



wwPDB EM Validation Summary Report ⓘ

Dec 28, 2024 – 12:31 PM EST

PDB ID : 6ZOO
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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

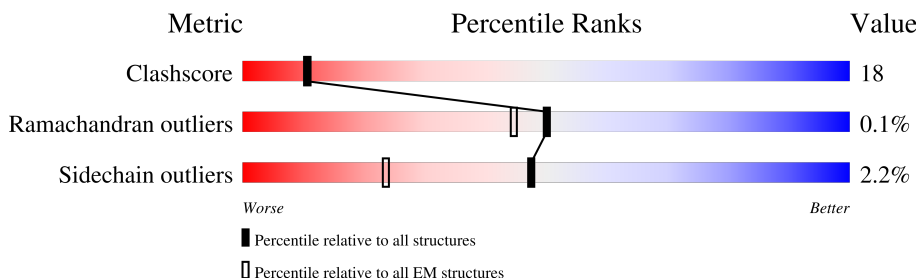
1 Overall quality at a glance

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	743	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% .

Continued on next page...

Continued from previous page...

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

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	601	X	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	1118	X	-	-	-
19	CLA	A	1119	X	-	-	-
19	CLA	A	1120	X	-	-	-
19	CLA	A	1121	X	-	-	-
19	CLA	A	1122	X	-	-	-
19	CLA	A	1123	X	-	-	-
19	CLA	A	1124	X	-	-	-
19	CLA	A	1125	X	-	-	-
19	CLA	A	1126	X	-	-	-
19	CLA	A	1127	X	-	-	-
19	CLA	A	1128	X	-	-	-
19	CLA	A	1129	X	-	-	-
19	CLA	A	1130	X	-	-	-
19	CLA	A	1131	X	-	-	-
19	CLA	A	1132	X	-	-	-
19	CLA	A	1133	X	-	-	-
19	CLA	A	1134	X	-	-	-
19	CLA	A	1135	X	-	-	-
19	CLA	A	1136	X	-	-	-
19	CLA	A	1137	X	-	-	-
19	CLA	A	1138	X	-	-	-
19	CLA	A	1139	X	-	-	-
19	CLA	A	1140	X	-	-	-
19	CLA	A	1141	X	-	-	-
19	CLA	B	1021	X	-	-	-
19	CLA	B	1022	X	-	-	-
19	CLA	B	1023	X	-	-	-
19	CLA	B	1201	X	-	-	-
19	CLA	B	1202	X	-	-	-
19	CLA	B	1203	X	-	-	-
19	CLA	B	1204	X	-	-	-
19	CLA	B	1205	X	-	-	-
19	CLA	B	1206	X	-	-	-
19	CLA	B	1207	X	-	-	-
19	CLA	B	1208	X	-	-	-
19	CLA	B	1209	X	-	-	-
19	CLA	B	1210	X	-	-	-
19	CLA	B	1211	X	-	-	-
19	CLA	B	1212	X	-	-	-
19	CLA	B	1213	X	-	-	-
19	CLA	B	1214	X	-	-	-
19	CLA	B	1215	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	1216	X	-	-	-
19	CLA	B	1217	X	-	-	-
19	CLA	B	1218	X	-	-	-
19	CLA	B	1219	X	-	-	-
19	CLA	B	1220	X	-	-	-
19	CLA	B	1221	X	-	-	-
19	CLA	B	1222	X	-	-	-
19	CLA	B	1223	X	-	-	-
19	CLA	B	1224	X	-	-	-
19	CLA	B	1225	X	-	-	-
19	CLA	B	1226	X	-	-	-
19	CLA	B	1227	X	-	-	-
19	CLA	B	1228	X	-	-	-
19	CLA	B	1229	X	-	-	-
19	CLA	B	1230	X	-	-	-
19	CLA	B	1231	X	-	-	-
19	CLA	B	1232	X	-	-	-
19	CLA	B	1234	X	-	-	-
19	CLA	B	1235	X	-	-	-
19	CLA	B	1236	X	-	-	-
19	CLA	B	1237	X	-	-	-
19	CLA	B	1238	X	-	-	-
19	CLA	B	1239	X	-	-	-
19	CLA	B	1240	X	-	-	-
19	CLA	F	1301	X	-	-	-
19	CLA	F	1302	X	-	-	-
19	CLA	G	1601	X	-	-	-
19	CLA	G	1602	X	-	-	-
19	CLA	G	1603	X	-	-	-
19	CLA	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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
28	LUT	3	502	X	-	-	-
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

Continued on next page...

Continued from previous page...

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		

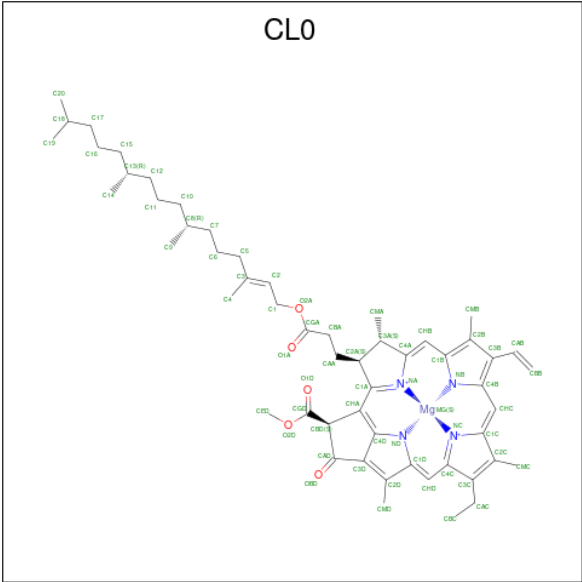
There are 3 discrepancies between the modelled and reference sequences:

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.

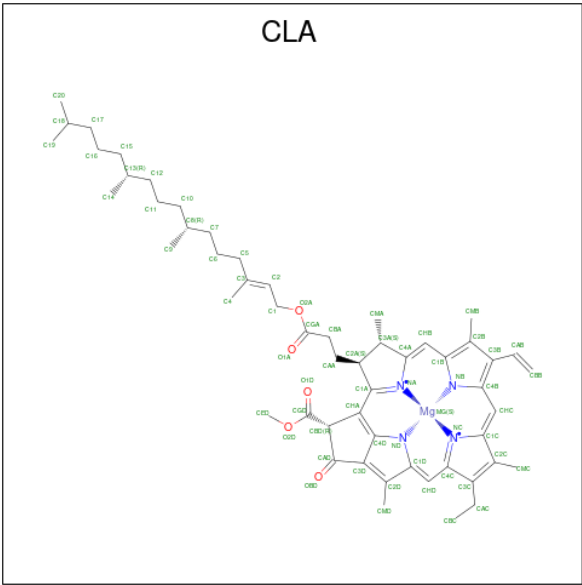
Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	99	Total	C	N	O	S	0	0
			728	460	115	150	3		

- Molecule 18 is CHLOROPHYLL A ISOMER (three-letter code: 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 (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

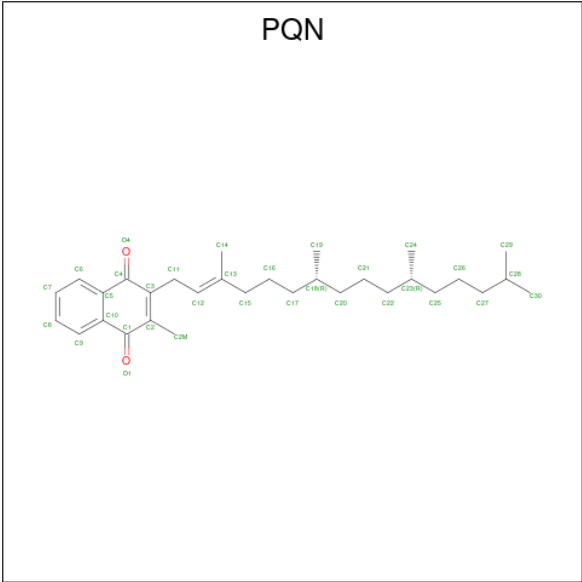
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	2	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	2	1	Total 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

Continued on next page...

Continued from previous page...

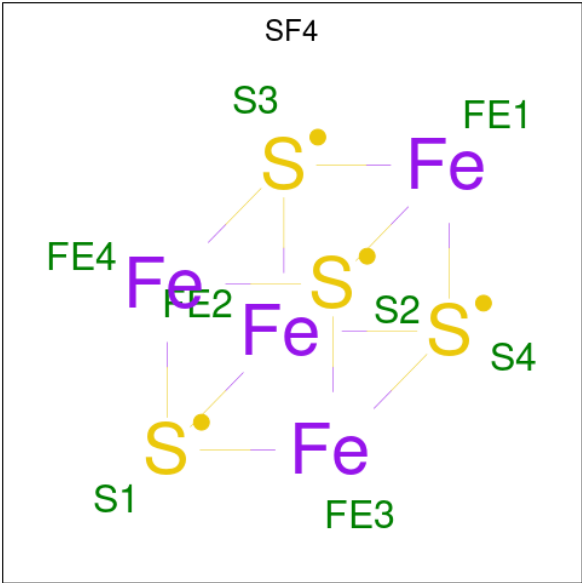
Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			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 (three-letter code: 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 (three-letter code: SF4) (formula: Fe₄S₄).



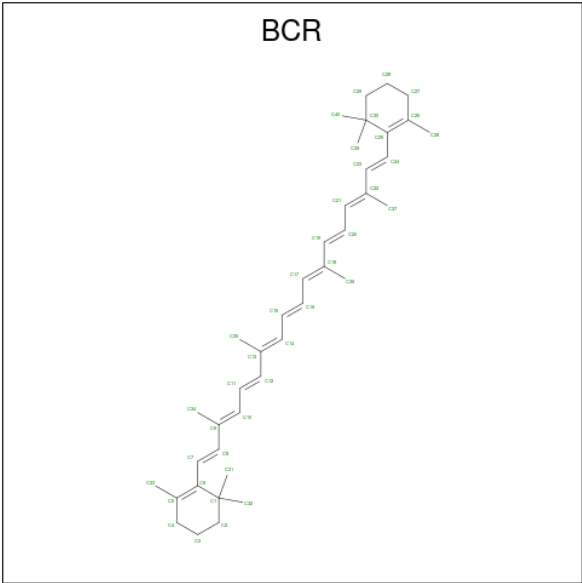
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	Fe	S	0
			8	4	4	
21	C	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

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

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



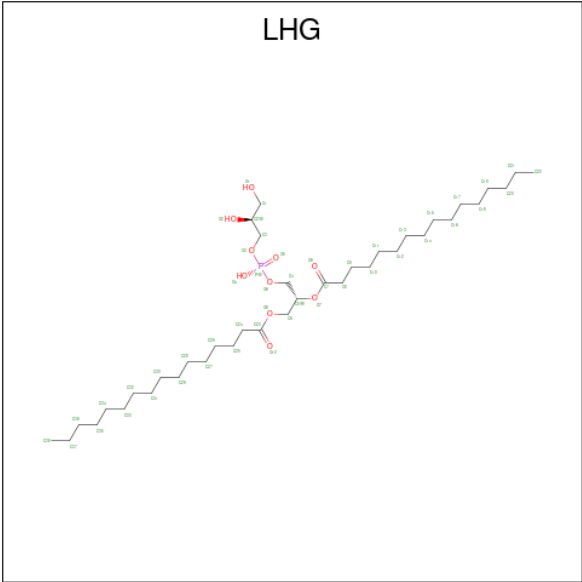
Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	A	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	
22	B	1	Total	C	0
			40	40	

Continued on next page...

Continued from previous page...

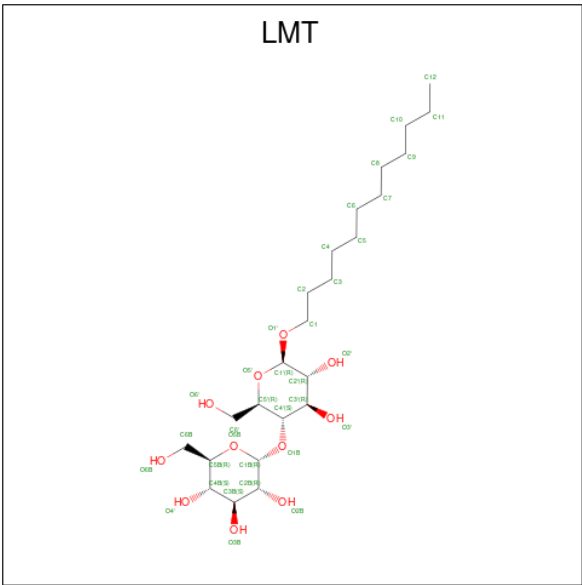
Mol	Chain	Residues	Atoms	AltConf
22	B	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	F	1	Total C 40 40	0
22	G	1	Total C 40 40	0
22	H	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	I	1	Total C 40 40	0
22	J	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	K	1	Total C 40 40	0
22	L	1	Total C 40 40	0
22	L	1	Total C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

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



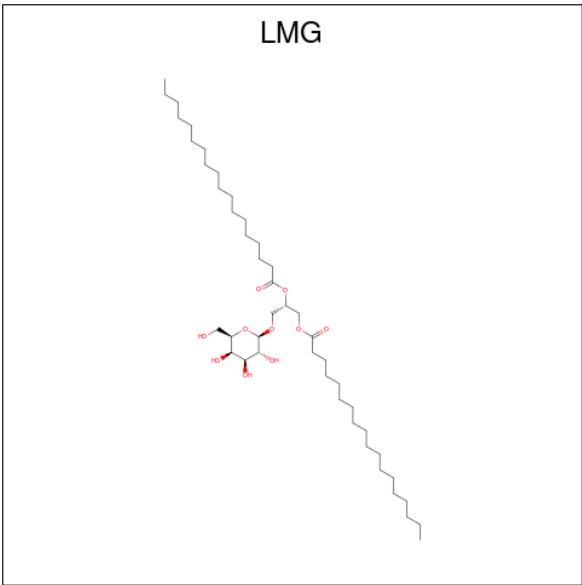
Mol	Chain	Residues	Atoms				AltConf
23	A	1	Total	C	O	P	0
			40	29	10	1	
23	A	1	Total	C	O	P	0
			49	38	10	1	
23	B	1	Total	C	O	P	0
			21	10	10	1	
23	B	1	Total	C	O	P	0
			49	38	10	1	
23	1	1	Total	C	O	P	0
			49	38	10	1	
23	2	1	Total	C	O	P	0
			35	24	10	1	
23	3	1	Total	C	O	P	0
			17	8	8	1	
23	4	1	Total	C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

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



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	O	0
			35	24	11	
24	B	1	Total	C	O	0
			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 (three-letter code: 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	

Continued on next page...

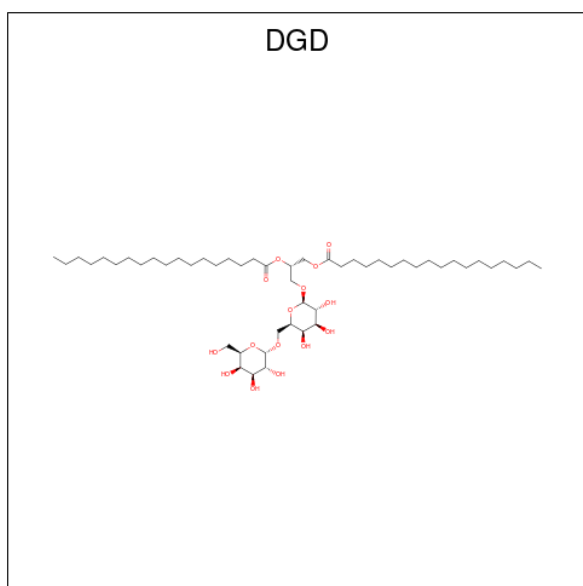
Continued from previous page...

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 (three-letter code: 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) (three-letter code: DGD) (formula: C₅₁H₉₆O₁₅).



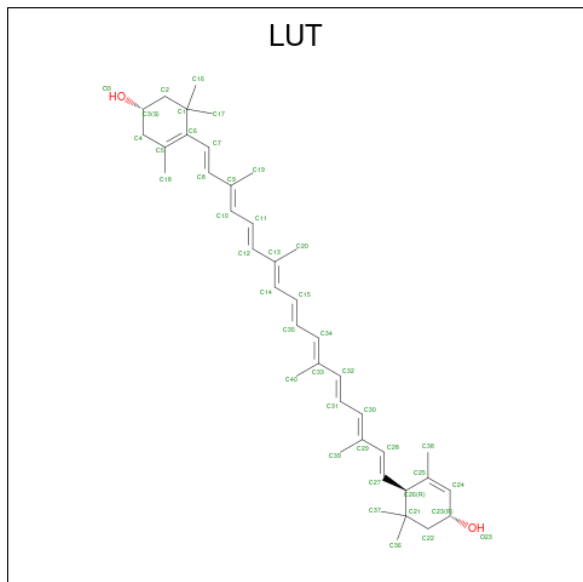
Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			61	46	15	
27	F	1	Total	C	O	0
			57	42	15	

Continued on next page...

Continued from previous page...

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 (three-letter code: LUT) (formula: $C_{40}H_{56}O_2$).



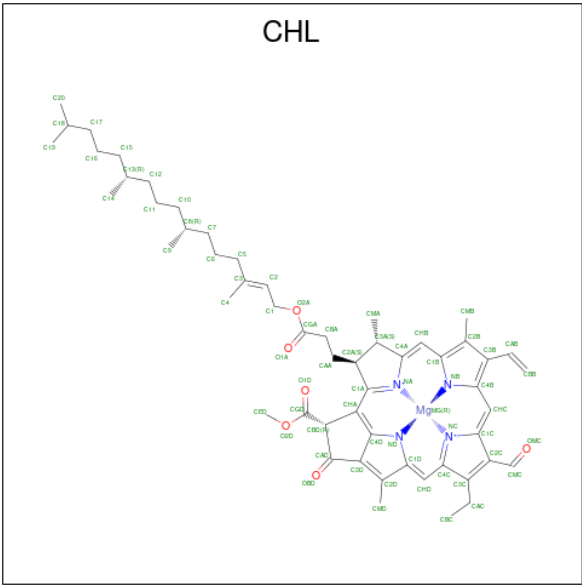
Mol	Chain	Residues	Atoms			AltConf
28	J	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	1	1	Total	C	O	0
			42	40	2	
28	2	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	
28	3	1	Total	C	O	0
			42	40	2	

Continued on next page...

Continued from previous page...

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 (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



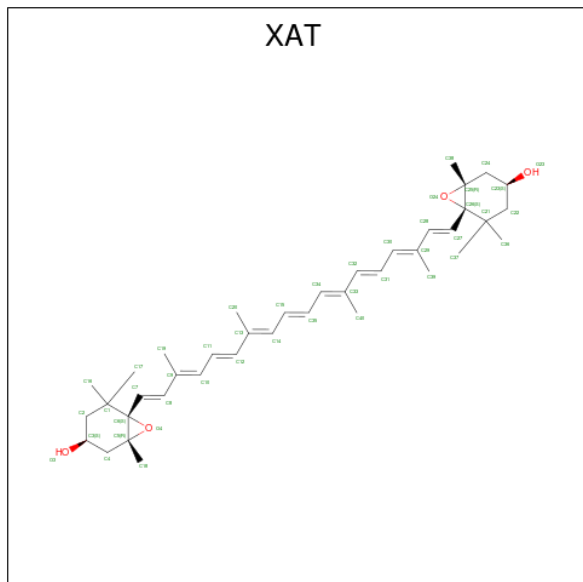
Mol	Chain	Residues	Atoms						AltConf
29	1	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	1	1	Total	C	Mg	N	O	0	
			47	36	1	4	6		
29	1	1	Total	C	Mg	N	O	0	
			61	50	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			56	45	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			48	37	1	4	6		
29	2	1	Total	C	Mg	N	O	0	
			46	35	1	4	6		
29	2	1	Total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

Continued on next page...

Continued from previous page...

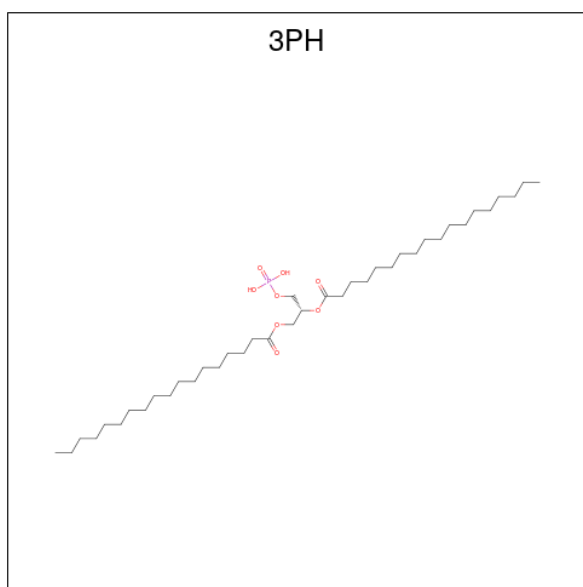
Mol	Chain	Residues	Atoms					AltConf
29	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
29	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- 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 (three-letter code: 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 (three-letter code: 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 (three-letter code: CU) (formula: Cu).

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

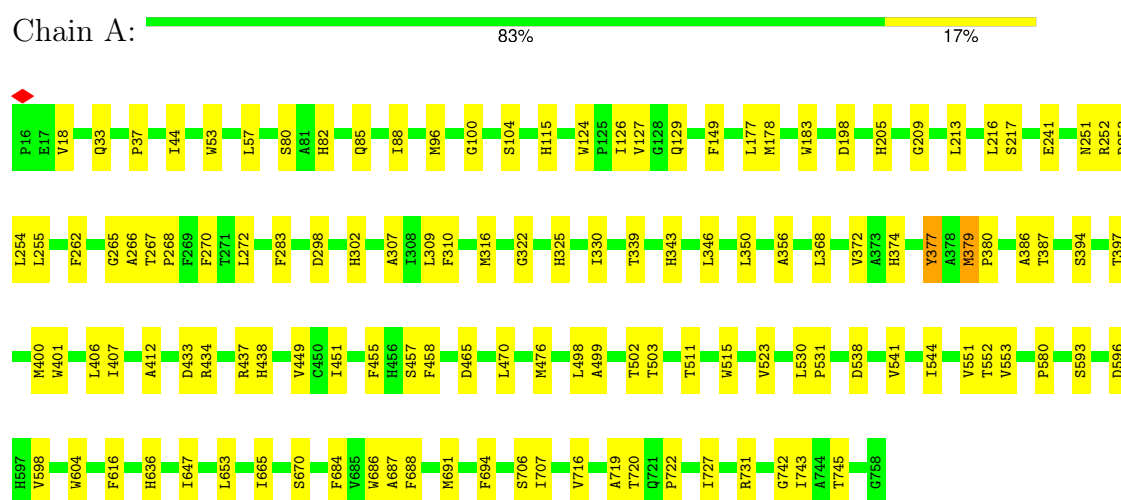
- Molecule 33 is water.

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

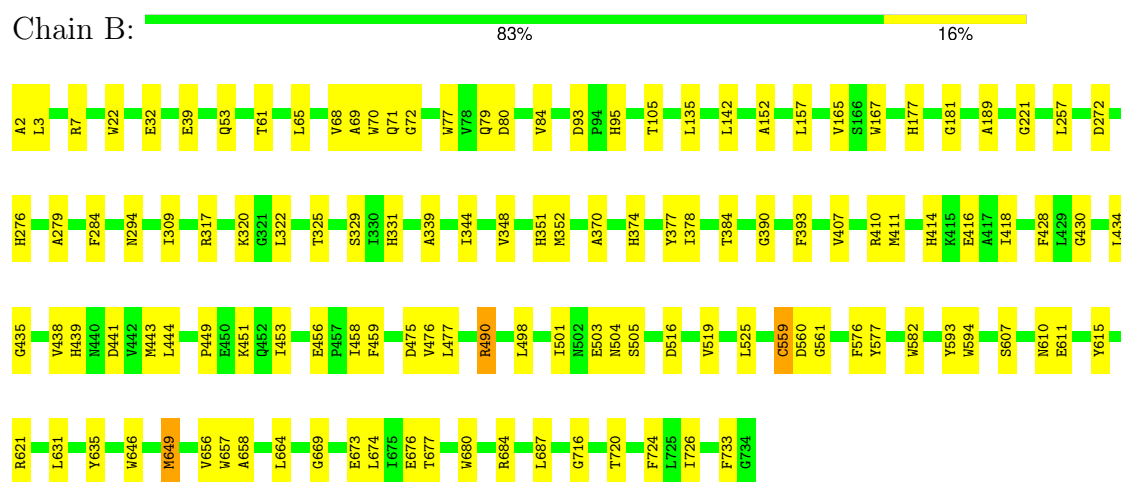
3 Residue-property plots

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

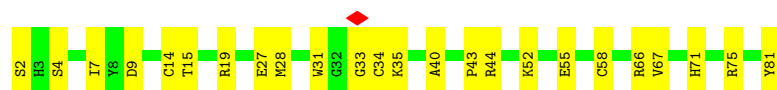


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

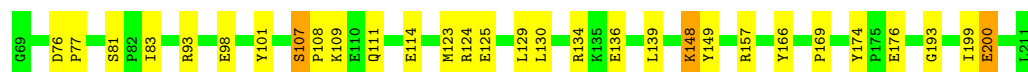
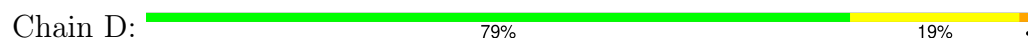


- Molecule 3: Photosystem I iron-sulfur center

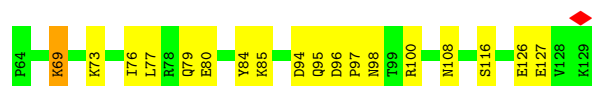




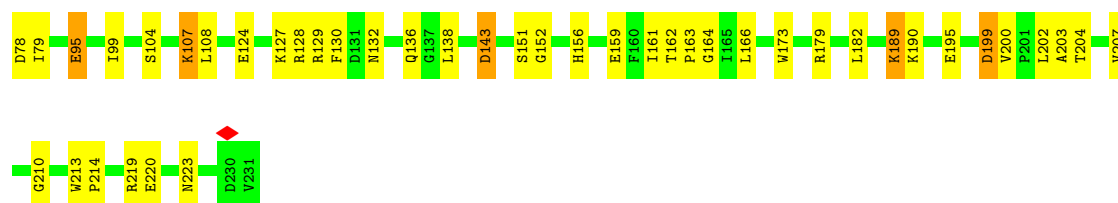
- Molecule 4: PsaD



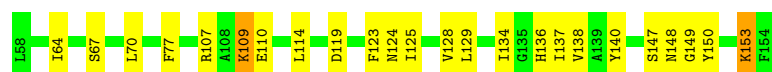
- Molecule 5: Putative uncharacterized protein



- Molecule 6: Photosystem I reaction center subunit III



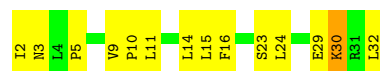
- Molecule 7: photosystem I reaction center



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



- Molecule 9: Photosystem I reaction center subunit VIII



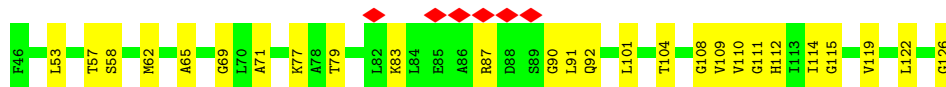
- Molecule 10: Photosystem I reaction center subunit IX

Chain J:  79% 21%




- Molecule 11: Photosystem I reaction center subunit X psaK

Chain K:  7% 68% 32%




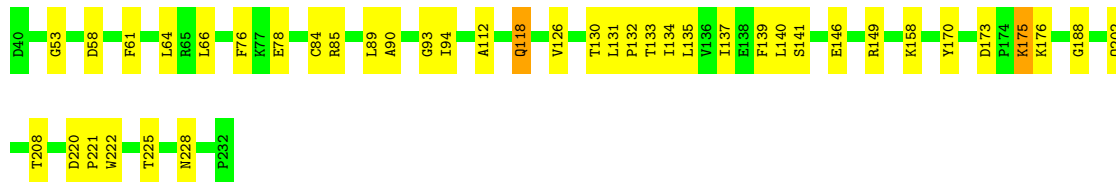
- Molecule 12: PsaL domain-containing protein

Chain L:  84% 16%



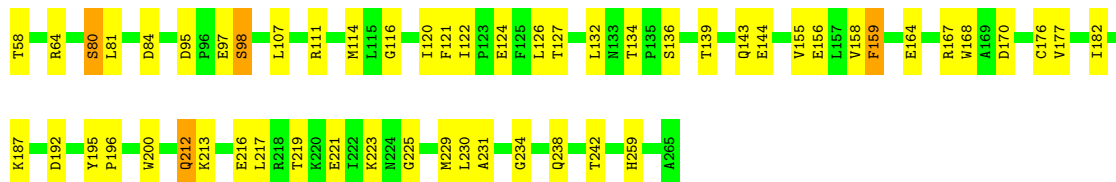
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain 1:  79% 20%



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

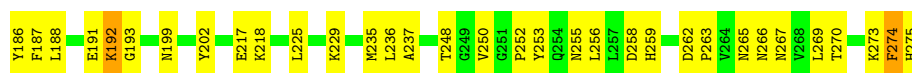
Chain 2:  74% 25%



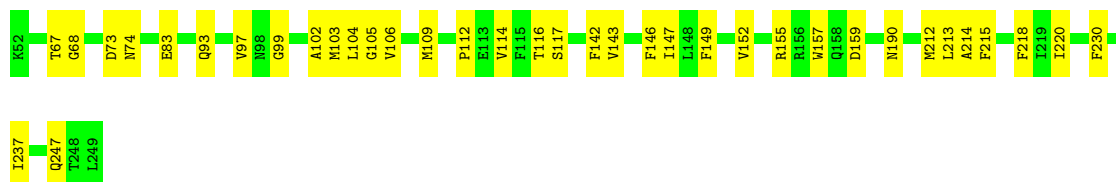
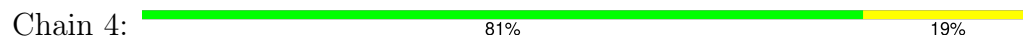
- Molecule 15: Chlorophyll a-b binding protein 3, chloroplastic

Chain 3:  68% 29%

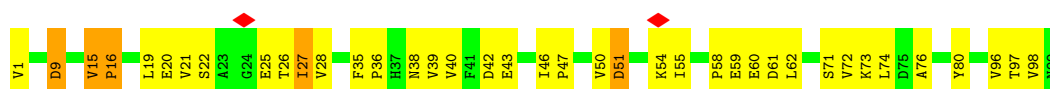




- Molecule 16: Chlorophyll a-b binding protein P4, chloroplastic



- Molecule 17: Plastocyanin, chloroplastic



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
Maximum map value	0.176	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0125	Depositor
Map size (\AA)	392.4, 392.4, 392.4	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.308, 1.308, 1.308	Depositor

5 Model quality

5.1 Standard geometry

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

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	9,14,15	0.97	1 (11%)	4,18,20	1.80	1 (25%)
1	SNK	A	115	1	9,14,15	1.00	1 (11%)	4,18,20	1.71	1 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	2.34	1.85	1.77
1	A	115	SNK	C02-S04	2.31	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	2.56	122.95	112.58
1	A	636	SNK	C01-C02-S04	2.53	122.85	112.58

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	N-CA-CB-CG
1	A	115	SNK	C-CA-CB-CG

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	A	1141	-	58,68,73	1.82	9 (15%)	68,107,113	1.93	14 (20%)
21	SF4	A	3001	2,1	0,12,12	-	-	-		
22	BCR	L	4020	-	41,41,41	1.59	4 (9%)	56,56,56	4.62	18 (32%)
22	BCR	F	4016	-	41,41,41	1.57	4 (9%)	56,56,56	4.48	17 (30%)
19	CLA	A	1105	-	58,68,73	1.82	8 (13%)	68,107,113	1.90	12 (17%)
24	LMT	2	808	-	36,36,36	1.12	5 (13%)	47,47,47	0.97	2 (4%)
29	CHL	2	610	-	54,64,74	0.89	2 (3%)	59,102,114	1.26	10 (16%)
22	BCR	J	4012	-	41,41,41	1.58	4 (9%)	56,56,56	4.72	17 (30%)
19	CLA	1	611	-	63,73,73	1.73	8 (12%)	74,113,113	1.82	12 (16%)
22	BCR	B	4006	-	41,41,41	1.58	4 (9%)	56,56,56	4.54	28 (50%)
19	CLA	B	1204	-	63,73,73	1.75	9 (14%)	74,113,113	1.84	15 (20%)
22	BCR	K	4002	-	41,41,41	1.56	4 (9%)	56,56,56	4.58	21 (37%)
22	BCR	A	4002	-	41,41,41	1.62	4 (9%)	56,56,56	4.46	22 (39%)
25	LMG	2	802	-	25,25,55	0.57	0	33,33,63	1.23	3 (9%)
19	CLA	4	606	-	48,58,73	1.97	7 (14%)	56,95,113	2.07	12 (21%)
19	CLA	A	1124	-	53,63,73	1.89	9 (16%)	62,101,113	1.96	13 (20%)
19	CLA	B	1216	-	63,73,73	1.69	8 (12%)	74,113,113	1.81	14 (18%)
19	CLA	A	1139	-	63,73,73	1.77	9 (14%)	74,113,113	1.87	15 (20%)
25	LMG	F	5002	-	47,47,55	1.09	4 (8%)	55,55,63	1.12	4 (7%)
27	DGD	3	803	-	52,52,67	0.94	3 (5%)	66,66,81	1.07	3 (4%)
22	BCR	A	4007	-	41,41,41	1.62	4 (9%)	56,56,56	4.76	20 (35%)
19	CLA	A	1129	-	63,73,73	1.73	9 (14%)	74,113,113	1.96	15 (20%)
19	CLA	B	1202	-	63,73,73	1.70	8 (12%)	74,113,113	1.97	16 (21%)
19	CLA	3	608	-	46,56,73	2.04	9 (19%)	53,92,113	2.13	12 (22%)
19	CLA	4	604	16	58,68,73	1.80	8 (13%)	68,107,113	1.99	14 (20%)
19	CLA	A	1121	-	58,68,73	1.80	9 (15%)	68,107,113	1.98	15 (22%)
19	CLA	B	1022	-	63,73,73	1.70	9 (14%)	74,113,113	1.86	16 (21%)
25	LMG	2	803	-	36,36,55	0.73	2 (5%)	44,44,63	1.08	2 (4%)
19	CLA	3	613	-	44,54,73	2.12	9 (20%)	51,90,113	2.13	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	L	1501	12	48,58,73	1.96	9 (18%)	56,95,113	2.16	15 (26%)
19	CLA	B	1229	-	63,73,73	1.73	8 (12%)	74,113,113	1.88	15 (20%)
19	CLA	A	1132	-	63,73,73	1.70	8 (12%)	74,113,113	1.88	15 (20%)
19	CLA	A	1136	-	63,73,73	1.72	9 (14%)	74,113,113	1.85	13 (17%)
19	CLA	B	1236	-	48,58,73	1.97	8 (16%)	56,95,113	2.13	16 (28%)
19	CLA	A	1117	-	63,73,73	1.69	8 (12%)	74,113,113	1.86	14 (18%)
22	BCR	G	4011	-	41,41,41	1.63	4 (9%)	56,56,56	4.63	21 (37%)
19	CLA	3	603	-	53,63,73	1.92	8 (15%)	62,101,113	2.12	16 (25%)
19	CLA	B	1205	-	63,73,73	1.70	8 (12%)	74,113,113	1.90	13 (17%)
19	CLA	B	1213	-	58,68,73	1.80	9 (15%)	68,107,113	1.92	13 (19%)
22	BCR	3	506	-	41,41,41	1.59	4 (9%)	56,56,56	4.66	21 (37%)
19	CLA	A	1138	-	63,73,73	1.68	9 (14%)	74,113,113	1.82	13 (17%)
19	CLA	A	1108	-	48,58,73	1.98	8 (16%)	56,95,113	2.13	13 (23%)
19	CLA	3	614	-	40,50,73	2.20	8 (20%)	45,85,113	2.22	9 (20%)
19	CLA	2	603	14	63,73,73	1.74	8 (12%)	74,113,113	1.87	14 (18%)
19	CLA	3	601	15	53,63,73	1.90	9 (16%)	62,101,113	1.98	13 (20%)
19	CLA	3	610	15	63,73,73	1.73	8 (12%)	74,113,113	1.85	14 (18%)
19	CLA	4	608	-	44,54,73	2.07	9 (20%)	51,90,113	2.11	13 (25%)
22	BCR	1	504	-	41,41,41	1.61	4 (9%)	56,56,56	4.81	19 (33%)
29	CHL	1	612	13	59,69,74	0.87	2 (3%)	65,108,114	1.12	8 (12%)
19	CLA	4	609	16	48,58,73	1.97	9 (18%)	56,95,113	2.07	13 (23%)
19	CLA	A	1137	-	63,73,73	1.73	9 (14%)	74,113,113	1.87	13 (17%)
25	LMG	B	5003	-	35,35,55	0.80	1 (2%)	43,43,63	1.16	4 (9%)
19	CLA	2	612	-	53,63,73	1.86	9 (16%)	62,101,113	1.97	12 (19%)
19	CLA	1	604	13	63,73,73	1.72	9 (14%)	74,113,113	1.85	13 (17%)
19	CLA	B	1203	2	63,73,73	1.73	8 (12%)	74,113,113	1.81	12 (16%)
22	BCR	K	4001	-	41,41,41	1.59	5 (12%)	56,56,56	4.75	16 (28%)
25	LMG	B	5004	-	33,33,55	0.53	0	41,41,63	1.23	5 (12%)
29	CHL	2	615	-	54,64,74	0.90	3 (5%)	59,102,114	1.32	11 (18%)
19	CLA	B	1220	-	53,63,73	1.85	9 (16%)	62,101,113	1.96	13 (20%)
19	CLA	B	1212	-	53,63,73	1.89	10 (18%)	62,101,113	2.08	15 (24%)
19	CLA	B	1224	-	63,73,73	1.70	9 (14%)	74,113,113	1.92	14 (18%)
19	CLA	A	1123	-	63,73,73	1.76	8 (12%)	74,113,113	1.89	11 (14%)
19	CLA	1	614	13	58,68,73	1.81	9 (15%)	68,107,113	1.88	13 (19%)
19	CLA	A	1126	-	63,73,73	1.71	8 (12%)	74,113,113	1.93	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DGD	G	5003	-	48,48,67	0.89	2 (4%)	62,62,81	0.98	3 (4%)
19	CLA	A	1135	-	49,59,73	1.95	8 (16%)	56,96,113	2.12	13 (23%)
25	LMG	F	5003	-	36,36,55	0.79	1 (2%)	44,44,63	1.03	2 (4%)
25	LMG	A	5006	-	50,50,55	1.18	5 (10%)	58,58,63	1.06	3 (5%)
19	CLA	3	607	-	50,60,73	1.95	8 (16%)	57,97,113	2.09	14 (24%)
19	CLA	A	1112	-	63,73,73	1.73	8 (12%)	74,113,113	1.87	14 (18%)
19	CLA	1	607	-	44,54,73	2.07	9 (20%)	51,90,113	2.16	10 (19%)
22	BCR	B	4004	-	41,41,41	1.61	4 (9%)	56,56,56	4.97	17 (30%)
25	LMG	F	5004	-	34,34,55	0.50	0	42,42,63	1.10	3 (7%)
19	CLA	A	1131	-	63,73,73	1.75	9 (14%)	74,113,113	1.79	13 (17%)
19	CLA	L	1503	-	48,58,73	1.98	9 (18%)	56,95,113	2.15	17 (30%)
19	CLA	2	602	-	50,60,73	1.94	8 (16%)	57,97,113	2.09	18 (31%)
19	CLA	B	1219	-	63,73,73	1.72	10 (15%)	74,113,113	1.91	12 (16%)
29	CHL	4	613	-	59,69,74	0.88	4 (6%)	65,108,114	1.11	8 (12%)
19	CLA	B	1207	-	63,73,73	1.71	10 (15%)	74,113,113	1.80	15 (20%)
25	LMG	F	5006	-	13,13,55	0.58	0	18,18,63	0.71	0
19	CLA	B	1211	-	63,73,73	1.67	8 (12%)	74,113,113	1.84	15 (20%)
19	CLA	B	1230	-	56,66,73	1.83	8 (14%)	65,104,113	2.03	16 (24%)
19	CLA	3	612	15	48,58,73	1.92	9 (18%)	56,95,113	2.12	13 (23%)
19	CLA	B	1210	-	63,73,73	1.72	10 (15%)	74,113,113	1.92	15 (20%)
19	CLA	A	1104	-	63,73,73	1.71	9 (14%)	74,113,113	1.88	15 (20%)
19	CLA	2	605	-	63,73,73	1.74	10 (15%)	74,113,113	1.87	13 (17%)
25	LMG	1	802	-	46,46,55	1.04	3 (6%)	54,54,63	1.02	2 (3%)
28	LUT	2	501	-	42,43,43	2.40	1 (2%)	51,60,60	2.14	18 (35%)
19	CLA	2	607	-	58,68,73	1.81	9 (15%)	68,107,113	2.06	16 (23%)
30	XAT	4	502	-	41,47,47	0.69	1 (2%)	54,74,74	1.76	15 (27%)
19	CLA	K	1402	-	58,68,73	1.80	8 (13%)	68,107,113	1.96	13 (19%)
19	CLA	A	1122	-	63,73,73	1.70	9 (14%)	74,113,113	1.90	14 (18%)
19	CLA	B	1023	-	63,73,73	1.72	7 (11%)	74,113,113	1.76	13 (17%)
19	CLA	F	1302	6	63,73,73	1.76	8 (12%)	74,113,113	1.88	15 (20%)
31	3PH	2	807	-	32,32,47	1.04	4 (12%)	35,37,52	1.20	2 (5%)
22	BCR	H	4021	-	41,41,41	1.59	4 (9%)	56,56,56	4.73	19 (33%)
19	CLA	4	601	16	58,68,73	1.83	9 (15%)	68,107,113	1.97	15 (22%)
25	LMG	B	5007	-	34,34,55	0.51	0	42,42,63	1.08	2 (4%)
22	BCR	I	4018	-	41,41,41	1.61	5 (12%)	56,56,56	4.60	25 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	CHL	4	610	-	45,55,74	1.02	4 (8%)	48,91,114	1.41	10 (20%)
23	LHG	4	801	-	34,34,48	0.47	0	37,40,54	1.20	3 (8%)
19	CLA	A	1116	-	54,64,73	1.84	10 (18%)	63,102,113	2.08	15 (23%)
19	CLA	B	1235	-	63,73,73	1.71	10 (15%)	74,113,113	1.90	14 (18%)
19	CLA	G	1603	-	63,73,73	1.73	8 (12%)	74,113,113	1.87	13 (17%)
25	LMG	2	805	-	30,30,55	0.56	0	38,38,63	1.09	3 (7%)
22	BCR	I	4020	-	41,41,41	1.61	4 (9%)	56,56,56	4.58	20 (35%)
19	CLA	B	1237	-	63,73,73	1.72	9 (14%)	74,113,113	1.81	12 (16%)
19	CLA	A	1109	-	63,73,73	1.72	9 (14%)	74,113,113	1.93	16 (21%)
19	CLA	J	1901	10	48,58,73	1.99	9 (18%)	56,95,113	2.07	13 (23%)
19	CLA	A	1133	-	63,73,73	1.73	9 (14%)	74,113,113	1.81	13 (17%)
19	CLA	A	1106	1	63,73,73	1.68	9 (14%)	74,113,113	1.94	16 (21%)
19	CLA	A	1120	-	58,68,73	1.81	8 (13%)	68,107,113	1.90	13 (19%)
19	CLA	B	1240	23	63,73,73	1.73	9 (14%)	74,113,113	1.86	14 (18%)
22	BCR	F	4014	-	41,41,41	1.60	4 (9%)	56,56,56	4.63	19 (33%)
19	CLA	B	1223	-	63,73,73	1.72	10 (15%)	74,113,113	1.92	16 (21%)
19	CLA	B	1222	33	63,73,73	1.67	9 (14%)	74,113,113	1.92	16 (21%)
19	CLA	1	603	-	53,63,73	1.88	8 (15%)	62,101,113	2.06	15 (24%)
28	LUT	1	502	-	42,43,43	2.41	1 (2%)	51,60,60	2.05	14 (27%)
19	CLA	1	606	-	48,58,73	2.00	8 (16%)	56,95,113	2.09	14 (25%)
22	BCR	L	4019	-	41,41,41	1.61	4 (9%)	56,56,56	4.75	20 (35%)
19	CLA	4	617	-	63,73,73	1.74	8 (12%)	74,113,113	1.90	16 (21%)
24	LMT	A	5004	-	36,36,36	1.13	5 (13%)	47,47,47	1.02	2 (4%)
19	CLA	A	1012	-	63,73,73	1.73	9 (14%)	74,113,113	1.84	14 (18%)
20	PQN	A	2001	-	34,34,34	0.38	0	43,45,45	1.15	3 (6%)
22	BCR	A	4011	-	41,41,41	1.58	4 (9%)	56,56,56	4.60	21 (37%)
27	DGD	J	5001	-	59,59,67	1.16	6 (10%)	73,73,81	1.01	2 (2%)
19	CLA	A	1110	-	53,63,73	1.88	8 (15%)	62,101,113	2.07	13 (20%)
19	CLA	A	1118	-	48,58,73	1.99	8 (16%)	56,95,113	2.11	13 (23%)
19	CLA	F	1301	-	63,73,73	1.75	9 (14%)	74,113,113	1.81	12 (16%)
27	DGD	F	5005	-	58,58,67	1.14	6 (10%)	72,72,81	1.04	5 (6%)
29	CHL	2	611	-	46,56,74	1.00	3 (6%)	49,92,114	1.33	9 (18%)
19	CLA	K	1403	-	46,56,73	2.05	9 (19%)	53,92,113	2.23	14 (26%)
19	CLA	B	1225	-	63,73,73	1.70	8 (12%)	74,113,113	1.85	13 (17%)
19	CLA	A	1134	1	53,63,73	1.86	8 (15%)	62,101,113	1.99	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	1226	-	63,73,73	1.72	8 (12%)	74,113,113	1.91	13 (17%)
19	CLA	B	1234	-	53,63,73	1.91	7 (13%)	62,101,113	2.01	12 (19%)
23	LHG	B	5001	19	20,20,48	0.59	0	23,26,54	1.53	3 (13%)
30	XAT	2	502	-	41,47,47	0.71	1 (2%)	54,74,74	1.99	14 (25%)
19	CLA	A	1127	-	63,73,73	1.70	8 (12%)	74,113,113	1.78	16 (21%)
19	CLA	A	1101	-	63,73,73	1.72	9 (14%)	74,113,113	1.91	16 (21%)
25	LMG	3	802	-	30,30,55	0.56	0	38,38,63	1.10	3 (7%)
19	CLA	1	613	-	43,53,73	2.12	10 (23%)	50,89,113	2.12	10 (20%)
19	CLA	B	1021	-	63,73,73	1.73	9 (14%)	74,113,113	1.92	14 (18%)
19	CLA	A	1114	-	44,54,73	2.10	9 (20%)	51,90,113	2.19	11 (21%)
19	CLA	B	1232	-	53,63,73	1.91	9 (16%)	62,101,113	1.97	12 (19%)
25	LMG	F	5001	-	30,30,55	0.53	0	38,38,63	1.07	2 (5%)
27	DGD	1	803	-	42,42,67	0.88	1 (2%)	56,56,81	1.01	2 (3%)
19	CLA	4	612	16	63,73,73	1.73	9 (14%)	74,113,113	1.81	13 (17%)
19	CLA	A	1130	-	53,63,73	1.88	9 (16%)	62,101,113	1.98	13 (20%)
19	CLA	G	1601	-	53,63,73	1.88	8 (15%)	62,101,113	2.03	15 (24%)
19	CLA	3	617	-	58,68,73	1.82	8 (13%)	68,107,113	1.91	13 (19%)
28	LUT	J	4013	-	42,43,43	2.40	1 (2%)	51,60,60	2.00	13 (25%)
19	CLA	B	1228	-	58,68,73	1.79	8 (13%)	68,107,113	1.99	16 (23%)
19	CLA	B	1231	-	58,68,73	1.80	8 (13%)	68,107,113	1.93	14 (20%)
23	LHG	B	5002	-	48,48,48	0.40	0	51,54,54	1.05	4 (7%)
19	CLA	3	605	-	53,63,73	1.94	10 (18%)	62,101,113	2.05	16 (25%)
19	CLA	1	605	-	63,73,73	1.74	8 (12%)	74,113,113	1.93	14 (18%)
19	CLA	3	602	-	50,60,73	1.95	9 (18%)	57,97,113	2.11	15 (26%)
19	CLA	1	602	13	44,54,73	2.07	8 (18%)	51,90,113	2.03	11 (21%)
22	BCR	2	503	-	41,41,41	1.66	5 (12%)	56,56,56	5.63	27 (48%)
28	LUT	3	501	-	42,43,43	2.44	1 (2%)	51,60,60	2.08	16 (31%)
25	LMG	G	5002	-	50,50,55	1.18	5 (10%)	58,58,63	1.18	4 (6%)
29	CHL	4	611	-	49,59,74	0.95	4 (8%)	53,96,114	1.36	11 (20%)
19	CLA	A	1111	-	63,73,73	1.70	9 (14%)	74,113,113	1.83	12 (16%)
23	LHG	1	801	-	48,48,48	0.40	0	51,54,54	0.98	2 (3%)
19	CLA	2	606	-	48,58,73	2.02	8 (16%)	56,95,113	2.06	12 (21%)
19	CLA	A	1125	-	63,73,73	1.71	9 (14%)	74,113,113	1.92	14 (18%)
19	CLA	B	1206	2	63,73,73	1.72	8 (12%)	74,113,113	1.87	12 (16%)
22	BCR	1	503	-	41,41,41	1.58	4 (9%)	56,56,56	4.83	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	DGD	4	802	-	51,51,67	0.95	2 (3%)	65,65,81	0.99	4 (6%)
19	CLA	A	1128	-	63,73,73	1.70	10 (15%)	74,113,113	1.88	16 (21%)
19	CLA	B	1221	-	63,73,73	1.71	9 (14%)	74,113,113	1.91	13 (17%)
19	CLA	B	1214	-	63,73,73	1.76	9 (14%)	74,113,113	1.88	14 (18%)
24	LMT	G	5005	-	32,32,36	1.18	4 (12%)	43,43,47	0.97	2 (4%)
19	CLA	B	1208	-	58,68,73	1.79	8 (13%)	68,107,113	1.87	13 (19%)
19	CLA	K	1401	-	43,53,73	2.11	9 (20%)	50,89,113	2.18	10 (20%)
22	BCR	A	4008	-	41,41,41	1.59	5 (12%)	56,56,56	4.60	25 (44%)
19	CLA	B	1238	33	63,73,73	1.73	7 (11%)	74,113,113	1.88	11 (14%)
19	CLA	B	1218	-	63,73,73	1.73	9 (14%)	74,113,113	1.88	15 (20%)
19	CLA	4	605	-	58,68,73	1.82	10 (17%)	68,107,113	1.95	15 (22%)
19	CLA	4	602	-	48,58,73	2.00	9 (18%)	56,95,113	2.09	15 (26%)
22	BCR	B	4010	-	41,41,41	1.58	4 (9%)	56,56,56	4.64	20 (35%)
19	CLA	G	1602	7	44,54,73	2.07	9 (20%)	51,90,113	2.16	12 (23%)
28	LUT	3	502	-	42,43,43	2.33	1 (2%)	51,60,60	1.78	16 (31%)
29	CHL	1	609	13	54,64,74	0.95	4 (7%)	59,102,114	1.30	10 (16%)
29	CHL	3	604	15	64,74,74	0.84	3 (4%)	71,114,114	1.24	9 (12%)
19	CLA	B	1239	-	63,73,73	1.77	8 (12%)	74,113,113	1.89	14 (18%)
25	LMG	2	804	-	30,30,55	0.54	0	38,38,63	1.09	2 (5%)
28	LUT	4	505	-	42,43,43	2.38	1 (2%)	51,60,60	2.37	19 (37%)
19	CLA	A	1013	-	63,73,73	1.69	9 (14%)	74,113,113	1.83	16 (21%)
19	CLA	1	608	-	44,54,73	2.08	9 (20%)	51,90,113	2.15	10 (19%)
19	CLA	2	604	14	63,73,73	1.73	8 (12%)	74,113,113	1.89	14 (18%)
19	CLA	A	1113	-	43,53,73	2.05	9 (20%)	50,89,113	2.11	13 (26%)
19	CLA	4	607	-	58,68,73	1.81	9 (15%)	68,107,113	1.93	13 (19%)
28	LUT	4	501	-	42,43,43	2.35	1 (2%)	51,60,60	2.14	17 (33%)
23	LHG	A	5002	-	48,48,48	0.40	0	51,54,54	1.12	4 (7%)
19	CLA	B	1209	-	44,54,73	2.07	9 (20%)	51,90,113	2.09	11 (21%)
19	CLA	B	1201	-	63,73,73	1.72	9 (14%)	74,113,113	1.84	14 (18%)
19	CLA	B	1215	-	63,73,73	1.65	8 (12%)	74,113,113	1.94	15 (20%)
19	CLA	A	1103	-	63,73,73	1.71	8 (12%)	74,113,113	1.89	12 (16%)
22	BCR	A	4003	-	41,41,41	1.59	4 (9%)	56,56,56	4.59	22 (39%)
19	CLA	1	601	13	63,73,73	1.72	9 (14%)	74,113,113	1.83	12 (16%)
24	LMT	B	5006	-	33,33,36	1.17	5 (15%)	44,44,47	0.93	2 (4%)
19	CLA	A	1119	-	63,73,73	1.74	8 (12%)	74,113,113	1.89	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	2	601	14	58,68,73	1.81	9 (15%)	68,107,113	2.00	16 (23%)
19	CLA	4	603	-	63,73,73	1.76	9 (14%)	74,113,113	1.92	13 (17%)
23	LHG	3	801	-	16,16,48	0.88	1 (6%)	17,20,54	0.69	0
25	LMG	G	5001	-	49,49,55	1.14	4 (8%)	57,57,63	1.22	4 (7%)
19	CLA	A	1115	-	63,73,73	1.74	9 (14%)	74,113,113	1.83	14 (18%)
19	CLA	2	608	-	48,58,73	2.00	8 (16%)	56,95,113	2.16	16 (28%)
25	LMG	G	5006	-	25,25,55	0.59	0	33,33,63	1.08	3 (9%)
23	LHG	2	801	-	34,34,48	0.46	0	37,40,54	1.11	3 (8%)
19	CLA	H	1701	-	58,68,73	1.81	8 (13%)	68,107,113	1.88	12 (17%)
22	BCR	B	4005	-	41,41,41	1.56	4 (9%)	56,56,56	4.56	17 (30%)
19	CLA	B	1227	-	63,73,73	1.73	8 (12%)	74,113,113	1.91	15 (20%)
19	CLA	L	1502	-	58,68,73	1.80	9 (15%)	68,107,113	1.99	16 (23%)
19	CLA	B	1217	-	44,54,73	2.01	8 (18%)	51,90,113	2.11	10 (19%)
19	CLA	A	1140	-	63,73,73	1.72	9 (14%)	74,113,113	1.86	15 (20%)
24	LMT	G	5004	-	36,36,36	1.12	5 (13%)	47,47,47	0.98	2 (4%)
19	CLA	A	1102	-	63,73,73	1.71	9 (14%)	74,113,113	2.00	17 (22%)
27	DGD	B	5005	-	62,62,67	1.21	6 (9%)	76,76,81	1.01	3 (3%)
21	SF4	C	3003	3	0,12,12	-	-	-	-	-
20	PQN	B	2002	-	34,34,34	0.42	0	43,45,45	1.15	3 (6%)
22	BCR	A	4017	-	41,41,41	1.60	4 (9%)	56,56,56	5.08	20 (35%)
24	LMT	B	5008	-	32,32,36	1.20	5 (15%)	43,43,47	1.00	3 (6%)
29	CHL	3	611	-	45,55,74	0.99	3 (6%)	48,91,114	1.39	11 (22%)
22	BCR	3	503	-	41,41,41	1.59	5 (12%)	56,56,56	4.46	18 (32%)
25	LMG	2	806	-	13,13,55	0.55	0	18,18,63	0.57	0
28	LUT	1	501	-	42,43,43	2.39	1 (2%)	51,60,60	2.10	20 (39%)
21	SF4	C	3002	3	0,12,12	-	-	-	-	-
23	LHG	A	5001	-	39,39,48	0.43	0	42,45,54	1.03	2 (4%)
19	CLA	3	606	-	48,58,73	1.98	8 (16%)	56,95,113	2.11	13 (23%)
29	CHL	2	613	-	44,54,74	0.97	2 (4%)	47,90,114	1.24	7 (14%)
18	CL0	A	1011	-	63,73,73	2.42	19 (30%)	74,113,113	2.38	22 (29%)
29	CHL	1	610	13	45,55,74	0.99	3 (6%)	48,91,114	1.34	11 (22%)
29	CHL	2	609	14	64,74,74	0.86	2 (3%)	71,114,114	1.12	10 (14%)
19	CLA	A	1107	1	63,73,73	1.75	8 (12%)	74,113,113	1.86	14 (18%)
22	BCR	B	4009	-	41,41,41	1.58	4 (9%)	56,56,56	4.36	21 (37%)
29	CHL	4	615	16	41,51,74	1.01	2 (4%)	42,86,114	1.44	9 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	K	1404	-	44,54,73	2.08	9 (20%)	51,90,113	2.04	10 (19%)

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	A	1141	-	1/1/14/20	13/31/109/115	-
22	BCR	L	4020	-	-	7/29/63/63	0/2/2/2
21	SF4	A	3001	2,1	-	-	0/6/5/5
22	BCR	F	4016	-	-	10/29/63/63	0/2/2/2
19	CLA	A	1105	-	1/1/14/20	13/31/109/115	-
24	LMT	2	808	-	-	4/21/61/61	0/2/2/2
29	CHL	2	610	-	4/4/18/26	2/27/125/137	-
22	BCR	J	4012	-	-	6/29/63/63	0/2/2/2
19	CLA	1	611	-	1/1/15/20	14/37/115/115	-
22	BCR	B	4006	-	-	3/29/63/63	0/2/2/2
19	CLA	B	1204	-	1/1/15/20	14/37/115/115	-
22	BCR	K	4002	-	-	5/29/63/63	0/2/2/2
22	BCR	A	4002	-	-	7/29/63/63	0/2/2/2
25	LMG	2	802	-	-	4/20/40/70	0/1/1/1
19	CLA	4	606	-	1/1/12/20	5/19/97/115	-
19	CLA	A	1124	-	1/1/13/20	8/25/103/115	-
19	CLA	B	1216	-	1/1/15/20	10/37/115/115	-
19	CLA	A	1139	-	1/1/15/20	14/37/115/115	-
25	LMG	F	5002	-	-	11/42/62/70	0/1/1/1
27	DGD	3	803	-	-	8/40/80/95	0/2/2/2
22	BCR	A	4007	-	-	10/29/63/63	0/2/2/2
19	CLA	A	1129	-	1/1/15/20	11/37/115/115	-
19	CLA	B	1202	-	1/1/15/20	17/37/115/115	-
19	CLA	3	608	-	1/1/11/20	6/17/95/115	-
19	CLA	4	604	16	1/1/14/20	7/31/109/115	-
19	CLA	A	1121	-	1/1/14/20	15/31/109/115	-
19	CLA	B	1022	-	1/1/15/20	8/37/115/115	-
25	LMG	2	803	-	-	12/31/51/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	3	613	-	1/1/11/20	6/15/93/115	-
19	CLA	L	1501	12	1/1/12/20	6/19/97/115	-
19	CLA	B	1229	-	1/1/15/20	13/37/115/115	-
19	CLA	A	1132	-	1/1/15/20	15/37/115/115	-
19	CLA	A	1136	-	1/1/15/20	18/37/115/115	-
19	CLA	B	1236	-	1/1/12/20	8/19/97/115	-
19	CLA	A	1117	-	1/1/15/20	13/37/115/115	-
22	BCR	G	4011	-	-	7/29/63/63	0/2/2/2
19	CLA	3	603	-	1/1/13/20	12/25/103/115	-
19	CLA	B	1205	-	1/1/15/20	13/37/115/115	-
19	CLA	B	1213	-	1/1/14/20	8/31/109/115	-
29	CHL	2	615	-	4/4/18/26	7/27/125/137	-
19	CLA	A	1138	-	1/1/15/20	15/37/115/115	-
19	CLA	A	1108	-	1/1/12/20	6/19/97/115	-
19	CLA	3	614	-	1/1/10/20	3/10/88/115	-
19	CLA	2	603	14	1/1/15/20	13/37/115/115	-
19	CLA	3	601	15	1/1/13/20	10/25/103/115	-
19	CLA	3	610	15	1/1/15/20	18/37/115/115	-
19	CLA	4	608	-	1/1/11/20	5/15/93/115	-
22	BCR	1	504	-	-	9/29/63/63	0/2/2/2
22	BCR	3	506	-	-	5/29/63/63	0/2/2/2
29	CHL	1	612	13	4/4/19/26	4/33/131/137	-
19	CLA	4	609	16	1/1/12/20	9/19/97/115	-
19	CLA	A	1137	-	1/1/15/20	17/37/115/115	-
25	LMG	B	5003	-	-	8/30/50/70	0/1/1/1
19	CLA	2	612	-	1/1/13/20	8/25/103/115	-
19	CLA	1	604	13	1/1/15/20	15/37/115/115	-
19	CLA	B	1203	2	1/1/15/20	12/37/115/115	-
22	BCR	K	4001	-	-	6/29/63/63	0/2/2/2
25	LMG	B	5004	-	-	10/28/48/70	0/1/1/1
19	CLA	B	1220	-	1/1/13/20	7/25/103/115	-
19	CLA	B	1212	-	1/1/13/20	12/25/103/115	-
19	CLA	B	1224	-	1/1/15/20	16/37/115/115	-
19	CLA	A	1123	-	1/1/15/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	1	614	13	1/1/14/20	16/31/109/115	-
19	CLA	A	1126	-	1/1/15/20	13/37/115/115	-
27	DGD	G	5003	-	-	11/36/76/95	0/2/2/2
19	CLA	A	1135	-	1/1/12/20	10/21/99/115	-
25	LMG	F	5003	-	-	11/31/51/70	0/1/1/1
25	LMG	A	5006	-	-	11/45/65/70	0/1/1/1
19	CLA	3	607	-	1/1/12/20	7/22/100/115	-
19	CLA	A	1112	-	1/1/15/20	18/37/115/115	-
19	CLA	1	607	-	1/1/11/20	7/15/93/115	-
22	BCR	B	4004	-	-	10/29/63/63	0/2/2/2
25	LMG	F	5004	-	-	8/29/49/70	0/1/1/1
19	CLA	A	1131	-	1/1/15/20	15/37/115/115	-
19	CLA	L	1503	-	1/1/12/20	6/19/97/115	-
19	CLA	2	602	-	1/1/12/20	7/22/100/115	-
19	CLA	B	1219	-	1/1/15/20	14/37/115/115	-
29	CHL	4	613	-	4/4/19/26	6/33/131/137	-
19	CLA	B	1207	-	1/1/15/20	13/37/115/115	-
25	LMG	F	5006	-	-	1/4/24/70	0/1/1/1
19	CLA	B	1211	-	1/1/15/20	16/37/115/115	-
19	CLA	B	1230	-	1/1/13/20	15/29/107/115	-
19	CLA	3	612	15	1/1/12/20	6/19/97/115	-
19	CLA	B	1210	-	1/1/15/20	9/37/115/115	-
19	CLA	A	1104	-	1/1/15/20	15/37/115/115	-
19	CLA	2	605	-	1/1/15/20	17/37/115/115	-
28	LUT	2	501	-	1/1/12/27	6/29/67/67	0/2/2/2
30	XAT	4	502	-	2/2/12/26	2/31/93/93	0/4/4/4
19	CLA	2	607	-	1/1/14/20	16/31/109/115	-
25	LMG	1	802	-	-	4/41/61/70	0/1/1/1
19	CLA	K	1402	-	1/1/14/20	16/31/109/115	-
19	CLA	A	1122	-	1/1/15/20	15/37/115/115	-
19	CLA	B	1023	-	1/1/15/20	16/37/115/115	-
19	CLA	F	1302	6	1/1/15/20	11/37/115/115	-
31	3PH	2	807	-	-	16/34/34/49	-
22	BCR	H	4021	-	-	8/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	4	601	16	1/1/14/20	13/31/109/115	-
25	LMG	B	5007	-	-	10/29/49/70	0/1/1/1
22	BCR	I	4018	-	-	7/29/63/63	0/2/2/2
29	CHL	4	610	-	3/3/16/26	3/17/115/137	-
23	LHG	4	801	-	-	21/39/39/53	-
19	CLA	A	1116	-	1/1/13/20	11/27/105/115	-
19	CLA	B	1235	-	1/1/15/20	11/37/115/115	-
19	CLA	G	1603	-	1/1/15/20	9/37/115/115	-
25	LMG	2	805	-	-	6/25/45/70	0/1/1/1
22	BCR	I	4020	-	-	14/29/63/63	0/2/2/2
19	CLA	B	1237	-	1/1/15/20	16/37/115/115	-
19	CLA	A	1109	-	1/1/15/20	18/37/115/115	-
19	CLA	J	1901	10	1/1/12/20	7/19/97/115	-
19	CLA	A	1133	-	1/1/15/20	18/37/115/115	-
19	CLA	A	1106	1	1/1/15/20	15/37/115/115	-
19	CLA	A	1120	-	1/1/14/20	14/31/109/115	-
19	CLA	B	1240	23	1/1/15/20	17/37/115/115	-
22	BCR	F	4014	-	-	8/29/63/63	0/2/2/2
19	CLA	B	1223	-	1/1/15/20	11/37/115/115	-
19	CLA	B	1222	33	1/1/15/20	18/37/115/115	-
19	CLA	1	603	-	1/1/13/20	8/25/103/115	-
28	LUT	1	502	-	1/1/12/27	5/29/67/67	0/2/2/2
19	CLA	1	606	-	1/1/12/20	5/19/97/115	-
22	BCR	L	4019	-	-	6/29/63/63	0/2/2/2
19	CLA	4	617	-	1/1/15/20	15/37/115/115	-
24	LMT	A	5004	-	-	7/21/61/61	0/2/2/2
19	CLA	A	1012	-	1/1/15/20	10/37/115/115	-
20	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
22	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
27	DGD	J	5001	-	-	11/47/87/95	0/2/2/2
19	CLA	A	1110	-	1/1/13/20	8/25/103/115	-
19	CLA	A	1118	-	1/1/12/20	6/19/97/115	-
19	CLA	F	1301	-	1/1/15/20	17/37/115/115	-
27	DGD	F	5005	-	-	15/46/86/95	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CHL	2	611	-	3/3/16/26	2/18/116/137	-
19	CLA	K	1403	-	1/1/11/20	10/17/95/115	-
19	CLA	B	1225	-	1/1/15/20	13/37/115/115	-
19	CLA	A	1134	1	1/1/13/20	8/25/103/115	-
19	CLA	B	1226	-	1/1/15/20	16/37/115/115	-
19	CLA	B	1234	-	1/1/13/20	7/25/103/115	-
23	LHG	B	5001	19	-	9/23/23/53	-
30	XAT	2	502	-	2/2/12/26	7/31/93/93	0/4/4/4
19	CLA	A	1127	-	1/1/15/20	14/37/115/115	-
19	CLA	A	1101	-	1/1/15/20	14/37/115/115	-
25	LMG	3	802	-	-	6/25/45/70	0/1/1/1
19	CLA	1	613	-	1/1/11/20	4/13/91/115	-
19	CLA	B	1021	-	1/1/15/20	5/37/115/115	-
19	CLA	A	1114	-	1/1/11/20	9/15/93/115	-
19	CLA	B	1232	-	1/1/13/20	11/25/103/115	-
25	LMG	F	5001	-	-	4/25/45/70	0/1/1/1
27	DGD	1	803	-	-	14/30/70/95	0/2/2/2
19	CLA	4	612	16	1/1/15/20	13/37/115/115	-
19	CLA	A	1130	-	1/1/13/20	4/25/103/115	-
19	CLA	G	1601	-	1/1/13/20	10/25/103/115	-
19	CLA	3	617	-	1/1/14/20	17/31/109/115	-
28	LUT	J	4013	-	1/1/12/27	4/29/67/67	0/2/2/2
19	CLA	B	1228	-	1/1/14/20	10/31/109/115	-
19	CLA	B	1231	-	1/1/14/20	6/31/109/115	-
23	LHG	B	5002	-	-	27/53/53/53	-
19	CLA	3	605	-	1/1/13/20	9/25/103/115	-
19	CLA	1	605	-	1/1/15/20	16/37/115/115	-
19	CLA	3	602	-	1/1/12/20	8/22/100/115	-
19	CLA	1	602	13	1/1/11/20	6/15/93/115	-
28	LUT	3	501	-	1/1/12/27	6/29/67/67	0/2/2/2
22	BCR	2	503	-	-	13/29/63/63	0/2/2/2
29	CHL	4	611	-	3/3/17/26	1/21/119/137	-
25	LMG	G	5002	-	-	17/45/65/70	0/1/1/1
19	CLA	A	1111	-	1/1/15/20	14/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	LHG	1	801	-	-	29/53/53/53	-
19	CLA	2	606	-	1/1/12/20	6/19/97/115	-
19	CLA	A	1125	-	1/1/15/20	13/37/115/115	-
19	CLA	B	1206	2	1/1/15/20	16/37/115/115	-
22	BCR	1	503	-	-	6/29/63/63	0/2/2/2
27	DGD	4	802	-	-	16/39/79/95	0/2/2/2
19	CLA	A	1128	-	1/1/15/20	15/37/115/115	-
19	CLA	B	1221	-	1/1/15/20	18/37/115/115	-
19	CLA	B	1214	-	1/1/15/20	12/37/115/115	-
24	LMT	G	5005	-	-	5/17/57/61	0/2/2/2
19	CLA	B	1208	-	1/1/14/20	14/31/109/115	-
19	CLA	K	1401	-	1/1/11/20	9/13/91/115	-
22	BCR	A	4008	-	-	10/29/63/63	0/2/2/2
19	CLA	B	1238	33	1/1/15/20	12/37/115/115	-
19	CLA	B	1218	-	1/1/15/20	7/37/115/115	-
19	CLA	4	605	-	1/1/14/20	10/31/109/115	-
19	CLA	4	602	-	1/1/12/20	5/19/97/115	-
22	BCR	B	4010	-	-	8/29/63/63	0/2/2/2
19	CLA	G	1602	7	1/1/11/20	7/15/93/115	-
28	LUT	3	502	-	1/1/12/27	2/29/67/67	0/2/2/2
29	CHL	1	609	13	4/4/18/26	3/27/125/137	-
29	CHL	3	604	15	4/4/20/26	8/39/137/137	-
19	CLA	B	1239	-	1/1/15/20	9/37/115/115	-
25	LMG	2	804	-	-	5/25/45/70	0/1/1/1
28	LUT	4	505	-	-	3/29/67/67	0/2/2/2
19	CLA	A	1013	-	1/1/15/20	12/37/115/115	-
19	CLA	1	608	-	1/1/11/20	7/15/93/115	-
19	CLA	2	604	14	1/1/15/20	16/37/115/115	-
19	CLA	A	1113	-	1/1/11/20	6/13/91/115	-
19	CLA	4	607	-	1/1/14/20	11/31/109/115	-
28	LUT	4	501	-	1/1/12/27	7/29/67/67	0/2/2/2
23	LHG	A	5002	-	-	27/53/53/53	-
19	CLA	B	1209	-	1/1/11/20	4/15/93/115	-
19	CLA	B	1201	-	1/1/15/20	13/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	1215	-	1/1/15/20	12/37/115/115	-
19	CLA	A	1103	-	1/1/15/20	15/37/115/115	-
22	BCR	A	4003	-	-	6/29/63/63	0/2/2/2
19	CLA	1	601	13	1/1/15/20	15/37/115/115	-
24	LMT	B	5006	-	-	4/18/58/61	0/2/2/2
19	CLA	A	1119	-	1/1/15/20	18/37/115/115	-
19	CLA	2	601	14	1/1/14/20	9/31/109/115	-
19	CLA	4	603	-	1/1/15/20	13/37/115/115	-
23	LHG	3	801	-	-	12/19/19/53	-
25	LMG	G	5001	-	-	16/44/64/70	0/1/1/1
19	CLA	A	1115	-	1/1/15/20	9/37/115/115	-
19	CLA	2	608	-	1/1/12/20	7/19/97/115	-
25	LMG	G	5006	-	-	11/20/40/70	0/1/1/1
23	LHG	2	801	-	-	18/39/39/53	-
19	CLA	H	1701	-	1/1/14/20	12/31/109/115	-
22	BCR	B	4005	-	-	10/29/63/63	0/2/2/2
19	CLA	B	1227	-	1/1/15/20	13/37/115/115	-
19	CLA	L	1502	-	1/1/14/20	11/31/109/115	-
19	CLA	B	1217	-	1/1/11/20	7/15/93/115	-
19	CLA	A	1140	-	1/1/15/20	7/37/115/115	-
24	LMT	G	5004	-	-	10/21/61/61	0/2/2/2
19	CLA	A	1102	-	1/1/15/20	21/37/115/115	-
27	DGD	B	5005	-	-	19/50/90/95	0/2/2/2
21	SF4	C	3003	3	-	-	0/6/5/5
20	PQN	B	2002	-	-	5/23/43/43	0/2/2/2
22	BCR	A	4017	-	-	9/29/63/63	0/2/2/2
24	LMT	B	5008	-	-	8/17/57/61	0/2/2/2
29	CHL	3	611	-	3/3/16/26	0/17/115/137	-
22	BCR	3	503	-	-	10/29/63/63	0/2/2/2
25	LMG	2	806	-	-	1/4/24/70	0/1/1/1
28	LUT	1	501	-	1/1/12/27	4/29/67/67	0/2/2/2
21	SF4	C	3002	3	-	-	0/6/5/5
23	LHG	A	5001	-	-	26/44/44/53	-
19	CLA	3	606	-	1/1/12/20	10/19/97/115	-
29	CHL	2	613	-	3/3/16/26	4/15/113/137	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CL0	A	1011	-	3/3/20/25	9/37/135/135	-
29	CHL	1	610	13	3/3/16/26	3/17/115/137	-
29	CHL	2	609	14	4/4/20/26	4/39/137/137	-
19	CLA	A	1107	1	1/1/15/20	14/37/115/115	-
22	BCR	B	4009	-	-	8/29/63/63	0/2/2/2
29	CHL	4	615	16	4/4/15/26	0/12/110/137	-
19	CLA	K	1404	-	1/1/11/20	5/15/93/115	-

The worst 5 of 1493 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	3	501	LUT	C24-C25	15.01	1.51	1.33
28	1	502	LUT	C24-C25	14.94	1.50	1.33
28	2	501	LUT	C24-C25	14.83	1.50	1.33
28	J	4013	LUT	C24-C25	14.80	1.50	1.33
28	1	501	LUT	C24-C25	14.75	1.50	1.33

The worst 5 of 2930 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	K	4001	BCR	C10-C11-C12	19.60	180.00	123.20
22	I	4018	BCR	C10-C11-C12	19.51	179.74	123.20
22	B	4005	BCR	C10-C11-C12	19.42	179.47	123.20
22	A	4017	BCR	C10-C11-C12	19.39	179.37	123.20
22	1	504	BCR	C10-C11-C12	19.20	178.82	123.20

5 of 206 chirality outliers are listed below:

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

5 of 2418 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	1011	CL0	C1A-C2A-CAA-CBA
18	A	1011	CL0	C3A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	A	1141	CLA	5	0
22	L	4020	BCR	10	0
22	F	4016	BCR	6	0
19	A	1105	CLA	2	0
24	2	808	LMT	1	0
29	2	610	CHL	2	0
22	J	4012	BCR	9	0
19	1	611	CLA	5	0
22	B	4006	BCR	11	0
19	B	1204	CLA	3	0
22	K	4002	BCR	9	0
22	A	4002	BCR	8	0
19	4	606	CLA	4	0
19	A	1124	CLA	3	0
19	B	1216	CLA	5	0
19	A	1139	CLA	6	0
25	F	5002	LMG	1	0
22	A	4007	BCR	5	0
19	A	1129	CLA	4	0
19	B	1202	CLA	4	0
19	3	608	CLA	3	0
19	4	604	CLA	7	0
19	A	1121	CLA	4	0
19	B	1022	CLA	9	0
19	3	613	CLA	4	0
19	L	1501	CLA	4	0
19	B	1229	CLA	8	0
19	A	1132	CLA	3	0
19	A	1136	CLA	2	0
19	B	1236	CLA	6	0
19	A	1117	CLA	3	0
22	G	4011	BCR	9	0
19	3	603	CLA	3	0
19	B	1205	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1213	CLA	5	0
22	3	506	BCR	9	0
19	A	1138	CLA	7	0
19	A	1108	CLA	10	0
19	3	614	CLA	3	0
19	2	603	CLA	6	0
19	3	601	CLA	11	0
19	3	610	CLA	3	0
19	4	608	CLA	4	0
22	1	504	BCR	3	0
29	1	612	CHL	2	0
19	4	609	CLA	1	0
19	A	1137	CLA	4	0
19	2	612	CLA	3	0
19	1	604	CLA	5	0
19	B	1203	CLA	4	0
22	K	4001	BCR	17	0
29	2	615	CHL	9	0
19	B	1220	CLA	3	0
19	B	1212	CLA	3	0
19	B	1224	CLA	4	0
19	A	1123	CLA	5	0
19	1	614	CLA	4	0
19	A	1126	CLA	7	0
27	G	5003	DGD	1	0
19	A	1135	CLA	8	0
25	A	5006	LMG	2	0
19	3	607	CLA	7	0
19	A	1112	CLA	6	0
19	1	607	CLA	2	0
22	B	4004	BCR	8	0
19	A	1131	CLA	1	0
19	L	1503	CLA	5	0
19	2	602	CLA	3	0
19	B	1219	CLA	6	0
29	4	613	CHL	2	0
19	B	1207	CLA	8	0
19	B	1211	CLA	8	0
19	B	1230	CLA	5	0
19	3	612	CLA	11	0
19	B	1210	CLA	6	0
19	A	1104	CLA	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	2	605	CLA	2	0
28	2	501	LUT	11	0
19	2	607	CLA	10	0
30	4	502	XAT	2	0
19	K	1402	CLA	3	0
19	A	1122	CLA	6	0
19	B	1023	CLA	5	0
19	F	1302	CLA	1	0
22	H	4021	BCR	10	0
19	4	601	CLA	9	0
22	I	4018	BCR	8	0
29	4	610	CHL	2	0
19	A	1116	CLA	4	0
19	B	1235	CLA	5	0
19	G	1603	CLA	5	0
22	I	4020	BCR	4	0
19	B	1237	CLA	1	0
19	A	1109	CLA	9	0
19	J	1901	CLA	3	0
19	A	1133	CLA	1	0
19	A	1106	CLA	3	0
19	A	1120	CLA	2	0
19	B	1240	CLA	6	0
22	F	4014	BCR	7	0
19	B	1223	CLA	4	0
19	B	1222	CLA	5	0
19	1	603	CLA	3	0
28	1	502	LUT	7	0
19	1	606	CLA	2	0
22	L	4019	BCR	9	0
19	4	617	CLA	7	0
19	A	1012	CLA	7	0
20	A	2001	PQN	2	0
22	A	4011	BCR	10	0
19	A	1110	CLA	4	0
19	A	1118	CLA	4	0
19	F	1301	CLA	2	0
27	F	5005	DGD	1	0
29	2	611	CHL	5	0
19	K	1403	CLA	3	0
19	B	1225	CLA	8	0
19	A	1134	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	1226	CLA	2	0
19	B	1234	CLA	6	0
30	2	502	XAT	6	0
19	A	1127	CLA	4	0
19	A	1101	CLA	5	0
19	1	613	CLA	7	0
19	B	1021	CLA	7	0
19	A	1114	CLA	3	0
19	B	1232	CLA	5	0
19	4	612	CLA	6	0
19	A	1130	CLA	2	0
19	G	1601	CLA	4	0
28	J	4013	LUT	12	0
19	B	1228	CLA	1	0
19	B	1231	CLA	5	0
19	3	605	CLA	4	0
19	1	605	CLA	7	0
19	3	602	CLA	4	0
22	2	503	BCR	10	0
28	3	501	LUT	13	0
25	G	5002	LMG	2	0
29	4	611	CHL	3	0
19	A	1111	CLA	4	0
19	2	606	CLA	6	0
19	A	1125	CLA	9	0
19	B	1206	CLA	8	0
22	1	503	BCR	6	0
27	4	802	DGD	1	0
19	A	1128	CLA	6	0
19	B	1221	CLA	5	0
19	B	1214	CLA	6	0
19	B	1208	CLA	5	0
19	K	1401	CLA	5	0
22	A	4008	BCR	4	0
19	B	1238	CLA	4	0
19	B	1218	CLA	5	0
19	4	605	CLA	2	0
19	4	602	CLA	3	0
22	B	4010	BCR	12	0
19	G	1602	CLA	3	0
28	3	502	LUT	13	0
29	1	609	CHL	2	0

Continued on next page...

Continued from previous page...

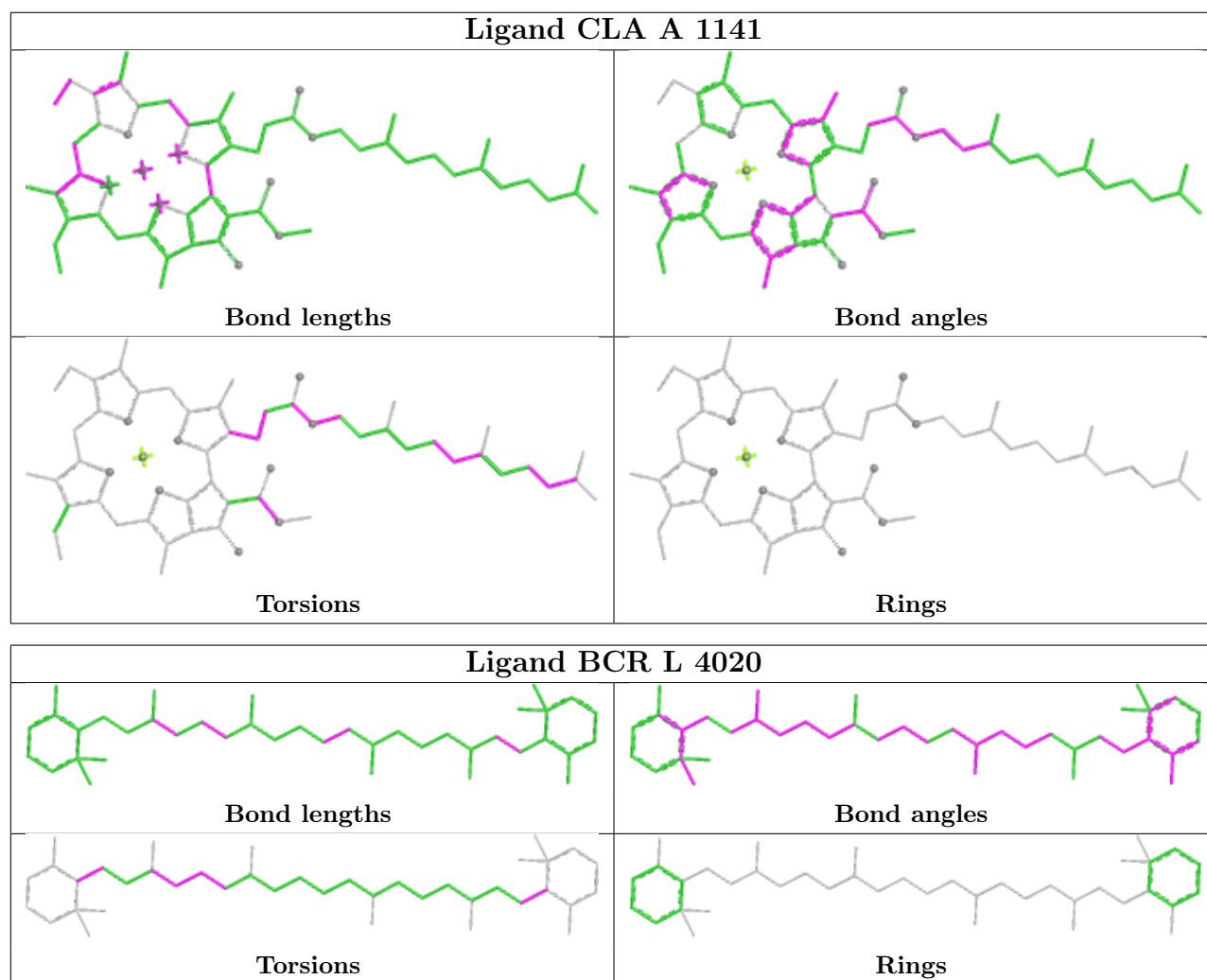
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	3	604	CHL	6	0
19	B	1239	CLA	6	0
28	4	505	LUT	6	0
19	A	1013	CLA	7	0
19	1	608	CLA	4	0
19	2	604	CLA	6	0
19	A	1113	CLA	6	0
19	4	607	CLA	8	0
28	4	501	LUT	17	0
19	B	1209	CLA	4	0
19	B	1201	CLA	2	0
19	B	1215	CLA	5	0
19	A	1103	CLA	5	0
22	A	4003	BCR	6	0
19	1	601	CLA	8	0
19	A	1119	CLA	8	0
19	2	601	CLA	13	0
19	4	603	CLA	7	0
23	3	801	LHG	1	0
19	A	1115	CLA	3	0
19	2	608	CLA	4	0
19	H	1701	CLA	6	0
22	B	4005	BCR	6	0
19	B	1227	CLA	5	0
19	L	1502	CLA	5	0
19	B	1217	CLA	3	0
19	A	1140	CLA	3	0
24	G	5004	LMT	4	0
19	A	1102	CLA	6	0
21	C	3003	SF4	1	0
20	B	2002	PQN	1	0
22	A	4017	BCR	9	0
24	B	5008	LMT	1	0
29	3	611	CHL	1	0
22	3	503	BCR	17	0
28	1	501	LUT	11	0
21	C	3002	SF4	1	0
23	A	5001	LHG	2	0
19	3	606	CLA	4	0
18	A	1011	CL0	3	0
29	1	610	CHL	5	0
29	2	609	CHL	3	0

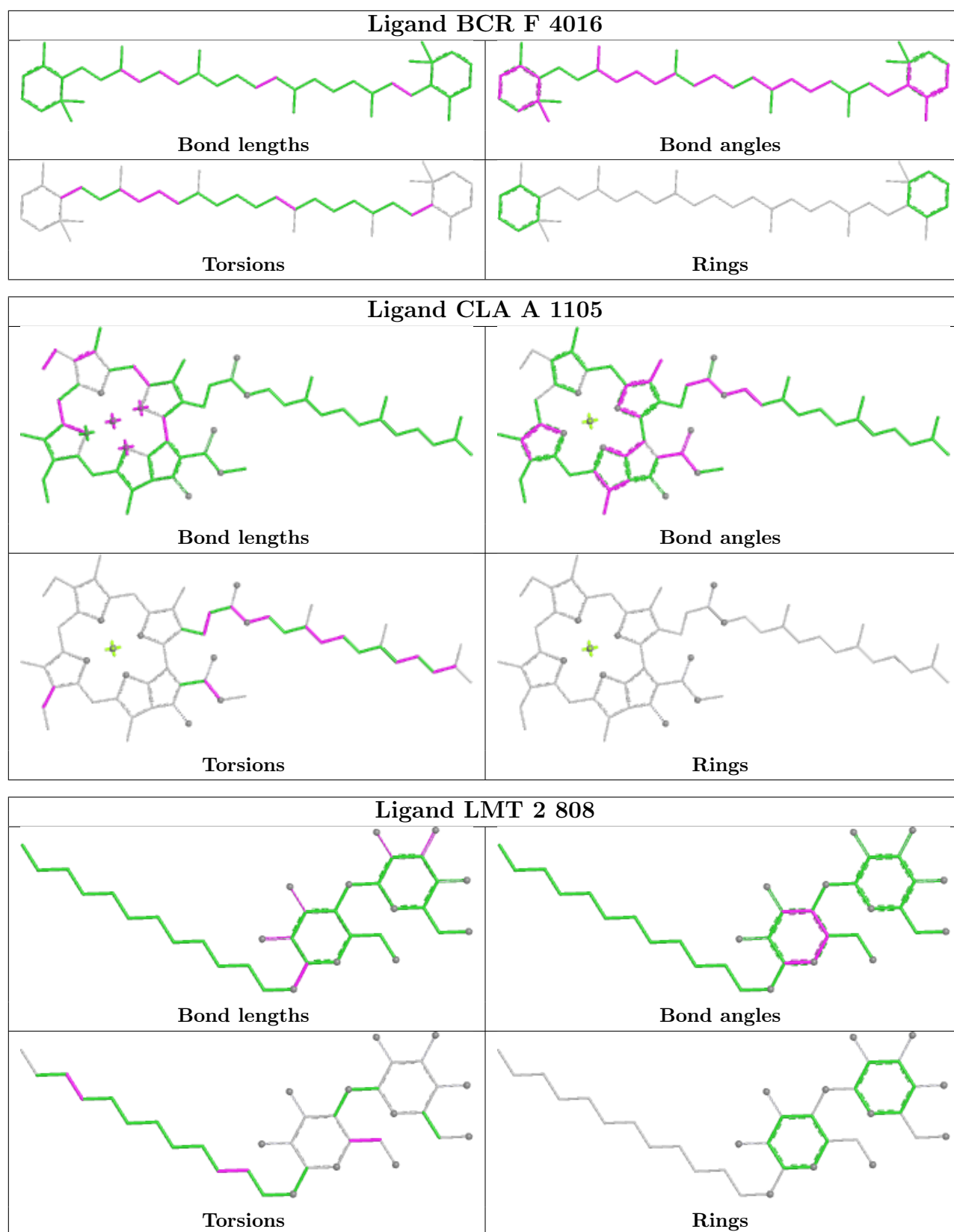
Continued on next page...

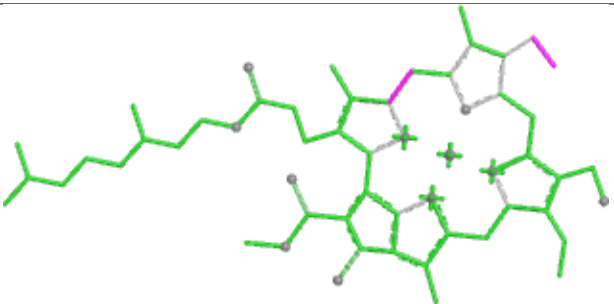
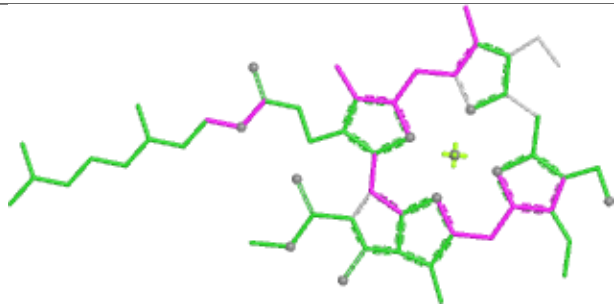
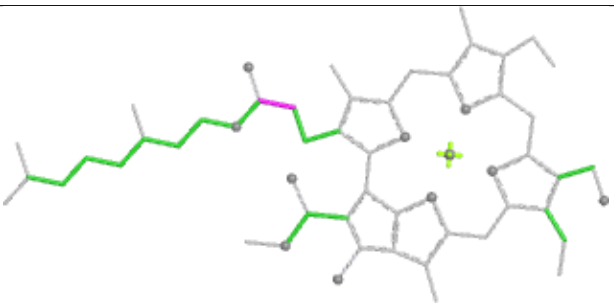
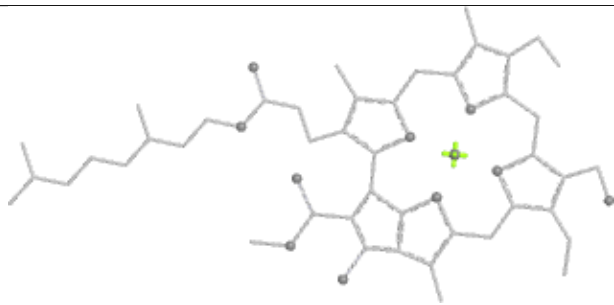
Continued from previous page...

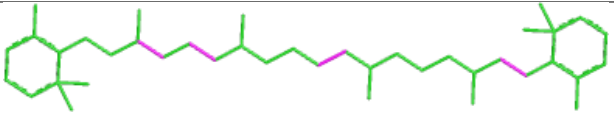
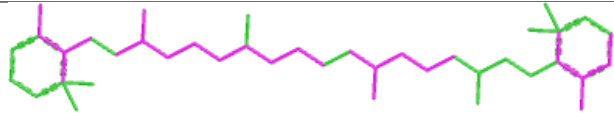
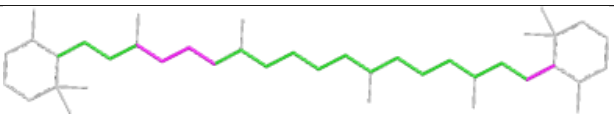
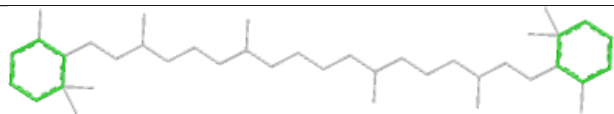
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	1107	CLA	2	0
22	B	4009	BCR	10	0

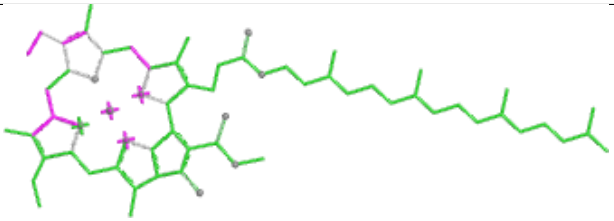
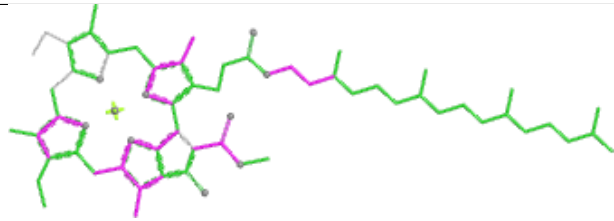
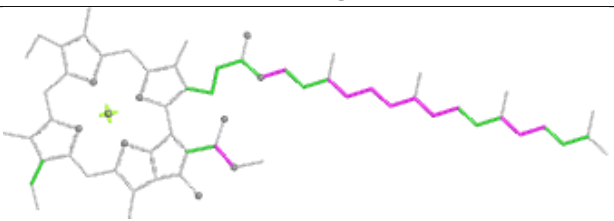
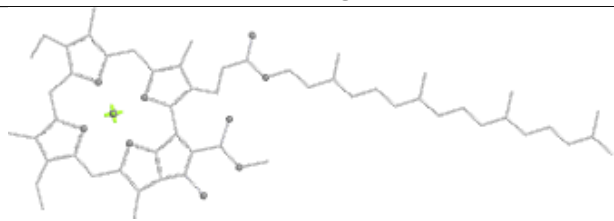
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

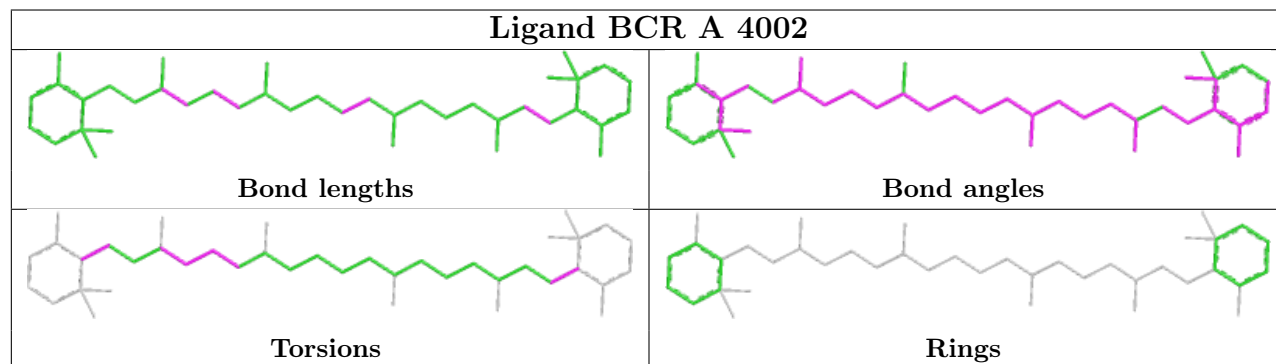
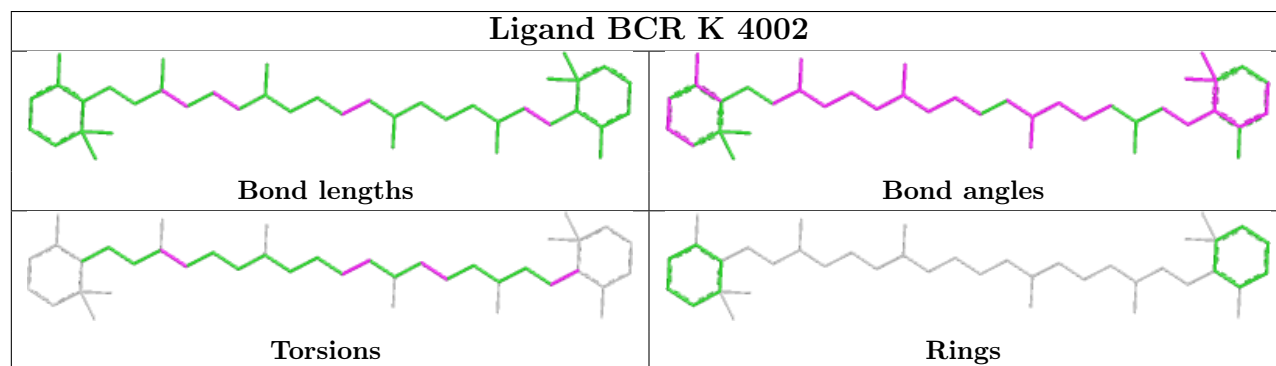
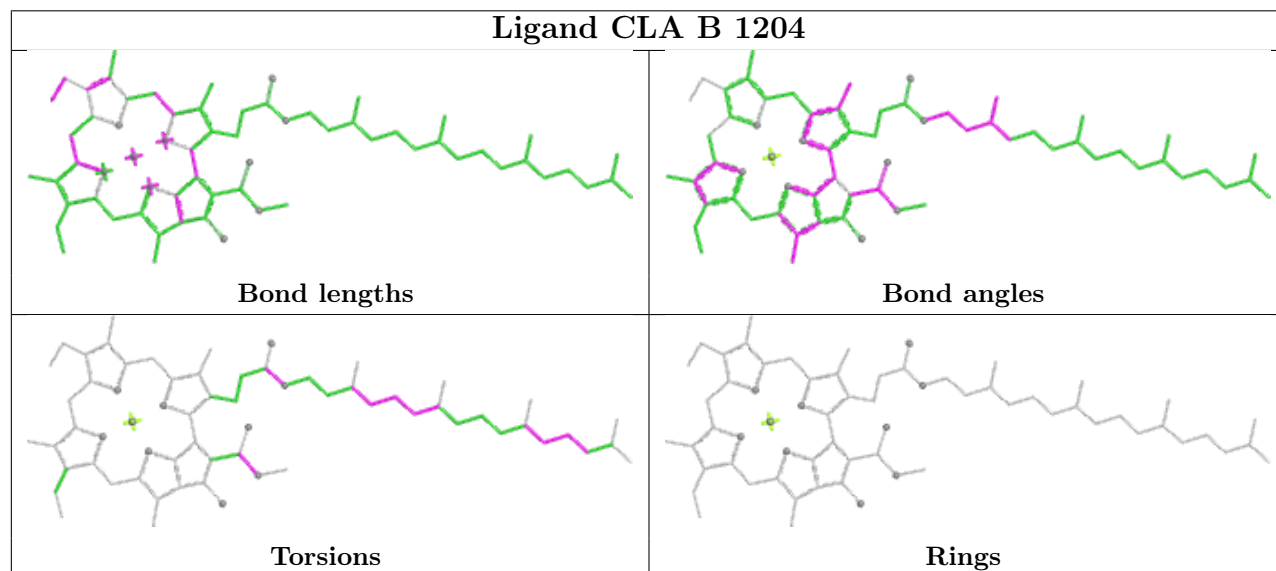
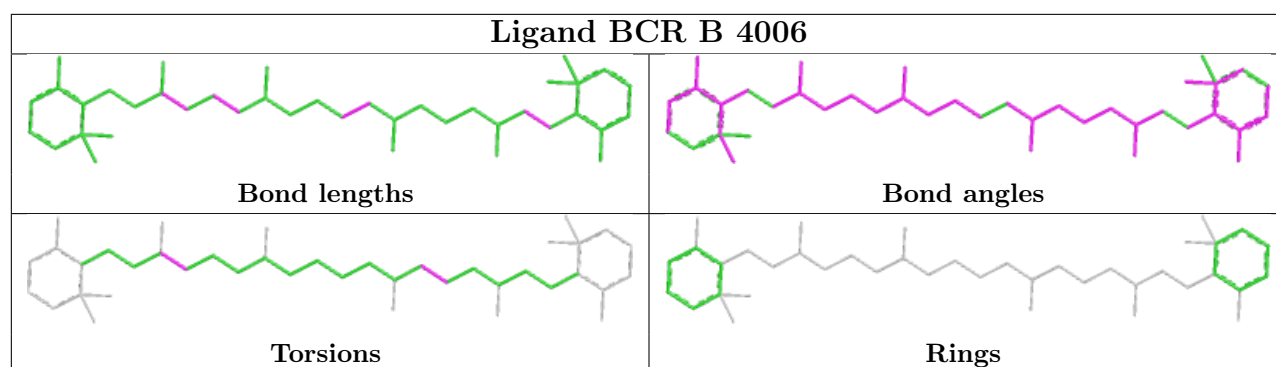


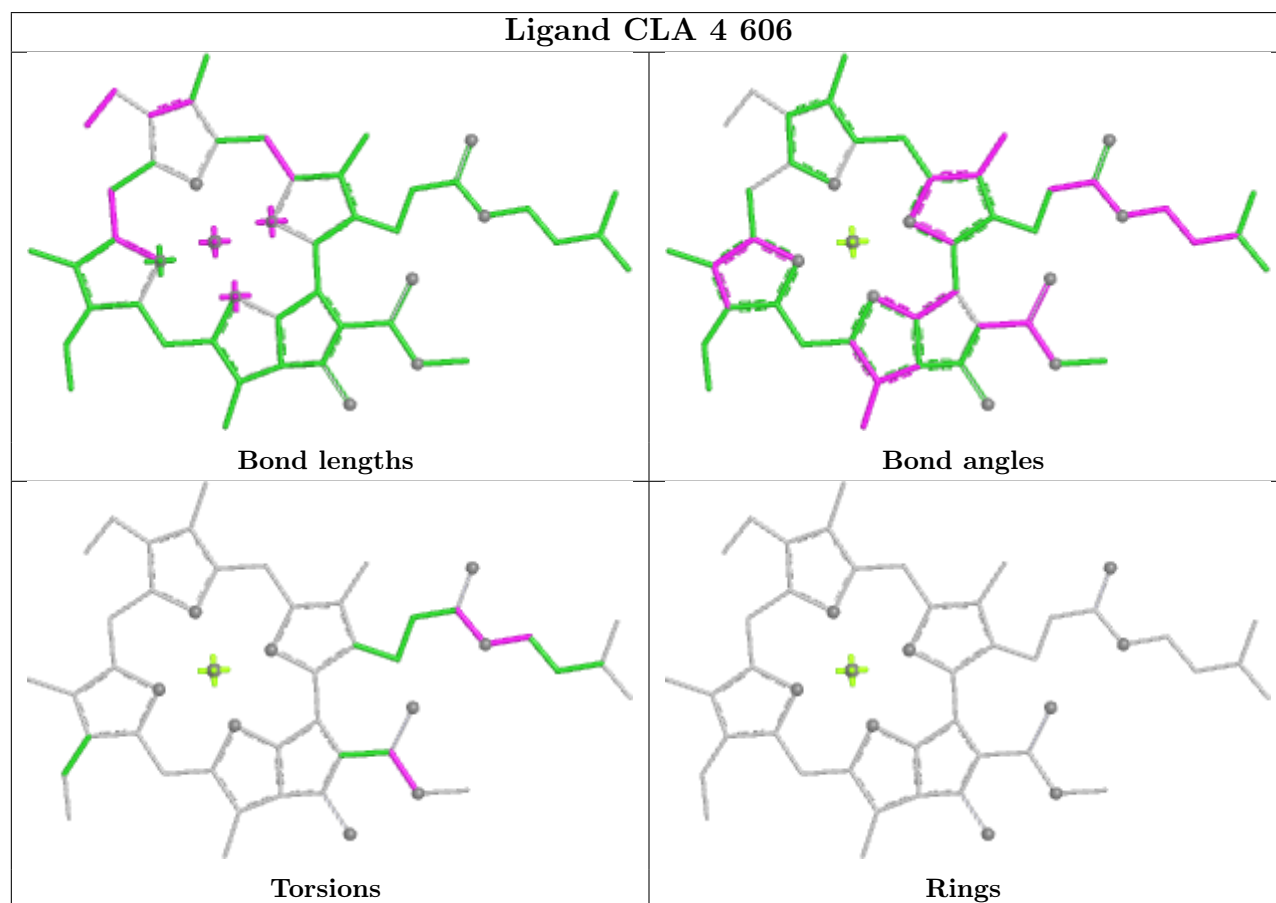
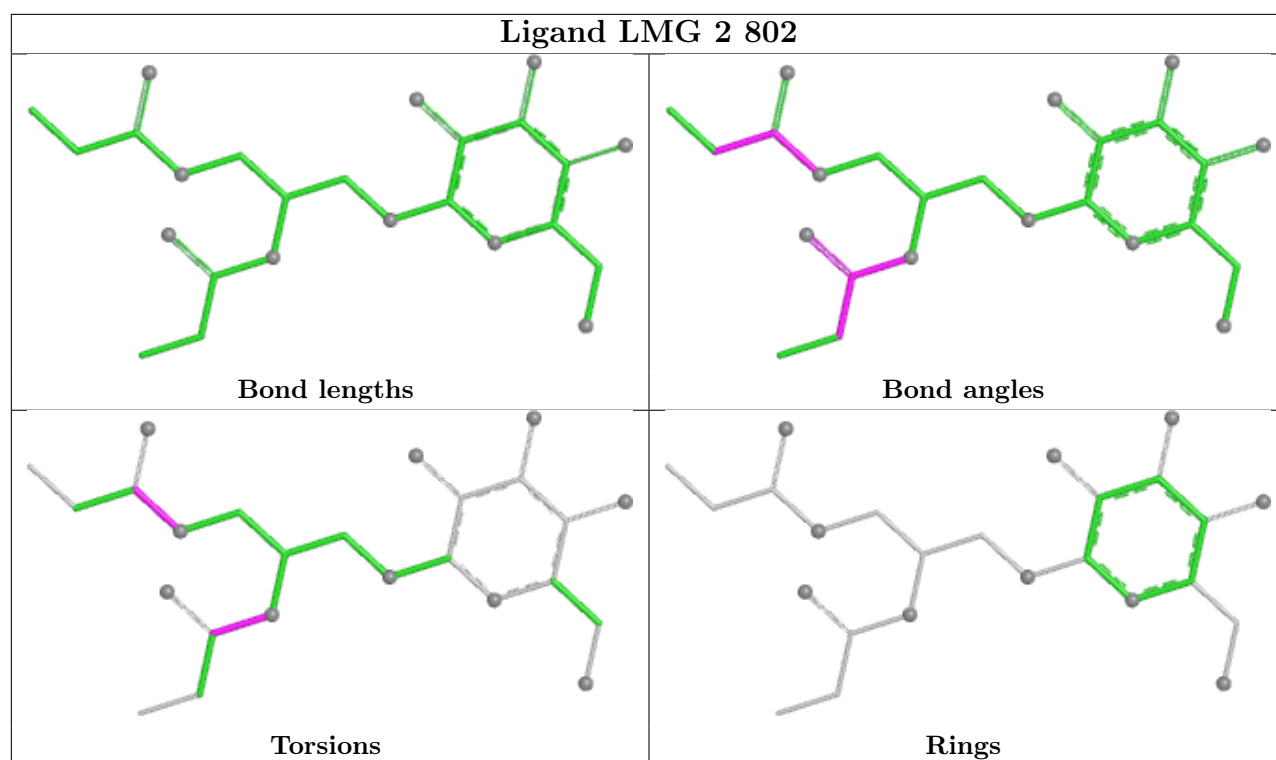


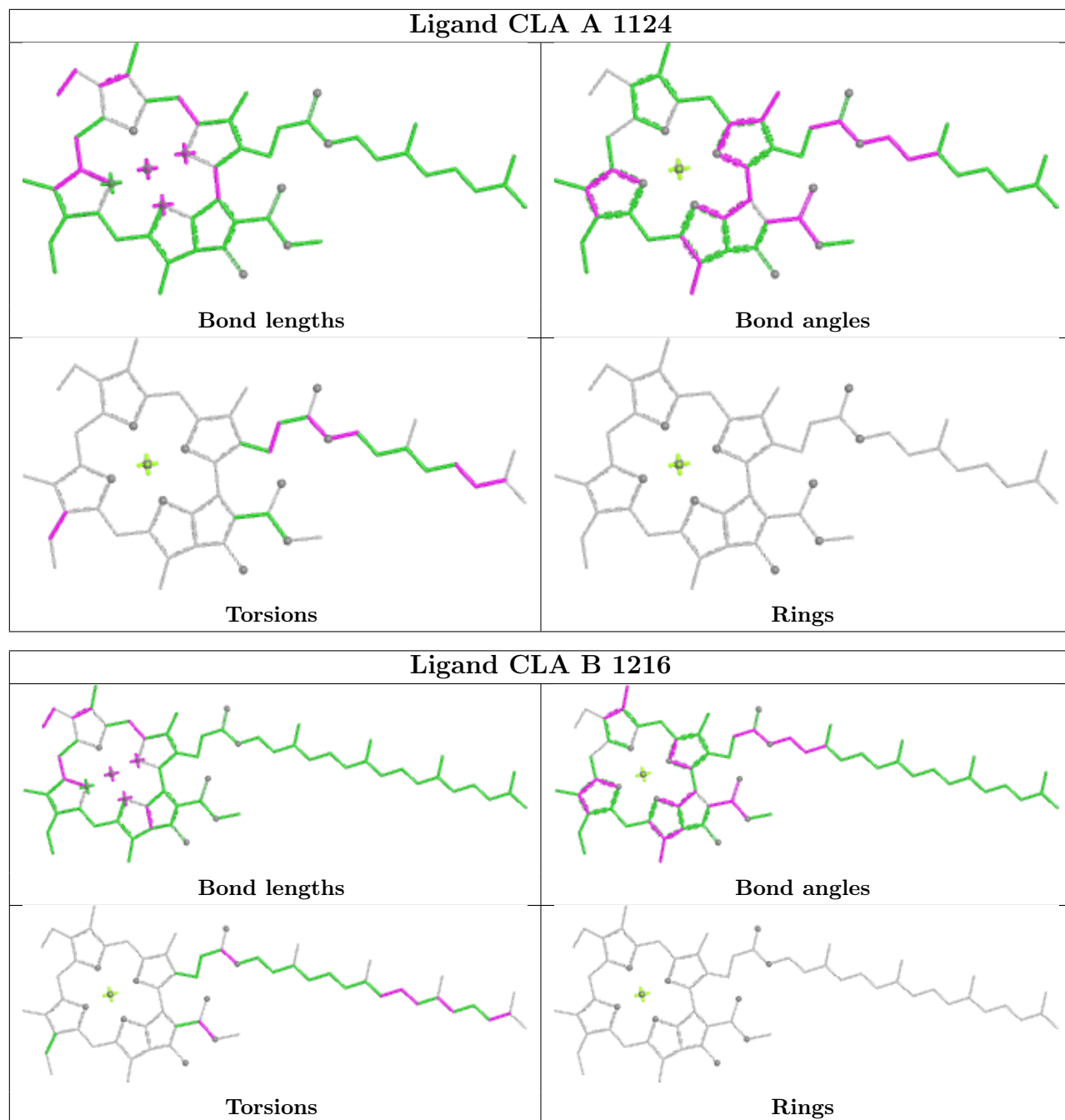
Ligand CHL 2 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

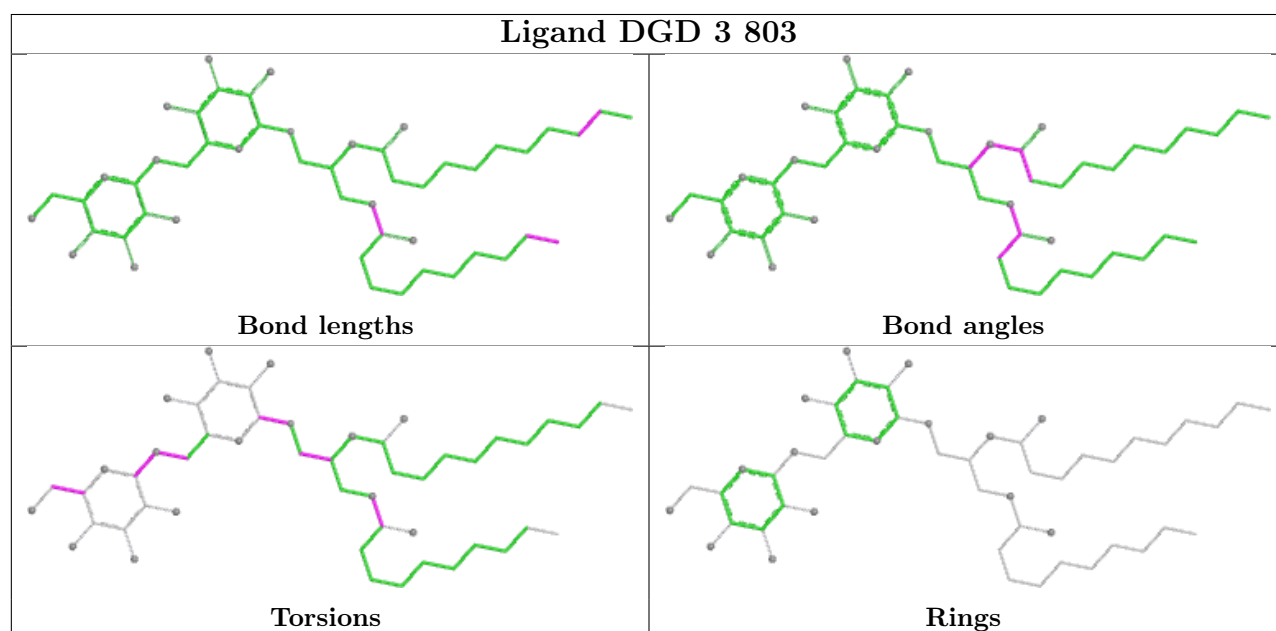
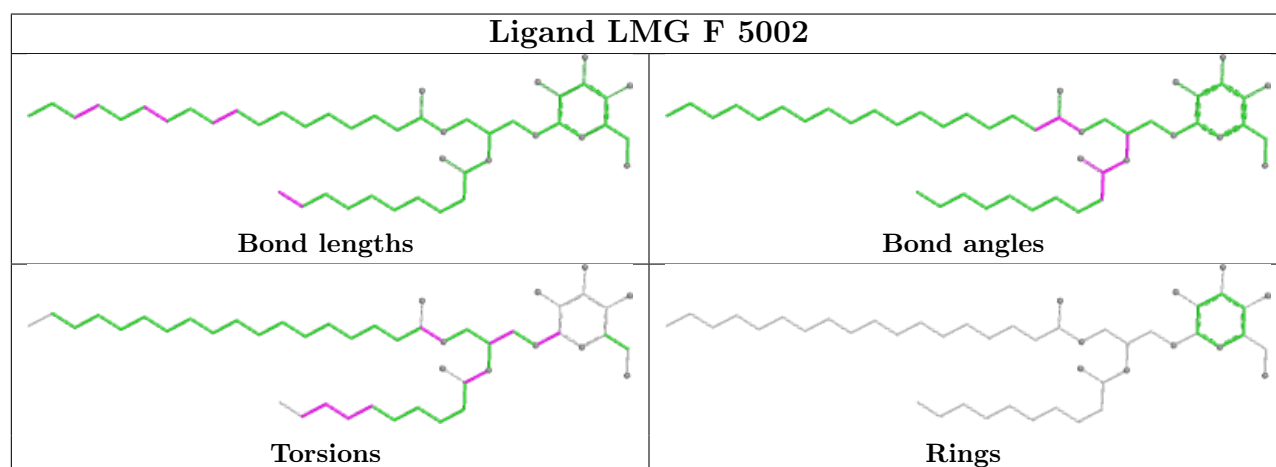
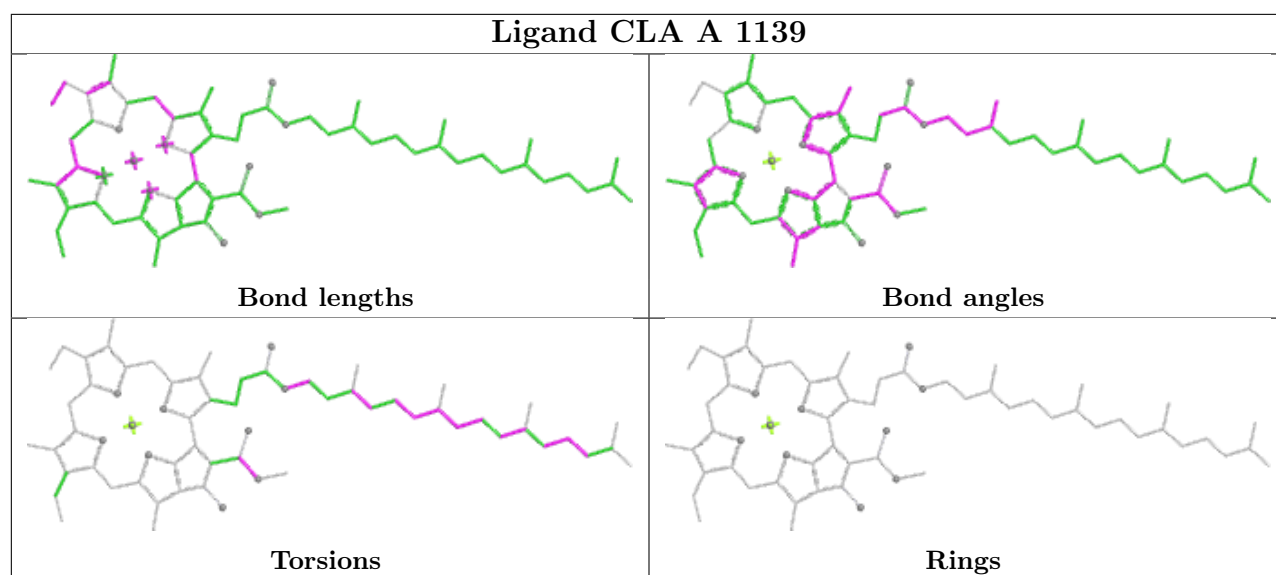
Ligand BCR J 4012	
	
Bond lengths	Bond angles
	
Torsions	Rings

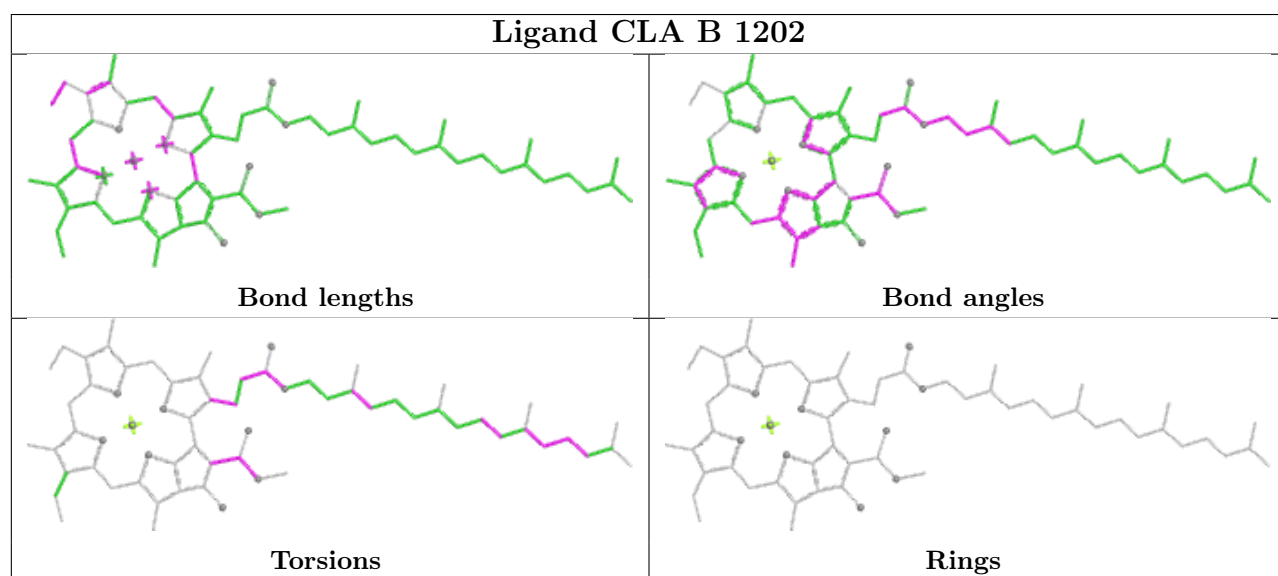
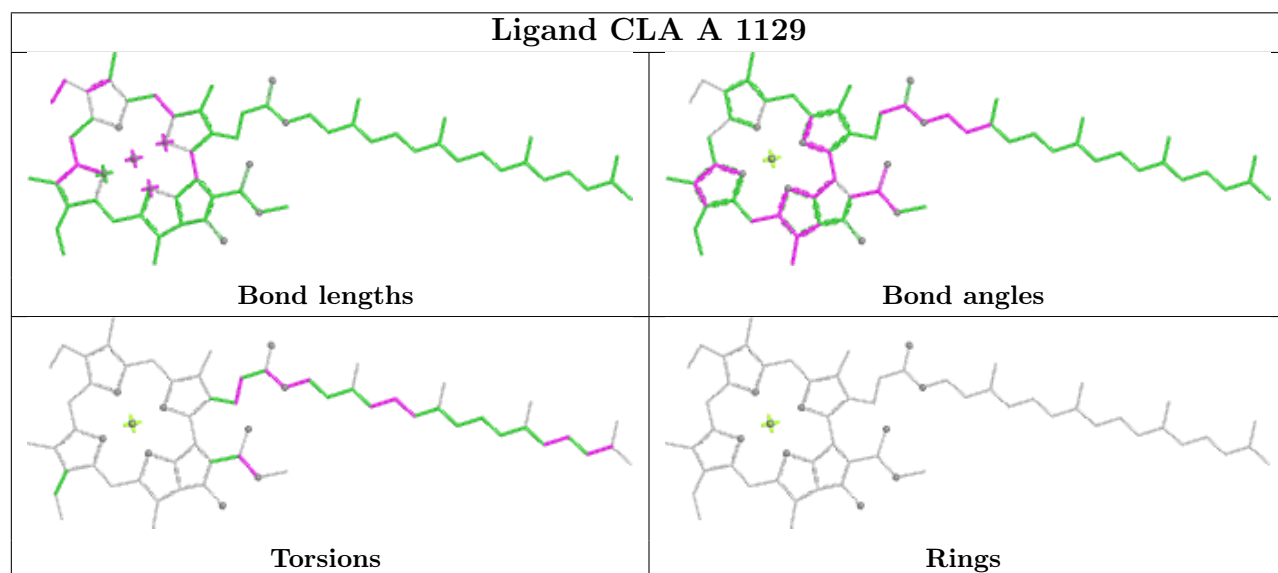
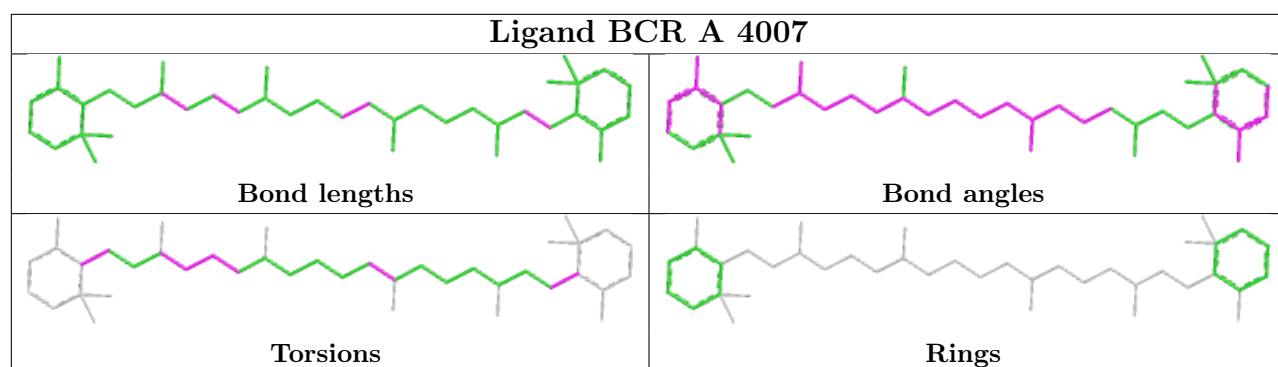
Ligand CLA 1 611	
	
Bond lengths	Bond angles
	
Torsions	Rings



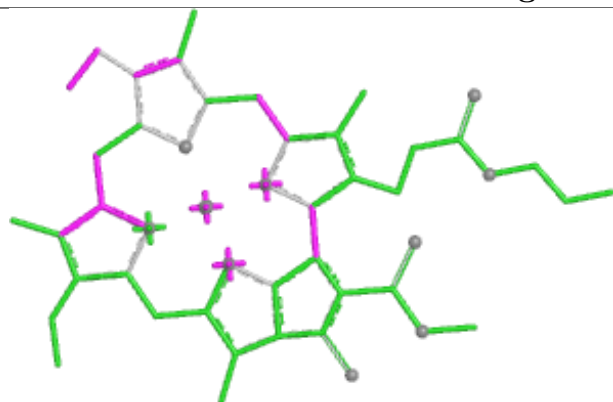




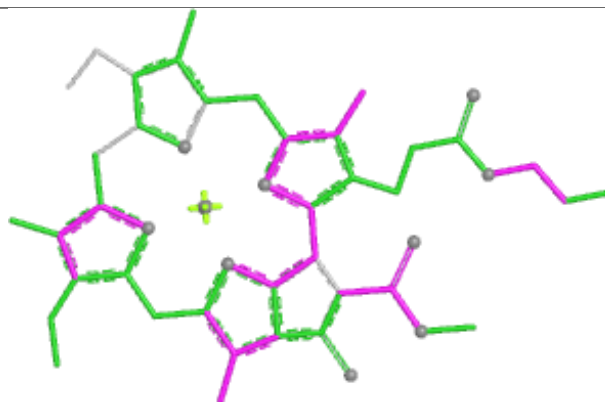




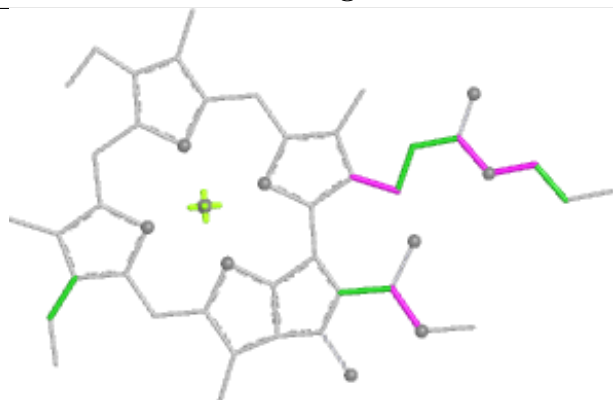
Ligand CLA 3 608



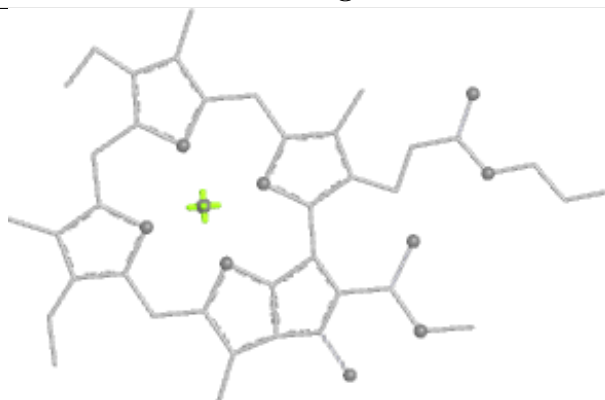
Bond lengths



Bond angles

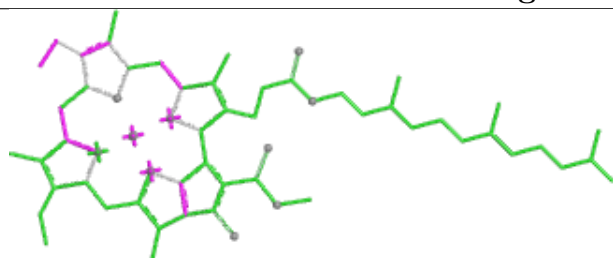


Torsions

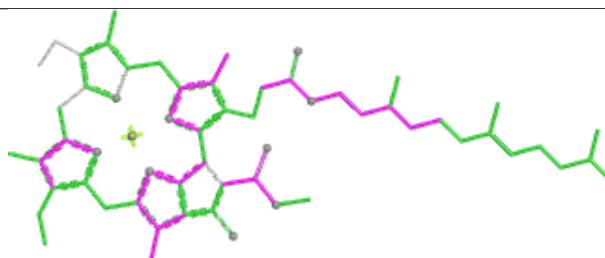


Rings

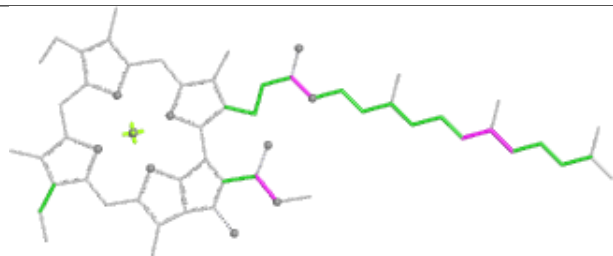
Ligand CLA 4 604



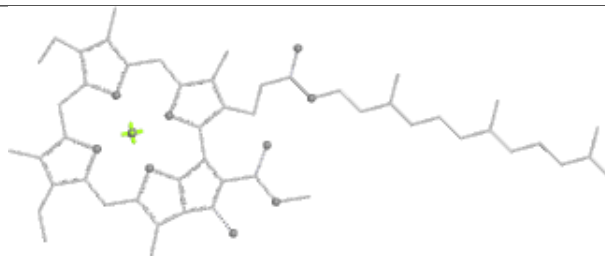
Bond lengths



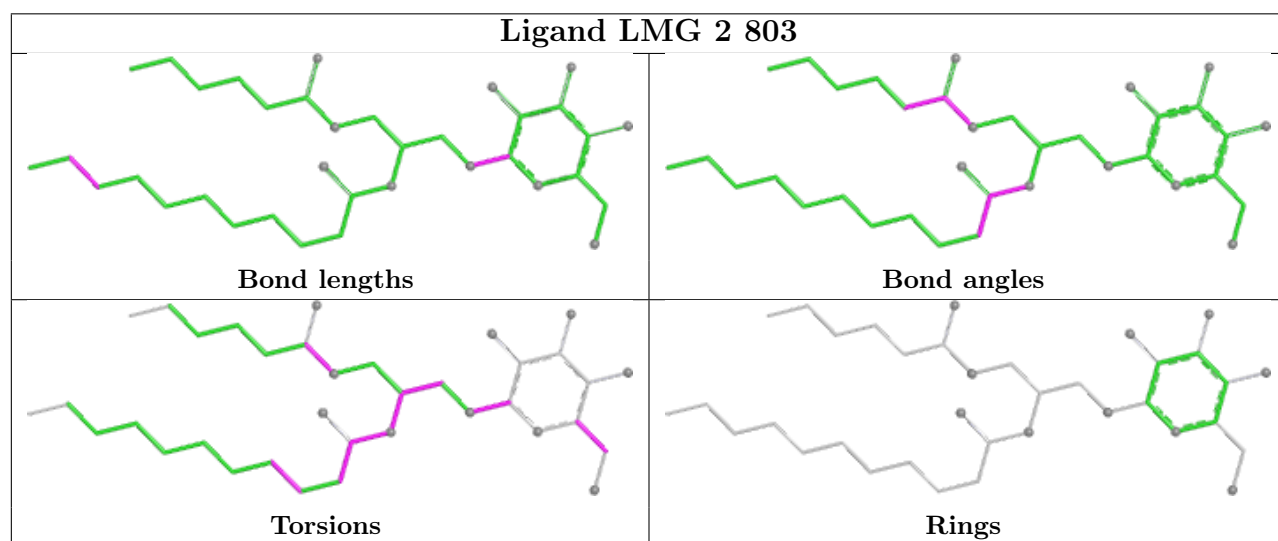
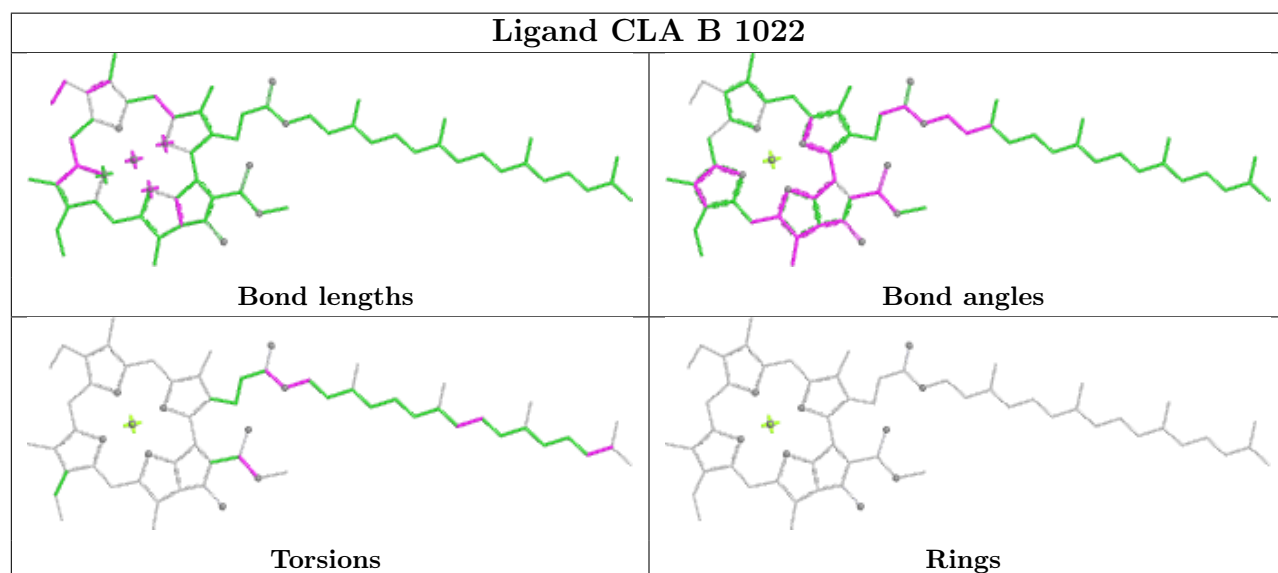
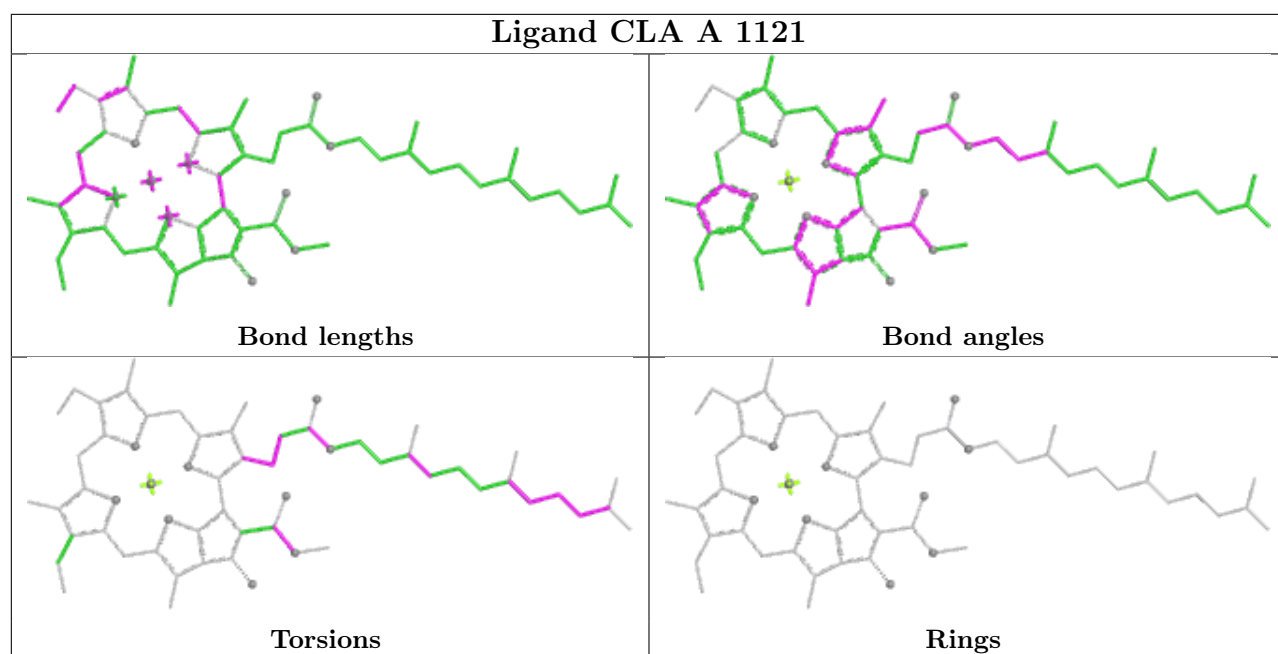
Bond angles



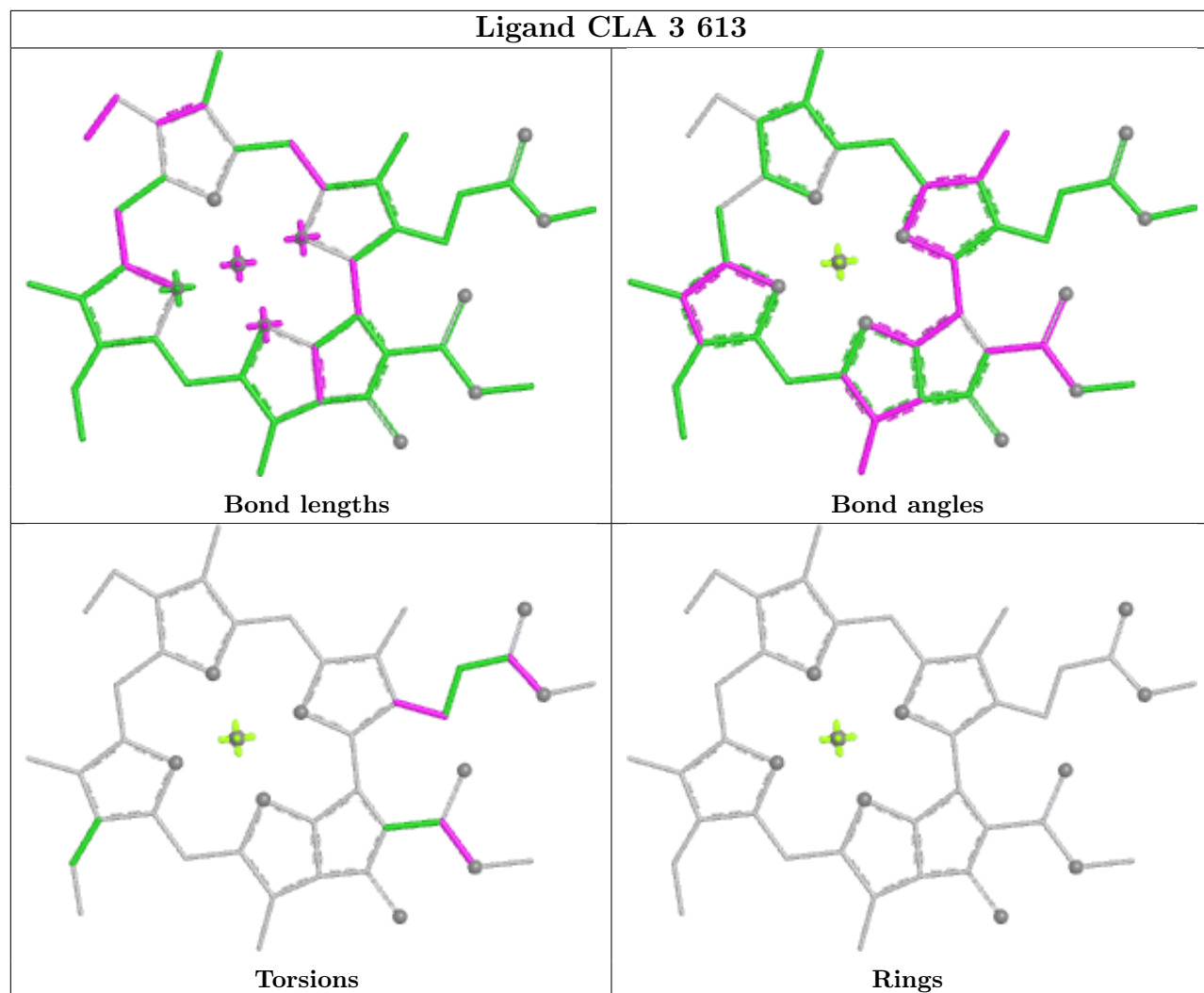
Torsions

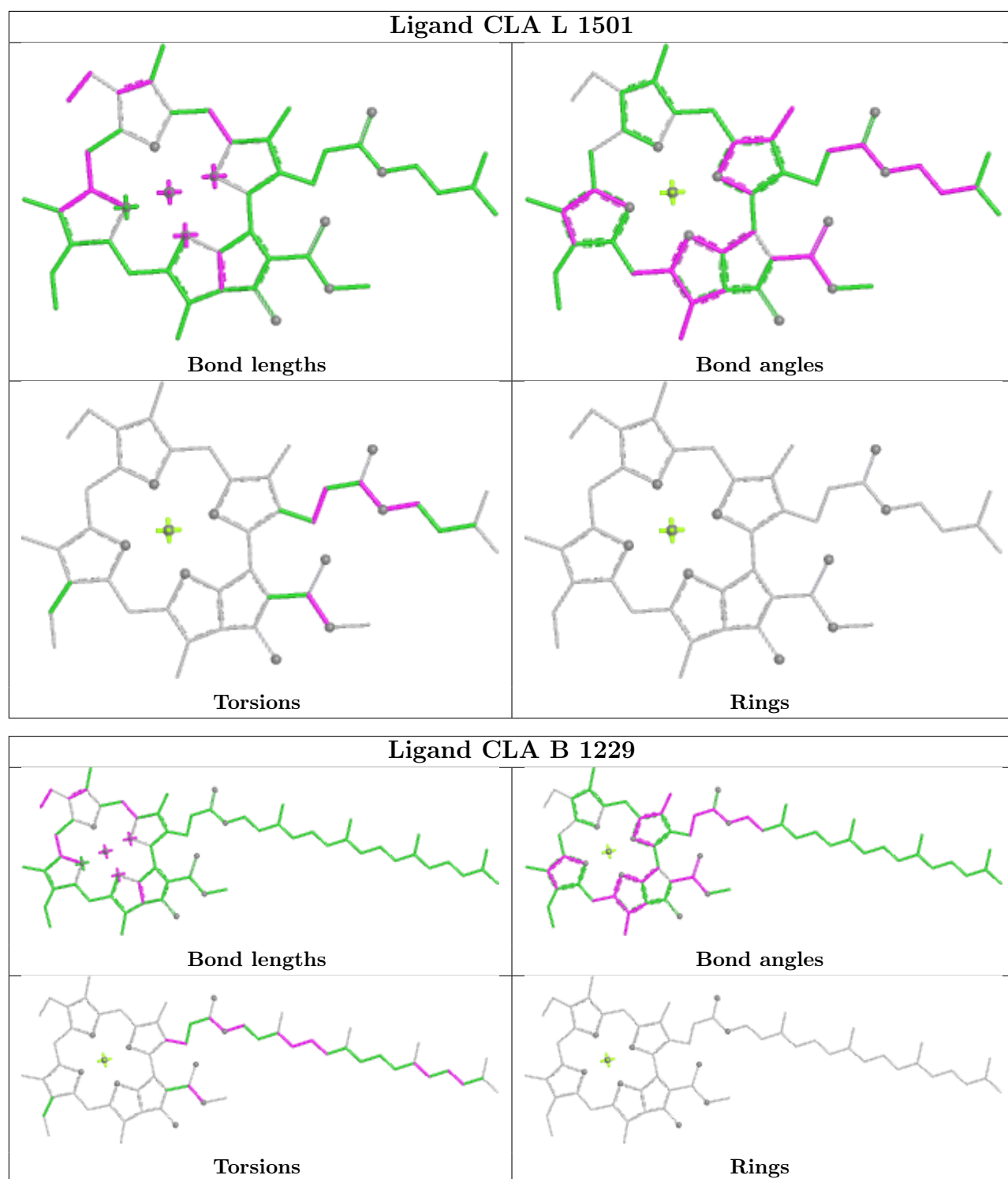


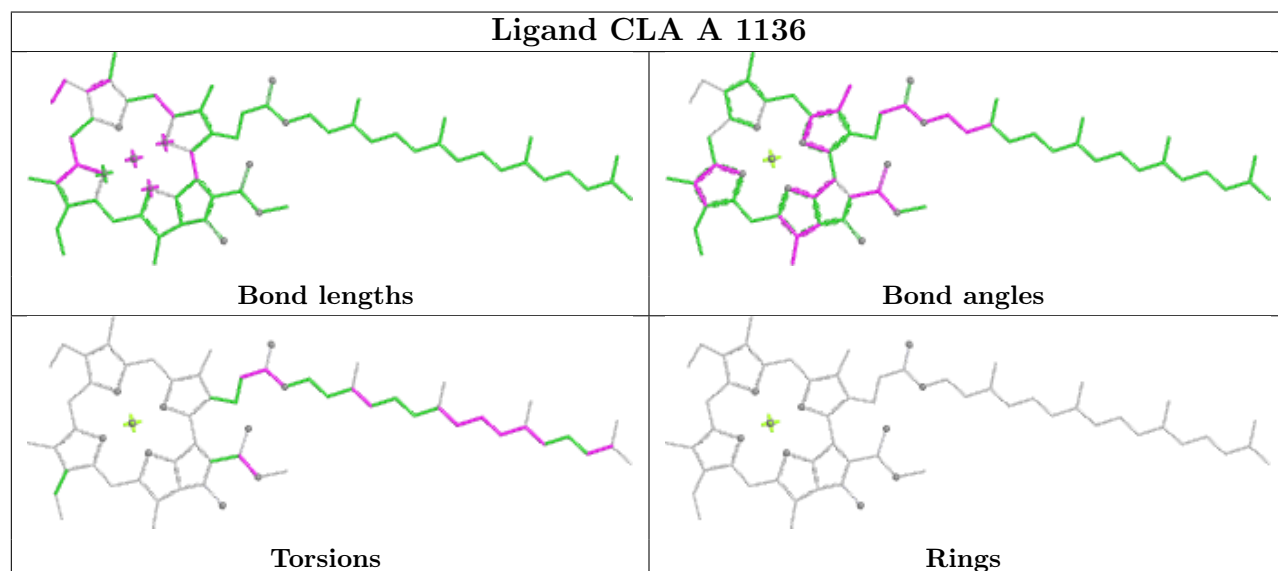
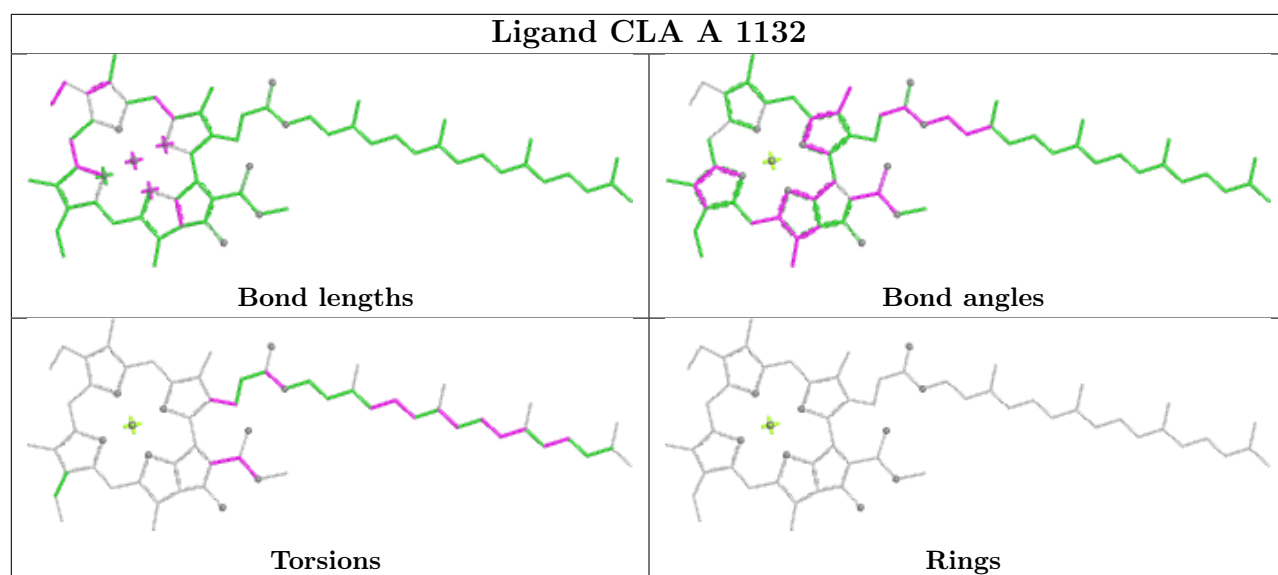
Rings

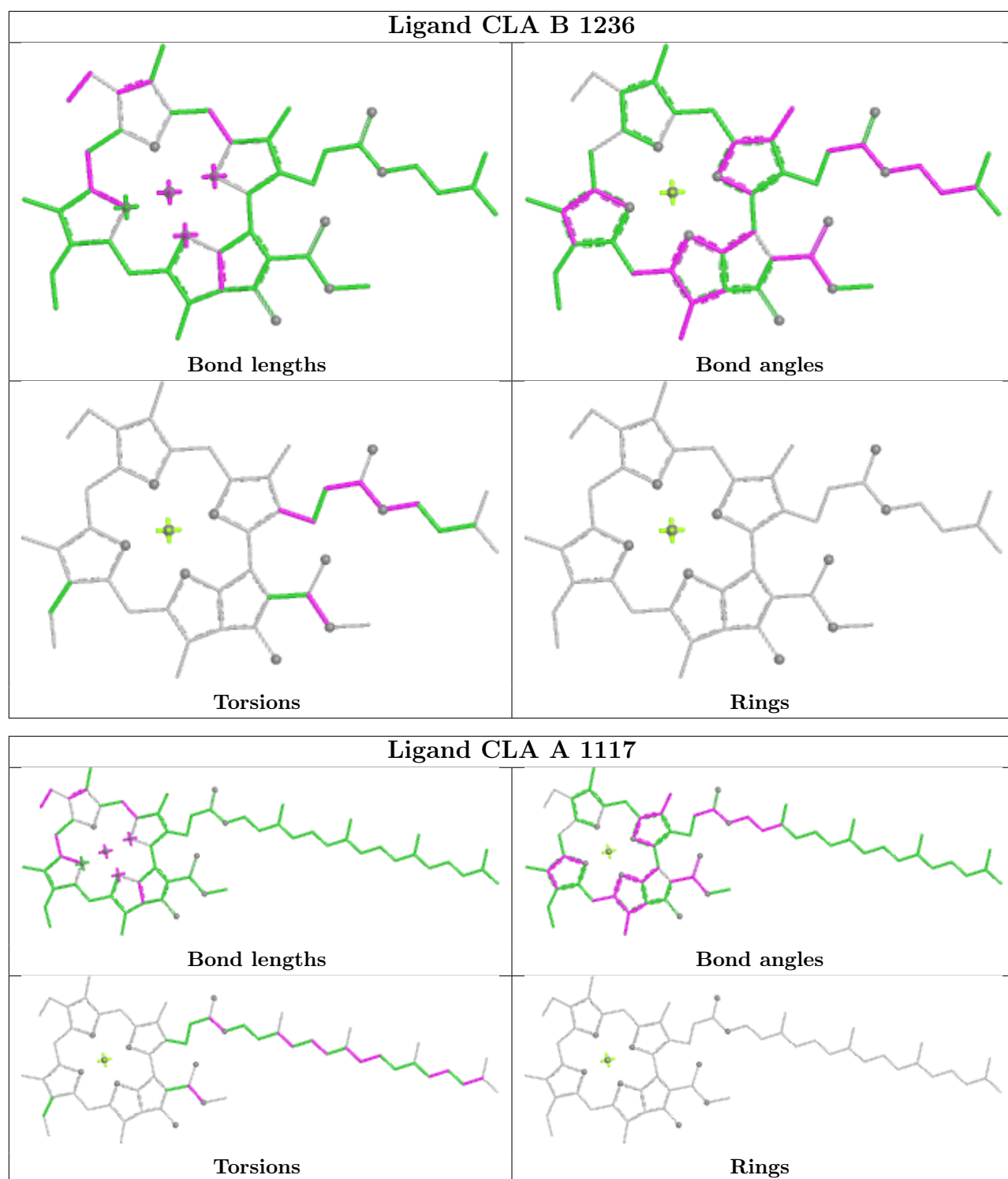


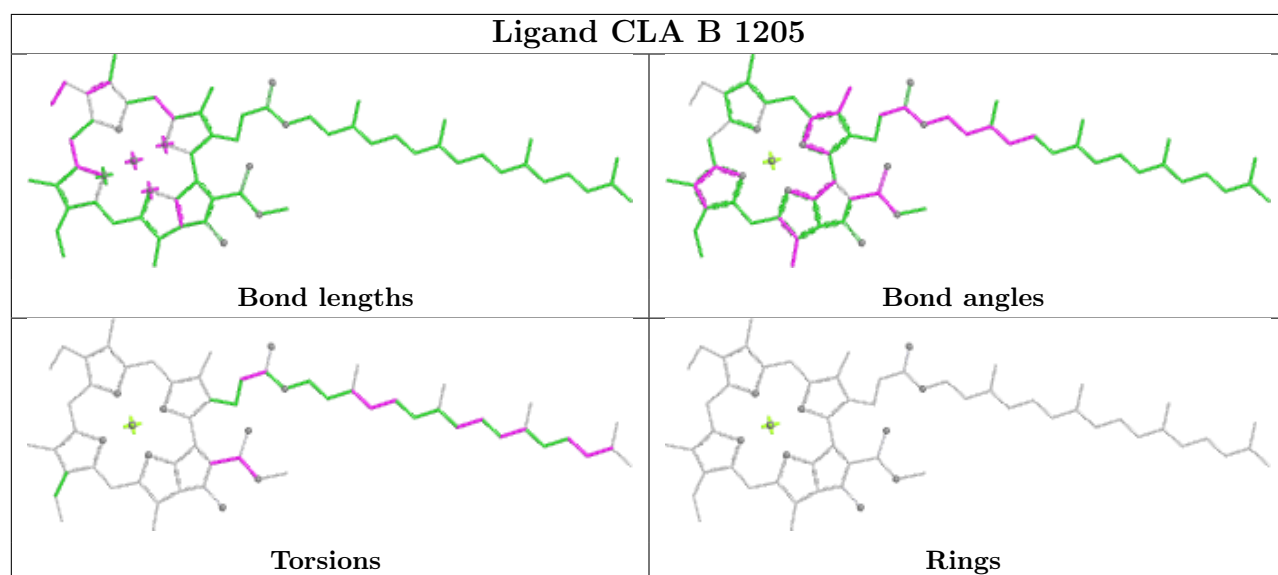
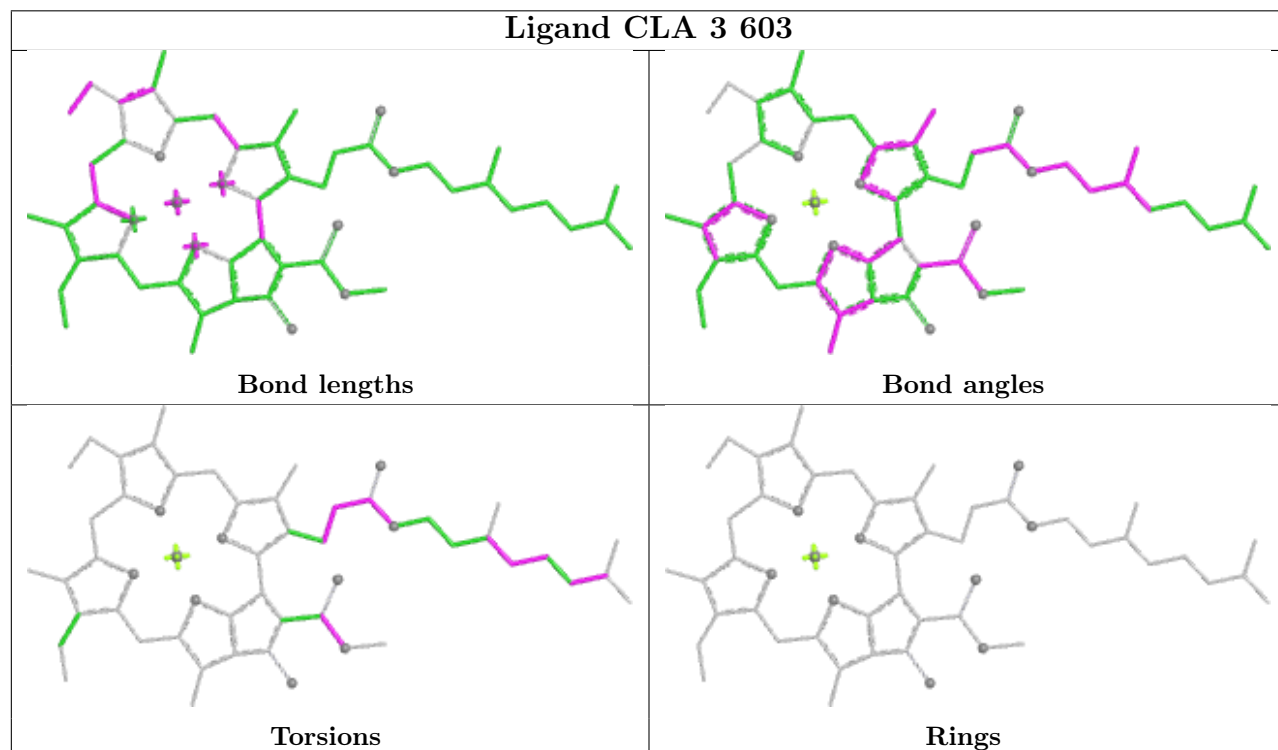
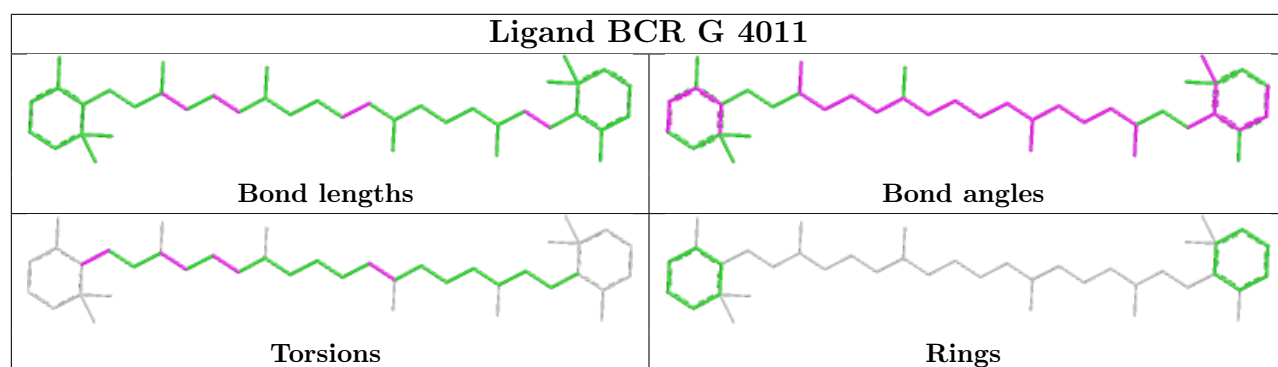
Ligand CLA 3 613

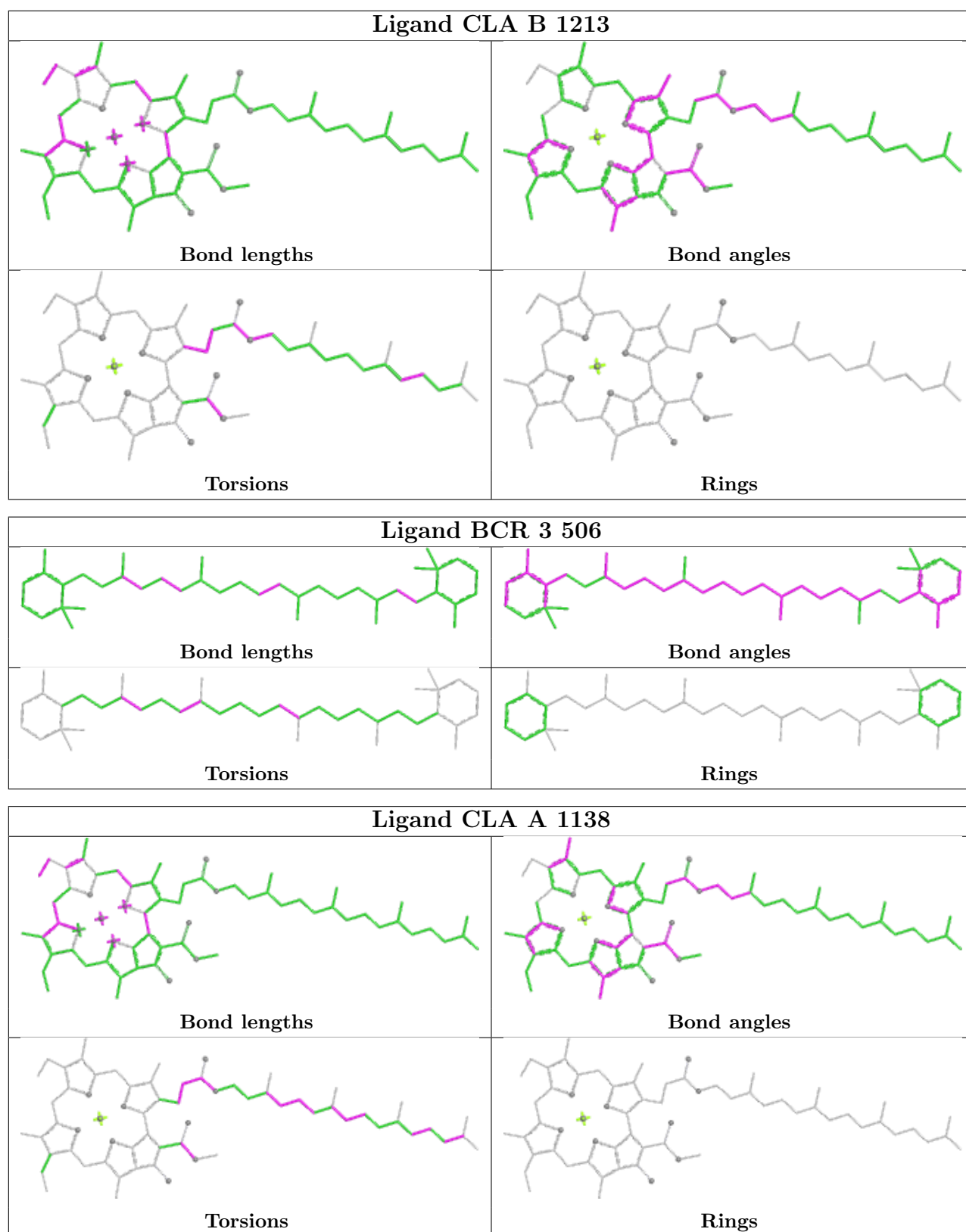


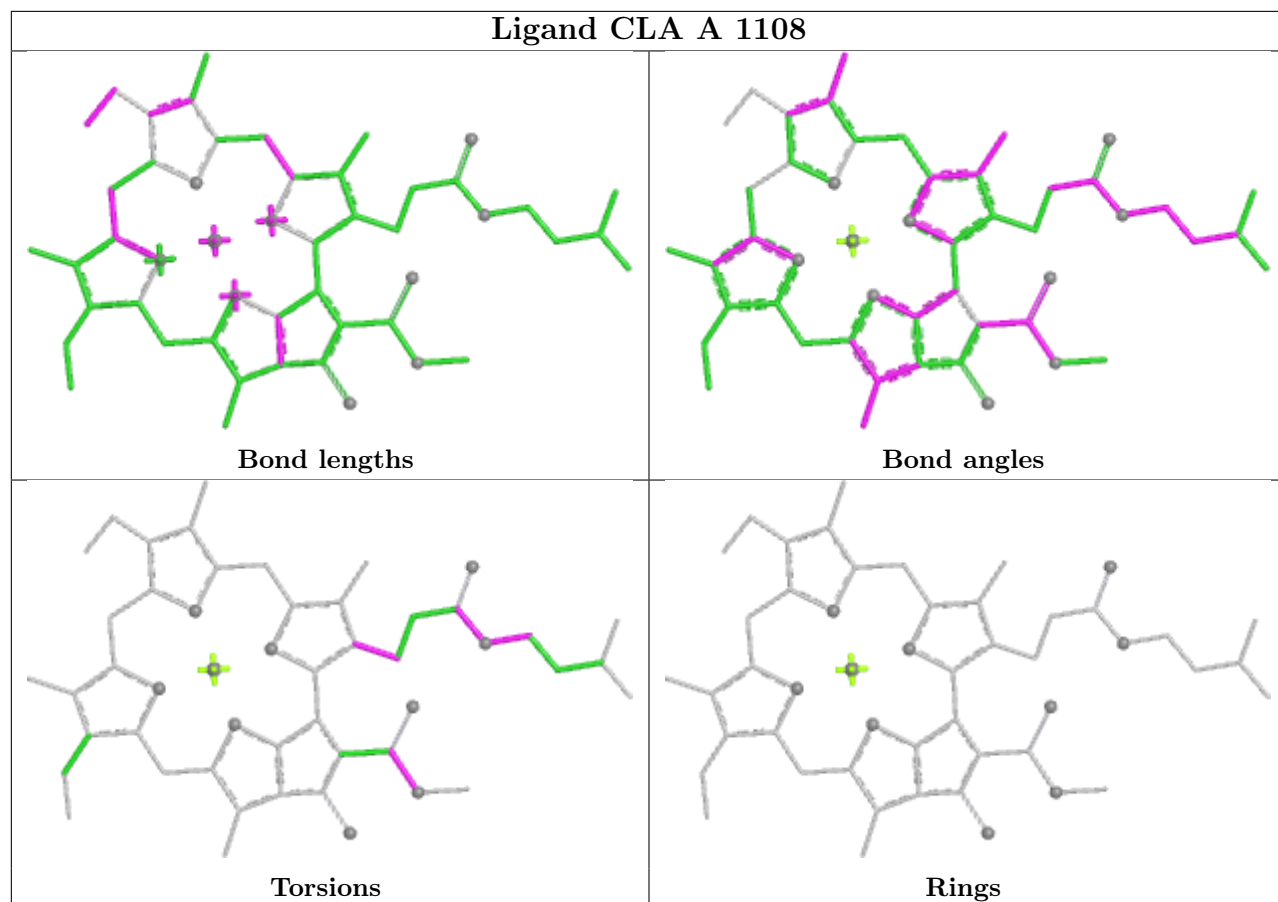




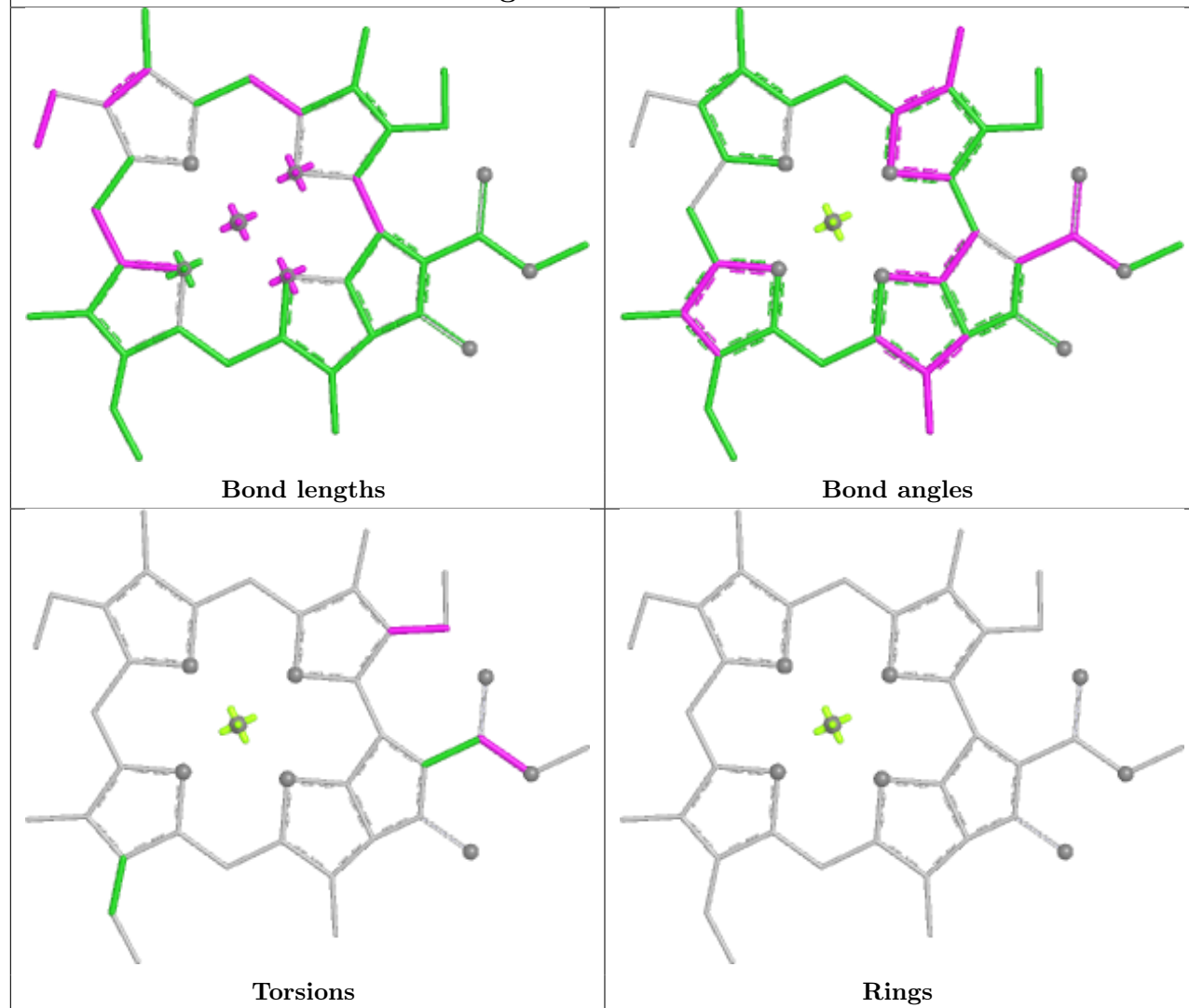




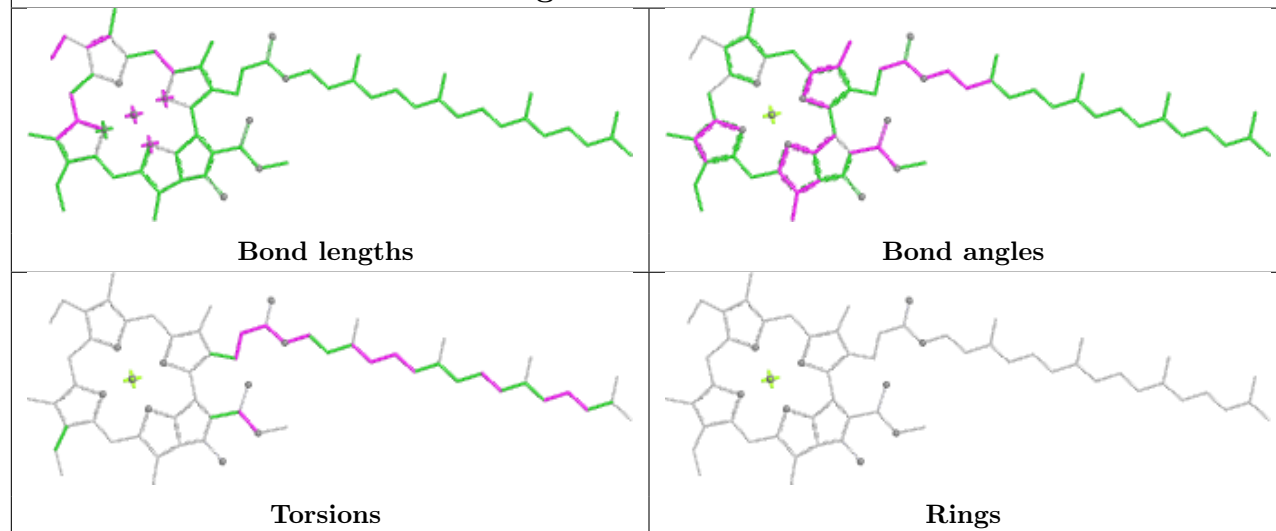


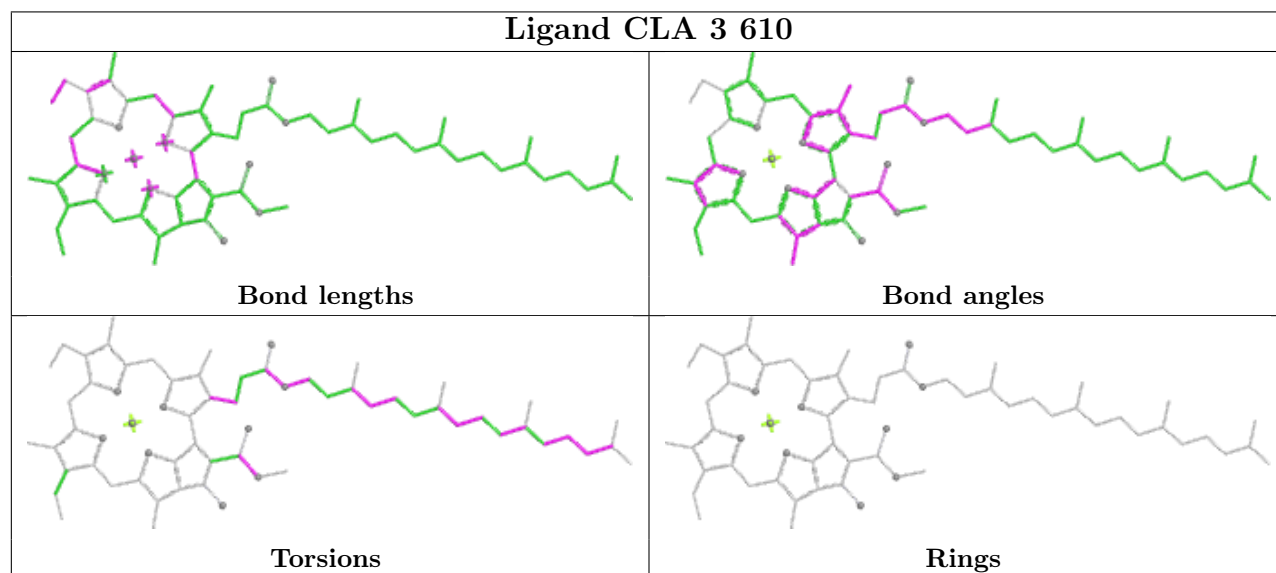
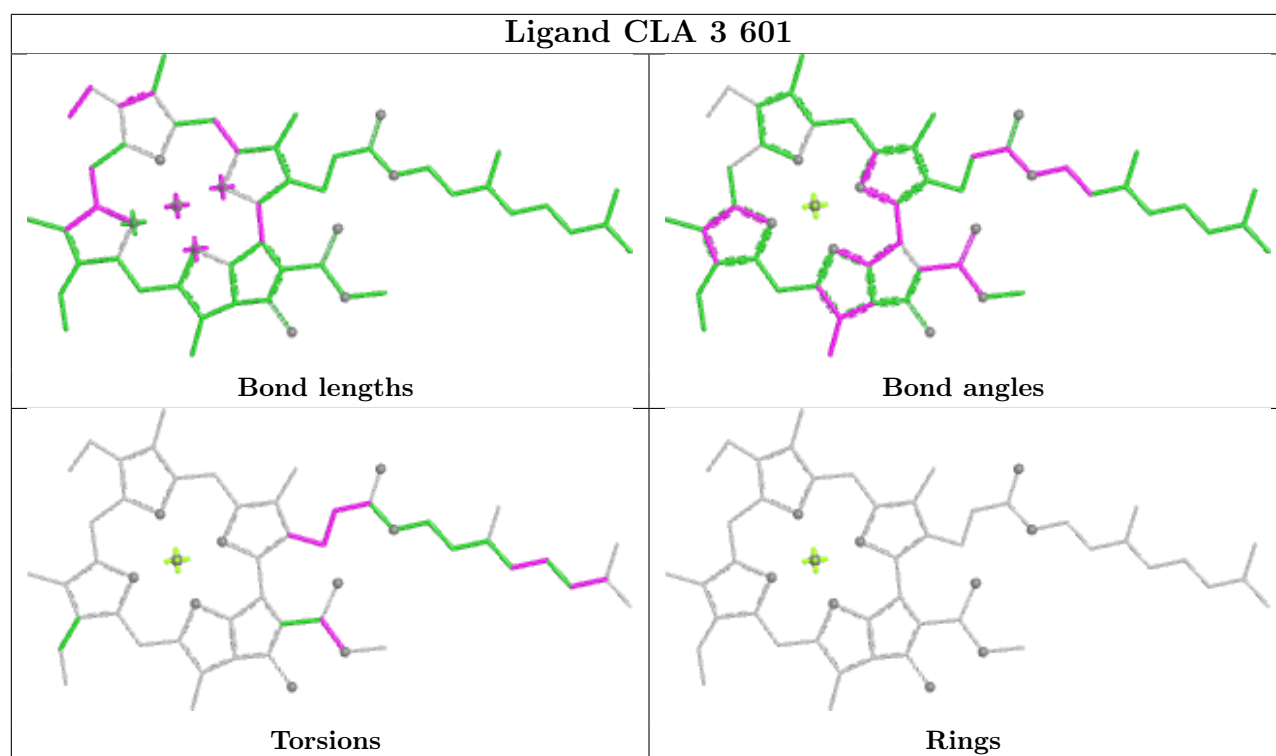


Ligand CLA 3 614

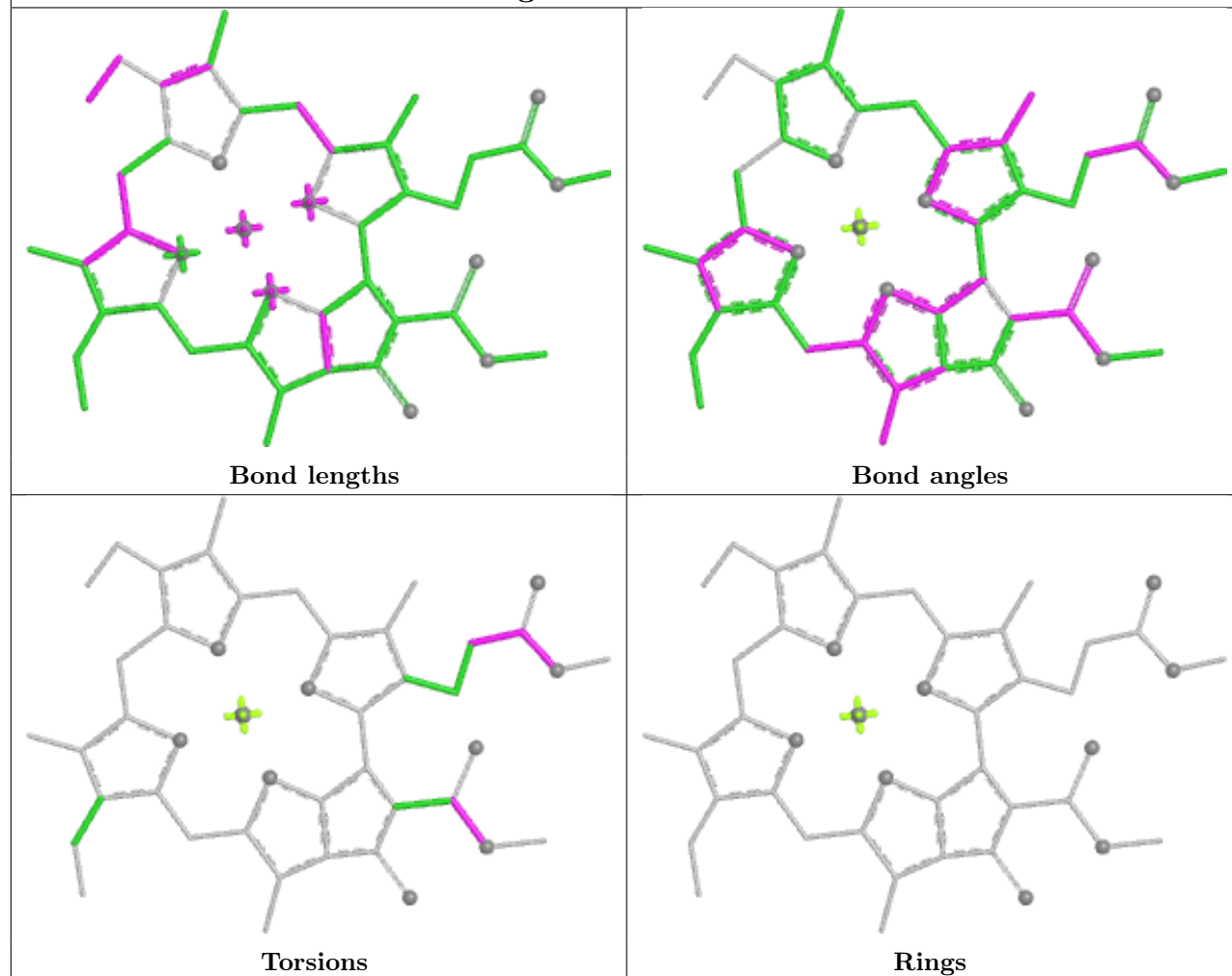


Ligand CLA 2 603

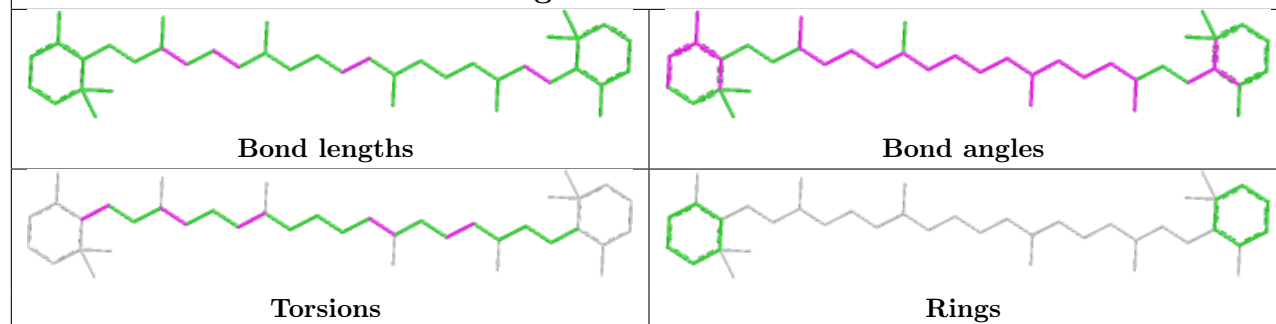


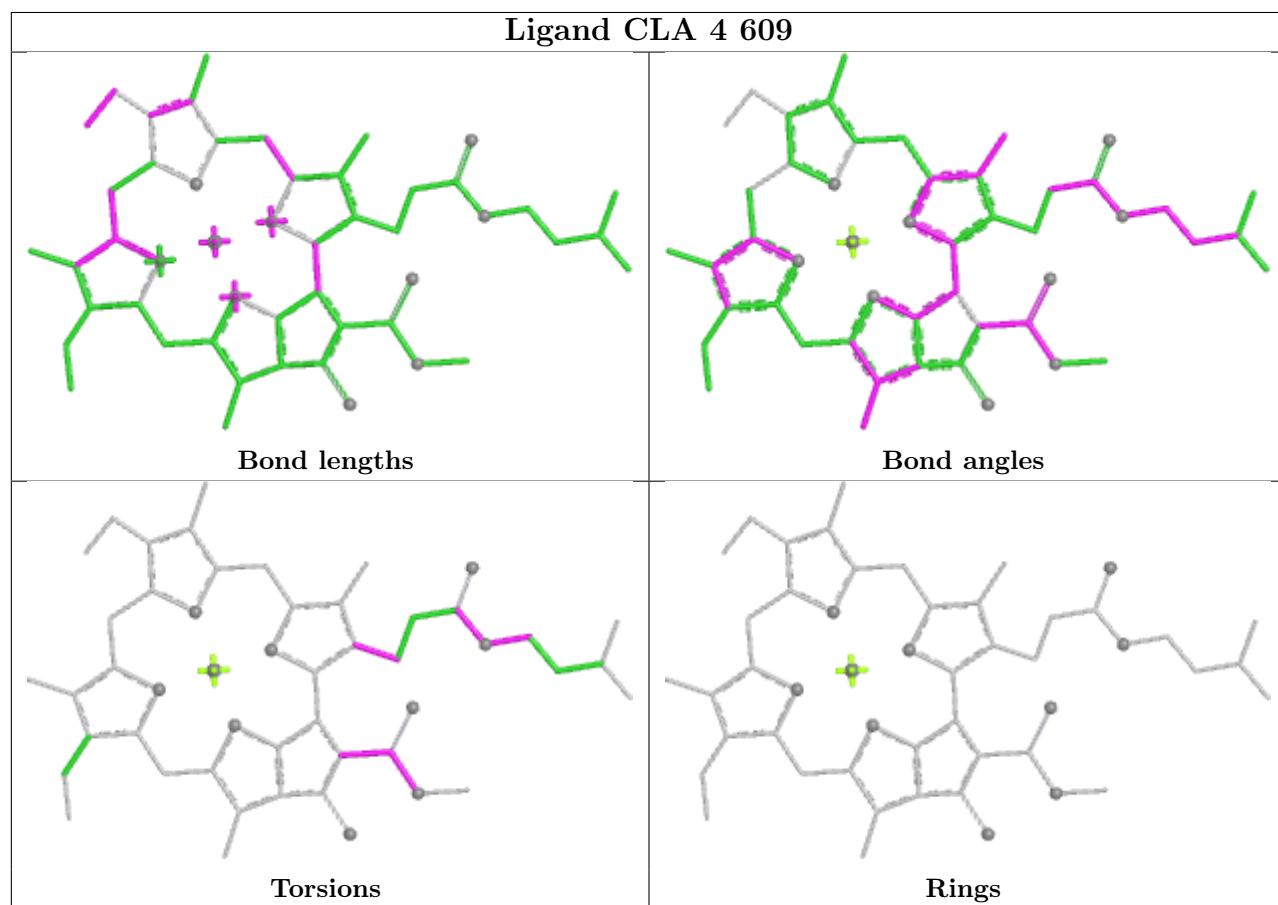
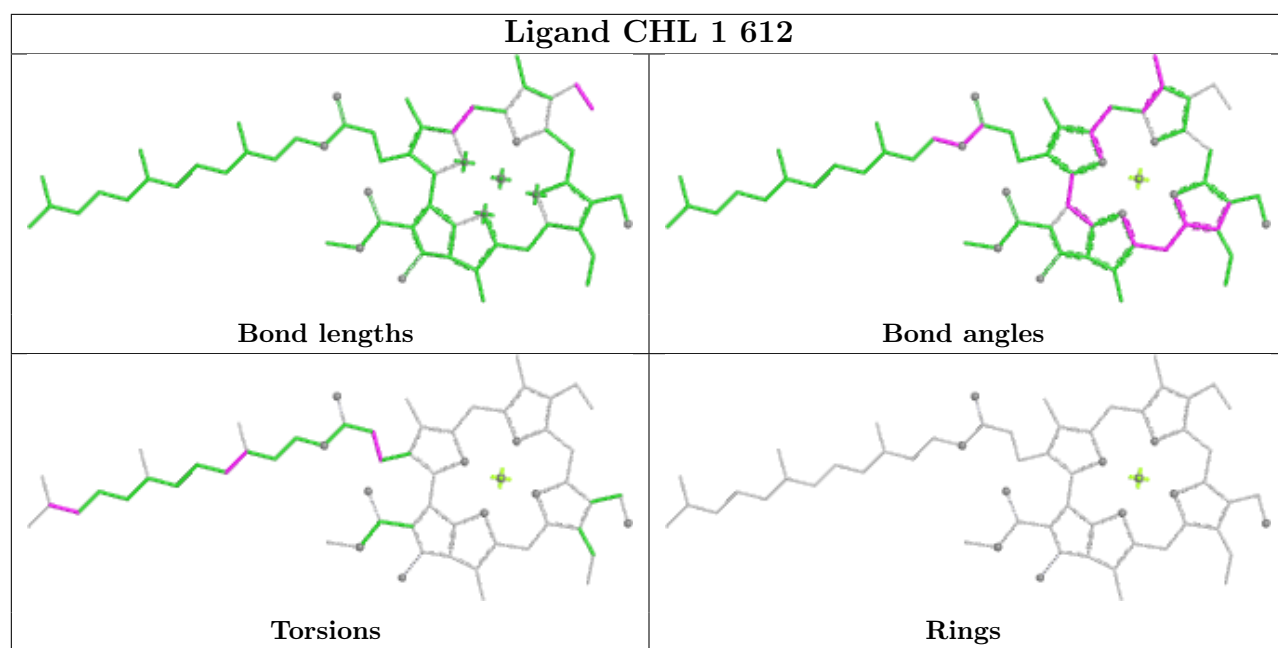


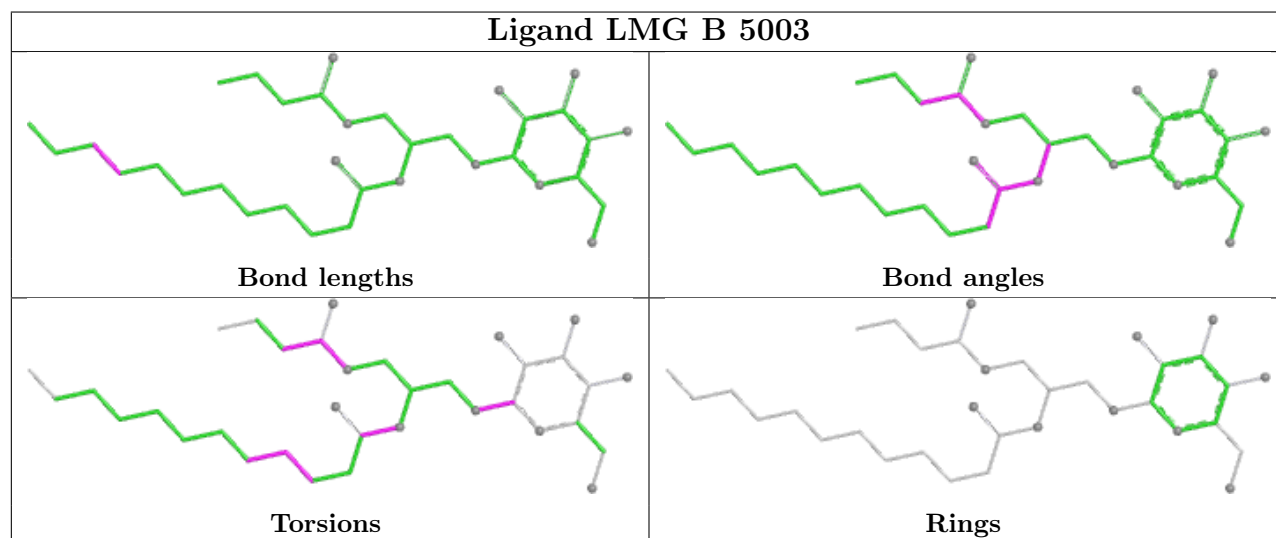
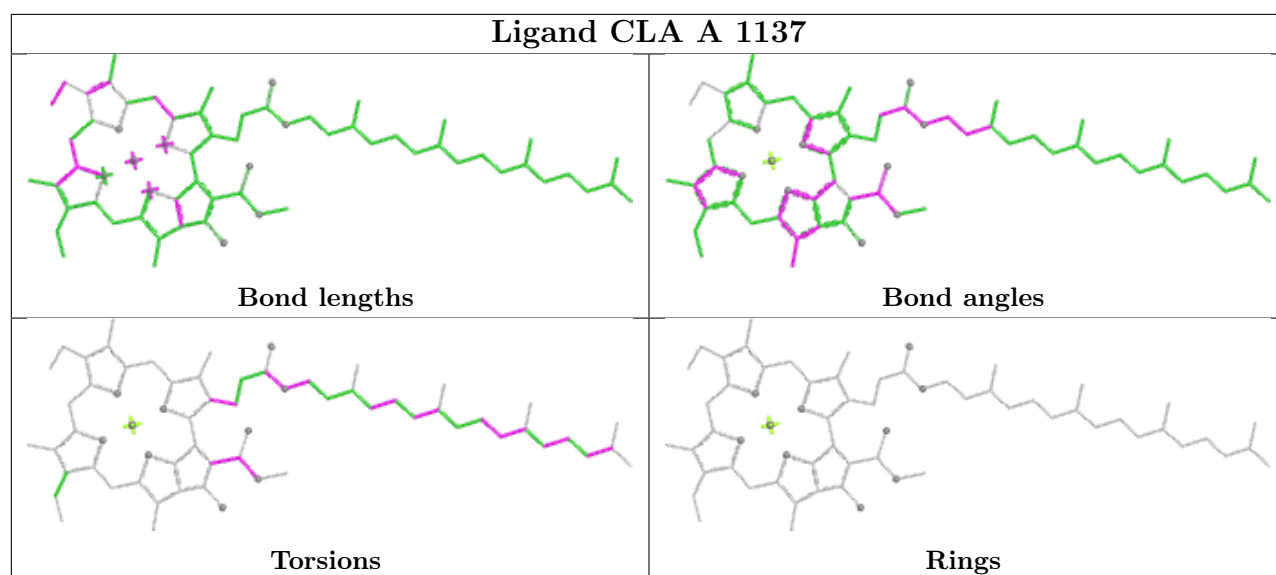
Ligand CLA 4 608

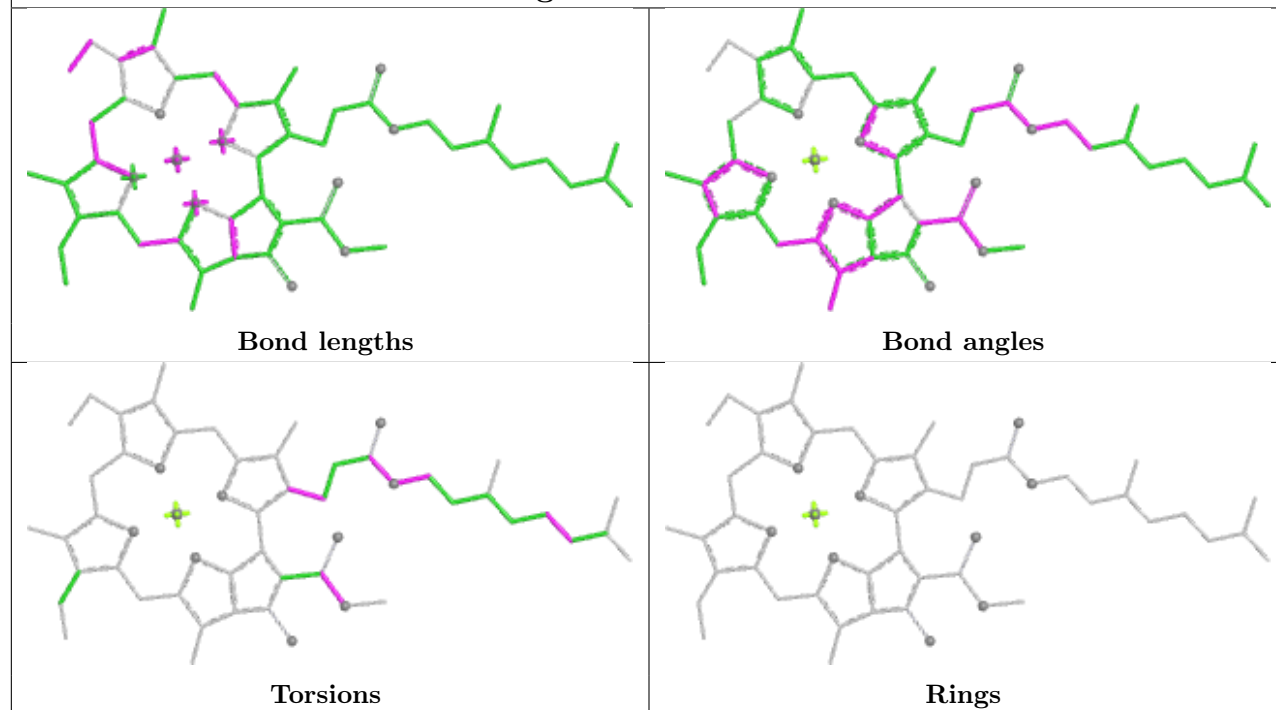
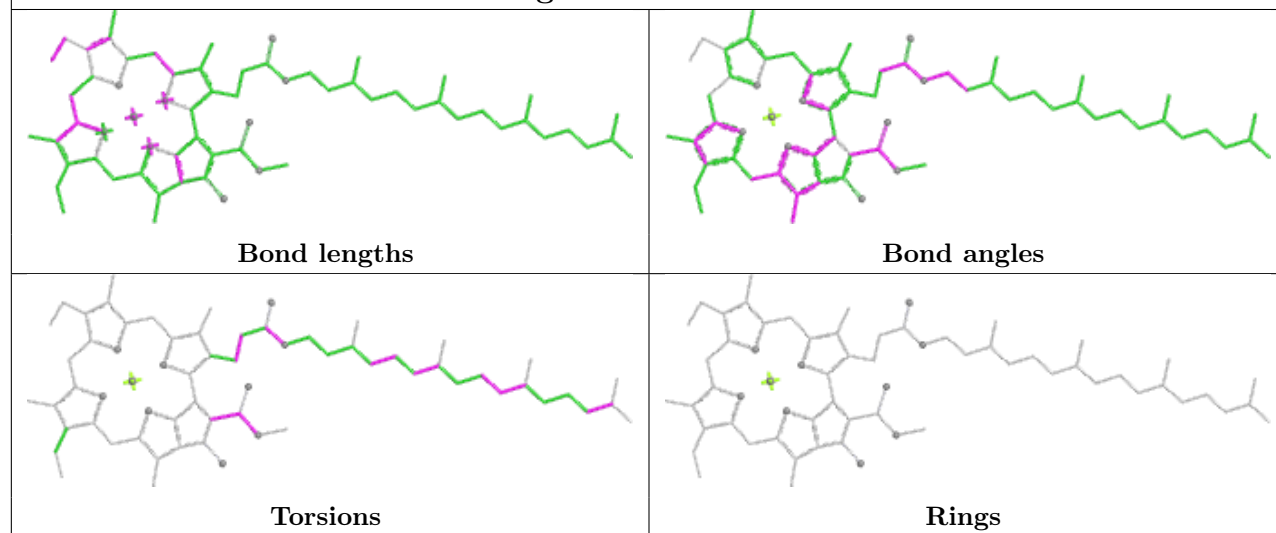


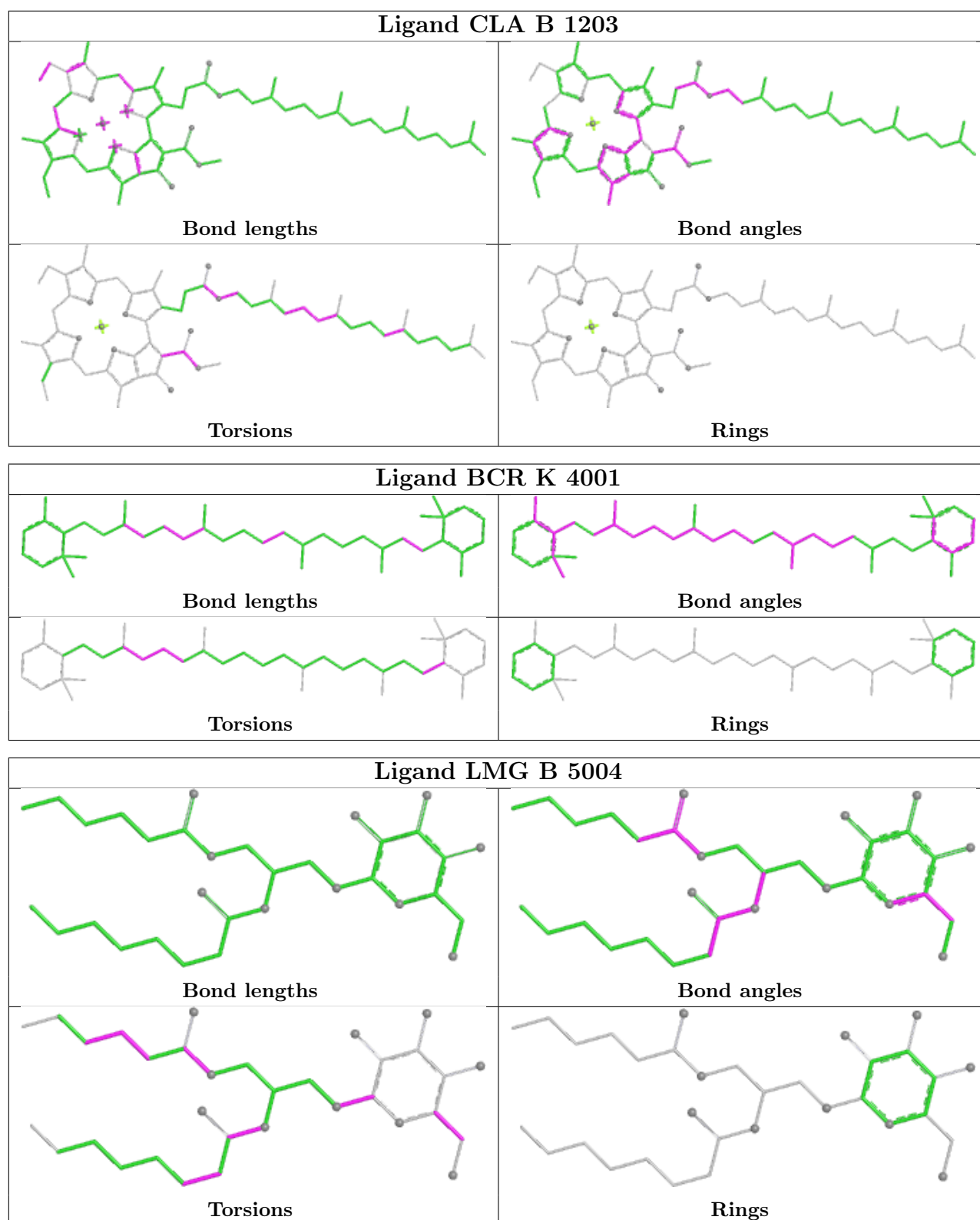
Ligand BCR 1 504

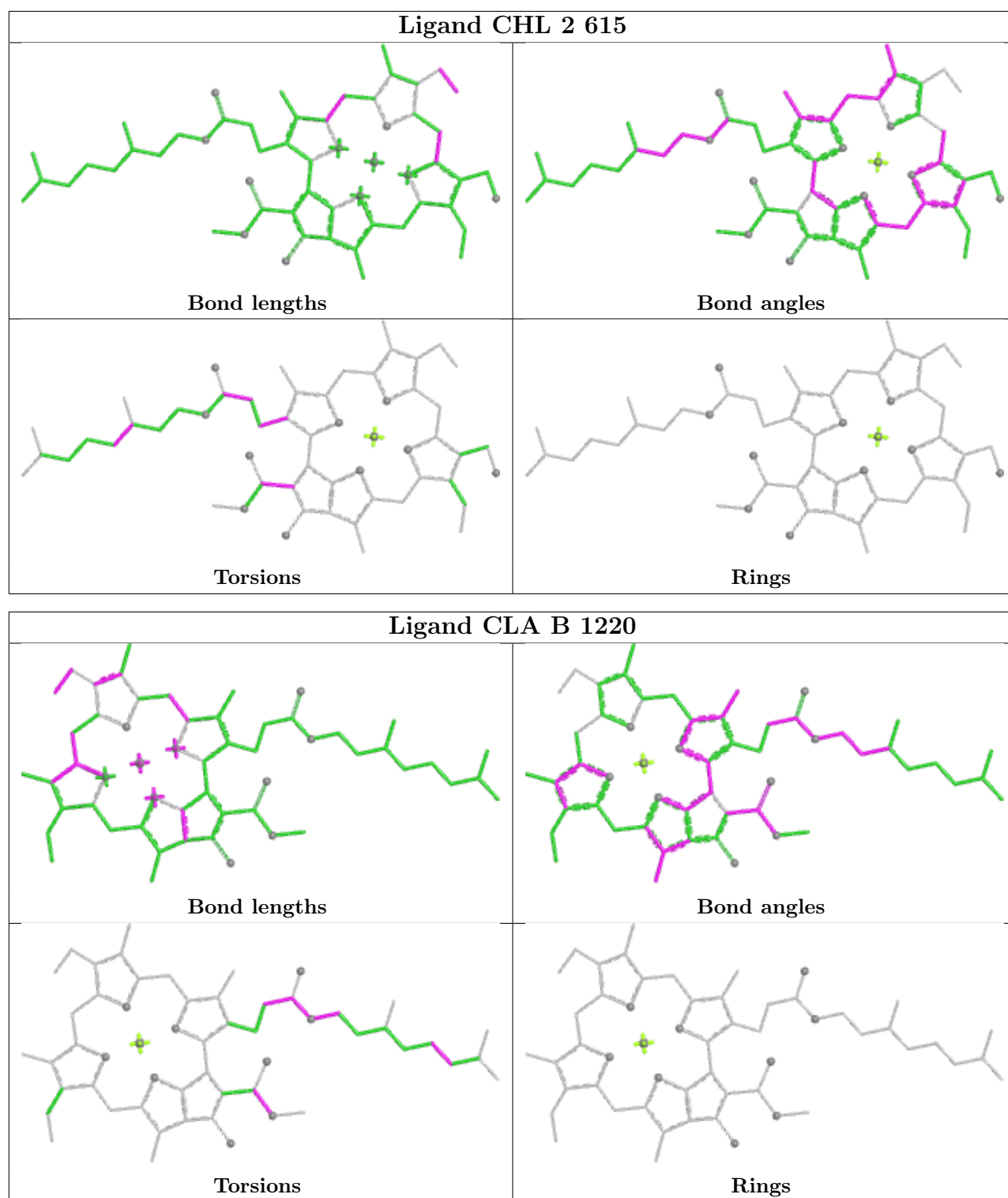


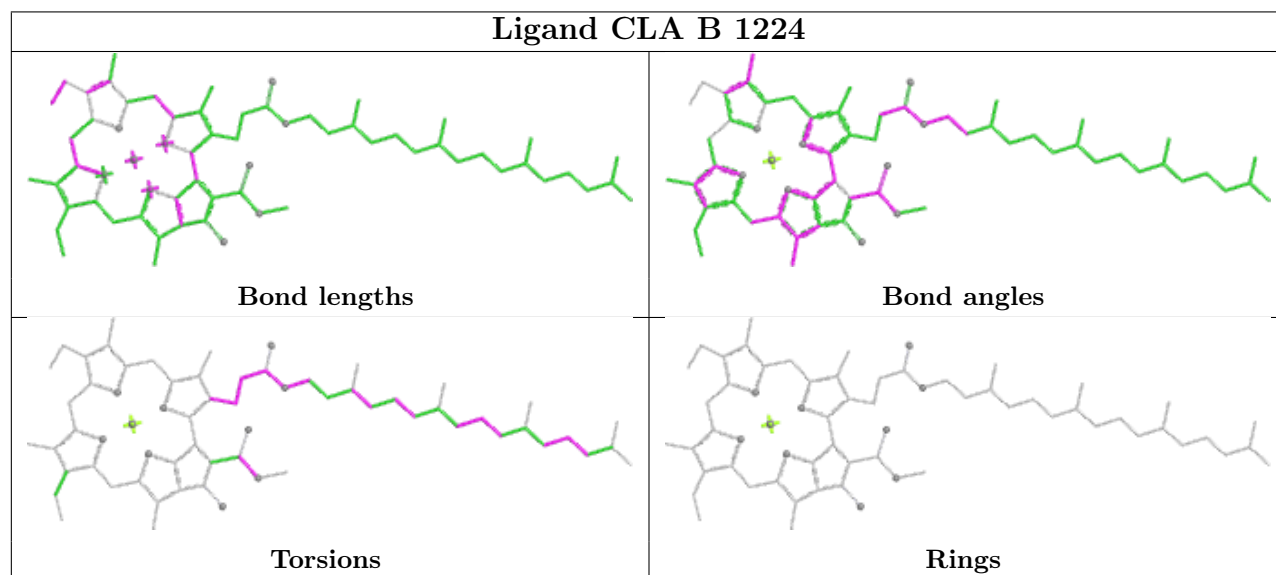
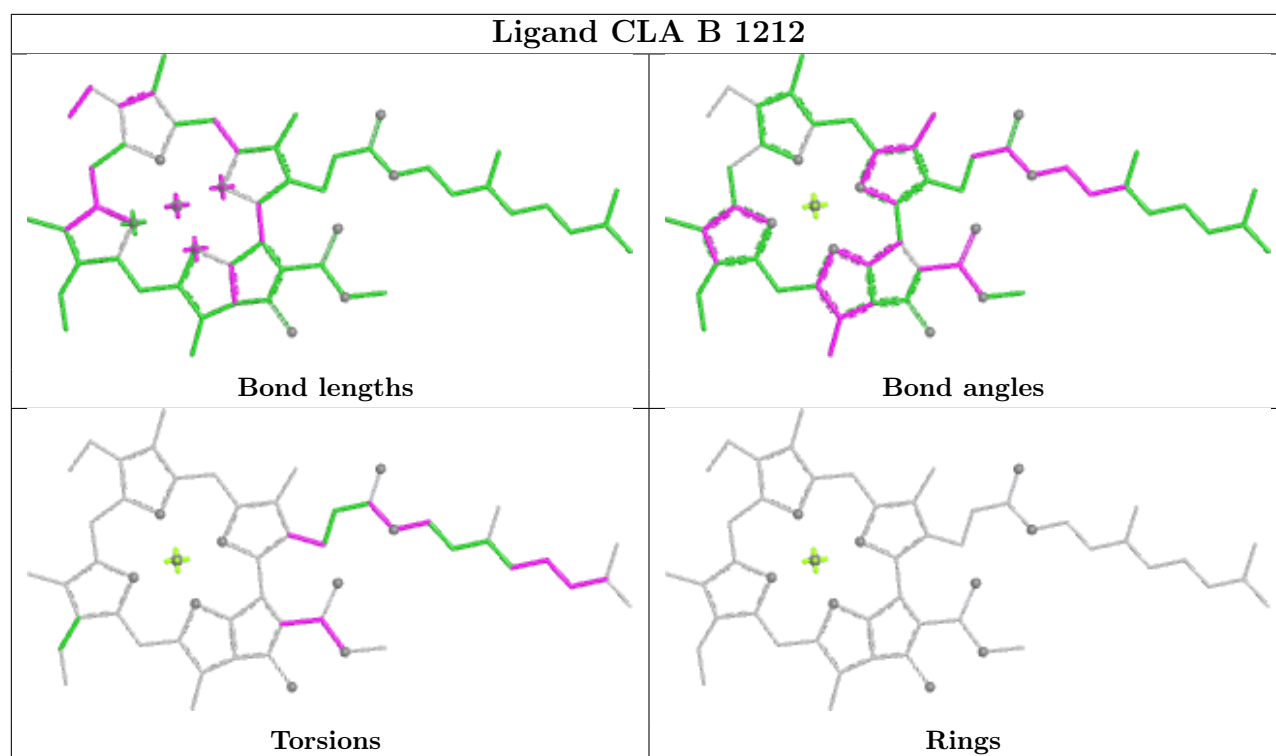


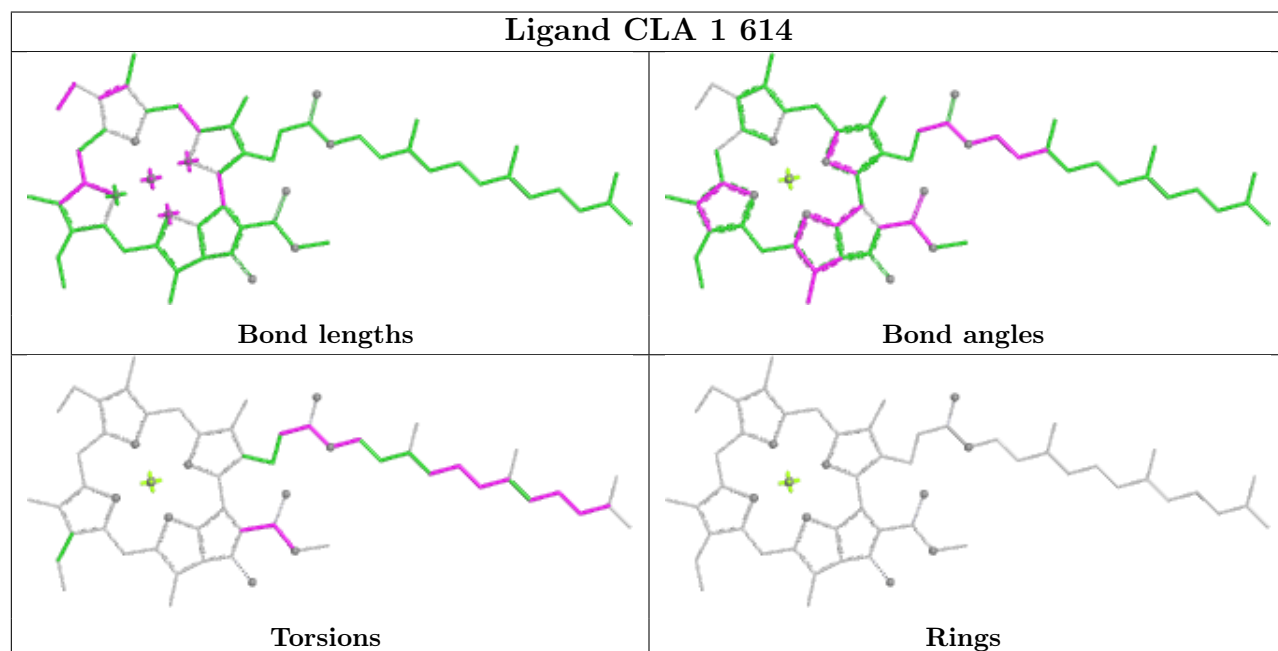
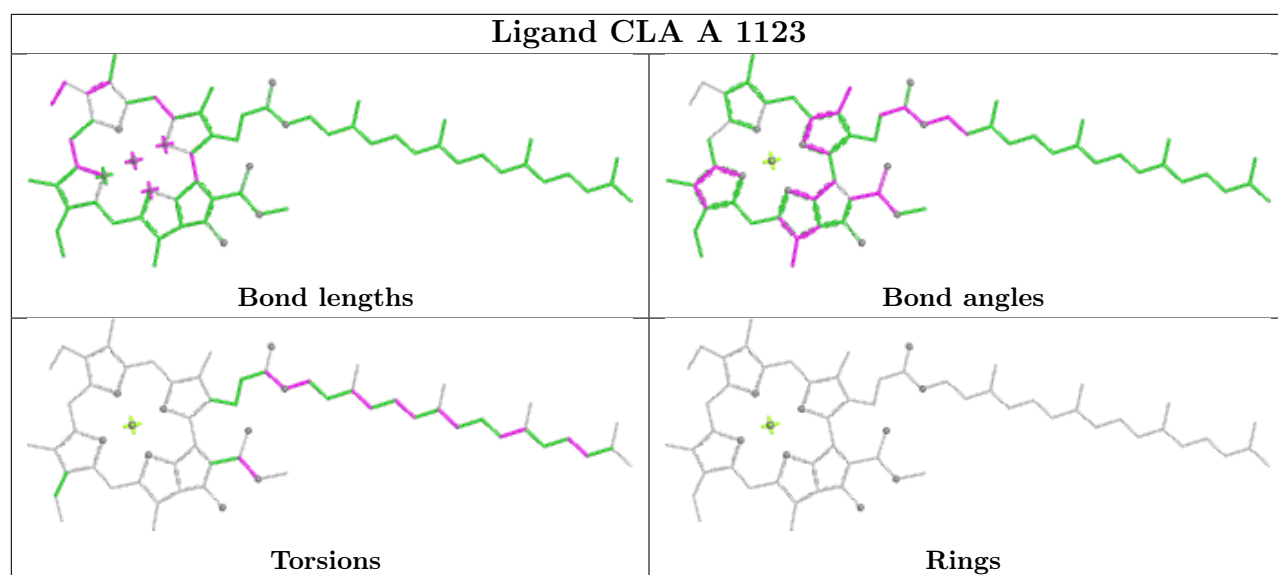


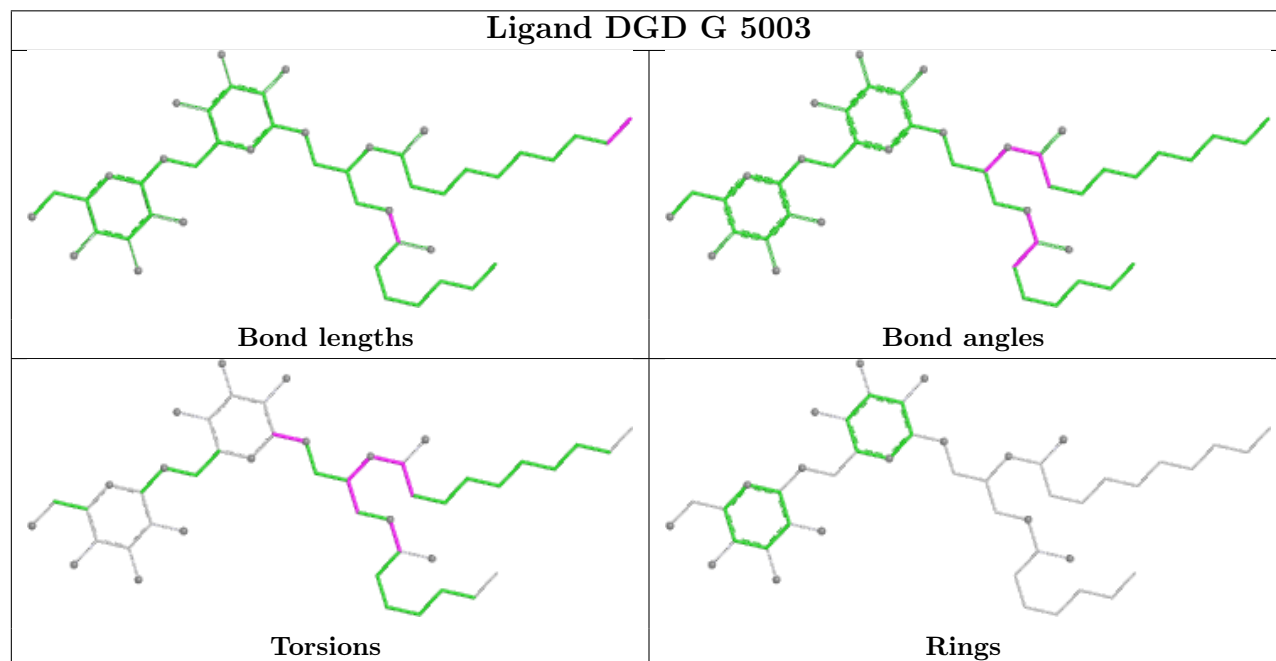
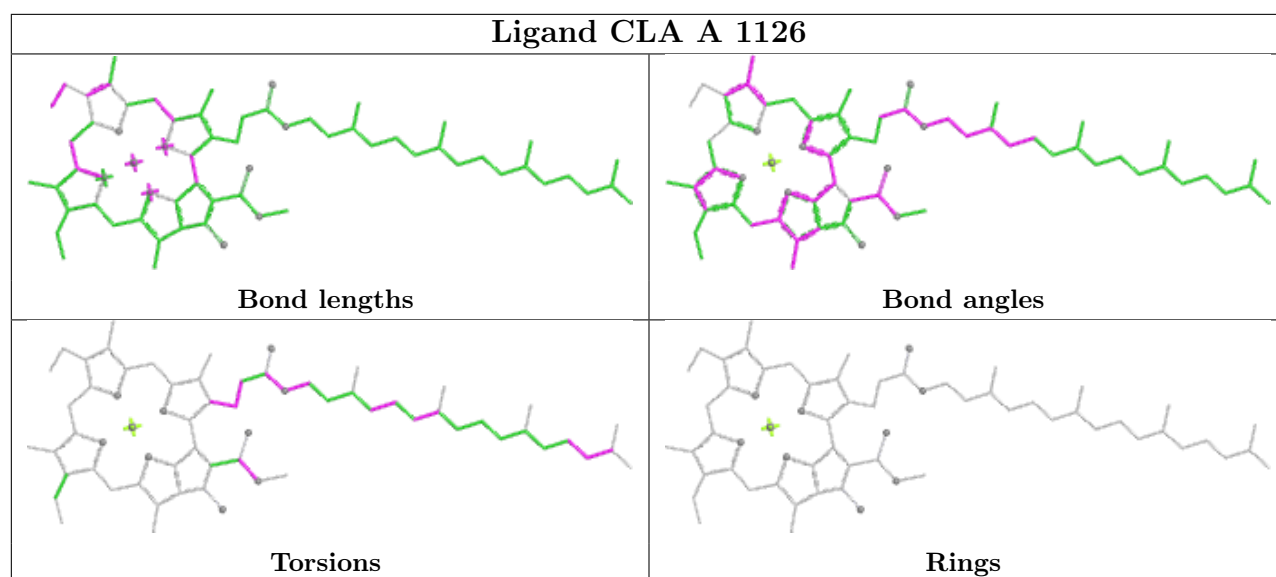
Ligand CLA 2 612**Ligand CLA 1 604**

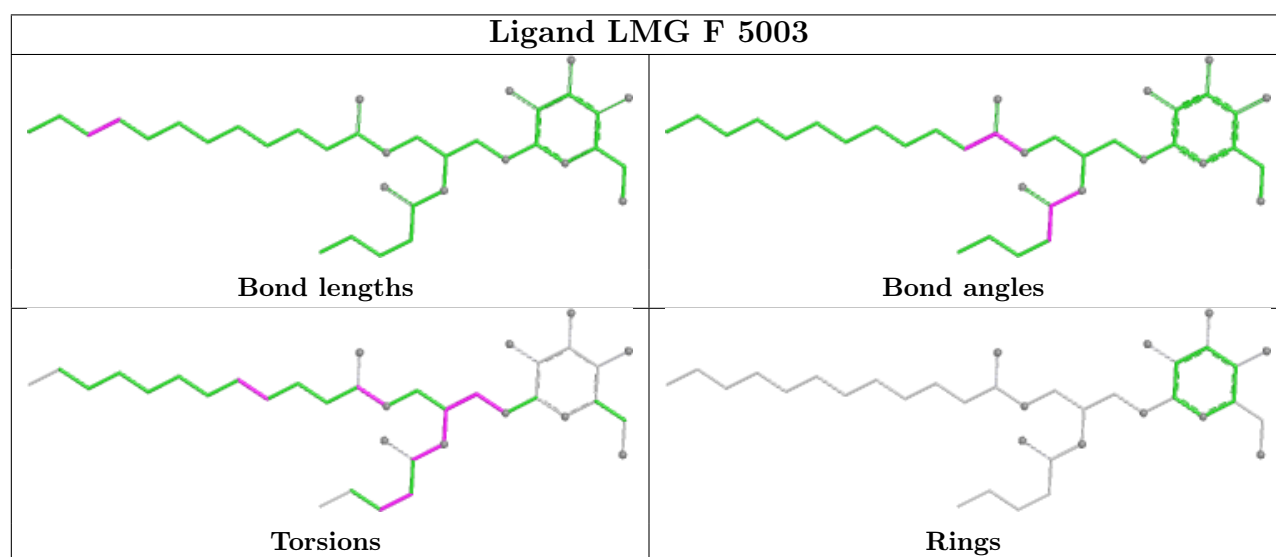
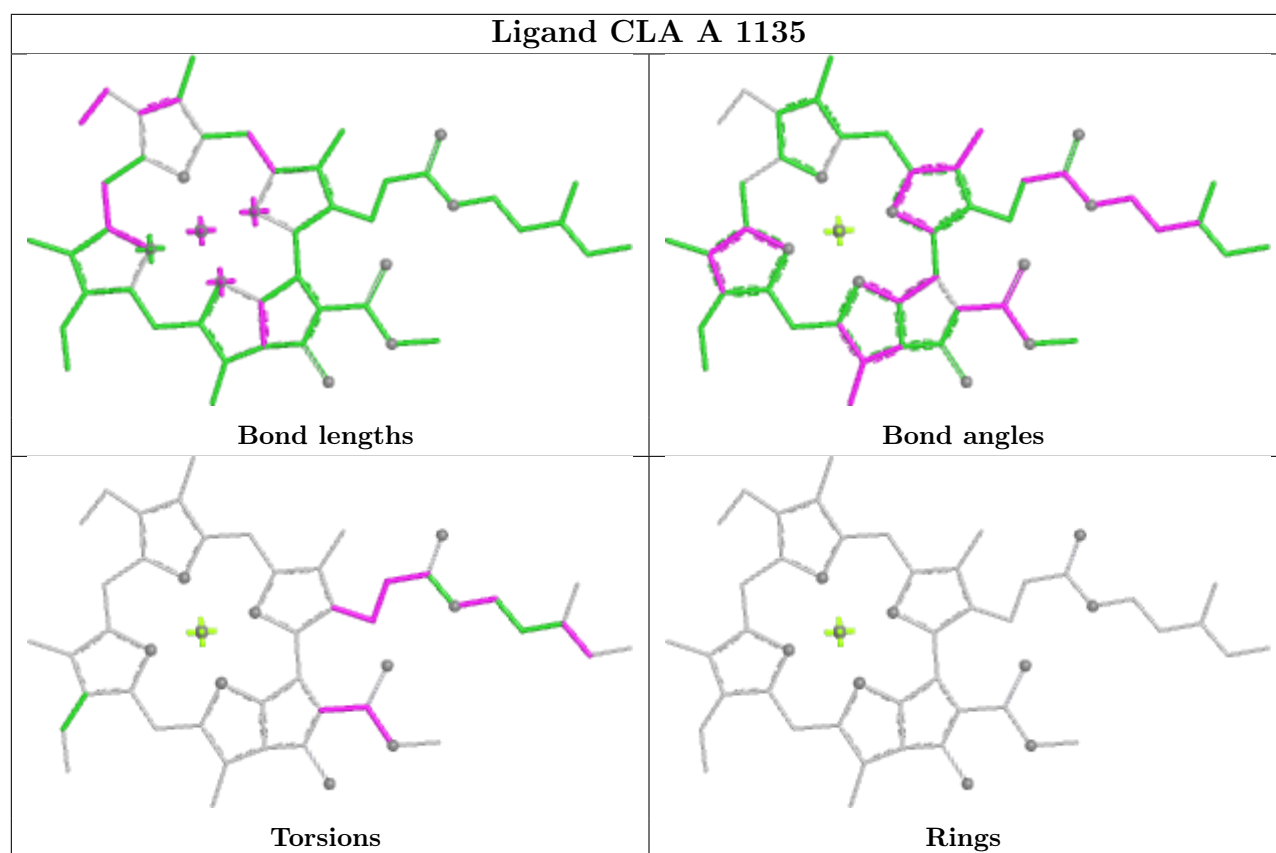


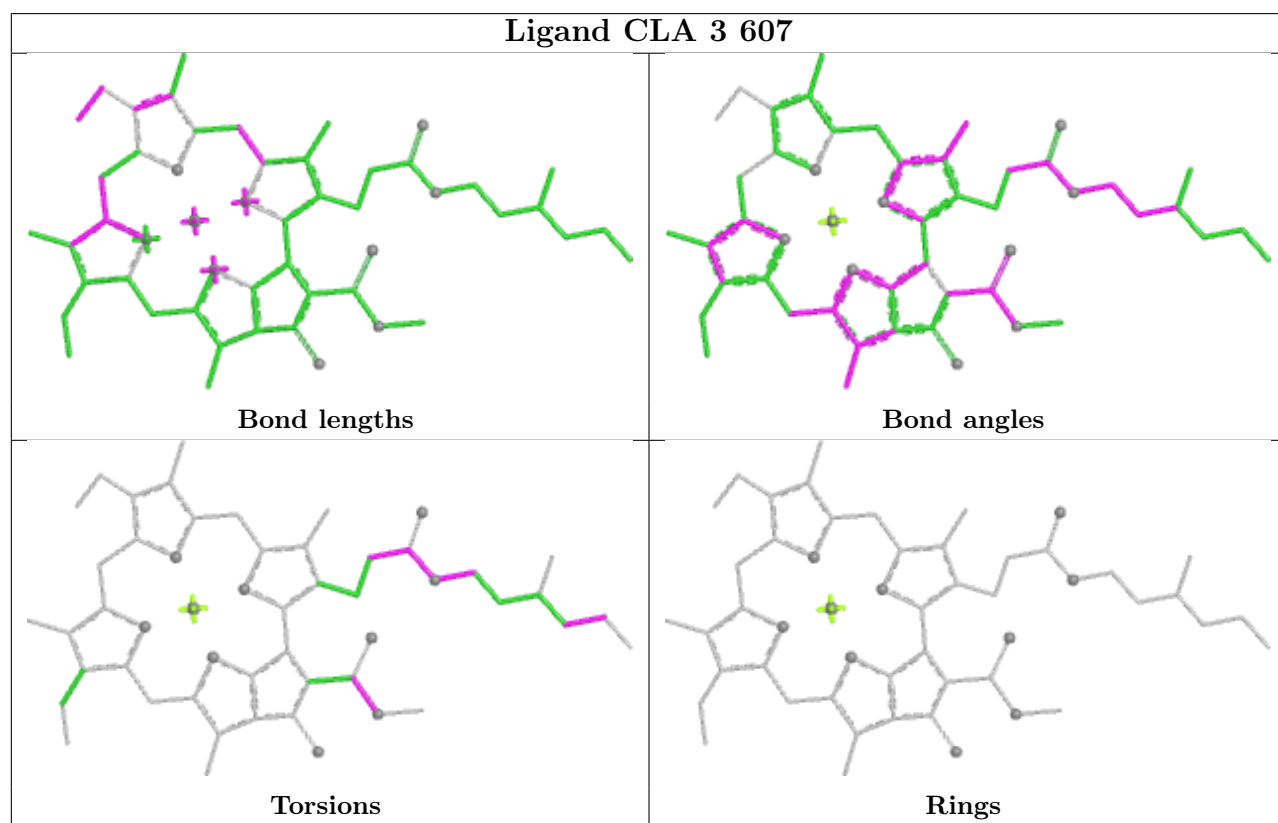
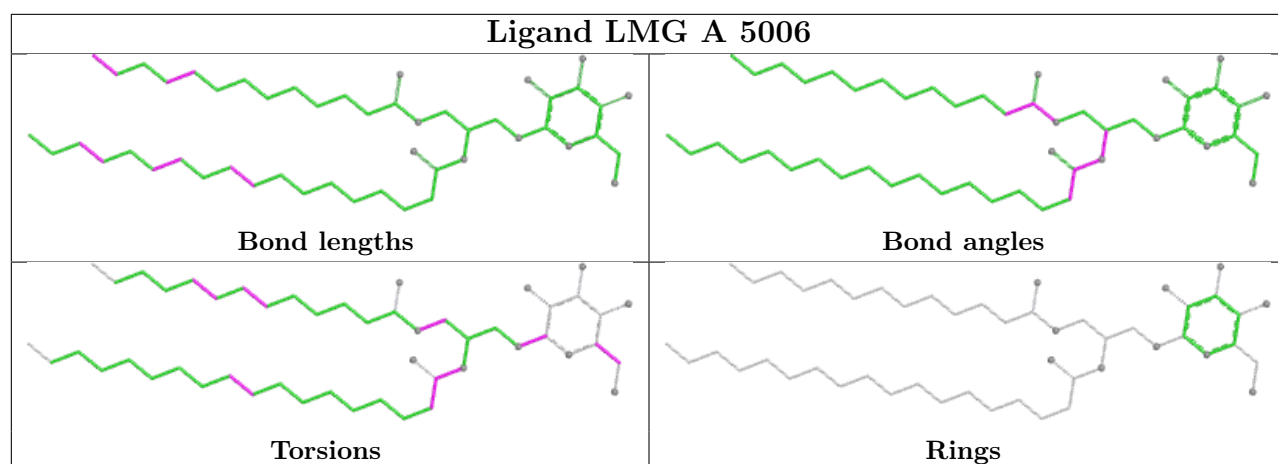


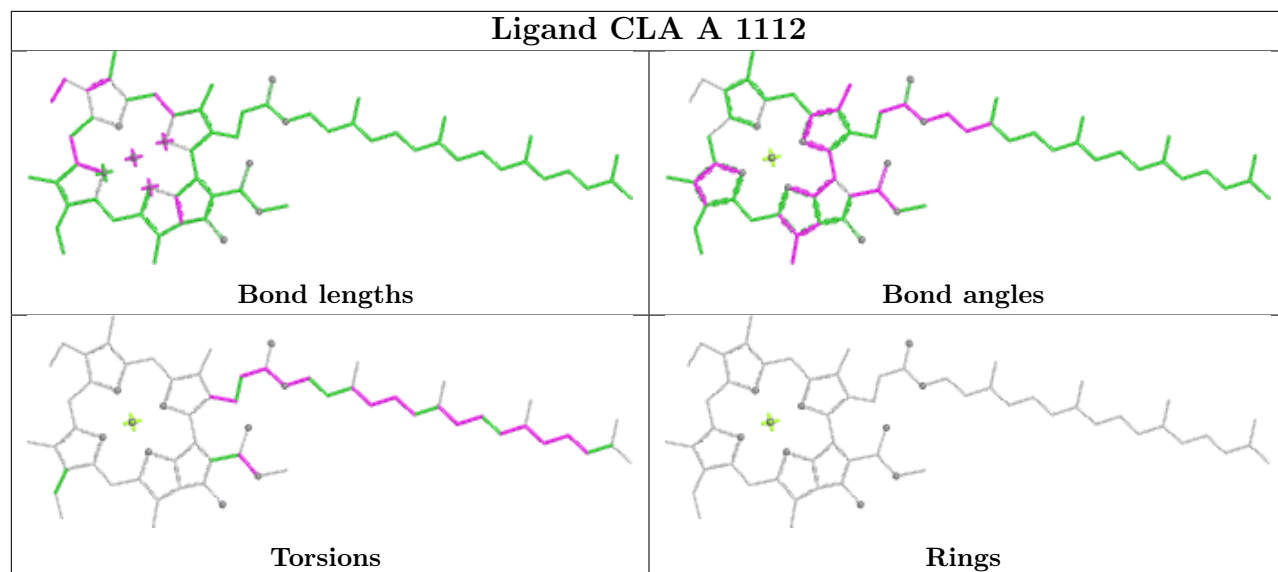
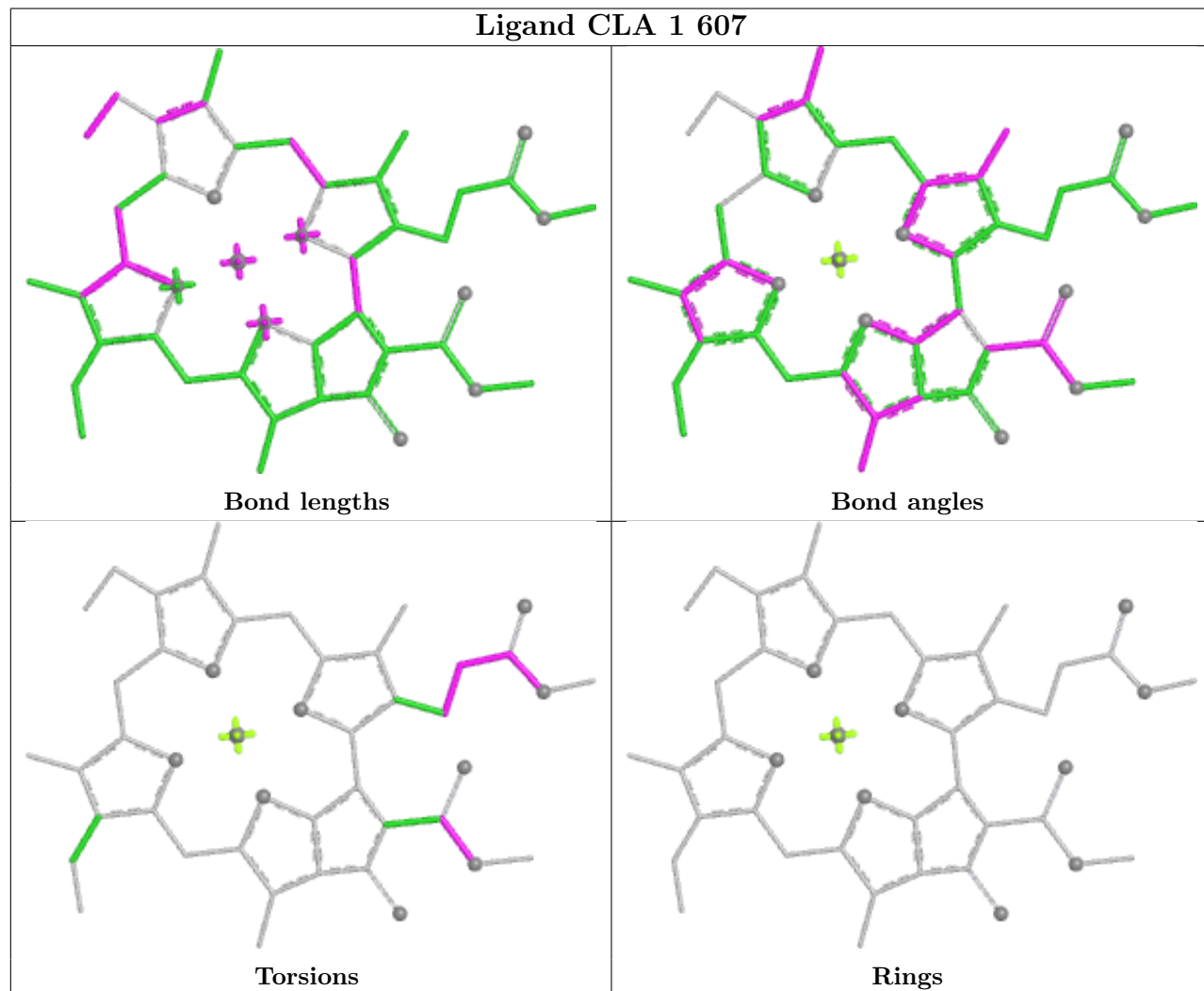


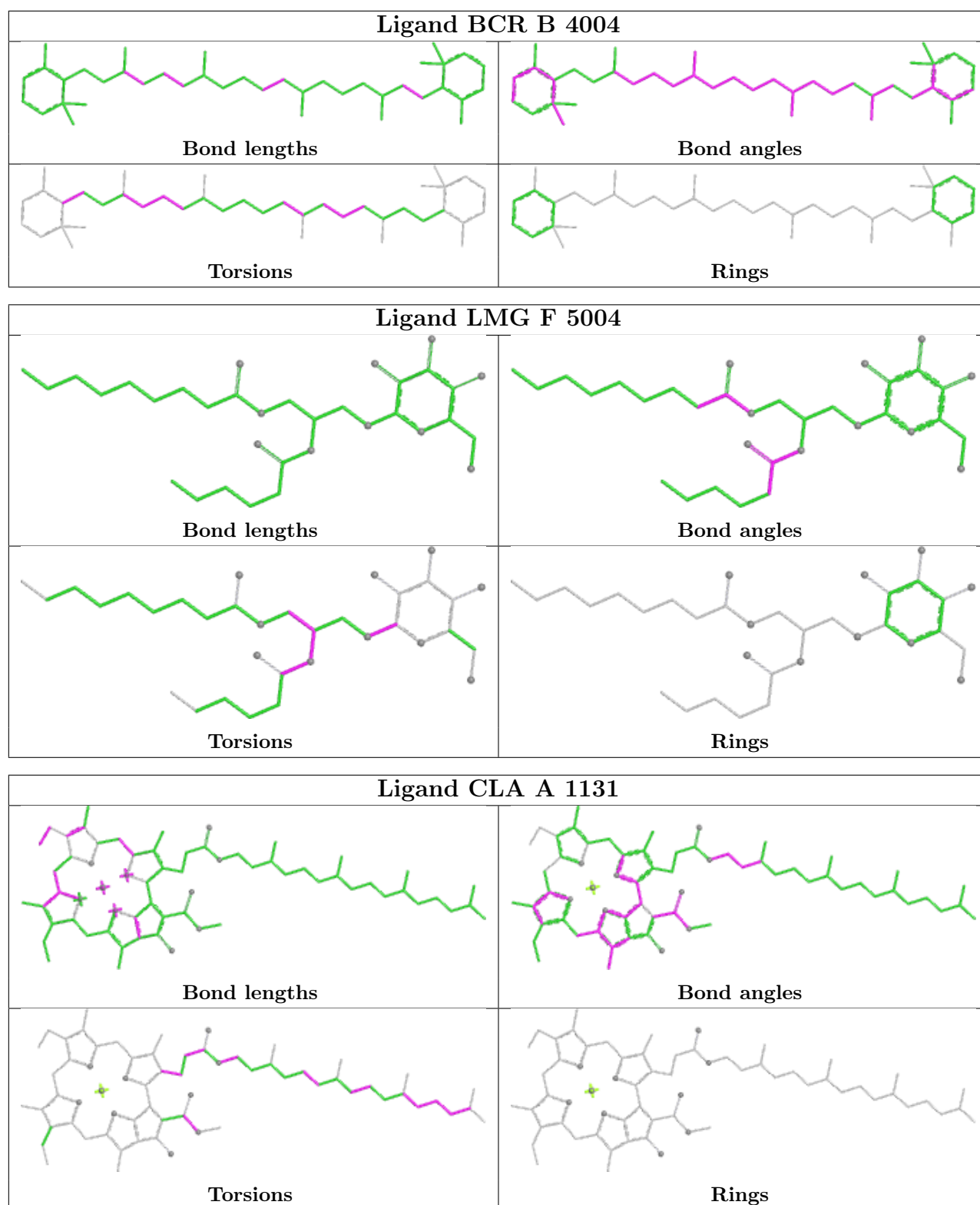


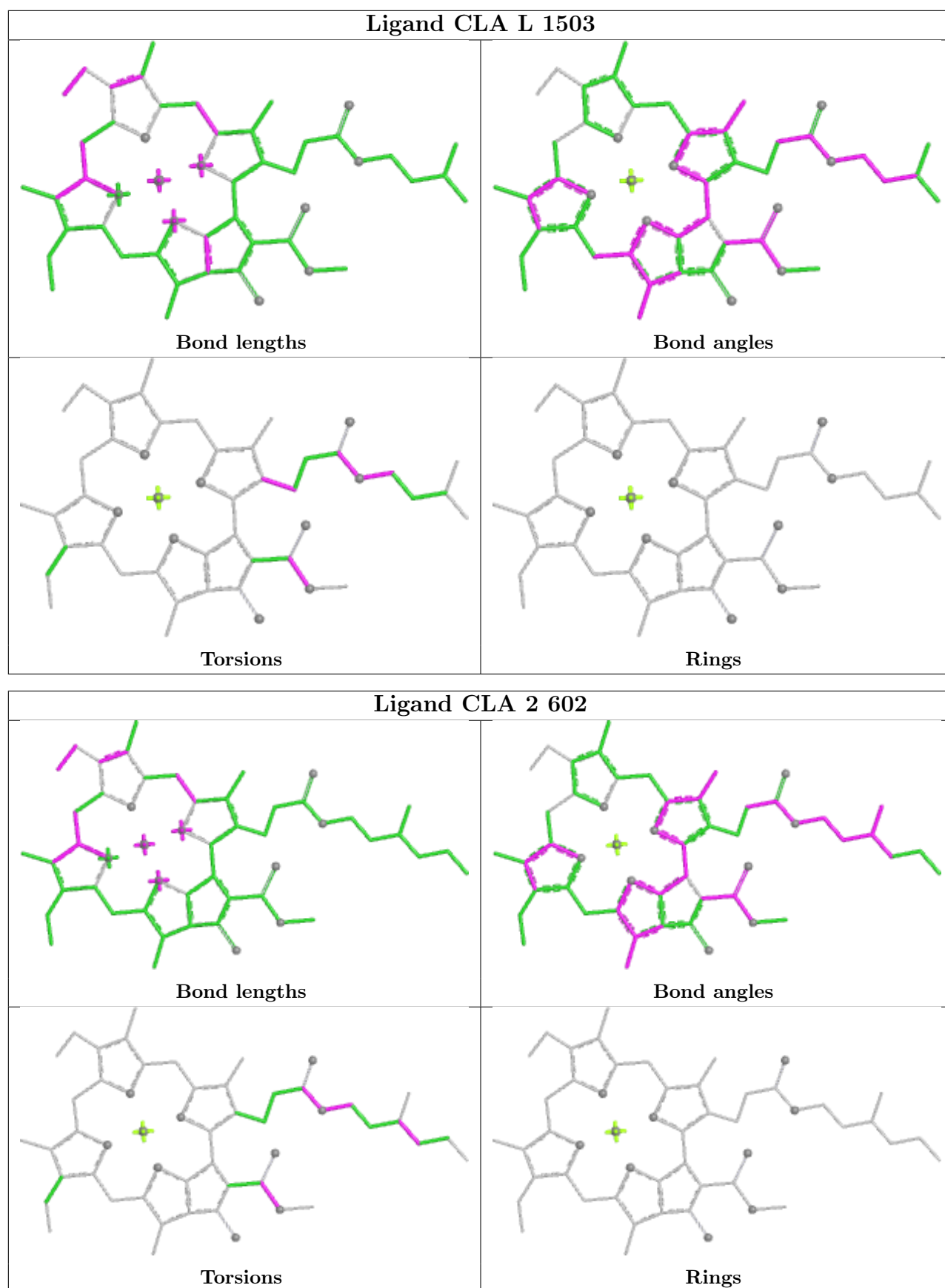


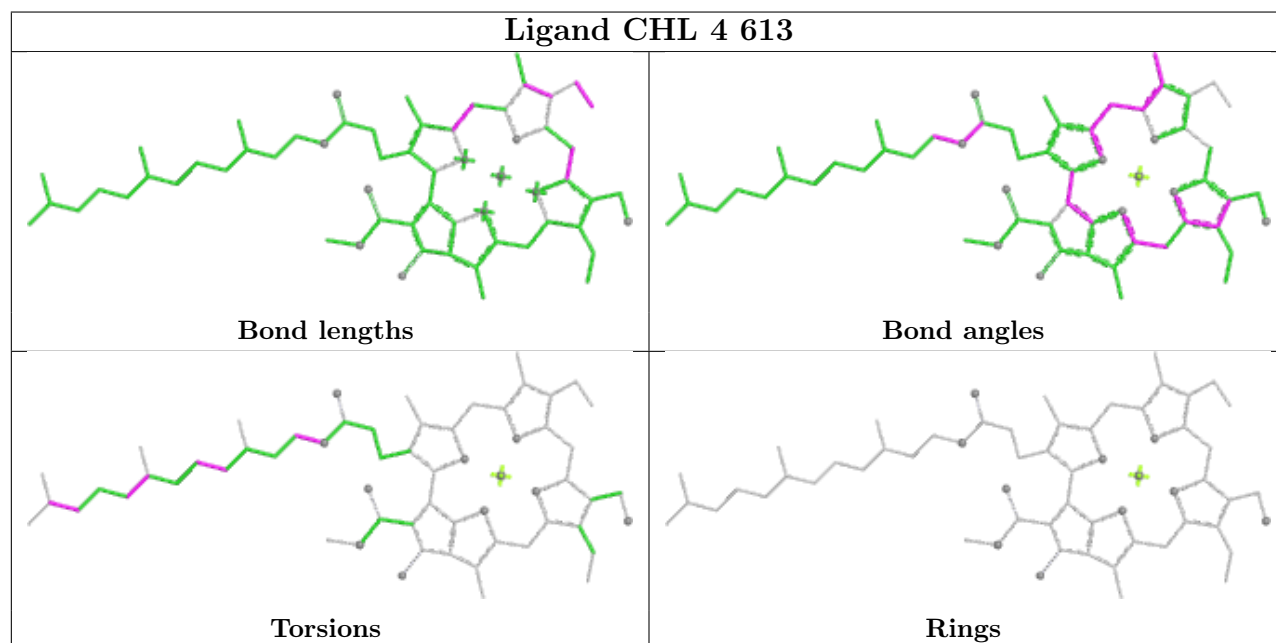
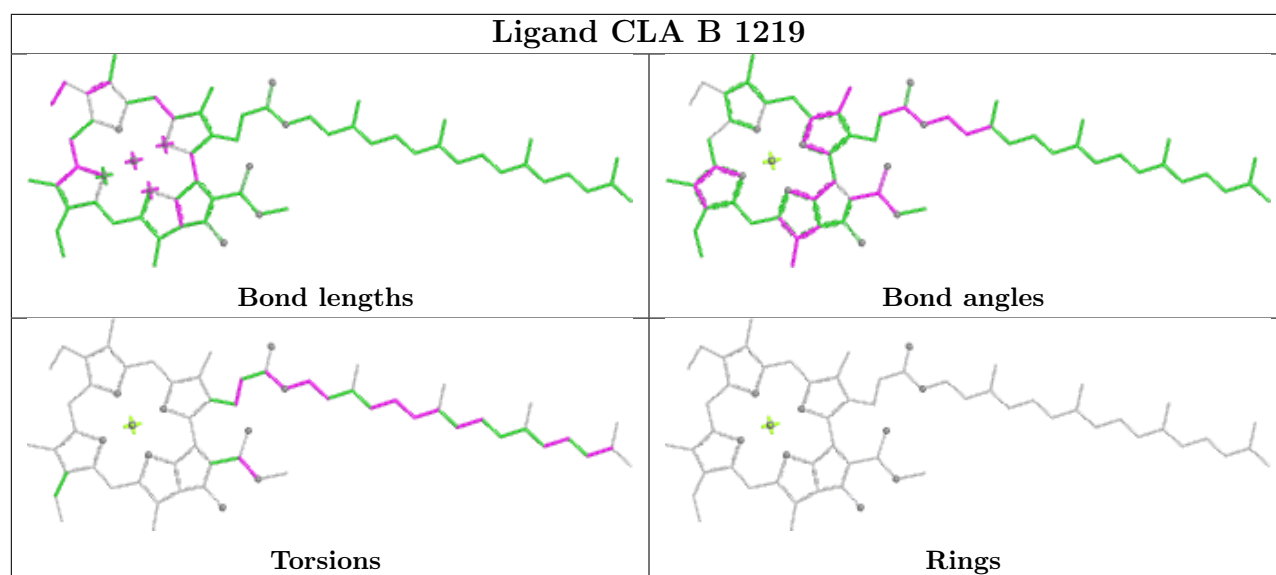


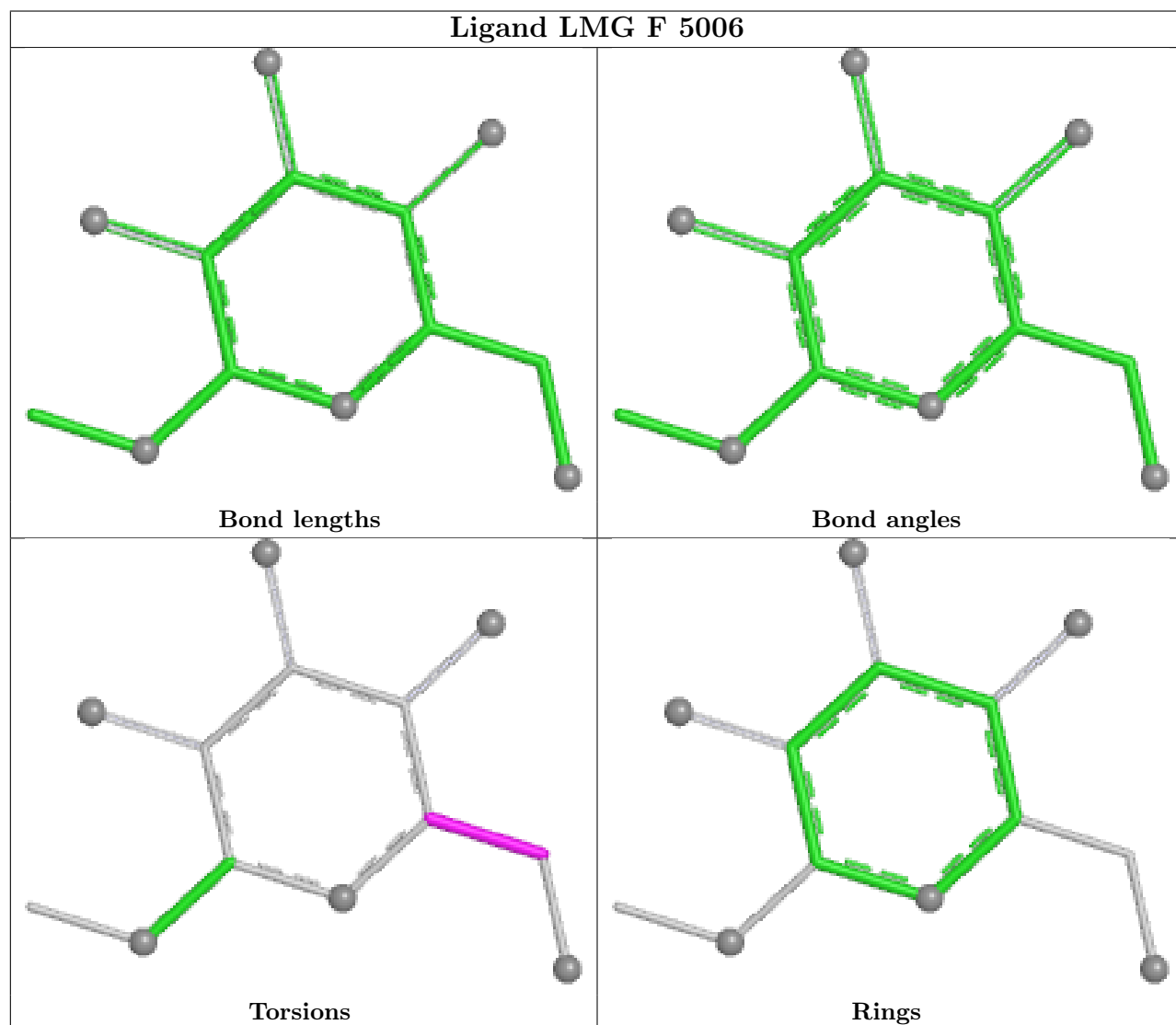
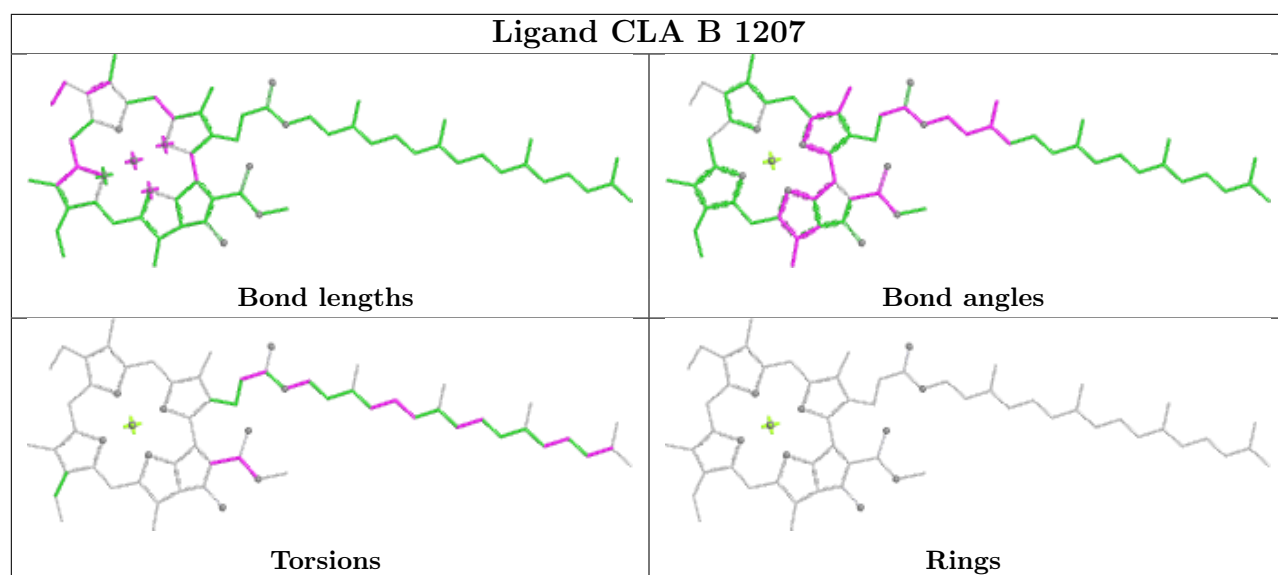


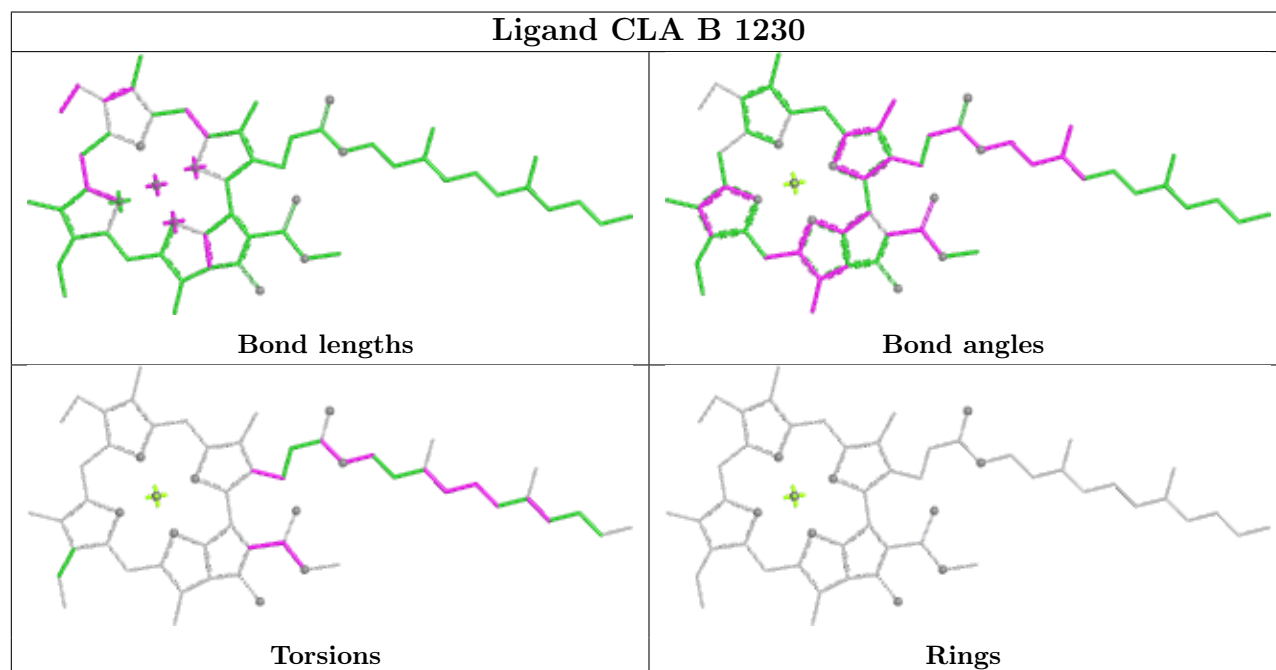
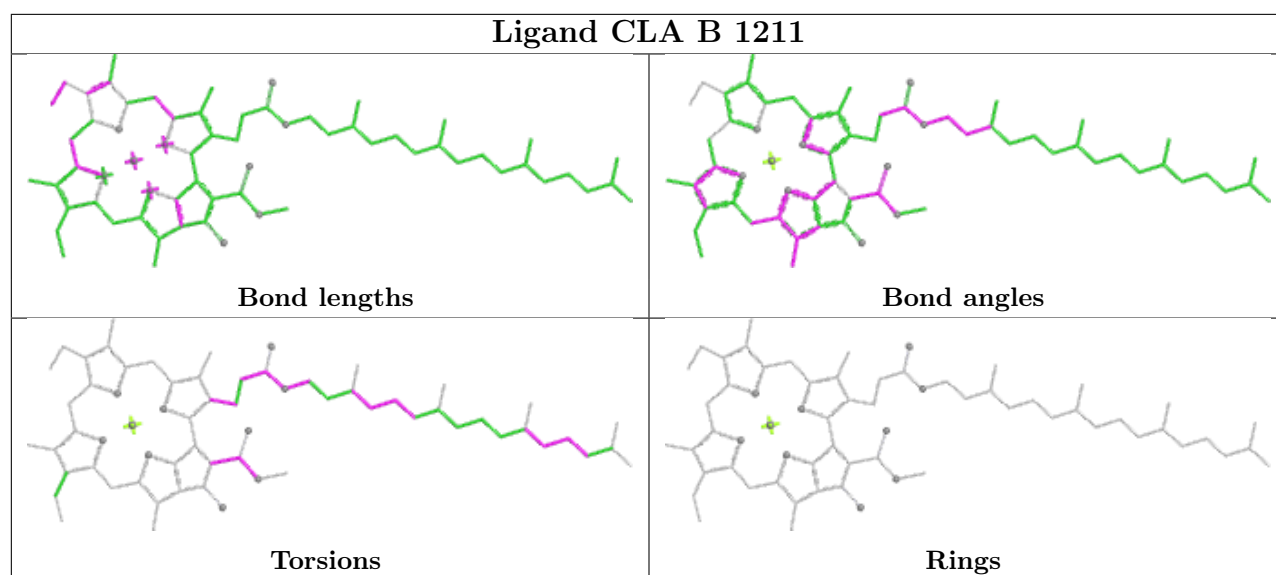
Ligand CLA A 1112**Ligand CLA 1 607**



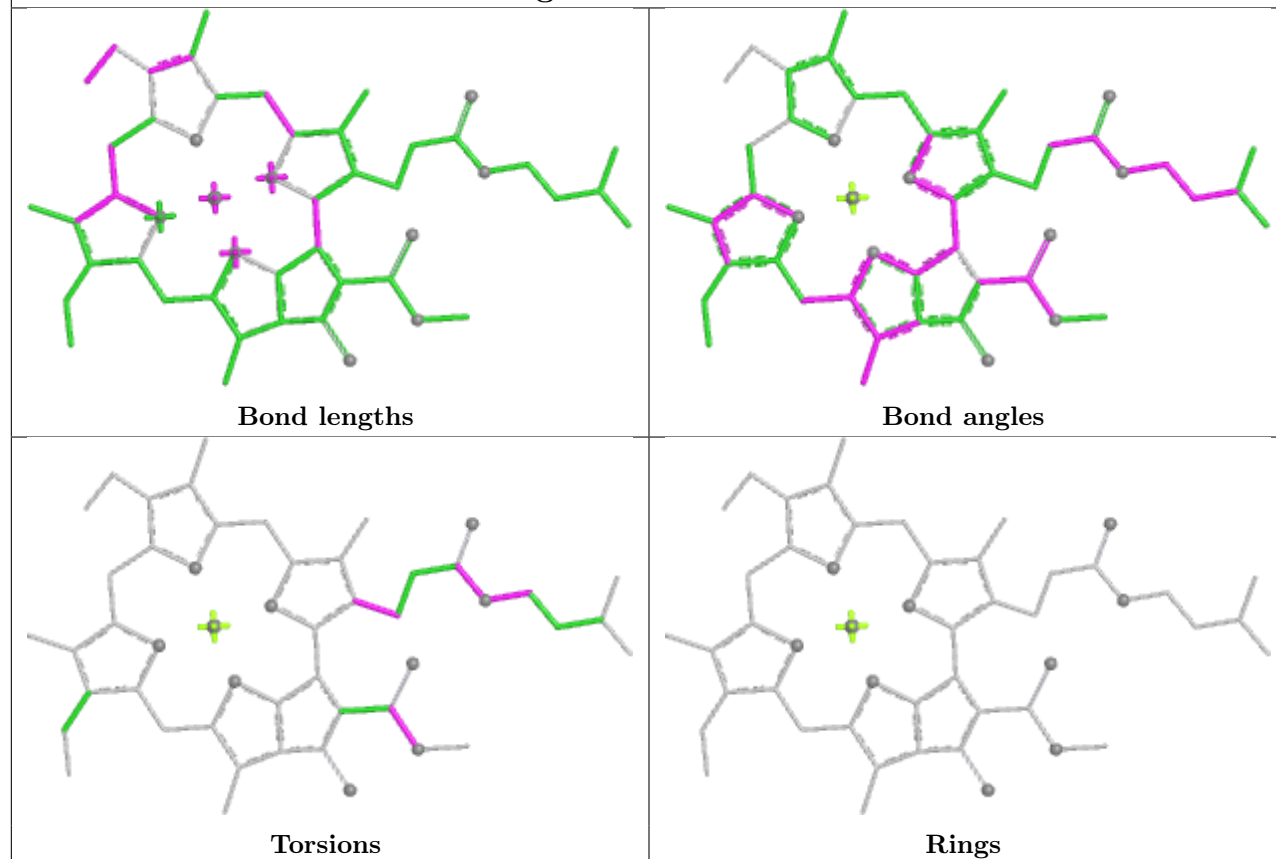




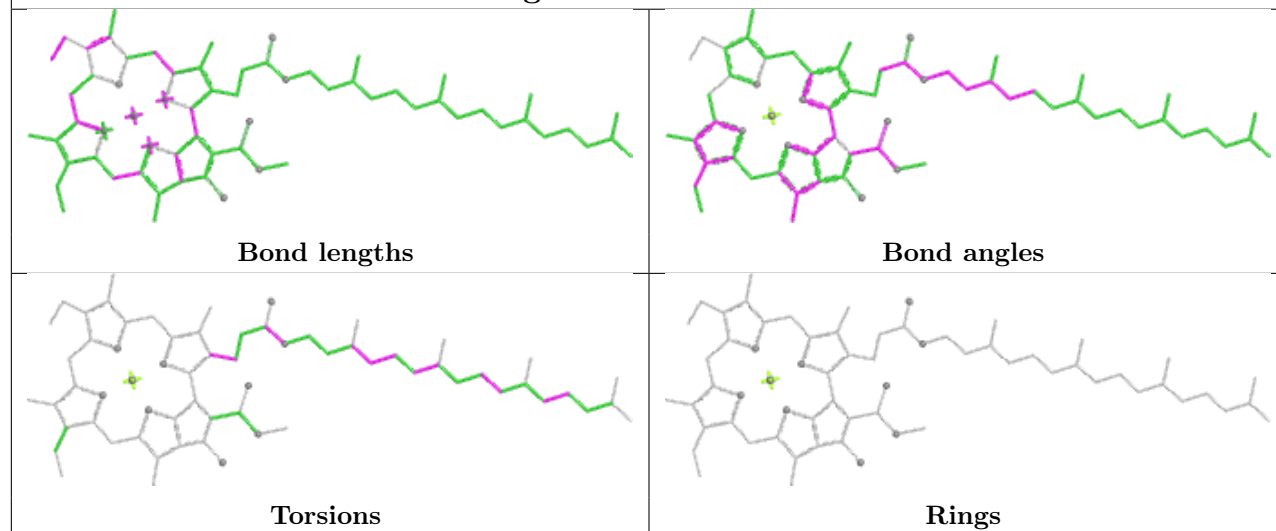


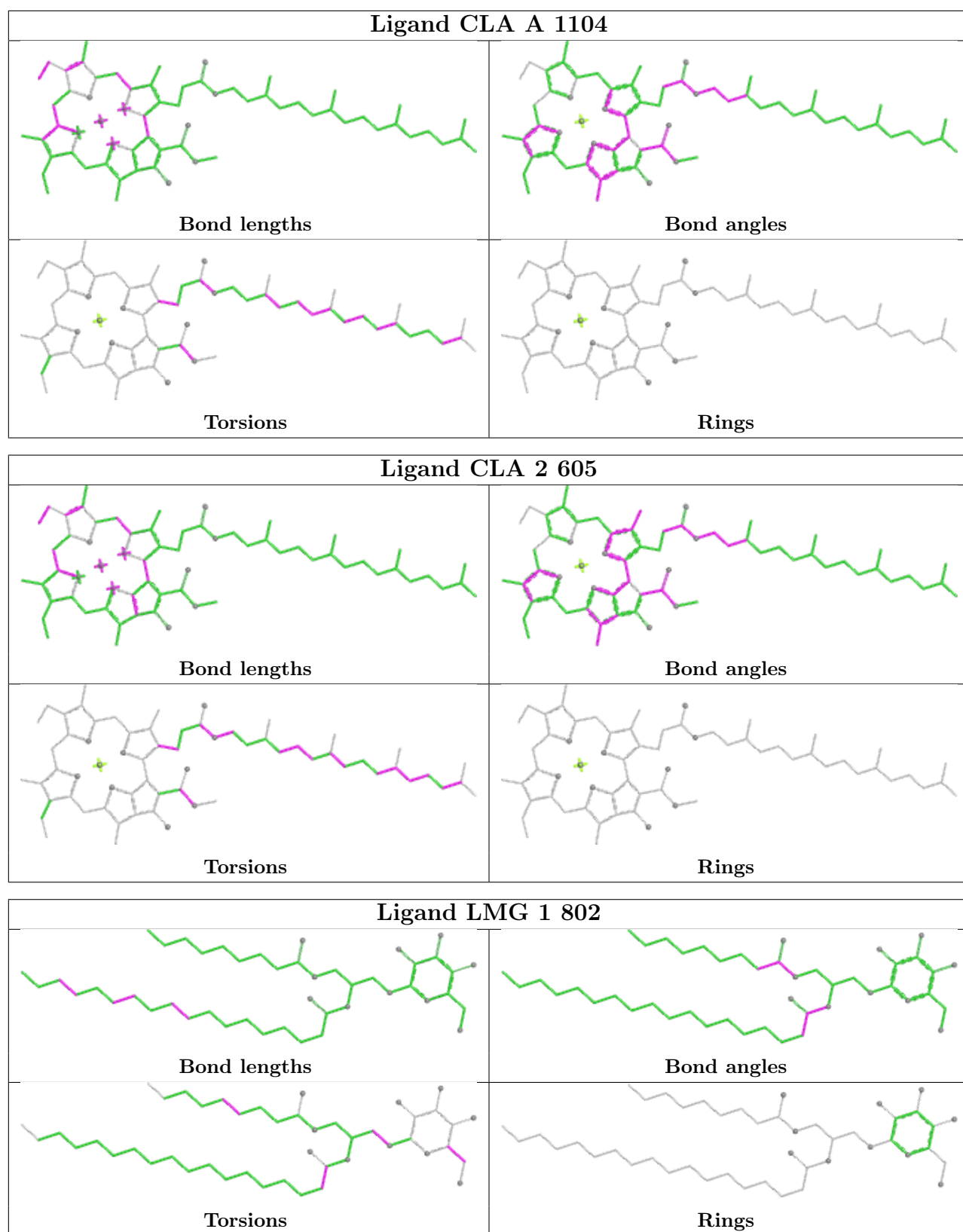


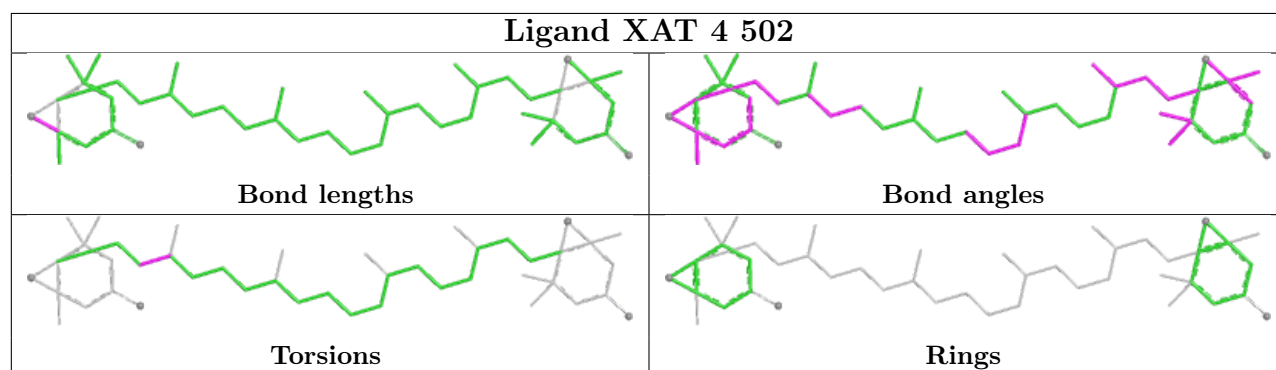
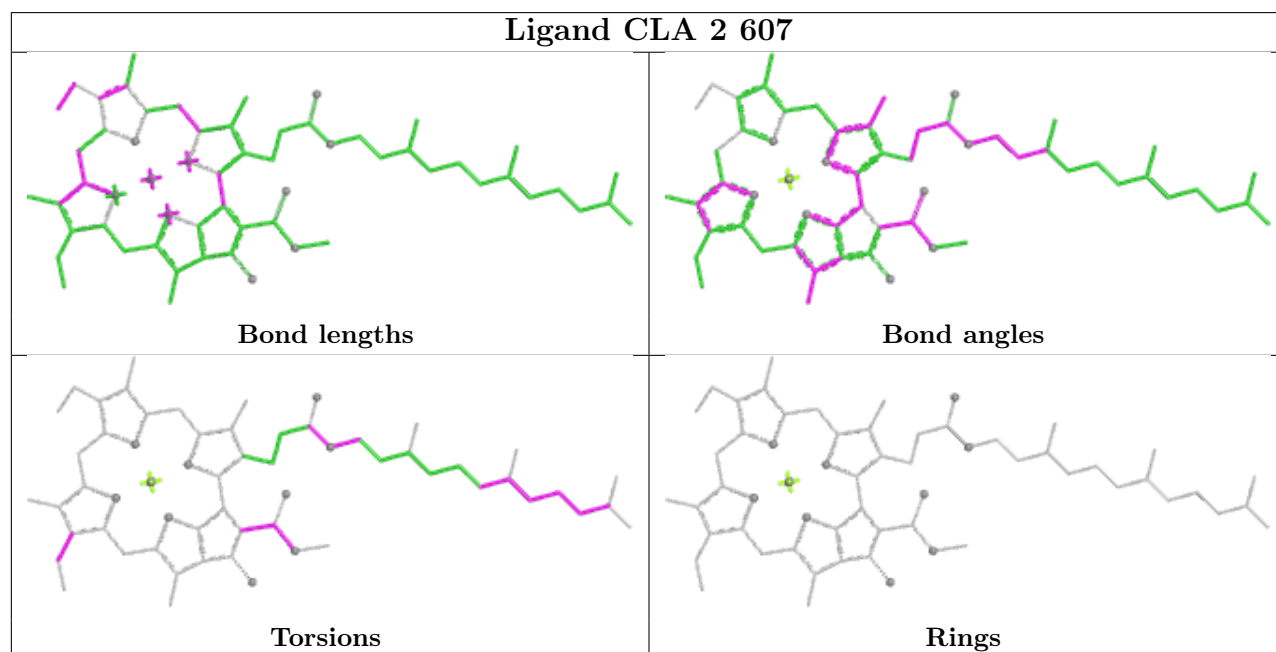
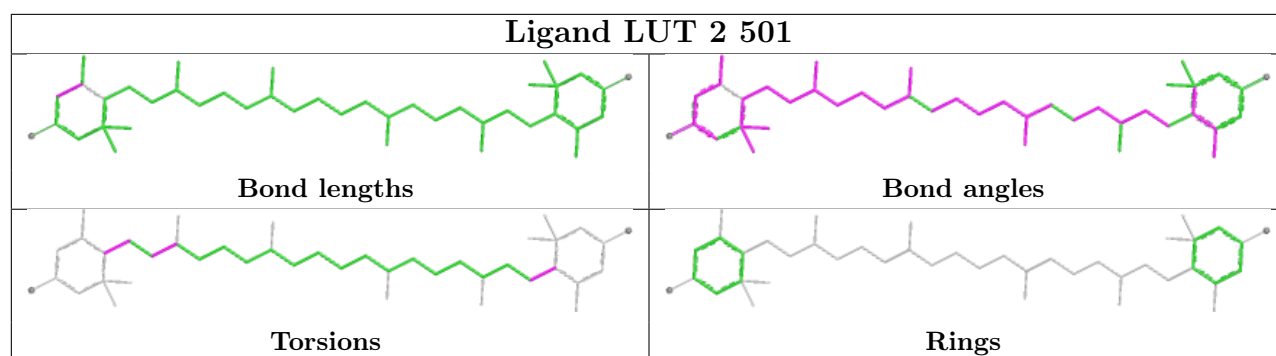
Ligand CLA 3 612

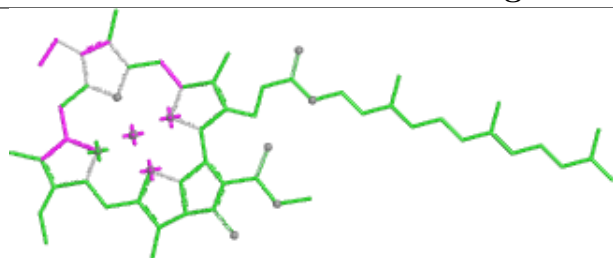


Ligand CLA B 1210

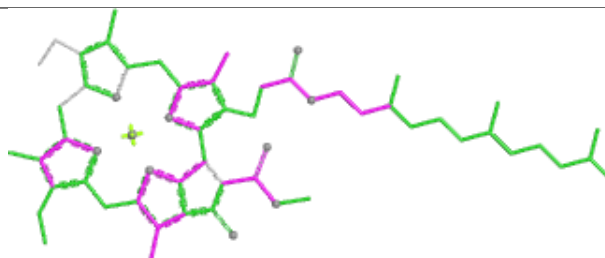




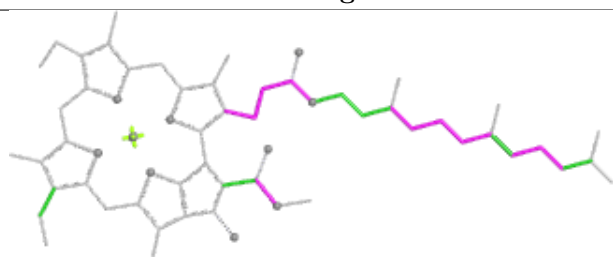


Ligand CLA K 1402

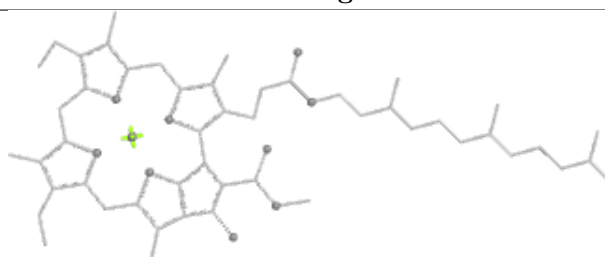
Bond lengths



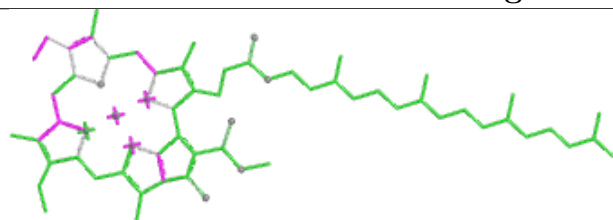
Bond angles



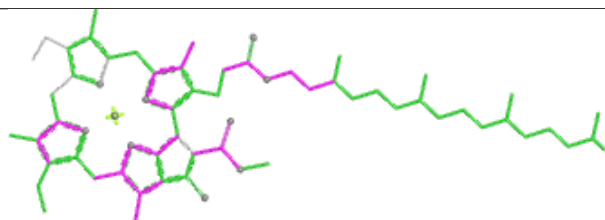
Torsions



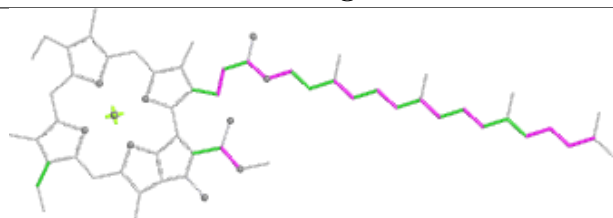
Rings

Ligand CLA A 1122

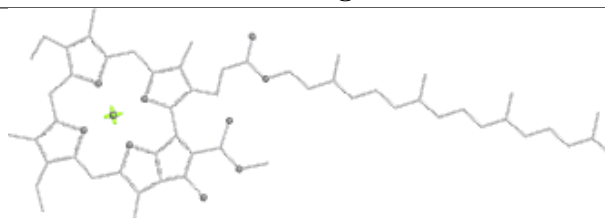
Bond lengths



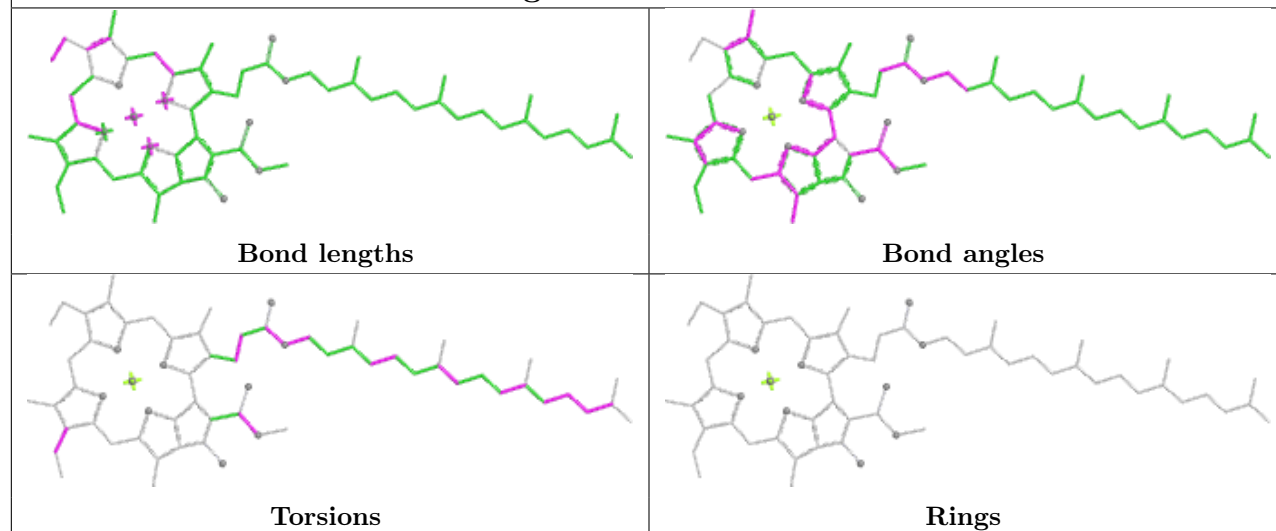
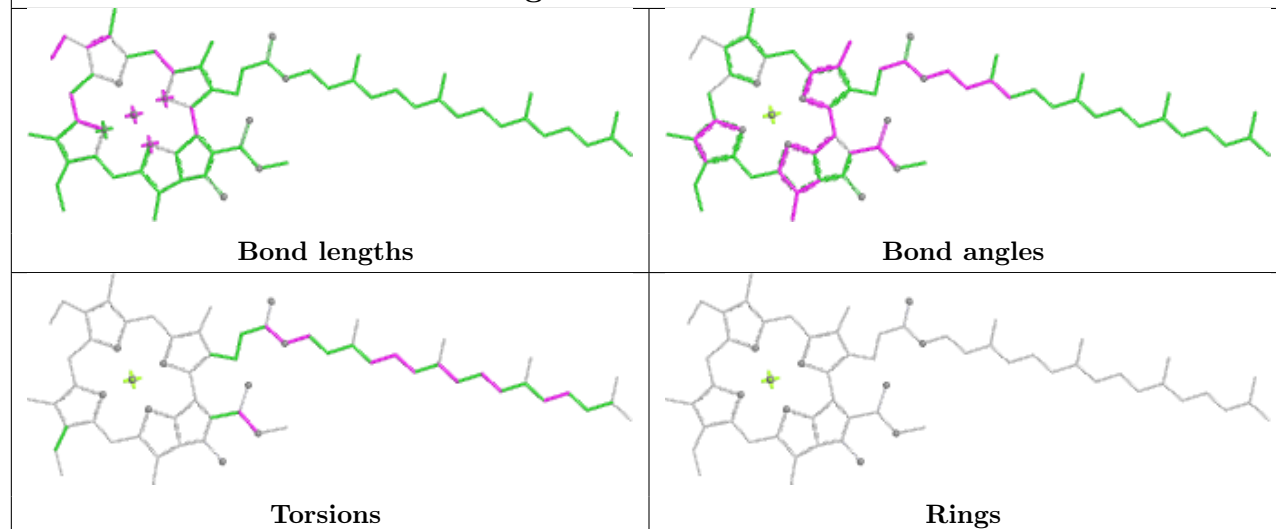
Bond angles

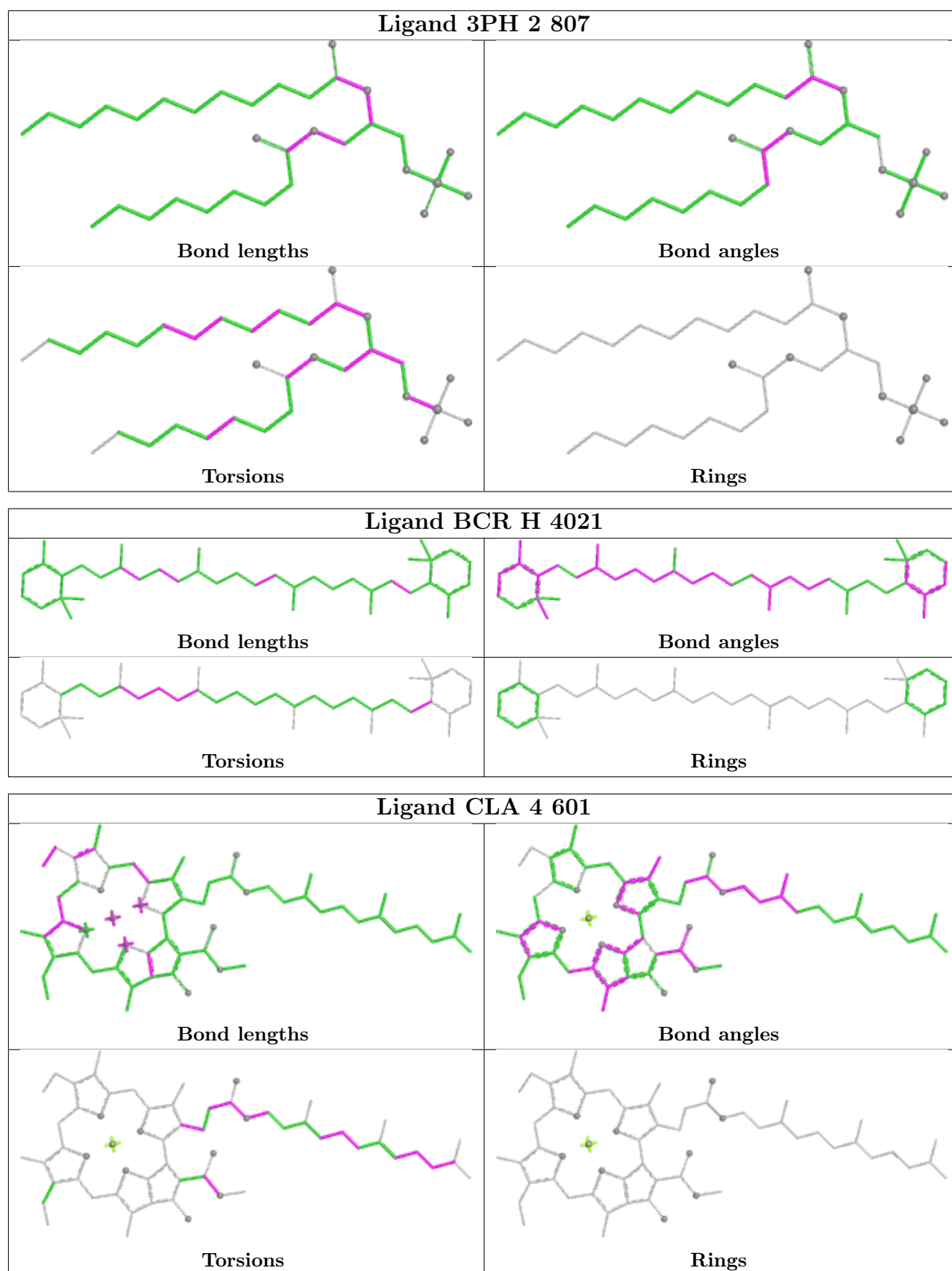


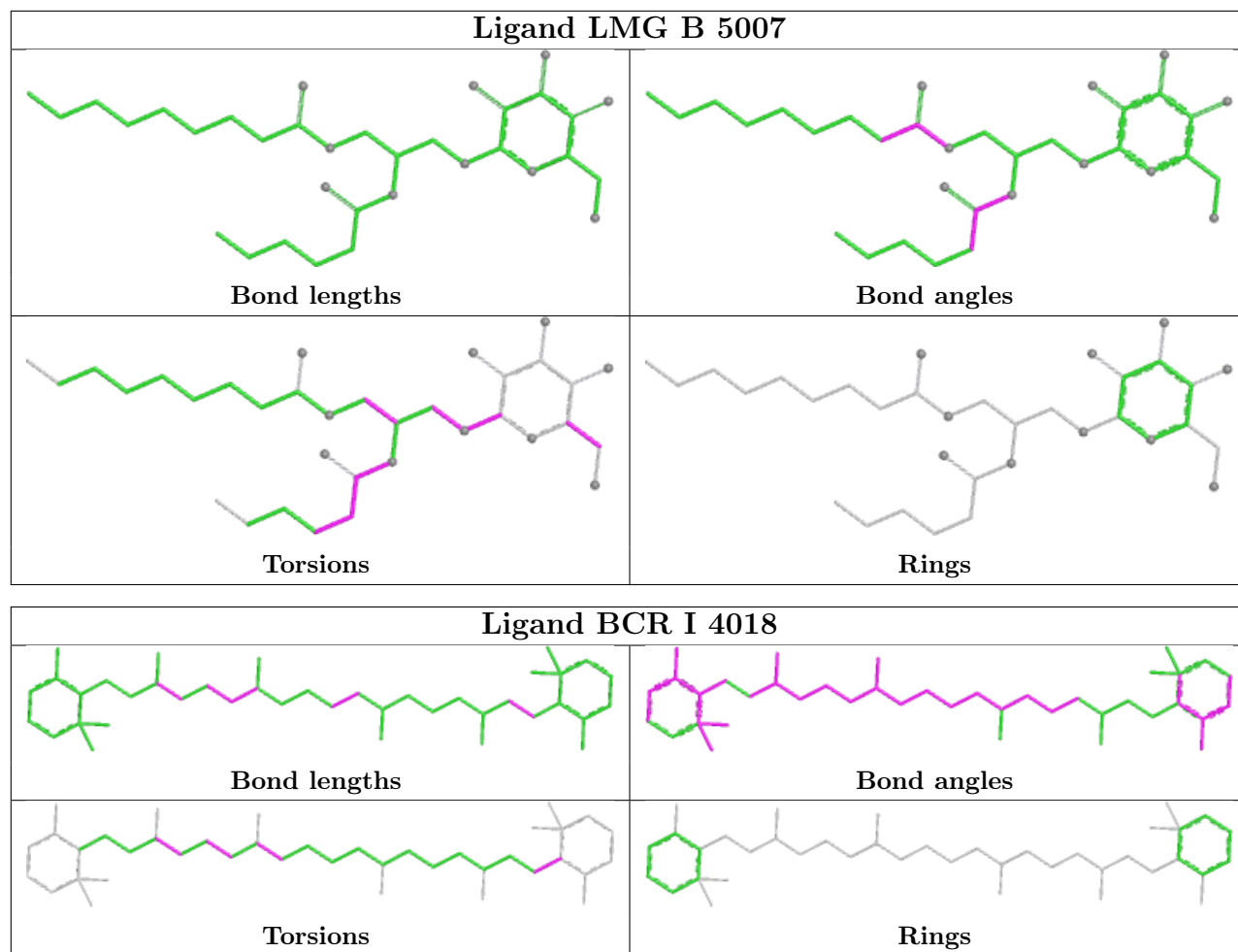
Torsions



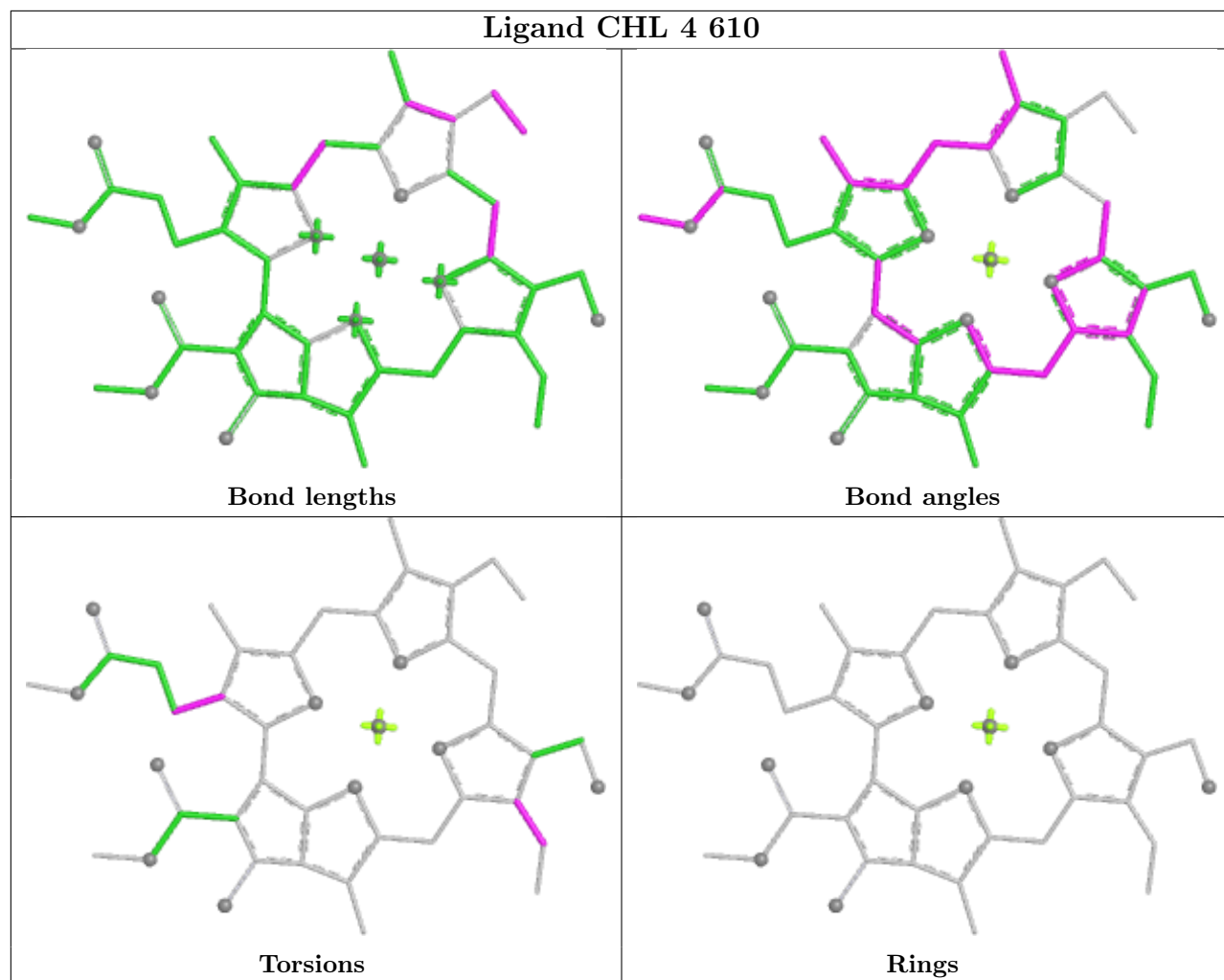
Rings

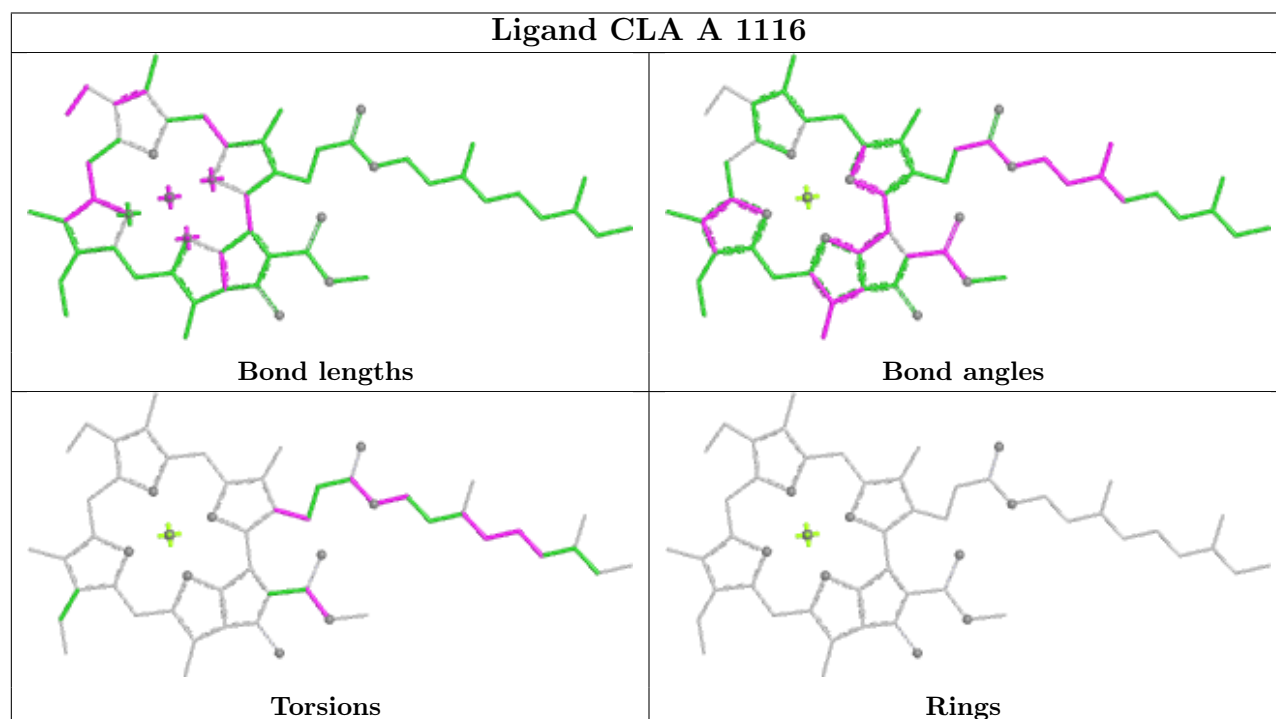
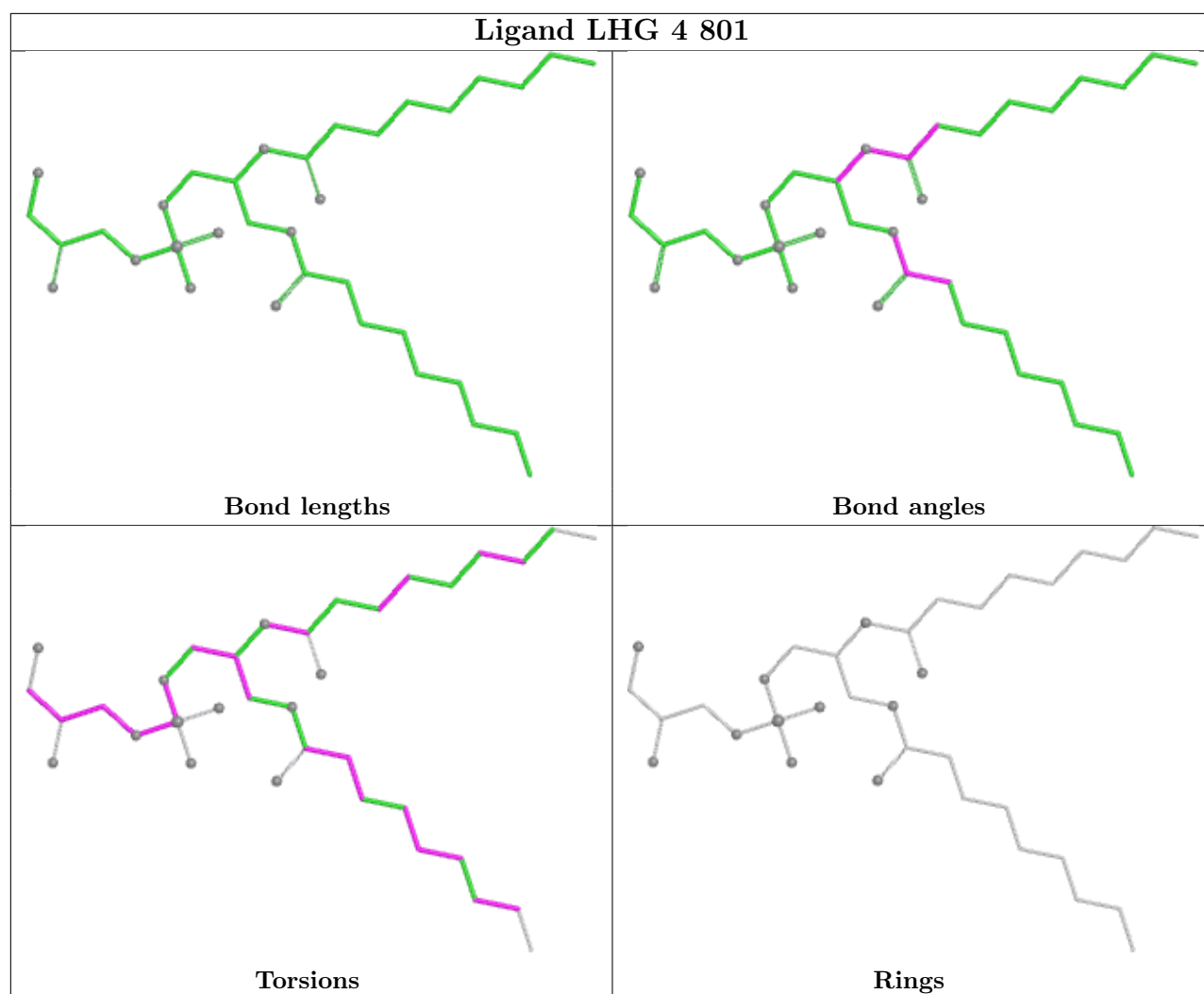
Ligand CLA B 1023**Ligand CLA F 1302**

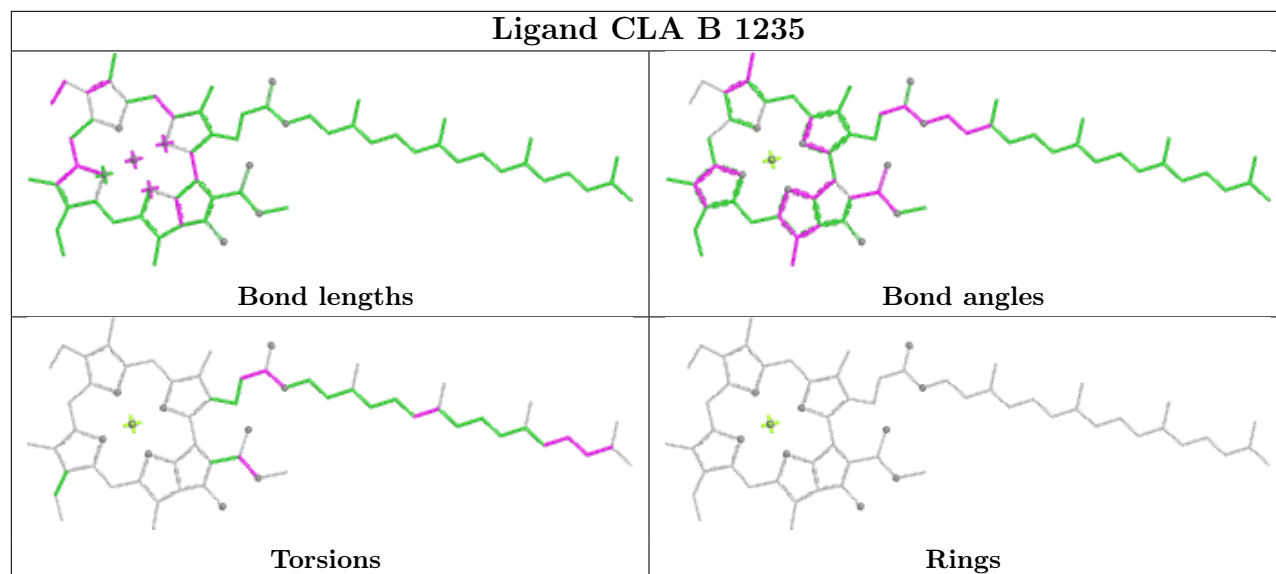
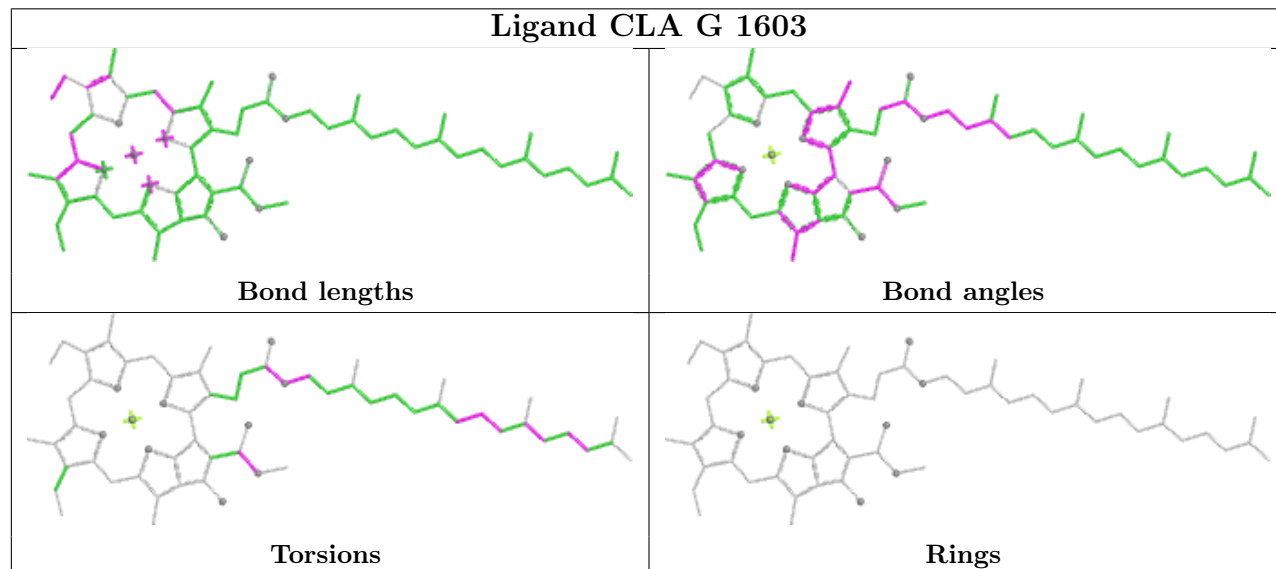


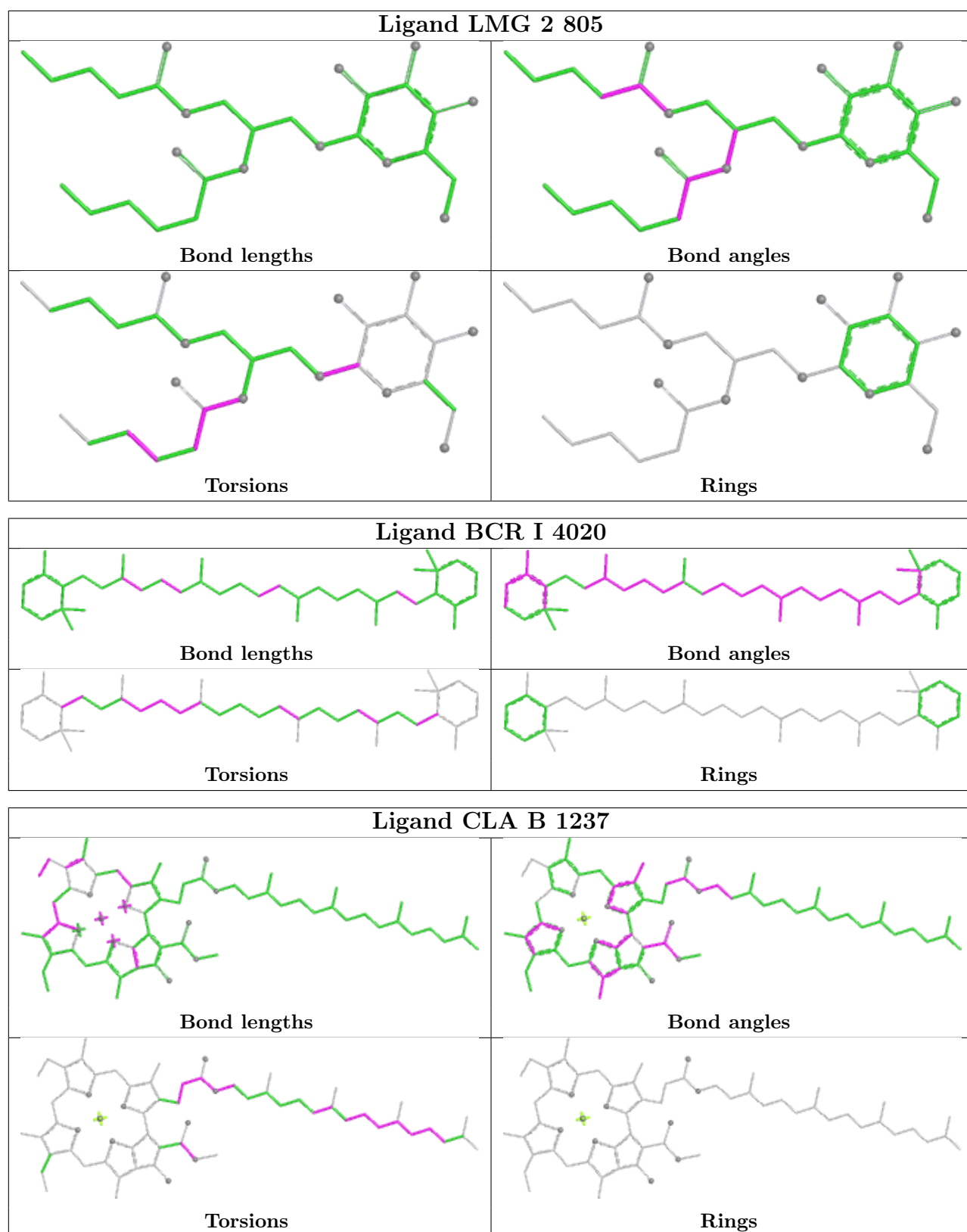


Ligand CHL 4 610

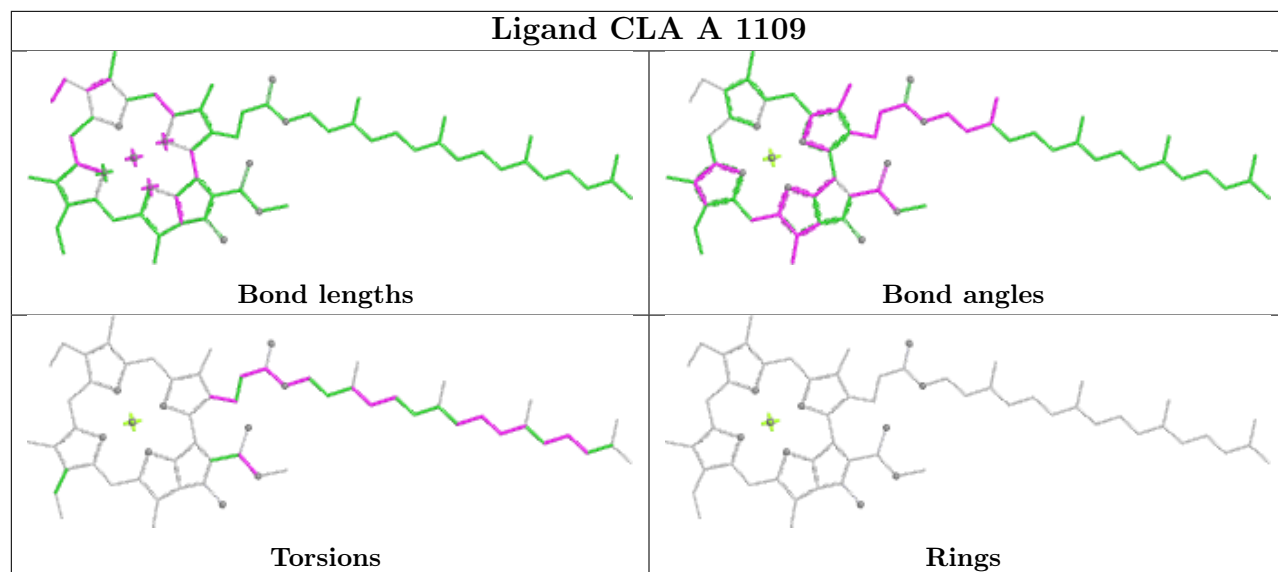




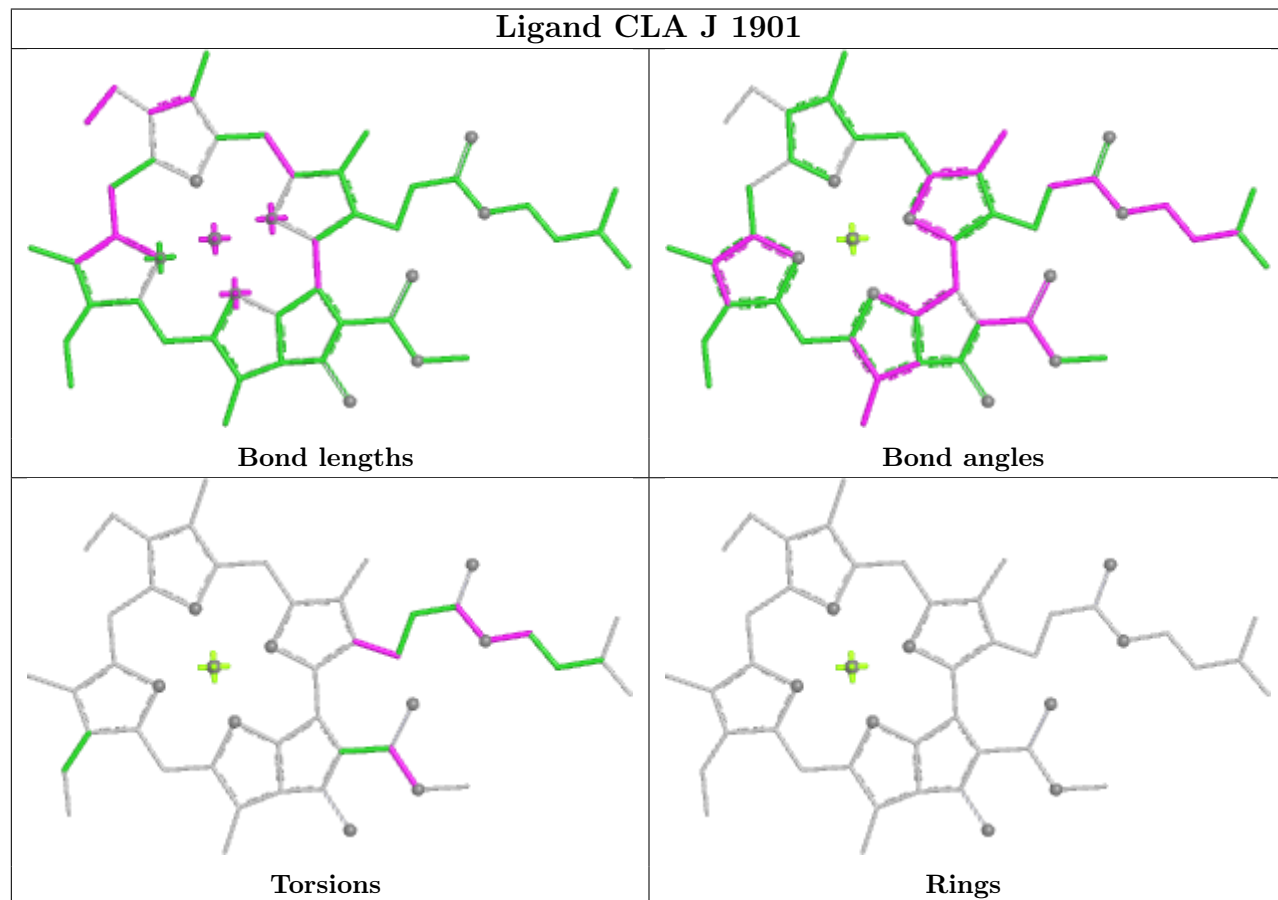
Ligand CLA B 1235**Ligand CLA G 1603**

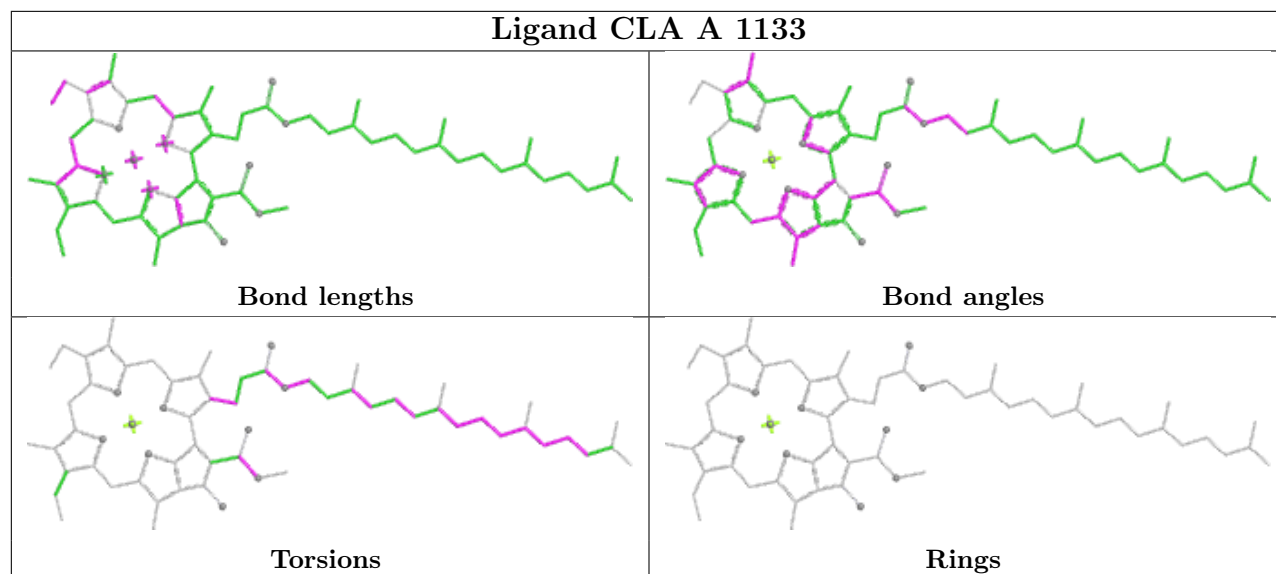
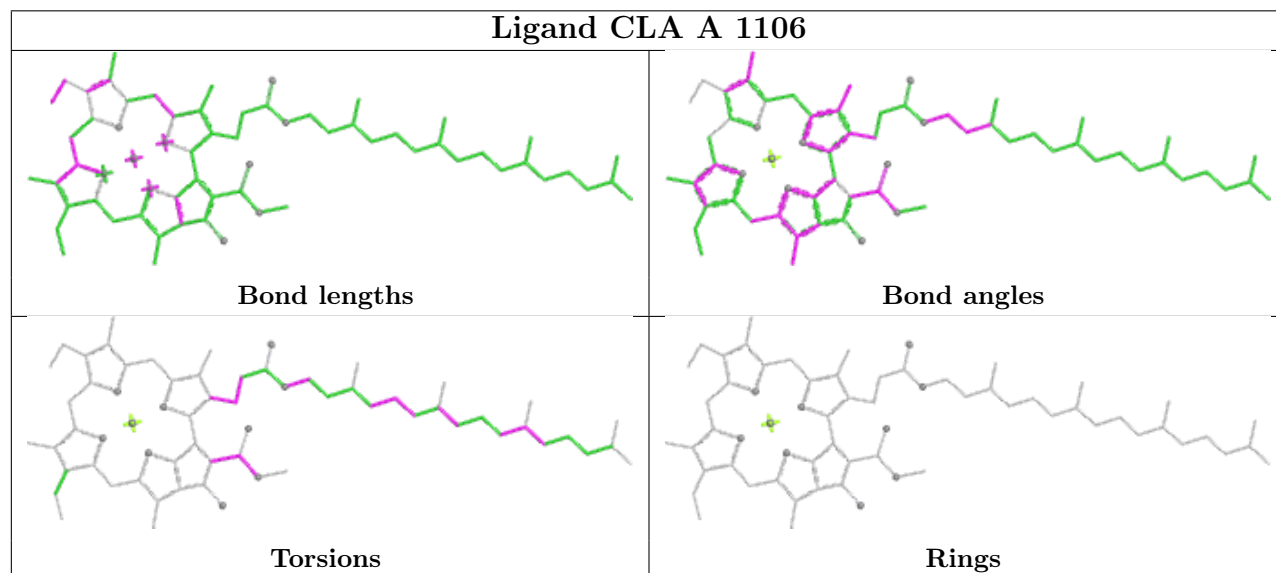


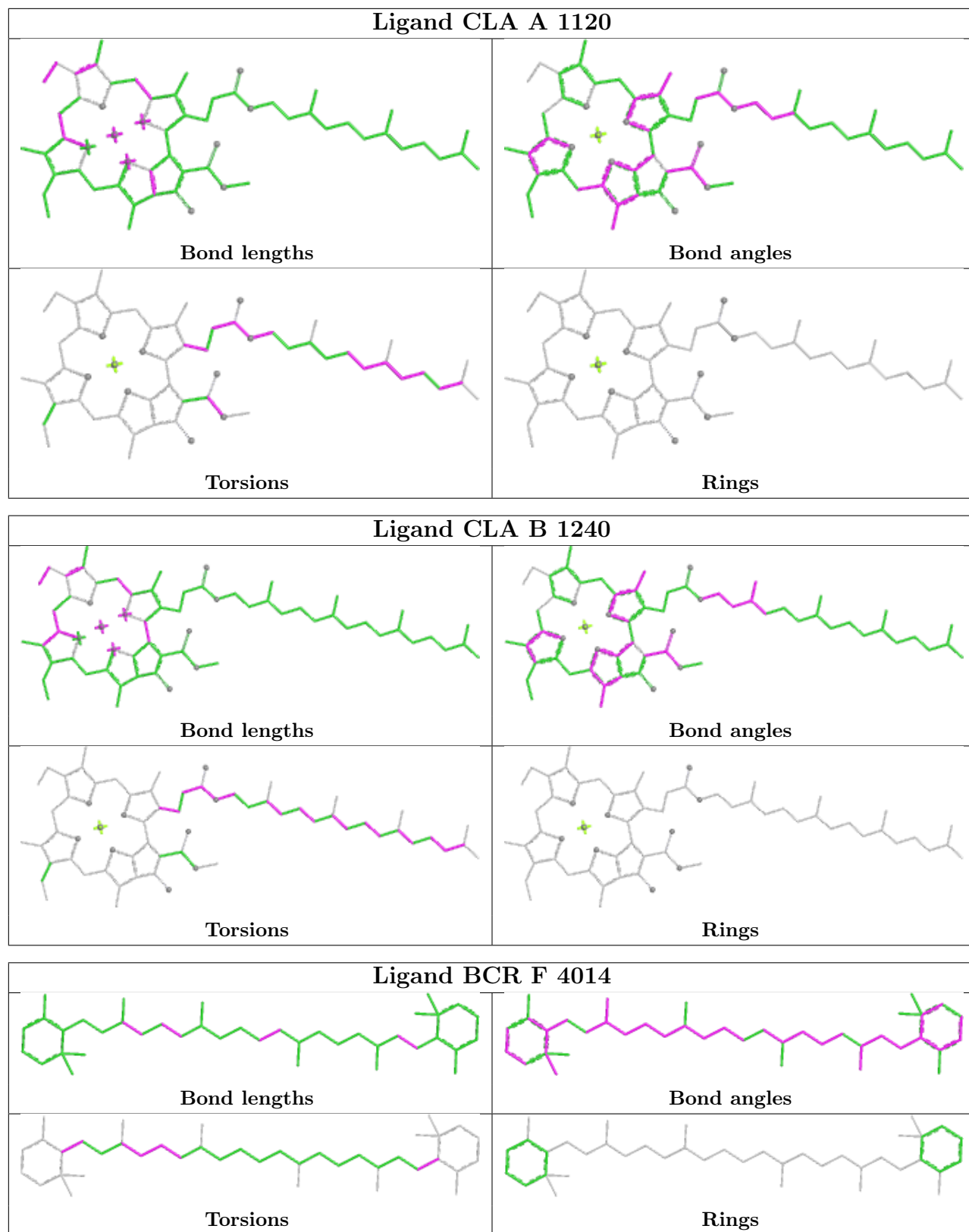
Ligand CLA A 1109

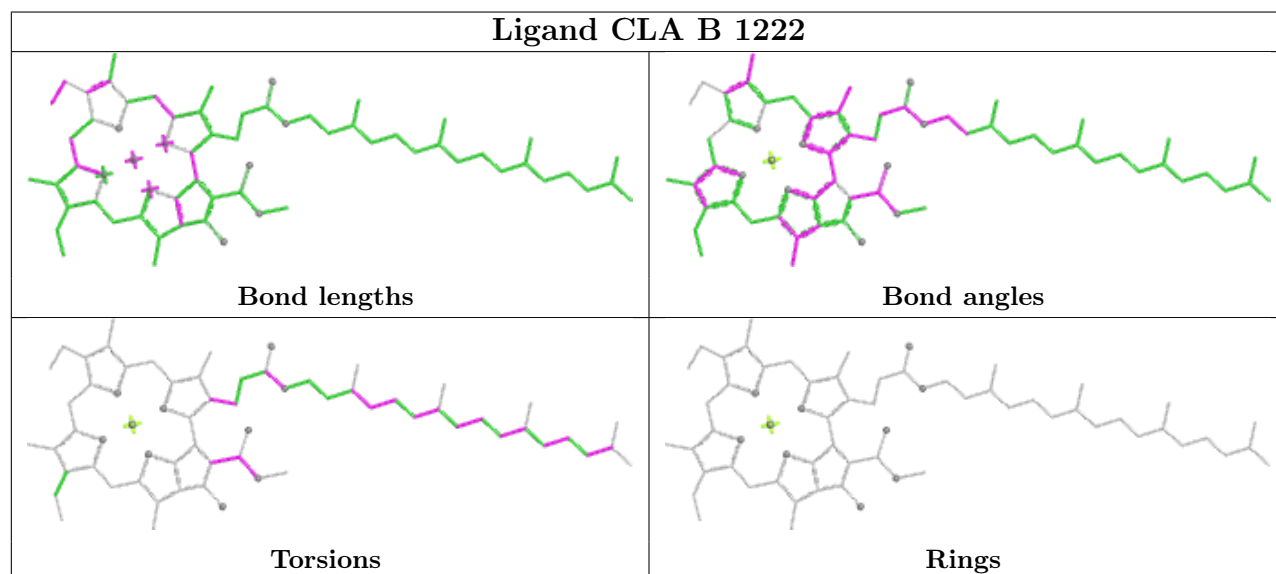
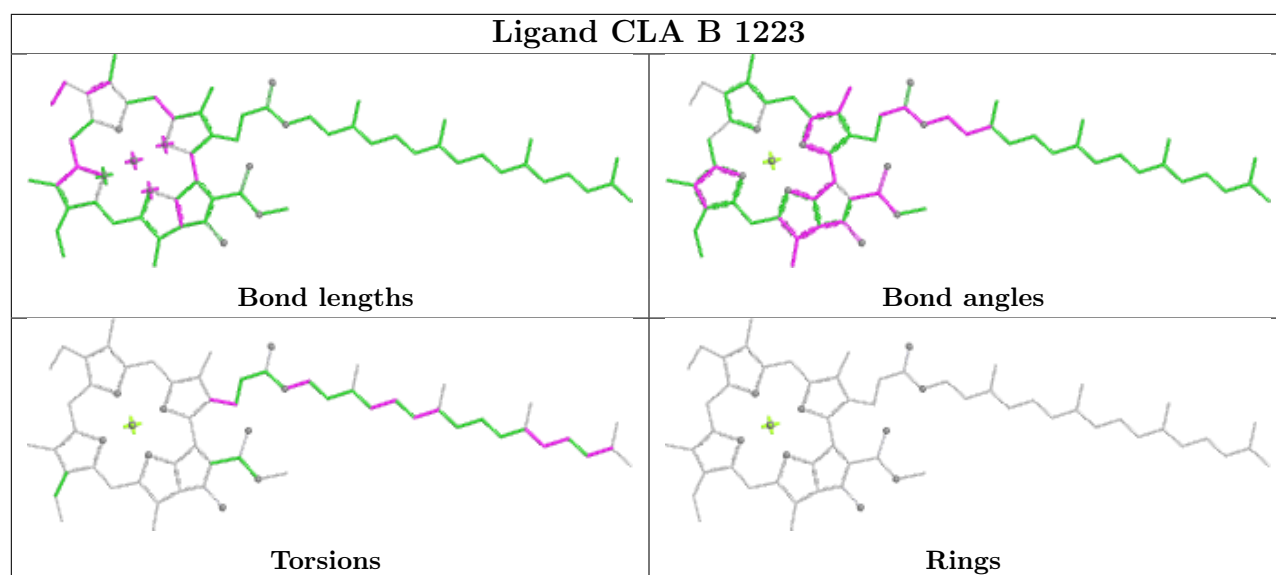


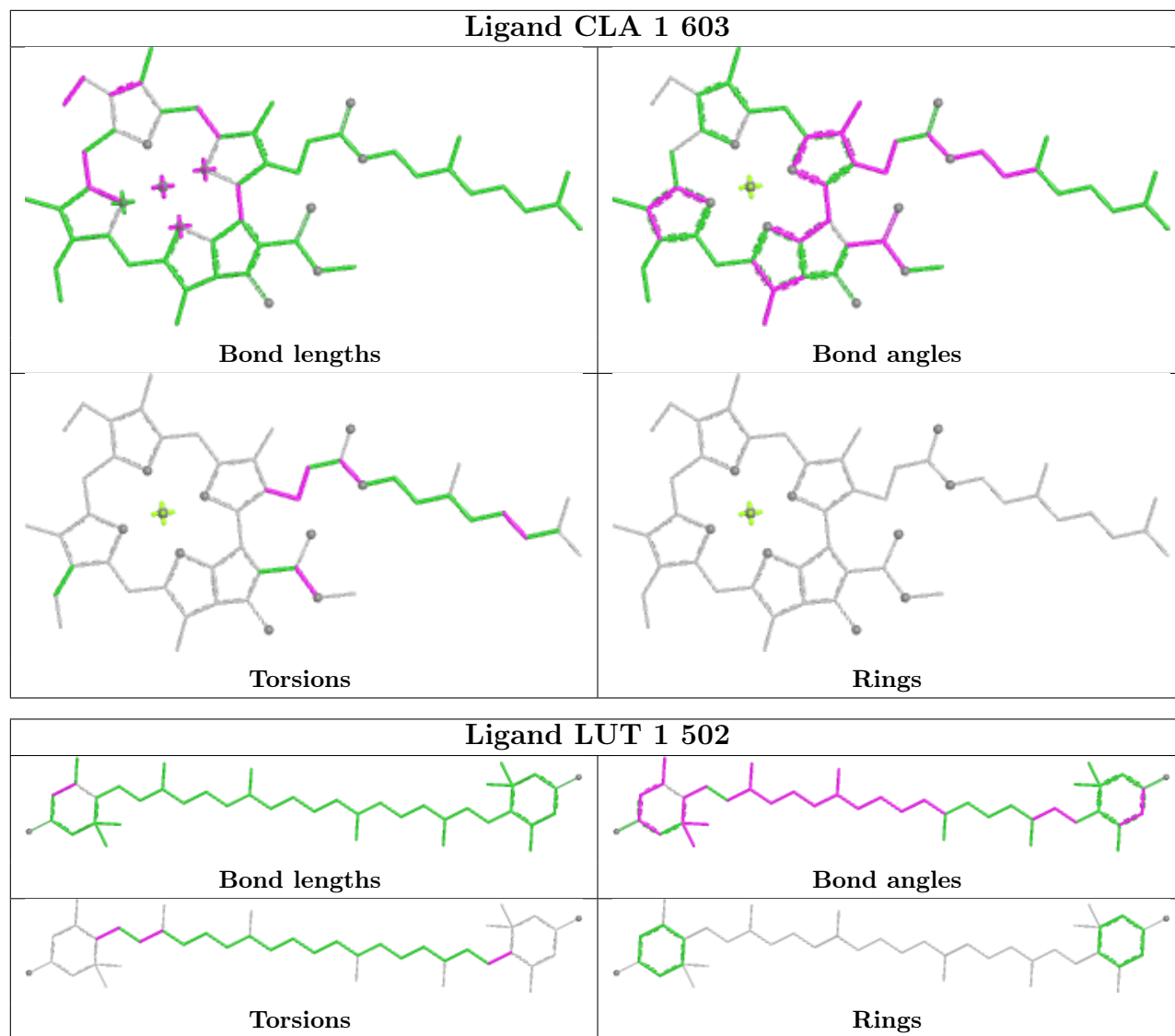
Ligand CLA J 1901



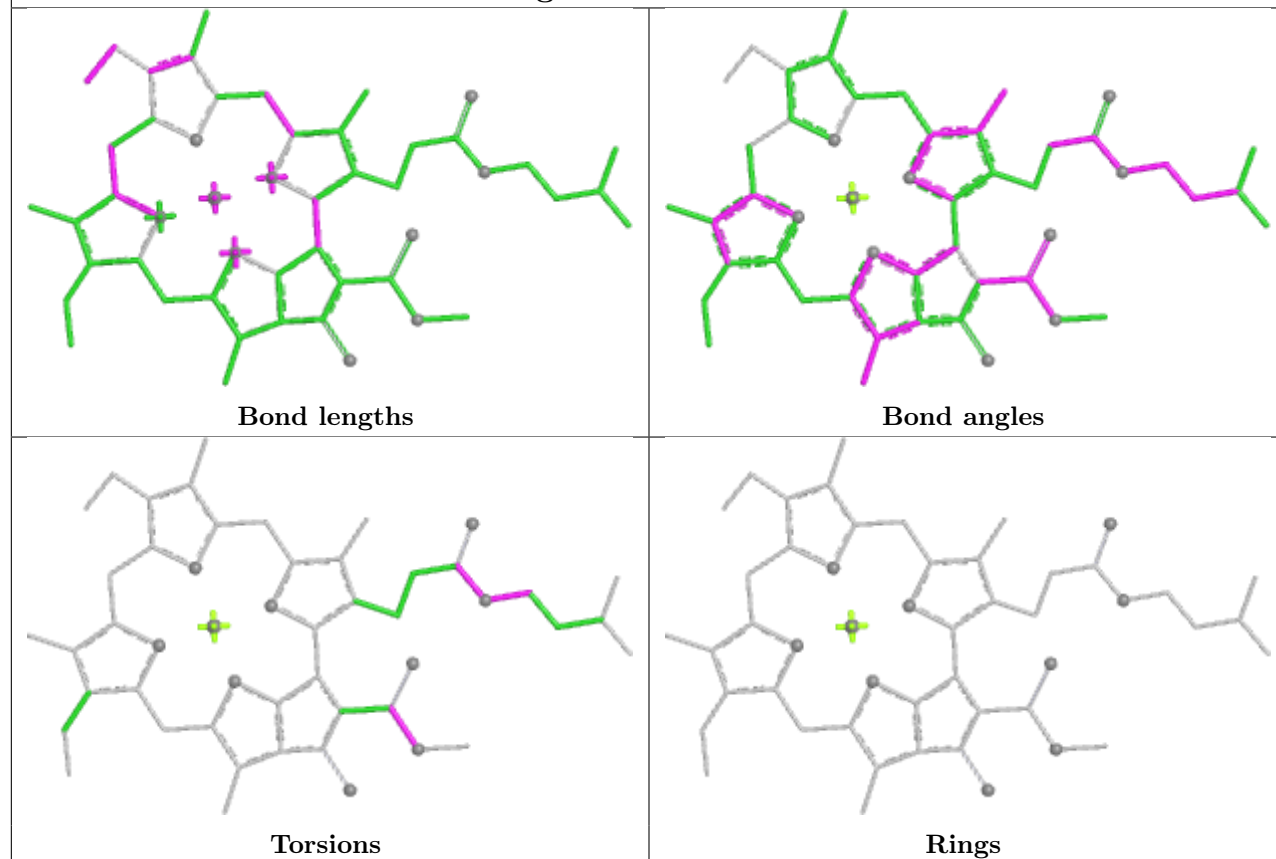
Ligand CLA A 1133**Ligand CLA A 1106**



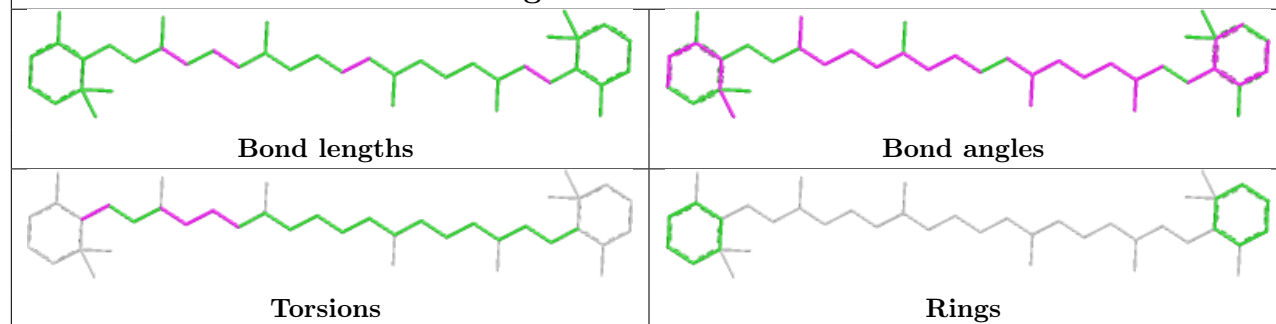


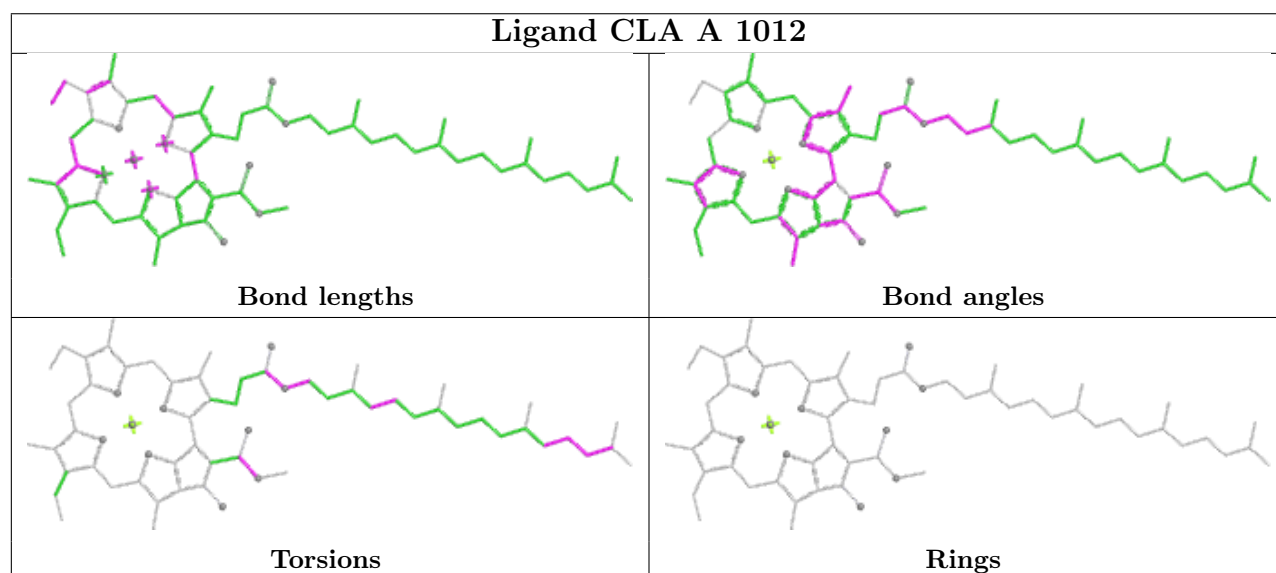
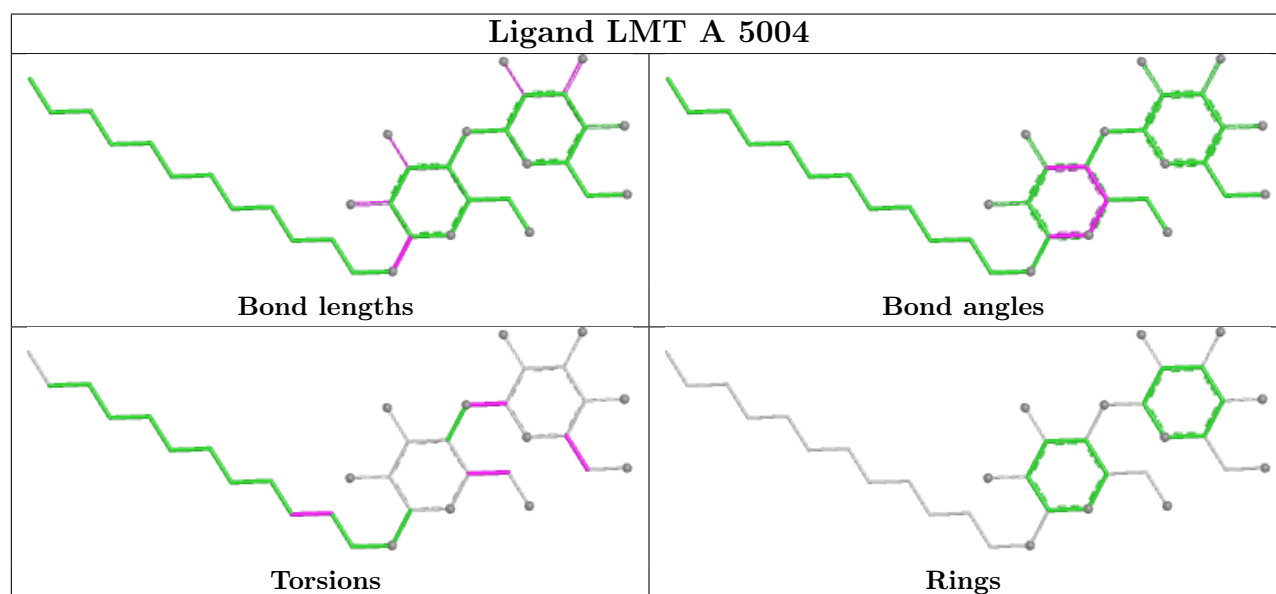
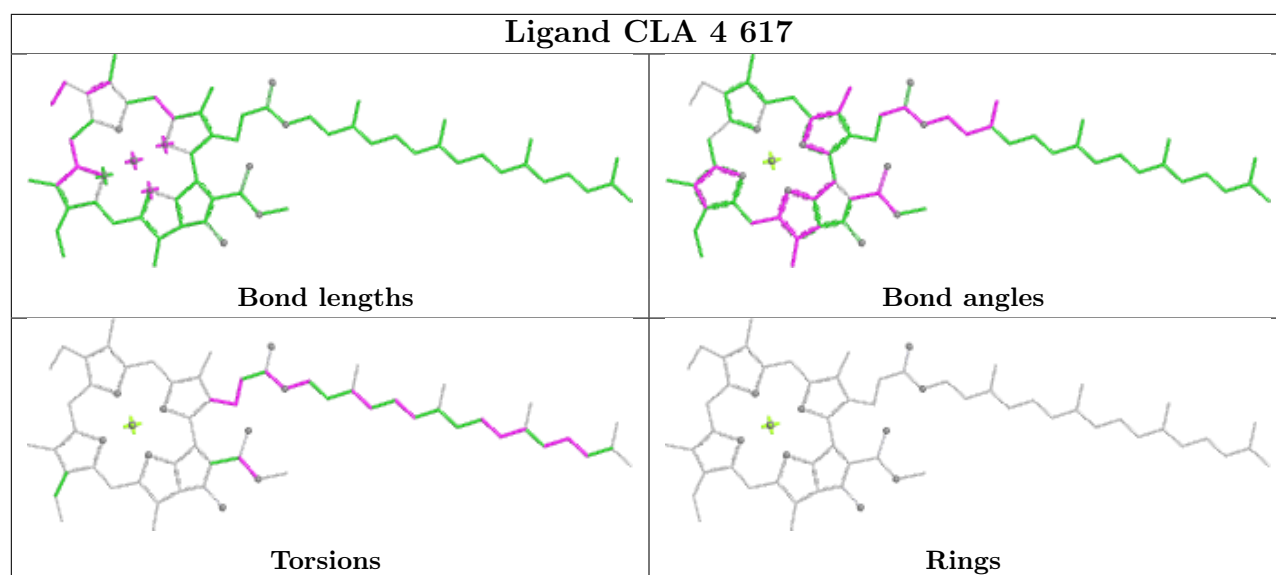


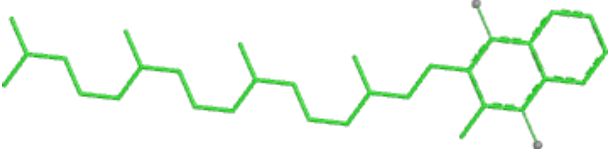
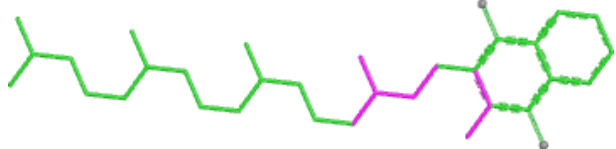
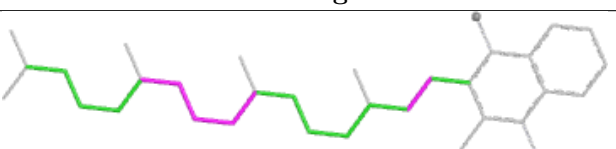
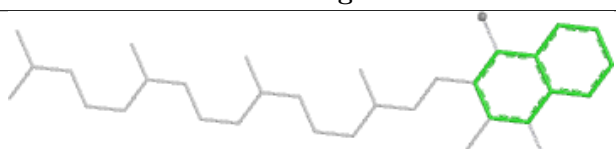
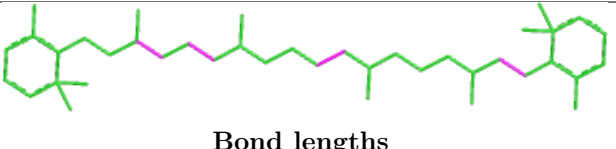
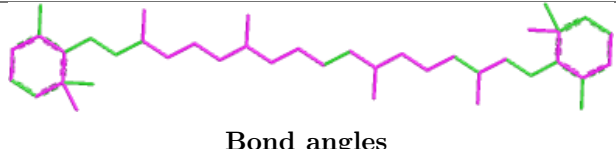
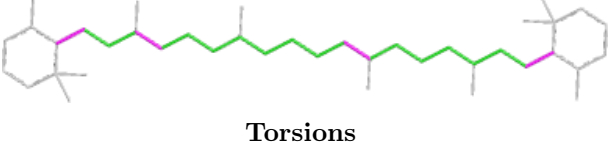
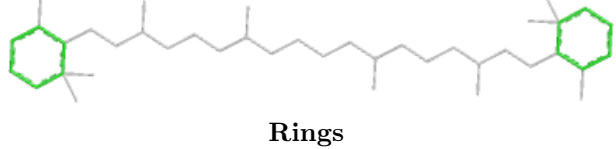
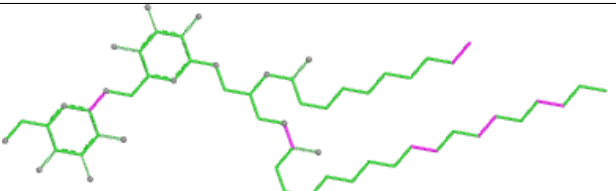
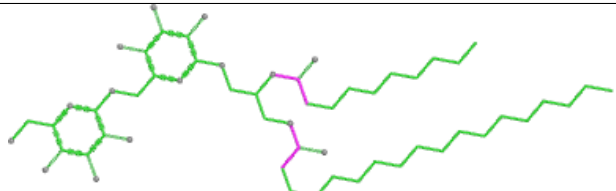
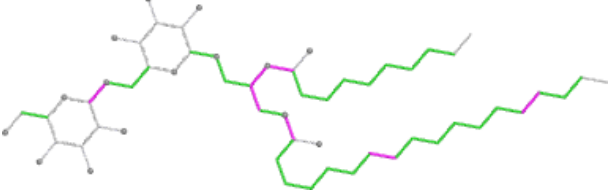
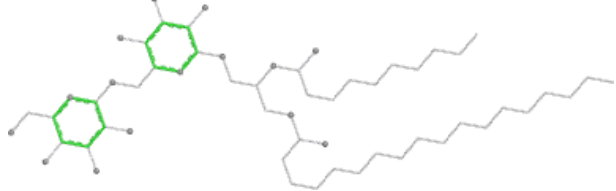
Ligand CLA 1 606

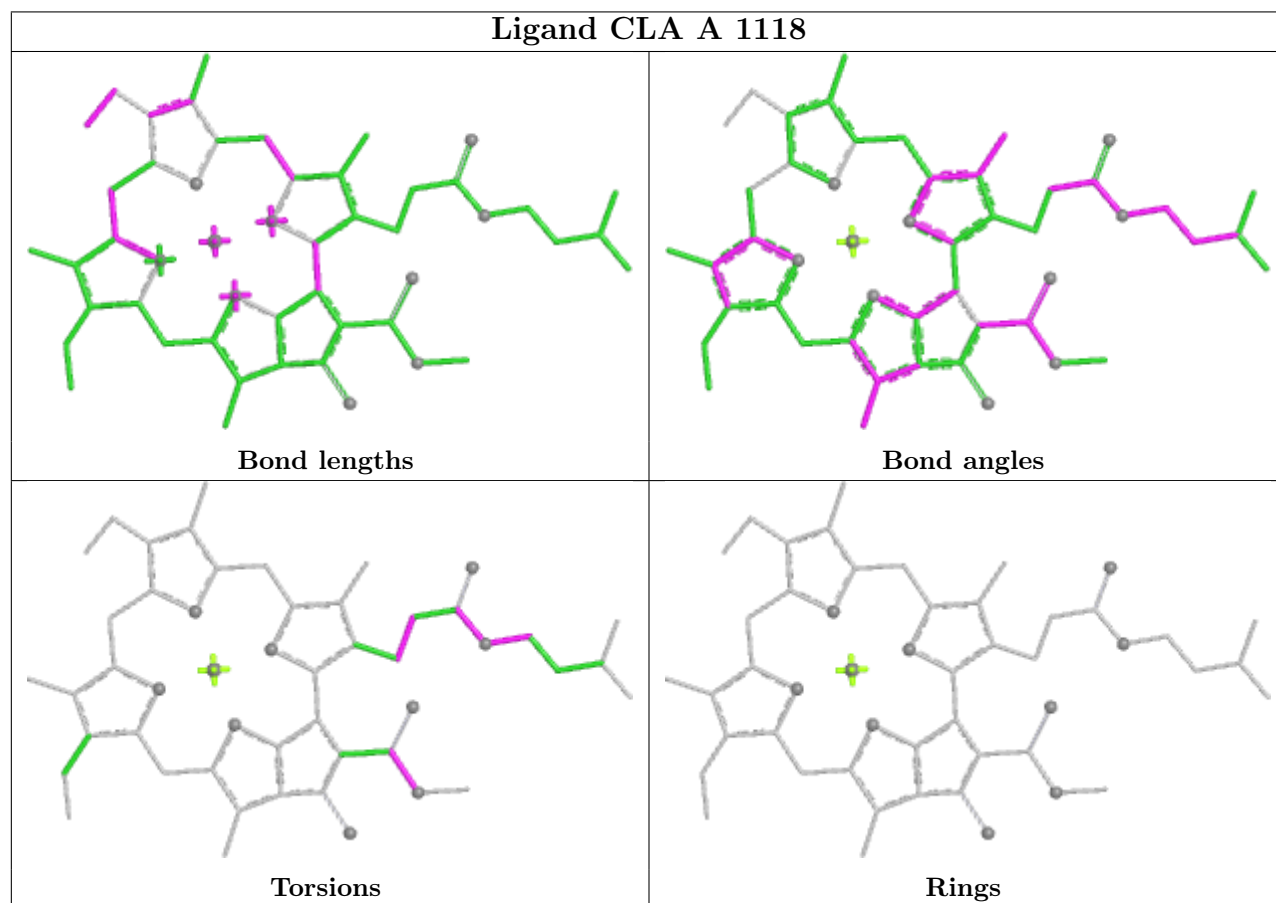
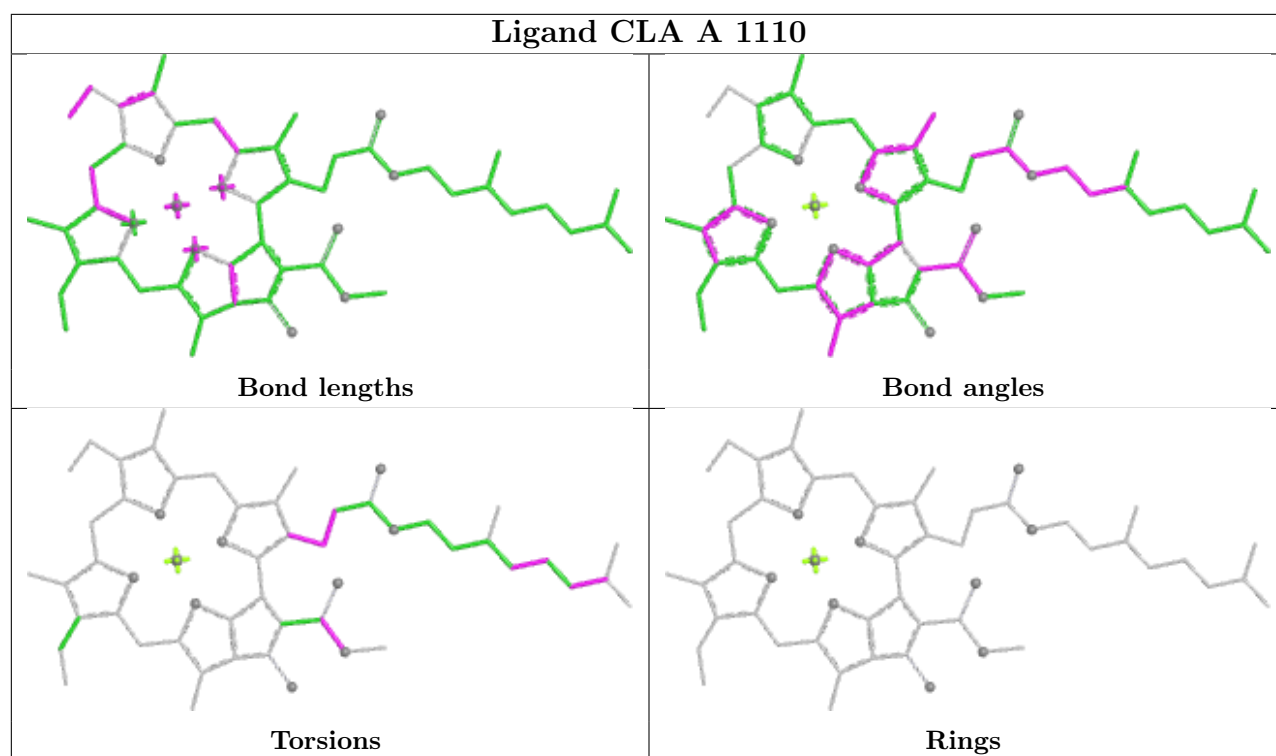


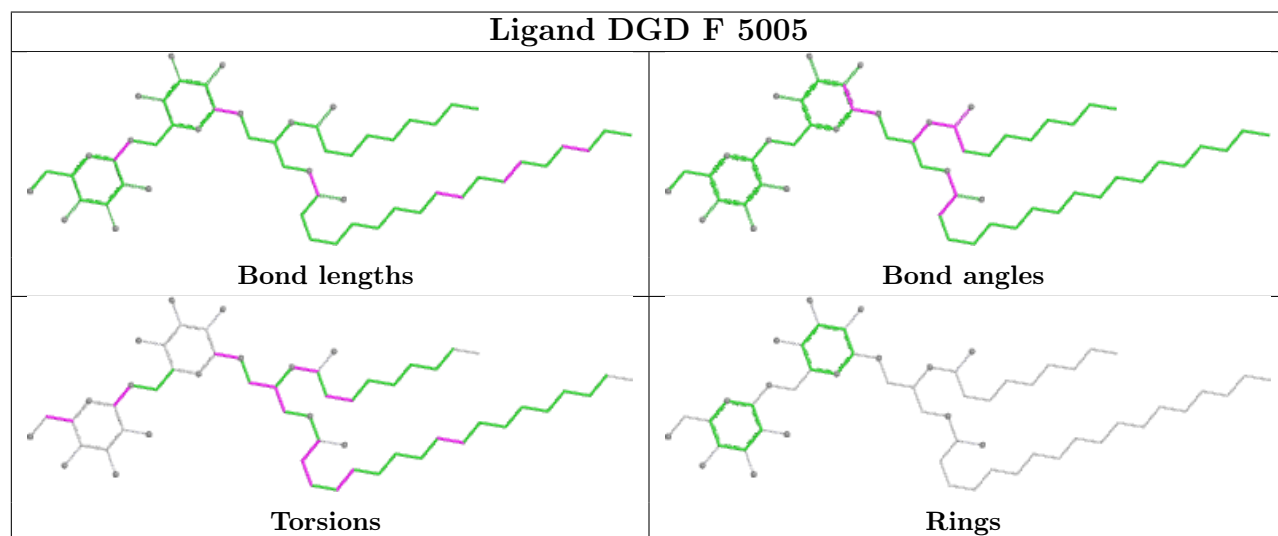
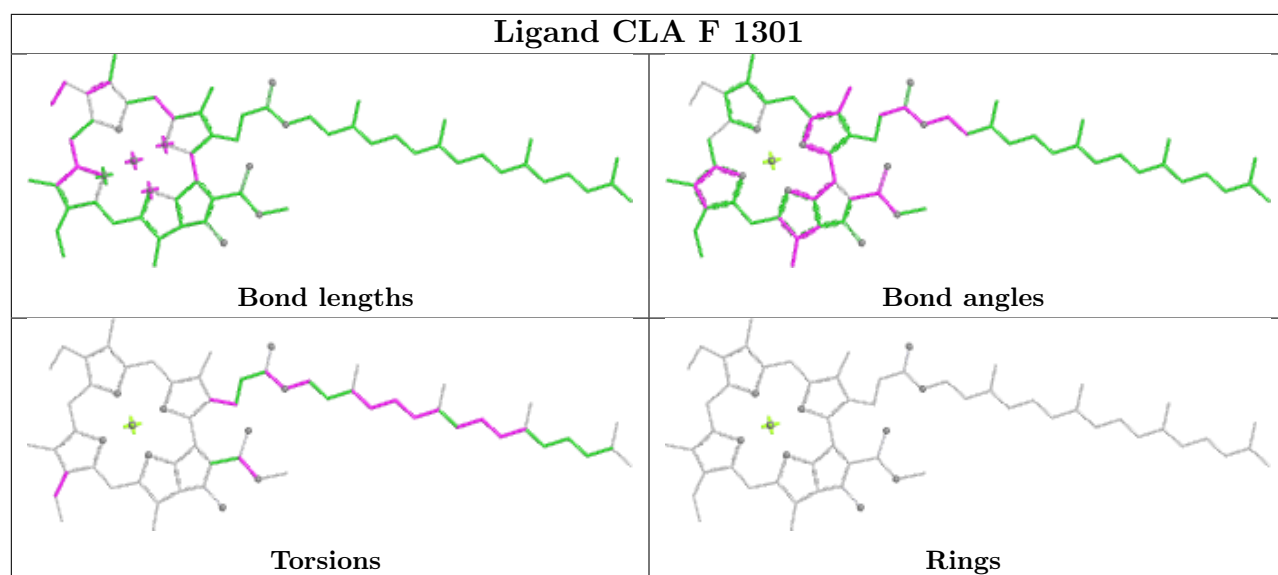
Ligand BCR L 4019



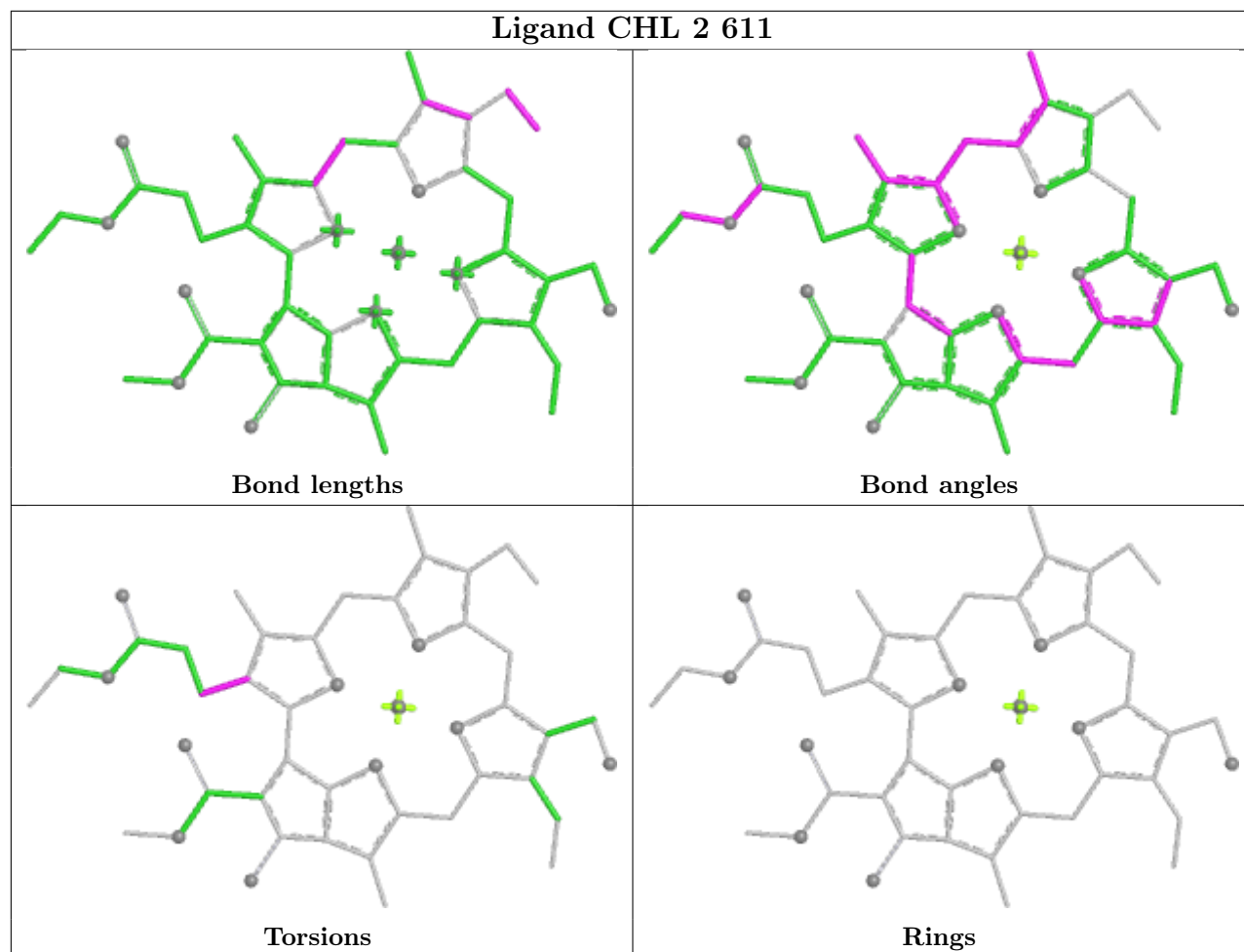


Ligand PQN A 2001	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 4011	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGD J 5001	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

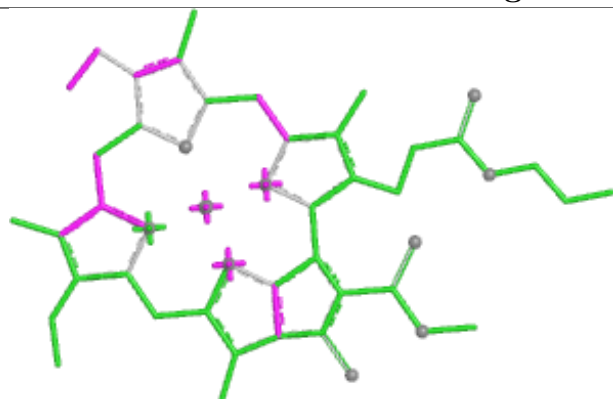




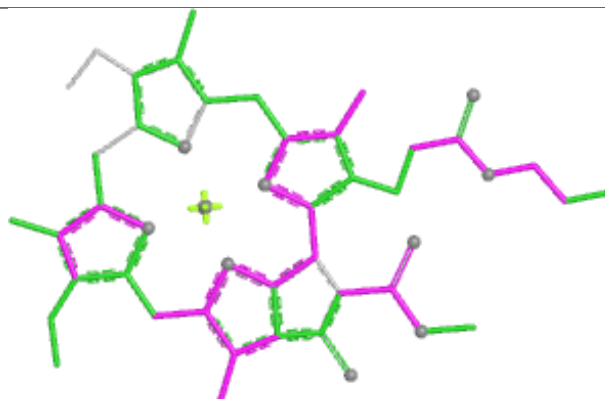
Ligand CHL 2 611



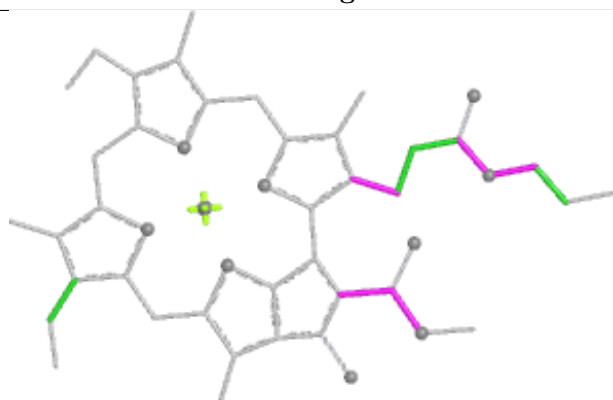
Ligand CLA K 1403



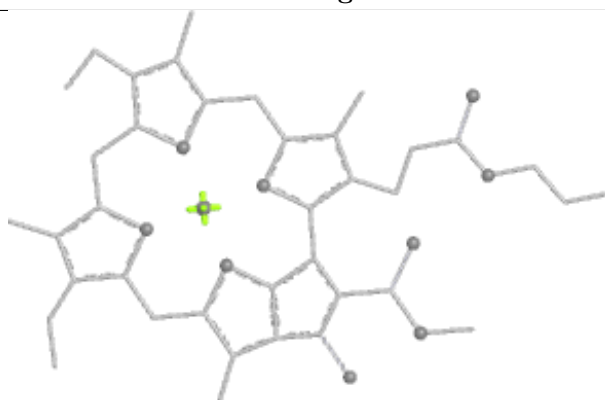
Bond lengths



Bond angles

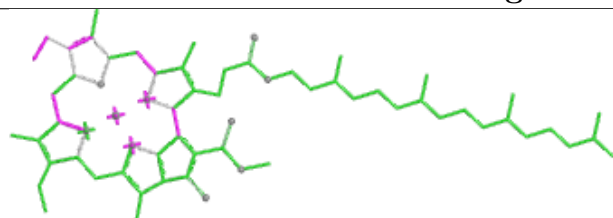


Torsions

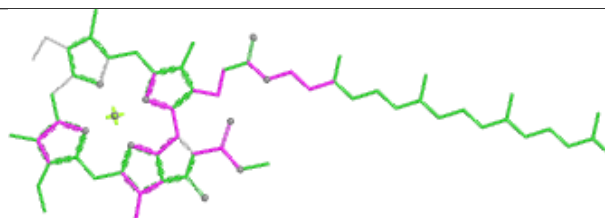


Rings

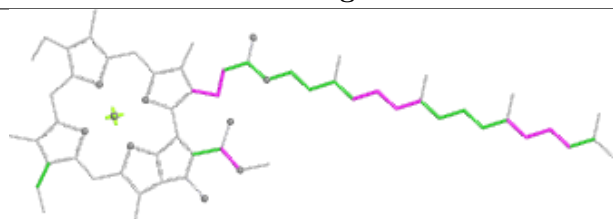
Ligand CLA B 1225



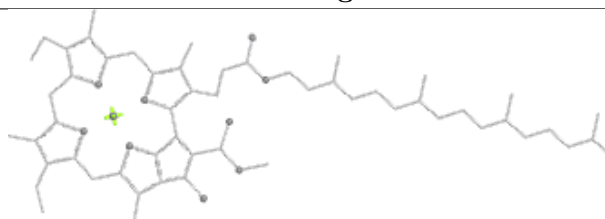
Bond lengths



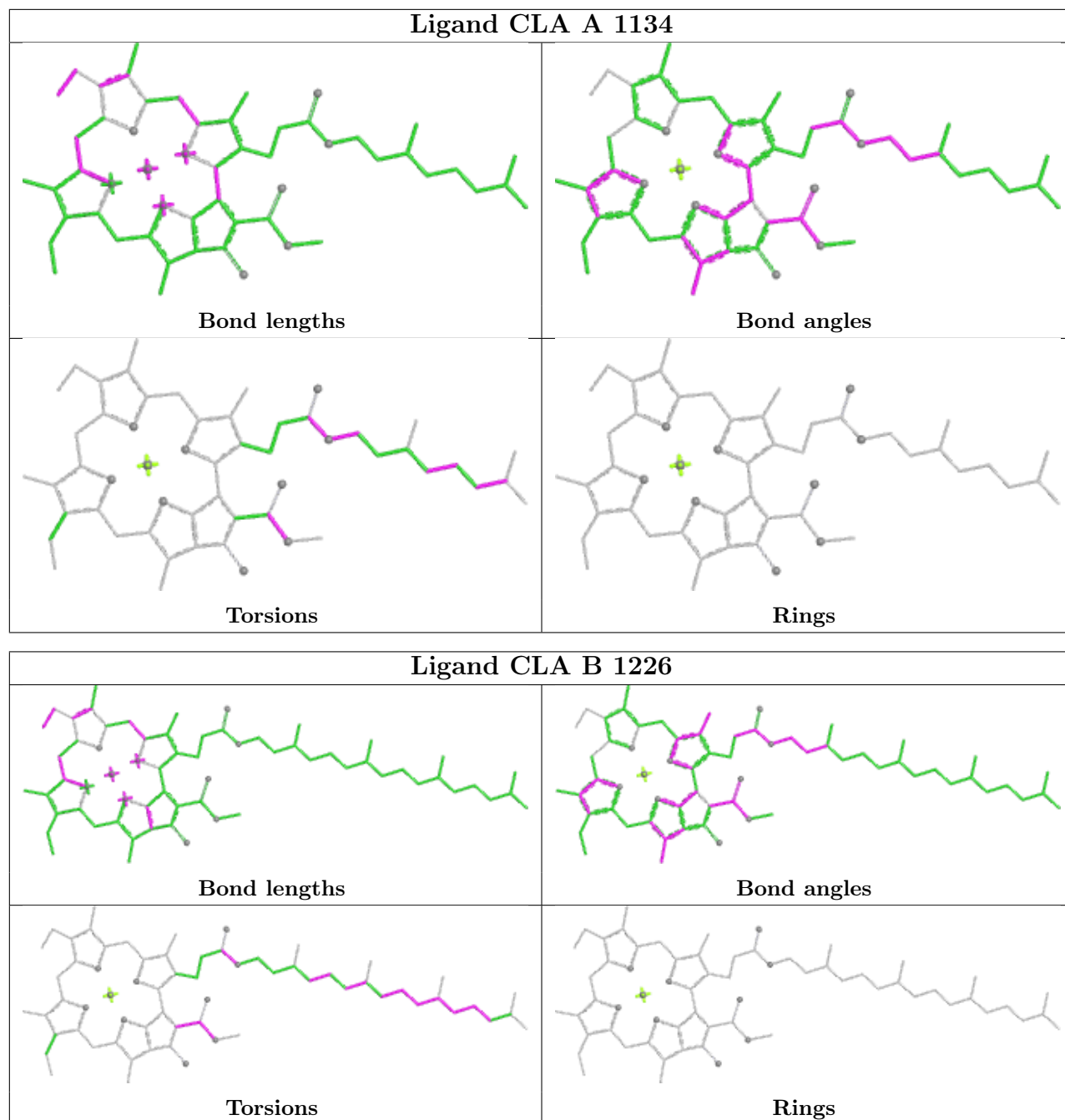
Bond angles

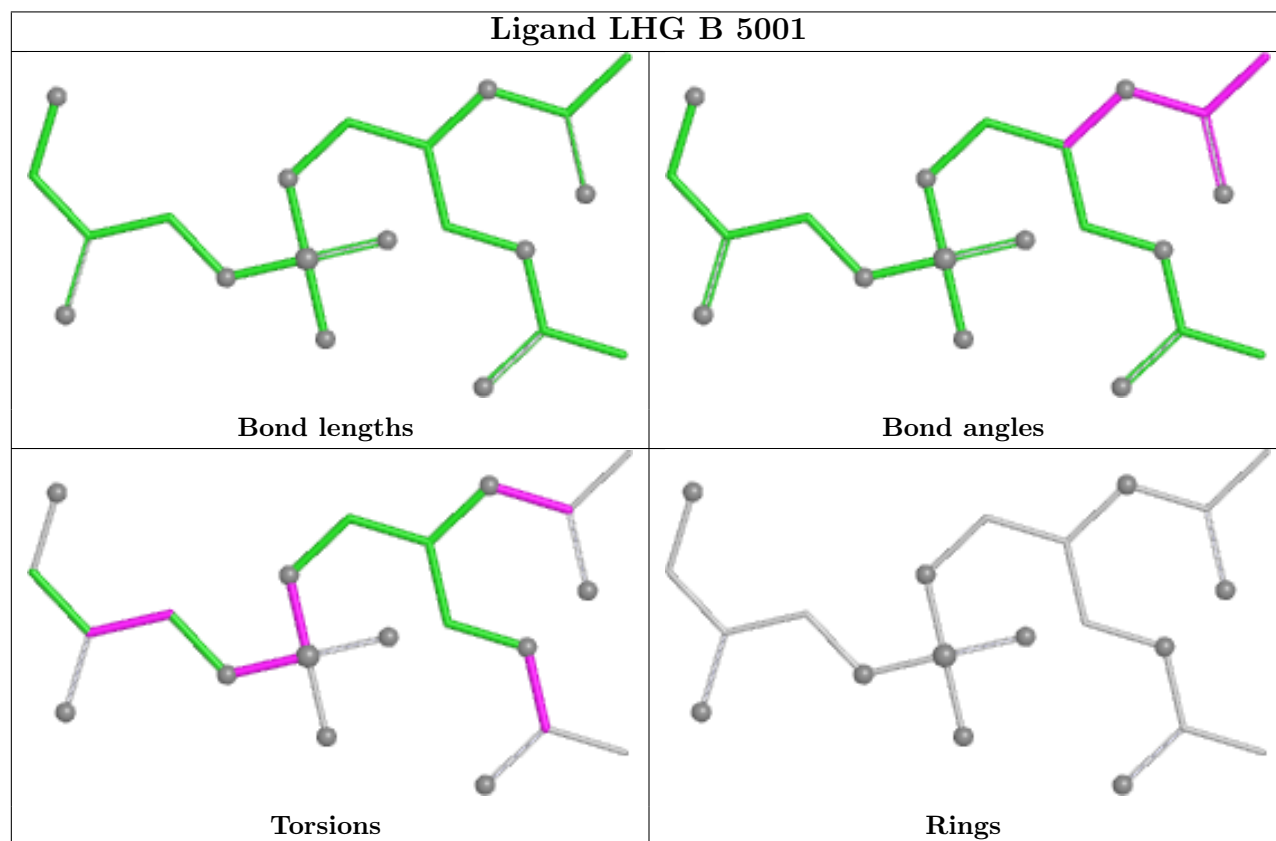
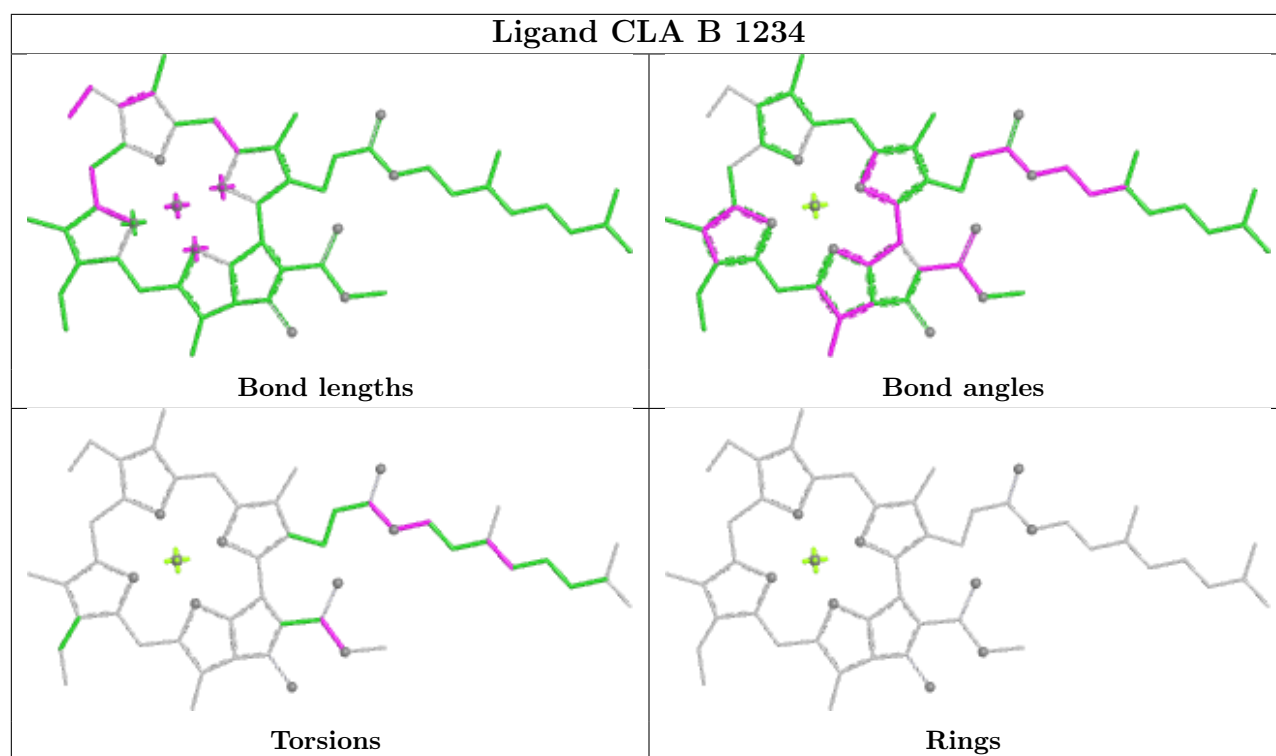


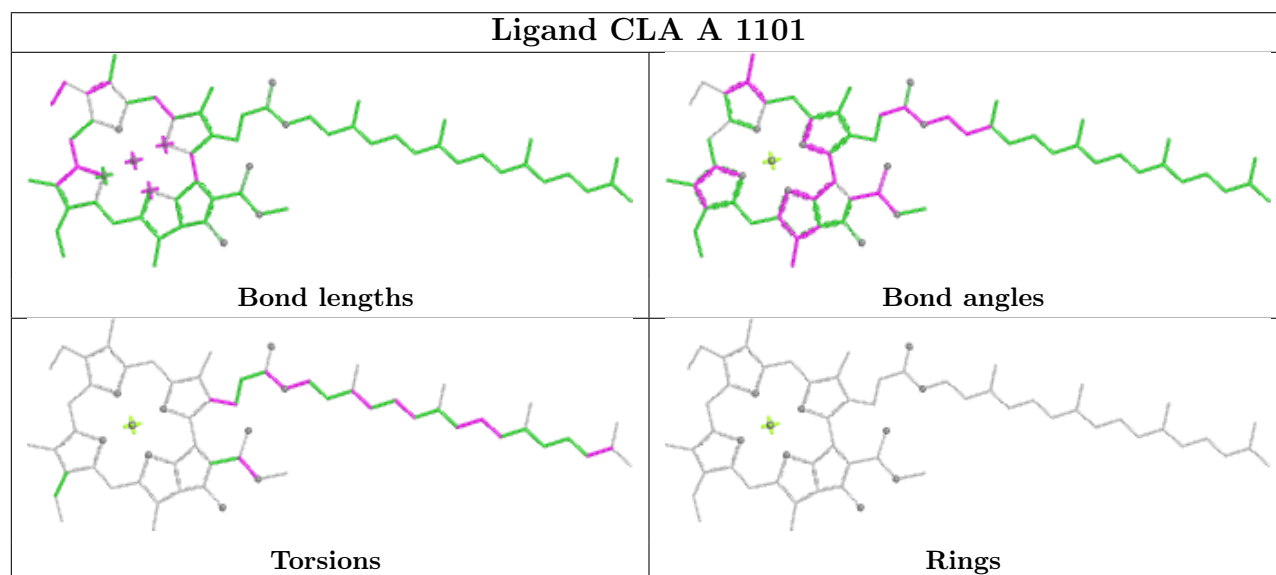
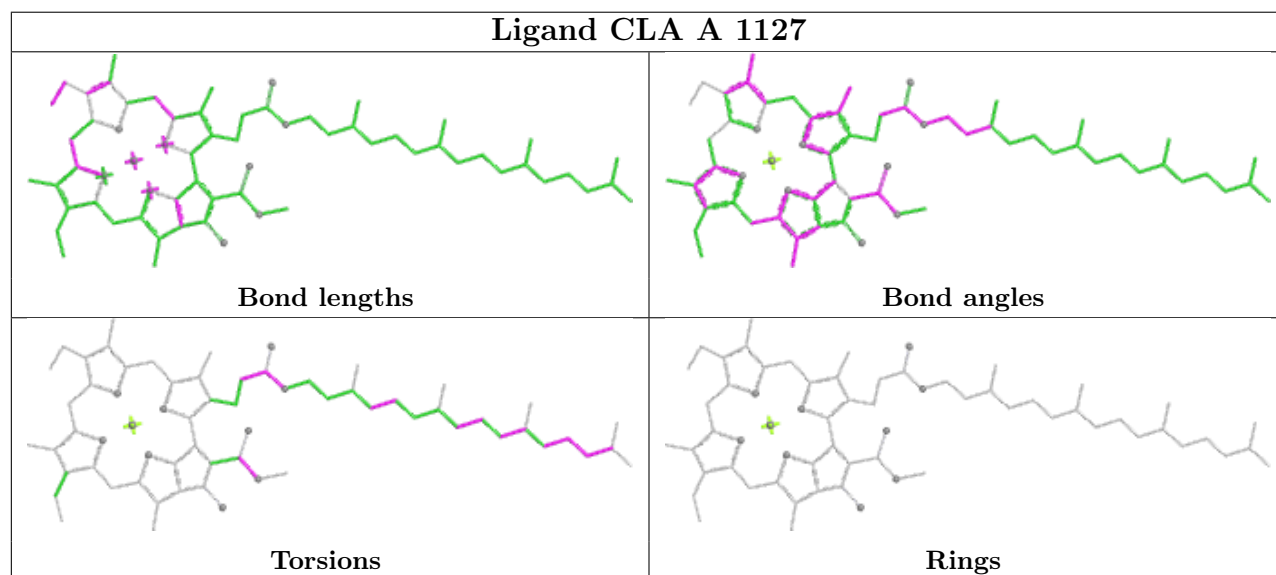
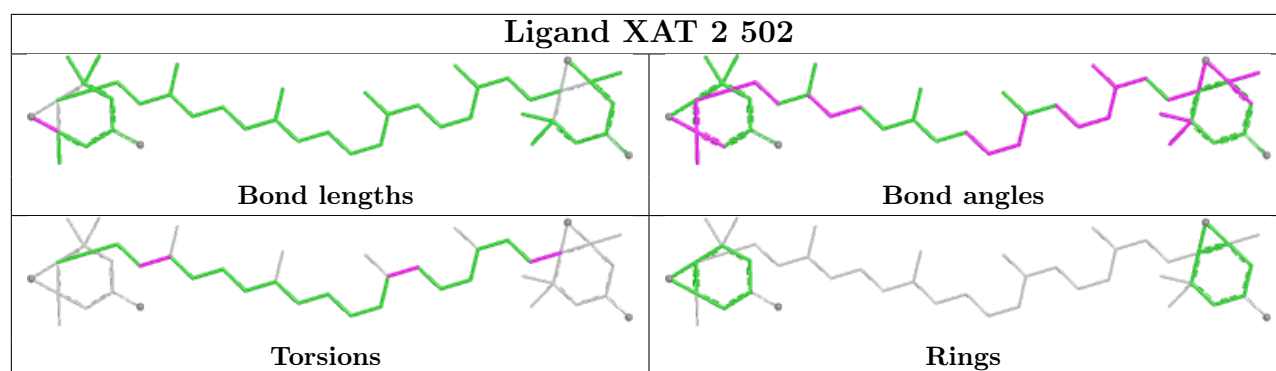
Torsions

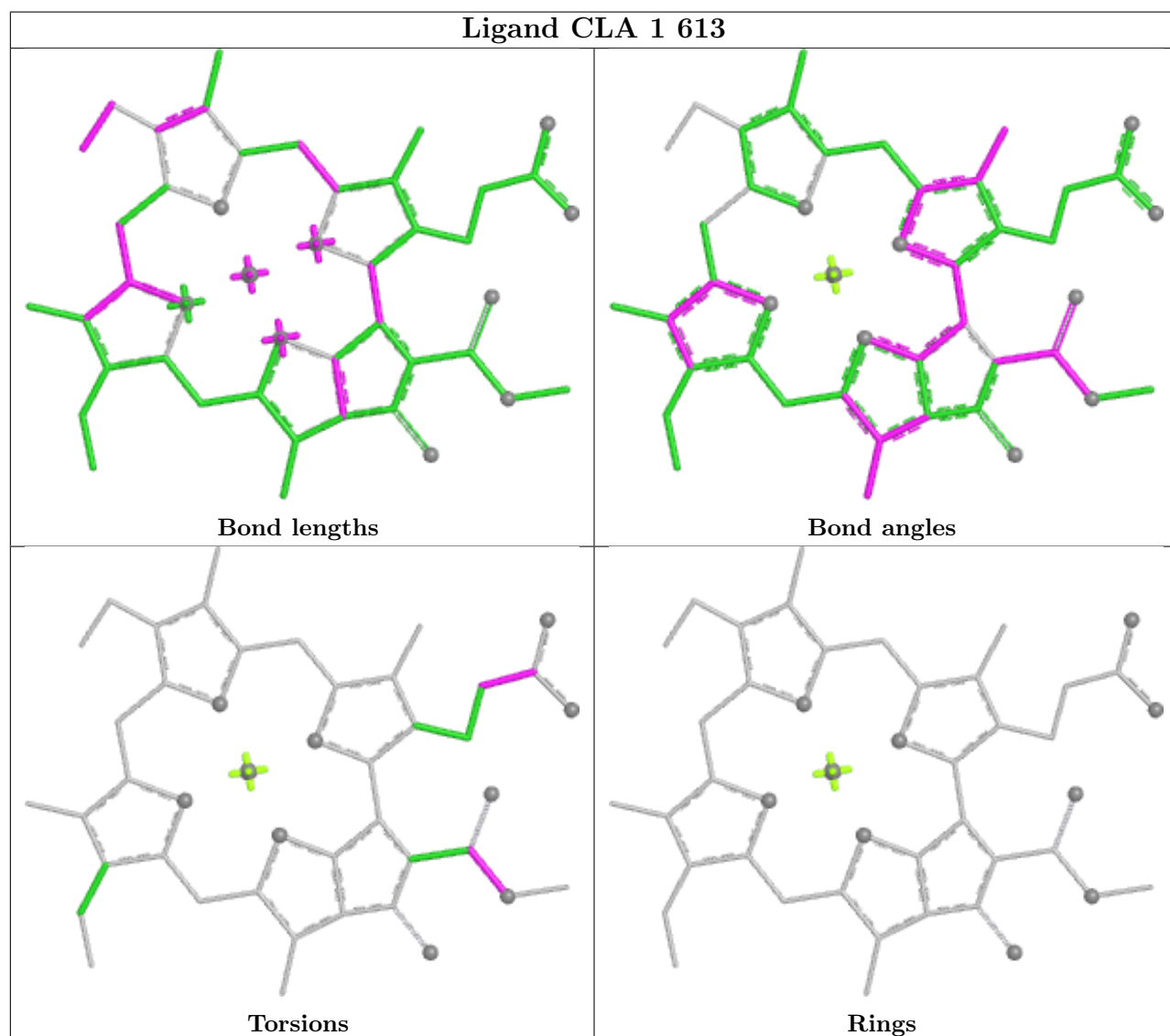
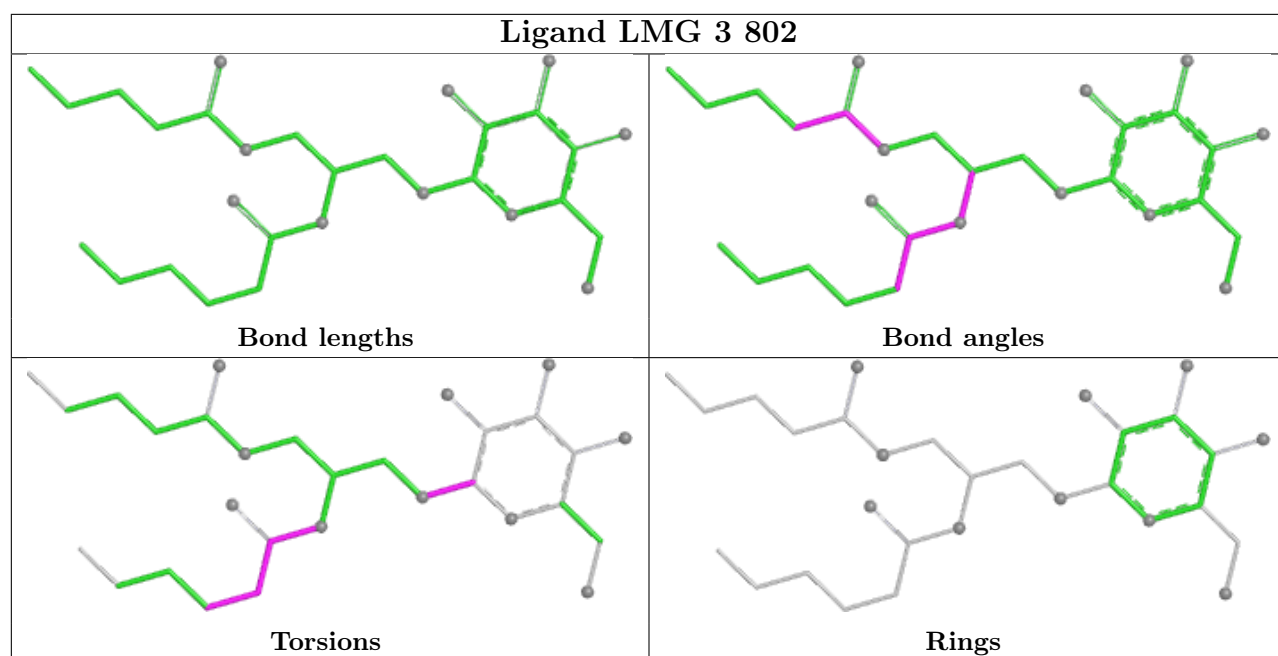


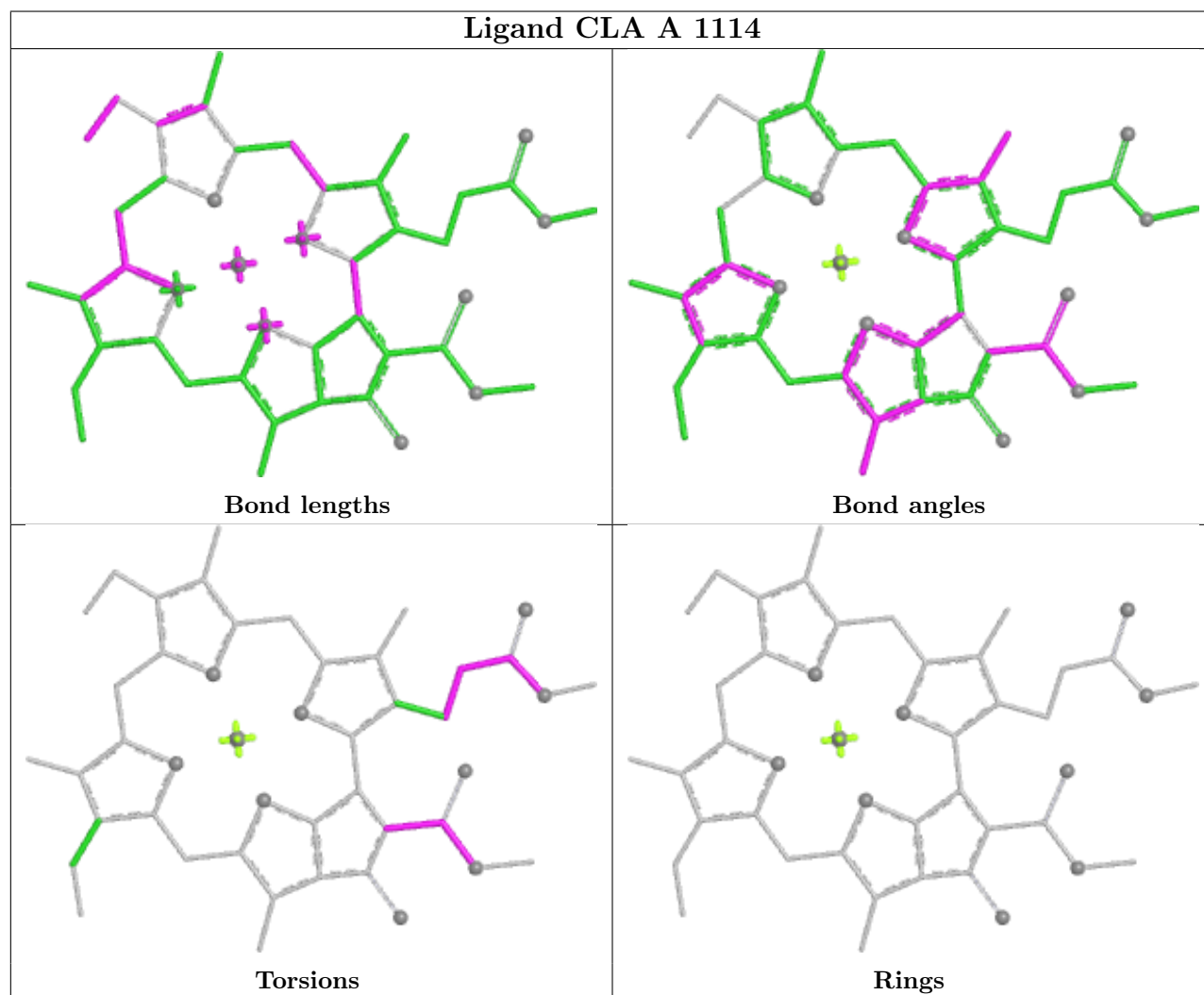
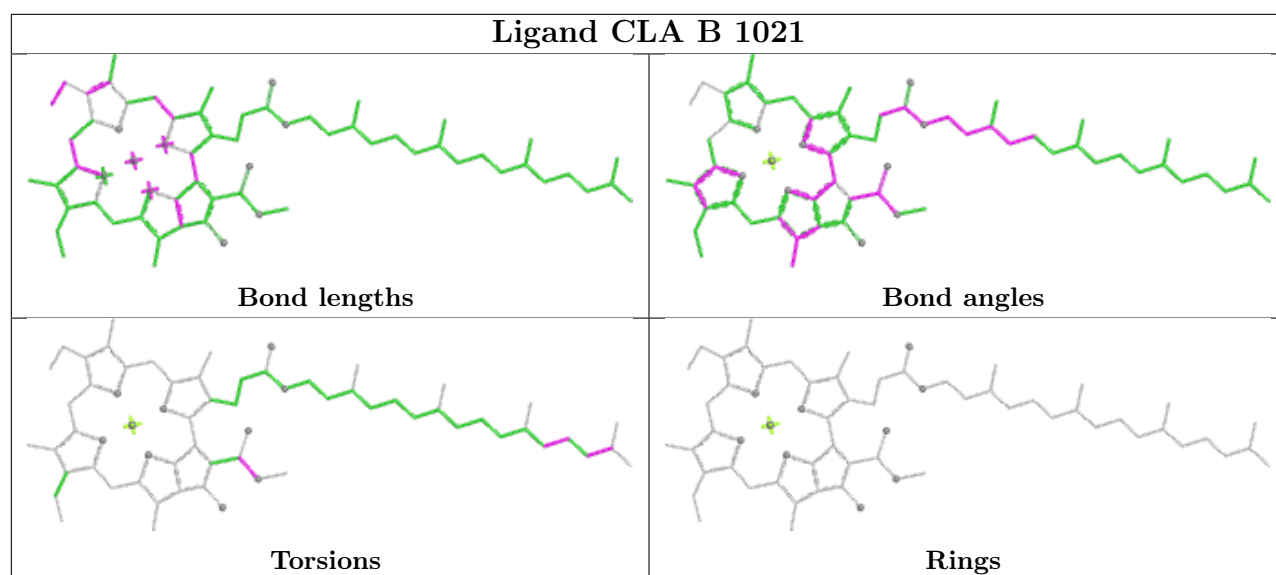
Rings

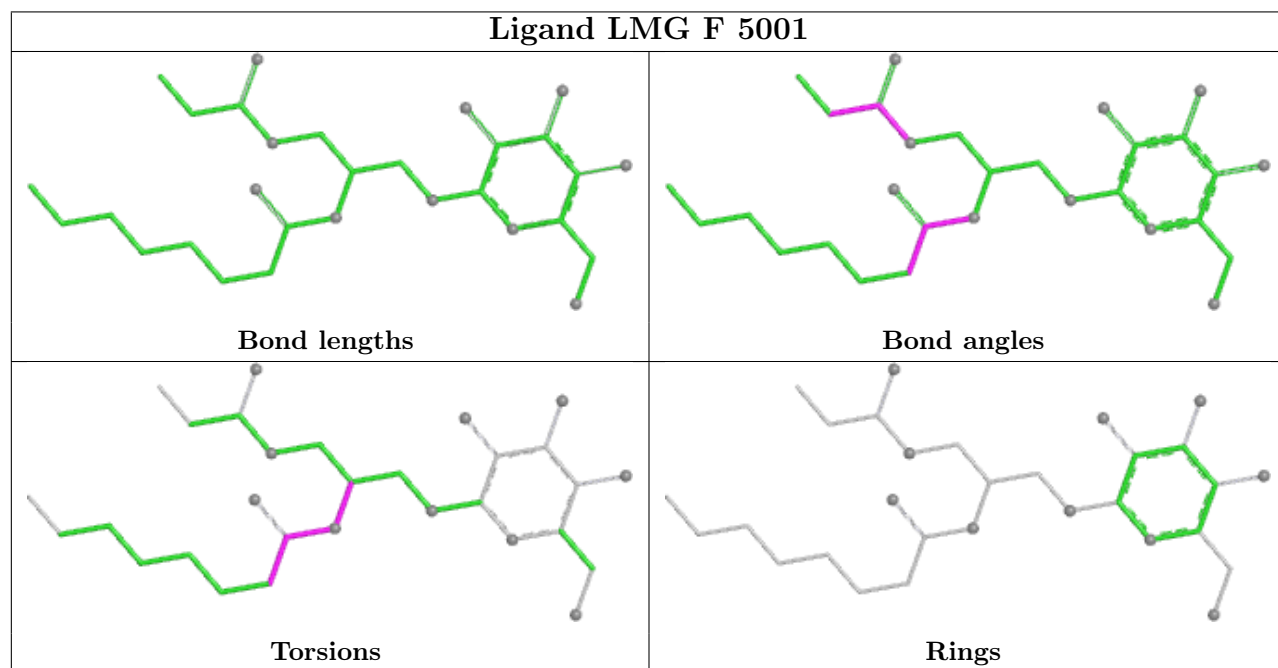
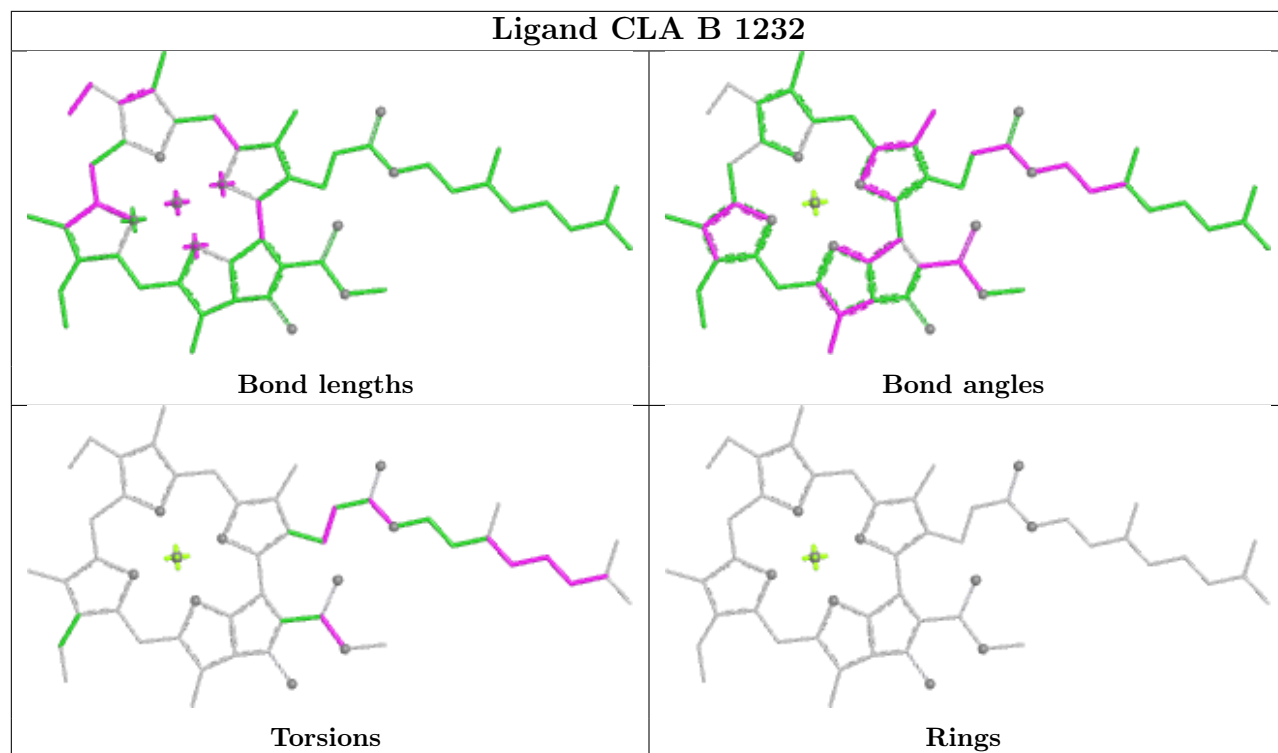


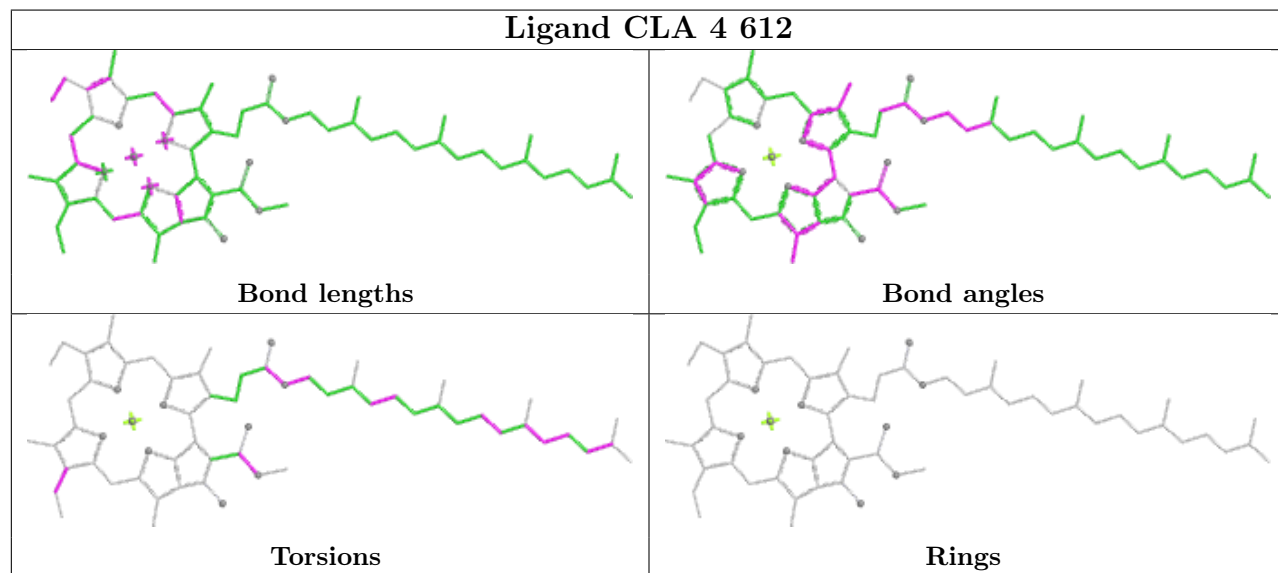
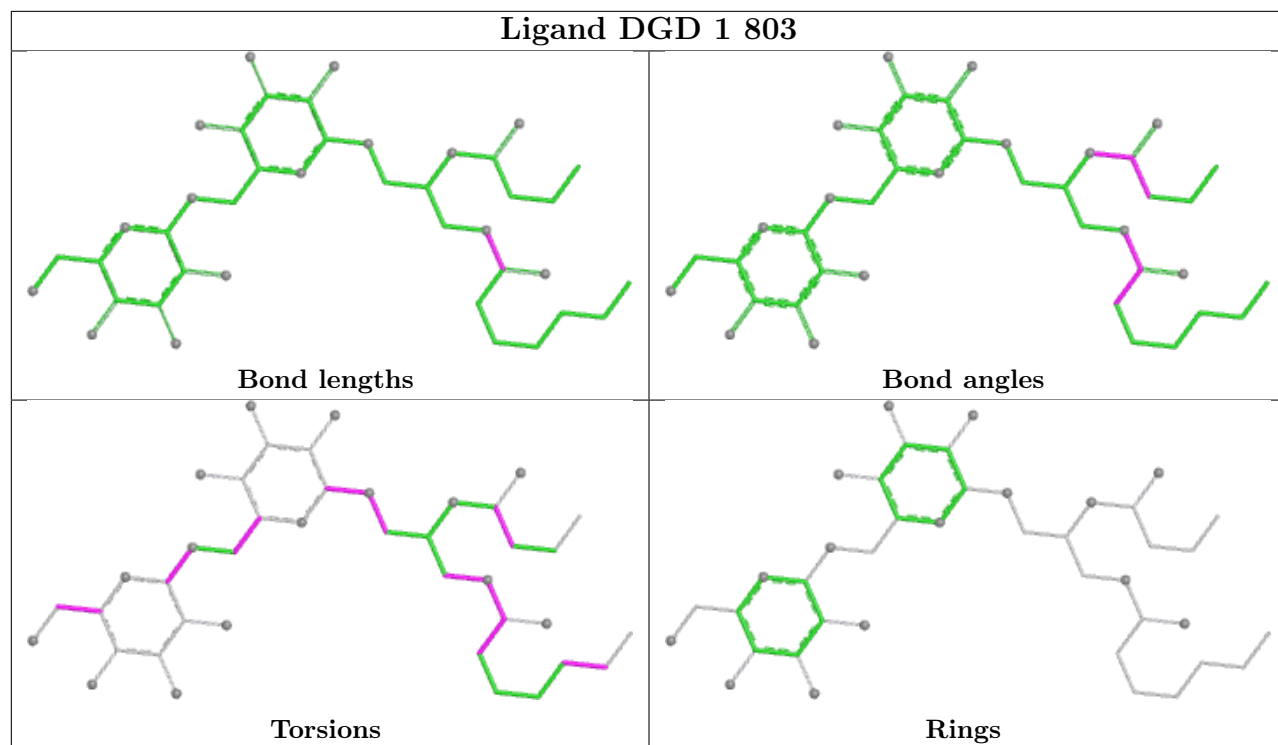




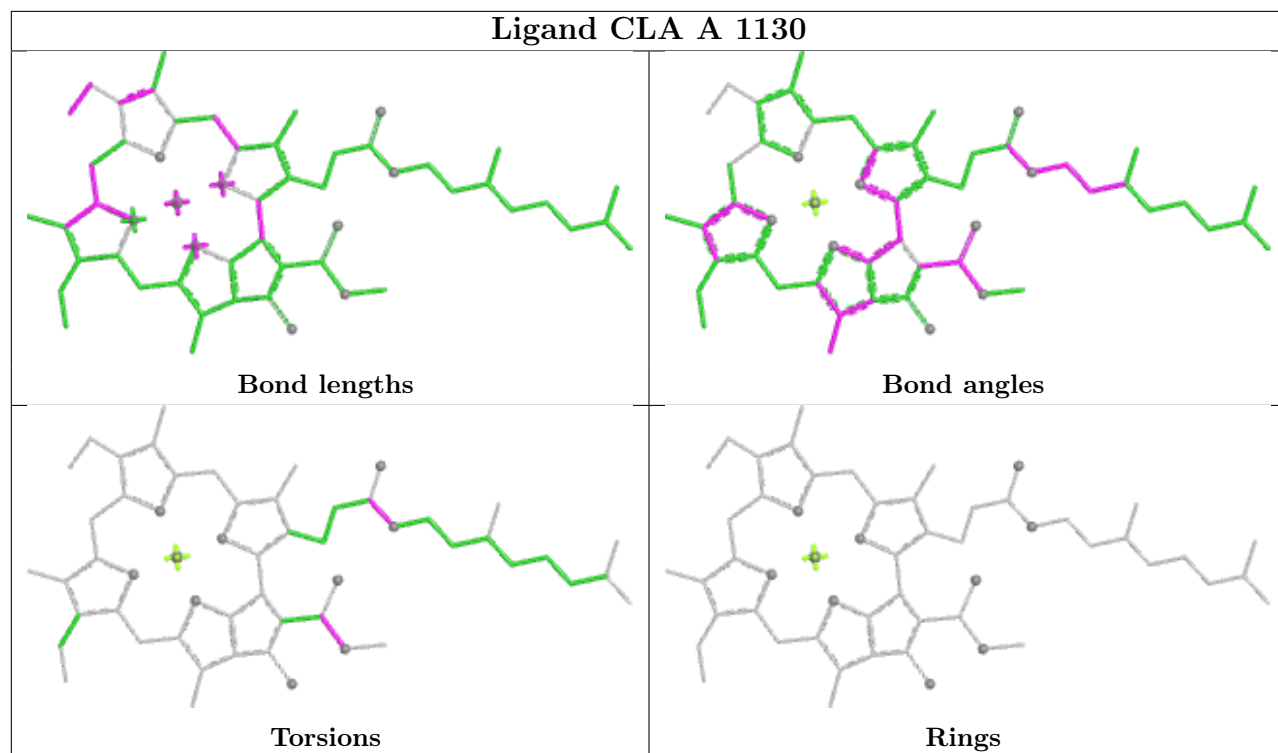




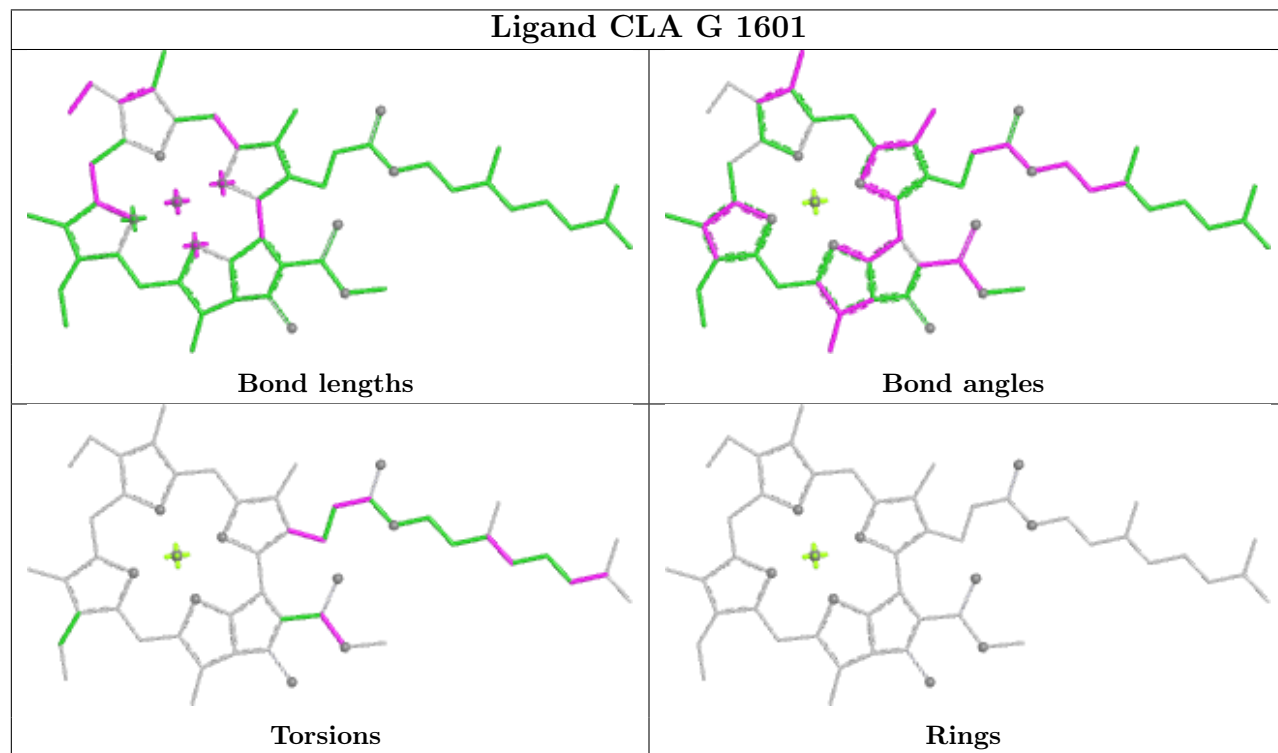


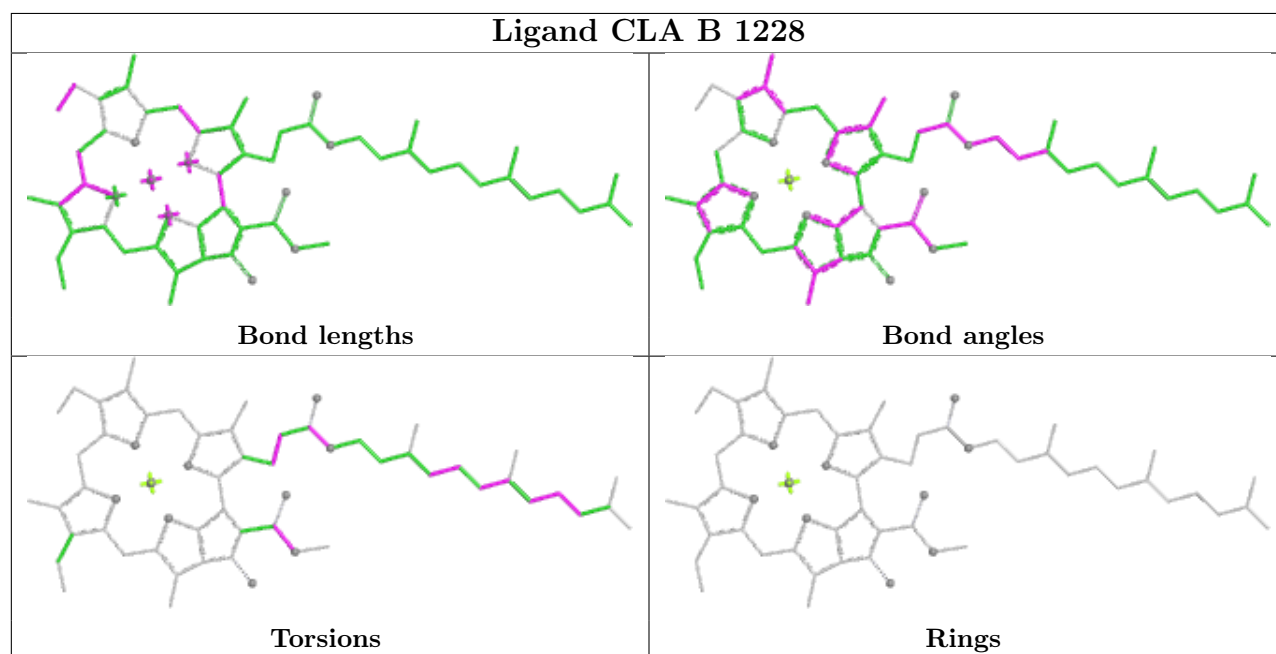
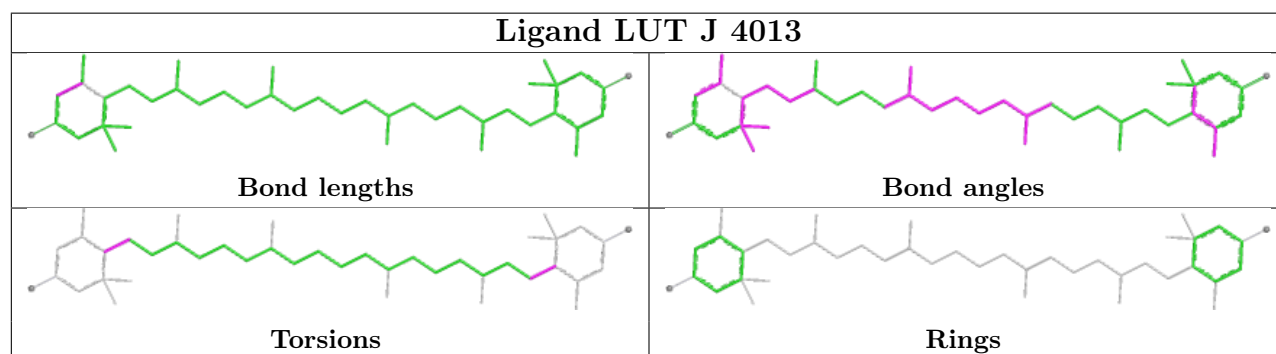
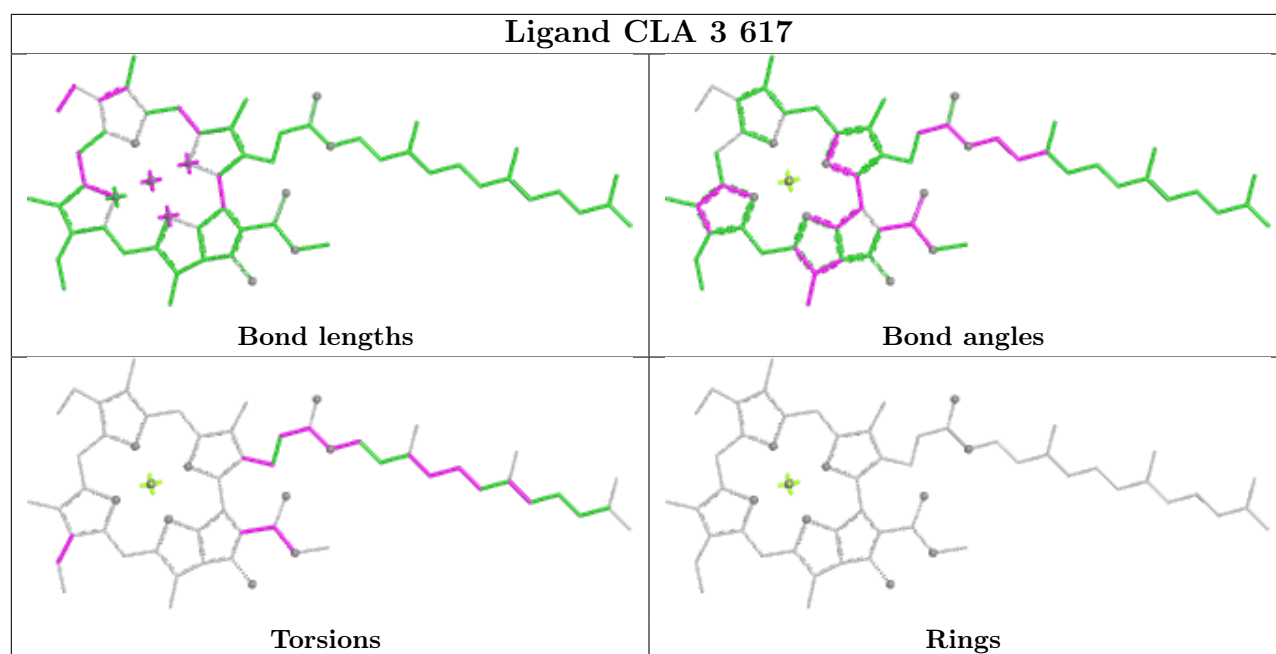


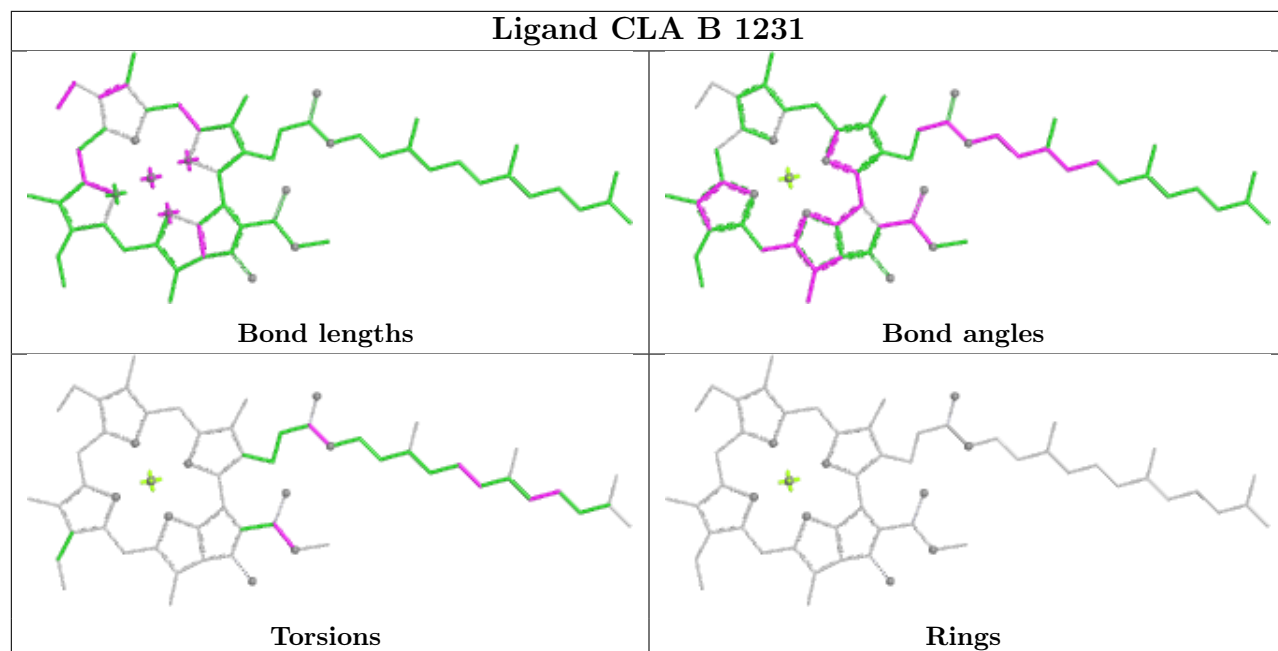
Ligand CLA A 1130

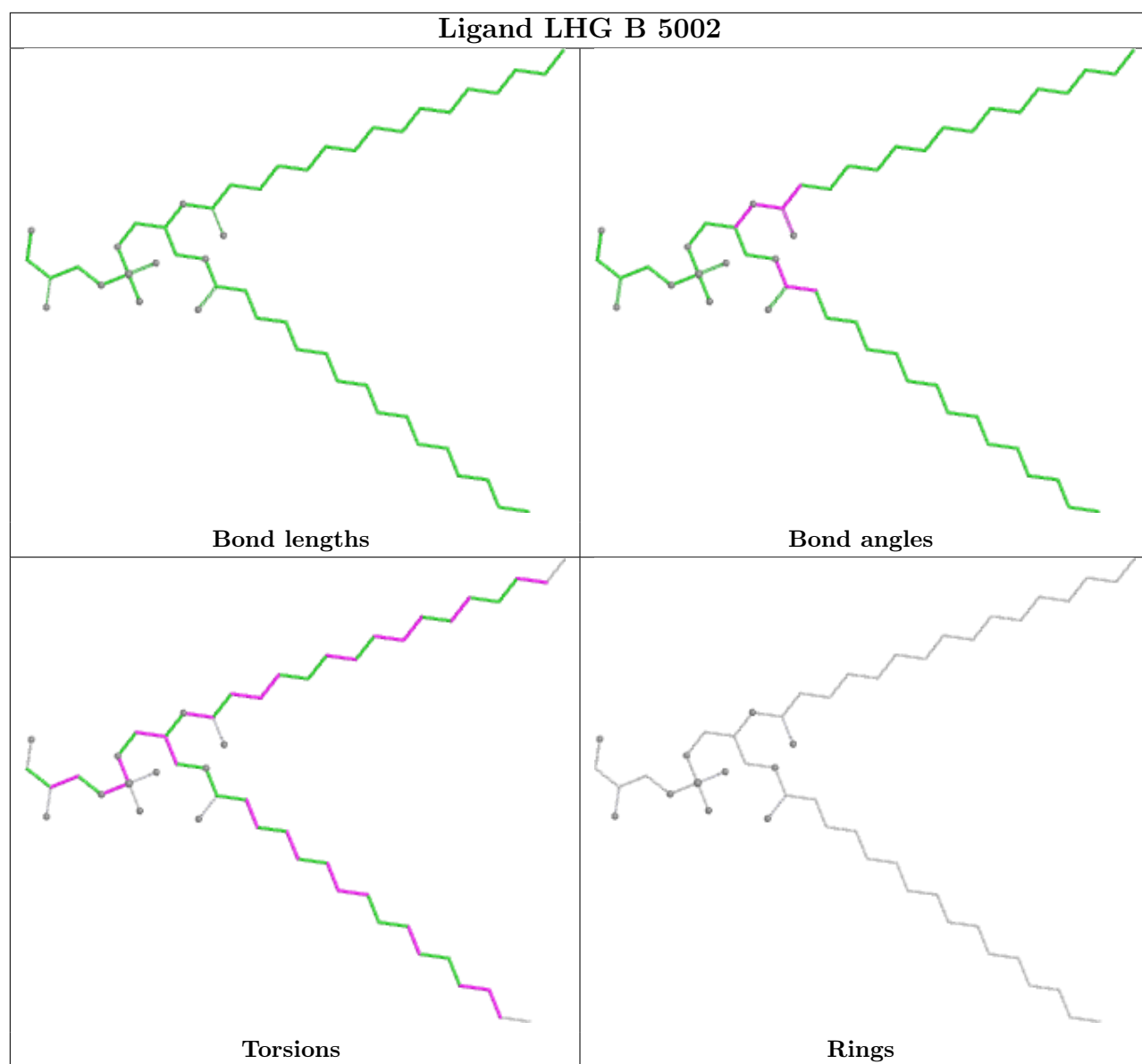


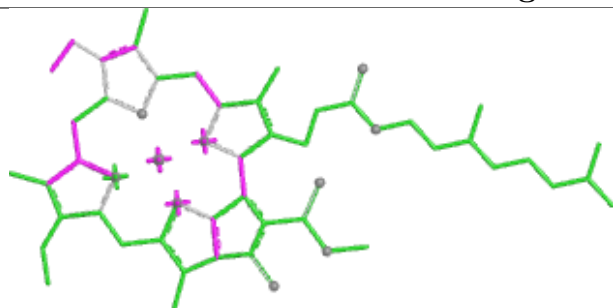
Ligand CLA G 1601



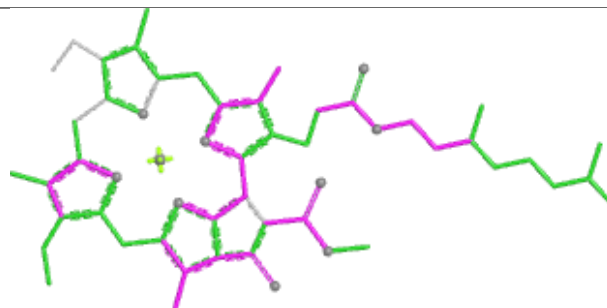




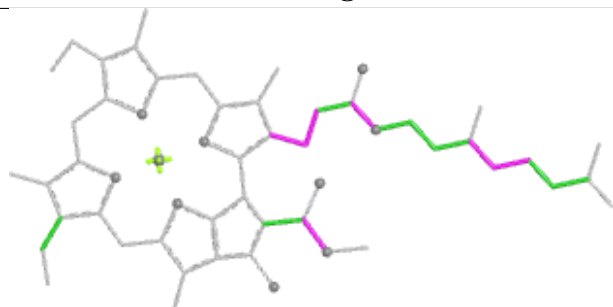


Ligand CLA 3 605

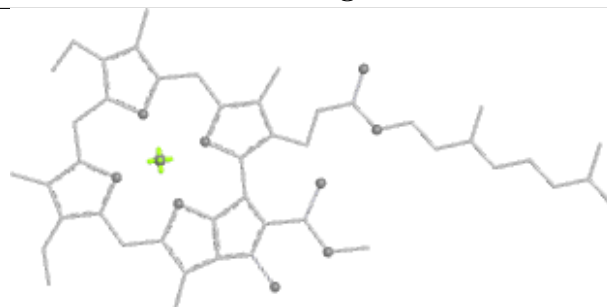
Bond lengths



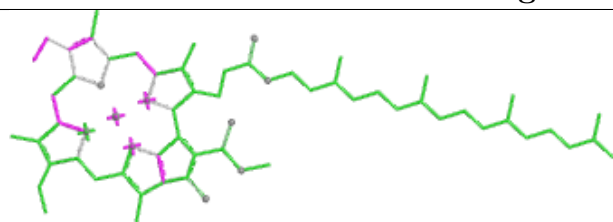
Bond angles



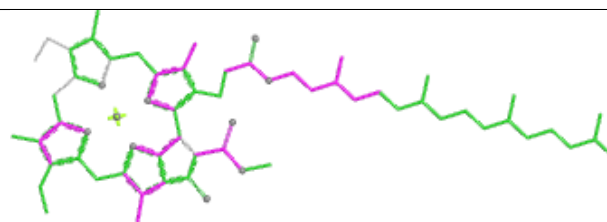
Torsions



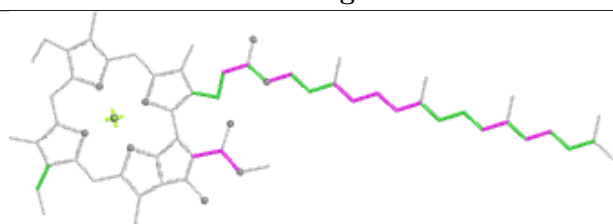
Rings

Ligand CLA 1 605

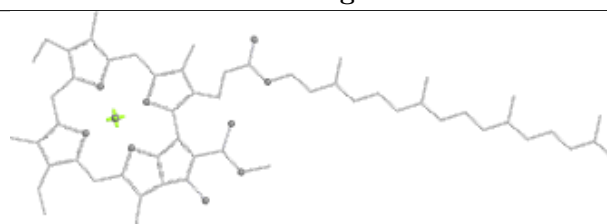
Bond lengths



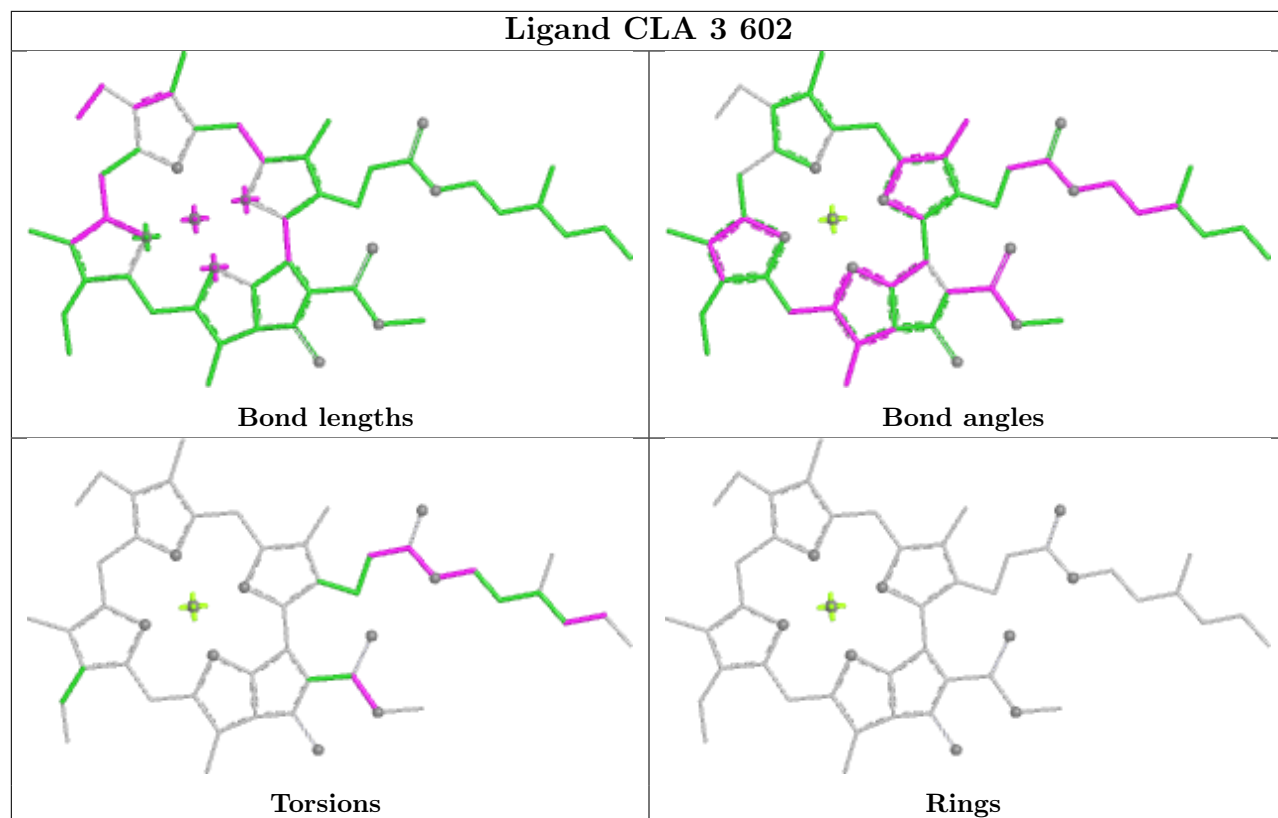
Bond angles

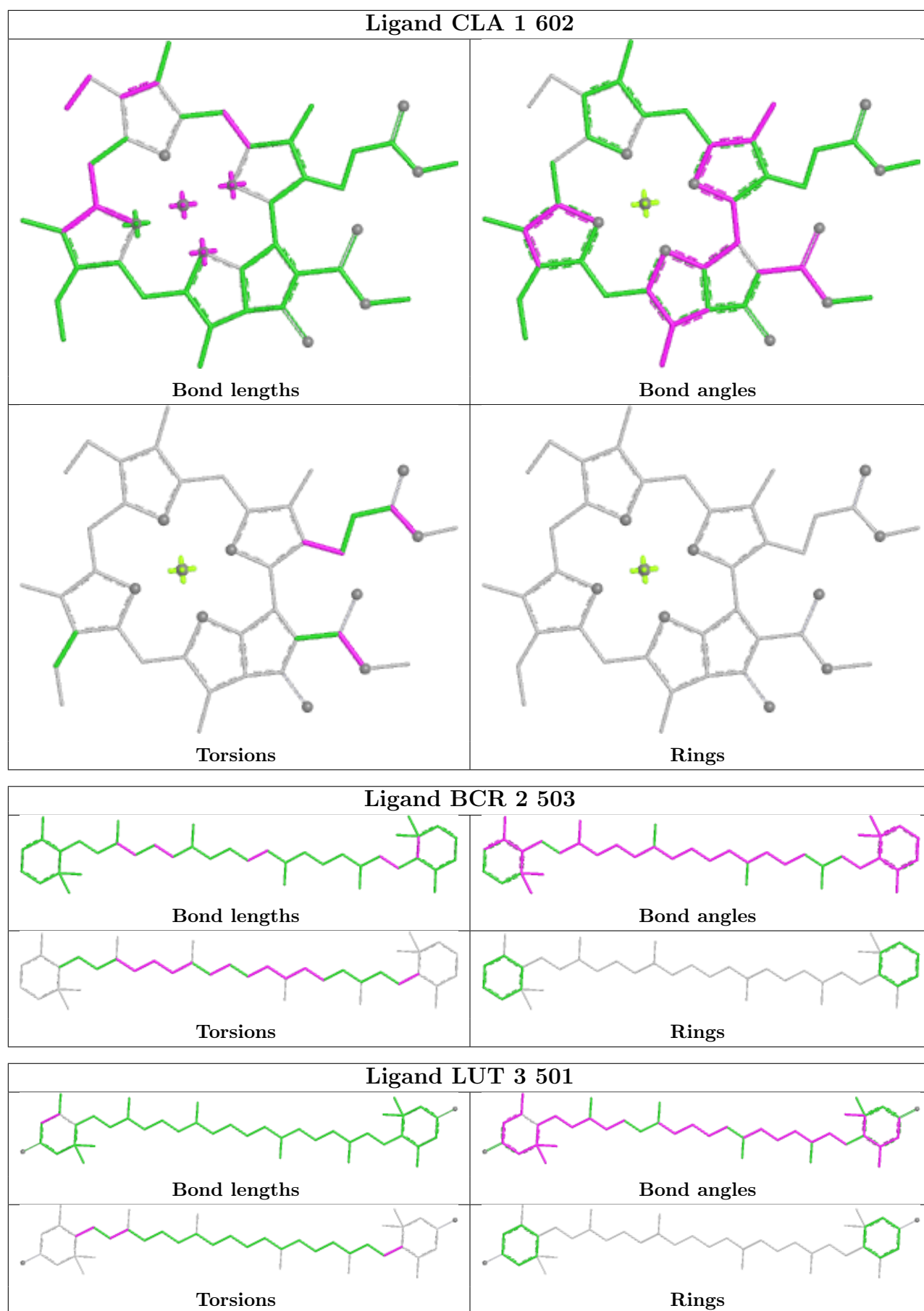


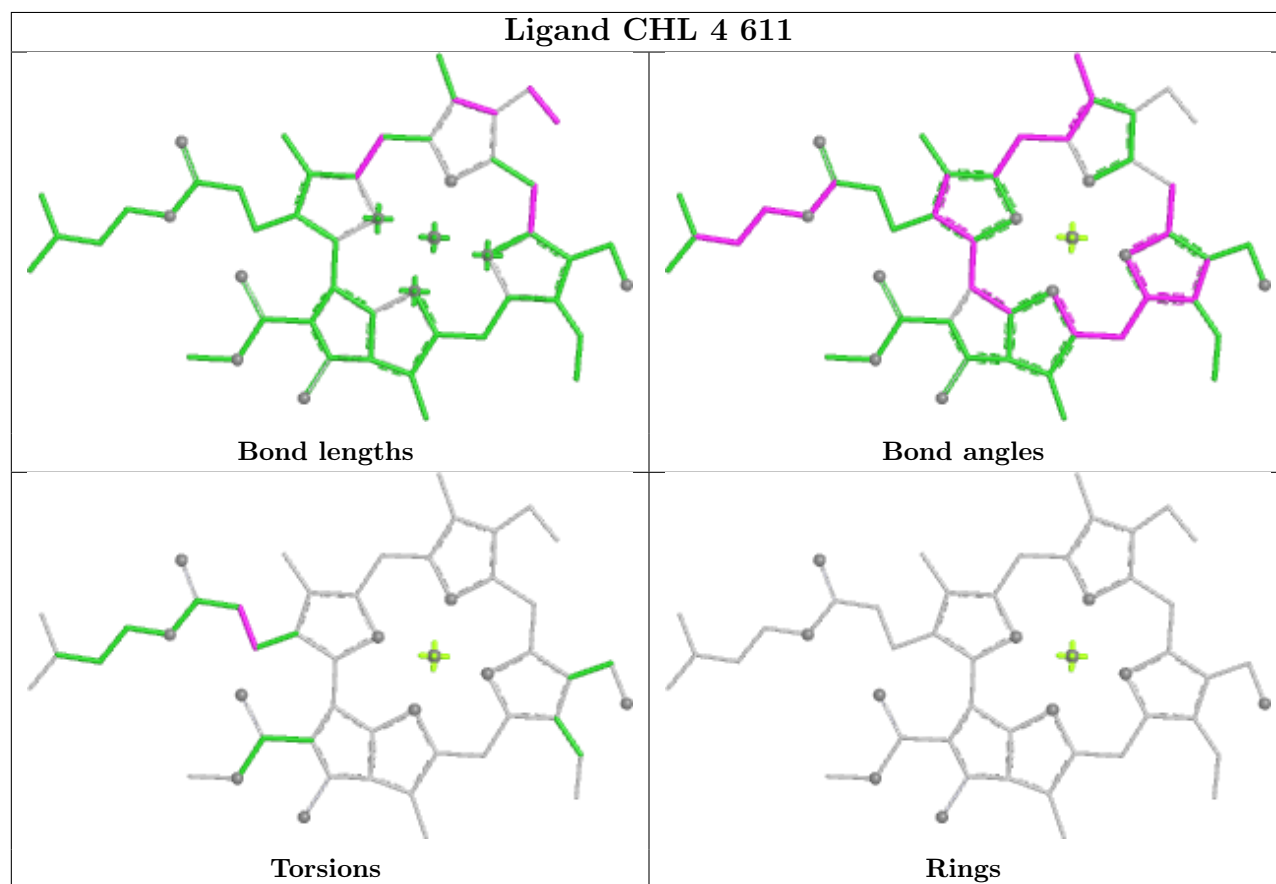
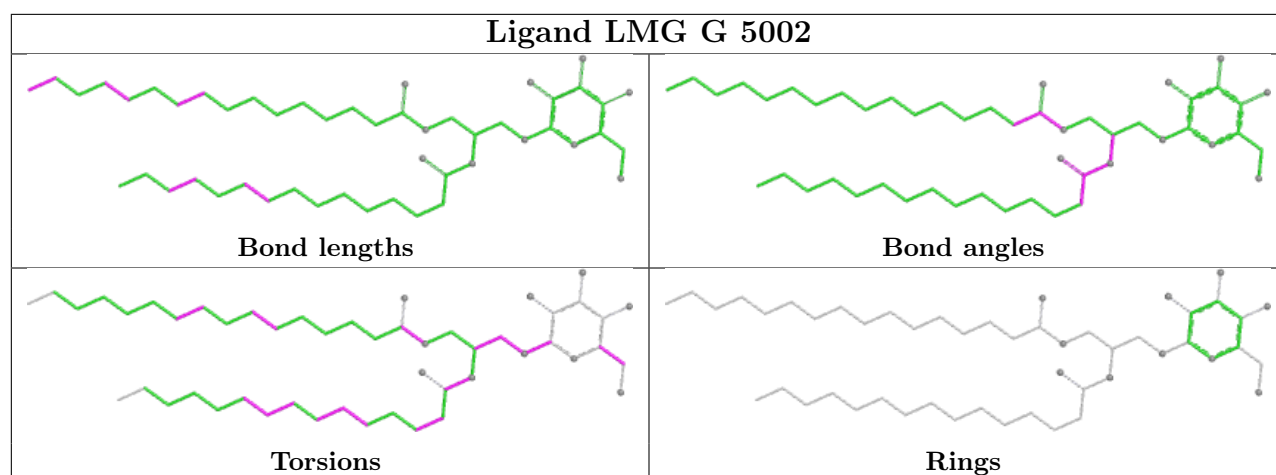
Torsions

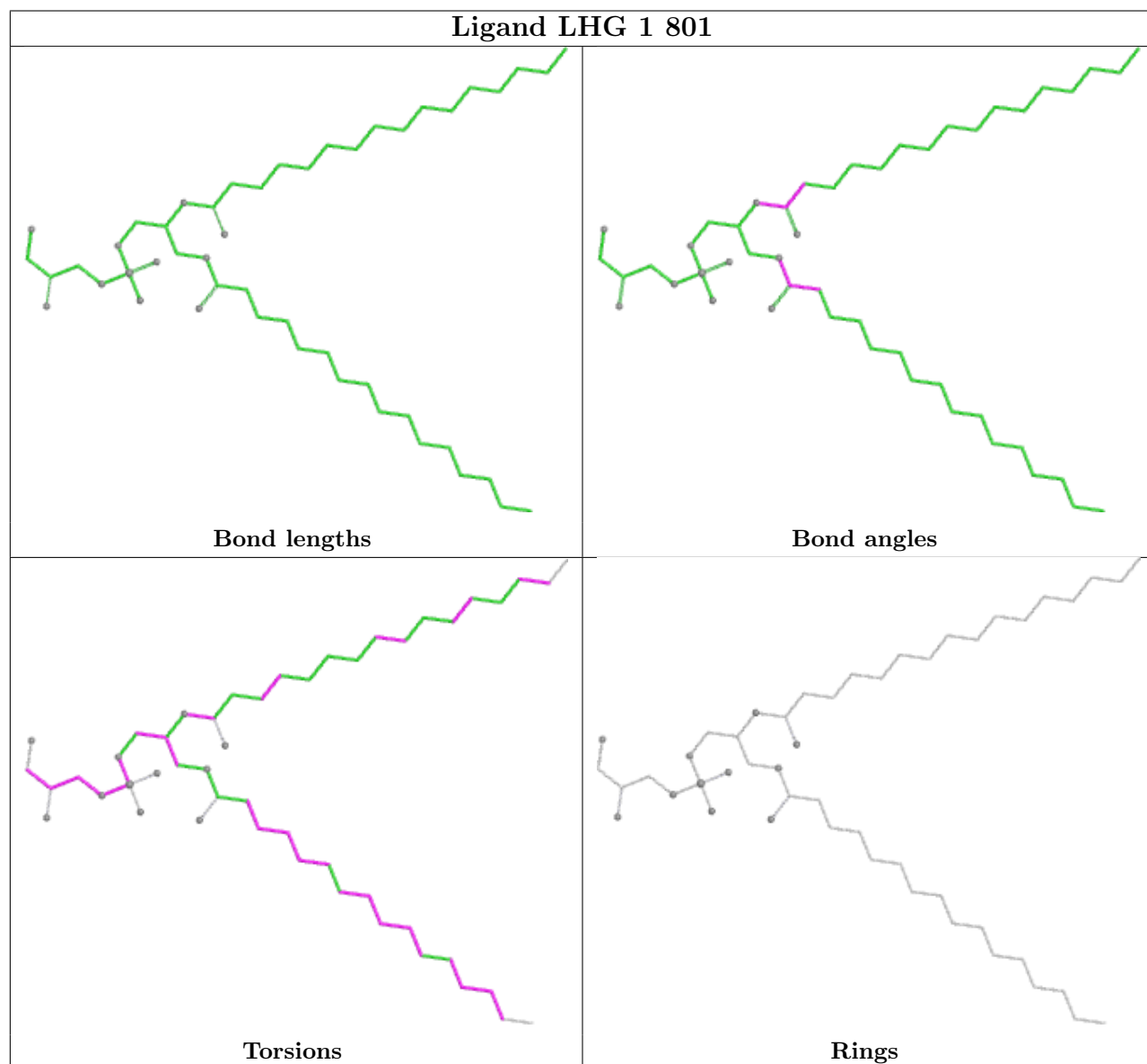
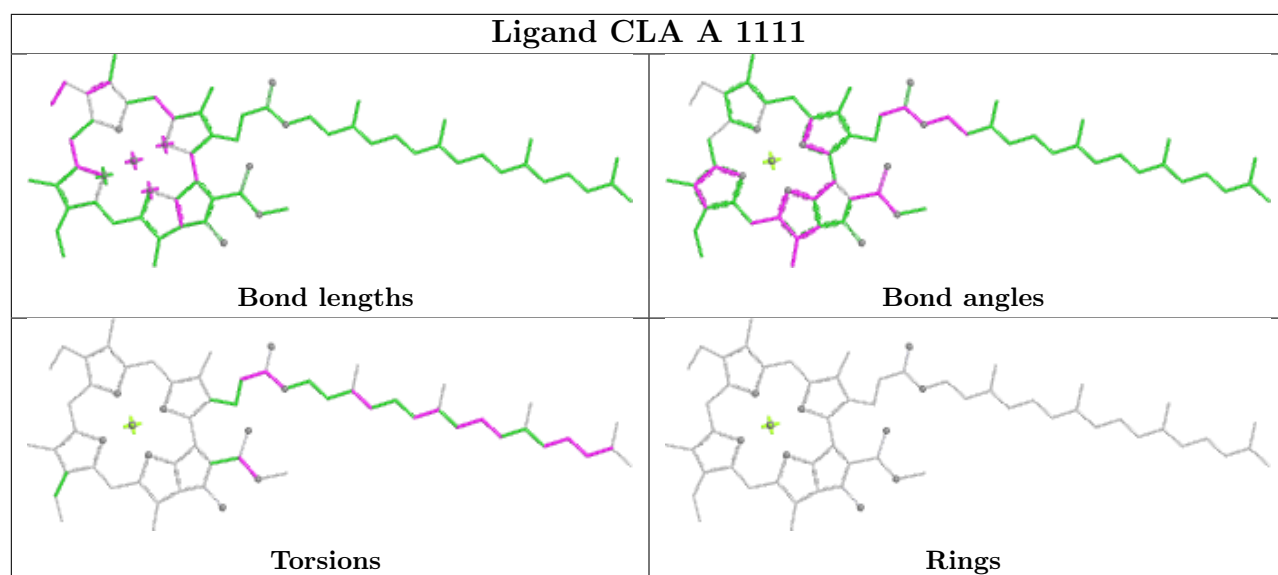


Rings

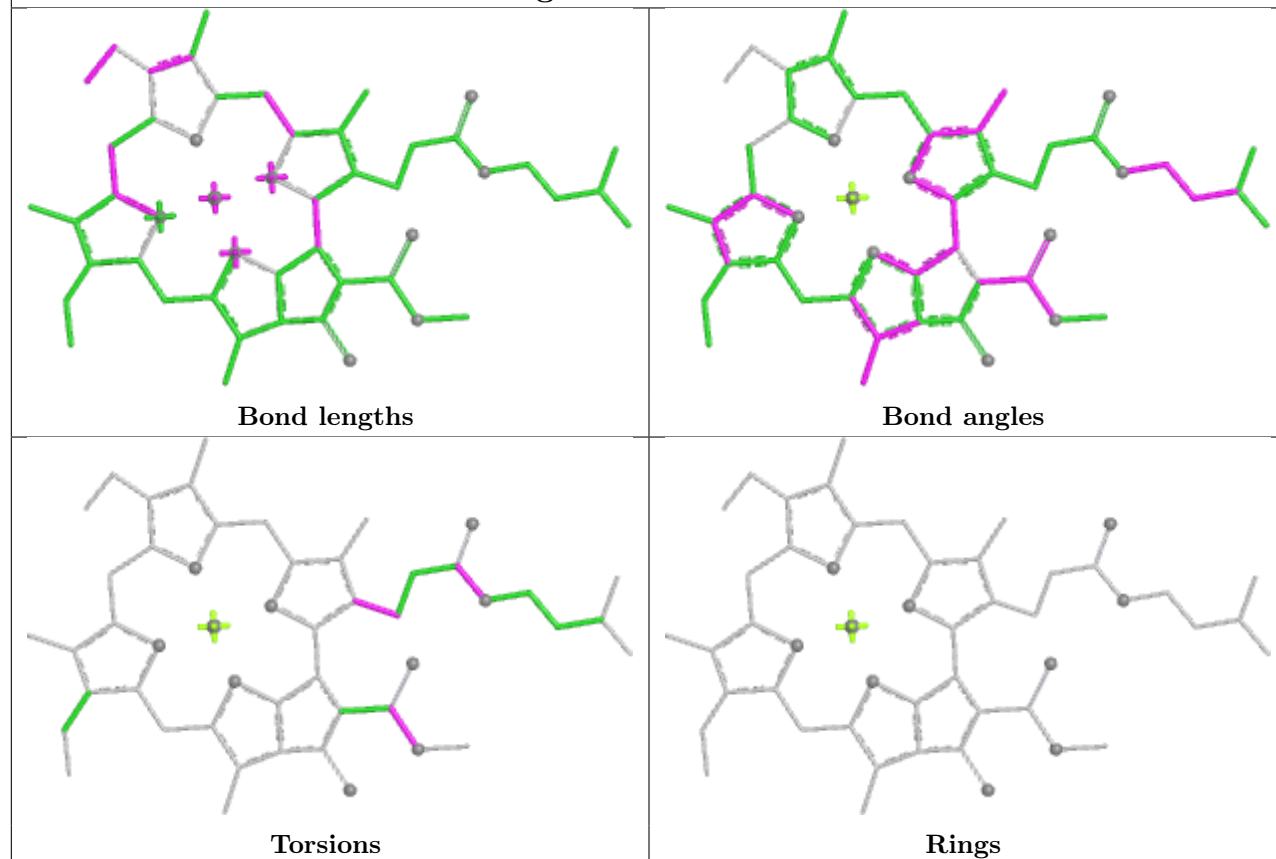




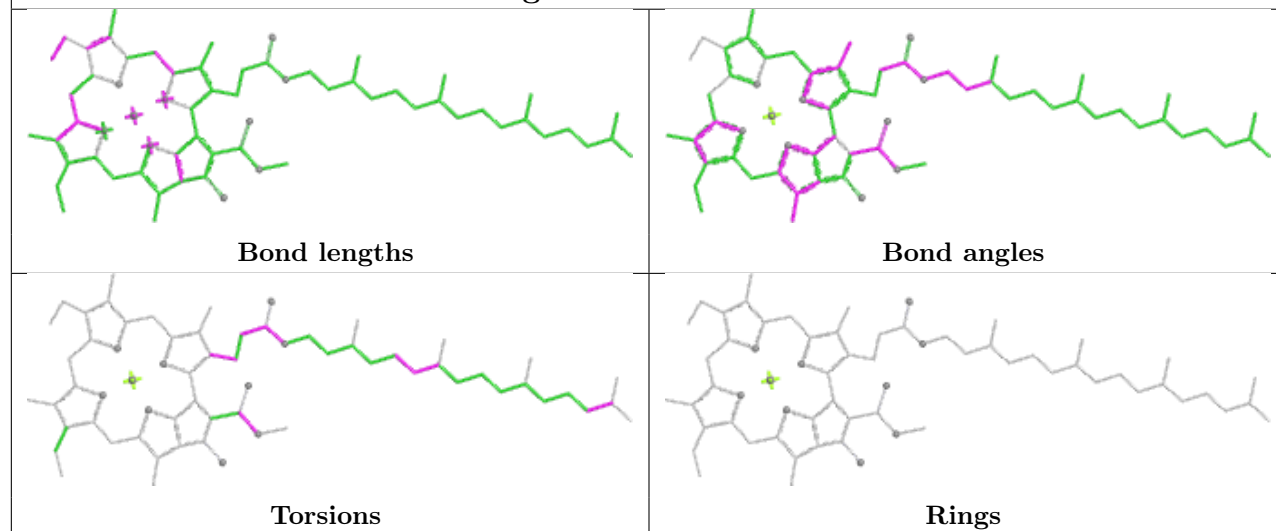


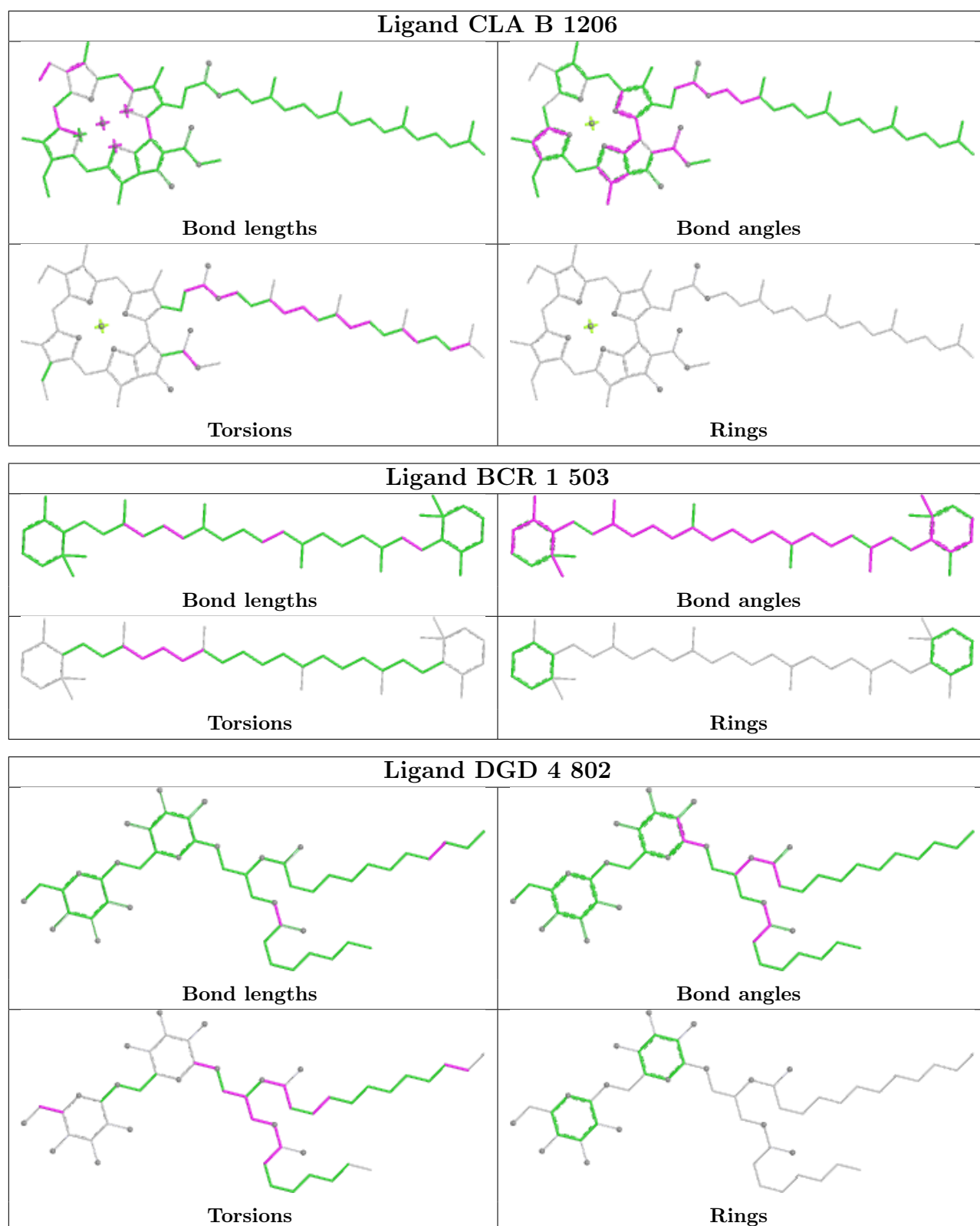


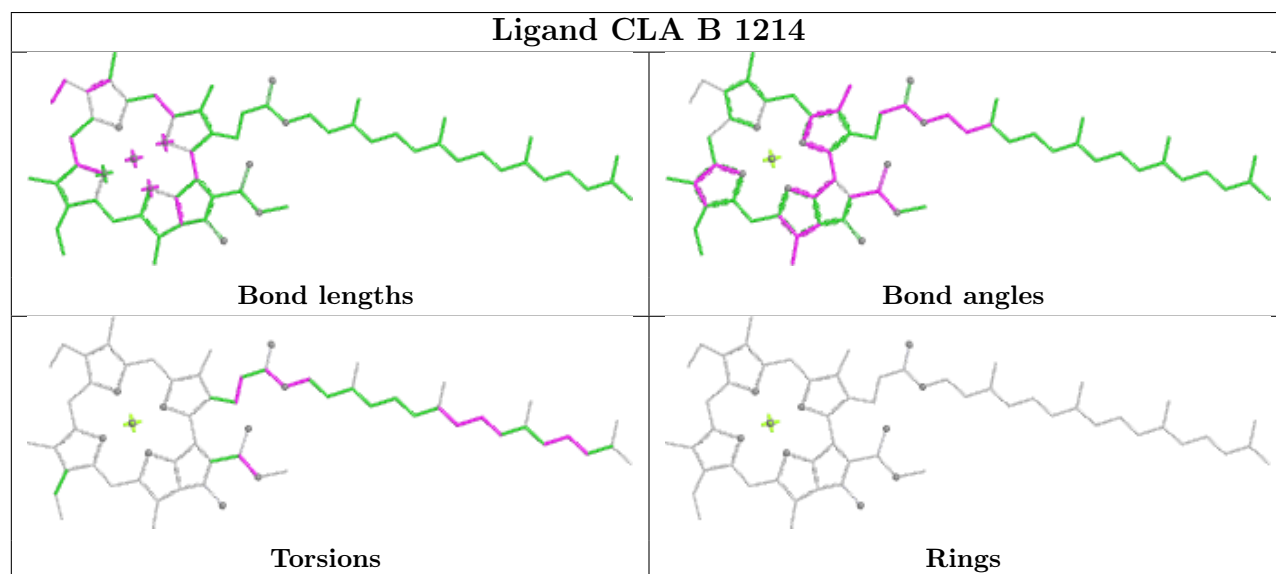
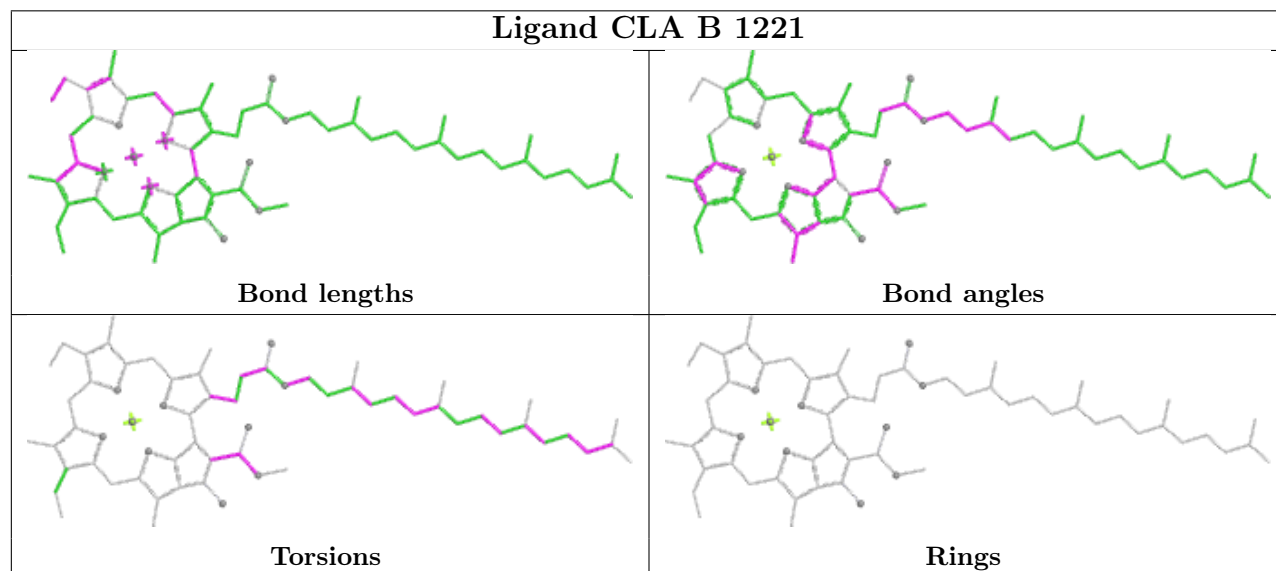
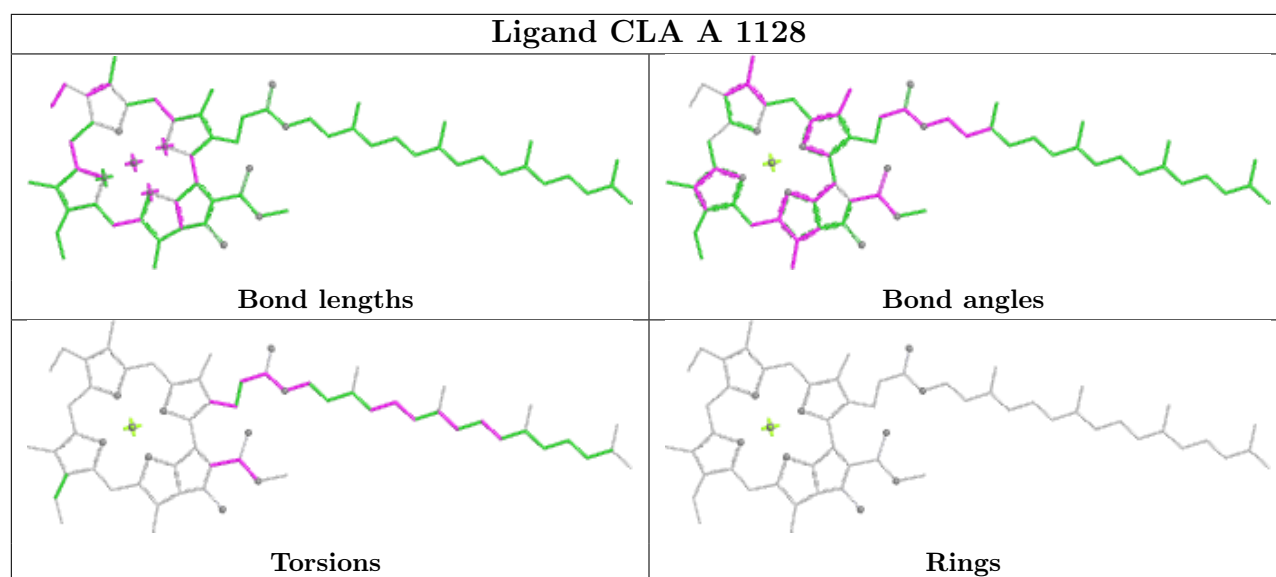
Ligand CLA 2 606

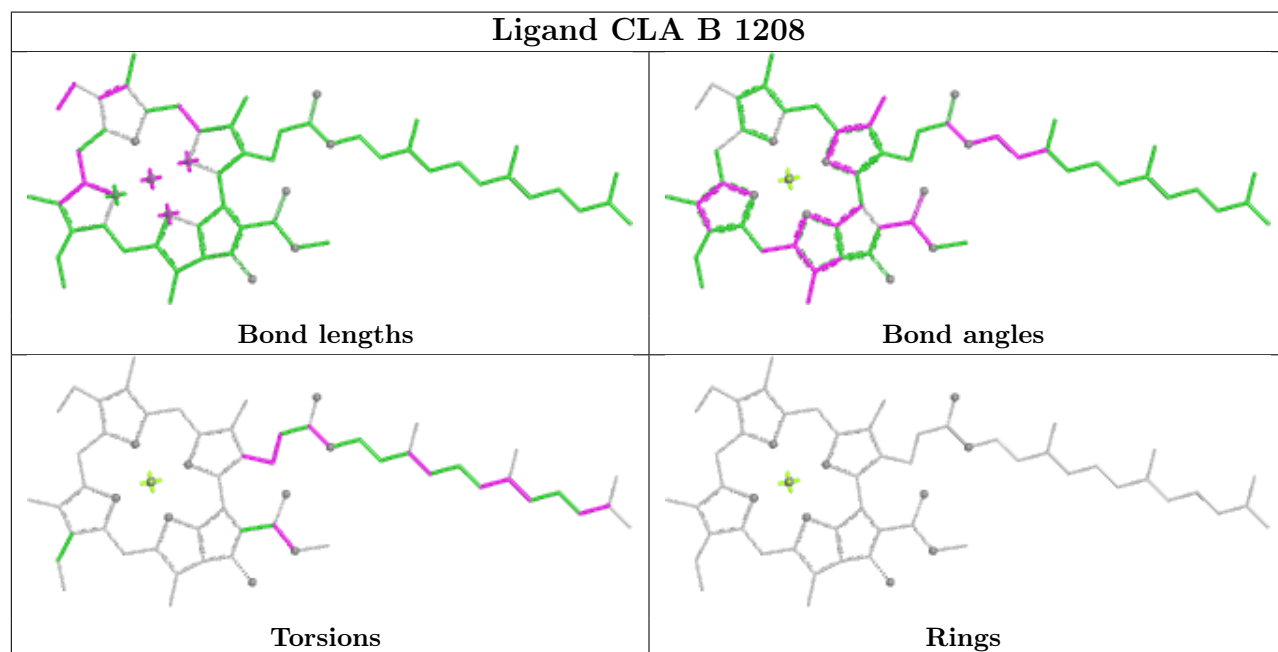
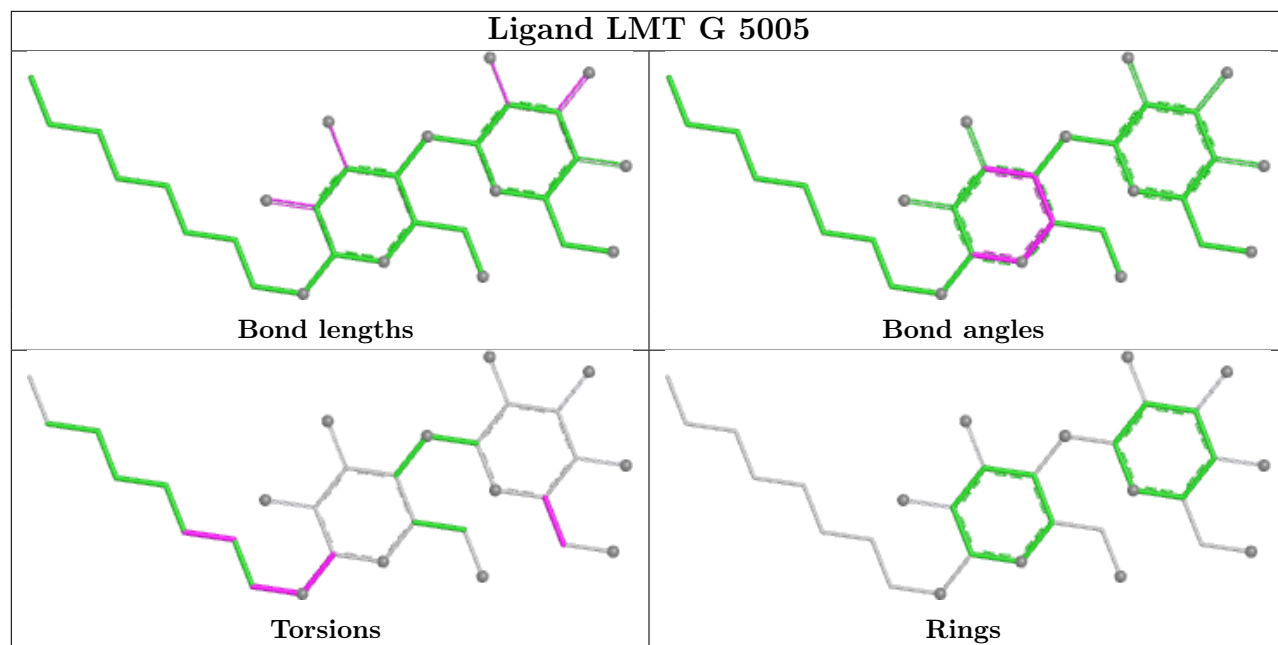


Ligand CLA A 1125

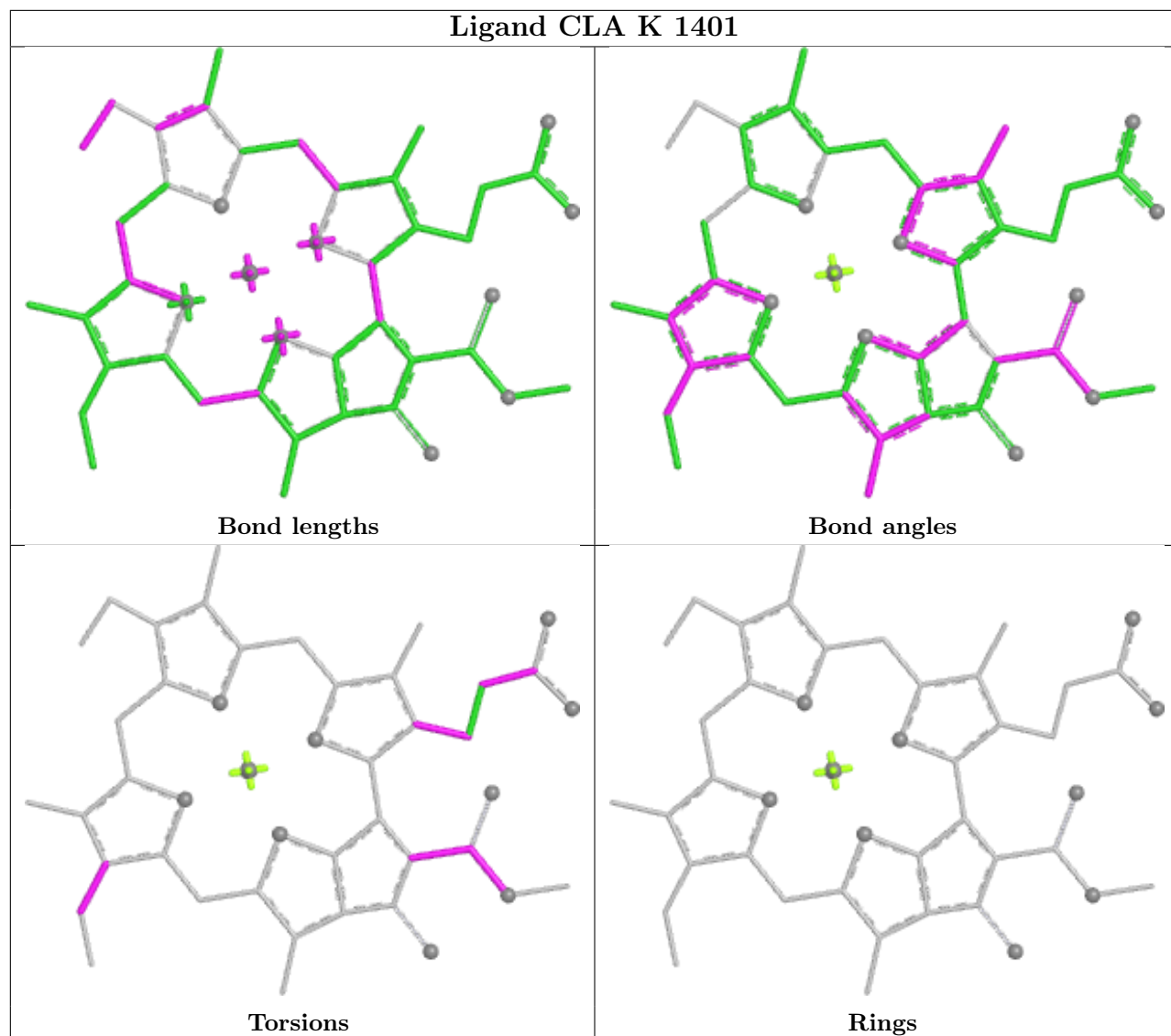




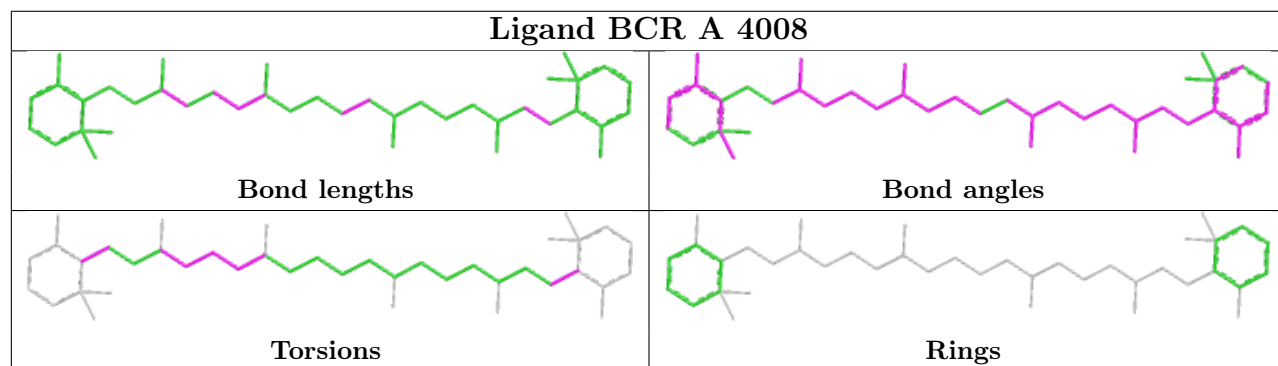


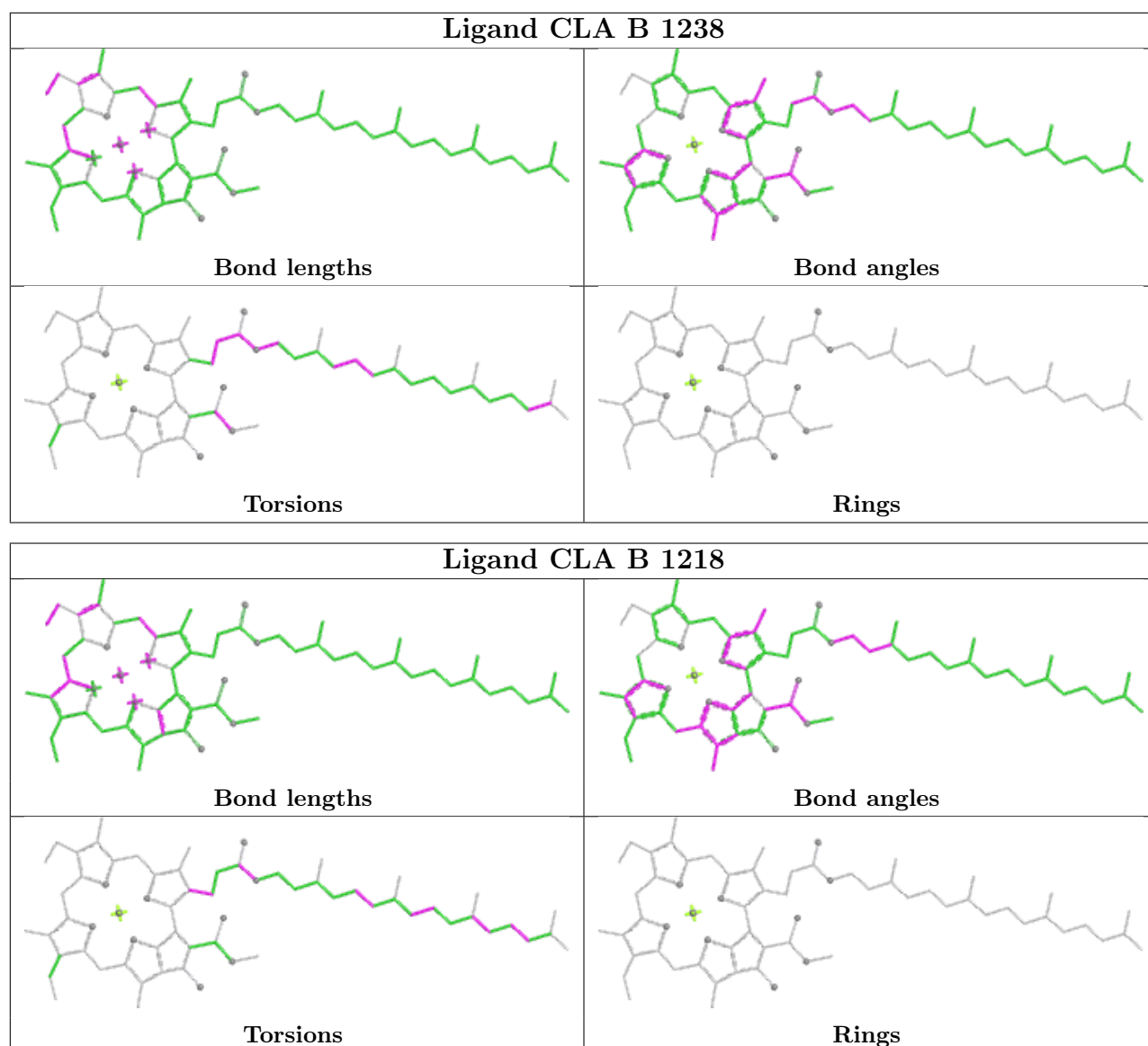


Ligand CLA K 1401

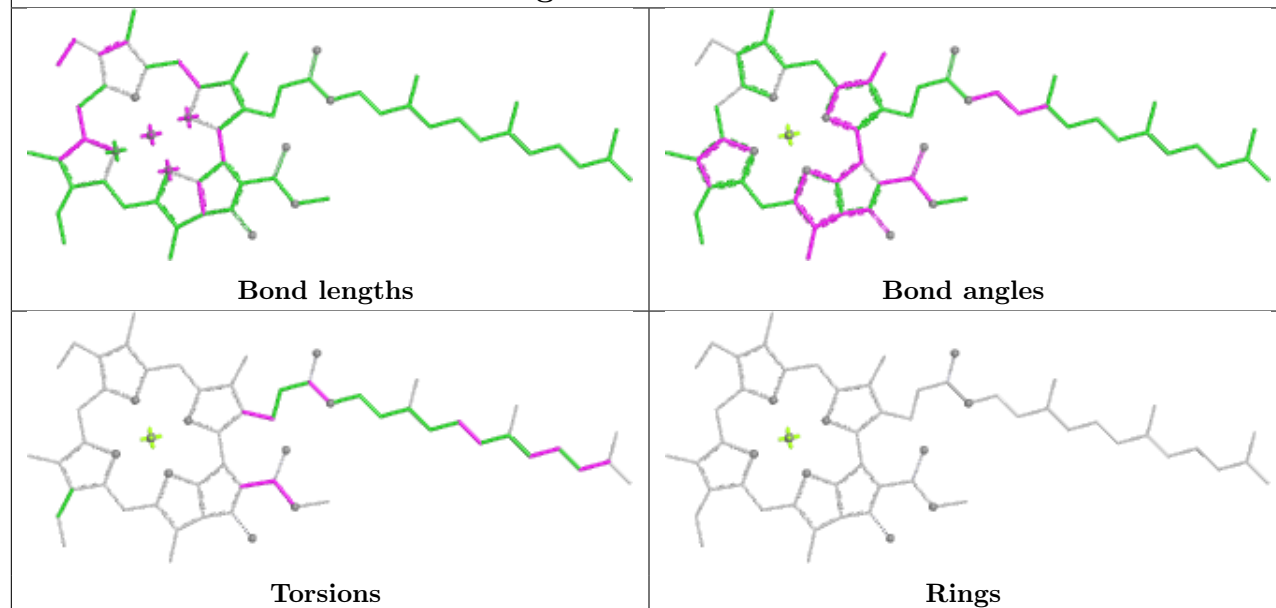


Ligand BCR A 4008

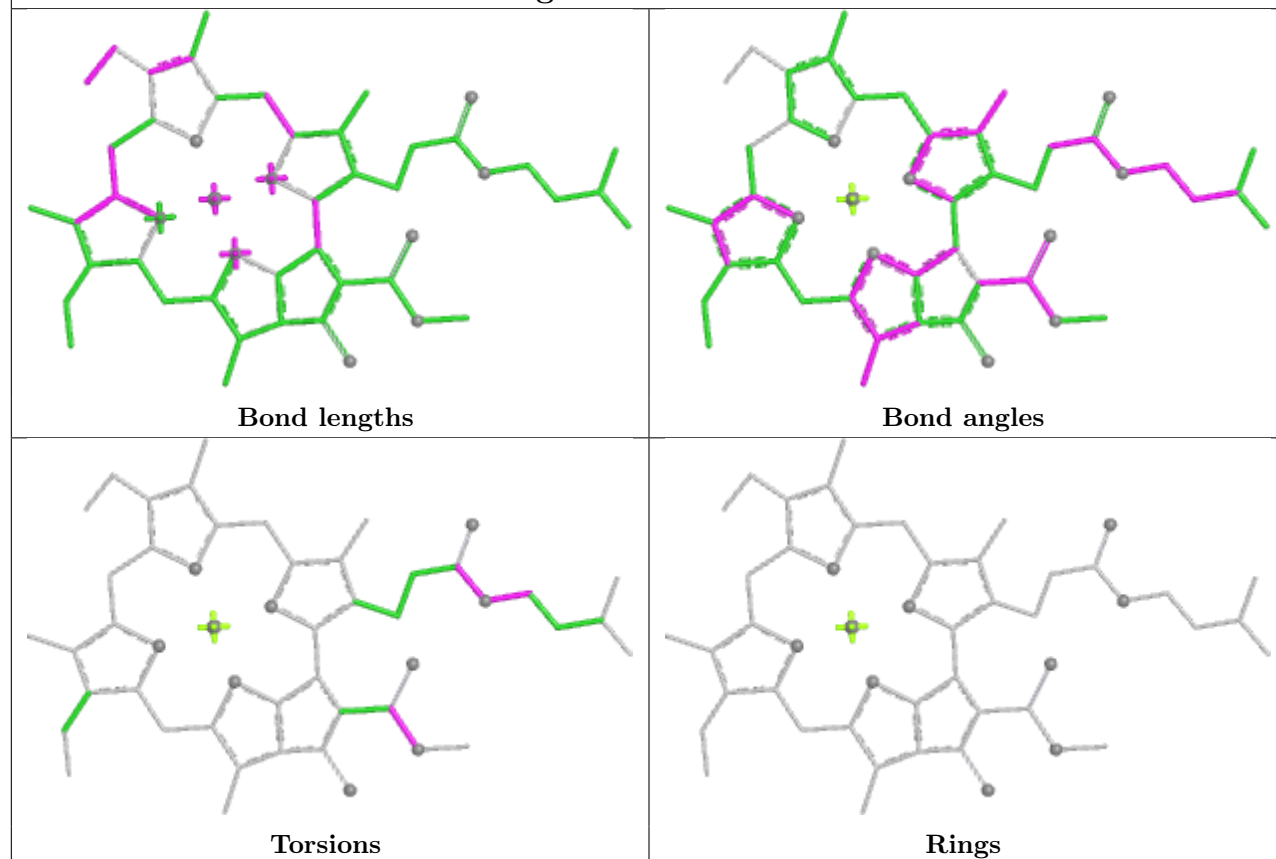


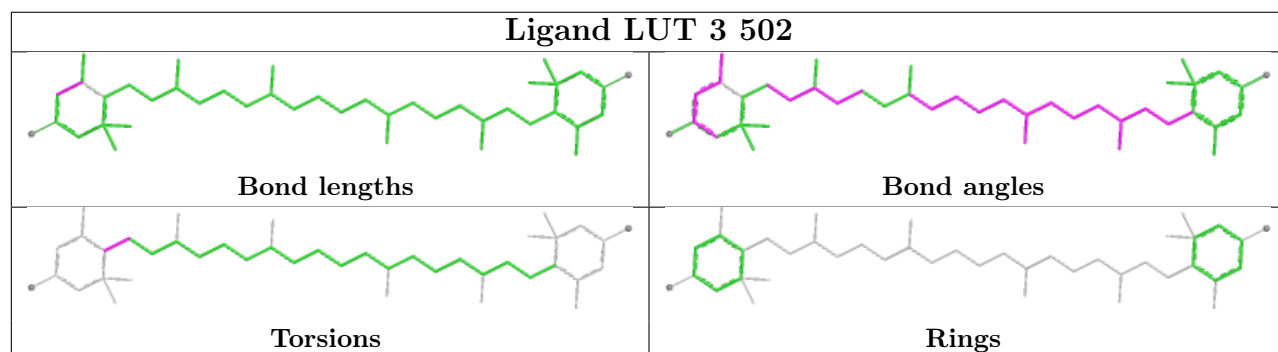
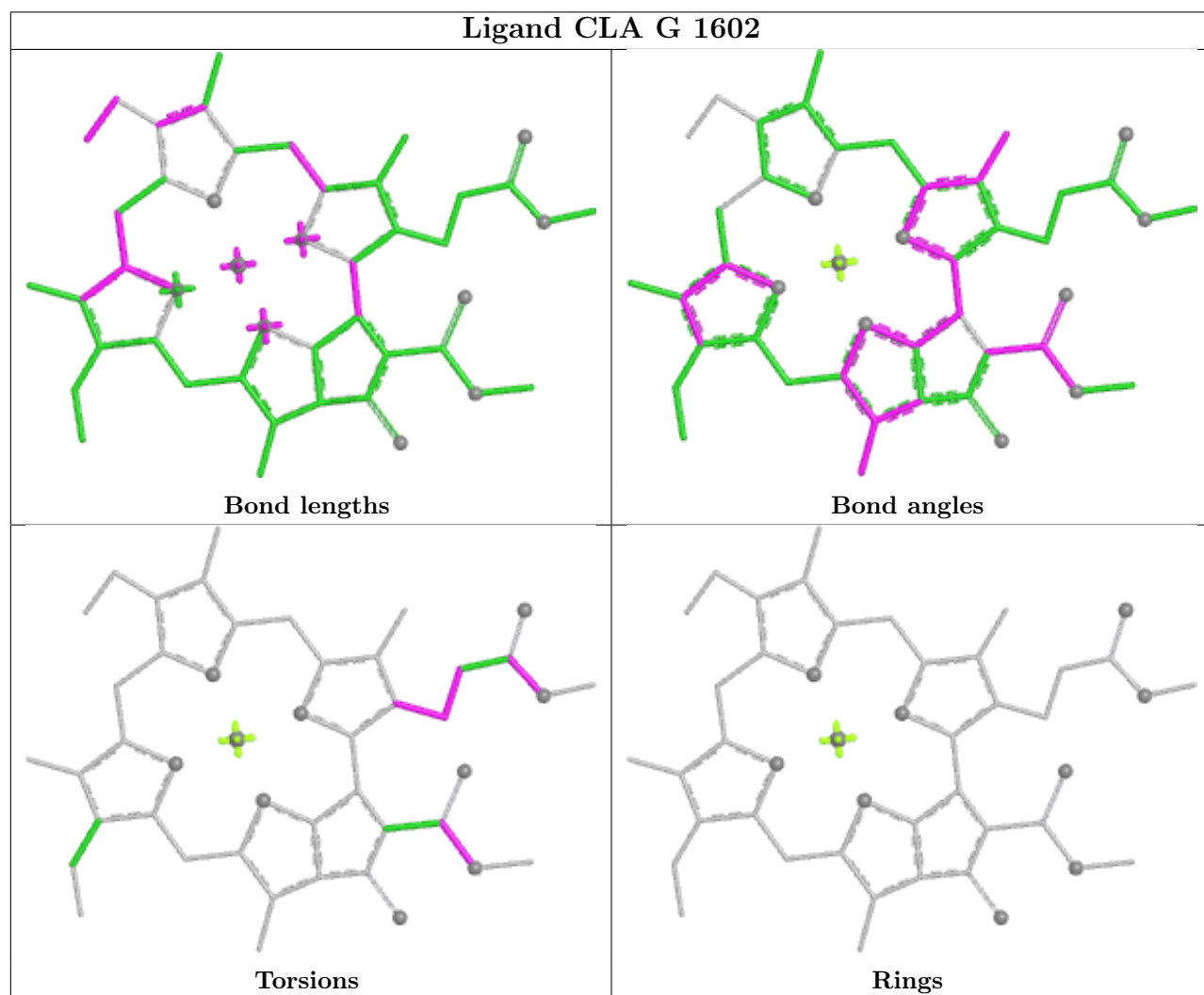
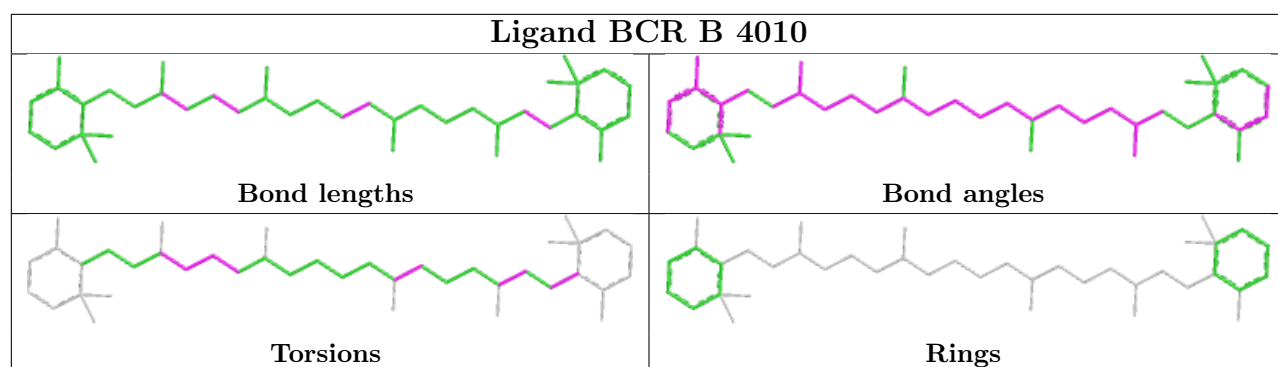


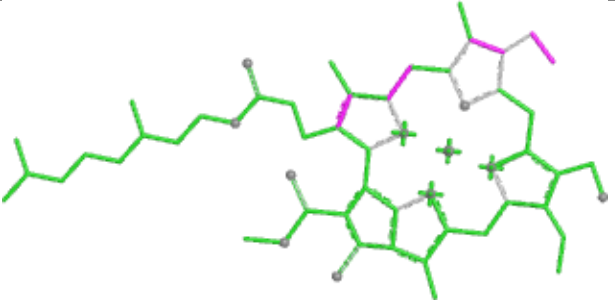
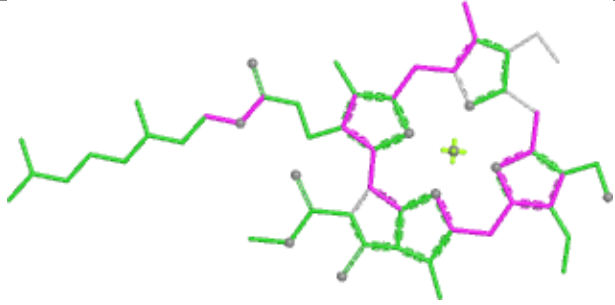
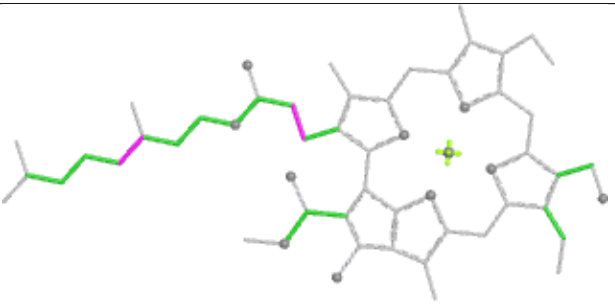
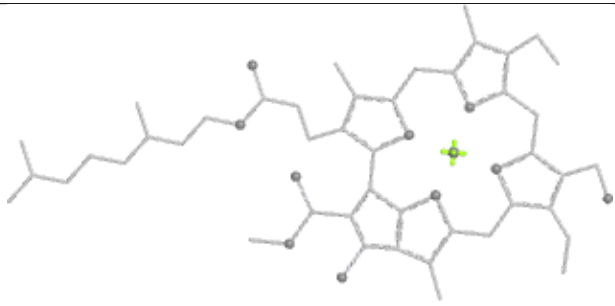
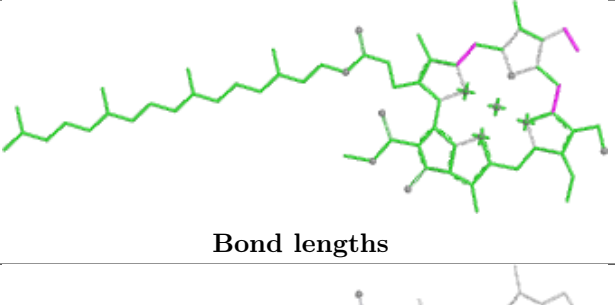
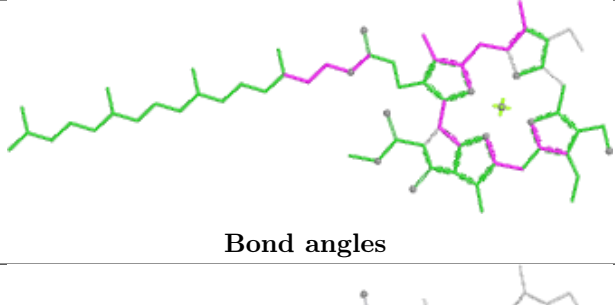
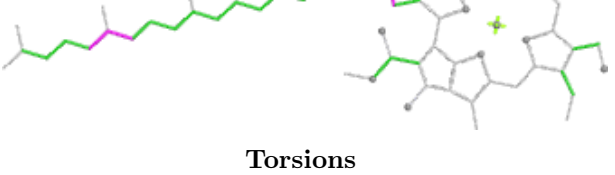

Ligand CLA 4 605

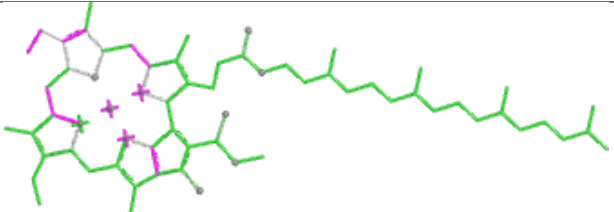
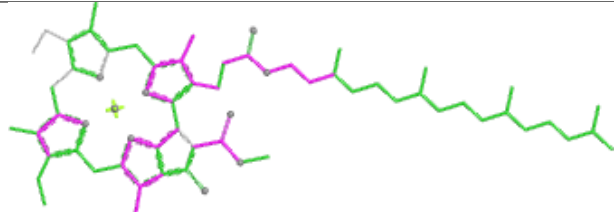
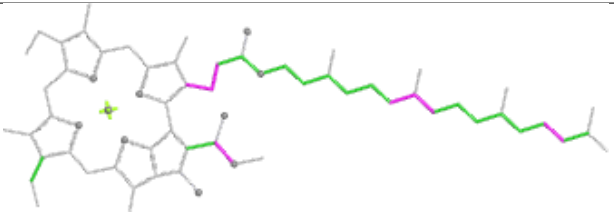
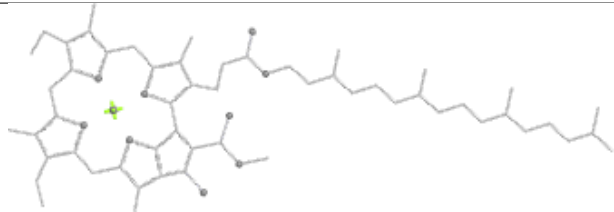


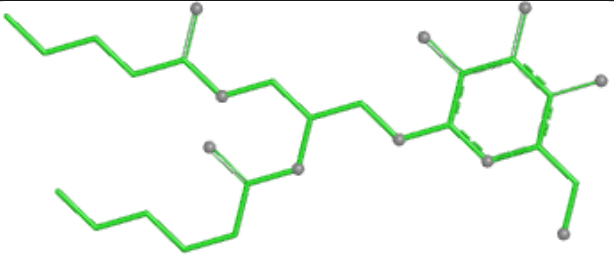
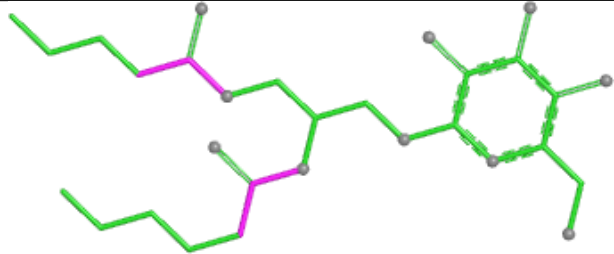
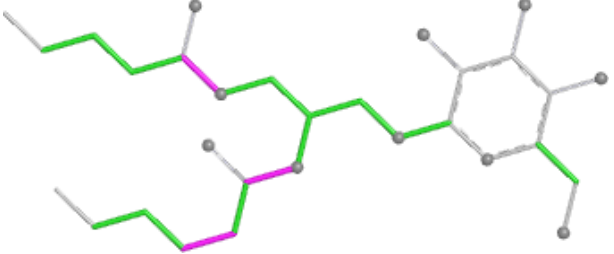
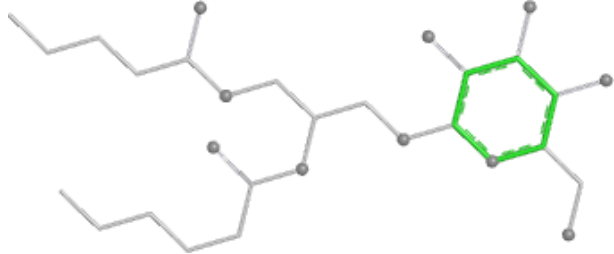
Ligand CLA 4 602

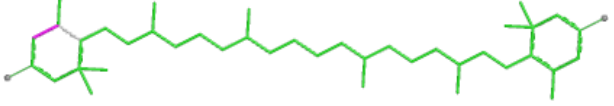
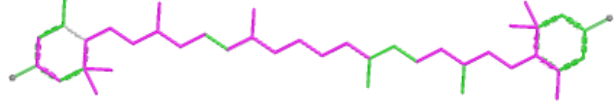
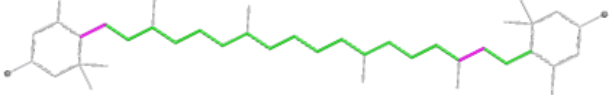
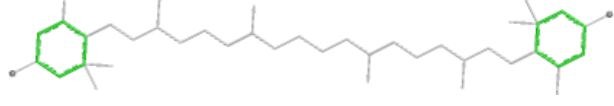


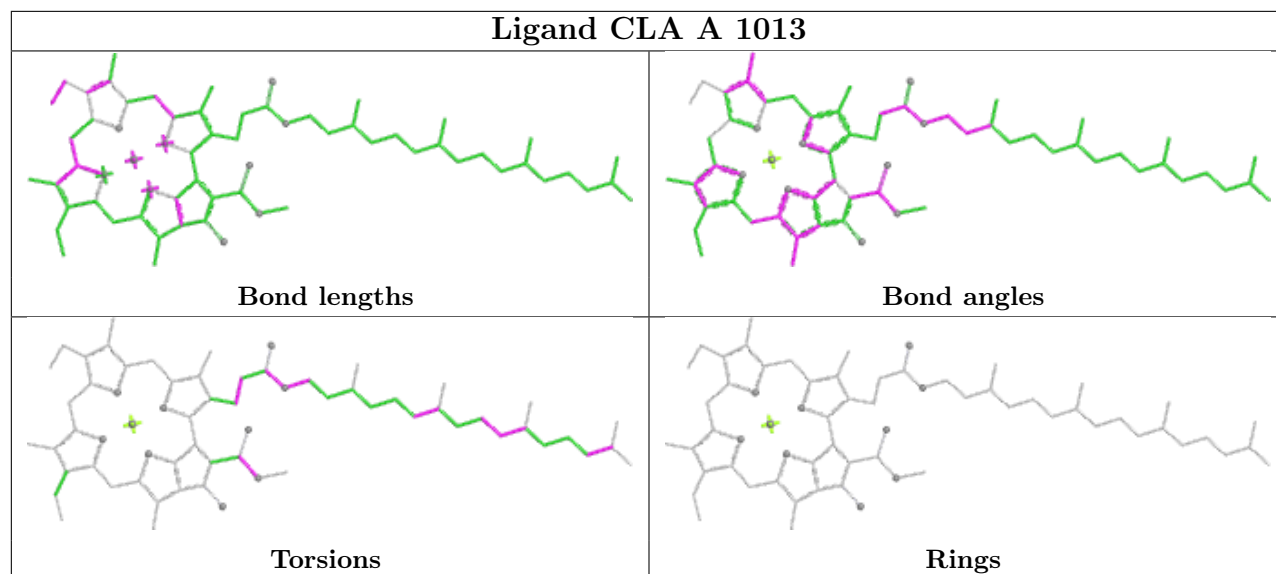
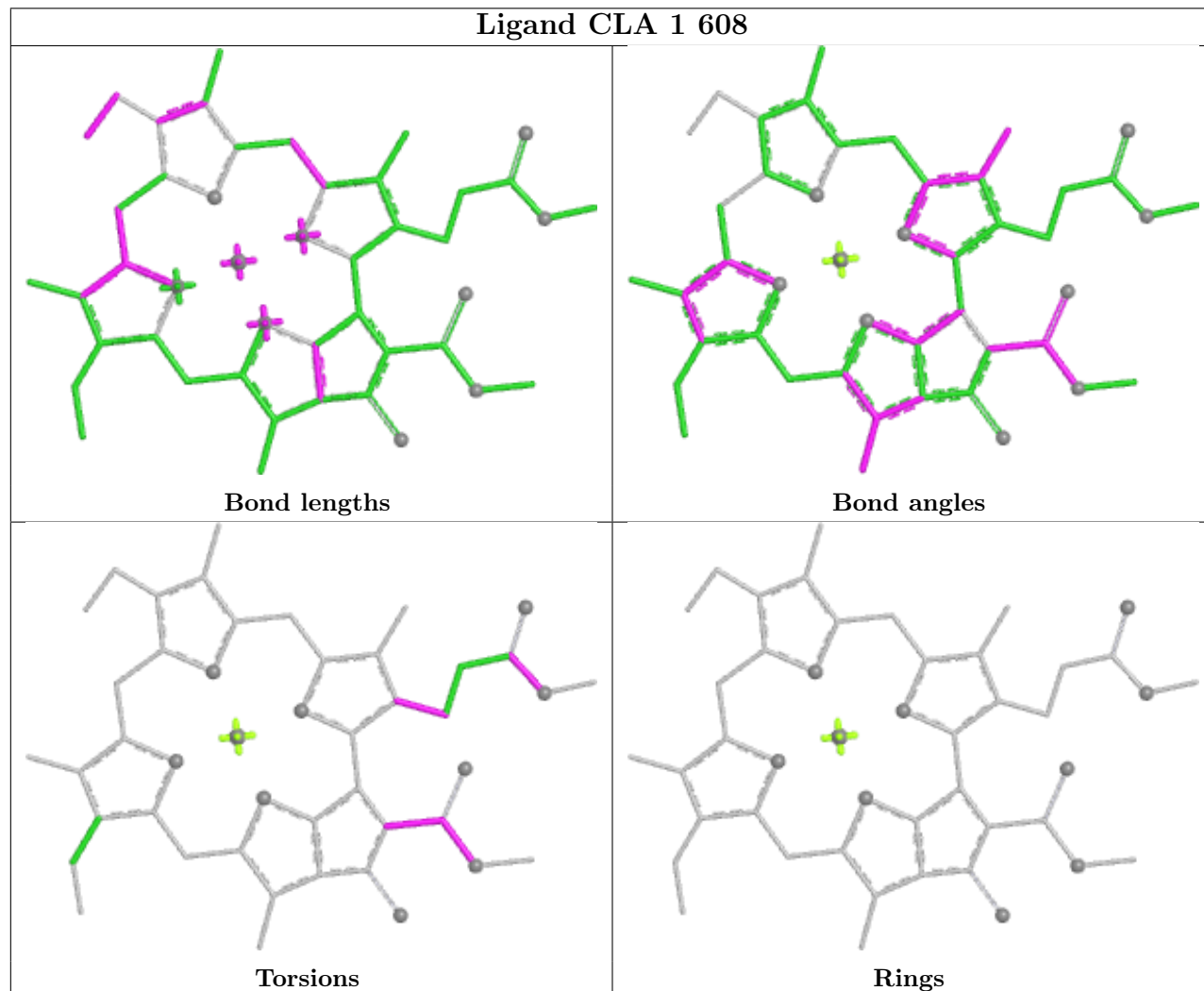


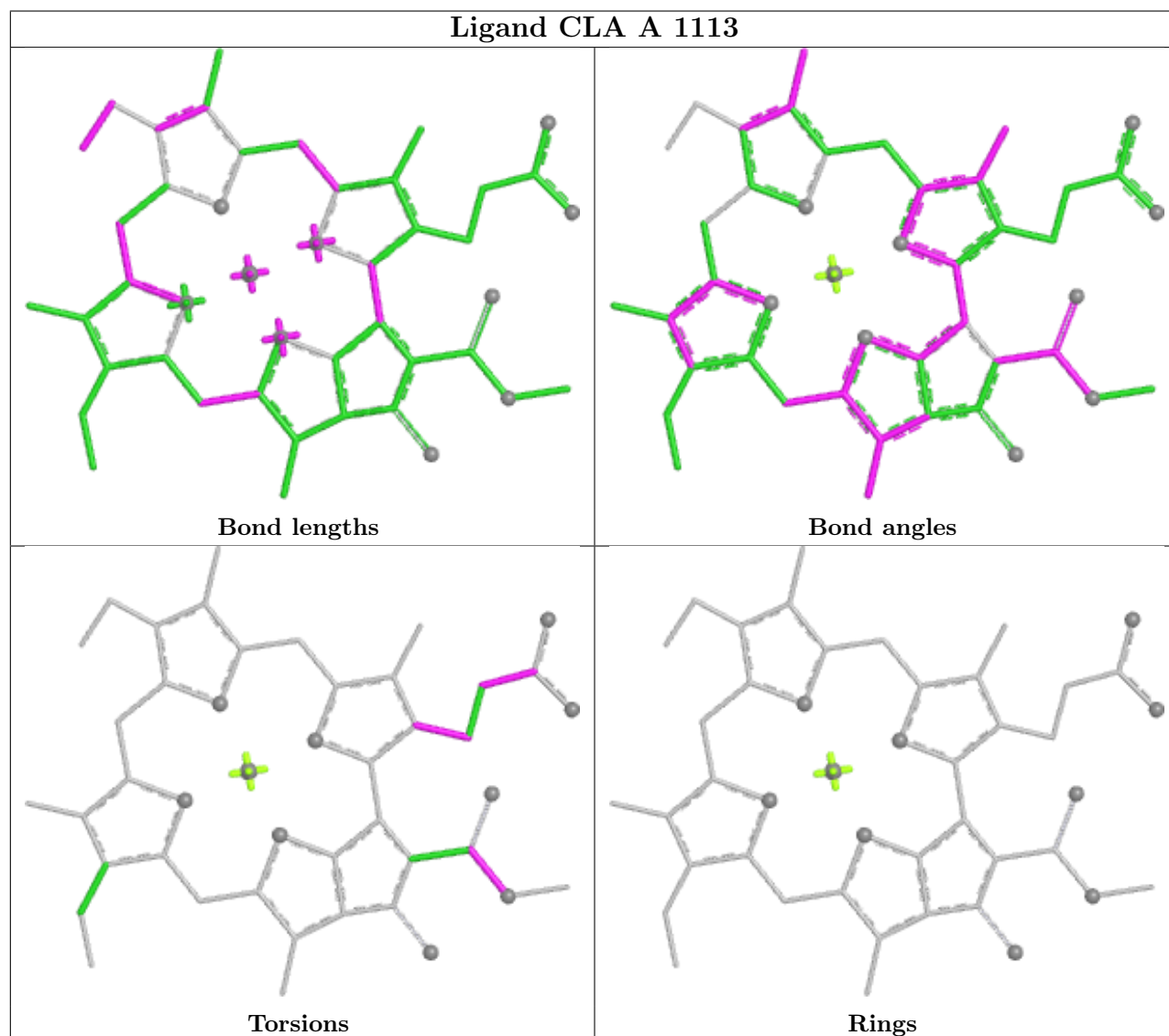
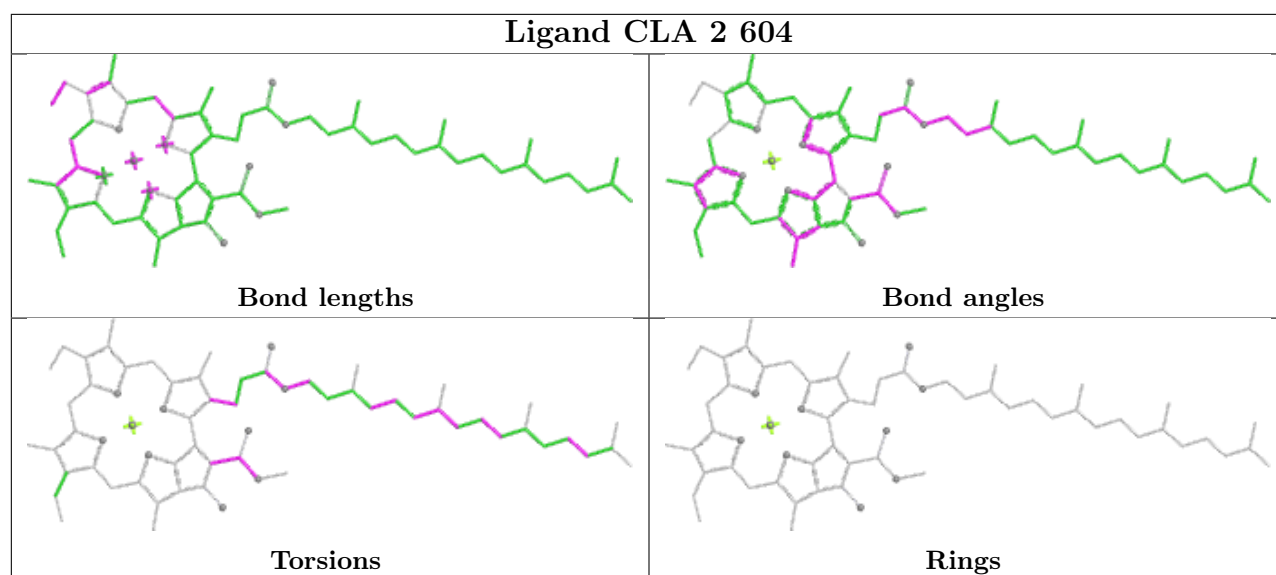
Ligand CHL 1 609	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CHL 3 604	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

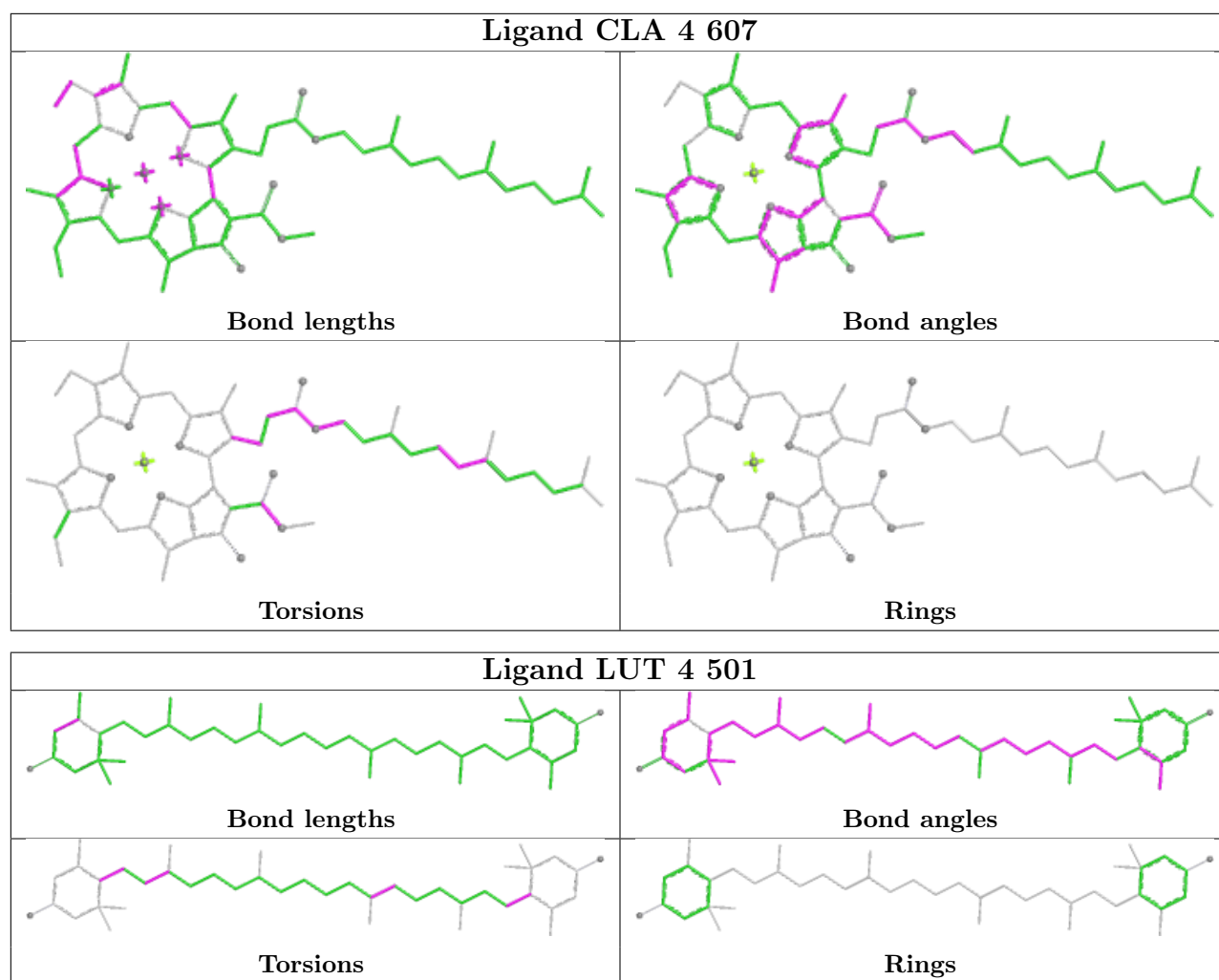
Ligand CLA B 1239	
	
Bond lengths	Bond angles
	
Torsions	Rings

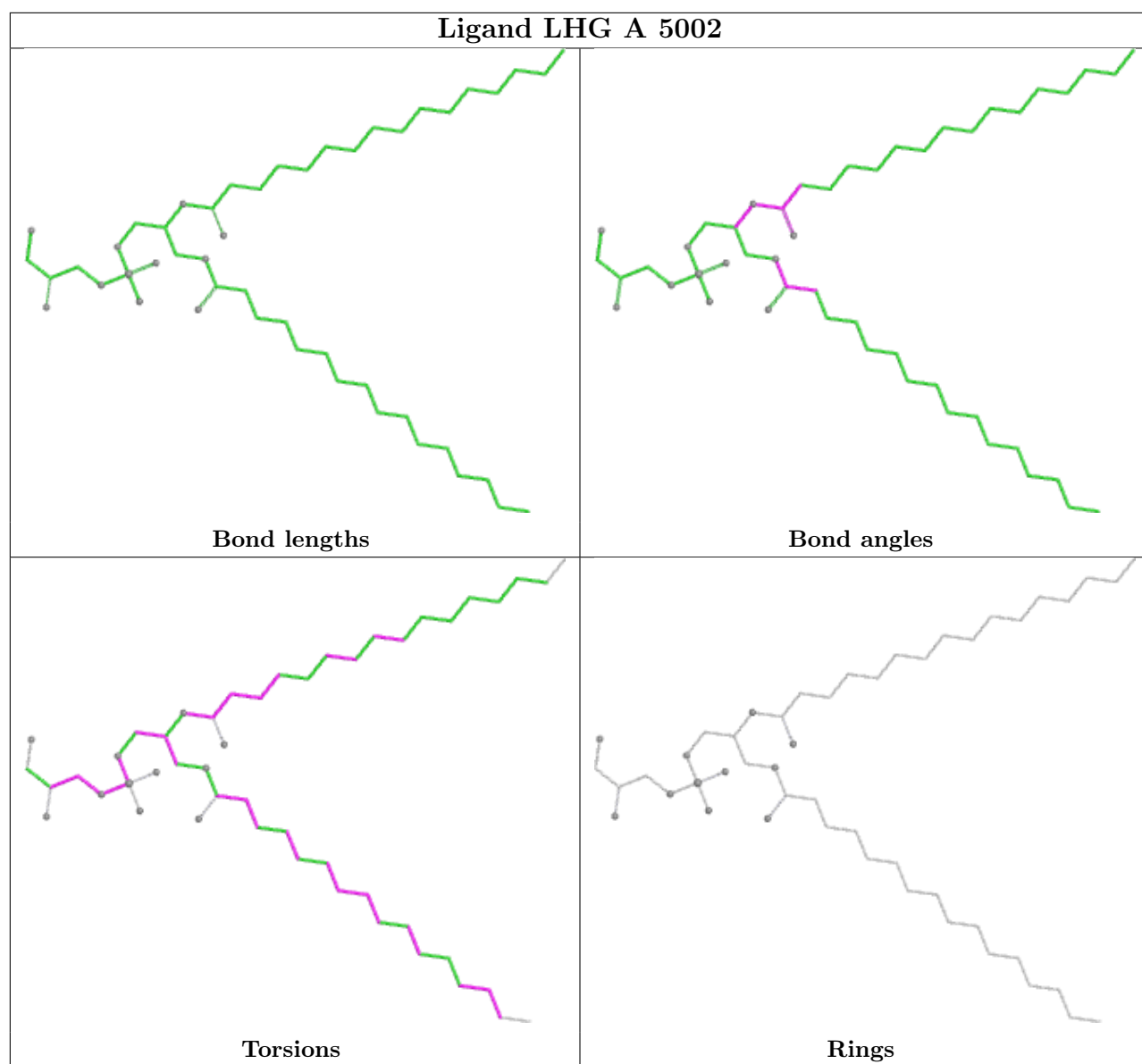
Ligand LMG 2 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 4 505	
	
Bond lengths	Bond angles
	
Torsions	Rings

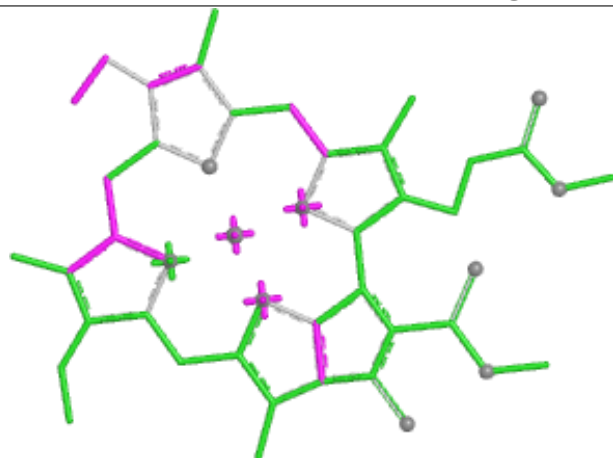
Ligand CLA A 1013**Ligand CLA 1 608**



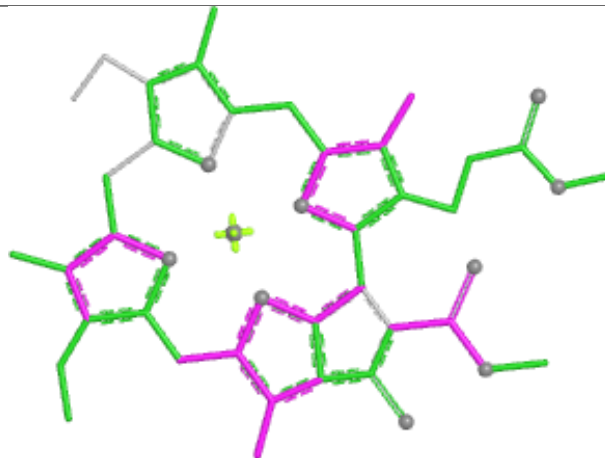




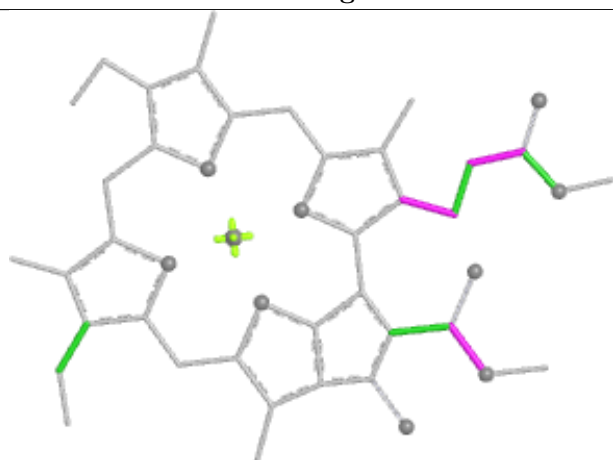
Ligand CLA B 1209



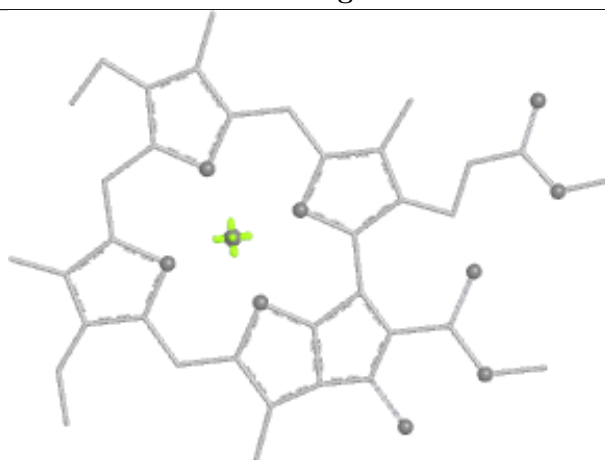
Bond lengths



Bond angles

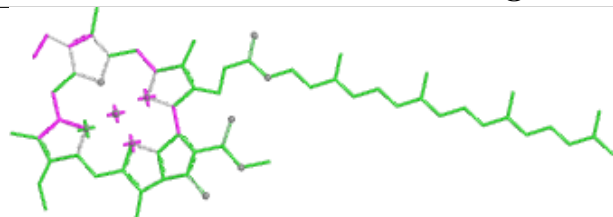


Torsions

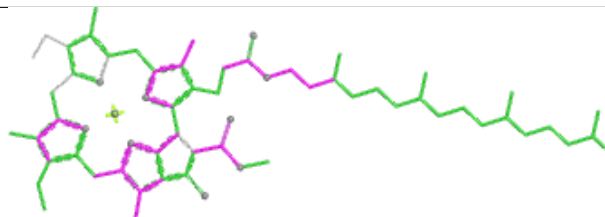


Rings

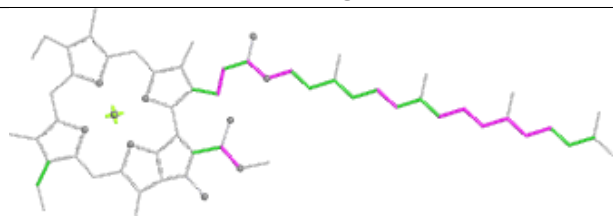
Ligand CLA B 1201



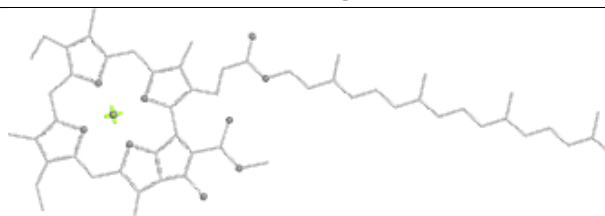
Bond lengths



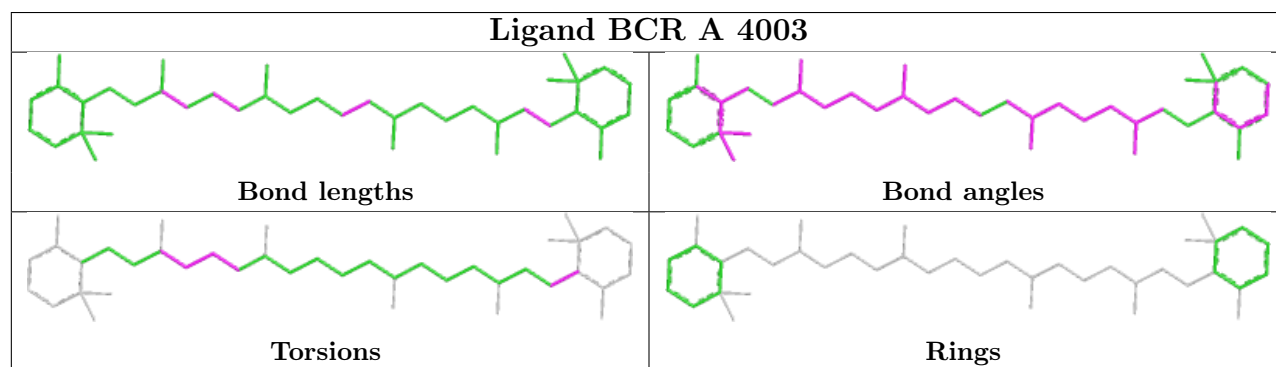
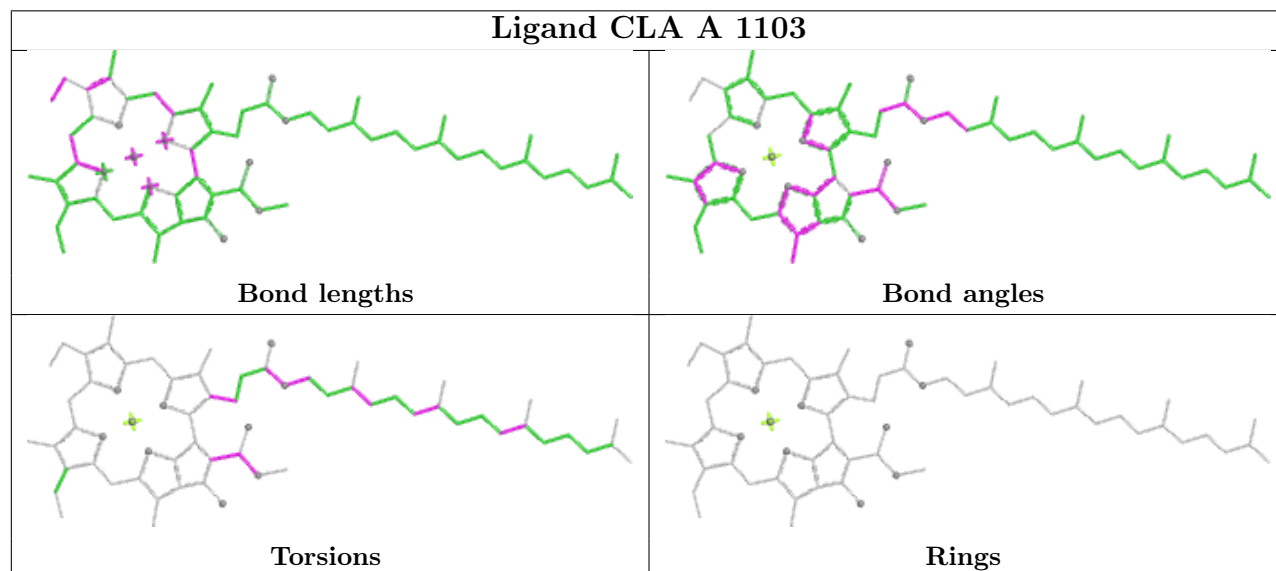
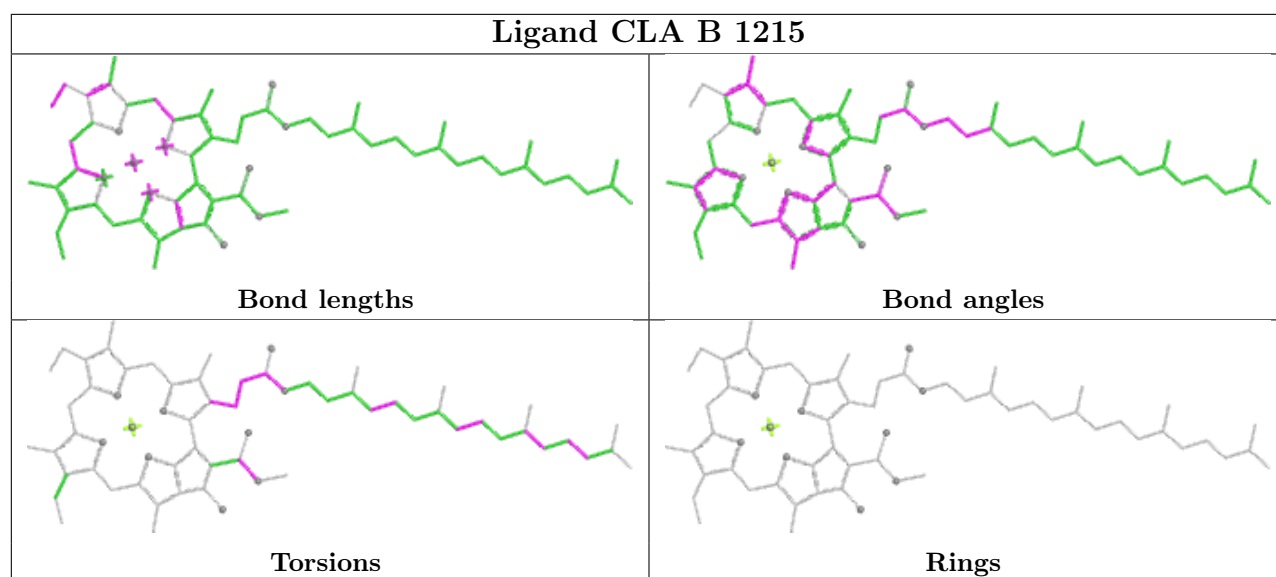
Bond angles

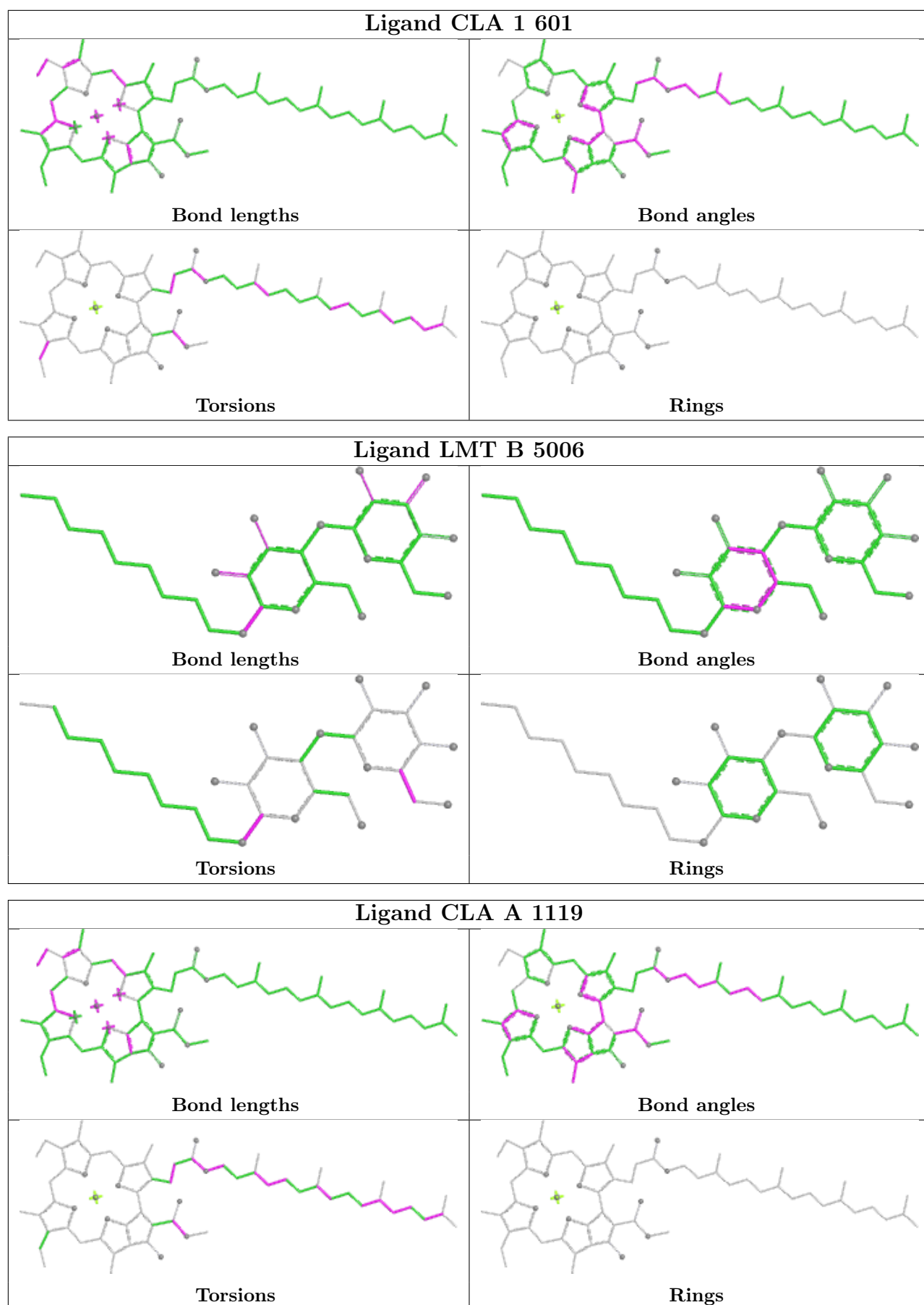


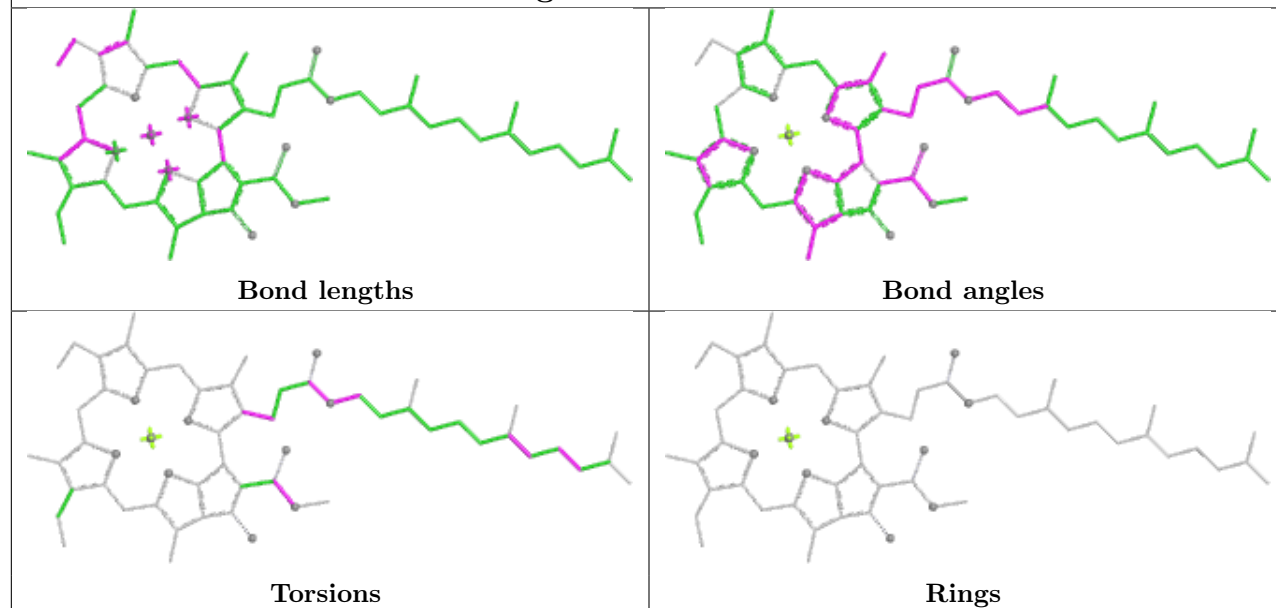
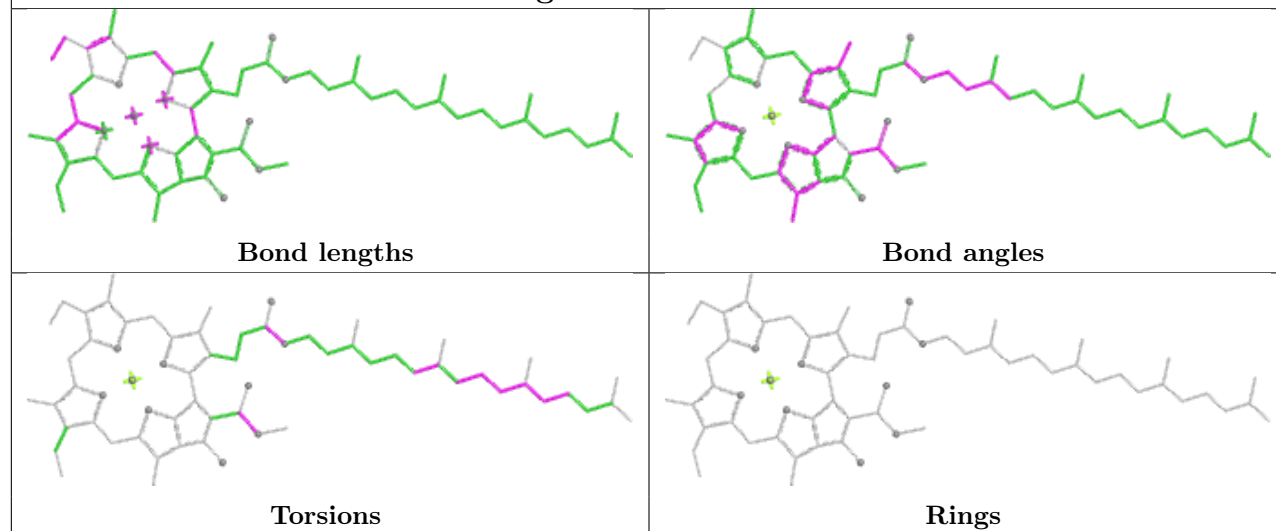
Torsions

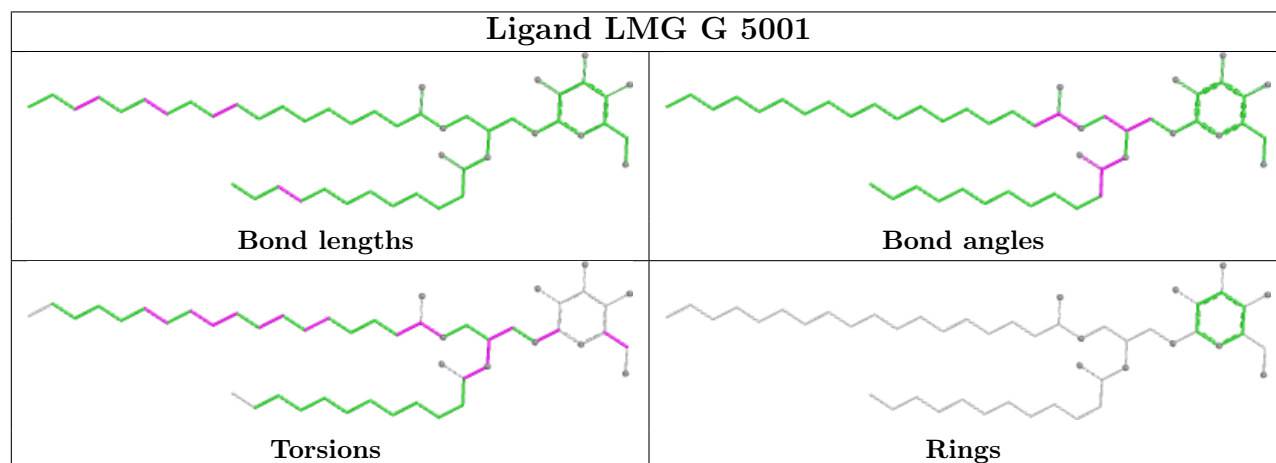
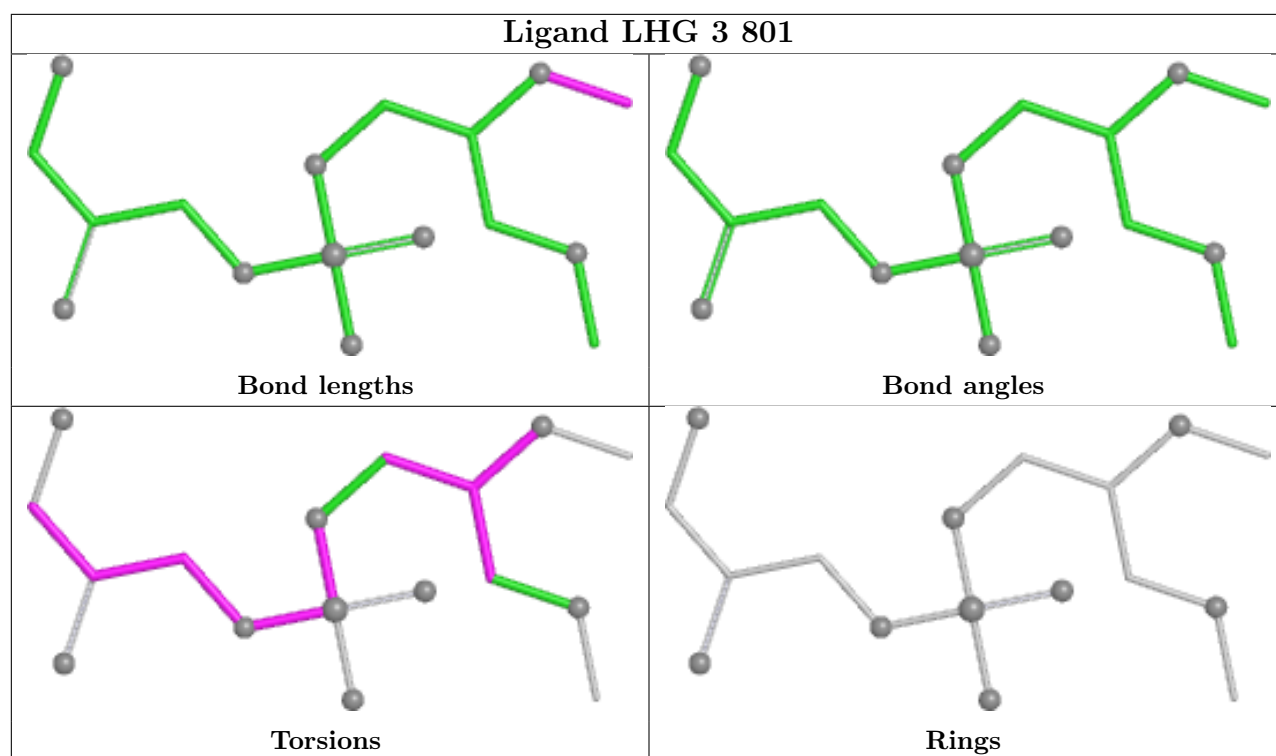


Rings

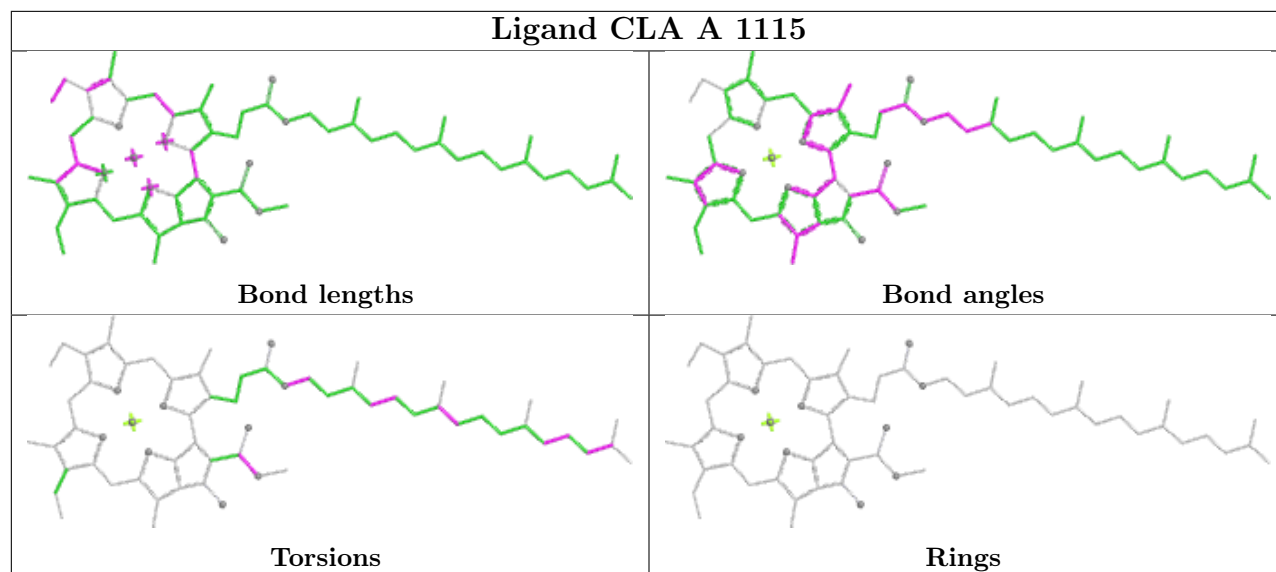




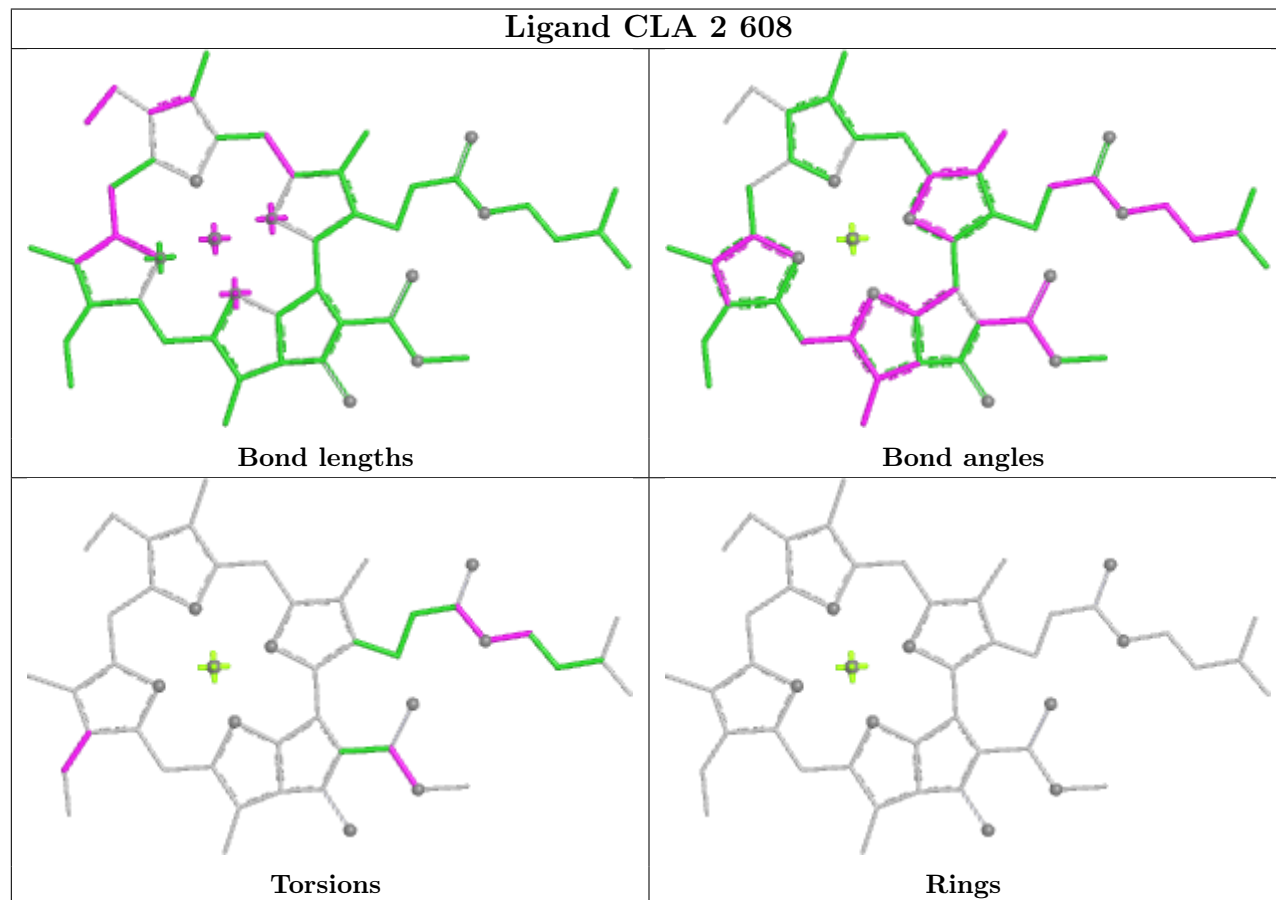
Ligand CLA 2 601**Ligand CLA 4 603**

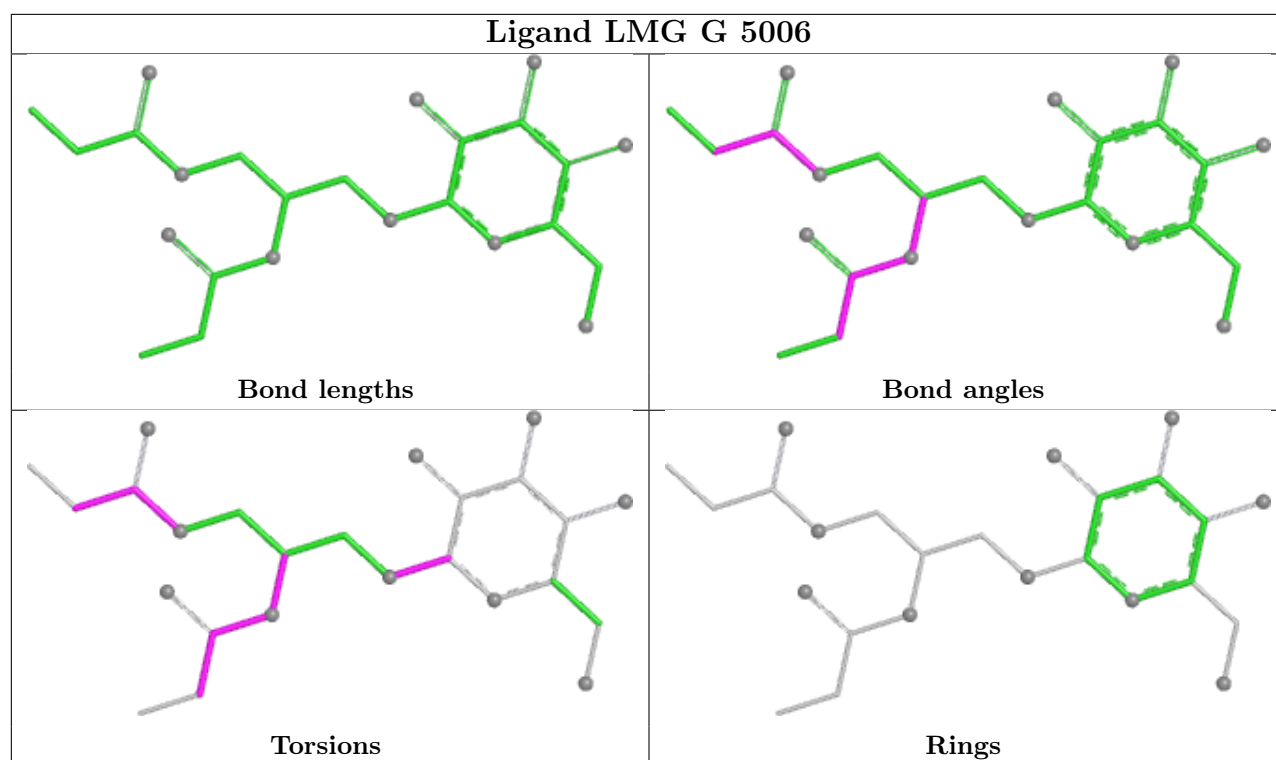


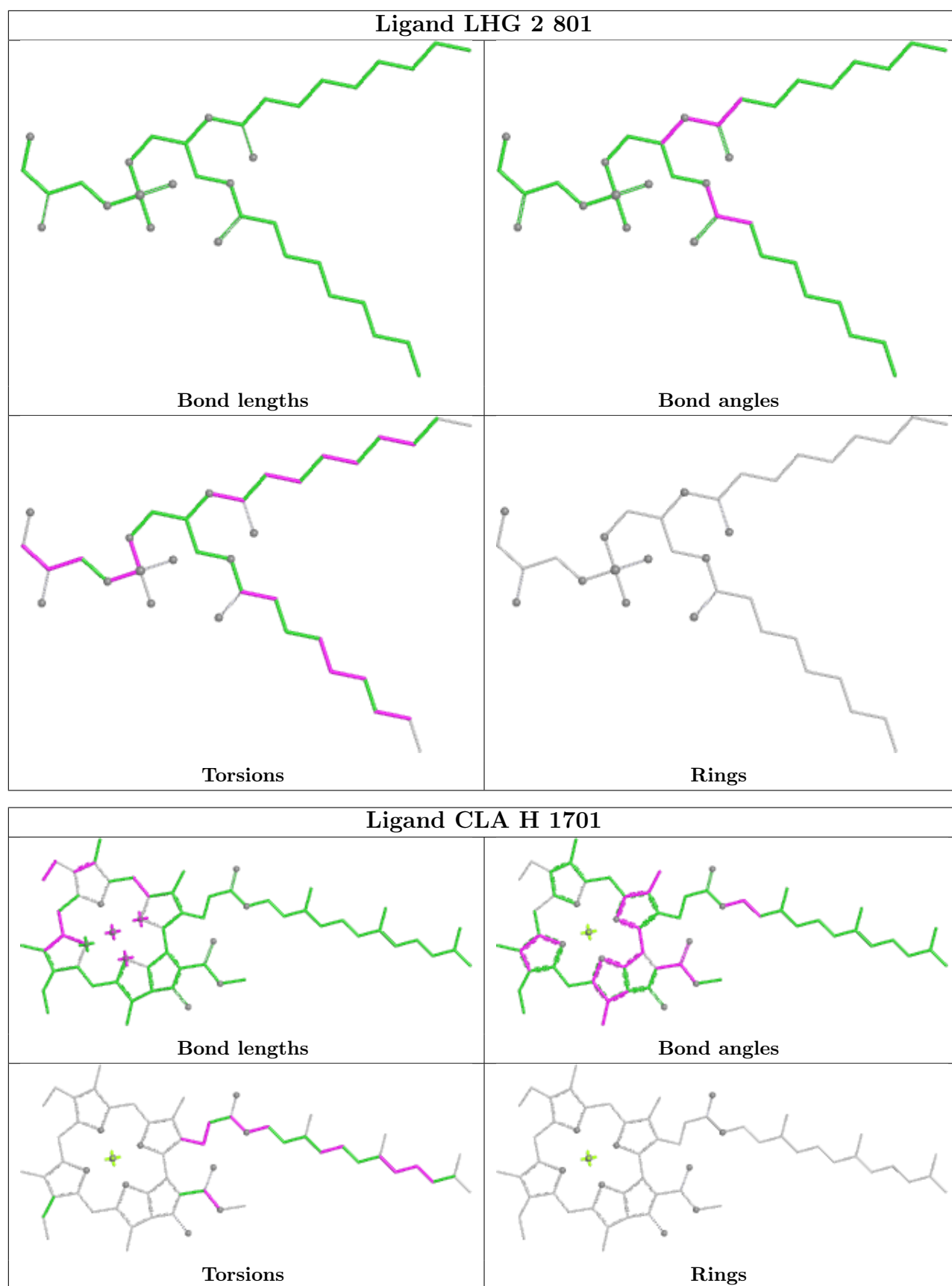
Ligand CLA A 1115

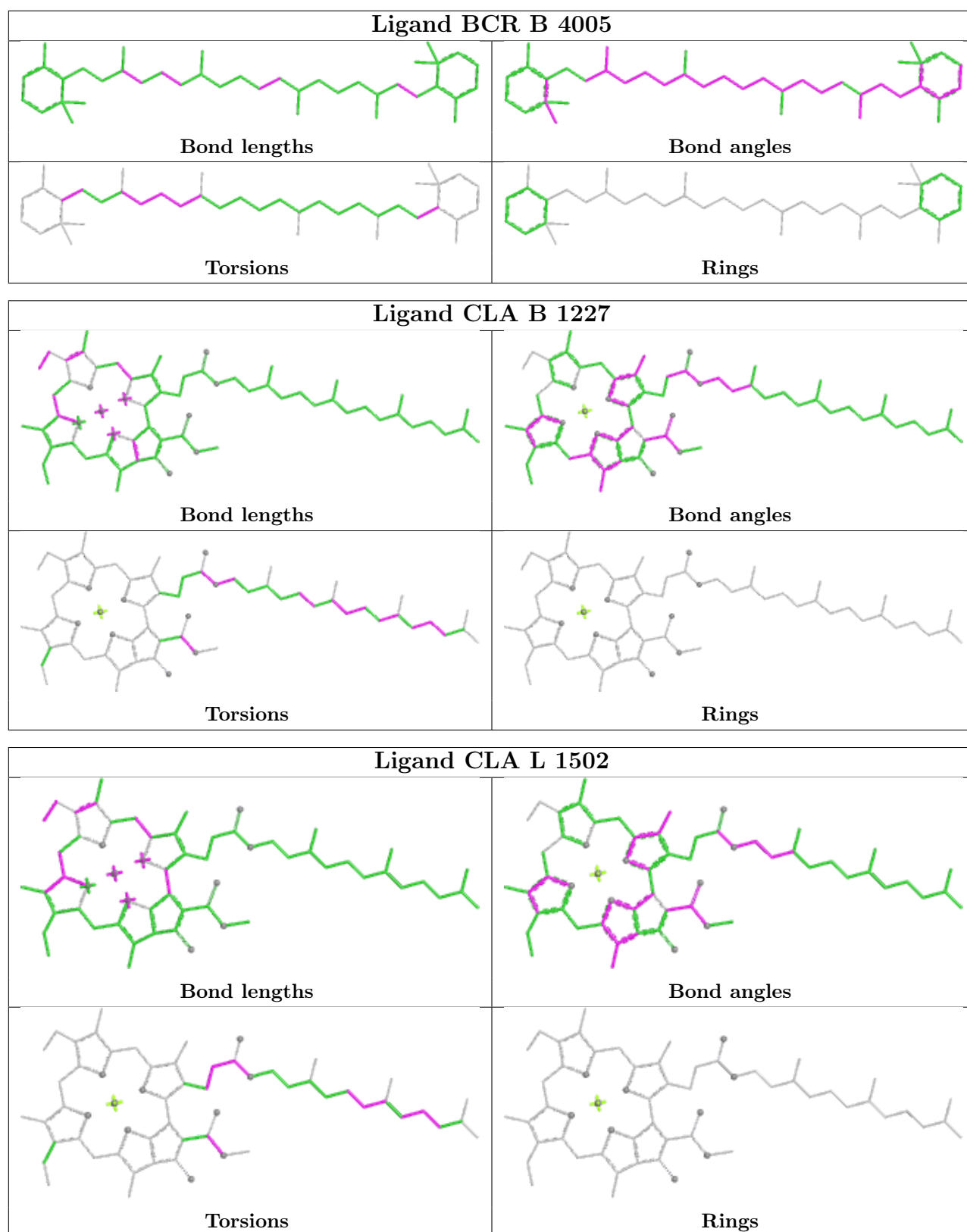


Ligand CLA 2 608

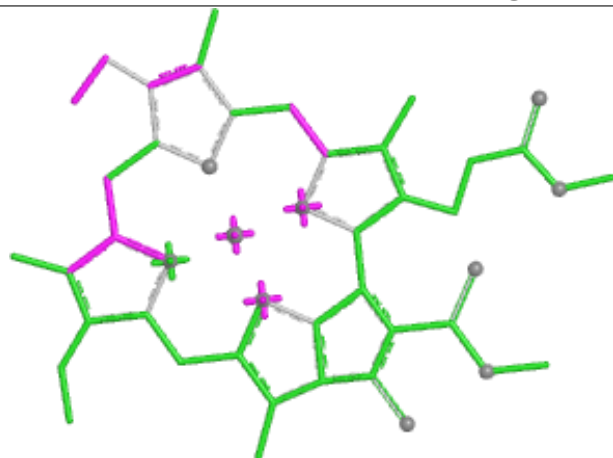




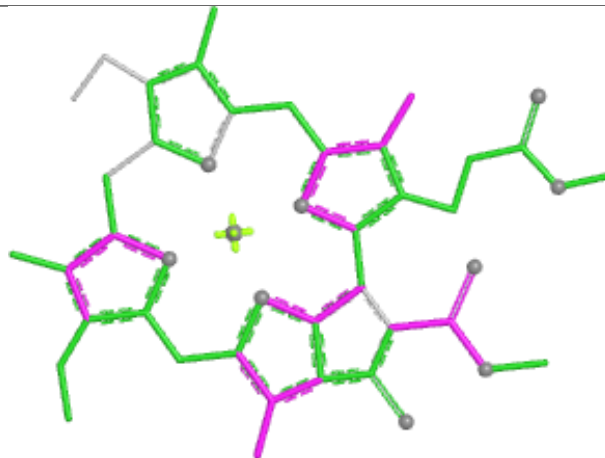




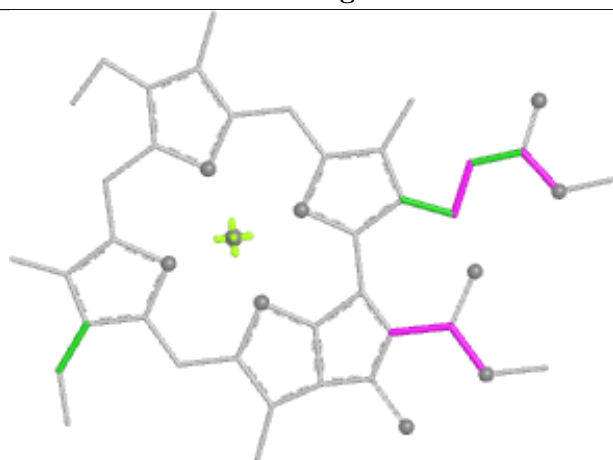
Ligand CLA B 1217



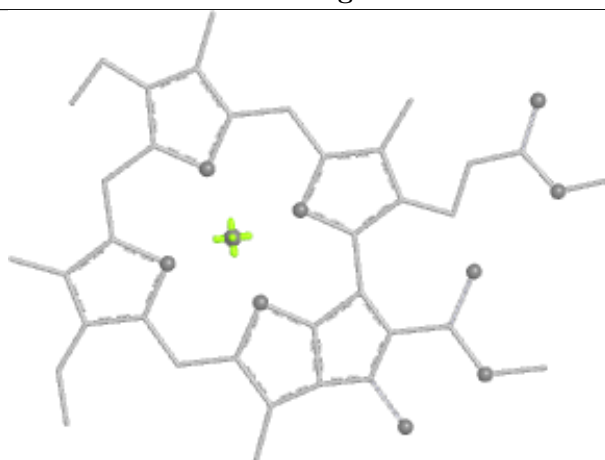
Bond lengths



Bond angles

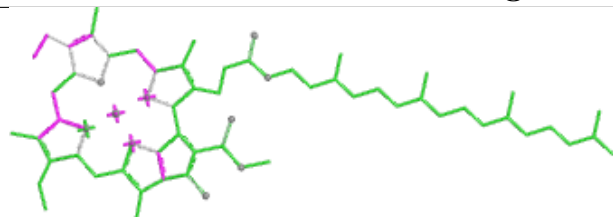


Torsions

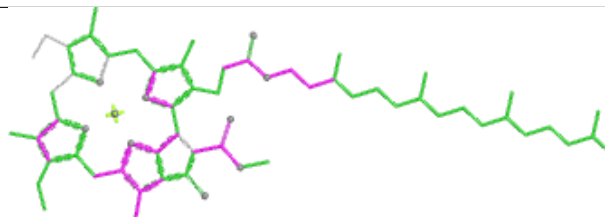


Rings

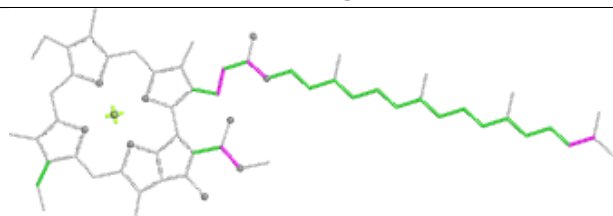
Ligand CLA A 1140



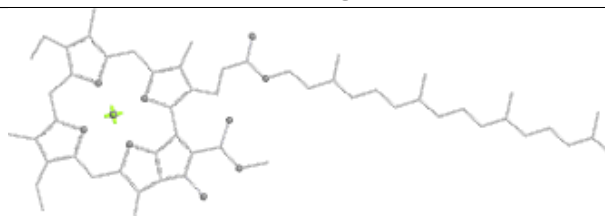
Bond lengths



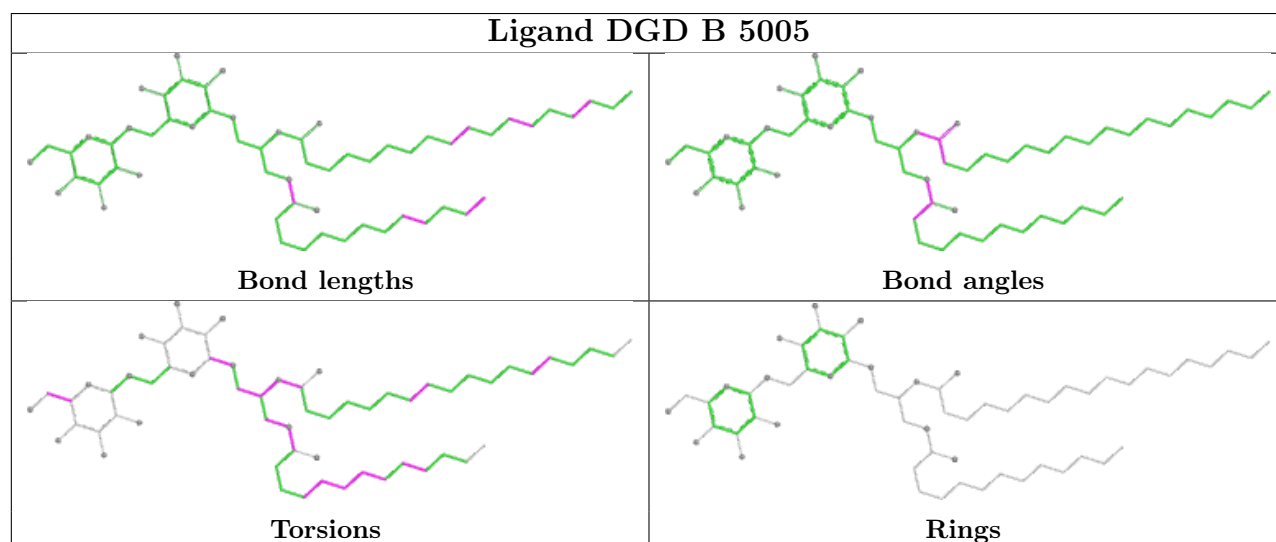
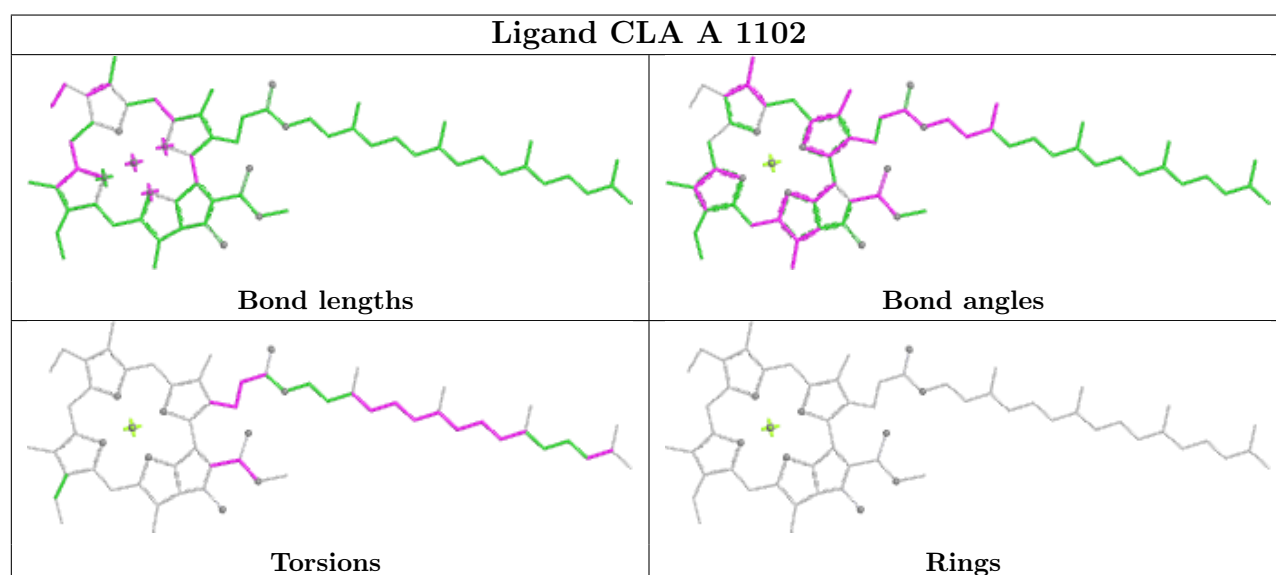
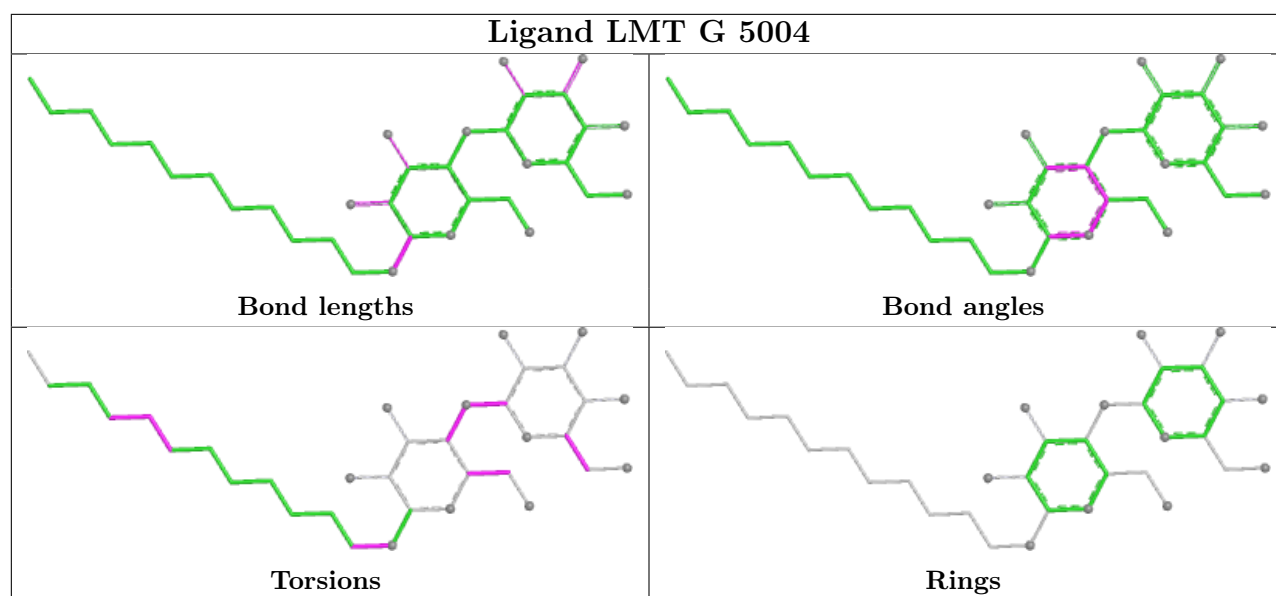
Bond angles

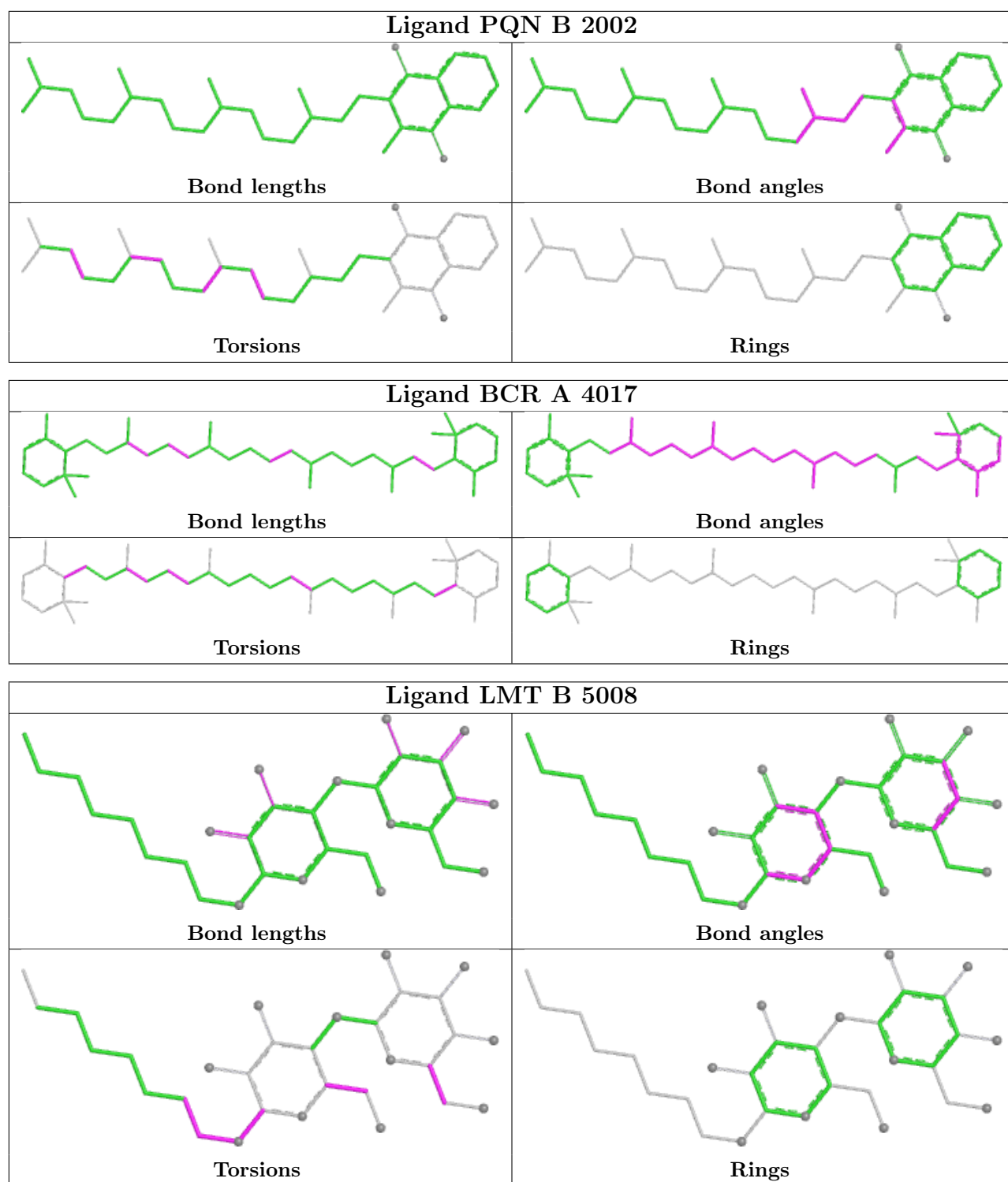


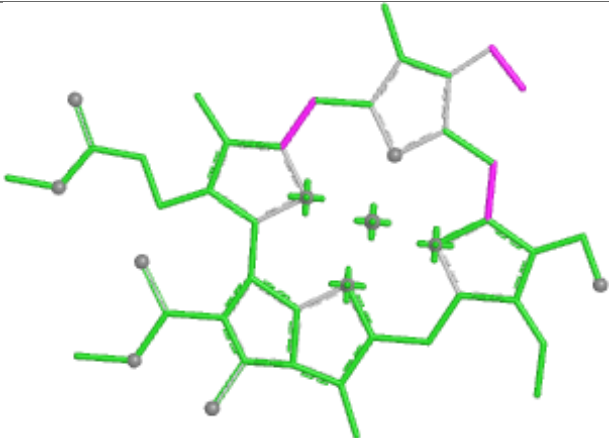
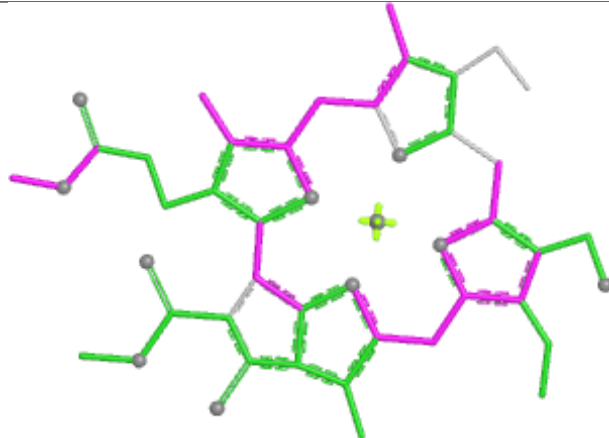
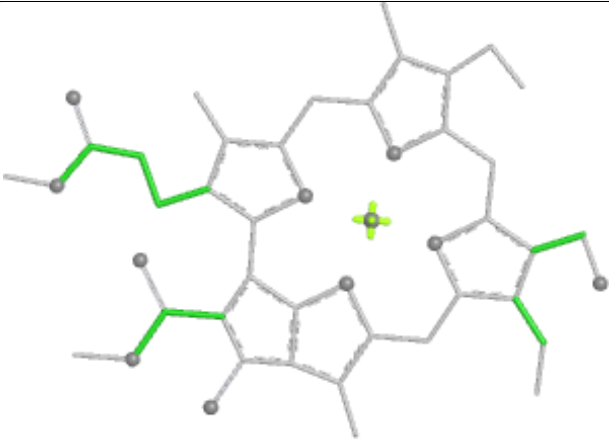

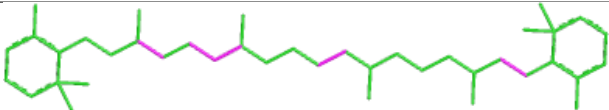
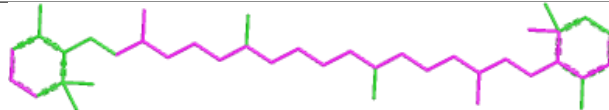
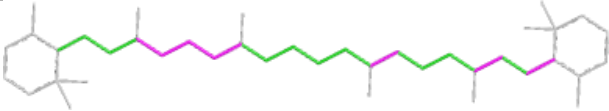
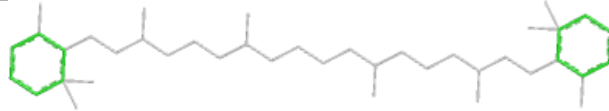
Torsions

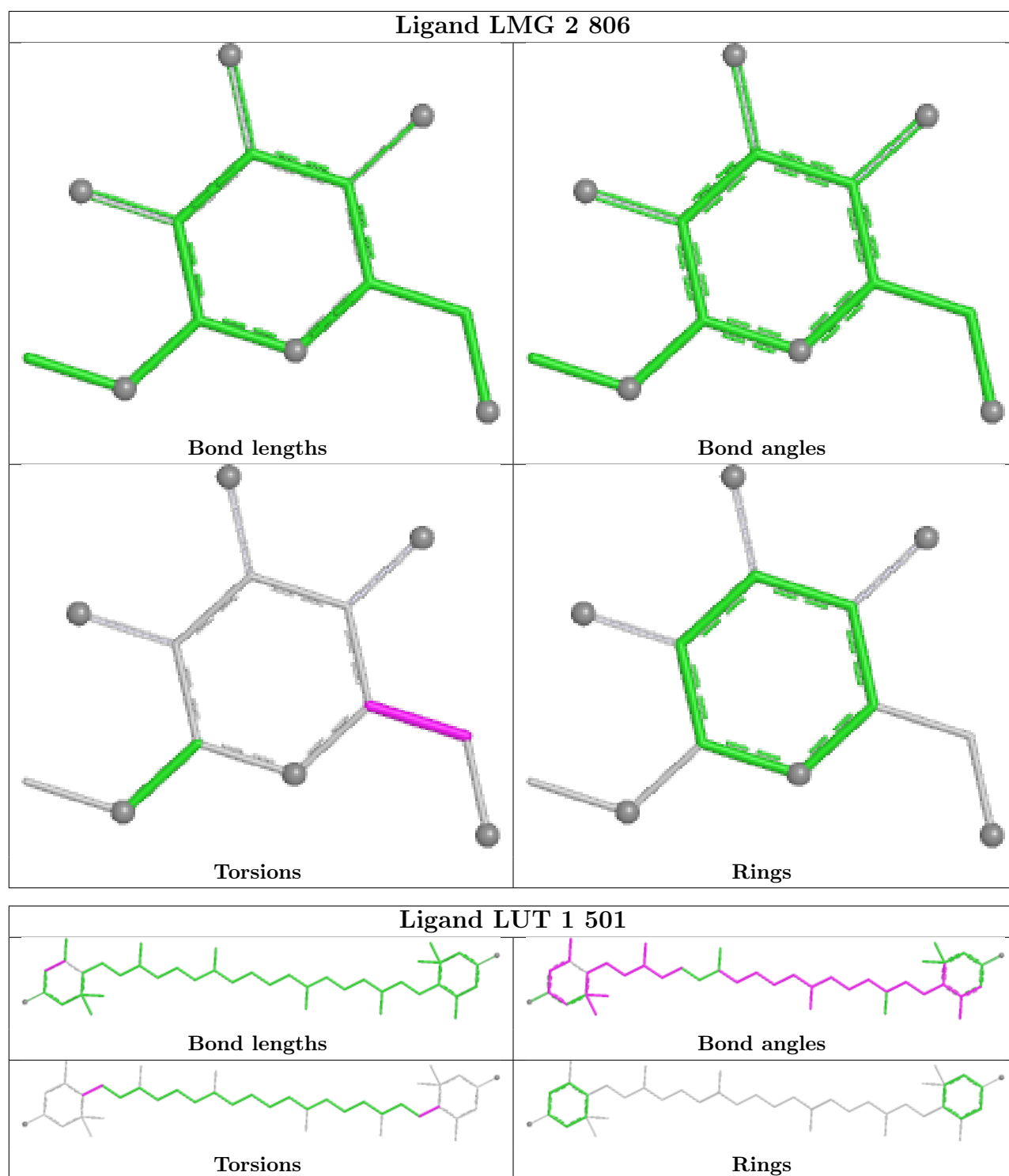


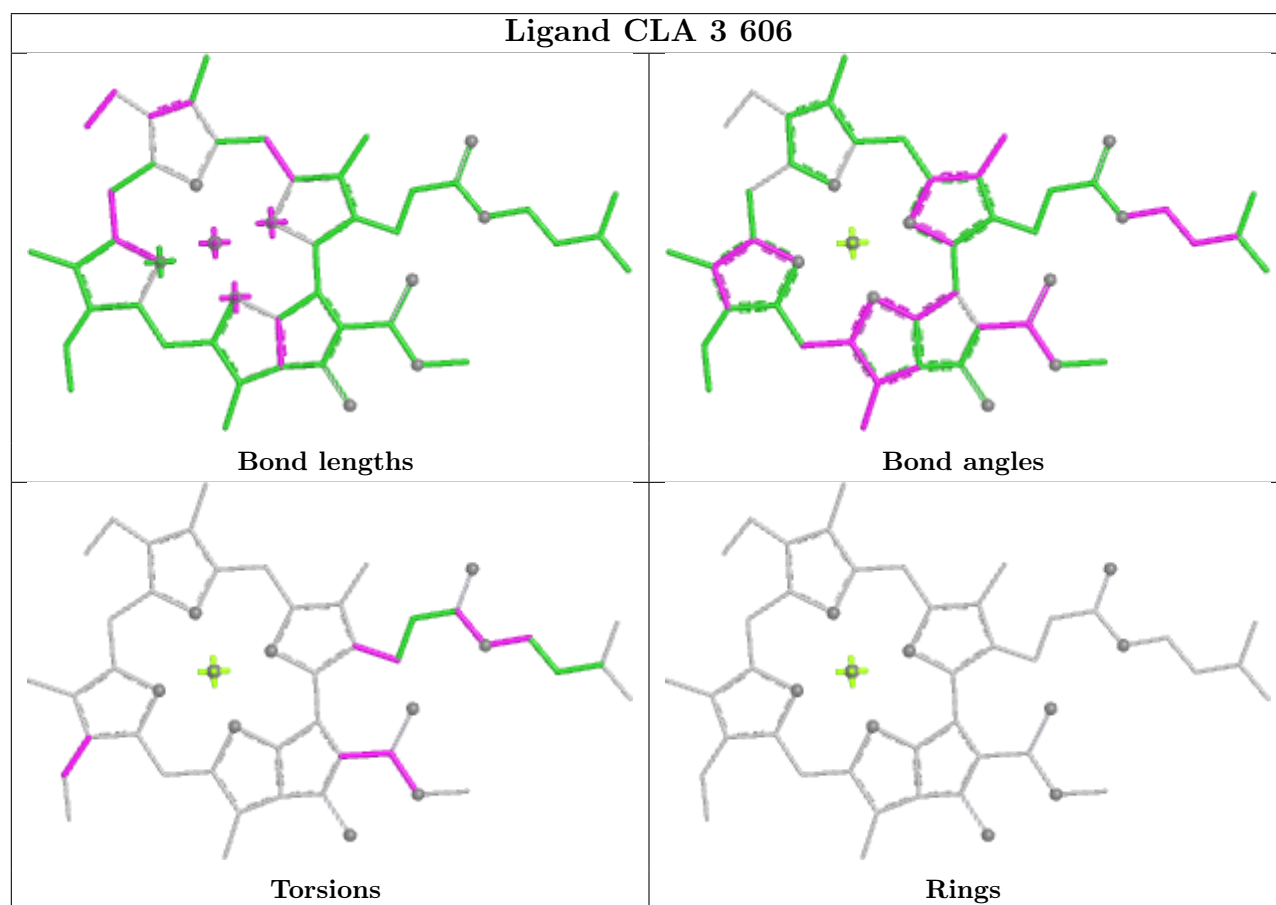
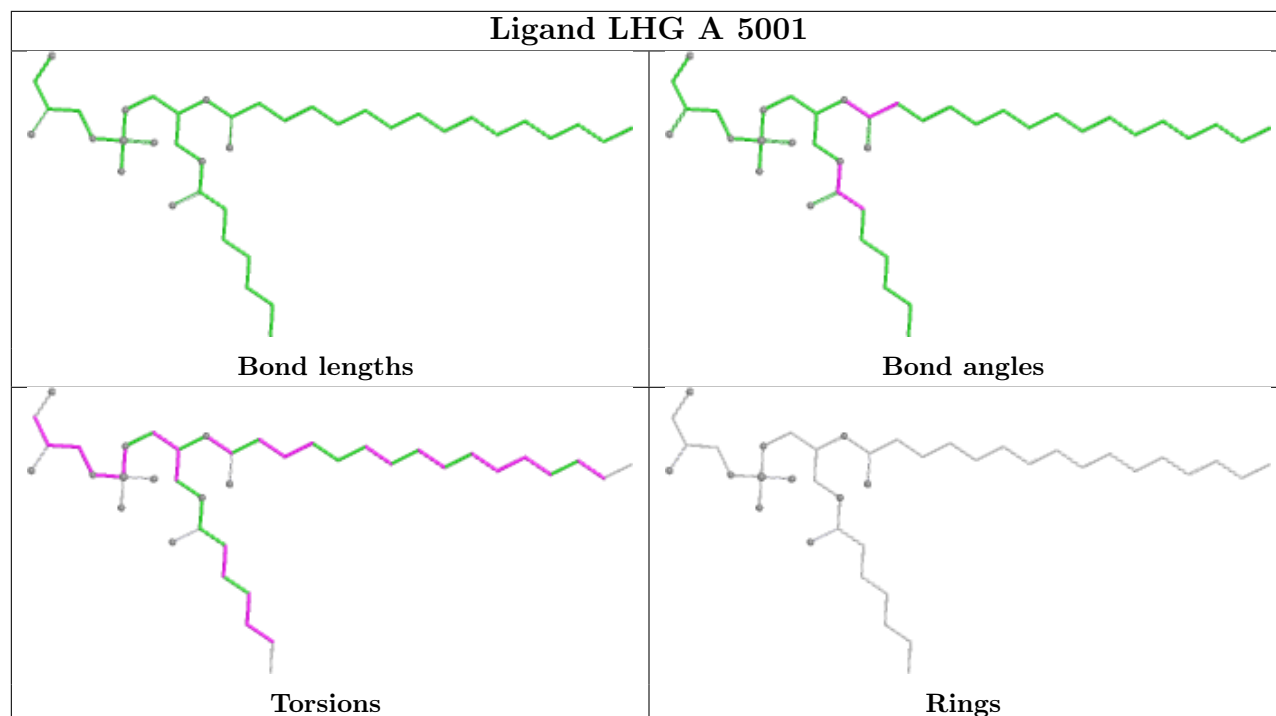
Rings



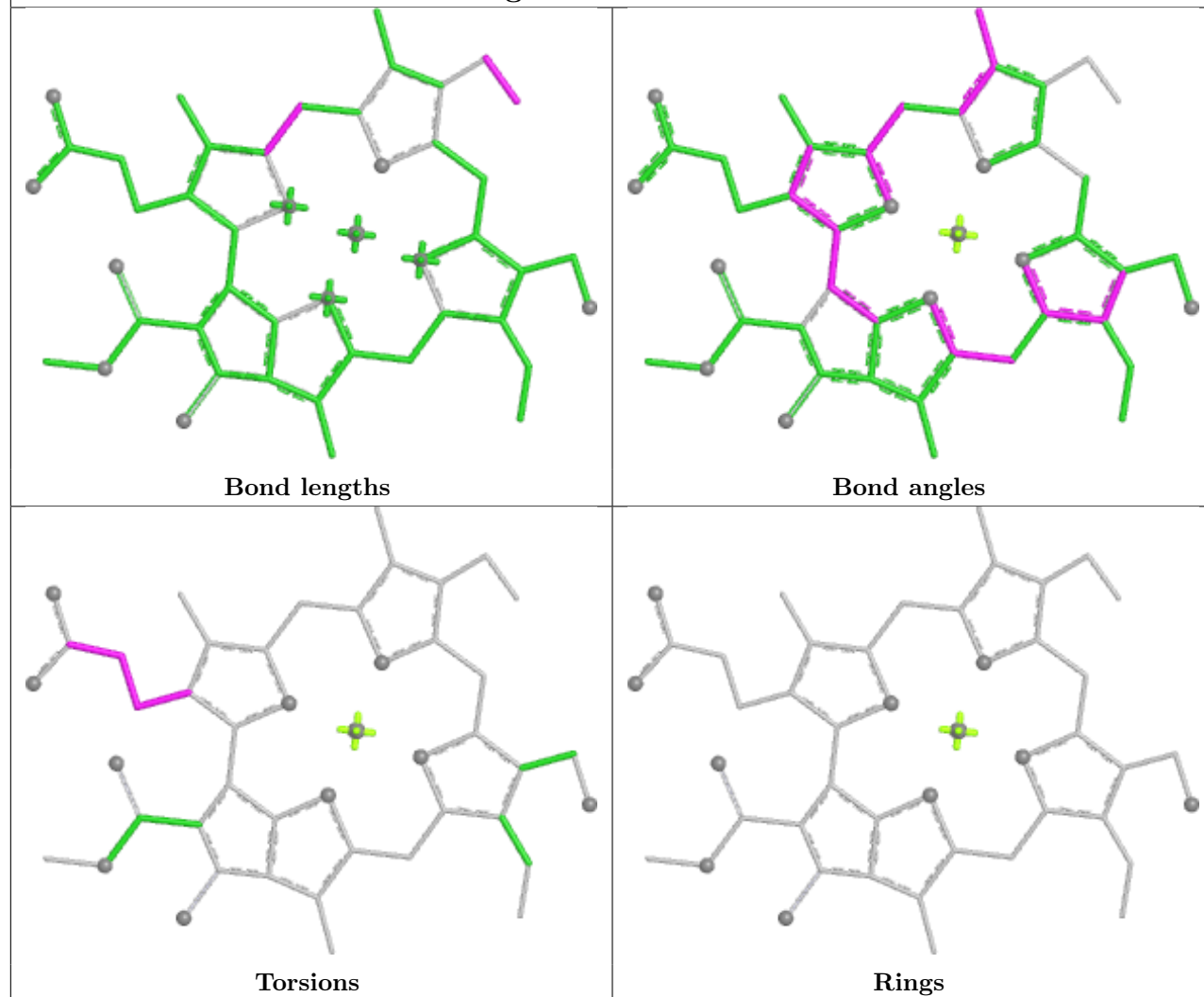


Ligand CHL 3 611	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR 3 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

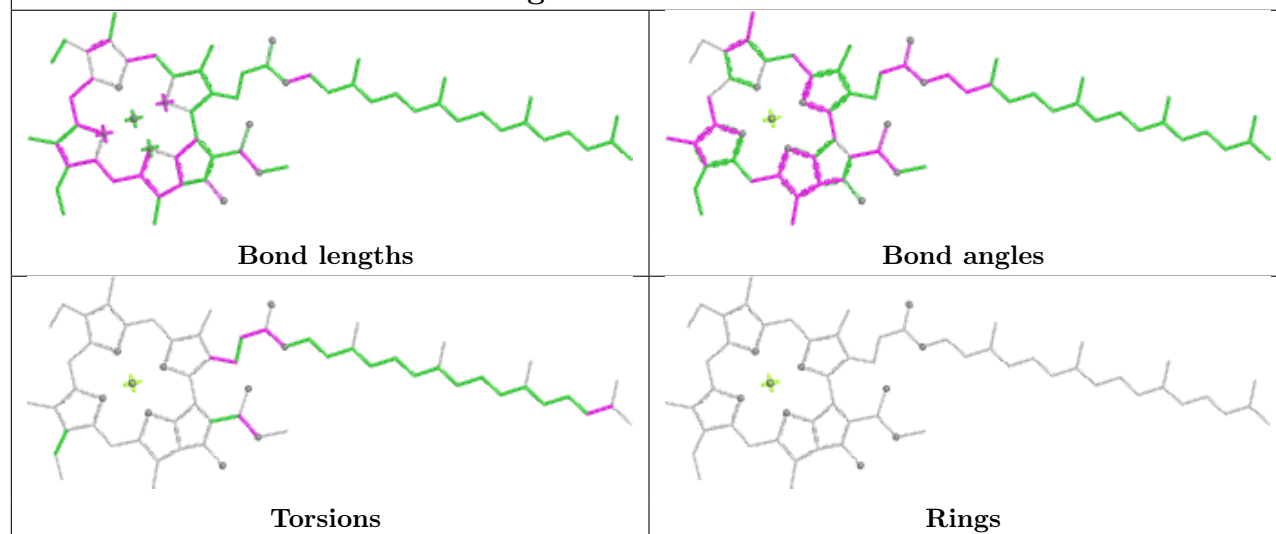




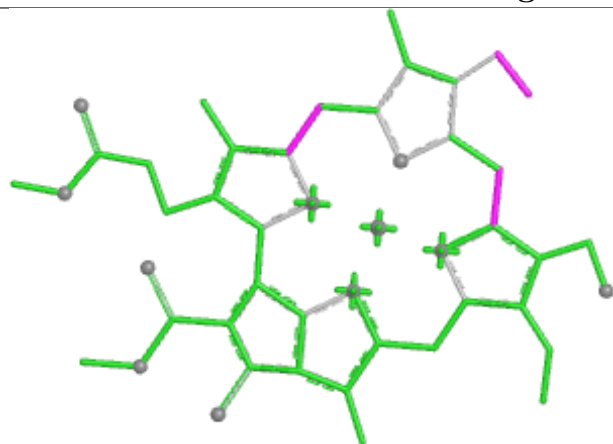
Ligand CHL 2 613



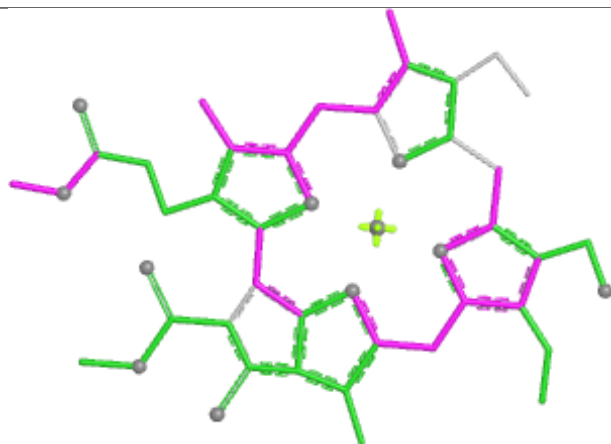
Ligand CL0 A 1011



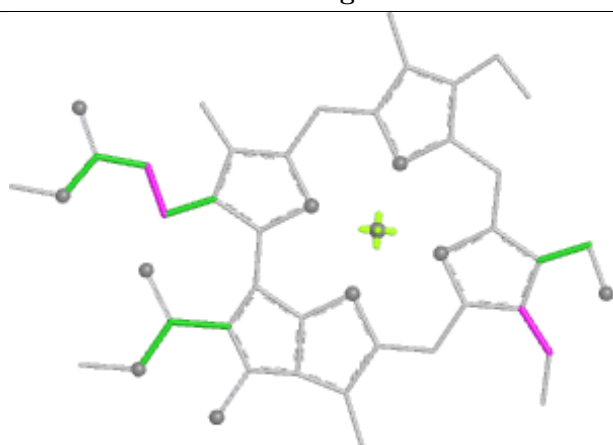
Ligand CHL 1 610



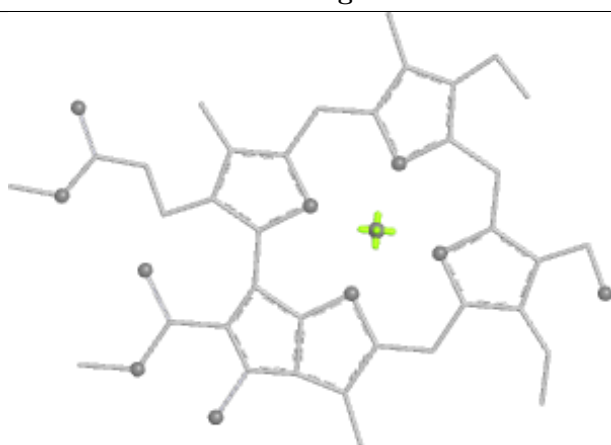
Bond lengths



Bond angles

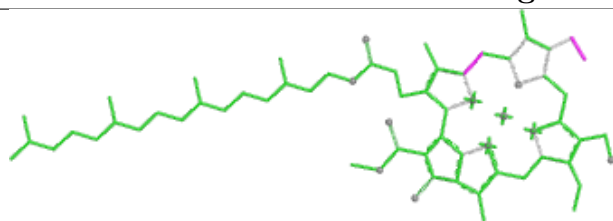


Torsions

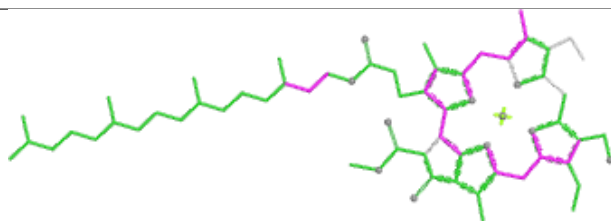


Rings

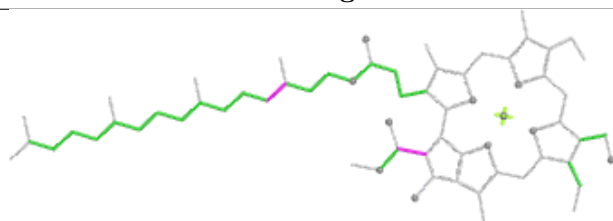
Ligand CHL 2 609



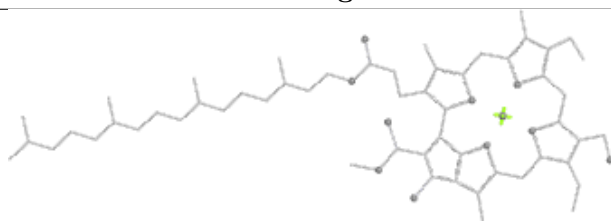
Bond lengths



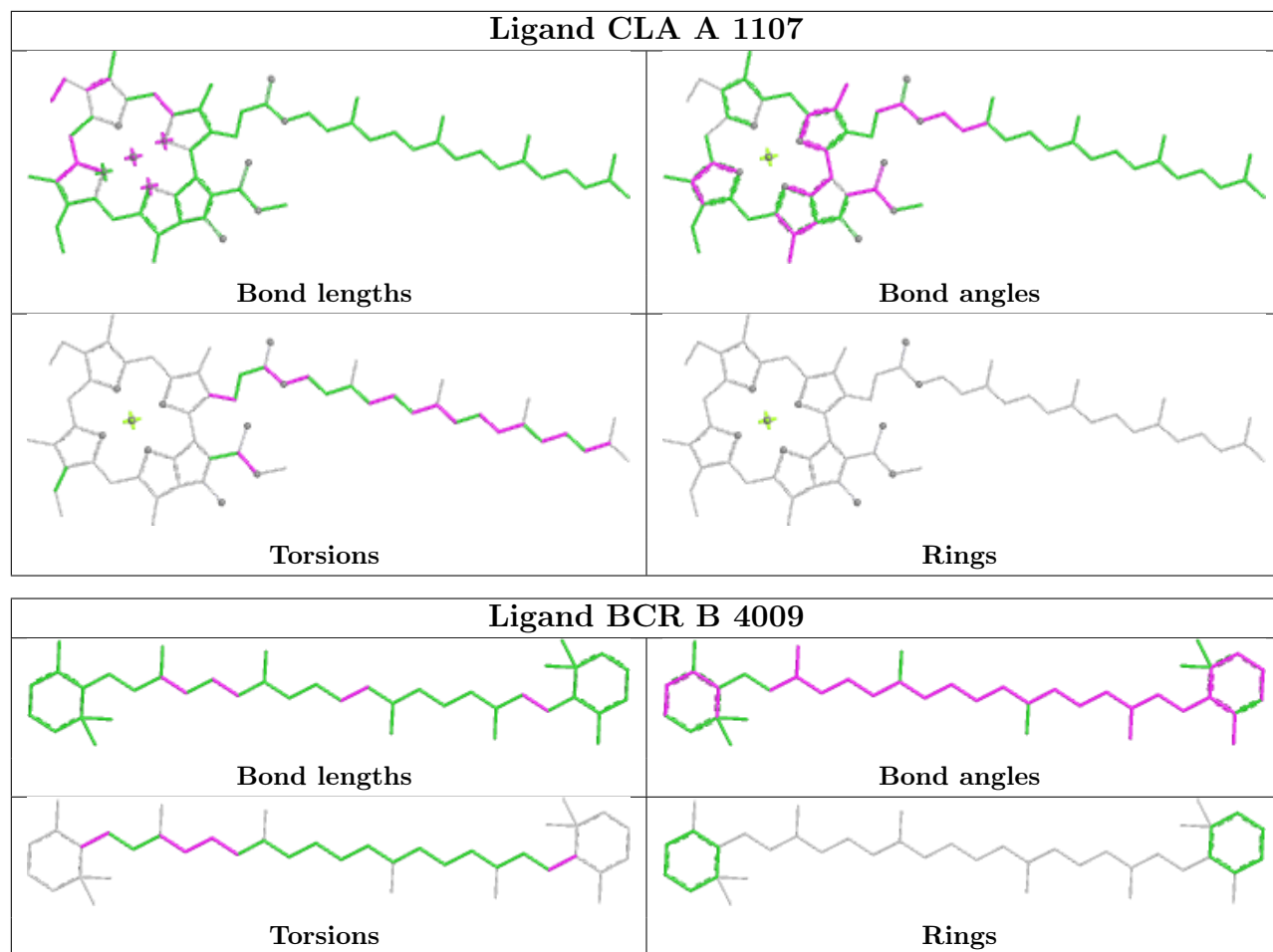
Bond angles



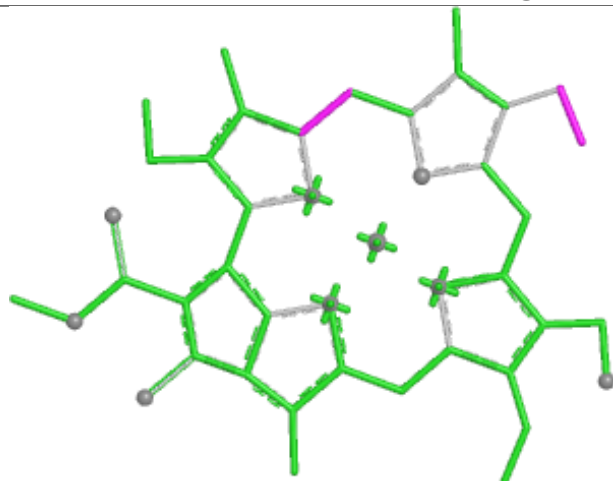
Torsions



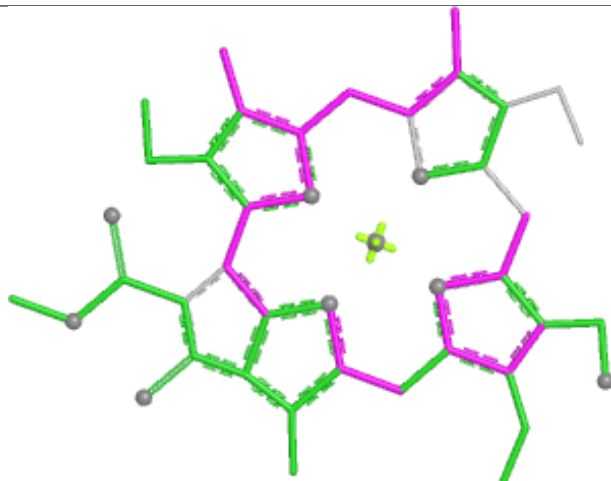
Rings



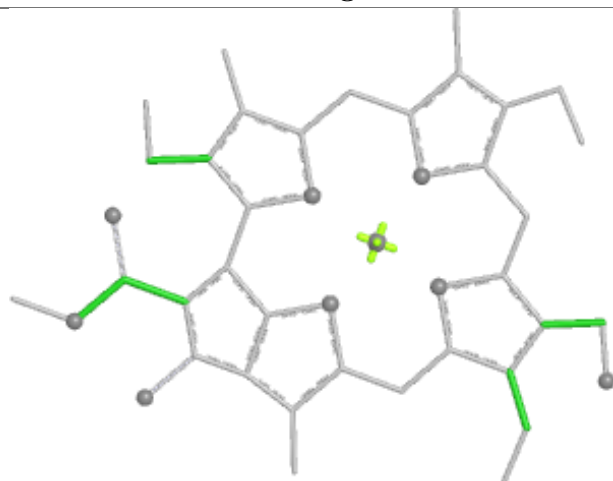
Ligand CHL 4 615



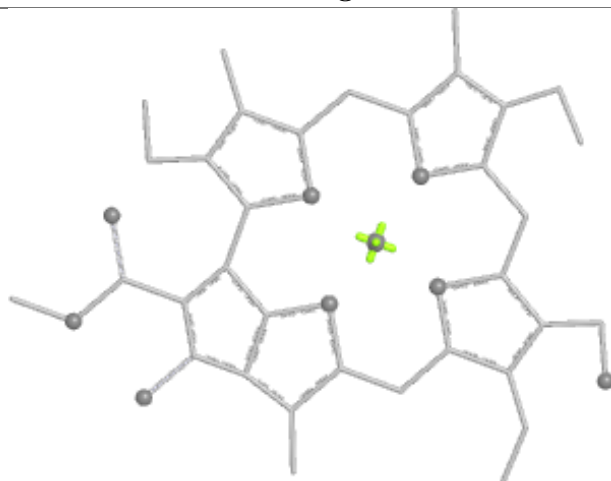
Bond lengths



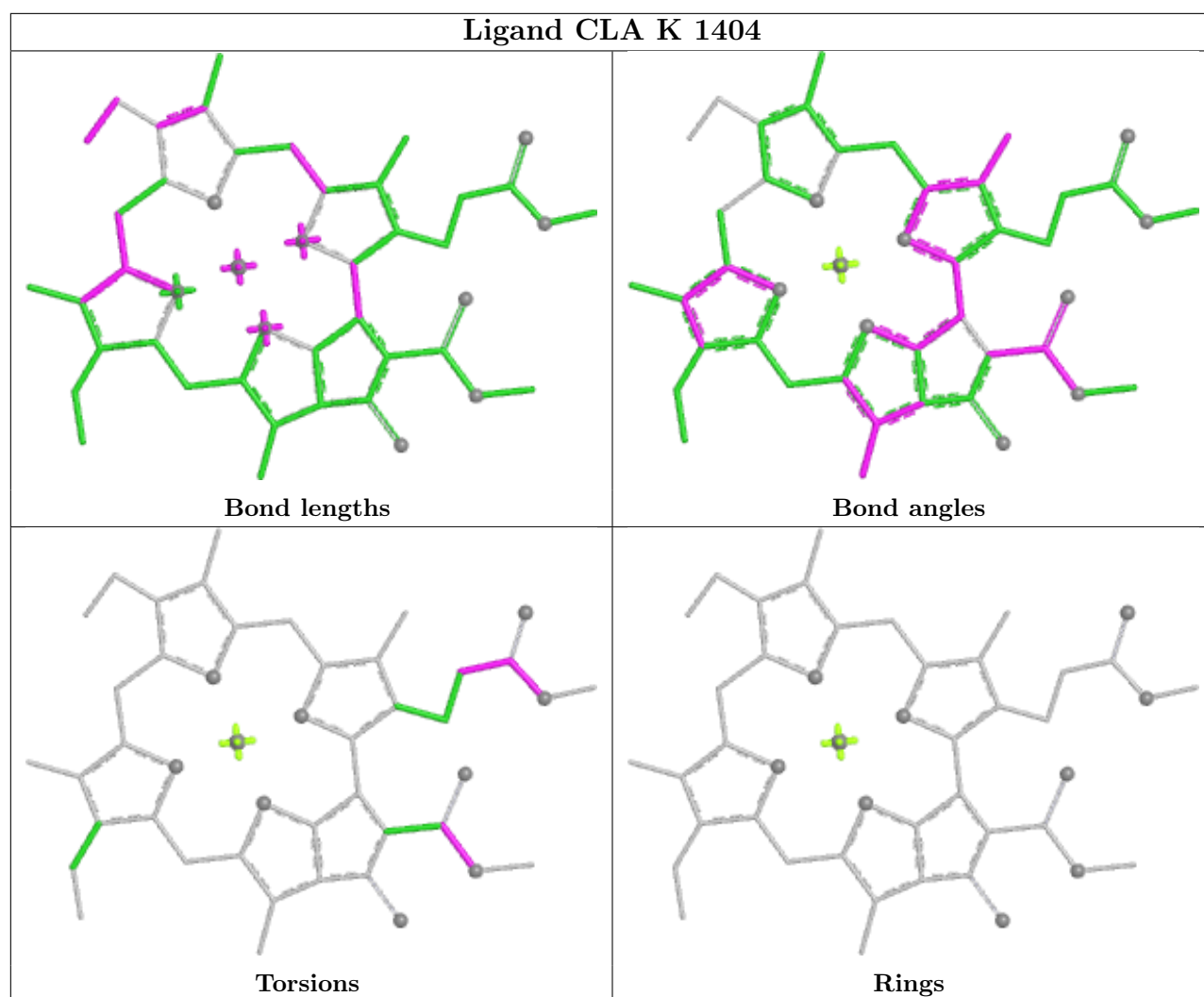
Bond angles



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.

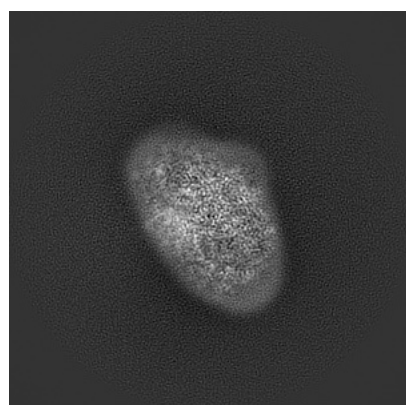
6 Map visualisation [i](#)

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.

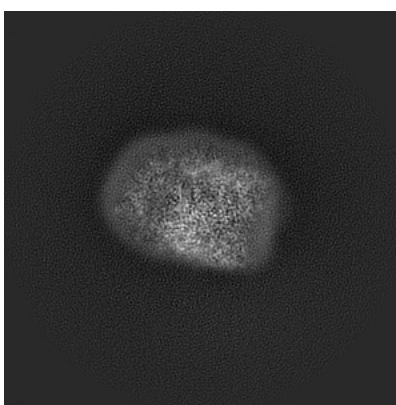
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

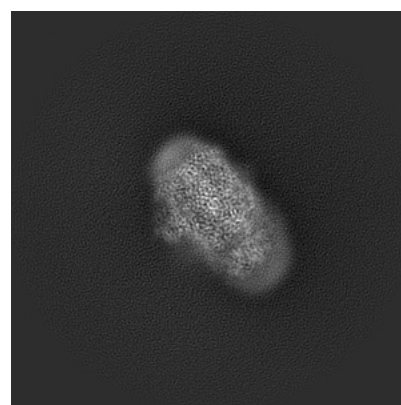
6.1.1 Primary map



X



Y

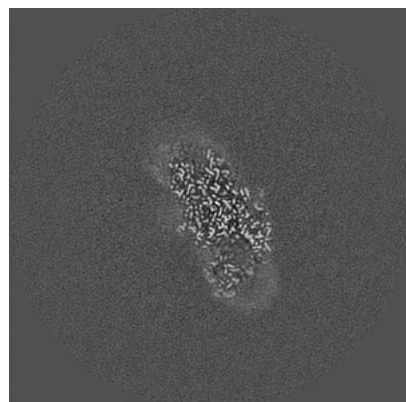


Z

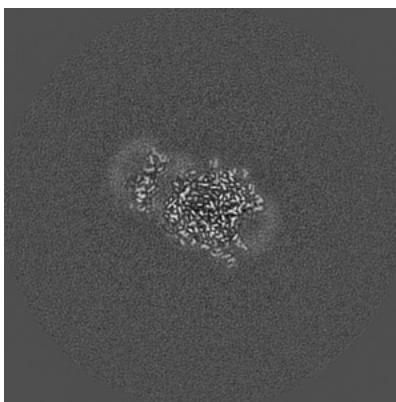
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

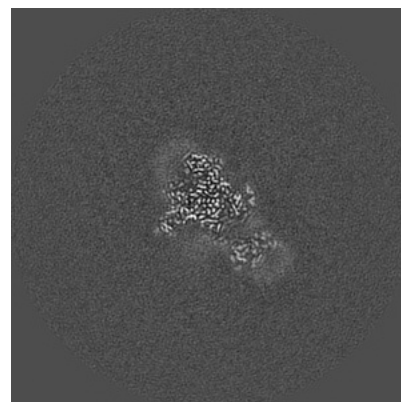
6.2.1 Primary map



X Index: 150



Y Index: 150

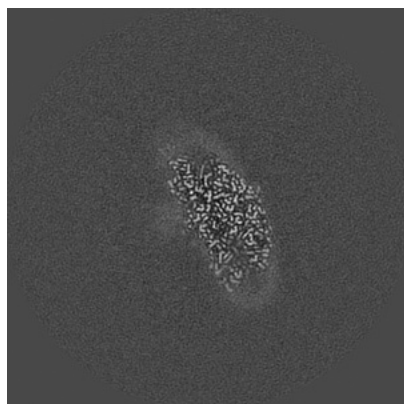


Z Index: 150

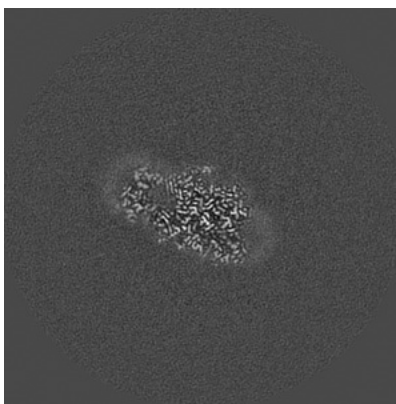
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

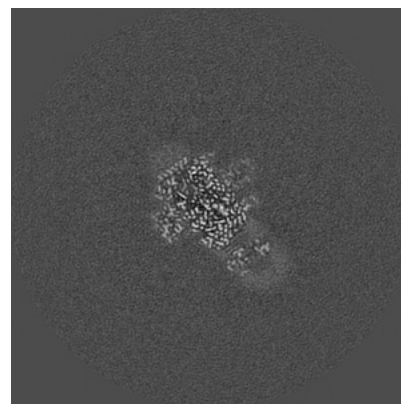
6.3.1 Primary map



X Index: 145



Y Index: 162

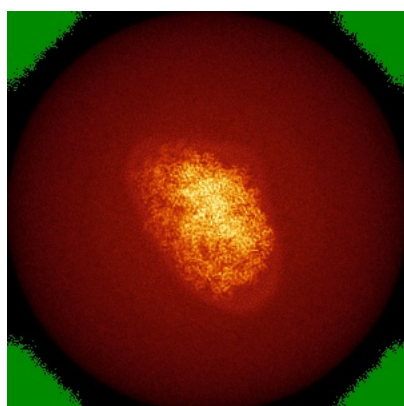


Z Index: 162

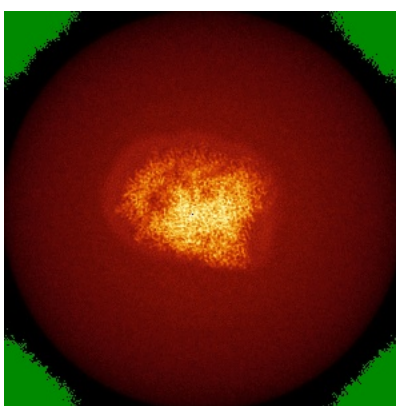
The images above show the largest variance slices of the map in three orthogonal directions.

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

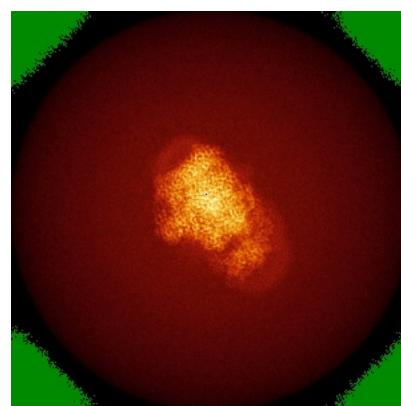
6.4.1 Primary map



X



Y

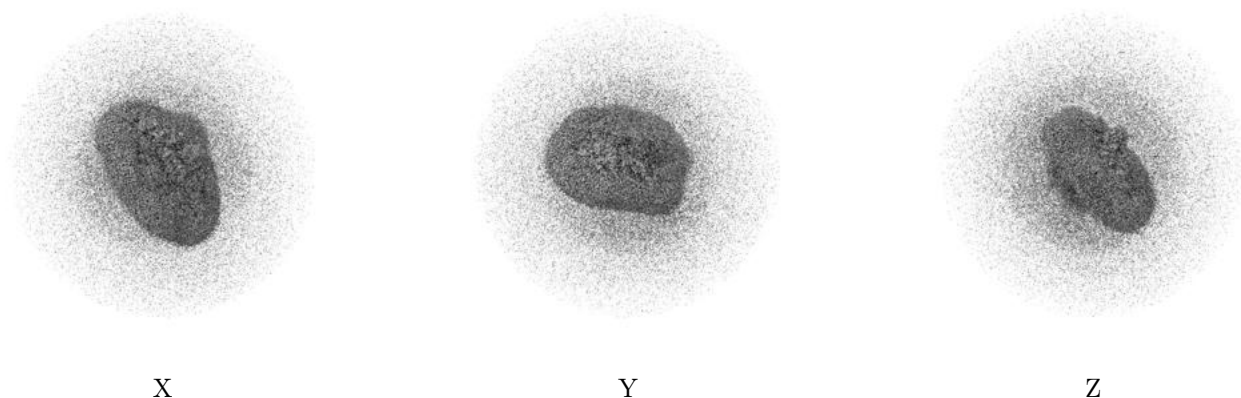


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

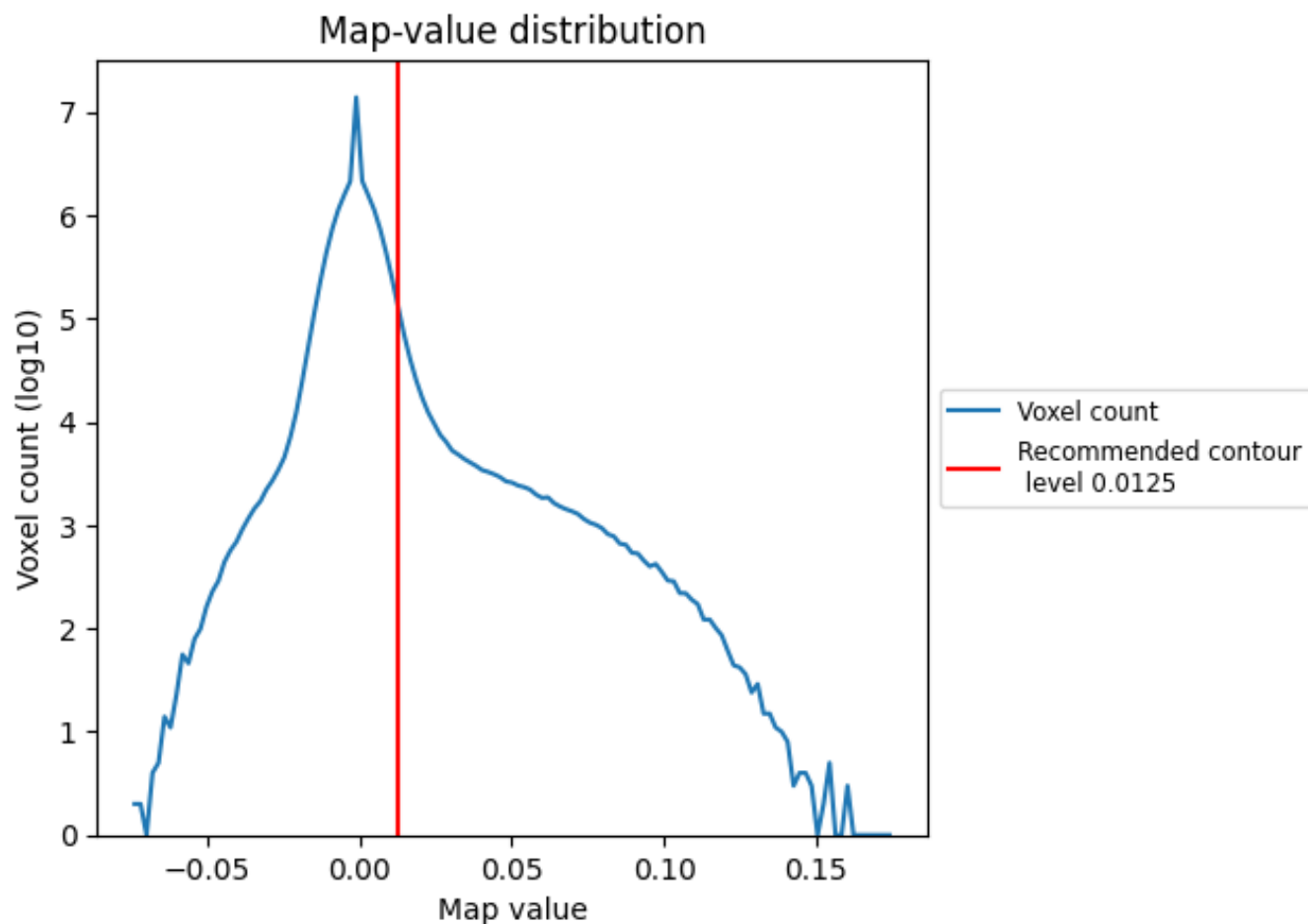
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

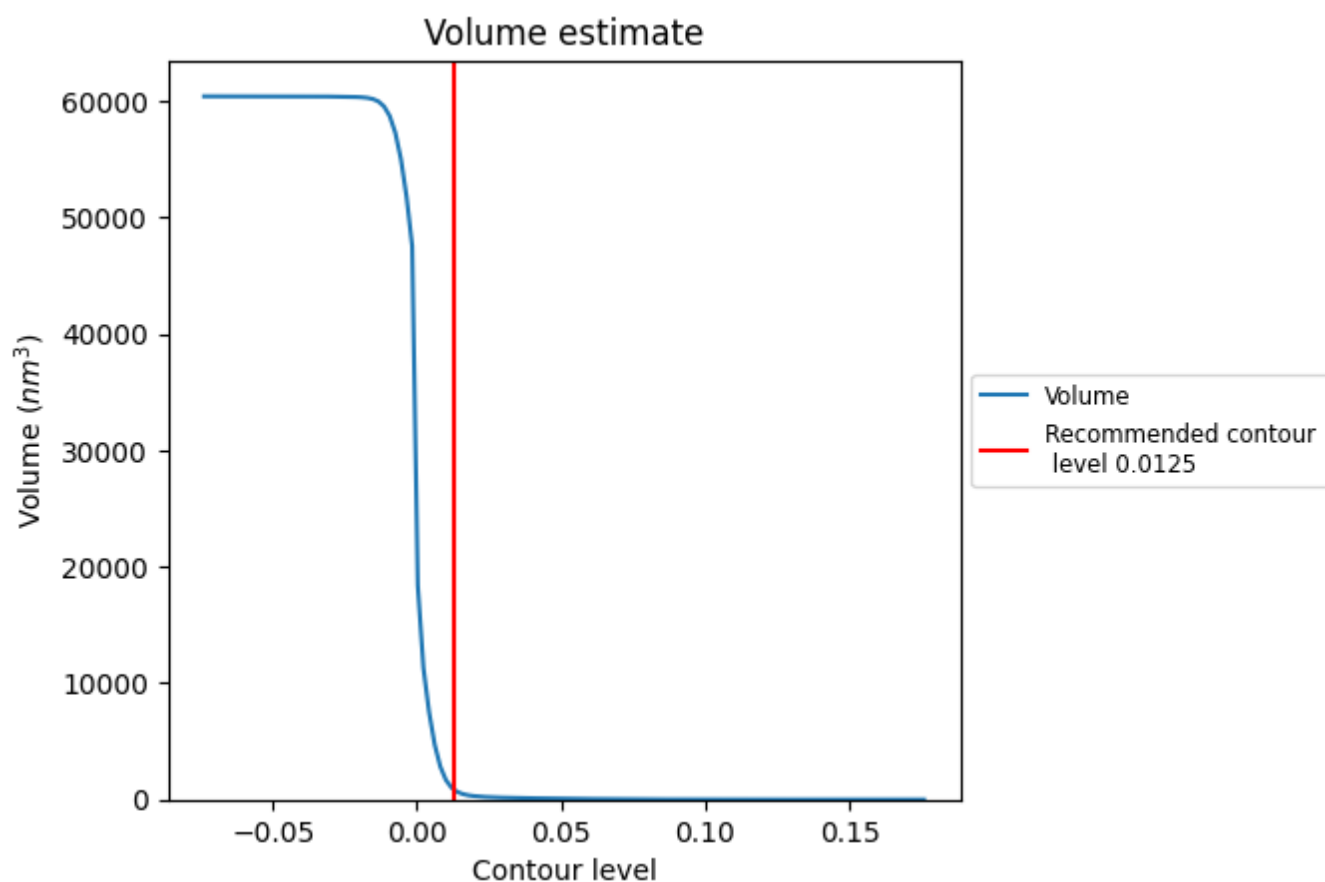
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

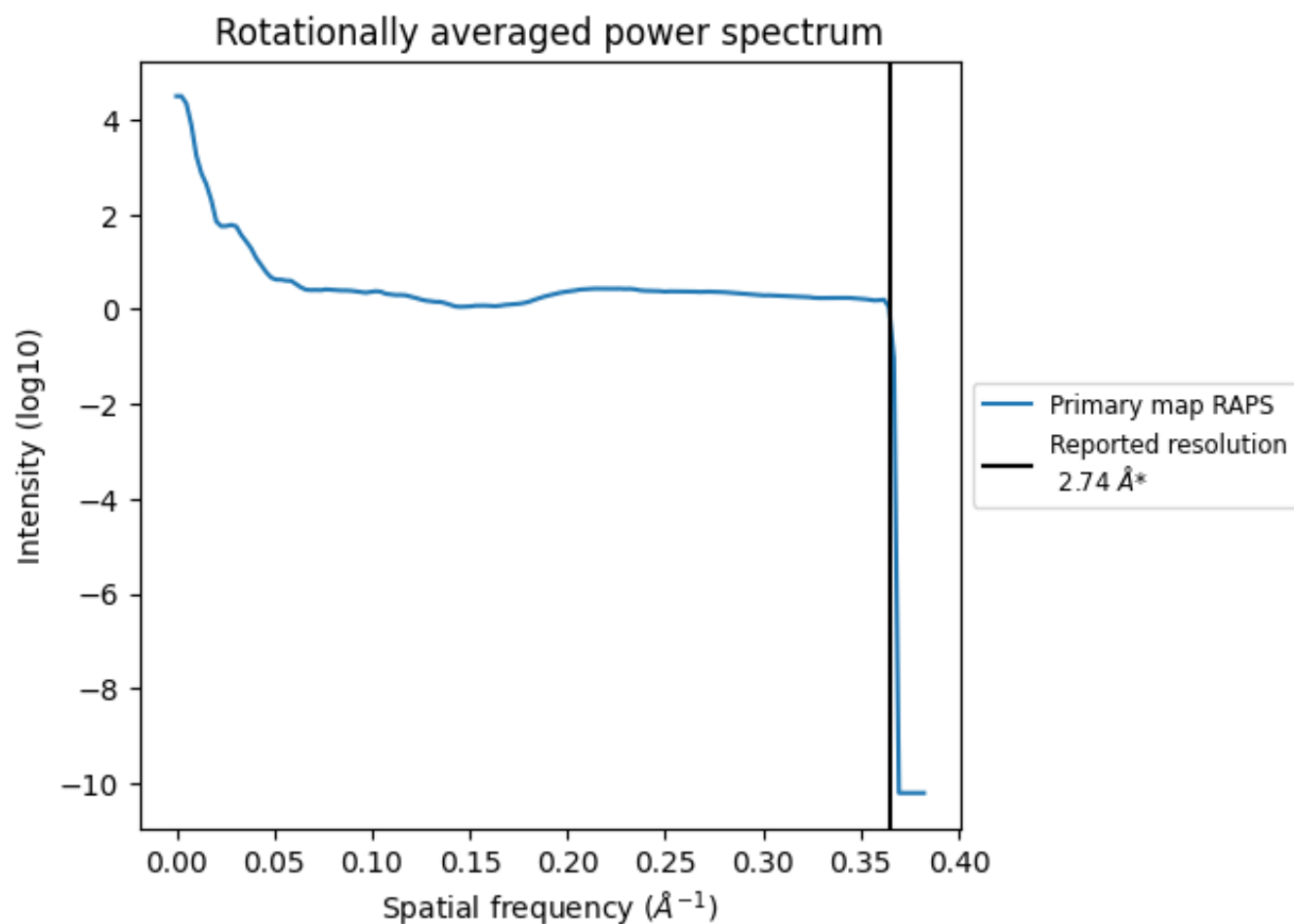
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 925 nm³; this corresponds to an approximate mass of 835 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

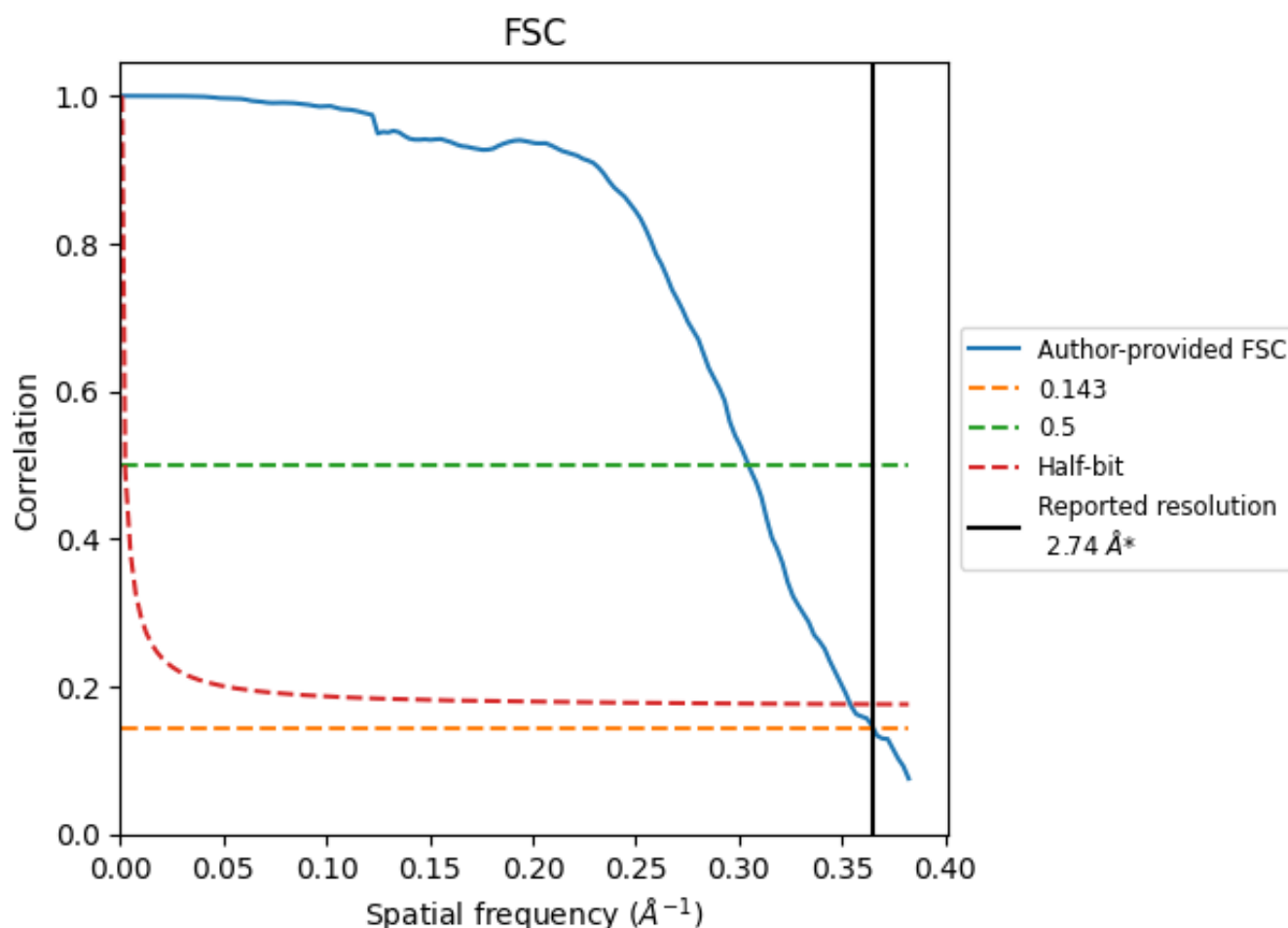


*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.365 \AA^{-1}

8.2 Resolution estimates [i](#)

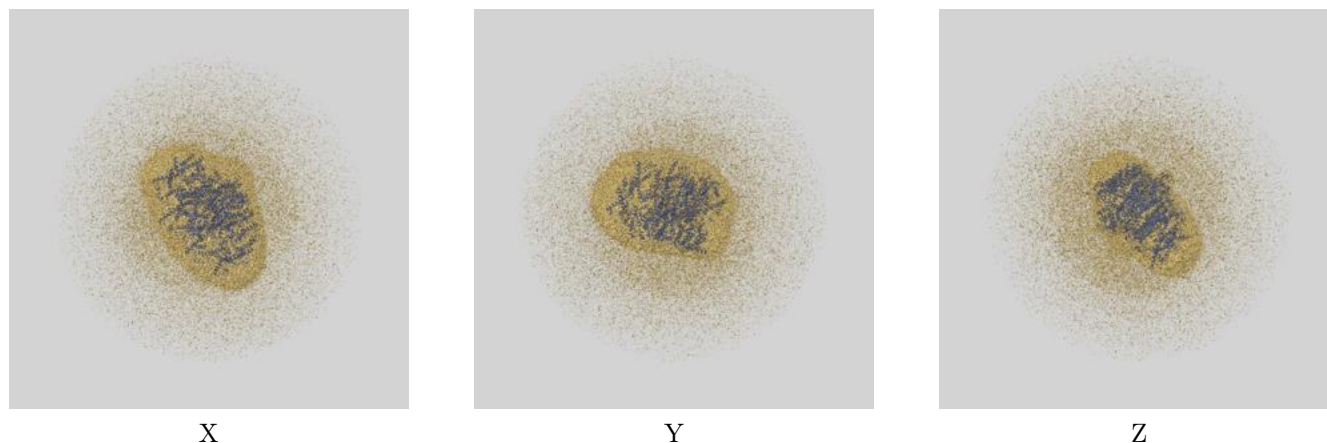
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.74	3.28	2.82
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

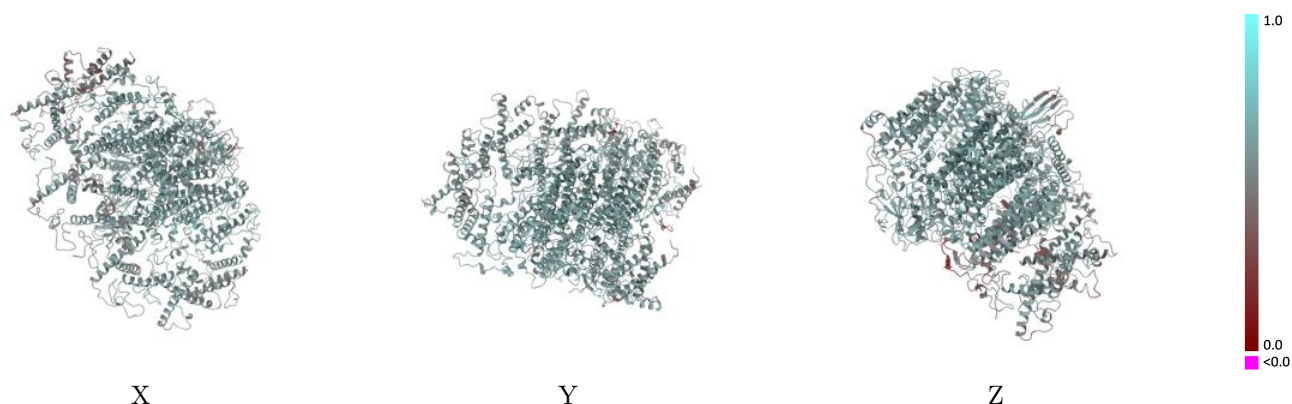
This section contains information regarding the fit between EMDB map EMD-11326 and PDB model 6ZOO. Per-residue inclusion information can be found in section [3](#) on page [32](#).

9.1 Map-model overlay [i](#)



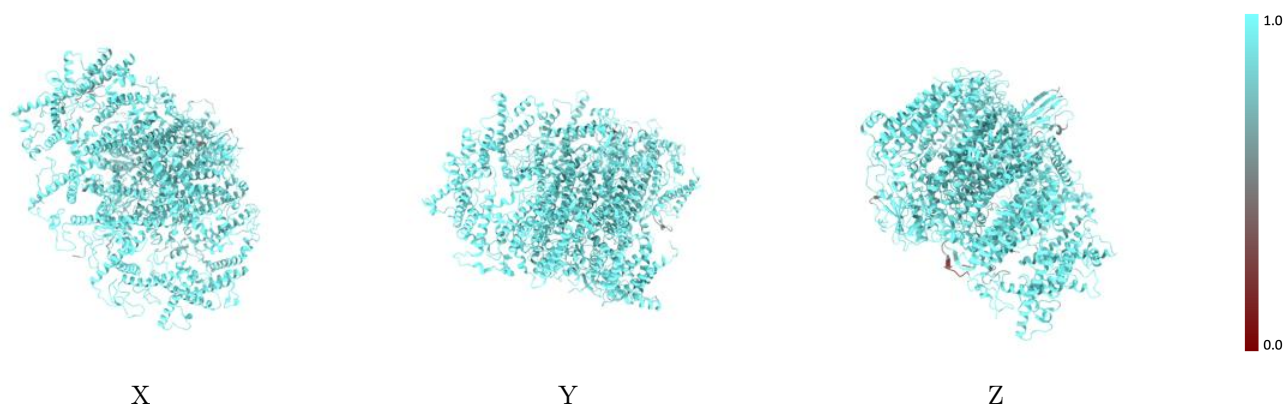
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



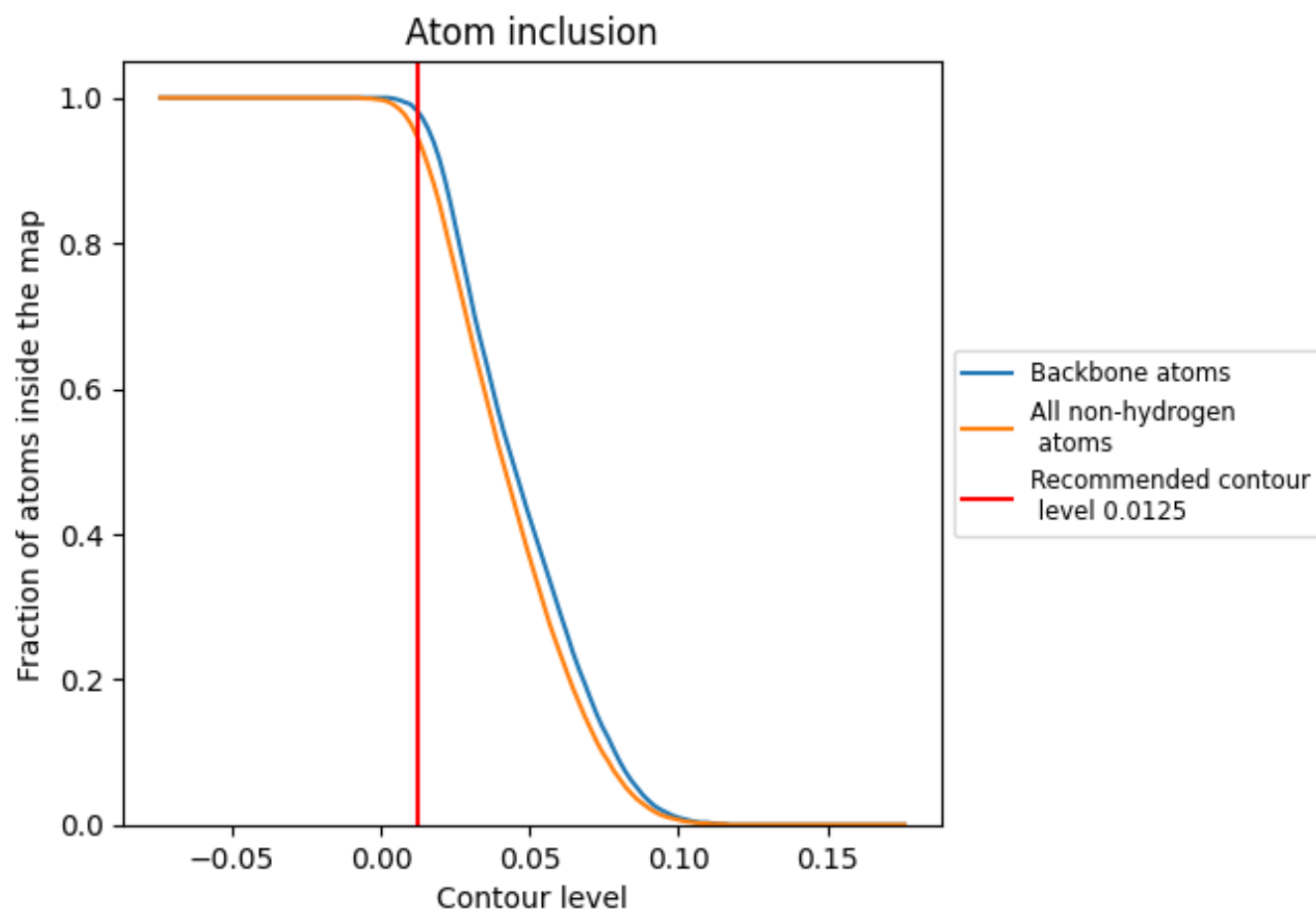
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0125).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9450	<div><div></div></div> 0.5600
1	<div><div></div></div> 0.9360	<div><div></div></div> 0.5350
2	<div><div></div></div> 0.9140	<div><div></div></div> 0.5030
3	<div><div></div></div> 0.9260	<div><div></div></div> 0.4950
4	<div><div></div></div> 0.9290	<div><div></div></div> 0.5310
A	<div><div></div></div> 0.9590	<div><div></div></div> 0.5920
B	<div><div></div></div> 0.9720	<div><div></div></div> 0.6050
C	<div><div></div></div> 0.9870	<div><div></div></div> 0.5950
D	<div><div></div></div> 0.9830	<div><div></div></div> 0.5900
E	<div><div></div></div> 0.9690	<div><div></div></div> 0.5560
F	<div><div></div></div> 0.9370	<div><div></div></div> 0.5620
G	<div><div></div></div> 0.9130	<div><div></div></div> 0.5220
H	<div><div></div></div> 0.9110	<div><div></div></div> 0.5050
I	<div><div></div></div> 0.9750	<div><div></div></div> 0.5800
J	<div><div></div></div> 0.9170	<div><div></div></div> 0.5090
K	<div><div></div></div> 0.8040	<div><div></div></div> 0.3930
L	<div><div></div></div> 0.9690	<div><div></div></div> 0.5600
P	<div><div></div></div> 0.8760	<div><div></div></div> 0.5280

