



wwPDB EM Validation Summary Report ⓘ

Apr 2, 2025 – 03:11 am BST

PDB ID : 6ZOO / pdb_00006zoo
EMDB ID : EMD-11326
Title : Photosystem I reduced Plastocyanin Complex
Authors : Nelson, N.; Caspy, I.; Shkolnisky, Y.
Deposited on : 2020-07-07
Resolution : 2.74 Å(reported)
Based on initial model : 6YEZ

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

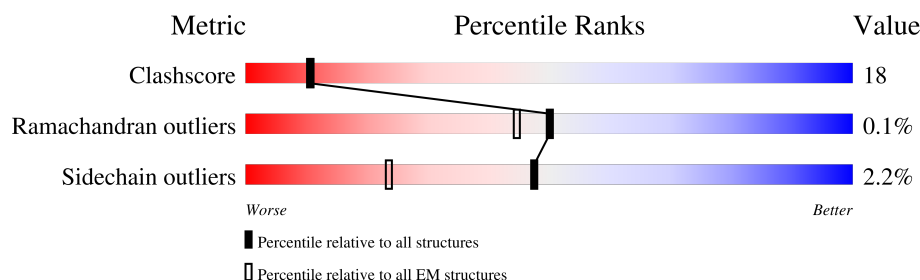
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 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	83% 17%
2	B	733	83% 16%
3	C	80	70% 30%
4	D	143	79% 19% .
5	E	66	73% 26% .
6	F	154	72% 25% .
7	G	97	75% 23% .
8	H	93	72% 26% .
9	I	31	55% 42% .

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Mol	Chain	Length	Quality of chain
10	J	42	 79% 21%
11	K	81	 68% 32%
12	L	159	 84% 16%
13	1	193	 79% 20% .
14	2	208	 74% 25% .
15	3	221	 68% 29% .
16	4	198	 81% 19%
17	P	99	 61% 34% 5%

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
1	SNK	A	636	X	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	602	X	-	-	-
19	CLA	3	603	X	-	-	-
19	CLA	3	605	X	-	-	-
19	CLA	3	606	X	-	-	-
19	CLA	3	607	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	605	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	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	-	-
19	CLA	B	1221	X	-	-	-
19	CLA	B	1222	X	-	-	-
19	CLA	B	1223	X	-	-	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	-	-
19	CLA	B	1226	X	-	-	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	-	-
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	-	-
19	CLA	B	1236	X	-	-	-
19	CLA	B	1237	X	-	-	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1239	X	-	-	-
19	CLA	B	1240	X	-	-	-
19	CLA	F	1301	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	G	1601	X	-	-	-
19	CLA	G	1602	X	-	-	-
19	CLA	G	1603	X	-	-	-
19	CLA	H	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	1	501	X	-	-	-
28	LUT	1	502	X	-	-	-
28	LUT	2	501	X	-	-	-
28	LUT	3	501	X	-	-	-
28	LUT	3	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	LUT	4	501	X	-	-	-
28	LUT	J	4013	X	-	-	-
29	CHL	1	609	X	-	-	-
29	CHL	1	610	X	-	-	-
29	CHL	1	612	X	-	-	-
29	CHL	2	609	X	-	-	-
29	CHL	2	610	X	-	-	-
29	CHL	2	611	X	-	-	-
29	CHL	2	613	X	-	-	-
29	CHL	2	615	X	-	-	-
29	CHL	3	604	X	-	-	-
29	CHL	3	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 38497 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
			5866	3843	998	1005	20		

- 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		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	69	GLY	-	insertion	UNP E1C9K8
D	70	PHE	-	insertion	UNP E1C9K8
D	71	THR	-	insertion	UNP E1C9K8
D	72	PRO	-	insertion	UNP E1C9K8
D	73	PRO	-	insertion	UNP E1C9K8
D	106	GLU	ASP	conflict	UNP E1C9K8
D	161	SER	ASN	conflict	UNP E1C9K8
D	180	PRO	ALA	conflict	UNP E1C9K8
D	187	VAL	GLN	conflict	UNP E1C9K8

- Molecule 5 is a protein called Putative uncharacterized protein.

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

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	64	PRO	-	insertion	UNP E1C9K6
E	65	PRO	-	insertion	UNP E1C9K6
E	79	GLN	LYS	conflict	UNP E1C9K6
E	125	VAL	ILE	conflict	UNP E1C9K6
E	126	GLU	VAL	conflict	UNP E1C9K6
E	129	LYS	GLU	conflict	UNP E1C9K6

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	80	ALA	SER	conflict	UNP A0A0M3KL12
F	87	ASP	GLU	conflict	UNP A0A0M3KL12
F	108	LEU	ILE	conflict	UNP A0A0M3KL12
F	111	PRO	ALA	conflict	UNP A0A0M3KL12
F	134	GLY	ALA	conflict	UNP A0A0M3KL12
F	188	ASP	GLU	conflict	UNP A0A0M3KL12
F	204	THR	SER	conflict	UNP A0A0M3KL12
F	205	GLY	ARG	conflict	UNP A0A0M3KL12

- Molecule 7 is a protein called photosystem I reaction center.

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

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	106	THR	SER	conflict	UNP A0A0M3KL13

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Chain	Residue	Modelled	Actual	Comment	Reference
G	112	VAL	ALA	conflict	UNP A0A0M3KL13
G	113	SER	GLY	conflict	UNP A0A0M3KL13
G	114	LEU	VAL	conflict	UNP A0A0M3KL13
G	115	LEU	SER	conflict	UNP A0A0M3KL13
G	118	ASN	-	insertion	UNP A0A0M3KL13
G	119	ASP	-	insertion	UNP A0A0M3KL13
G	120	PRO	-	insertion	UNP A0A0M3KL13
G	121	VAL	-	insertion	UNP A0A0M3KL13
G	122	GLY	ALA	conflict	UNP A0A0M3KL13
G	123	PHE	ALA	conflict	UNP A0A0M3KL13
G	124	ASN	ALA	conflict	UNP A0A0M3KL13
G	125	ILE	LEU	conflict	UNP A0A0M3KL13

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	H	93	Total	C	N	O	0	0
			712	466	112	134		

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

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

- Molecule 10 is a protein called 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 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	159	Total	C	N	O	S	0	0
			1197	788	191	217	1		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

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

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	40	ASP	HIS	conflict	UNP Q01667
1	45	GLN	GLU	conflict	UNP Q01667
1	49	SER	ALA	conflict	UNP Q01667
1	65	ARG	GLY	conflict	UNP Q01667
1	71	GLU	ALA	conflict	UNP Q01667
1	76	PHE	TYR	conflict	UNP Q01667
1	102	LEU	TYR	conflict	UNP Q01667
1	136	VAL	ALA	conflict	UNP Q01667
1	141	SER	ALA	conflict	UNP Q01667
1	177	PHE	LEU	conflict	UNP Q01667
1	178	HIS	GLU	conflict	UNP Q01667
1	180	TYR	LEU	conflict	UNP Q01667
1	182	ILE	VAL	conflict	UNP Q01667
1	185	VAL	ILE	conflict	UNP Q01667
1	198	ILE	PHE	conflict	UNP Q01667
1	225	THR	ASN	conflict	UNP Q01667
1	228	ASN	ASP	conflict	UNP Q01667
1	229	VAL	ILE	conflict	UNP Q01667
1	230	LEU	VAL	conflict	UNP Q01667

- 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		

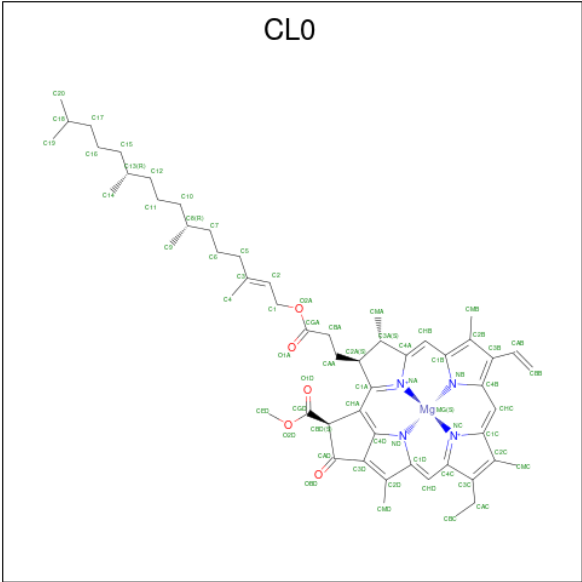
There are 3 discrepancies between the modelled and reference sequences:

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 Plastocyanin, chloroplastic.

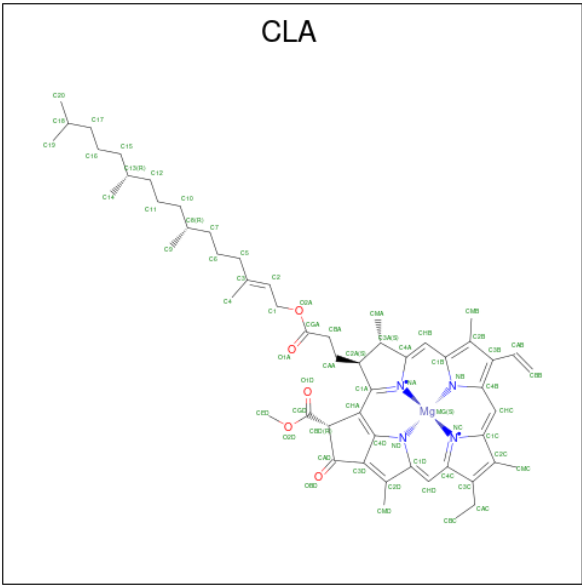
Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	99	Total	C	N	O	S	0	0
			728	460	115	150	3		

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



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

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



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

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

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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 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 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 50	C 40	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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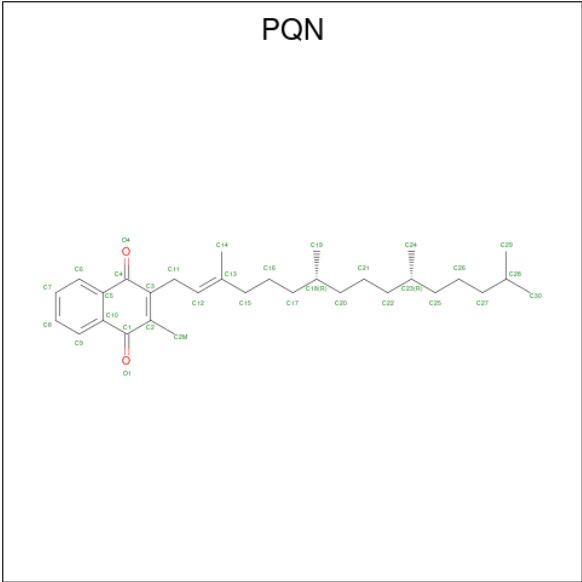
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total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

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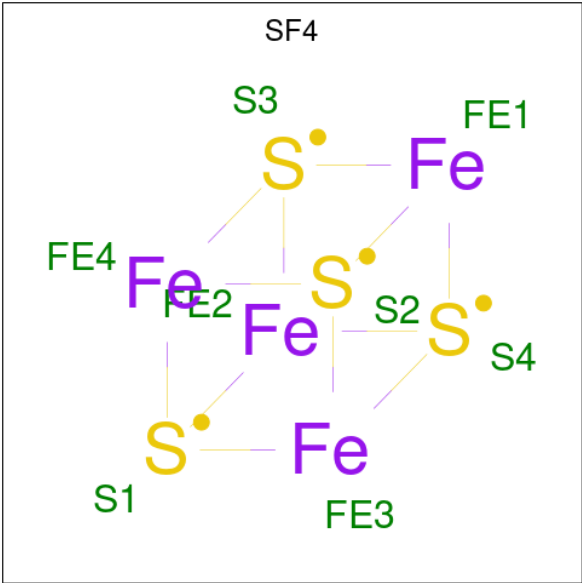
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			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
			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: Fe₄S₄).



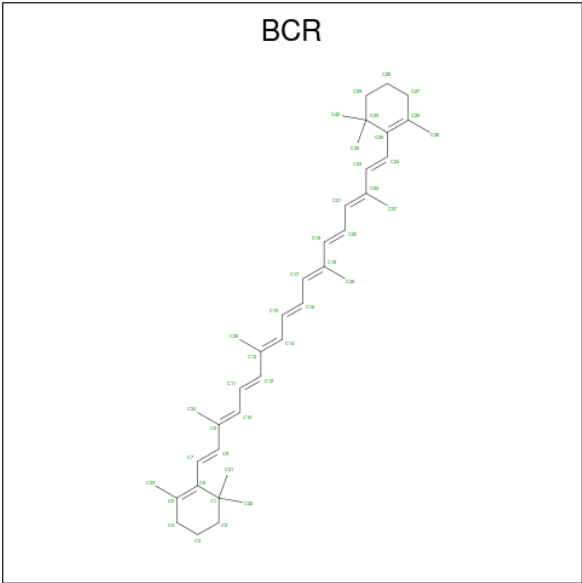
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 22 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



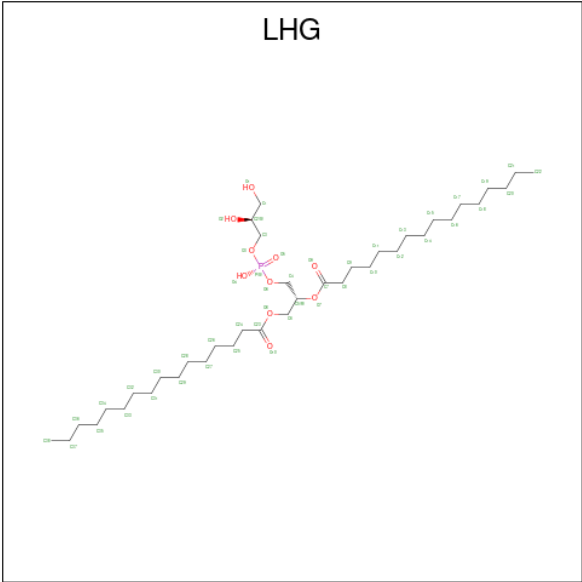
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

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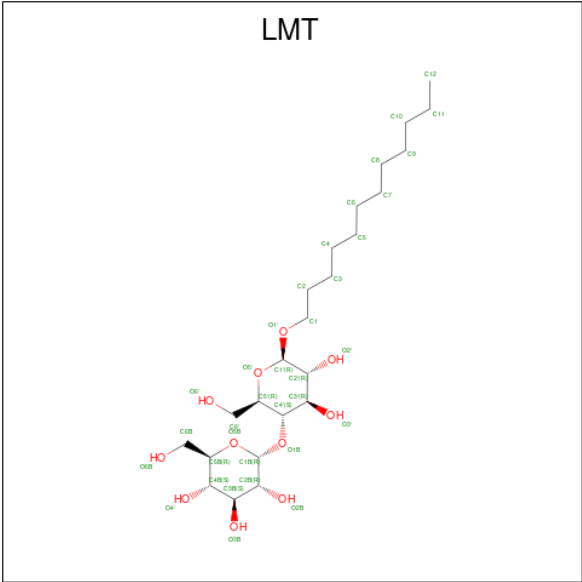
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	H	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C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

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



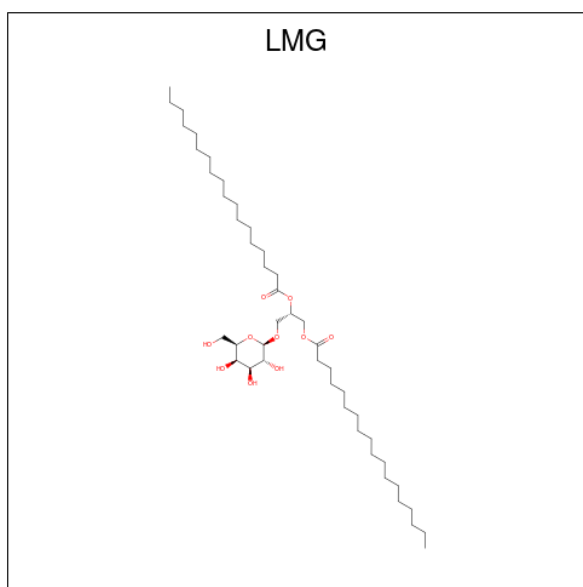
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			21	10	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	3	1	Total	C	O	P	0
			17	8	8	1	
23	4	1	Total	C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

- Molecule 24 is DODECYL-BETA-D-MALTOSIDE (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
			31	20	11	
24	B	1	Total	C	O	0
			32	21	11	
24	G	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			31	20	11	
24	2	1	Total	C	O	0
			35	24	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
			25	15	10	
25	G	1	Total	C	O	0
			49	39	10	
25	G	1	Total	C	O	0
			50	40	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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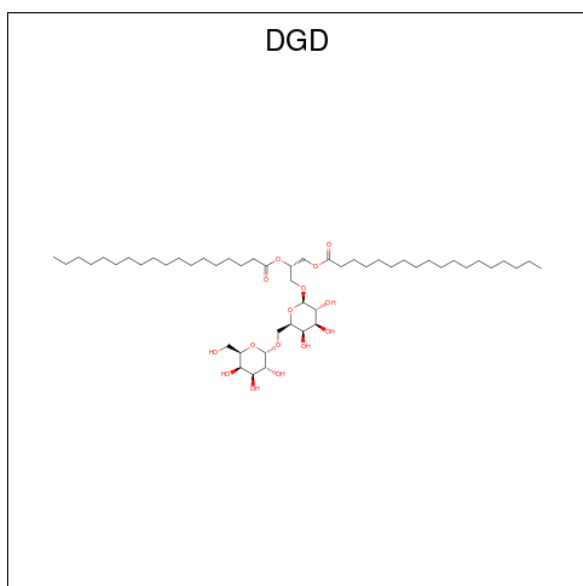
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Mol	Chain	Residues	Atoms			AltConf
25	2	1	Total	C	O	0
			36	26	10	
25	2	1	Total	C	O	0
			30	20	10	
25	2	1	Total	C	O	0
			30	20	10	
25	2	1	Total	C	O	0
			13	7	6	
25	3	1	Total	C	O	0
			30	20	10	

- 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).



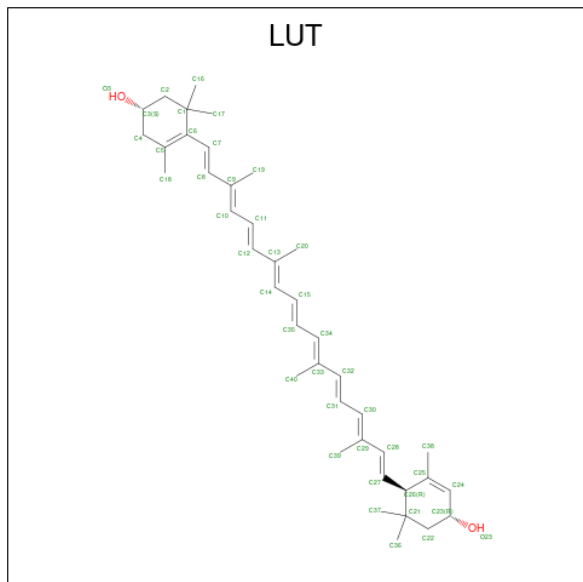
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			61	46	15	
27	F	1	Total	C	O	0
			57	42	15	

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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
			50	35	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).



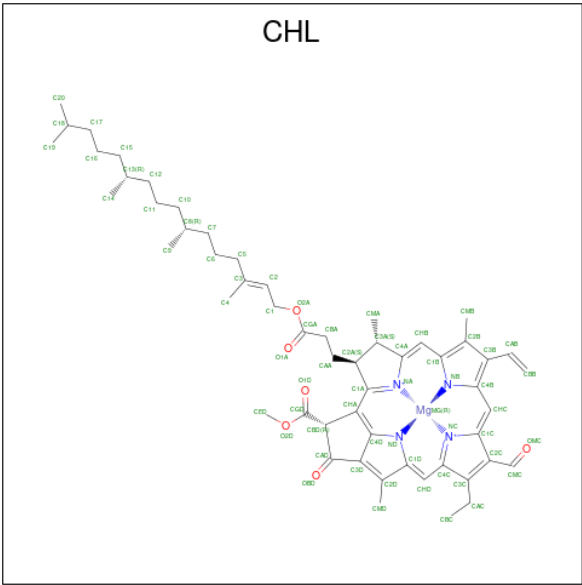
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	

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

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



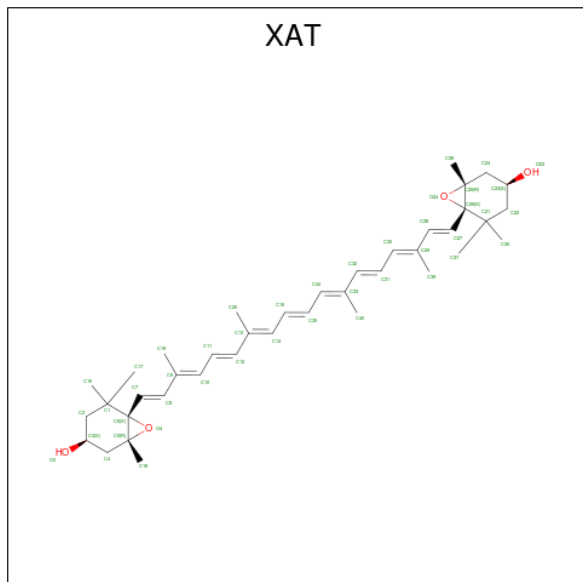
Mol	Chain	Residues	Atoms					AltConf
29	1	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
29	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
29	2	1	Total	C	Mg	N	O	0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

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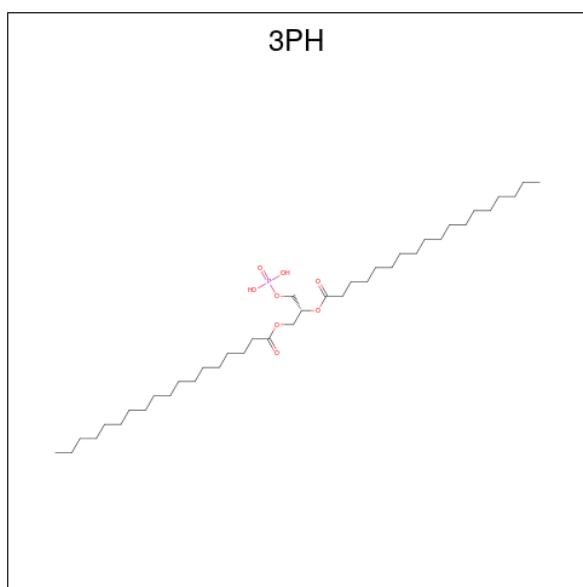
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- 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 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: C₃₉H₇₇O₈P).



Mol	Chain	Residues	Atoms				AltConf
31	2	1	Total	C	O	P	0
			33	24	8	1	

- Molecule 32 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

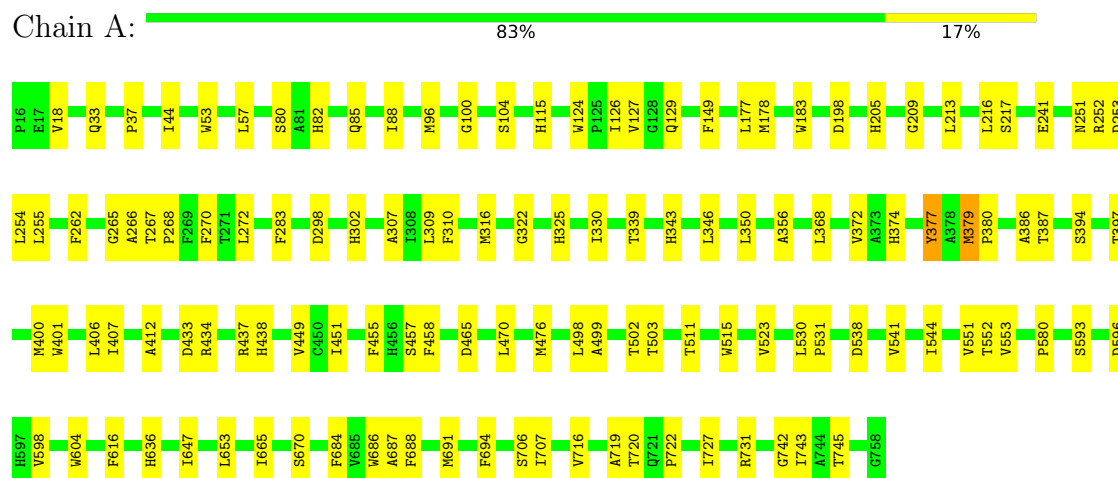
- Molecule 33 is water.

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

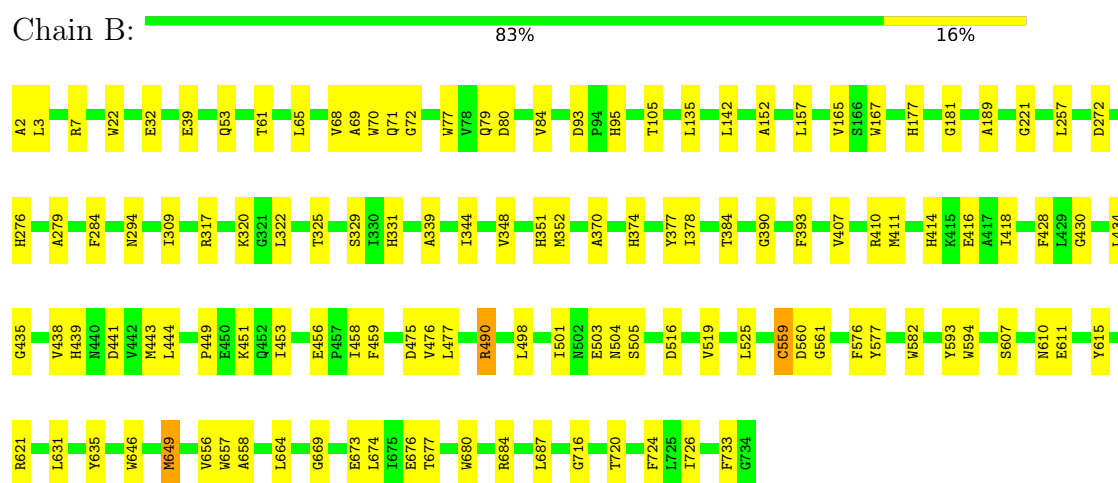
3 Residue-property plots

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.

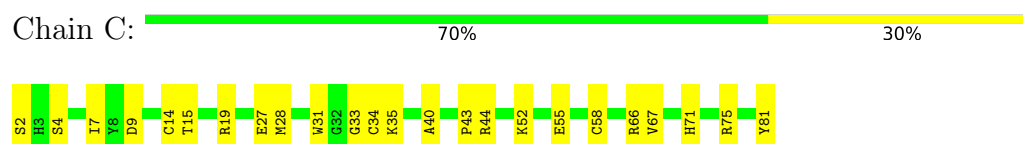
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

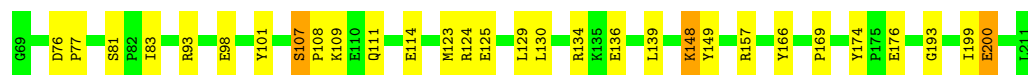


- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: PsadD

Chain D:  79% 19%



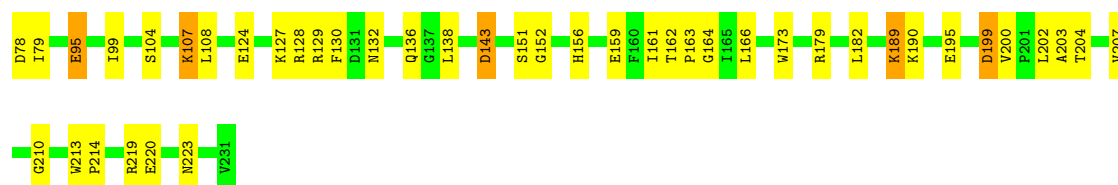
- Molecule 5: Putative uncharacterized protein

Chain E:  73% 26%




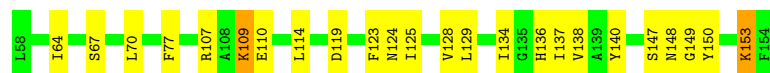
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  72% 25%



- Molecule 7: photosystem I reaction center

Chain G:  75% 23%



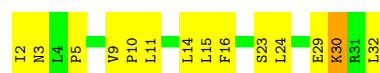
- Molecule 8: Photosystem I reaction center subunit VI,Photosystem I reaction center subunit VI

Chain H:  72% 26%




- Molecule 9: Photosystem I reaction center subunit VIII

Chain I:  55% 42%



- Molecule 10: Photosystem I reaction center subunit IX

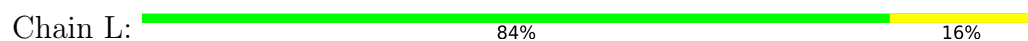
Chain J:  79% 21%



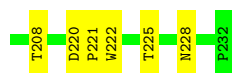
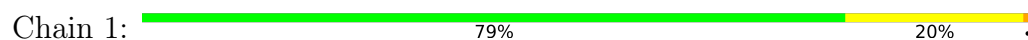
- Molecule 11: Photosystem I reaction center subunit X psaK



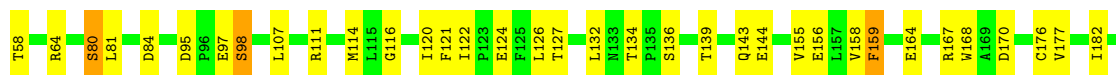
- Molecule 12: PsaL domain-containing protein



- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic




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

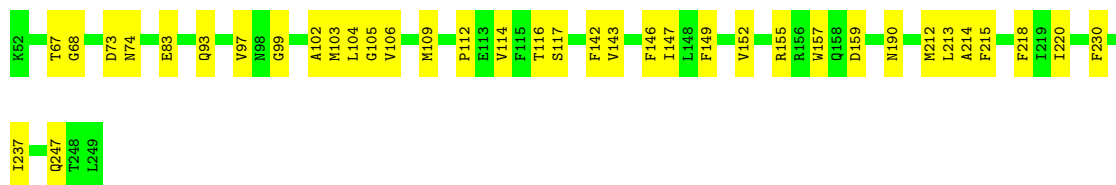


- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic



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

Chain 4:  81% 19%



● Molecule 17: Plastocyanin, chloroplastic

Chain P:  61% 34% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	104127	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 ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.26	0/6033	0.45	0/8228
2	B	0.27	0/6069	0.46	0/8286
3	C	0.25	0/625	0.53	0/846
4	D	0.27	0/1163	0.50	0/1572
5	E	0.27	0/540	0.50	0/734
6	F	0.26	0/1234	0.48	0/1670
7	G	0.26	0/776	0.46	0/1054
8	H	0.27	0/733	0.44	0/995
9	I	0.29	0/246	0.44	0/335
10	J	0.28	0/349	0.45	0/476
11	K	0.26	0/576	0.47	0/779
12	L	0.26	0/1232	0.45	0/1684
13	1	0.27	0/1558	0.44	0/2125
14	2	0.26	0/1679	0.45	0/2302
15	3	0.29	0/1760	0.48	0/2390
16	4	0.26	0/1608	0.41	0/2191
17	P	0.73	2/743 (0.3%)	0.82	1/1009 (0.1%)
All	All	0.29	2/26924 (0.0%)	0.47	1/36676 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0
15	3	0	1
All	All	1	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	P	16	PRO	N-CA	12.99	1.69	1.47
17	P	15	VAL	C-N	5.79	1.45	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	16	PRO	CA-N-CD	-7.58	100.89	111.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	636	SNK	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
15	3	86	PRO	Peptide

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	5866	0	5705	138	0
2	B	5857	0	5653	124	0
3	C	612	0	591	24	0
4	D	1132	0	1141	40	0
5	E	528	0	528	19	0
6	F	1206	0	1231	34	0
7	G	757	0	743	32	0
8	H	712	0	701	36	0
9	I	240	0	264	25	0
10	J	338	0	345	13	0
11	K	569	0	596	41	0
12	L	1197	0	1197	37	0
13	1	1508	0	1489	41	0
14	2	1620	0	1557	72	0
15	3	1706	0	1661	100	0
16	4	1559	0	1527	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	P	728	0	699	58	0
18	A	65	0	72	3	0
19	1	608	0	564	46	0
19	2	522	0	501	51	0
19	3	630	0	539	52	0
19	4	631	0	600	51	0
19	A	2643	0	2752	186	0
19	B	2610	0	2750	183	0
19	F	130	0	144	3	0
19	G	166	0	152	12	0
19	H	60	0	59	6	0
19	J	50	0	38	3	0
19	K	199	0	159	11	0
19	L	160	0	137	14	0
20	A	33	0	46	2	0
20	B	33	0	46	1	0
21	A	8	0	0	0	0
21	C	16	0	0	2	0
22	1	80	0	103	9	0
22	2	40	0	51	10	0
22	3	80	0	105	25	0
22	A	240	0	311	42	0
22	B	200	0	261	46	0
22	F	80	0	104	13	0
22	G	40	0	52	9	0
22	H	40	0	52	10	0
22	I	80	0	104	10	0
22	J	40	0	52	9	0
22	K	80	0	104	26	0
22	L	80	0	104	19	0
23	1	49	0	74	0	0
23	2	35	0	40	0	0
23	3	17	0	12	1	0
23	4	35	0	40	0	0
23	A	89	0	127	2	0
23	B	70	0	86	0	0
24	2	35	0	45	1	0
24	A	35	0	45	0	0
24	B	63	0	70	1	0
24	G	66	0	79	4	0
25	1	46	0	65	0	0
25	2	134	0	133	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	3	30	0	30	0	0
25	A	50	0	73	2	0
25	B	102	0	114	0	0
25	F	160	0	188	1	0
25	G	124	0	161	2	0
26	A	1	0	0	0	0
26	B	1	0	0	0	0
27	1	41	0	40	0	0
27	3	51	0	60	0	0
27	4	50	0	58	1	0
27	B	61	0	83	0	0
27	F	57	0	75	1	0
27	G	47	0	52	1	0
27	J	58	0	77	0	0
28	1	84	0	110	18	0
28	2	42	0	55	11	0
28	3	84	0	110	26	0
28	4	84	0	110	23	0
28	J	42	0	55	12	0
29	1	164	0	135	9	0
29	2	272	0	225	19	0
29	3	113	0	99	7	0
29	4	202	0	152	5	0
30	2	44	0	56	6	0
30	4	44	0	56	2	0
31	2	33	0	39	0	0
32	P	1	0	0	0	0
33	B	2	0	0	0	0
All	All	38497	0	38619	1421	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 18.

The worst 5 of 1421 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)
1:A:377:TYR:OH	19:A:1135:CLA:HBC3	1.26	1.35
17:P:16:PRO:CA	17:P:16:PRO:N	1.69	1.32
12:L:204:LEU:HD21	19:L:1503:CLA:HED1	1.26	1.14
17:P:55:ILE:HG22	17:P:72:VAL:CG2	1.78	1.13
5:E:96:ASP:OD2	5:E:97:PRO:O	1.69	1.11

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/743 (100%)	710 (96%)	29 (4%)	0	100	100
2	B	731/733 (100%)	698 (96%)	33 (4%)	0	100	100
3	C	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
4	D	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	19	33
5	E	64/66 (97%)	59 (92%)	5 (8%)	0	100	100
6	F	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
7	G	95/97 (98%)	94 (99%)	1 (1%)	0	100	100
8	H	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
9	I	29/31 (94%)	26 (90%)	3 (10%)	0	100	100
10	J	40/42 (95%)	40 (100%)	0	0	100	100
11	K	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
12	L	157/159 (99%)	147 (94%)	10 (6%)	0	100	100
13	1	191/193 (99%)	182 (95%)	9 (5%)	0	100	100
14	2	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
15	3	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	14	27
16	4	196/198 (99%)	183 (93%)	13 (7%)	0	100	100
17	P	97/99 (98%)	87 (90%)	9 (9%)	1 (1%)	13	23
All	All	3305/3341 (99%)	3135 (95%)	166 (5%)	4 (0%)	50	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	3	86	PRO
15	3	87	GLU

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Mol	Chain	Res	Type
4	D	107	SER
17	P	50	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	602/602 (100%)	600 (100%)	2 (0%)	91	95
2	B	598/598 (100%)	594 (99%)	4 (1%)	81	89
3	C	69/69 (100%)	67 (97%)	2 (3%)	37	58
4	D	122/122 (100%)	118 (97%)	4 (3%)	33	54
5	E	58/58 (100%)	55 (95%)	3 (5%)	19	35
6	F	125/126 (99%)	116 (93%)	9 (7%)	12	21
7	G	82/82 (100%)	78 (95%)	4 (5%)	21	38
8	H	75/75 (100%)	70 (93%)	5 (7%)	13	24
9	I	27/27 (100%)	25 (93%)	2 (7%)	11	20
10	J	35/35 (100%)	34 (97%)	1 (3%)	37	58
11	K	59/59 (100%)	58 (98%)	1 (2%)	56	73
12	L	126/126 (100%)	126 (100%)	0	100	100
13	1	158/158 (100%)	155 (98%)	3 (2%)	52	71
14	2	167/167 (100%)	157 (94%)	10 (6%)	16	28
15	3	171/172 (99%)	167 (98%)	4 (2%)	45	66
16	4	164/164 (100%)	162 (99%)	2 (1%)	67	82
17	P	79/79 (100%)	74 (94%)	5 (6%)	15	27
All	All	2717/2719 (100%)	2656 (98%)	61 (2%)	47	68

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	51	LYS

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Mol	Chain	Res	Type
16	4	117	SER
10	J	15	SER
16	4	83	GLU
17	P	51	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
11	K	112	HIS
14	2	212	GLN
15	3	199	ASN
2	B	89	HIS
1	A	251	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	SNK	A	636	1	8,14,15	1.00	1 (12%)	5,18,20	1.75	1 (20%)
1	SNK	A	115	1	8,14,15	1.03	1 (12%)	5,18,20	1.71	1 (20%)

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
1	SNK	A	636	1	1/1/2/3	5/5/10/12	0/1/1/1
1	SNK	A	115	1	-	3/5/10/12	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	636	SNK	C02-S04	2.28	1.85	1.77
1	A	115	SNK	C02-S04	2.25	1.85	1.77

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SNK	C01-C02-S04	2.90	122.95	112.32
1	A	636	SNK	C01-C02-S04	2.87	122.85	112.32

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	636	SNK	CA

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	115	SNK	C01-C02-S04-CD2
1	A	115	SNK	O03-C02-S04-CD2
1	A	636	SNK	O-C-CA-CB
1	A	636	SNK	C01-C02-S04-CD2
1	A	636	SNK	O03-C02-S04-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 243 ligands modelled in this entry, 3 are monoatomic - leaving 240 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
19	CLA	B	1202	-	65,73,73	1.33	8 (12%)	76,113,113	2.00	16 (21%)
19	CLA	4	608	-	46,54,73	1.61	9 (19%)	53,90,113	2.10	12 (22%)
23	LHG	4	801	-	34,34,48	0.47	0	37,40,54	1.18	3 (8%)
21	SF4	C	3003	3	0,12,12	-	-	-		
27	DGD	J	5001	-	59,59,67	1.08	6 (10%)	73,73,81	1.00	2 (2%)
19	CLA	B	1213	-	60,68,73	1.40	9 (15%)	70,107,113	1.94	14 (20%)
19	CLA	B	1207	-	65,73,73	1.37	9 (13%)	76,113,113	1.83	15 (19%)
19	CLA	2	602	-	52,60,73	1.51	8 (15%)	60,97,113	2.09	18 (30%)
22	BCR	F	4014	-	41,41,41	1.83	4 (9%)	56,56,56	4.45	20 (35%)
25	LMG	G	5001	-	49,49,55	1.02	4 (8%)	57,57,63	1.20	4 (7%)
19	CLA	A	1127	-	65,73,73	1.35	8 (12%)	76,113,113	1.81	14 (18%)
19	CLA	3	613	-	46,54,73	1.61	9 (19%)	53,90,113	2.12	12 (22%)
19	CLA	A	1117	-	65,73,73	1.35	8 (12%)	76,113,113	1.88	15 (19%)
22	BCR	B	4010	-	41,41,41	1.81	4 (9%)	56,56,56	4.47	21 (37%)
29	CHL	1	610	13	47,55,74	0.99	2 (4%)	50,91,114	1.39	11 (22%)
24	LMT	B	5008	-	32,32,36	1.23	5 (15%)	43,43,47	0.99	3 (6%)
22	BCR	2	503	-	41,41,41	1.89	5 (12%)	56,56,56	5.43	26 (46%)
19	CLA	A	1134	1	55,63,73	1.47	8 (14%)	64,101,113	2.01	12 (18%)
25	LMG	F	5004	-	34,34,55	0.49	0	42,42,63	1.09	3 (7%)
25	LMG	B	5003	-	35,35,55	0.74	1 (2%)	43,43,63	1.15	4 (9%)
19	CLA	B	1219	-	65,73,73	1.36	9 (13%)	76,113,113	1.93	14 (18%)
19	CLA	3	601	15	55,63,73	1.48	9 (16%)	64,101,113	2.01	16 (25%)
19	CLA	A	1141	-	60,68,73	1.41	9 (15%)	70,107,113	1.95	15 (21%)
25	LMG	G	5002	-	50,50,55	1.05	5 (10%)	58,58,63	1.16	4 (6%)
23	LHG	A	5002	-	48,48,48	0.40	0	51,54,54	1.10	4 (7%)
19	CLA	1	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.84	12 (15%)
19	CLA	B	1235	-	65,73,73	1.34	10 (15%)	76,113,113	1.92	15 (19%)
19	CLA	B	1240	23	65,73,73	1.36	8 (12%)	76,113,113	1.88	16 (21%)
19	CLA	A	1108	-	50,58,73	1.54	8 (16%)	58,95,113	2.15	15 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1204	-	65,73,73	1.38	9 (13%)	76,113,113	1.87	14 (18%)
19	CLA	1	608	-	46,54,73	1.61	8 (17%)	53,90,113	2.13	12 (22%)
19	CLA	B	1021	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	16 (21%)
29	CHL	4	615	16	43,51,74	1.00	2 (4%)	45,86,114	1.49	9 (20%)
19	CLA	B	1224	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	15 (19%)
22	BCR	J	4012	-	41,41,41	1.82	4 (9%)	56,56,56	4.54	17 (30%)
19	CLA	2	601	14	60,68,73	1.42	9 (15%)	70,107,113	2.02	17 (24%)
19	CLA	A	1138	-	65,73,73	1.35	9 (13%)	76,113,113	1.84	15 (19%)
19	CLA	B	1215	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	15 (19%)
22	BCR	I	4018	-	41,41,41	1.78	5 (12%)	56,56,56	4.44	25 (44%)
19	CLA	B	1226	-	65,73,73	1.35	7 (10%)	76,113,113	1.94	16 (21%)
19	CLA	B	1234	-	55,63,73	1.47	7 (12%)	64,101,113	2.03	14 (21%)
19	CLA	L	1503	-	50,58,73	1.54	9 (18%)	58,95,113	2.18	18 (31%)
21	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
25	LMG	2	802	-	25,25,55	0.56	0	33,33,63	1.37	3 (9%)
19	CLA	B	1218	-	65,73,73	1.36	9 (13%)	76,113,113	1.89	15 (19%)
19	CLA	B	1231	-	60,68,73	1.41	9 (15%)	70,107,113	1.95	14 (20%)
19	CLA	B	1223	-	65,73,73	1.36	10 (15%)	76,113,113	1.93	18 (23%)
27	DGD	3	803	-	52,52,67	0.90	3 (5%)	66,66,81	1.07	3 (4%)
19	CLA	B	1022	-	65,73,73	1.36	8 (12%)	76,113,113	1.88	15 (19%)
19	CLA	A	1103	-	65,73,73	1.33	7 (10%)	76,113,113	1.92	13 (17%)
19	CLA	F	1301	-	65,73,73	1.36	9 (13%)	76,113,113	1.84	14 (18%)
28	LUT	J	4013	-	42,43,43	2.30	1 (2%)	51,60,60	2.02	13 (25%)
25	LMG	F	5006	-	13,13,55	0.57	0	18,18,63	0.71	0
18	CL0	A	1011	-	65,73,73	2.35	18 (27%)	76,113,113	2.45	19 (25%)
25	LMG	B	5004	-	33,33,55	0.52	0	41,41,63	1.21	4 (9%)
23	LHG	A	5001	-	39,39,48	0.43	0	42,45,54	1.02	2 (4%)
19	CLA	G	1602	7	46,54,73	1.61	8 (17%)	53,90,113	2.15	14 (26%)
19	CLA	4	604	16	60,68,73	1.40	8 (13%)	70,107,113	2.00	16 (22%)
19	CLA	A	1136	-	65,73,73	1.37	9 (13%)	76,113,113	1.87	15 (19%)
19	CLA	B	1212	-	55,63,73	1.46	10 (18%)	64,101,113	2.10	16 (25%)
28	LUT	4	505	-	42,43,43	2.28	1 (2%)	51,60,60	2.38	20 (39%)
27	DGD	F	5005	-	58,58,67	1.06	6 (10%)	72,72,81	1.03	4 (5%)
19	CLA	1	605	-	65,73,73	1.36	8 (12%)	76,113,113	1.96	14 (18%)
29	CHL	1	609	13	56,64,74	0.94	3 (5%)	61,102,114	1.35	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	B	4005	-	41,41,41	1.79	4 (9%)	56,56,56	4.39	17 (30%)
19	CLA	B	1205	-	65,73,73	1.36	8 (12%)	76,113,113	1.92	15 (19%)
19	CLA	B	1201	-	65,73,73	1.35	8 (12%)	76,113,113	1.86	15 (19%)
19	CLA	A	1124	-	55,63,73	1.48	8 (14%)	64,101,113	1.97	15 (23%)
19	CLA	A	1126	-	65,73,73	1.38	9 (13%)	76,113,113	1.94	18 (23%)
19	CLA	1	602	13	46,54,73	1.60	8 (17%)	53,90,113	2.02	12 (22%)
22	BCR	A	4003	-	41,41,41	1.81	4 (9%)	56,56,56	4.41	22 (39%)
19	CLA	1	604	13	65,73,73	1.36	9 (13%)	76,113,113	1.87	14 (18%)
29	CHL	4	613	-	61,69,74	0.88	3 (4%)	67,108,114	1.16	8 (11%)
19	CLA	3	603	-	55,63,73	1.49	9 (16%)	64,101,113	2.15	16 (25%)
19	CLA	B	1238	33	65,73,73	1.36	8 (12%)	76,113,113	1.90	13 (17%)
19	CLA	3	602	-	52,60,73	1.52	8 (15%)	60,97,113	2.14	17 (28%)
25	LMG	F	5003	-	36,36,55	0.72	1 (2%)	44,44,63	1.02	2 (4%)
19	CLA	3	614	-	42,50,73	1.69	8 (19%)	48,85,113	2.19	11 (22%)
19	CLA	A	1105	-	60,68,73	1.43	9 (15%)	70,107,113	1.92	13 (18%)
22	BCR	I	4020	-	41,41,41	1.86	4 (9%)	56,56,56	4.42	20 (35%)
27	DGD	4	802	-	51,51,67	0.92	2 (3%)	65,65,81	0.98	3 (4%)
19	CLA	A	1119	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	17 (22%)
23	LHG	2	801	-	34,34,48	0.46	0	37,40,54	1.09	3 (8%)
19	CLA	A	1012	-	65,73,73	1.37	8 (12%)	76,113,113	1.85	16 (21%)
19	CLA	B	1225	-	65,73,73	1.34	7 (10%)	76,113,113	1.87	16 (21%)
19	CLA	A	1107	1	65,73,73	1.35	7 (10%)	76,113,113	1.89	15 (19%)
19	CLA	A	1129	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	16 (21%)
19	CLA	1	606	-	50,58,73	1.54	8 (16%)	58,95,113	2.11	15 (25%)
22	BCR	B	4004	-	41,41,41	1.87	4 (9%)	56,56,56	4.79	18 (32%)
29	CHL	1	612	13	61,69,74	0.87	2 (3%)	67,108,114	1.17	7 (10%)
19	CLA	A	1116	-	56,64,73	1.49	10 (17%)	65,102,113	2.09	17 (26%)
19	CLA	4	617	-	65,73,73	1.33	8 (12%)	76,113,113	1.93	16 (21%)
22	BCR	F	4016	-	41,41,41	1.80	4 (9%)	56,56,56	4.31	16 (28%)
19	CLA	3	606	-	50,58,73	1.53	8 (16%)	58,95,113	2.13	14 (24%)
19	CLA	A	1120	-	60,68,73	1.41	9 (15%)	70,107,113	1.92	13 (18%)
22	BCR	L	4020	-	41,41,41	1.80	4 (9%)	56,56,56	4.44	18 (32%)
22	BCR	3	503	-	41,41,41	1.82	5 (12%)	56,56,56	4.29	19 (33%)
19	CLA	A	1101	-	65,73,73	1.34	9 (13%)	76,113,113	1.93	17 (22%)
19	CLA	A	1118	-	50,58,73	1.55	9 (18%)	58,95,113	2.13	14 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1236	-	50,58,73	1.54	8 (16%)	58,95,113	2.16	16 (27%)
25	LMG	2	803	-	36,36,55	0.69	2 (5%)	44,44,63	1.06	2 (4%)
29	CHL	2	610	-	56,64,74	0.87	2 (3%)	61,102,114	1.30	10 (16%)
29	CHL	4	611	-	51,59,74	0.96	3 (5%)	55,96,114	1.42	11 (20%)
19	CLA	B	1217	-	46,54,73	1.59	7 (15%)	53,90,113	2.10	13 (24%)
25	LMG	G	5006	-	25,25,55	0.58	0	33,33,63	1.17	3 (9%)
19	CLA	B	1221	-	65,73,73	1.36	9 (13%)	76,113,113	1.94	14 (18%)
19	CLA	B	1210	-	65,73,73	1.36	10 (15%)	76,113,113	1.94	17 (22%)
25	LMG	F	5001	-	30,30,55	0.52	0	38,38,63	1.09	2 (5%)
19	CLA	G	1603	-	65,73,73	1.36	8 (12%)	76,113,113	1.89	15 (19%)
19	CLA	A	1132	-	65,73,73	1.36	9 (13%)	76,113,113	1.90	14 (18%)
25	LMG	2	804	-	30,30,55	0.53	0	38,38,63	1.08	2 (5%)
27	DGD	1	803	-	42,42,67	0.87	1 (2%)	56,56,81	0.99	2 (3%)
29	CHL	2	609	14	66,74,74	0.85	2 (3%)	73,114,114	1.16	9 (12%)
19	CLA	A	1109	-	65,73,73	1.37	10 (15%)	76,113,113	1.98	17 (22%)
19	CLA	B	1230	-	58,66,73	1.44	9 (15%)	67,104,113	2.05	17 (25%)
19	CLA	K	1402	-	60,68,73	1.41	8 (13%)	70,107,113	1.98	15 (21%)
22	BCR	1	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.65	21 (37%)
28	LUT	1	502	-	42,43,43	2.31	1 (2%)	51,60,60	2.18	15 (29%)
19	CLA	A	1133	-	65,73,73	1.36	9 (13%)	76,113,113	1.84	14 (18%)
22	BCR	A	4008	-	41,41,41	1.79	4 (9%)	56,56,56	4.42	25 (44%)
19	CLA	B	1229	-	65,73,73	1.35	7 (10%)	76,113,113	1.89	16 (21%)
19	CLA	A	1123	-	65,73,73	1.36	9 (13%)	76,113,113	1.91	13 (17%)
29	CHL	2	611	-	48,56,74	1.00	3 (6%)	51,92,114	1.39	10 (19%)
19	CLA	B	1206	2	65,73,73	1.36	8 (12%)	76,113,113	1.89	13 (17%)
31	3PH	2	807	-	32,32,47	1.03	4 (12%)	36,37,52	1.17	2 (5%)
19	CLA	A	1130	-	55,63,73	1.48	9 (16%)	64,101,113	2.00	12 (18%)
19	CLA	4	601	16	60,68,73	1.41	9 (15%)	70,107,113	2.01	16 (22%)
19	CLA	A	1122	-	65,73,73	1.38	9 (13%)	76,113,113	1.93	16 (21%)
19	CLA	A	1106	1	65,73,73	1.34	9 (13%)	76,113,113	1.96	18 (23%)
19	CLA	J	1901	10	50,58,73	1.56	9 (18%)	58,95,113	2.09	14 (24%)
24	LMT	2	808	-	36,36,36	1.15	5 (13%)	47,47,47	0.96	2 (4%)
19	CLA	A	1114	-	46,54,73	1.61	9 (19%)	53,90,113	2.17	12 (22%)
19	CLA	F	1302	6	65,73,73	1.35	8 (12%)	76,113,113	1.90	16 (21%)
19	CLA	1	614	13	60,68,73	1.43	8 (13%)	70,107,113	1.90	14 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	1139	-	65,73,73	1.37	9 (13%)	76,113,113	1.90	16 (21%)
19	CLA	A	1137	-	65,73,73	1.37	9 (13%)	76,113,113	1.89	15 (19%)
22	BCR	K	4001	-	41,41,41	1.80	5 (12%)	56,56,56	4.56	15 (26%)
19	CLA	1	613	-	45,53,73	1.64	10 (22%)	52,89,113	2.11	12 (23%)
20	PQN	A	2001	-	34,34,34	0.36	0	42,45,45	1.14	3 (7%)
29	CHL	2	615	-	56,64,74	0.90	2 (3%)	61,102,114	1.36	11 (18%)
19	CLA	4	609	16	50,58,73	1.56	9 (18%)	58,95,113	2.09	15 (25%)
19	CLA	3	608	-	48,56,73	1.59	8 (16%)	55,92,113	2.12	13 (23%)
19	CLA	A	1113	-	45,53,73	1.61	8 (17%)	52,89,113	2.10	14 (26%)
23	LHG	3	801	-	16,16,48	0.87	1 (6%)	17,20,54	0.67	0
19	CLA	B	1237	-	65,73,73	1.37	9 (13%)	76,113,113	1.83	13 (17%)
19	CLA	A	1104	-	65,73,73	1.34	9 (13%)	76,113,113	1.90	15 (19%)
22	BCR	1	503	-	41,41,41	1.83	4 (9%)	56,56,56	4.66	22 (39%)
28	LUT	3	502	-	42,43,43	2.24	1 (2%)	51,60,60	1.93	17 (33%)
29	CHL	2	613	-	46,54,74	0.96	2 (4%)	49,90,114	1.30	7 (14%)
30	XAT	2	502	-	39,47,47	0.68	1 (2%)	54,74,74	2.05	12 (22%)
22	BCR	L	4019	-	41,41,41	1.84	4 (9%)	56,56,56	4.58	19 (33%)
19	CLA	2	604	14	65,73,73	1.36	8 (12%)	76,113,113	1.92	14 (18%)
28	LUT	3	501	-	42,43,43	2.33	1 (2%)	51,60,60	2.20	17 (33%)
19	CLA	4	606	-	50,58,73	1.55	8 (16%)	58,95,113	2.09	14 (24%)
19	CLA	A	1128	-	65,73,73	1.35	9 (13%)	76,113,113	1.90	17 (22%)
28	LUT	4	501	-	42,43,43	2.25	1 (2%)	51,60,60	2.26	17 (33%)
19	CLA	B	1222	33	65,73,73	1.34	8 (12%)	76,113,113	1.94	16 (21%)
19	CLA	B	1227	-	65,73,73	1.36	8 (12%)	76,113,113	1.93	16 (21%)
19	CLA	2	603	14	65,73,73	1.35	8 (12%)	76,113,113	1.90	14 (18%)
19	CLA	3	605	-	55,63,73	1.49	10 (18%)	64,101,113	2.07	17 (26%)
25	LMG	F	5002	-	47,47,55	0.97	4 (8%)	55,55,63	1.10	3 (5%)
25	LMG	2	806	-	13,13,55	0.55	0	18,18,63	0.56	0
19	CLA	A	1013	-	65,73,73	1.33	8 (12%)	76,113,113	1.86	16 (21%)
23	LHG	B	5002	-	48,48,48	0.40	0	51,54,54	1.04	4 (7%)
29	CHL	4	610	-	47,55,74	1.02	2 (4%)	50,91,114	1.45	10 (20%)
19	CLA	B	1211	-	65,73,73	1.34	8 (12%)	76,113,113	1.86	13 (17%)
20	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.15	3 (7%)
25	LMG	1	802	-	46,46,55	0.94	3 (6%)	54,54,63	1.01	2 (3%)
19	CLA	B	1214	-	65,73,73	1.36	10 (15%)	76,113,113	1.90	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	SF4	C	3002	3	0,12,12	-	-	-		
22	BCR	3	506	-	41,41,41	1.84	4 (9%)	56,56,56	4.49	21 (37%)
23	LHG	B	5001	19	20,20,48	0.58	0	23,26,54	1.48	2 (8%)
30	XAT	4	502	-	39,47,47	0.66	1 (2%)	54,74,74	1.71	13 (24%)
19	CLA	B	1208	-	60,68,73	1.43	8 (13%)	70,107,113	1.89	13 (18%)
19	CLA	L	1502	-	60,68,73	1.43	9 (15%)	70,107,113	2.03	17 (24%)
22	BCR	A	4017	-	41,41,41	1.80	4 (9%)	56,56,56	4.93	20 (35%)
29	CHL	3	611	-	47,55,74	0.99	2 (4%)	50,91,114	1.45	11 (22%)
19	CLA	B	1239	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	15 (19%)
23	LHG	1	801	-	48,48,48	0.39	0	51,54,54	0.96	2 (3%)
19	CLA	A	1112	-	65,73,73	1.37	8 (12%)	76,113,113	1.88	14 (18%)
24	LMT	A	5004	-	36,36,36	1.16	6 (16%)	47,47,47	1.01	2 (4%)
19	CLA	2	605	-	65,73,73	1.35	9 (13%)	76,113,113	1.89	15 (19%)
19	CLA	4	603	-	65,73,73	1.37	9 (13%)	76,113,113	1.95	15 (19%)
19	CLA	4	602	-	50,58,73	1.54	9 (18%)	58,95,113	2.12	16 (27%)
19	CLA	L	1501	12	50,58,73	1.54	9 (18%)	58,95,113	2.19	16 (27%)
22	BCR	A	4011	-	41,41,41	1.79	4 (9%)	56,56,56	4.43	22 (39%)
25	LMG	2	805	-	30,30,55	0.55	0	38,38,63	1.08	2 (5%)
28	LUT	1	501	-	42,43,43	2.29	1 (2%)	51,60,60	2.23	20 (39%)
22	BCR	A	4007	-	41,41,41	1.85	4 (9%)	56,56,56	4.59	21 (37%)
19	CLA	B	1216	-	65,73,73	1.36	9 (13%)	76,113,113	1.84	15 (19%)
19	CLA	2	607	-	60,68,73	1.43	9 (15%)	70,107,113	2.07	17 (24%)
19	CLA	K	1404	-	46,54,73	1.62	9 (19%)	53,90,113	2.03	12 (22%)
19	CLA	B	1209	-	46,54,73	1.60	9 (19%)	53,90,113	2.08	12 (22%)
19	CLA	A	1115	-	65,73,73	1.36	9 (13%)	76,113,113	1.85	15 (19%)
19	CLA	3	607	-	52,60,73	1.52	8 (15%)	60,97,113	2.13	16 (26%)
19	CLA	A	1135	-	51,59,73	1.52	8 (15%)	59,96,113	2.13	13 (22%)
19	CLA	K	1401	-	45,53,73	1.62	8 (17%)	52,89,113	2.17	12 (23%)
19	CLA	B	1023	-	65,73,73	1.37	7 (10%)	76,113,113	1.80	14 (18%)
22	BCR	G	4011	-	41,41,41	1.86	4 (9%)	56,56,56	4.46	23 (41%)
19	CLA	K	1403	-	48,56,73	1.59	9 (18%)	55,92,113	2.22	15 (27%)
19	CLA	1	601	13	65,73,73	1.38	8 (12%)	76,113,113	1.86	14 (18%)
22	BCR	B	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.40	28 (50%)
19	CLA	1	603	-	55,63,73	1.49	9 (16%)	64,101,113	2.08	16 (25%)
19	CLA	3	610	15	65,73,73	1.35	8 (12%)	76,113,113	1.88	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	BCR	B	4009	-	41,41,41	1.81	4 (9%)	56,56,56	4.20	19 (33%)
24	LMT	G	5004	-	36,36,36	1.15	6 (16%)	47,47,47	0.97	2 (4%)
25	LMG	A	5006	-	50,50,55	1.05	5 (10%)	58,58,63	1.05	3 (5%)
19	CLA	B	1232	-	55,63,73	1.50	9 (16%)	64,101,113	2.00	14 (21%)
19	CLA	A	1111	-	65,73,73	1.35	9 (13%)	76,113,113	1.84	12 (15%)
25	LMG	3	802	-	30,30,55	0.55	0	38,38,63	1.08	3 (7%)
19	CLA	A	1121	-	60,68,73	1.42	9 (15%)	70,107,113	2.02	15 (21%)
27	DGD	B	5005	-	62,62,67	1.11	5 (8%)	76,76,81	0.99	3 (3%)
19	CLA	A	1131	-	65,73,73	1.36	7 (10%)	76,113,113	1.82	14 (18%)
19	CLA	B	1220	-	55,63,73	1.48	9 (16%)	64,101,113	1.98	15 (23%)
19	CLA	4	605	-	60,68,73	1.42	9 (15%)	70,107,113	1.97	16 (22%)
19	CLA	2	606	-	50,58,73	1.56	9 (18%)	58,95,113	2.08	14 (24%)
29	CHL	3	604	15	66,74,74	0.83	2 (3%)	73,114,114	1.28	9 (12%)
19	CLA	A	1102	-	65,73,73	1.35	9 (13%)	76,113,113	2.02	18 (23%)
19	CLA	4	607	-	60,68,73	1.42	8 (13%)	70,107,113	1.95	16 (22%)
27	DGD	G	5003	-	48,48,67	0.86	2 (4%)	62,62,81	0.97	3 (4%)
19	CLA	3	617	-	60,68,73	1.43	9 (15%)	70,107,113	1.93	15 (21%)
19	CLA	3	612	15	50,58,73	1.53	8 (16%)	58,95,113	2.14	14 (24%)
19	CLA	2	608	-	50,58,73	1.56	8 (16%)	58,95,113	2.18	16 (27%)
19	CLA	4	612	16	65,73,73	1.37	10 (15%)	76,113,113	1.83	13 (17%)
22	BCR	K	4002	-	41,41,41	1.80	4 (9%)	56,56,56	4.41	21 (37%)
24	LMT	B	5006	-	33,33,36	1.20	5 (15%)	44,44,47	0.93	2 (4%)
19	CLA	H	1701	-	60,68,73	1.40	8 (13%)	70,107,113	1.90	13 (18%)
19	CLA	A	1140	-	65,73,73	1.36	8 (12%)	76,113,113	1.88	14 (18%)
19	CLA	B	1228	-	60,68,73	1.40	7 (11%)	70,107,113	2.01	17 (24%)
22	BCR	H	4021	-	41,41,41	1.84	4 (9%)	56,56,56	4.55	19 (33%)
25	LMG	B	5007	-	34,34,55	0.51	0	42,42,63	1.07	2 (4%)
19	CLA	G	1601	-	55,63,73	1.46	7 (12%)	64,101,113	2.06	16 (25%)
22	BCR	A	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.30	22 (39%)
24	LMT	G	5005	-	32,32,36	1.21	5 (15%)	43,43,47	0.96	2 (4%)
28	LUT	2	501	-	42,43,43	2.29	1 (2%)	51,60,60	2.24	17 (33%)
19	CLA	A	1125	-	65,73,73	1.36	8 (12%)	76,113,113	1.94	16 (21%)
19	CLA	2	612	-	55,63,73	1.46	9 (16%)	64,101,113	2.00	13 (20%)
19	CLA	B	1203	2	65,73,73	1.35	9 (13%)	76,113,113	1.84	14 (18%)
19	CLA	A	1110	-	55,63,73	1.47	6 (10%)	64,101,113	2.12	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	1	607	-	46,54,73	1.59	8 (17%)	53,90,113	2.15	12 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1202	-	1/1/15/20	19/37/115/115	-
19	CLA	4	608	-	1/1/11/20	7/15/93/115	-
23	LHG	4	801	-	-	21/39/39/53	-
21	SF4	C	3003	3	-	-	0/6/5/5
27	DGD	J	5001	-	-	11/47/87/95	0/2/2/2
19	CLA	B	1213	-	1/1/14/20	8/31/109/115	-
19	CLA	B	1207	-	1/1/15/20	15/37/115/115	-
19	CLA	2	602	-	1/1/12/20	7/22/100/115	-
22	BCR	F	4014	-	-	8/29/63/63	0/2/2/2
25	LMG	G	5001	-	-	16/44/64/70	0/1/1/1
19	CLA	A	1127	-	1/1/15/20	16/37/115/115	-
19	CLA	3	613	-	1/1/11/20	6/15/93/115	-
19	CLA	A	1117	-	1/1/15/20	15/37/115/115	-
29	CHL	1	610	13	3/3/16/26	5/17/115/137	-
22	BCR	B	4010	-	-	8/29/63/63	0/2/2/2
24	LMT	B	5008	-	-	8/17/57/61	0/2/2/2
22	BCR	2	503	-	-	14/29/63/63	0/2/2/2
19	CLA	A	1134	1	1/1/13/20	10/25/103/115	-
25	LMG	F	5004	-	-	8/29/49/70	0/1/1/1
25	LMG	B	5003	-	-	9/30/50/70	0/1/1/1
19	CLA	B	1219	-	1/1/15/20	16/37/115/115	-
19	CLA	3	601	15	1/1/13/20	12/25/103/115	-
19	CLA	A	1141	-	1/1/14/20	17/31/109/115	-
25	LMG	G	5002	-	-	18/45/65/70	0/1/1/1
23	LHG	A	5002	-	-	28/53/53/53	-
19	CLA	1	611	-	1/1/15/20	17/37/115/115	-
19	CLA	B	1235	-	1/1/15/20	13/37/115/115	-
19	CLA	B	1240	23	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	1108	-	1/1/12/20	8/19/97/115	-
19	CLA	B	1204	-	1/1/15/20	16/37/115/115	-
19	CLA	1	608	-	1/1/11/20	7/15/93/115	-
19	CLA	B	1021	-	1/1/15/20	8/37/115/115	-
29	CHL	4	615	16	4/4/15/26	0/12/110/137	-
19	CLA	B	1224	-	1/1/15/20	19/37/115/115	-
22	BCR	J	4012	-	-	6/29/63/63	0/2/2/2
19	CLA	2	601	14	1/1/14/20	9/31/109/115	-
19	CLA	A	1138	-	1/1/15/20	18/37/115/115	-
19	CLA	B	1215	-	1/1/15/20	12/37/115/115	-
22	BCR	I	4018	-	-	7/29/63/63	0/2/2/2
19	CLA	B	1226	-	1/1/15/20	16/37/115/115	-
19	CLA	B	1234	-	1/1/13/20	8/25/103/115	-
19	CLA	L	1503	-	1/1/12/20	8/19/97/115	-
21	SF4	A	3001	2,1	-	-	0/6/5/5
25	LMG	2	802	-	-	4/20/40/70	0/1/1/1
19	CLA	B	1218	-	1/1/15/20	11/37/115/115	-
19	CLA	B	1231	-	1/1/14/20	6/31/109/115	-
19	CLA	B	1223	-	1/1/15/20	12/37/115/115	-
27	DGD	3	803	-	-	8/40/80/95	0/2/2/2
19	CLA	B	1022	-	1/1/15/20	7/37/115/115	-
19	CLA	A	1103	-	1/1/15/20	18/37/115/115	-
19	CLA	F	1301	-	1/1/15/20	17/37/115/115	-
28	LUT	J	4013	-	1/1/12/27	5/29/67/67	0/2/2/2
25	LMG	F	5006	-	-	1/4/24/70	0/1/1/1
18	CL0	A	1011	-	3/3/20/25	9/37/135/135	-
25	LMG	B	5004	-	-	10/28/48/70	0/1/1/1
23	LHG	A	5001	-	-	26/44/44/53	-
19	CLA	G	1602	7	1/1/11/20	9/15/93/115	-
19	CLA	4	604	16	1/1/14/20	7/31/109/115	-
19	CLA	A	1136	-	1/1/15/20	20/37/115/115	-
19	CLA	B	1212	-	1/1/13/20	12/25/103/115	-
28	LUT	4	505	-	-	3/29/67/67	0/2/2/2
27	DGD	F	5005	-	-	15/46/86/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	605	-	1/1/15/20	16/37/115/115	-
29	CHL	1	609	13	4/4/18/26	3/27/125/137	-
22	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
19	CLA	B	1205	-	1/1/15/20	13/37/115/115	-
19	CLA	B	1201	-	1/1/15/20	17/37/115/115	-
19	CLA	A	1124	-	1/1/13/20	8/25/103/115	-
19	CLA	A	1126	-	1/1/15/20	16/37/115/115	-
19	CLA	1	602	13	1/1/11/20	6/15/93/115	-
29	CHL	4	613	-	4/4/19/26	6/33/131/137	-
19	CLA	1	604	13	1/1/15/20	15/37/115/115	-
22	BCR	A	4003	-	-	6/29/63/63	0/2/2/2
19	CLA	3	603	-	1/1/13/20	12/25/103/115	-
19	CLA	B	1238	33	1/1/15/20	12/37/115/115	-
19	CLA	3	602	-	1/1/12/20	8/22/100/115	-
25	LMG	F	5003	-	-	13/31/51/70	0/1/1/1
19	CLA	3	614	-	1/1/10/20	3/10/88/115	-
19	CLA	A	1105	-	1/1/14/20	13/31/109/115	-
22	BCR	I	4020	-	-	14/29/63/63	0/2/2/2
27	DGD	4	802	-	-	17/39/79/95	0/2/2/2
19	CLA	A	1119	-	1/1/15/20	21/37/115/115	-
23	LHG	2	801	-	-	18/39/39/53	-
19	CLA	A	1012	-	1/1/15/20	10/37/115/115	-
19	CLA	B	1225	-	1/1/15/20	15/37/115/115	-
19	CLA	A	1107	1	1/1/15/20	15/37/115/115	-
19	CLA	A	1129	-	1/1/15/20	11/37/115/115	-
19	CLA	1	606	-	1/1/12/20	5/19/97/115	-
29	CHL	1	612	13	4/4/19/26	4/33/131/137	-
22	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
19	CLA	A	1116	-	1/1/13/20	11/27/105/115	-
19	CLA	4	617	-	1/1/15/20	18/37/115/115	-
22	BCR	F	4016	-	-	10/29/63/63	0/2/2/2
19	CLA	3	606	-	1/1/12/20	11/19/97/115	-
19	CLA	A	1120	-	1/1/14/20	16/31/109/115	-
22	BCR	L	4020	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	3	503	-	-	10/29/63/63	0/2/2/2
19	CLA	A	1101	-	1/1/15/20	16/37/115/115	-
19	CLA	A	1118	-	1/1/12/20	7/19/97/115	-
19	CLA	B	1236	-	1/1/12/20	8/19/97/115	-
29	CHL	2	610	-	4/4/18/26	2/27/125/137	-
29	CHL	4	611	-	3/3/17/26	1/21/119/137	-
25	LMG	2	803	-	-	12/31/51/70	0/1/1/1
19	CLA	B	1217	-	1/1/11/20	7/15/93/115	-
25	LMG	G	5006	-	-	10/20/40/70	0/1/1/1
19	CLA	B	1221	-	1/1/15/20	18/37/115/115	-
19	CLA	B	1210	-	1/1/15/20	11/37/115/115	-
25	LMG	F	5001	-	-	4/25/45/70	0/1/1/1
19	CLA	G	1603	-	1/1/15/20	9/37/115/115	-
19	CLA	A	1132	-	1/1/15/20	15/37/115/115	-
29	CHL	2	609	14	4/4/20/26	7/39/137/137	-
25	LMG	2	804	-	-	5/25/45/70	0/1/1/1
27	DGD	1	803	-	-	14/30/70/95	0/2/2/2
19	CLA	A	1109	-	1/1/15/20	18/37/115/115	-
19	CLA	B	1230	-	1/1/13/20	15/29/107/115	-
19	CLA	K	1402	-	1/1/14/20	18/31/109/115	-
28	LUT	1	502	-	1/1/12/27	5/29/67/67	0/2/2/2
22	BCR	1	504	-	-	9/29/63/63	0/2/2/2
19	CLA	A	1133	-	1/1/15/20	21/37/115/115	-
22	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
19	CLA	B	1229	-	1/1/15/20	13/37/115/115	-
19	CLA	A	1123	-	1/1/15/20	15/37/115/115	-
29	CHL	2	611	-	3/3/16/26	3/18/116/137	-
19	CLA	B	1206	2	1/1/15/20	16/37/115/115	-
31	3PH	2	807	-	-	16/34/34/49	-
19	CLA	A	1130	-	1/1/13/20	6/25/103/115	-
19	CLA	4	601	16	1/1/14/20	16/31/109/115	-
19	CLA	A	1122	-	1/1/15/20	18/37/115/115	-
19	CLA	A	1106	1	1/1/15/20	15/37/115/115	-
19	CLA	J	1901	10	1/1/12/20	7/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMT	2	808	-	-	4/21/61/61	0/2/2/2
19	CLA	A	1114	-	1/1/11/20	9/15/93/115	-
19	CLA	F	1302	6	1/1/15/20	13/37/115/115	-
19	CLA	1	614	13	1/1/14/20	16/31/109/115	-
19	CLA	A	1139	-	1/1/15/20	15/37/115/115	-
19	CLA	A	1137	-	1/1/15/20	19/37/115/115	-
22	BCR	K	4001	-	-	6/29/63/63	0/2/2/2
19	CLA	1	613	-	1/1/11/20	6/13/91/115	-
29	CHL	2	615	-	4/4/18/26	7/27/125/137	-
20	PQN	A	2001	-	-	6/23/43/43	0/2/2/2
19	CLA	4	609	16	1/1/12/20	9/19/97/115	-
19	CLA	3	608	-	1/1/11/20	6/17/95/115	-
19	CLA	A	1113	-	1/1/11/20	8/13/91/115	-
23	LHG	3	801	-	-	15/19/19/53	-
19	CLA	B	1237	-	1/1/15/20	20/37/115/115	-
19	CLA	A	1104	-	1/1/15/20	17/37/115/115	-
28	LUT	3	502	-	1/1/12/27	1/29/67/67	0/2/2/2
22	BCR	1	503	-	-	6/29/63/63	0/2/2/2
29	CHL	2	613	-	3/3/16/26	4/15/113/137	-
30	XAT	2	502	-	2/2/12/26	7/31/93/93	0/4/4/4
22	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
19	CLA	2	604	14	1/1/15/20	18/37/115/115	-
28	LUT	3	501	-	1/1/12/27	6/29/67/67	0/2/2/2
19	CLA	4	606	-	1/1/12/20	7/19/97/115	-
19	CLA	A	1128	-	1/1/15/20	15/37/115/115	-
28	LUT	4	501	-	1/1/12/27	7/29/67/67	0/2/2/2
19	CLA	B	1222	33	1/1/15/20	19/37/115/115	-
19	CLA	B	1227	-	1/1/15/20	12/37/115/115	-
19	CLA	2	603	14	1/1/15/20	16/37/115/115	-
19	CLA	3	605	-	1/1/13/20	11/25/103/115	-
29	CHL	4	610	-	3/3/16/26	3/17/115/137	-
25	LMG	F	5002	-	-	11/42/62/70	0/1/1/1
19	CLA	A	1013	-	1/1/15/20	14/37/115/115	-
23	LHG	B	5002	-	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	2	806	-	-	1/4/24/70	0/1/1/1
19	CLA	B	1211	-	1/1/15/20	18/37/115/115	-
20	PQN	B	2002	-	-	6/23/43/43	0/2/2/2
25	LMG	1	802	-	-	4/41/61/70	0/1/1/1
19	CLA	B	1214	-	1/1/15/20	12/37/115/115	-
23	LHG	B	5001	19	-	9/23/23/53	-
22	BCR	3	506	-	-	5/29/63/63	0/2/2/2
21	SF4	C	3002	3	-	-	0/6/5/5
30	XAT	4	502	-	2/2/12/26	2/31/93/93	0/4/4/4
19	CLA	B	1208	-	1/1/14/20	14/31/109/115	-
19	CLA	L	1502	-	1/1/14/20	15/31/109/115	-
29	CHL	3	611	-	3/3/16/26	0/17/115/137	-
22	BCR	A	4017	-	-	9/29/63/63	0/2/2/2
19	CLA	B	1239	-	1/1/15/20	10/37/115/115	-
23	LHG	1	801	-	-	30/53/53/53	-
19	CLA	A	1112	-	1/1/15/20	21/37/115/115	-
24	LMT	A	5004	-	-	7/21/61/61	0/2/2/2
19	CLA	2	605	-	1/1/15/20	17/37/115/115	-
19	CLA	4	603	-	1/1/15/20	13/37/115/115	-
19	CLA	4	602	-	1/1/12/20	7/19/97/115	-
19	CLA	L	1501	12	1/1/12/20	10/19/97/115	-
22	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
25	LMG	2	805	-	-	6/25/45/70	0/1/1/1
28	LUT	1	501	-	1/1/12/27	4/29/67/67	0/2/2/2
22	BCR	A	4007	-	-	10/29/63/63	0/2/2/2
19	CLA	B	1216	-	1/1/15/20	12/37/115/115	-
19	CLA	2	607	-	1/1/14/20	13/31/109/115	-
19	CLA	K	1404	-	1/1/11/20	5/15/93/115	-
19	CLA	B	1209	-	1/1/11/20	4/15/93/115	-
19	CLA	A	1115	-	1/1/15/20	12/37/115/115	-
19	CLA	3	607	-	1/1/12/20	9/22/100/115	-
19	CLA	A	1135	-	1/1/12/20	11/21/99/115	-
19	CLA	K	1401	-	1/1/11/20	8/13/91/115	-
19	CLA	B	1023	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	BCR	G	4011	-	-	7/29/63/63	0/2/2/2
19	CLA	K	1403	-	1/1/11/20	8/17/95/115	-
19	CLA	1	601	13	1/1/15/20	16/37/115/115	-
22	BCR	B	4006	-	-	3/29/63/63	0/2/2/2
19	CLA	1	603	-	1/1/13/20	10/25/103/115	-
19	CLA	3	610	15	1/1/15/20	19/37/115/115	-
22	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
24	LMT	G	5004	-	-	10/21/61/61	0/2/2/2
25	LMG	A	5006	-	-	10/45/65/70	0/1/1/1
19	CLA	B	1232	-	1/1/13/20	11/25/103/115	-
19	CLA	A	1111	-	1/1/15/20	17/37/115/115	-
25	LMG	3	802	-	-	6/25/45/70	0/1/1/1
19	CLA	A	1121	-	1/1/14/20	15/31/109/115	-
27	DGD	B	5005	-	-	19/50/90/95	0/2/2/2
19	CLA	A	1131	-	1/1/15/20	17/37/115/115	-
19	CLA	B	1220	-	1/1/13/20	9/25/103/115	-
19	CLA	4	605	-	1/1/14/20	10/31/109/115	-
19	CLA	2	606	-	1/1/12/20	8/19/97/115	-
29	CHL	3	604	15	4/4/20/26	10/39/137/137	-
19	CLA	A	1102	-	1/1/15/20	22/37/115/115	-
19	CLA	4	607	-	1/1/14/20	14/31/109/115	-
27	DGD	G	5003	-	-	11/36/76/95	0/2/2/2
19	CLA	3	617	-	1/1/14/20	18/31/109/115	-
19	CLA	3	612	15	1/1/12/20	7/19/97/115	-
19	CLA	2	608	-	1/1/12/20	8/19/97/115	-
19	CLA	4	612	16	1/1/15/20	14/37/115/115	-
22	BCR	K	4002	-	-	5/29/63/63	0/2/2/2
24	LMT	B	5006	-	-	4/18/58/61	0/2/2/2
19	CLA	H	1701	-	1/1/14/20	12/31/109/115	-
19	CLA	A	1140	-	1/1/15/20	7/37/115/115	-
19	CLA	B	1228	-	1/1/14/20	13/31/109/115	-
22	BCR	H	4021	-	-	8/29/63/63	0/2/2/2
25	LMG	B	5007	-	-	10/29/49/70	0/1/1/1
19	CLA	G	1601	-	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	2	501	-	1/1/12/27	6/29/67/67	0/2/2/2
22	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
24	LMT	G	5005	-	-	5/17/57/61	0/2/2/2
19	CLA	A	1125	-	1/1/15/20	15/37/115/115	-
19	CLA	2	612	-	1/1/13/20	8/25/103/115	-
19	CLA	B	1203	2	1/1/15/20	11/37/115/115	-
19	CLA	A	1110	-	1/1/13/20	8/25/103/115	-
19	CLA	1	607	-	1/1/11/20	9/15/93/115	-

The worst 5 of 1464 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	3	501	LUT	C24-C25	14.33	1.51	1.33
28	1	502	LUT	C24-C25	14.27	1.50	1.33
28	2	501	LUT	C24-C25	14.15	1.50	1.33
28	J	4013	LUT	C24-C25	14.13	1.50	1.33
28	1	501	LUT	C24-C25	14.08	1.50	1.33

The worst 5 of 3078 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	4001	BCR	C10-C11-C12	18.19	180.00	123.22
22	I	4018	BCR	C10-C11-C12	18.11	179.74	123.22
22	A	4017	BCR	C16-C15-C14	18.06	160.47	123.47
22	B	4005	BCR	C10-C11-C12	18.03	179.47	123.22
22	A	4017	BCR	C10-C11-C12	17.99	179.37	123.22

5 of 206 chirality outliers are listed below:

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

5 of 2603 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1011	CL0	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	A	1011	CL0	C3A-C2A-CAA-CBA
19	A	1012	CLA	CBD-CGD-O2D-CED
19	A	1013	CLA	C2-C1-O2A-CGA
19	A	1013	CLA	CBD-CGD-O2D-CED

There are no ring outliers.

204 monomers are involved in 906 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1202	CLA	4	0
19	4	608	CLA	4	0
21	C	3003	SF4	1	0
19	B	1213	CLA	5	0
19	B	1207	CLA	8	0
19	2	602	CLA	3	0
22	F	4014	BCR	7	0
19	A	1127	CLA	4	0
19	3	613	CLA	4	0
19	A	1117	CLA	3	0
22	B	4010	BCR	12	0
29	1	610	CHL	5	0
24	B	5008	LMT	1	0
22	2	503	BCR	10	0
19	A	1134	CLA	3	0
19	B	1219	CLA	6	0
19	3	601	CLA	11	0
19	A	1141	CLA	5	0
25	G	5002	LMG	2	0
19	1	611	CLA	5	0
19	B	1235	CLA	5	0
19	B	1240	CLA	6	0
19	A	1108	CLA	10	0
19	B	1204	CLA	3	0
19	1	608	CLA	4	0
19	B	1021	CLA	7	0
19	B	1224	CLA	4	0
22	J	4012	BCR	9	0
19	2	601	CLA	13	0
19	A	1138	CLA	7	0
19	B	1215	CLA	5	0
22	I	4018	BCR	8	0
19	B	1226	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1234	CLA	6	0
19	L	1503	CLA	5	0
19	B	1218	CLA	5	0
19	B	1231	CLA	5	0
19	B	1223	CLA	4	0
19	B	1022	CLA	9	0
19	A	1103	CLA	5	0
19	F	1301	CLA	2	0
28	J	4013	LUT	12	0
18	A	1011	CL0	3	0
23	A	5001	LHG	2	0
19	G	1602	CLA	3	0
19	4	604	CLA	7	0
19	A	1136	CLA	2	0
19	B	1212	CLA	3	0
28	4	505	LUT	6	0
27	F	5005	DGD	1	0
19	1	605	CLA	7	0
29	1	609	CHL	2	0
22	B	4005	BCR	6	0
19	B	1205	CLA	5	0
19	B	1201	CLA	2	0
19	A	1124	CLA	3	0
19	A	1126	CLA	7	0
22	A	4003	BCR	6	0
19	1	604	CLA	5	0
29	4	613	CHL	2	0
19	3	603	CLA	3	0
19	B	1238	CLA	4	0
19	3	602	CLA	4	0
19	3	614	CLA	3	0
19	A	1105	CLA	2	0
22	I	4020	BCR	4	0
27	4	802	DGD	1	0
19	A	1119	CLA	8	0
19	A	1012	CLA	7	0
19	B	1225	CLA	8	0
19	A	1107	CLA	2	0
19	A	1129	CLA	4	0
19	1	606	CLA	2	0
22	B	4004	BCR	8	0
29	1	612	CHL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1116	CLA	4	0
19	4	617	CLA	7	0
22	F	4016	BCR	6	0
19	3	606	CLA	4	0
19	A	1120	CLA	2	0
22	L	4020	BCR	10	0
22	3	503	BCR	17	0
19	A	1101	CLA	5	0
19	A	1118	CLA	4	0
19	B	1236	CLA	6	0
29	2	610	CHL	2	0
29	4	611	CHL	3	0
19	B	1217	CLA	3	0
19	B	1221	CLA	5	0
19	B	1210	CLA	6	0
19	G	1603	CLA	5	0
19	A	1132	CLA	3	0
29	2	609	CHL	3	0
19	A	1109	CLA	9	0
19	B	1230	CLA	5	0
19	K	1402	CLA	3	0
22	1	504	BCR	3	0
28	1	502	LUT	7	0
19	A	1133	CLA	1	0
22	A	4008	BCR	4	0
19	B	1229	CLA	8	0
19	A	1123	CLA	5	0
29	2	611	CHL	5	0
19	B	1206	CLA	8	0
19	A	1130	CLA	2	0
19	4	601	CLA	9	0
19	A	1122	CLA	6	0
19	A	1106	CLA	3	0
19	J	1901	CLA	3	0
24	2	808	LMT	1	0
19	A	1114	CLA	3	0
19	F	1302	CLA	1	0
19	1	614	CLA	4	0
19	A	1139	CLA	6	0
19	A	1137	CLA	4	0
22	K	4001	BCR	17	0
19	1	613	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	2001	PQN	2	0
29	2	615	CHL	9	0
19	4	609	CLA	1	0
19	3	608	CLA	3	0
19	A	1113	CLA	6	0
23	3	801	LHG	1	0
19	B	1237	CLA	1	0
19	A	1104	CLA	12	0
22	1	503	BCR	6	0
28	3	502	LUT	13	0
30	2	502	XAT	6	0
22	L	4019	BCR	9	0
19	2	604	CLA	6	0
28	3	501	LUT	13	0
19	4	606	CLA	4	0
19	A	1128	CLA	6	0
28	4	501	LUT	17	0
19	B	1222	CLA	5	0
19	B	1227	CLA	5	0
19	2	603	CLA	6	0
19	3	605	CLA	4	0
25	F	5002	LMG	1	0
19	A	1013	CLA	7	0
29	4	610	CHL	2	0
19	B	1211	CLA	8	0
20	B	2002	PQN	1	0
19	B	1214	CLA	6	0
21	C	3002	SF4	1	0
22	3	506	BCR	9	0
30	4	502	XAT	2	0
19	B	1208	CLA	5	0
19	L	1502	CLA	5	0
22	A	4017	BCR	9	0
29	3	611	CHL	1	0
19	B	1239	CLA	6	0
19	A	1112	CLA	6	0
19	2	605	CLA	2	0
19	4	603	CLA	7	0
19	4	602	CLA	3	0
19	L	1501	CLA	4	0
22	A	4011	BCR	10	0
28	1	501	LUT	11	0

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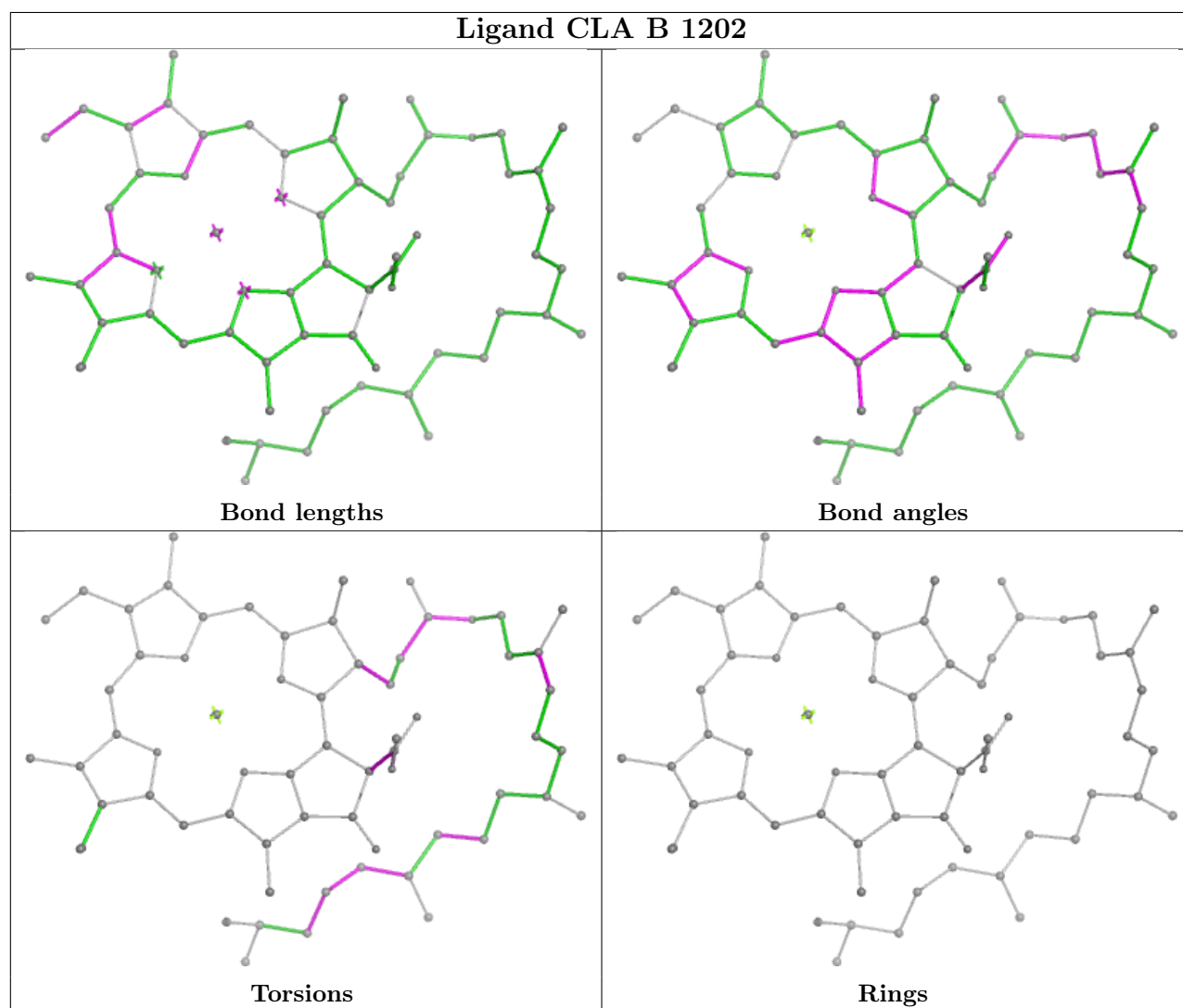
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A	4007	BCR	5	0
19	B	1216	CLA	5	0
19	2	607	CLA	10	0
19	B	1209	CLA	4	0
19	A	1115	CLA	3	0
19	3	607	CLA	7	0
19	A	1135	CLA	8	0
19	K	1401	CLA	5	0
19	B	1023	CLA	5	0
22	G	4011	BCR	9	0
19	K	1403	CLA	3	0
19	1	601	CLA	8	0
22	B	4006	BCR	11	0
19	1	603	CLA	3	0
19	3	610	CLA	3	0
22	B	4009	BCR	10	0
24	G	5004	LMT	4	0
25	A	5006	LMG	2	0
19	B	1232	CLA	5	0
19	A	1111	CLA	4	0
19	A	1121	CLA	4	0
19	A	1131	CLA	1	0
19	B	1220	CLA	3	0
19	4	605	CLA	2	0
19	2	606	CLA	6	0
29	3	604	CHL	6	0
19	A	1102	CLA	6	0
19	4	607	CLA	8	0
27	G	5003	DGD	1	0
19	3	612	CLA	11	0
19	2	608	CLA	4	0
19	4	612	CLA	6	0
22	K	4002	BCR	9	0
19	H	1701	CLA	6	0
19	A	1140	CLA	3	0
19	B	1228	CLA	1	0
22	H	4021	BCR	10	0
19	G	1601	CLA	4	0
22	A	4002	BCR	8	0
28	2	501	LUT	11	0
19	A	1125	CLA	9	0
19	2	612	CLA	3	0

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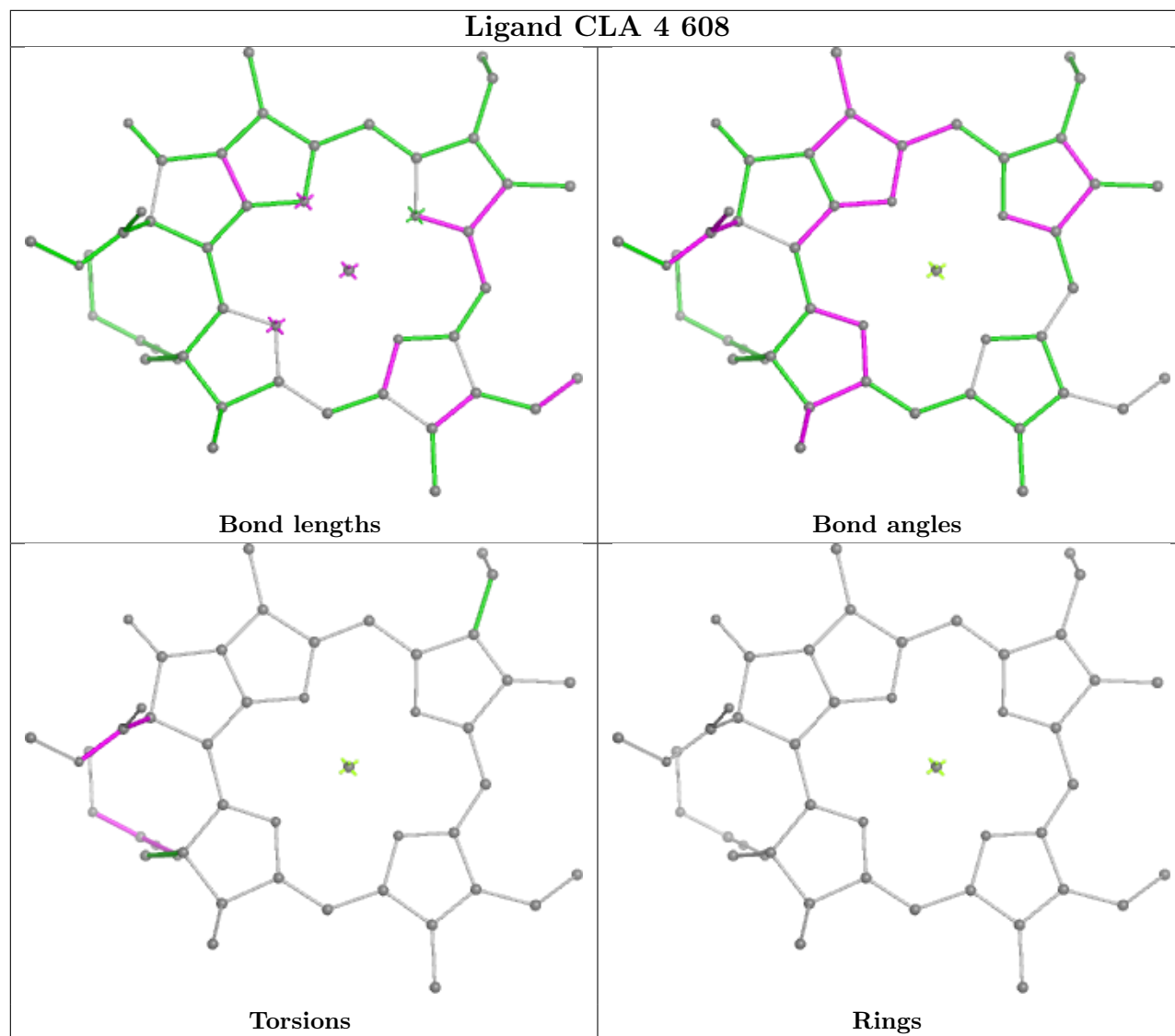
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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19	A	1110	CLA	4	0
19	1	607	CLA	2	0

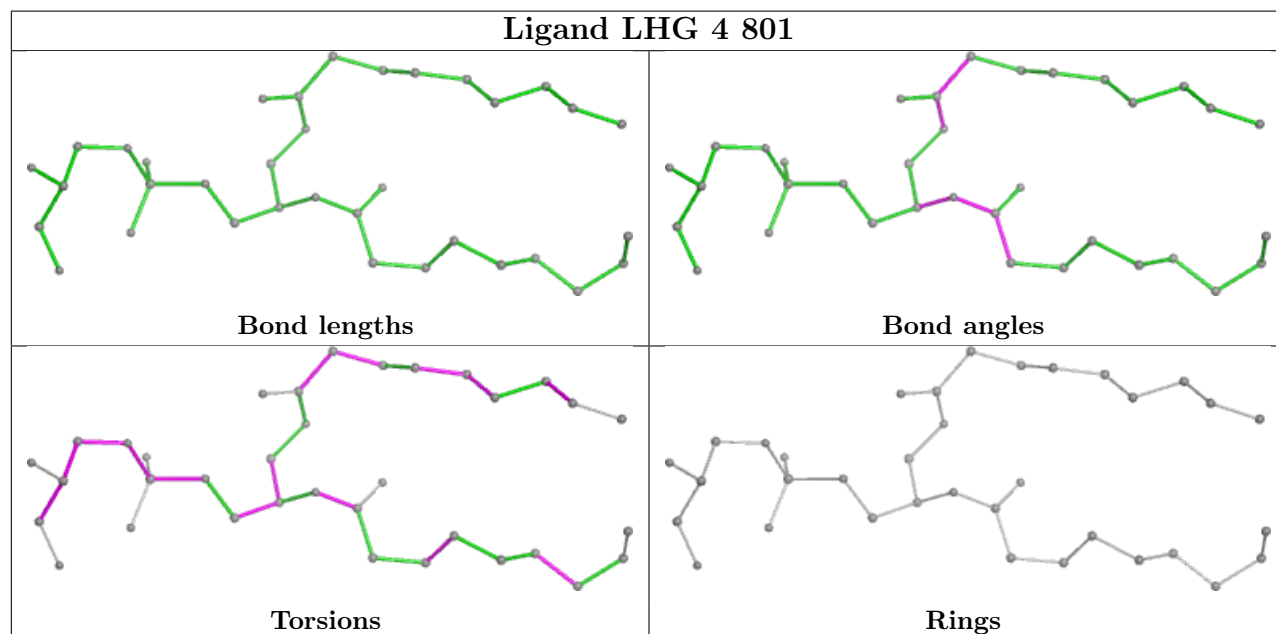
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

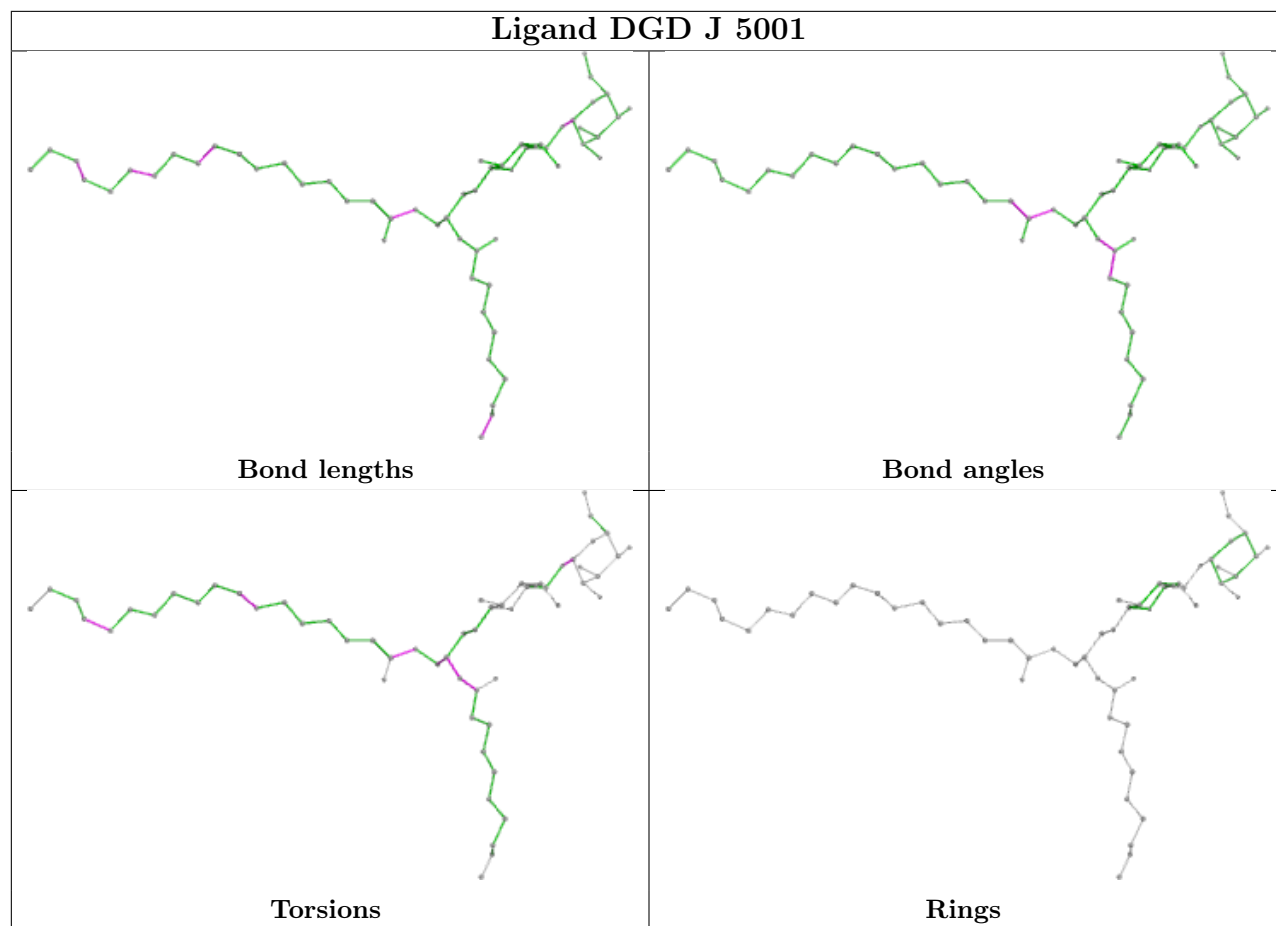


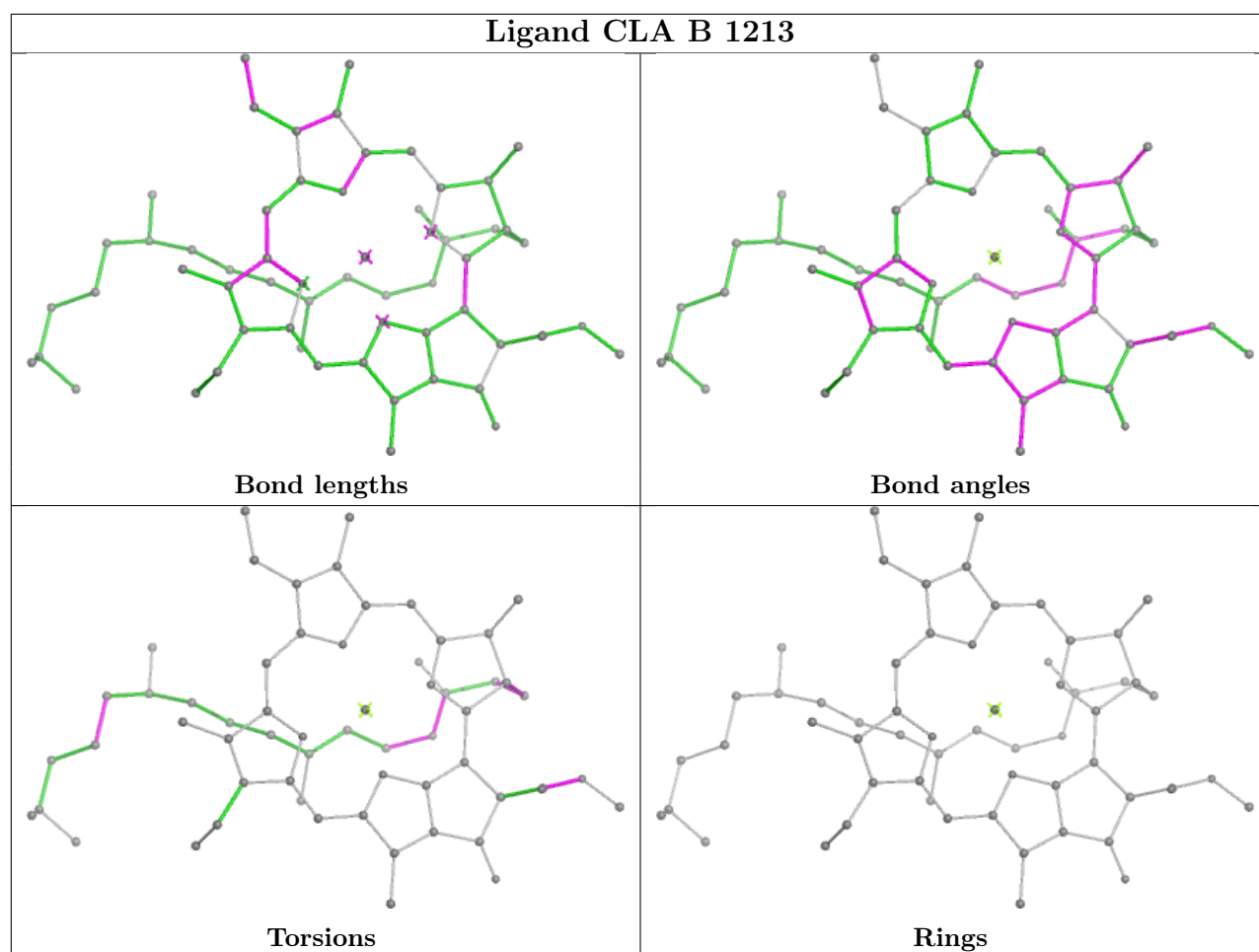
Ligand CLA 4 608

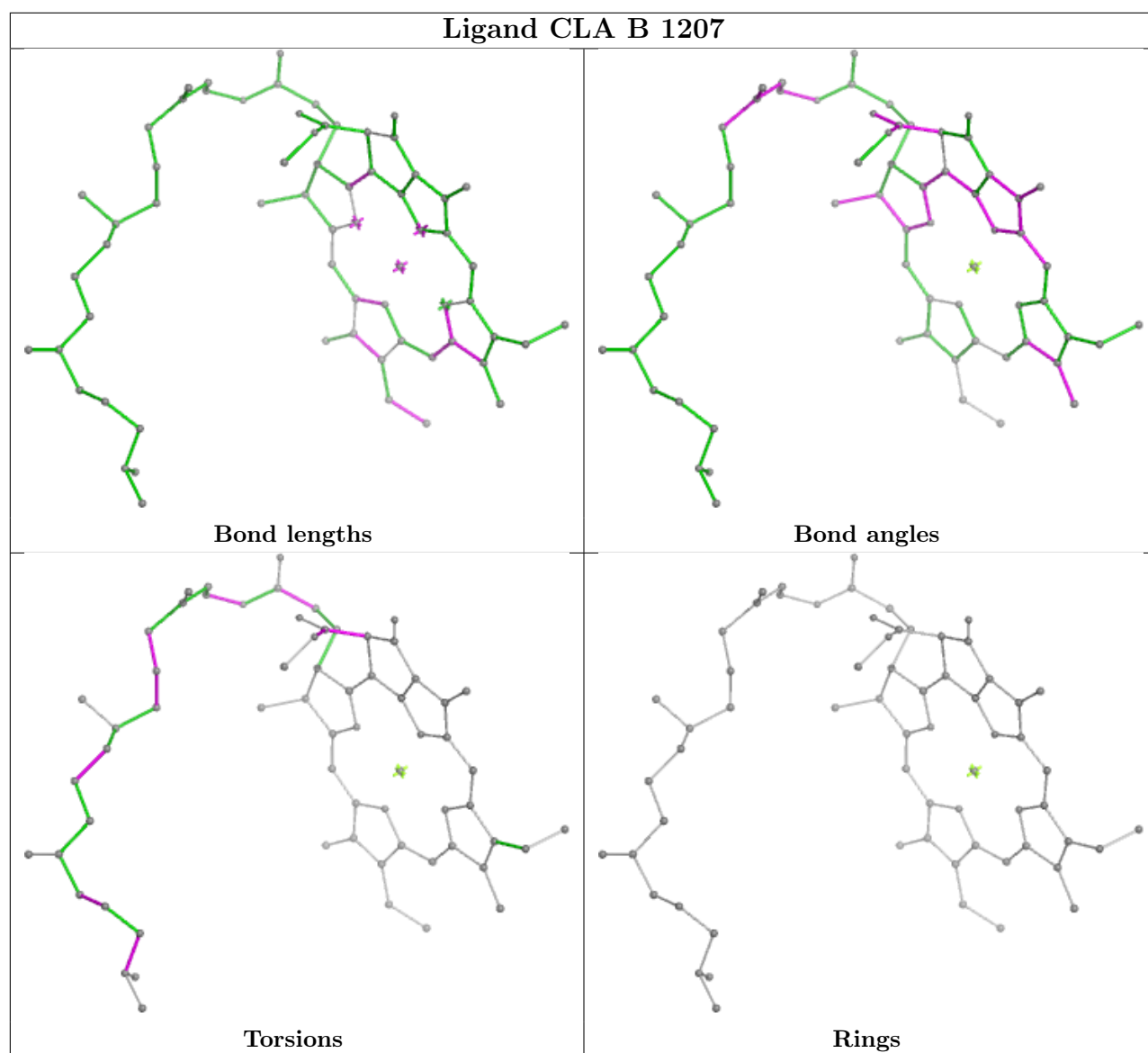


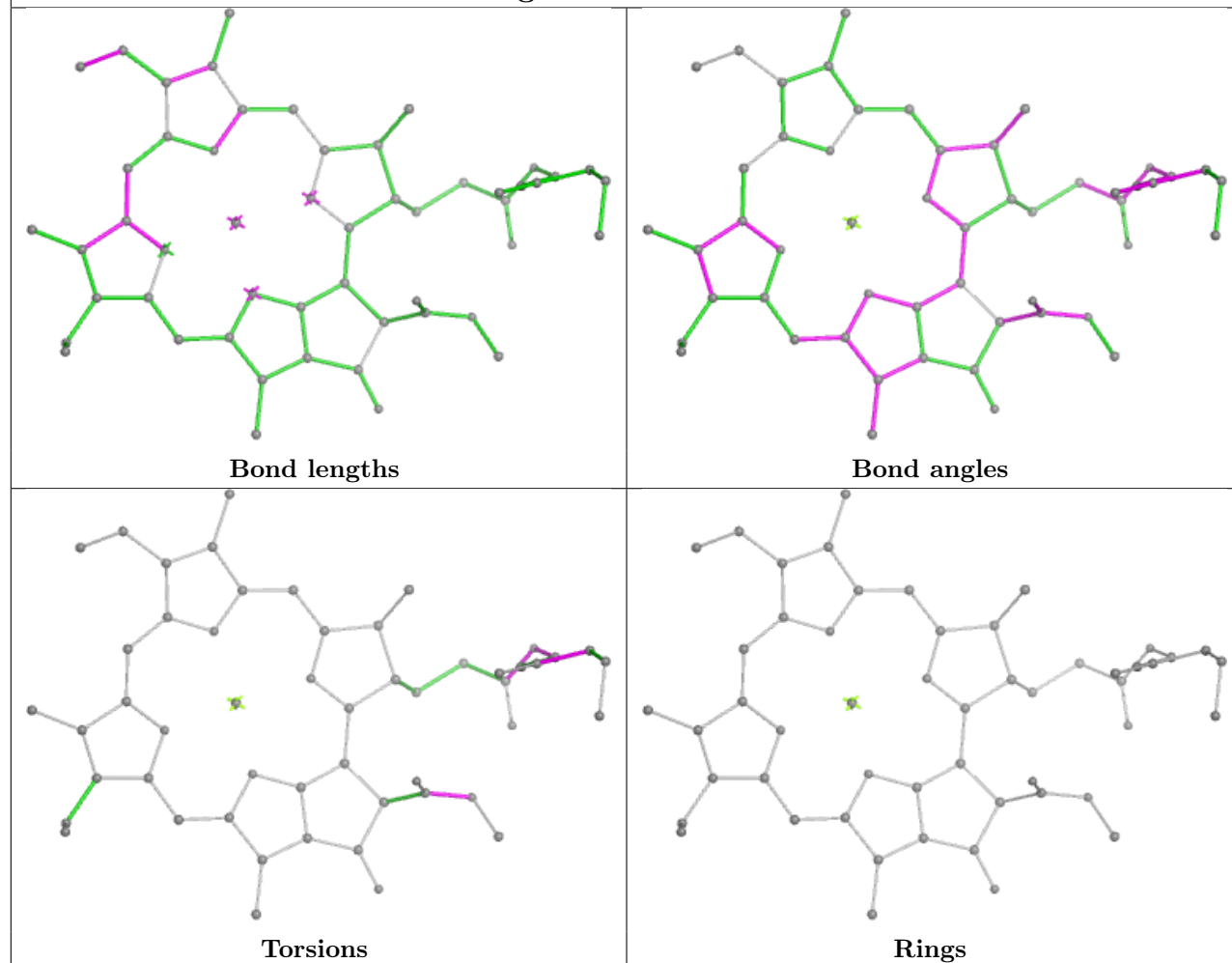
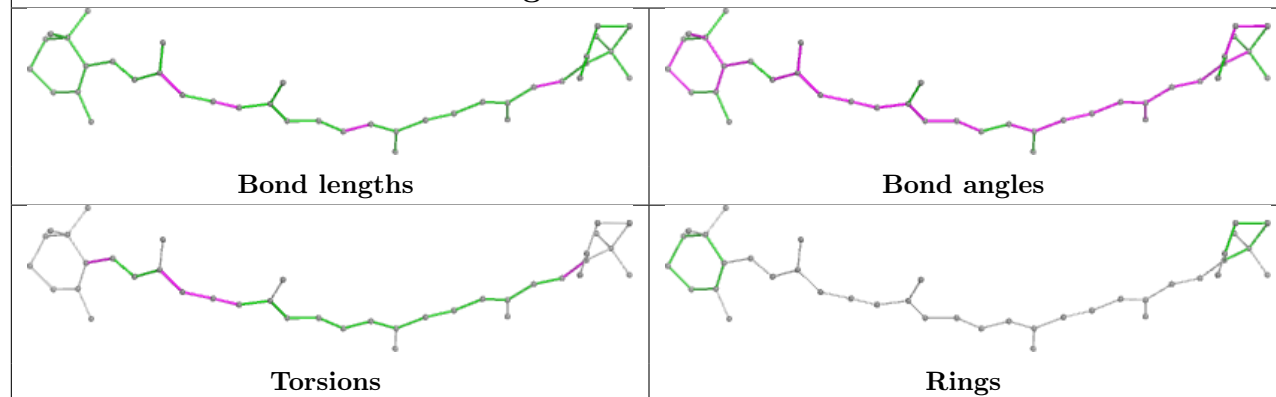
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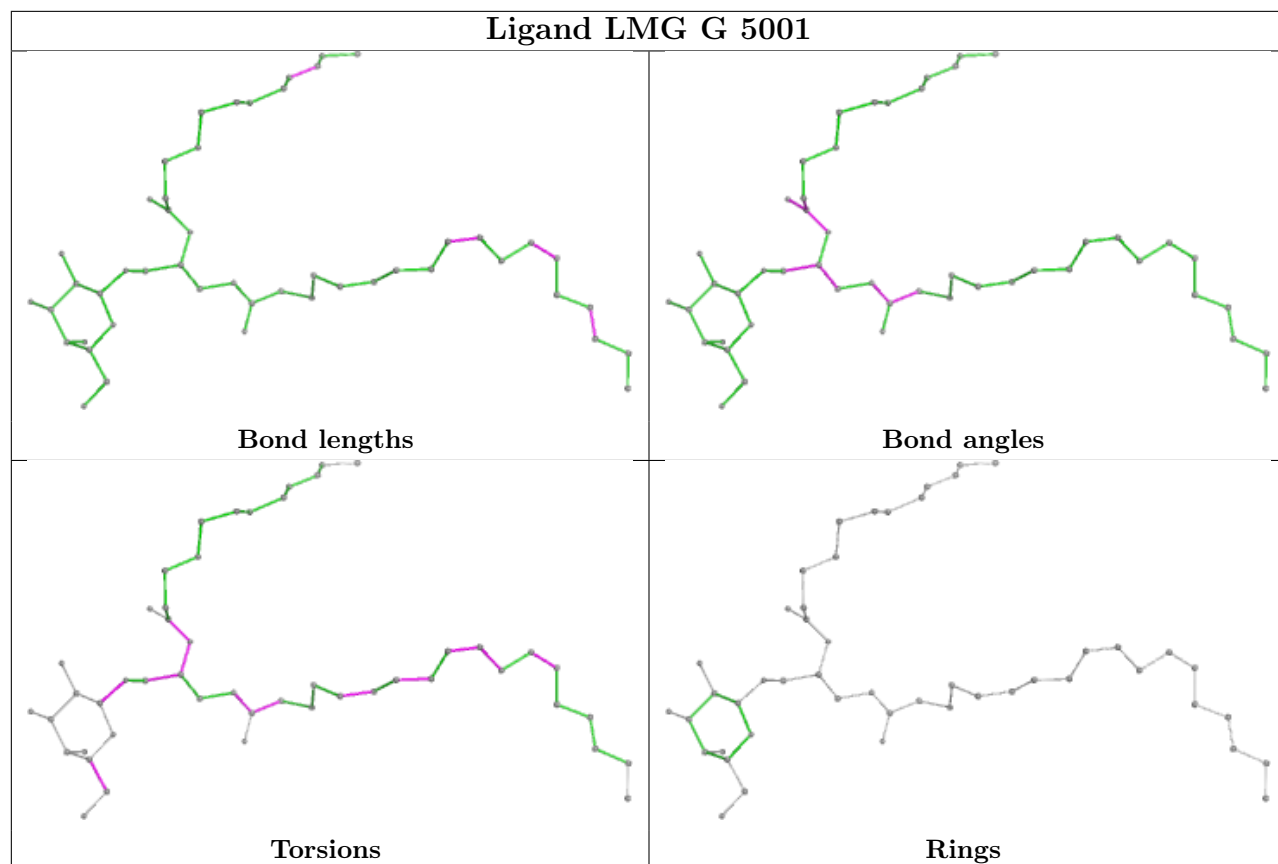


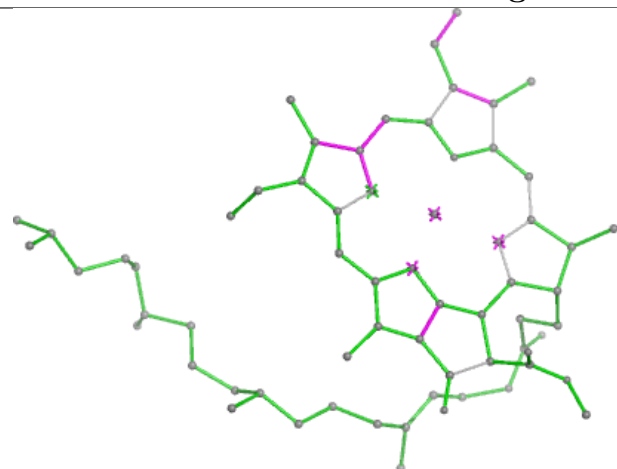
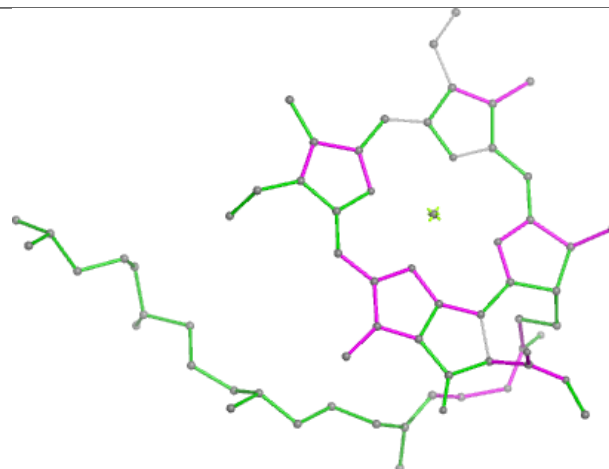
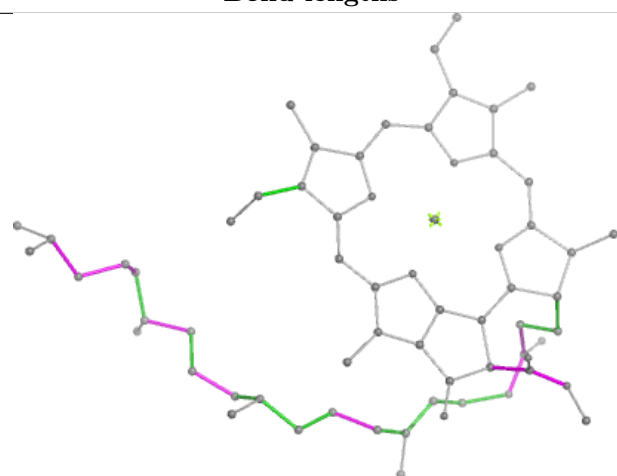
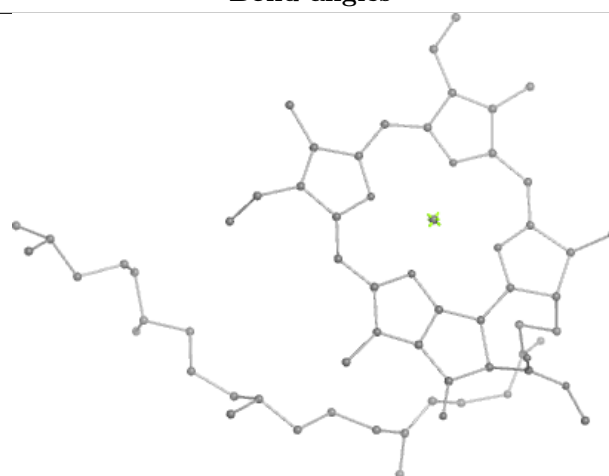




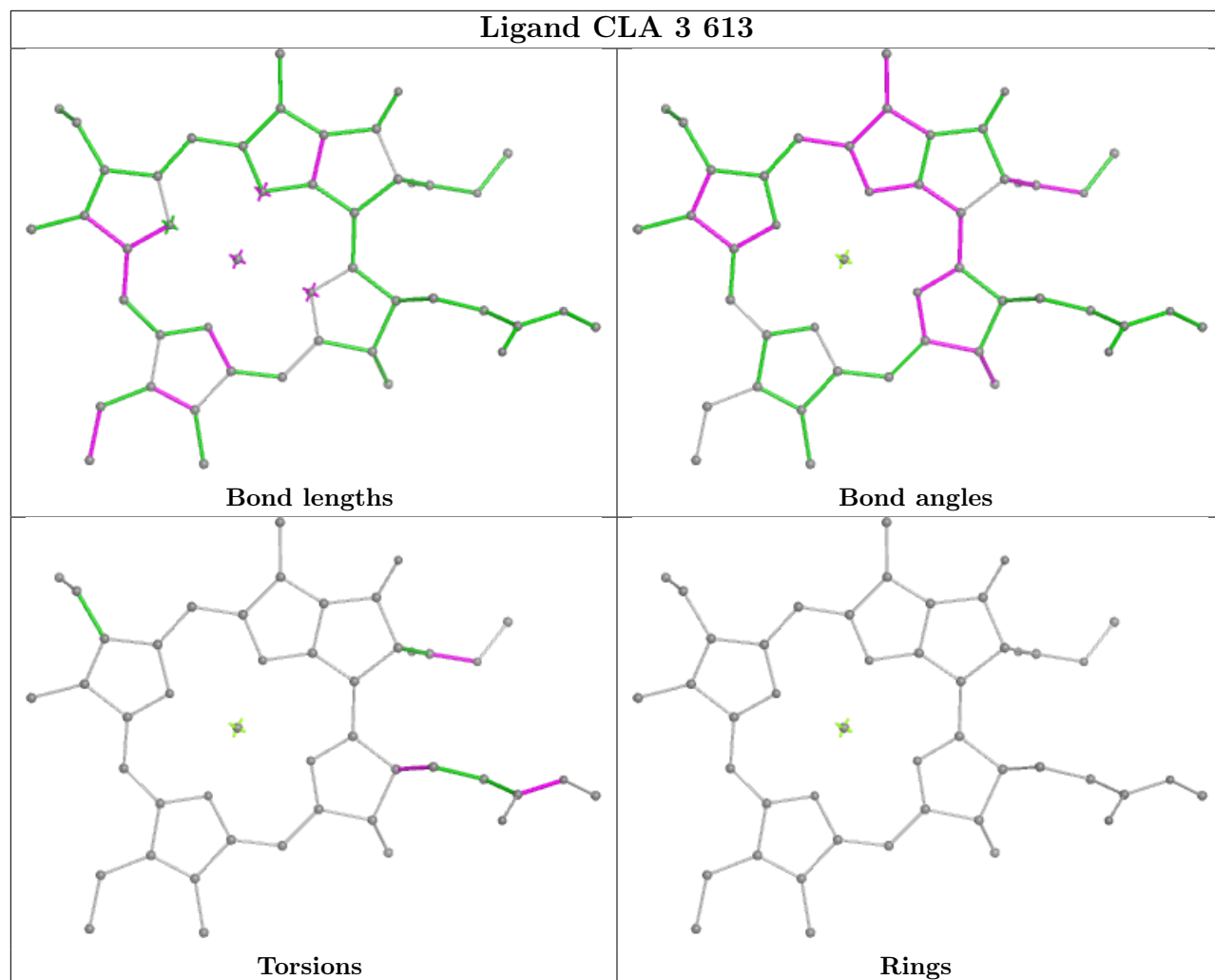


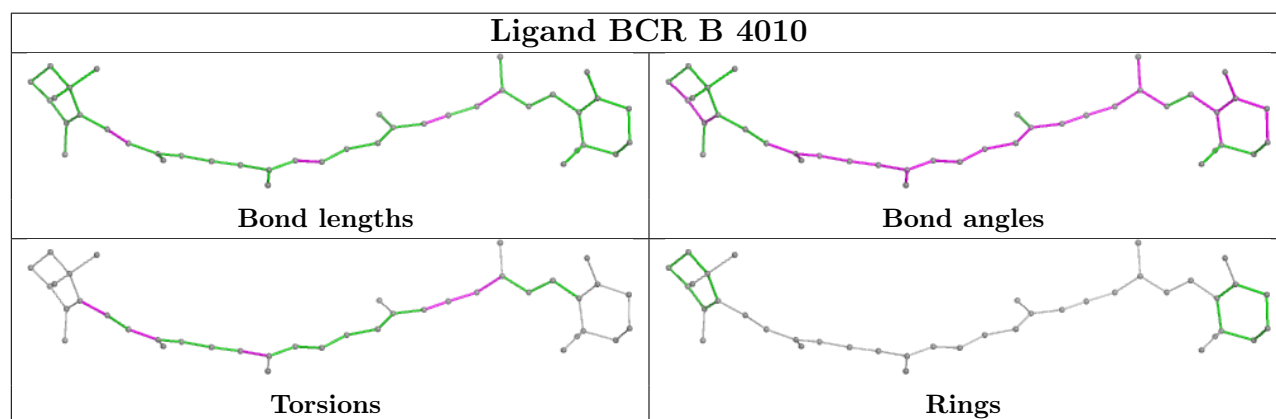
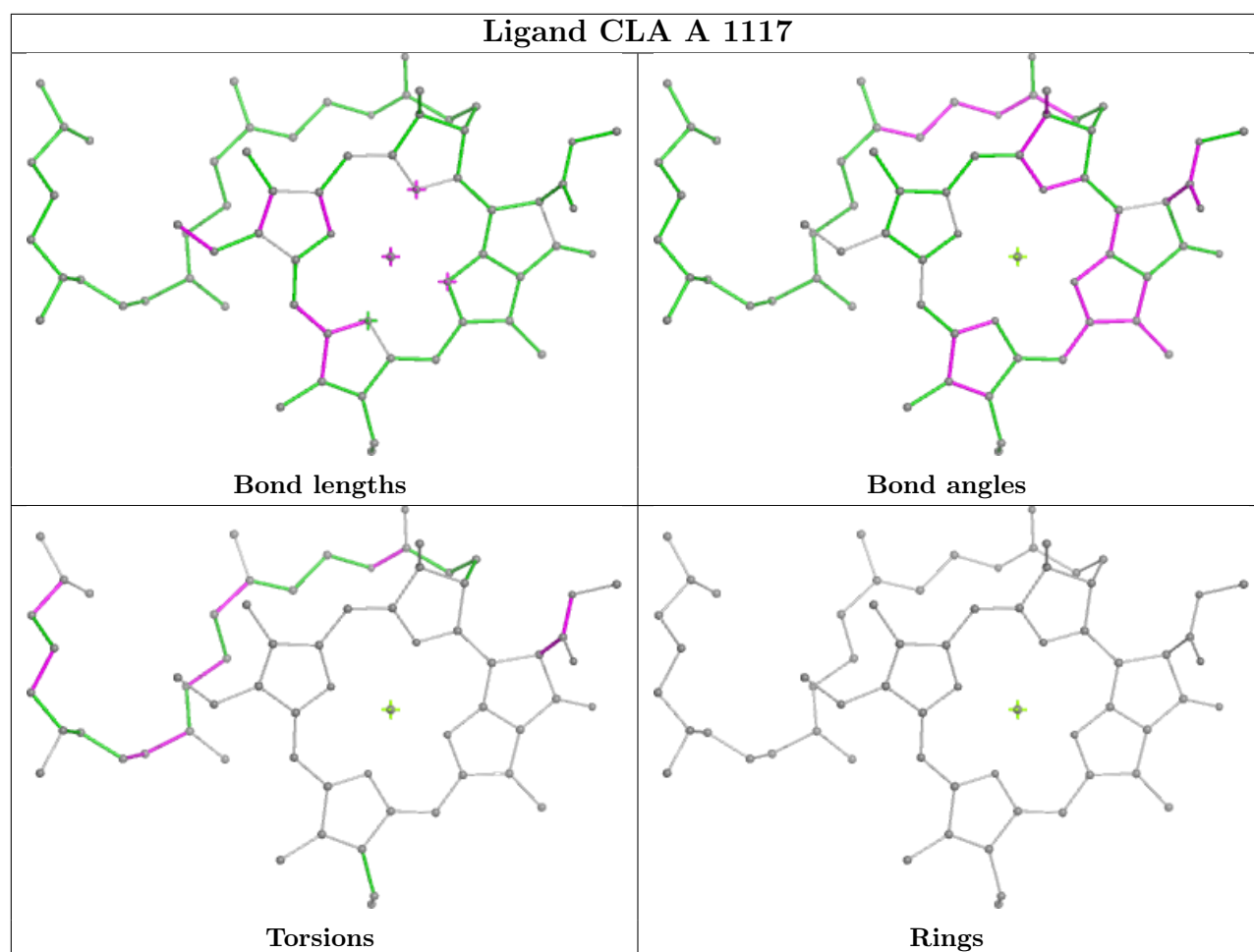
Ligand CLA 2 602**Ligand BCR F 4014**



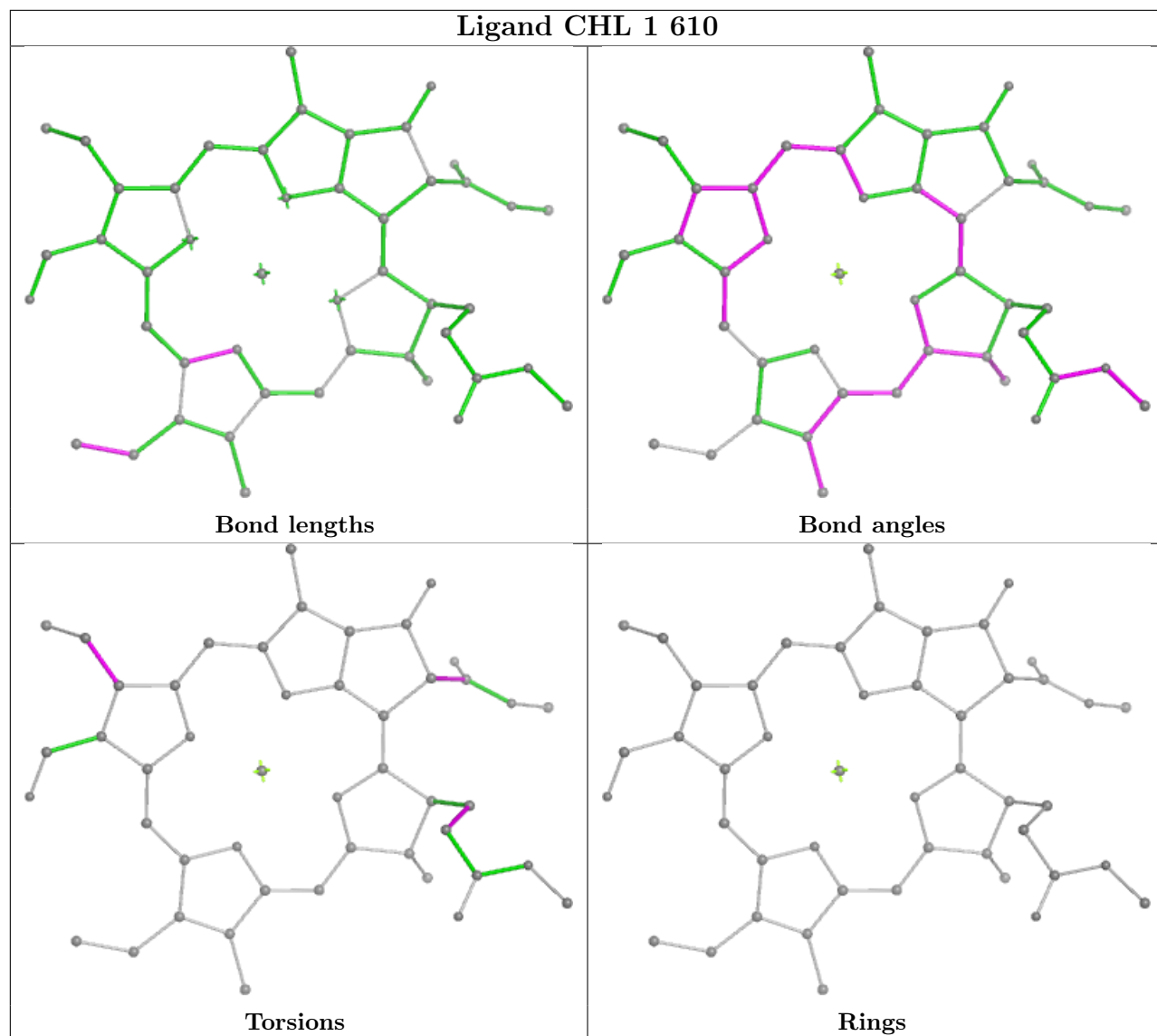
Ligand CLA A 1127**Bond lengths****Bond angles****Torsions****Rings**

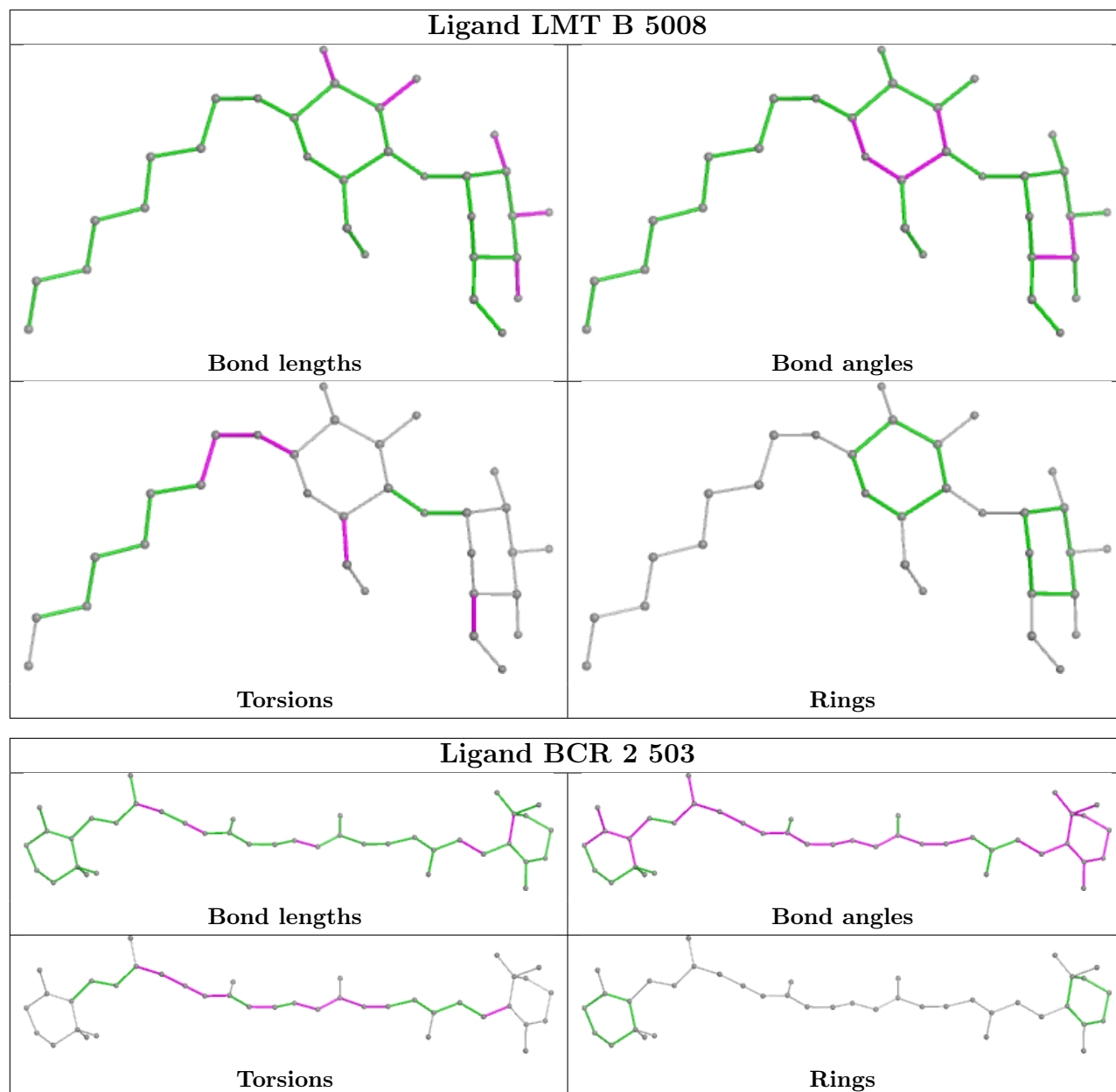
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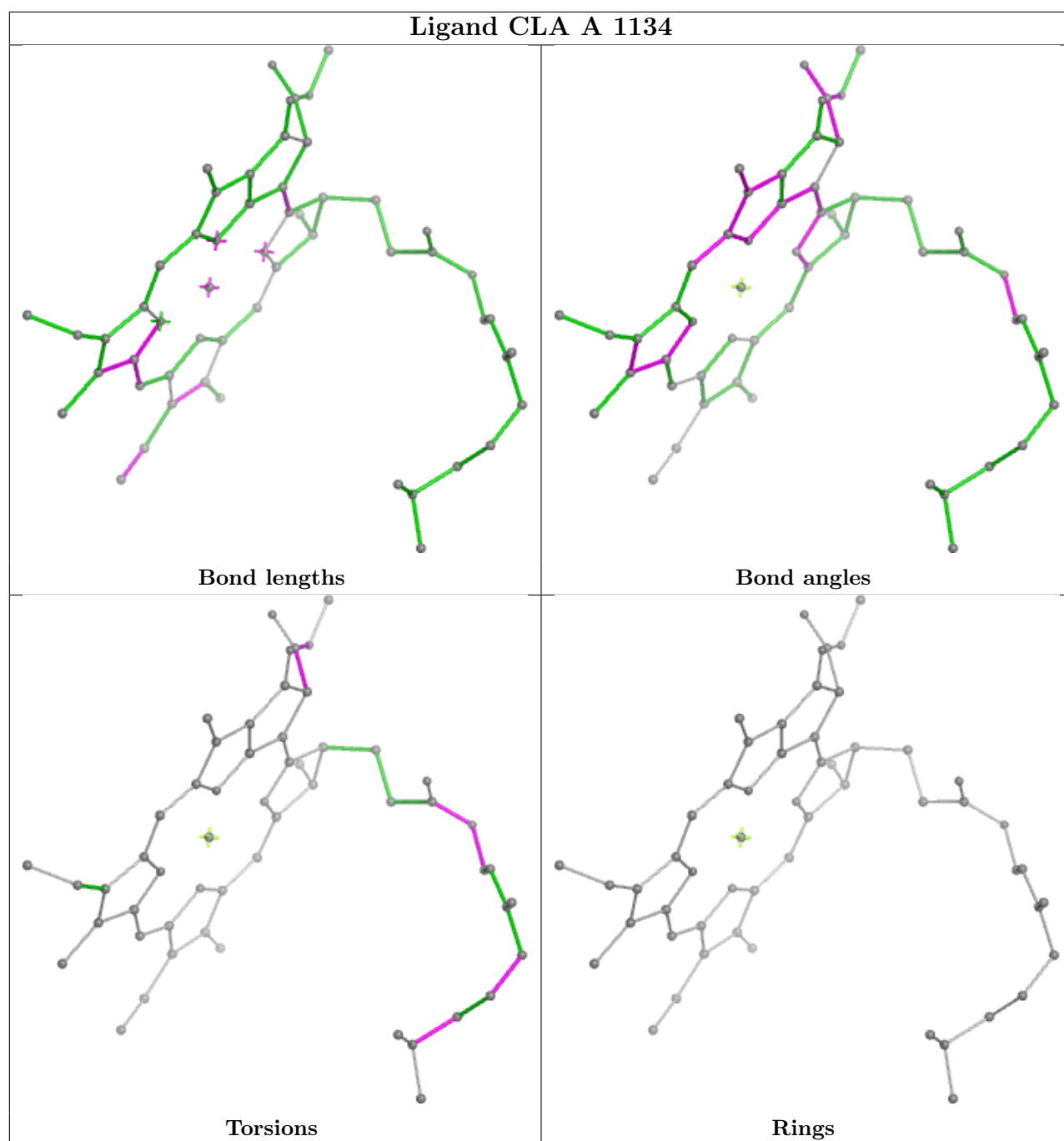


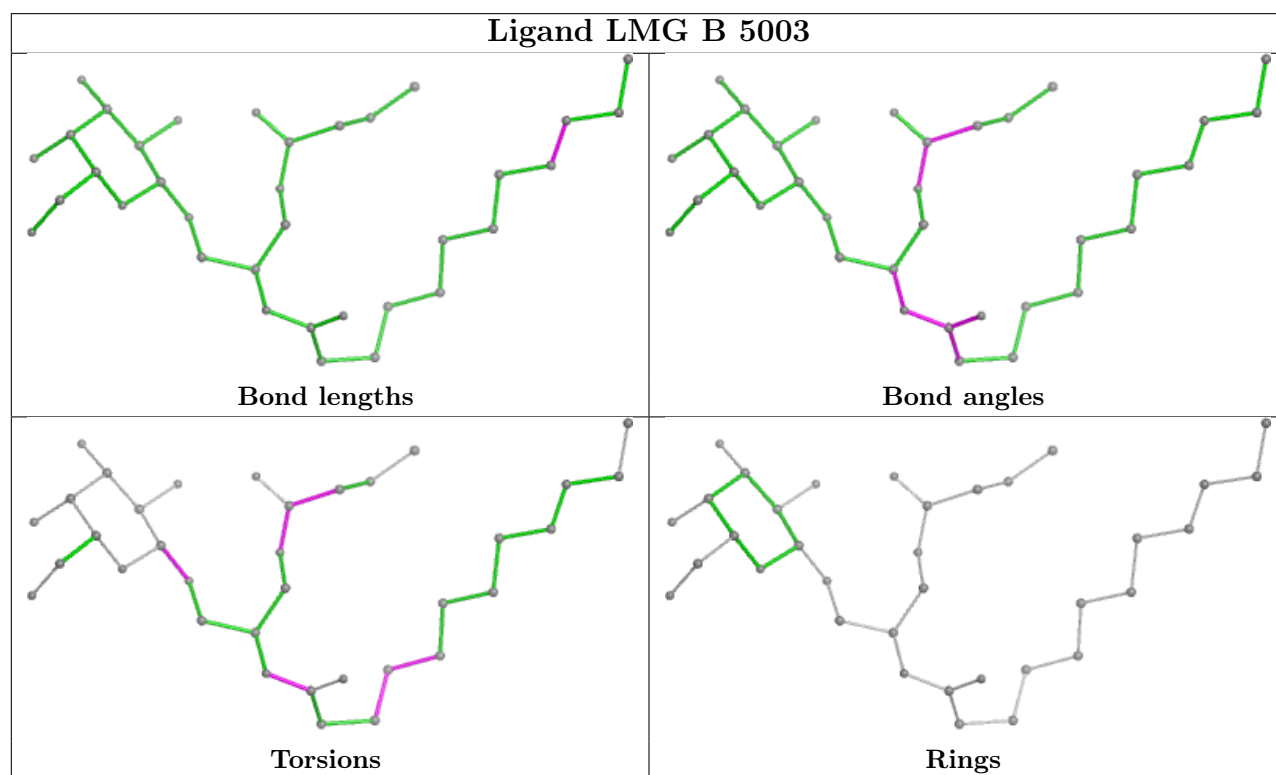
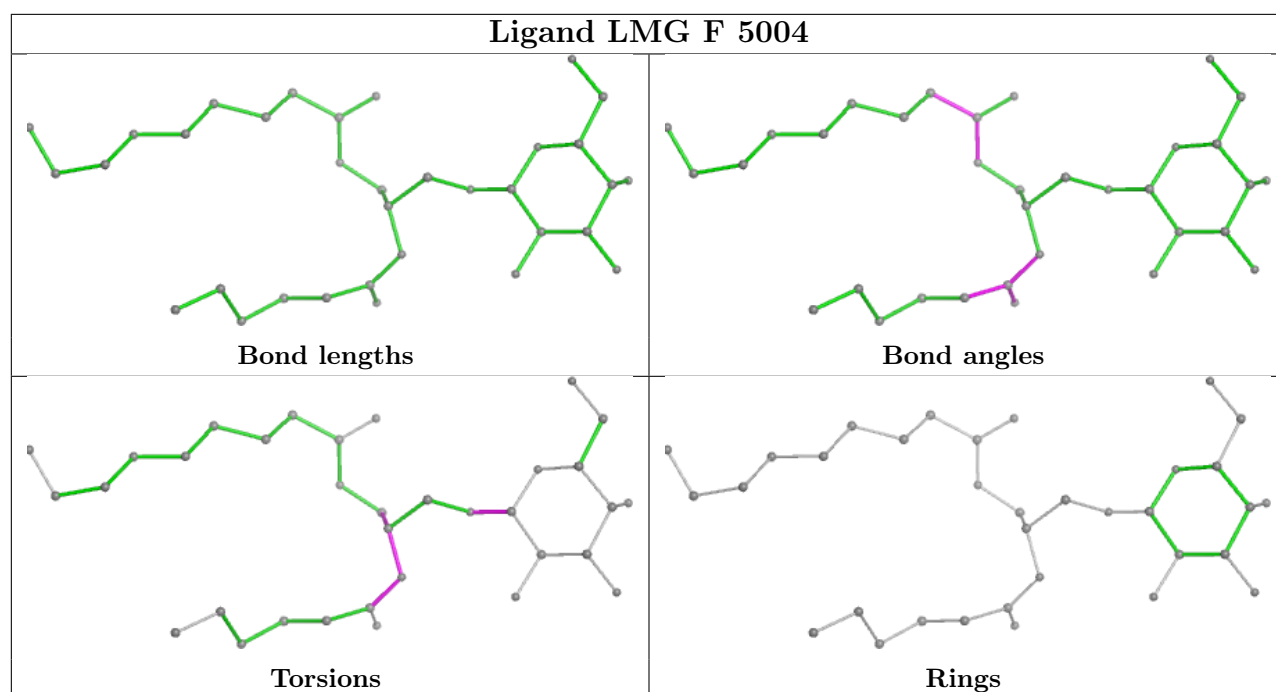


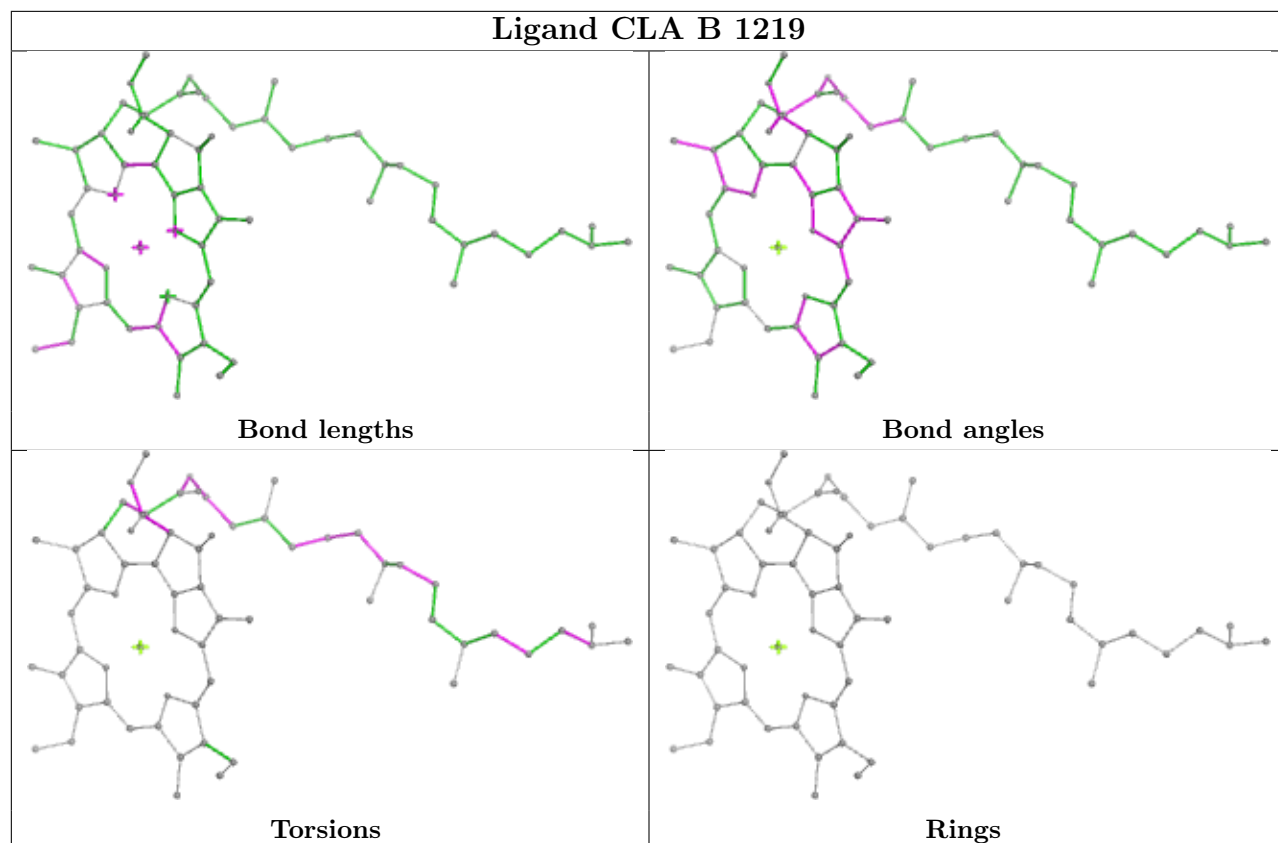
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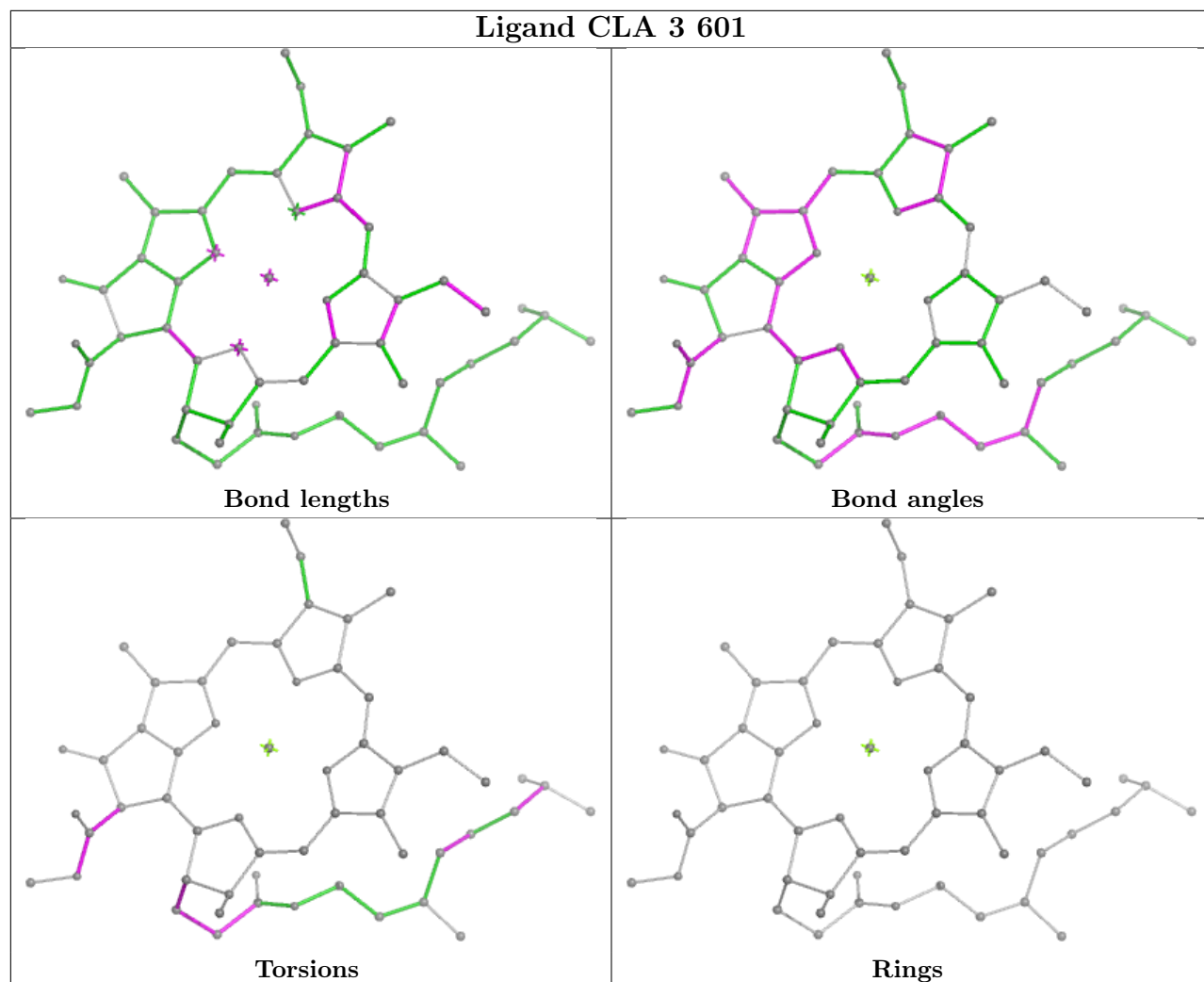


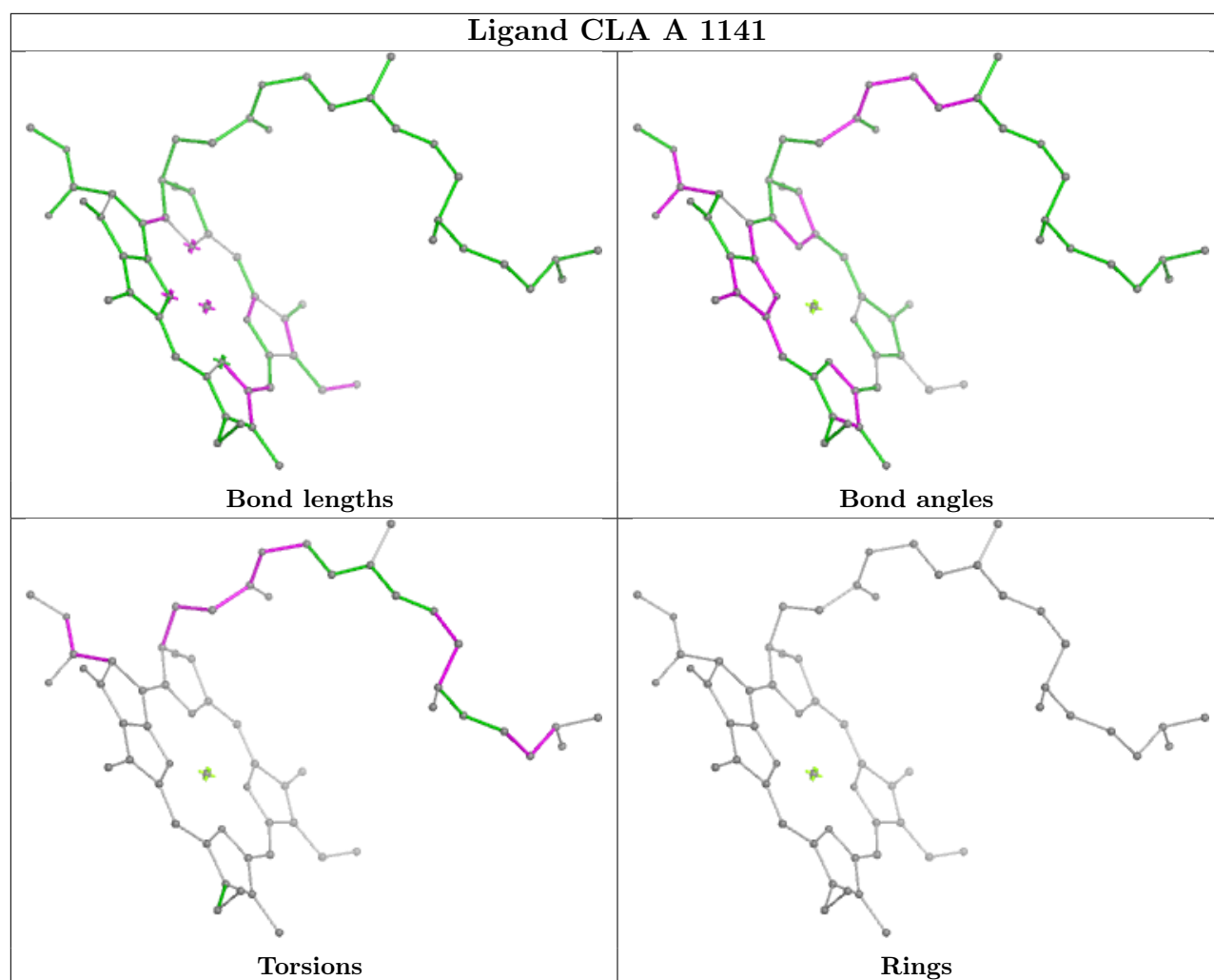




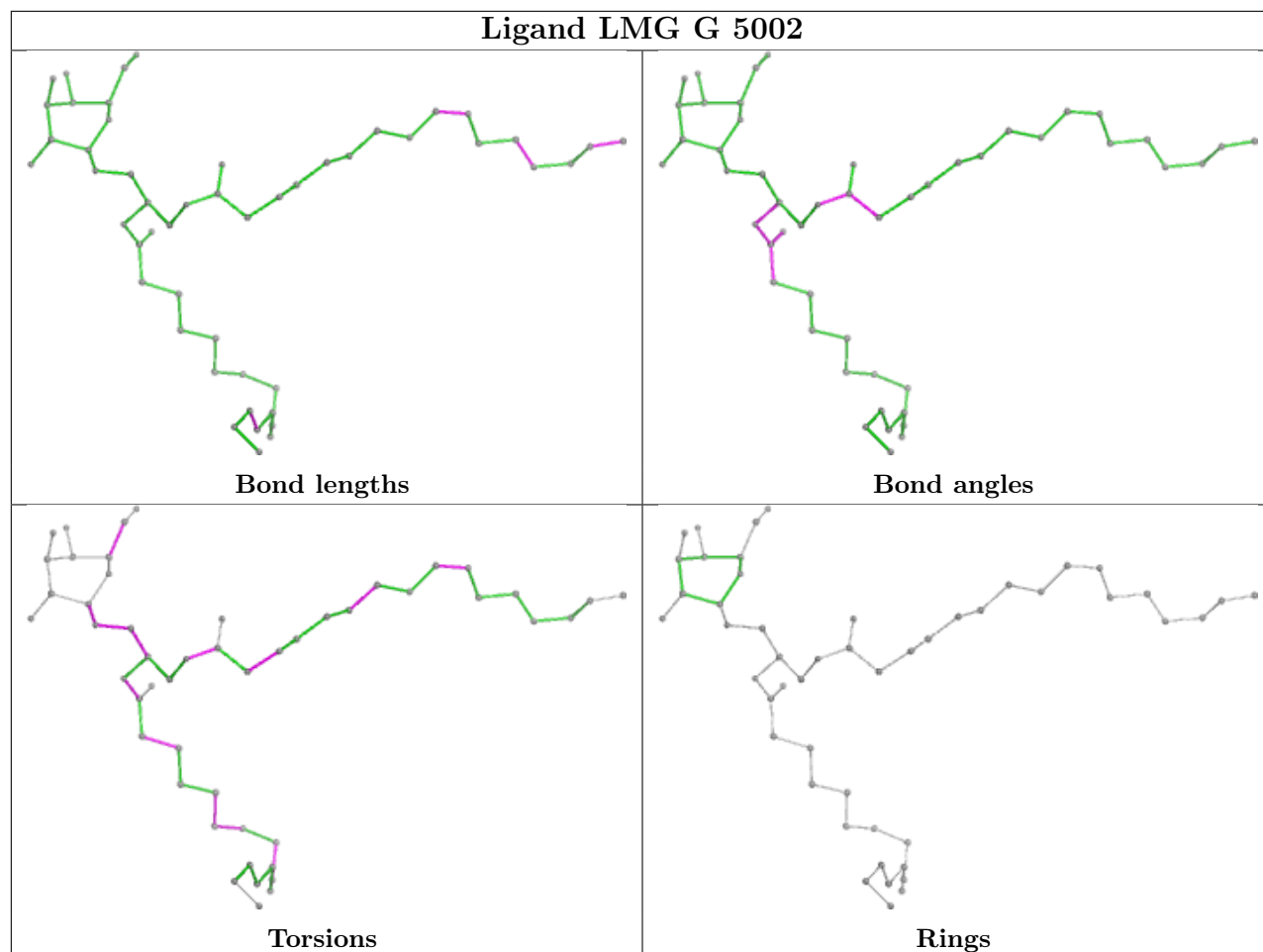


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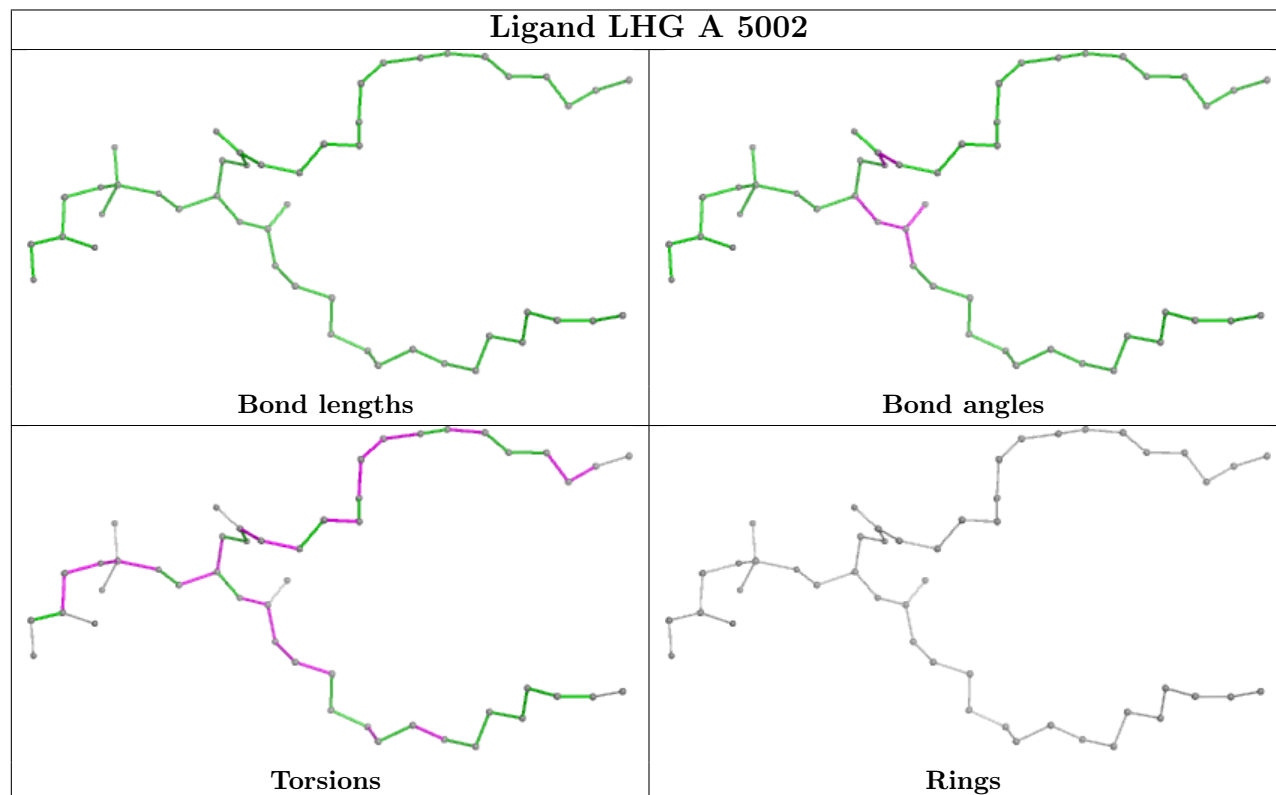


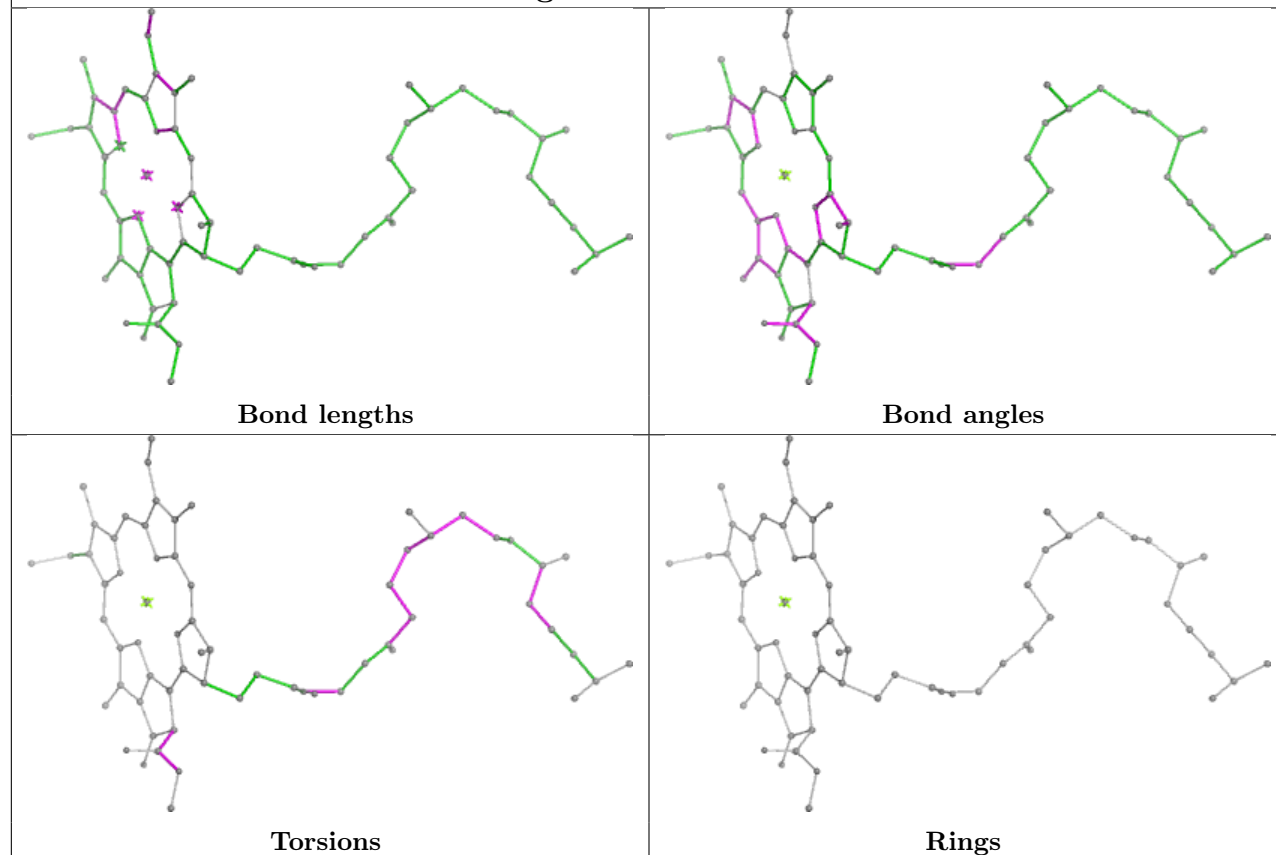
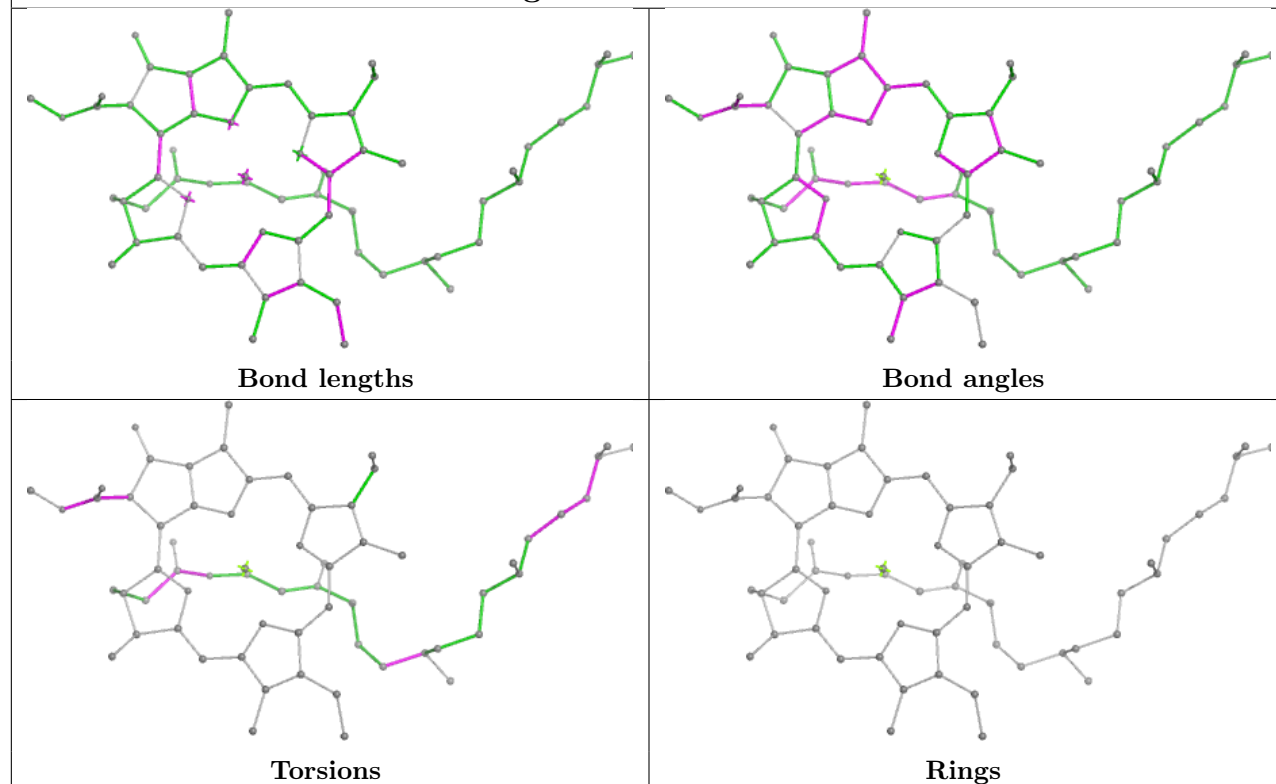


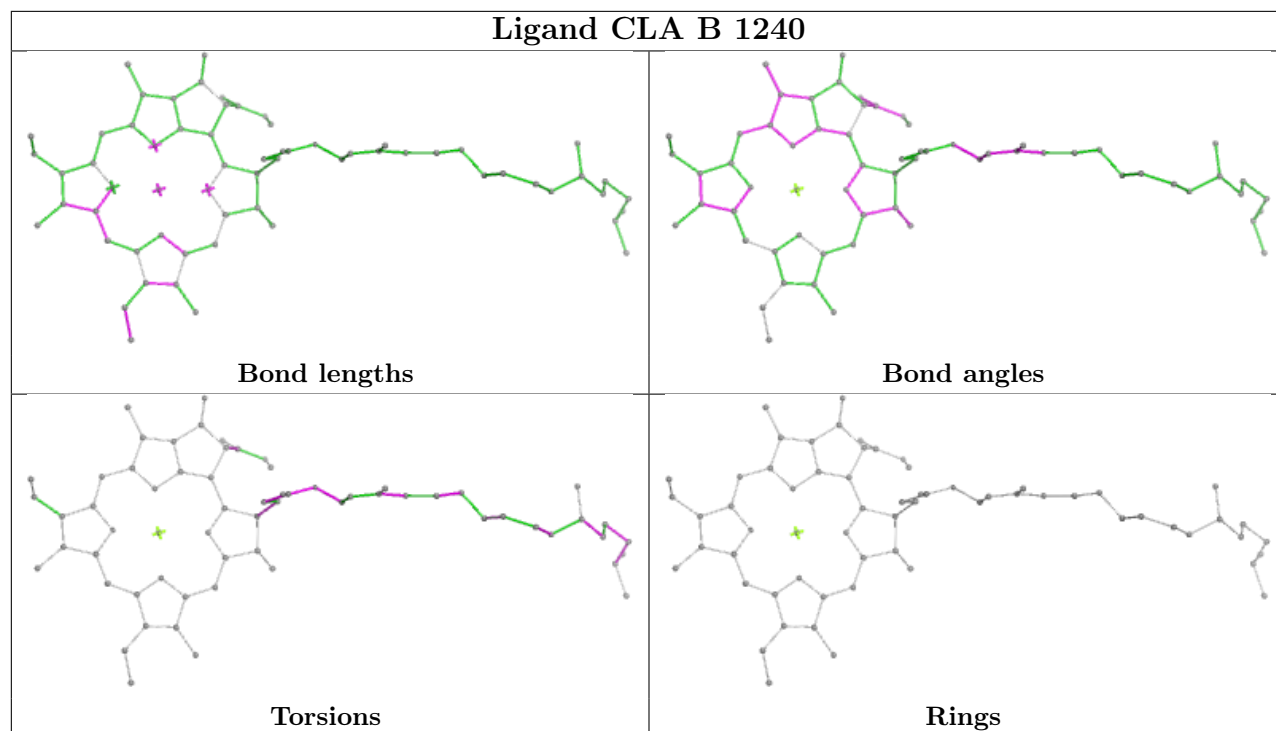
Ligand LMG G 5002

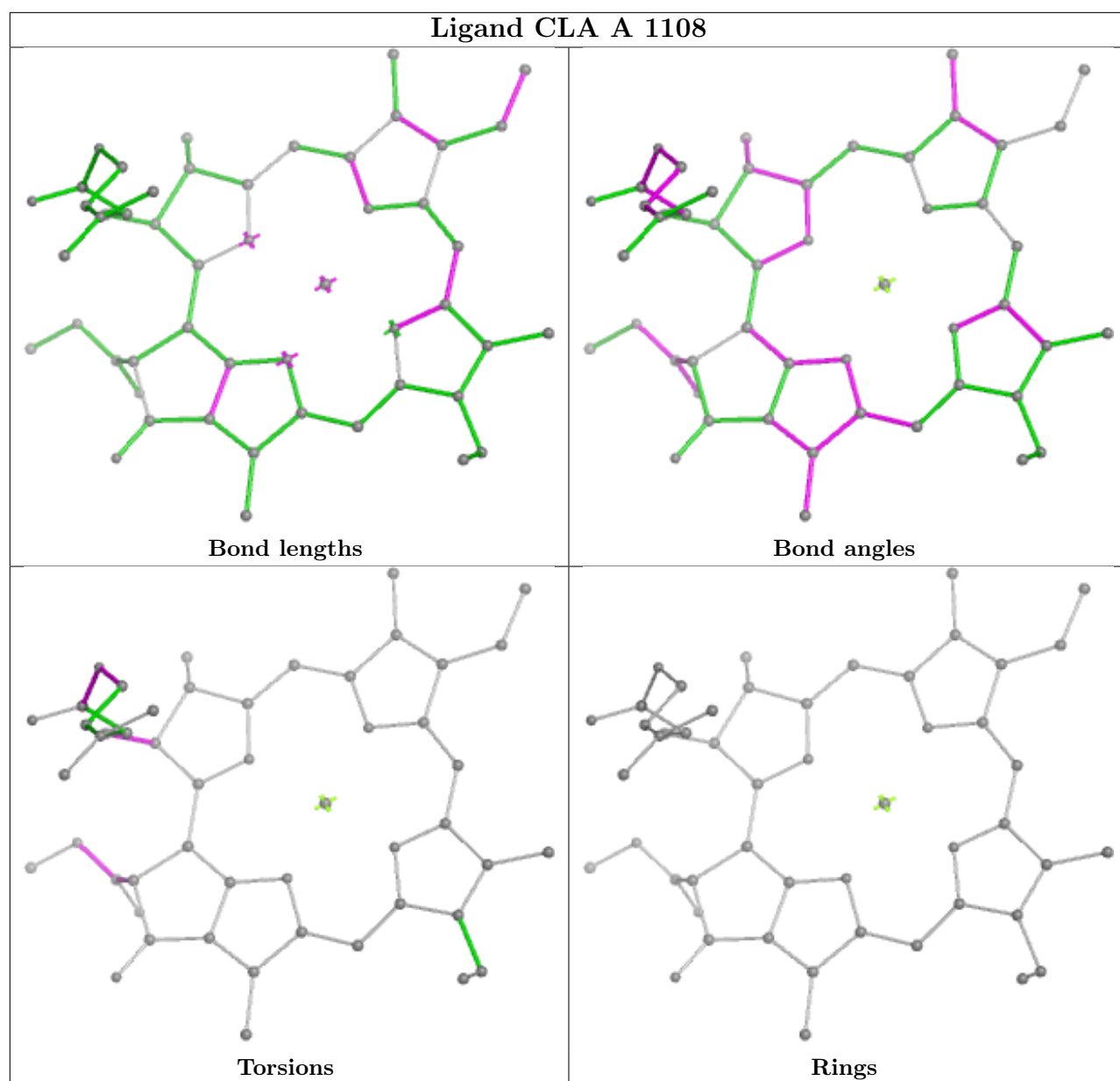


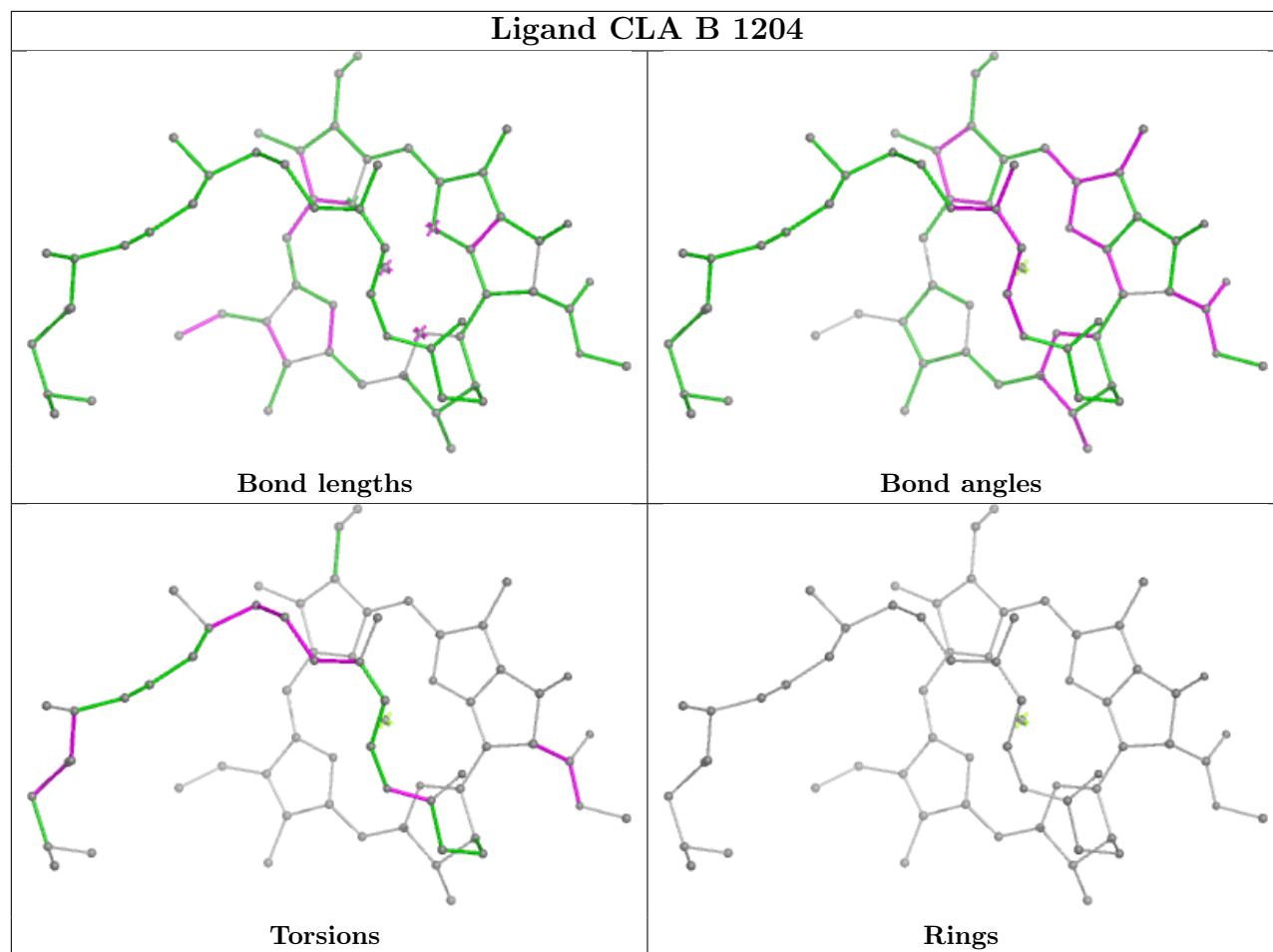
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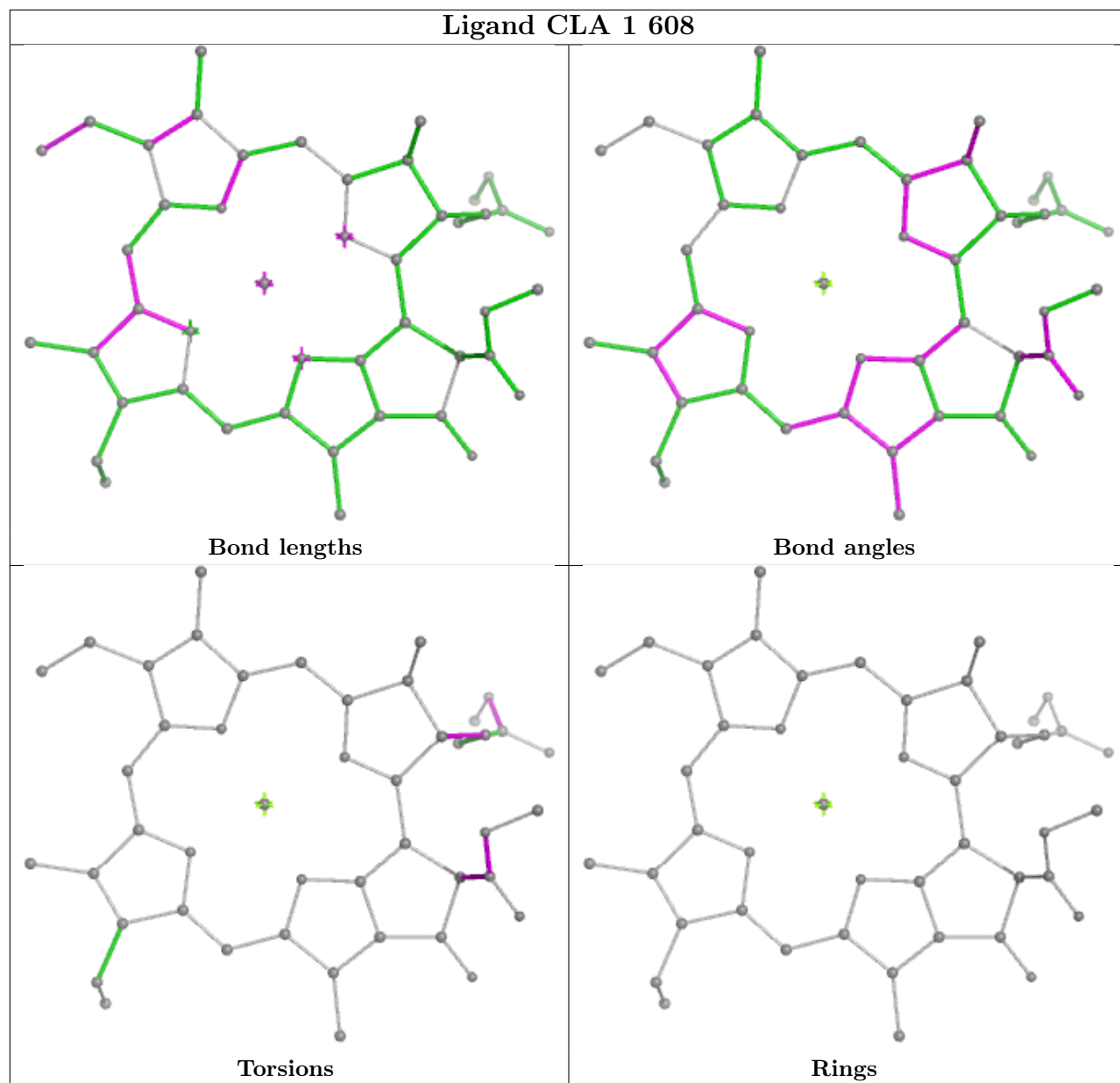
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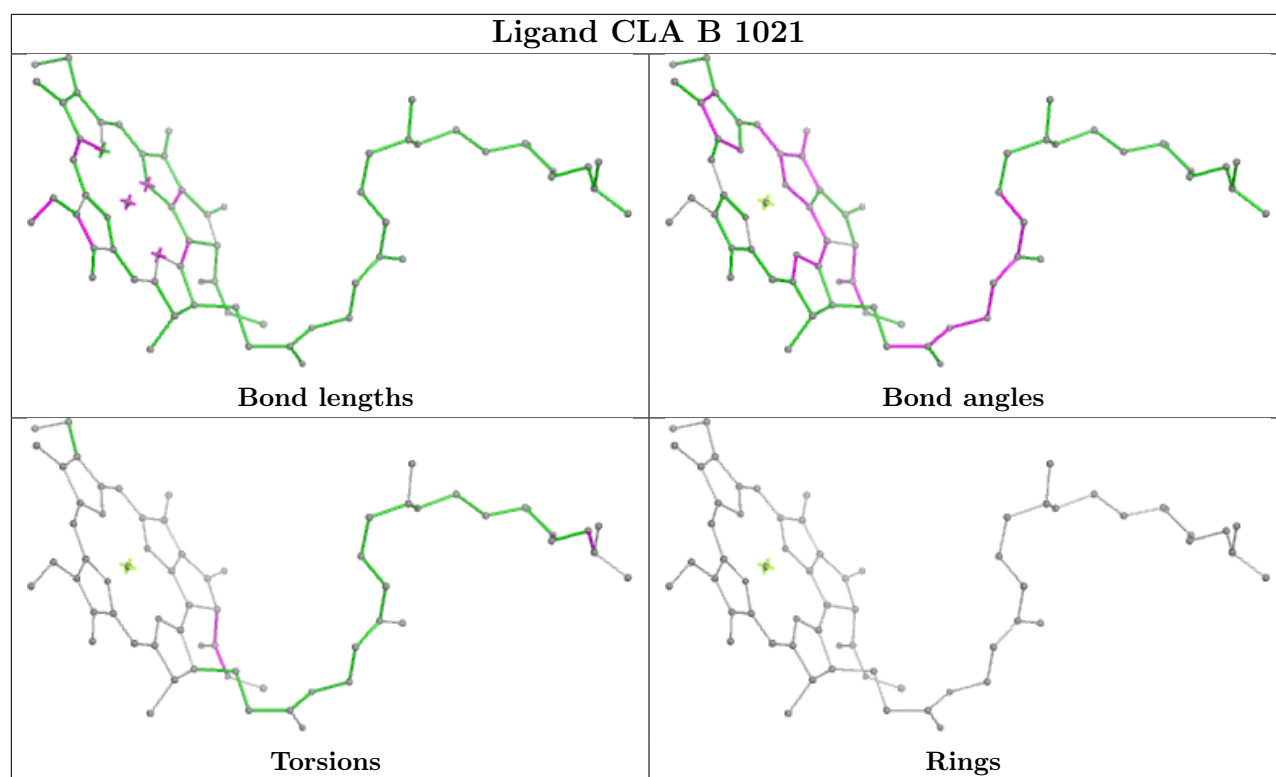




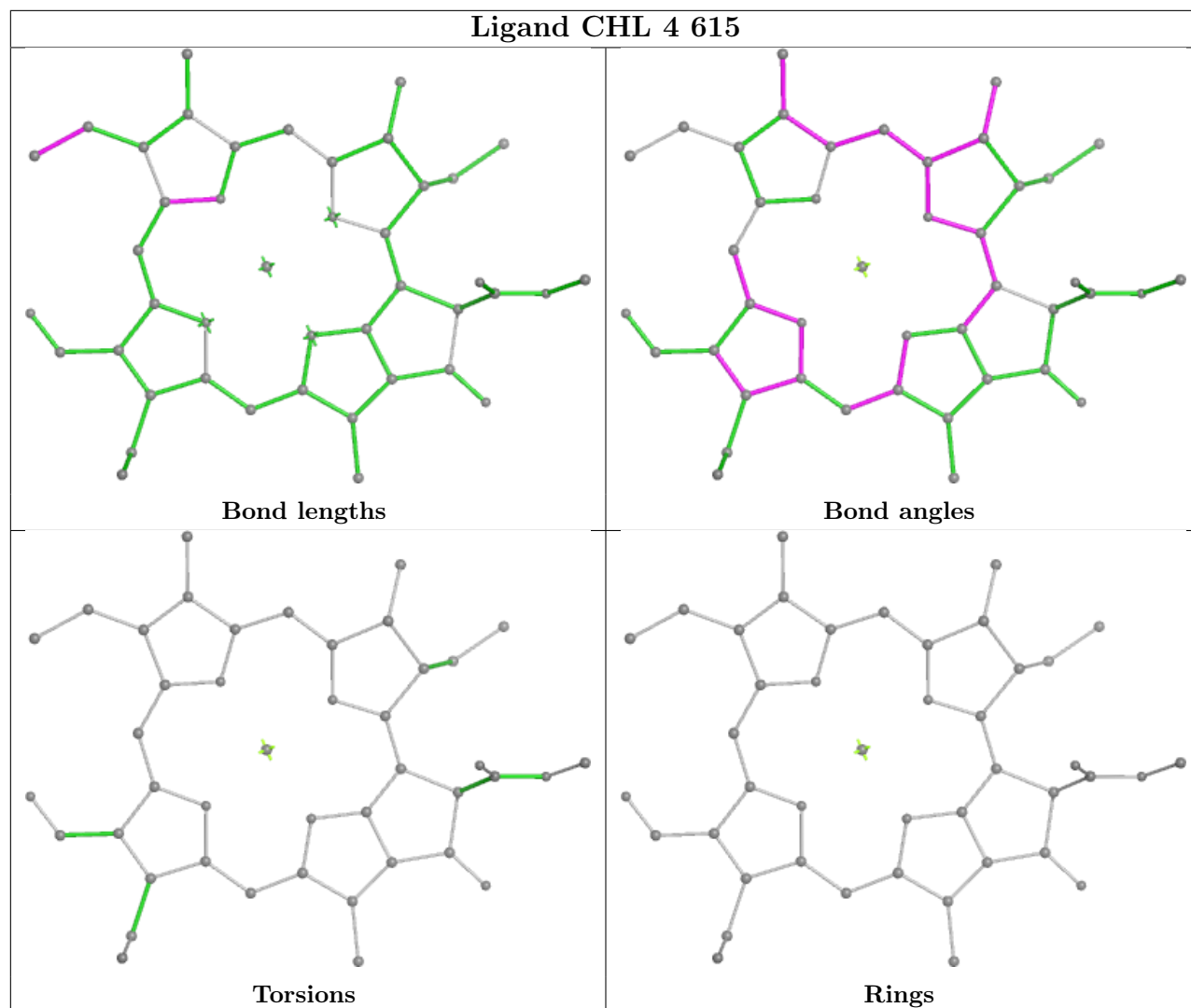


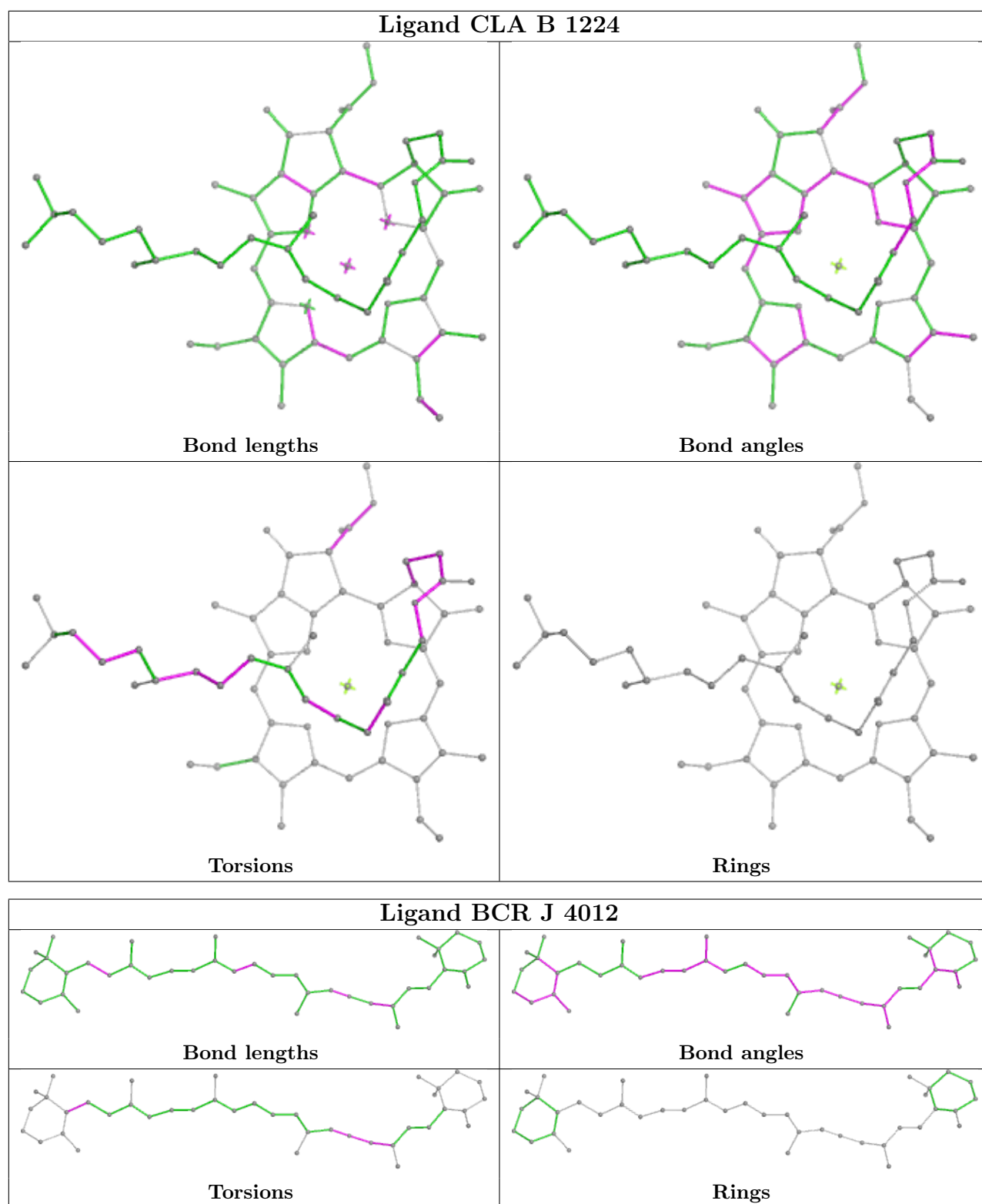
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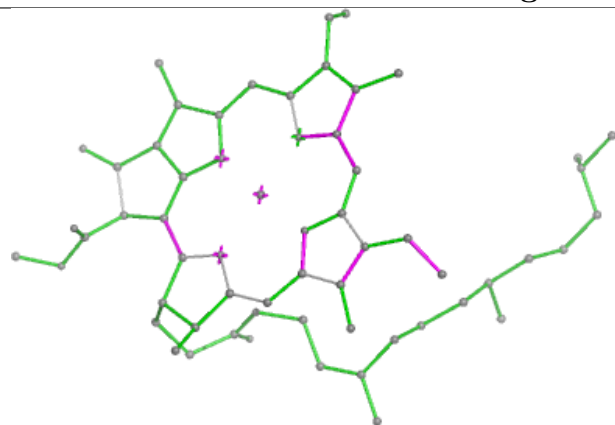


Ligand CHL 4 615

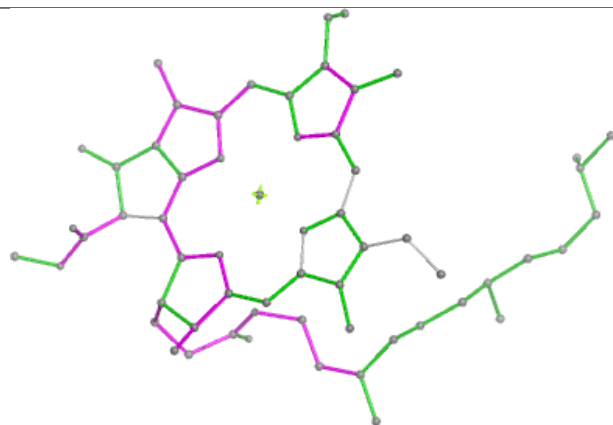




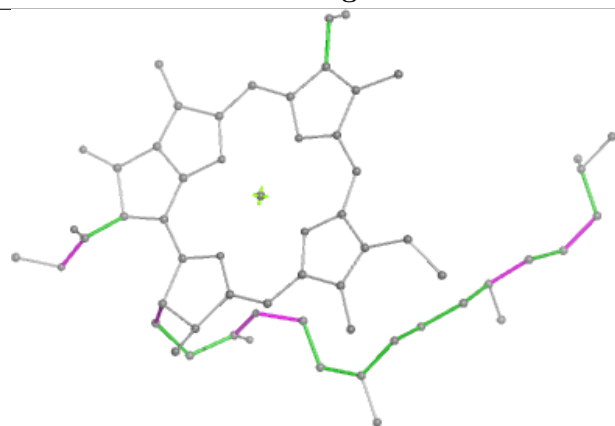
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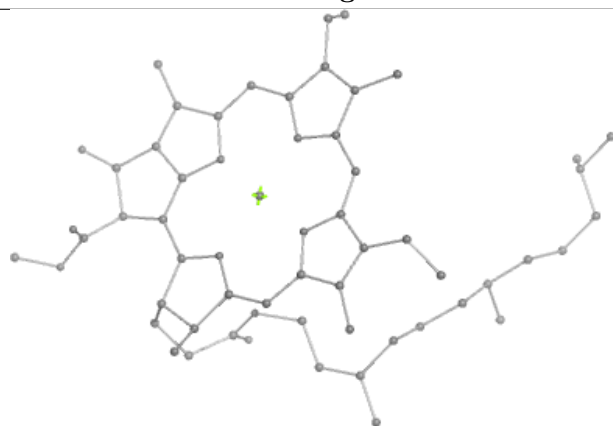
Bond lengths



Bond angles

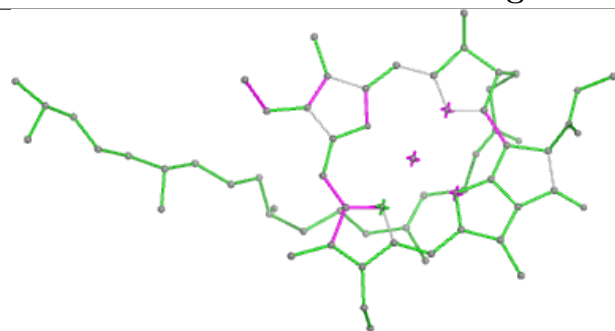


Torsions

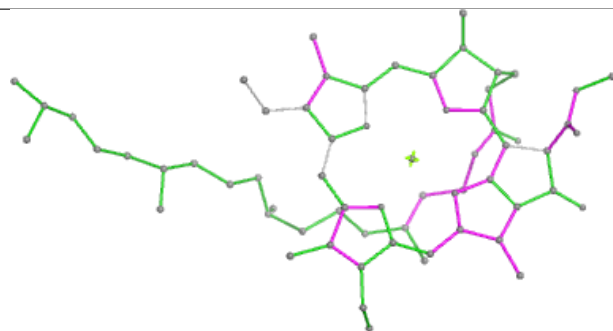


Rings

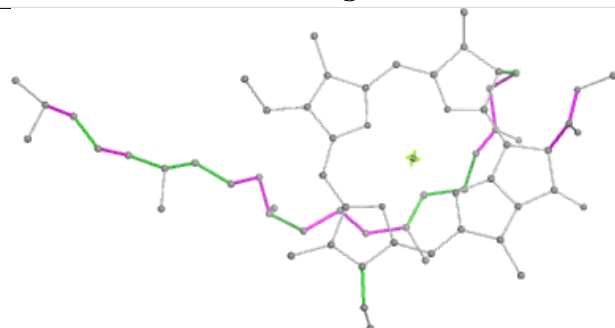
Ligand CLA A 1138



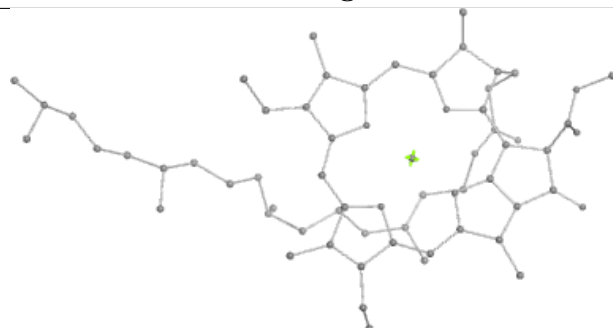
Bond lengths



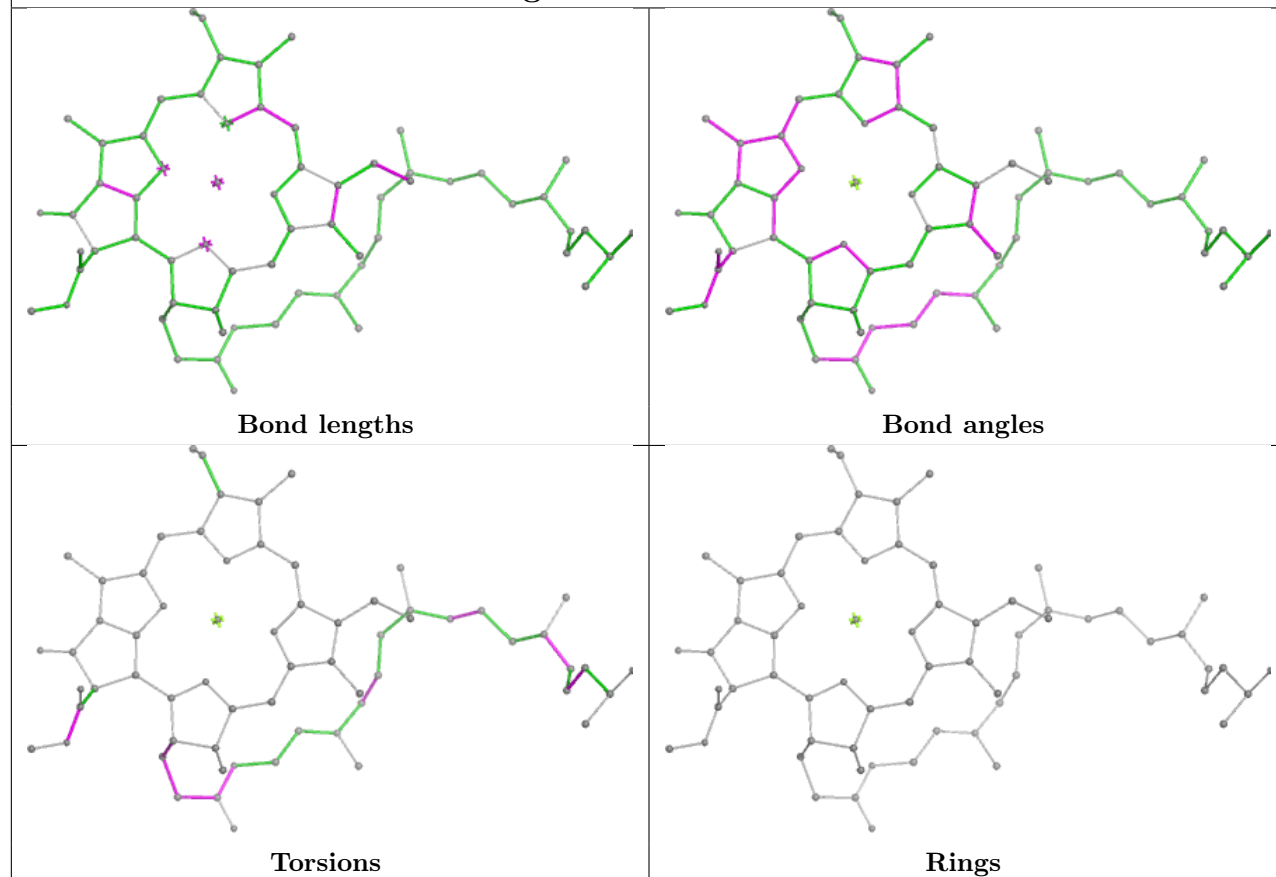
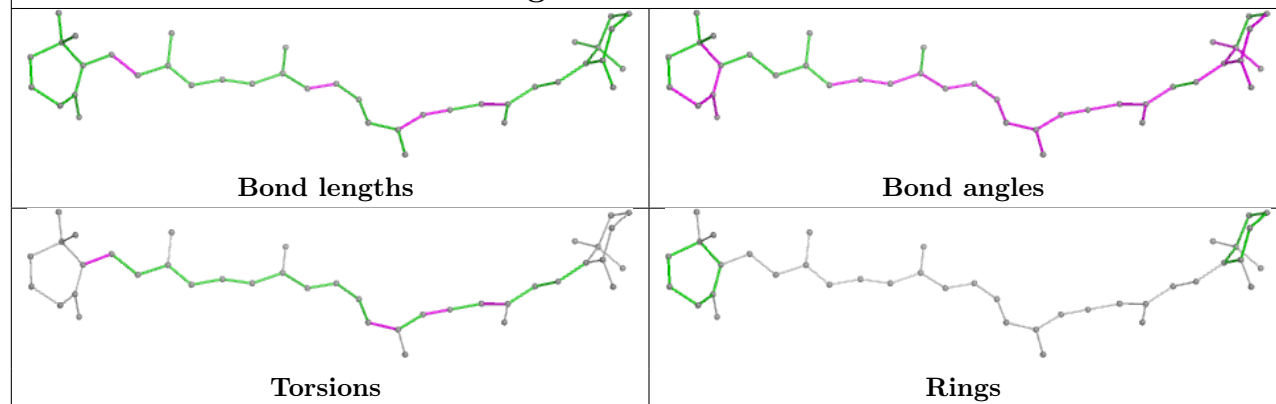
Bond angles

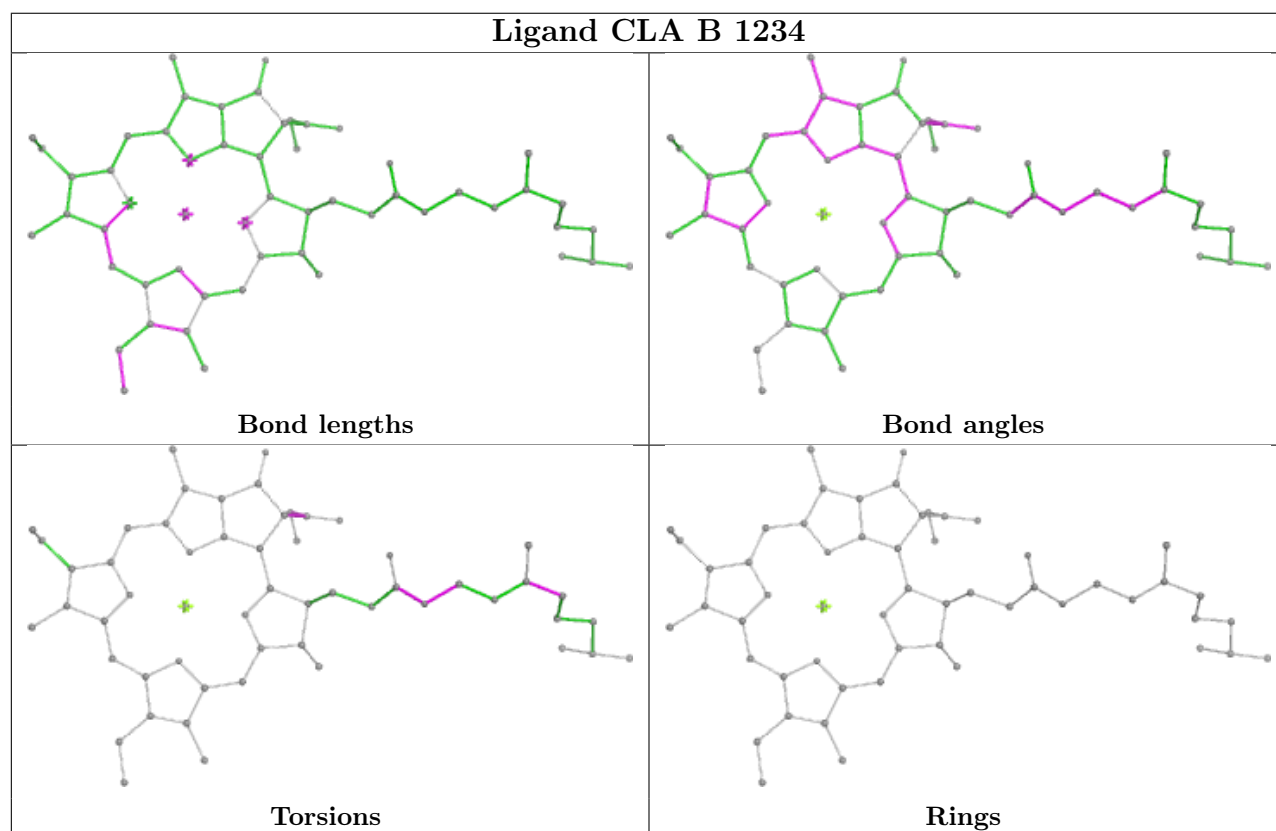
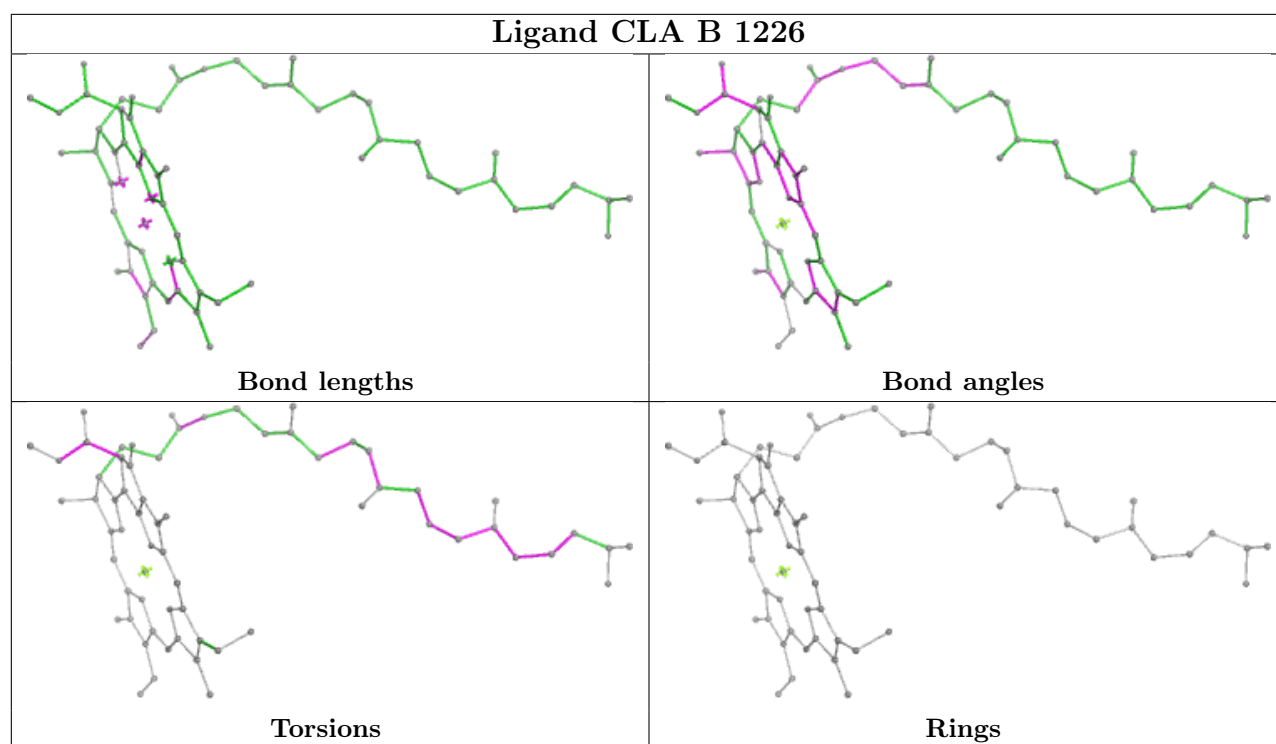


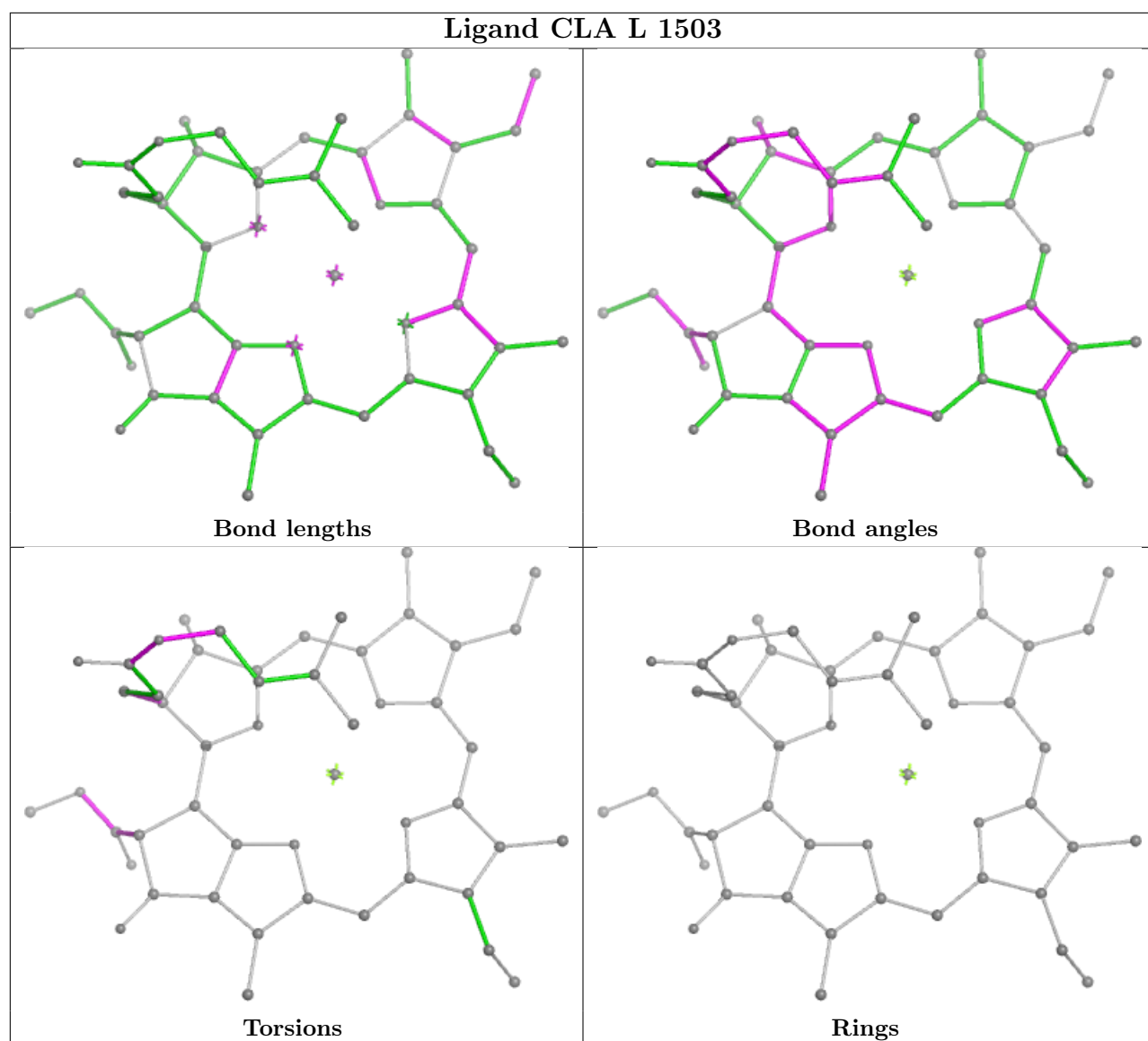
Torsions

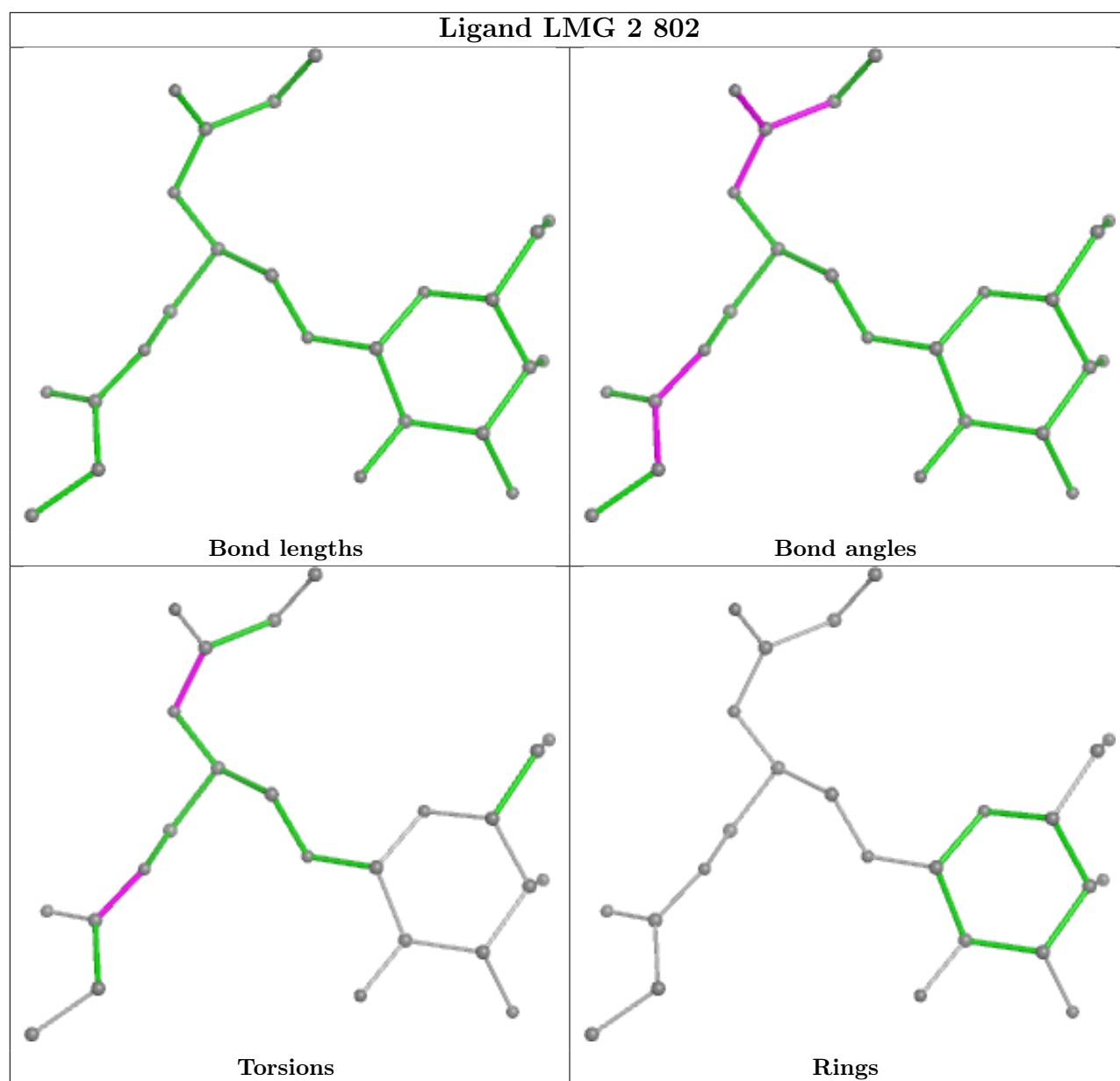


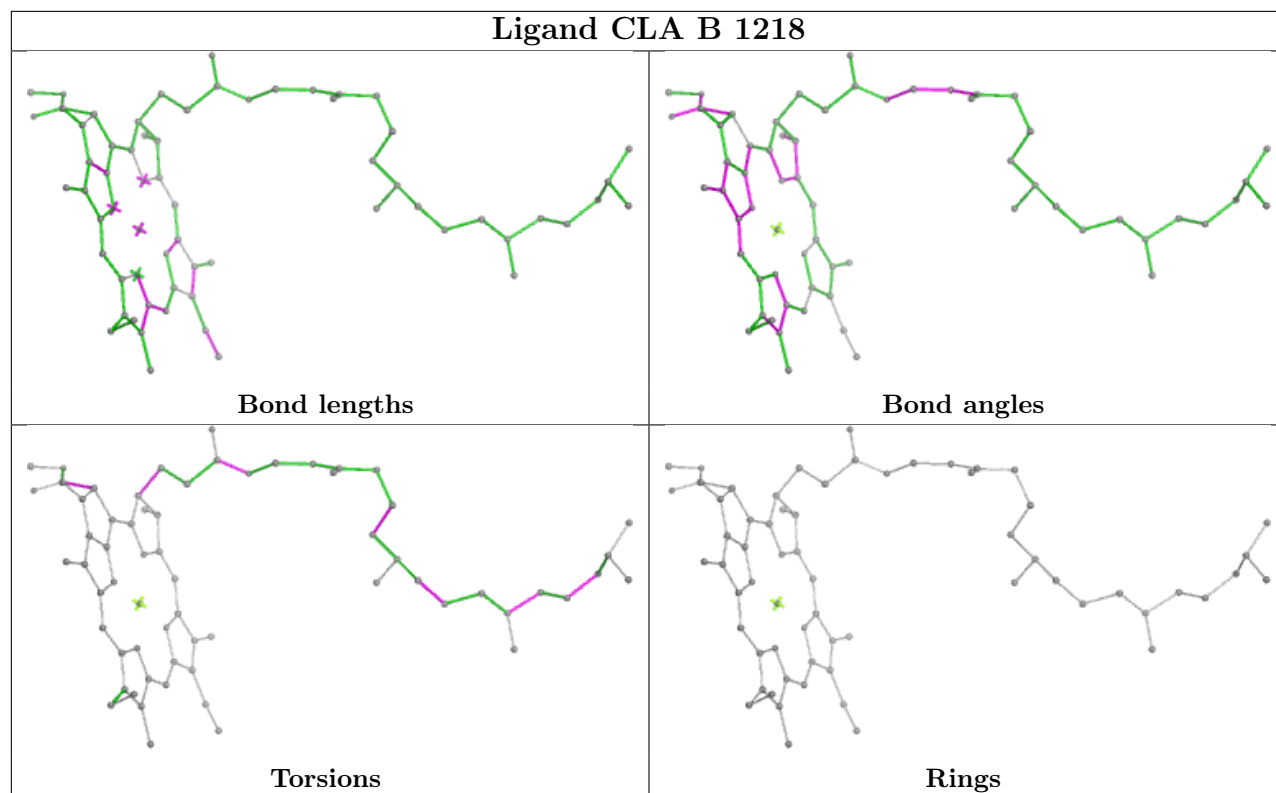
Rings

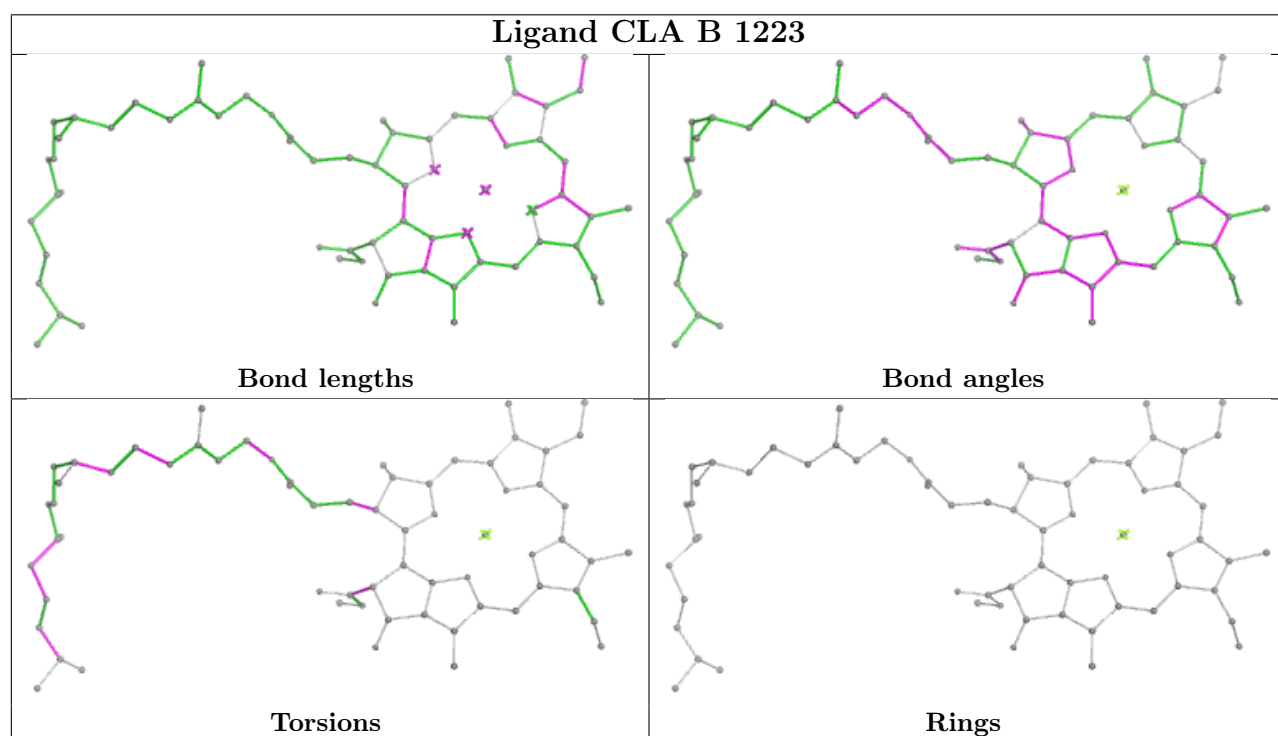
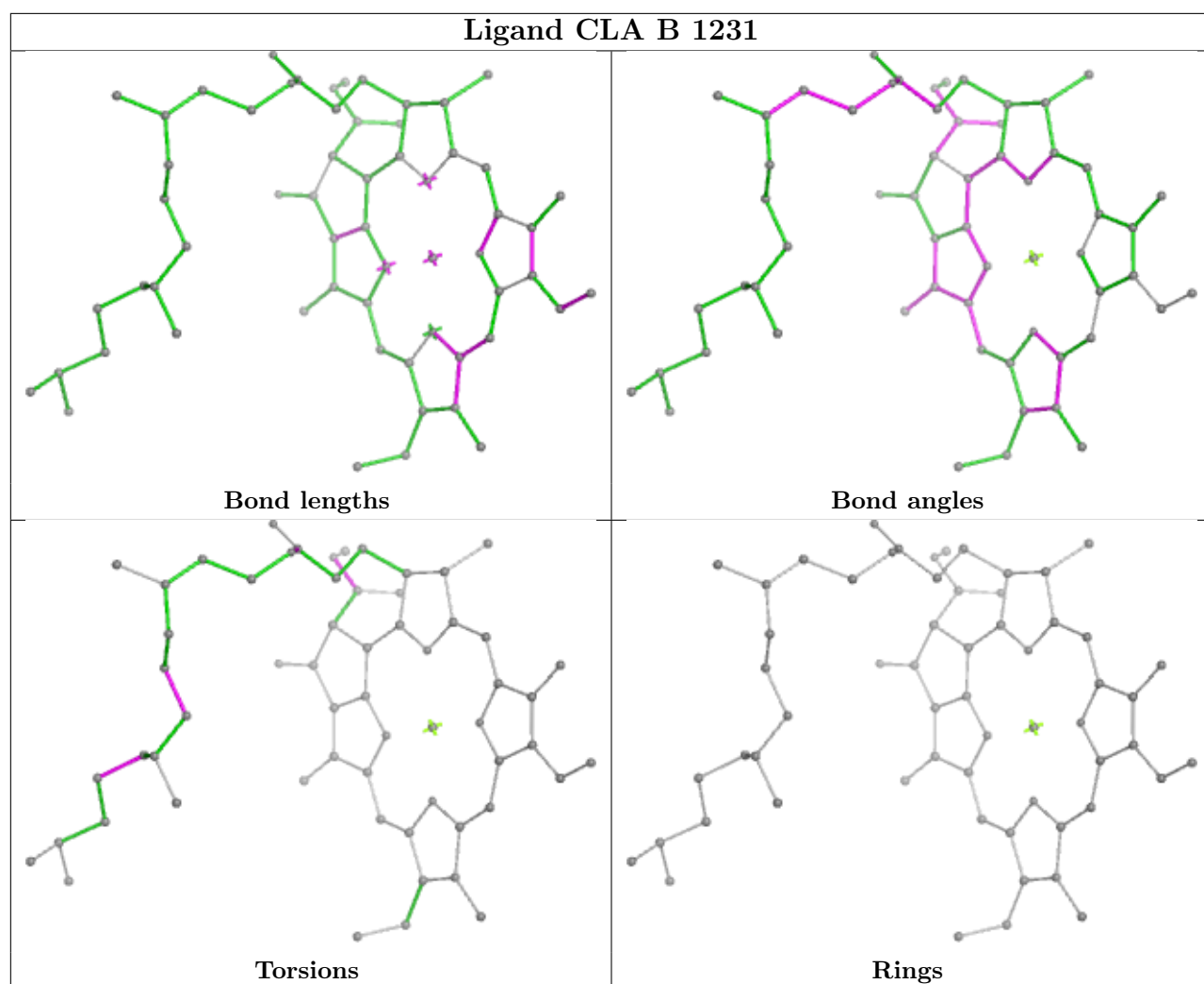
Ligand CLA B 1215**Ligand BCR I 4018**

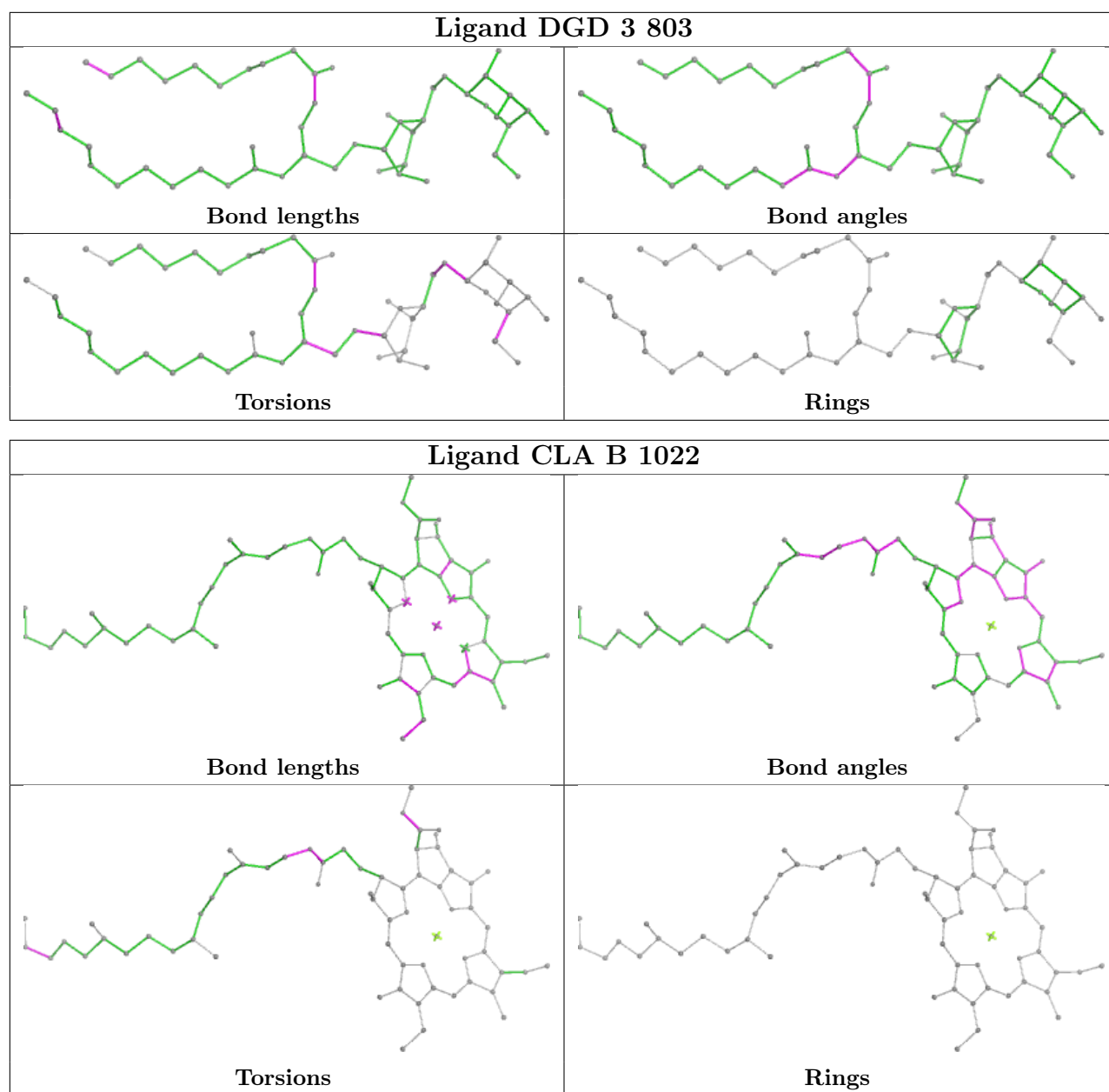


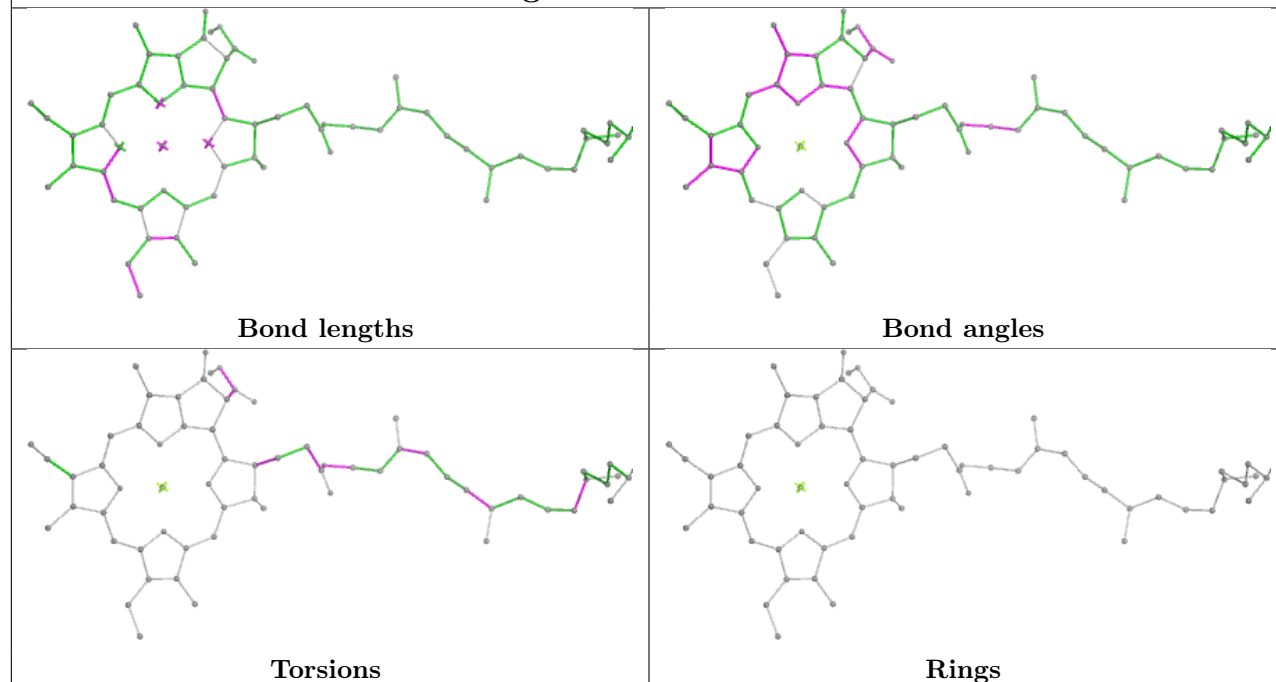
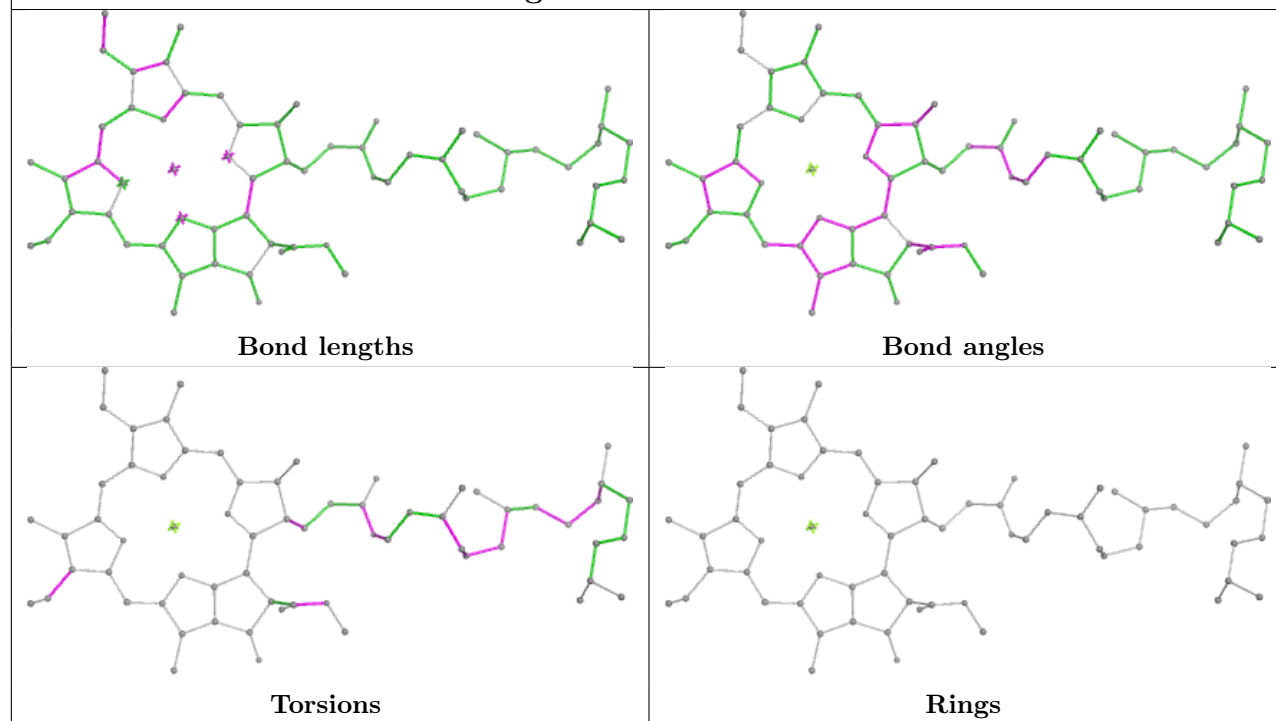


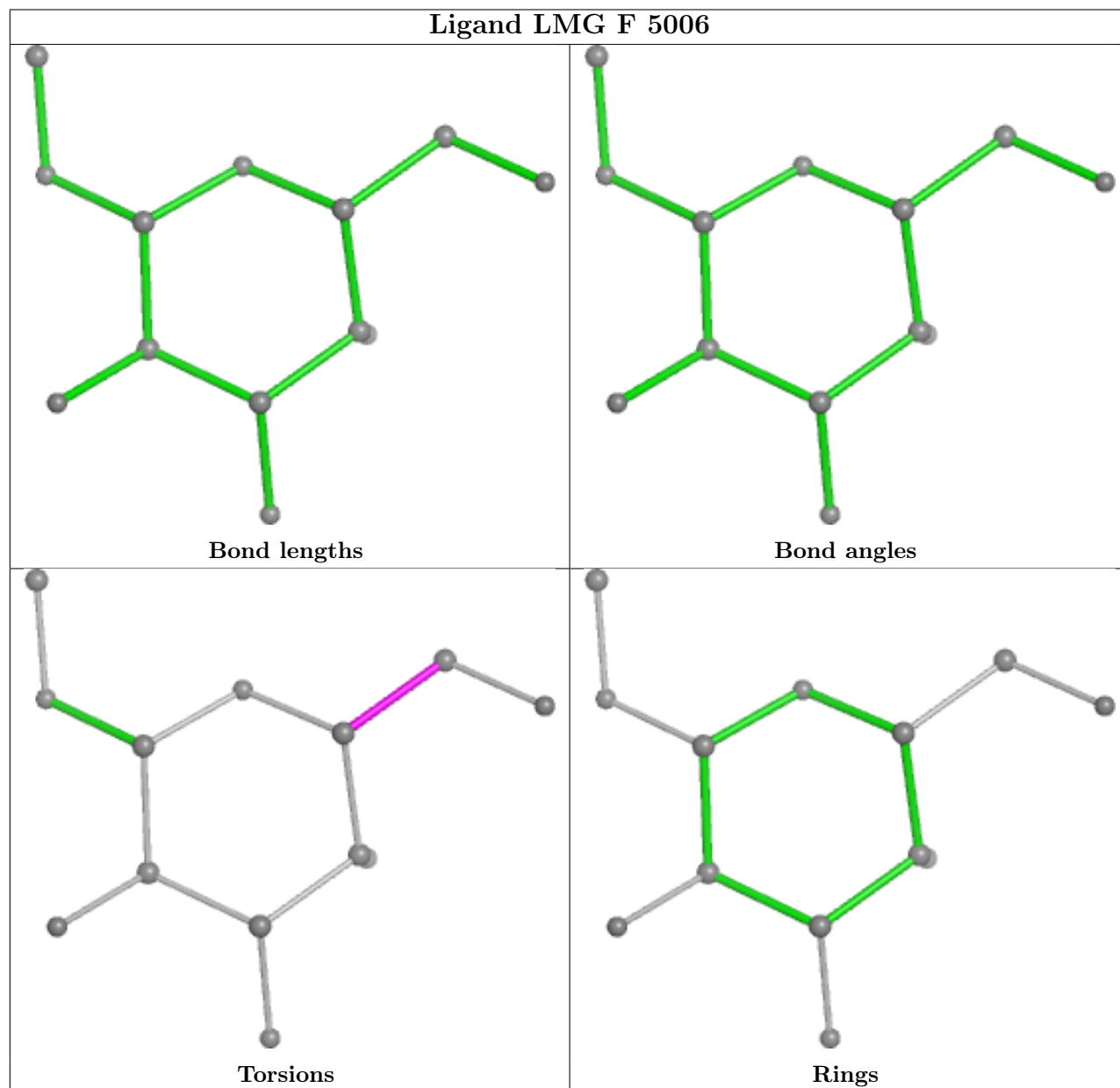
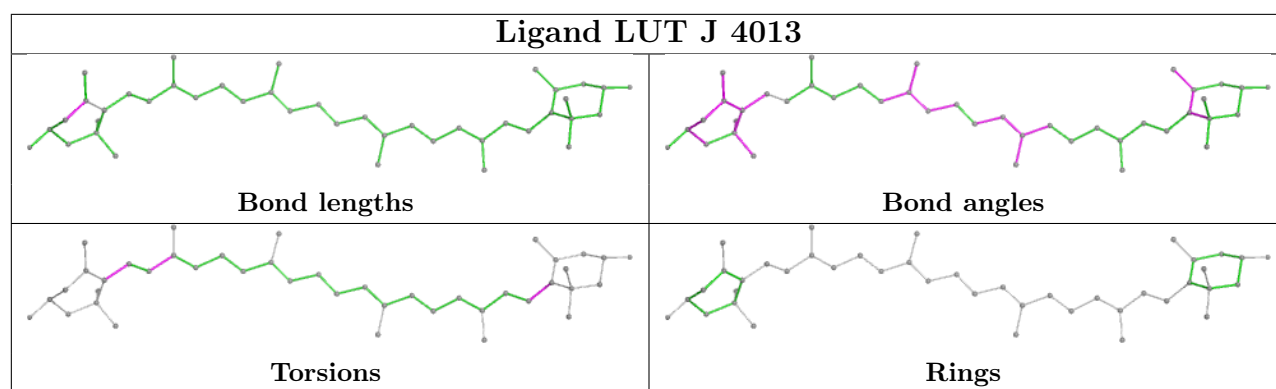


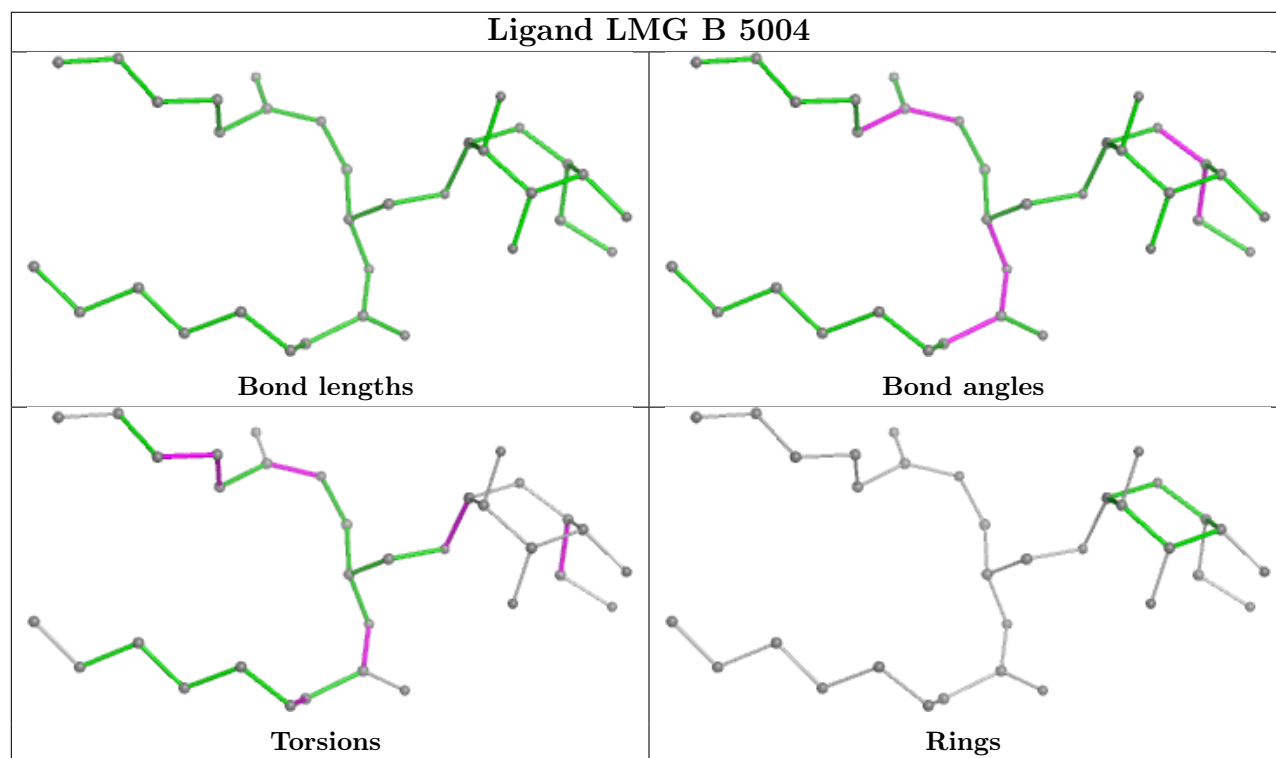
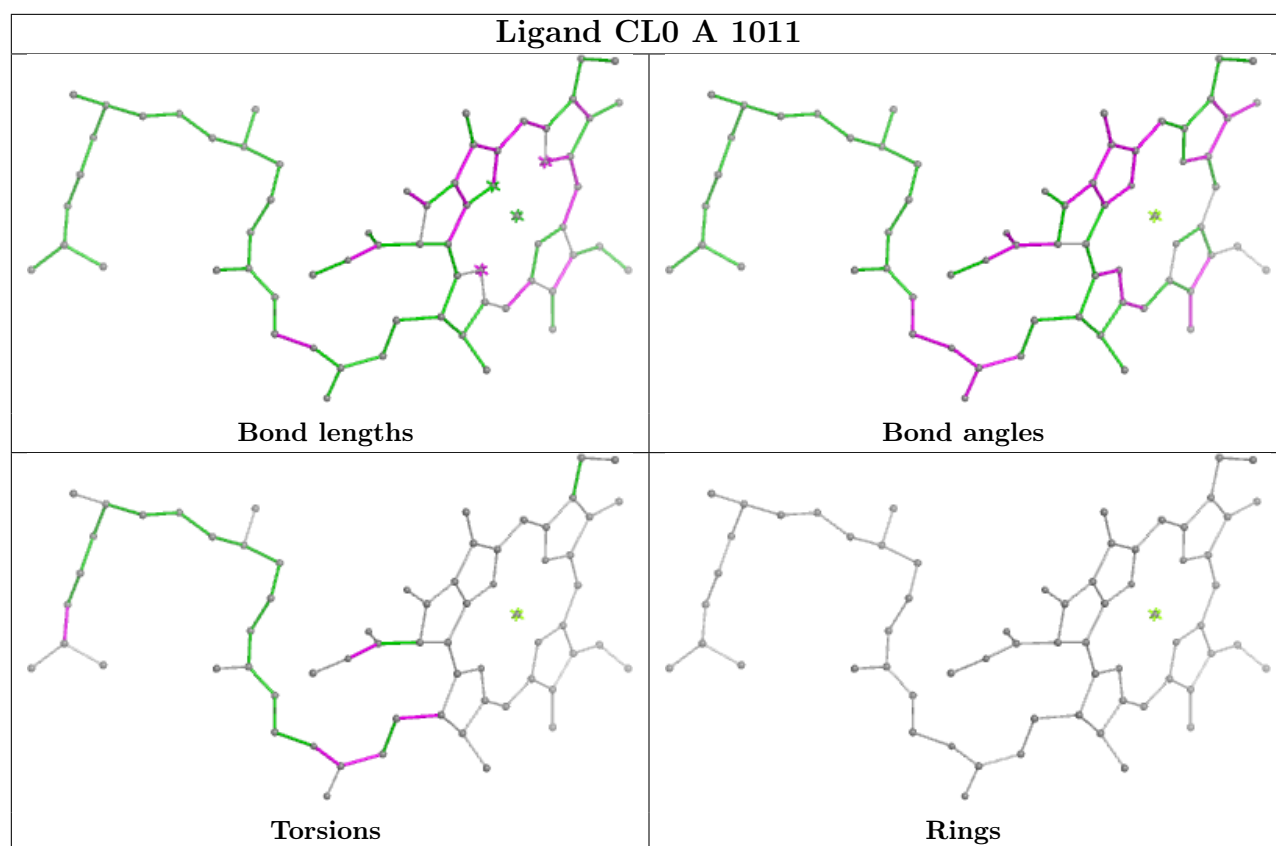


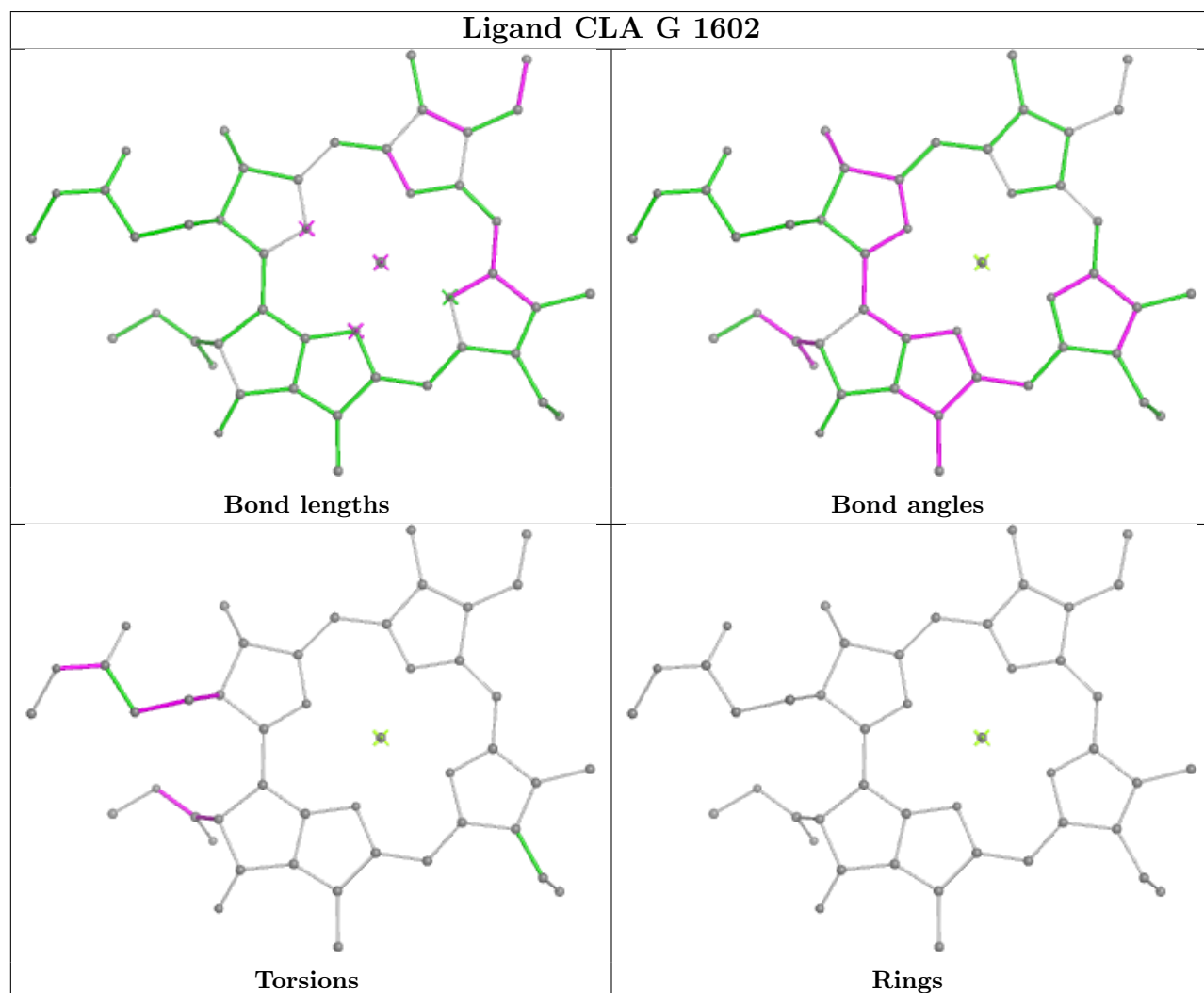
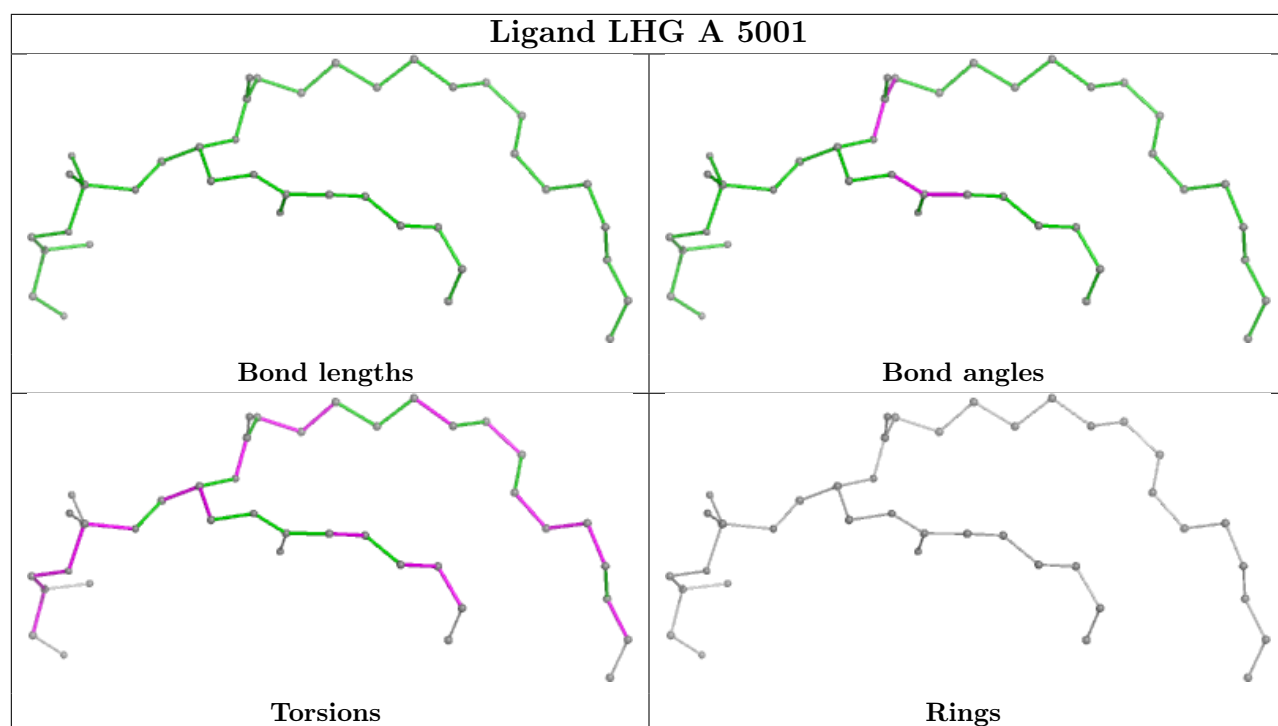


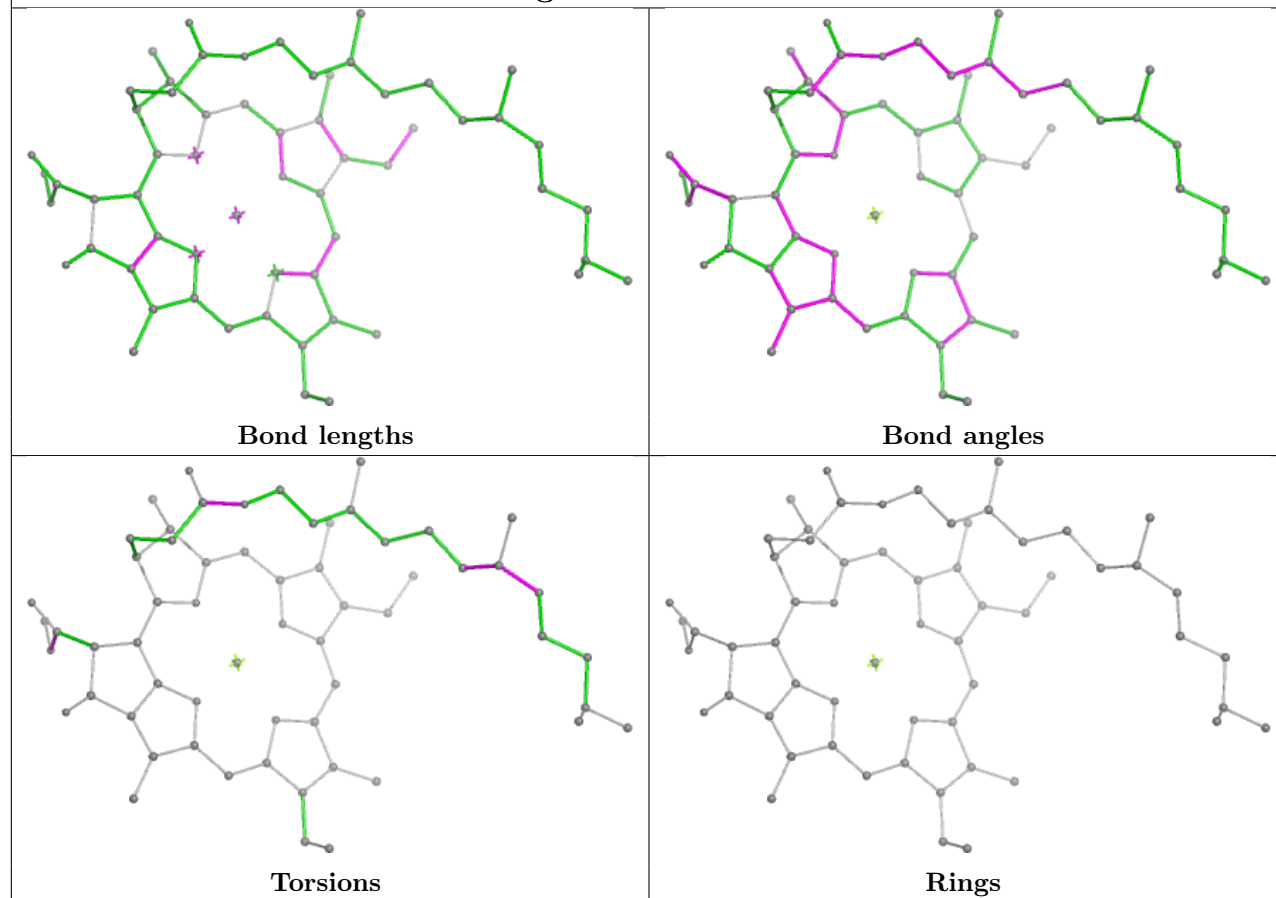
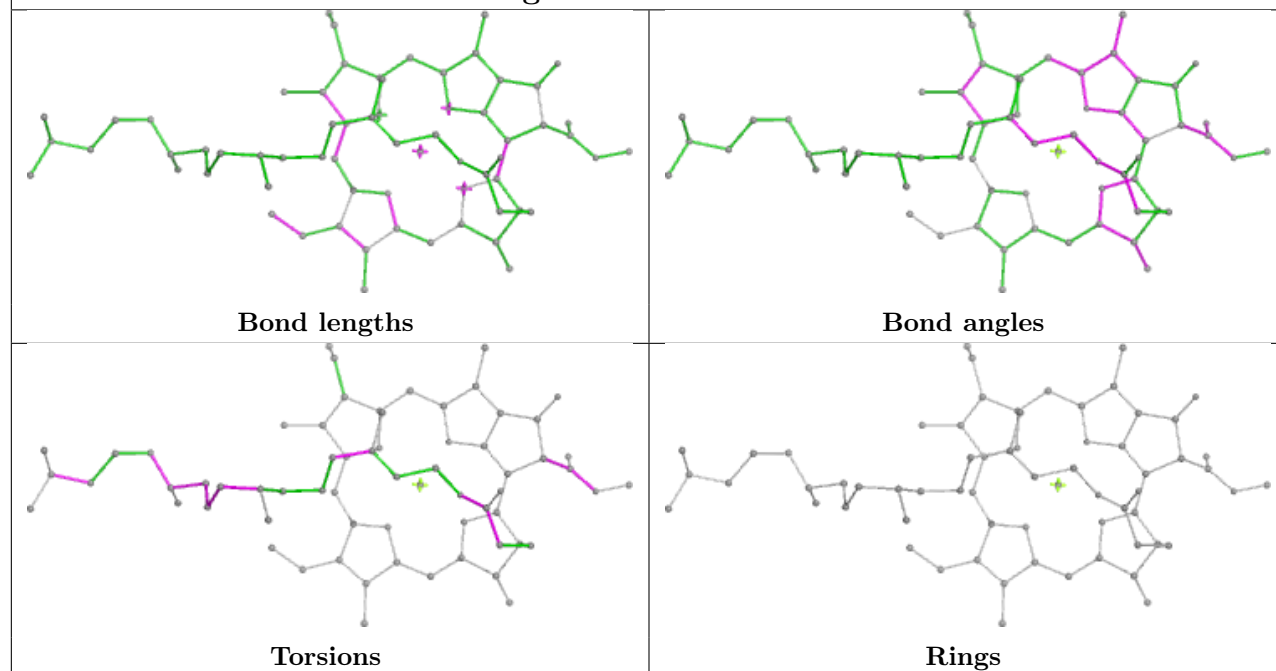


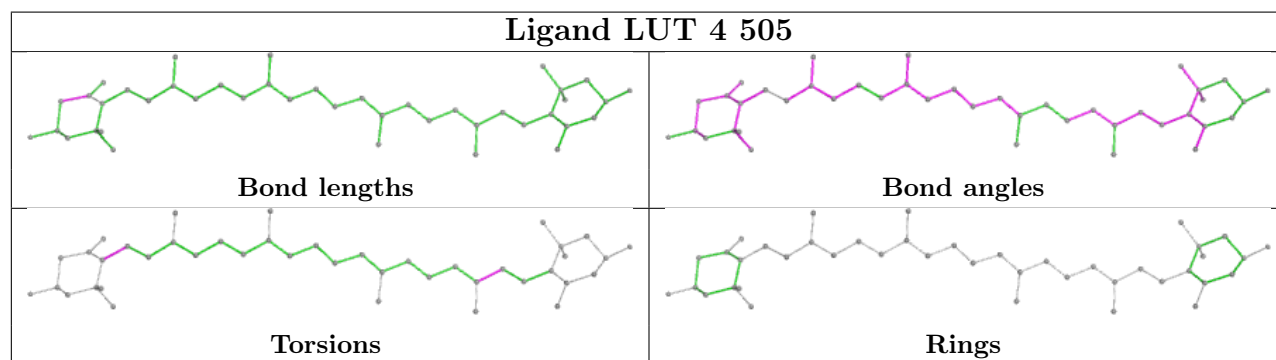
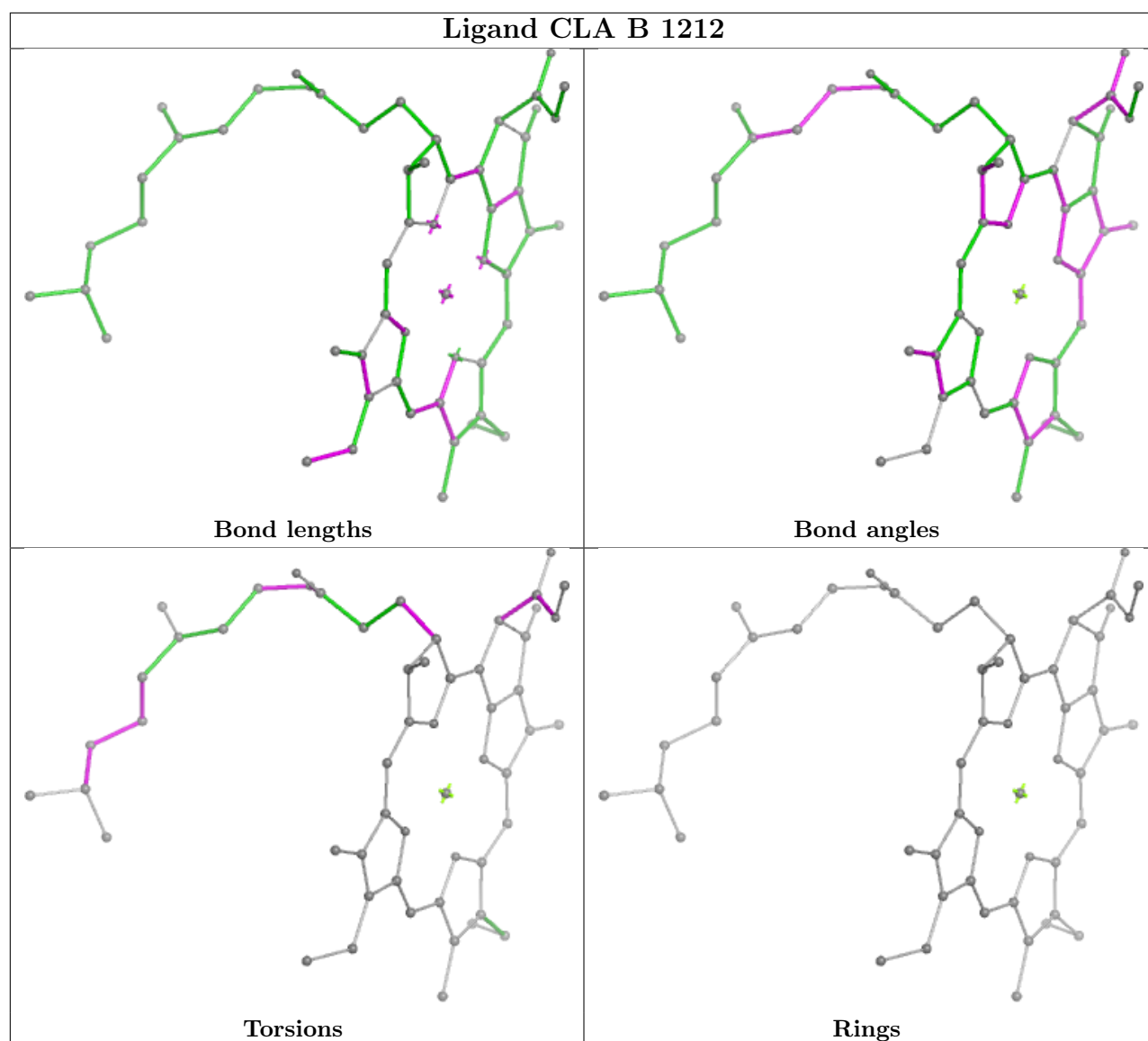
Ligand CLA A 1103**Ligand CLA F 1301**

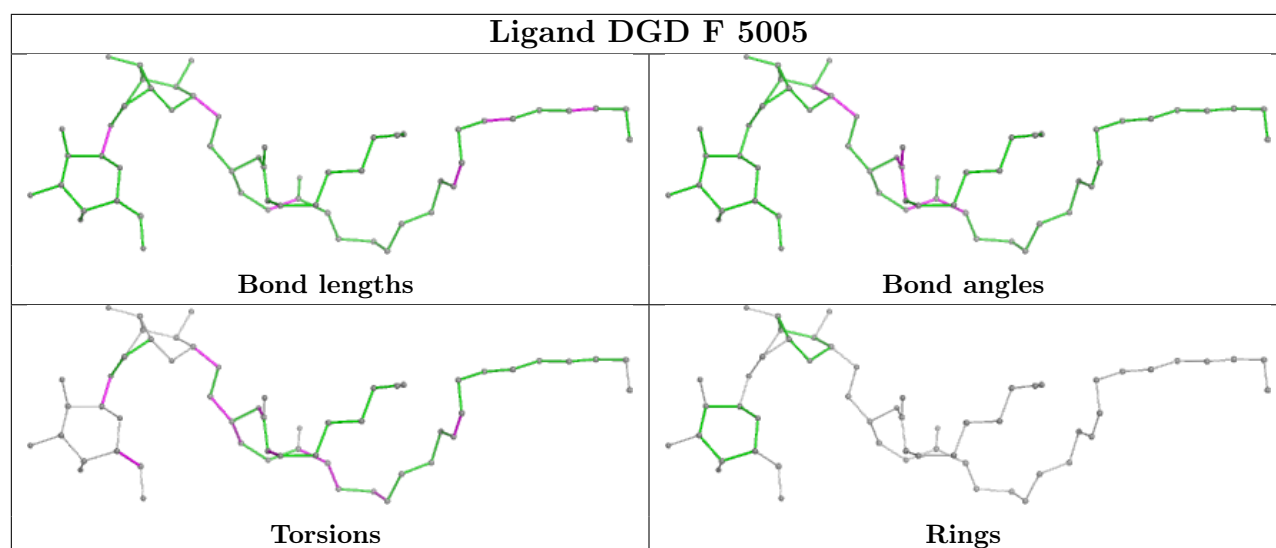




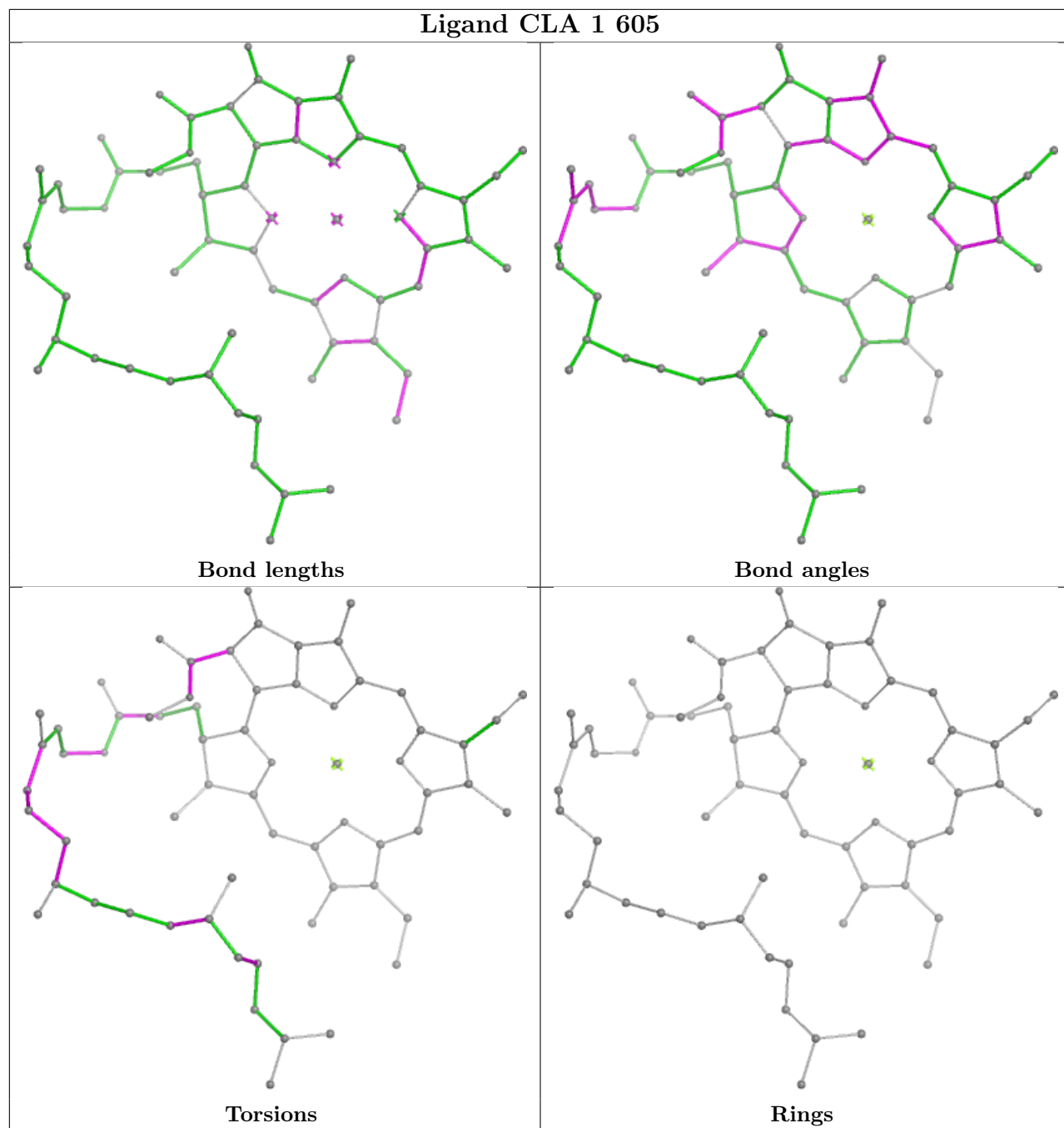


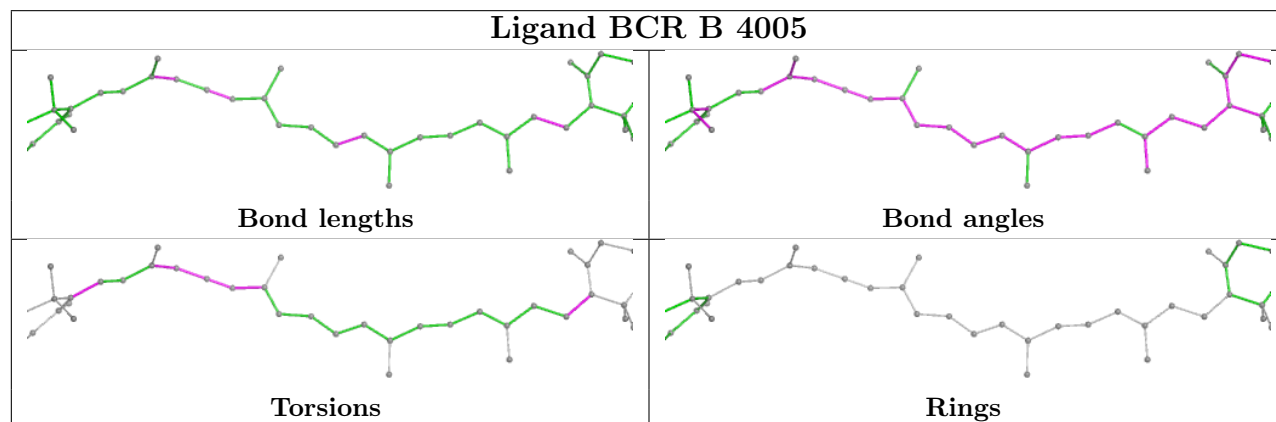
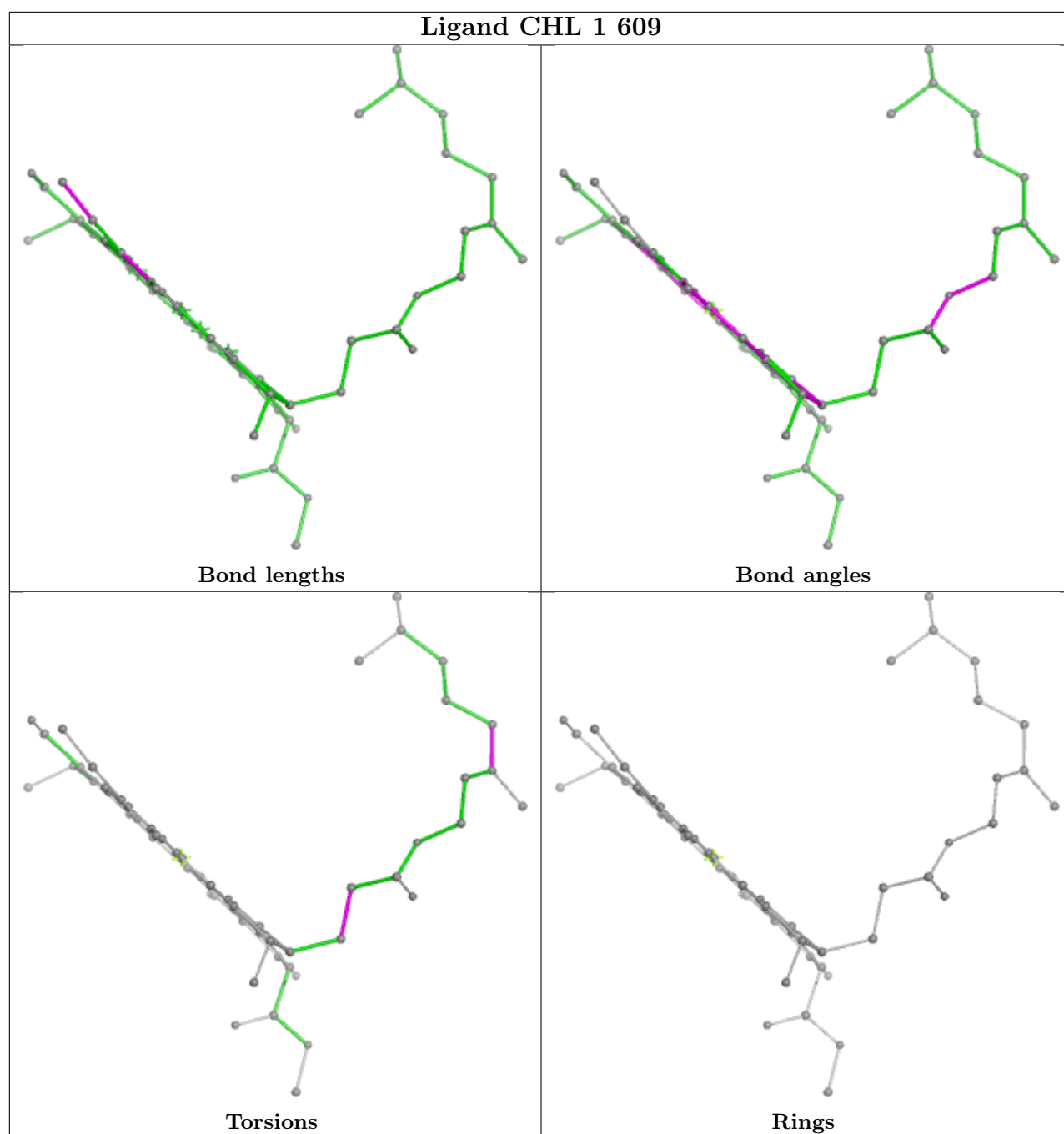
Ligand CLA 4 604**Ligand CLA A 1136**

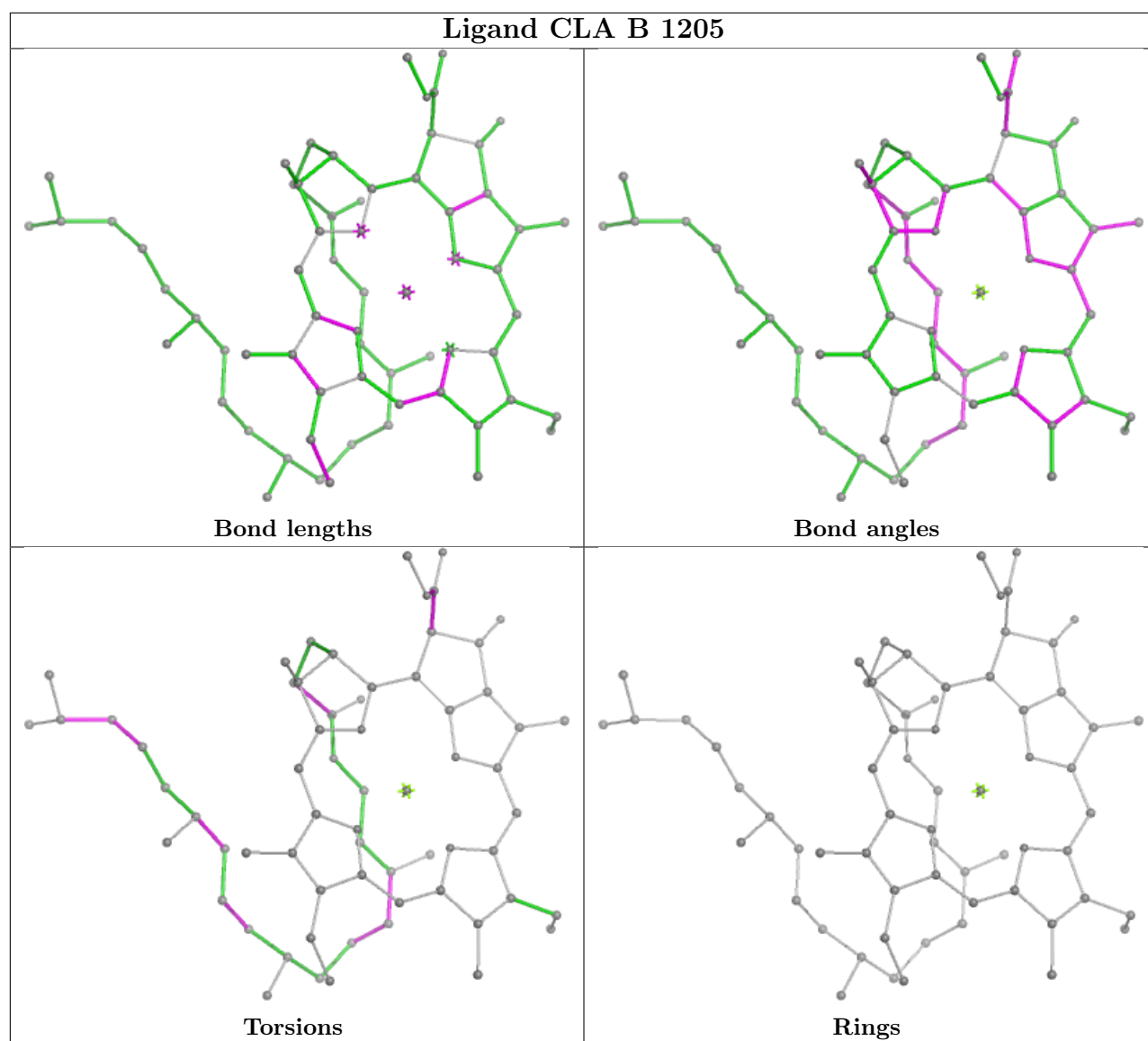


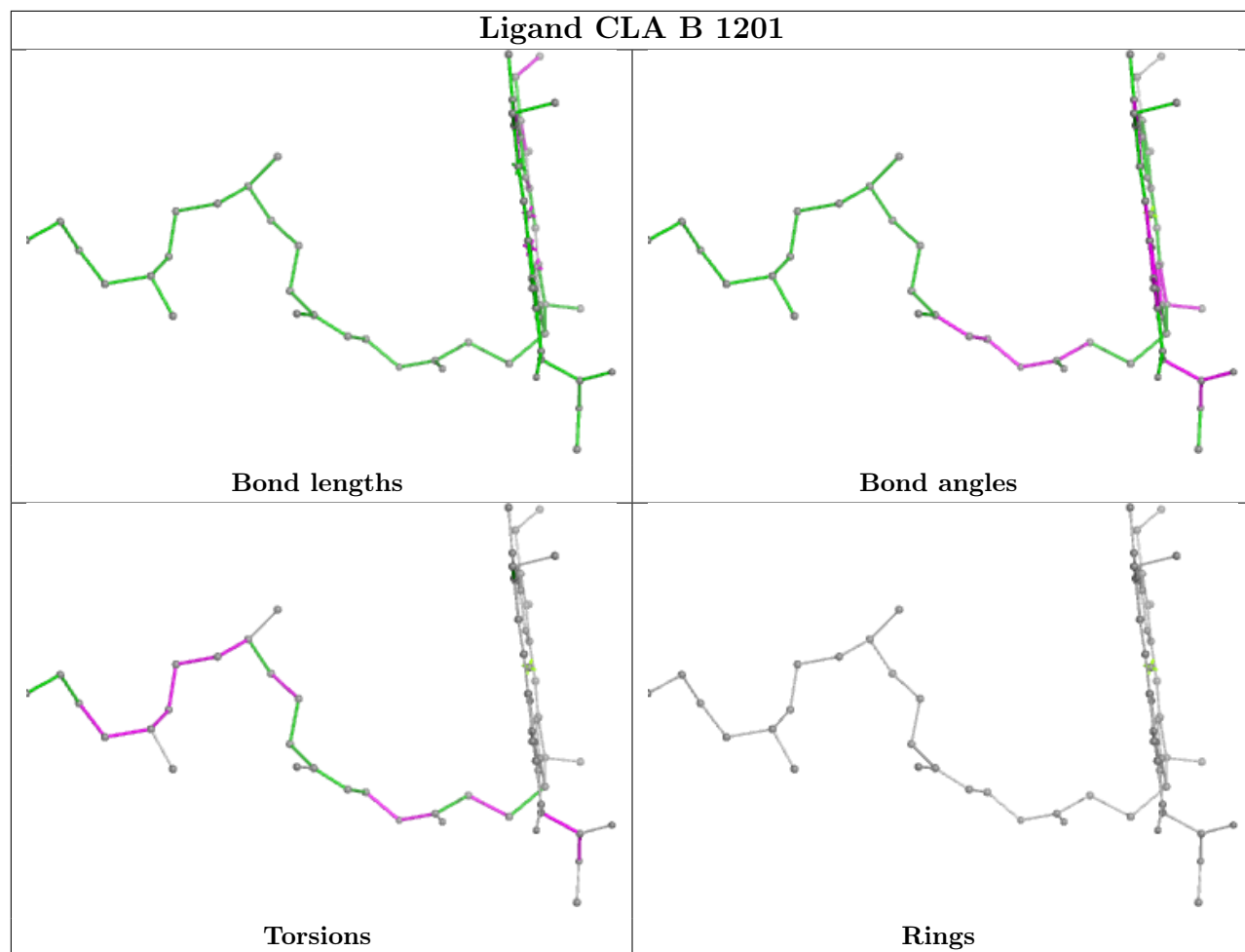


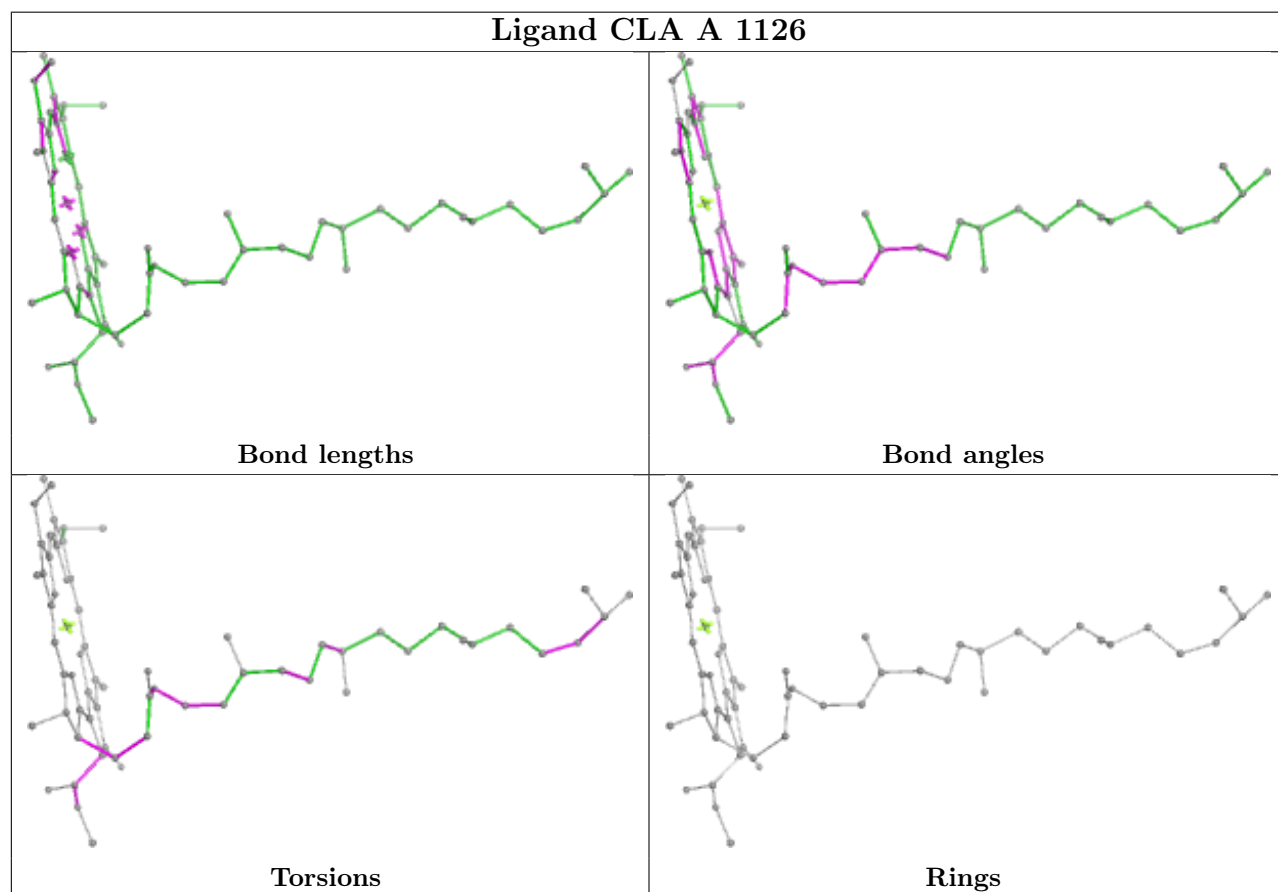
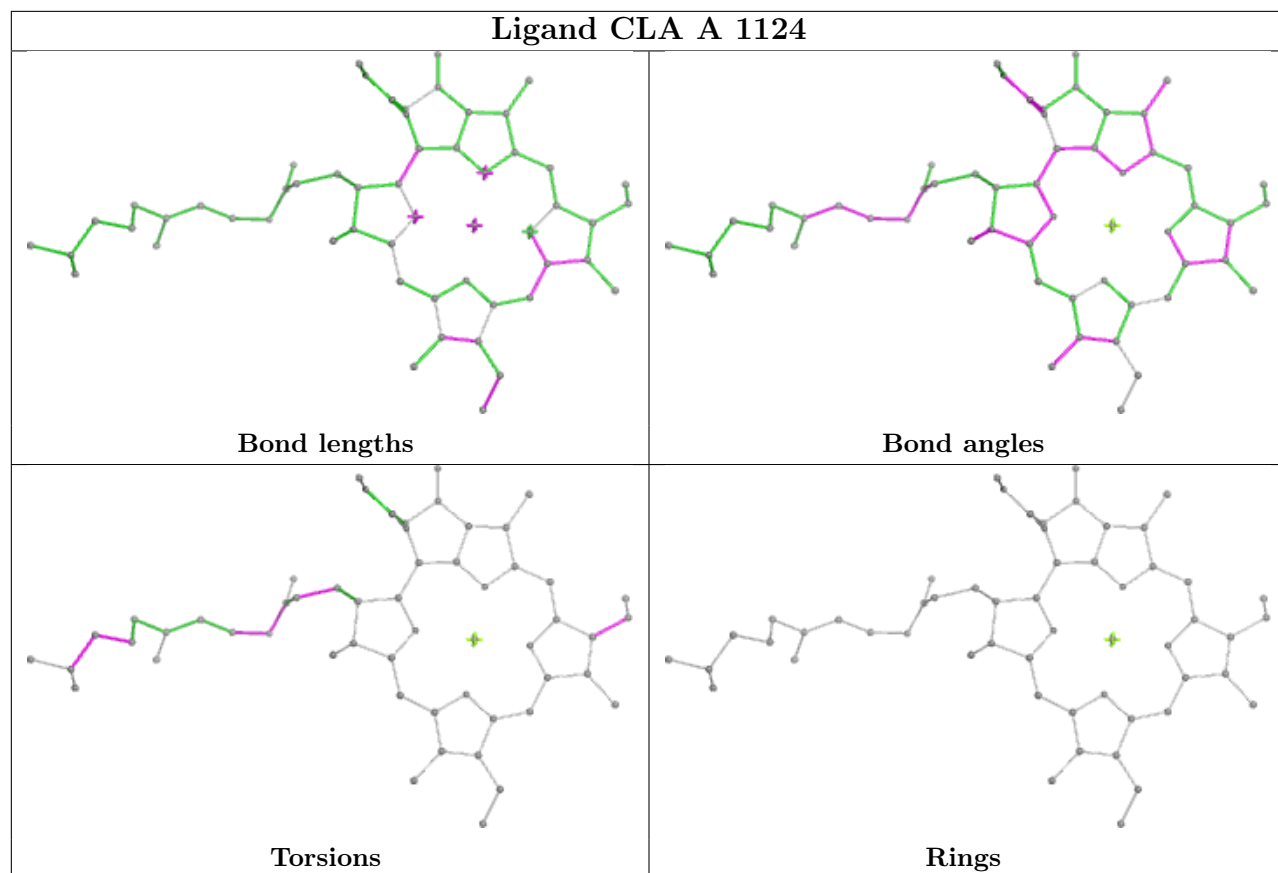
Ligand CLA 1 605



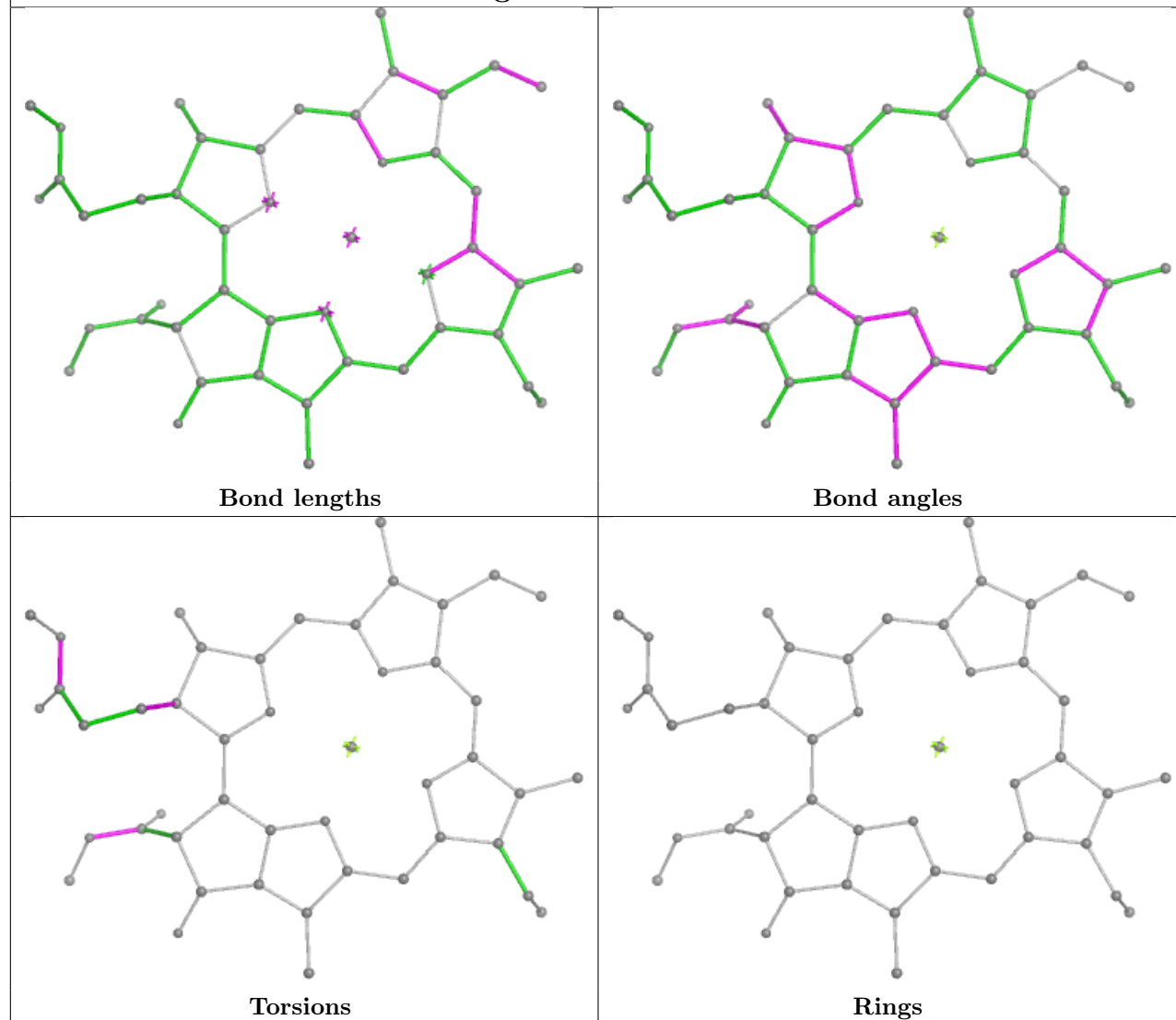




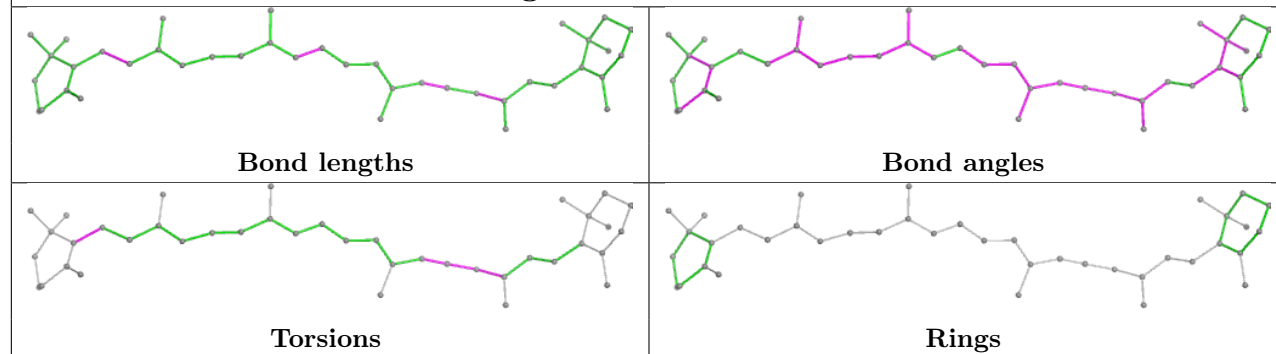


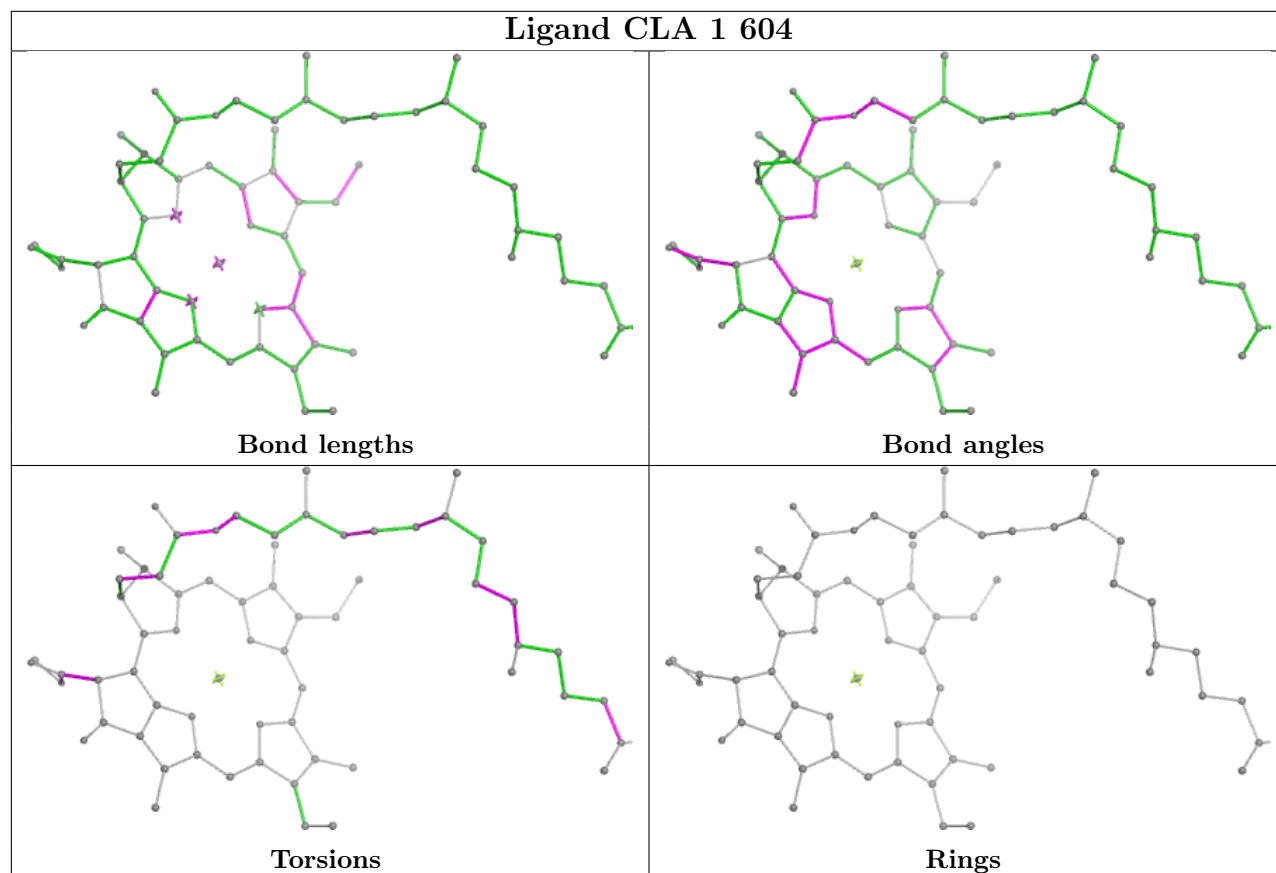
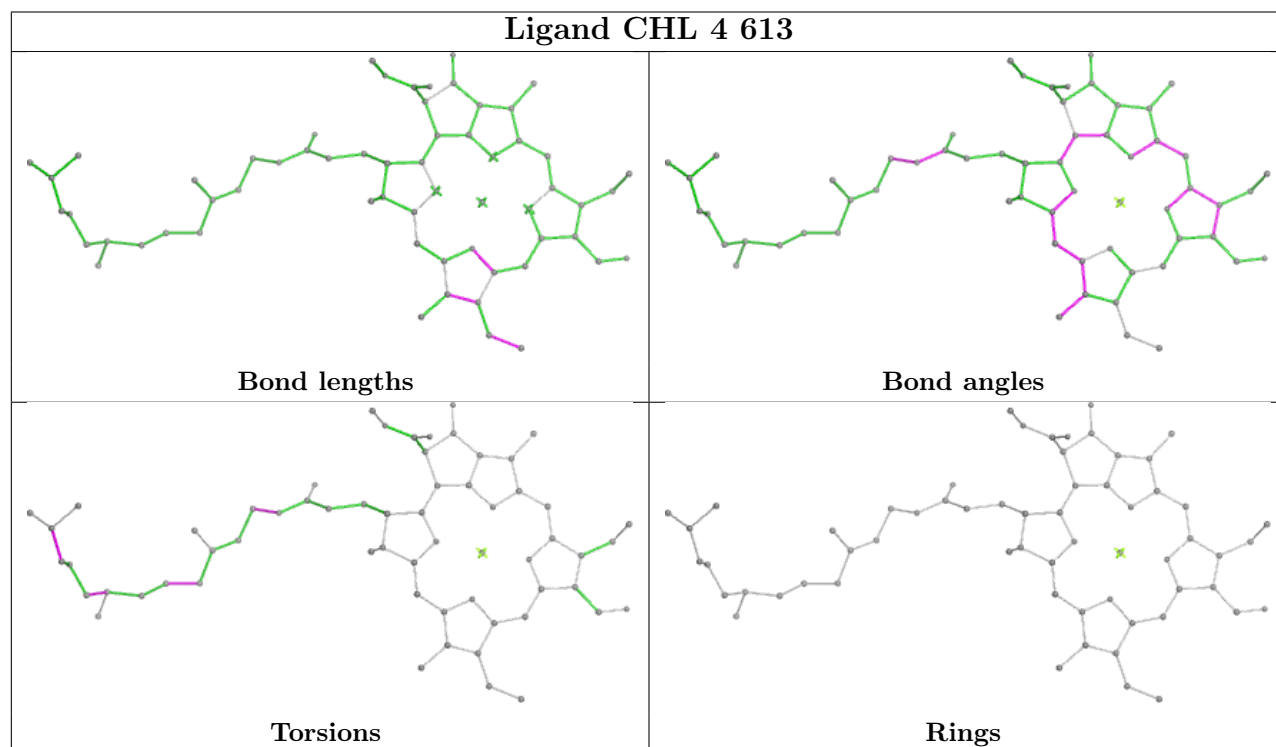


Ligand CLA 1 602

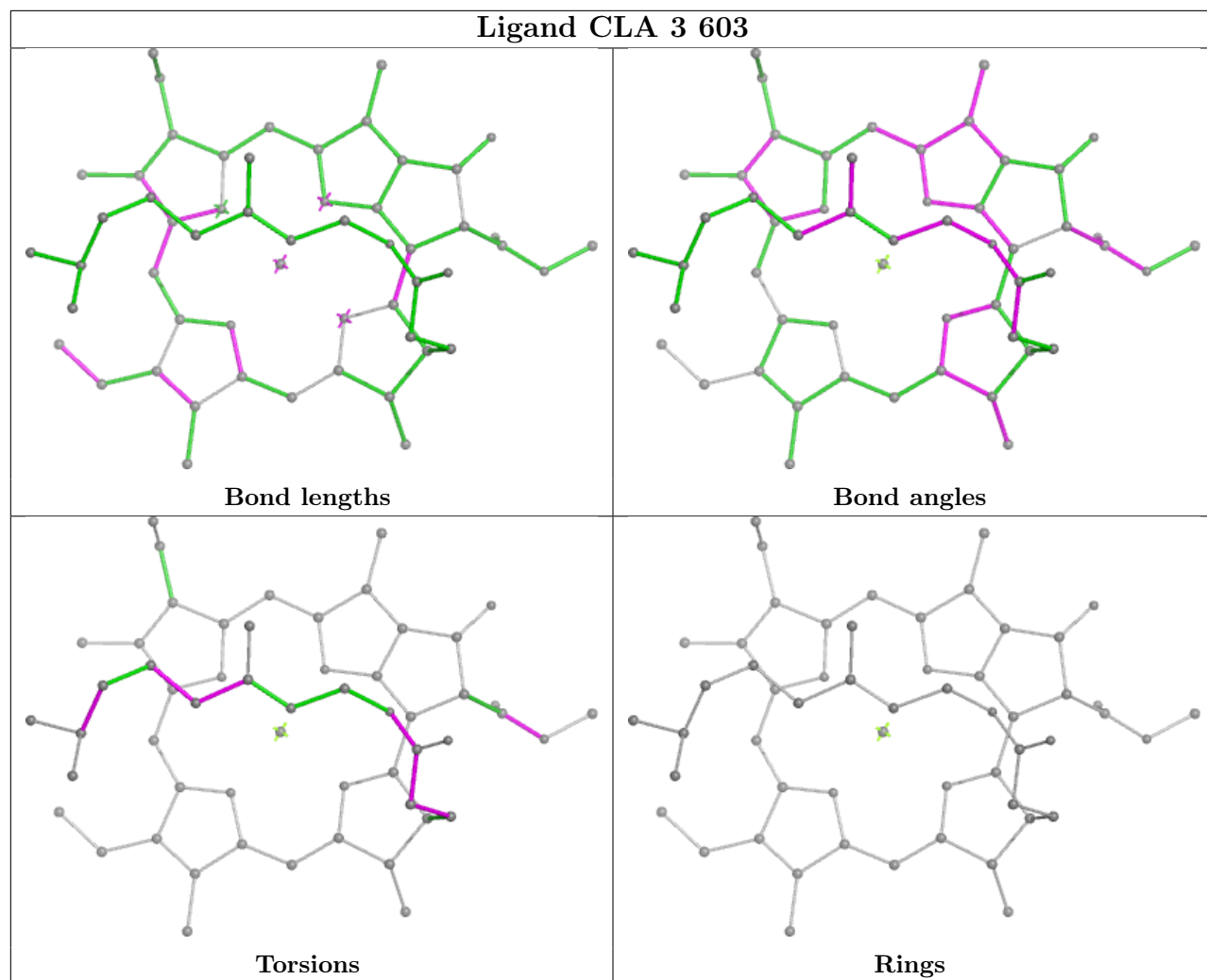


Ligand BCR A 4003

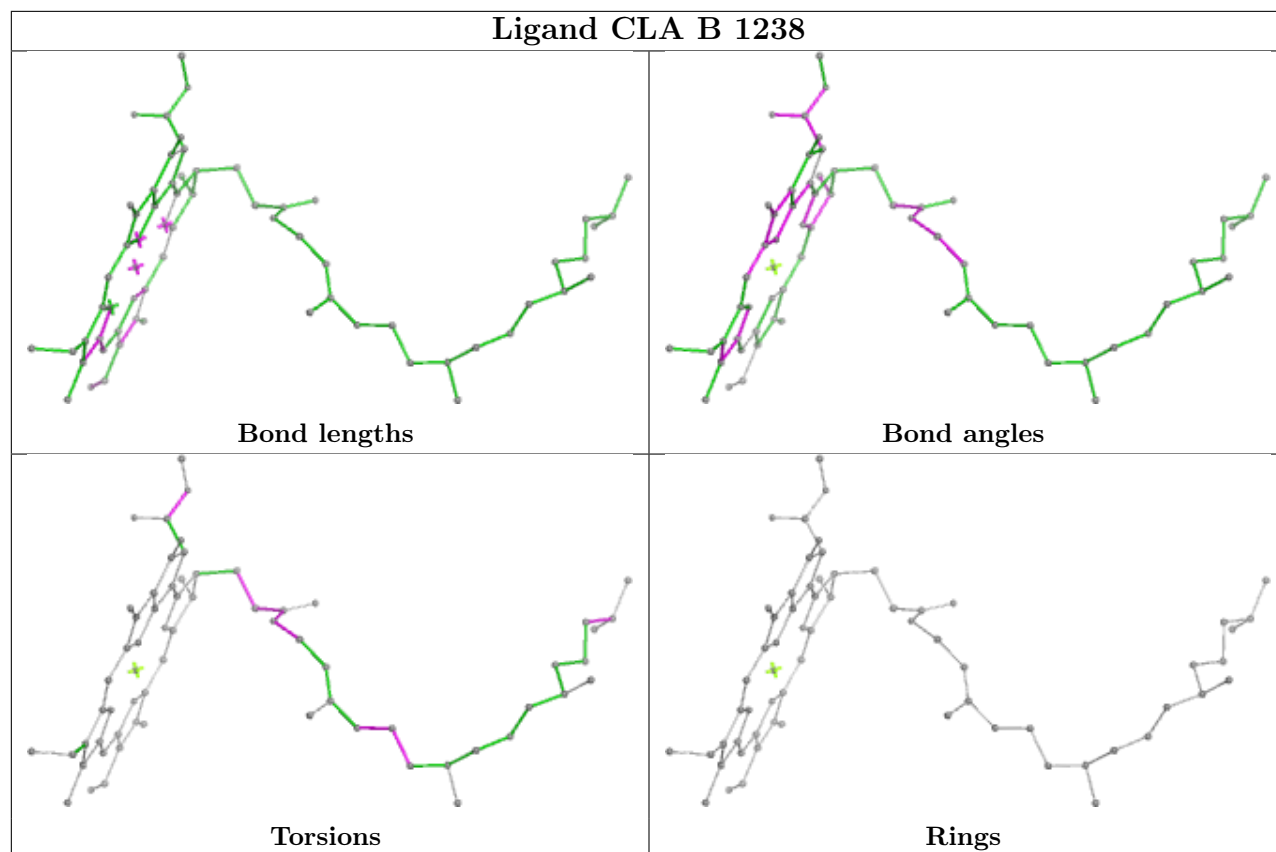


Ligand CLA 1 604**Ligand CHL 4 613**

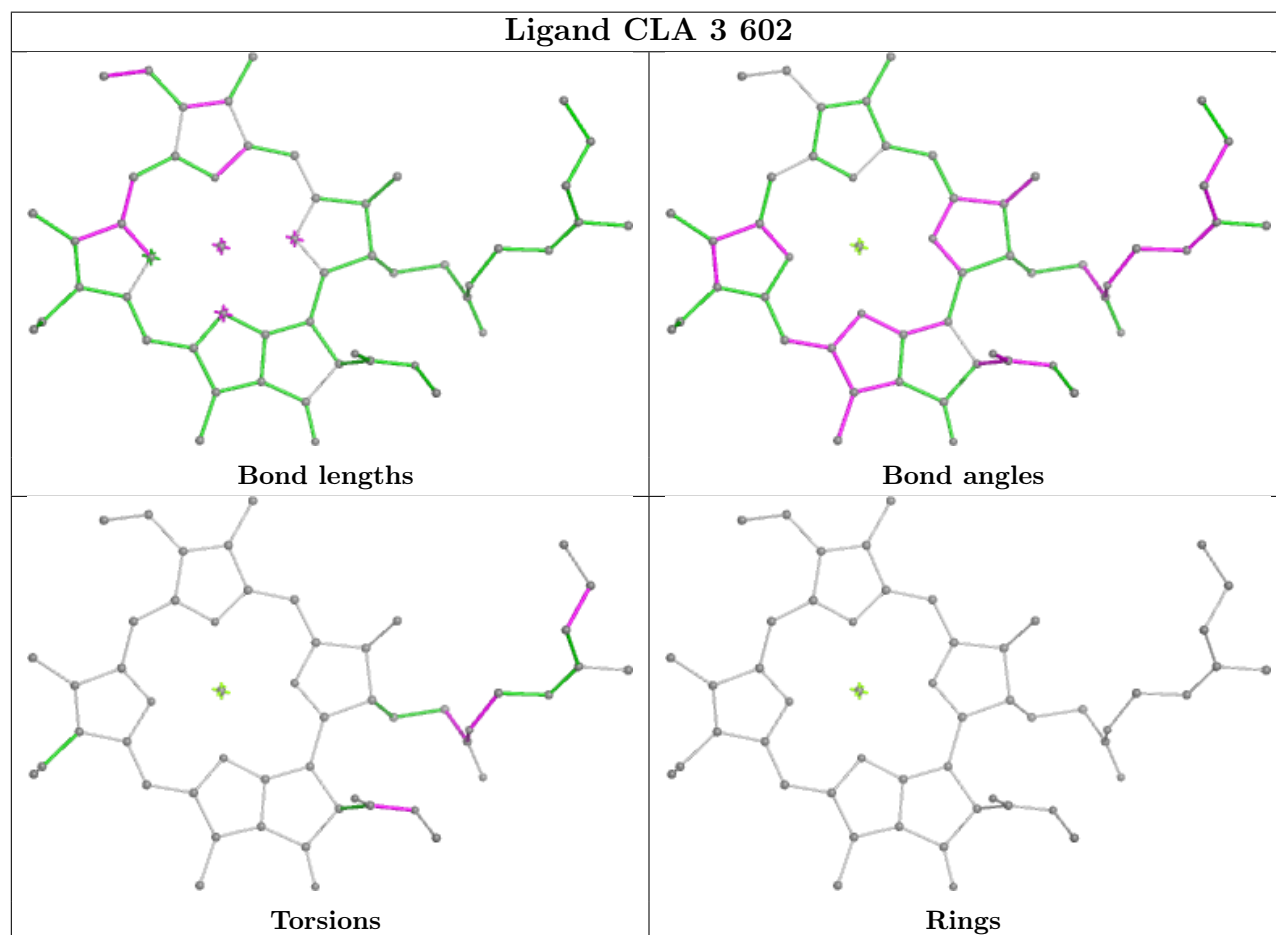
Ligand CLA 3 603

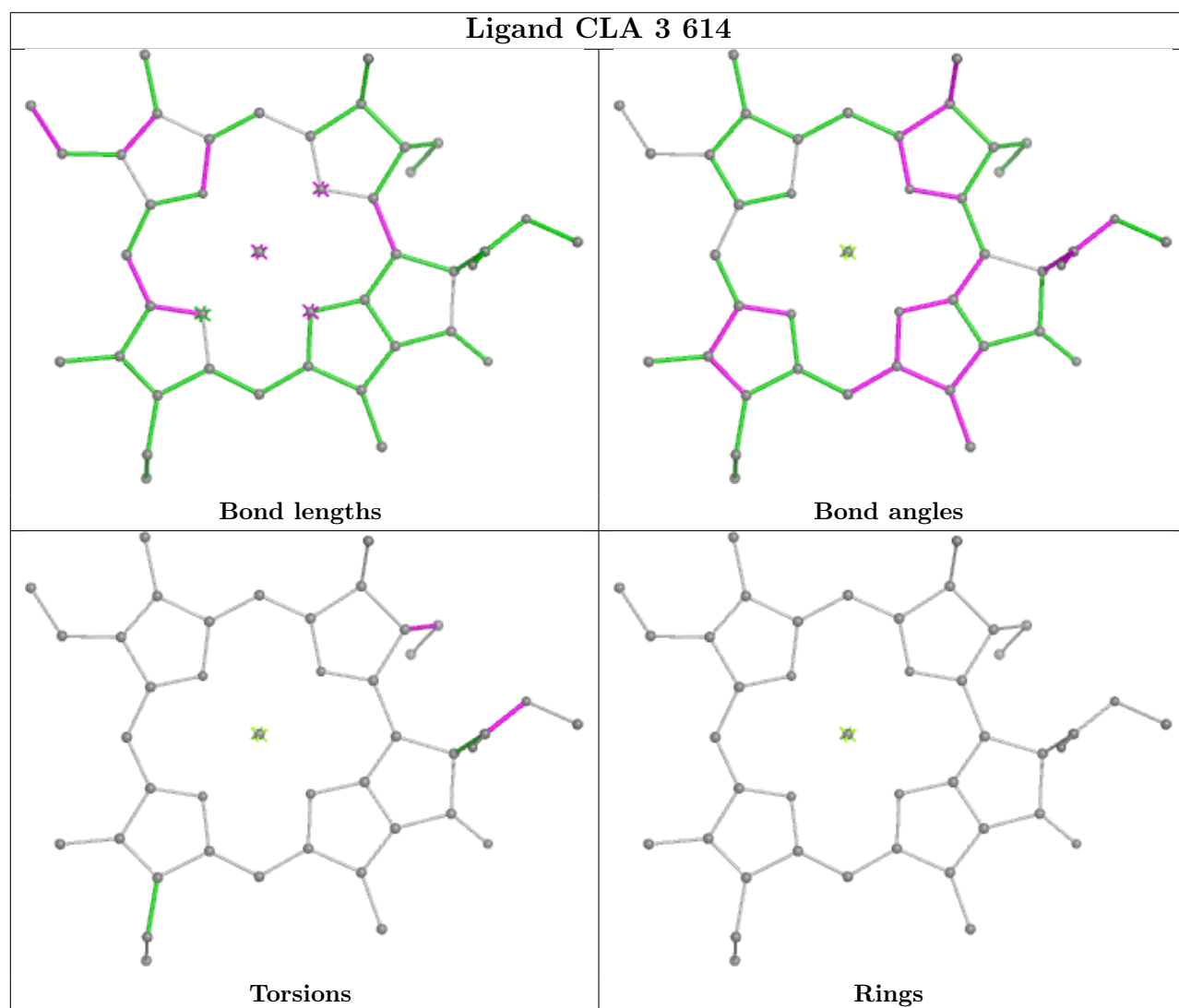
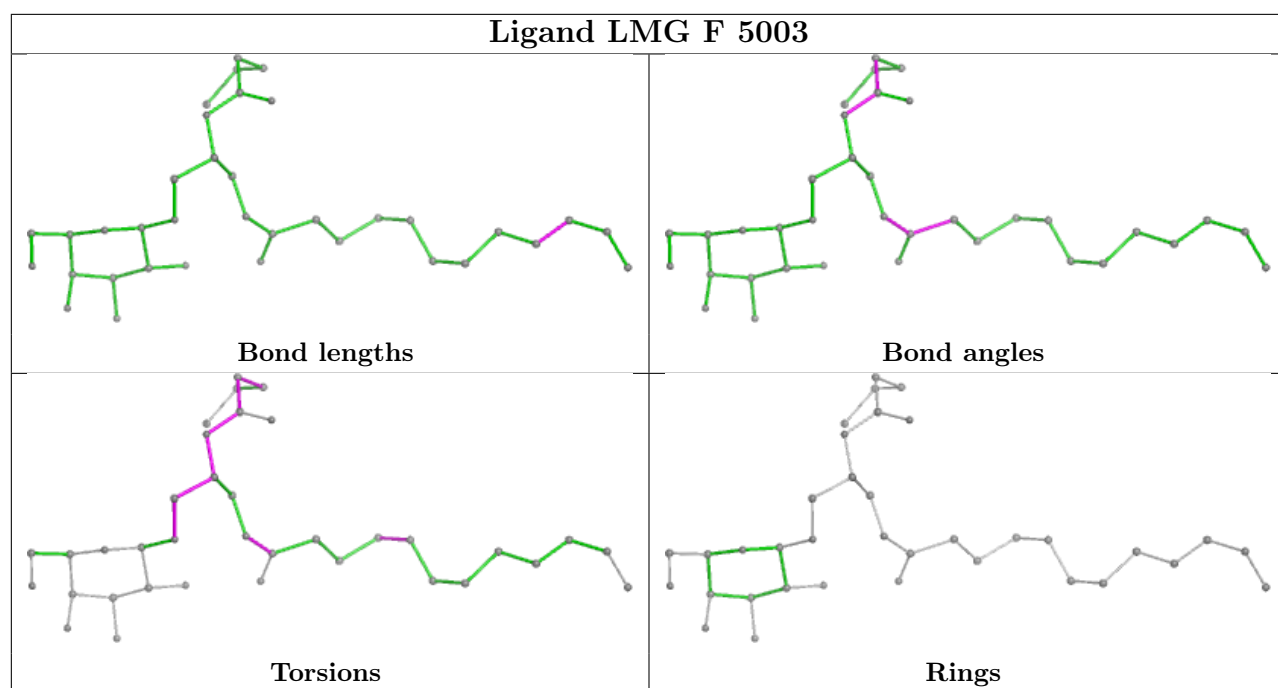


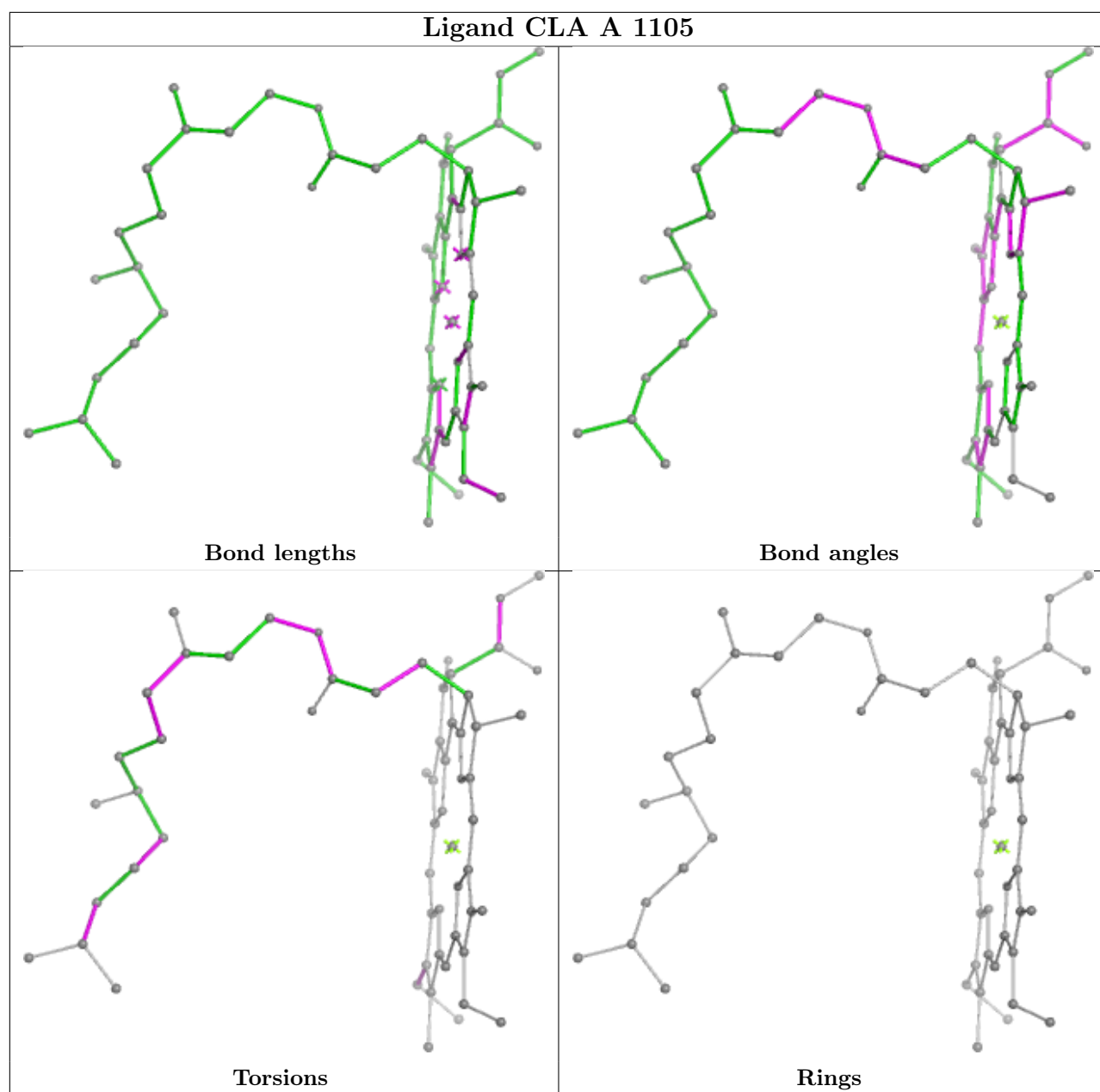
Ligand CLA B 1238

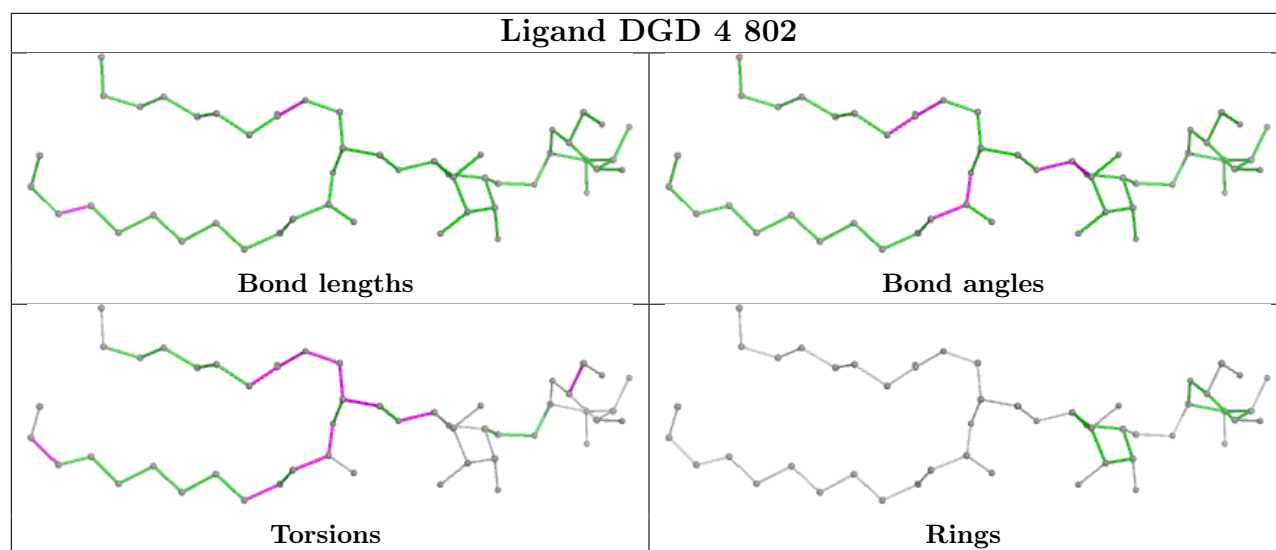
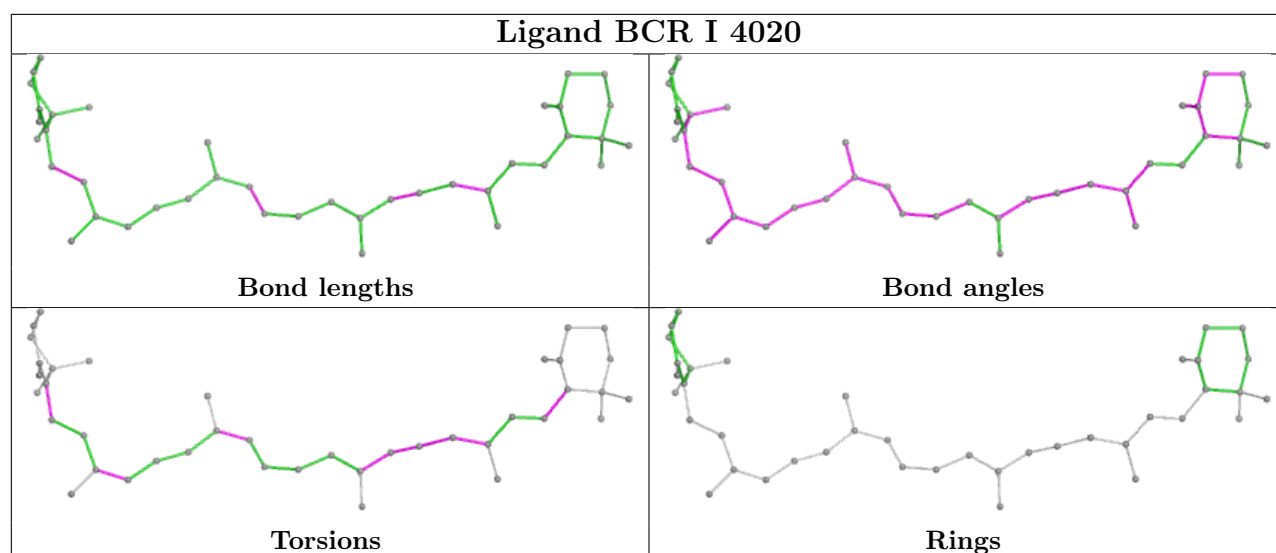


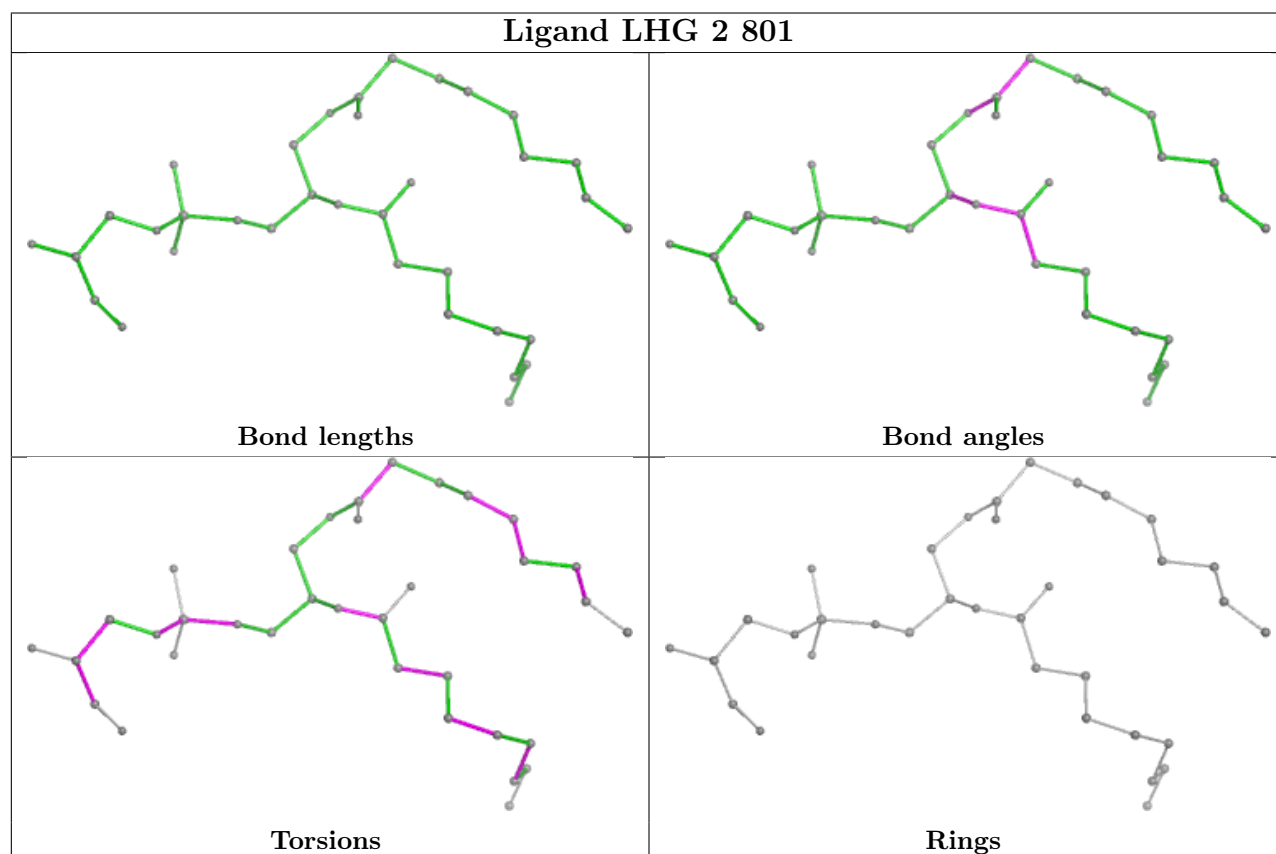
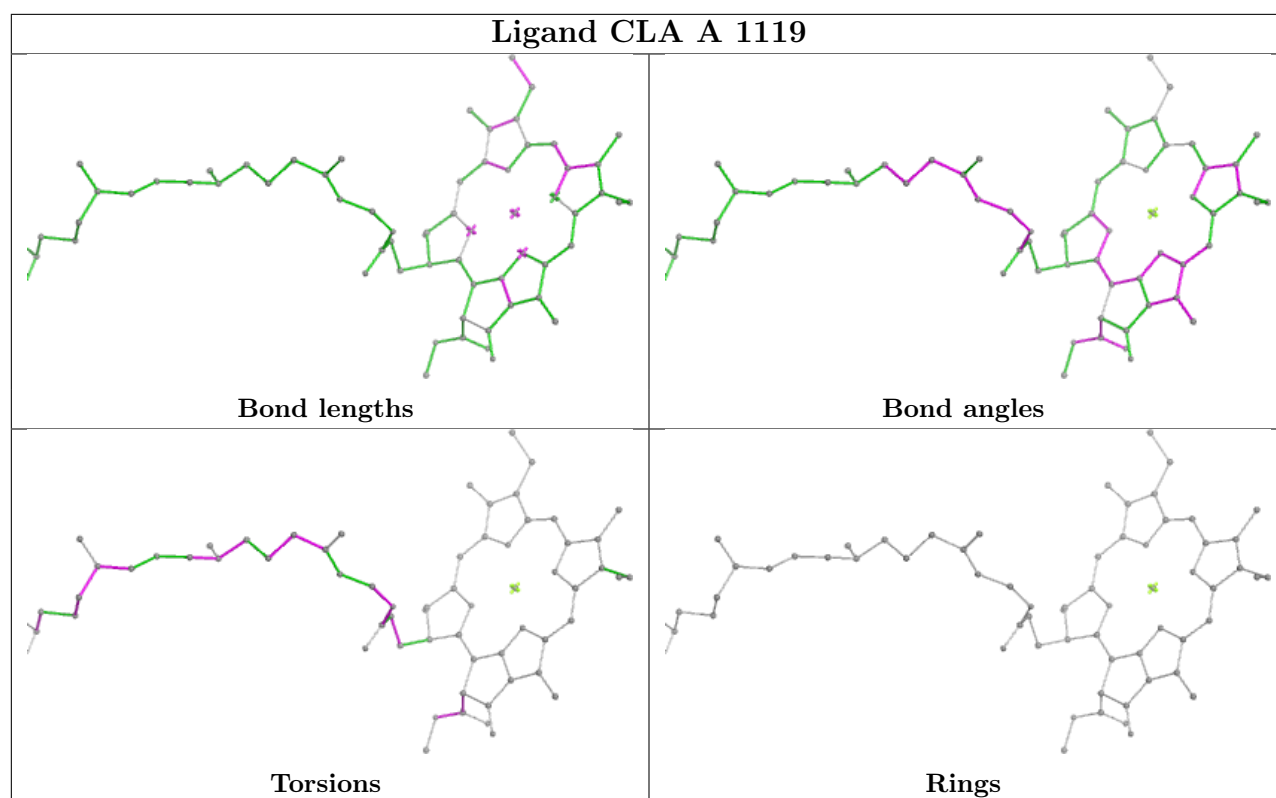
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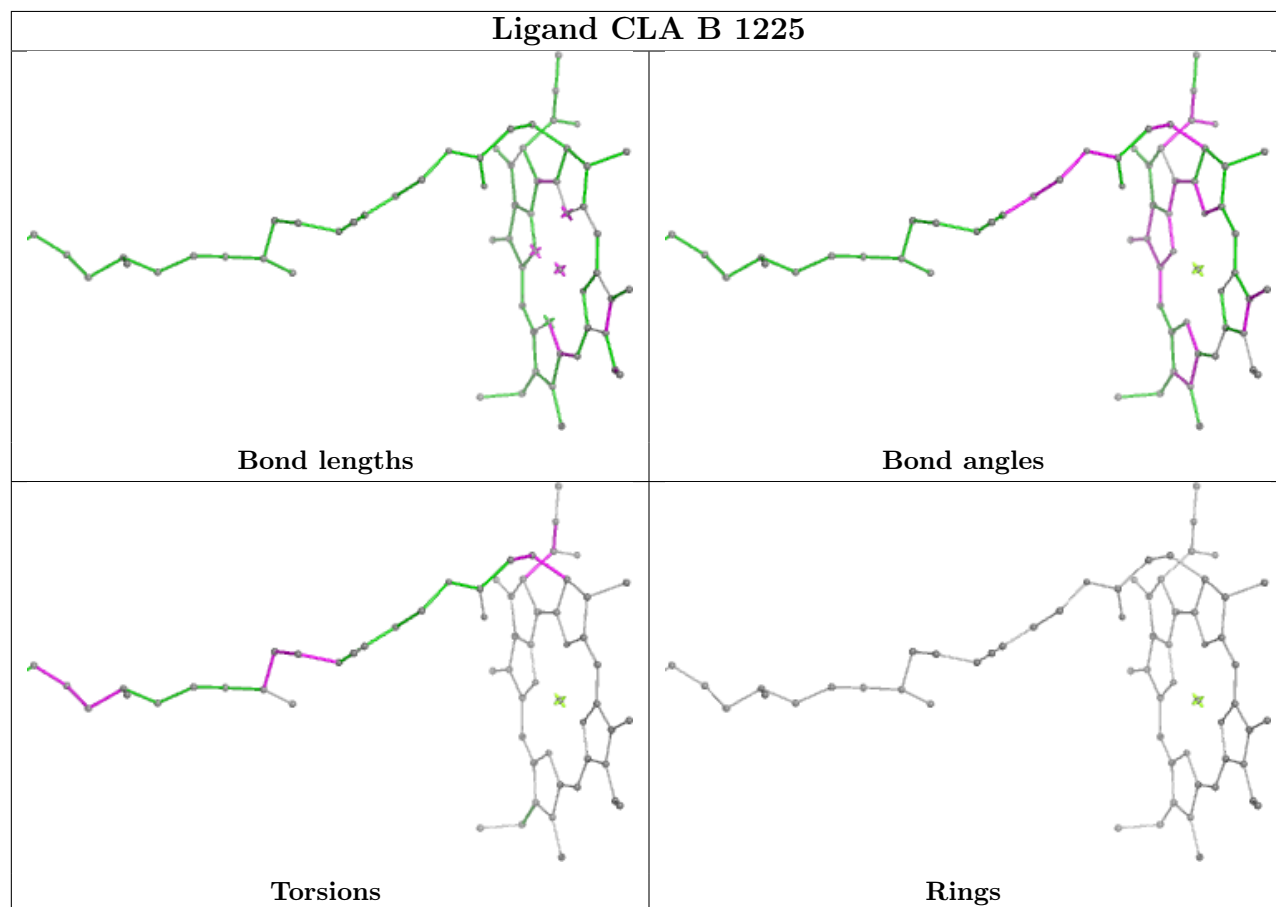
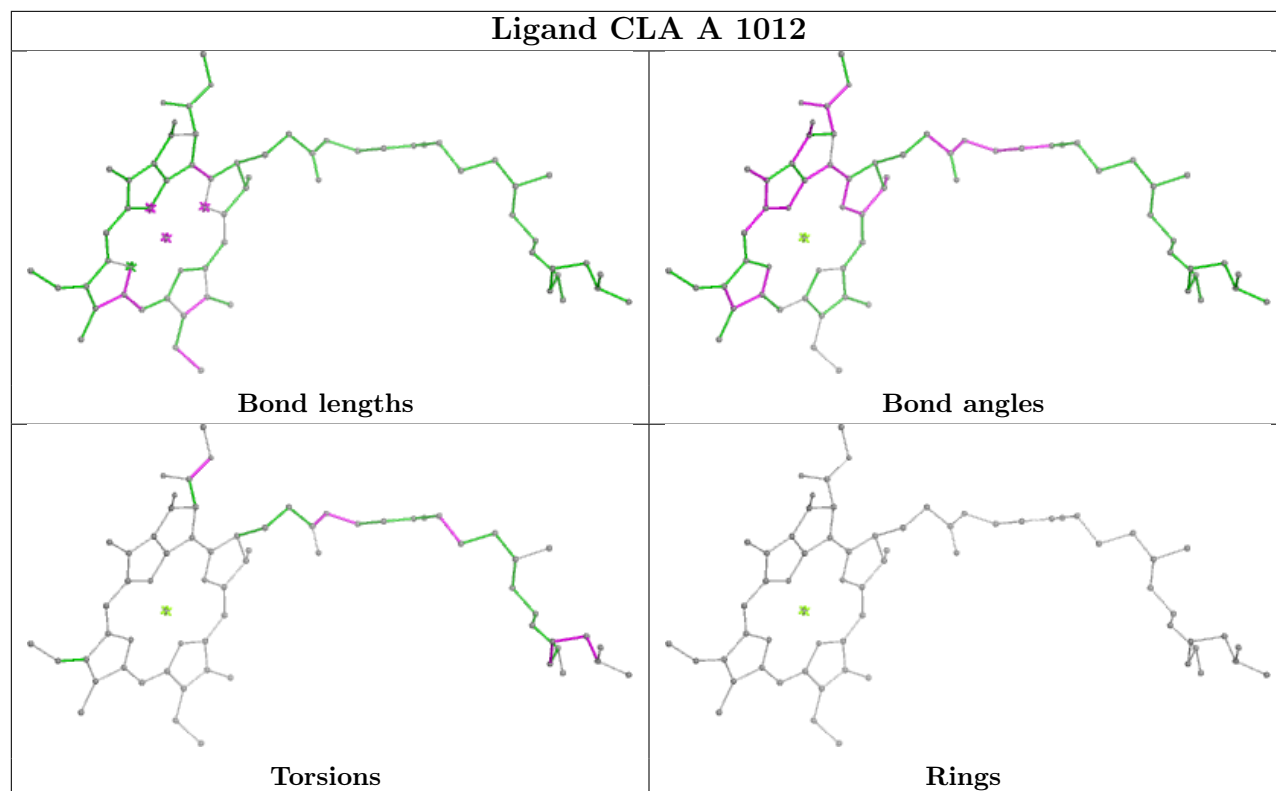


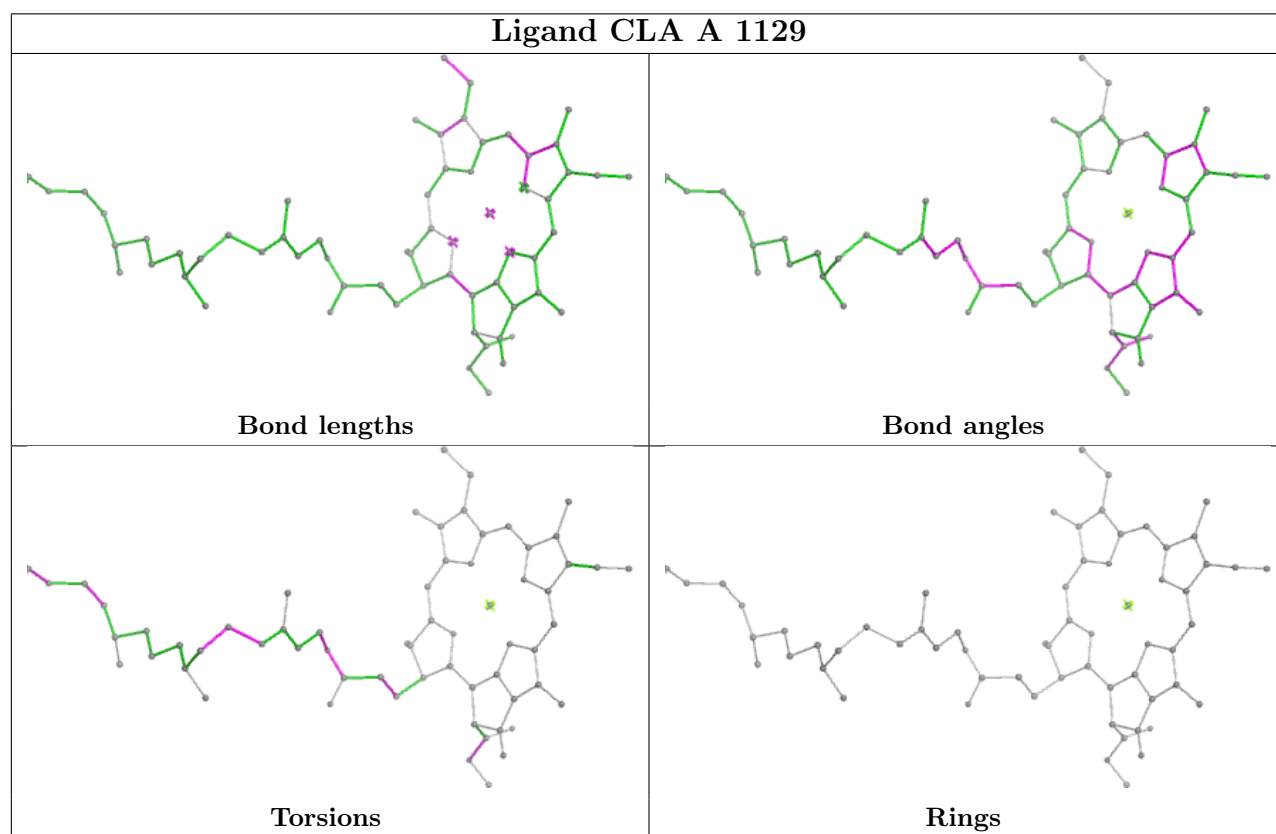
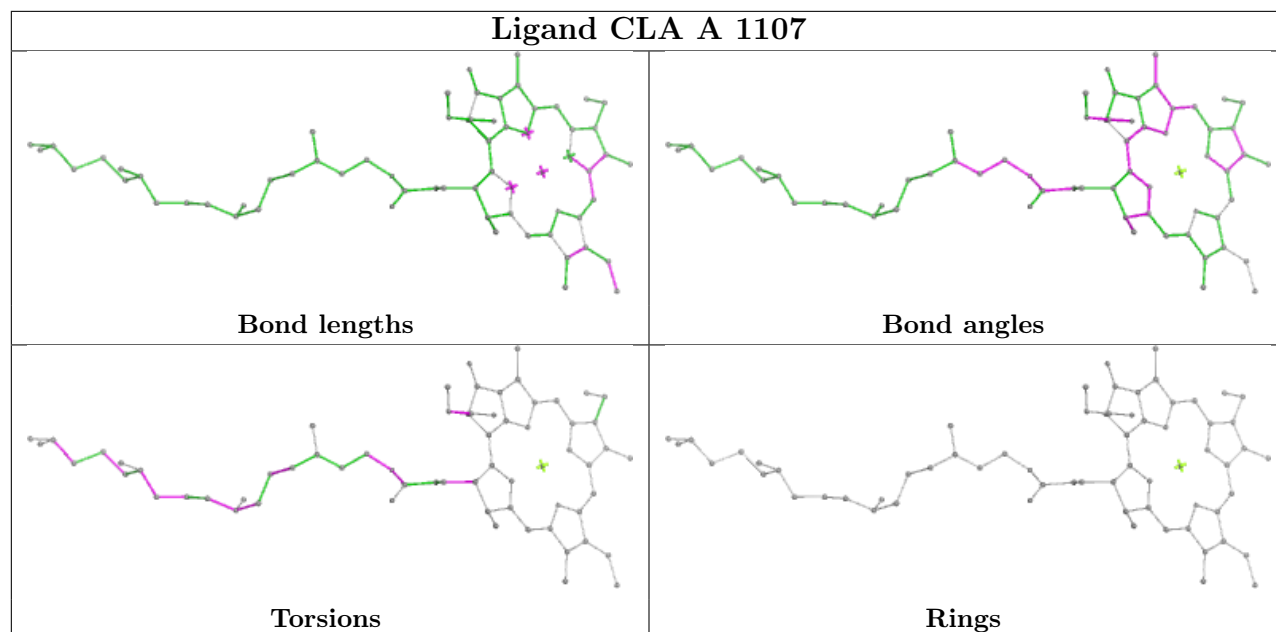




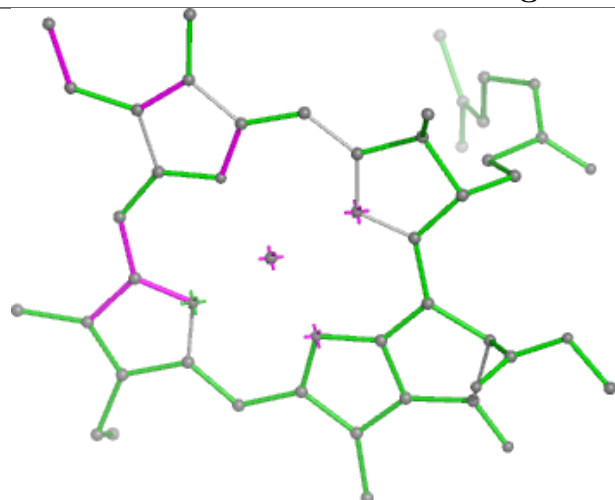




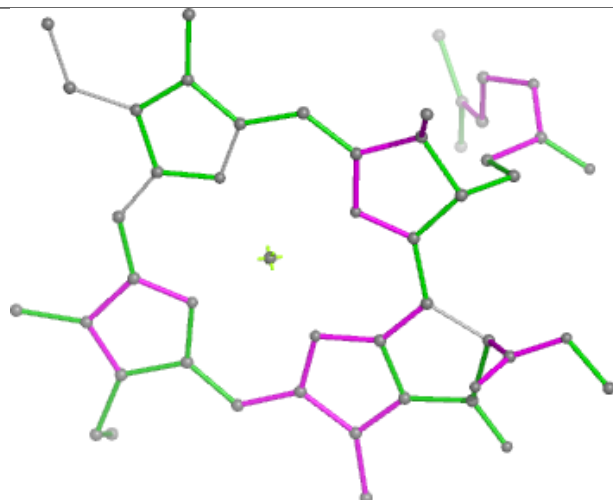




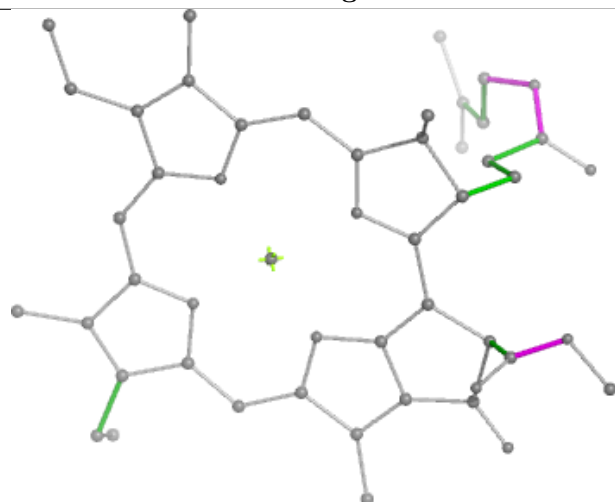
Ligand CLA 1 606



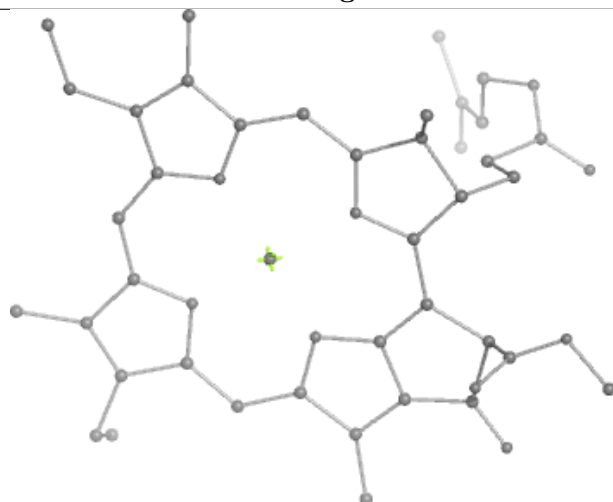
Bond lengths



Bond angles

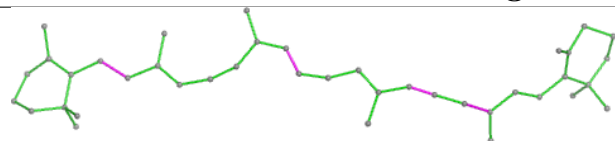


Torsions

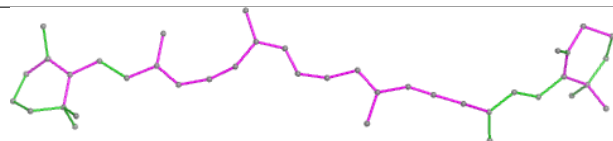


Rings

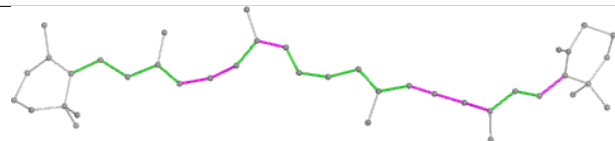
Ligand BCR B 4004



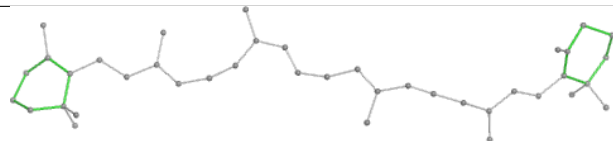
Bond lengths



Bond angles

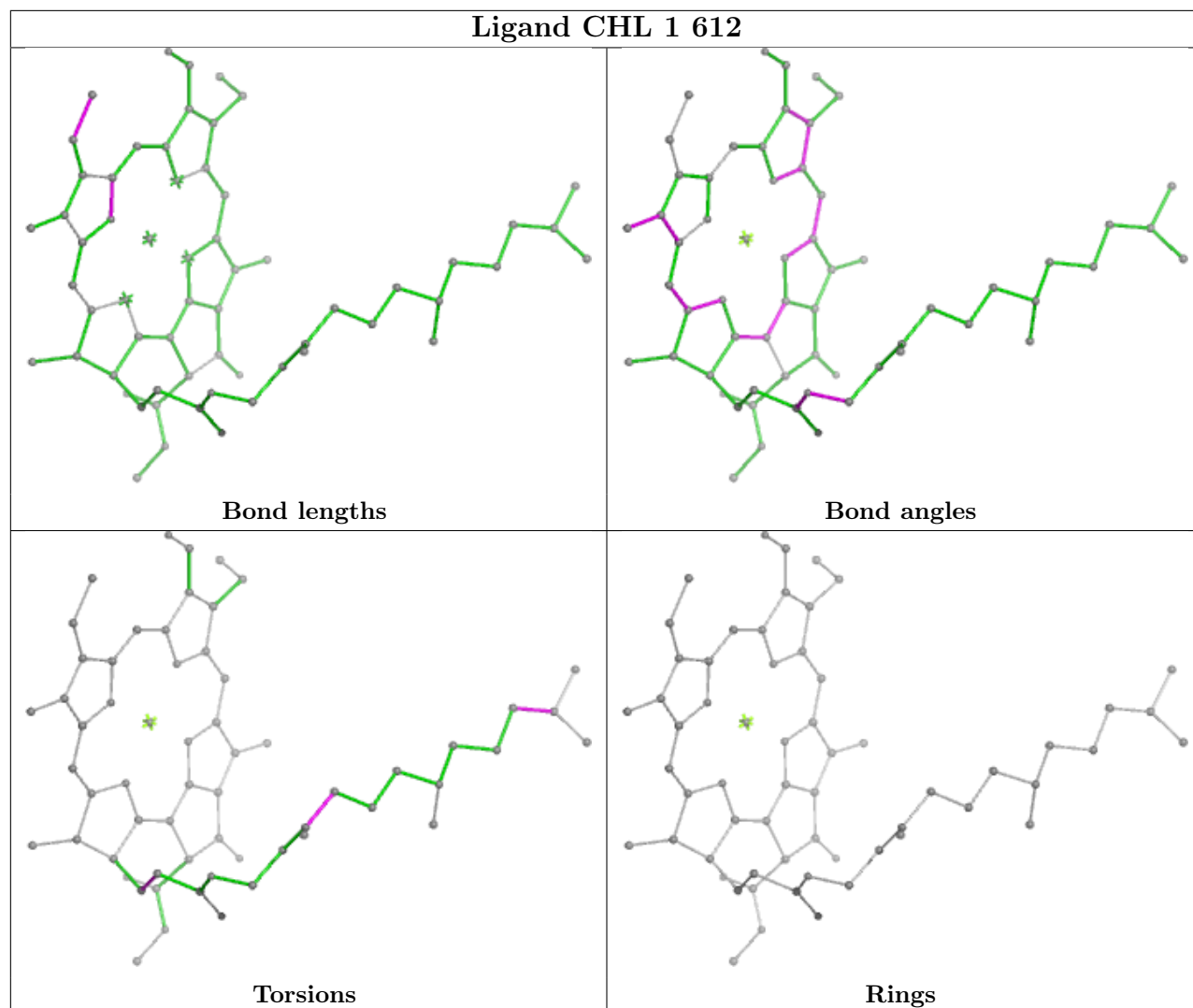


Torsions

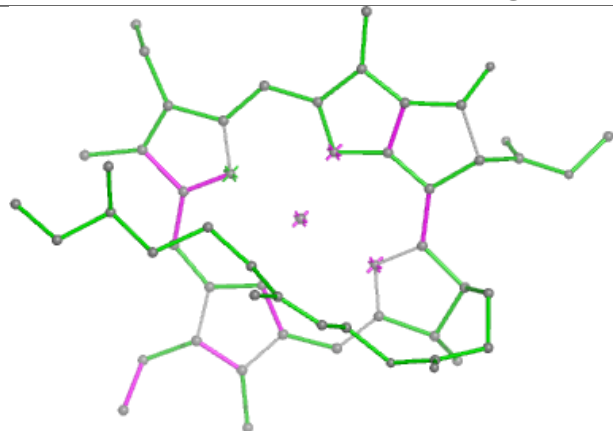


Rings

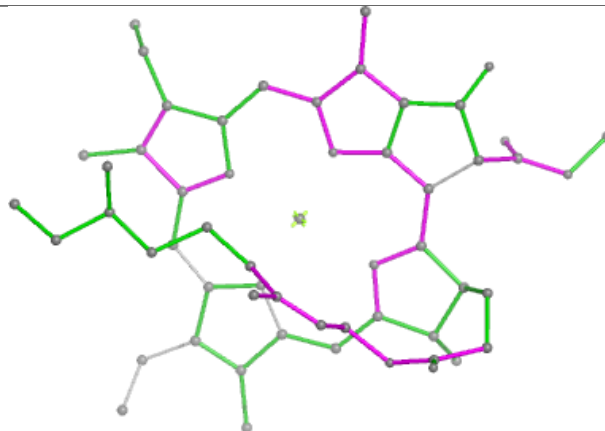
Ligand CHL 1 612



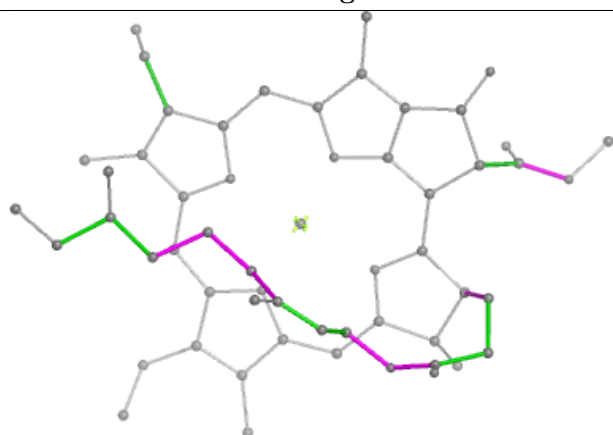
Ligand CLA A 1116



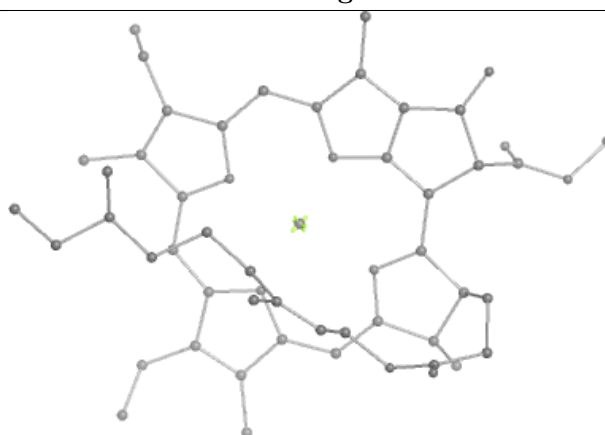
Bond lengths



Bond angles

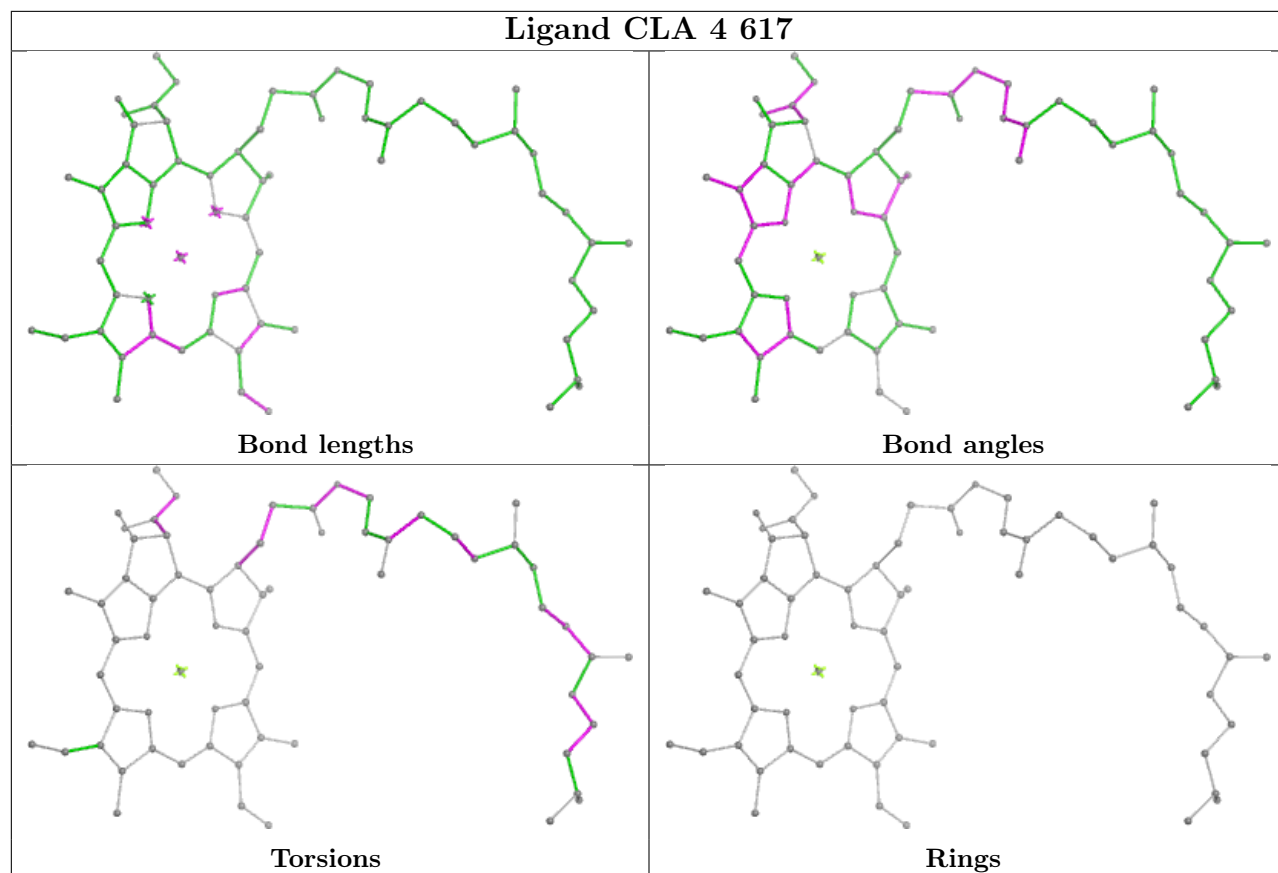


Torsions

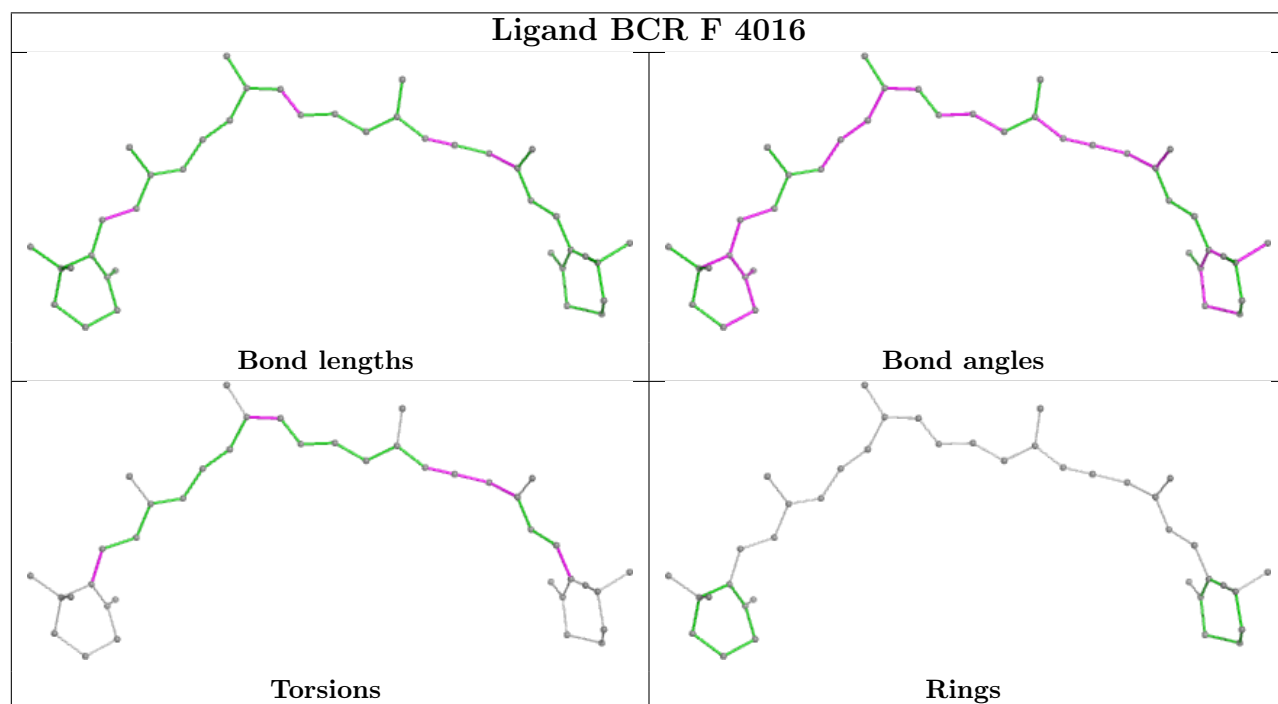


Rings

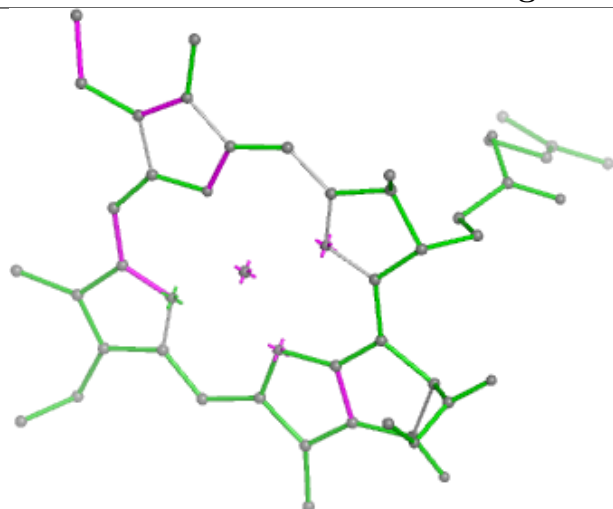
Ligand CLA 4 617



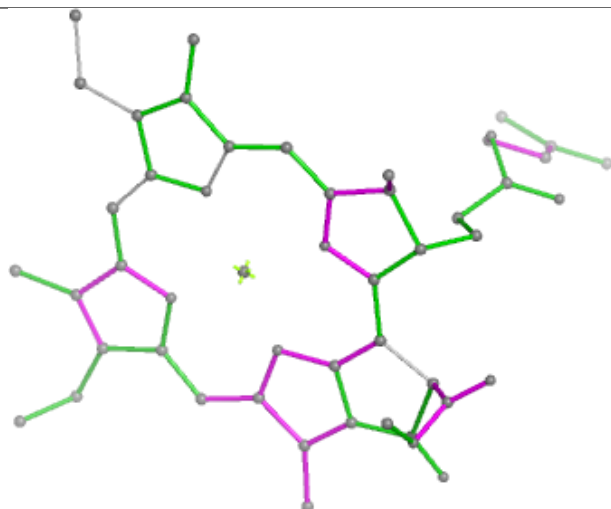
Ligand BCR F 4016



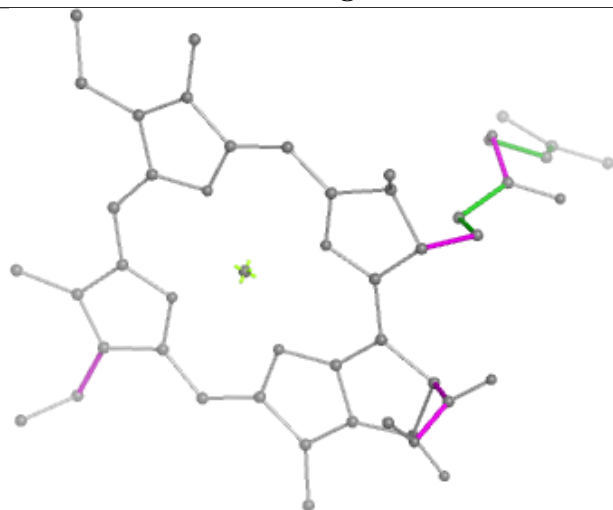
Ligand CLA 3 606



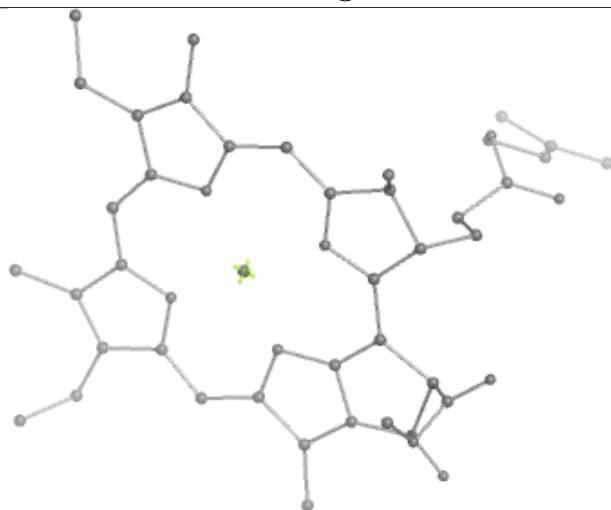
Bond lengths



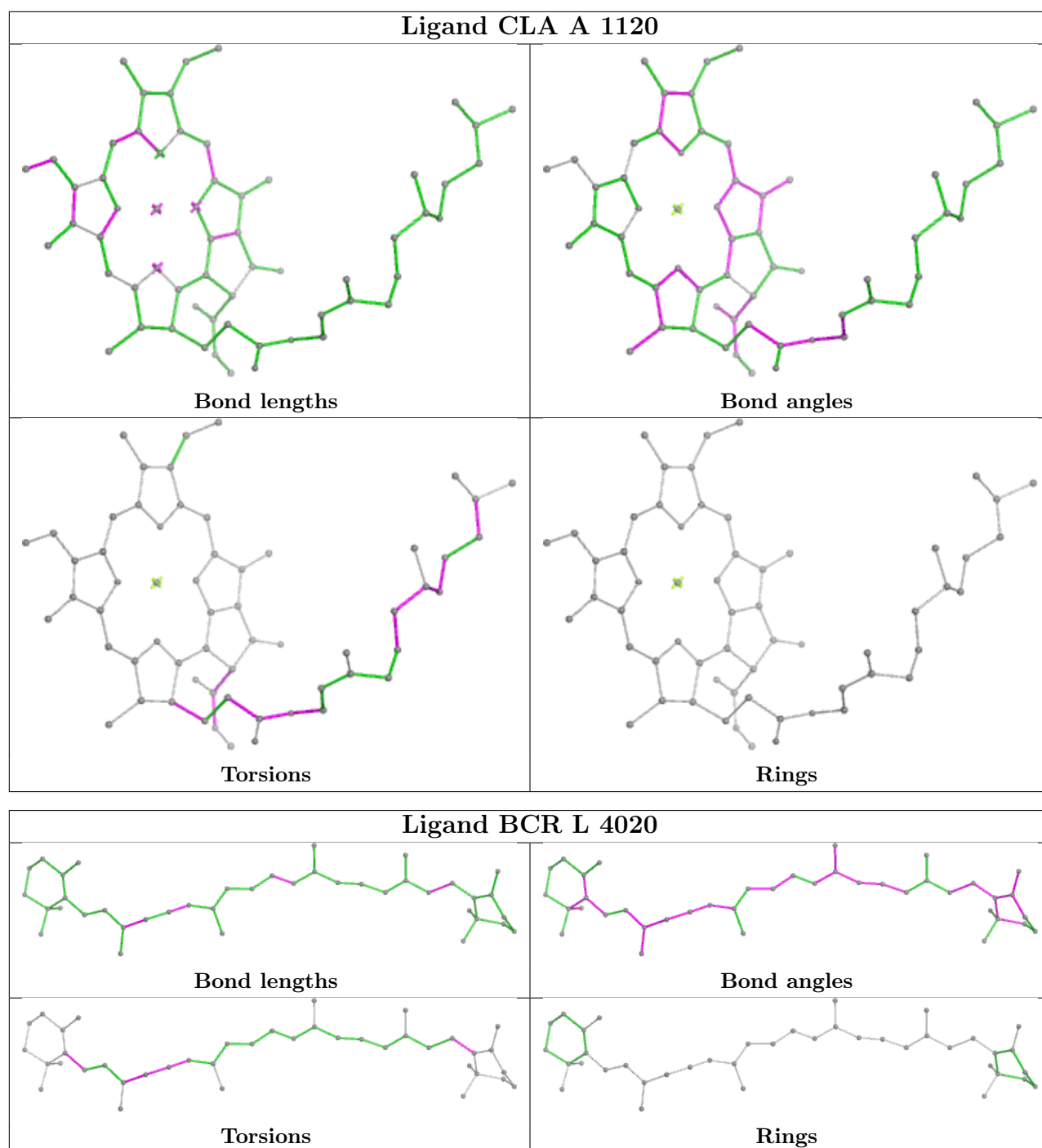
Bond angles

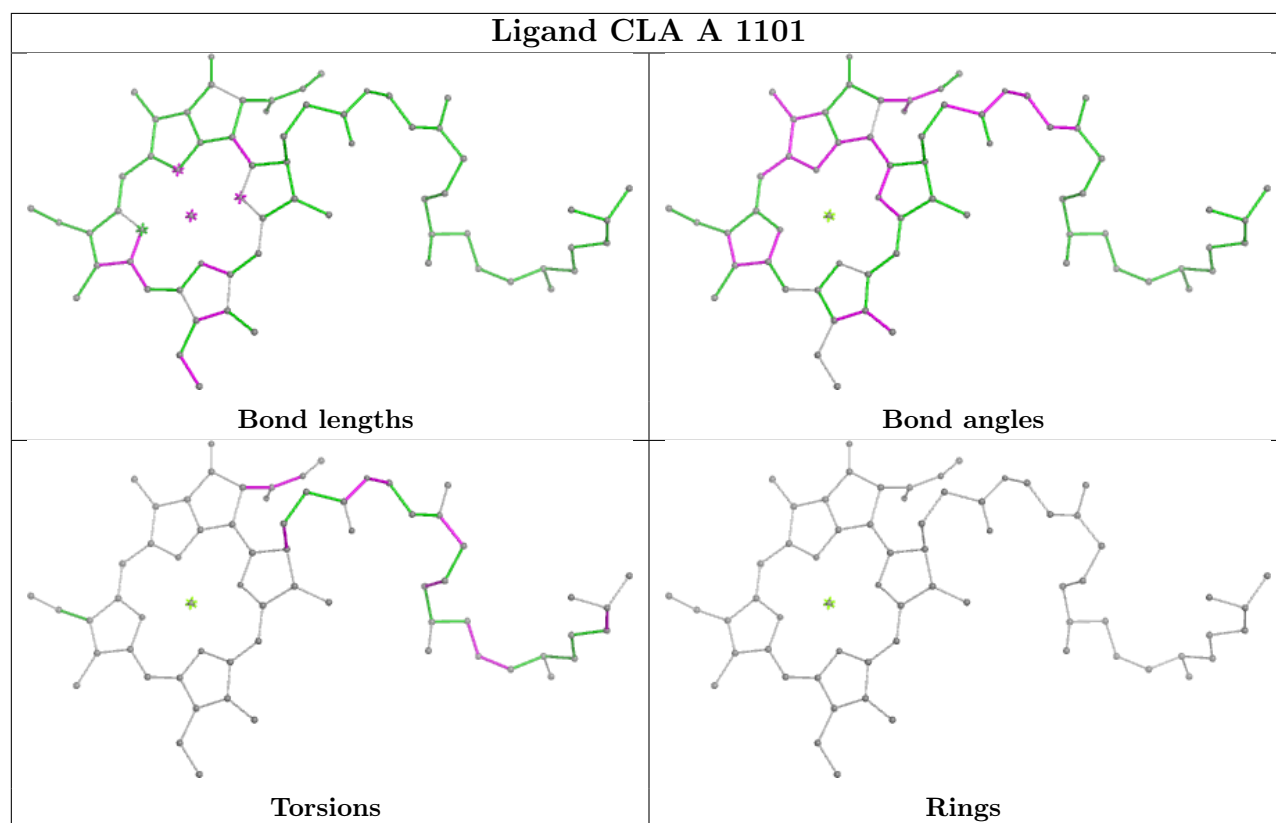
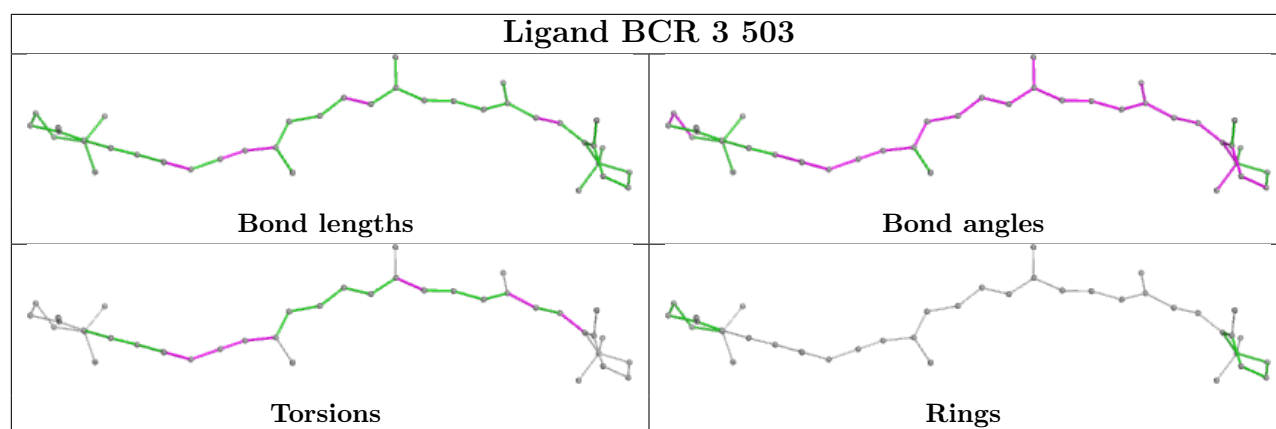


Torsions

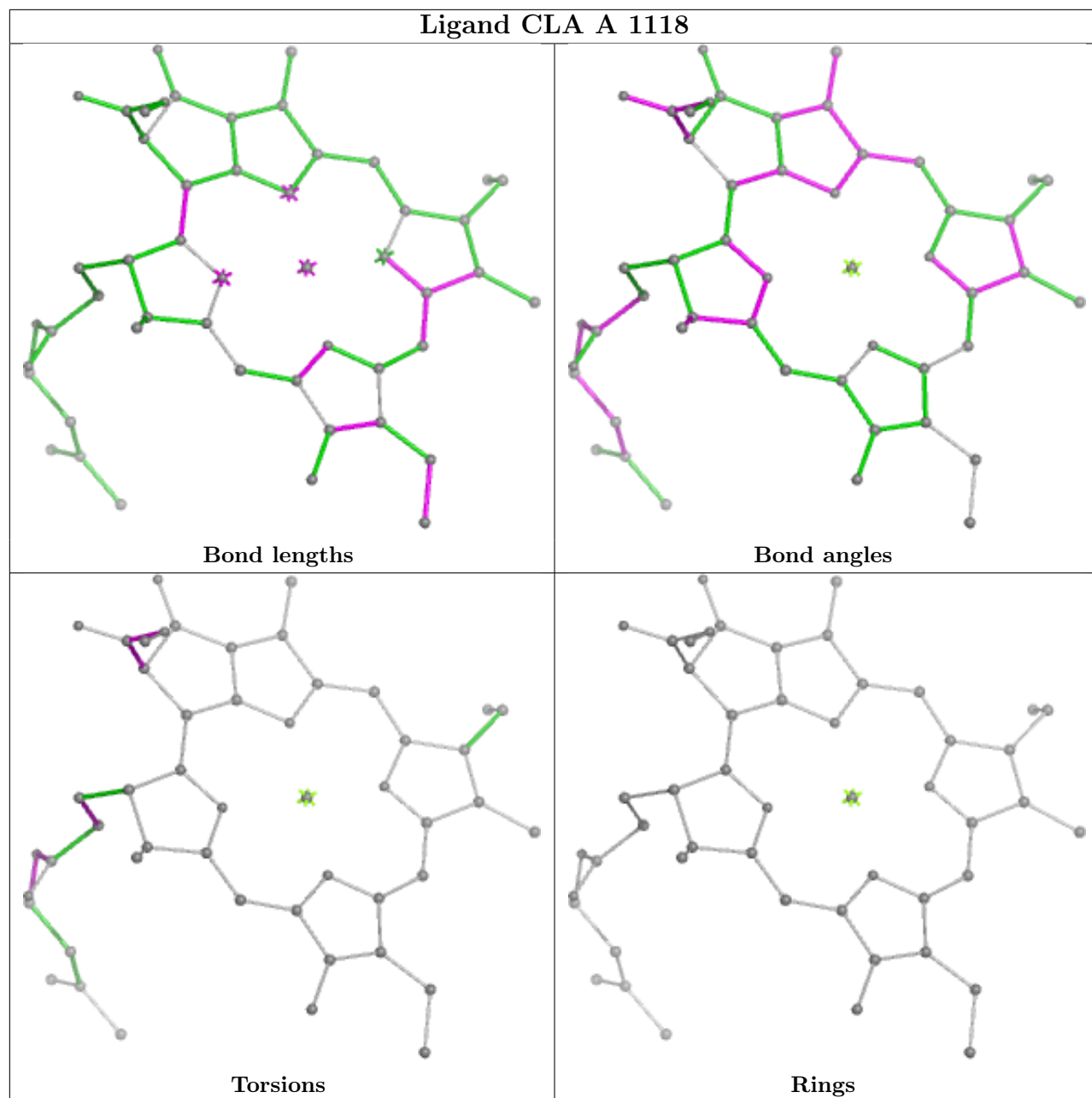


Rings

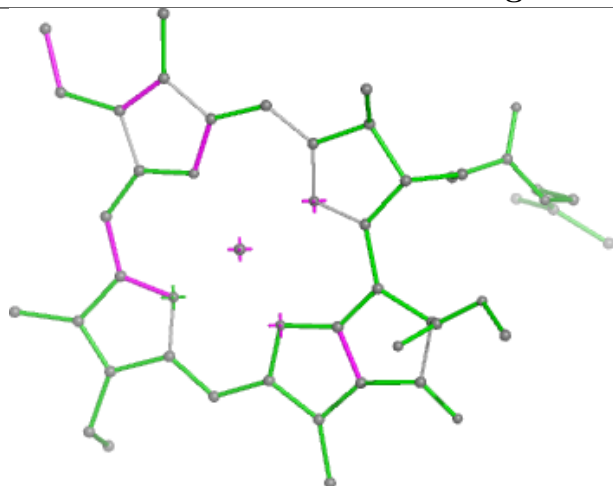




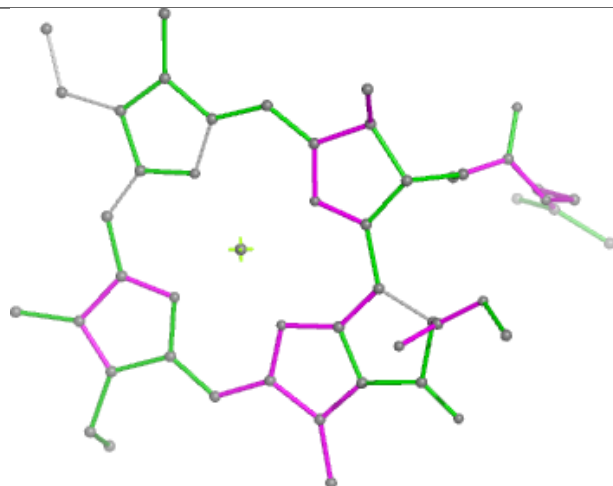
Ligand CLA A 1118



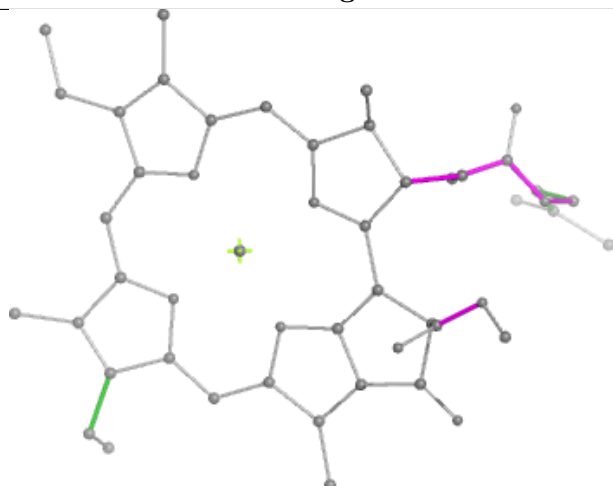
Ligand CLA B 1236



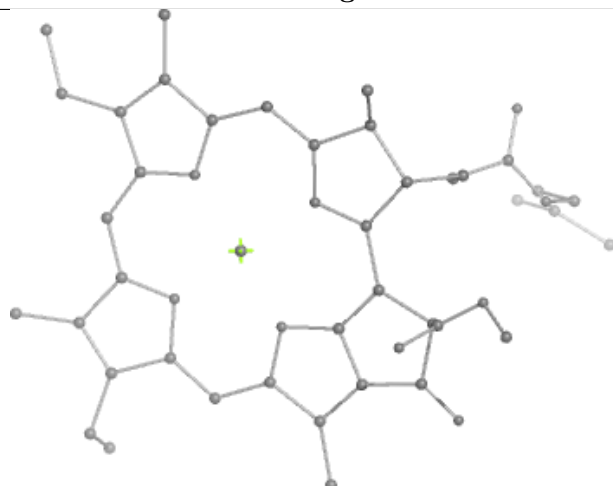
Bond lengths



Bond angles

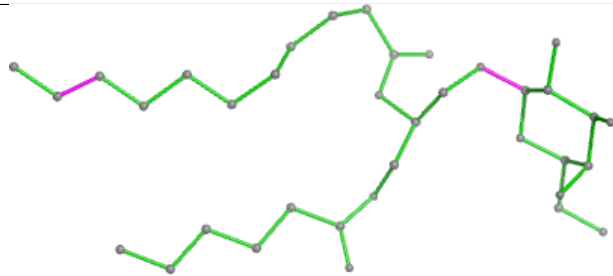


Torsions

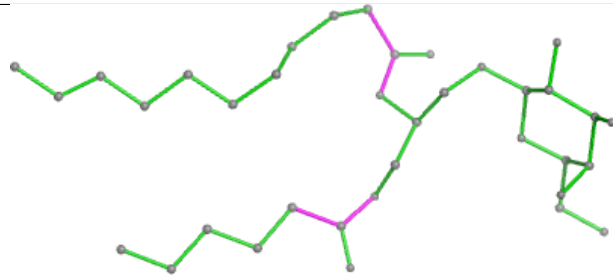


Rings

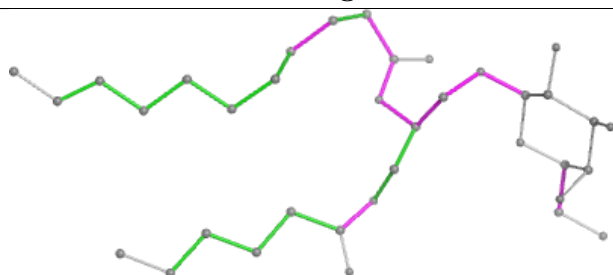
Ligand LMG 2 803



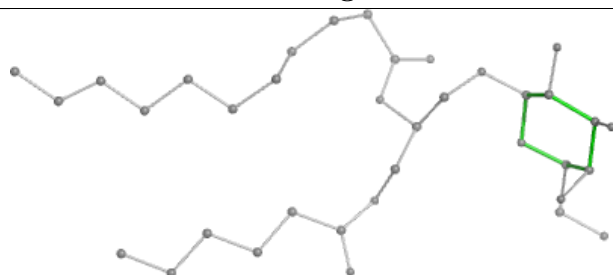
Bond lengths



Bond angles

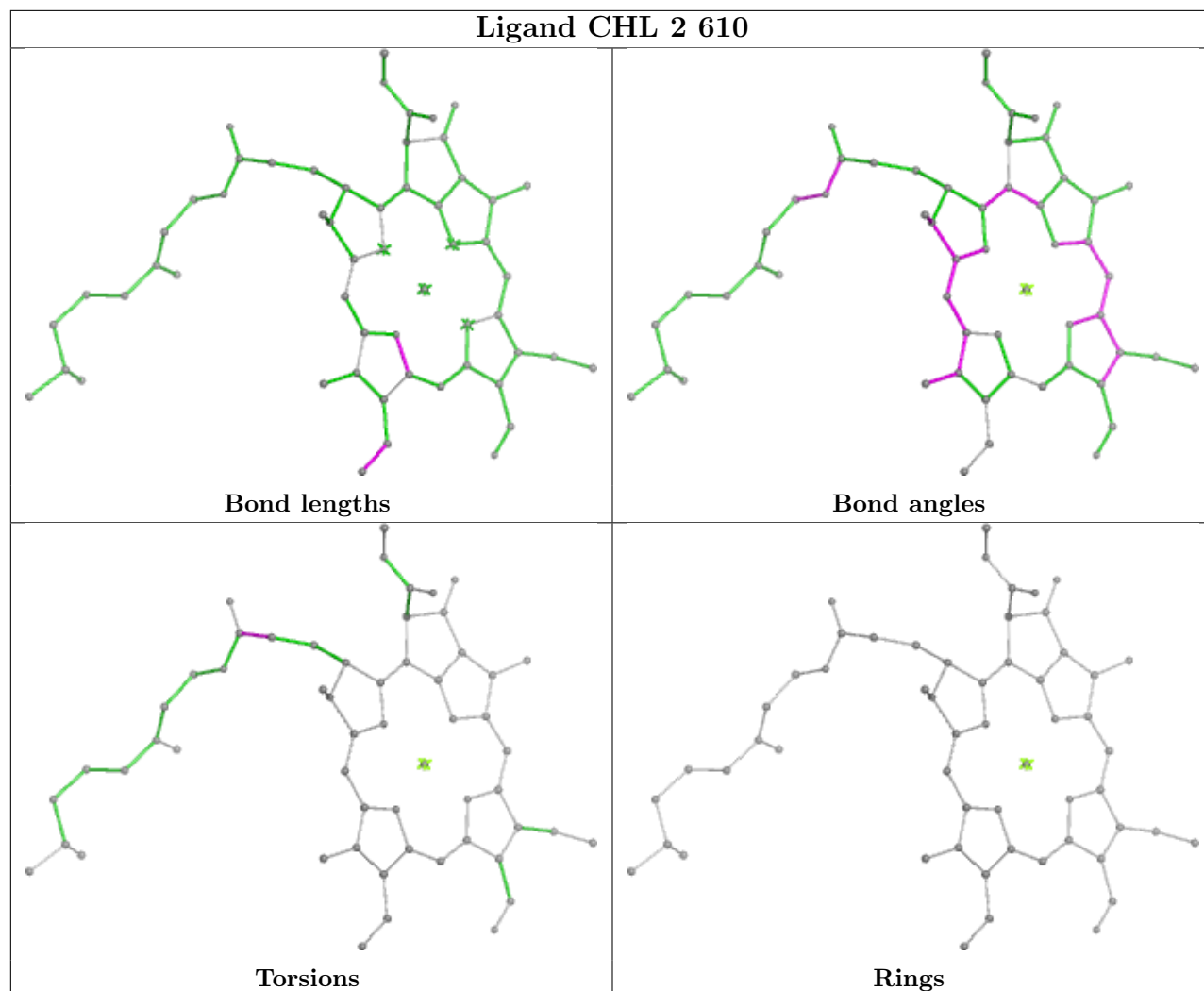


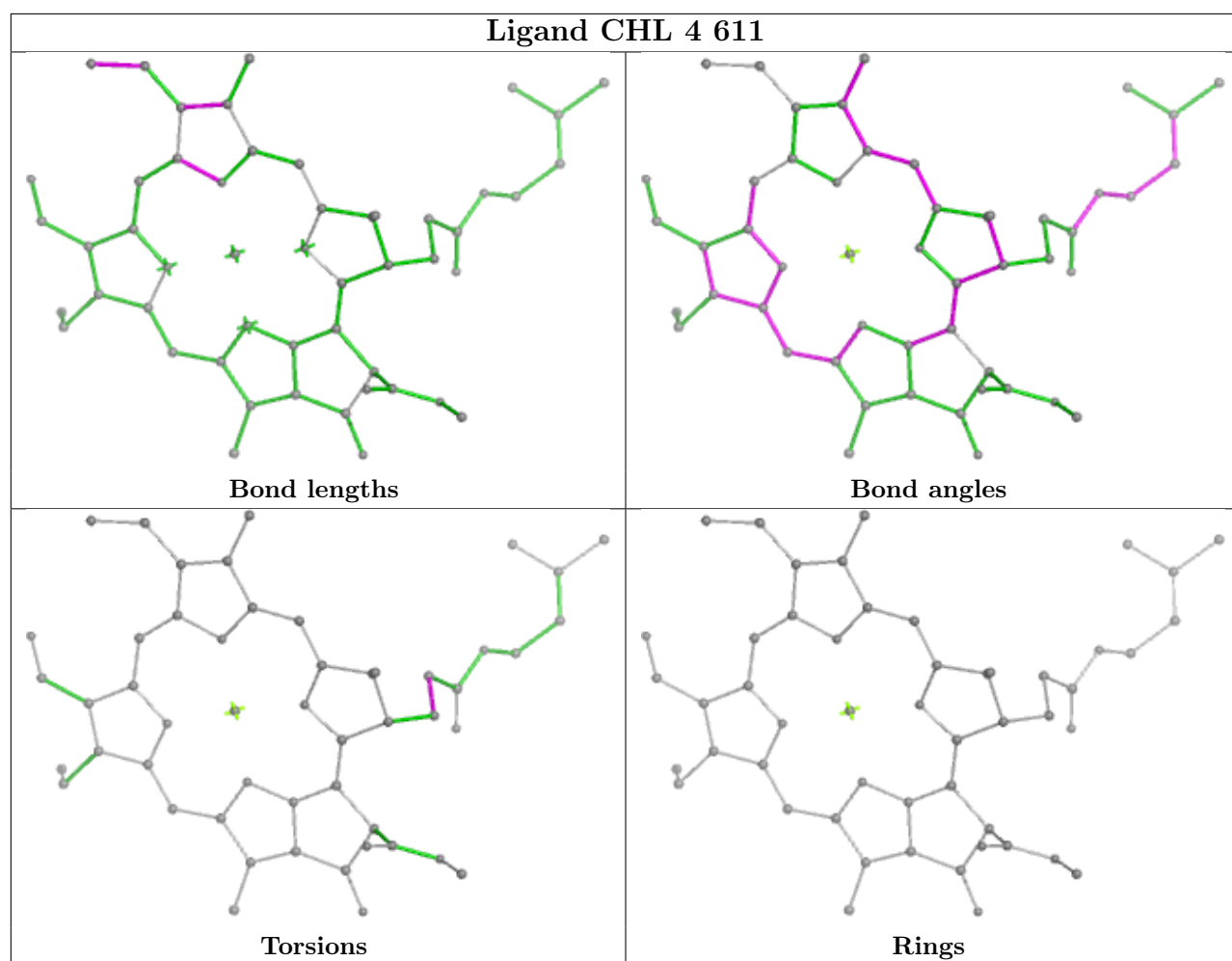
Torsions

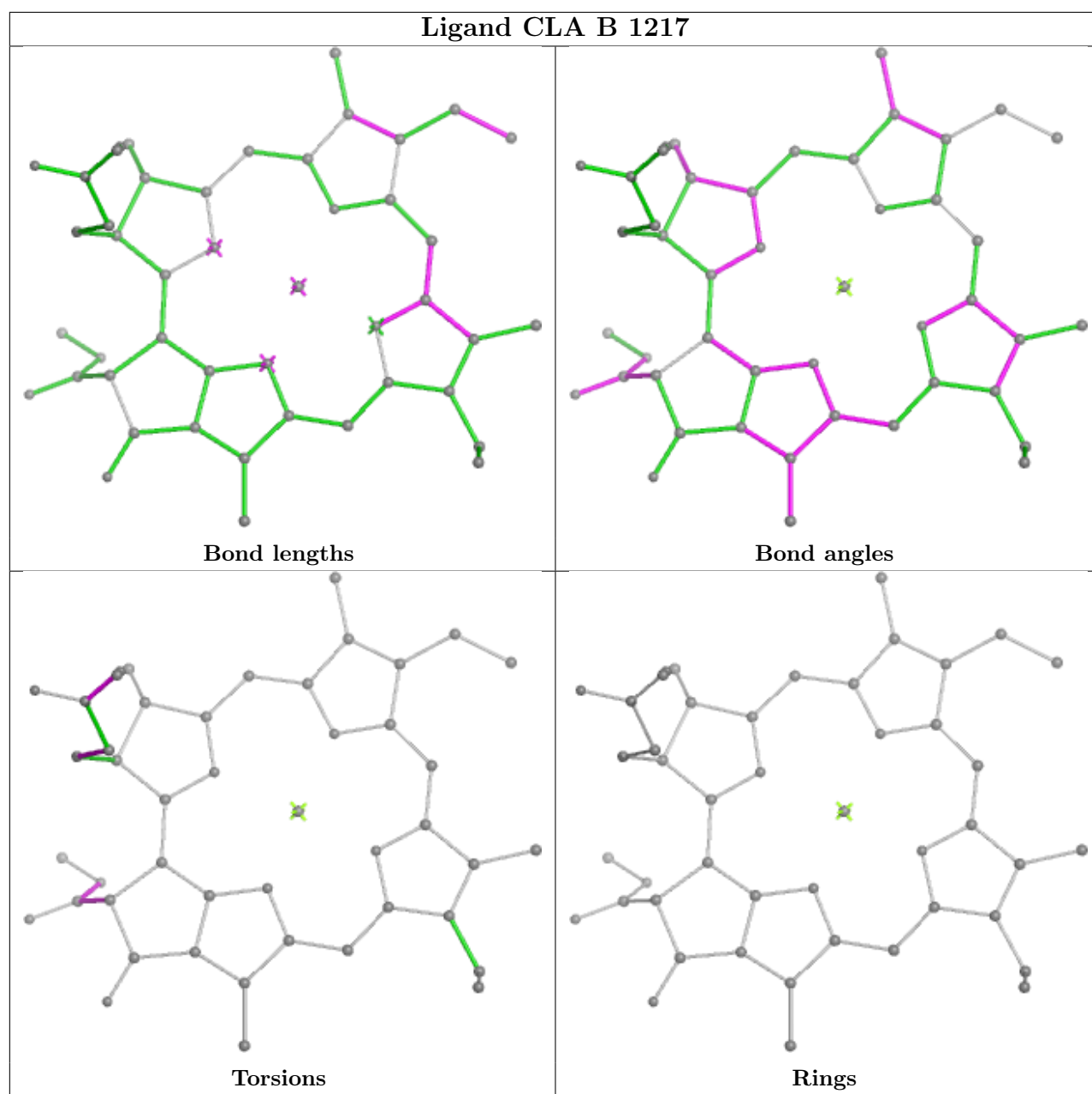


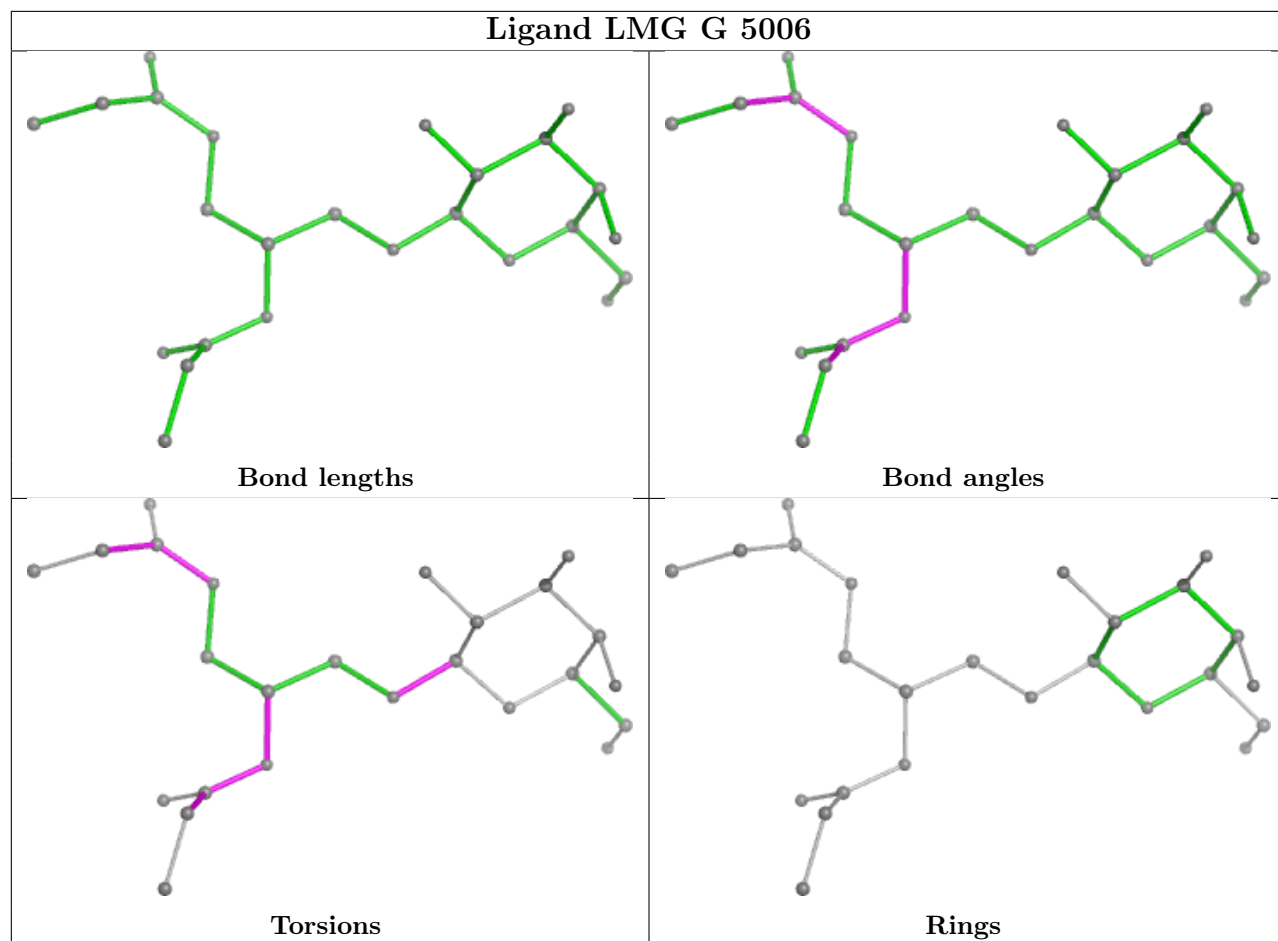
Rings

Ligand CHL 2 610

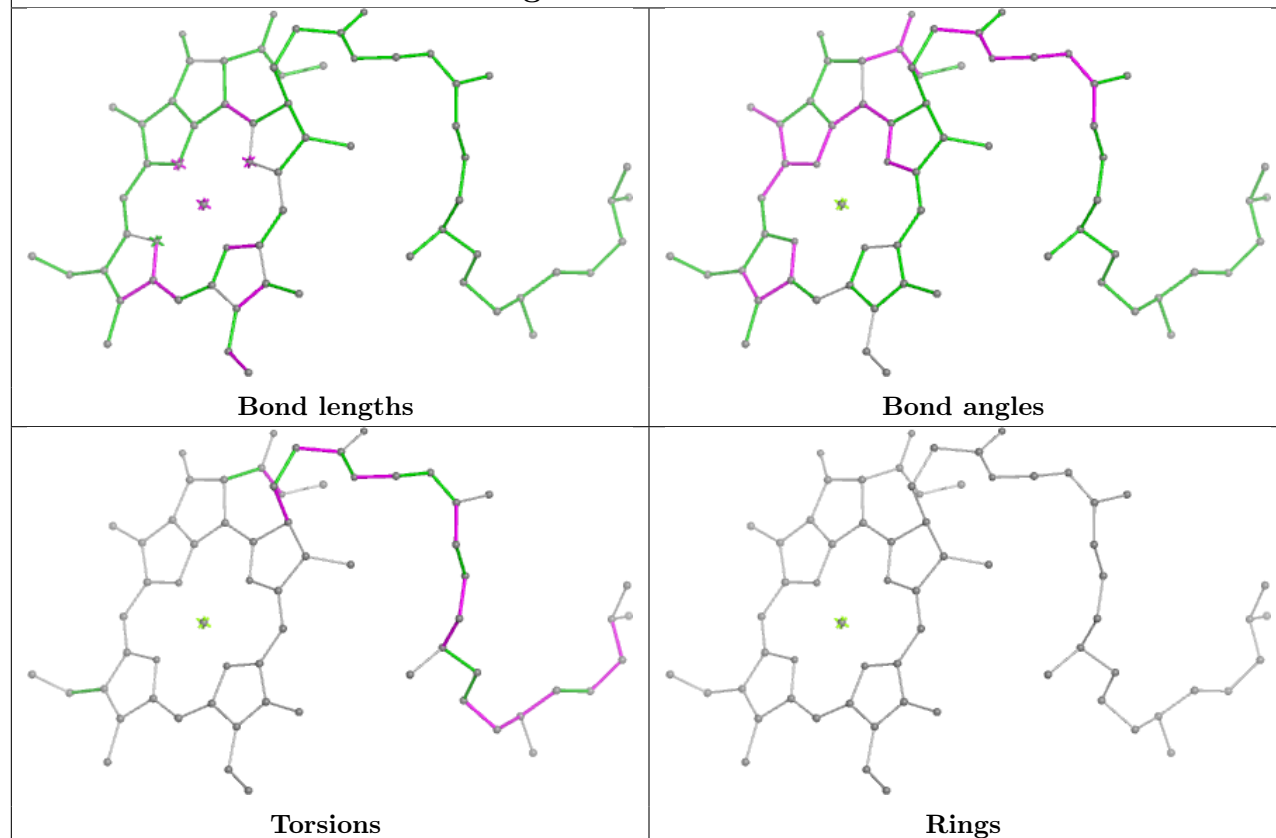




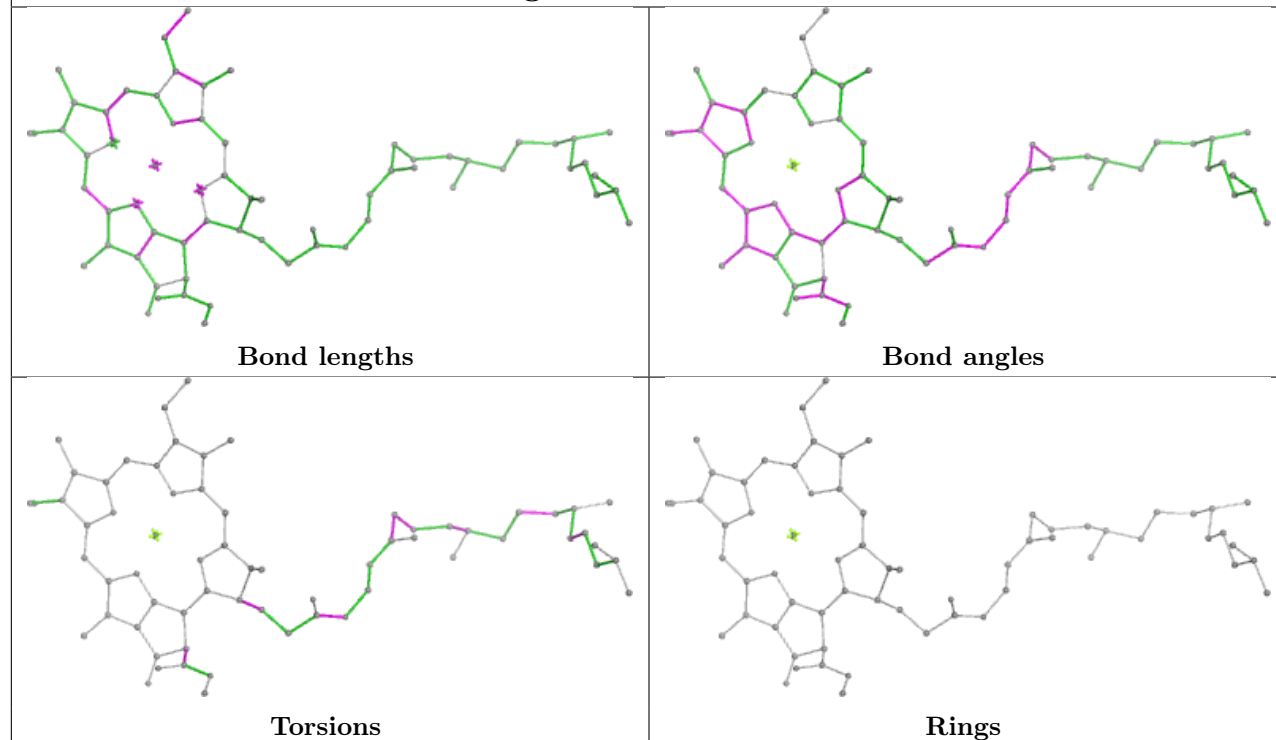


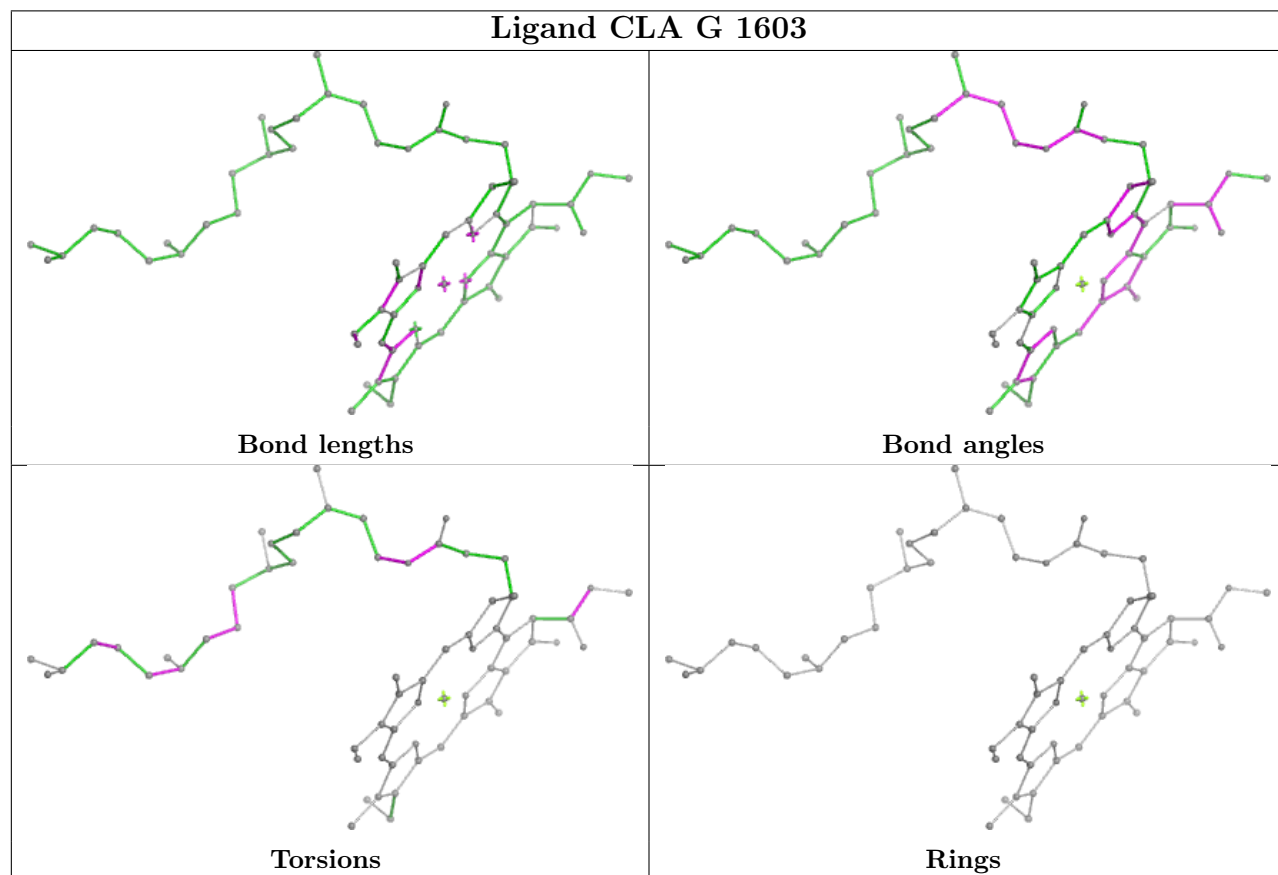
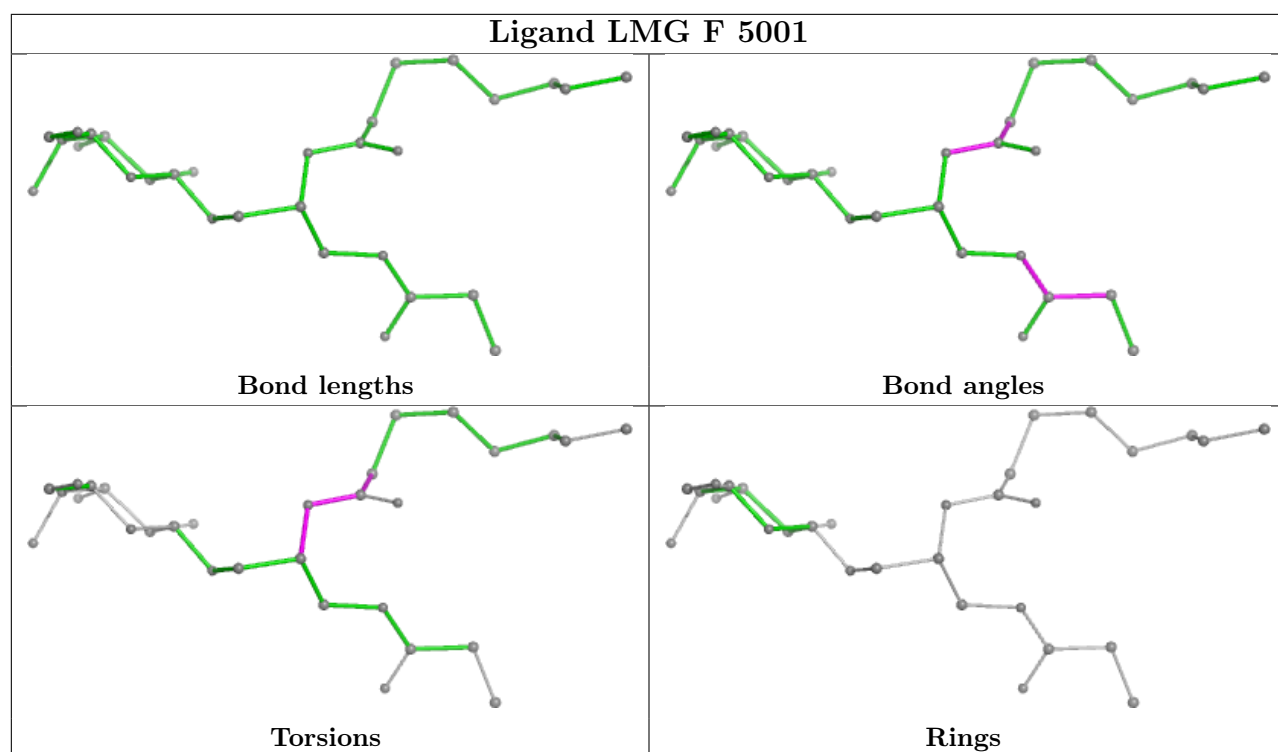


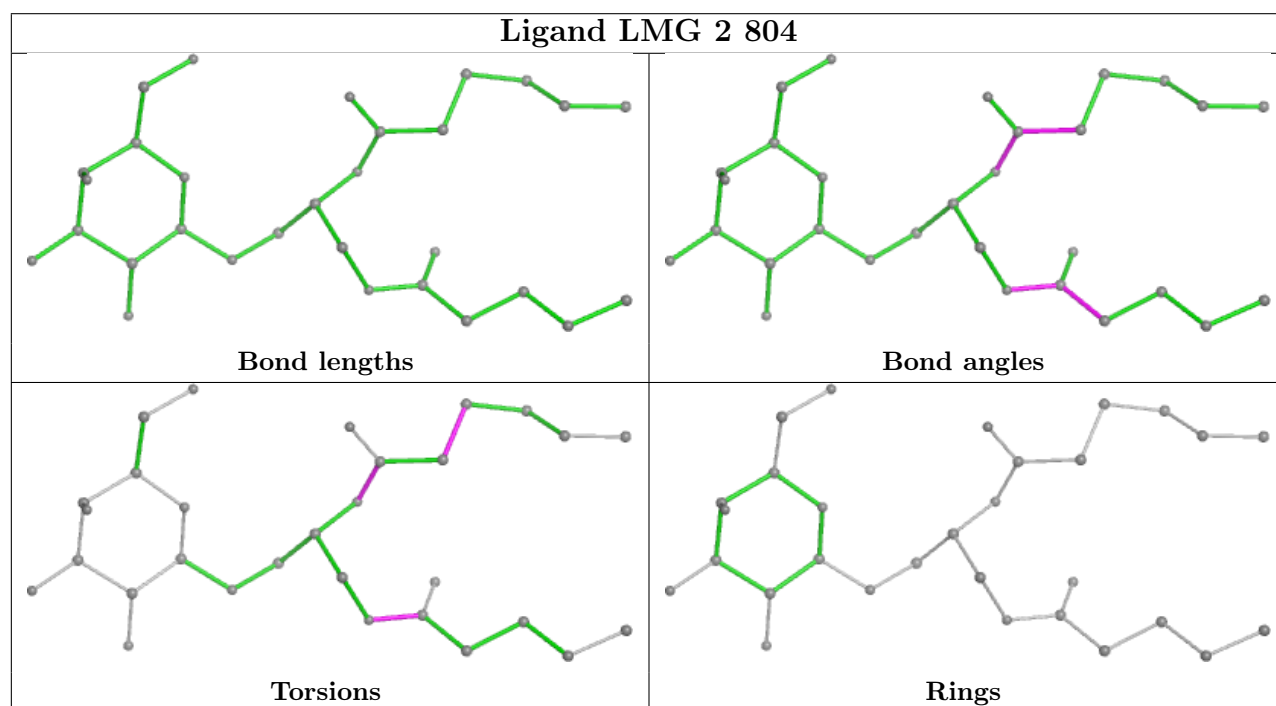
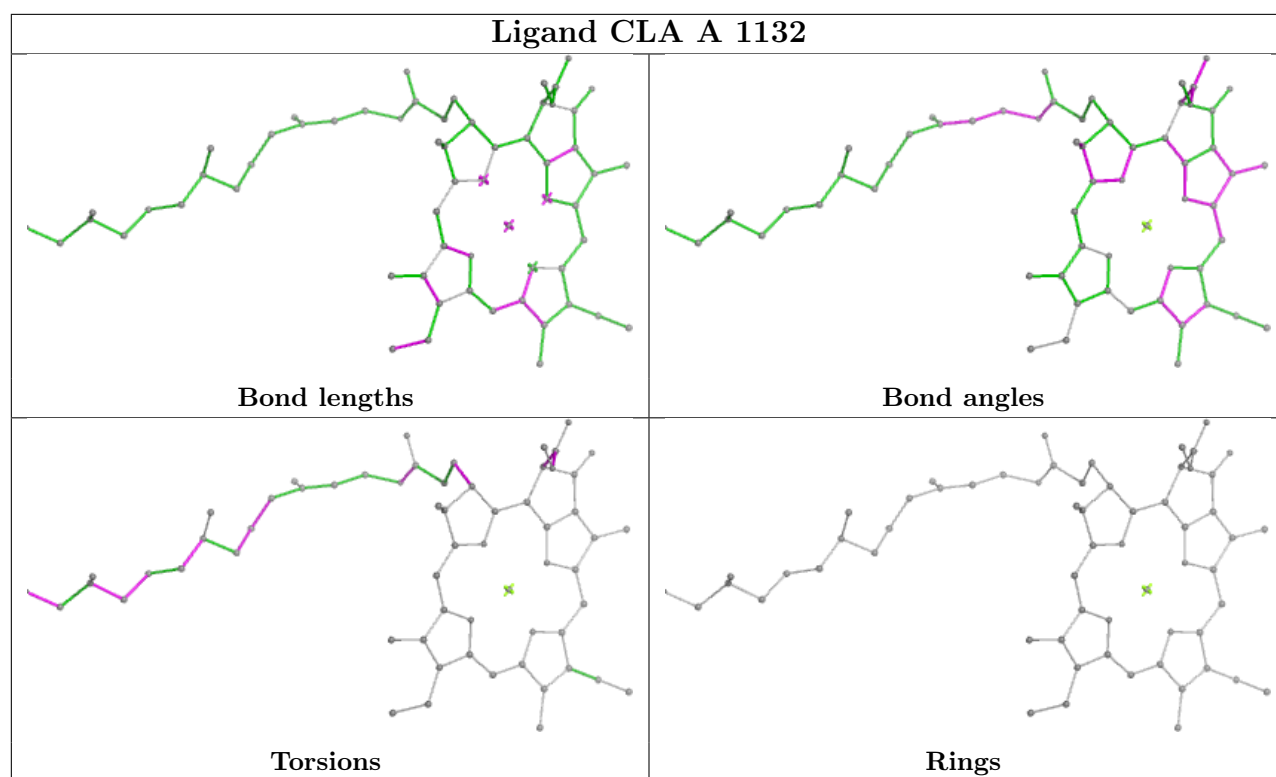
Ligand CLA B 1221



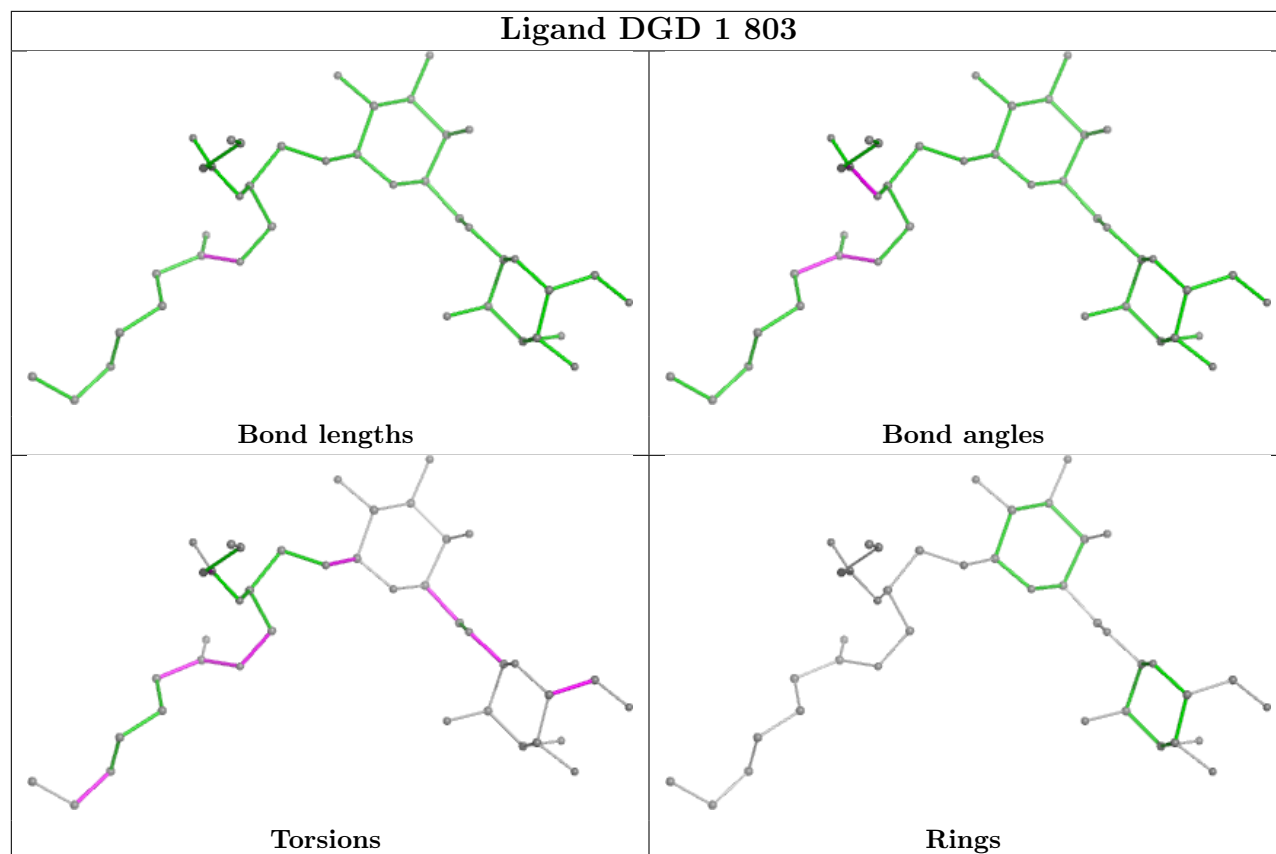
Ligand CLA B 1210



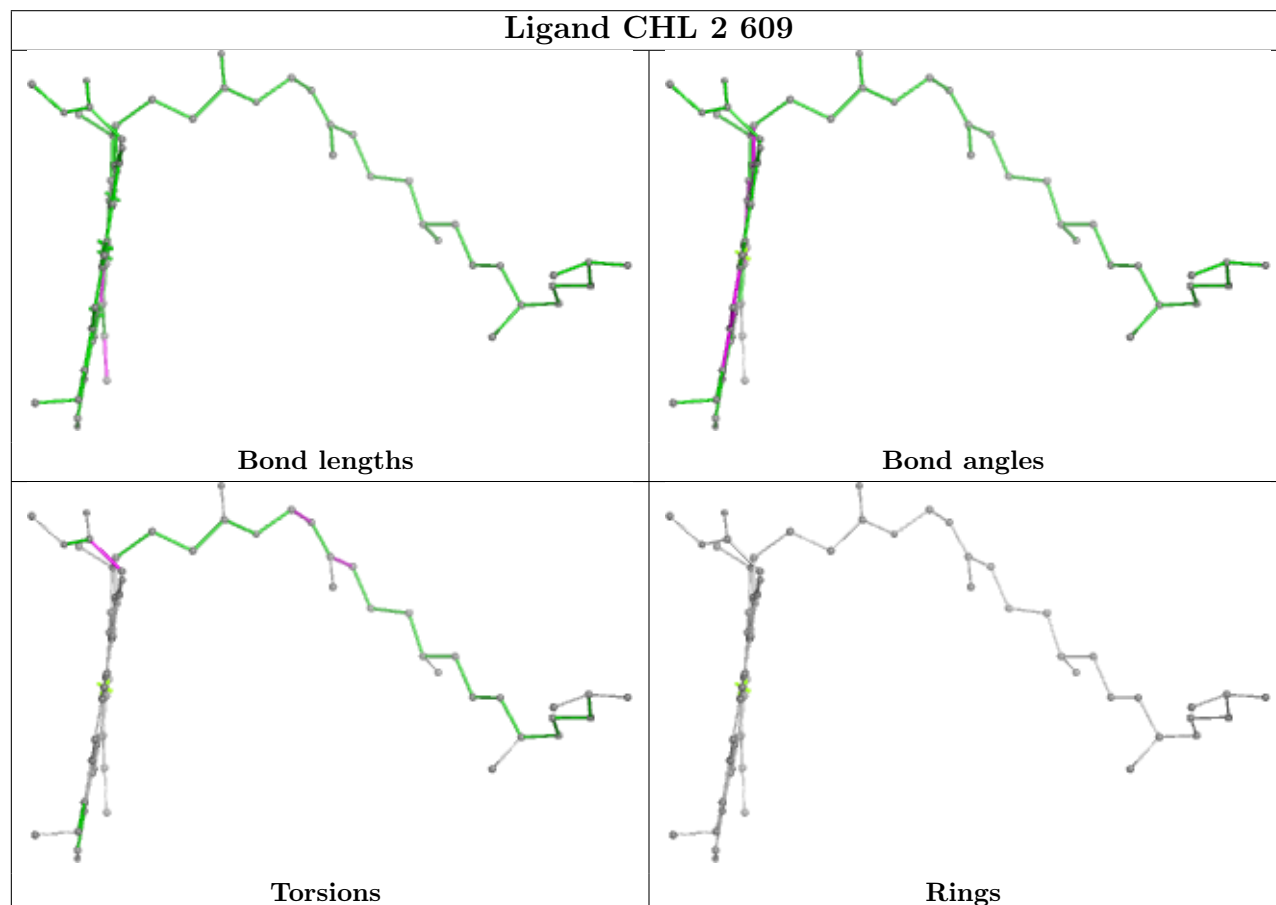


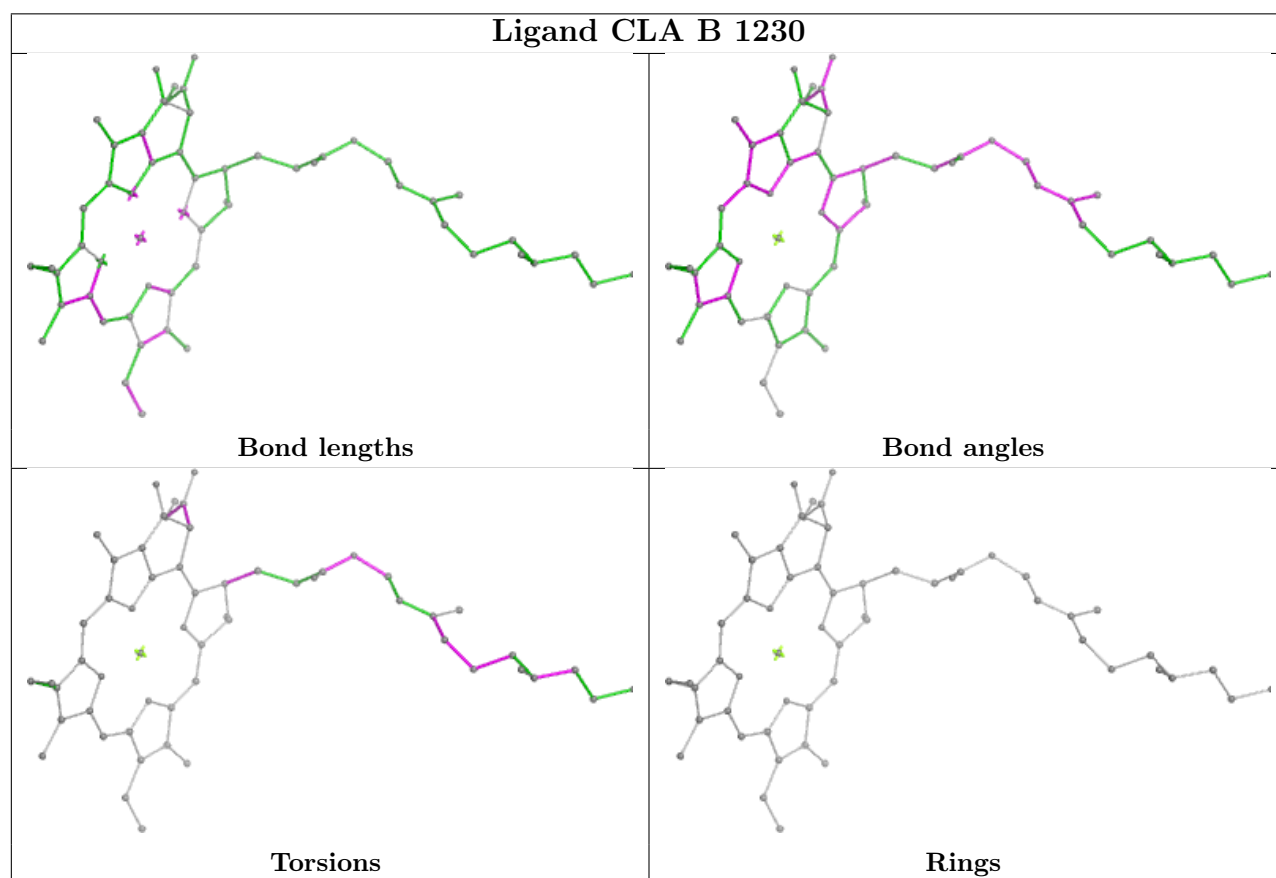
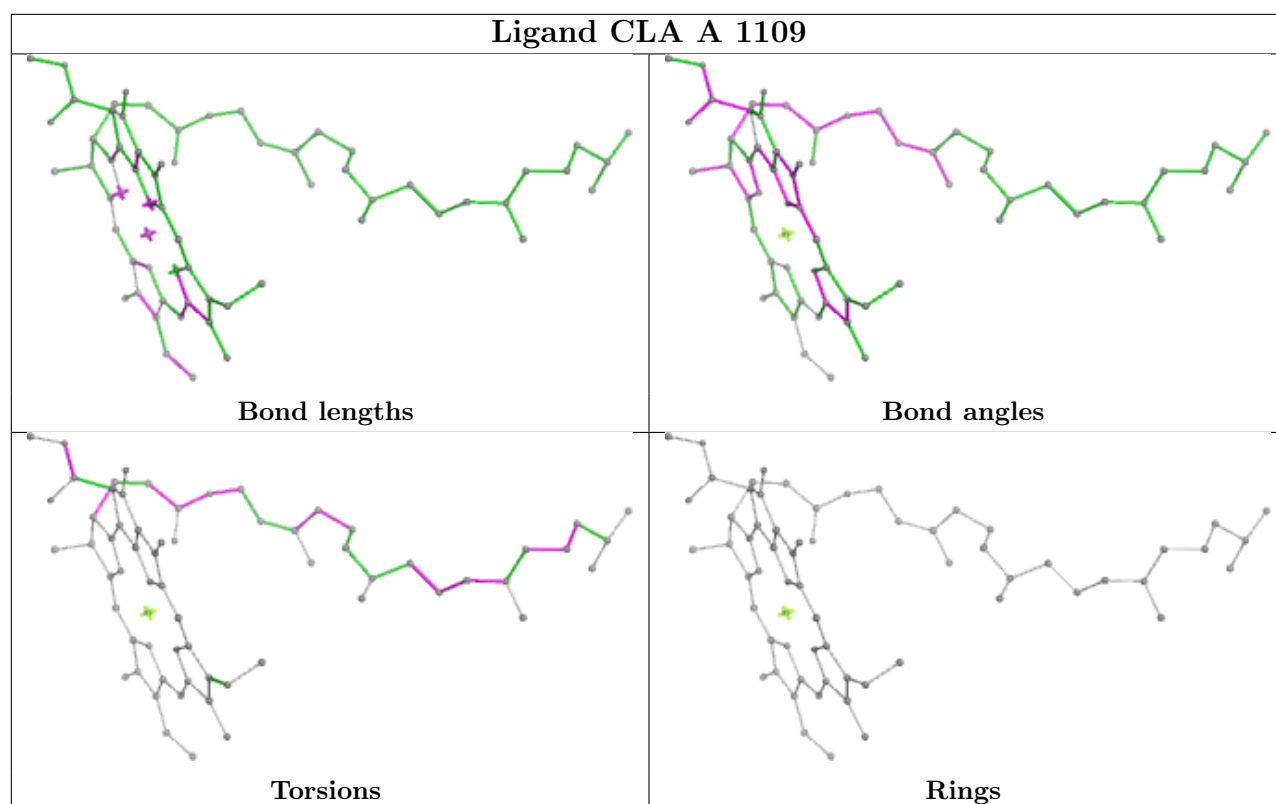


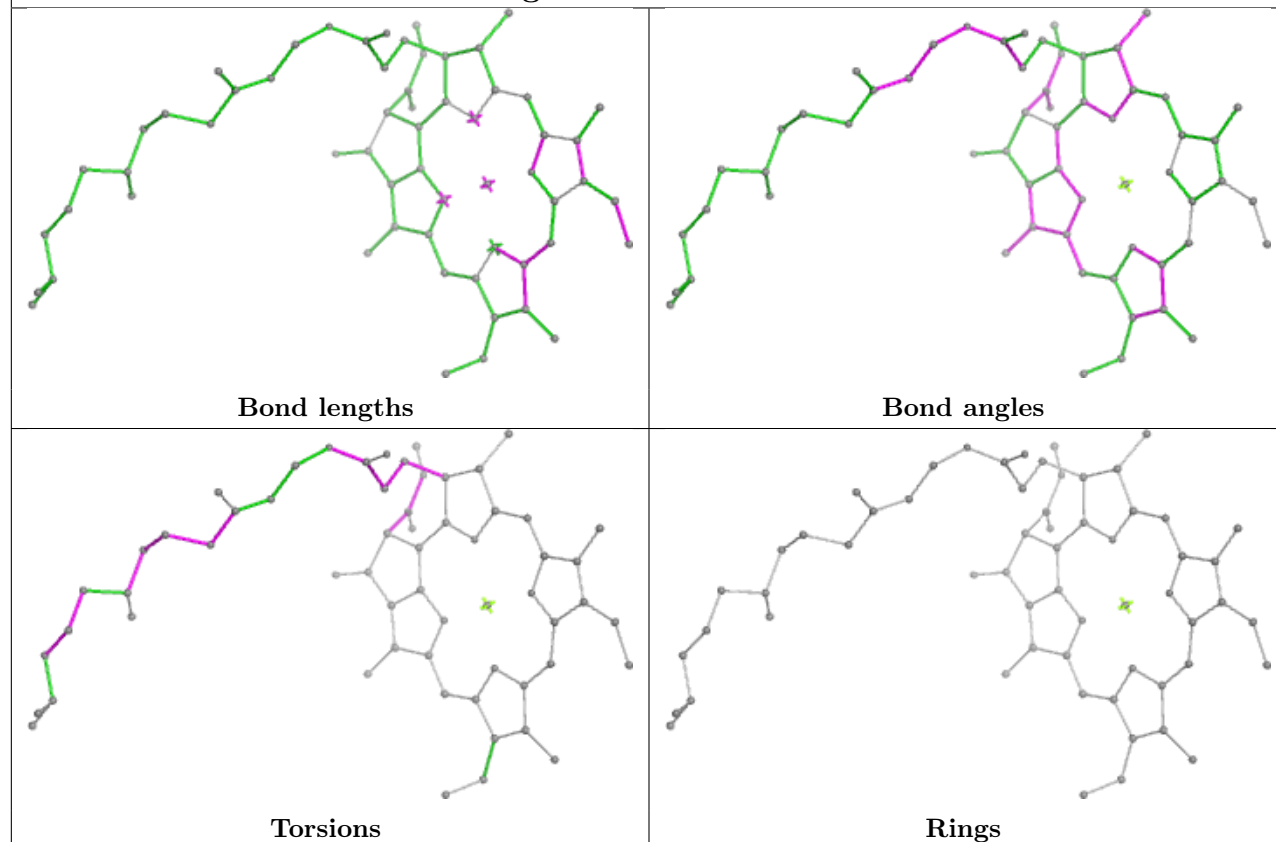
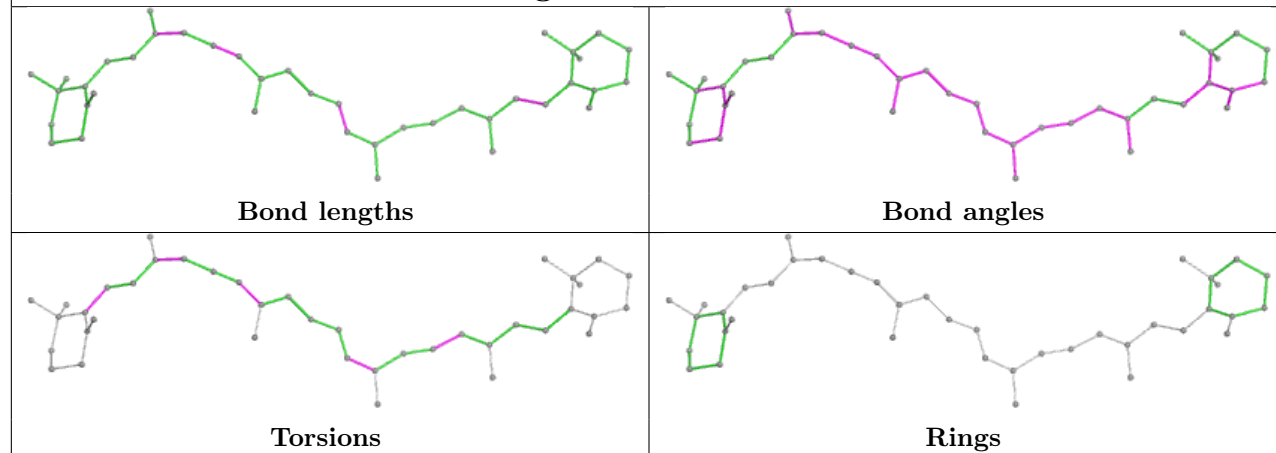
Ligand DGD 1 803

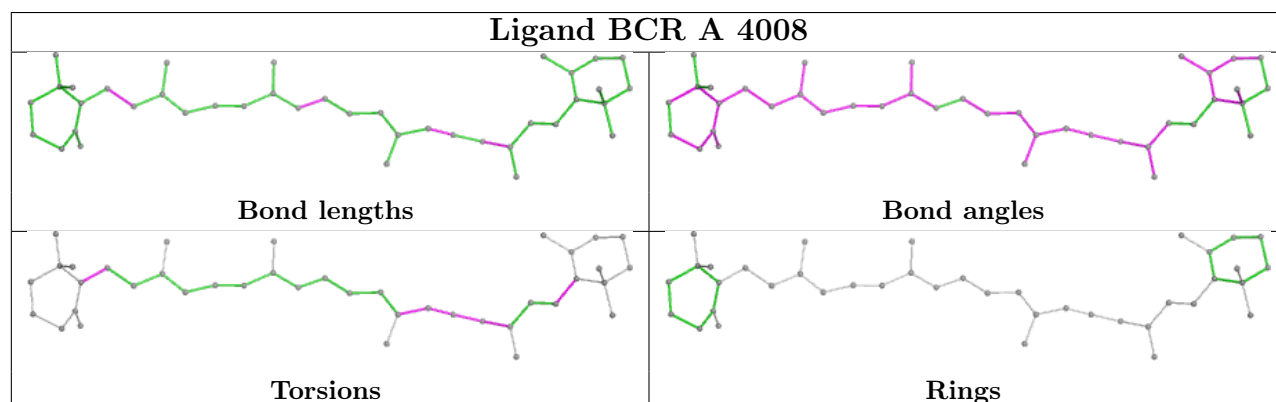
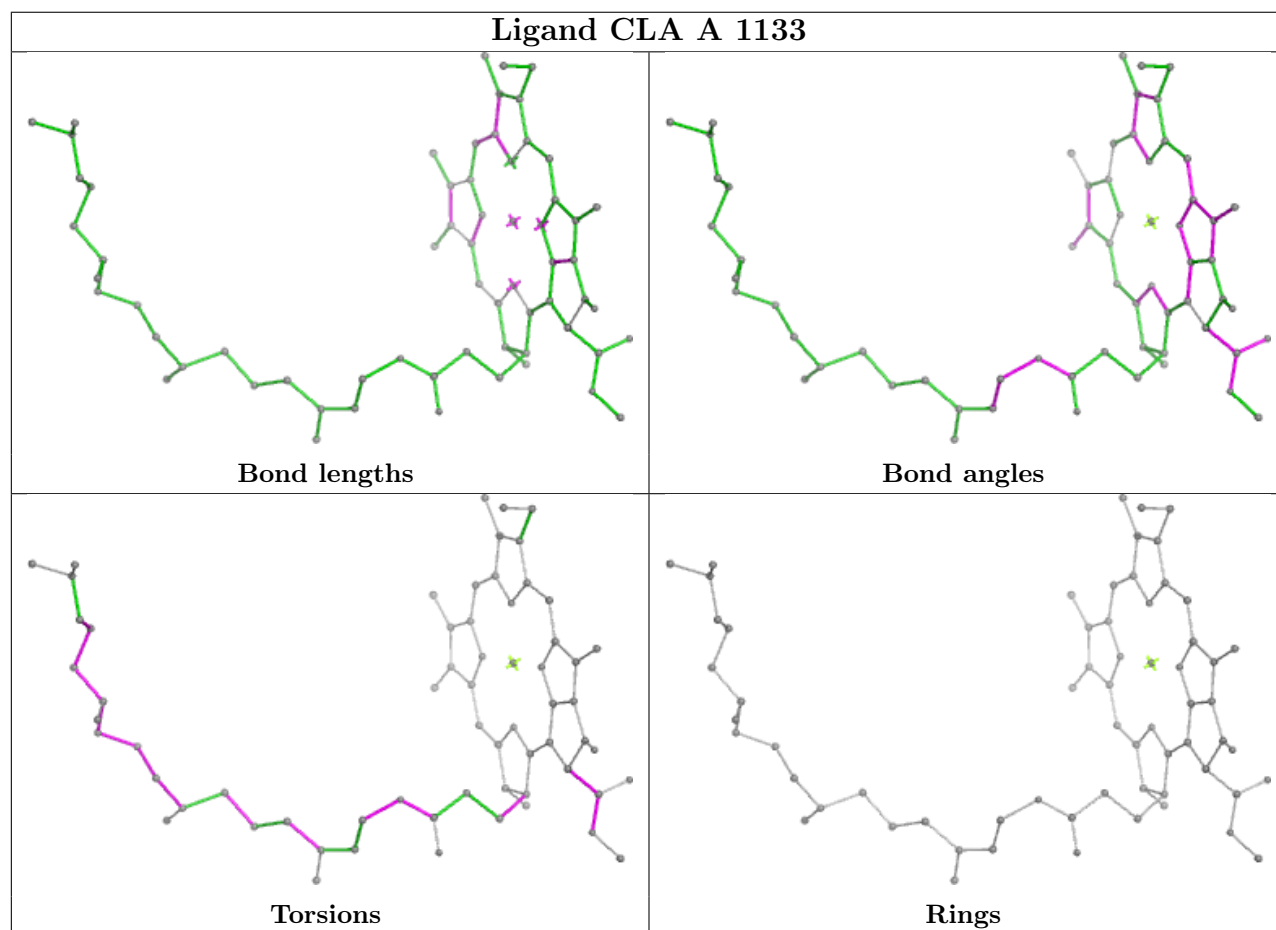
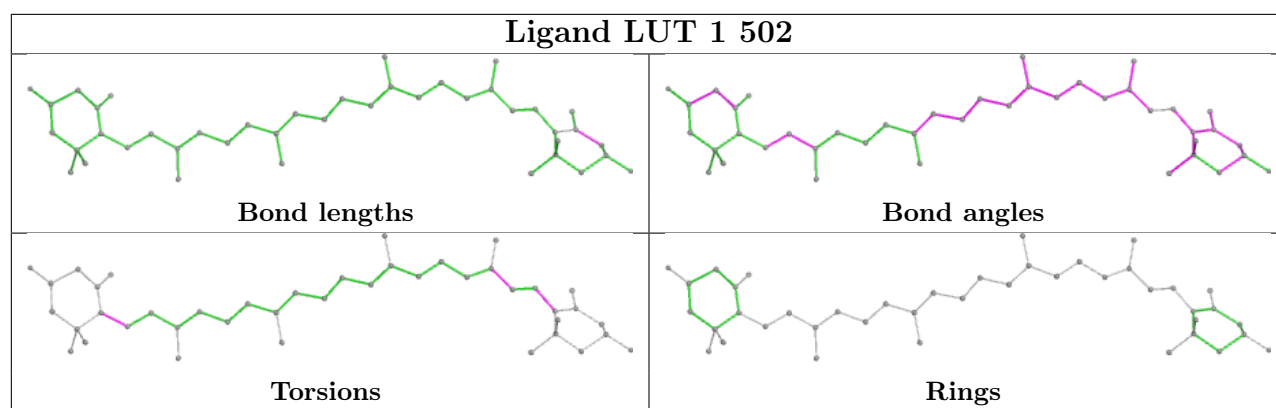


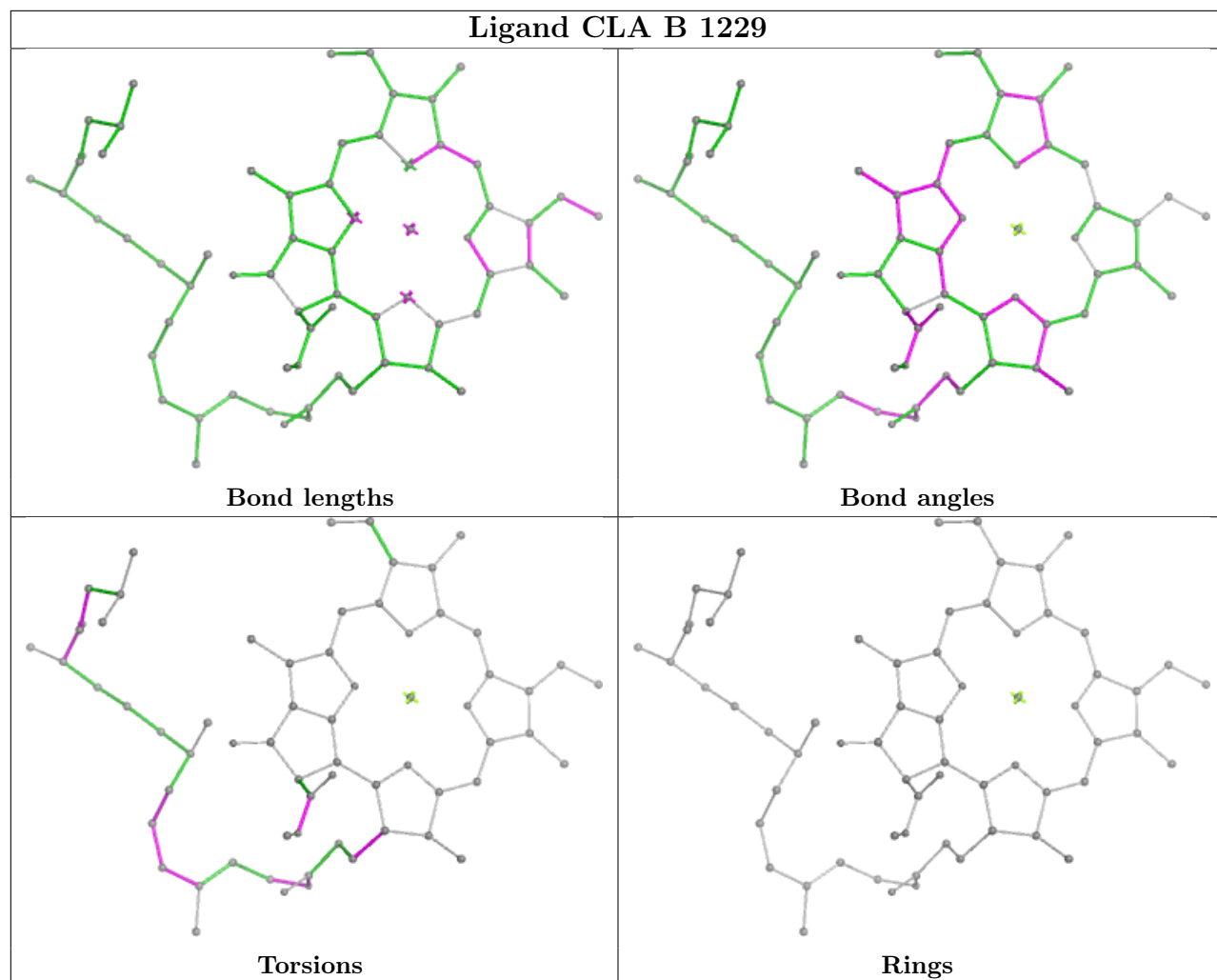
Ligand CHL 2 609

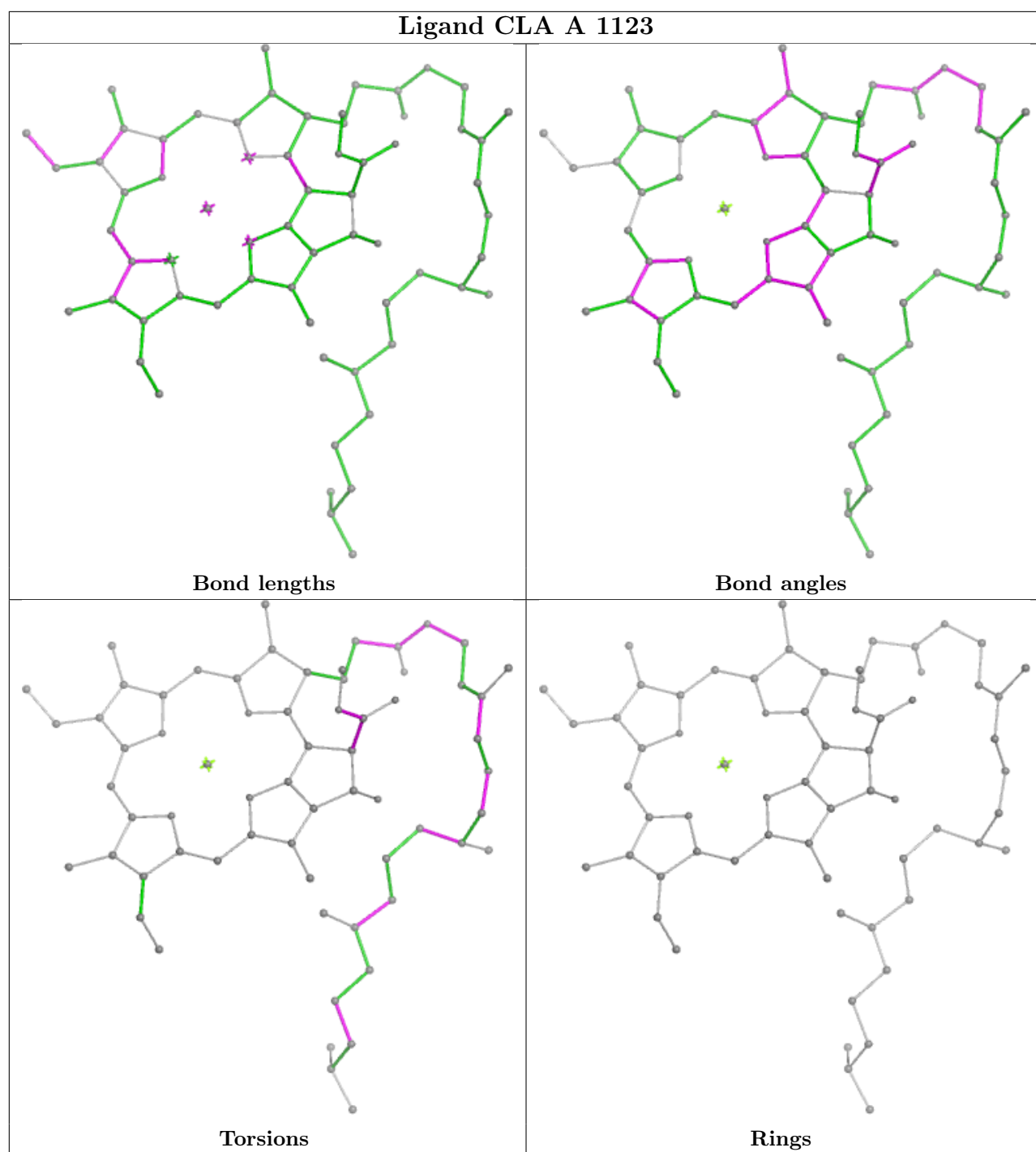




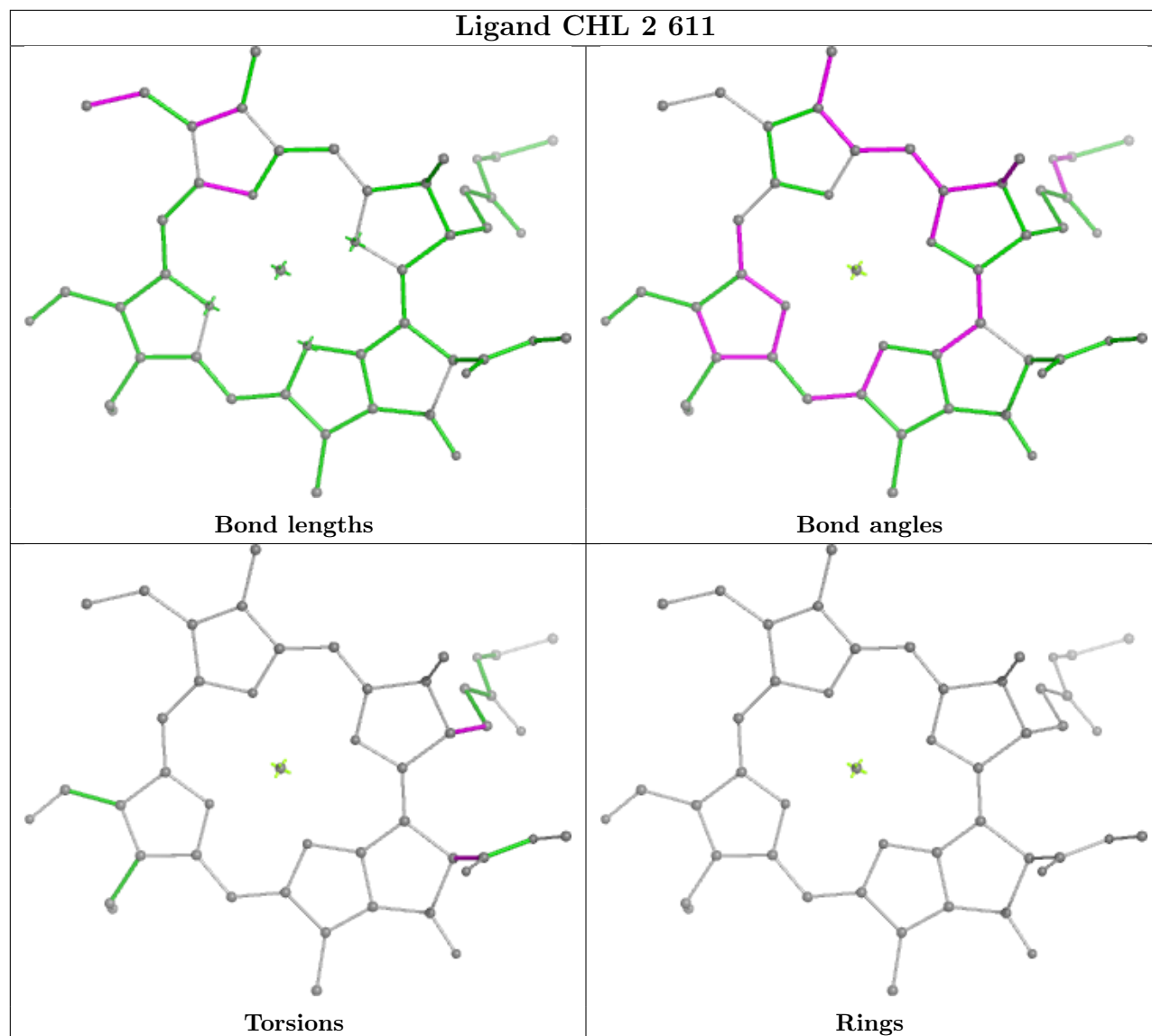
Ligand CLA K 1402**Ligand BCR 1 504**

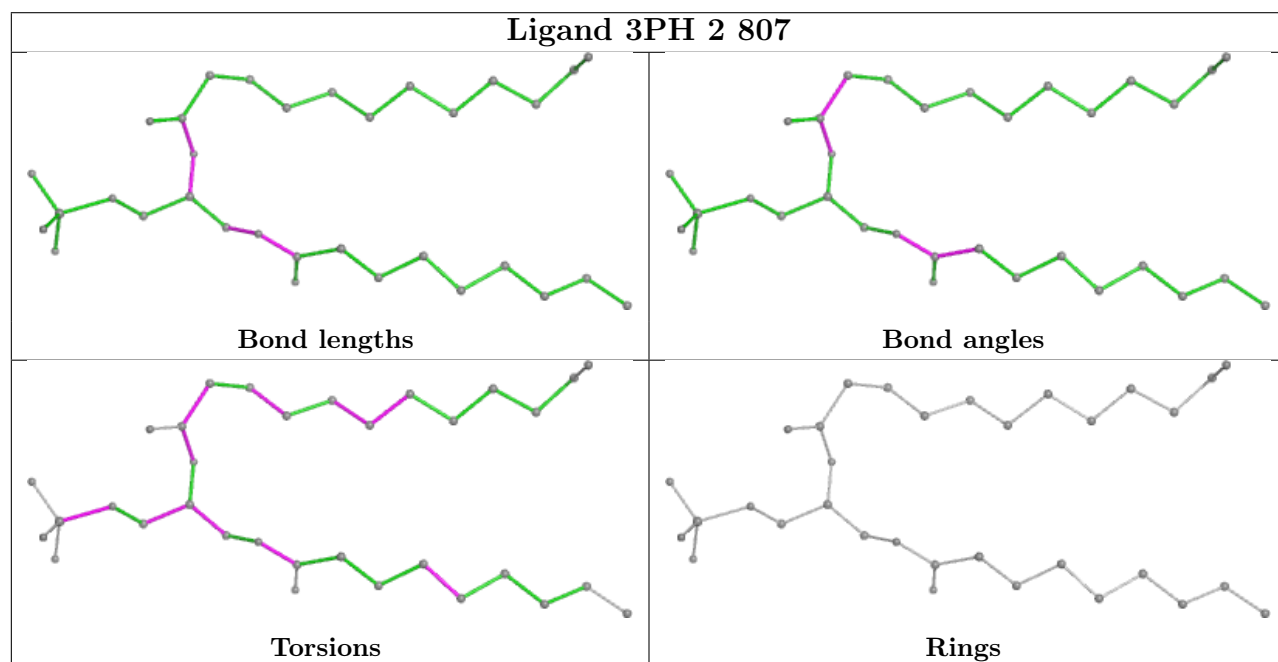
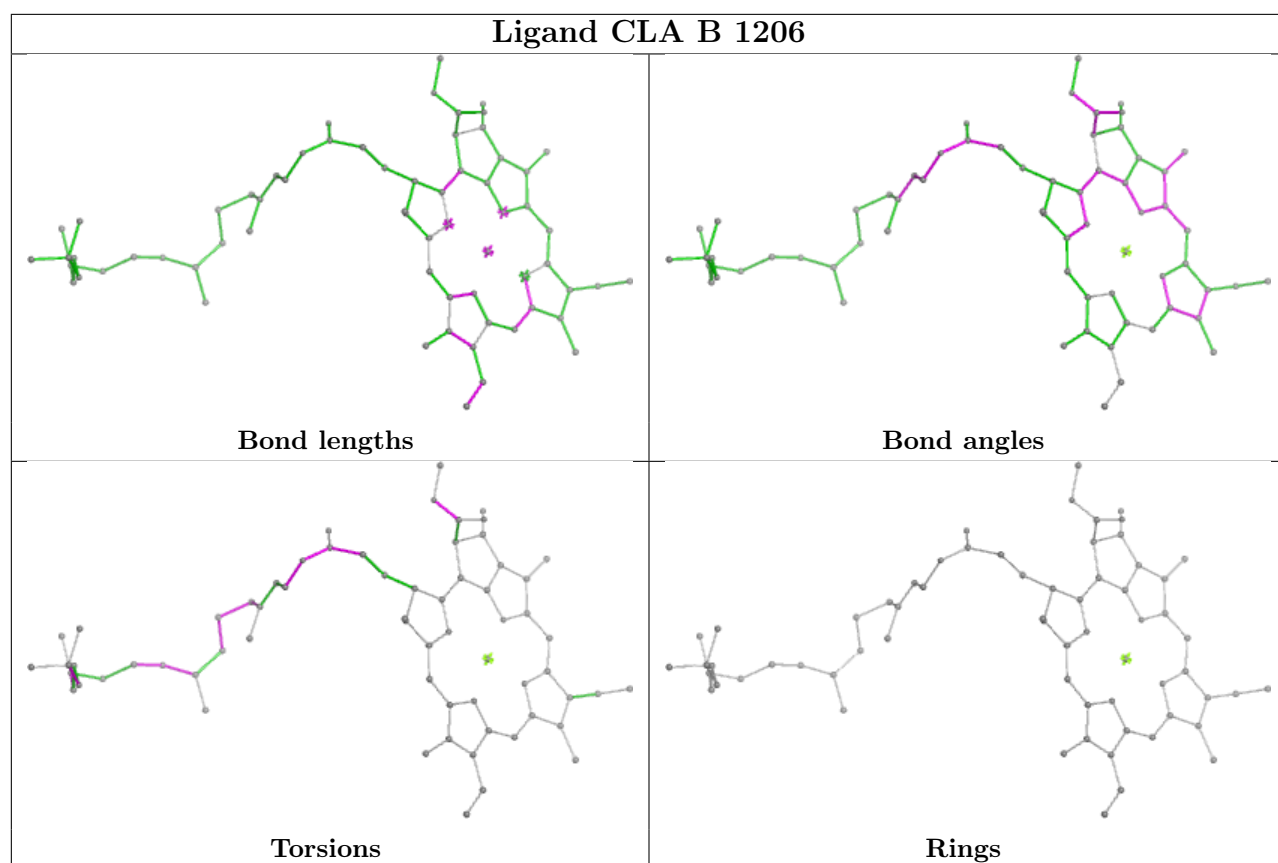


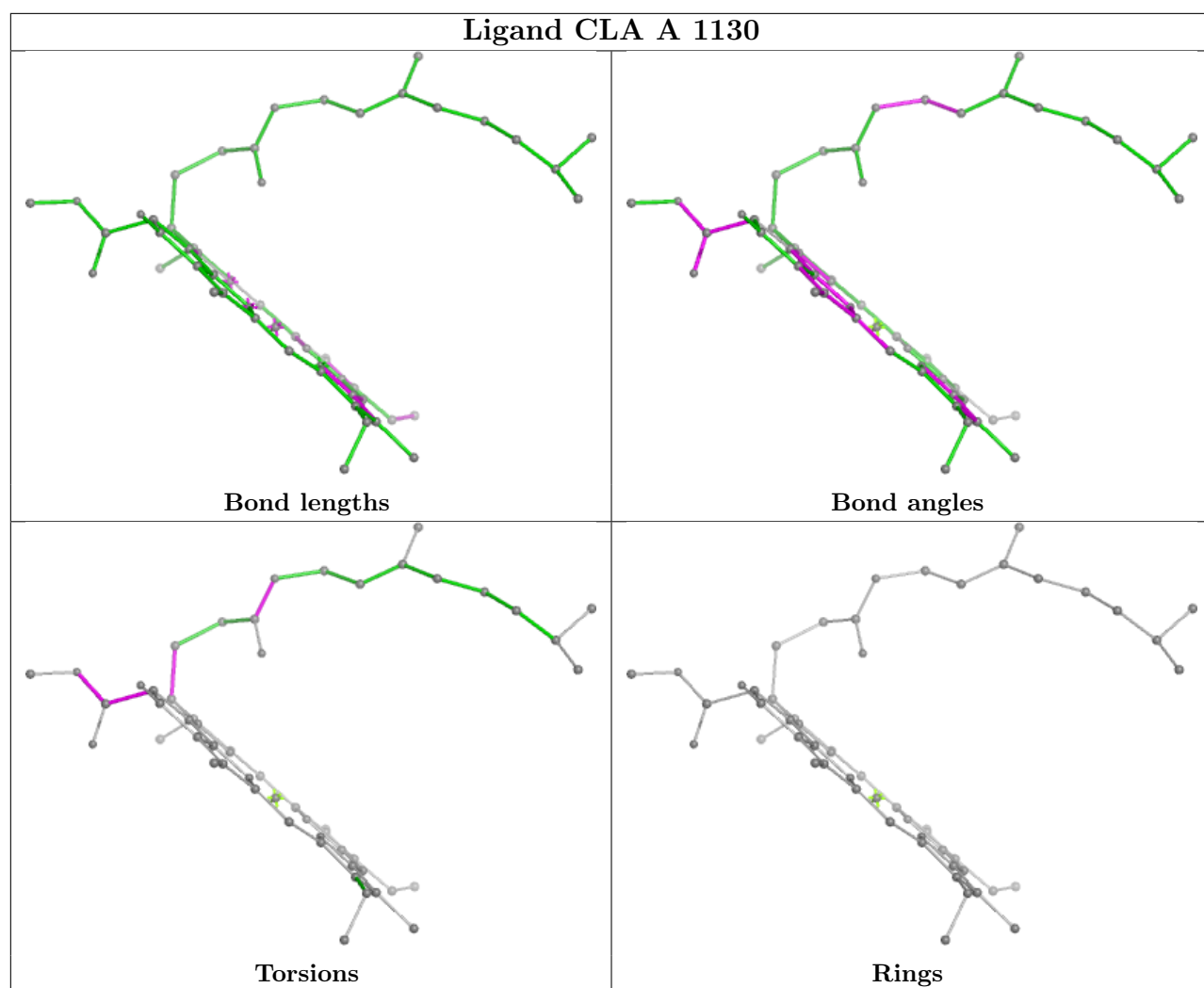


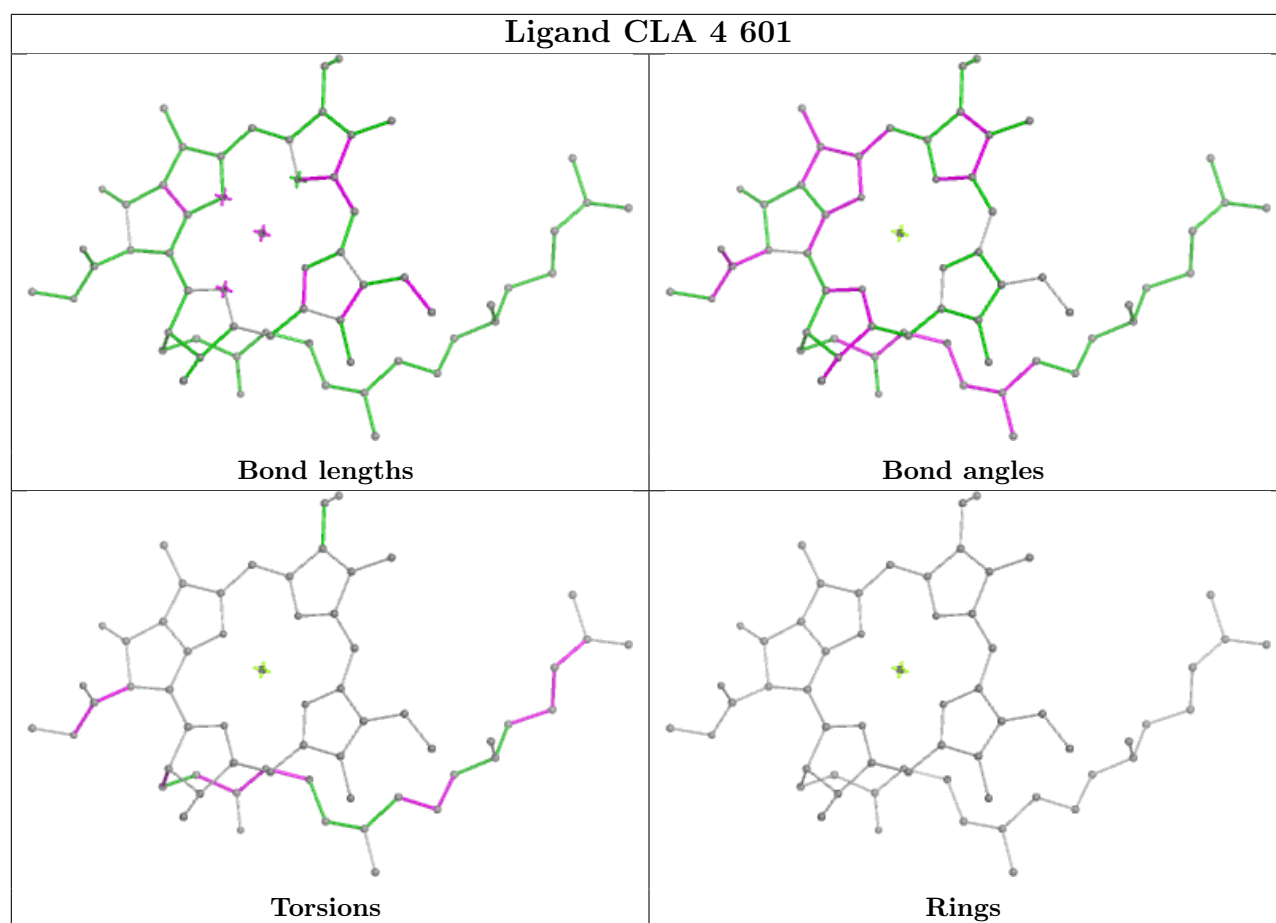


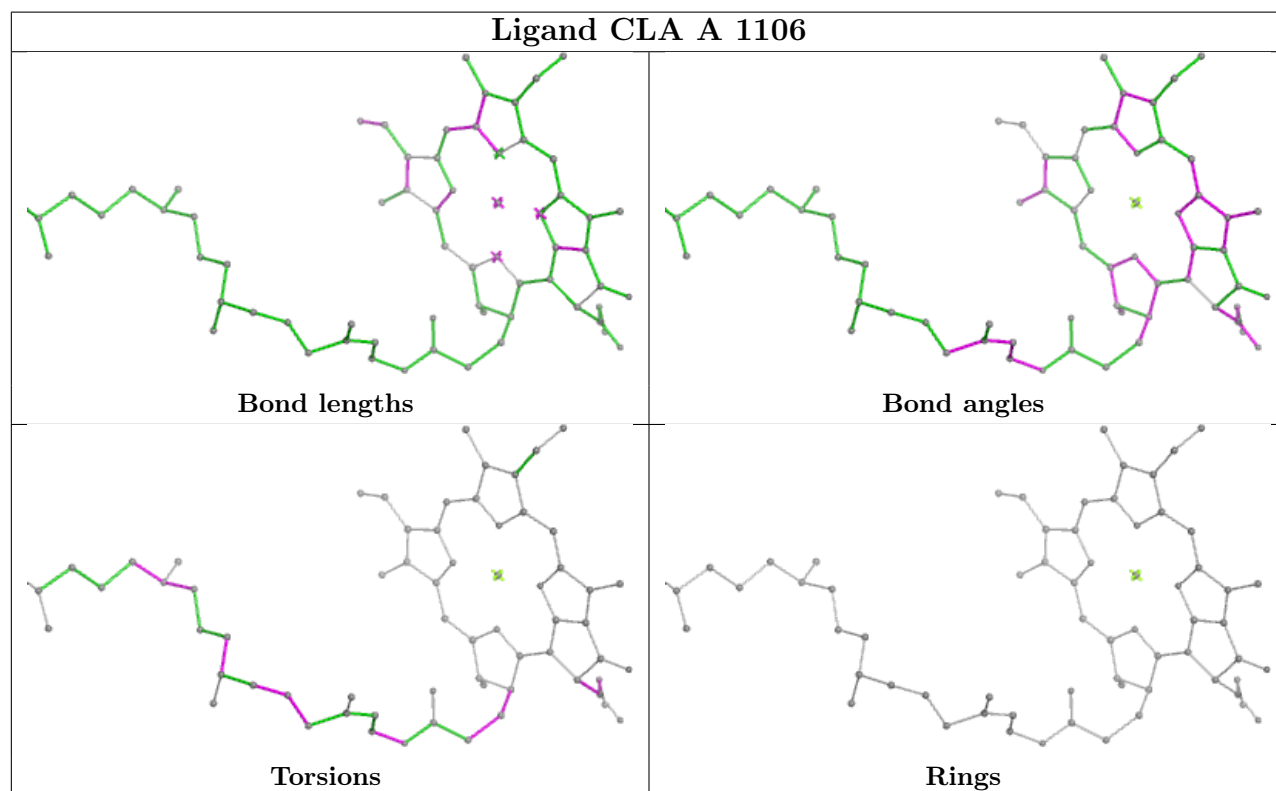
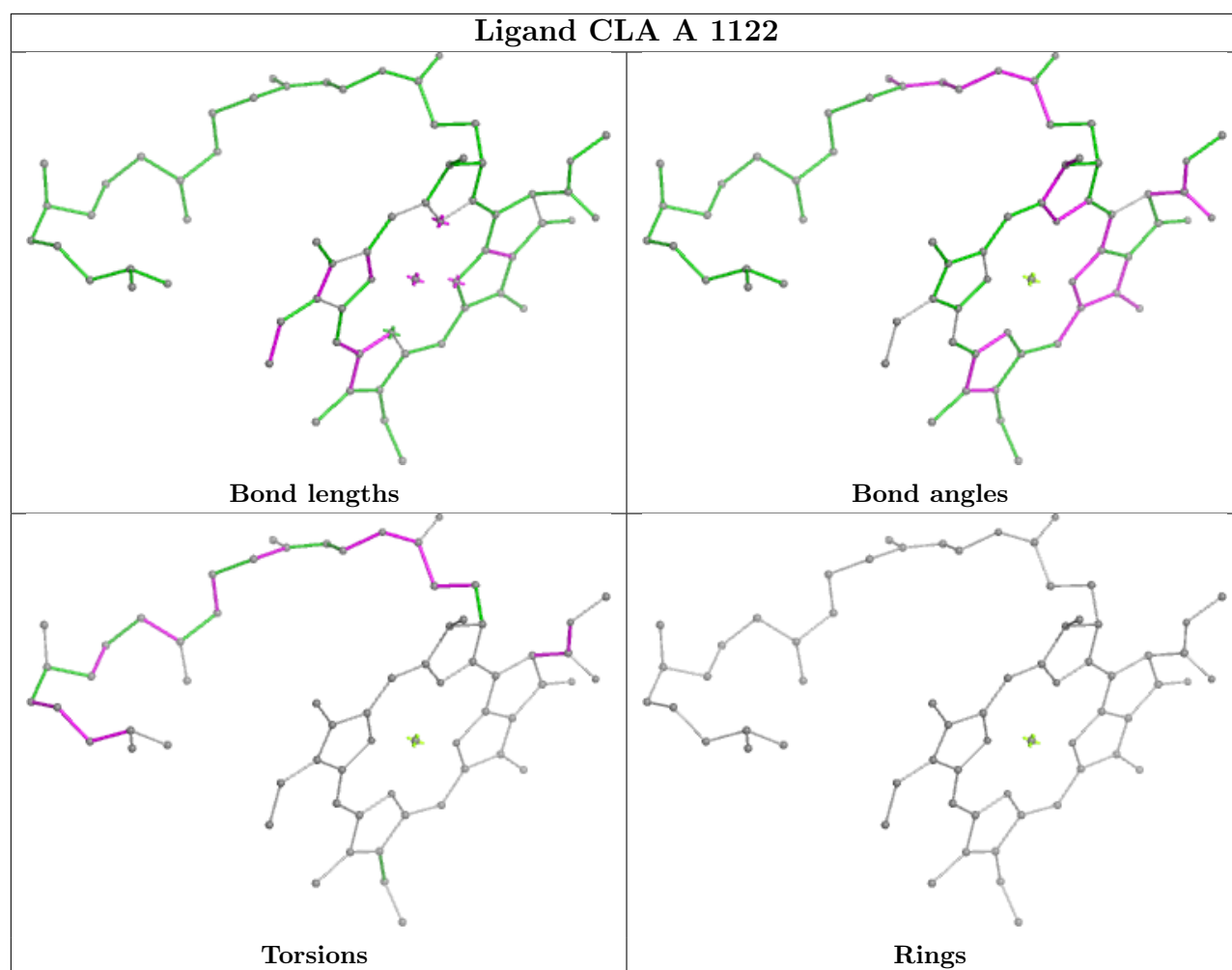
Ligand CHL 2 611

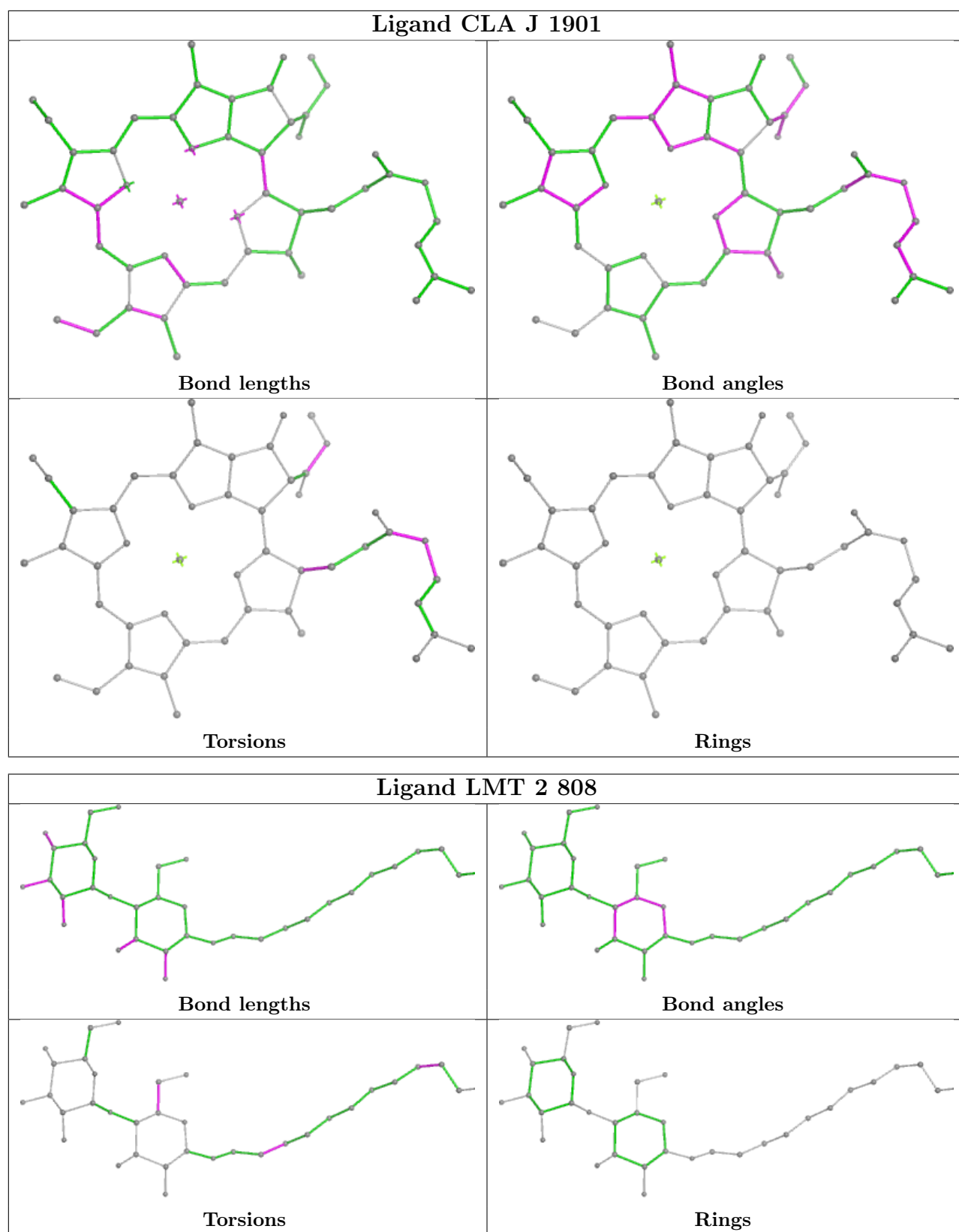


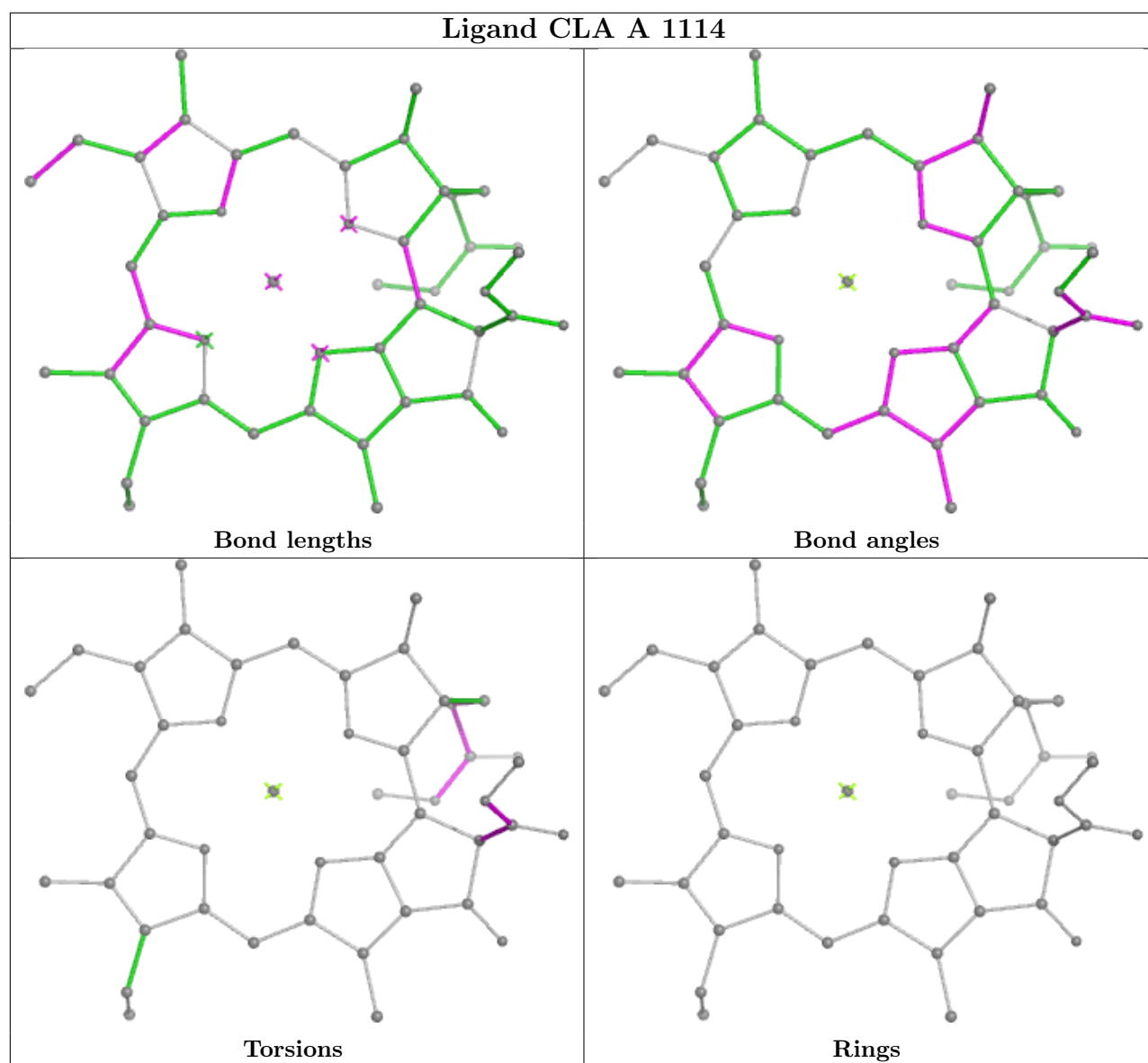


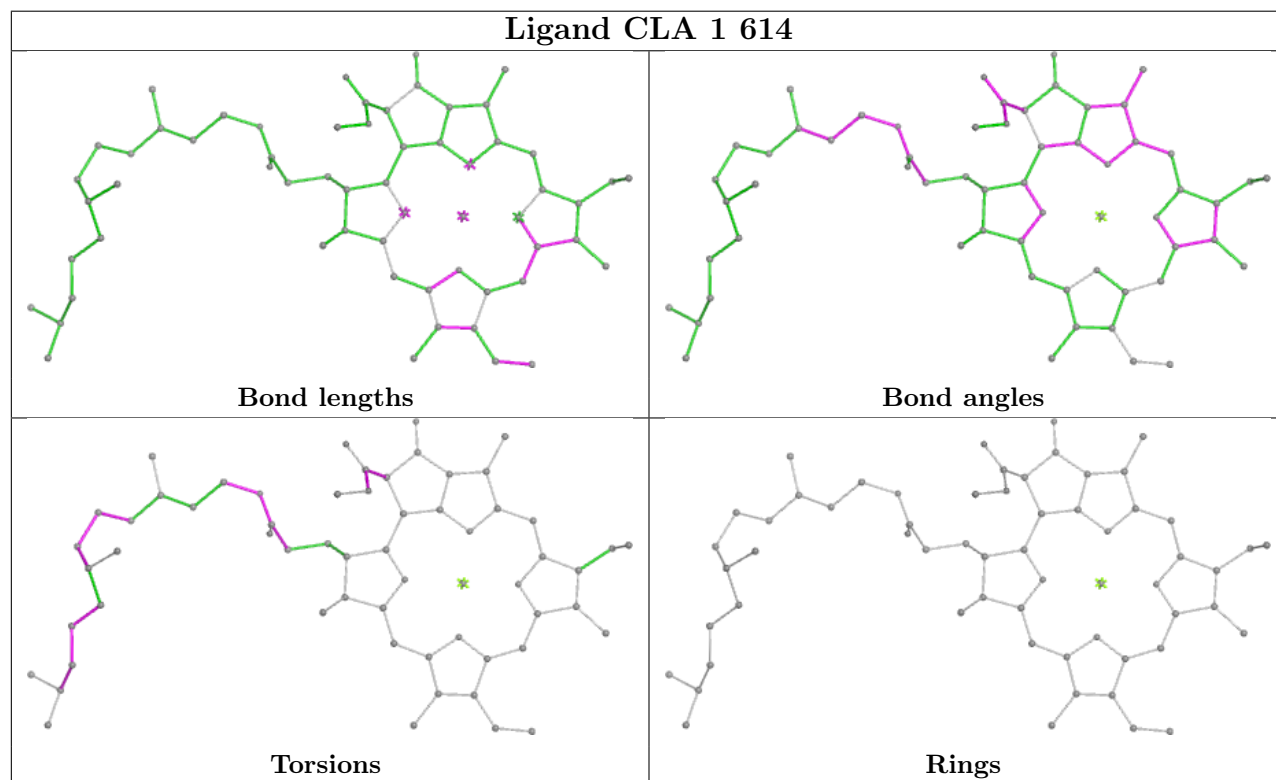
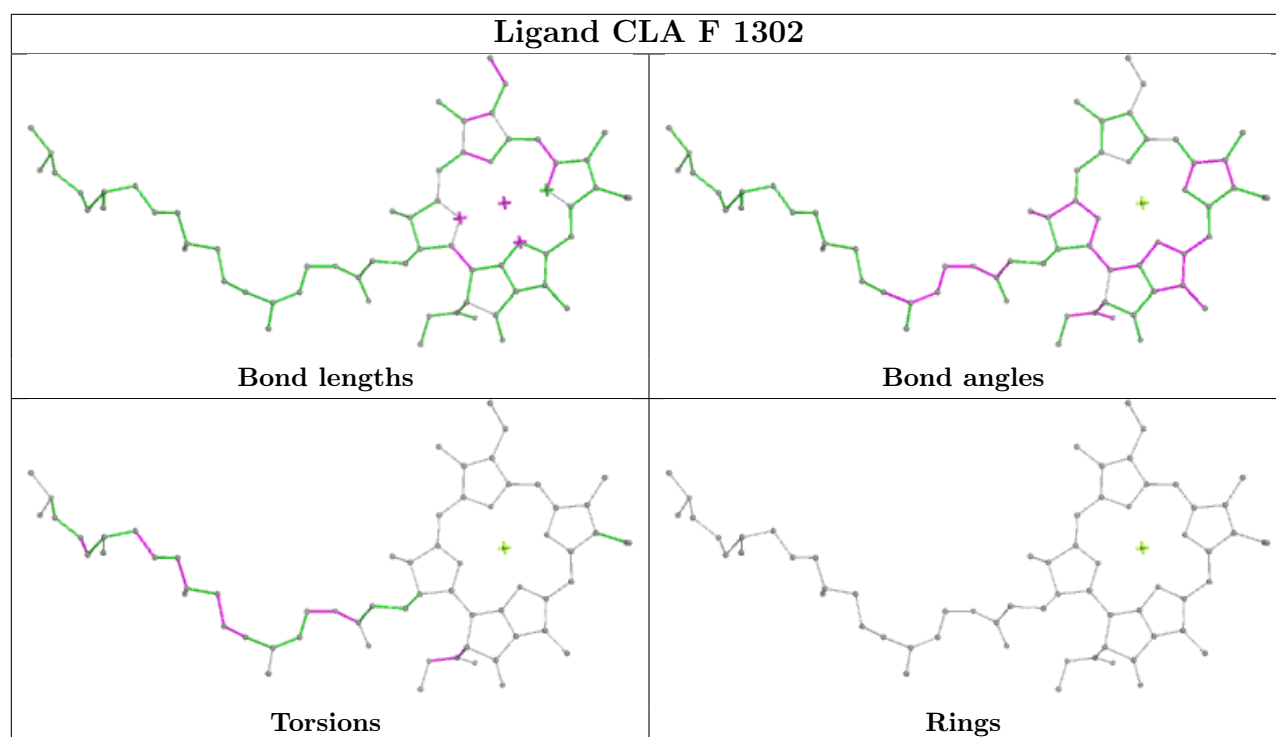


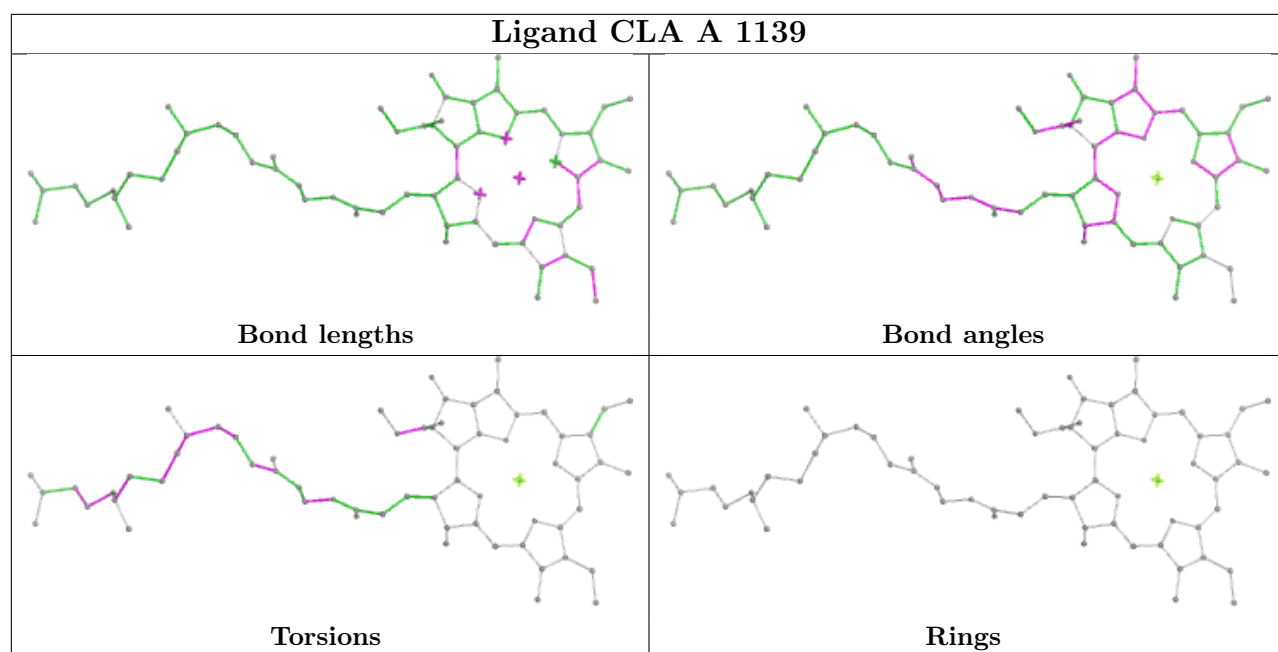


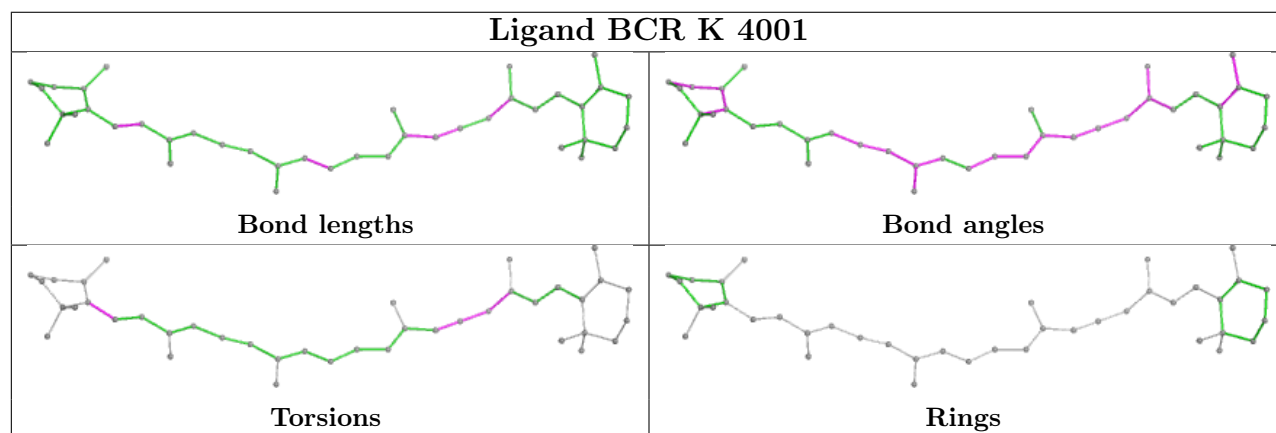
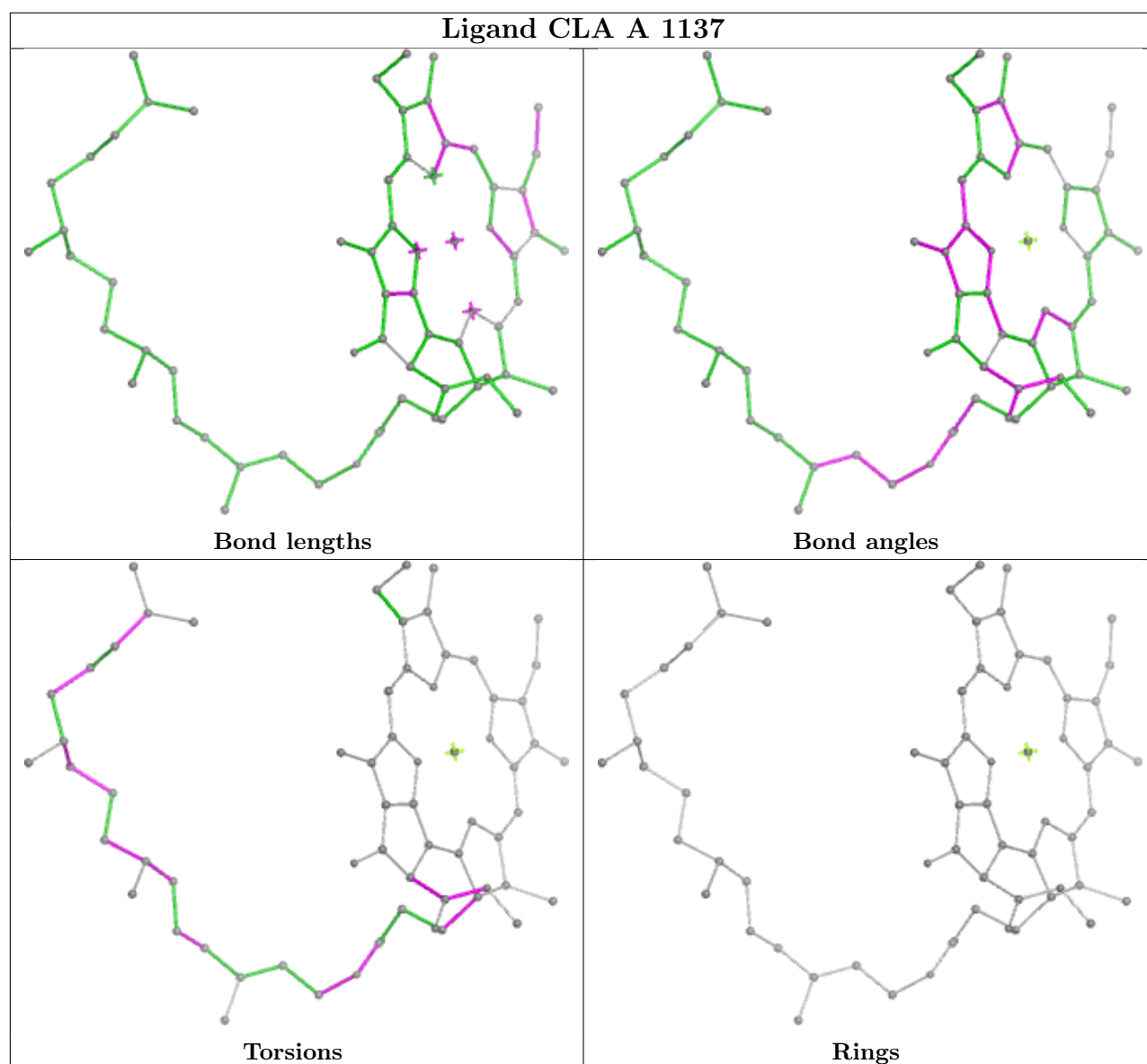




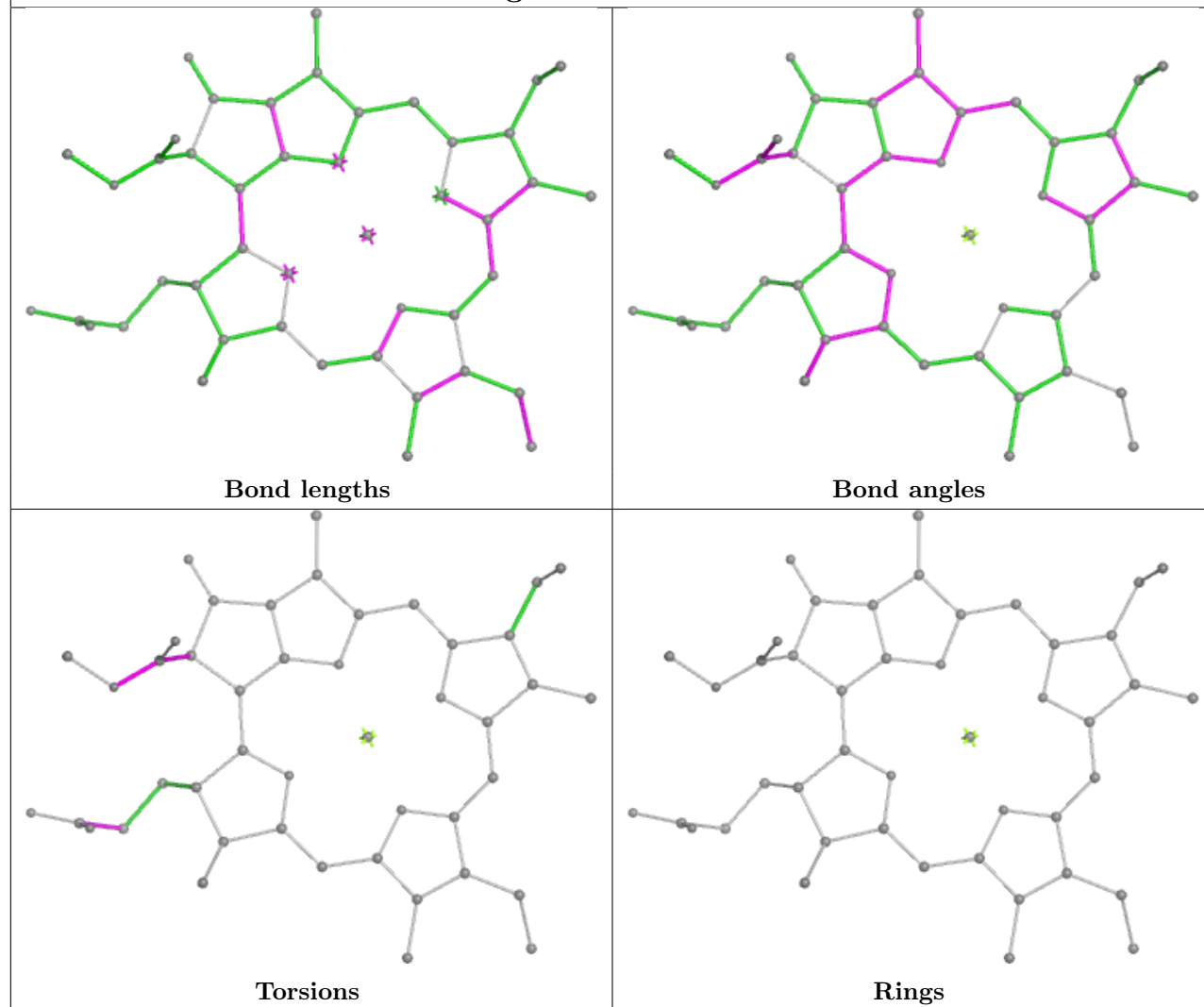




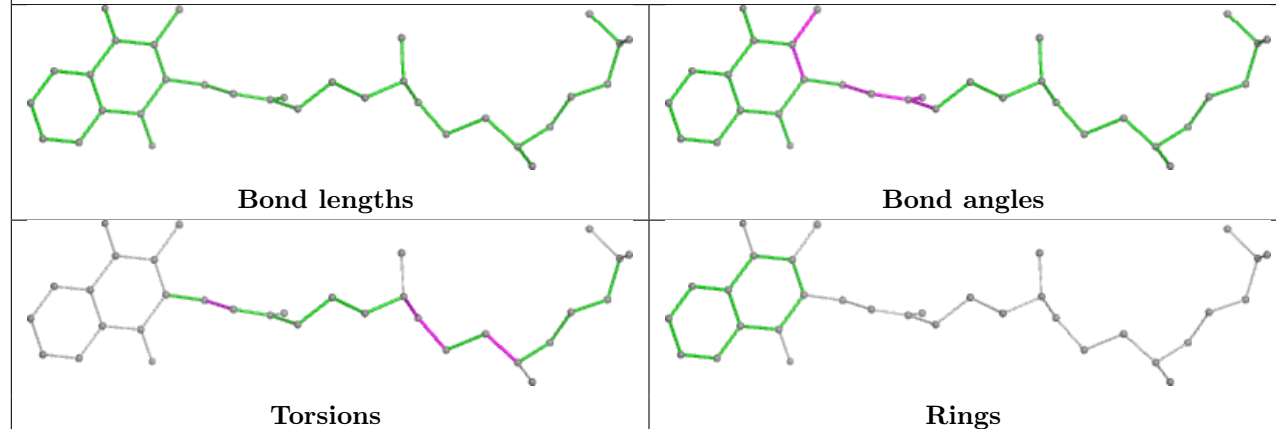


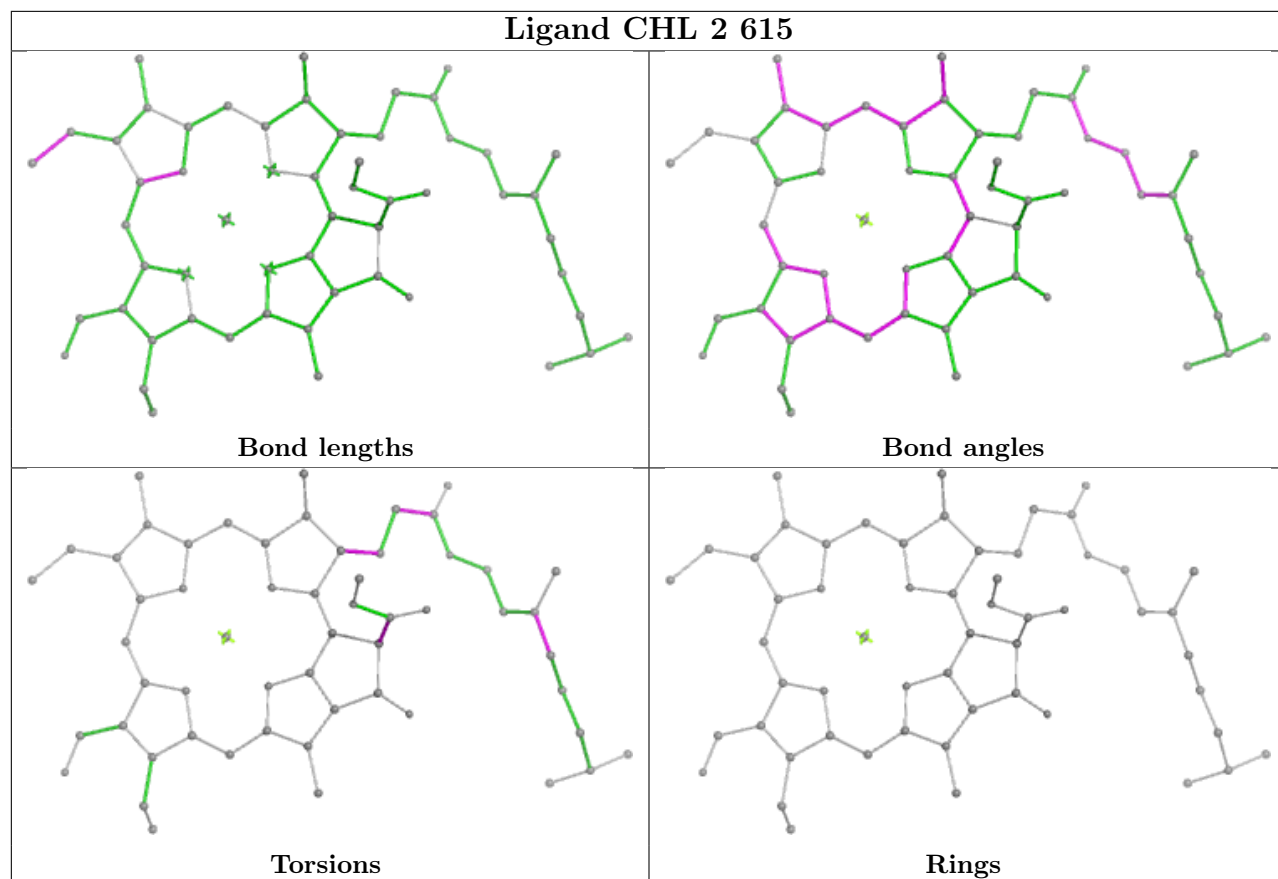


Ligand CLA 1 613

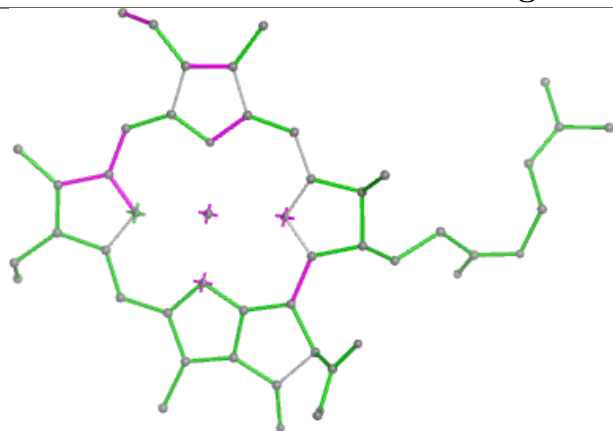


Ligand PQN A 2001

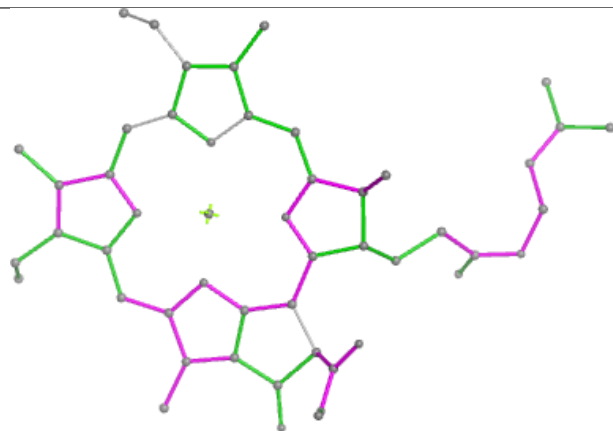




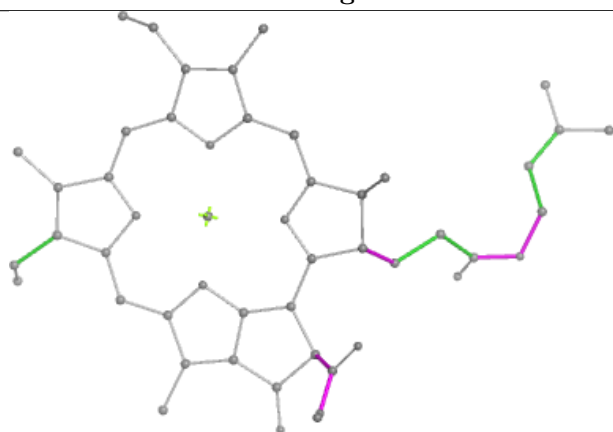
Ligand CLA 4 609



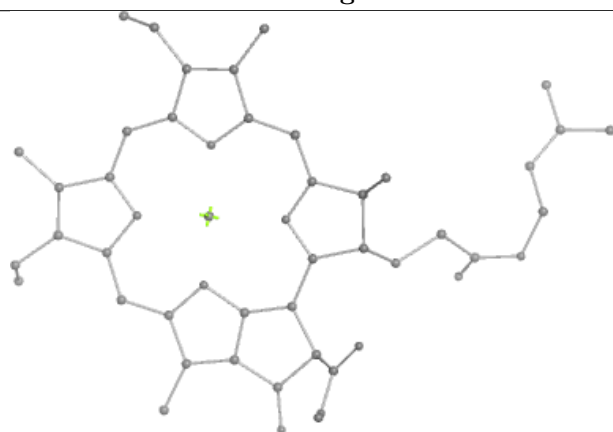
Bond lengths



Bond angles

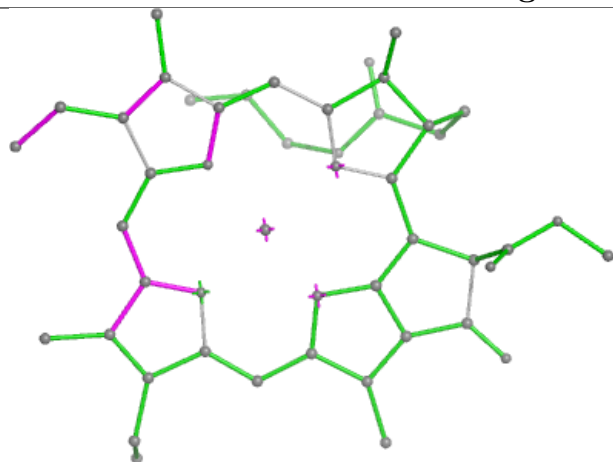


Torsions

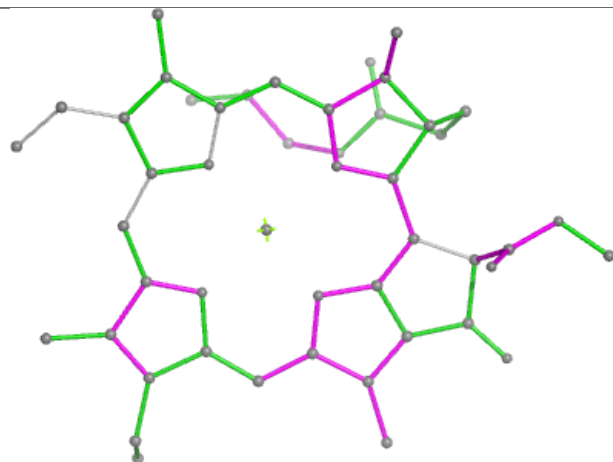


Rings

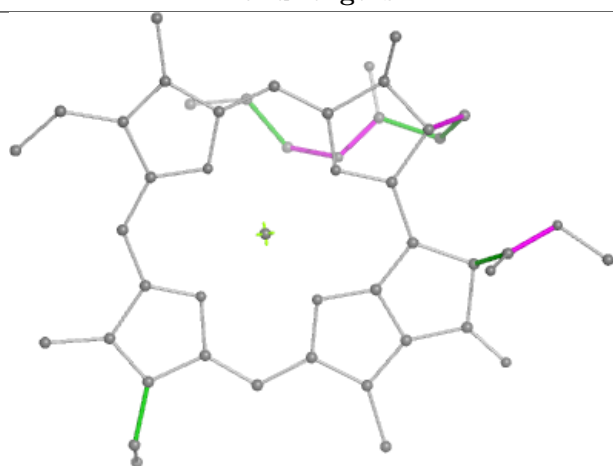
Ligand CLA 3 608



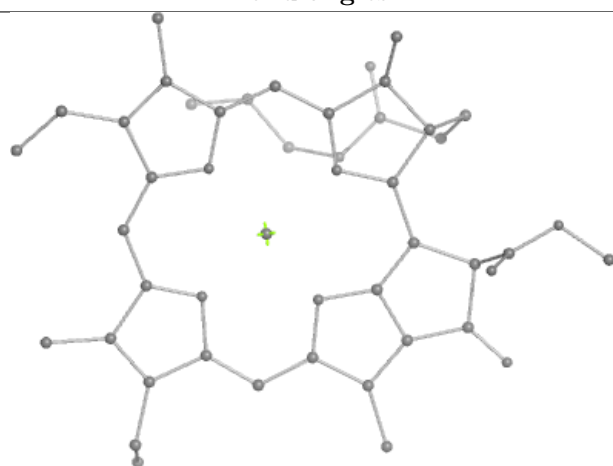
Bond lengths



Bond angles

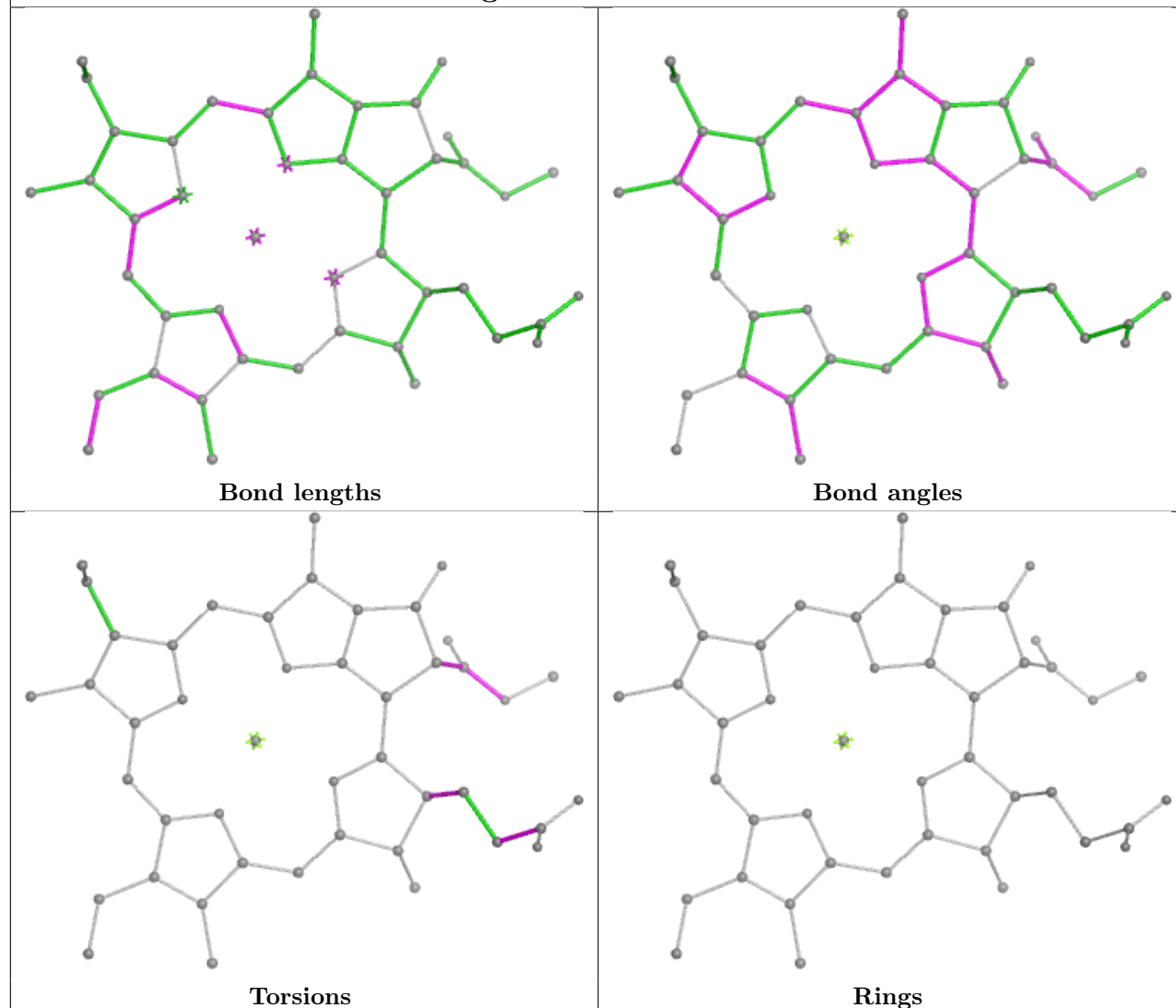


Torsions

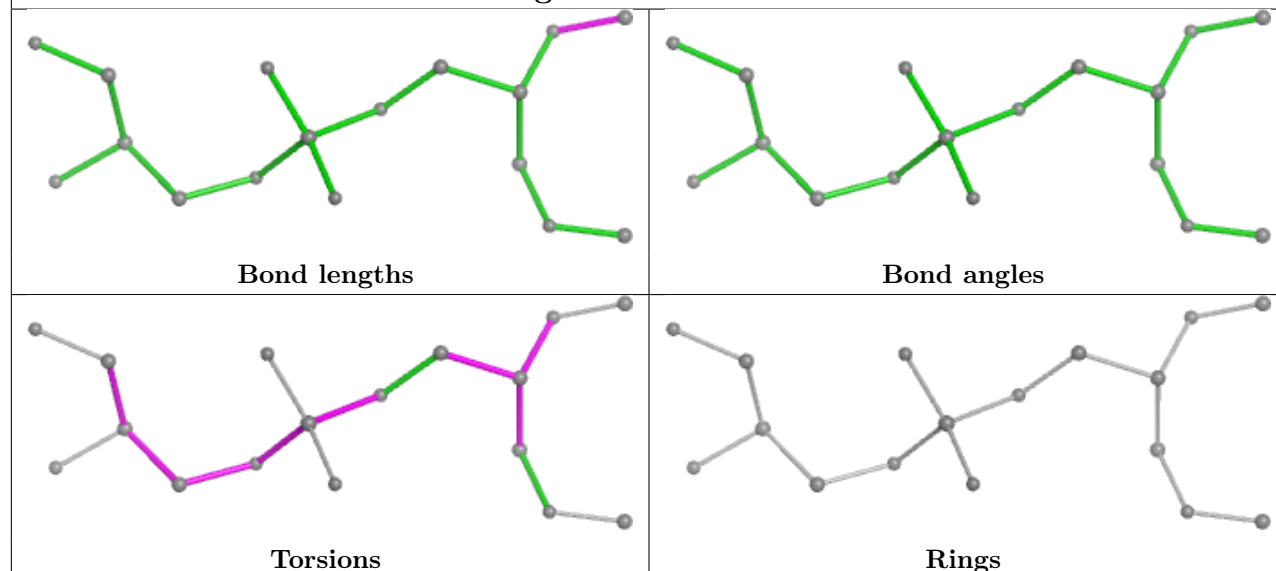


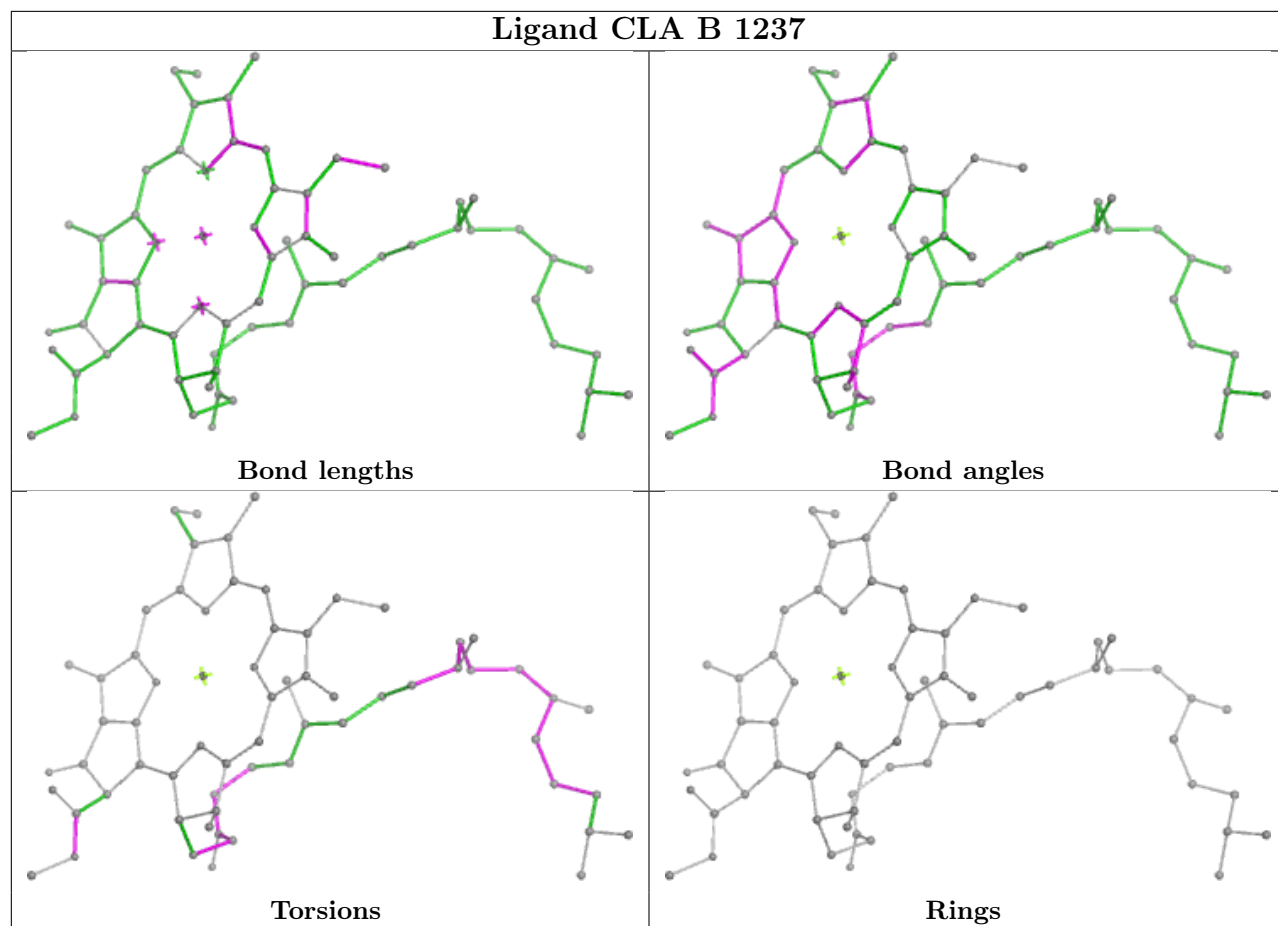
Rings

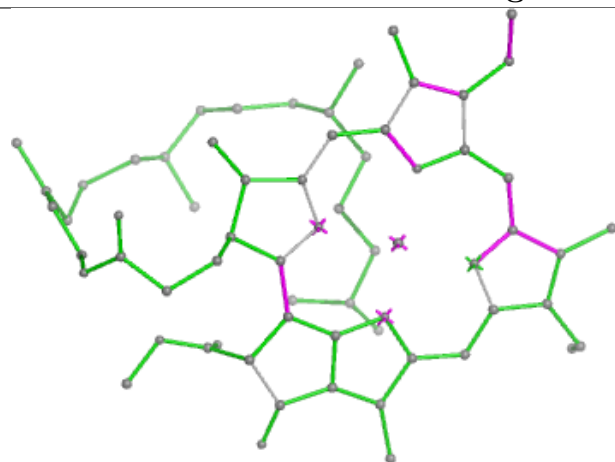
Ligand CLA A 1113



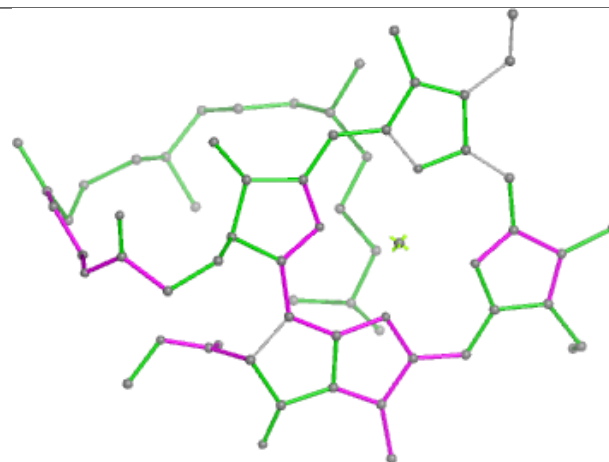
Ligand LHG 3 801



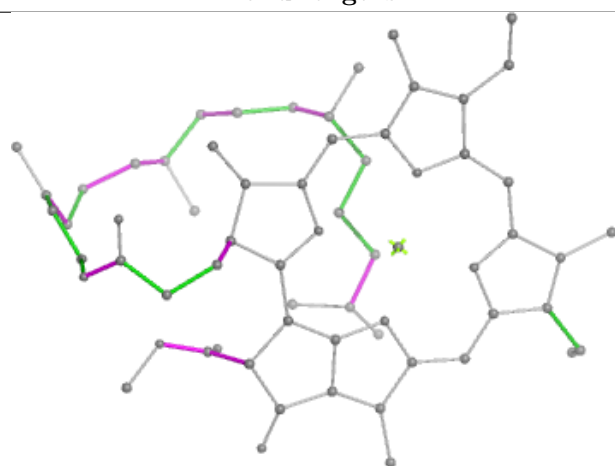


Ligand CLA A 1104

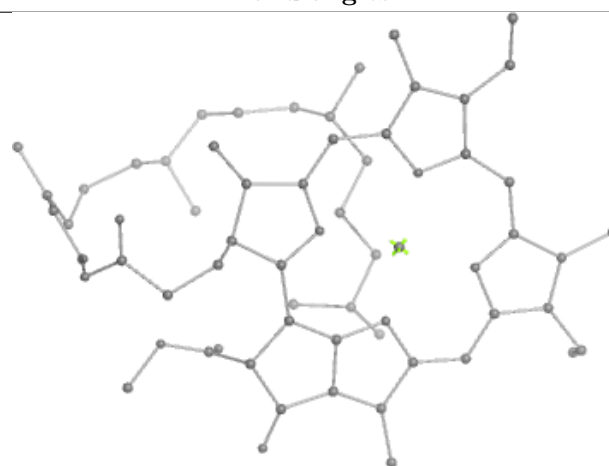
Bond lengths



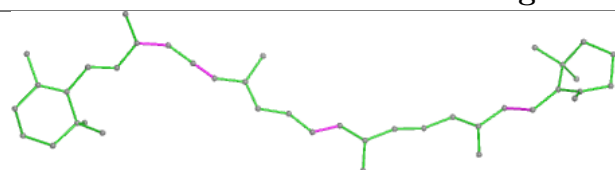
Bond angles



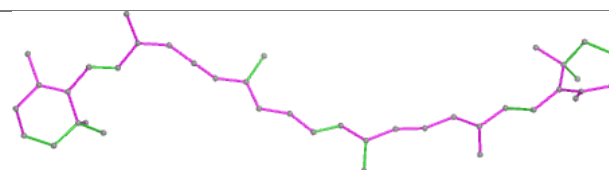
Torsions



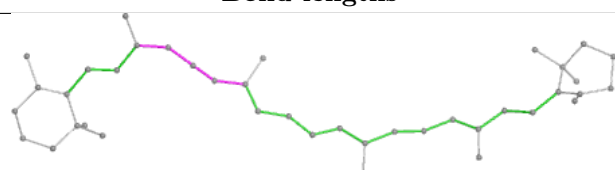
Rings

Ligand BCR 1 503

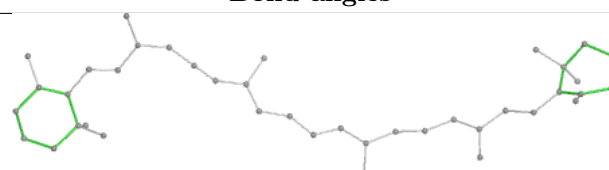
Bond lengths



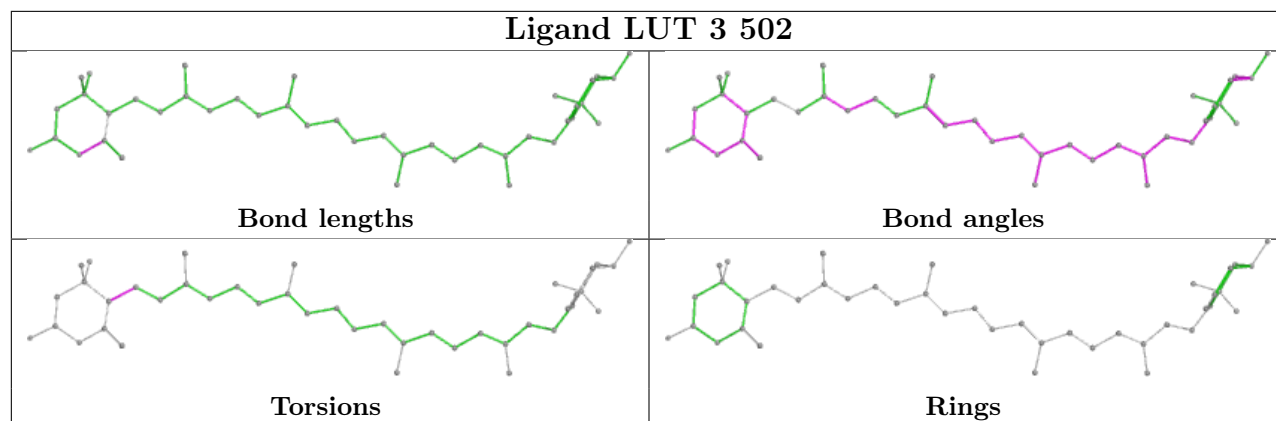
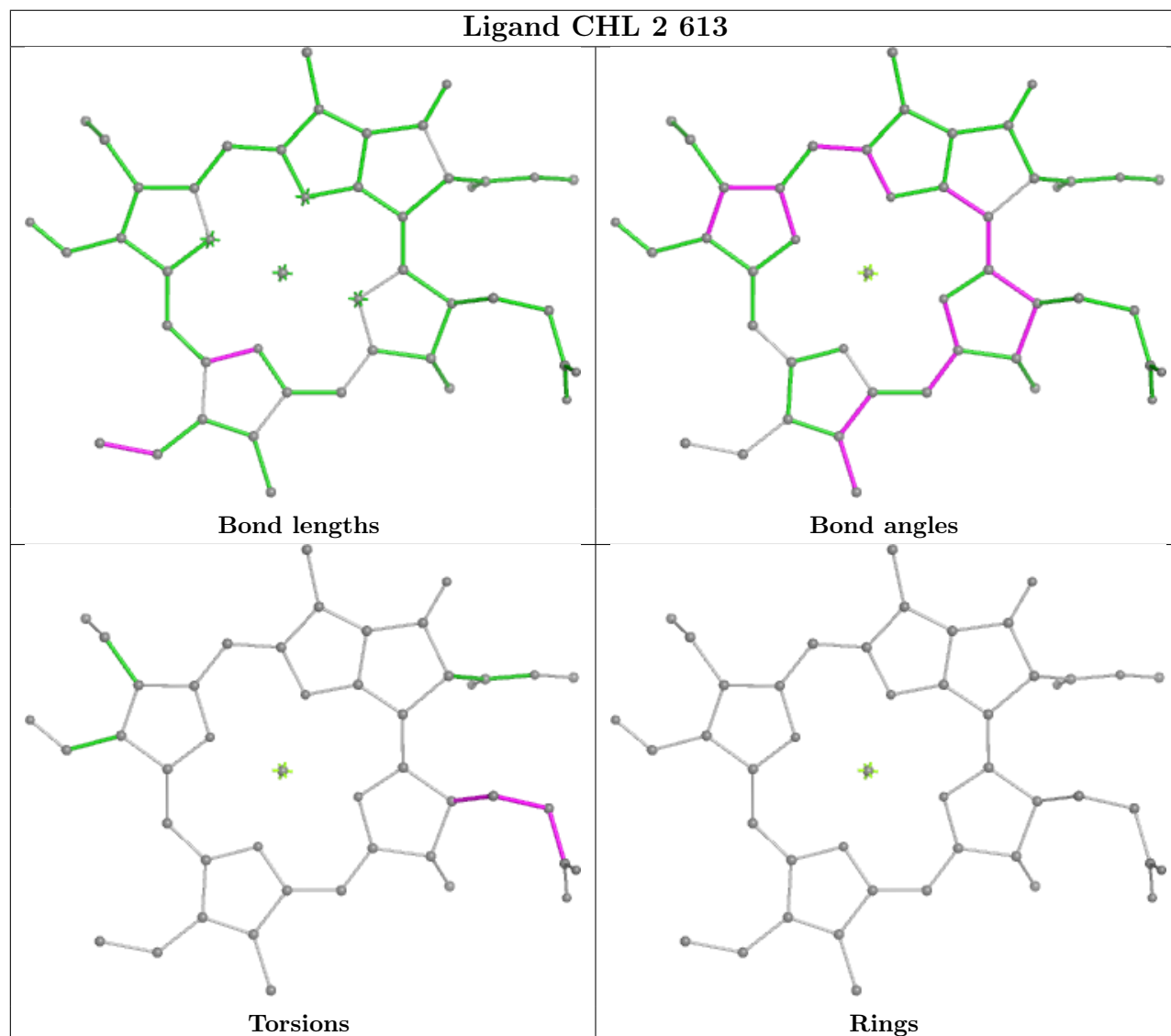
Bond angles

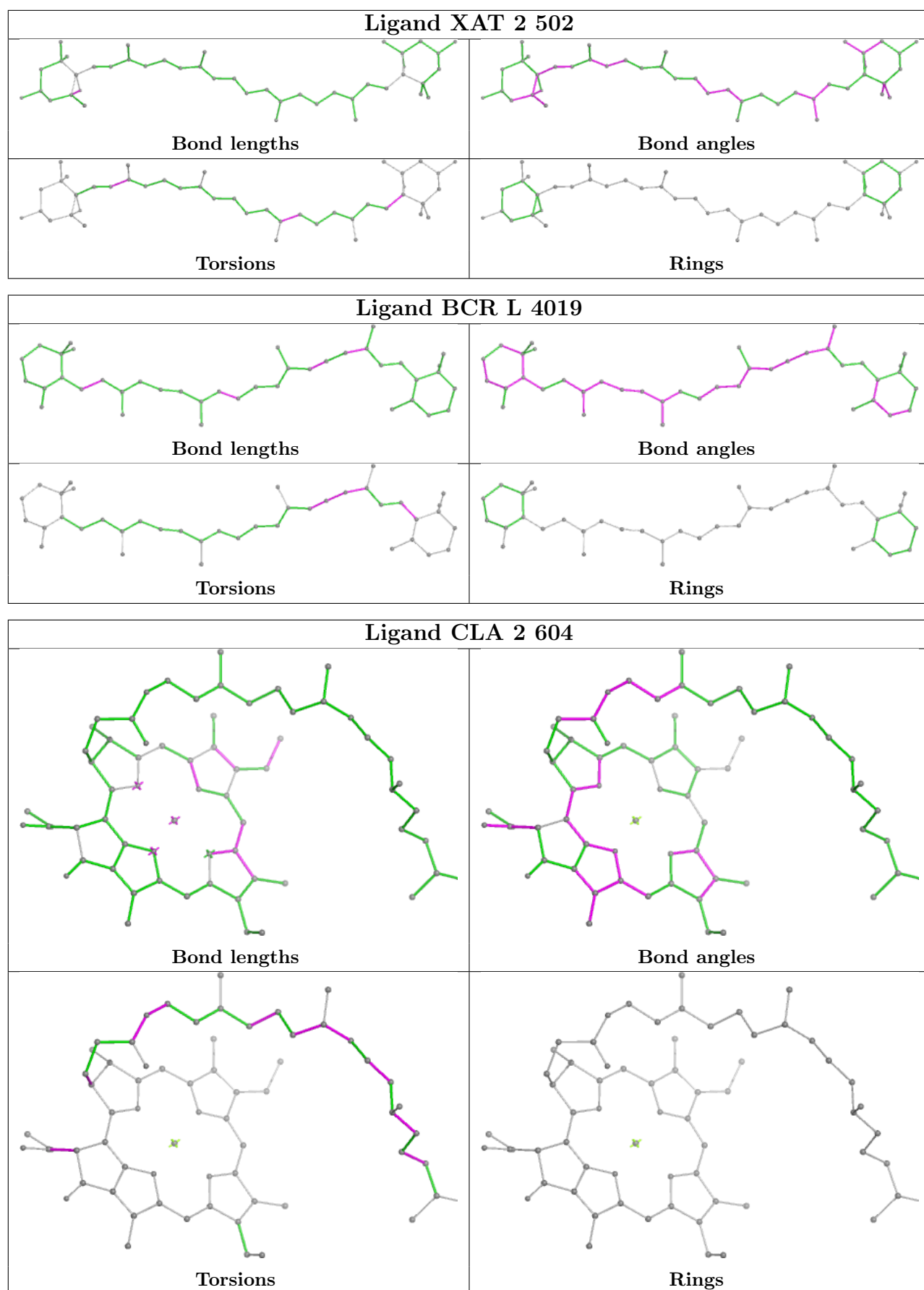


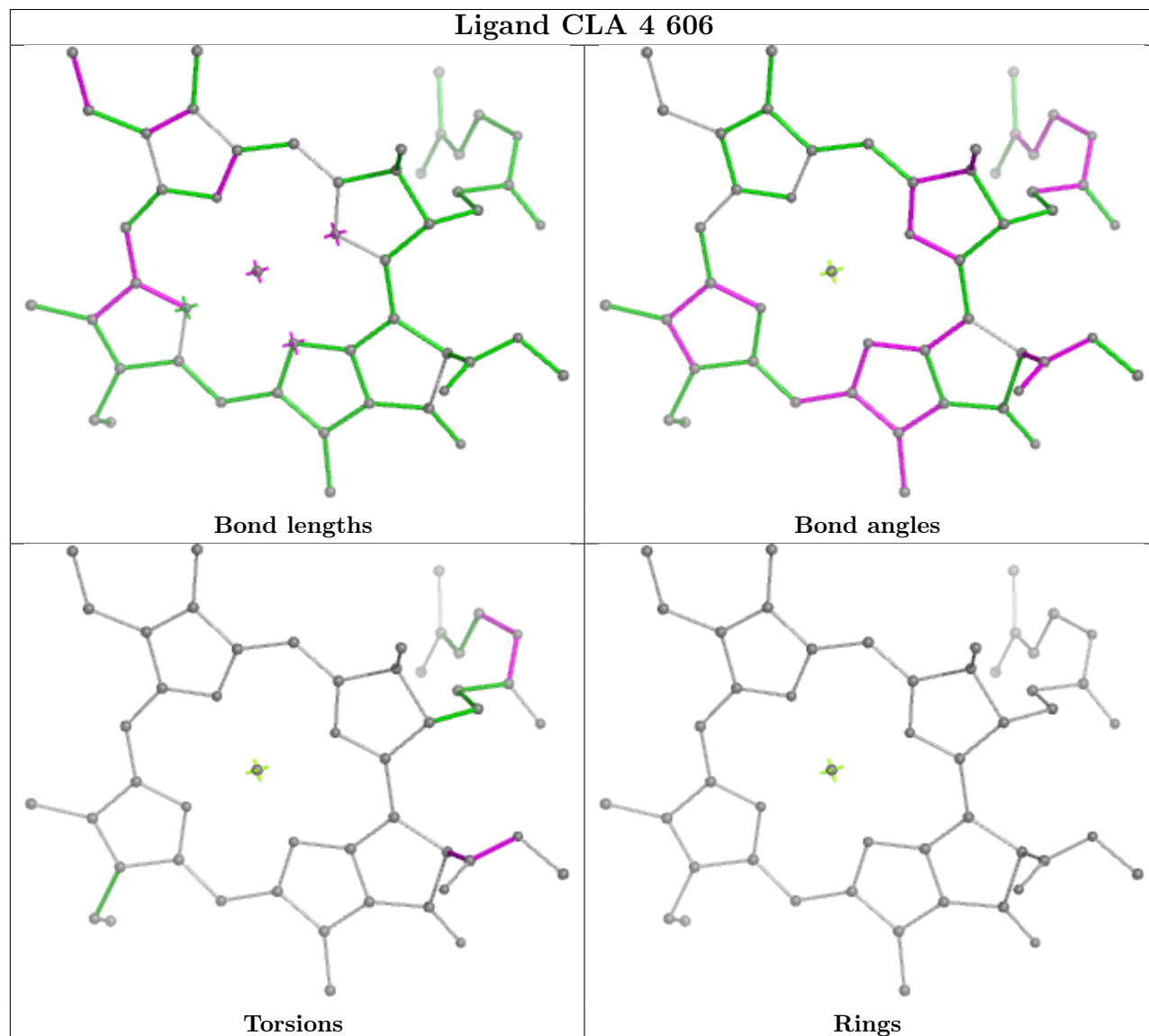
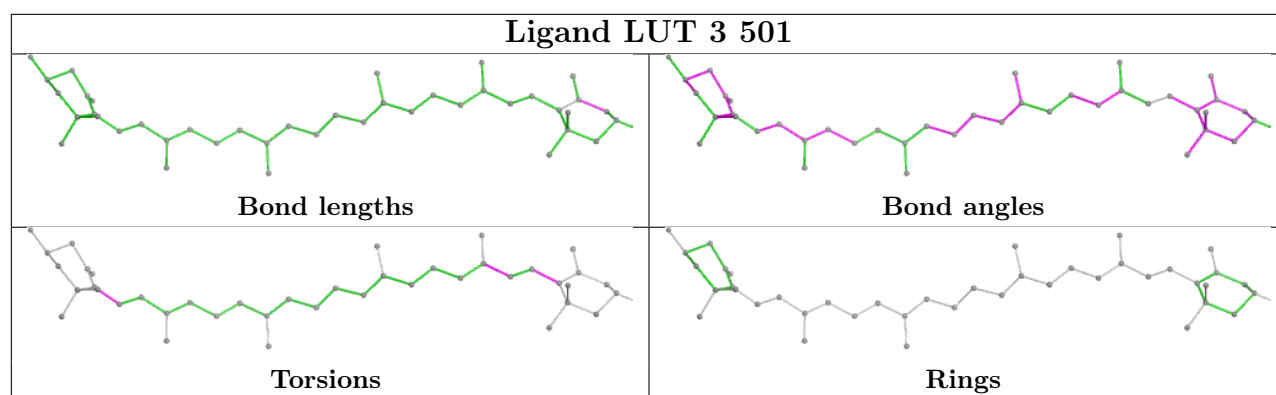
Torsions

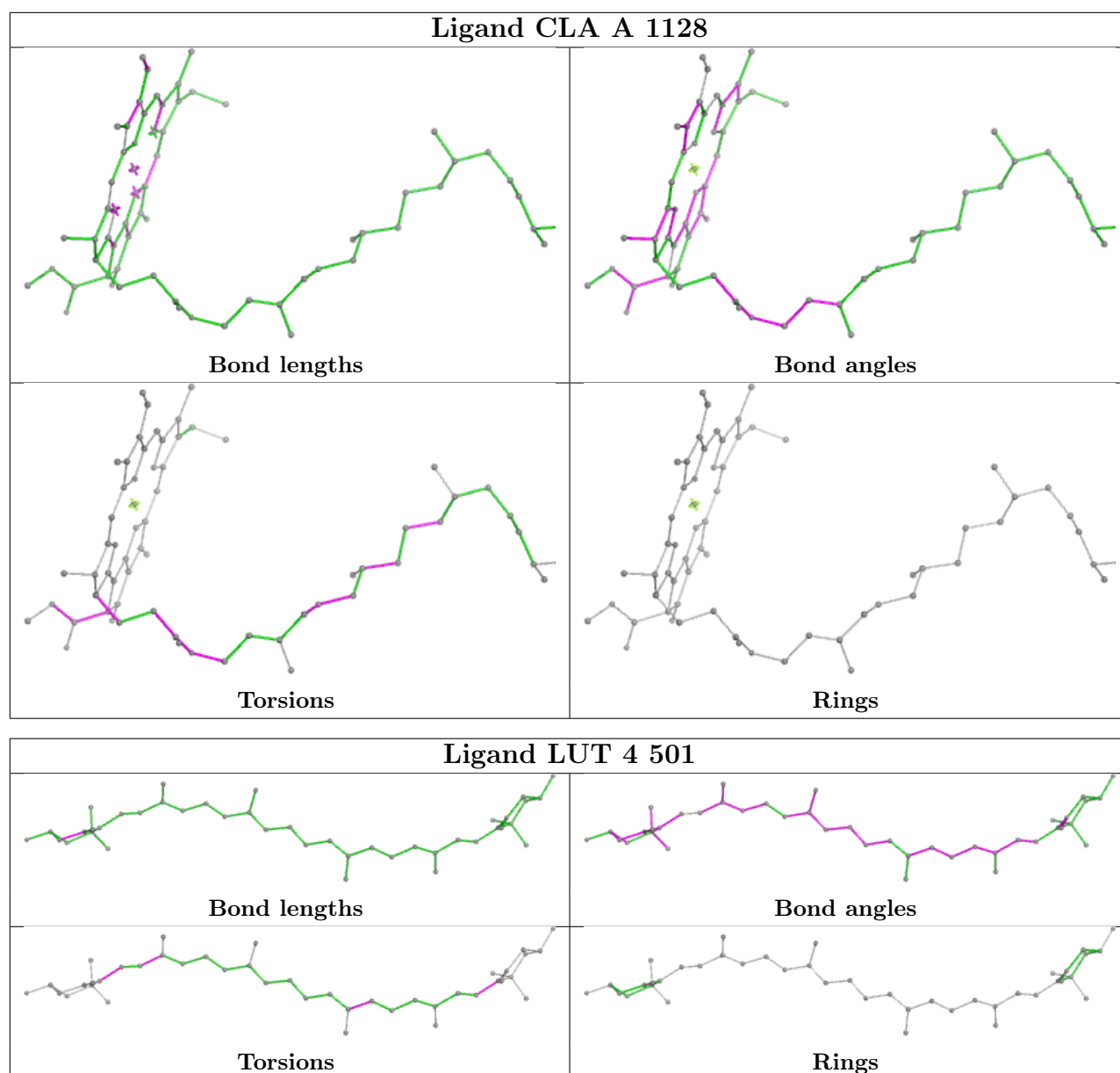


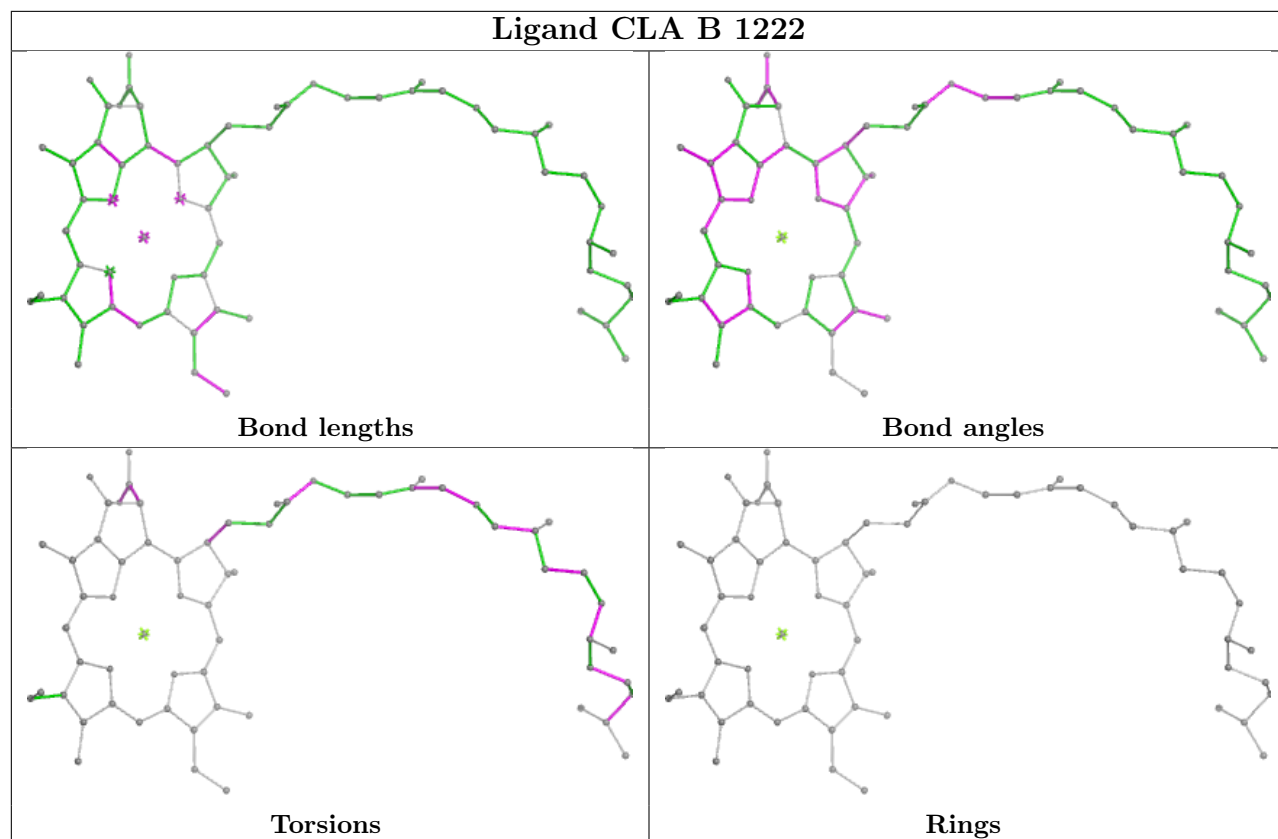
Rings

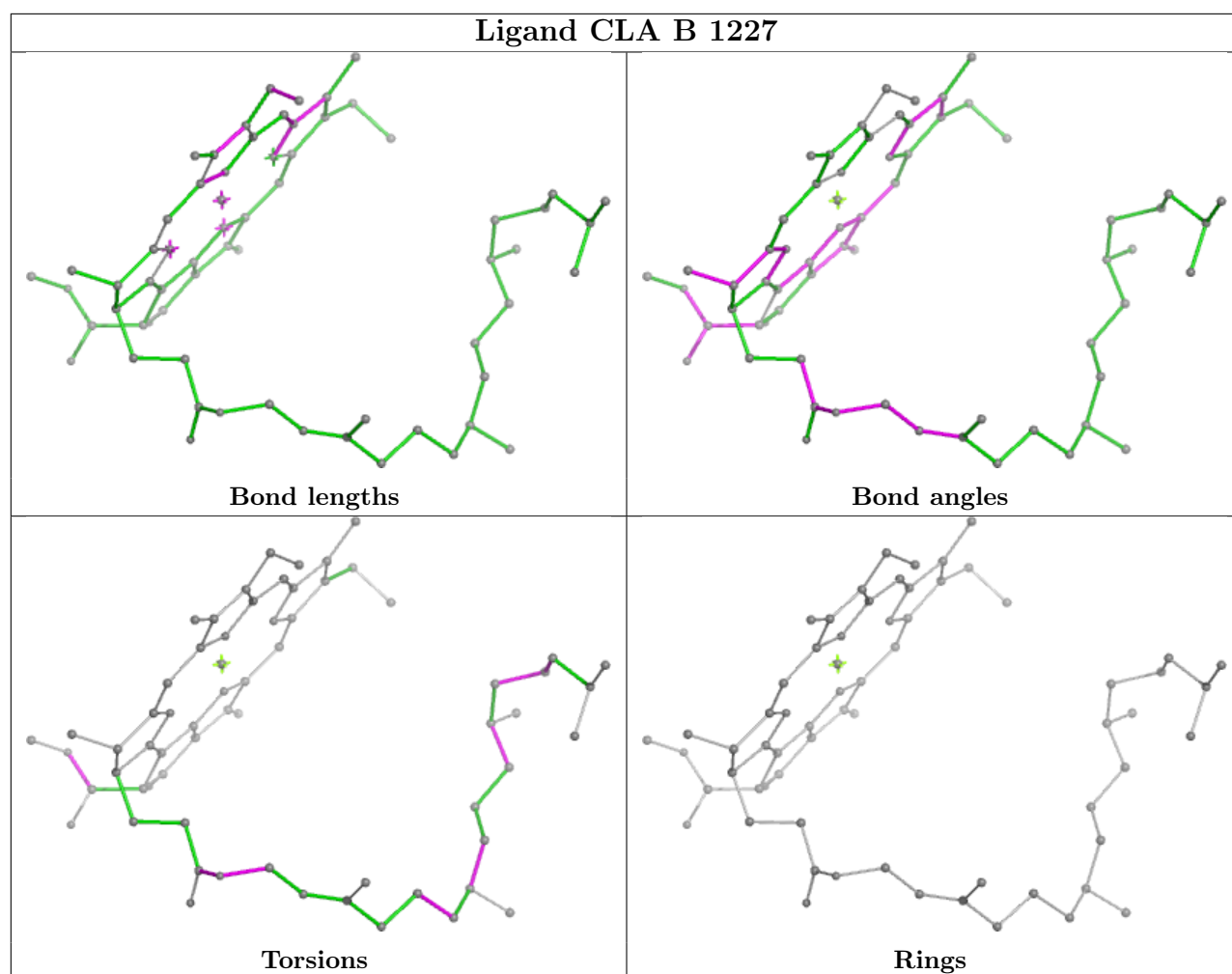
Ligand LUT 3 502**Ligand CHL 2 613**



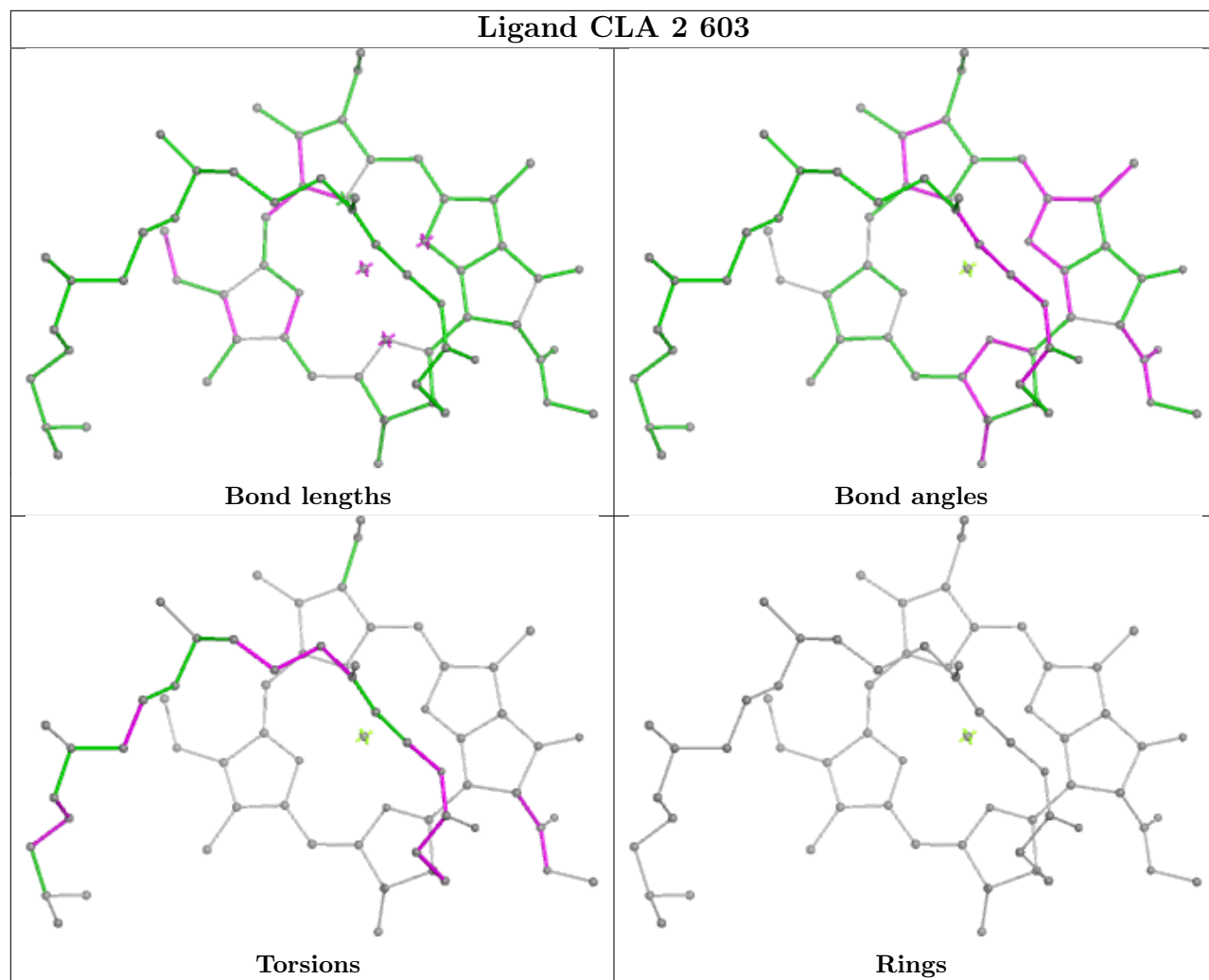




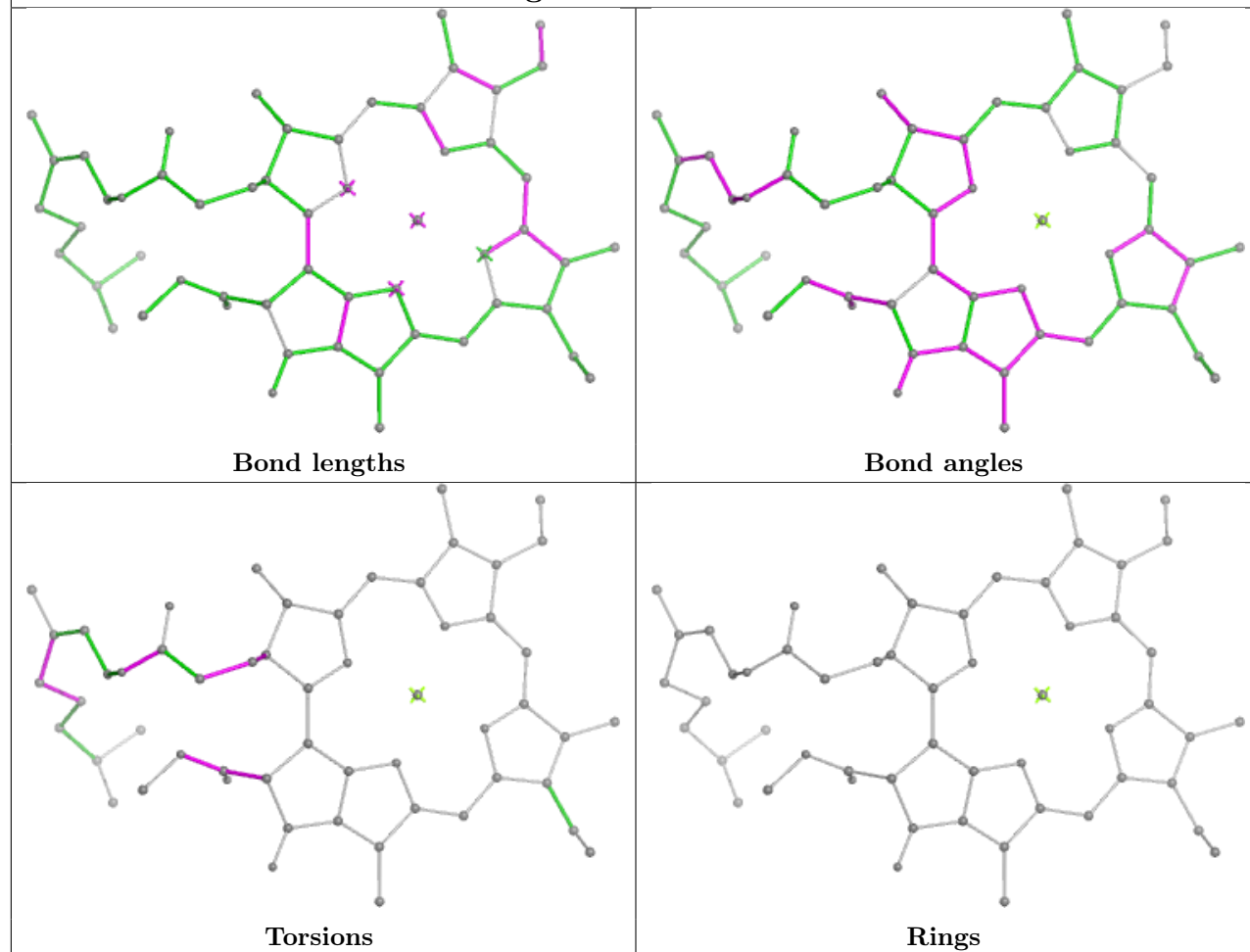




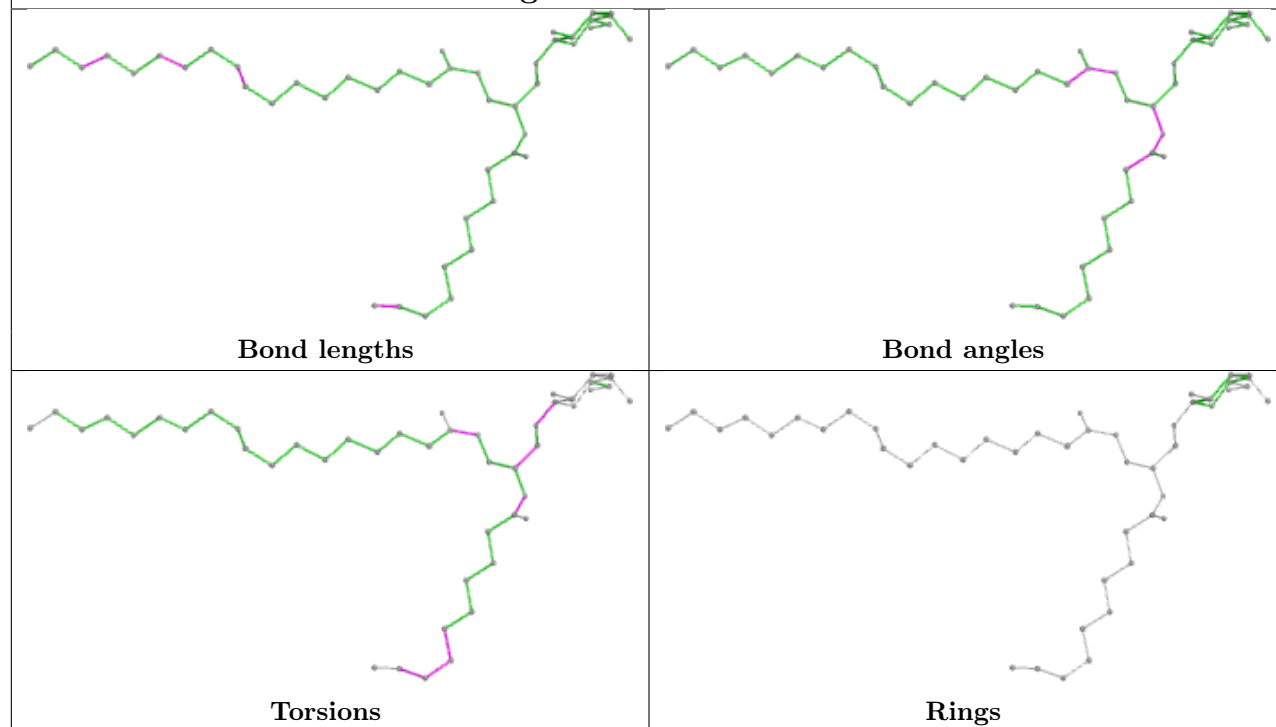
Ligand CLA 2 603

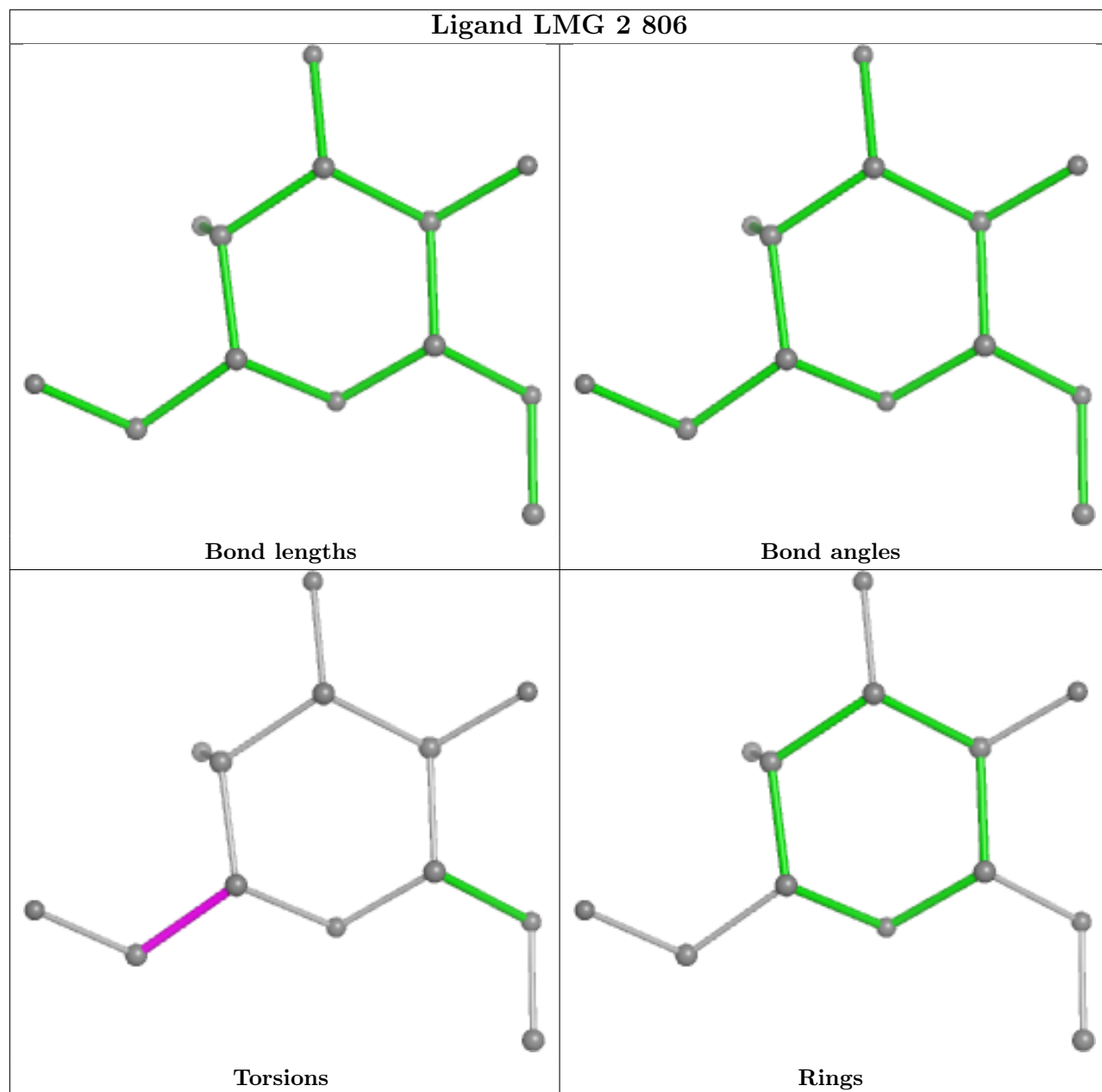


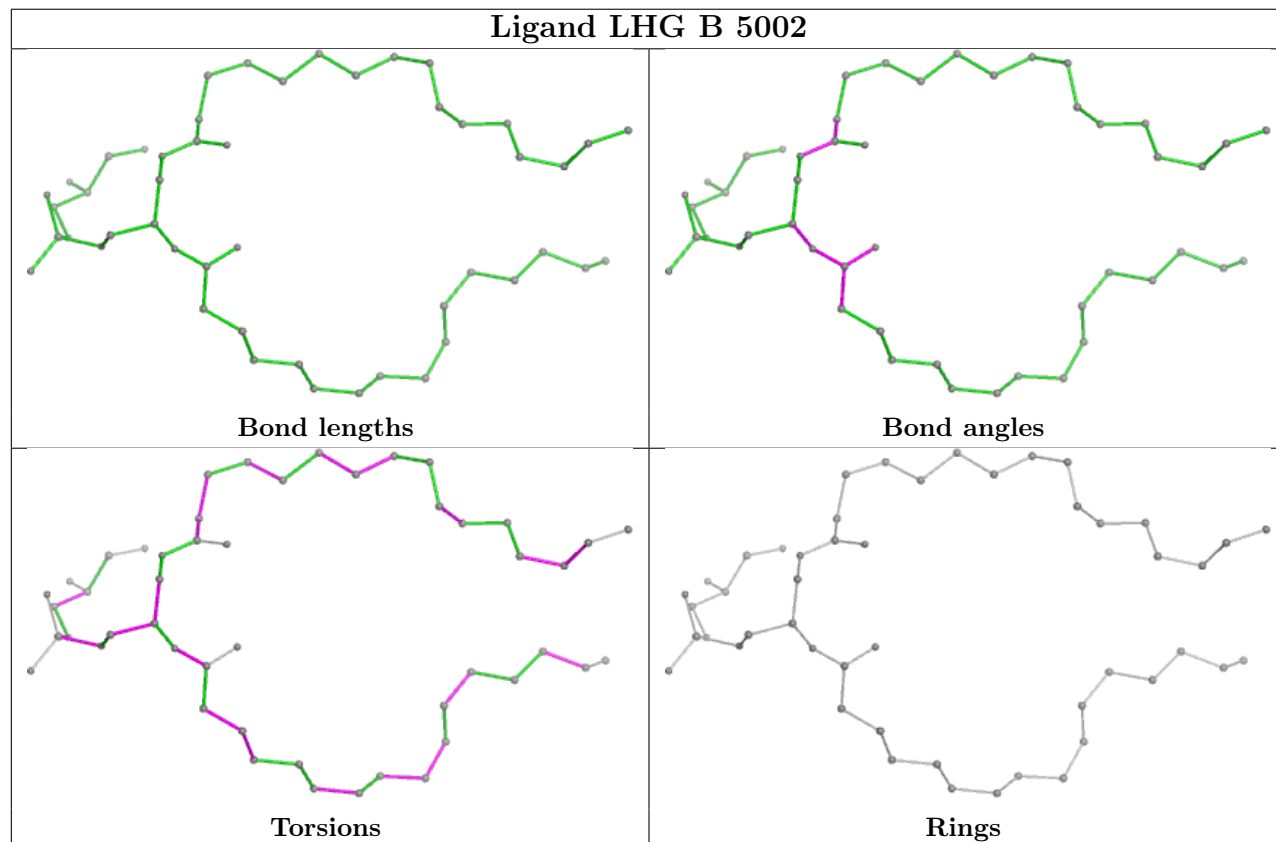
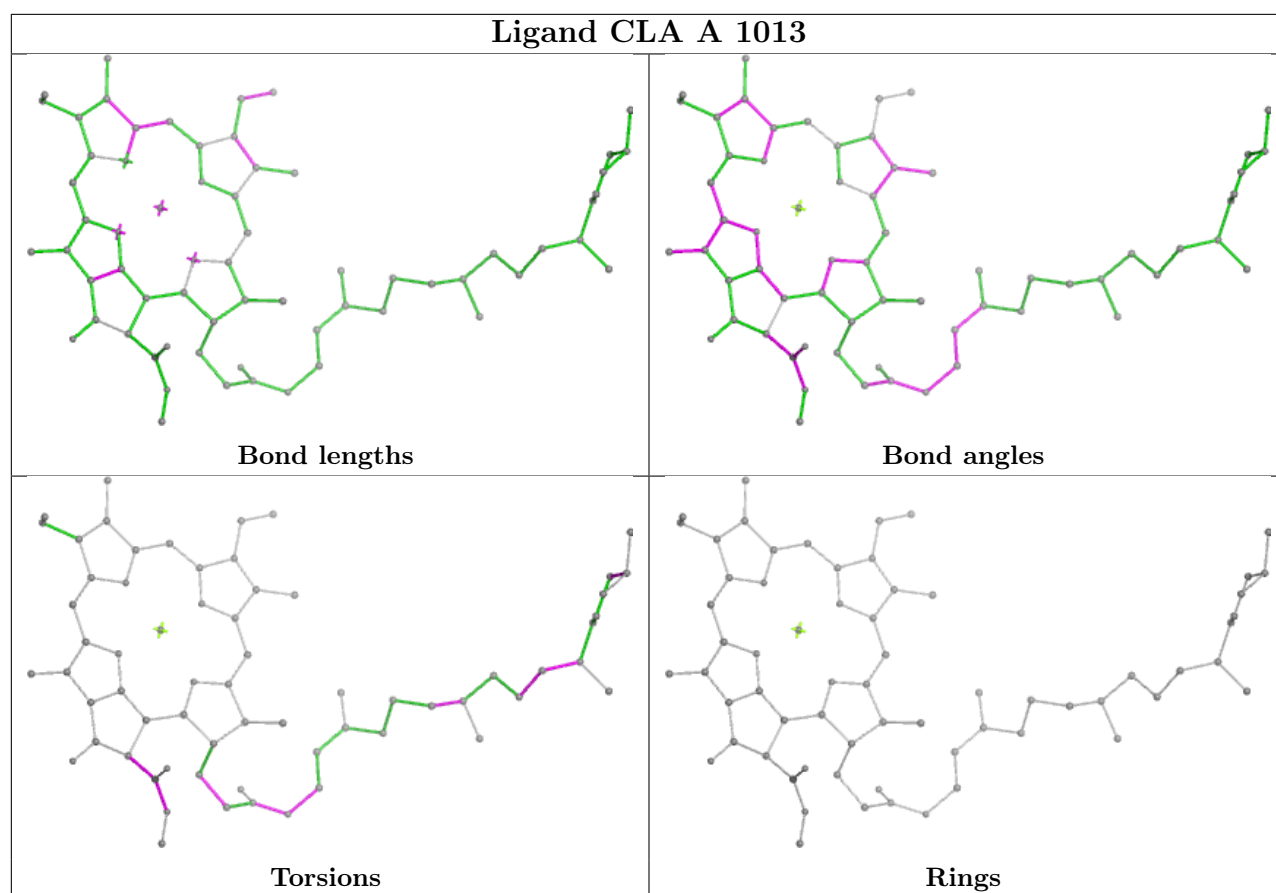
Ligand CLA 3 605



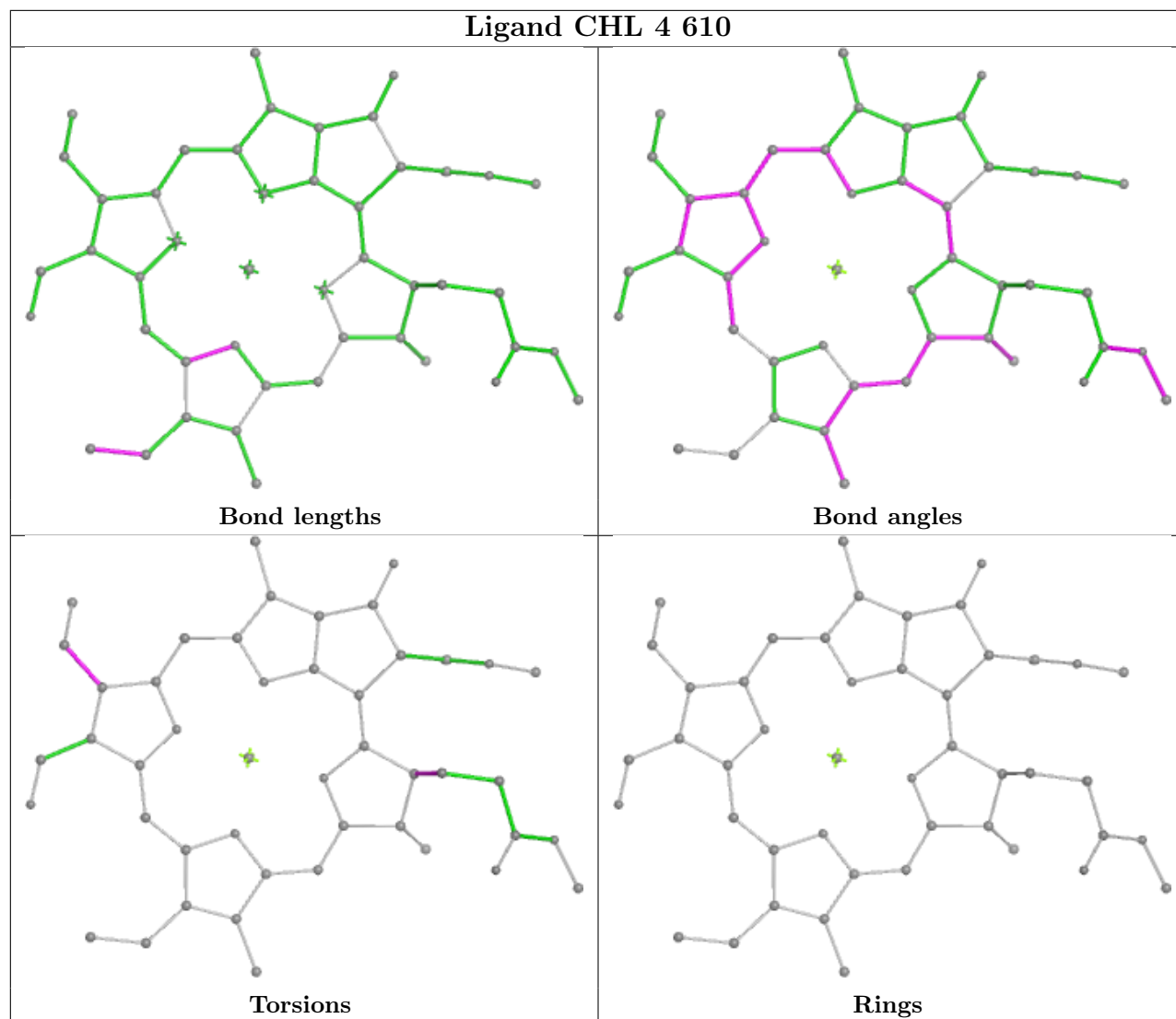
Ligand LMG F 5002

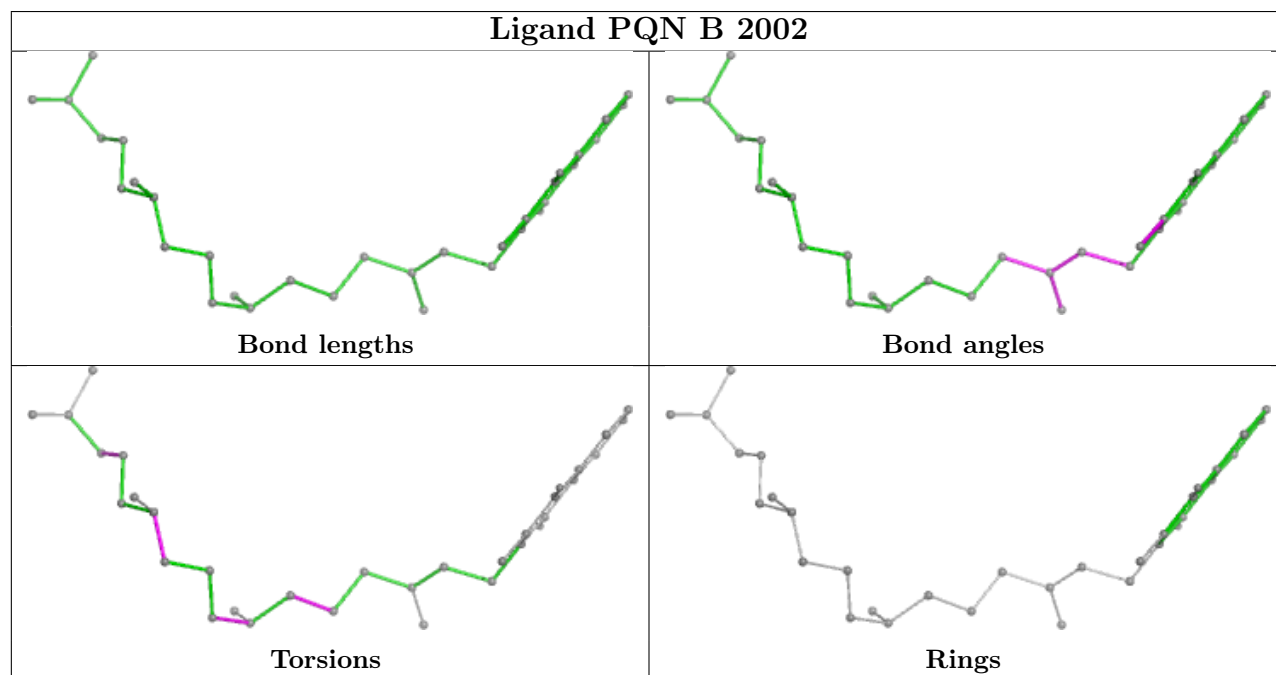
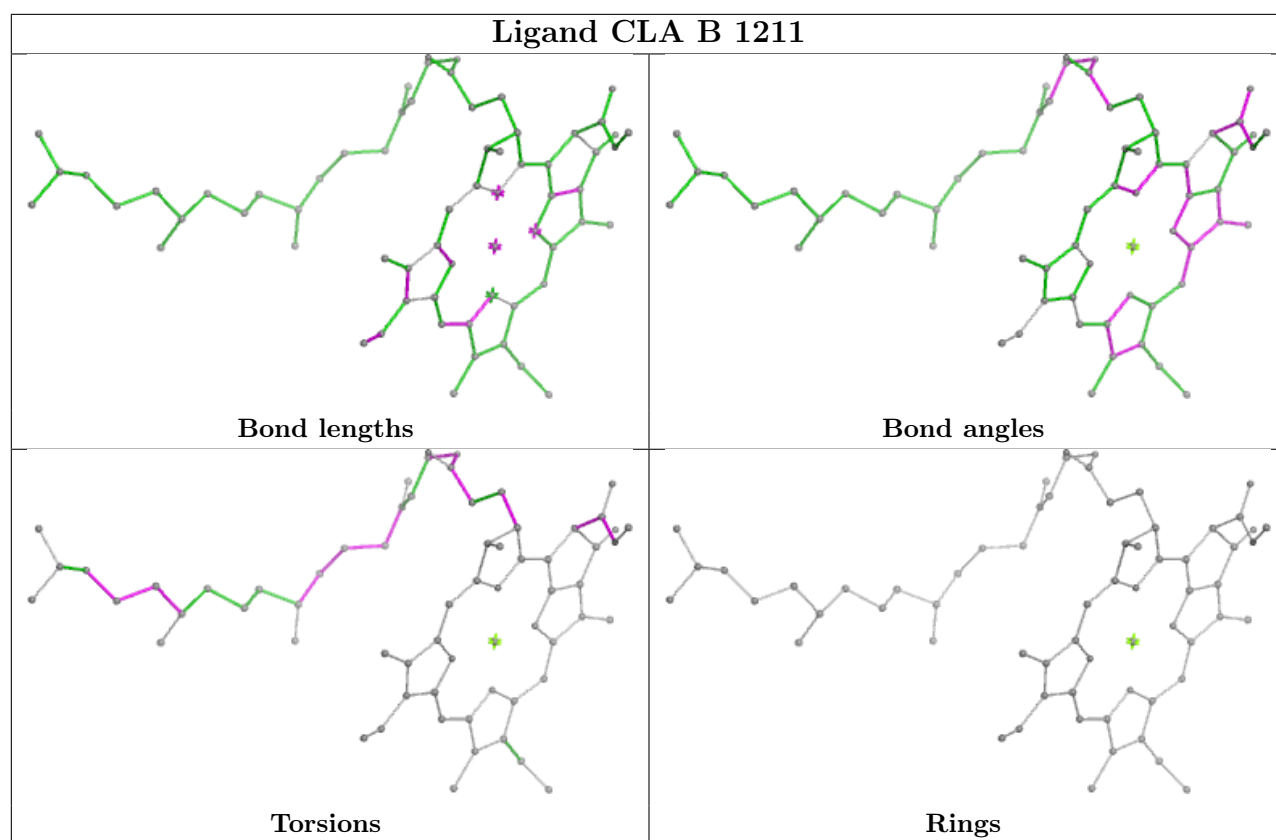


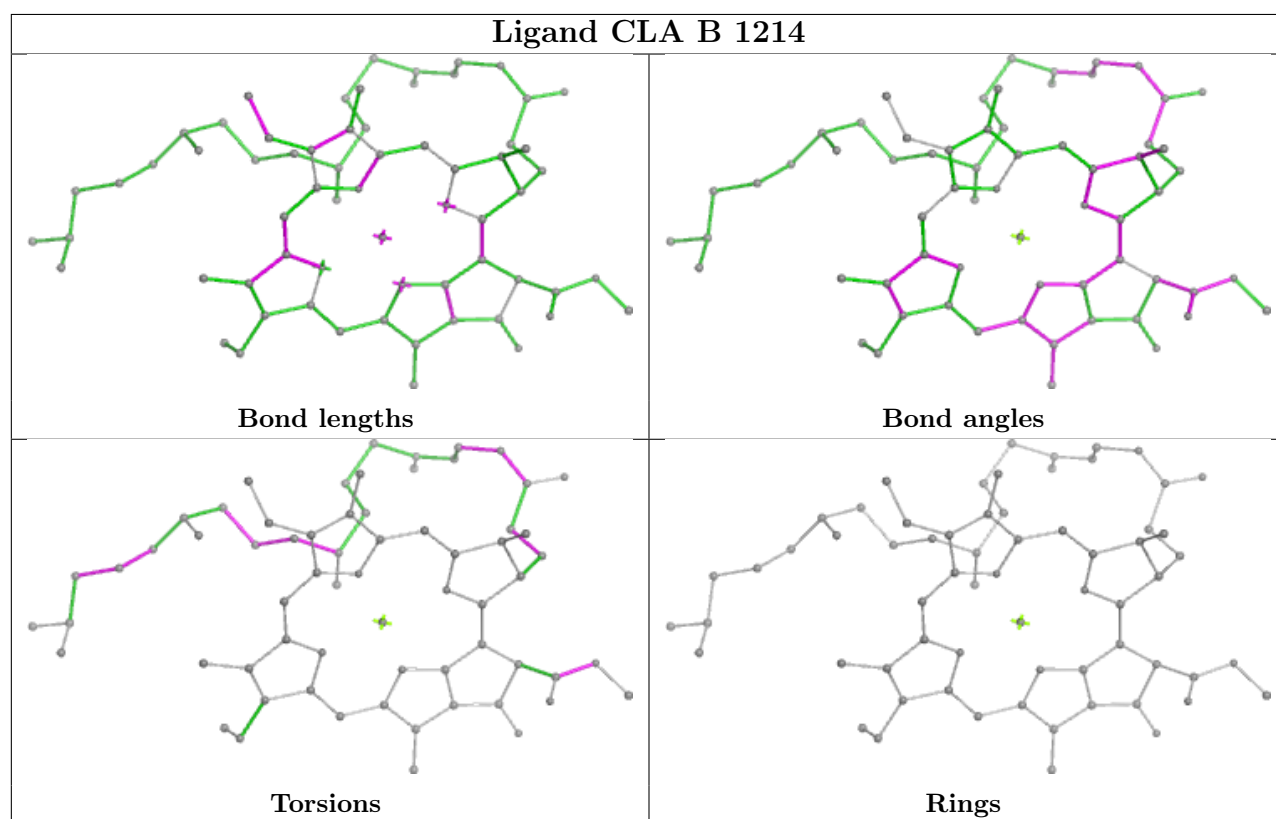
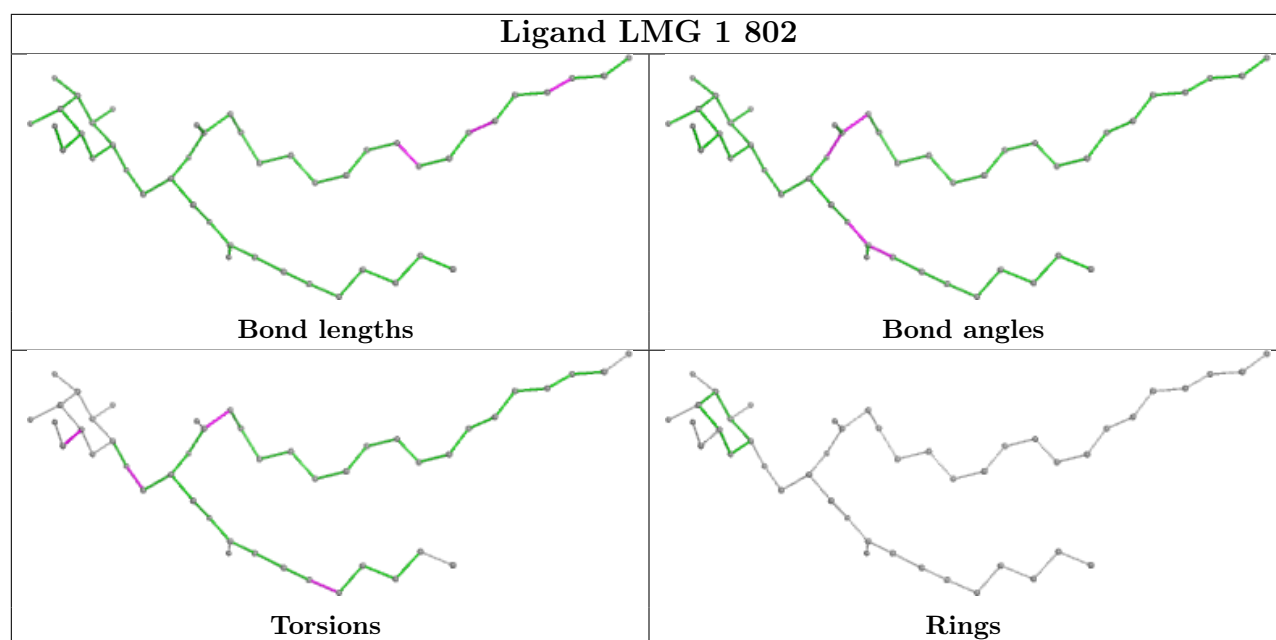


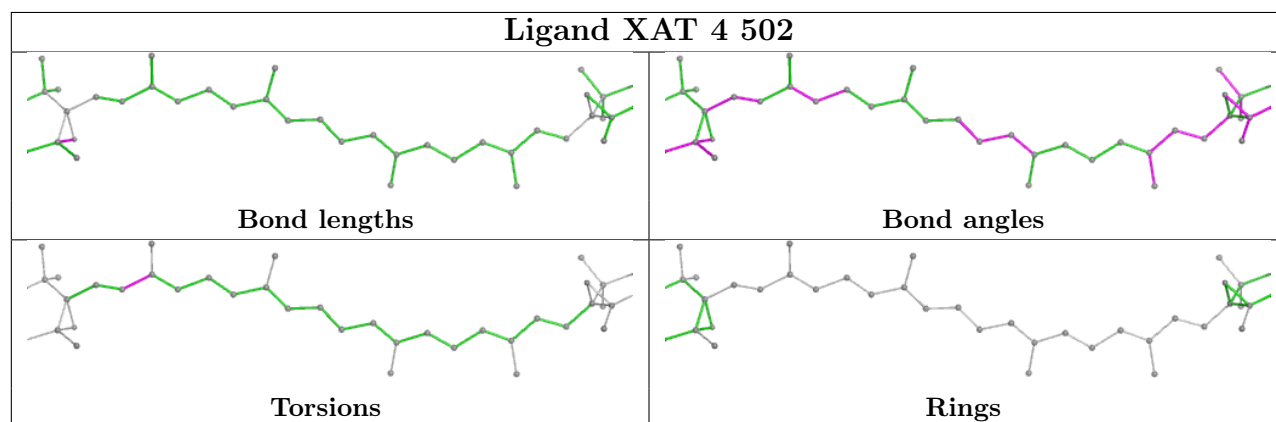
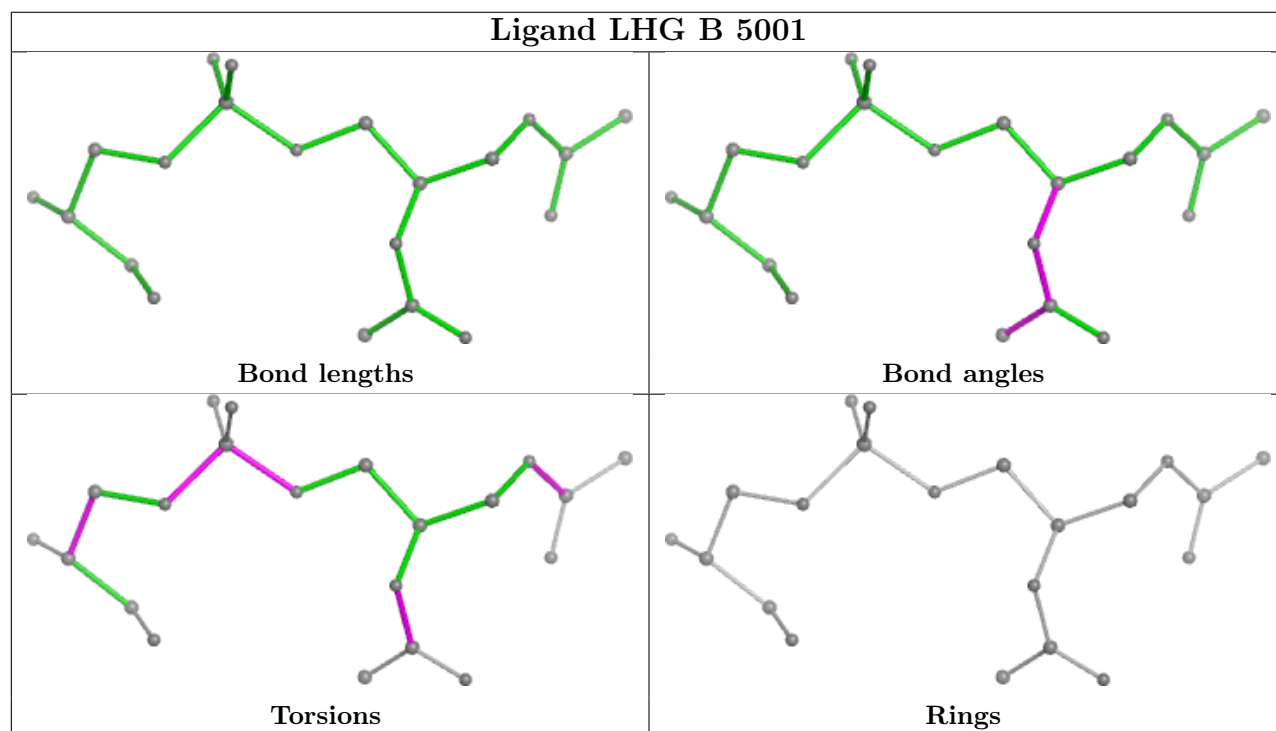
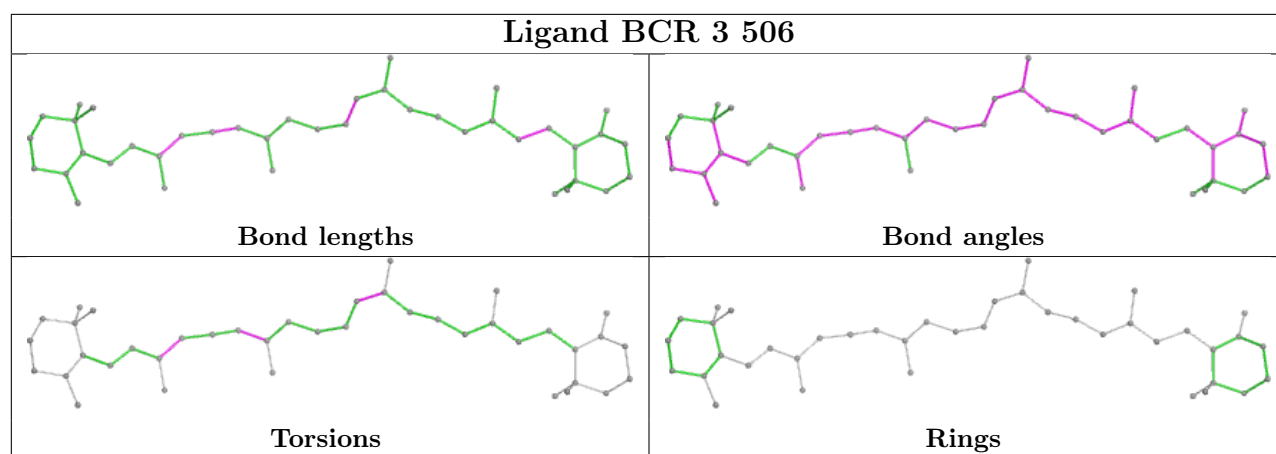


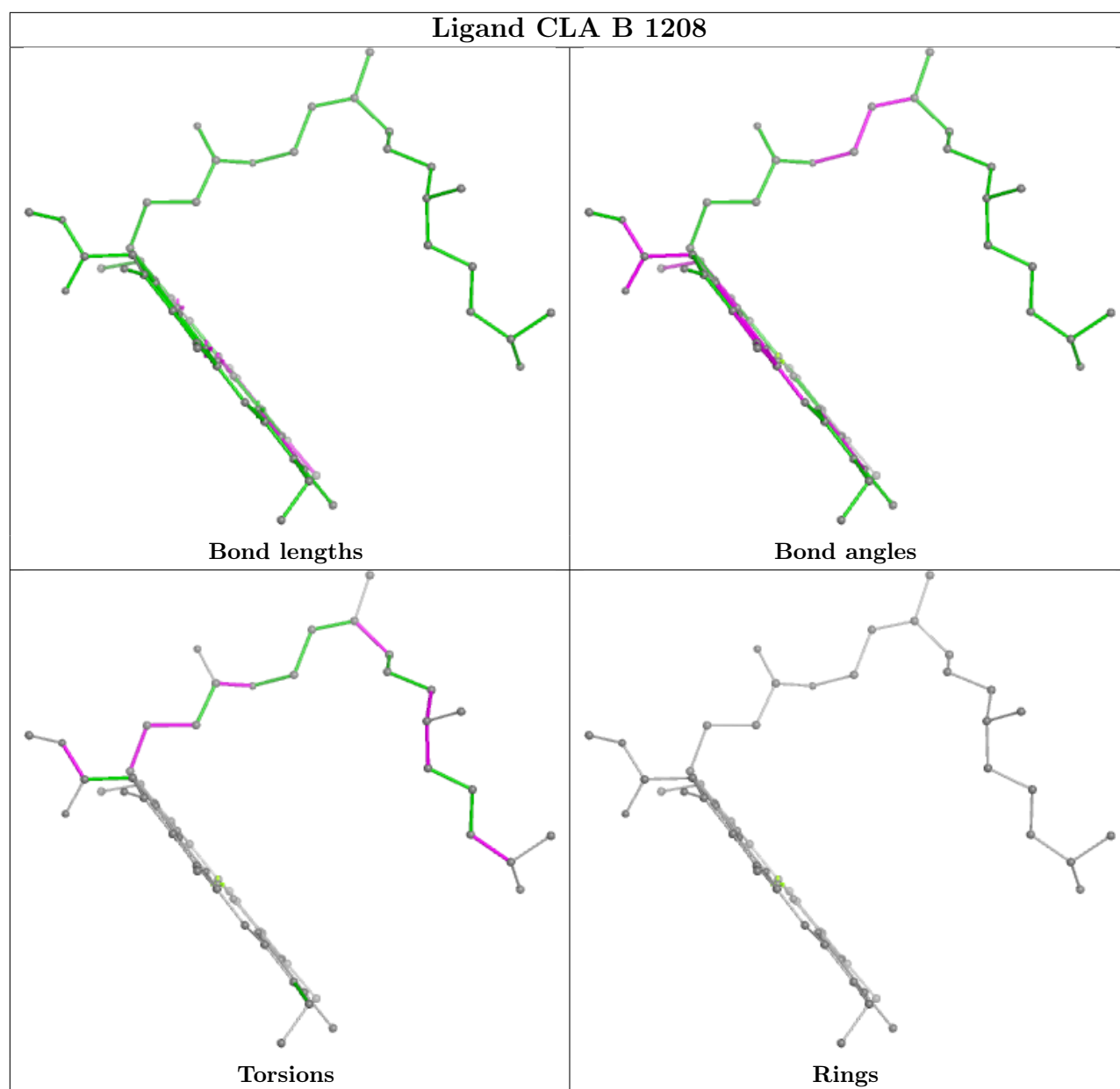
Ligand CHL 4 610

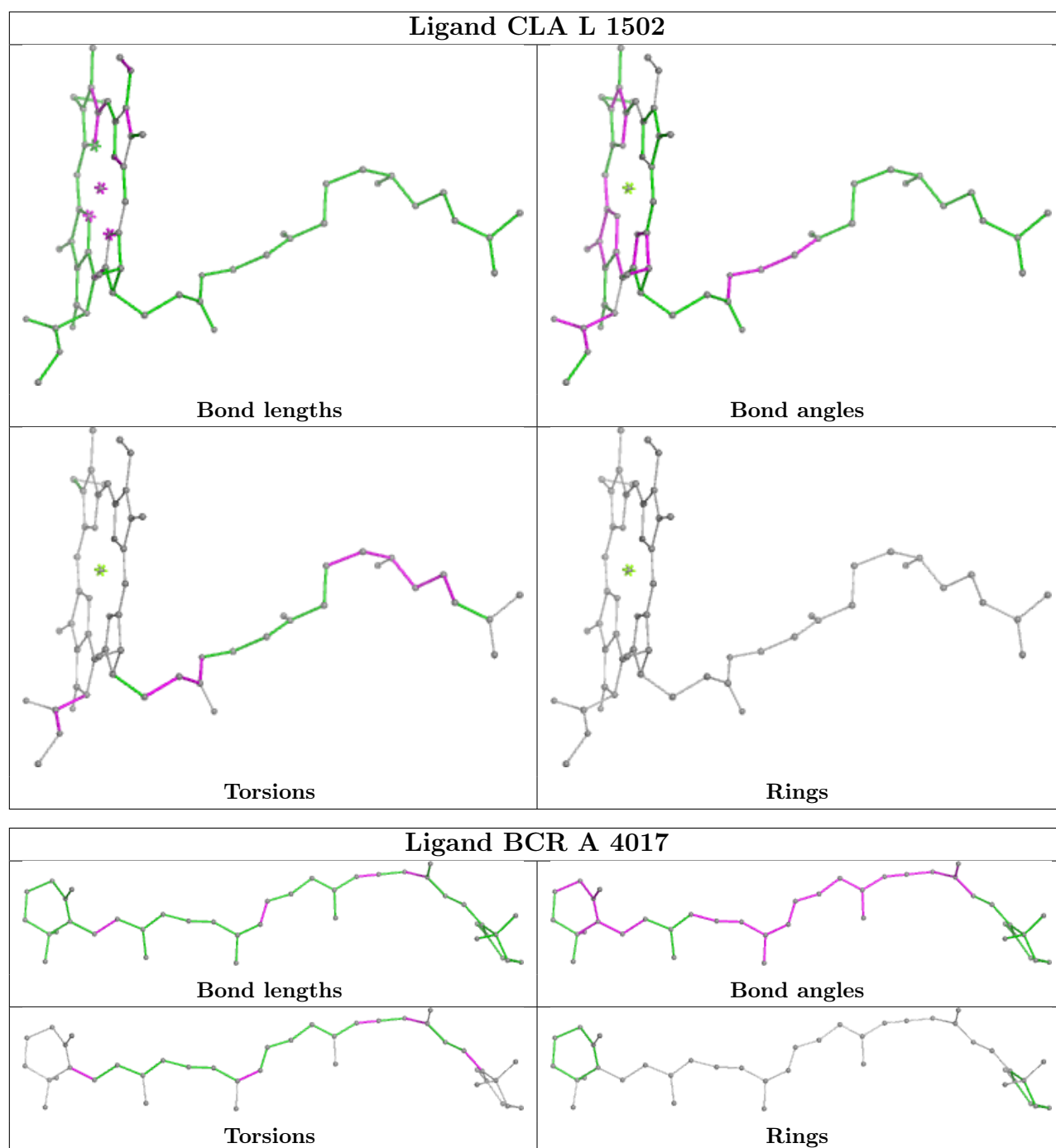




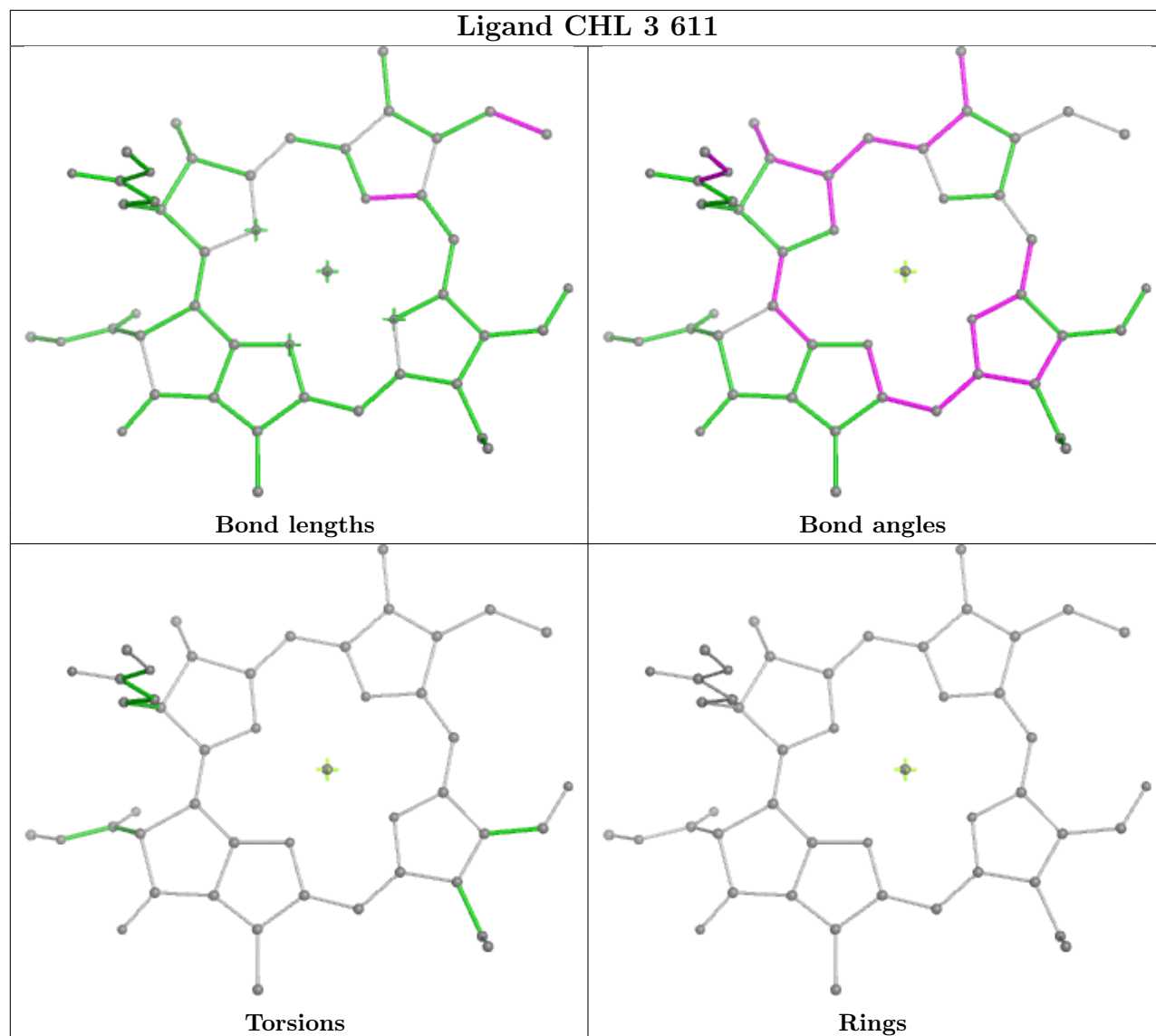


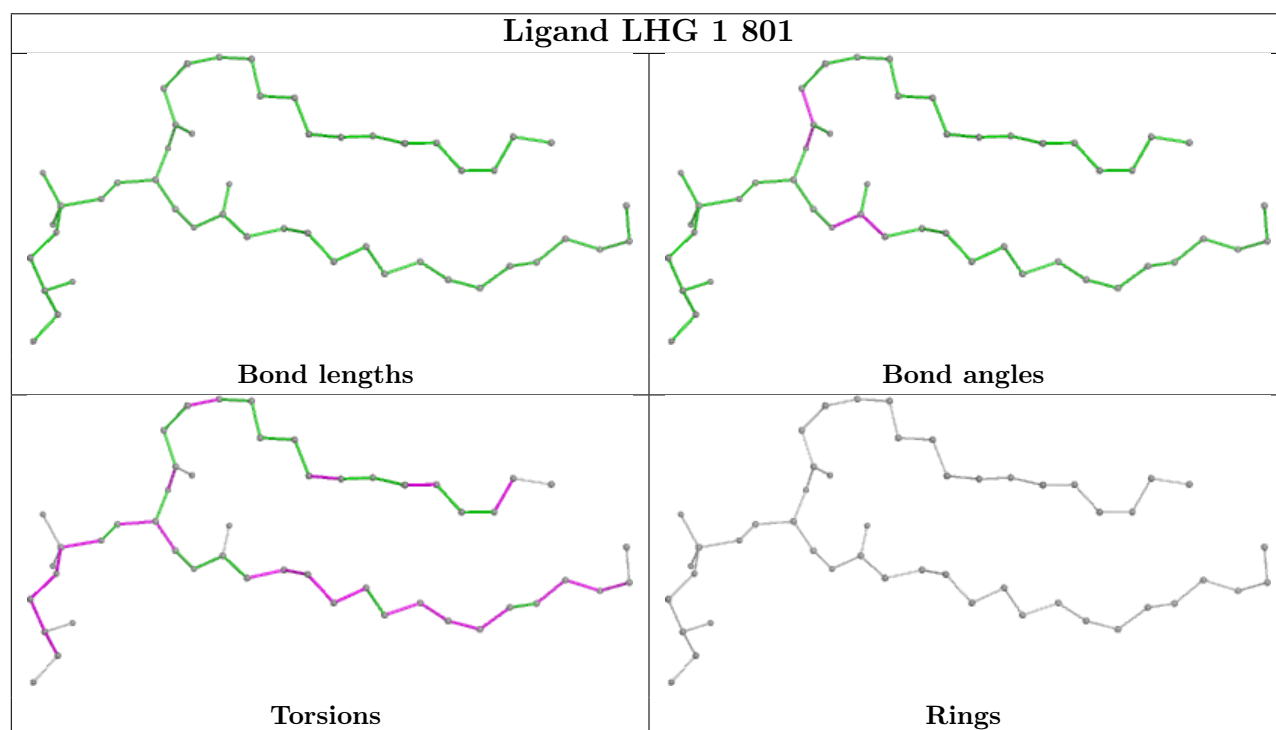
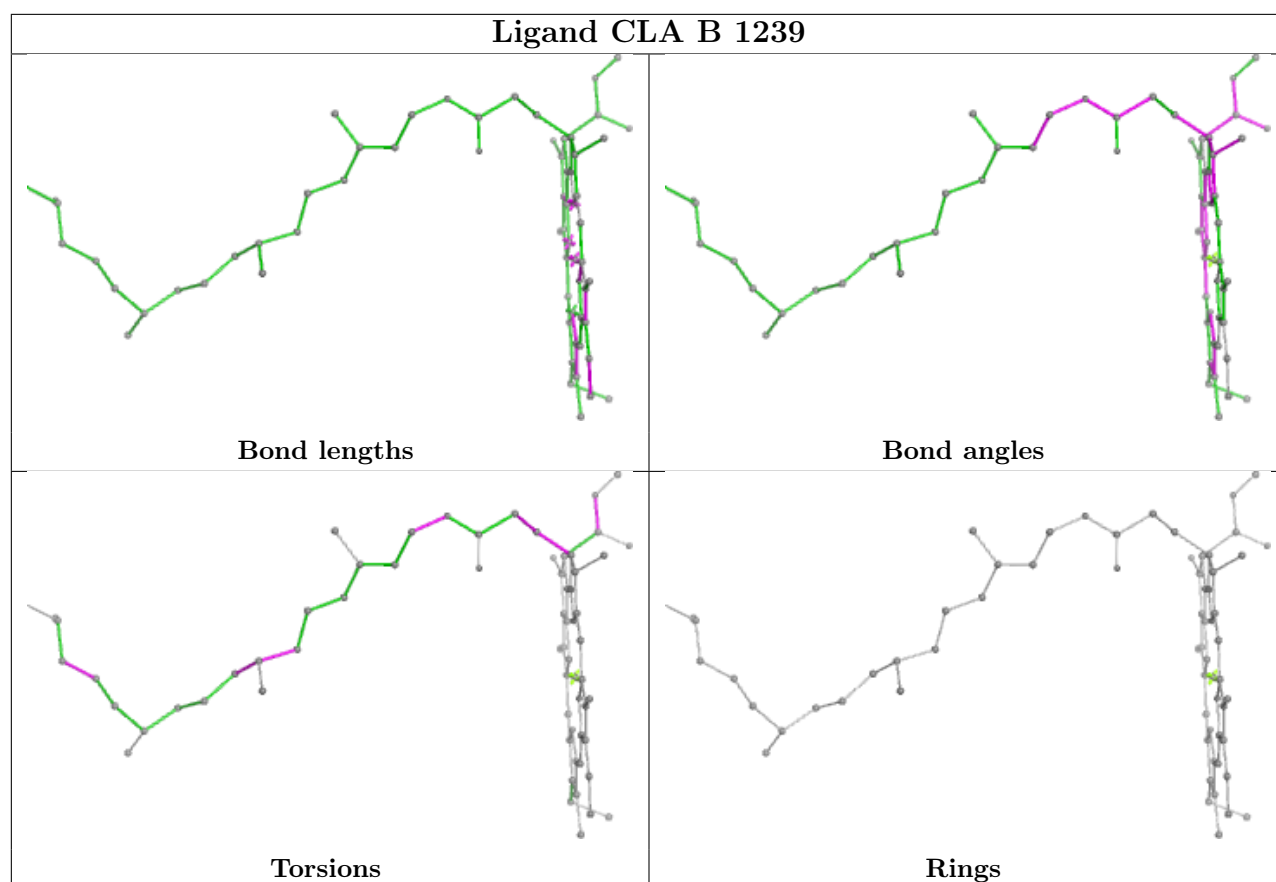


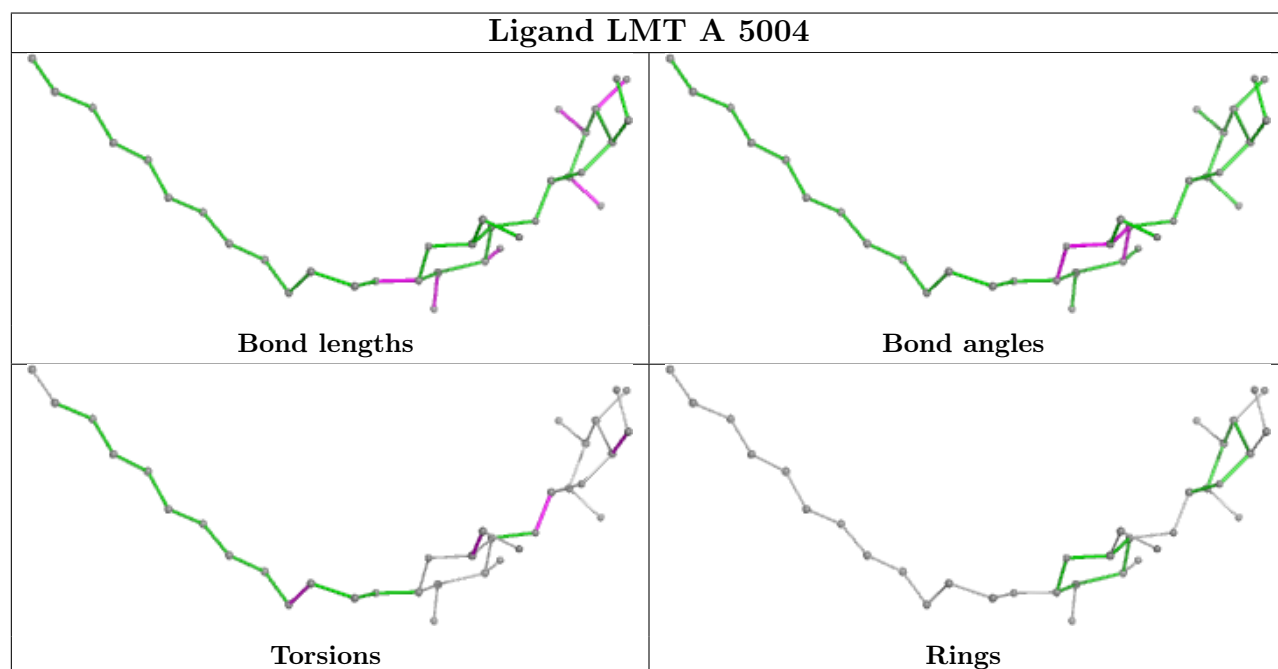
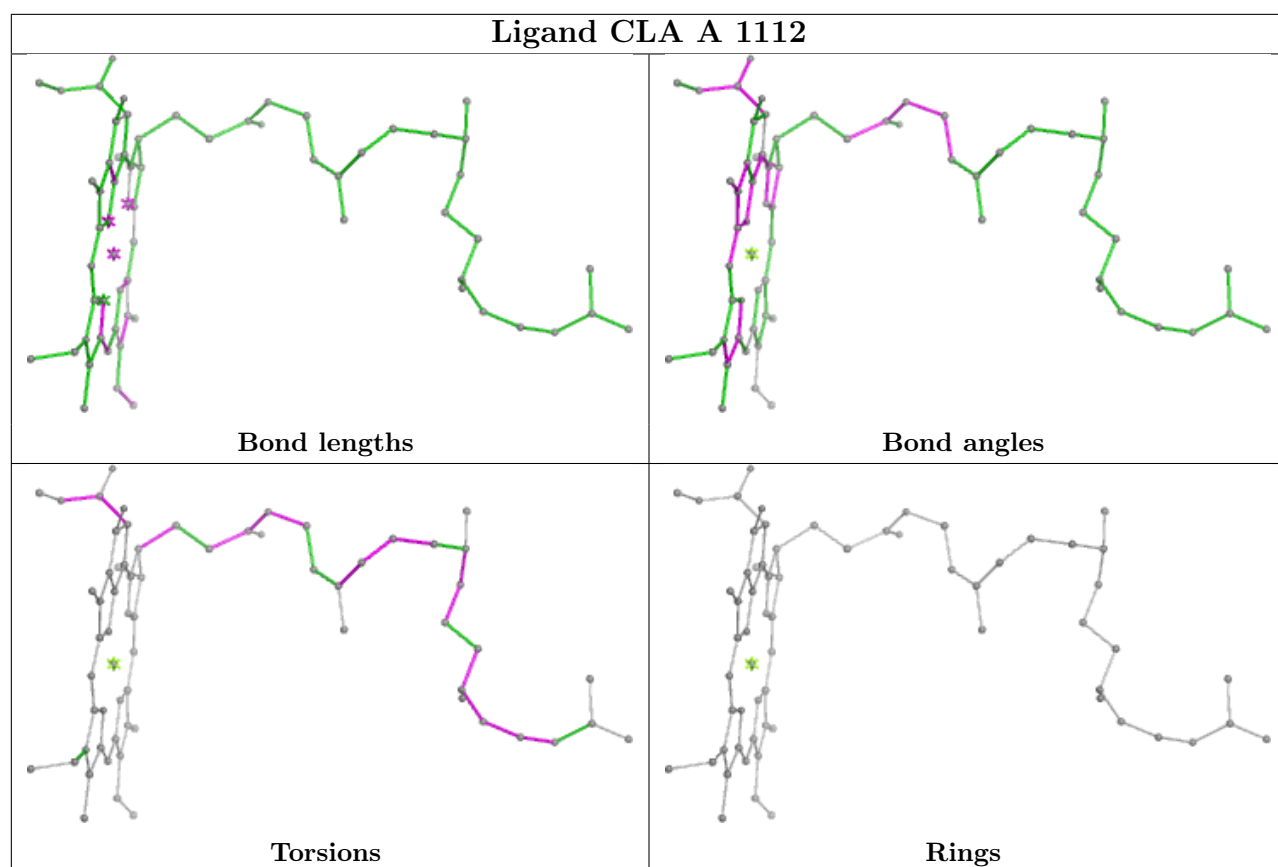




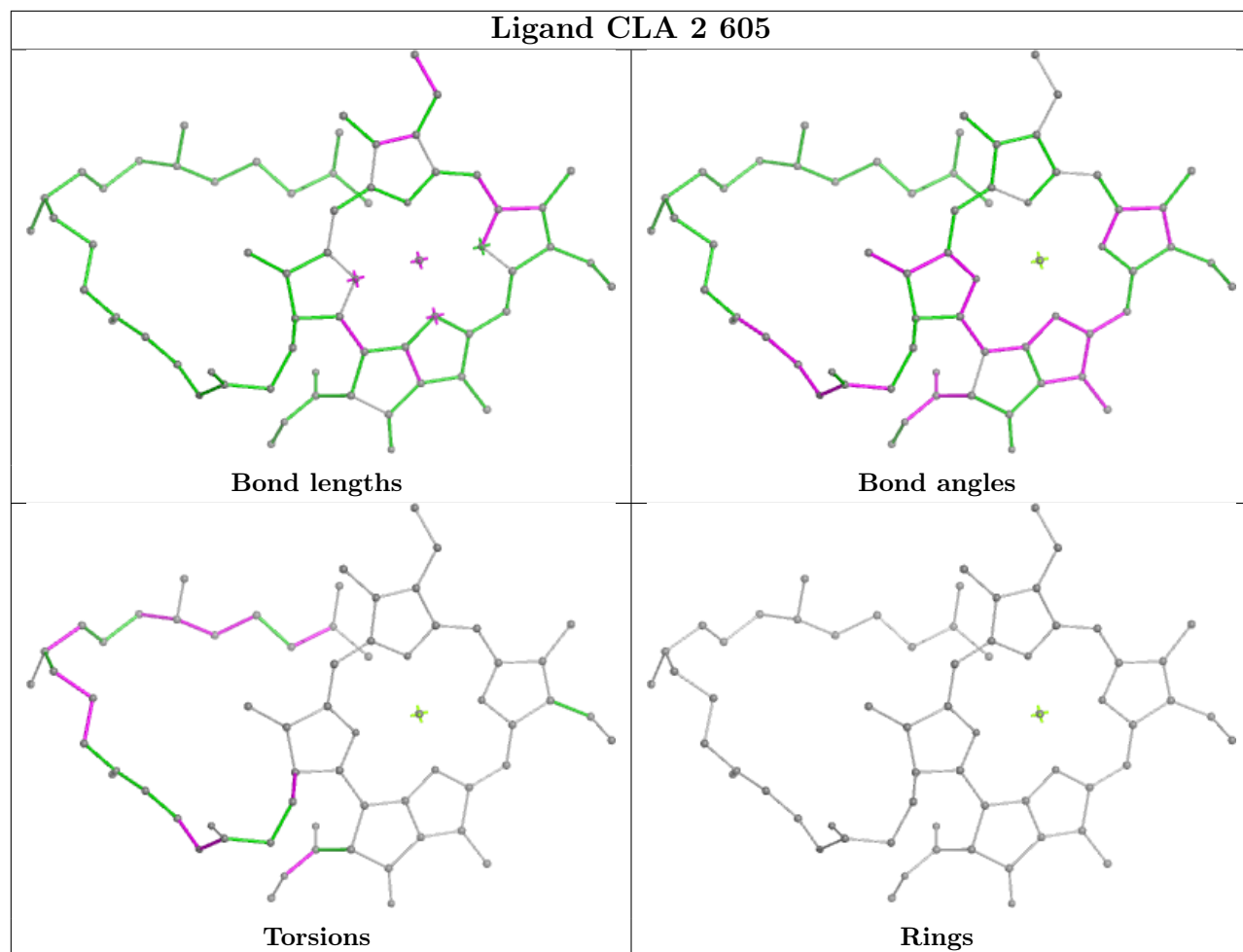
Ligand CHL 3 611

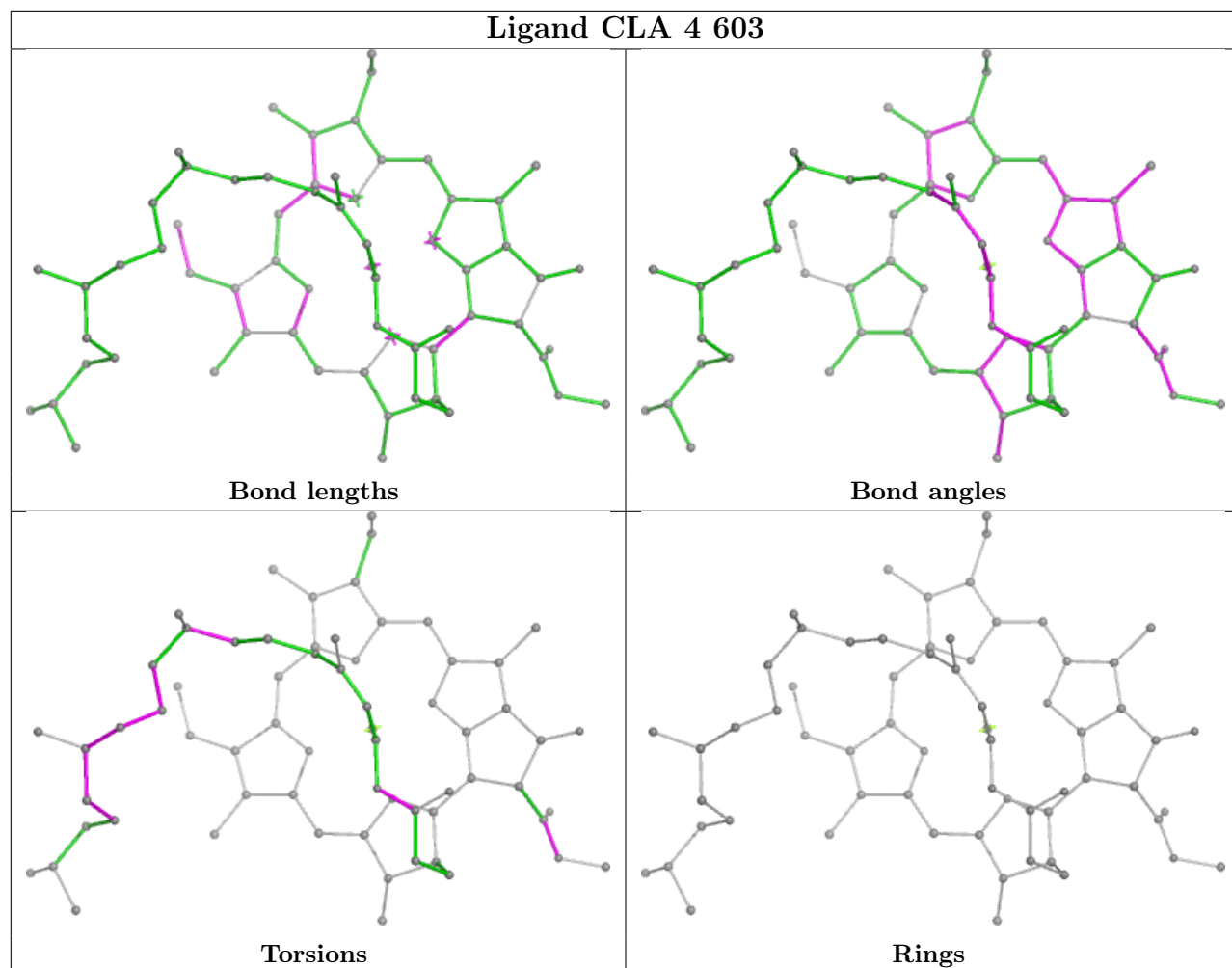




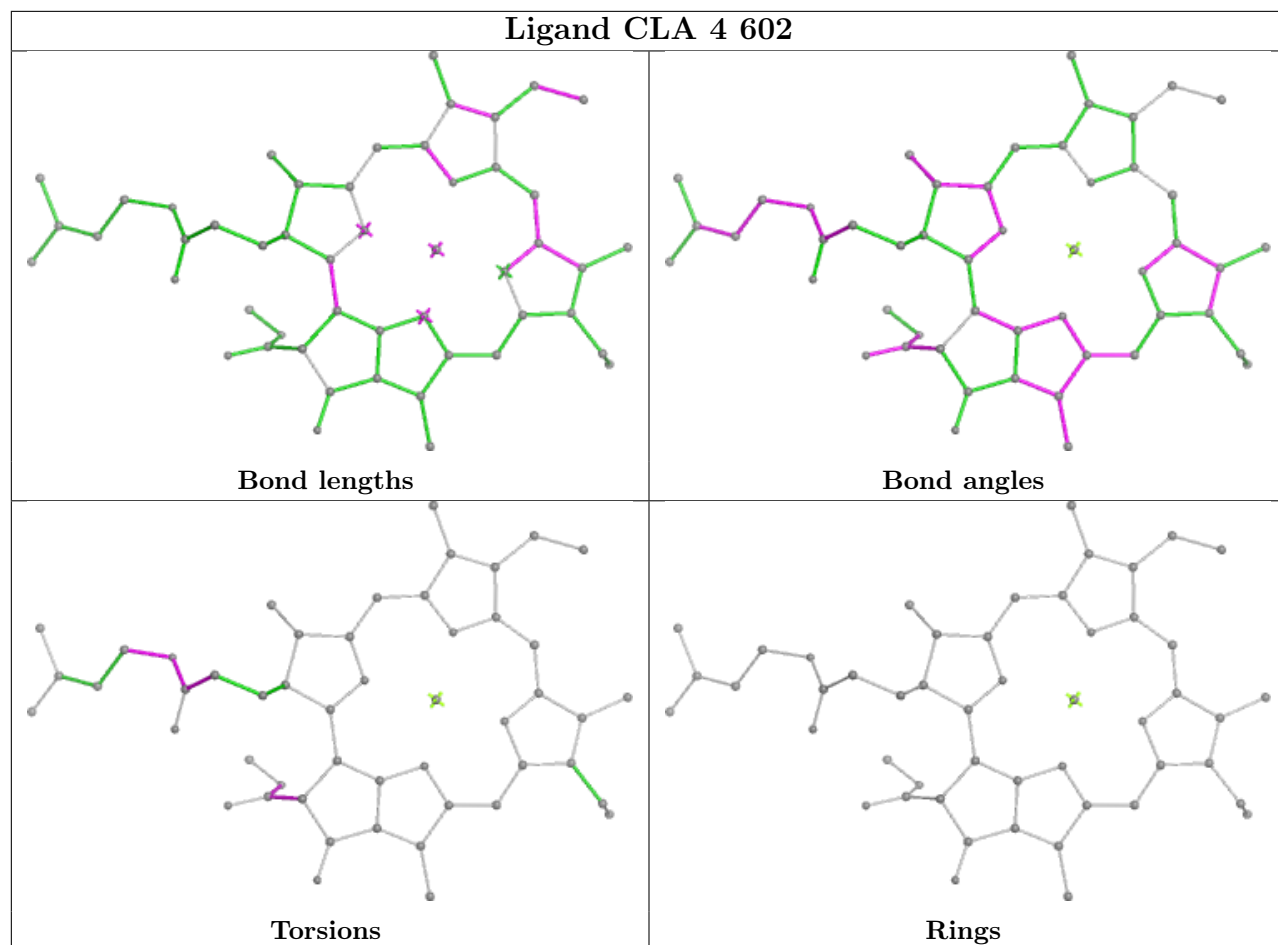


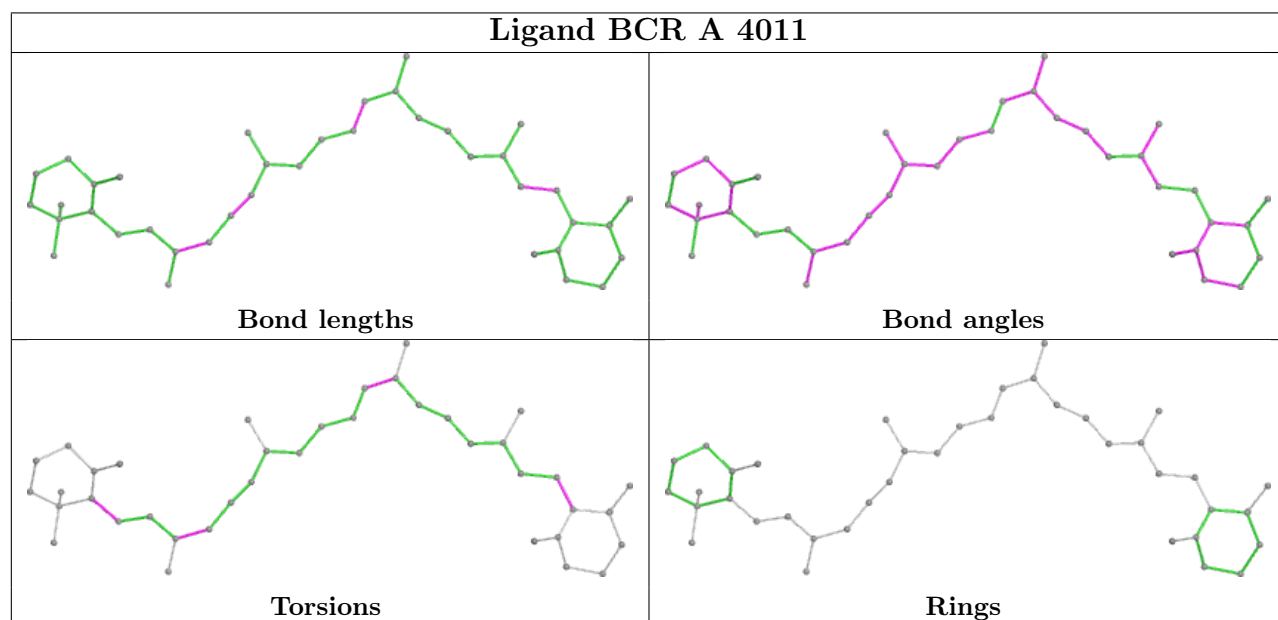
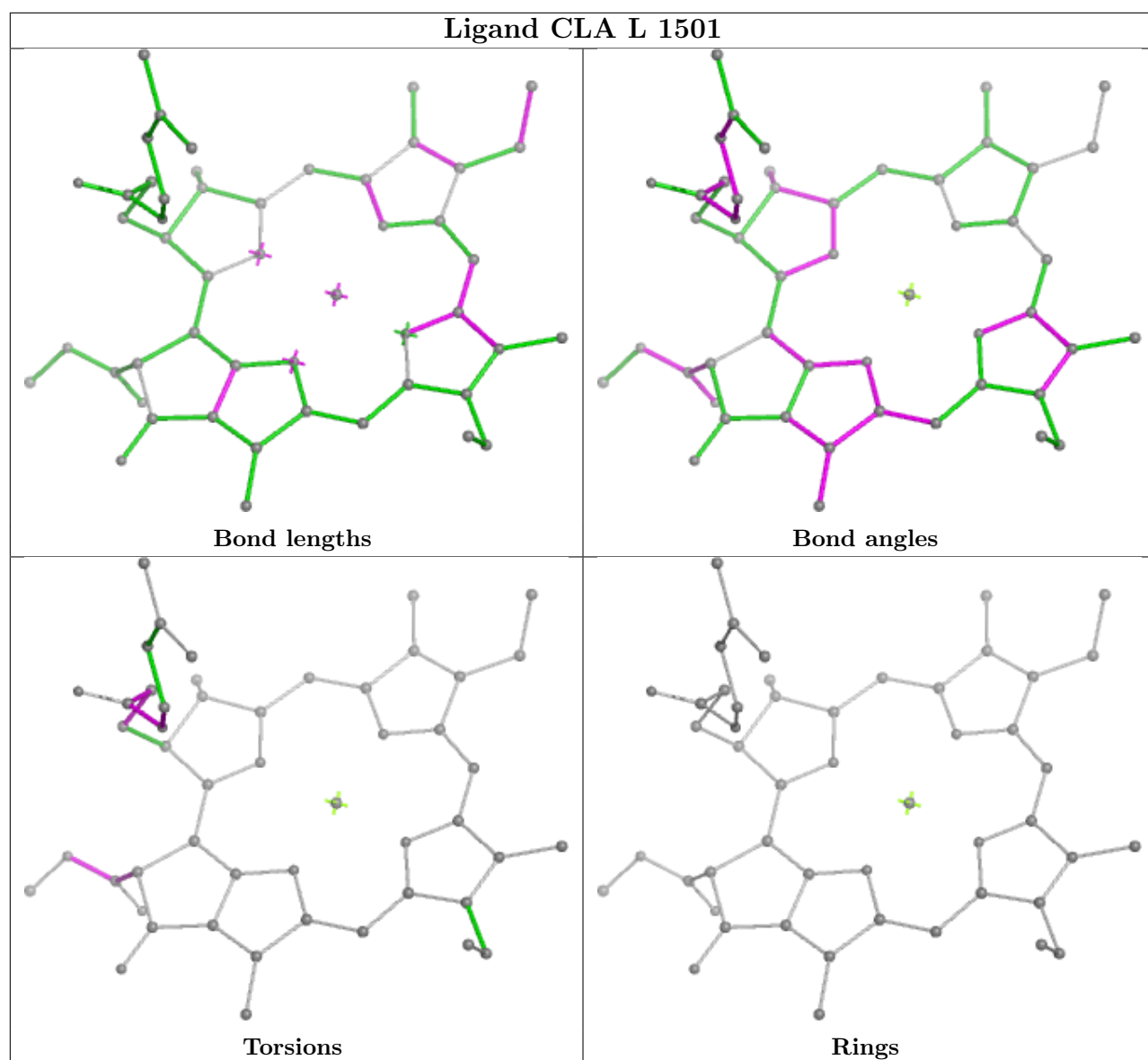
Ligand CLA 2 605

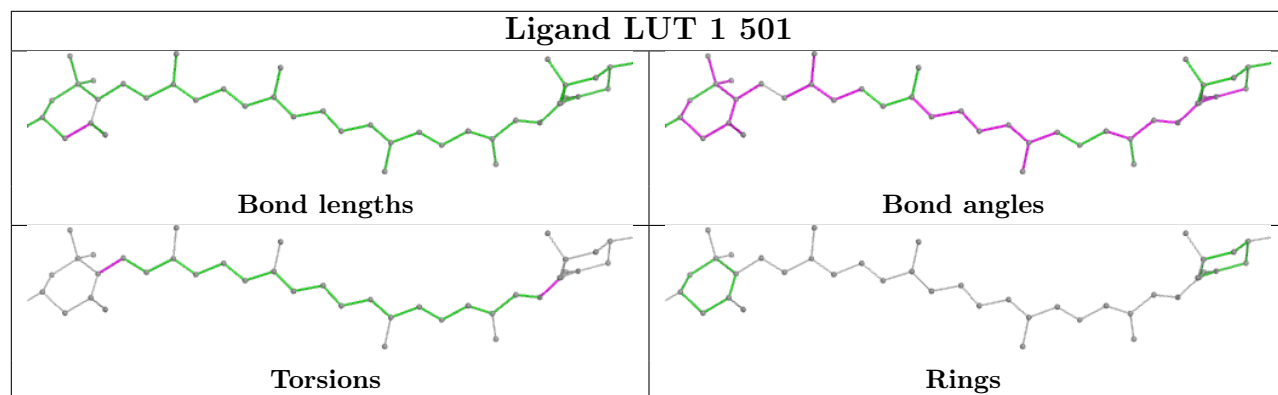
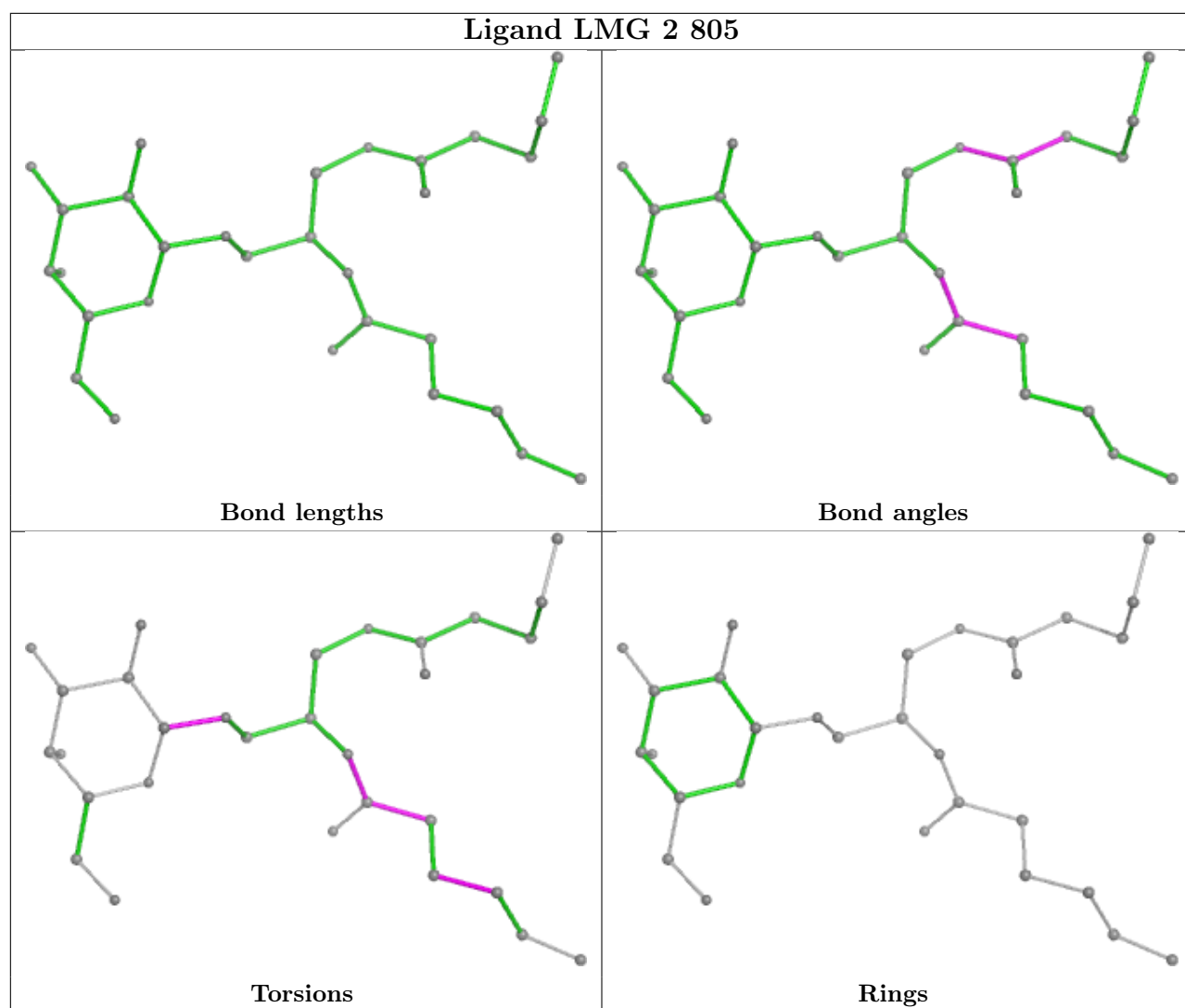


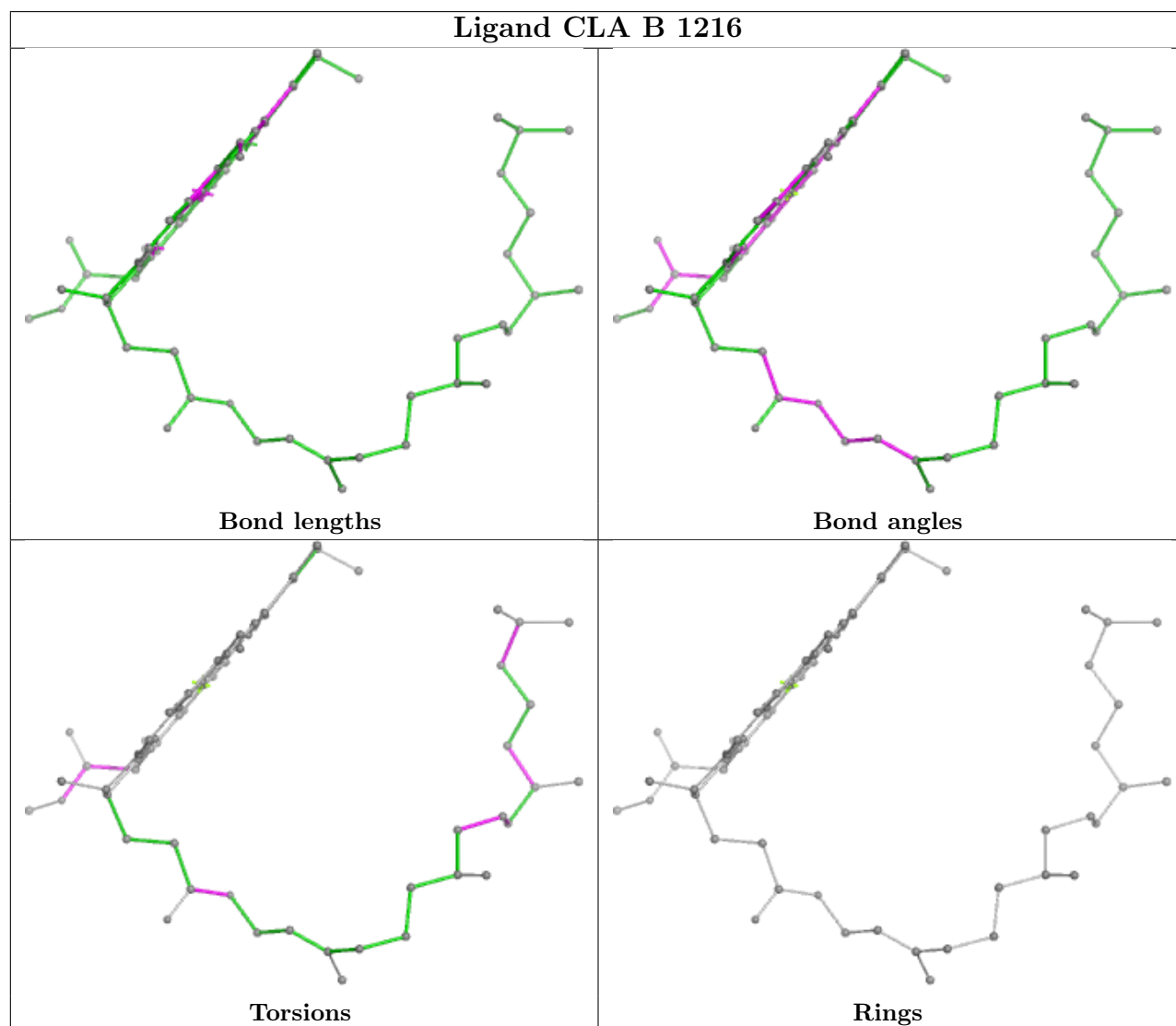
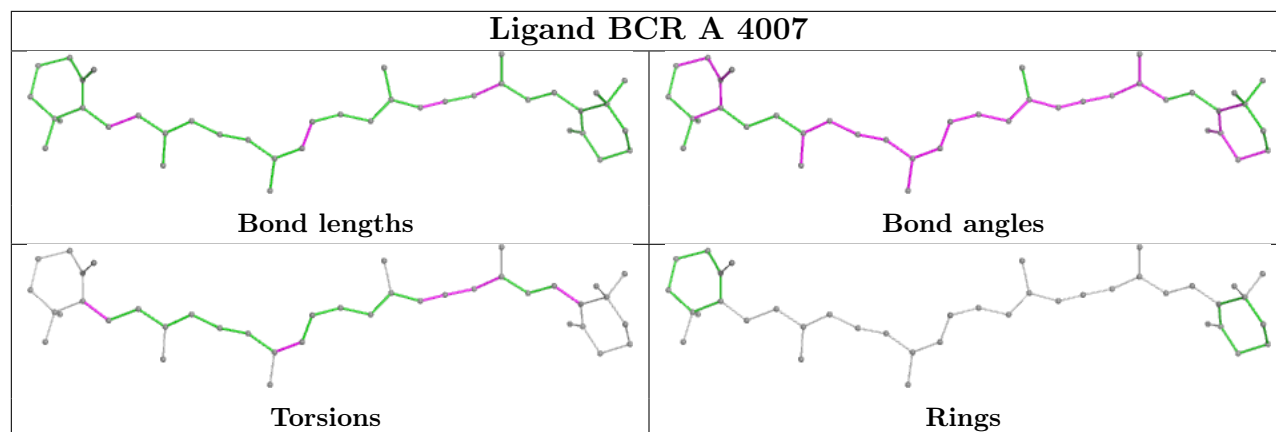
Ligand CLA 4 603

Ligand CLA 4 602

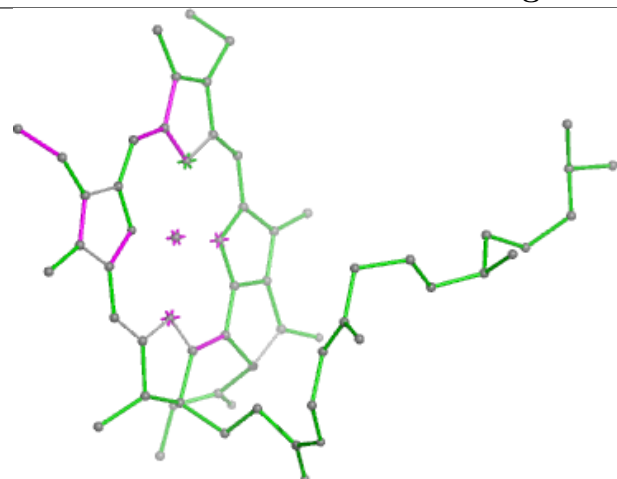




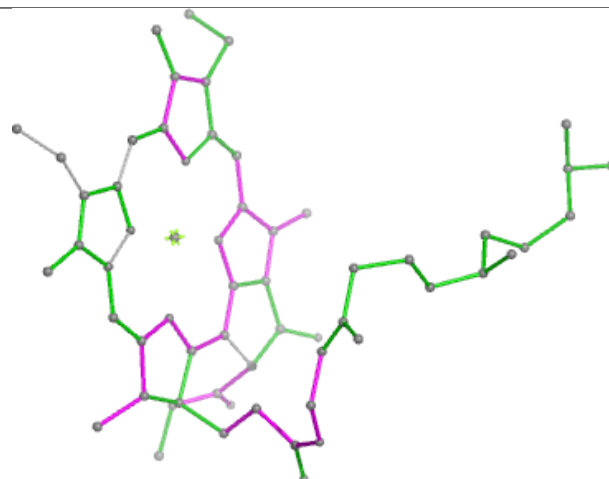




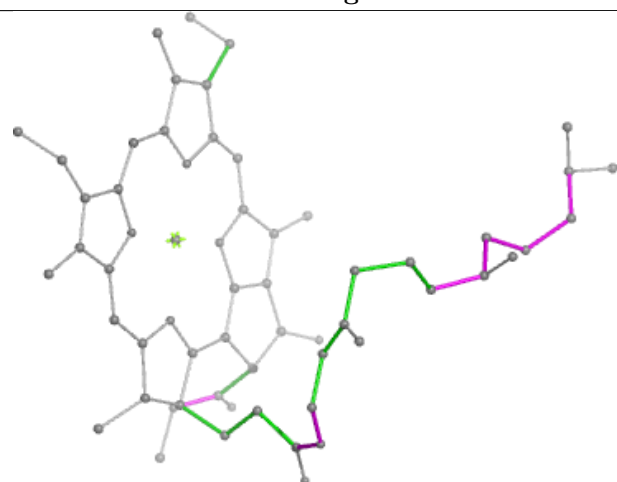
Ligand CLA 2 607



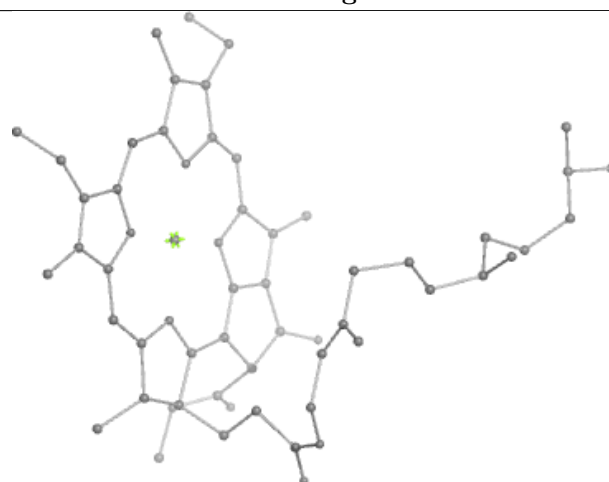
Bond lengths



Bond angles

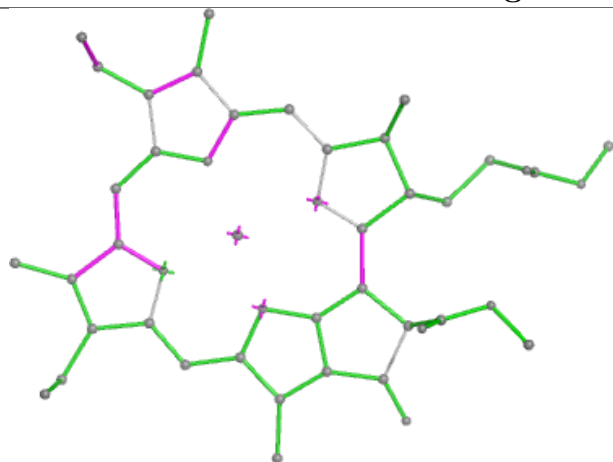


Torsions

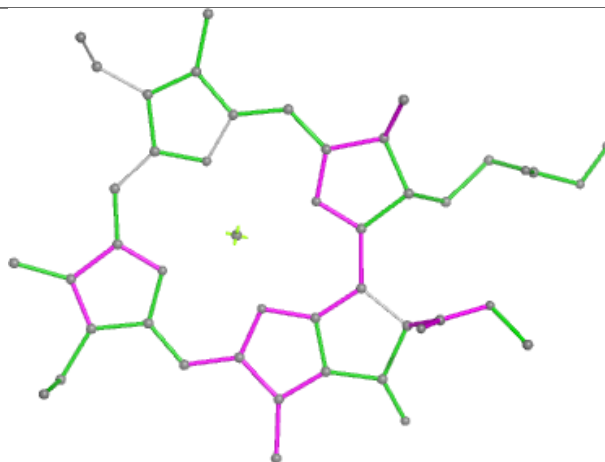


Rings

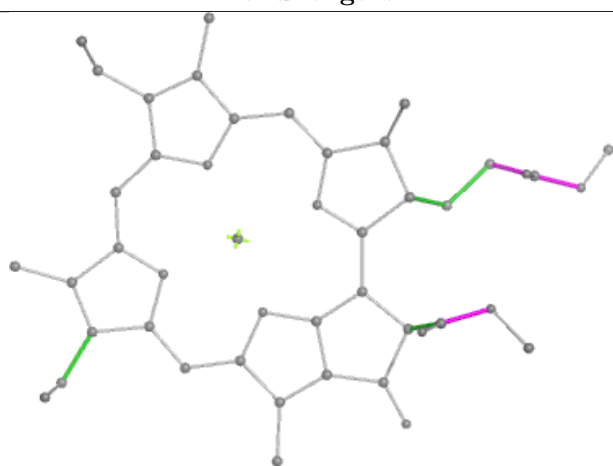
Ligand CLA K 1404



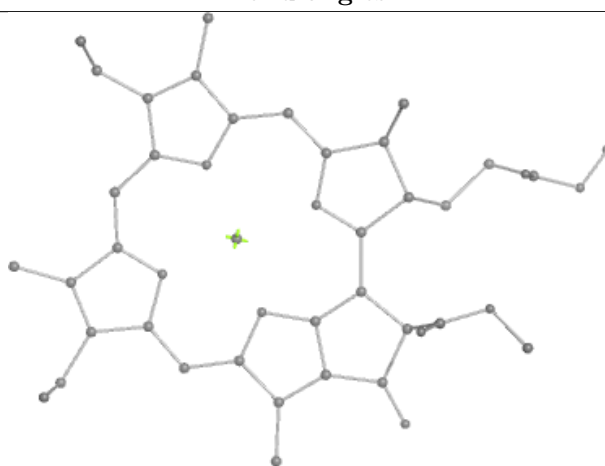
Bond lengths



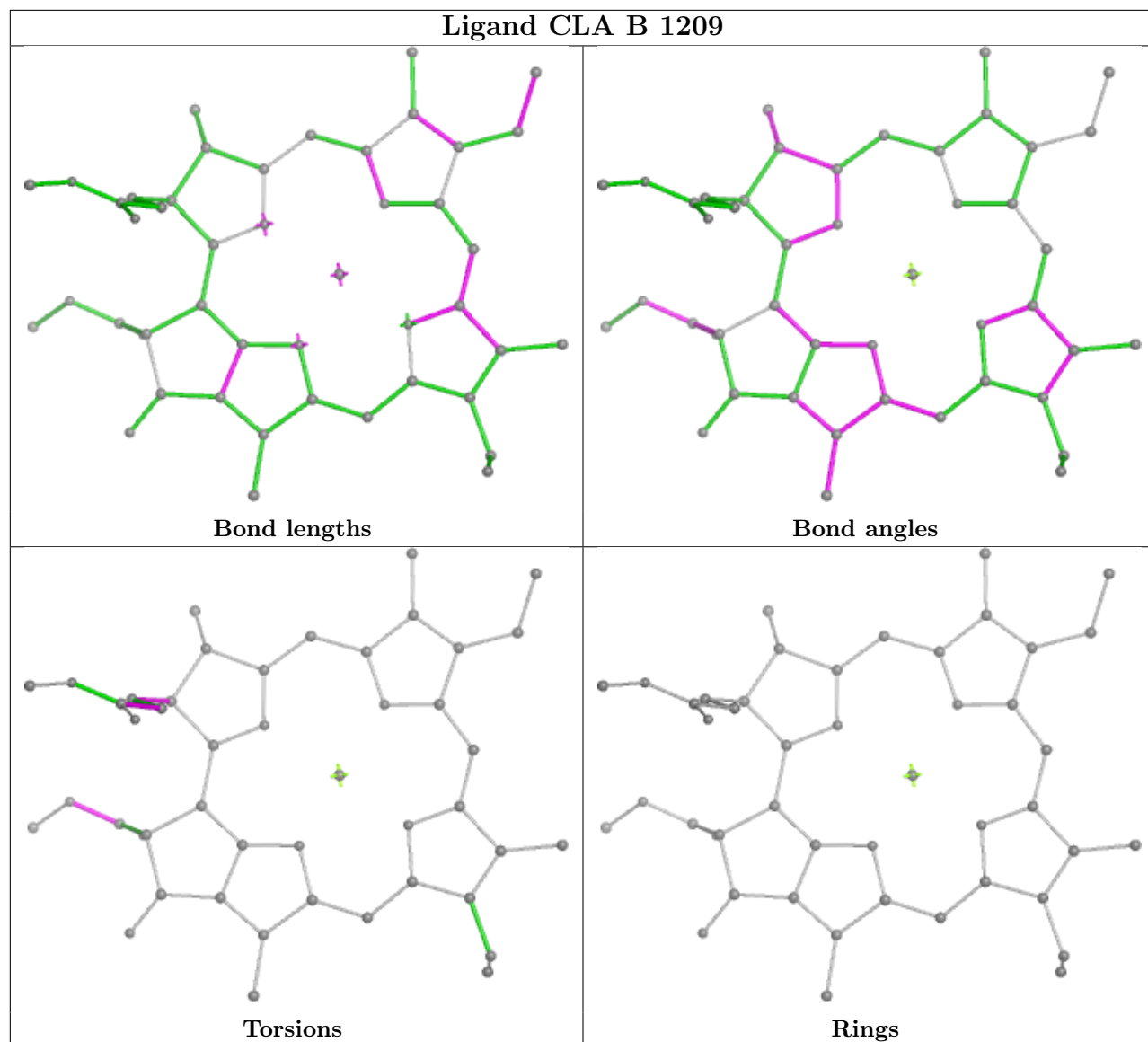
Bond angles

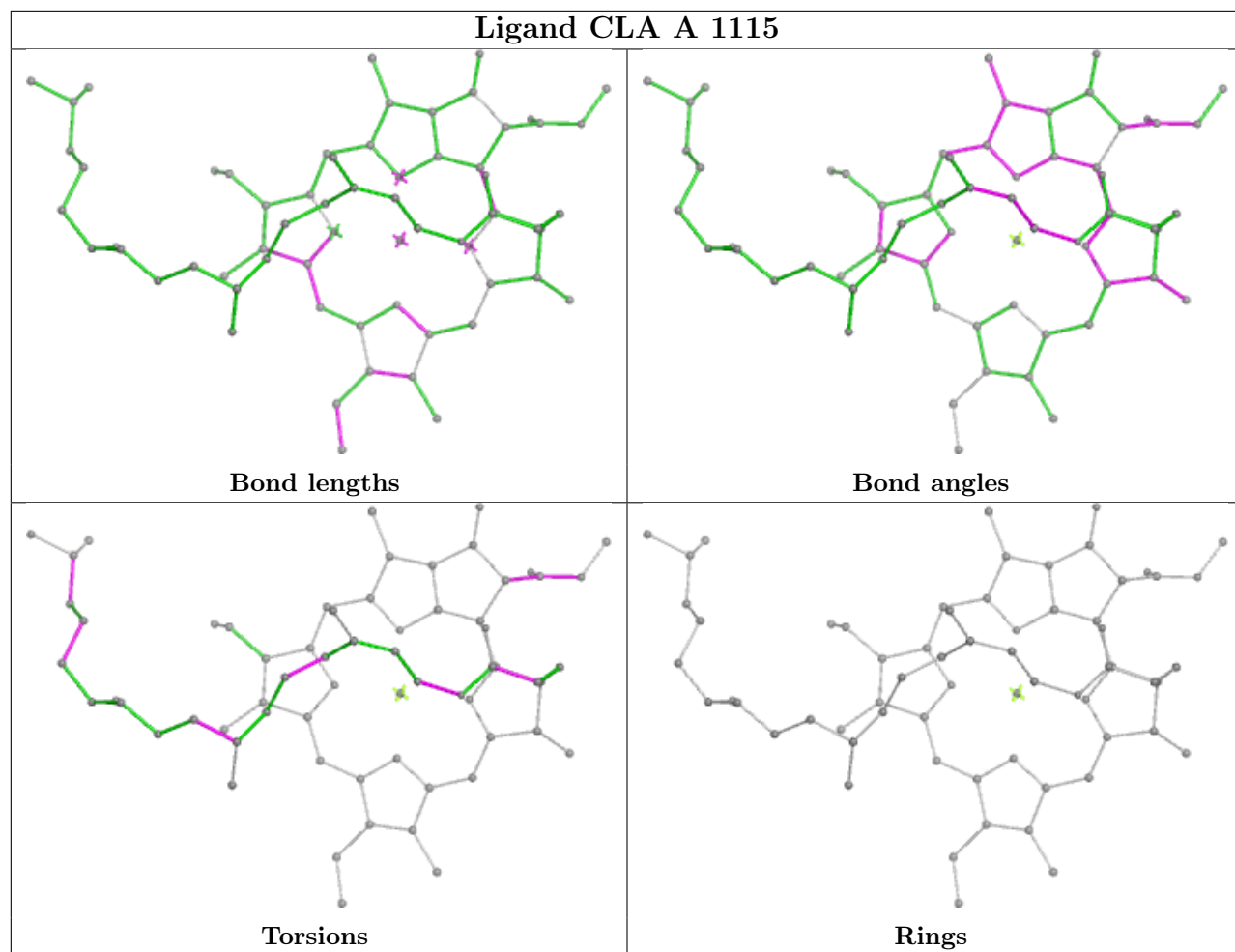


Torsions

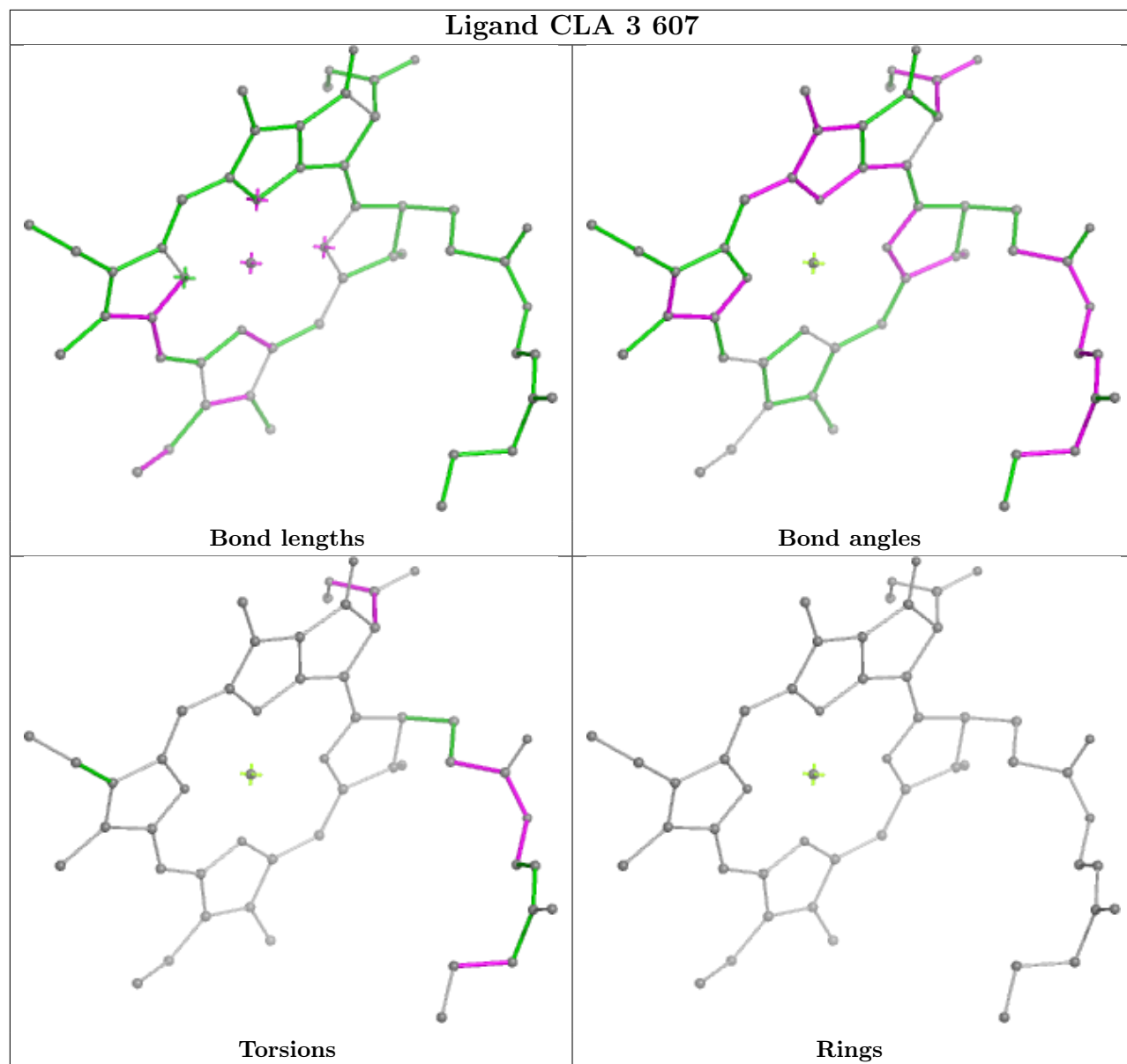


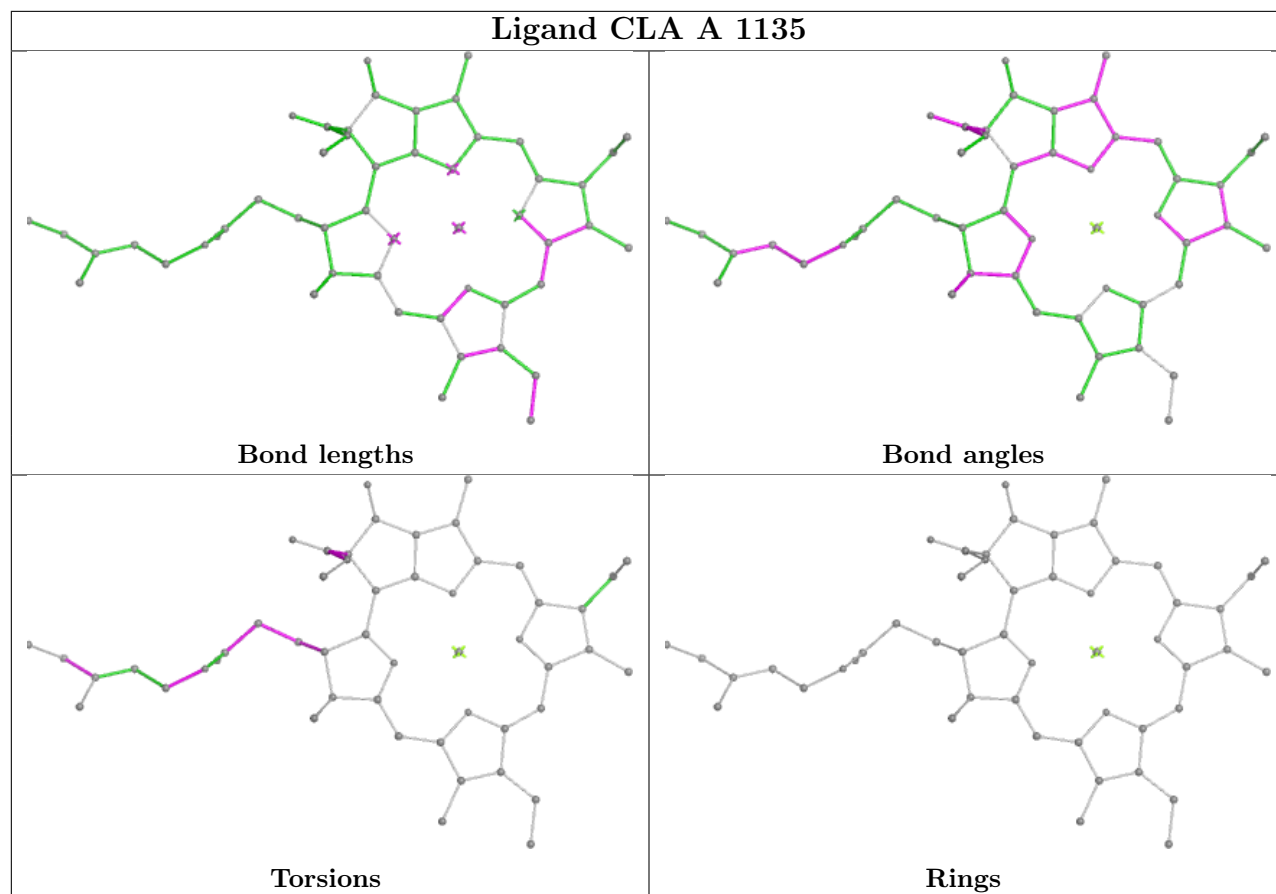
Rings



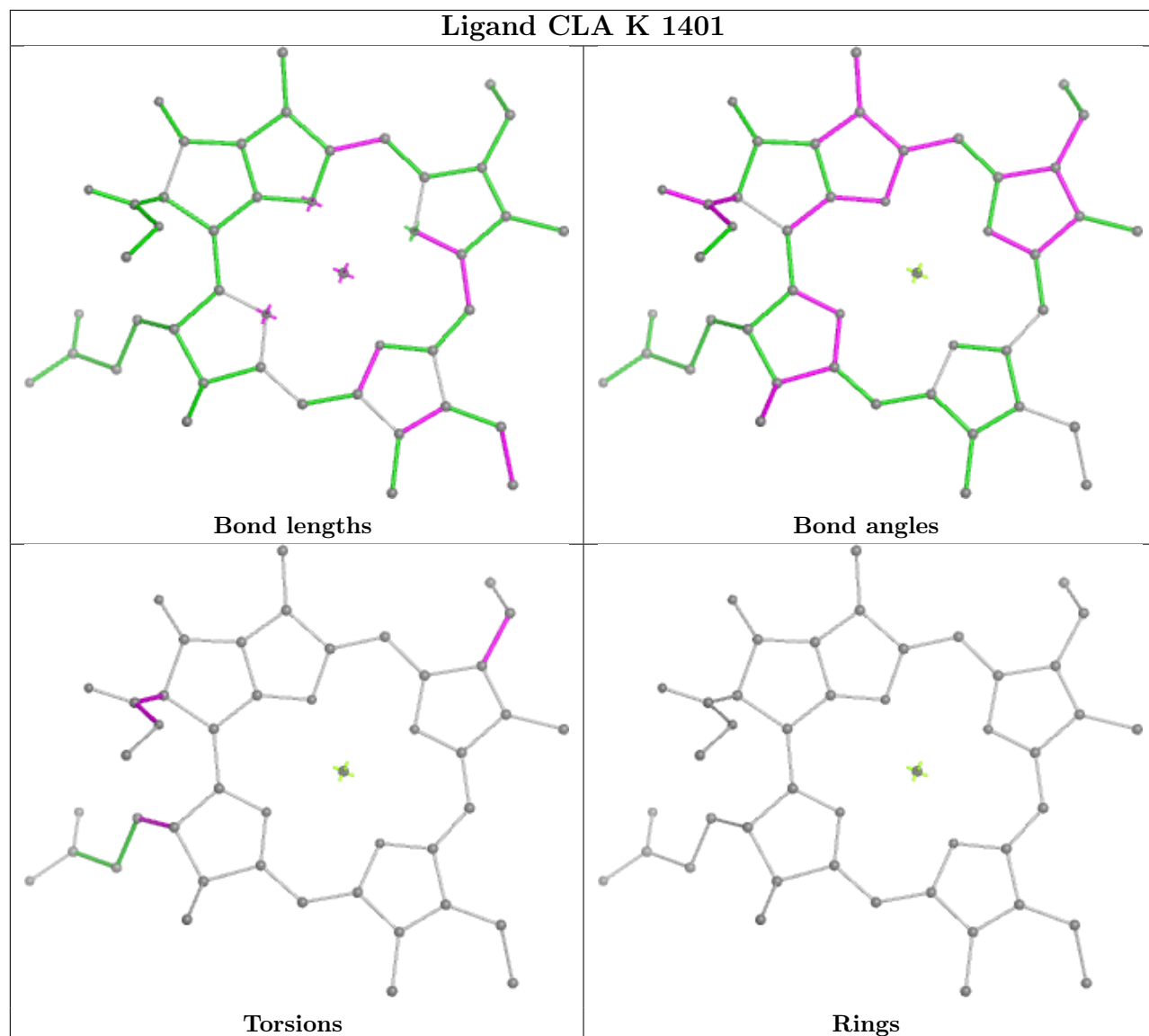


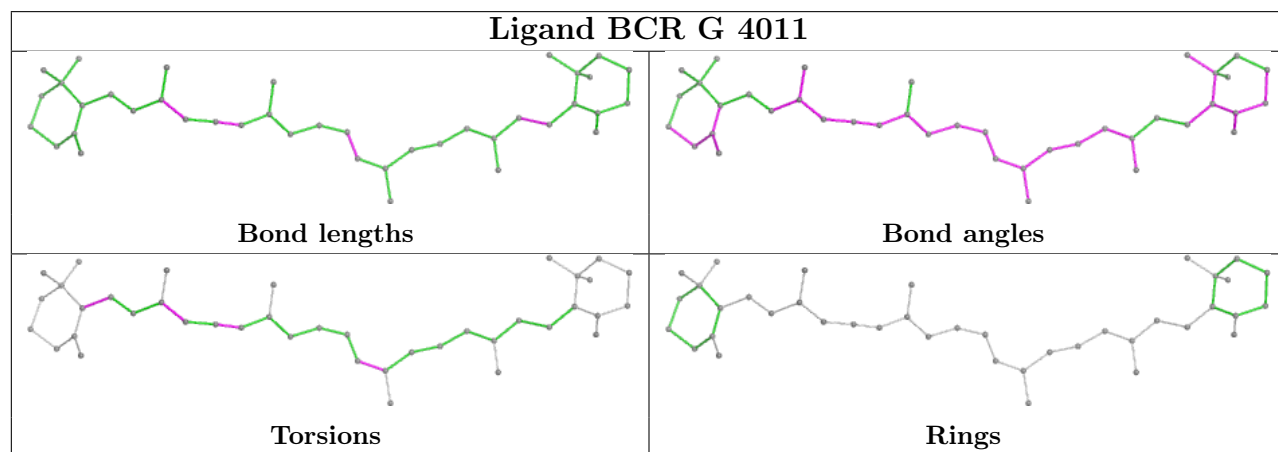
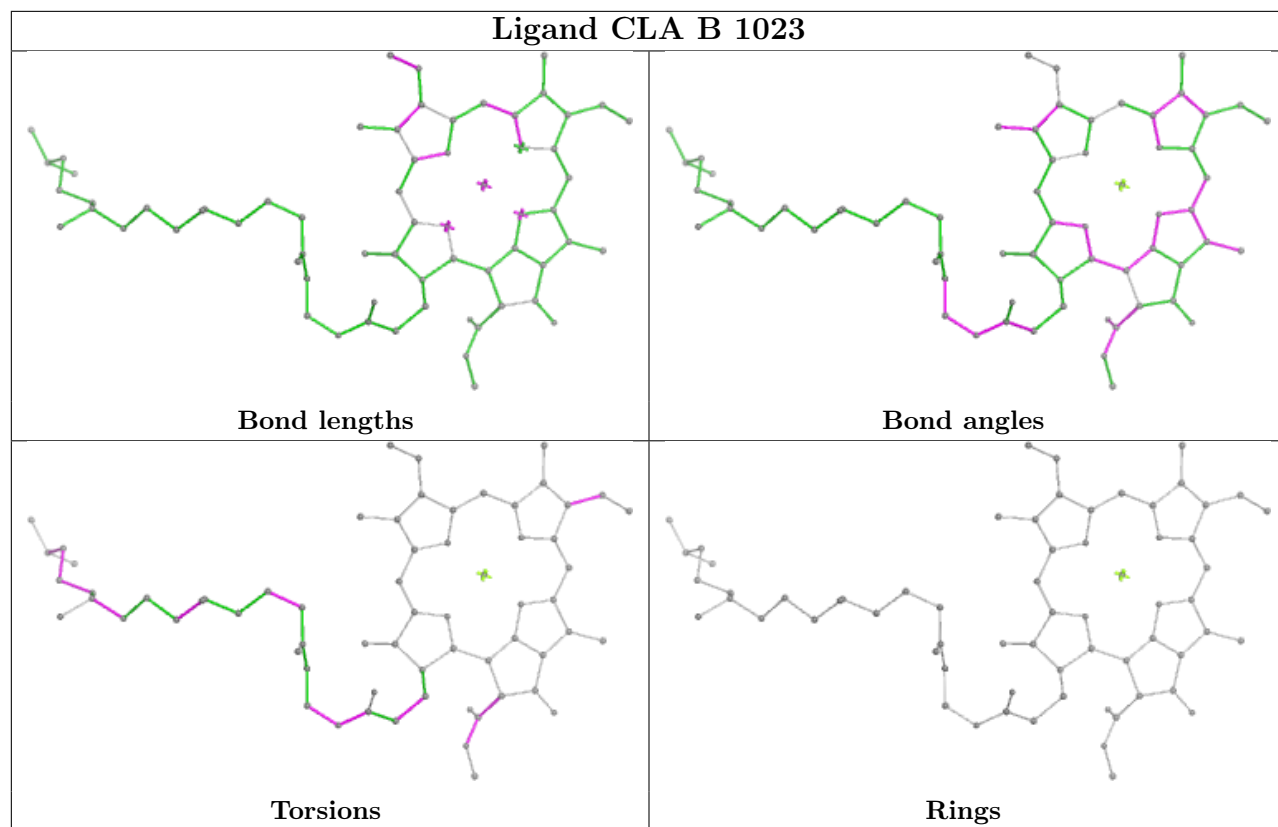
Ligand CLA 3 607

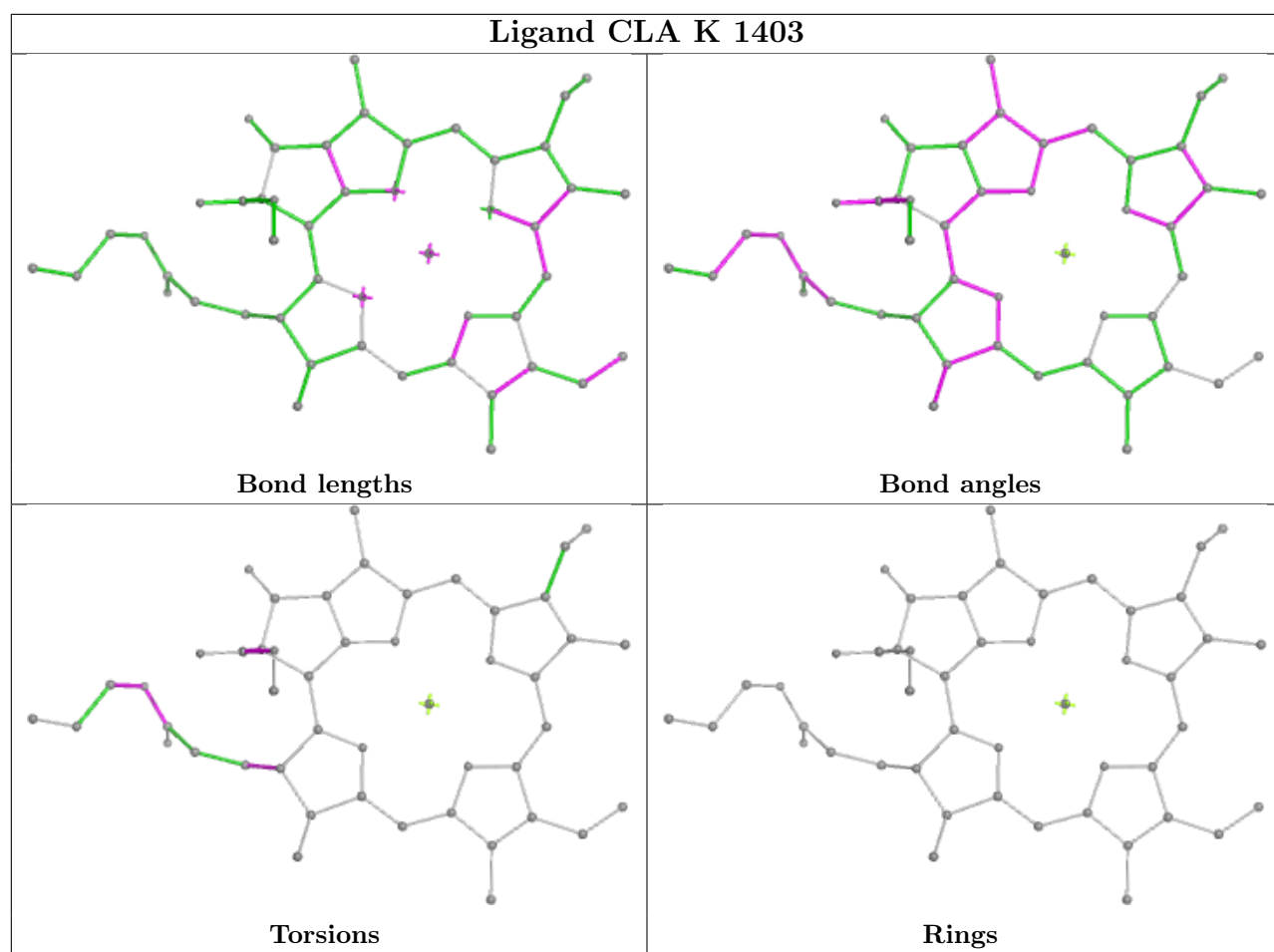


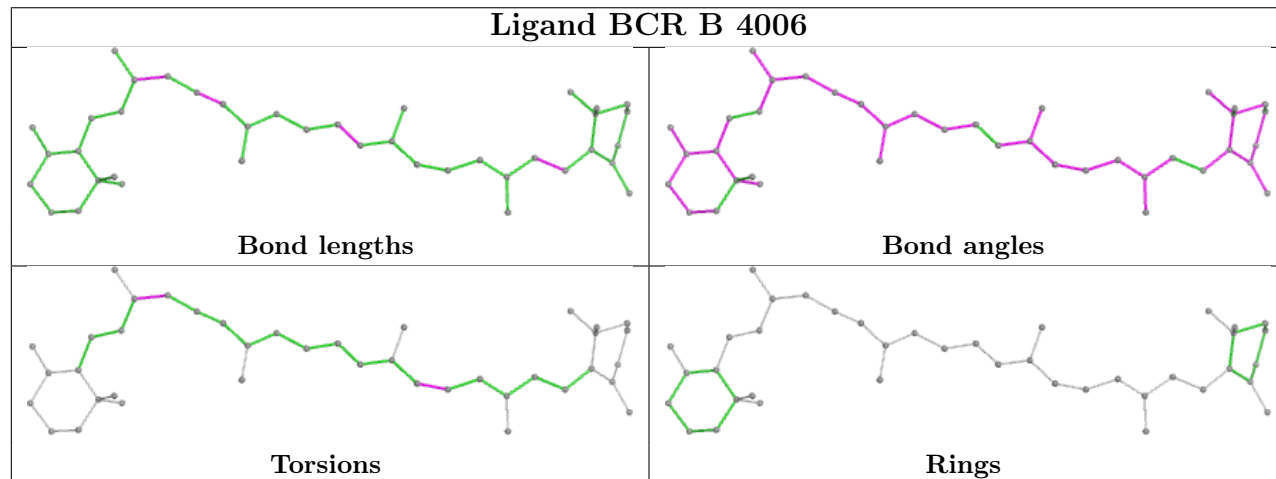
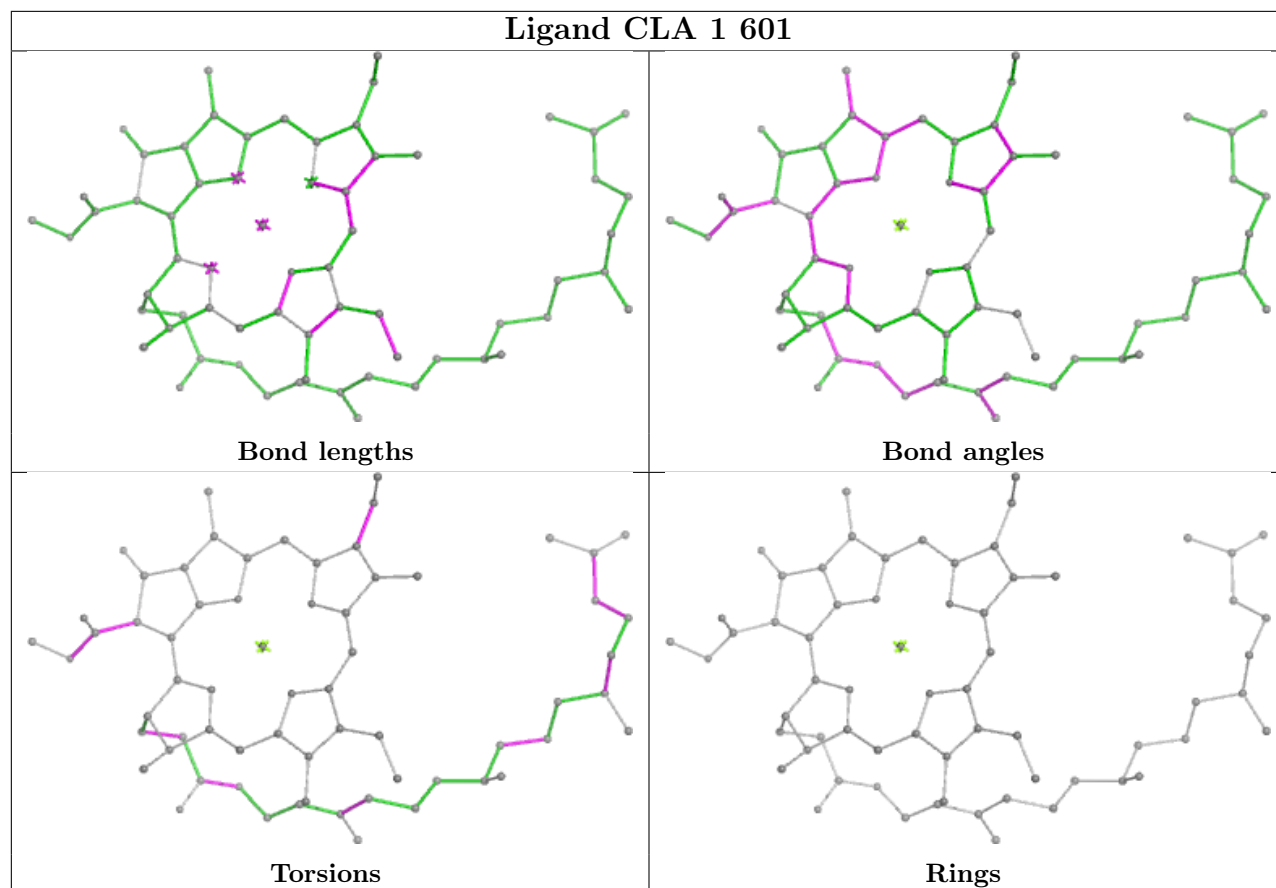


Ligand CLA K 1401

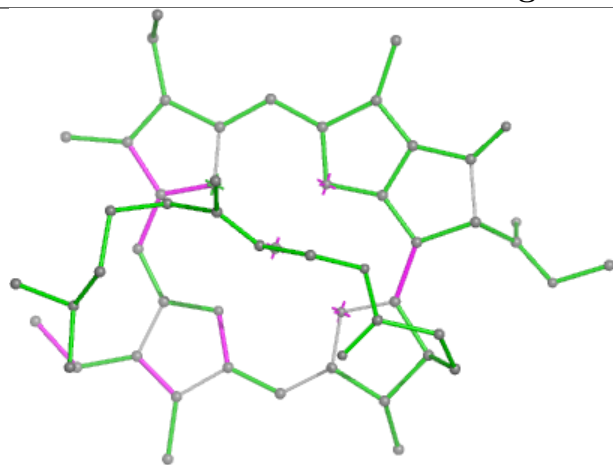




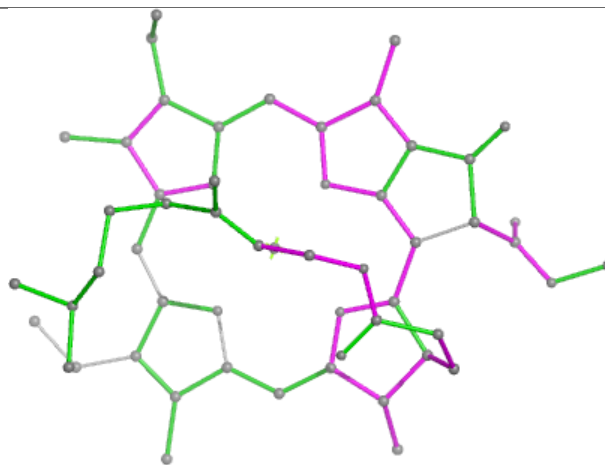




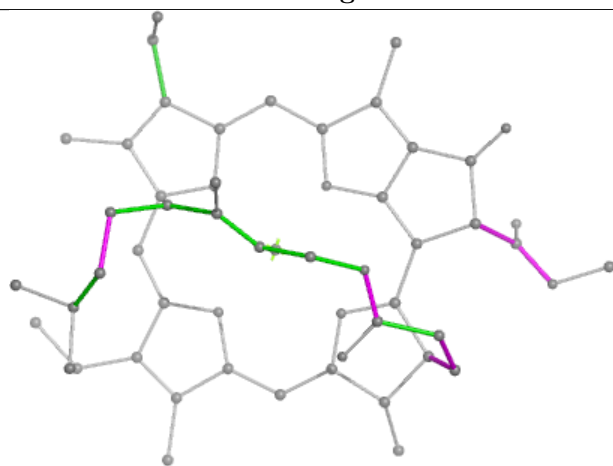
Ligand CLA 1 603



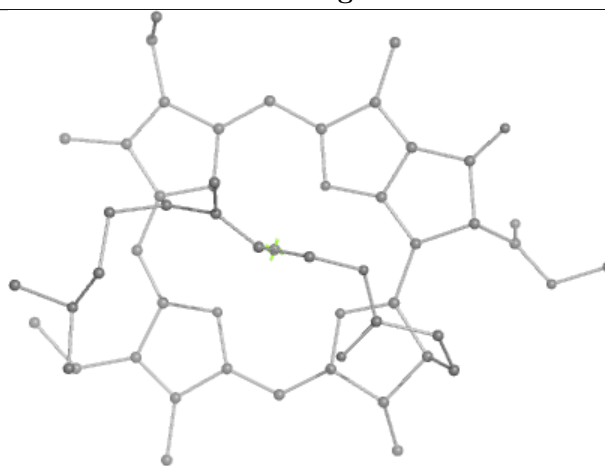
Bond lengths



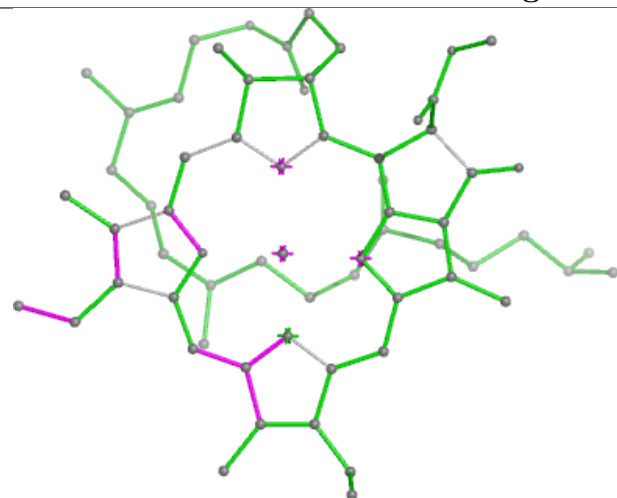
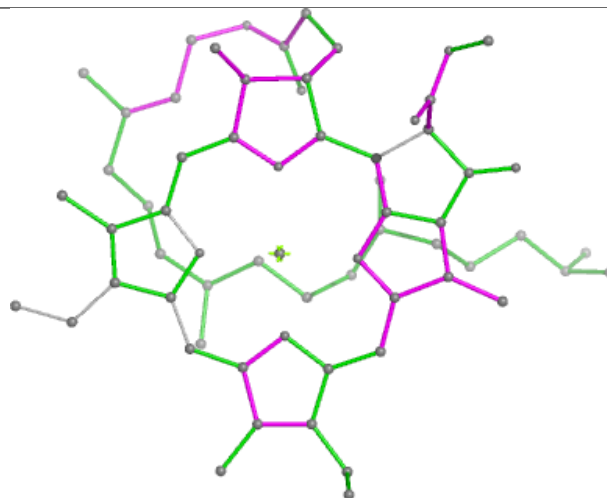
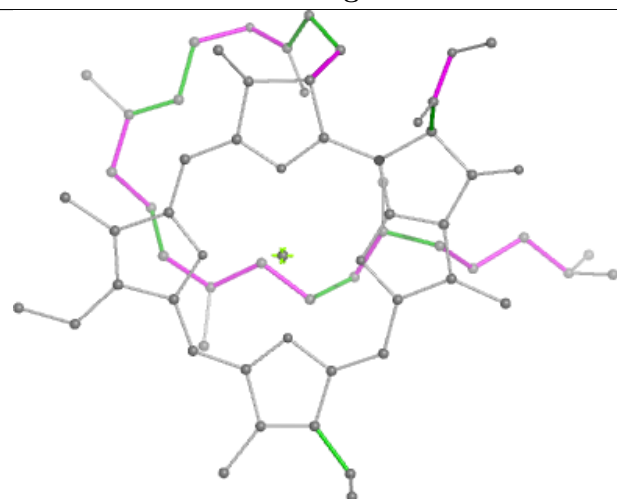
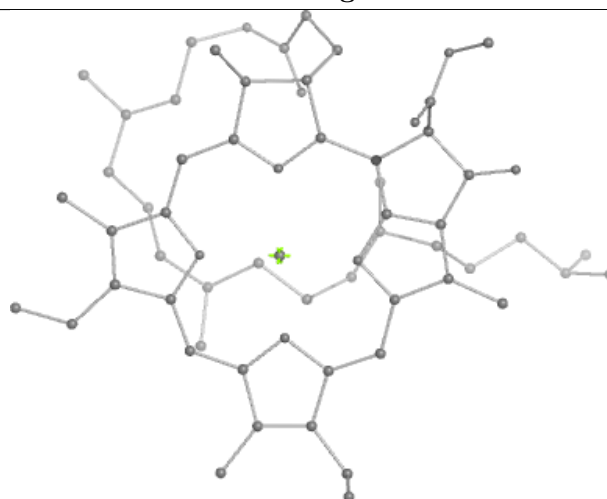
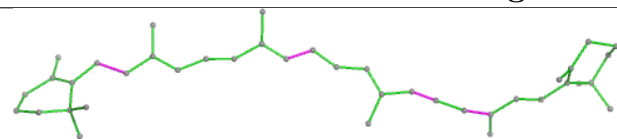
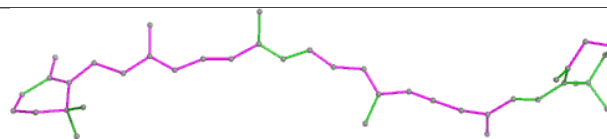
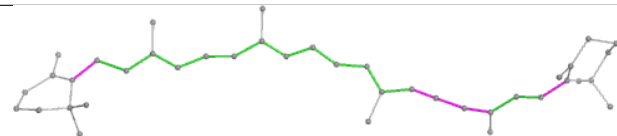
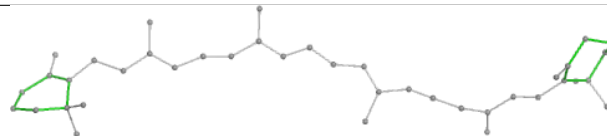
Bond angles

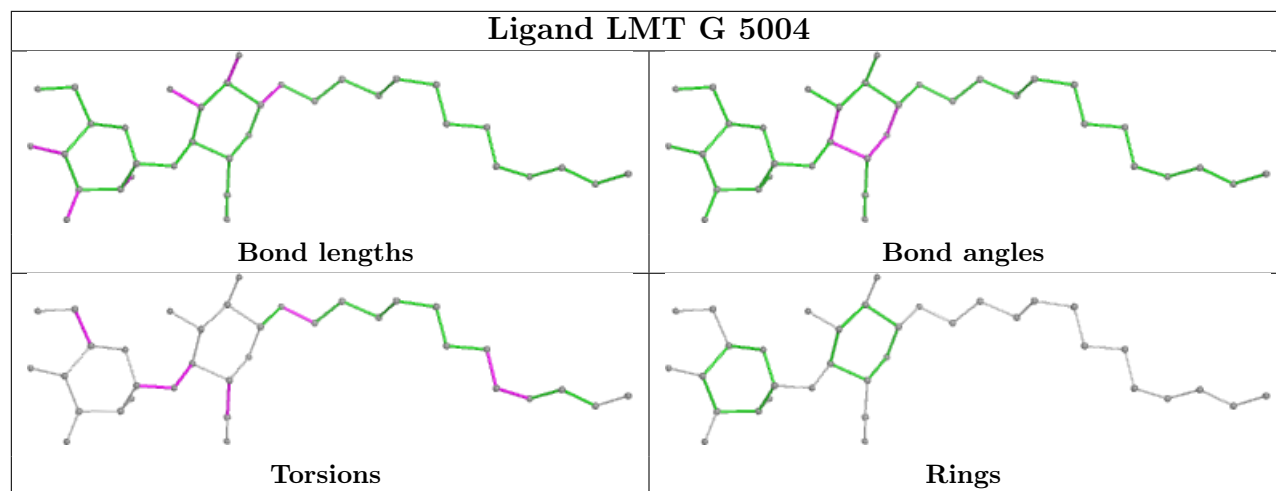


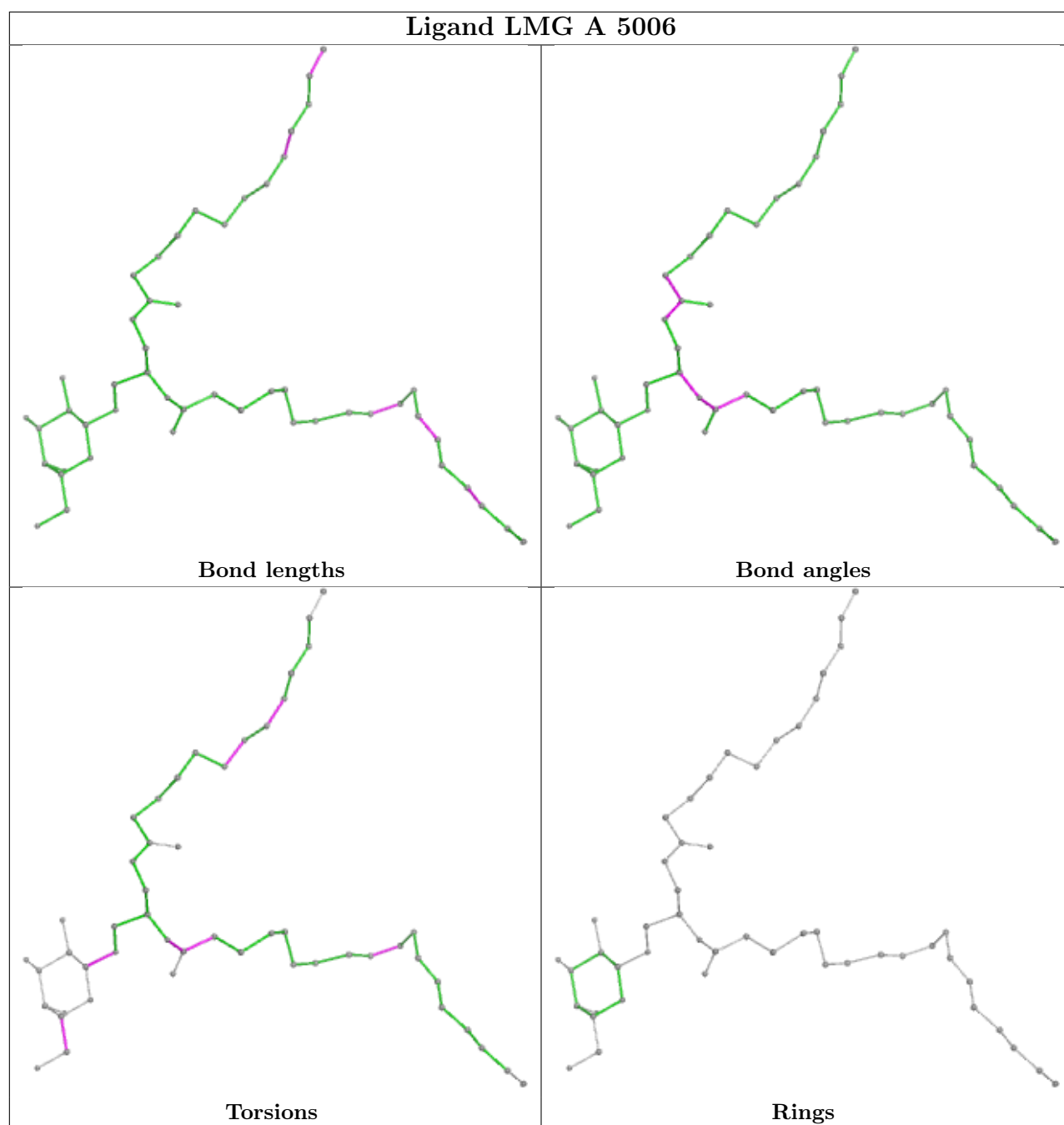
Torsions

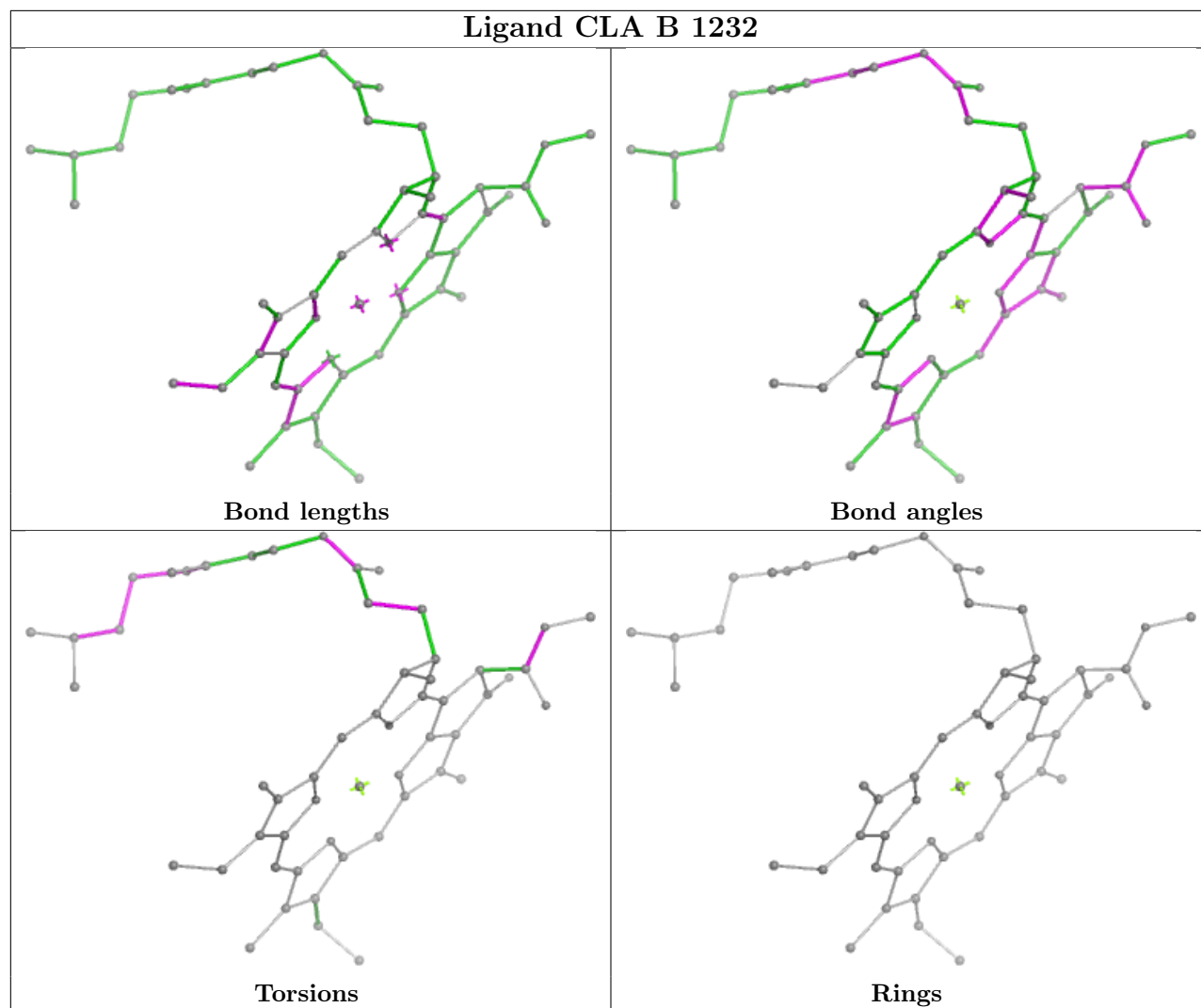


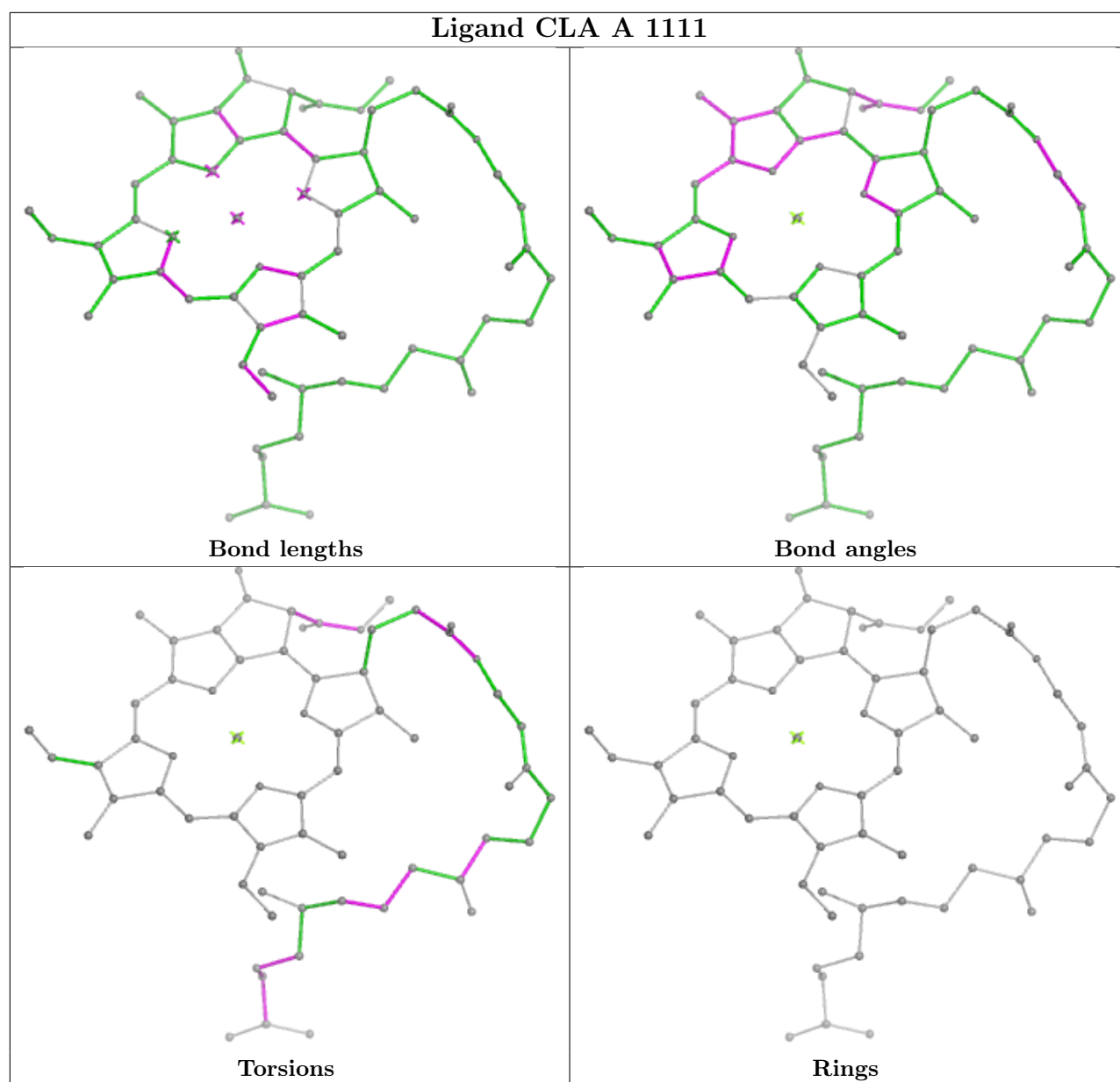
Rings

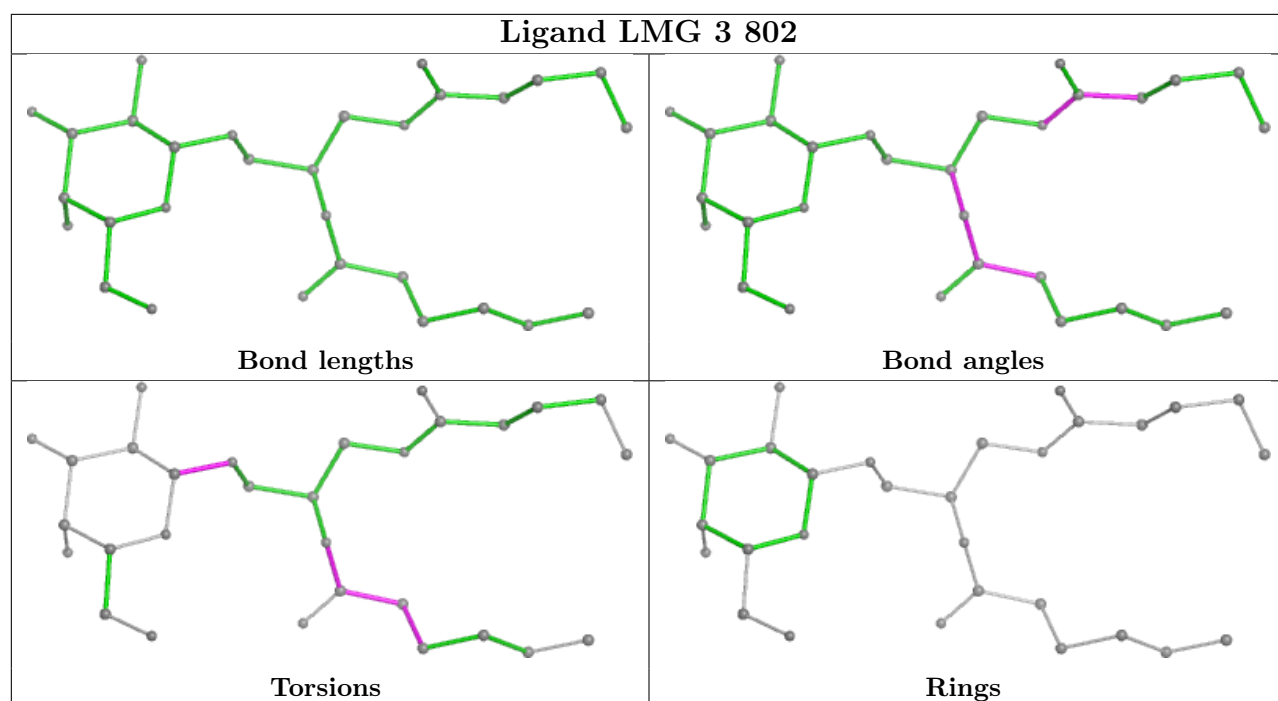
Ligand CLA 3 610**Bond lengths****Bond angles****Torsions****Rings****Ligand BCR B 4009****Bond lengths****Bond angles****Torsions****Rings**

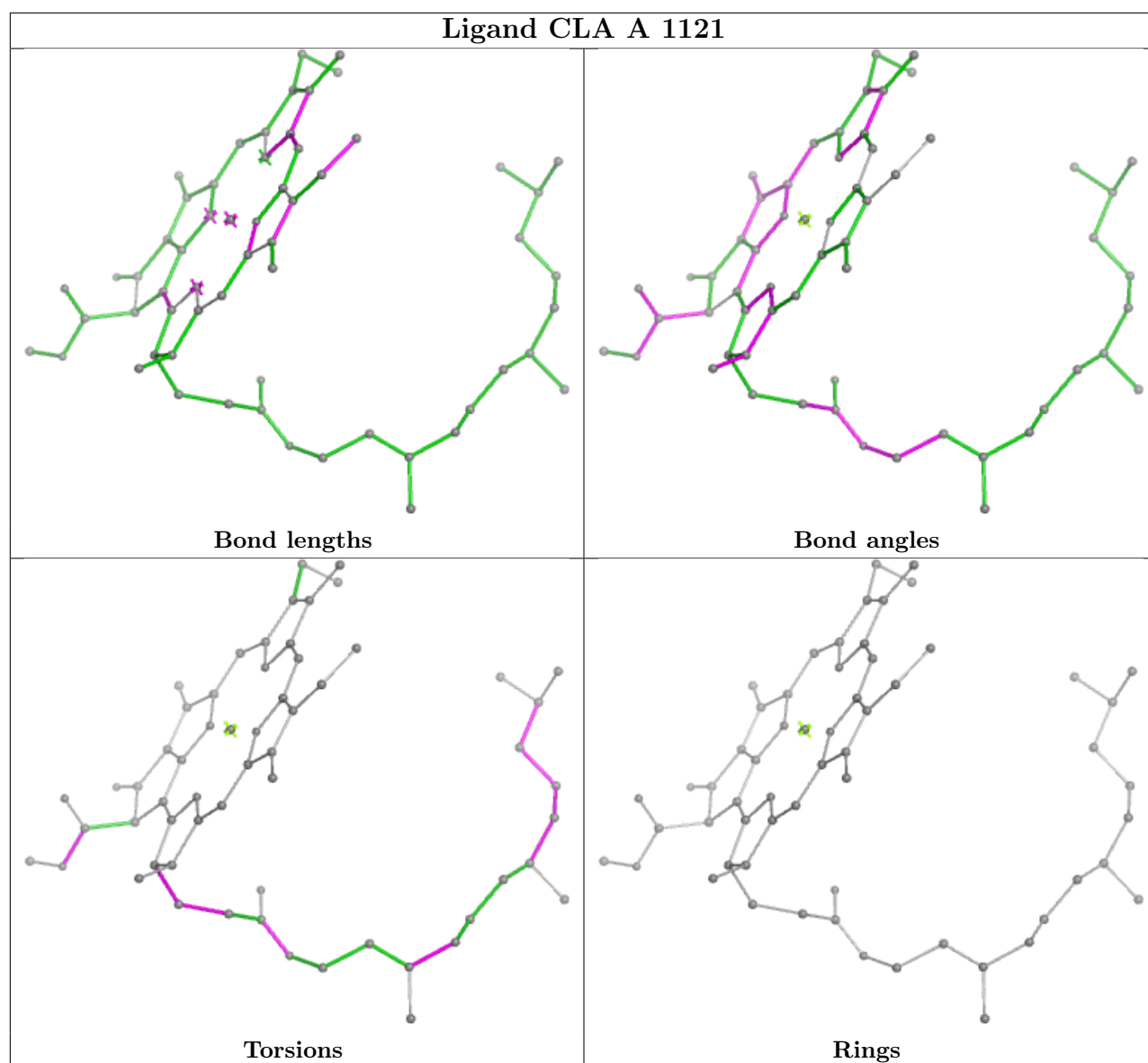


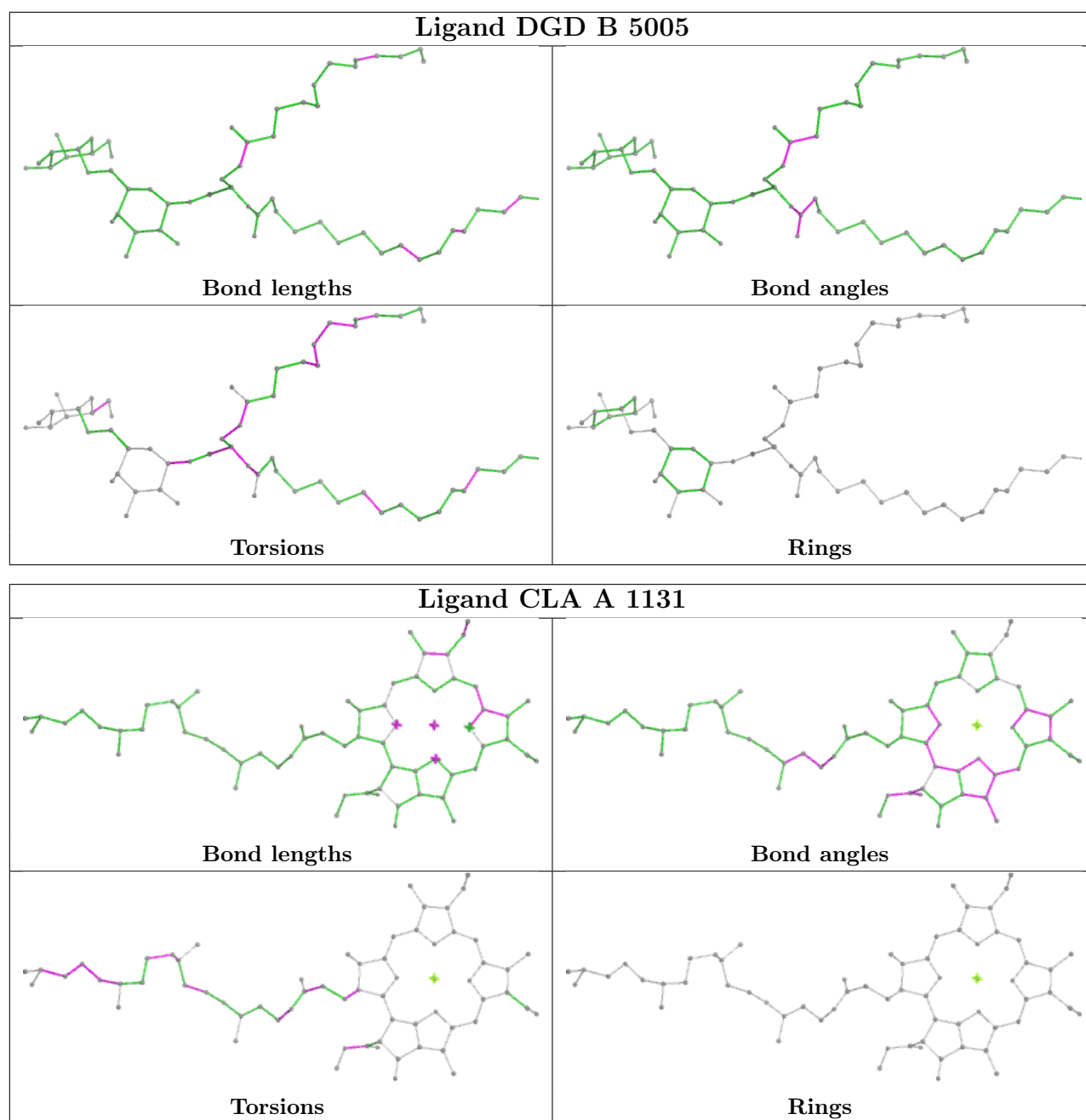


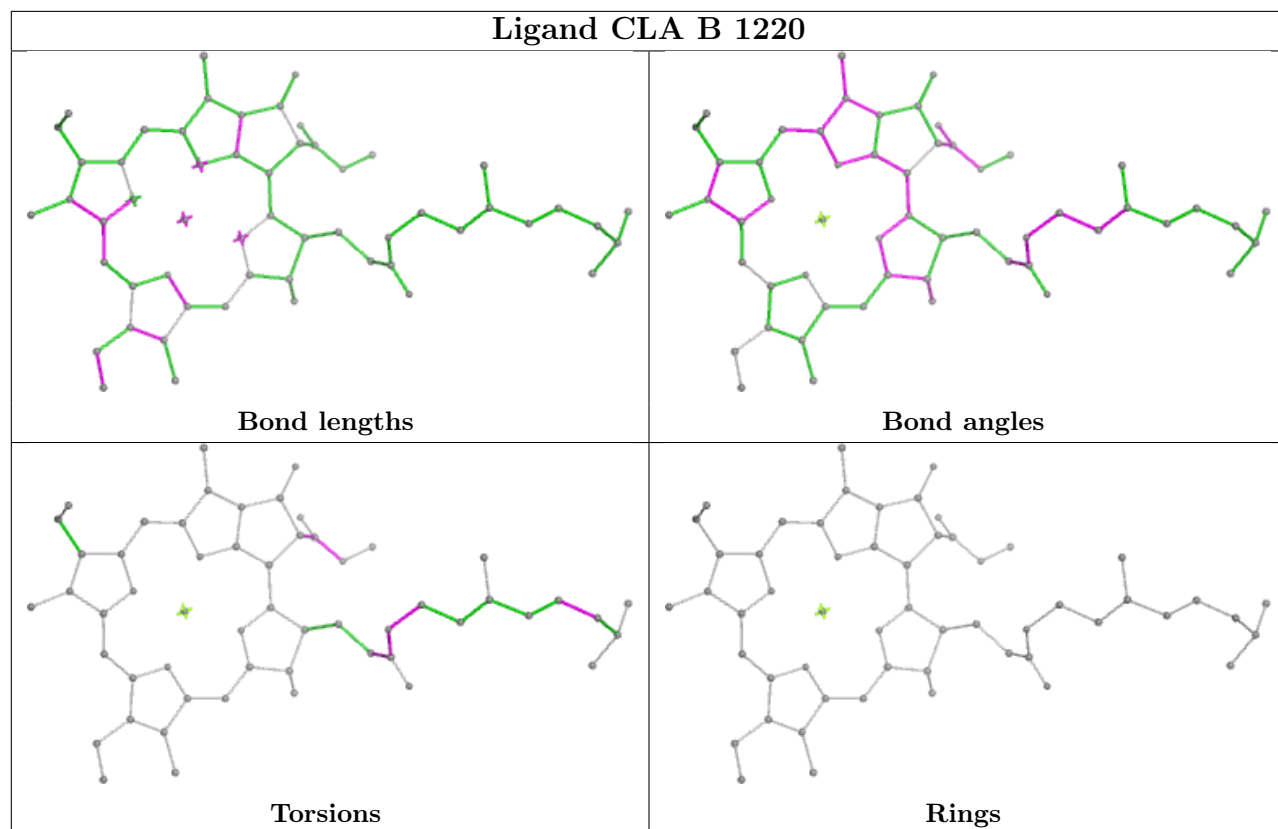




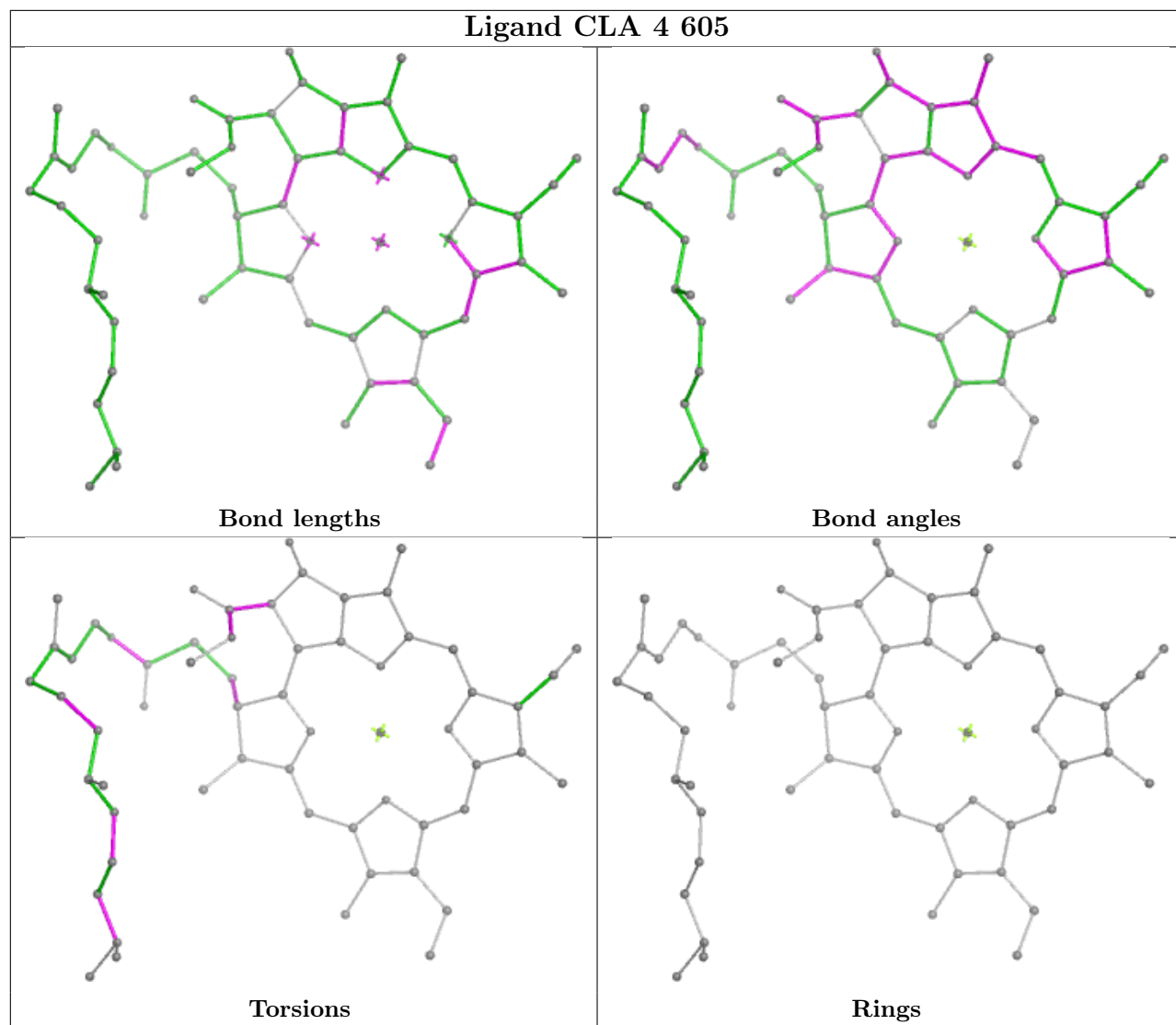




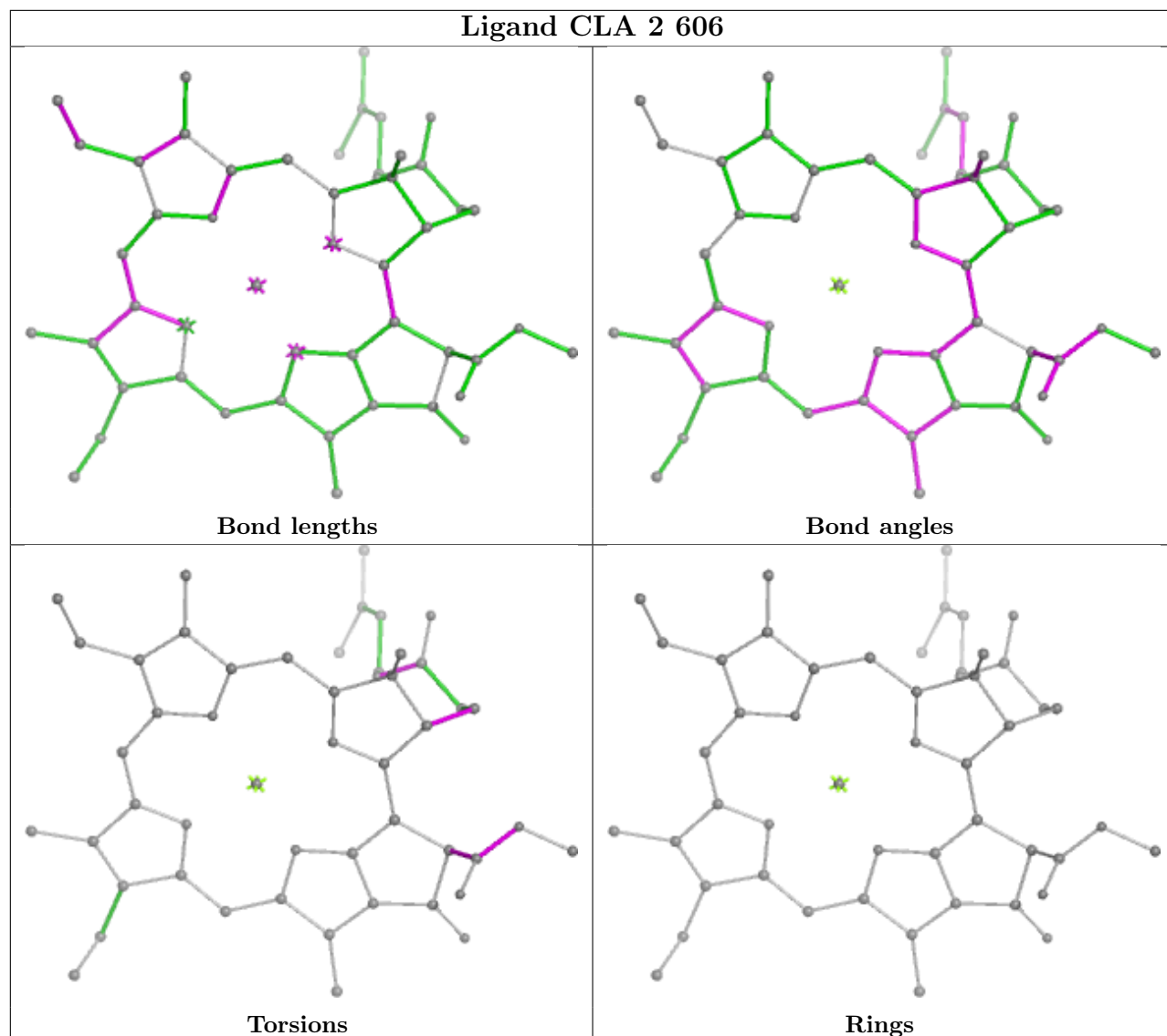


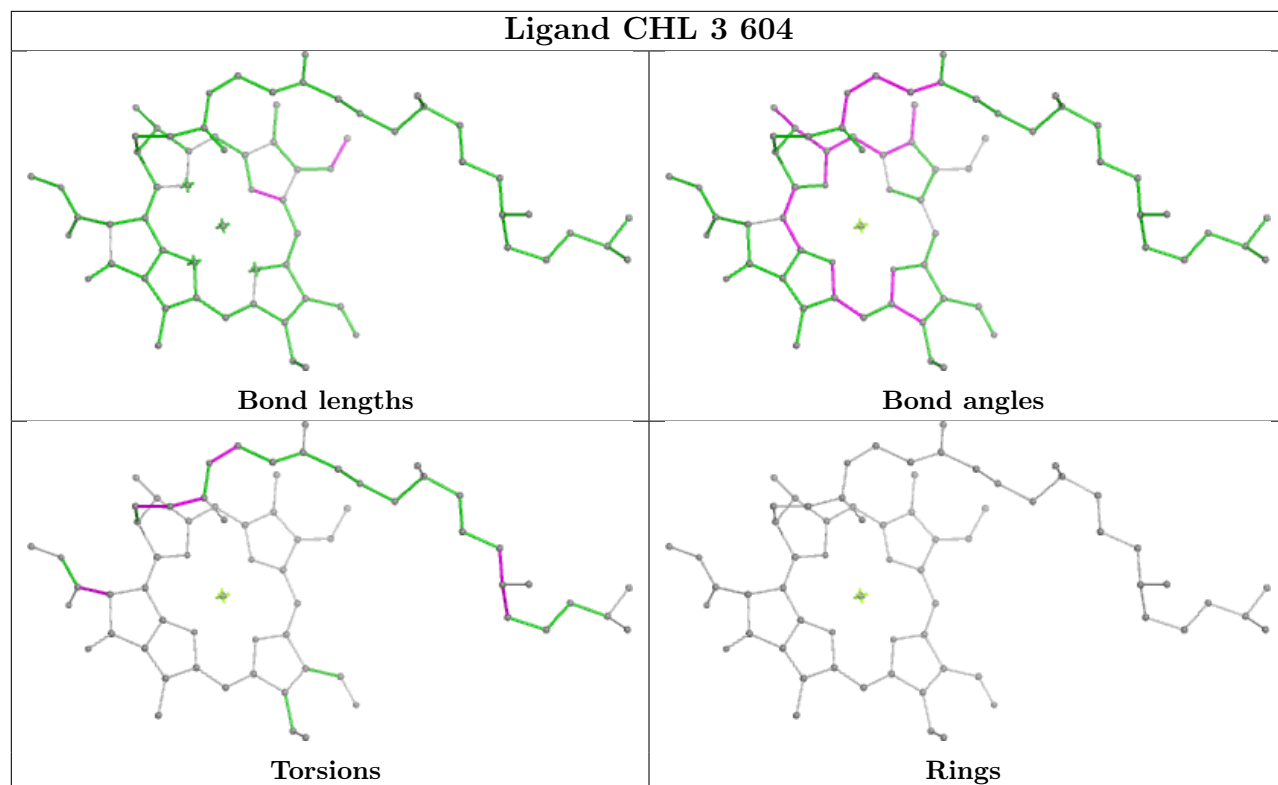
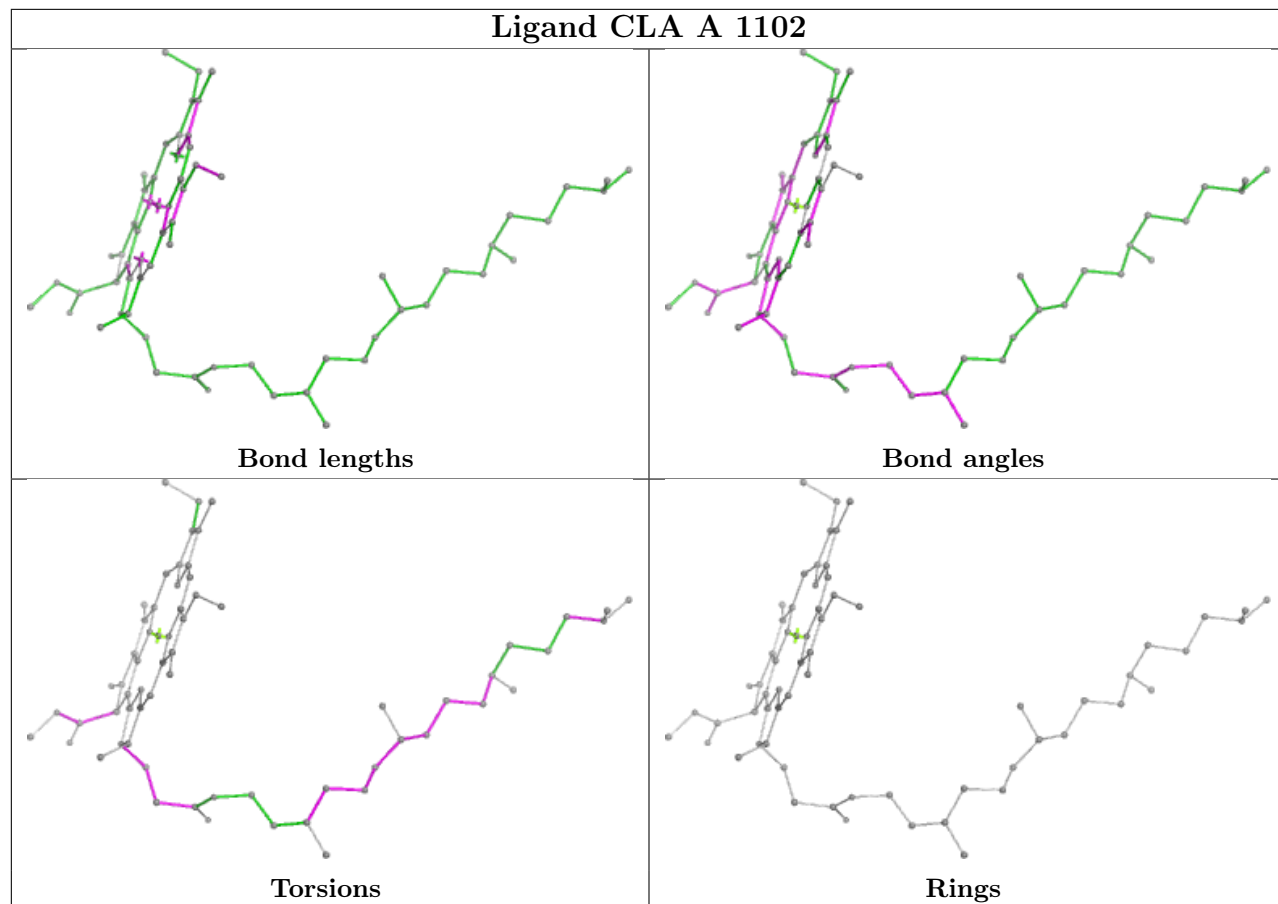


Ligand CLA 4 605

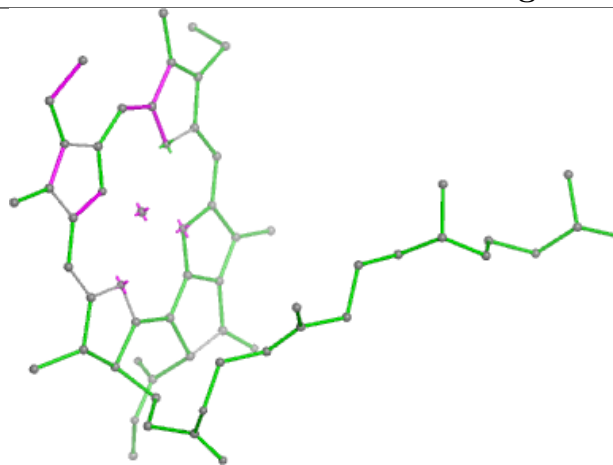


Ligand CLA 2 606

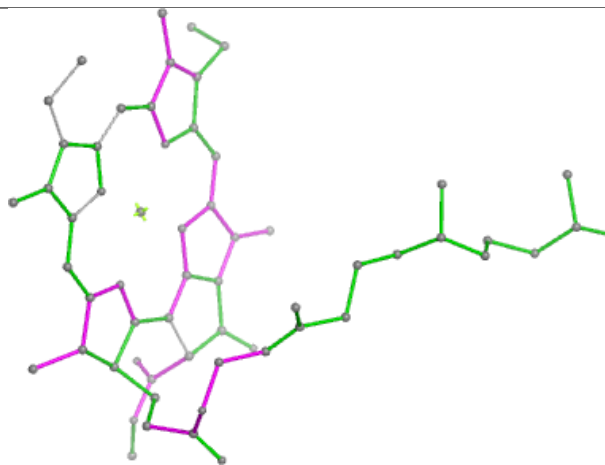


Ligand CHL 3 604**Ligand CLA A 1102**

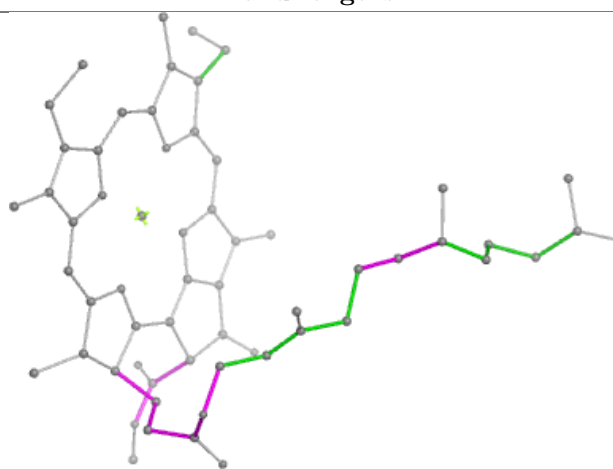
Ligand CLA 4 607



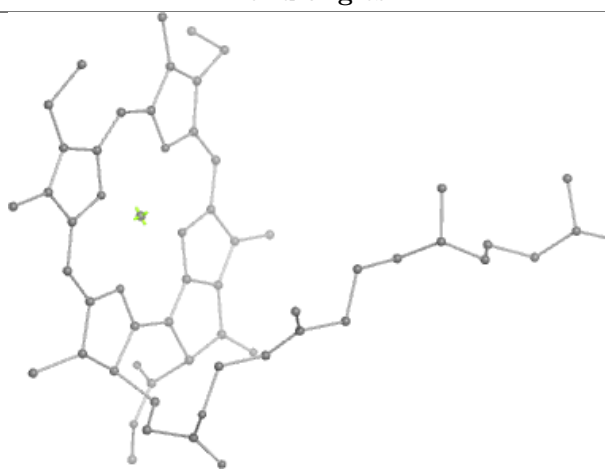
Bond lengths



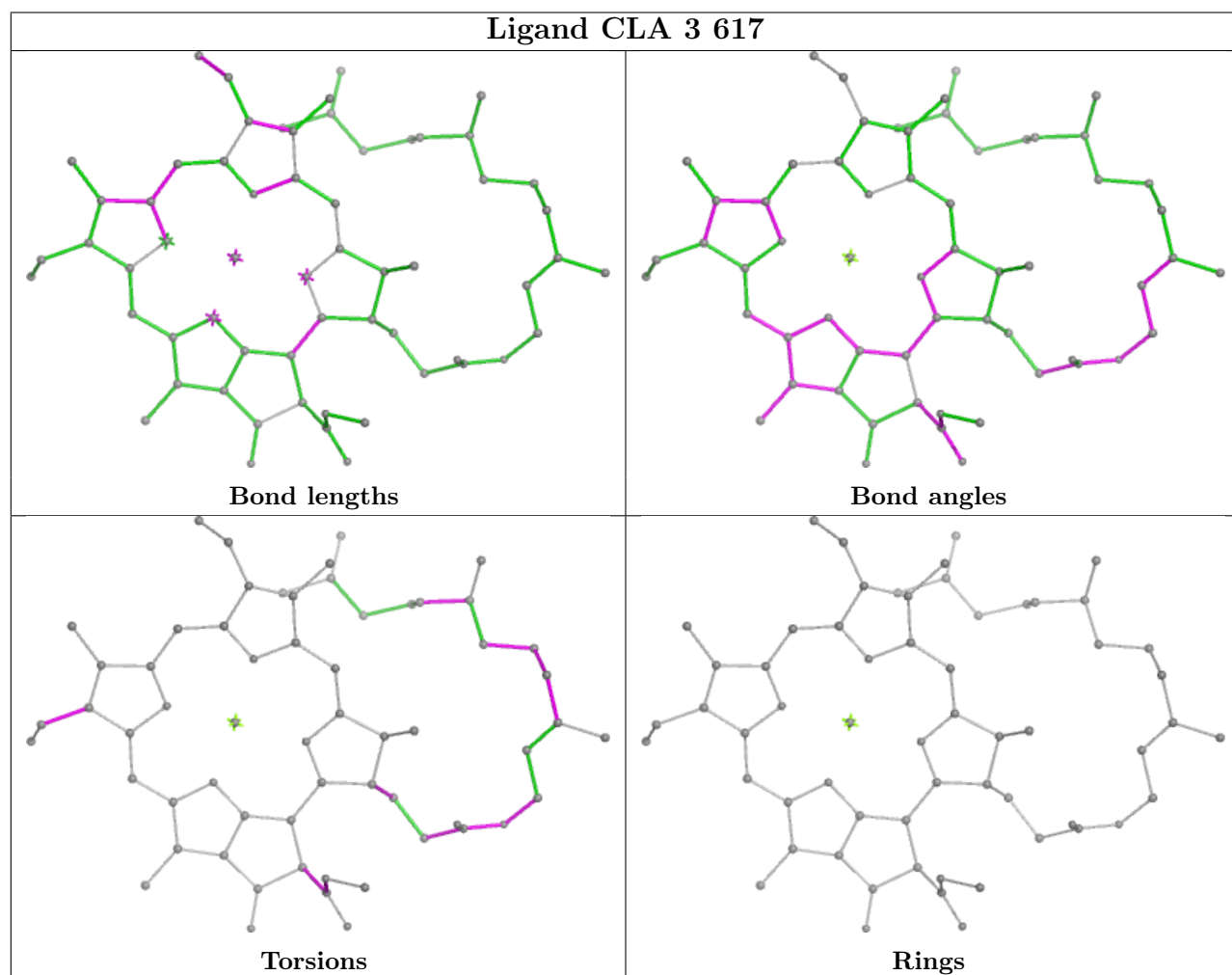
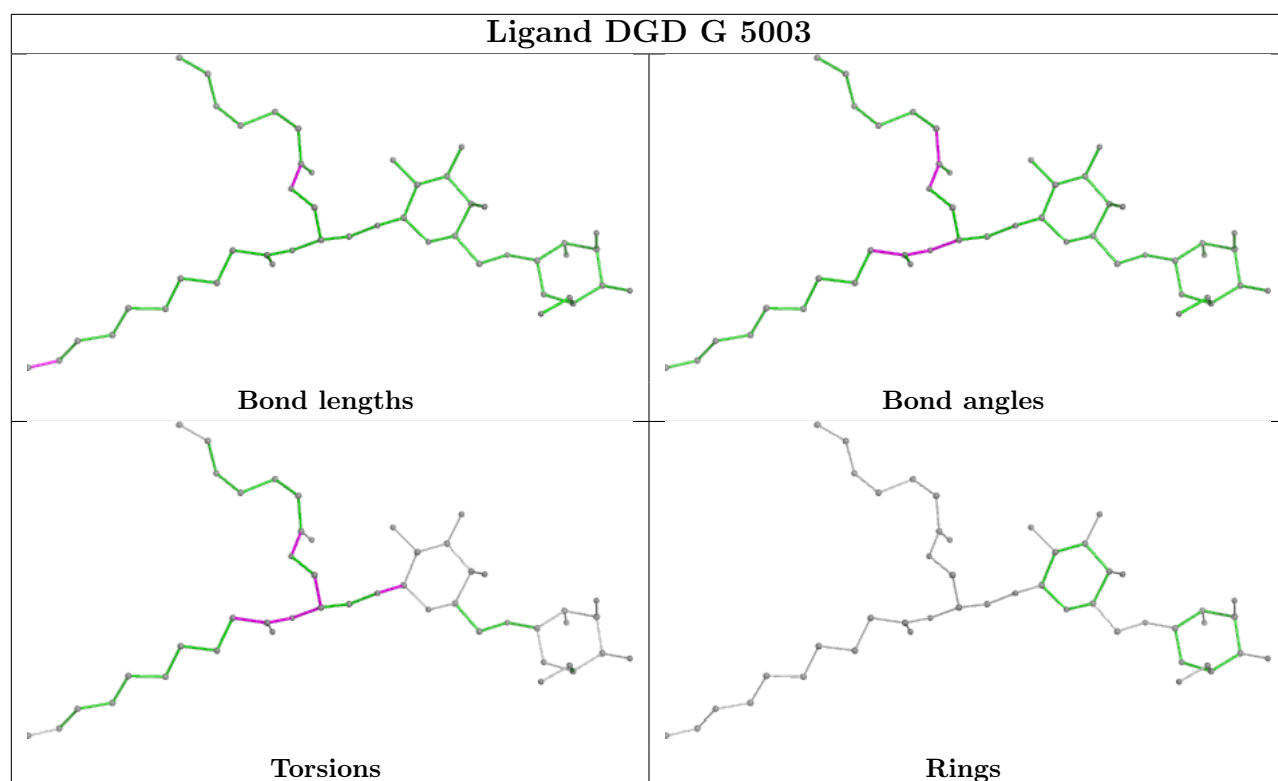
Bond angles



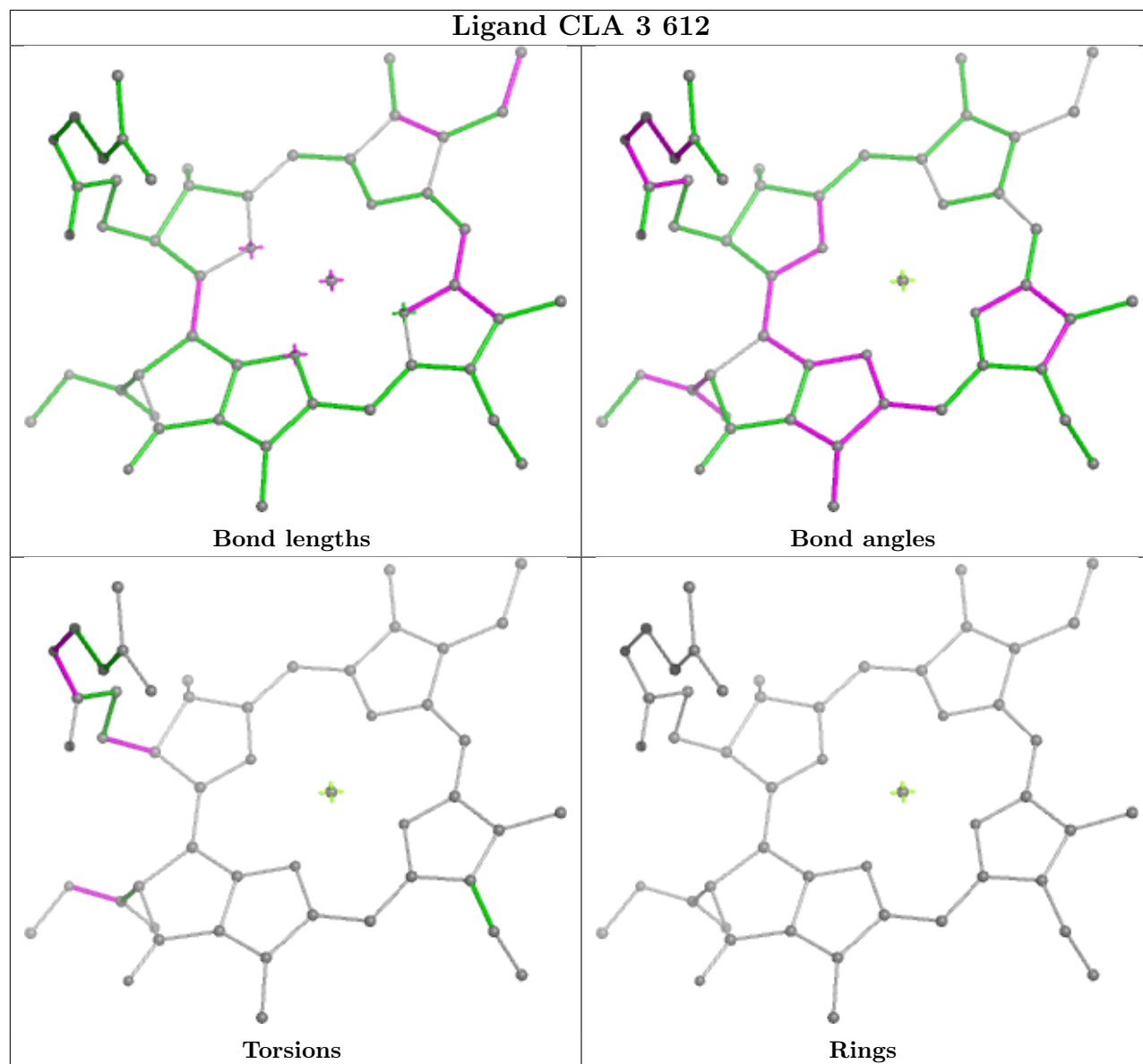
Torsions



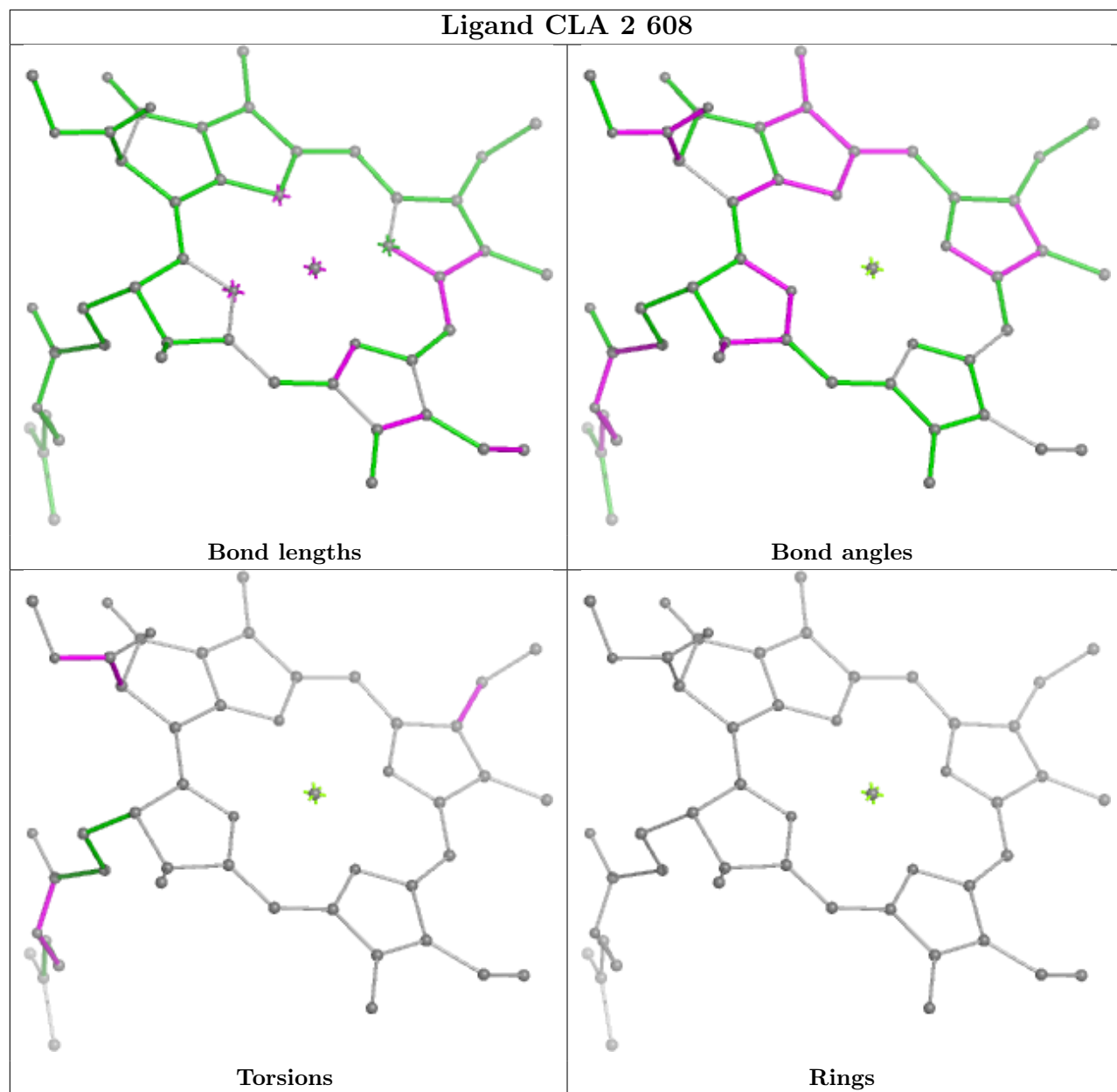
Rings

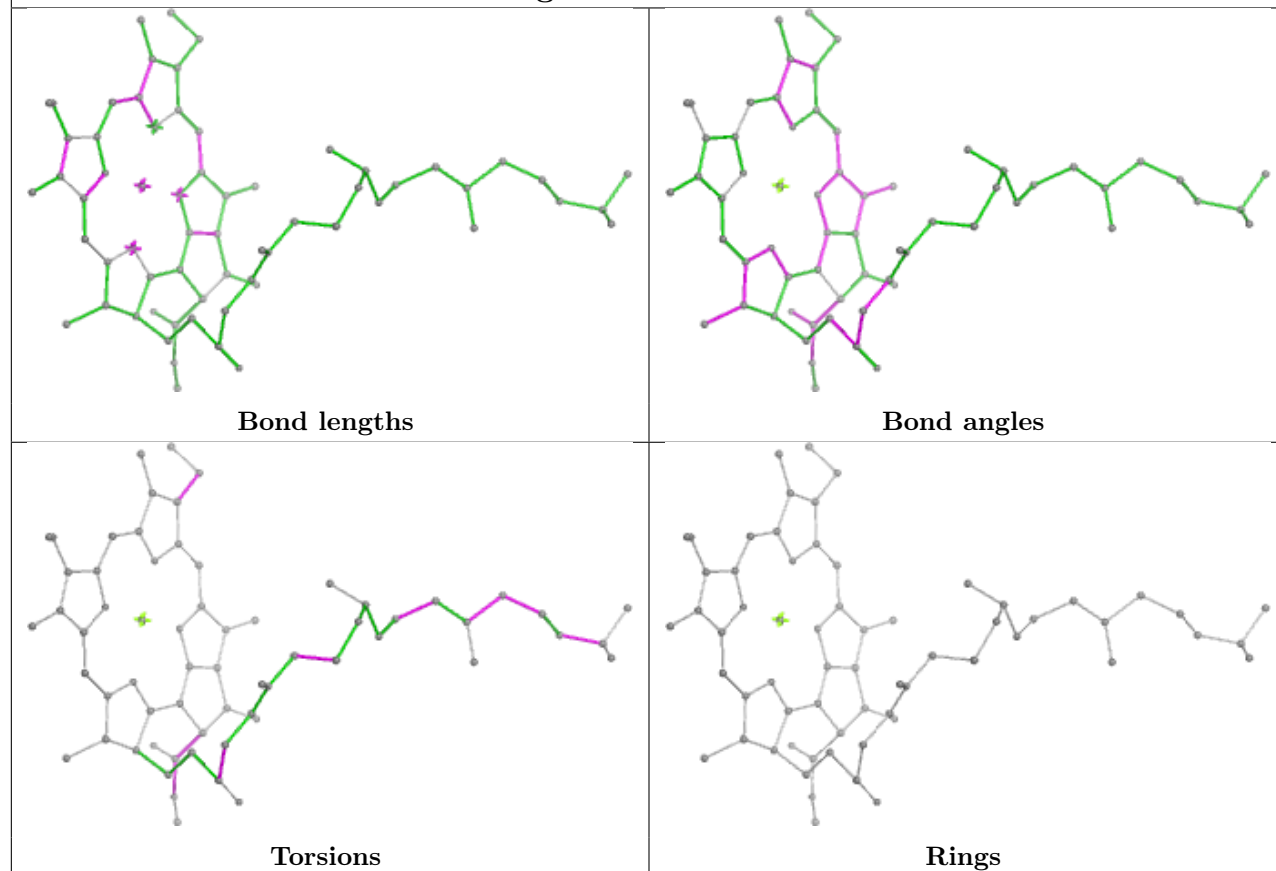
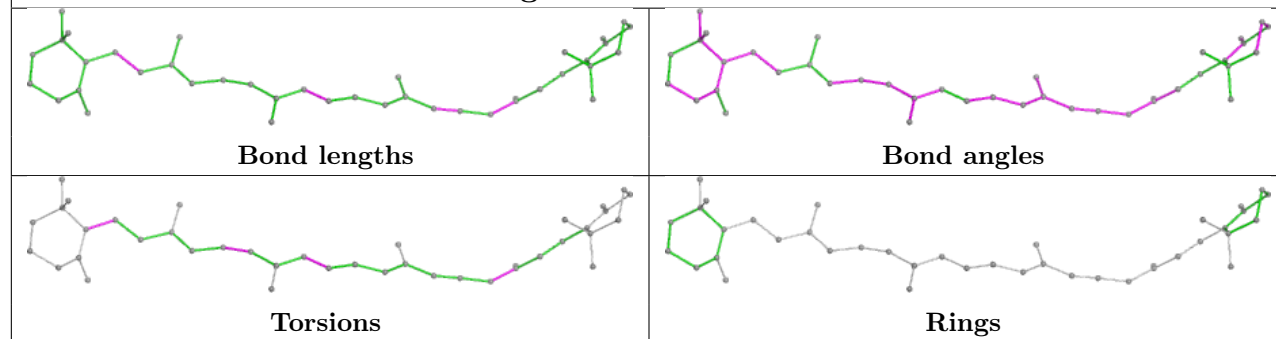


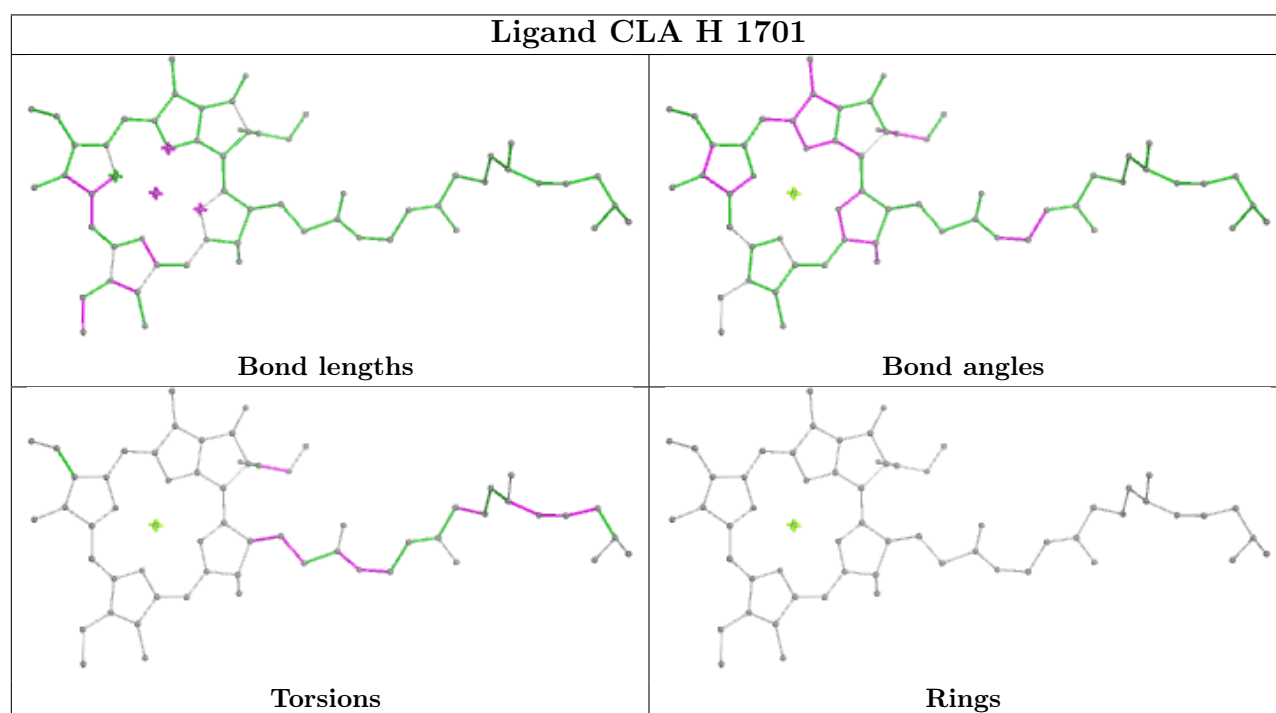
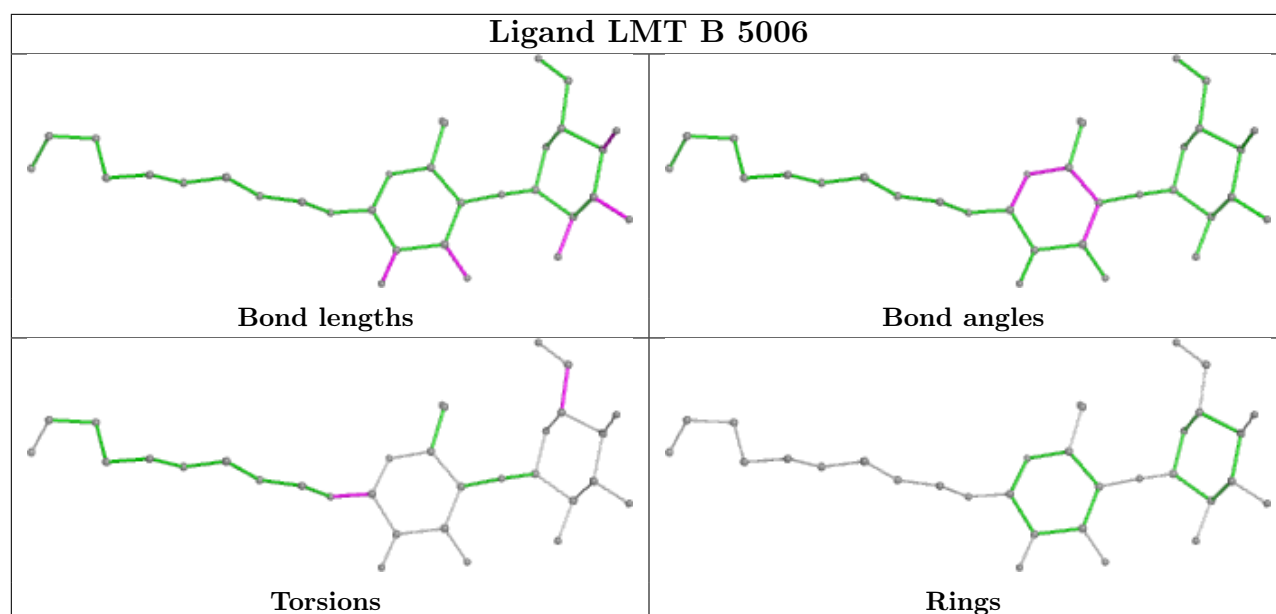
Ligand CLA 3 612

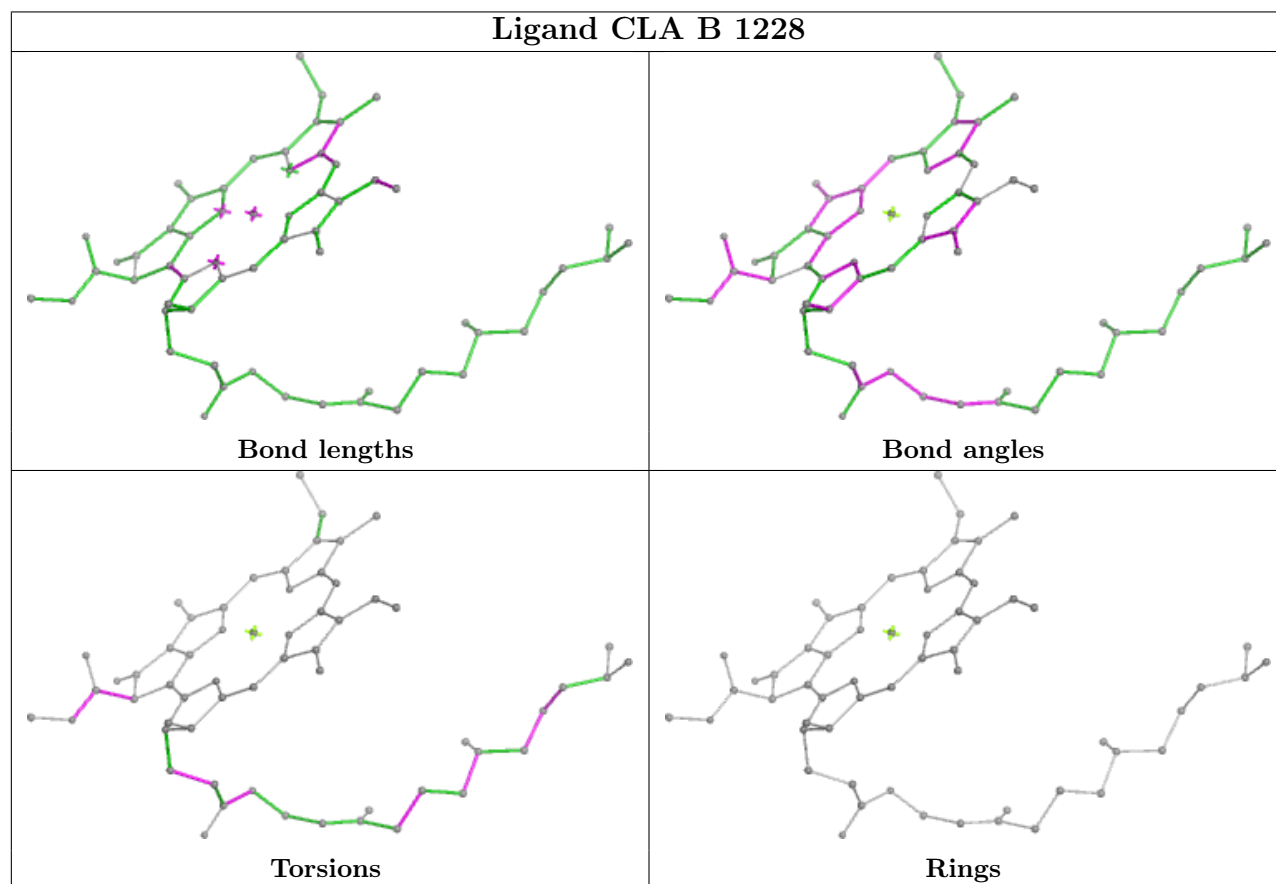
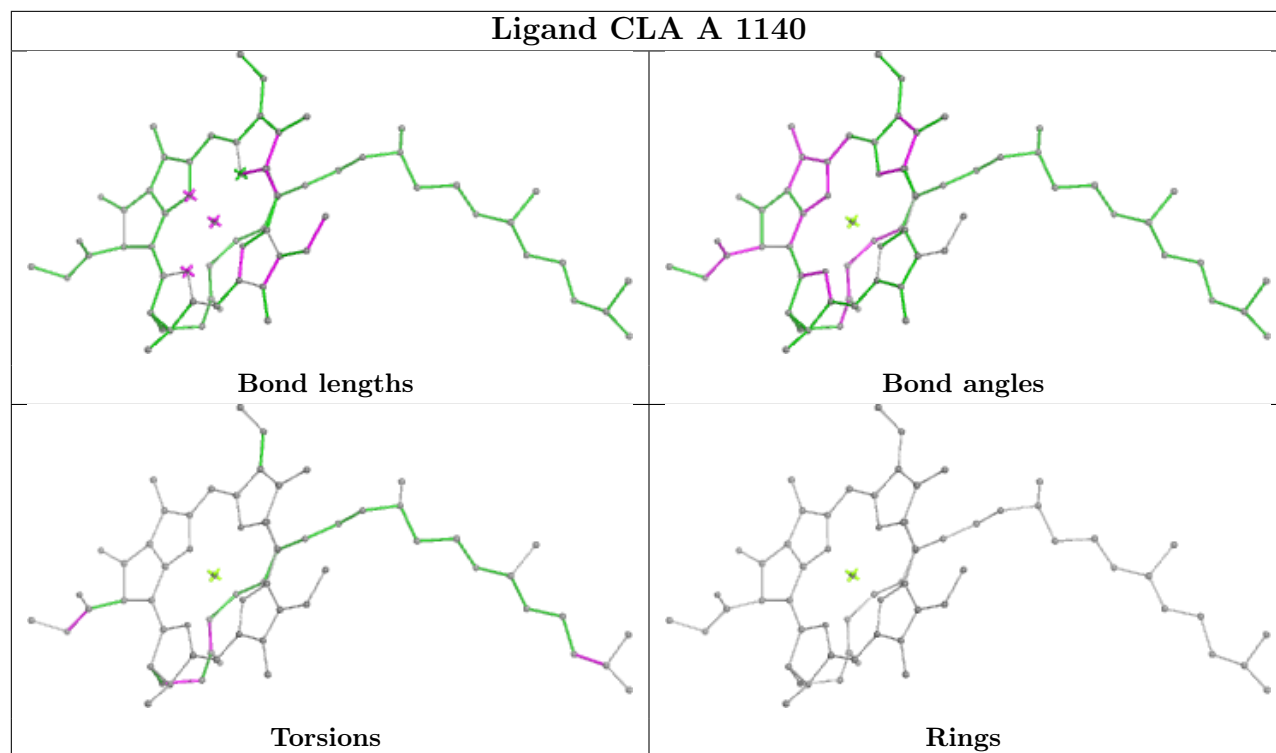


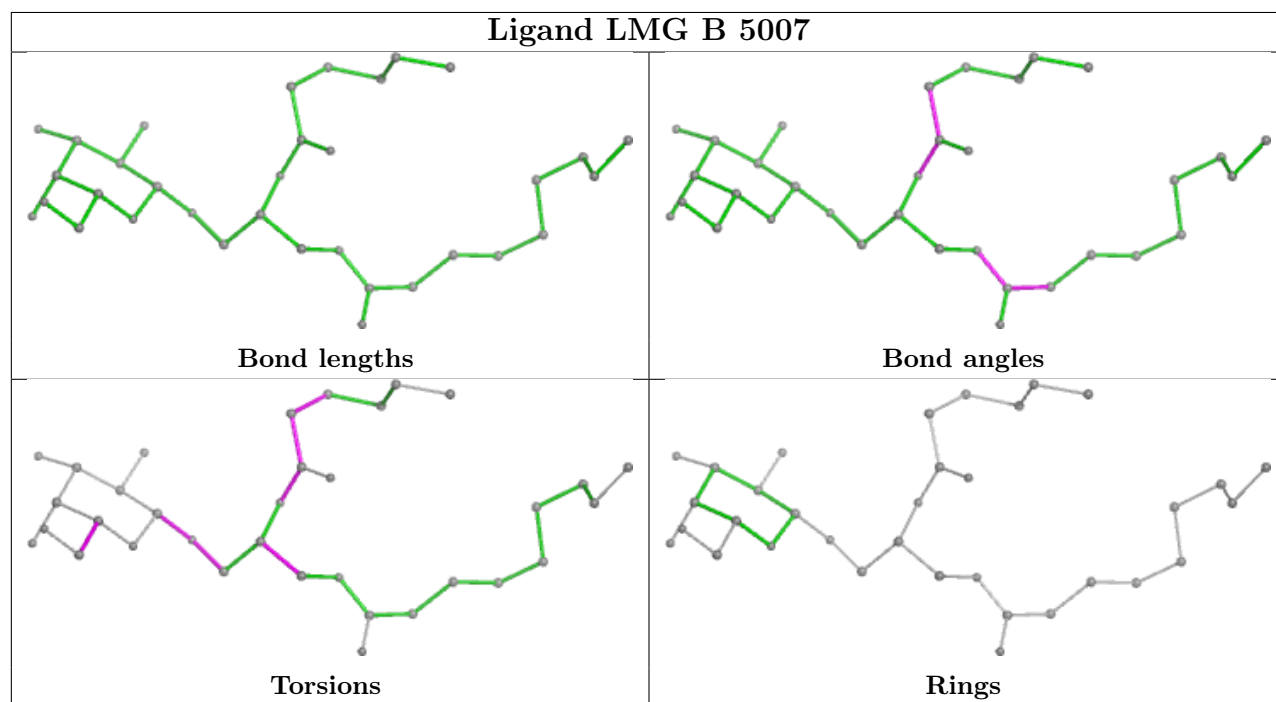
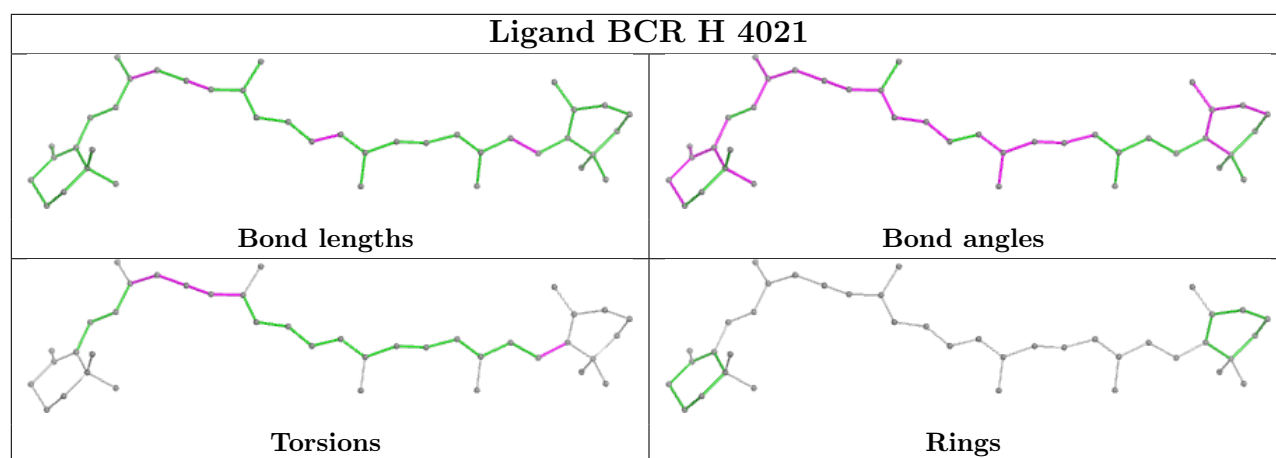
Ligand CLA 2 608

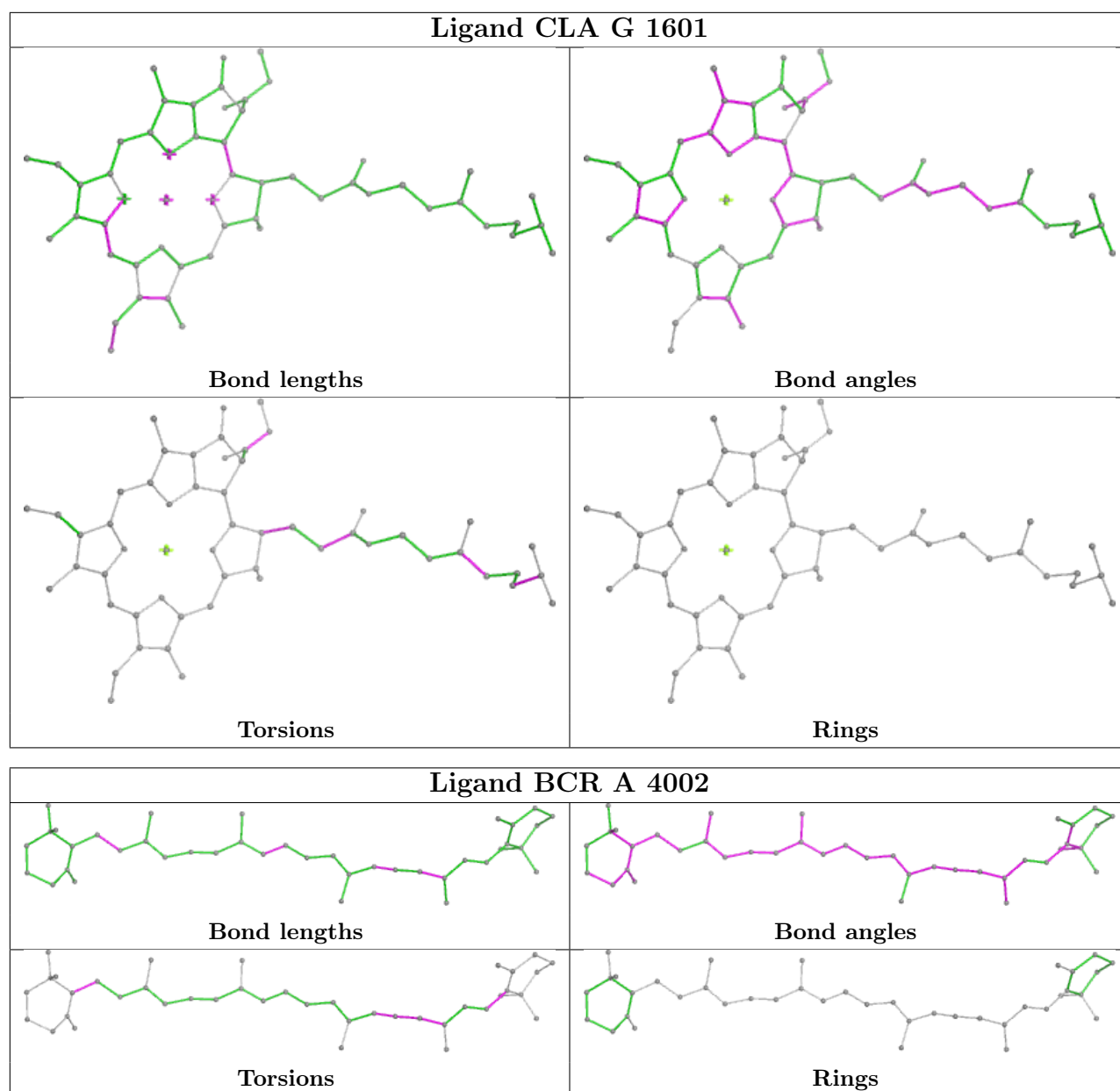


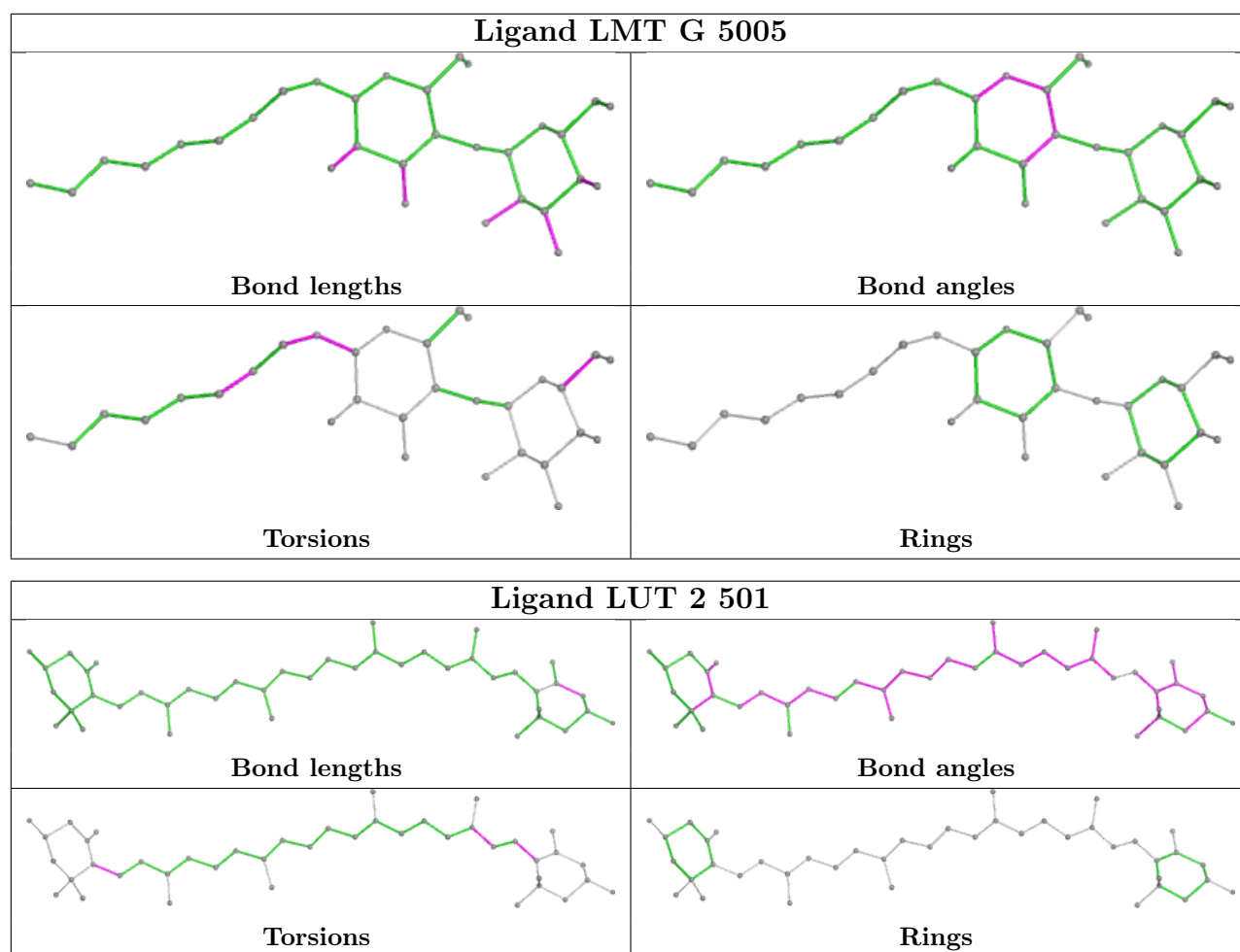
Ligand CLA 4 612**Ligand BCR K 4002**

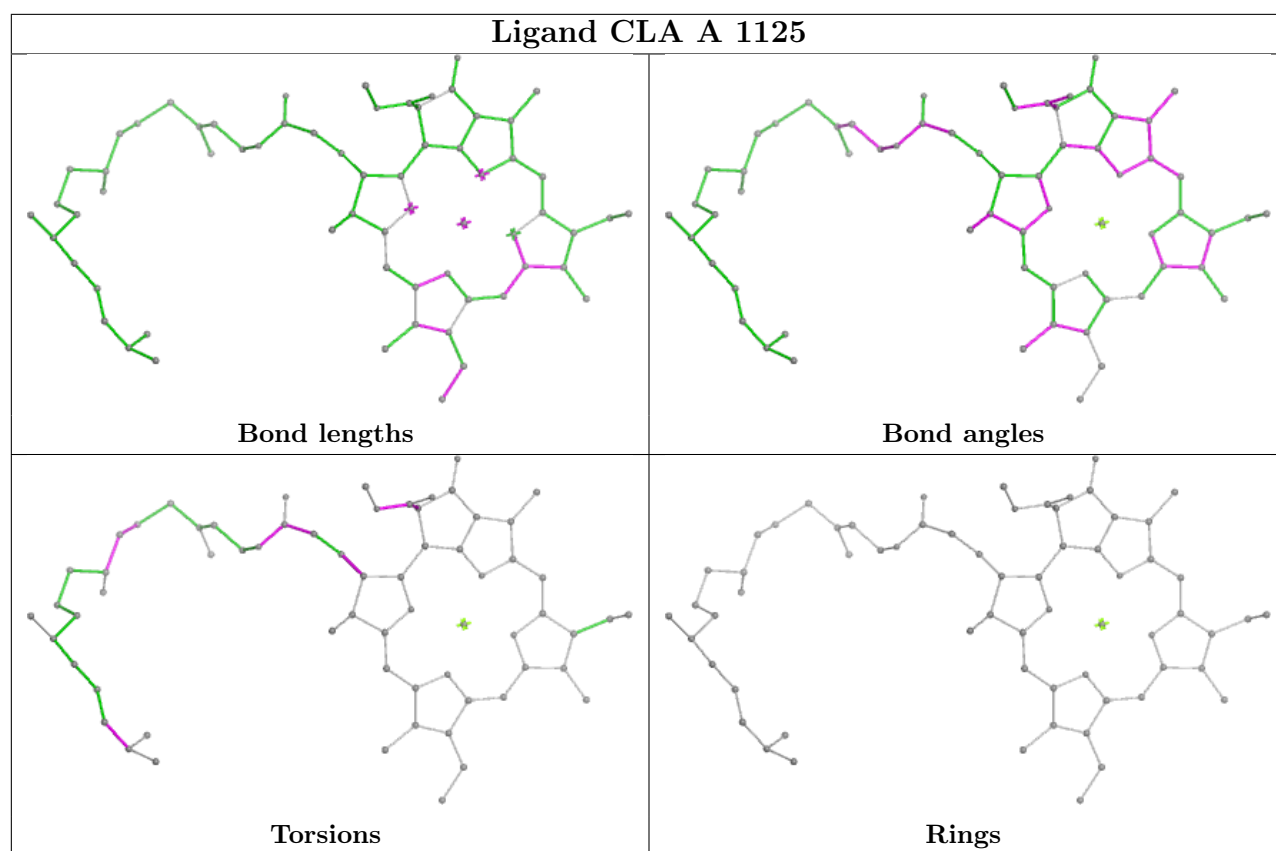




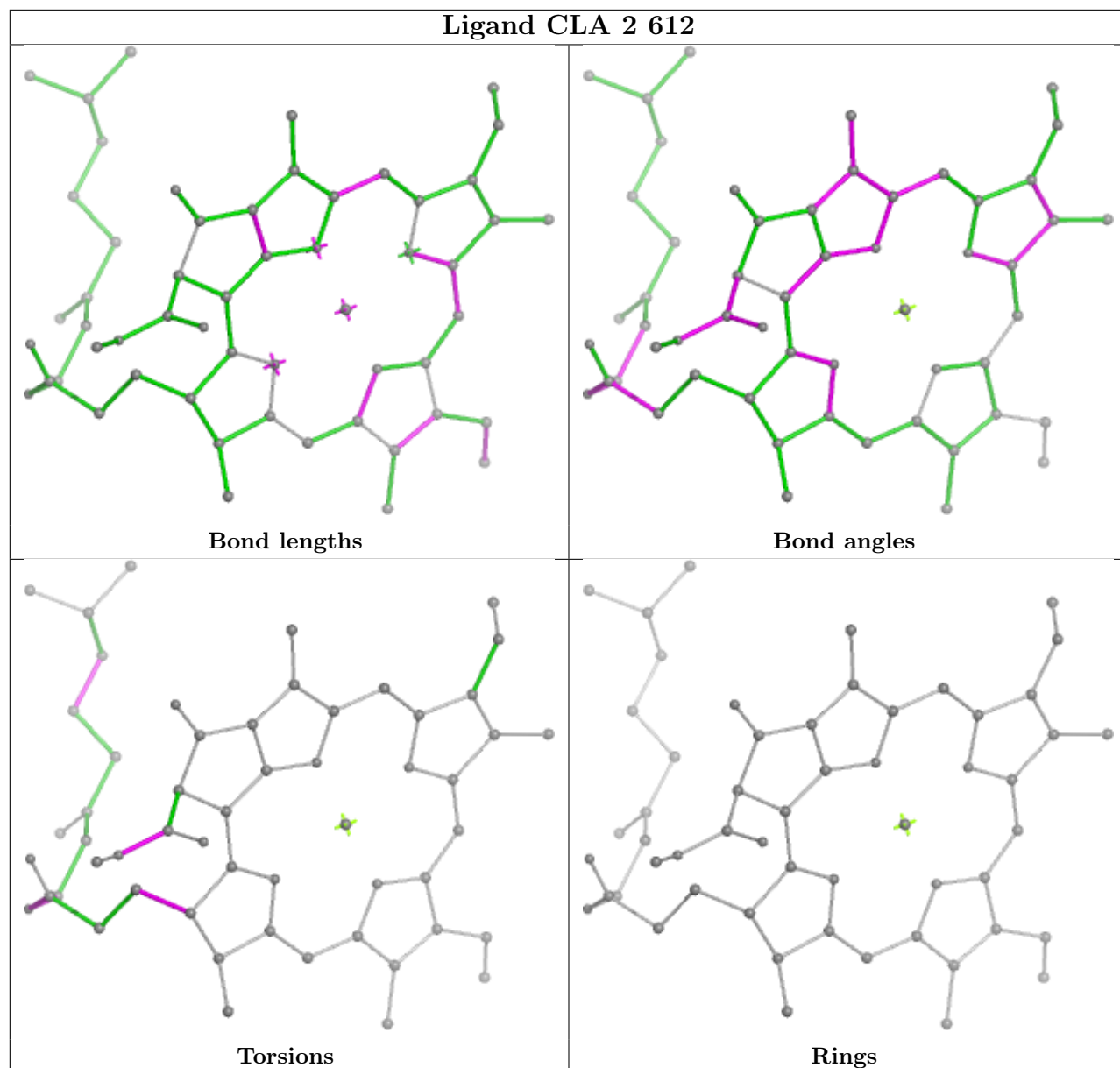


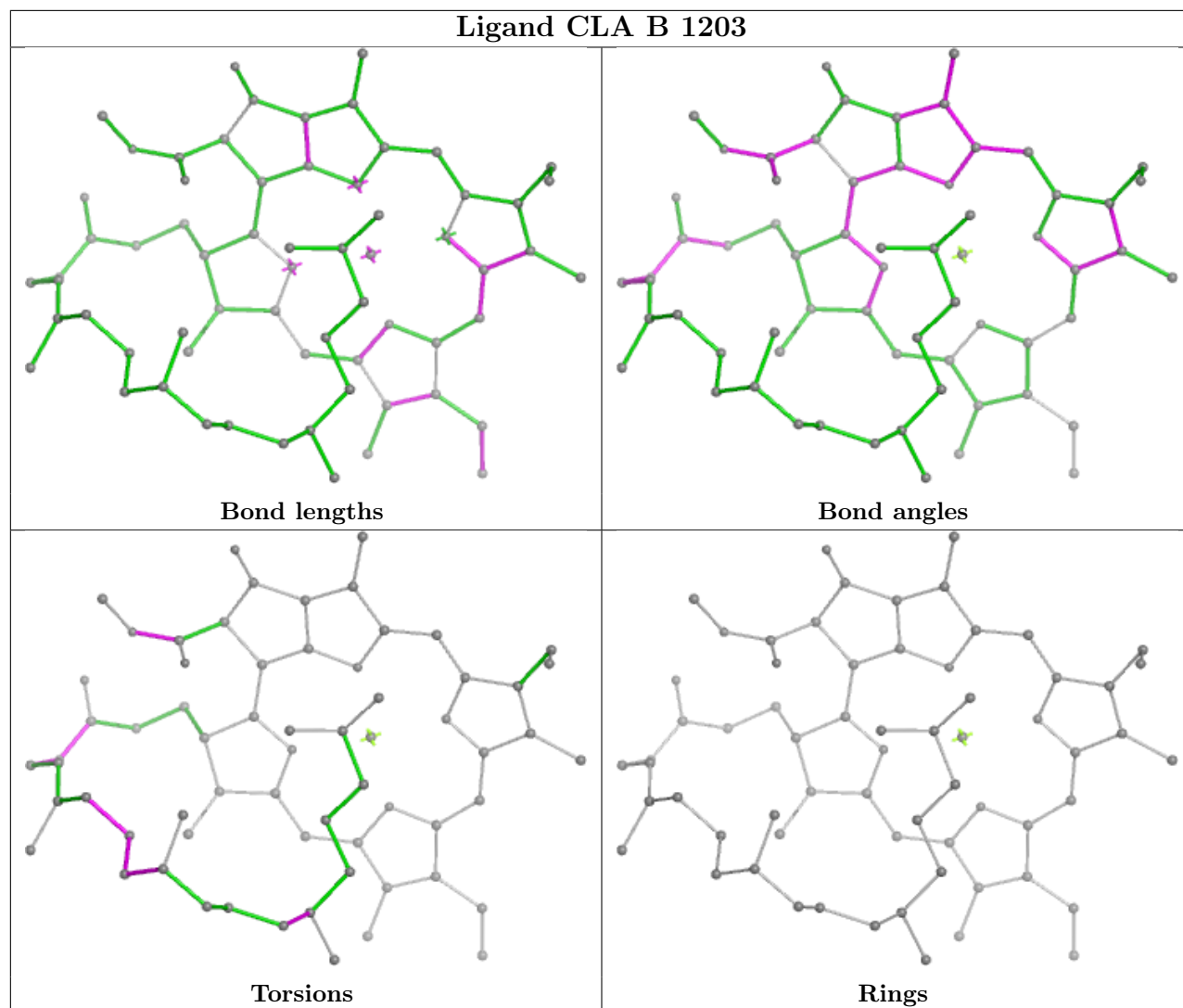




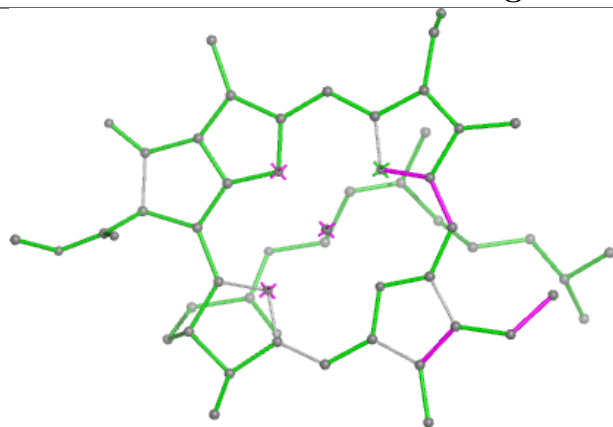


Ligand CLA 2 612

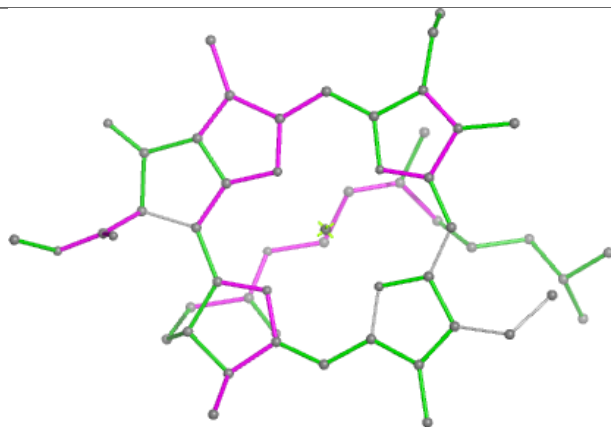




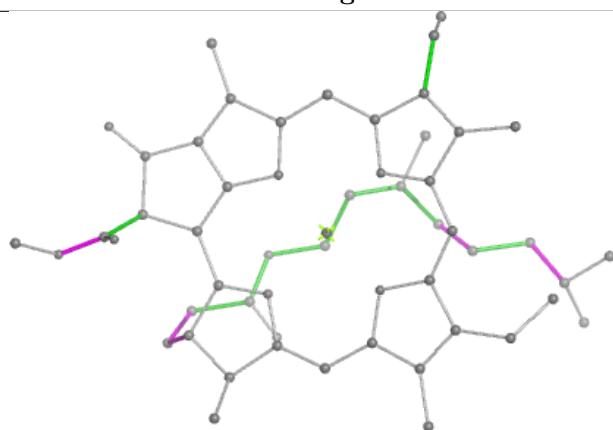
Ligand CLA A 1110



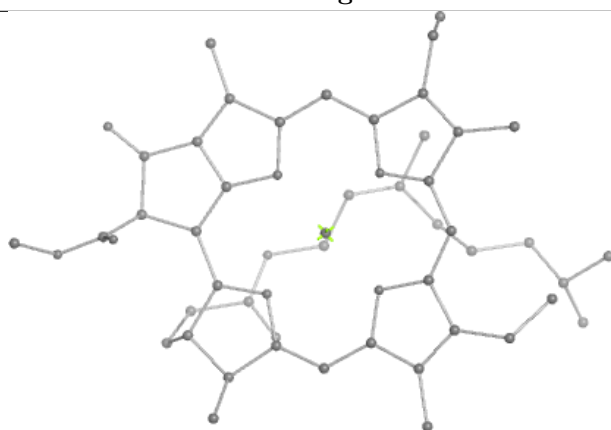
Bond lengths



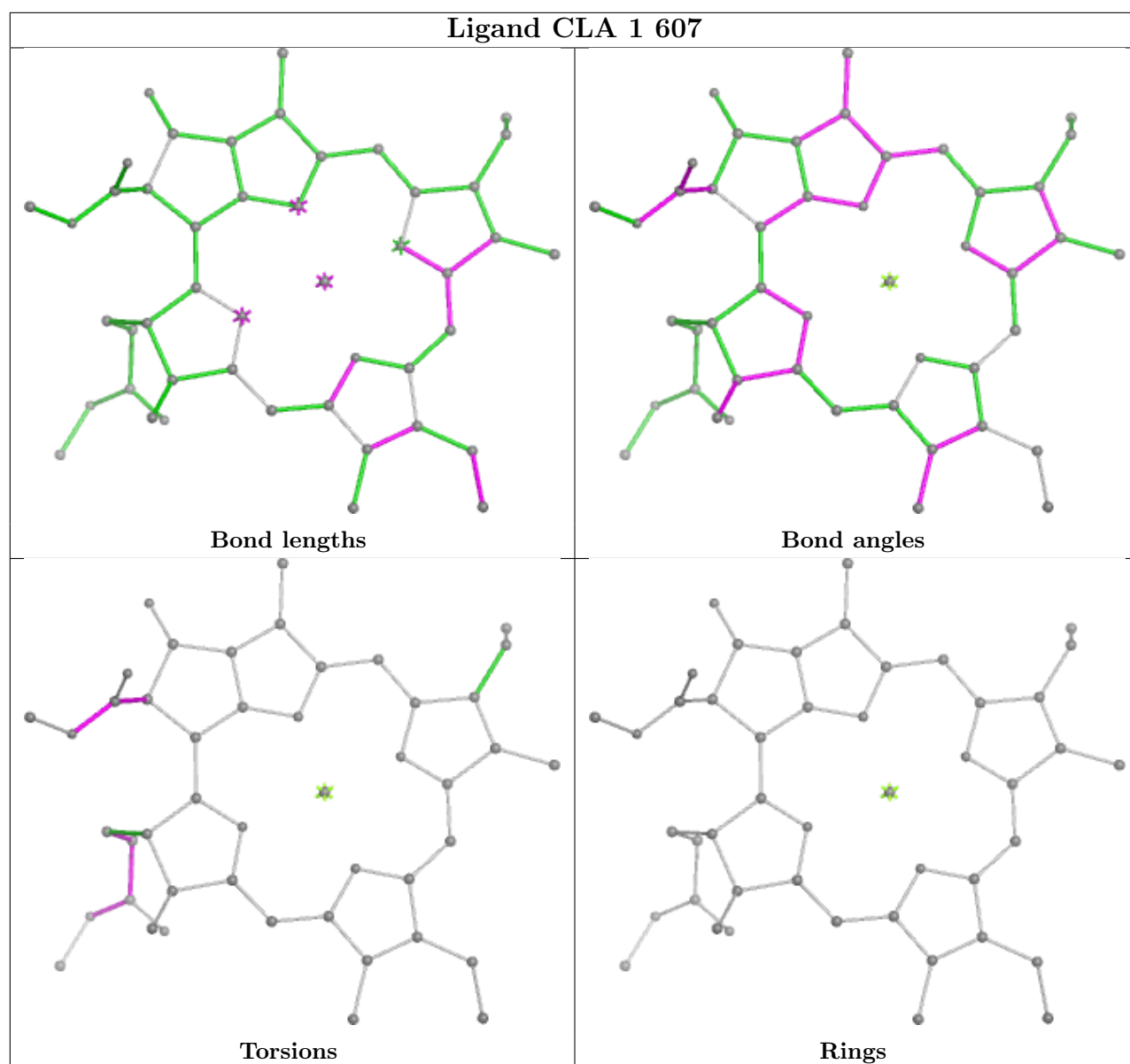
Bond angles



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-11326. 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.