



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2024 – 09:38 pm BST

PDB ID : 6YEZ
EMDB ID : EMD-10798
Title : Plant PSI-ferredoxin-plastocyanin supercomplex
Authors : Caspy, I.; Nelson, N.; Shkolnisky, Y.; Klaiman, D.; Sheinker, A.
Deposited on : 2020-03-25
Resolution : 2.70 Å(reported)
Based on initial model : 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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

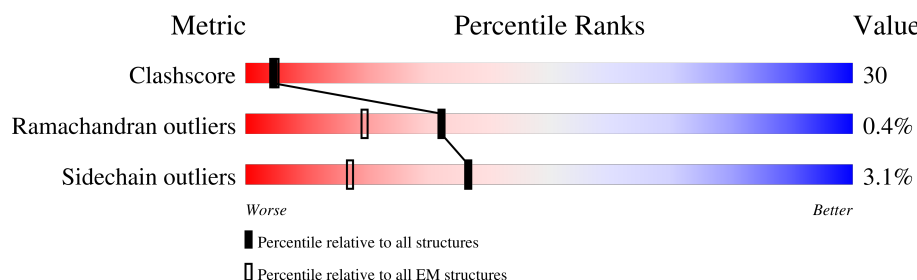
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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





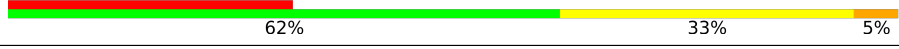
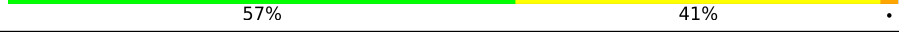
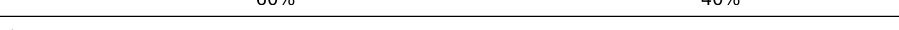
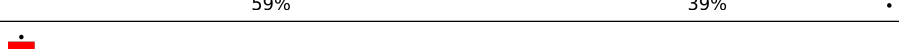
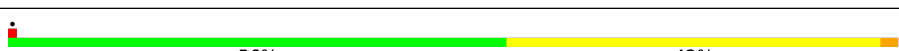
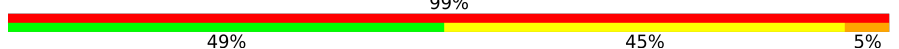


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	743	
2	B	733	
3	C	80	
4	D	143	
5	E	66	
6	F	154	
7	G	97	
8	H	93	

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Mol	Chain	Length	Quality of chain
9	I	31	
10	J	42	
11	K	81	
12	L	159	
13	1	193	
14	2	208	
15	3	221	
16	4	198	
17	N	97	
18	P	99	

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	2	612	X	-	-	-
20	CLA	3	601	X	-	-	-
20	CLA	3	602	X	-	-	-
20	CLA	3	603	X	-	-	-
20	CLA	3	605	X	-	-	-
20	CLA	3	606	X	-	-	-
20	CLA	3	608	X	-	-	-
20	CLA	3	610	X	-	-	-
20	CLA	3	612	X	-	-	-
20	CLA	3	613	X	-	-	-
20	CLA	3	614	X	-	-	-
20	CLA	3	617	X	-	-	-
20	CLA	4	601	X	-	X	-
20	CLA	4	602	X	-	-	-
20	CLA	4	603	X	-	-	-
20	CLA	4	604	X	-	X	-
20	CLA	4	606	X	-	-	-
20	CLA	4	607	X	-	-	-
20	CLA	4	608	X	-	-	-
20	CLA	4	609	X	-	-	-
20	CLA	4	612	X	-	X	-
20	CLA	4	617	X	-	-	-
20	CLA	A	1012	X	-	-	-
20	CLA	A	1013	X	-	-	-
20	CLA	A	1101	X	-	-	-
20	CLA	A	1102	X	-	-	-
20	CLA	A	1103	X	-	-	-
20	CLA	A	1104	X	-	-	-
20	CLA	A	1105	X	-	-	-
20	CLA	A	1106	X	-	-	-
20	CLA	A	1107	X	-	-	-
20	CLA	A	1108	X	-	-	-
20	CLA	A	1109	X	-	-	-
20	CLA	A	1110	X	-	-	-
20	CLA	A	1111	X	-	-	-
20	CLA	A	1112	X	-	-	-
20	CLA	A	1113	X	-	-	-
20	CLA	A	1114	X	-	-	-
20	CLA	A	1115	X	-	-	-
20	CLA	A	1116	X	-	-	-
20	CLA	A	1117	X	-	-	-
20	CLA	A	1118	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	1119	X	-	-	-
20	CLA	A	1120	X	-	-	-
20	CLA	A	1121	X	-	-	-
20	CLA	A	1122	X	-	-	-
20	CLA	A	1123	X	-	-	-
20	CLA	A	1124	X	-	-	-
20	CLA	A	1125	X	-	-	-
20	CLA	A	1126	X	-	X	-
20	CLA	A	1127	X	-	-	-
20	CLA	A	1128	X	-	-	-
20	CLA	A	1129	X	-	-	-
20	CLA	A	1130	X	-	-	-
20	CLA	A	1131	X	-	-	-
20	CLA	A	1132	X	-	X	-
20	CLA	A	1133	X	-	-	-
20	CLA	A	1134	X	-	-	-
20	CLA	A	1135	X	-	-	-
20	CLA	A	1136	X	-	-	-
20	CLA	A	1137	X	-	-	-
20	CLA	A	1138	X	-	-	-
20	CLA	A	1139	X	-	-	-
20	CLA	A	1140	X	-	-	-
20	CLA	A	1141	X	-	-	-
20	CLA	B	1021	X	-	-	-
20	CLA	B	1022	X	-	-	-
20	CLA	B	1023	X	-	-	-
20	CLA	B	1201	X	-	-	-
20	CLA	B	1202	X	-	-	-
20	CLA	B	1203	X	-	-	-
20	CLA	B	1204	X	-	-	-
20	CLA	B	1205	X	-	-	-
20	CLA	B	1206	X	-	-	-
20	CLA	B	1207	X	-	-	-
20	CLA	B	1208	X	-	-	-
20	CLA	B	1209	X	-	-	-
20	CLA	B	1210	X	-	-	-
20	CLA	B	1211	X	-	-	-
20	CLA	B	1212	X	-	-	-
20	CLA	B	1213	X	-	-	-
20	CLA	B	1214	X	-	-	-
20	CLA	B	1215	X	-	-	-
20	CLA	B	1216	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	1217	X	-	-	-
20	CLA	B	1218	X	-	-	-
20	CLA	B	1219	X	-	-	-
20	CLA	B	1220	X	-	-	-
20	CLA	B	1221	X	-	-	-
20	CLA	B	1222	X	-	-	-
20	CLA	B	1223	X	-	-	-
20	CLA	B	1224	X	-	-	-
20	CLA	B	1225	X	-	-	-
20	CLA	B	1226	X	-	-	-
20	CLA	B	1227	X	-	-	-
20	CLA	B	1228	X	-	-	-
20	CLA	B	1229	X	-	-	-
20	CLA	B	1230	X	-	-	-
20	CLA	B	1231	X	-	-	-
20	CLA	B	1232	X	-	-	-
20	CLA	B	1234	X	-	-	-
20	CLA	B	1235	X	-	-	-
20	CLA	B	1236	X	-	-	-
20	CLA	B	1237	X	-	-	-
20	CLA	B	1238	X	-	-	-
20	CLA	B	1239	X	-	-	-
20	CLA	B	1240	X	-	-	-
20	CLA	F	1301	X	-	-	-
20	CLA	F	1302	X	-	-	-
20	CLA	G	1601	X	-	-	-
20	CLA	G	1602	X	-	-	-
20	CLA	G	1603	X	-	-	-
20	CLA	H	1701	X	-	X	-
20	CLA	J	1901	X	-	-	-
20	CLA	K	1401	X	-	-	-
20	CLA	K	1402	X	-	-	-
20	CLA	K	1403	X	-	-	-
20	CLA	K	1404	X	-	-	-
20	CLA	L	1501	X	-	-	-
20	CLA	L	1502	X	-	-	-
20	CLA	L	1503	X	-	-	-
22	BCR	2	503	-	-	X	-
22	BCR	H	4021	-	-	X	-
22	BCR	L	4019	-	-	X	-
25	SF4	C	3003	-	-	X	-
29	LUT	1	502	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	LUT	2	501	X	-	-	-
29	LUT	3	502	X	-	-	-
30	CHL	1	609	X	-	-	-
30	CHL	1	610	X	-	-	-
30	CHL	1	612	X	-	-	-
30	CHL	2	609	X	-	X	-
30	CHL	2	610	X	-	-	-
30	CHL	2	611	X	-	-	-
30	CHL	2	613	X	-	-	-
30	CHL	2	615	X	-	-	-
30	CHL	3	604	X	-	-	-
30	CHL	3	607	X	-	-	-
30	CHL	3	611	X	-	-	-
30	CHL	4	610	X	-	-	-
30	CHL	4	611	X	-	-	-
30	CHL	4	613	X	-	-	-
30	CHL	4	615	X	-	-	-
31	XAT	2	502	X	-	-	-
31	XAT	4	502	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 39217 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	93	Total	C	N	O	0	0
			712	466	112	134		

- 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 PsaJ.

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

- 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	159	Total	C	N	O	S	0	0
			1197	788	191	217	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 a protein called Plastocyanin, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	P	99	Total	C	N	O	S	0	0
			728	460	115	150	3		

- Molecule 19 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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

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

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

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

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Mol	Chain	Residues	Atoms					AltConf
20	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	K	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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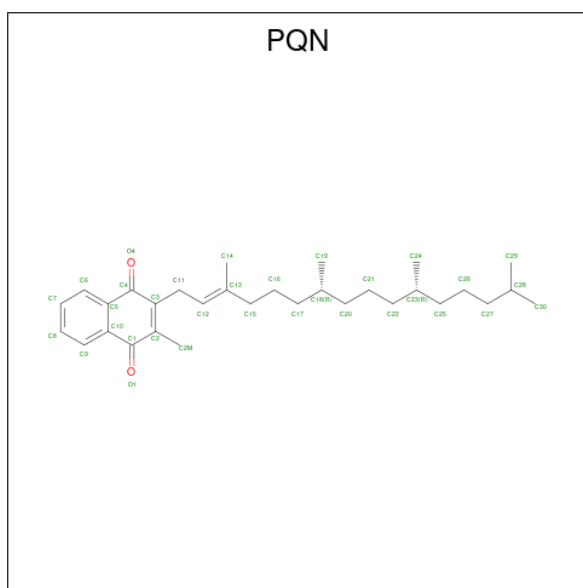
Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 48	C 38	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 42	C 34	Mg 1	N 4	O 3	0

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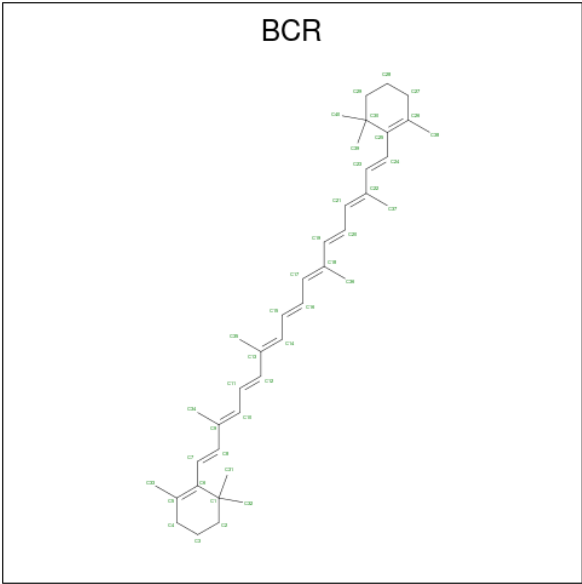
Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 21 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 22 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



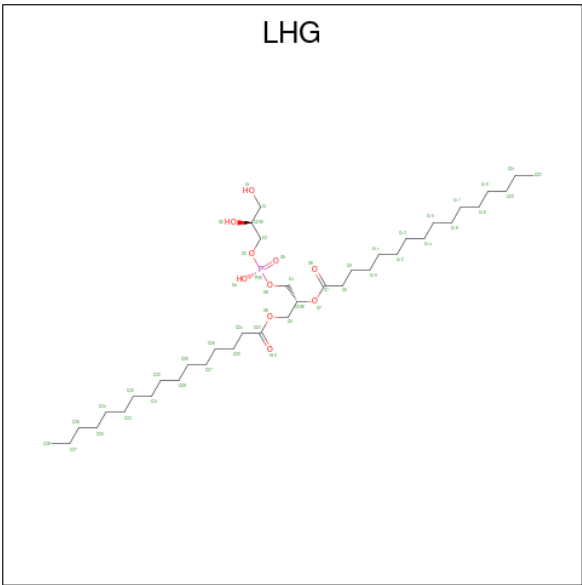
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

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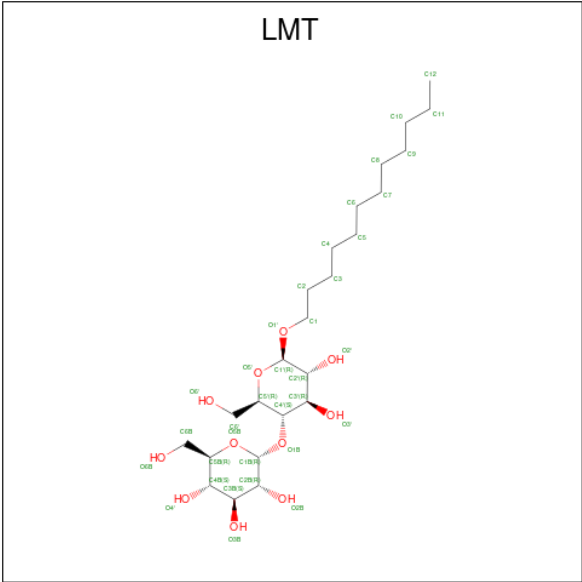
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	H	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 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 (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



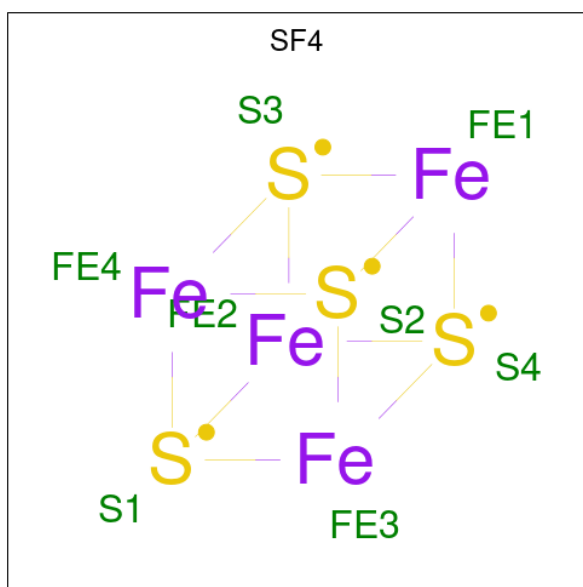
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			21	10	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	3	1	Total	C	O	P	0
			17	8	8	1	
23	4	1	Total	C	O	P	0
			35	24	10	1	

- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



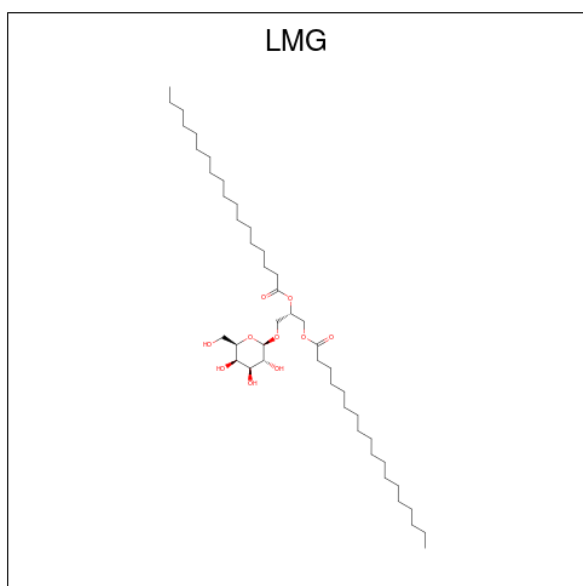
Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			32	21	11	
24	B	1	Total	C	O	0
			31	20	11	
24	G	1	Total	C	O	0
			31	20	11	
24	G	1	Total	C	O	0
			35	24	11	
24	2	1	Total	C	O	0
			35	24	11	

- Molecule 25 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

- Molecule 26 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			50	40	10	
26	B	1	Total	C	O	0
			35	25	10	
26	B	1	Total	C	O	0
			33	23	10	
26	B	1	Total	C	O	0
			34	24	10	
26	F	1	Total	C	O	0
			47	37	10	
26	F	1	Total	C	O	0
			36	26	10	
26	F	1	Total	C	O	0
			34	24	10	
26	F	1	Total	C	O	0
			13	7	6	
26	F	1	Total	C	O	0
			30	20	10	
26	G	1	Total	C	O	0
			25	15	10	
26	G	1	Total	C	O	0
			49	39	10	
26	G	1	Total	C	O	0
			50	40	10	
26	1	1	Total	C	O	0
			46	36	10	
26	2	1	Total	C	O	0
			25	15	10	
26	2	1	Total	C	O	0
			36	26	10	
26	2	1	Total	C	O	0
			30	20	10	
26	2	1	Total	C	O	0
			30	20	10	
26	2	1	Total	C	O	0
			13	7	6	
26	3	1	Total	C	O	0
			30	20	10	

- Molecule 27 is CALCIUM ION (three-letter code: CA) (formula: Ca).

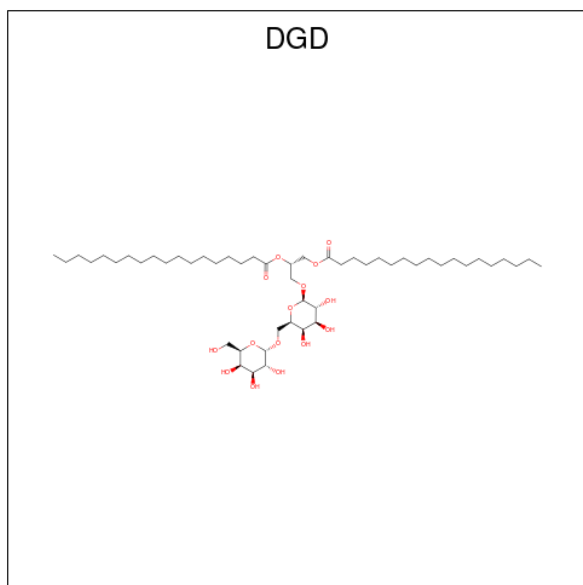
Mol	Chain	Residues	Atoms		AltConf
27	A	1	Total	Ca	0
			1	1	

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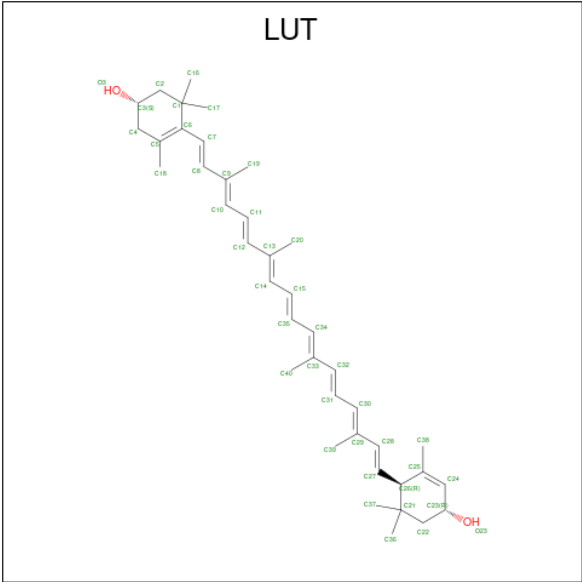
Mol	Chain	Residues	Atoms		AltConf
27	B	1	Total	Ca	0
			1	1	

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



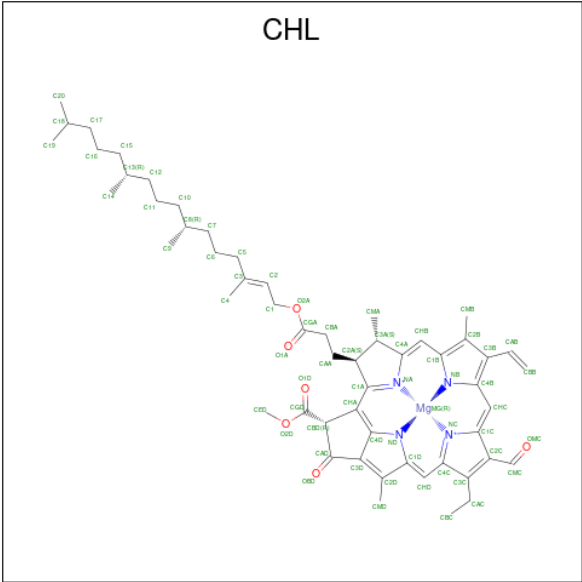
Mol	Chain	Residues	Atoms			AltConf
28	B	1	Total	C	O	0
			61	46	15	
28	F	1	Total	C	O	0
			57	42	15	
28	G	1	Total	C	O	0
			47	32	15	
28	J	1	Total	C	O	0
			58	43	15	
28	1	1	Total	C	O	0
			41	26	15	
28	3	1	Total	C	O	0
			51	36	15	
28	4	1	Total	C	O	0
			51	36	15	

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
29	J	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	1	1	Total	C	O	0
			42	40	2	
29	2	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	3	1	Total	C	O	0
			42	40	2	
29	4	1	Total	C	O	0
			42	40	2	

- Molecule 30 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



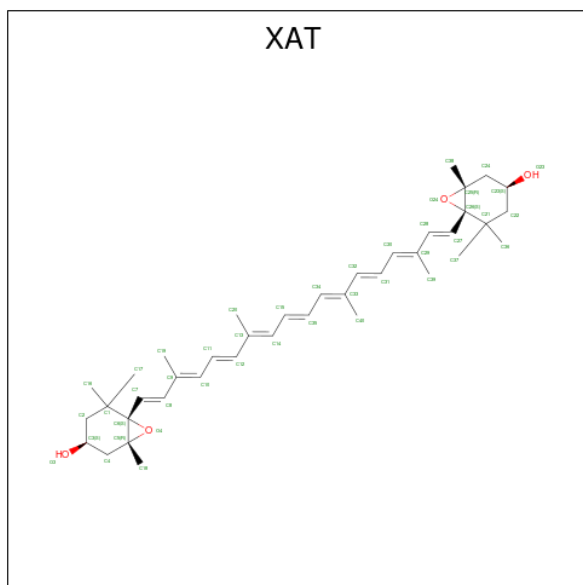
Mol	Chain	Residues	Atoms					AltConf
30	1	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	1	1	Total 61	C 50	Mg 1	N 4	O 6	0
30	1	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	2	1	Total 48	C 37	Mg 1	N 4	O 6	0
30	2	1	Total 46	C 35	Mg 1	N 4	O 6	0
30	2	1	Total 56	C 45	Mg 1	N 4	O 6	0
30	2	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
30	3	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	3	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	4	1	Total 47	C 36	Mg 1	N 4	O 6	0
30	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
30	4	1	Total 61	C 50	Mg 1	N 4	O 6	0

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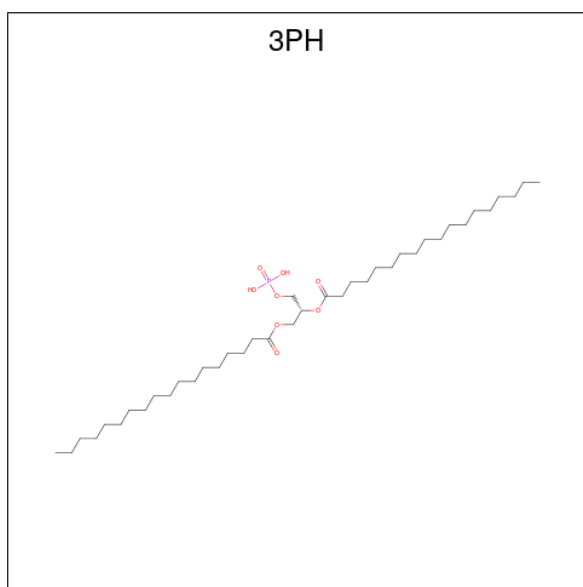
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
30	4	1	43	34	1	4	4	0

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



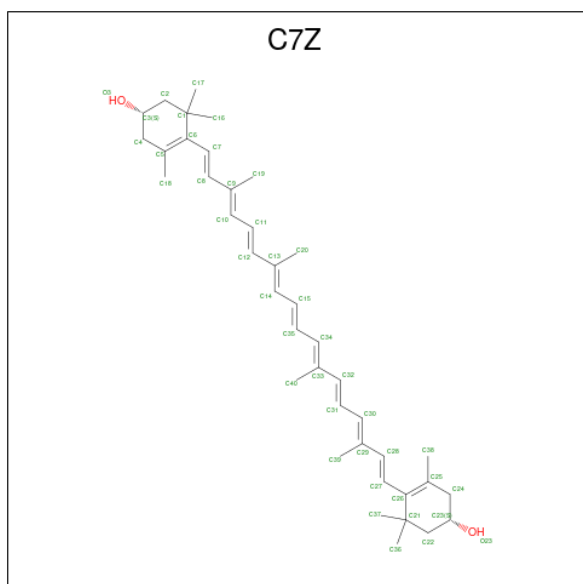
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
31	2	1	44	40	4	0
31	4	1	44	40	4	0

- Molecule 32 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P).



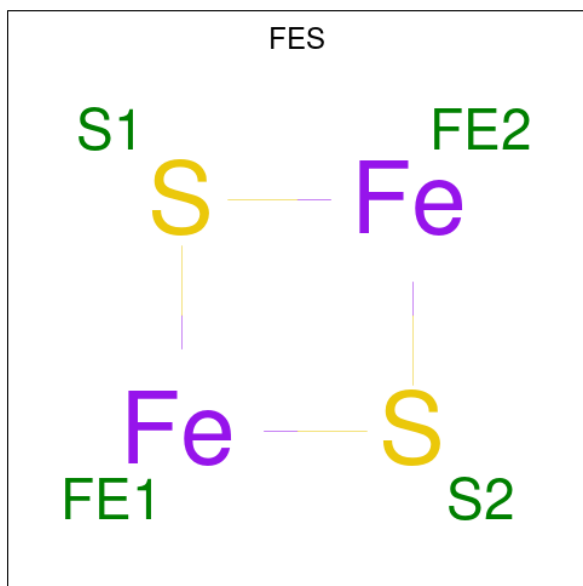
Mol	Chain	Residues	Atoms				AltConf
32	2	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 33 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms				AltConf
33	4	1	Total	C	O		0
			42	40	2		

- Molecule 34 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



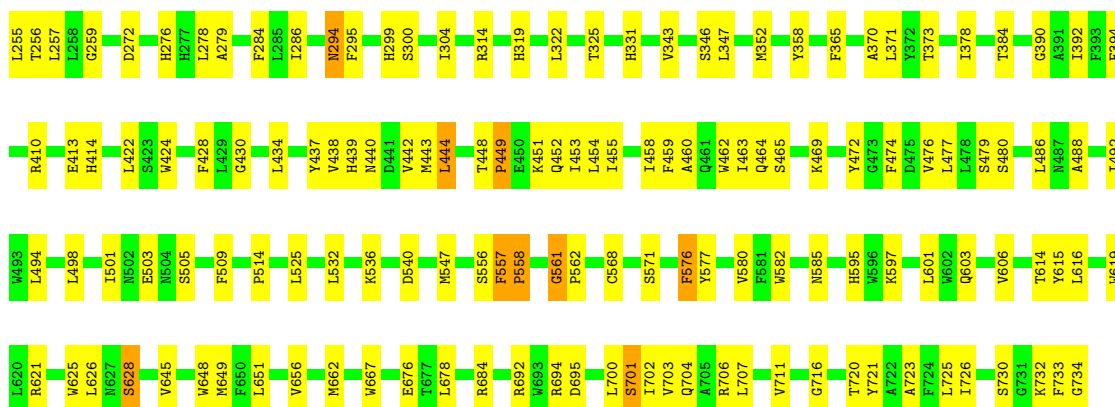
Mol	Chain	Residues	Atoms			AltConf
34	N	1	Total	Fe	S	0
			4	2	2	

- Molecule 35 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
35	P	1	Total	Cu	0
			1	1	

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		AltConf
36	B	2	Total	O	0
			2	2	



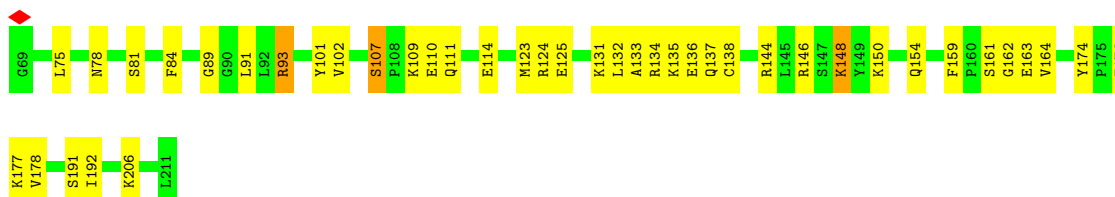
• Molecule 3: Photosystem I iron-sulfur center

Chain C: 68% 31%



• Molecule 4: PsaD

Chain D: 71% 27%



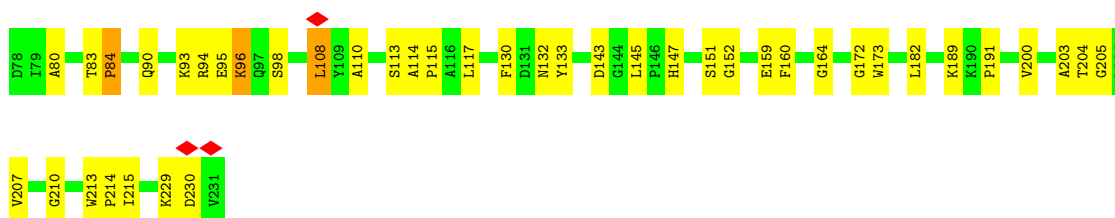
• Molecule 5: PsaE

Chain E: 5% 86% 12%



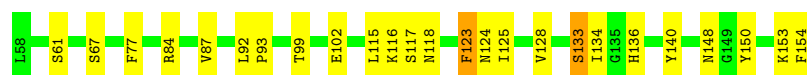
• Molecule 6: PsaF

Chain F: 73% 25%



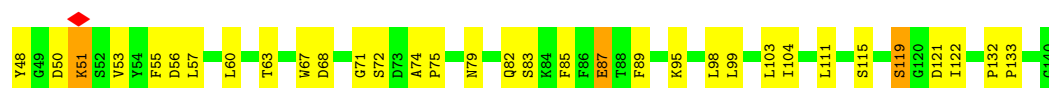
• Molecule 7: PsaG

Chain G:  74% 24% .



• Molecule 8: PsaH

Chain H:  65% 32% .



• Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  58% 39% .



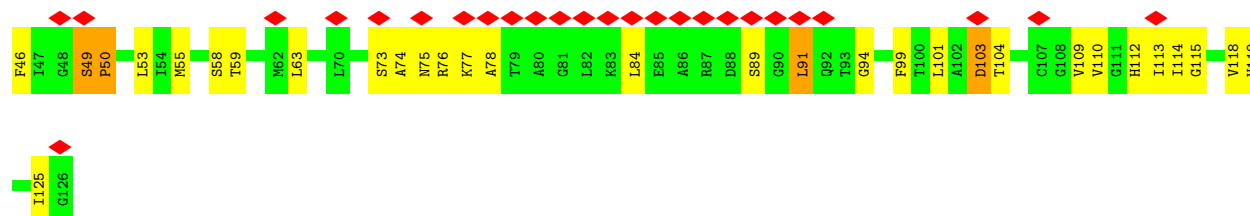
• Molecule 10: PsaJ

Chain J:  62% 38%



• Molecule 11: Photosystem I reaction center subunit X psaK

Chain K:  32% 62% 5%



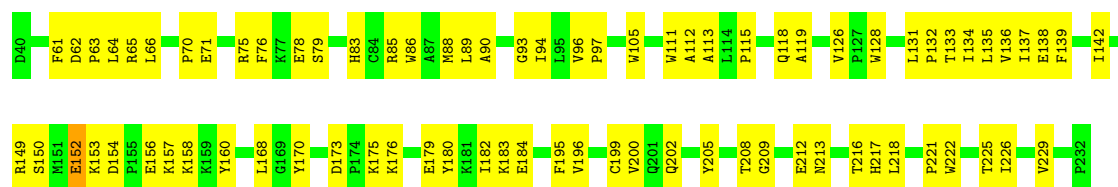
• Molecule 12: PsaL

Chain L:  57% 41% .



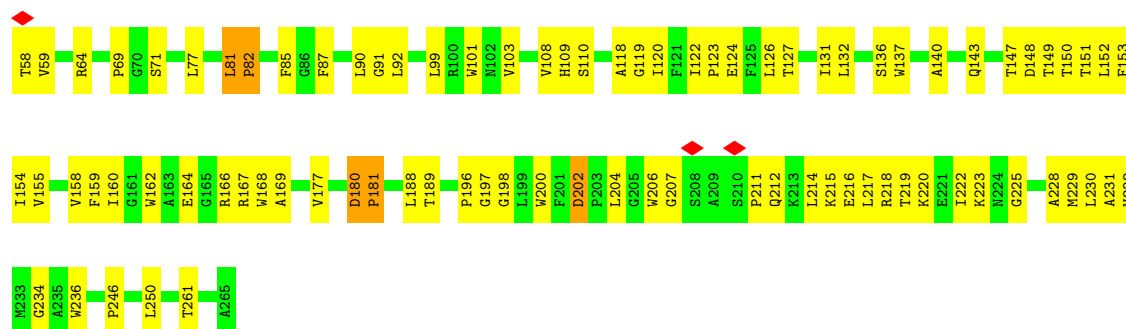
• Molecule 13: Lhca1

Chain 1:  60% 40%



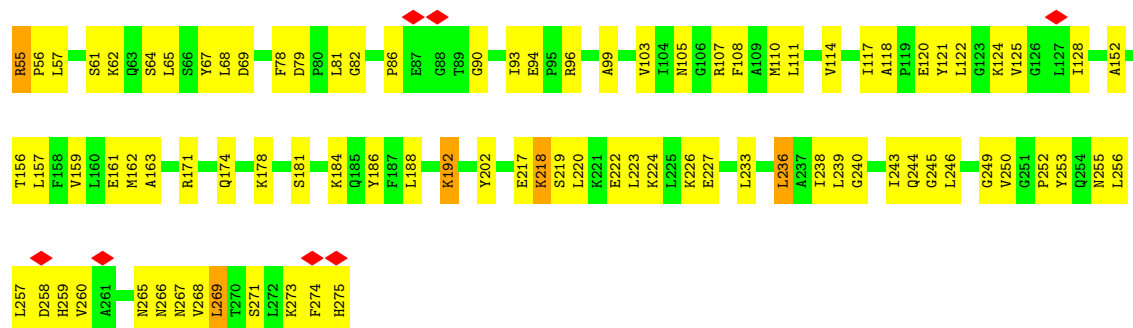
• Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 2:  59% 39%



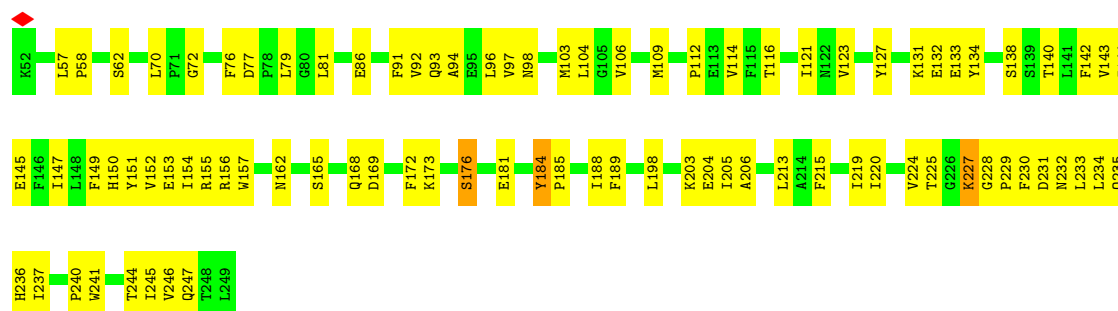
• Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:  60% 38%



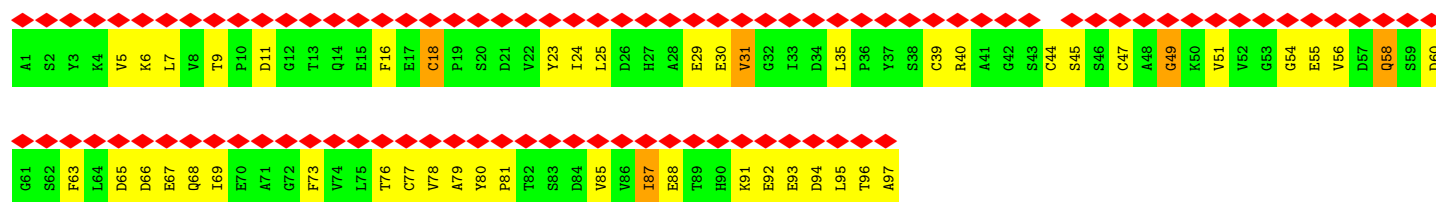
• Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4:  56% 42%



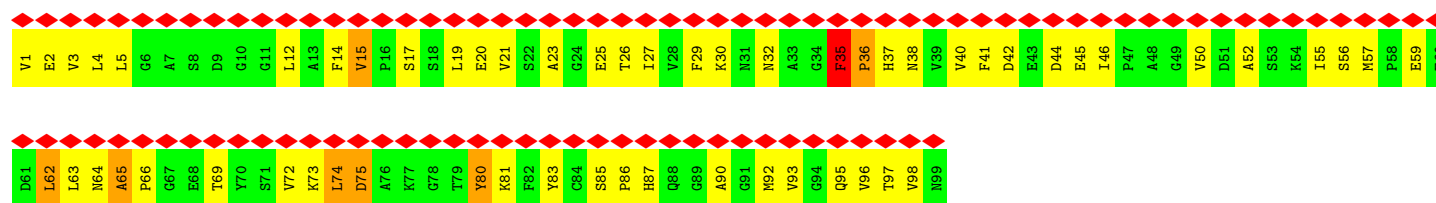
- Molecule 17: Ferredoxin-1, chloroplastic

Chain N: 



- Molecule 18: Plastocyanin, chloroplastic

Chain P: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	102216	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 ($e^-/\text{\AA}^2$)	47.05	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	Depositor
Map size (\AA)	246.6, 246.6, 246.6	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, XAT, CL0, CA, CLA, BCR, LMG, CU, CHL, LHG, C7Z, LUT, DGD, LMT, FES, 3PH, PQN

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	0.55	4/6057 (0.1%)	0.51	2/8264 (0.0%)
2	B	0.54	5/6069 (0.1%)	0.51	2/8286 (0.0%)
3	C	0.77	2/625 (0.3%)	0.65	1/846 (0.1%)
4	D	0.42	0/1163	0.52	0/1572
5	E	0.43	0/540	0.49	0/734
6	F	0.65	2/1234 (0.2%)	0.60	1/1670 (0.1%)
7	G	0.40	0/776	0.47	0/1054
8	H	0.47	0/733	0.52	0/995
9	I	0.40	0/246	0.57	0/335
10	J	0.43	0/349	0.46	0/476
11	K	0.48	0/576	0.62	0/779
12	L	0.64	2/1232 (0.2%)	0.62	1/1684 (0.1%)
13	1	0.39	0/1558	0.49	0/2125
14	2	0.68	4/1679 (0.2%)	0.60	2/2302 (0.1%)
15	3	0.49	1/1760 (0.1%)	0.60	1/2390 (0.0%)
16	4	0.50	1/1608 (0.1%)	0.53	0/2191
17	N	0.83	2/736 (0.3%)	1.04	4/1000 (0.4%)
18	P	0.94	3/743 (0.4%)	0.78	1/1009 (0.1%)
All	All	0.56	26/27684 (0.1%)	0.57	15/37712 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	P	0	2

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37	PRO	N-CA	13.91	1.70	1.47
14	2	82	PRO	N-CA	13.88	1.70	1.47
1	A	570	PRO	N-CA	13.70	1.70	1.47
6	F	84	PRO	N-CA	13.69	1.70	1.47
2	B	449	PRO	N-CA	13.62	1.70	1.47

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	N	49	GLY	O-C-N	-12.13	103.28	122.70
17	N	40	ARG	NE-CZ-NH2	-9.45	115.58	120.30
2	B	558	PRO	CA-N-CD	-9.05	98.83	111.50
17	N	49	GLY	C-N-CA	8.93	144.01	121.70
1	A	570	PRO	CA-N-CD	-8.19	100.04	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	P	15	VAL	Peptide
18	P	35	PHE	Peptide

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	345	0
2	B	5857	0	5653	223	0
3	C	612	0	591	28	0
4	D	1132	0	1141	47	0
5	E	528	0	528	5	0
6	F	1206	0	1231	48	0
7	G	757	0	743	22	0
8	H	712	0	701	37	0
9	I	240	0	264	31	0
10	J	338	0	345	31	0
11	K	569	0	596	41	0
12	L	1197	0	1197	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1	1508	0	1489	118	0
14	2	1620	0	1557	132	0
15	3	1706	0	1661	124	0
16	4	1559	0	1527	141	0
17	N	724	0	672	71	0
18	P	728	0	699	85	0
19	A	65	0	72	12	0
20	1	608	0	563	103	0
20	2	522	0	499	105	0
20	3	578	0	495	70	0
20	4	631	0	595	170	0
20	A	2643	0	2749	387	0
20	B	2610	0	2747	268	0
20	F	130	0	144	20	0
20	G	166	0	153	21	0
20	H	60	0	58	21	0
20	J	50	0	38	7	0
20	K	199	0	158	17	0
20	L	160	0	134	52	0
21	A	33	0	46	7	0
21	B	33	0	46	3	0
22	1	80	0	105	5	0
22	2	40	0	53	24	0
22	3	80	0	105	14	0
22	A	240	0	316	27	0
22	B	200	0	265	20	0
22	F	80	0	105	11	0
22	G	40	0	53	5	0
22	H	40	0	53	21	0
22	I	80	0	105	17	0
22	J	40	0	53	5	0
22	K	80	0	106	17	0
22	L	80	0	106	47	0
23	1	49	0	74	11	0
23	2	35	0	40	7	0
23	3	17	0	12	0	0
23	4	35	0	40	11	0
23	A	89	0	127	3	0
23	B	70	0	86	6	0
24	2	35	0	46	8	0
24	A	35	0	45	1	0
24	B	63	0	68	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	G	66	0	79	0	0
25	A	8	0	0	0	0
25	C	16	0	0	3	0
26	1	46	0	65	8	0
26	2	134	0	133	17	0
26	3	30	0	30	0	0
26	A	50	0	73	3	0
26	B	102	0	114	16	0
26	F	160	0	188	7	0
26	G	124	0	161	14	0
27	A	1	0	0	0	0
27	B	1	0	0	0	0
28	1	41	0	40	1	0
28	3	51	0	60	3	0
28	4	51	0	60	4	0
28	B	61	0	83	7	0
28	F	57	0	75	18	0
28	G	47	0	52	3	0
28	J	58	0	77	10	0
29	1	84	0	110	40	0
29	2	42	0	55	13	0
29	3	84	0	110	9	0
29	4	42	0	55	20	0
29	J	42	0	55	10	0
30	1	164	0	134	32	0
30	2	272	0	223	50	0
30	3	164	0	136	13	0
30	4	202	0	152	11	0
31	2	44	0	56	14	0
31	4	44	0	56	14	0
32	2	33	0	39	5	0
33	4	42	0	0	4	0
34	N	4	0	0	0	0
35	P	1	0	0	0	0
36	B	2	0	0	0	0
All	All	39217	0	39245	2384	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 30.

The worst 5 of 2384 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)
2:B:558:PRO:N	2:B:558:PRO:CA	1.69	1.44
14:2:181:PRO:CA	14:2:181:PRO:N	1.70	1.43
6:F:84:PRO:N	6:F:84:PRO:CA	1.70	1.41
1:A:570:PRO:N	1:A:570:PRO:CA	1.70	1.41
3:C:22:PRO:CA	3:C:22:PRO:N	1.69	1.38

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/743 (100%)	713 (96%)	25 (3%)	3 (0%)	30	55
2	B	731/733 (100%)	700 (96%)	31 (4%)	0	100	100
3	C	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
4	D	141/143 (99%)	136 (96%)	5 (4%)	0	100	100
5	E	64/66 (97%)	58 (91%)	6 (9%)	0	100	100
6	F	152/154 (99%)	145 (95%)	7 (5%)	0	100	100
7	G	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
8	H	91/93 (98%)	83 (91%)	7 (8%)	1 (1%)	12	30
9	I	29/31 (94%)	26 (90%)	3 (10%)	0	100	100
10	J	40/42 (95%)	40 (100%)	0	0	100	100
11	K	79/81 (98%)	71 (90%)	6 (8%)	2 (2%)	4	12
12	L	157/159 (99%)	146 (93%)	10 (6%)	1 (1%)	22	45
13	1	191/193 (99%)	185 (97%)	6 (3%)	0	100	100
14	2	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	25	49
15	3	219/221 (99%)	197 (90%)	22 (10%)	0	100	100
16	4	196/198 (99%)	188 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	N	95/97 (98%)	82 (86%)	11 (12%)	2 (2%)	5	15
18	P	97/99 (98%)	85 (88%)	10 (10%)	2 (2%)	5	15
All	All	3402/3438 (99%)	3214 (94%)	176 (5%)	12 (0%)	32	55

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	639	GLY
11	K	50	PRO
12	L	209	LEU
17	N	66	ASP
1	A	580	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/604 (100%)	589 (98%)	15 (2%)	42	72
2	B	598/598 (100%)	580 (97%)	18 (3%)	36	65
3	C	69/69 (100%)	68 (99%)	1 (1%)	62	84
4	D	122/122 (100%)	115 (94%)	7 (6%)	17	40
5	E	58/58 (100%)	56 (97%)	2 (3%)	32	61
6	F	125/126 (99%)	123 (98%)	2 (2%)	58	82
7	G	82/82 (100%)	78 (95%)	4 (5%)	21	47
8	H	75/75 (100%)	71 (95%)	4 (5%)	19	43
9	I	27/27 (100%)	25 (93%)	2 (7%)	11	28
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	59/59 (100%)	57 (97%)	2 (3%)	32	61
12	L	126/126 (100%)	121 (96%)	5 (4%)	27	55
13	1	158/158 (100%)	154 (98%)	4 (2%)	42	72
14	2	167/167 (100%)	165 (99%)	2 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	3	171/172 (99%)	166 (97%)	5 (3%)	37	67
16	4	164/164 (100%)	156 (95%)	8 (5%)	21	47
17	N	82/82 (100%)	78 (95%)	4 (5%)	21	47
18	P	79/79 (100%)	76 (96%)	3 (4%)	28	56
All	All	2801/2803 (100%)	2713 (97%)	88 (3%)	37	64

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	79	VAL
15	3	236	LEU
12	L	151	SER
13	1	175	LYS
16	4	133	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
18	P	95	GLN
17	N	58	GLN
12	L	61	ASN
8	H	79	ASN
14	2	238	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 244 ligands modelled in this entry, 3 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$
20	CLA	3	614	-	42,50,73	1.68	7 (16%)	48,85,113	2.27	13 (27%)
20	CLA	K	1402	-	60,68,73	1.40	8 (13%)	70,107,113	2.09	19 (27%)
26	LMG	F	5006	-	13,13,55	0.54	0	18,18,63	0.77	0
20	CLA	A	1012	-	65,73,73	1.42	7 (10%)	76,113,113	2.01	15 (19%)
20	CLA	A	1129	-	65,73,73	1.38	7 (10%)	76,113,113	2.00	16 (21%)
20	CLA	B	1216	-	65,73,73	1.36	7 (10%)	76,113,113	1.92	16 (21%)
33	C7Z	4	505	-	43,43,43	5.25	17 (39%)	58,60,60	5.54	32 (55%)
20	CLA	A	1116	-	56,64,73	1.50	8 (14%)	65,102,113	2.11	17 (26%)
22	BCR	A	4003	-	41,41,41	1.86	4 (9%)	56,56,56	4.23	20 (35%)
29	LUT	4	501	-	42,43,43	2.40	4 (9%)	51,60,60	2.17	15 (29%)
24	LMT	2	808	-	36,36,36	0.41	0	47,47,47	0.73	1 (2%)
20	CLA	4	612	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	16 (21%)
20	CLA	3	610	15	65,73,73	1.34	7 (10%)	76,113,113	2.00	19 (25%)
26	LMG	A	5006	-	50,50,55	1.04	5 (10%)	58,58,63	1.19	3 (5%)
20	CLA	K	1404	11	46,54,73	1.61	9 (19%)	53,90,113	2.09	12 (22%)
20	CLA	A	1121	-	60,68,73	1.45	7 (11%)	70,107,113	2.08	16 (22%)
20	CLA	B	1210	-	65,73,73	1.42	8 (12%)	76,113,113	2.09	21 (27%)
20	CLA	1	607	-	46,54,73	1.62	7 (15%)	53,90,113	2.12	13 (24%)
31	XAT	4	502	-	39,47,47	0.78	1 (2%)	54,74,74	2.07	13 (24%)
20	CLA	A	1110	-	55,63,73	1.51	7 (12%)	64,101,113	2.17	19 (29%)
20	CLA	A	1135	-	51,59,73	1.55	7 (13%)	59,96,113	2.25	17 (28%)
20	CLA	A	1137	-	65,73,73	1.39	7 (10%)	76,113,113	1.98	16 (21%)
26	LMG	G	5002	-	50,50,55	1.06	4 (8%)	58,58,63	1.21	4 (6%)
30	CHL	2	610	-	56,64,74	0.89	3 (5%)	61,102,114	1.41	11 (18%)
20	CLA	K	1401	-	45,53,73	1.60	7 (15%)	52,89,113	2.16	13 (25%)
20	CLA	B	1213	-	60,68,73	1.44	7 (11%)	70,107,113	2.01	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LUT	2	501	-	42,43,43	2.34	3 (7%)	51,60,60	2.42	17 (33%)
22	BCR	A	4017	-	41,41,41	1.84	5 (12%)	56,56,56	4.79	19 (33%)
20	CLA	A	1128	-	65,73,73	1.40	7 (10%)	76,113,113	2.07	18 (23%)
20	CLA	B	1239	-	65,73,73	1.42	7 (10%)	76,113,113	1.98	19 (25%)
22	BCR	L	4019	-	41,41,41	1.92	4 (9%)	56,56,56	4.38	17 (30%)
22	BCR	1	503	-	41,41,41	1.86	4 (9%)	56,56,56	4.19	14 (25%)
20	CLA	A	1117	-	65,73,73	1.39	8 (12%)	76,113,113	1.93	16 (21%)
20	CLA	B	1214	-	65,73,73	1.41	8 (12%)	76,113,113	2.01	16 (21%)
20	CLA	1	605	-	65,73,73	1.34	7 (10%)	76,113,113	2.17	18 (23%)
20	CLA	1	614	13	60,68,73	1.44	7 (11%)	70,107,113	2.07	17 (24%)
20	CLA	3	606	-	50,58,73	1.58	9 (18%)	58,95,113	2.13	13 (22%)
20	CLA	A	1103	-	65,73,73	1.37	8 (12%)	76,113,113	2.11	19 (25%)
20	CLA	A	1115	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	13 (17%)
20	CLA	1	604	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	17 (22%)
30	CHL	4	613	-	61,69,74	1.08	4 (6%)	67,108,114	1.38	12 (17%)
20	CLA	A	1108	-	50,58,73	1.60	8 (16%)	58,95,113	2.21	19 (32%)
20	CLA	4	607	-	60,68,73	1.40	8 (13%)	70,107,113	2.03	18 (25%)
30	CHL	1	610	13	47,55,74	1.12	4 (8%)	50,91,114	1.31	8 (16%)
20	CLA	B	1235	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	20 (26%)
20	CLA	4	601	16	60,68,73	1.39	7 (11%)	70,107,113	2.01	16 (22%)
23	LHG	B	5001	20	20,20,48	0.59	0	23,26,54	1.48	2 (8%)
26	LMG	F	5003	-	36,36,55	0.72	1 (2%)	44,44,63	1.08	3 (6%)
22	BCR	A	4008	-	41,41,41	1.87	6 (14%)	56,56,56	4.05	17 (30%)
20	CLA	3	603	15	55,63,73	1.50	7 (12%)	64,101,113	2.19	18 (28%)
30	CHL	2	615	-	56,64,74	0.92	3 (5%)	61,102,114	1.44	13 (21%)
20	CLA	F	1301	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)
23	LHG	A	5002	-	48,48,48	0.38	0	51,54,54	1.13	5 (9%)
22	BCR	3	506	-	41,41,41	1.92	4 (9%)	56,56,56	4.40	18 (32%)
20	CLA	A	1113	-	45,53,73	1.62	7 (15%)	52,89,113	2.17	15 (28%)
20	CLA	B	1022	-	65,73,73	1.44	8 (12%)	76,113,113	1.94	16 (21%)
20	CLA	H	1701	8	60,68,73	1.39	8 (13%)	70,107,113	2.01	16 (22%)
20	CLA	A	1114	-	46,54,73	1.64	7 (15%)	53,90,113	2.16	14 (26%)
22	BCR	3	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.41	17 (30%)
20	CLA	3	605	-	55,63,73	1.49	7 (12%)	64,101,113	2.20	19 (29%)
25	SF4	C	3002	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	1023	-	65,73,73	1.42	9 (13%)	76,113,113	1.92	16 (21%)
26	LMG	B	5004	-	33,33,55	0.54	0	41,41,63	1.32	6 (14%)
20	CLA	A	1122	-	65,73,73	1.39	7 (10%)	76,113,113	1.95	14 (18%)
20	CLA	A	1131	-	65,73,73	1.39	8 (12%)	76,113,113	1.97	17 (22%)
30	CHL	2	609	-	66,74,74	0.85	3 (4%)	73,114,114	1.33	12 (16%)
30	CHL	4	610	-	47,55,74	1.16	5 (10%)	50,91,114	1.56	12 (24%)
20	CLA	G	1601	-	55,63,73	1.51	6 (10%)	64,101,113	2.10	19 (29%)
20	CLA	B	1231	-	60,68,73	1.45	8 (13%)	70,107,113	2.10	15 (21%)
20	CLA	B	1228	-	60,68,73	1.41	7 (11%)	70,107,113	2.05	14 (20%)
20	CLA	B	1222	36	65,73,73	1.37	8 (12%)	76,113,113	2.06	20 (26%)
22	BCR	B	4010	-	41,41,41	1.84	5 (12%)	56,56,56	4.26	15 (26%)
26	LMG	1	802	-	46,46,55	0.94	3 (6%)	54,54,63	1.07	2 (3%)
26	LMG	2	806	-	13,13,55	0.57	0	18,18,63	0.56	0
22	BCR	A	4007	-	41,41,41	1.87	6 (14%)	56,56,56	4.37	16 (28%)
20	CLA	4	617	-	65,73,73	1.32	8 (12%)	76,113,113	2.04	15 (19%)
23	LHG	4	801	-	34,34,48	0.42	0	37,40,54	1.14	3 (8%)
25	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
20	CLA	4	609	16	50,58,73	1.53	7 (14%)	58,95,113	2.21	16 (27%)
20	CLA	A	1119	-	65,73,73	1.39	8 (12%)	76,113,113	2.01	20 (26%)
20	CLA	A	1123	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	19 (25%)
22	BCR	I	4020	-	41,41,41	1.86	4 (9%)	56,56,56	4.36	16 (28%)
20	CLA	2	612	-	55,63,73	1.46	7 (12%)	64,101,113	2.13	16 (25%)
28	DGD	1	803	-	42,42,67	0.86	1 (2%)	56,56,81	1.05	3 (5%)
22	BCR	G	4011	-	41,41,41	1.87	4 (9%)	56,56,56	4.56	18 (32%)
24	LMT	B	5008	-	32,32,36	1.31	6 (18%)	43,43,47	1.02	3 (6%)
22	BCR	B	4009	-	41,41,41	1.82	4 (9%)	56,56,56	4.20	14 (25%)
29	LUT	1	502	-	42,43,43	2.40	2 (4%)	51,60,60	2.15	11 (21%)
20	CLA	A	1102	-	65,73,73	1.38	7 (10%)	76,113,113	2.02	17 (22%)
20	CLA	B	1226	-	65,73,73	1.40	7 (10%)	76,113,113	2.11	18 (23%)
20	CLA	2	601	-	60,68,73	1.43	7 (11%)	70,107,113	1.96	16 (22%)
20	CLA	B	1209	-	46,54,73	1.56	7 (15%)	53,90,113	2.14	13 (24%)
20	CLA	B	1201	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	15 (19%)
20	CLA	A	1127	-	65,73,73	1.40	9 (13%)	76,113,113	1.96	18 (23%)
20	CLA	A	1130	-	55,63,73	1.47	7 (12%)	64,101,113	2.10	18 (28%)
20	CLA	3	608	-	48,56,73	1.55	8 (16%)	55,92,113	2.19	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	LMT	A	5004	-	36,36,36	1.21	7 (19%)	47,47,47	1.08	3 (6%)
30	CHL	3	604	-	66,74,74	0.89	2 (3%)	73,114,114	1.39	9 (12%)
30	CHL	2	613	-	46,54,74	1.00	3 (6%)	49,90,114	1.48	9 (18%)
20	CLA	A	1111	-	65,73,73	1.38	8 (12%)	76,113,113	2.06	19 (25%)
20	CLA	1	603	-	55,63,73	1.49	7 (12%)	64,101,113	2.20	19 (29%)
20	CLA	3	617	-	60,68,73	1.38	7 (11%)	70,107,113	2.03	17 (24%)
23	LHG	3	801	30	16,16,48	0.83	1 (6%)	17,20,54	0.68	0
26	LMG	2	804	-	30,30,55	0.54	0	38,38,63	1.14	3 (7%)
20	CLA	1	613	-	45,53,73	1.68	7 (15%)	52,89,113	2.02	13 (25%)
20	CLA	3	613	-	46,54,73	1.59	7 (15%)	53,90,113	2.17	14 (26%)
23	LHG	1	801	-	48,48,48	0.44	0	51,54,54	1.20	3 (5%)
20	CLA	A	1140	-	65,73,73	1.38	7 (10%)	76,113,113	1.94	17 (22%)
20	CLA	B	1204	-	65,73,73	1.38	8 (12%)	76,113,113	2.01	17 (22%)
20	CLA	B	1229	-	65,73,73	1.37	8 (12%)	76,113,113	2.06	20 (26%)
20	CLA	J	1901	10	50,58,73	1.55	9 (18%)	58,95,113	2.25	17 (29%)
20	CLA	B	1208	-	60,68,73	1.44	7 (11%)	70,107,113	1.96	14 (20%)
23	LHG	2	801	20	34,34,48	0.44	0	37,40,54	1.13	2 (5%)
20	CLA	B	1207	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	17 (22%)
30	CHL	4	615	-	43,51,74	1.03	2 (4%)	45,86,114	1.41	9 (20%)
20	CLA	1	602	13	46,54,73	1.63	8 (17%)	53,90,113	2.07	14 (26%)
20	CLA	G	1603	-	65,73,73	1.37	9 (13%)	76,113,113	2.16	18 (23%)
20	CLA	2	607	23	60,68,73	1.38	6 (10%)	70,107,113	2.13	19 (27%)
28	DGD	G	5003	-	48,48,67	0.84	1 (2%)	62,62,81	1.01	2 (3%)
20	CLA	A	1126	-	65,73,73	1.42	8 (12%)	76,113,113	1.95	16 (21%)
20	CLA	L	1502	-	60,68,73	1.38	7 (11%)	70,107,113	2.06	17 (24%)
20	CLA	2	603	14	65,73,73	1.37	9 (13%)	76,113,113	1.99	18 (23%)
20	CLA	B	1211	-	65,73,73	1.37	8 (12%)	76,113,113	2.07	19 (25%)
22	BCR	B	4004	-	41,41,41	1.93	4 (9%)	56,56,56	4.84	23 (41%)
28	DGD	B	5005	-	62,62,67	1.11	6 (9%)	76,76,81	1.03	4 (5%)
30	CHL	4	611	-	51,59,74	1.05	3 (5%)	55,96,114	1.46	12 (21%)
22	BCR	B	4006	-	41,41,41	1.87	4 (9%)	56,56,56	4.24	21 (37%)
23	LHG	B	5002	-	48,48,48	0.40	0	51,54,54	1.10	3 (5%)
20	CLA	B	1218	-	65,73,73	1.37	7 (10%)	76,113,113	2.00	16 (21%)
29	LUT	3	501	-	42,43,43	2.35	2 (4%)	51,60,60	2.20	18 (35%)
20	CLA	4	608	-	46,54,73	1.58	8 (17%)	53,90,113	2.18	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	A	1141	23	60,68,73	1.40	7 (11%)	70,107,113	2.02	18 (25%)
23	LHG	A	5001	20	39,39,48	0.45	0	42,45,54	1.25	4 (9%)
22	BCR	L	4020	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	18 (32%)
20	CLA	F	1302	6	65,73,73	1.37	7 (10%)	76,113,113	1.92	14 (18%)
24	LMT	G	5005	-	32,32,36	1.23	5 (15%)	43,43,47	1.02	2 (4%)
20	CLA	4	603	-	65,73,73	1.33	7 (10%)	76,113,113	1.88	15 (19%)
24	LMT	G	5004	-	36,36,36	1.20	6 (16%)	47,47,47	1.05	3 (6%)
20	CLA	A	1109	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
26	LMG	F	5001	-	30,30,55	0.52	0	38,38,63	1.21	2 (5%)
21	PQN	A	2001	-	34,34,34	0.37	0	42,45,45	1.26	4 (9%)
26	LMG	2	802	-	25,25,55	0.53	0	33,33,63	1.27	3 (9%)
20	CLA	B	1230	-	58,66,73	1.44	7 (12%)	67,104,113	2.15	18 (26%)
20	CLA	1	601	13	65,73,73	1.36	7 (10%)	76,113,113	2.07	20 (26%)
20	CLA	B	1203	-	65,73,73	1.37	7 (10%)	76,113,113	1.96	17 (22%)
20	CLA	4	602	-	50,58,73	1.52	8 (16%)	58,95,113	2.12	16 (27%)
20	CLA	A	1133	-	65,73,73	1.39	8 (12%)	76,113,113	1.91	17 (22%)
20	CLA	2	602	-	52,60,73	1.51	8 (15%)	60,97,113	2.15	17 (28%)
22	BCR	K	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.35	15 (26%)
20	CLA	A	1138	-	65,73,73	1.38	8 (12%)	76,113,113	1.93	15 (19%)
20	CLA	G	1602	-	46,54,73	1.65	7 (15%)	53,90,113	2.14	17 (32%)
20	CLA	L	1501	12	50,58,73	1.52	8 (16%)	58,95,113	2.22	16 (27%)
26	LMG	G	5006	-	25,25,55	0.56	0	33,33,63	1.34	4 (12%)
20	CLA	A	1132	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	16 (21%)
20	CLA	1	611	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	16 (21%)
28	DGD	F	5005	-	58,58,67	1.05	4 (6%)	72,72,81	1.12	5 (6%)
22	BCR	J	4012	-	41,41,41	1.85	4 (9%)	56,56,56	4.21	19 (33%)
20	CLA	B	1221	-	65,73,73	1.39	7 (10%)	76,113,113	2.09	22 (28%)
20	CLA	A	1107	1	65,73,73	1.35	7 (10%)	76,113,113	2.09	19 (25%)
20	CLA	4	604	-	60,68,73	1.40	8 (13%)	70,107,113	2.06	16 (22%)
28	DGD	4	802	-	52,52,67	0.89	2 (3%)	66,66,81	1.03	2 (3%)
20	CLA	B	1234	-	55,63,73	1.51	8 (14%)	64,101,113	2.11	16 (25%)
26	LMG	2	803	-	36,36,55	0.64	1 (2%)	44,44,63	1.05	3 (6%)
20	CLA	A	1104	-	65,73,73	1.39	8 (12%)	76,113,113	2.05	19 (25%)
20	CLA	B	1212	-	55,63,73	1.48	8 (14%)	64,101,113	2.17	16 (25%)
20	CLA	B	1205	-	65,73,73	1.38	7 (10%)	76,113,113	2.03	18 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	1220	-	55,63,73	1.50	8 (14%)	64,101,113	2.08	13 (20%)
34	FES	N	101	17	0,4,4	-	-	-		
22	BCR	I	4018	-	41,41,41	1.94	4 (9%)	56,56,56	3.88	19 (33%)
21	PQN	B	2002	-	34,34,34	0.41	0	42,45,45	1.28	4 (9%)
22	BCR	H	4021	-	41,41,41	1.87	4 (9%)	56,56,56	4.40	17 (30%)
26	LMG	G	5001	-	49,49,55	1.00	4 (8%)	57,57,63	1.17	5 (8%)
29	LUT	3	502	-	42,43,43	2.32	1 (2%)	51,60,60	2.10	13 (25%)
30	CHL	1	612	-	61,69,74	1.05	4 (6%)	67,108,114	1.37	11 (16%)
20	CLA	1	606	-	50,58,73	1.57	7 (14%)	58,95,113	2.25	20 (34%)
20	CLA	B	1238	36	65,73,73	1.33	8 (12%)	76,113,113	1.98	15 (19%)
22	BCR	K	4002	-	41,41,41	1.87	4 (9%)	56,56,56	4.47	18 (32%)
20	CLA	A	1105	-	60,68,73	1.42	8 (13%)	70,107,113	2.13	17 (24%)
20	CLA	B	1237	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	20 (26%)
24	LMT	B	5006	-	33,33,36	1.24	6 (18%)	44,44,47	1.00	3 (6%)
26	LMG	F	5004	-	34,34,55	0.46	0	42,42,63	1.12	2 (4%)
20	CLA	A	1106	1	65,73,73	1.38	8 (12%)	76,113,113	2.03	19 (25%)
22	BCR	F	4016	-	41,41,41	1.87	5 (12%)	56,56,56	4.29	15 (26%)
20	CLA	B	1219	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	17 (22%)
20	CLA	A	1125	-	65,73,73	1.38	8 (12%)	76,113,113	2.09	20 (26%)
30	CHL	2	611	-	48,56,74	1.00	3 (6%)	51,92,114	1.55	11 (21%)
20	CLA	A	1120	-	60,68,73	1.44	7 (11%)	70,107,113	2.01	14 (20%)
19	CL0	A	1011	-	65,73,73	2.18	16 (24%)	76,113,113	2.50	25 (32%)
20	CLA	B	1236	-	50,58,73	1.57	7 (14%)	58,95,113	2.26	17 (29%)
20	CLA	B	1227	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	18 (23%)
20	CLA	B	1240	23	65,73,73	1.39	8 (12%)	76,113,113	2.10	21 (27%)
20	CLA	2	608	-	50,58,73	1.60	7 (14%)	58,95,113	2.33	17 (29%)
20	CLA	4	605	-	60,68,73	1.46	7 (11%)	70,107,113	2.01	19 (27%)
29	LUT	J	4013	-	42,43,43	2.26	2 (4%)	51,60,60	2.41	18 (35%)
28	DGD	J	5001	-	59,59,67	1.06	6 (10%)	73,73,81	1.02	2 (2%)
20	CLA	1	608	-	46,54,73	1.62	7 (15%)	53,90,113	2.23	14 (26%)
20	CLA	B	1021	-	65,73,73	1.40	9 (13%)	76,113,113	2.03	19 (25%)
20	CLA	A	1101	-	65,73,73	1.33	8 (12%)	76,113,113	2.01	17 (22%)
20	CLA	B	1217	-	46,54,73	1.64	7 (15%)	53,90,113	2.17	13 (24%)
22	BCR	A	4002	-	41,41,41	1.85	5 (12%)	56,56,56	4.24	17 (30%)
26	LMG	F	5002	-	47,47,55	0.97	4 (8%)	55,55,63	1.20	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	3	607	23	51,59,74	0.99	3 (5%)	55,96,114	1.39	10 (18%)
22	BCR	1	504	-	41,41,41	1.90	4 (9%)	56,56,56	4.66	14 (25%)
26	LMG	2	805	-	30,30,55	0.52	0	38,38,63	1.08	2 (5%)
20	CLA	A	1139	-	65,73,73	1.38	8 (12%)	76,113,113	2.02	18 (23%)
26	LMG	B	5007	-	34,34,55	0.50	0	42,42,63	1.07	3 (7%)
31	XAT	2	502	-	39,47,47	0.80	1 (2%)	54,74,74	2.23	15 (27%)
22	BCR	2	503	-	41,41,41	1.95	5 (12%)	56,56,56	5.26	27 (48%)
20	CLA	A	1013	-	65,73,73	1.40	7 (10%)	76,113,113	1.94	20 (26%)
26	LMG	3	802	-	30,30,55	0.56	0	38,38,63	1.14	3 (7%)
28	DGD	3	803	-	52,52,67	0.89	2 (3%)	66,66,81	1.14	4 (6%)
20	CLA	B	1215	-	65,73,73	1.37	8 (12%)	76,113,113	2.12	20 (26%)
20	CLA	3	612	-	50,58,73	1.53	8 (16%)	58,95,113	2.20	15 (25%)
20	CLA	2	606	-	50,58,73	1.53	7 (14%)	58,95,113	2.24	18 (31%)
20	CLA	L	1503	-	50,58,73	1.53	7 (14%)	58,95,113	2.19	17 (29%)
20	CLA	B	1223	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	19 (25%)
20	CLA	4	606	-	50,58,73	1.55	6 (12%)	58,95,113	2.23	19 (32%)
25	SF4	C	3003	3	0,12,12	-	-	-	-	-
20	CLA	3	602	-	52,60,73	1.53	8 (15%)	60,97,113	2.24	18 (30%)
20	CLA	3	601	-	55,63,73	1.46	7 (12%)	64,101,113	2.24	21 (32%)
29	LUT	1	501	-	42,43,43	2.38	2 (4%)	51,60,60	2.02	16 (31%)
22	BCR	F	4014	-	41,41,41	1.84	4 (9%)	56,56,56	4.27	17 (30%)
20	CLA	A	1124	-	55,63,73	1.50	8 (14%)	64,101,113	2.13	17 (26%)
26	LMG	B	5003	-	35,35,55	0.73	1 (2%)	43,43,63	1.13	3 (6%)
22	BCR	A	4011	-	41,41,41	1.86	5 (12%)	56,56,56	4.30	19 (33%)
20	CLA	A	1118	-	50,58,73	1.56	7 (14%)	58,95,113	2.33	18 (31%)
20	CLA	K	1403	-	48,56,73	1.58	7 (14%)	55,92,113	2.22	16 (29%)
22	BCR	B	4005	-	41,41,41	1.86	4 (9%)	56,56,56	4.33	17 (30%)
20	CLA	A	1112	-	65,73,73	1.39	7 (10%)	76,113,113	1.96	18 (23%)
20	CLA	B	1232	-	55,63,73	1.53	7 (12%)	64,101,113	2.15	19 (29%)
20	CLA	A	1134	1	55,63,73	1.50	7 (12%)	64,101,113	2.08	14 (21%)
20	CLA	B	1206	2	65,73,73	1.39	7 (10%)	76,113,113	2.00	17 (22%)
20	CLA	B	1224	-	65,73,73	1.39	7 (10%)	76,113,113	2.01	16 (21%)
20	CLA	B	1202	-	65,73,73	1.37	7 (10%)	76,113,113	1.99	19 (25%)
20	CLA	2	605	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	20 (26%)
20	CLA	A	1136	-	65,73,73	1.39	7 (10%)	76,113,113	1.90	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	1	609	13	56,64,74	0.93	3 (5%)	61,102,114	1.41	10 (16%)
32	3PH	2	807	-	32,32,47	1.01	4 (12%)	36,37,52	1.20	2 (5%)
20	CLA	B	1225	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	18 (23%)
20	CLA	2	604	14	65,73,73	1.34	8 (12%)	76,113,113	1.97	17 (22%)
30	CHL	3	611	-	47,55,74	1.17	3 (6%)	50,91,114	1.54	11 (22%)

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
20	CLA	3	614	-	1/1/10/20	3/10/88/115	-
20	CLA	K	1402	-	1/1/14/20	20/31/109/115	-
26	LMG	F	5006	-	-	1/4/24/70	0/1/1/1
20	CLA	A	1012	-	1/1/15/20	20/37/115/115	-
20	CLA	A	1129	-	1/1/15/20	15/37/115/115	-
20	CLA	B	1216	-	1/1/15/20	12/37/115/115	-
33	C7Z	4	505	-	-	16/29/67/67	0/2/2/2
20	CLA	A	1116	-	1/1/13/20	11/27/105/115	-
22	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
29	LUT	4	501	-	-	5/29/67/67	0/2/2/2
24	LMT	2	808	-	-	2/21/61/61	0/2/2/2
20	CLA	4	612	-	1/1/15/20	17/37/115/115	-
20	CLA	3	610	15	1/1/15/20	21/37/115/115	-
26	LMG	A	5006	-	-	11/45/65/70	0/1/1/1
20	CLA	K	1404	11	1/1/11/20	5/15/93/115	-
20	CLA	A	1121	-	1/1/14/20	14/31/109/115	-
20	CLA	B	1210	-	1/1/15/20	16/37/115/115	-
20	CLA	1	607	-	1/1/11/20	7/15/93/115	-
31	XAT	4	502	-	2/2/12/26	2/31/93/93	0/4/4/4
20	CLA	A	1110	-	1/1/13/20	6/25/103/115	-
20	CLA	A	1135	-	1/1/12/20	8/21/99/115	-
20	CLA	A	1137	-	1/1/15/20	18/37/115/115	-
26	LMG	G	5002	-	-	18/45/65/70	0/1/1/1
30	CHL	2	610	-	4/4/18/26	4/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	K	1401	-	1/1/11/20	8/13/91/115	-
20	CLA	B	1213	-	1/1/14/20	8/31/109/115	-
29	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
22	BCR	A	4017	-	-	6/29/63/63	0/2/2/2
20	CLA	A	1128	-	1/1/15/20	16/37/115/115	-
20	CLA	B	1239	-	1/1/15/20	20/37/115/115	-
22	BCR	L	4019	-	-	14/29/63/63	0/2/2/2
22	BCR	1	503	-	-	16/29/63/63	0/2/2/2
20	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
20	CLA	B	1214	-	1/1/15/20	14/37/115/115	-
20	CLA	1	605	-	1/1/15/20	18/37/115/115	-
20	CLA	1	614	13	1/1/14/20	15/31/109/115	-
20	CLA	3	606	-	1/1/12/20	12/19/97/115	-
20	CLA	A	1103	-	1/1/15/20	22/37/115/115	-
20	CLA	A	1115	-	1/1/15/20	22/37/115/115	-
20	CLA	1	604	-	1/1/15/20	17/37/115/115	-
30	CHL	4	613	-	4/4/19/26	8/33/131/137	-
20	CLA	A	1108	-	1/1/12/20	7/19/97/115	-
20	CLA	4	607	-	1/1/14/20	15/31/109/115	-
30	CHL	1	610	13	3/3/16/26	7/17/115/137	-
20	CLA	B	1235	-	1/1/15/20	17/37/115/115	-
20	CLA	4	601	16	1/1/14/20	14/31/109/115	-
23	LHG	B	5001	20	-	14/23/23/53	-
26	LMG	F	5003	-	-	6/31/51/70	0/1/1/1
22	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
20	CLA	3	603	15	1/1/13/20	15/25/103/115	-
30	CHL	2	615	-	4/4/18/26	5/27/125/137	-
20	CLA	F	1301	-	1/1/15/20	17/37/115/115	-
23	LHG	A	5002	-	-	37/53/53/53	-
22	BCR	3	506	-	-	14/29/63/63	0/2/2/2
20	CLA	A	1113	-	1/1/11/20	9/13/91/115	-
20	CLA	B	1022	-	1/1/15/20	4/37/115/115	-
20	CLA	H	1701	8	1/1/14/20	17/31/109/115	-
20	CLA	A	1114	-	1/1/11/20	8/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	3	503	-	-	15/29/63/63	0/2/2/2
20	CLA	3	605	-	1/1/13/20	8/25/103/115	-
25	SF4	C	3002	3	-	-	0/6/5/5
20	CLA	B	1023	-	1/1/15/20	11/37/115/115	-
26	LMG	B	5004	-	-	13/28/48/70	0/1/1/1
20	CLA	A	1122	-	1/1/15/20	16/37/115/115	-
20	CLA	A	1131	-	1/1/15/20	11/37/115/115	-
30	CHL	2	609	-	4/4/20/26	9/39/137/137	-
30	CHL	4	610	-	3/3/16/26	2/17/115/137	-
20	CLA	G	1601	-	1/1/13/20	9/25/103/115	-
20	CLA	B	1231	-	1/1/14/20	10/31/109/115	-
20	CLA	B	1228	-	1/1/14/20	16/31/109/115	-
20	CLA	B	1222	36	1/1/15/20	22/37/115/115	-
22	BCR	B	4010	-	-	13/29/63/63	0/2/2/2
26	LMG	1	802	-	-	8/41/61/70	0/1/1/1
26	LMG	2	806	-	-	1/4/24/70	0/1/1/1
22	BCR	A	4007	-	-	9/29/63/63	0/2/2/2
20	CLA	4	617	-	1/1/15/20	20/37/115/115	-
23	LHG	4	801	-	-	19/39/39/53	-
25	SF4	A	3001	2,1	-	-	0/6/5/5
20	CLA	4	609	16	1/1/12/20	10/19/97/115	-
20	CLA	A	1119	-	1/1/15/20	18/37/115/115	-
20	CLA	A	1123	-	1/1/15/20	15/37/115/115	-
22	BCR	I	4020	-	-	15/29/63/63	0/2/2/2
20	CLA	2	612	-	1/1/13/20	12/25/103/115	-
28	DGD	1	803	-	-	15/30/70/95	0/2/2/2
22	BCR	G	4011	-	-	9/29/63/63	0/2/2/2
24	LMT	B	5008	-	-	8/17/57/61	0/2/2/2
22	BCR	B	4009	-	-	9/29/63/63	0/2/2/2
29	LUT	1	502	-	-	5/29/67/67	0/2/2/2
20	CLA	A	1102	-	1/1/15/20	23/37/115/115	-
20	CLA	B	1226	-	1/1/15/20	20/37/115/115	-
20	CLA	2	601	-	1/1/14/20	12/31/109/115	-
20	CLA	B	1209	-	1/1/11/20	6/15/93/115	-
20	CLA	B	1201	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1127	-	1/1/15/20	19/37/115/115	-
20	CLA	A	1130	-	1/1/13/20	12/25/103/115	-
20	CLA	3	608	-	1/1/11/20	4/17/95/115	-
30	CHL	3	604	-	4/4/20/26	12/39/137/137	-
24	LMT	A	5004	-	-	9/21/61/61	0/2/2/2
30	CHL	2	613	-	3/3/16/26	6/15/113/137	-
20	CLA	A	1111	-	1/1/15/20	20/37/115/115	-
20	CLA	1	603	-	1/1/13/20	10/25/103/115	-
20	CLA	3	617	-	1/1/14/20	12/31/109/115	-
23	LHG	3	801	30	-	13/19/19/53	-
26	LMG	2	804	-	-	8/25/45/70	0/1/1/1
20	CLA	1	613	-	1/1/11/20	6/13/91/115	-
20	CLA	3	613	-	1/1/11/20	7/15/93/115	-
23	LHG	1	801	-	-	29/53/53/53	-
20	CLA	A	1140	-	1/1/15/20	12/37/115/115	-
20	CLA	B	1204	-	1/1/15/20	22/37/115/115	-
20	CLA	B	1229	-	1/1/15/20	12/37/115/115	-
20	CLA	J	1901	10	1/1/12/20	8/19/97/115	-
20	CLA	B	1208	-	1/1/14/20	13/31/109/115	-
23	LHG	2	801	20	-	19/39/39/53	-
20	CLA	B	1207	-	1/1/15/20	24/37/115/115	-
30	CHL	4	615	-	3/3/15/26	2/12/110/137	-
20	CLA	1	602	13	1/1/11/20	6/15/93/115	-
20	CLA	G	1603	-	1/1/15/20	17/37/115/115	-
20	CLA	2	607	23	1/1/14/20	15/31/109/115	-
28	DGD	G	5003	-	-	11/36/76/95	0/2/2/2
20	CLA	A	1126	-	1/1/15/20	21/37/115/115	-
20	CLA	L	1502	-	1/1/14/20	21/31/109/115	-
20	CLA	2	603	14	1/1/15/20	15/37/115/115	-
20	CLA	B	1211	-	1/1/15/20	22/37/115/115	-
22	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
30	CHL	4	611	-	3/3/17/26	2/21/119/137	-
28	DGD	B	5005	-	-	19/50/90/95	0/2/2/2
22	BCR	B	4006	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	B	5002	-	-	30/53/53/53	-
20	CLA	B	1218	-	1/1/15/20	10/37/115/115	-
29	LUT	3	501	-	-	5/29/67/67	0/2/2/2
20	CLA	4	608	-	1/1/11/20	6/15/93/115	-
20	CLA	A	1141	23	1/1/14/20	14/31/109/115	-
23	LHG	A	5001	20	-	22/44/44/53	-
22	BCR	L	4020	-	-	9/29/63/63	0/2/2/2
20	CLA	F	1302	6	1/1/15/20	17/37/115/115	-
24	LMT	G	5005	-	-	6/17/57/61	0/2/2/2
20	CLA	4	603	-	1/1/15/20	17/37/115/115	-
24	LMT	G	5004	-	-	10/21/61/61	0/2/2/2
20	CLA	A	1109	-	1/1/15/20	13/37/115/115	-
26	LMG	F	5001	-	-	7/25/45/70	0/1/1/1
21	PQN	A	2001	-	-	3/23/43/43	0/2/2/2
26	LMG	2	802	-	-	8/20/40/70	0/1/1/1
20	CLA	B	1230	-	1/1/13/20	14/29/107/115	-
20	CLA	1	601	13	1/1/15/20	20/37/115/115	-
20	CLA	B	1203	-	1/1/15/20	15/37/115/115	-
20	CLA	4	602	-	1/1/12/20	7/19/97/115	-
20	CLA	A	1133	-	1/1/15/20	15/37/115/115	-
20	CLA	2	602	-	1/1/12/20	8/22/100/115	-
22	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
20	CLA	A	1138	-	1/1/15/20	17/37/115/115	-
20	CLA	G	1602	-	1/1/11/20	8/15/93/115	-
20	CLA	L	1501	12	1/1/12/20	12/19/97/115	-
26	LMG	G	5006	-	-	11/20/40/70	0/1/1/1
20	CLA	A	1132	-	1/1/15/20	13/37/115/115	-
20	CLA	1	611	-	1/1/15/20	14/37/115/115	-
28	DGD	F	5005	-	-	18/46/86/95	0/2/2/2
22	BCR	J	4012	-	-	12/29/63/63	0/2/2/2
20	CLA	B	1221	-	1/1/15/20	21/37/115/115	-
20	CLA	A	1107	1	1/1/15/20	17/37/115/115	-
20	CLA	4	604	-	1/1/14/20	16/31/109/115	-
28	DGD	4	802	-	-	17/40/80/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1234	-	1/1/13/20	9/25/103/115	-
26	LMG	2	803	-	-	12/31/51/70	0/1/1/1
20	CLA	A	1104	-	1/1/15/20	17/37/115/115	-
20	CLA	B	1212	-	1/1/13/20	9/25/103/115	-
20	CLA	B	1205	-	1/1/15/20	16/37/115/115	-
20	CLA	B	1220	-	1/1/13/20	12/25/103/115	-
34	FES	N	101	17	-	-	0/1/1/1
29	LUT	3	502	-	1/1/12/27	11/29/67/67	0/2/2/2
21	PQN	B	2002	-	-	8/23/43/43	0/2/2/2
22	BCR	H	4021	-	-	12/29/63/63	0/2/2/2
30	CHL	1	612	-	4/4/19/26	8/33/131/137	-
22	BCR	I	4018	-	-	14/29/63/63	0/2/2/2
26	LMG	G	5001	-	-	21/44/64/70	0/1/1/1
20	CLA	1	606	-	1/1/12/20	7/19/97/115	-
20	CLA	B	1238	36	1/1/15/20	17/37/115/115	-
22	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
20	CLA	A	1105	-	1/1/14/20	19/31/109/115	-
20	CLA	B	1237	-	1/1/15/20	21/37/115/115	-
24	LMT	B	5006	-	-	7/18/58/61	0/2/2/2
26	LMG	F	5004	-	-	8/29/49/70	0/1/1/1
20	CLA	A	1106	1	1/1/15/20	19/37/115/115	-
22	BCR	F	4016	-	-	15/29/63/63	0/2/2/2
20	CLA	B	1219	-	1/1/15/20	20/37/115/115	-
20	CLA	A	1125	-	1/1/15/20	18/37/115/115	-
30	CHL	2	611	-	3/3/16/26	3/18/116/137	-
20	CLA	A	1120	-	1/1/14/20	15/31/109/115	-
19	CL0	A	1011	-	3/3/20/25	7/37/135/135	-
20	CLA	B	1236	-	1/1/12/20	10/19/97/115	-
20	CLA	B	1227	-	1/1/15/20	13/37/115/115	-
20	CLA	B	1240	23	1/1/15/20	20/37/115/115	-
20	CLA	2	608	-	1/1/12/20	7/19/97/115	-
20	CLA	4	605	-	-	13/31/109/115	-
29	LUT	J	4013	-	-	7/29/67/67	0/2/2/2
28	DGD	J	5001	-	-	13/47/87/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	608	-	1/1/11/20	5/15/93/115	-
20	CLA	B	1021	-	1/1/15/20	16/37/115/115	-
20	CLA	A	1101	-	1/1/15/20	18/37/115/115	-
20	CLA	B	1217	-	1/1/11/20	5/15/93/115	-
22	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
26	LMG	F	5002	-	-	11/42/62/70	0/1/1/1
30	CHL	3	607	23	3/3/17/26	6/21/119/137	-
22	BCR	1	504	-	-	14/29/63/63	0/2/2/2
26	LMG	2	805	-	-	8/25/45/70	0/1/1/1
20	CLA	A	1139	-	1/1/15/20	14/37/115/115	-
26	LMG	B	5007	-	-	11/29/49/70	0/1/1/1
31	XAT	2	502	-	2/2/12/26	4/31/93/93	0/4/4/4
22	BCR	2	503	-	-	14/29/63/63	0/2/2/2
20	CLA	A	1013	-	1/1/15/20	18/37/115/115	-
26	LMG	3	802	-	-	14/25/45/70	0/1/1/1
28	DGD	3	803	-	-	10/40/80/95	0/2/2/2
20	CLA	B	1215	-	1/1/15/20	16/37/115/115	-
20	CLA	3	612	-	1/1/12/20	11/19/97/115	-
20	CLA	2	606	-	1/1/12/20	9/19/97/115	-
20	CLA	L	1503	-	1/1/12/20	9/19/97/115	-
20	CLA	B	1223	-	1/1/15/20	14/37/115/115	-
20	CLA	4	606	-	1/1/12/20	7/19/97/115	-
25	SF4	C	3003	3	-	-	0/6/5/5
20	CLA	3	602	-	1/1/12/20	9/22/100/115	-
20	CLA	3	601	-	1/1/13/20	14/25/103/115	-
29	LUT	1	501	-	-	3/29/67/67	0/2/2/2
22	BCR	F	4014	-	-	9/29/63/63	0/2/2/2
20	CLA	A	1124	-	1/1/13/20	8/25/103/115	-
26	LMG	B	5003	-	-	8/30/50/70	0/1/1/1
22	BCR	A	4011	-	-	16/29/63/63	0/2/2/2
20	CLA	A	1118	-	1/1/12/20	7/19/97/115	-
20	CLA	K	1403	-	1/1/11/20	9/17/95/115	-
22	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
20	CLA	A	1112	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1232	-	1/1/13/20	13/25/103/115	-
20	CLA	A	1134	1	1/1/13/20	14/25/103/115	-
20	CLA	B	1206	2	1/1/15/20	20/37/115/115	-
20	CLA	B	1224	-	1/1/15/20	18/37/115/115	-
20	CLA	B	1202	-	1/1/15/20	15/37/115/115	-
20	CLA	2	605	-	1/1/15/20	22/37/115/115	-
20	CLA	A	1136	-	1/1/15/20	14/37/115/115	-
30	CHL	1	609	13	4/4/18/26	0/27/125/137	-
32	3PH	2	807	-	-	16/34/34/49	-
20	CLA	B	1225	-	1/1/15/20	16/37/115/115	-
20	CLA	2	604	14	1/1/15/20	17/37/115/115	-
30	CHL	3	611	-	3/3/16/26	0/17/115/137	-

The worst 5 of 1347 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	1	502	LUT	C24-C25	14.56	1.51	1.33
33	4	505	C7Z	C34-C33	14.48	1.55	1.35
33	4	505	C7Z	C30-C29	14.33	1.54	1.35
29	4	501	LUT	C24-C25	14.28	1.50	1.33
29	1	501	LUT	C24-C25	14.27	1.50	1.33

The worst 5 of 3346 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	A	4017	BCR	C16-C15-C14	18.16	160.67	123.47
22	H	4021	BCR	C10-C11-C12	18.10	179.72	123.22
22	B	4004	BCR	C11-C10-C9	17.84	152.77	127.31
22	3	506	BCR	C10-C11-C12	17.71	178.49	123.22
22	1	504	BCR	C10-C11-C12	17.60	178.15	123.22

5 of 201 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1011	CL0	NA
19	A	1011	CL0	ND
19	A	1011	CL0	NC
20	A	1101	CLA	ND
20	A	1102	CLA	ND

5 of 2969 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1101	CLA	C2-C1-O2A-CGA
20	A	1101	CLA	CHA-CBD-CGD-O1D
20	A	1101	CLA	CHA-CBD-CGD-O2D
20	A	1102	CLA	C3A-C2A-CAA-CBA
20	A	1103	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

229 monomers are involved in 1607 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	3	614	CLA	1	0
20	K	1402	CLA	3	0
20	A	1012	CLA	11	0
20	A	1129	CLA	2	0
20	B	1216	CLA	7	0
33	4	505	C7Z	4	0
20	A	1116	CLA	13	0
29	4	501	LUT	20	0
24	2	808	LMT	8	0
20	4	612	CLA	21	0
20	3	610	CLA	3	0
26	A	5006	LMG	3	0
20	K	1404	CLA	3	0
20	A	1121	CLA	3	0
20	B	1210	CLA	11	0
20	1	607	CLA	1	0
31	4	502	XAT	14	0
20	A	1110	CLA	8	0
20	A	1135	CLA	5	0
20	A	1137	CLA	4	0
26	G	5002	LMG	8	0
30	2	610	CHL	16	0
20	K	1401	CLA	11	0
20	B	1213	CLA	3	0
29	2	501	LUT	13	0
22	A	4017	BCR	8	0
20	A	1128	CLA	5	0
20	B	1239	CLA	8	0
22	L	4019	BCR	28	0
22	1	503	BCR	1	0
20	A	1117	CLA	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1214	CLA	9	0
20	1	605	CLA	9	0
20	1	614	CLA	5	0
20	3	606	CLA	7	0
20	A	1103	CLA	18	0
20	A	1115	CLA	10	0
20	1	604	CLA	15	0
30	4	613	CHL	5	0
20	A	1108	CLA	5	0
20	4	607	CLA	12	0
30	1	610	CHL	10	0
20	B	1235	CLA	5	0
20	4	601	CLA	36	0
23	B	5001	LHG	2	0
26	F	5003	LMG	3	0
22	A	4008	BCR	4	0
20	3	603	CLA	10	0
30	2	615	CHL	4	0
20	F	1301	CLA	12	0
23	A	5002	LHG	2	0
22	3	506	BCR	3	0
20	A	1113	CLA	19	0
20	B	1022	CLA	11	0
20	H	1701	CLA	21	0
20	A	1114	CLA	3	0
22	3	503	BCR	11	0
20	3	605	CLA	6	0
25	C	3002	SF4	1	0
20	B	1023	CLA	3	0
26	B	5004	LMG	2	0
20	A	1122	CLA	8	0
20	A	1131	CLA	10	0
30	2	609	CHL	21	0
30	4	610	CHL	3	0
20	G	1601	CLA	6	0
20	B	1231	CLA	5	0
20	B	1228	CLA	4	0
20	B	1222	CLA	8	0
22	B	4010	BCR	3	0
26	1	802	LMG	8	0
22	A	4007	BCR	5	0
20	4	617	CLA	12	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	4	801	LHG	11	0
20	4	609	CLA	16	0
20	A	1119	CLA	13	0
20	A	1123	CLA	10	0
22	I	4020	BCR	10	0
20	2	612	CLA	14	0
28	1	803	DGD	1	0
22	G	4011	BCR	5	0
24	B	5008	LMT	1	0
22	B	4009	BCR	4	0
29	1	502	LUT	34	0
20	A	1102	CLA	6	0
20	B	1226	CLA	7	0
20	2	601	CLA	8	0
20	B	1209	CLA	4	0
20	B	1201	CLA	5	0
20	A	1127	CLA	12	0
20	A	1130	CLA	3	0
20	3	608	CLA	5	0
24	A	5004	LMT	1	0
30	3	604	CHL	3	0
30	2	613	CHL	5	0
20	A	1111	CLA	13	0
20	1	603	CLA	20	0
20	3	617	CLA	18	0
26	2	804	LMG	2	0
20	1	613	CLA	9	0
20	3	613	CLA	2	0
23	1	801	LHG	11	0
20	A	1140	CLA	7	0
20	B	1204	CLA	9	0
20	B	1229	CLA	8	0
20	J	1901	CLA	7	0
20	B	1208	CLA	3	0
23	2	801	LHG	7	0
20	B	1207	CLA	12	0
30	4	615	CHL	3	0
20	1	602	CLA	2	0
20	G	1603	CLA	13	0
20	2	607	CLA	9	0
28	G	5003	DGD	3	0
20	A	1126	CLA	22	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	1502	CLA	18	0
20	2	603	CLA	9	0
20	B	1211	CLA	11	0
22	B	4004	BCR	5	0
28	B	5005	DGD	7	0
30	4	611	CHL	1	0
22	B	4006	BCR	5	0
23	B	5002	LHG	4	0
20	B	1218	CLA	9	0
29	3	501	LUT	5	0
20	4	608	CLA	14	0
20	A	1141	CLA	3	0
23	A	5001	LHG	1	0
22	L	4020	BCR	19	0
20	F	1302	CLA	8	0
20	4	603	CLA	16	0
20	A	1109	CLA	15	0
26	F	5001	LMG	1	0
21	A	2001	PQN	7	0
26	2	802	LMG	10	0
20	B	1230	CLA	9	0
20	1	601	CLA	13	0
20	B	1203	CLA	4	0
20	4	602	CLA	18	0
20	A	1133	CLA	12	0
20	2	602	CLA	3	0
22	K	4001	BCR	9	0
20	A	1138	CLA	4	0
20	G	1602	CLA	2	0
20	L	1501	CLA	18	0
26	G	5006	LMG	1	0
20	A	1132	CLA	27	0
20	1	611	CLA	10	0
28	F	5005	DGD	18	0
22	J	4012	BCR	5	0
20	B	1221	CLA	4	0
20	A	1107	CLA	10	0
20	4	604	CLA	26	0
28	4	802	DGD	4	0
20	B	1234	CLA	12	0
26	2	803	LMG	4	0
20	A	1104	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1212	CLA	5	0
20	B	1205	CLA	9	0
20	B	1220	CLA	3	0
22	I	4018	BCR	8	0
21	B	2002	PQN	3	0
22	H	4021	BCR	21	0
26	G	5001	LMG	5	0
29	3	502	LUT	4	0
30	1	612	CHL	6	0
20	1	606	CLA	10	0
20	B	1238	CLA	9	0
22	K	4002	BCR	8	0
20	A	1105	CLA	12	0
20	B	1237	CLA	20	0
20	A	1106	CLA	11	0
22	F	4016	BCR	9	0
20	B	1219	CLA	5	0
20	A	1125	CLA	11	0
30	2	611	CHL	5	0
20	A	1120	CLA	4	0
19	A	1011	CL0	12	0
20	B	1236	CLA	2	0
20	B	1227	CLA	7	0
20	B	1240	CLA	9	0
20	2	608	CLA	10	0
20	4	605	CLA	12	0
29	J	4013	LUT	10	0
28	J	5001	DGD	10	0
20	1	608	CLA	10	0
20	B	1021	CLA	11	0
20	A	1101	CLA	16	0
20	B	1217	CLA	1	0
22	A	4002	BCR	3	0
26	F	5002	LMG	3	0
30	3	607	CHL	1	0
22	1	504	BCR	4	0
26	2	805	LMG	1	0
20	A	1139	CLA	11	0
26	B	5007	LMG	1	0
31	2	502	XAT	14	0
22	2	503	BCR	24	0
20	A	1013	CLA	13	0

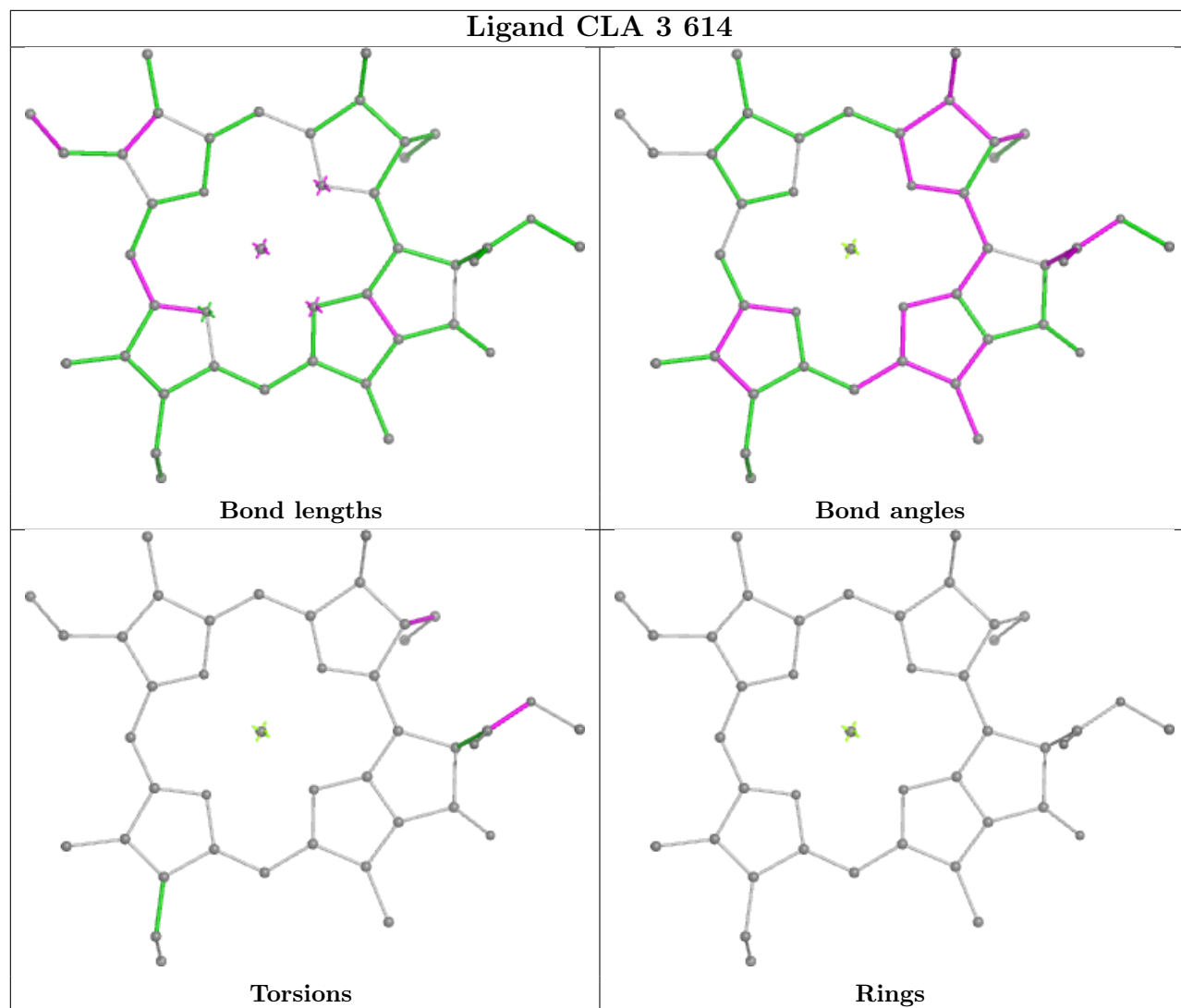
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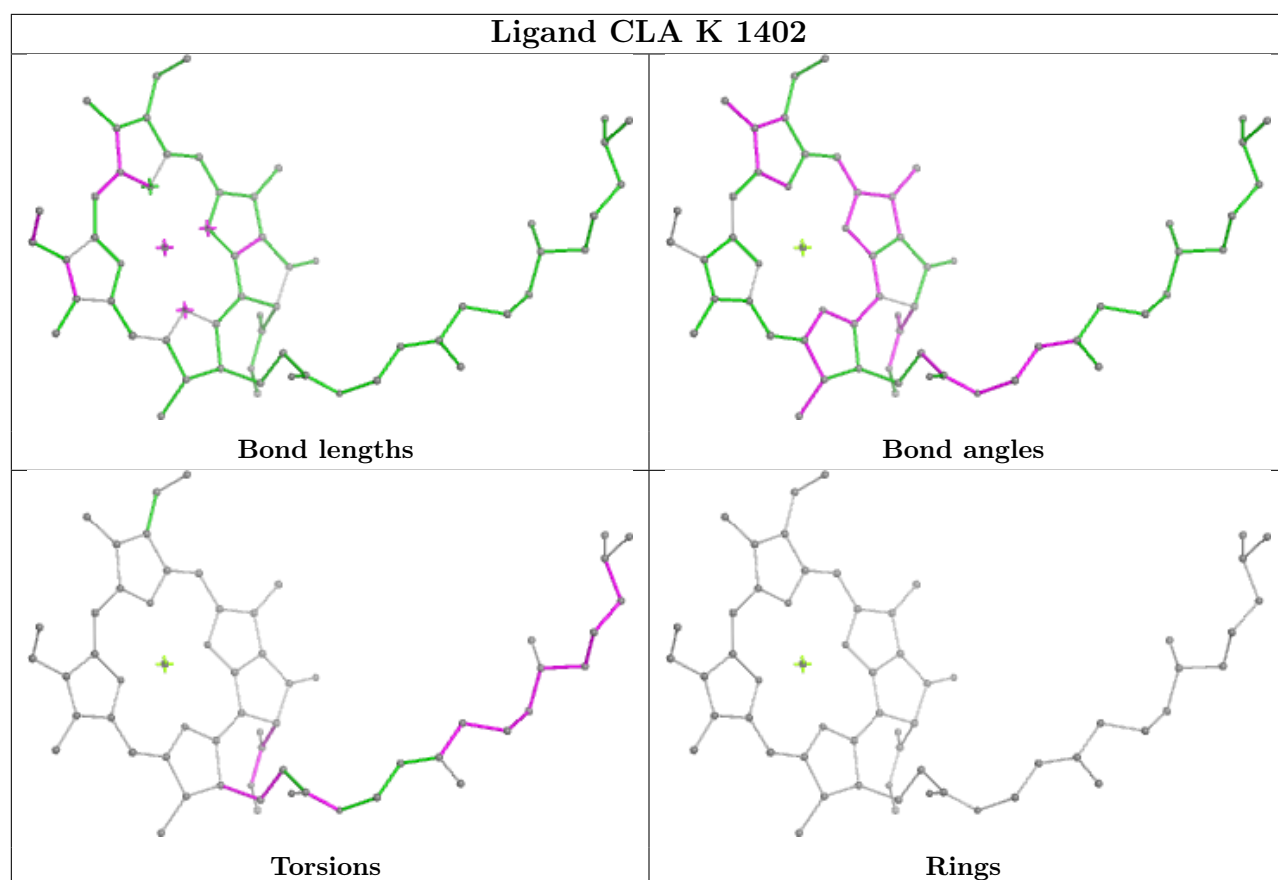
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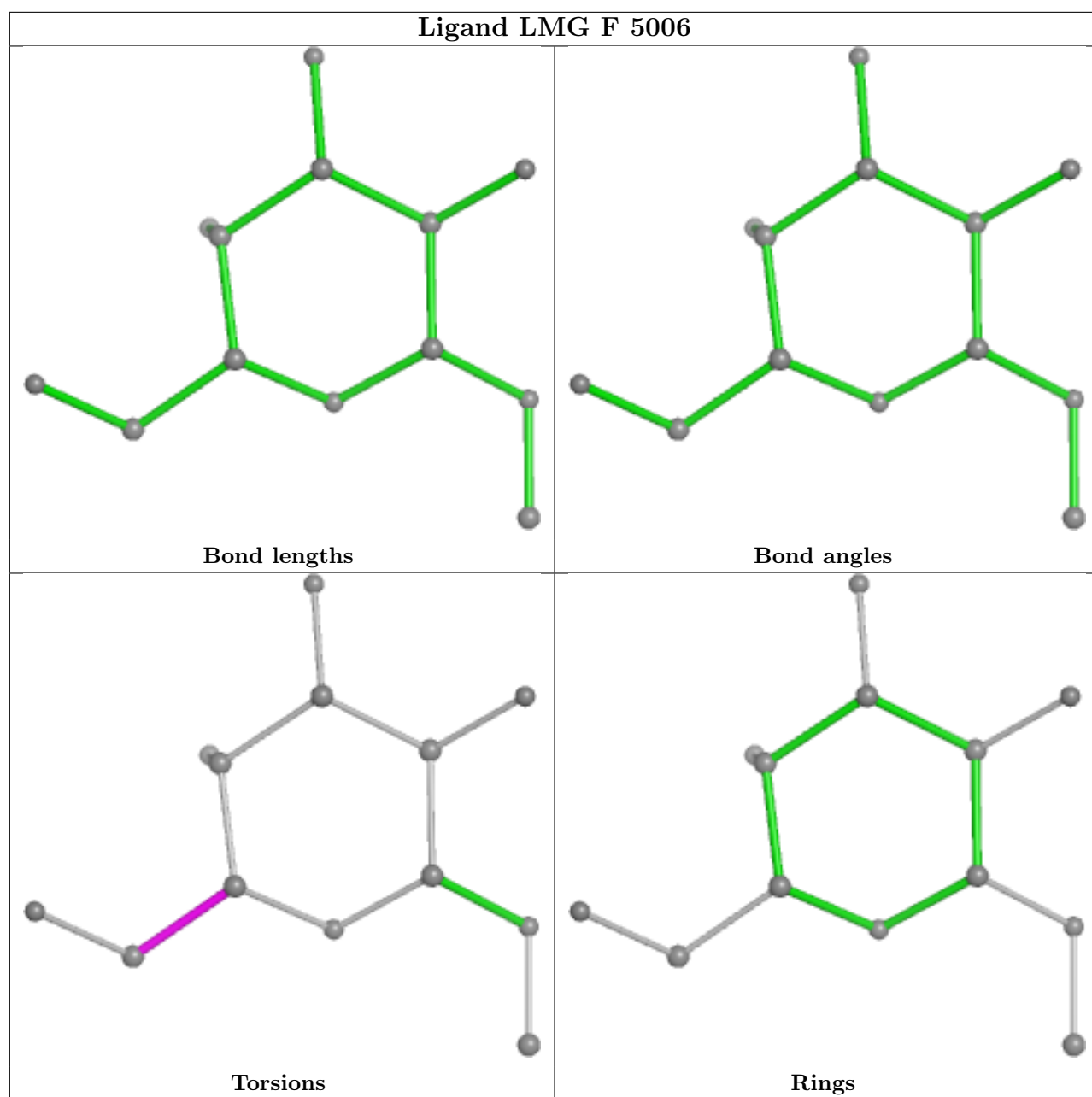
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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20	B	1215	CLA	4	0
20	3	612	CLA	9	0
20	2	606	CLA	21	0
20	L	1503	CLA	17	0
20	B	1223	CLA	6	0
20	4	606	CLA	4	0
25	C	3003	SF4	2	0
20	3	602	CLA	2	0
20	3	601	CLA	13	0
29	1	501	LUT	6	0
22	F	4014	BCR	2	0
20	A	1124	CLA	4	0
26	B	5003	LMG	13	0
22	A	4011	BCR	7	0
20	A	1118	CLA	3	0
22	B	4005	BCR	3	0
20	A	1112	CLA	15	0
20	B	1232	CLA	10	0
20	A	1134	CLA	10	0
20	B	1206	CLA	10	0
20	B	1224	CLA	5	0
20	B	1202	CLA	7	0
20	2	605	CLA	11	0
20	A	1136	CLA	12	0
30	1	609	CHL	16	0
32	2	807	3PH	5	0
20	B	1225	CLA	11	0
20	2	604	CLA	25	0
30	3	611	CHL	9	0

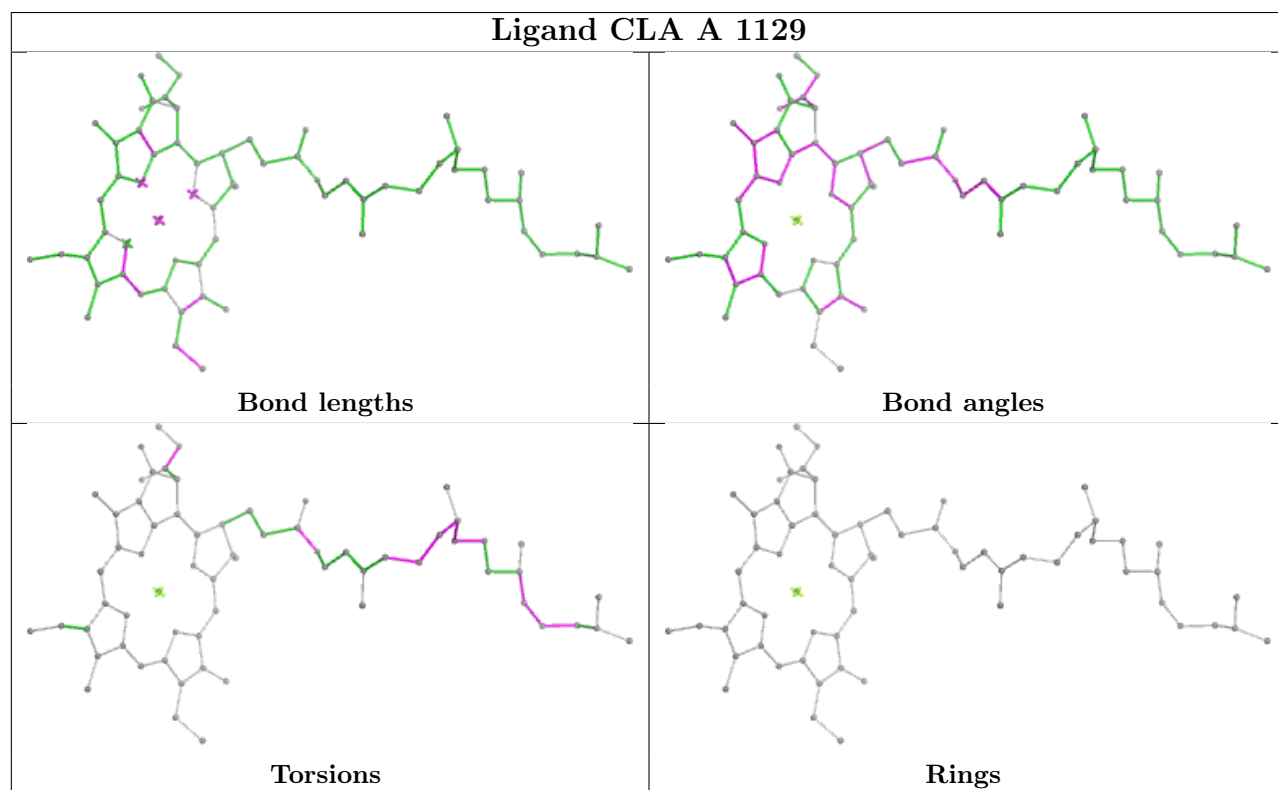
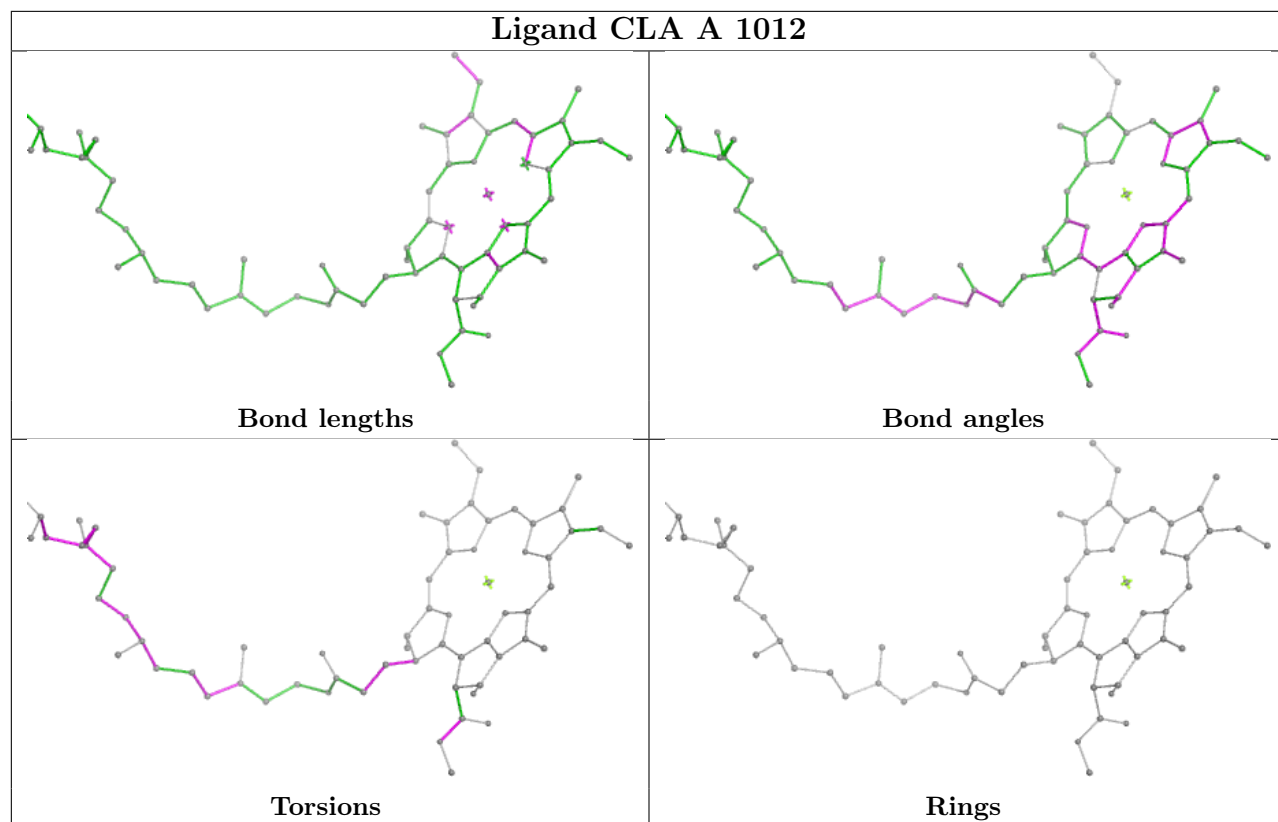
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

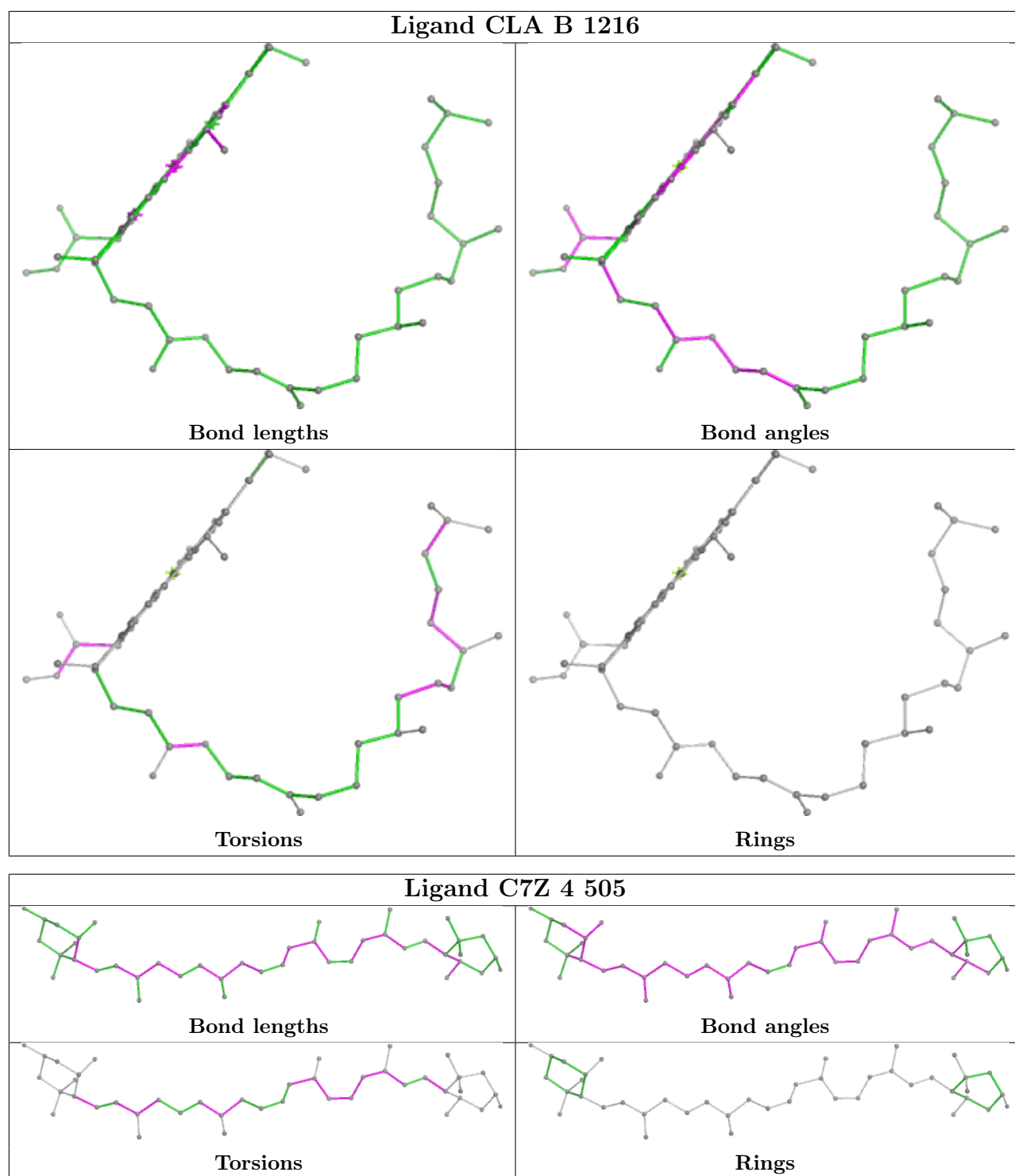
Ligand CLA 3 614

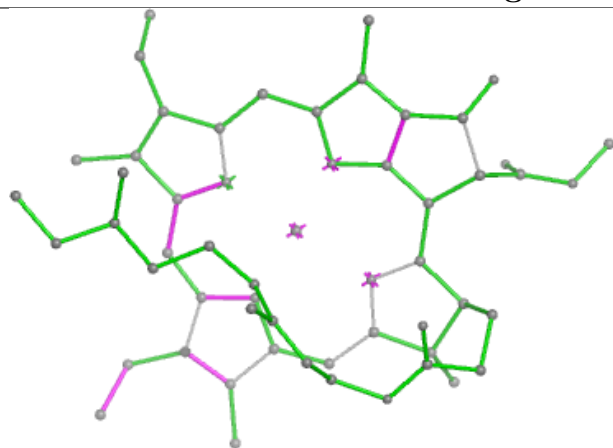




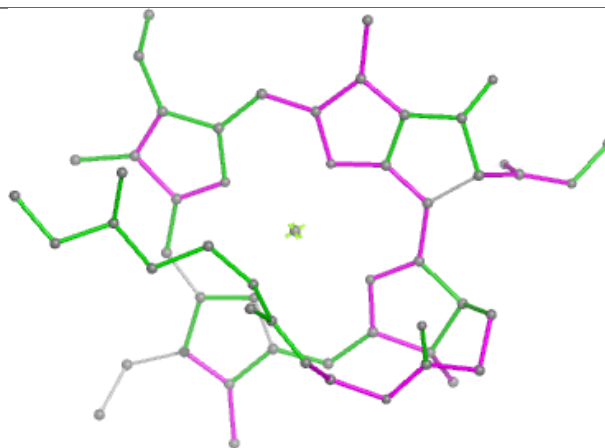




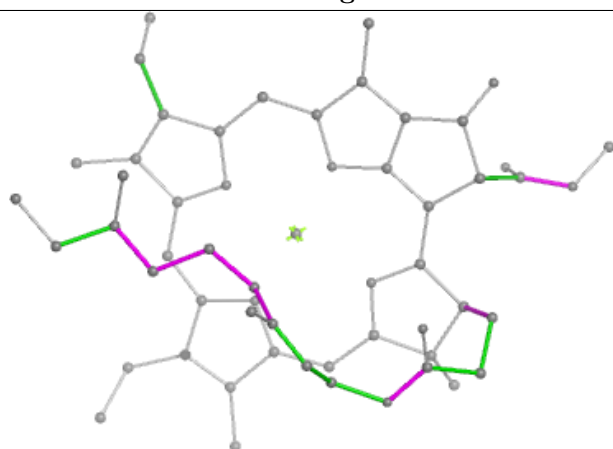


Ligand CLA A 1116

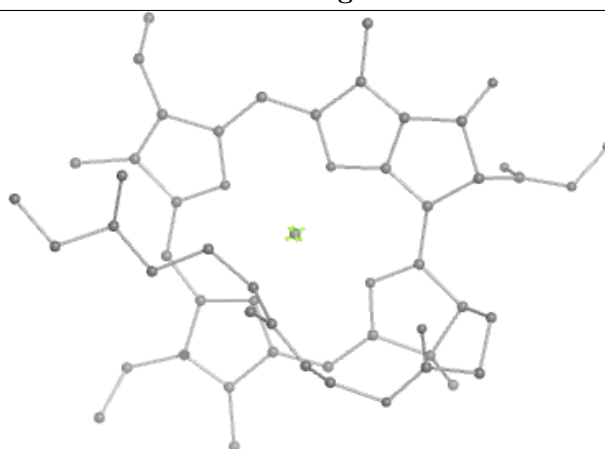
Bond lengths



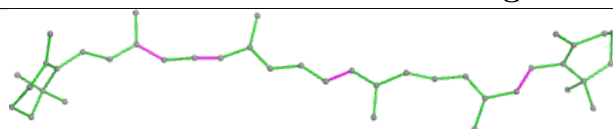
Bond angles



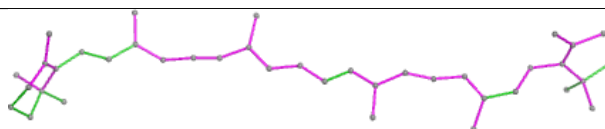
Torsions



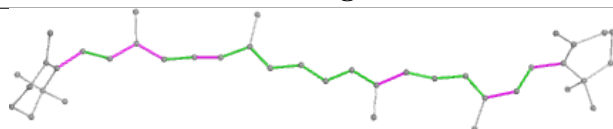
Rings

Ligand BCR A 4003

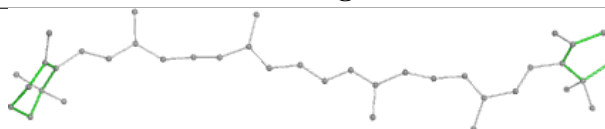
Bond lengths



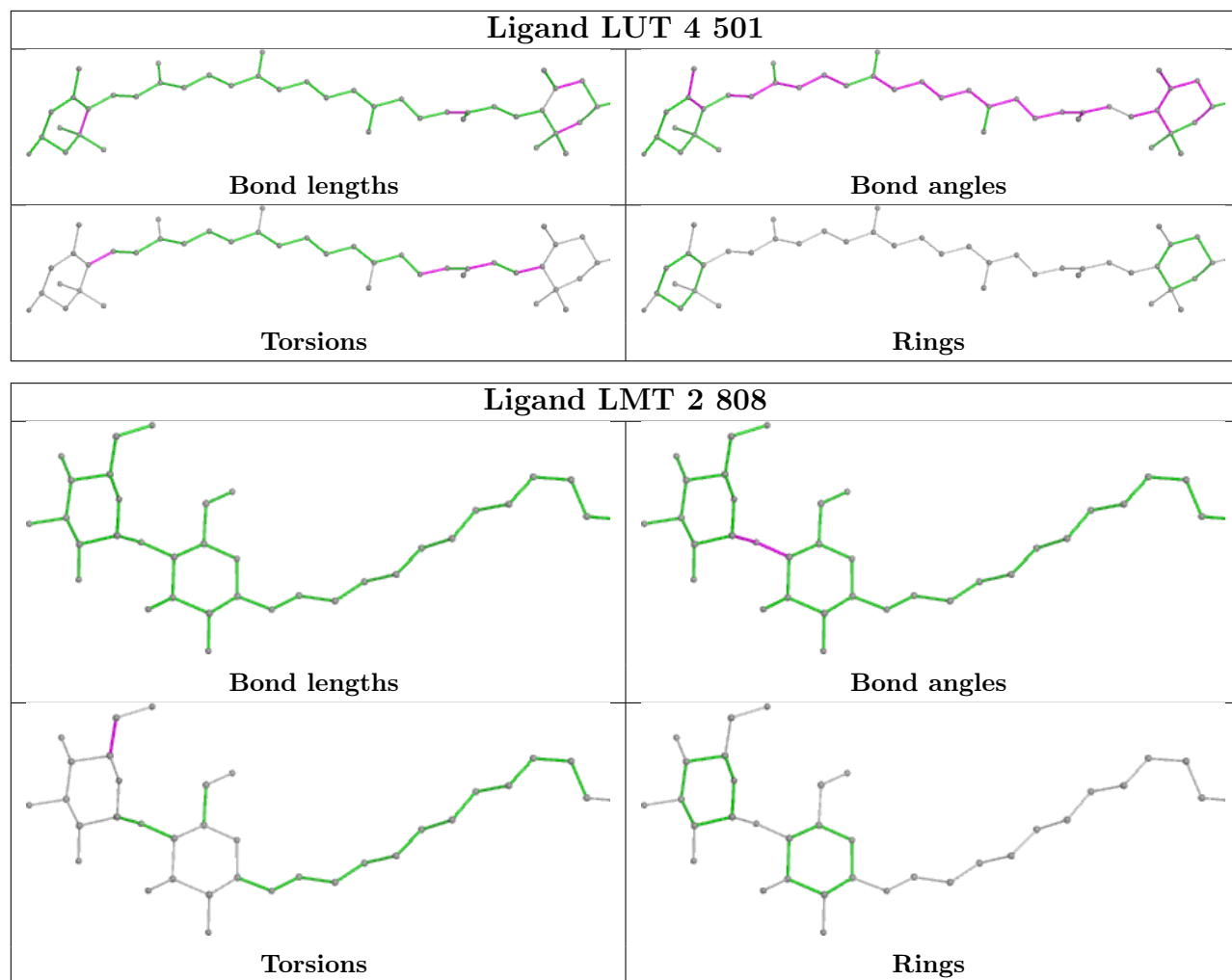
Bond angles

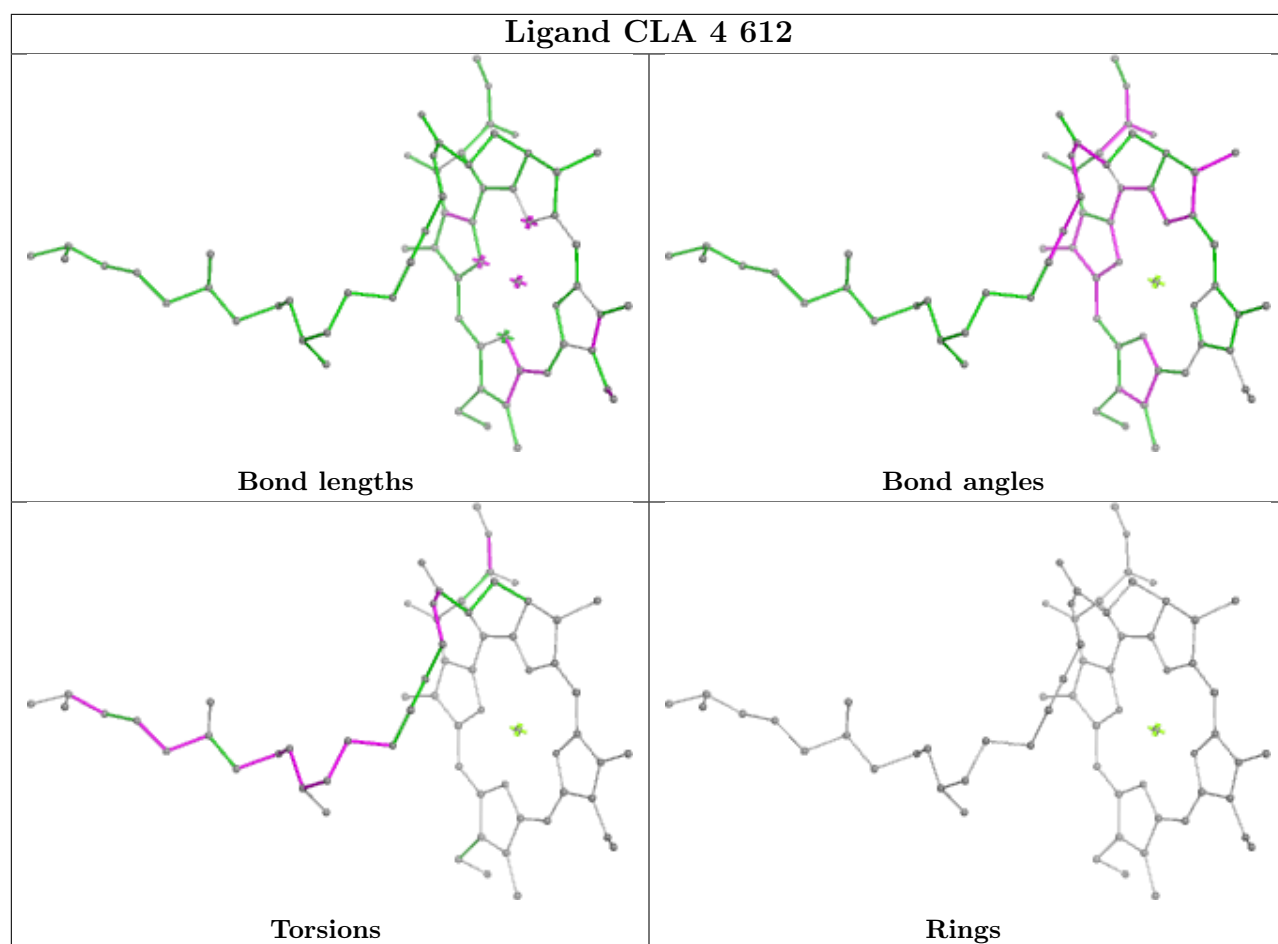


Torsions

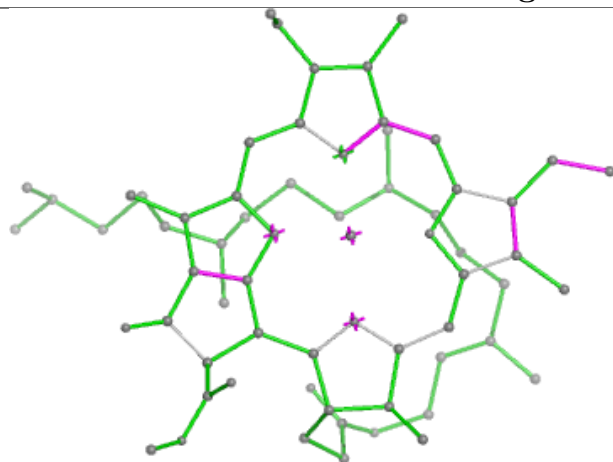


Rings

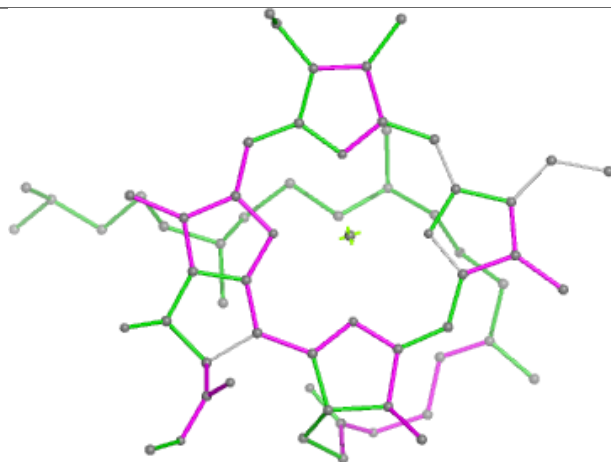




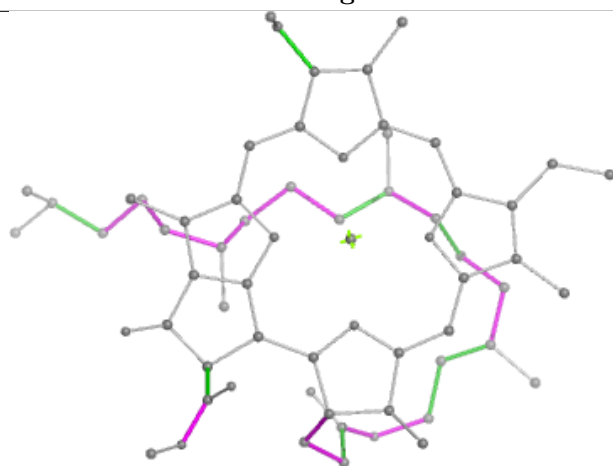
Ligand CLA 3 610



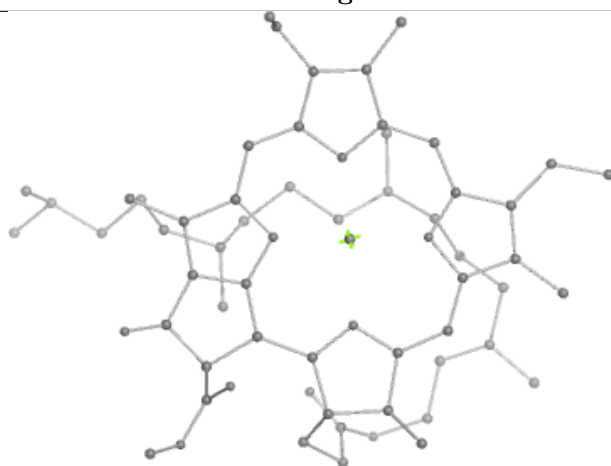
Bond lengths



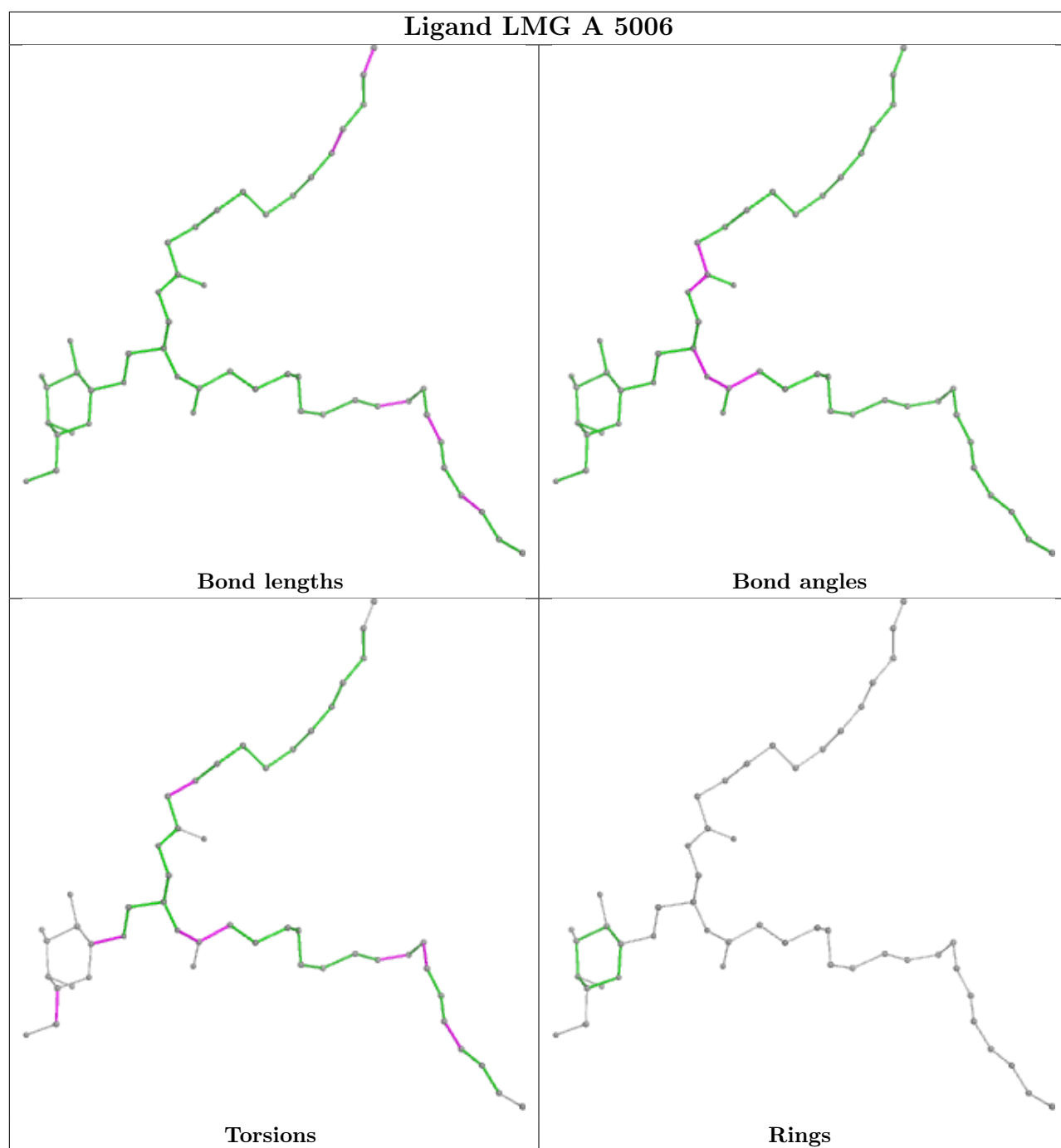
Bond angles



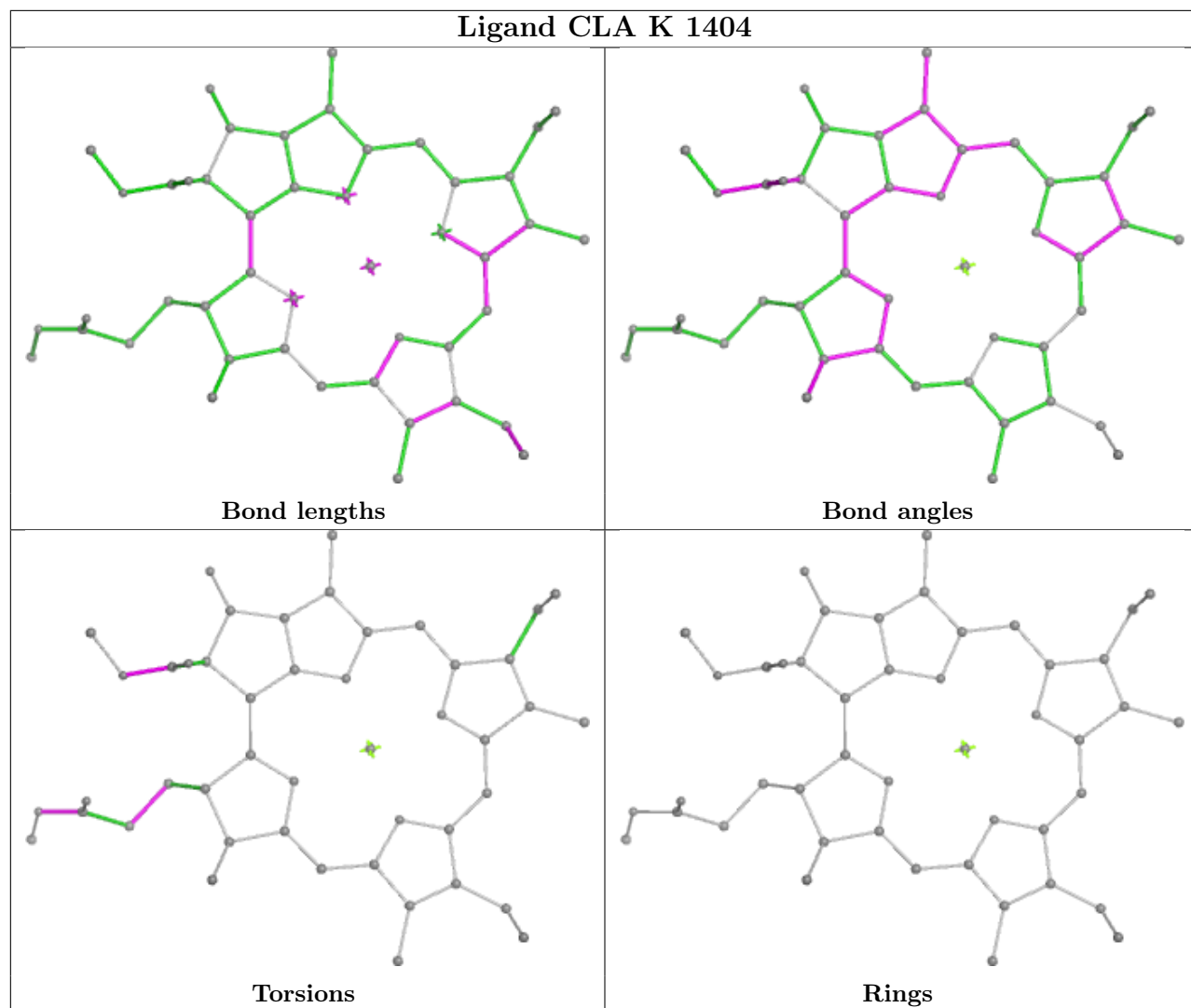
Torsions

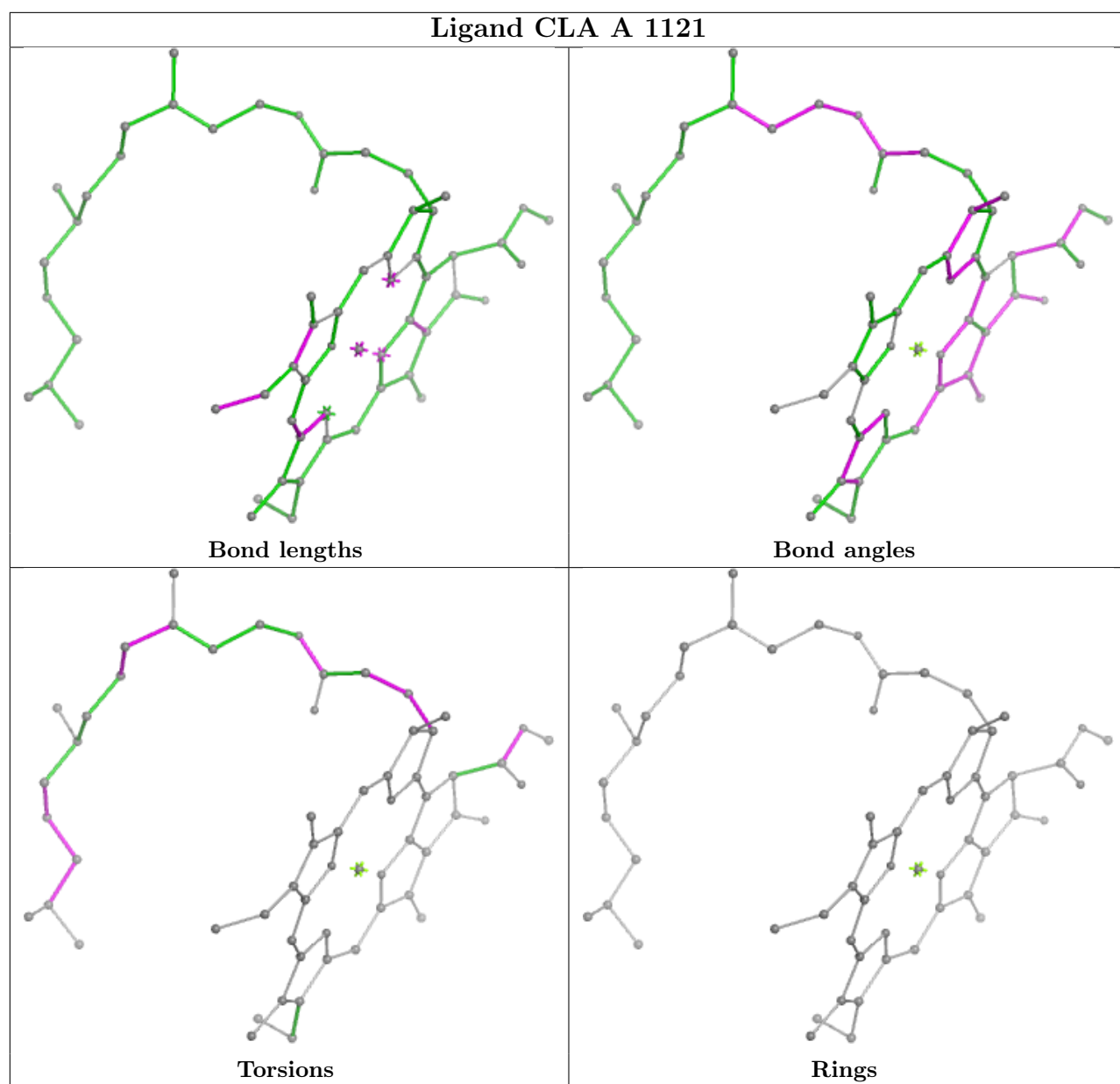


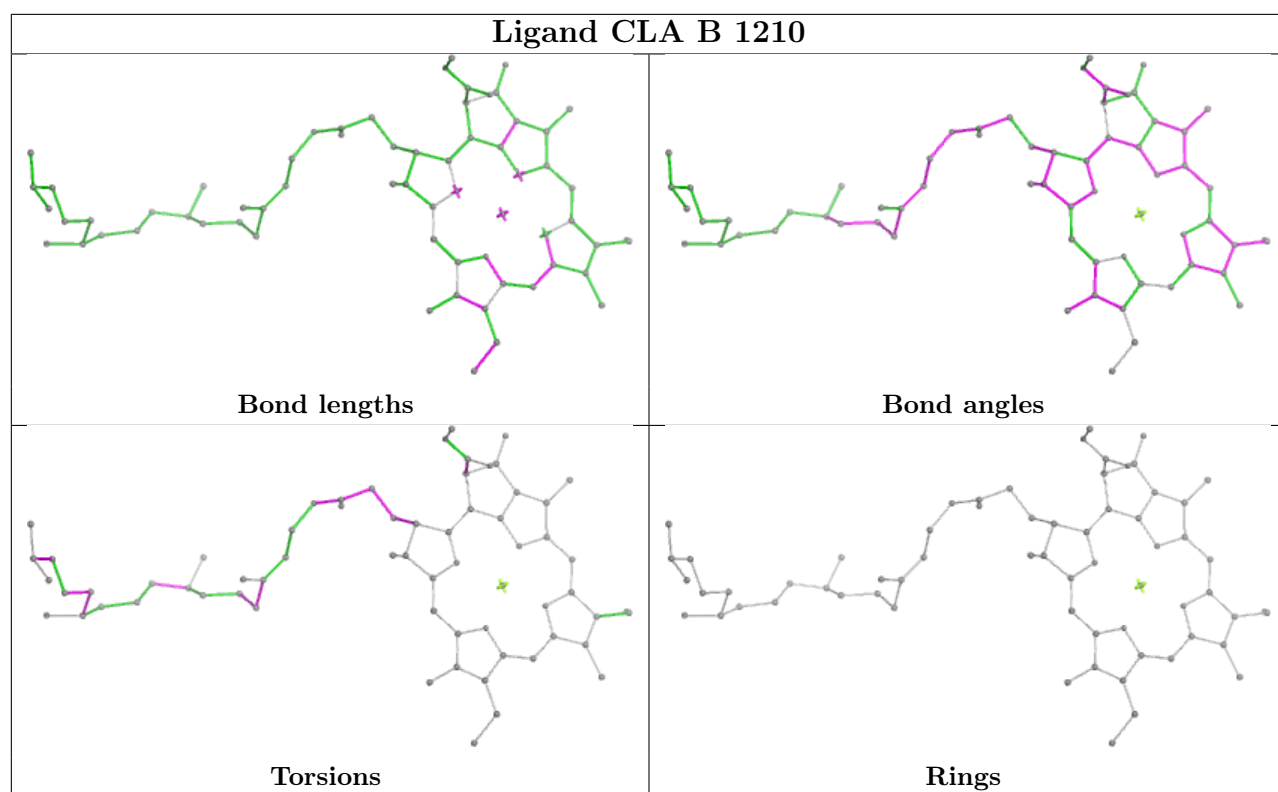
Rings



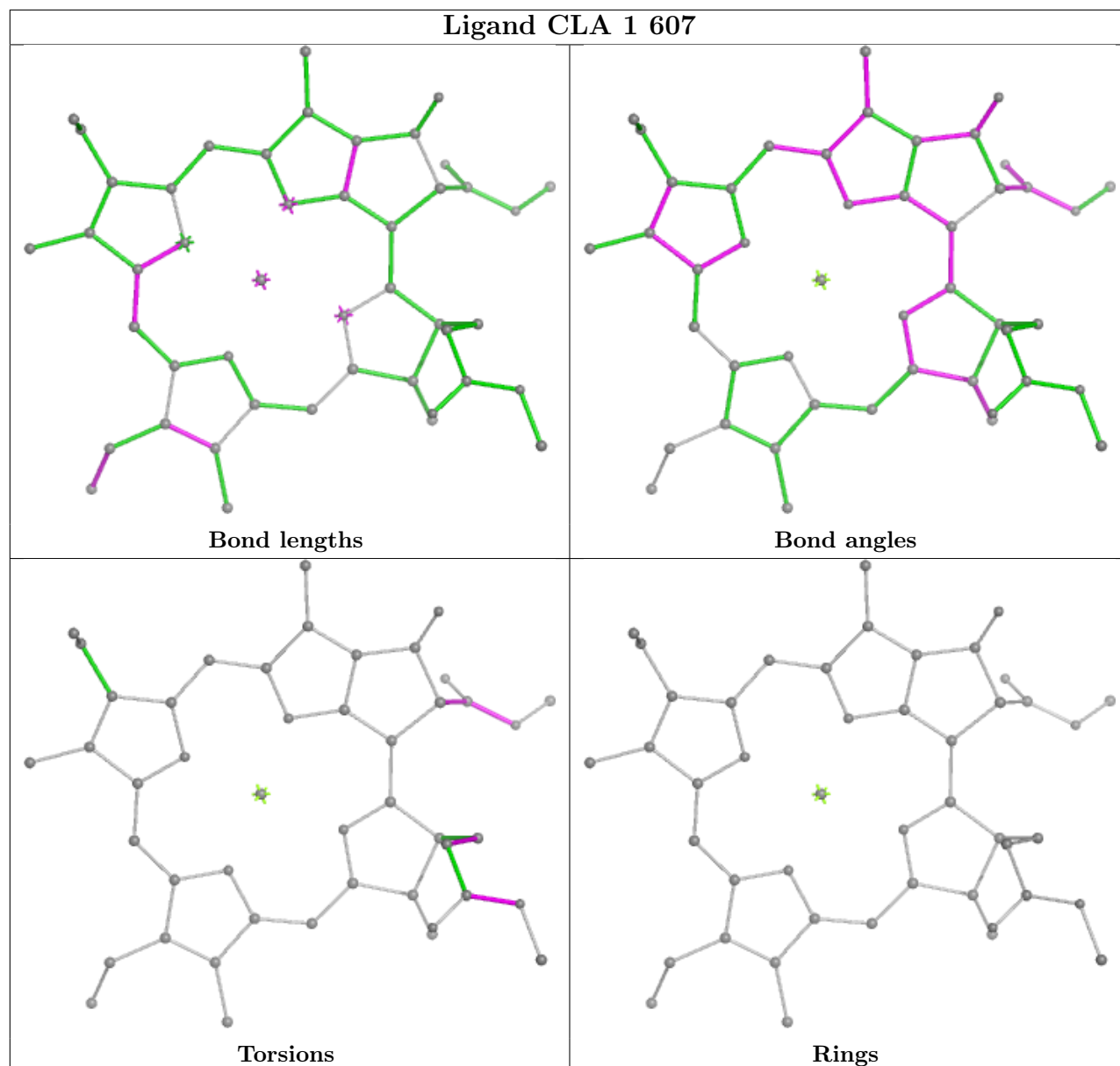
Ligand CLA K 1404



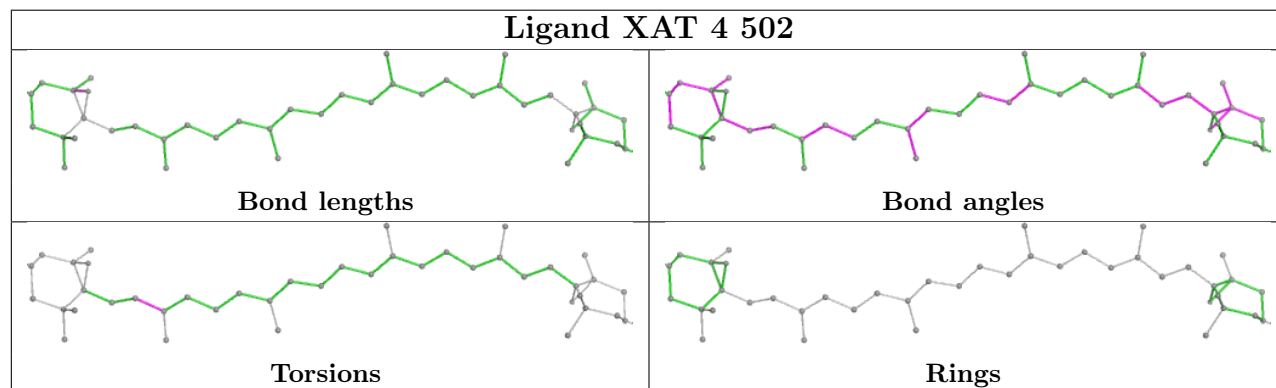


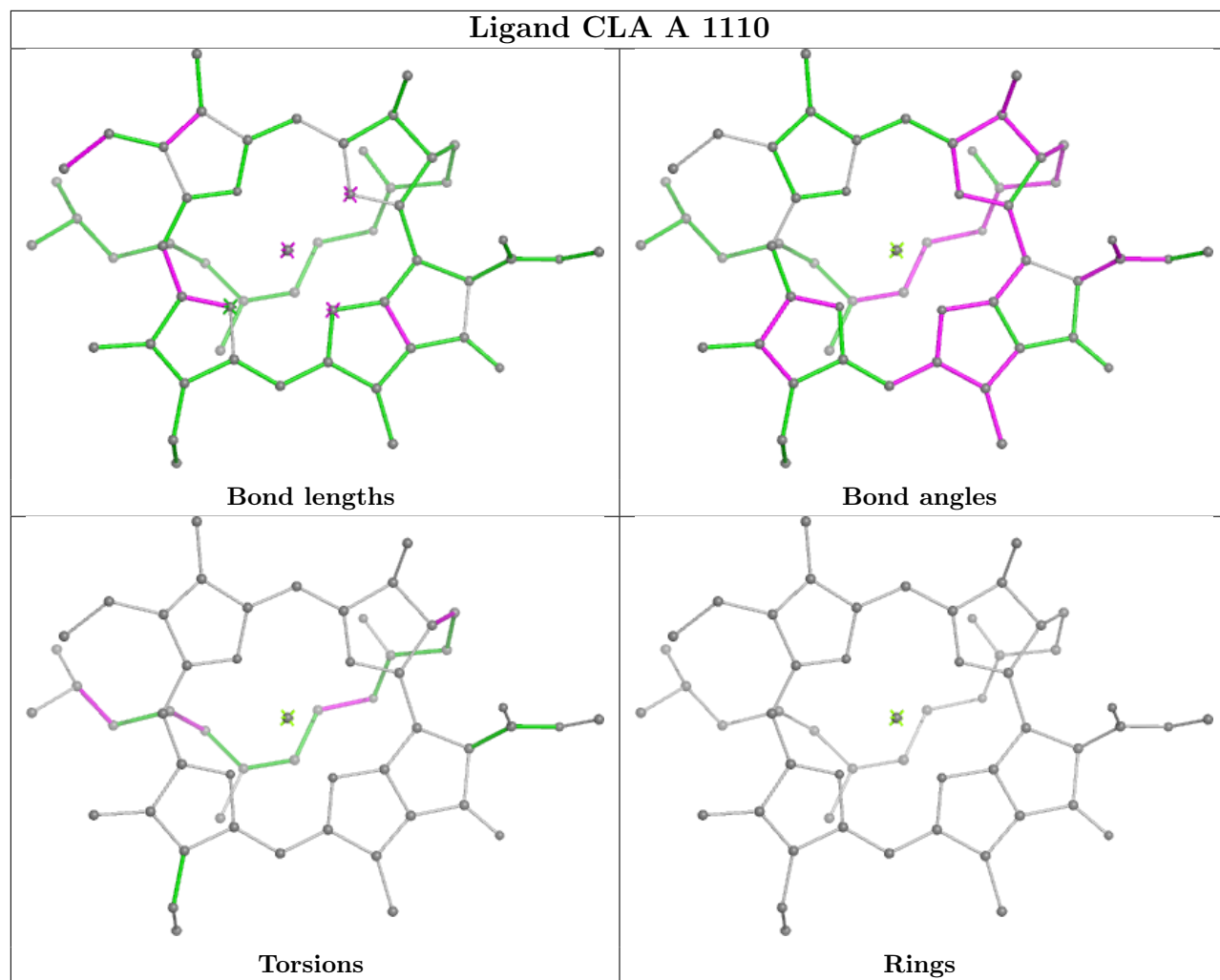


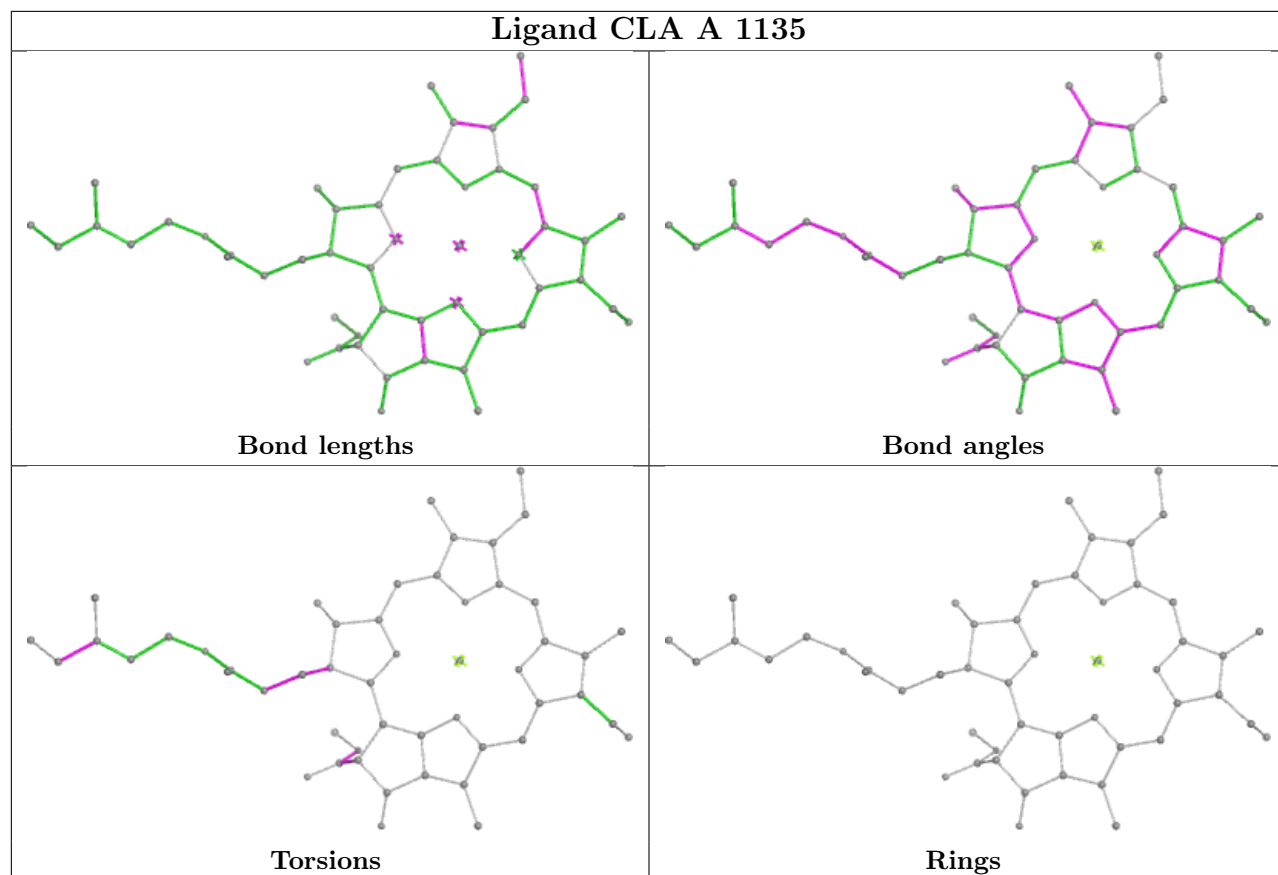
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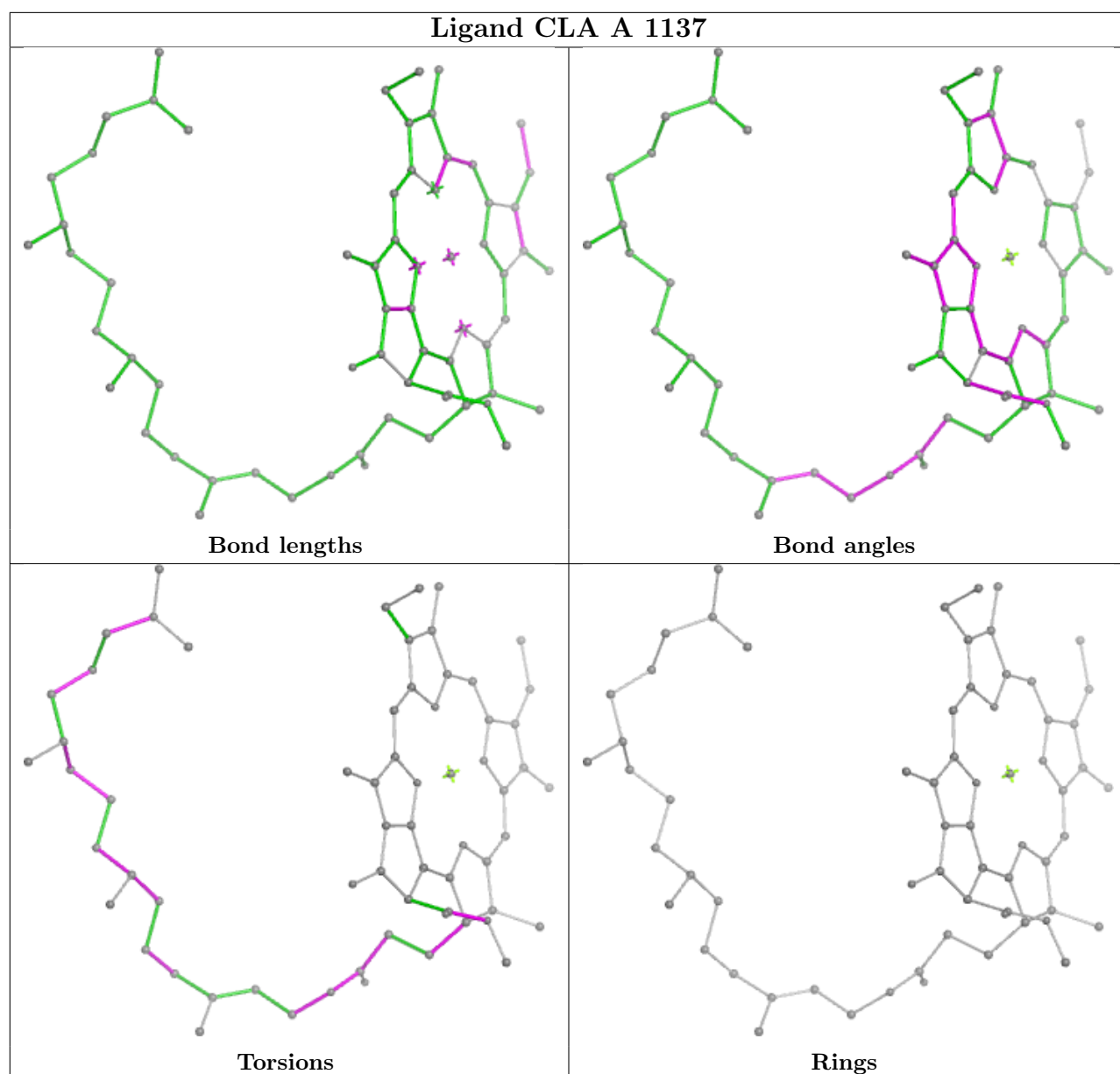


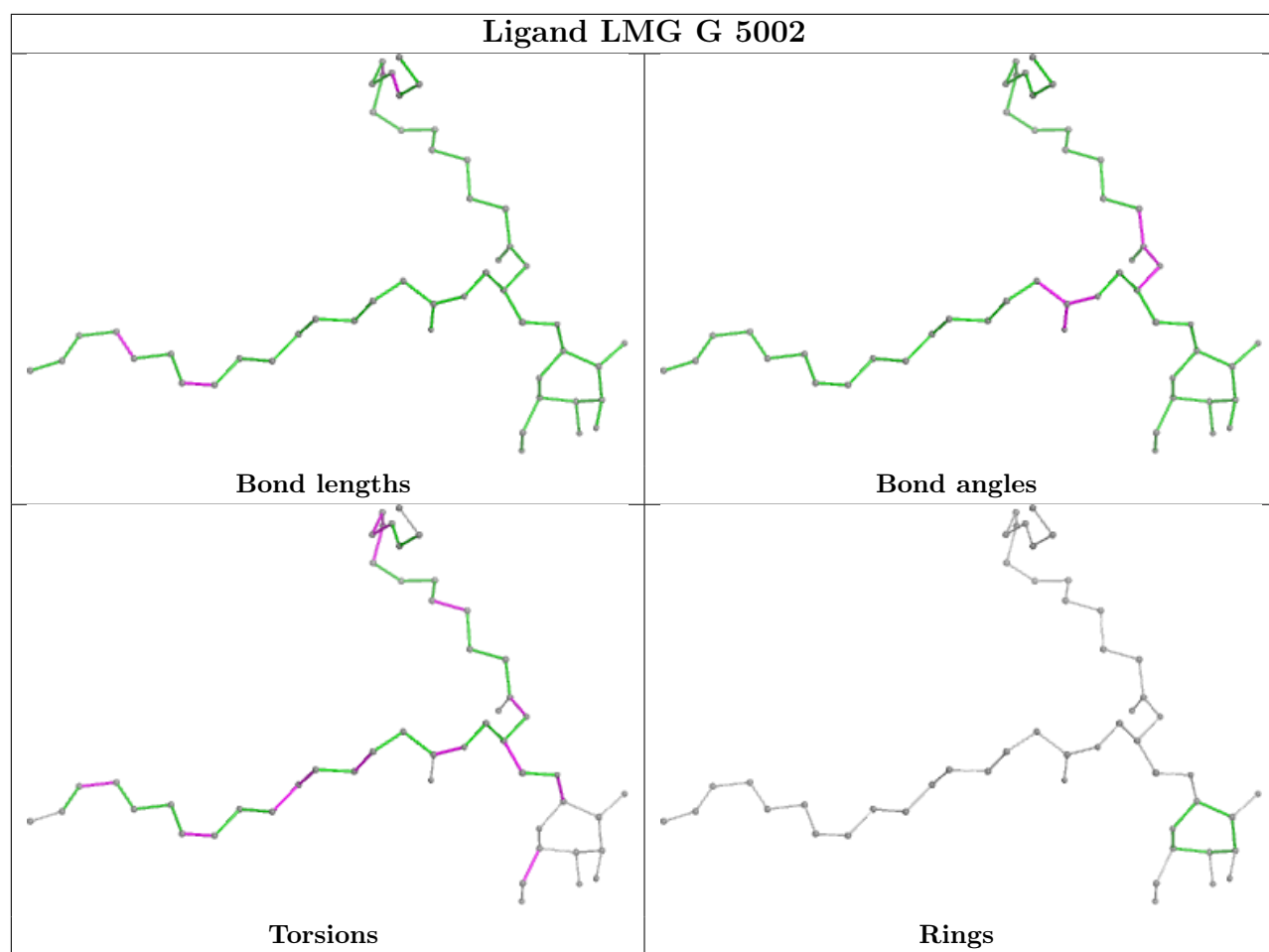
Ligand XAT 4 502

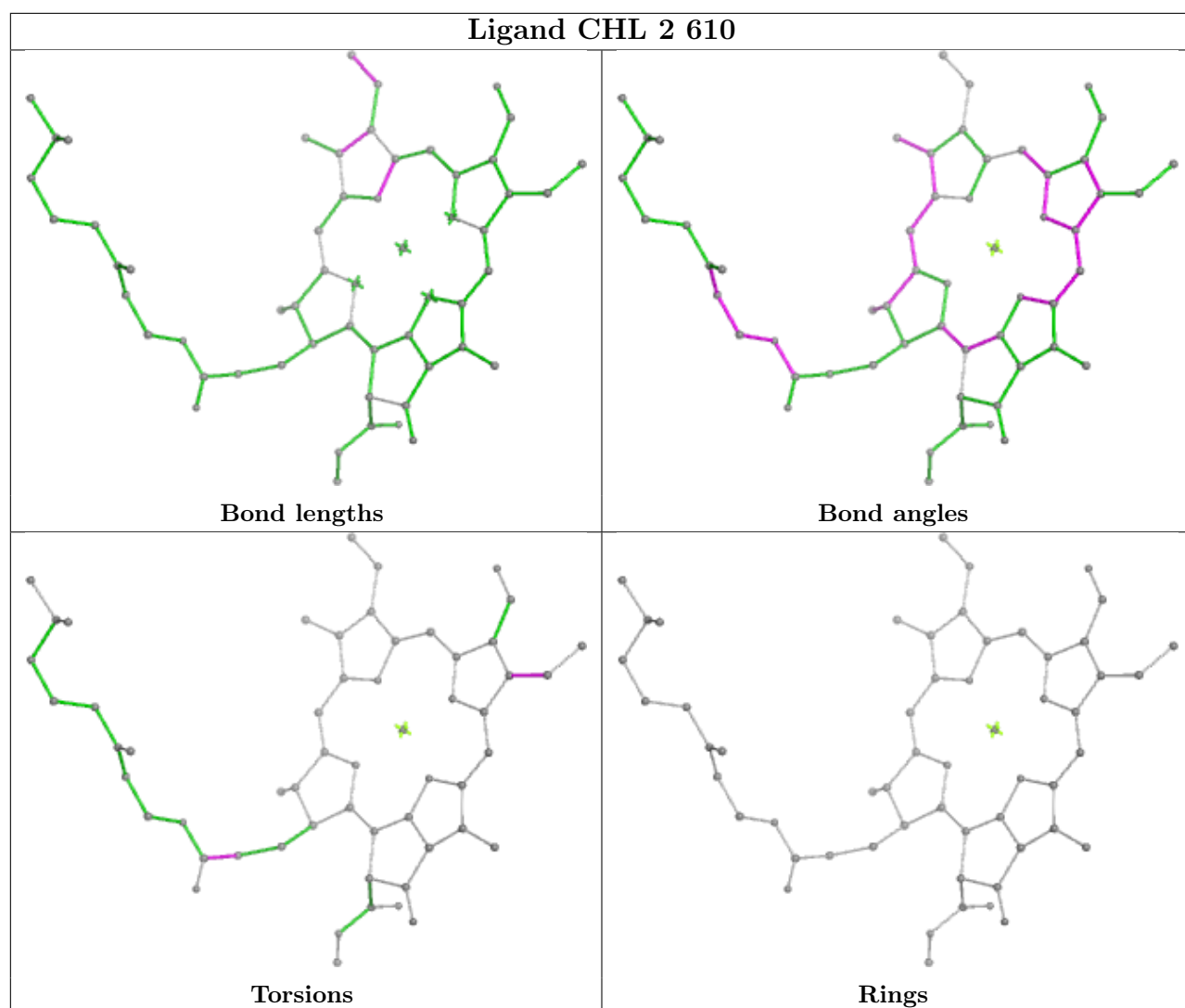


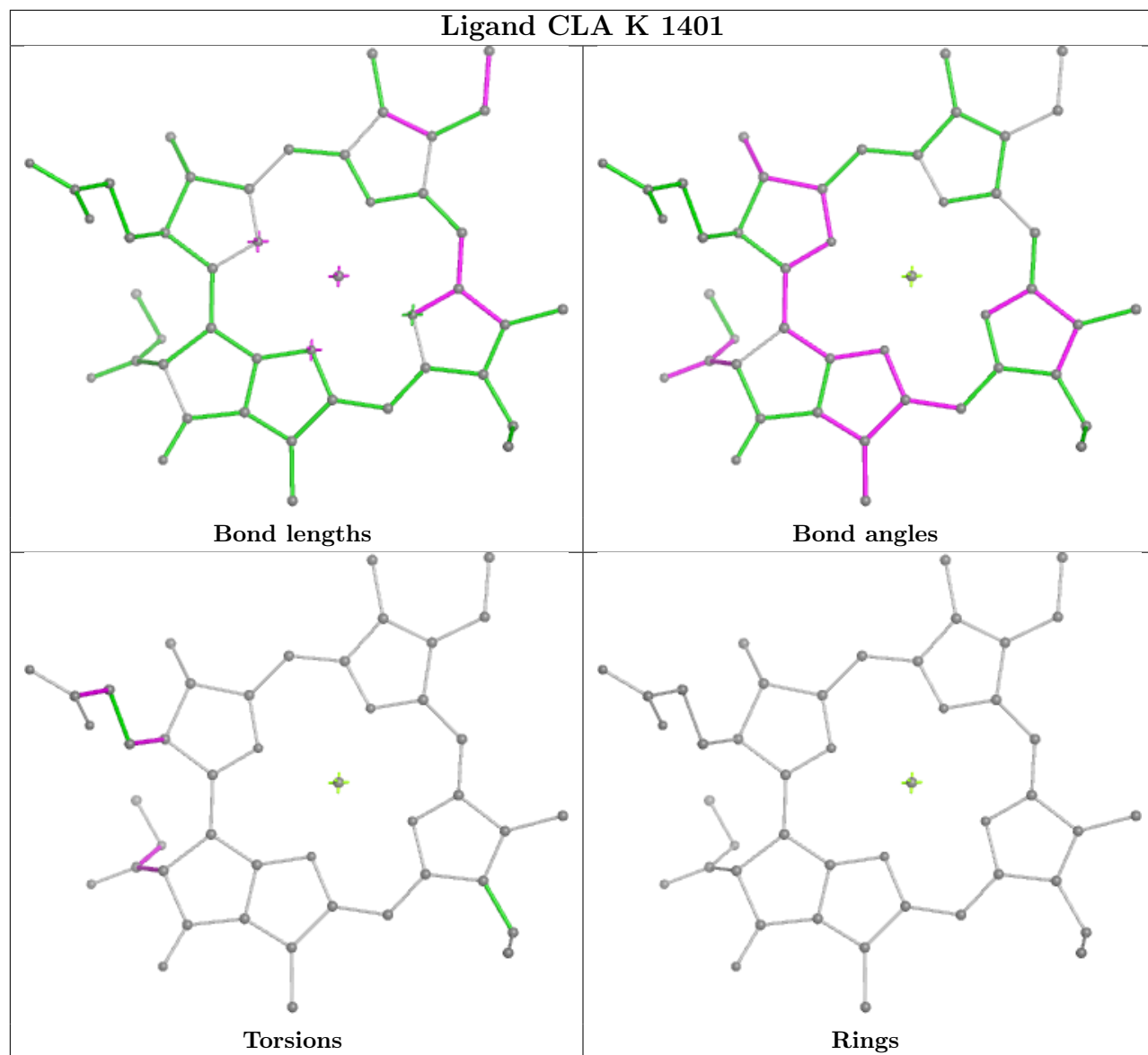


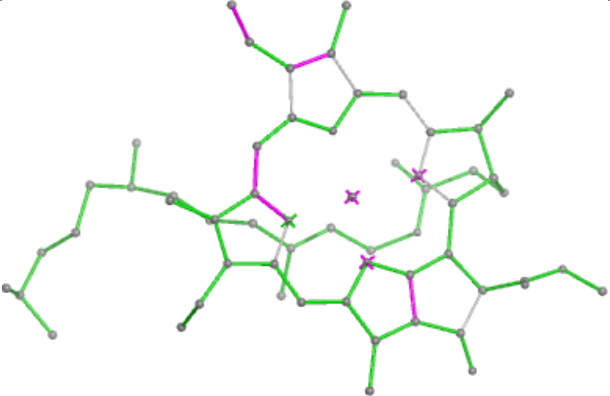
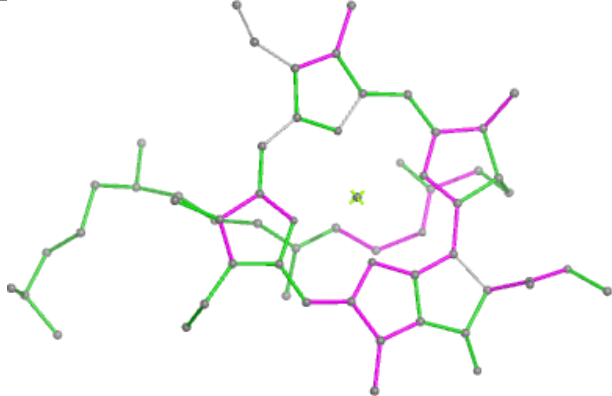
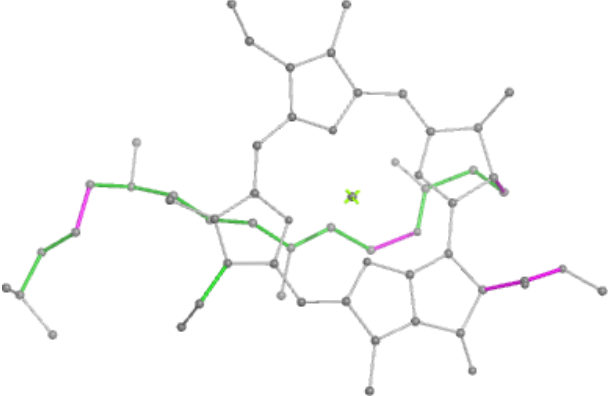
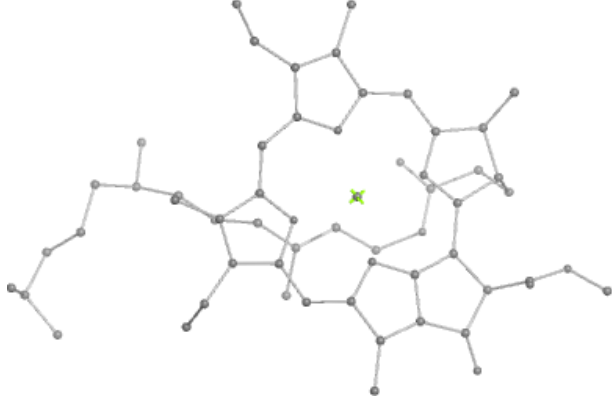
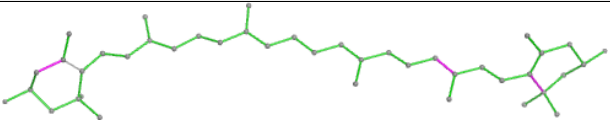
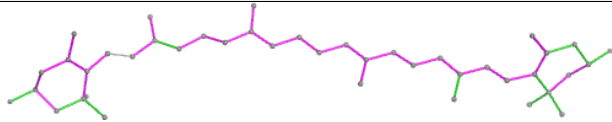
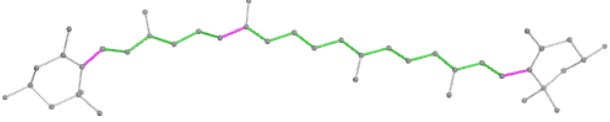
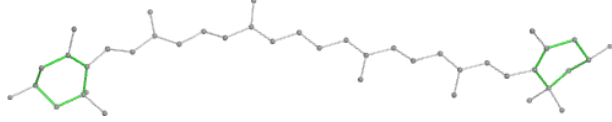
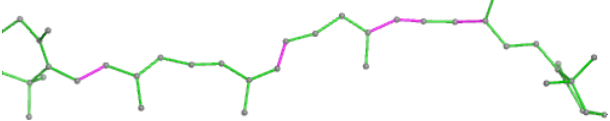
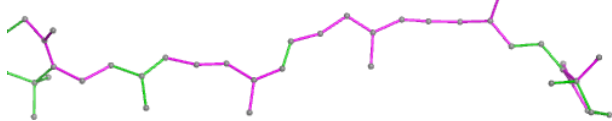
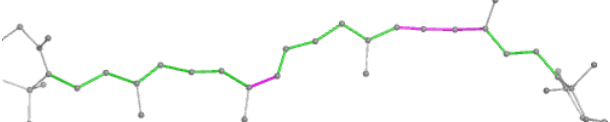



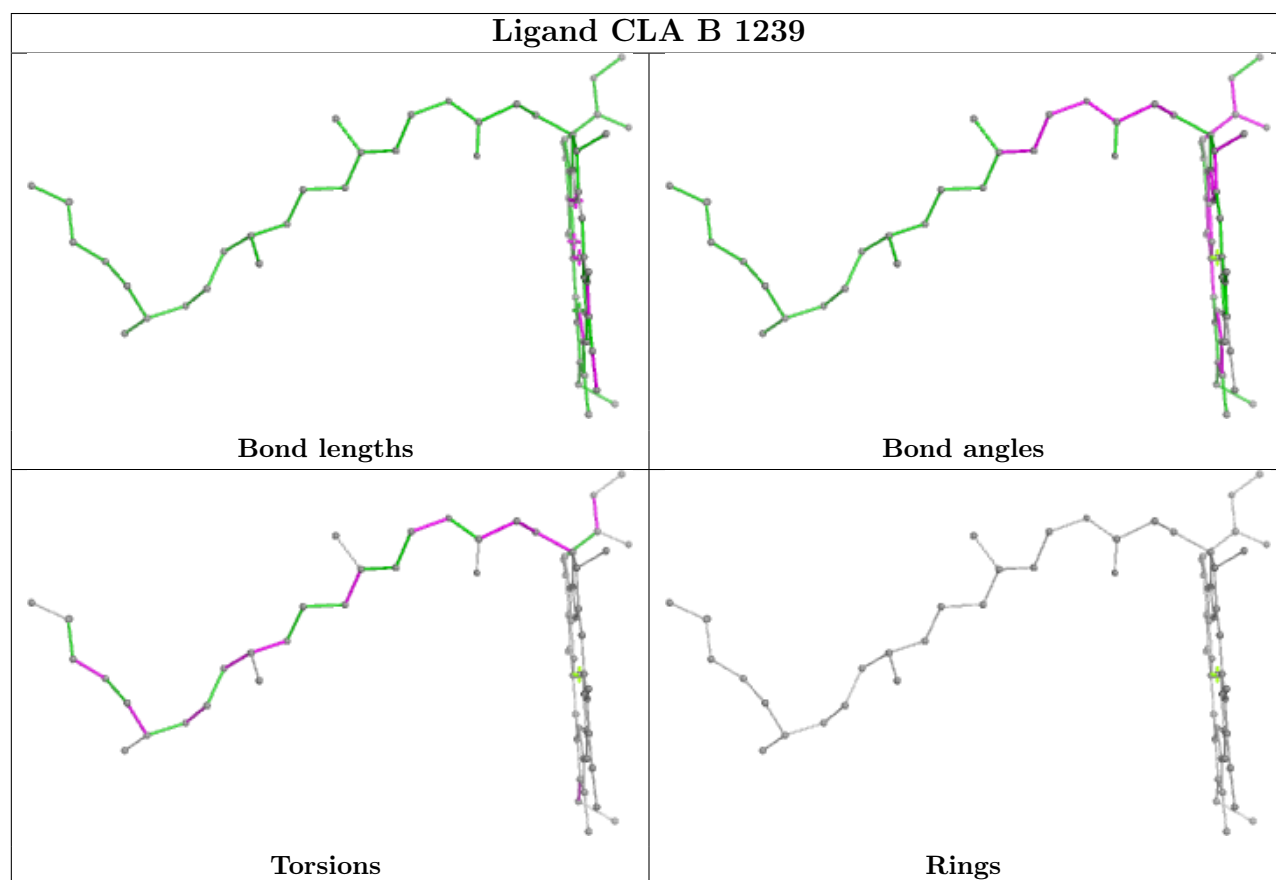
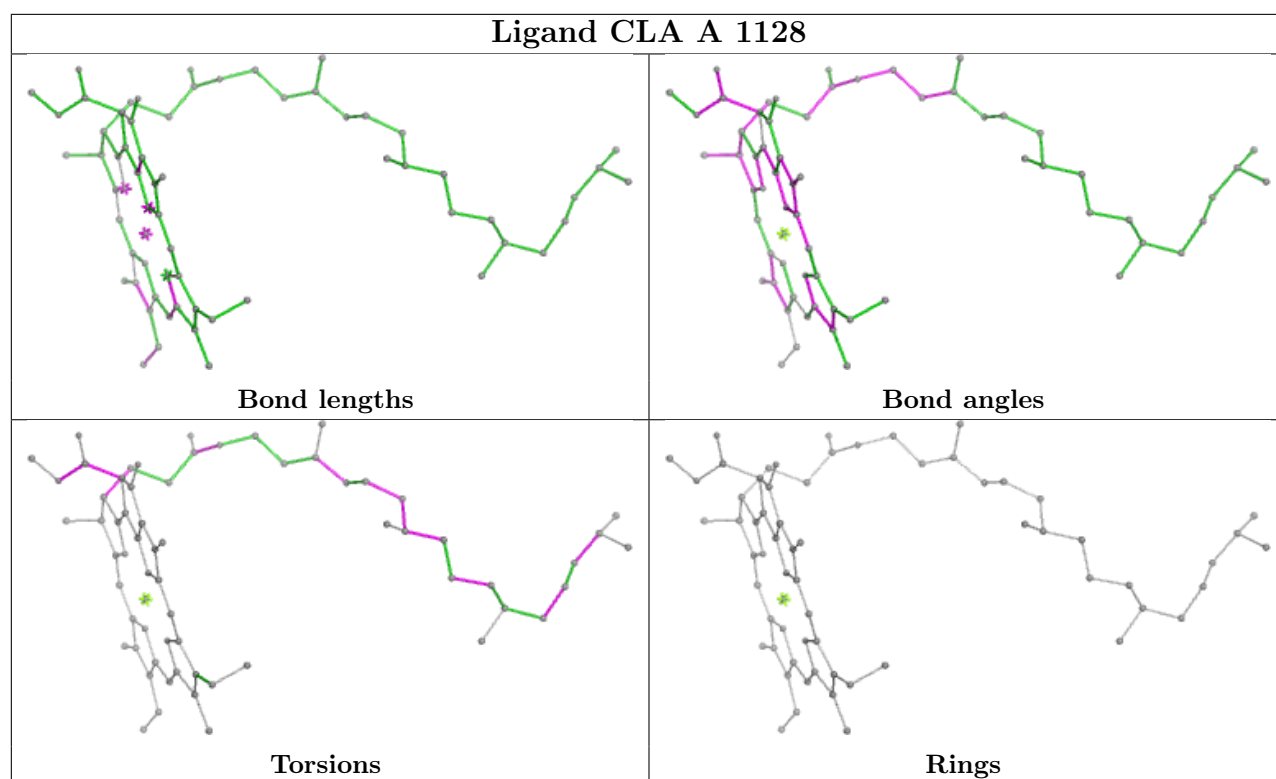


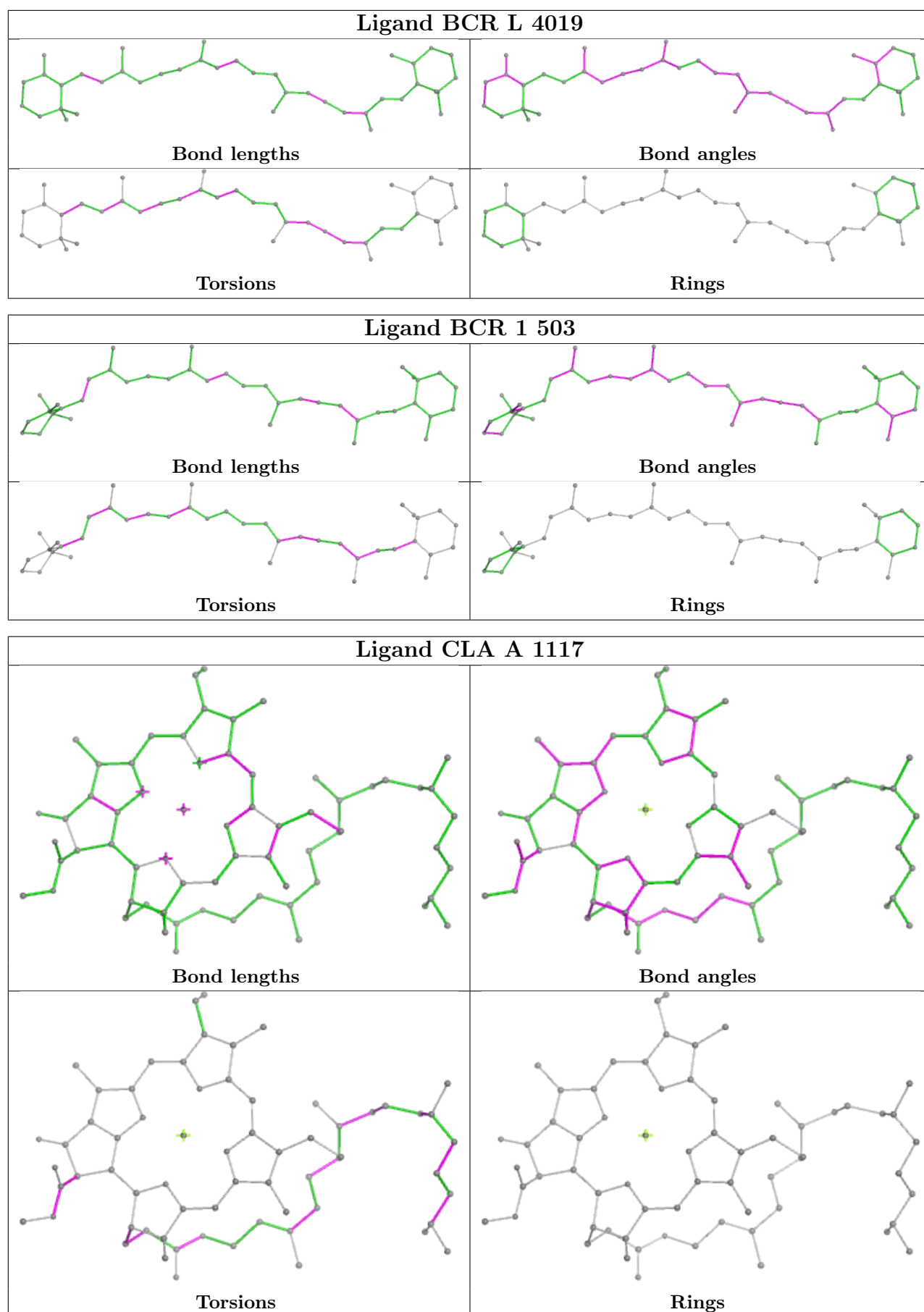


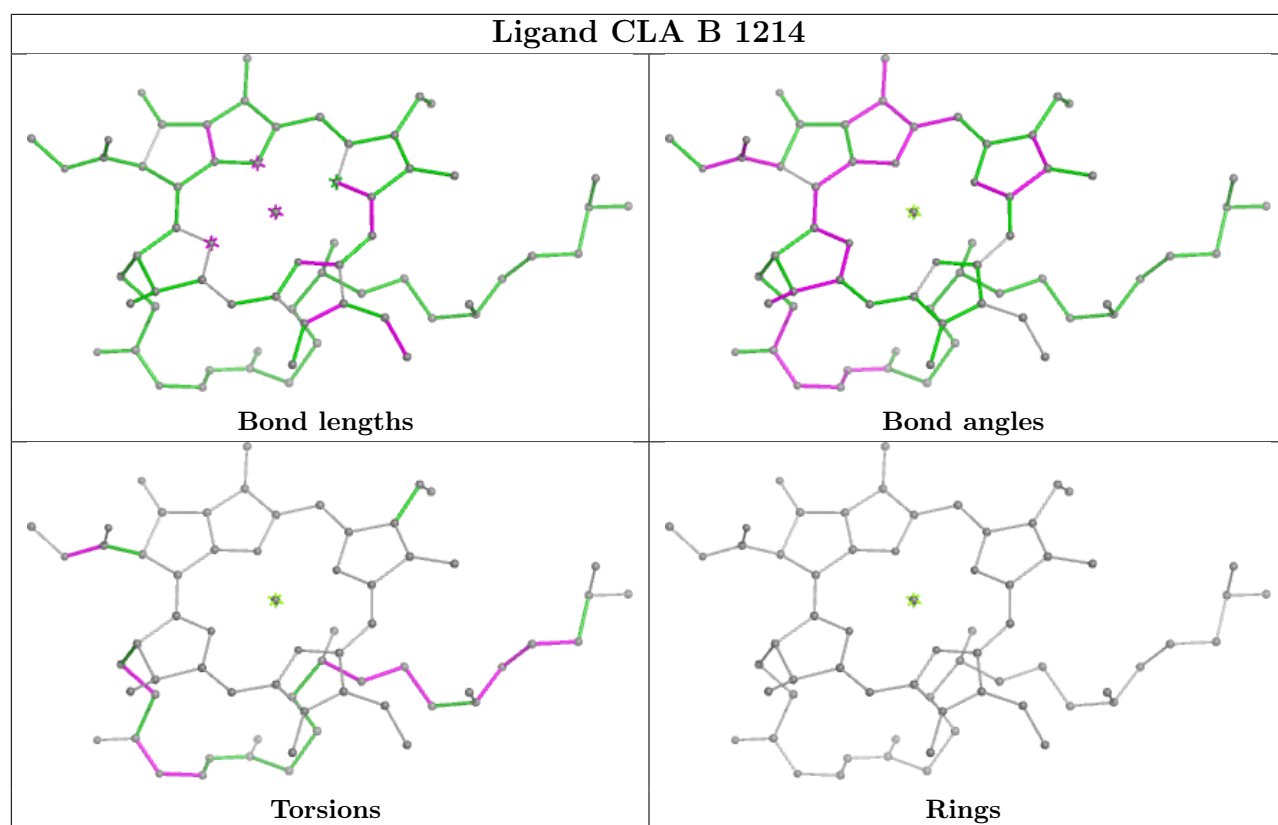


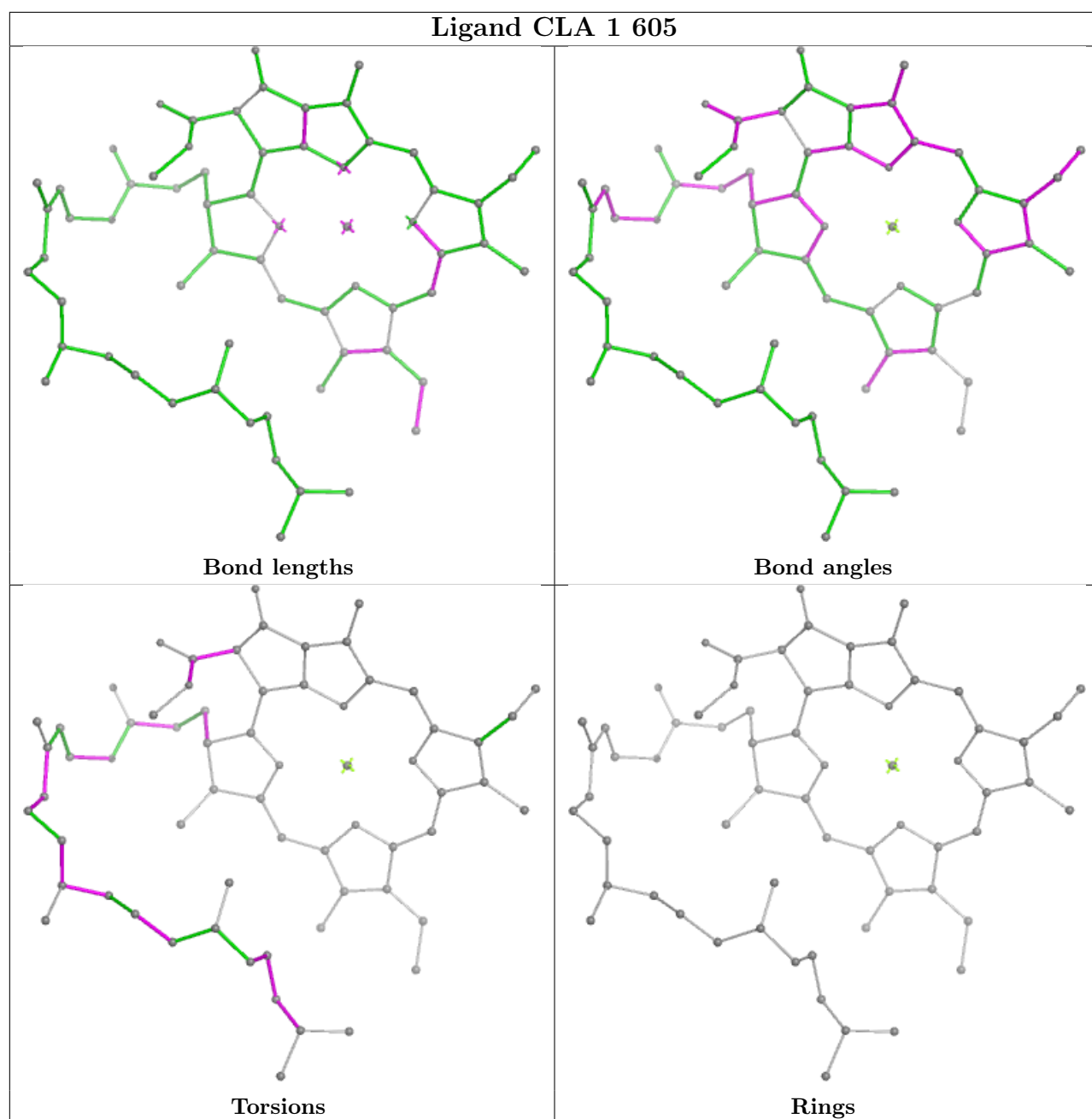


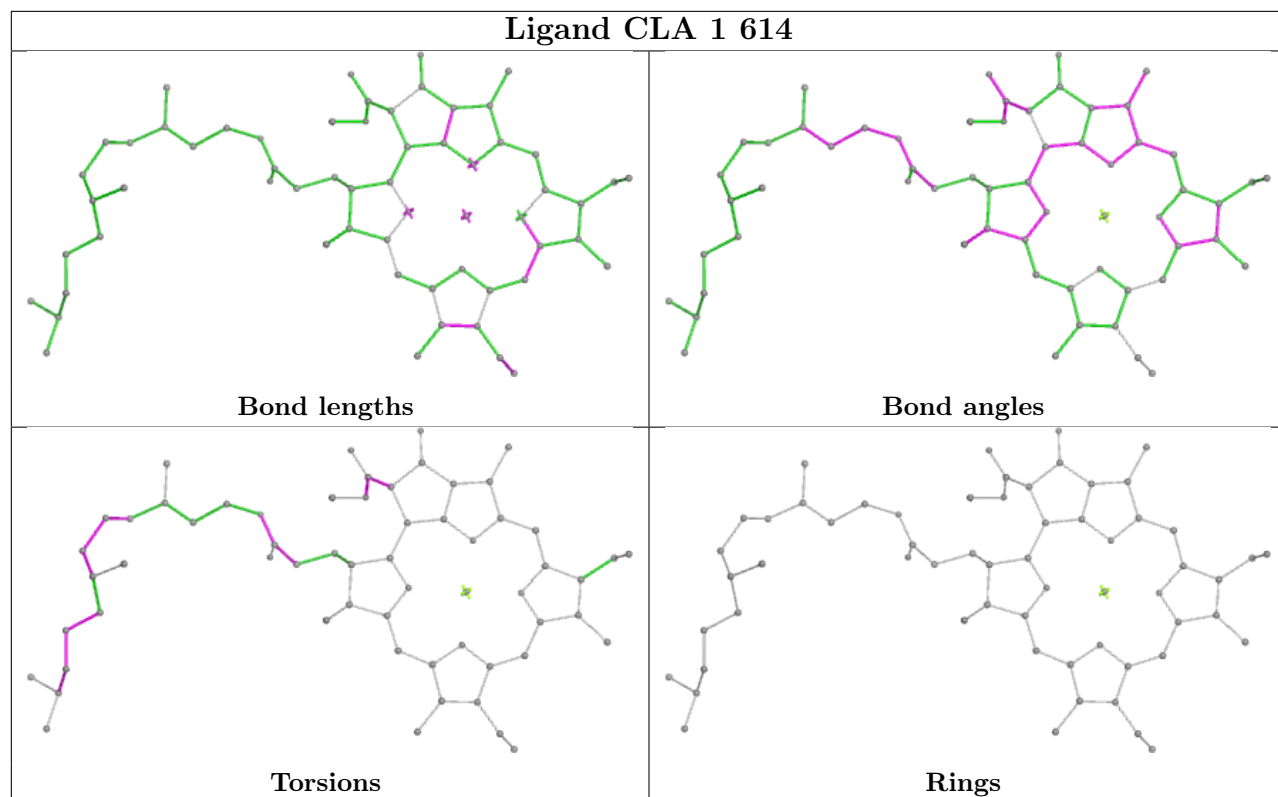
Ligand CLA B 1213	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand LUT 2 501	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR A 4017	
	
Bond lengths	Bond angles
	
Torsions	Rings



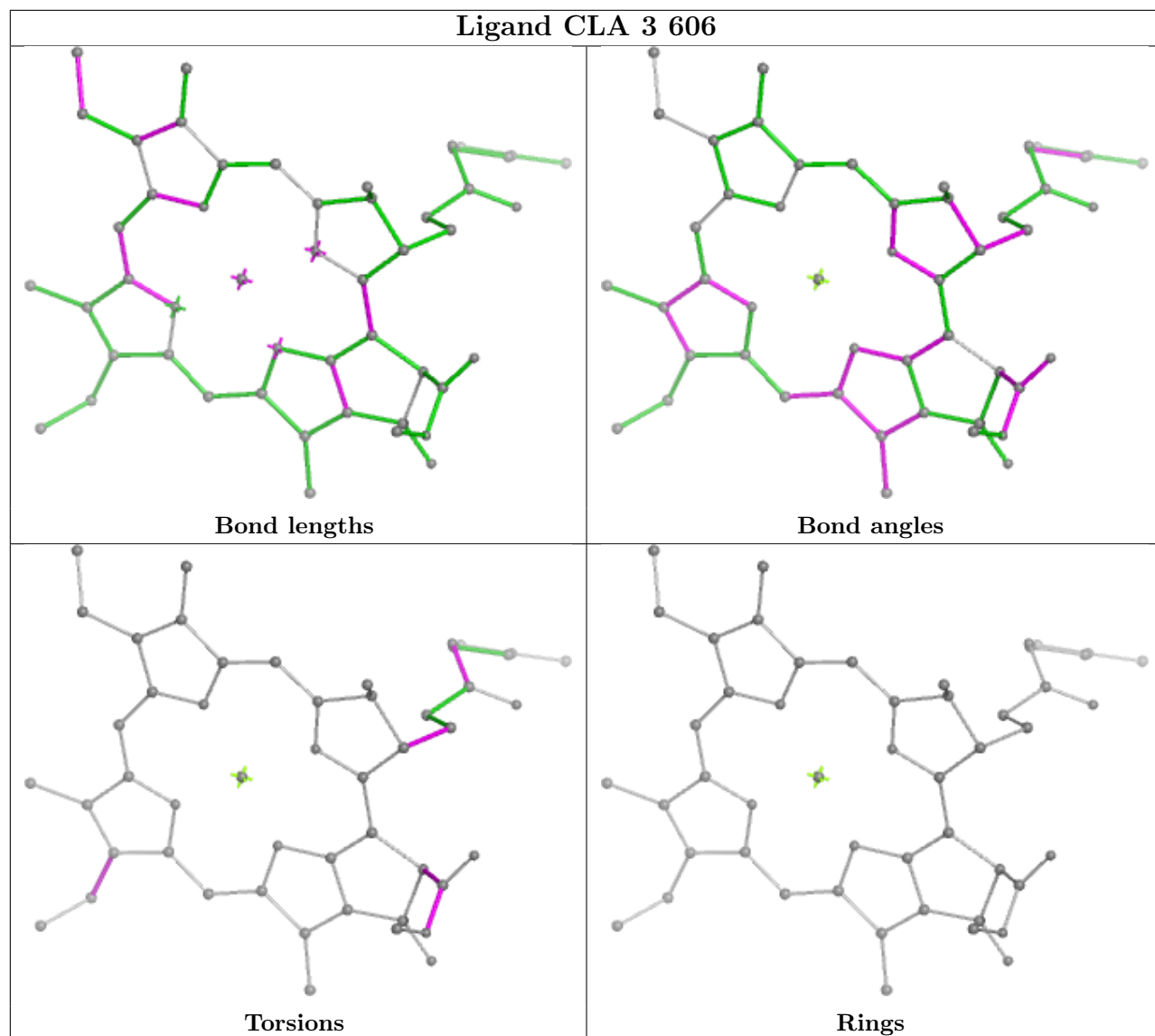


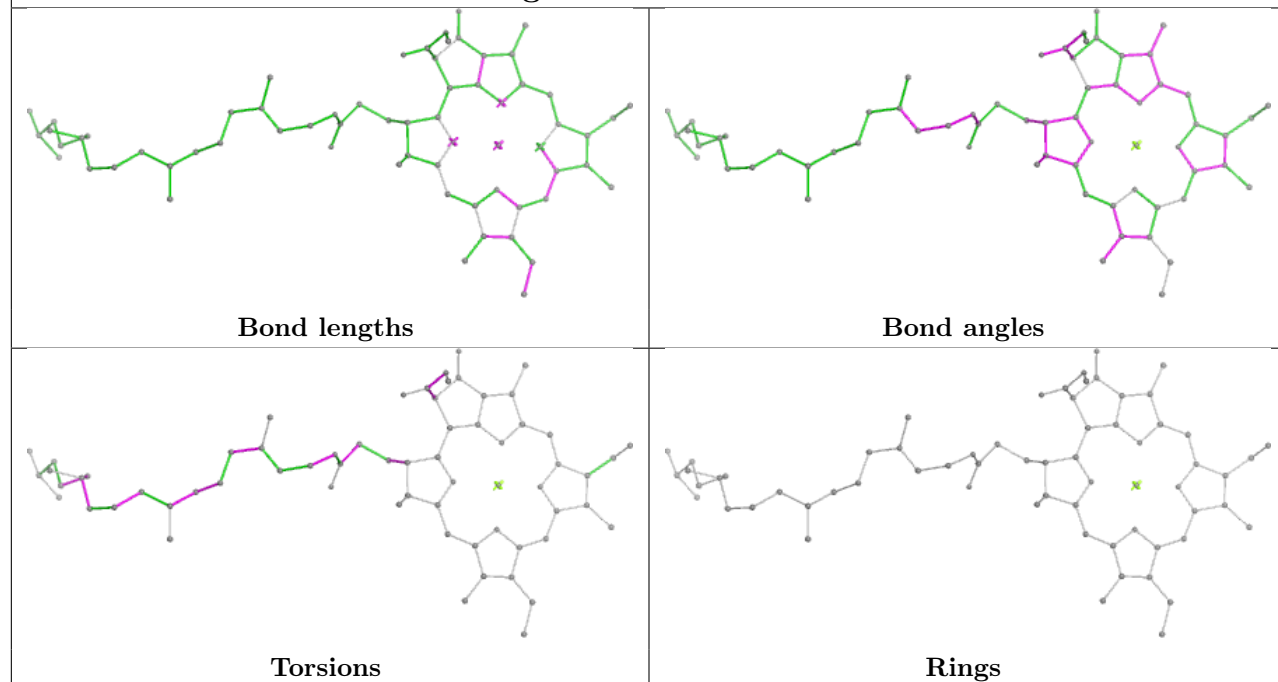
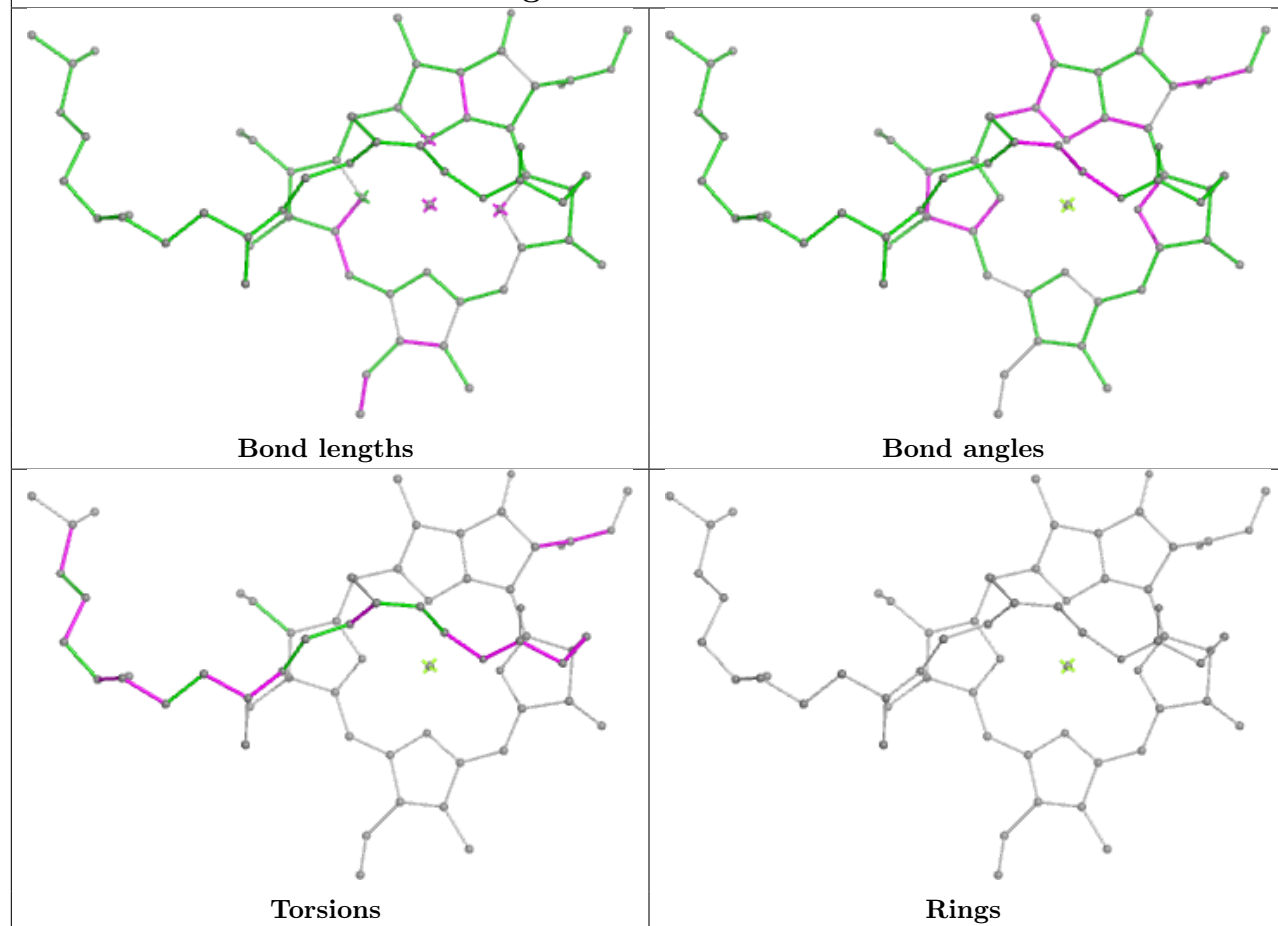


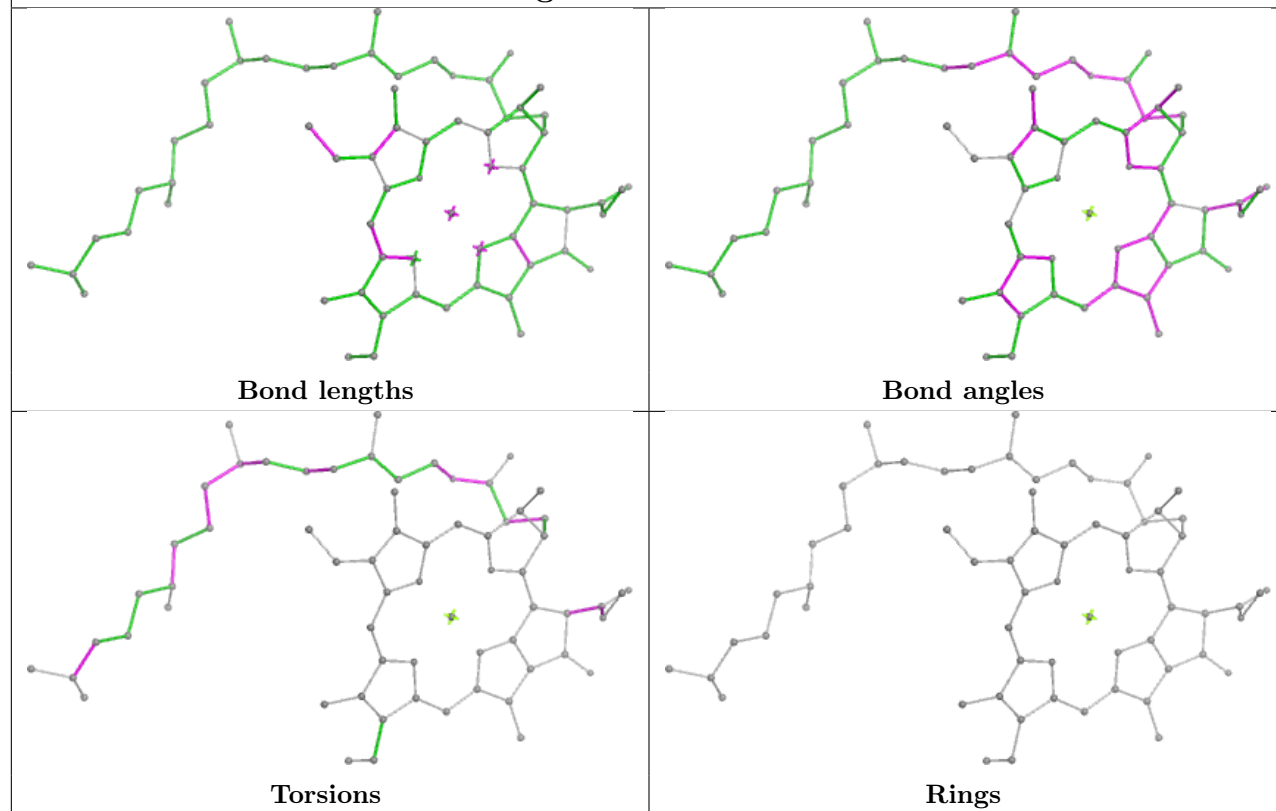
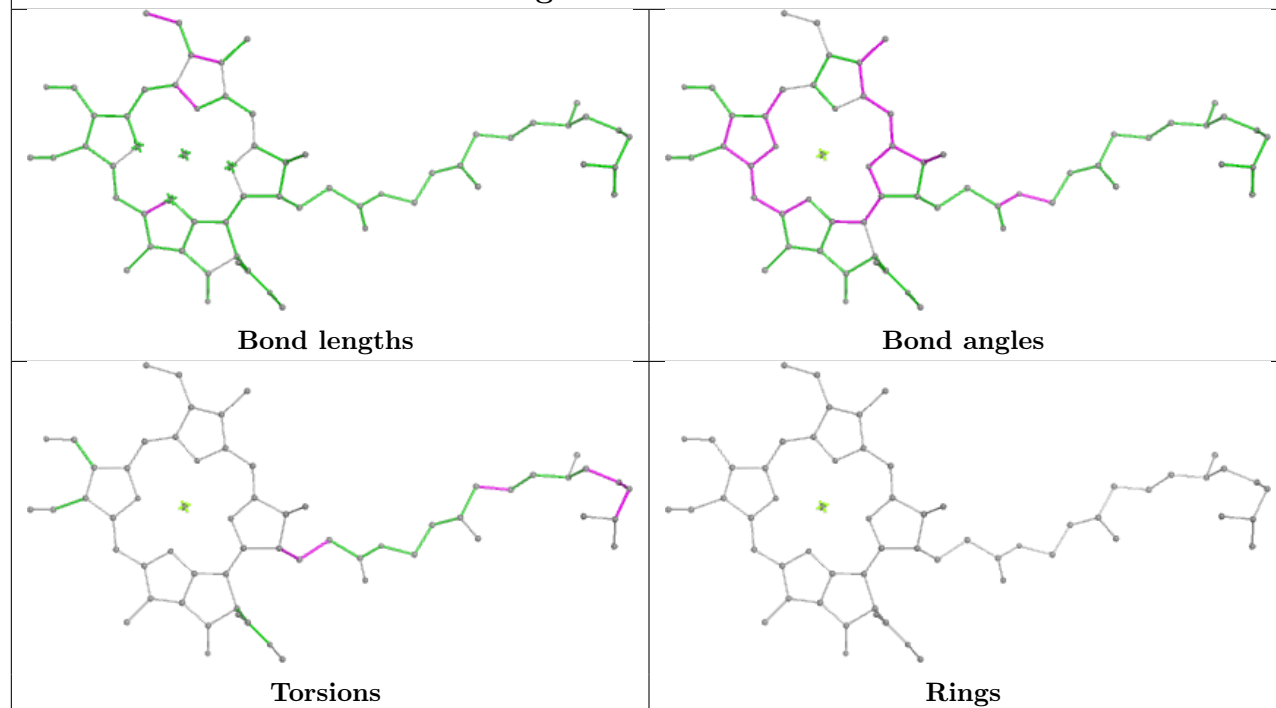


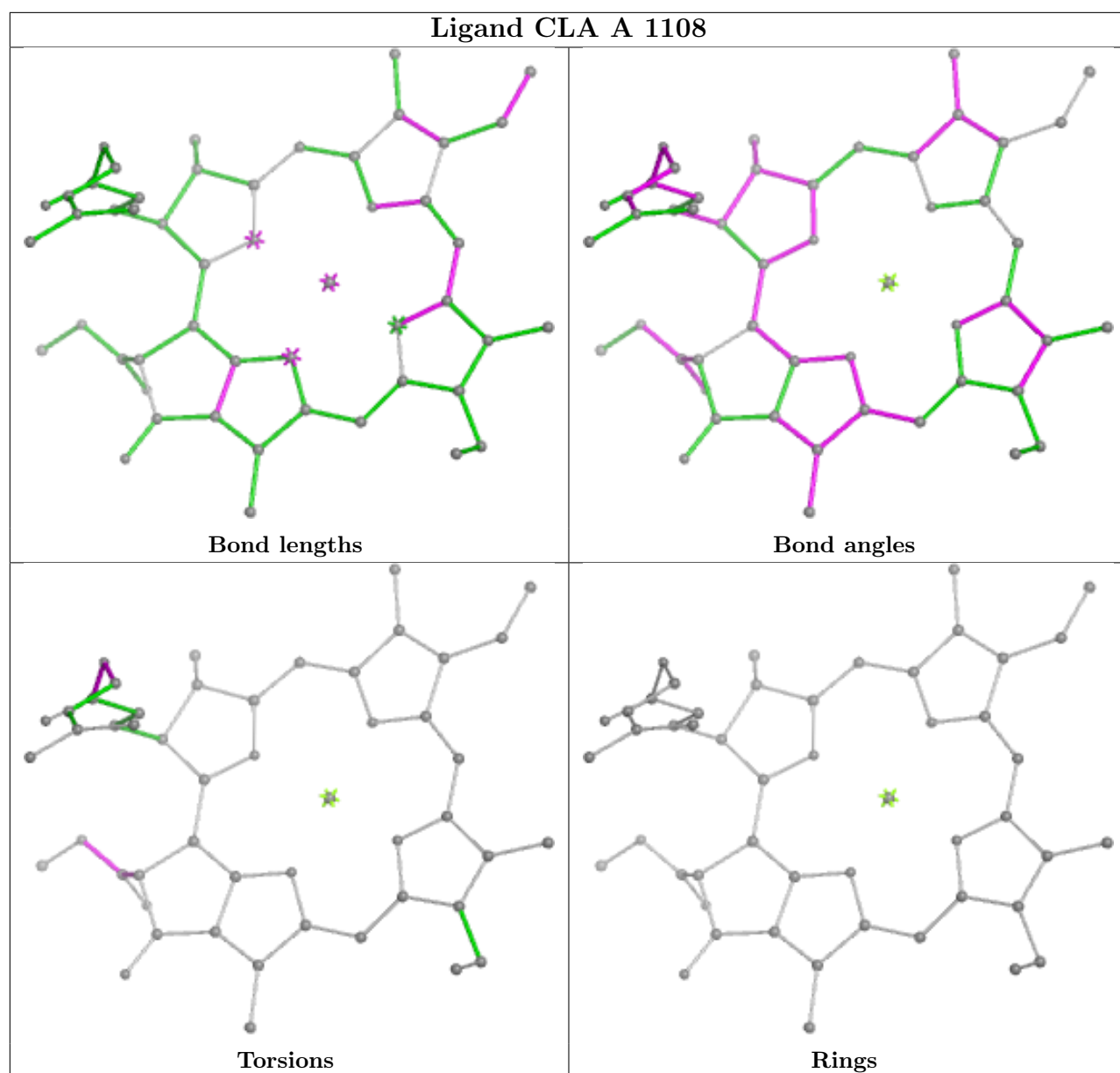


Ligand CLA 3 606

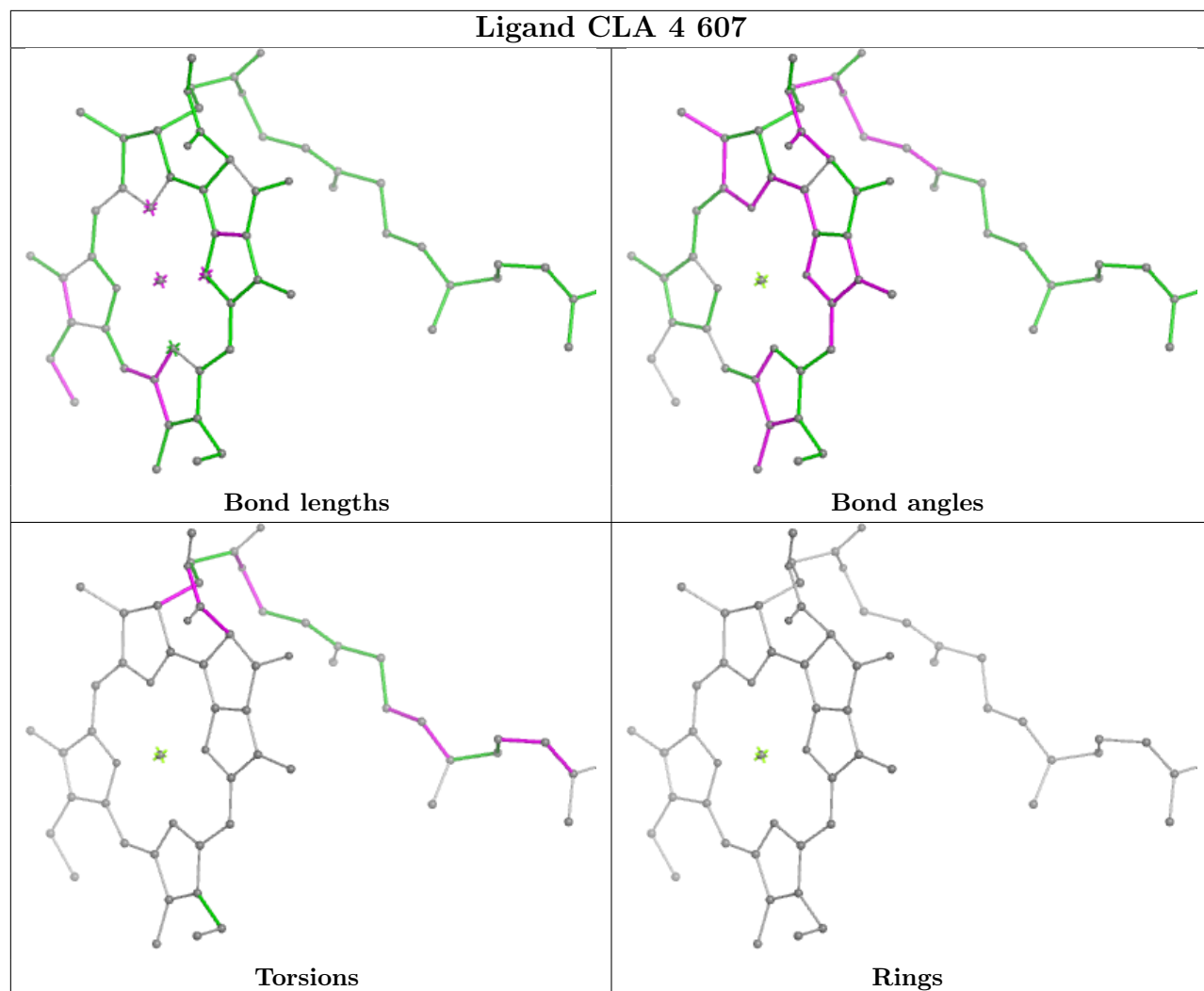


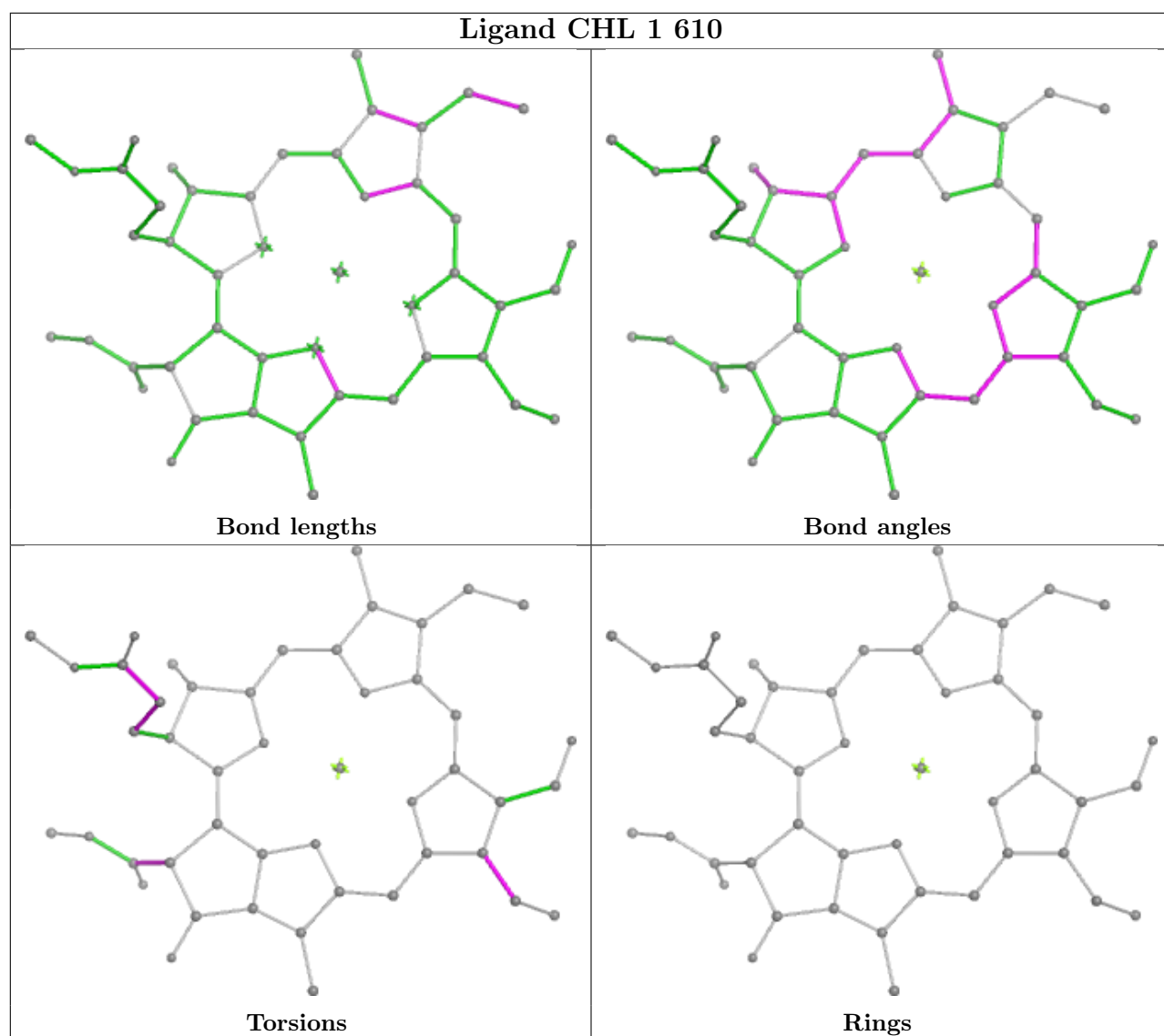
Ligand CLA A 1103**Ligand CLA A 1115**

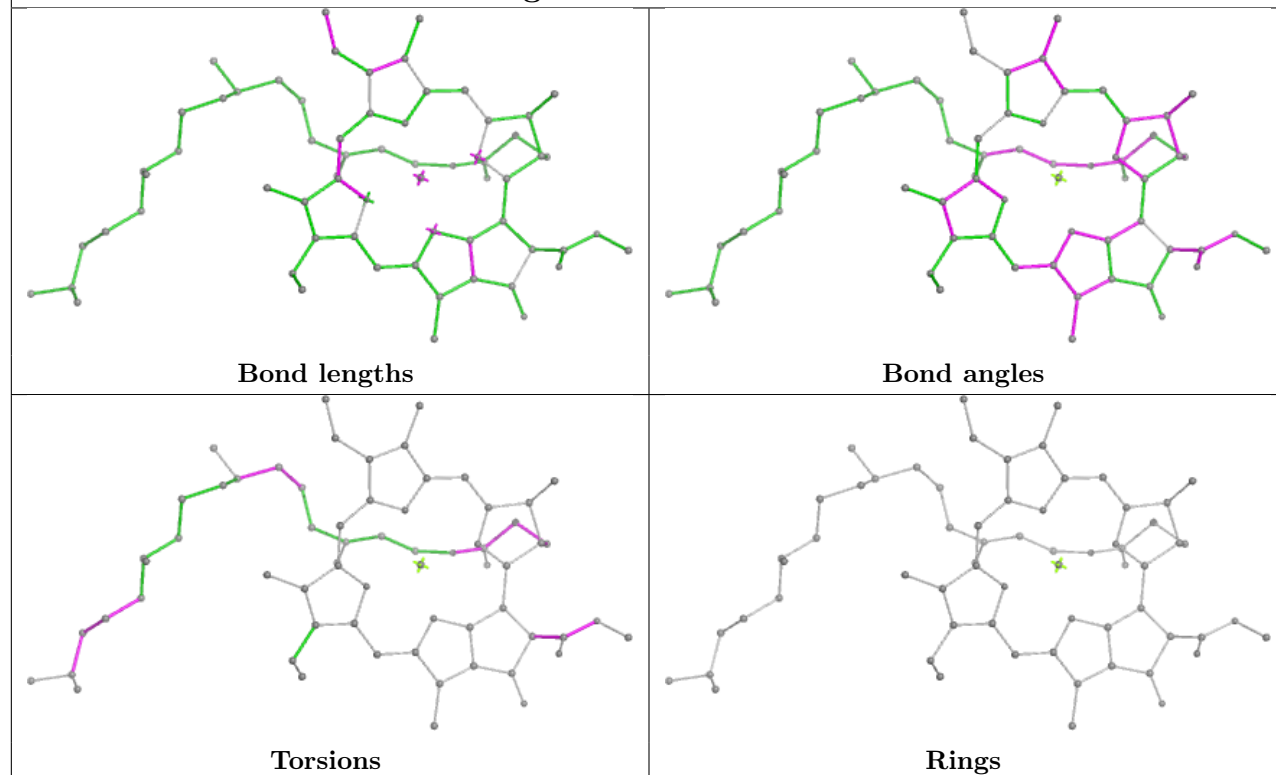
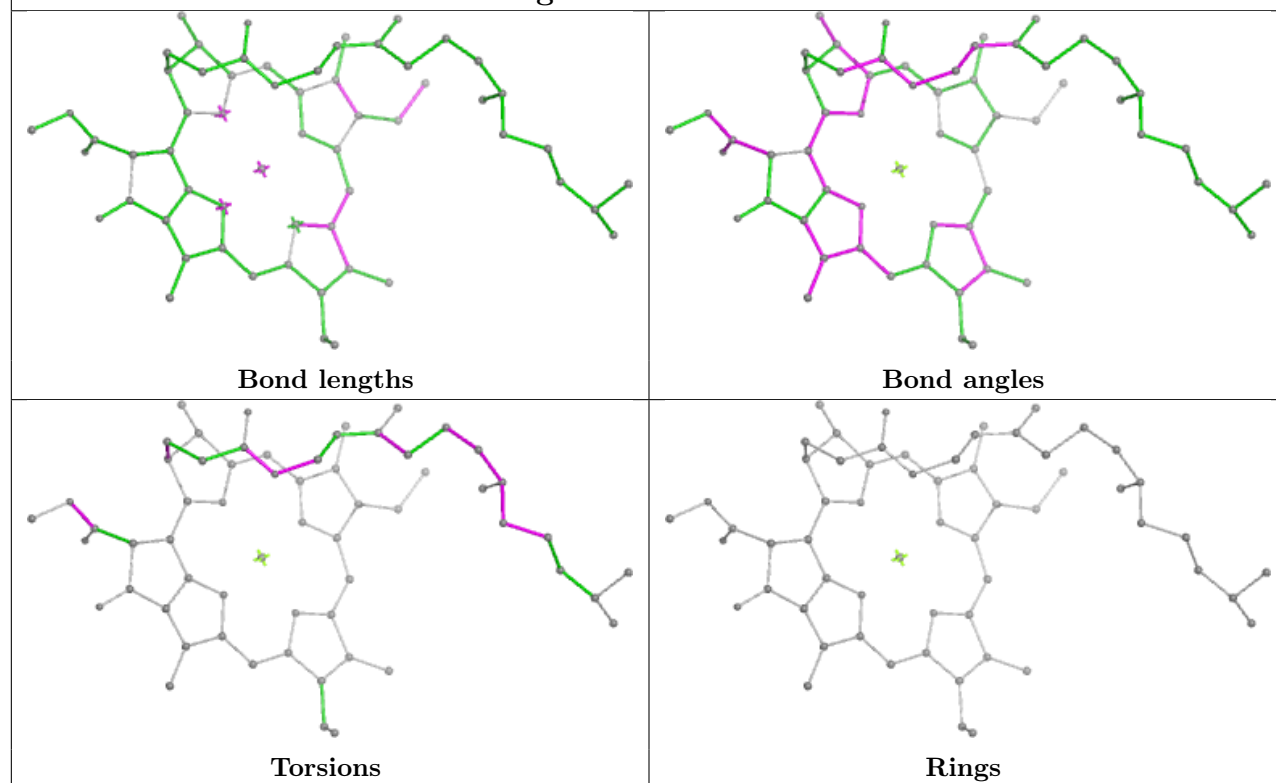
Ligand CLA 1 604**Ligand CHL 4 613**

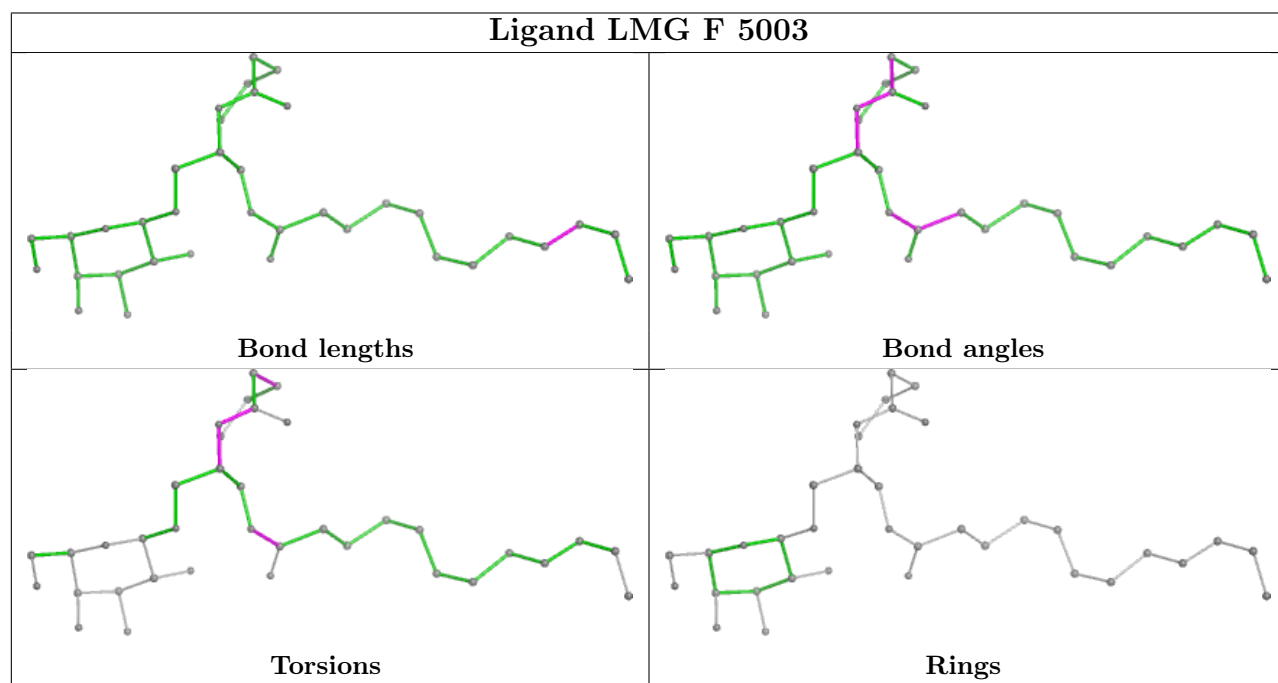
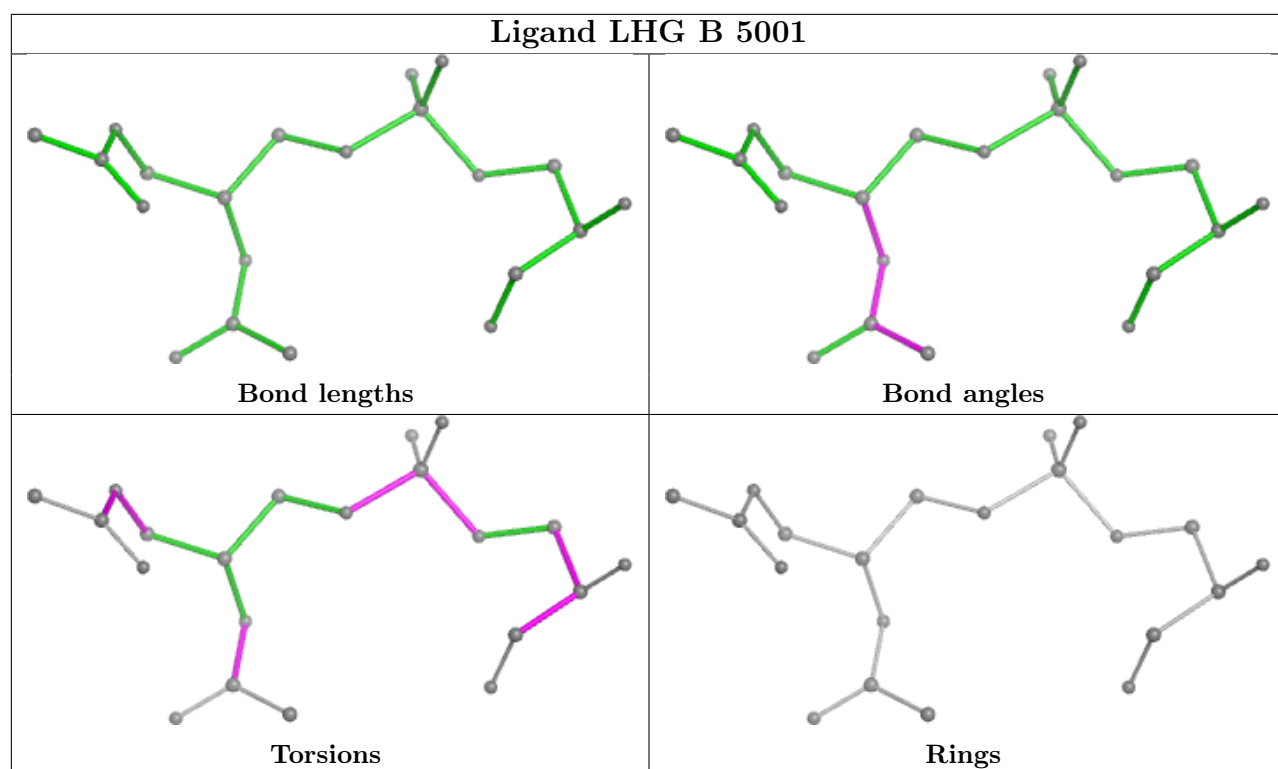


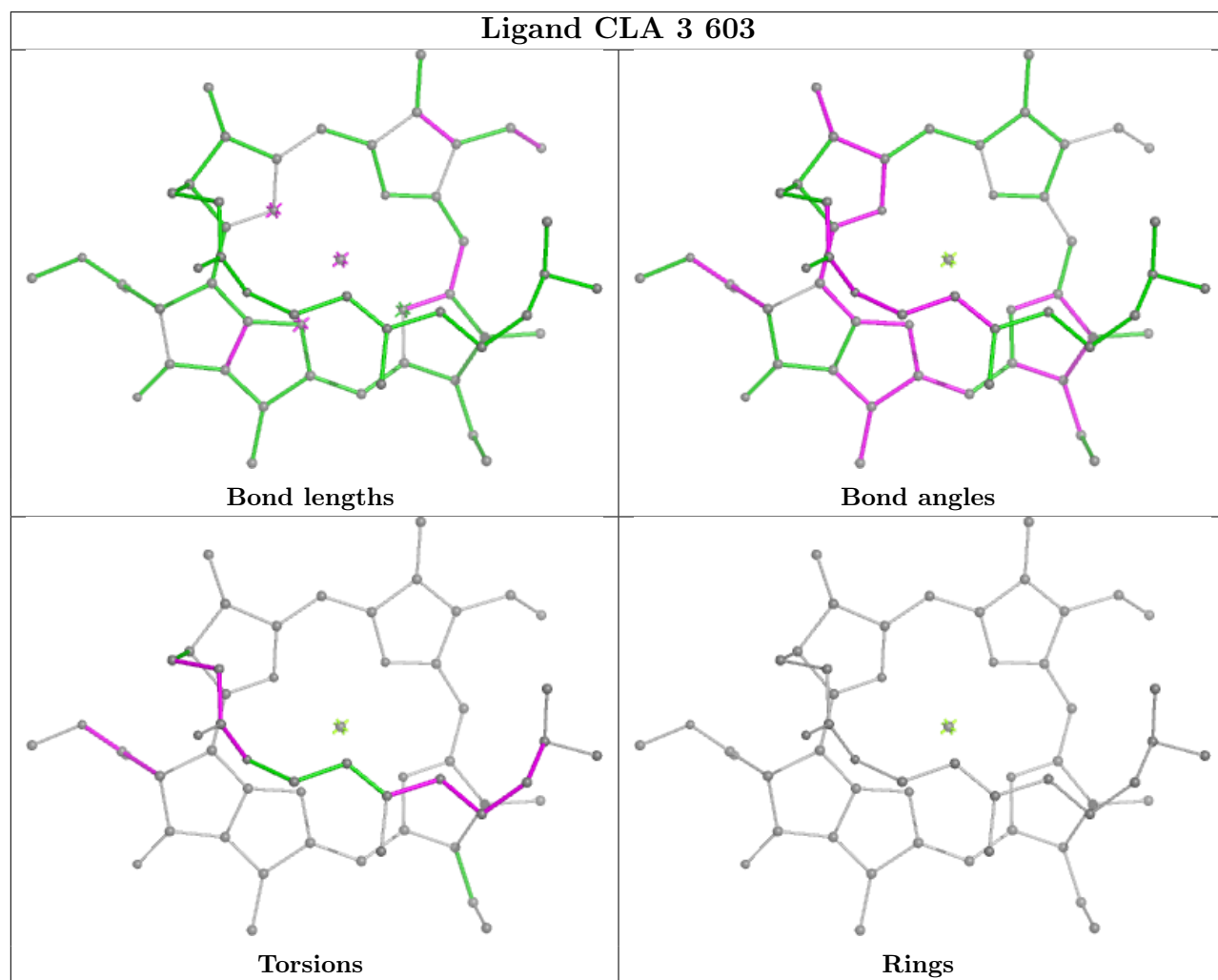
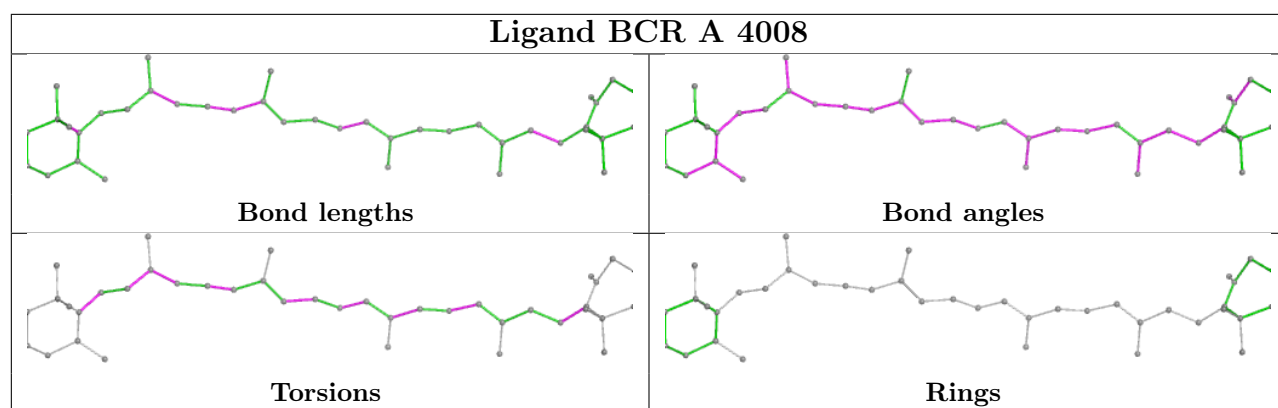
Ligand CLA 4 607



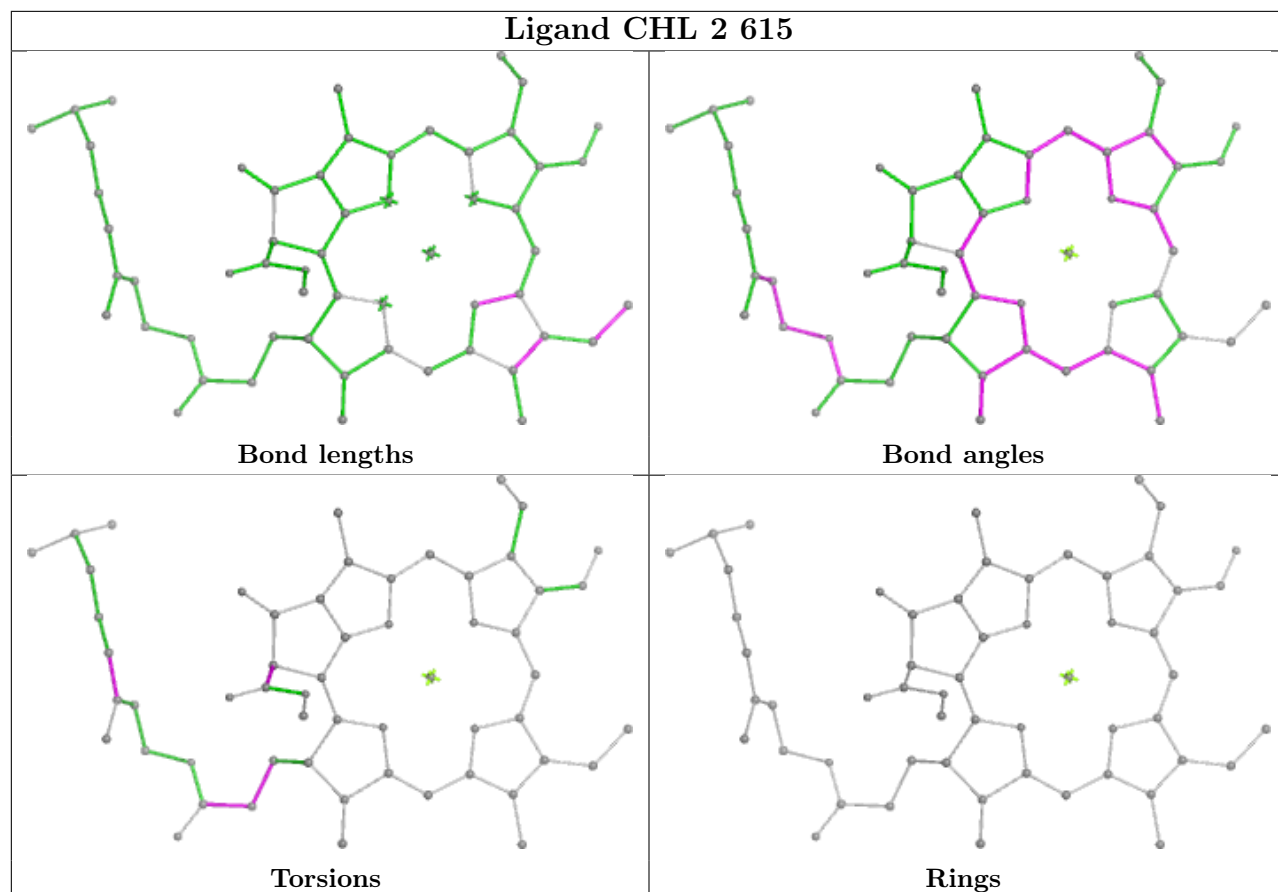


Ligand CLA B 1235**Ligand CLA 4 601**

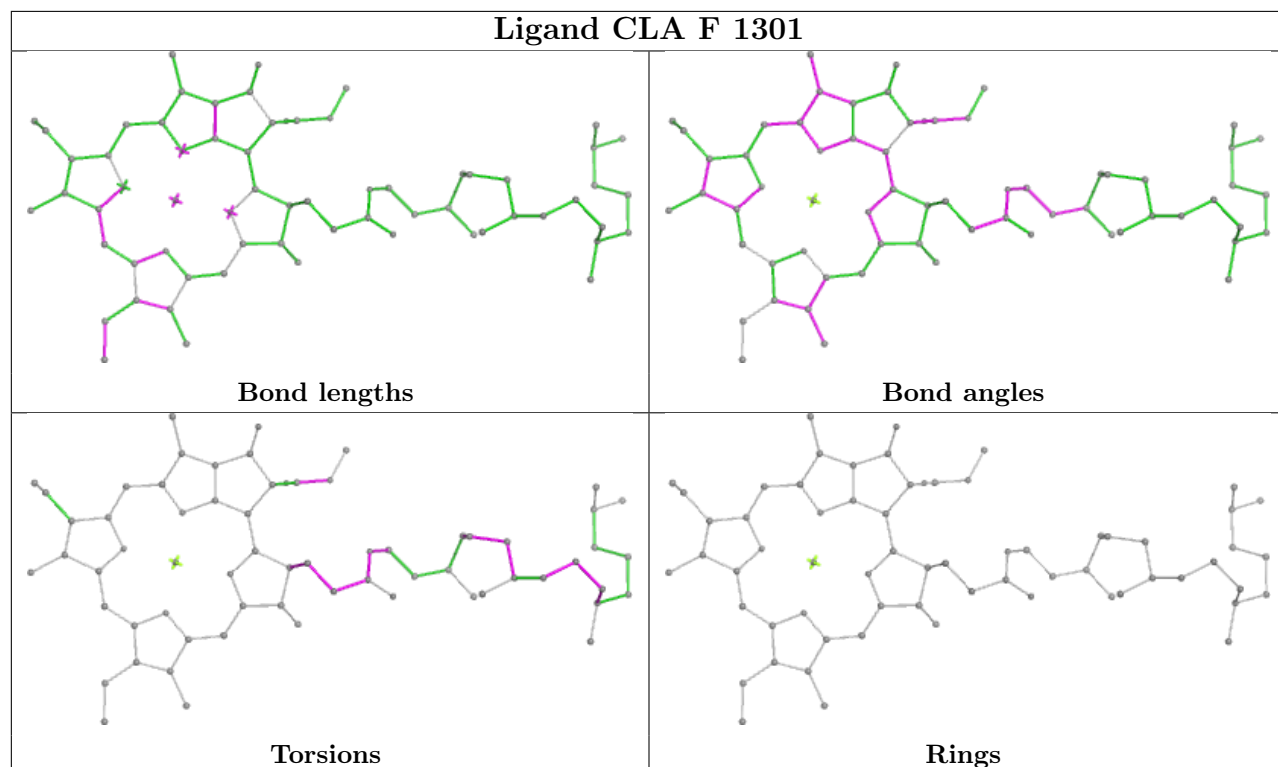


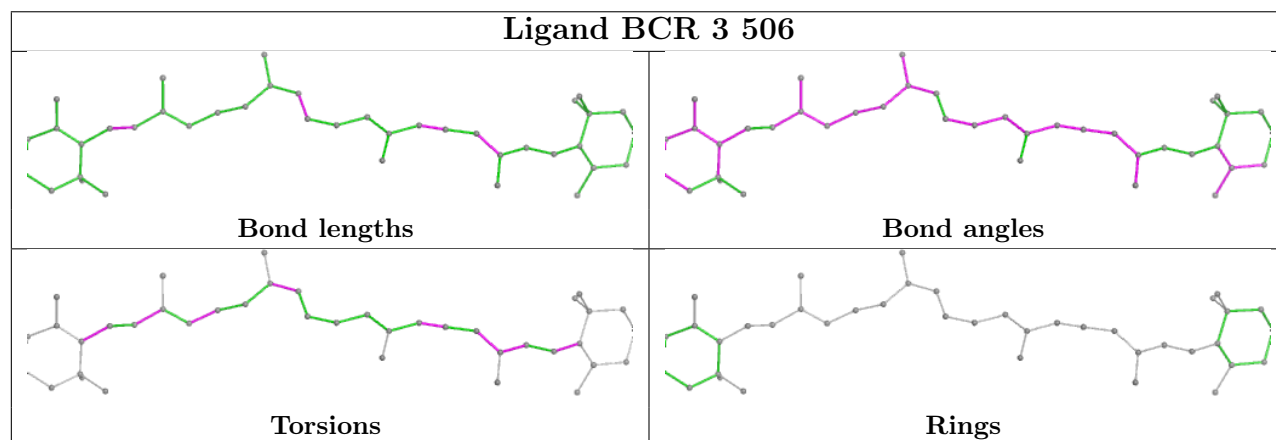
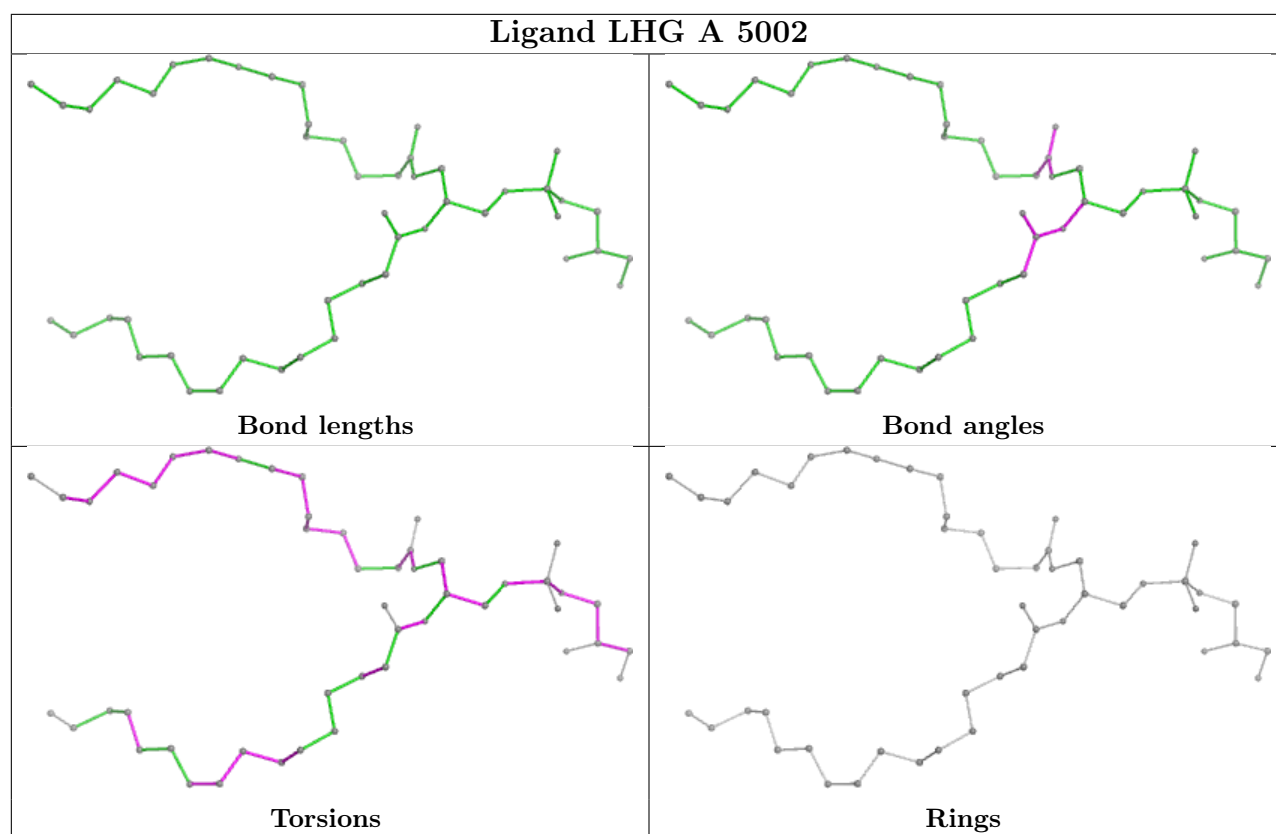


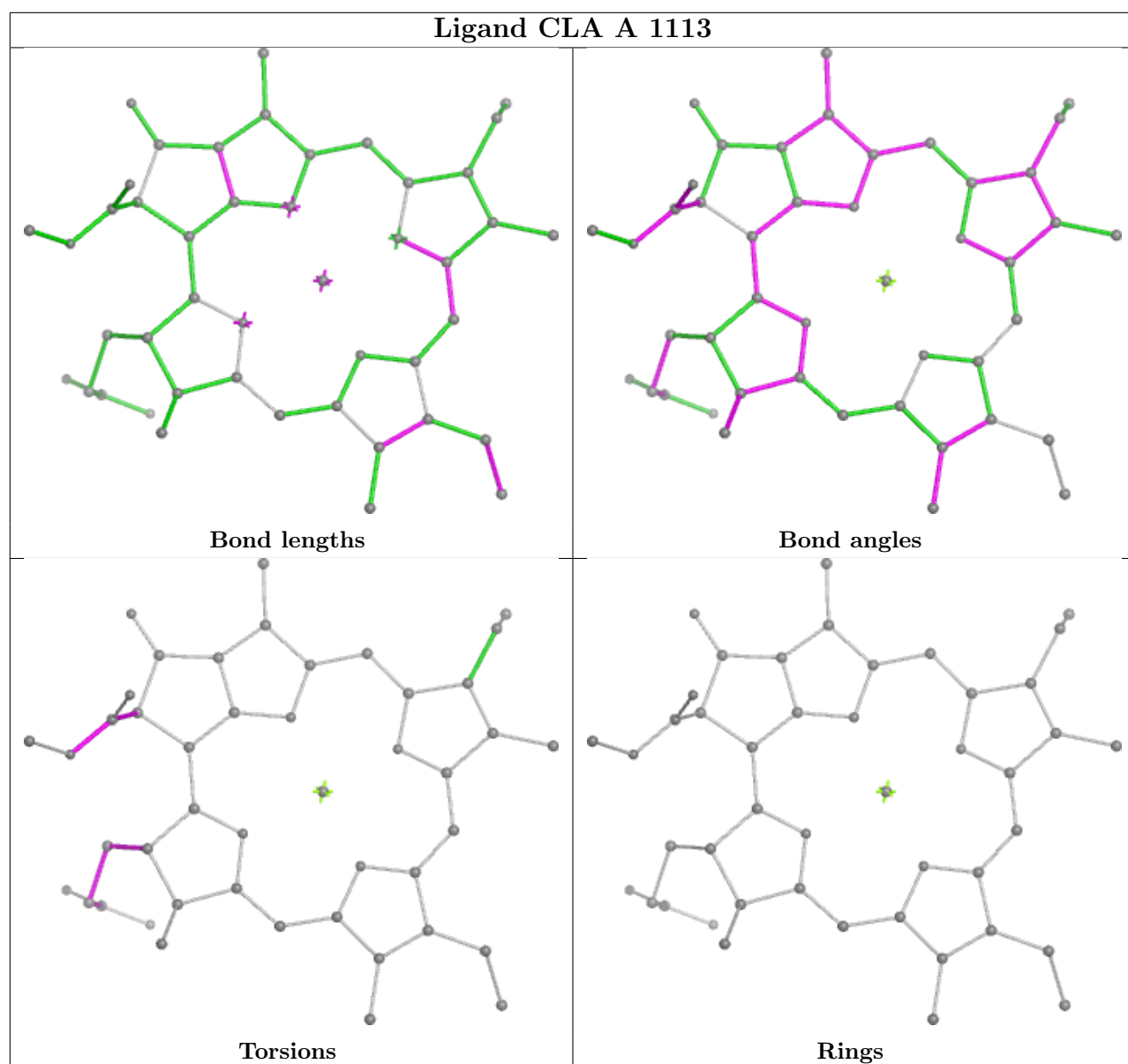
Ligand CHL 2 615

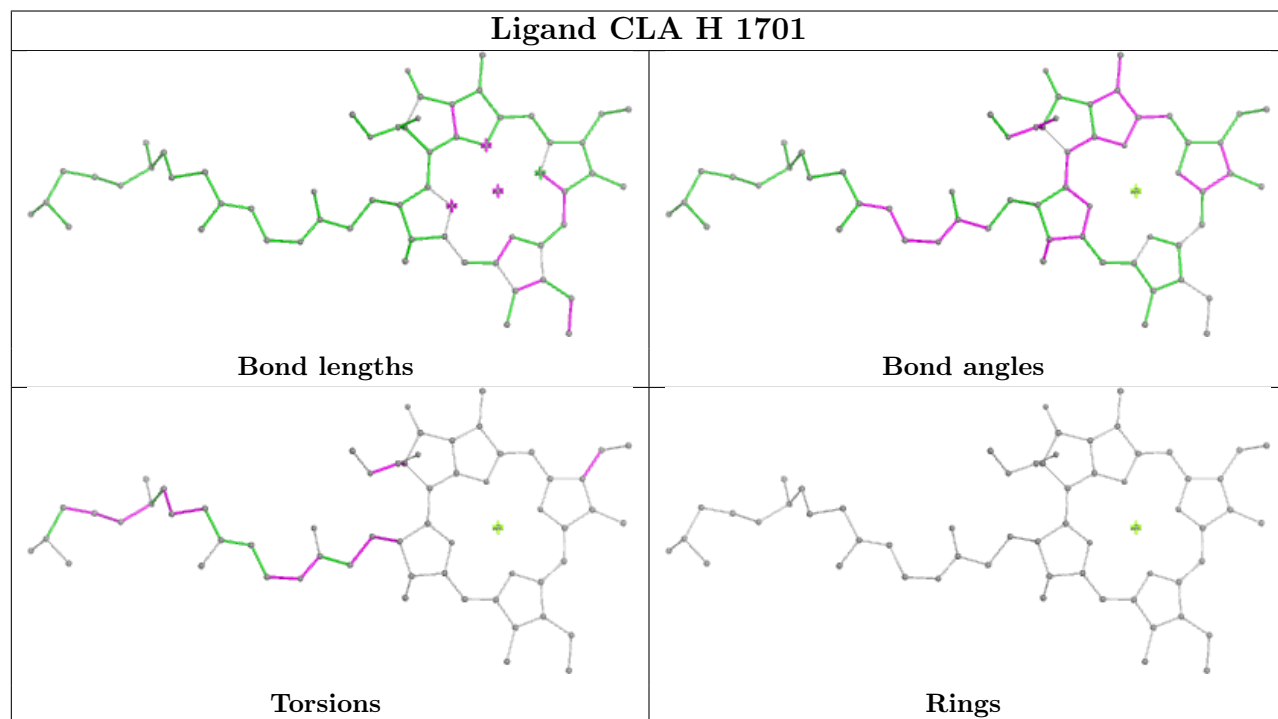
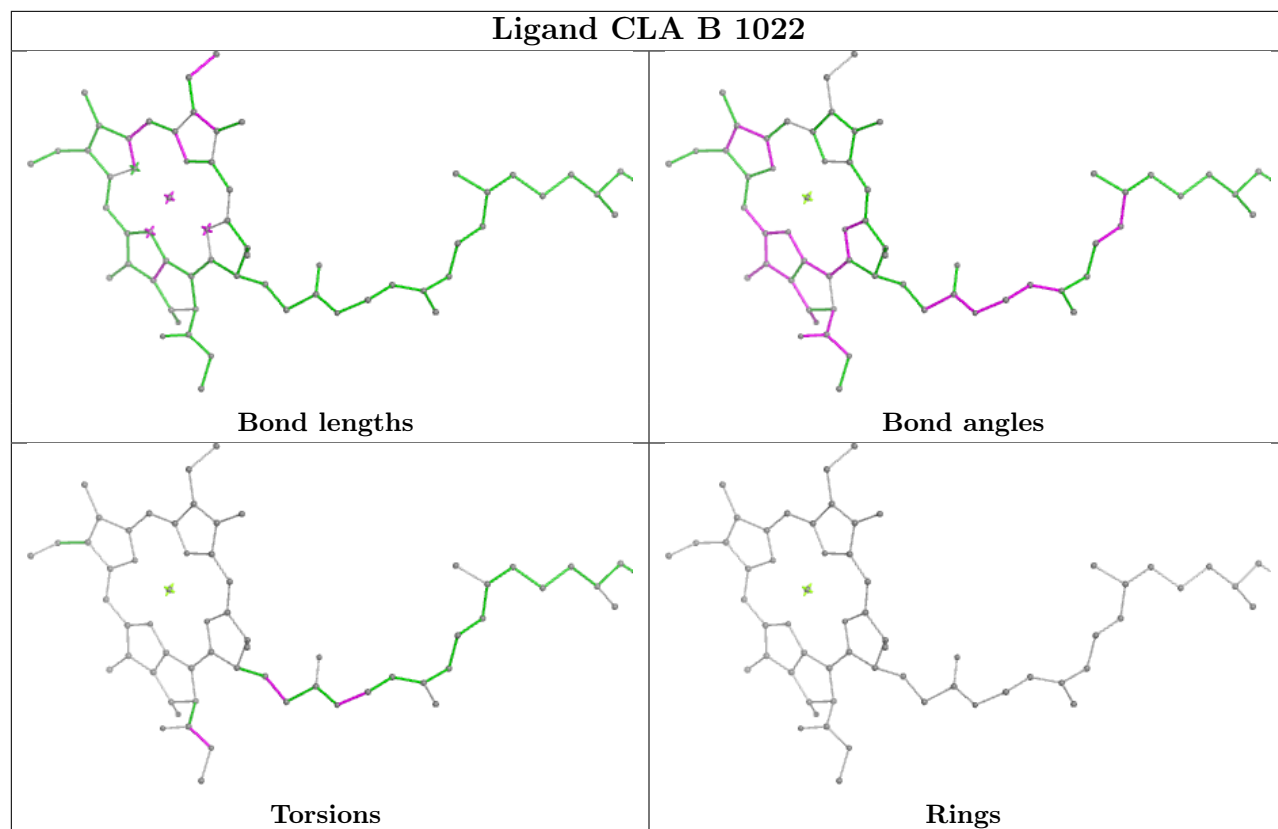


Ligand CLA F 1301

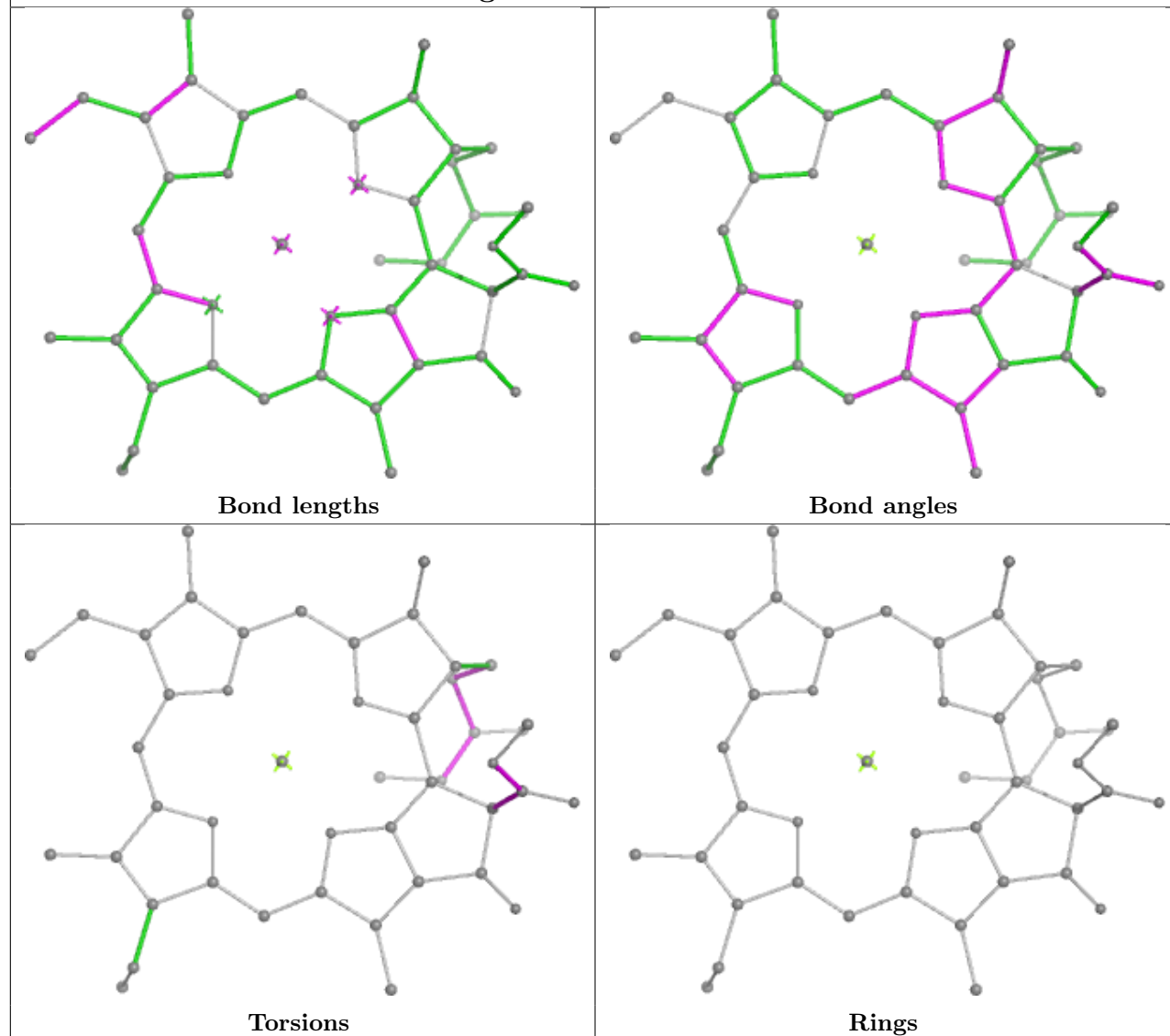




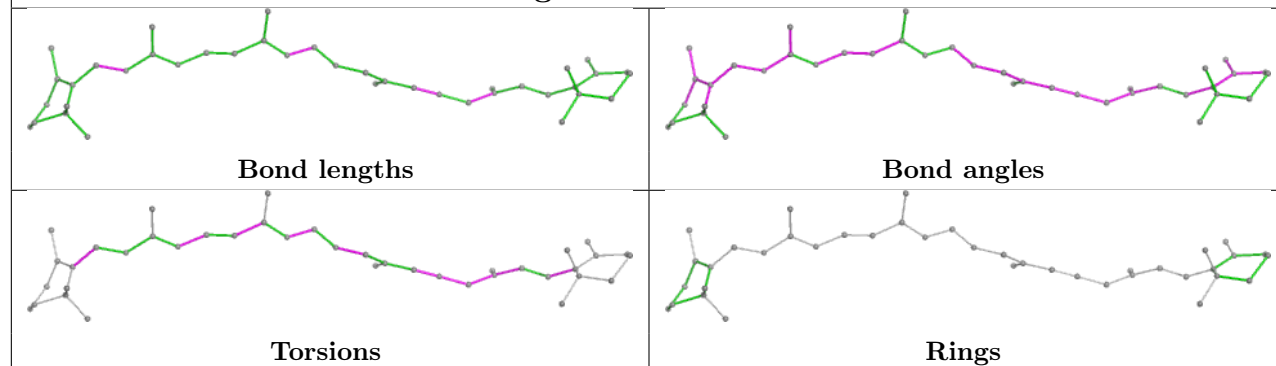




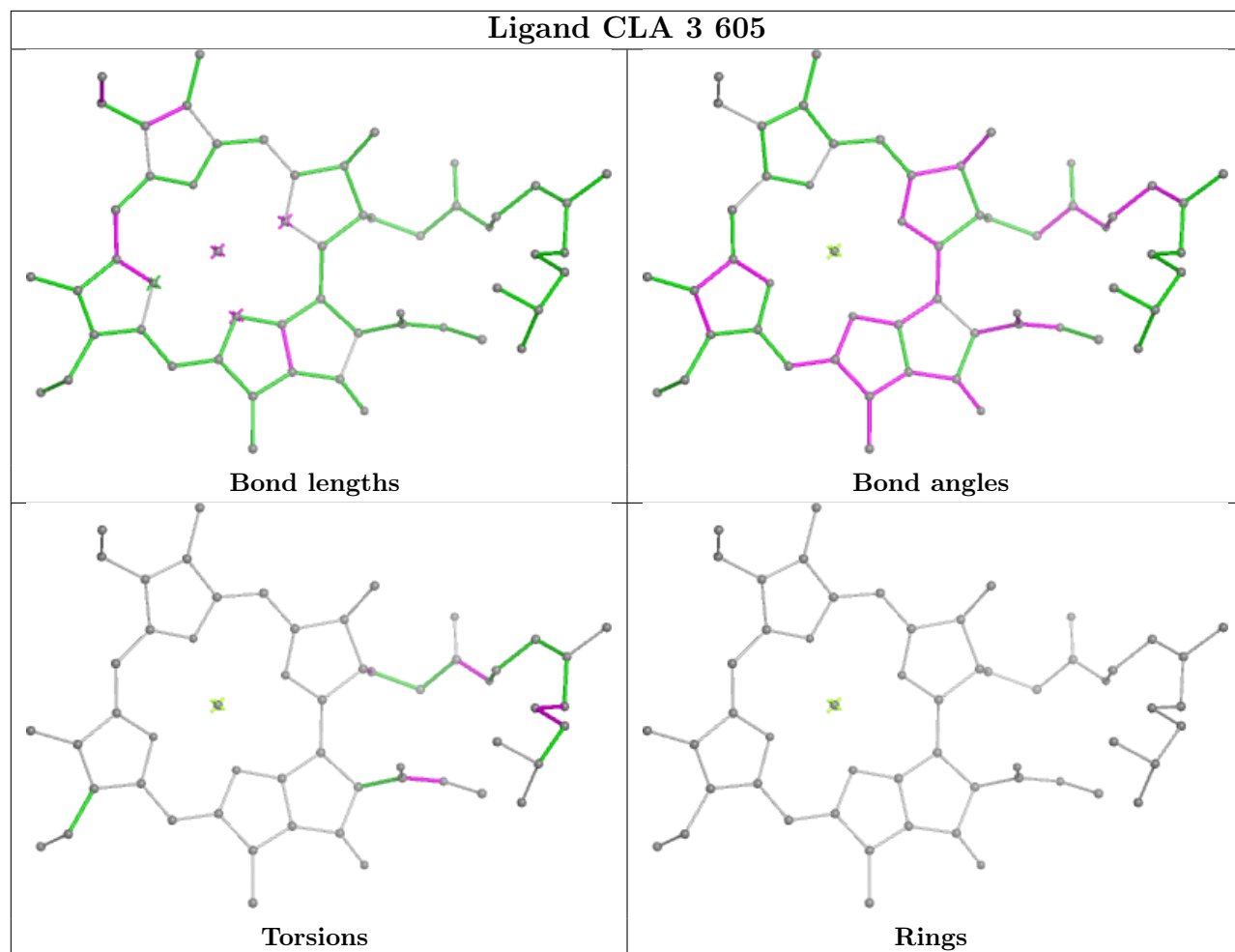
Ligand CLA A 1114

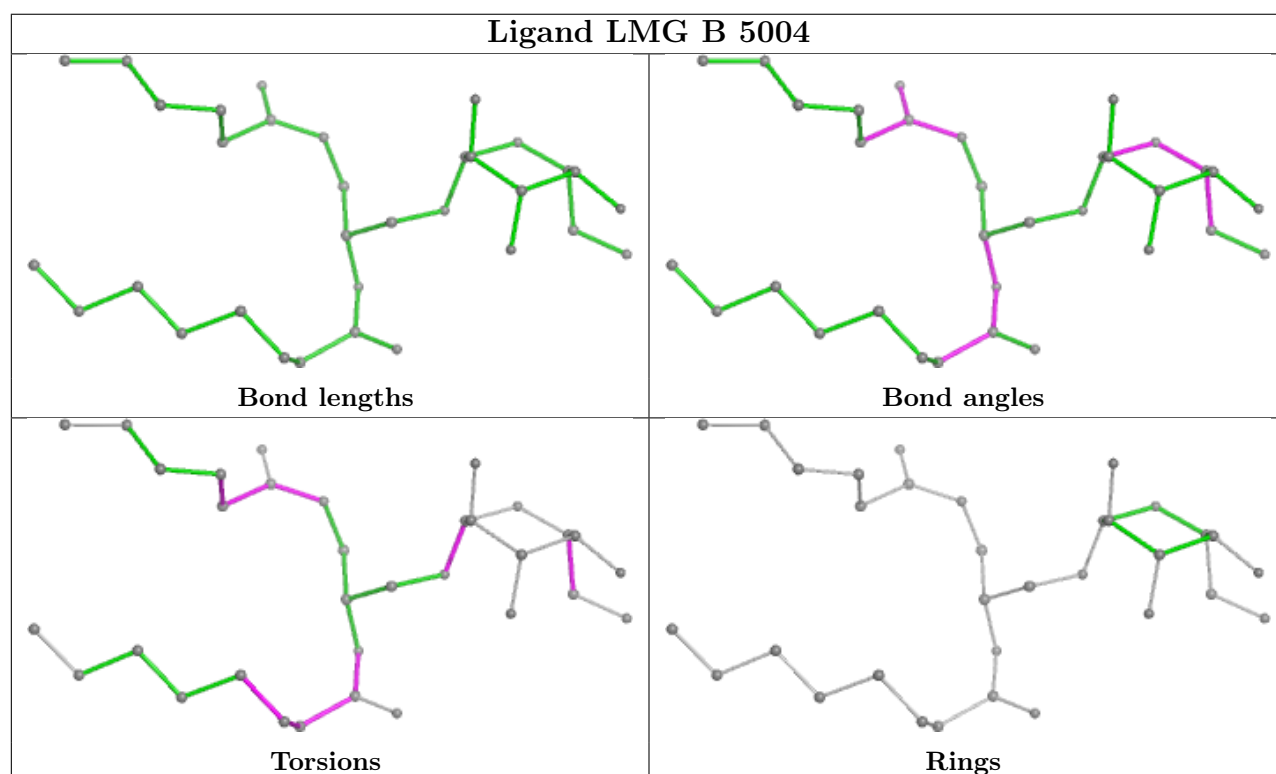
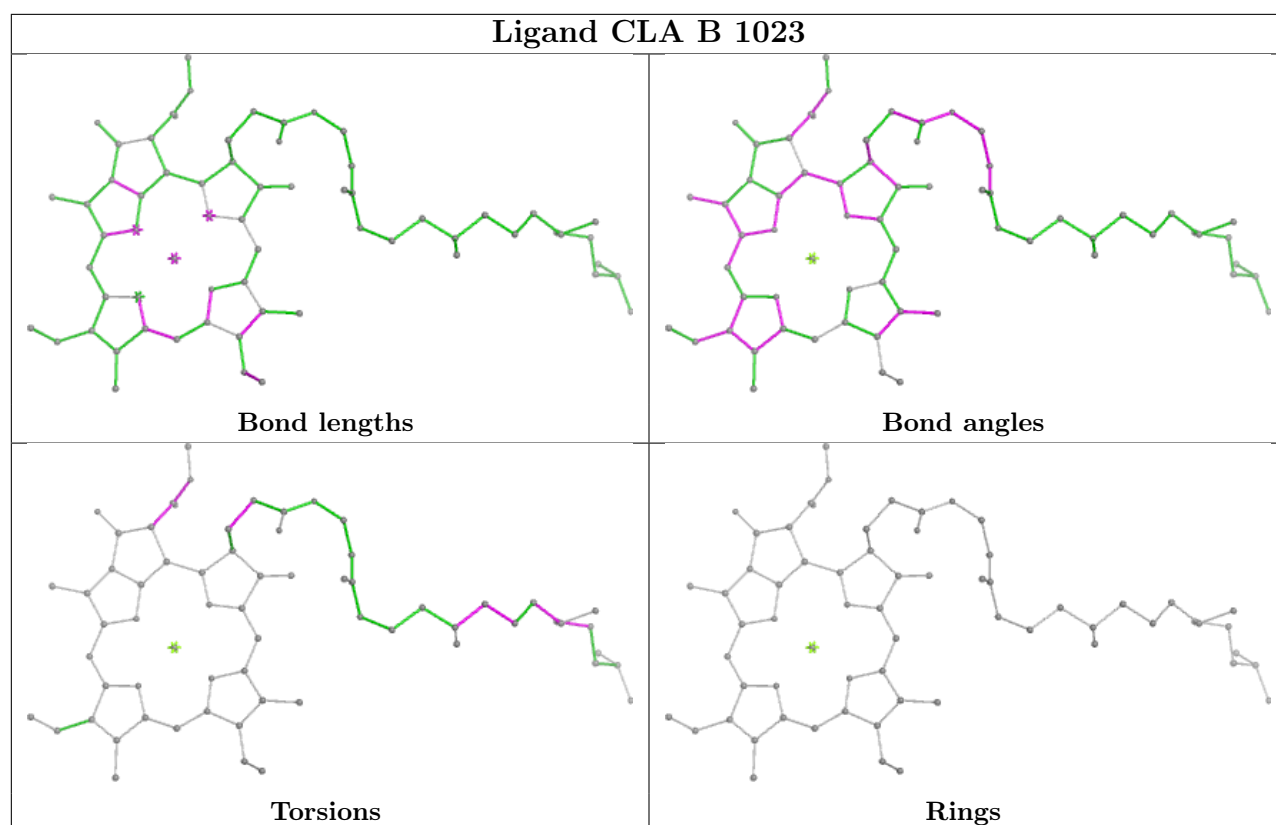


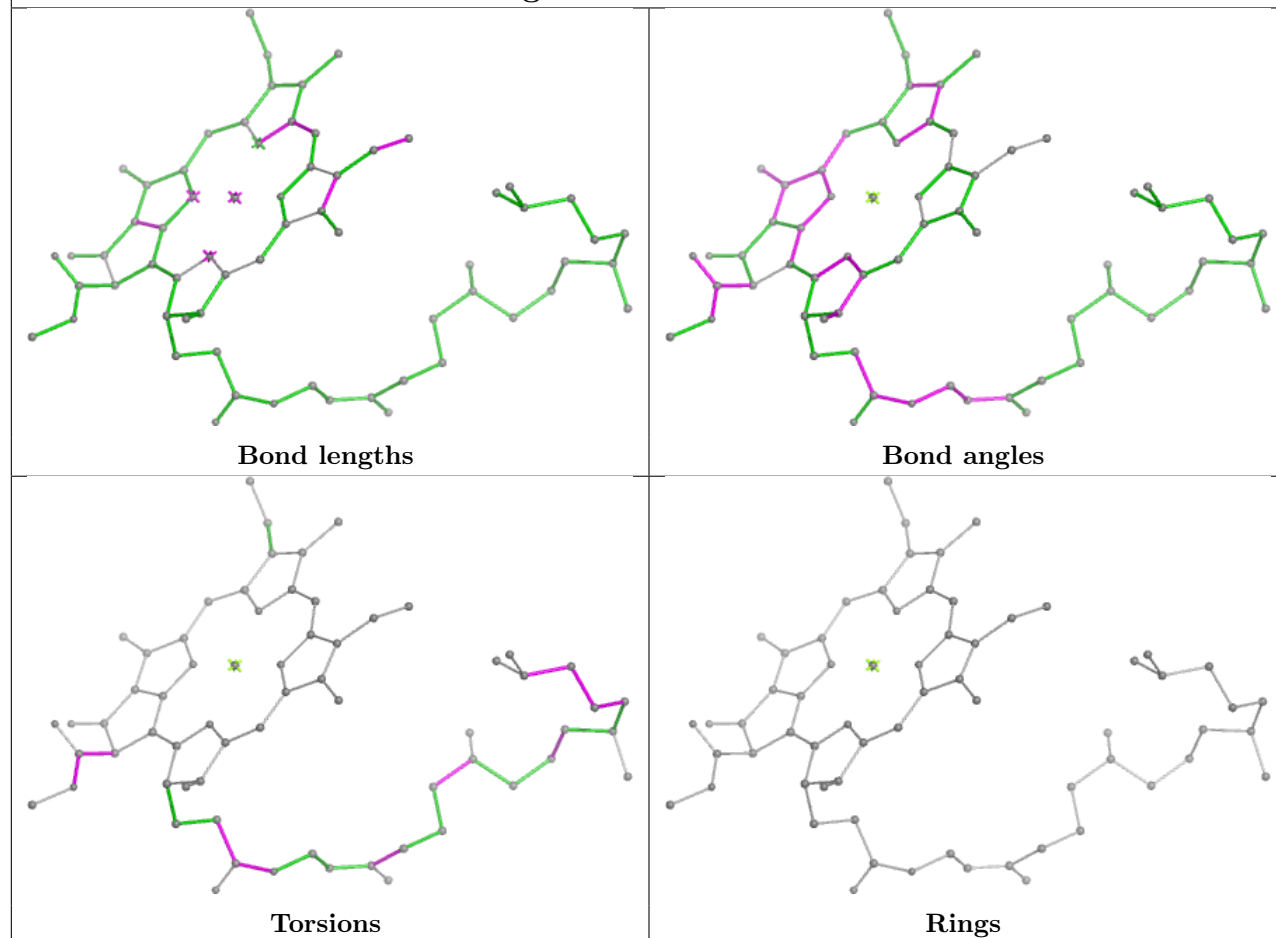
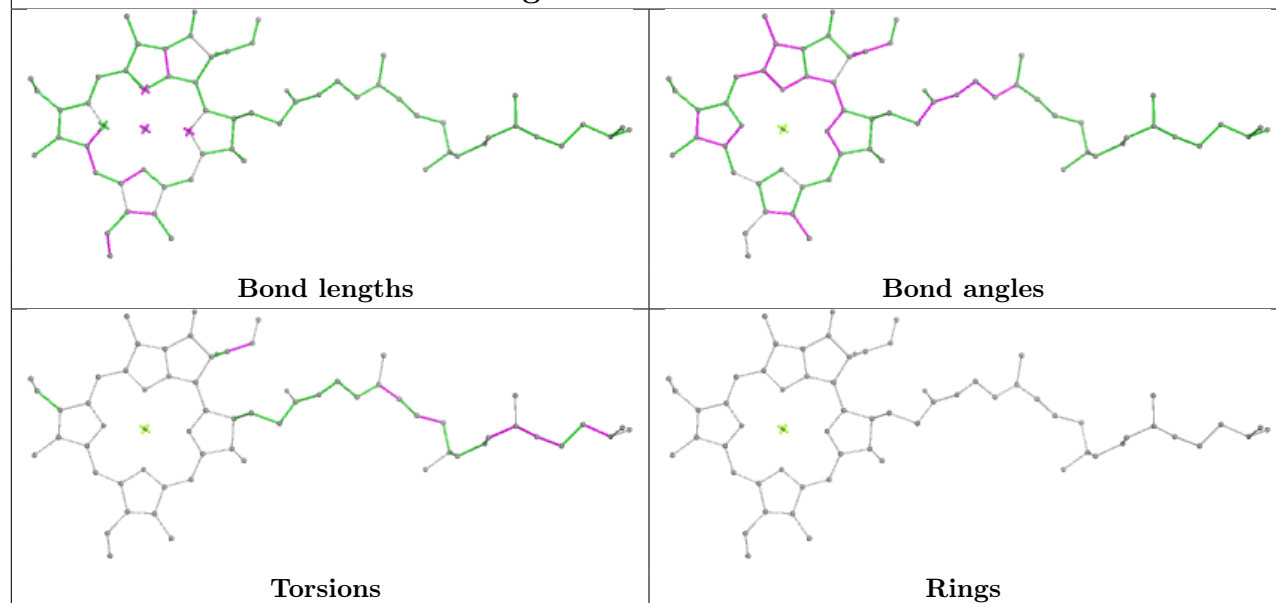
Ligand BCR 3 503

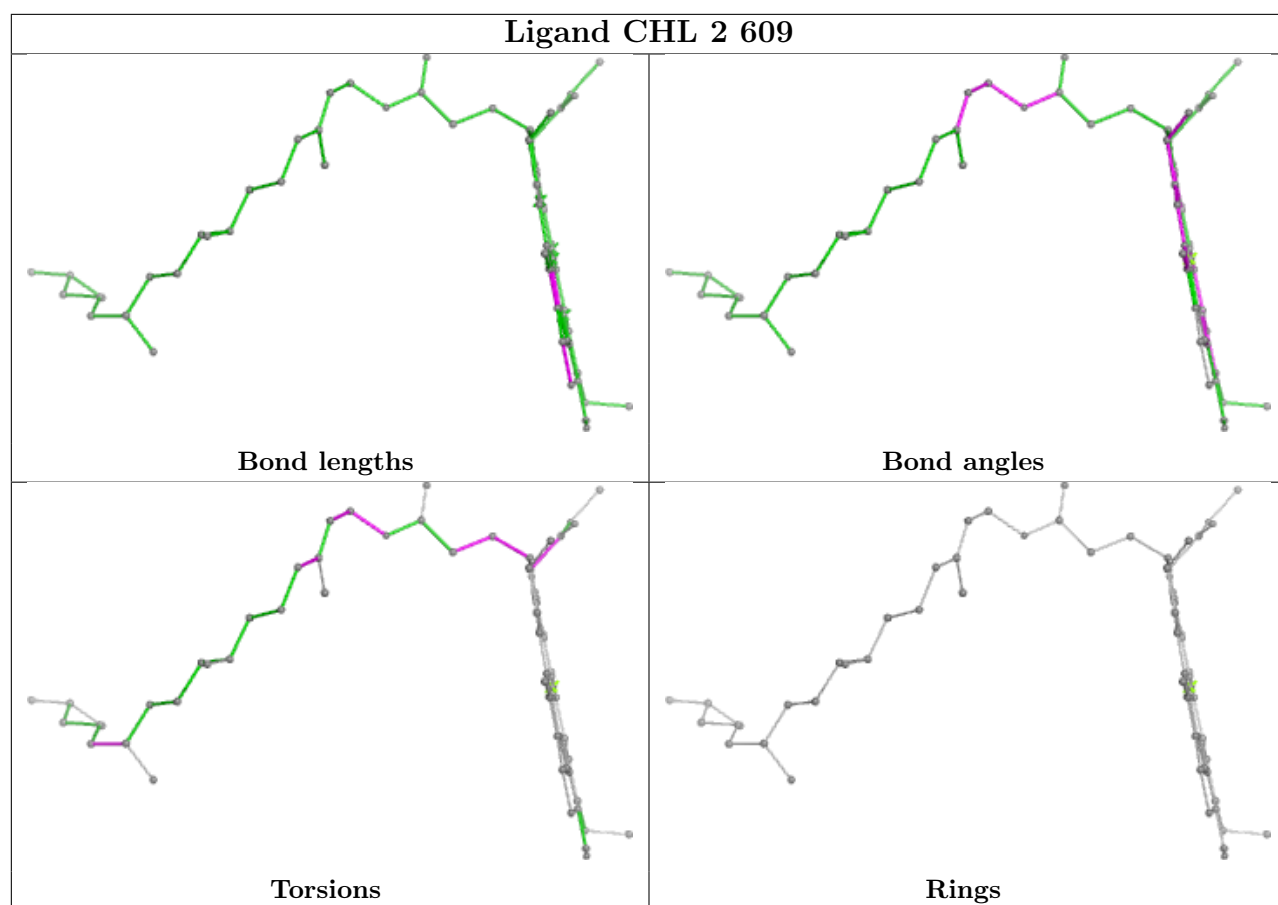


Ligand CLA 3 605

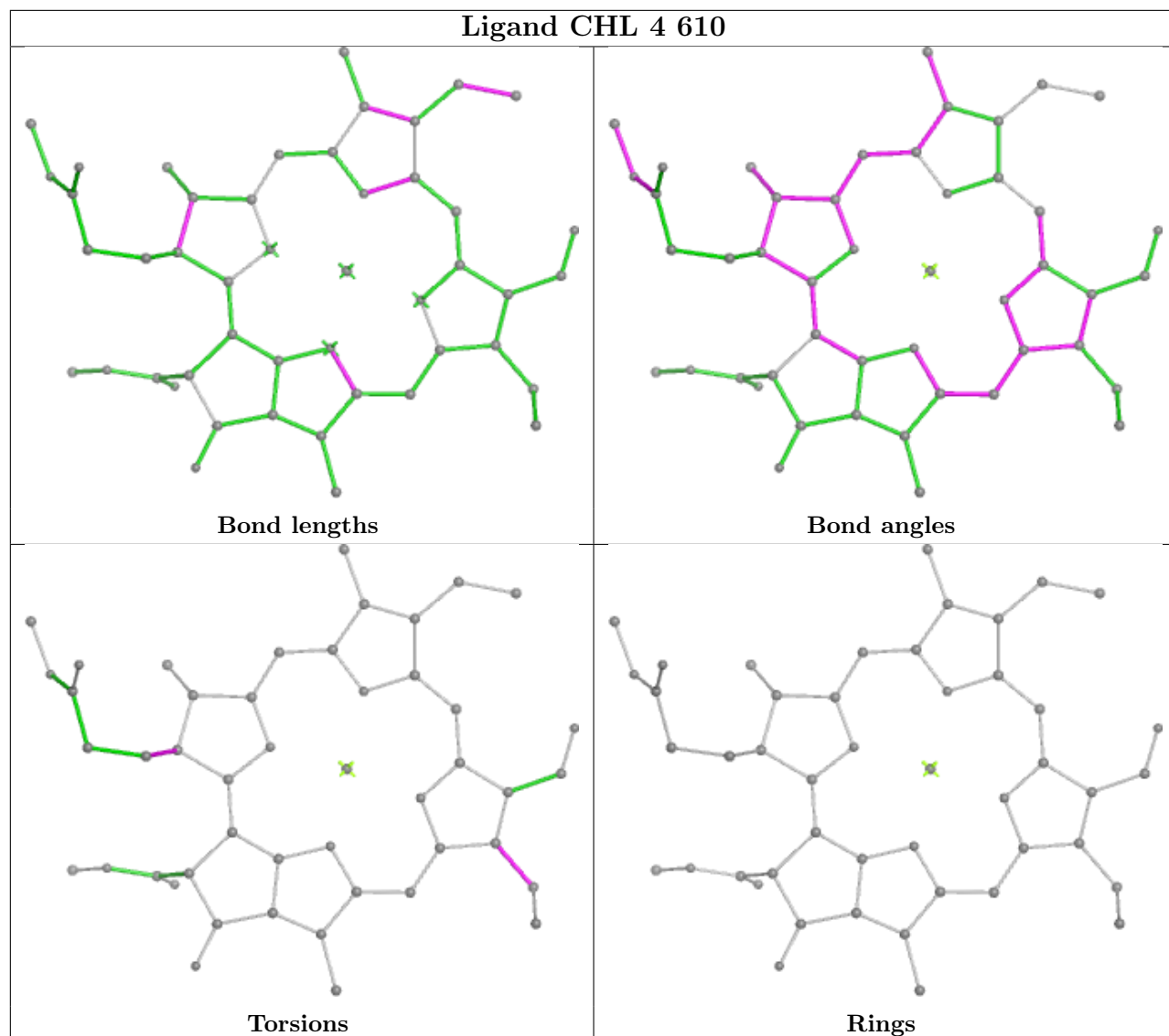


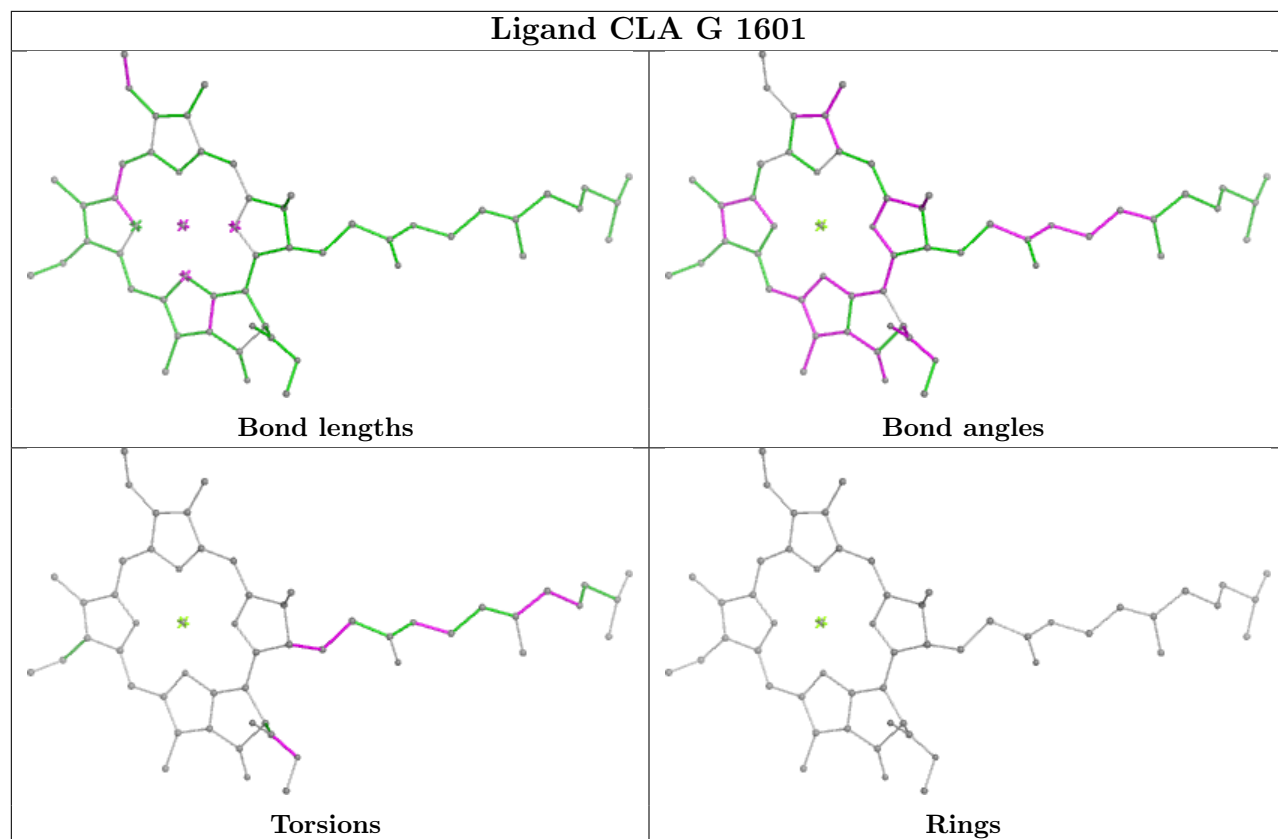


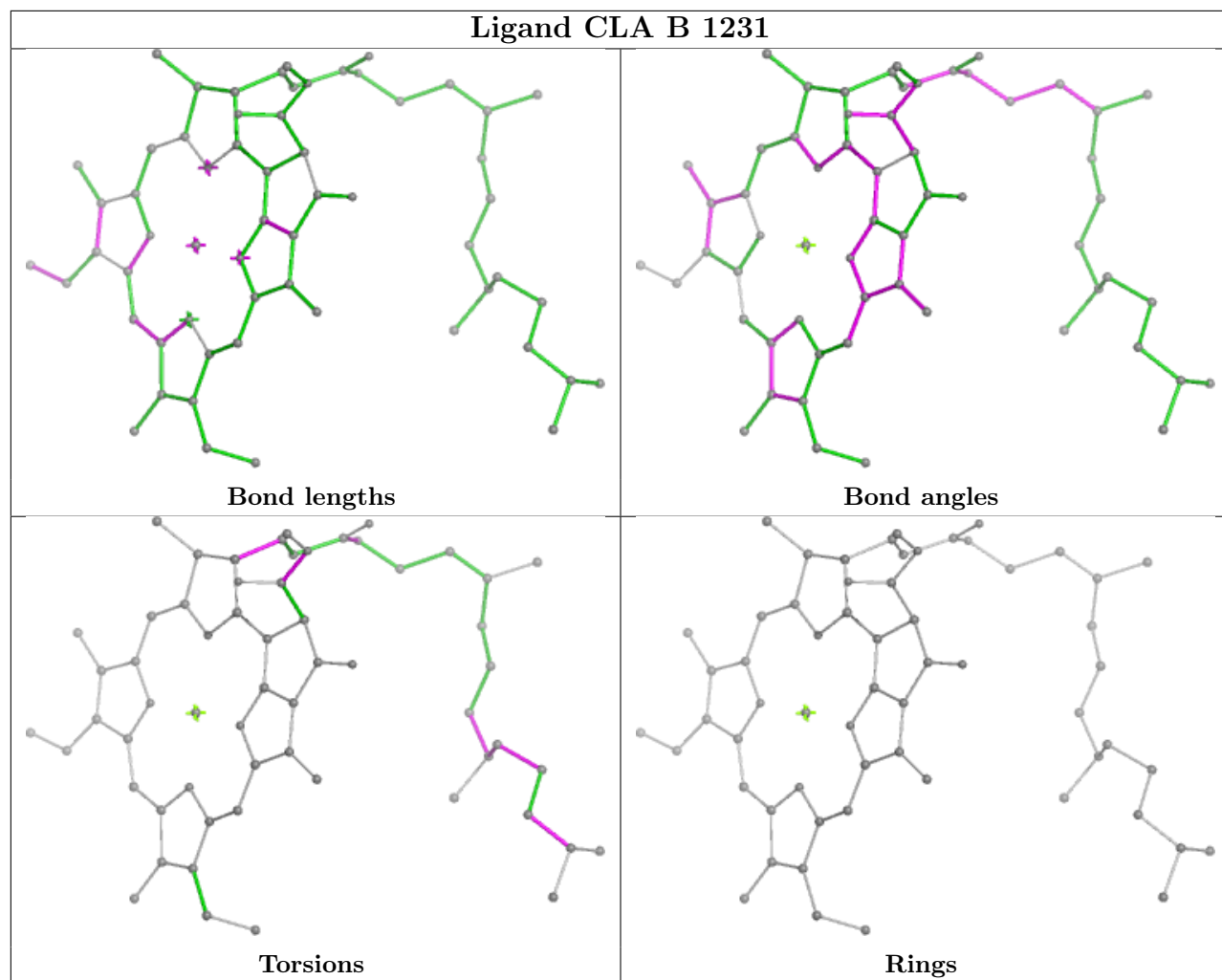
Ligand CLA A 1122**Ligand CLA A 1131**

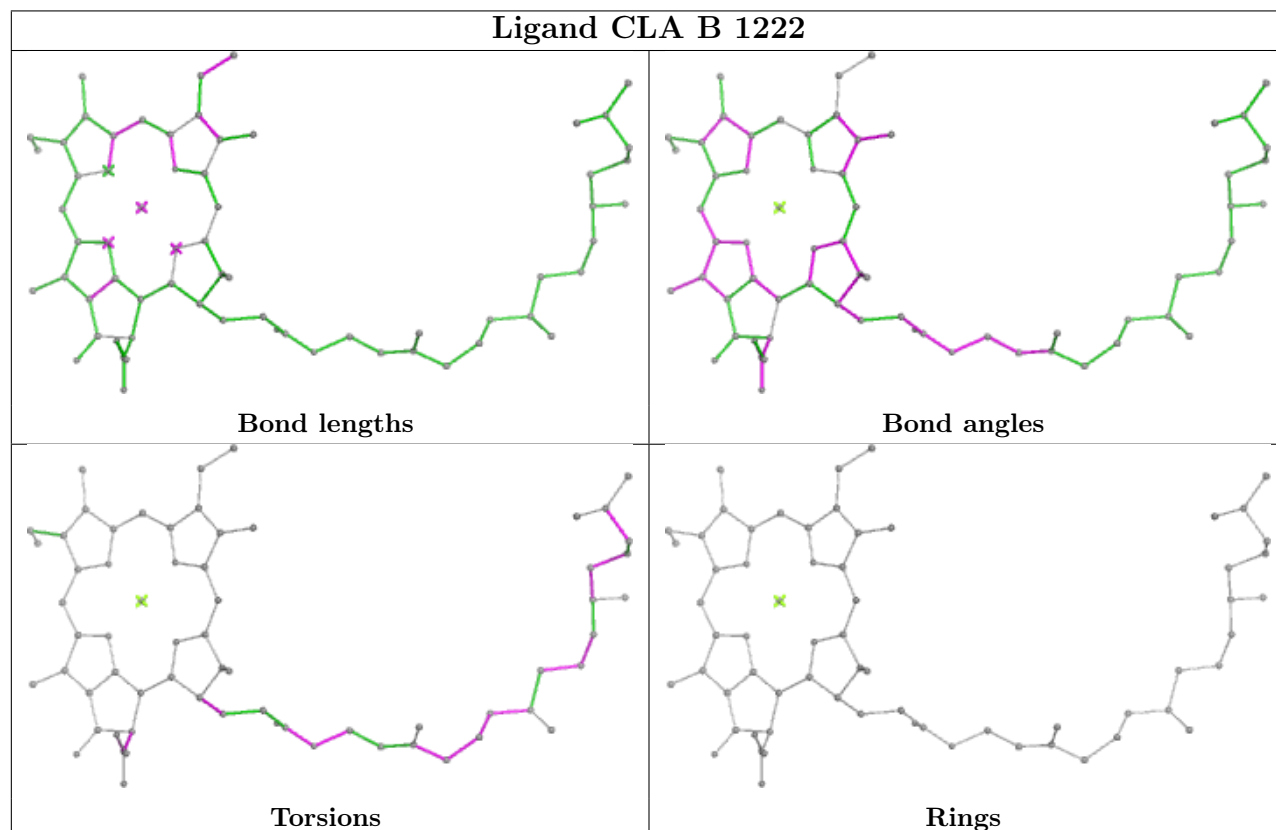
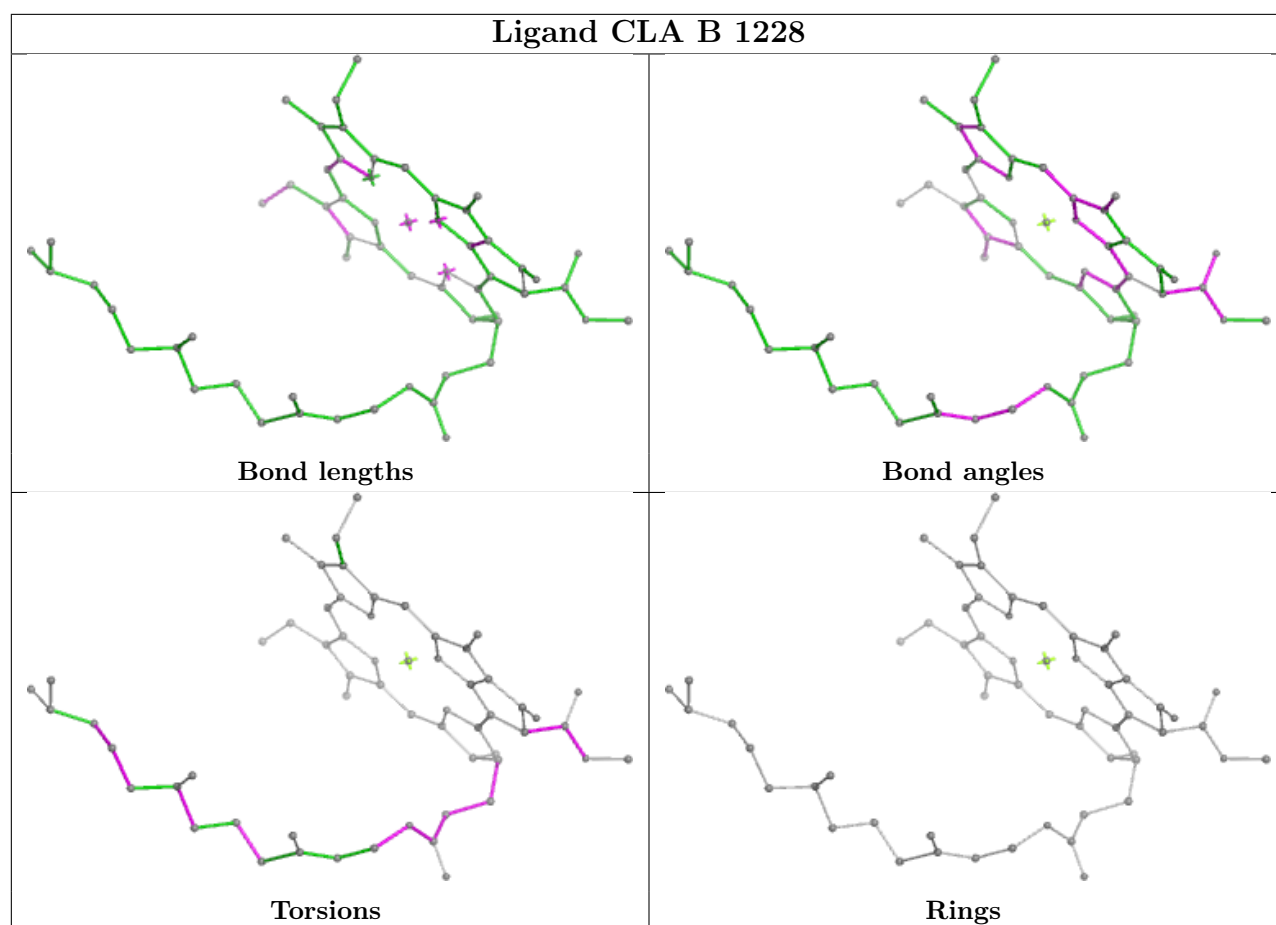


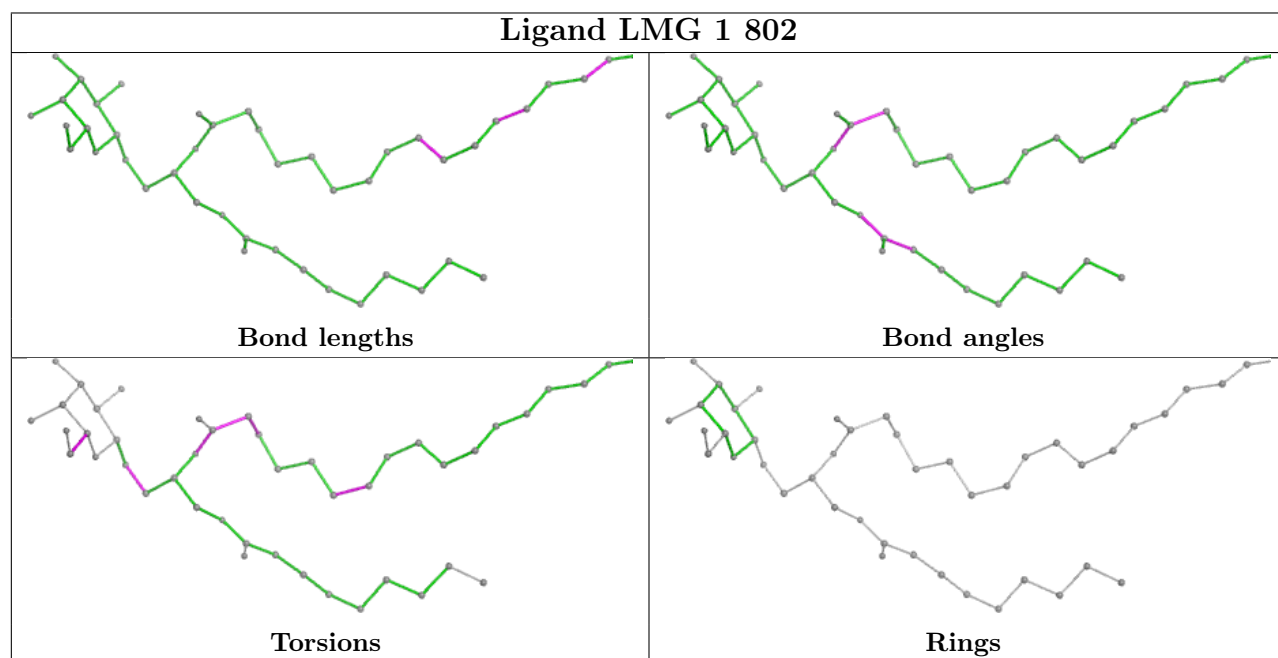
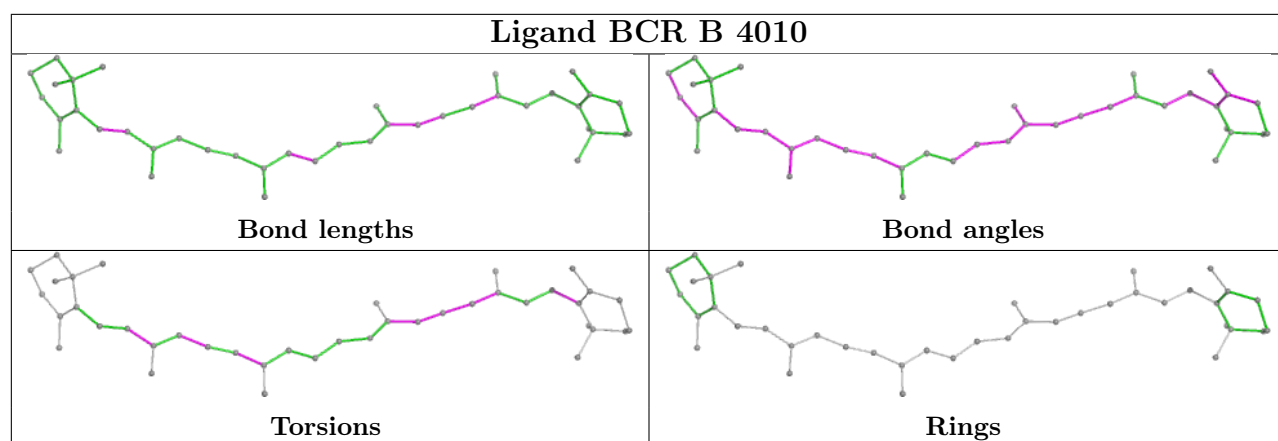
Ligand CHL 4 610

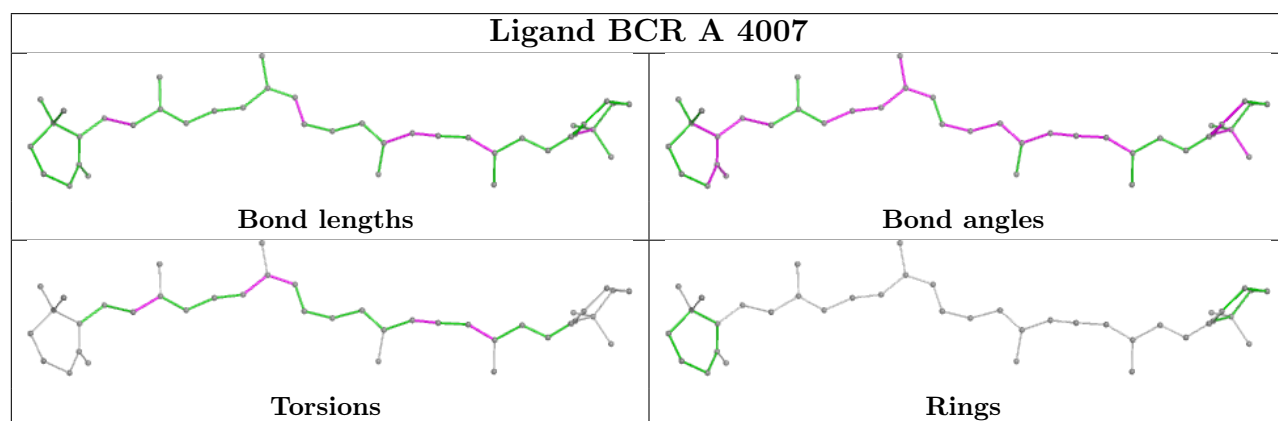
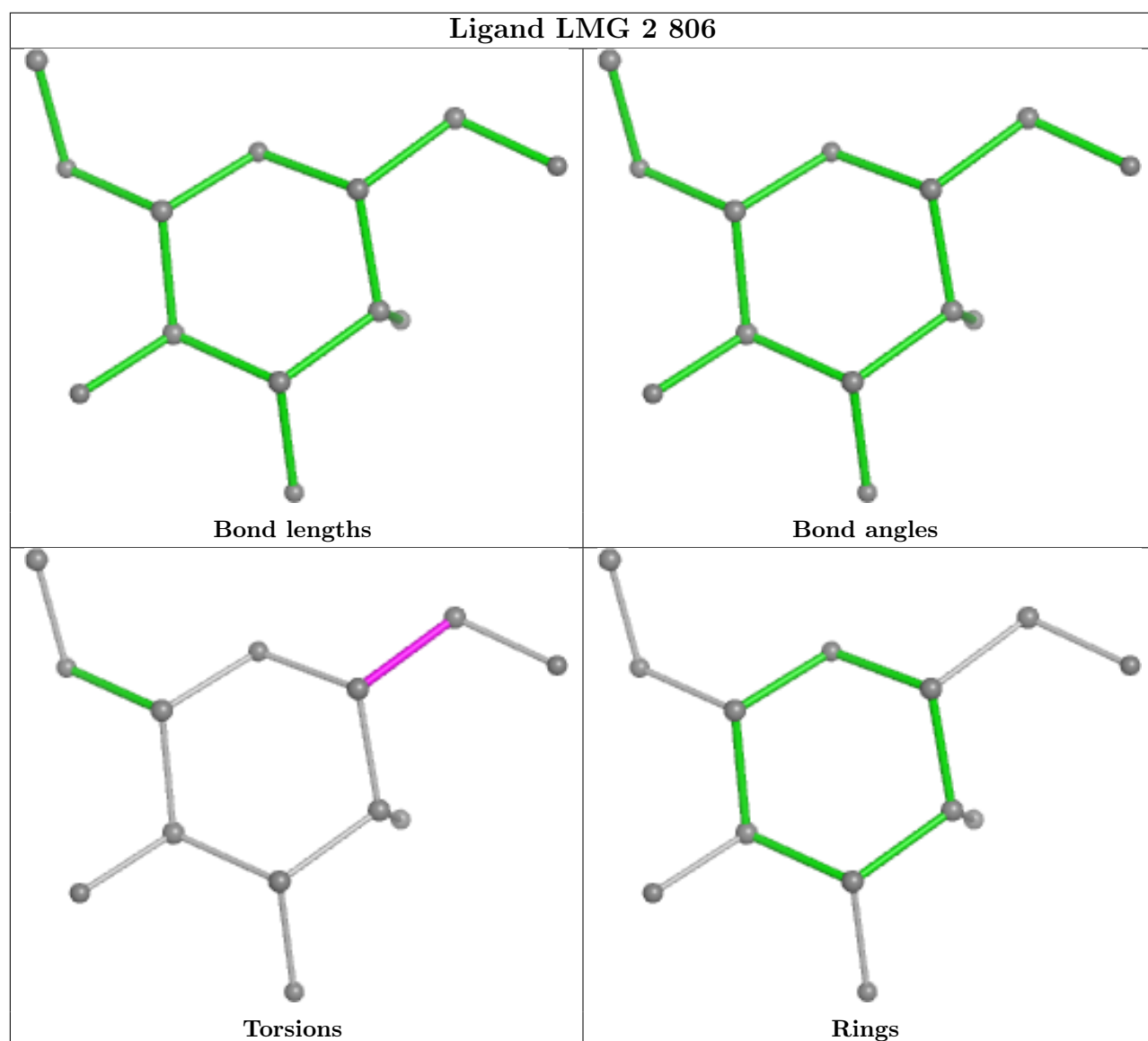


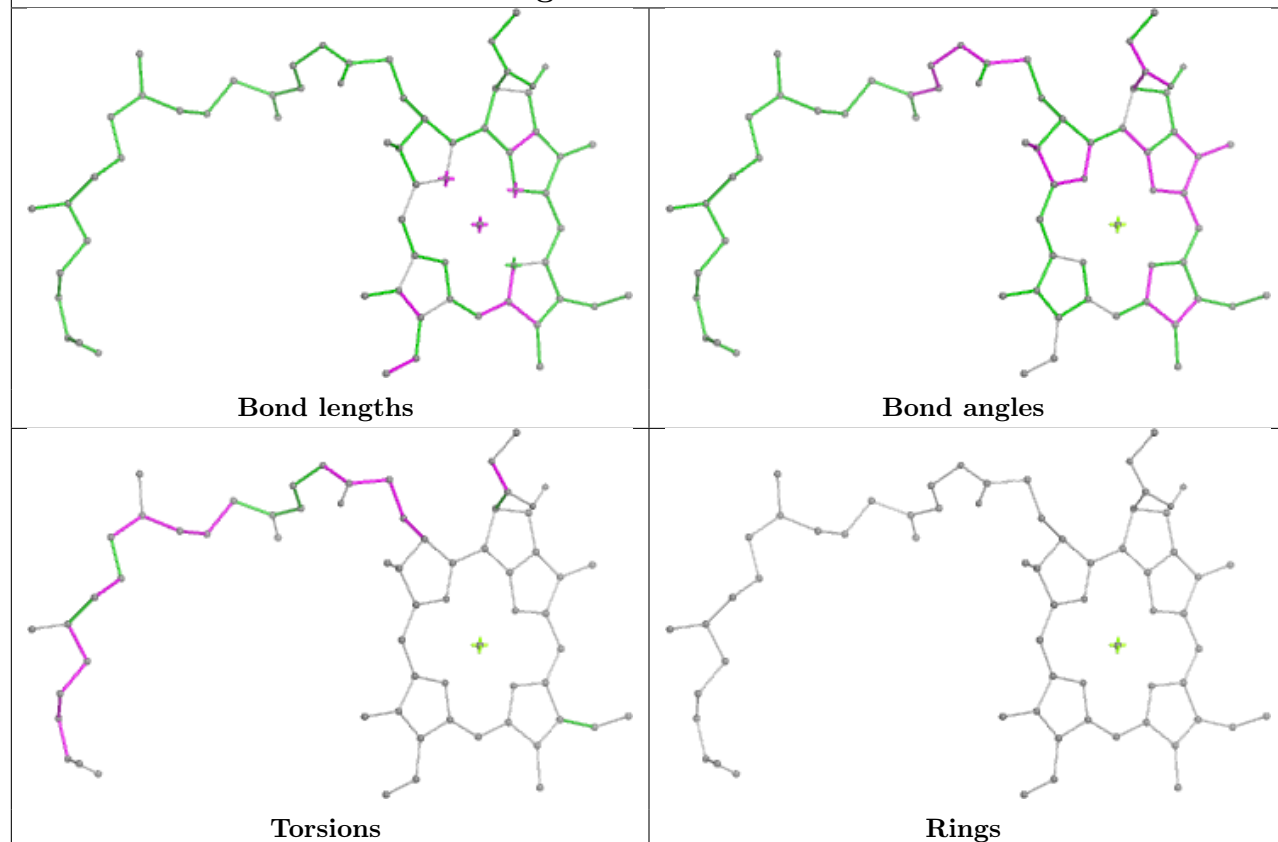
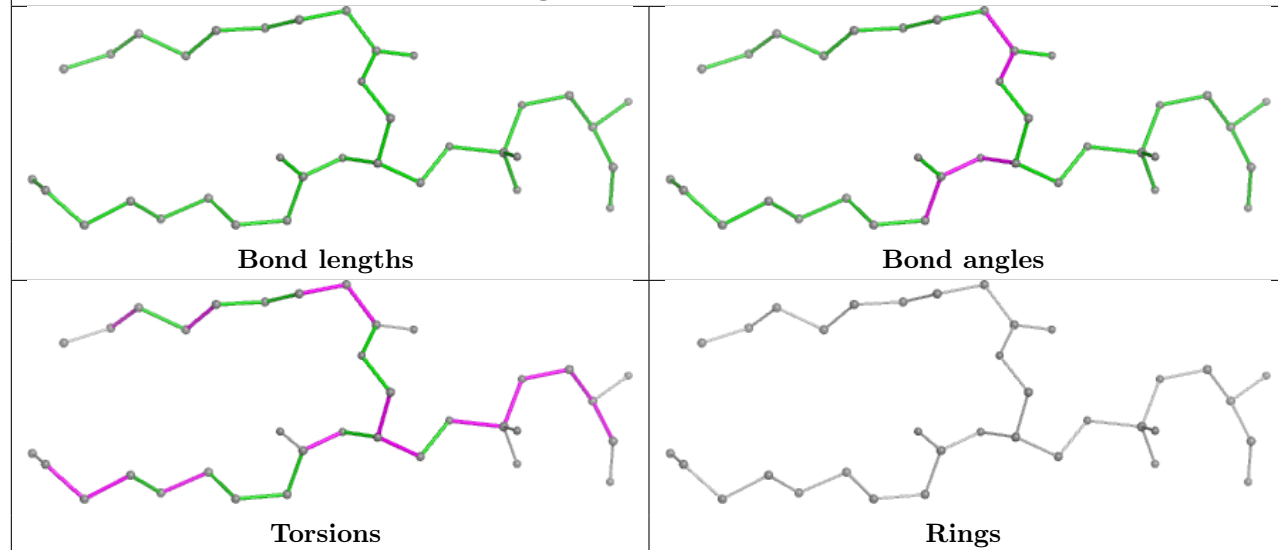




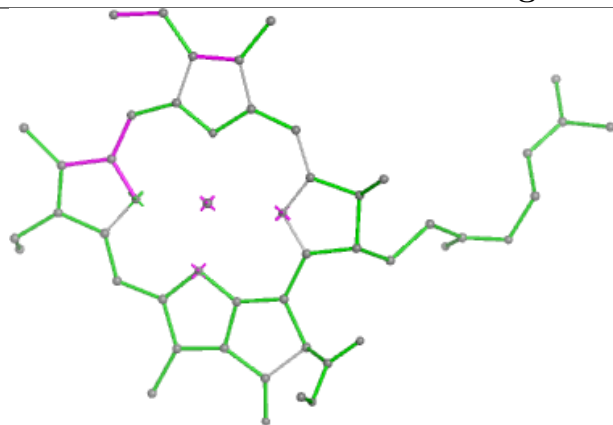




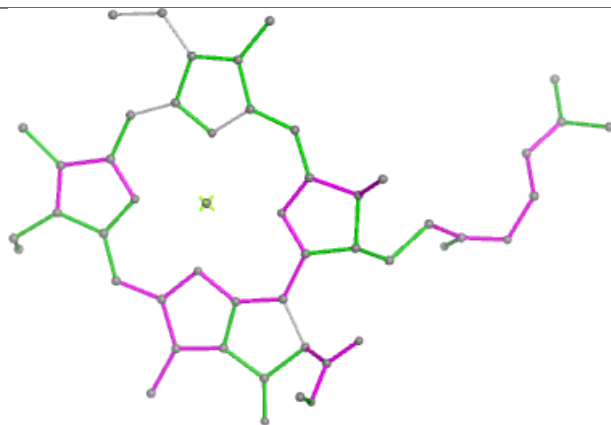


Ligand CLA 4 617**Ligand LHG 4 801**

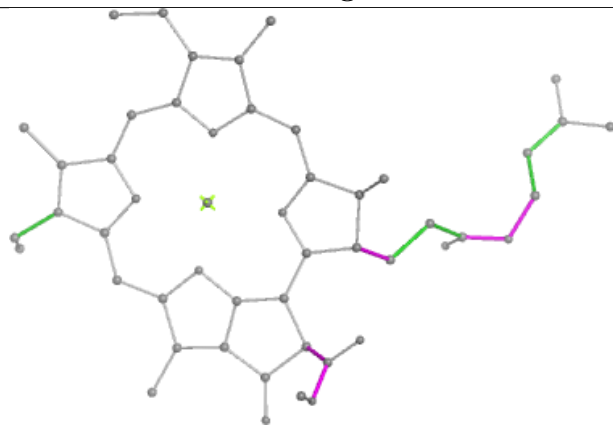
Ligand CLA 4 609



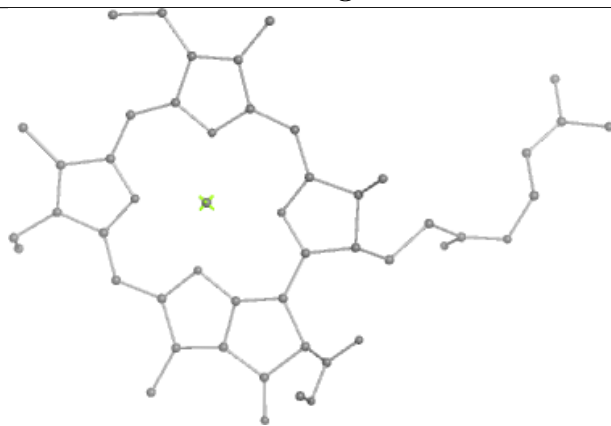
Bond lengths



Bond angles

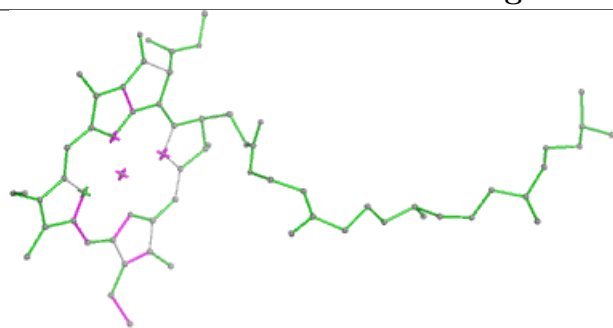


Torsions

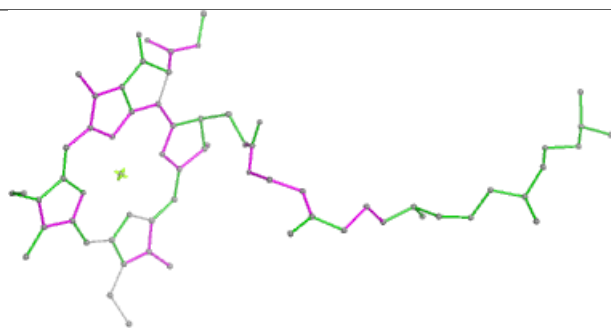


Rings

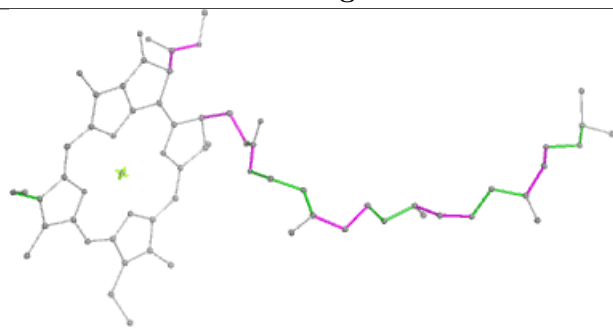
Ligand CLA A 1119



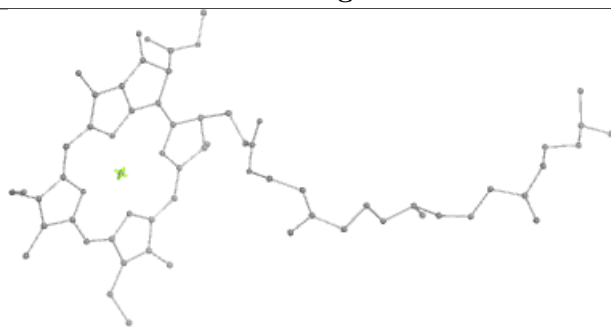
Bond lengths



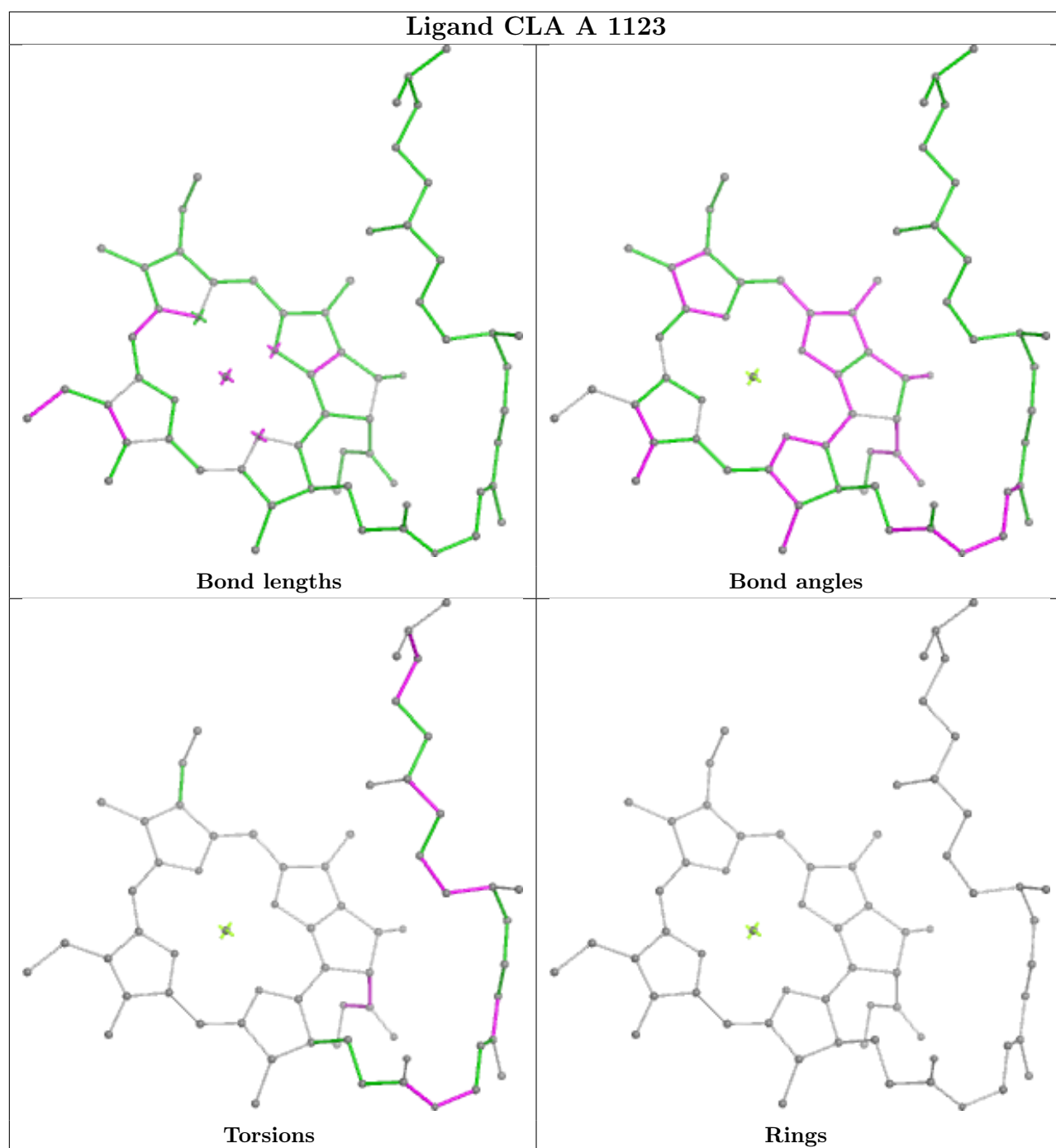
Bond angles

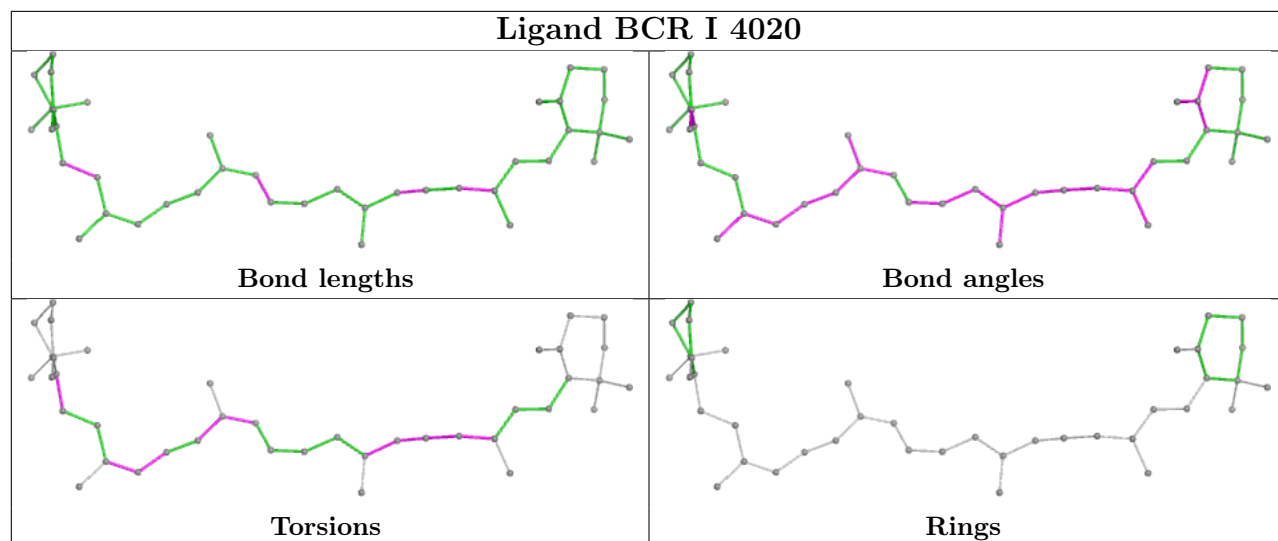


Torsions

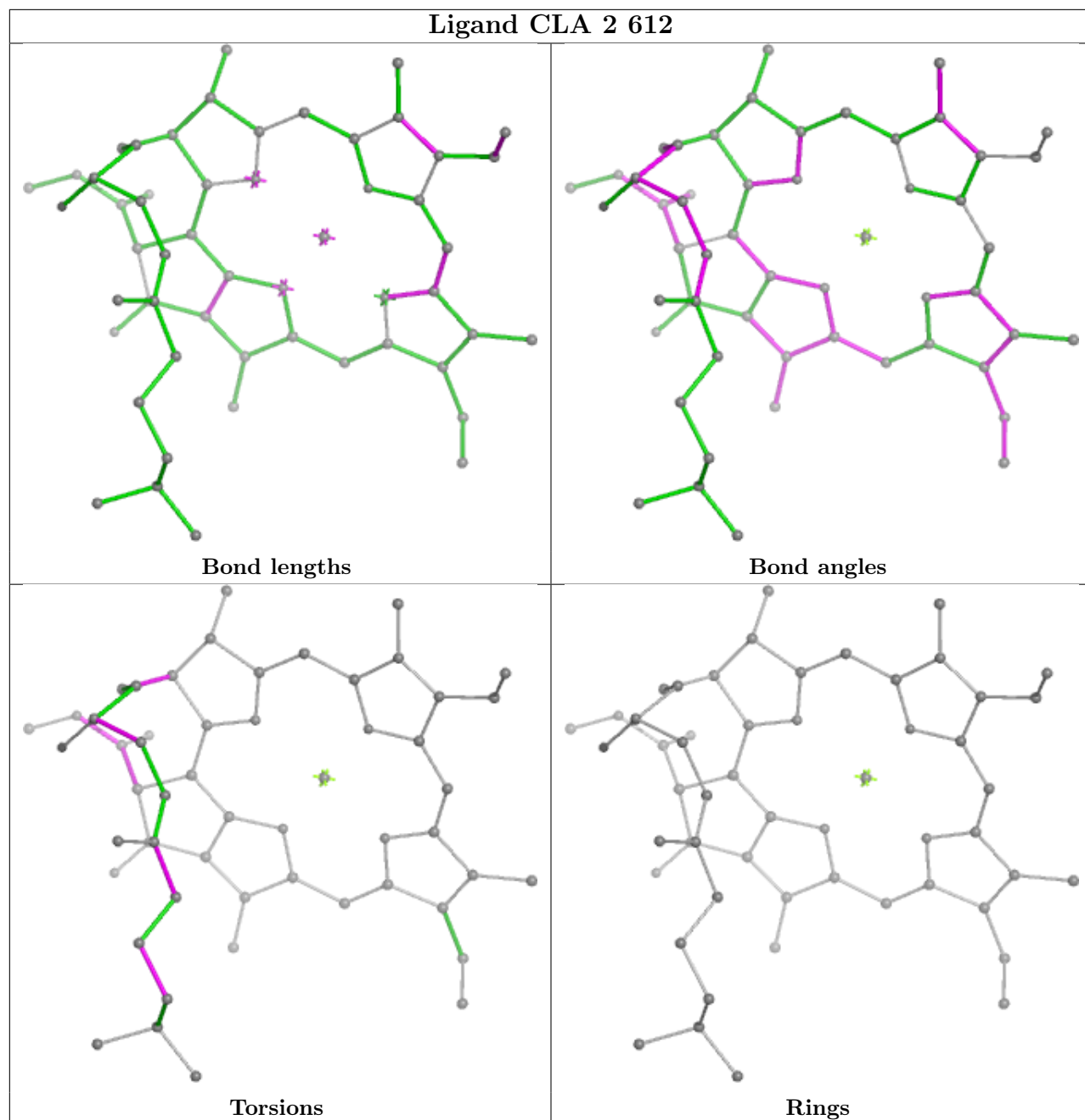


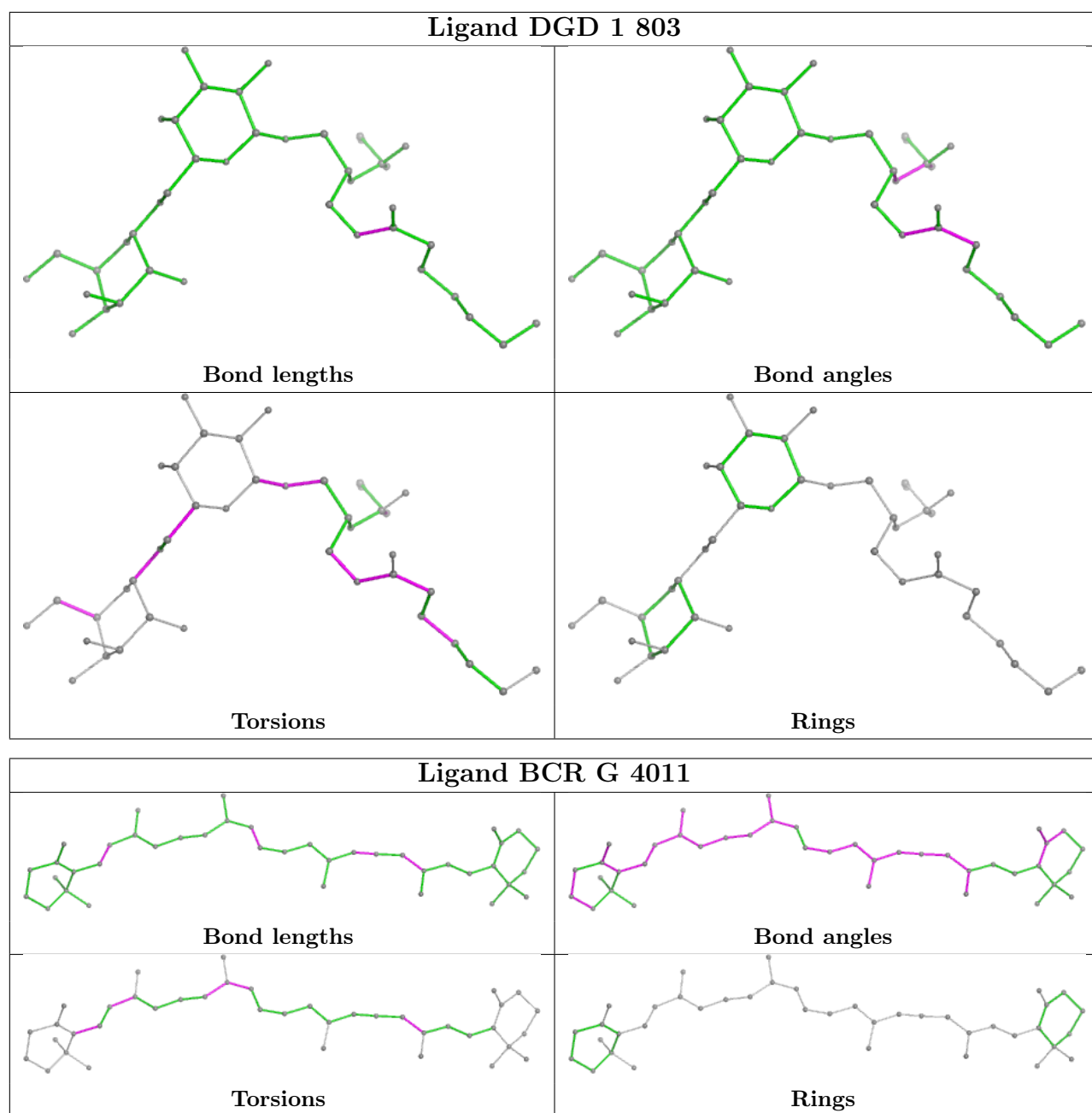
Rings

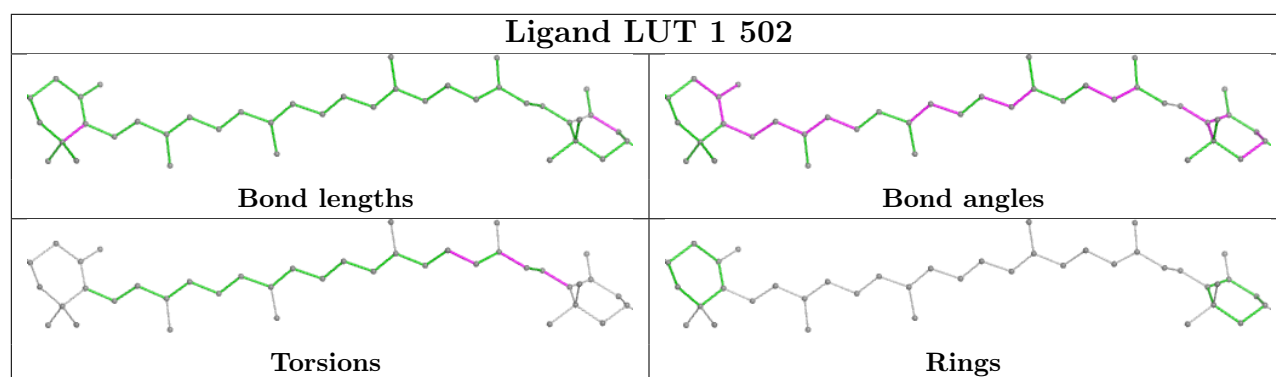
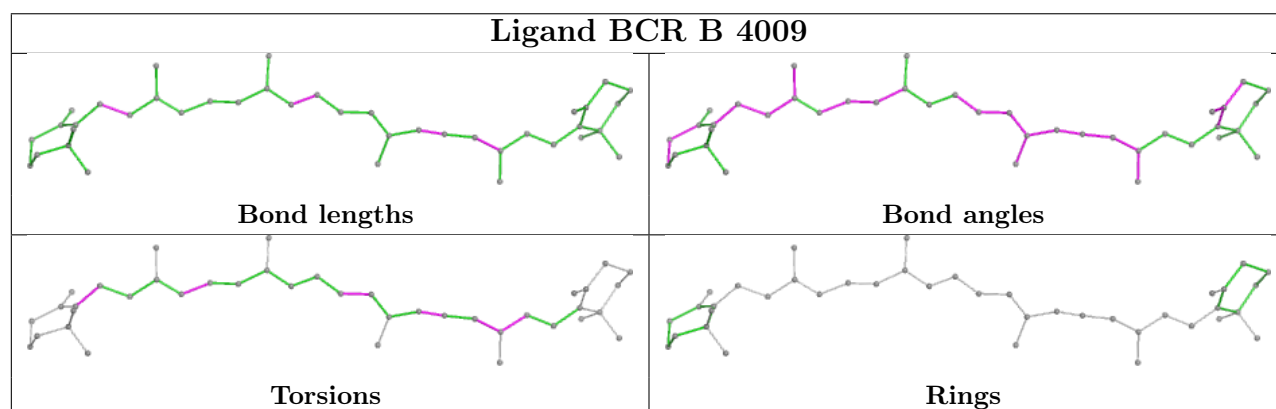
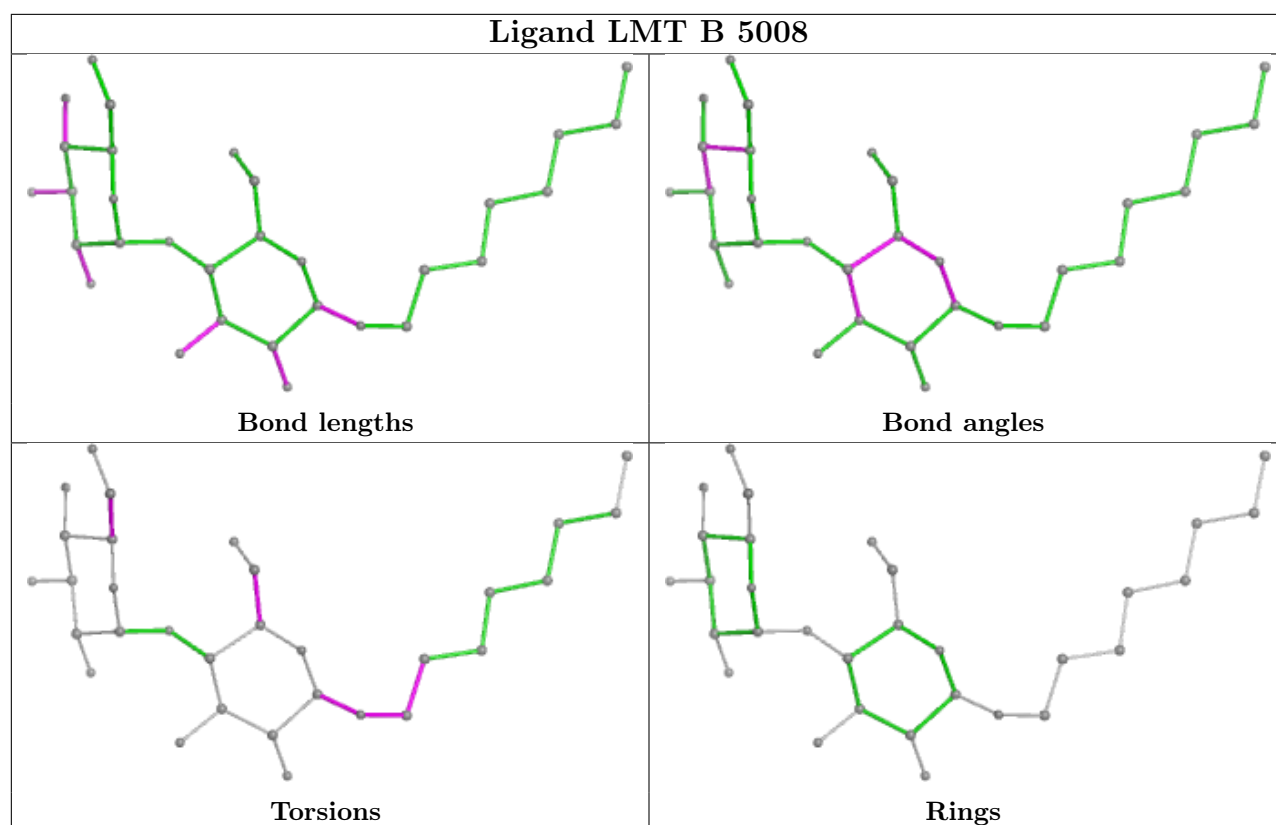


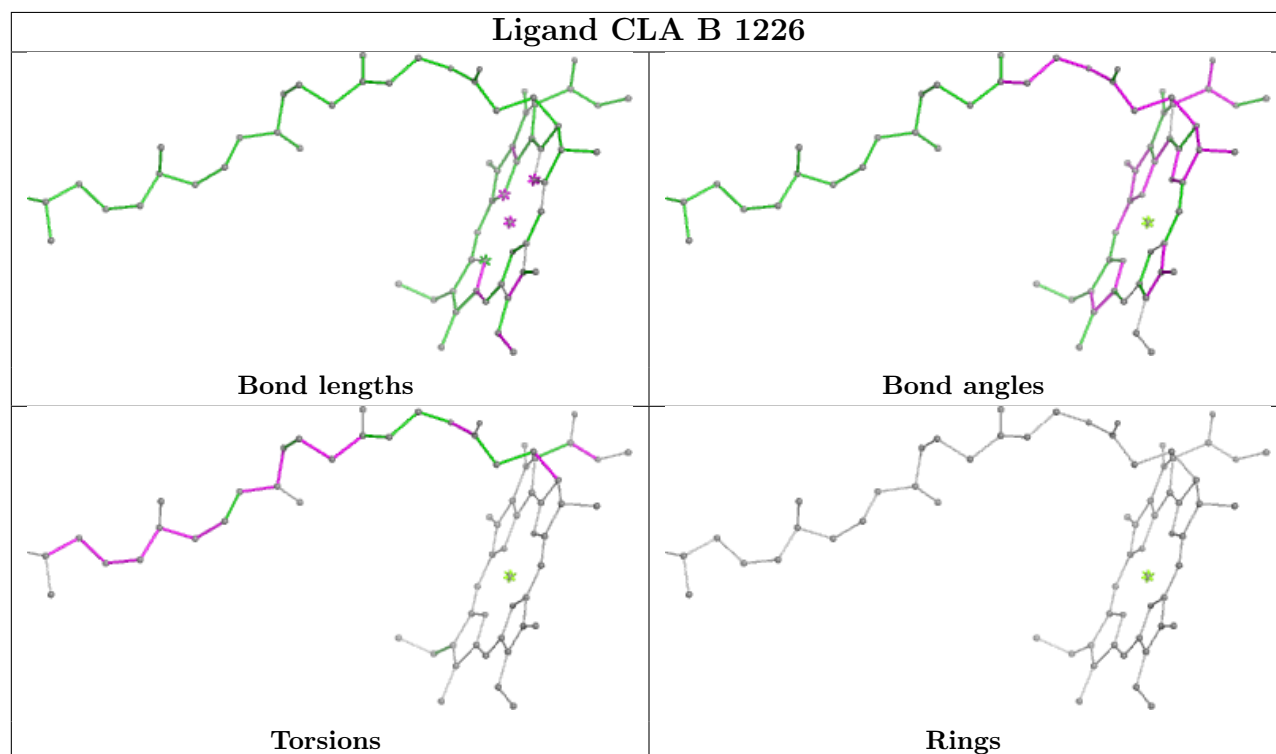
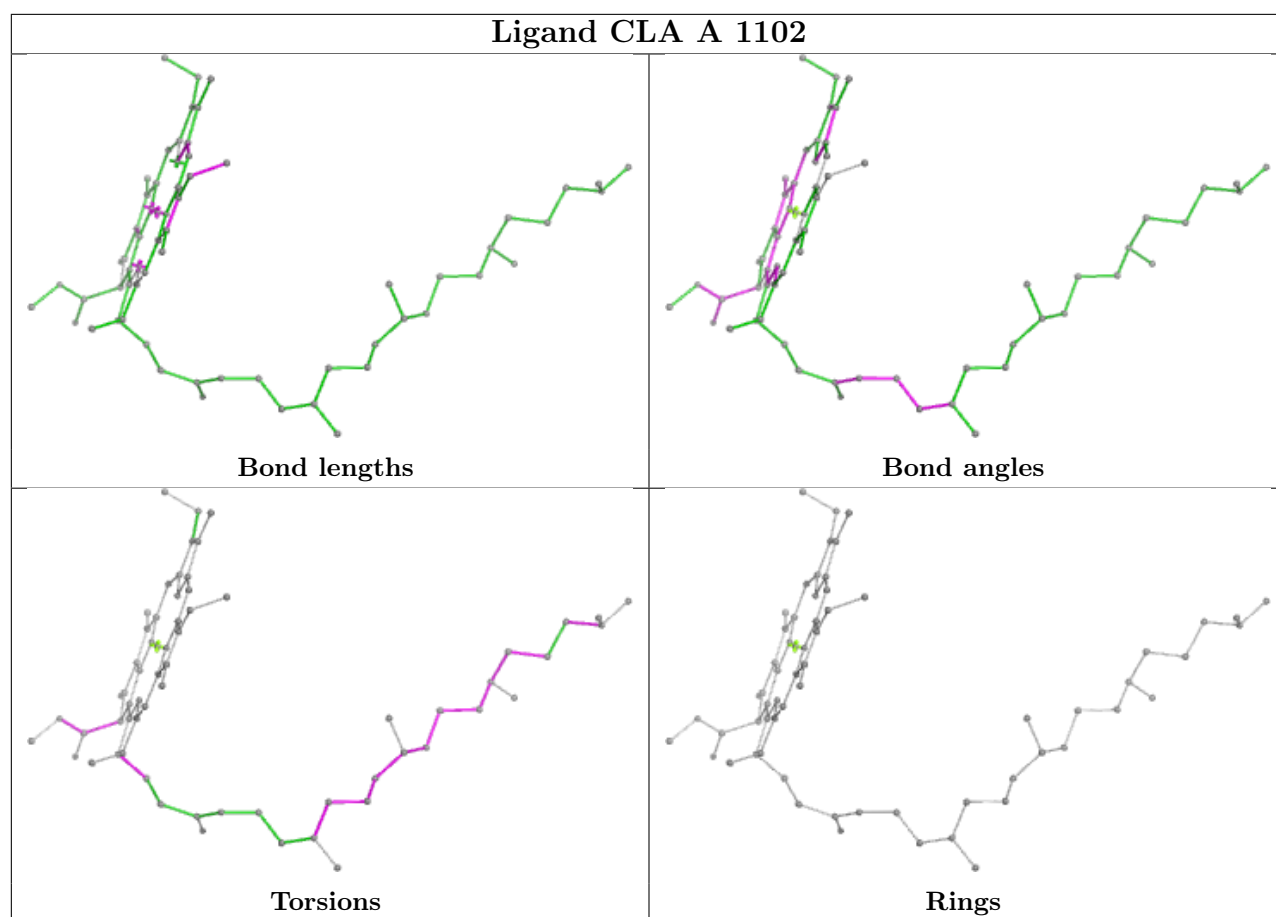


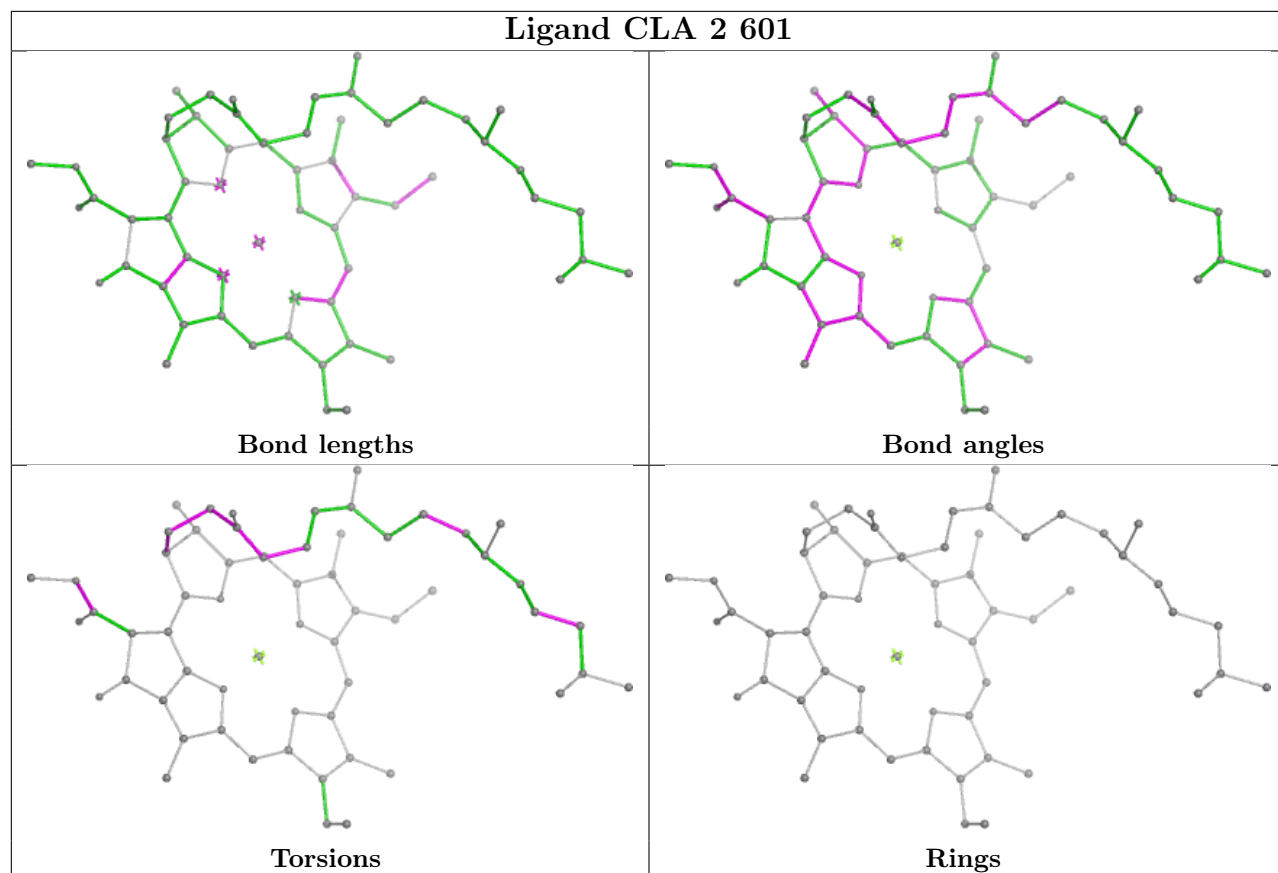
Ligand CLA 2 612

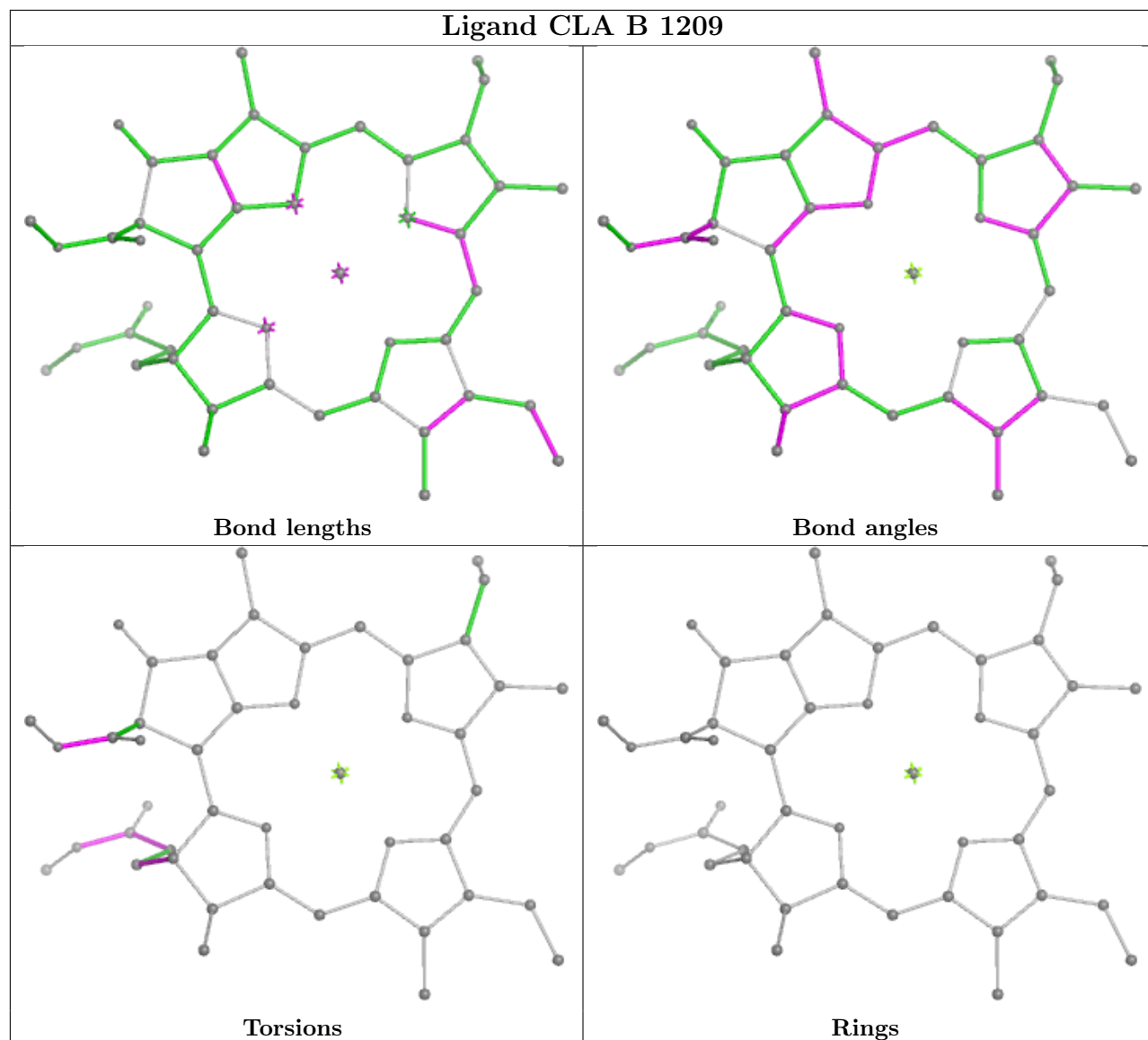


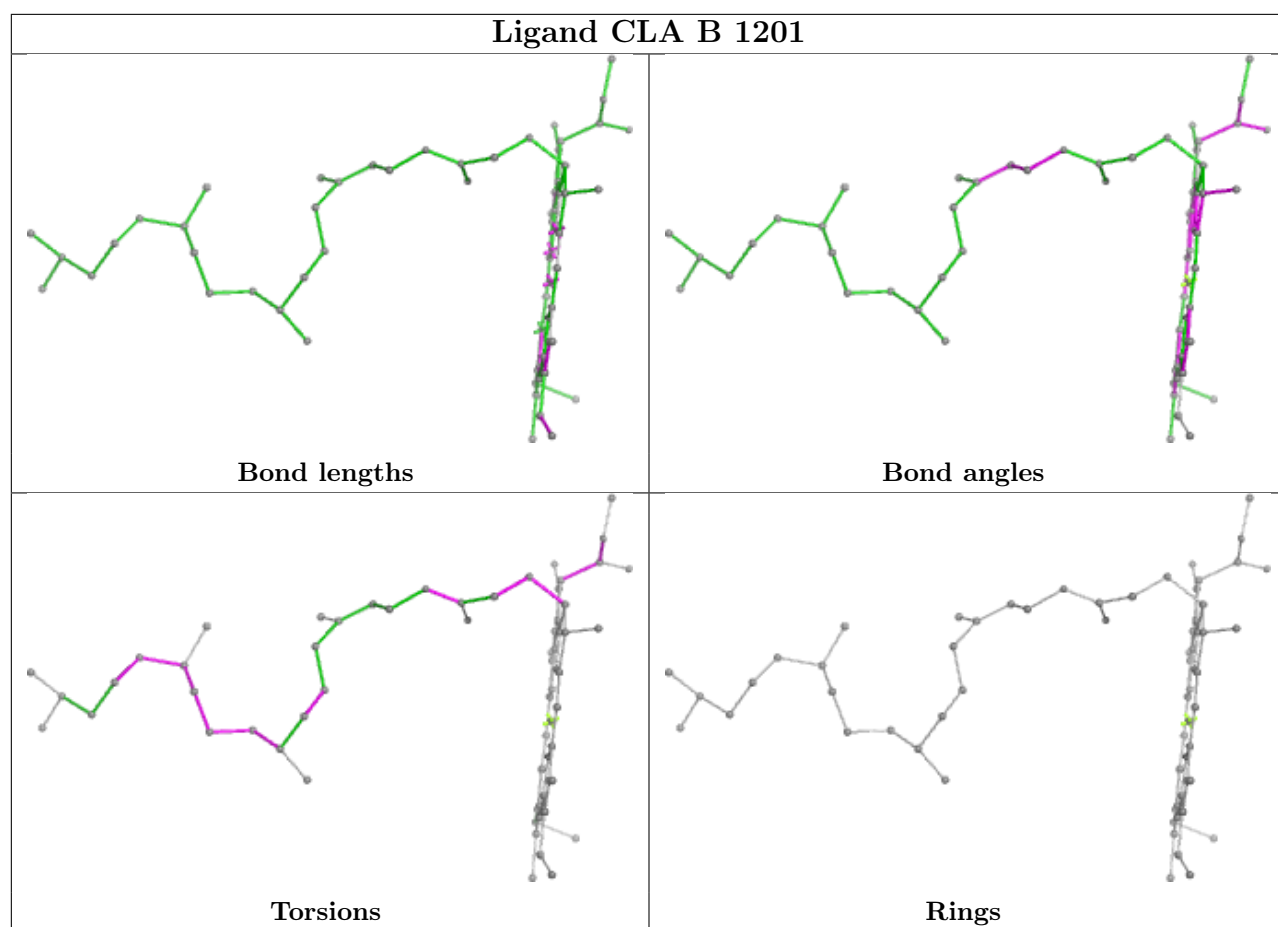




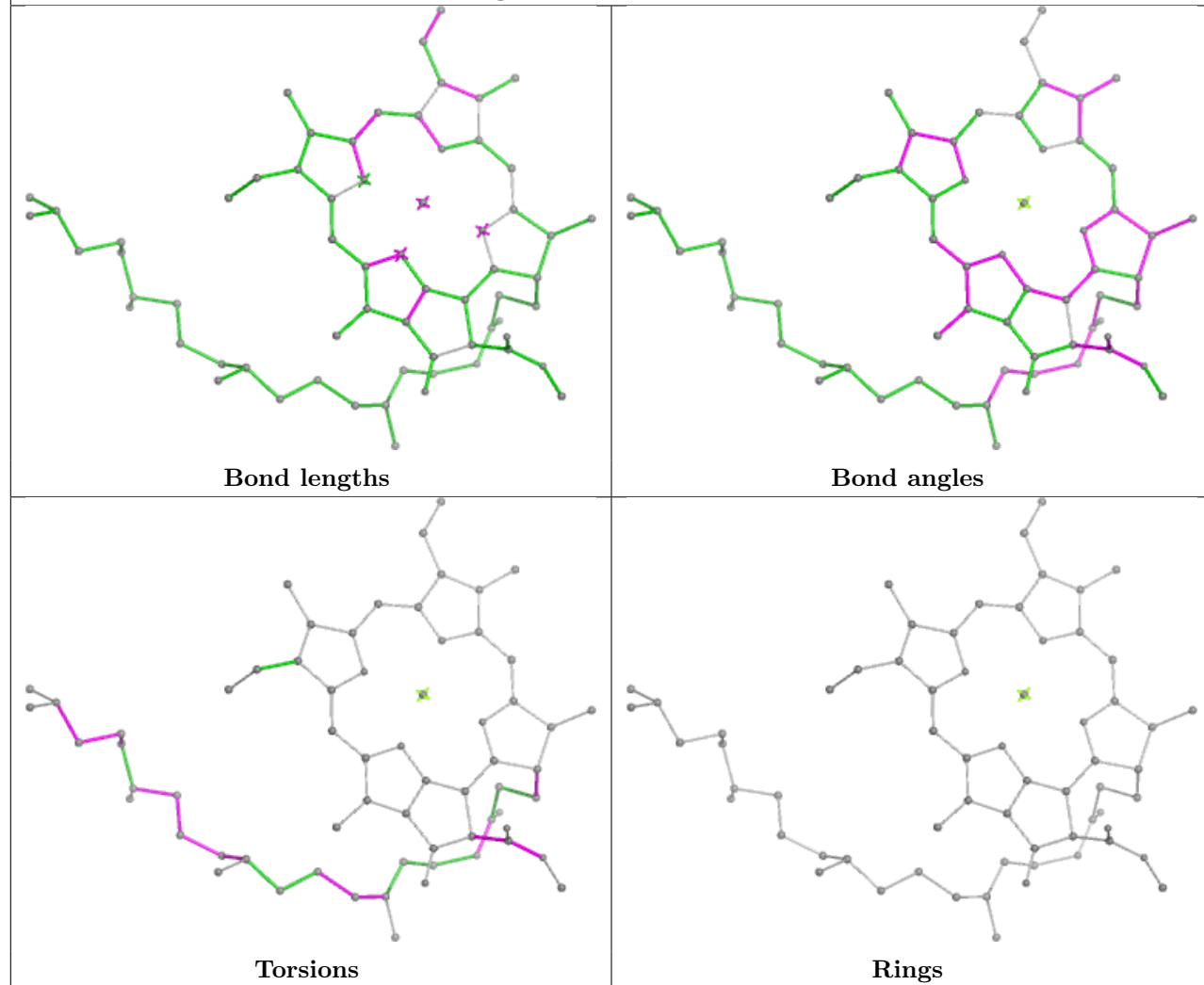


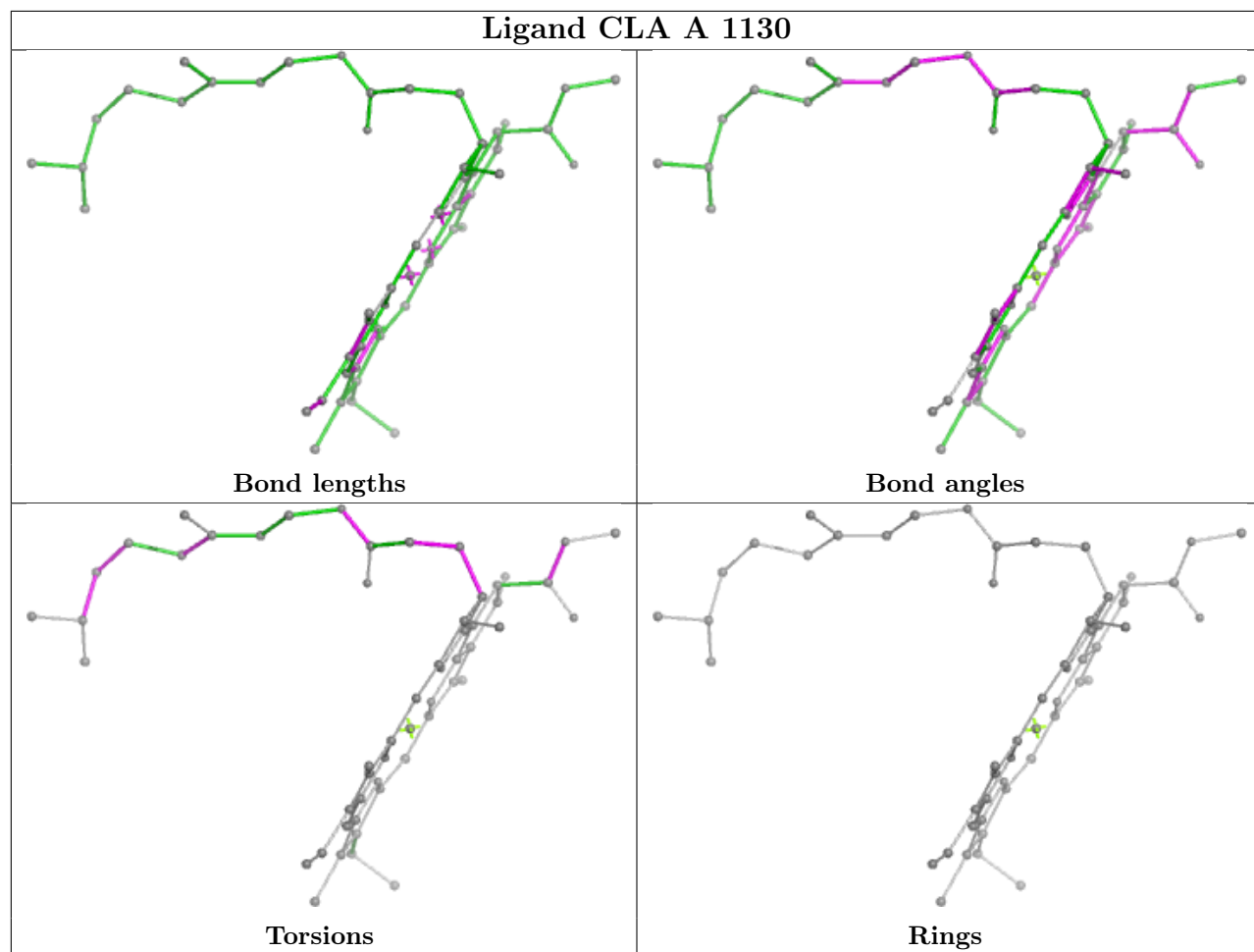




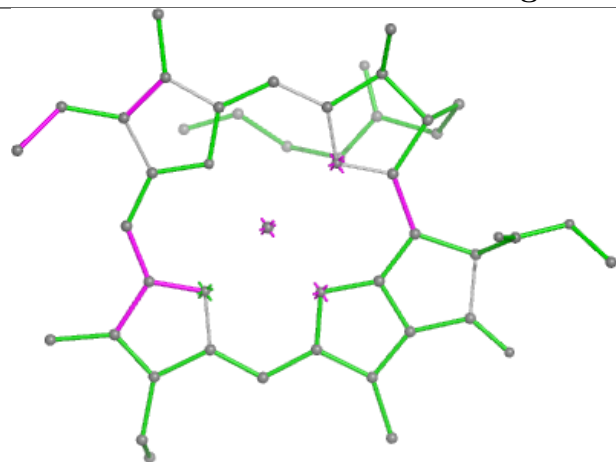


Ligand CLA A 1127

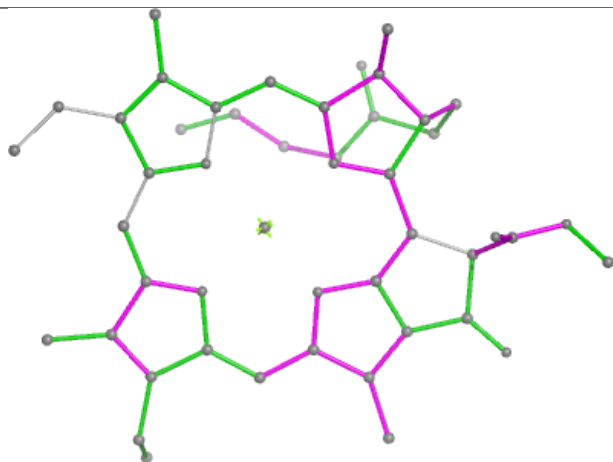




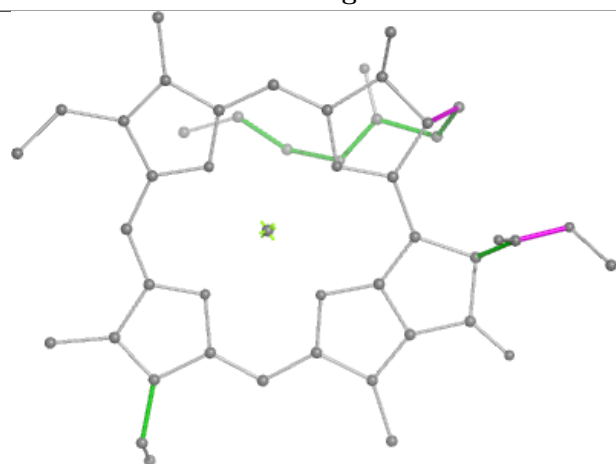
Ligand CLA 3 608



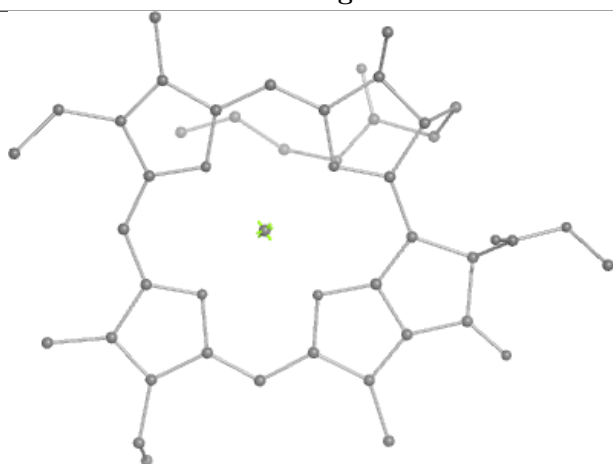
Bond lengths



Bond angles

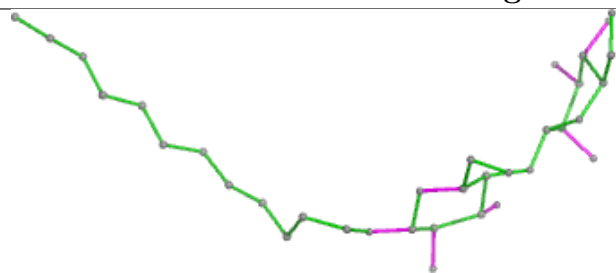


Torsions

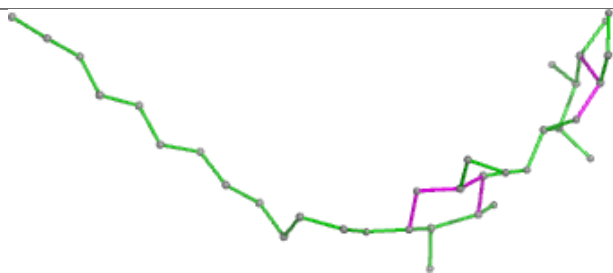


Rings

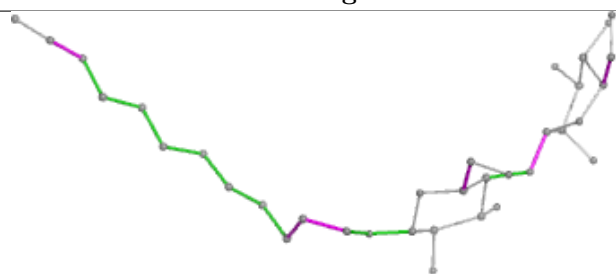
Ligand LMT A 5004



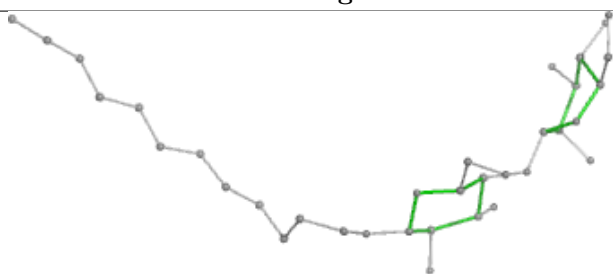
Bond lengths



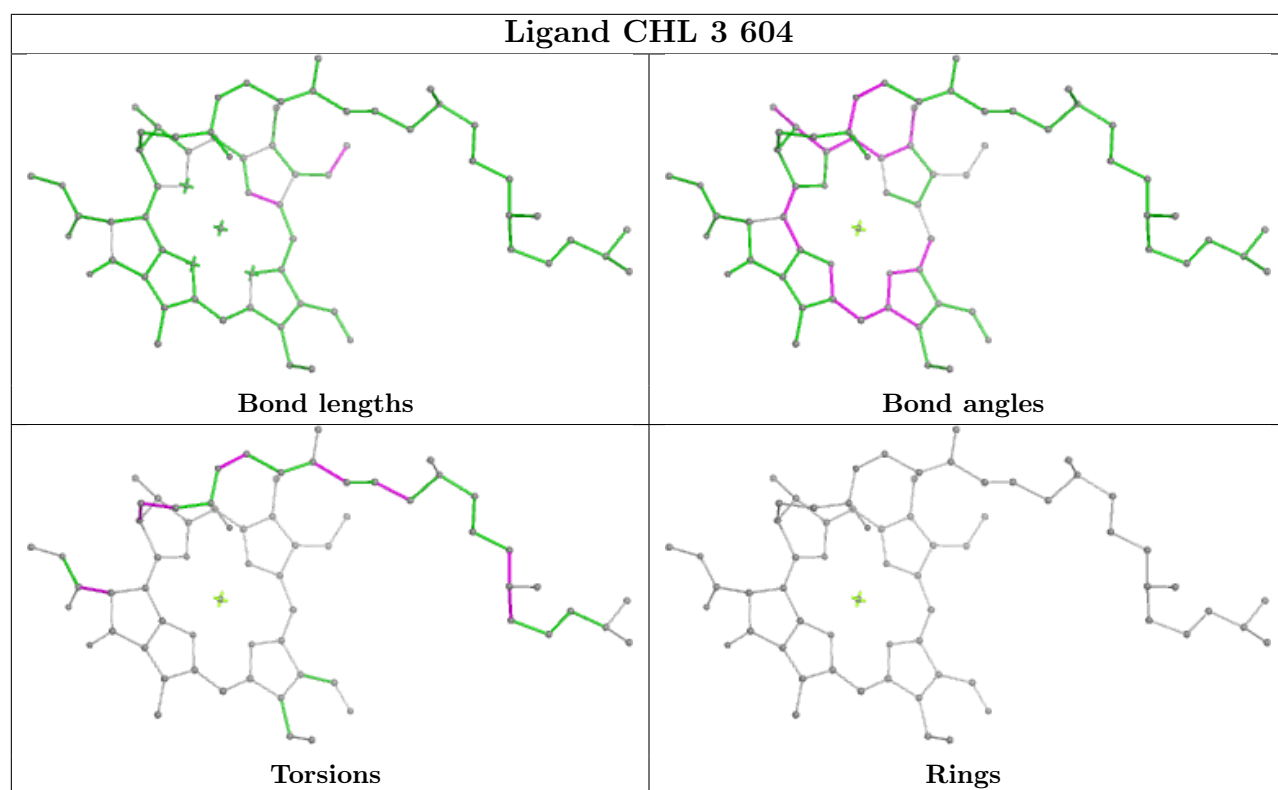
Bond angles



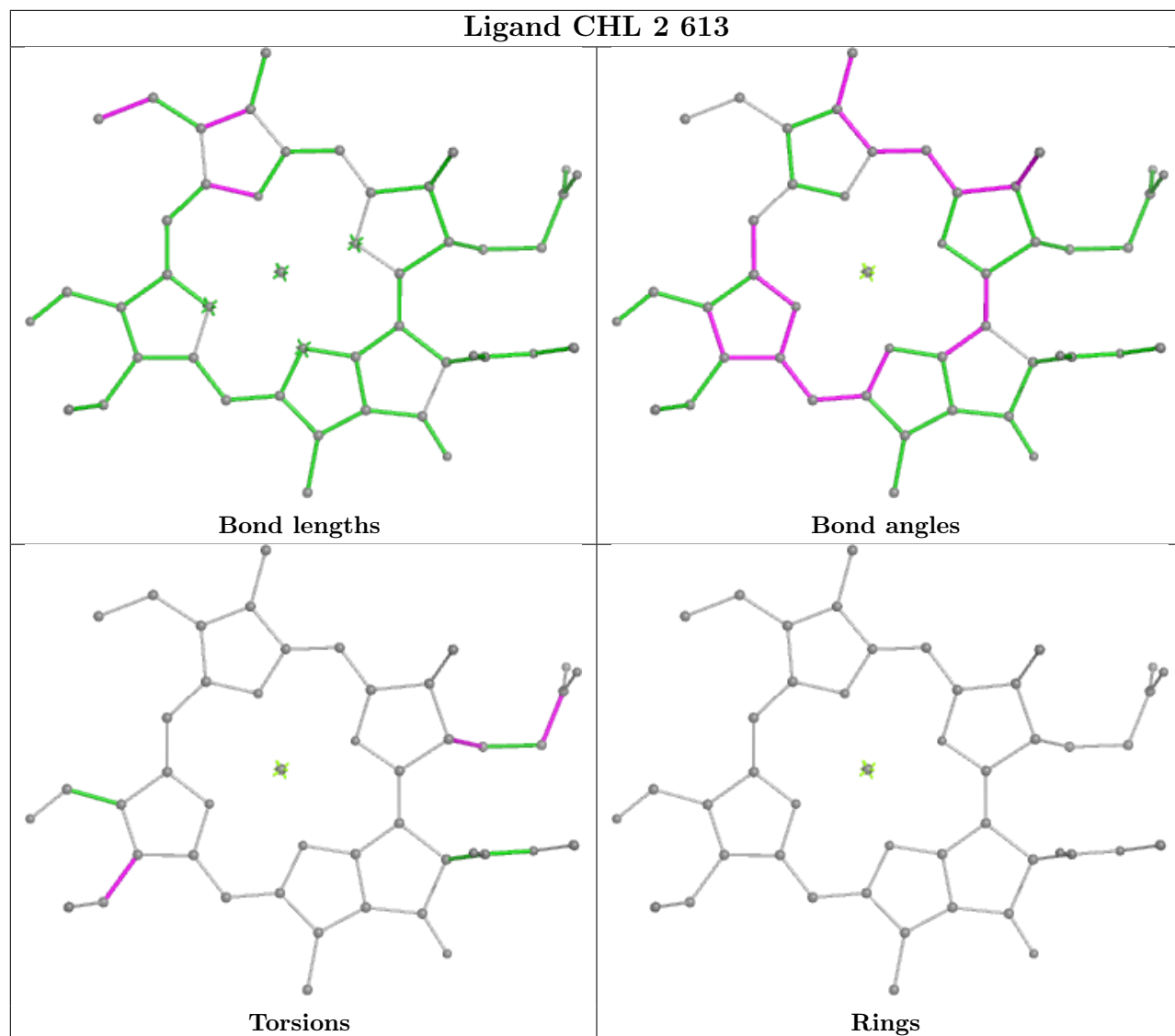
Torsions

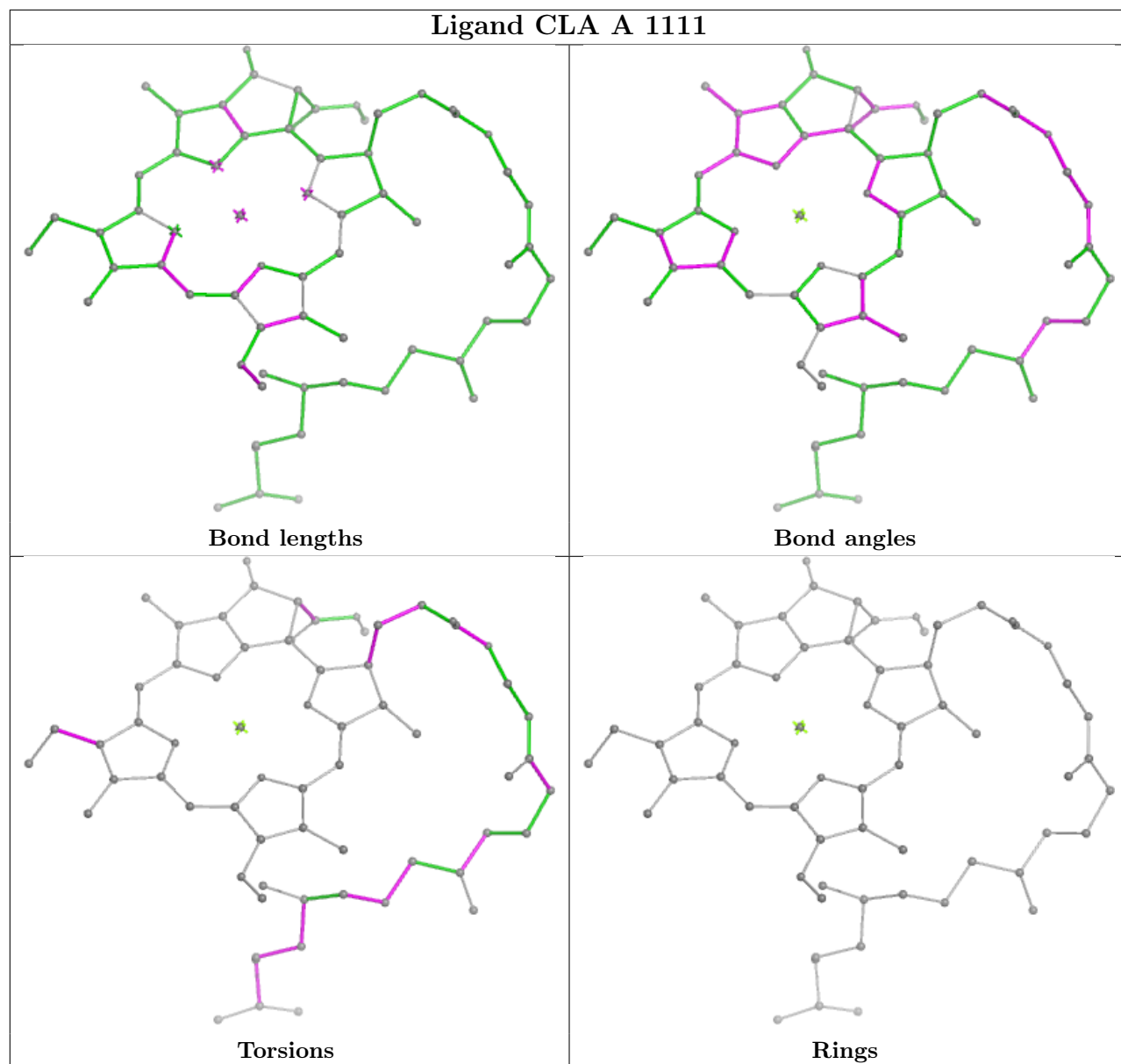


Rings

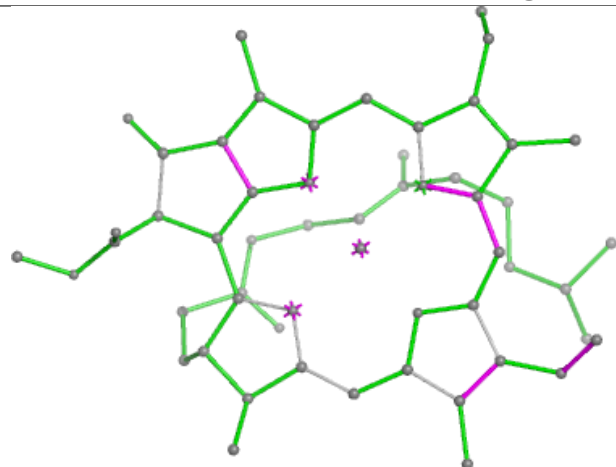


Ligand CHL 2 613

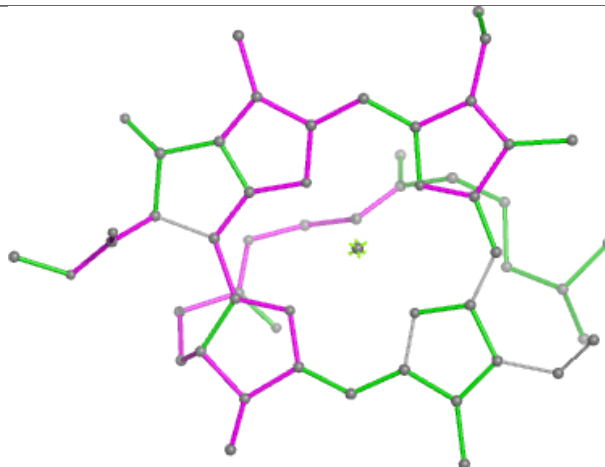




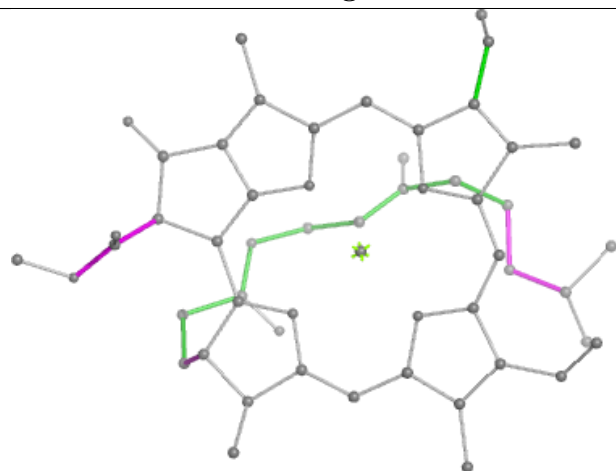
Ligand CLA 1 603



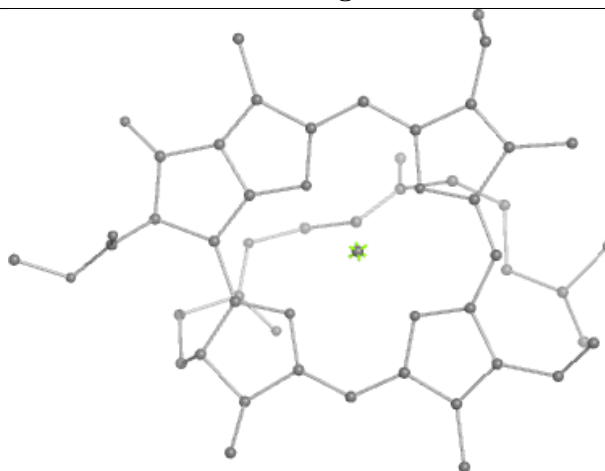
Bond lengths



Bond angles

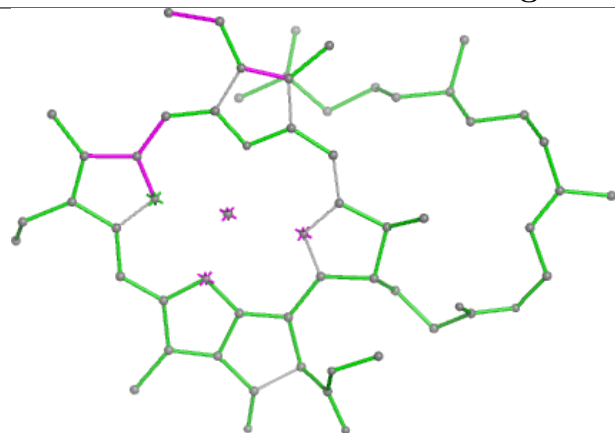


Torsions

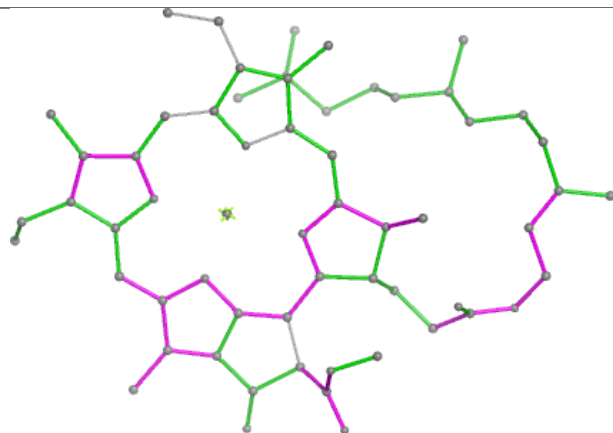


Rings

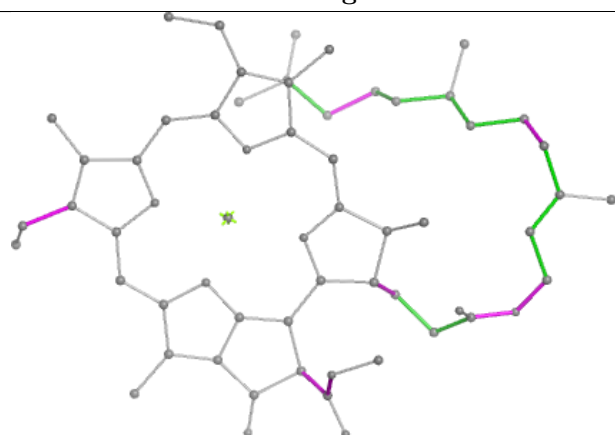
Ligand CLA 3 617



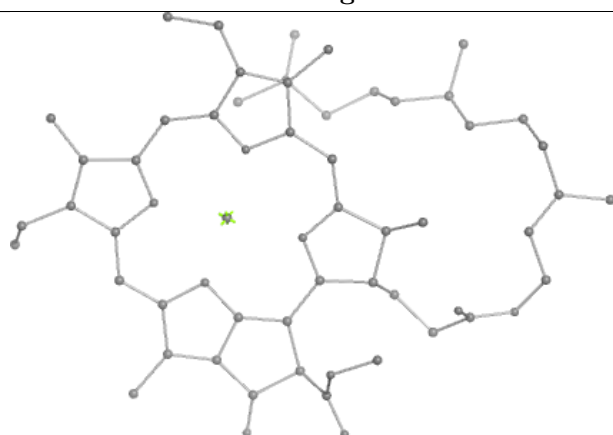
Bond lengths



Bond angles

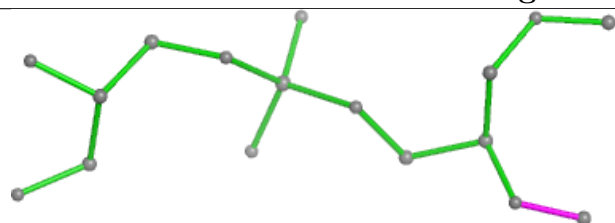


Torsions

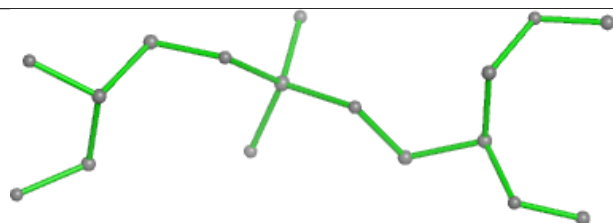


Rings

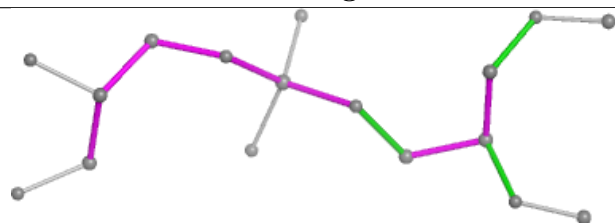
Ligand LHG 3 801



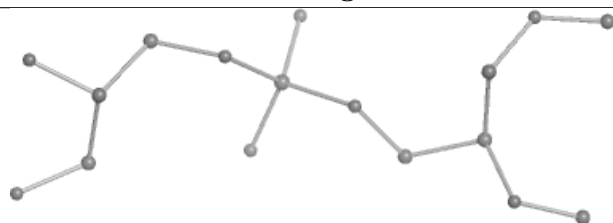
Bond lengths



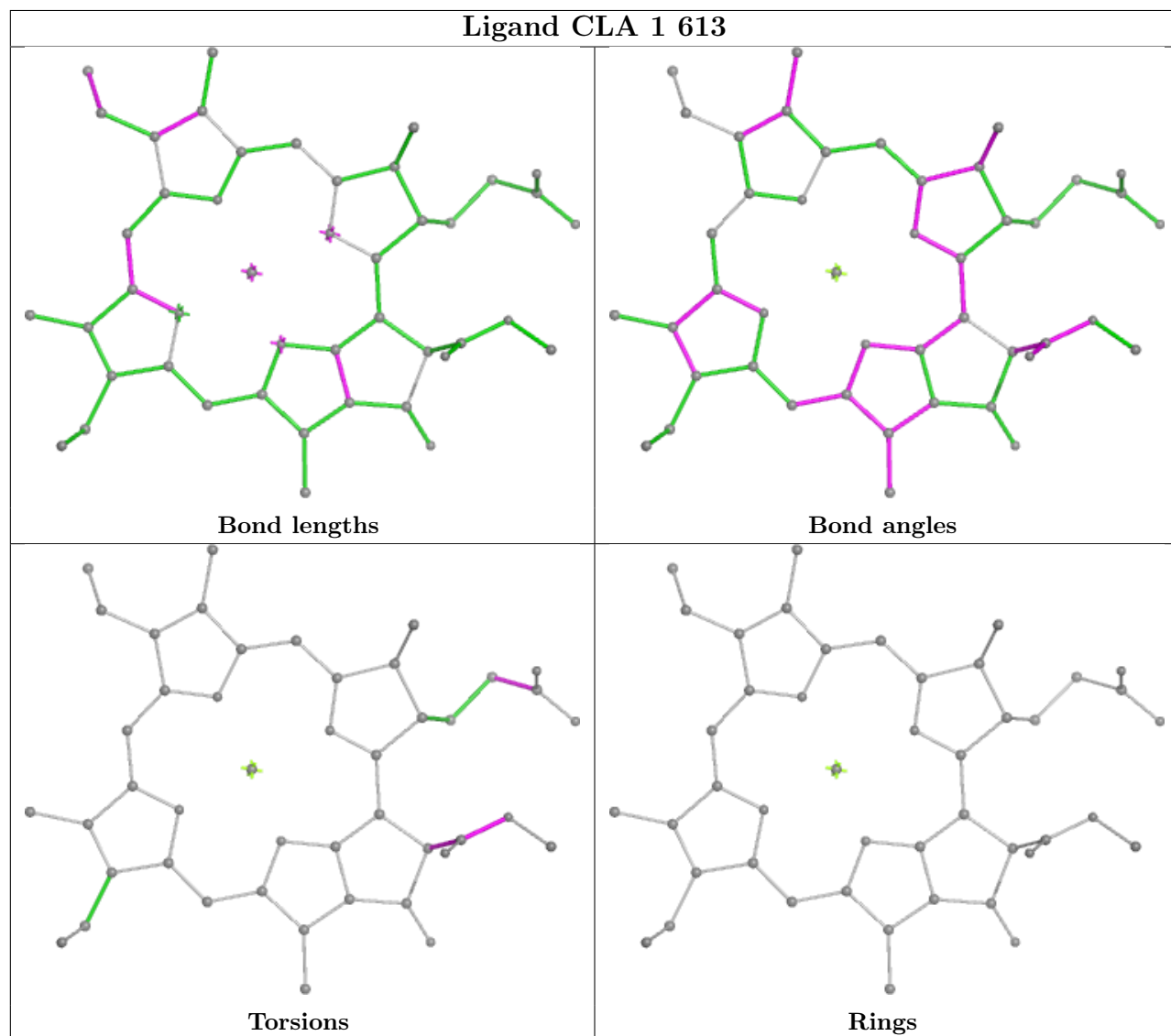
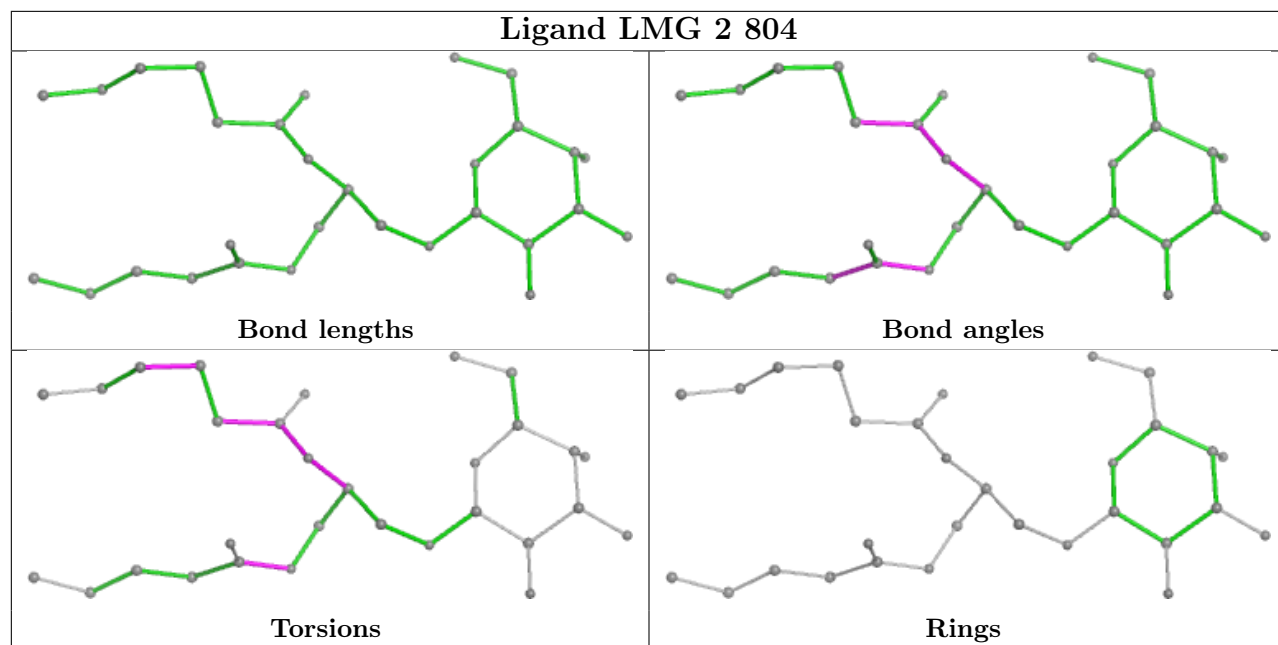
Bond angles



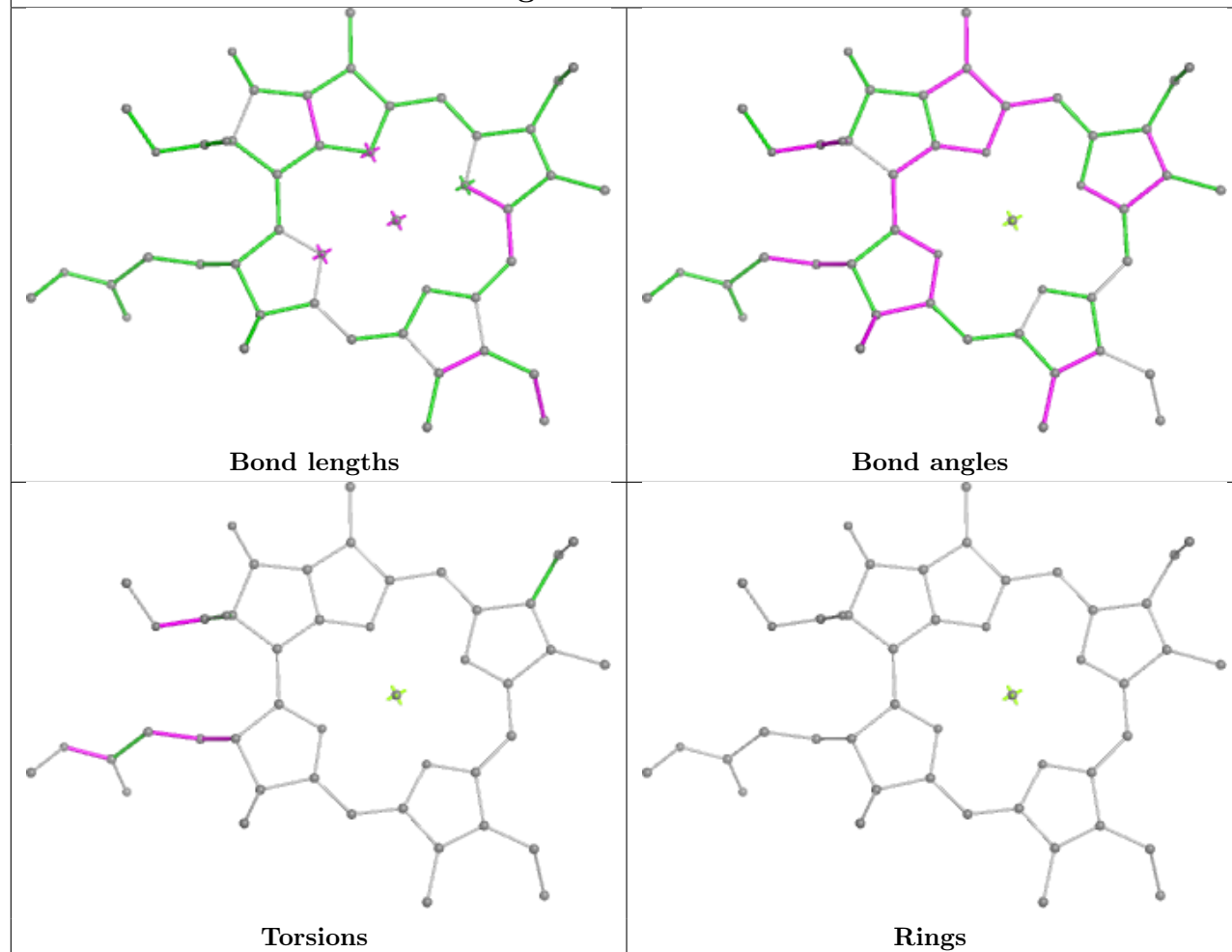
Torsions



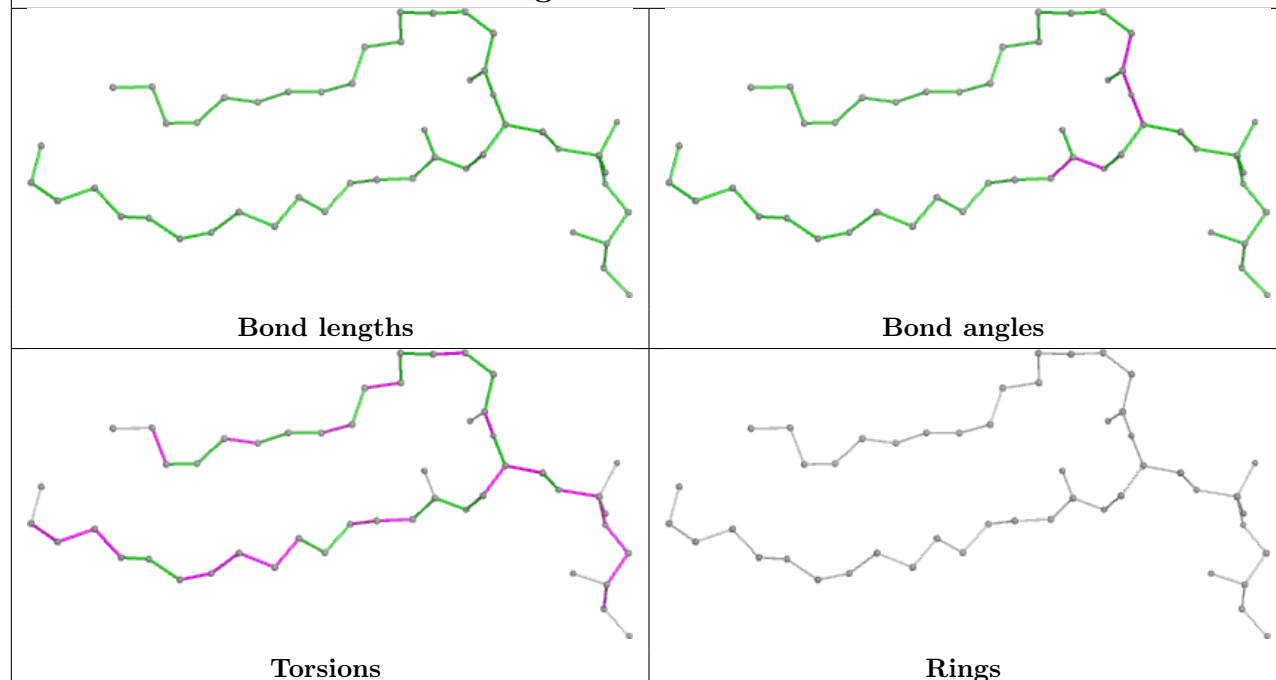
Rings

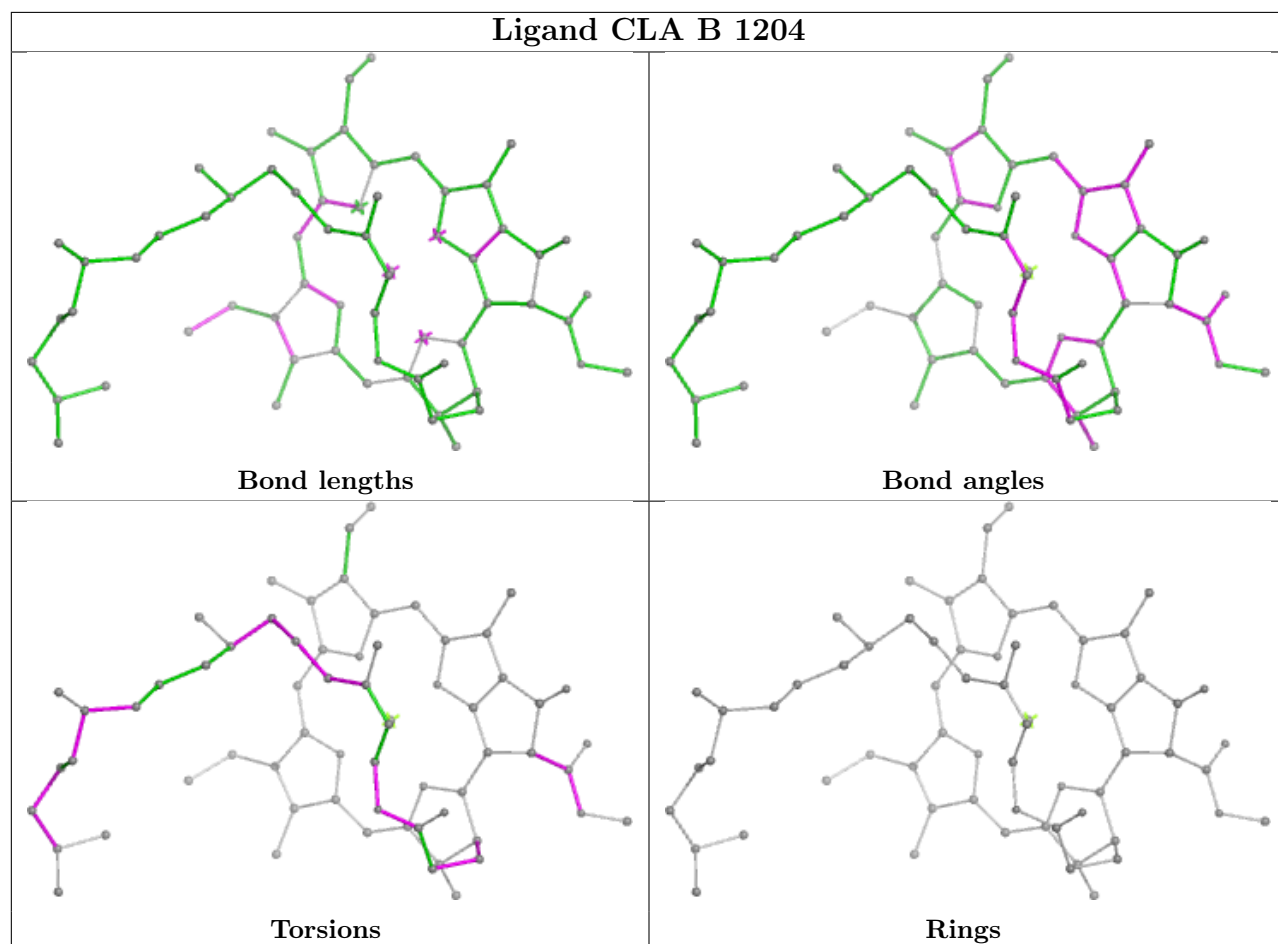
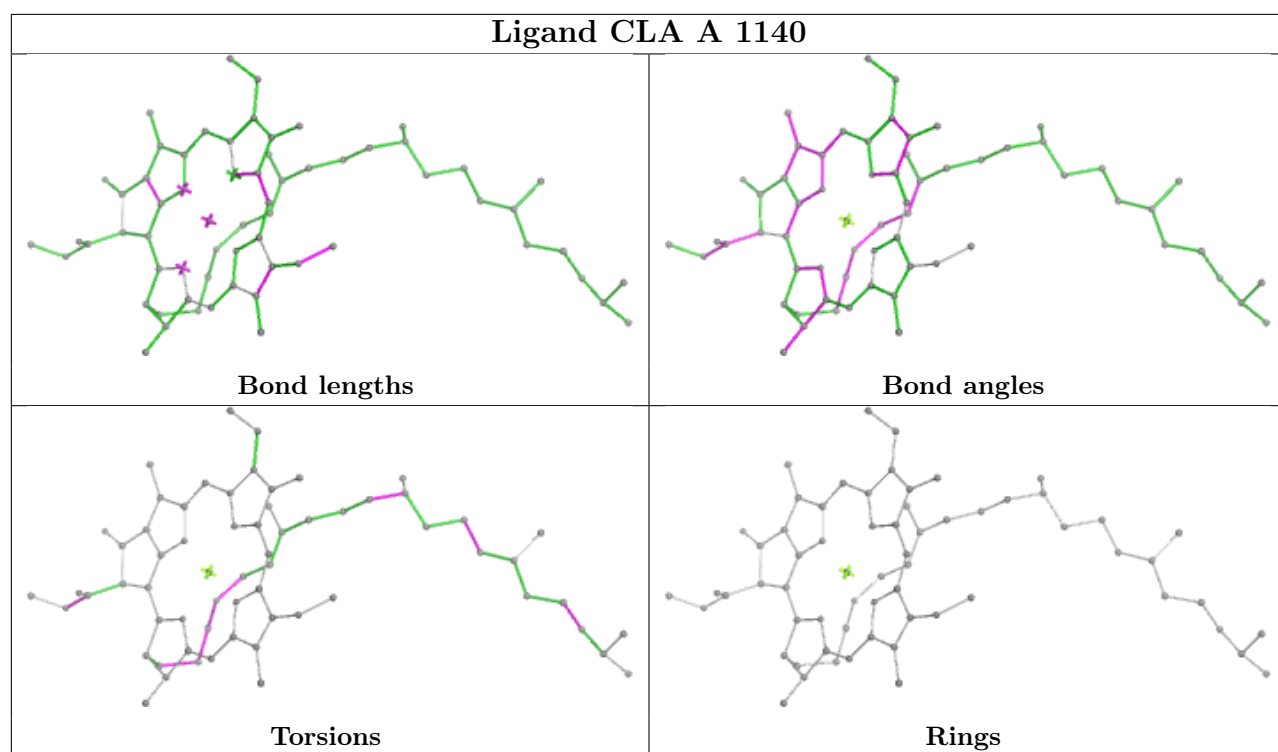


Ligand CLA 3 613

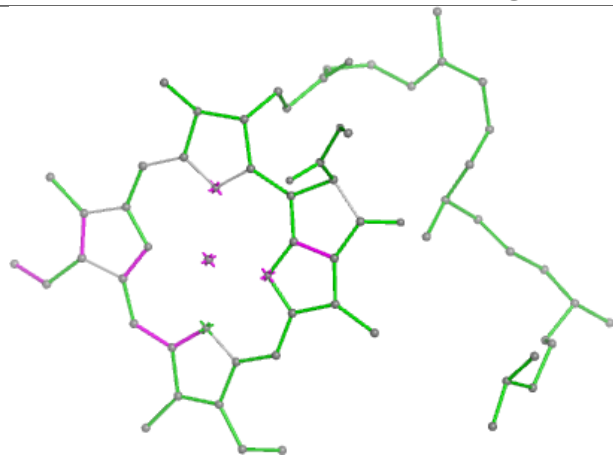


Ligand LHG 1 801

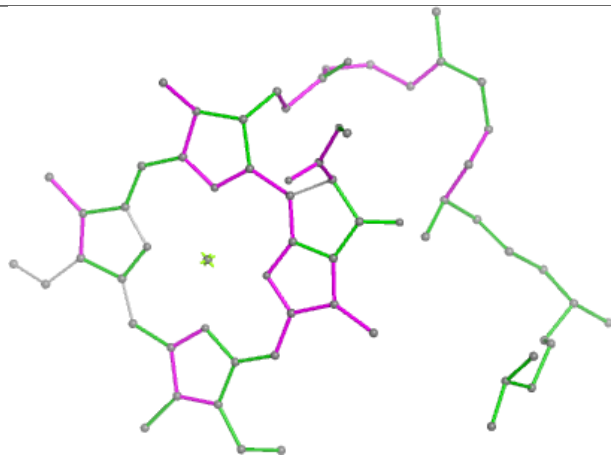




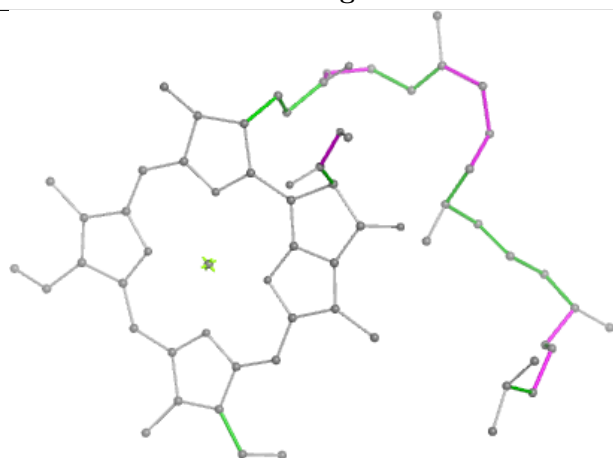
Ligand CLA B 1229



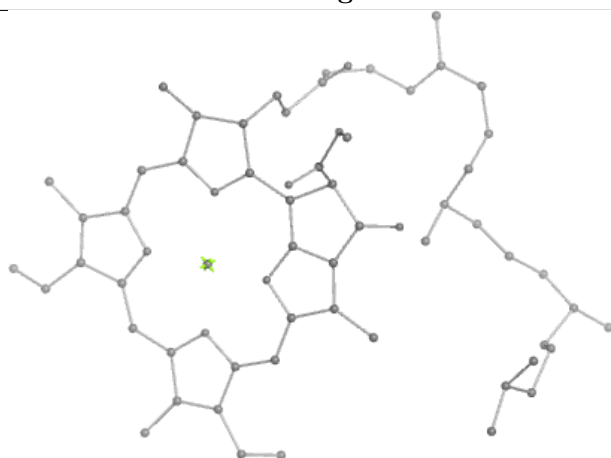
Bond lengths



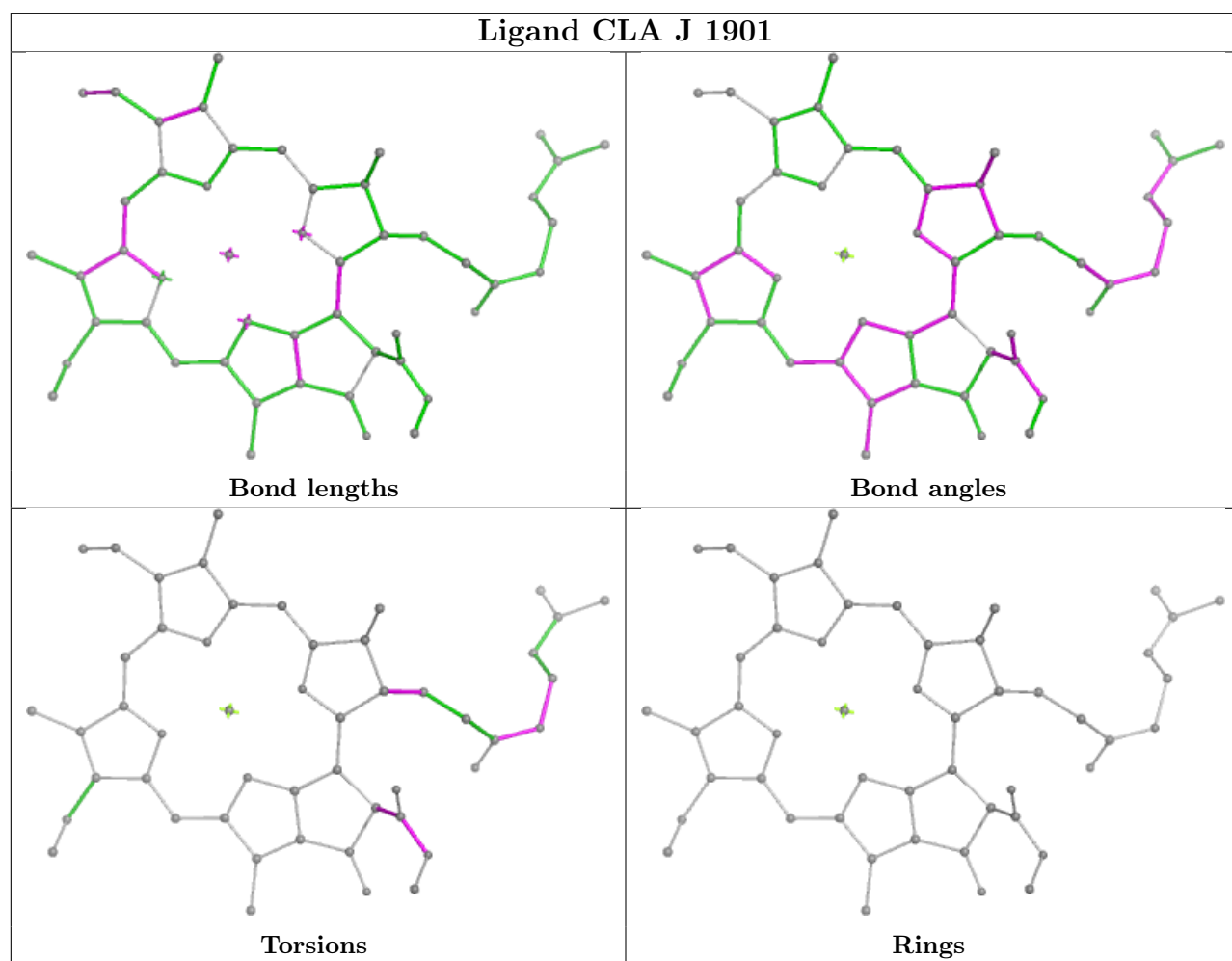
Bond angles

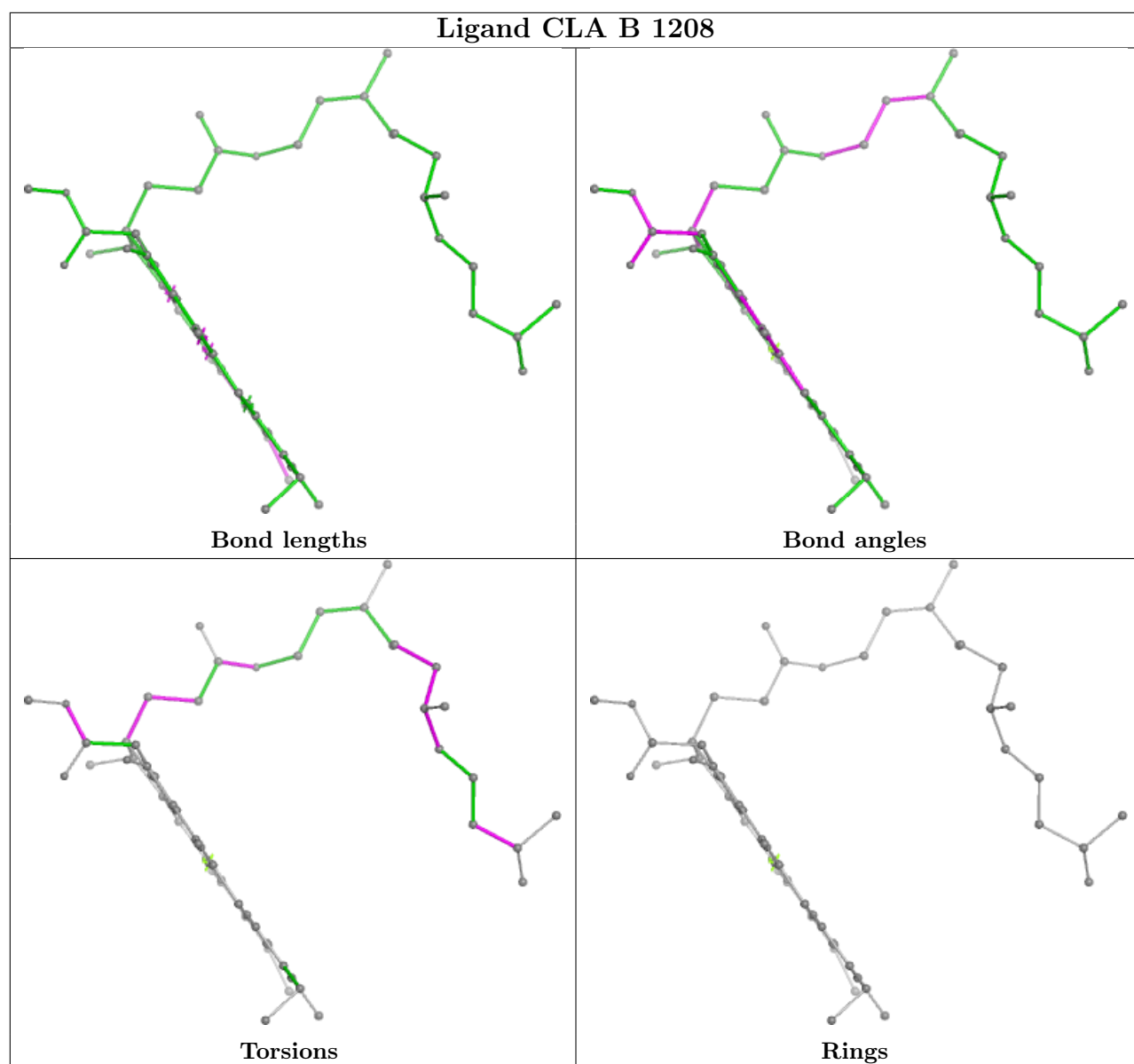


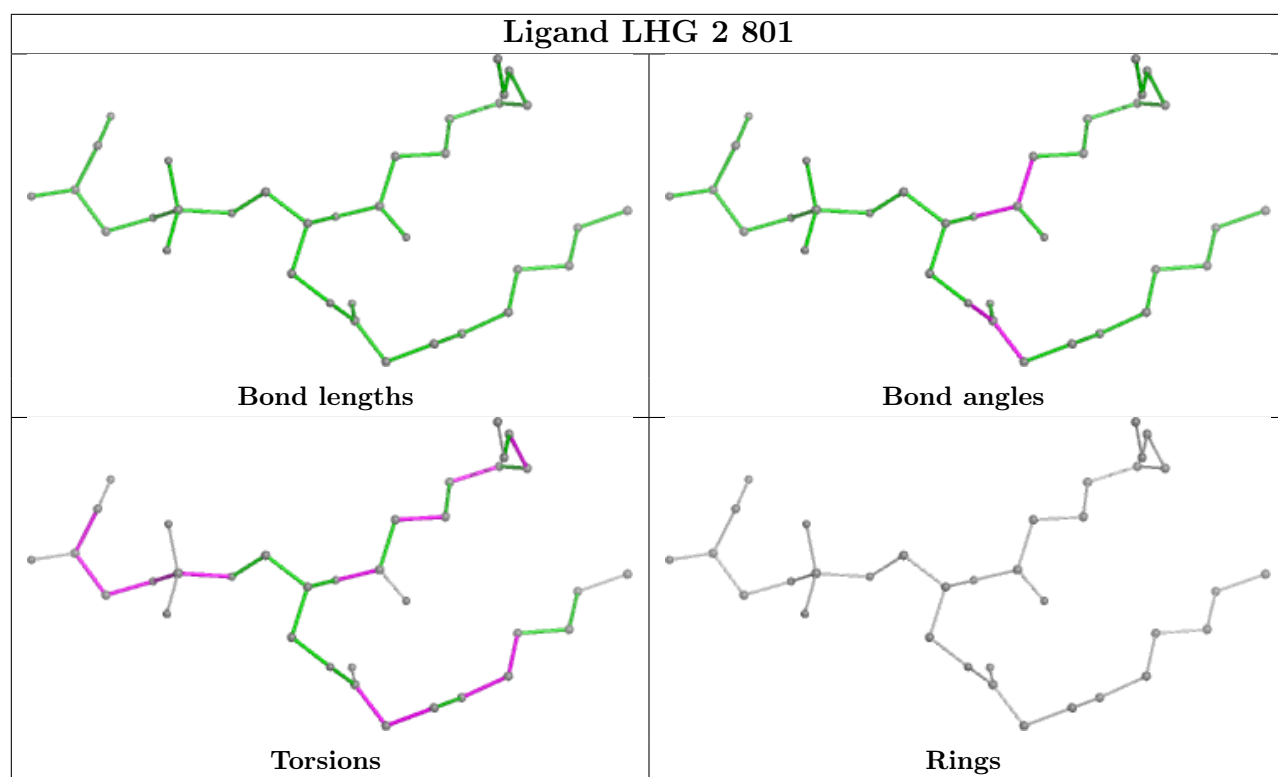
Torsions

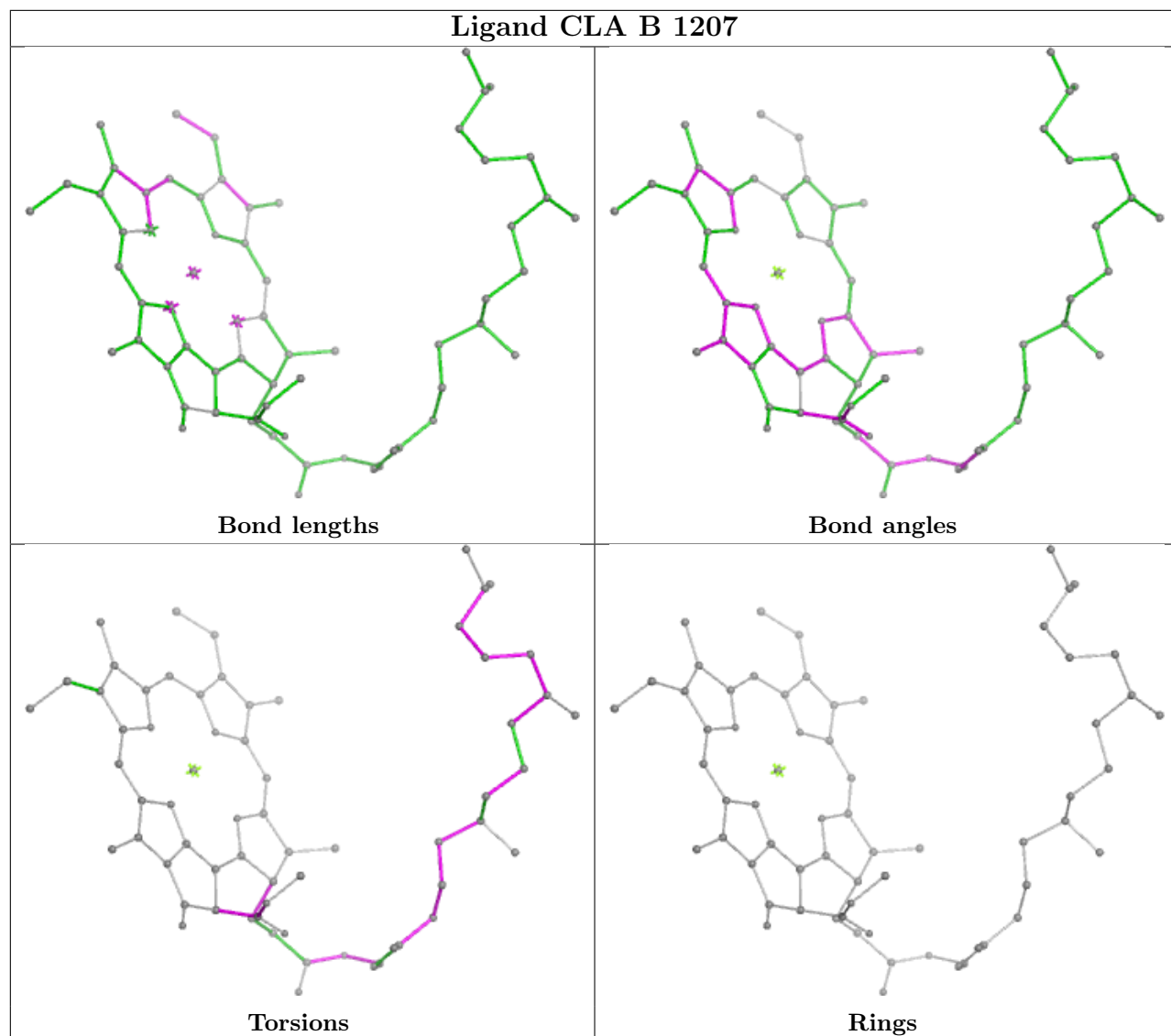


Rings

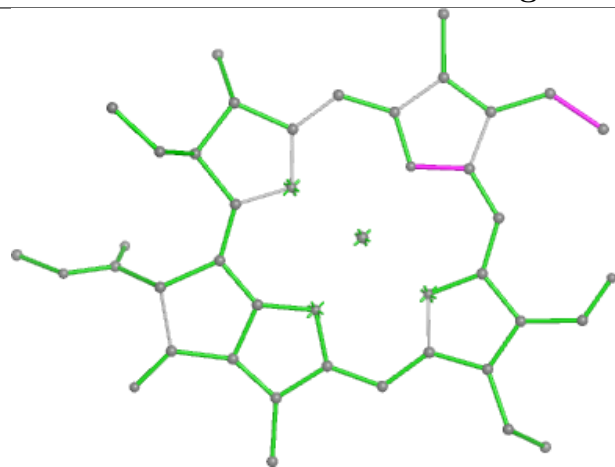




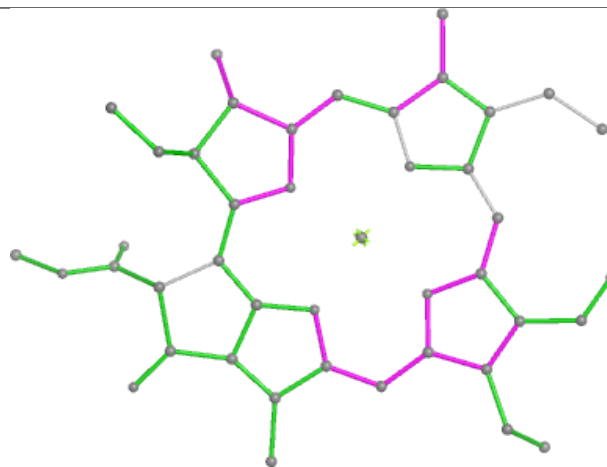




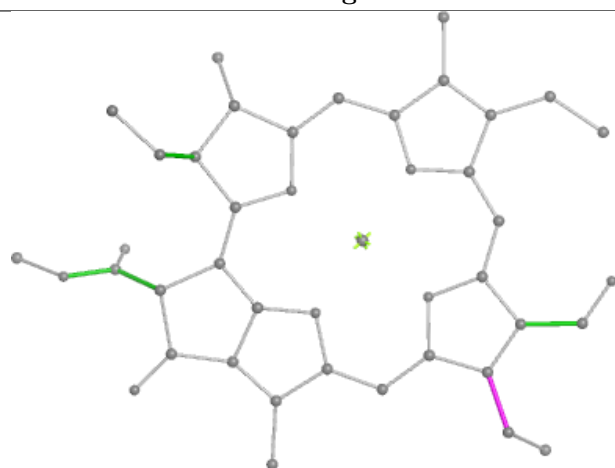
Ligand CHL 4 615



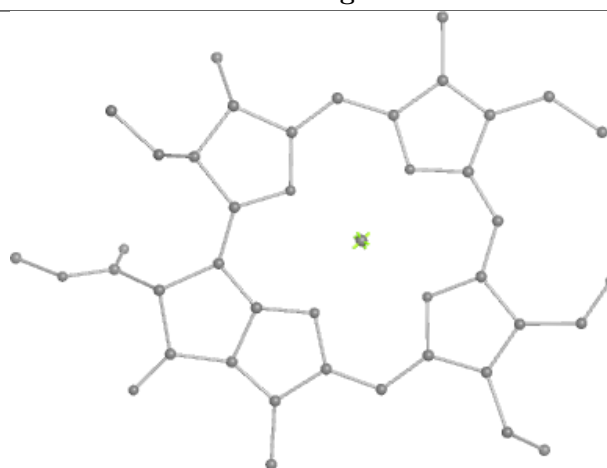
Bond lengths



Bond angles

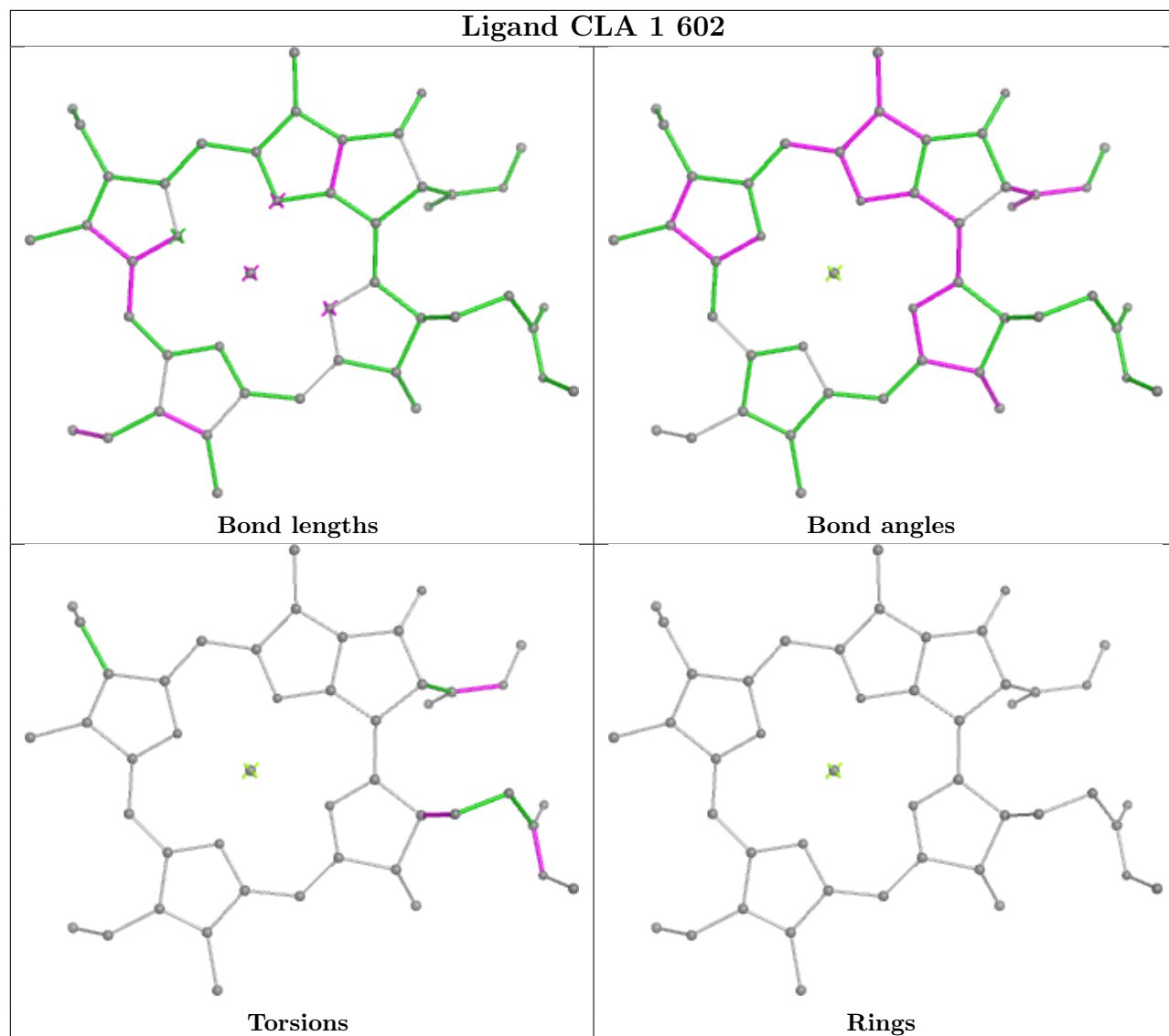


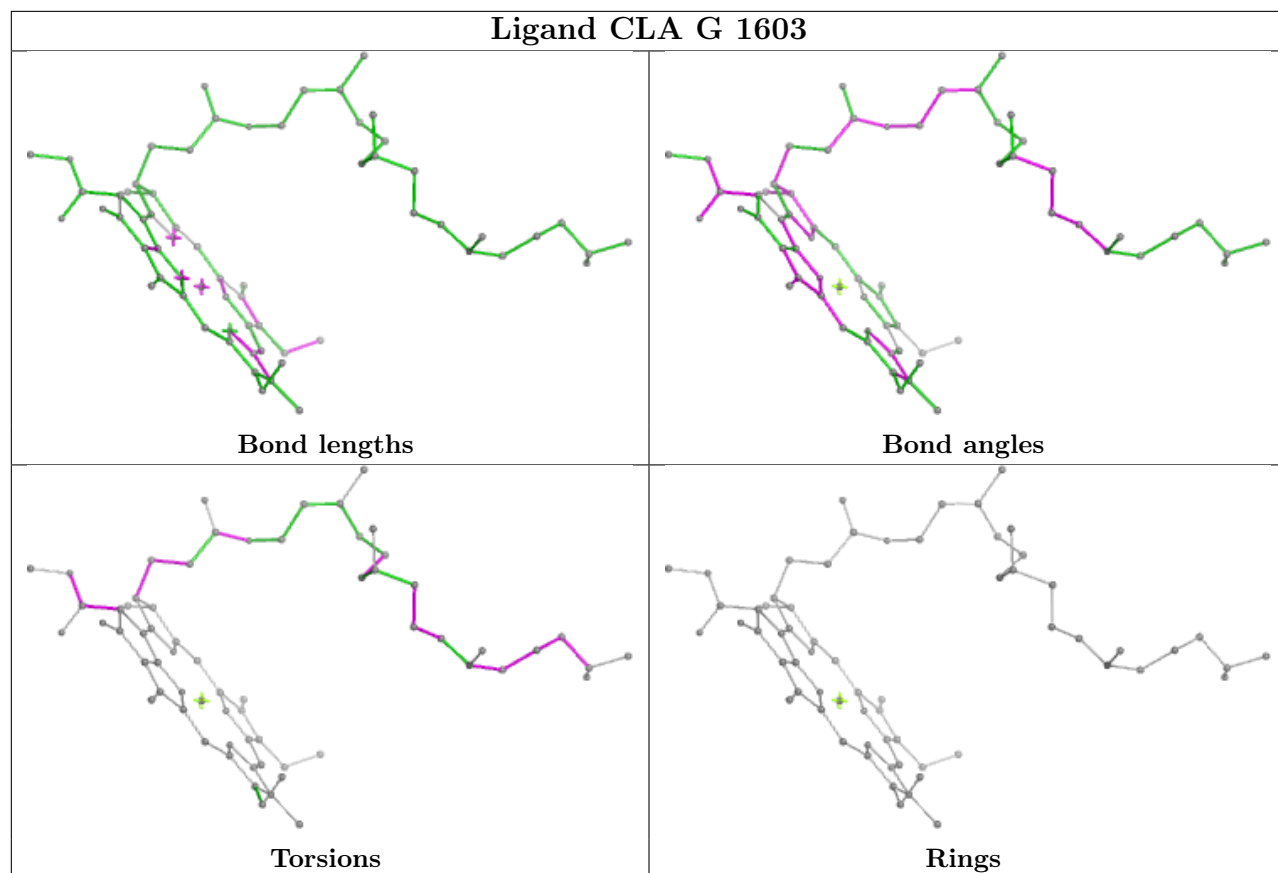
Torsions



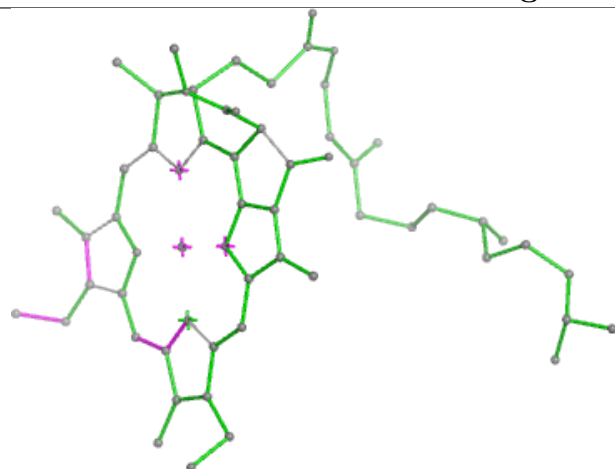
Rings

Ligand CLA 1 602

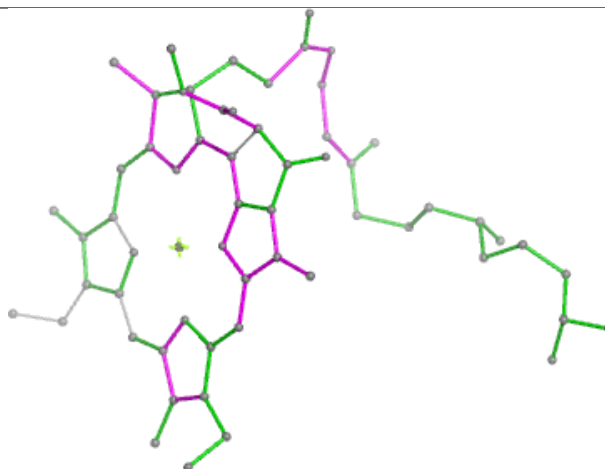




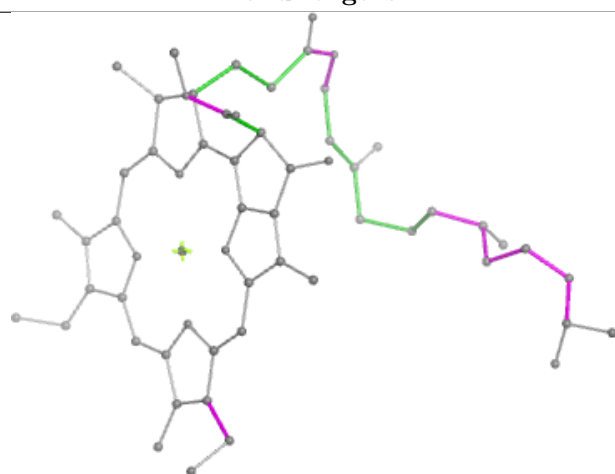
Ligand CLA 2 607



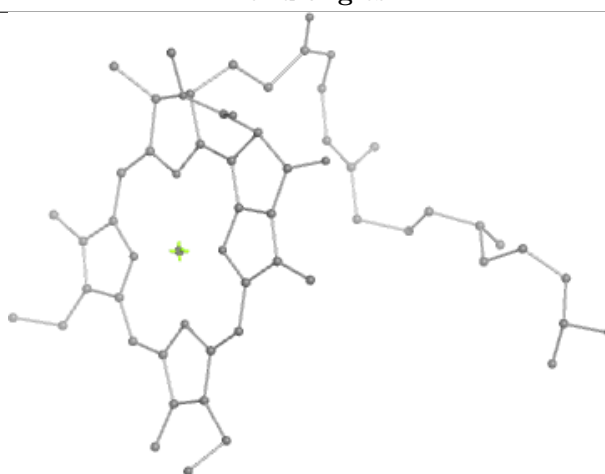
Bond lengths



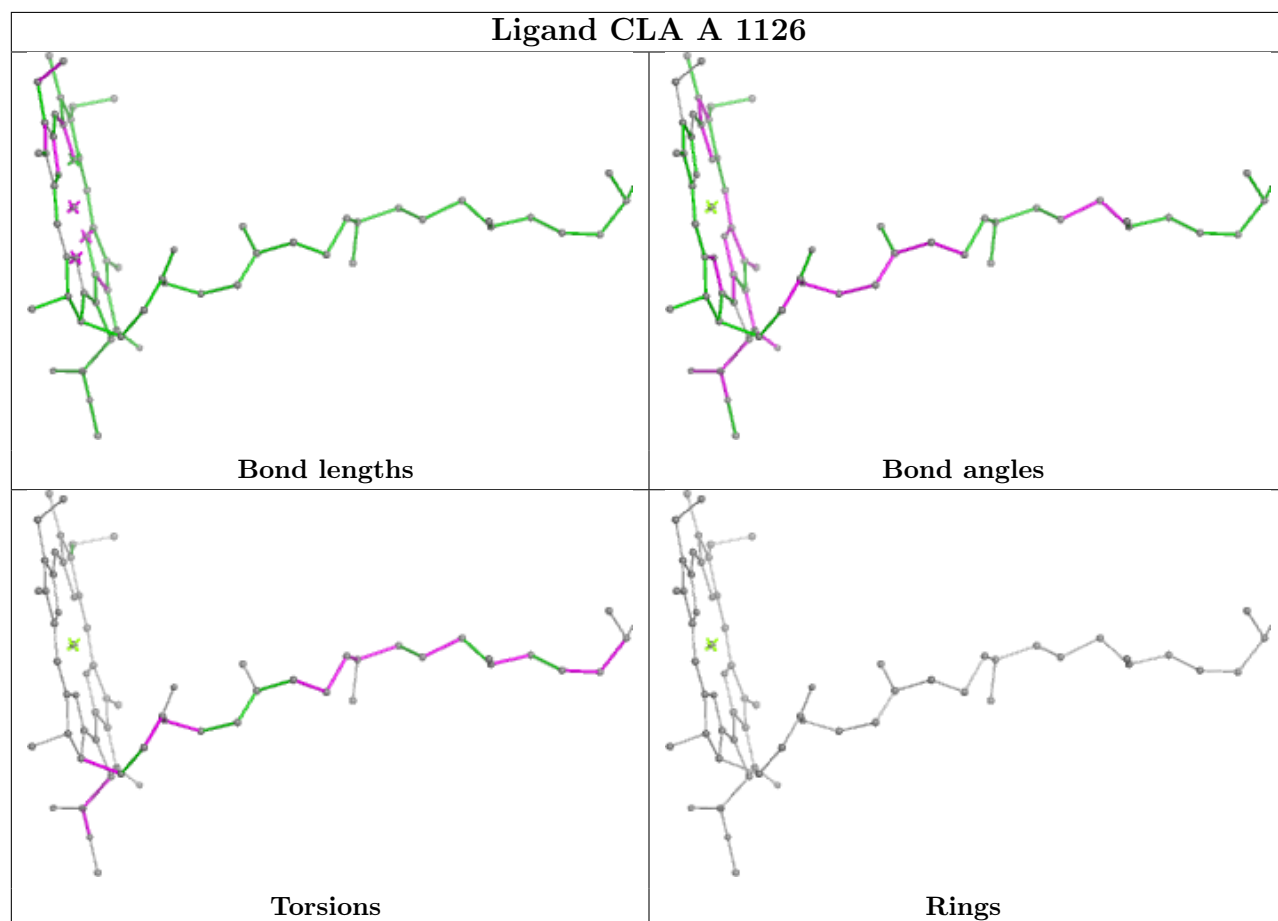
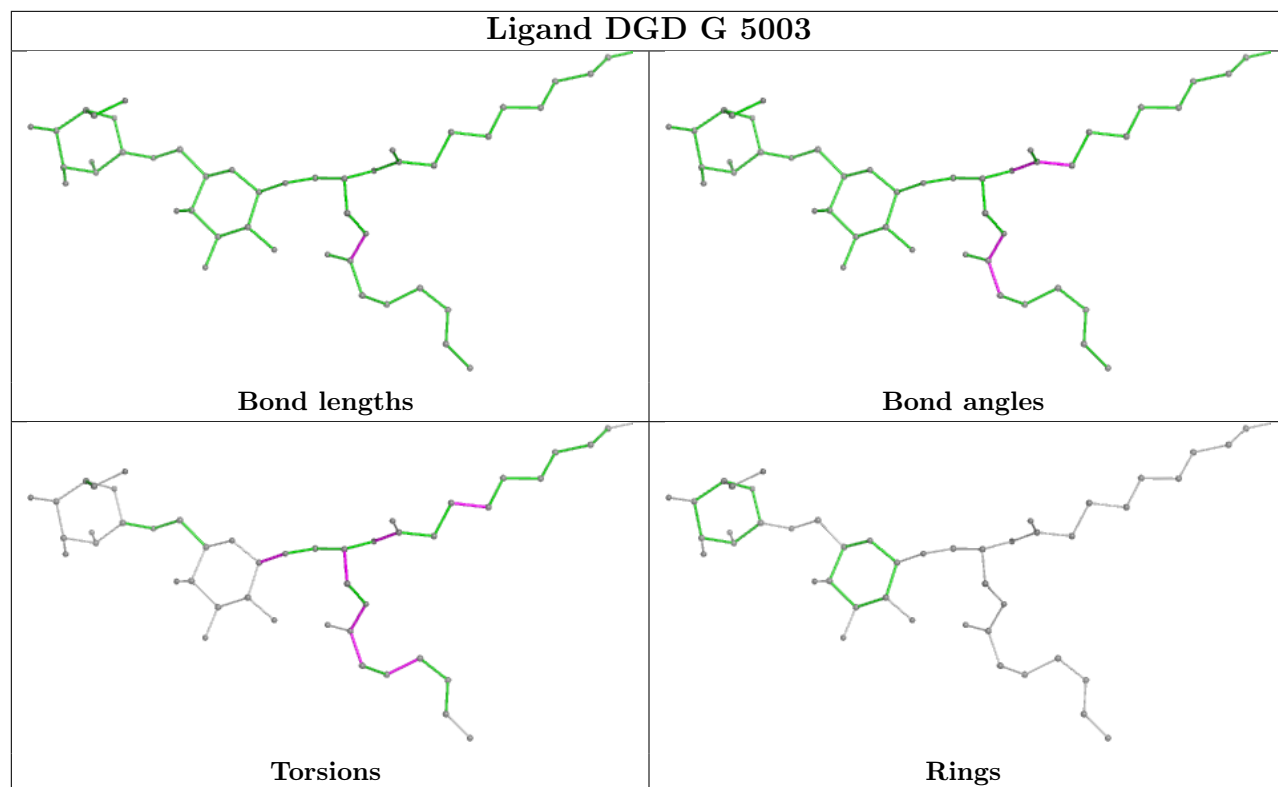
Bond angles

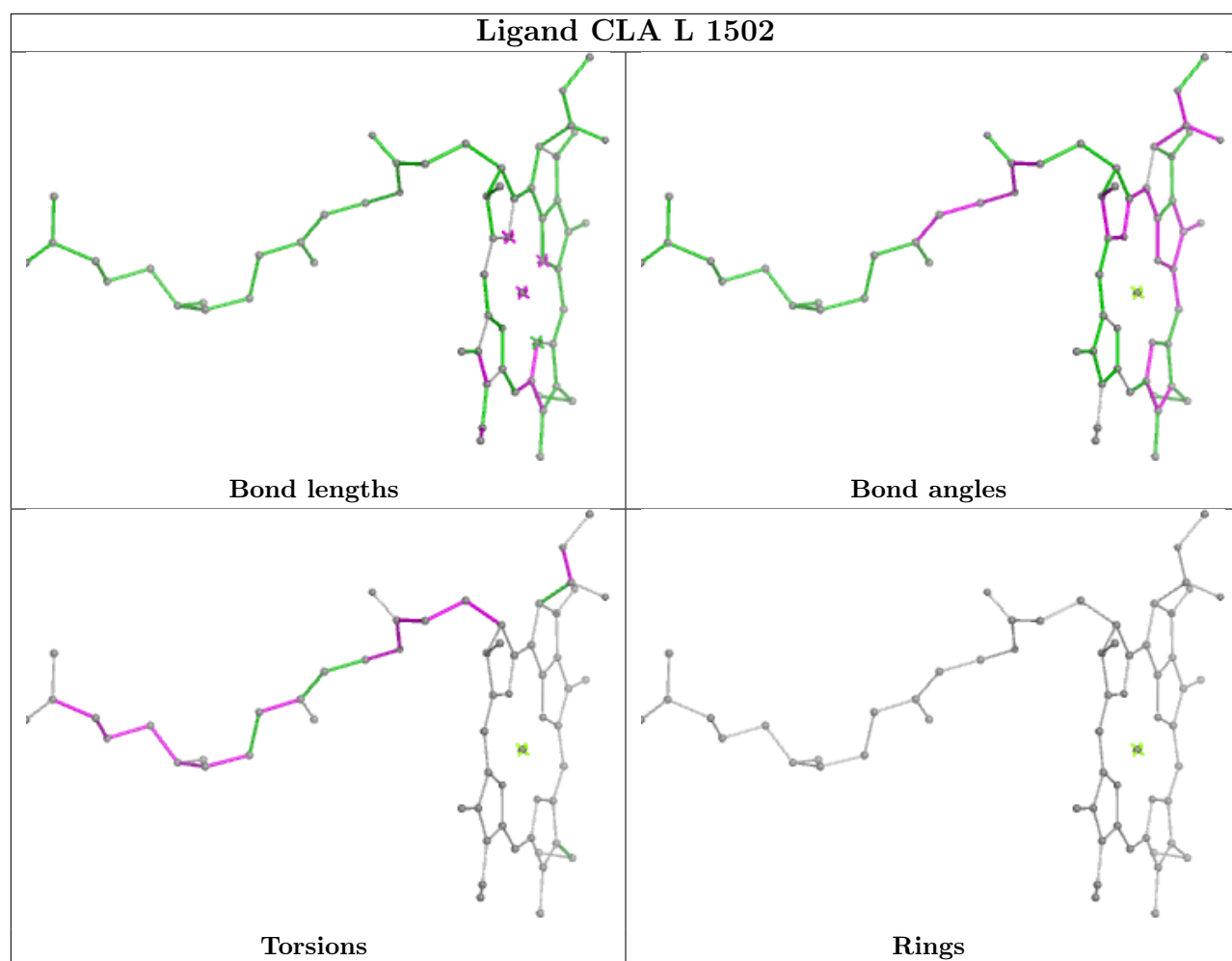


Torsions

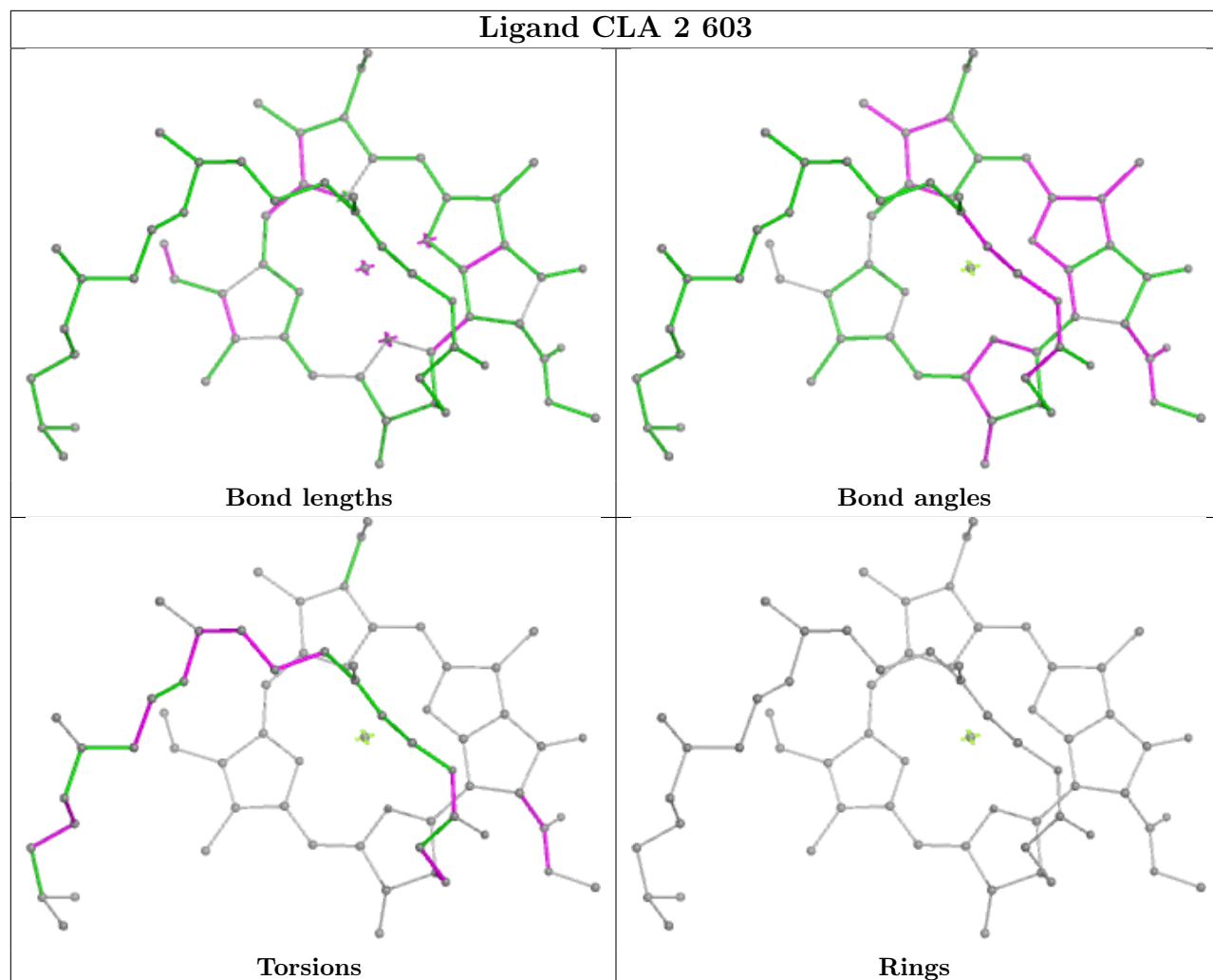


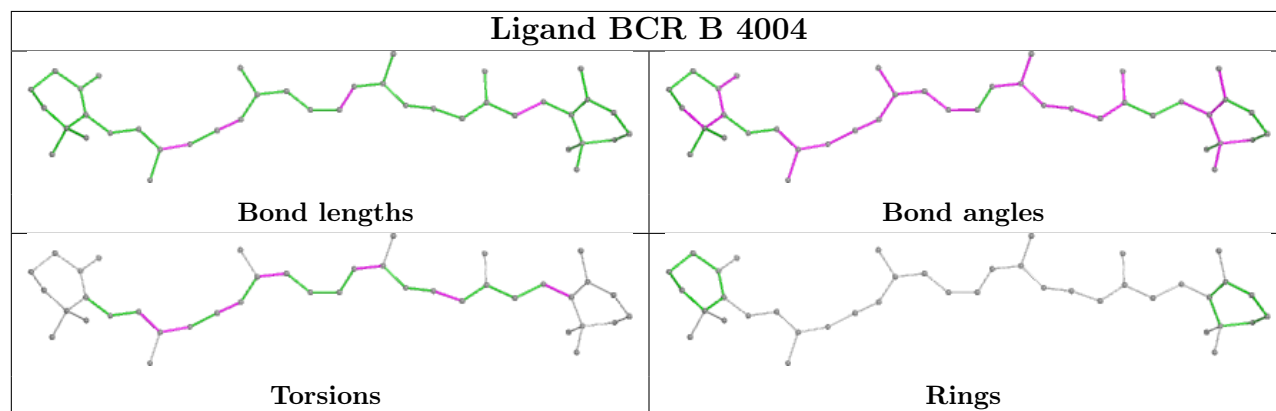
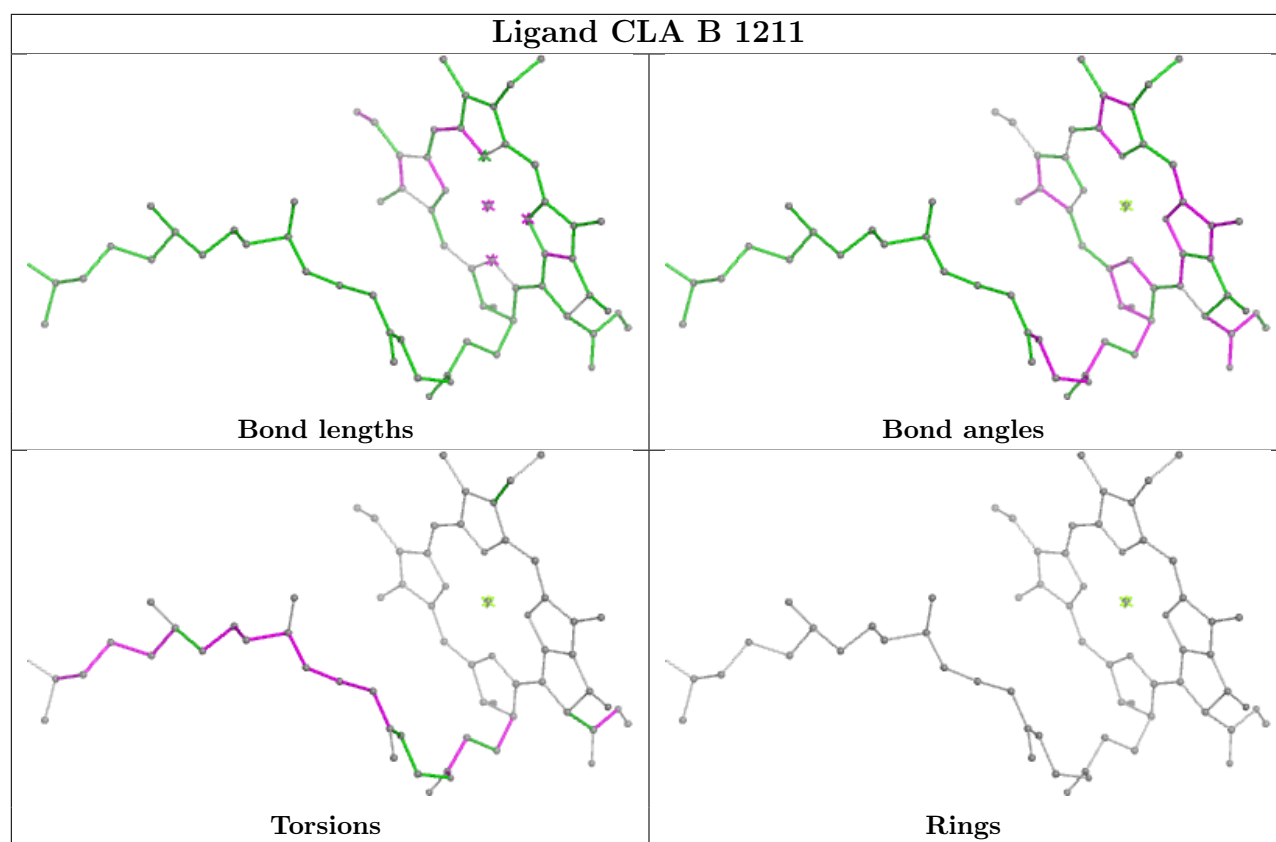
Rings

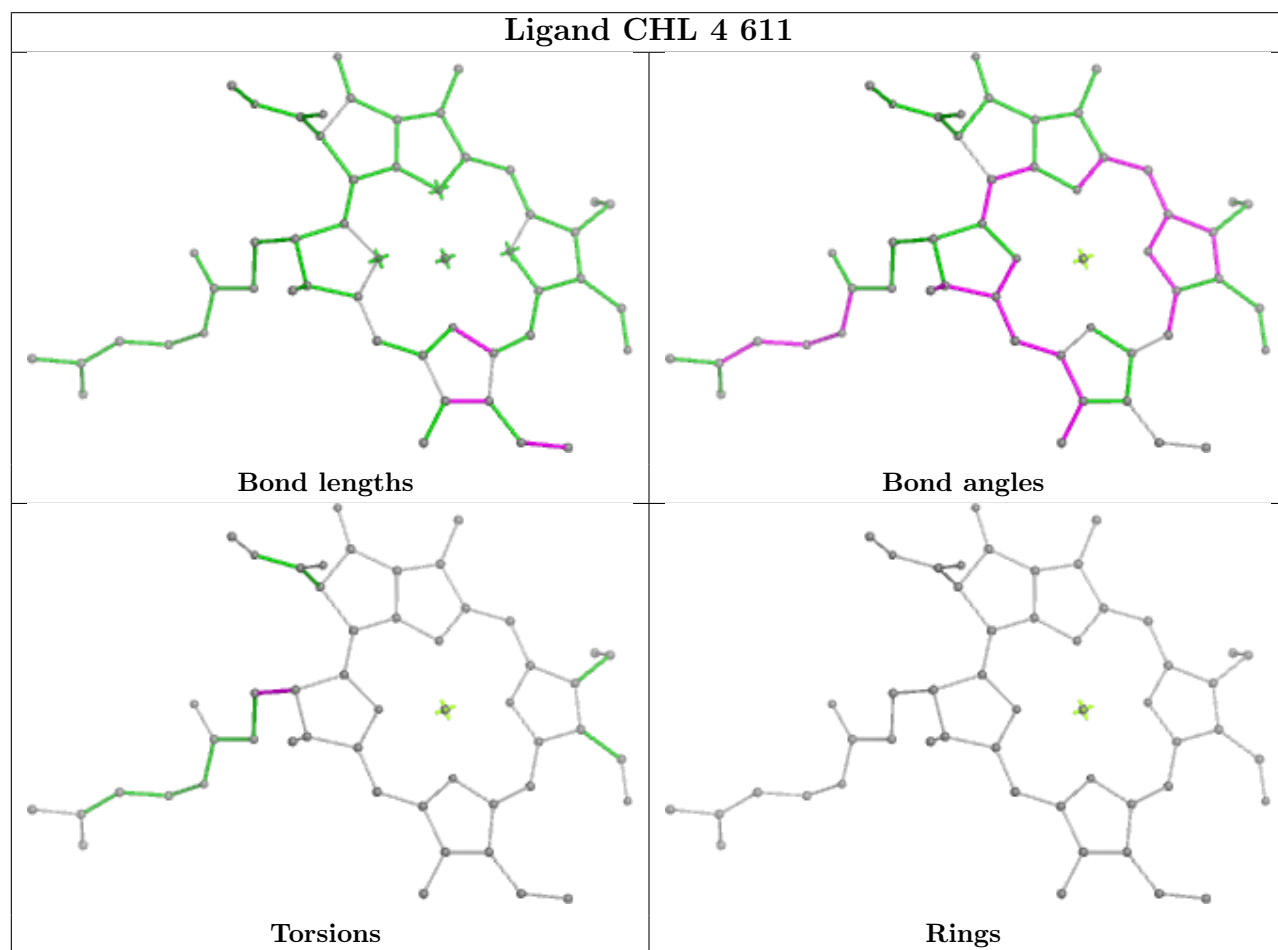
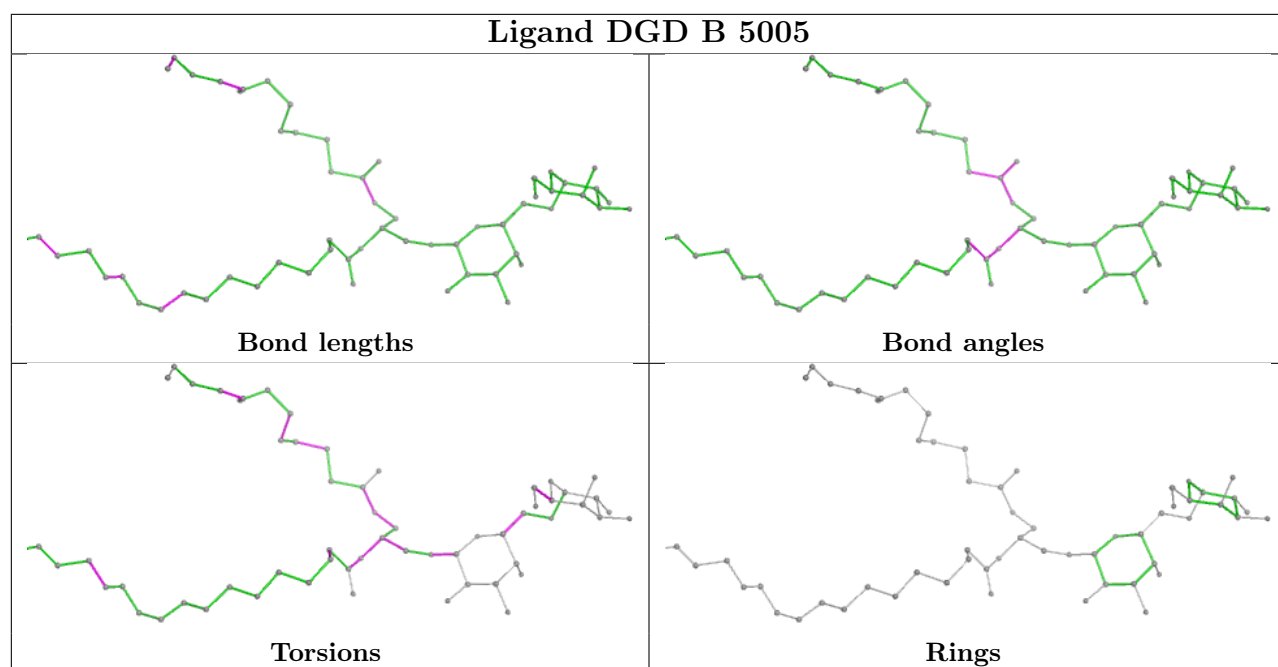


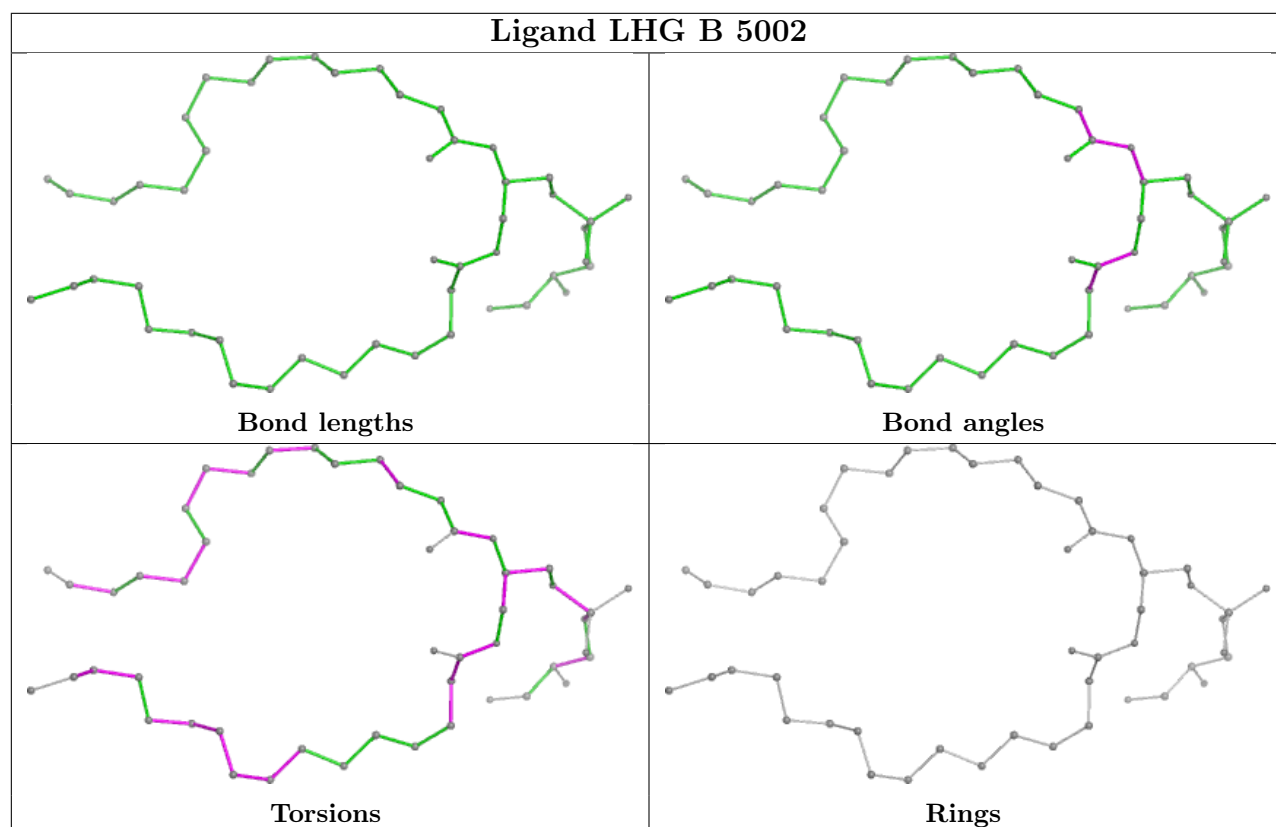
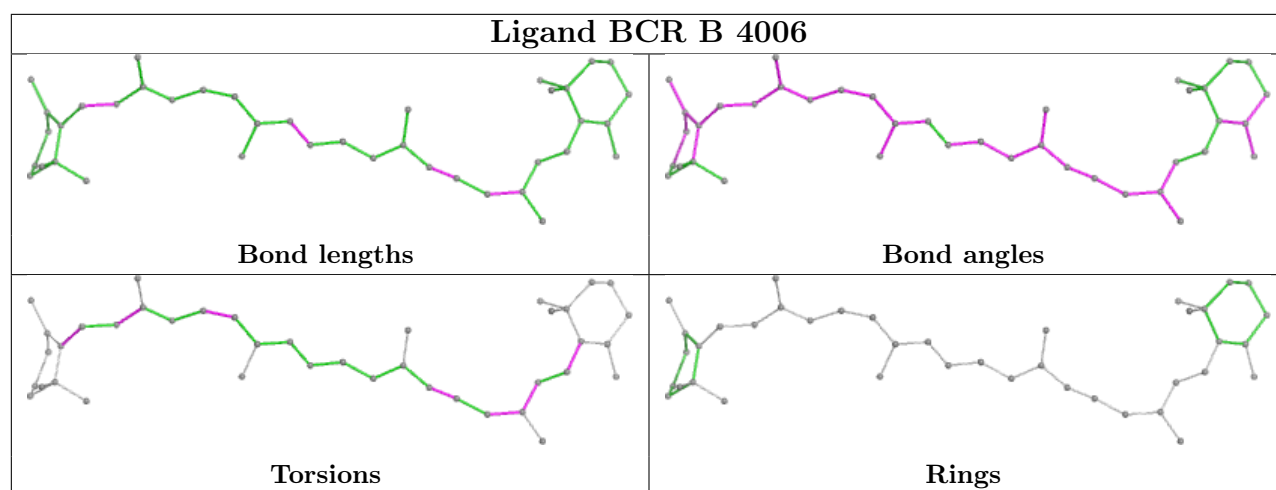


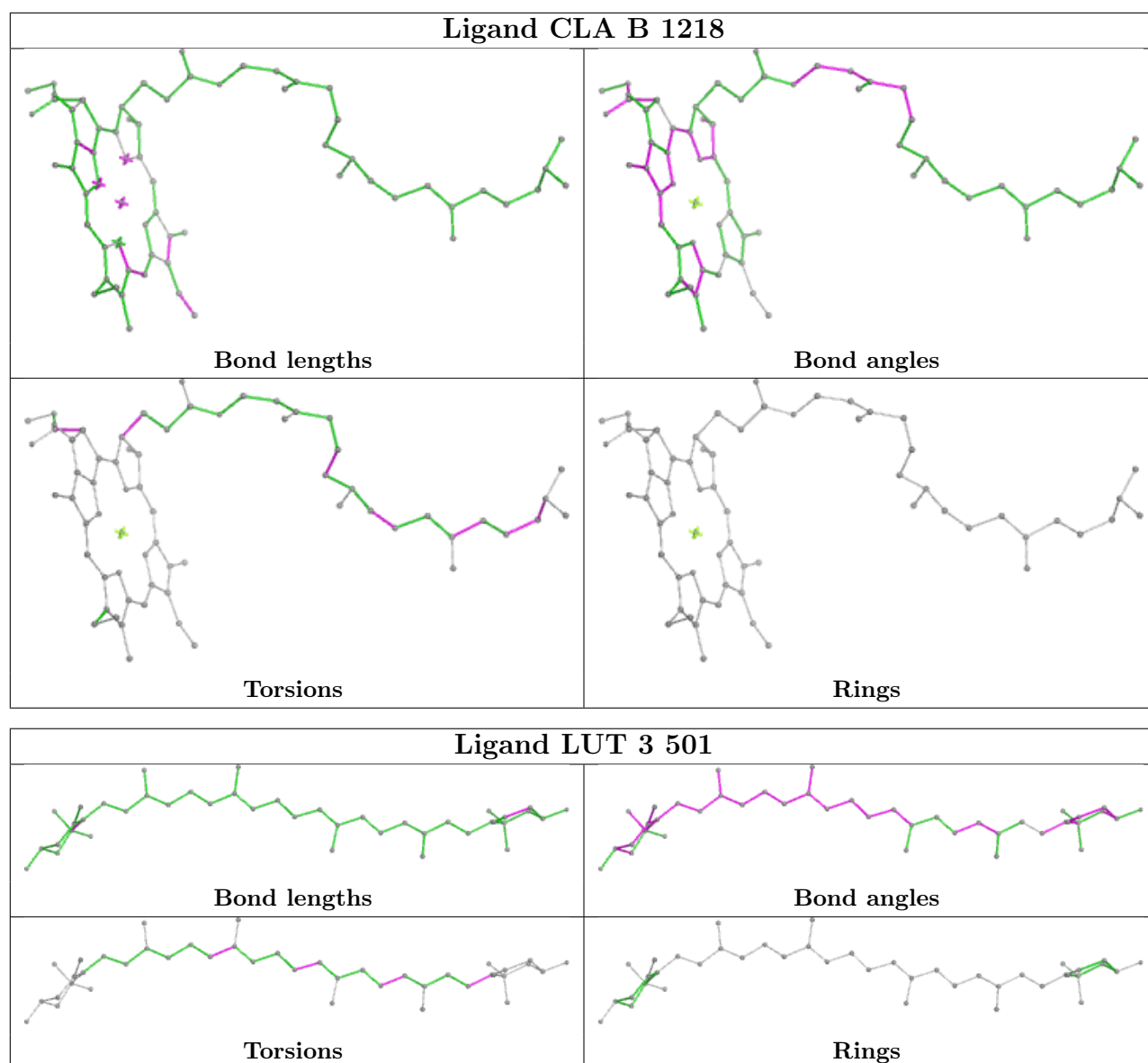
Ligand CLA 2 603



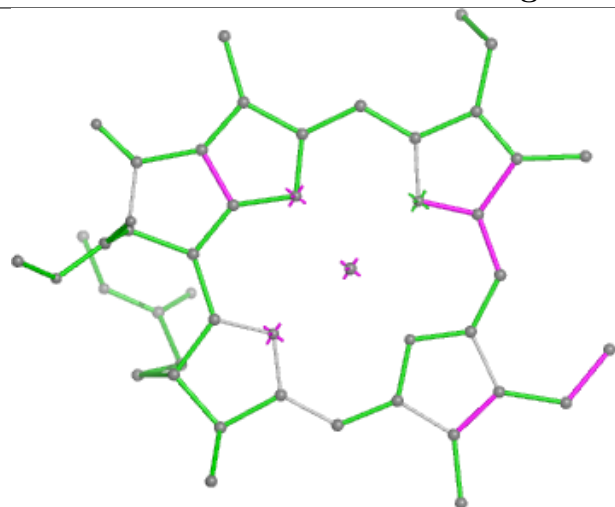




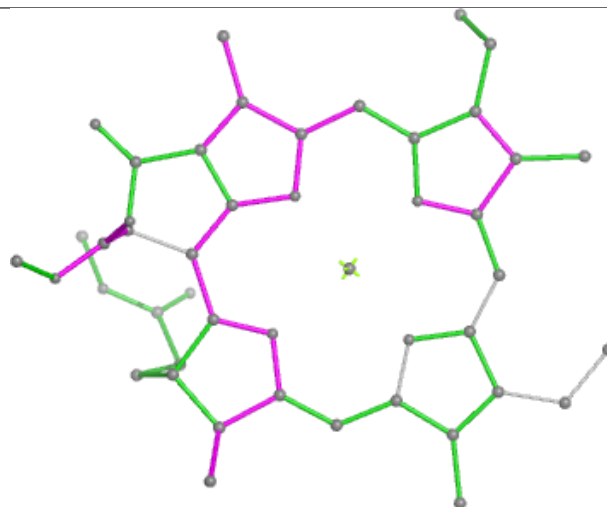




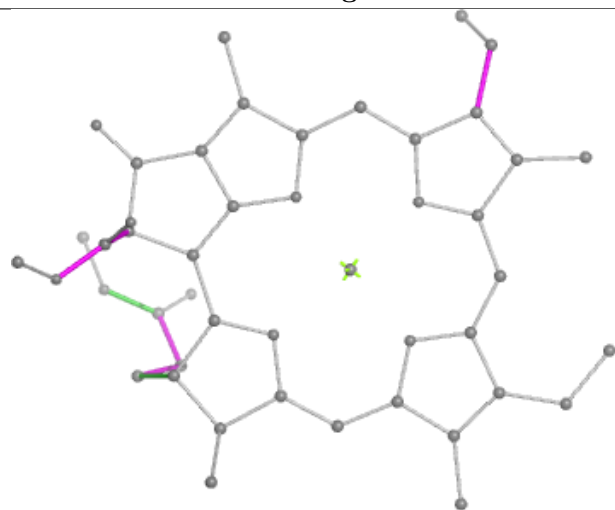
Ligand CLA 4 608



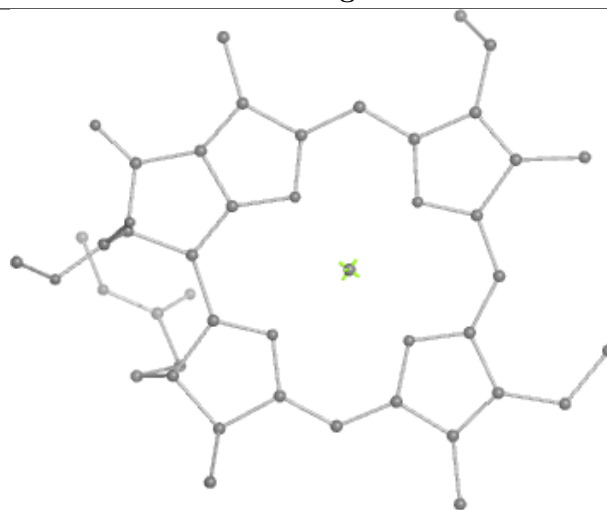
Bond lengths



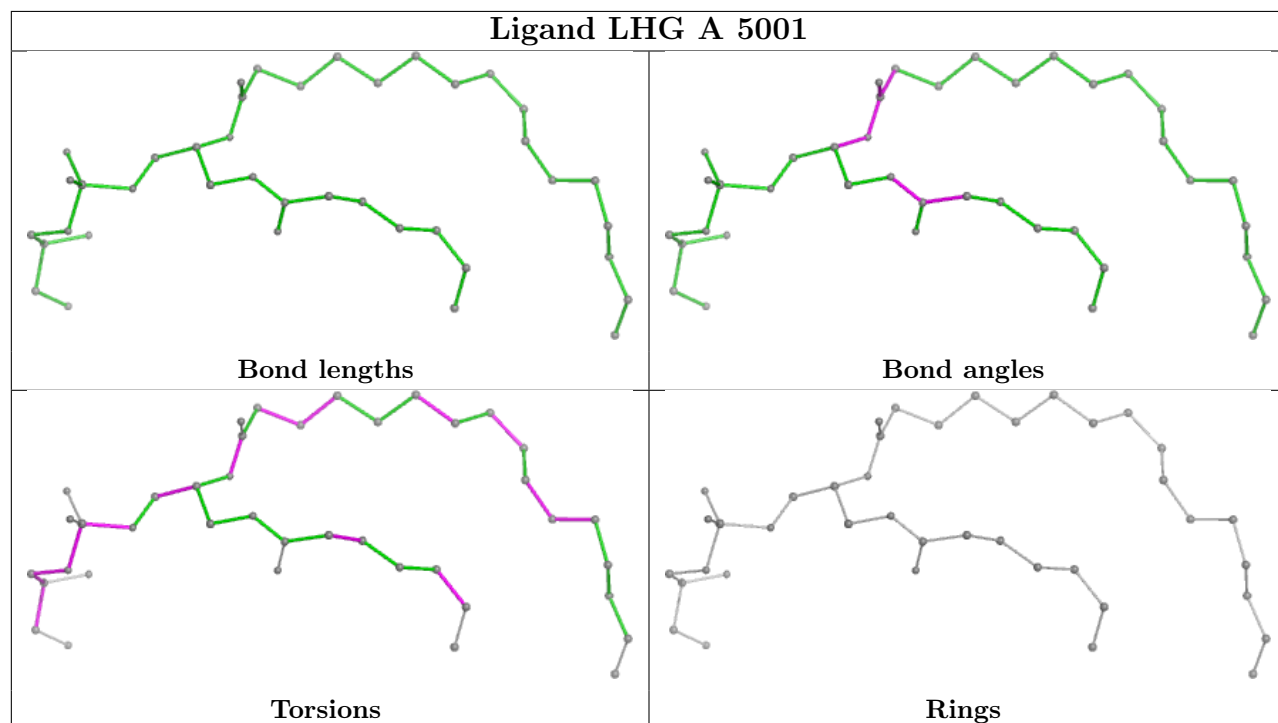
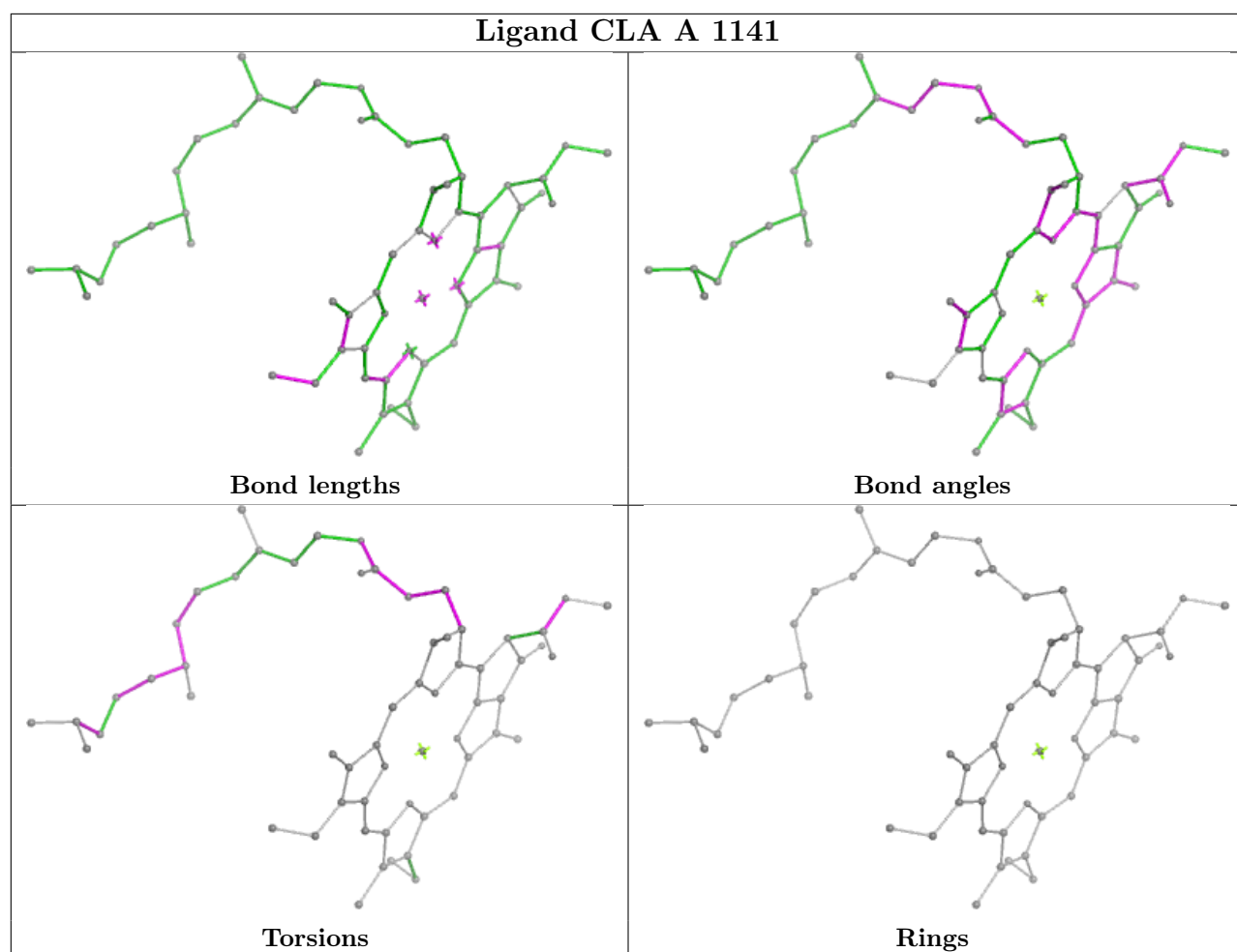
Bond angles

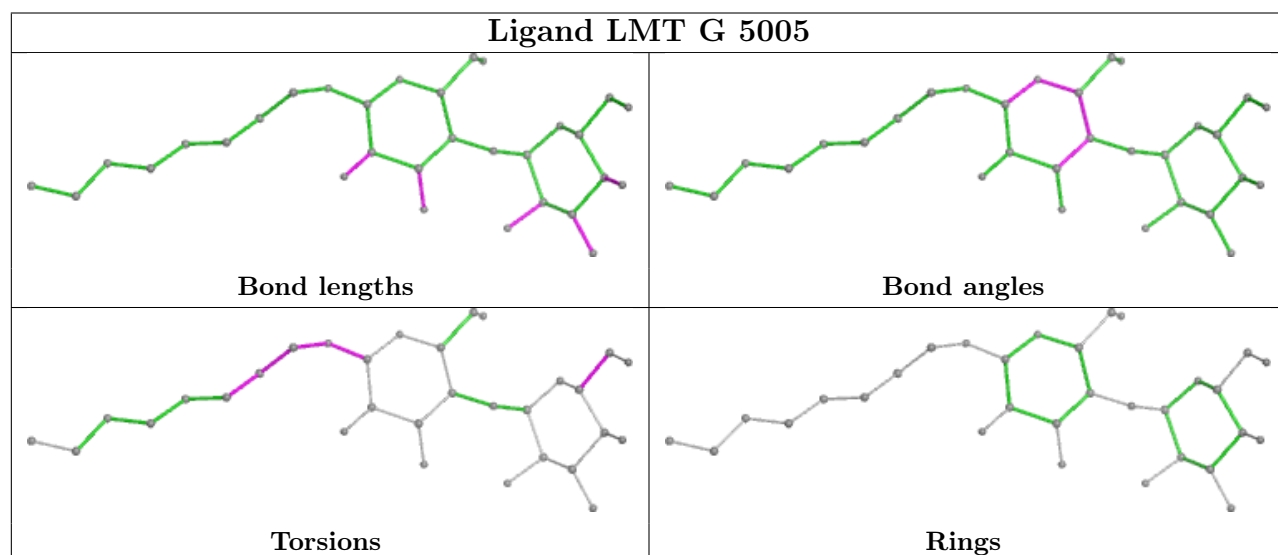
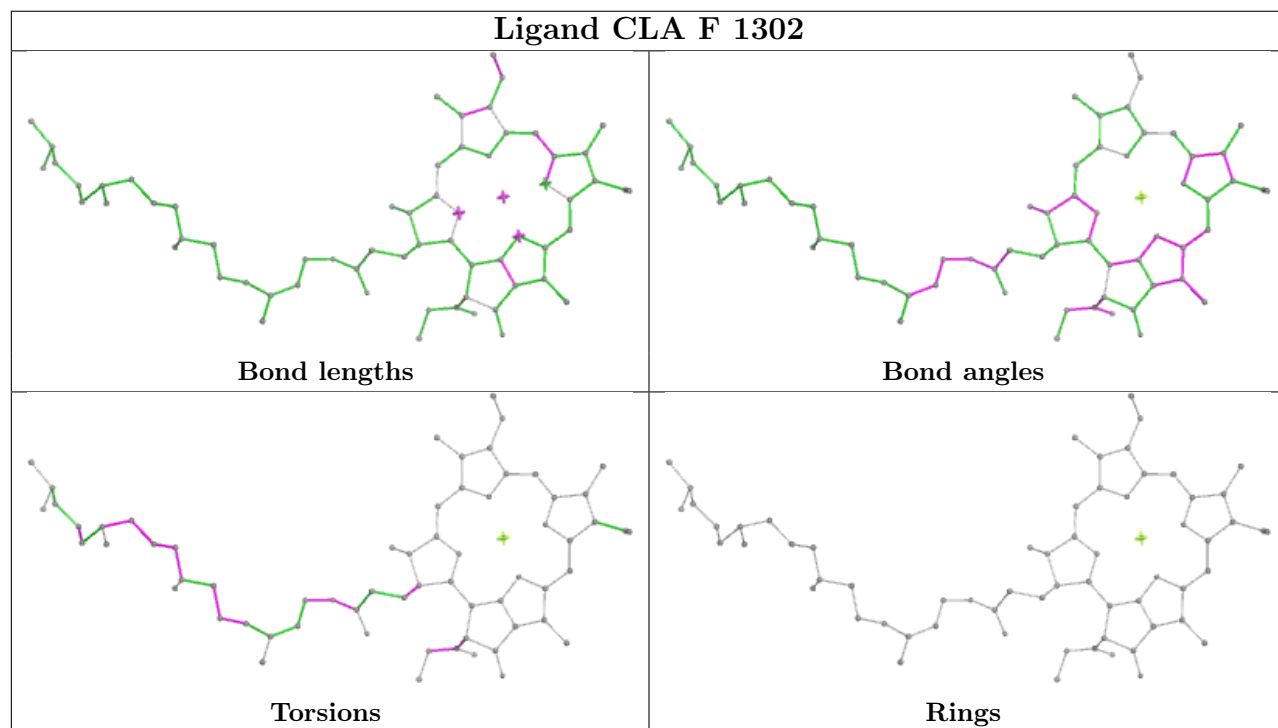
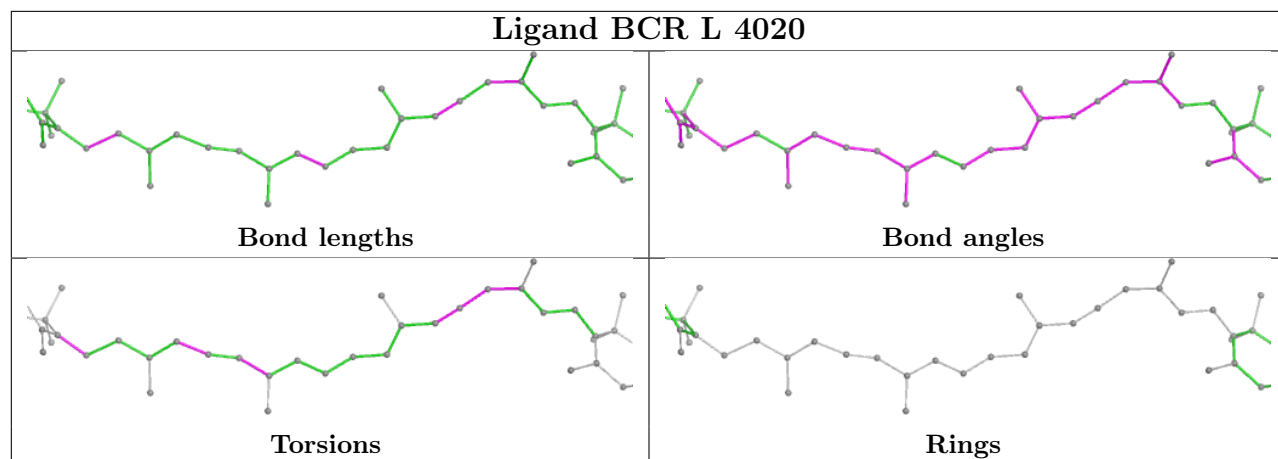


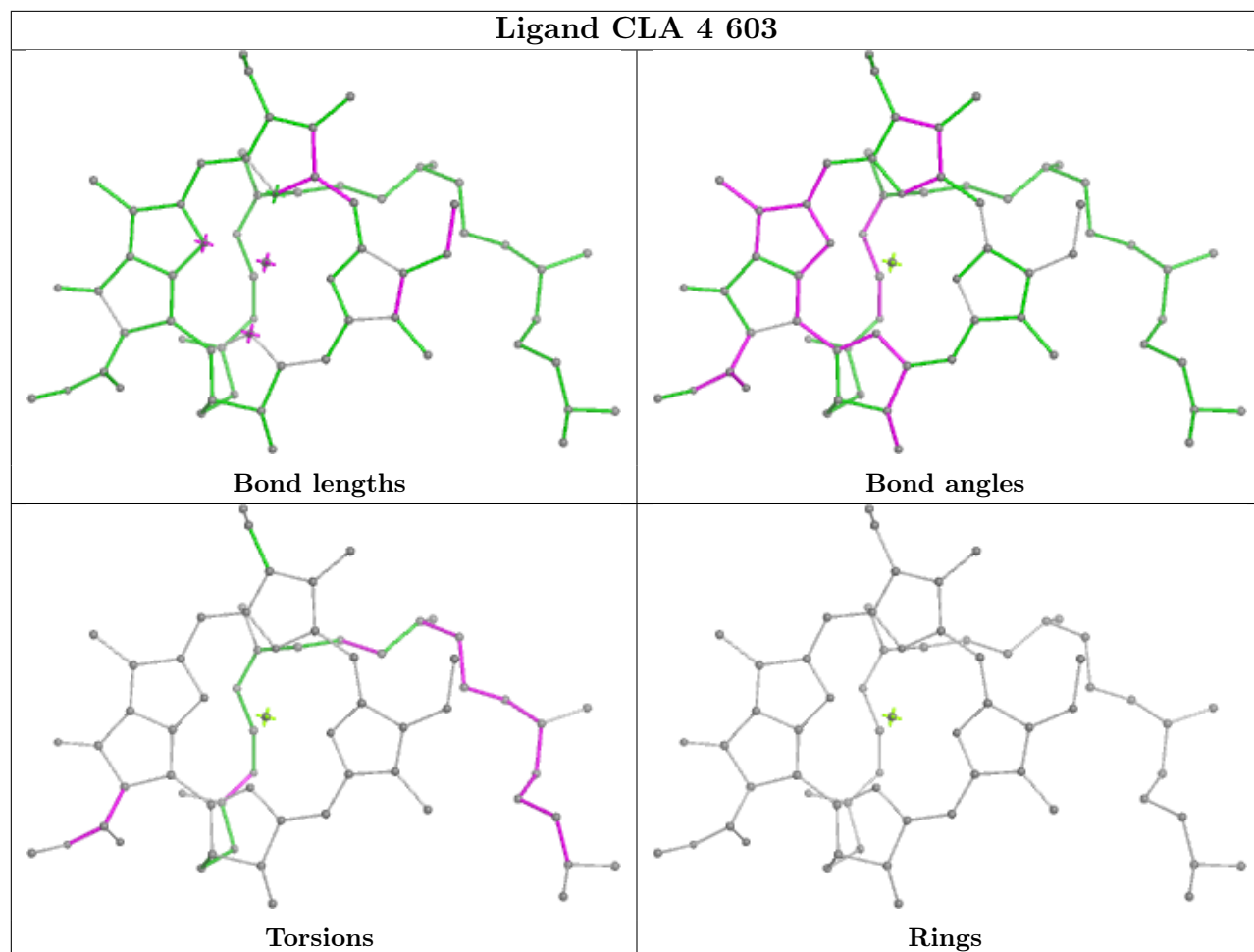
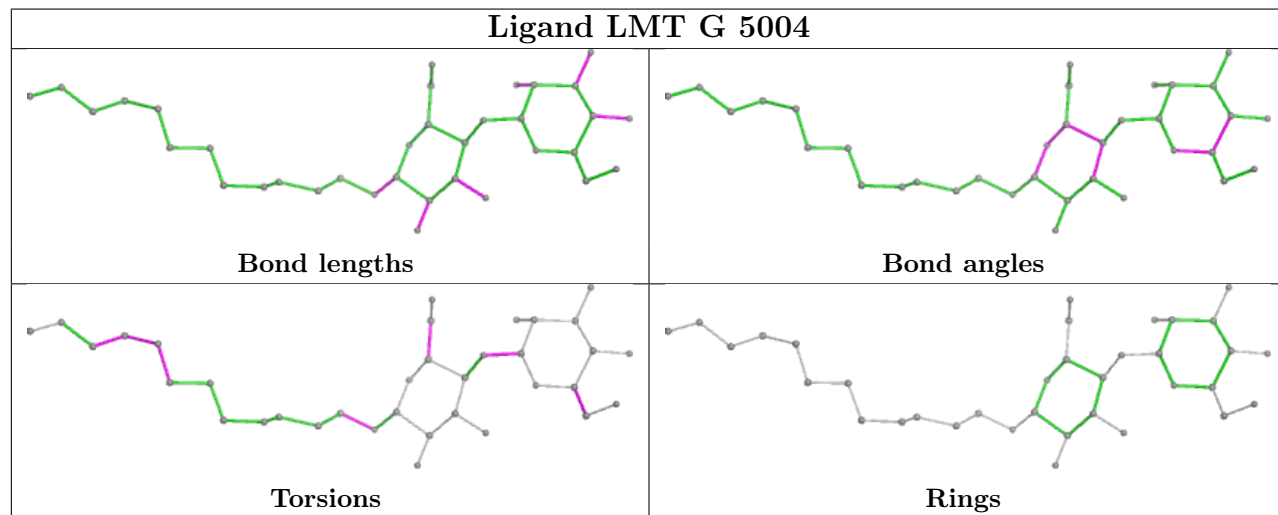
Torsions

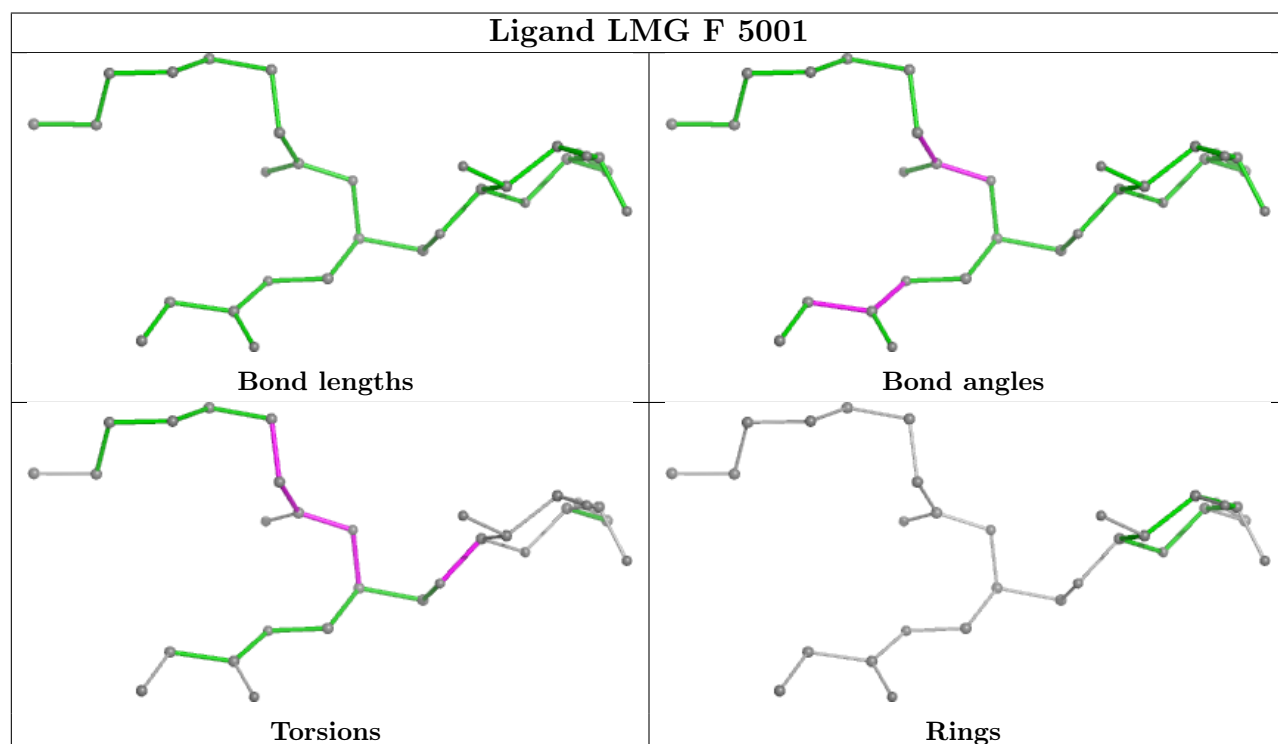
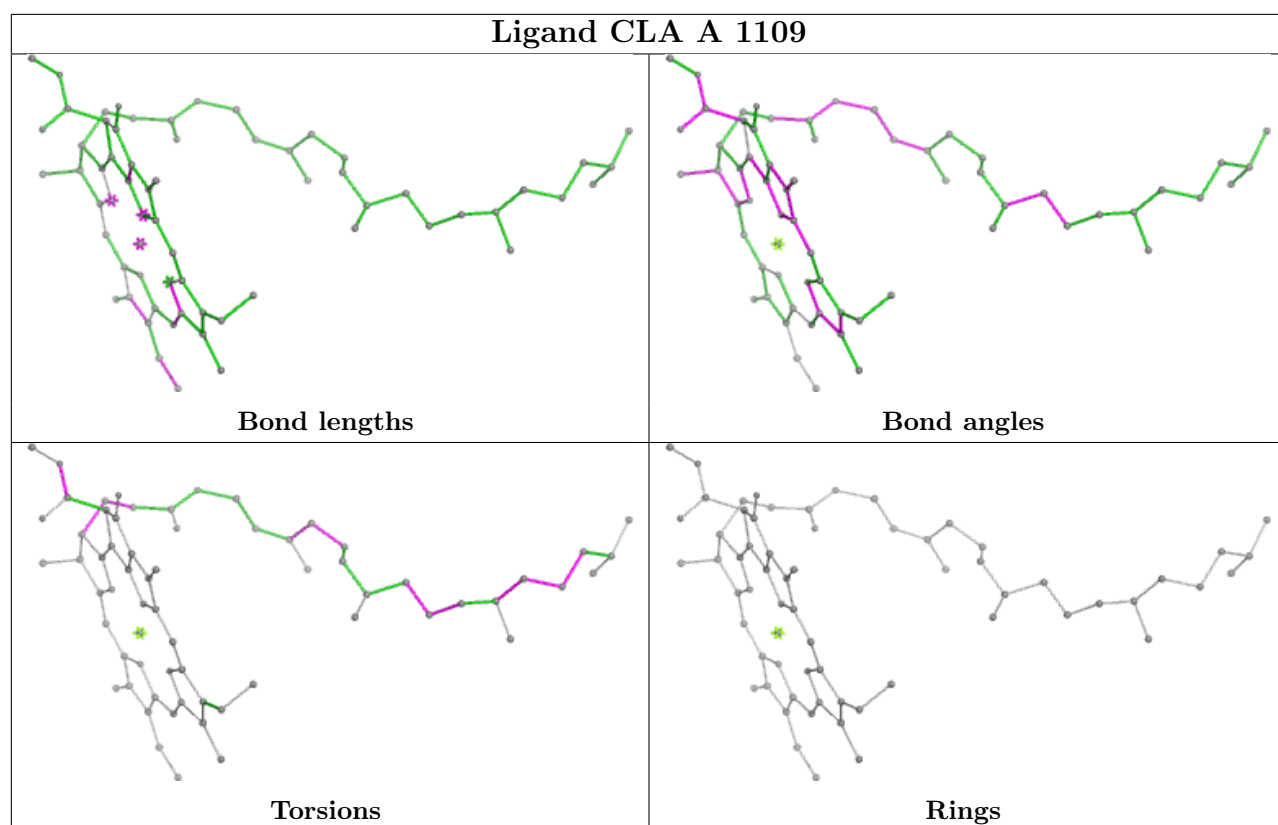


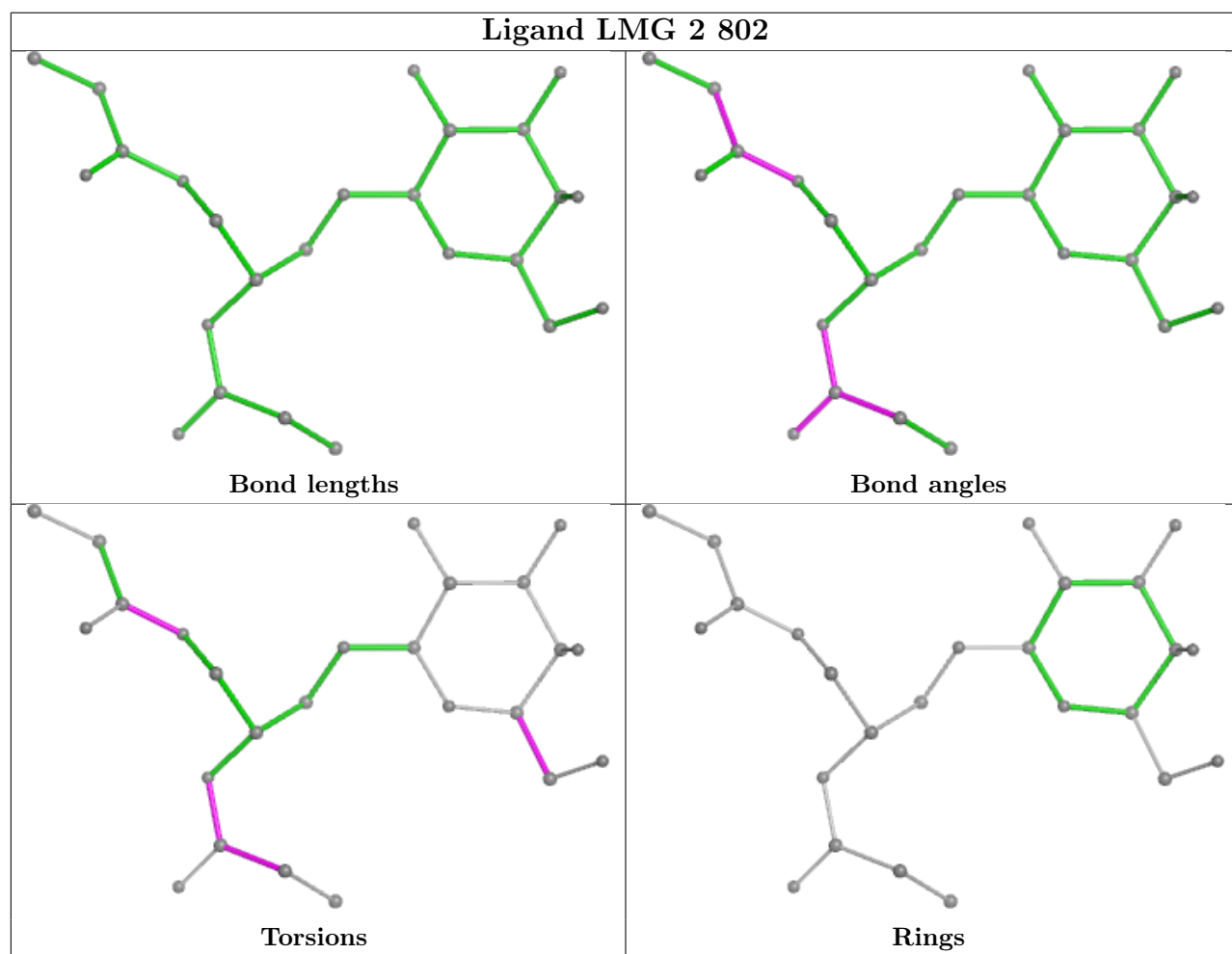
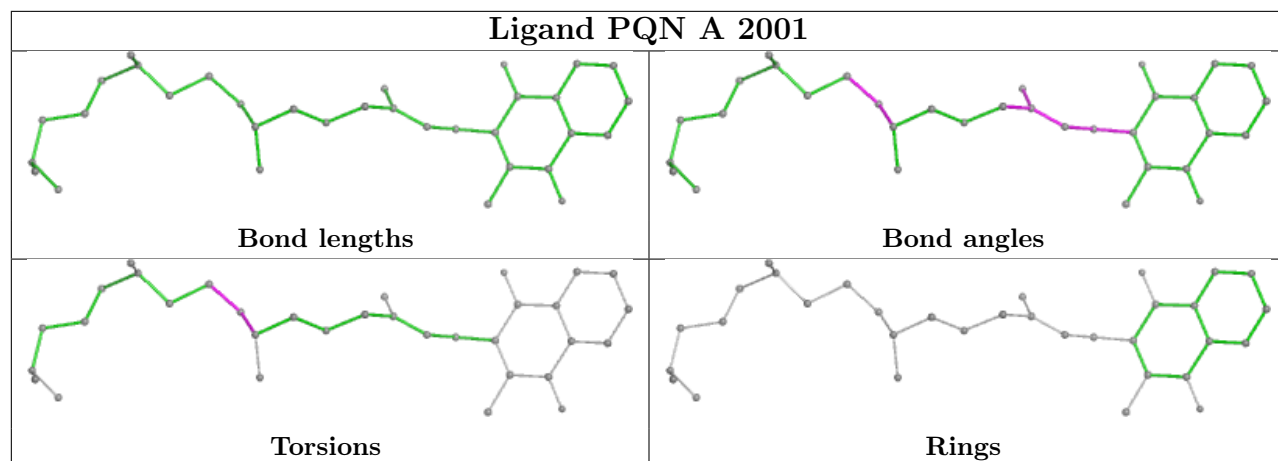
Rings

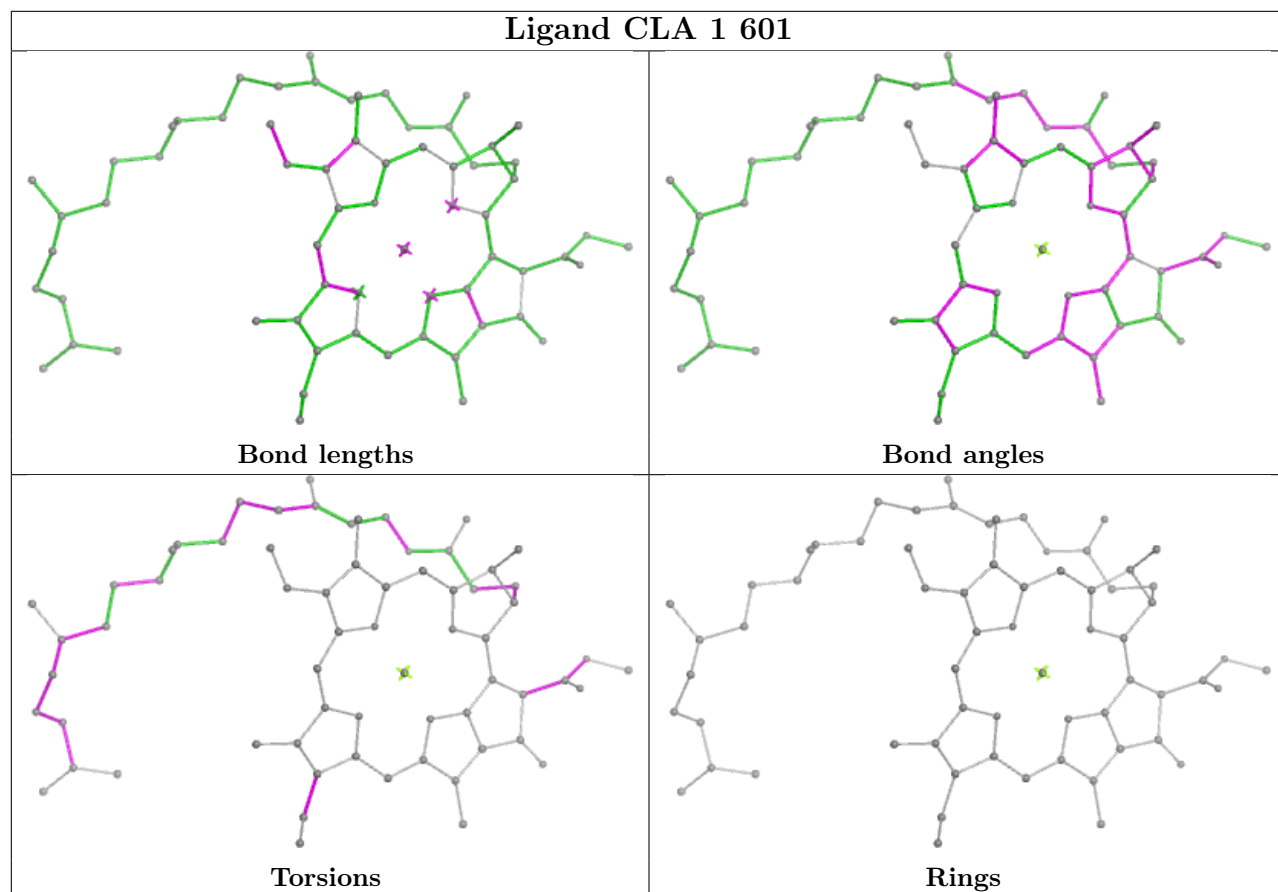
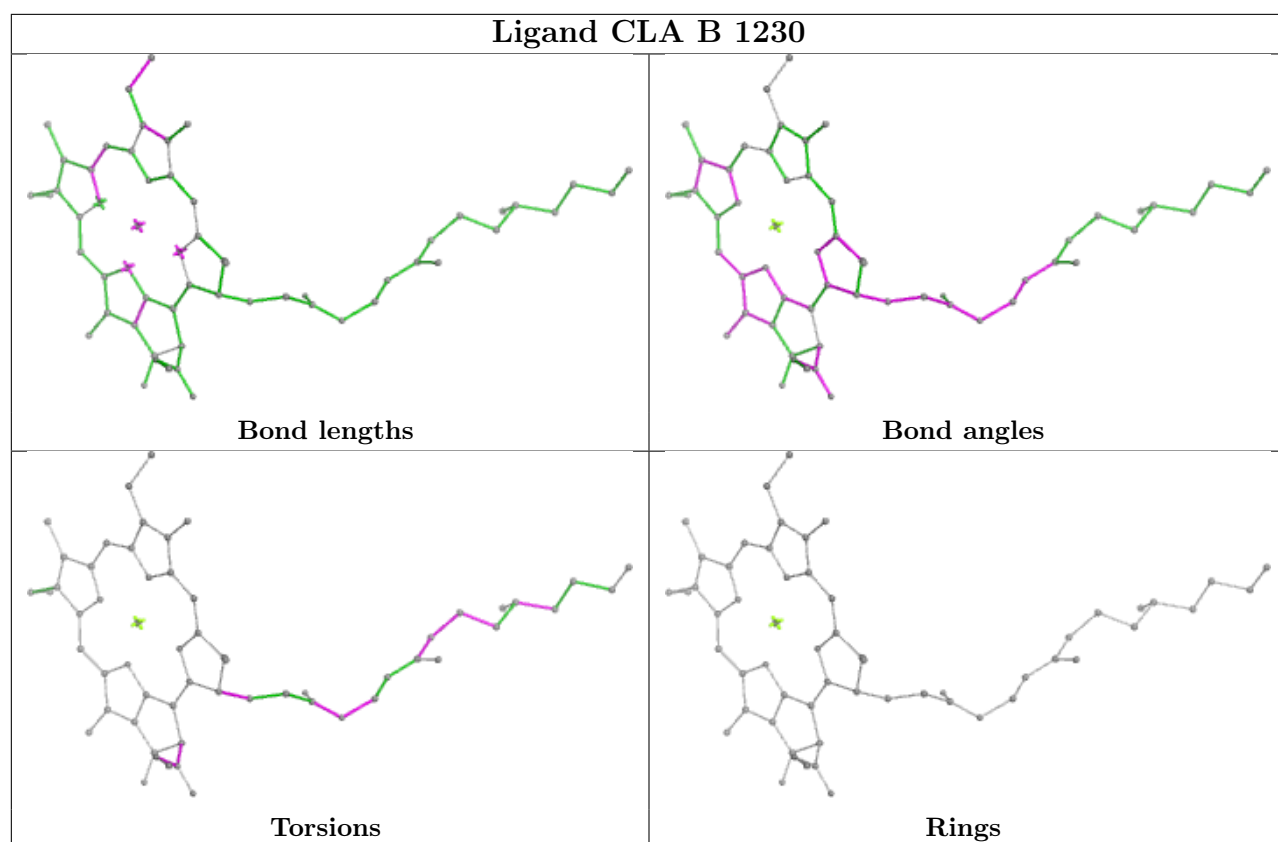


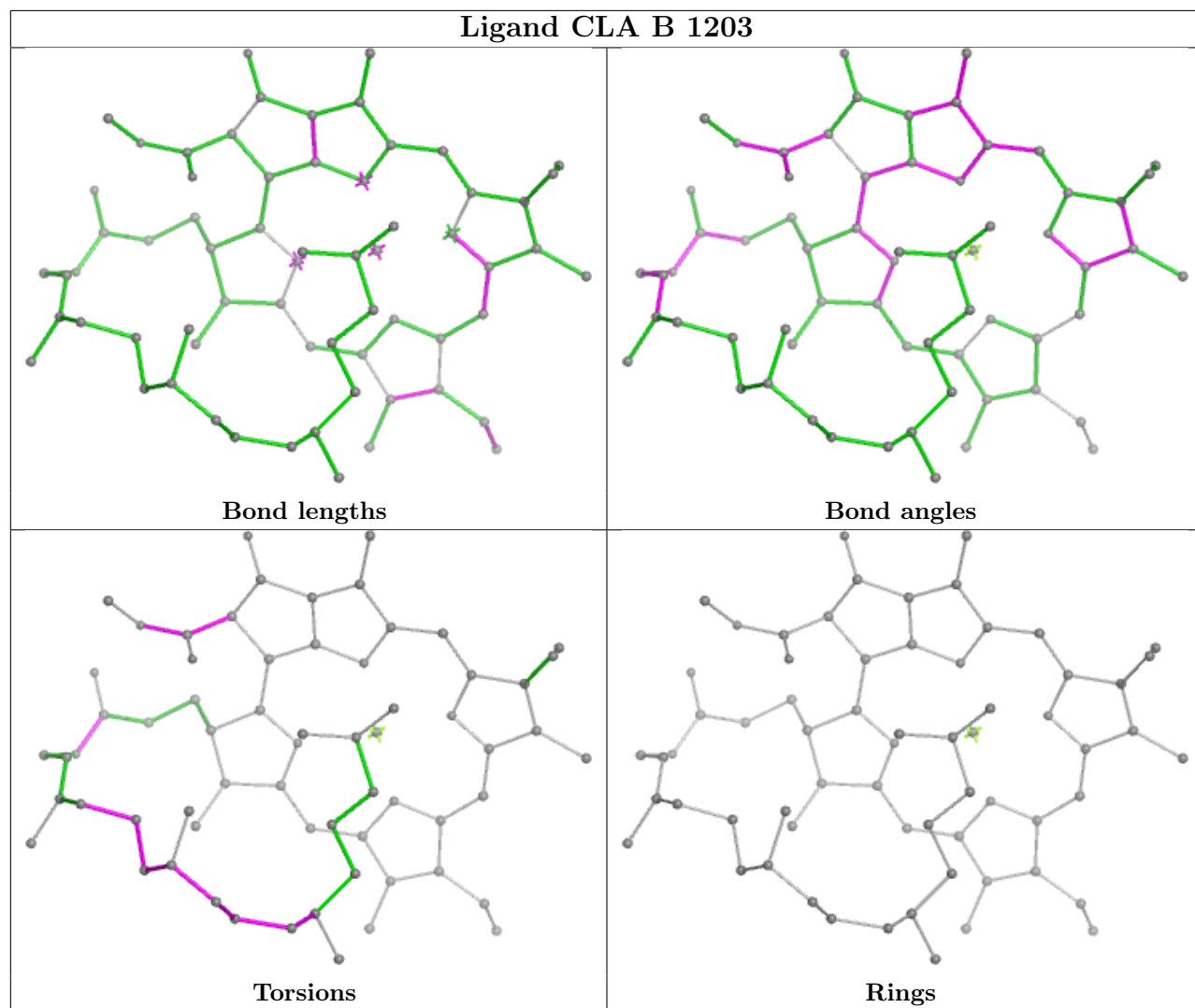


Ligand CLA 4 603**Ligand LMT G 5004**

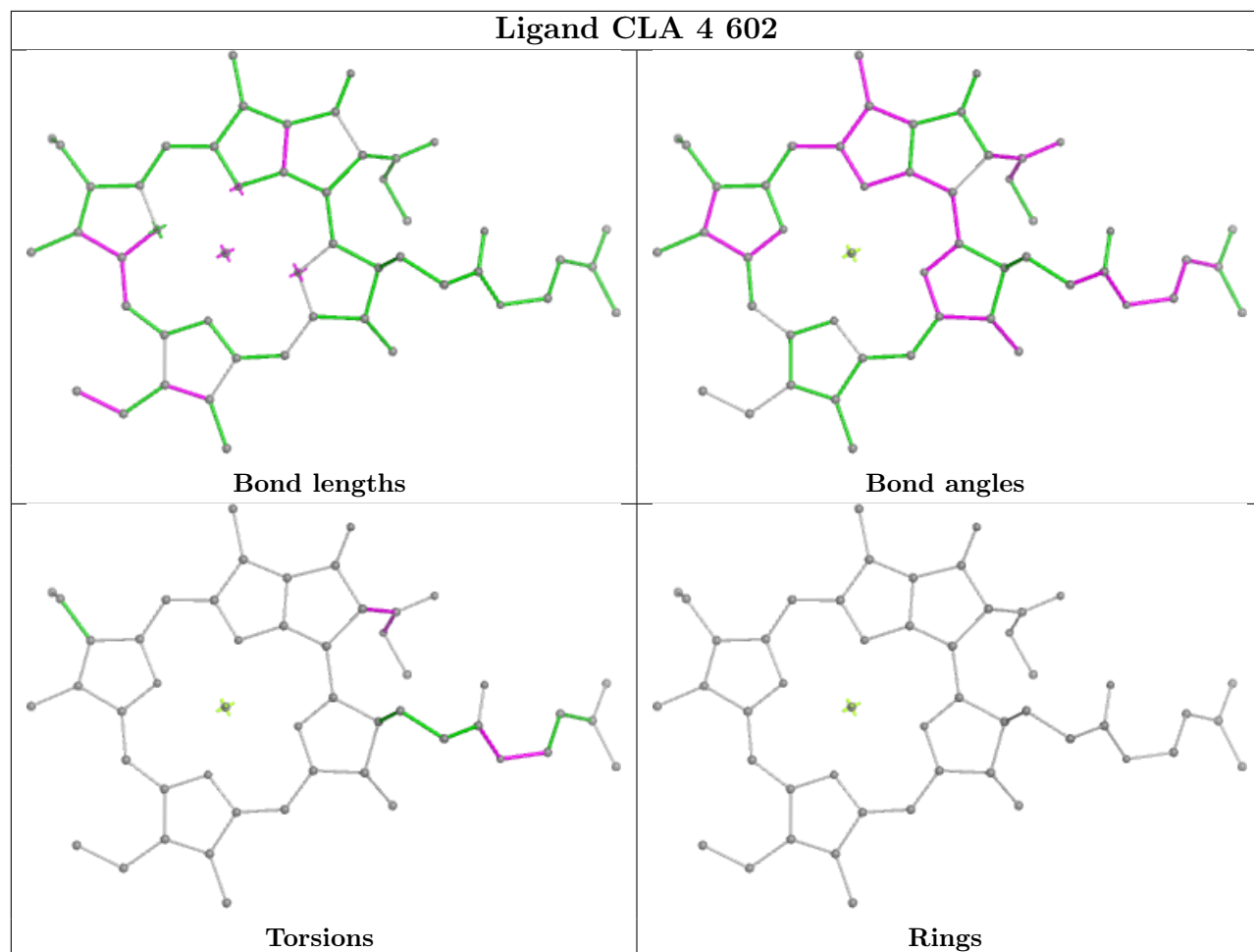


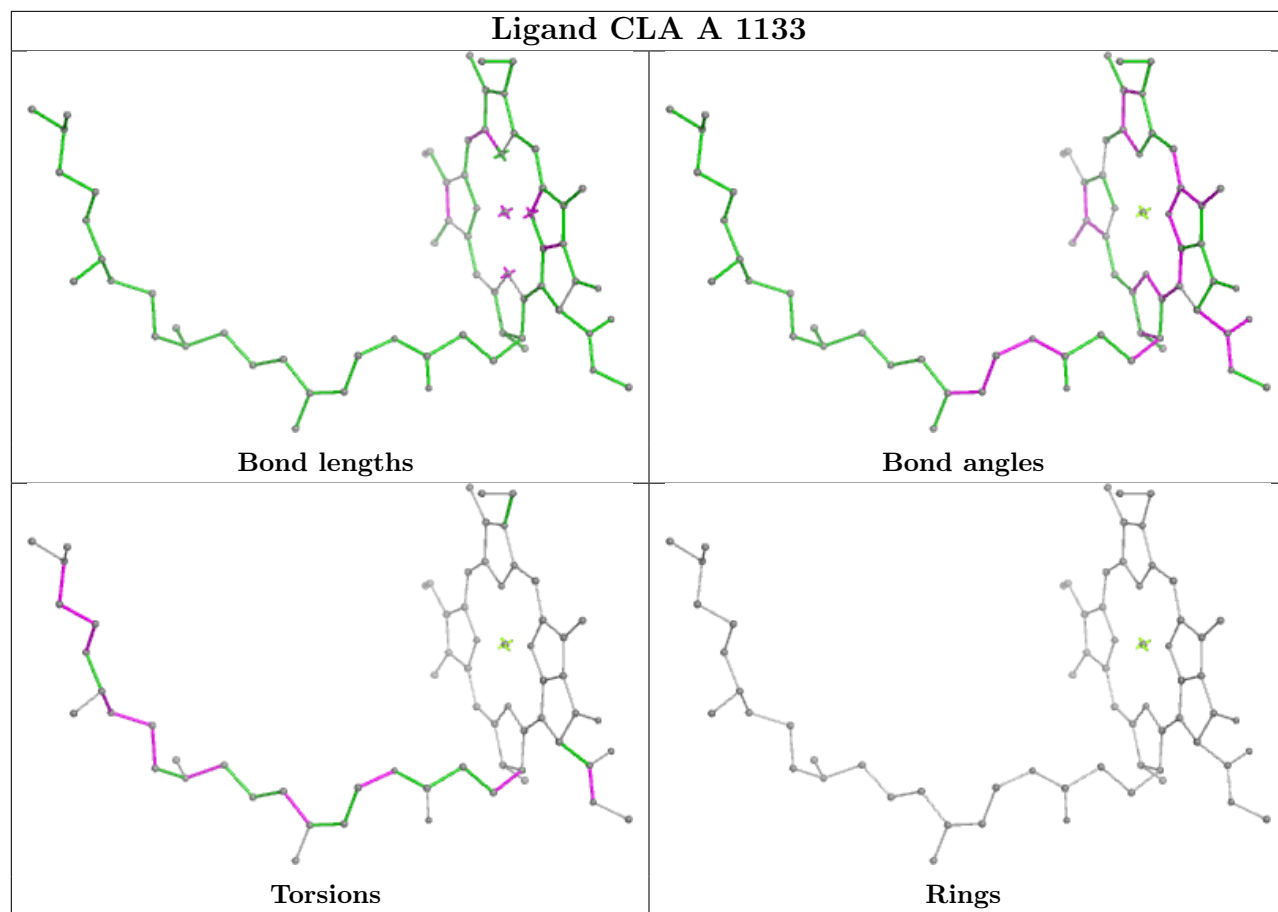




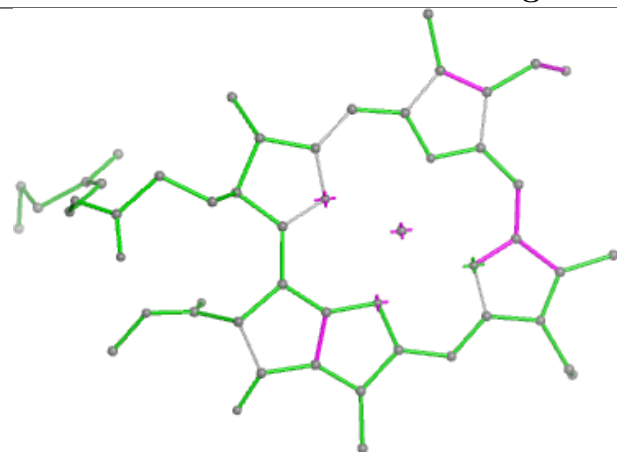


Ligand CLA 4 602

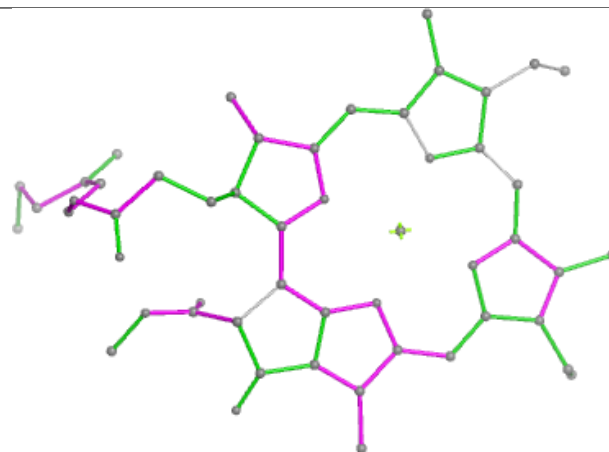




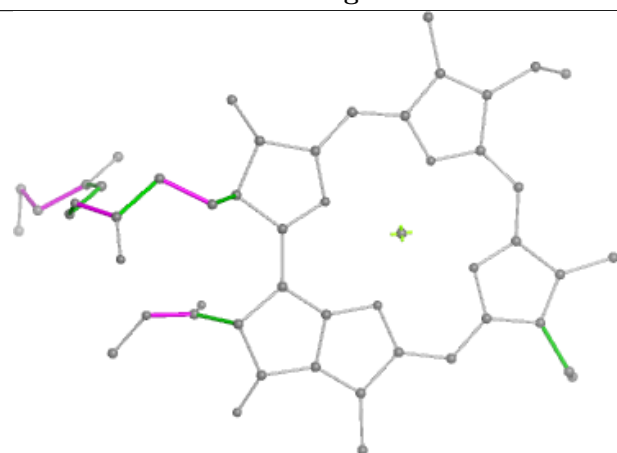
Ligand CLA 2 602



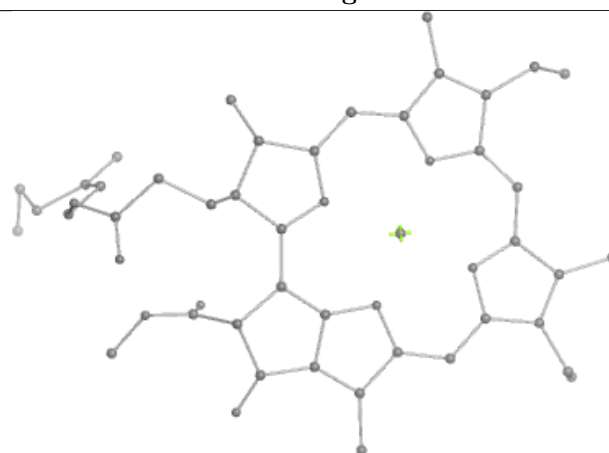
Bond lengths



Bond angles

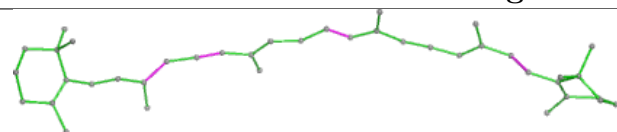


Torsions

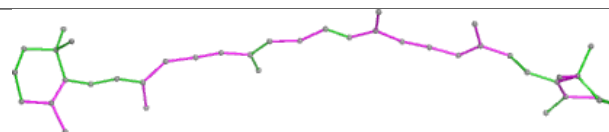


Rings

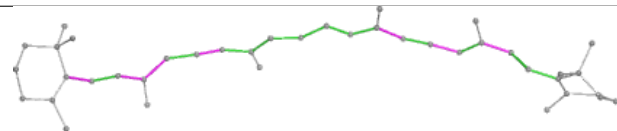
Ligand BCR K 4001



Bond lengths



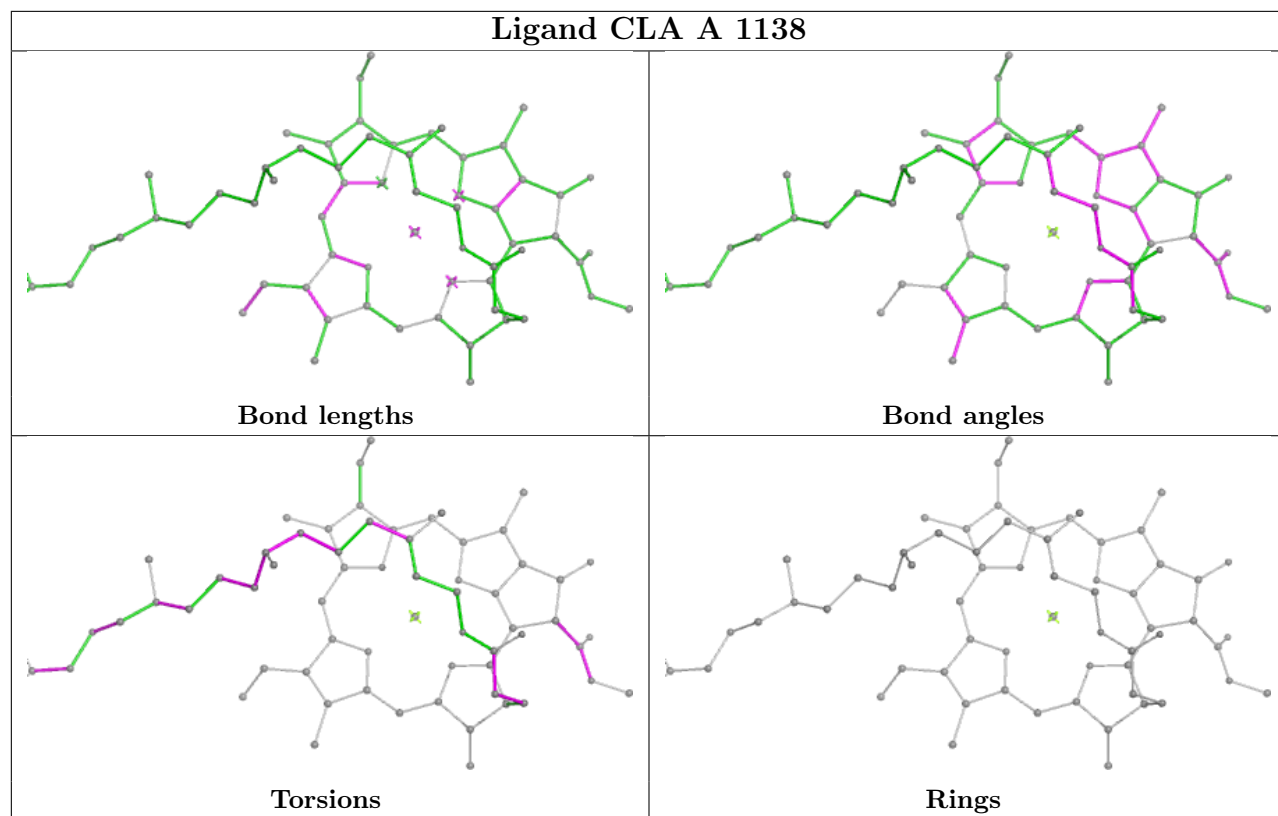
Bond angles



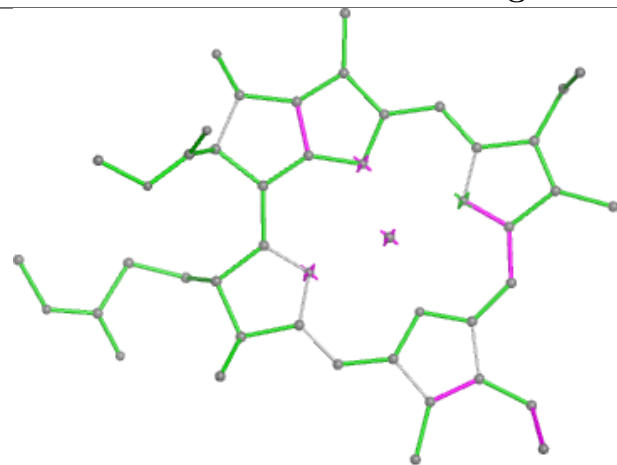
Torsions



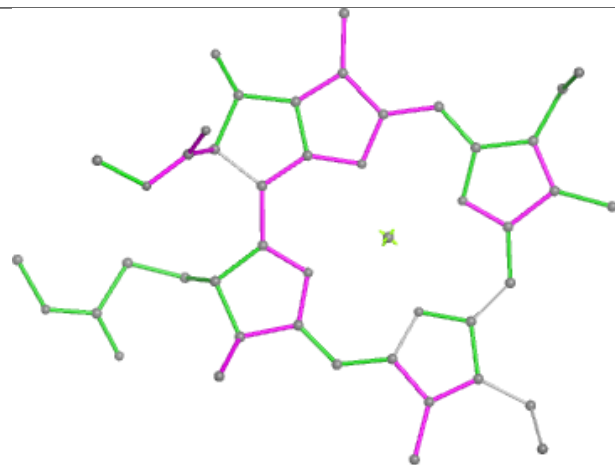
Rings



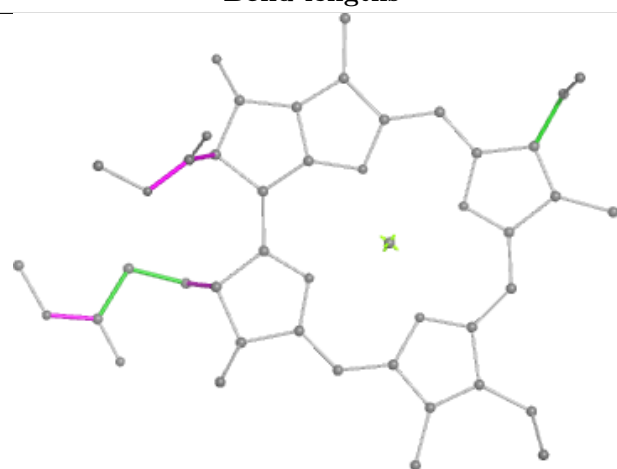
Ligand CLA G 1602



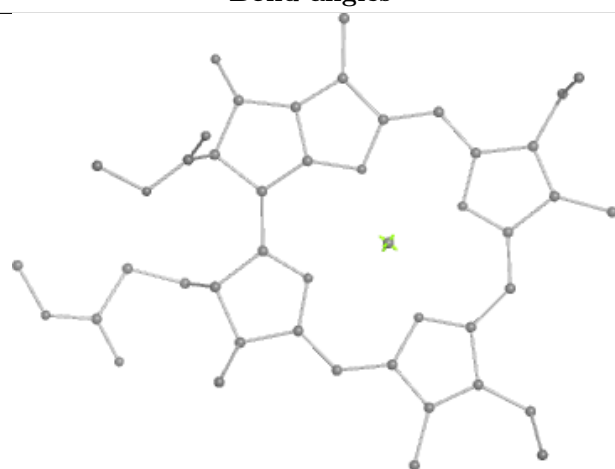
Bond lengths



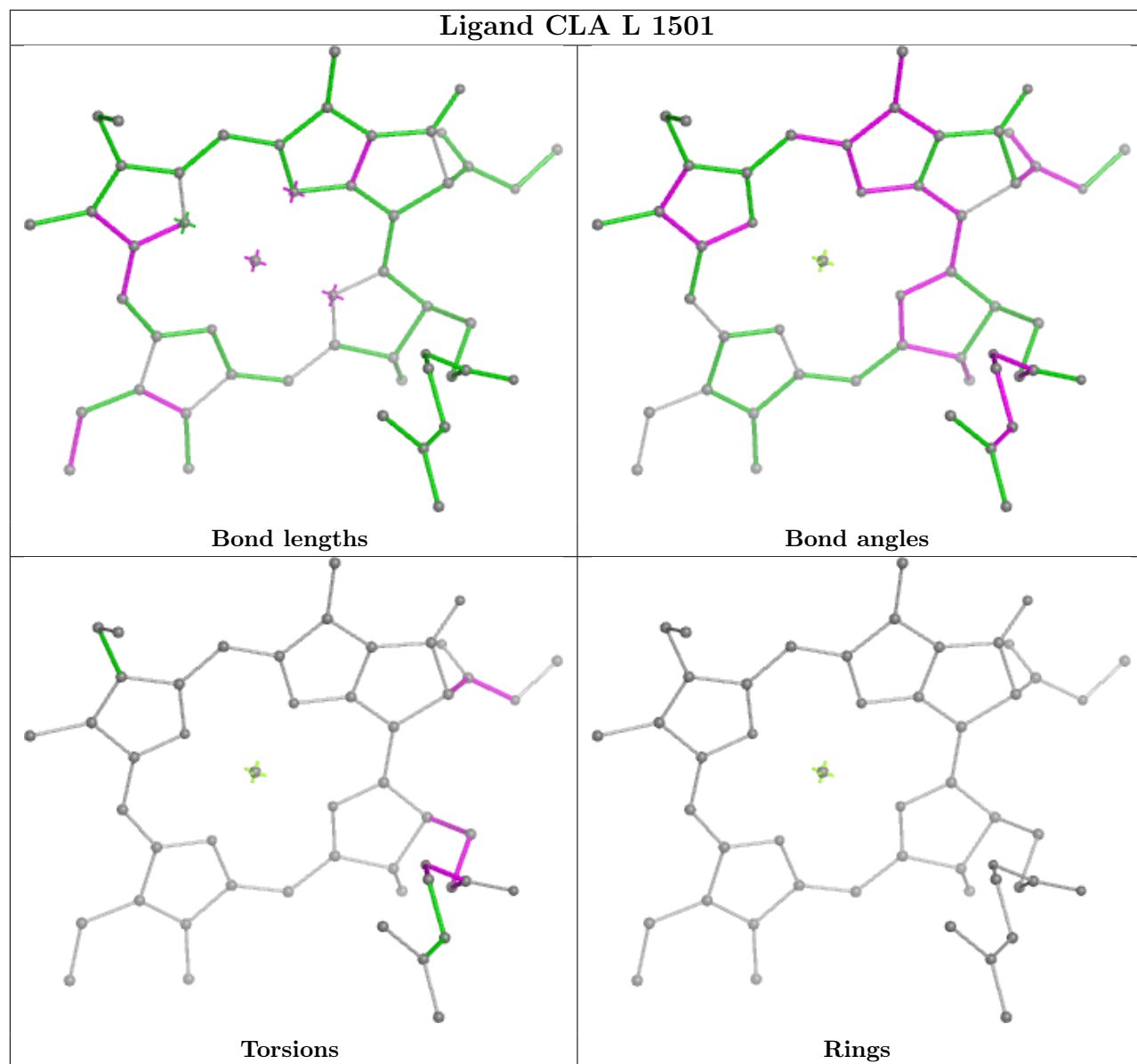
Bond angles



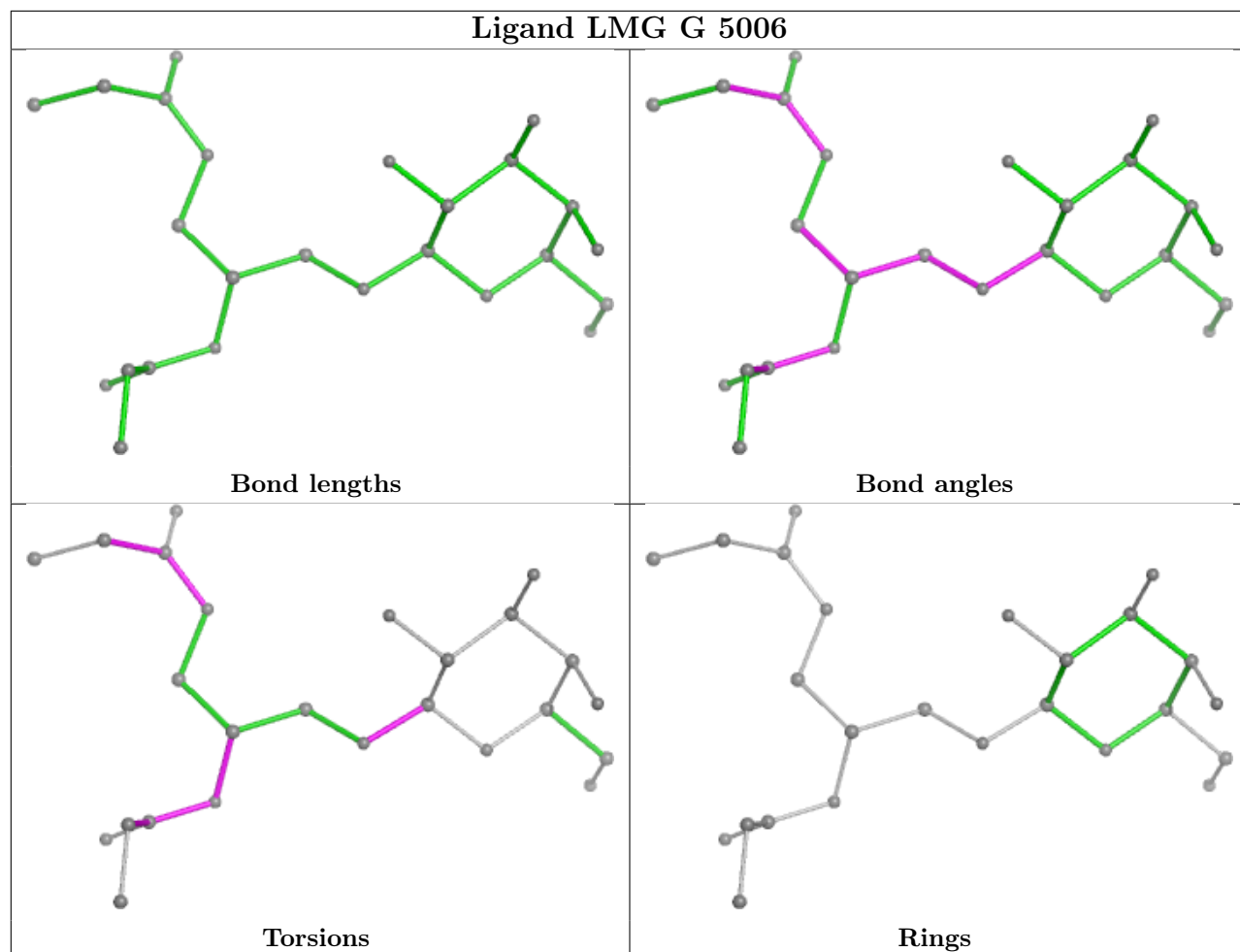
Torsions



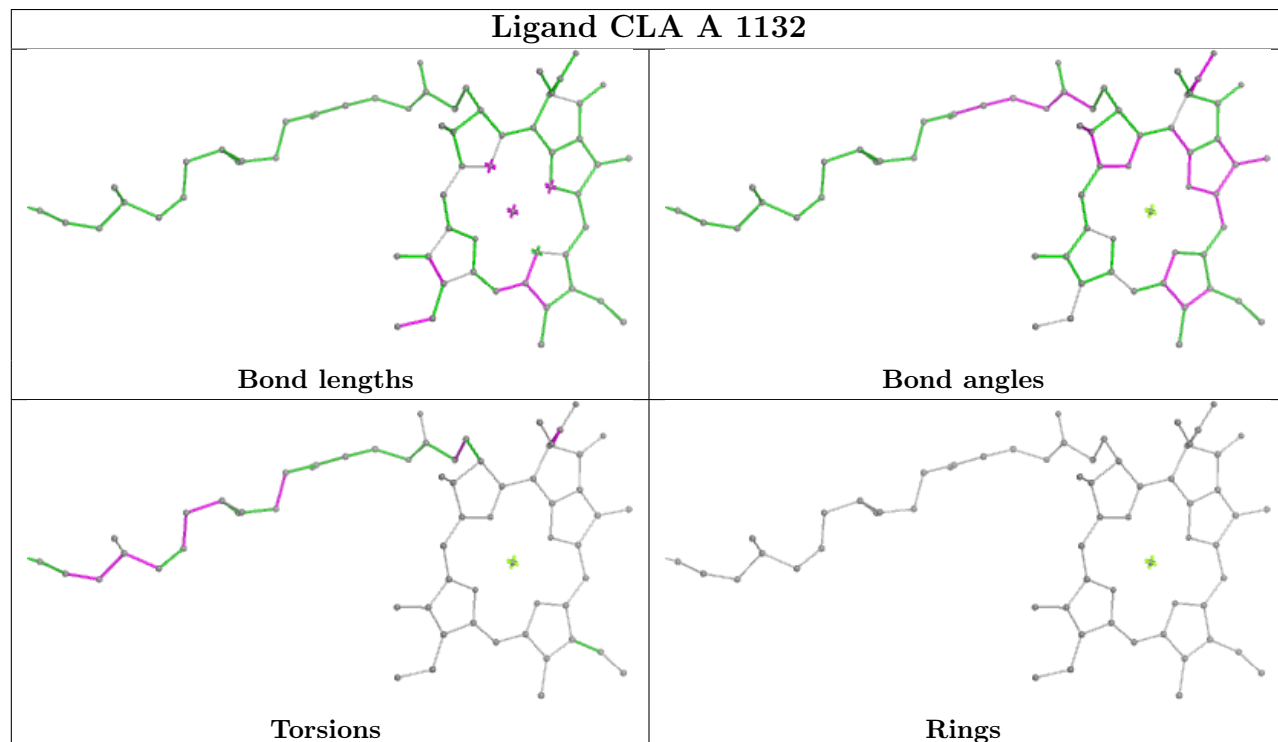
Rings

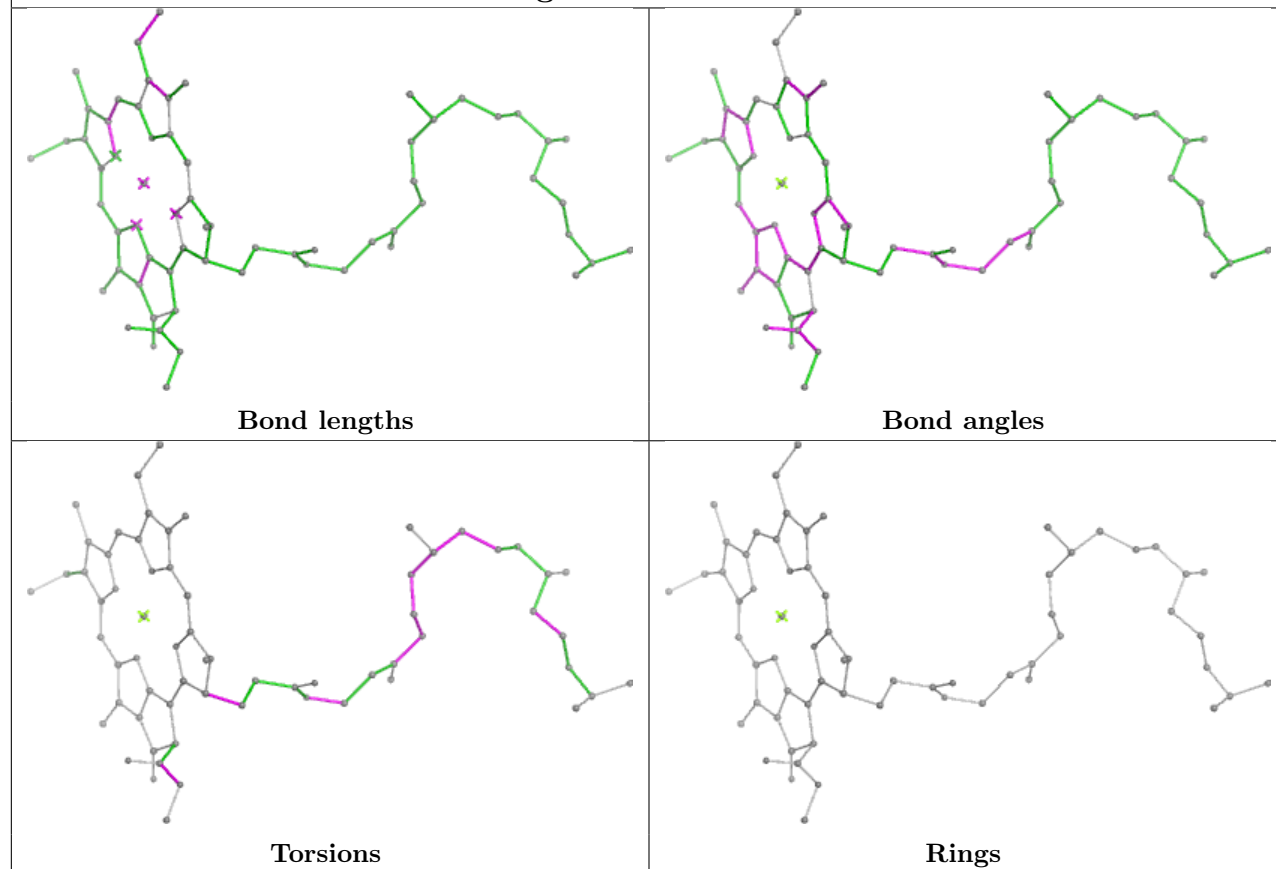
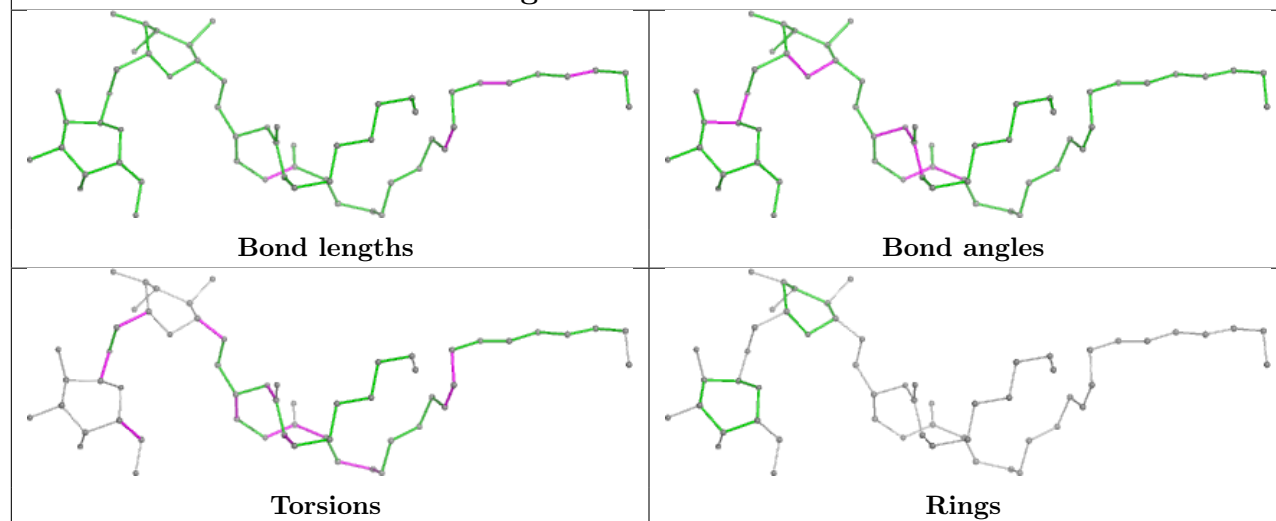


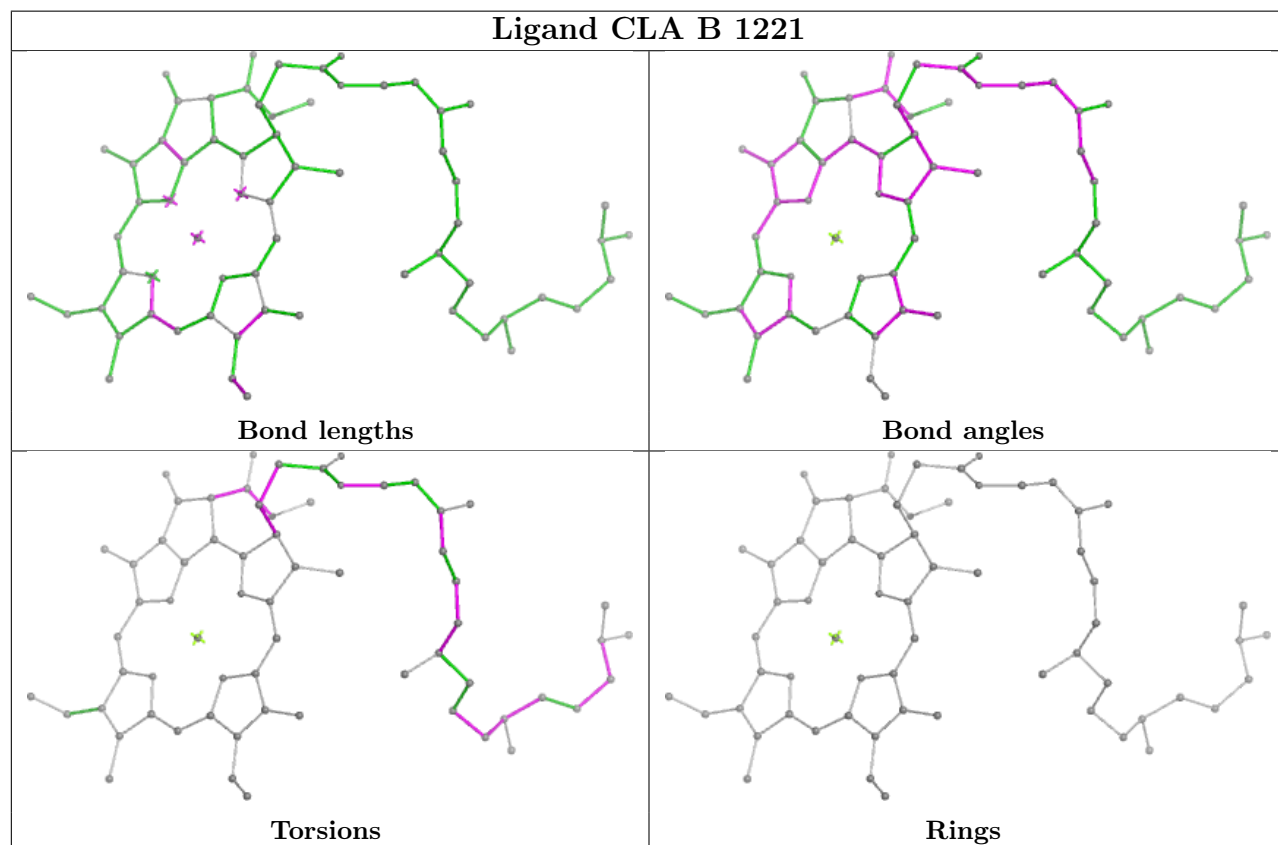
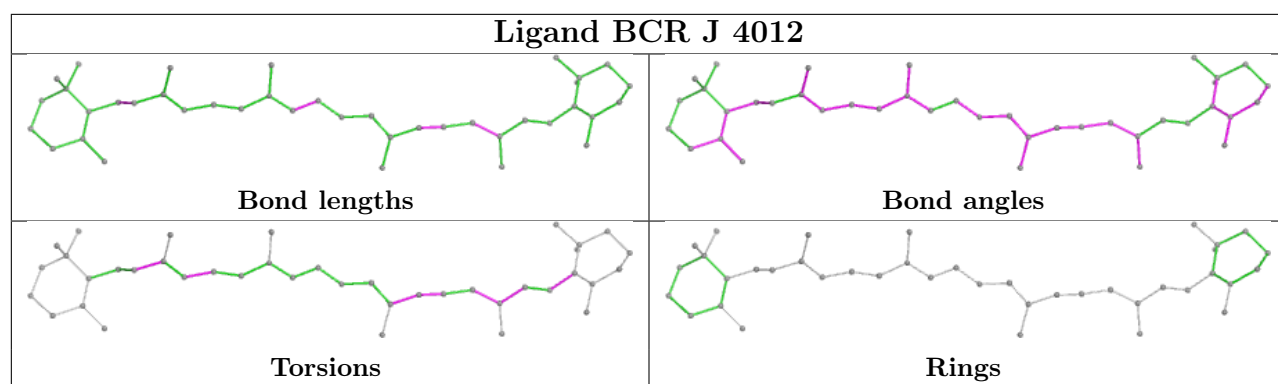
Ligand LMG G 5006

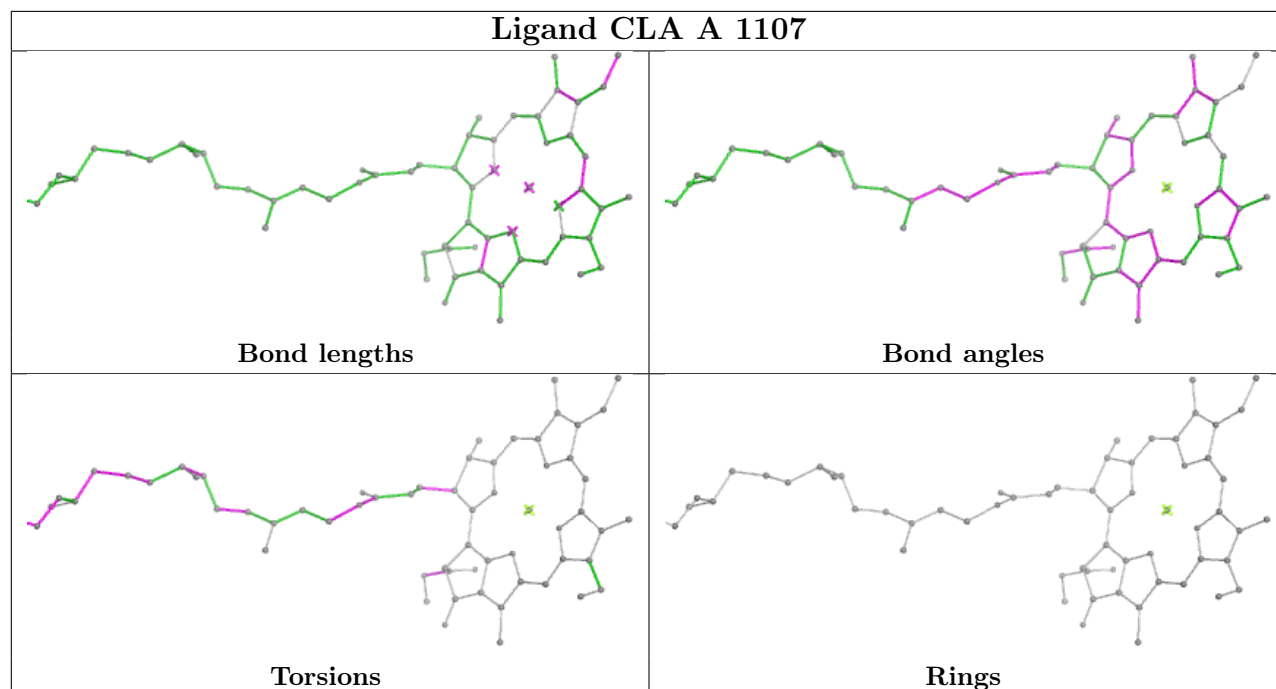
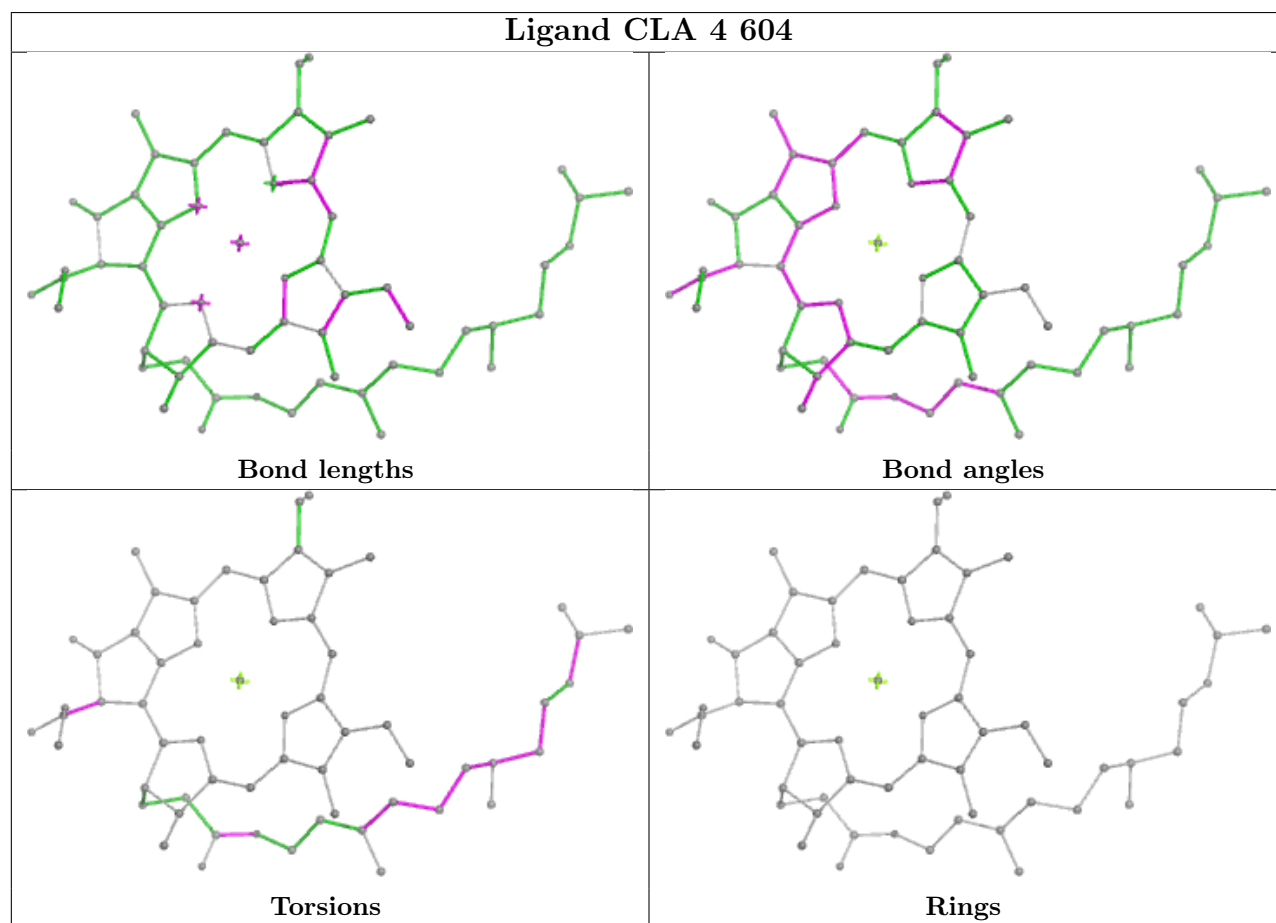


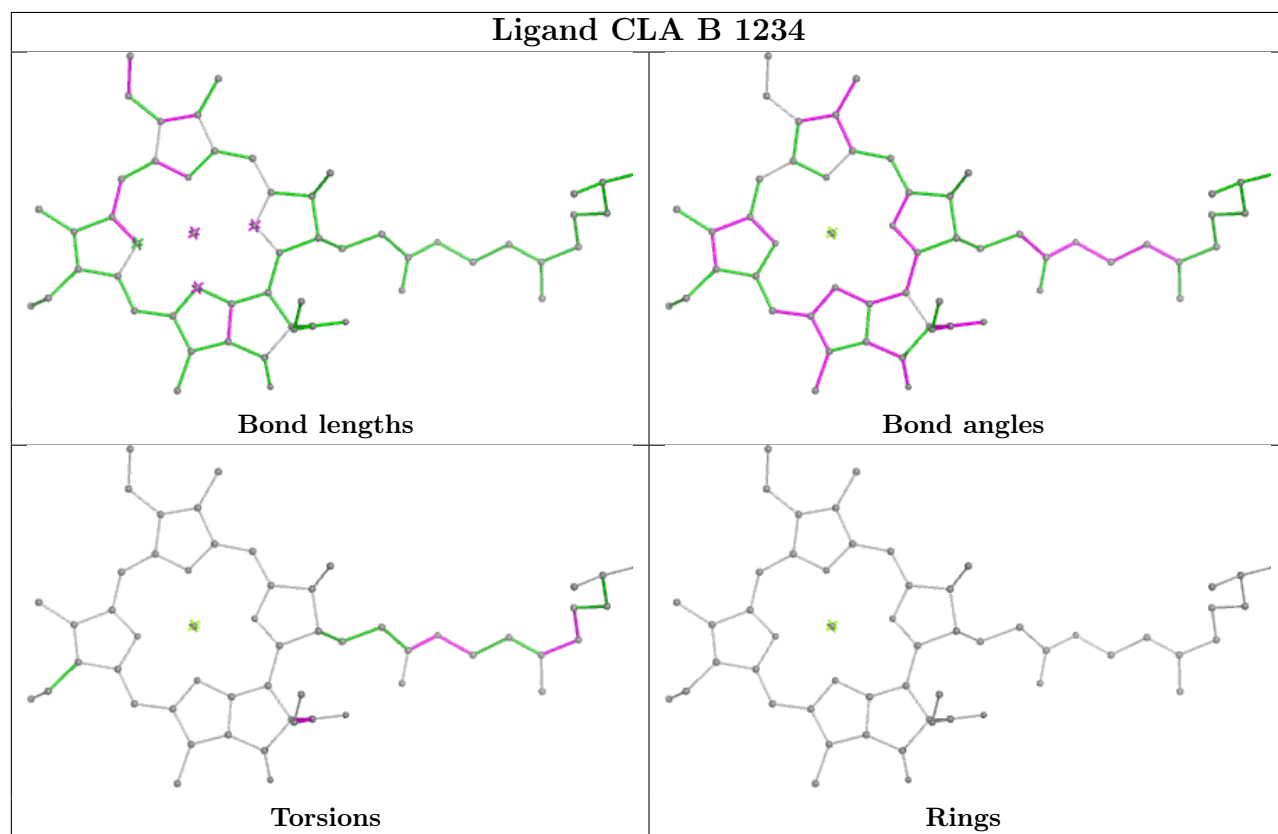
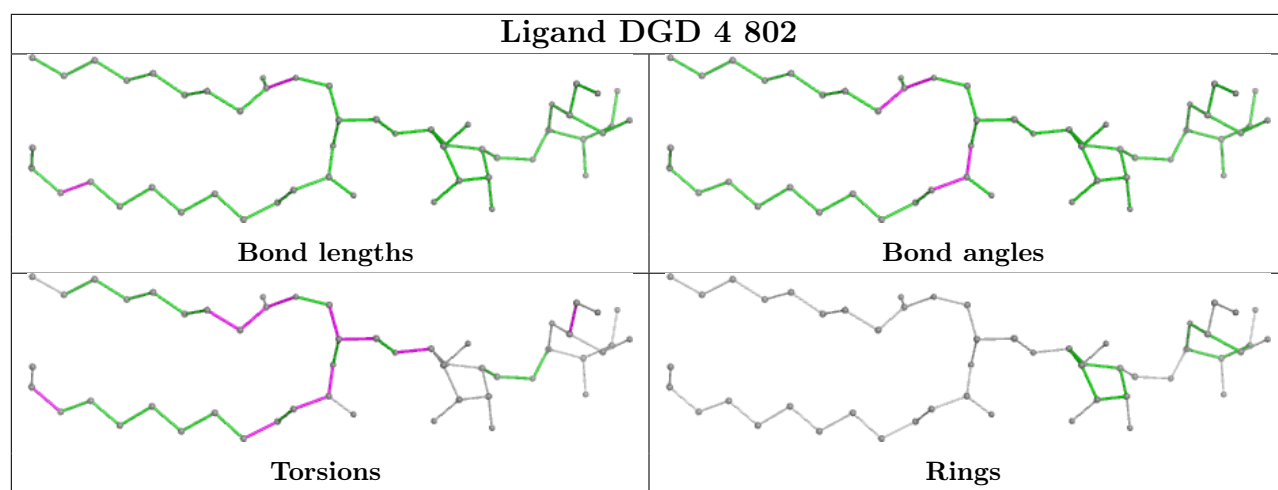
Ligand CLA A 1132

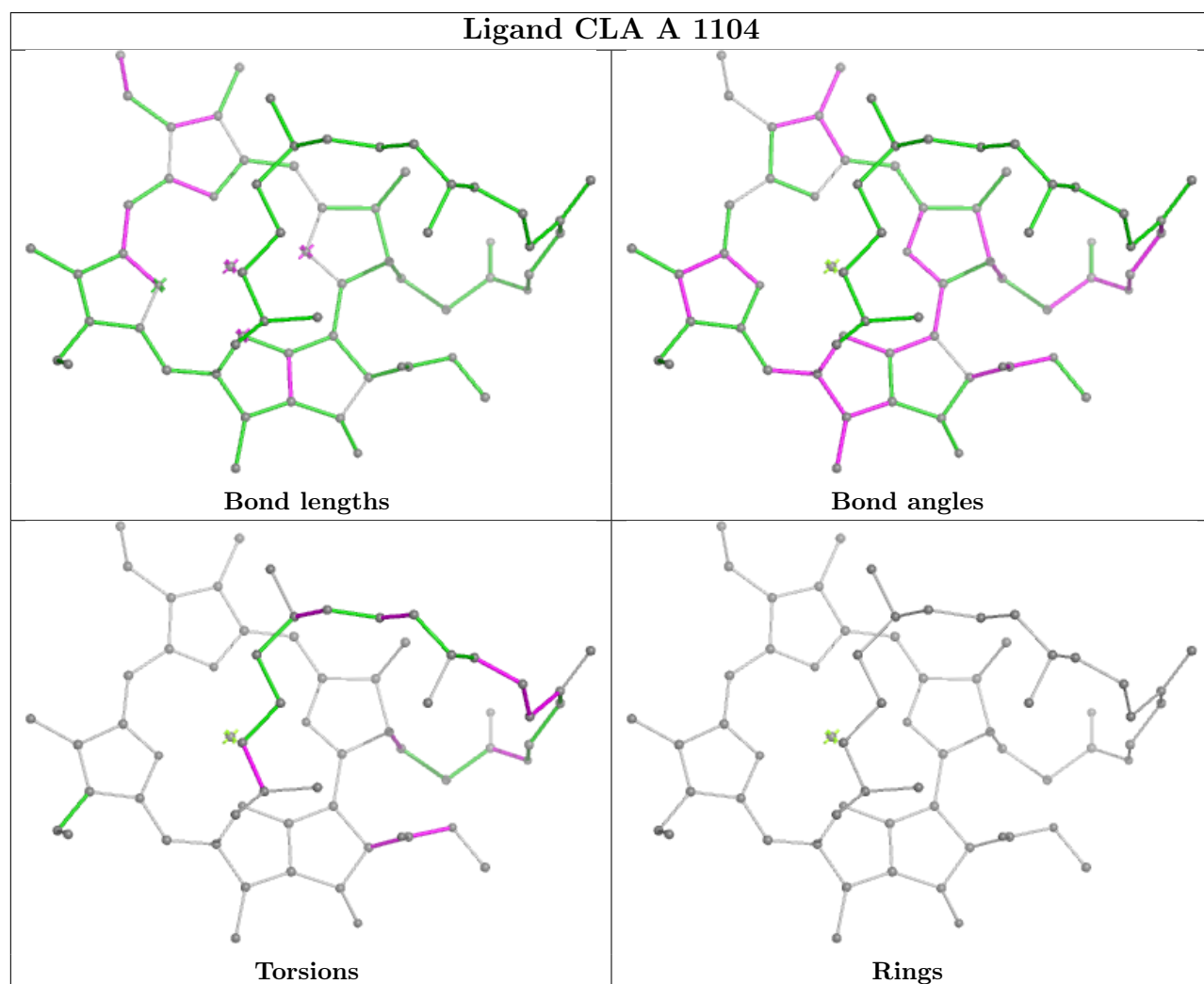
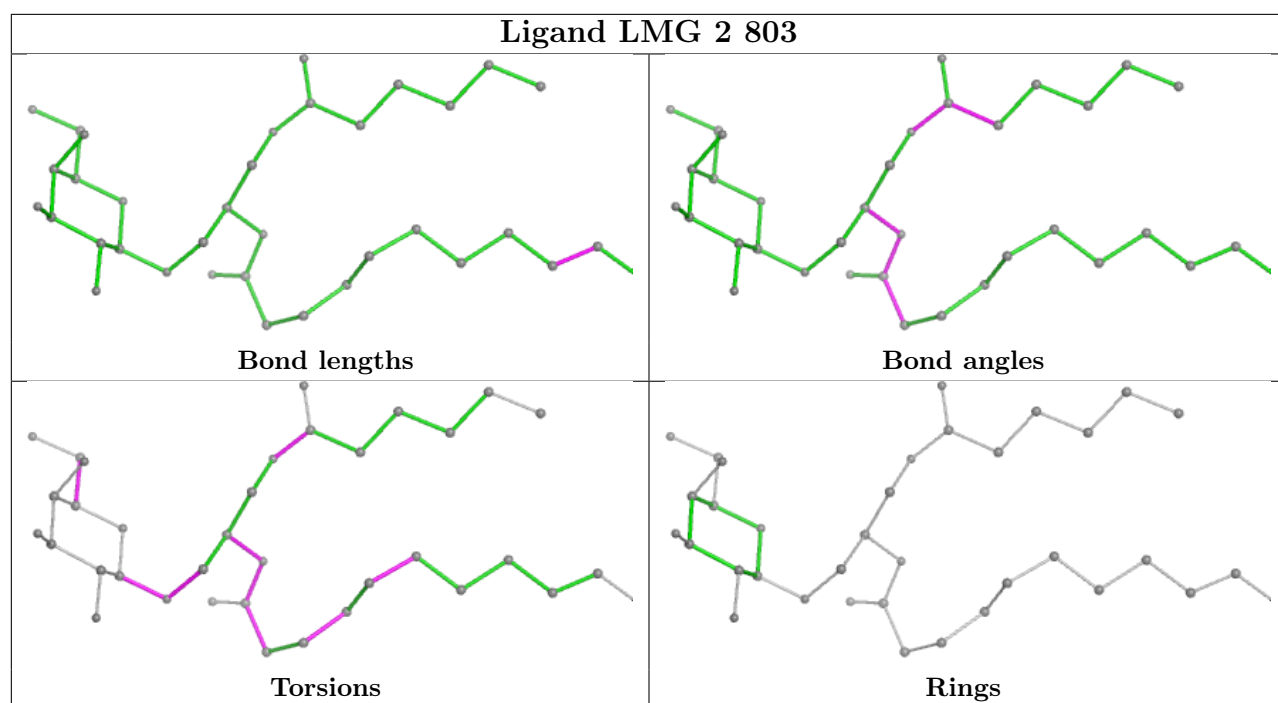


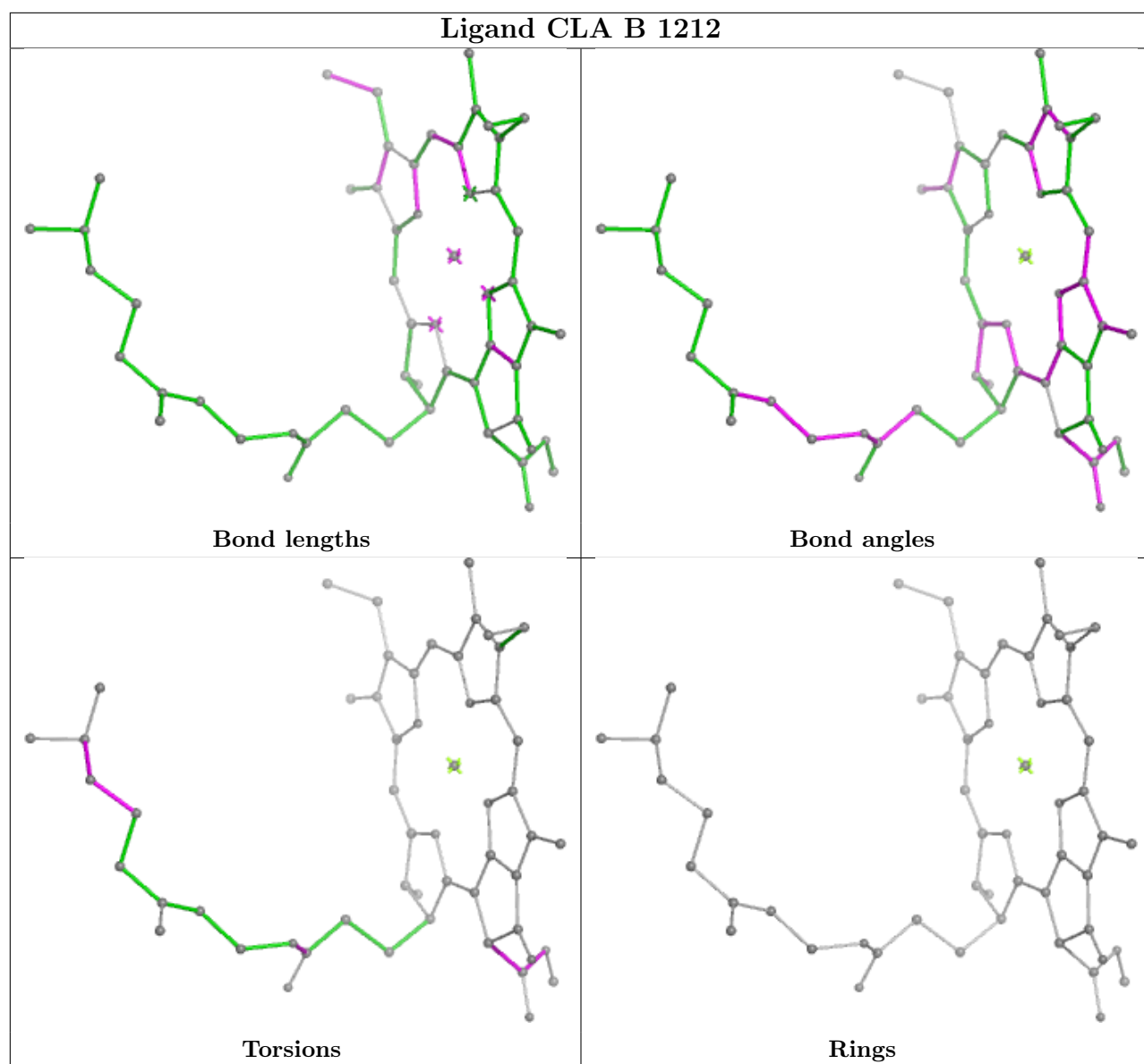
Ligand CLA 1 611**Ligand DGD F 5005**

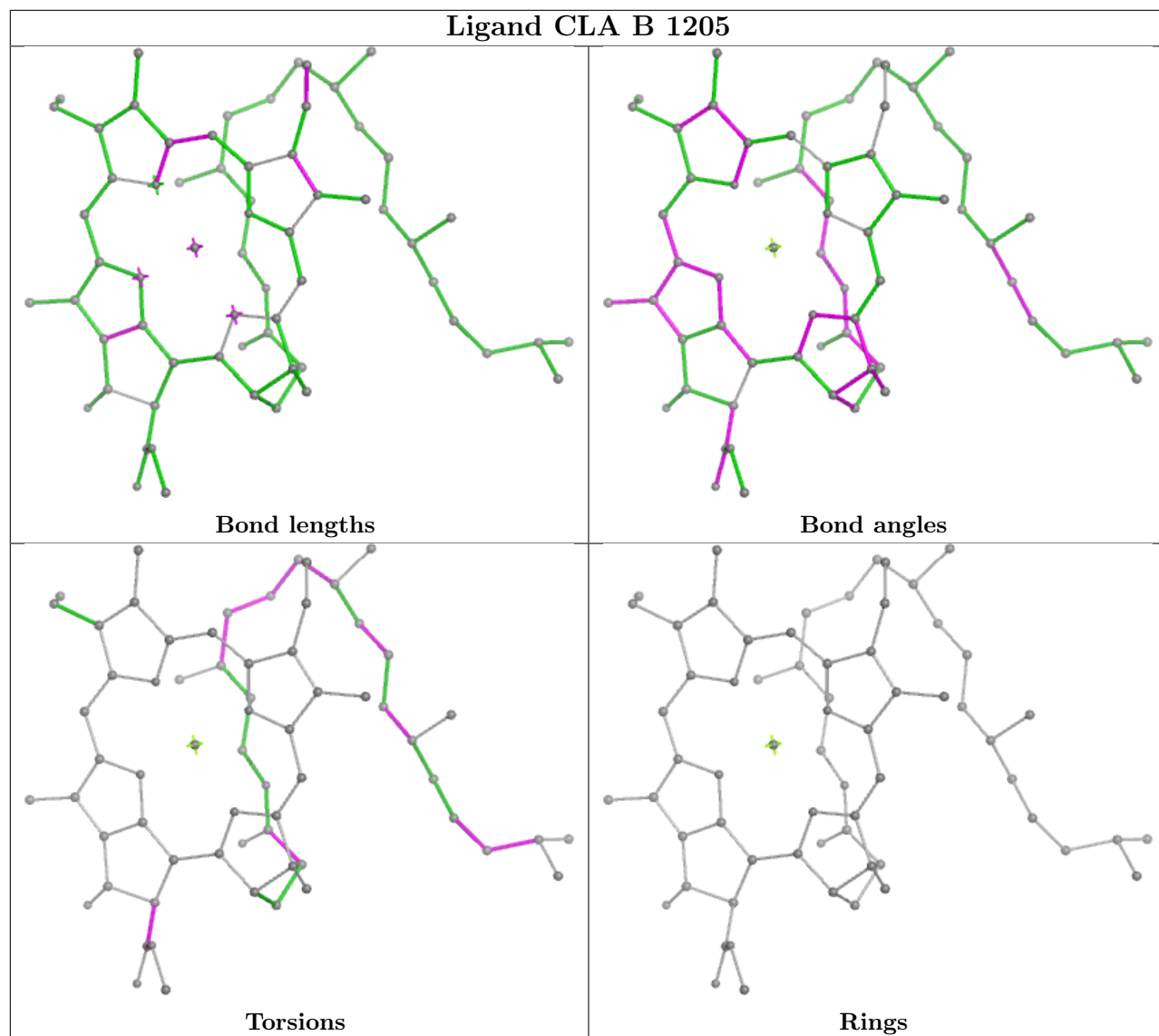


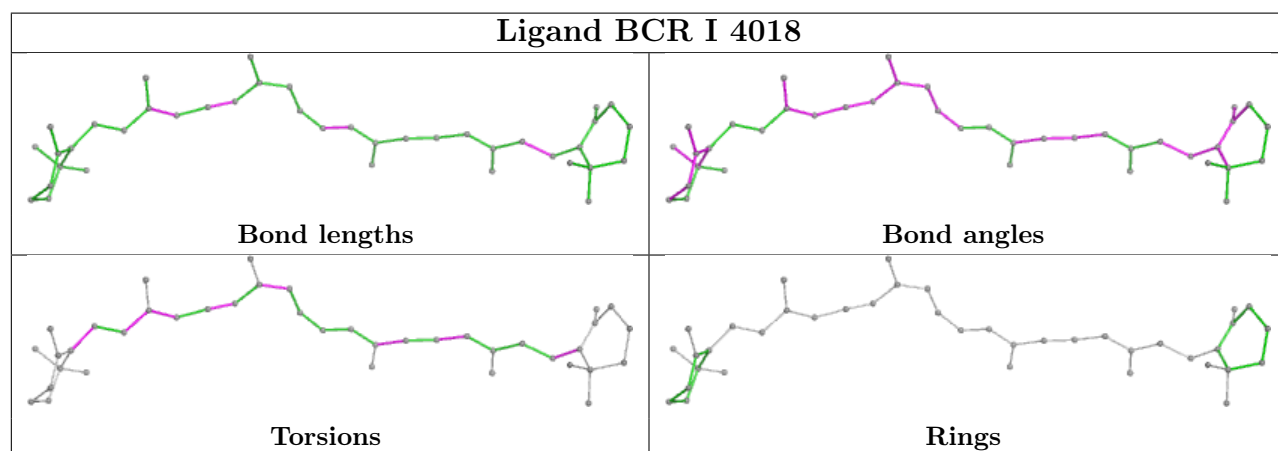
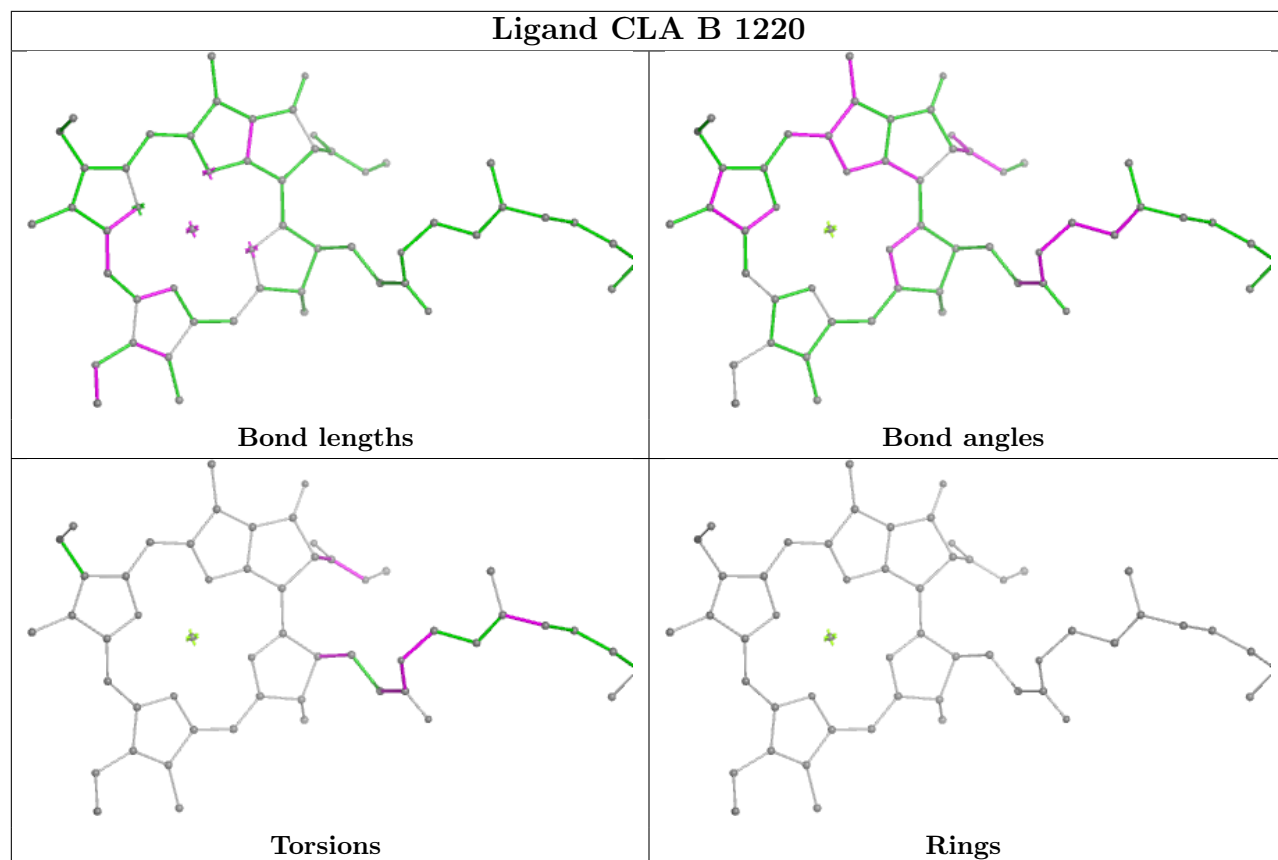
Ligand CLA A 1107**Ligand CLA 4 604**

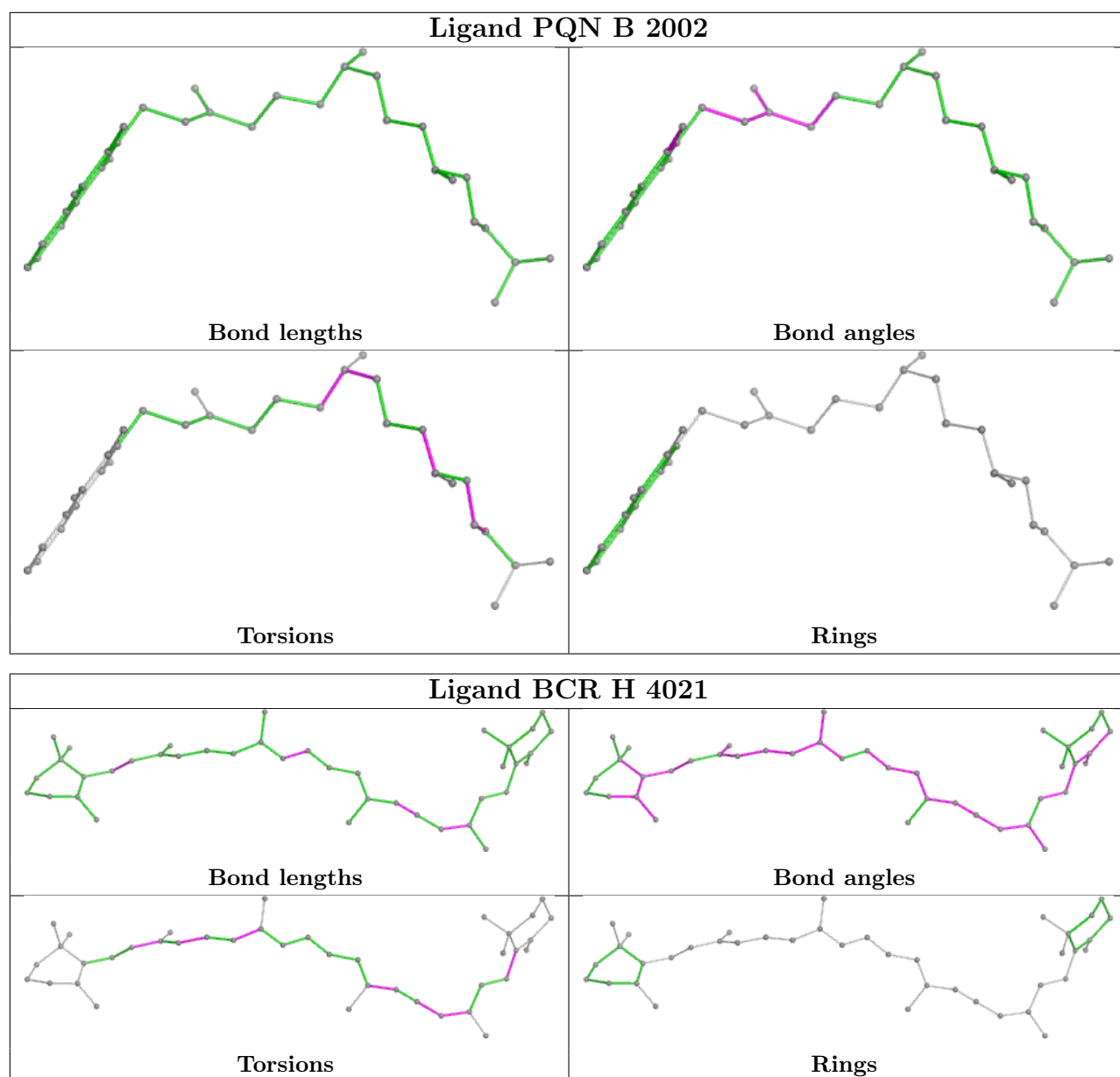


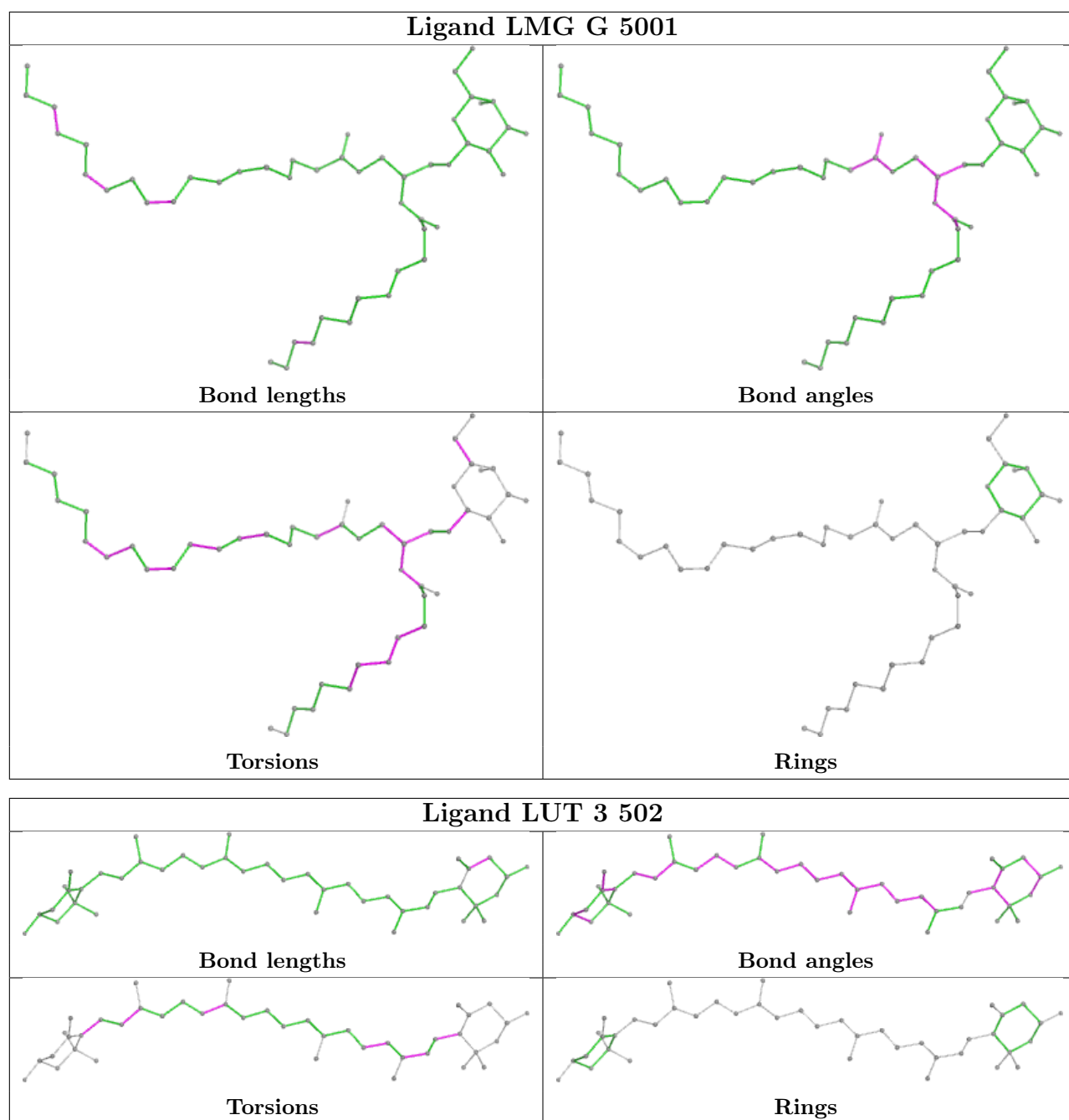




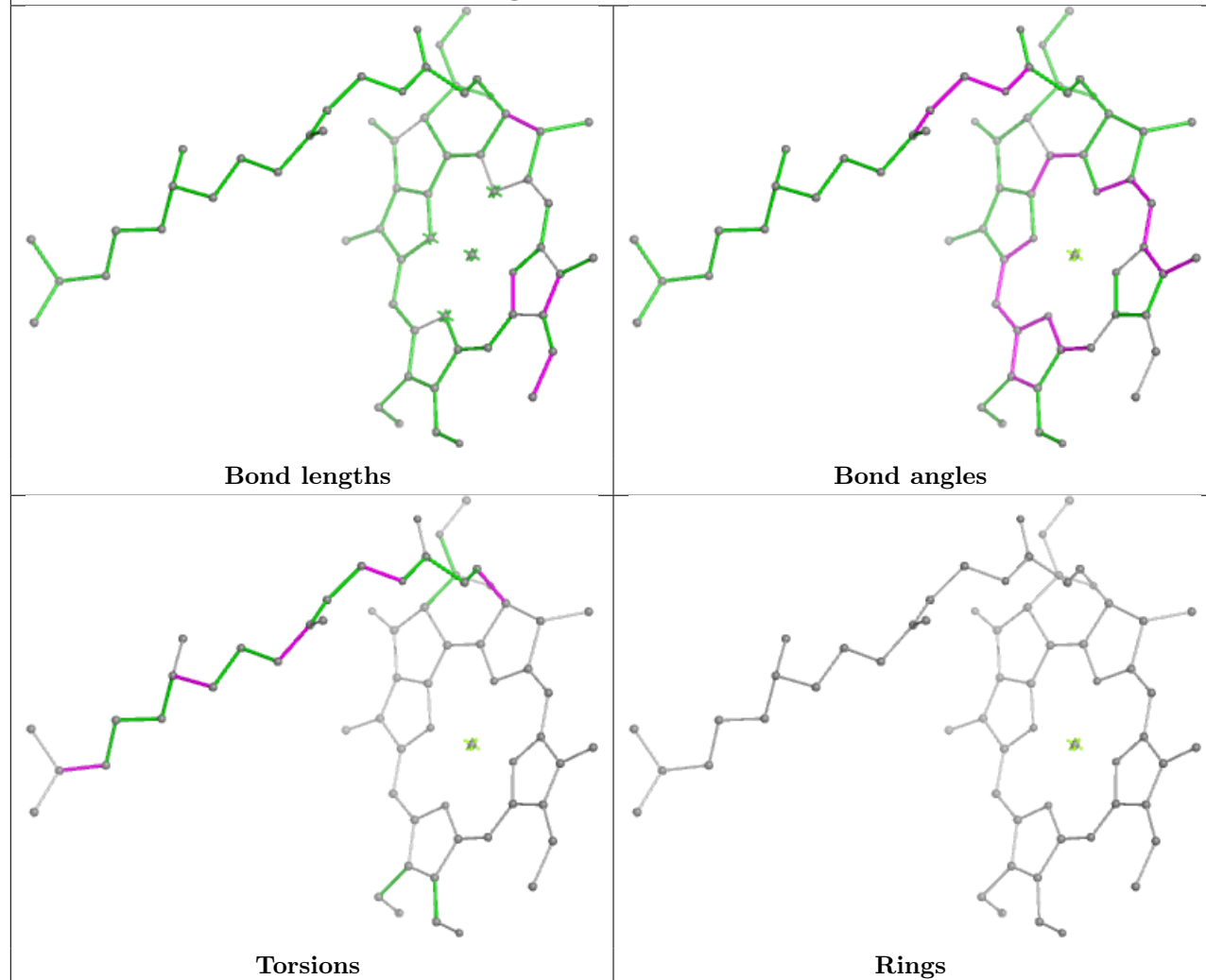




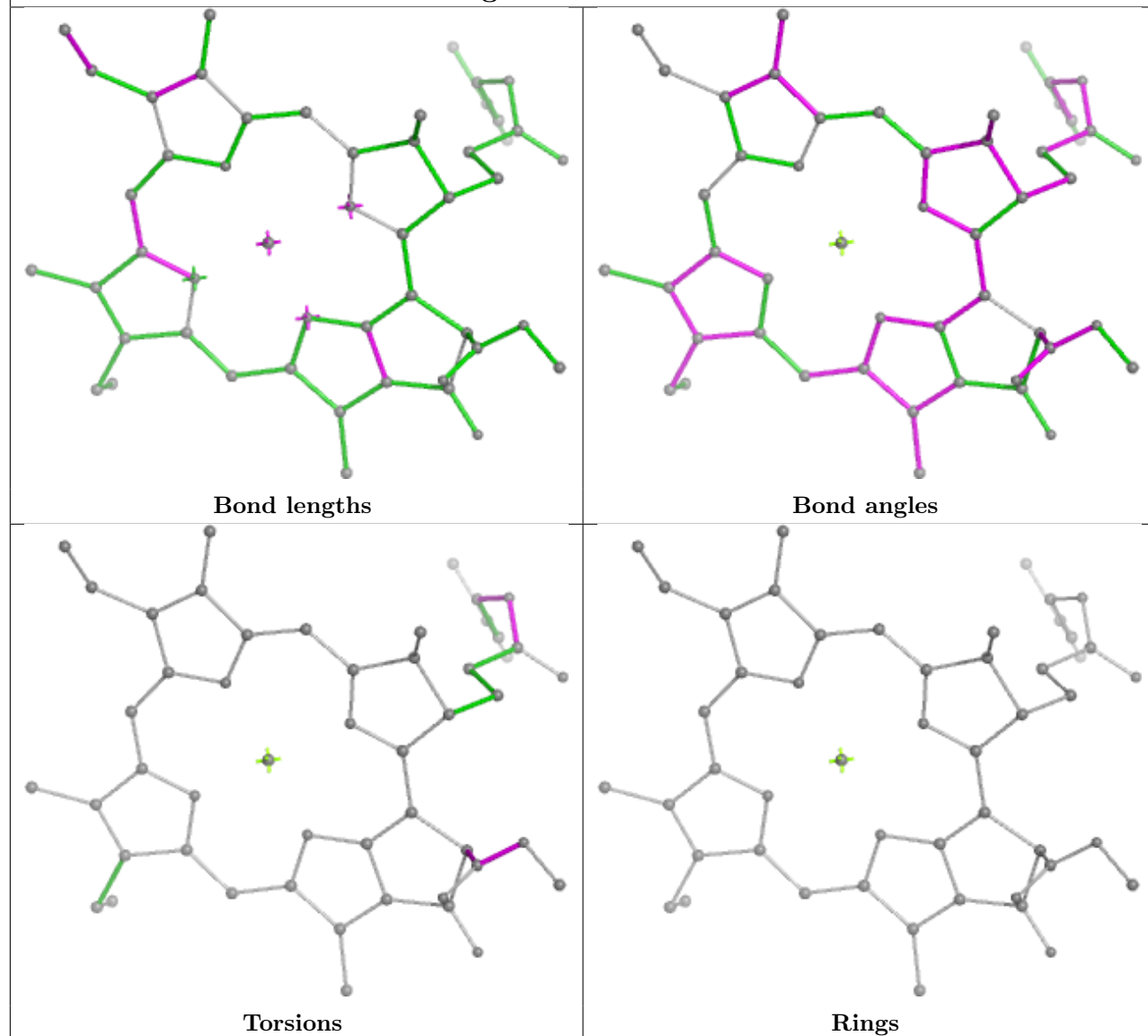


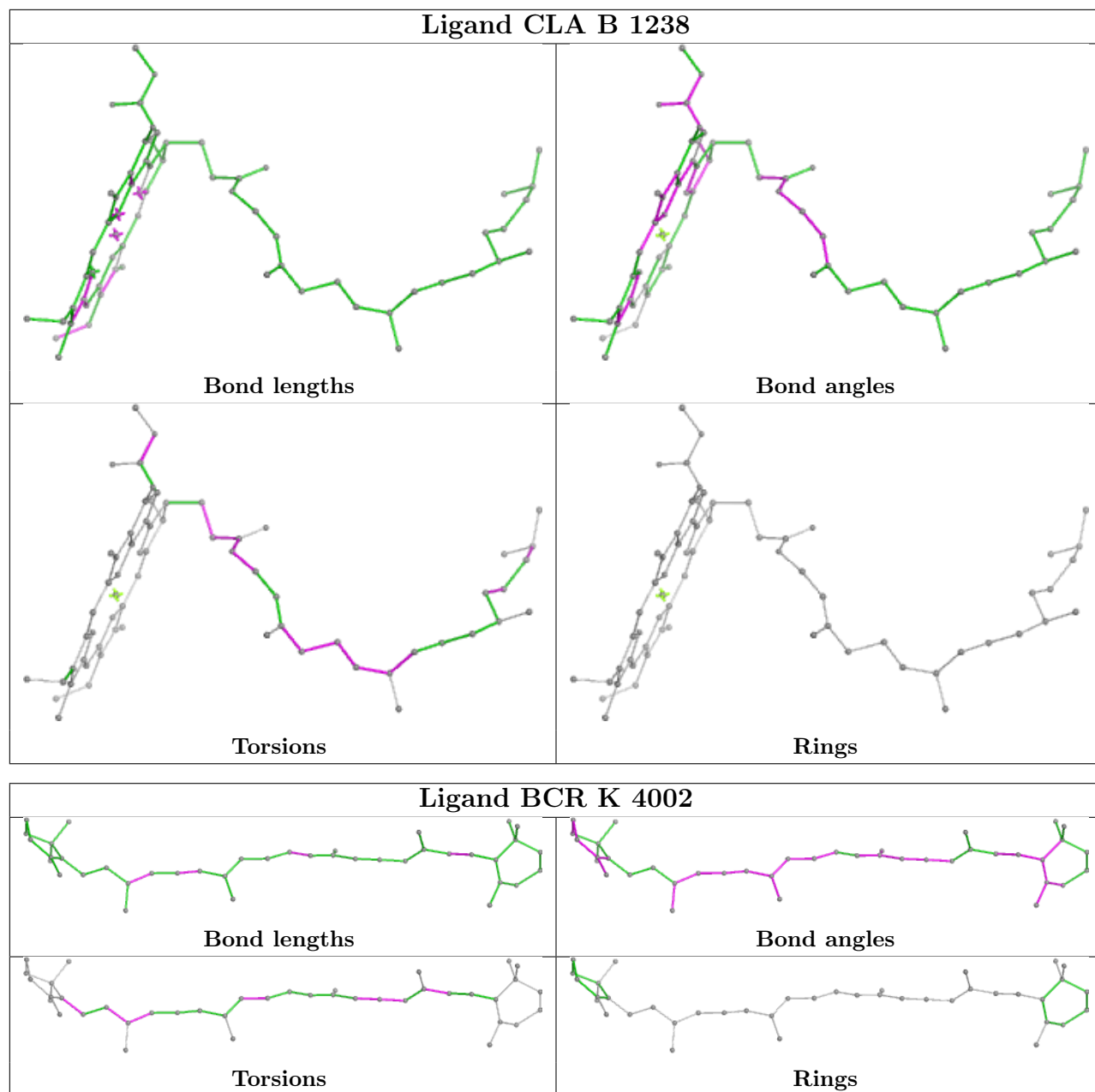


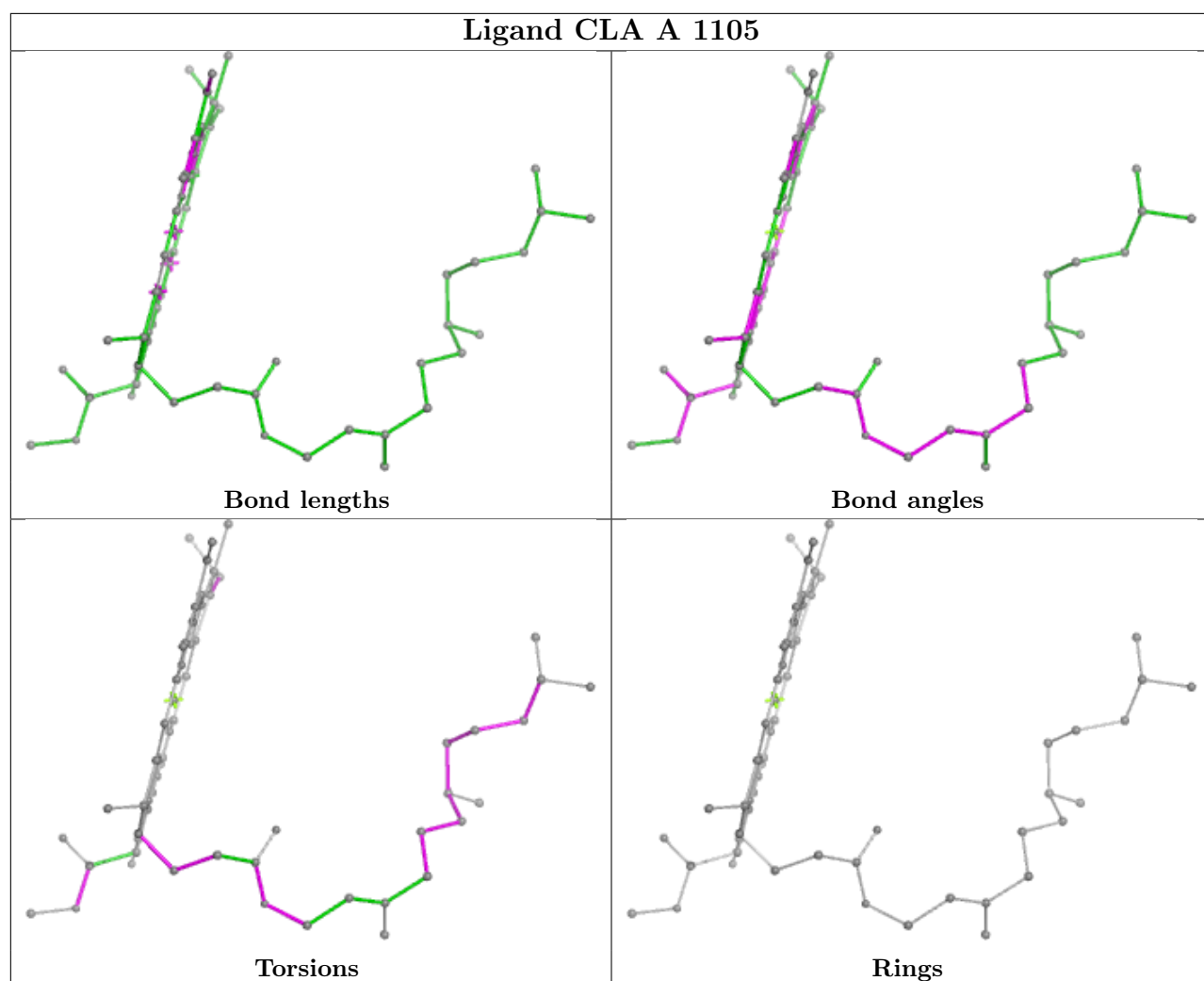
Ligand CHL 1 612

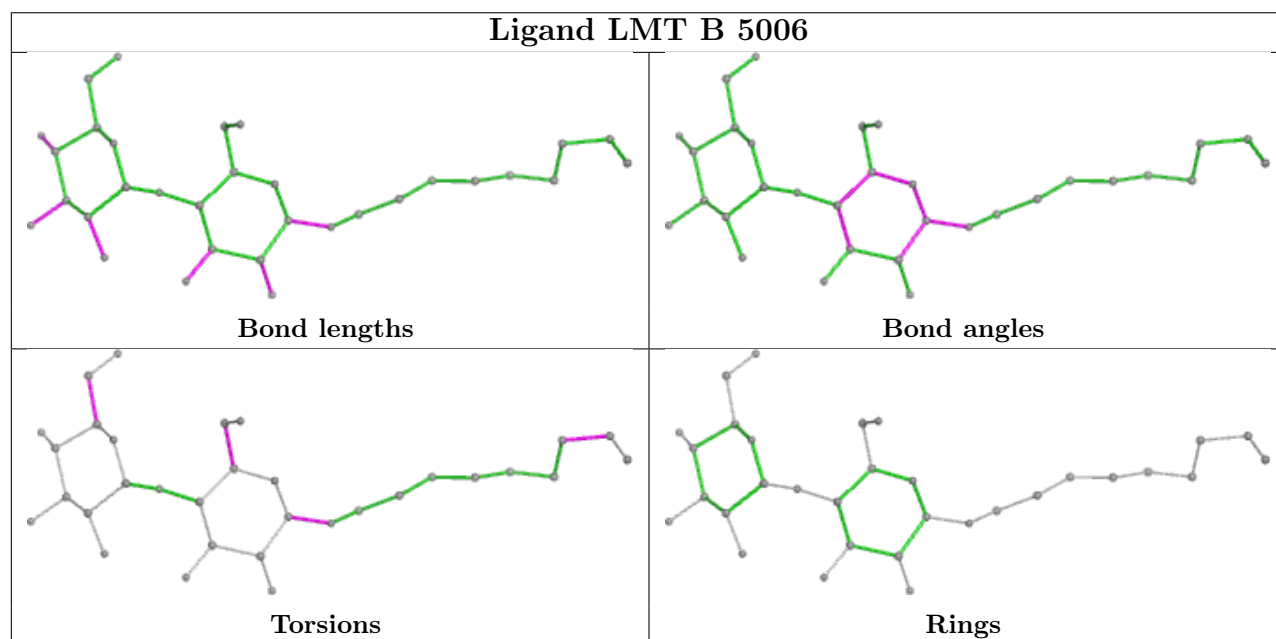
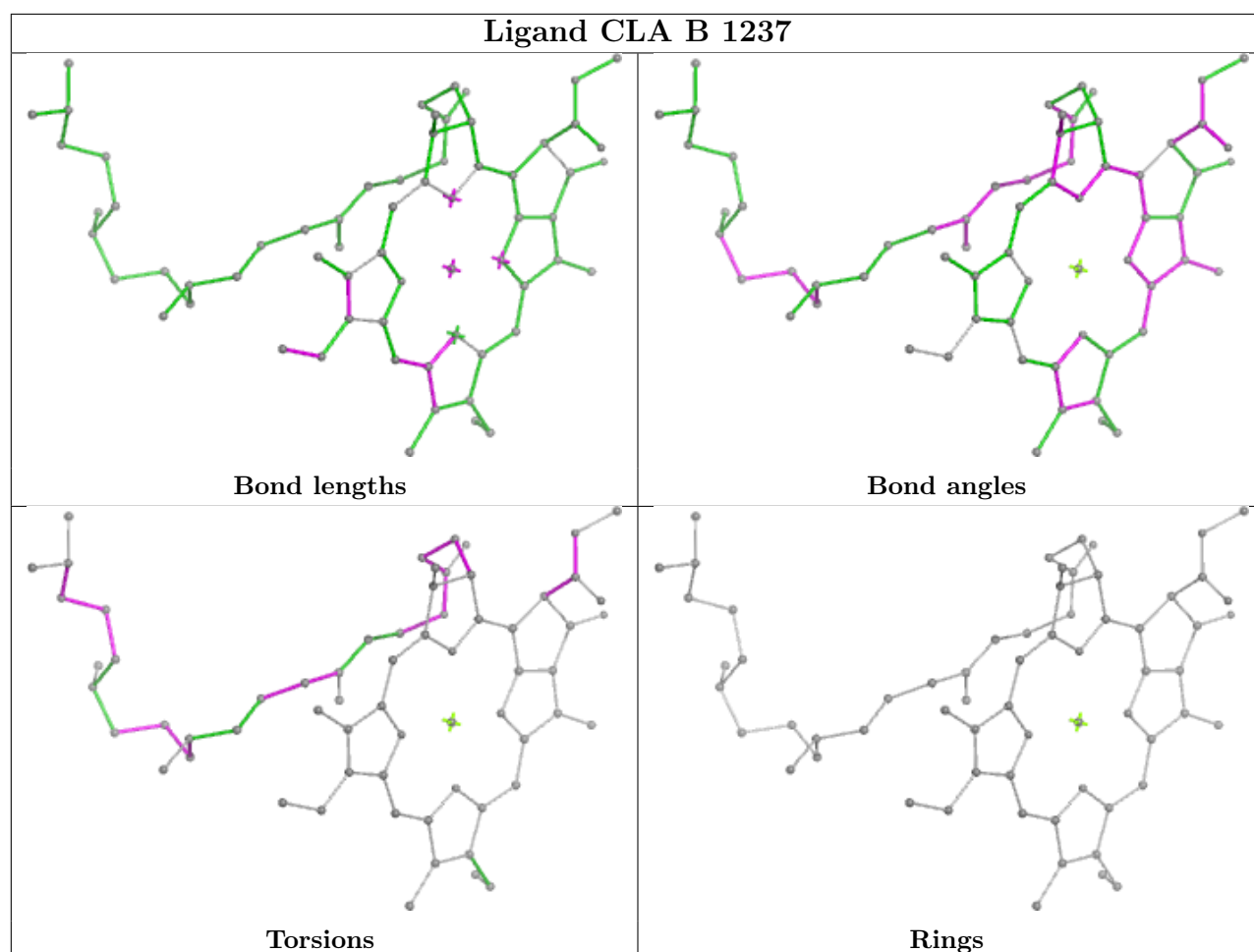


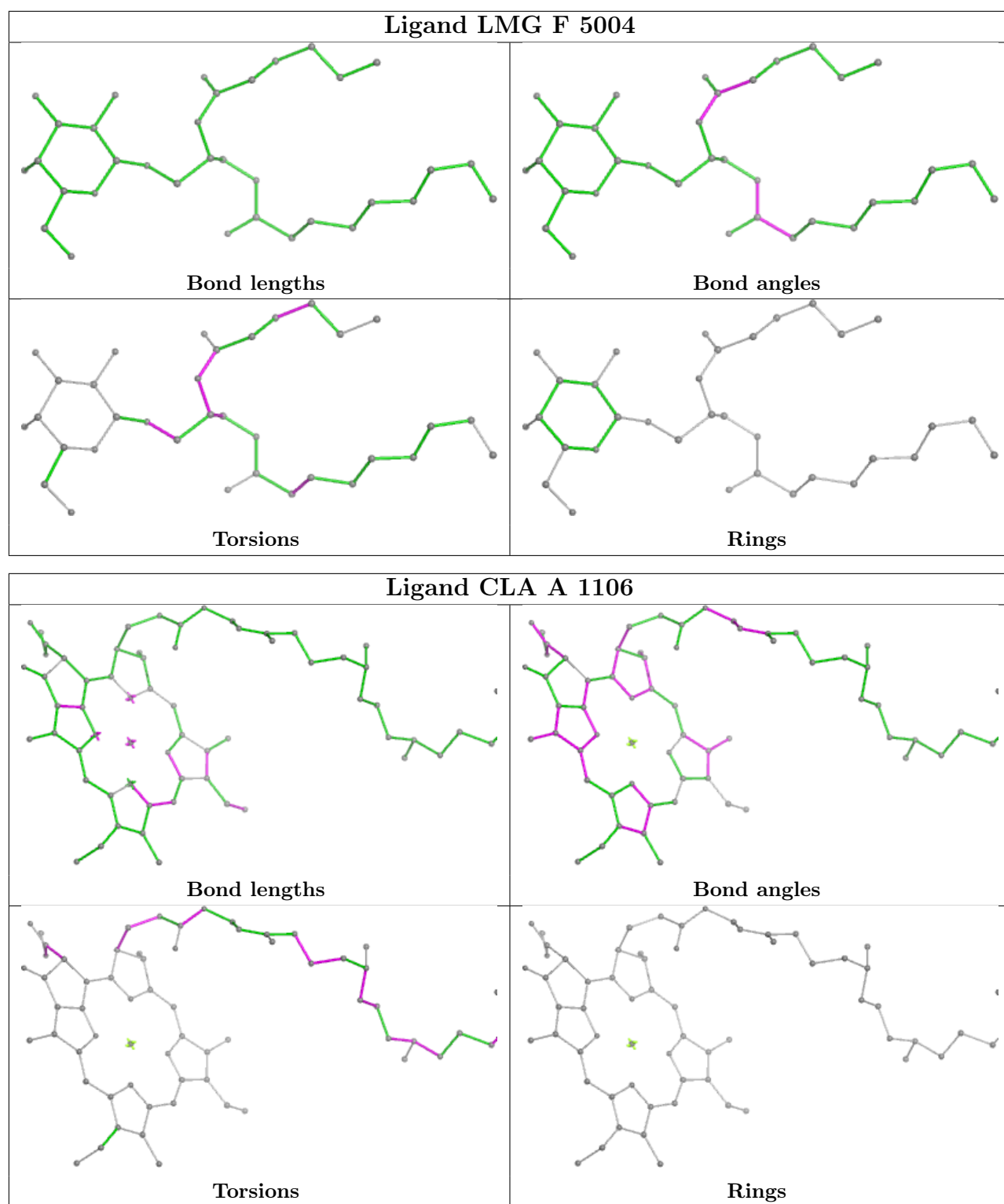
Ligand CLA 1 606

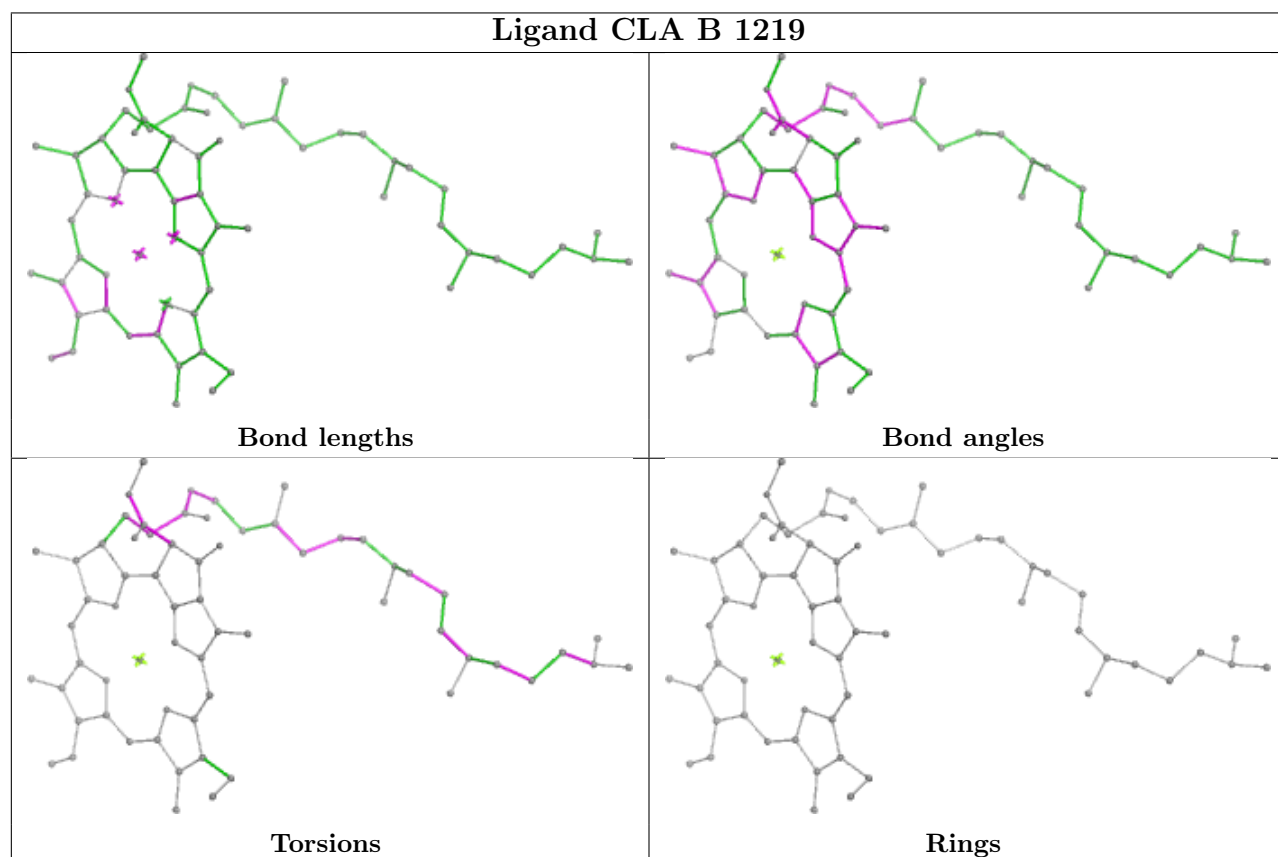
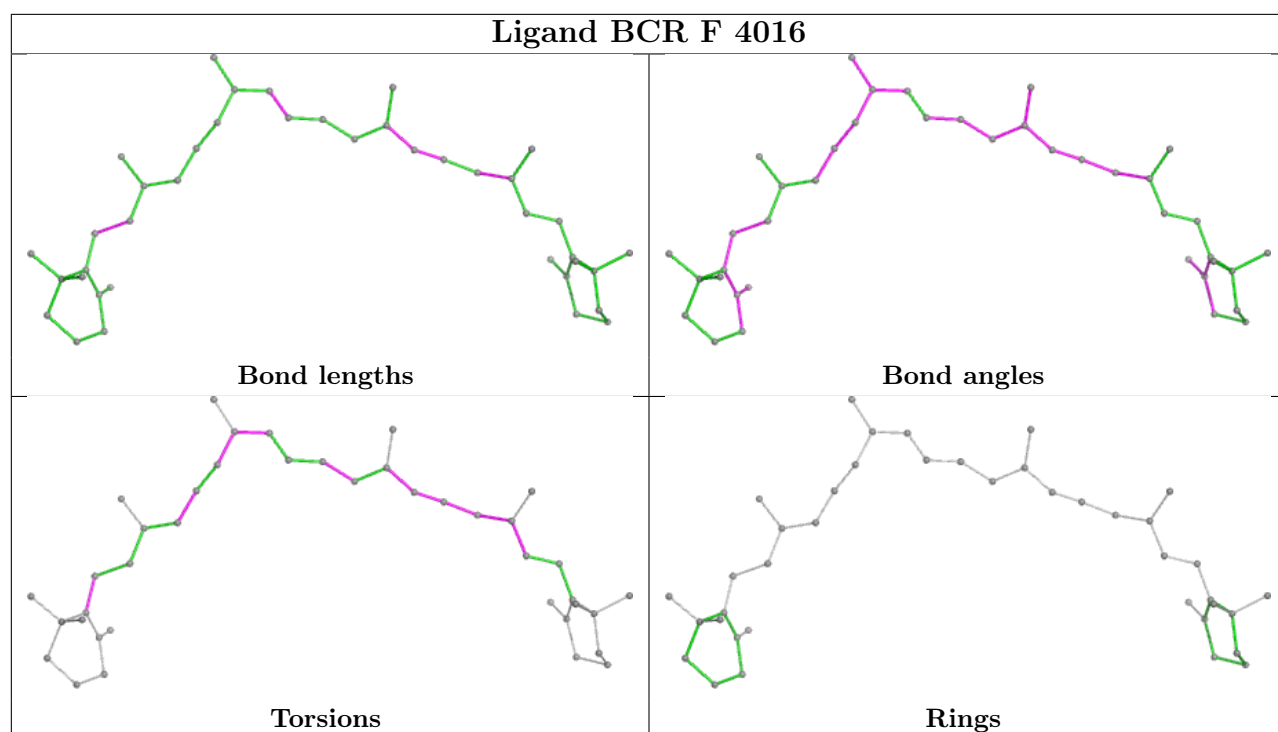


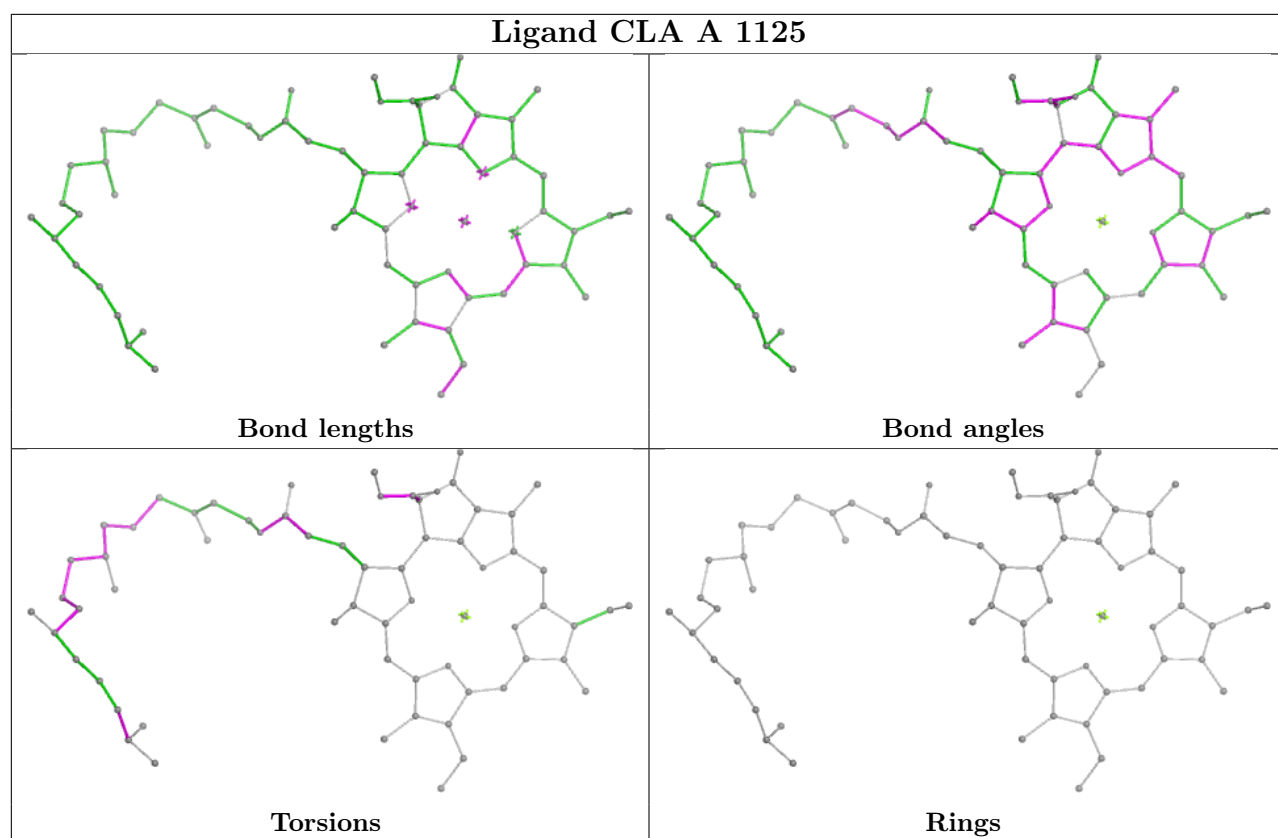




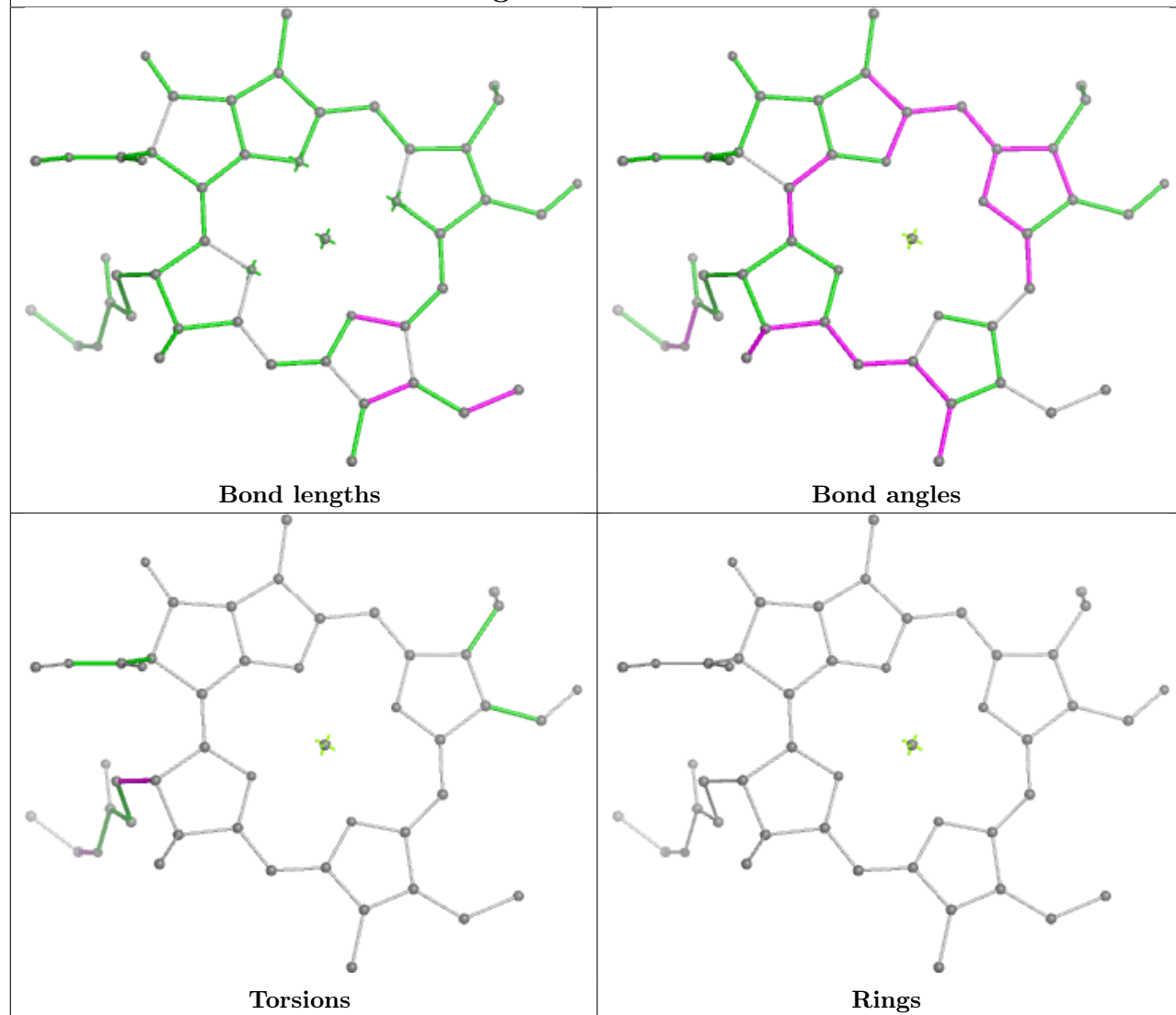


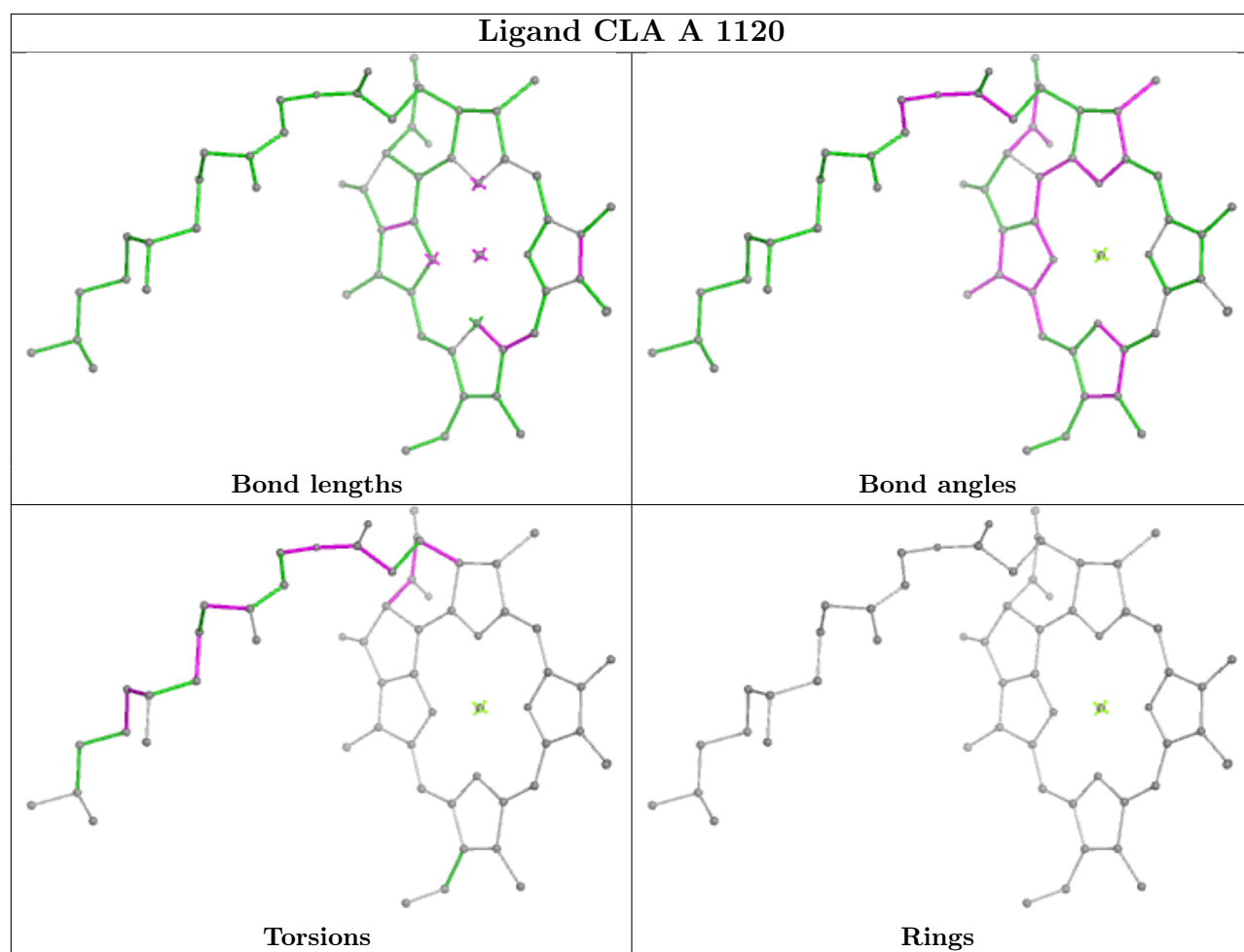


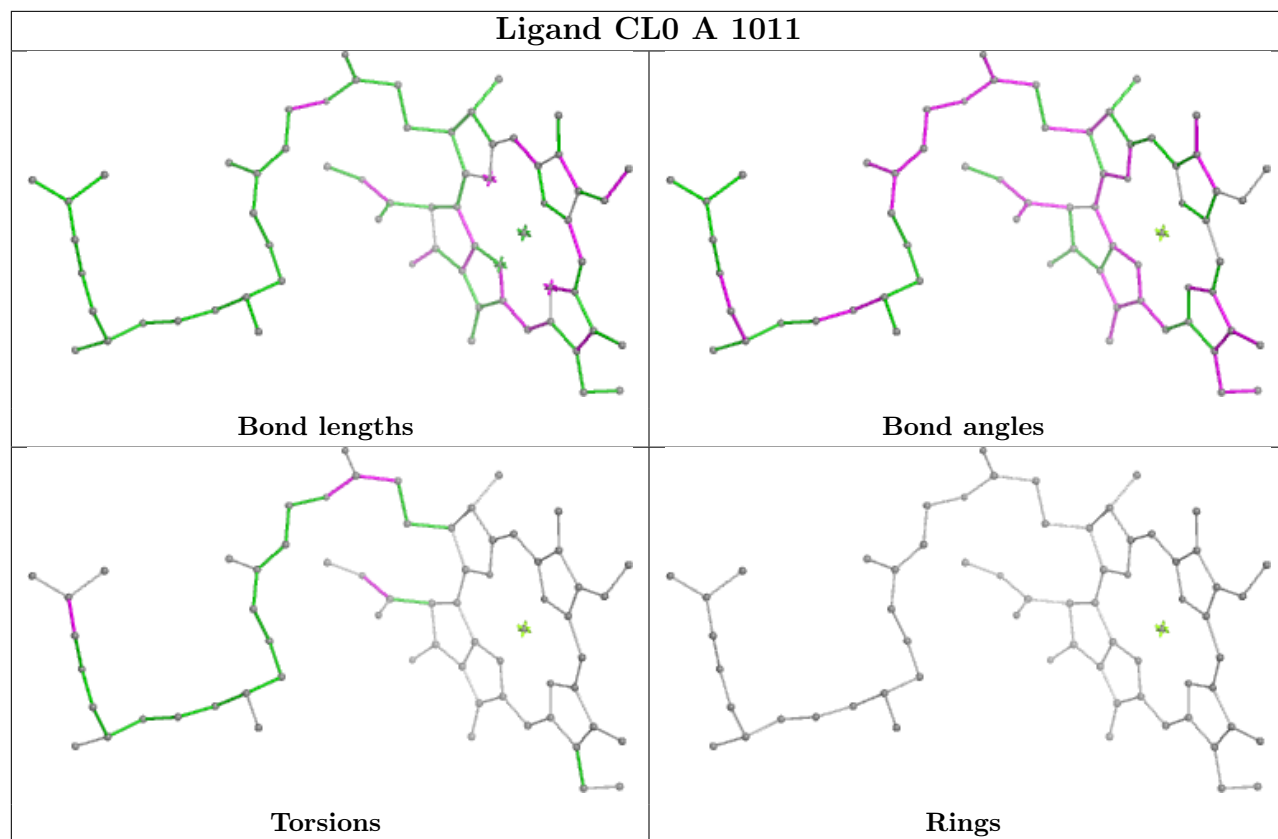




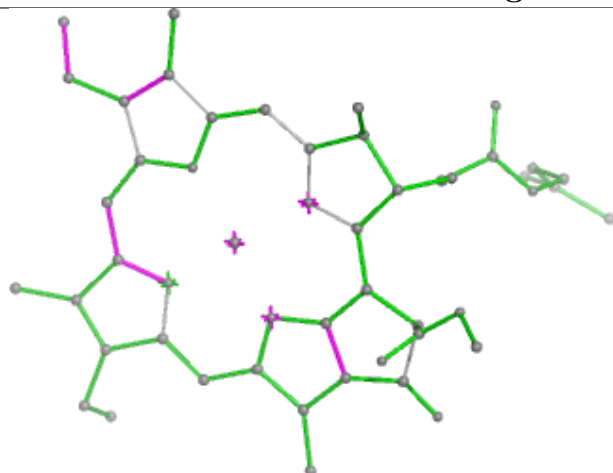
Ligand CHL 2 611



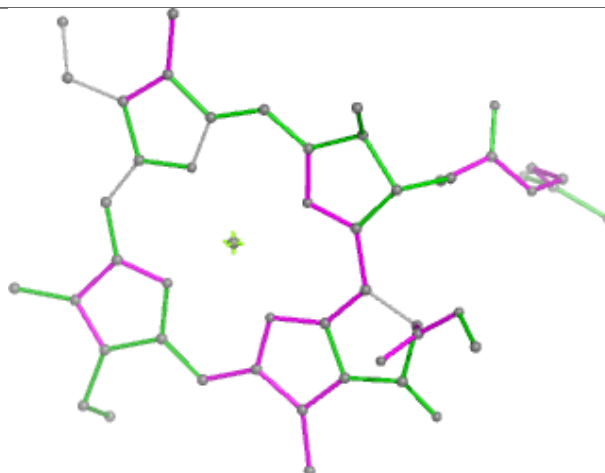




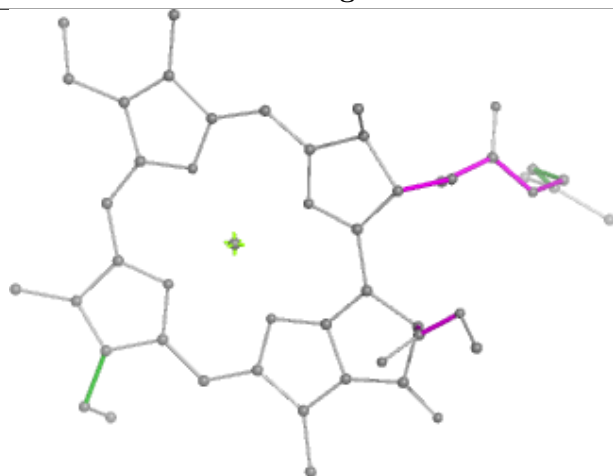
Ligand CLA B 1236



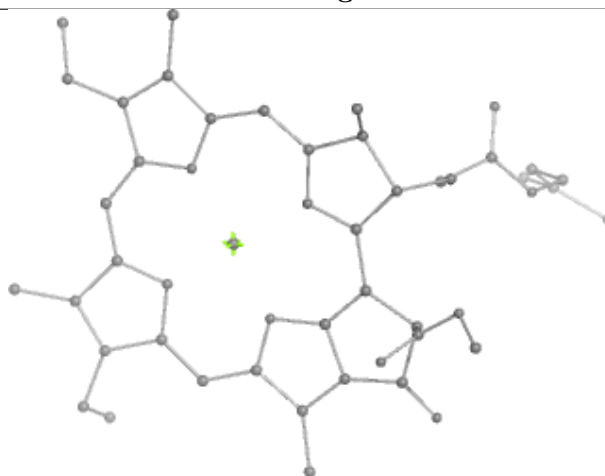
Bond lengths



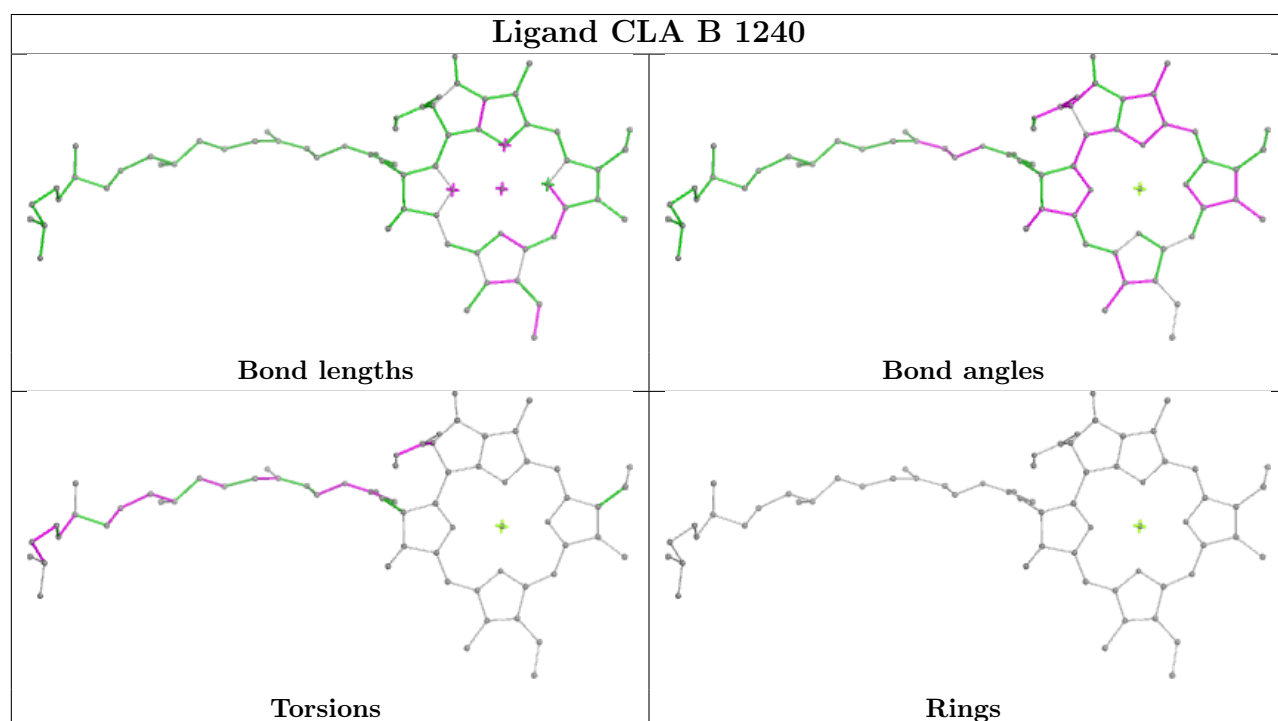
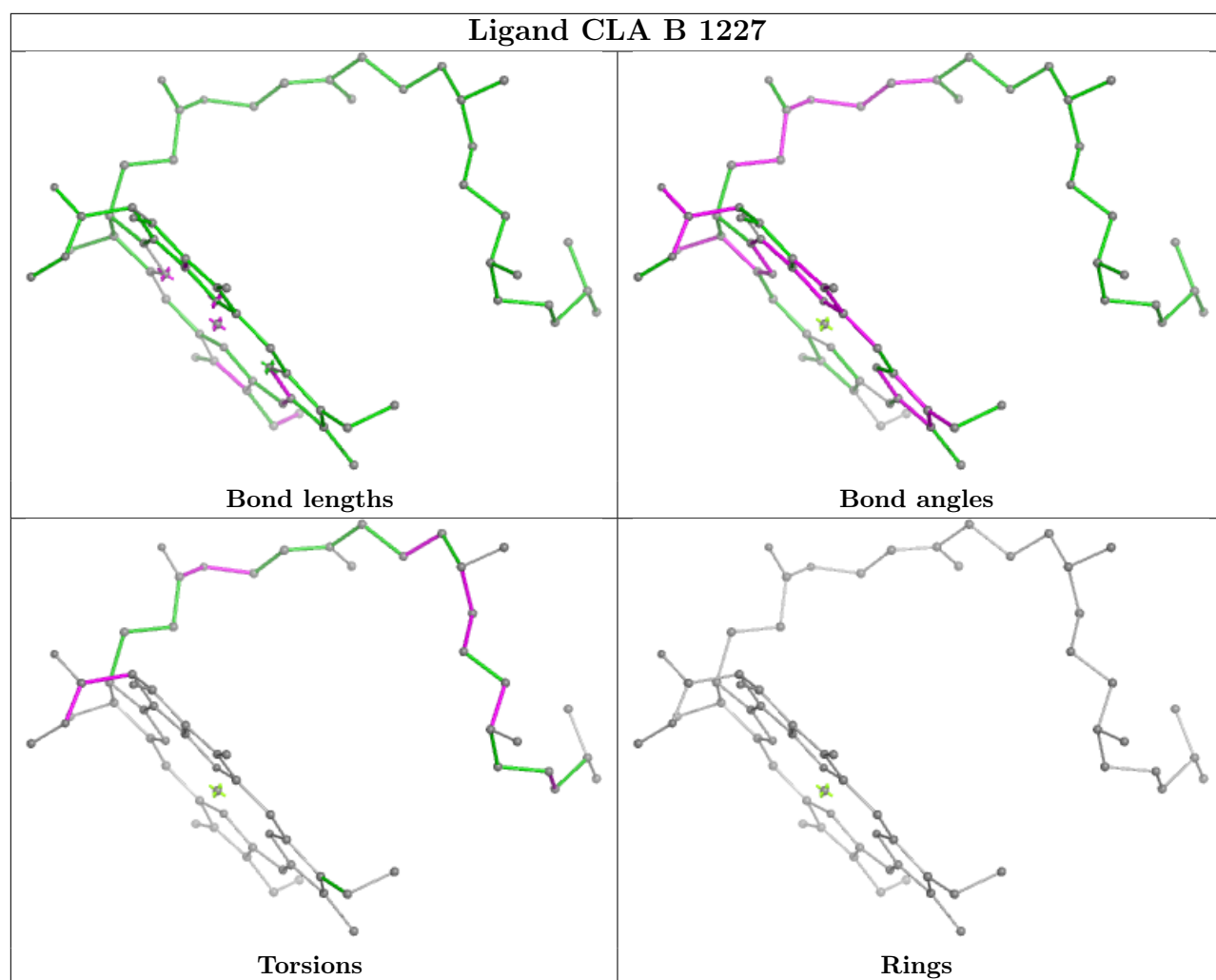
Bond angles



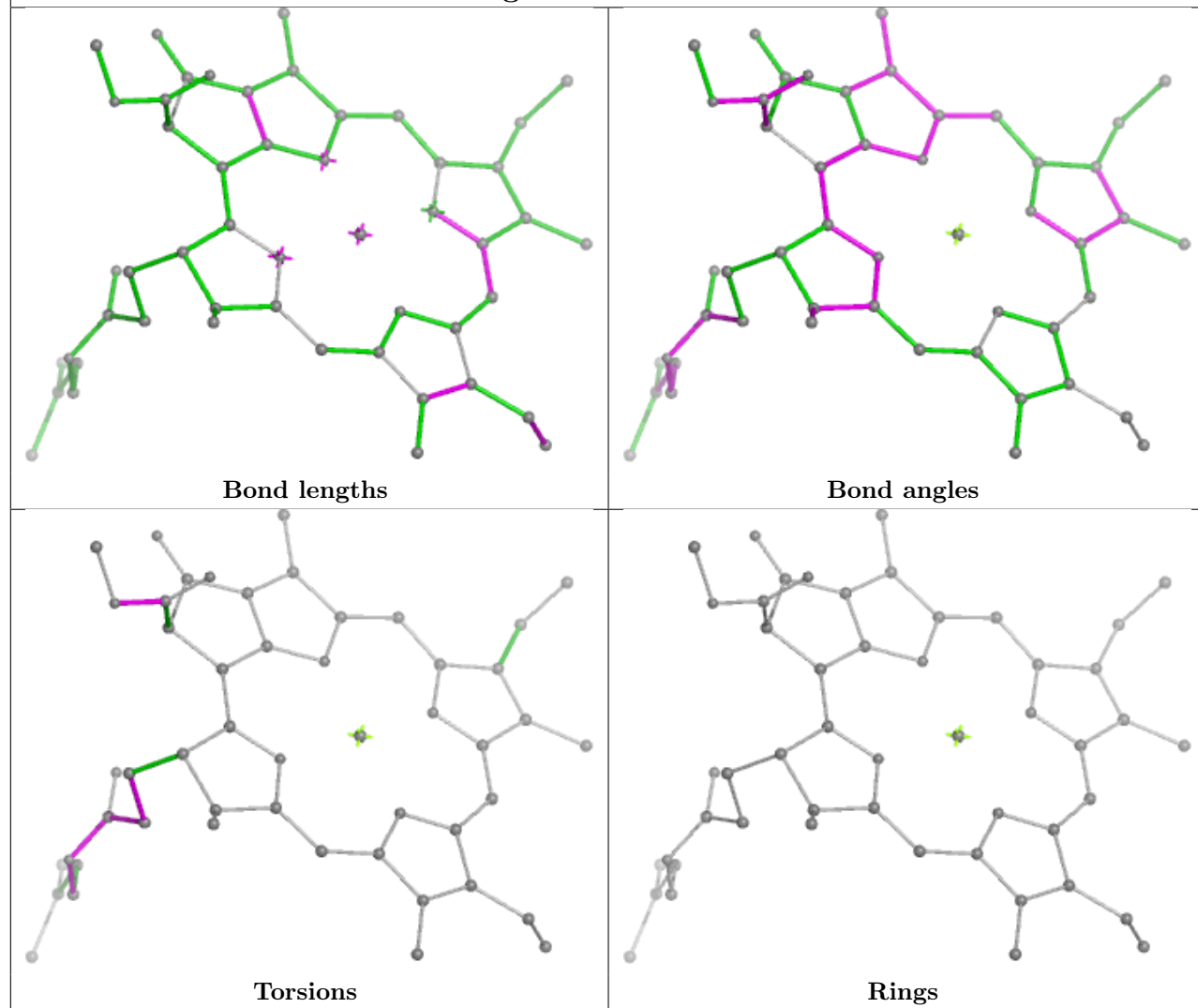
Torsions

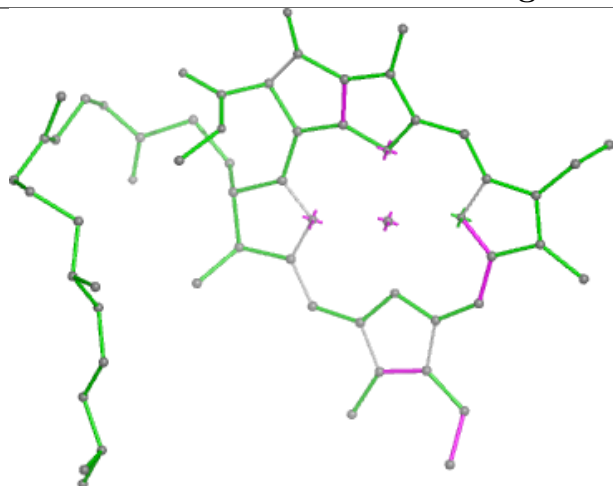


Rings

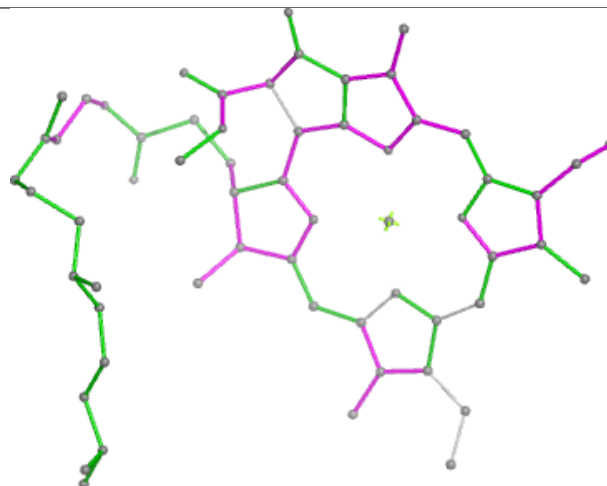


Ligand CLA 2 608

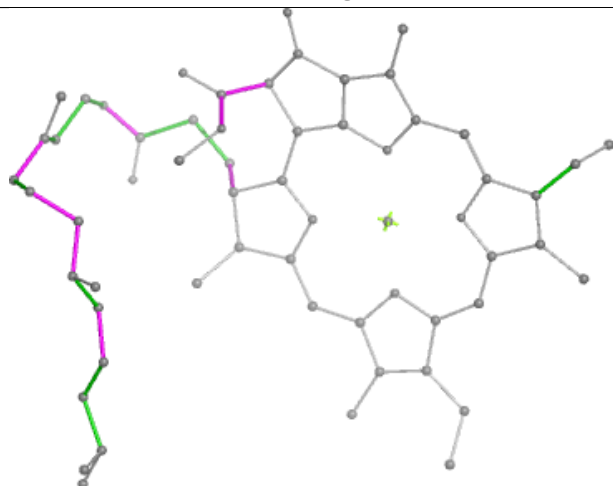


Ligand CLA 4 605

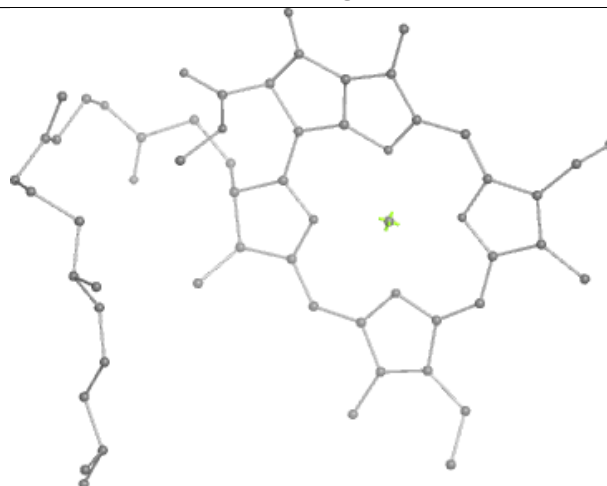
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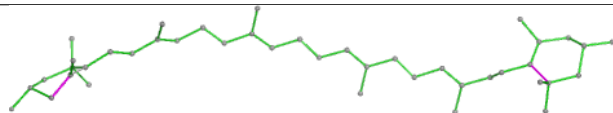
Bond angles



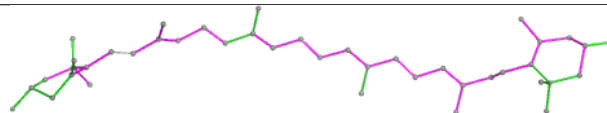
Torsions



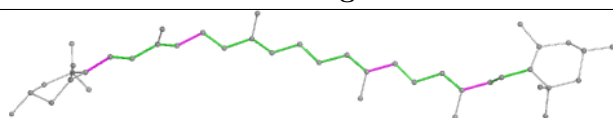
Rings

Ligand LUT J 4013

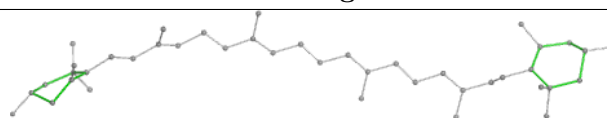
Bond lengths



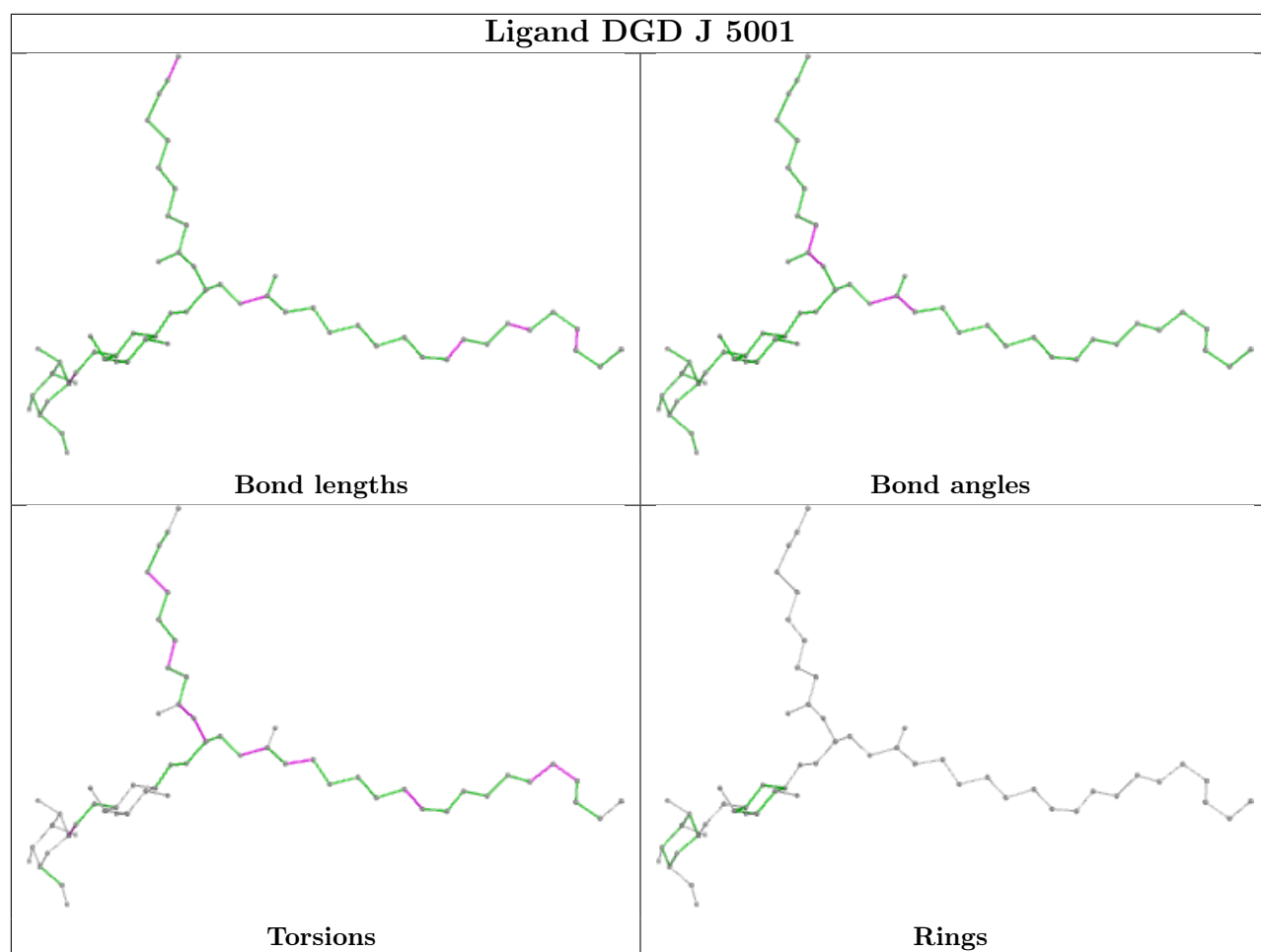
Bond angles



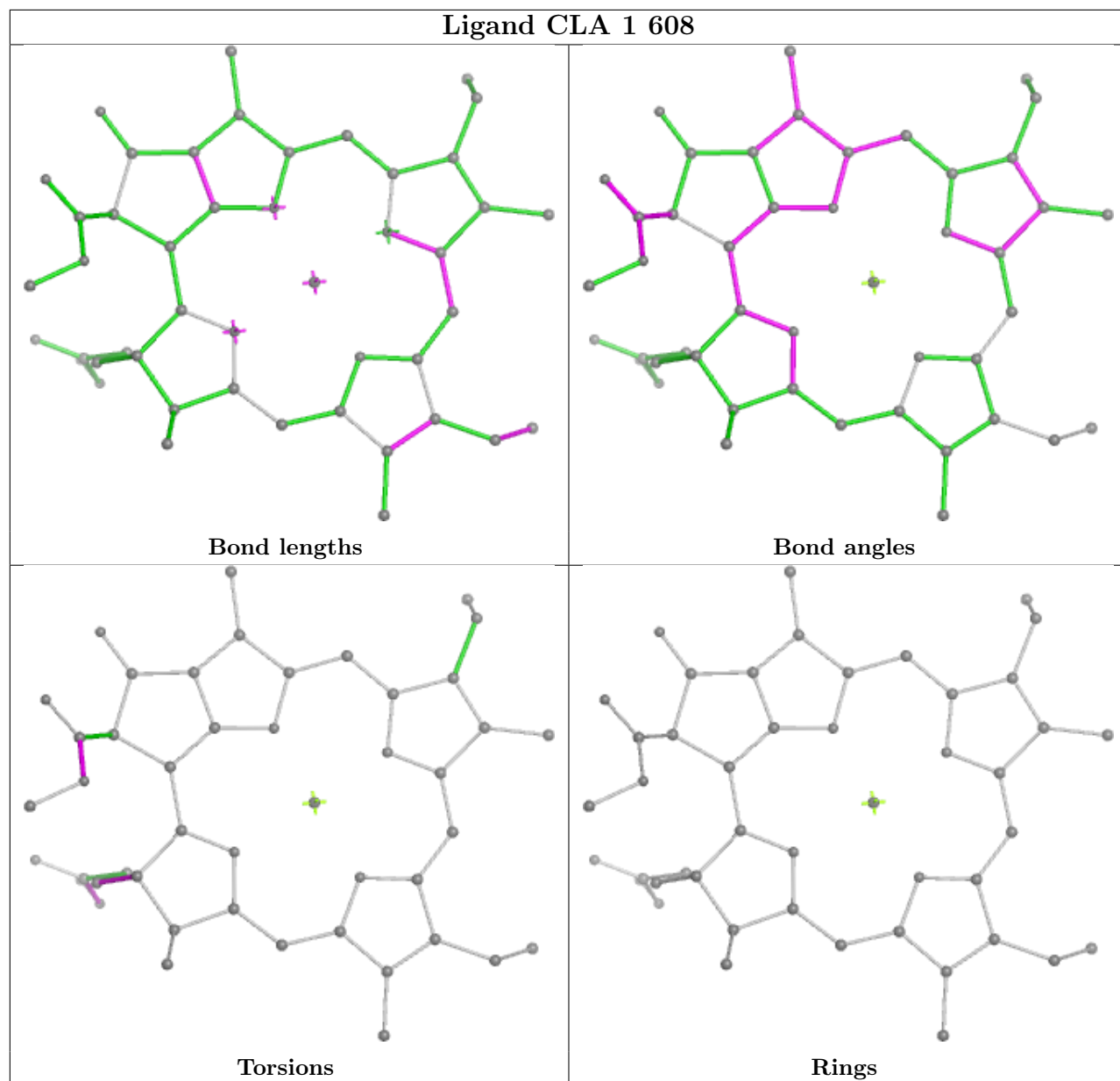
Torsions

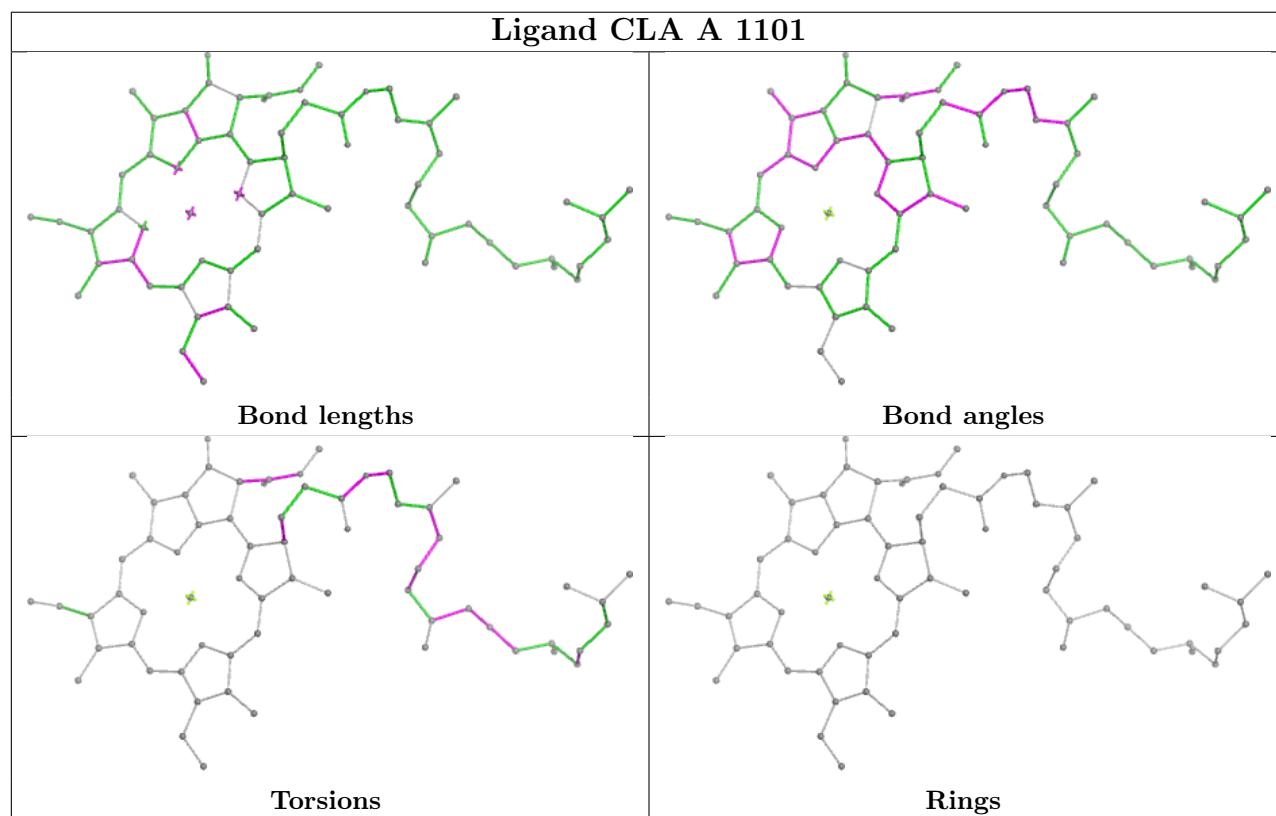
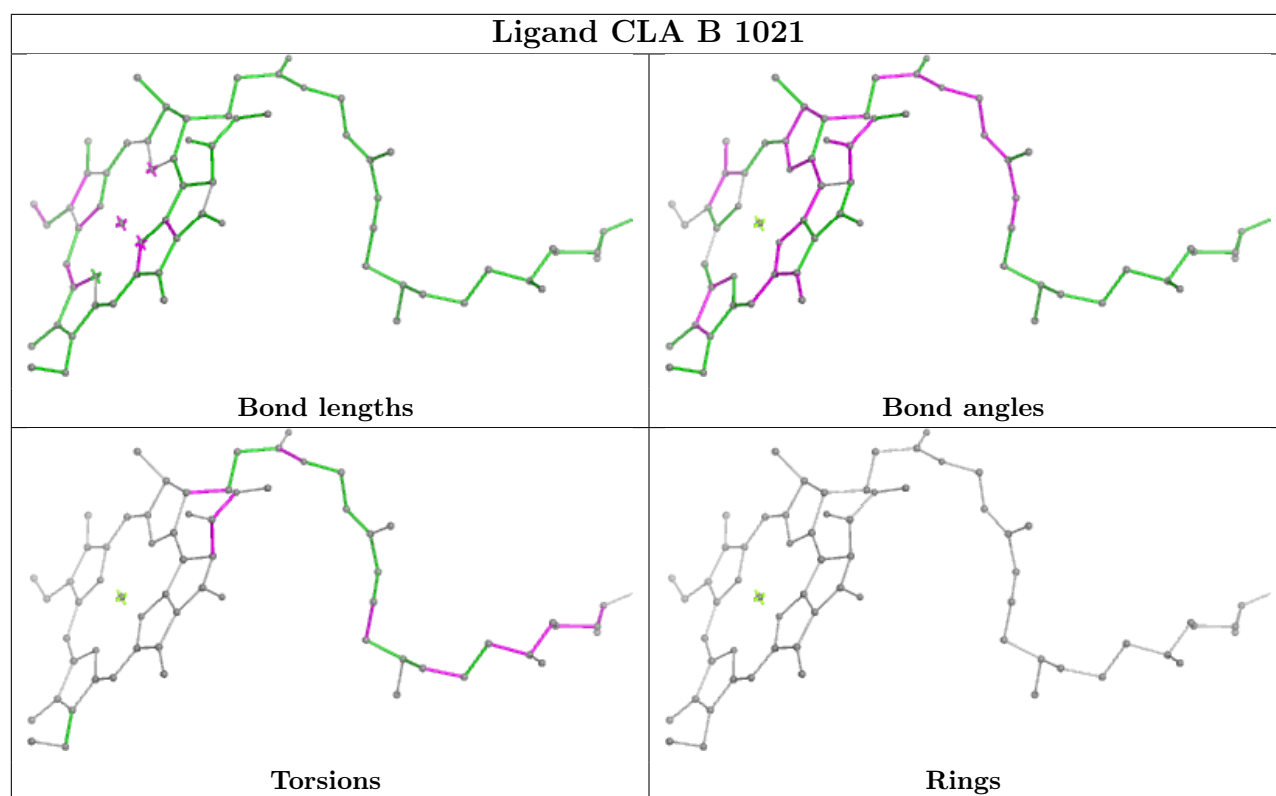


Rings

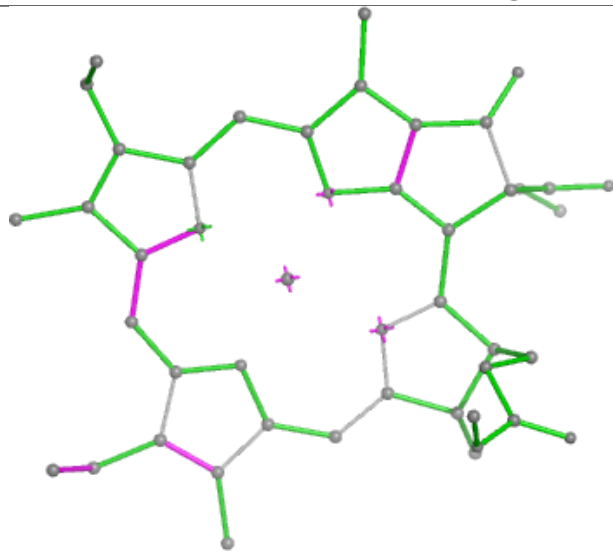


Ligand CLA 1 608

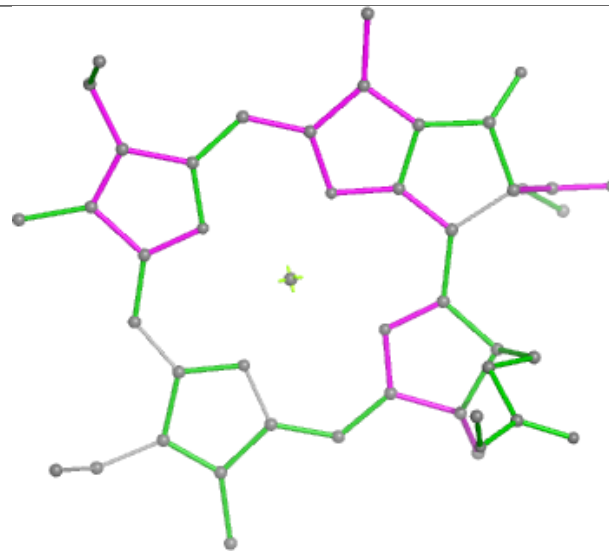




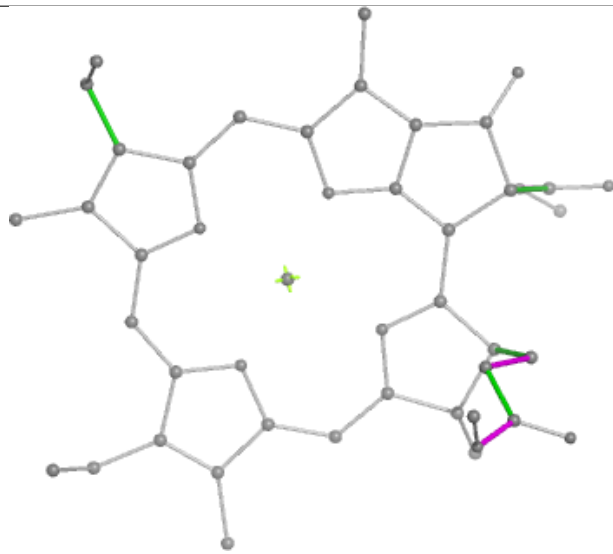
Ligand CLA B 1217



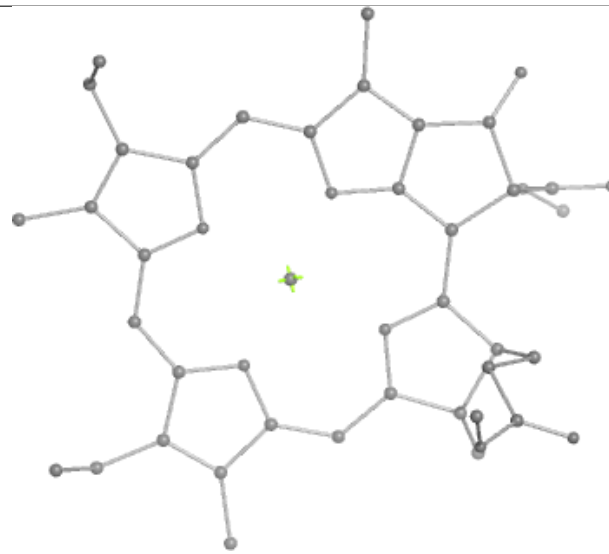
Bond lengths



Bond angles

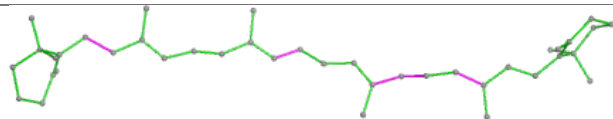


Torsions

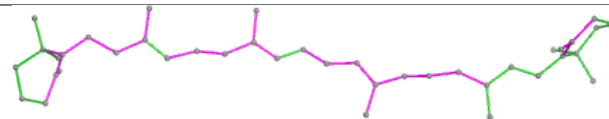


Rings

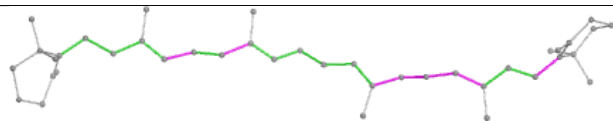
Ligand BCR A 4002



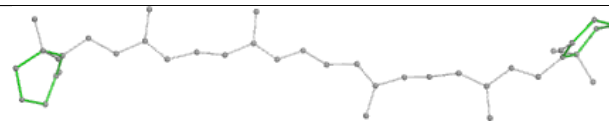
Bond lengths



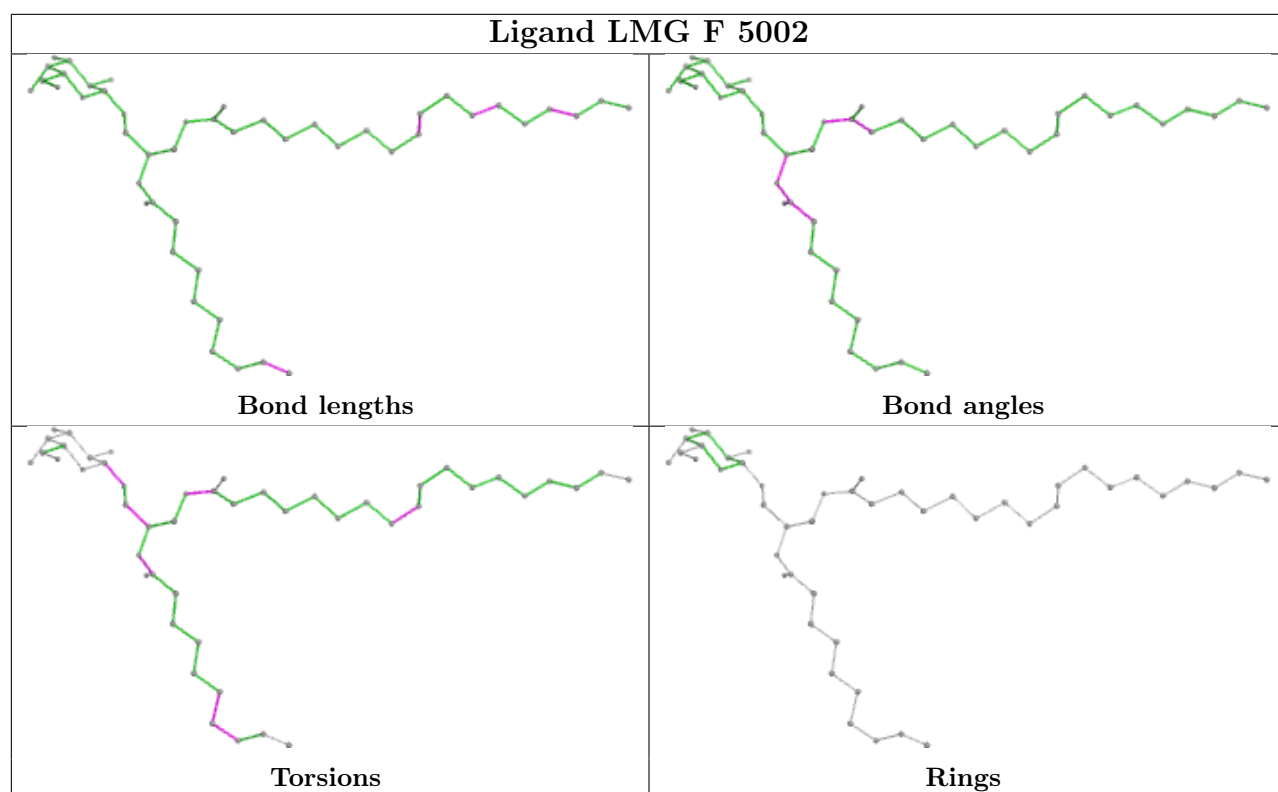
Bond angles



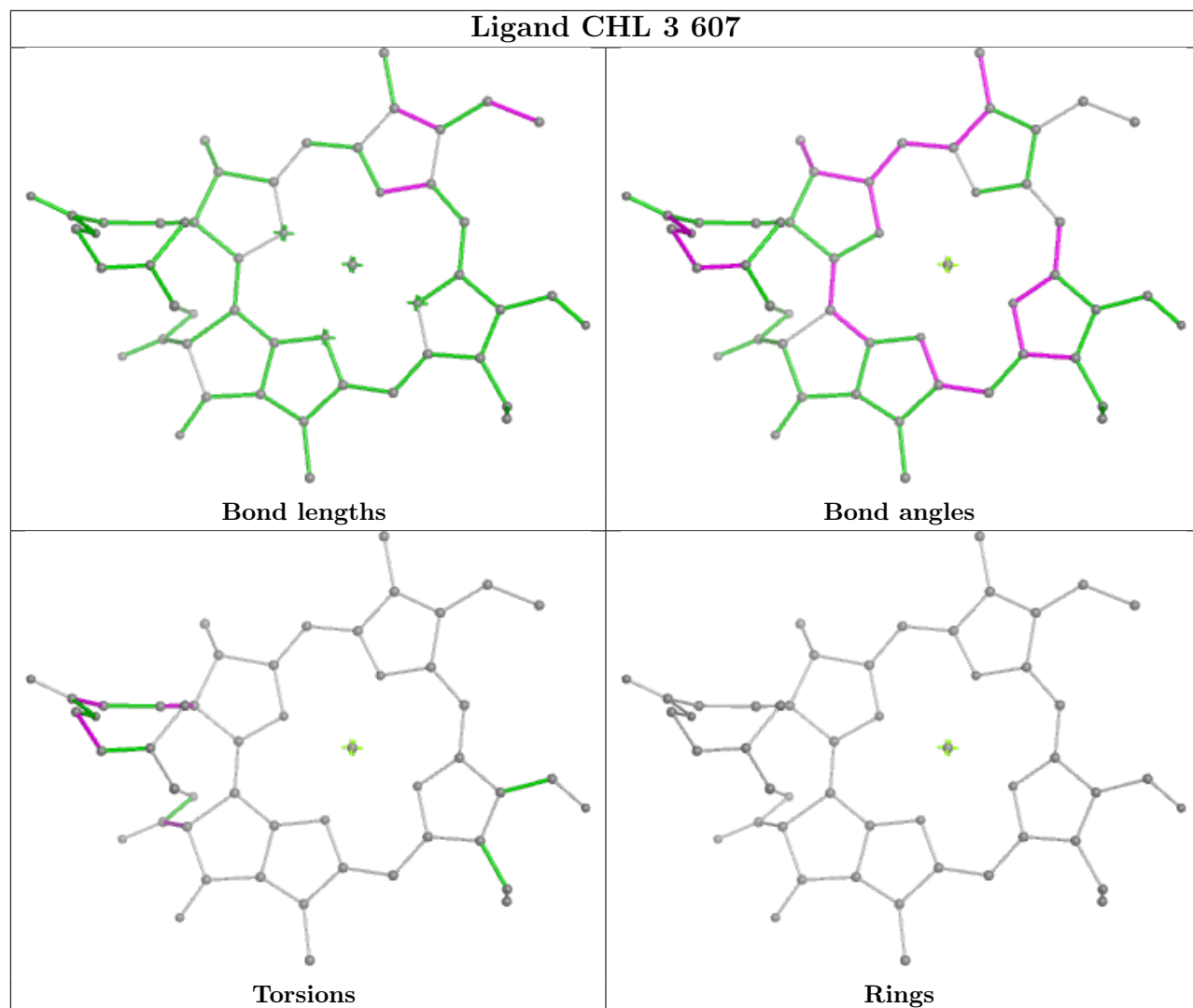
Torsions



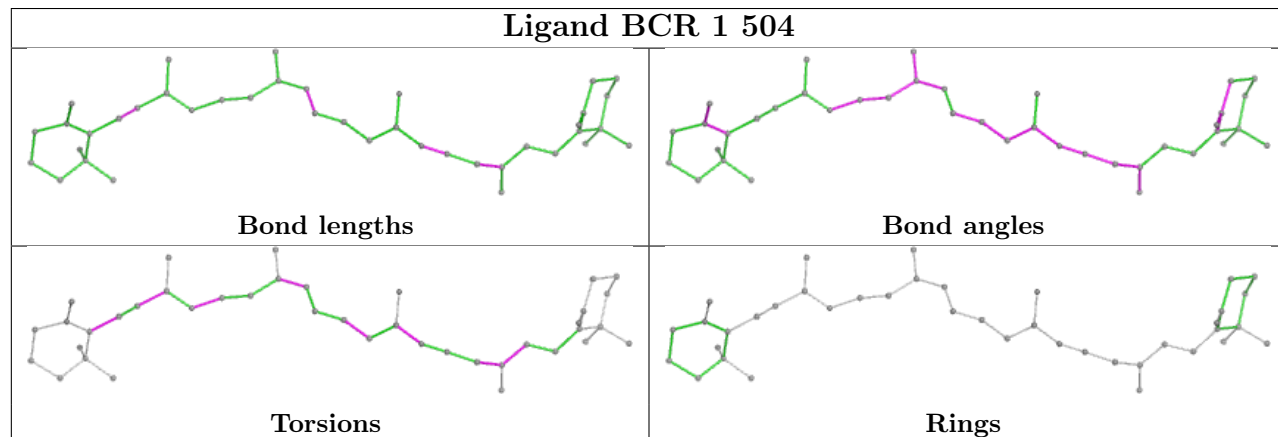
Rings

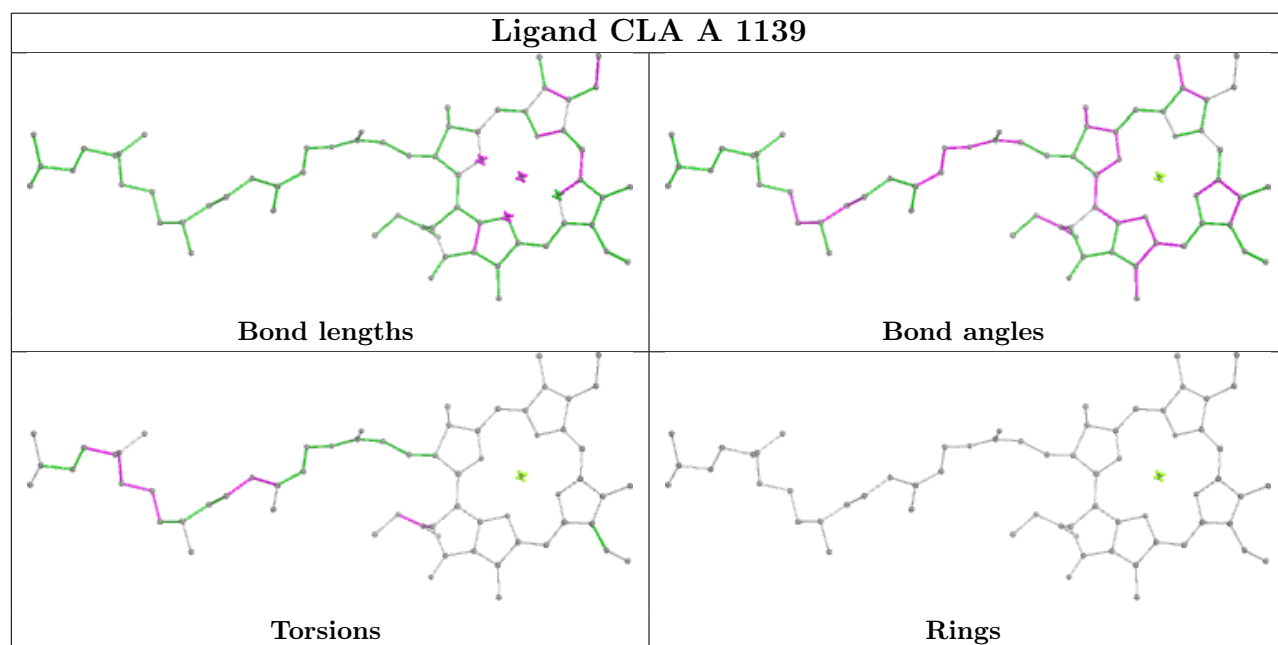
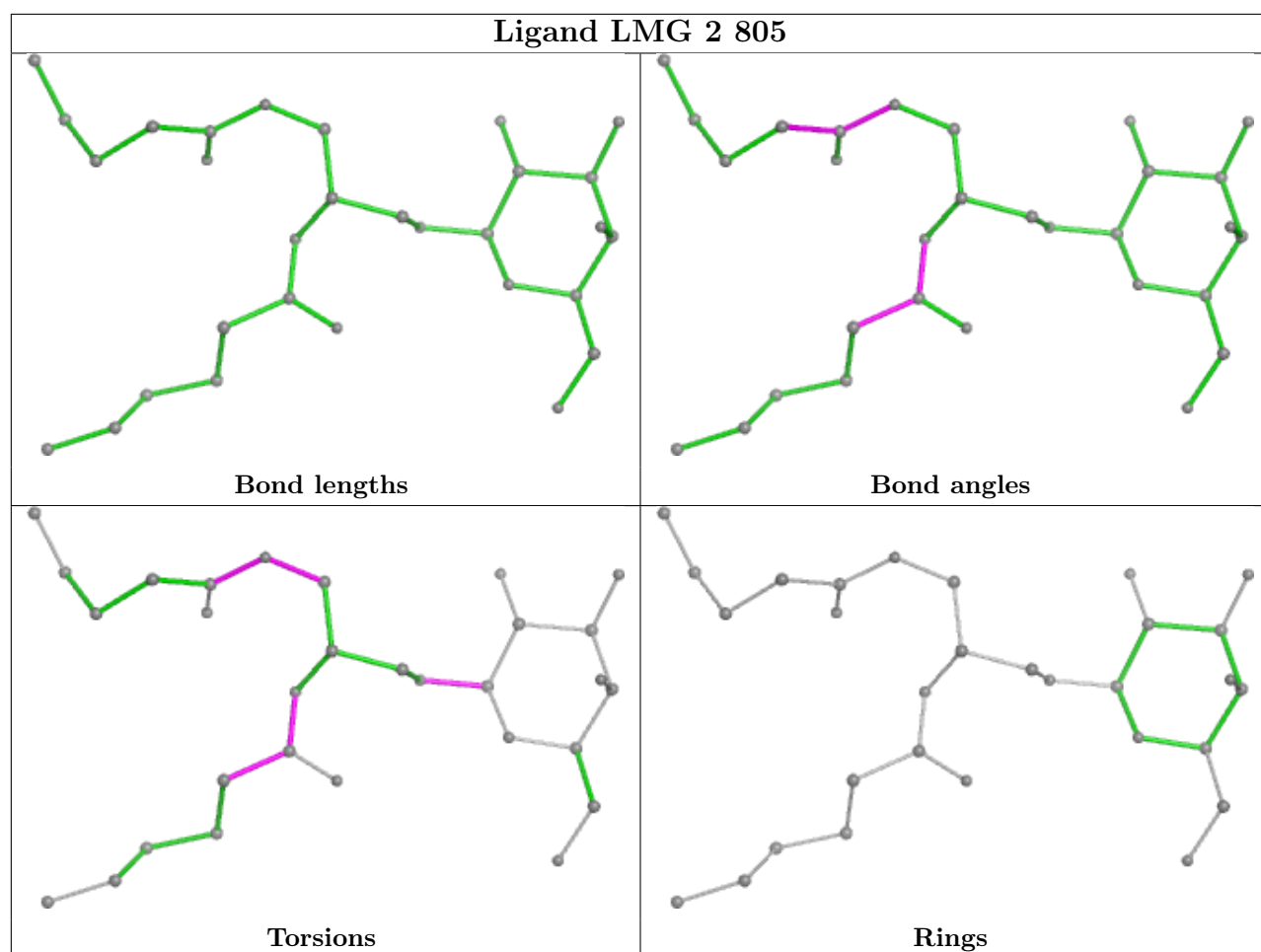


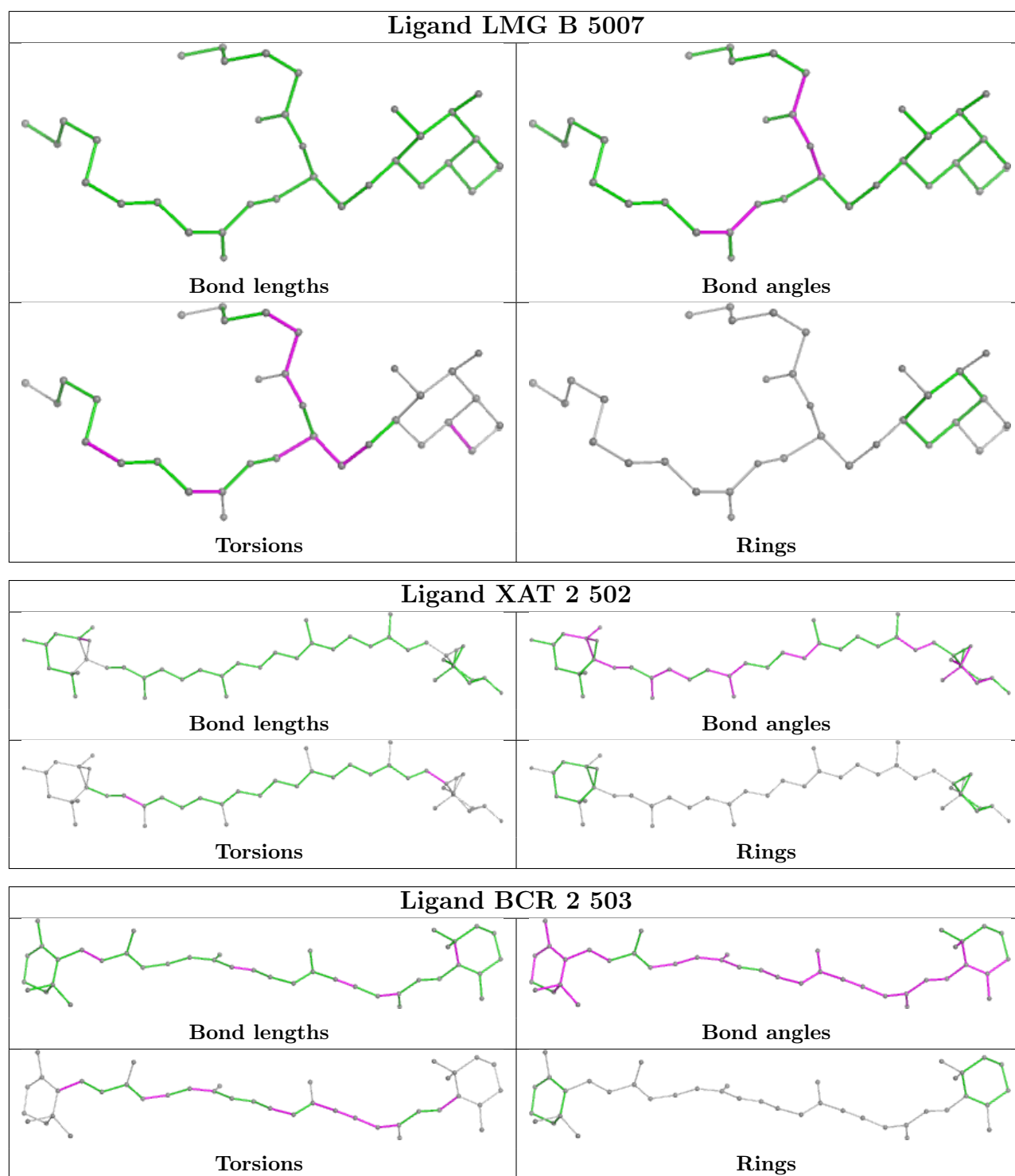
Ligand CHL 3 607

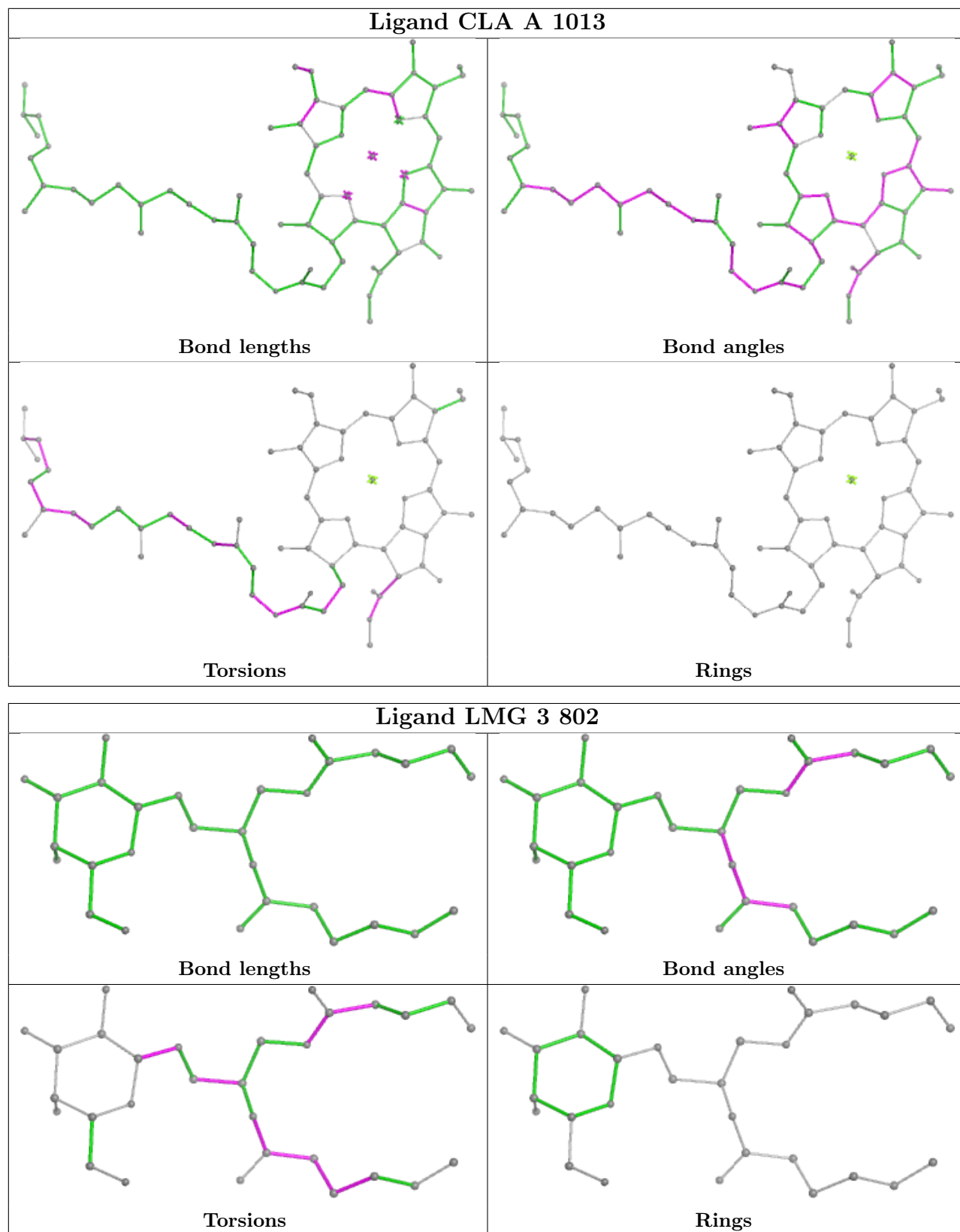


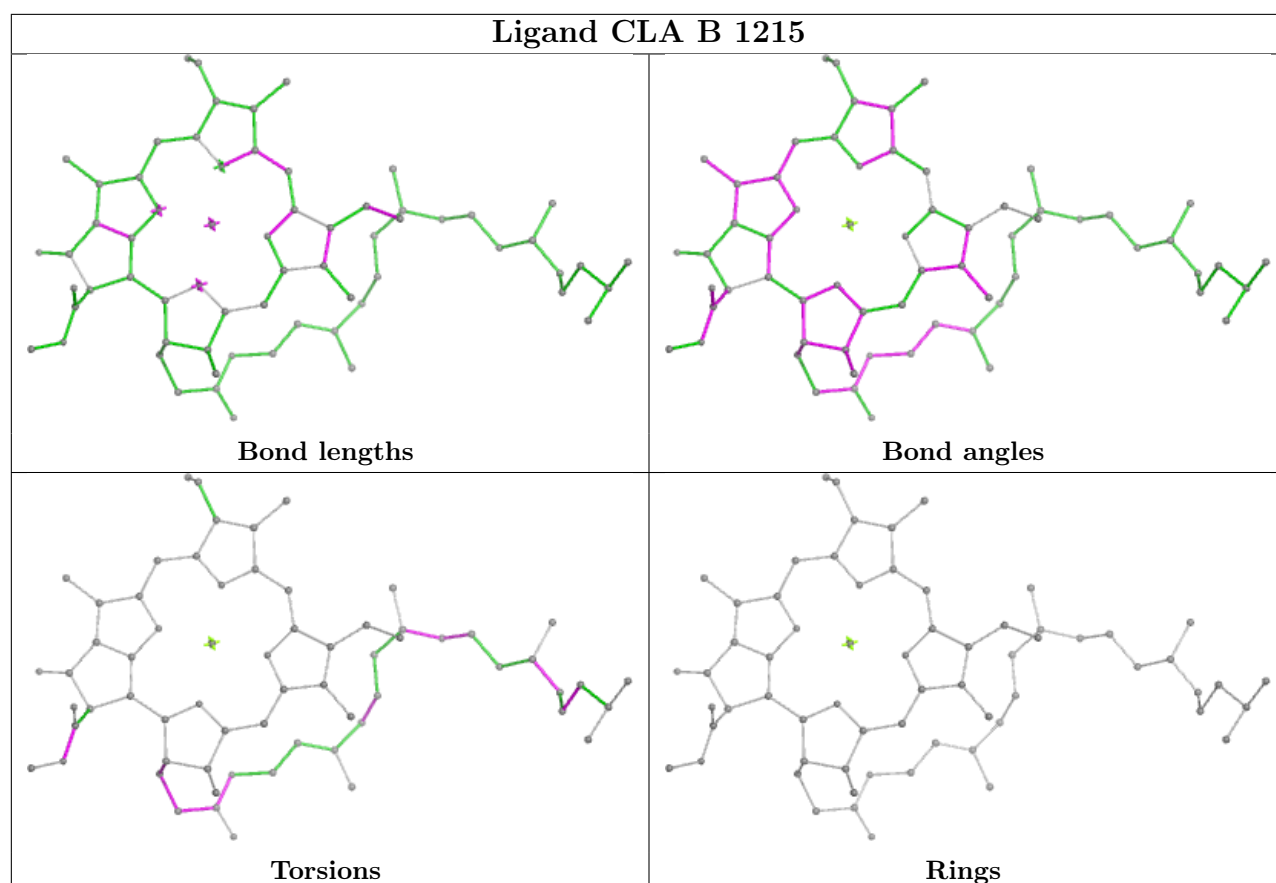
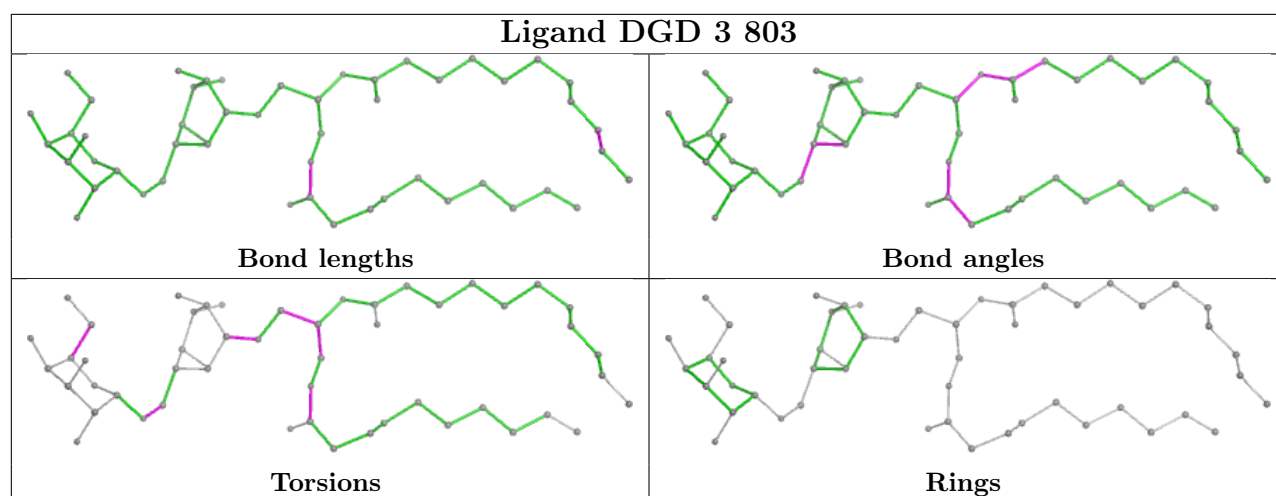
Ligand BCR 1 504



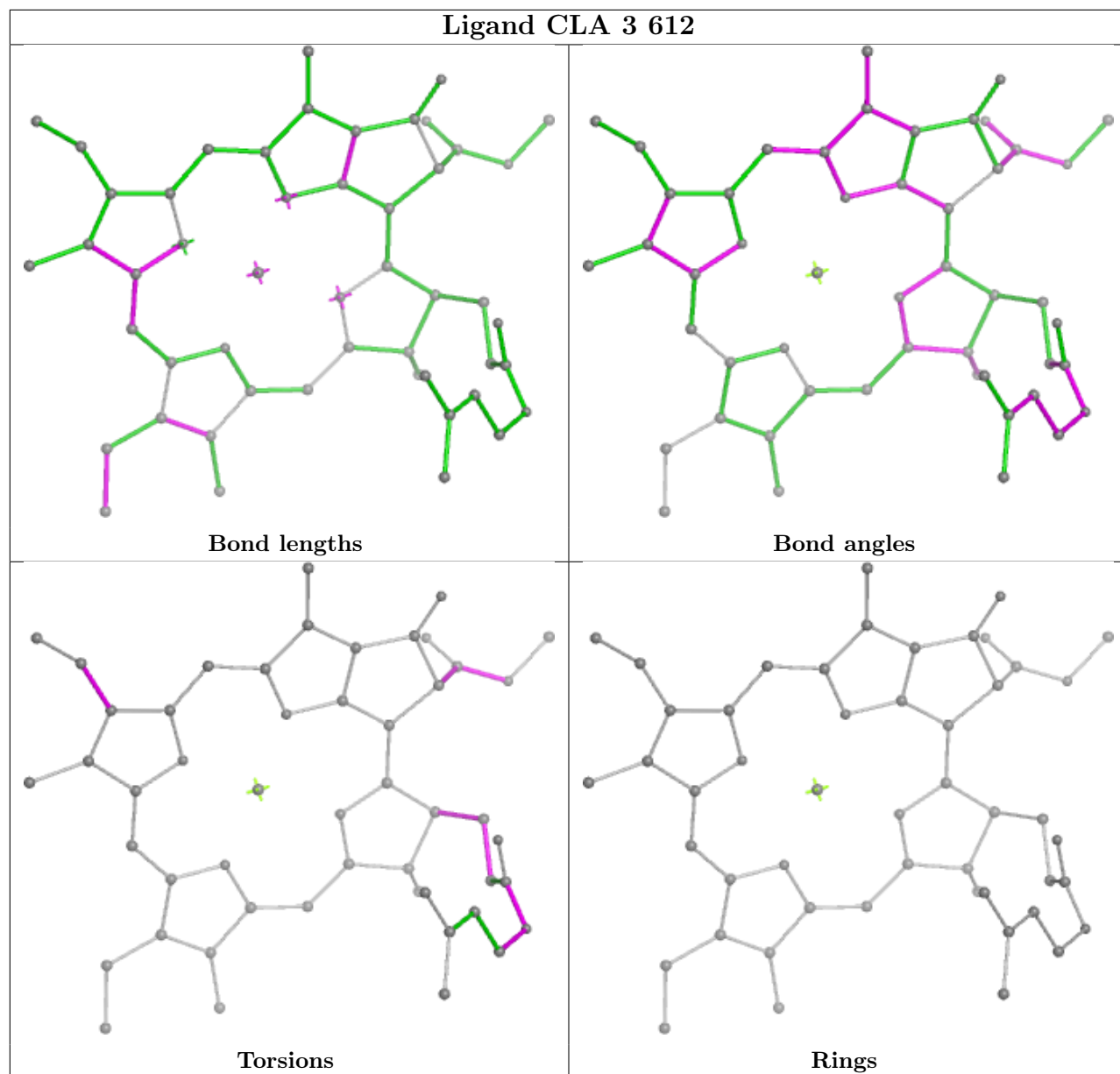




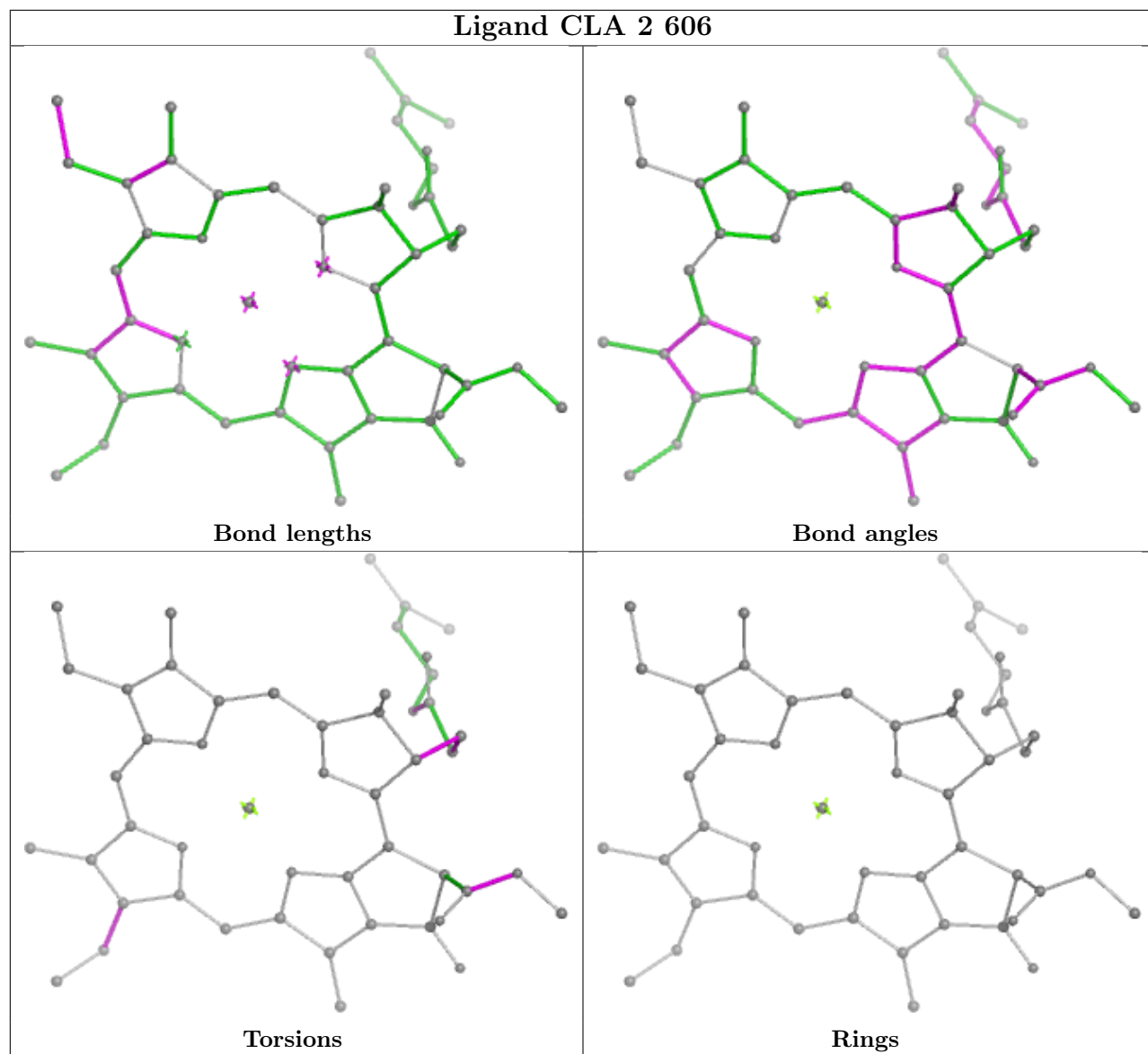


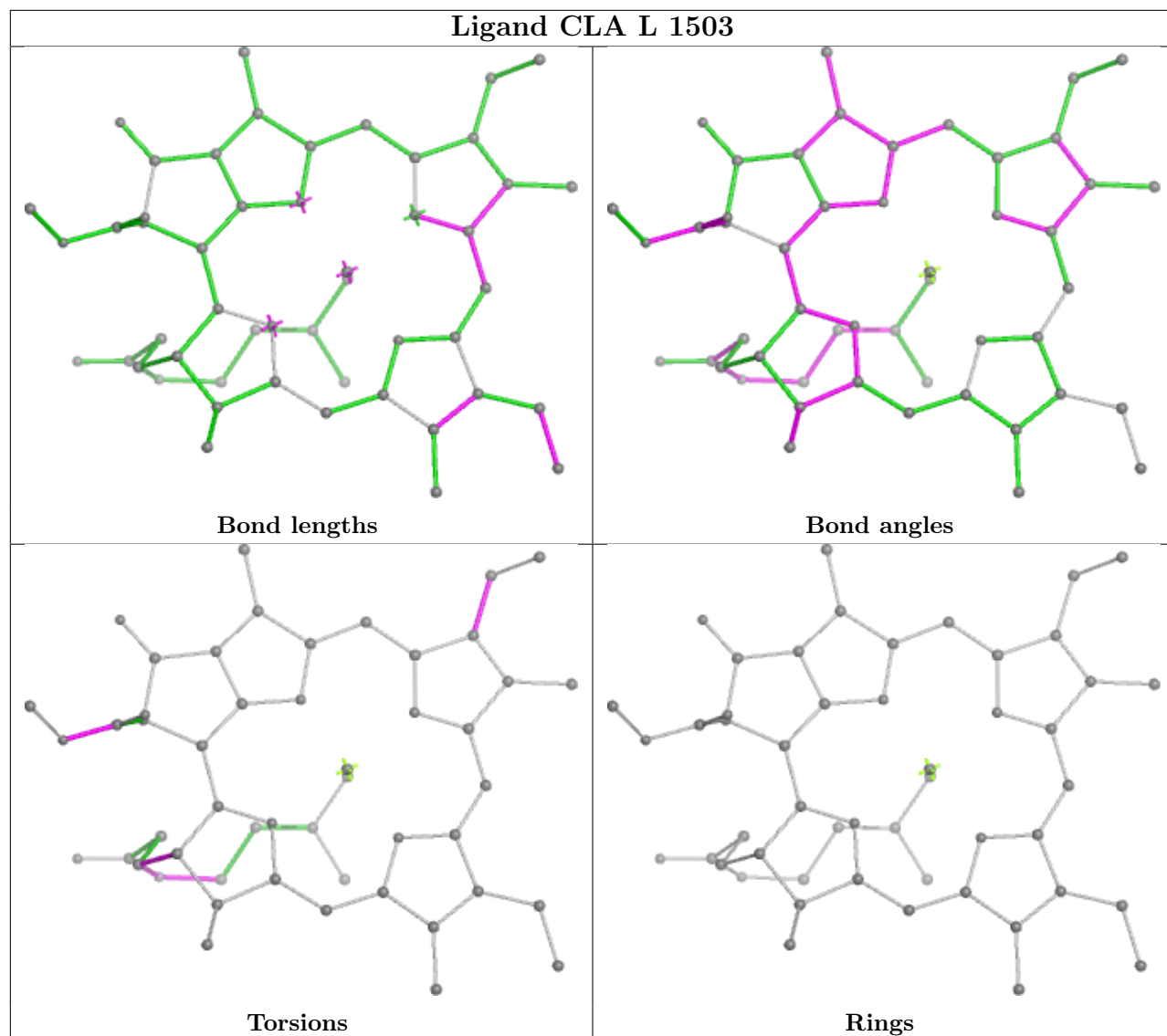


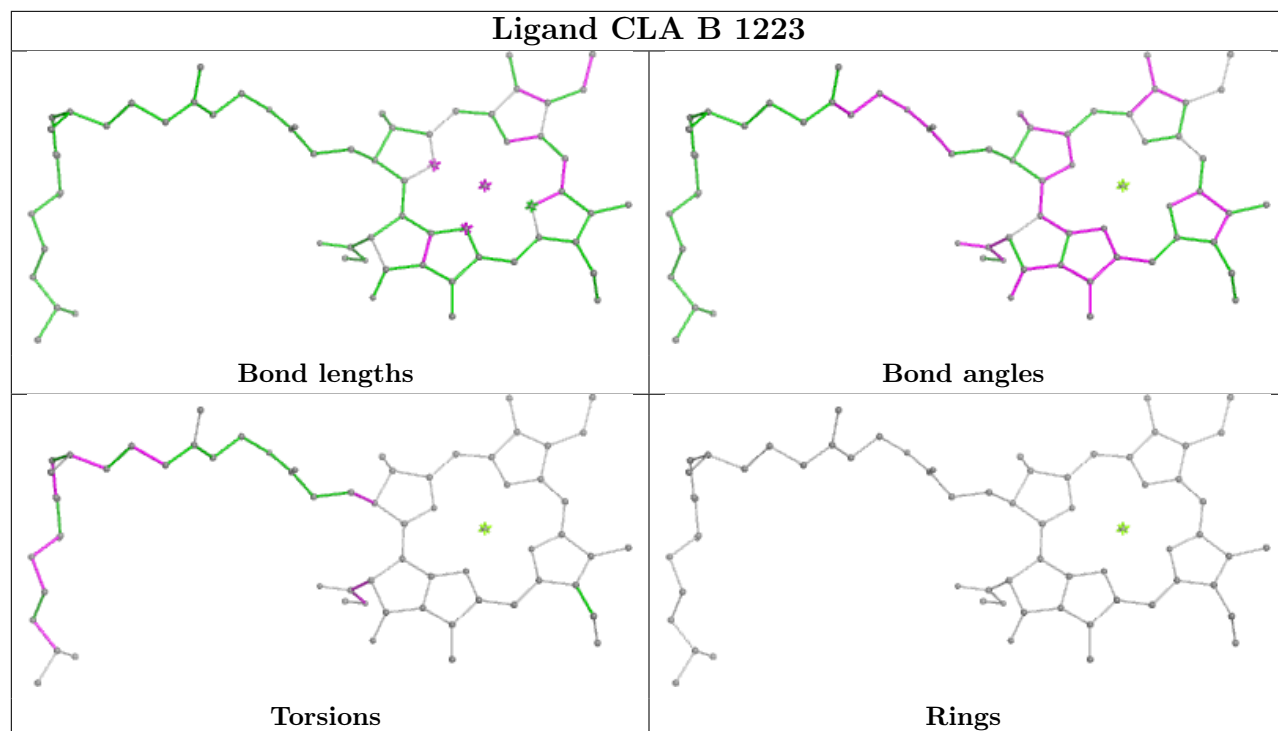
Ligand CLA 3 612



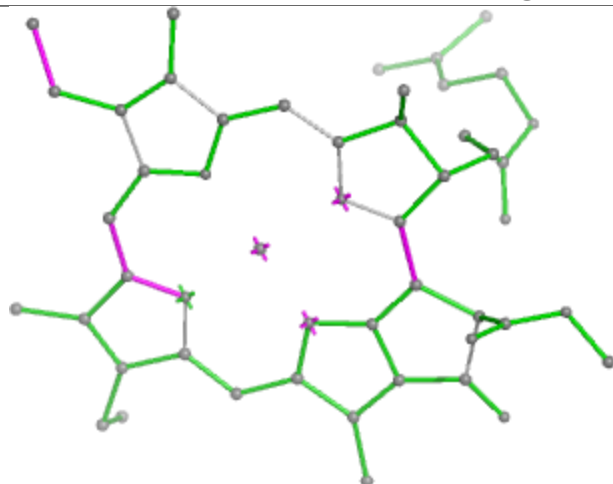
Ligand CLA 2 606



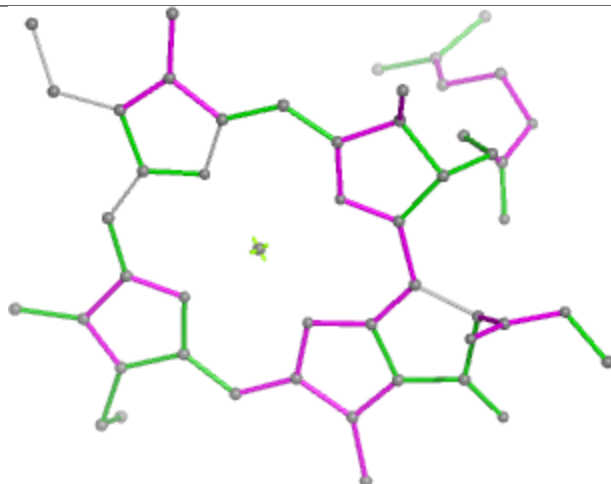




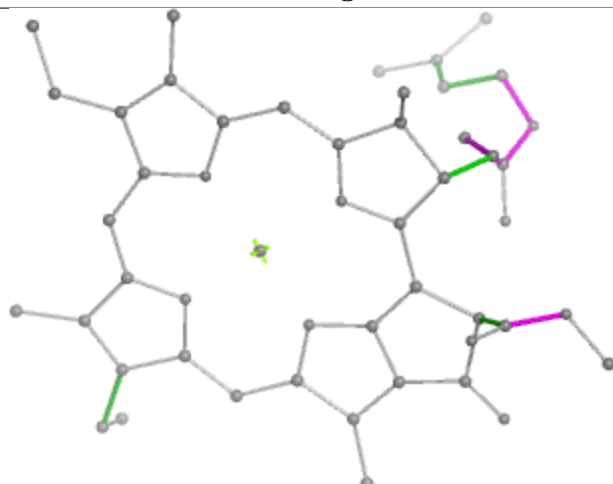
Ligand CLA 4 606



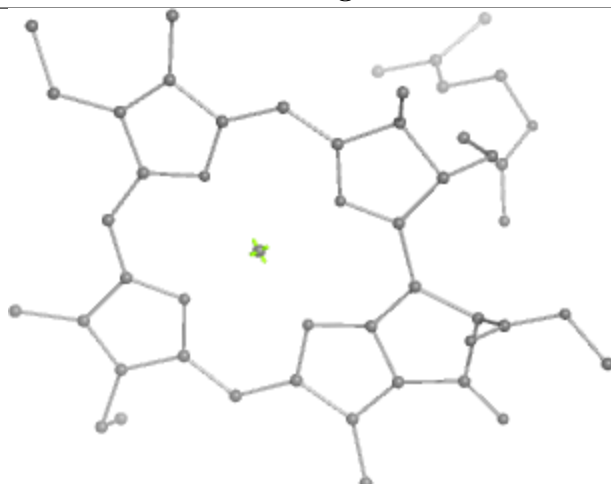
Bond lengths



Bond angles

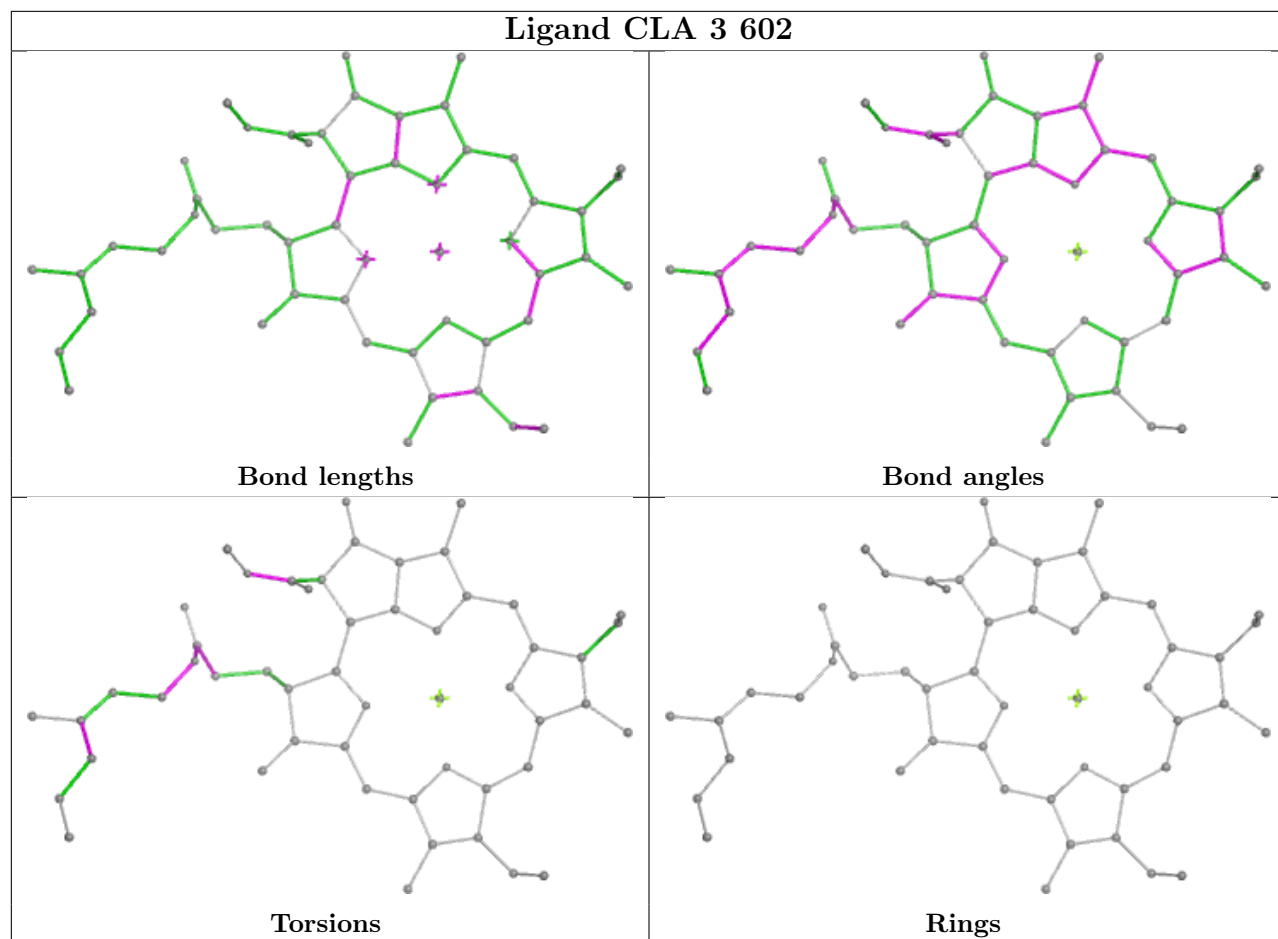


Torsions

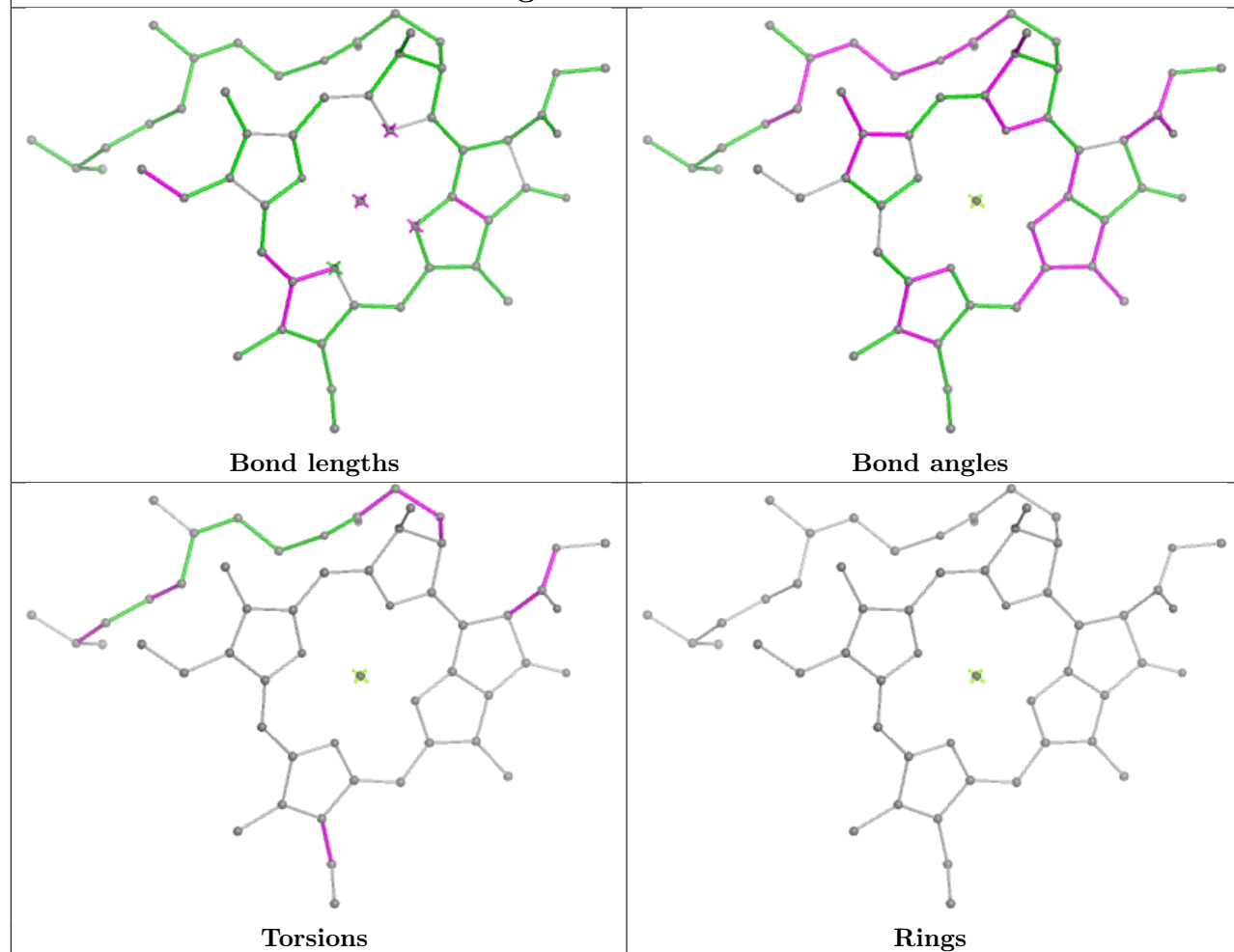


Rings

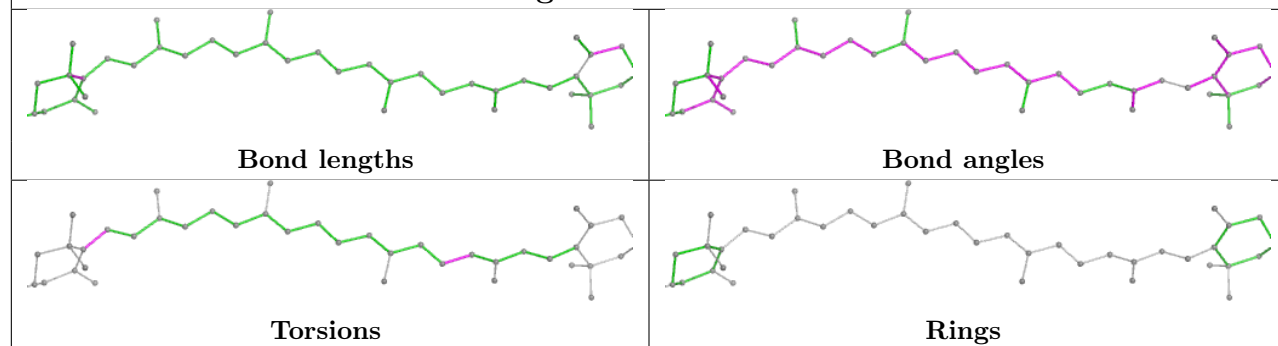
Ligand CLA 3 602

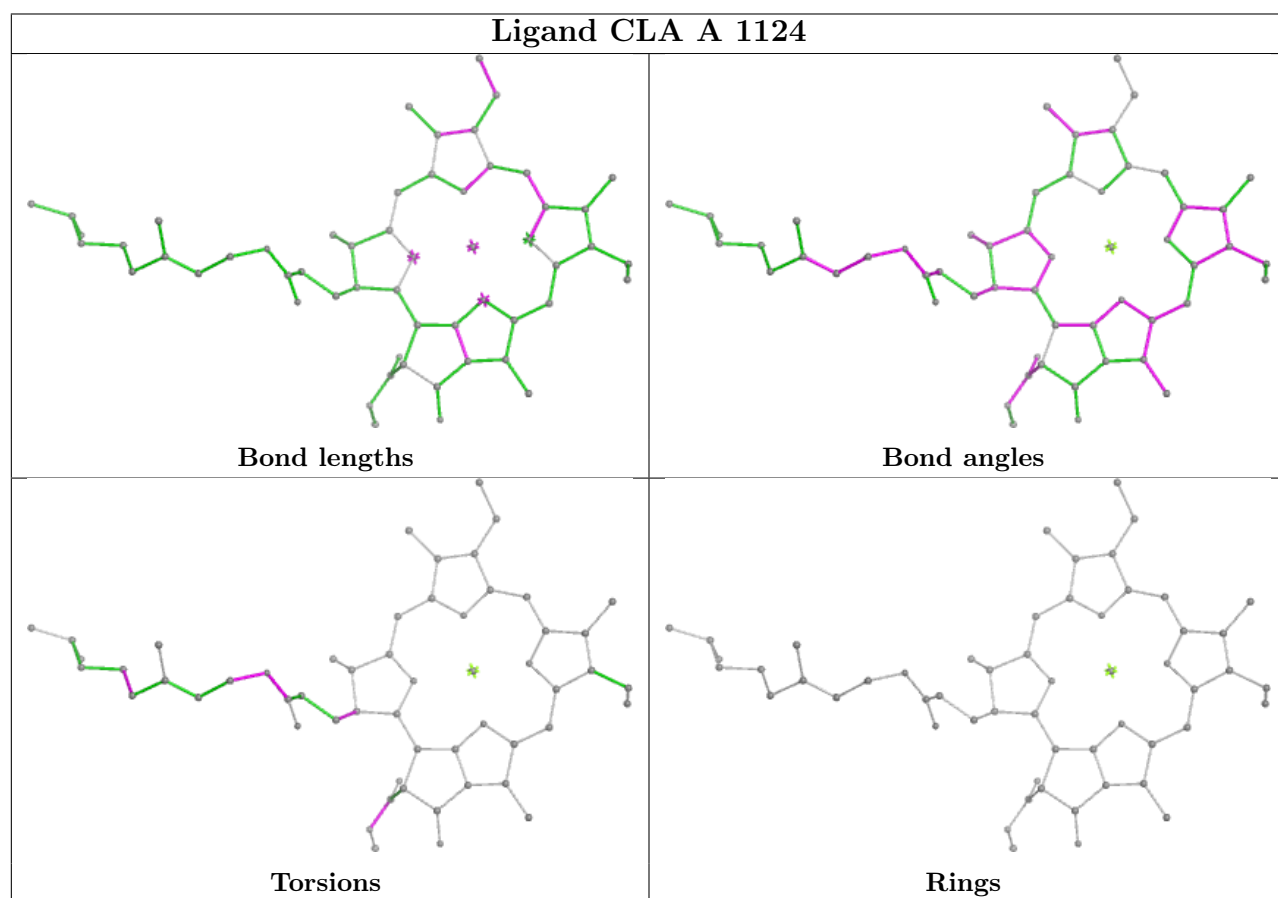
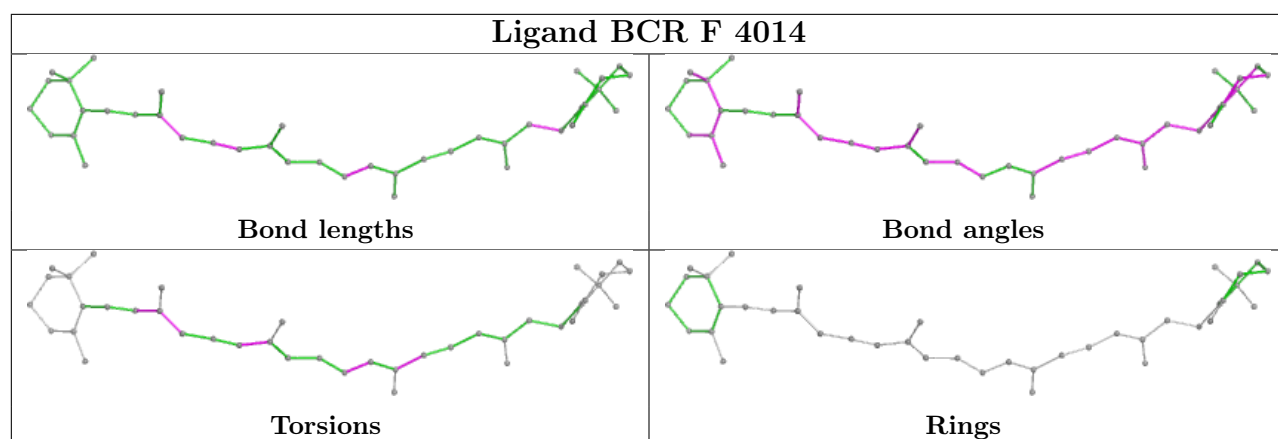


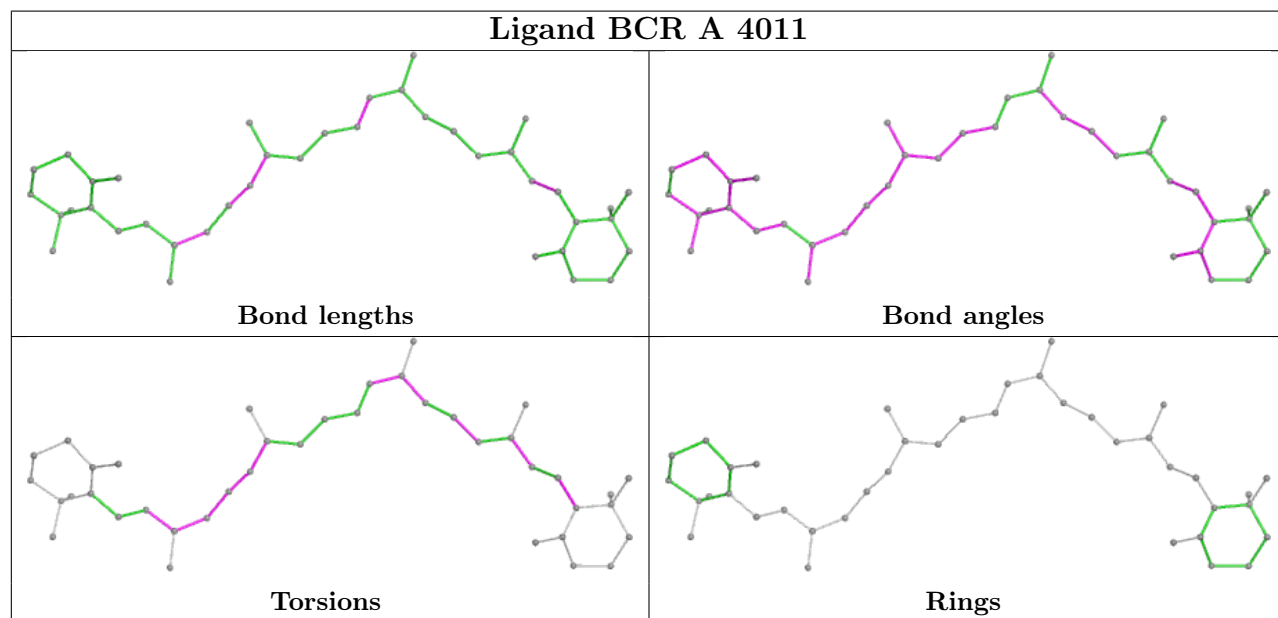
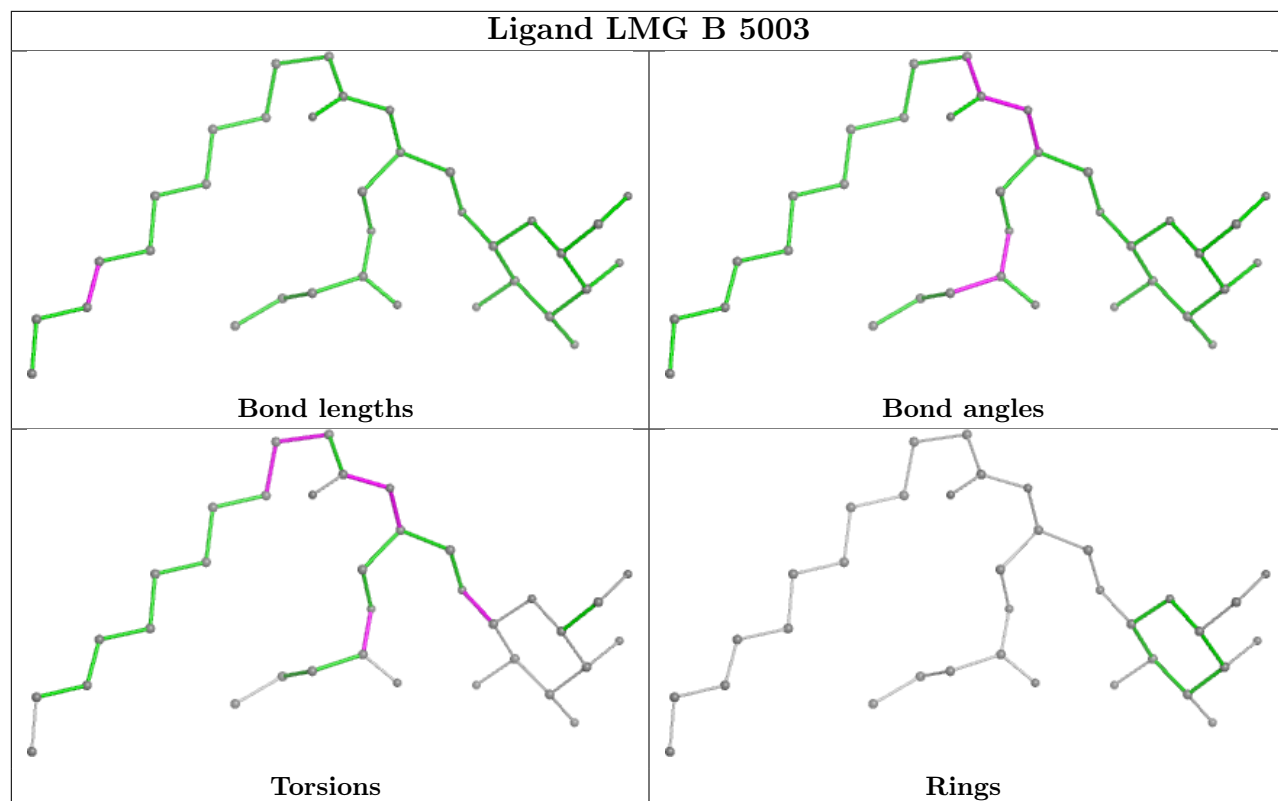
Ligand CLA 3 601



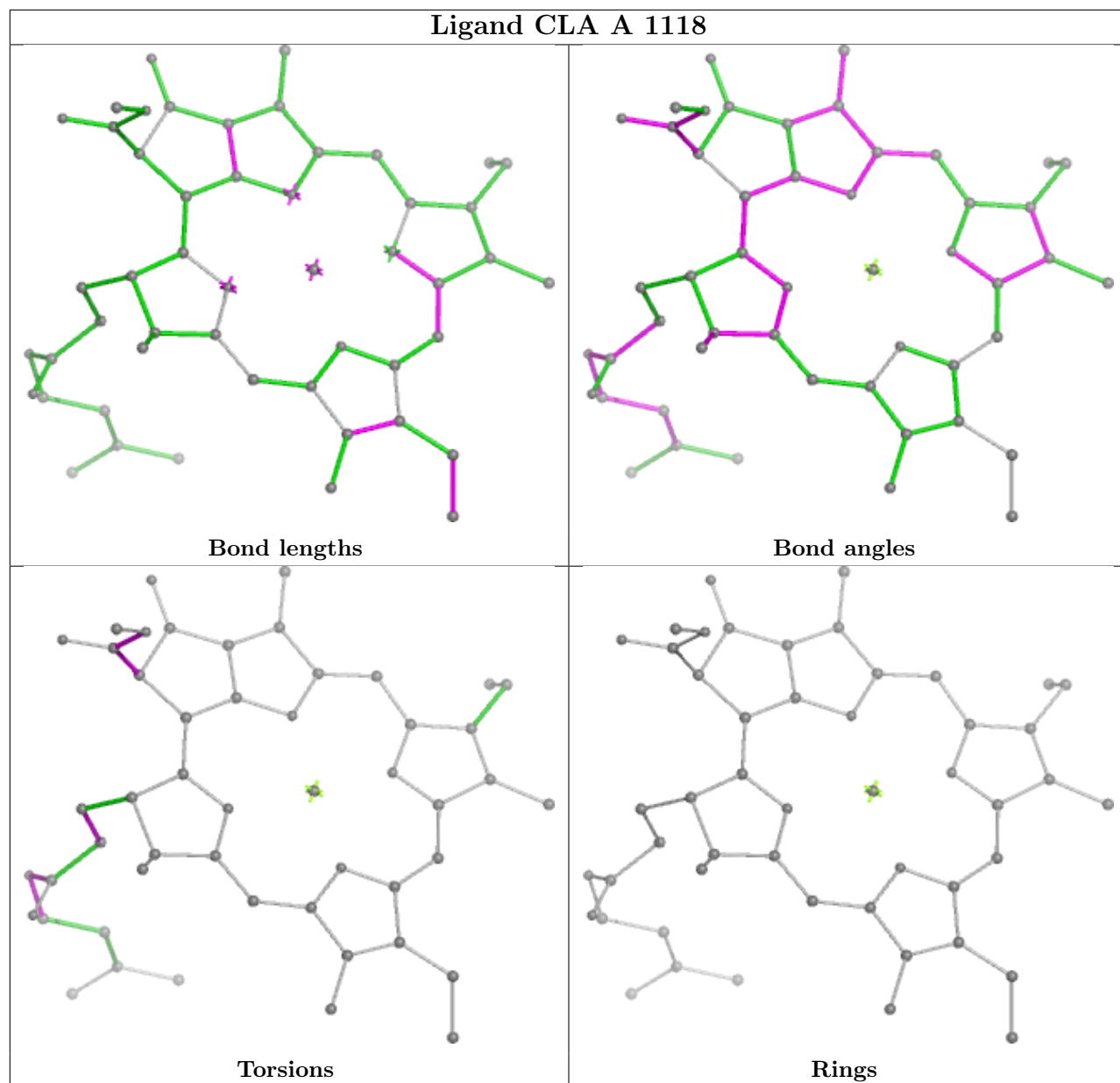
Ligand LUT 1 501

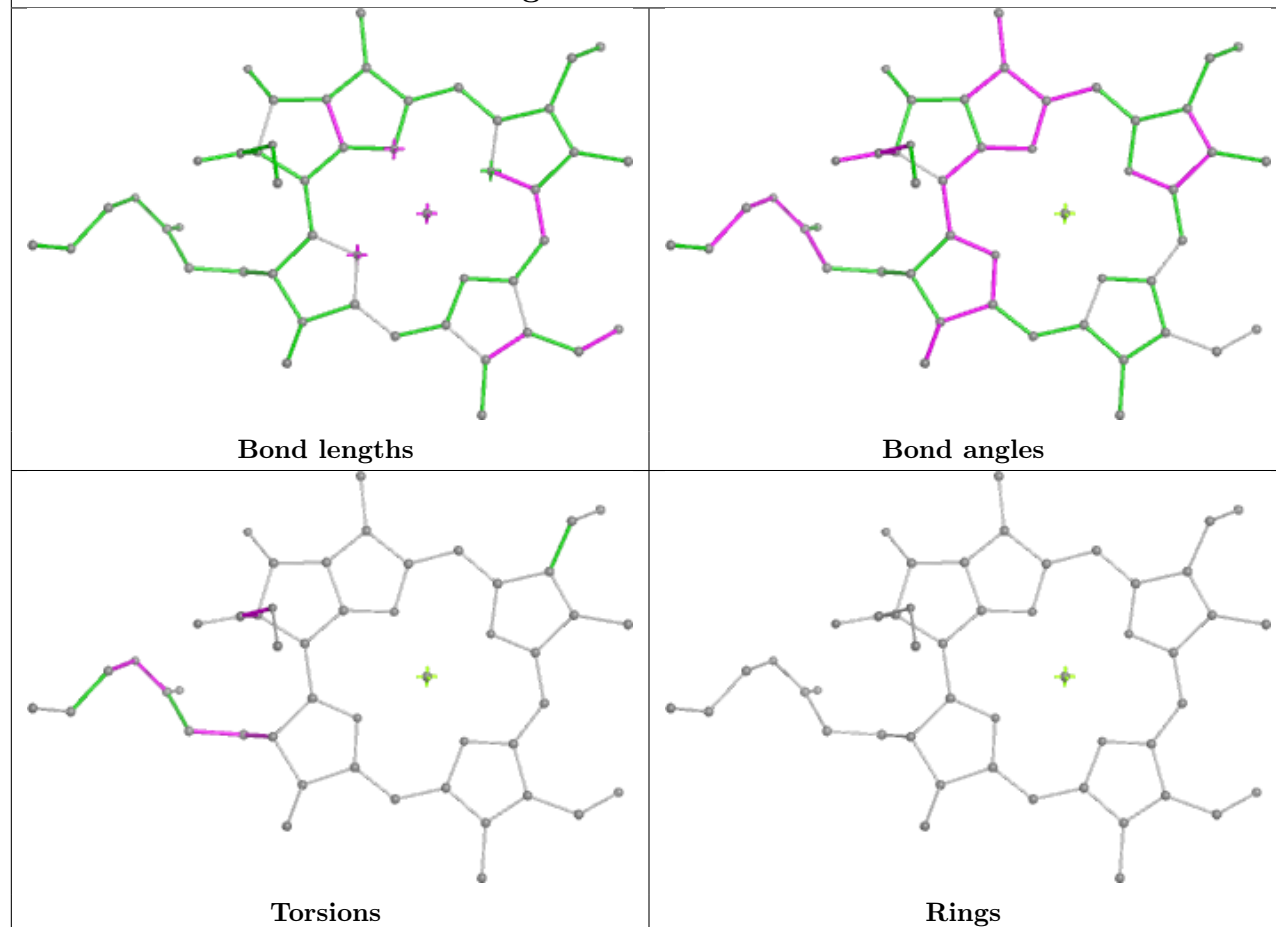
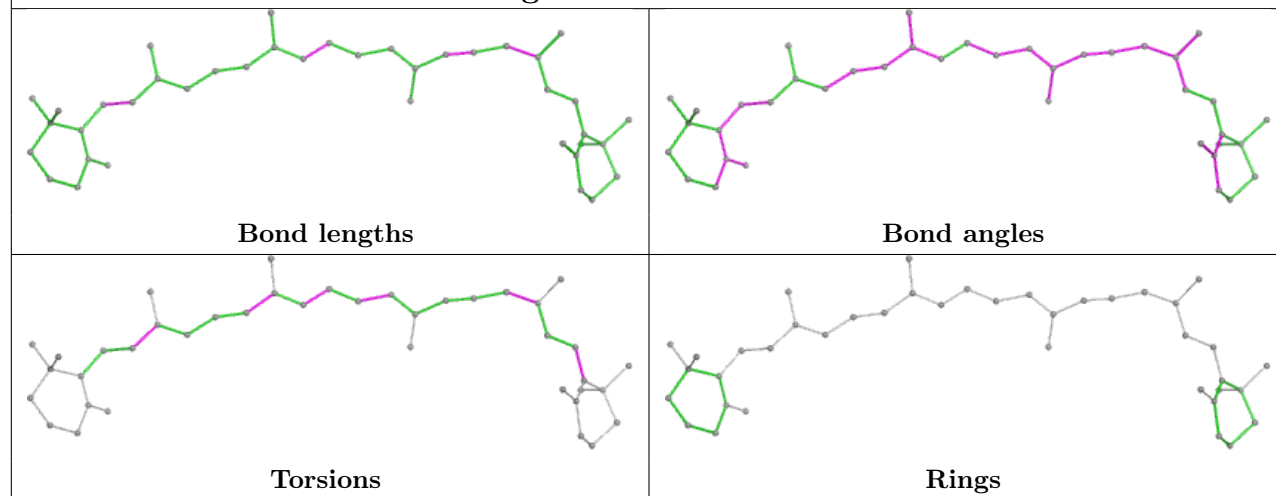


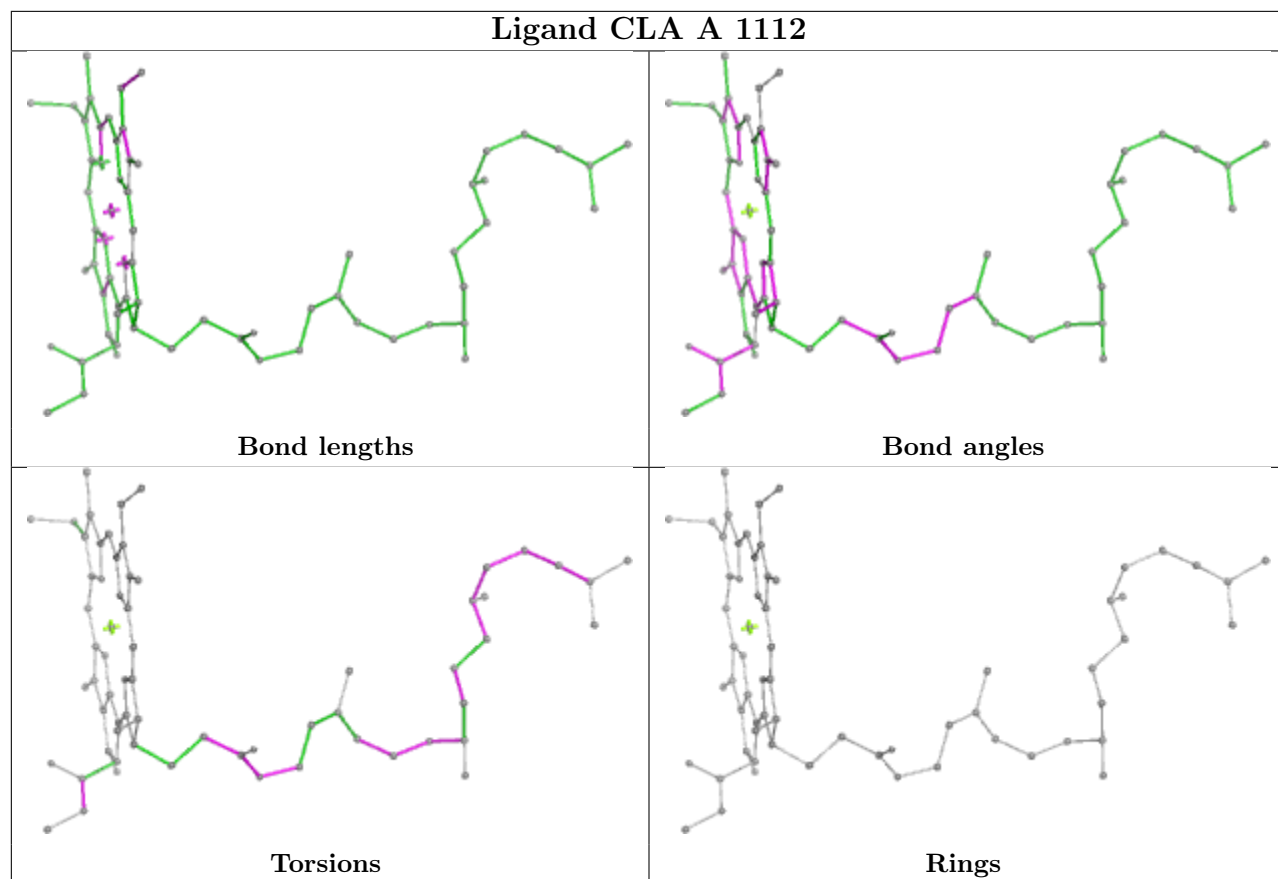


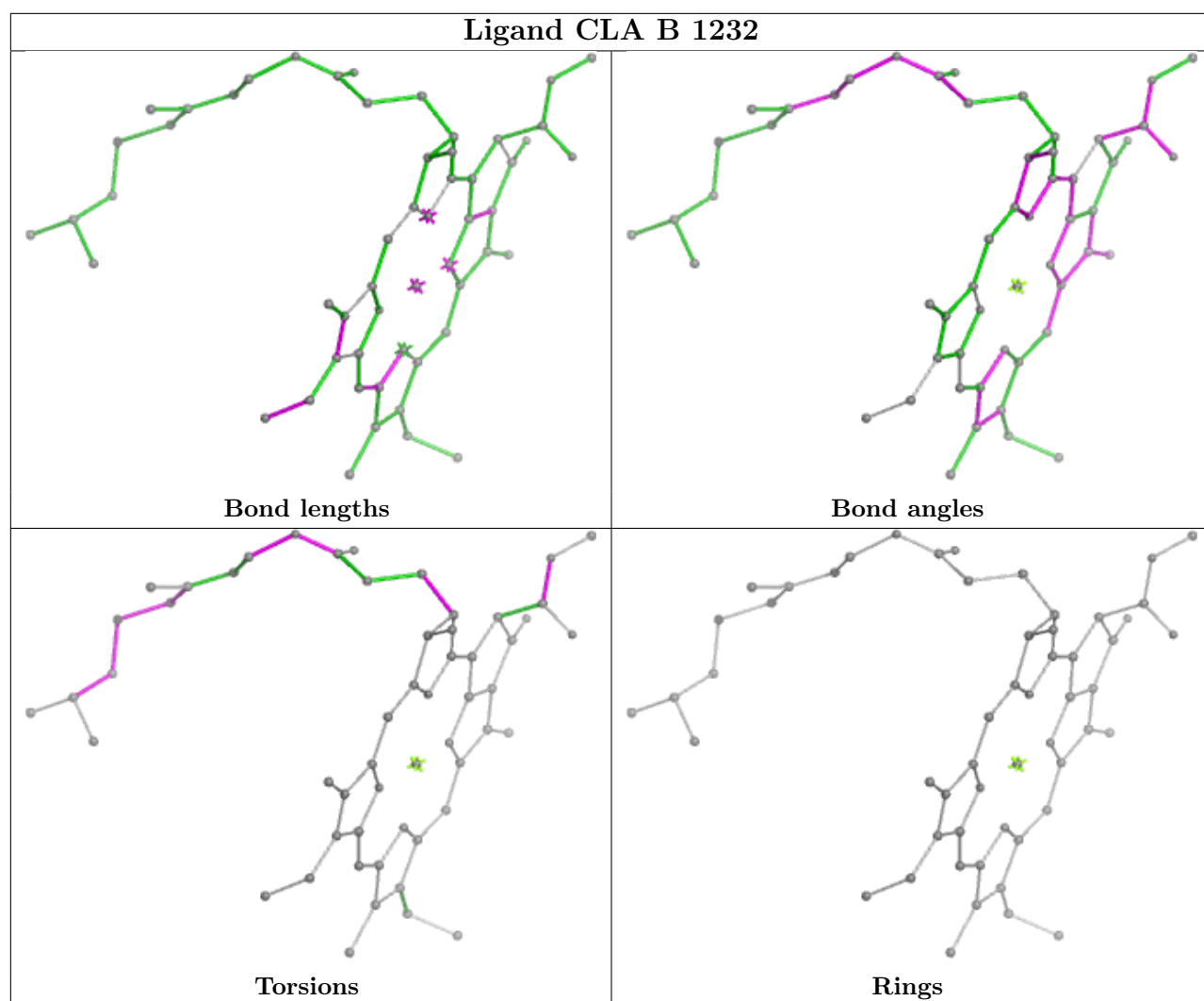


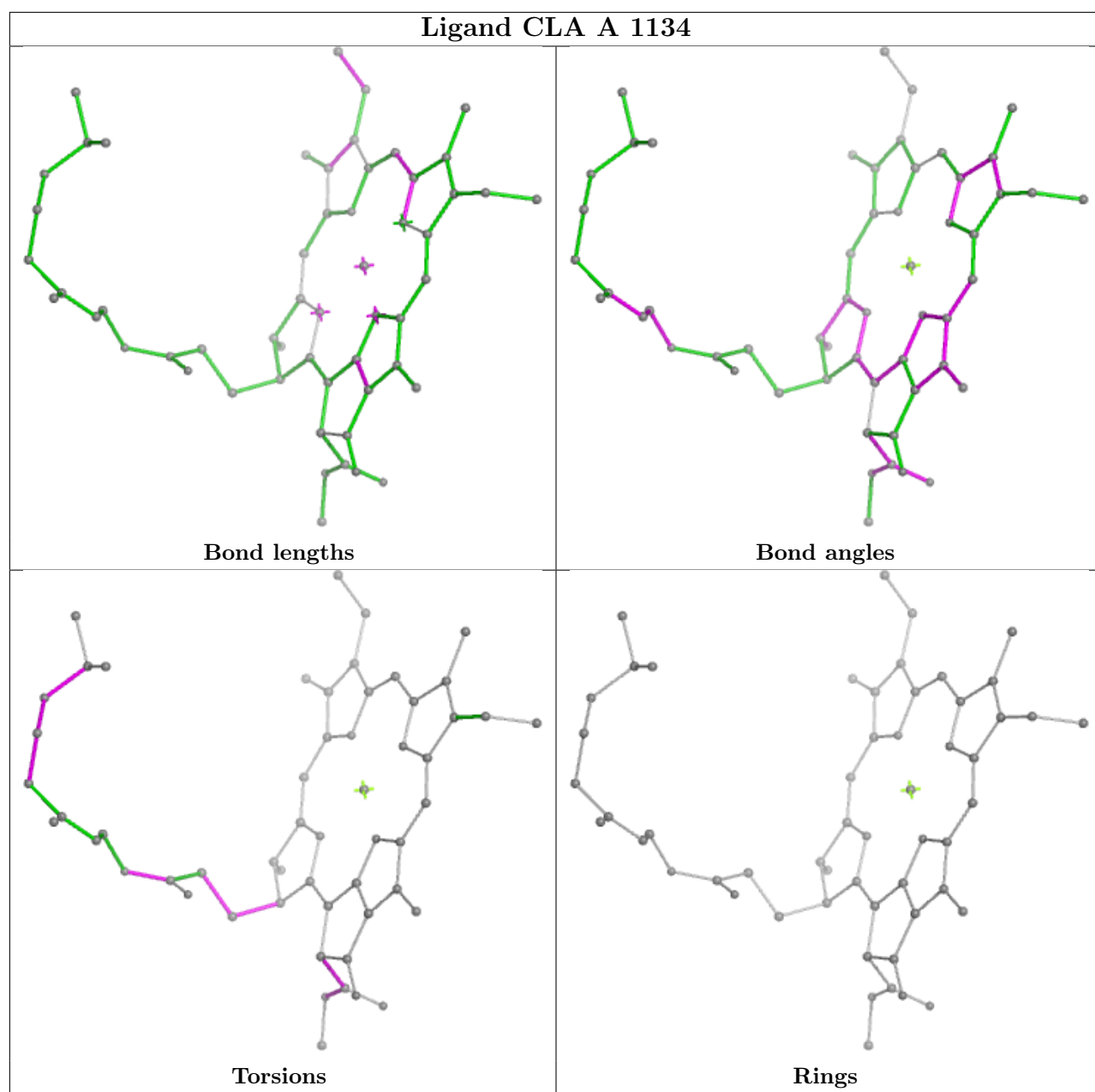
Ligand CLA A 1118

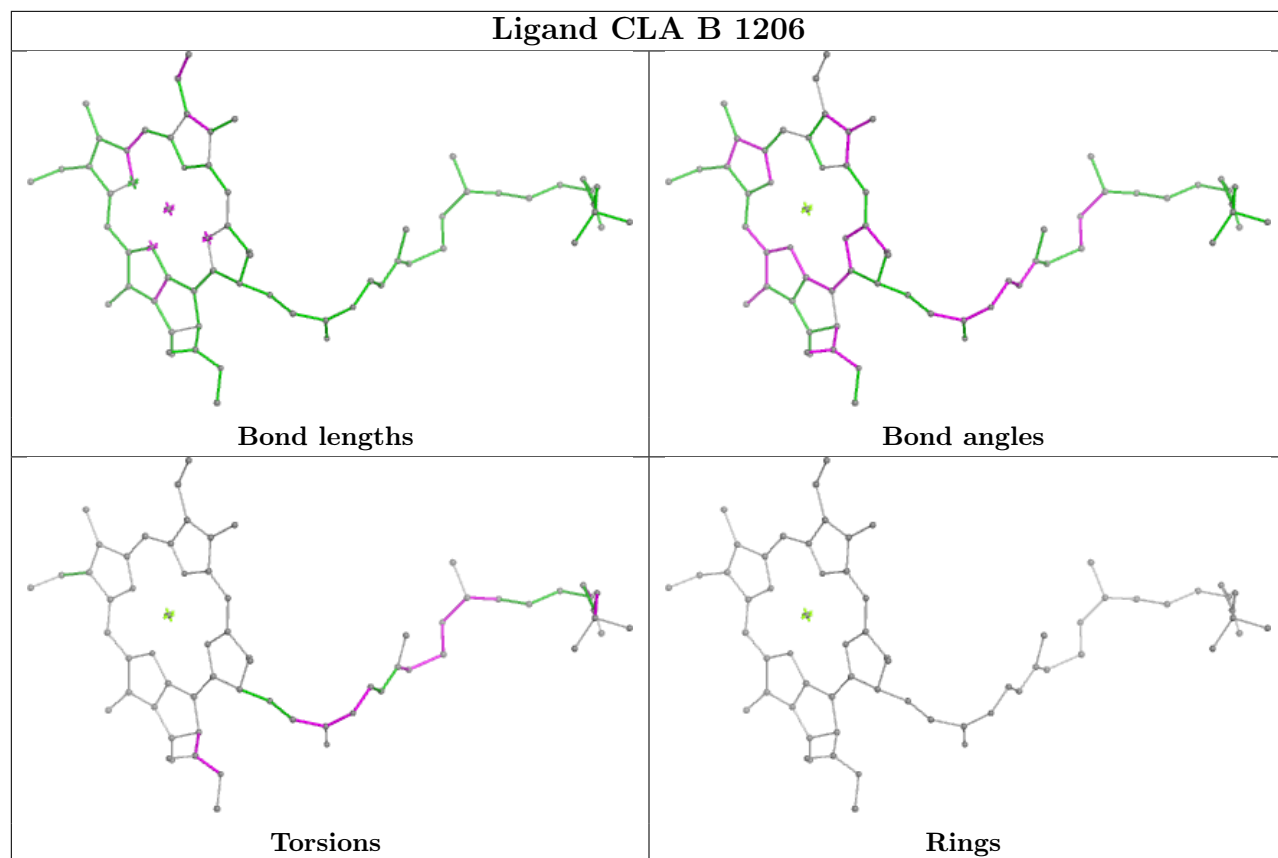


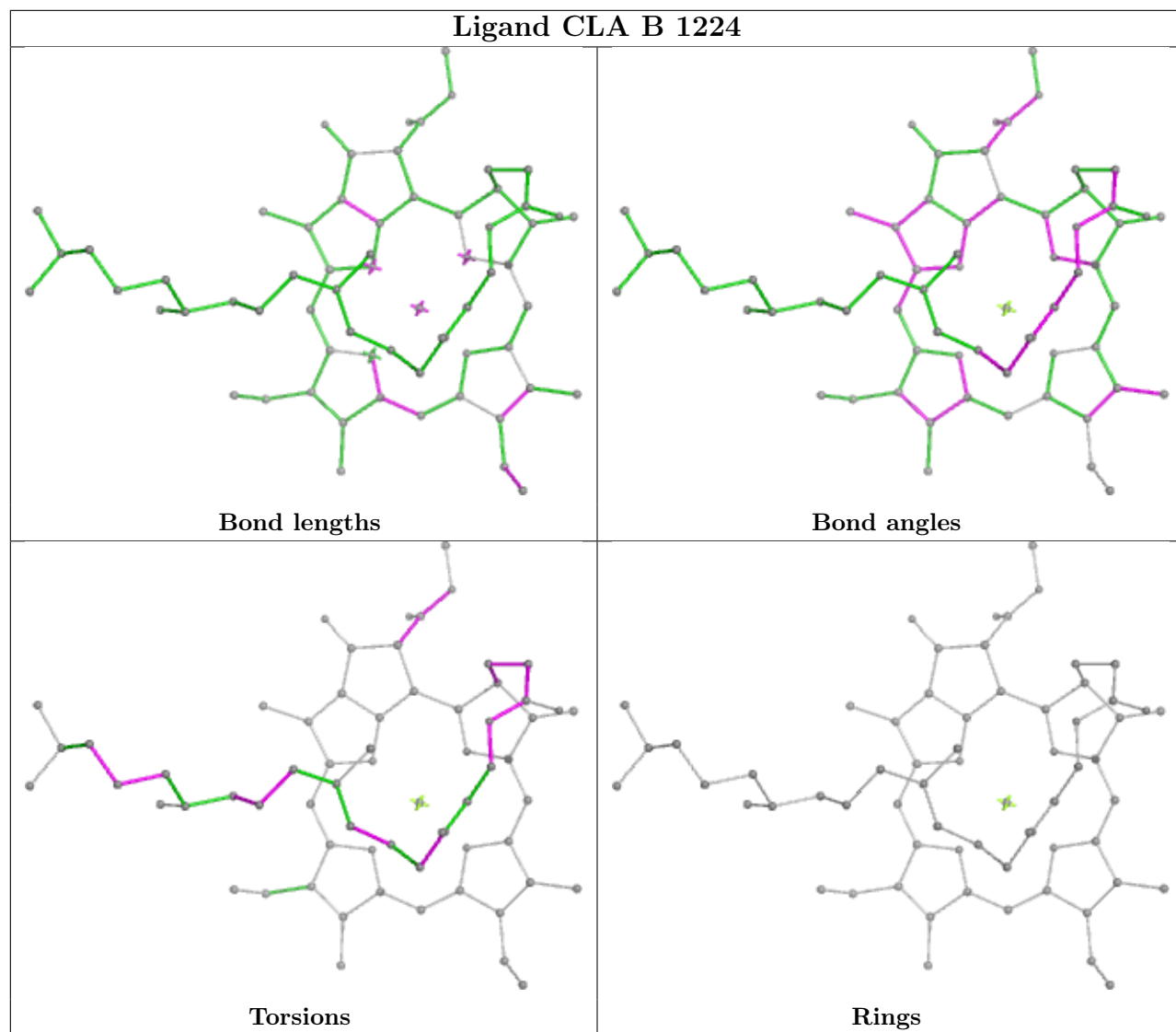
Ligand CLA K 1403**Ligand BCR B 4005**

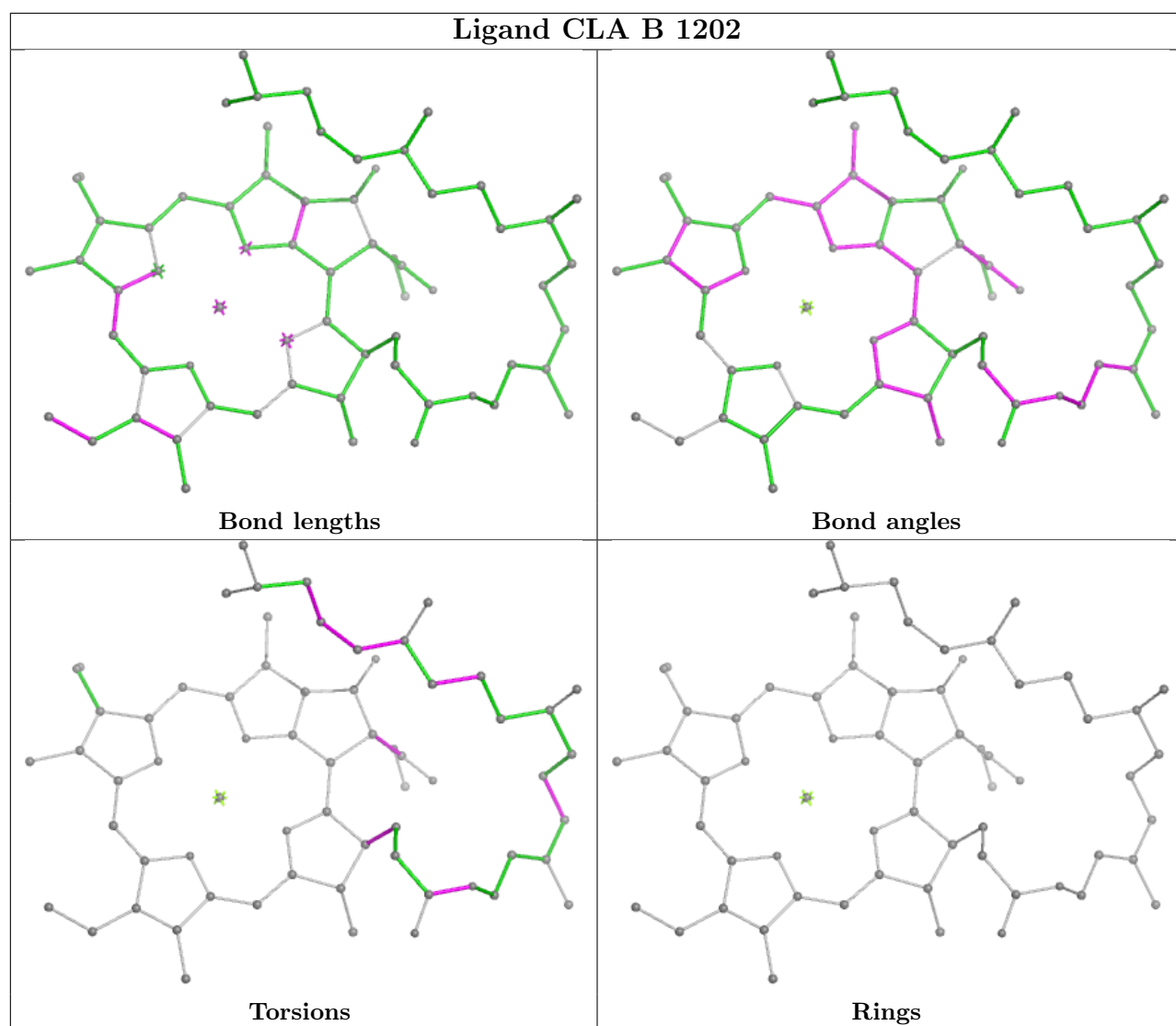




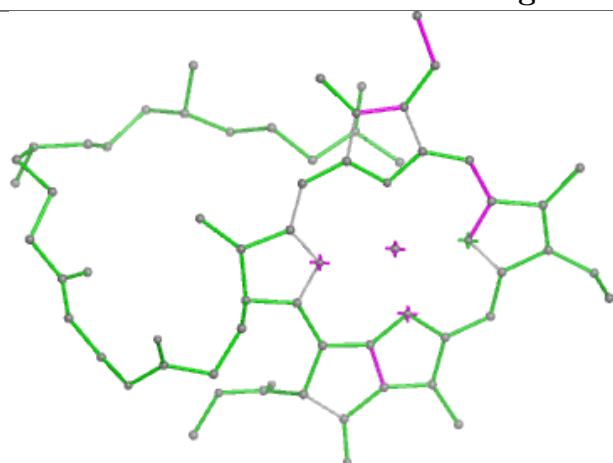




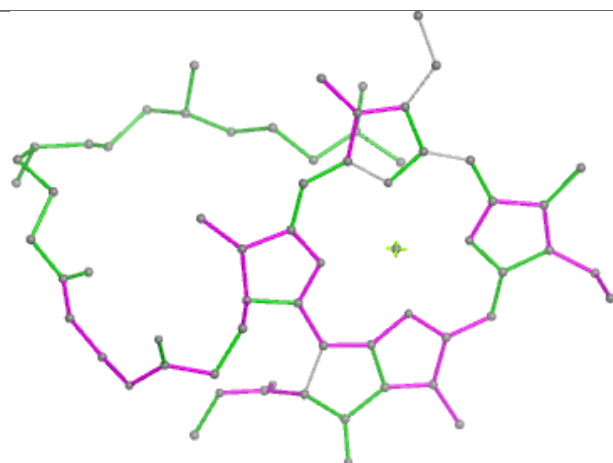




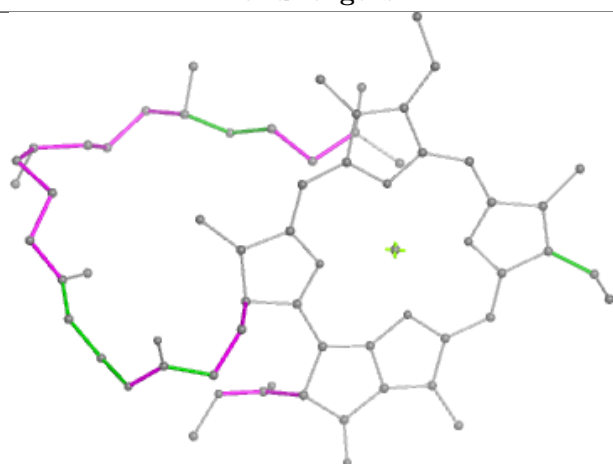
Ligand CLA 2 605



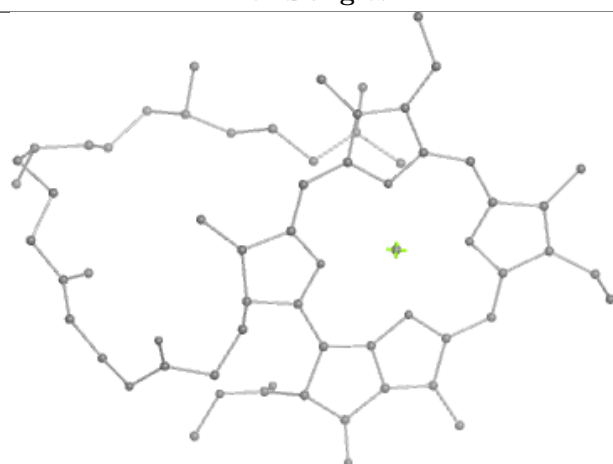
Bond lengths



Bond angles

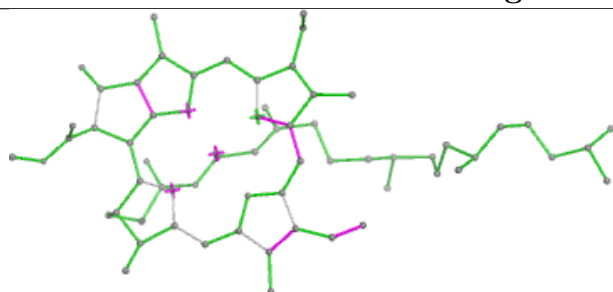


Torsions

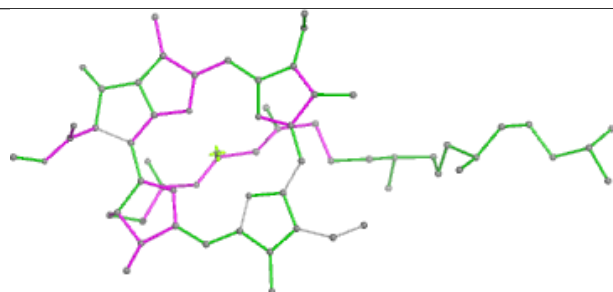


Rings

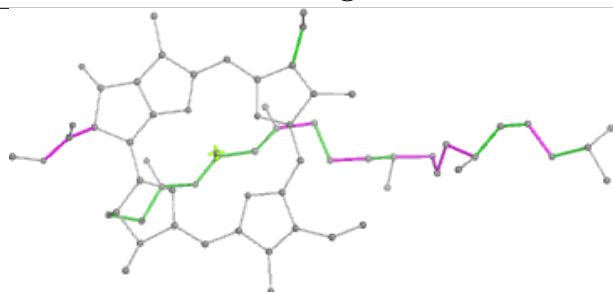
Ligand CLA A 1136



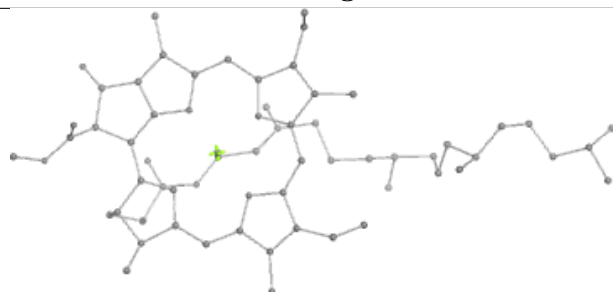
Bond lengths



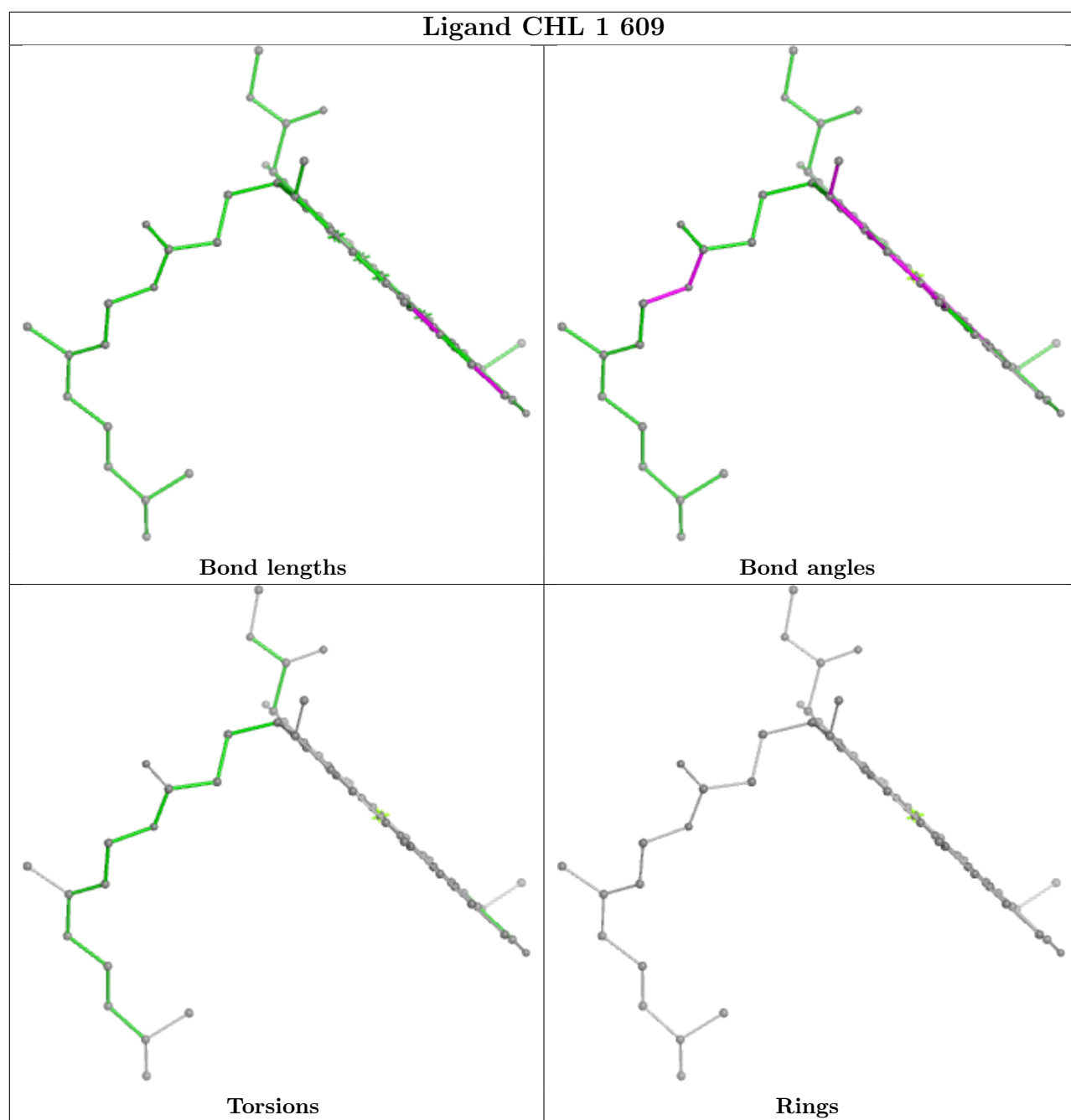
Bond angles

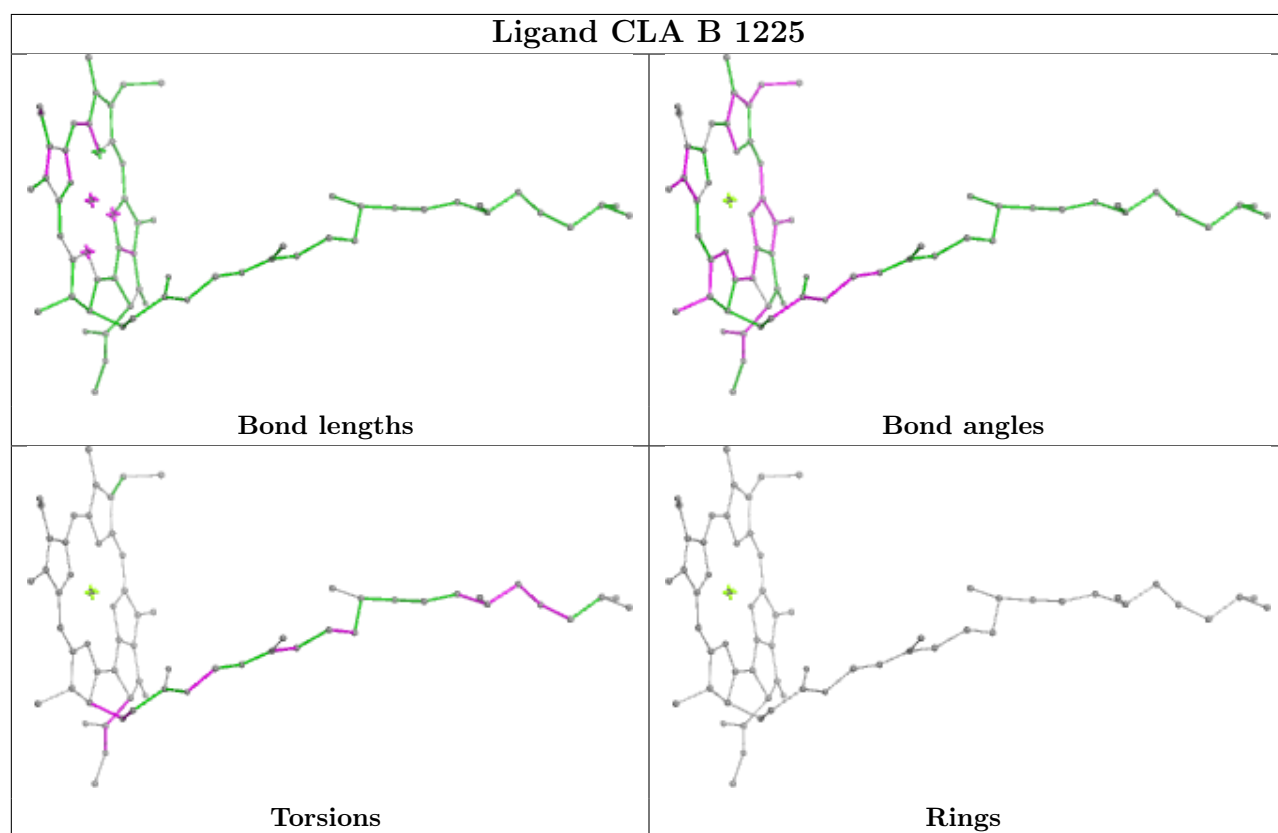
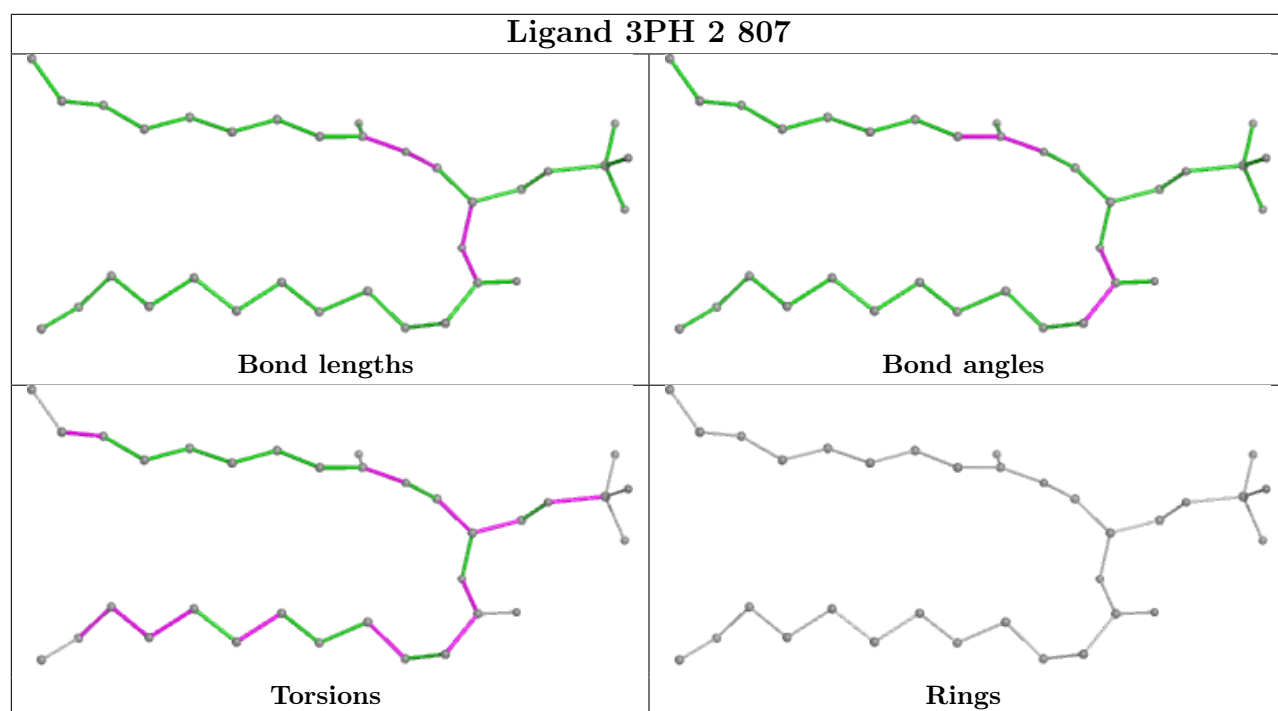


Torsions

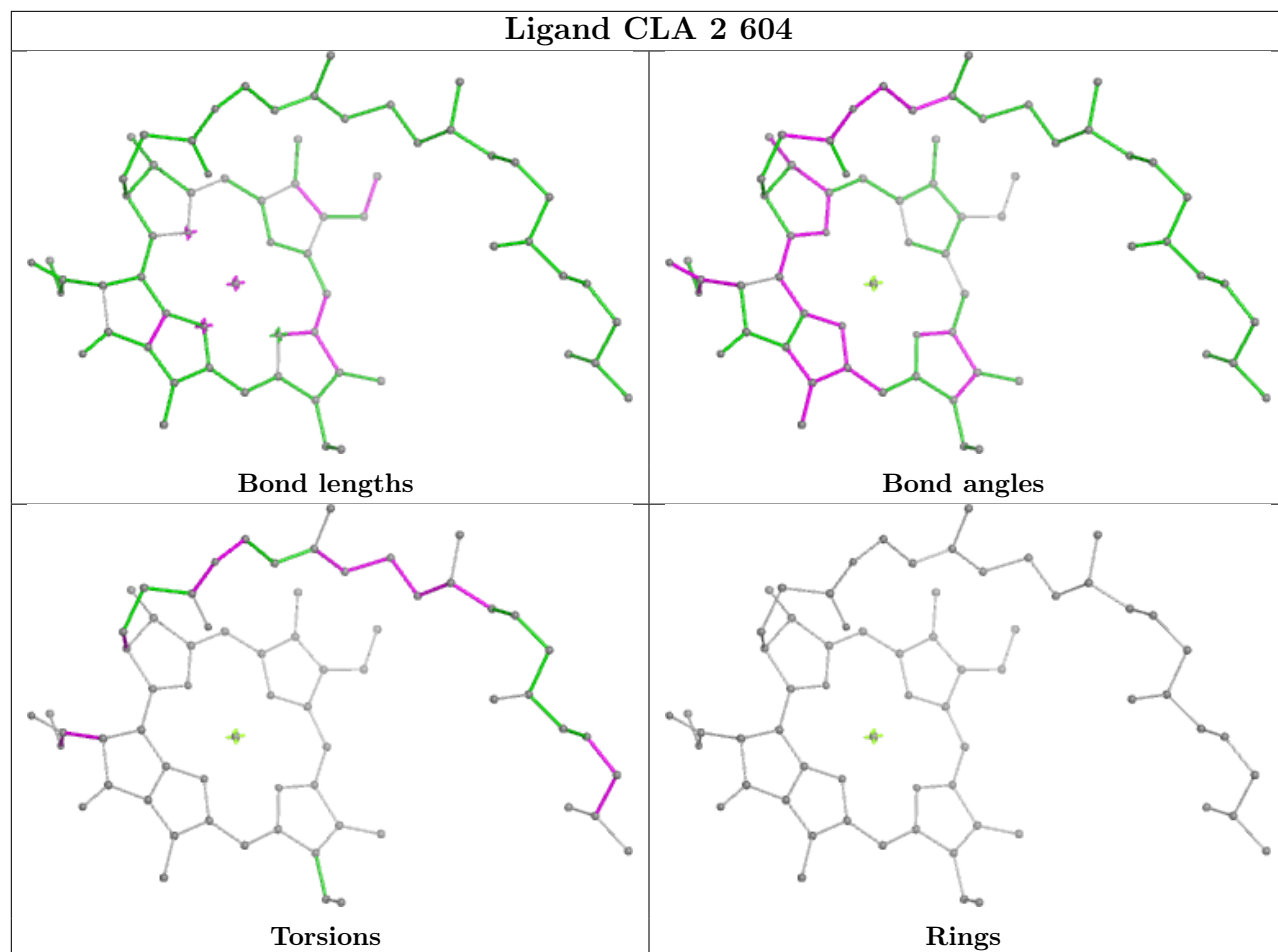


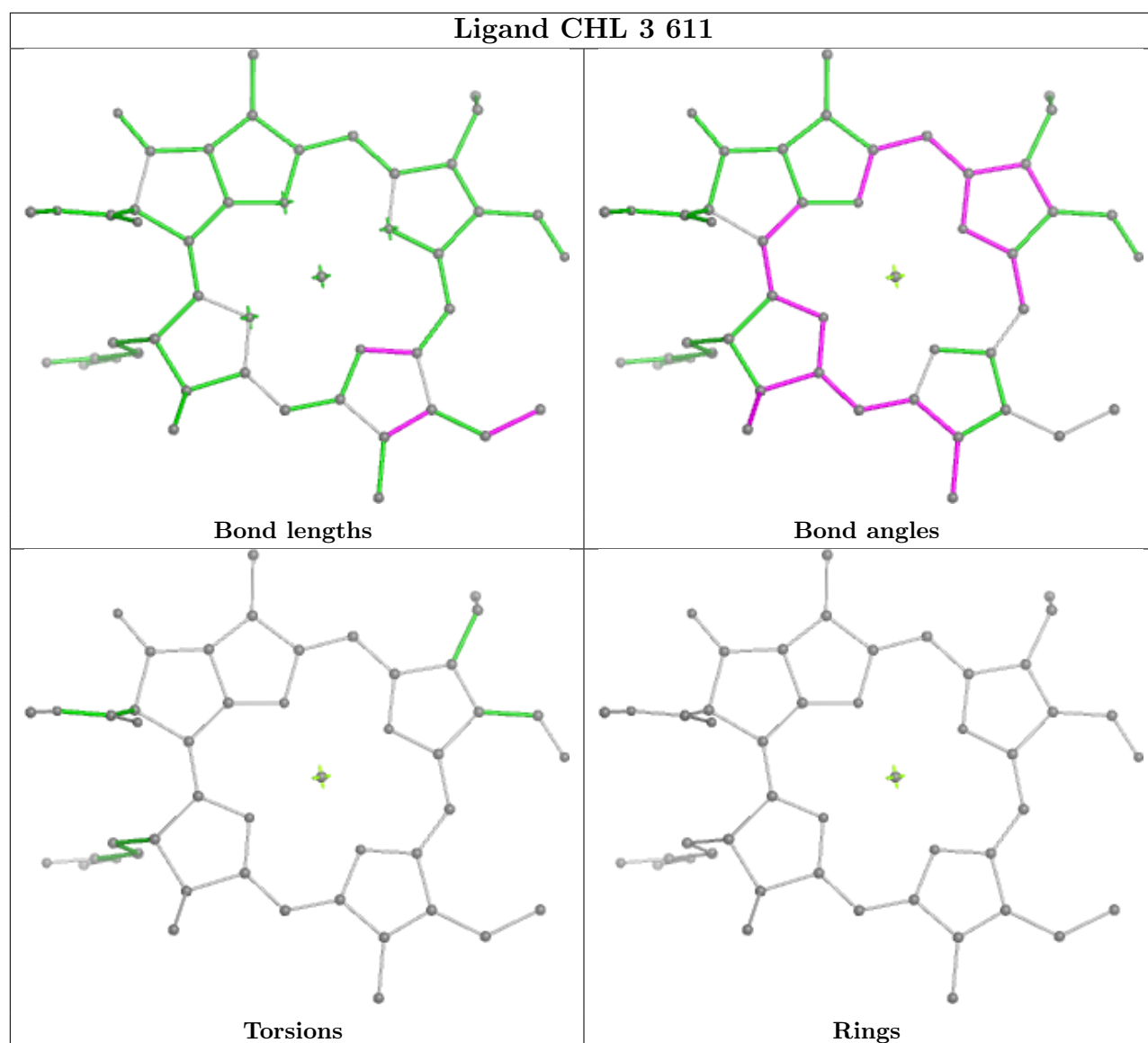
Rings





Ligand CLA 2 604





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
17	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	35:LEU	C	36:PRO	N	1.19

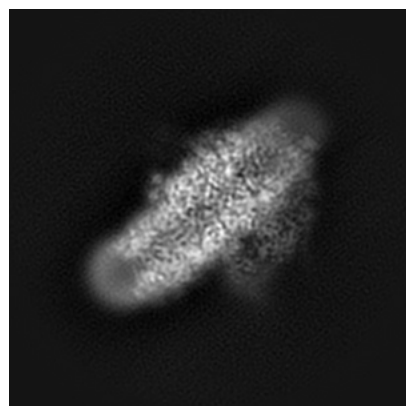
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10798. These allow visual inspection of the internal detail of the map and identification of artifacts.

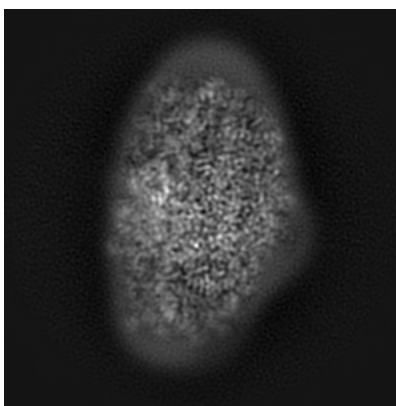
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

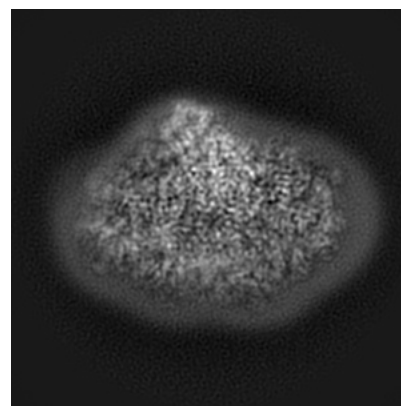
6.1.1 Primary map



X

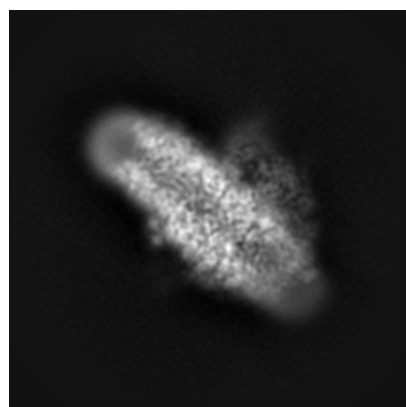


Y

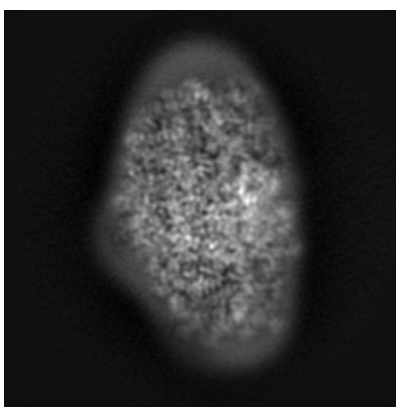


Z

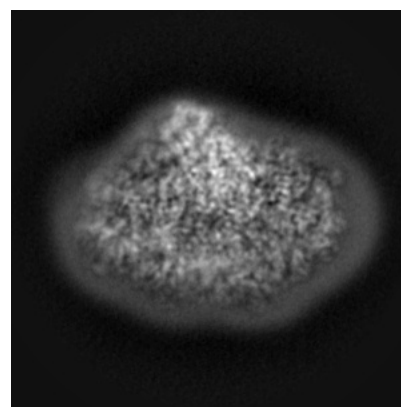
6.1.2 Raw map



X



Y

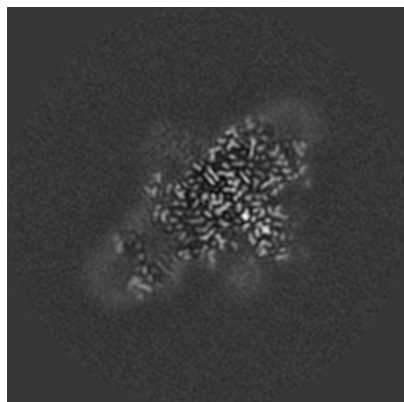


Z

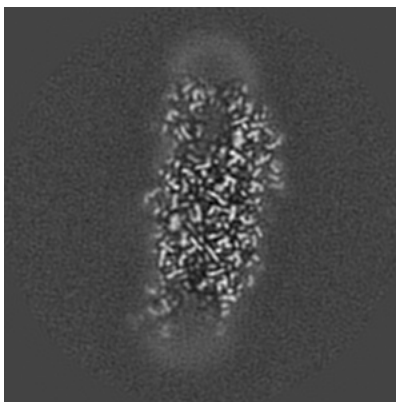
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

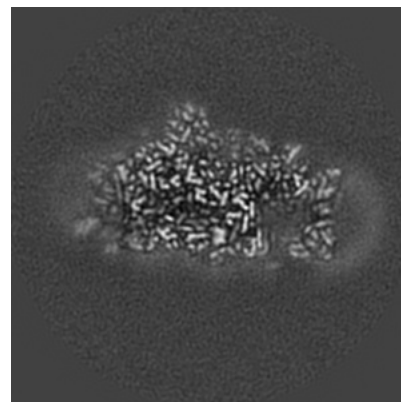
6.2.1 Primary map



X Index: 150

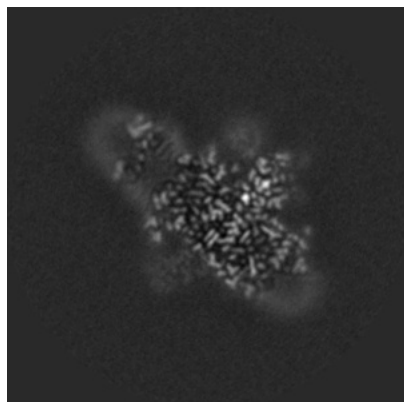


Y Index: 150

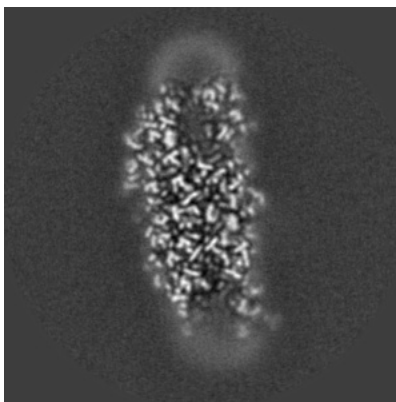


Z Index: 150

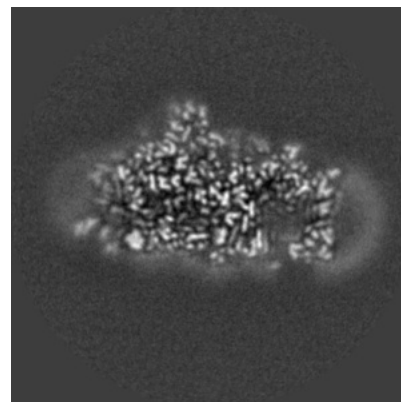
6.2.2 Raw map



X Index: 150



Y Index: 150

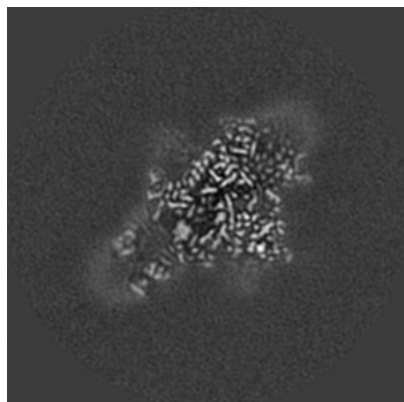


Z Index: 150

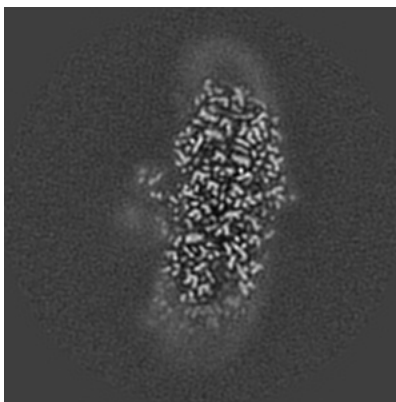
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

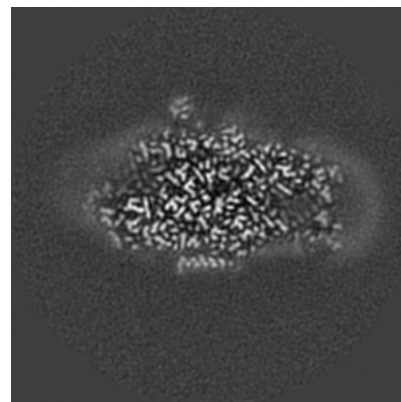
6.3.1 Primary map



X Index: 154

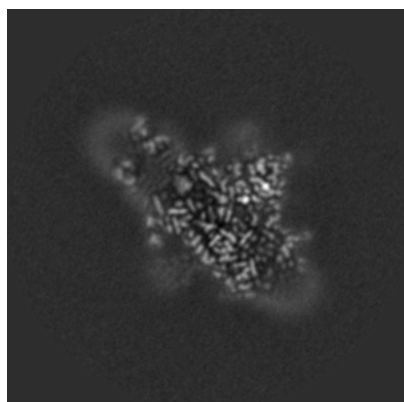


Y Index: 164

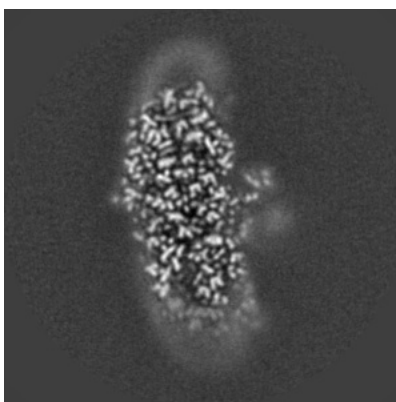


Z Index: 161

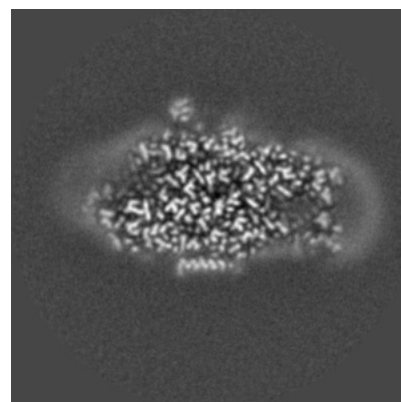
6.3.2 Raw map



X Index: 153



Y Index: 164

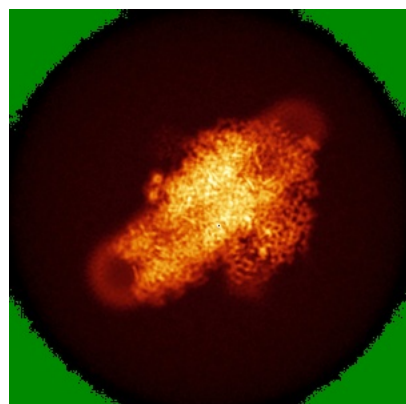


Z Index: 138

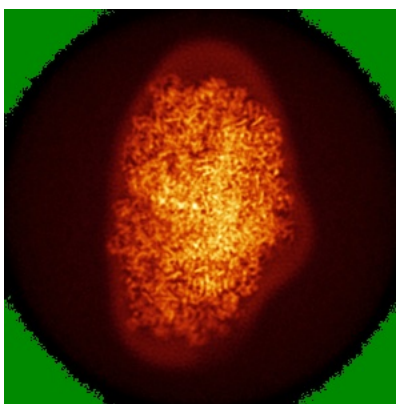
The images above show the largest variance slices of the map in three orthogonal directions.

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

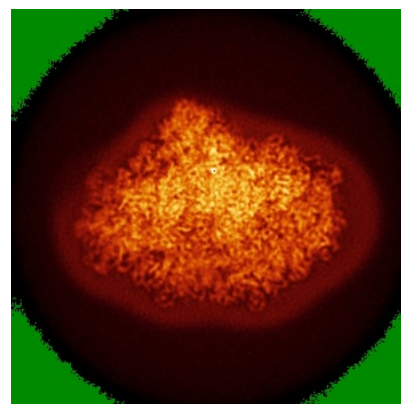
6.4.1 Primary map



X

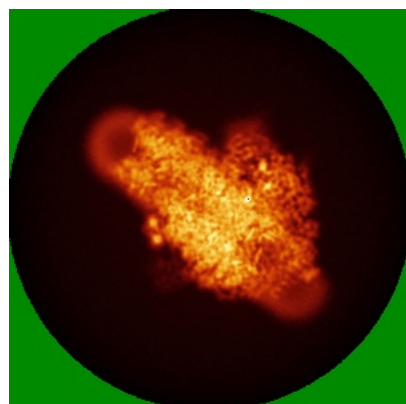


Y

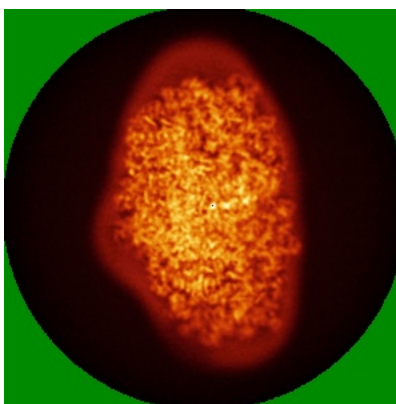


Z

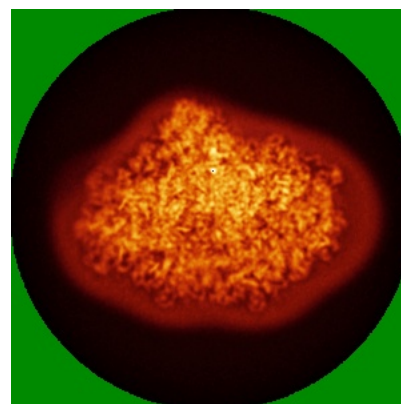
6.4.2 Raw map



X



Y

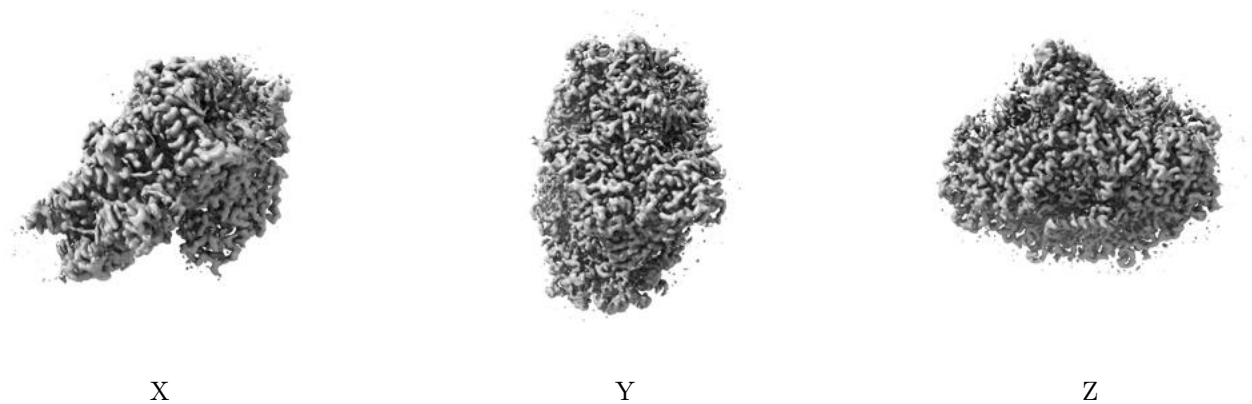


Z

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

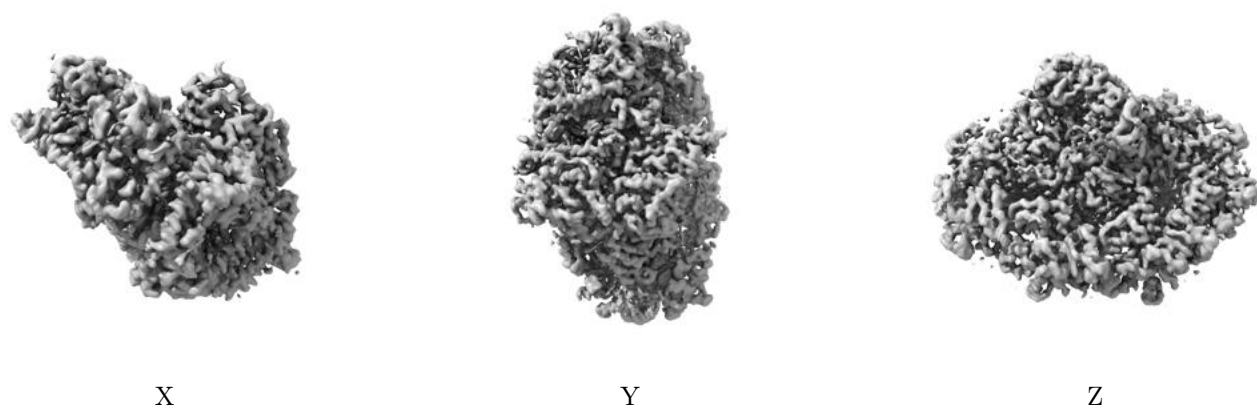
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

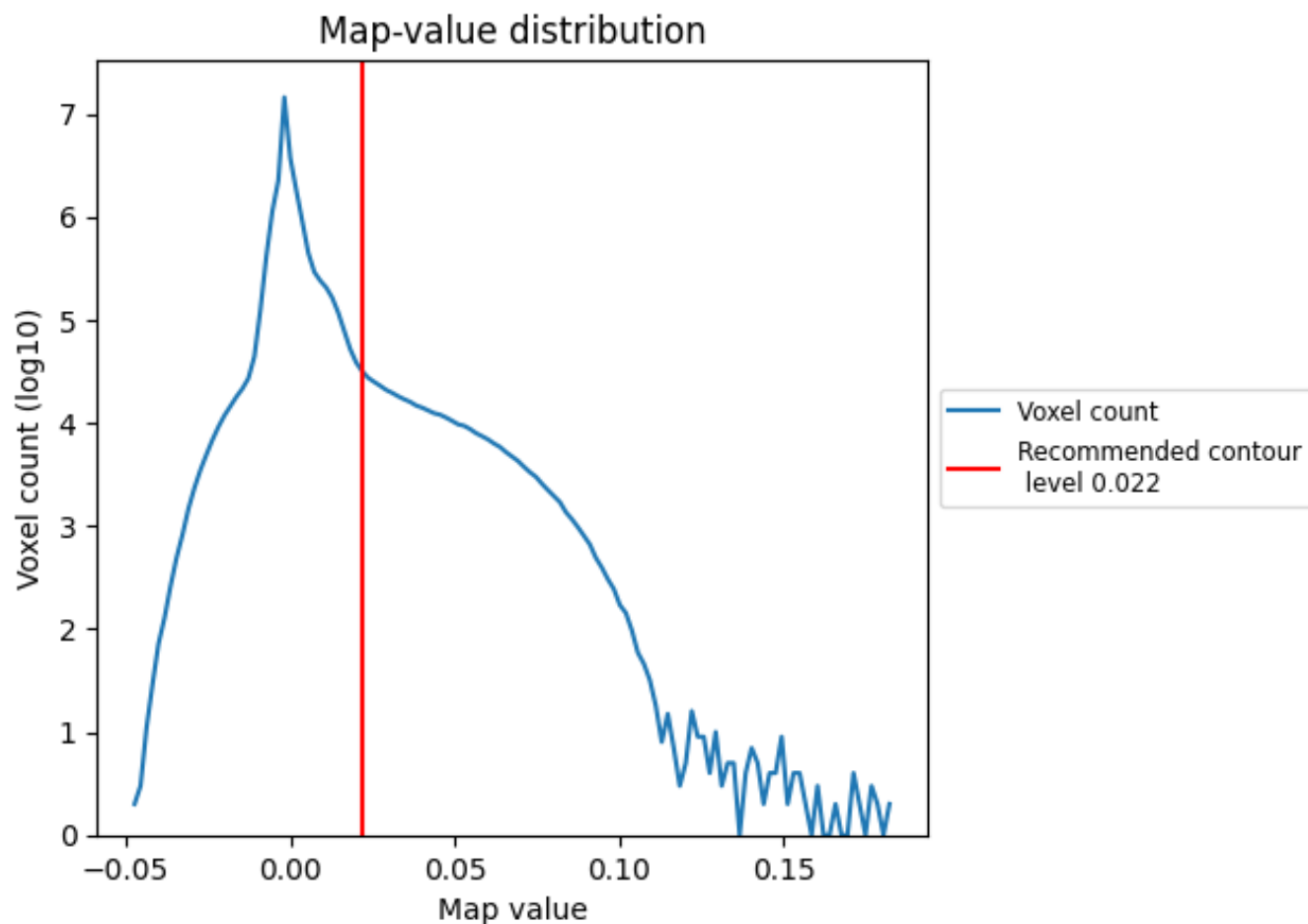
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

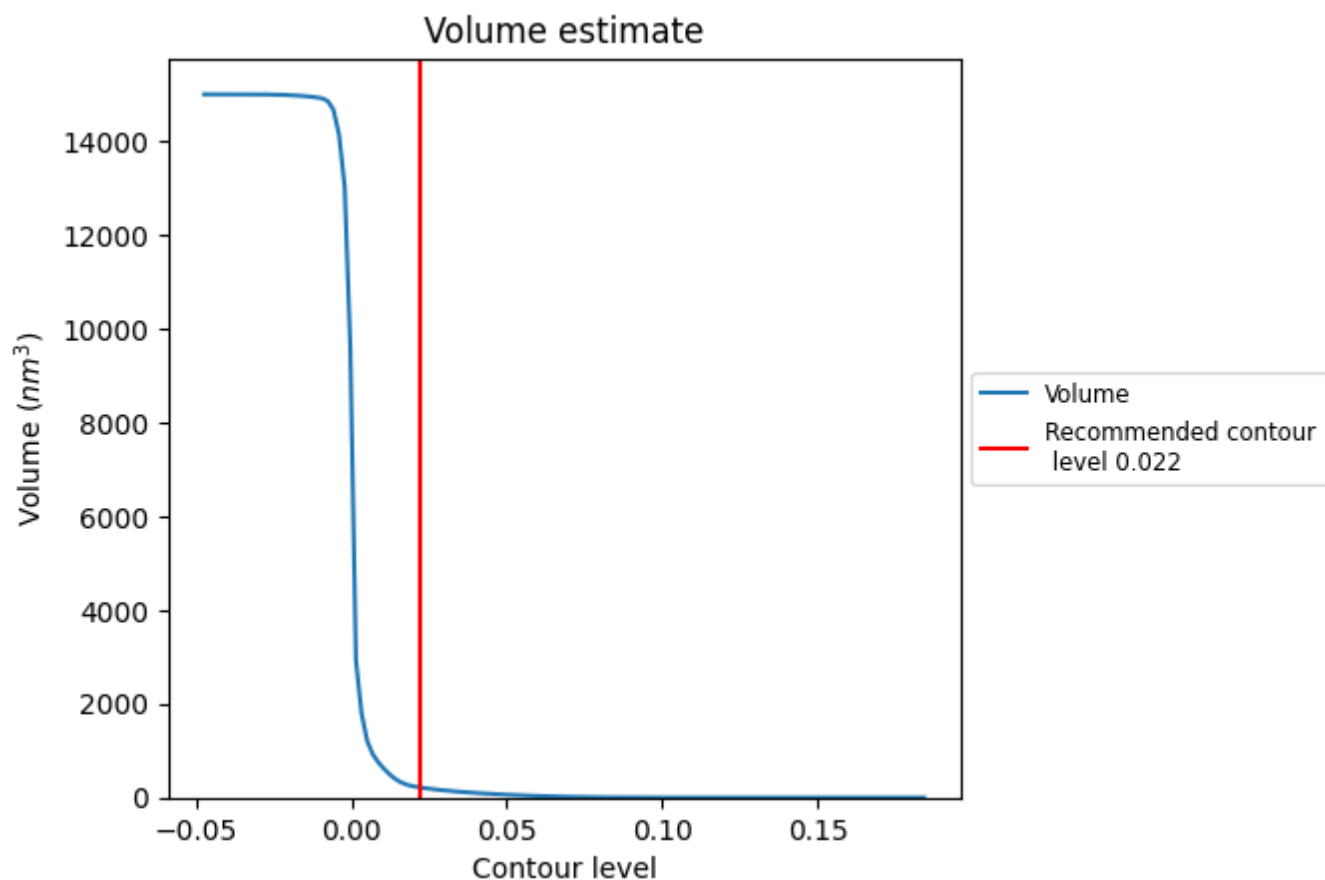
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

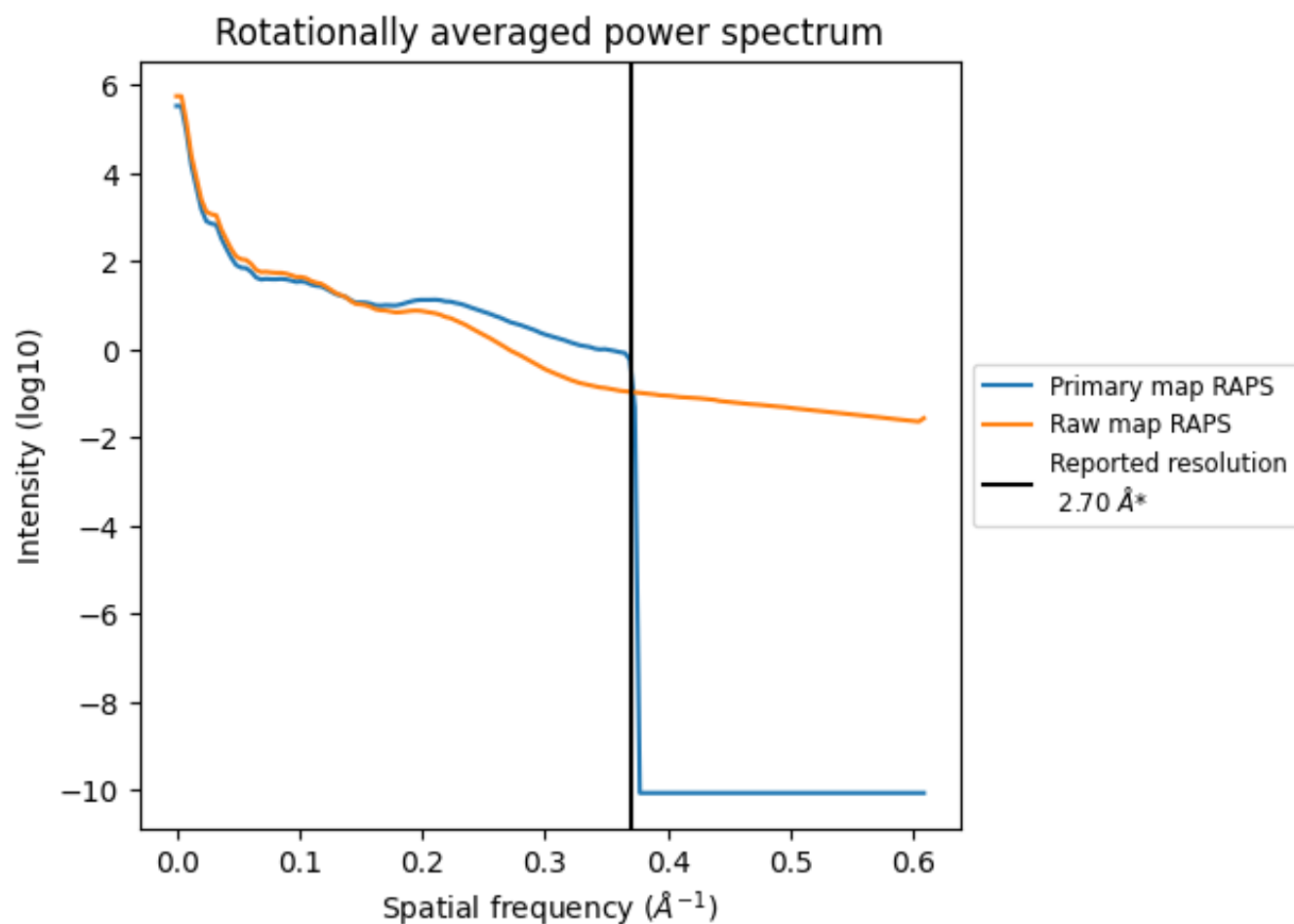
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 215 nm³; this corresponds to an approximate mass of 195 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 ⓘ

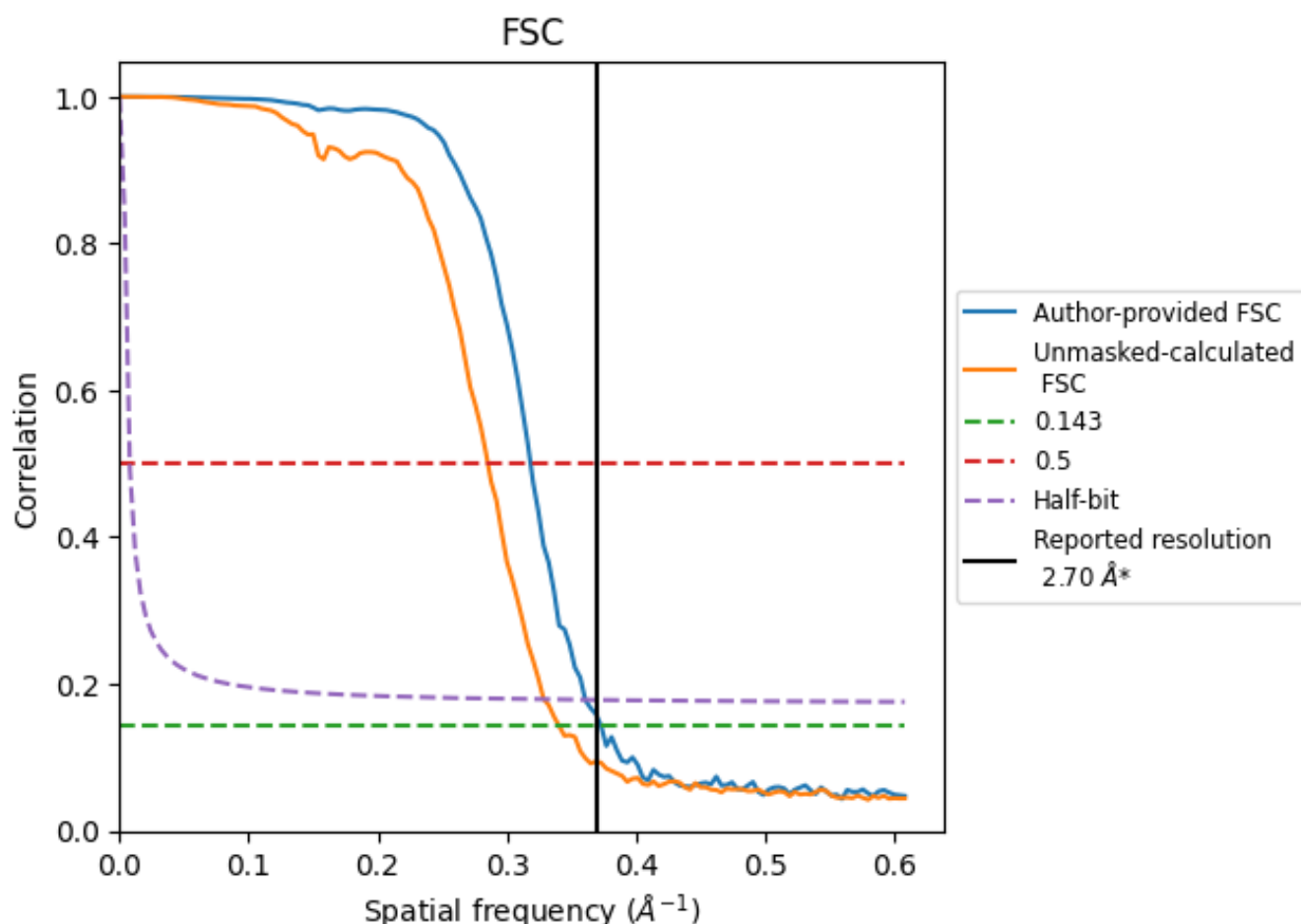


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

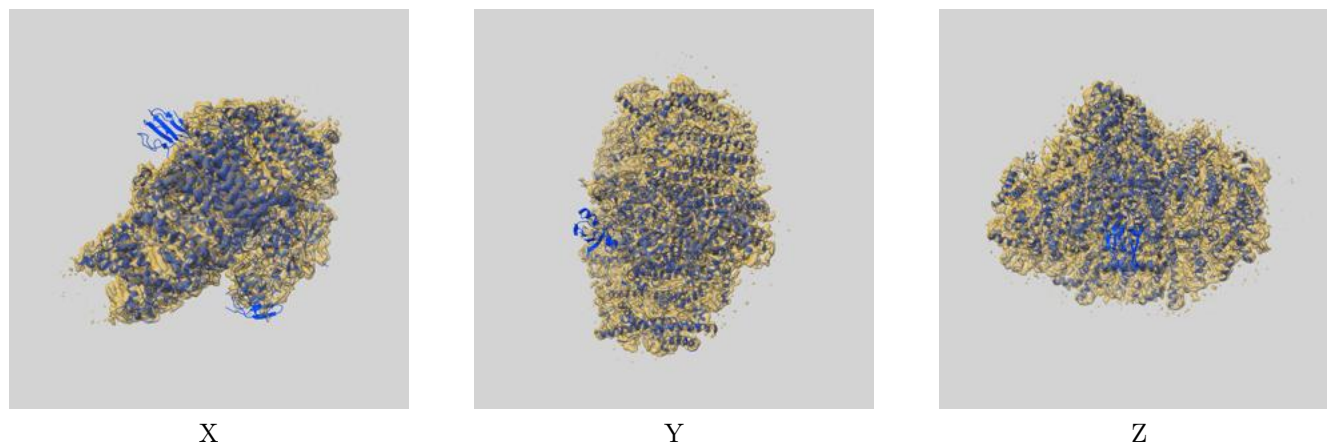
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.68	3.14	2.77
Unmasked-calculated*	2.94	3.50	3.04

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

9 Map-model fit [i](#)

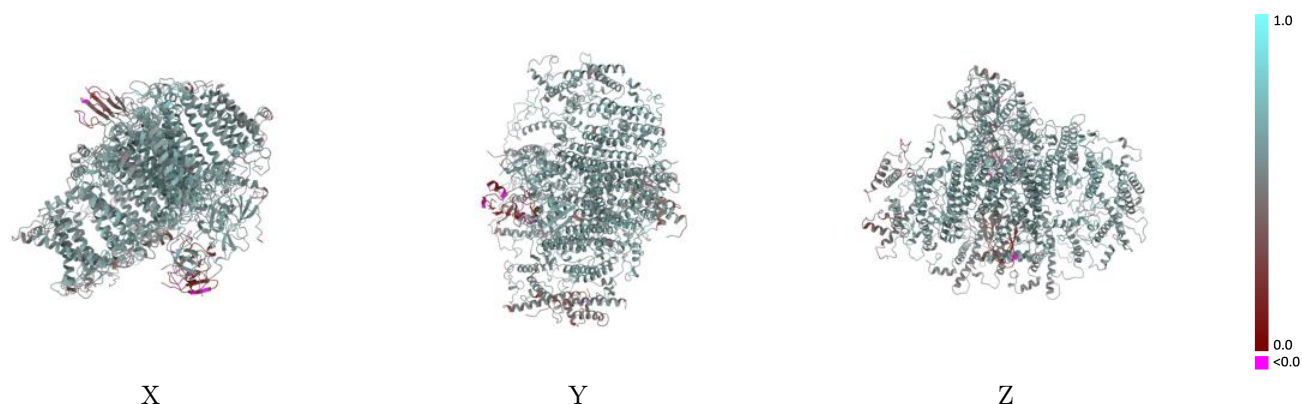
This section contains information regarding the fit between EMDB map EMD-10798 and PDB model 6YEZ. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



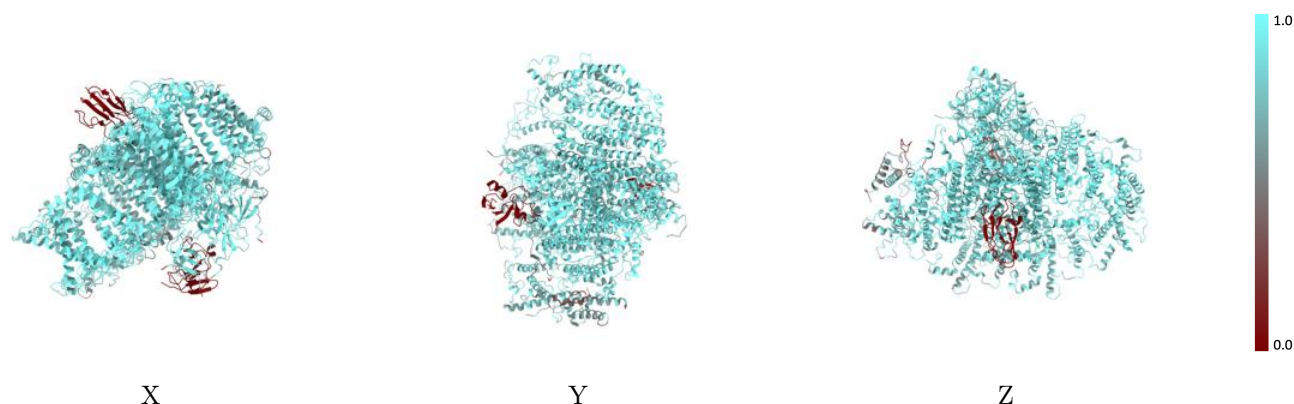
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



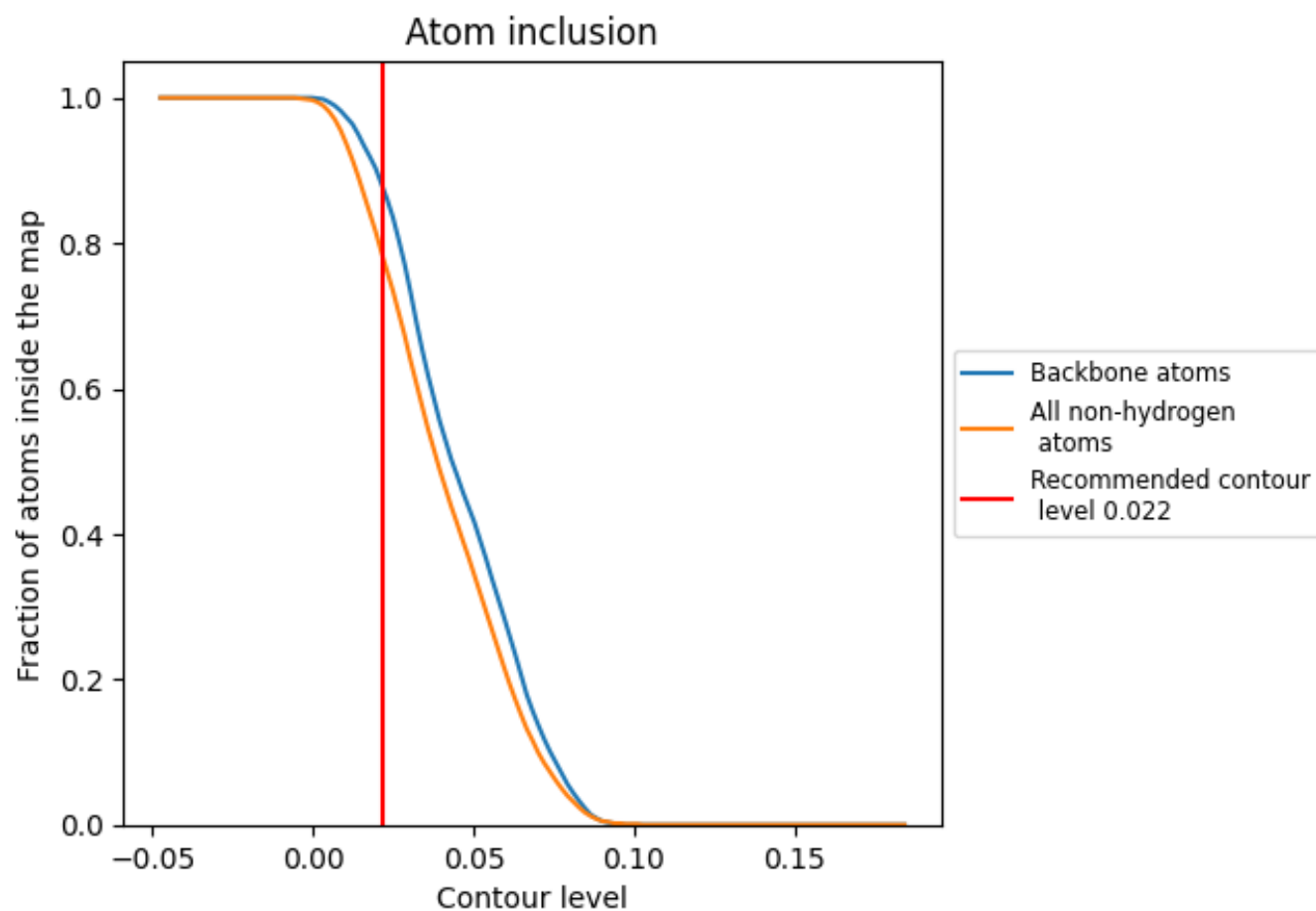
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 78% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7780	<div></div> 0.5360
1	<div></div> 0.7920	<div></div> 0.5340
2	<div></div> 0.7140	<div></div> 0.4750
3	<div></div> 0.7210	<div></div> 0.4840
4	<div></div> 0.7870	<div></div> 0.5180
A	<div></div> 0.8470	<div></div> 0.5710
B	<div></div> 0.8780	<div></div> 0.5920
C	<div></div> 0.9270	<div></div> 0.5930
D	<div></div> 0.8900	<div></div> 0.5660
E	<div></div> 0.8310	<div></div> 0.5480
F	<div></div> 0.7670	<div></div> 0.5400
G	<div></div> 0.7330	<div></div> 0.5090
H	<div></div> 0.7480	<div></div> 0.4990
I	<div></div> 0.7890	<div></div> 0.5460
J	<div></div> 0.7540	<div></div> 0.5320
K	<div></div> 0.4650	<div></div> 0.4130
L	<div></div> 0.8330	<div></div> 0.5480
N	<div></div> 0.0570	<div></div> 0.2140
P	<div></div> 0.0040	<div></div> 0.3360

1.0

0.0

<0.0