



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 07:13 pm BST

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

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.dev117
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 : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

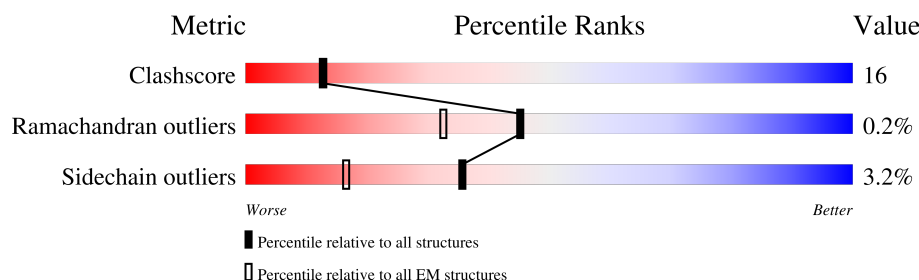
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.50 Å.

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









Metric	Whole archive (#Entries)	EM structures (#Entries)
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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	743	82% 17%
2	B	733	78% 21% .
3	C	80	90% 9% .
4	D	143	77% 22% .
5	E	66	88% 12%
6	F	154	73% 26% .
7	G	97	82% 15% .
8	H	88	68% 30% .
9	I	31	81% 16% .

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Mol	Chain	Length	Quality of chain
10	J	42	
11	K	81	
12	L	157	
13	1	193	
14	2	208	
15	3	221	
16	4	198	
17	N	97	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	CL0	A	1011	X	-	-	-
19	CLA	1	601	X	-	-	-
19	CLA	1	602	X	-	-	-
19	CLA	1	603	X	-	-	-
19	CLA	1	604	X	-	-	-
19	CLA	1	605	X	-	-	-
19	CLA	1	606	X	-	-	-
19	CLA	1	607	X	-	-	-
19	CLA	1	608	X	-	-	-
19	CLA	1	611	X	-	-	-
19	CLA	1	613	X	-	-	-
19	CLA	1	614	X	-	-	-
19	CLA	2	601	X	-	-	-
19	CLA	2	602	X	-	-	-
19	CLA	2	603	X	-	-	-
19	CLA	2	604	X	-	-	-
19	CLA	2	605	X	-	-	-
19	CLA	2	606	X	-	-	-
19	CLA	2	607	X	-	-	-
19	CLA	2	608	X	-	-	-
19	CLA	2	612	X	-	-	-
19	CLA	3	601	X	-	-	-
19	CLA	3	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	603	X	-	-	-
19	CLA	3	606	X	-	-	-
19	CLA	3	608	X	-	-	-
19	CLA	3	610	X	-	-	-
19	CLA	3	612	X	-	-	-
19	CLA	3	613	X	-	-	-
19	CLA	3	614	X	-	-	-
19	CLA	3	617	X	-	-	-
19	CLA	4	601	X	-	-	-
19	CLA	4	602	X	-	-	-
19	CLA	4	603	X	-	-	-
19	CLA	4	604	X	-	-	-
19	CLA	4	606	X	-	-	-
19	CLA	4	607	X	-	-	-
19	CLA	4	608	X	-	-	-
19	CLA	4	609	X	-	-	-
19	CLA	4	612	X	-	-	-
19	CLA	4	617	X	-	-	-
19	CLA	A	1012	X	-	-	-
19	CLA	A	1013	X	-	-	-
19	CLA	A	1101	X	-	-	-
19	CLA	A	1102	X	-	-	-
19	CLA	A	1103	X	-	-	-
19	CLA	A	1104	X	-	-	-
19	CLA	A	1105	X	-	-	-
19	CLA	A	1106	X	-	-	-
19	CLA	A	1107	X	-	-	-
19	CLA	A	1108	X	-	-	-
19	CLA	A	1109	X	-	-	-
19	CLA	A	1110	X	-	-	-
19	CLA	A	1111	X	-	-	-
19	CLA	A	1112	X	-	-	-
19	CLA	A	1113	X	-	-	-
19	CLA	A	1114	X	-	-	-
19	CLA	A	1115	X	-	-	-
19	CLA	A	1116	X	-	-	-
19	CLA	A	1117	X	-	-	-
19	CLA	A	1118	X	-	-	-
19	CLA	A	1119	X	-	-	-
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1123	X	-	-	-
19	CLA	A	1124	X	-	-	-
19	CLA	A	1125	X	-	-	-
19	CLA	A	1126	X	-	-	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	-	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1130	X	-	-	-
19	CLA	A	1131	X	-	-	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	-	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	-	-
19	CLA	A	1136	X	-	-	-
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	-	-
19	CLA	A	1139	X	-	-	-
19	CLA	A	1140	X	-	-	-
19	CLA	A	1141	X	-	-	-
19	CLA	B	1021	X	-	-	-
19	CLA	B	1022	X	-	-	-
19	CLA	B	1023	X	-	-	-
19	CLA	B	1201	X	-	-	-
19	CLA	B	1202	X	-	-	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1204	X	-	-	-
19	CLA	B	1205	X	-	-	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1207	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	-	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1213	X	-	-	-
19	CLA	B	1214	X	-	-	-
19	CLA	B	1215	X	-	-	-
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1221	X	-	-	-
19	CLA	B	1222	X	-	-	-
19	CLA	B	1223	X	-	-	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	-	-
19	CLA	B	1226	X	-	-	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	-	-
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	-	-
19	CLA	B	1236	X	-	-	-
19	CLA	B	1237	X	-	-	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1239	X	-	-	-
19	CLA	B	1240	X	-	-	-
19	CLA	F	1301	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	G	1601	X	-	-	-
19	CLA	G	1602	X	-	-	-
19	CLA	G	1603	X	-	-	-
19	CLA	G	1701	X	-	-	-
19	CLA	J	1901	X	-	-	-
19	CLA	K	1401	X	-	-	-
19	CLA	K	1402	X	-	-	-
19	CLA	K	1403	X	-	-	-
19	CLA	K	1404	X	-	-	-
19	CLA	L	1501	X	-	-	-
19	CLA	L	1502	X	-	-	-
19	CLA	L	1503	X	-	-	-
28	LUT	2	501	X	-	-	-
28	LUT	3	502	X	-	-	-
28	LUT	J	4013	X	-	-	-
29	CHL	1	609	X	-	-	-
29	CHL	1	610	X	-	-	-
29	CHL	1	612	X	-	-	-
29	CHL	2	609	X	-	-	-
29	CHL	2	610	X	-	-	-
29	CHL	2	611	X	-	-	-

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

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 38469 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	743	Total	C	N	O	S	0	0
			5858	3839	998	1003	18		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			612	379	107	115	11		

- Molecule 4 is a protein called PsaD.

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

- Molecule 5 is a protein called PsaE.

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

- Molecule 6 is a protein called PsaF.

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

- Molecule 7 is a protein called PsaG.

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

- Molecule 8 is a protein called PsaH.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 12 is a protein called PsaL.

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

- Molecule 13 is a protein called Lhca1.

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

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

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

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

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

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

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

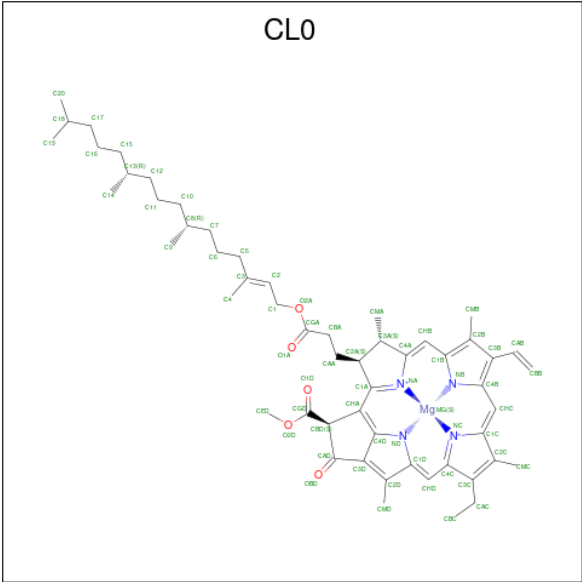
There are 3 discrepancies between the modelled and reference sequences:

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

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

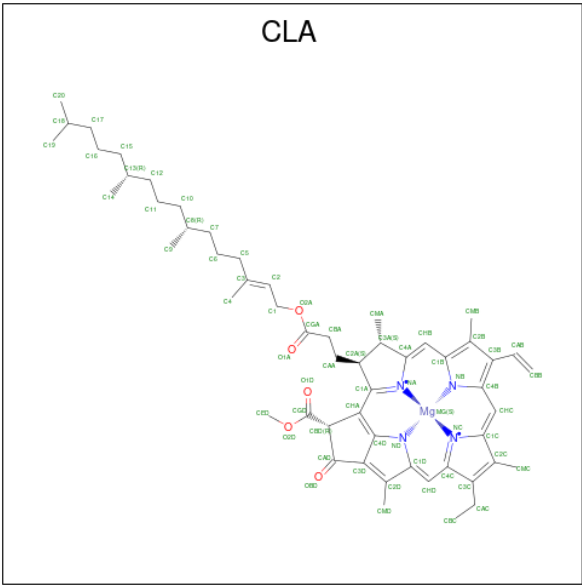
Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	97	Total	C	N	O	S	0	0
			724	448	111	160	5		

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



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

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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

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

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

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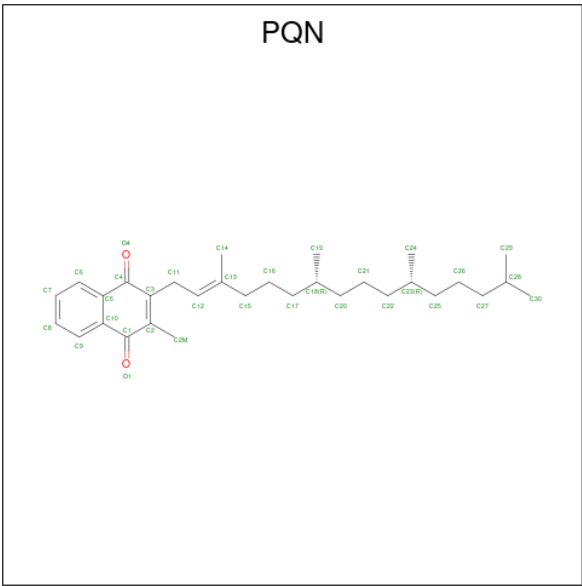
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	2	1	Total	C	Mg	N	O	0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

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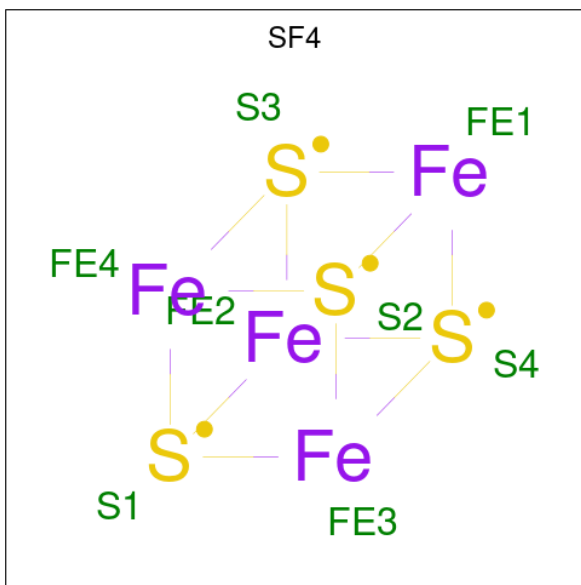
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0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

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



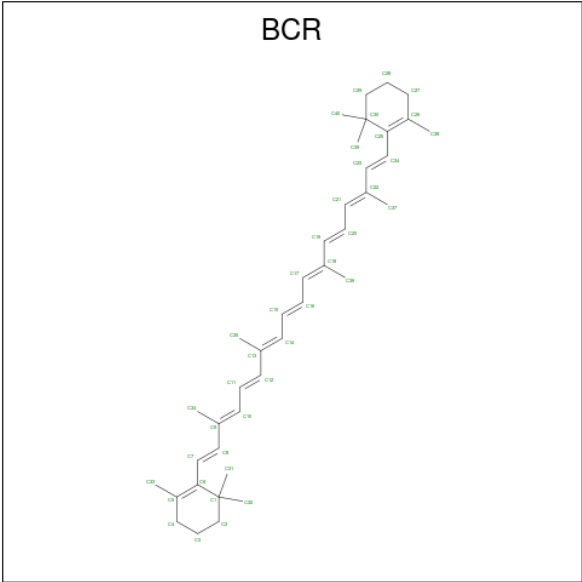
Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			33	31	2	
20	B	1	Total	C	O	0
			33	31	2	

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



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

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



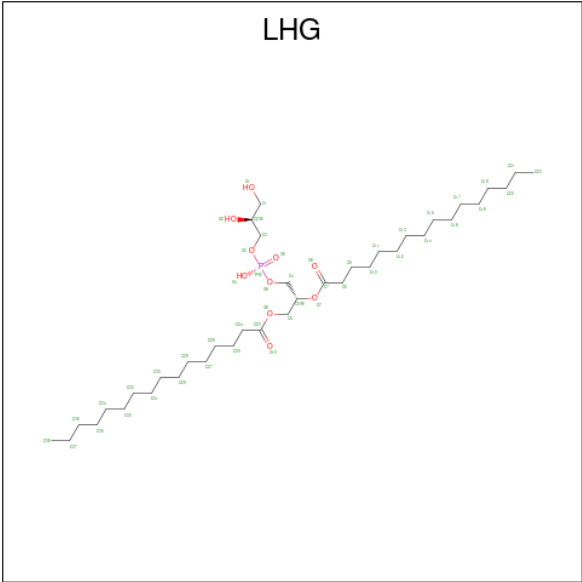
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40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

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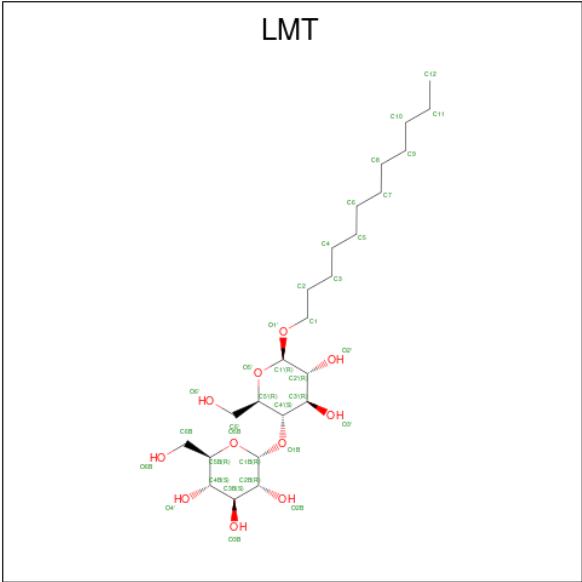
Mol	Chain	Residues	Atoms	AltConf
22	G	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	1	1	Total C 40 40	0
22	1	1	Total C 40 40	0
22	2	1	Total C 40 40	0
22	3	1	Total C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

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



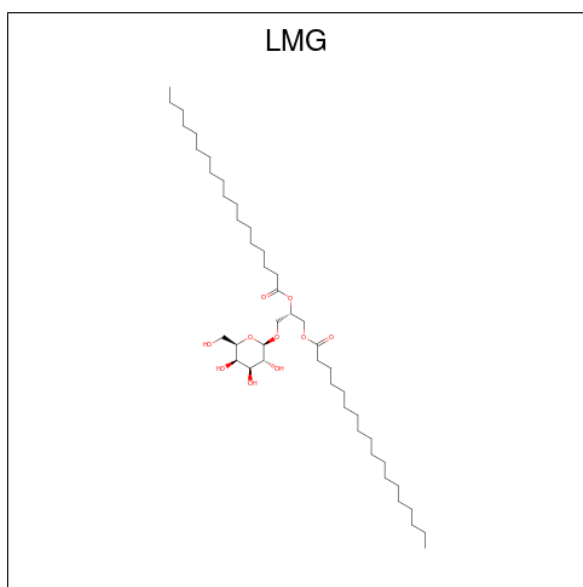
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			21	10	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	2	1	Total	C	O	P	0
			33	22	10	1	
23	3	1	Total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

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



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

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



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

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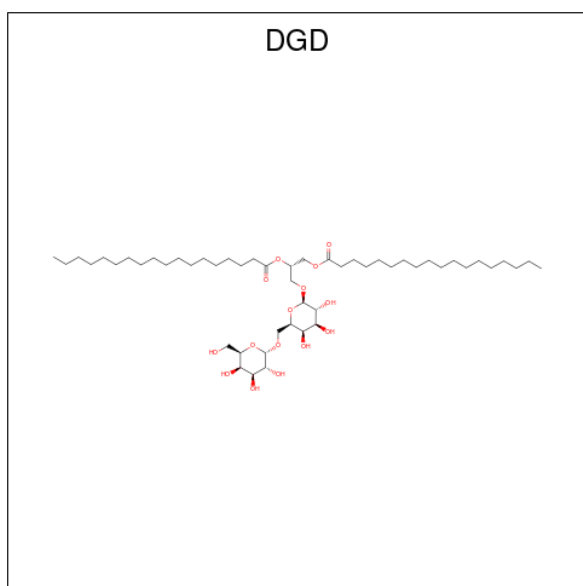
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Mol	Chain	Residues	Atoms			AltConf
25	2	1	Total	C	O	0
			36	26	10	
25	2	1	Total	C	O	0
			30	20	10	
25	2	1	Total	C	O	0
			13	7	6	
25	2	1	Total	C	O	0
			13	7	6	
25	3	1	Total	C	O	0
			30	20	10	

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

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

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



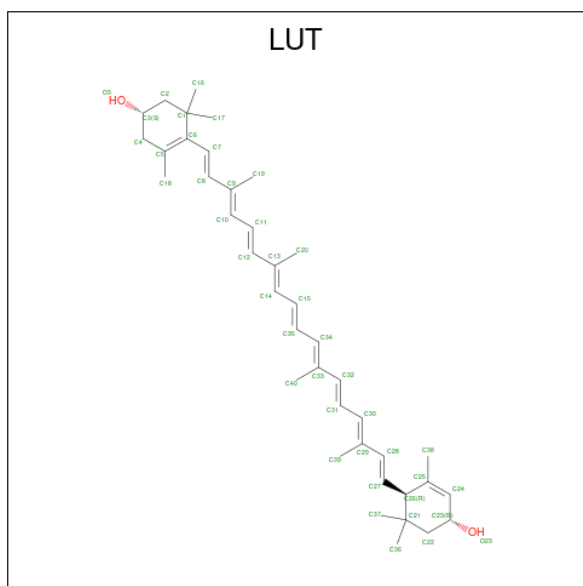
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			61	46	15	
27	F	1	Total	C	O	0
			57	42	15	

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

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



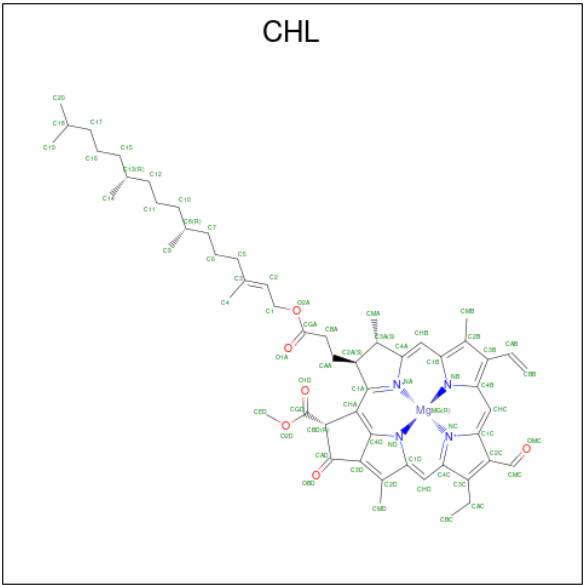
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	

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

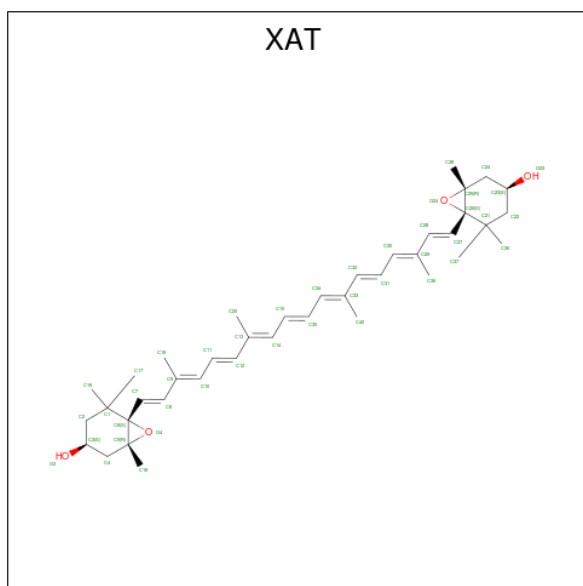
- Molecule 29 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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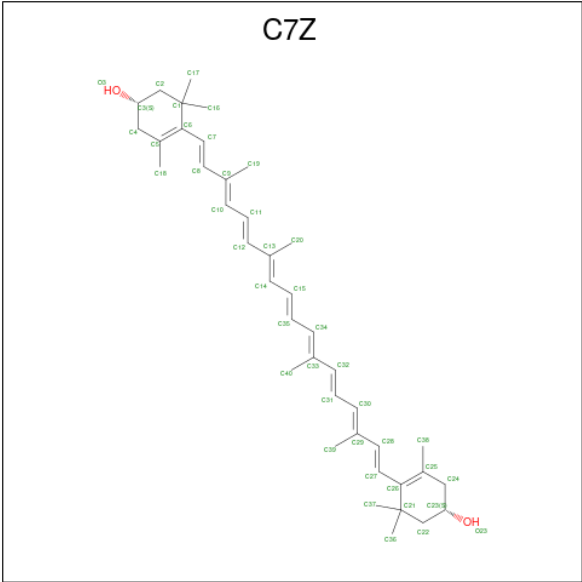
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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



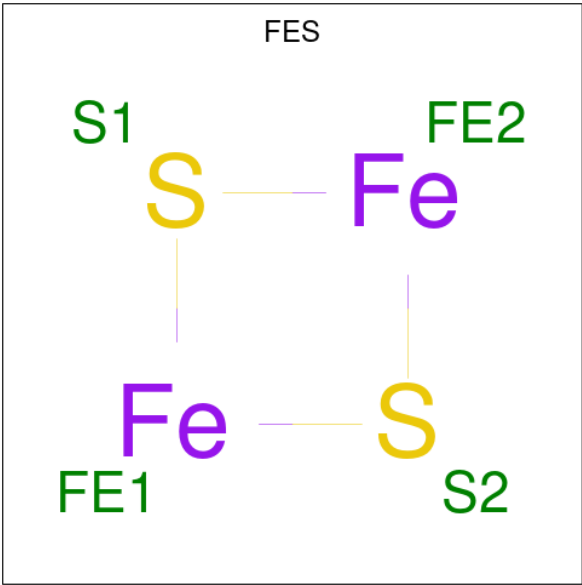
Mol	Chain	Residues	Atoms			AltConf
30	2	1	Total	C	O	0
			44	40	4	
30	4	1	Total	C	O	0
			44	40	4	

- Molecule 31 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E}, 15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



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

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



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

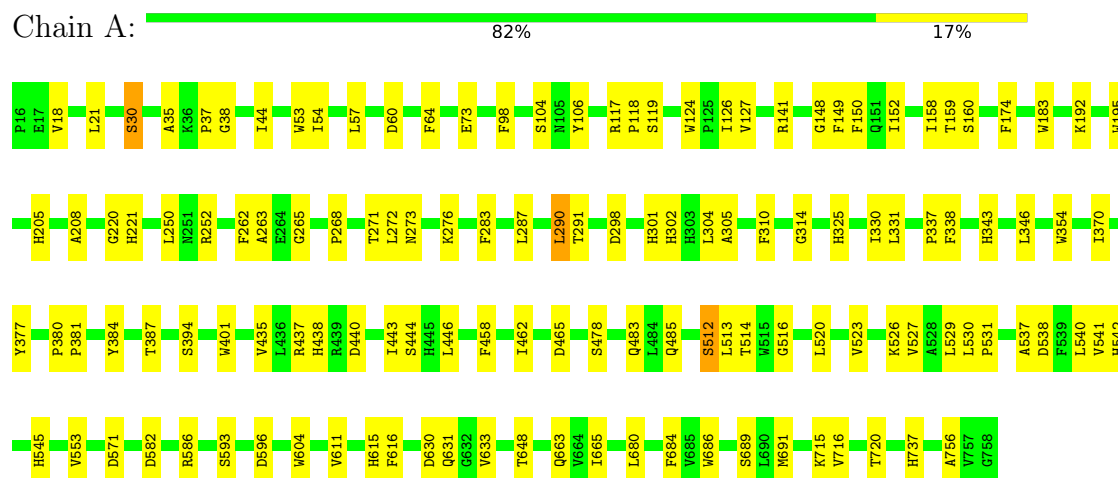
- Molecule 33 is water.

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

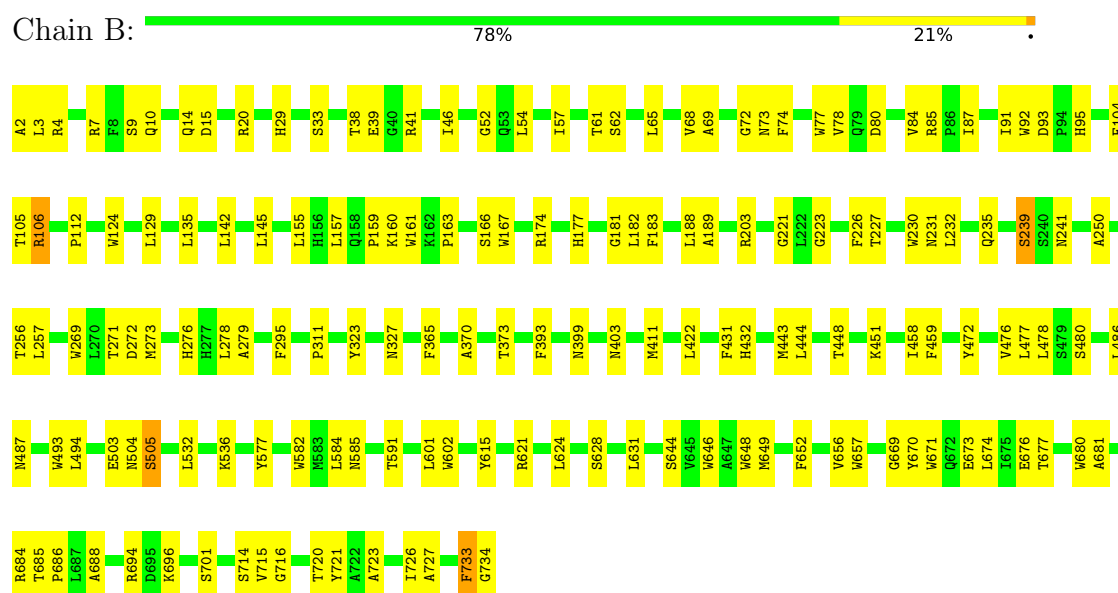
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

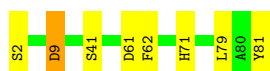


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center





- Molecule 4: PsaD

Chain D: 77% 22%



- Molecule 5: PsaE

Chain E: 88% 12%



- Molecule 6: PsaF

Chain F: 73% 26%



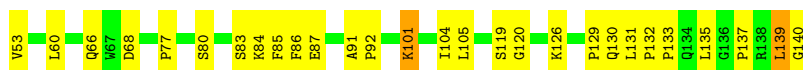
- Molecule 7: PsaG

Chain G: 82% 15%



- Molecule 8: PsaH

Chain H: 68% 30%




- Molecule 9: Photosystem I reaction center subunit VIII

Chain I: 81% 16%



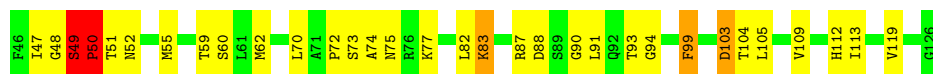
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  88% 12%



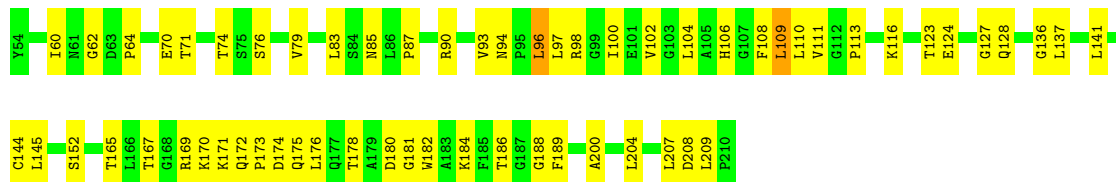
- Molecule 11: Photosystem I reaction center subunit X psaK

Chain K:  60% 33%



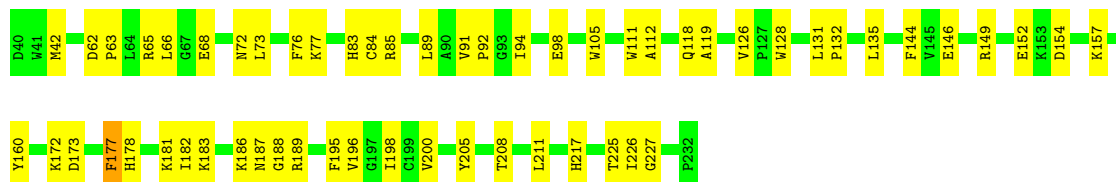
- Molecule 12: PsaL

Chain L:  62% 37%



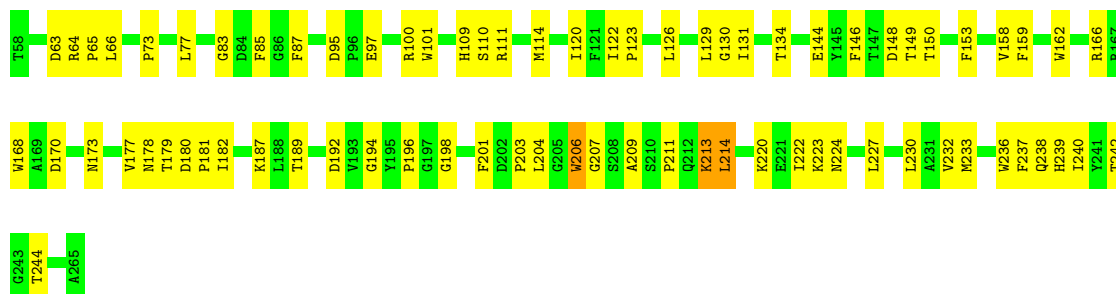
- Molecule 13: Lhca1

Chain 1:  70% 29%



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

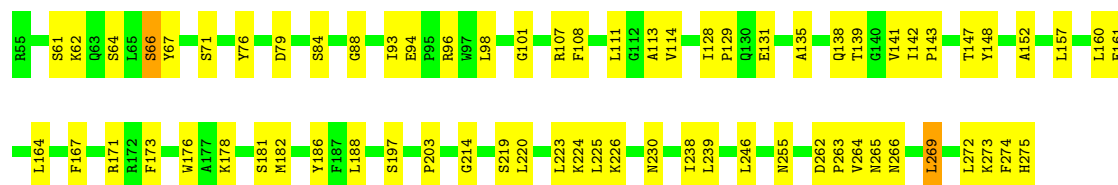
Chain 2:  64% 34%



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

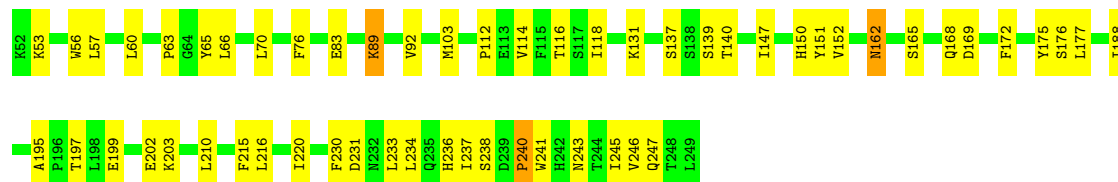
Chain 3:  69% 30%





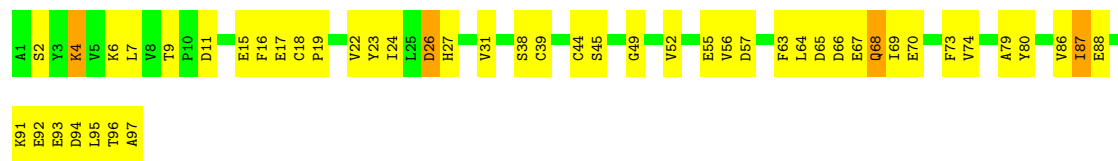
- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic

Chain 4: 72% 27% .



- Molecule 17: Ferredoxin-1, chloroplastic

Chain N: 51% 45% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	269657	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.075	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, C7Z, FES, CA, CHL, DGD, LMG, LMT, CLA, BCR, SF4, LHG, XAT, LUT, 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	0.41	1/6057 (0.0%)	0.49	0/8264
2	B	0.38	0/6069	0.49	0/8286
3	C	0.36	0/625	0.51	0/846
4	D	0.38	0/1163	0.53	0/1572
5	E	0.39	0/540	0.48	0/734
6	F	0.49	1/1234 (0.1%)	0.57	0/1670
7	G	0.36	0/776	0.47	0/1054
8	H	0.36	0/693	0.57	0/942
9	I	0.36	0/246	0.49	0/335
10	J	0.34	0/349	0.43	0/476
11	K	0.71	2/576 (0.3%)	0.66	1/779 (0.1%)
12	L	0.35	0/1207	0.51	0/1651
13	1	0.34	0/1558	0.47	0/2125
14	2	0.38	0/1679	0.52	0/2302
15	3	0.35	0/1760	0.50	0/2390
16	4	0.37	0/1608	0.47	0/2191
17	N	0.42	0/736	0.60	0/1000
All	All	0.40	4/26876 (0.0%)	0.50	1/36617 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	K	50	PRO	N-CA	13.71	1.70	1.47
1	A	117	ARG	C-N	8.93	1.51	1.34
6	F	83	THR	C-N	8.57	1.50	1.34
11	K	49	SER	C-N	6.03	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	50	PRO	CA-N-CD	-7.88	100.47	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	108	0
2	B	5857	0	5653	140	0
3	C	612	0	591	5	0
4	D	1132	0	1141	24	0
5	E	528	0	528	4	0
6	F	1206	0	1231	33	0
7	G	757	0	743	17	0
8	H	673	0	667	27	0
9	I	240	0	264	12	0
10	J	338	0	345	6	0
11	K	569	0	596	37	0
12	L	1174	0	1183	52	0
13	1	1508	0	1489	54	0
14	2	1620	0	1557	70	0
15	3	1706	0	1661	60	0
16	4	1559	0	1527	55	0
17	N	724	0	672	73	0
18	A	65	0	72	6	0
19	1	608	0	565	49	0
19	2	522	0	503	46	0
19	3	578	0	497	37	0
19	4	631	0	600	46	0
19	A	2643	0	2751	183	0
19	B	2610	0	2750	180	0
19	F	130	0	144	8	0
19	G	226	0	212	14	0
19	J	50	0	39	0	0
19	K	199	0	158	19	0
19	L	160	0	136	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	33	0	46	0	0
20	B	33	0	46	4	0
21	A	8	0	0	0	0
21	C	16	0	0	0	0
22	1	80	0	105	8	0
22	2	40	0	53	10	0
22	3	80	0	105	6	0
22	A	240	0	316	17	0
22	B	200	0	264	14	0
22	F	80	0	104	5	0
22	G	80	0	105	8	0
22	I	80	0	105	6	0
22	J	40	0	53	1	0
22	K	80	0	106	12	0
22	L	80	0	106	7	0
23	1	49	0	74	8	0
23	2	68	0	76	4	0
23	3	17	0	12	0	0
23	A	89	0	127	5	0
23	B	70	0	86	9	0
24	A	35	0	45	3	0
24	B	63	0	69	4	0
24	G	66	0	77	2	0
24	J	25	0	22	0	0
25	1	46	0	65	3	0
25	2	117	0	114	9	0
25	3	30	0	30	0	0
25	A	50	0	73	5	0
25	B	102	0	114	5	0
25	F	160	0	188	13	0
25	G	124	0	161	8	0
26	A	1	0	0	0	0
26	B	1	0	0	0	0
27	1	41	0	40	1	0
27	3	51	0	60	3	0
27	4	102	0	120	6	0
27	B	61	0	83	7	0
27	F	57	0	75	7	0
27	G	47	0	52	4	0
27	J	58	0	77	4	0
28	1	84	0	110	16	0
28	2	42	0	55	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	3	84	0	110	4	0
28	4	42	0	55	6	0
28	J	42	0	55	4	0
29	1	164	0	133	19	0
29	2	272	0	226	21	0
29	3	164	0	137	18	0
29	4	202	0	151	13	0
30	2	44	0	56	10	0
30	4	44	0	56	6	0
31	4	42	0	0	0	0
32	N	4	0	0	1	0
33	1	5	0	0	2	0
33	2	2	0	0	0	0
33	3	3	0	0	0	0
33	4	1	0	0	0	0
33	A	13	0	0	1	0
33	B	15	0	0	0	0
33	C	2	0	0	0	0
33	D	1	0	0	0	0
33	F	3	0	0	0	0
33	G	4	0	0	1	0
33	I	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	L	3	0	0	1	0
All	All	38469	0	38492	1259	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

The worst 5 of 1259 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:50:PRO:N	11:K:50:PRO:CA	1.70	1.36
17:N:73:PHE:CG	17:N:95:LEU:HD23	1.75	1.19
17:N:64:LEU:CD2	17:N:69:ILE:HD11	1.80	1.12
14:2:182:ILE:HG12	19:4:607:CLA:HMB1	1.35	1.09
11:K:49:SER:H	11:K:50:PRO:CD	1.65	1.09

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%)	715 (96%)	26 (4%)	0	100	100
2	B	731/733 (100%)	698 (96%)	33 (4%)	0	100	100
3	C	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
4	D	141/143 (99%)	131 (93%)	10 (7%)	0	100	100
5	E	64/66 (97%)	61 (95%)	3 (5%)	0	100	100
6	F	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	19	35
7	G	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
8	H	86/88 (98%)	78 (91%)	8 (9%)	0	100	100
9	I	29/31 (94%)	29 (100%)	0	0	100	100
10	J	40/42 (95%)	40 (100%)	0	0	100	100
11	K	79/81 (98%)	70 (89%)	6 (8%)	3 (4%)	2	3
12	L	155/157 (99%)	143 (92%)	12 (8%)	0	100	100
13	1	191/193 (99%)	175 (92%)	16 (8%)	0	100	100
14	2	206/208 (99%)	178 (86%)	26 (13%)	2 (1%)	13	25
15	3	219/221 (99%)	190 (87%)	29 (13%)	0	100	100
16	4	196/198 (99%)	181 (92%)	15 (8%)	0	100	100
17	N	95/97 (98%)	84 (88%)	9 (10%)	2 (2%)	5	10
All	All	3298/3332 (99%)	3082 (94%)	208 (6%)	8 (0%)	45	64

5 of 8 Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	604/604 (100%)	590 (98%)	14 (2%)	45	72
2	B	598/598 (100%)	583 (98%)	15 (2%)	42	69
3	C	69/69 (100%)	67 (97%)	2 (3%)	37	64
4	D	122/122 (100%)	119 (98%)	3 (2%)	42	69
5	E	58/58 (100%)	57 (98%)	1 (2%)	56	79
6	F	125/126 (99%)	123 (98%)	2 (2%)	58	80
7	G	82/82 (100%)	76 (93%)	6 (7%)	11	24
8	H	71/71 (100%)	68 (96%)	3 (4%)	25	49
9	I	27/27 (100%)	26 (96%)	1 (4%)	29	55
10	J	35/35 (100%)	35 (100%)	0	100	100
11	K	59/59 (100%)	55 (93%)	4 (7%)	13	27
12	L	124/124 (100%)	119 (96%)	5 (4%)	27	51
13	1	158/158 (100%)	155 (98%)	3 (2%)	52	77
14	2	167/167 (100%)	157 (94%)	10 (6%)	16	33
15	3	171/172 (99%)	165 (96%)	6 (4%)	31	57
16	4	164/164 (100%)	158 (96%)	6 (4%)	29	55
17	N	82/82 (100%)	75 (92%)	7 (8%)	8	18
All	All	2716/2718 (100%)	2628 (97%)	88 (3%)	36	60

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

Mol	Chain	Res	Type
13	1	131	LEU
15	3	108	PHE
14	2	65	PRO
14	2	192	ASP
16	4	53	LYS

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

sidechains are listed below:

Mol	Chain	Res	Type
7	G	95	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
28	LUT	1	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.81	10 (19%)
19	CLA	3	602	-	52,60,73	1.53	8 (15%)	60,97,113	2.10	18 (30%)
19	CLA	B	1238	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	18 (23%)
29	CHL	3	604	-	66,74,74	0.89	4 (6%)	73,114,114	1.41	10 (13%)
19	CLA	B	1231	-	60,68,73	1.43	7 (11%)	70,107,113	2.00	16 (22%)
19	CLA	A	1113	-	45,53,73	1.65	8 (17%)	52,89,113	2.19	15 (28%)
19	CLA	1	607	-	46,54,73	1.59	7 (15%)	53,90,113	2.12	13 (24%)
19	CLA	4	605	-	60,68,73	1.48	8 (13%)	70,107,113	2.05	20 (28%)
22	BCR	A	4011	-	41,41,41	1.83	4 (9%)	56,56,56	4.29	17 (30%)
31	C7Z	4	505	-	43,43,43	5.44	17 (39%)	58,60,60	5.32	31 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	G	1603	-	65,73,73	1.37	8 (12%)	76,113,113	2.02	16 (21%)
29	CHL	1	612	-	61,69,74	0.94	3 (4%)	67,108,114	1.27	11 (16%)
19	CLA	3	617	-	60,68,73	1.41	6 (10%)	70,107,113	1.98	18 (25%)
22	BCR	B	4005	-	41,41,41	1.85	5 (12%)	56,56,56	4.27	16 (28%)
19	CLA	B	1202	-	65,73,73	1.36	7 (10%)	76,113,113	1.84	18 (23%)
19	CLA	4	604	-	60,68,73	1.41	7 (11%)	70,107,113	2.18	18 (25%)
19	CLA	A	1121	-	60,68,73	1.44	8 (13%)	70,107,113	1.99	18 (25%)
19	CLA	B	1213	-	60,68,73	1.45	7 (11%)	70,107,113	2.06	17 (24%)
27	DGD	G	5003	-	48,48,67	0.85	2 (4%)	62,62,81	1.14	3 (4%)
19	CLA	1	613	-	45,53,73	1.64	8 (17%)	52,89,113	2.06	14 (26%)
23	LHG	2	807	-	32,32,48	0.45	0	35,38,54	1.22	2 (5%)
29	CHL	2	609	14	66,74,74	0.97	4 (6%)	73,114,114	1.31	10 (13%)
19	CLA	4	602	-	50,58,73	1.53	8 (16%)	58,95,113	2.33	18 (31%)
22	BCR	B	4006	-	41,41,41	1.88	4 (9%)	56,56,56	4.18	25 (44%)
19	CLA	1	601	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	17 (22%)
29	CHL	2	611	-	48,56,74	1.17	5 (10%)	51,92,114	1.39	10 (19%)
23	LHG	A	5002	-	48,48,48	0.41	0	51,54,54	1.10	3 (5%)
19	CLA	B	1225	-	65,73,73	1.38	8 (12%)	76,113,113	1.89	14 (18%)
20	PQN	B	2002	-	34,34,34	0.32	0	42,45,45	1.18	2 (4%)
19	CLA	1	611	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
19	CLA	A	1141	-	60,68,73	1.43	7 (11%)	70,107,113	2.16	18 (25%)
25	LMG	F	5003	-	36,36,55	0.71	1 (2%)	44,44,63	1.04	2 (4%)
19	CLA	B	1216	-	65,73,73	1.35	8 (12%)	76,113,113	1.95	17 (22%)
19	CLA	A	1133	-	65,73,73	1.35	7 (10%)	76,113,113	1.99	18 (23%)
19	CLA	A	1137	-	65,73,73	1.39	8 (12%)	76,113,113	1.92	16 (21%)
22	BCR	B	4009	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	16 (28%)
19	CLA	2	607	-	60,68,73	1.42	8 (13%)	70,107,113	2.07	18 (25%)
19	CLA	4	617	-	65,73,73	1.36	7 (10%)	76,113,113	1.94	17 (22%)
19	CLA	2	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.00	17 (22%)
19	CLA	B	1209	-	46,54,73	1.60	7 (15%)	53,90,113	2.20	14 (26%)
19	CLA	3	614	-	42,50,73	1.68	9 (21%)	48,85,113	2.19	16 (33%)
29	CHL	3	611	-	47,55,74	1.17	5 (10%)	50,91,114	1.50	9 (18%)
29	CHL	1	609	13	56,64,74	1.06	6 (10%)	61,102,114	1.31	9 (14%)
29	CHL	2	610	-	56,64,74	0.88	2 (3%)	61,102,114	1.43	15 (24%)
19	CLA	B	1203	2	65,73,73	1.36	7 (10%)	76,113,113	1.87	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	F	4016	-	41,41,41	1.84	5 (12%)	56,56,56	4.19	12 (21%)
19	CLA	A	1119	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	15 (19%)
25	LMG	2	803	-	36,36,55	0.68	2 (5%)	44,44,63	1.06	3 (6%)
25	LMG	B	5004	-	33,33,55	0.55	1 (3%)	41,41,63	1.23	4 (9%)
22	BCR	F	4014	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	13 (23%)
32	FES	N	101	17	0,4,4	-	-	-		
19	CLA	B	1223	-	65,73,73	1.38	7 (10%)	76,113,113	1.96	17 (22%)
19	CLA	B	1222	33	65,73,73	1.36	7 (10%)	76,113,113	2.13	16 (21%)
22	BCR	I	4018	-	41,41,41	1.81	5 (12%)	56,56,56	4.24	21 (37%)
22	BCR	A	4007	-	41,41,41	1.84	4 (9%)	56,56,56	4.41	19 (33%)
19	CLA	A	1138	-	65,73,73	1.35	8 (12%)	76,113,113	1.88	16 (21%)
19	CLA	B	1206	-	65,73,73	1.34	8 (12%)	76,113,113	2.02	14 (18%)
19	CLA	A	1115	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	13 (17%)
23	LHG	A	5001	-	39,39,48	0.44	0	42,45,54	1.12	3 (7%)
19	CLA	A	1103	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	19 (25%)
19	CLA	B	1227	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	14 (18%)
19	CLA	A	1012	-	65,73,73	1.41	7 (10%)	76,113,113	2.10	16 (21%)
27	DGD	4	801	-	52,52,67	0.95	4 (7%)	66,66,81	1.30	8 (12%)
24	LMT	G	5005	-	32,32,36	1.29	6 (18%)	43,43,47	1.13	5 (11%)
19	CLA	A	1118	-	50,58,73	1.56	8 (16%)	58,95,113	2.30	16 (27%)
19	CLA	B	1218	-	65,73,73	1.39	9 (13%)	76,113,113	2.01	19 (25%)
19	CLA	1	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	17 (22%)
19	CLA	2	604	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	19 (25%)
22	BCR	A	4003	-	41,41,41	1.83	4 (9%)	56,56,56	4.20	16 (28%)
23	LHG	B	5002	-	48,48,48	0.39	0	51,54,54	1.08	3 (5%)
19	CLA	B	1237	-	65,73,73	1.35	7 (10%)	76,113,113	1.98	16 (21%)
19	CLA	A	1116	-	56,64,73	1.49	7 (12%)	65,102,113	2.05	16 (24%)
19	CLA	B	1217	-	46,54,73	1.65	8 (17%)	53,90,113	2.16	15 (28%)
22	BCR	K	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	14 (25%)
27	DGD	B	5005	-	62,62,67	1.10	6 (9%)	76,76,81	1.09	4 (5%)
19	CLA	B	1229	-	65,73,73	1.37	7 (10%)	76,113,113	2.01	15 (19%)
29	CHL	4	611	-	51,59,74	1.12	4 (7%)	55,96,114	1.74	13 (23%)
19	CLA	A	1111	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	17 (22%)
19	CLA	B	1221	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	16 (21%)
19	CLA	A	1109	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LMG	A	5006	-	50,50,55	1.06	5 (10%)	58,58,63	1.22	5 (8%)
19	CLA	L	1501	-	50,58,73	1.52	7 (14%)	58,95,113	2.32	19 (32%)
25	LMG	2	806	-	13,13,55	0.53	0	18,18,63	0.55	0
19	CLA	B	1226	-	65,73,73	1.37	8 (12%)	76,113,113	2.09	18 (23%)
19	CLA	B	1230	-	58,66,73	1.44	7 (12%)	67,104,113	2.14	18 (26%)
22	BCR	A	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.24	22 (39%)
22	BCR	B	4004	-	41,41,41	1.97	4 (9%)	56,56,56	5.07	22 (39%)
28	LUT	1	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.99	14 (27%)
19	CLA	1	606	-	50,58,73	1.54	8 (16%)	58,95,113	2.23	18 (31%)
22	BCR	1	504	-	41,41,41	1.89	4 (9%)	56,56,56	4.63	22 (39%)
19	CLA	A	1126	-	65,73,73	1.39	7 (10%)	76,113,113	1.97	15 (19%)
19	CLA	K	1402	-	60,68,73	1.44	9 (15%)	70,107,113	2.09	17 (24%)
23	LHG	3	801	-	16,16,48	0.87	1 (6%)	17,20,54	0.67	0
19	CLA	B	1212	-	55,63,73	1.48	8 (14%)	64,101,113	2.21	19 (29%)
19	CLA	3	610	15	65,73,73	1.34	8 (12%)	76,113,113	1.97	17 (22%)
29	CHL	4	613	-	61,69,74	1.00	3 (4%)	67,108,114	1.27	10 (14%)
19	CLA	A	1104	1	65,73,73	1.36	7 (10%)	76,113,113	2.02	18 (23%)
19	CLA	3	606	-	50,58,73	1.56	8 (16%)	58,95,113	2.26	18 (31%)
19	CLA	3	603	-	55,63,73	1.46	8 (14%)	64,101,113	2.12	17 (26%)
19	CLA	B	1208	-	60,68,73	1.42	7 (11%)	70,107,113	2.00	17 (24%)
19	CLA	B	1220	-	55,63,73	1.51	7 (12%)	64,101,113	2.00	17 (26%)
21	SF4	C	3002	3	0,12,12	-	-	-	-	-
22	BCR	J	4012	-	41,41,41	1.83	4 (9%)	56,56,56	4.23	17 (30%)
29	CHL	4	615	-	43,51,74	1.06	2 (4%)	45,86,114	1.52	10 (22%)
19	CLA	A	1120	-	60,68,73	1.40	7 (11%)	70,107,113	2.07	16 (22%)
19	CLA	A	1130	-	55,63,73	1.46	7 (12%)	64,101,113	2.15	18 (28%)
19	CLA	B	1215	-	65,73,73	1.35	7 (10%)	76,113,113	2.17	18 (23%)
28	LUT	J	4013	-	42,43,43	2.27	1 (2%)	51,60,60	1.98	12 (23%)
22	BCR	3	503	-	41,41,41	1.86	4 (9%)	56,56,56	4.39	16 (28%)
29	CHL	2	615	-	56,64,74	0.93	3 (5%)	61,102,114	1.54	11 (18%)
19	CLA	A	1124	33	55,63,73	1.47	8 (14%)	64,101,113	2.20	18 (28%)
19	CLA	A	1114	-	46,54,73	1.63	7 (15%)	53,90,113	2.18	14 (26%)
20	PQN	A	2001	-	34,34,34	0.32	0	42,45,45	1.24	4 (9%)
24	LMT	A	5004	-	36,36,36	1.19	6 (16%)	47,47,47	1.21	4 (8%)
19	CLA	B	1235	-	65,73,73	1.33	8 (12%)	76,113,113	1.99	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	608	-	46,54,73	1.61	8 (17%)	53,90,113	2.05	12 (22%)
19	CLA	B	1207	-	65,73,73	1.39	8 (12%)	76,113,113	1.99	17 (22%)
19	CLA	B	1211	-	65,73,73	1.34	6 (9%)	76,113,113	2.09	21 (27%)
24	LMT	B	5006	-	33,33,36	1.23	5 (15%)	44,44,47	1.04	4 (9%)
25	LMG	G	5001	-	49,49,55	0.99	4 (8%)	57,57,63	1.25	4 (7%)
19	CLA	3	608	-	48,56,73	1.60	9 (18%)	55,92,113	2.21	16 (29%)
19	CLA	4	612	16	65,73,73	1.37	7 (10%)	76,113,113	1.98	18 (23%)
19	CLA	2	605	-	65,73,73	1.36	7 (10%)	76,113,113	2.11	17 (22%)
19	CLA	A	1125	-	65,73,73	1.36	7 (10%)	76,113,113	1.96	16 (21%)
28	LUT	4	501	-	42,43,43	2.36	1 (2%)	51,60,60	2.02	16 (31%)
19	CLA	A	1101	-	65,73,73	1.36	8 (12%)	76,113,113	2.19	19 (25%)
19	CLA	4	603	-	65,73,73	1.38	7 (10%)	76,113,113	1.91	17 (22%)
21	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
19	CLA	J	1901	33	50,58,73	1.54	9 (18%)	58,95,113	2.12	16 (27%)
19	CLA	B	1201	-	65,73,73	1.36	8 (12%)	76,113,113	2.05	18 (23%)
19	CLA	A	1110	-	55,63,73	1.48	8 (14%)	64,101,113	2.10	18 (28%)
22	BCR	A	4017	-	41,41,41	1.86	5 (12%)	56,56,56	4.83	18 (32%)
23	LHG	2	801	-	34,34,48	0.49	0	37,40,54	1.18	4 (10%)
19	CLA	4	606	-	50,58,73	1.56	7 (14%)	58,95,113	2.17	16 (27%)
19	CLA	2	601	-	60,68,73	1.42	9 (15%)	70,107,113	2.00	16 (22%)
19	CLA	1	614	13	60,68,73	1.42	9 (15%)	70,107,113	2.11	19 (27%)
22	BCR	2	503	-	41,41,41	1.90	4 (9%)	56,56,56	4.98	24 (42%)
19	CLA	A	1117	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	16 (21%)
19	CLA	A	1131	-	65,73,73	1.40	7 (10%)	76,113,113	1.97	15 (19%)
19	CLA	B	1228	-	60,68,73	1.41	7 (11%)	70,107,113	2.04	14 (20%)
19	CLA	B	1023	-	65,73,73	1.40	7 (10%)	76,113,113	1.97	18 (23%)
19	CLA	2	606	-	50,58,73	1.55	7 (14%)	58,95,113	2.33	17 (29%)
28	LUT	3	501	-	42,43,43	2.37	1 (2%)	51,60,60	2.04	14 (27%)
25	LMG	1	802	-	46,46,55	0.94	3 (6%)	54,54,63	1.10	3 (5%)
22	BCR	G	4011	-	41,41,41	1.85	4 (9%)	56,56,56	4.54	20 (35%)
29	CHL	4	610	-	47,55,74	1.04	3 (6%)	50,91,114	1.44	8 (16%)
19	CLA	A	1132	-	65,73,73	1.41	8 (12%)	76,113,113	2.03	18 (23%)
19	CLA	A	1107	1	65,73,73	1.36	6 (9%)	76,113,113	2.03	20 (26%)
19	CLA	A	1106	1	65,73,73	1.36	7 (10%)	76,113,113	2.02	16 (21%)
19	CLA	G	1601	-	55,63,73	1.48	8 (14%)	64,101,113	2.14	18 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	4	601	16	60,68,73	1.43	7 (11%)	70,107,113	2.08	17 (24%)
19	CLA	A	1134	1	55,63,73	1.49	8 (14%)	64,101,113	2.18	16 (25%)
25	LMG	G	5002	-	50,50,55	1.05	5 (10%)	58,58,63	1.18	3 (5%)
19	CLA	1	604	-	65,73,73	1.38	8 (12%)	76,113,113	1.94	18 (23%)
19	CLA	A	1013	-	65,73,73	1.36	7 (10%)	76,113,113	1.87	18 (23%)
25	LMG	3	802	-	30,30,55	0.57	1 (3%)	38,38,63	1.16	4 (10%)
29	CHL	3	607	-	51,59,74	1.00	3 (5%)	55,96,114	1.30	7 (12%)
25	LMG	2	802	-	25,25,55	0.58	0	33,33,63	1.22	3 (9%)
19	CLA	A	1139	-	65,73,73	1.37	7 (10%)	76,113,113	2.08	21 (27%)
19	CLA	L	1502	-	60,68,73	1.41	8 (13%)	70,107,113	2.05	17 (24%)
19	CLA	F	1301	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	16 (21%)
19	CLA	B	1234	-	55,63,73	1.50	8 (14%)	64,101,113	2.10	17 (26%)
25	LMG	F	5001	-	30,30,55	0.54	0	38,38,63	1.16	2 (5%)
19	CLA	B	1204	-	65,73,73	1.40	7 (10%)	76,113,113	1.84	12 (15%)
25	LMG	2	804	-	30,30,55	0.52	0	38,38,63	1.20	3 (7%)
29	CHL	1	610	13	47,55,74	1.10	4 (8%)	50,91,114	1.54	9 (18%)
22	BCR	I	4020	-	41,41,41	1.89	5 (12%)	56,56,56	4.45	15 (26%)
22	BCR	L	4020	-	41,41,41	1.87	4 (9%)	56,56,56	4.27	17 (30%)
19	CLA	A	1122	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	16 (21%)
19	CLA	A	1112	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	19 (25%)
25	LMG	2	805	-	13,13,55	0.53	0	18,18,63	0.68	0
19	CLA	1	602	13	46,54,73	1.61	8 (17%)	53,90,113	2.16	13 (24%)
19	CLA	A	1129	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	13 (17%)
19	CLA	3	601	15	55,63,73	1.46	6 (10%)	64,101,113	2.14	17 (26%)
24	LMT	G	5004	-	36,36,36	1.21	6 (16%)	47,47,47	1.20	3 (6%)
19	CLA	A	1140	-	65,73,73	1.37	7 (10%)	76,113,113	1.88	16 (21%)
19	CLA	1	608	-	46,54,73	1.64	8 (17%)	53,90,113	2.27	13 (24%)
19	CLA	A	1123	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	16 (21%)
19	CLA	F	1302	6	65,73,73	1.34	7 (10%)	76,113,113	2.01	15 (19%)
21	SF4	C	3003	3	0,12,12	-	-	-	-	-
24	LMT	B	5008	-	32,32,36	1.27	5 (15%)	43,43,47	0.96	2 (4%)
19	CLA	B	1205	-	65,73,73	1.40	7 (10%)	76,113,113	1.96	14 (18%)
18	CL0	A	1011	-	65,73,73	2.20	17 (26%)	76,113,113	2.43	21 (27%)
22	BCR	A	4008	-	41,41,41	1.85	4 (9%)	56,56,56	4.13	17 (30%)
22	BCR	K	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.36	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1022	-	65,73,73	1.40	7 (10%)	76,113,113	1.96	16 (21%)
19	CLA	A	1136	-	65,73,73	1.33	8 (12%)	76,113,113	2.02	16 (21%)
19	CLA	B	1210	-	65,73,73	1.33	7 (10%)	76,113,113	2.11	20 (26%)
23	LHG	1	801	-	48,48,48	0.40	0	51,54,54	1.14	4 (7%)
19	CLA	4	607	-	60,68,73	1.43	8 (13%)	70,107,113	1.88	15 (21%)
25	LMG	F	5002	-	47,47,55	0.98	3 (6%)	55,55,63	1.22	4 (7%)
27	DGD	F	5005	-	58,58,67	1.05	5 (8%)	72,72,81	1.17	5 (6%)
23	LHG	B	5001	-	20,20,48	0.62	0	23,26,54	1.60	3 (13%)
19	CLA	1	603	-	55,63,73	1.50	8 (14%)	64,101,113	2.23	18 (28%)
19	CLA	3	612	15	50,58,73	1.53	8 (16%)	58,95,113	2.28	15 (25%)
22	BCR	L	4019	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	16 (28%)
19	CLA	A	1105	-	60,68,73	1.43	6 (10%)	70,107,113	2.07	16 (22%)
19	CLA	A	1127	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	16 (21%)
19	CLA	B	1219	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	B	1239	-	65,73,73	1.40	9 (13%)	76,113,113	1.99	15 (19%)
22	BCR	3	506	-	41,41,41	1.86	4 (9%)	56,56,56	4.43	16 (28%)
27	DGD	4	802	-	52,52,67	0.90	2 (3%)	66,66,81	1.02	2 (3%)
19	CLA	4	609	16	50,58,73	1.54	8 (16%)	58,95,113	2.28	16 (27%)
30	XAT	4	502	-	39,47,47	0.80	1 (2%)	54,74,74	1.75	15 (27%)
19	CLA	A	1135	-	51,59,73	1.52	8 (15%)	59,96,113	2.25	18 (30%)
19	CLA	K	1401	-	45,53,73	1.61	10 (22%)	52,89,113	2.15	13 (25%)
30	XAT	2	502	-	39,47,47	0.75	1 (2%)	54,74,74	2.42	15 (27%)
19	CLA	A	1128	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	17 (22%)
22	BCR	G	4021	-	41,41,41	1.89	4 (9%)	56,56,56	4.36	18 (32%)
19	CLA	B	1214	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	16 (21%)
27	DGD	1	803	-	42,42,67	0.87	1 (2%)	56,56,81	1.10	3 (5%)
19	CLA	L	1503	33	50,58,73	1.54	9 (18%)	58,95,113	2.27	19 (32%)
24	LMT	J	5003	-	26,26,36	1.34	5 (19%)	37,37,47	1.14	3 (8%)
19	CLA	2	608	-	50,58,73	1.54	8 (16%)	58,95,113	2.20	18 (31%)
22	BCR	B	4010	-	41,41,41	1.86	4 (9%)	56,56,56	4.17	13 (23%)
25	LMG	F	5006	-	13,13,55	0.53	0	18,18,63	0.75	0
19	CLA	2	612	-	55,63,73	1.49	7 (12%)	64,101,113	2.12	14 (21%)
27	DGD	3	803	-	52,52,67	0.86	3 (5%)	66,66,81	1.11	3 (4%)
25	LMG	B	5003	-	35,35,55	0.74	1 (2%)	43,43,63	1.17	5 (11%)
19	CLA	B	1240	-	65,73,73	1.36	7 (10%)	76,113,113	2.07	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LMG	B	5007	-	34,34,55	0.49	0	42,42,63	1.18	3 (7%)
19	CLA	B	1236	-	50,58,73	1.56	7 (14%)	58,95,113	2.24	17 (29%)
22	BCR	1	503	-	41,41,41	1.86	4 (9%)	56,56,56	4.23	17 (30%)
19	CLA	2	602	-	52,60,73	1.55	8 (15%)	60,97,113	2.10	18 (30%)
25	LMG	F	5004	-	34,34,55	0.46	0	42,42,63	1.13	2 (4%)
28	LUT	2	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.20	15 (29%)
27	DGD	J	5001	-	59,59,67	1.04	5 (8%)	73,73,81	1.00	2 (2%)
19	CLA	A	1108	-	50,58,73	1.57	7 (14%)	58,95,113	2.19	19 (32%)
19	CLA	B	1224	-	65,73,73	1.38	7 (10%)	76,113,113	1.95	18 (23%)
19	CLA	G	1602	7	46,54,73	1.59	8 (17%)	53,90,113	2.17	16 (30%)
19	CLA	B	1021	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	18 (23%)
19	CLA	K	1403	11	48,56,73	1.60	9 (18%)	55,92,113	2.35	17 (30%)
19	CLA	A	1102	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	16 (21%)
19	CLA	B	1232	-	55,63,73	1.52	8 (14%)	64,101,113	2.17	18 (28%)
19	CLA	3	605	15	55,63,73	1.53	9 (16%)	64,101,113	2.10	18 (28%)
29	CHL	2	613	-	46,54,74	1.08	3 (6%)	49,90,114	1.37	8 (16%)
25	LMG	G	5006	-	25,25,55	0.56	0	33,33,63	1.32	2 (6%)
19	CLA	K	1404	-	46,54,73	1.65	9 (19%)	53,90,113	1.97	13 (24%)
19	CLA	3	613	-	46,54,73	1.64	8 (17%)	53,90,113	2.18	13 (24%)
19	CLA	G	1701	-	60,68,73	1.42	8 (13%)	70,107,113	2.04	15 (21%)
28	LUT	3	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.99	13 (25%)

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
28	LUT	1	501	-	-	2/29/67/67	0/2/2/2
19	CLA	3	602	-	1/1/12/20	9/22/100/115	-
19	CLA	B	1238	-	1/1/15/20	24/37/115/115	-
29	CHL	3	604	-	4/4/20/26	11/39/137/137	-
19	CLA	B	1231	-	1/1/14/20	11/31/109/115	-
19	CLA	A	1113	-	1/1/11/20	7/13/91/115	-
19	CLA	1	607	-	1/1/11/20	4/15/93/115	-
19	CLA	4	605	-	-	15/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	A	4011	-	-	11/29/63/63	0/2/2/2
31	C7Z	4	505	-	-	17/29/67/67	0/2/2/2
19	CLA	G	1603	-	1/1/15/20	17/37/115/115	-
29	CHL	1	612	-	4/4/19/26	6/33/131/137	-
19	CLA	3	617	-	1/1/14/20	14/31/109/115	-
22	BCR	B	4005	-	-	9/29/63/63	0/2/2/2
19	CLA	B	1202	-	1/1/15/20	15/37/115/115	-
19	CLA	4	604	-	1/1/14/20	13/31/109/115	-
19	CLA	A	1121	-	1/1/14/20	13/31/109/115	-
19	CLA	B	1213	-	1/1/14/20	6/31/109/115	-
27	DGD	G	5003	-	-	11/36/76/95	0/2/2/2
19	CLA	1	613	-	1/1/11/20	4/13/91/115	-
23	LHG	2	807	-	-	19/37/37/53	-
29	CHL	2	609	14	4/4/20/26	8/39/137/137	-
19	CLA	4	602	-	1/1/12/20	8/19/97/115	-
22	BCR	B	4006	-	-	12/29/63/63	0/2/2/2
19	CLA	1	601	-	1/1/15/20	15/37/115/115	-
29	CHL	2	611	-	3/3/16/26	5/18/116/137	-
23	LHG	A	5002	-	-	39/53/53/53	-
19	CLA	B	1225	-	1/1/15/20	18/37/115/115	-
20	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
19	CLA	1	611	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1141	-	1/1/14/20	11/31/109/115	-
25	LMG	F	5003	-	-	13/31/51/70	0/1/1/1
19	CLA	B	1216	-	1/1/15/20	16/37/115/115	-
19	CLA	A	1133	-	1/1/15/20	21/37/115/115	-
19	CLA	A	1137	-	1/1/15/20	17/37/115/115	-
22	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
19	CLA	2	607	-	1/1/14/20	14/31/109/115	-
19	CLA	4	617	-	1/1/15/20	17/37/115/115	-
19	CLA	2	603	-	1/1/15/20	17/37/115/115	-
19	CLA	B	1209	-	1/1/11/20	6/15/93/115	-
19	CLA	3	614	-	1/1/10/20	3/10/88/115	-
29	CHL	3	611	-	3/3/16/26	1/17/115/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	1	609	13	4/4/18/26	4/27/125/137	-
29	CHL	2	610	-	4/4/18/26	3/27/125/137	-
19	CLA	B	1203	2	1/1/15/20	15/37/115/115	-
22	BCR	F	4016	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1119	-	1/1/15/20	14/37/115/115	-
25	LMG	2	803	-	-	14/31/51/70	0/1/1/1
25	LMG	B	5004	-	-	16/28/48/70	0/1/1/1
22	BCR	F	4014	-	-	10/29/63/63	0/2/2/2
32	FES	N	101	17	-	-	0/1/1/1
19	CLA	B	1223	-	1/1/15/20	16/37/115/115	-
19	CLA	B	1222	33	1/1/15/20	18/37/115/115	-
22	BCR	I	4018	-	-	13/29/63/63	0/2/2/2
22	BCR	A	4007	-	-	4/29/63/63	0/2/2/2
19	CLA	A	1138	-	1/1/15/20	14/37/115/115	-
19	CLA	B	1206	-	1/1/15/20	18/37/115/115	-
19	CLA	A	1115	-	1/1/15/20	23/37/115/115	-
23	LHG	A	5001	-	-	24/44/44/53	-
19	CLA	A	1103	-	1/1/15/20	26/37/115/115	-
19	CLA	B	1227	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1012	-	1/1/15/20	19/37/115/115	-
27	DGD	4	801	-	-	17/40/80/95	0/2/2/2
24	LMT	G	5005	-	-	7/17/57/61	0/2/2/2
19	CLA	A	1118	-	1/1/12/20	4/19/97/115	-
19	CLA	B	1218	-	1/1/15/20	13/37/115/115	-
19	CLA	1	605	-	1/1/15/20	16/37/115/115	-
19	CLA	2	604	-	1/1/15/20	15/37/115/115	-
29	CHL	4	611	-	3/3/17/26	0/21/119/137	-
22	BCR	A	4003	-	-	8/29/63/63	0/2/2/2
19	CLA	B	1237	-	1/1/15/20	20/37/115/115	-
19	CLA	A	1116	-	1/1/13/20	15/27/105/115	-
19	CLA	B	1217	-	1/1/11/20	7/15/93/115	-
22	BCR	K	4001	-	-	9/29/63/63	0/2/2/2
23	LHG	B	5002	-	-	31/53/53/53	-
19	CLA	B	1229	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	DGD	B	5005	-	-	25/50/90/95	0/2/2/2
19	CLA	A	1111	-	1/1/15/20	17/37/115/115	-
19	CLA	B	1221	-	1/1/15/20	19/37/115/115	-
19	CLA	A	1109	-	1/1/15/20	10/37/115/115	-
25	LMG	A	5006	-	-	16/45/65/70	0/1/1/1
19	CLA	L	1501	-	1/1/12/20	6/19/97/115	-
25	LMG	2	806	-	-	1/4/24/70	0/1/1/1
19	CLA	B	1226	-	1/1/15/20	24/37/115/115	-
19	CLA	B	1230	-	1/1/13/20	11/29/107/115	-
22	BCR	A	4002	-	-	12/29/63/63	0/2/2/2
22	BCR	B	4004	-	-	8/29/63/63	0/2/2/2
28	LUT	1	502	-	-	2/29/67/67	0/2/2/2
19	CLA	1	606	-	1/1/12/20	7/19/97/115	-
22	BCR	1	504	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1126	-	1/1/15/20	21/37/115/115	-
19	CLA	K	1402	-	1/1/14/20	24/31/109/115	-
23	LHG	3	801	-	-	7/19/19/53	-
19	CLA	B	1212	-	1/1/13/20	12/25/103/115	-
19	CLA	3	610	15	1/1/15/20	20/37/115/115	-
29	CHL	4	613	-	4/4/19/26	8/33/131/137	-
19	CLA	A	1104	1	1/1/15/20	17/37/115/115	-
19	CLA	3	606	-	1/1/12/20	11/19/97/115	-
19	CLA	3	603	-	1/1/13/20	13/25/103/115	-
19	CLA	B	1208	-	1/1/14/20	12/31/109/115	-
19	CLA	B	1220	-	1/1/13/20	9/25/103/115	-
21	SF4	C	3002	3	-	-	0/6/5/5
22	BCR	J	4012	-	-	11/29/63/63	0/2/2/2
29	CHL	4	615	-	3/3/15/26	0/12/110/137	-
19	CLA	A	1120	-	1/1/14/20	12/31/109/115	-
19	CLA	A	1130	-	1/1/13/20	14/25/103/115	-
19	CLA	B	1215	-	1/1/15/20	18/37/115/115	-
28	LUT	J	4013	-	1/1/12/27	4/29/67/67	0/2/2/2
29	CHL	2	615	-	4/4/18/26	8/27/125/137	-
22	BCR	3	503	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1124	33	1/1/13/20	8/25/103/115	-
19	CLA	A	1114	-	1/1/11/20	9/15/93/115	-
20	PQN	A	2001	-	-	4/23/43/43	0/2/2/2
24	LMT	A	5004	-	-	7/21/61/61	0/2/2/2
19	CLA	B	1235	-	1/1/15/20	17/37/115/115	-
19	CLA	4	608	-	1/1/11/20	8/15/93/115	-
19	CLA	B	1207	-	1/1/15/20	19/37/115/115	-
19	CLA	B	1211	-	1/1/15/20	19/37/115/115	-
24	LMT	B	5006	-	-	9/18/58/61	0/2/2/2
25	LMG	G	5001	-	-	21/44/64/70	0/1/1/1
19	CLA	3	608	-	1/1/11/20	6/17/95/115	-
19	CLA	4	612	16	1/1/15/20	14/37/115/115	-
19	CLA	2	605	-	1/1/15/20	20/37/115/115	-
19	CLA	A	1125	-	1/1/15/20	17/37/115/115	-
28	LUT	4	501	-	-	5/29/67/67	0/2/2/2
19	CLA	A	1101	-	1/1/15/20	21/37/115/115	-
19	CLA	4	603	-	1/1/15/20	15/37/115/115	-
21	SF4	A	3001	1,2	-	-	0/6/5/5
19	CLA	J	1901	33	1/1/12/20	7/19/97/115	-
19	CLA	B	1201	-	1/1/15/20	18/37/115/115	-
19	CLA	A	1110	-	1/1/13/20	7/25/103/115	-
22	BCR	A	4017	-	-	8/29/63/63	0/2/2/2
23	LHG	2	801	-	-	21/39/39/53	-
19	CLA	4	606	-	1/1/12/20	7/19/97/115	-
19	CLA	2	601	-	1/1/14/20	13/31/109/115	-
19	CLA	1	614	13	1/1/14/20	15/31/109/115	-
22	BCR	2	503	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
19	CLA	A	1131	-	1/1/15/20	14/37/115/115	-
19	CLA	B	1228	-	1/1/14/20	14/31/109/115	-
19	CLA	B	1023	-	1/1/15/20	10/37/115/115	-
19	CLA	2	606	-	1/1/12/20	6/19/97/115	-
28	LUT	3	501	-	-	4/29/67/67	0/2/2/2
25	LMG	1	802	-	-	13/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	G	4011	-	-	10/29/63/63	0/2/2/2
29	CHL	4	610	-	3/3/16/26	7/17/115/137	-
19	CLA	A	1132	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1107	1	1/1/15/20	18/37/115/115	-
19	CLA	A	1106	1	1/1/15/20	17/37/115/115	-
19	CLA	G	1601	-	1/1/13/20	8/25/103/115	-
19	CLA	4	601	16	1/1/14/20	16/31/109/115	-
19	CLA	A	1134	1	1/1/13/20	13/25/103/115	-
25	LMG	G	5002	-	-	20/45/65/70	0/1/1/1
19	CLA	1	604	-	1/1/15/20	16/37/115/115	-
19	CLA	A	1013	-	1/1/15/20	22/37/115/115	-
25	LMG	3	802	-	-	9/25/45/70	0/1/1/1
29	CHL	3	607	-	3/3/17/26	6/21/119/137	-
25	LMG	2	802	-	-	8/20/40/70	0/1/1/1
19	CLA	A	1139	-	1/1/15/20	17/37/115/115	-
19	CLA	L	1502	-	1/1/14/20	15/31/109/115	-
19	CLA	F	1301	-	1/1/15/20	18/37/115/115	-
19	CLA	B	1234	-	1/1/13/20	12/25/103/115	-
25	LMG	F	5001	-	-	9/25/45/70	0/1/1/1
19	CLA	B	1204	-	1/1/15/20	20/37/115/115	-
25	LMG	2	804	-	-	9/25/45/70	0/1/1/1
29	CHL	1	610	13	3/3/16/26	2/17/115/137	-
22	BCR	I	4020	-	-	11/29/63/63	0/2/2/2
22	BCR	L	4020	-	-	9/29/63/63	0/2/2/2
19	CLA	A	1122	-	1/1/15/20	17/37/115/115	-
19	CLA	A	1112	-	1/1/15/20	22/37/115/115	-
25	LMG	2	805	-	-	2/4/24/70	0/1/1/1
19	CLA	1	602	13	1/1/11/20	6/15/93/115	-
19	CLA	A	1129	-	1/1/15/20	18/37/115/115	-
19	CLA	3	601	15	1/1/13/20	10/25/103/115	-
24	LMT	G	5004	-	-	11/21/61/61	0/2/2/2
19	CLA	A	1140	-	1/1/15/20	9/37/115/115	-
19	CLA	1	608	-	1/1/11/20	7/15/93/115	-
19	CLA	A	1123	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	F	1302	6	1/1/15/20	19/37/115/115	-
24	LMT	B	5008	-	-	7/17/57/61	0/2/2/2
21	SF4	C	3003	3	-	-	0/6/5/5
19	CLA	B	1205	-	1/1/15/20	10/37/115/115	-
18	CL0	A	1011	-	3/3/20/25	8/37/135/135	-
22	BCR	A	4008	-	-	13/29/63/63	0/2/2/2
22	BCR	K	4002	-	-	11/29/63/63	0/2/2/2
19	CLA	B	1022	-	1/1/15/20	10/37/115/115	-
19	CLA	A	1136	-	1/1/15/20	19/37/115/115	-
19	CLA	B	1210	-	1/1/15/20	16/37/115/115	-
23	LHG	1	801	-	-	30/53/53/53	-
19	CLA	4	607	-	1/1/14/20	16/31/109/115	-
25	LMG	F	5002	-	-	10/42/62/70	0/1/1/1
27	DGD	F	5005	-	-	20/46/86/95	0/2/2/2
23	LHG	B	5001	-	-	12/23/23/53	-
19	CLA	1	603	-	1/1/13/20	7/25/103/115	-
19	CLA	3	612	15	1/1/12/20	9/19/97/115	-
22	BCR	L	4019	-	-	12/29/63/63	0/2/2/2
19	CLA	A	1105	-	1/1/14/20	18/31/109/115	-
19	CLA	A	1127	-	1/1/15/20	19/37/115/115	-
19	CLA	B	1219	-	1/1/15/20	20/37/115/115	-
19	CLA	B	1239	-	1/1/15/20	19/37/115/115	-
22	BCR	3	506	-	-	14/29/63/63	0/2/2/2
27	DGD	4	802	-	-	16/40/80/95	0/2/2/2
19	CLA	4	609	16	1/1/12/20	10/19/97/115	-
30	XAT	4	502	-	2/2/12/26	6/31/93/93	0/4/4/4
19	CLA	A	1135	-	1/1/12/20	10/21/99/115	-
19	CLA	K	1401	-	1/1/11/20	6/13/91/115	-
30	XAT	2	502	-	1/1/12/26	5/31/93/93	0/4/4/4
19	CLA	A	1128	-	1/1/15/20	13/37/115/115	-
22	BCR	G	4021	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1214	-	1/1/15/20	14/37/115/115	-
27	DGD	1	803	-	-	12/30/70/95	0/2/2/2
19	CLA	L	1503	33	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	J	5003	-	-	6/11/51/61	0/2/2/2
19	CLA	2	608	-	1/1/12/20	10/19/97/115	-
22	BCR	B	4010	-	-	12/29/63/63	0/2/2/2
25	LMG	F	5006	-	-	1/4/24/70	0/1/1/1
19	CLA	2	612	-	1/1/13/20	11/25/103/115	-
27	DGD	3	803	-	-	10/40/80/95	0/2/2/2
25	LMG	B	5003	-	-	9/30/50/70	0/1/1/1
19	CLA	B	1240	-	1/1/15/20	18/37/115/115	-
28	LUT	2	501	-	1/1/12/27	5/29/67/67	0/2/2/2
19	CLA	B	1236	-	1/1/12/20	10/19/97/115	-
22	BCR	1	503	-	-	17/29/63/63	0/2/2/2
19	CLA	2	602	-	1/1/12/20	8/22/100/115	-
25	LMG	B	5007	-	-	9/29/49/70	0/1/1/1
25	LMG	F	5004	-	-	9/29/49/70	0/1/1/1
27	DGD	J	5001	-	-	12/47/87/95	0/2/2/2
19	CLA	A	1108	-	1/1/12/20	7/19/97/115	-
19	CLA	B	1224	-	1/1/15/20	15/37/115/115	-
19	CLA	G	1602	7	1/1/11/20	8/15/93/115	-
19	CLA	B	1021	-	1/1/15/20	10/37/115/115	-
19	CLA	K	1403	11	1/1/11/20	9/17/95/115	-
19	CLA	A	1102	-	1/1/15/20	25/37/115/115	-
19	CLA	B	1232	-	1/1/13/20	13/25/103/115	-
29	CHL	2	613	-	3/3/16/26	4/15/113/137	-
19	CLA	3	605	15	-	10/25/103/115	-
25	LMG	G	5006	-	-	10/20/40/70	0/1/1/1
19	CLA	K	1404	-	1/1/11/20	6/15/93/115	-
19	CLA	3	613	-	1/1/11/20	6/15/93/115	-
19	CLA	G	1701	-	1/1/14/20	12/31/109/115	-
28	LUT	3	502	-	1/1/12/27	8/29/67/67	0/2/2/2

The worst 5 of 1364 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	505	C7Z	C10-C9	14.87	1.55	1.35
31	4	505	C7Z	C34-C33	14.83	1.55	1.35
31	4	505	C7Z	C14-C13	14.73	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	4	505	C7Z	C30-C29	14.67	1.55	1.35
28	3	501	LUT	C24-C25	14.53	1.51	1.33

The worst 5 of 3279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	4004	BCR	C11-C10-C9	19.37	154.96	127.31
22	A	4017	BCR	C16-C15-C14	18.15	160.66	123.47
22	1	504	BCR	C10-C11-C12	17.64	178.27	123.22
22	G	4021	BCR	C10-C11-C12	17.50	177.83	123.22
22	I	4018	BCR	C10-C11-C12	17.47	177.72	123.22

5 of 200 chirality outliers are listed below:

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

5 of 2925 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A	1012	CLA	C2-C3-C5-C6
19	A	1012	CLA	C4-C3-C5-C6
19	A	1013	CLA	C2-C1-O2A-CGA
19	A	1013	CLA	C2-C3-C5-C6
19	A	1013	CLA	C4-C3-C5-C6

There are no ring outliers.

222 monomers are involved in 798 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	1	501	LUT	9	0
19	3	602	CLA	5	0
19	B	1238	CLA	7	0
29	3	604	CHL	8	0
19	B	1231	CLA	2	0
19	A	1113	CLA	6	0
19	1	607	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	4	605	CLA	9	0
22	A	4011	BCR	3	0
19	G	1603	CLA	4	0
29	1	612	CHL	6	0
19	3	617	CLA	3	0
22	B	4005	BCR	1	0
19	B	1202	CLA	6	0
19	4	604	CLA	5	0
19	A	1121	CLA	7	0
19	B	1213	CLA	5	0
27	G	5003	DGD	4	0
19	1	613	CLA	6	0
23	2	807	LHG	2	0
29	2	609	CHL	3	0
19	4	602	CLA	3	0
22	B	4006	BCR	5	0
19	1	601	CLA	12	0
29	2	611	CHL	5	0
23	A	5002	LHG	2	0
19	B	1225	CLA	5	0
20	B	2002	PQN	4	0
19	1	611	CLA	4	0
19	A	1141	CLA	4	0
25	F	5003	LMG	1	0
19	B	1216	CLA	2	0
19	A	1133	CLA	3	0
19	A	1137	CLA	4	0
22	B	4009	BCR	3	0
19	2	607	CLA	2	0
19	4	617	CLA	3	0
19	2	603	CLA	10	0
19	B	1209	CLA	3	0
19	3	614	CLA	2	0
29	3	611	CHL	4	0
29	1	609	CHL	6	0
29	2	610	CHL	7	0
19	B	1203	CLA	3	0
22	F	4016	BCR	5	0
19	A	1119	CLA	7	0
25	2	803	LMG	6	0
32	N	101	FES	1	0
19	B	1223	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1222	CLA	9	0
22	I	4018	BCR	3	0
22	A	4007	BCR	4	0
19	A	1138	CLA	3	0
19	B	1206	CLA	5	0
19	A	1115	CLA	9	0
23	A	5001	LHG	3	0
19	A	1103	CLA	8	0
19	B	1227	CLA	5	0
19	A	1012	CLA	8	0
27	4	801	DGD	3	0
19	B	1218	CLA	5	0
19	1	605	CLA	5	0
19	2	604	CLA	12	0
22	A	4003	BCR	2	0
23	B	5002	LHG	5	0
19	B	1237	CLA	7	0
19	A	1116	CLA	9	0
22	K	4001	BCR	5	0
27	B	5005	DGD	7	0
19	B	1229	CLA	5	0
29	4	611	CHL	1	0
19	A	1111	CLA	9	0
19	B	1221	CLA	4	0
19	A	1109	CLA	10	0
25	A	5006	LMG	5	0
19	L	1501	CLA	4	0
25	2	806	LMG	1	0
19	B	1226	CLA	5	0
19	B	1230	CLA	6	0
22	A	4002	BCR	3	0
22	B	4004	BCR	4	0
28	1	502	LUT	7	0
19	1	606	CLA	1	0
22	1	504	BCR	2	0
19	A	1126	CLA	7	0
19	K	1402	CLA	2	0
19	B	1212	CLA	2	0
19	3	610	CLA	6	0
29	4	613	CHL	8	0
19	A	1104	CLA	4	0
19	3	606	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	3	603	CLA	3	0
19	B	1208	CLA	5	0
19	B	1220	CLA	3	0
22	J	4012	BCR	1	0
29	4	615	CHL	3	0
19	A	1120	CLA	4	0
19	A	1130	CLA	2	0
19	B	1215	CLA	2	0
28	J	4013	LUT	4	0
22	3	503	BCR	3	0
29	2	615	CHL	5	0
19	A	1124	CLA	3	0
19	A	1114	CLA	3	0
24	A	5004	LMT	3	0
19	B	1235	CLA	6	0
19	4	608	CLA	2	0
19	B	1207	CLA	10	0
19	B	1211	CLA	4	0
24	B	5006	LMT	3	0
25	G	5001	LMG	3	0
19	3	608	CLA	1	0
19	4	612	CLA	5	0
19	2	605	CLA	6	0
19	A	1125	CLA	4	0
28	4	501	LUT	6	0
19	A	1101	CLA	4	0
19	4	603	CLA	7	0
19	B	1201	CLA	5	0
19	A	1110	CLA	5	0
22	A	4017	BCR	5	0
23	2	801	LHG	2	0
19	4	606	CLA	3	0
19	2	601	CLA	7	0
19	1	614	CLA	3	0
22	2	503	BCR	10	0
19	A	1117	CLA	2	0
19	A	1131	CLA	3	0
19	B	1228	CLA	1	0
19	B	1023	CLA	5	0
19	2	606	CLA	5	0
28	3	501	LUT	2	0
25	1	802	LMG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	G	4011	BCR	4	0
29	4	610	CHL	3	0
19	A	1132	CLA	2	0
19	A	1107	CLA	4	0
19	A	1106	CLA	6	0
19	G	1601	CLA	3	0
19	4	601	CLA	3	0
19	A	1134	CLA	3	0
25	G	5002	LMG	5	0
19	1	604	CLA	8	0
19	A	1013	CLA	9	0
29	3	607	CHL	6	0
25	2	802	LMG	2	0
19	A	1139	CLA	3	0
19	L	1502	CLA	5	0
19	F	1301	CLA	4	0
19	B	1234	CLA	7	0
25	F	5001	LMG	1	0
19	B	1204	CLA	6	0
29	1	610	CHL	7	0
22	I	4020	BCR	3	0
19	A	1122	CLA	6	0
19	A	1112	CLA	8	0
19	1	602	CLA	4	0
19	A	1129	CLA	2	0
19	3	601	CLA	9	0
24	G	5004	LMT	2	0
19	A	1140	CLA	3	0
19	A	1123	CLA	5	0
19	F	1302	CLA	4	0
24	B	5008	LMT	1	0
19	B	1205	CLA	4	0
18	A	1011	CL0	6	0
22	A	4008	BCR	2	0
22	K	4002	BCR	7	0
19	B	1022	CLA	4	0
19	A	1136	CLA	9	0
19	B	1210	CLA	7	0
23	1	801	LHG	8	0
19	4	607	CLA	7	0
25	F	5002	LMG	8	0
27	F	5005	DGD	7	0

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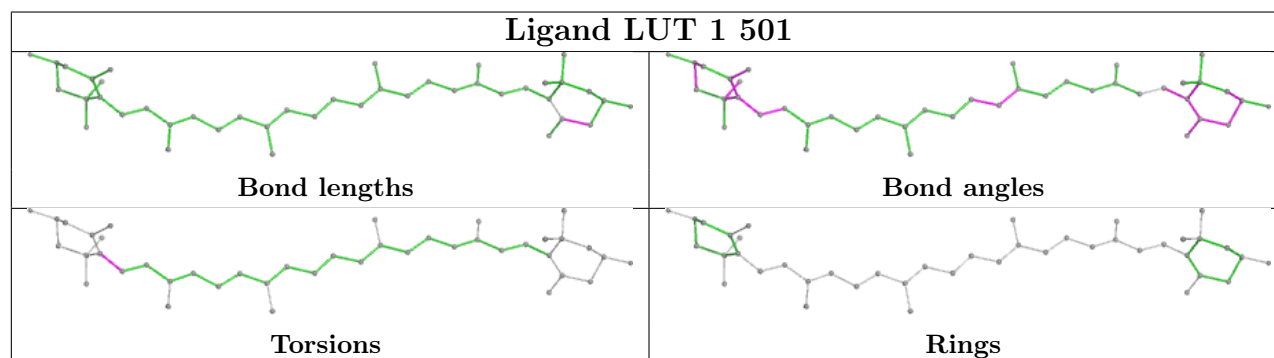
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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19	1	603	CLA	6	0
19	3	612	CLA	4	0
22	L	4019	BCR	7	0
19	A	1105	CLA	8	0
19	A	1127	CLA	1	0
19	B	1219	CLA	9	0
19	B	1239	CLA	7	0
22	3	506	BCR	3	0
27	4	802	DGD	3	0
19	4	609	CLA	3	0
30	4	502	XAT	6	0
19	A	1135	CLA	6	0
19	K	1401	CLA	11	0
30	2	502	XAT	10	0
19	A	1128	CLA	3	0
22	G	4021	BCR	4	0
19	B	1214	CLA	6	0
27	1	803	DGD	1	0
19	L	1503	CLA	5	0
19	2	608	CLA	2	0
22	B	4010	BCR	1	0
25	F	5006	LMG	1	0
19	2	612	CLA	5	0
27	3	803	DGD	3	0
25	B	5003	LMG	3	0
19	B	1240	CLA	12	0
25	B	5007	LMG	2	0
19	B	1236	CLA	1	0
22	1	503	BCR	6	0
19	2	602	CLA	3	0
25	F	5004	LMG	2	0
28	2	501	LUT	4	0
27	J	5001	DGD	4	0
19	A	1108	CLA	2	0
19	B	1224	CLA	7	0
19	G	1602	CLA	3	0
19	B	1021	CLA	4	0
19	K	1403	CLA	2	0
19	A	1102	CLA	7	0
19	B	1232	CLA	3	0
19	3	605	CLA	4	0

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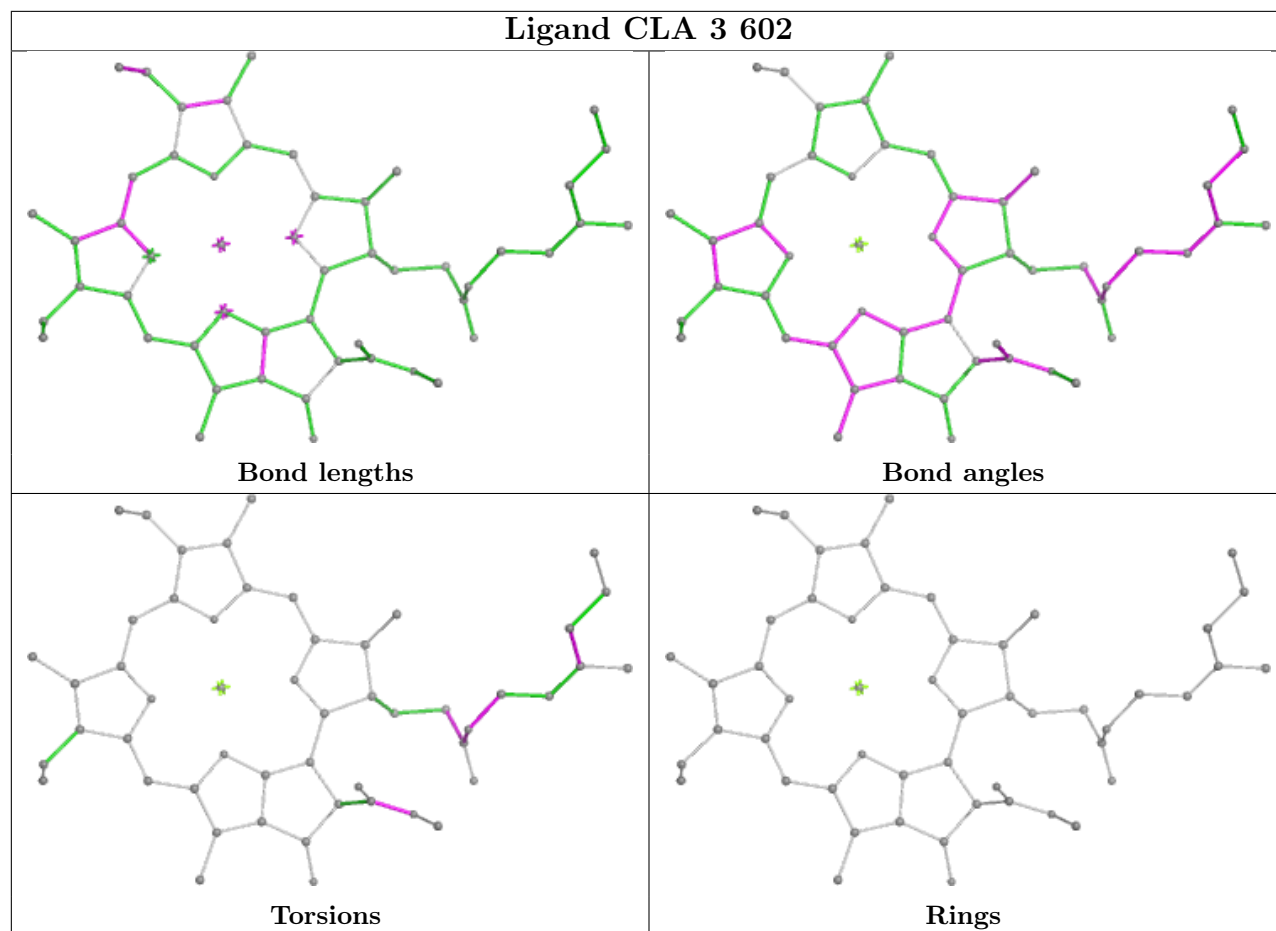
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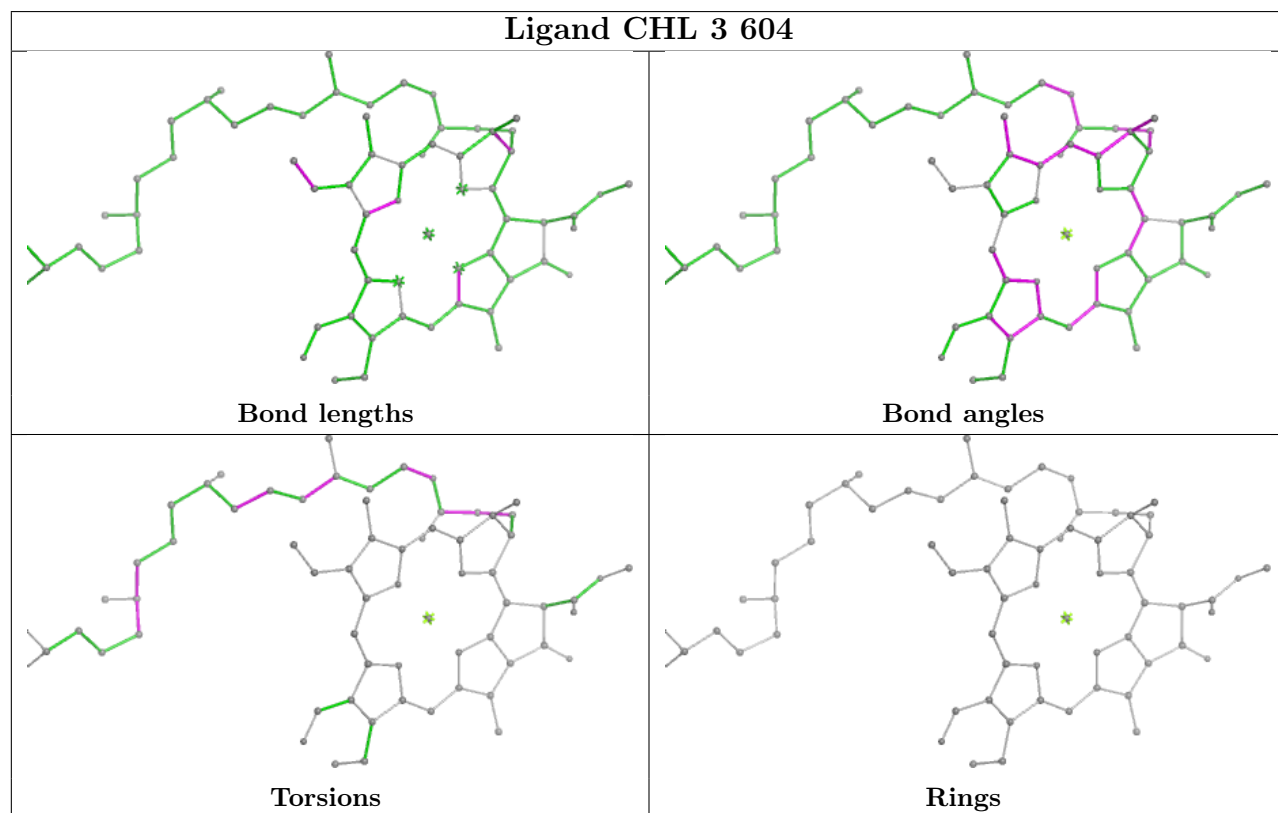
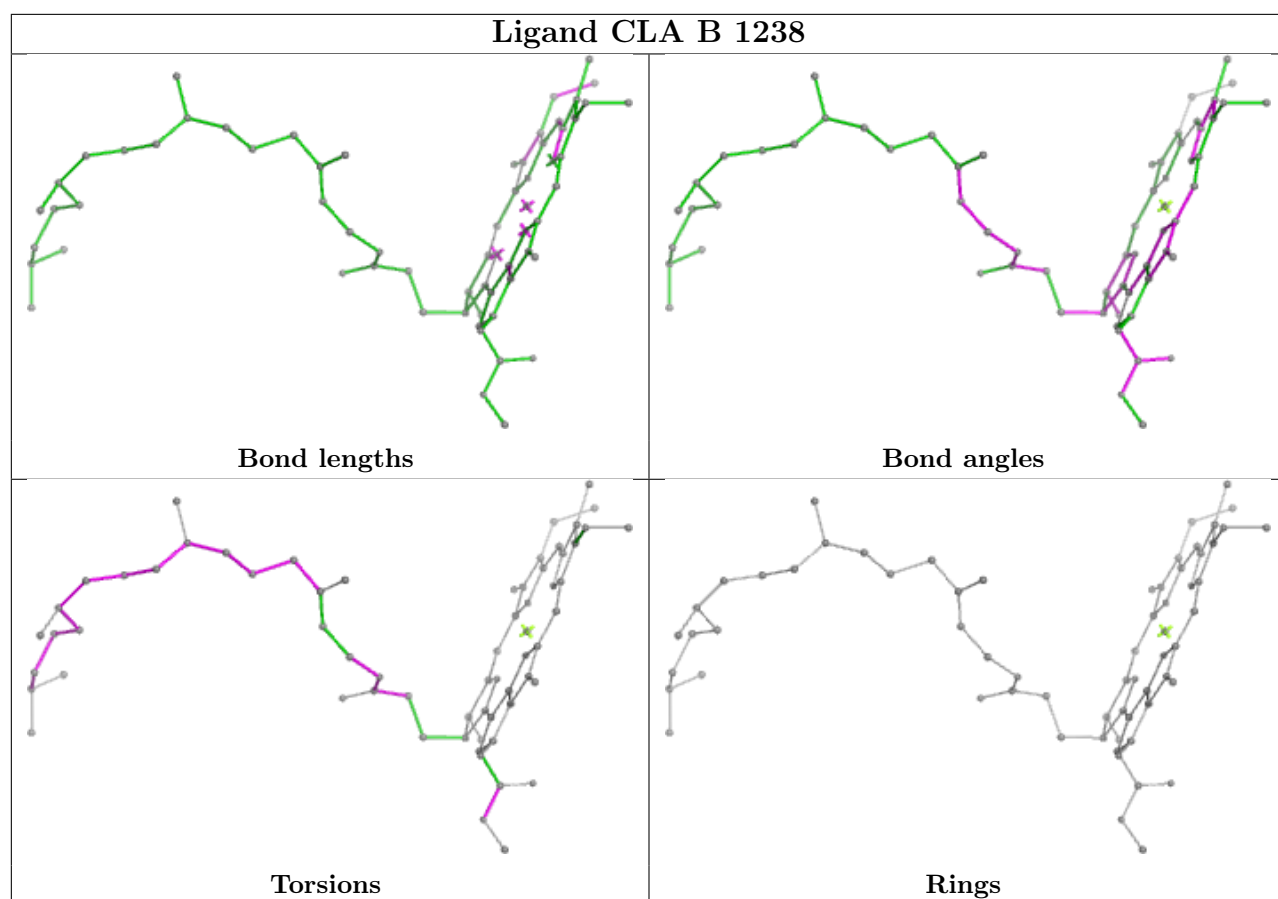
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	2	613	CHL	1	0
19	K	1404	CLA	4	0
19	3	613	CLA	3	0
19	G	1701	CLA	4	0
28	3	502	LUT	2	0

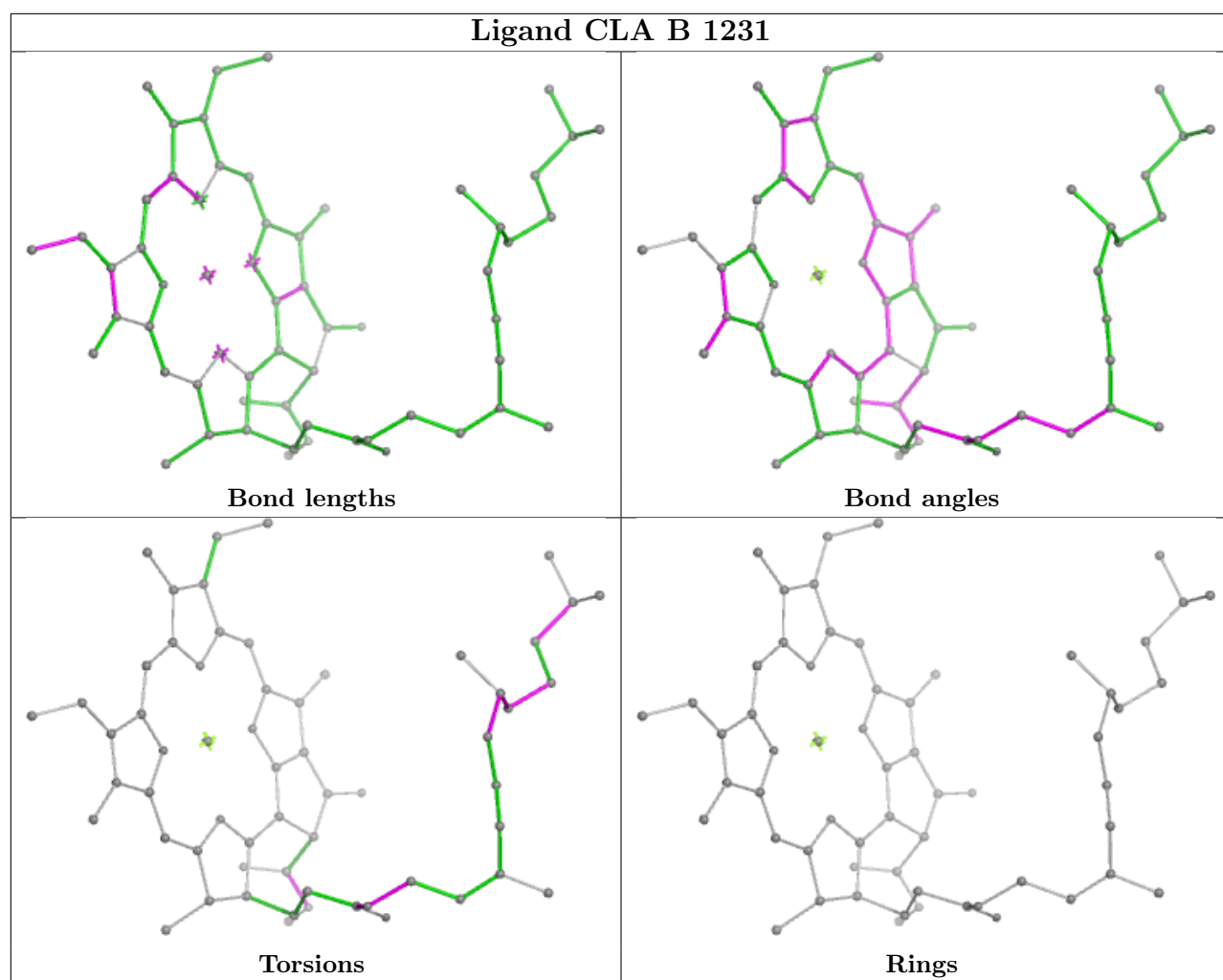
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

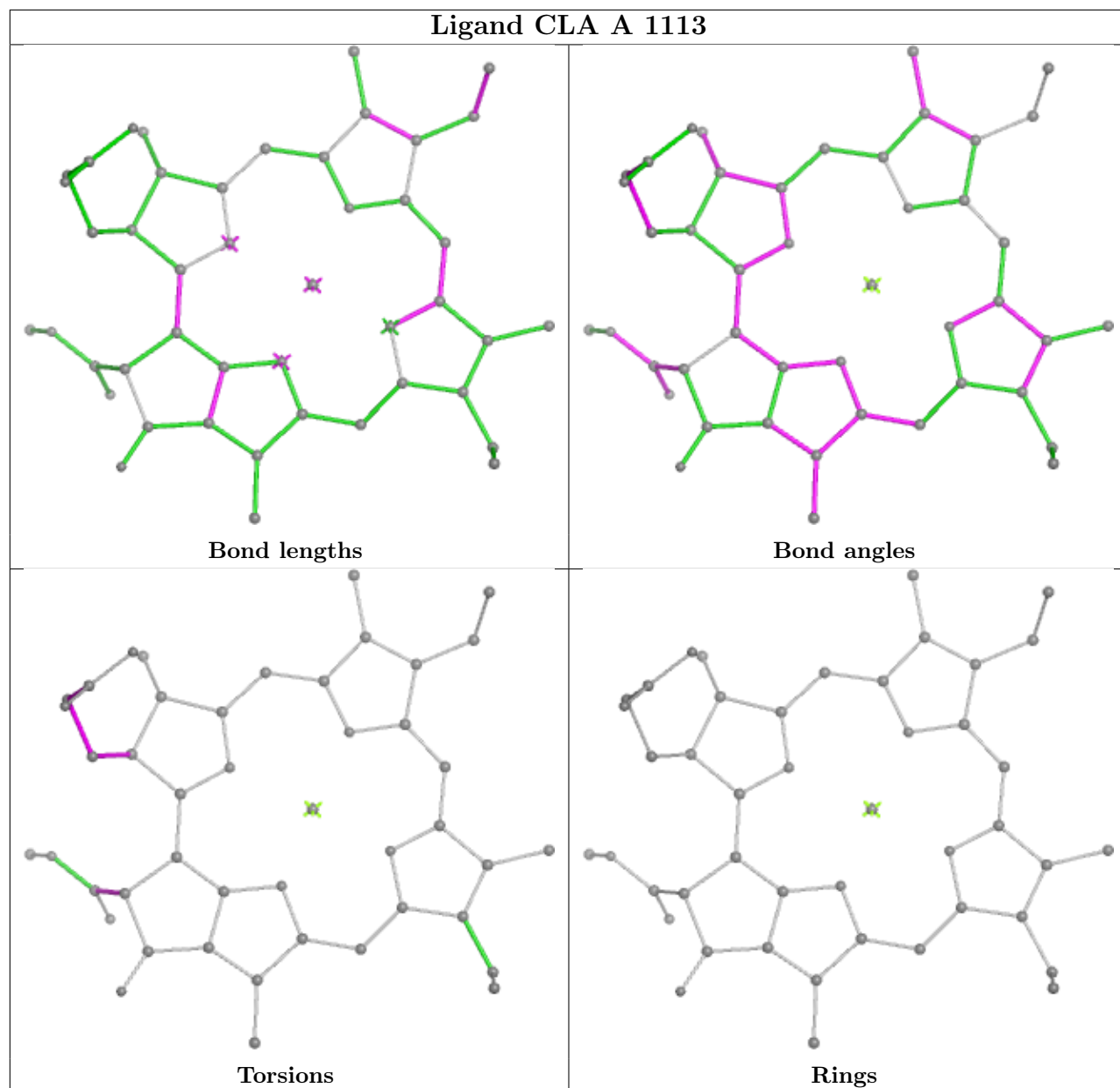


Ligand CLA 3 602

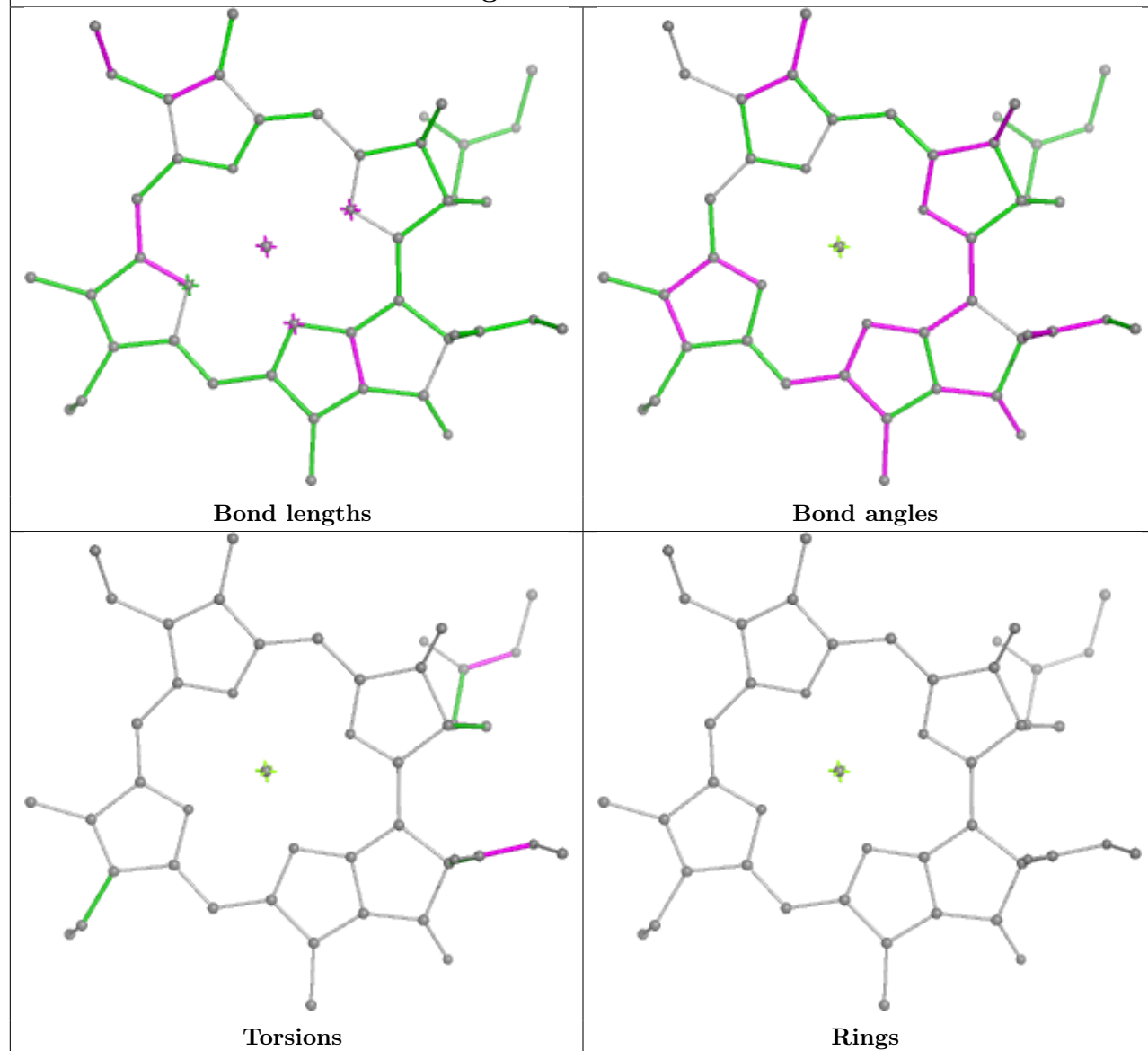


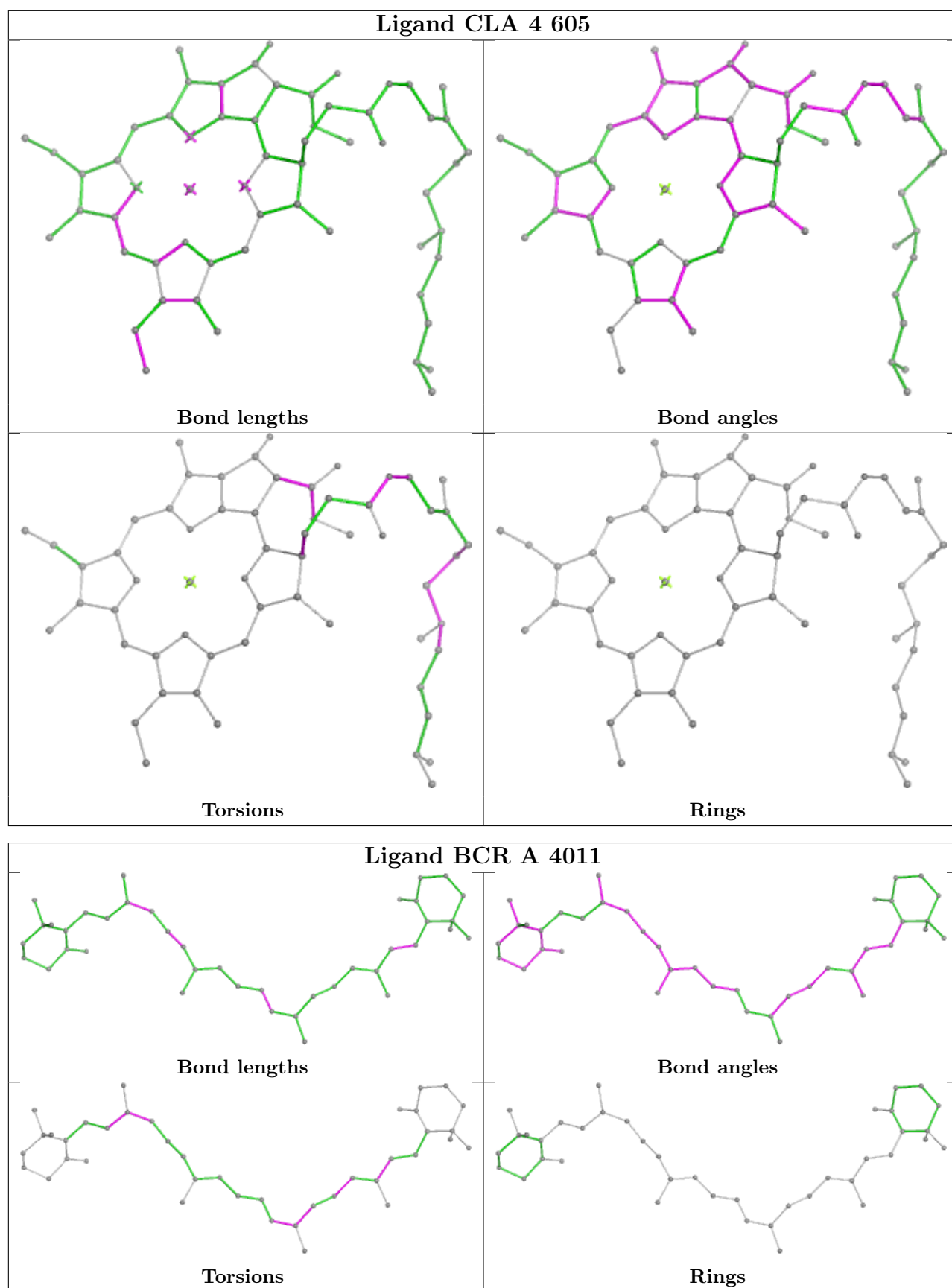


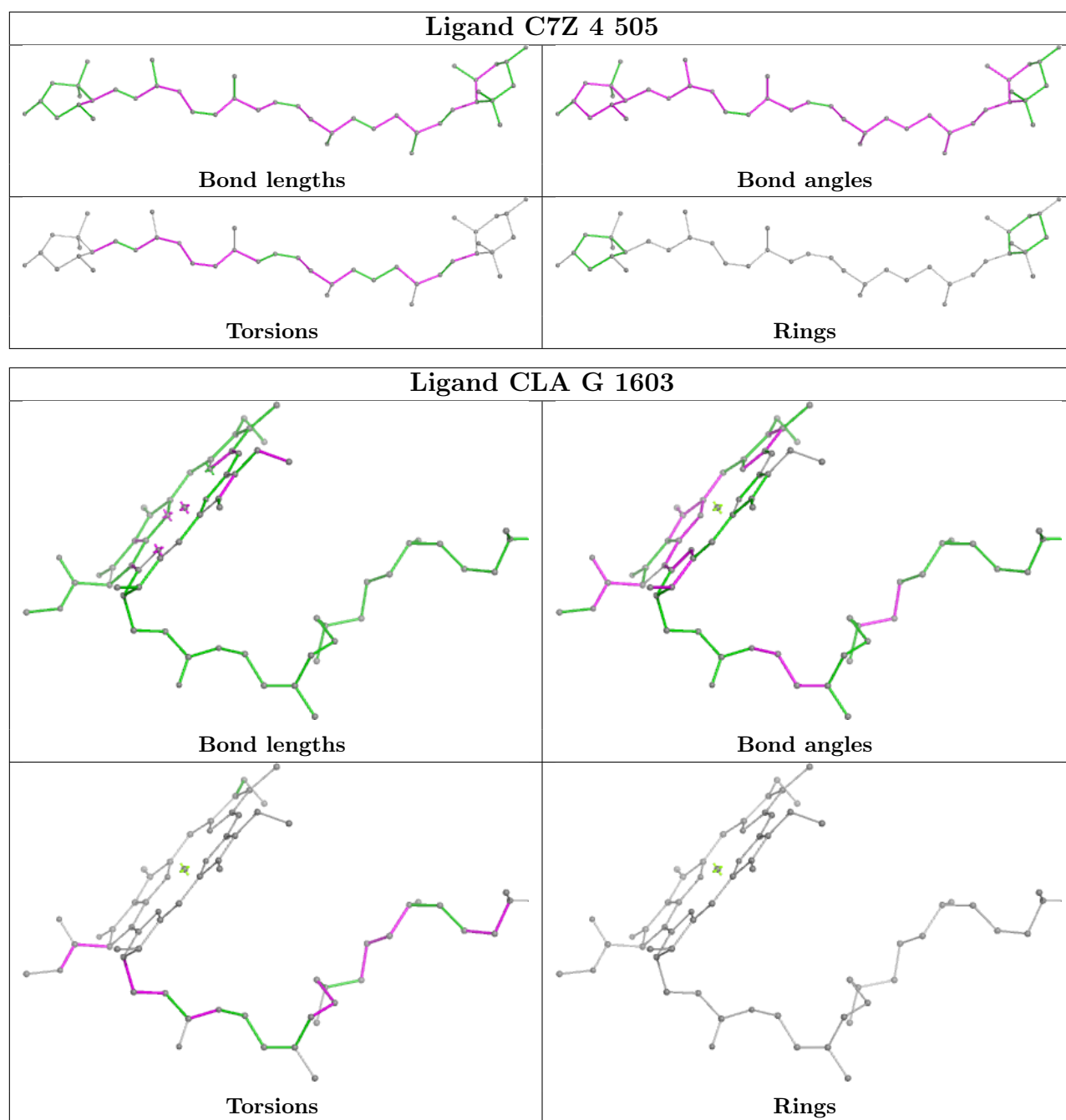


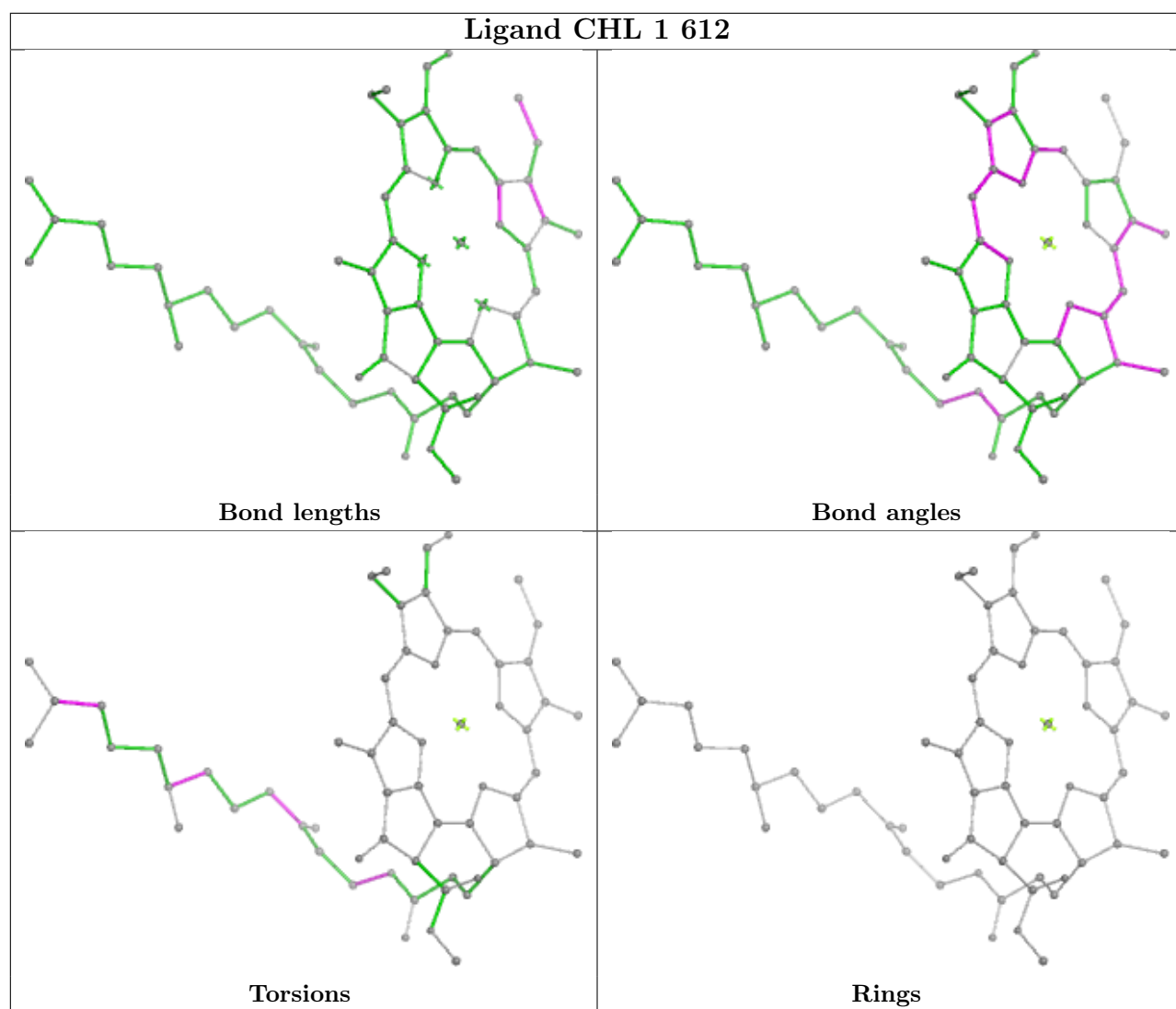


Ligand CLA 1 607

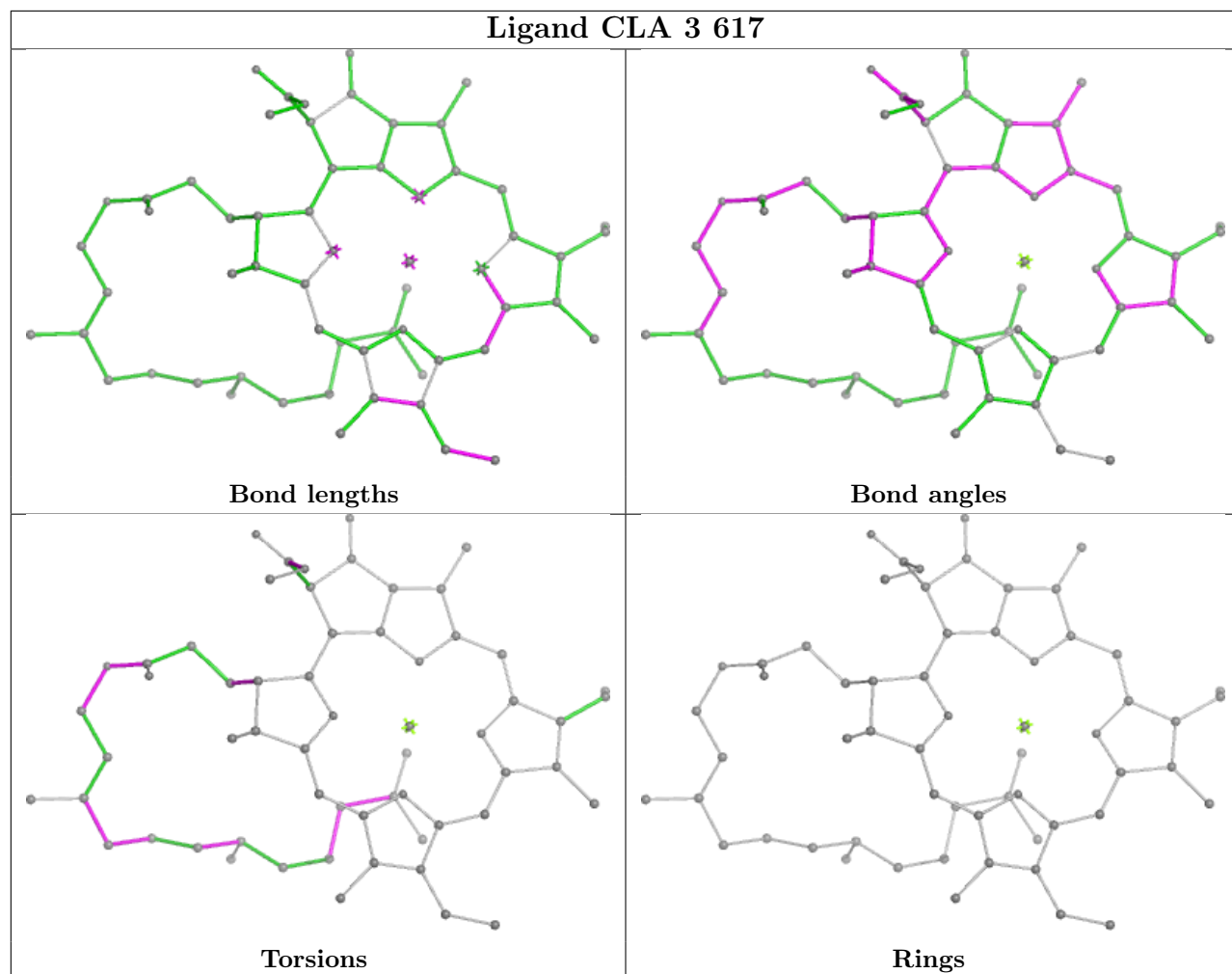




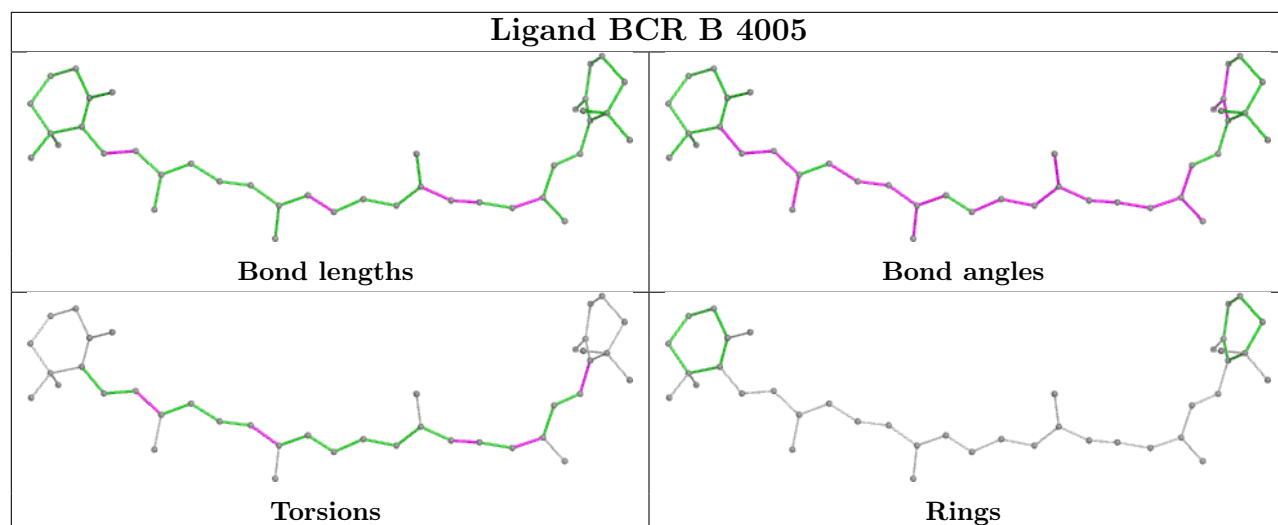


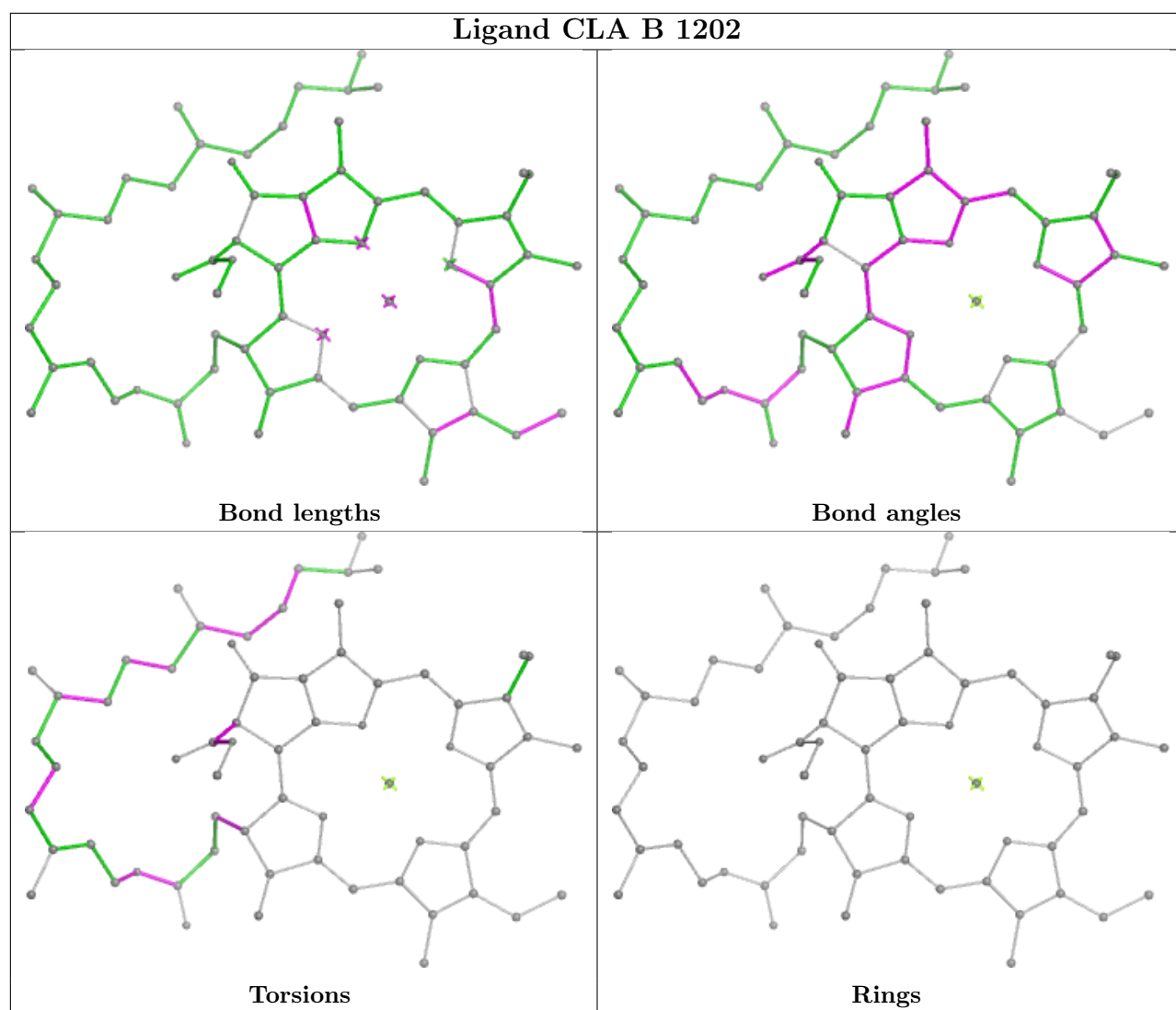


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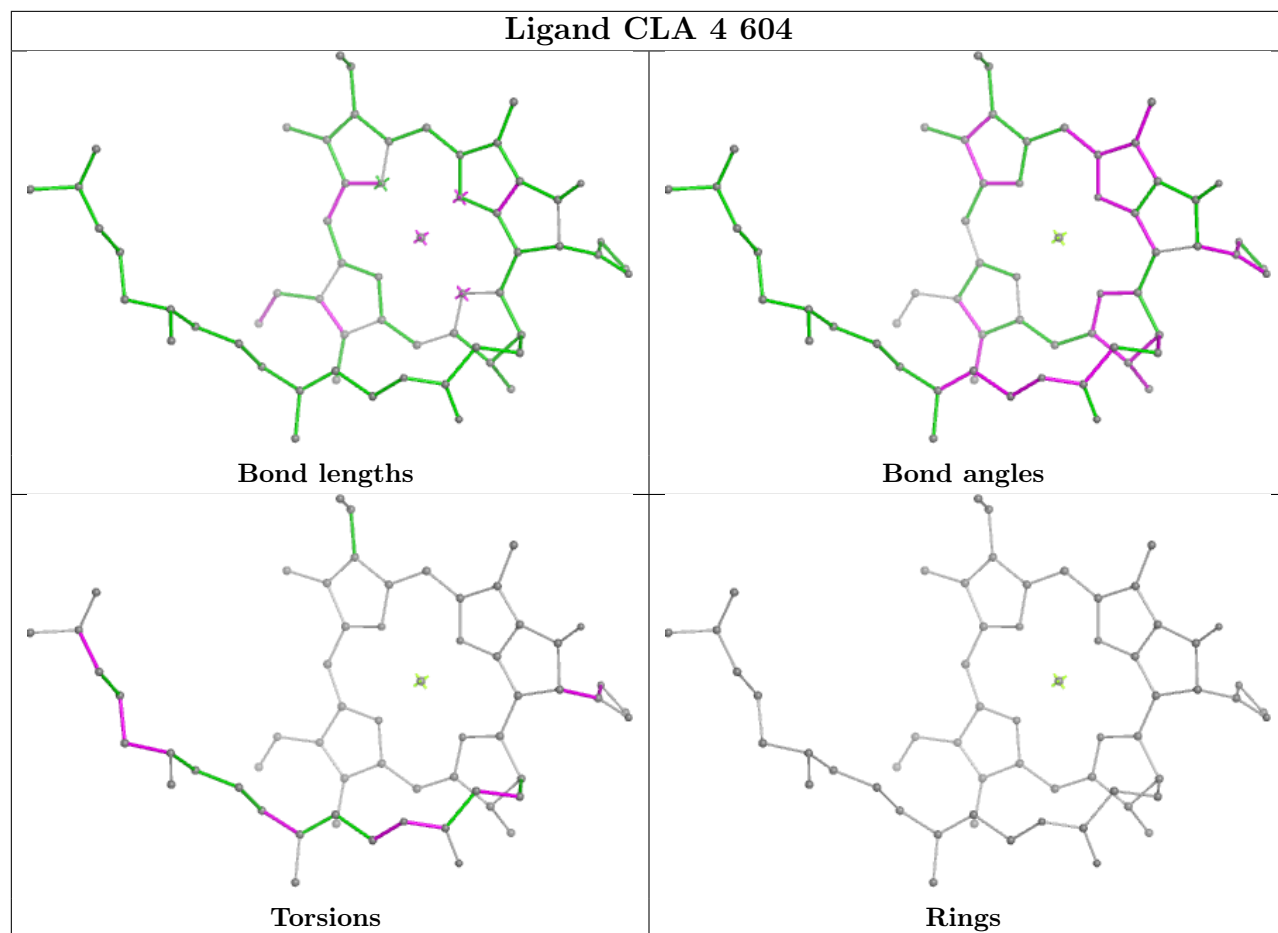


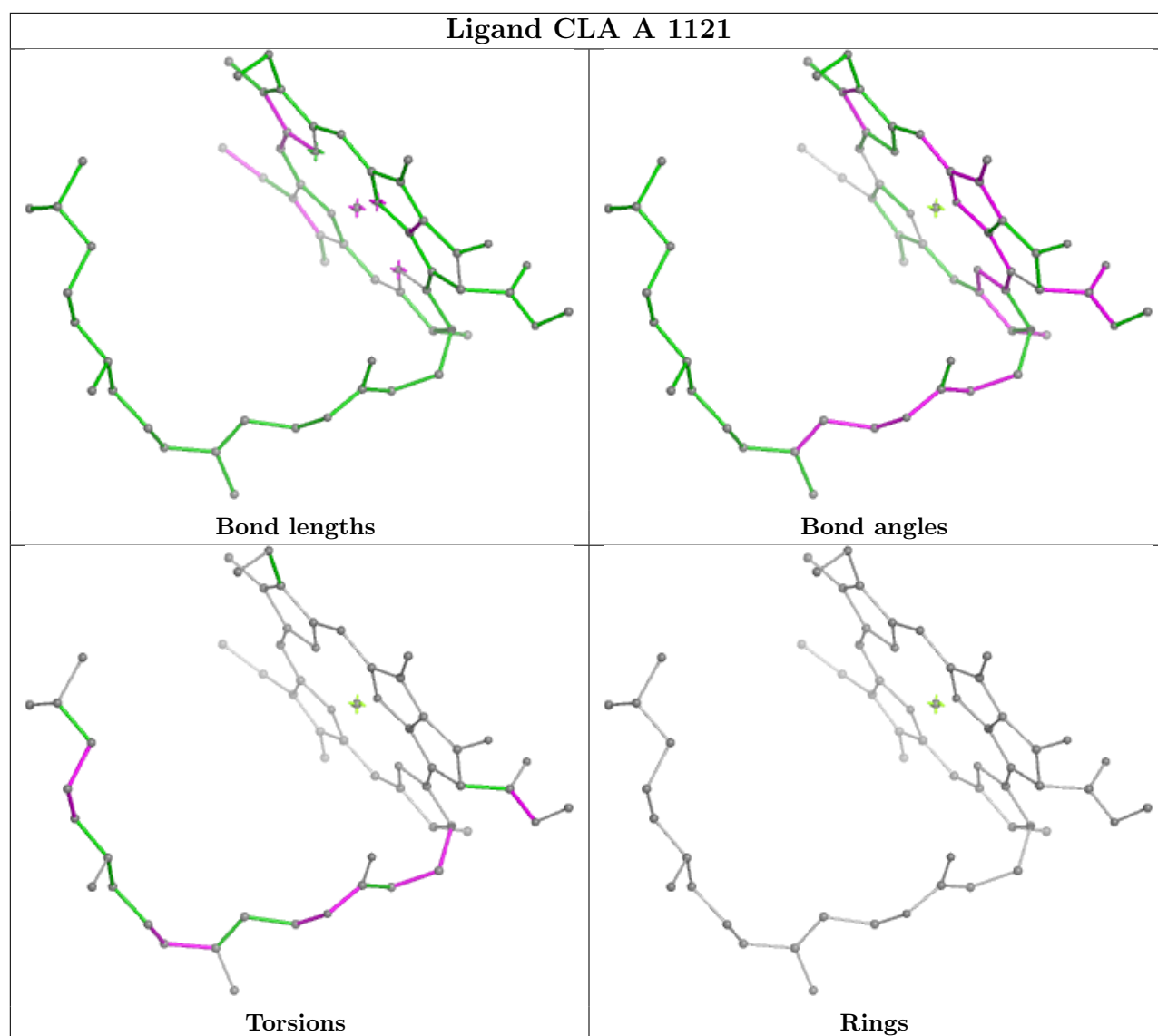
Ligand BCR B 4005

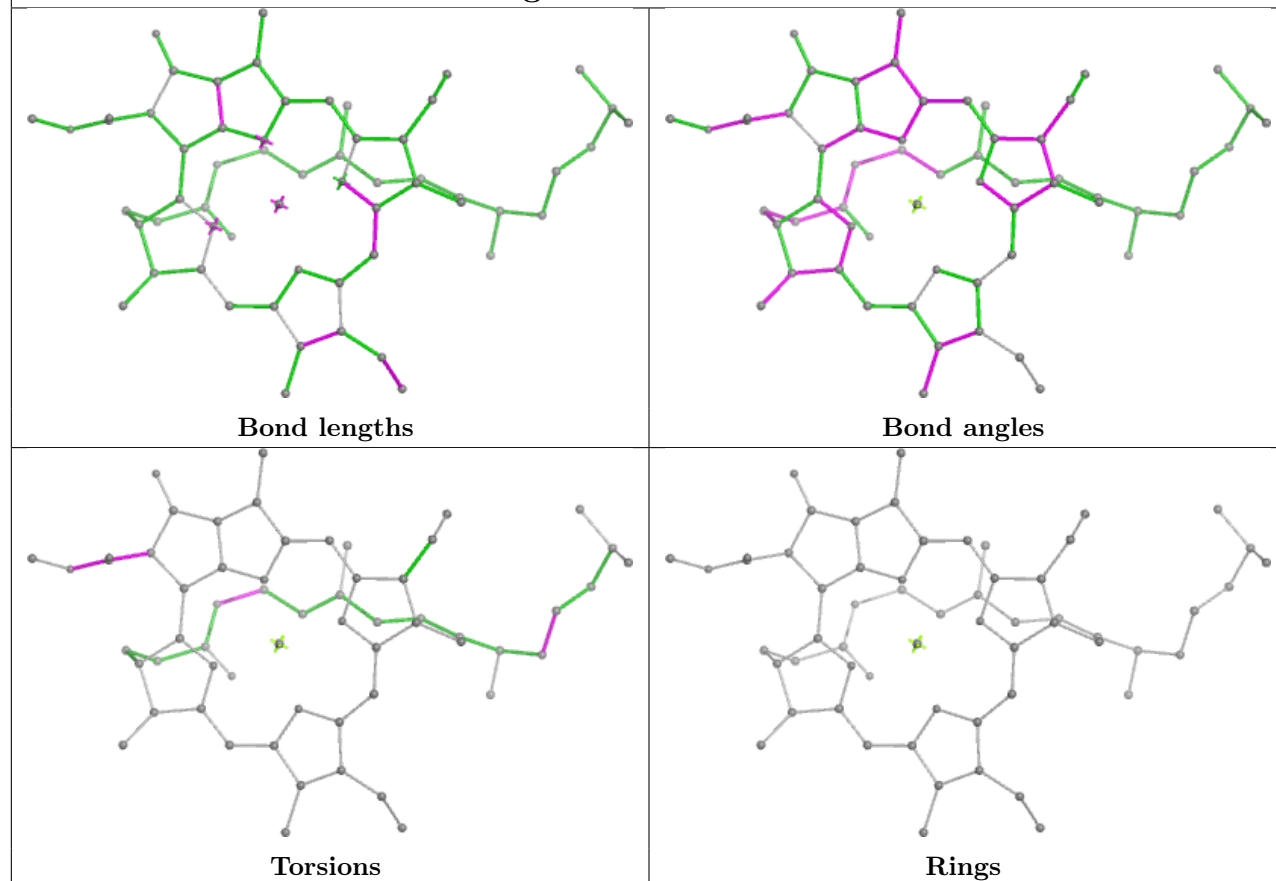
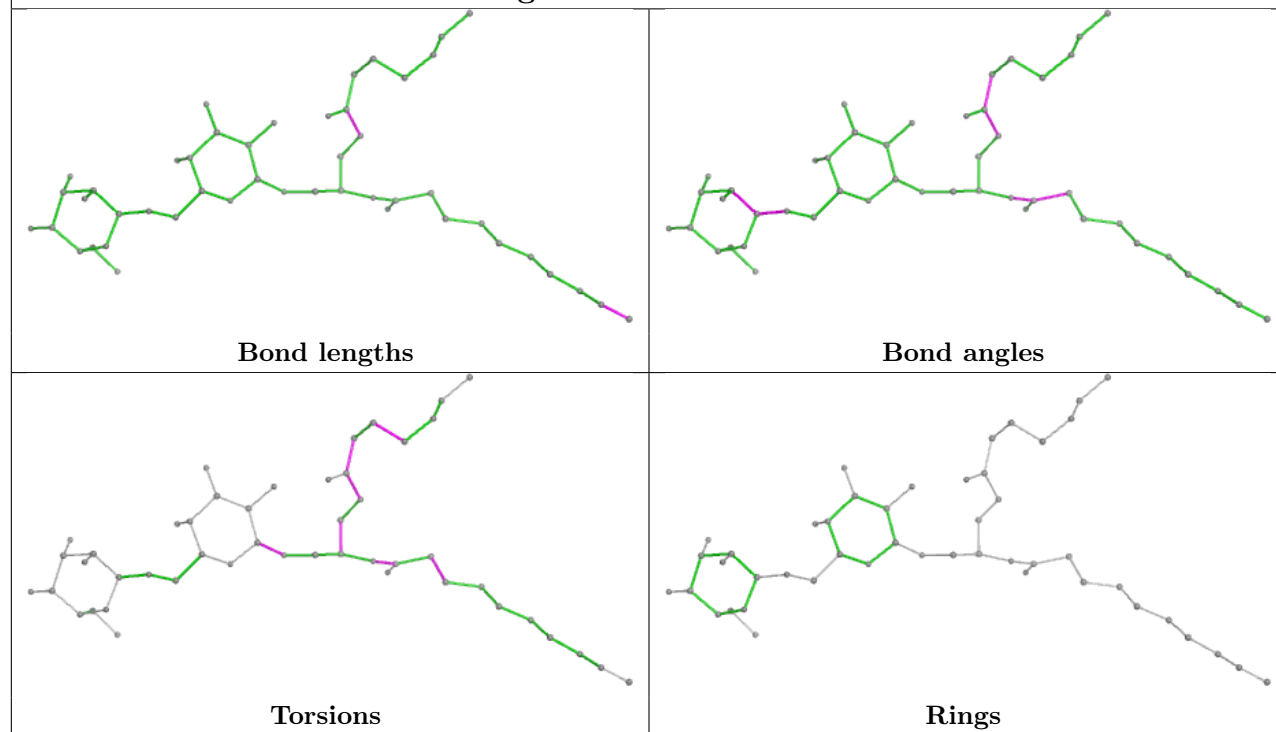




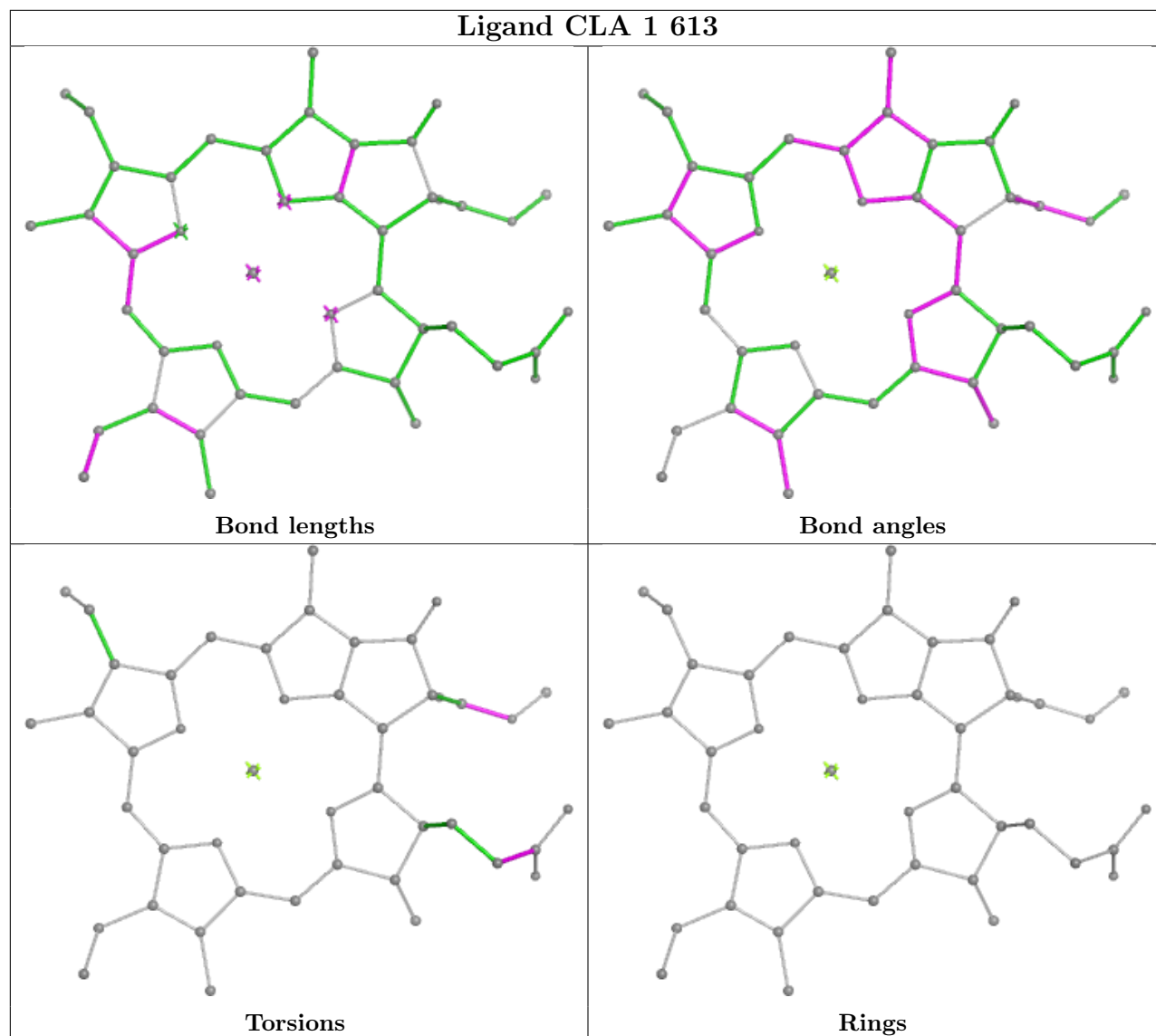
Ligand CLA 4 604

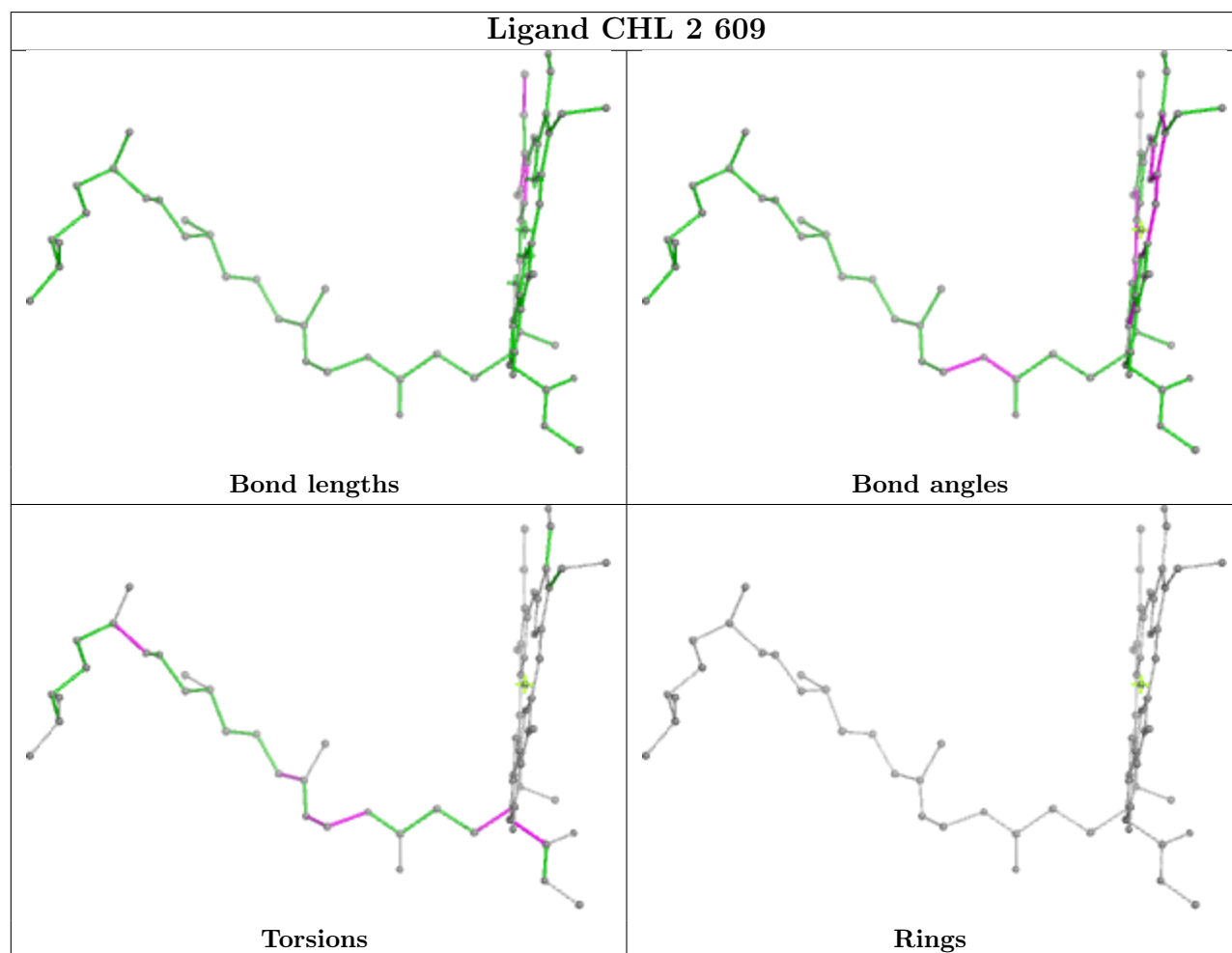
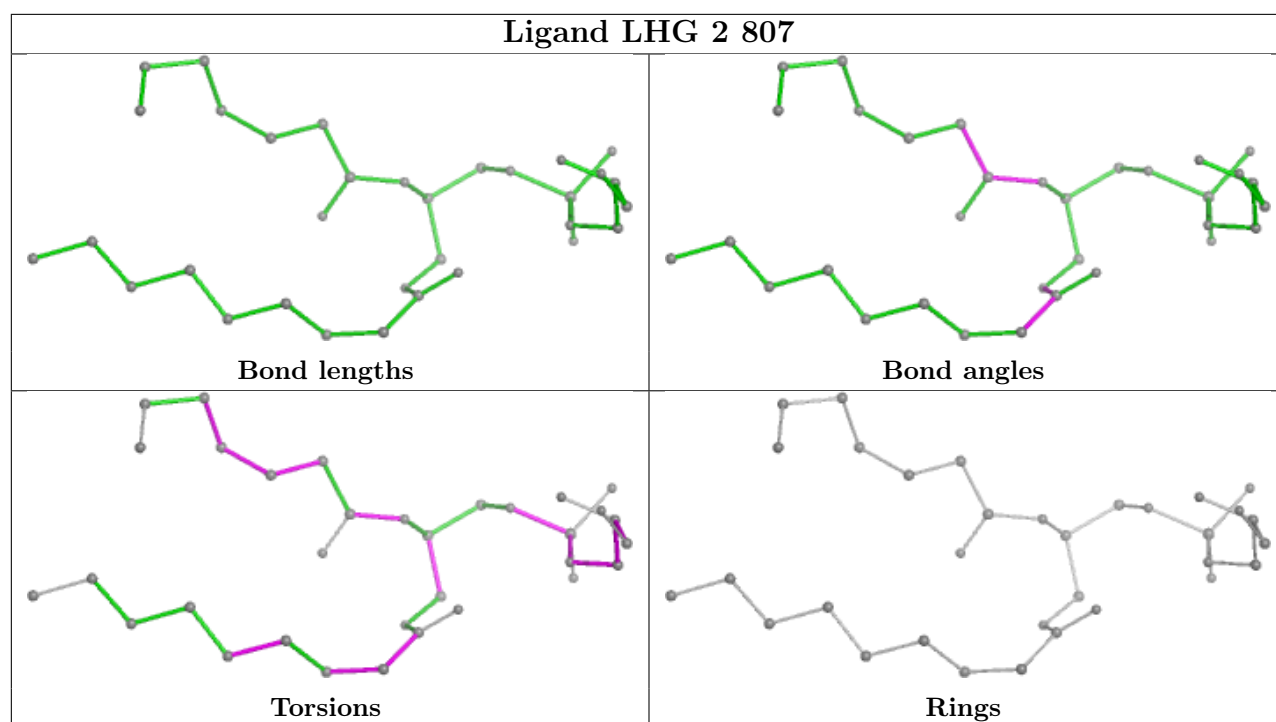


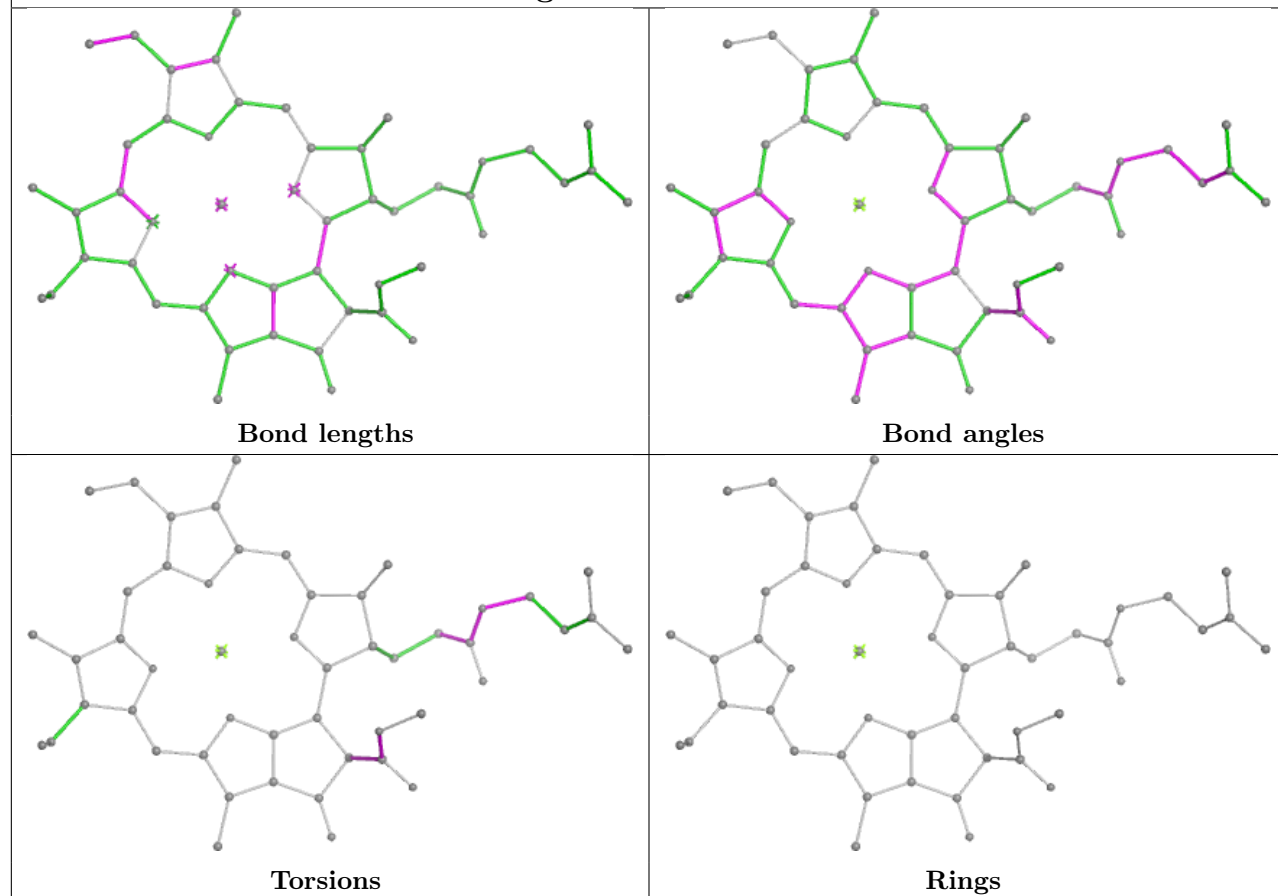
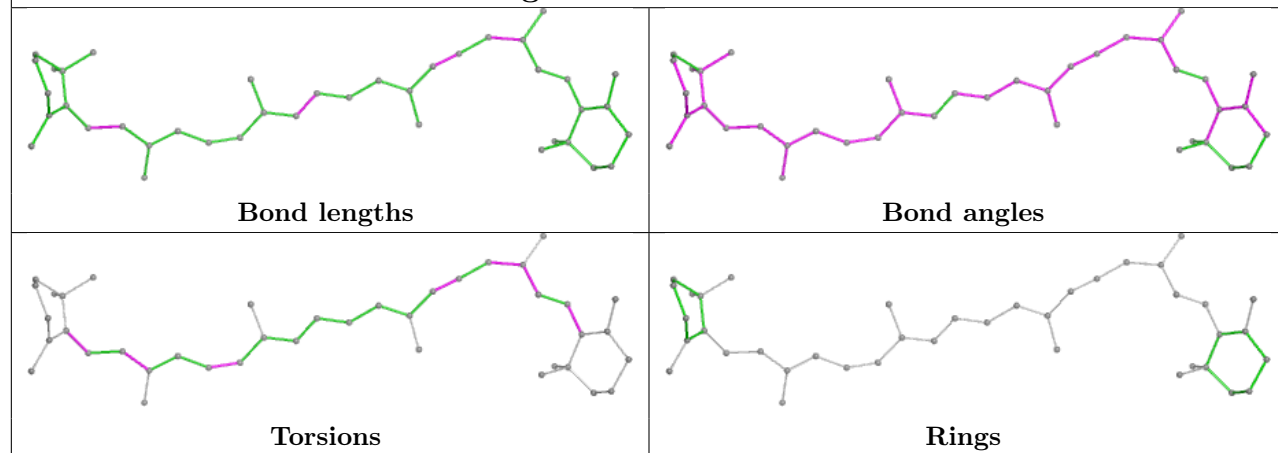


Ligand CLA B 1213**Ligand DGD G 5003**

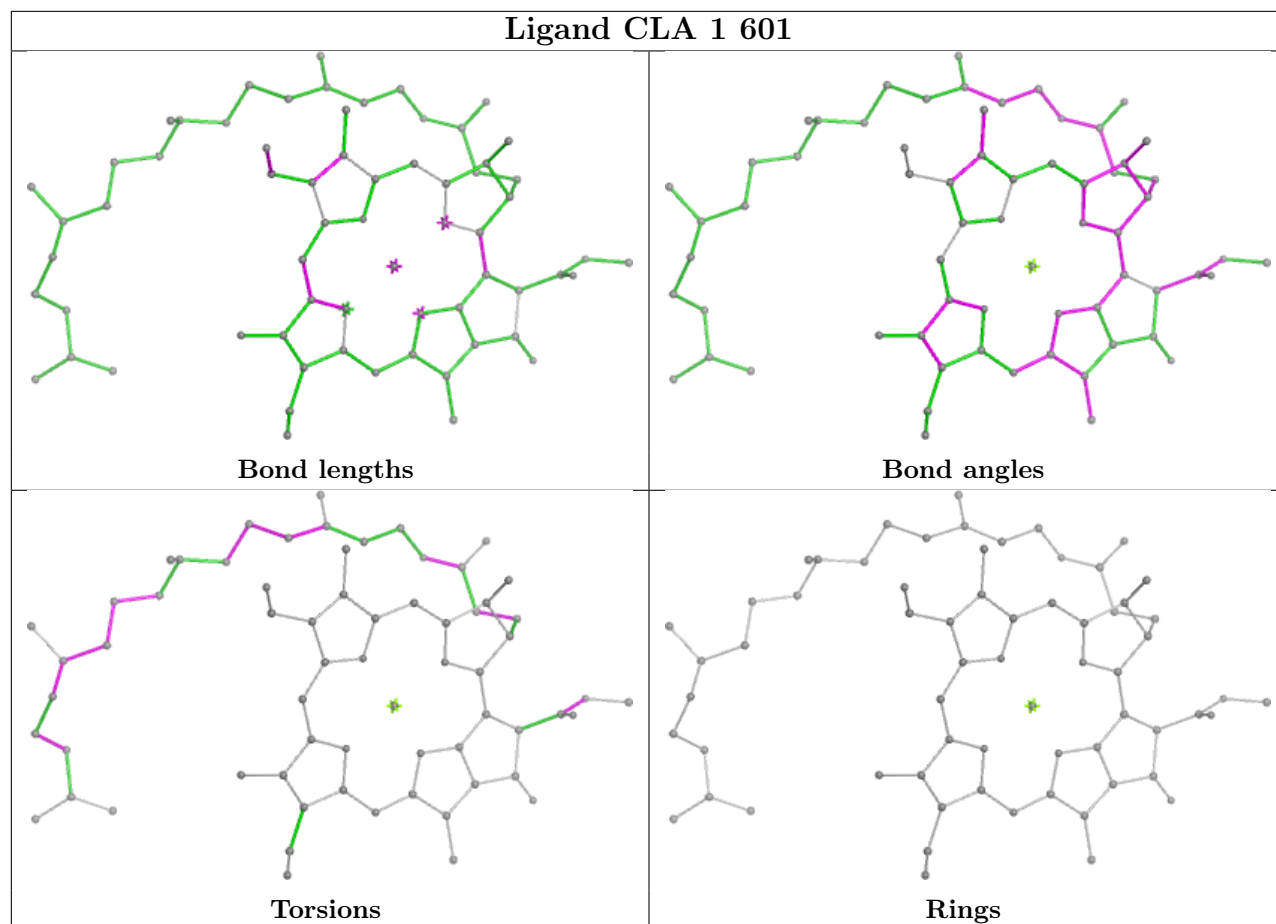
Ligand CLA 1 613



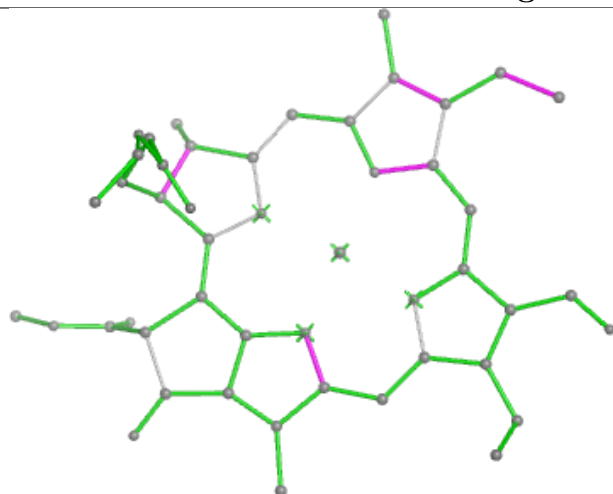


Ligand CLA 4 602**Ligand BCR B 4006**

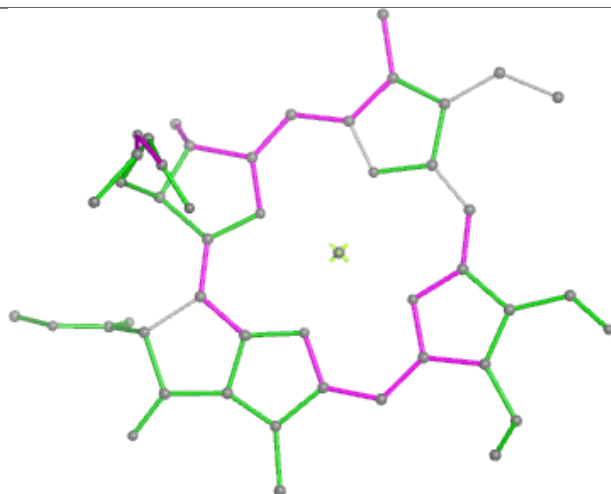
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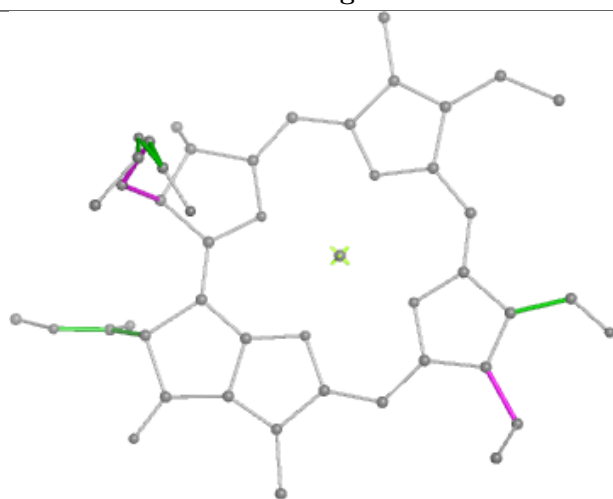
Ligand CHL 2 611



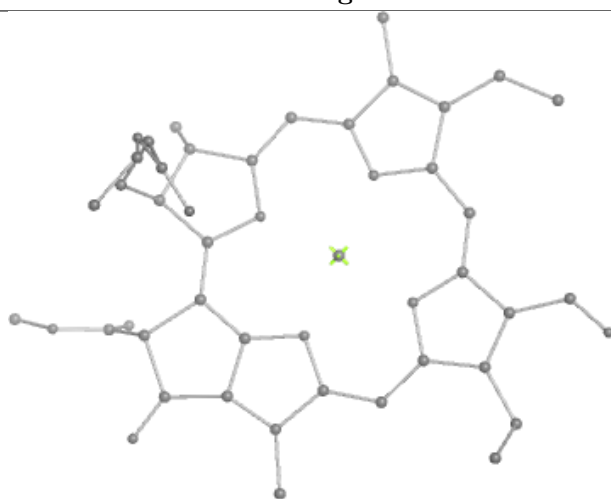
Bond lengths



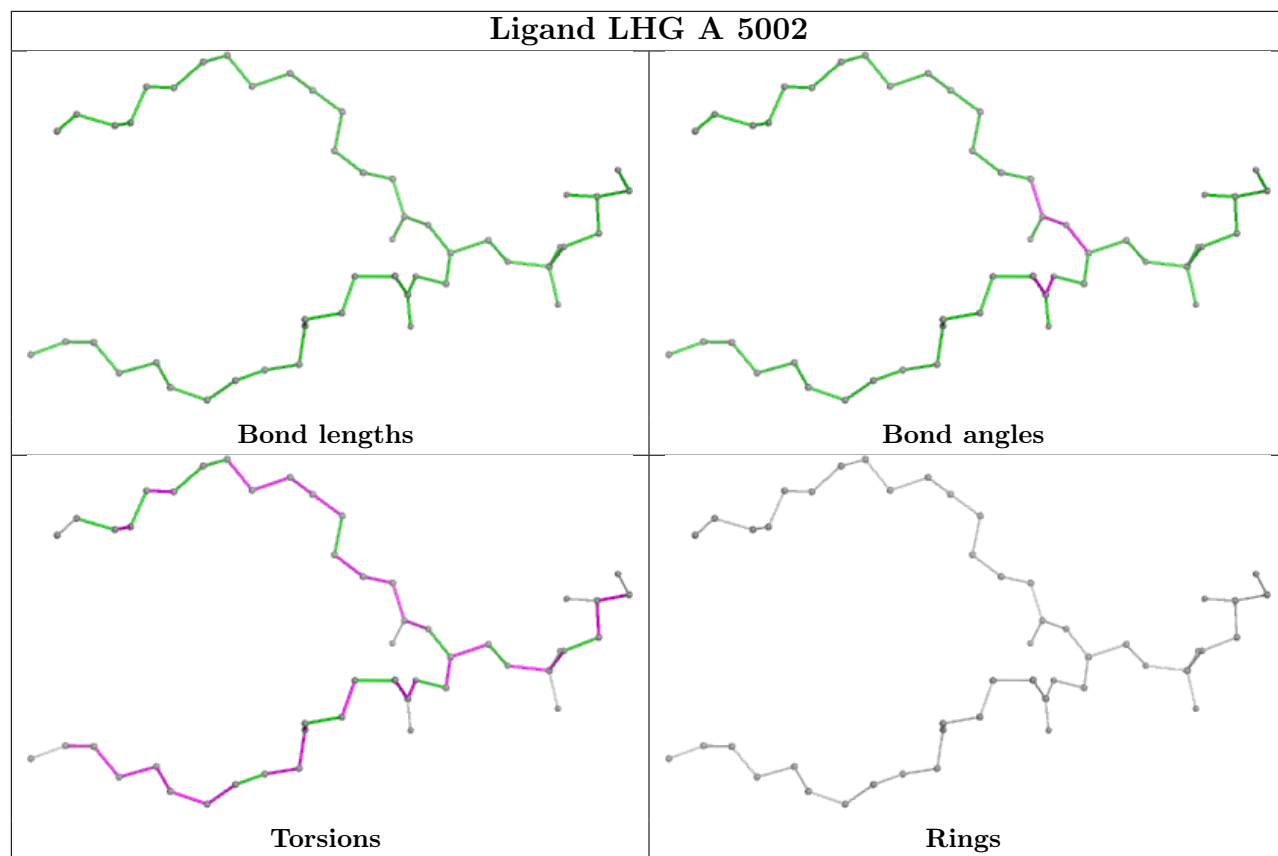
Bond angles

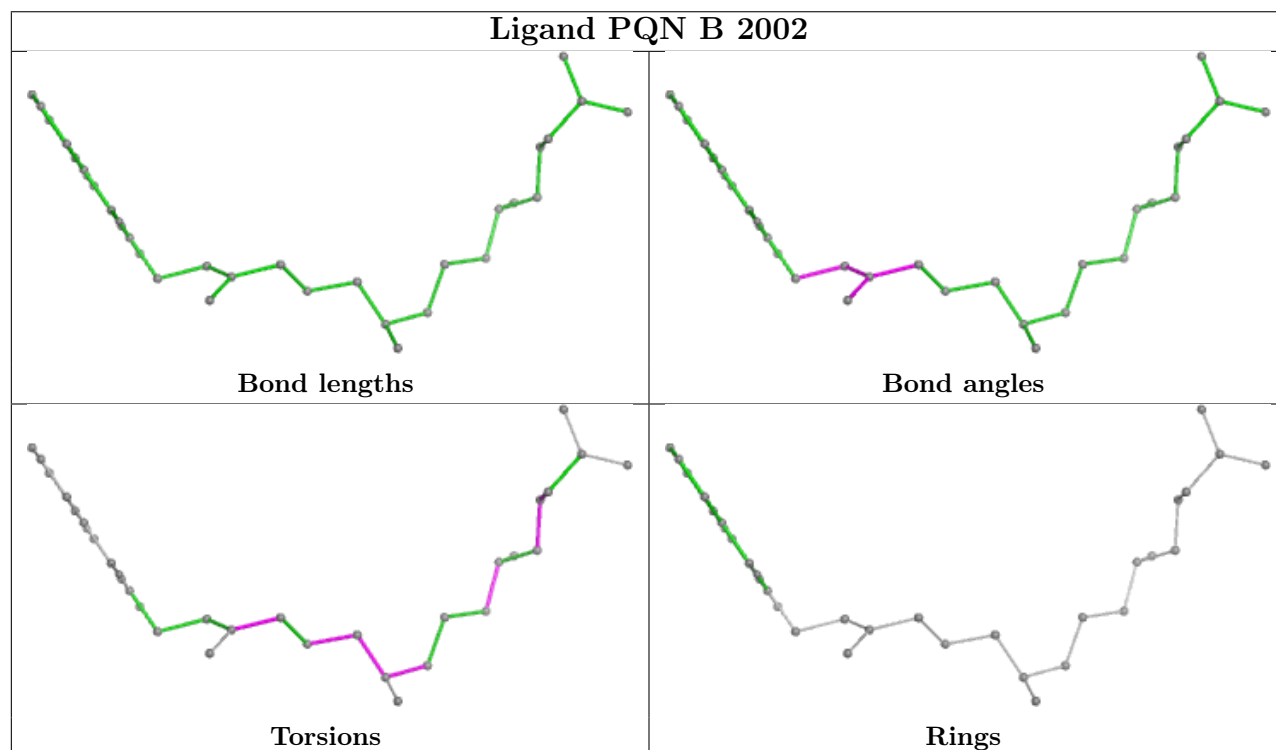
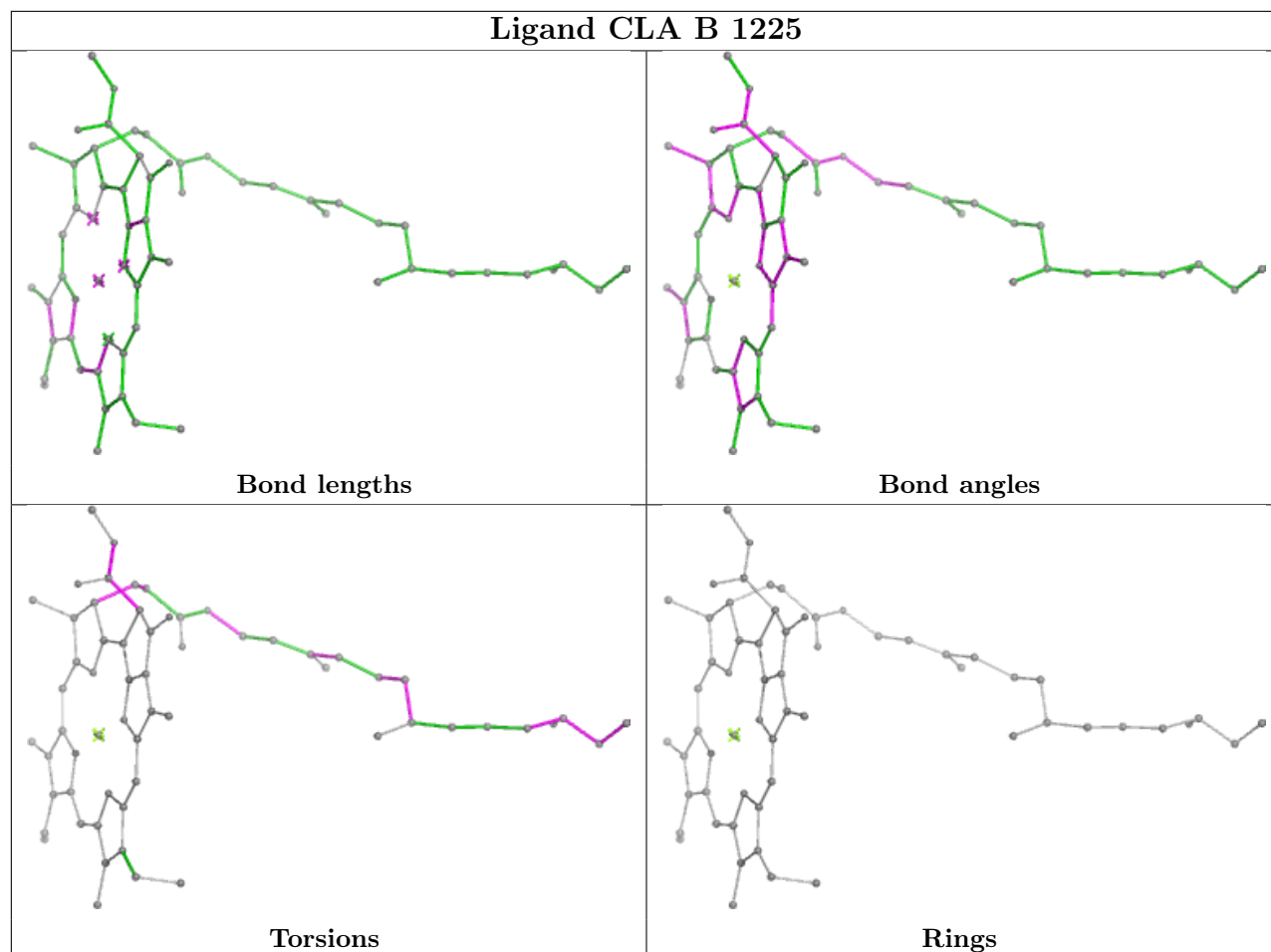


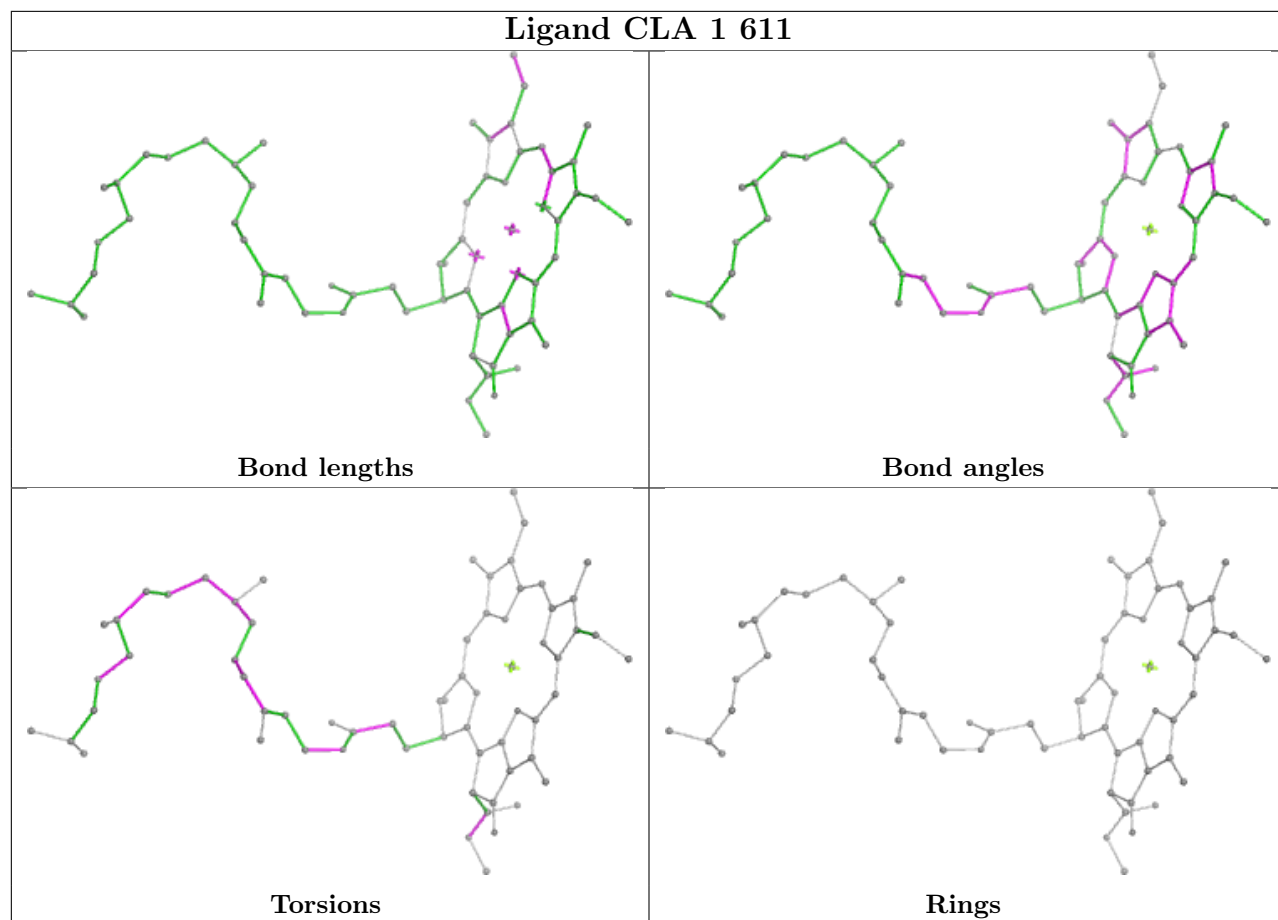
Torsions

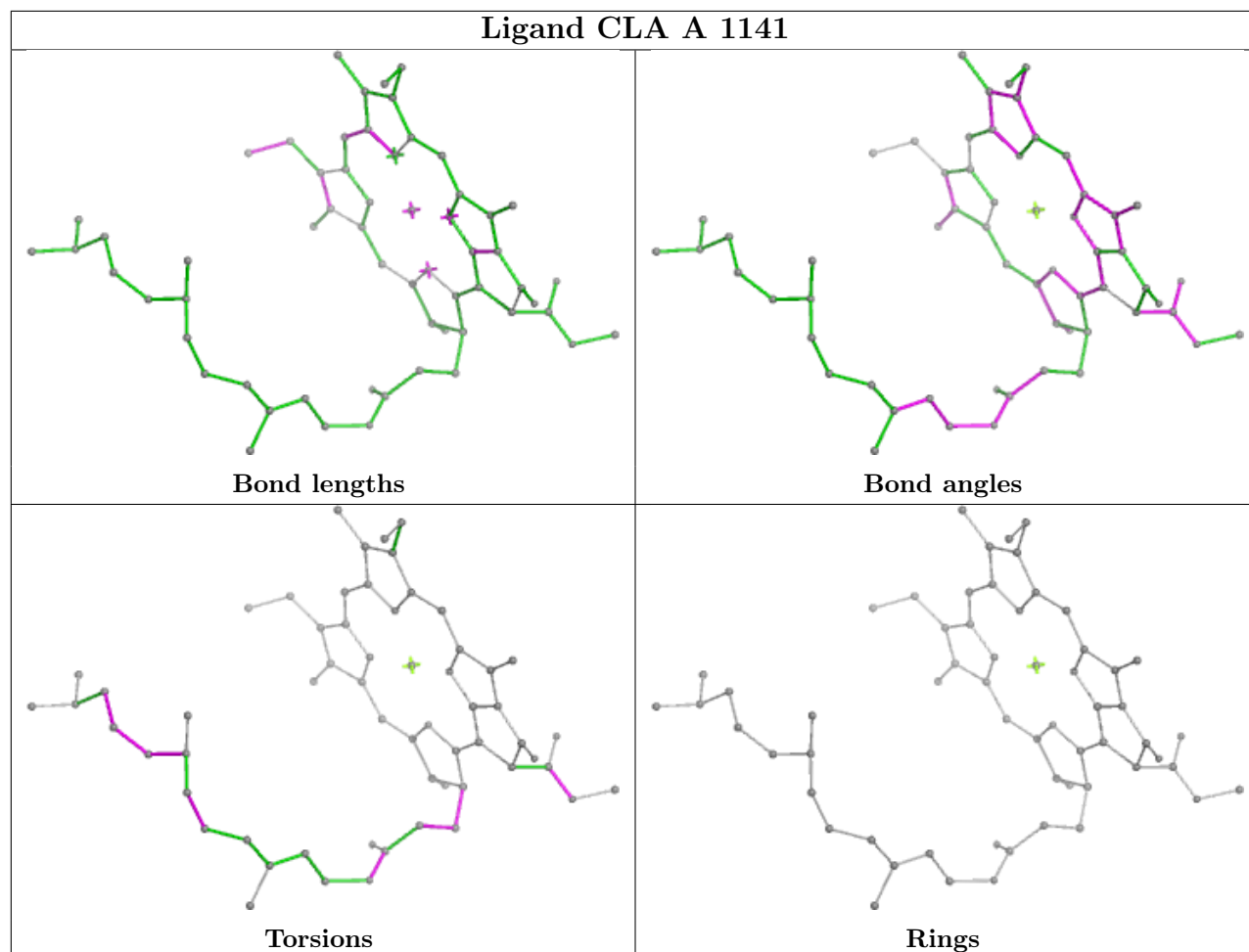
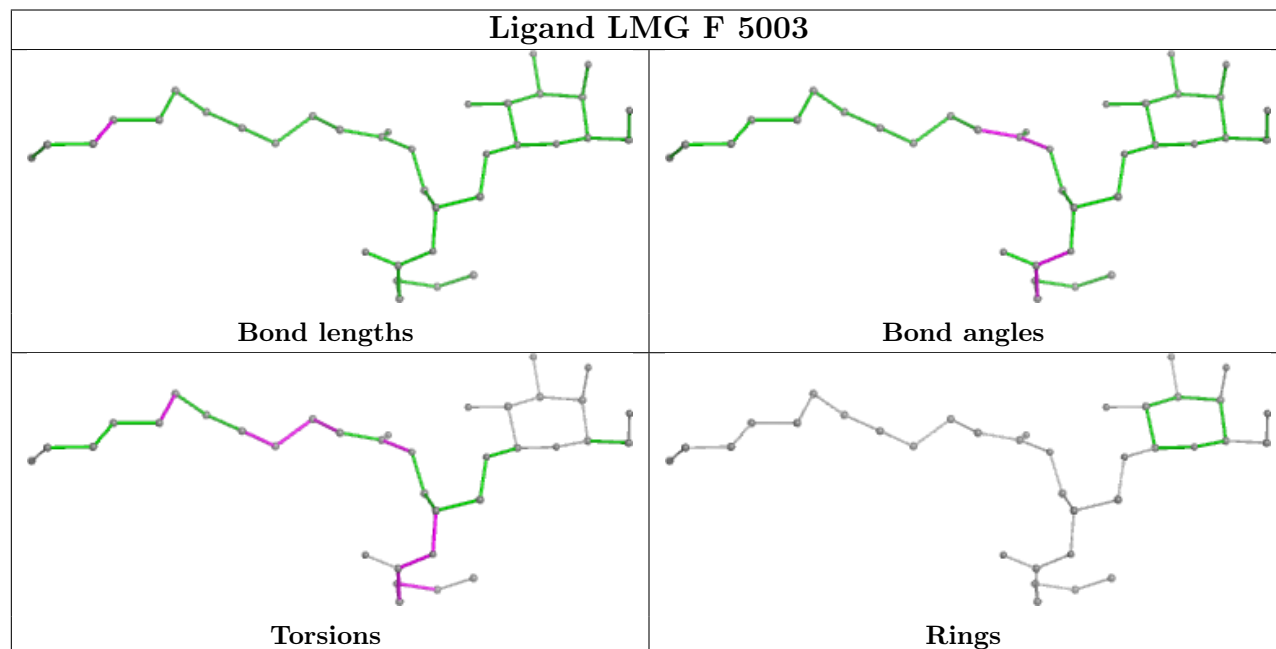


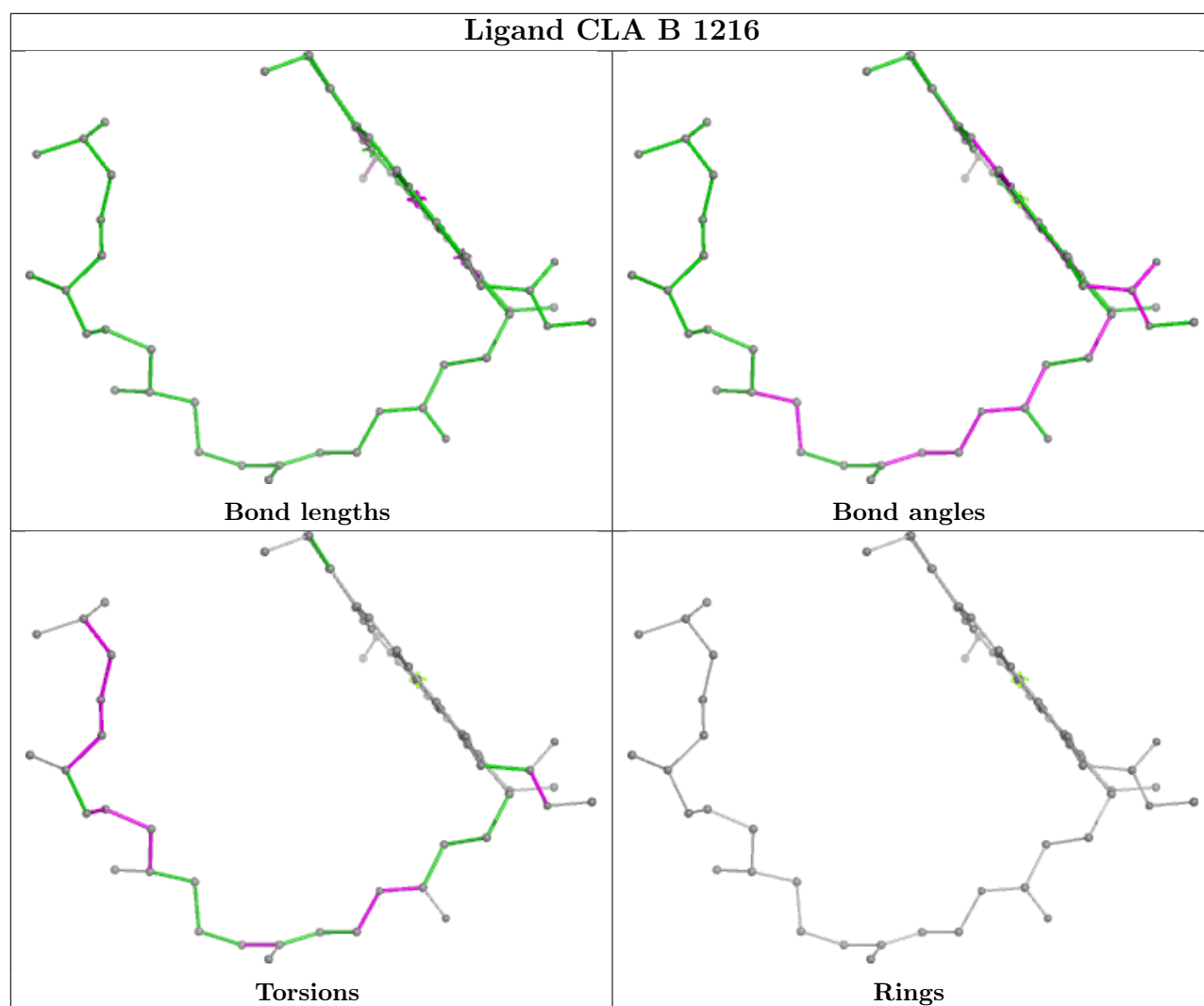
Rings

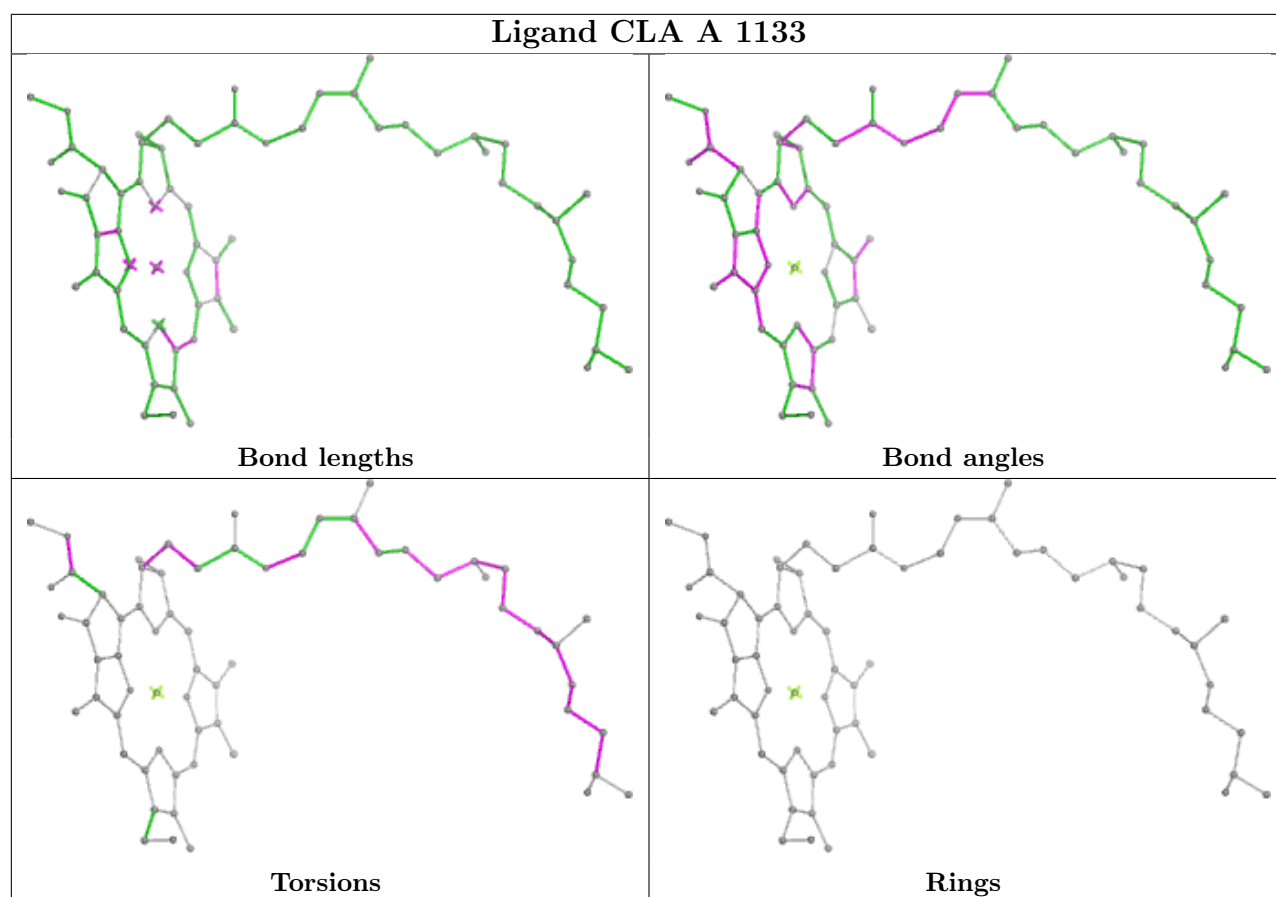


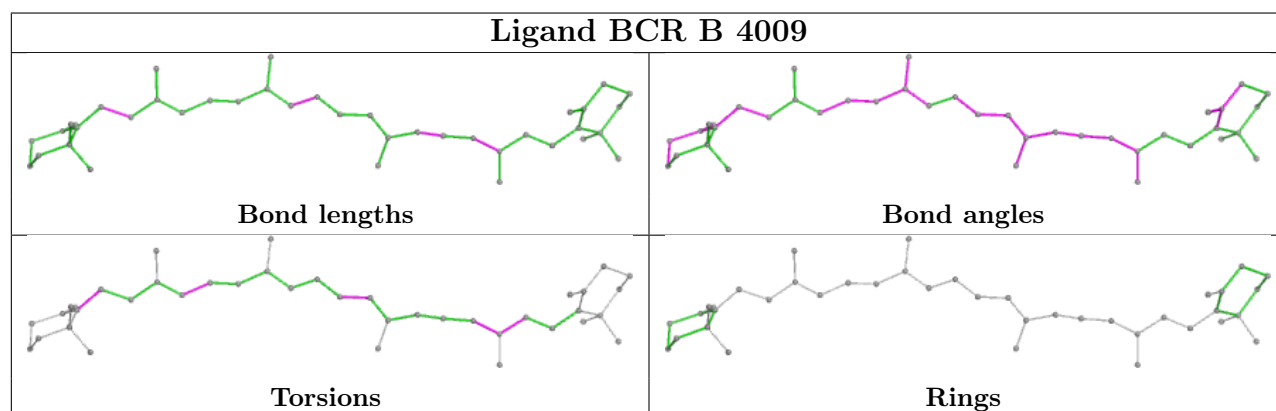
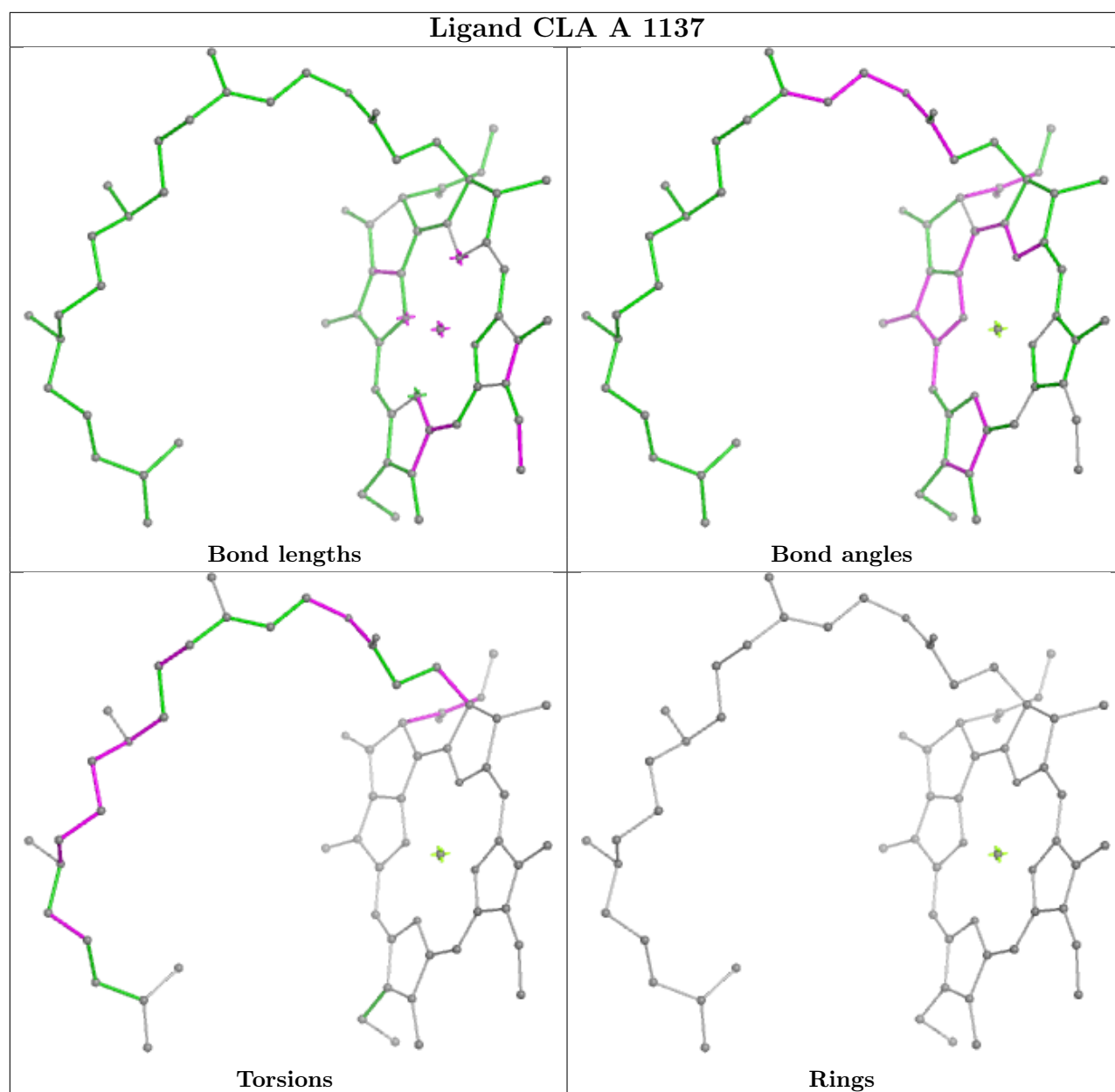




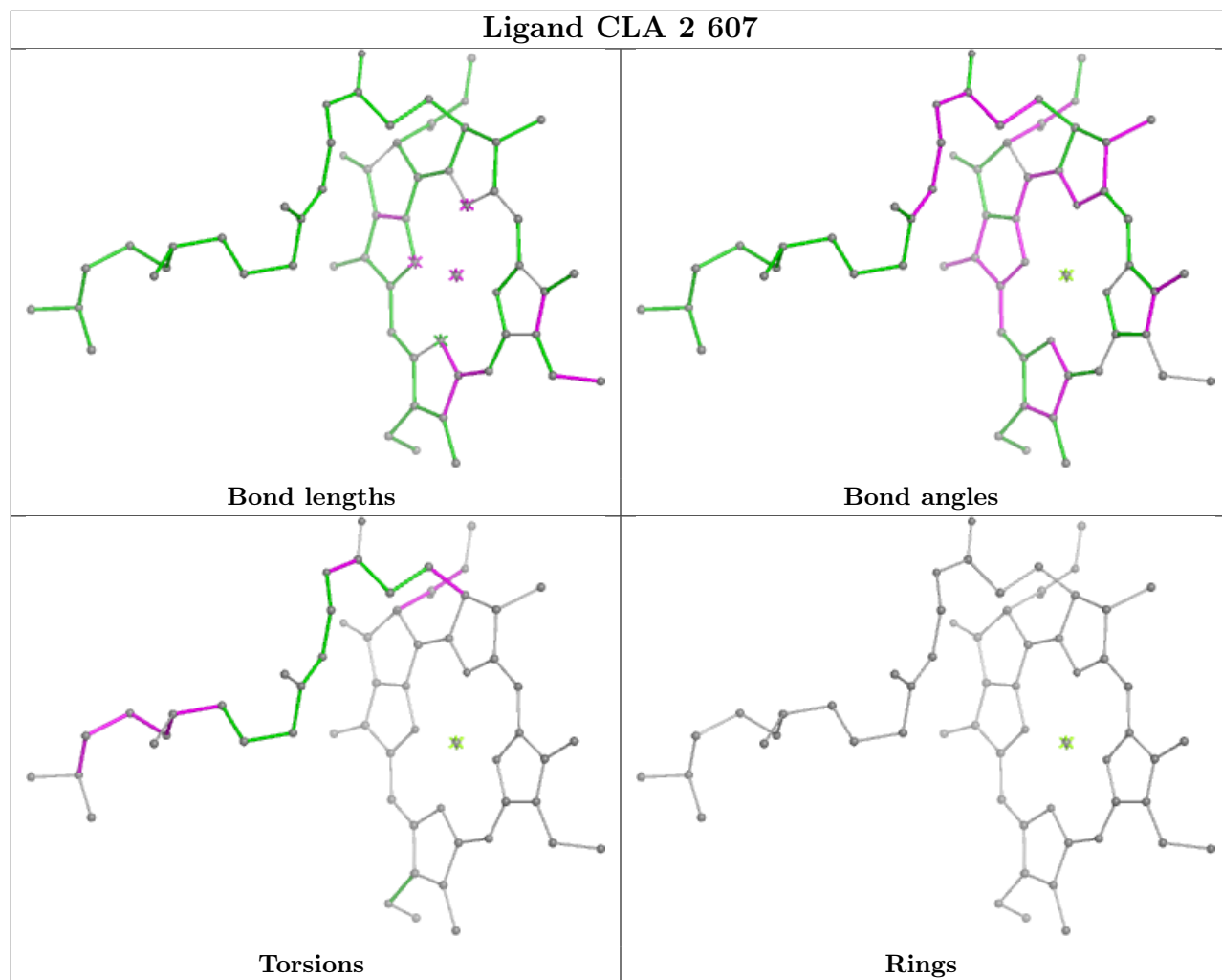
Ligand CLA A 1141**Ligand LMG F 5003**

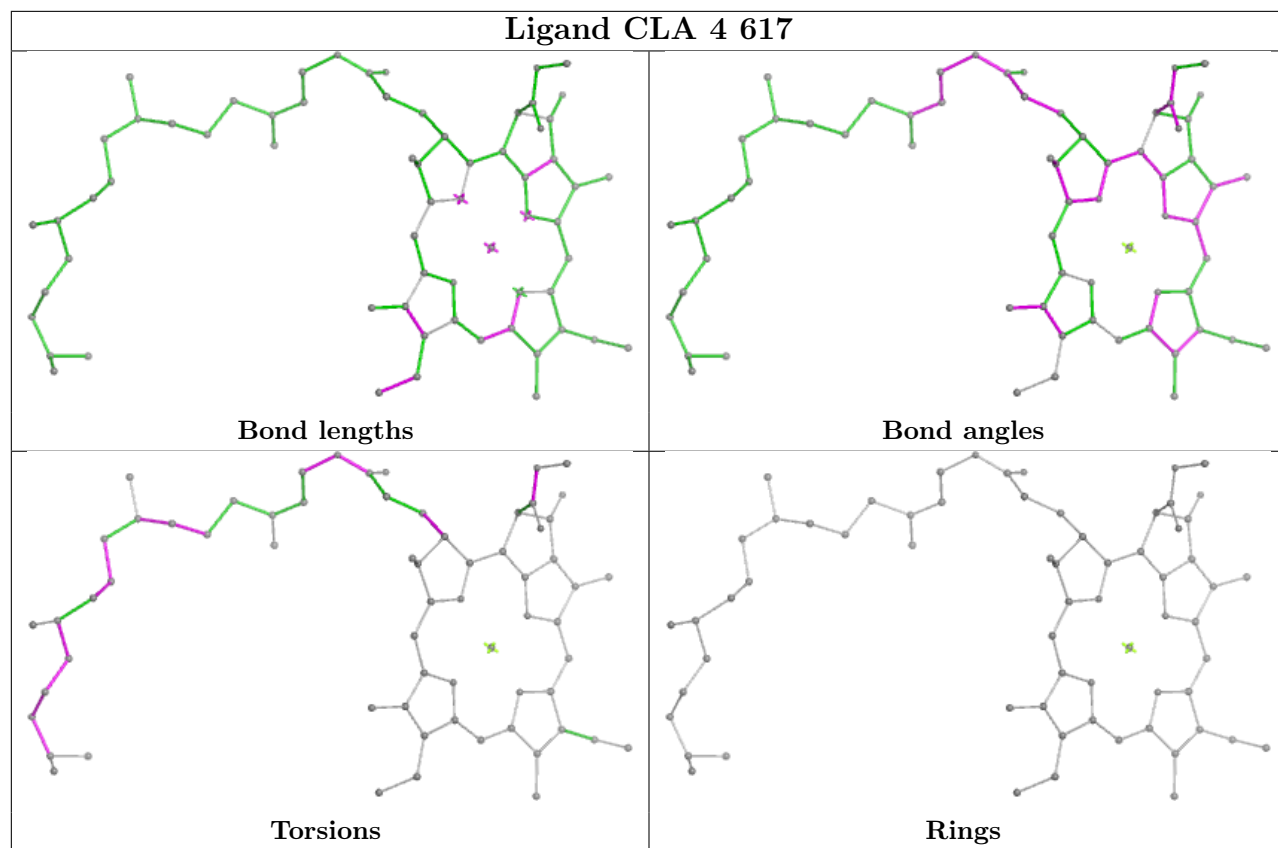




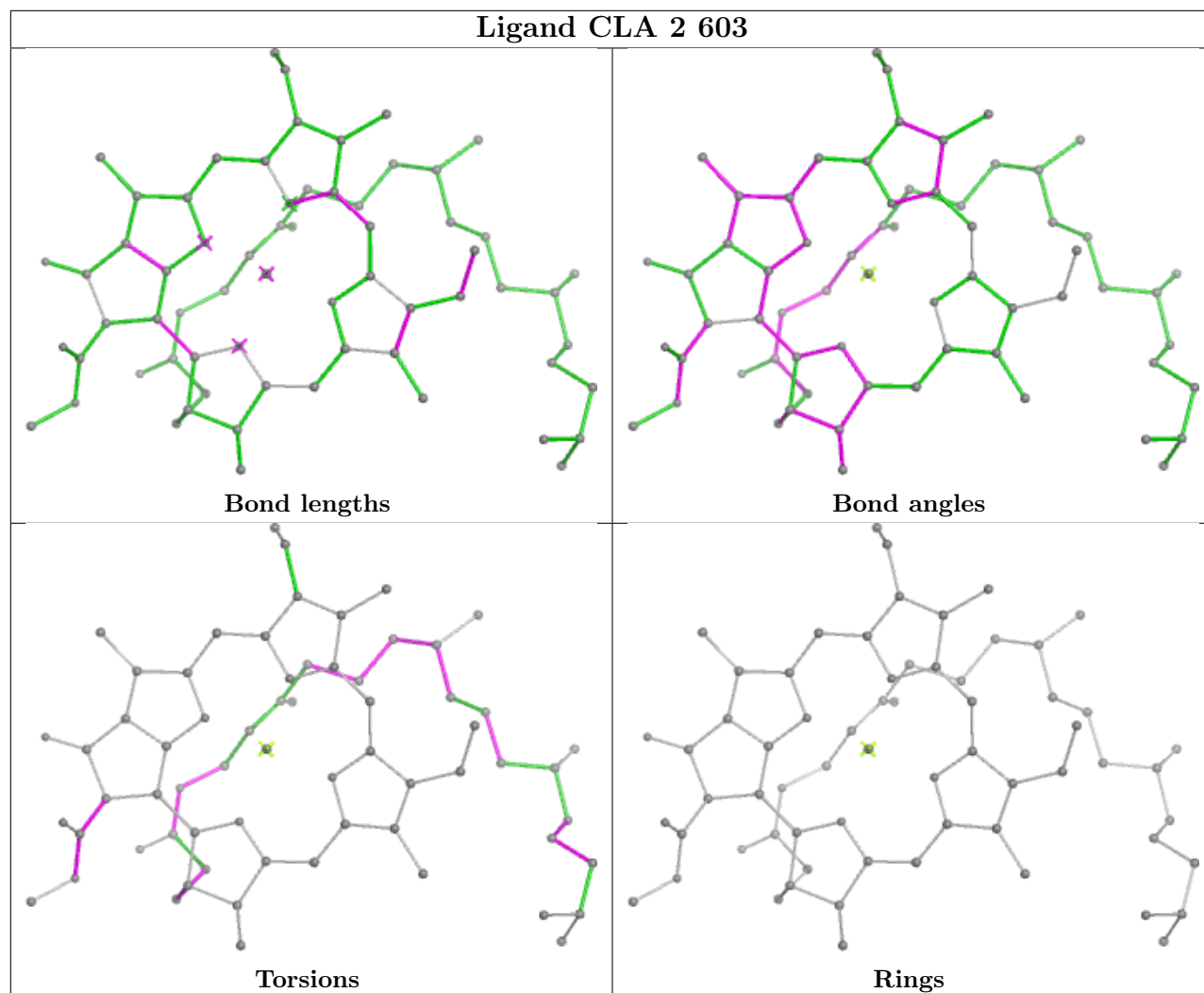


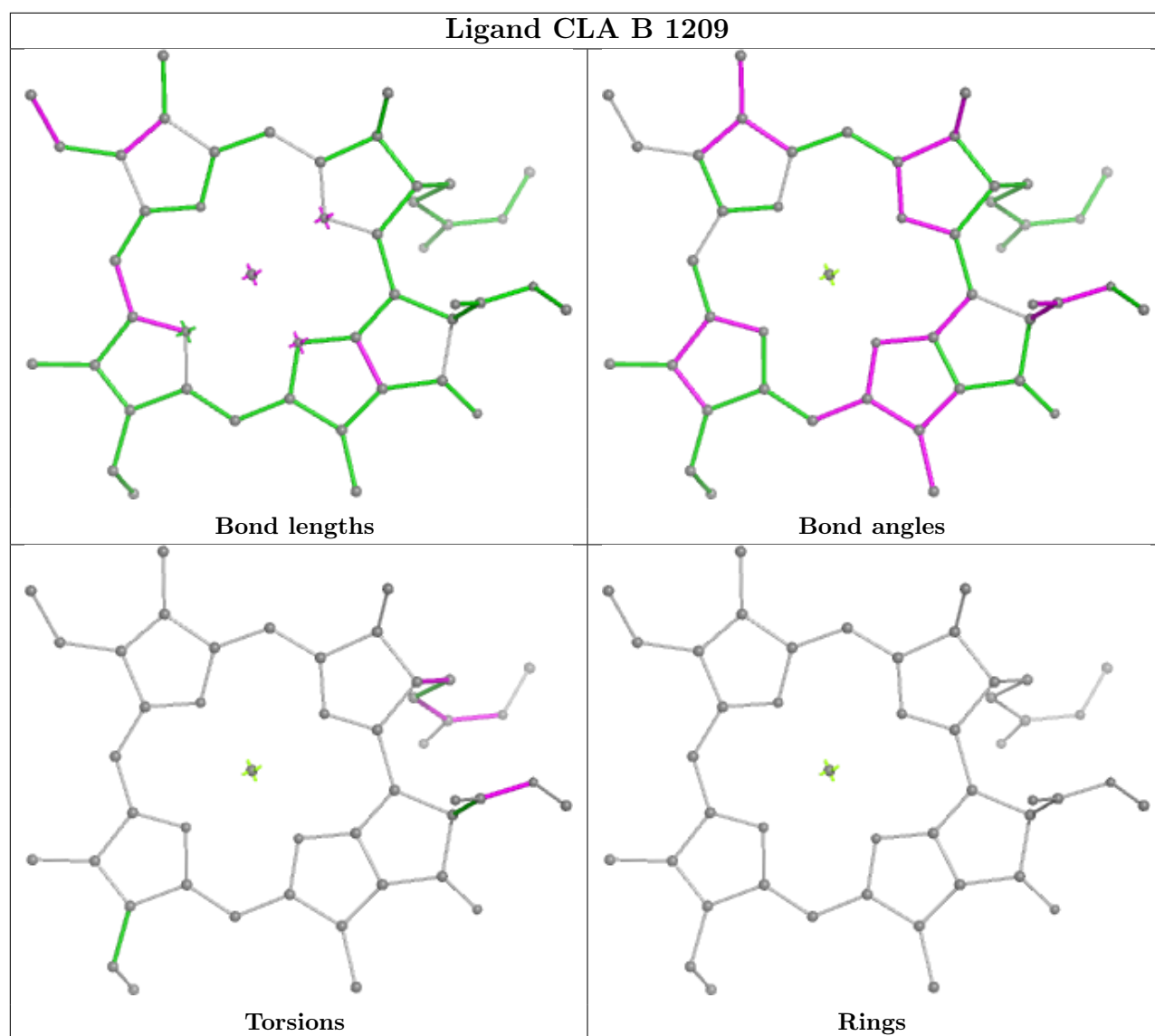
Ligand CLA 2 607



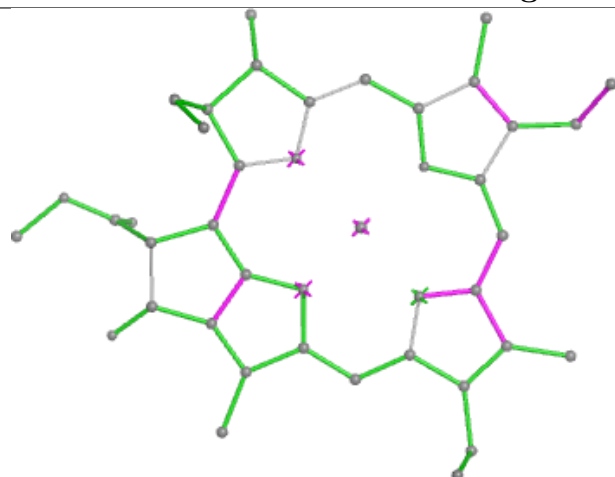


Ligand CLA 2 603

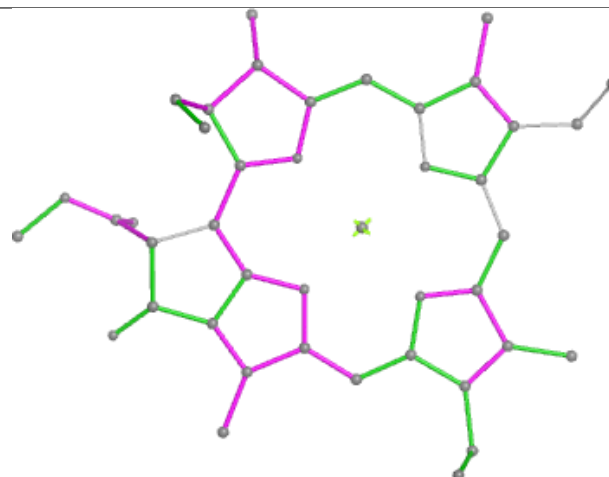




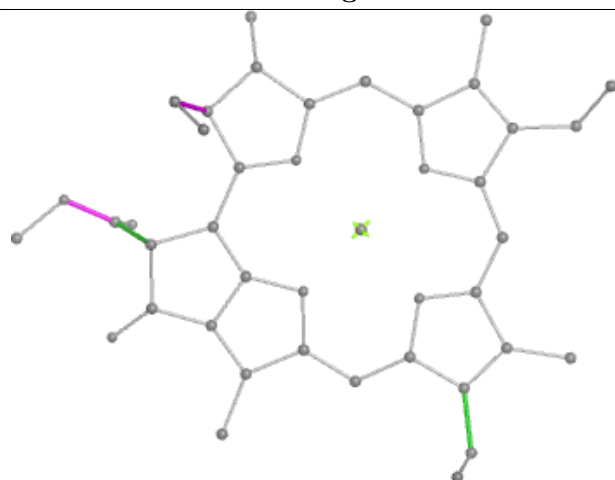
Ligand CLA 3 614



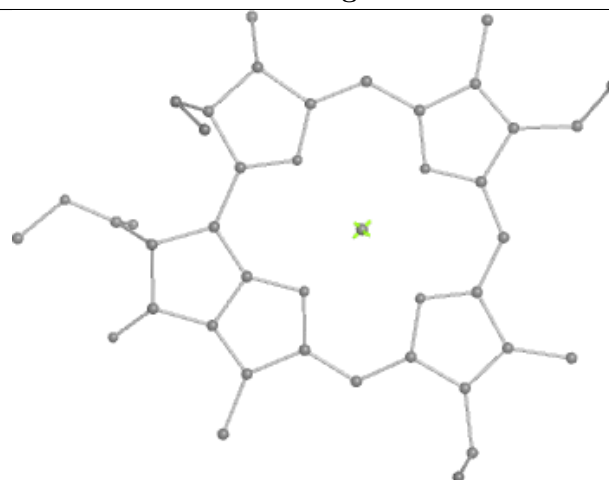
Bond lengths



Bond angles

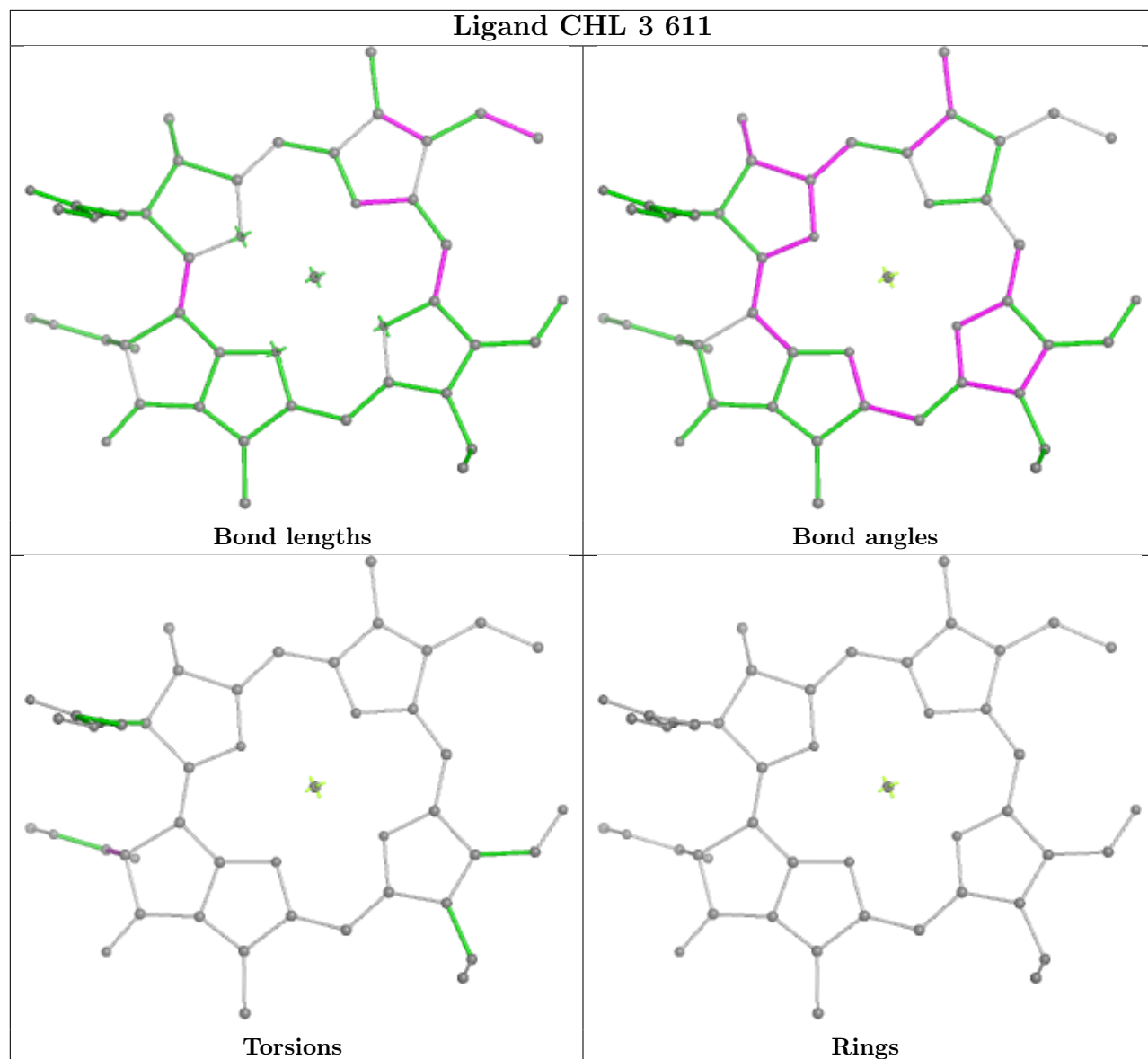


Torsions

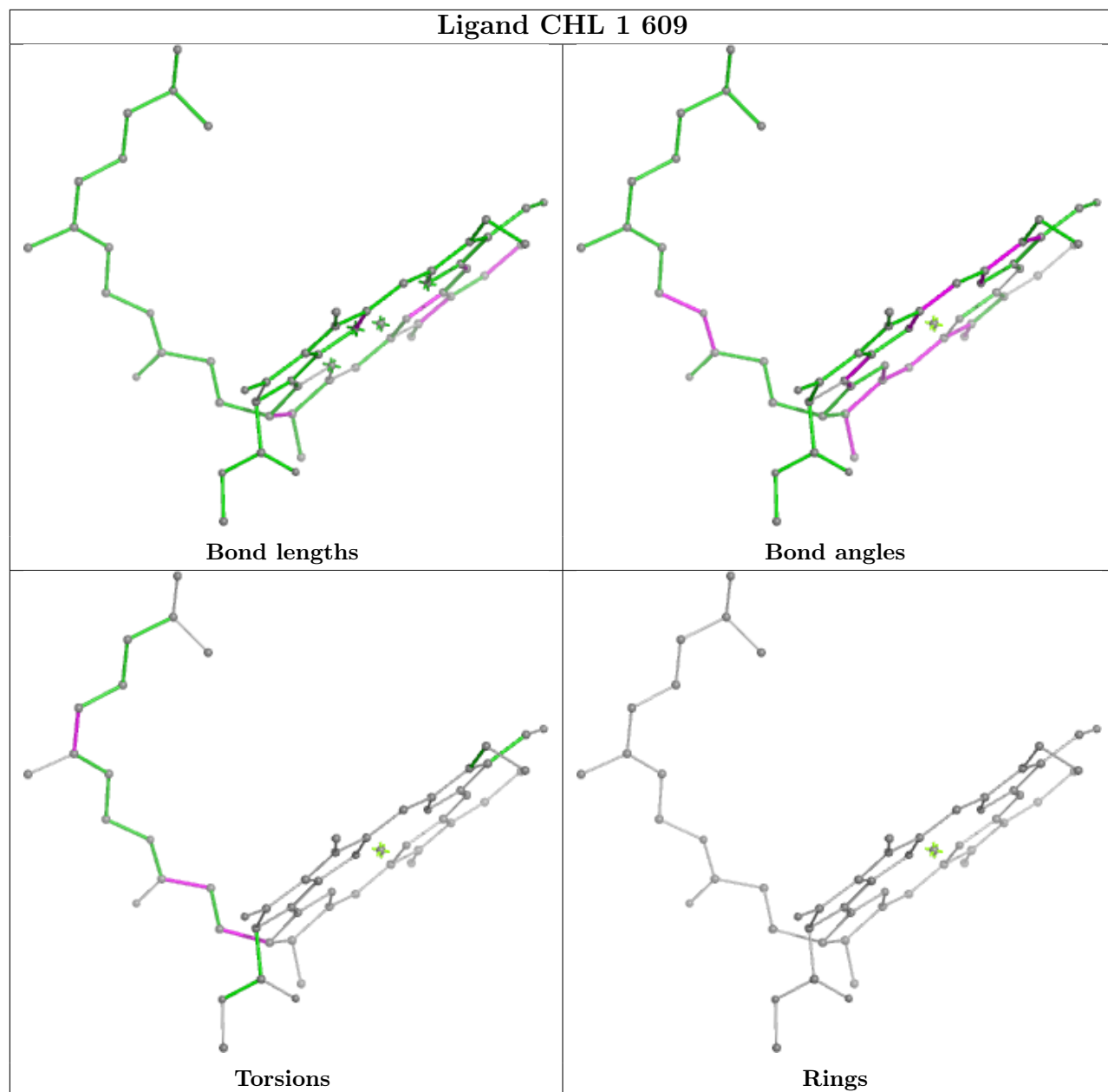


Rings

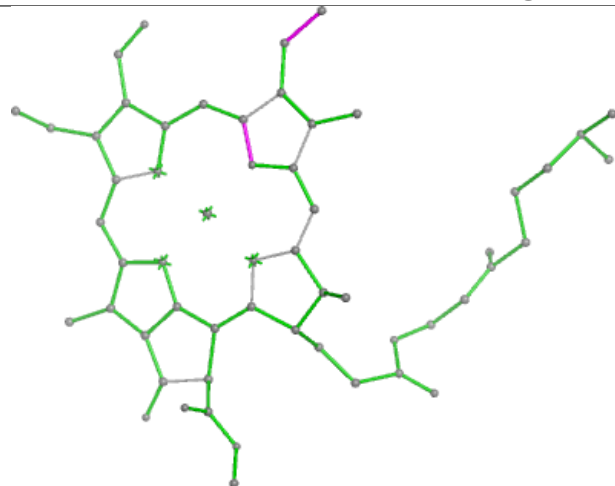
Ligand CHL 3 611



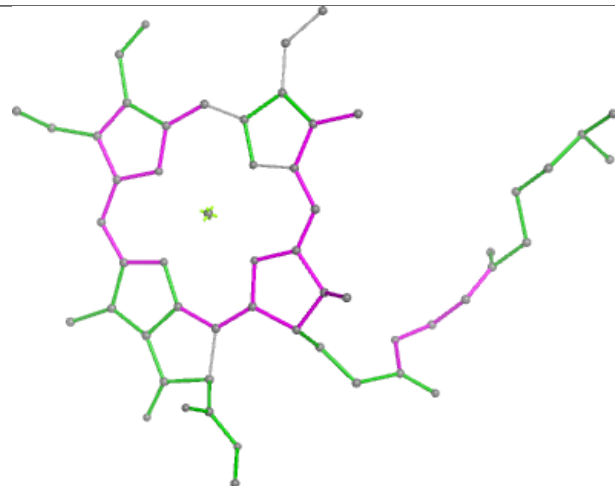
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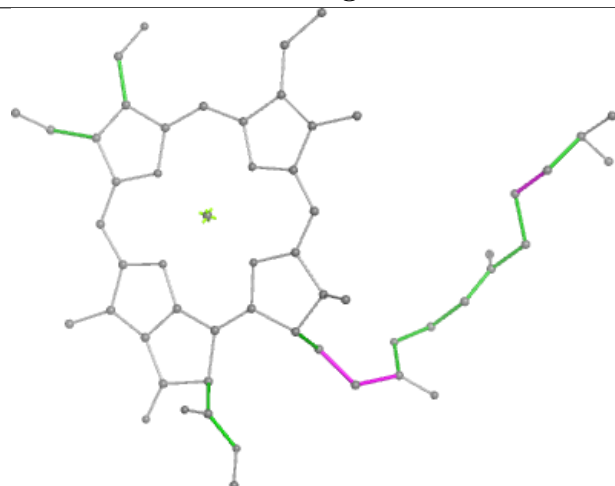
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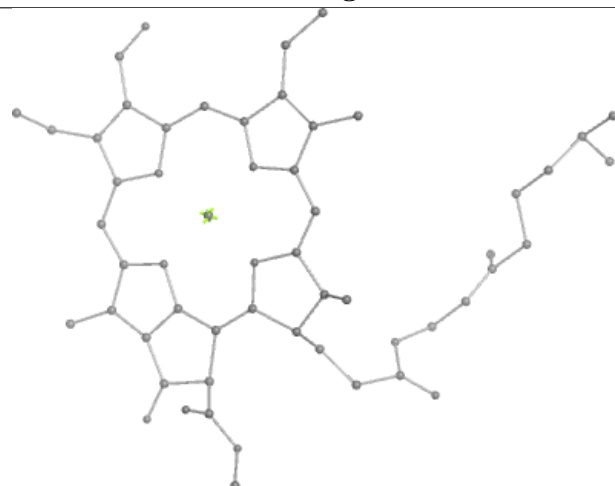
Bond lengths



Bond angles

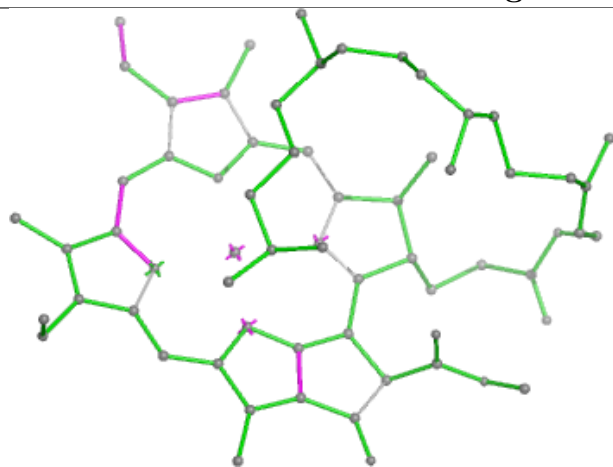


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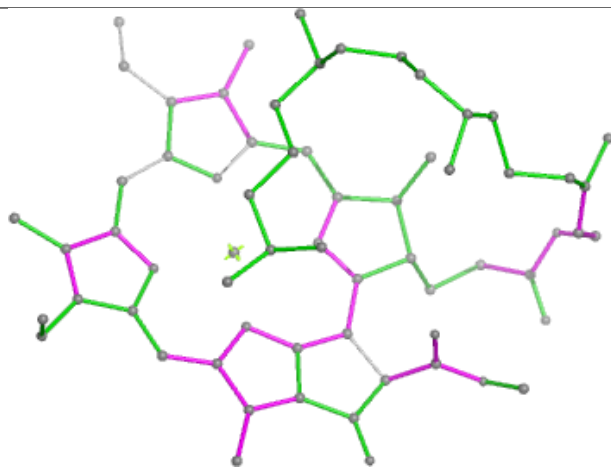


Rings

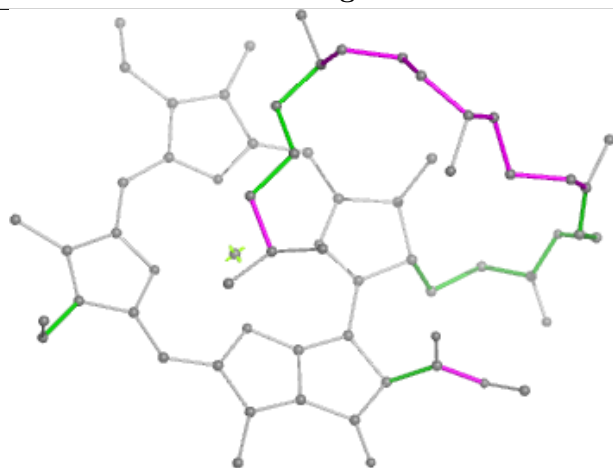
Ligand CLA B 1203



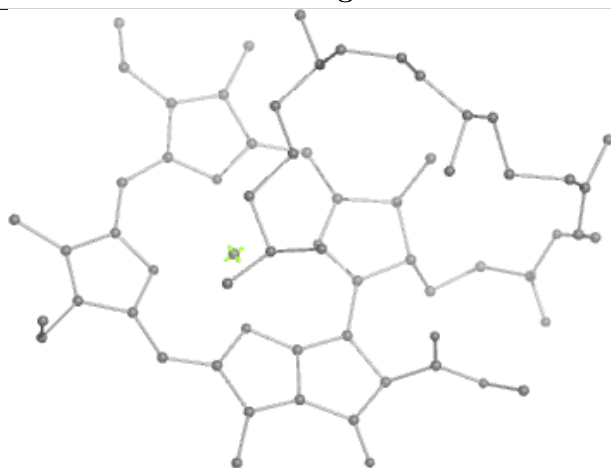
Bond lengths



Bond angles

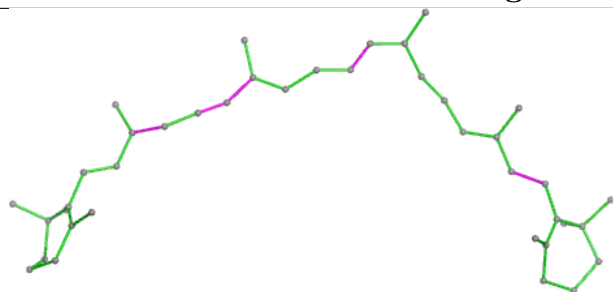


Torsions

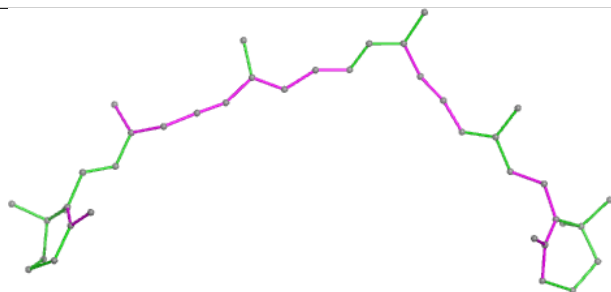


Rings

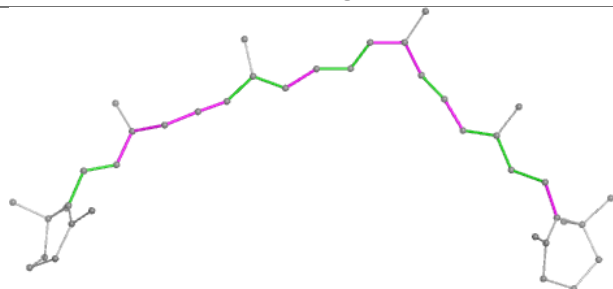
Ligand BCR F 4016



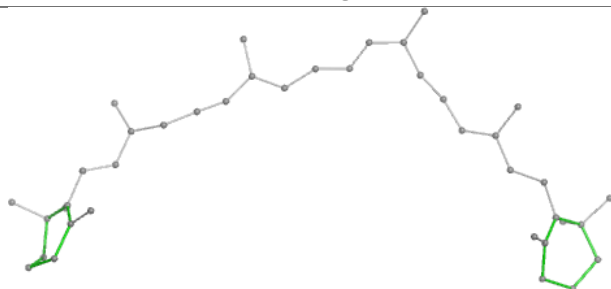
Bond lengths



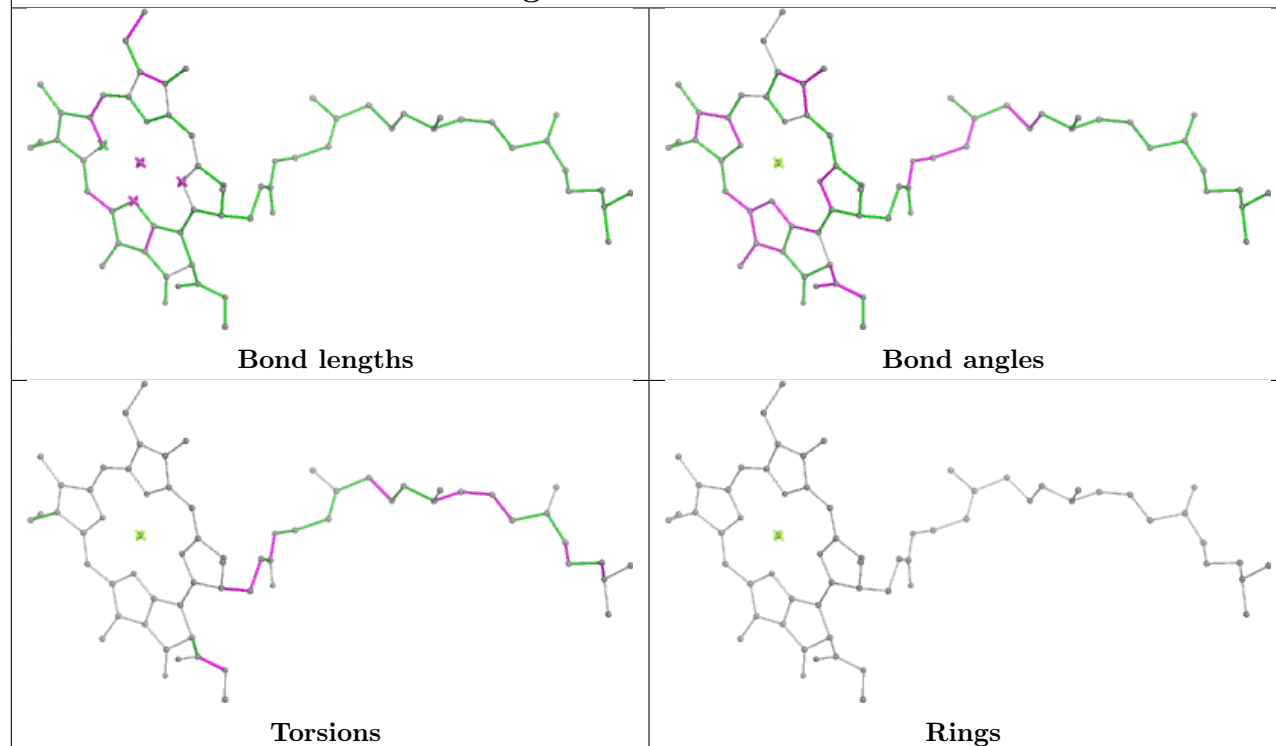
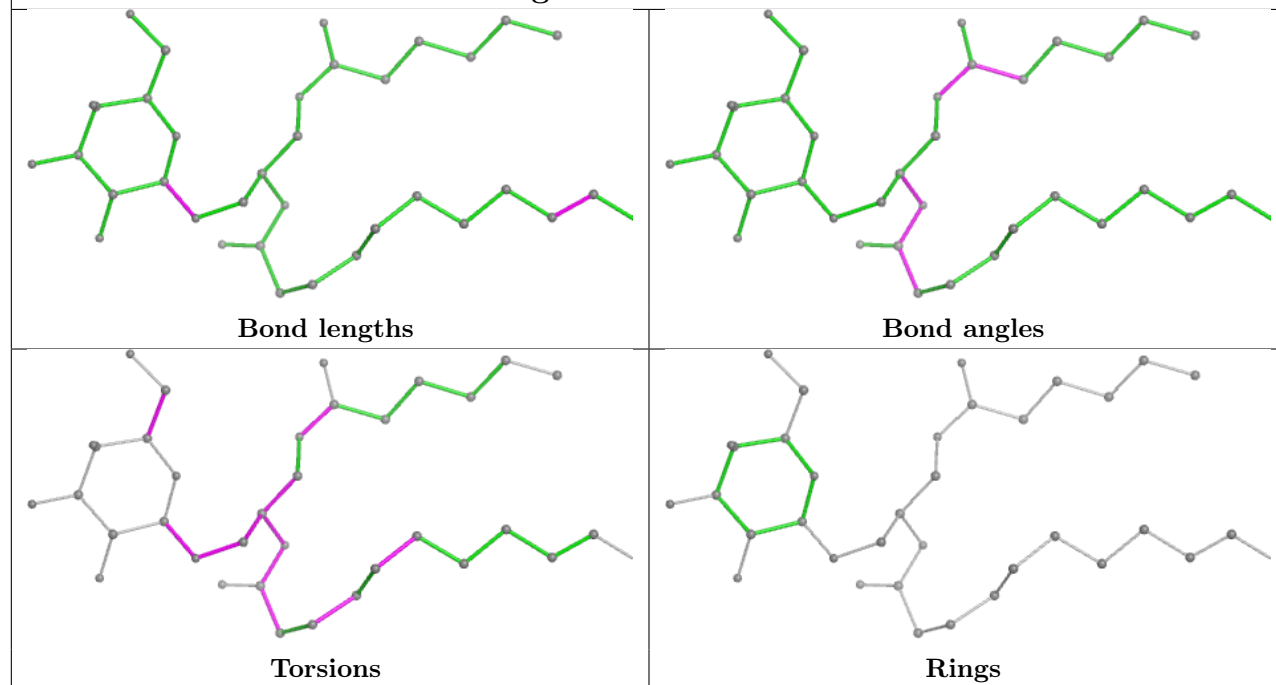
Bond angles

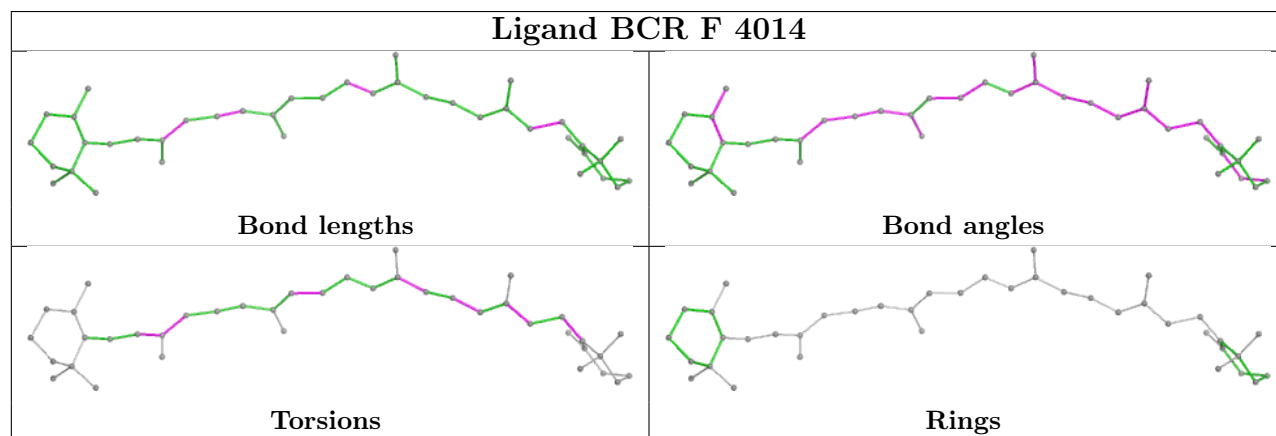
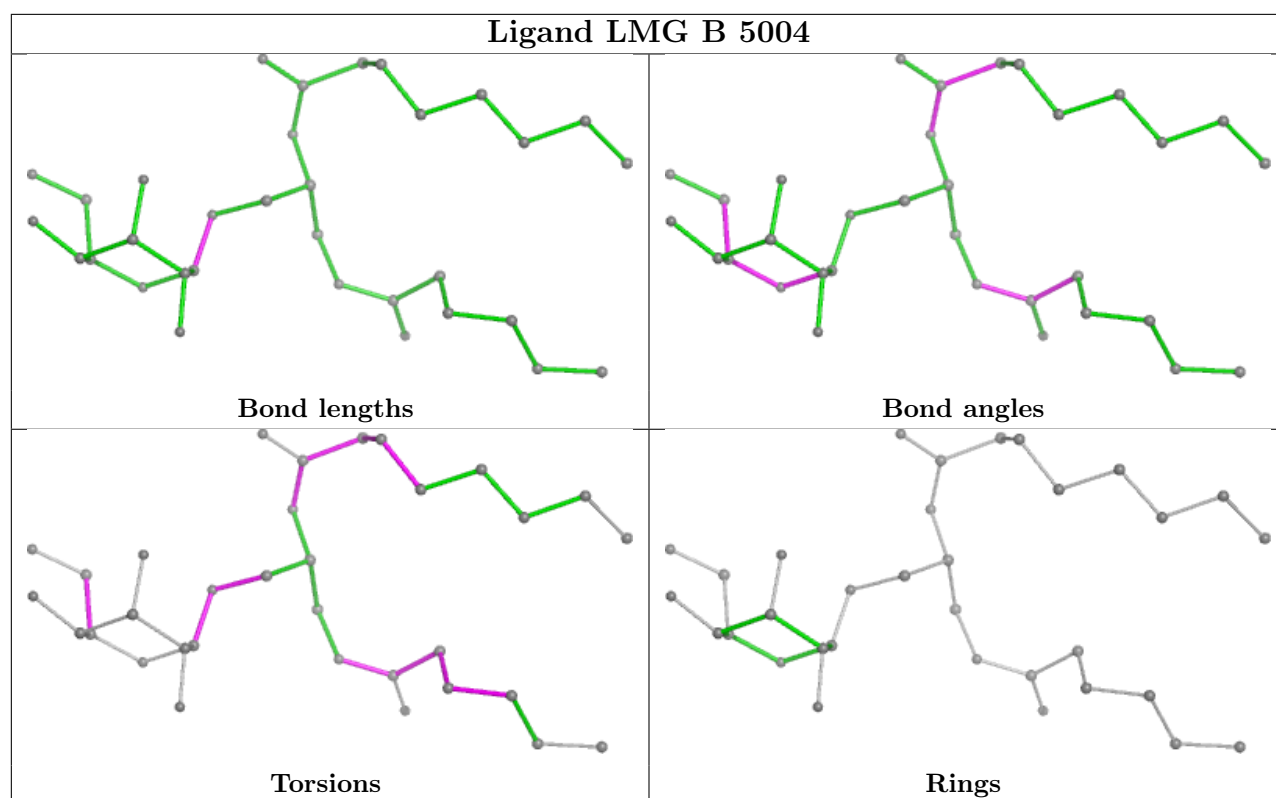


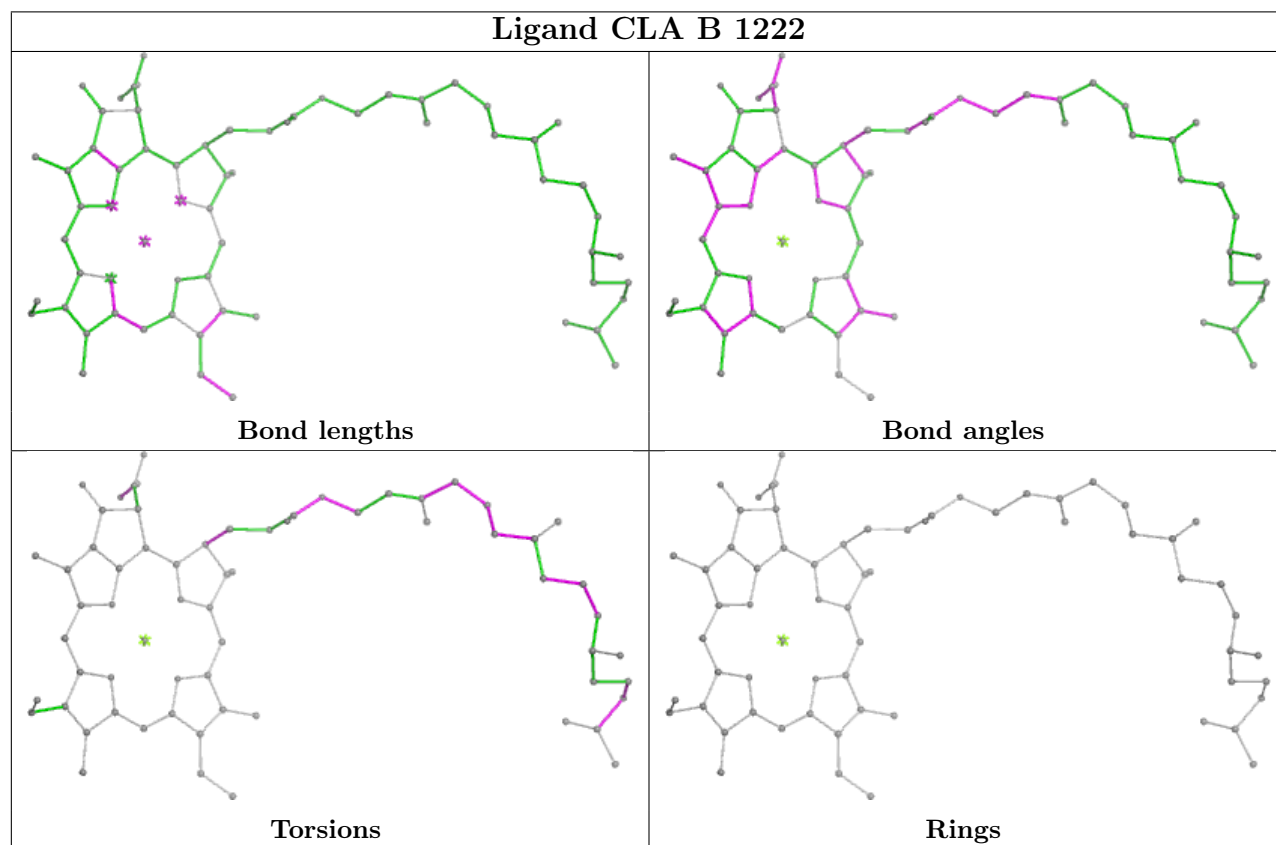
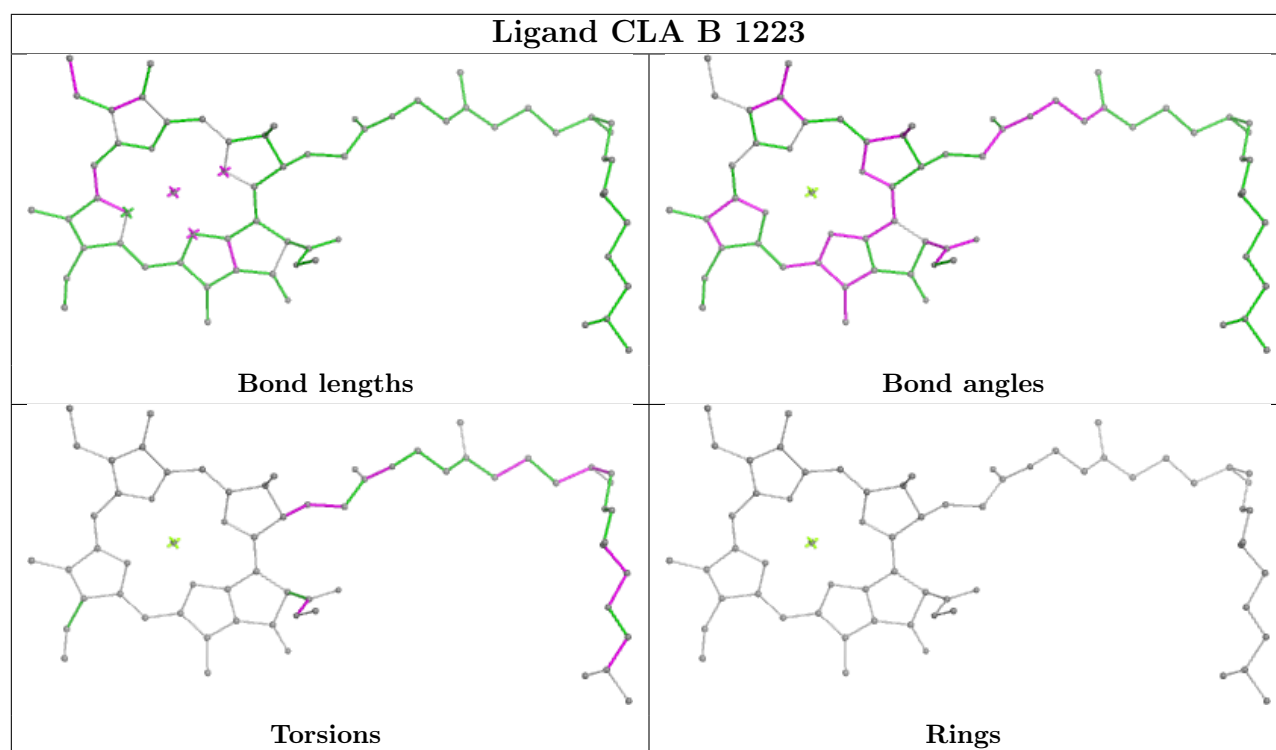
Torsions

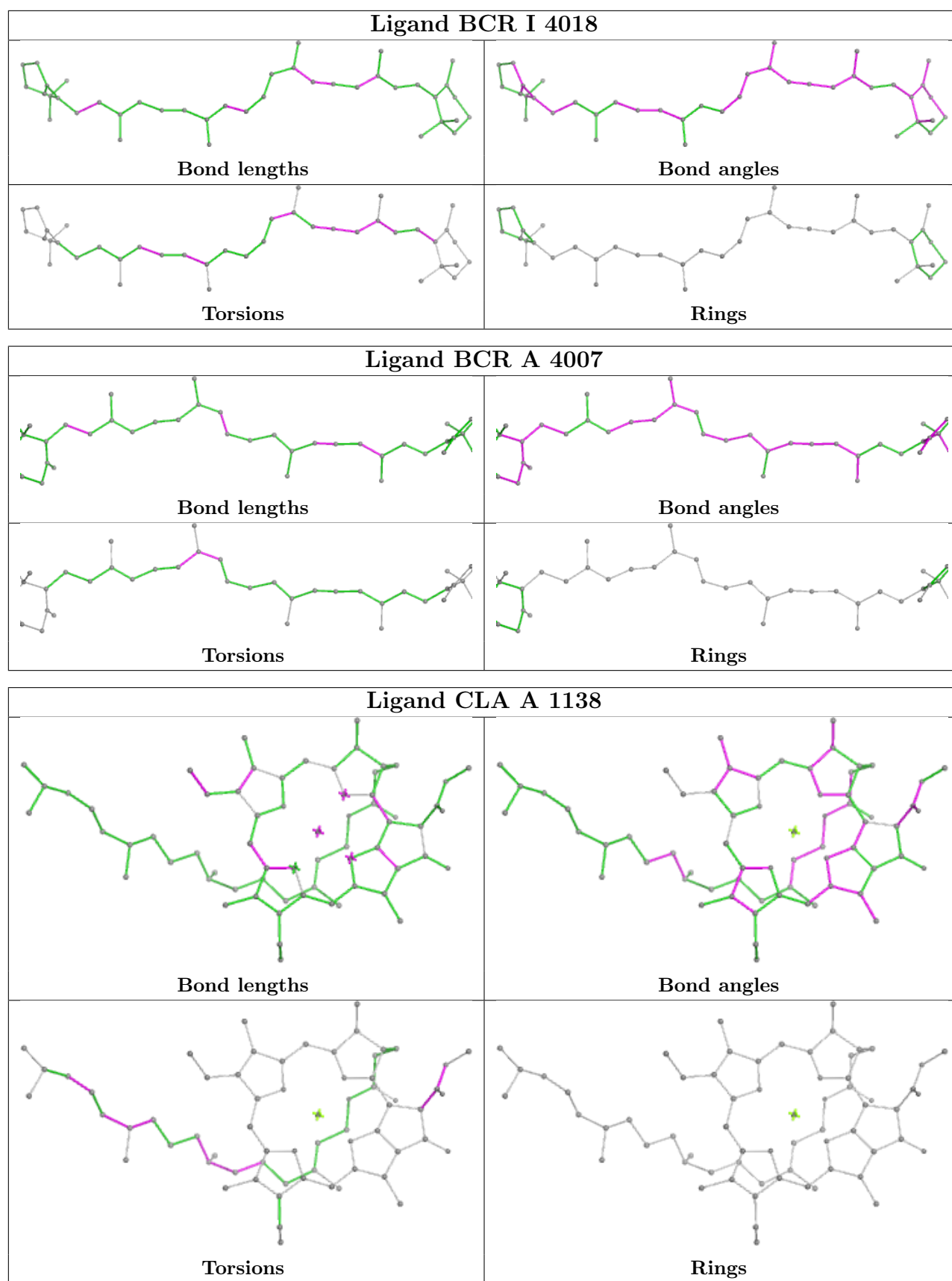


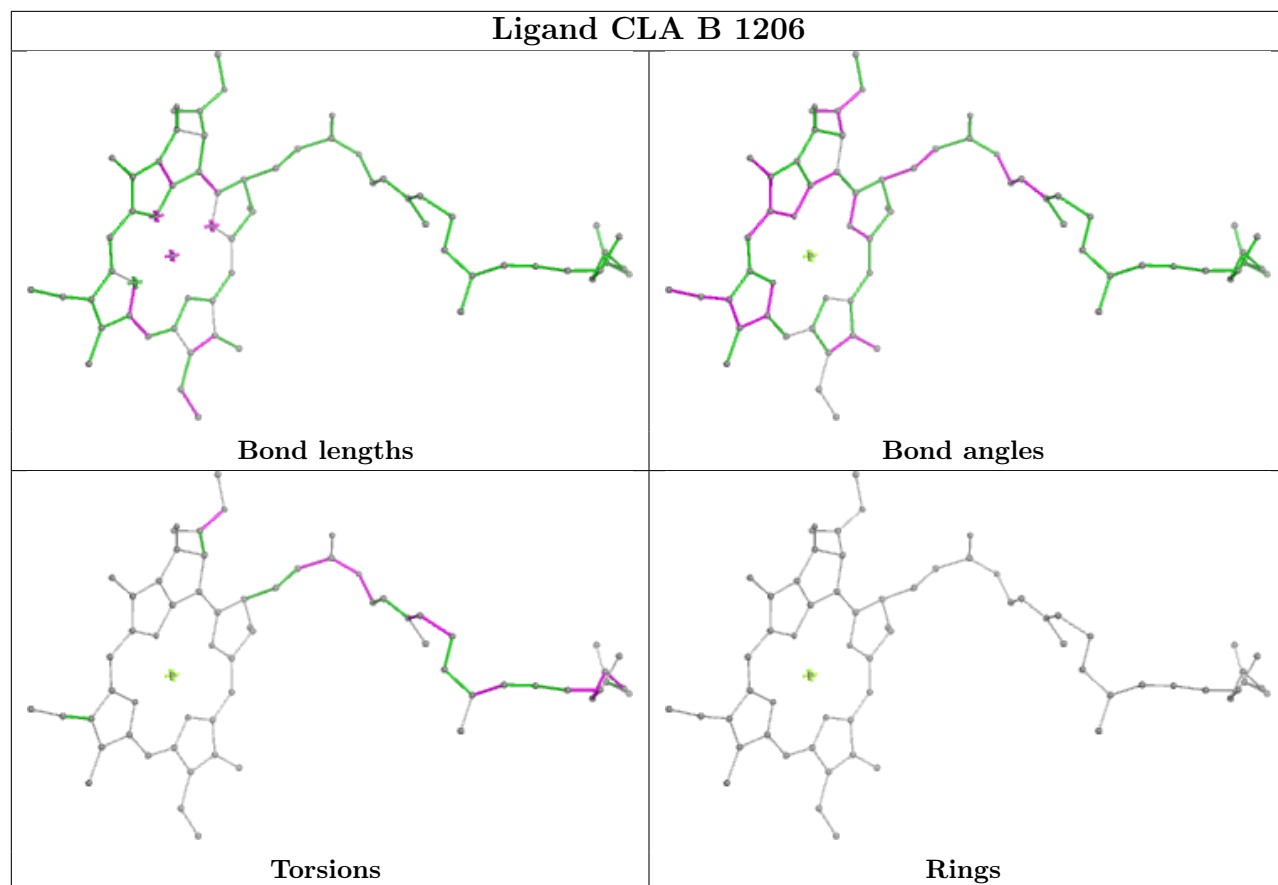
Rings

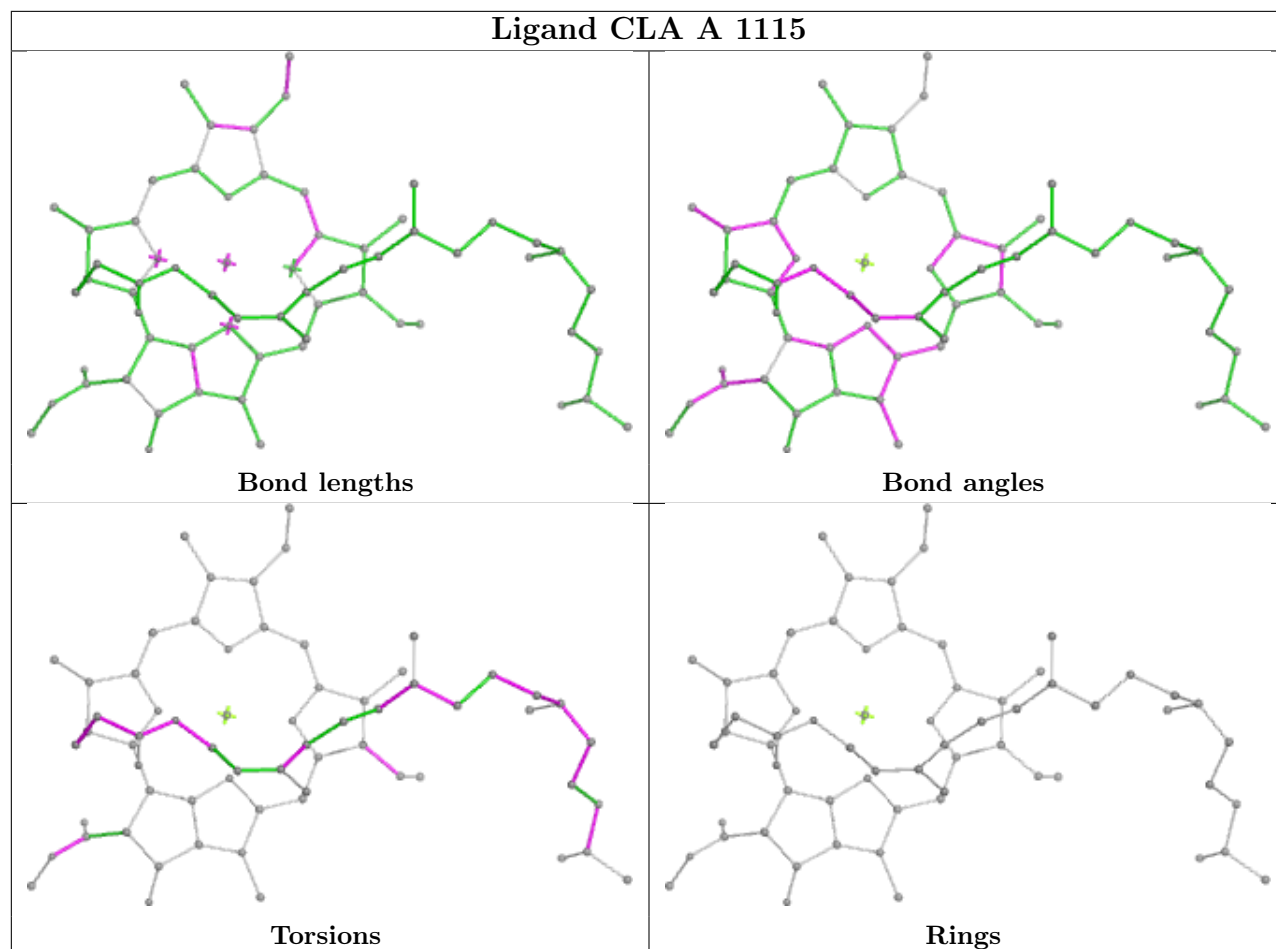
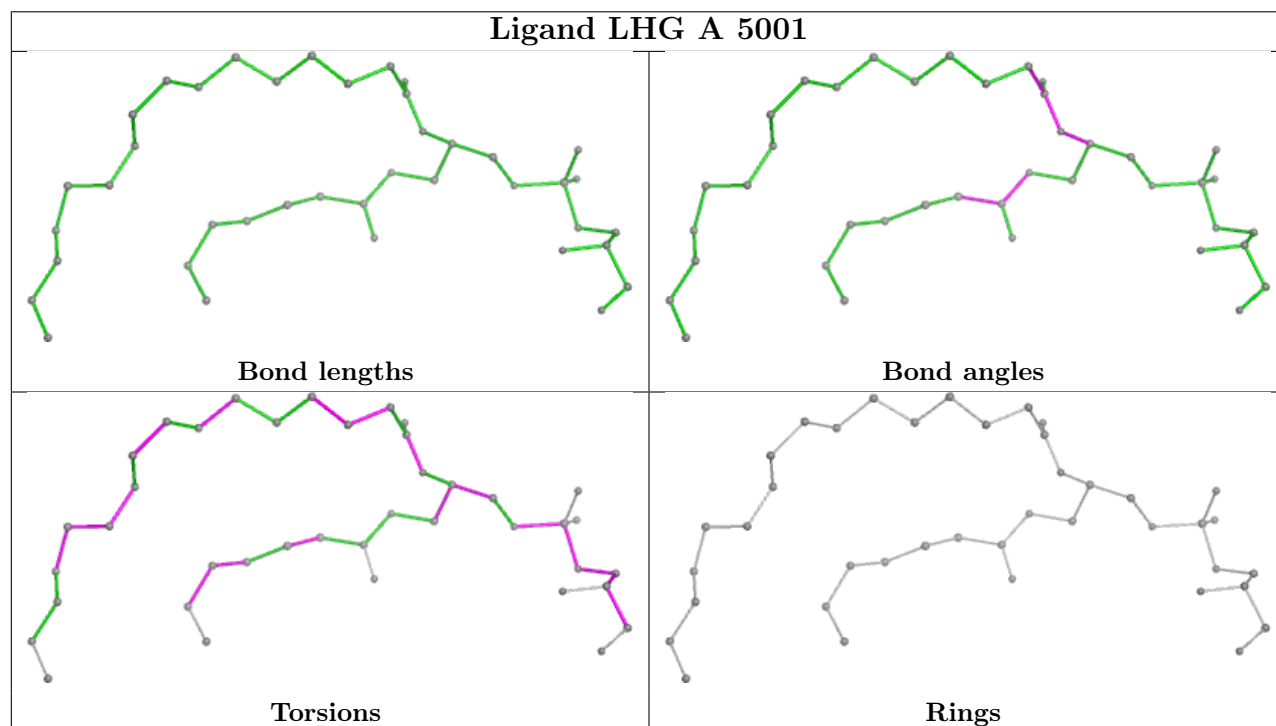
Ligand CLA A 1119**Ligand LMG 2 803**

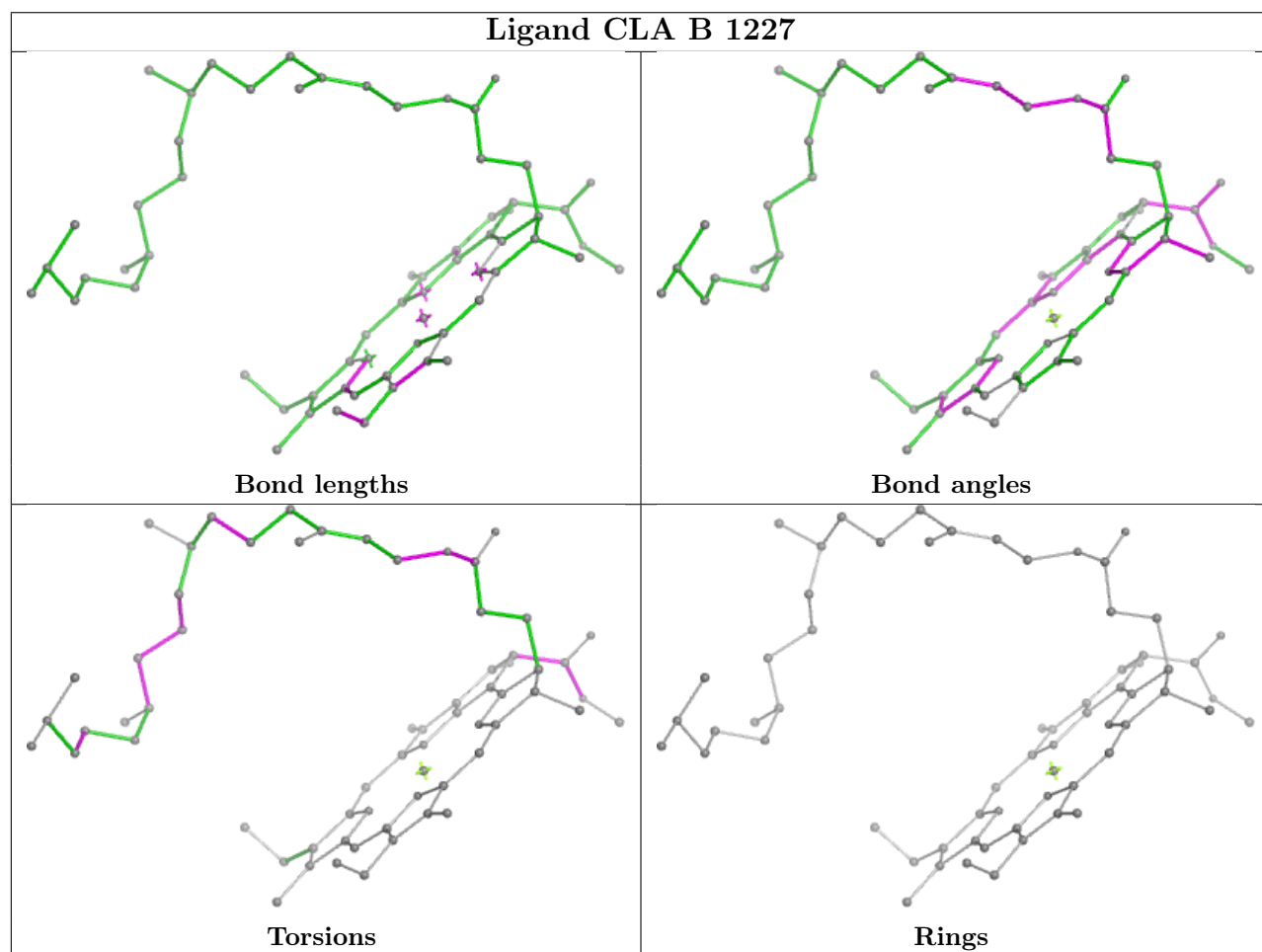
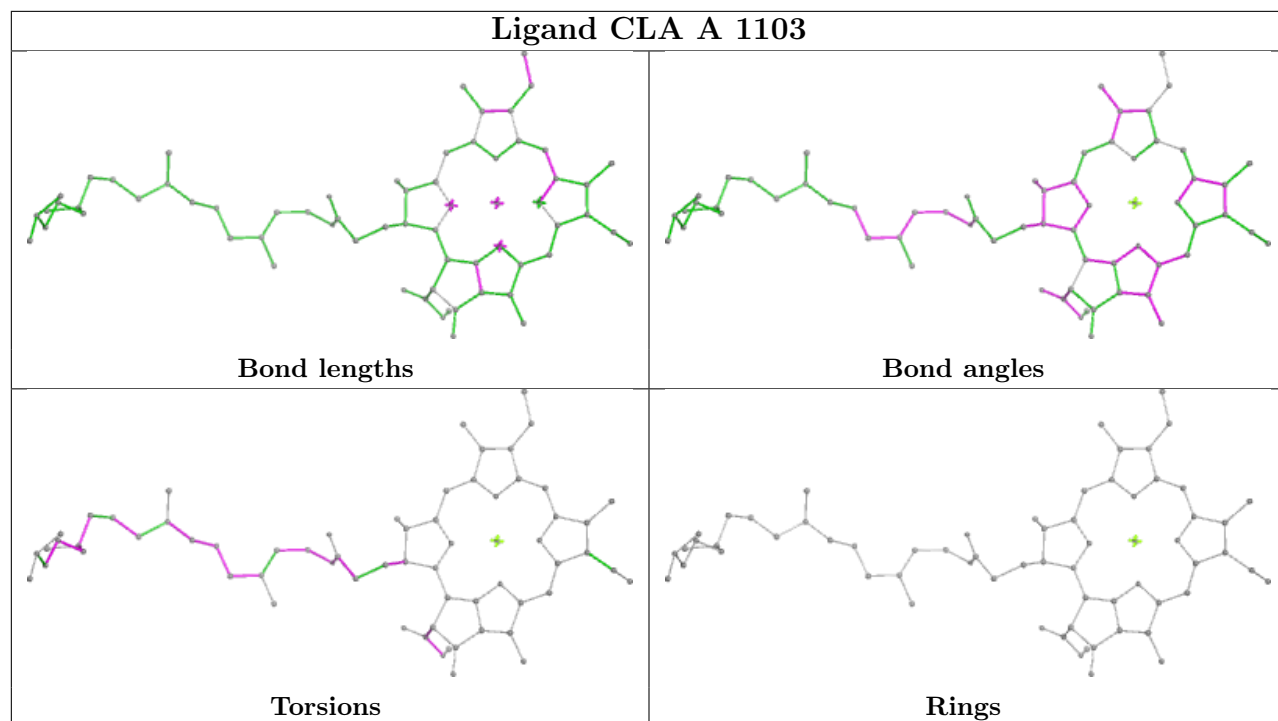


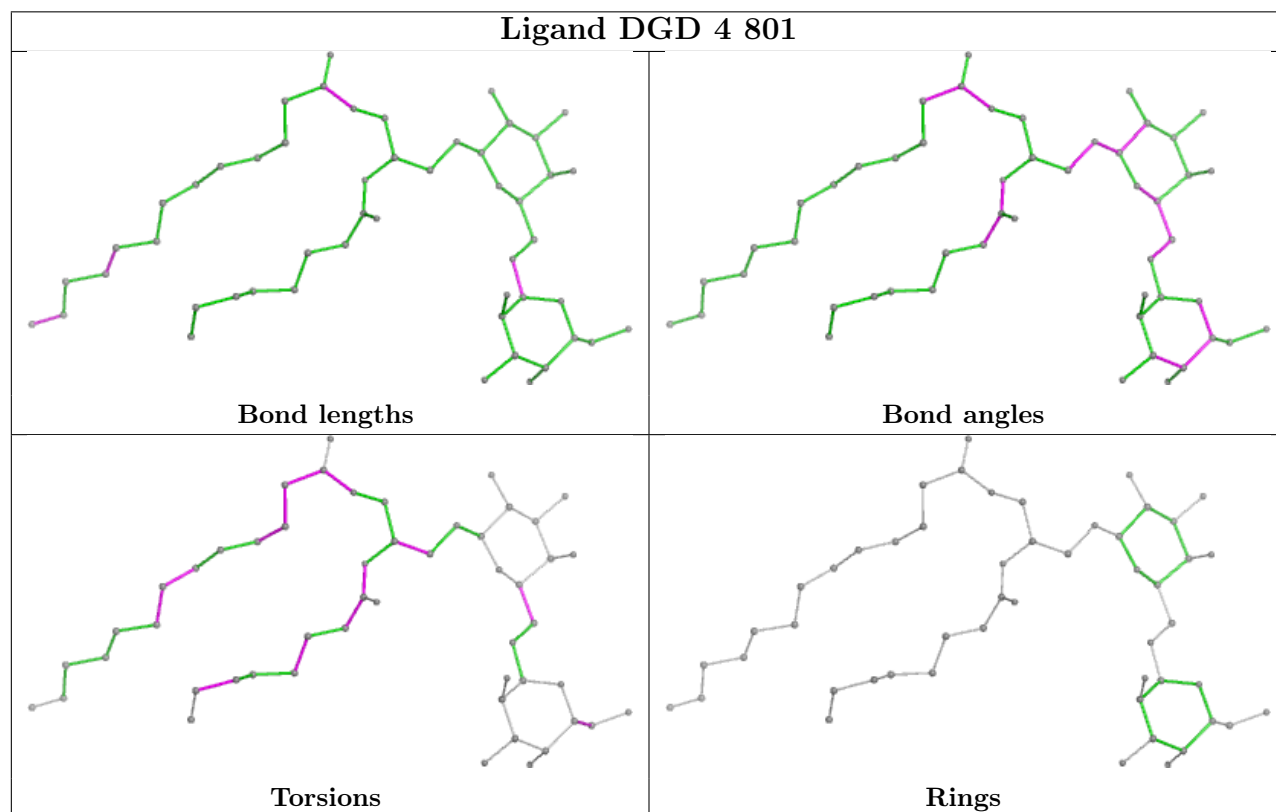
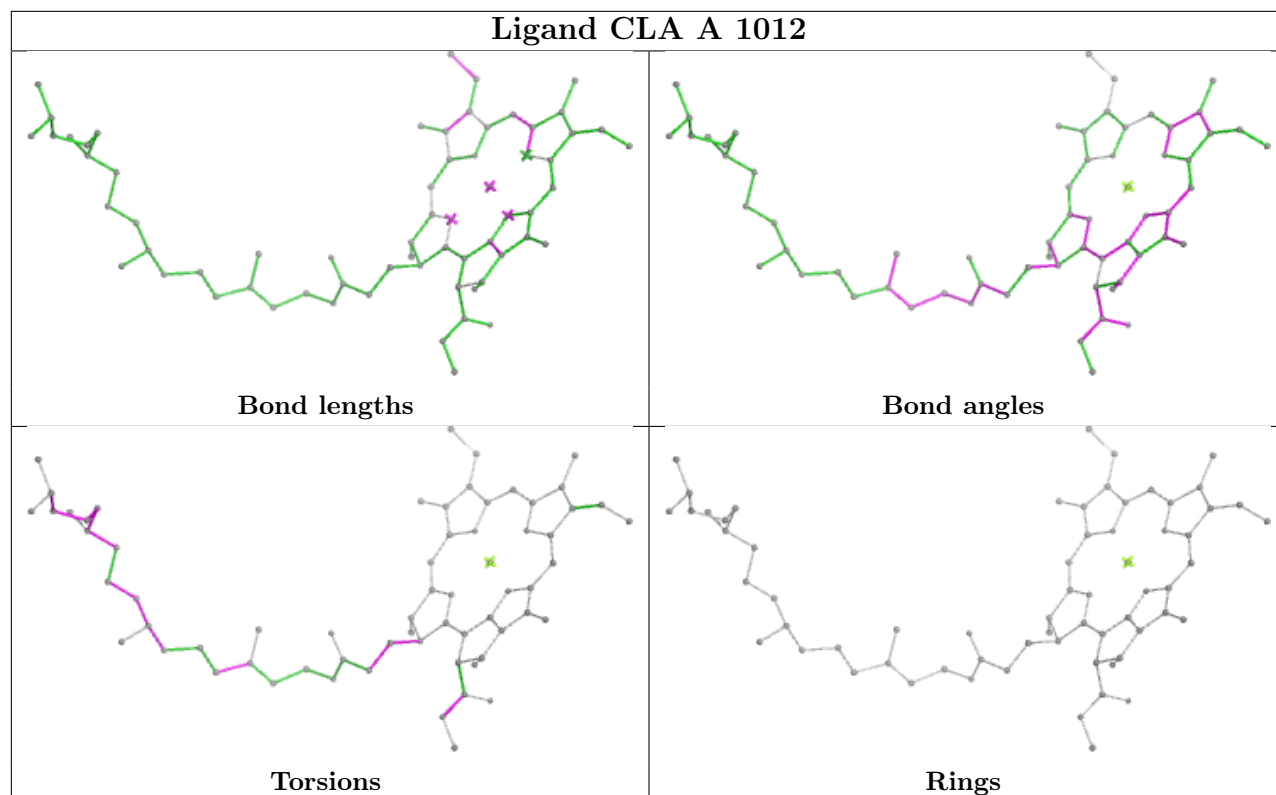




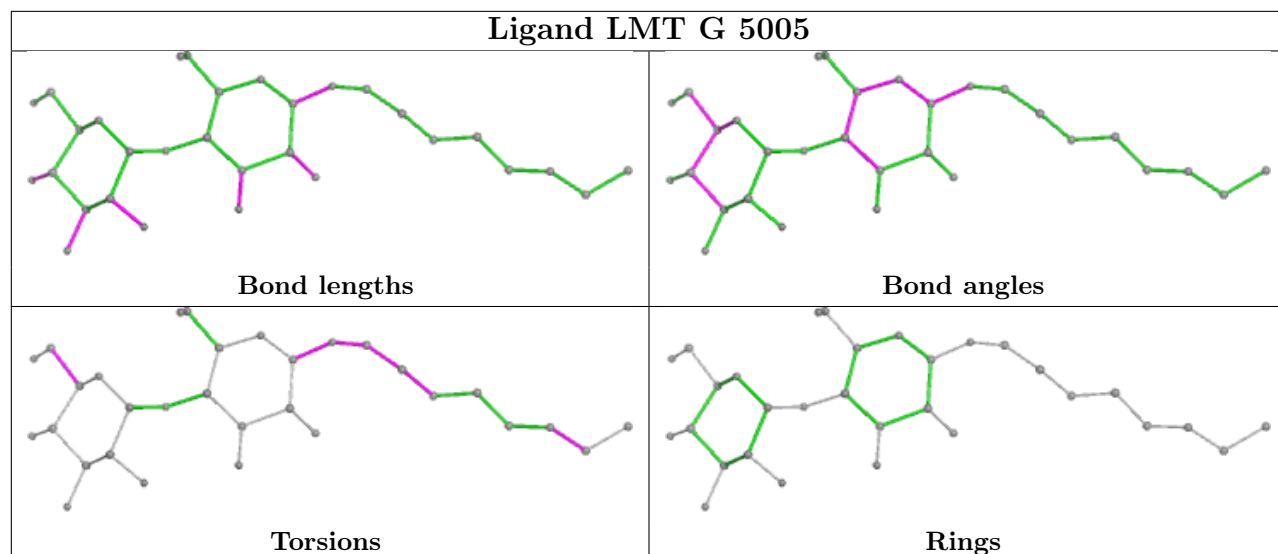


Ligand CLA A 1115**Ligand LHG A 5001**

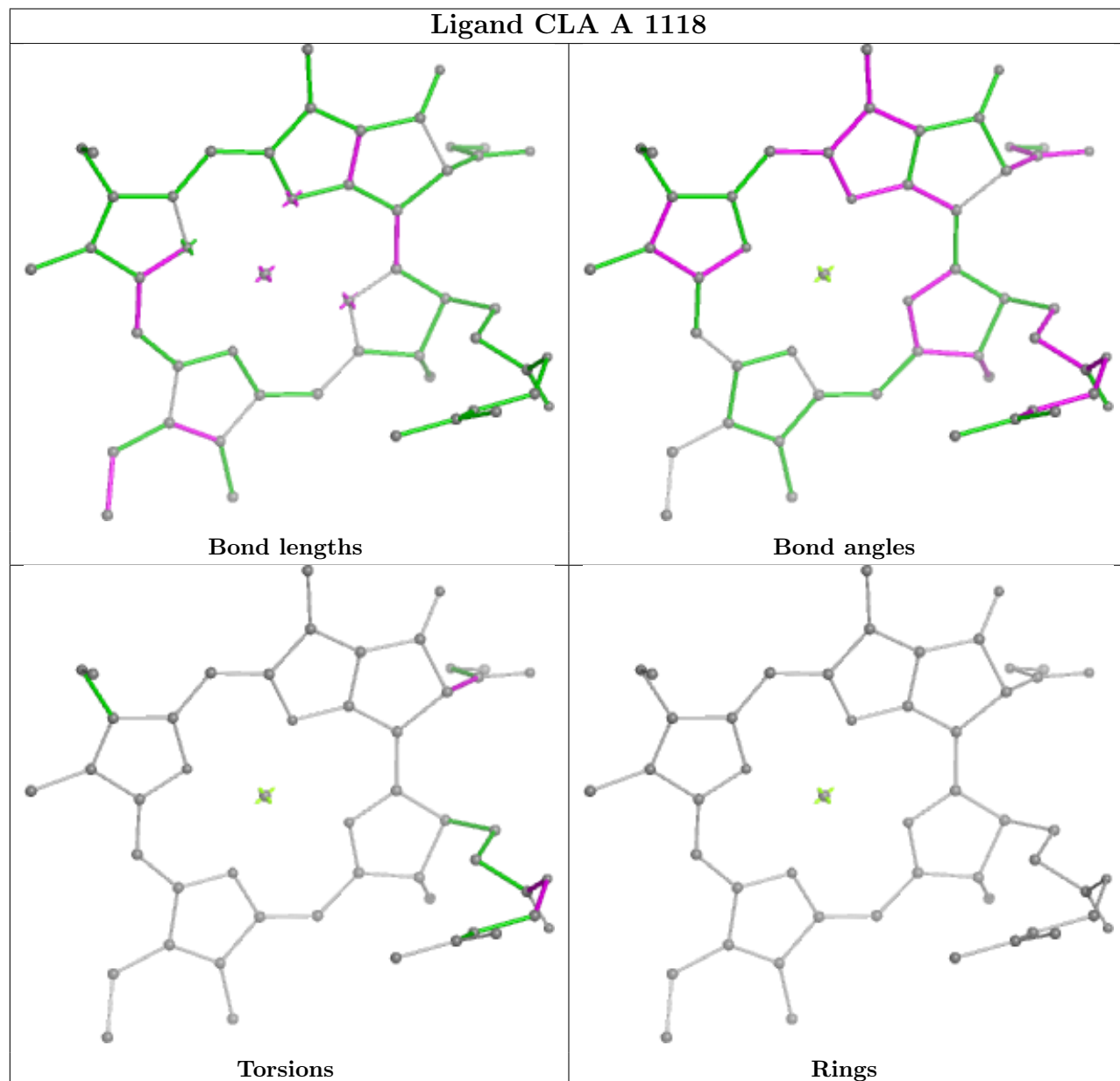


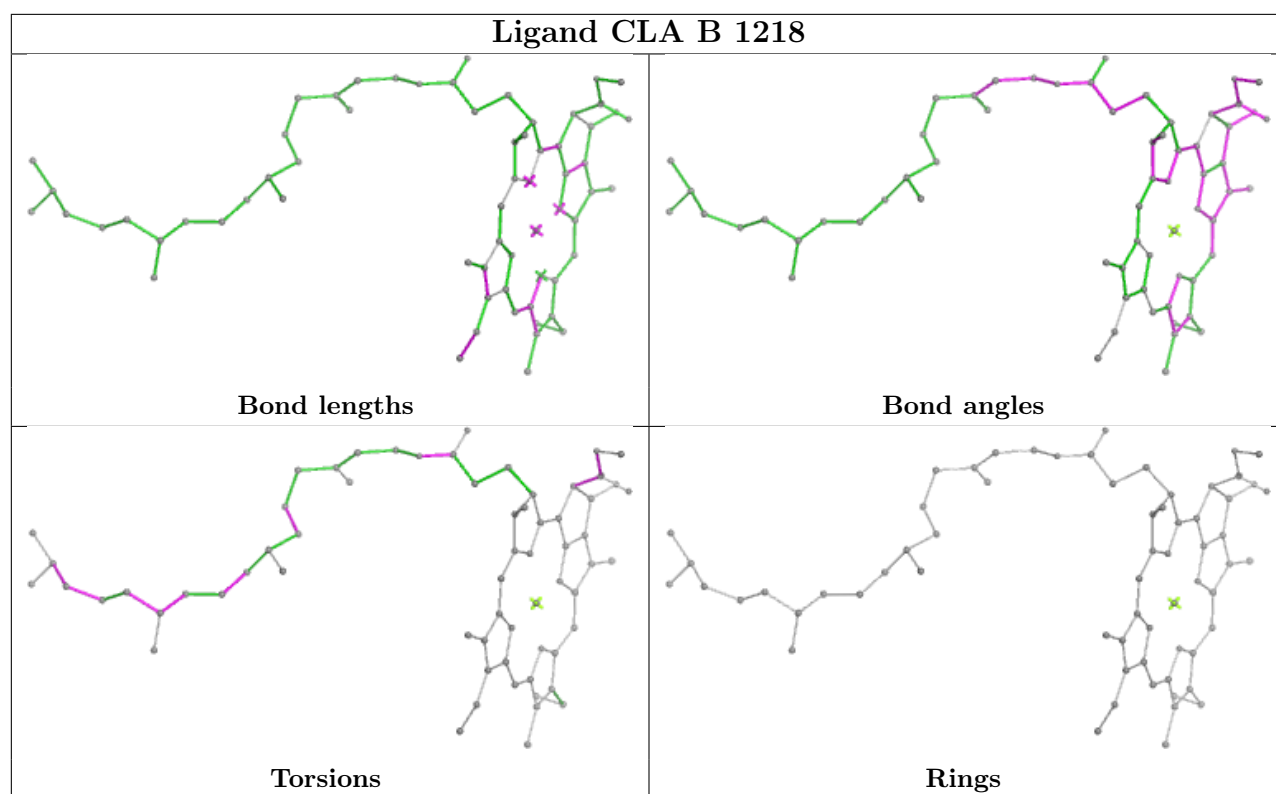


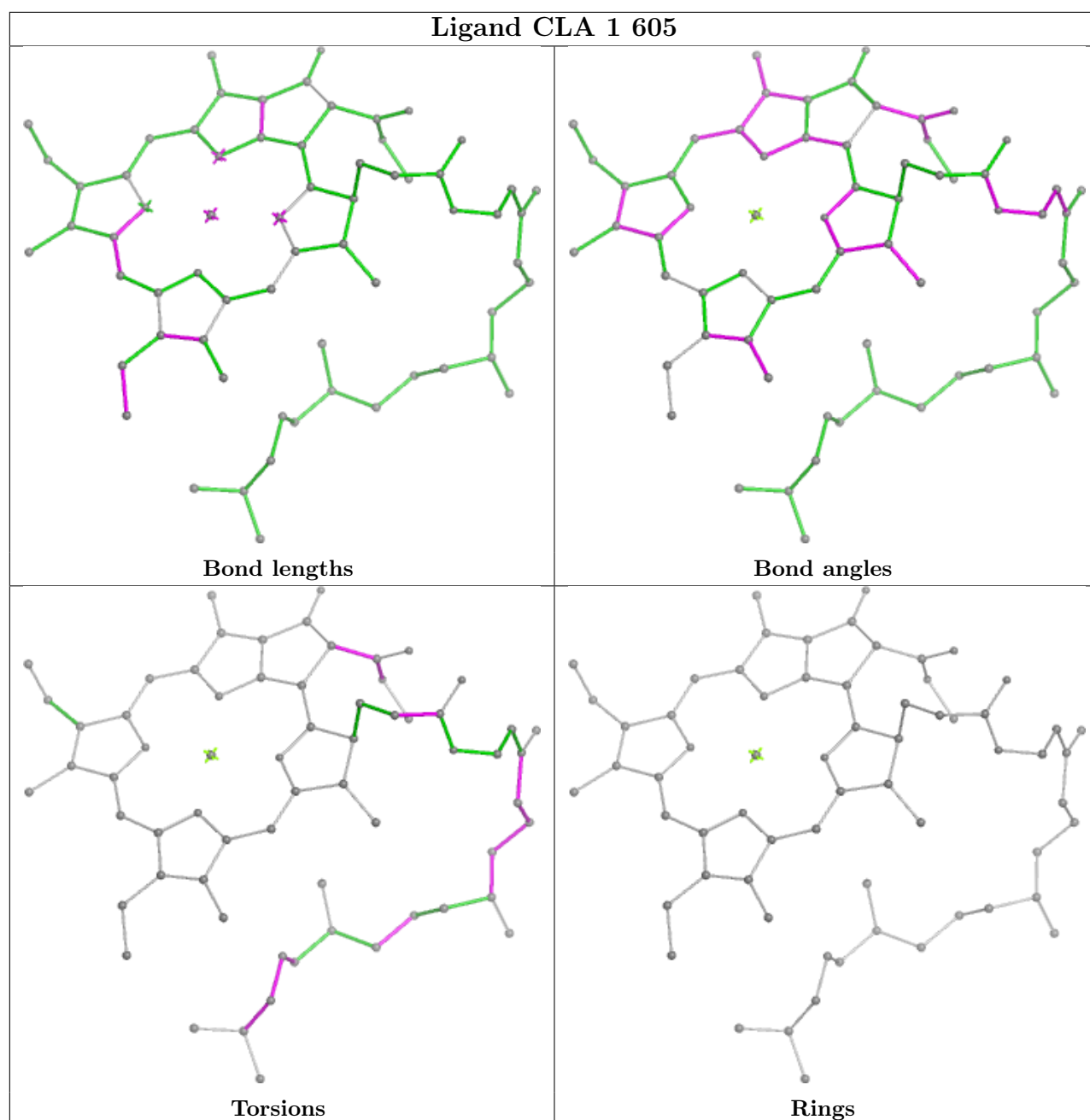
Ligand LMT G 5005

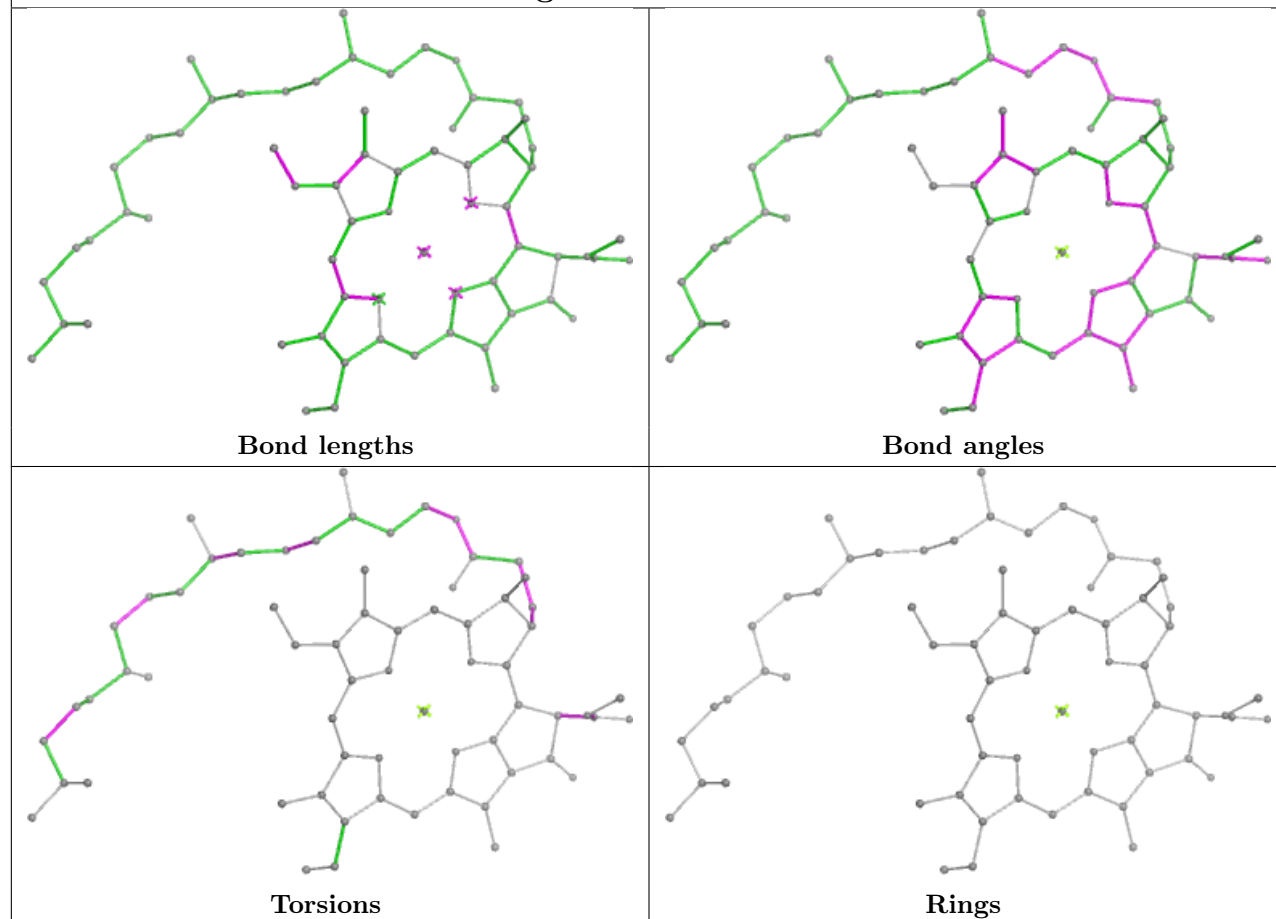
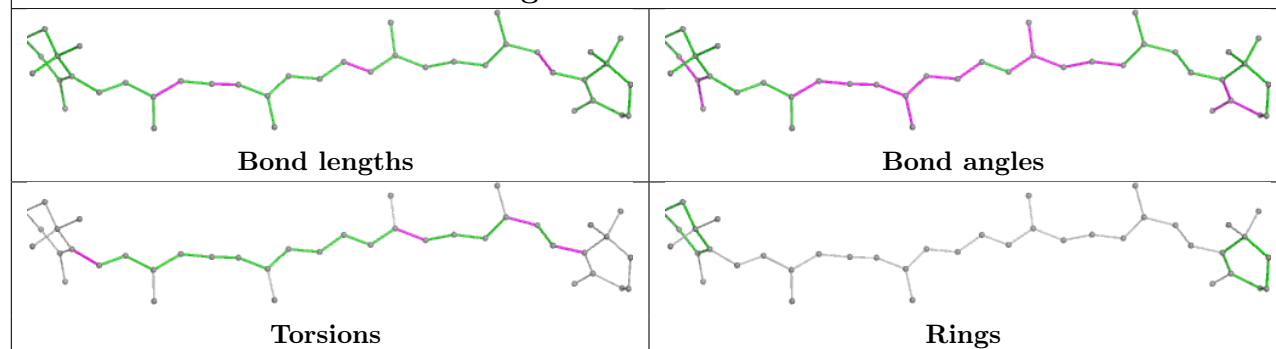


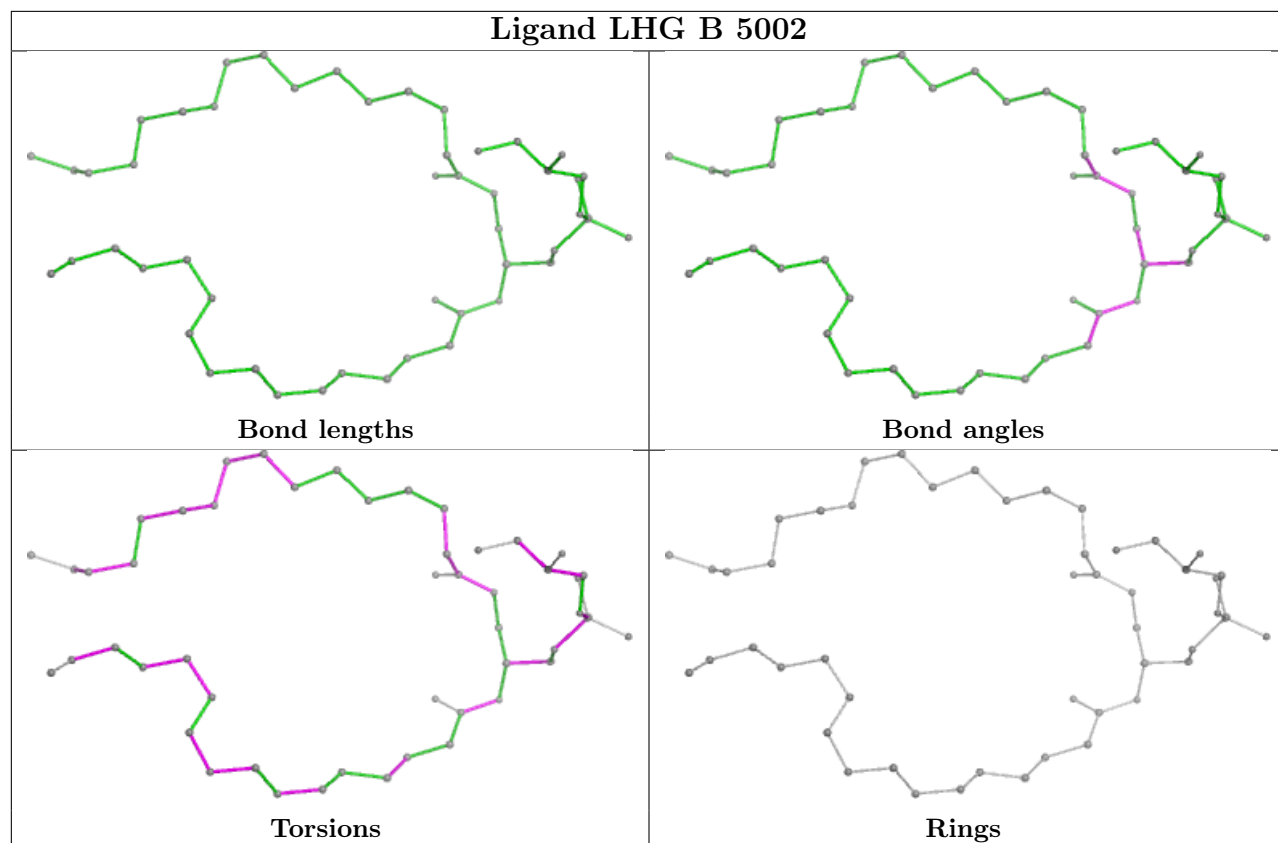
Ligand CLA A 1118

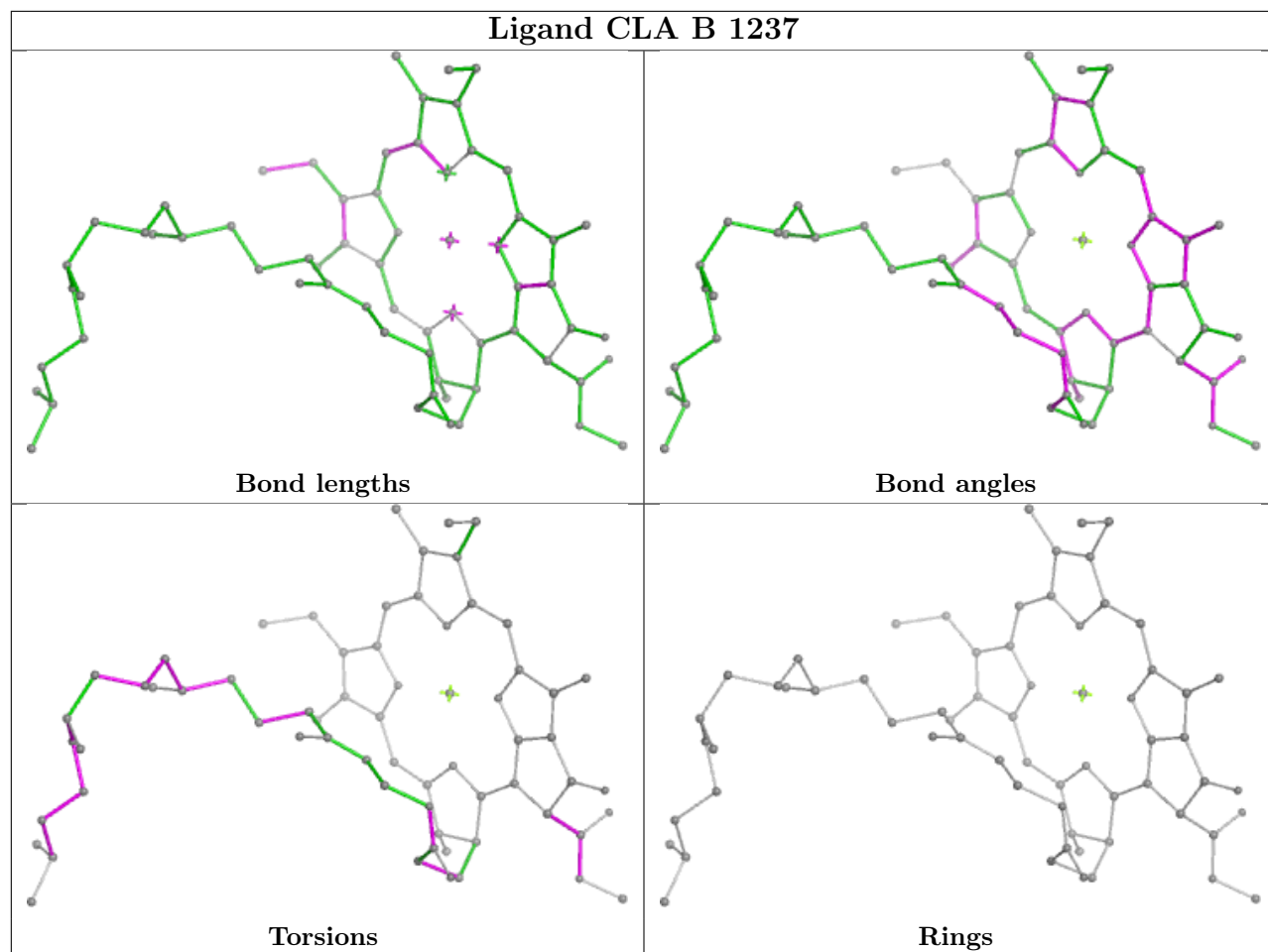


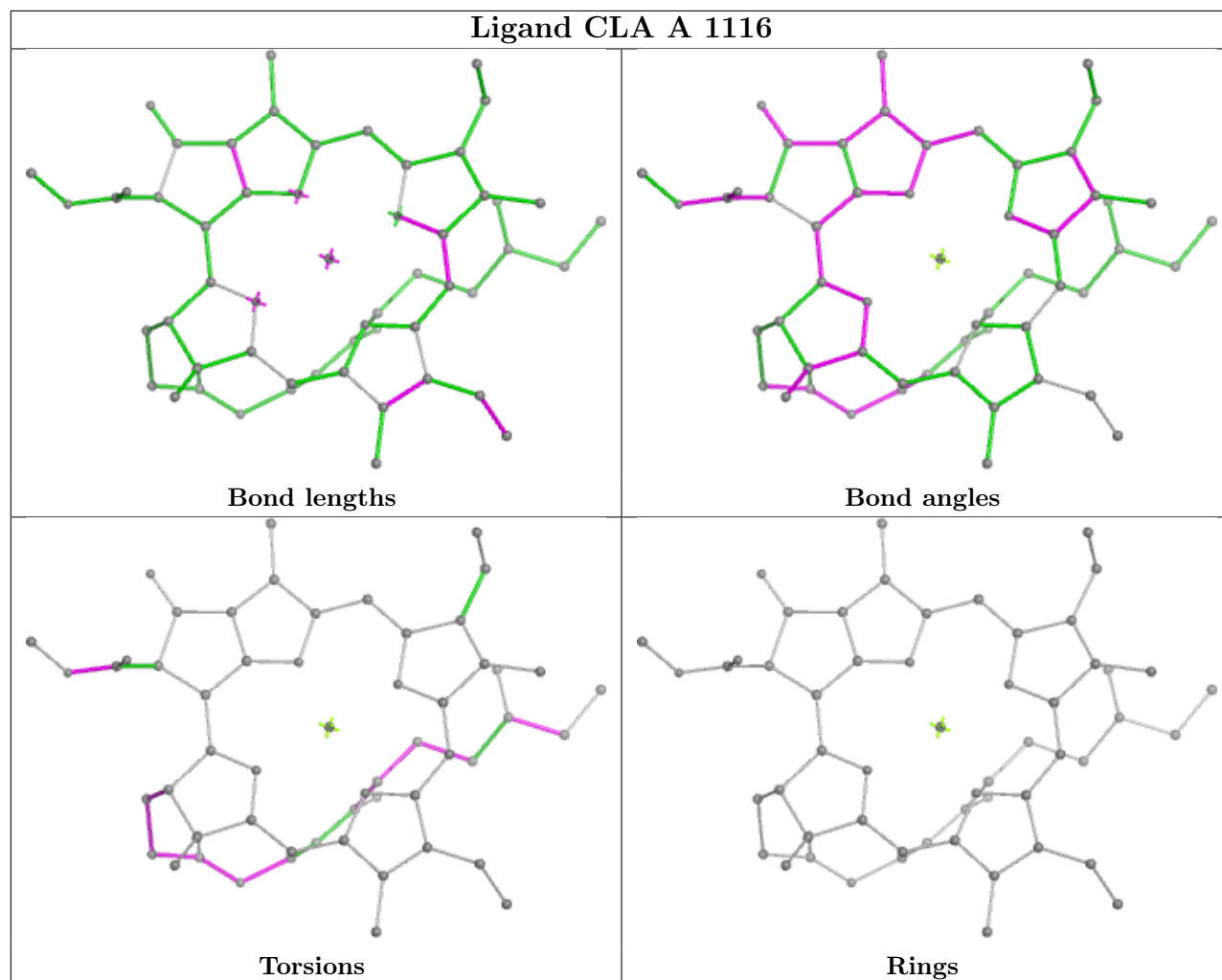


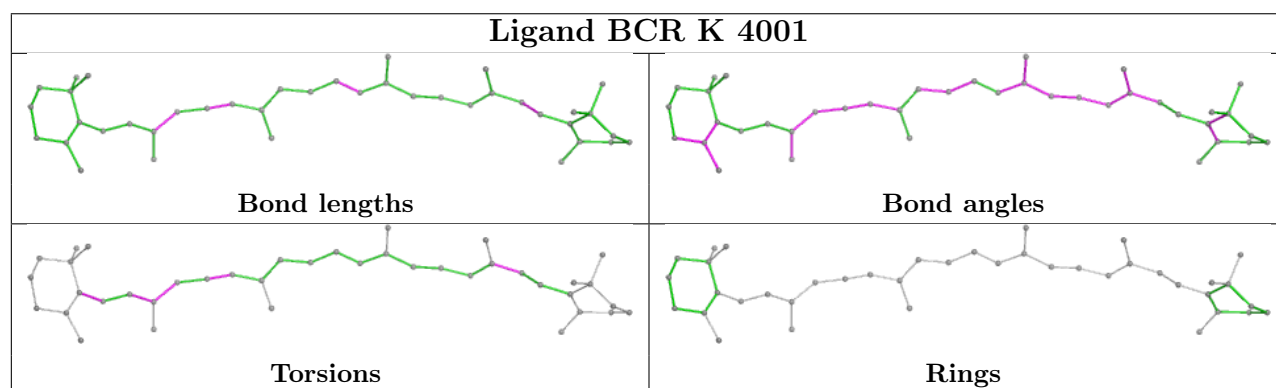
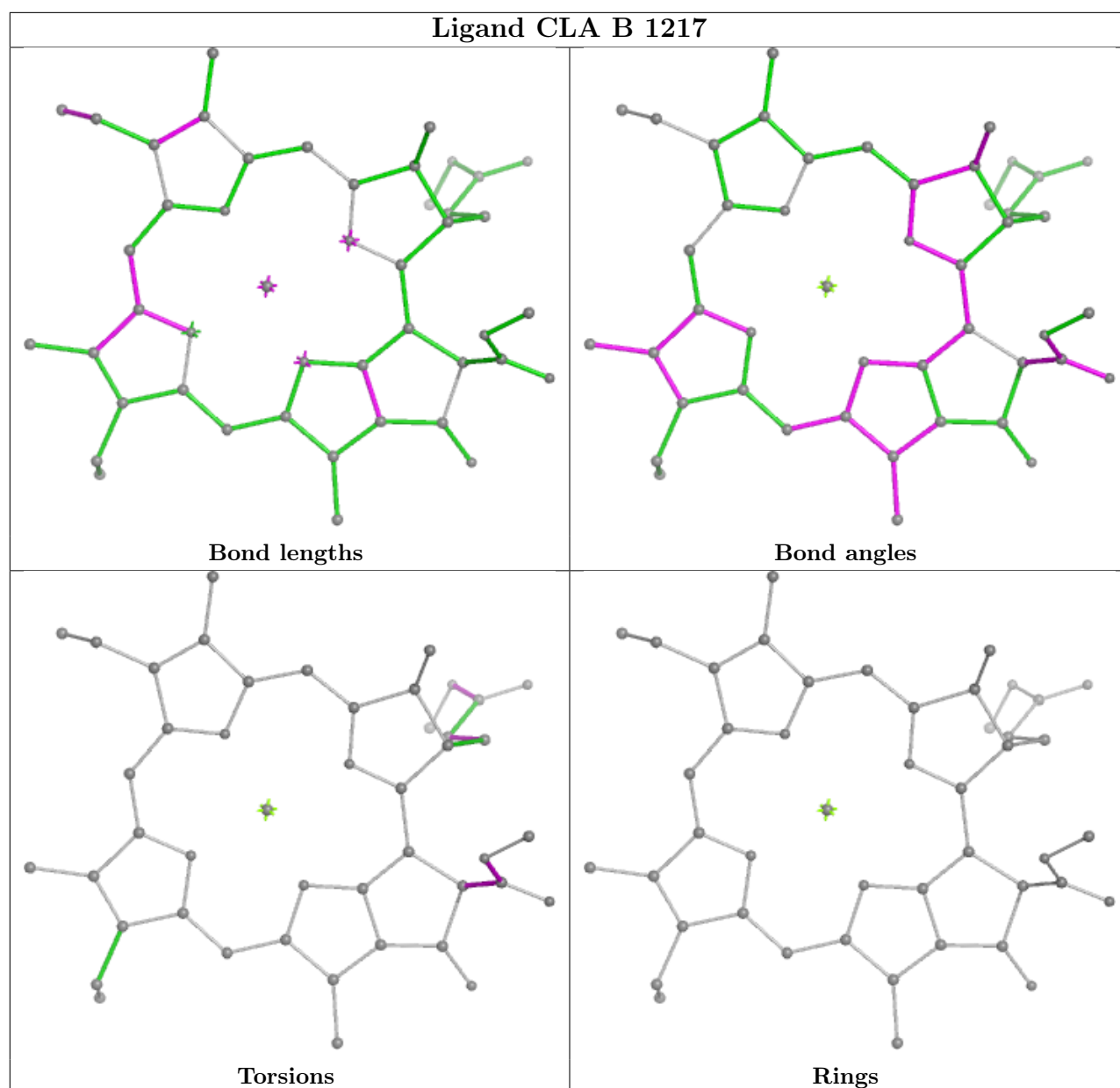


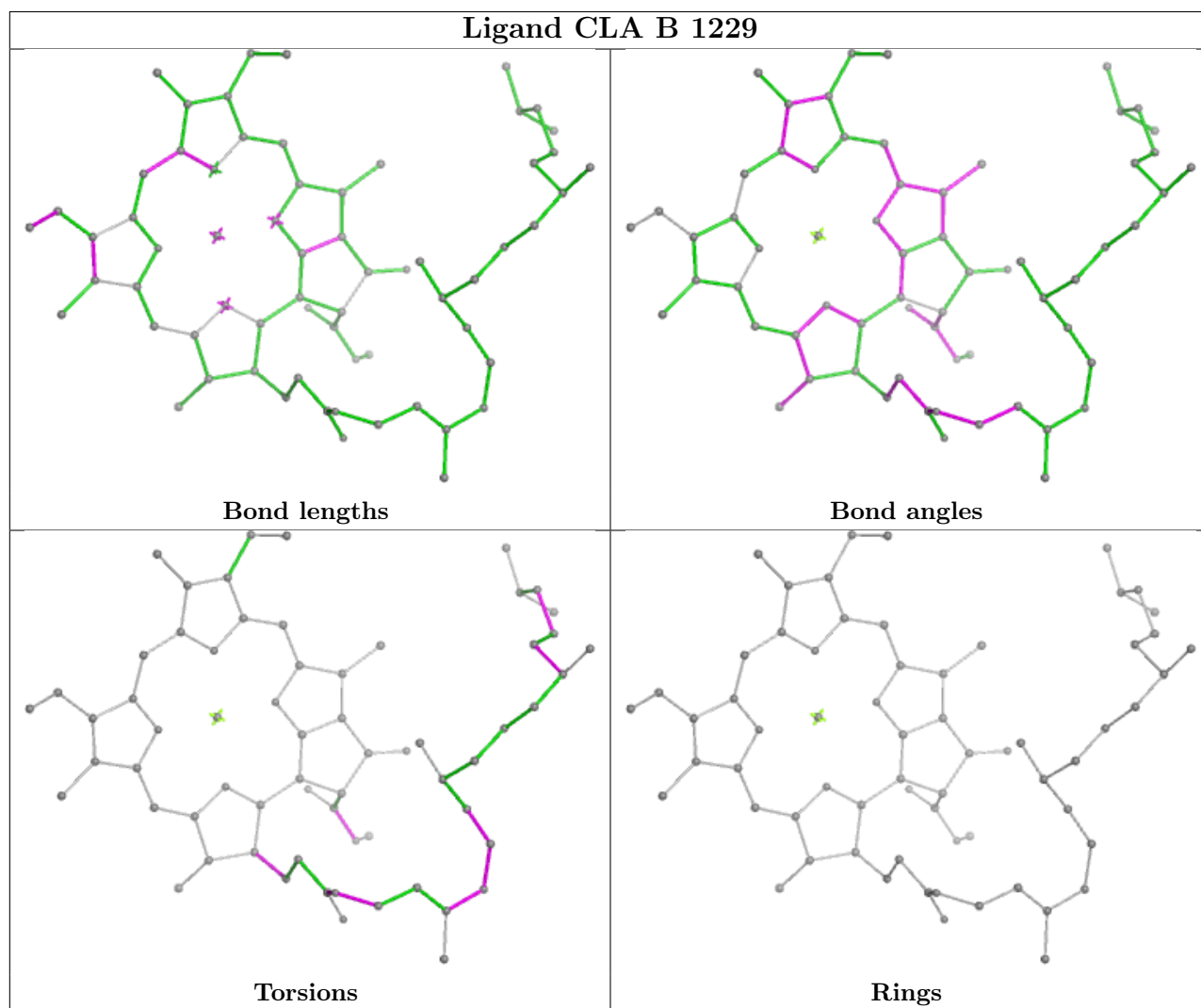
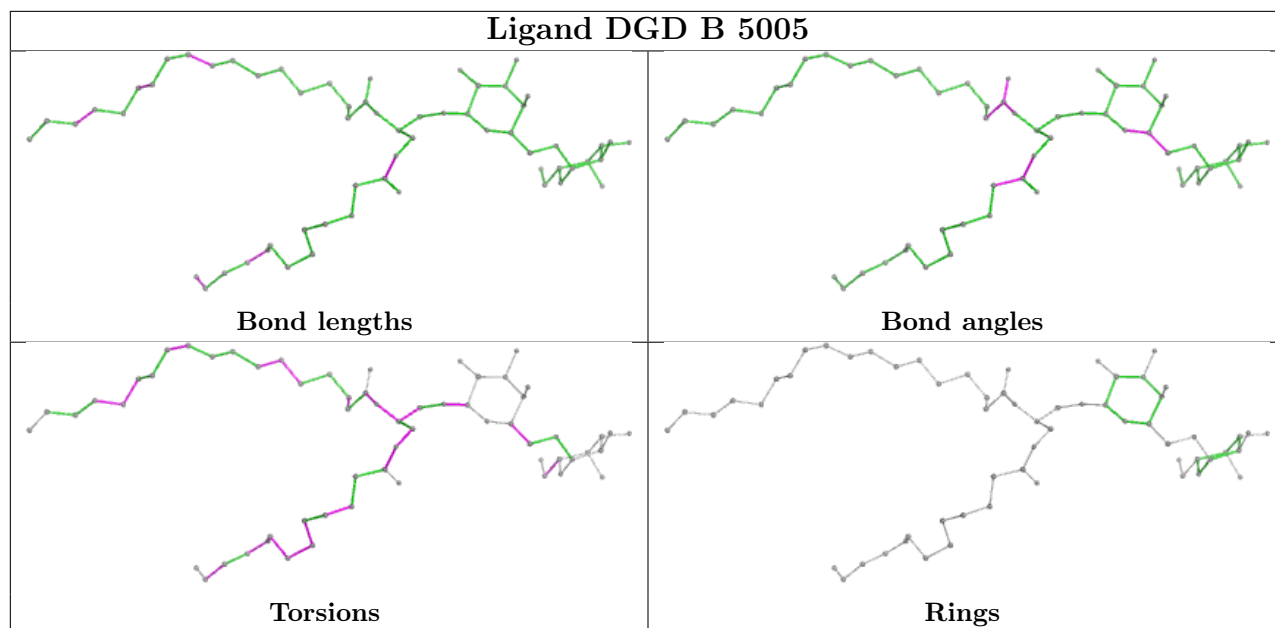
Ligand CLA 2 604**Ligand BCR A 4003**



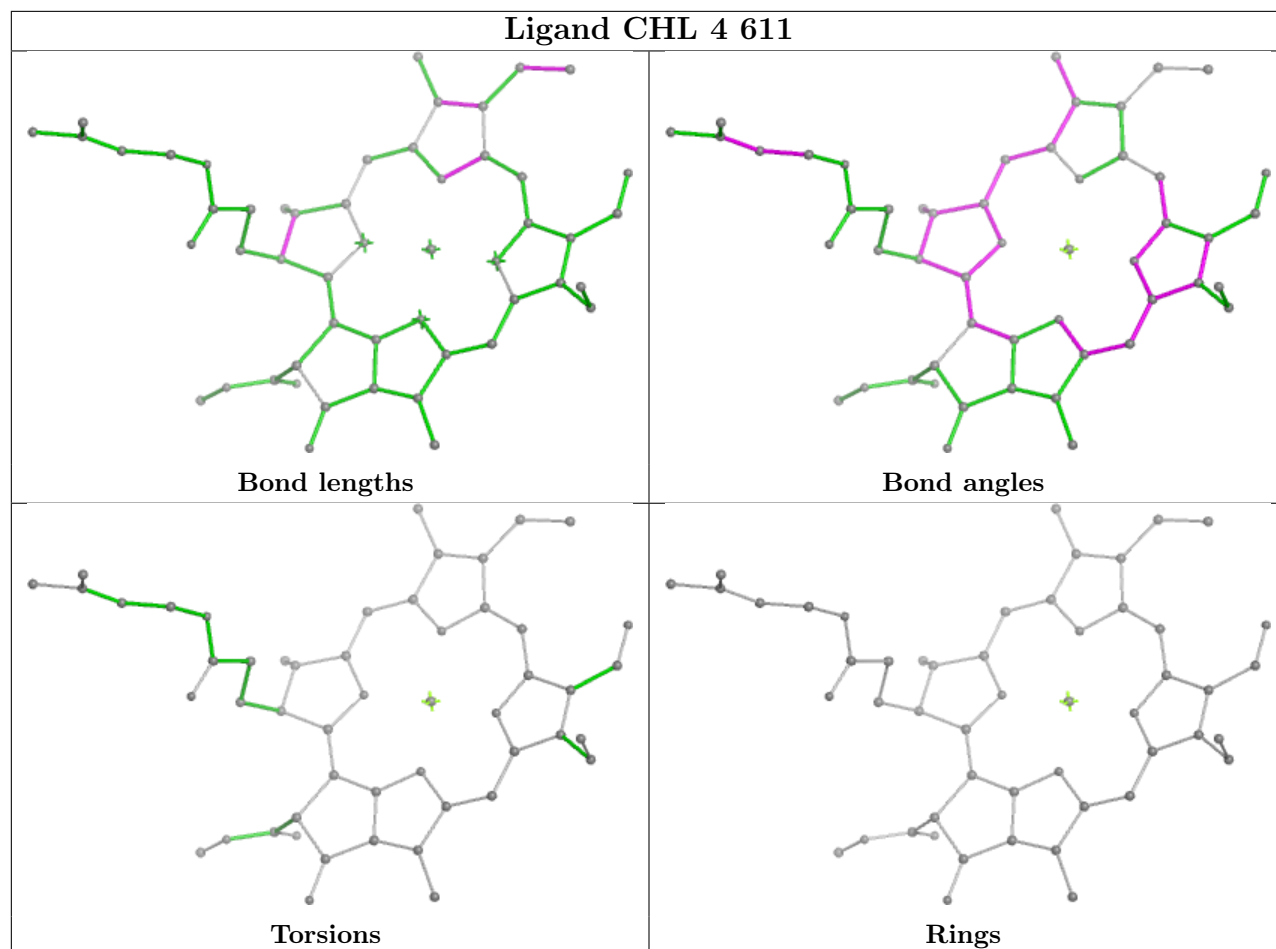


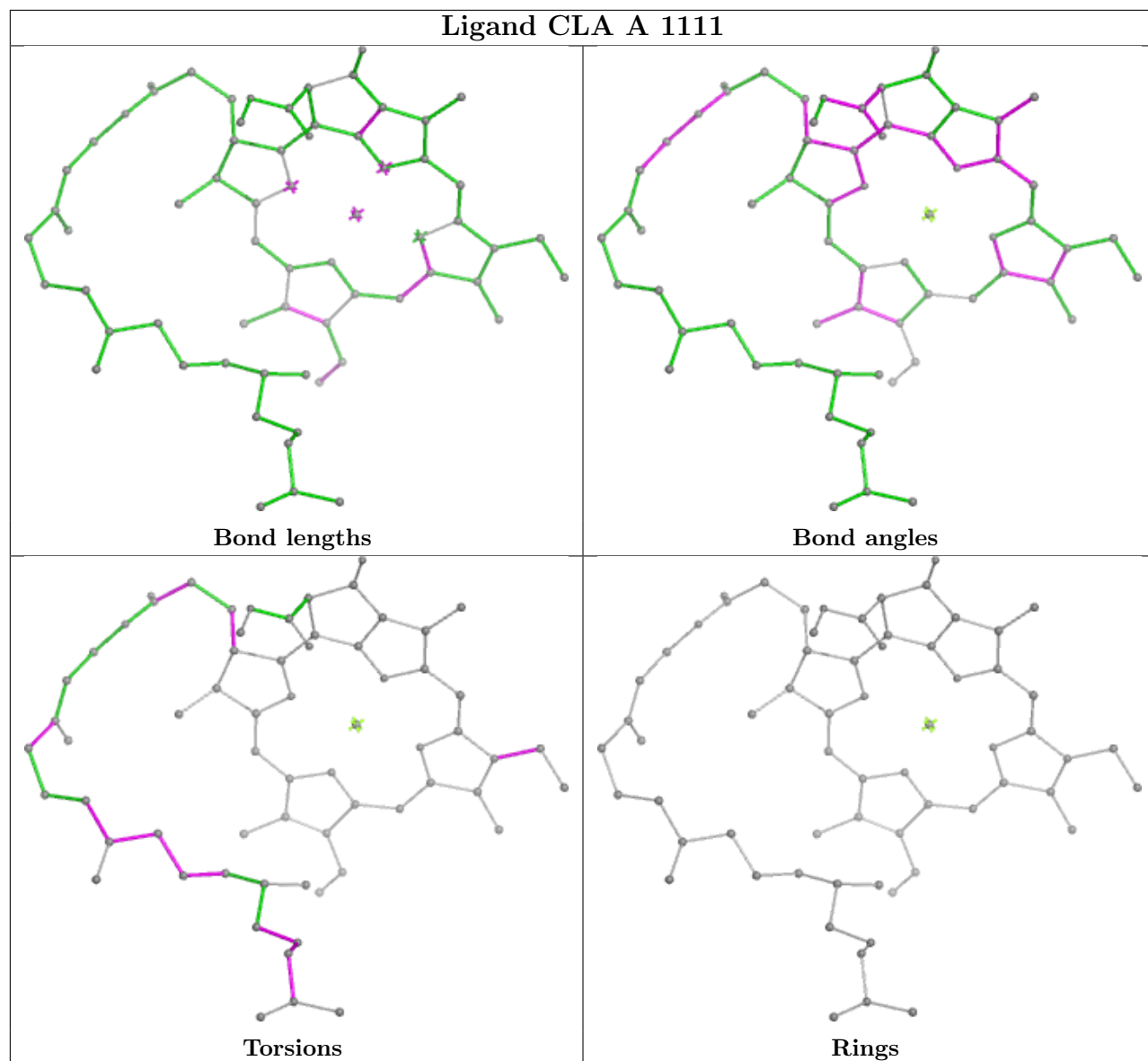


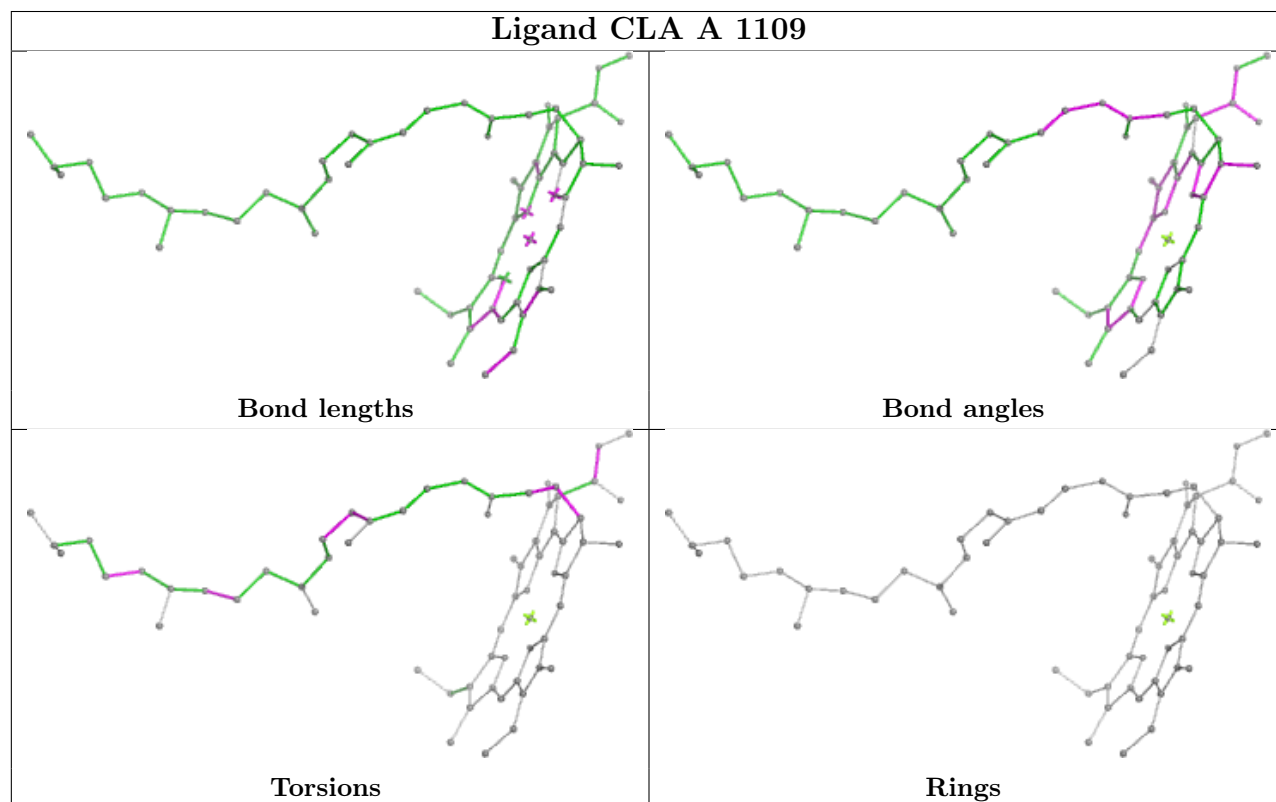
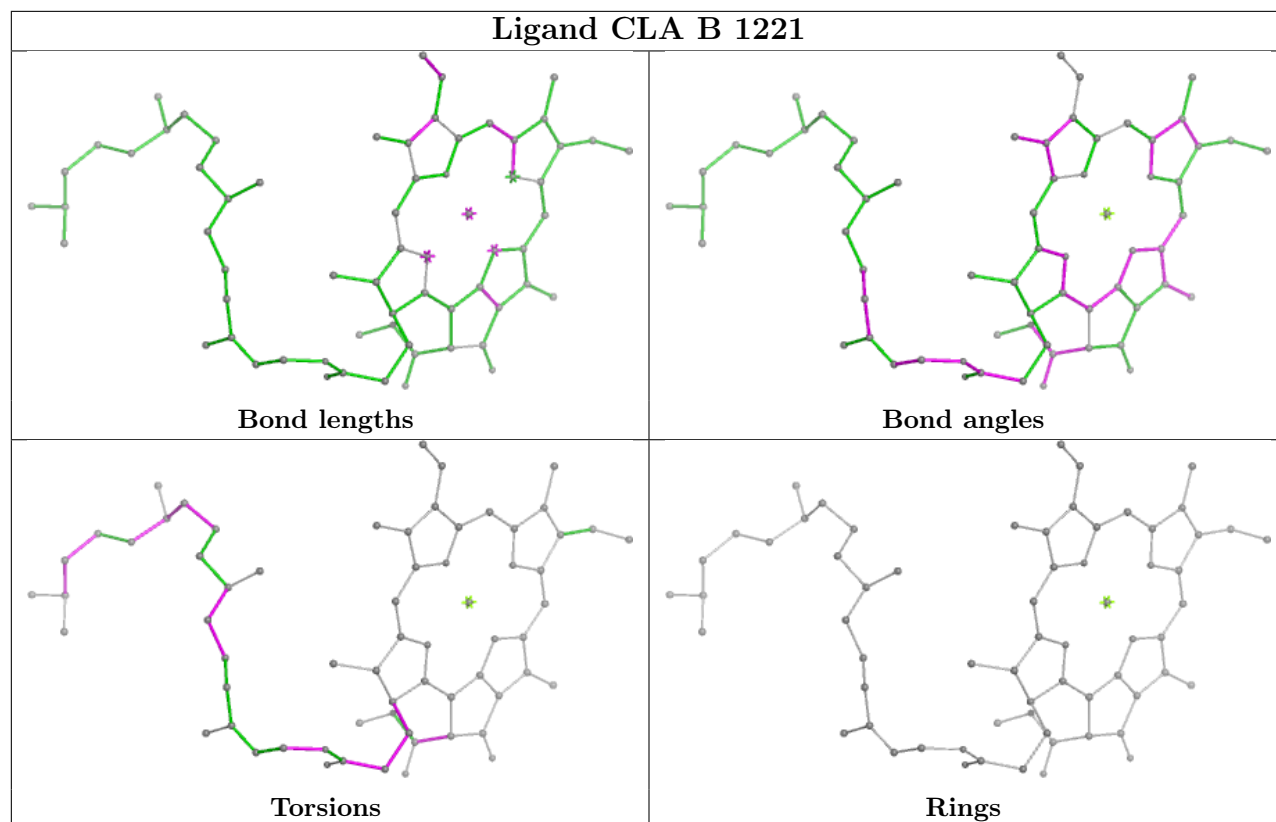


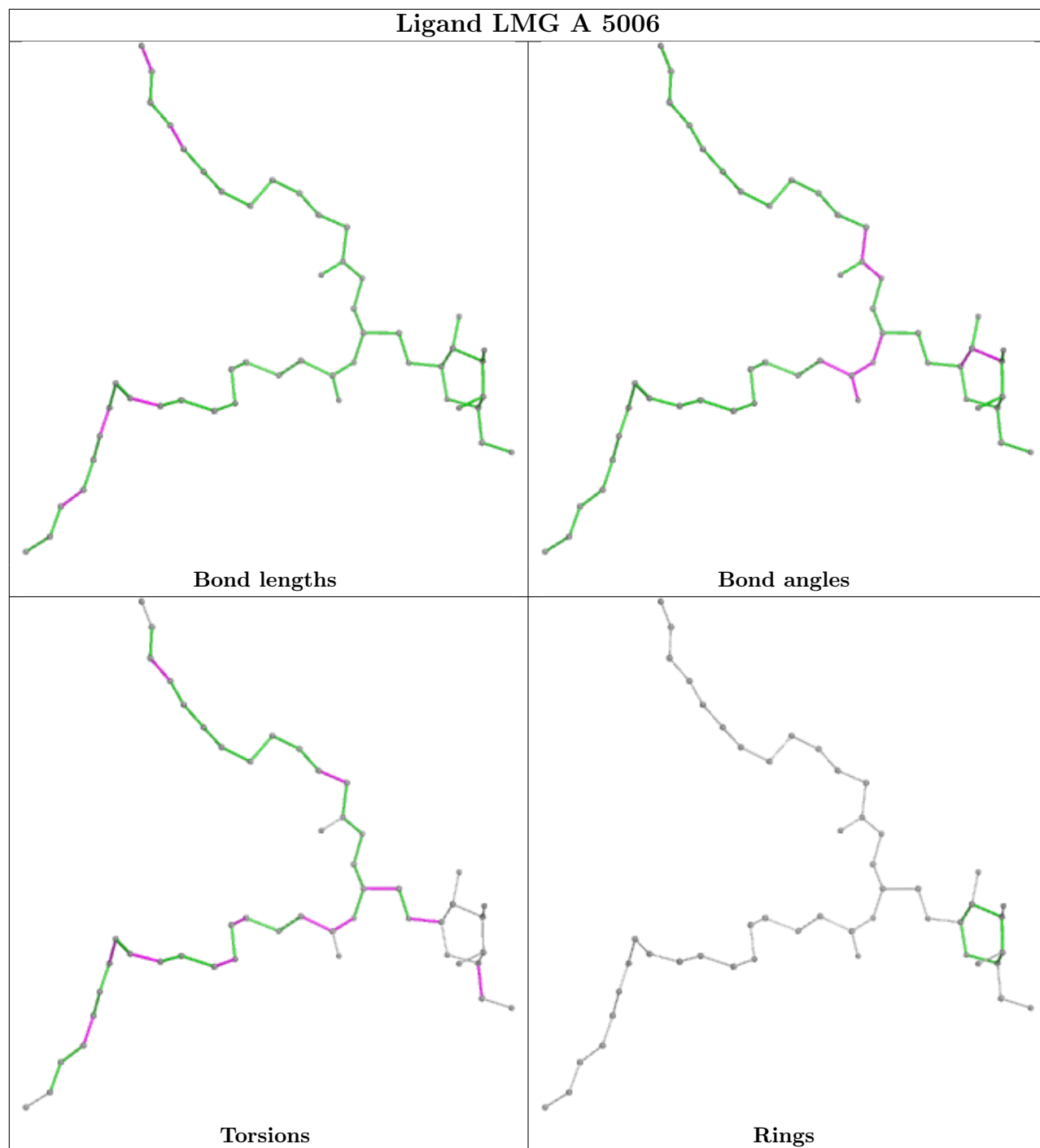


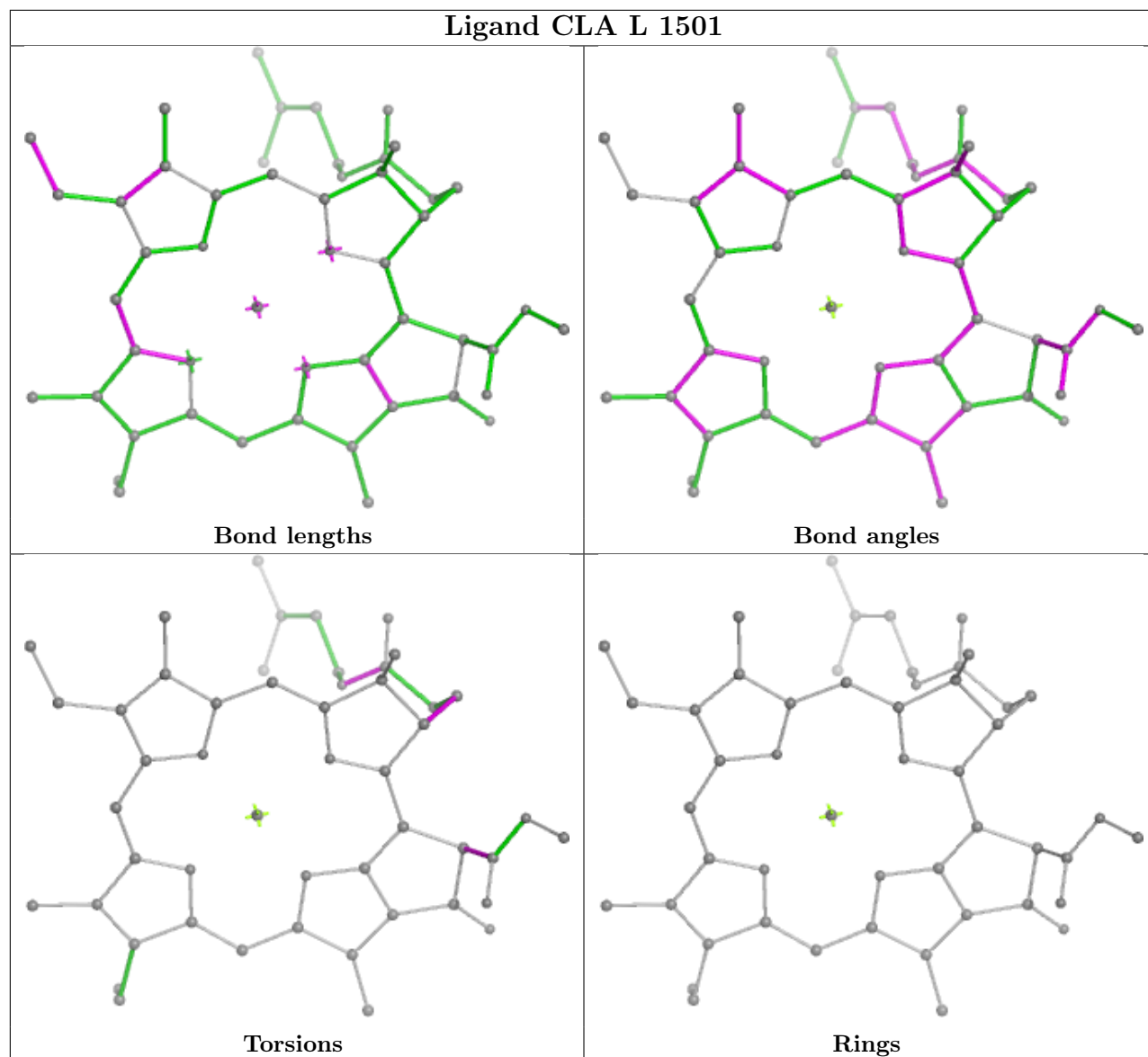
Ligand CHL 4 611

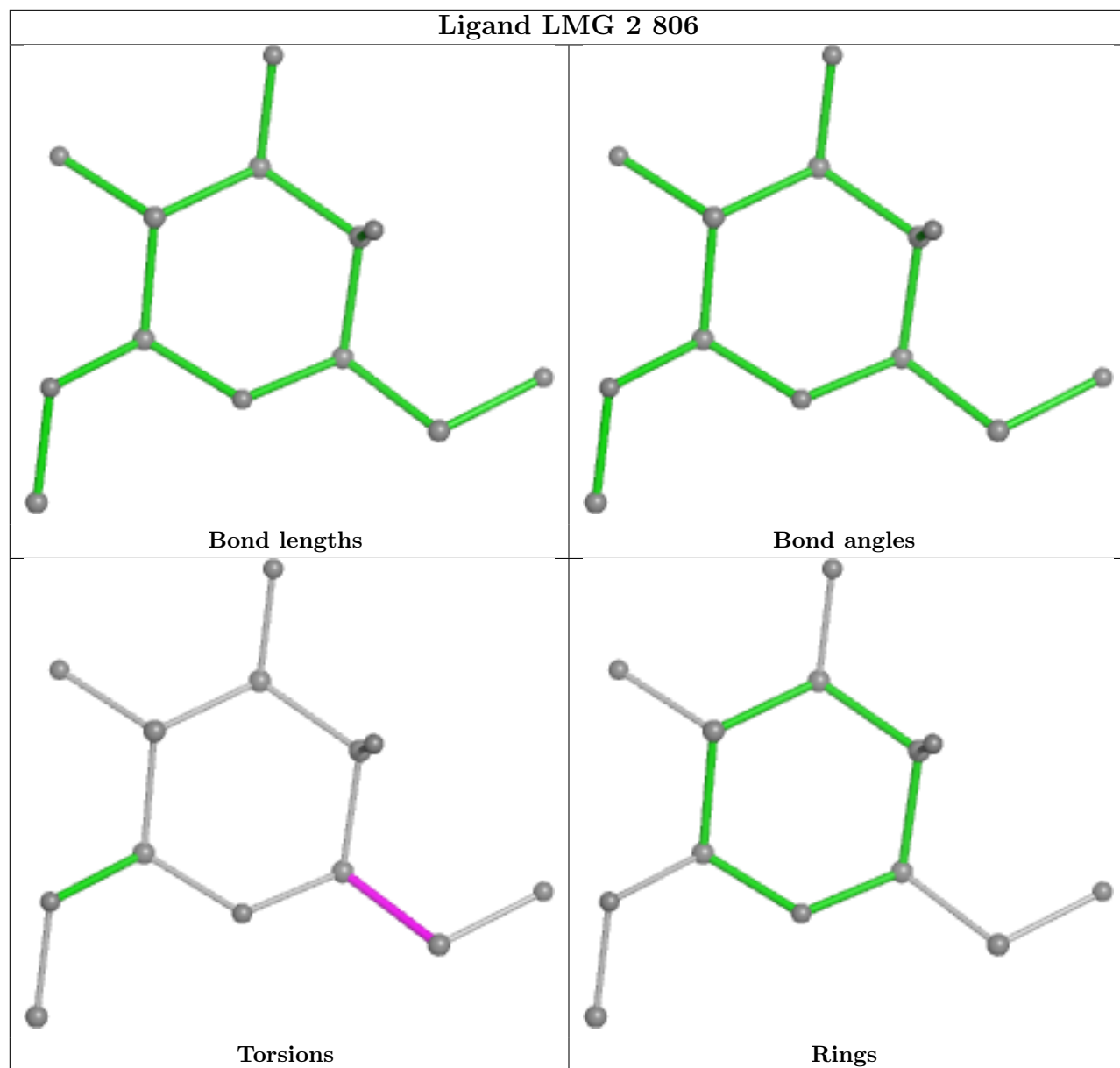


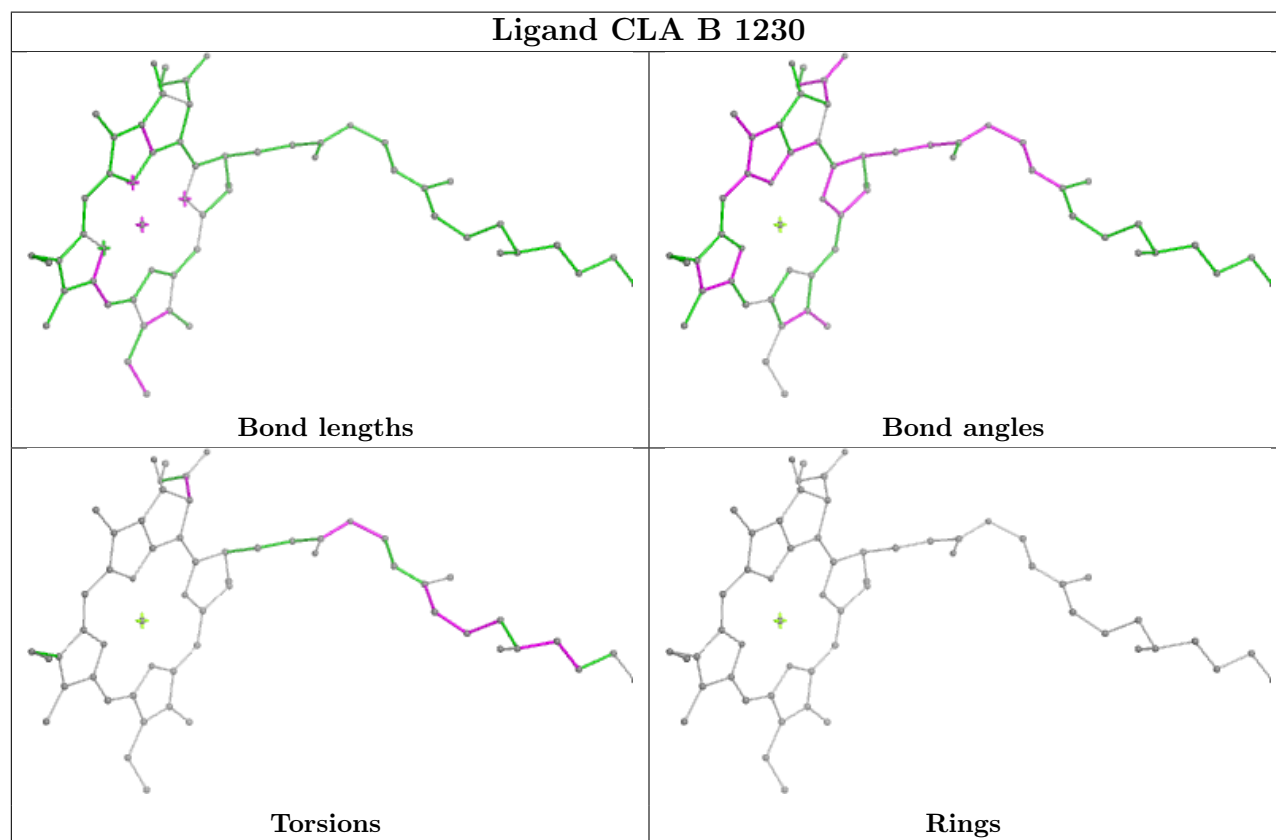
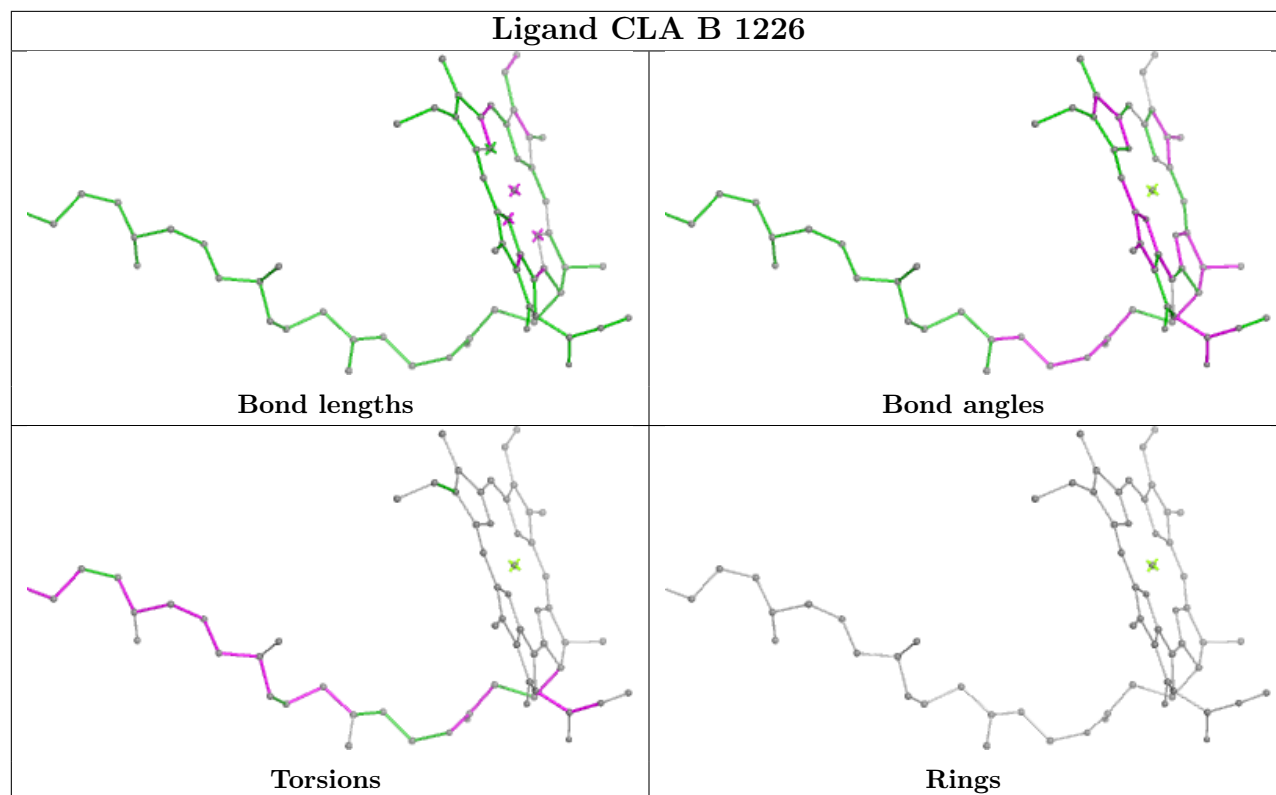


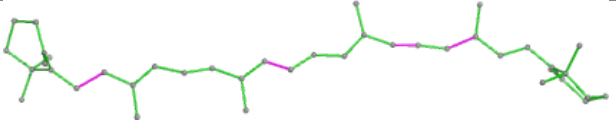
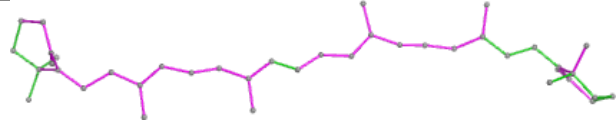
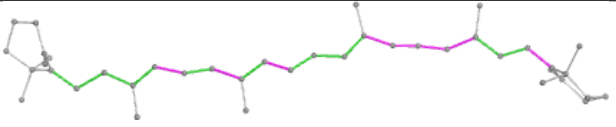



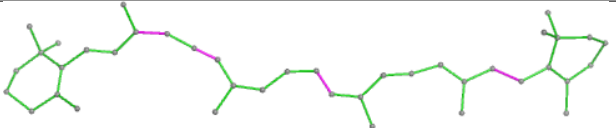
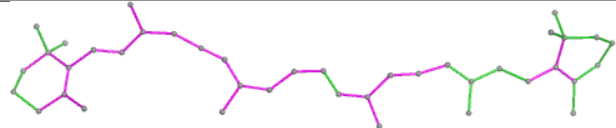
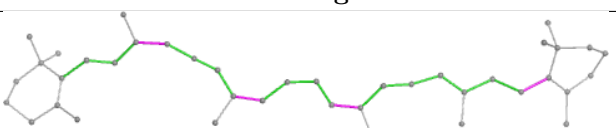



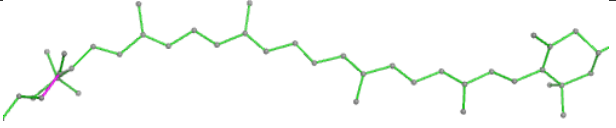
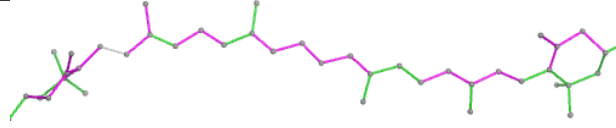
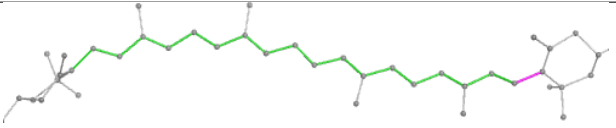
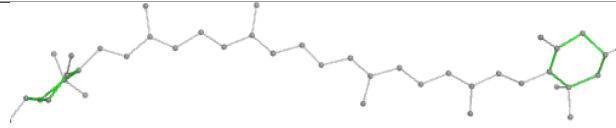




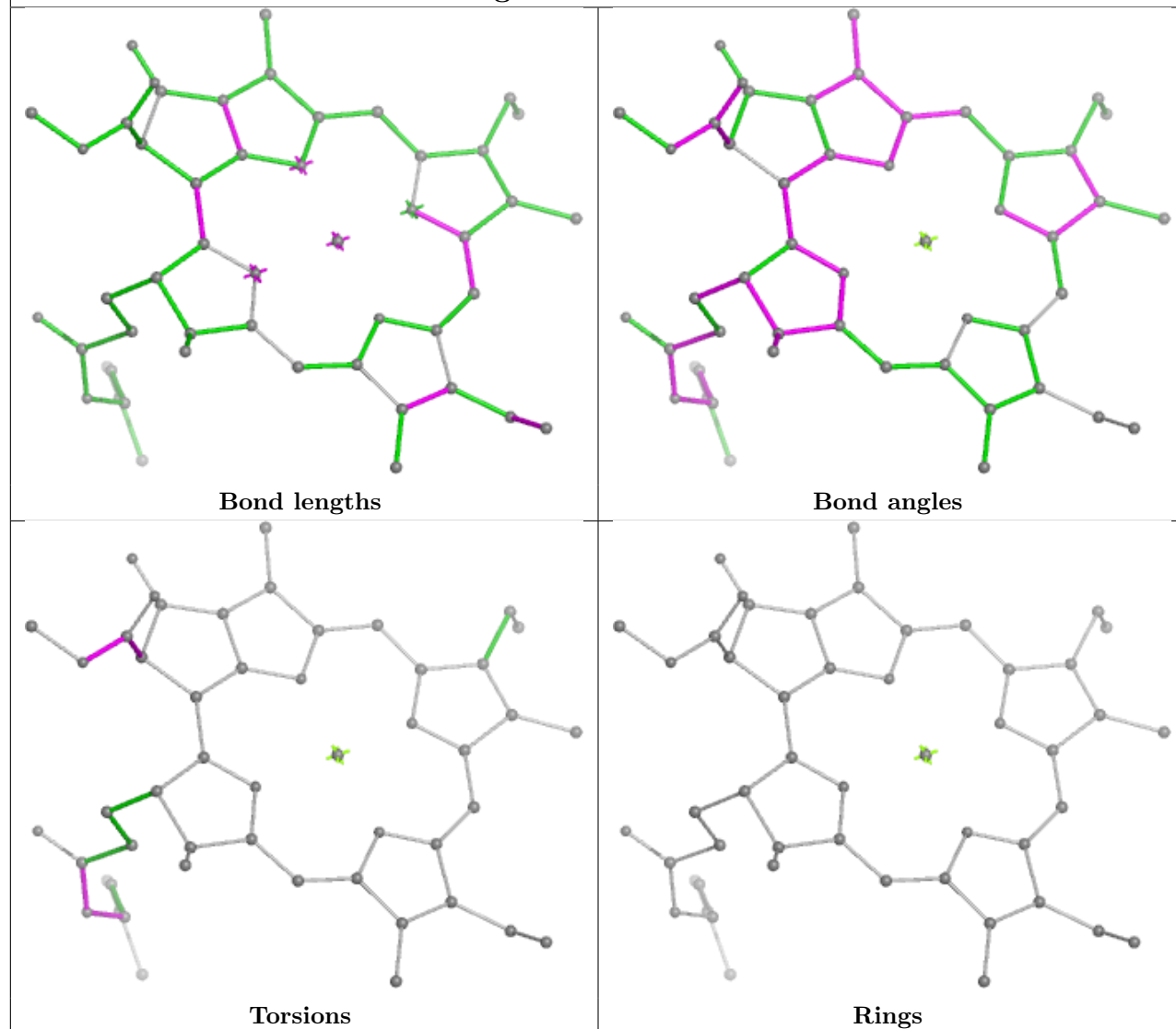


Ligand BCR A 4002	
	Bond lengths
	Bond angles
	Torsions
	Rings

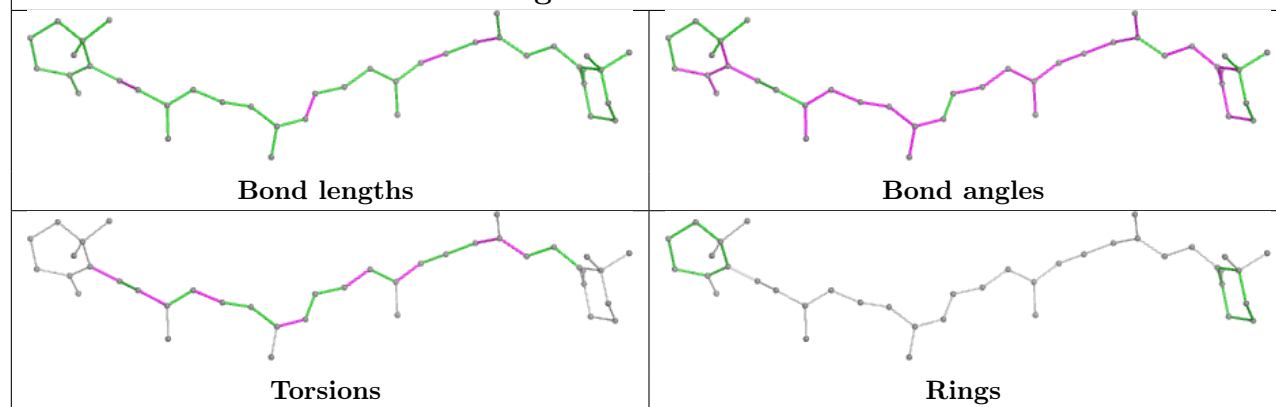
Ligand BCR B 4004	
	Bond lengths
	Bond angles
	Torsions
	Rings

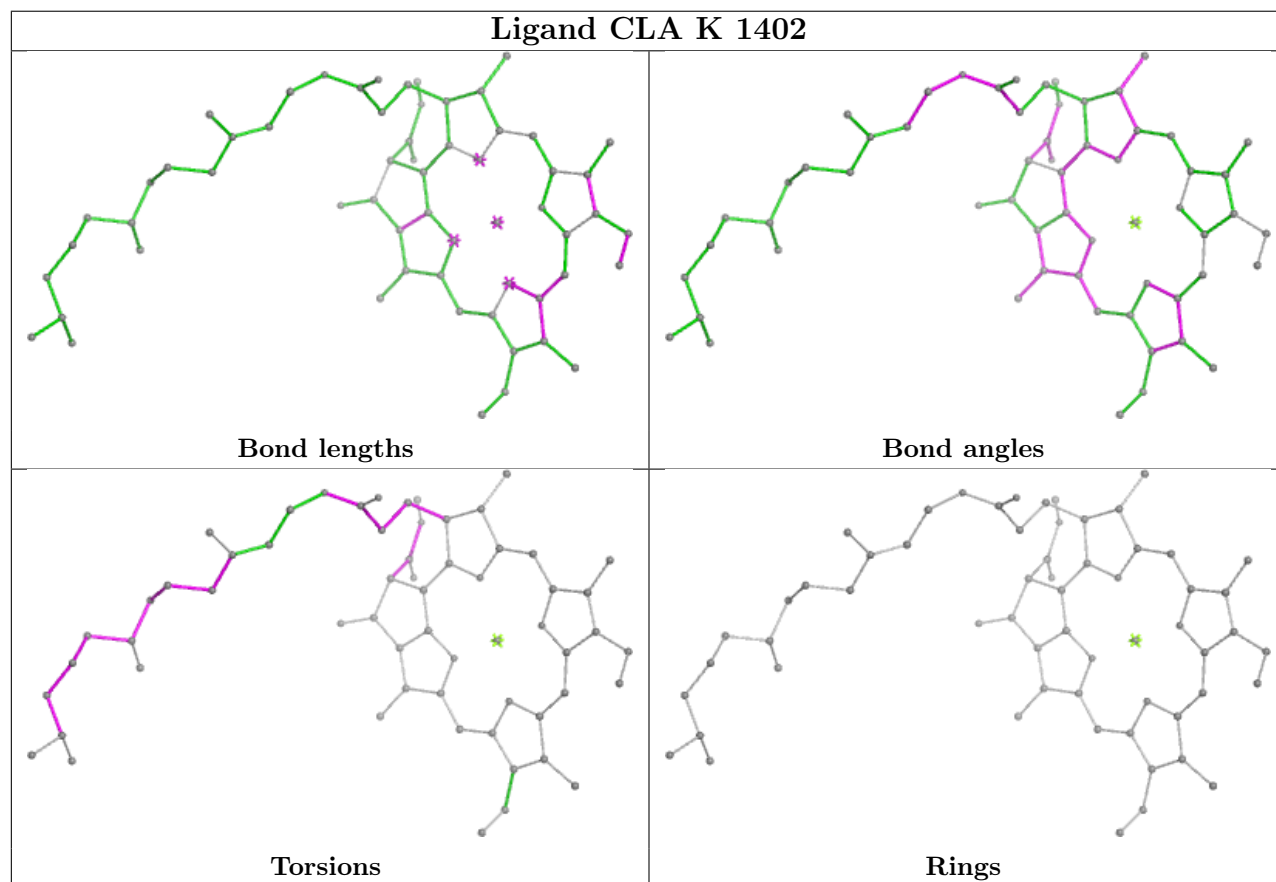
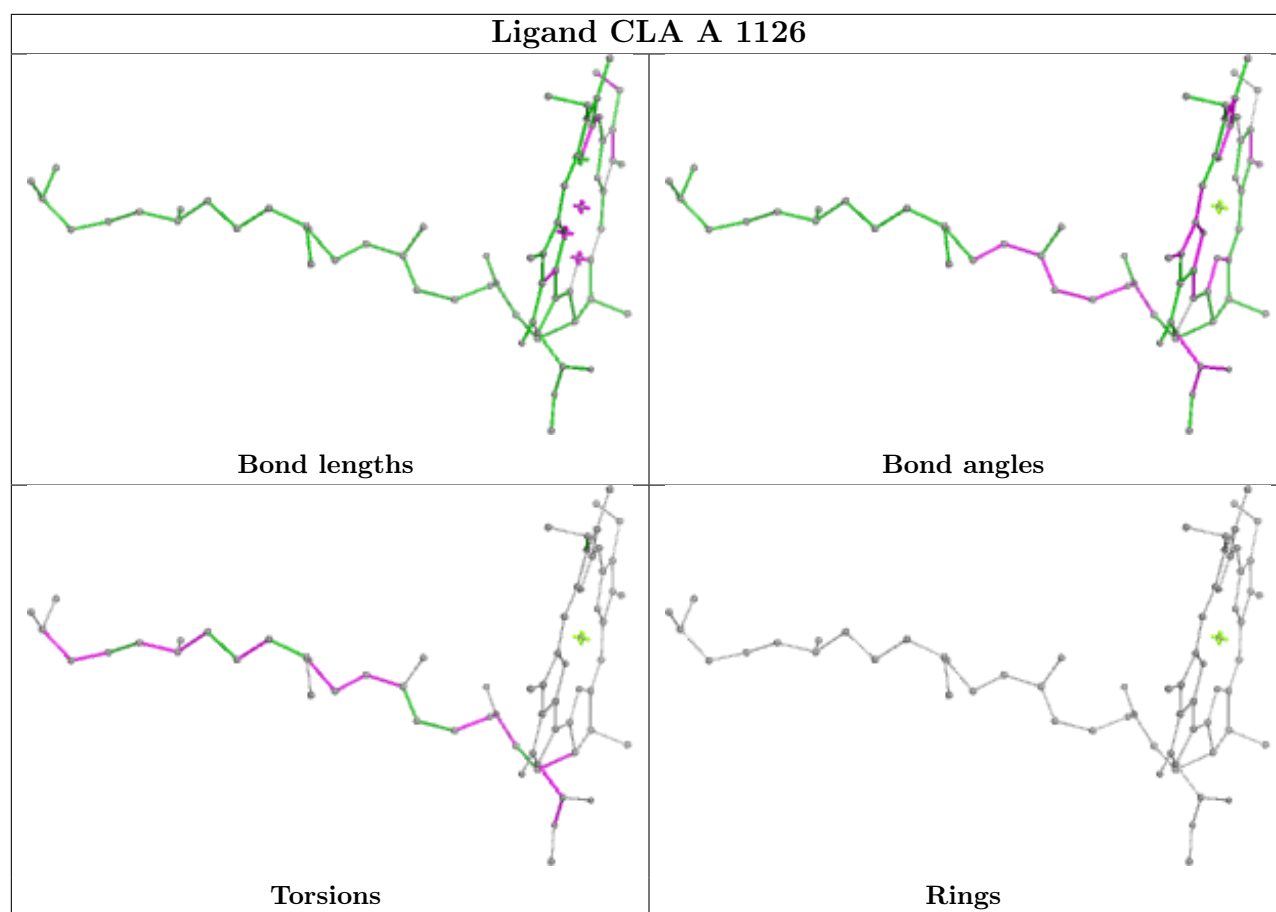
Ligand LUT 1 502	
	Bond lengths
	Bond angles
	Torsions
	Rings

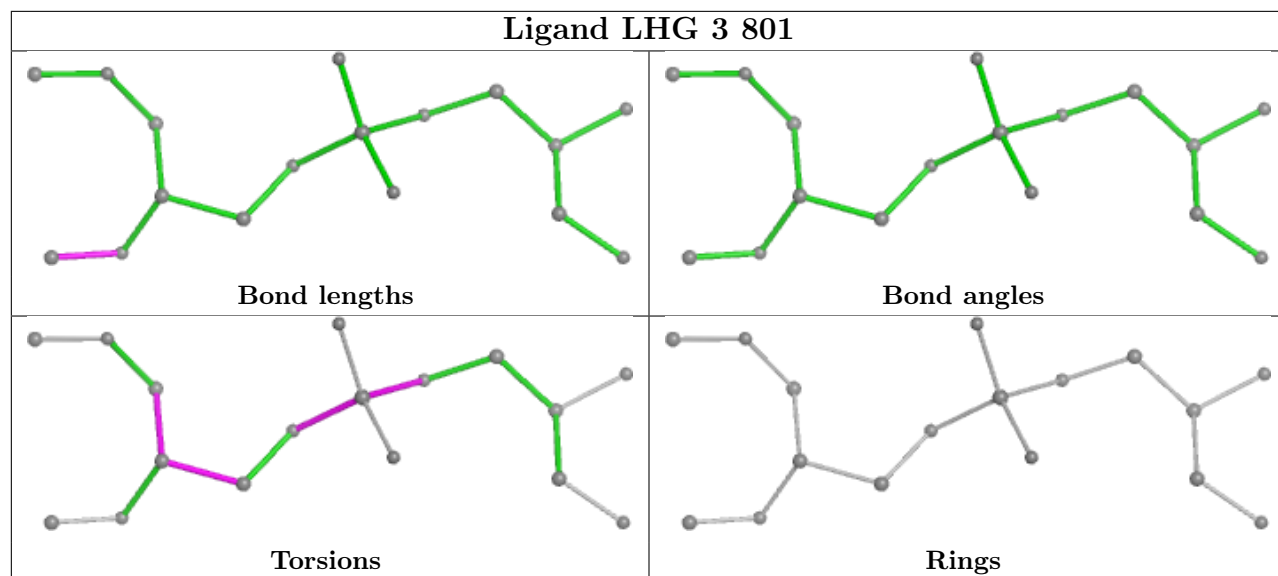
Ligand CLA 1 606

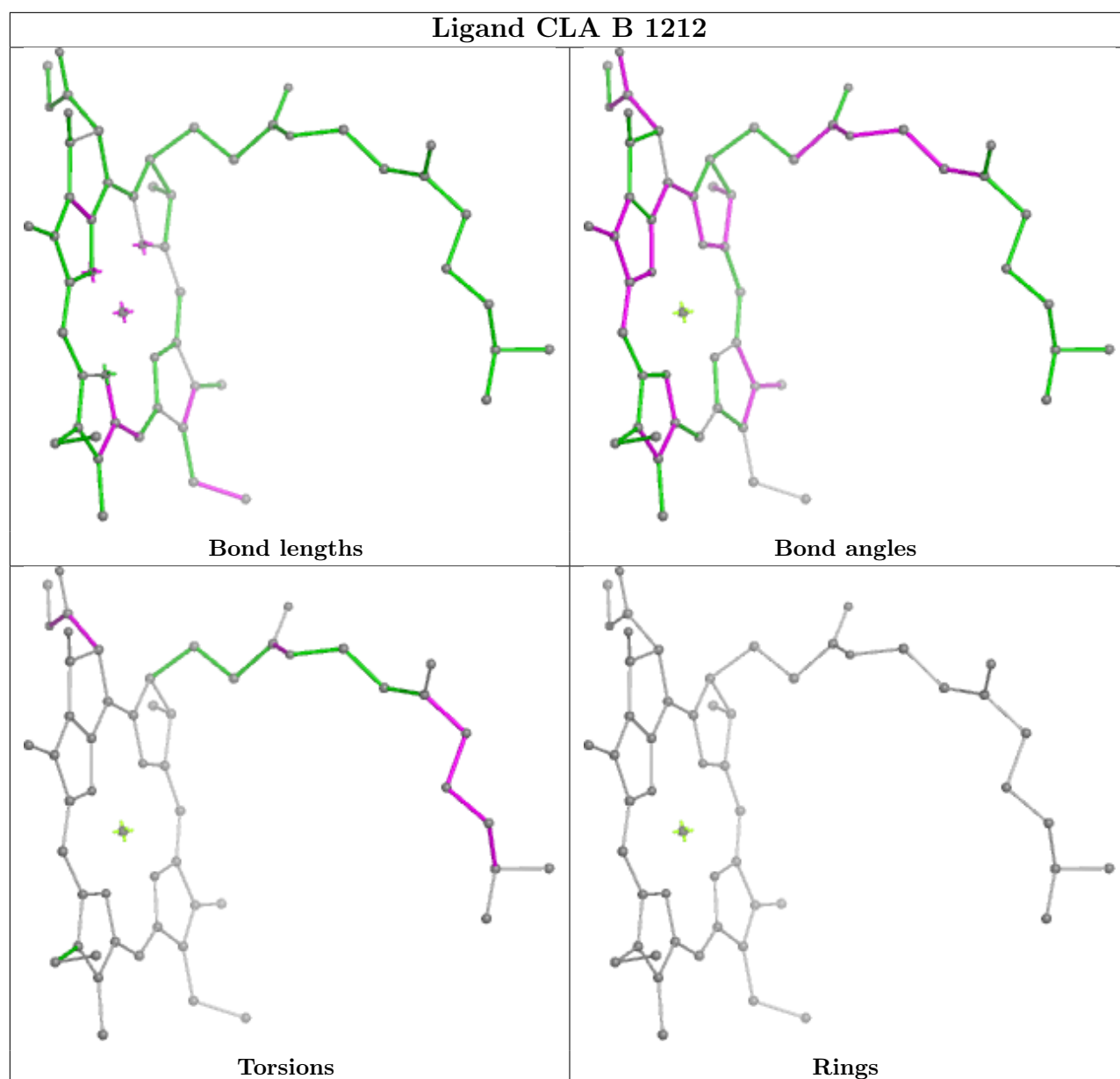


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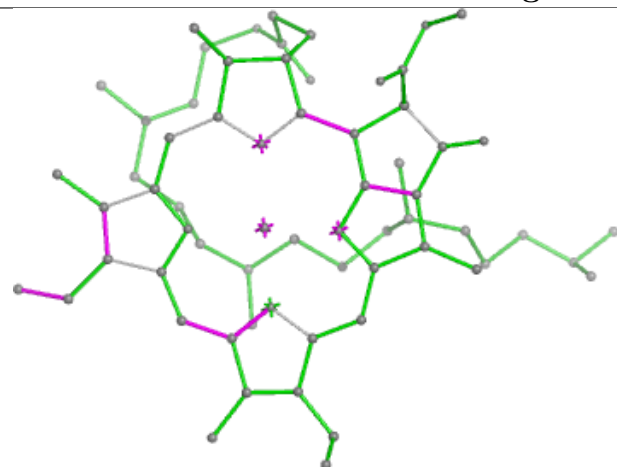




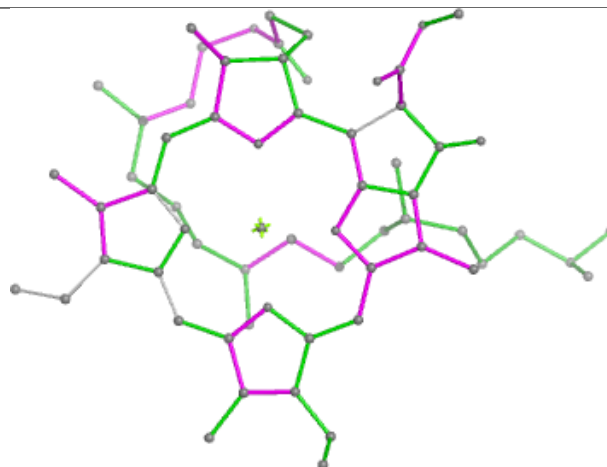




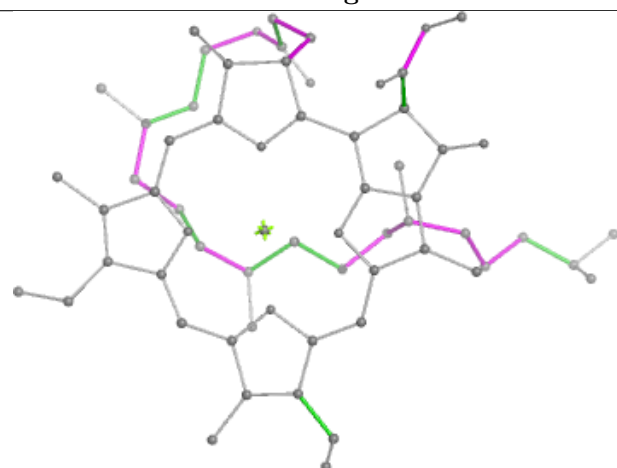
Ligand CLA 3 610



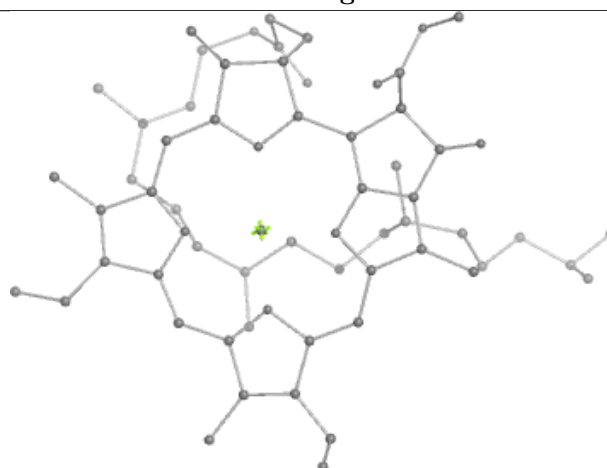
Bond lengths



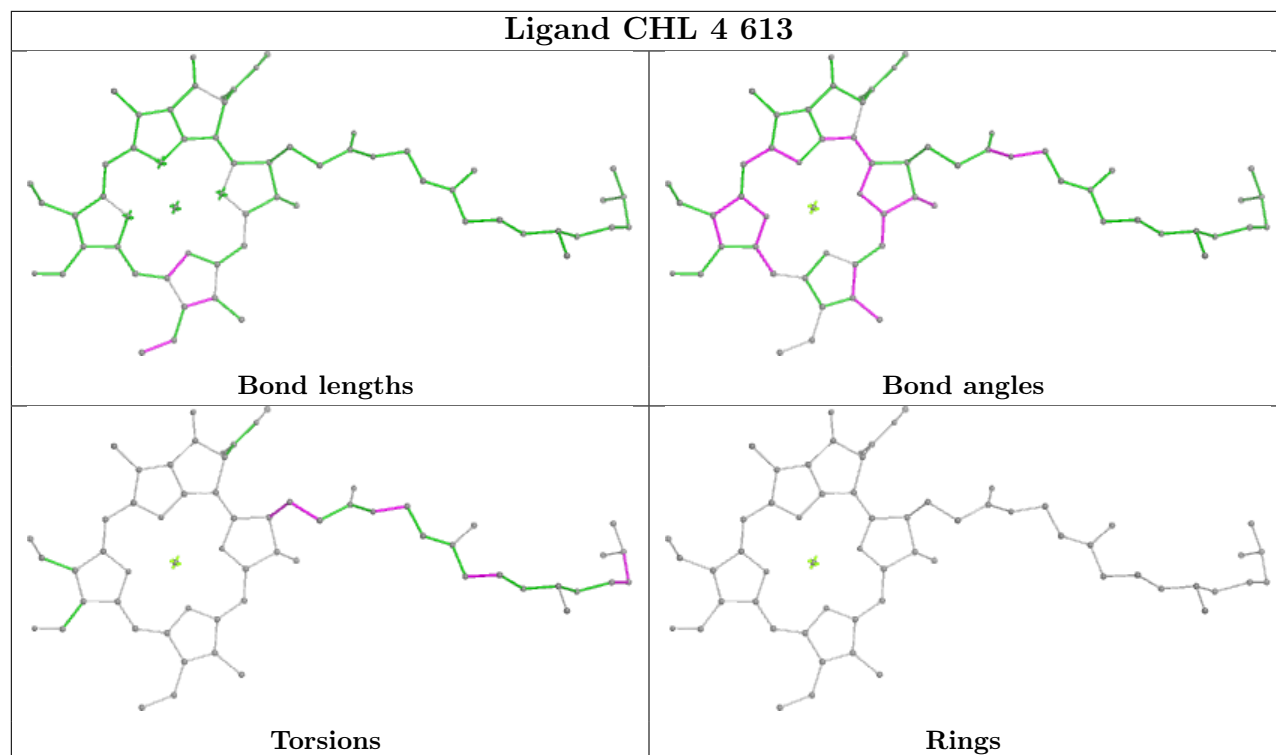
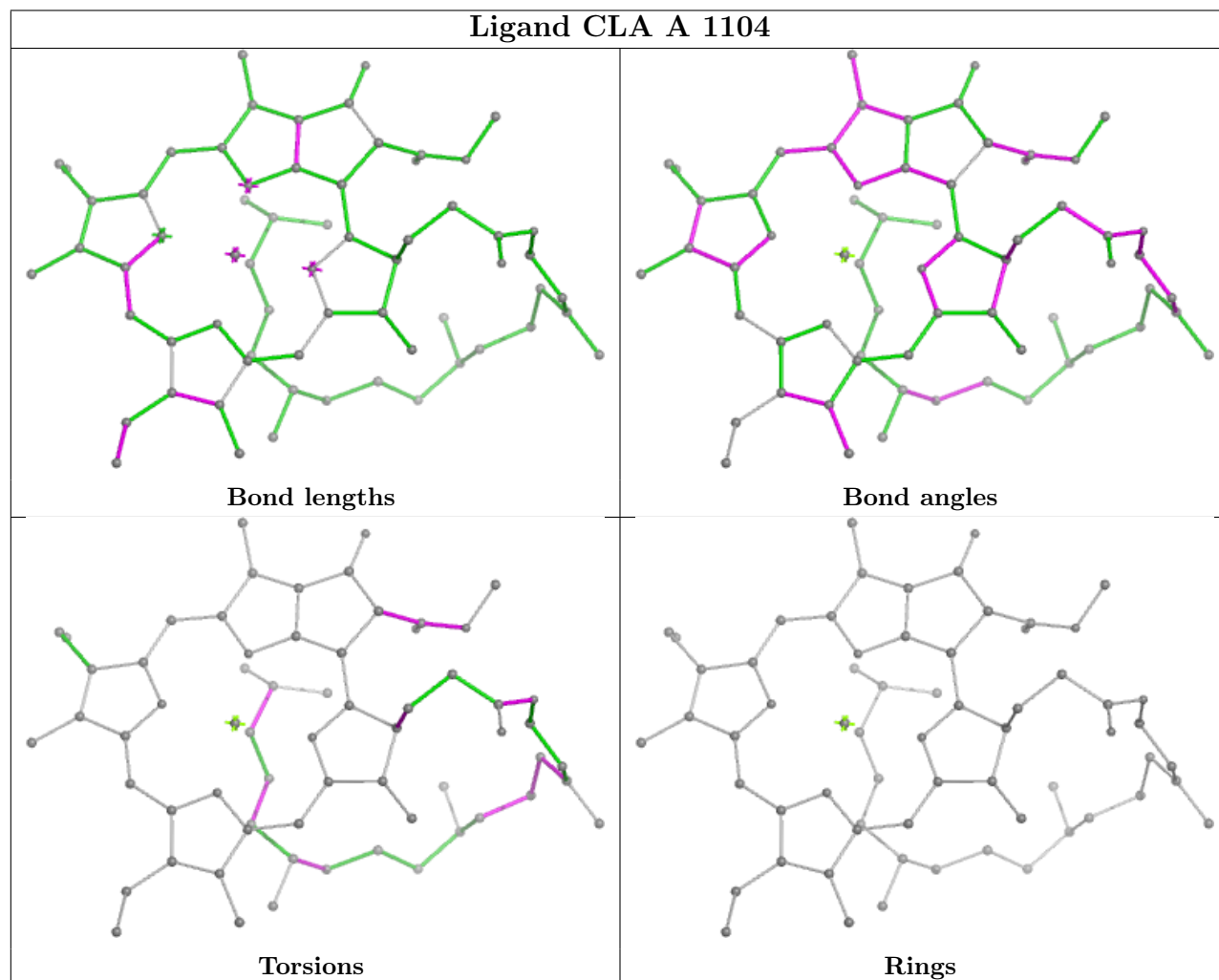
Bond angles



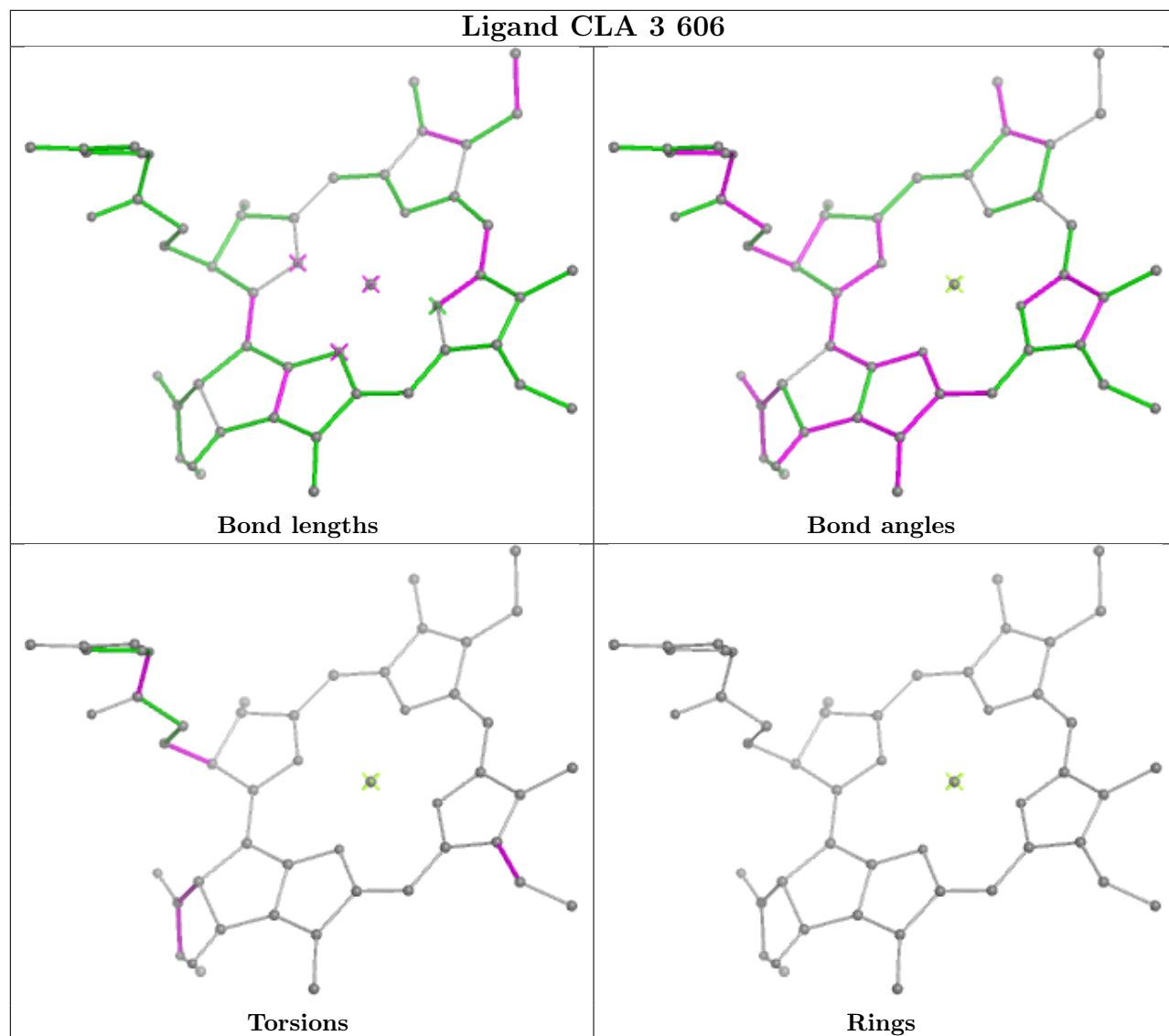
Torsions

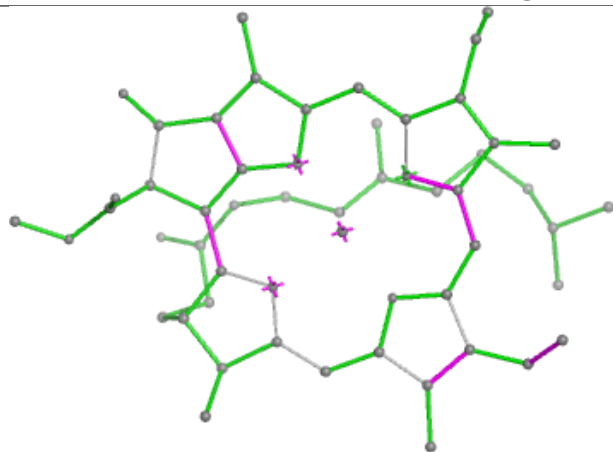
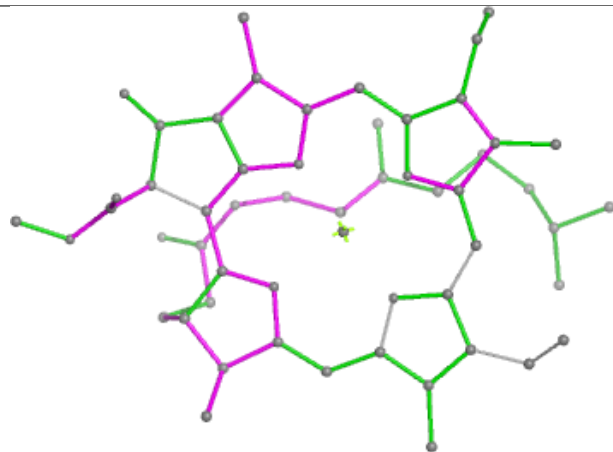
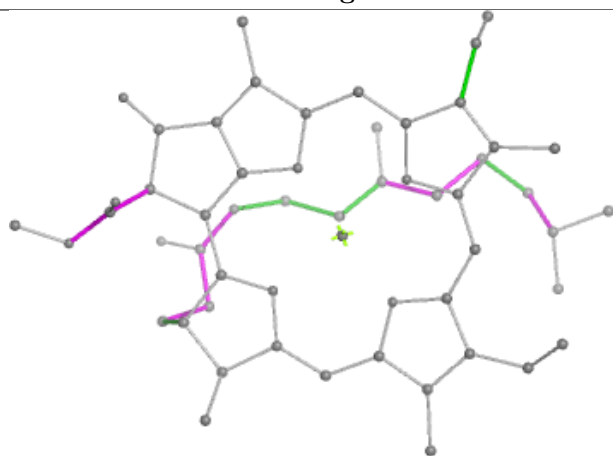
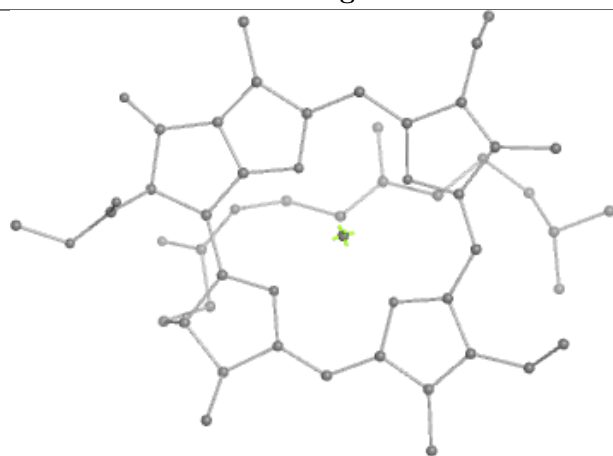


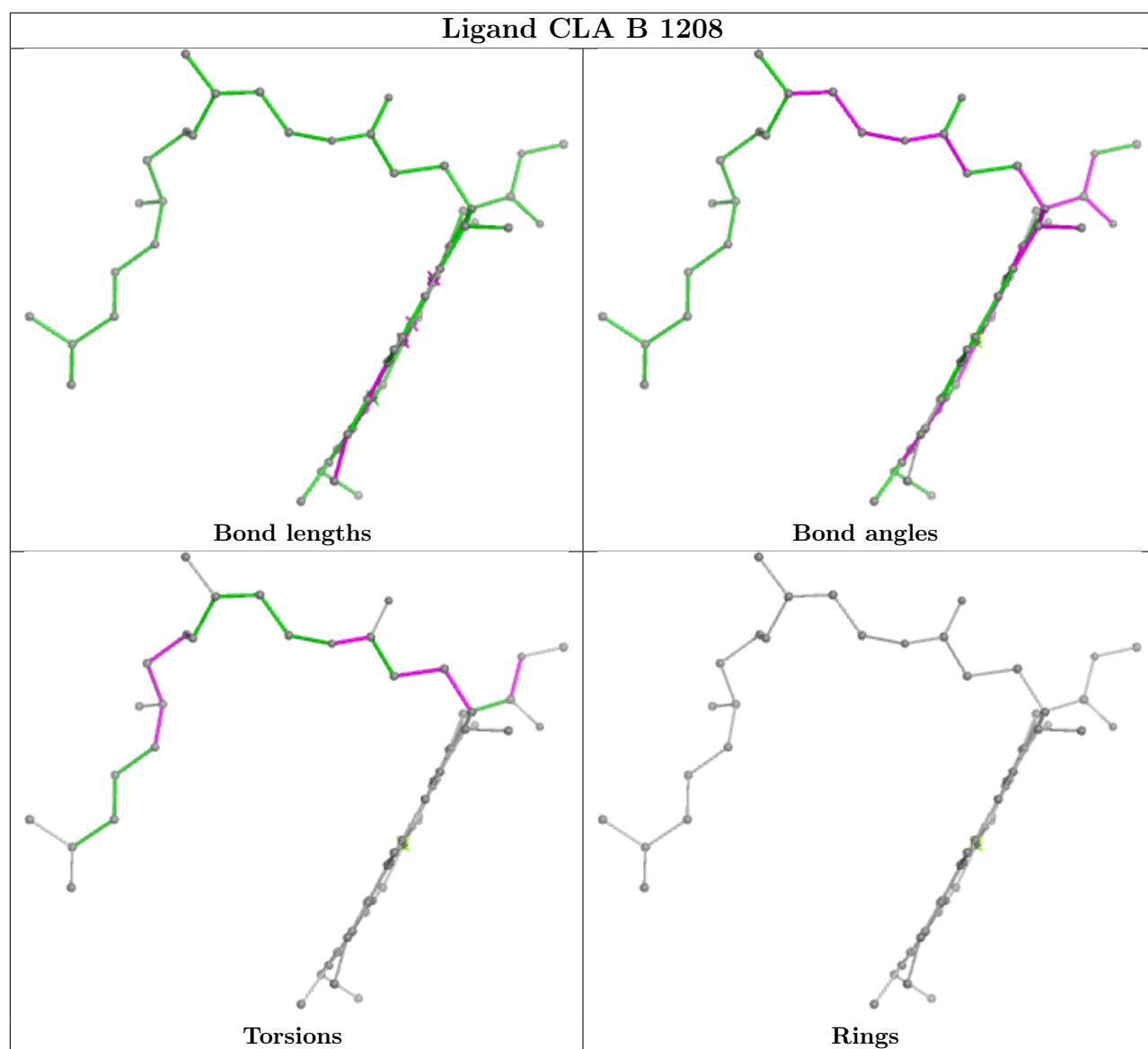
Rings

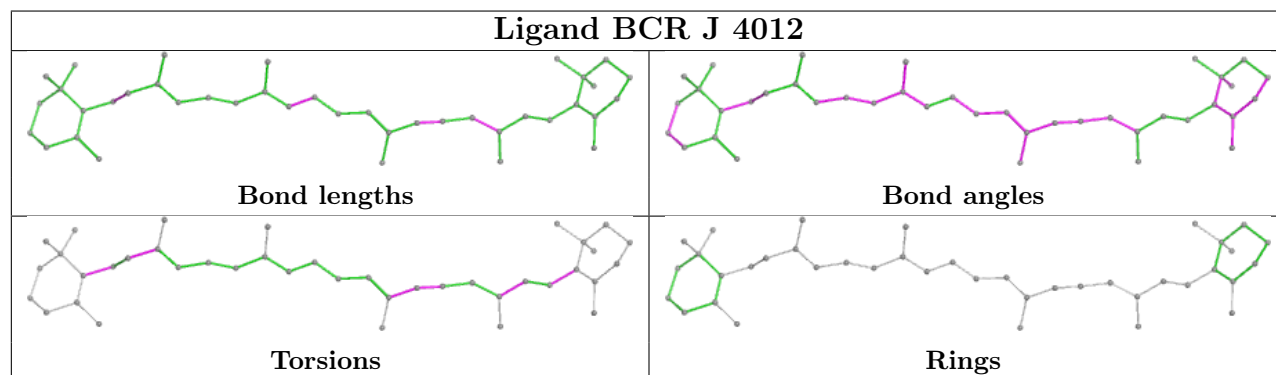
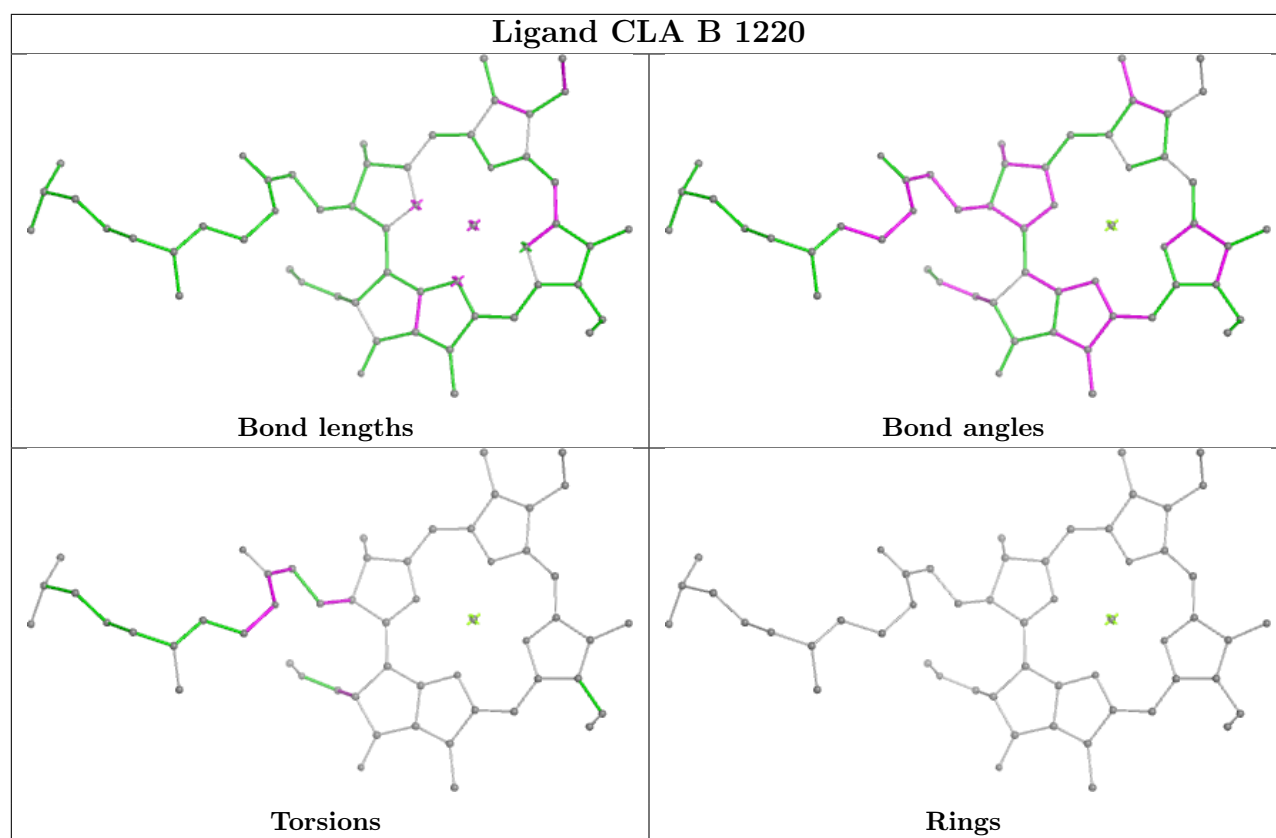
Ligand CHL 4 613**Ligand CLA A 1104**

Ligand CLA 3 606

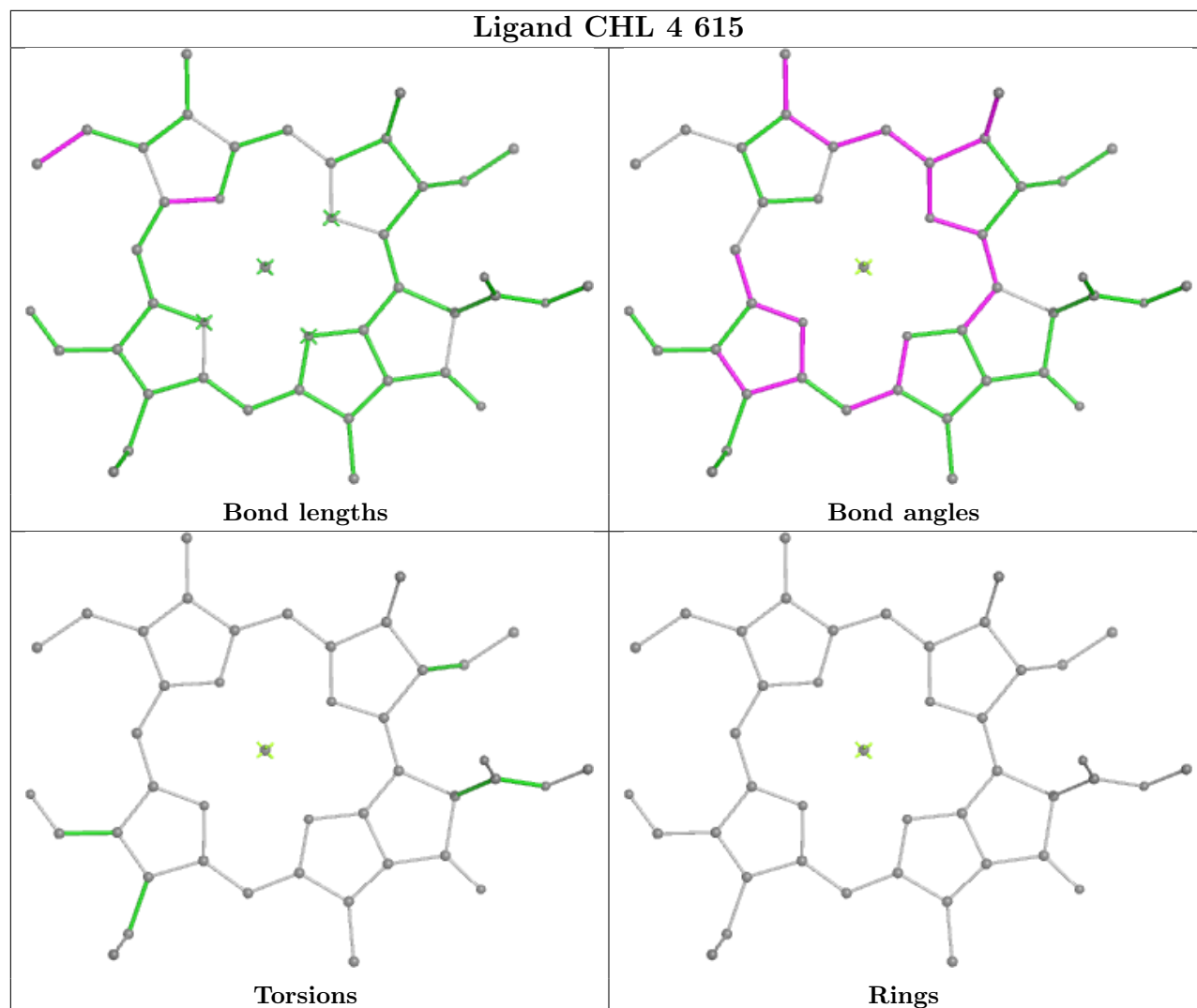


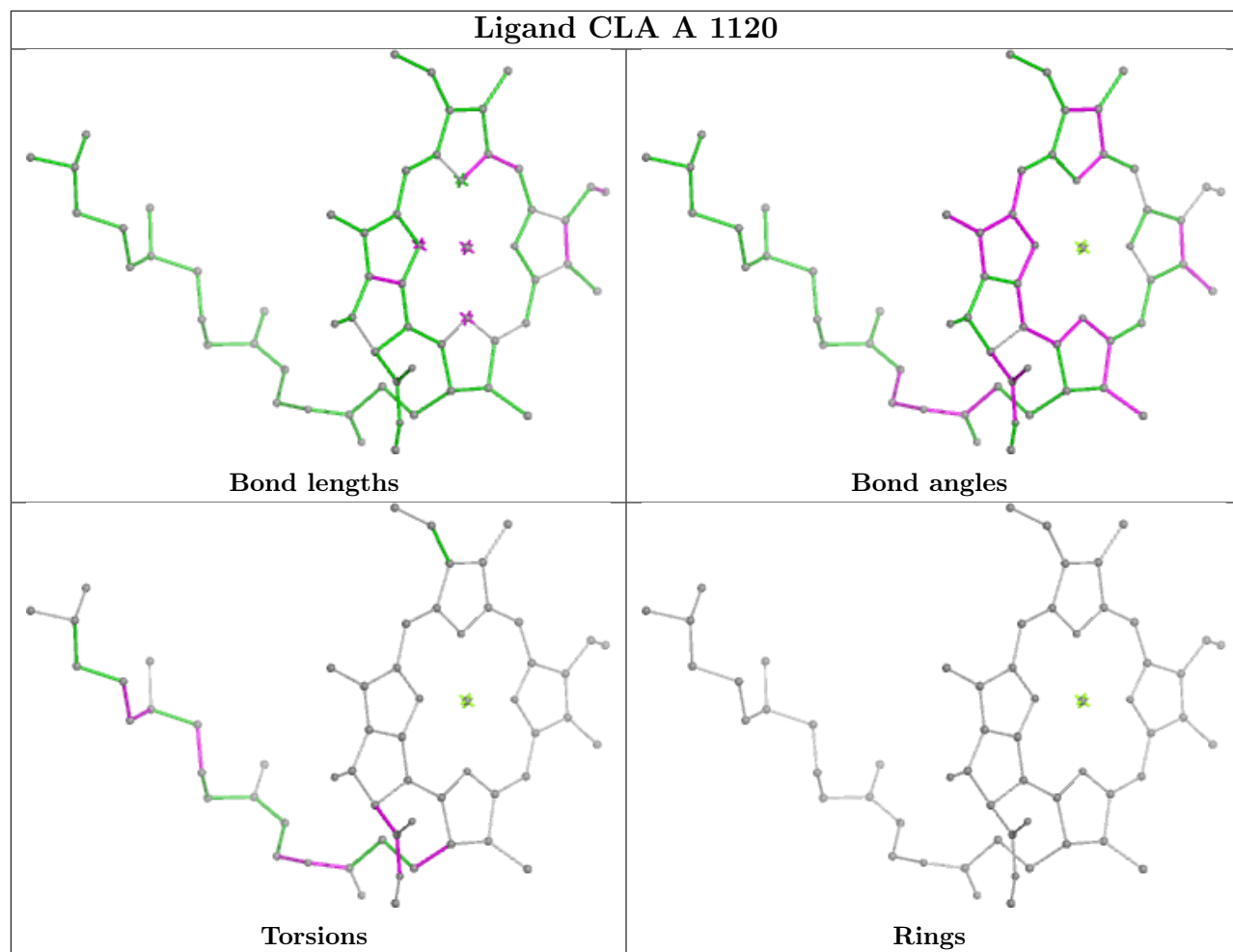
Ligand CLA 3 603**Bond lengths****Bond angles****Torsions****Rings**

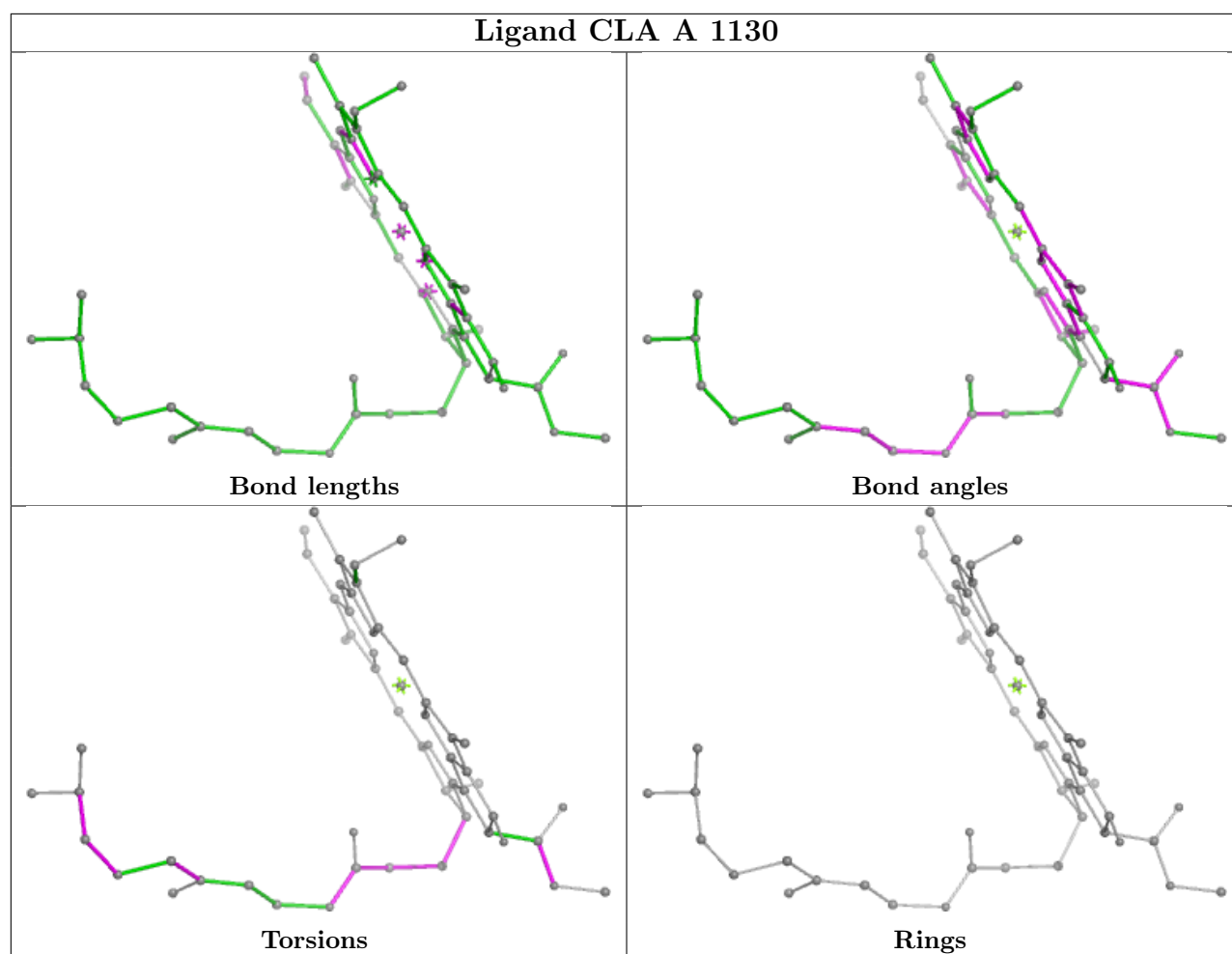


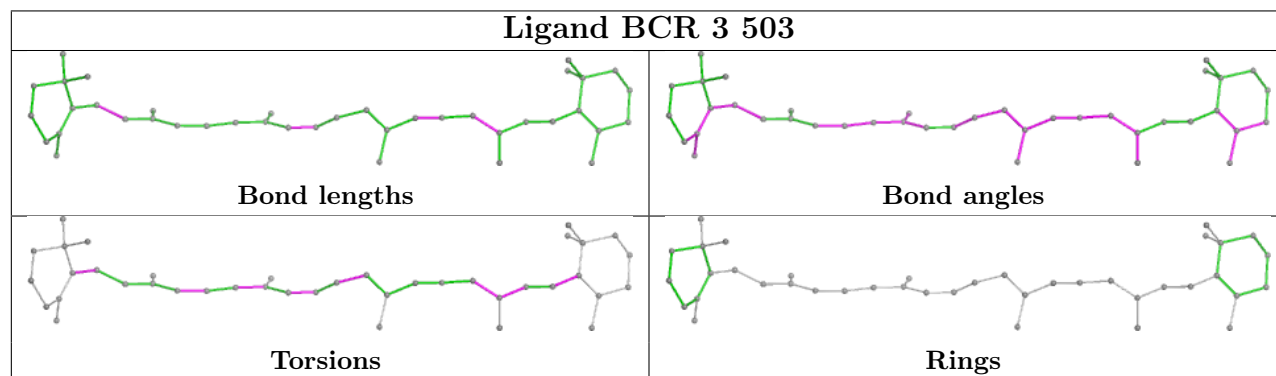
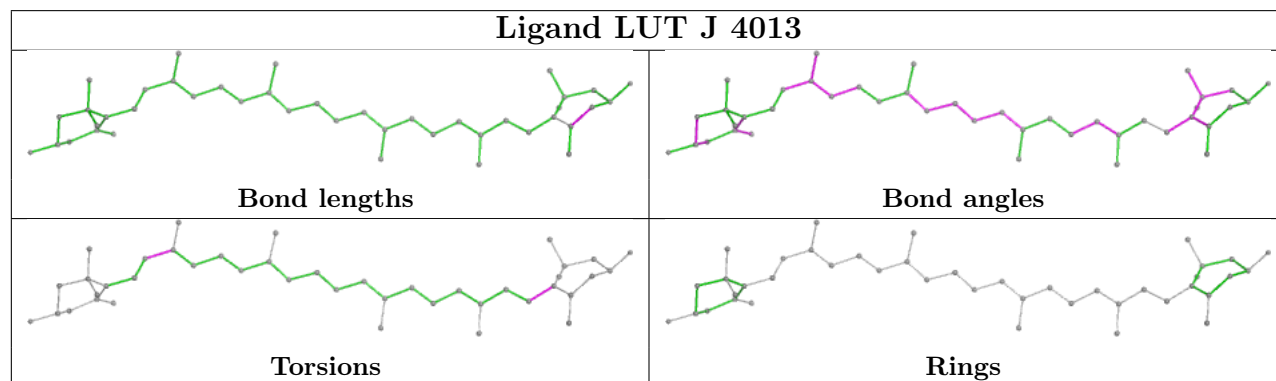
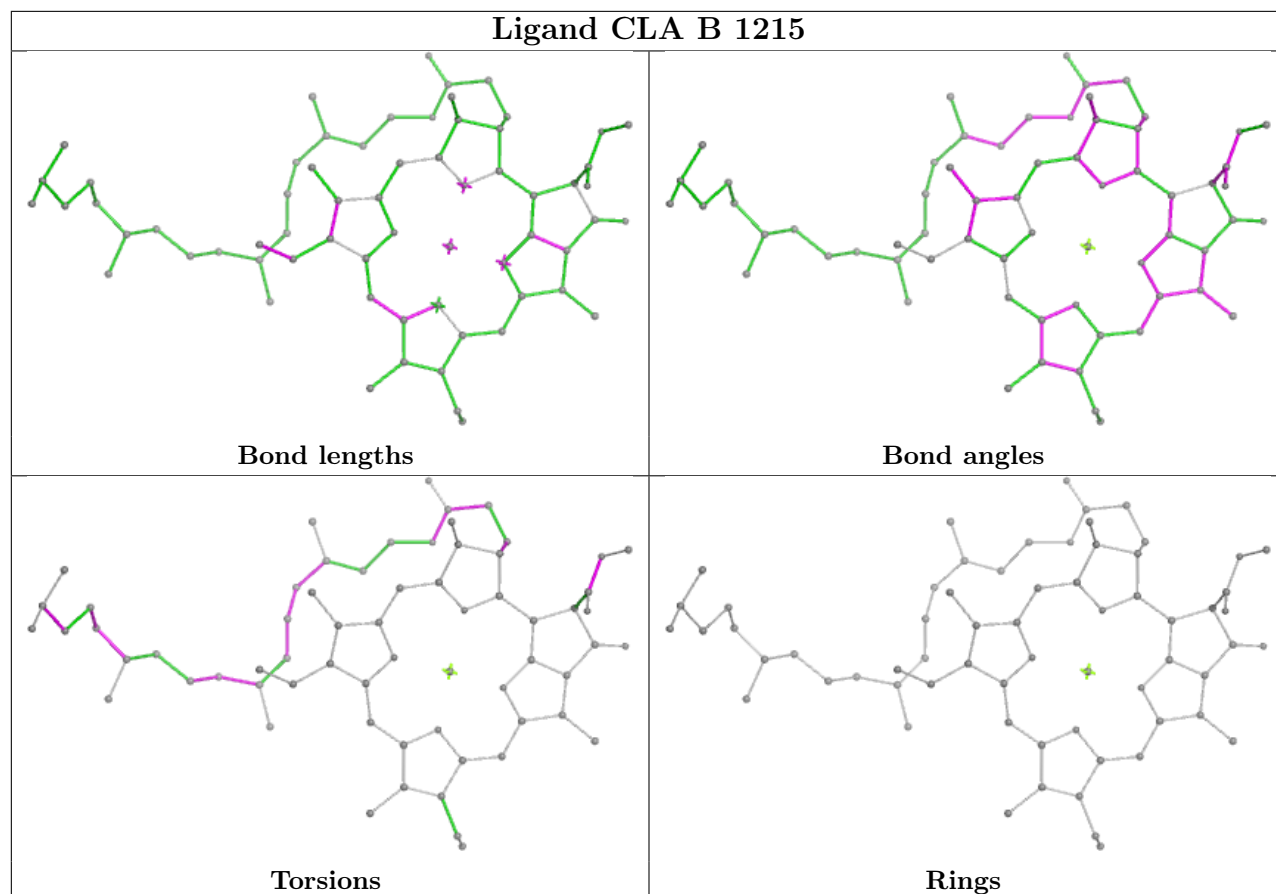


Ligand CHL 4 615

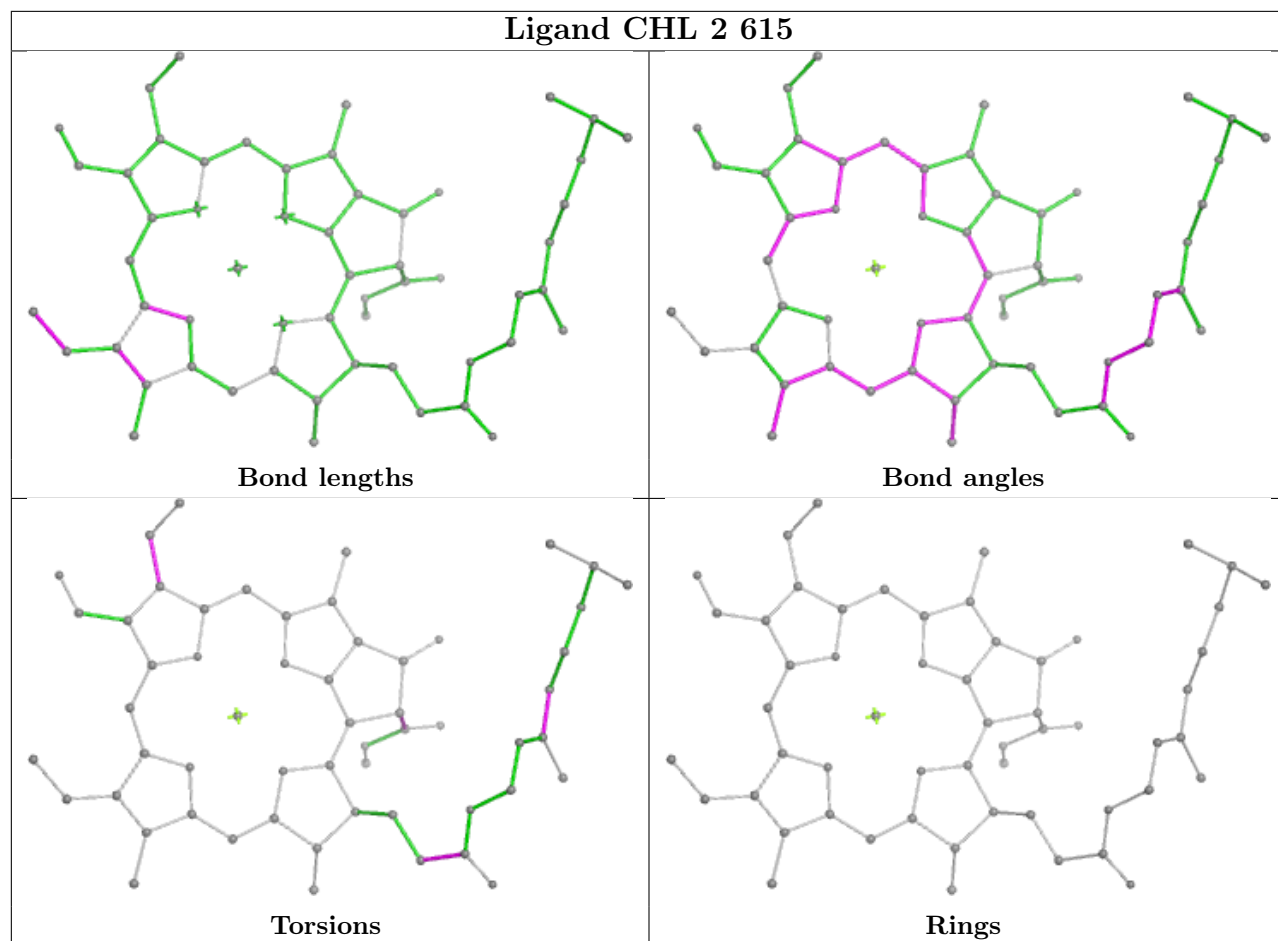


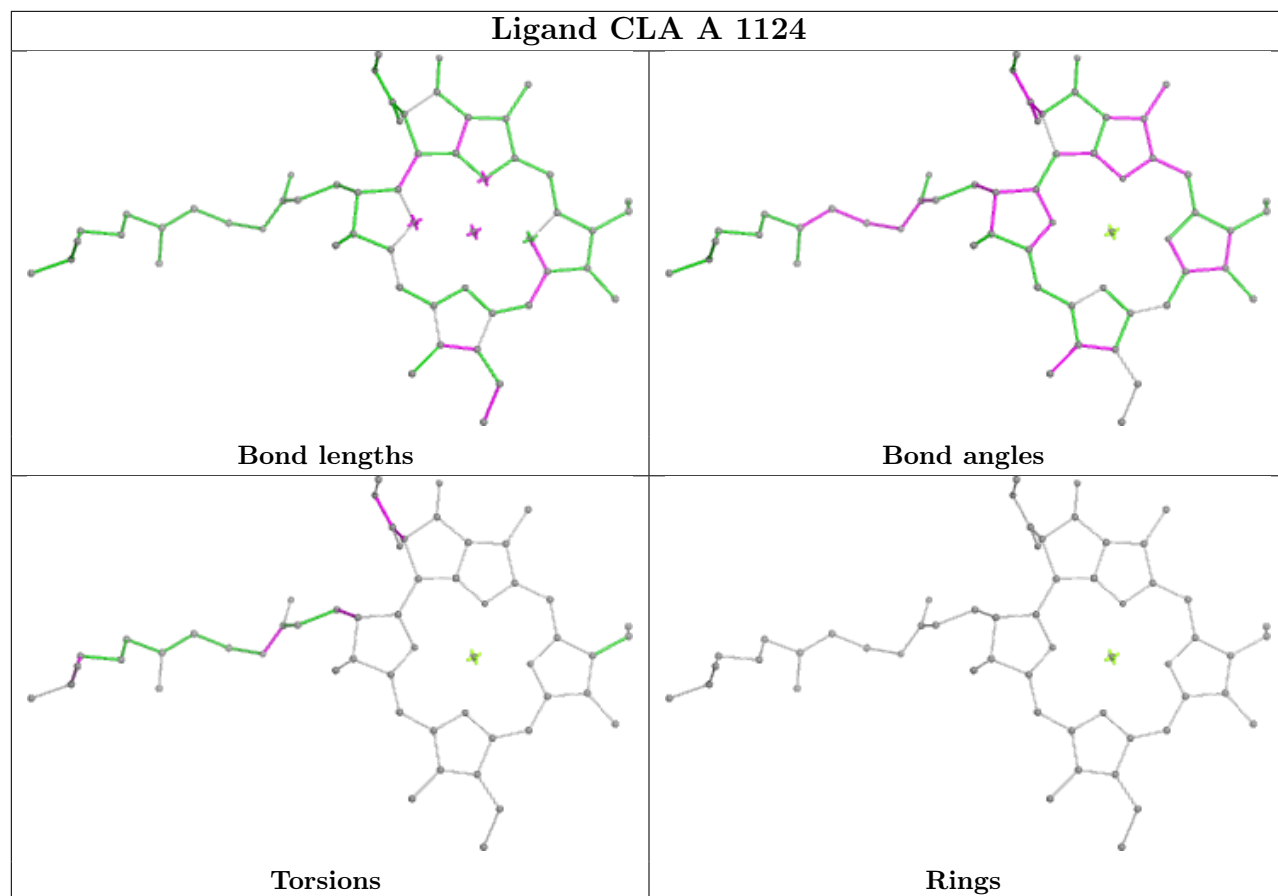




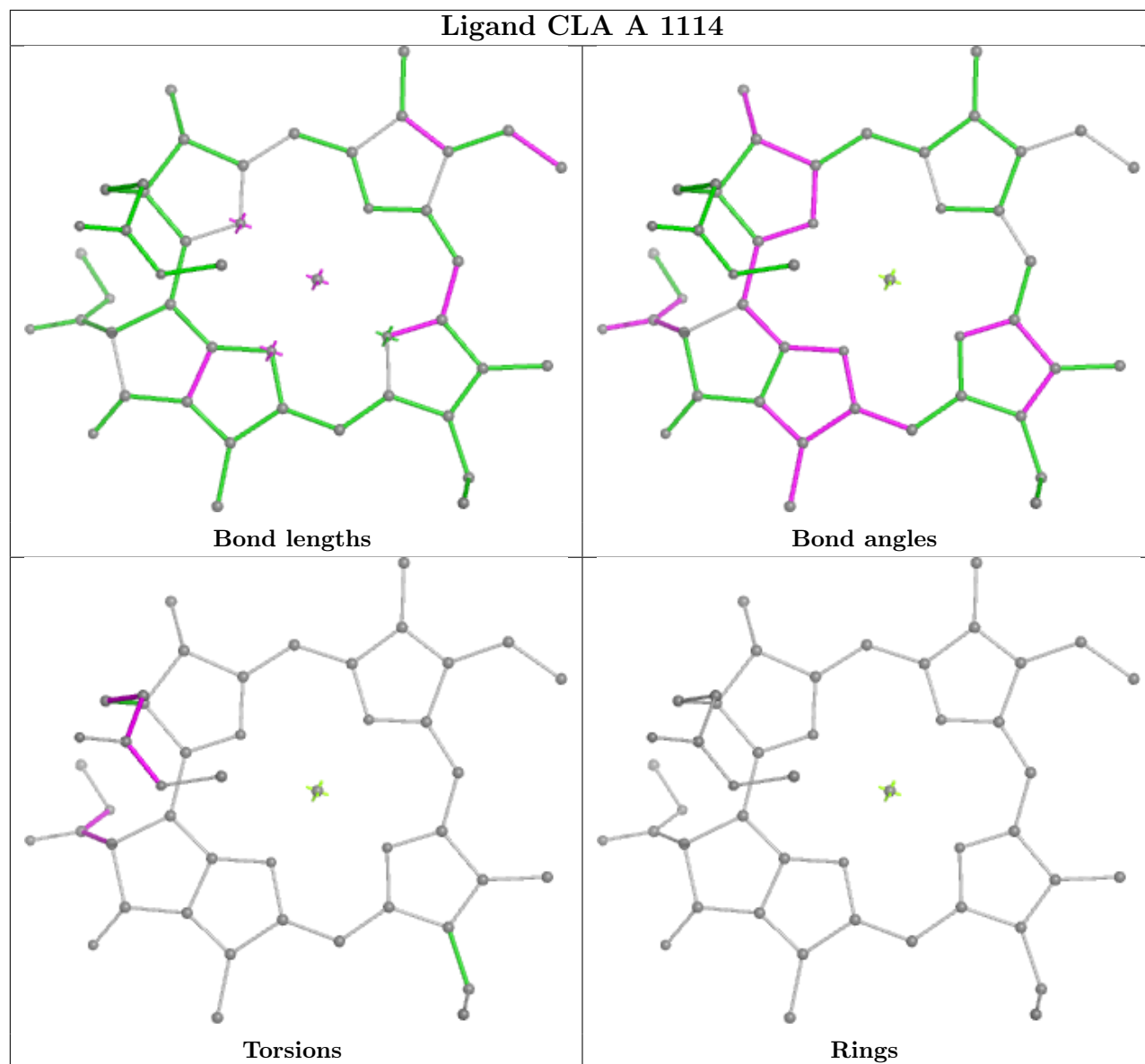


Ligand CHL 2 615

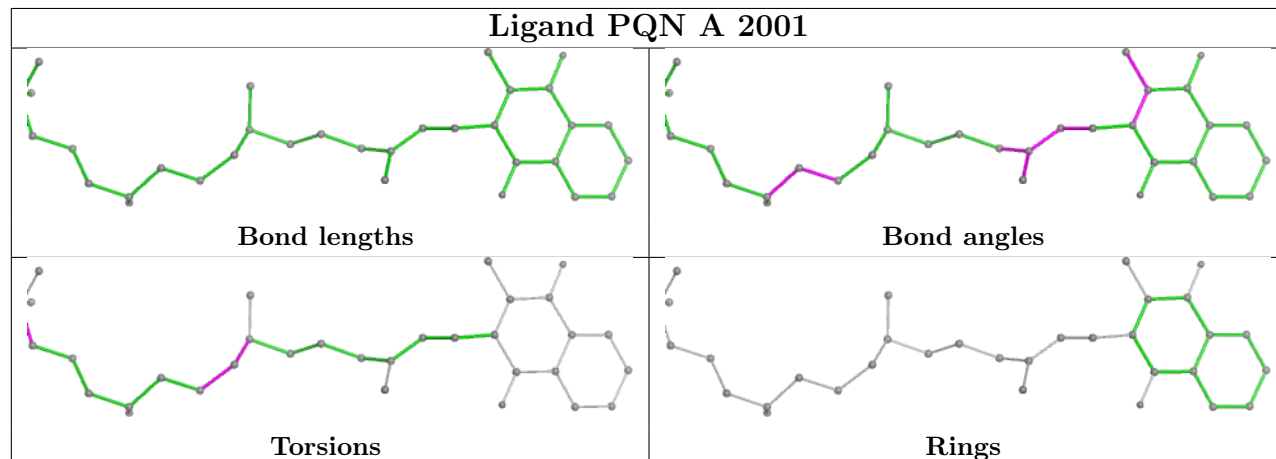


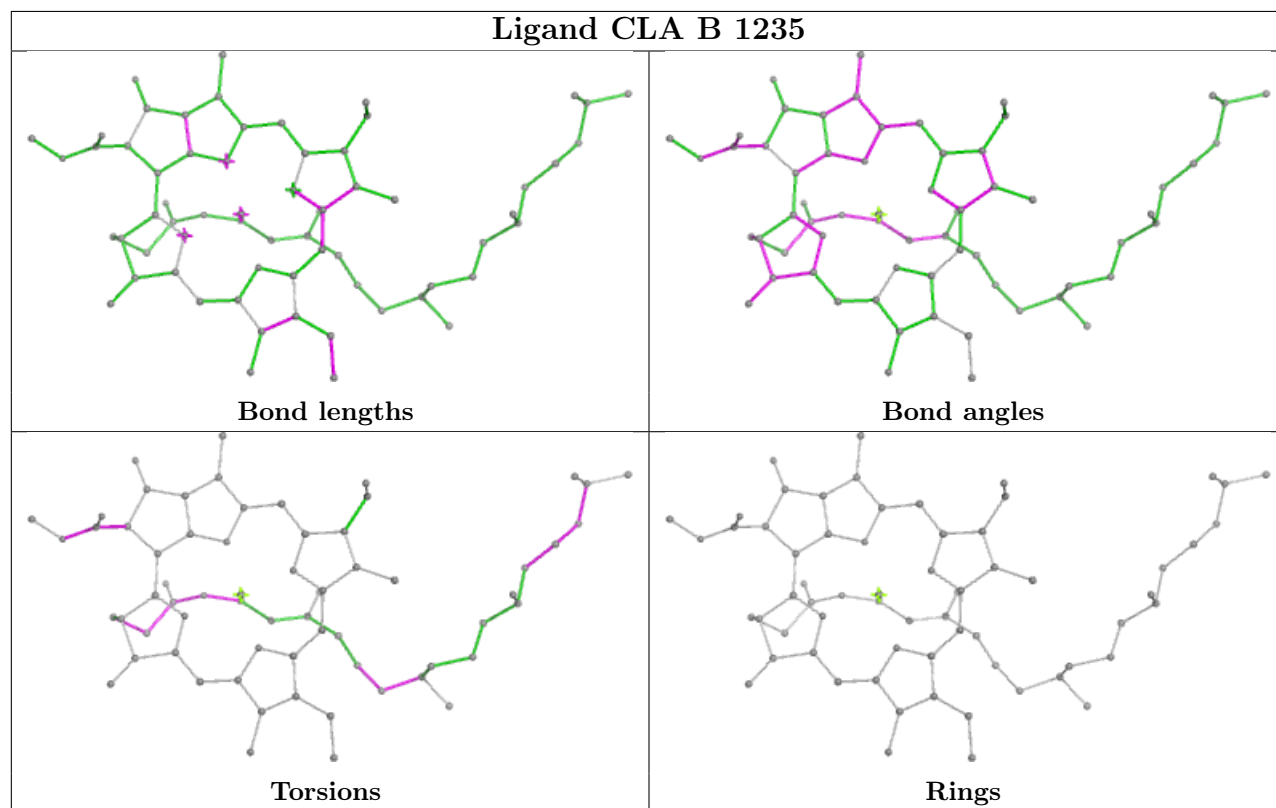
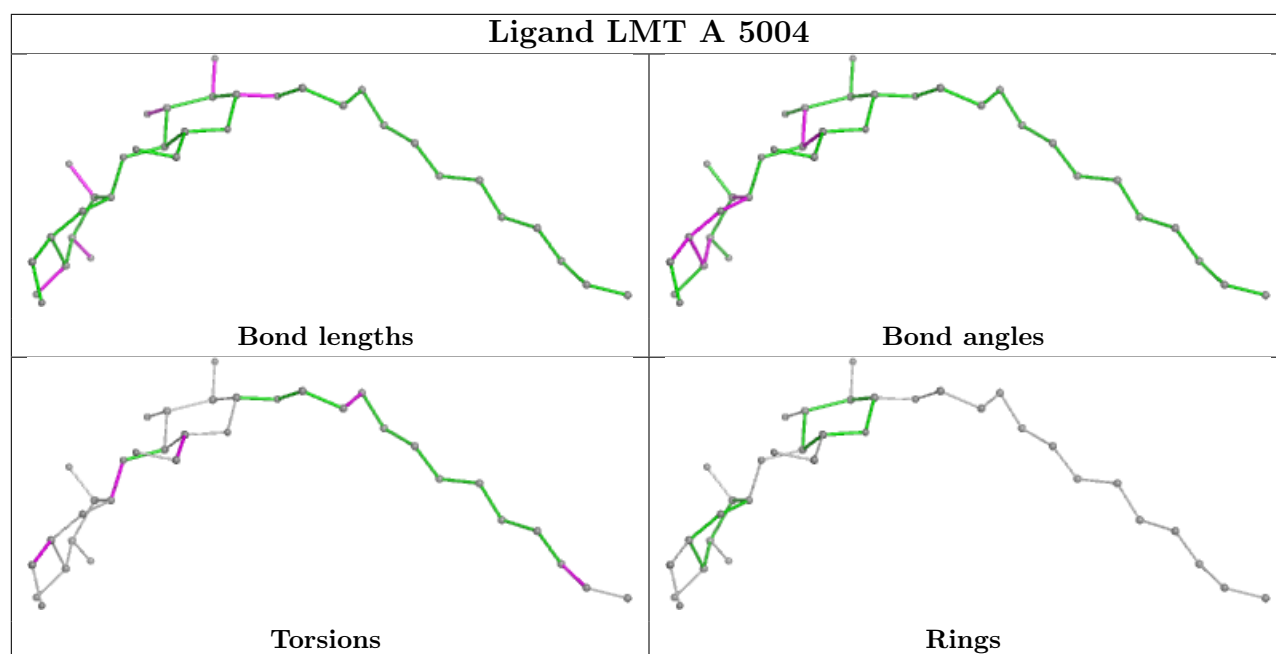


Ligand CLA A 1114

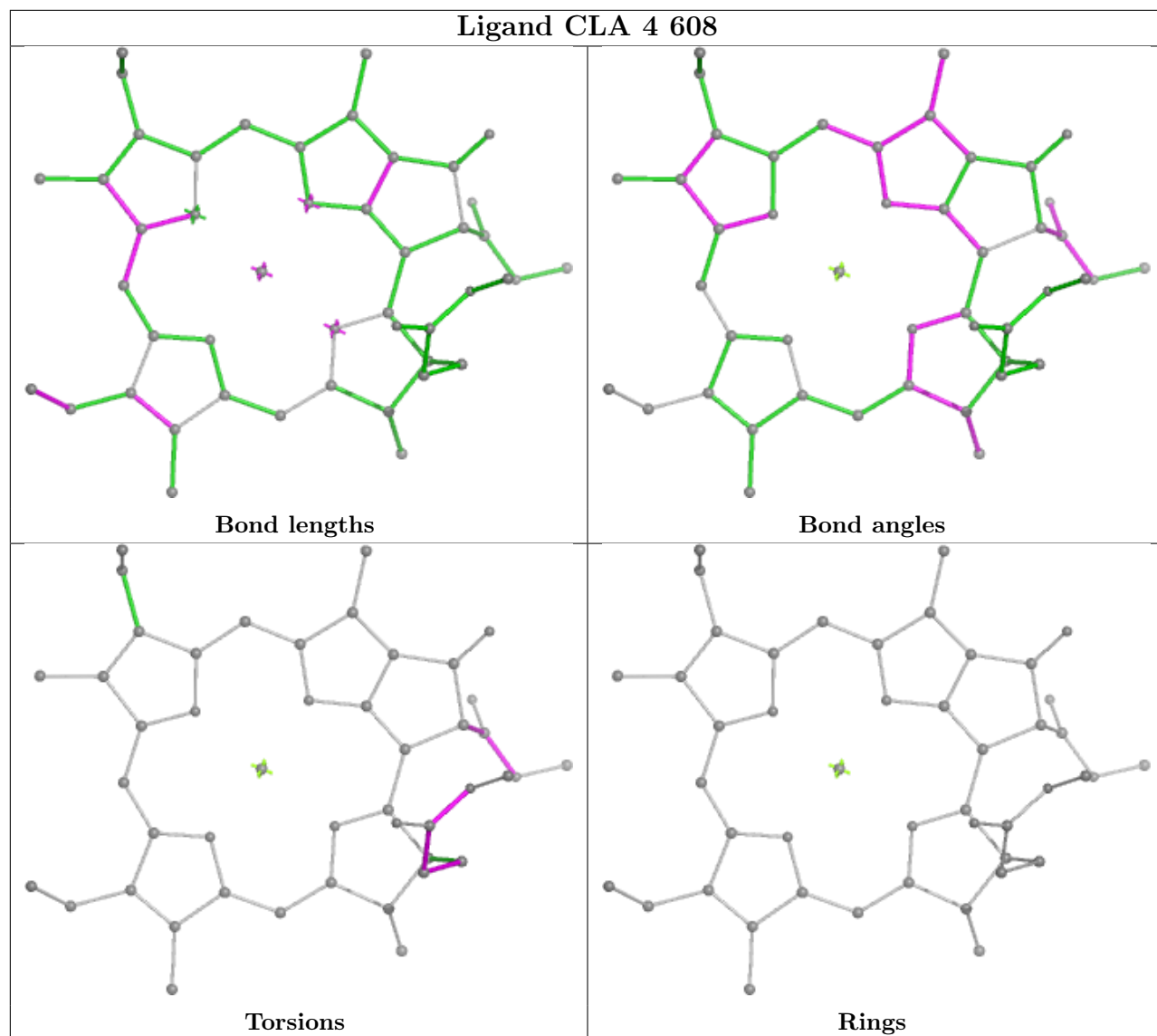


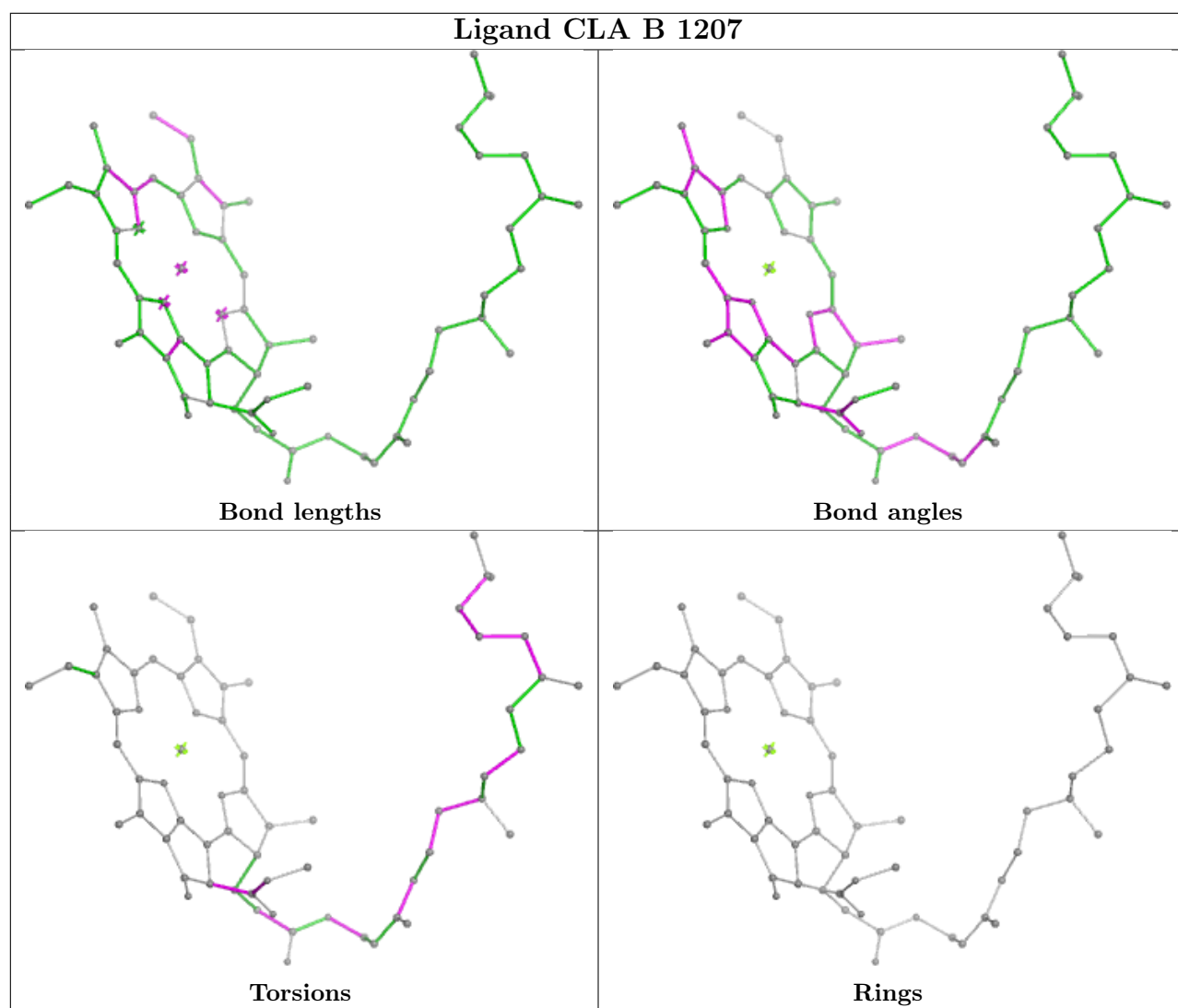
Ligand PQN A 2001

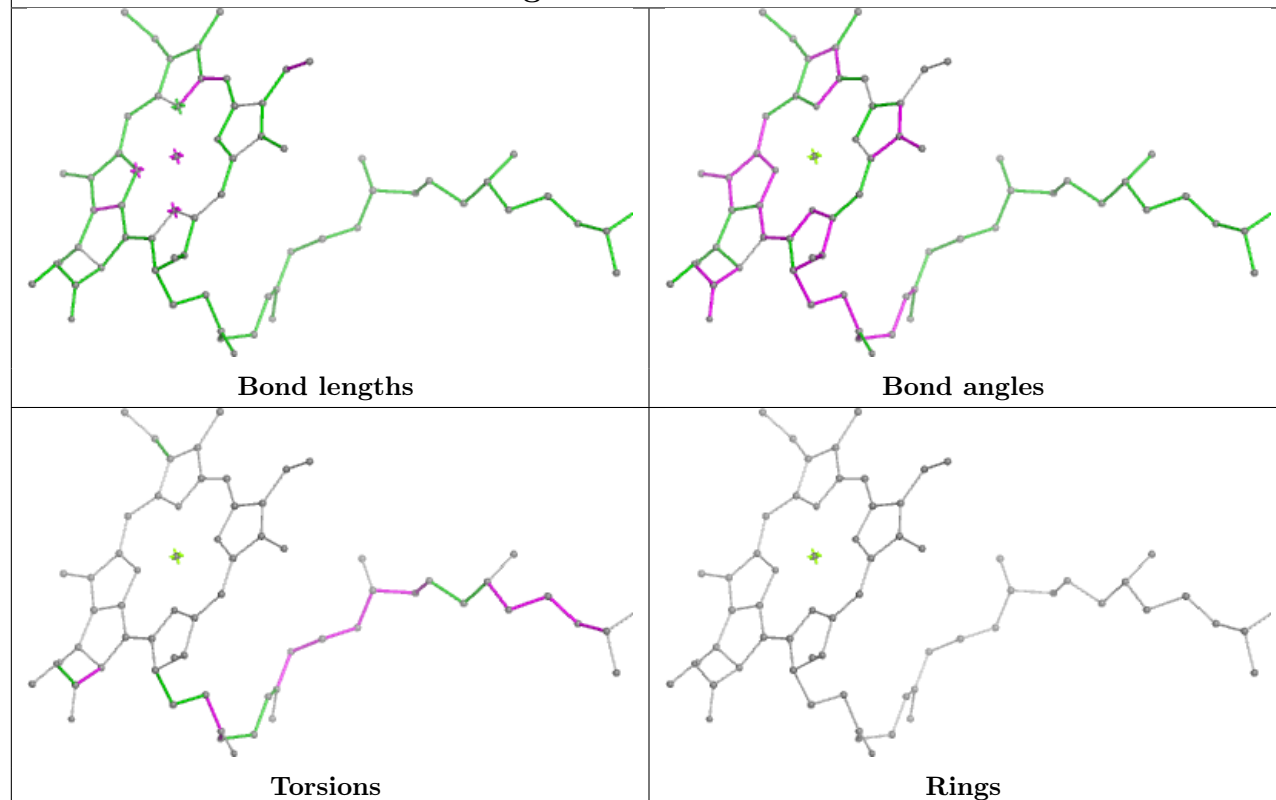
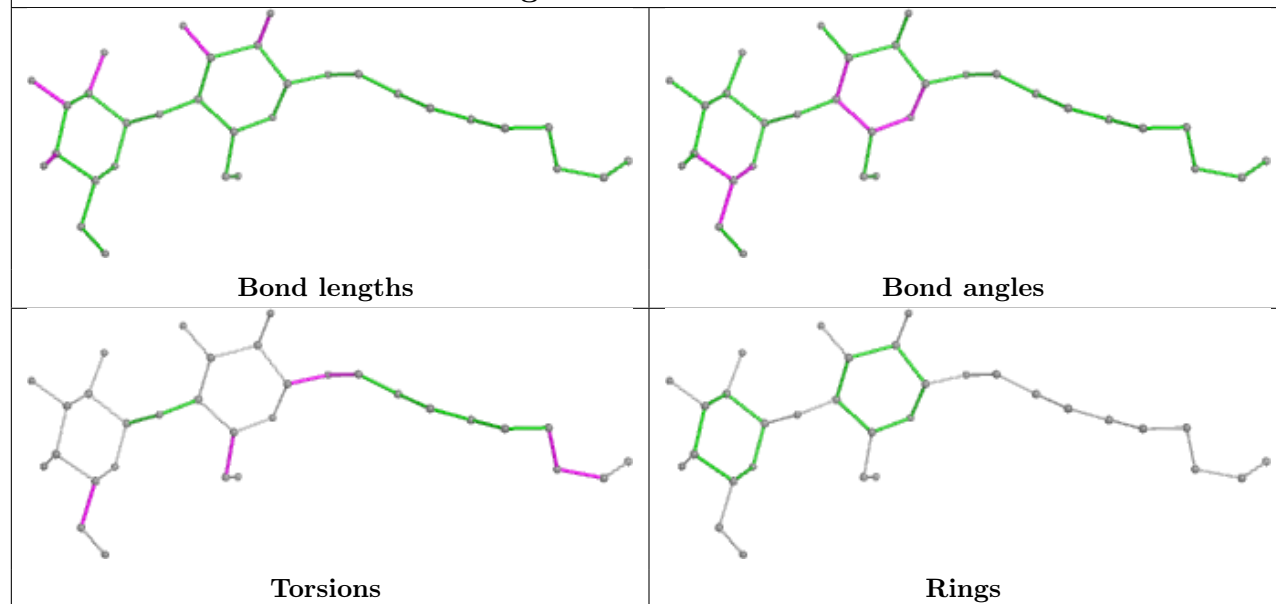


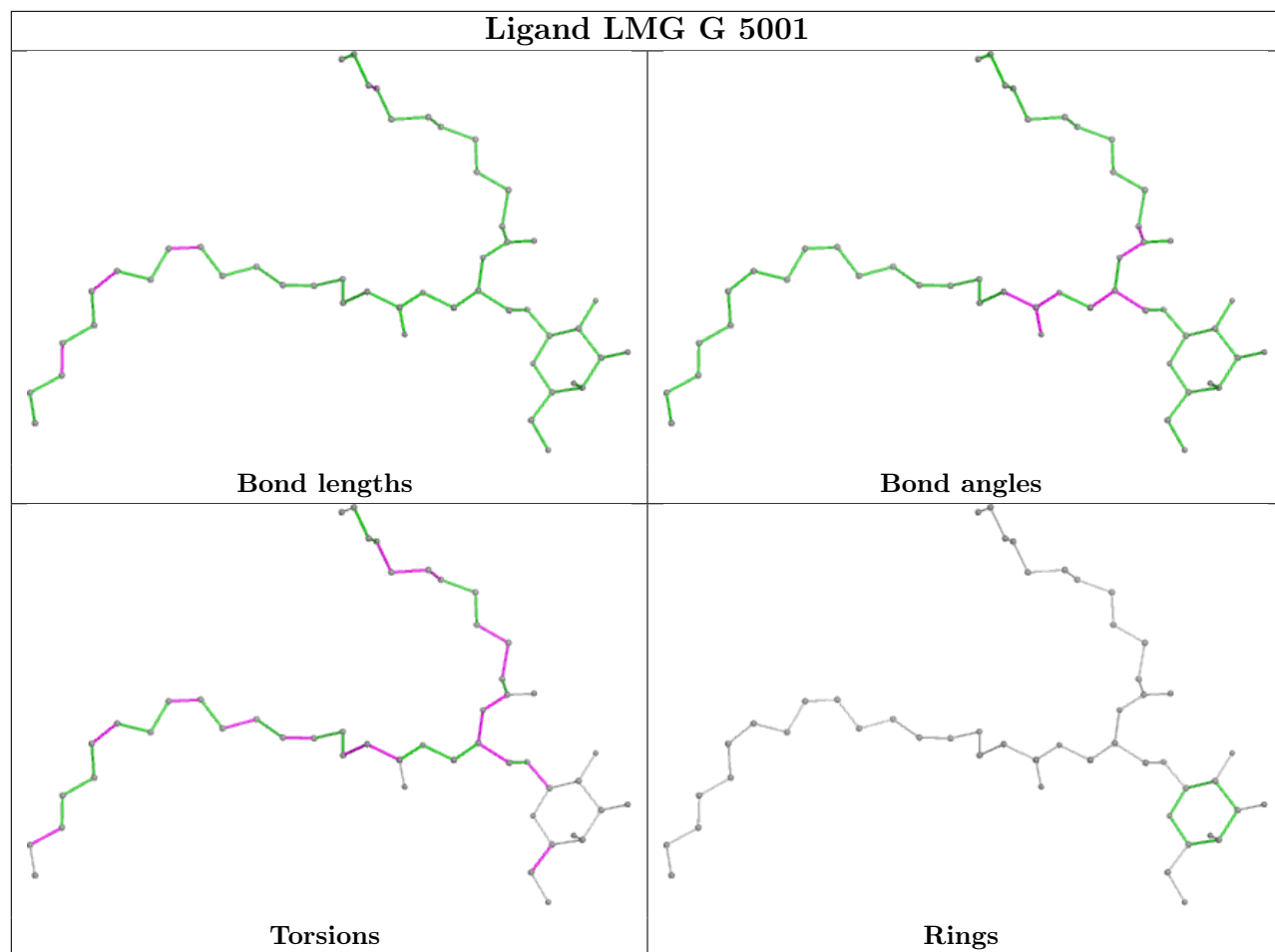


Ligand CLA 4 608

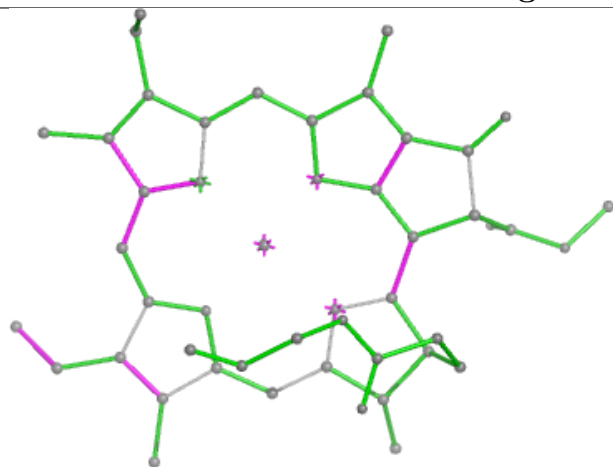




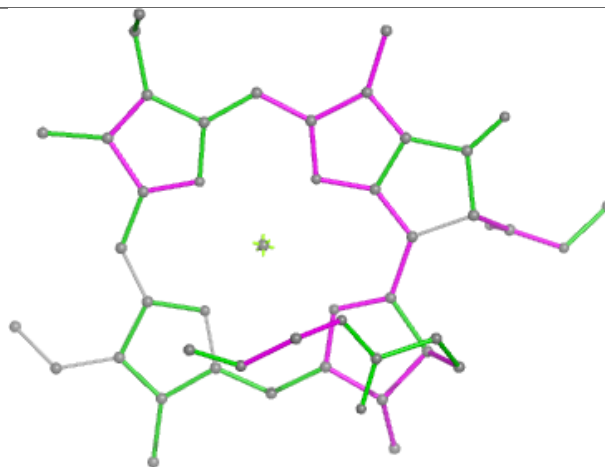
Ligand CLA B 1211**Ligand LMT B 5006**



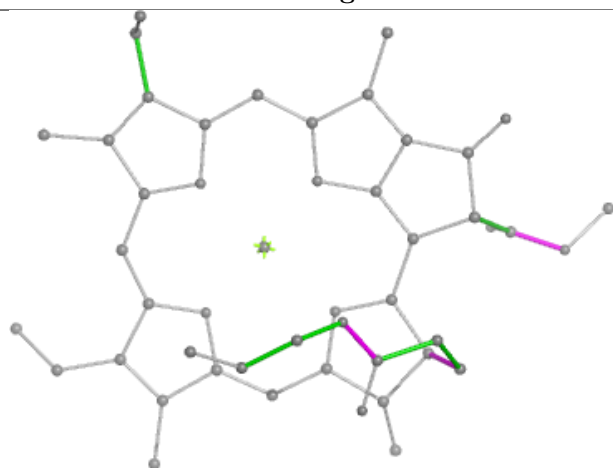
Ligand CLA 3 608



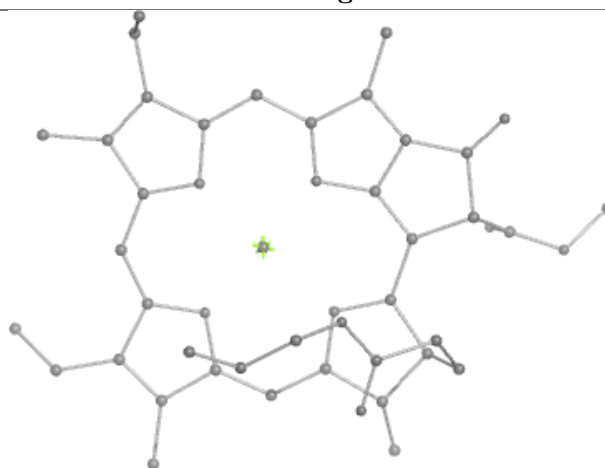
Bond lengths



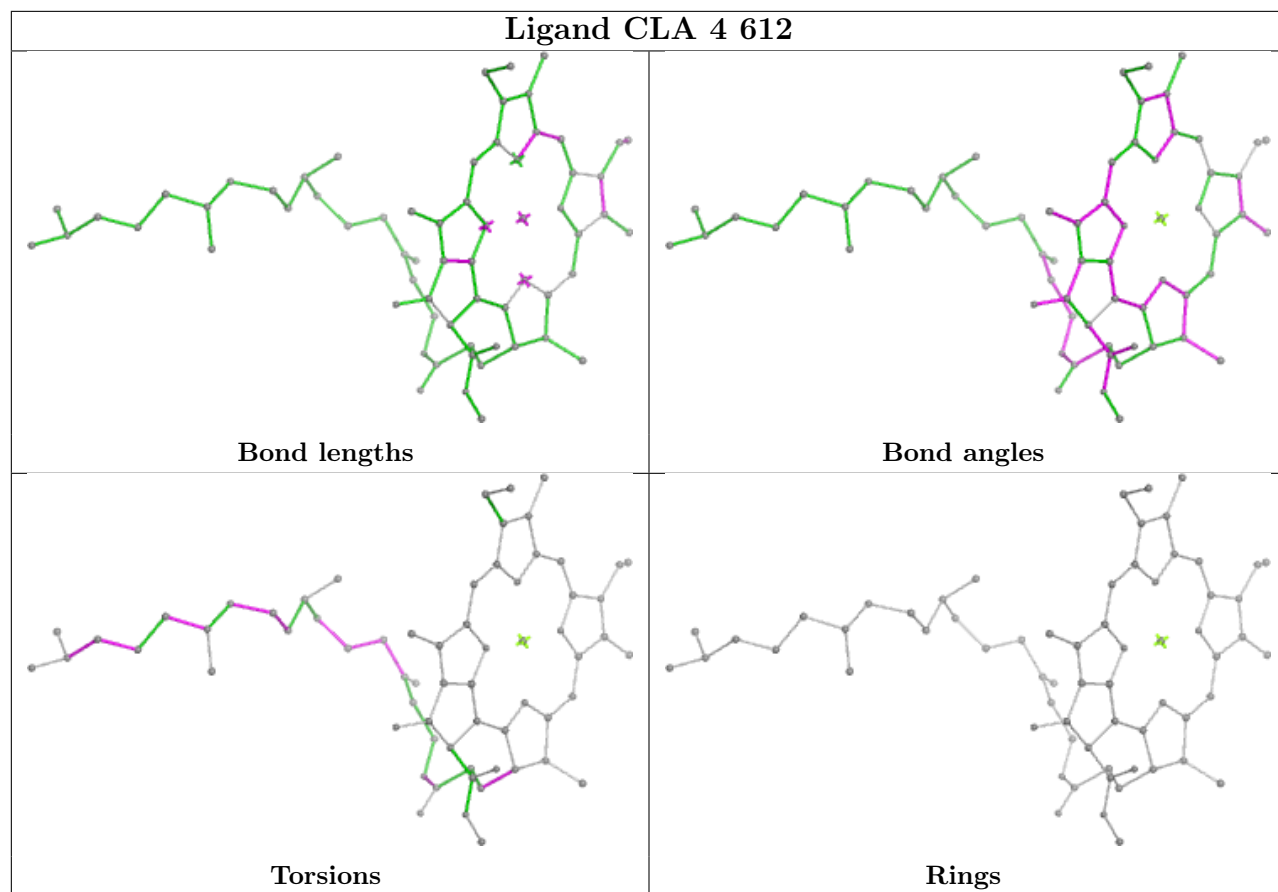
Bond angles



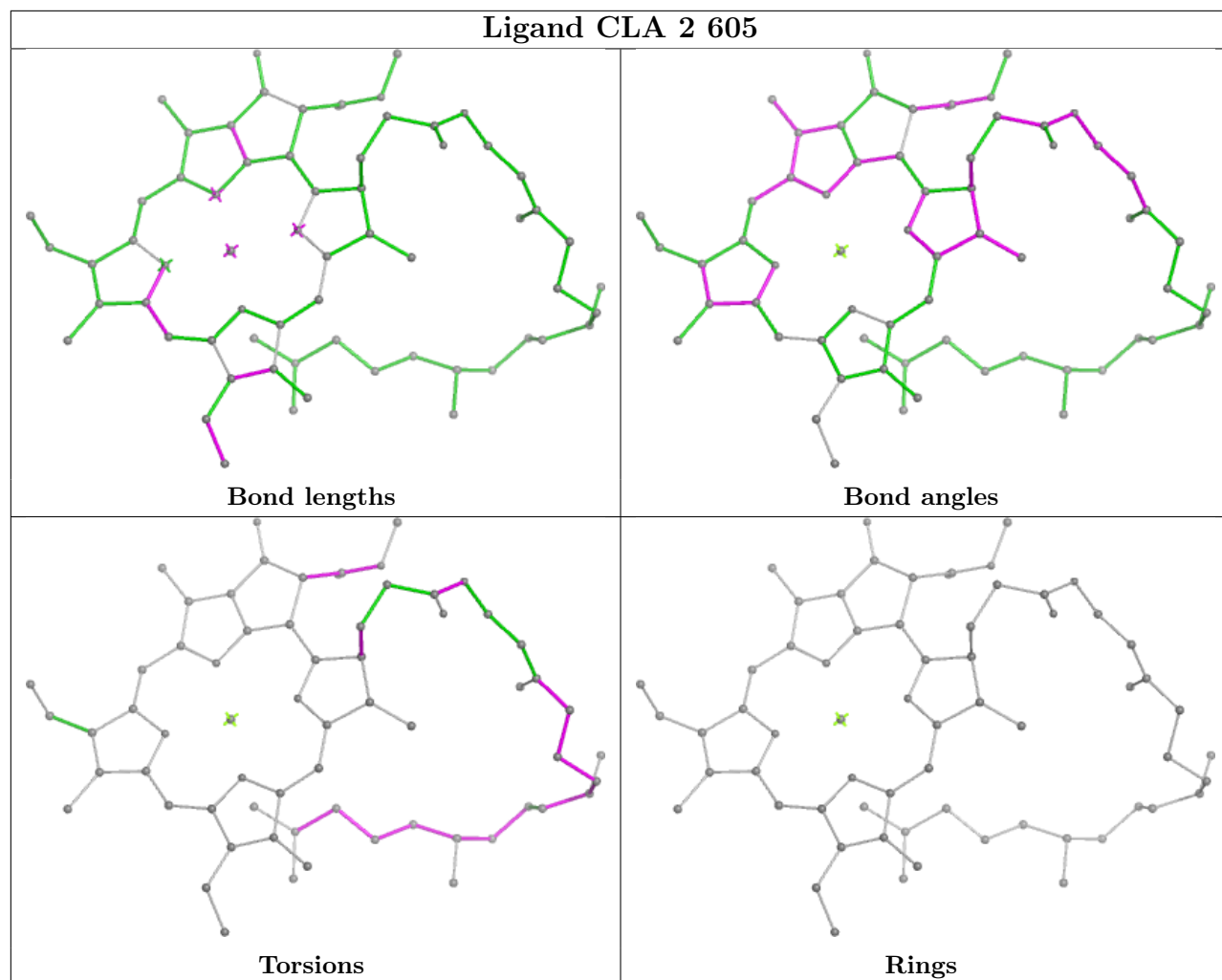
Torsions

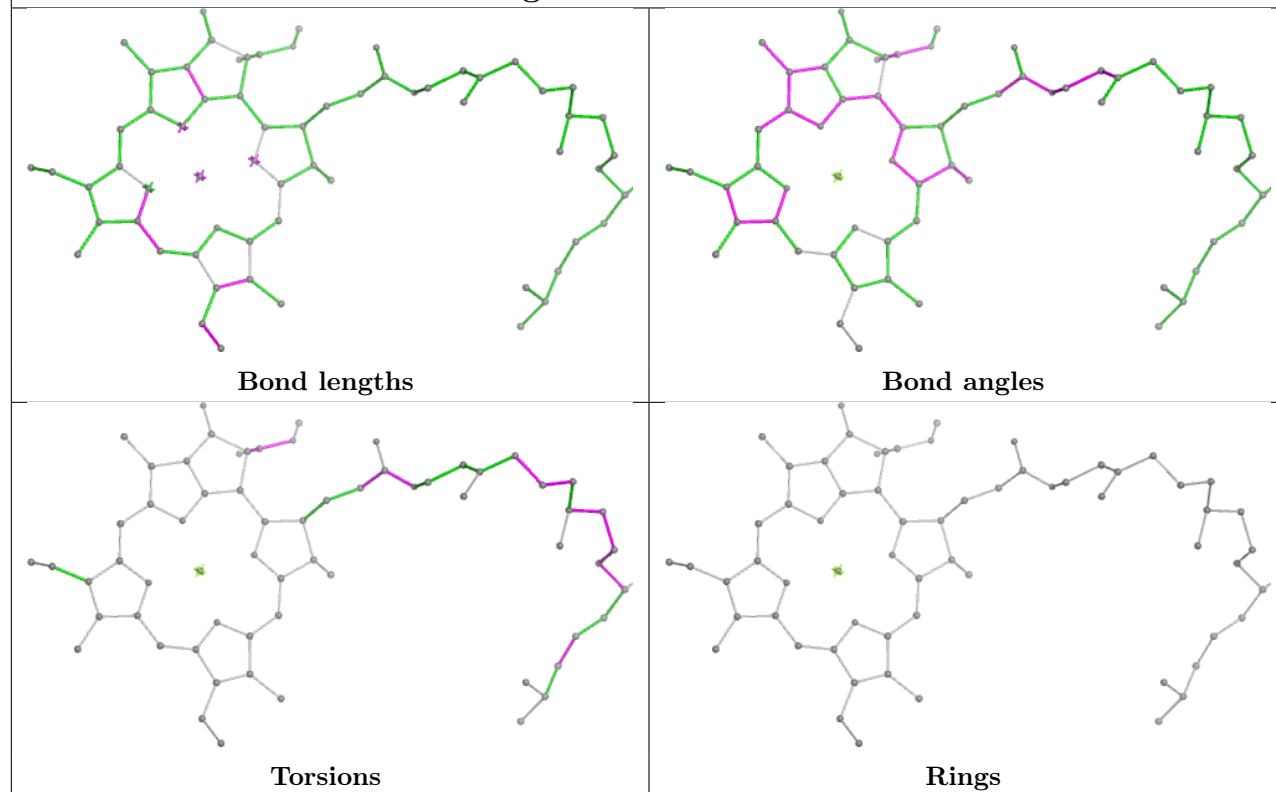
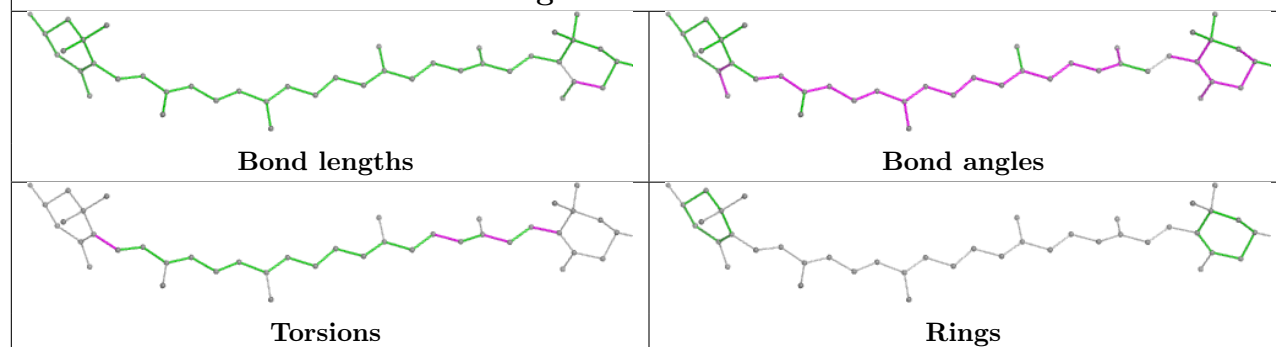


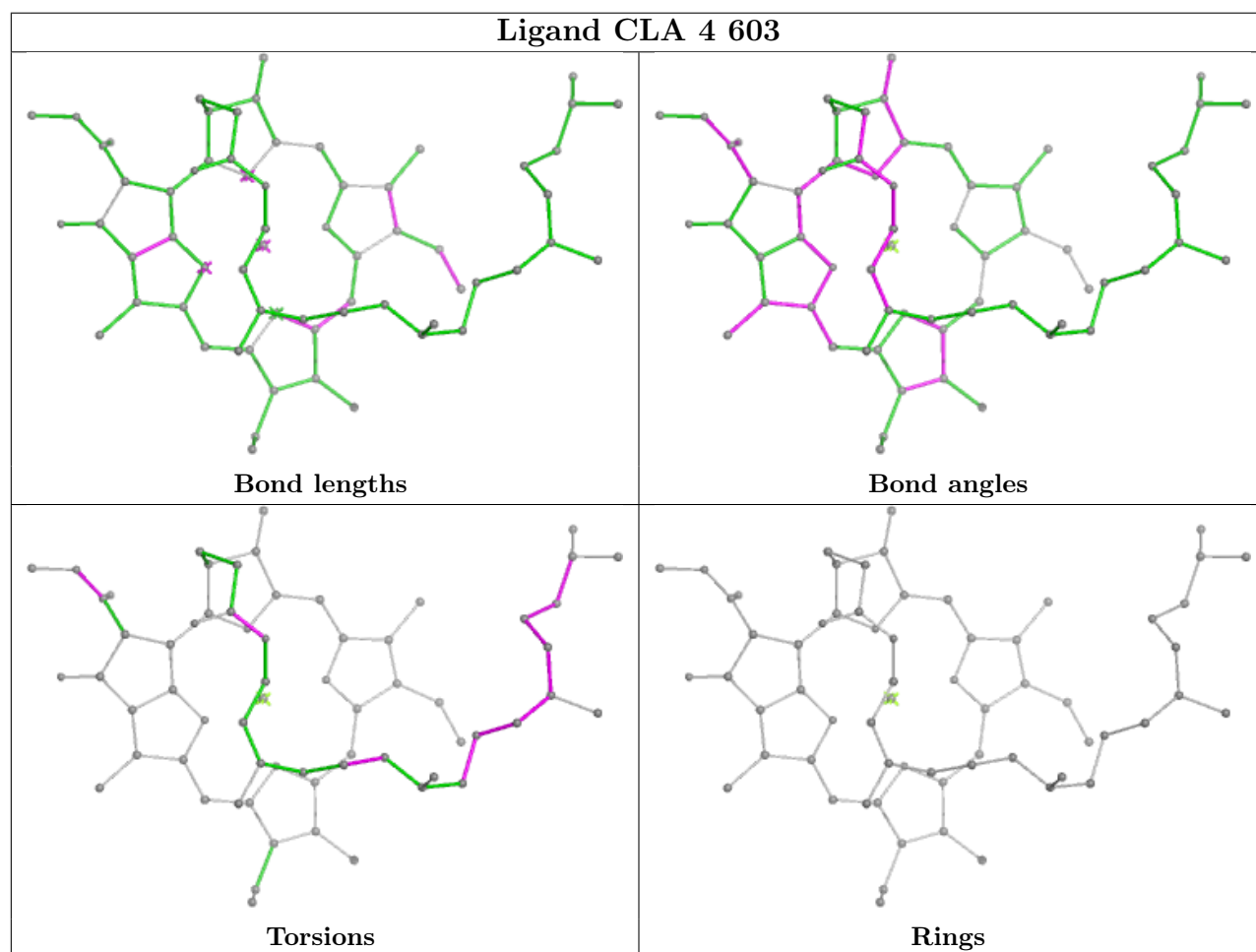
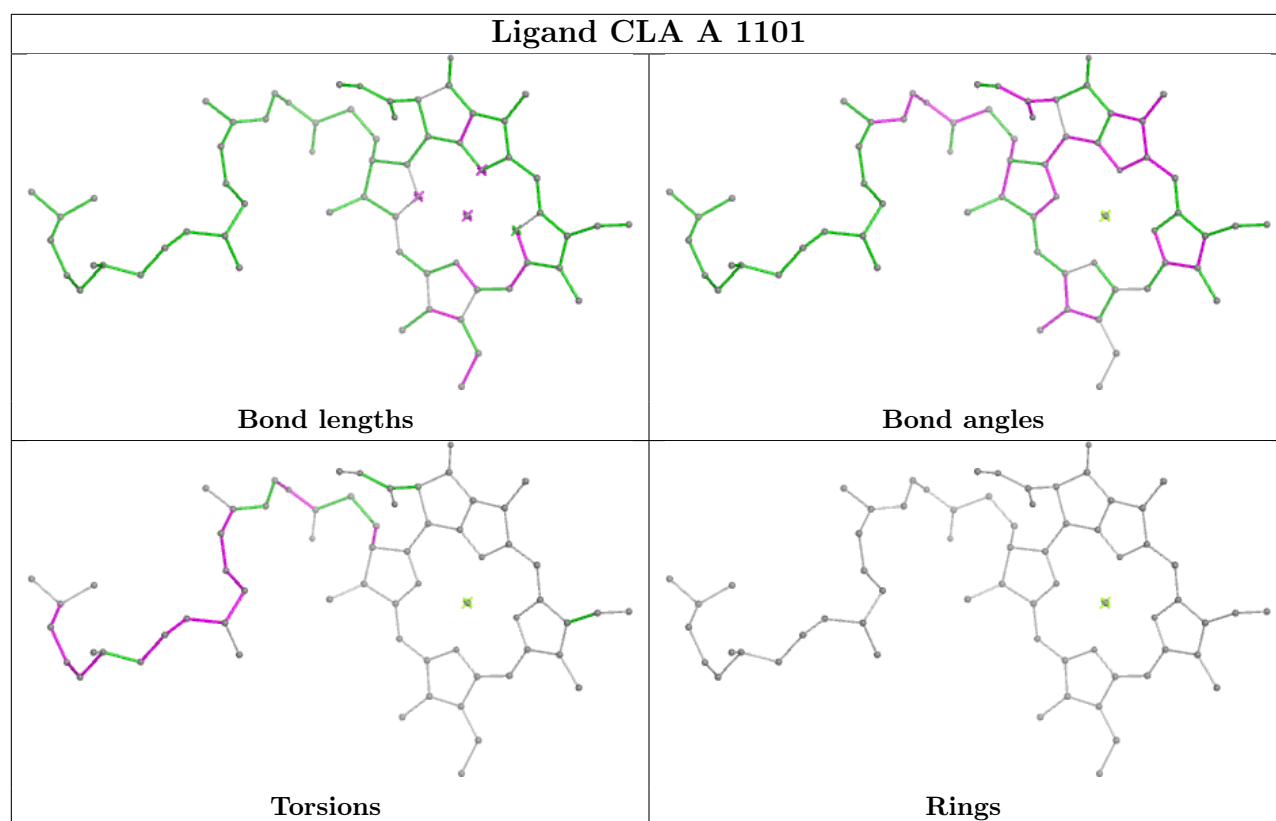
Rings

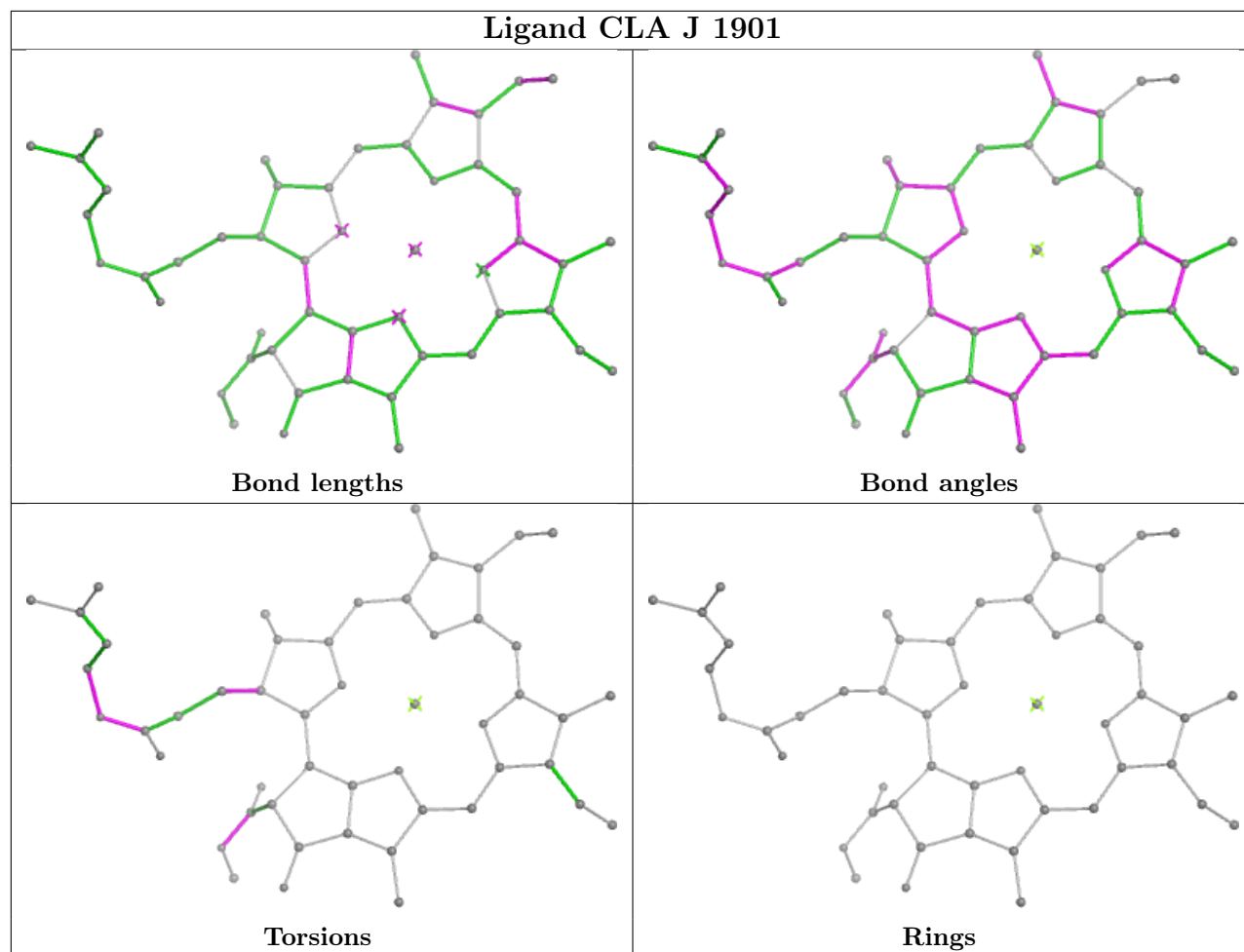


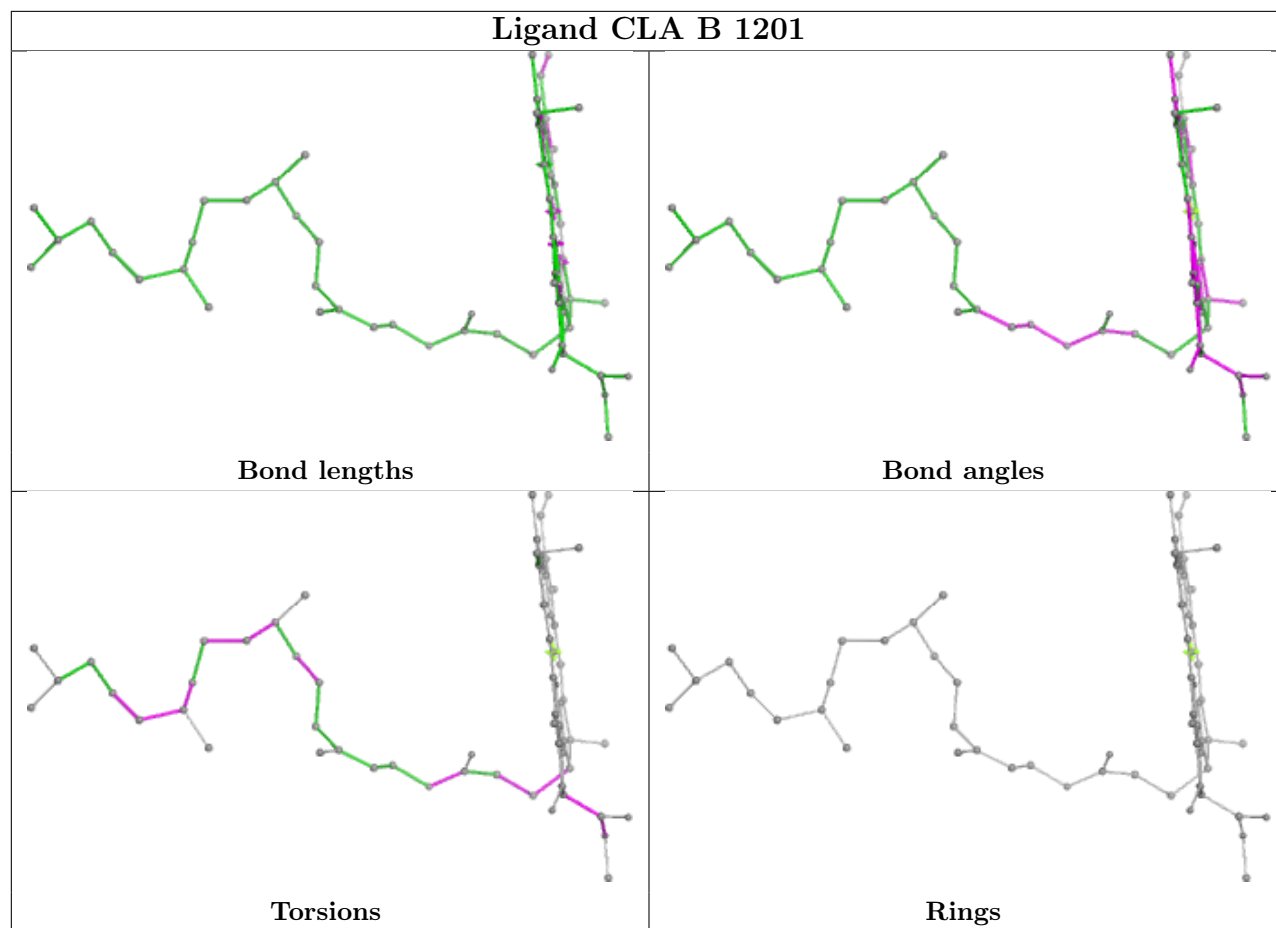
Ligand CLA 2 605

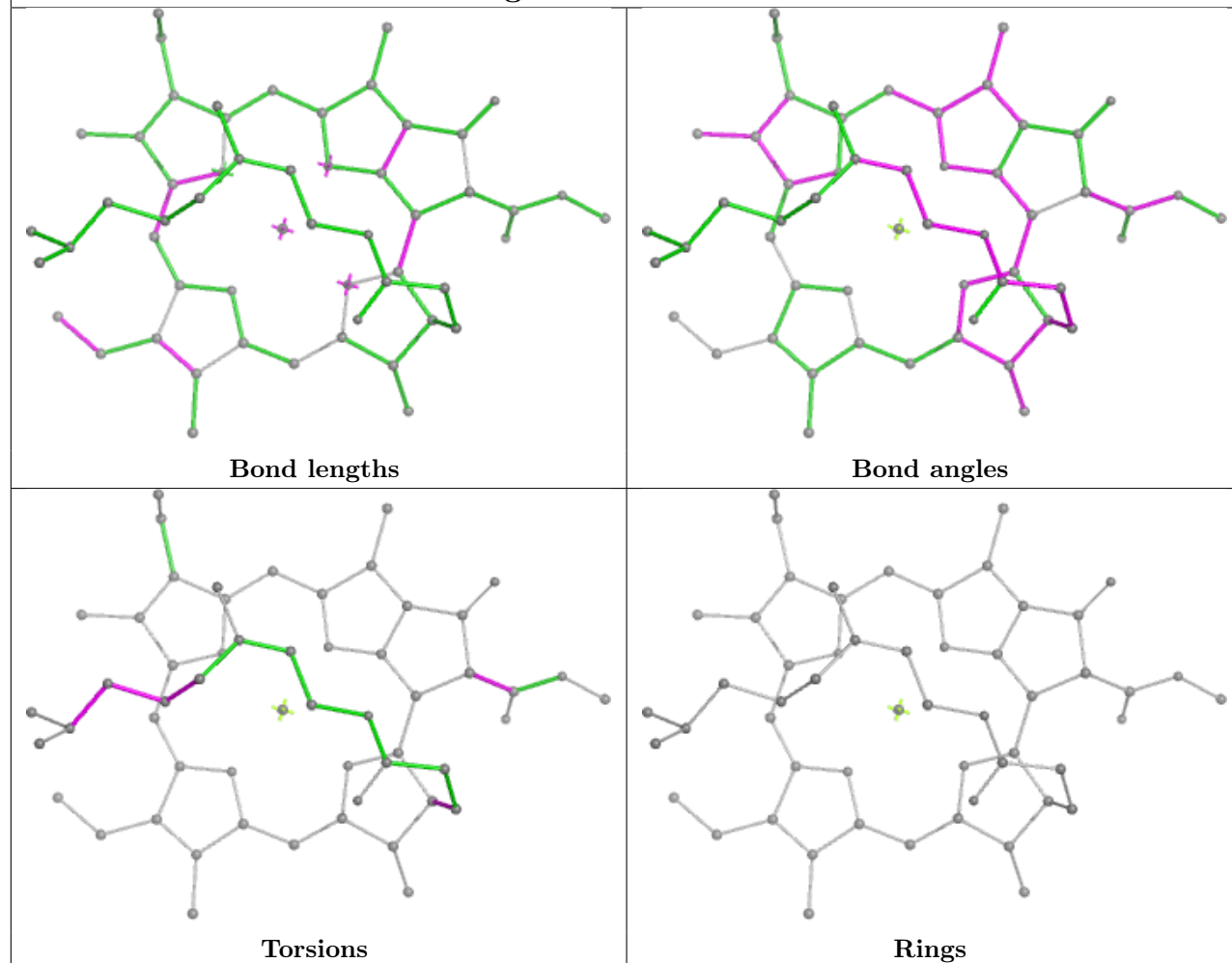
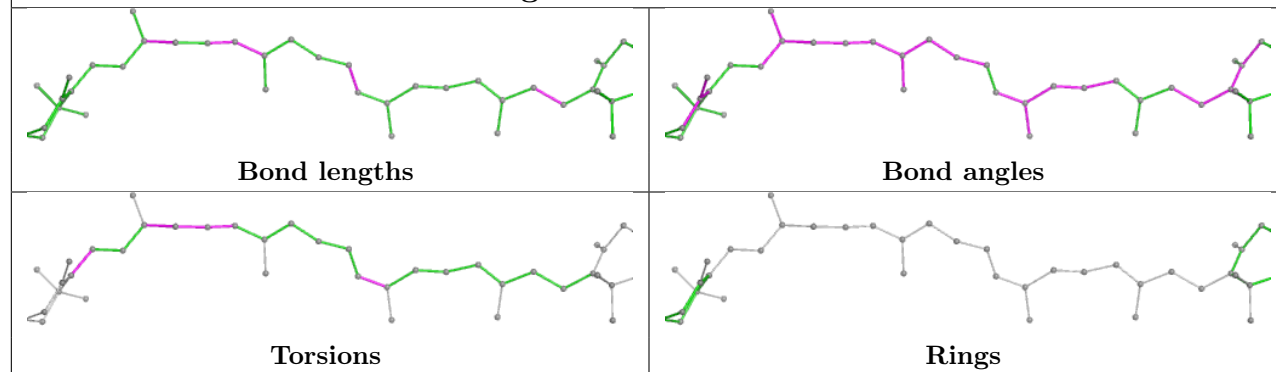


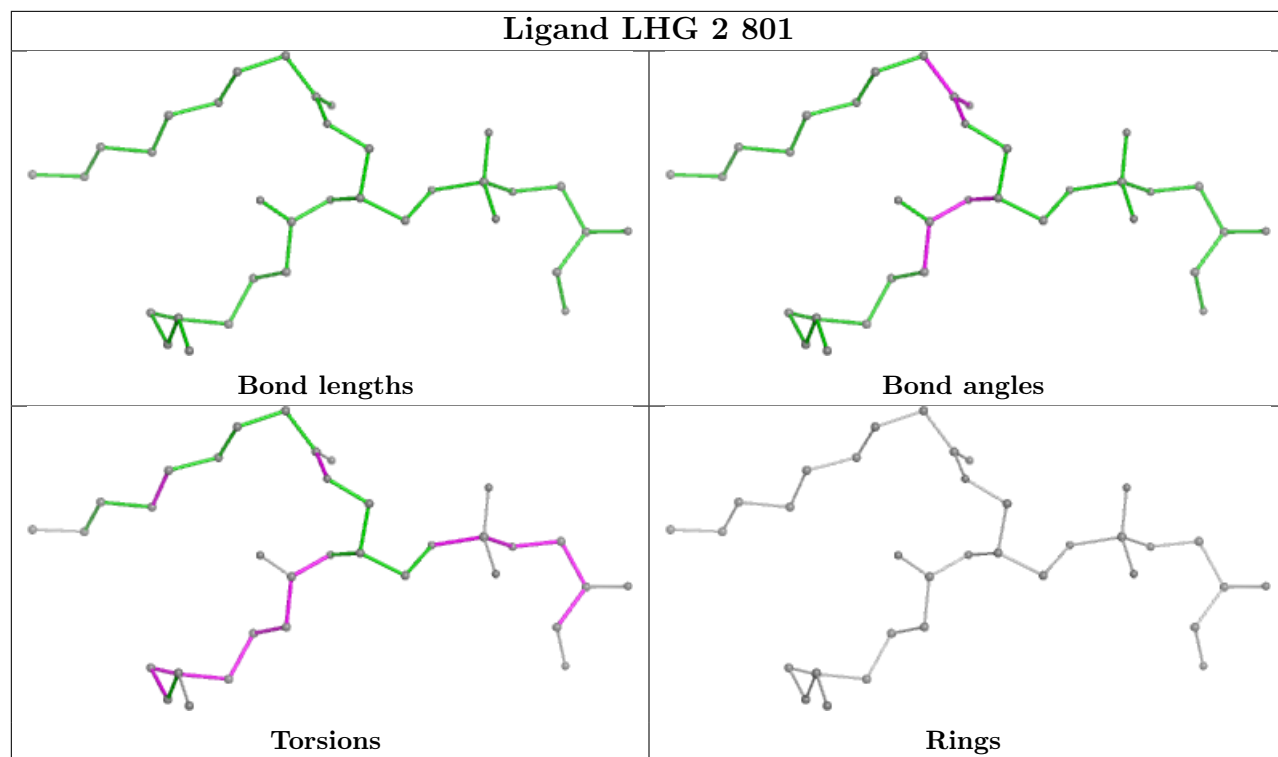
Ligand CLA A 1125**Ligand LUT 4 501**



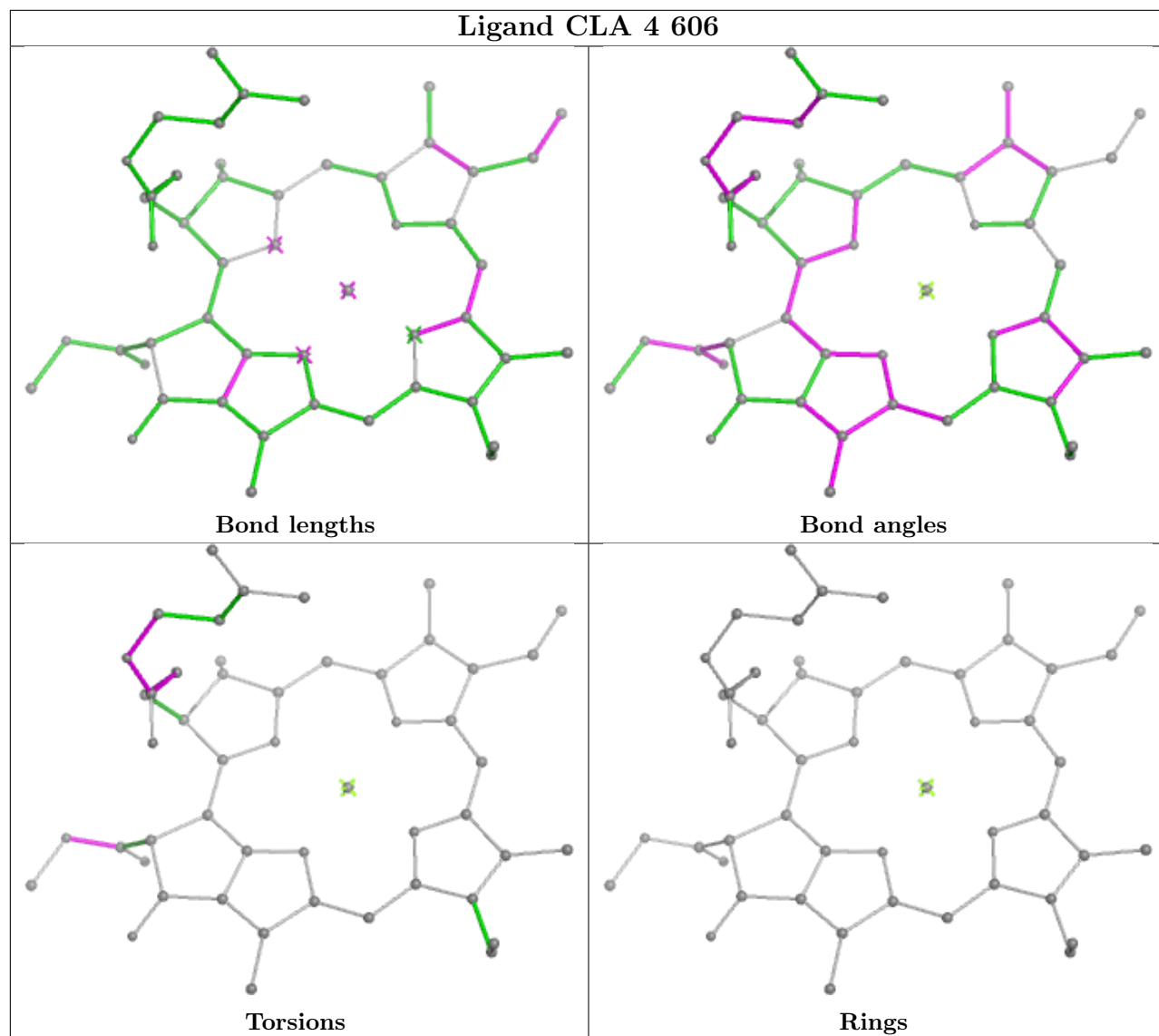


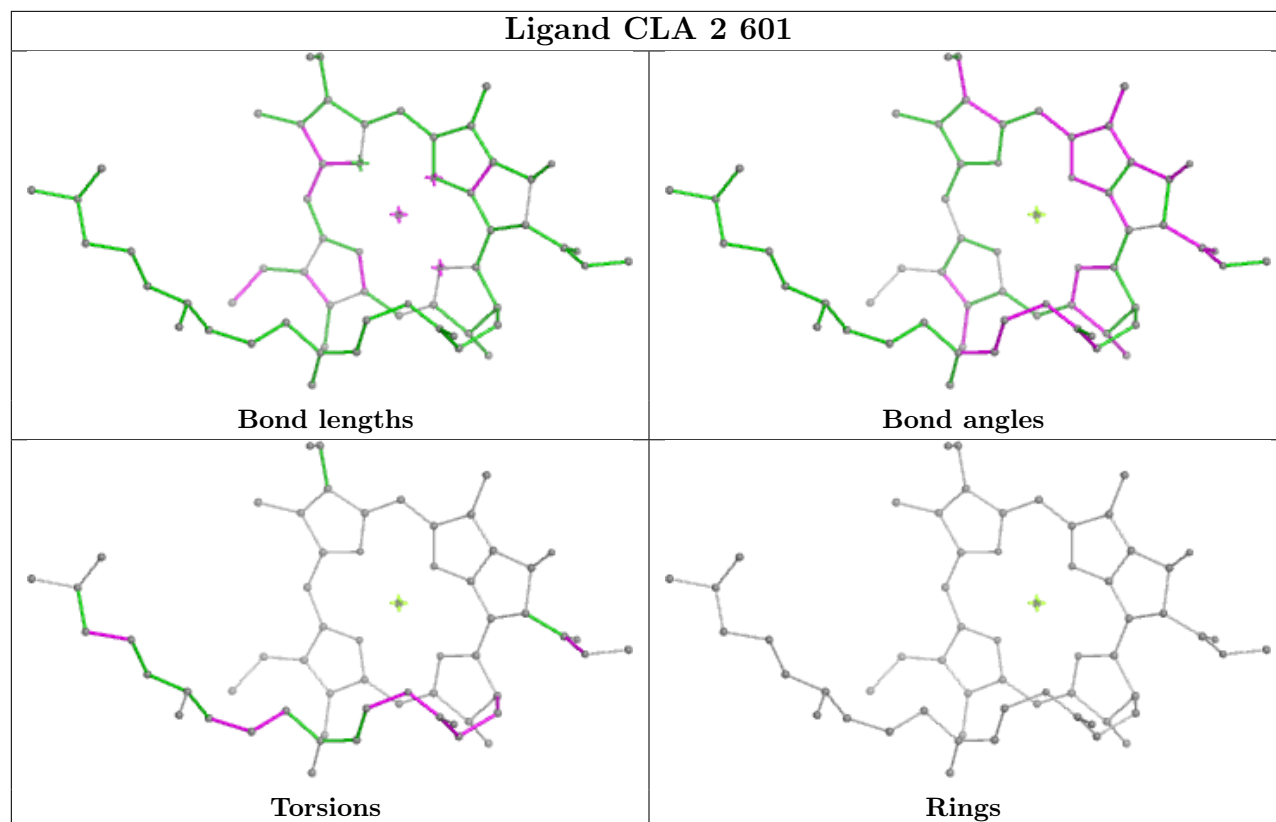
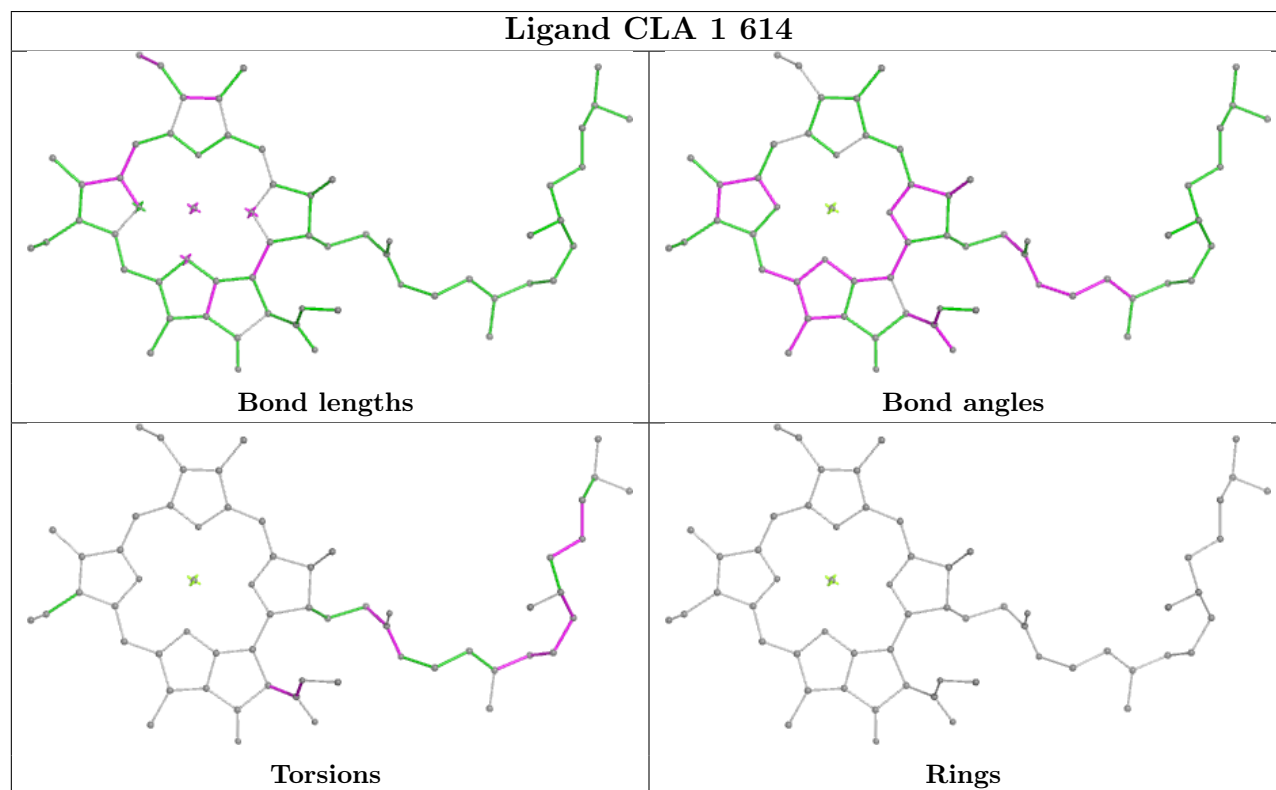


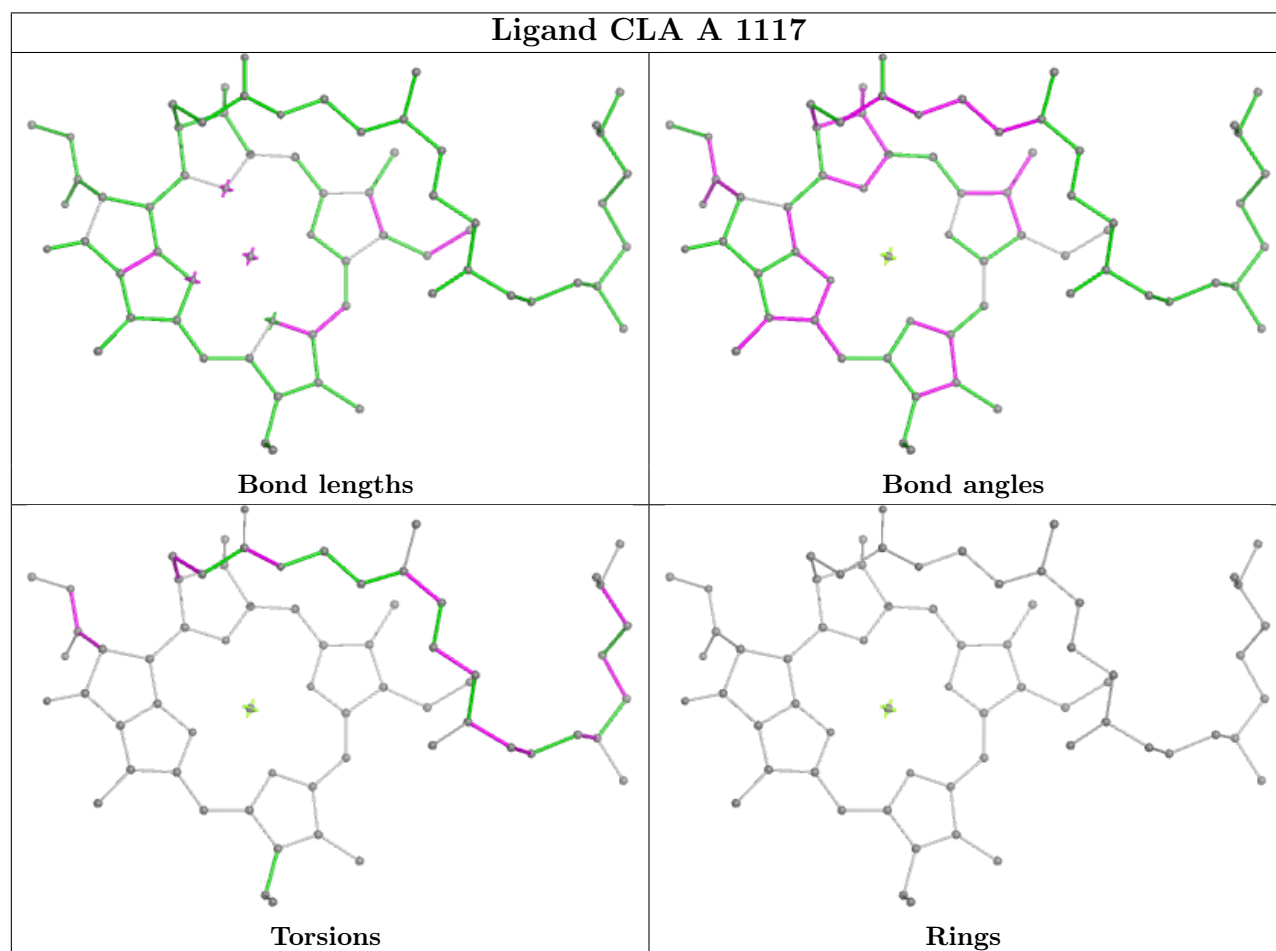
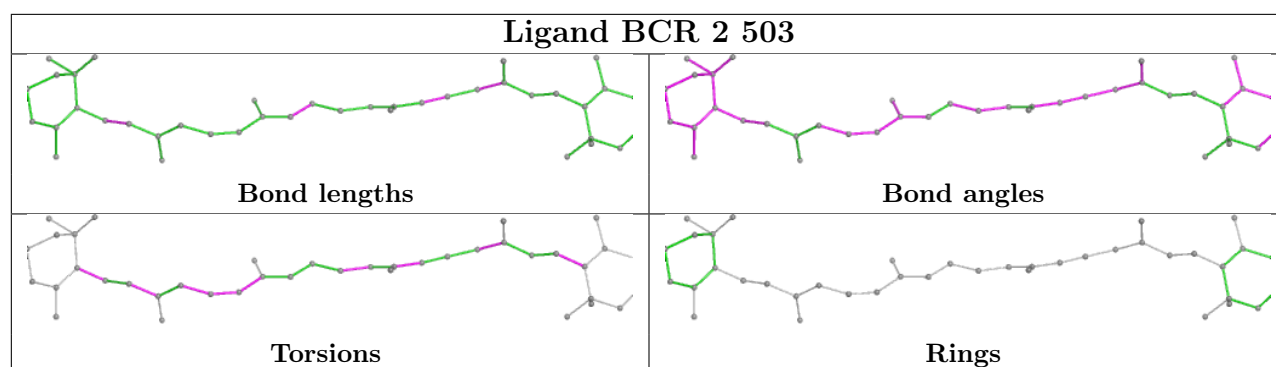
Ligand CLA A 1110**Ligand BCR A 4017**

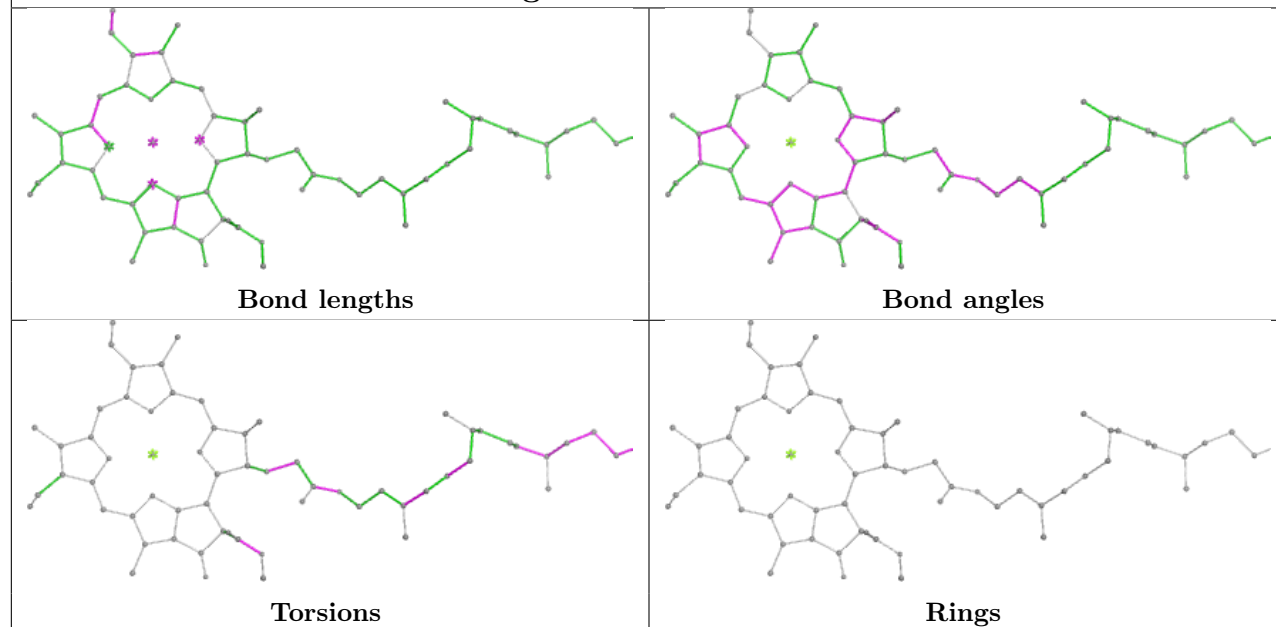
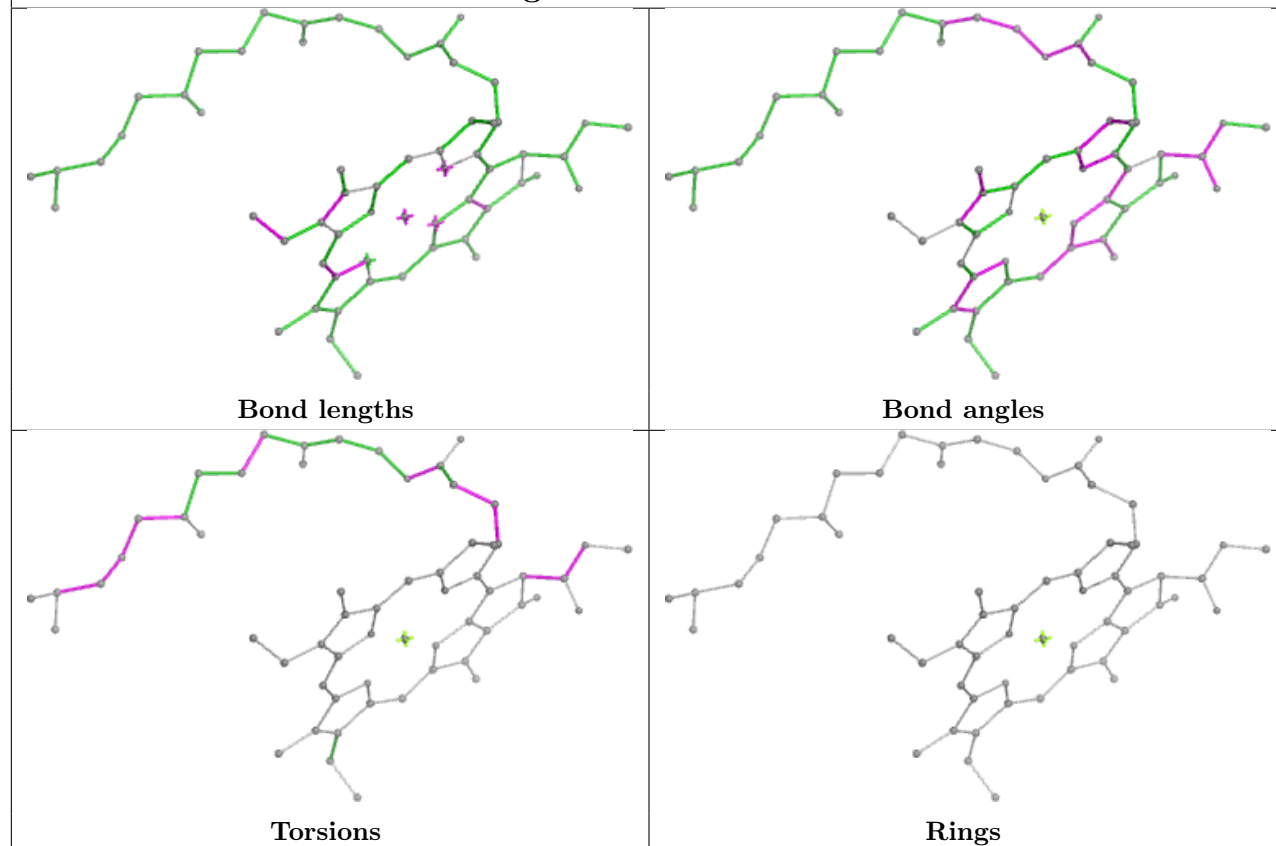


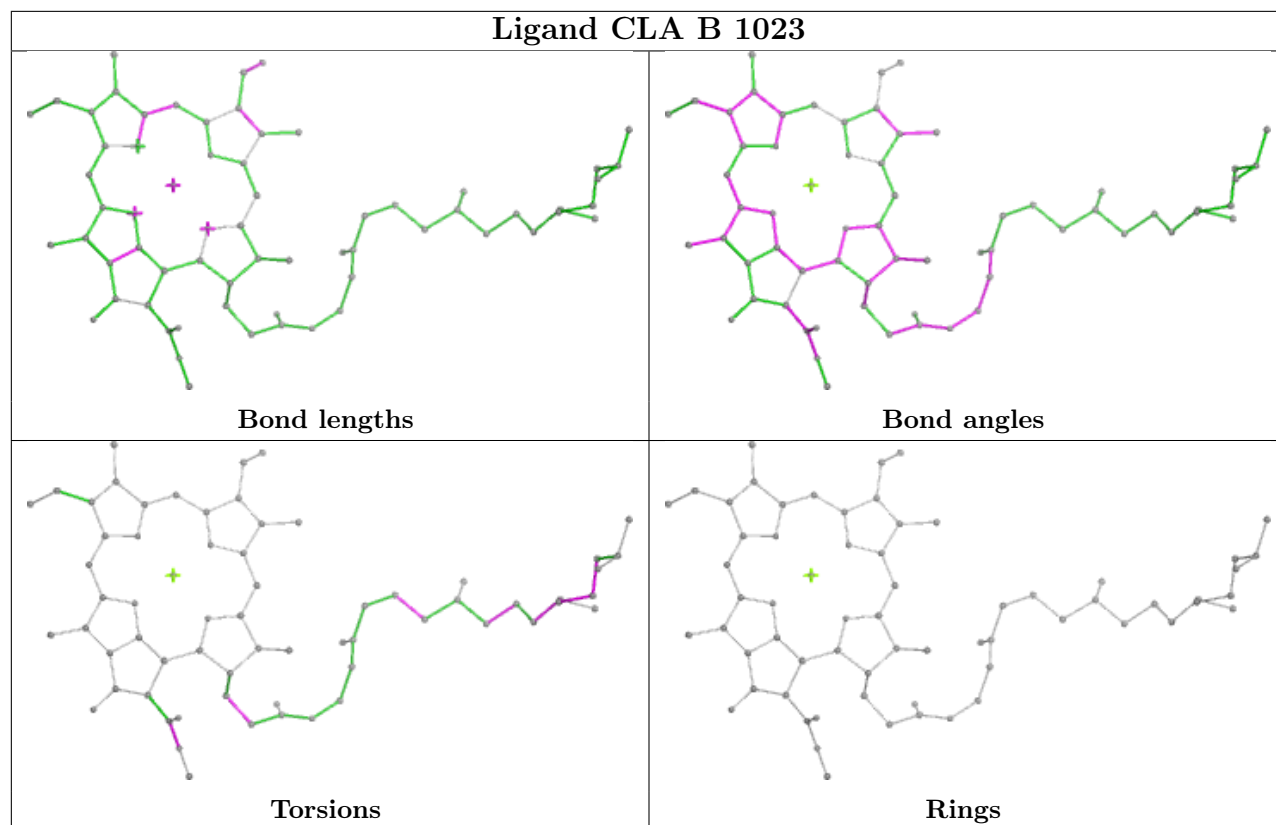
Ligand CLA 4 606



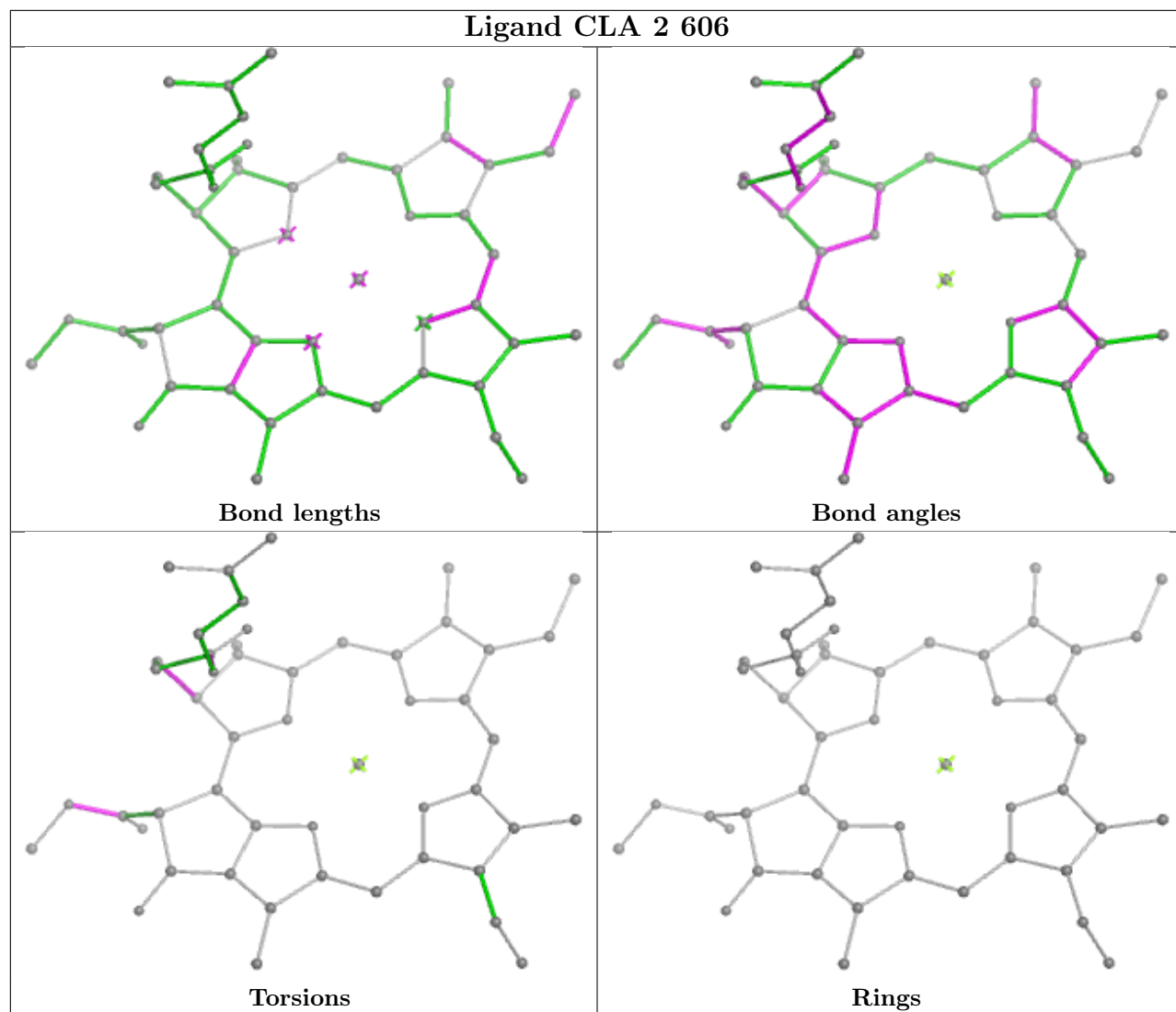
Ligand CLA 2 601**Ligand CLA 1 614**



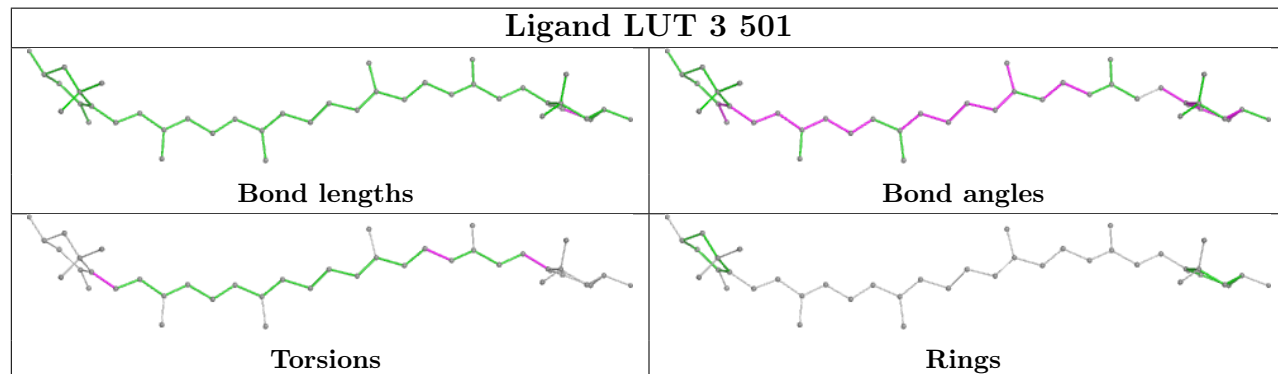
Ligand CLA A 1131**Ligand CLA B 1228**

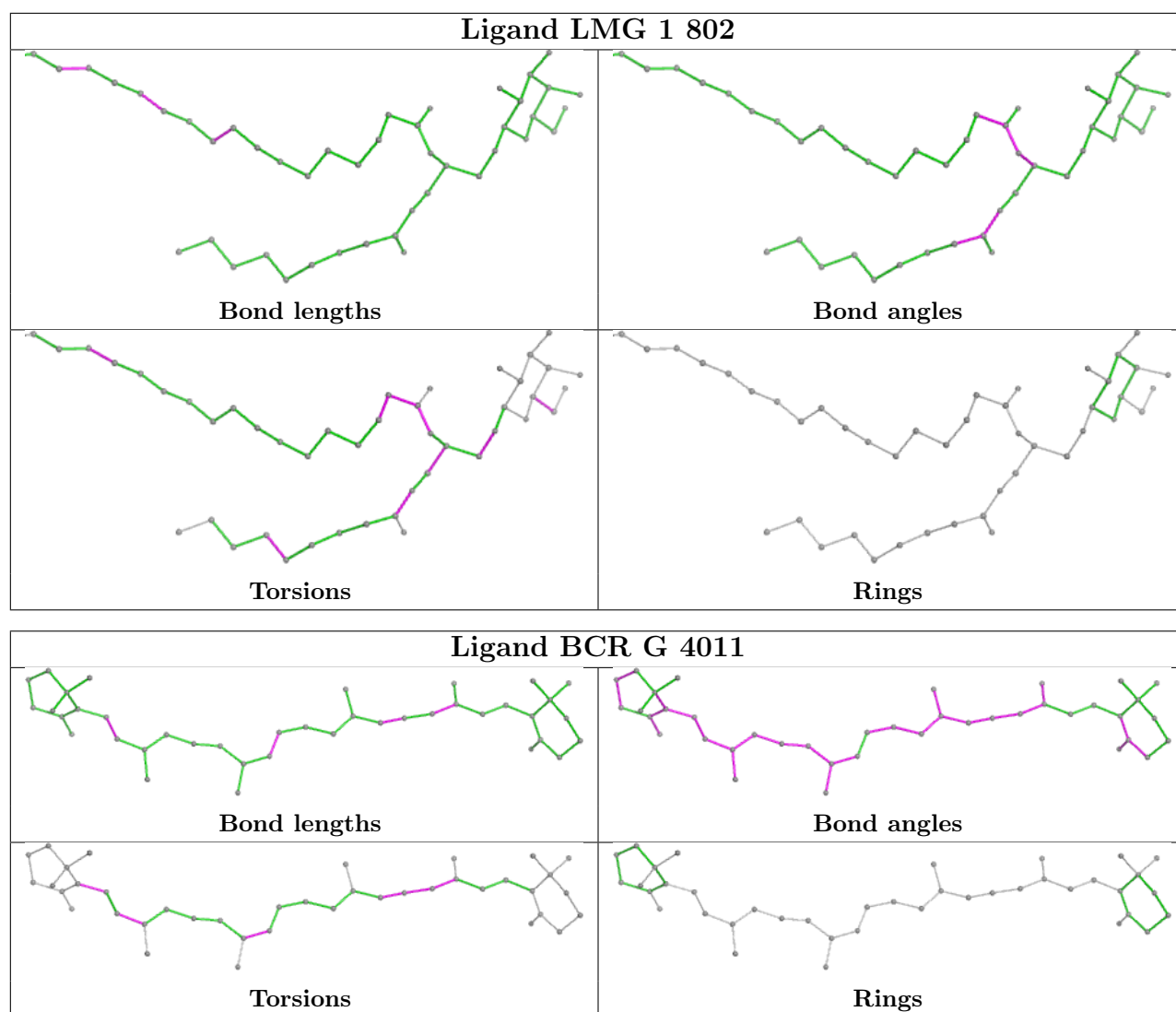


Ligand CLA 2 606

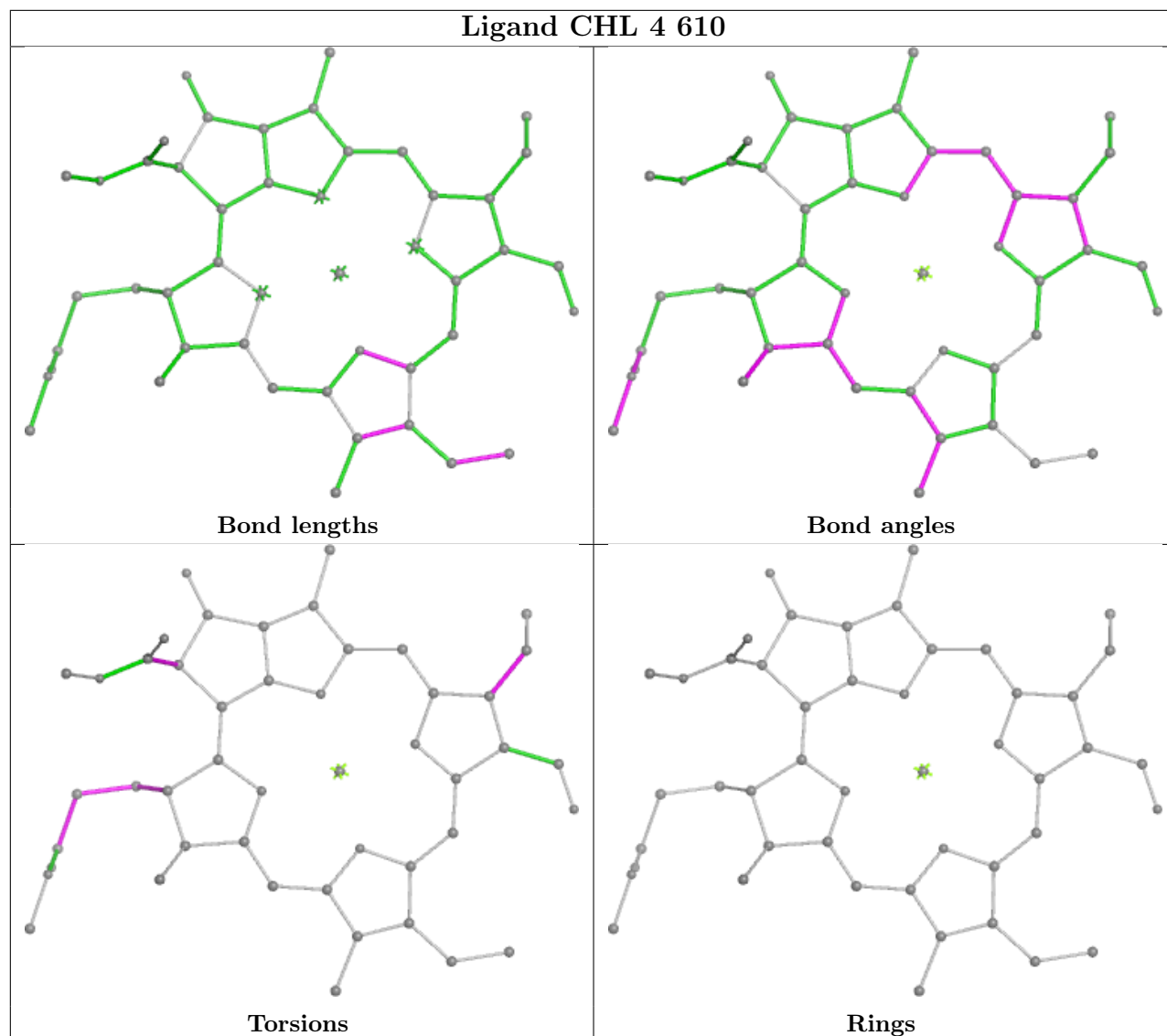


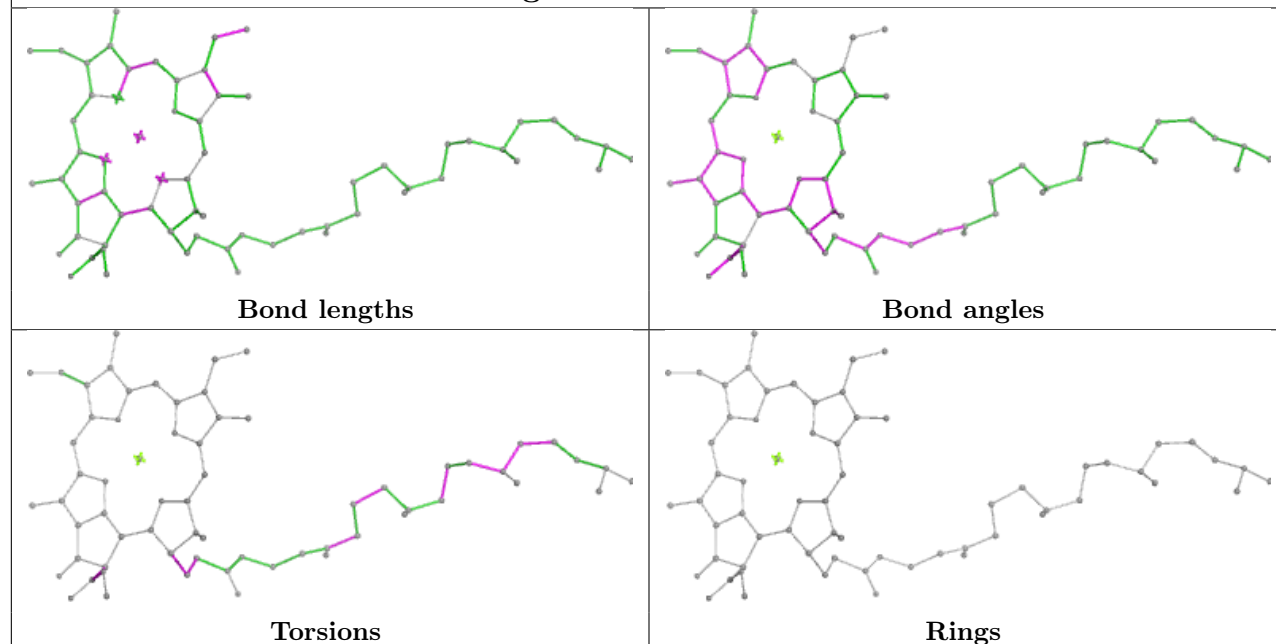
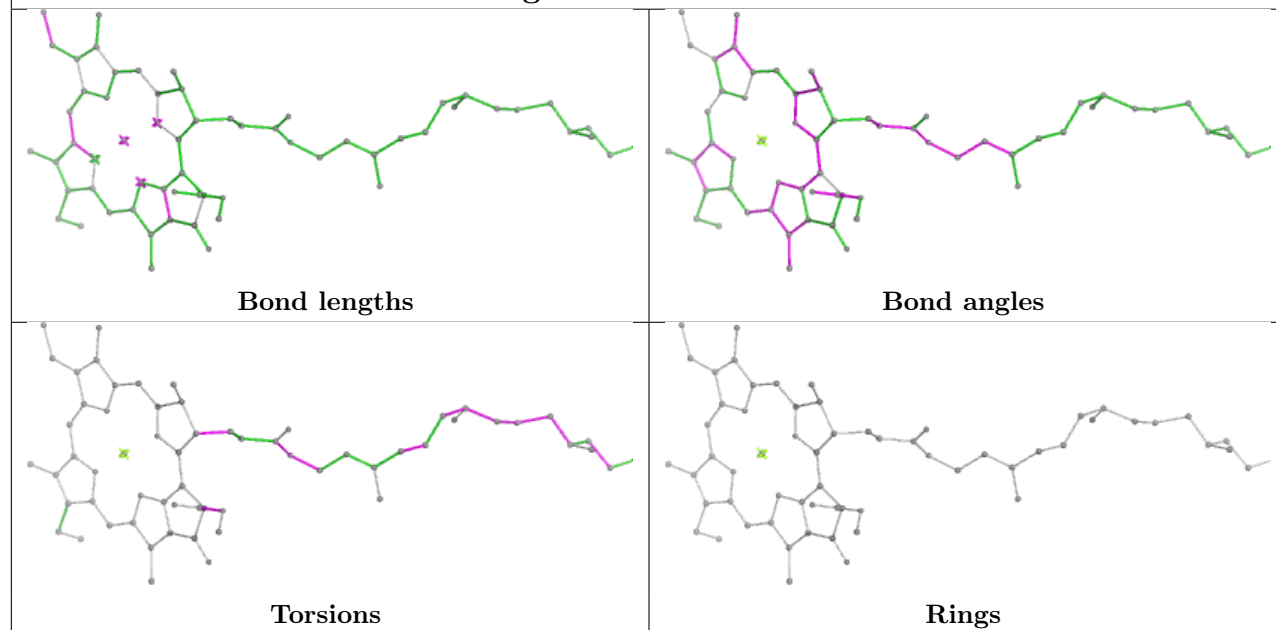
Ligand LUT 3 501

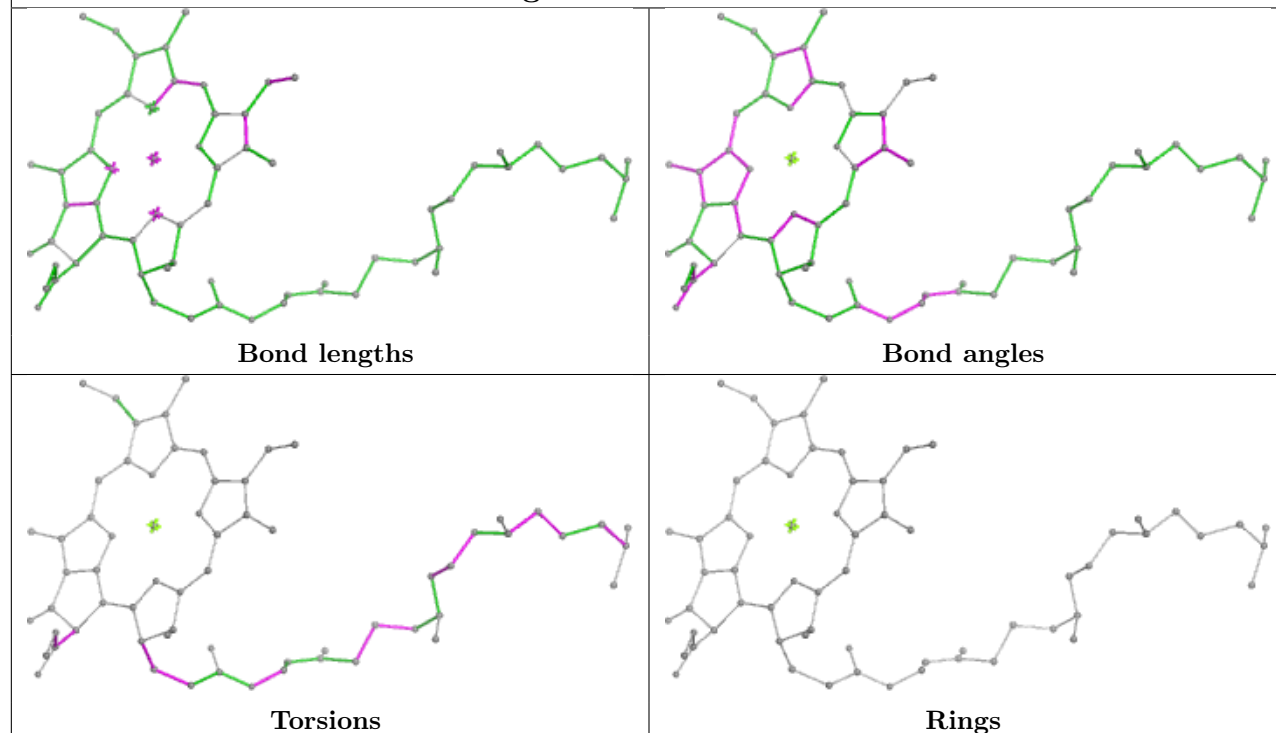
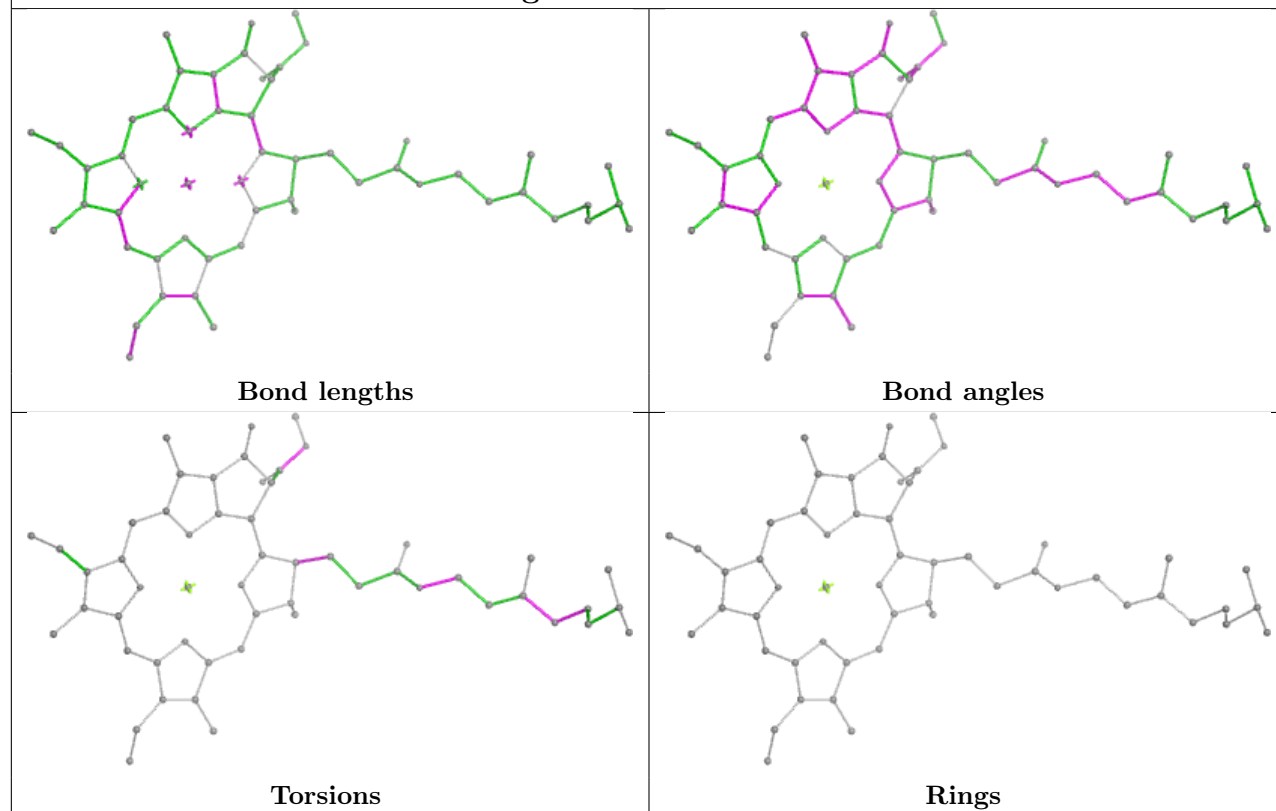


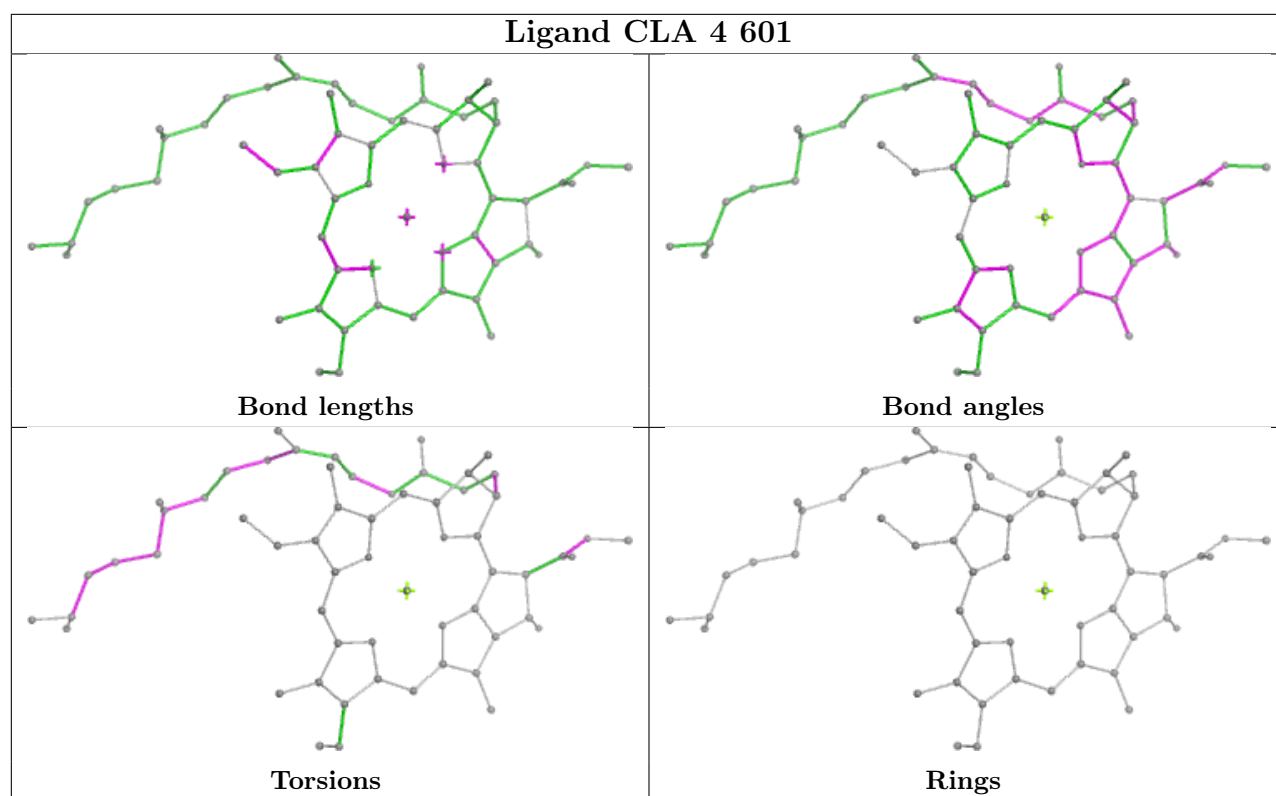


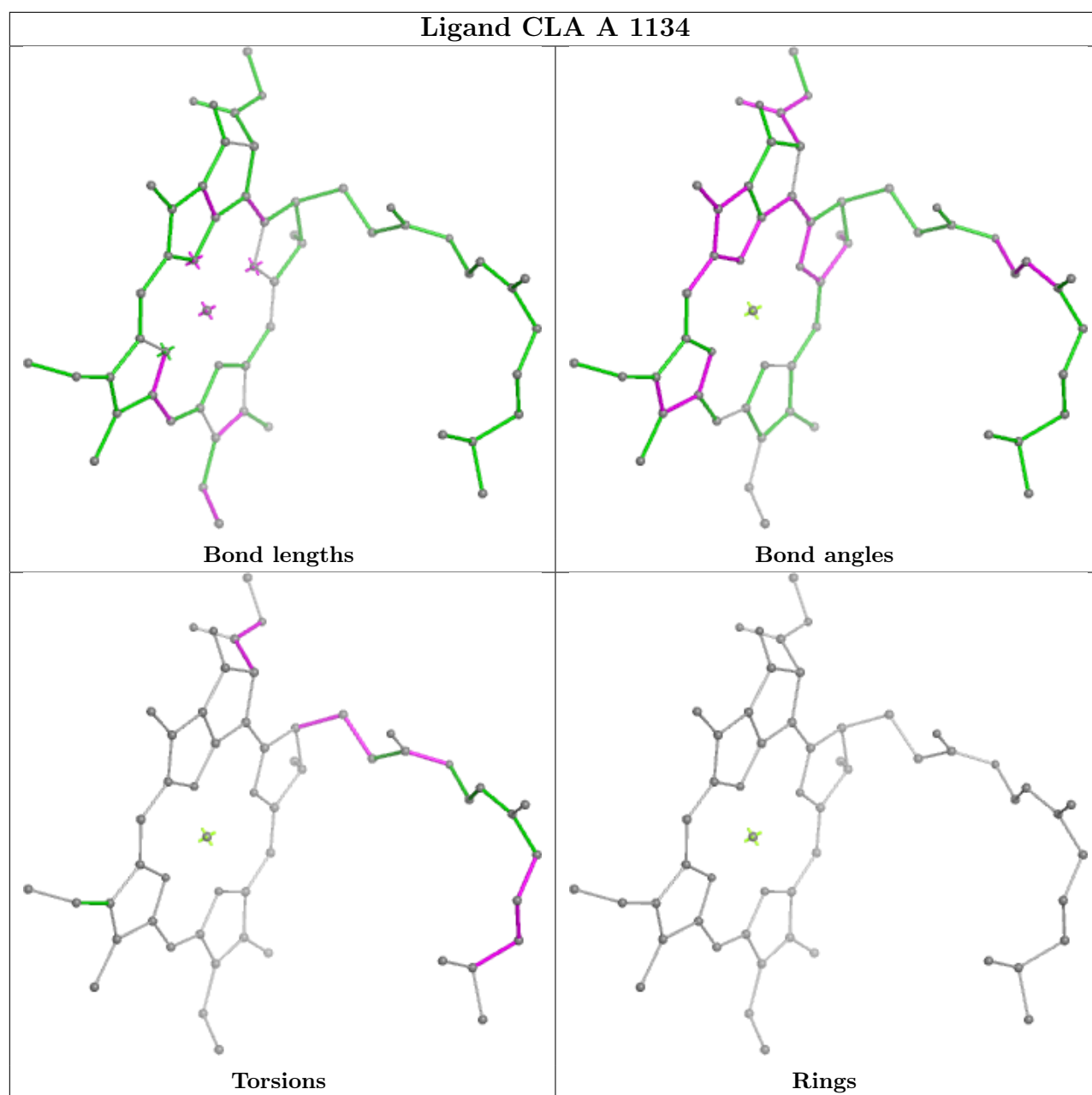
Ligand CHL 4 610

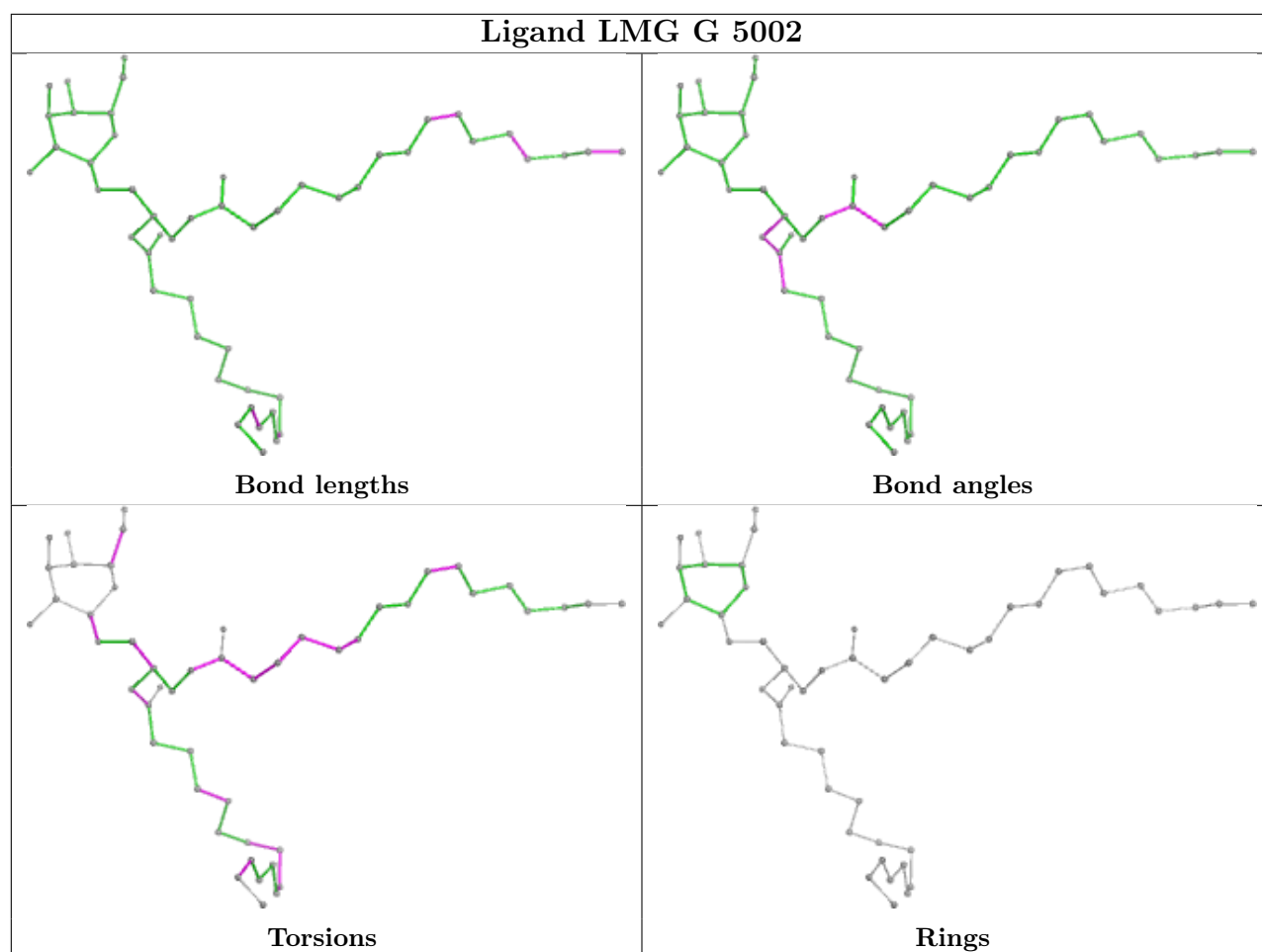


Ligand CLA A 1132**Ligand CLA A 1107**

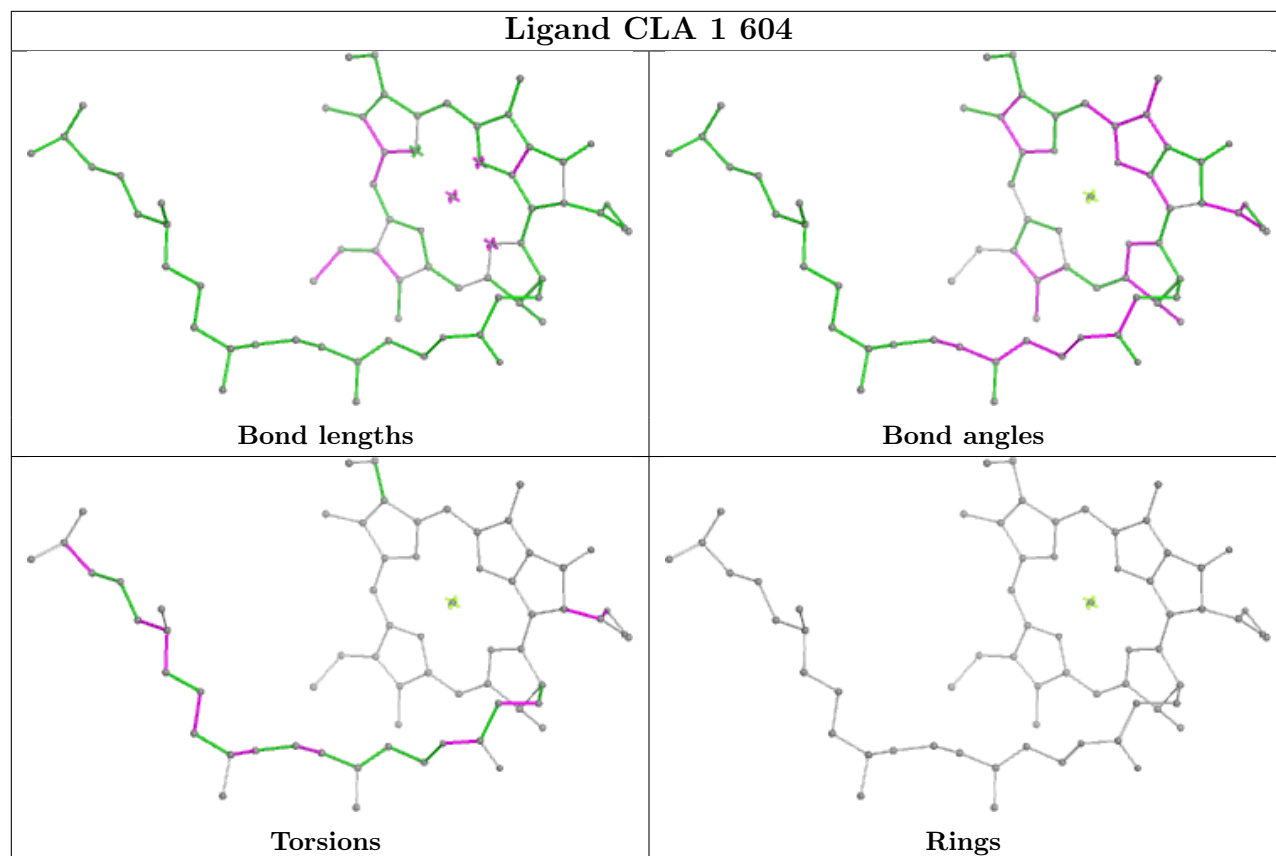
Ligand CLA A 1106**Ligand CLA G 1601**



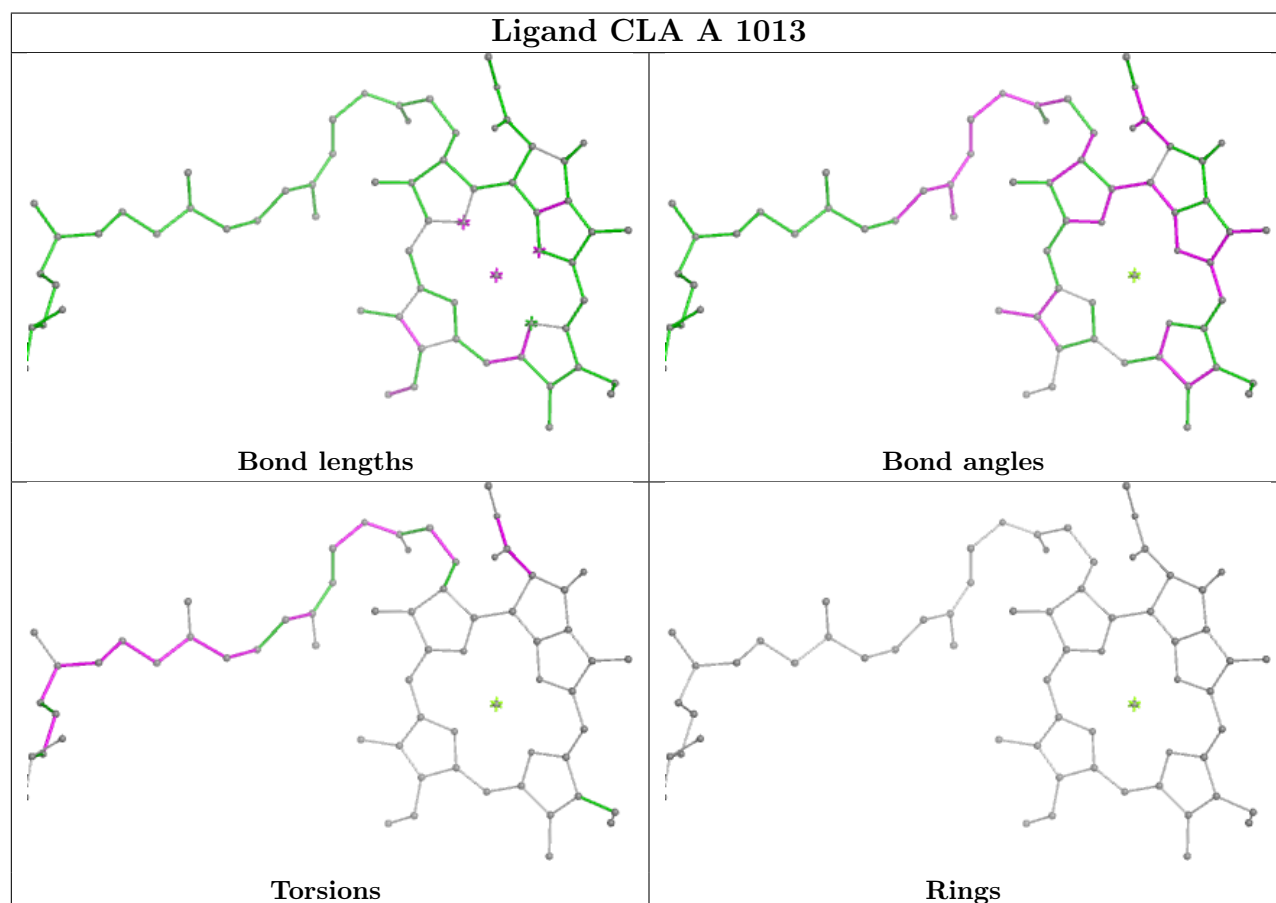


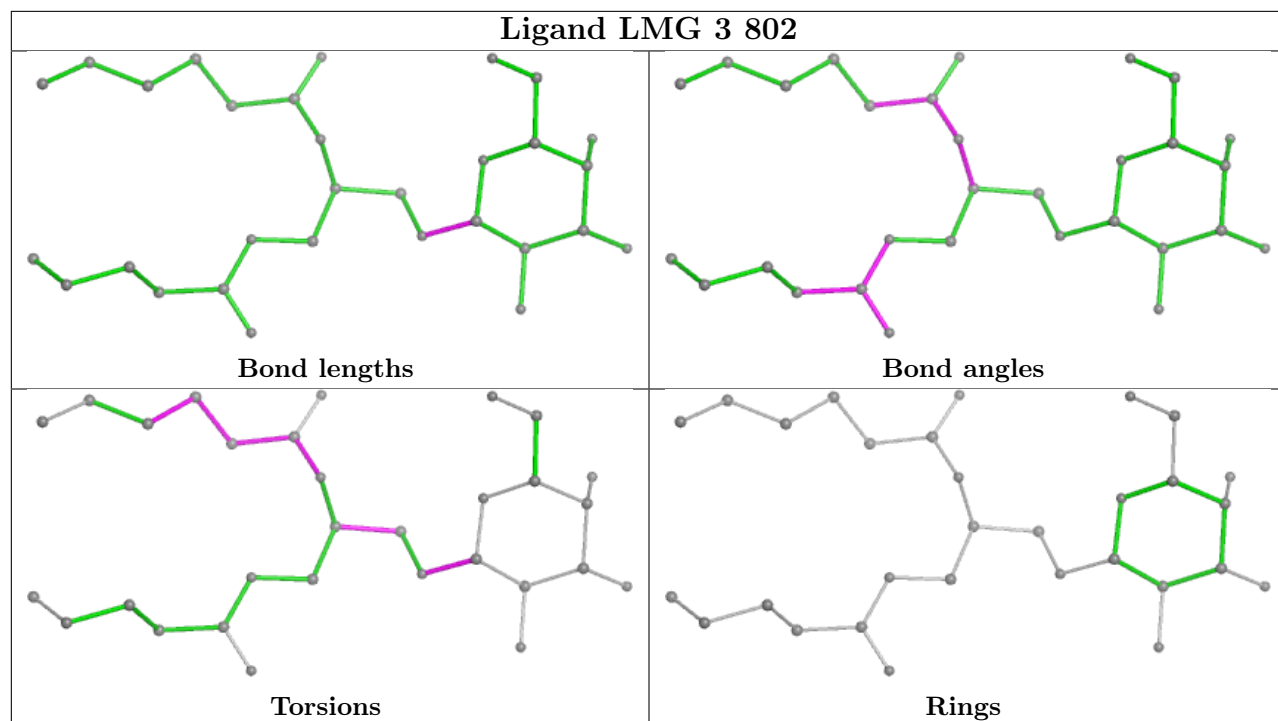


Ligand CLA 1 604

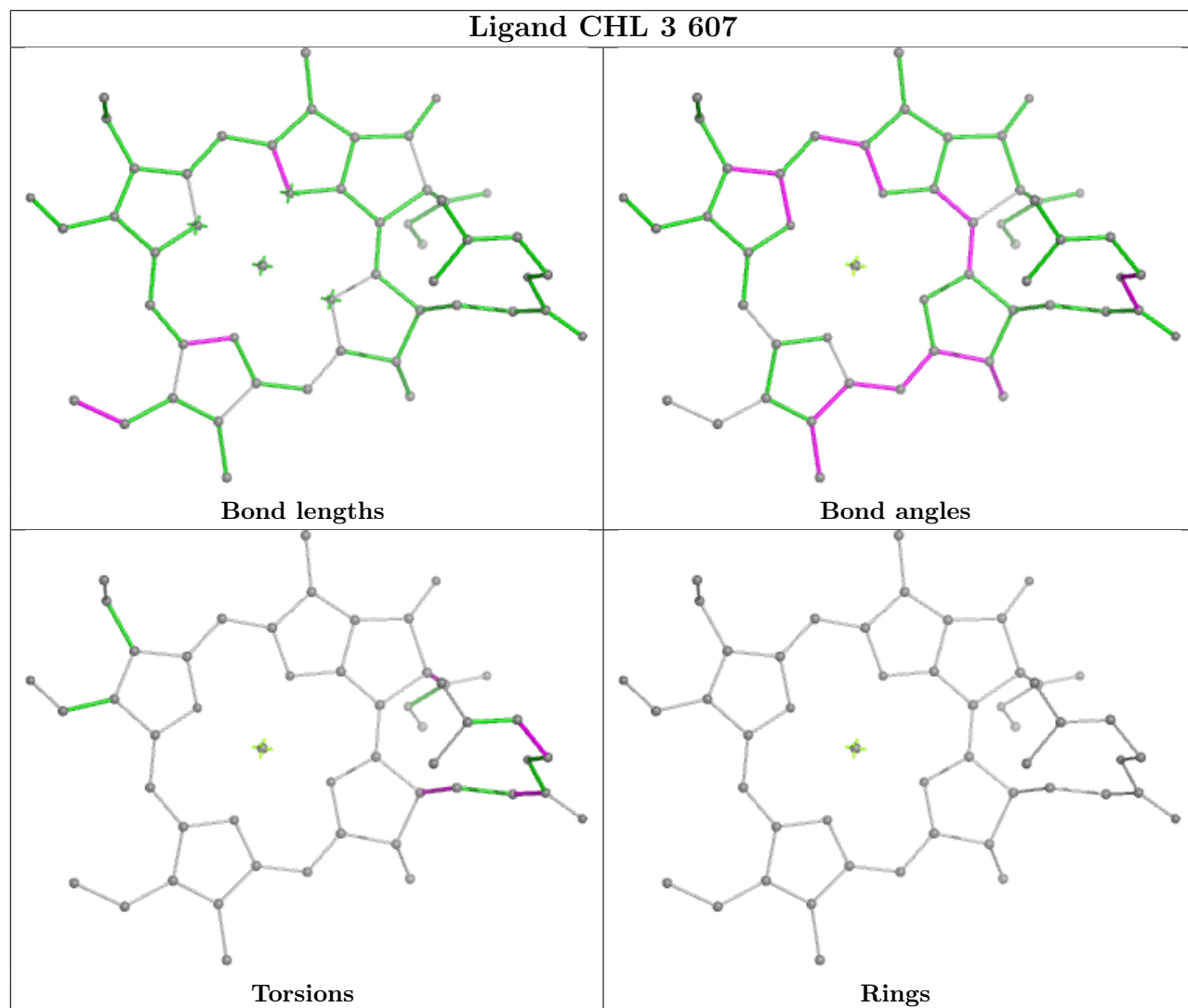


Ligand CLA A 1013

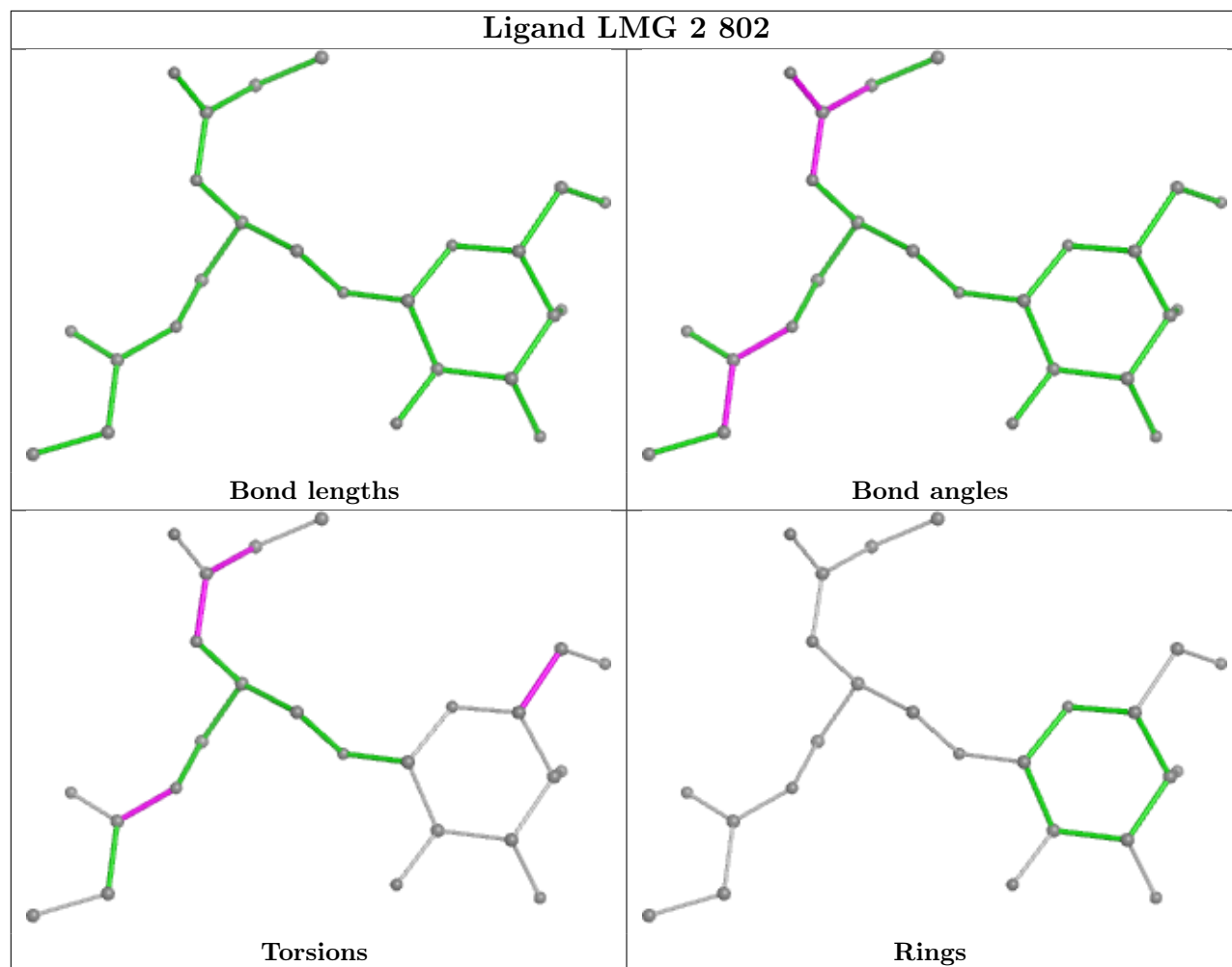




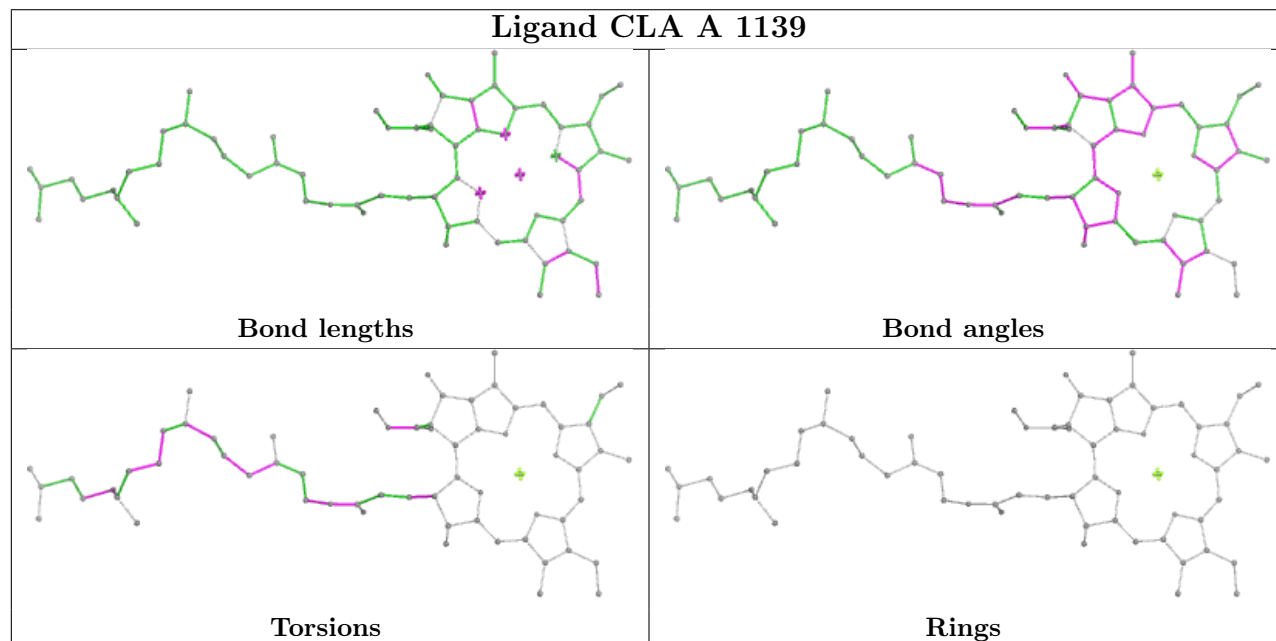
Ligand CHL 3 607

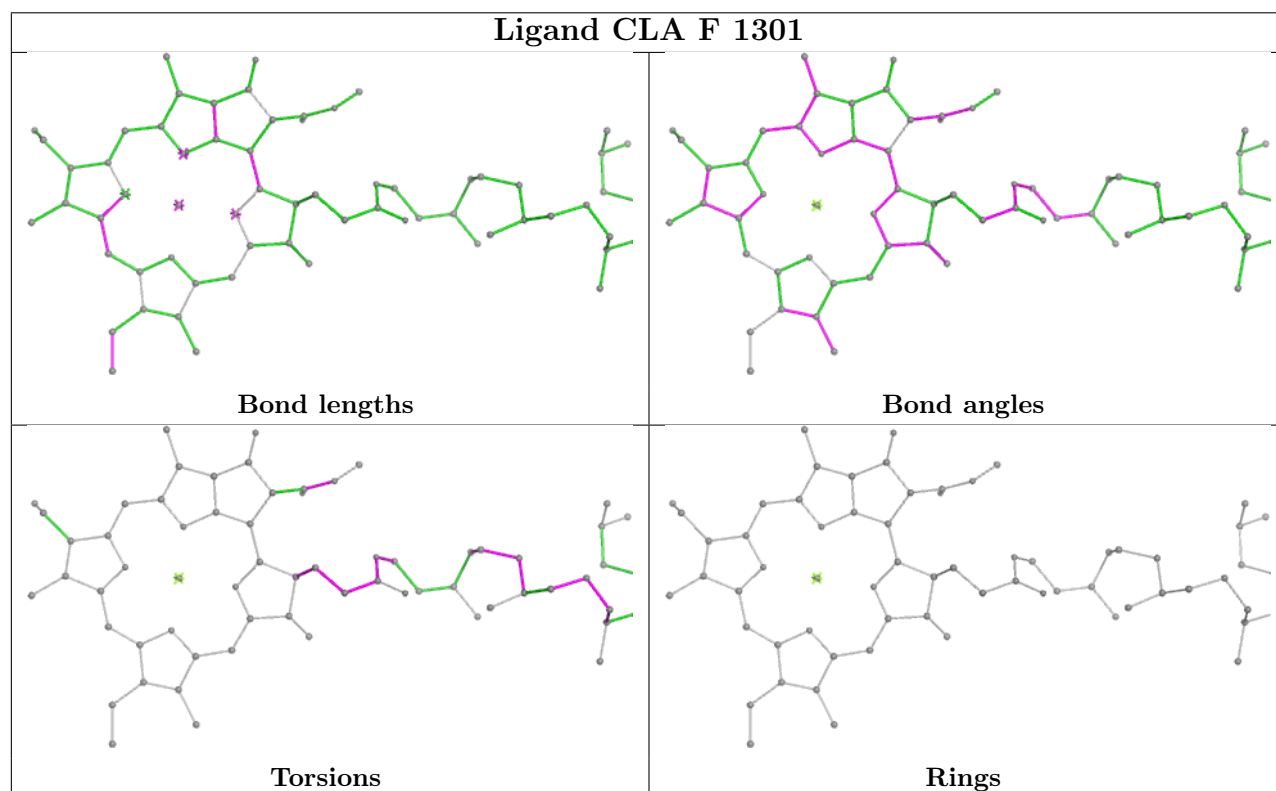
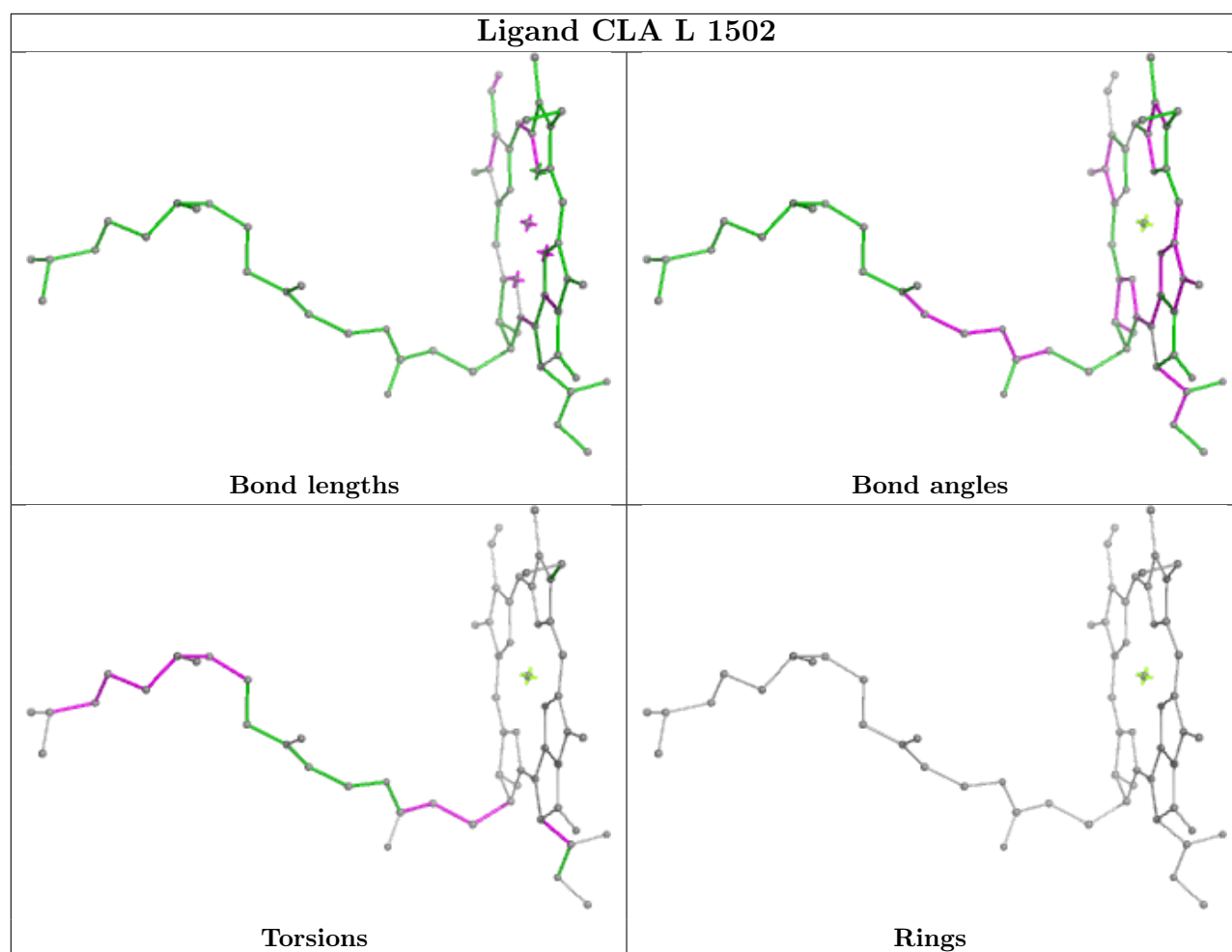


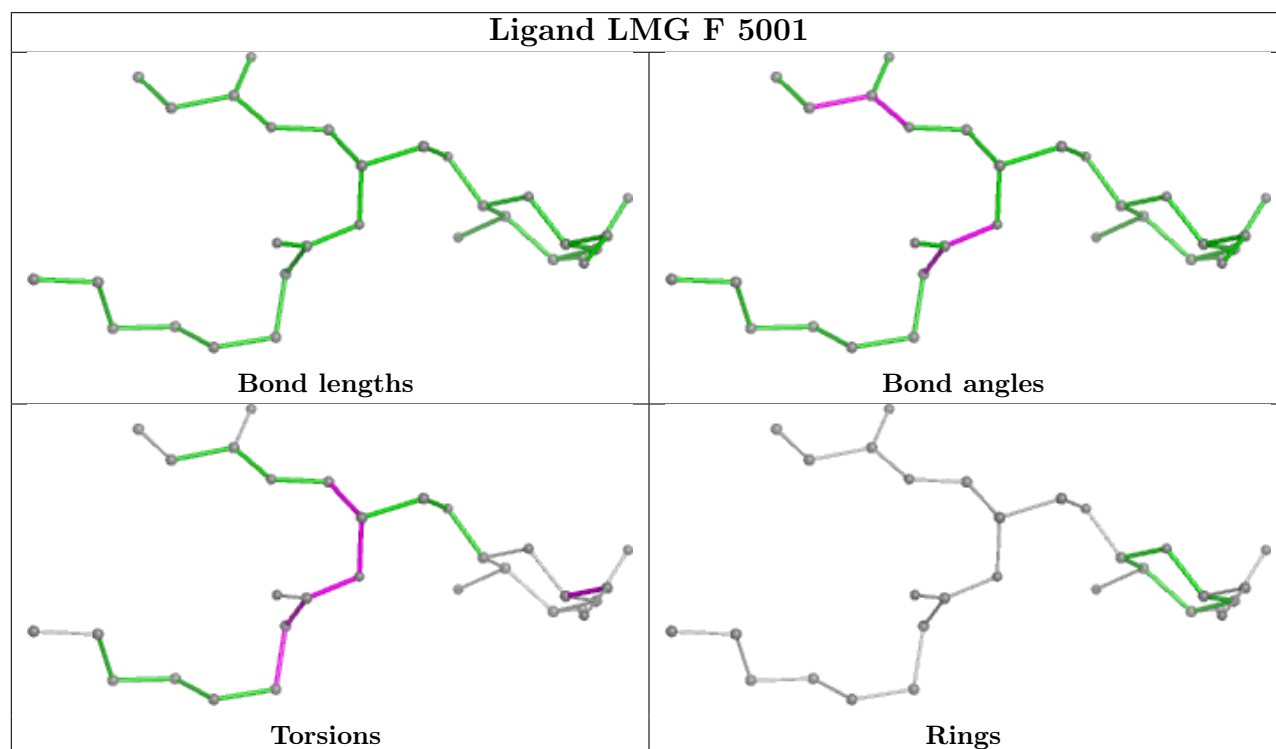
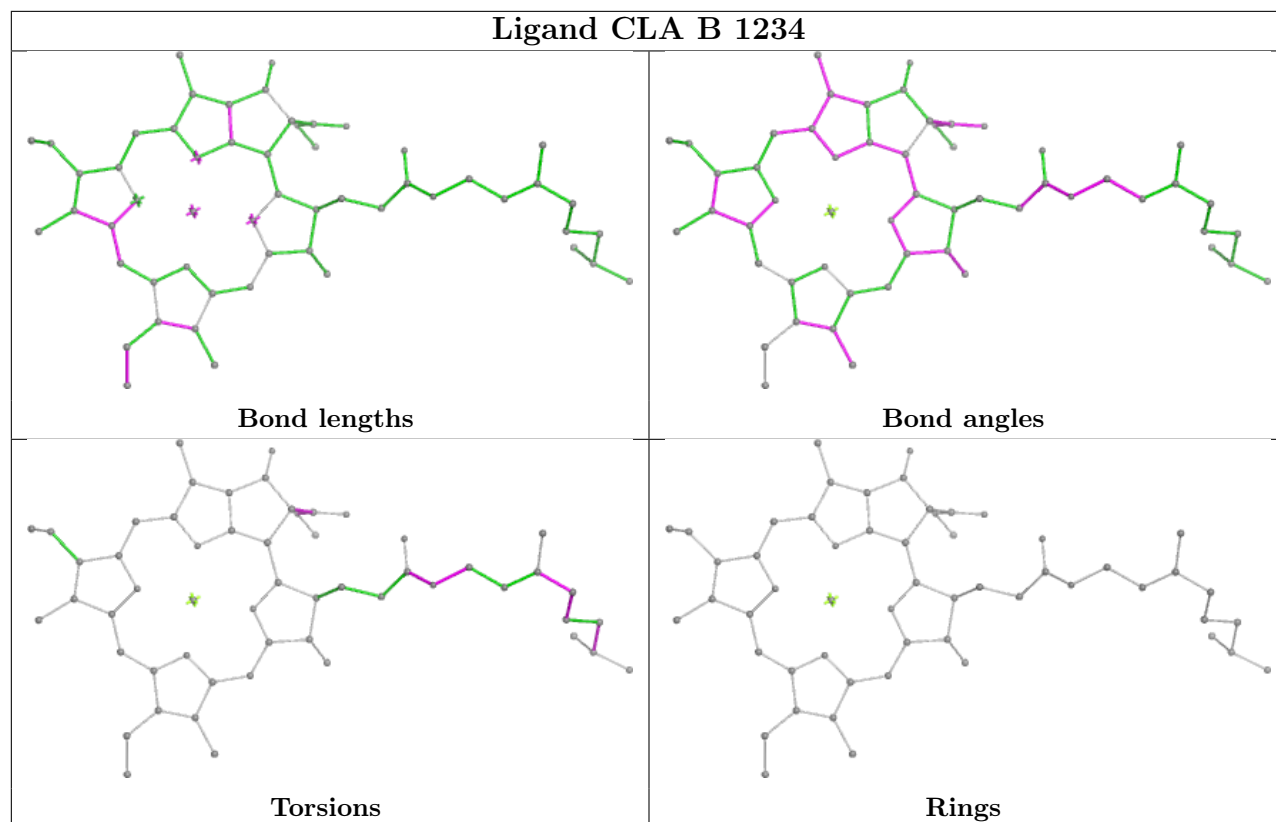
Ligand LMG 2 802

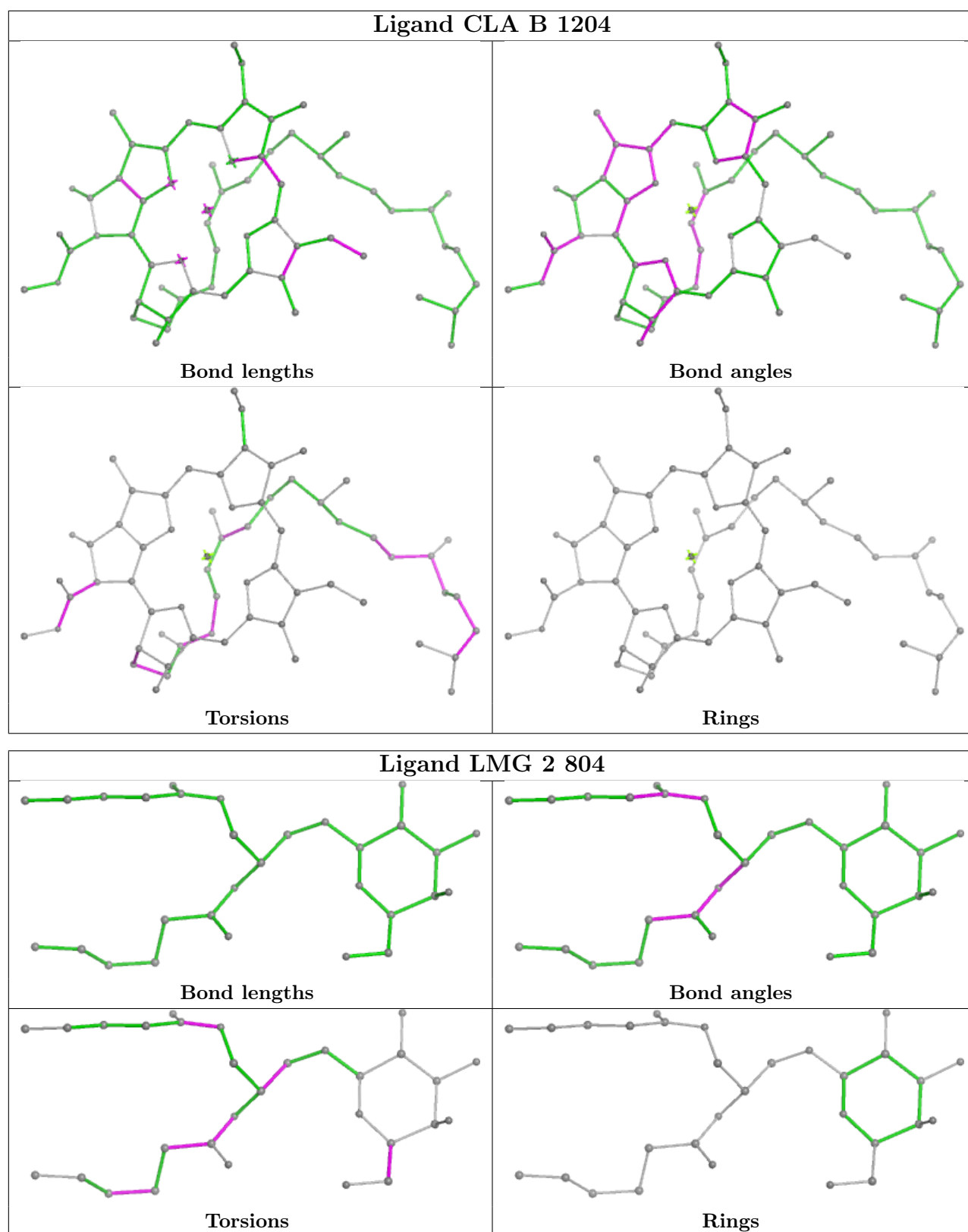


Ligand CLA A 1139

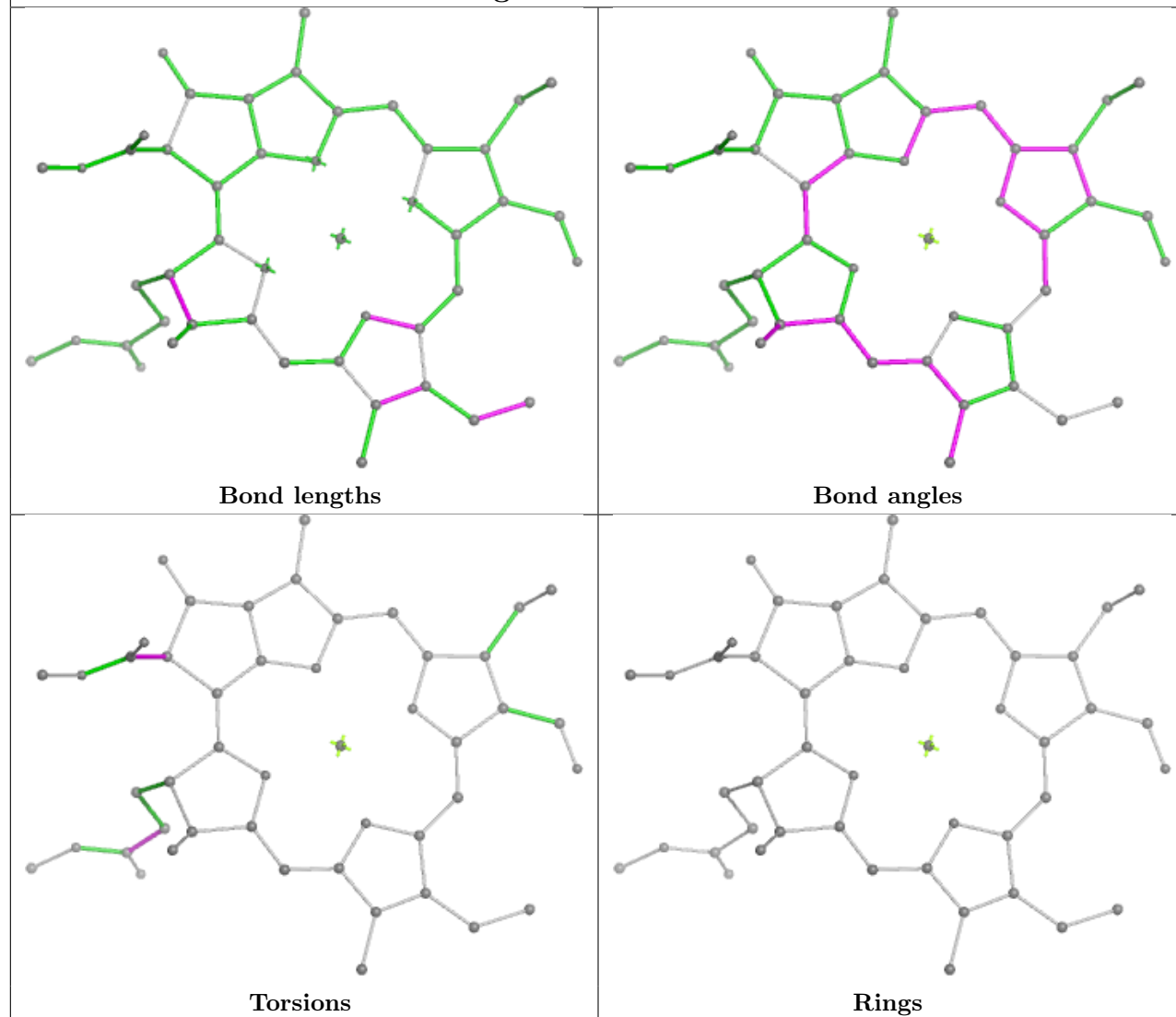




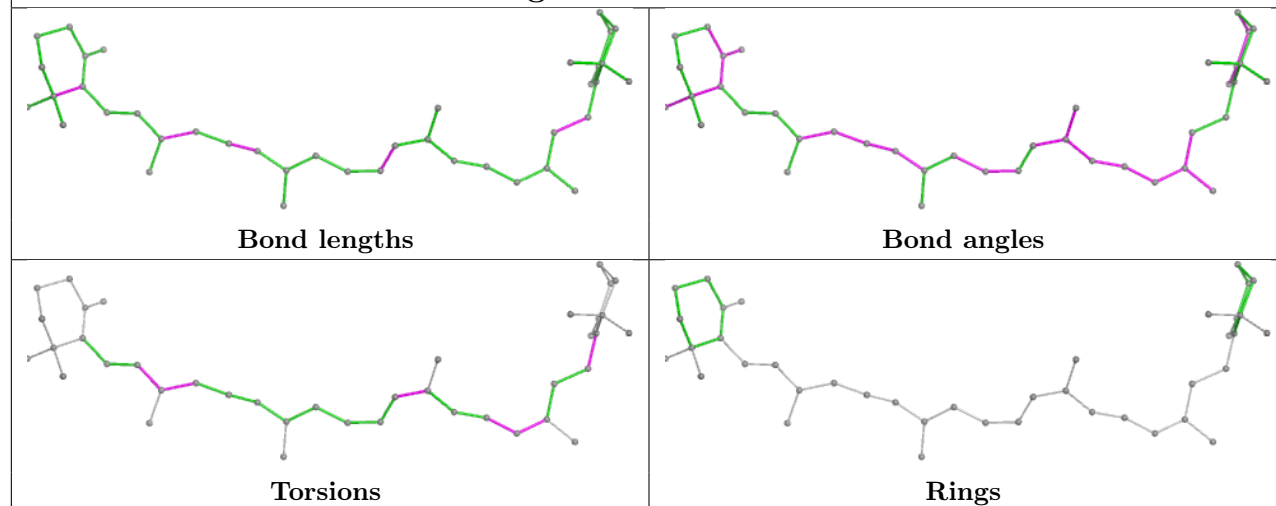


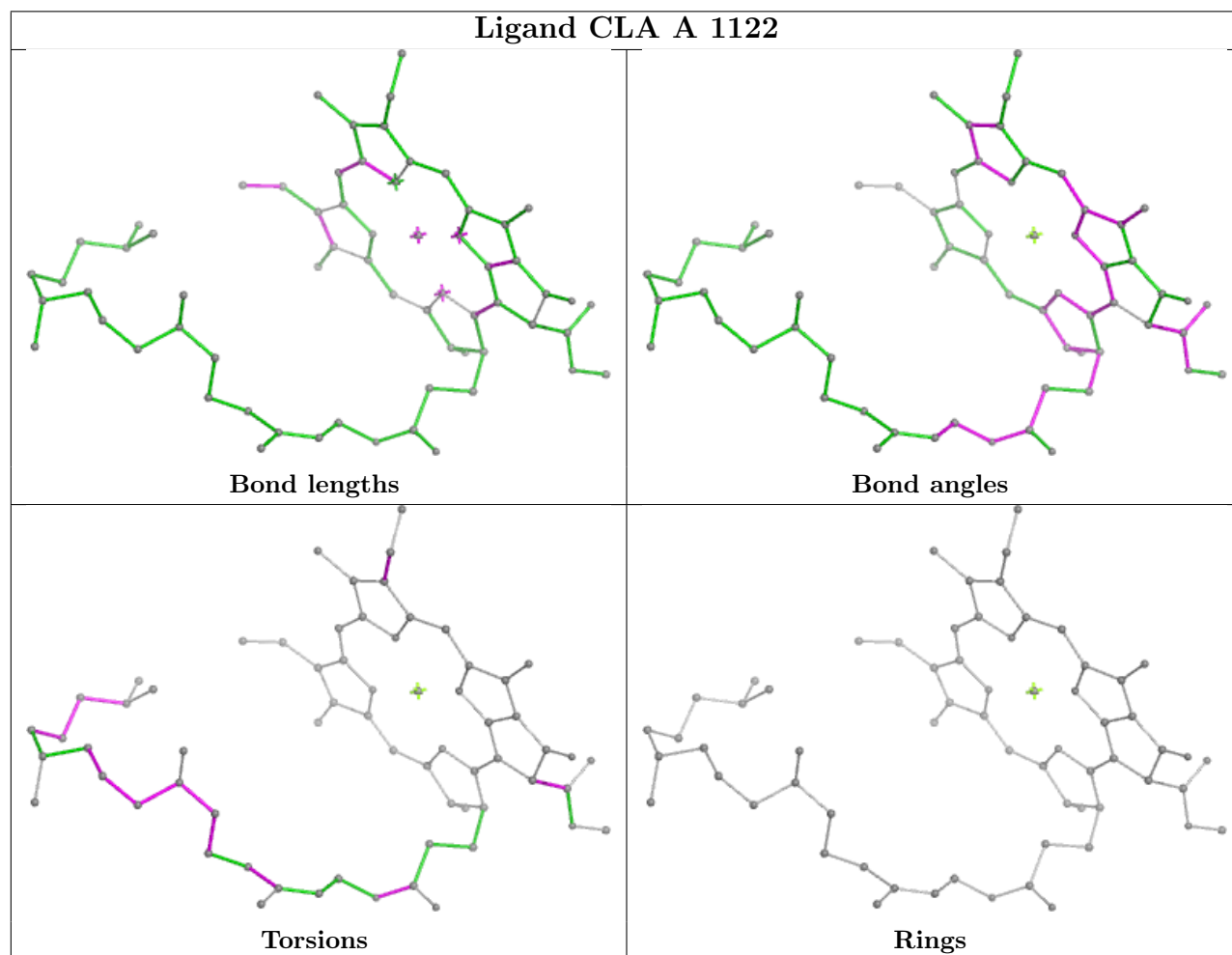
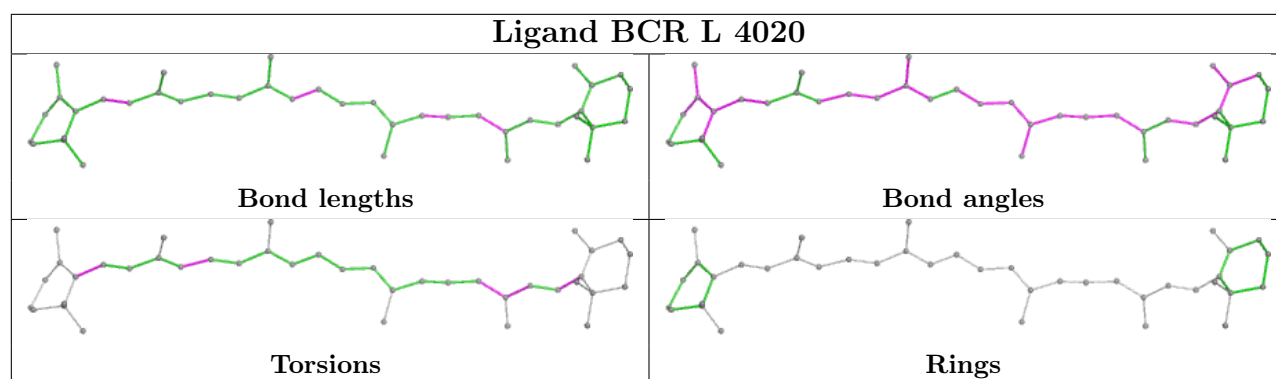


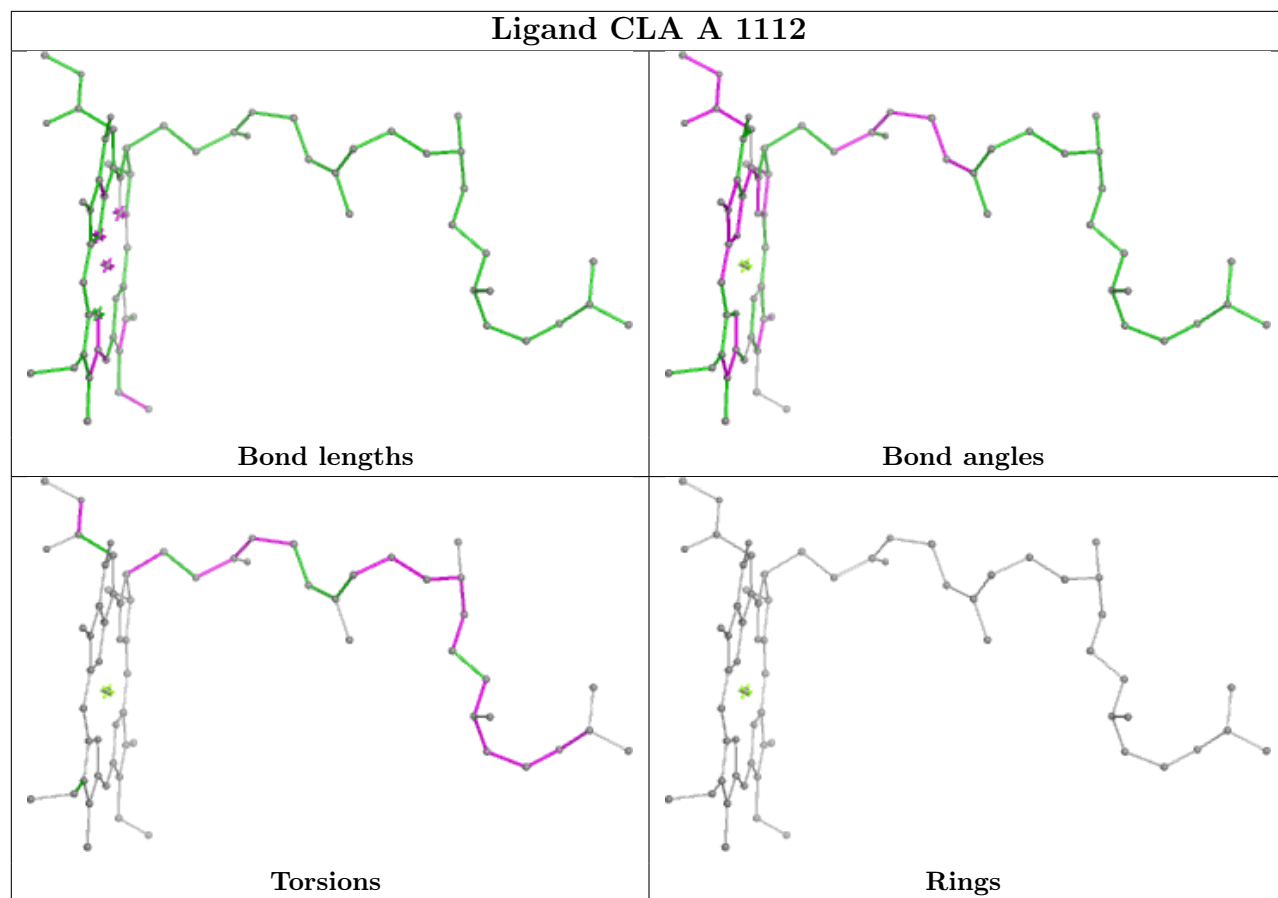
Ligand CHL 1 610

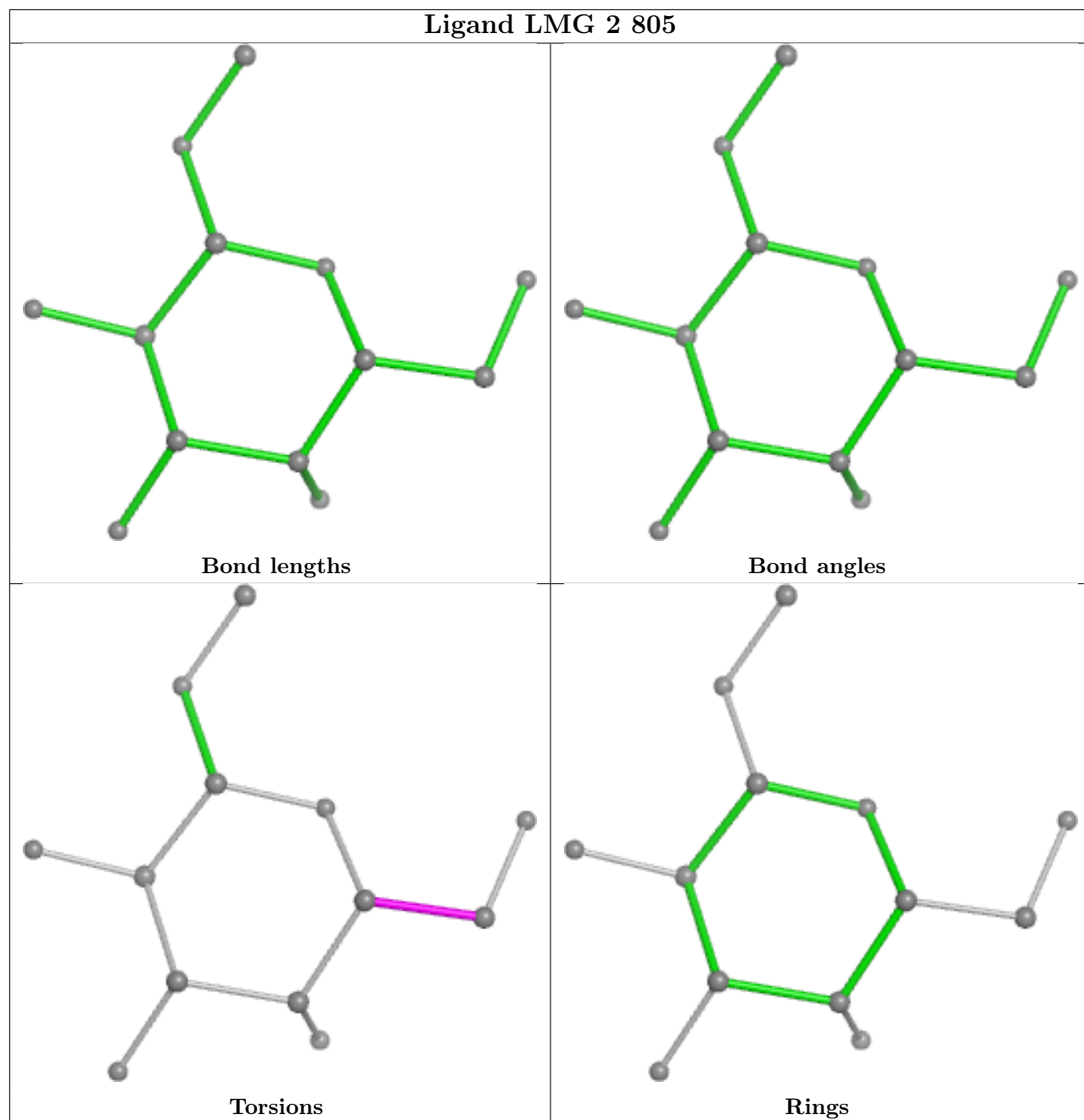


Ligand BCR I 4020

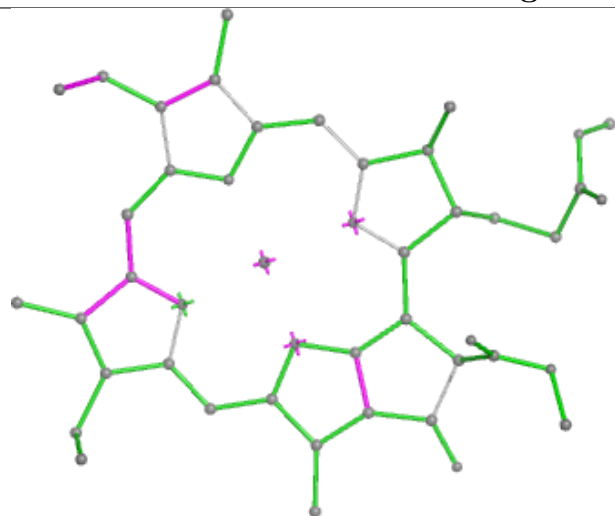




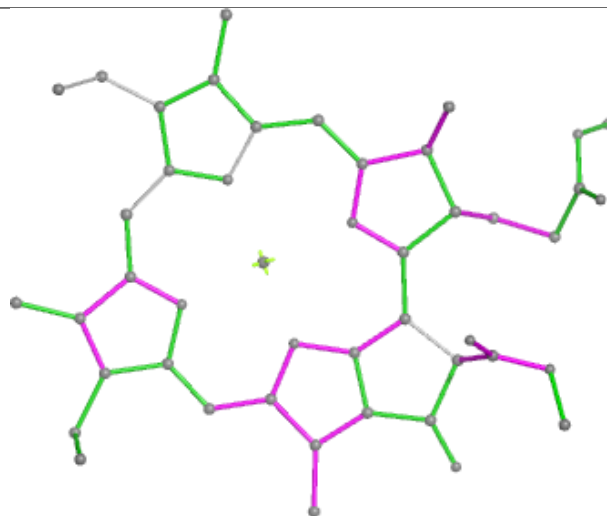




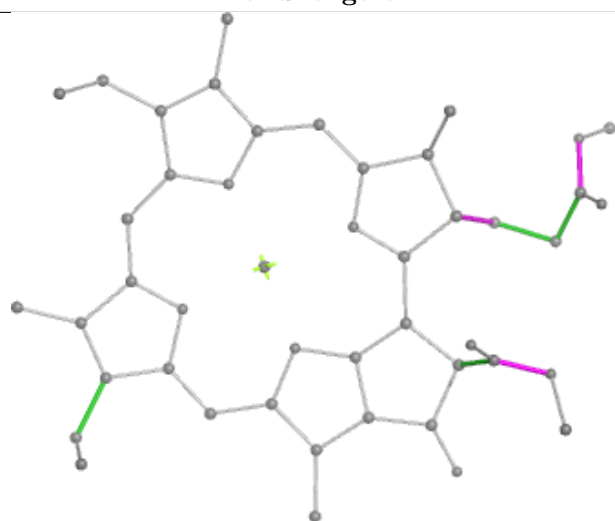
Ligand CLA 1 602



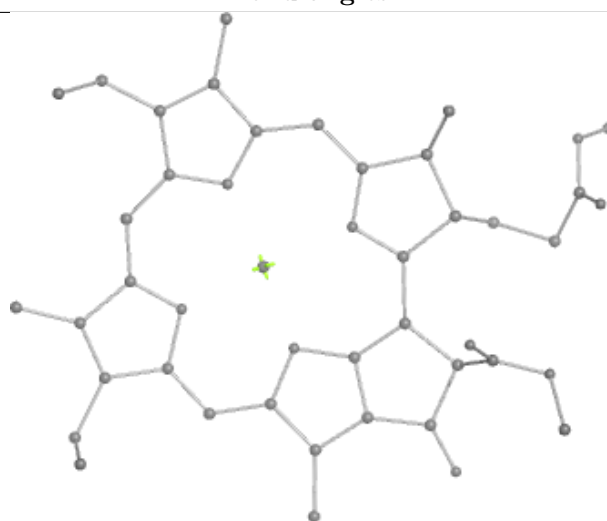
Bond lengths



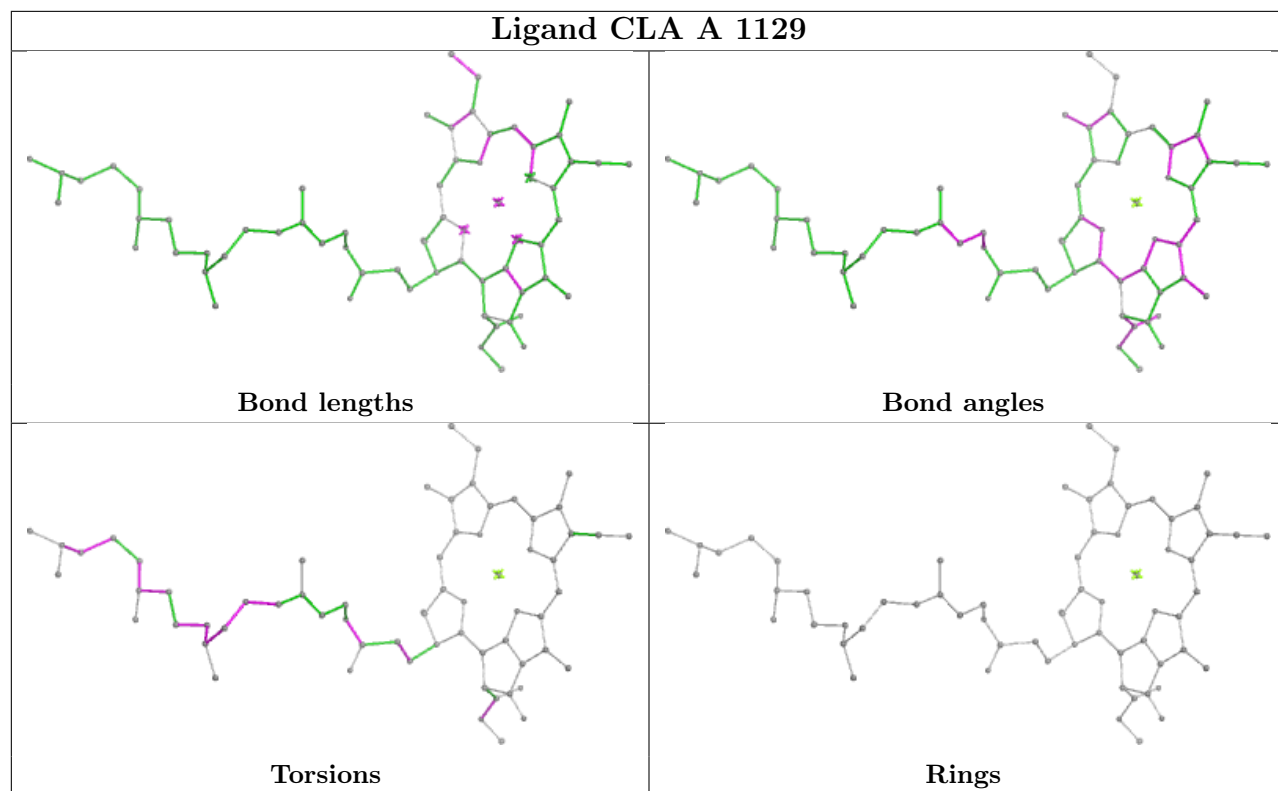
Bond angles



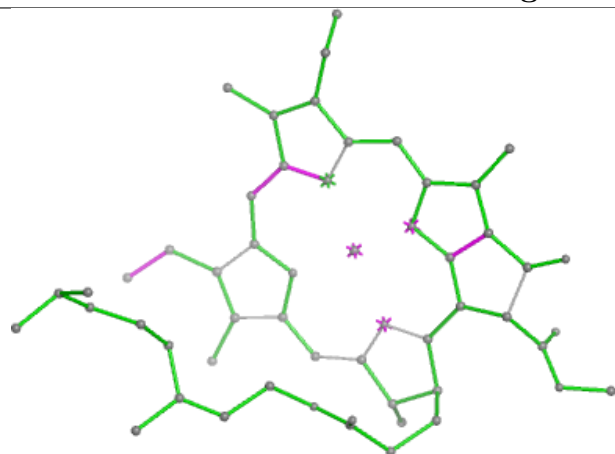
Torsions



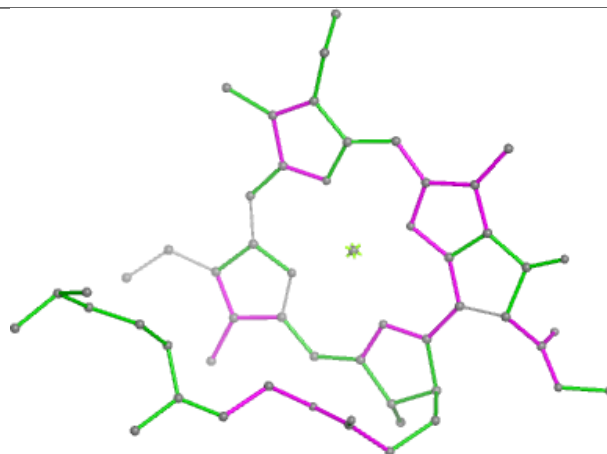
Rings



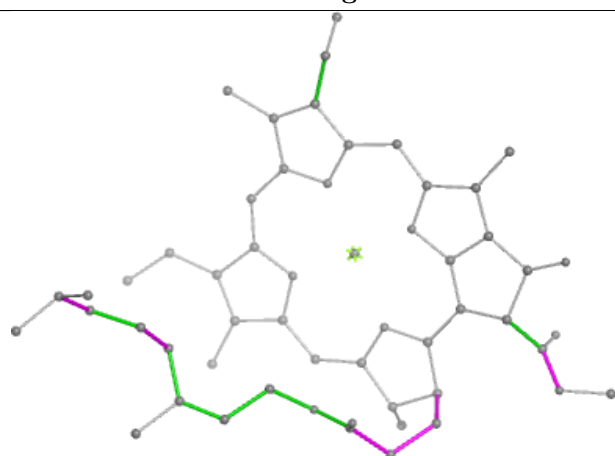
Ligand CLA 3 601



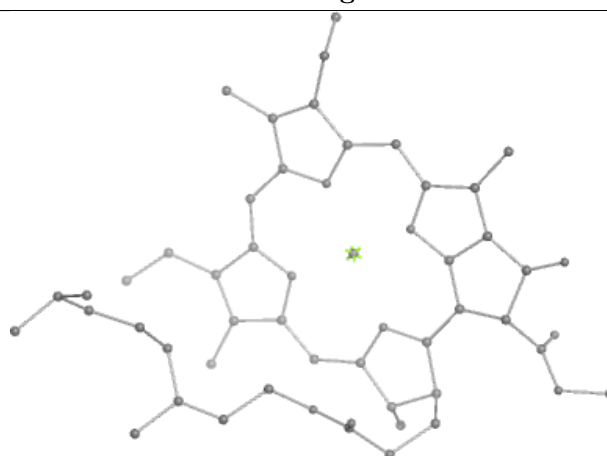
Bond lengths



Bond angles

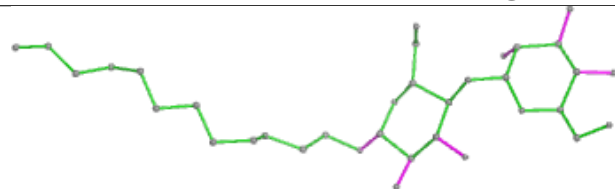


Torsions

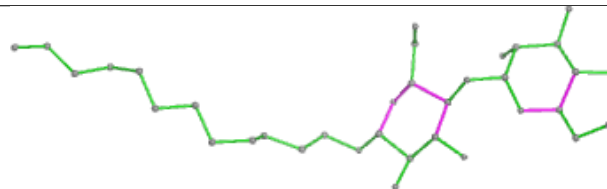


Rings

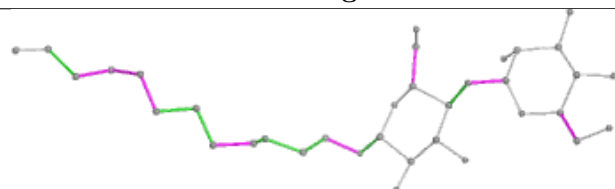
Ligand LMT G 5004



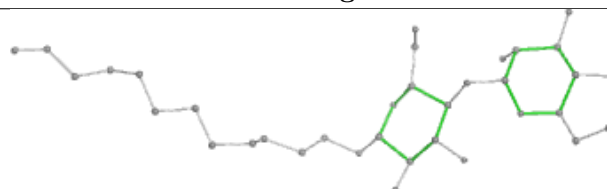
Bond lengths



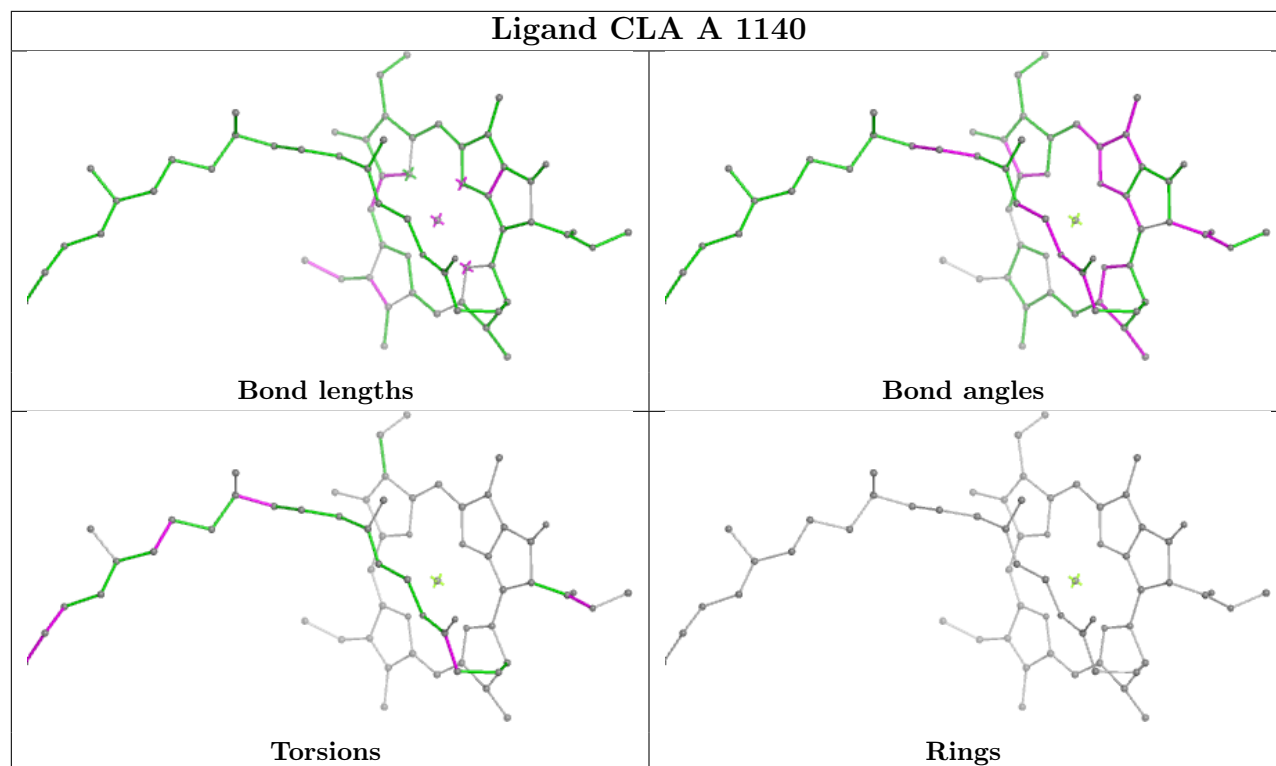
Bond angles



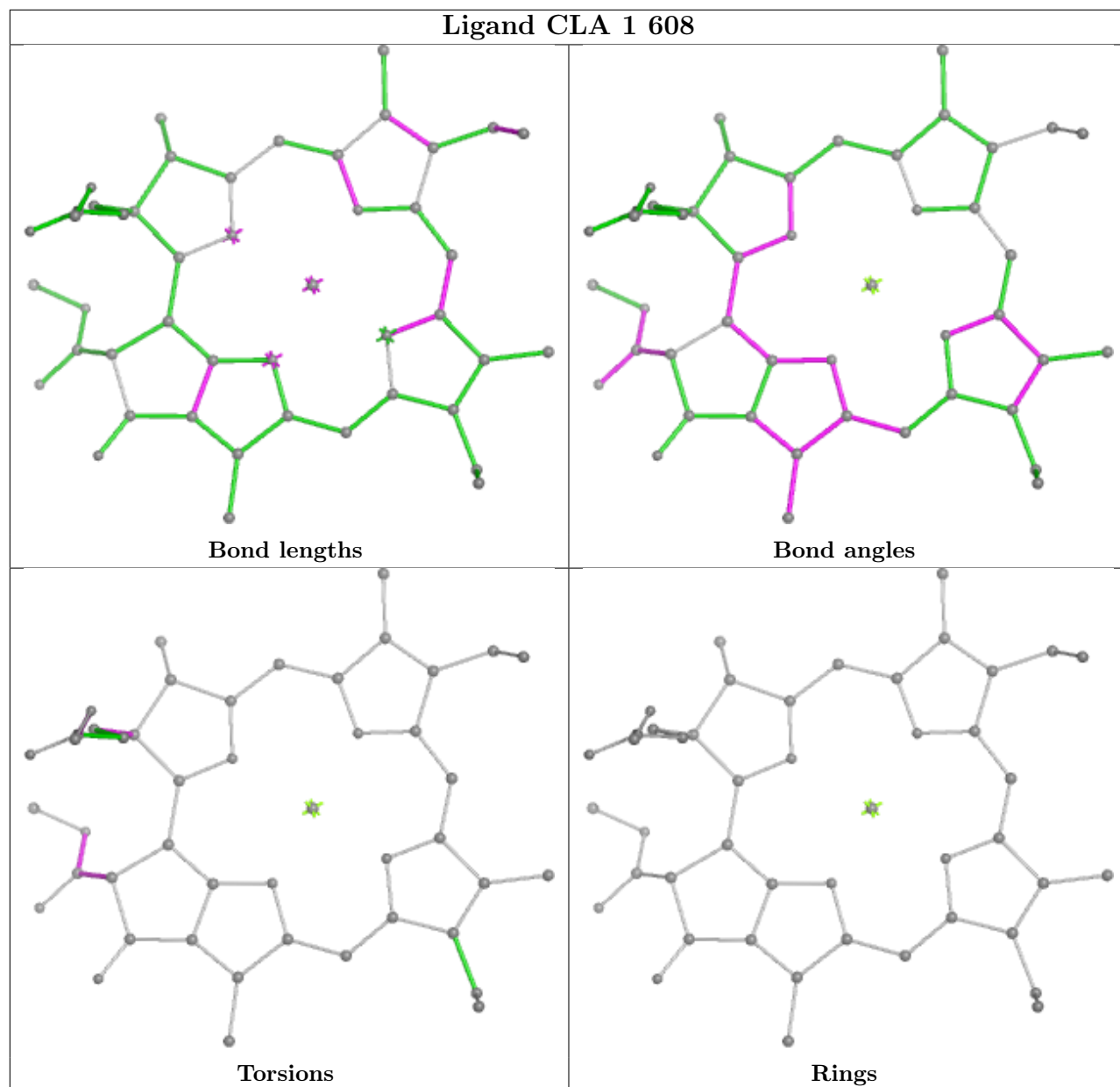
Torsions



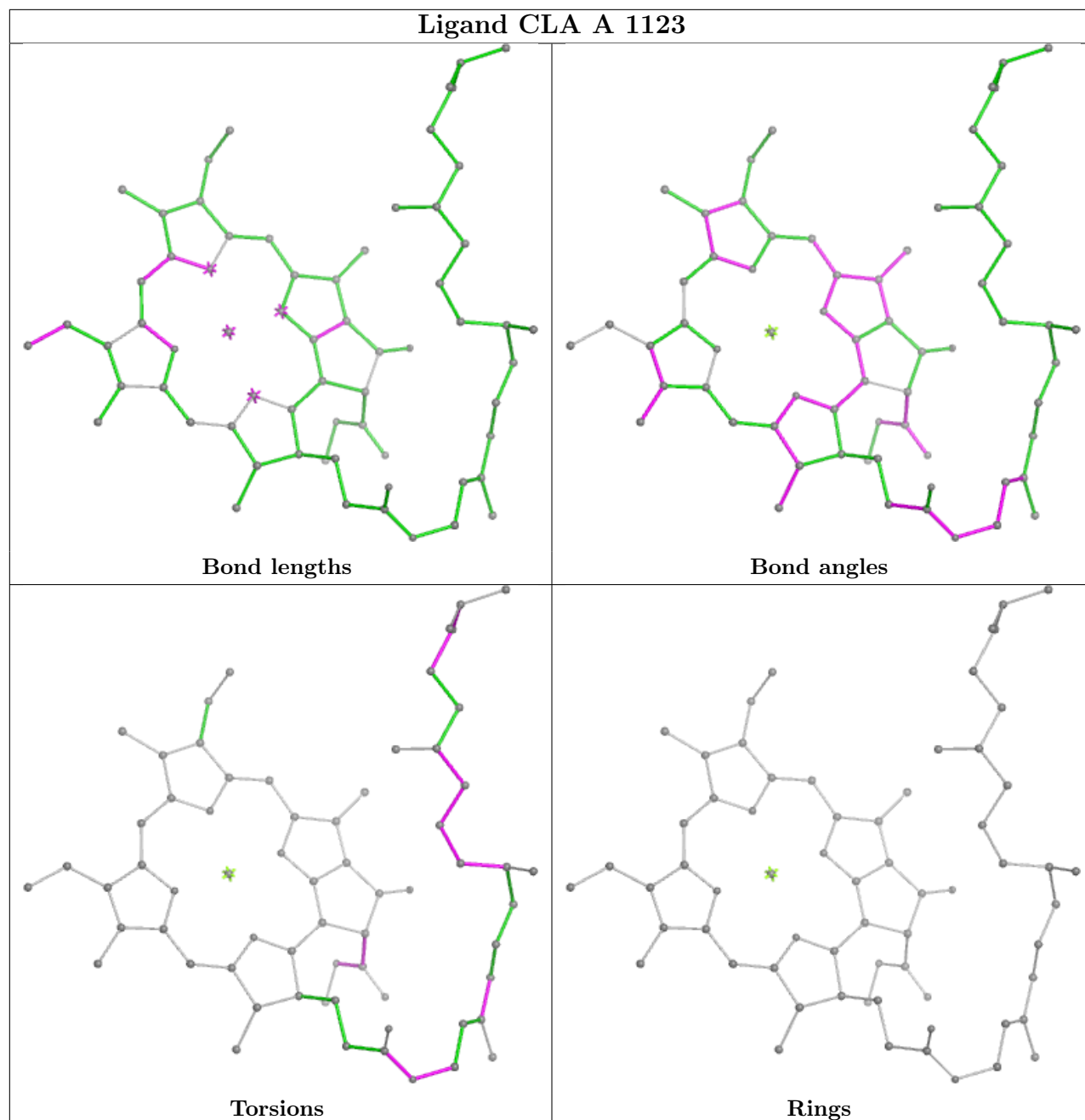
Rings

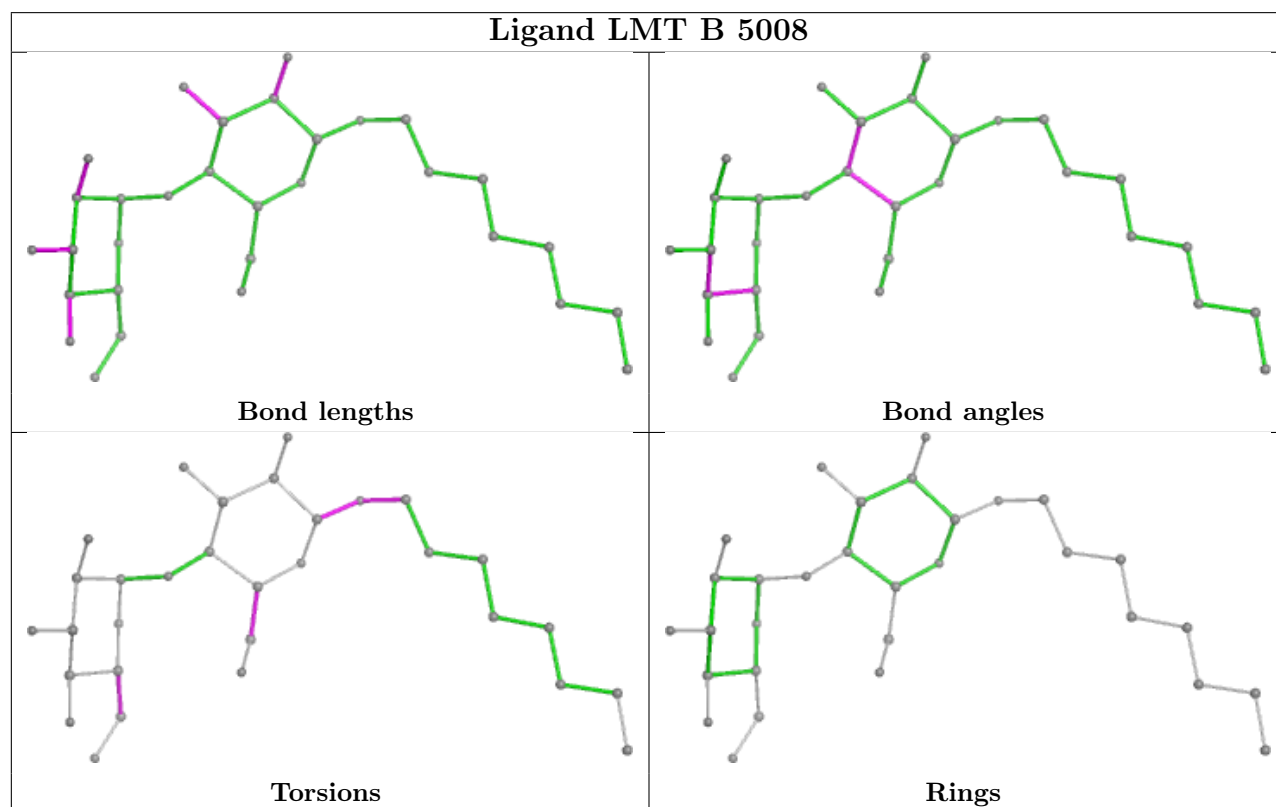
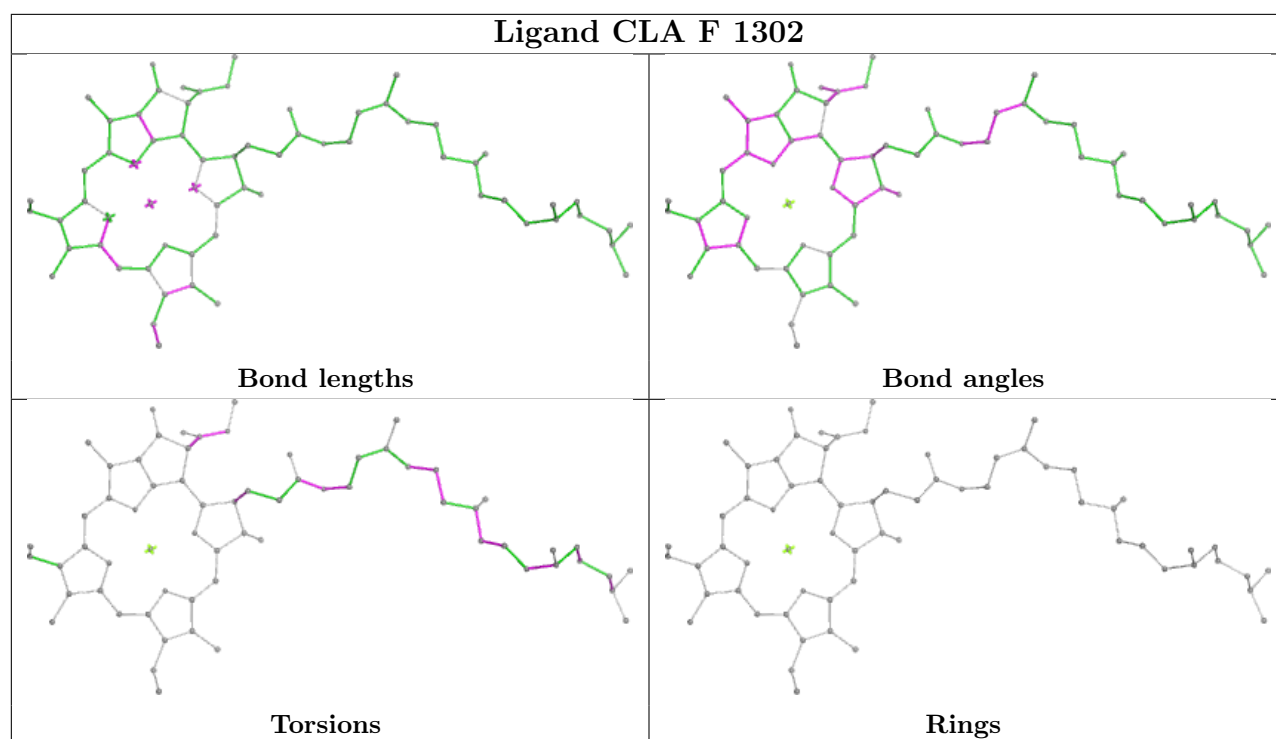


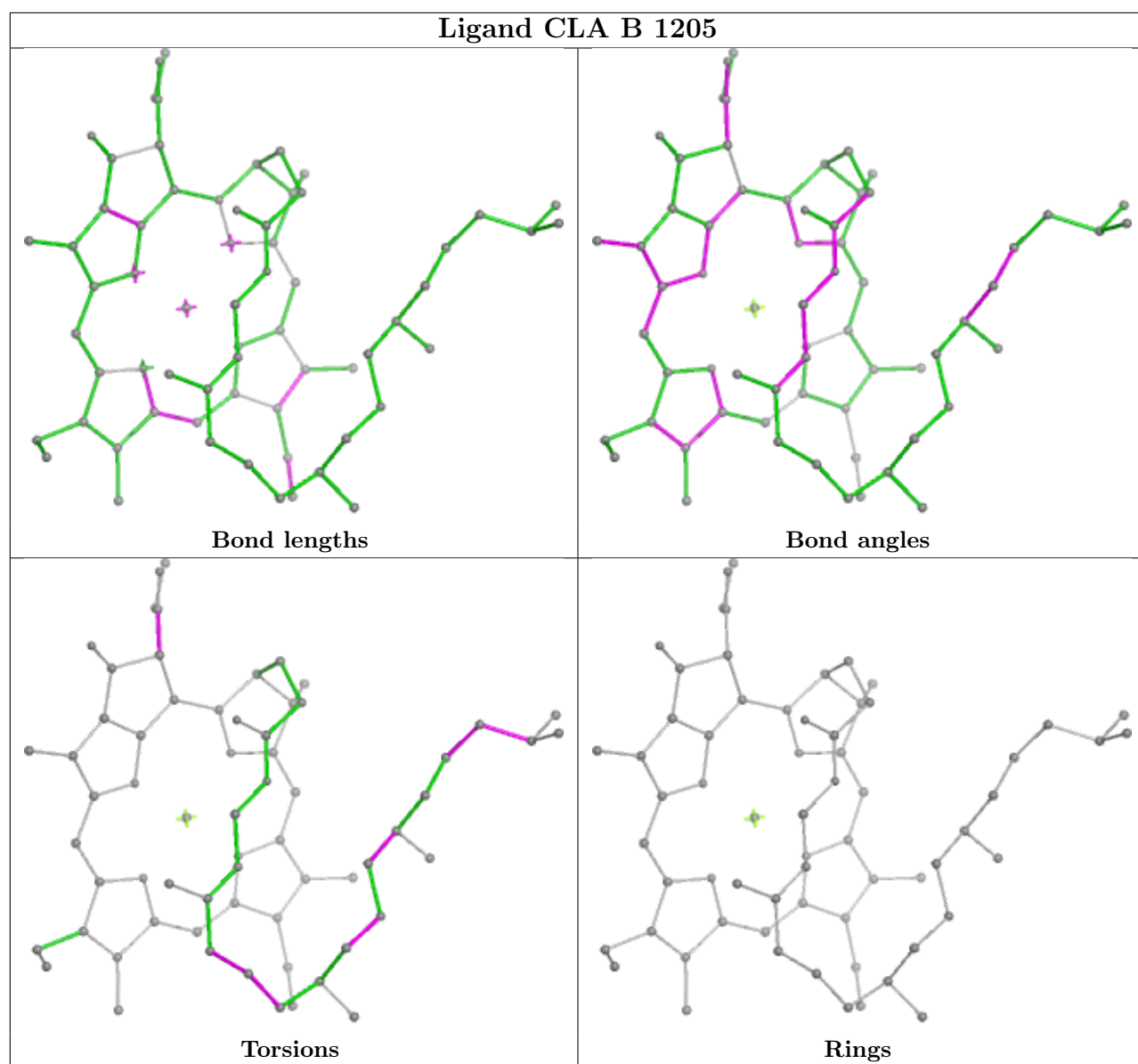
Ligand CLA 1 608

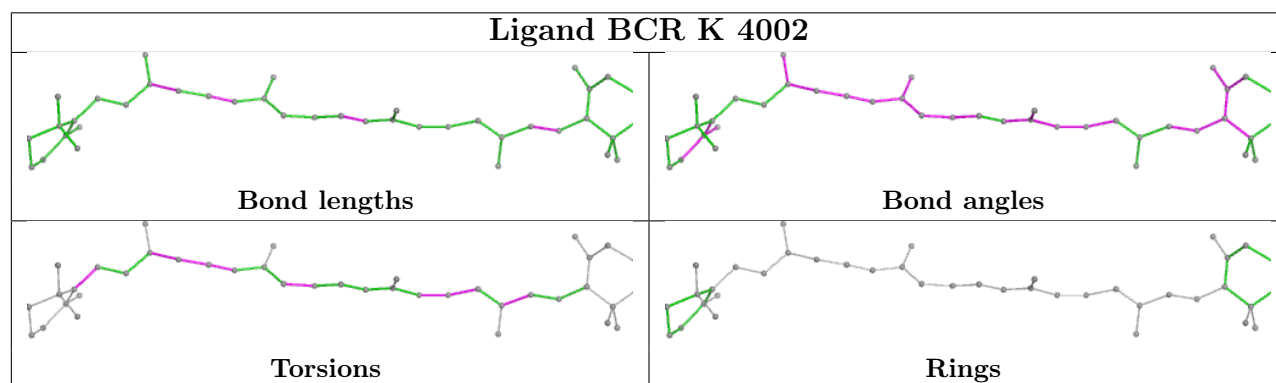
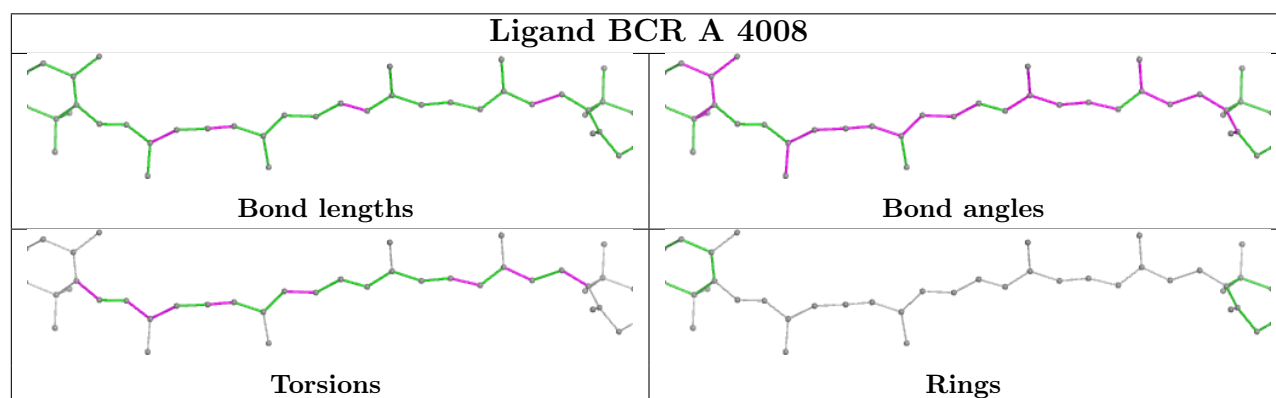
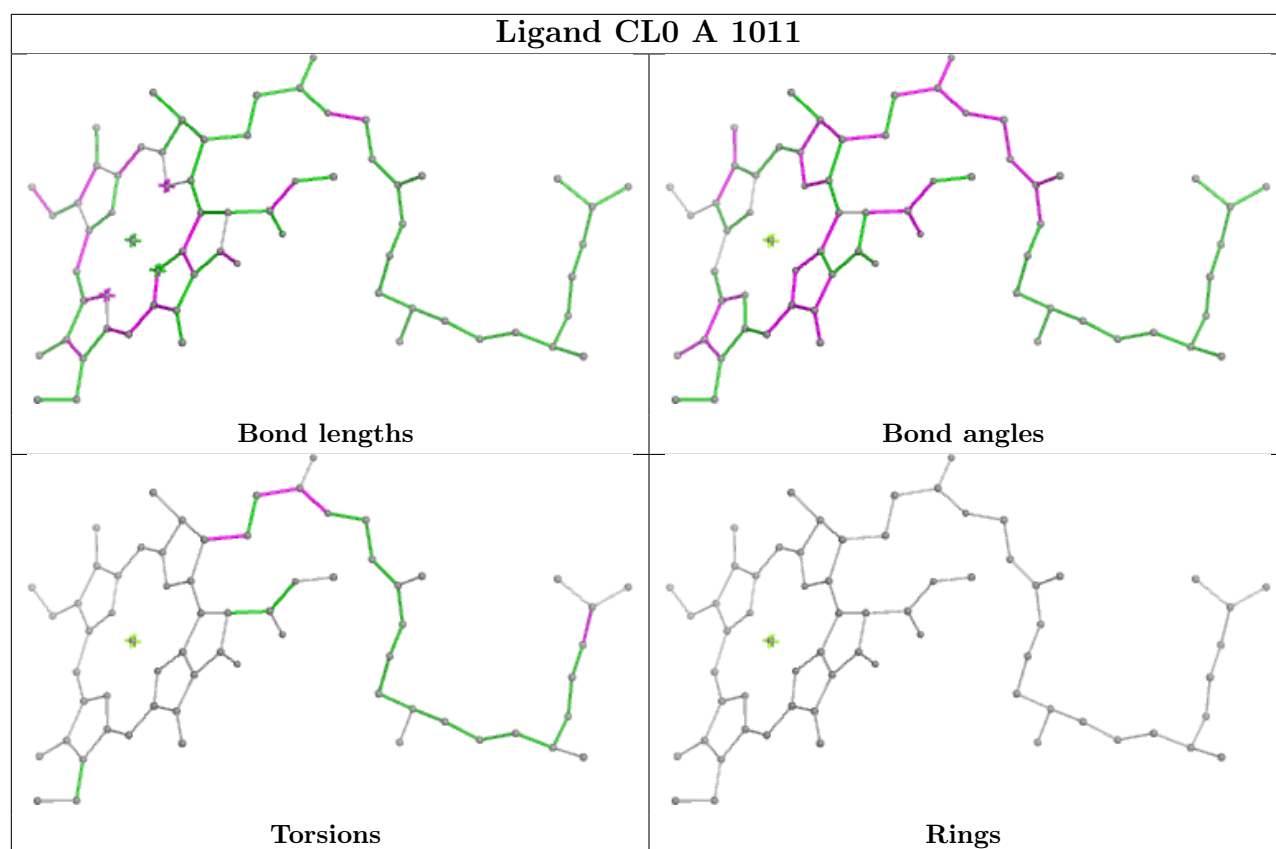


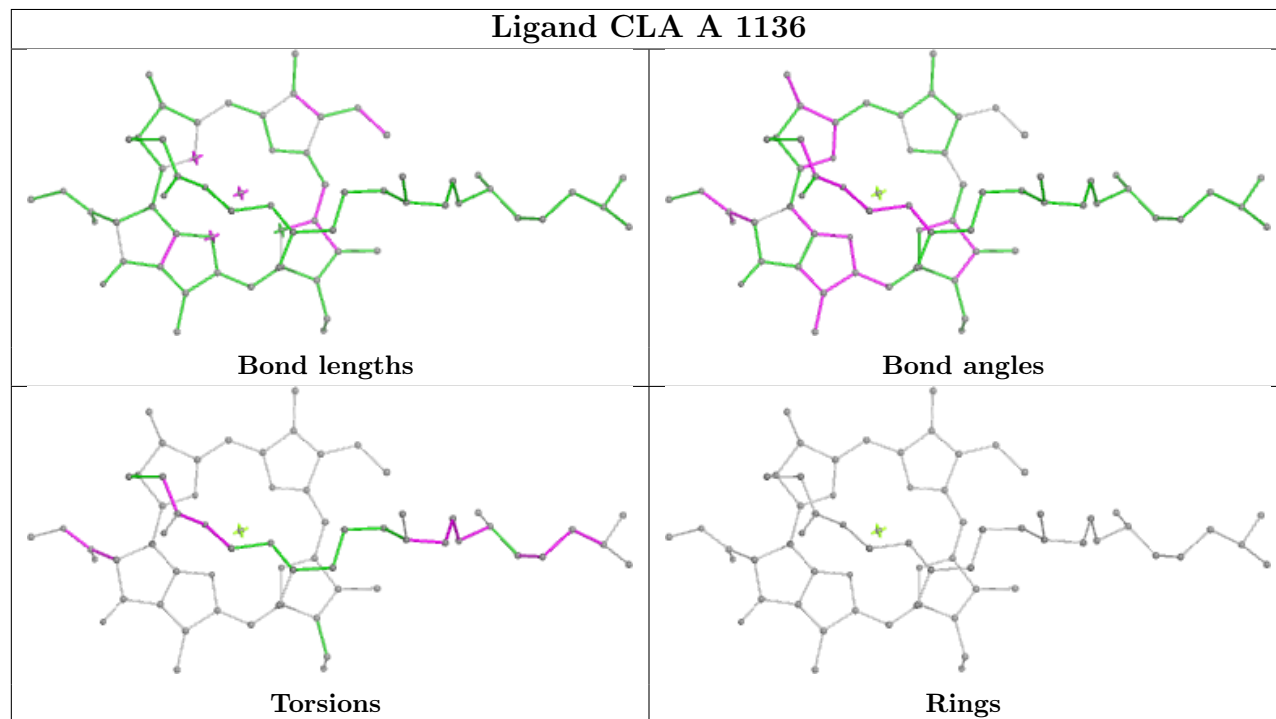
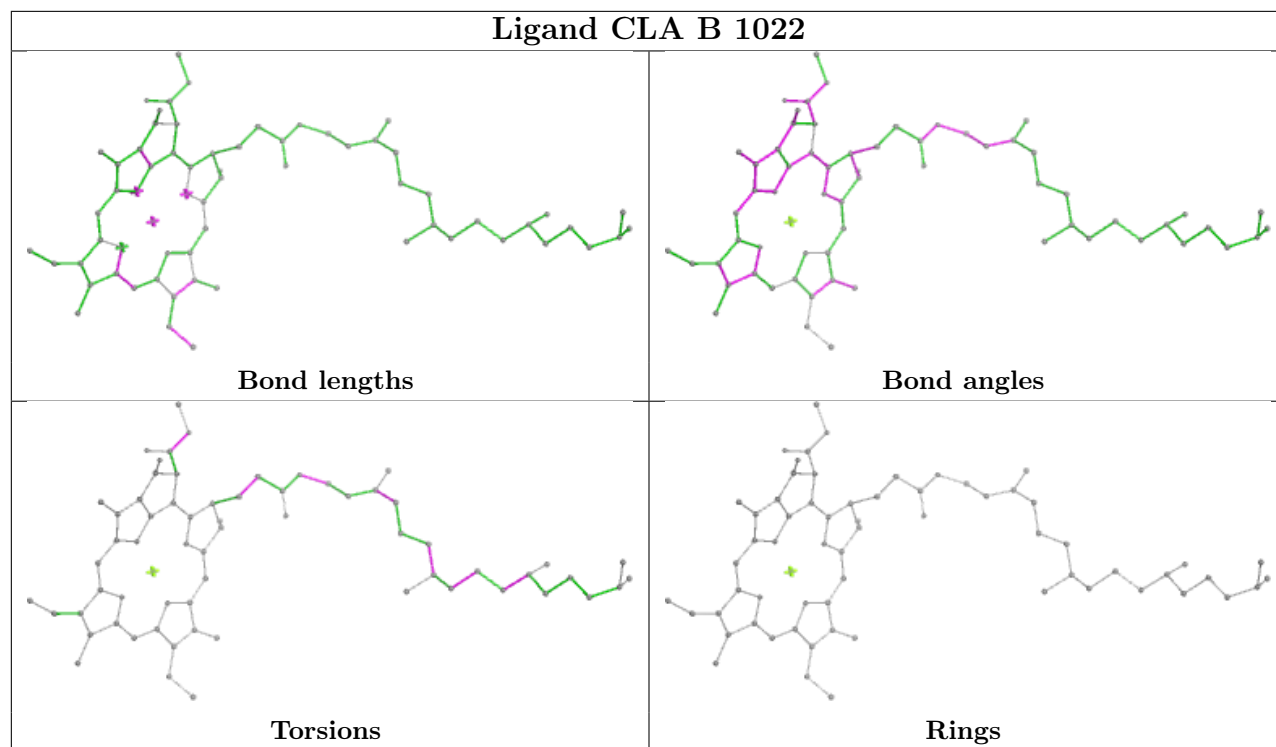
Ligand CLA A 1123

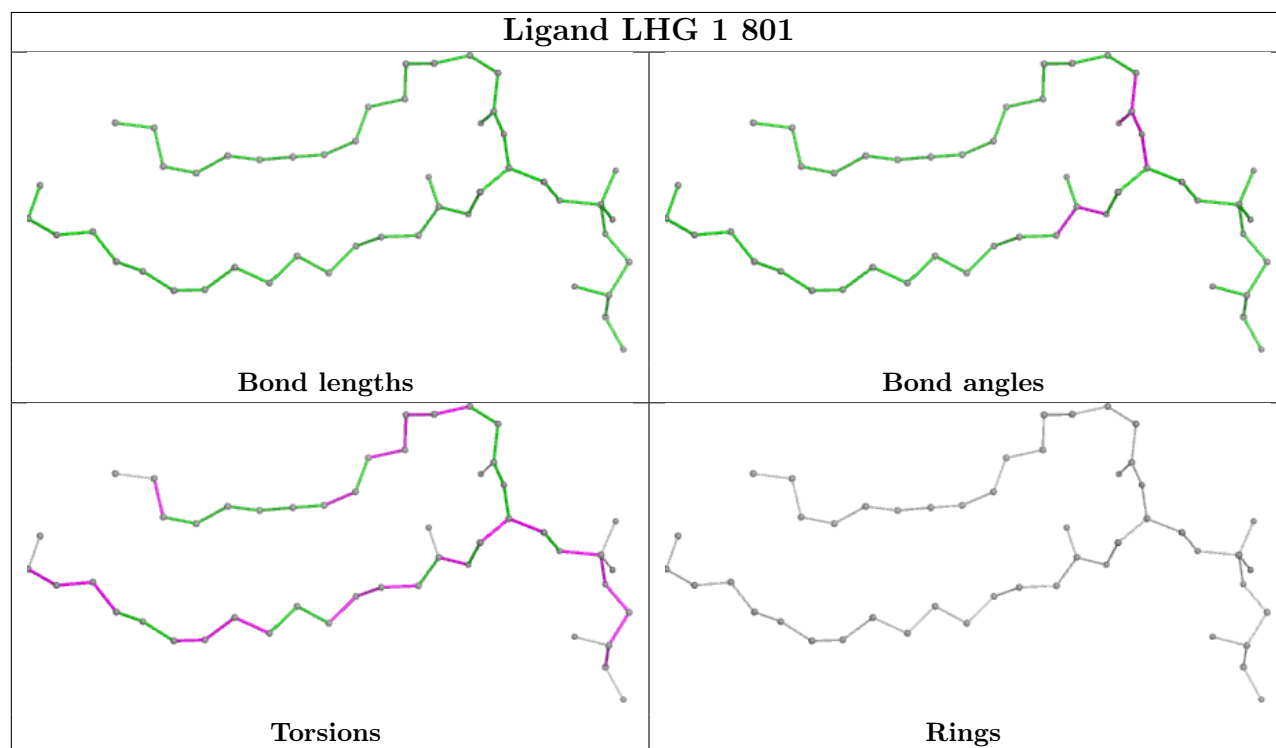
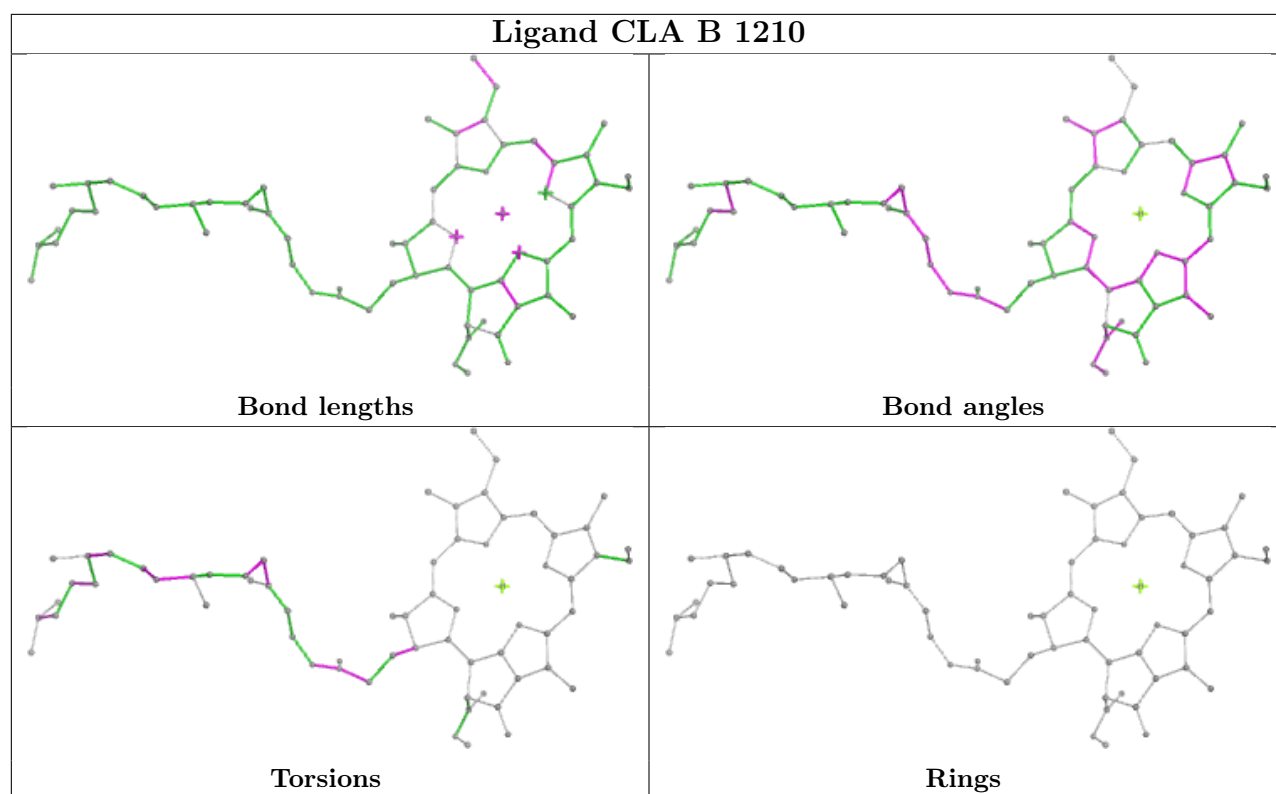


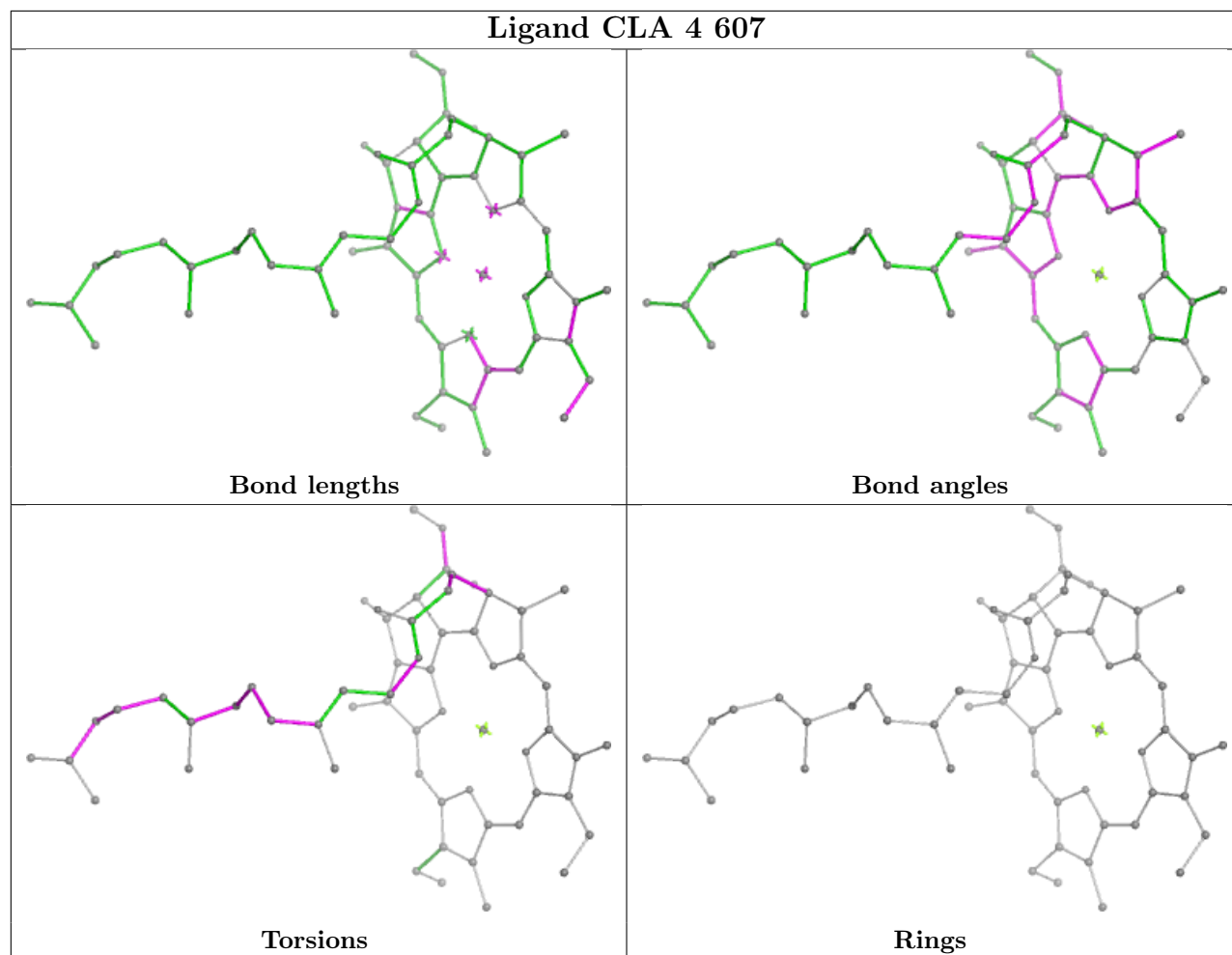
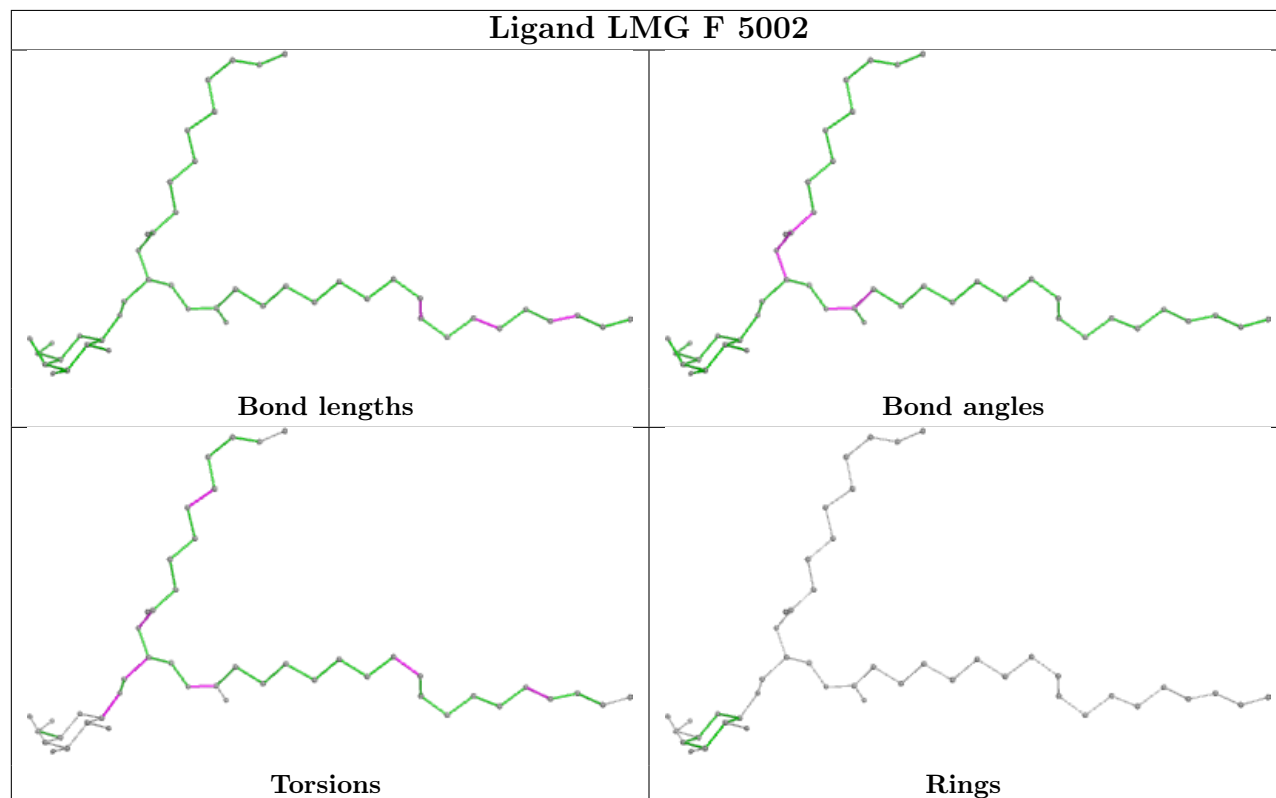


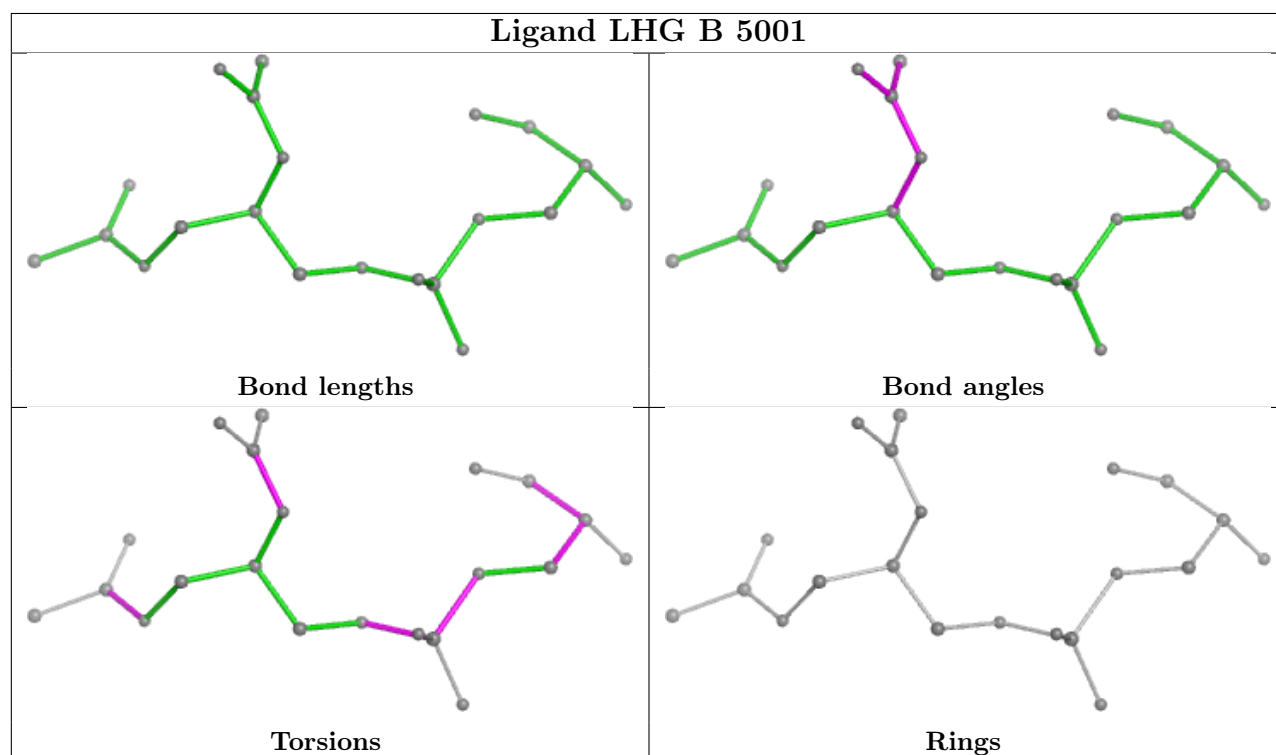
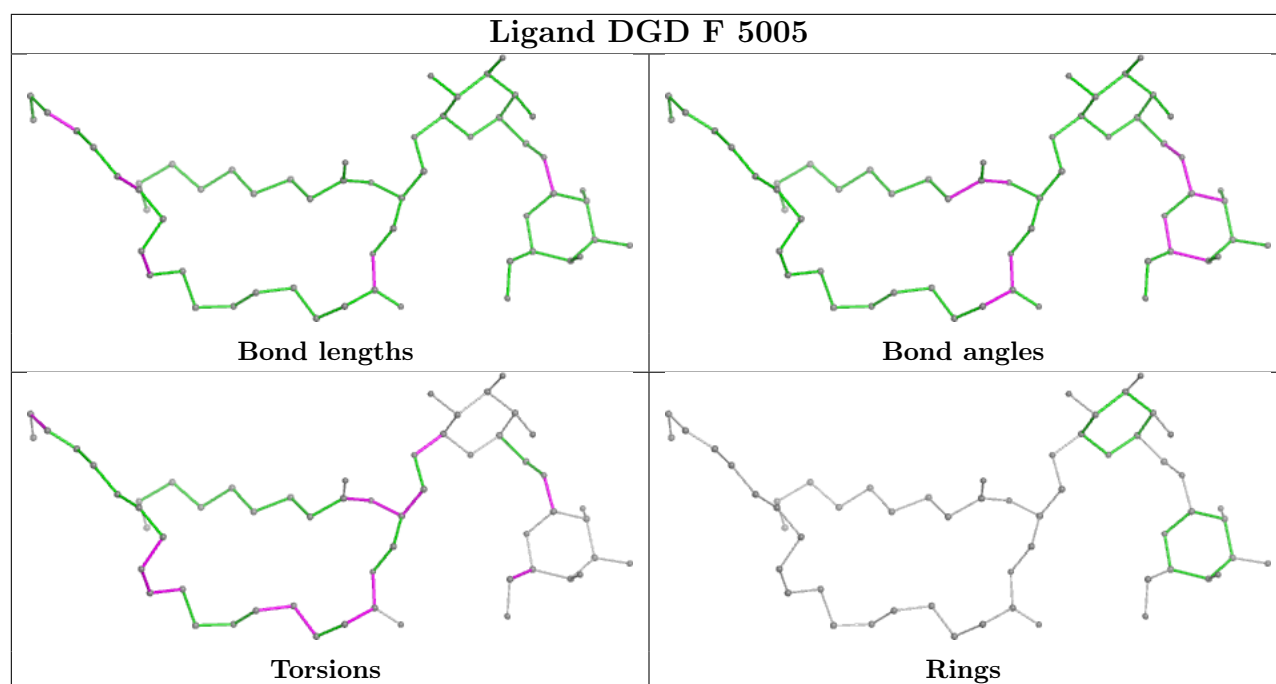




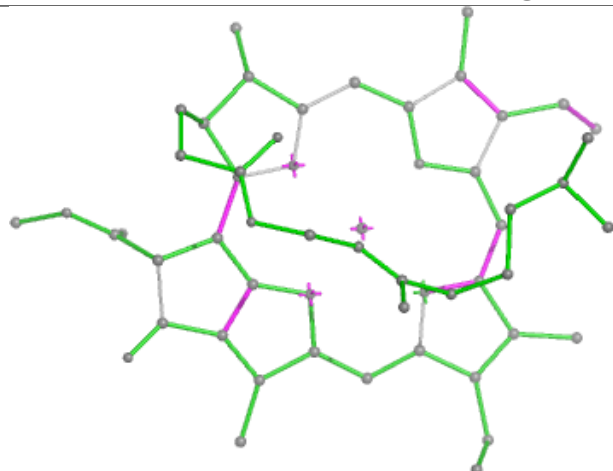




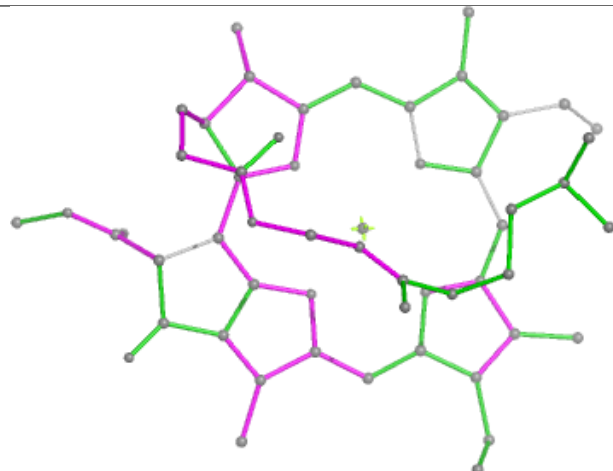
Ligand CLA 4 607**Ligand LMG F 5002**



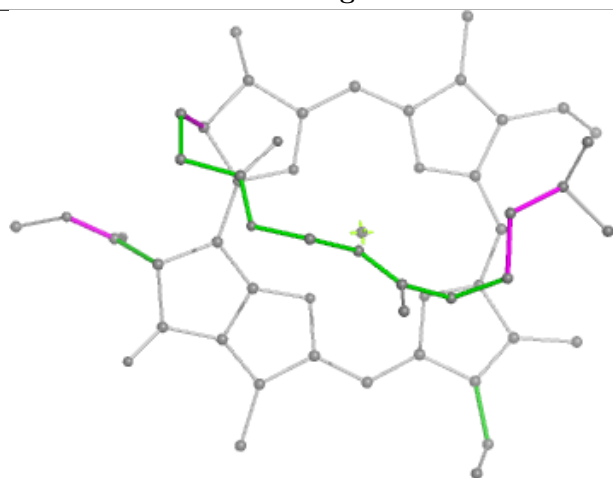
Ligand CLA 1 603



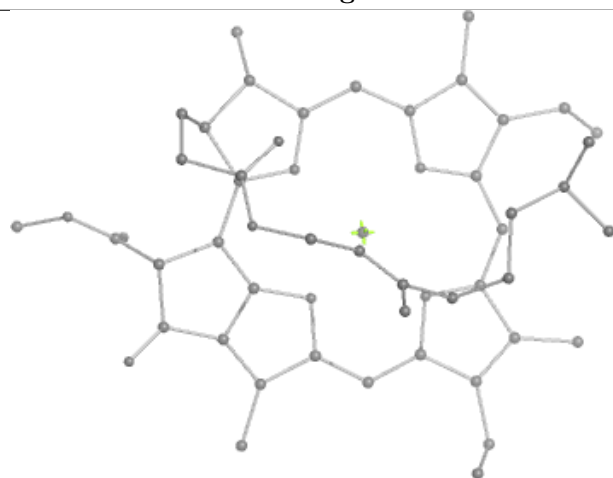
Bond lengths



Bond angles

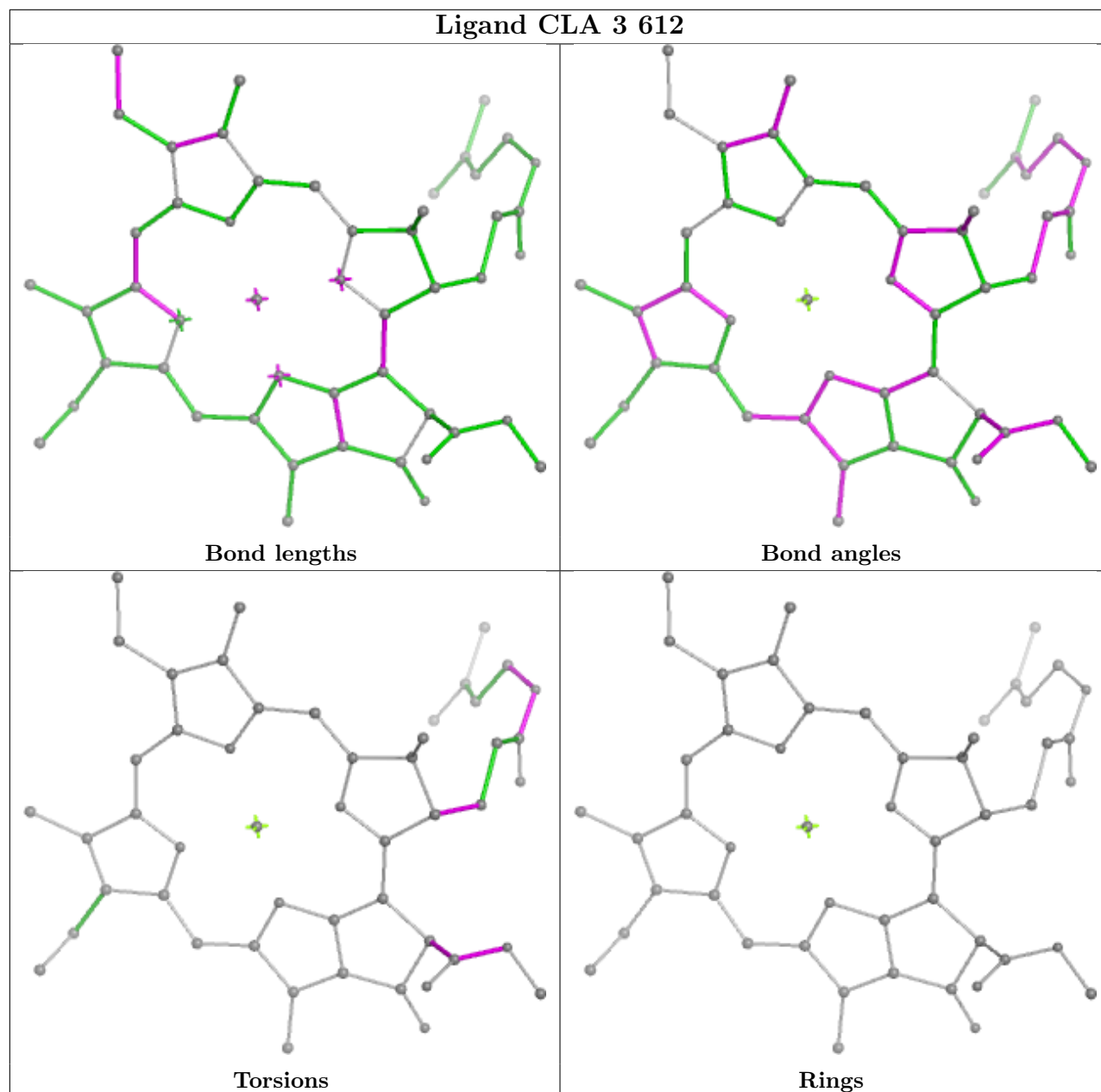


Torsions

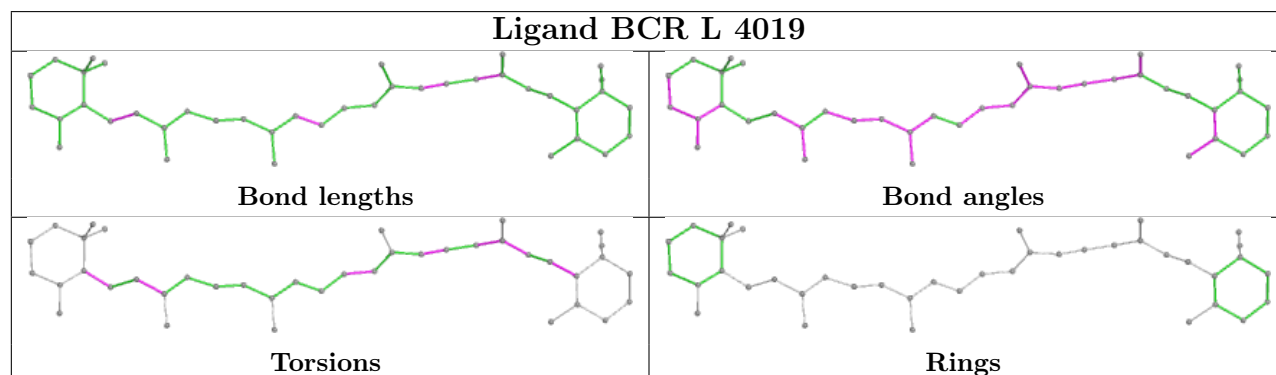


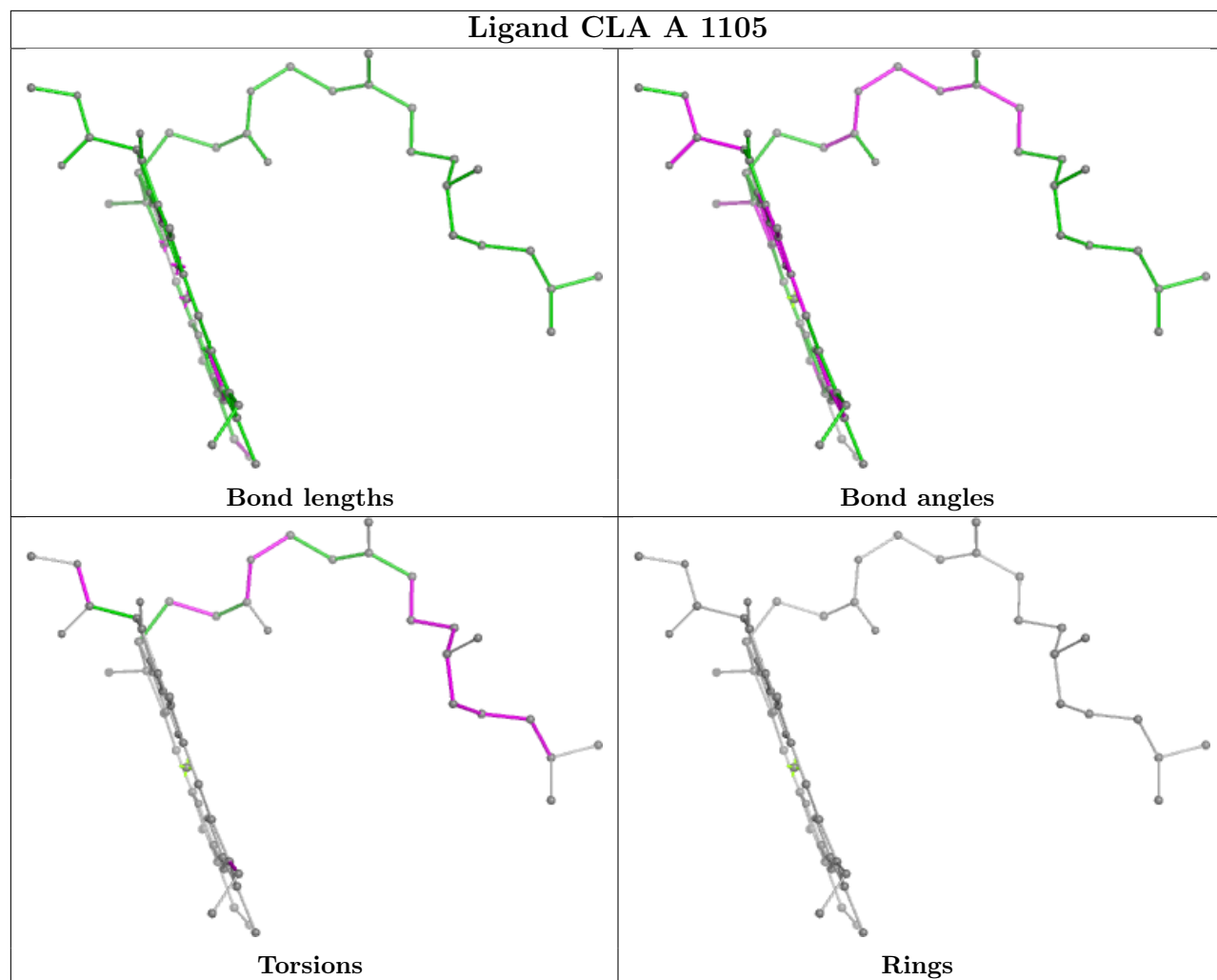
Rings

Ligand CLA 3 612

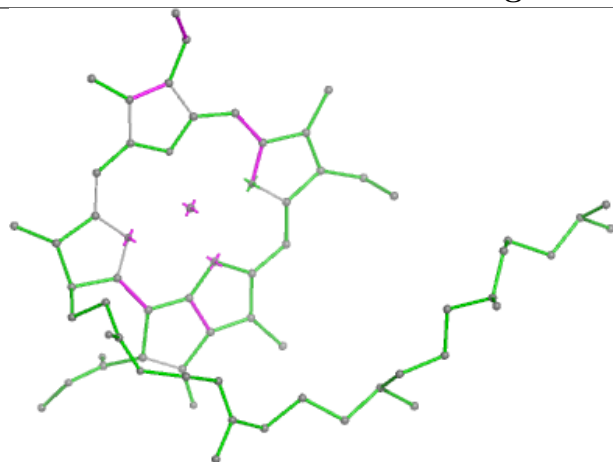


Ligand BCR L 4019

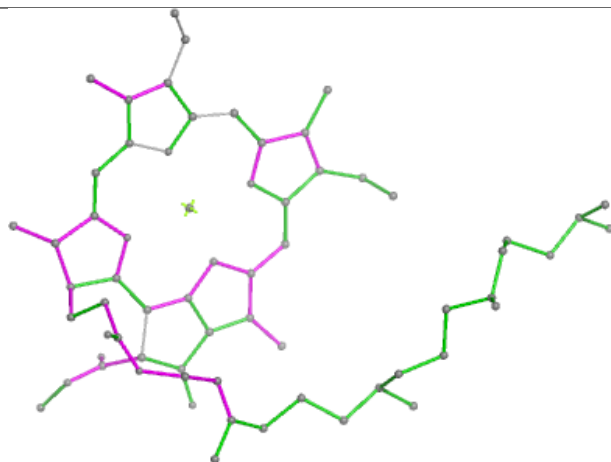




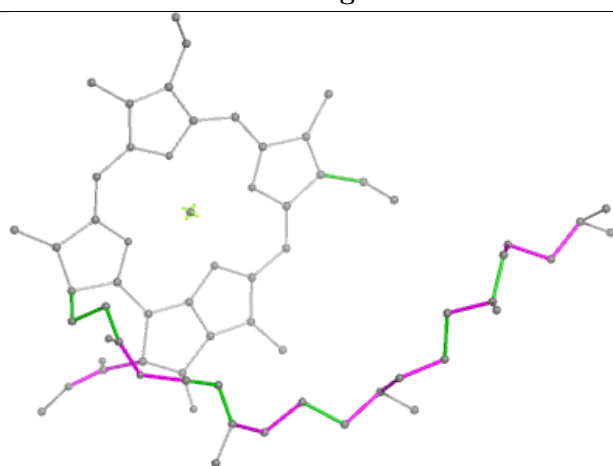
Ligand CLA A 1127



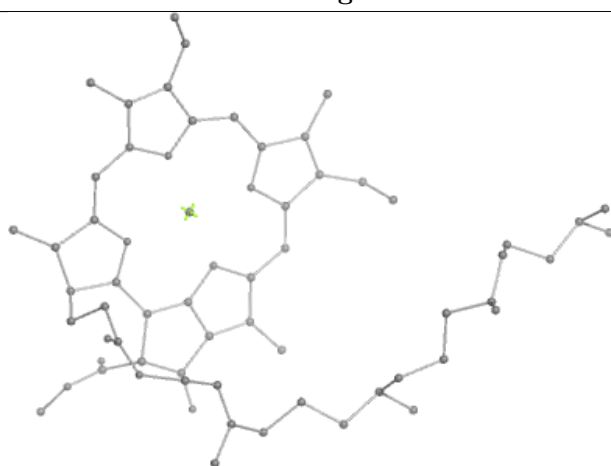
Bond lengths



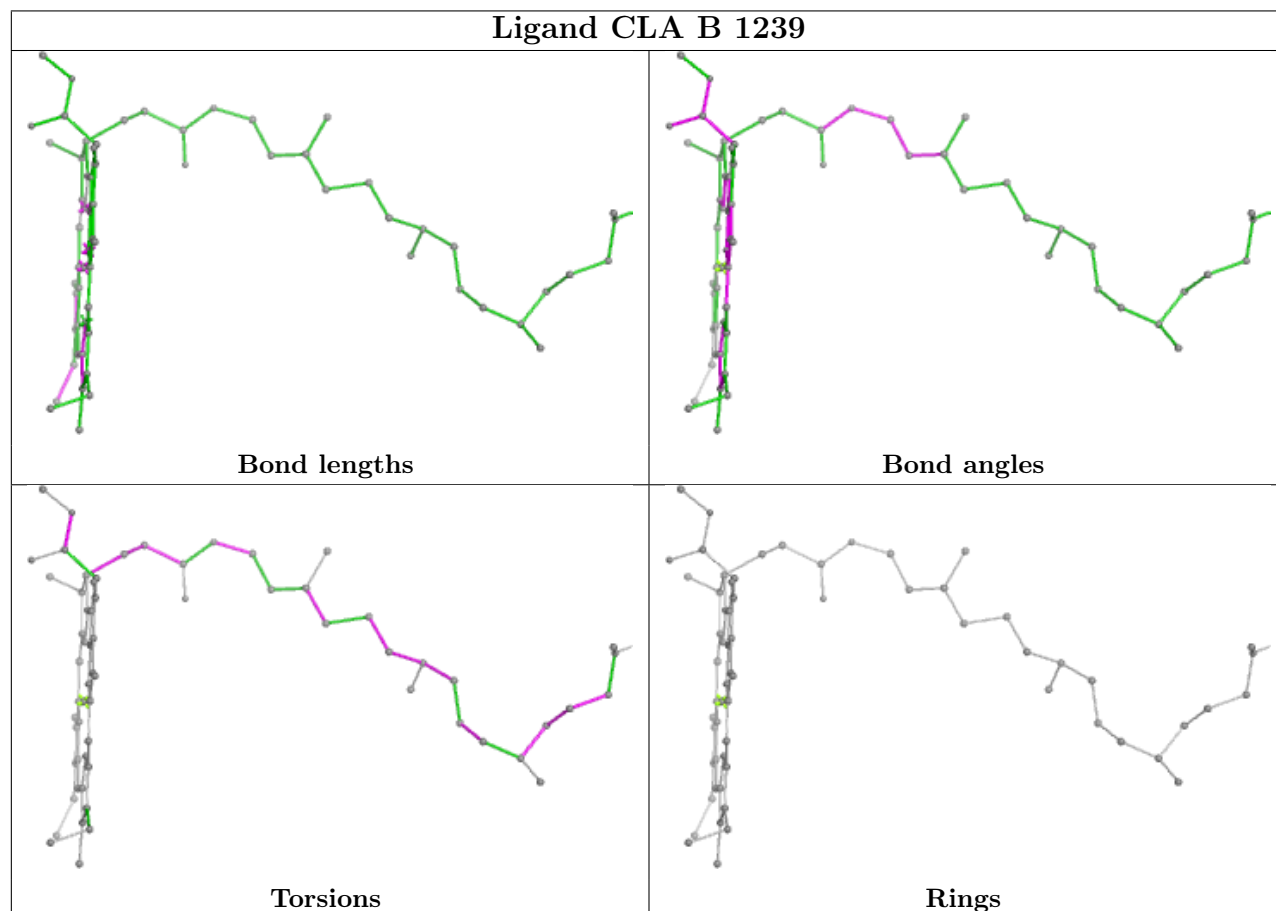
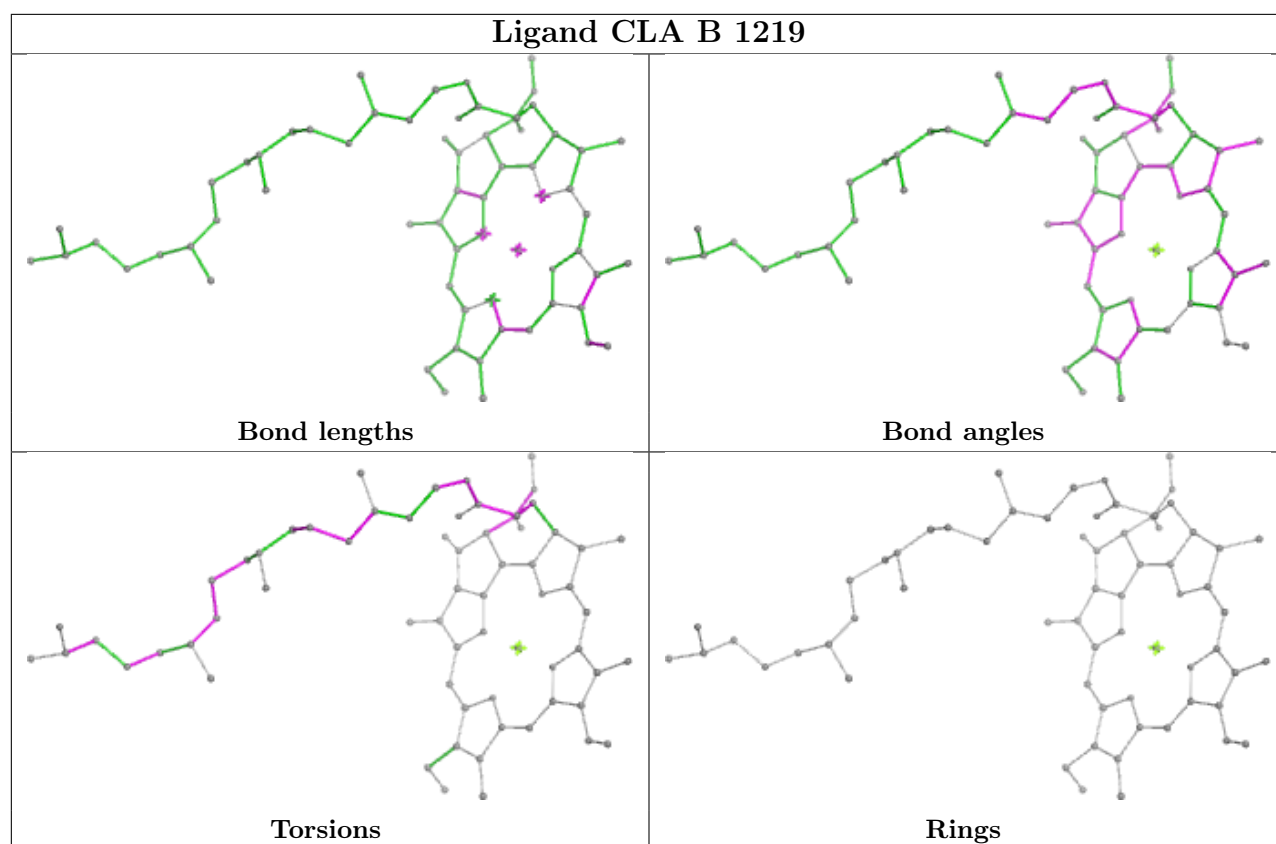
Bond angles

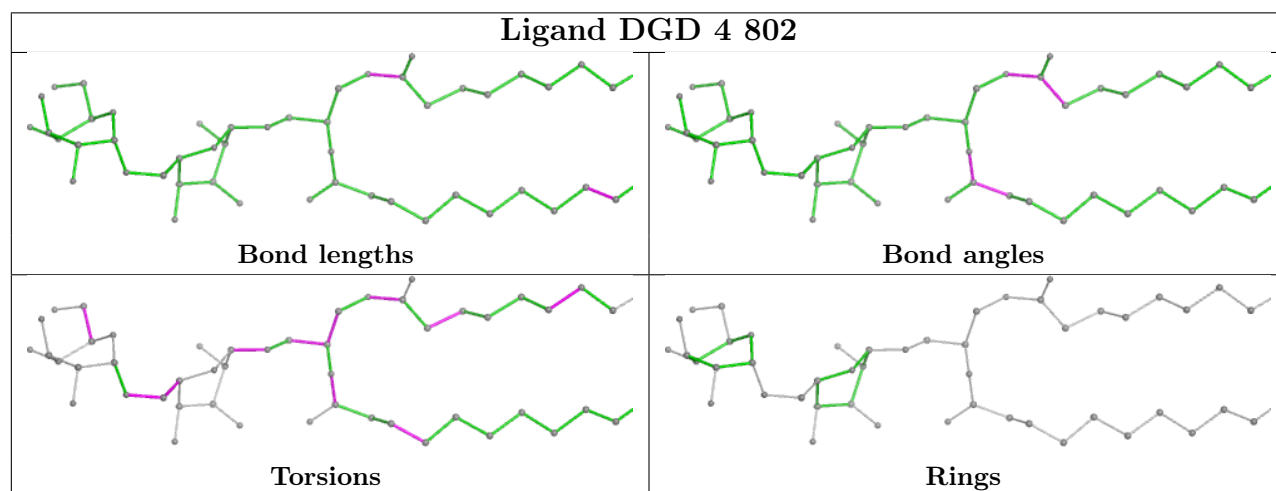
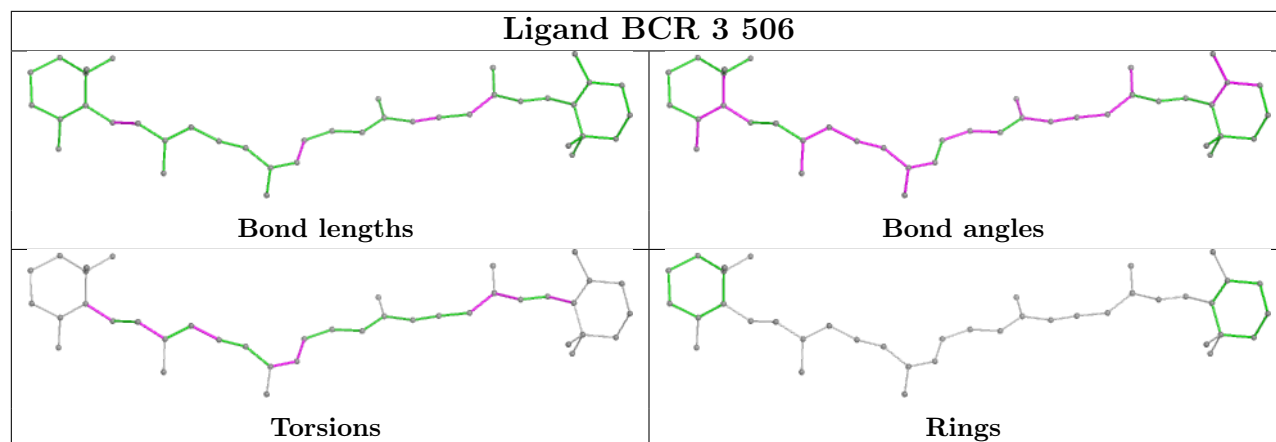


Torsions

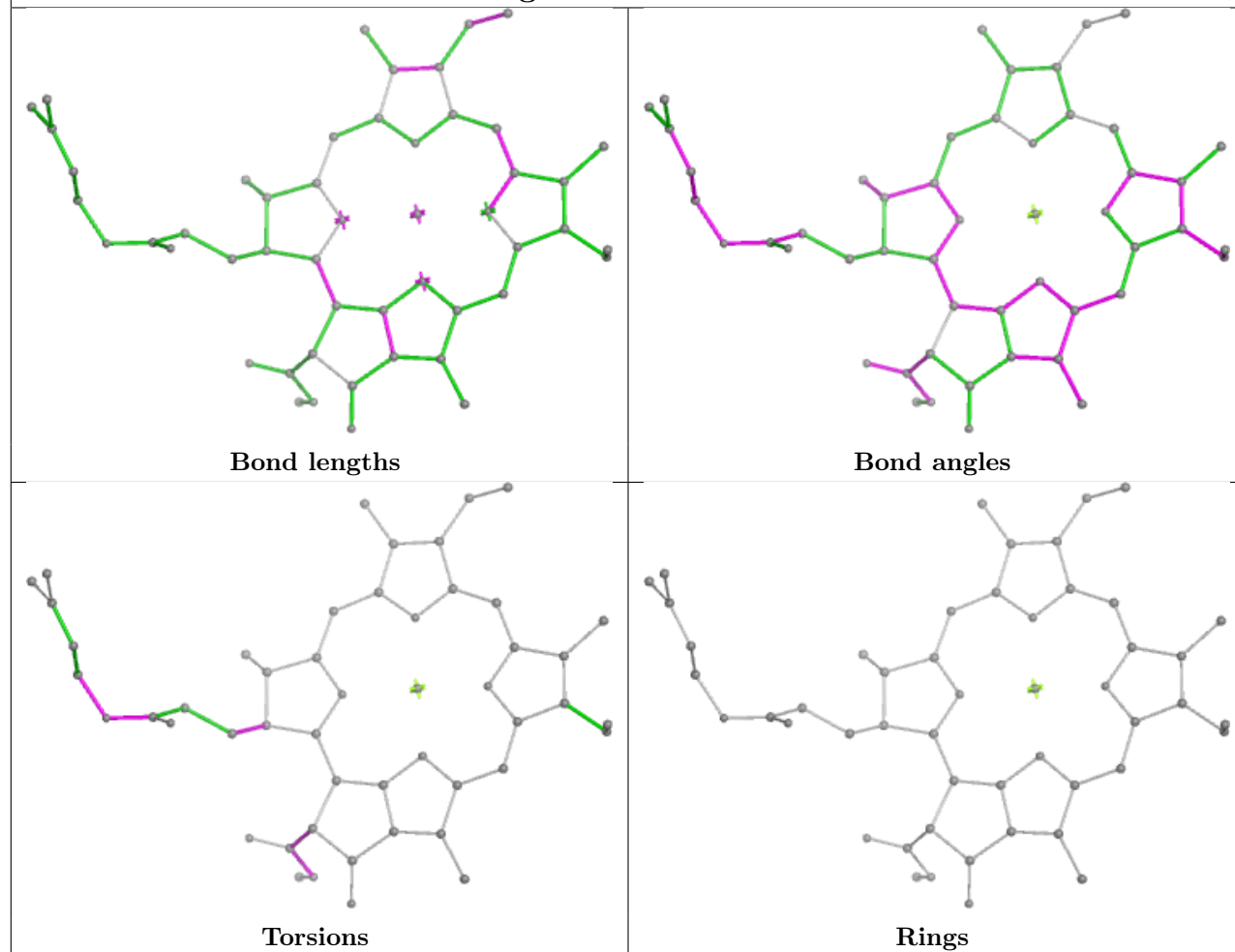


Rings

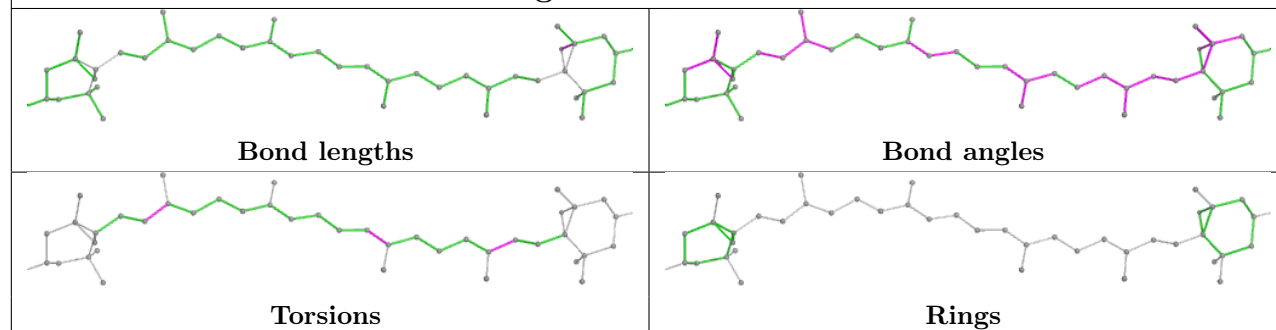


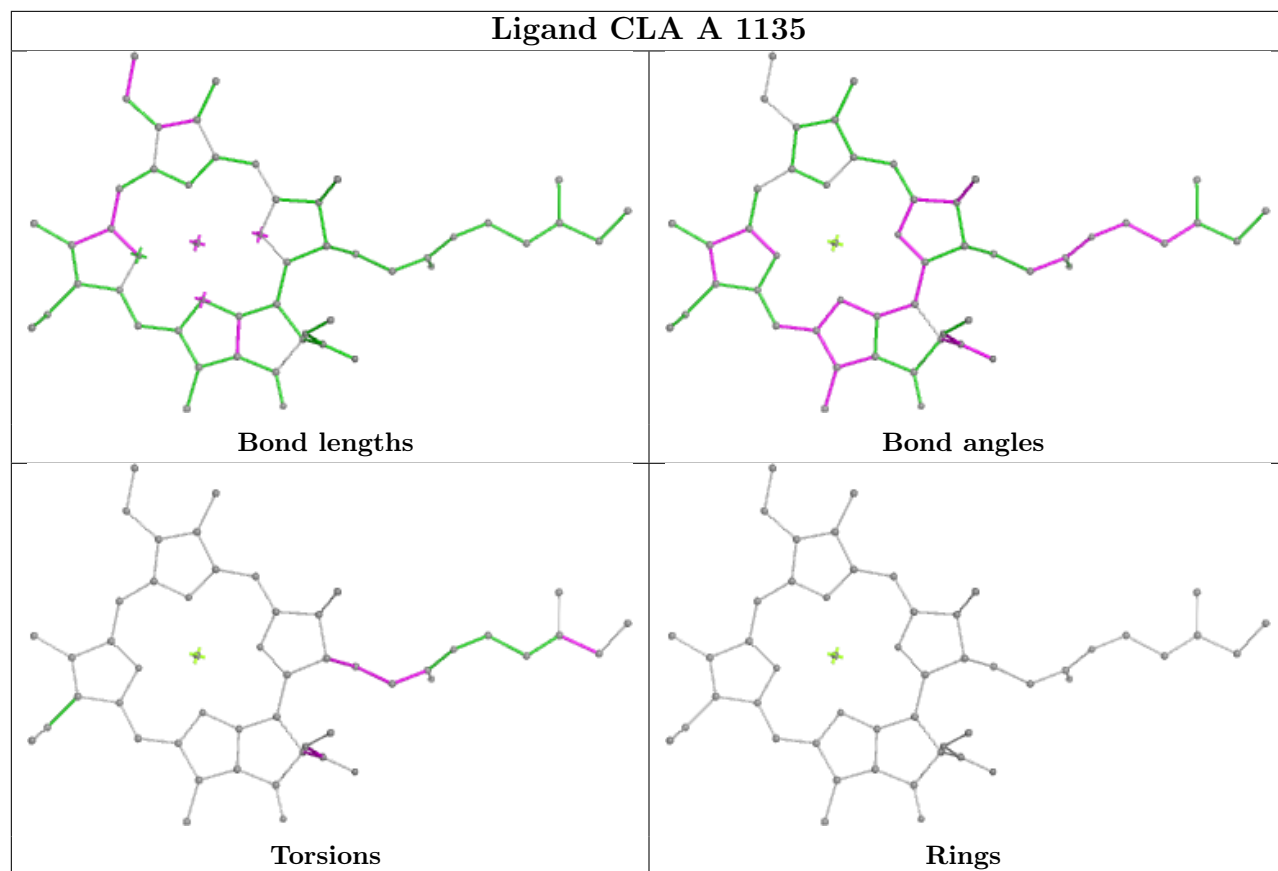


Ligand CLA 4 609

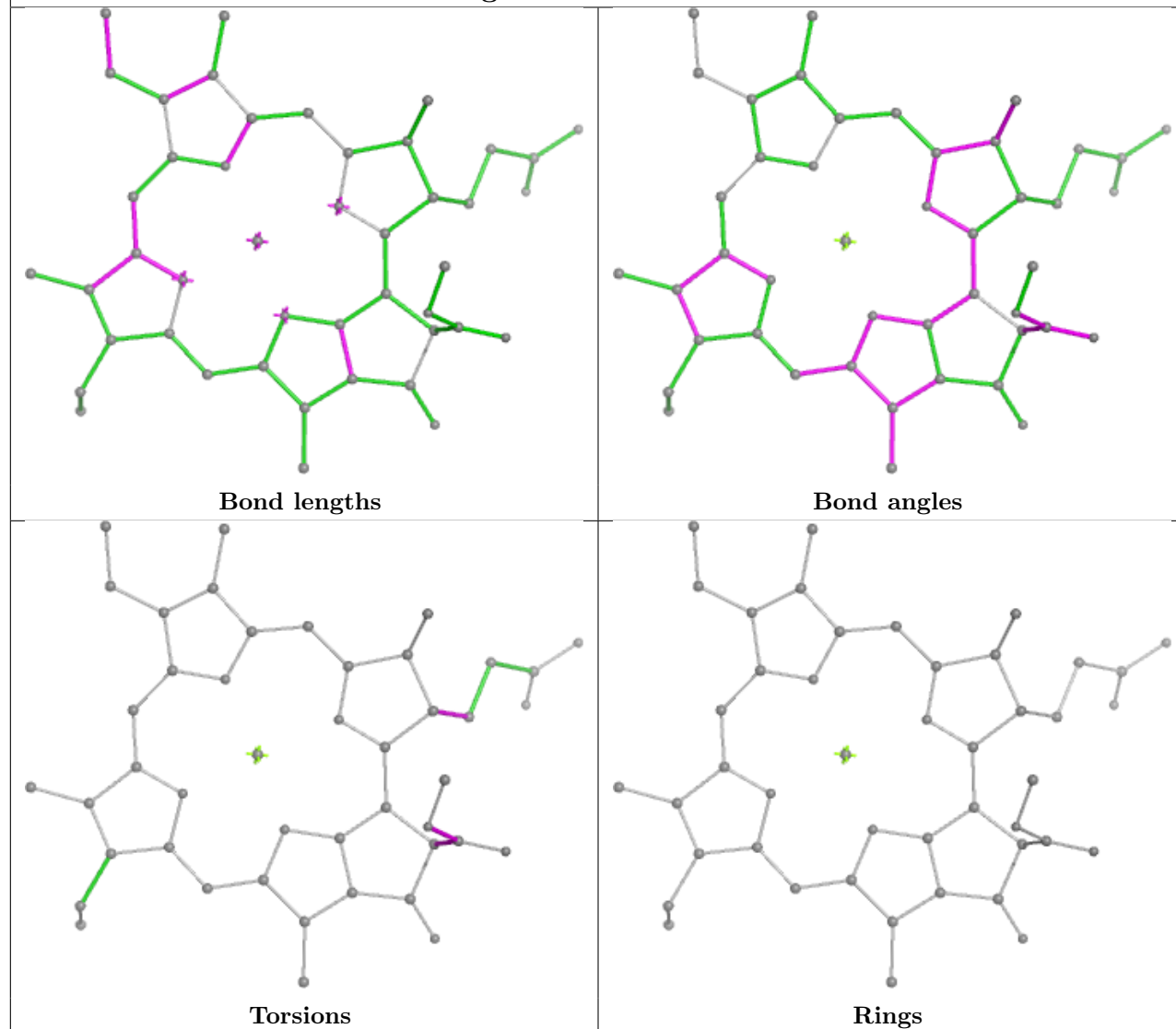


Ligand XAT 4 502

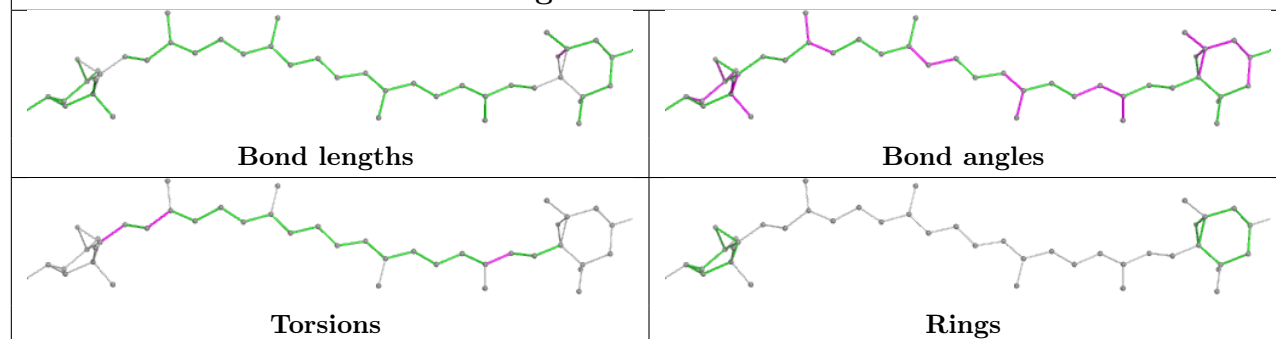


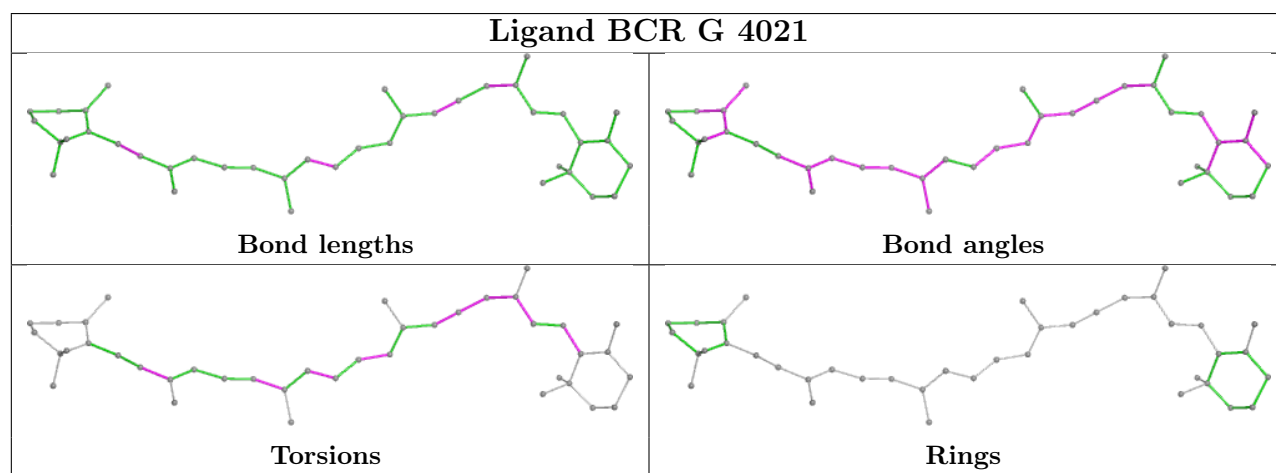
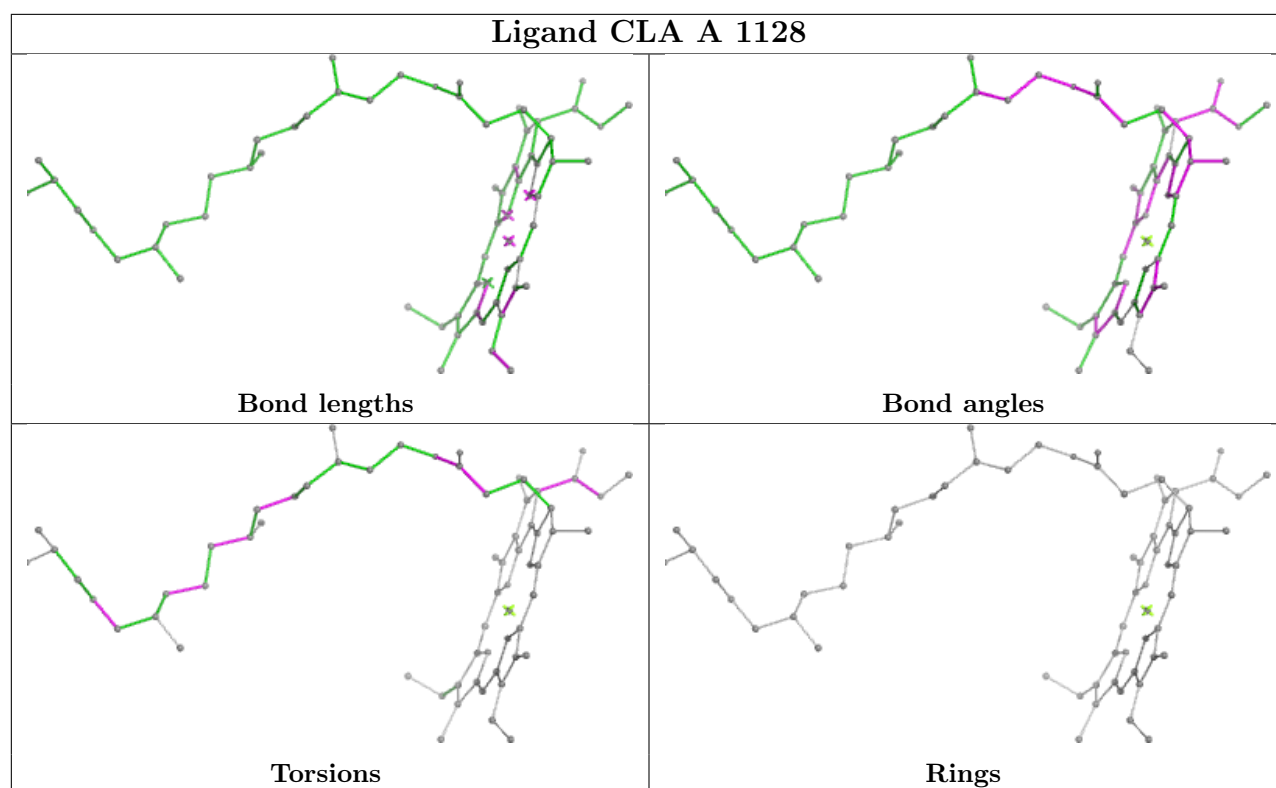


Ligand CLA K 1401

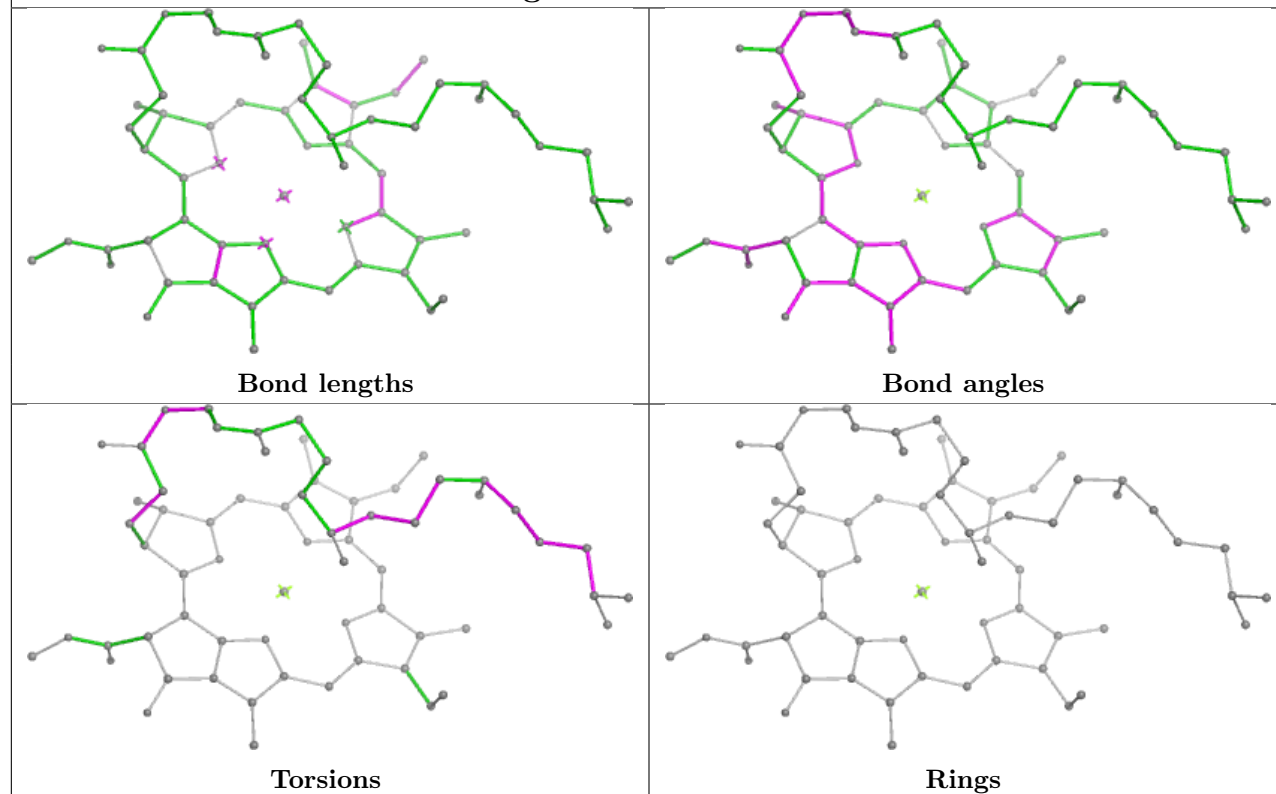


Ligand XAT 2 502

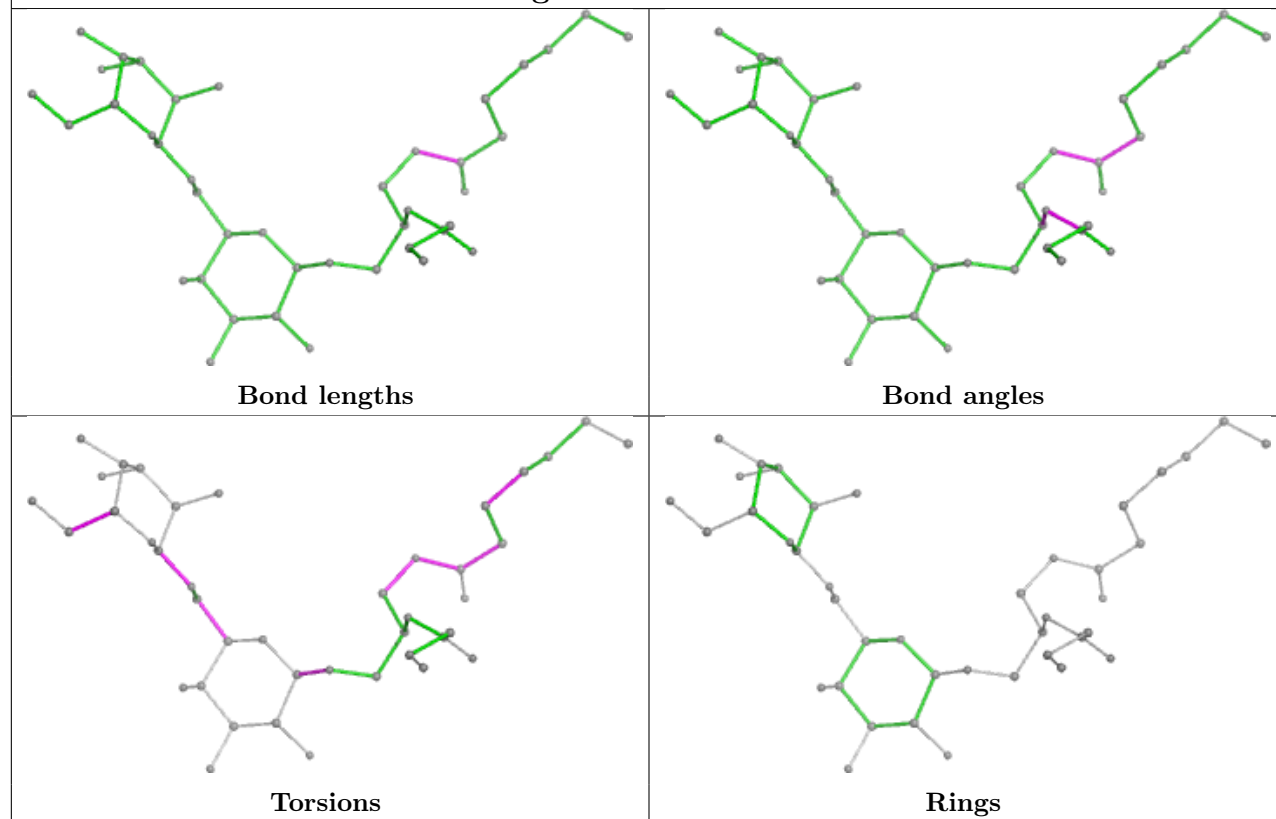


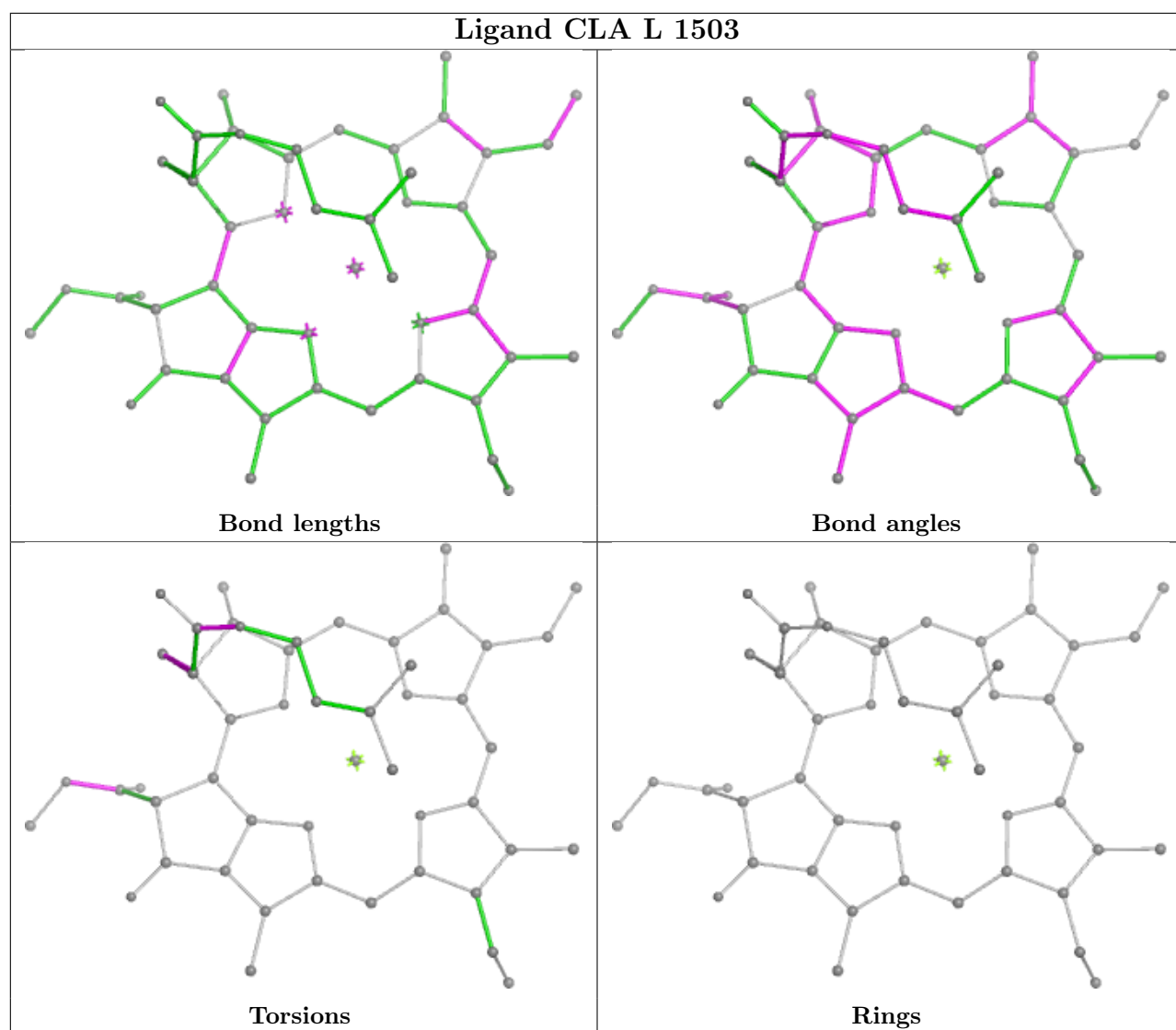


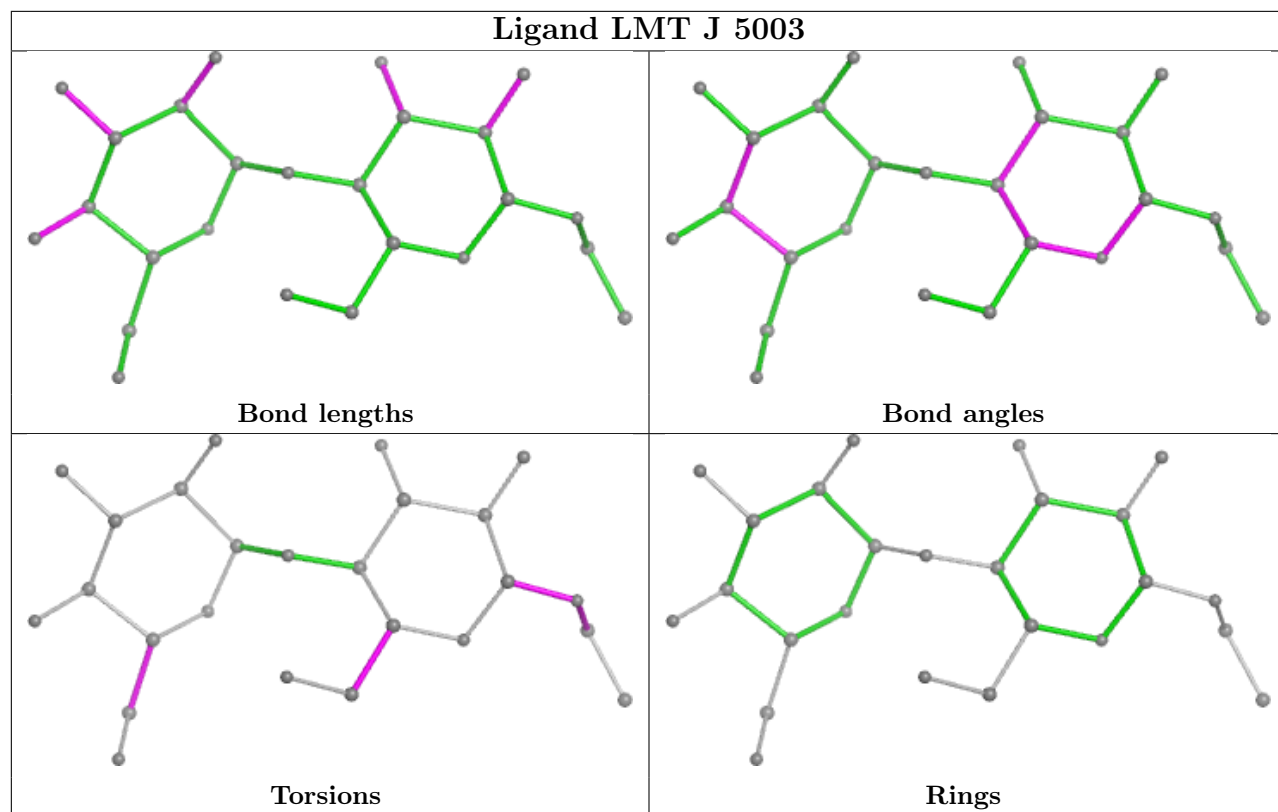
Ligand CLA B 1214



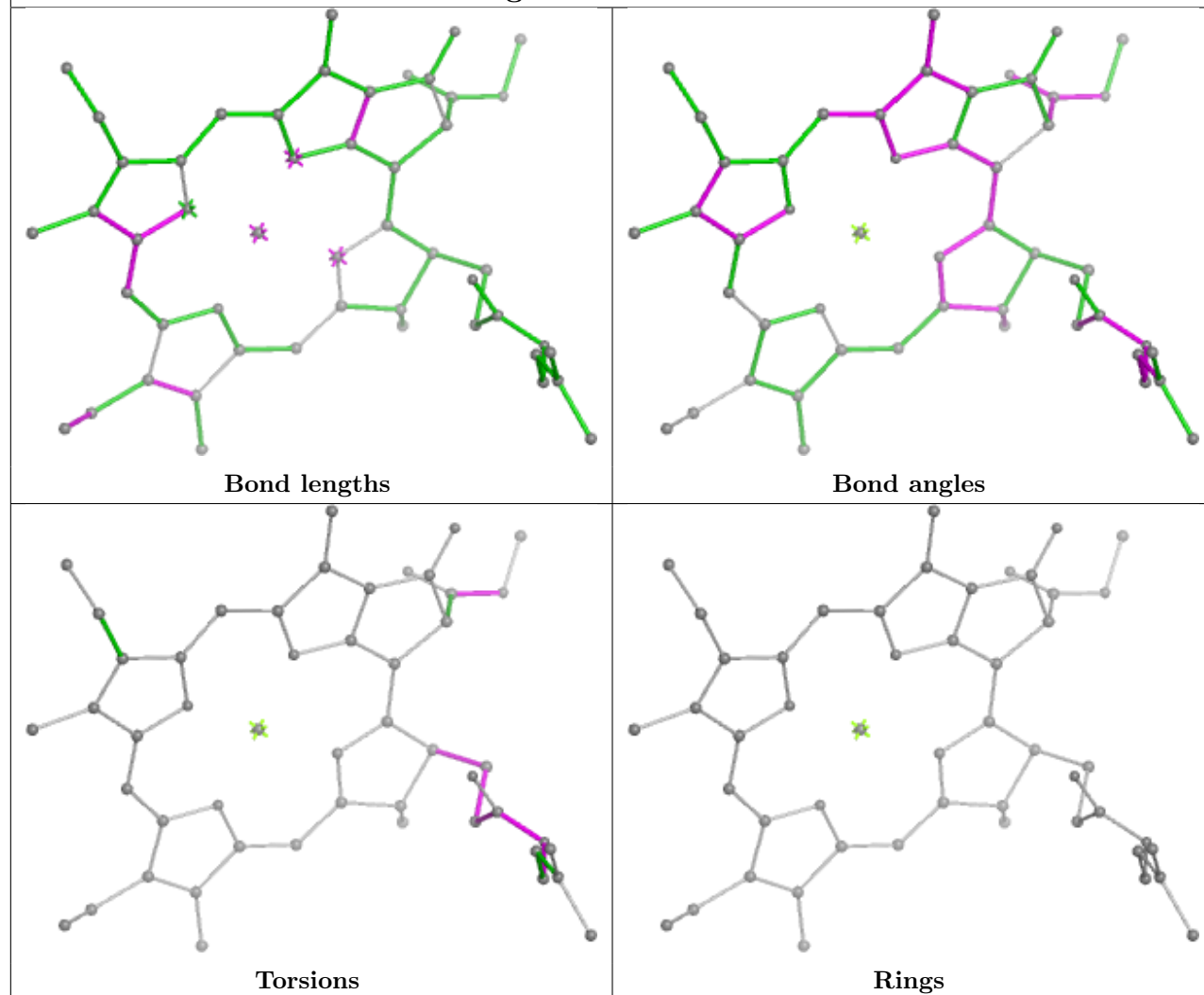
Ligand DGD 1 803



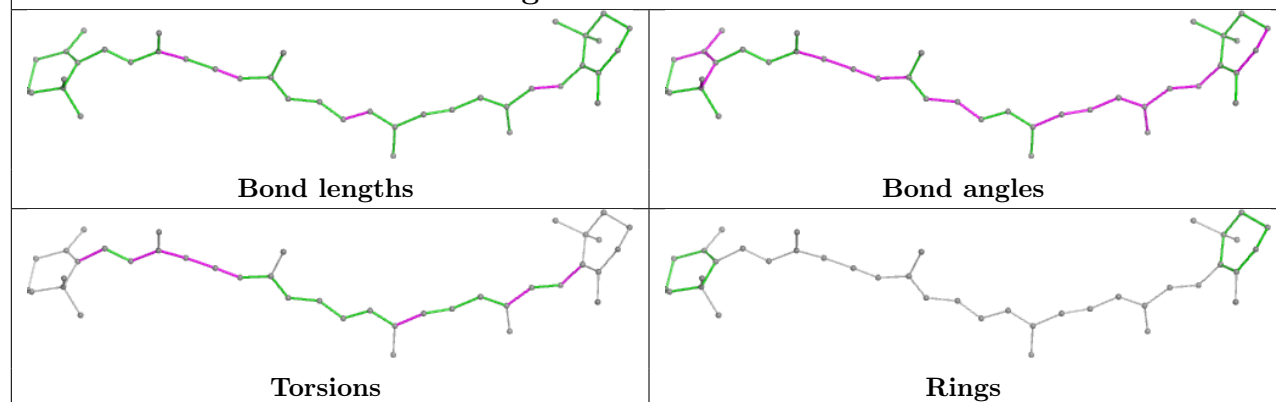


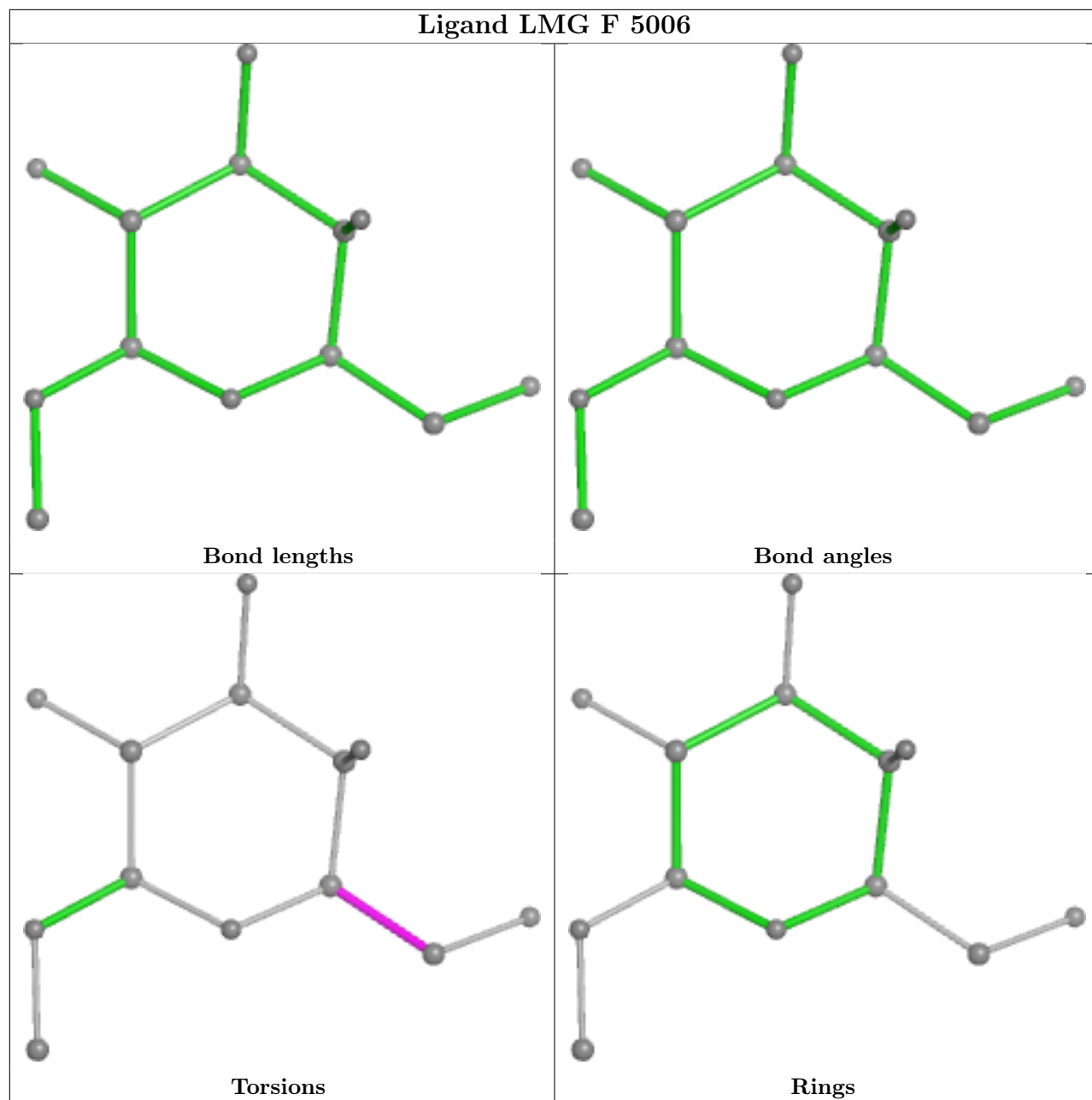


Ligand CLA 2 608

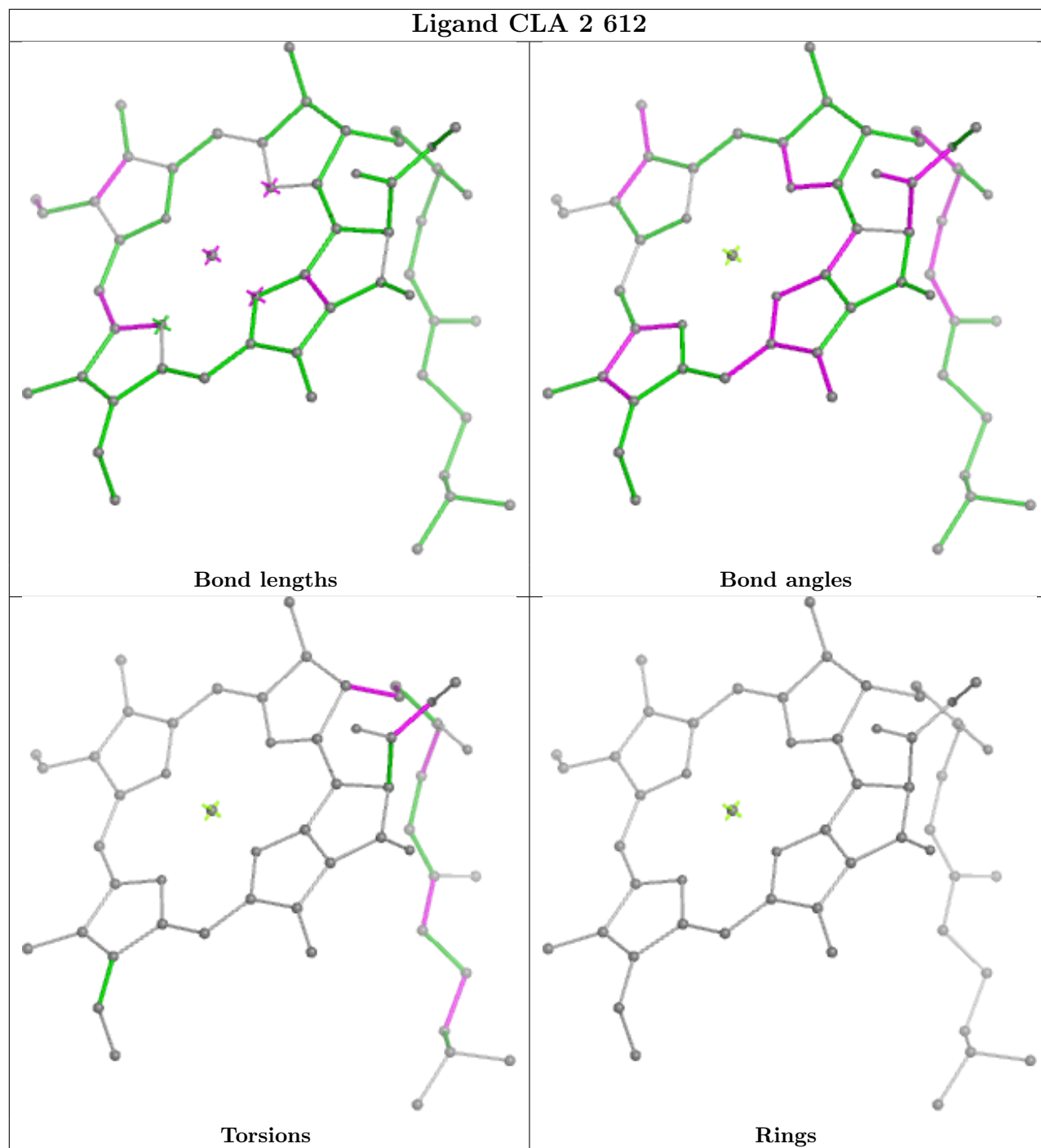


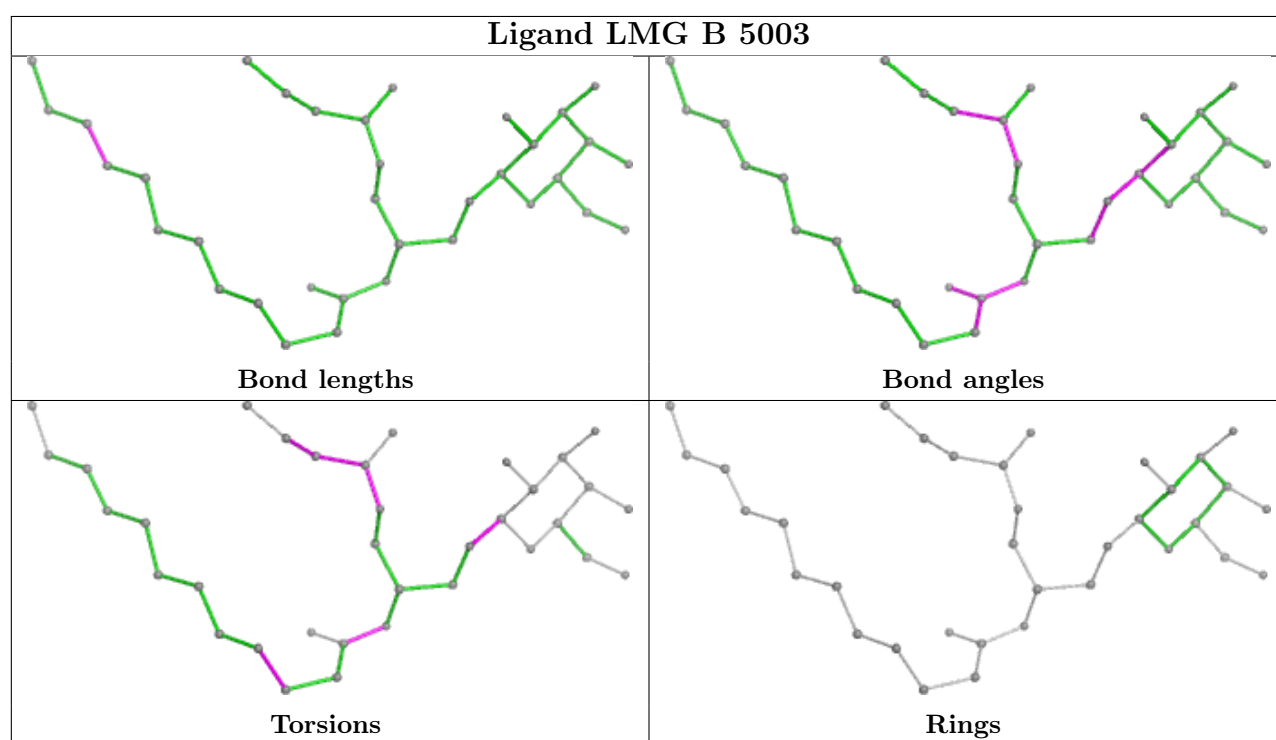
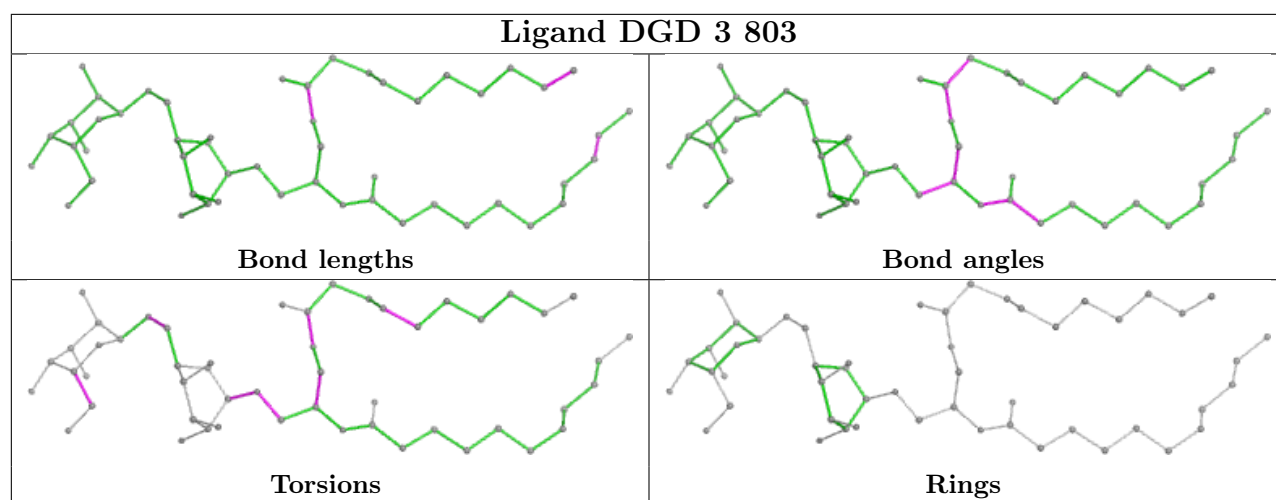
Ligand BCR B 4010

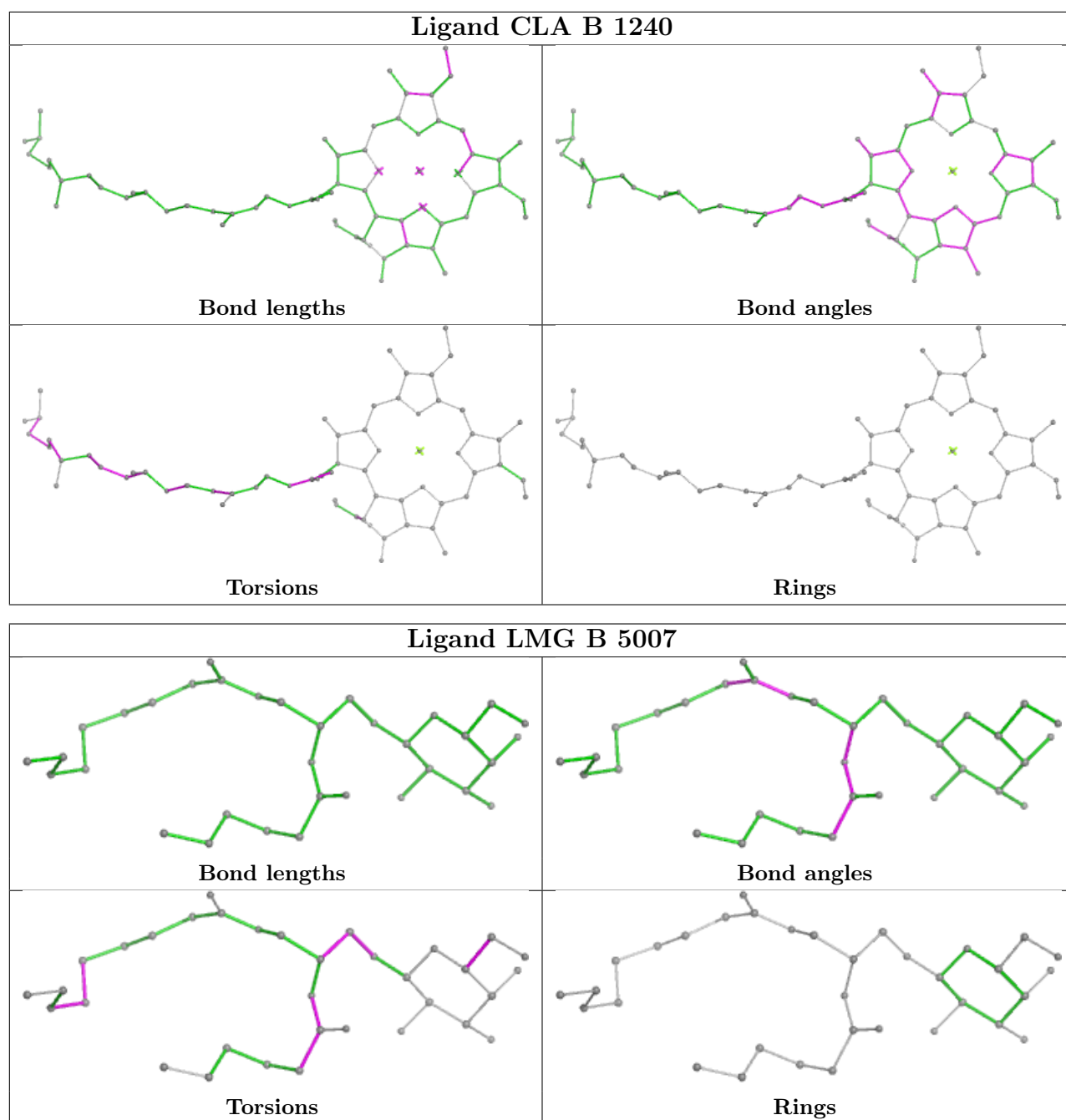


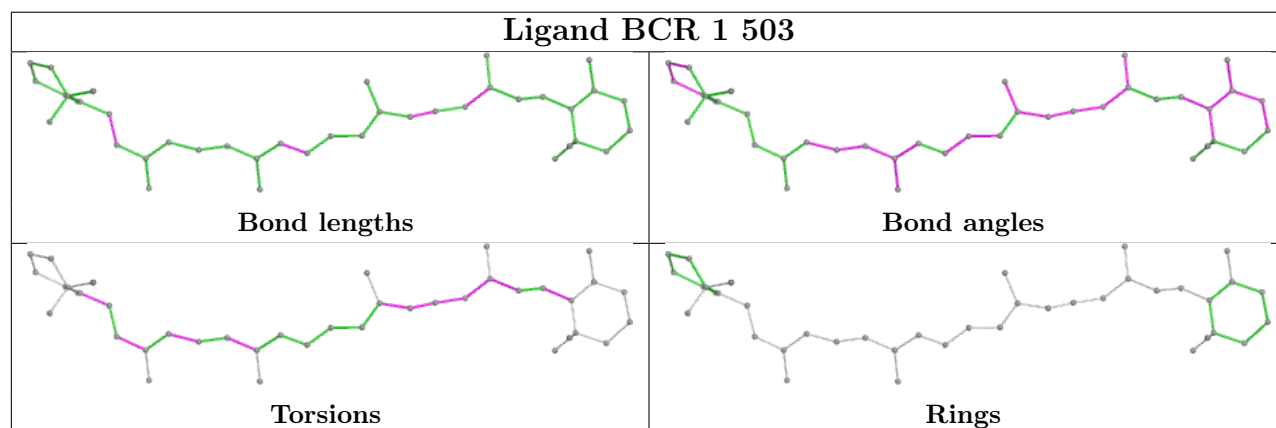
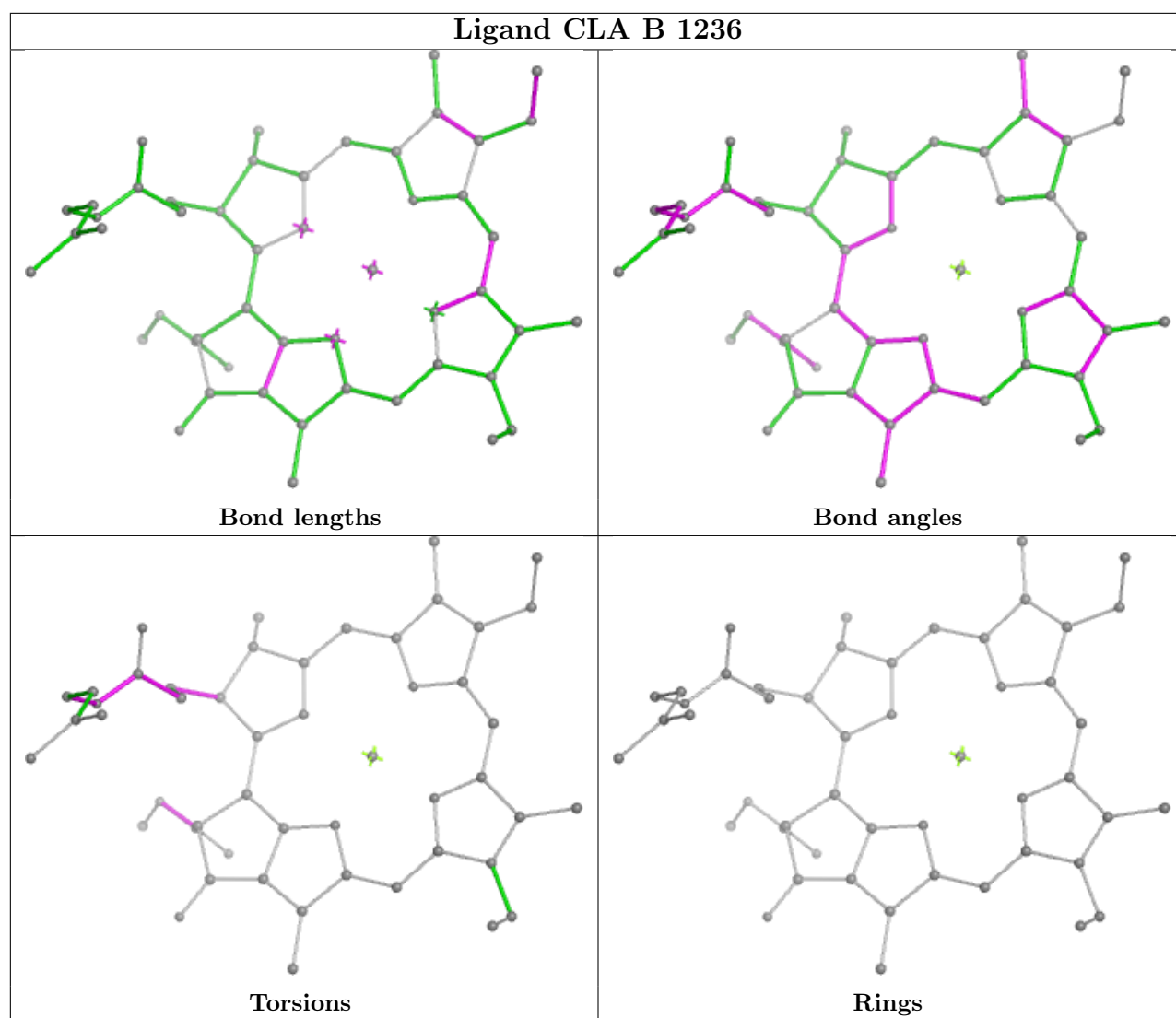


Ligand CLA 2 612

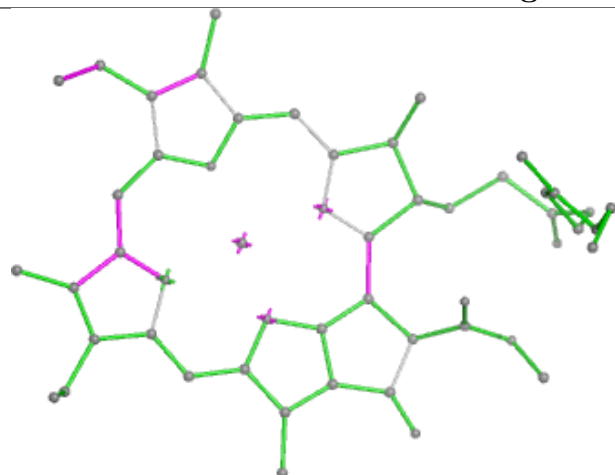




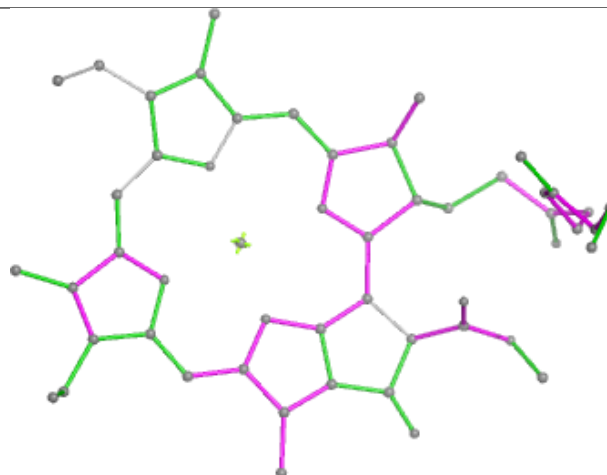




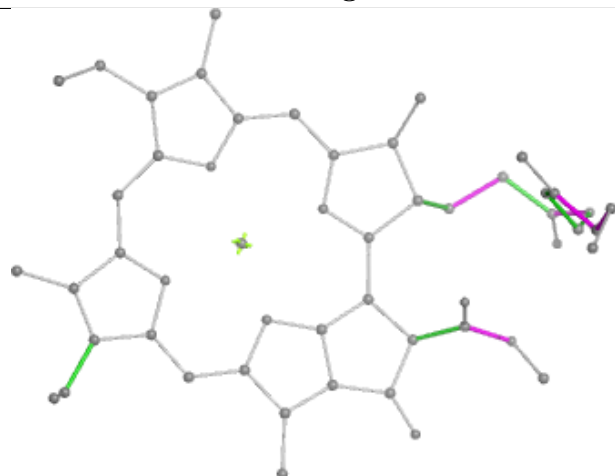
Ligand CLA 2 602



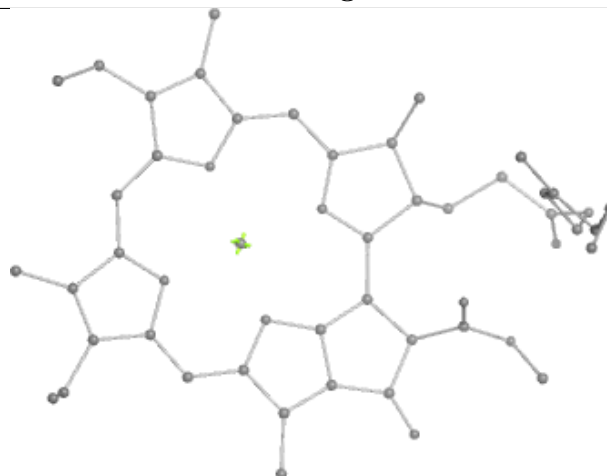
Bond lengths



Bond angles

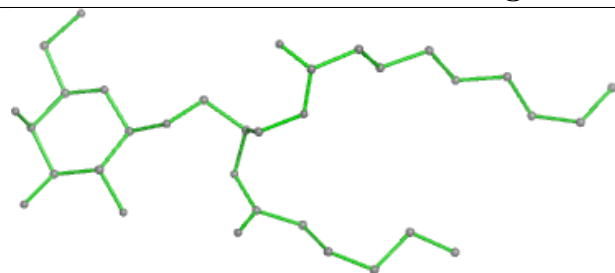


Torsions

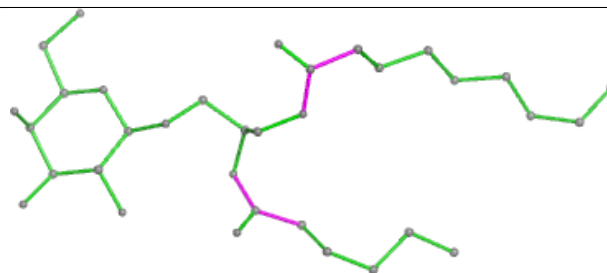


Rings

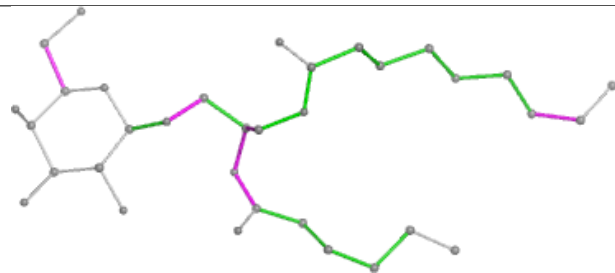
Ligand LMG F 5004



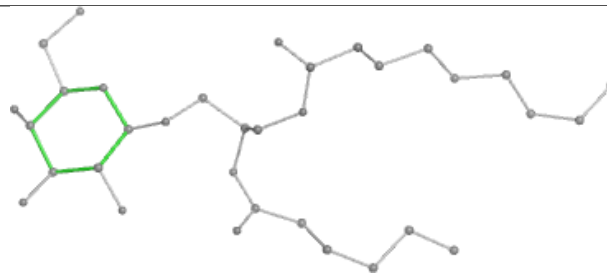
Bond lengths



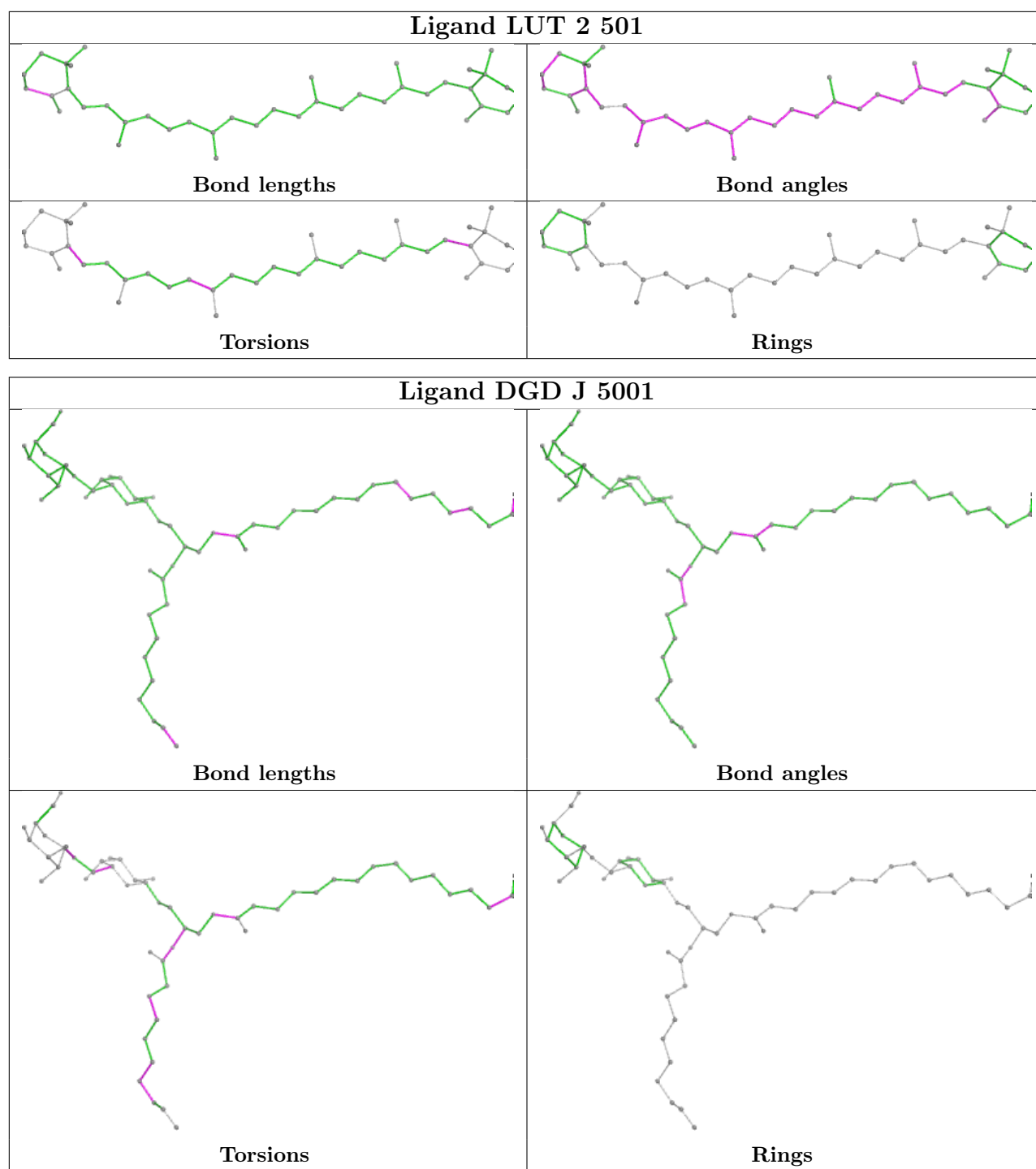
Bond angles



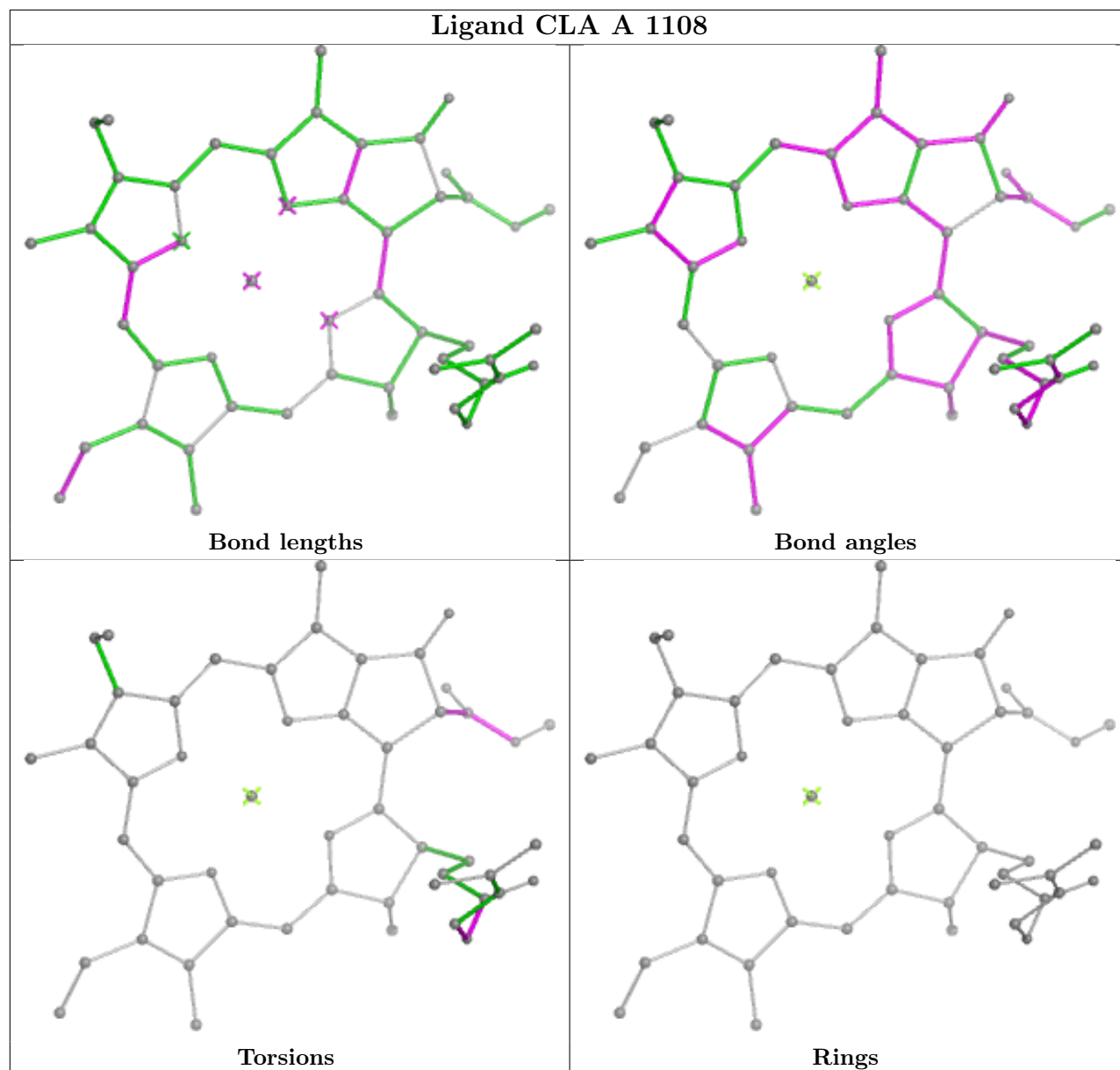
Torsions

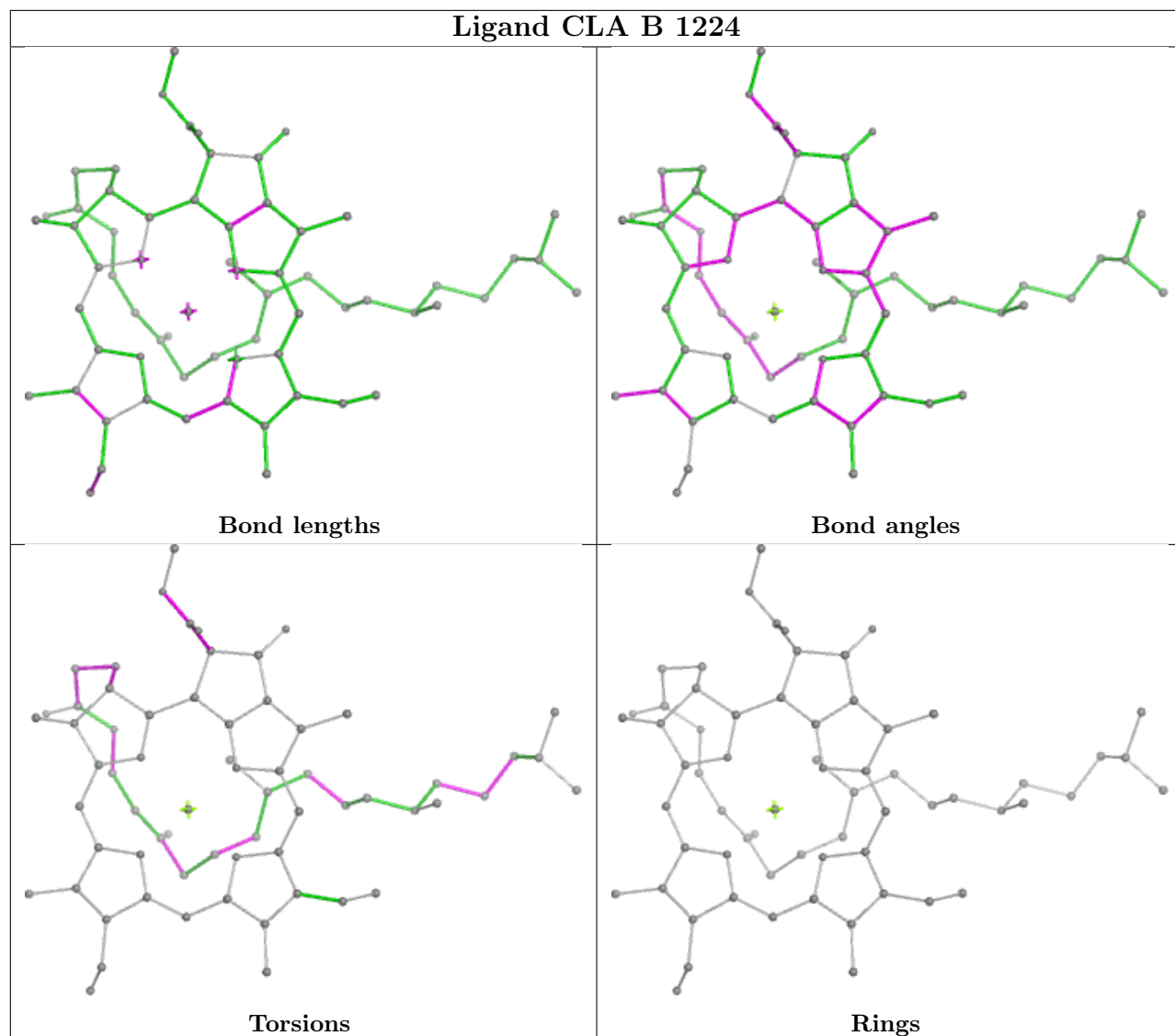


Rings

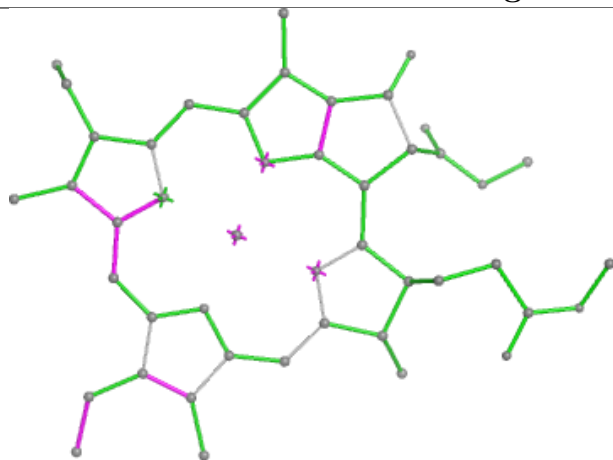


Ligand CLA A 1108

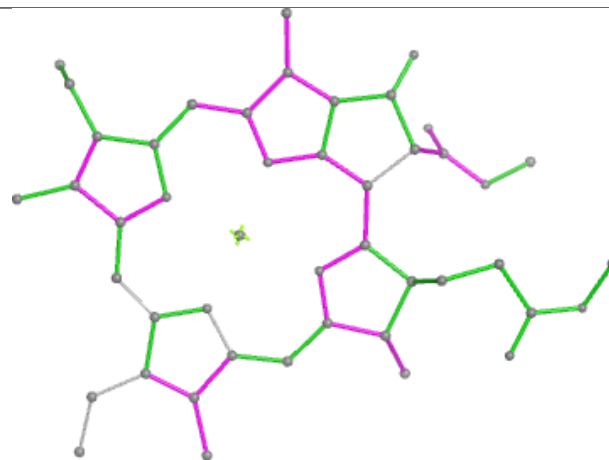




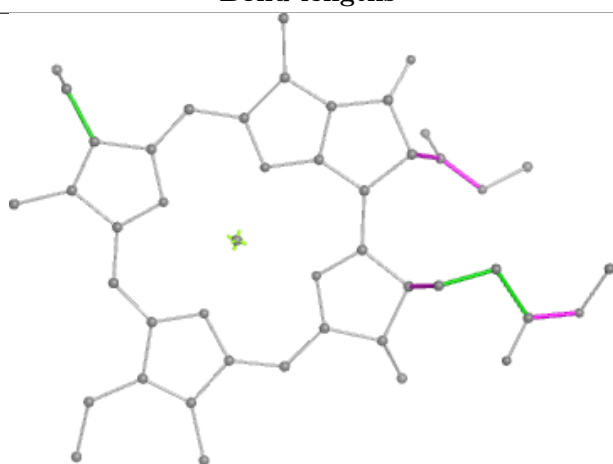
Ligand CLA G 1602



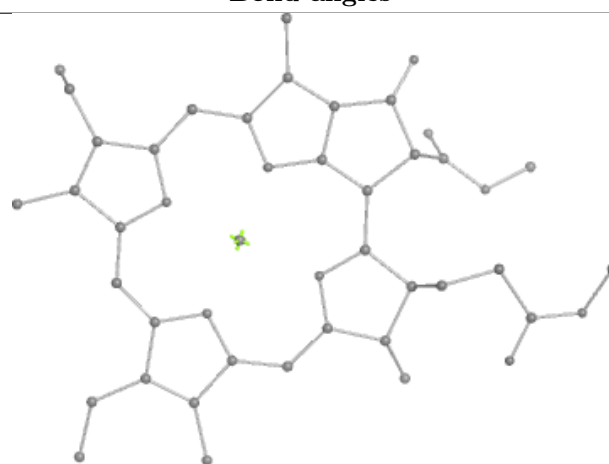
Bond lengths



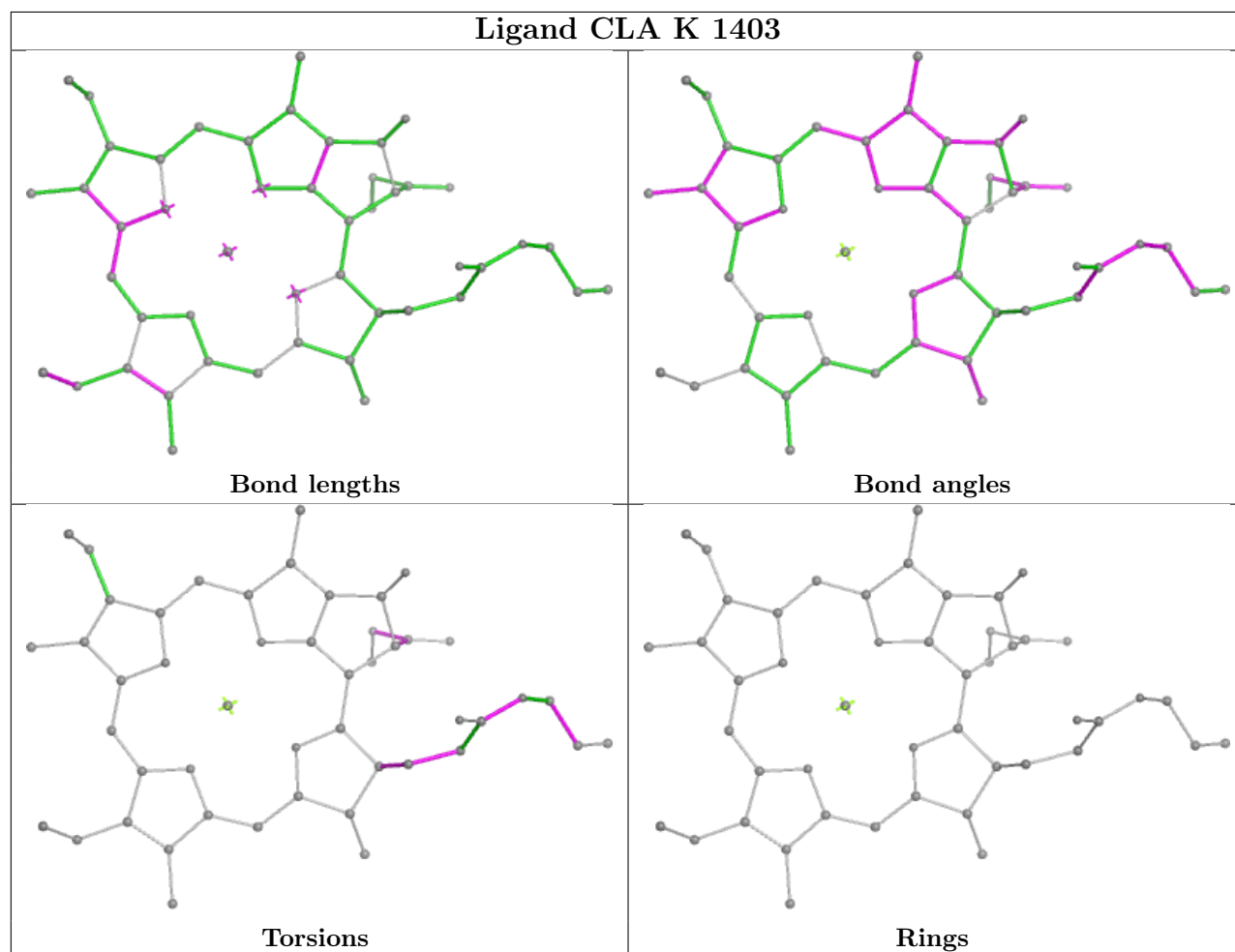
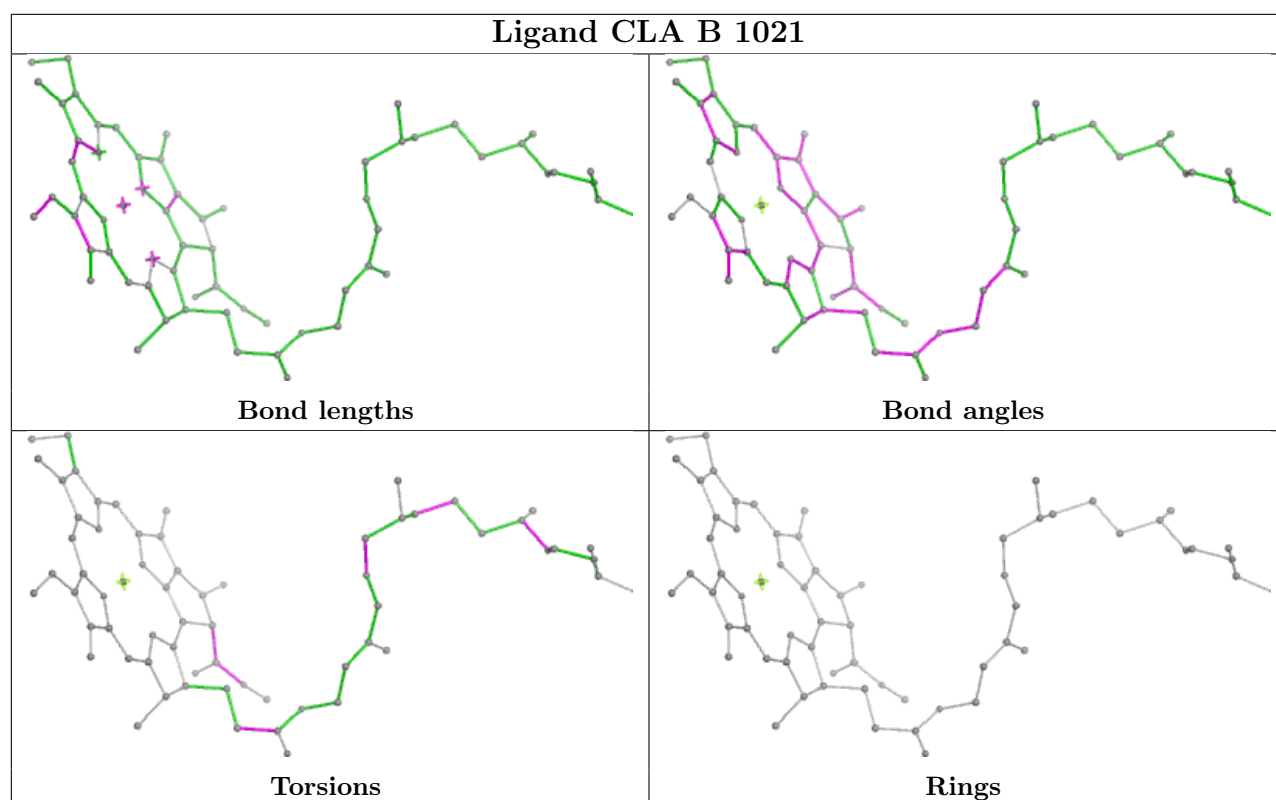
Bond angles

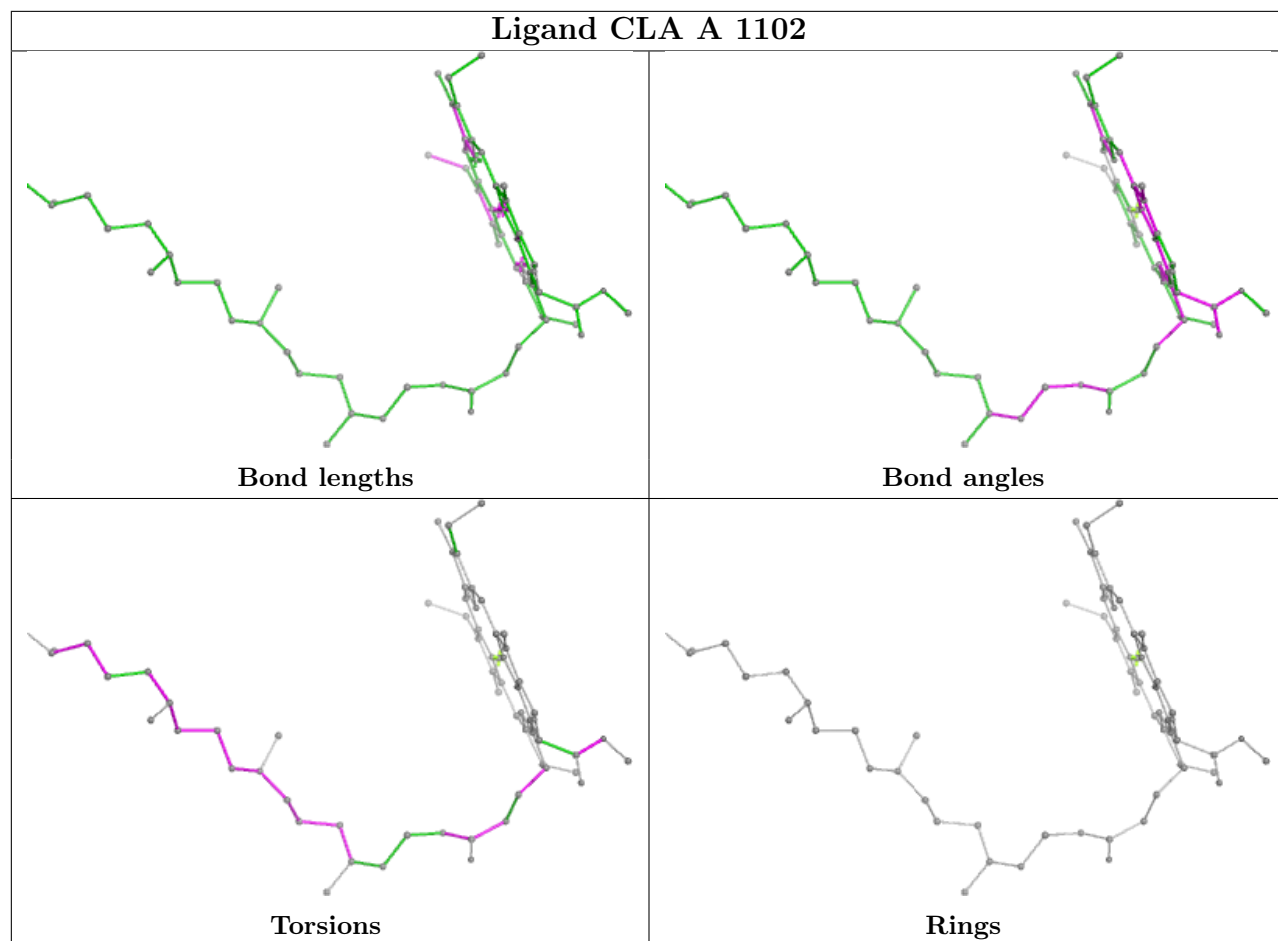


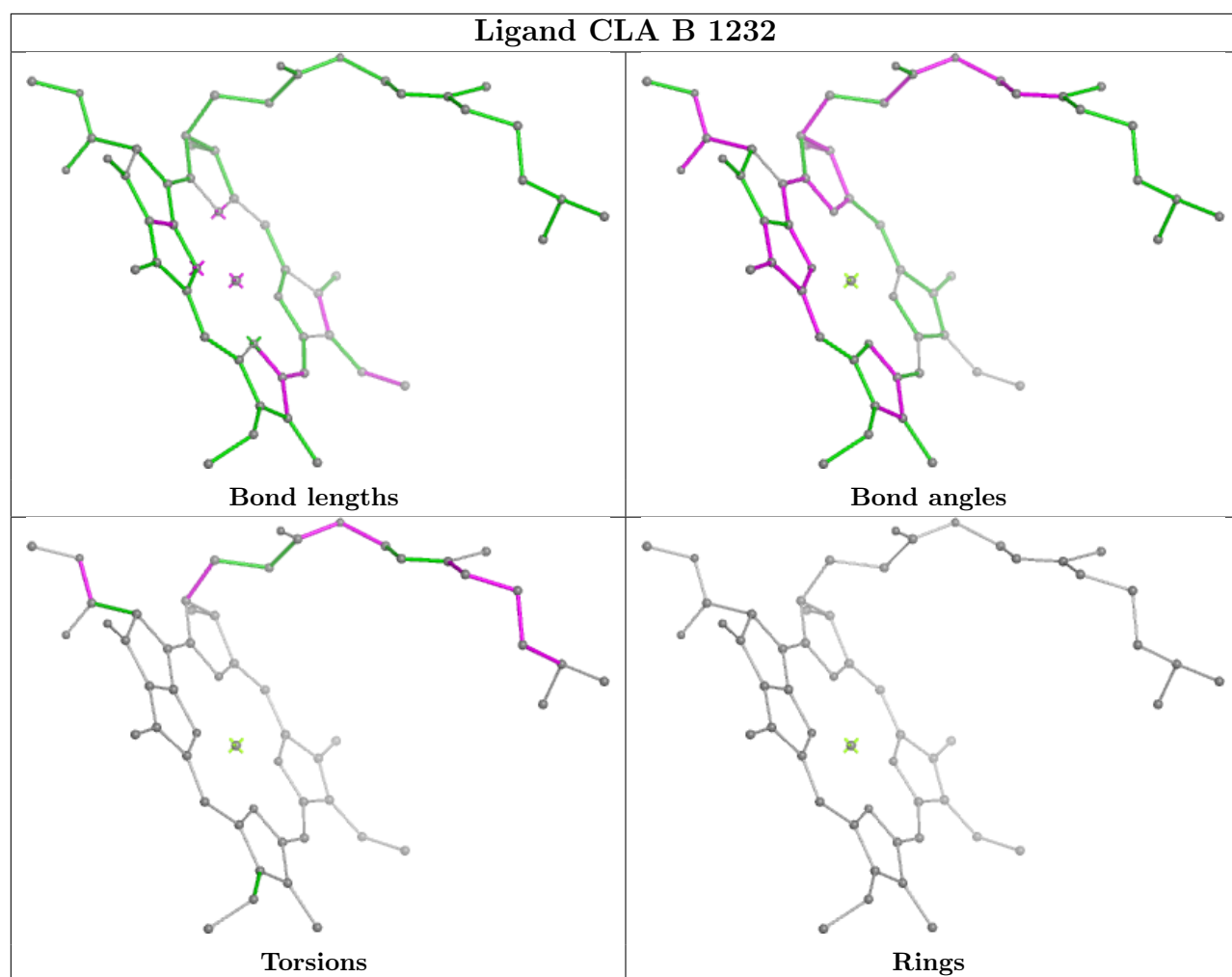
Torsions



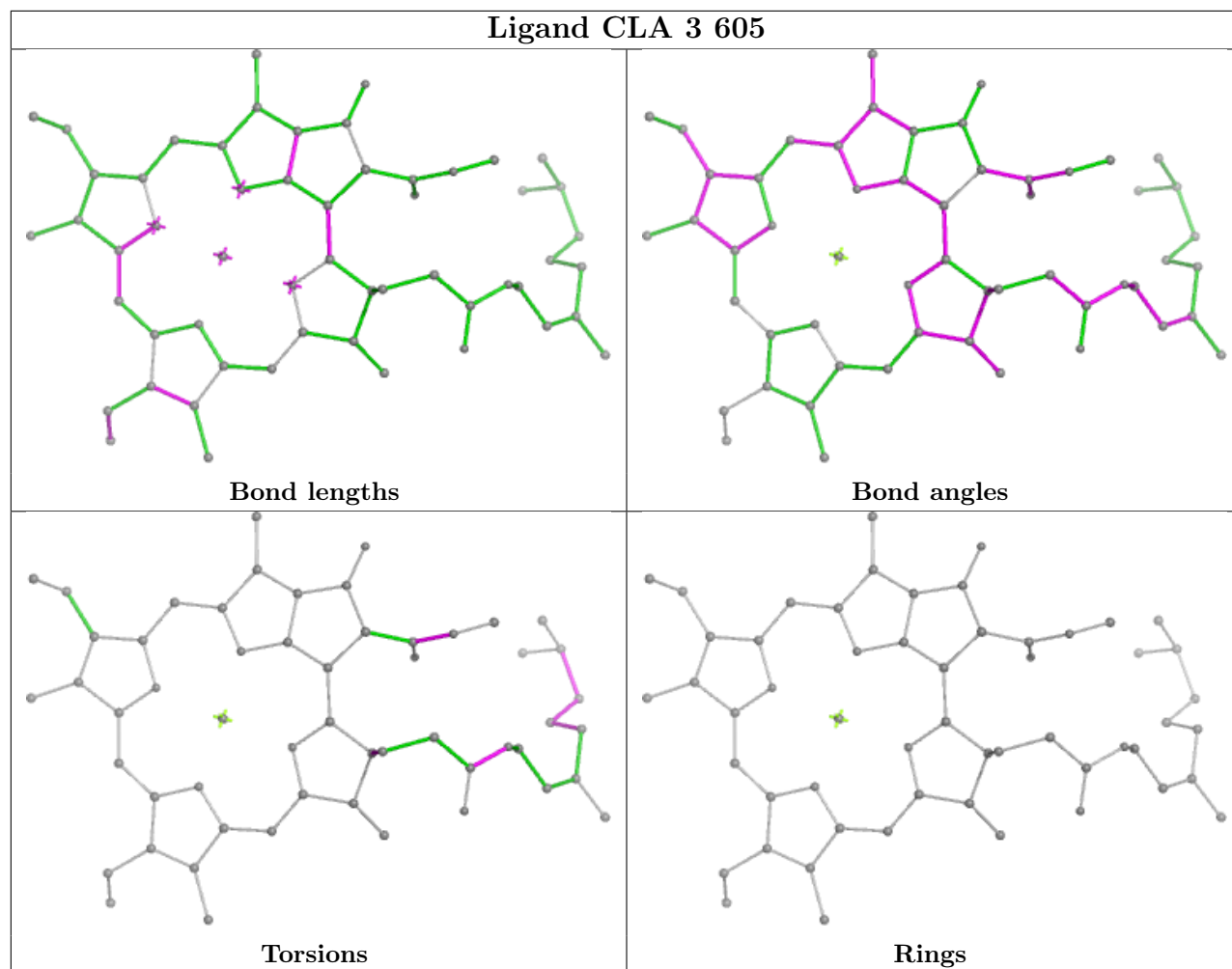
Rings



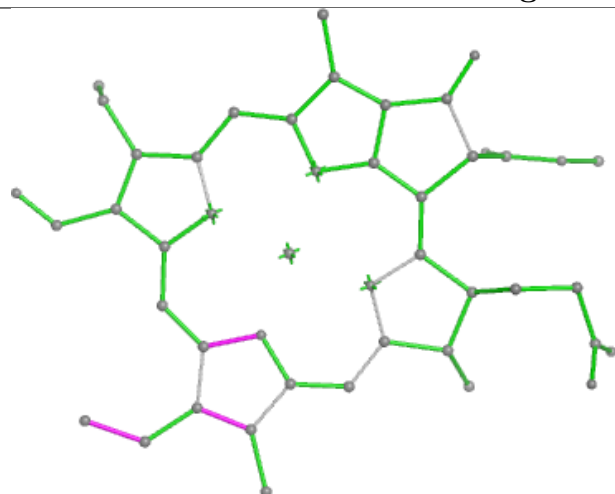




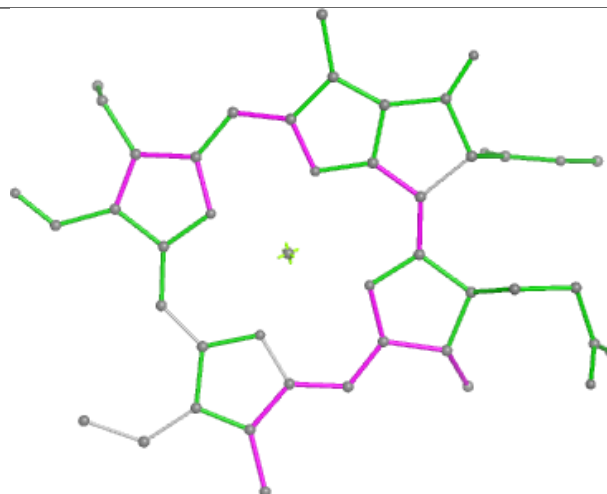
Ligand CLA 3 605



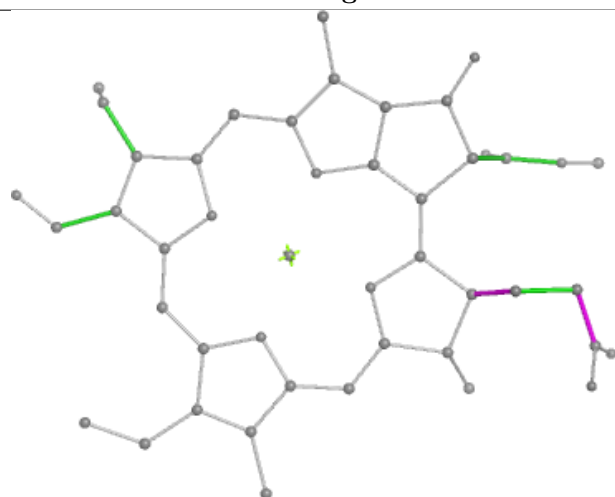
Ligand CHL 2 613



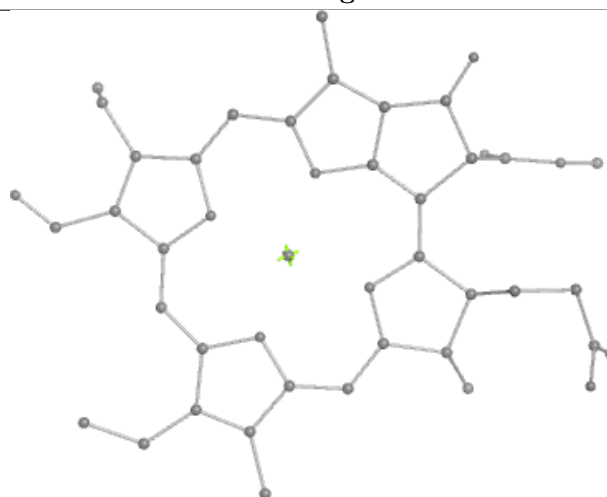
Bond lengths



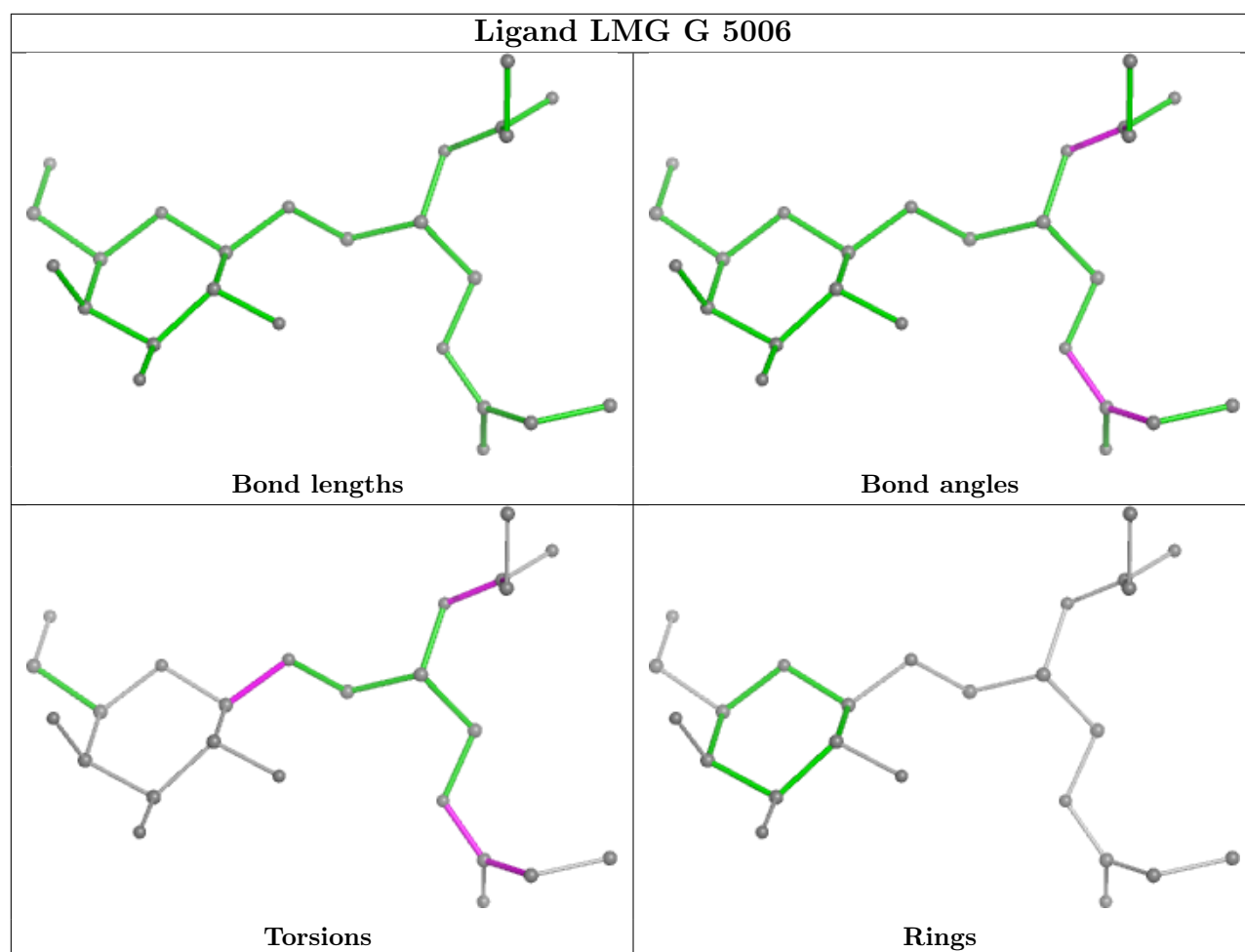
Bond angles



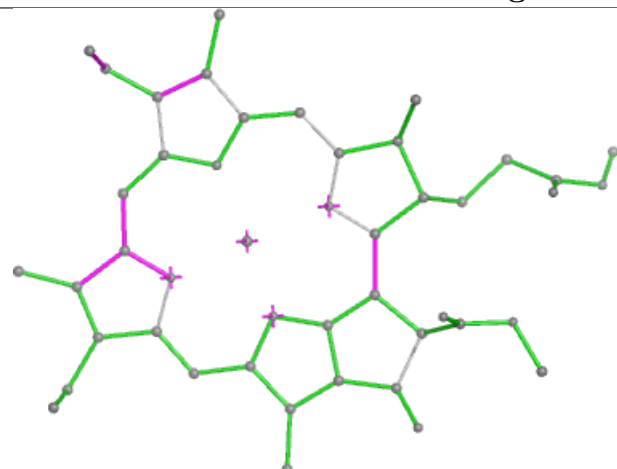
Torsions



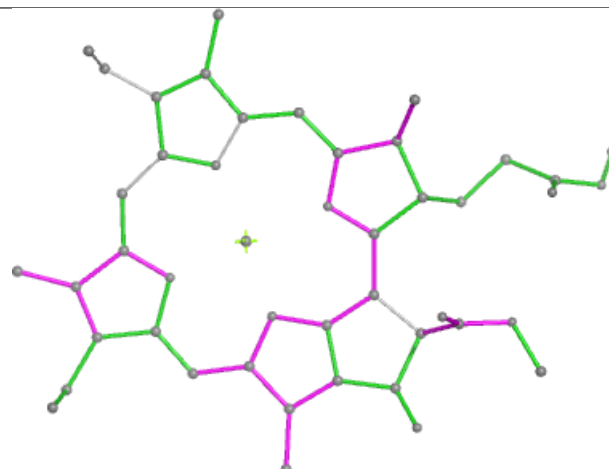
Rings



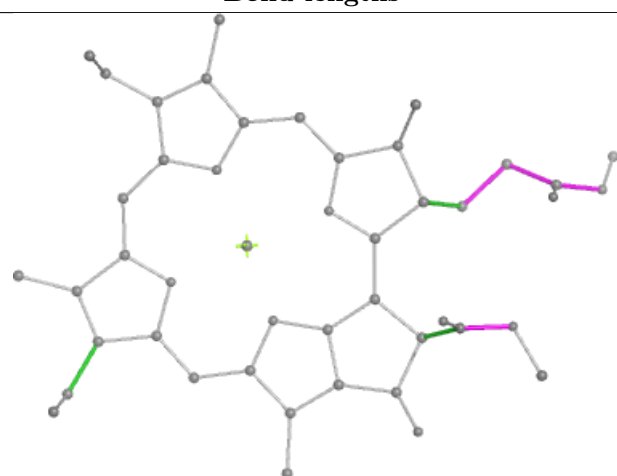
Ligand CLA K 1404



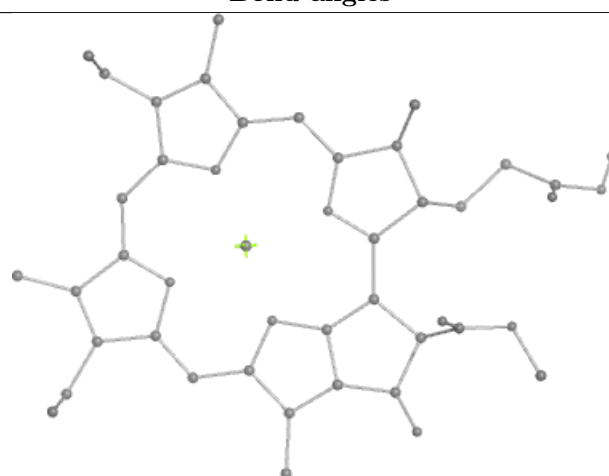
Bond lengths



Bond angles

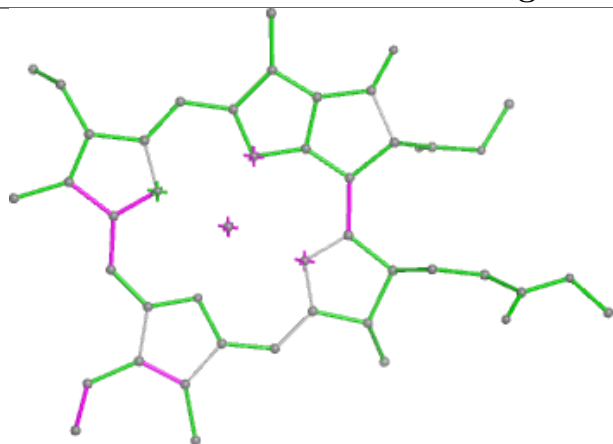


Torsions

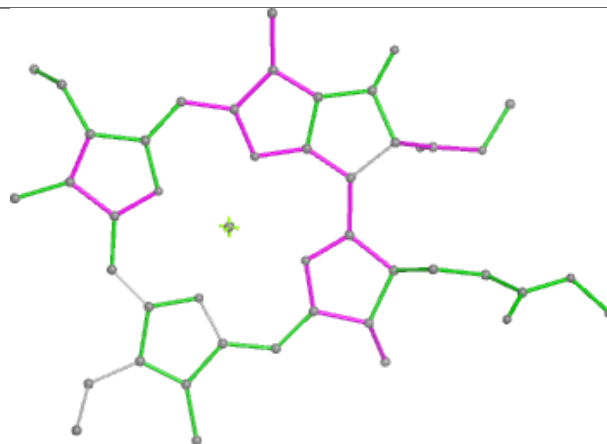


Rings

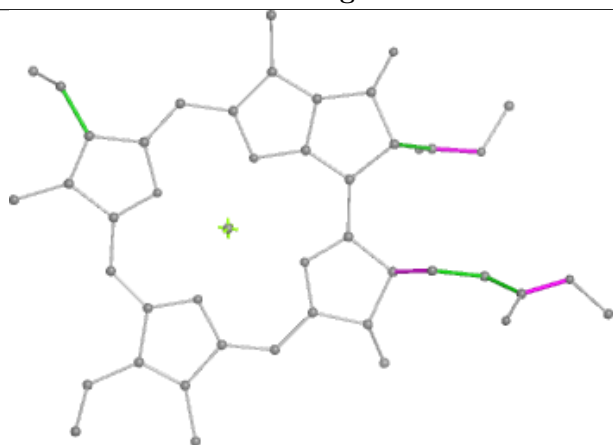
Ligand CLA 3 613



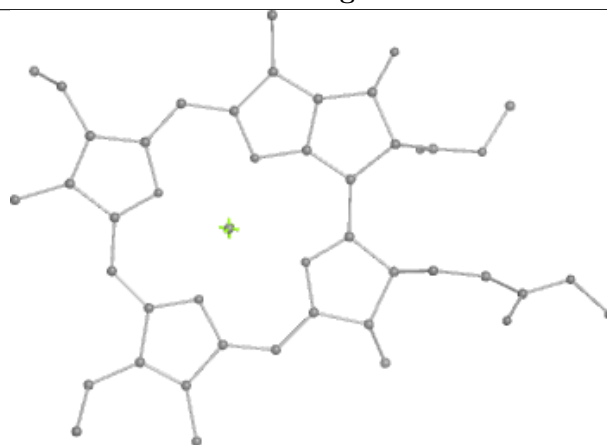
Bond lengths



Bond angles

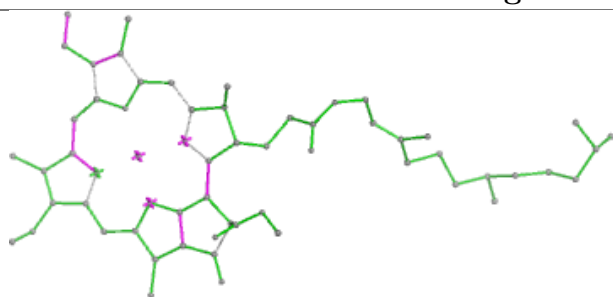


Torsions

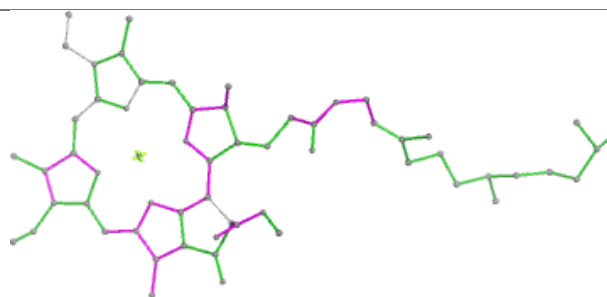


Rings

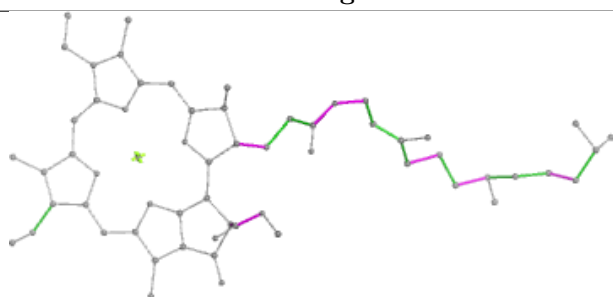
Ligand CLA G 1701



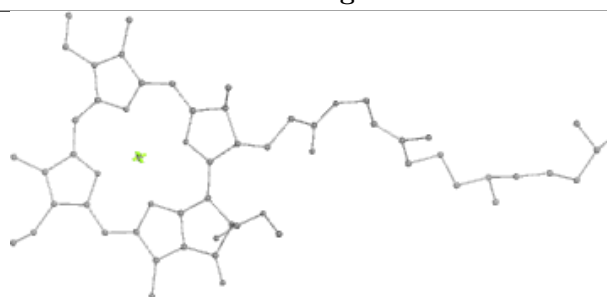
Bond lengths



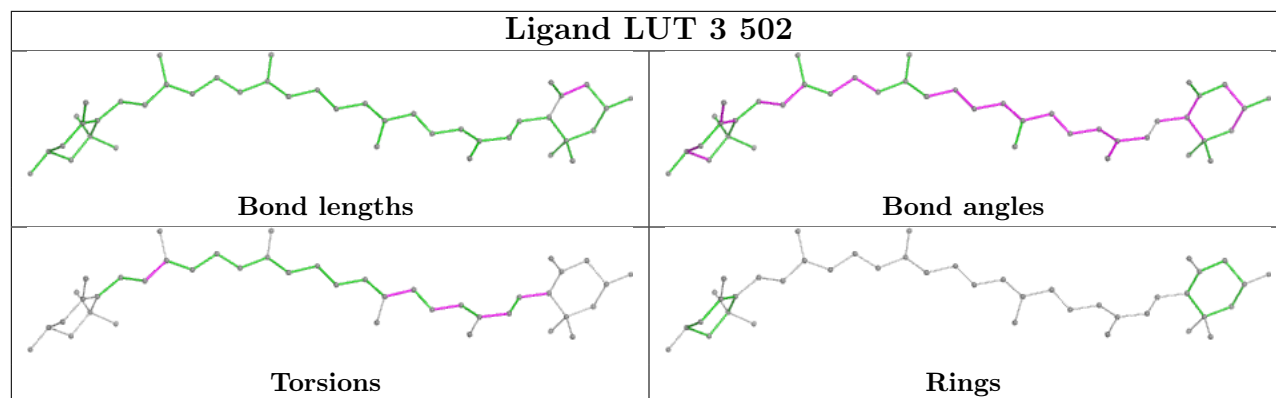
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

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

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.