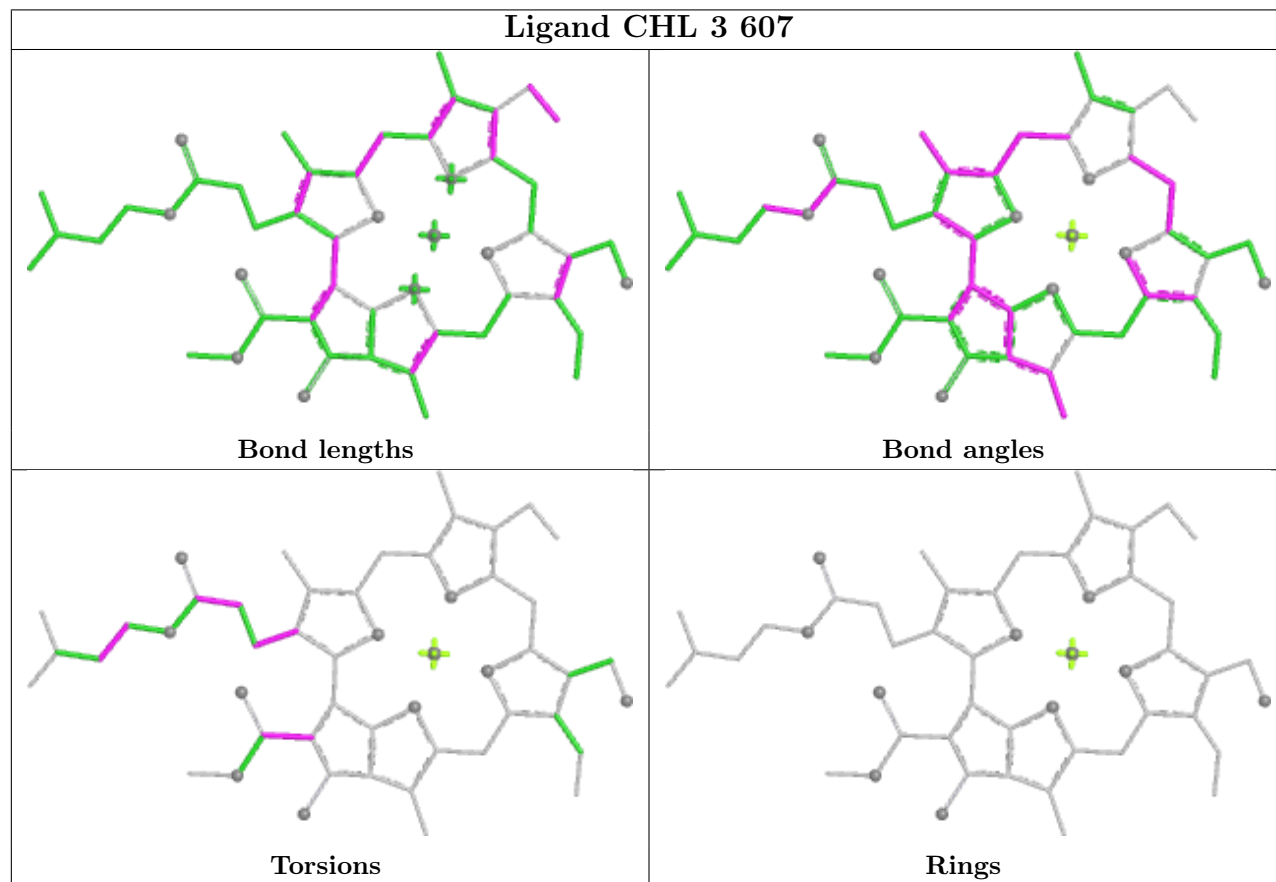




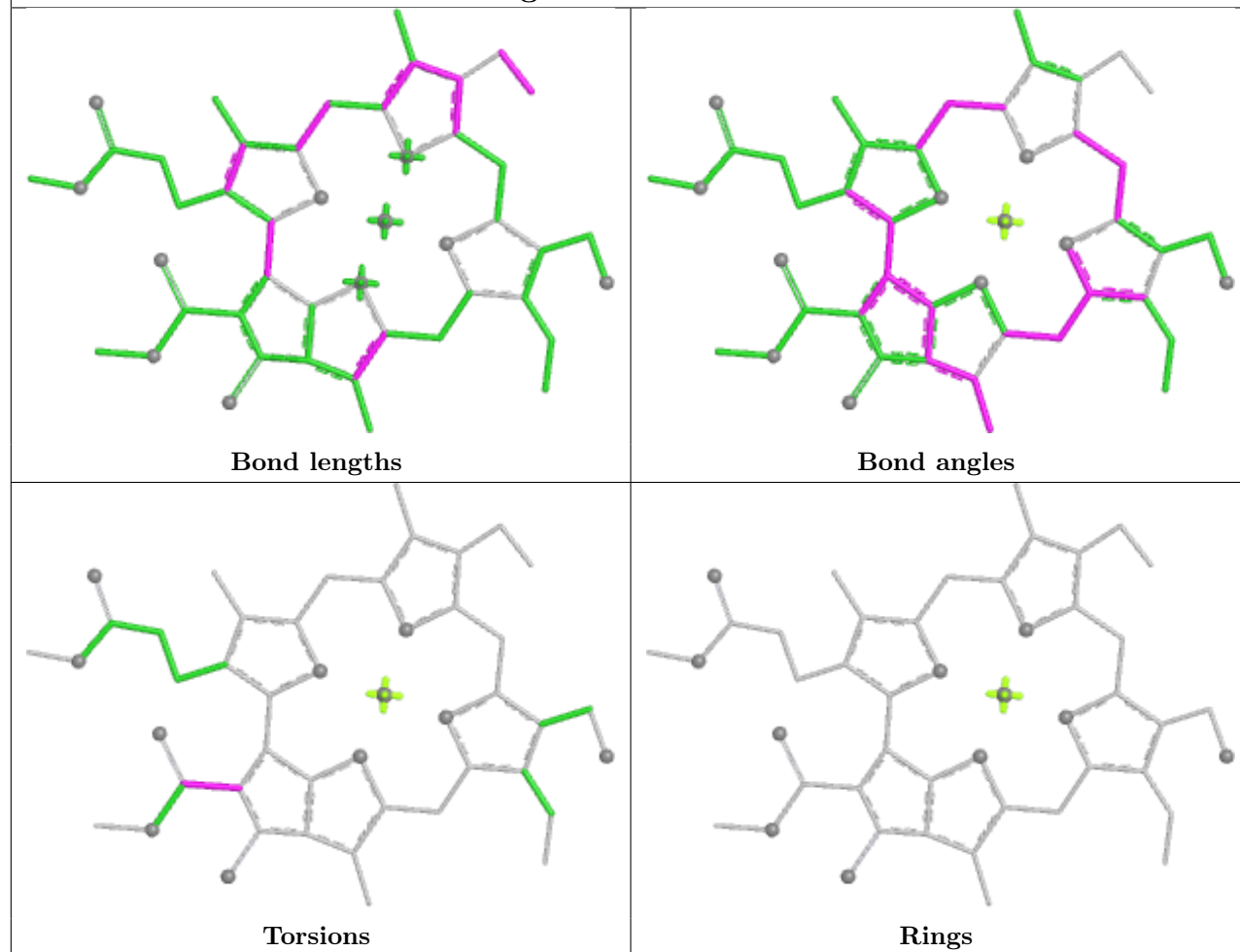
Ligand CLA 3 603



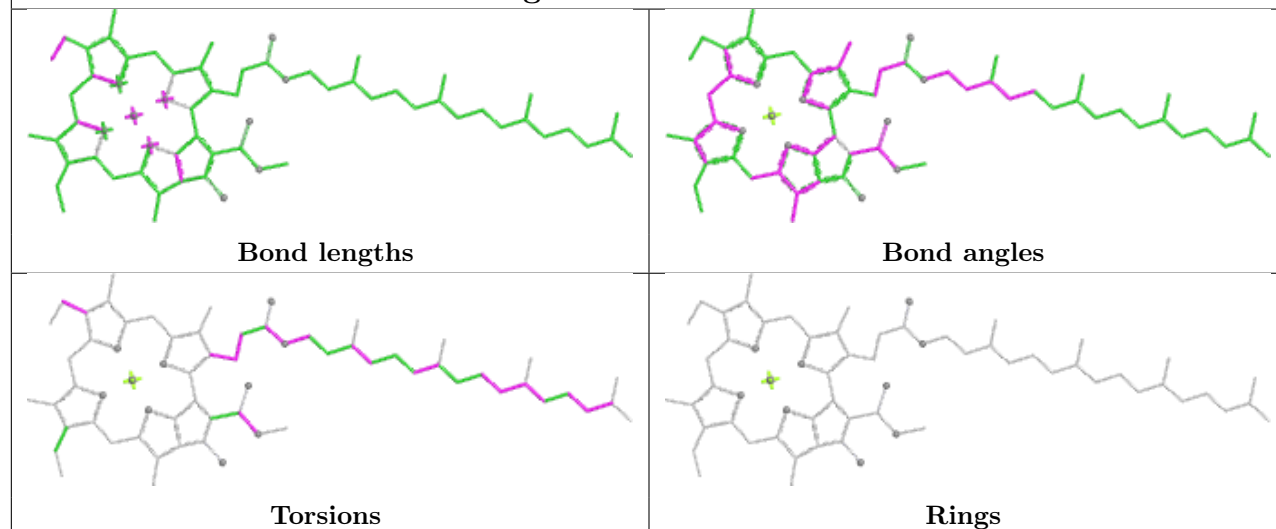
Ligand CHL 3 607

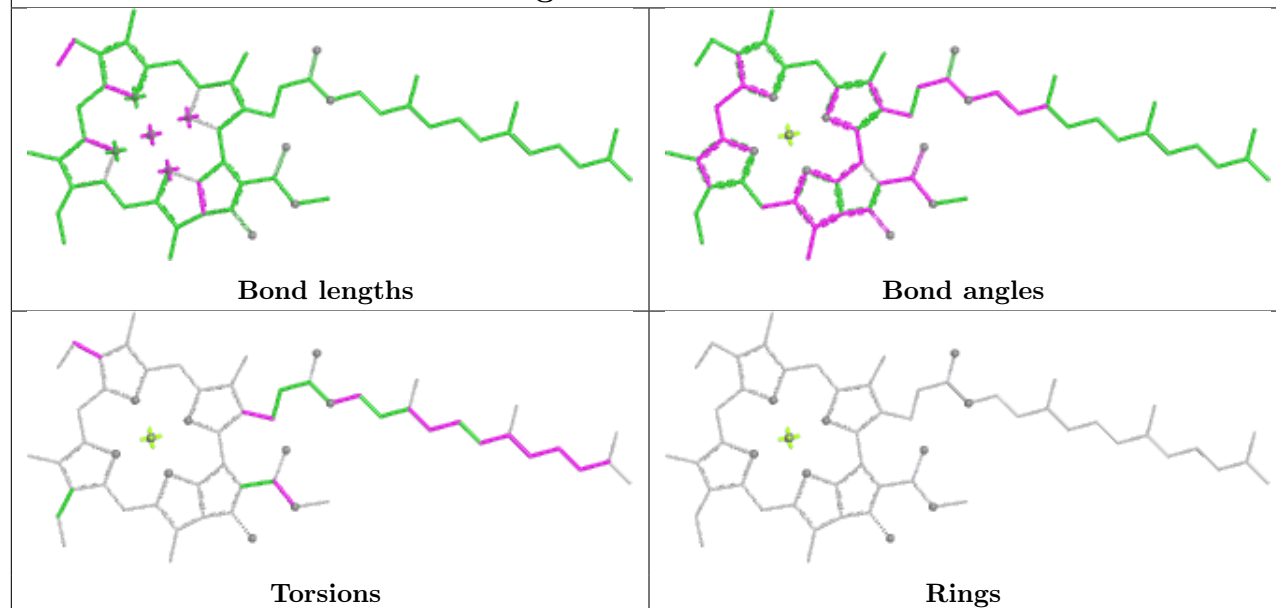
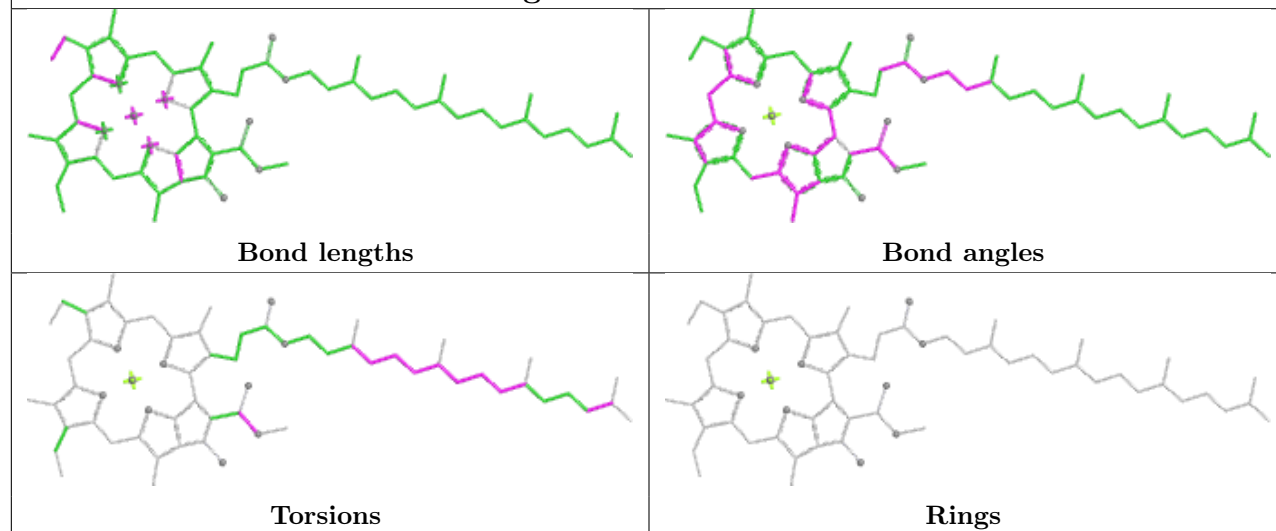


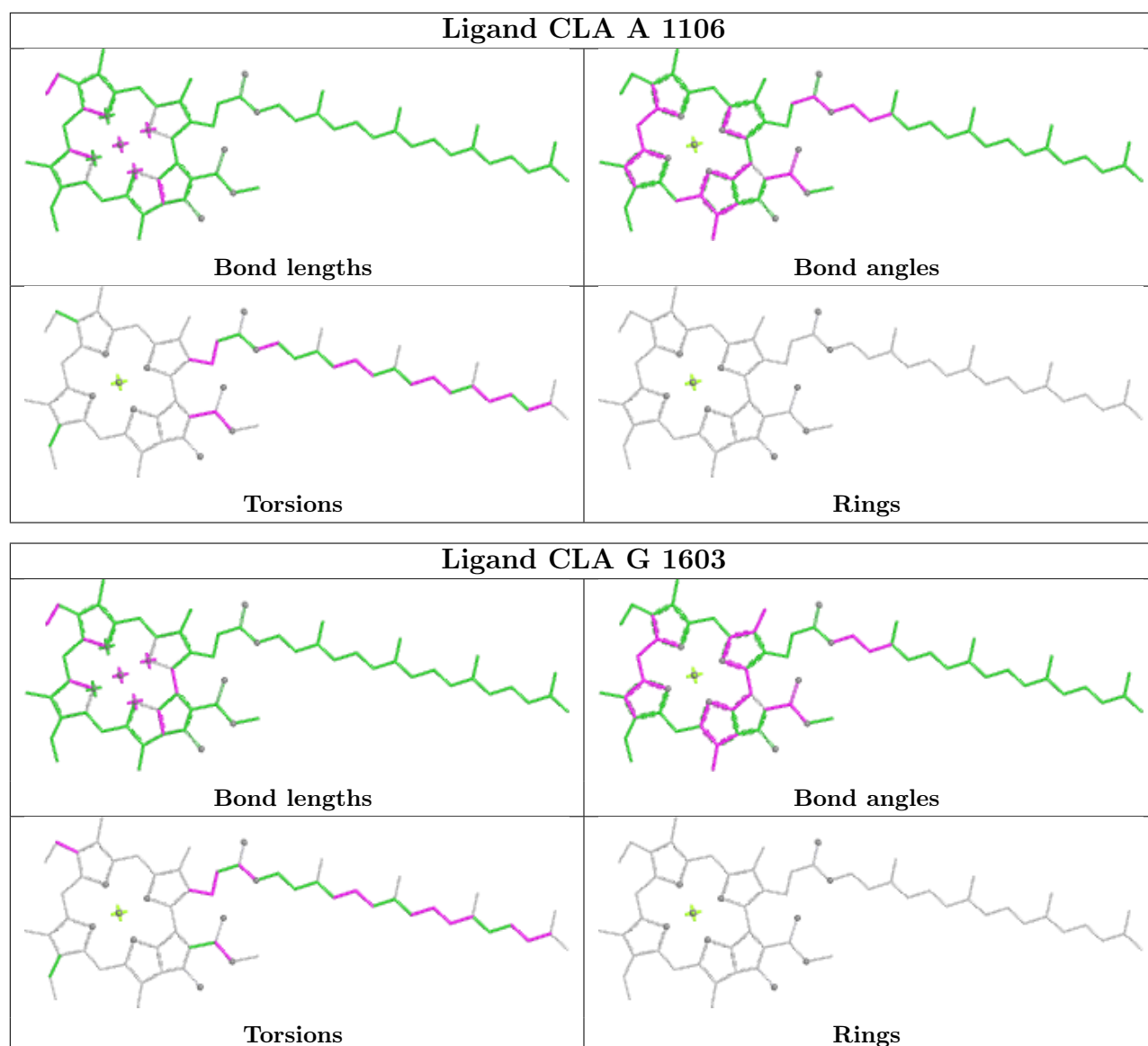
Ligand CHL 3 611

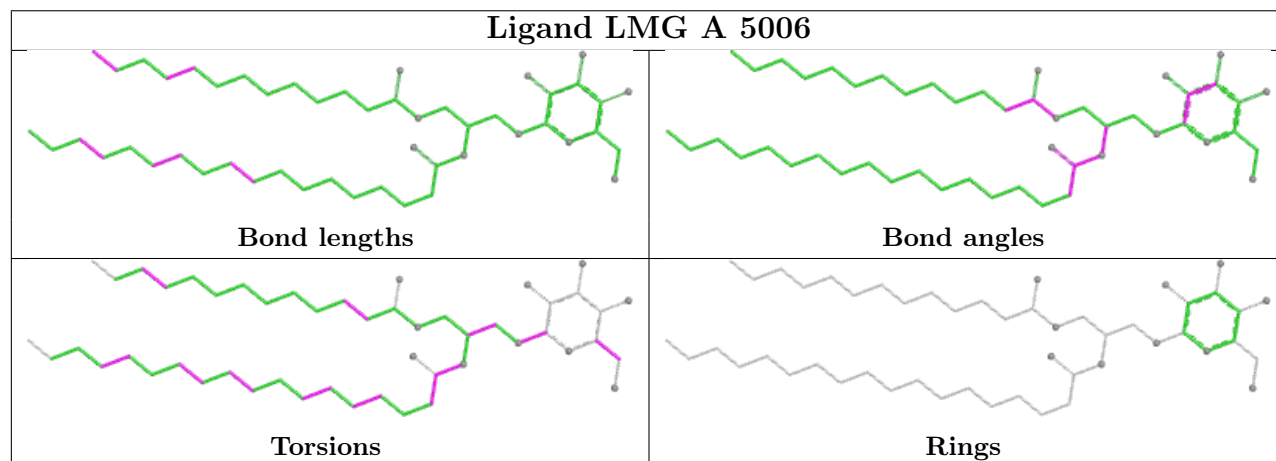
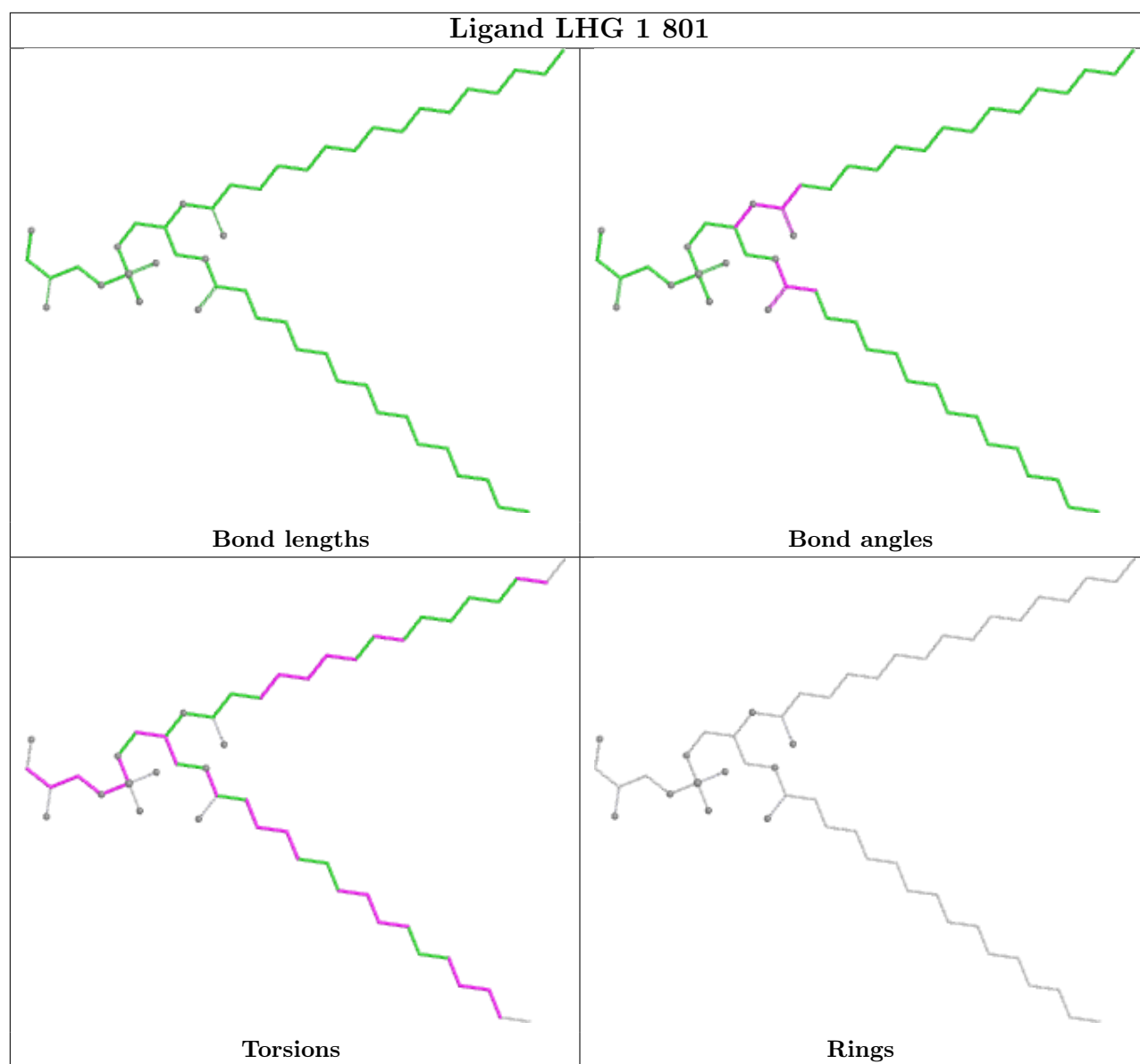


Ligand CLA B 1204

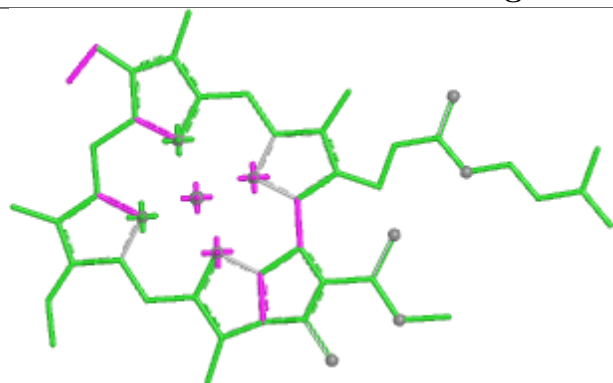


Ligand CLA 4 601**Ligand CLA B 1203**

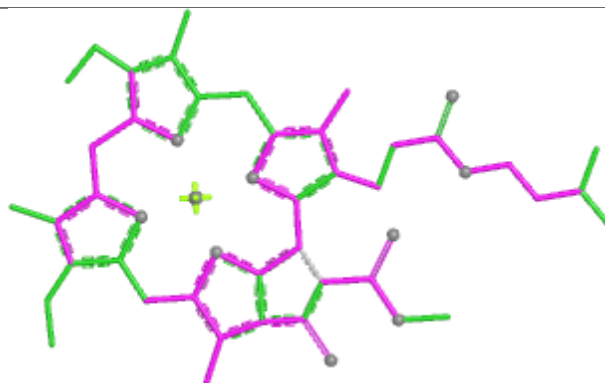




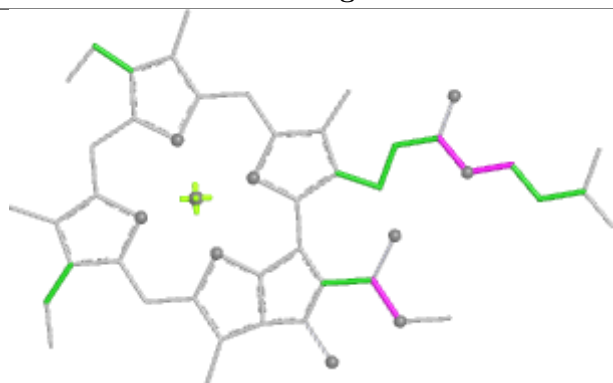
Ligand CLA A 1108



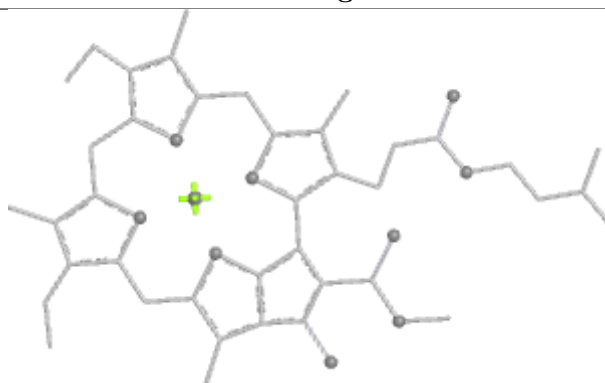
Bond lengths



Bond angles

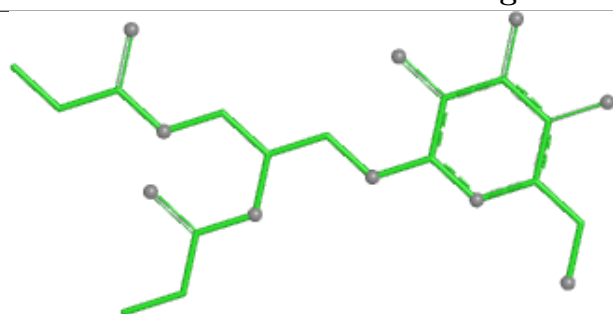


Torsions

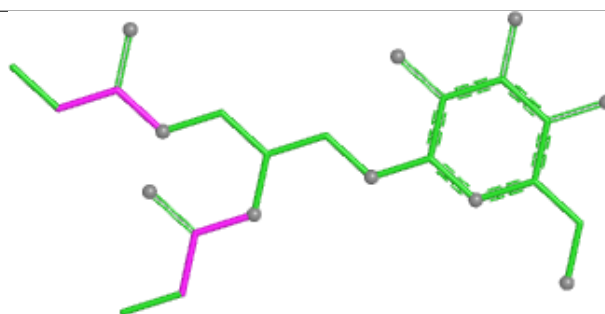


Rings

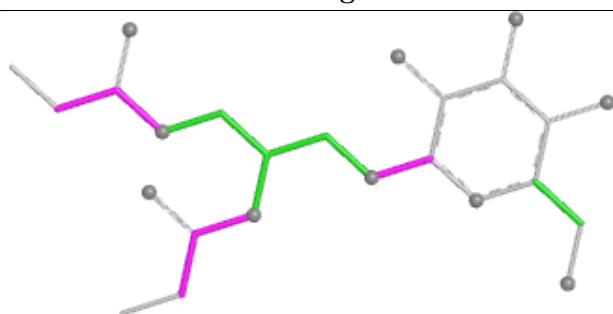
Ligand LMG G 5006



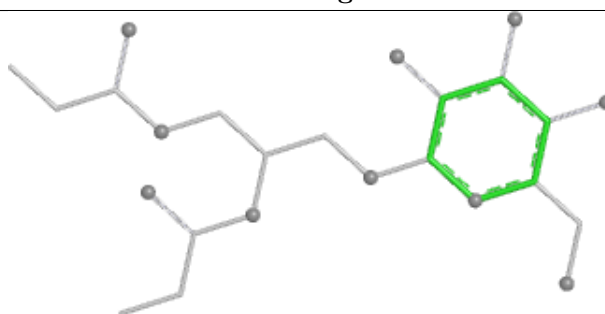
Bond lengths



Bond angles

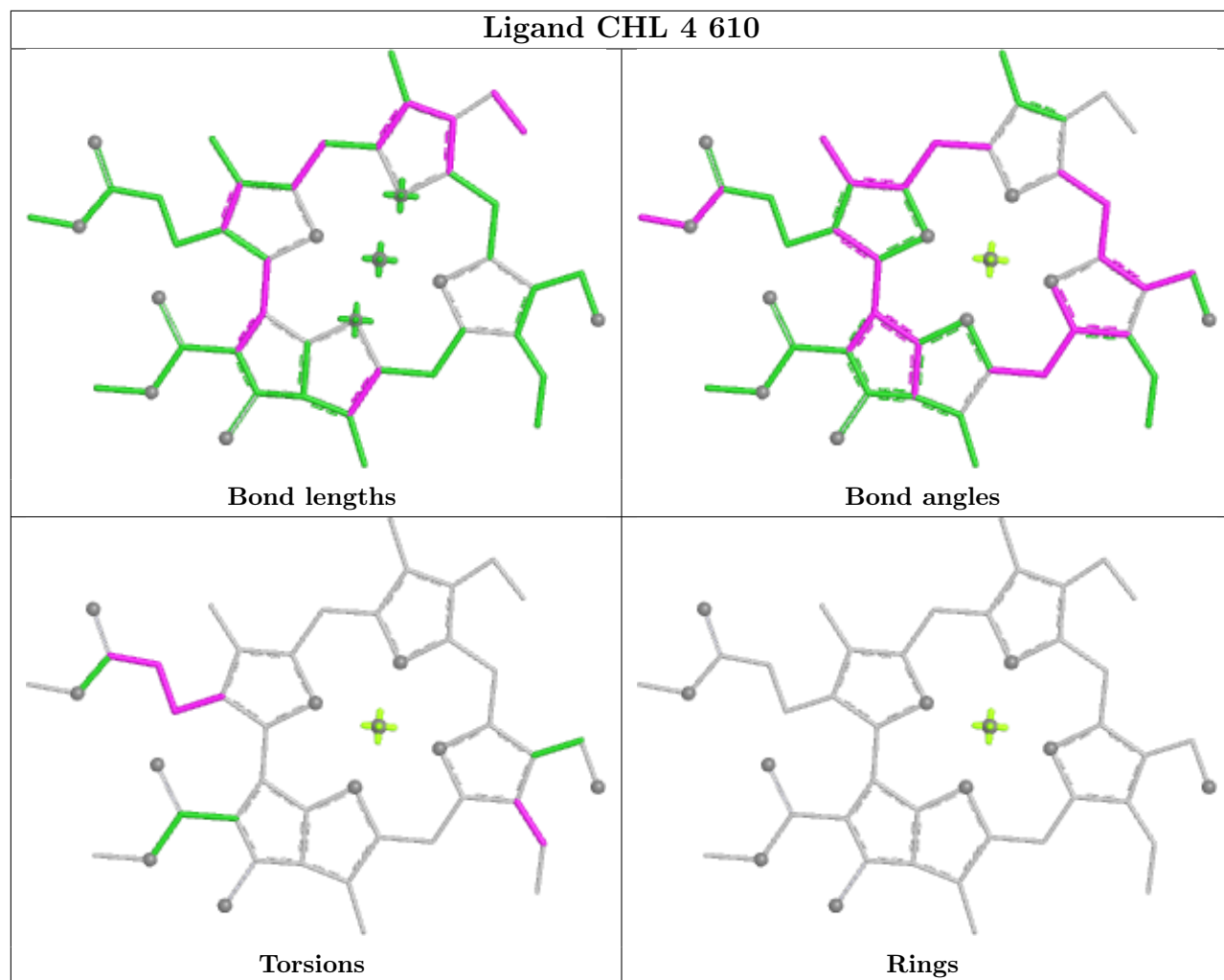


Torsions

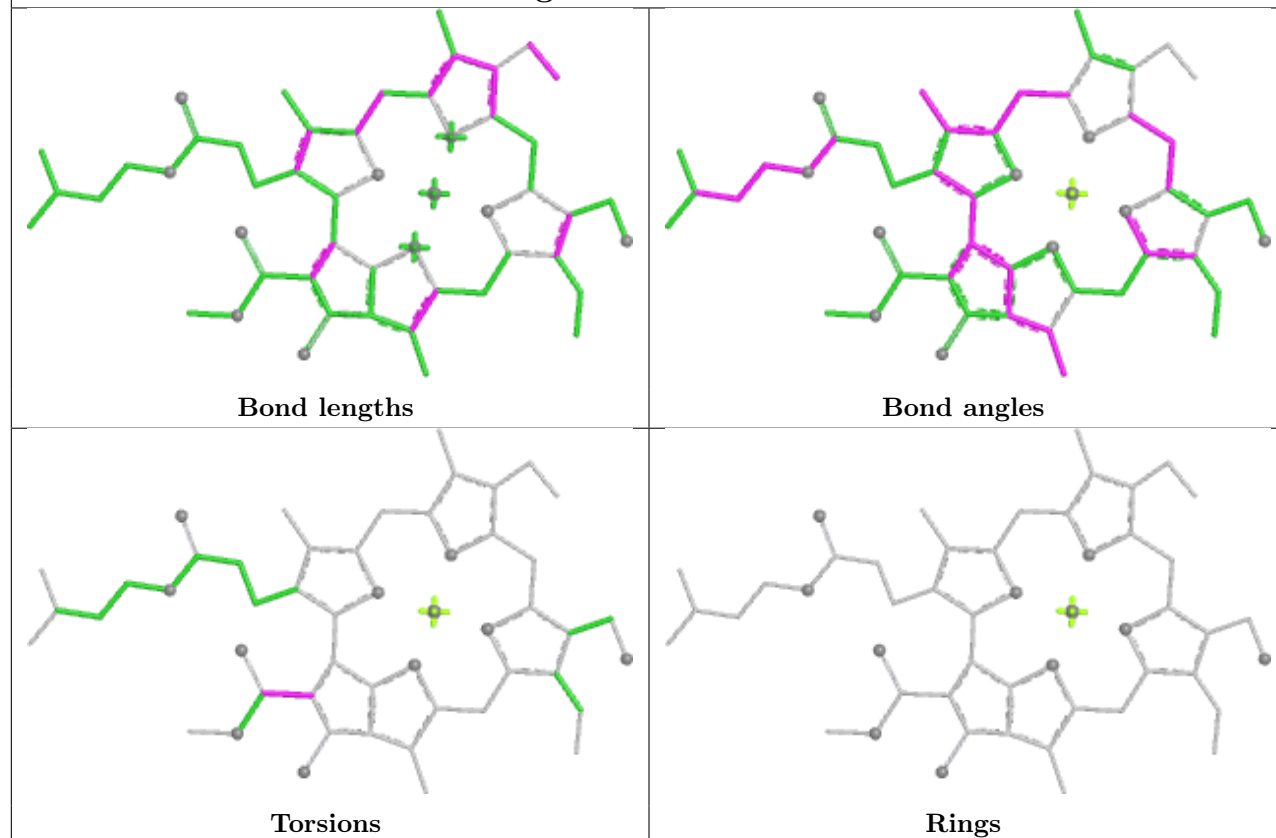


Rings

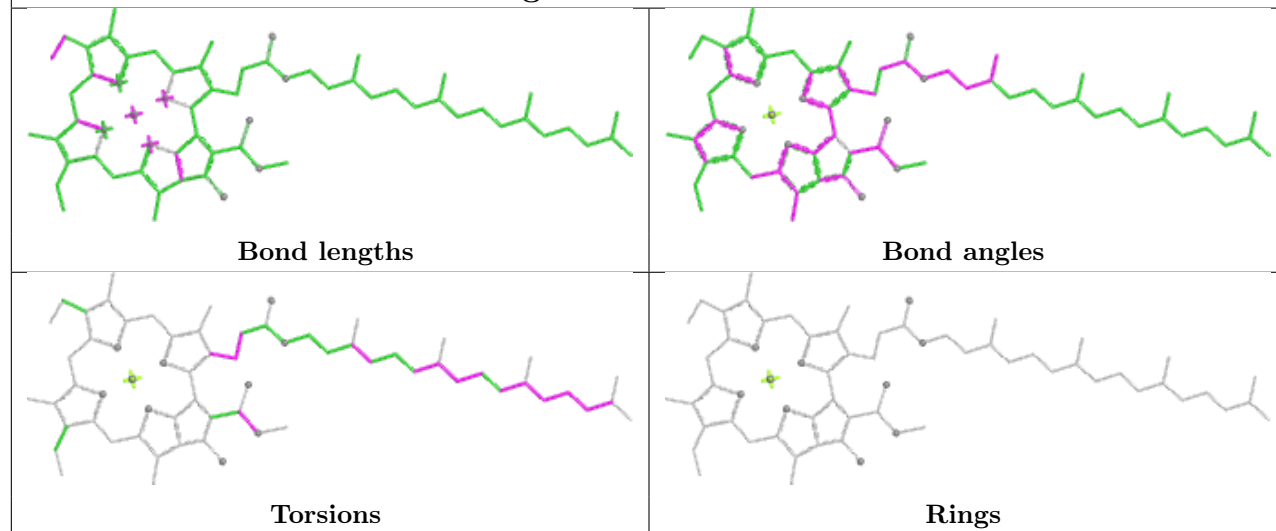
Ligand CHL 4 610

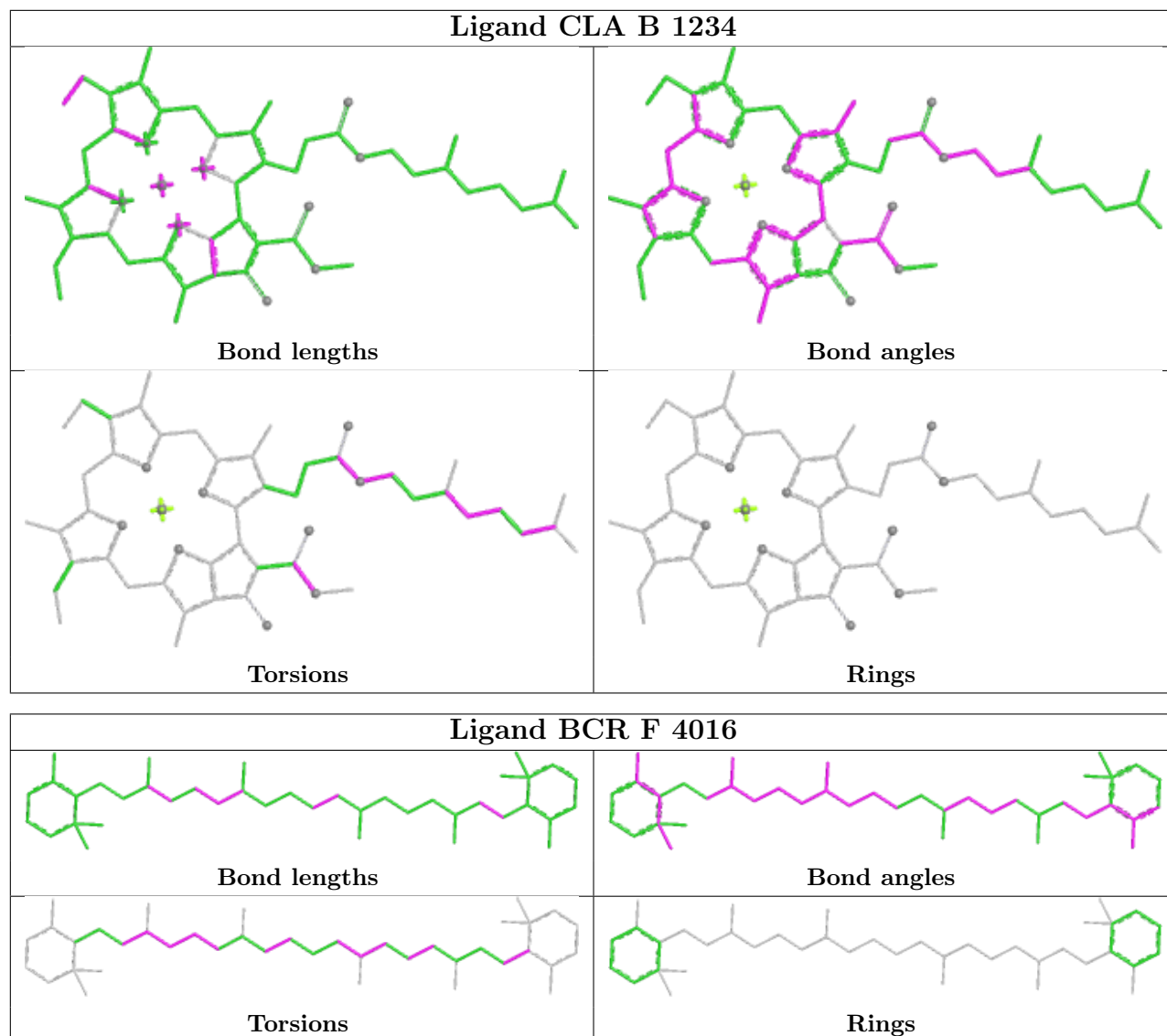


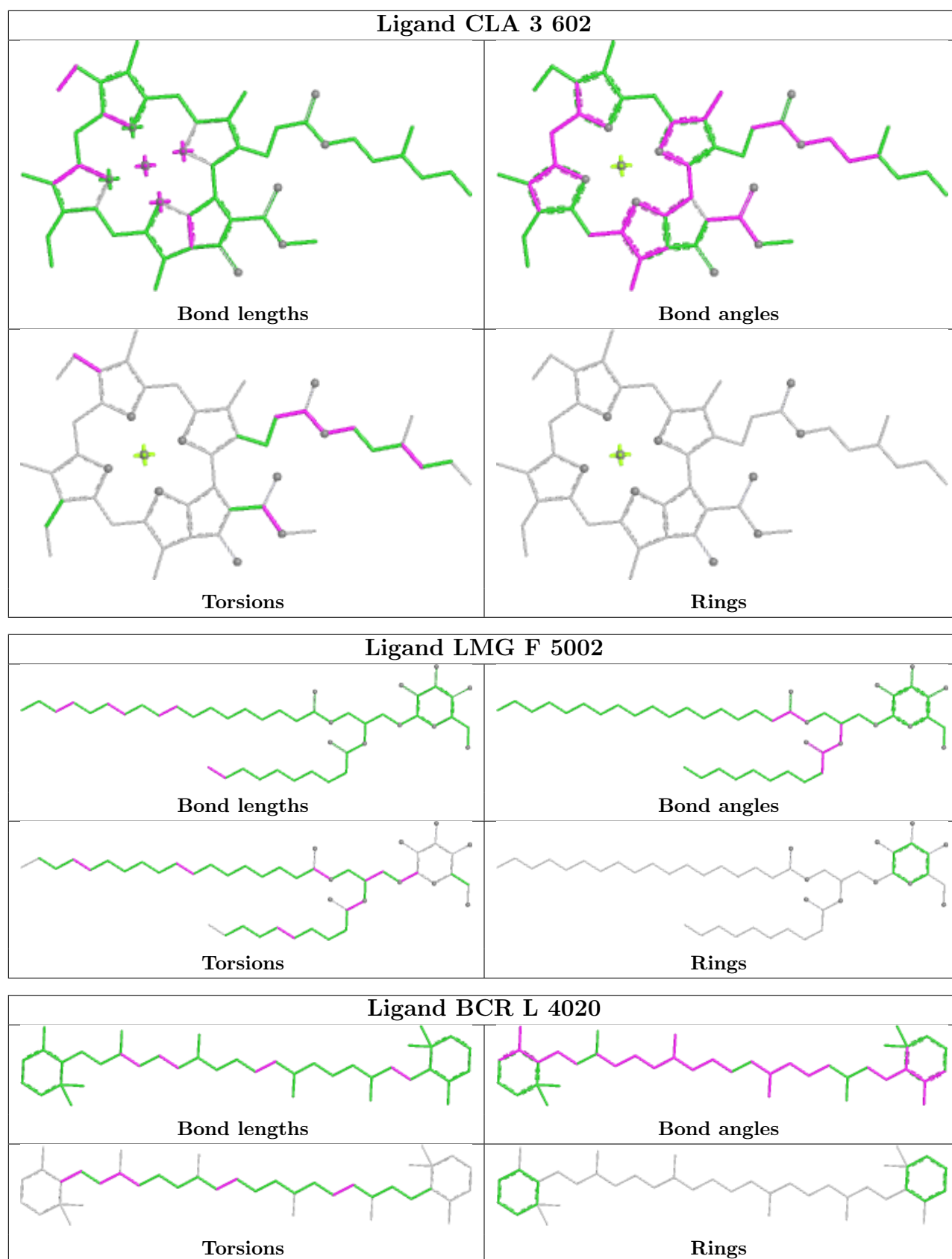
Ligand CHL 4 611

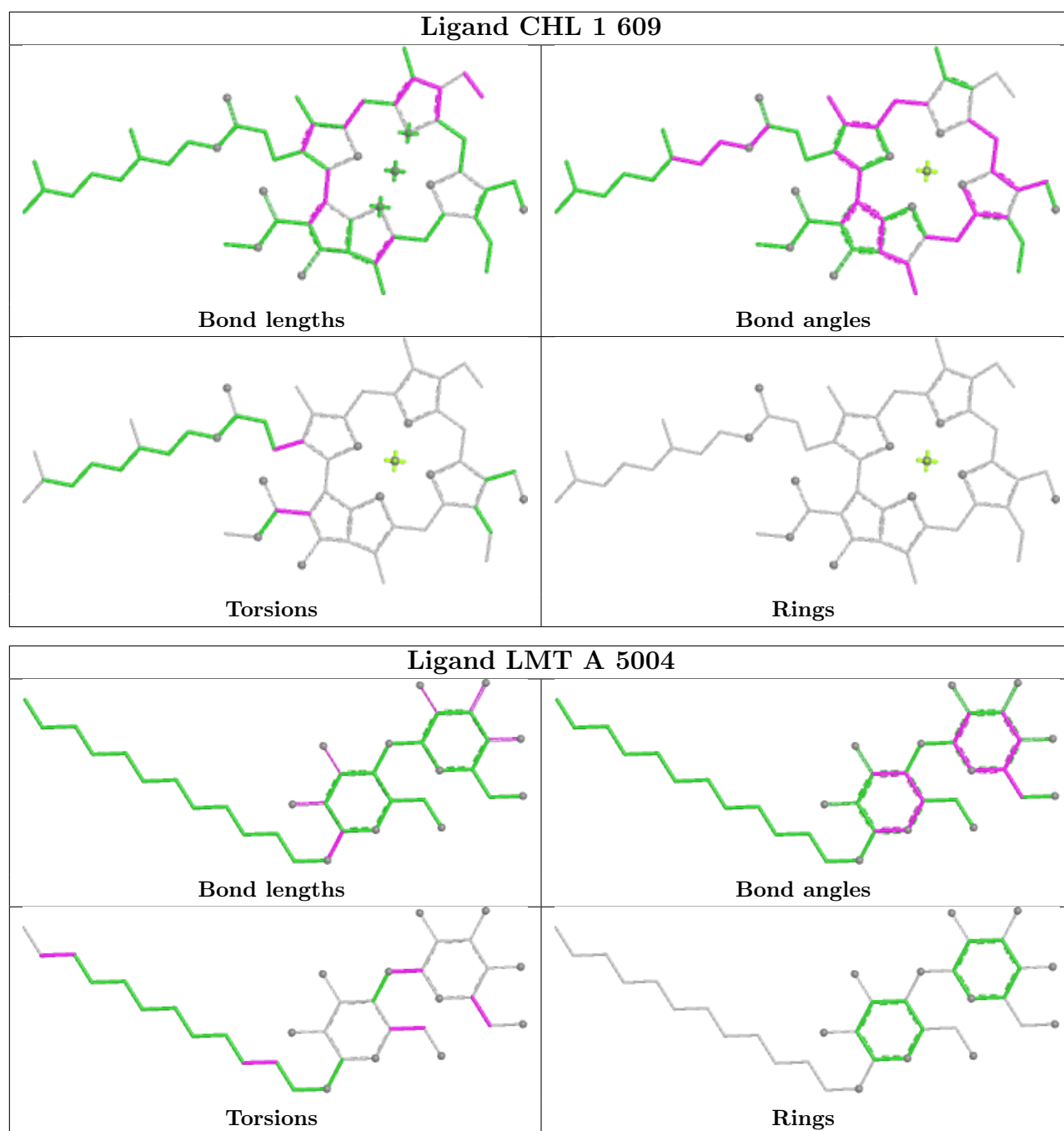


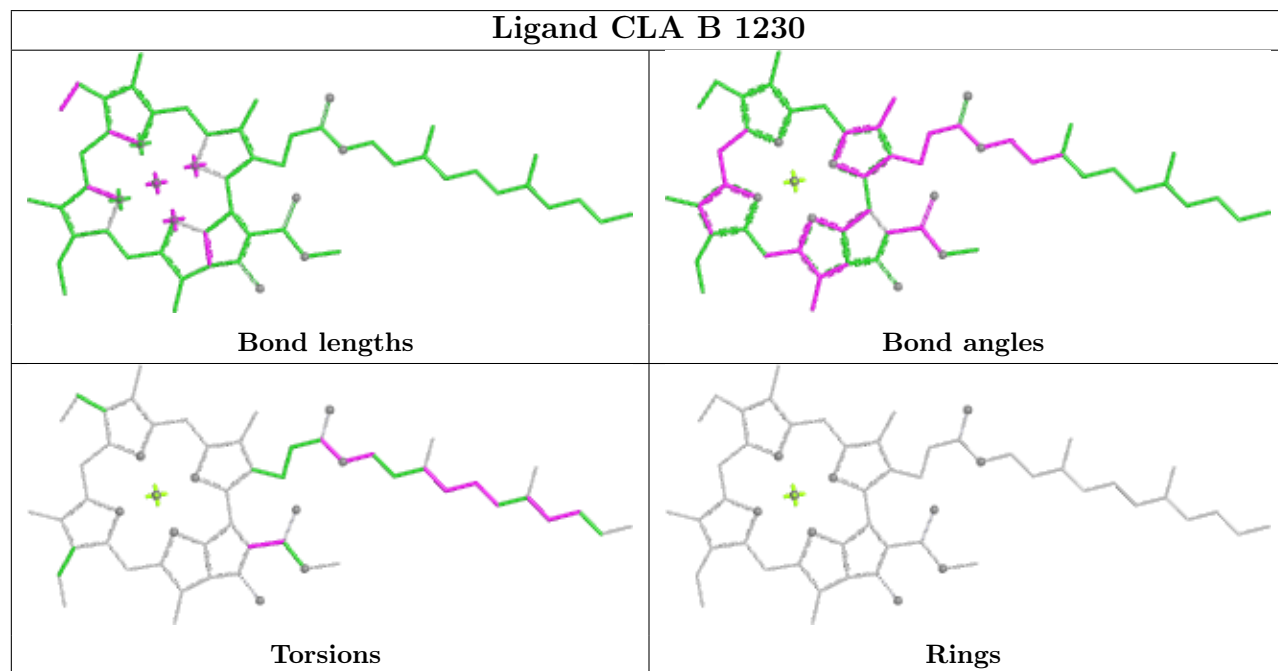
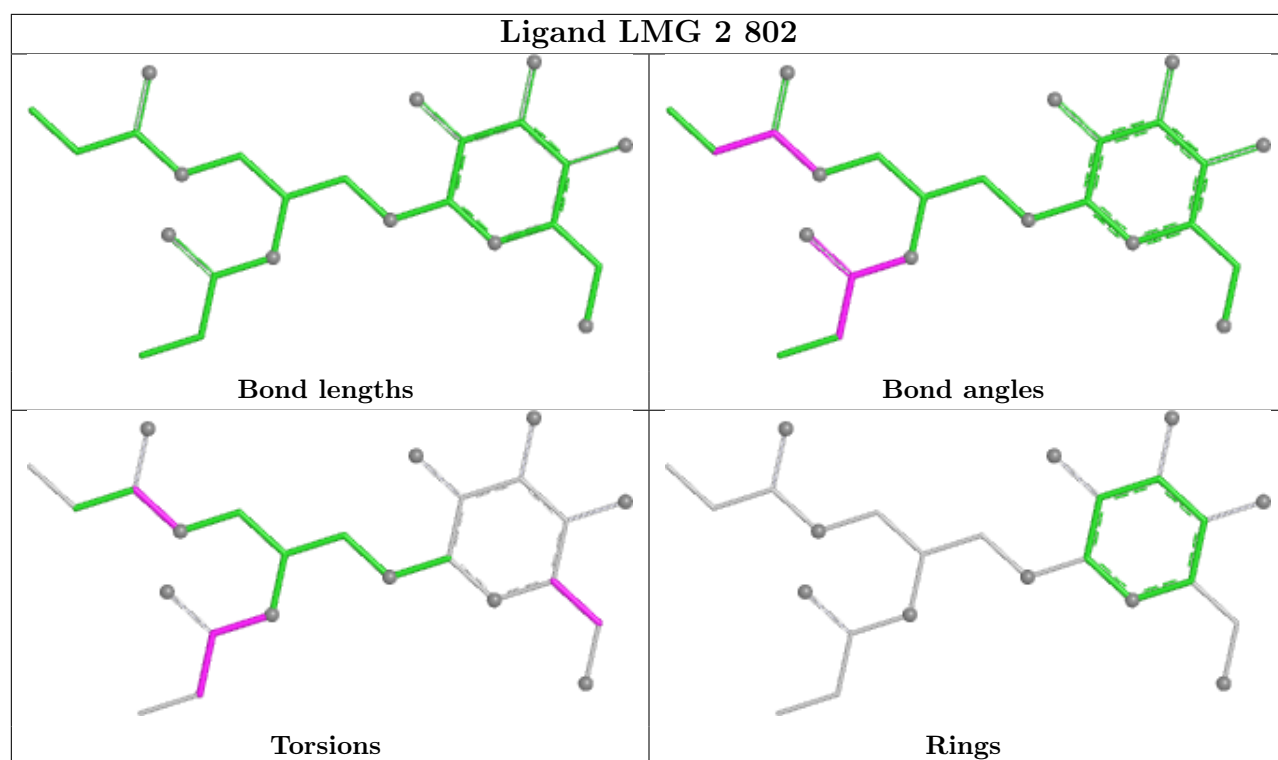
Ligand CLA A 1012

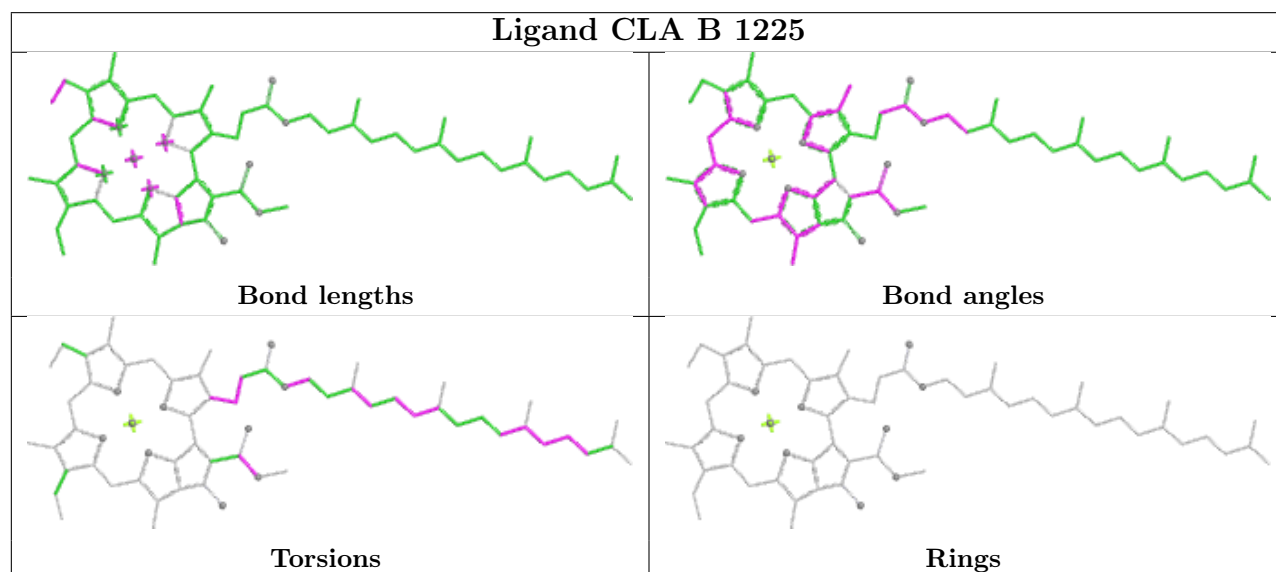
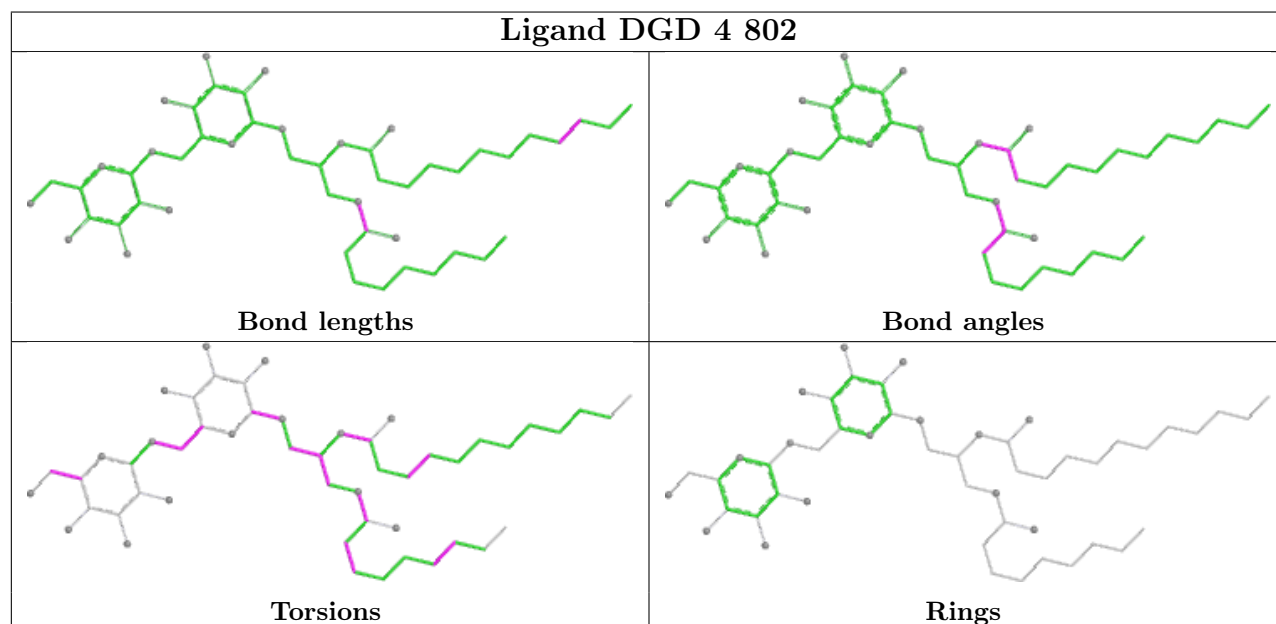
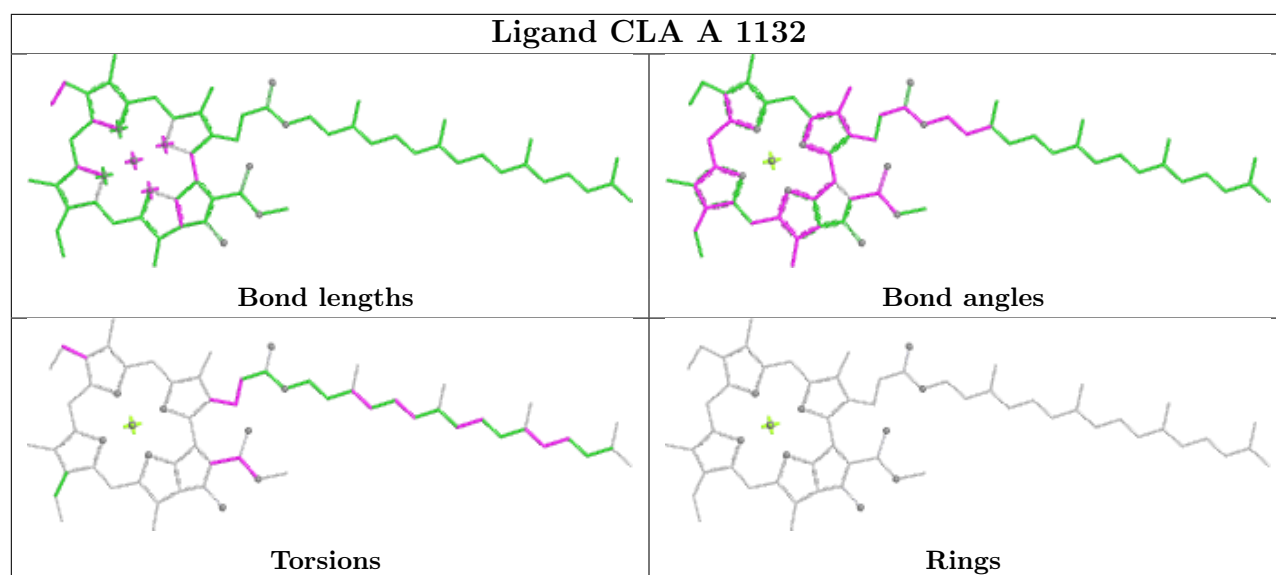


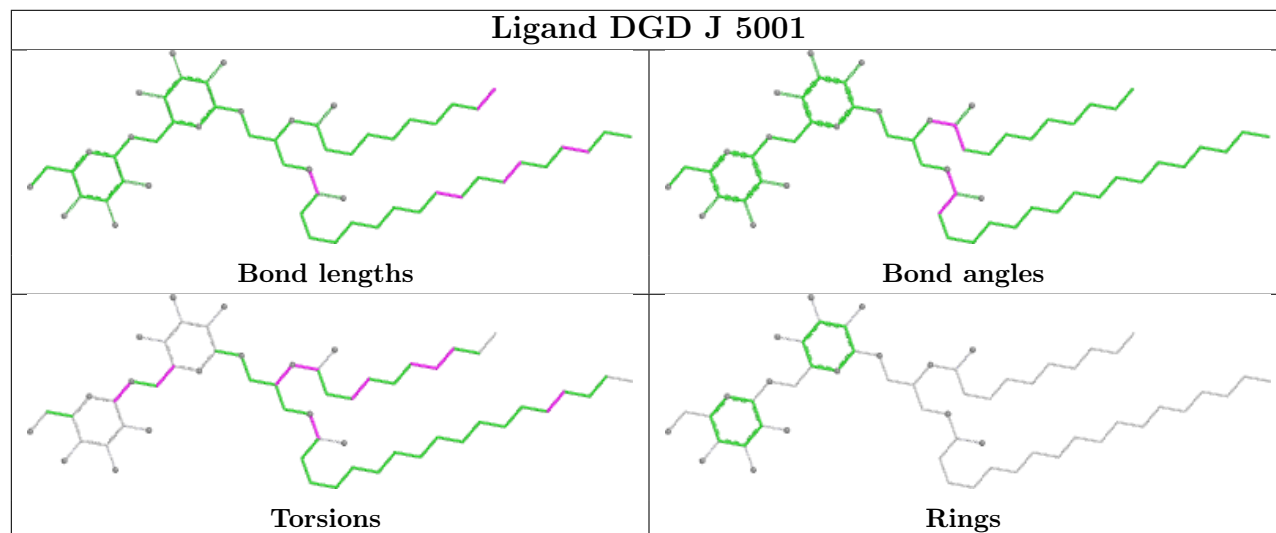
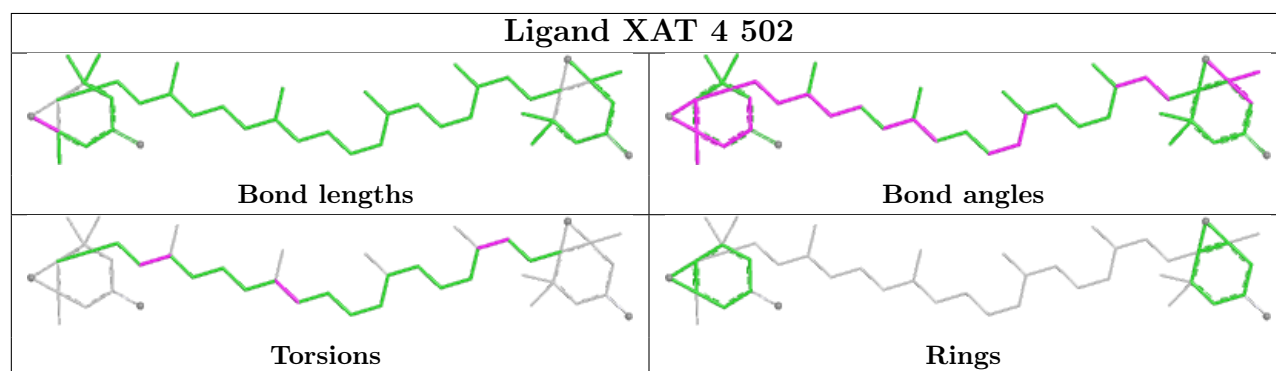
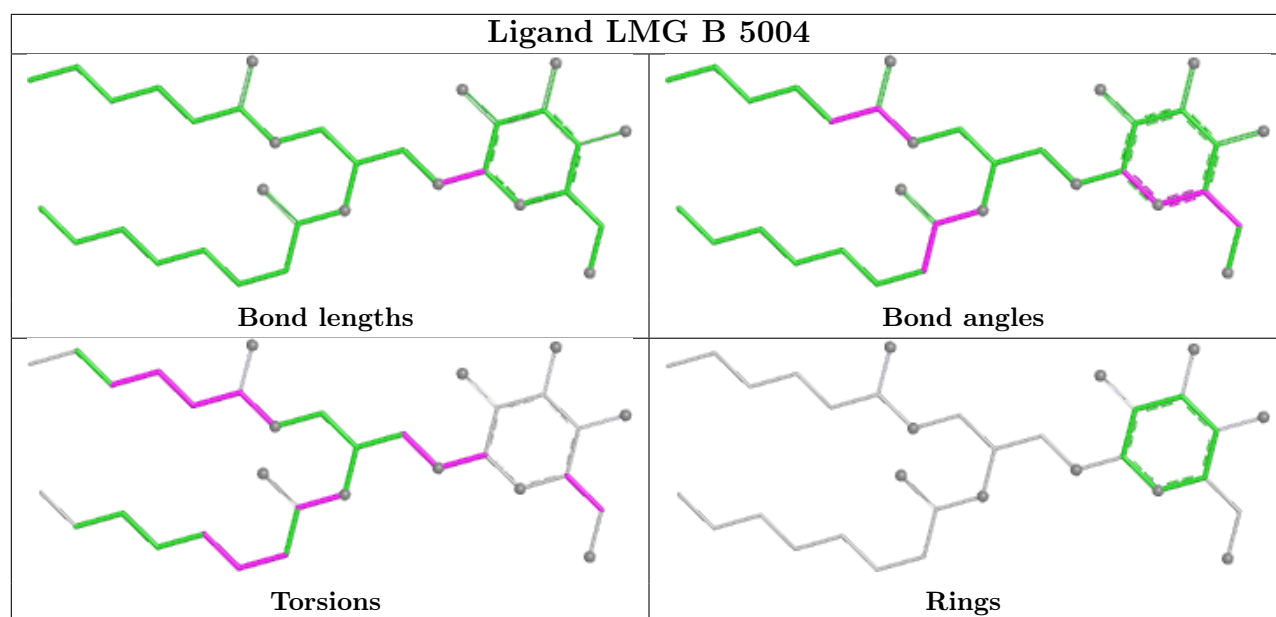


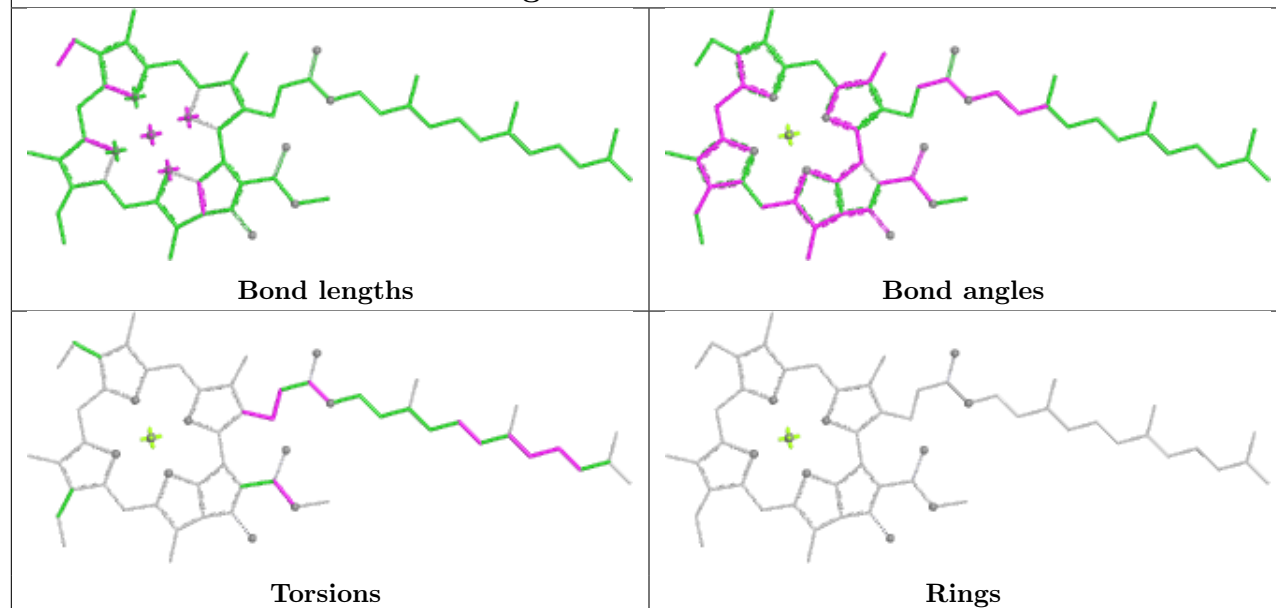
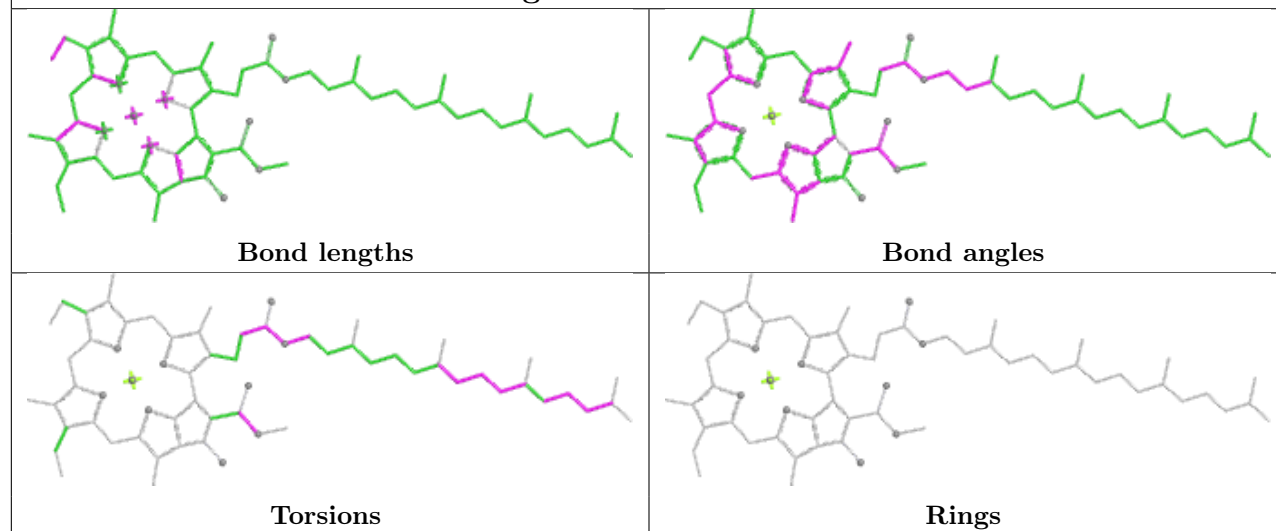




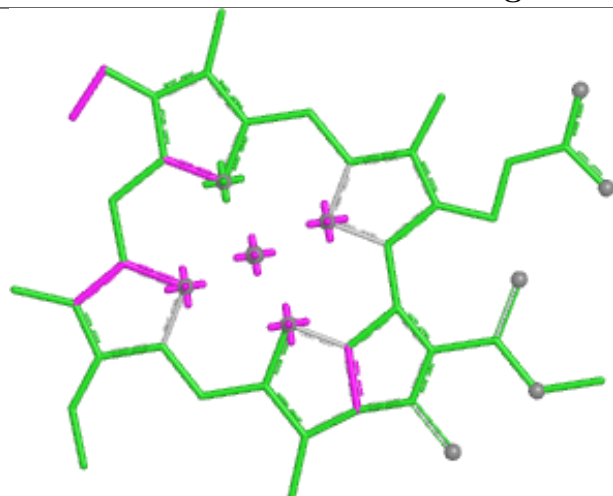




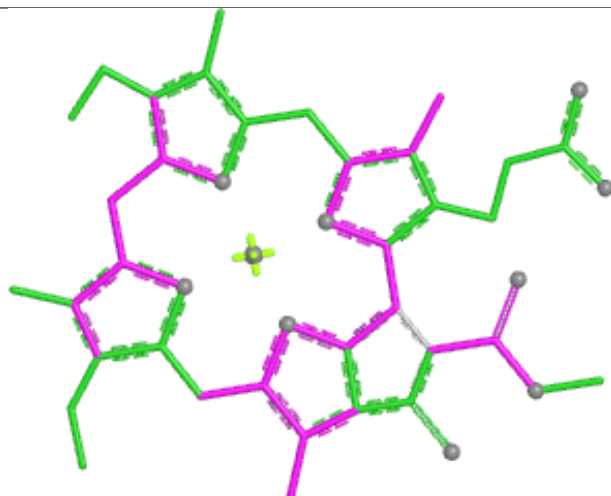


Ligand CLA A 1141**Ligand CLA A 1136**

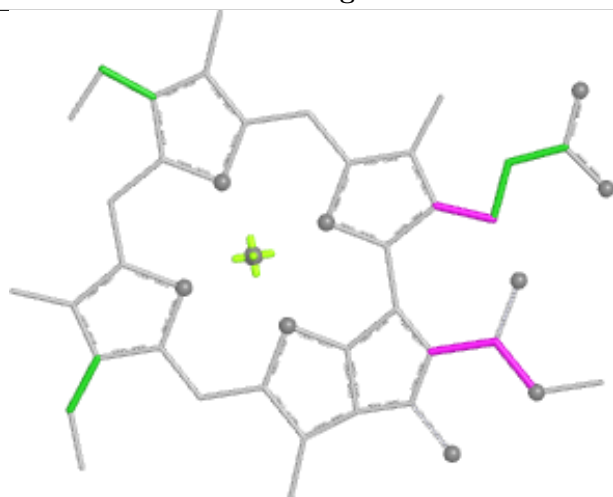
Ligand CLA K 1401



Bond lengths



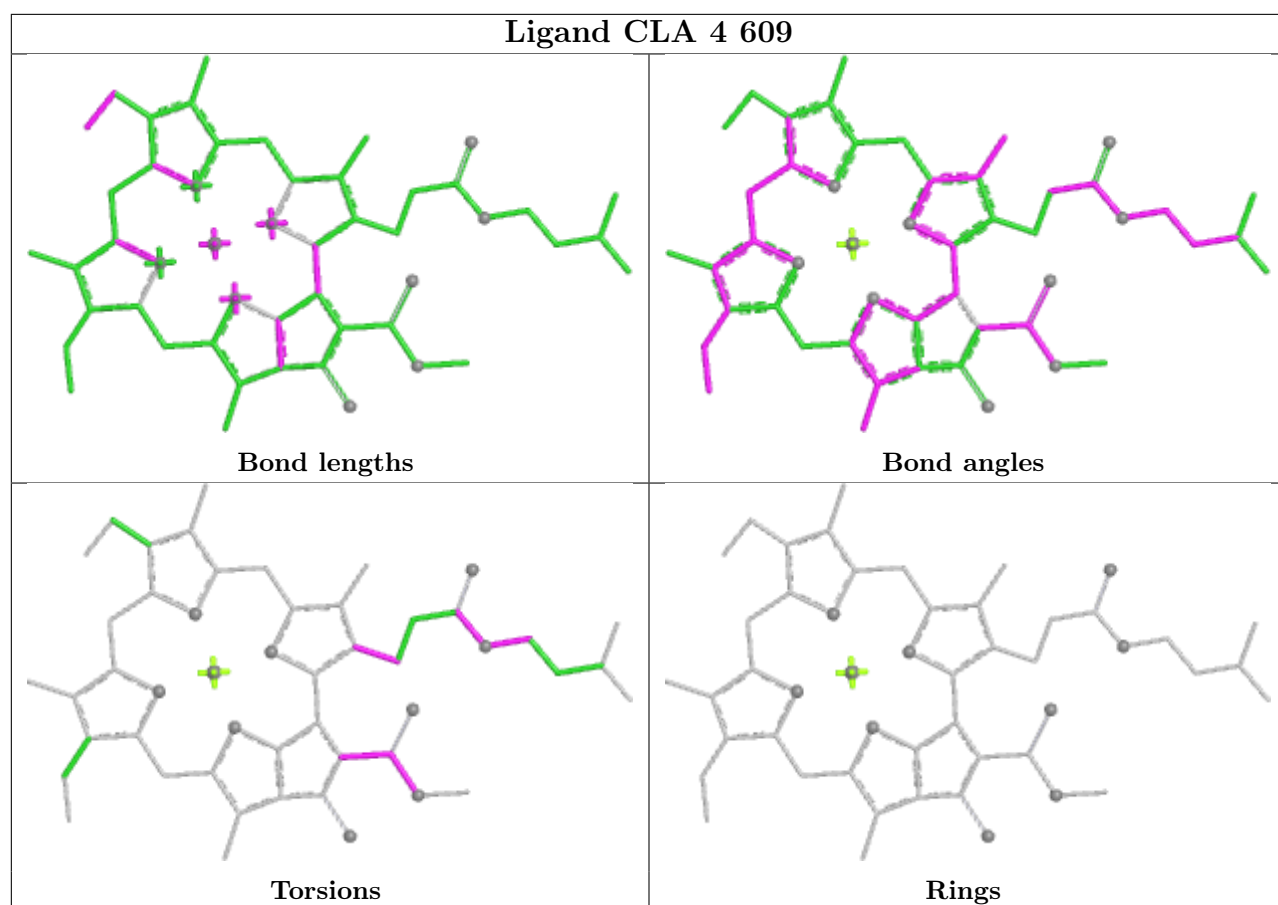
Bond angles

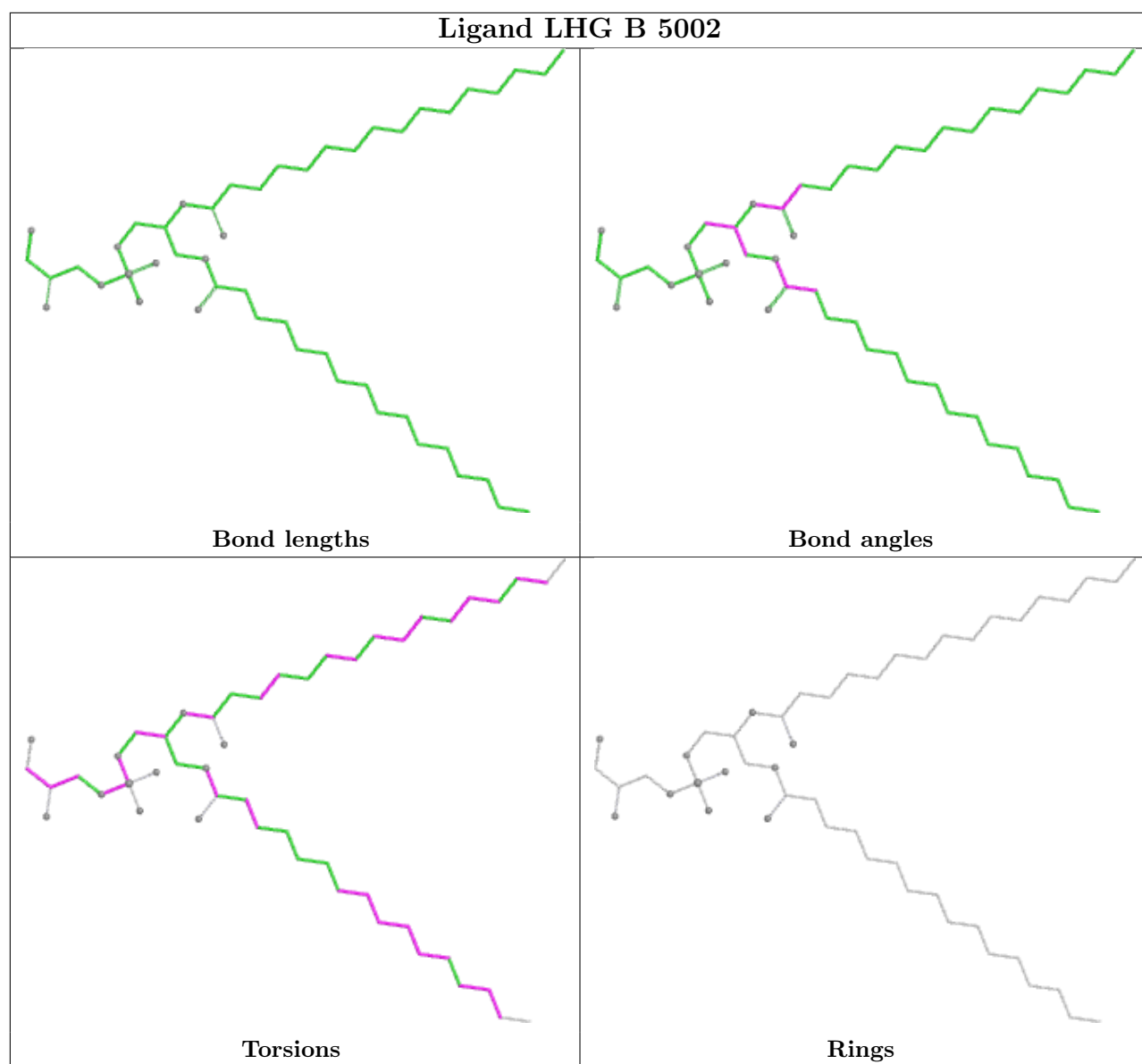


Torsions

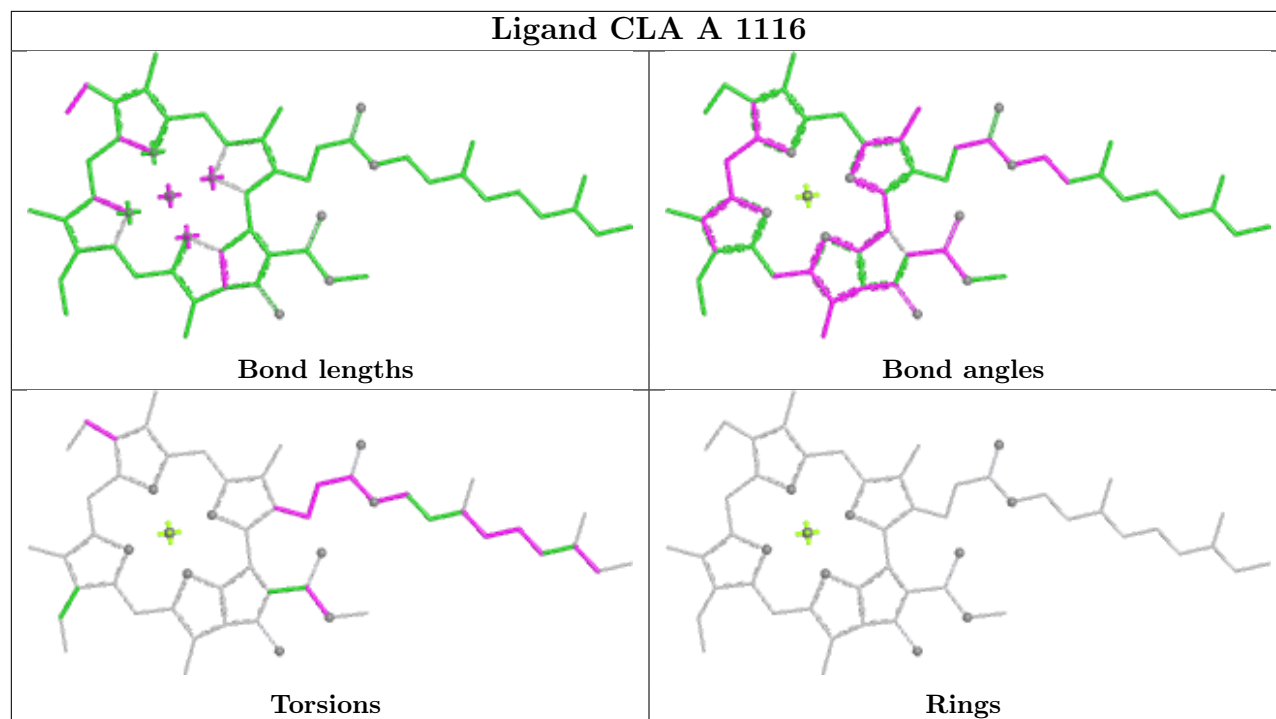


Rings

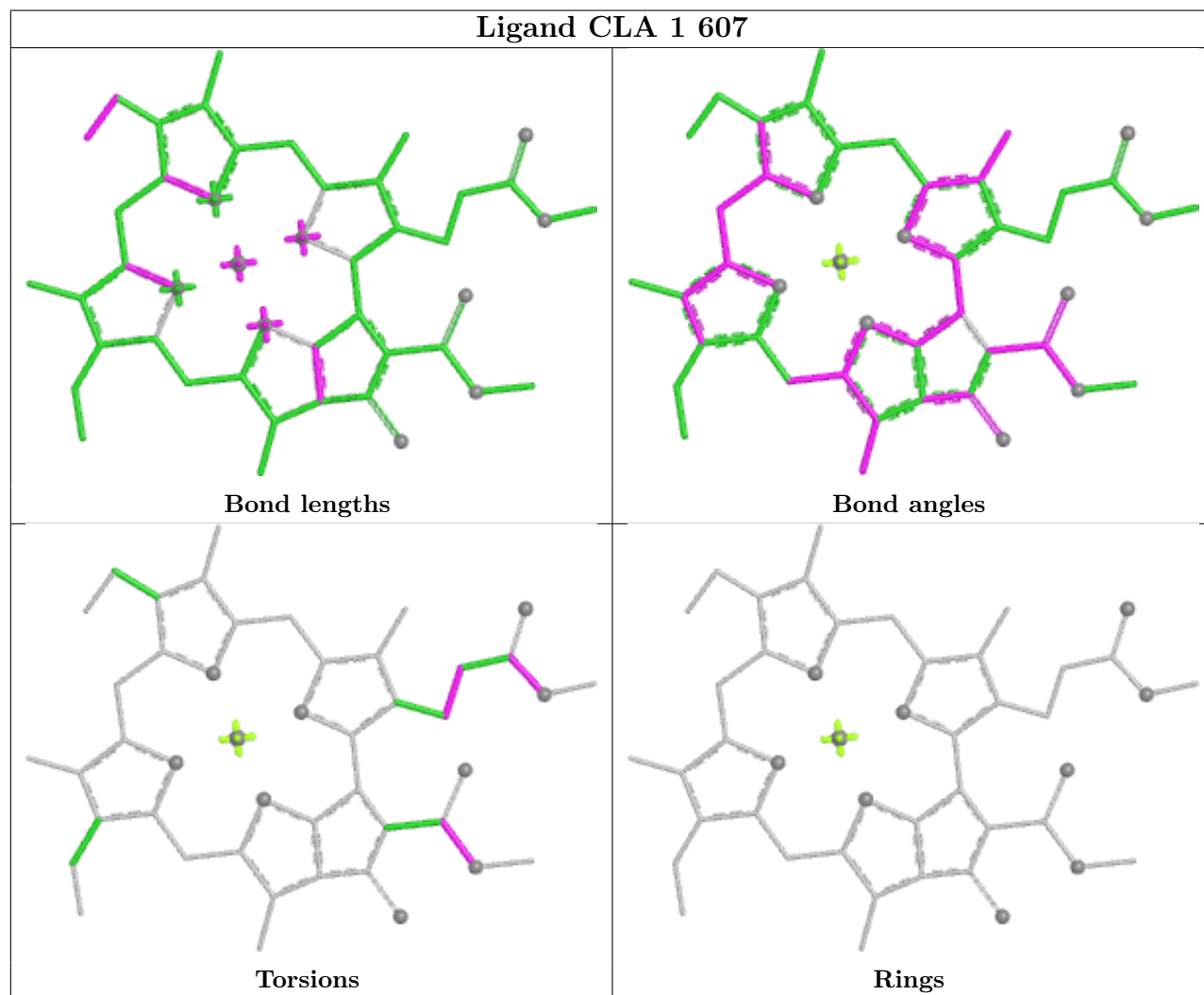




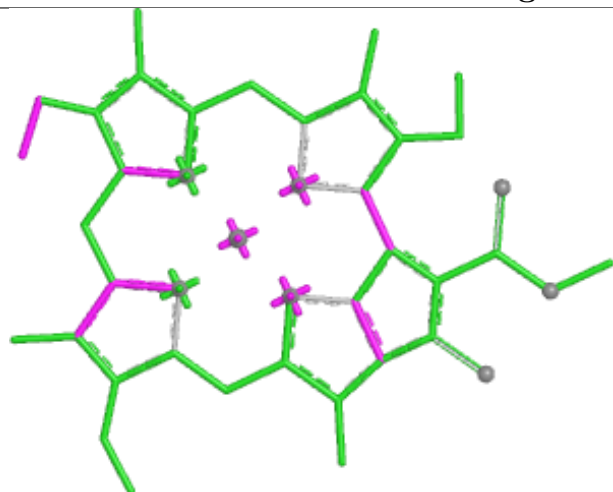
Ligand CLA A 1116



Ligand CLA 1 607



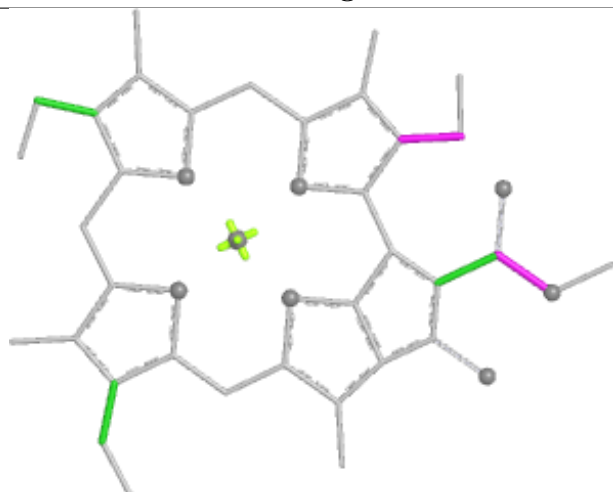
Ligand CLA 3 614



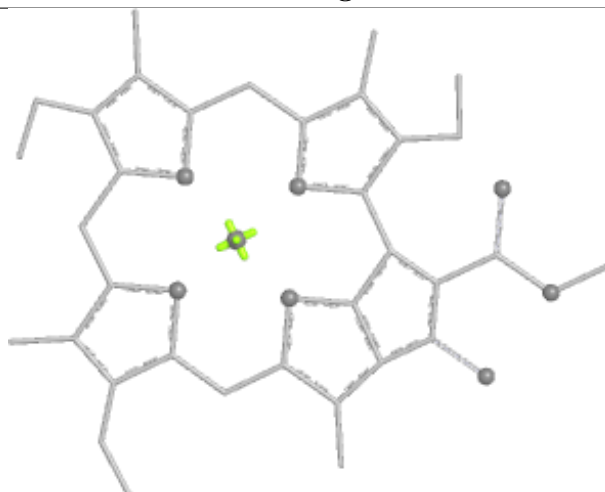
Bond lengths



Bond angles

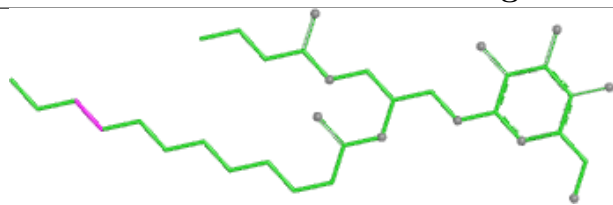


Torsions

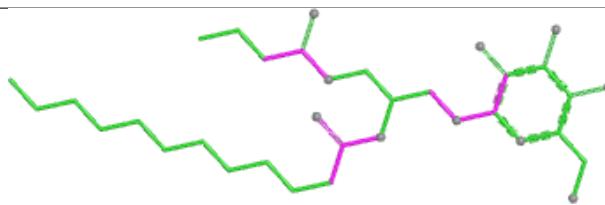


Rings

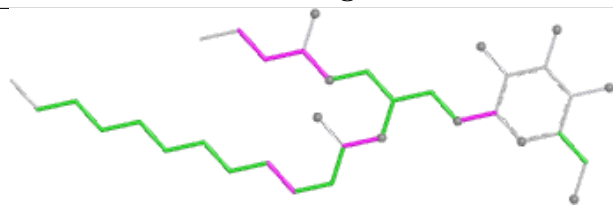
Ligand LMG B 5003



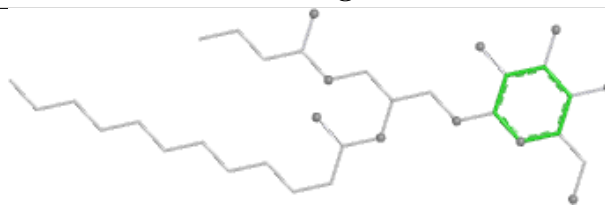
Bond lengths



Bond angles

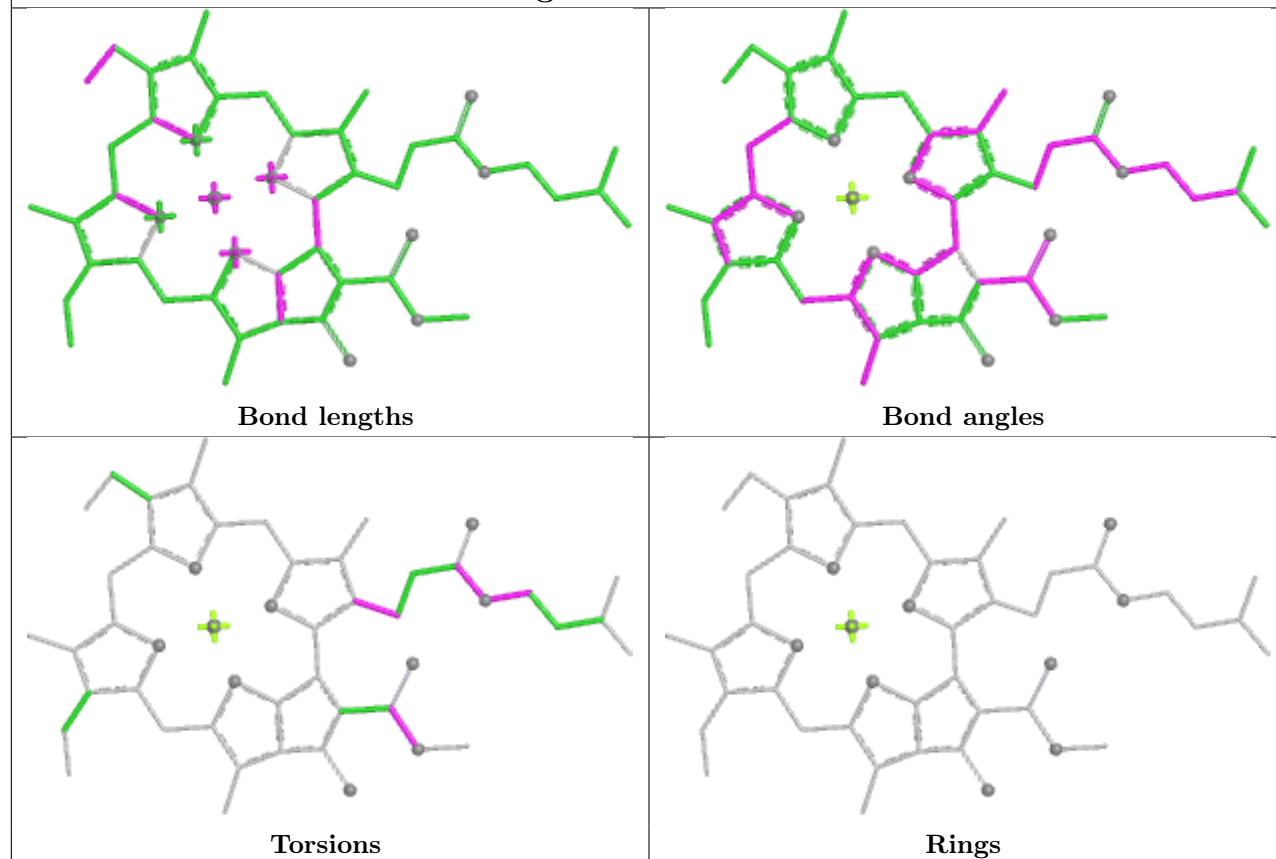


Torsions

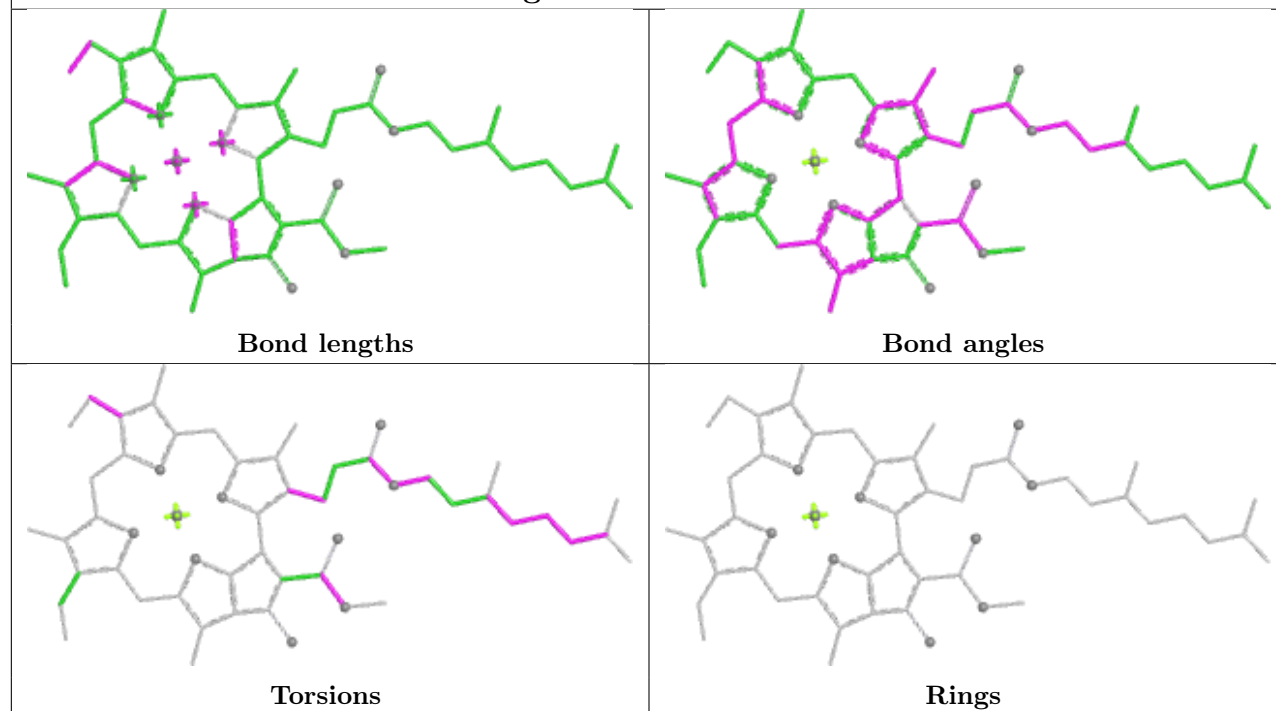


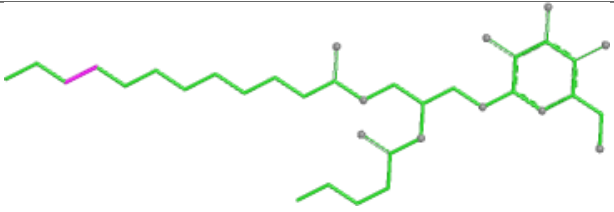
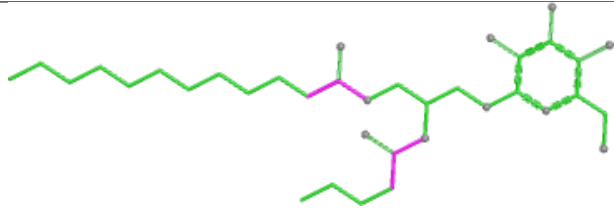
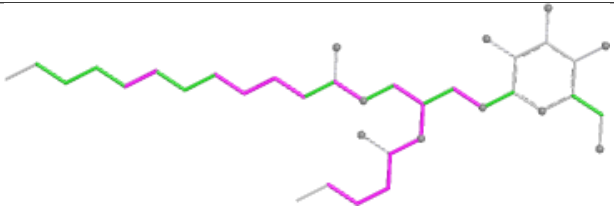
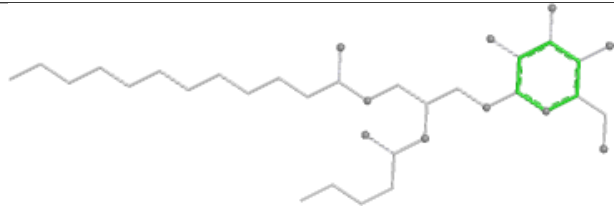
Rings

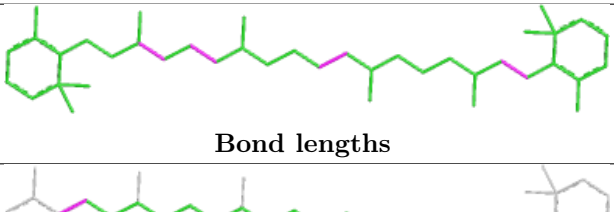
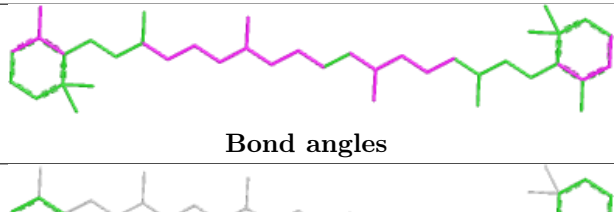
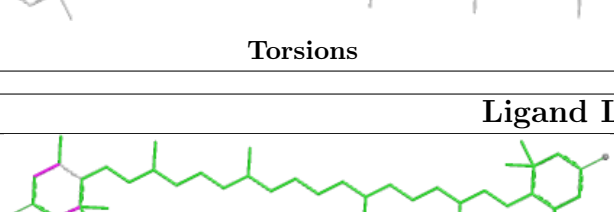
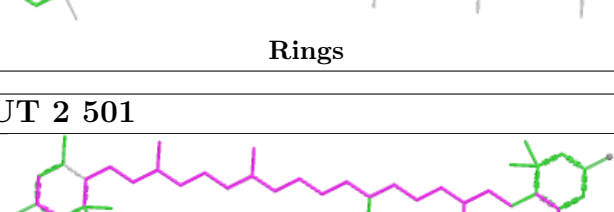
Ligand CLA 3 612

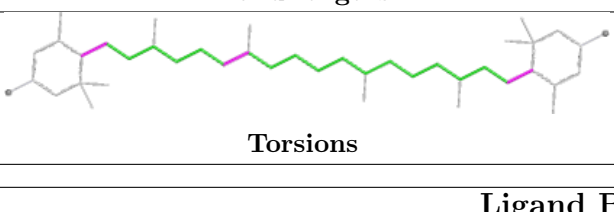
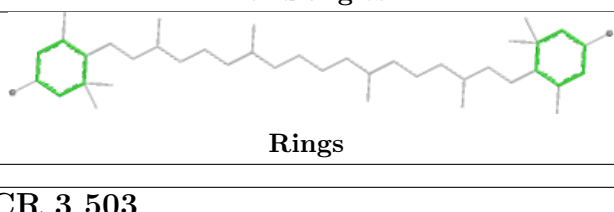
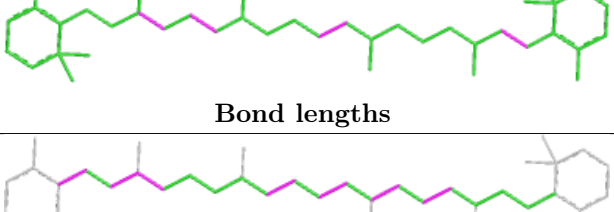
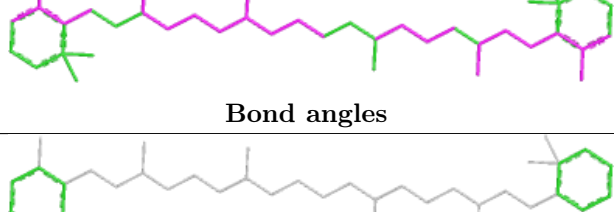


Ligand CLA B 1232

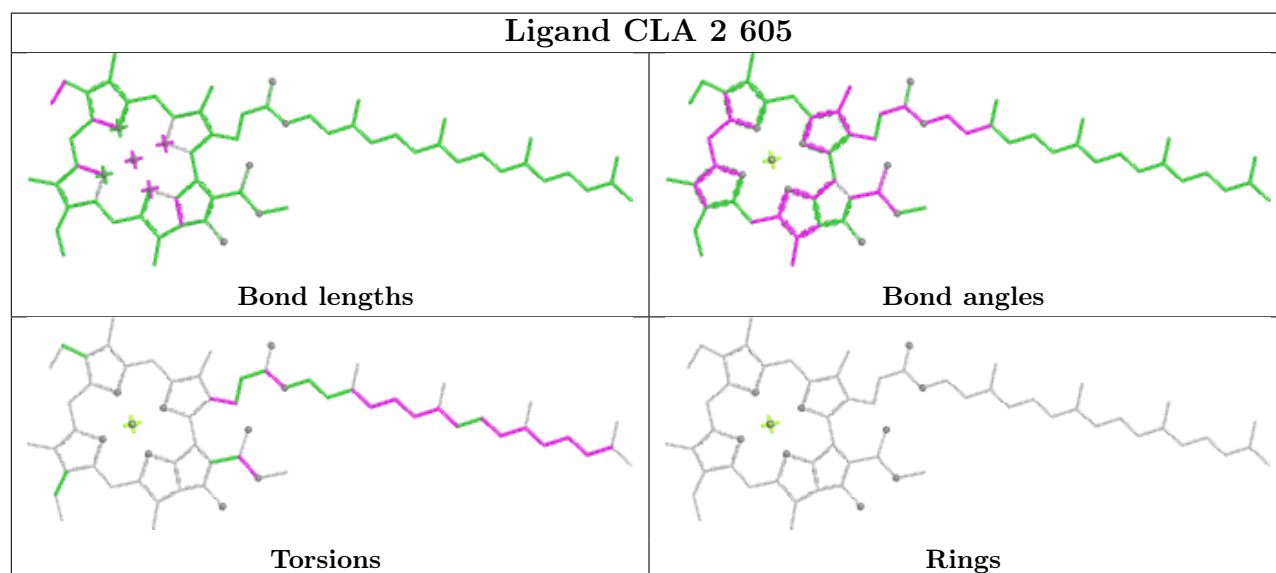
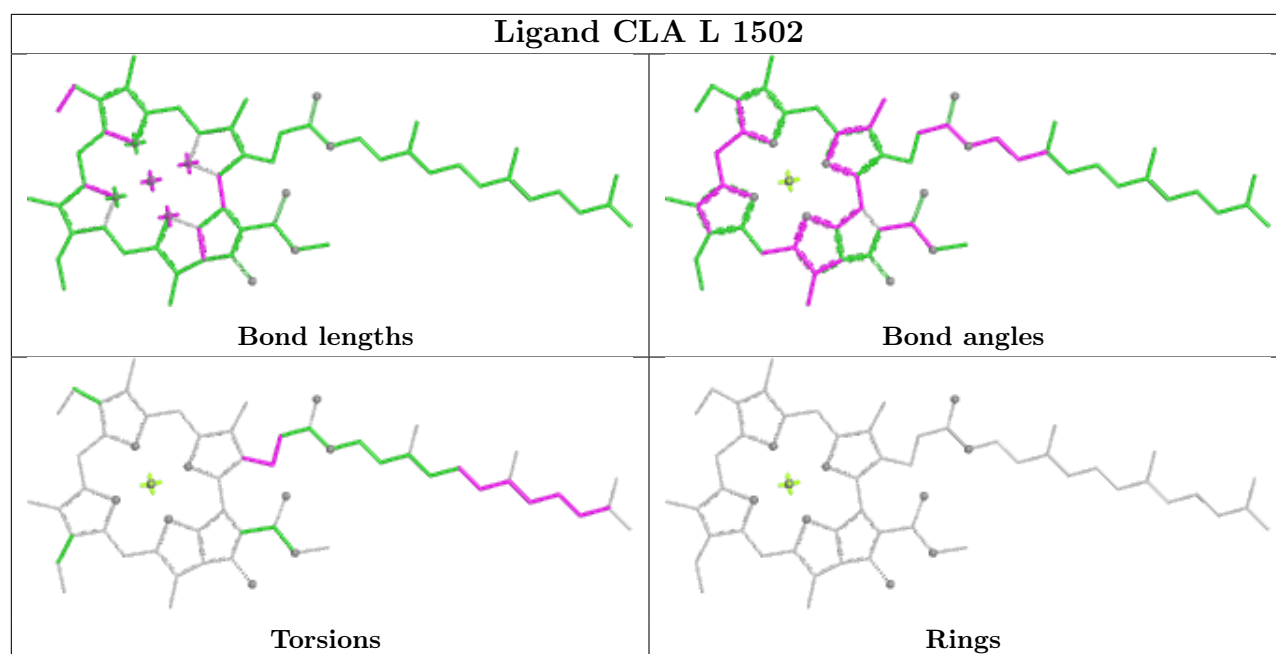


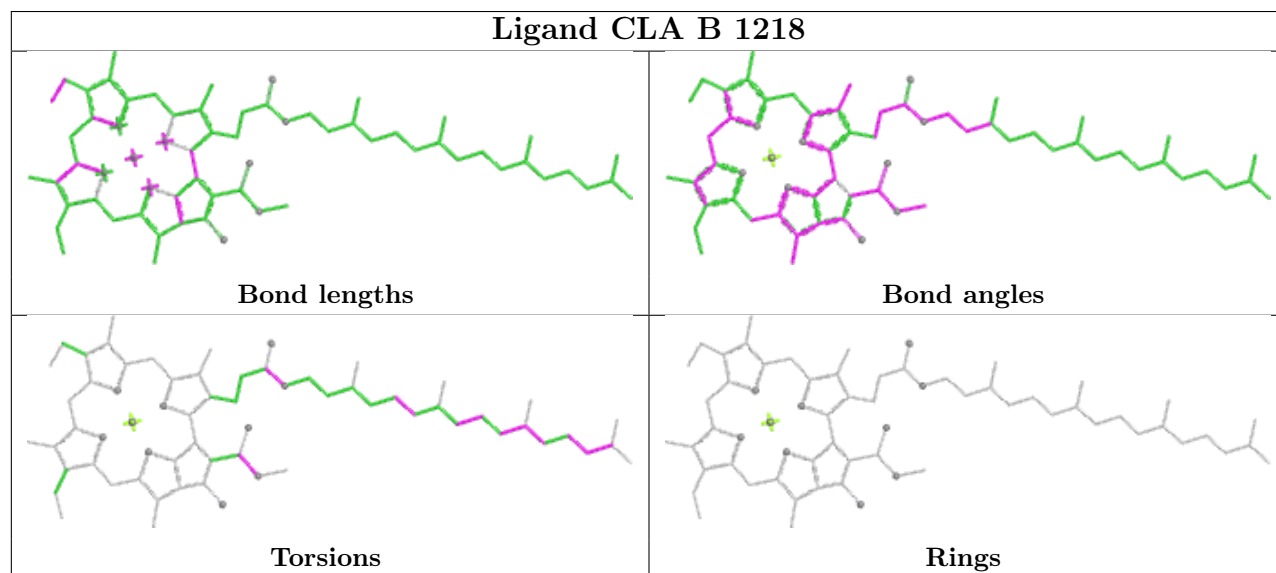
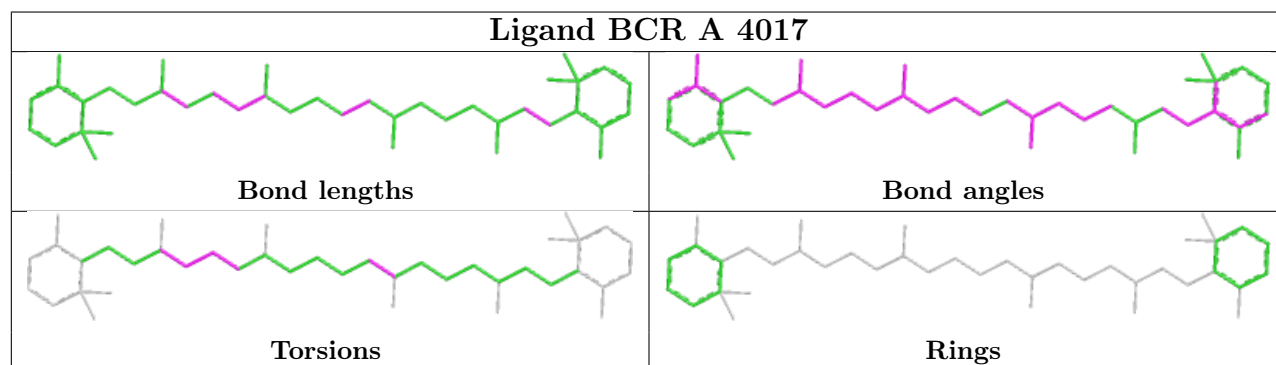
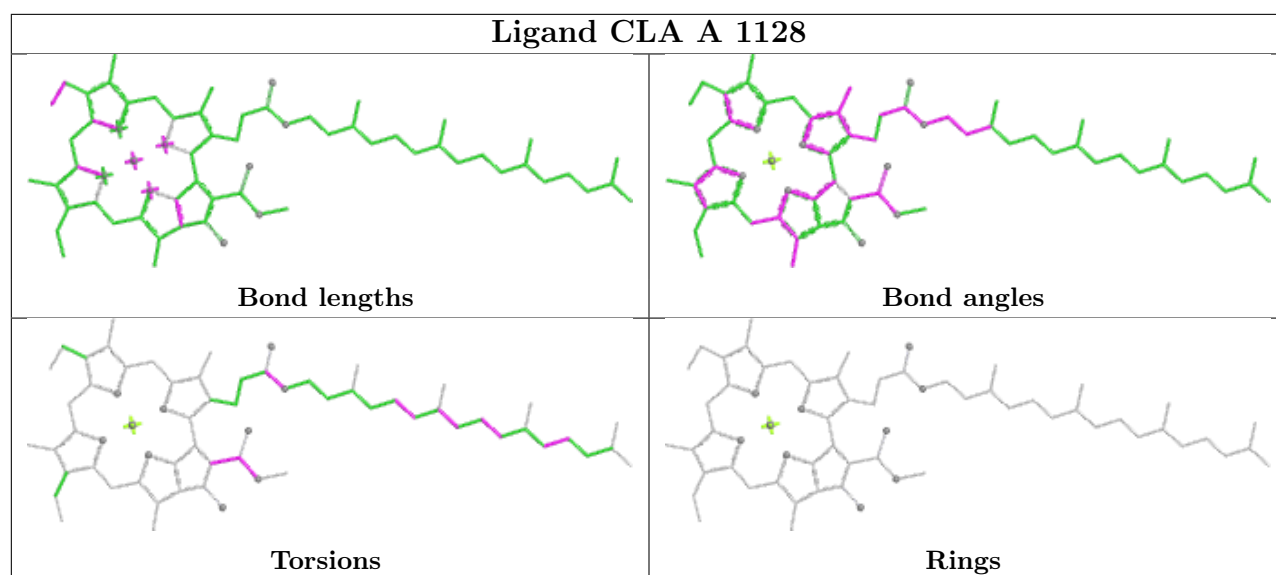
Ligand LMG F 5003	
	
Bond lengths	Bond angles
	
Torsions	Rings

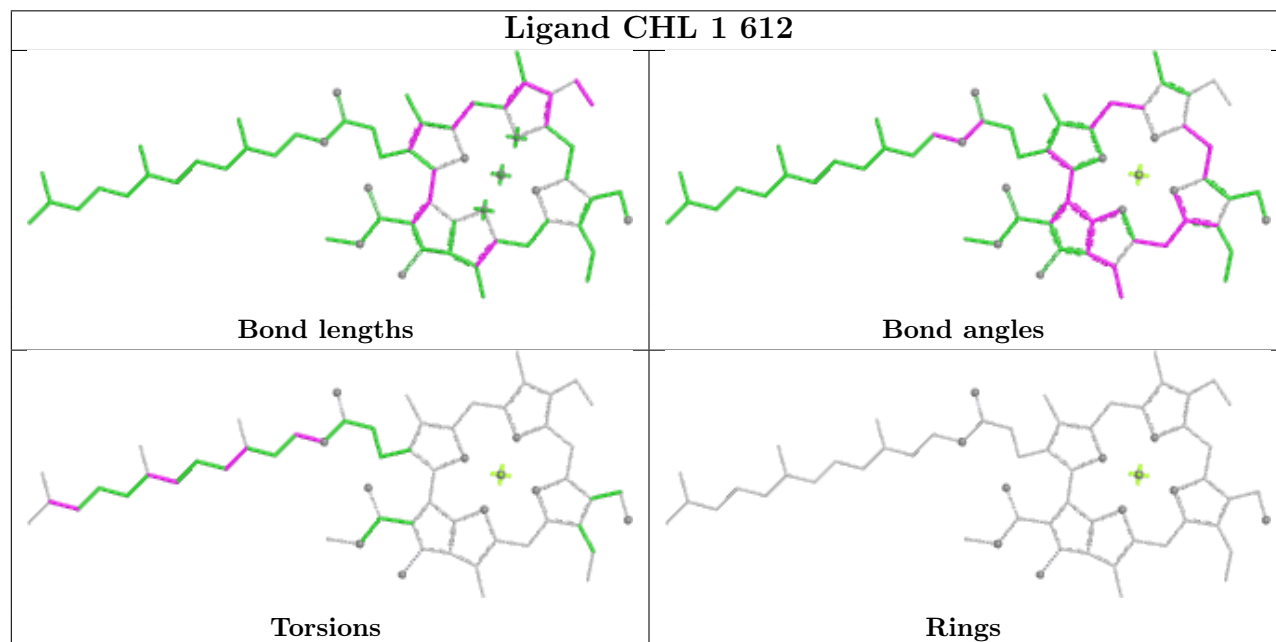
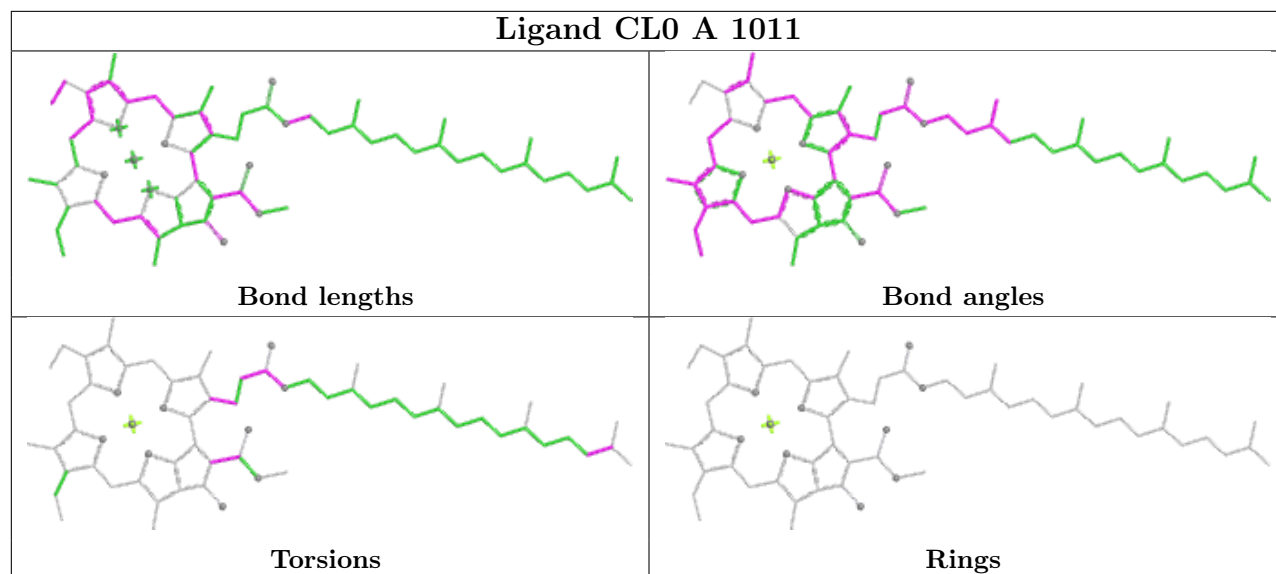
Ligand BCR A 4003	
	
Bond lengths	Bond angles
	
Torsions	Rings

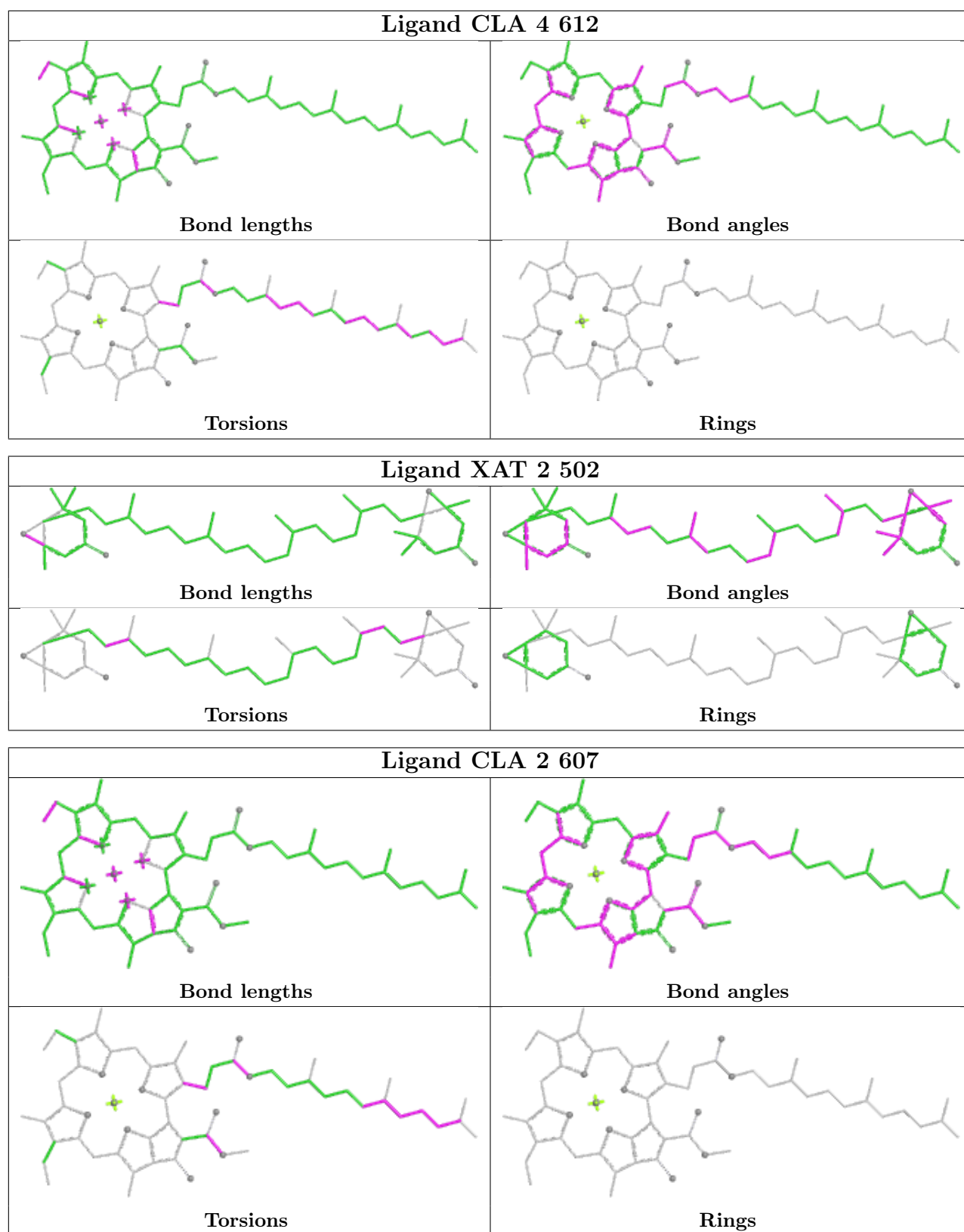
Ligand LUT 2 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

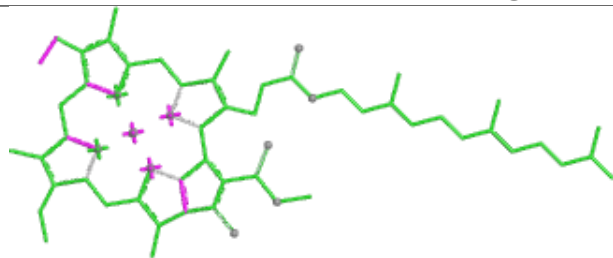
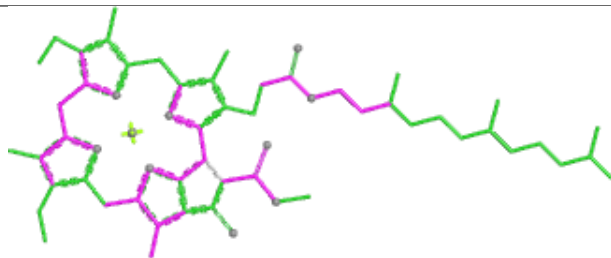
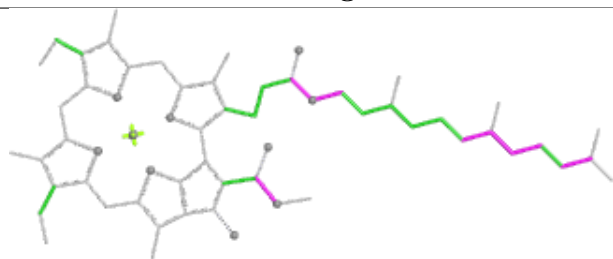
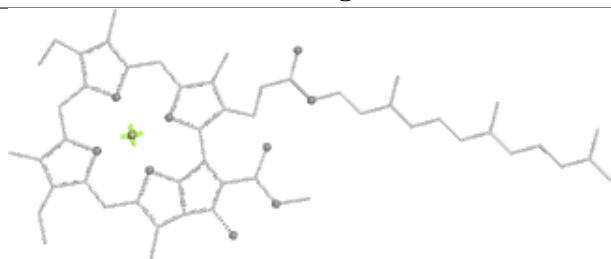
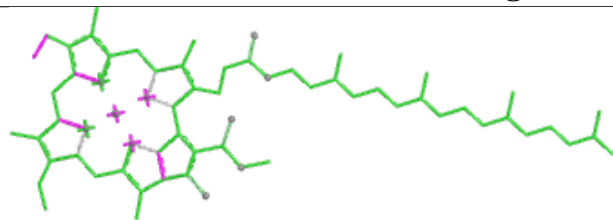
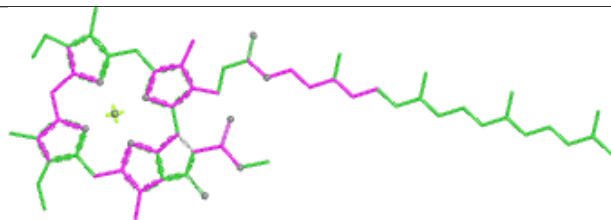
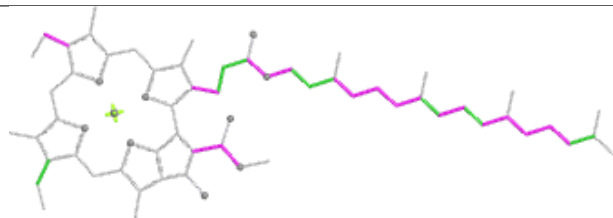
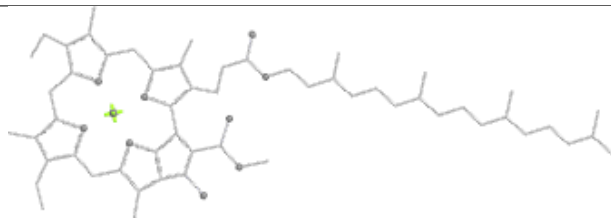
Ligand BCR 3 503	
	
Bond lengths	Bond angles
Torsions	Rings

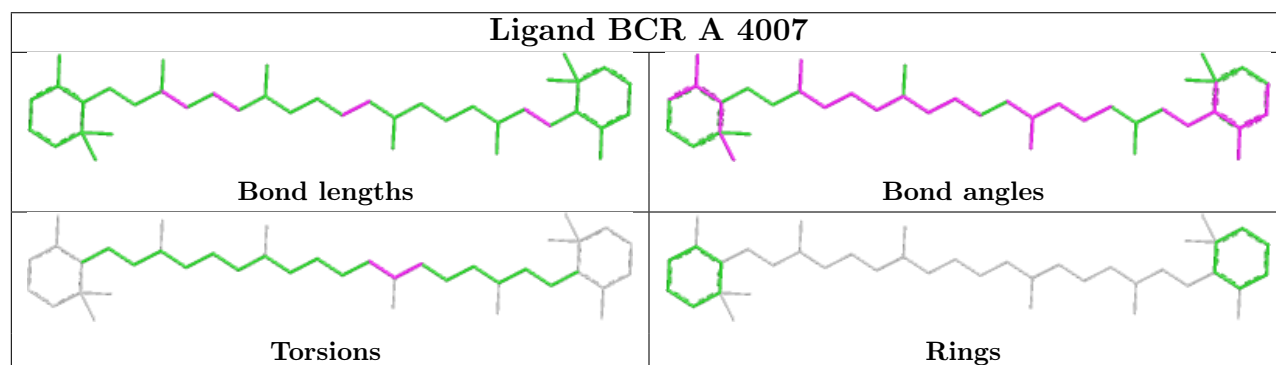
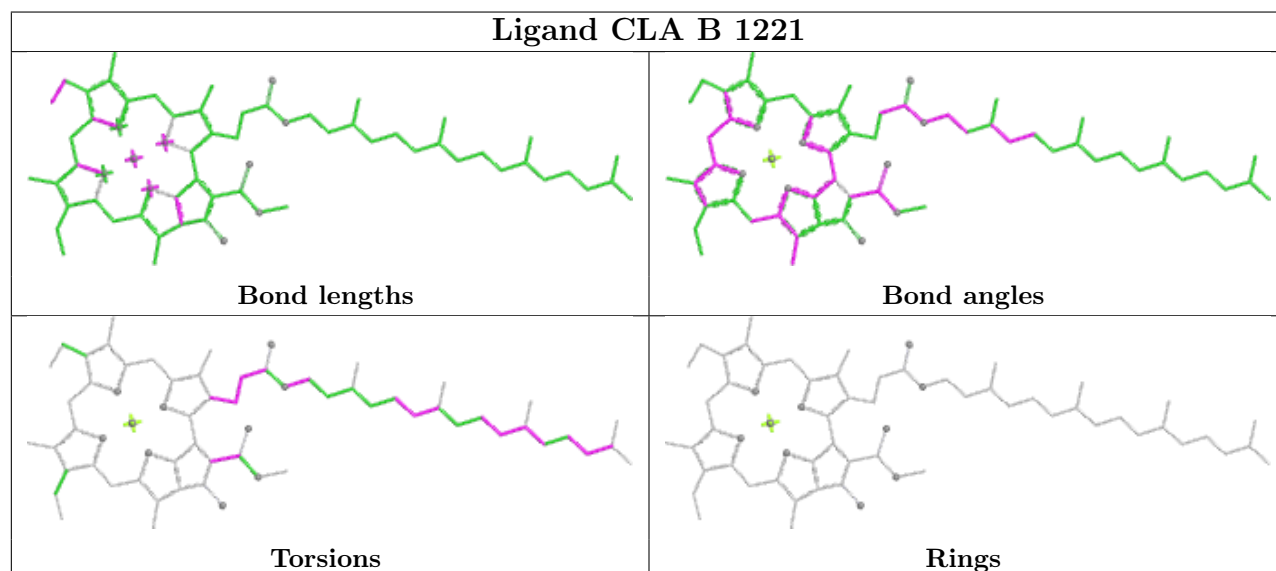
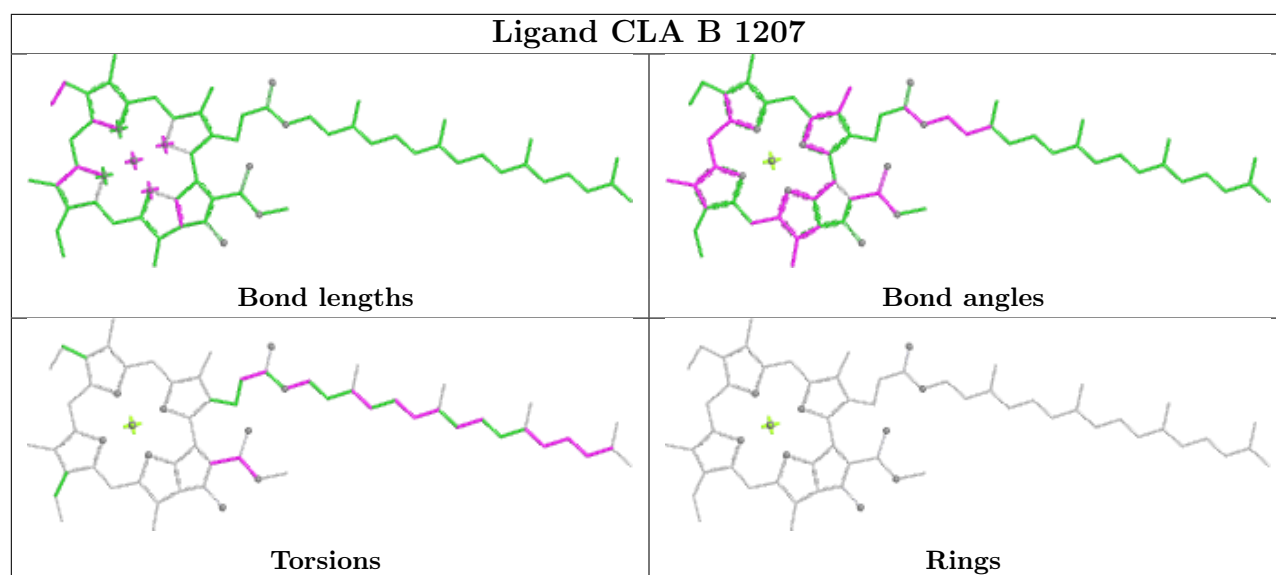


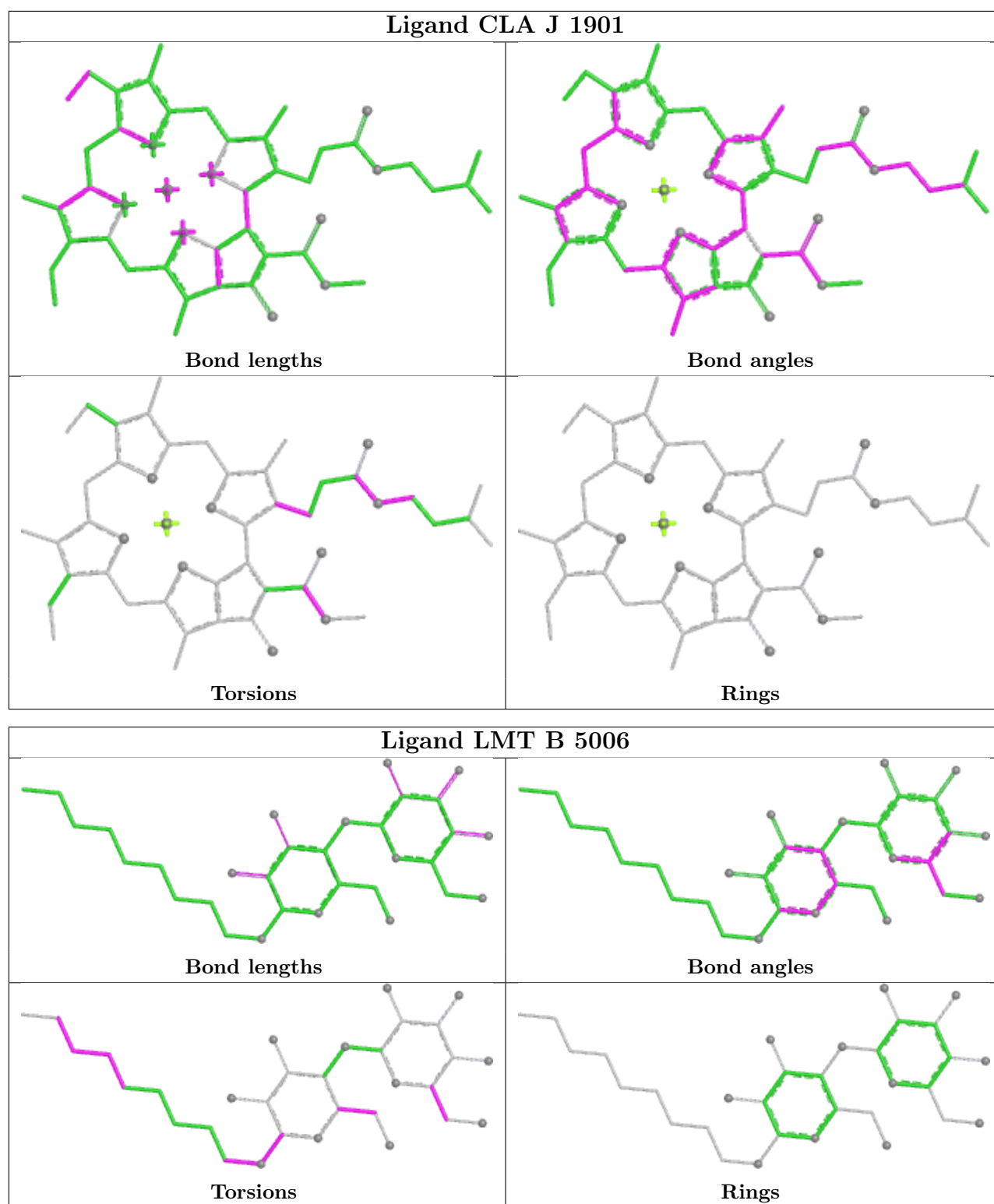


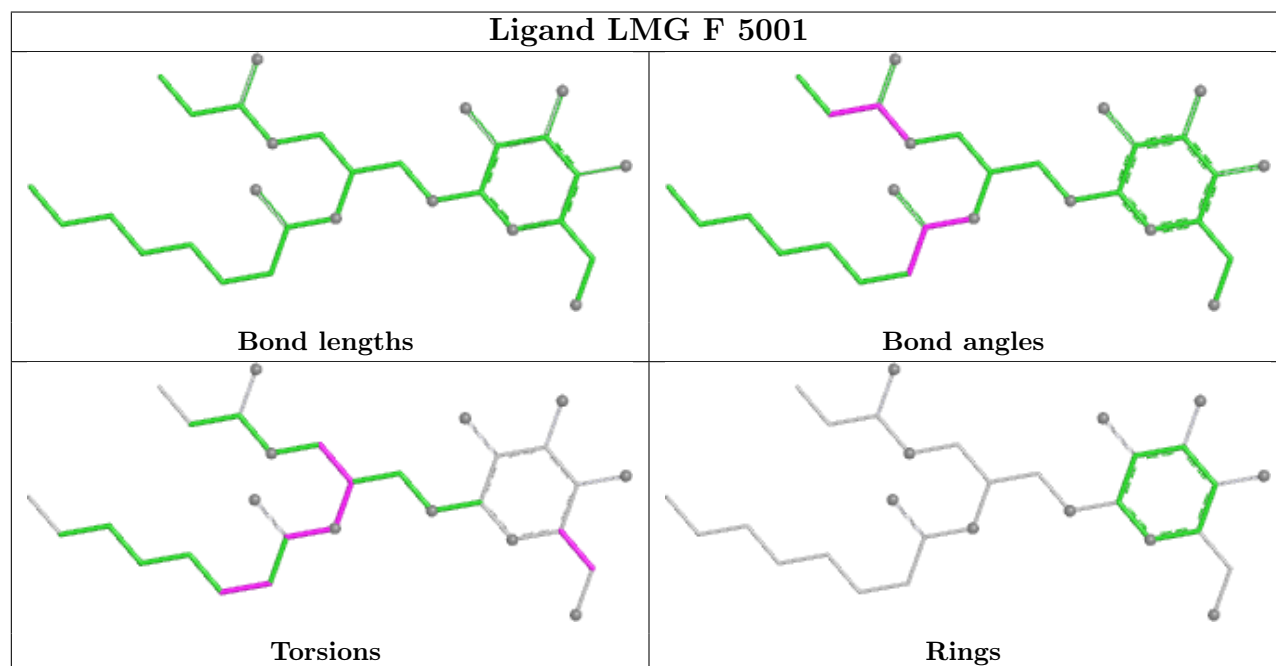
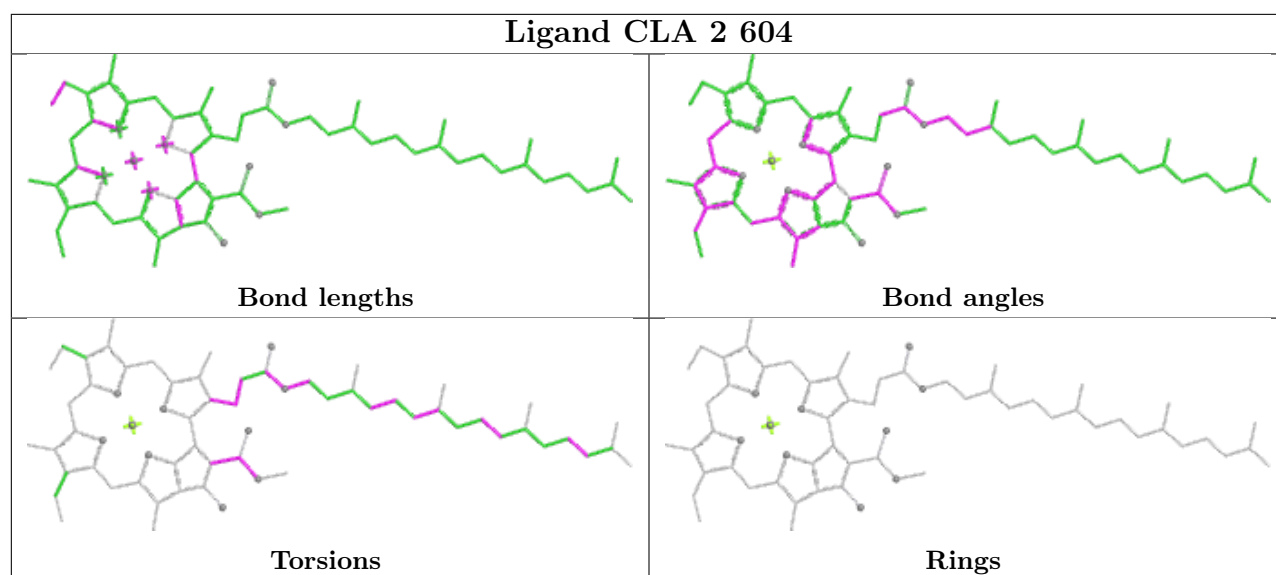


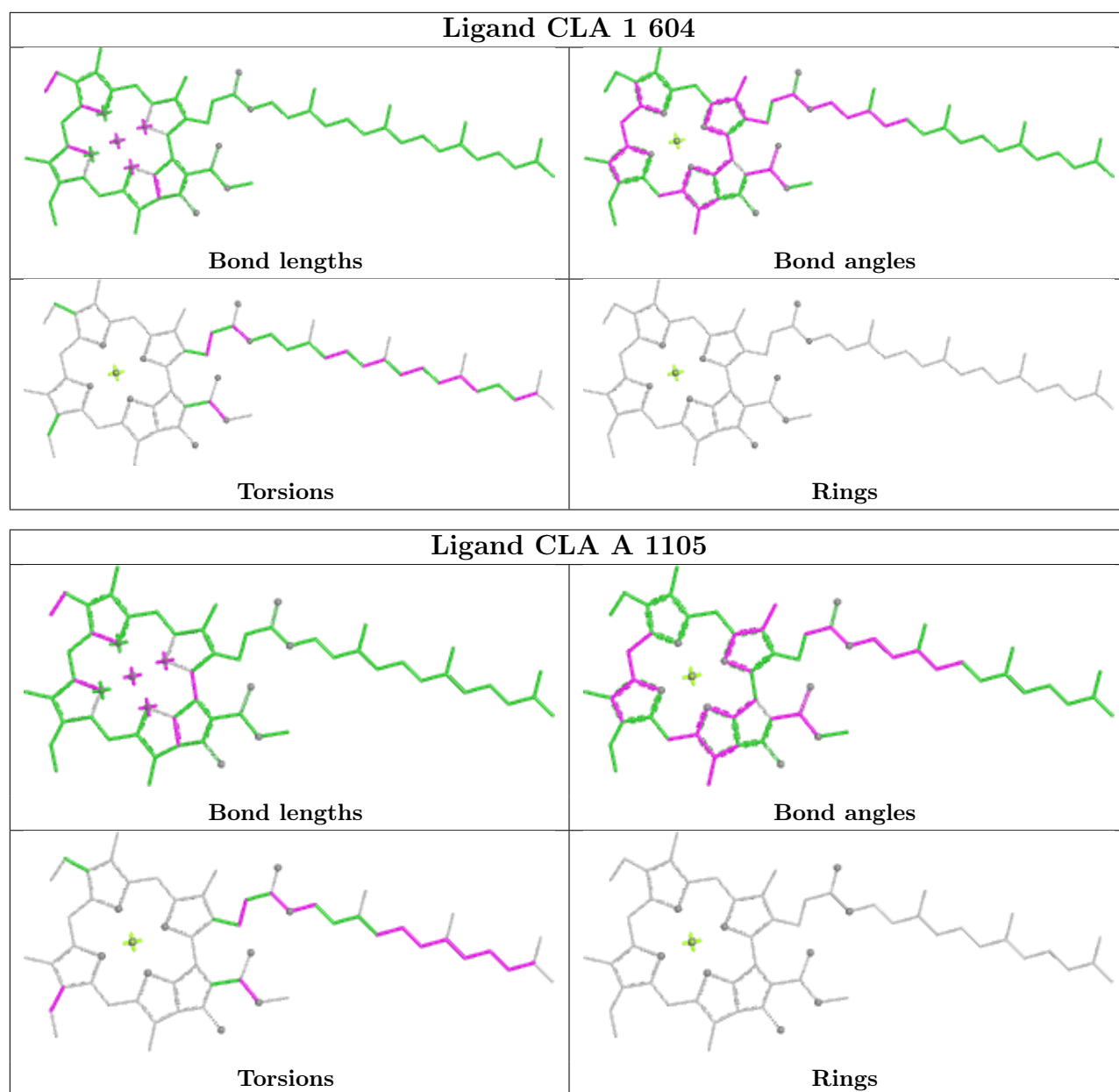


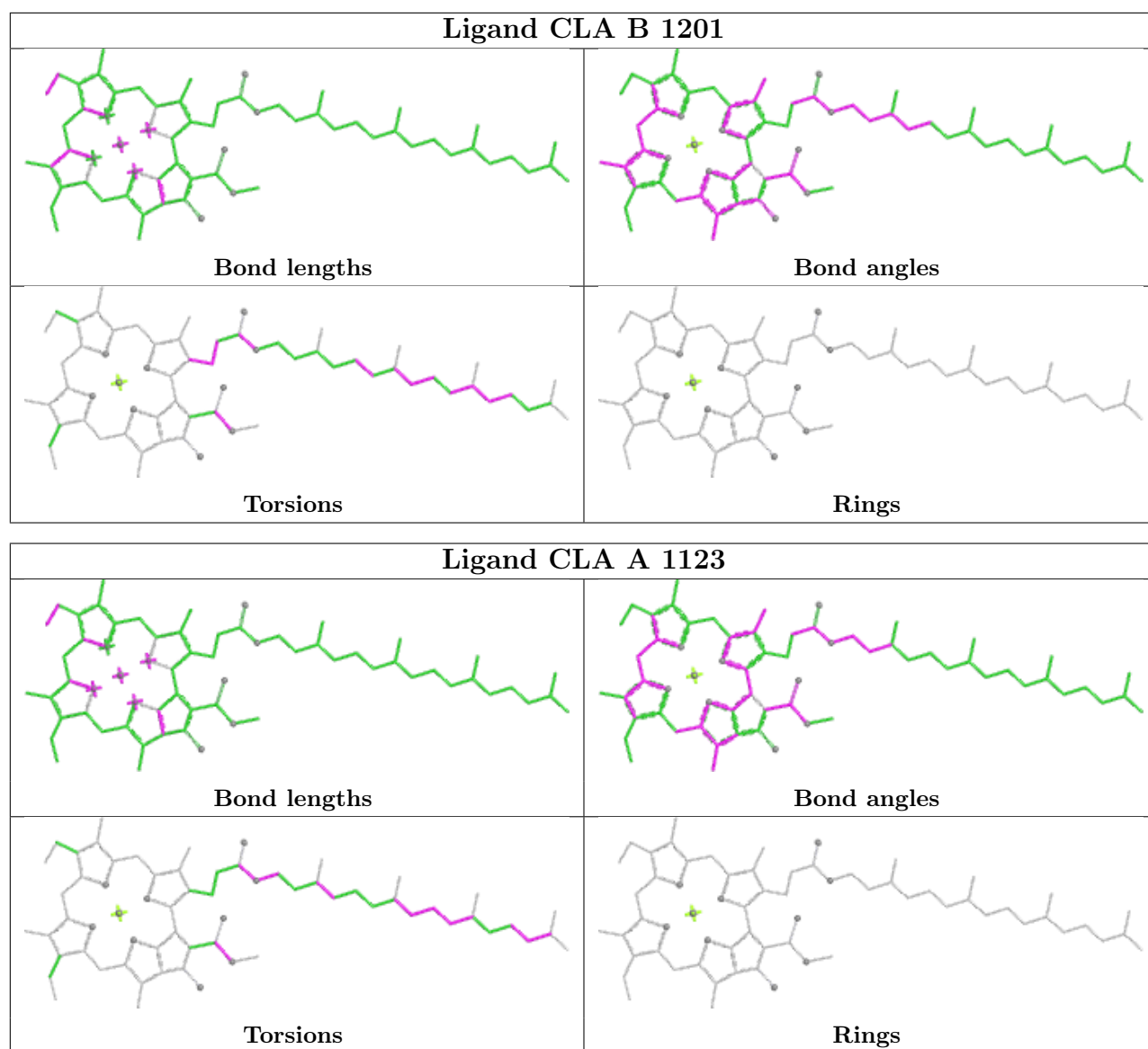
Ligand CLA B 1231**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1103****Bond lengths****Bond angles****Torsions****Rings**

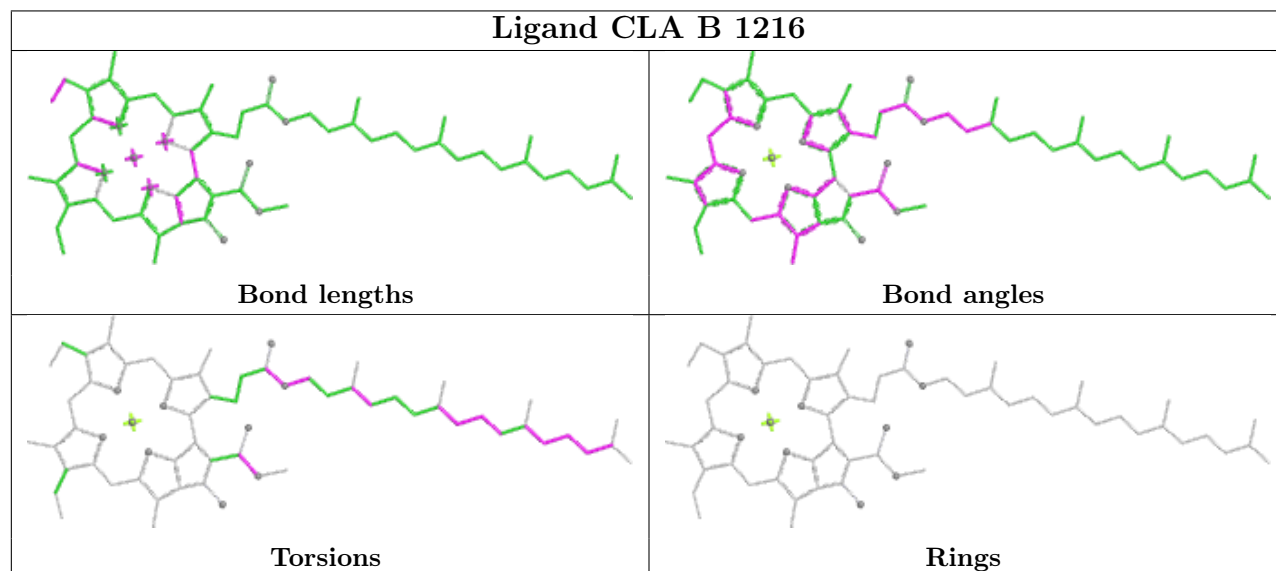
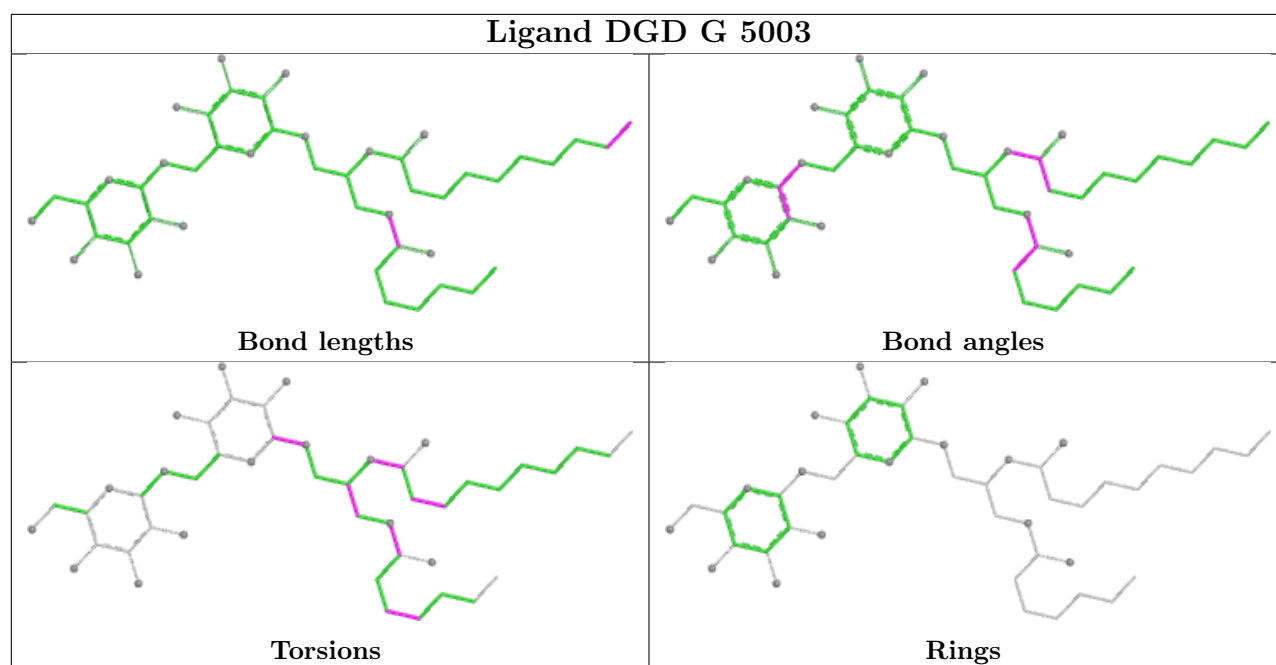


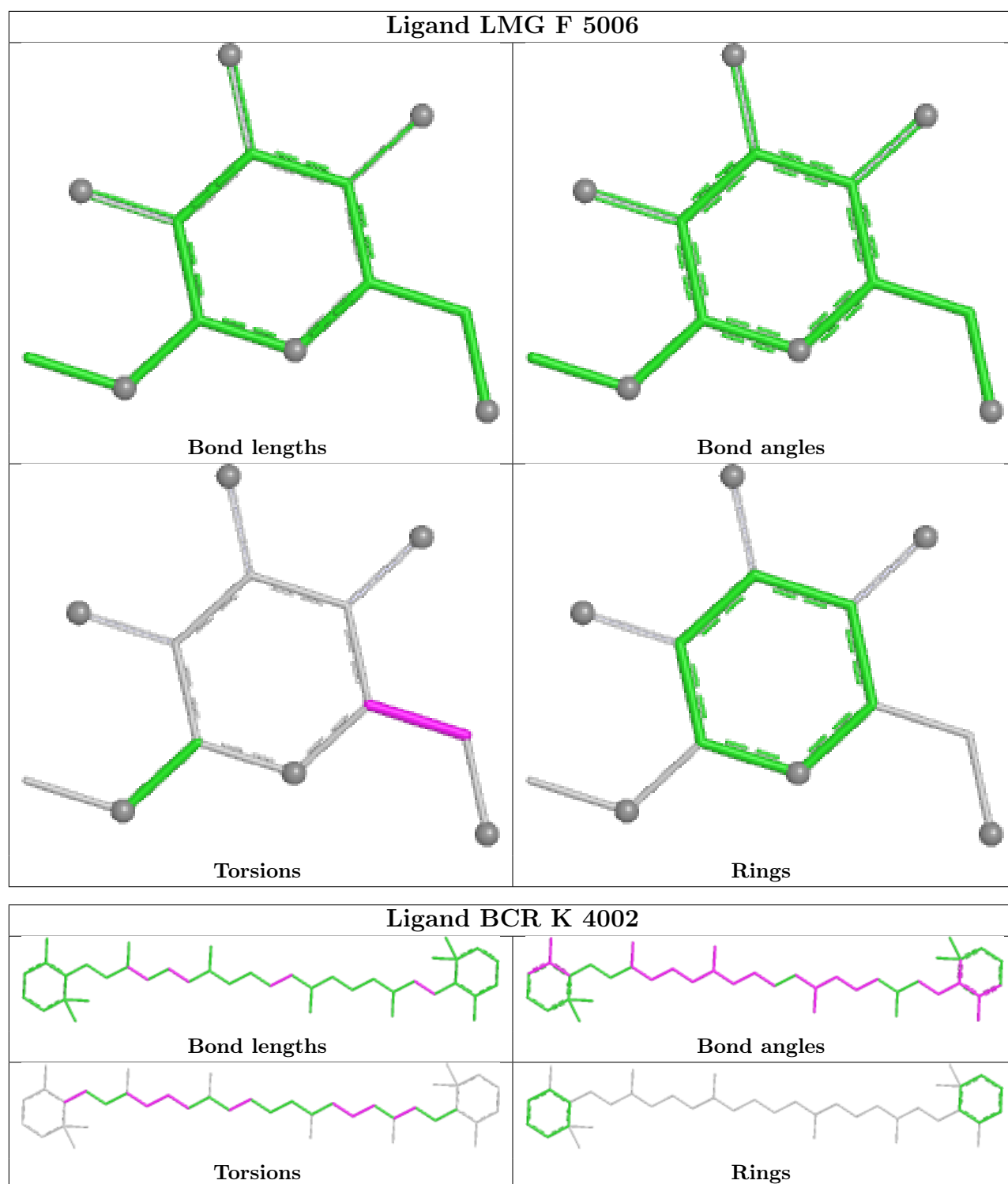


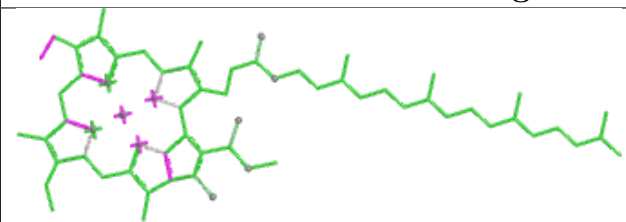
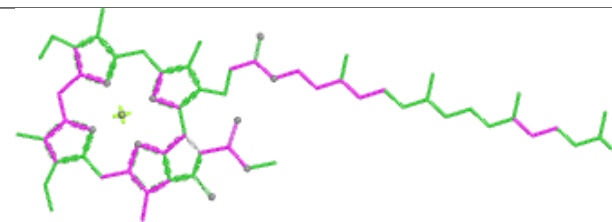
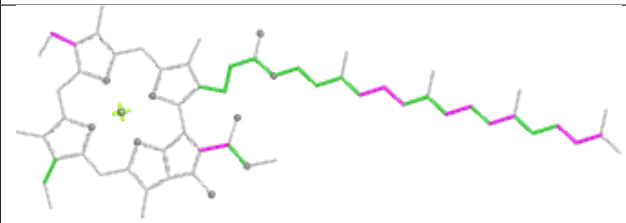
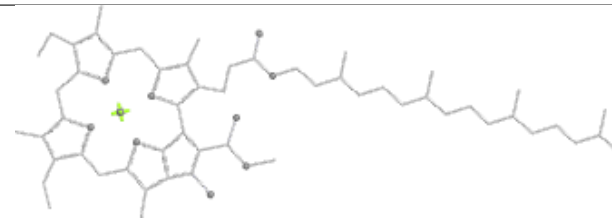


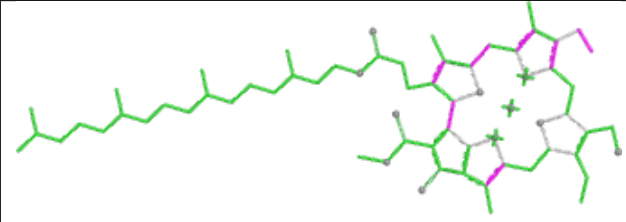
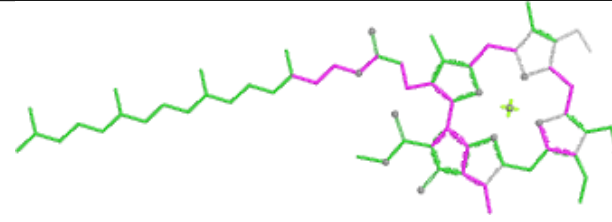
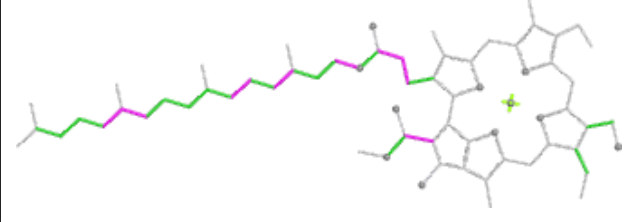
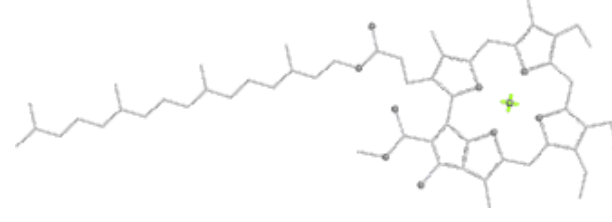


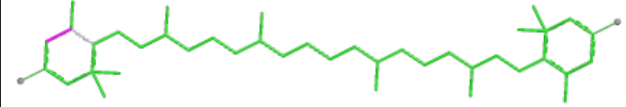
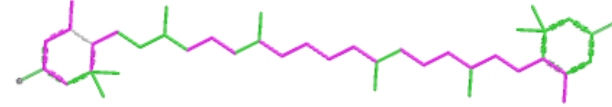
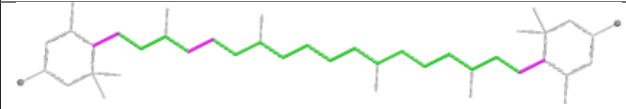
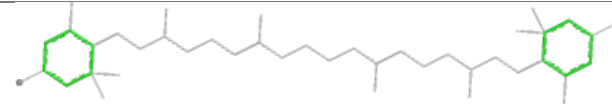


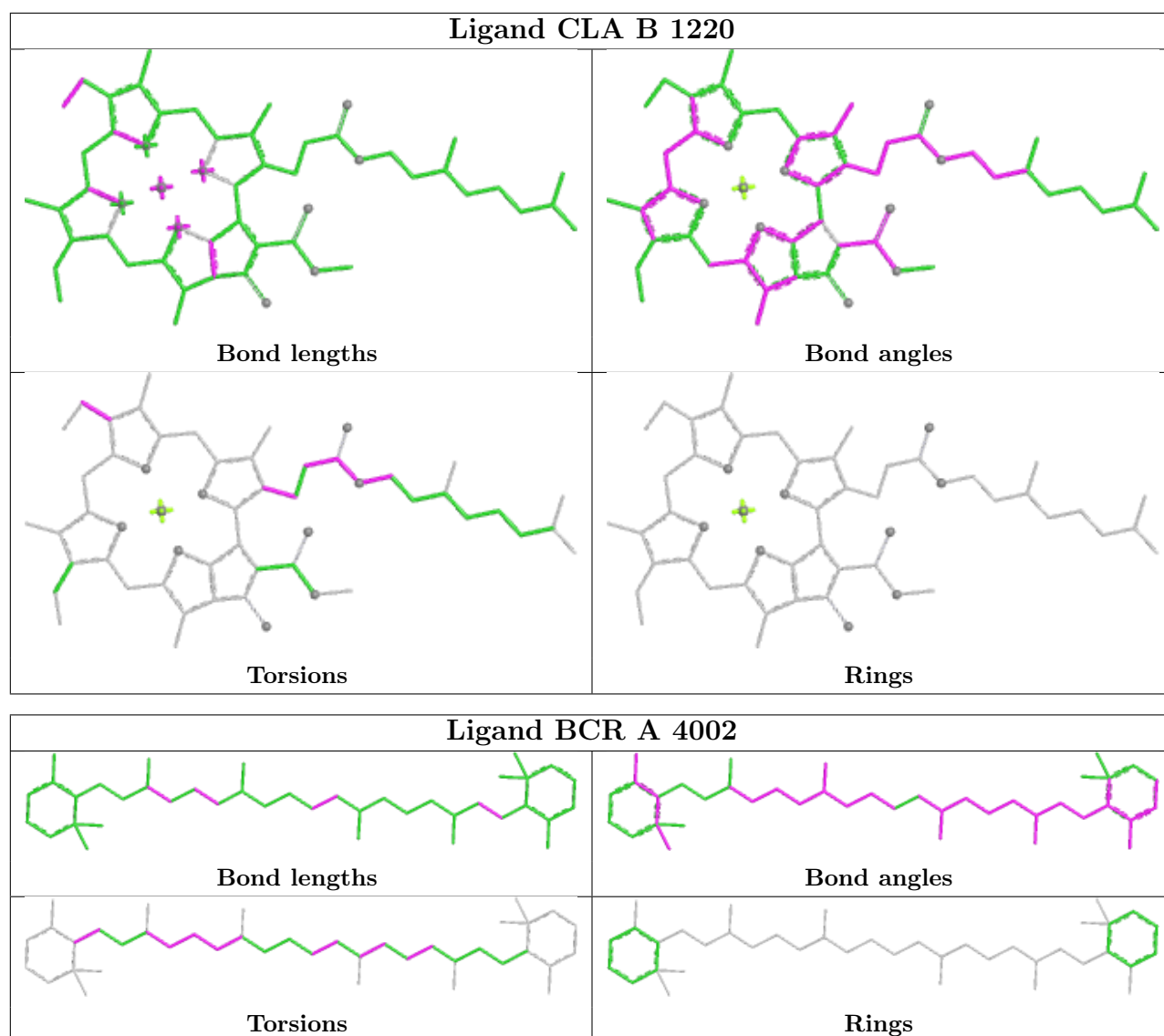




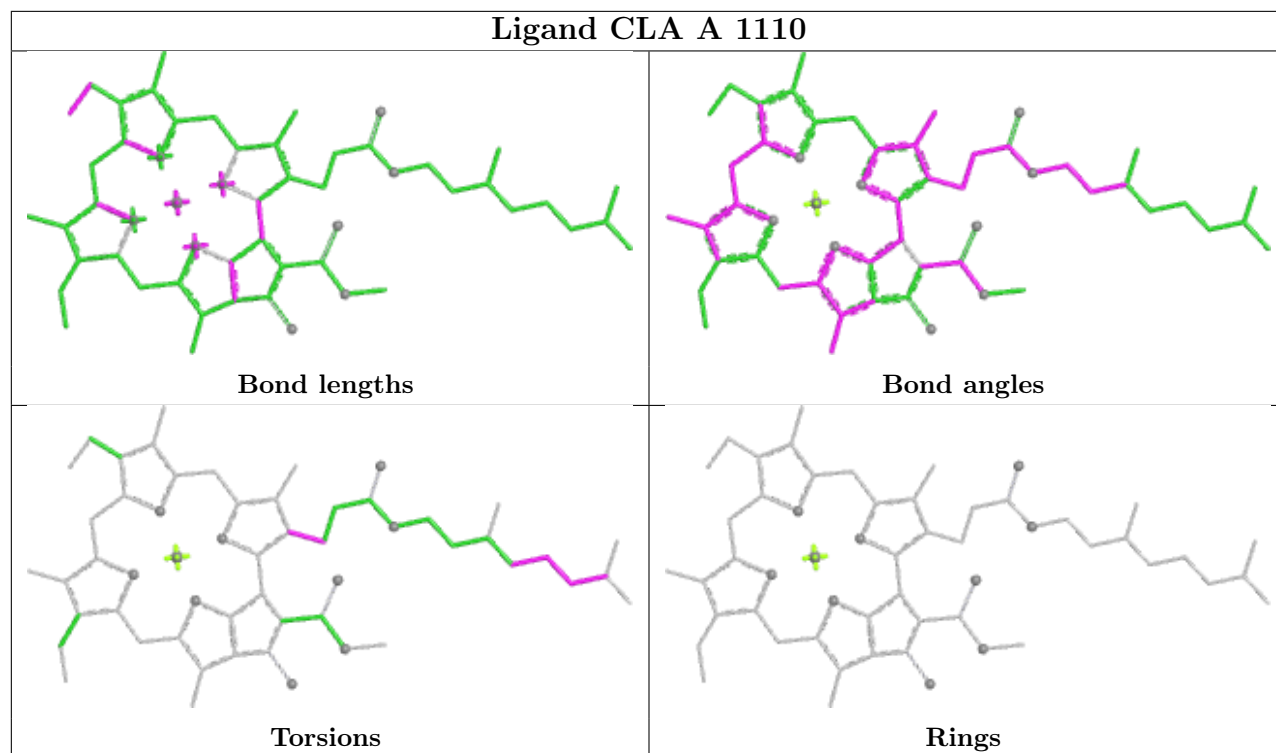
Ligand CLA B 1205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL 3 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

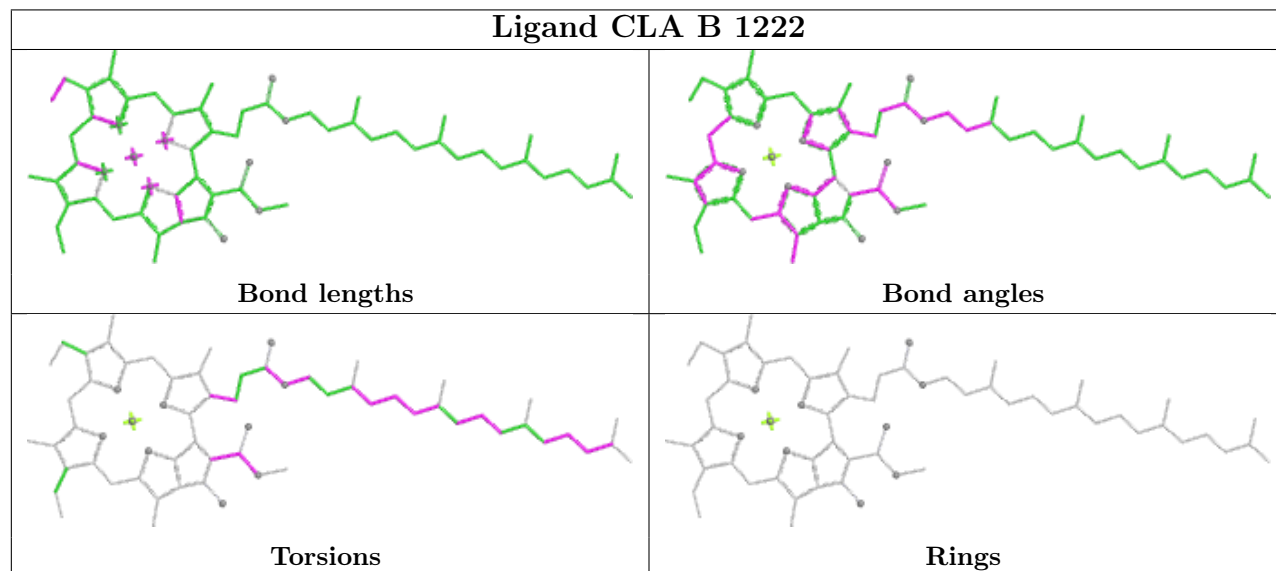
Ligand LUT 3 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

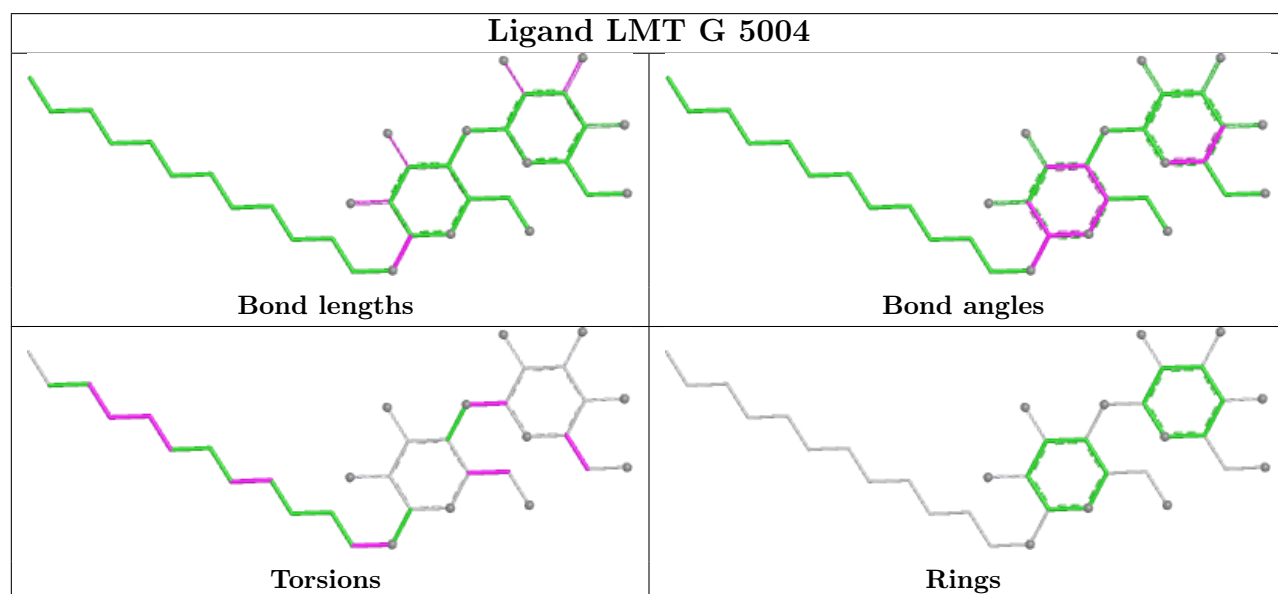
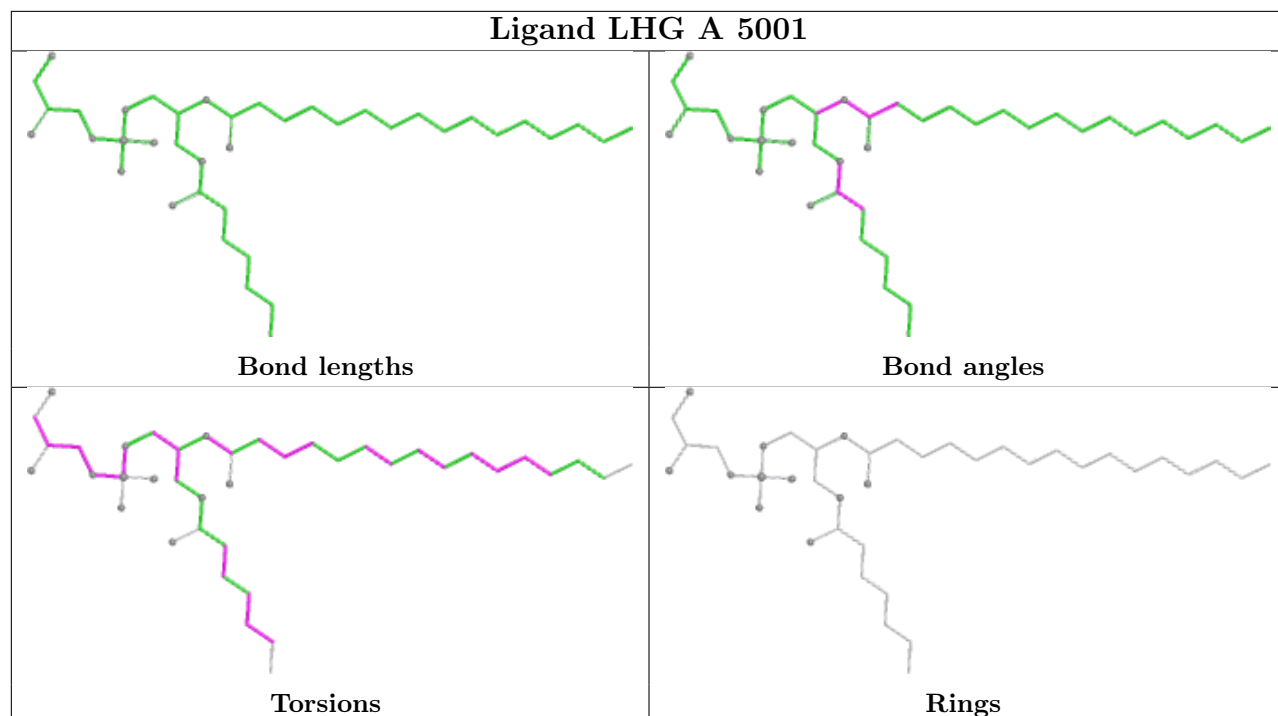


Ligand CLA A 1110

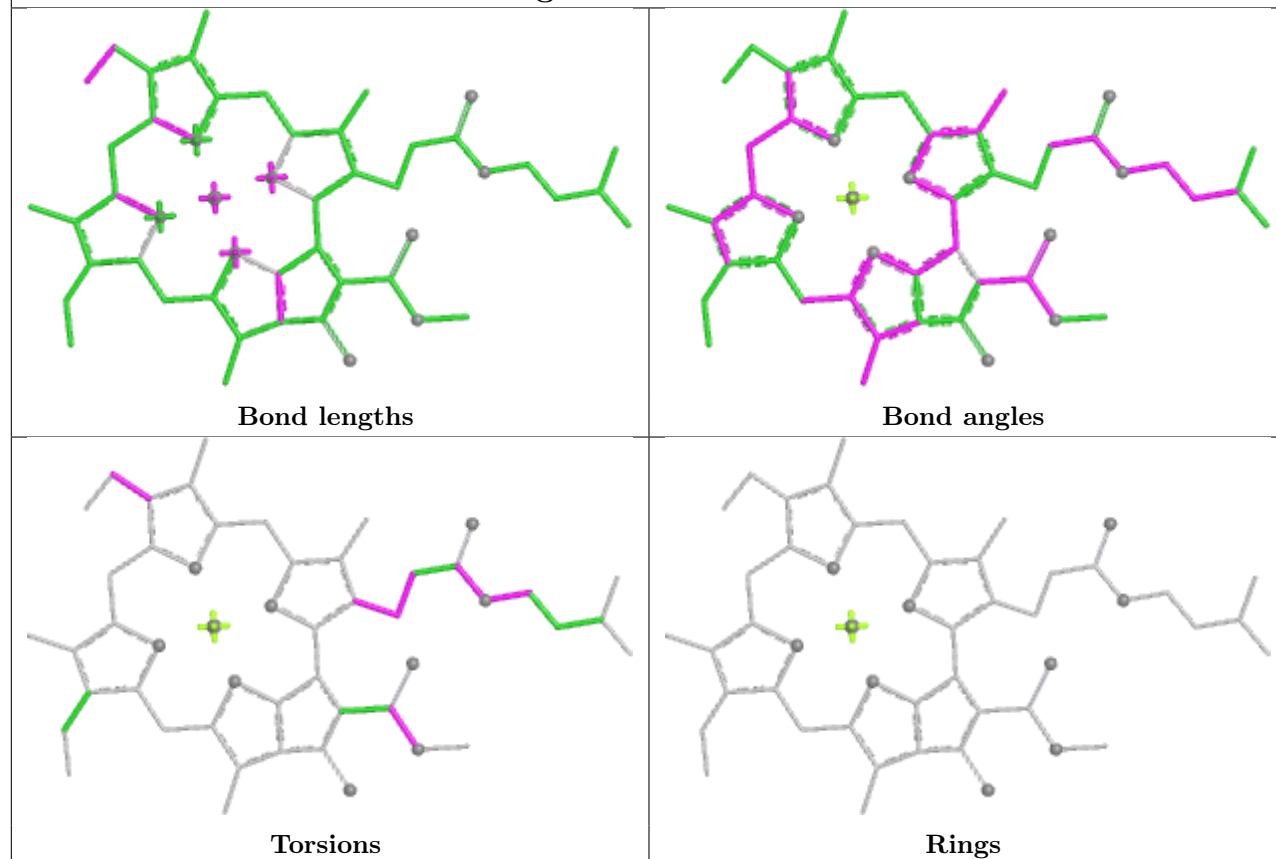


Ligand CLA B 1222

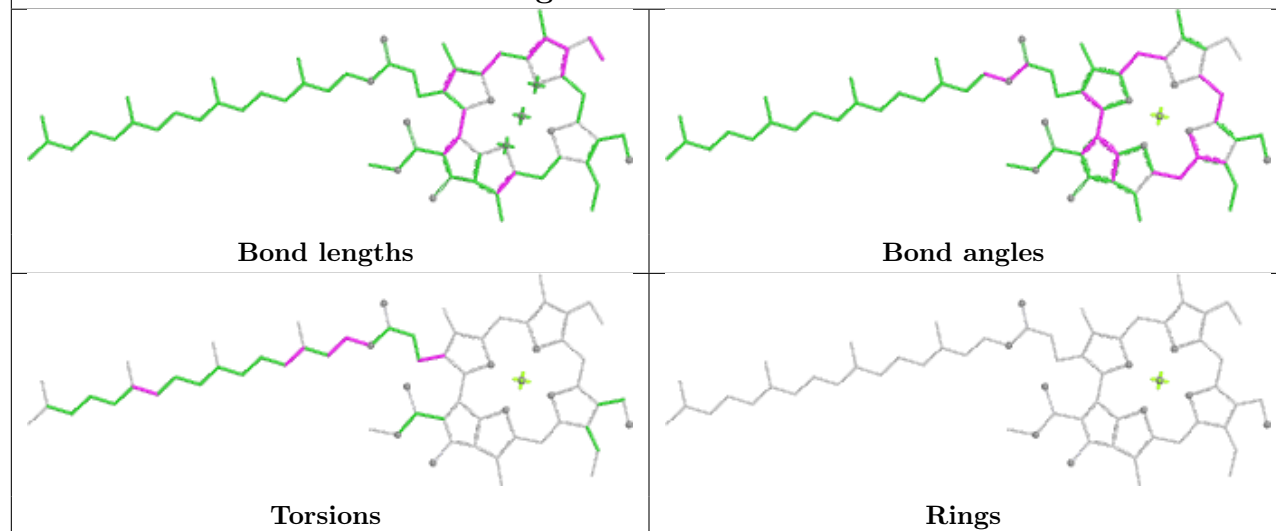


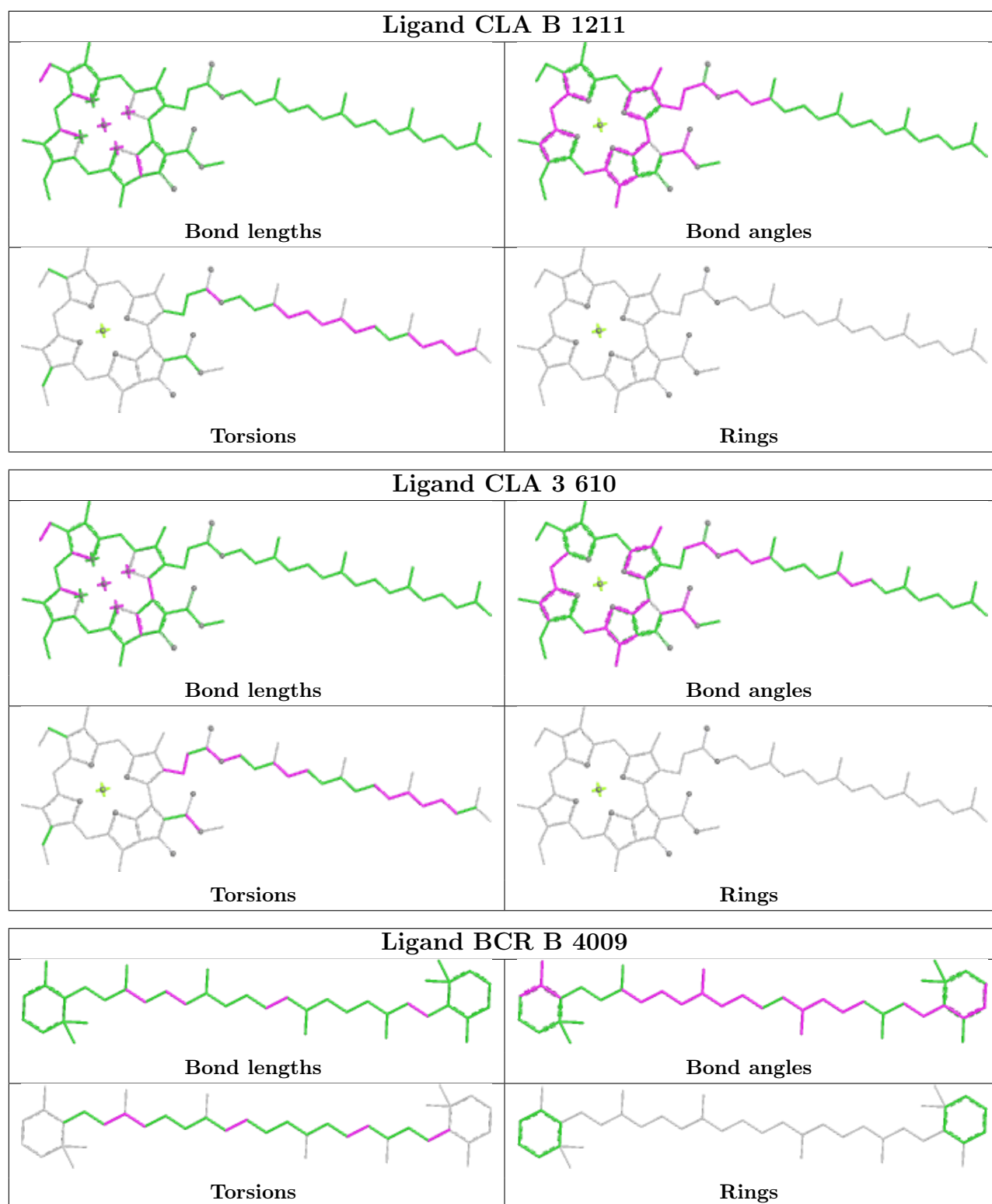


Ligand CLA 2 608



Ligand CHL 2 609





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

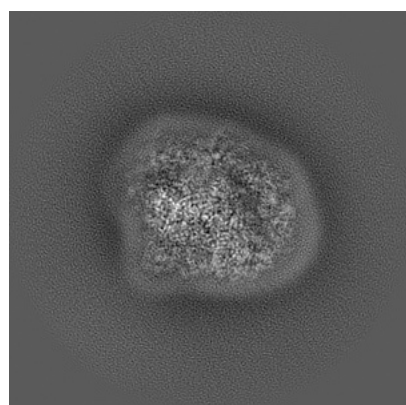
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10746. These allow visual inspection of the internal detail of the map and identification of artifacts.

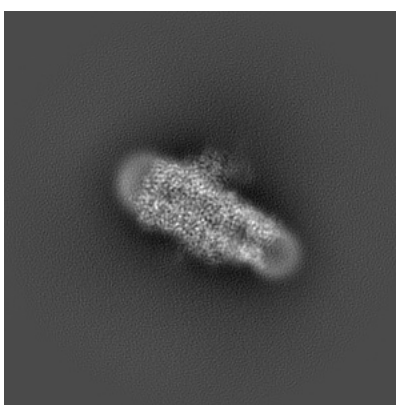
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

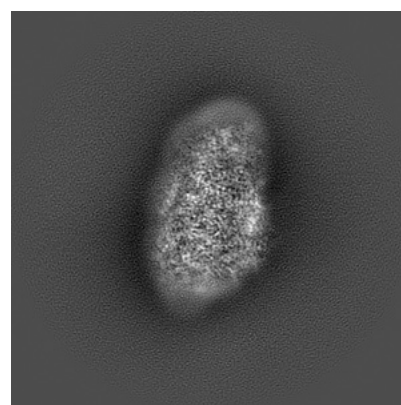
6.1.1 Primary map



X



Y

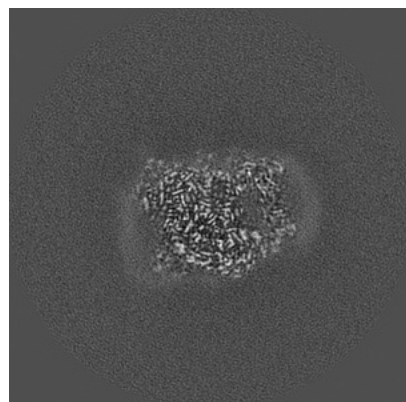


Z

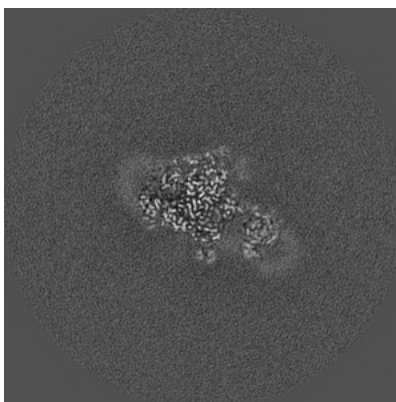
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

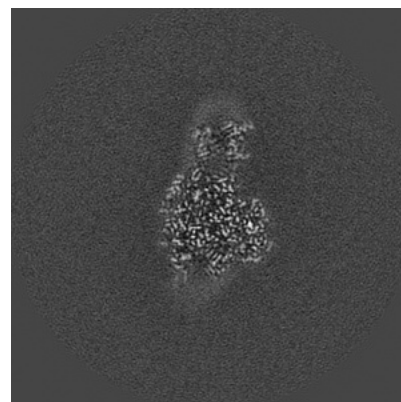
6.2.1 Primary map



X Index: 165



Y Index: 165

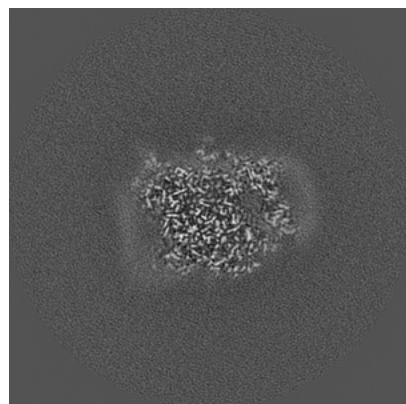


Z Index: 165

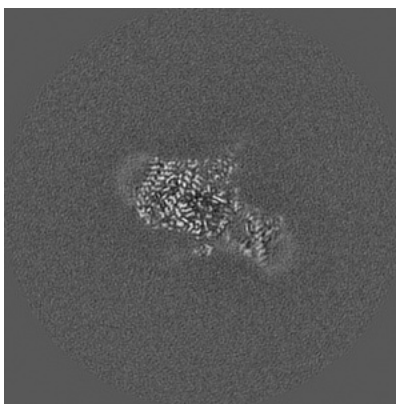
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

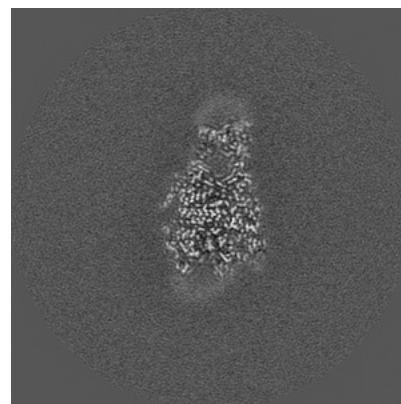
6.3.1 Primary map



X Index: 163



Y Index: 172

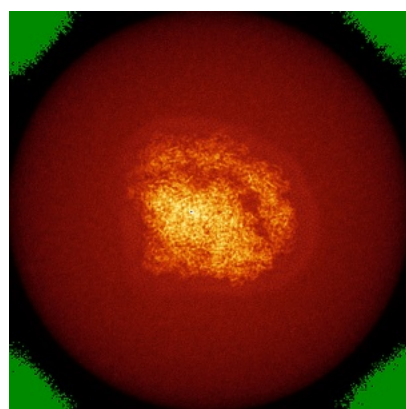


Z Index: 159

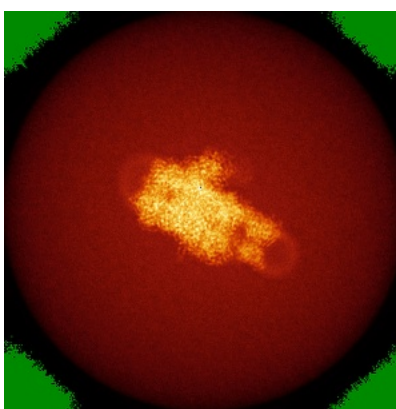
The images above show the largest variance slices of the map in three orthogonal directions.

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

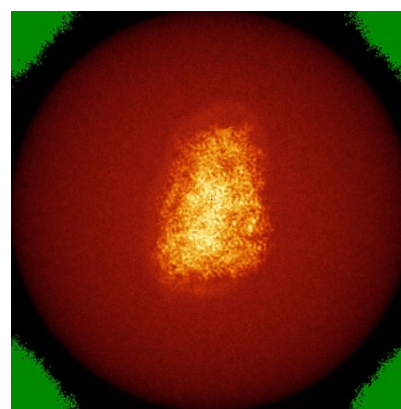
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

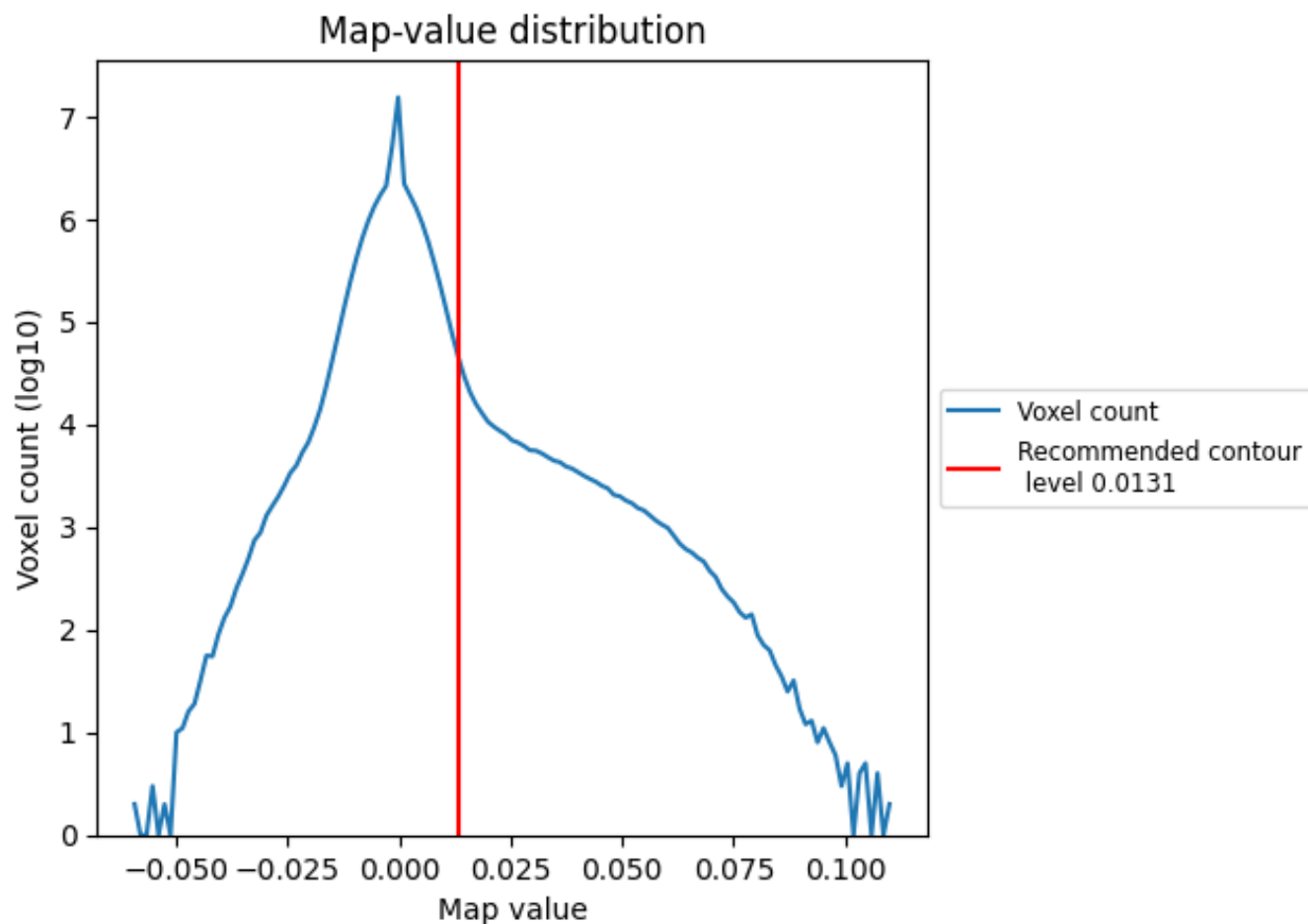
6.6 Mask visualisation

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

7 Map analysis [i](#)

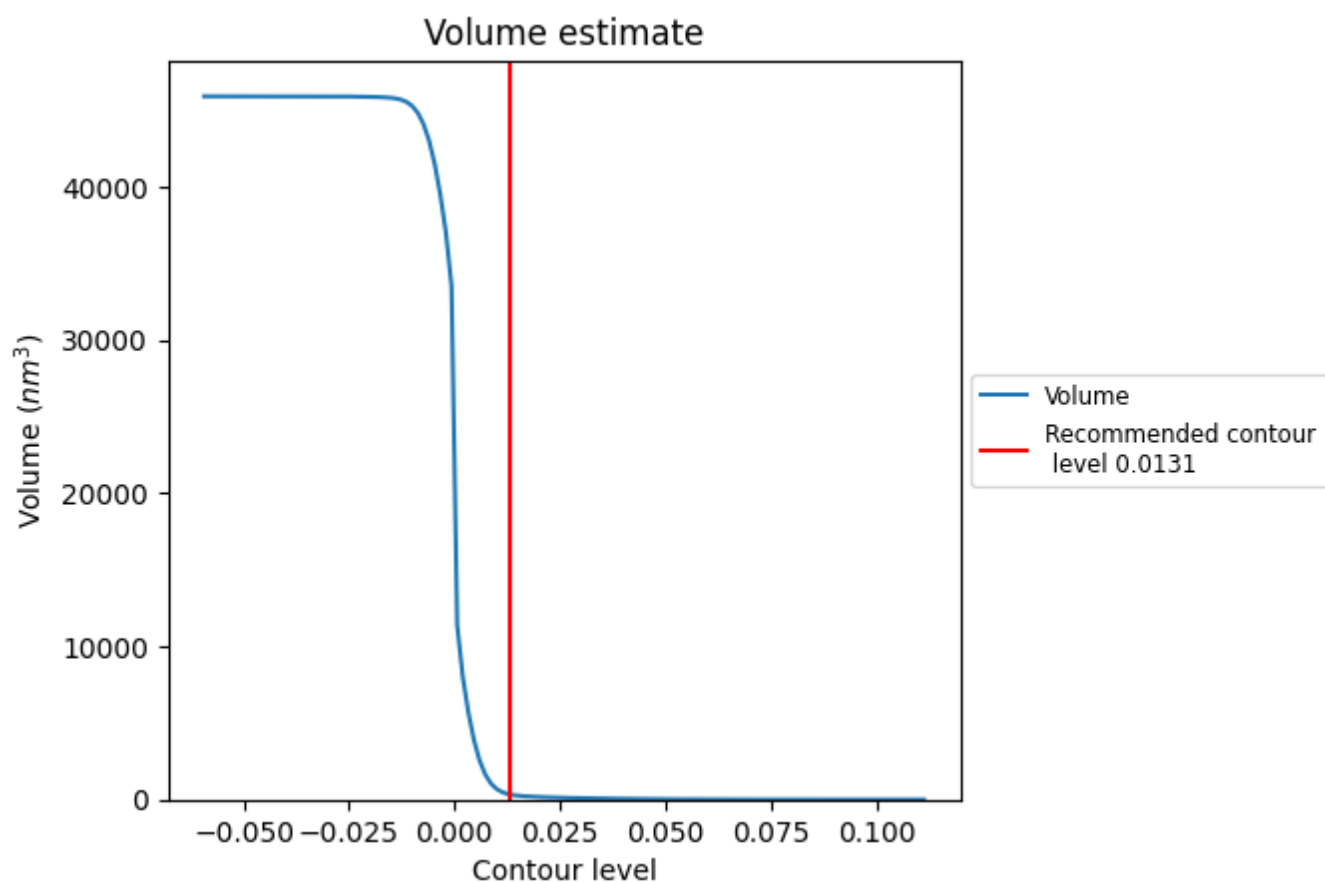
This section contains the results of statistical analysis of the map.

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.

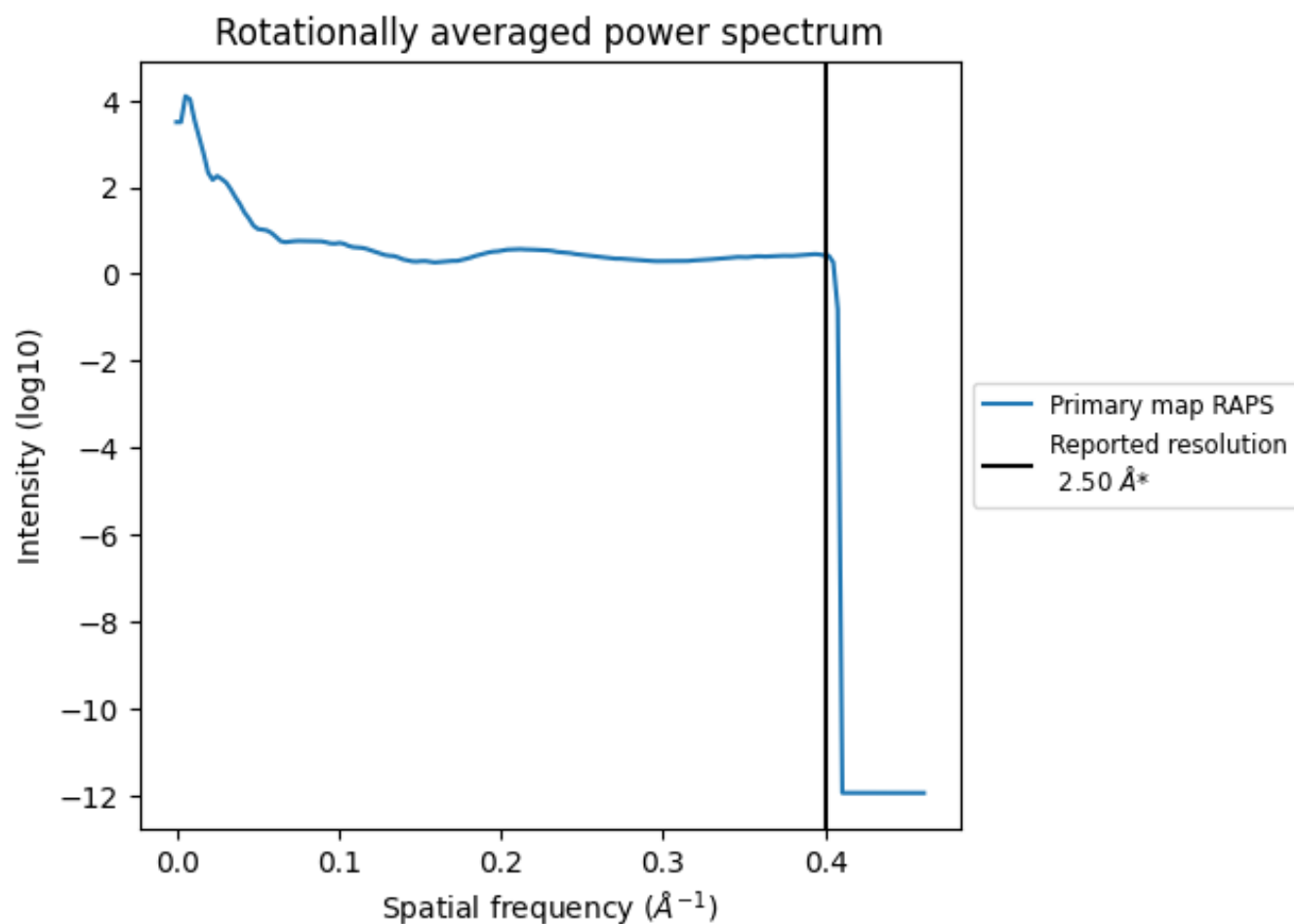
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 305 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 ⓘ

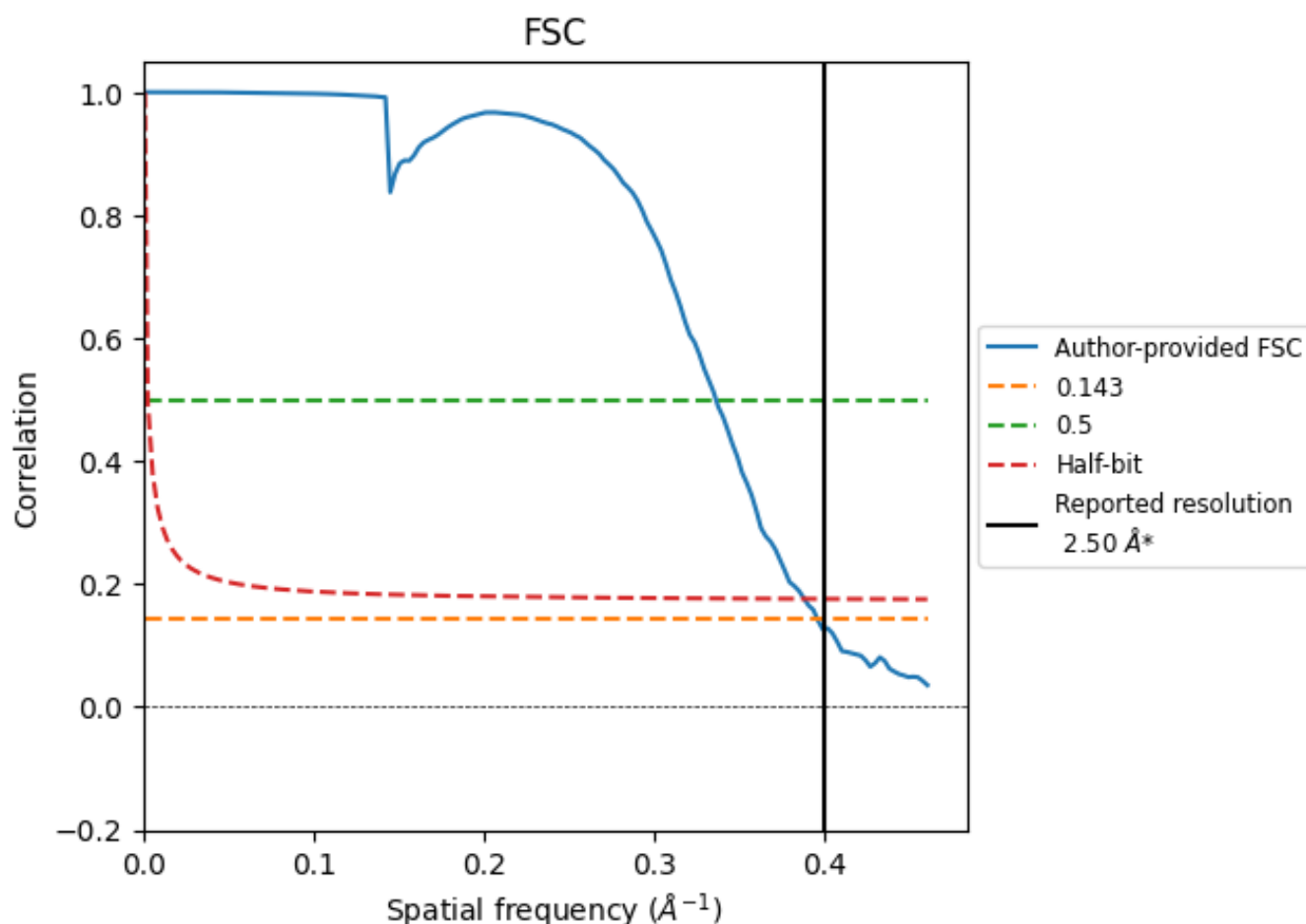


*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.52	2.97	2.57
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

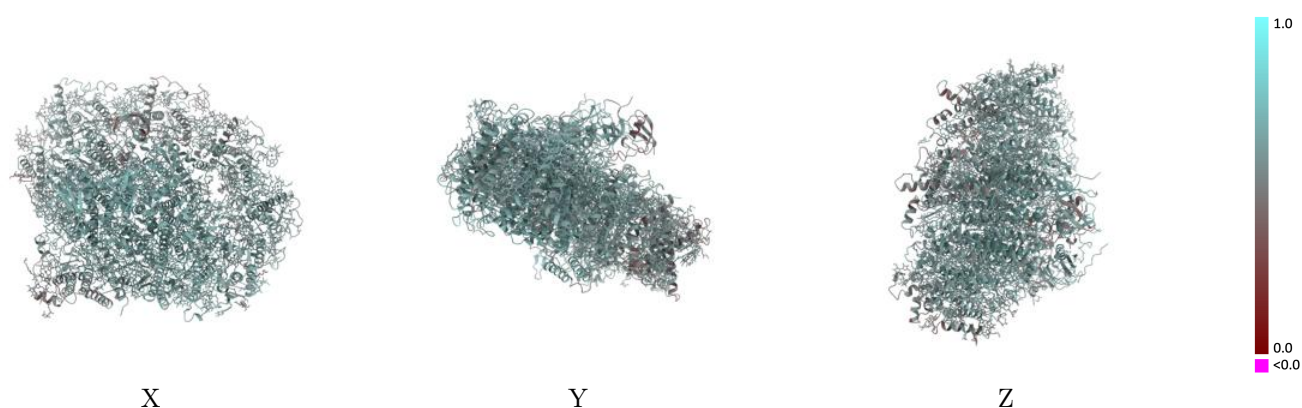
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10746 and PDB model 6YAC. Per-residue inclusion information can be found in section 3 on page 31.

9.1 Map-model overlay [i](#)

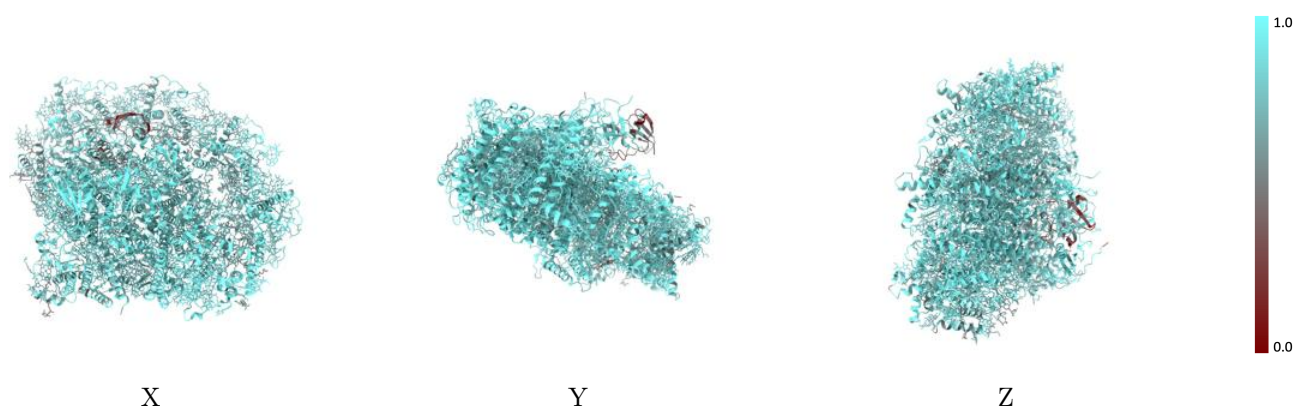
This section was not generated.

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



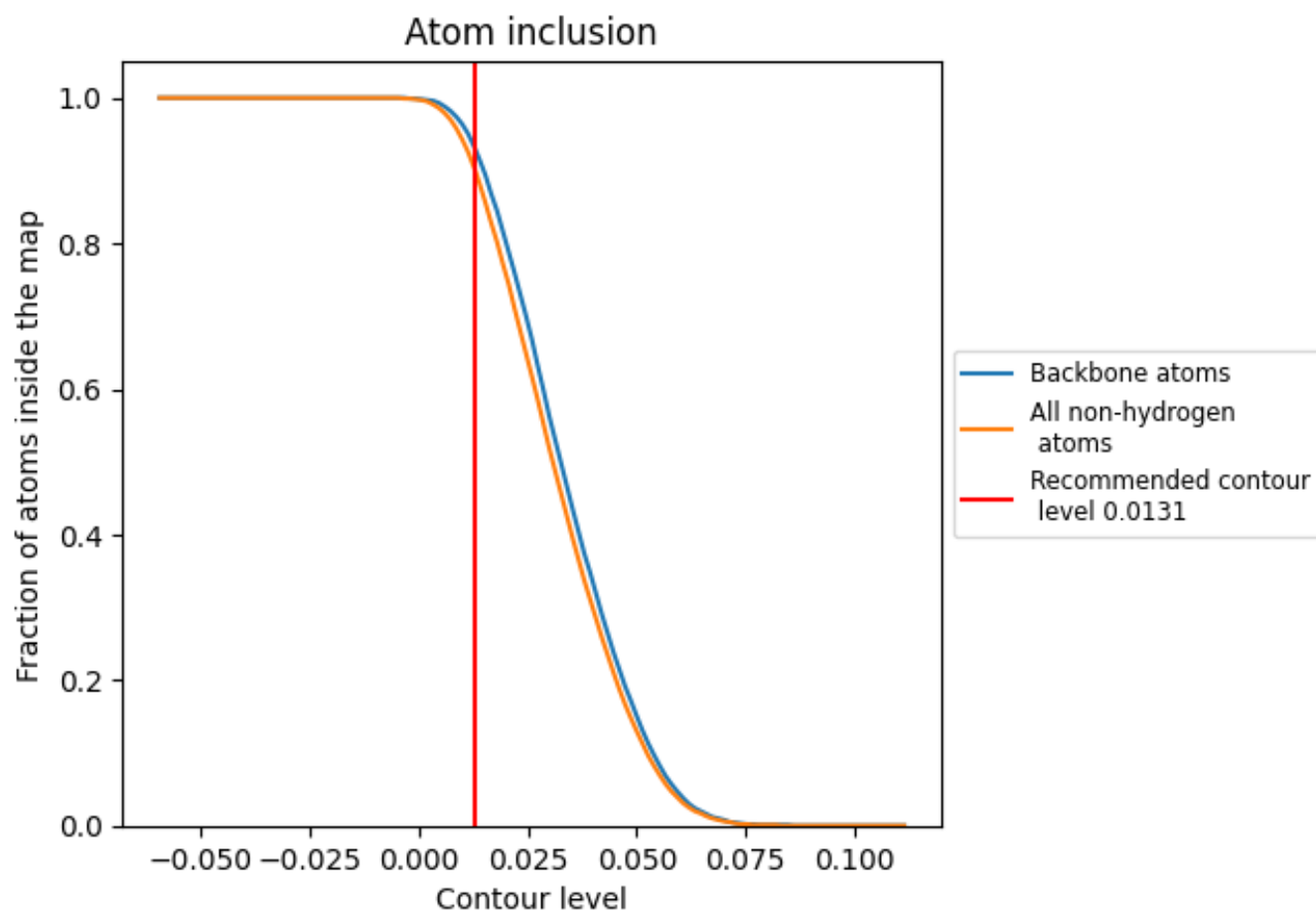
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0131).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.0131) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8980	0.6010
1	0.8920	0.5840
2	0.8360	0.5290
3	0.8600	0.5540
4	0.8750	0.5560
A	0.9430	0.6420
B	0.9480	0.6440
C	0.9940	0.6600
D	0.9470	0.6240
E	0.9090	0.6250
F	0.8750	0.6040
G	0.8350	0.5770
H	0.8310	0.5350
I	0.8680	0.5780
J	0.8520	0.5930
K	0.7140	0.5190
L	0.8560	0.5440
N	0.4970	0.4580

1.0

0.0

<0.0