



## wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 08:15 am BST

PDB ID : 7BLX  
EMDB ID : EMD-12227  
Title : Photosystem I of a temperature sensitive mutant *Chlamydomonas reinhardtii*  
Authors : Caspy, I.; Nelson, N.  
Deposited on : 2021-01-19  
Resolution : 3.15 Å(reported)  
Based on initial model : 6JO5

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

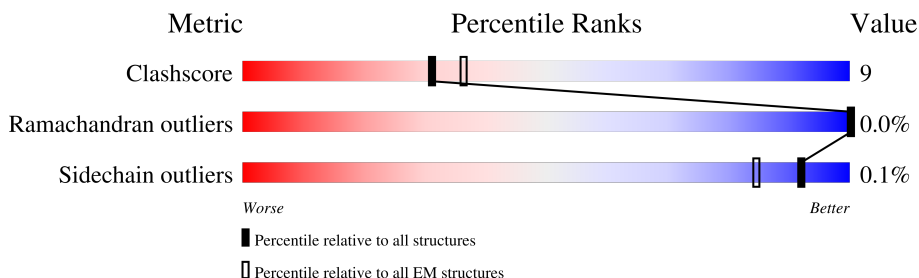
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.15 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  $\geq 3$ , 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	741	<div> <div>17%</div> <div>86%</div> <div>14%</div> </div>
2	B	733	<div> <div>21%</div> <div>85%</div> <div>15%</div> </div>
3	C	80	<div> <div>21%</div> <div>92%</div> <div>8%</div> </div>
4	D	144	<div> <div>47%</div> <div>94%</div> <div>6%</div> </div>
5	E	63	<div> <div>38%</div> <div>97%</div> <div>.</div> </div>
6	F	165	<div> <div>38%</div> <div>91%</div> <div>9%</div> </div>
7	G	91	<div> <div>77%</div> <div>71%</div> <div>10%</div> <div>19%</div> </div>
8	I	37	<div> <div>70%</div> <div>86%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
9	J	39	
10	K	84	
11	L	126	
12	1	194	
12	Z	194	
13	3	219	
14	7	213	
15	8	217	
16	4	210	
17	5	227	
18	6	229	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CL0	A	1011	X	-	-	-
20	CLA	1	601	X	-	-	-
20	CLA	1	602	X	-	-	-
20	CLA	1	603	X	-	-	-
20	CLA	1	604	X	-	-	-
20	CLA	1	605	X	-	-	-
20	CLA	1	606	X	-	-	-
20	CLA	1	607	X	-	-	-
20	CLA	1	608	X	-	-	-
20	CLA	1	611	X	-	-	-
20	CLA	1	612	X	-	-	-
20	CLA	1	613	X	-	-	-
20	CLA	1	615	X	-	-	-
20	CLA	3	601	X	-	-	-
20	CLA	3	602	X	-	-	-
20	CLA	3	603	X	-	-	-
20	CLA	3	604	X	-	-	-
20	CLA	3	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	3	606	X	-	-	-
20	CLA	3	607	X	-	-	-
20	CLA	3	608	X	-	-	-
20	CLA	3	610	X	-	-	-
20	CLA	3	612	X	-	-	-
20	CLA	3	613	X	-	-	-
20	CLA	3	616	X	-	-	-
20	CLA	3	618	X	-	-	-
20	CLA	4	601	X	-	-	-
20	CLA	4	602	X	-	-	-
20	CLA	4	603	X	-	-	-
20	CLA	4	604	X	-	-	-
20	CLA	4	605	X	-	-	-
20	CLA	4	606	X	-	-	-
20	CLA	4	607	X	-	-	-
20	CLA	4	608	X	-	-	-
20	CLA	4	609	X	-	-	-
20	CLA	4	612	X	-	-	-
20	CLA	4	615	X	-	-	-
20	CLA	5	601	X	-	-	-
20	CLA	5	602	X	-	-	-
20	CLA	5	603	X	-	-	-
20	CLA	5	604	X	-	-	-
20	CLA	5	605	X	-	-	-
20	CLA	5	606	X	-	-	-
20	CLA	5	607	X	-	-	-
20	CLA	5	608	X	-	-	-
20	CLA	5	609	X	-	-	-
20	CLA	5	612	X	-	-	-
20	CLA	5	613	X	-	-	-
20	CLA	5	615	X	-	-	-
20	CLA	5	618	X	-	-	-
20	CLA	5	622	X	-	-	-
20	CLA	6	601	X	-	-	-
20	CLA	6	602	X	-	-	-
20	CLA	6	603	X	-	-	-
20	CLA	6	604	X	-	-	-
20	CLA	6	605	X	-	-	-
20	CLA	6	606	X	-	-	-
20	CLA	6	607	X	-	-	-
20	CLA	6	608	X	-	-	-
20	CLA	6	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	6	612	X	-	-	-
20	CLA	6	615	X	-	-	-
20	CLA	6	618	X	-	-	-
20	CLA	6	619	X	-	-	-
20	CLA	7	601	X	-	-	-
20	CLA	7	602	X	-	-	-
20	CLA	7	603	X	-	-	-
20	CLA	7	604	X	-	-	-
20	CLA	7	605	X	-	-	-
20	CLA	7	606	X	-	-	-
20	CLA	7	607	X	-	-	-
20	CLA	7	608	X	-	-	-
20	CLA	7	609	X	-	-	-
20	CLA	7	611	X	-	-	-
20	CLA	7	612	X	-	-	-
20	CLA	7	613	X	-	-	-
20	CLA	7	615	X	-	-	-
20	CLA	7	616	X	-	-	-
20	CLA	8	601	X	-	-	-
20	CLA	8	602	X	-	-	-
20	CLA	8	603	X	-	-	-
20	CLA	8	604	X	-	-	-
20	CLA	8	605	X	-	-	-
20	CLA	8	606	X	-	-	-
20	CLA	8	607	X	-	-	-
20	CLA	8	608	X	-	-	-
20	CLA	8	609	X	-	-	-
20	CLA	8	611	X	-	-	-
20	CLA	8	612	X	-	-	-
20	CLA	8	615	X	-	-	-
20	CLA	A	1012	X	-	-	-
20	CLA	A	1013	X	-	-	-
20	CLA	A	1101	X	-	-	-
20	CLA	A	1102	X	-	-	-
20	CLA	A	1103	X	-	-	-
20	CLA	A	1104	X	-	-	-
20	CLA	A	1105	X	-	-	-
20	CLA	A	1106	X	-	-	-
20	CLA	A	1107	X	-	-	-
20	CLA	A	1108	X	-	-	-
20	CLA	A	1109	X	-	-	-
20	CLA	A	1110	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	1111	X	-	-	-
20	CLA	A	1112	X	-	-	-
20	CLA	A	1113	X	-	-	-
20	CLA	A	1114	X	-	-	-
20	CLA	A	1115	X	-	-	-
20	CLA	A	1116	X	-	-	-
20	CLA	A	1117	X	-	-	-
20	CLA	A	1118	X	-	-	-
20	CLA	A	1119	X	-	-	-
20	CLA	A	1120	X	-	-	-
20	CLA	A	1121	X	-	-	-
20	CLA	A	1122	X	-	-	-
20	CLA	A	1123	X	-	-	-
20	CLA	A	1124	X	-	-	-
20	CLA	A	1125	X	-	-	-
20	CLA	A	1126	X	-	-	-
20	CLA	A	1127	X	-	-	-
20	CLA	A	1128	X	-	-	-
20	CLA	A	1129	X	-	-	-
20	CLA	A	1130	X	-	-	-
20	CLA	A	1131	X	-	-	-
20	CLA	A	1132	X	-	-	-
20	CLA	A	1133	X	-	-	-
20	CLA	A	1134	X	-	-	-
20	CLA	A	1135	X	-	-	-
20	CLA	A	1136	X	-	-	-
20	CLA	A	1137	X	-	-	-
20	CLA	A	1138	X	-	-	-
20	CLA	A	1139	X	-	-	-
20	CLA	A	1140	X	-	-	-
20	CLA	A	1141	X	-	-	-
20	CLA	B	1021	X	-	-	-
20	CLA	B	1022	X	-	-	-
20	CLA	B	1023	X	-	-	-
20	CLA	B	1201	X	-	-	-
20	CLA	B	1202	X	-	-	-
20	CLA	B	1203	X	-	-	-
20	CLA	B	1204	X	-	-	-
20	CLA	B	1205	X	-	-	-
20	CLA	B	1206	X	-	-	-
20	CLA	B	1207	X	-	-	-
20	CLA	B	1208	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	1209	X	-	-	-
20	CLA	B	1210	X	-	-	-
20	CLA	B	1211	X	-	-	-
20	CLA	B	1212	X	-	-	-
20	CLA	B	1213	X	-	-	-
20	CLA	B	1214	X	-	-	-
20	CLA	B	1215	X	-	-	-
20	CLA	B	1216	X	-	-	-
20	CLA	B	1217	X	-	-	-
20	CLA	B	1218	X	-	-	-
20	CLA	B	1219	X	-	-	-
20	CLA	B	1220	X	-	-	-
20	CLA	B	1221	X	-	-	-
20	CLA	B	1222	X	-	-	-
20	CLA	B	1223	X	-	-	-
20	CLA	B	1224	X	-	-	-
20	CLA	B	1225	X	-	-	-
20	CLA	B	1226	X	-	-	-
20	CLA	B	1227	X	-	-	-
20	CLA	B	1228	X	-	-	-
20	CLA	B	1229	X	-	-	-
20	CLA	B	1230	X	-	-	-
20	CLA	B	1231	X	-	-	-
20	CLA	B	1232	X	-	-	-
20	CLA	B	1234	X	-	-	-
20	CLA	B	1235	X	-	-	-
20	CLA	B	1236	X	-	-	-
20	CLA	B	1237	X	-	-	-
20	CLA	B	1238	X	-	-	-
20	CLA	B	1239	X	-	-	-
20	CLA	B	1240	X	-	-	-
20	CLA	B	1241	X	-	-	-
20	CLA	F	1301	X	-	-	-
20	CLA	F	1302	X	-	-	-
20	CLA	G	1601	X	-	-	-
20	CLA	G	1602	X	-	-	-
20	CLA	J	1901	X	-	-	-
20	CLA	K	1401	X	-	-	-
20	CLA	K	1402	X	-	-	-
20	CLA	K	1403	X	-	-	-
20	CLA	K	1404	X	-	-	-
20	CLA	L	1502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	L	1503	X	-	-	-
20	CLA	Z	601	X	-	-	-
20	CLA	Z	602	X	-	-	-
20	CLA	Z	603	X	-	-	-
20	CLA	Z	604	X	-	-	-
20	CLA	Z	605	X	-	-	-
20	CLA	Z	606	X	-	-	-
20	CLA	Z	607	X	-	-	-
20	CLA	Z	608	X	-	-	-
20	CLA	Z	611	X	-	-	-
20	CLA	Z	612	X	-	-	-
20	CLA	Z	615	X	-	-	-
33	RRX	F	4001	X	-	-	-
34	C7Z	1	503	X	-	-	-
34	C7Z	5	505	X	-	-	-
34	C7Z	J	4002	X	-	-	-
37	CHL	1	609	X	-	-	-
37	CHL	1	610	X	-	-	-
37	CHL	3	611	X	-	-	-
37	CHL	4	610	X	-	-	-
37	CHL	4	611	X	-	-	-
37	CHL	4	613	X	-	-	-
37	CHL	4	617	X	-	-	-
37	CHL	5	610	X	-	-	-
37	CHL	5	611	X	-	-	-
37	CHL	5	617	X	-	-	-
37	CHL	6	610	X	-	-	-
37	CHL	6	611	X	-	-	-
37	CHL	6	613	X	-	-	-
37	CHL	6	617	X	-	-	-
37	CHL	7	610	X	-	-	-
37	CHL	8	610	X	-	-	-
37	CHL	8	613	X	-	-	-
37	CHL	Z	609	X	-	-	-
37	CHL	Z	610	X	-	-	-
37	CHL	Z	613	X	-	-	-
39	QTB	Z	504	X	-	-	-

## 2 Entry composition

There are 43 unique types of molecules in this entry. The entry contains 47524 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	741	Total	C	N	O	S	0	0
			5820	3805	993	1000	22		

- 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
			5825	3825	977	1005	18		

- 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
			601	369	103	117	12		

- Molecule 4 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1135	725	201	202	7		

- Molecule 5 is a protein called Photosystem I reaction center subunit IV, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	63	Total	C	N	O	0	0
			497	316	87	94		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	G	74	Total	C	N	O	0	0
			550	354	94	102		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	37	Total	C	N	O	S	0	0
			282	195	39	47	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	39	Total	C	N	O	S	0	0
			321	219	45	56	1		

- Molecule 10 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	84	Total	C	N	O	S	0	0
			571	362	98	109	2		

- Molecule 11 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	126	Total	C	N	O	S	0	0
			914	595	148	168	3		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	PRO	deletion	UNP A8IL32
L	?	-	SER	deletion	UNP A8IL32
L	?	-	ILE	deletion	UNP A8IL32
L	?	-	GLY	deletion	UNP A8IL32
L	?	-	VAL	deletion	UNP A8IL32
L	?	-	LYS	deletion	UNP A8IL32
L	?	-	THR	deletion	UNP A8IL32
L	?	-	LEU	deletion	UNP A8IL32
L	?	-	SER	deletion	UNP A8IL32
L	?	-	GLY	deletion	UNP A8IL32
L	?	-	ARG	deletion	UNP A8IL32

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	SER	deletion	UNP A8IL32

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
12	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	3	219	Total	C	N	O	S	0	0
			1674	1092	270	304	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	213	Total	C	N	O	S	0	0
			1650	1072	274	298	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	8	217	Total	C	N	O	S	0	0
			1650	1073	280	293	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	4	210	Total	C	N	O	S	0	0
			1628	1068	262	293	5		

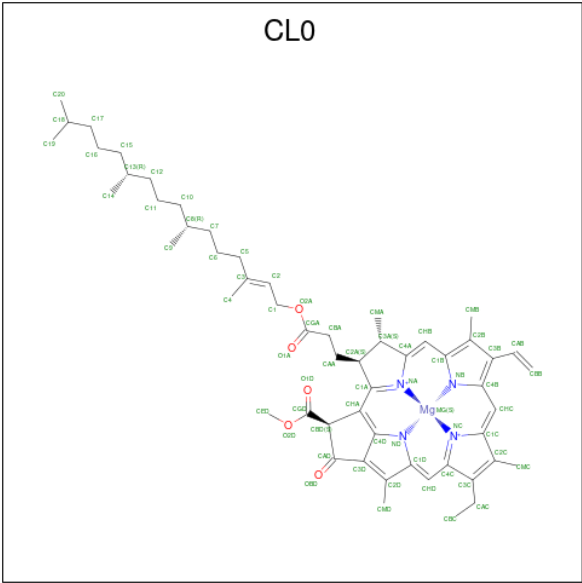
- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	5	227	Total	C	N	O	S	0	0
			1775	1154	297	316	8		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

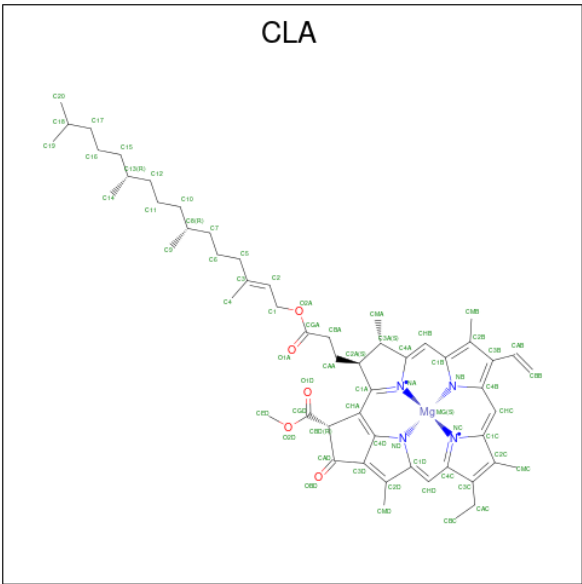
Mol	Chain	Residues	Atoms					AltConf	Trace
18	6	229	Total	C	N	O	S	0	0
			1766	1164	292	304	6		

- Molecule 19 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

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





Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
20	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	G	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	J	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	K	1	Total 49	C 39	Mg 1	N 4	O 5	0
20	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
20	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
20	Z	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	Z	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	3	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	7	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
20	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	7	1	Total 42	C 34	Mg 1	N 4	O 3	0
20	7	1	Total 58	C 48	Mg 1	N 4	O 5	0
20	7	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 62	C 52	Mg 1	N 4	O 5	0
20	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	8	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	4	1	Total 41	C 33	Mg 1	N 4	O 3	0

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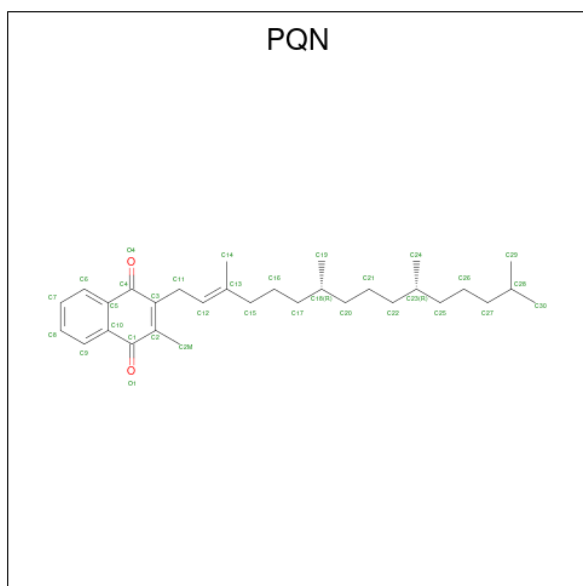
Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
20	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	5	1	Total 61	C 51	Mg 1	N 4	O 5	0
20	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
20	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
20	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
20	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
20	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
20	6	1	Total 52	C 42	Mg 1	N 4	O 5	0
20	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
20	6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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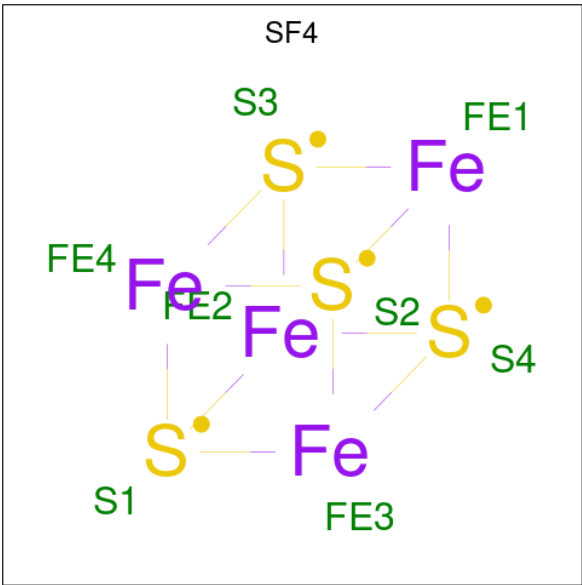
Mol	Chain	Residues	Atoms					AltConf
20	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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



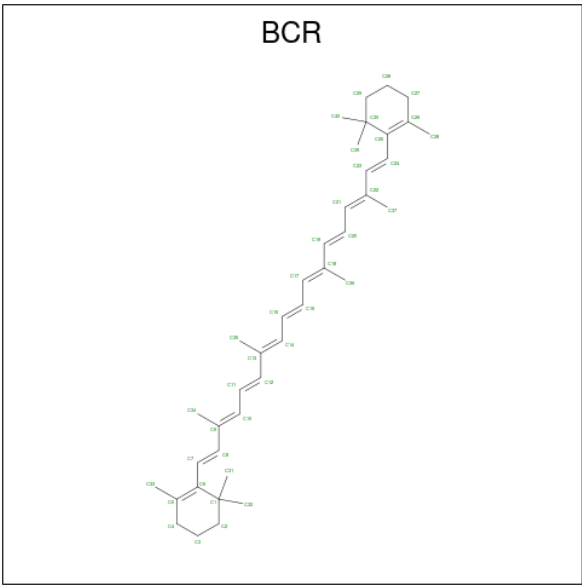
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			33	31	2	
21	B	1	Total	C	O	0
			33	31	2	

- Molecule 22 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



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

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).



Mol	Chain	Residues	Atoms		AltConf
23	A	1	Total	C	0
			40	40	

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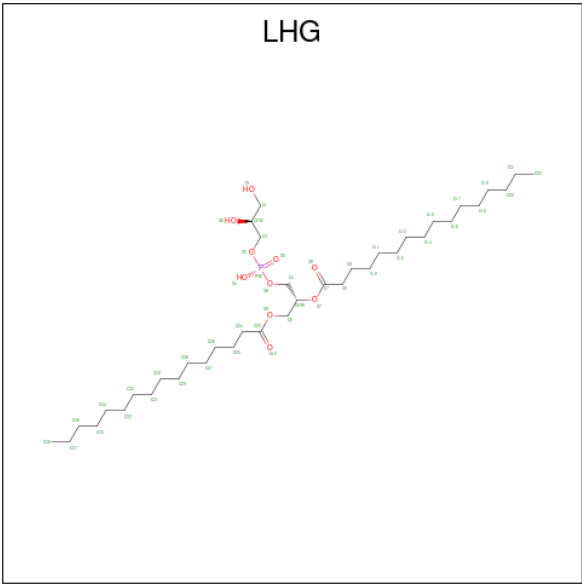
Mol	Chain	Residues	Atoms	AltConf
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
23	3	1	Total	C	0
			40	40	
23	7	1	Total	C	0
			40	40	
23	7	1	Total	C	0
			40	40	
23	8	1	Total	C	0
			40	40	
23	4	1	Total	C	0
			40	40	
23	5	1	Total	C	0
			40	40	
23	5	1	Total	C	0
			40	40	
23	6	1	Total	C	0
			40	40	
23	6	1	Total	C	0
			40	40	

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
24	A	1	Total	C	O	P	0
			35	24	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	

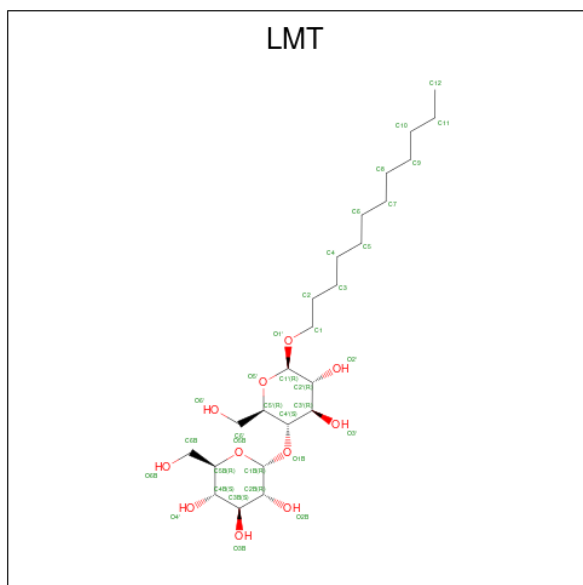
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Mol	Chain	Residues	Atoms				AltConf
24	B	1	Total 23	C 12	O 10	P 1	0
24	B	1	Total 20	C 9	O 10	P 1	0
24	B	1	Total 33	C 22	O 10	P 1	0
24	1	1	Total 43	C 32	O 10	P 1	0
24	Z	1	Total 43	C 32	O 10	P 1	0
24	3	1	Total 20	C 9	O 10	P 1	0
24	7	1	Total 37	C 26	O 10	P 1	0
24	8	1	Total 38	C 27	O 10	P 1	0
24	4	1	Total 49	C 38	O 10	P 1	0
24	4	1	Total 32	C 21	O 10	P 1	0
24	5	1	Total 37	C 26	O 10	P 1	0
24	6	1	Total 49	C 38	O 10	P 1	0

- # NKP

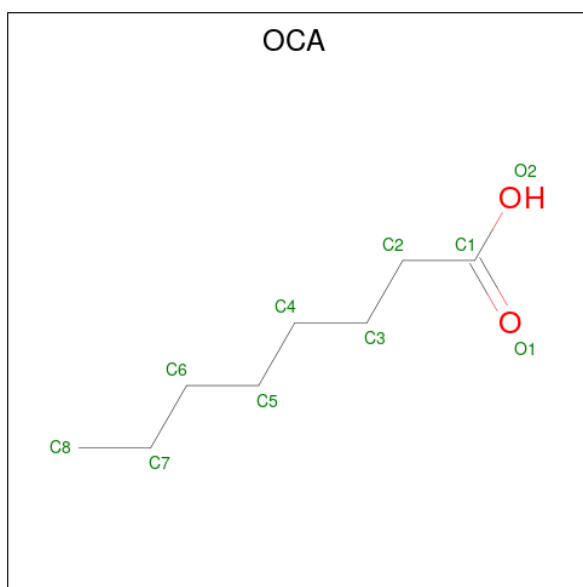
Mol	Chain	Residues	Atoms				AltConf
25	A	1	Total	C	O	P	0
			29	21	7	1	
25	3	1	Total	C	O	P	0
			16	8	7	1	
25	8	1	Total	C	O	P	0
			29	21	7	1	

- Molecule 26 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



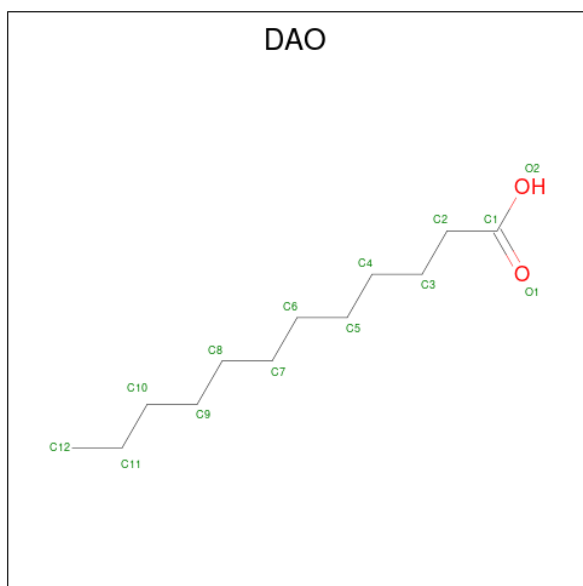
Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	C	O	0
			35	24	11	
26	B	1	Total	C	O	0
			35	24	11	
26	B	1	Total	C	O	0
			35	24	11	
26	F	1	Total	C	O	0
			35	24	11	
26	1	1	Total	C	O	0
			35	24	11	
26	8	1	Total	C	O	0
			35	24	11	
26	4	1	Total	C	O	0
			35	24	11	

- Molecule 27 is OCTANOIC ACID (CAPRYLIC ACID) (three-letter code: OCA) (formula:  $C_8H_{16}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			10	8	2	

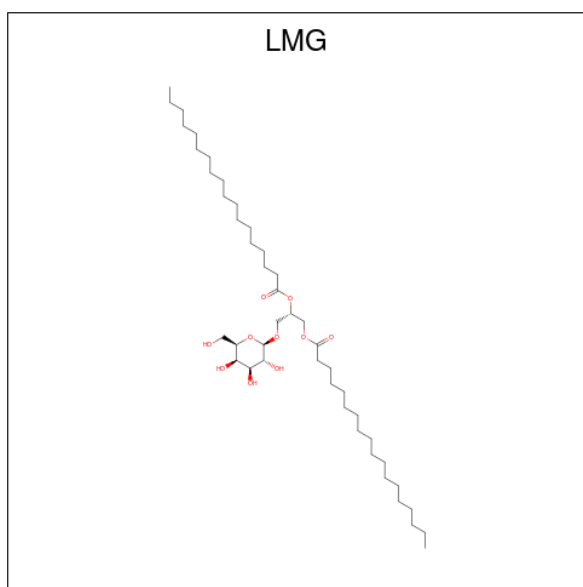
- Molecule 28 is LAURIC ACID (three-letter code: DAO) (formula:  $C_{12}H_{24}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			14	12	2	

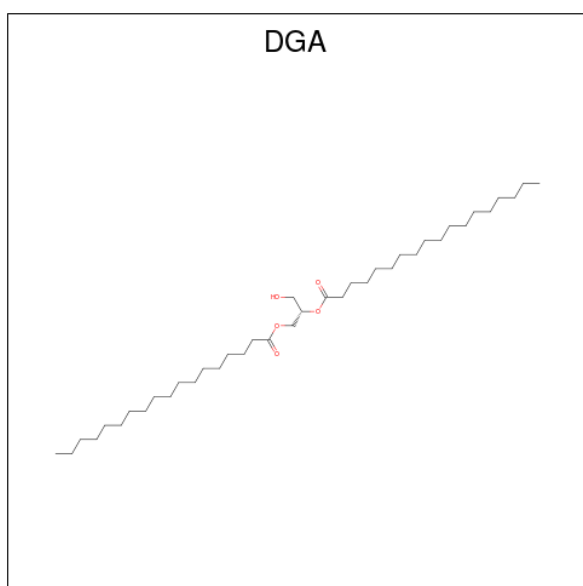
- Molecule 29 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).





Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			29	19	10	
29	J	1	Total	C	O	0
			35	25	10	

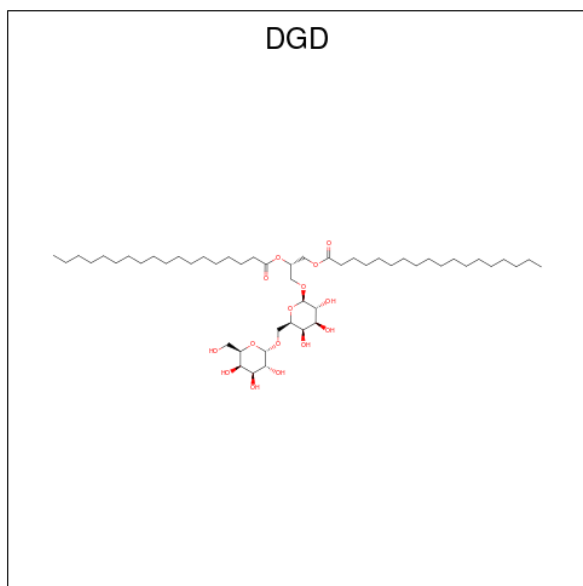
- Molecule 30 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	C	O	0
			44	39	5	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD)

(formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).

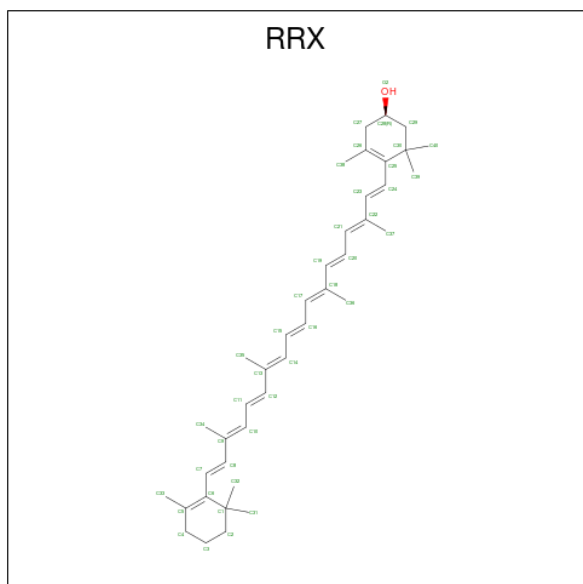


Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			66	51	15	

- Molecule 32 is CALCIUM ION (three-letter code: CA) (formula: Ca).

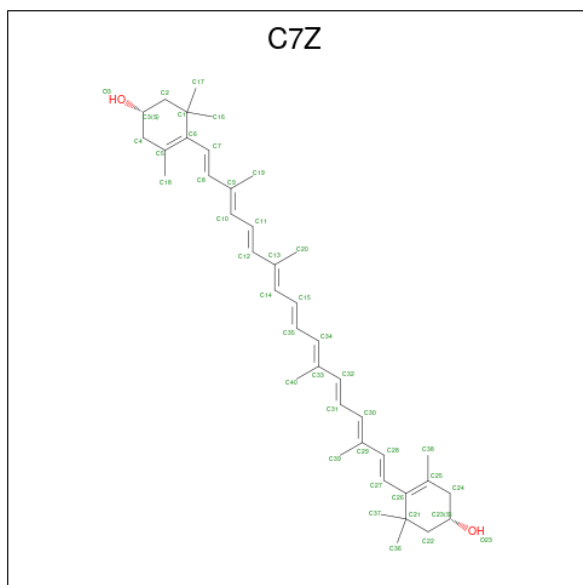
Mol	Chain	Residues	Atoms		AltConf
32	B	1	Total	Ca	0
			1	1	

- Molecule 33 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



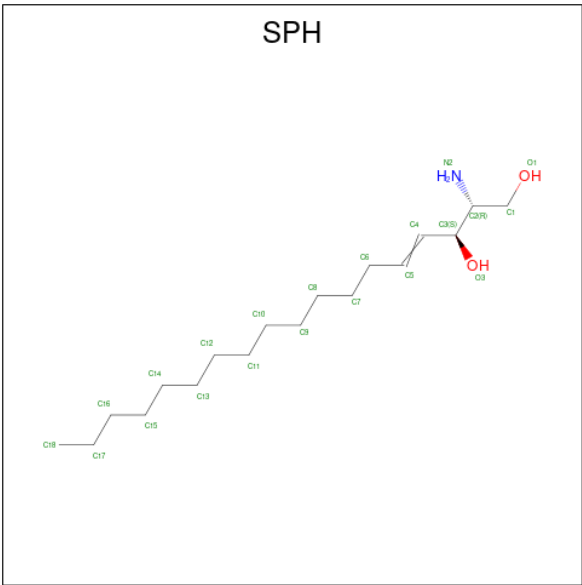
Mol	Chain	Residues	Atoms			AltConf
33	F	1	Total	C	O	0
			41	40	1	

- Molecule 34 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (three-letter code: C7Z) (formula:  $C_{40}H_{56}O_2$ ).



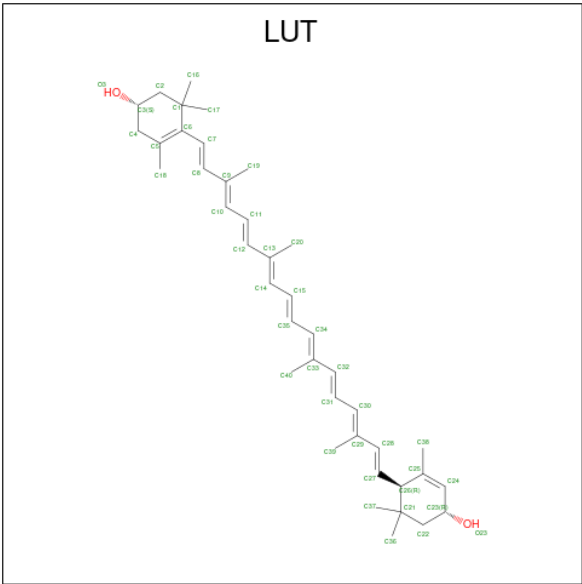
Mol	Chain	Residues	Atoms			AltConf
34	J	1	Total	C	O	0
			42	40	2	
34	1	1	Total	C	O	0
			42	40	2	
34	5	1	Total	C	O	0
			42	40	2	

- Molecule 35 is SPHINGOSINE (three-letter code: SPH) (formula:  $C_{18}H_{37}NO_2$ ).



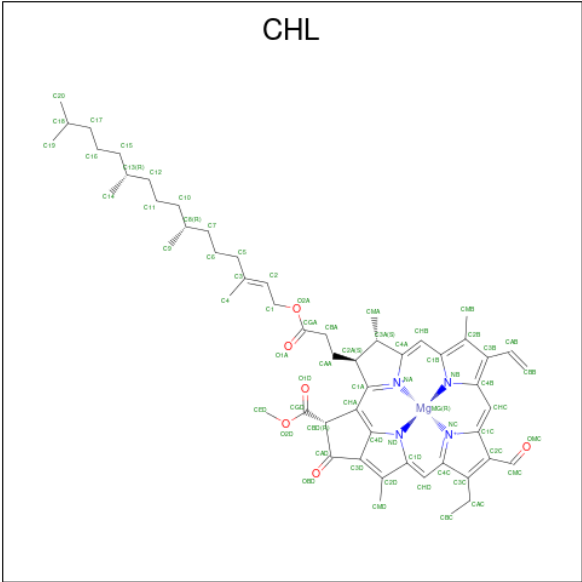
Mol	Chain	Residues	Atoms				AltConf
35	K	1	Total	C	N	O	0
			21	18	1	2	
35	7	1	Total	C	N	O	0
			21	18	1	2	
35	7	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 36 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
36	1	1	Total	C	O	0
			42	40	2	
36	1	1	Total	C	O	0
			42	40	2	
36	Z	1	Total	C	O	0
			42	40	2	
36	Z	1	Total	C	O	0
			42	40	2	
36	Z	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	3	1	Total	C	O	0
			42	40	2	
36	7	1	Total	C	O	0
			42	40	2	
36	7	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	8	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	4	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	5	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	
36	6	1	Total	C	O	0
			42	40	2	

- Molecule 37 is CHLOROPHYLL B (three-letter code: CHL) (formula:  $C_{55}H_{70}MgN_4O_6$ ).



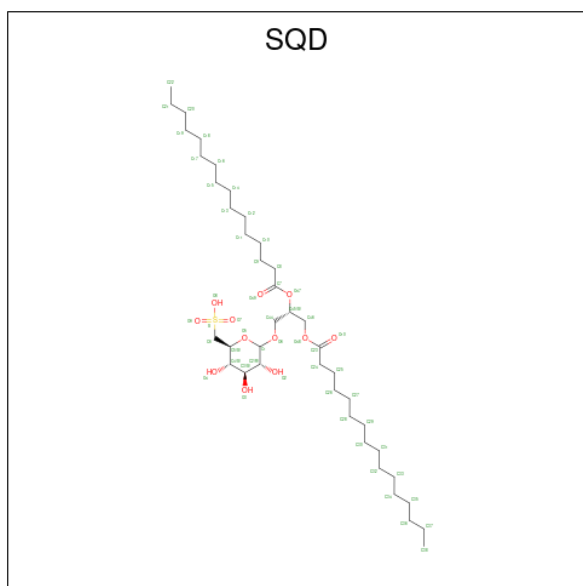
Mol	Chain	Residues	Atoms					AltConf
37	1	1	Total 48	C 37	Mg 1	N 4	O 6	0
37	1	1	Total 58	C 47	Mg 1	N 4	O 6	0
37	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
37	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	3	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	7	1	Total 54	C 43	Mg 1	N 4	O 6	0
37	8	1	Total 56	C 45	Mg 1	N 4	O 6	0
37	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
37	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
37	4	1	Total 51	C 40	Mg 1	N 4	O 6	0
37	4	1	Total 56	C 45	Mg 1	N 4	O 6	0
37	4	1	Total 43	C 34	Mg 1	N 4	O 4	0
37	5	1	Total 66	C 55	Mg 1	N 4	O 6	0

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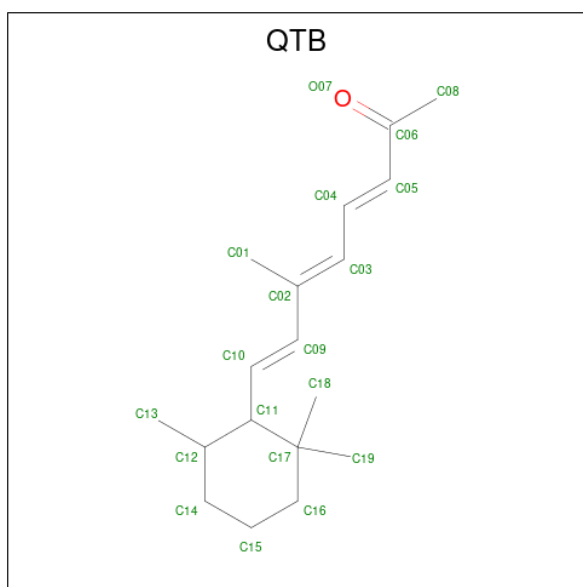
Mol	Chain	Residues	Atoms					AltConf
37	5	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
37	5	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
37	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
37	6	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
37	6	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
37	6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

- Molecule 38 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



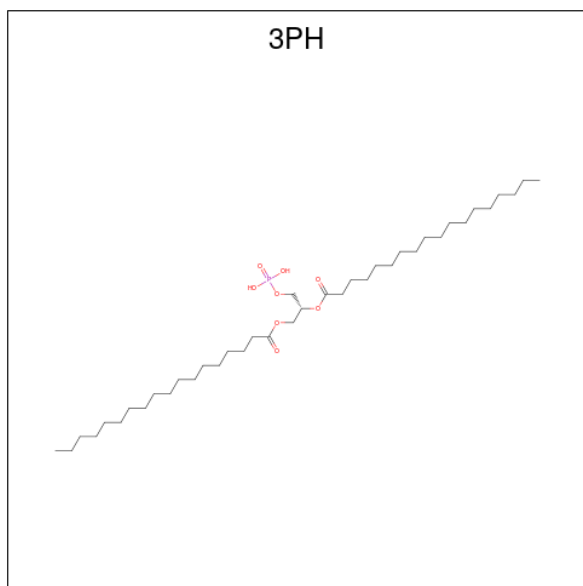
Mol	Chain	Residues	Atoms				AltConf
38	1	1	Total	C	O	S	0
			48	35	12	1	

- Molecule 39 is (3 {E},5 {E},7 {E})-6-methyl-8-[(6 {R})-2,2,6-trimethylcyclohexyl]octa-3,5,7-trien-2-one (three-letter code: QTB) (formula: C<sub>18</sub>H<sub>28</sub>O).



Mol	Chain	Residues	Atoms			AltConf
39	Z	1	Total	C	O	0
			19	18	1	

- Molecule 40 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula:  $C_{39}H_{77}O_8P$ ).



Mol	Chain	Residues	Atoms				AltConf
40	7	1	Total	C	O	P	0
			39	30	8	1	
40	8	1	Total	C	O	P	0
			30	21	8	1	

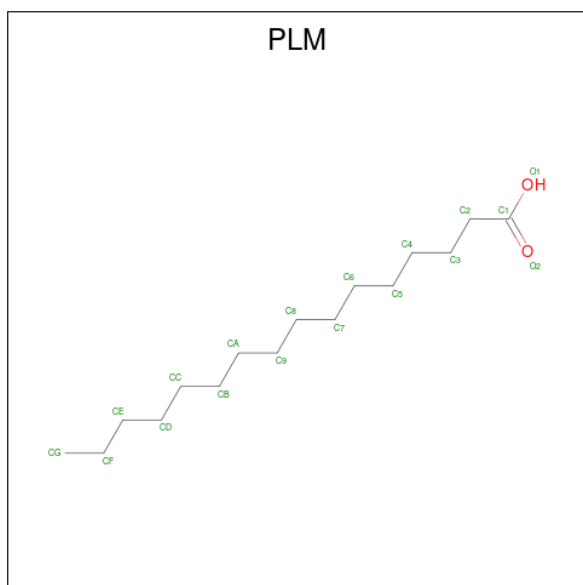
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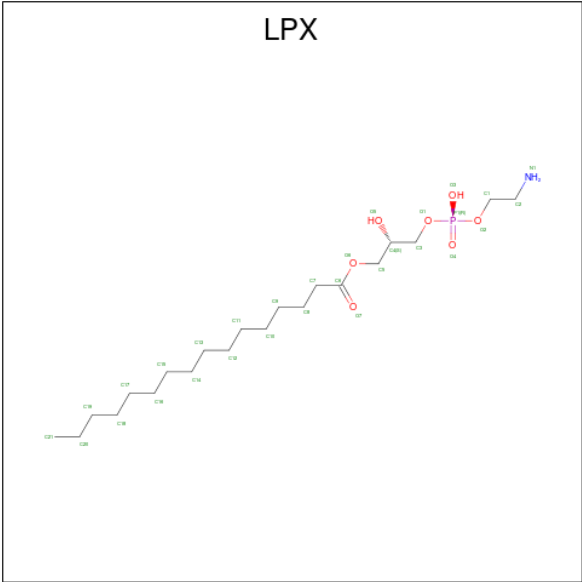
Mol	Chain	Residues	Atoms				AltConf
40	5	1	Total	C	O	P	0
			23	14	8	1	
40	6	1	Total	C	O	P	0
			29	20	8	1	

- Molecule 41 is PALMITIC ACID (three-letter code: PLM) (formula:  $C_{16}H_{32}O_2$ ).



Mol	Chain	Residues	Atoms			AltConf
41	7	1	Total	C	O	0
			18	16	2	

- Molecule 42 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula:  $C_{21}H_{44}NO_7P$ ).



Mol	Chain	Residues	Atoms					AltConf
42	8	1	Total	C	N	O	P	0
			30	21	1	7	1	

- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	A	3	Total	O	0
			3	3	
43	A	10	Total	O	0
			10	10	
43	A	17	Total	O	0
			17	17	
43	A	7	Total	O	0
			7	7	
43	A	6	Total	O	0
			6	6	
43	A	3	Total	O	0
			3	3	
43	A	5	Total	O	0
			5	5	
43	A	14	Total	O	0
			14	14	
43	A	3	Total	O	0
			3	3	
43	A	16	Total	O	0
			16	16	
43	A	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	A	1	Total O 1 1	0
43	B	2	Total O 2 2	0
43	B	1	Total O 1 1	0
43	B	1	Total O 1 1	0
43	B	1	Total O 1 1	0
43	B	5	Total O 5 5	0
43	B	15	Total O 15 15	0
43	B	4	Total O 4 4	0
43	B	12	Total O 12 12	0
43	B	18	Total O 18 18	0
43	B	2	Total O 2 2	0
43	B	15	Total O 15 15	0
43	B	3	Total O 3 3	0
43	C	1	Total O 1 1	0
43	C	1	Total O 1 1	0
43	C	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
43	C	1	Total 1	O 1	0
43	C	2	Total 2	O 2	0
43	C	8	Total 8	O 8	0
43	C	1	Total 1	O 1	0
43	C	1	Total 1	O 1	0
43	C	1	Total 1	O 1	0
43	C	1	Total 1	O 1	0
43	C	1	Total 1	O 1	0
43	D	1	Total 1	O 1	0
43	D	1	Total 1	O 1	0
43	D	1	Total 1	O 1	0
43	D	1	Total 1	O 1	0
43	D	1	Total 1	O 1	0
43	D	1	Total 1	O 1	0
43	D	1	Total 1	O 1	0
43	D	1	Total 1	O 1	0
43	D	2	Total 2	O 2	0
43	D	2	Total 2	O 2	0
43	D	1	Total 1	O 1	0
43	E	1	Total 1	O 1	0
43	E	1	Total 1	O 1	0
43	E	1	Total 1	O 1	0

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Mol	Chain	Residues	Atoms	AltConf
43	E	4	Total O 4 4	0
43	F	1	Total O 1 1	0
43	F	1	Total O 1 1	0
43	F	1	Total O 1 1	0
43	F	3	Total O 3 3	0
43	F	6	Total O 6 6	0
43	F	1	Total O 1 1	0
43	F	1	Total O 1 1	0
43	J	1	Total O 1 1	0
43	J	2	Total O 2 2	0
43	K	1	Total O 1 1	0
43	K	1	Total O 1 1	0
43	L	1	Total O 1 1	0
43	L	4	Total O 4 4	0
43	1	15	Total O 15 15	0
43	1	1	Total O 1 1	0
43	Z	8	Total O 8 8	0
43	3	16	Total O 16 16	0
43	3	1	Total O 1 1	0
43	7	18	Total O 18 18	0
43	8	1	Total O 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
43	8	15	Total 15	O 15	0
43	4	7	Total 7	O 7	0
43	5	9	Total 9	O 9	0
43	6	8	Total 8	O 8	0

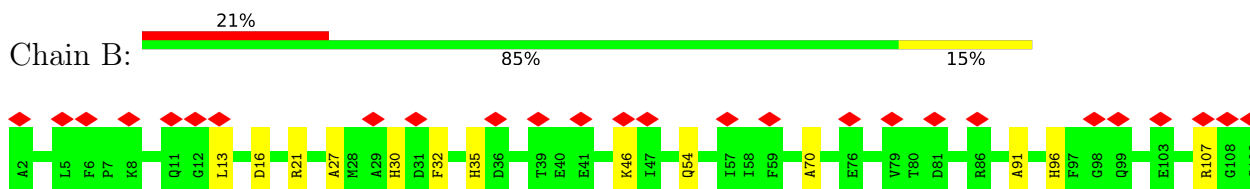
### 3 Residue-property plots

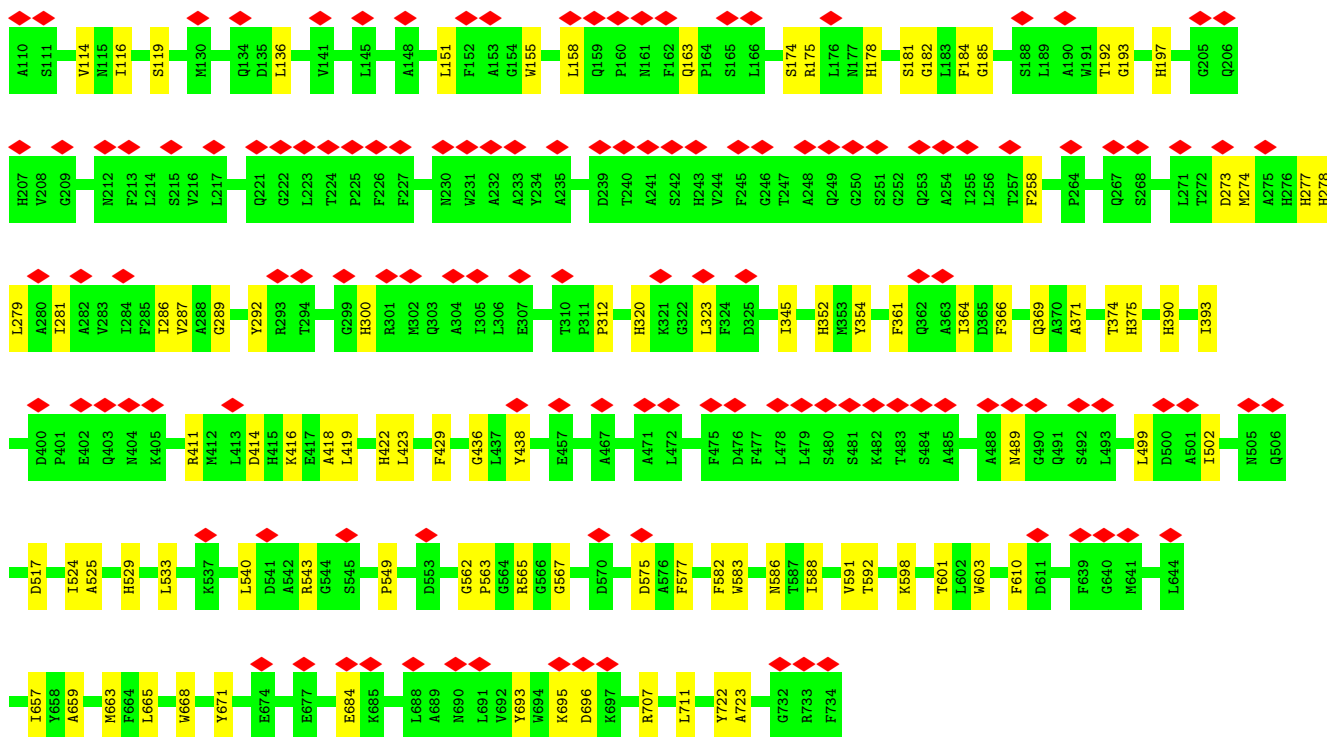
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

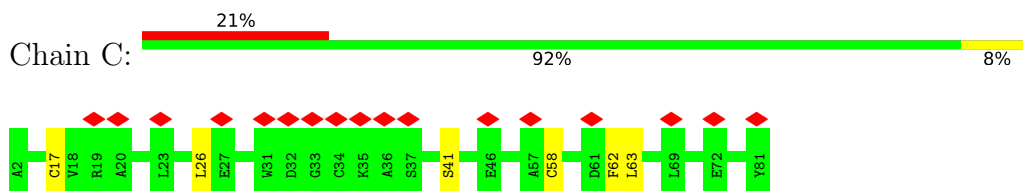


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

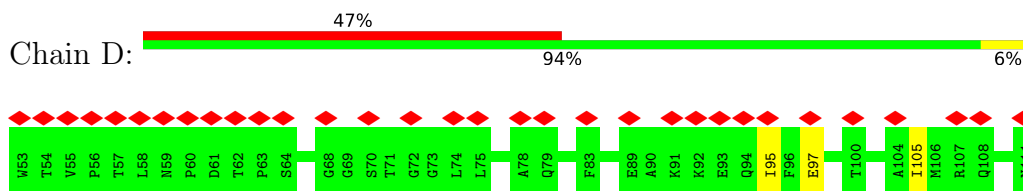




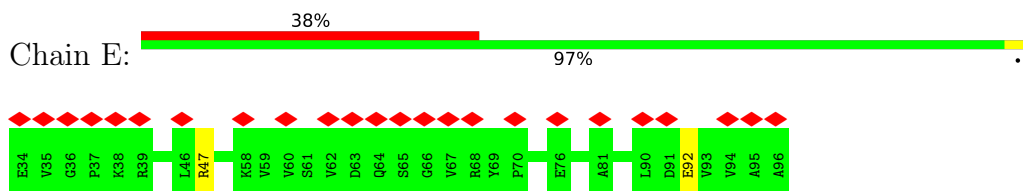
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Photosystem I reaction center subunit II, chloroplastic

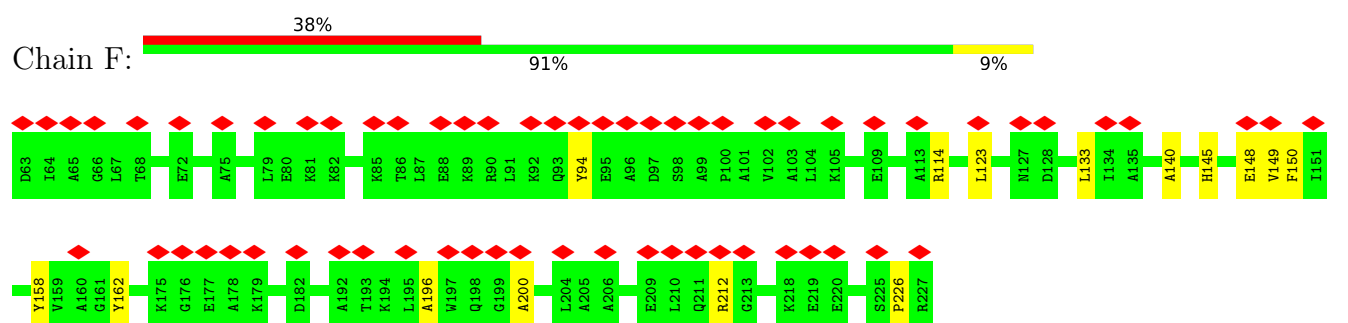


• Molecule 5: Photosystem I reaction center subunit IV, chloroplastic

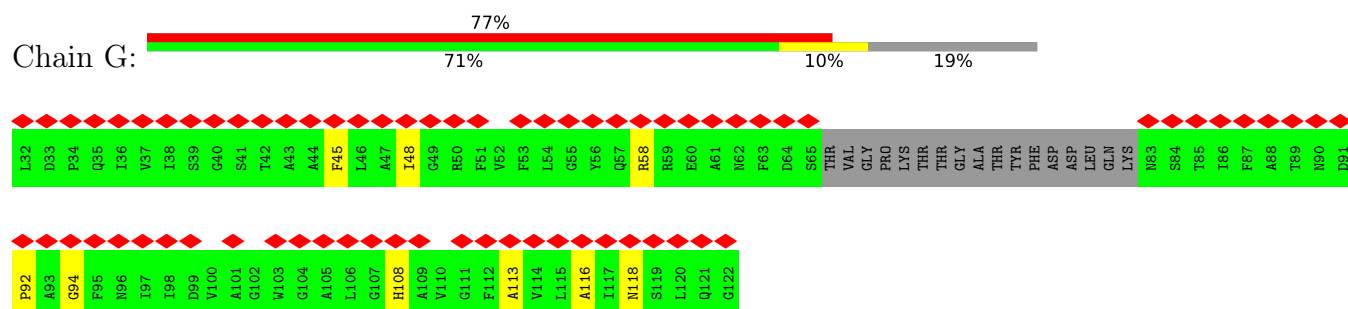


• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

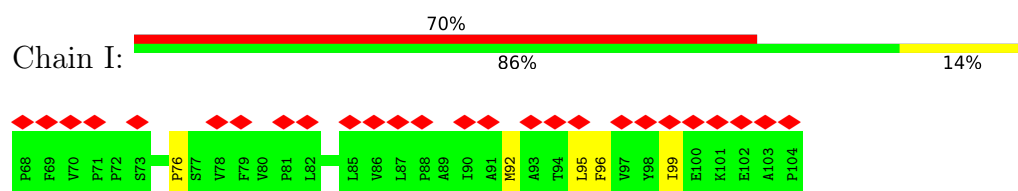




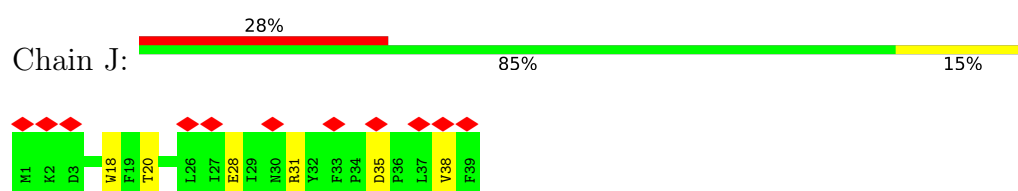
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



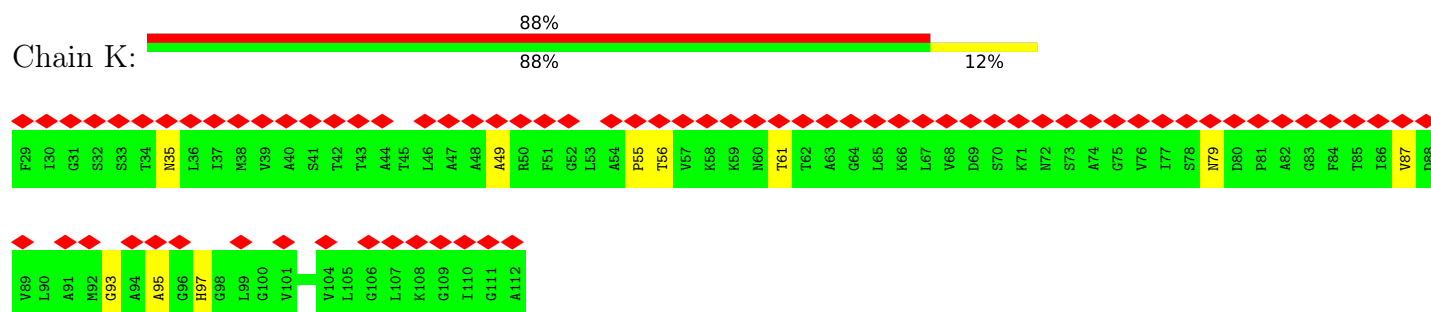
- Molecule 8: Photosystem I reaction center subunit VIII



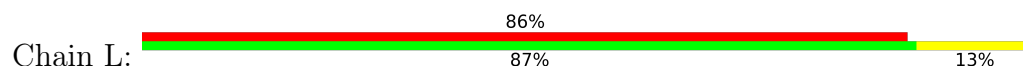
- Molecule 9: Photosystem I reaction center subunit IX

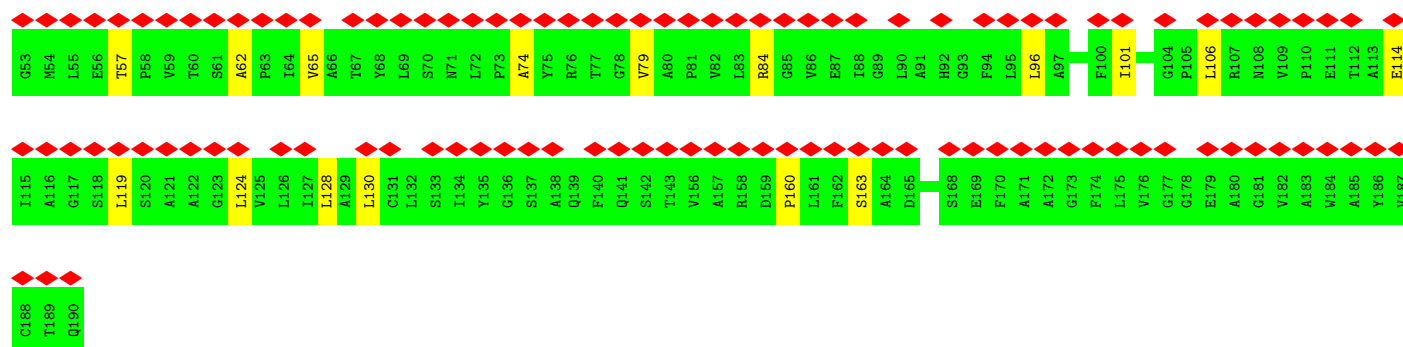


- Molecule 10: Photosystem I reaction center subunit psaK, chloroplastic



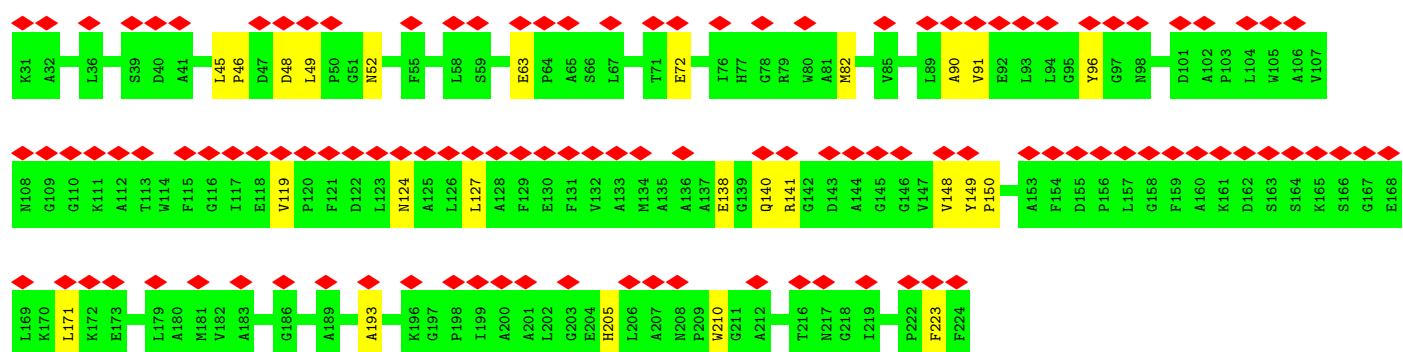
- Molecule 11: PSI subunit V





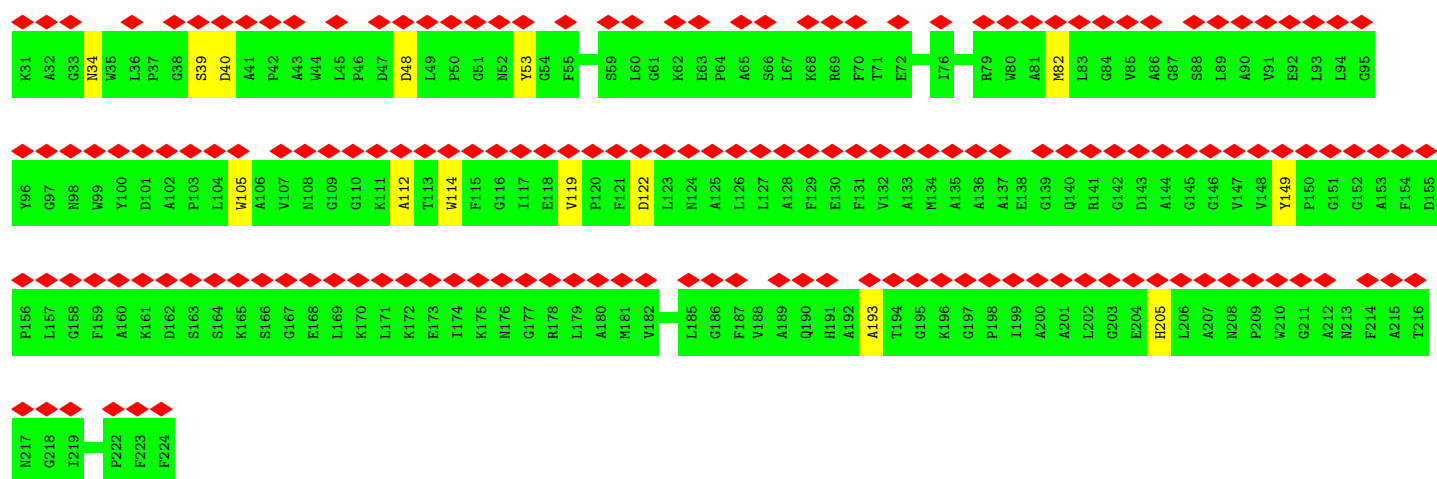
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain 1:



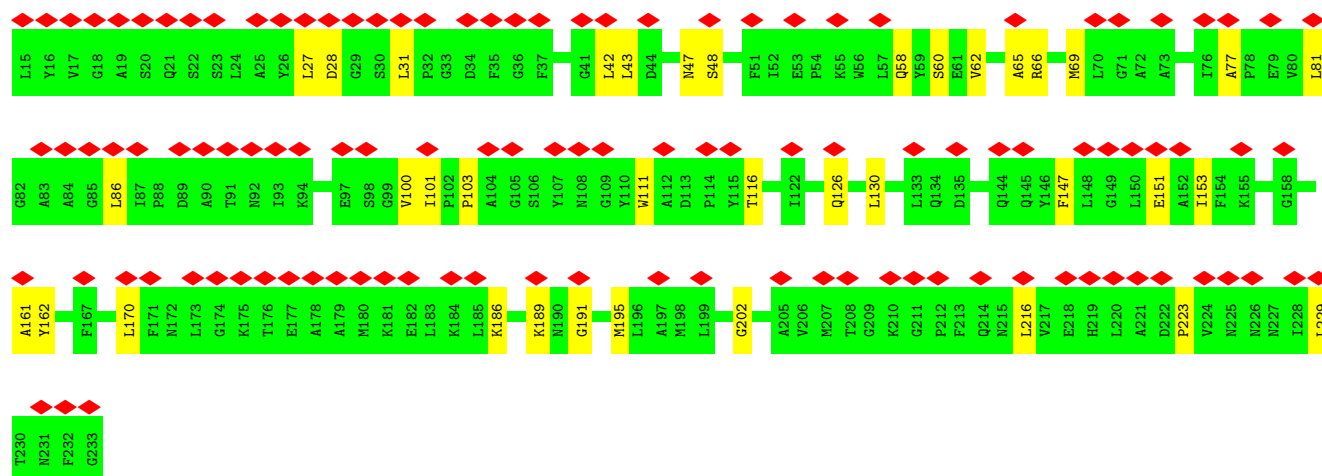
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

Chain Z:



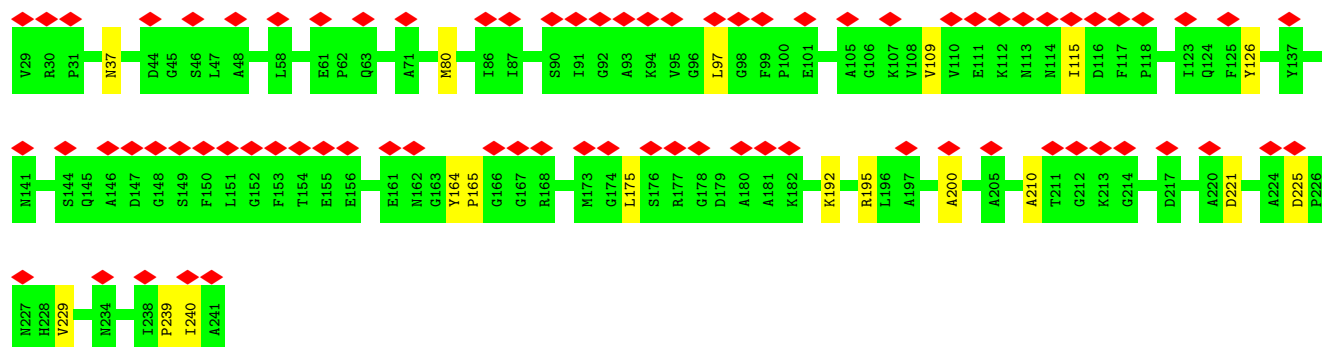
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic

Chain 3:



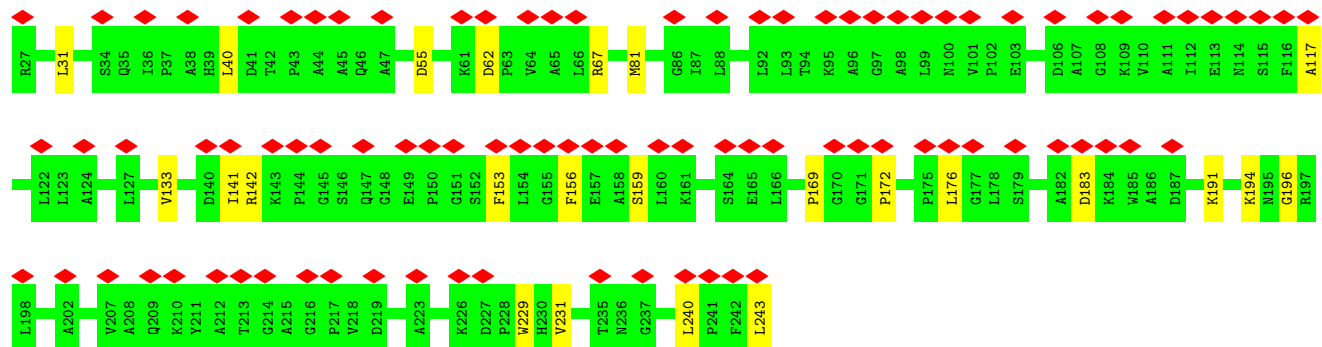
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic

Chain 7: 37% 92% 8%



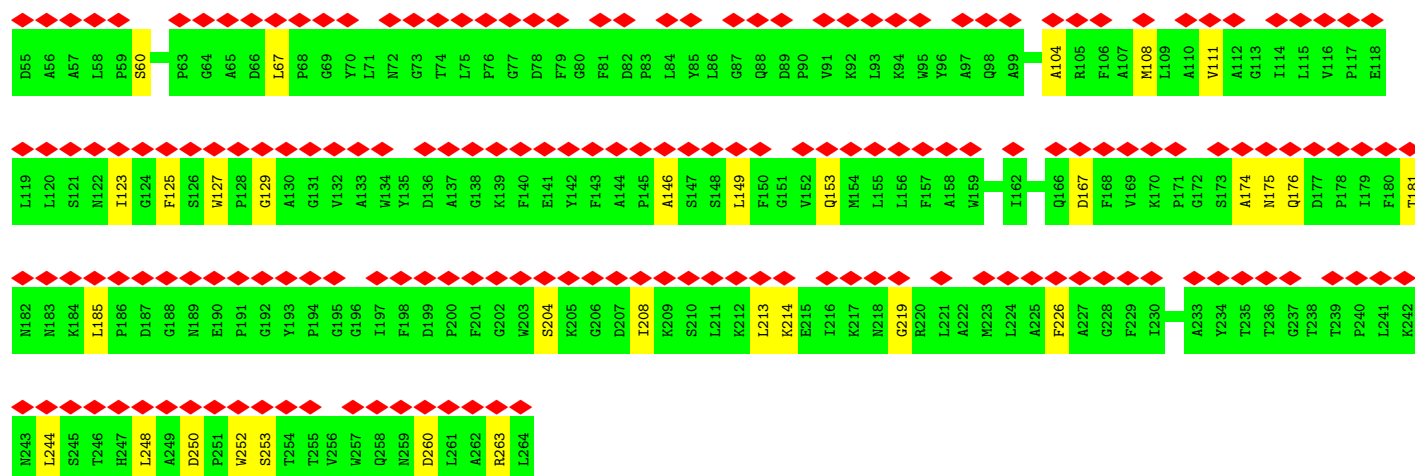
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 42% 89% 11%

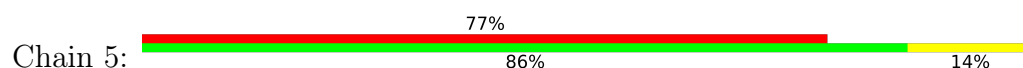


- Molecule 16: Chlorophyll a-b binding protein, chloroplastic

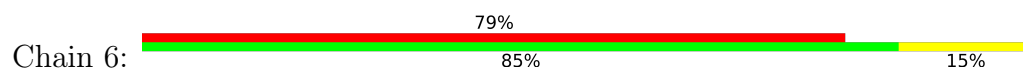
Chain 4: 85% 85% 15%



• Molecule 17: Chlorophyll a-b binding protein, chloroplastic



• Molecule 18: Chlorophyll a-b binding protein, chloroplastic



I217	F218	S219	K220	A221	A222	V223	V224	P225	G226	Q227	A228	V229	A230	P231	P232	C233	K234	I235	P236	A237	S238	V239	S240	Y241	K242	G243	I244	E245	I246	P247	T248	P249	C250	F251	L252	Q253	G254	L255	W256	P257
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17311	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 ( $e^-/\text{\AA}^2$ )	46.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.019	Depositor
Map size ( $\text{\AA}$ )	264.64, 264.64, 264.64	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.827, 0.827, 0.827	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BCR, CLA, DGA, CL0, LUT, OCA, 3PH, LPX, SF4, QTB, LMG, C7Z, SNC, CHL, PQN, DGD, DAO, LHG, CA, RRX, SPH, PLM, NKP, SQD, LMT

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	0.32	0/6016	0.52	0/8201
2	B	0.32	0/6037	0.53	0/8242
3	C	0.29	0/611	0.59	0/826
4	D	0.31	0/1154	0.57	0/1556
5	E	0.31	0/507	0.52	0/689
6	F	0.31	0/1292	0.54	0/1747
7	G	0.28	0/561	0.48	0/760
8	I	0.31	0/294	0.53	0/406
9	J	0.33	0/332	0.52	0/454
10	K	0.28	0/576	0.49	0/779
11	L	0.29	0/935	0.50	0/1277
12	1	0.29	0/1491	0.48	0/2028
12	Z	0.28	0/1491	0.46	0/2028
13	3	0.32	0/1722	0.51	0/2336
14	7	0.31	0/1702	0.48	0/2310
15	8	0.30	0/1701	0.47	0/2315
16	4	0.30	0/1683	0.50	0/2296
17	5	0.30	0/1830	0.49	0/2492
18	6	0.29	0/1828	0.50	0/2497
All	All	0.31	0/31763	0.51	0/43239

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5820	0	5670	82	0
2	B	5825	0	5579	84	0
3	C	601	0	581	4	0
4	D	1135	0	1148	4	0
5	E	497	0	491	1	0
6	F	1266	0	1301	13	0
7	G	550	0	532	7	0
8	I	282	0	292	5	0
9	J	321	0	322	5	0
10	K	571	0	606	10	0
11	L	914	0	921	11	0
12	1	1445	0	1396	21	0
12	Z	1445	0	1396	12	0
13	3	1674	0	1633	33	0
14	7	1650	0	1589	17	0
15	8	1650	0	1629	19	0
16	4	1628	0	1576	23	0
17	5	1775	0	1746	32	0
18	6	1766	0	1765	30	0
19	A	65	0	72	3	0
20	1	712	0	712	29	0
20	3	748	0	720	28	0
20	4	613	0	566	24	0
20	5	799	0	757	34	0
20	6	759	0	741	37	0
20	7	790	0	751	32	0
20	8	694	0	672	22	0
20	A	2699	0	2866	146	0
20	B	2680	0	2834	130	0
20	F	110	0	105	8	0
20	G	96	0	72	2	0
20	J	42	0	30	0	0
20	K	205	0	168	9	0
20	L	115	0	110	4	0
20	Z	622	0	584	22	0
21	A	33	0	46	0	0
21	B	33	0	46	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	A	8	0	0	0	0
22	C	16	0	0	1	0
23	3	160	0	212	11	0
23	4	40	0	53	1	0
23	5	80	0	105	3	0
23	6	80	0	106	6	0
23	7	80	0	106	5	0
23	8	40	0	53	2	0
23	A	200	0	264	19	0
23	B	280	0	370	20	0
23	G	40	0	53	3	0
23	I	40	0	52	2	0
23	J	40	0	53	3	0
23	K	80	0	106	5	0
23	L	80	0	106	6	0
24	1	43	0	56	2	0
24	3	20	0	12	0	0
24	4	81	0	108	3	0
24	5	37	0	44	2	0
24	6	49	0	74	4	0
24	7	37	0	44	2	0
24	8	38	0	46	2	0
24	A	84	0	114	4	0
24	B	76	0	64	2	0
24	Z	43	0	56	0	0
25	3	16	0	12	1	0
25	8	29	0	39	0	0
25	A	29	0	39	0	0
26	1	35	0	45	1	0
26	4	35	0	43	2	0
26	8	35	0	45	1	0
26	A	35	0	42	2	0
26	B	70	0	89	2	0
26	F	35	0	45	0	0
27	A	10	0	15	0	0
28	A	14	0	23	0	0
29	A	29	0	28	0	0
29	J	35	0	40	0	0
30	A	44	0	76	4	0
31	B	66	0	96	5	0
32	B	1	0	0	0	0
33	F	41	0	56	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	1	42	0	0	0	0
34	5	42	0	0	0	0
34	J	42	0	0	0	0
35	7	42	0	74	3	0
35	K	21	0	37	2	0
36	1	84	0	110	4	0
36	3	84	0	110	11	0
36	4	84	0	110	9	0
36	5	84	0	110	11	0
36	6	84	0	110	5	0
36	7	84	0	110	1	0
36	8	84	0	110	5	0
36	Z	126	0	165	4	0
37	1	106	0	82	5	0
37	3	66	0	69	5	0
37	4	201	0	146	7	0
37	5	160	0	133	9	0
37	6	206	0	157	8	0
37	7	54	0	42	3	0
37	8	122	0	115	6	0
37	Z	178	0	168	10	0
38	1	48	0	62	1	0
39	Z	19	0	0	0	0
40	5	23	0	19	0	0
40	6	29	0	31	0	0
40	7	39	0	51	5	0
40	8	30	0	33	0	0
41	7	18	0	31	0	0
42	8	30	0	43	0	0
43	1	16	0	0	0	0
43	3	17	0	0	0	0
43	4	7	0	0	0	0
43	5	9	0	0	1	0
43	6	8	0	0	0	0
43	7	18	0	0	0	0
43	8	16	0	0	0	0
43	A	91	0	0	2	0
43	B	79	0	0	0	0
43	C	19	0	0	1	0
43	D	12	0	0	0	0
43	E	7	0	0	0	0
43	F	14	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	J	3	0	0	0	0
43	K	2	0	0	0	0
43	L	5	0	0	0	0
43	Z	8	0	0	0	0
All	All	47524	0	47243	816	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 9.

The worst 5 of 816 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)
36:4:502:LUT:H32	20:4:604:CLA:HAB	1.44	0.98
20:B:1220:CLA:HAB	20:B:1227:CLA:HMD2	1.53	0.91
20:B:1201:CLA:HMA2	20:B:1241:CLA:HMD2	1.66	0.77
20:5:605:CLA:H52	20:5:622:CLA:HAB	1.66	0.77
1:A:396:TRP:CD1	20:A:1126:CLA:HAB	2.23	0.74

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	739/741 (100%)	716 (97%)	23 (3%)	0	100	100
2	B	731/733 (100%)	705 (96%)	26 (4%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	141/144 (98%)	136 (96%)	5 (4%)	0	100	100
5	E	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
6	F	163/165 (99%)	157 (96%)	5 (3%)	1 (1%)	22	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	70/91 (77%)	70 (100%)	0	0	100	100
8	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
9	J	37/39 (95%)	36 (97%)	1 (3%)	0	100	100
10	K	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
11	L	122/126 (97%)	119 (98%)	3 (2%)	0	100	100
12	1	192/194 (99%)	182 (95%)	10 (5%)	0	100	100
12	Z	192/194 (99%)	189 (98%)	3 (2%)	0	100	100
13	3	217/219 (99%)	209 (96%)	8 (4%)	0	100	100
14	7	211/213 (99%)	205 (97%)	6 (3%)	0	100	100
15	8	215/217 (99%)	208 (97%)	7 (3%)	0	100	100
16	4	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
17	5	225/227 (99%)	221 (98%)	4 (2%)	0	100	100
18	6	227/229 (99%)	222 (98%)	5 (2%)	0	100	100
All	All	3946/4006 (98%)	3820 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	150	PHE

### 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	601/601 (100%)	601 (100%)	0	100	100
2	B	596/596 (100%)	596 (100%)	0	100	100
3	C	69/69 (100%)	69 (100%)	0	100	100
4	D	120/120 (100%)	119 (99%)	1 (1%)	79	89
5	E	54/54 (100%)	54 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	127/127 (100%)	127 (100%)	0	100	100
7	G	54/68 (79%)	54 (100%)	0	100	100
8	I	31/31 (100%)	31 (100%)	0	100	100
9	J	35/35 (100%)	35 (100%)	0	100	100
10	K	58/58 (100%)	58 (100%)	0	100	100
11	L	92/92 (100%)	92 (100%)	0	100	100
12	1	137/137 (100%)	137 (100%)	0	100	100
12	Z	137/137 (100%)	137 (100%)	0	100	100
13	3	167/167 (100%)	167 (100%)	0	100	100
14	7	164/164 (100%)	164 (100%)	0	100	100
15	8	163/163 (100%)	163 (100%)	0	100	100
16	4	164/165 (99%)	164 (100%)	0	100	100
17	5	184/184 (100%)	184 (100%)	0	100	100
18	6	183/183 (100%)	182 (100%)	1 (0%)	86	92
All	All	3136/3151 (100%)	3134 (100%)	2 (0%)	92	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	189	ARG
18	6	133	ARG

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

Mol	Chain	Res	Type
12	1	52	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
4	SNC	D	137	4	4,7,8	1.00	0	1,7,9	3.26	1 (100%)

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
4	SNC	D	137	4	-	0/0/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	137	SNC	CA-CB-SG	-3.26	105.99	112.76

There are no chirality outliers.

There are no torsion outliers.

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 317 ligands modelled in this entry, 1 is monoatomic - leaving 316 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	B	1226	-	65,73,73	1.39	8 (12%)	76,113,113	2.19	22 (28%)
20	CLA	7	601	-	60,68,73	1.44	9 (15%)	70,107,113	2.12	19 (27%)
20	CLA	B	1022	43	65,73,73	1.38	7 (10%)	76,113,113	1.95	18 (23%)
23	BCR	L	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.27	13 (23%)
20	CLA	B	1229	-	65,73,73	1.36	9 (13%)	76,113,113	1.99	20 (26%)
20	CLA	7	603	-	65,73,73	1.38	9 (13%)	76,113,113	2.16	20 (26%)
20	CLA	B	1239	-	65,73,73	1.34	8 (12%)	76,113,113	2.09	15 (19%)
36	LUT	6	501	-	42,43,43	2.36	1 (2%)	51,60,60	1.85	11 (21%)
20	CLA	A	1104	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	19 (25%)
20	CLA	7	616	-	60,68,73	1.39	8 (13%)	70,107,113	2.20	16 (22%)
20	CLA	8	615	15	46,54,73	1.60	8 (17%)	53,90,113	2.19	15 (28%)
23	BCR	4	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.23	16 (28%)
20	CLA	3	608	-	45,53,73	1.63	8 (17%)	52,89,113	2.18	13 (25%)
23	BCR	B	4007	-	41,41,41	1.83	4 (9%)	56,56,56	4.18	16 (28%)
20	CLA	4	615	-	41,49,73	1.68	6 (14%)	47,84,113	2.33	17 (36%)
20	CLA	A	1131	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	15 (19%)
20	CLA	K	1403	-	49,57,73	1.55	7 (14%)	55,93,113	2.22	16 (29%)
23	BCR	B	4003	-	41,41,41	1.84	4 (9%)	56,56,56	4.30	18 (32%)
20	CLA	L	1502	-	65,73,73	1.35	9 (13%)	76,113,113	2.04	18 (23%)
20	CLA	1	615	12	65,73,73	1.40	8 (12%)	76,113,113	1.85	14 (18%)
20	CLA	B	1217	-	56,64,73	1.47	8 (14%)	65,102,113	2.06	15 (23%)
20	CLA	4	606	-	50,58,73	1.55	10 (20%)	58,95,113	2.29	17 (29%)
20	CLA	B	1236	-	65,73,73	1.37	9 (13%)	76,113,113	2.00	15 (19%)
36	LUT	Z	501	-	42,43,43	2.29	1 (2%)	51,60,60	1.91	11 (21%)
20	CLA	A	1107	1	65,73,73	1.34	8 (12%)	76,113,113	2.03	20 (26%)
24	LHG	7	801	-	36,36,48	0.46	0	39,42,54	1.17	3 (7%)
34	C7Z	1	503	-	43,43,43	5.38	26 (60%)	58,60,60	2.36	20 (34%)
20	CLA	A	1120	-	55,63,73	1.44	8 (14%)	64,101,113	2.27	20 (31%)
37	CHL	3	611	-	66,74,74	1.00	3 (4%)	73,114,114	1.21	10 (13%)
20	CLA	A	1123	-	65,73,73	1.36	8 (12%)	76,113,113	2.01	16 (21%)
20	CLA	B	1021	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	B	1224	-	65,73,73	1.38	8 (12%)	76,113,113	2.03	17 (22%)
36	LUT	7	501	-	42,43,43	2.35	1 (2%)	51,60,60	1.90	12 (23%)
20	CLA	8	605	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	17 (22%)
20	CLA	A	1116	-	60,68,73	1.43	8 (13%)	70,107,113	2.10	22 (31%)
20	CLA	Z	607	-	57,65,73	1.46	8 (14%)	66,103,113	2.06	15 (22%)
26	LMT	B	6101	-	36,36,36	1.18	5 (13%)	47,47,47	1.11	5 (10%)
20	CLA	5	609	-	65,73,73	1.37	10 (15%)	76,113,113	1.90	15 (19%)
20	CLA	6	604	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	21 (27%)
36	LUT	Z	502	-	42,43,43	2.29	1 (2%)	51,60,60	1.98	13 (25%)
20	CLA	3	618	-	46,54,73	1.61	8 (17%)	53,90,113	2.14	13 (24%)
20	CLA	4	605	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	16 (21%)
20	CLA	A	1114	-	61,69,73	1.41	8 (13%)	71,108,113	2.08	16 (22%)
20	CLA	A	1141	24	52,60,73	1.53	6 (11%)	60,97,113	2.26	19 (31%)
21	PQN	B	2002	-	34,34,34	0.40	0	42,45,45	1.09	2 (4%)
26	LMT	8	805	-	36,36,36	1.20	5 (13%)	47,47,47	1.01	1 (2%)
20	CLA	F	1301	-	65,73,73	1.36	7 (10%)	76,113,113	2.02	19 (25%)
35	SPH	K	5001	-	19,20,20	0.66	0	18,21,21	1.00	0
37	CHL	Z	613	-	46,54,74	0.97	2 (4%)	49,90,114	1.37	7 (14%)
20	CLA	B	1204	-	65,73,73	1.36	9 (13%)	76,113,113	2.01	16 (21%)
20	CLA	A	1110	-	65,73,73	1.37	7 (10%)	76,113,113	2.08	15 (19%)
23	BCR	3	504	-	41,41,41	1.83	5 (12%)	56,56,56	4.28	15 (26%)
41	PLM	7	805	-	17,17,17	0.58	0	17,17,17	1.04	0
23	BCR	G	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.30	15 (26%)
20	CLA	6	612	-	50,58,73	1.55	8 (16%)	58,95,113	2.25	17 (29%)
20	CLA	B	1023	-	65,73,73	1.34	8 (12%)	76,113,113	2.02	17 (22%)
26	LMT	B	5005	-	36,36,36	1.24	5 (13%)	47,47,47	1.15	4 (8%)
31	DGD	B	5003	-	67,67,67	1.18	7 (10%)	81,81,81	1.07	6 (7%)
20	CLA	7	611	-	50,58,73	1.51	7 (14%)	58,95,113	2.34	19 (32%)
36	LUT	8	501	-	42,43,43	2.30	1 (2%)	51,60,60	1.95	14 (27%)
20	CLA	A	1121	-	65,73,73	1.37	7 (10%)	76,113,113	2.00	18 (23%)
23	BCR	6	503	-	41,41,41	1.85	4 (9%)	56,56,56	4.37	15 (26%)
35	SPH	7	803	-	19,20,20	0.66	0	18,21,21	0.90	0
20	CLA	6	615	-	61,69,73	1.40	7 (11%)	71,108,113	2.13	18 (25%)
36	LUT	6	502	-	42,43,43	2.38	1 (2%)	51,60,60	1.88	16 (31%)
20	CLA	A	1103	-	65,73,73	1.31	7 (10%)	76,113,113	2.07	18 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	8	611	-	50,58,73	1.51	7 (14%)	58,95,113	2.37	19 (32%)
36	LUT	1	501	-	42,43,43	2.31	1 (2%)	51,60,60	1.80	10 (19%)
20	CLA	A	1101	-	65,73,73	1.35	7 (10%)	76,113,113	1.98	17 (22%)
20	CLA	B	1207	-	65,73,73	1.35	7 (10%)	76,113,113	2.03	17 (22%)
20	CLA	3	602	-	46,54,73	1.60	8 (17%)	53,90,113	2.05	11 (20%)
20	CLA	B	1232	-	45,53,73	1.67	9 (20%)	52,89,113	2.11	11 (21%)
30	DGA	A	5005	-	43,43,43	1.14	3 (6%)	45,45,45	1.48	3 (6%)
20	CLA	7	602	-	50,58,73	1.52	8 (16%)	58,95,113	2.21	15 (25%)
34	C7Z	5	505	-	43,43,43	5.43	26 (60%)	58,60,60	2.17	17 (29%)
20	CLA	6	605	-	55,63,73	1.47	8 (14%)	64,101,113	2.19	19 (29%)
37	CHL	5	611	-	51,59,74	0.90	2 (3%)	55,96,114	1.43	10 (18%)
20	CLA	6	619	18	65,73,73	1.34	6 (9%)	76,113,113	2.02	17 (22%)
29	LMG	J	5001	-	35,35,55	0.46	0	43,43,63	1.13	2 (4%)
23	BCR	3	503	-	41,41,41	1.83	5 (12%)	56,56,56	4.19	16 (28%)
20	CLA	1	611	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	19 (25%)
20	CLA	A	1138	-	65,73,73	1.33	8 (12%)	76,113,113	2.14	17 (22%)
23	BCR	K	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	14 (25%)
26	LMT	1	803	-	36,36,36	1.17	5 (13%)	47,47,47	0.99	1 (2%)
24	LHG	B	5002	-	19,19,48	0.84	1 (5%)	20,24,54	1.34	1 (5%)
20	CLA	A	1109	-	65,73,73	1.37	8 (12%)	76,113,113	2.02	17 (22%)
20	CLA	8	601	15	60,68,73	1.41	8 (13%)	70,107,113	2.11	18 (25%)
40	3PH	5	802	-	22,22,47	1.24	4 (18%)	26,27,52	1.35	2 (7%)
20	CLA	1	605	-	55,63,73	1.47	8 (14%)	64,101,113	2.11	17 (26%)
20	CLA	7	615	14	58,66,73	1.44	9 (15%)	67,104,113	2.05	15 (22%)
36	LUT	7	502	-	42,43,43	2.30	1 (2%)	51,60,60	1.96	12 (23%)
20	CLA	B	1208	-	56,64,73	1.45	8 (14%)	65,102,113	2.18	17 (26%)
20	CLA	1	603	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	18 (23%)
38	SQD	1	802	-	47,48,54	0.83	0	56,59,65	0.94	2 (3%)
20	CLA	B	1219	-	59,67,73	1.44	8 (13%)	68,105,113	2.15	19 (27%)
20	CLA	4	604	-	60,68,73	1.40	7 (11%)	70,107,113	2.04	18 (25%)
39	QTB	Z	504	-	19,19,19	2.50	5 (26%)	20,26,26	2.80	8 (40%)
24	LHG	6	801	-	48,48,48	0.40	0	51,54,54	1.02	3 (5%)
24	LHG	Z	801	-	42,42,48	0.41	0	45,48,54	1.16	4 (8%)
20	CLA	4	602	-	52,60,73	1.53	7 (13%)	60,97,113	2.19	15 (25%)
37	CHL	8	610	-	56,64,74	0.92	2 (3%)	61,102,114	1.40	12 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	6	607	-	55,63,73	1.46	8 (14%)	64,101,113	2.08	19 (29%)
20	CLA	B	1220	-	65,73,73	1.36	7 (10%)	76,113,113	1.92	15 (19%)
23	BCR	A	4005	-	41,41,41	1.83	5 (12%)	56,56,56	4.17	11 (19%)
23	BCR	B	4006	-	41,41,41	1.81	4 (9%)	56,56,56	4.21	17 (30%)
26	LMT	A	5006	-	36,36,36	1.22	6 (16%)	47,47,47	1.04	1 (2%)
20	CLA	Z	603	-	50,58,73	1.56	9 (18%)	58,95,113	2.24	17 (29%)
20	CLA	3	601	-	65,73,73	1.36	9 (13%)	76,113,113	2.06	17 (22%)
23	BCR	B	4004	-	41,41,41	1.82	4 (9%)	56,56,56	4.25	14 (25%)
37	CHL	6	613	-	56,64,74	0.87	2 (3%)	61,102,114	1.26	9 (14%)
20	CLA	5	606	-	50,58,73	1.55	8 (16%)	58,95,113	2.23	16 (27%)
37	CHL	Z	610	-	66,74,74	0.79	2 (3%)	73,114,114	1.22	11 (15%)
20	CLA	B	1238	-	65,73,73	1.35	9 (13%)	76,113,113	2.06	18 (23%)
23	BCR	L	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.30	16 (28%)
21	PQN	A	2001	-	34,34,34	0.39	0	42,45,45	1.15	2 (4%)
20	CLA	8	612	-	46,54,73	1.60	9 (19%)	53,90,113	2.05	13 (24%)
20	CLA	B	1234	-	60,68,73	1.41	7 (11%)	70,107,113	2.08	18 (25%)
23	BCR	J	4001	-	41,41,41	1.81	4 (9%)	56,56,56	4.27	17 (30%)
20	CLA	B	1241	-	65,73,73	1.40	11 (16%)	76,113,113	1.97	16 (21%)
40	3PH	8	806	-	29,29,47	1.09	4 (13%)	33,34,52	1.11	2 (6%)
20	CLA	7	605	-	61,69,73	1.38	8 (13%)	71,108,113	2.07	19 (26%)
20	CLA	A	1113	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	16 (21%)
20	CLA	B	1213	-	65,73,73	1.35	9 (13%)	76,113,113	2.15	23 (30%)
20	CLA	Z	611	-	55,63,73	1.49	10 (18%)	64,101,113	2.14	17 (26%)
34	C7Z	J	4002	-	43,43,43	5.36	27 (62%)	58,60,60	2.29	20 (34%)
23	BCR	5	504	-	41,41,41	1.83	5 (12%)	56,56,56	4.57	21 (37%)
23	BCR	7	504	-	41,41,41	1.85	4 (9%)	56,56,56	4.41	17 (30%)
20	CLA	G	1602	-	46,54,73	1.60	9 (19%)	53,90,113	2.27	15 (28%)
20	CLA	1	612	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	18 (23%)
25	NKP	3	802	-	15,15,28	2.07	3 (20%)	18,19,32	1.52	2 (11%)
20	CLA	B	1223	-	65,73,73	1.38	7 (10%)	76,113,113	1.99	18 (23%)
36	LUT	Z	503	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	11 (21%)
20	CLA	5	612	-	65,73,73	1.33	7 (10%)	76,113,113	1.93	16 (21%)
24	LHG	A	5002	-	48,48,48	0.40	0	51,54,54	1.07	3 (5%)
37	CHL	6	610	-	56,64,74	0.88	2 (3%)	61,102,114	1.40	12 (19%)
20	CLA	6	609	18	65,73,73	1.36	7 (10%)	76,113,113	1.94	15 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	3	616	-	56,64,73	1.46	7 (12%)	65,102,113	2.17	16 (24%)
23	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.36	12 (21%)
20	CLA	7	604	-	65,73,73	1.36	7 (10%)	76,113,113	1.95	18 (23%)
20	CLA	A	1136	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	17 (22%)
20	CLA	A	1105	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
23	BCR	B	4005	-	41,41,41	1.89	4 (9%)	56,56,56	4.48	17 (30%)
20	CLA	Z	604	-	65,73,73	1.34	8 (12%)	76,113,113	2.03	19 (25%)
20	CLA	A	1125	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	21 (27%)
24	LHG	B	5001	-	22,22,48	0.55	0	25,28,54	1.30	2 (8%)
20	CLA	A	1119	-	65,73,73	1.36	7 (10%)	76,113,113	1.87	16 (21%)
20	CLA	B	1215	-	60,68,73	1.40	8 (13%)	70,107,113	2.03	17 (24%)
20	CLA	5	607	-	61,69,73	1.41	8 (13%)	71,108,113	2.01	17 (23%)
20	CLA	B	1211	-	60,68,73	1.42	7 (11%)	70,107,113	1.96	15 (21%)
24	LHG	3	801	-	19,19,48	0.91	1 (5%)	20,24,54	1.44	1 (5%)
20	CLA	L	1503	-	50,58,73	1.53	8 (16%)	58,95,113	2.23	18 (31%)
23	BCR	7	503	-	41,41,41	1.82	4 (9%)	56,56,56	4.28	14 (25%)
23	BCR	A	4003	-	41,41,41	1.80	4 (9%)	56,56,56	4.35	20 (35%)
20	CLA	A	1127	-	65,73,73	1.38	7 (10%)	76,113,113	1.85	16 (21%)
20	CLA	5	615	17	50,58,73	1.55	7 (14%)	58,95,113	2.23	16 (27%)
20	CLA	6	606	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	17 (22%)
20	CLA	A	1140	-	65,73,73	1.37	8 (12%)	76,113,113	1.91	15 (19%)
20	CLA	B	1210	-	65,73,73	1.36	6 (9%)	76,113,113	2.02	18 (23%)
20	CLA	8	607	-	55,63,73	1.50	7 (12%)	64,101,113	2.08	14 (21%)
40	3PH	7	802	-	38,38,47	0.98	3 (7%)	42,43,52	1.16	2 (4%)
37	CHL	1	610	-	48,56,74	0.93	2 (4%)	51,92,114	1.36	10 (19%)
20	CLA	4	608	-	55,63,73	1.49	9 (16%)	64,101,113	2.08	16 (25%)
25	NKP	8	802	-	28,28,28	1.51	2 (7%)	31,32,32	1.25	3 (9%)
20	CLA	5	603	-	56,64,73	1.45	7 (12%)	65,102,113	2.23	15 (23%)
36	LUT	3	501	-	42,43,43	2.31	1 (2%)	51,60,60	1.94	12 (23%)
20	CLA	4	609	16	60,68,73	1.42	8 (13%)	70,107,113	2.03	17 (24%)
20	CLA	B	1231	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	16 (21%)
20	CLA	6	601	-	60,68,73	1.42	8 (13%)	70,107,113	2.10	21 (30%)
20	CLA	3	610	13	60,68,73	1.43	8 (13%)	70,107,113	2.03	18 (25%)
20	CLA	A	1117	-	65,73,73	1.34	7 (10%)	76,113,113	2.09	18 (23%)
20	CLA	3	604	-	60,68,73	1.45	8 (13%)	70,107,113	2.17	21 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	5	613	-	55,63,73	1.50	8 (14%)	64,101,113	2.06	17 (26%)
23	BCR	A	4004	-	41,41,41	1.81	4 (9%)	56,56,56	4.37	16 (28%)
23	BCR	A	4001	-	41,41,41	1.85	4 (9%)	56,56,56	4.14	12 (21%)
20	CLA	8	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.17	20 (26%)
23	BCR	3	506	-	41,41,41	1.87	4 (9%)	56,56,56	4.48	15 (26%)
20	CLA	B	1216	-	65,73,73	1.38	9 (13%)	76,113,113	1.90	14 (18%)
37	CHL	8	613	-	66,74,74	0.95	4 (6%)	73,114,114	1.18	10 (13%)
20	CLA	A	1129	-	50,58,73	1.55	8 (16%)	58,95,113	2.18	14 (24%)
36	LUT	4	501	-	42,43,43	2.37	1 (2%)	51,60,60	1.94	13 (25%)
26	LMT	F	5001	-	36,36,36	1.21	6 (16%)	47,47,47	0.92	1 (2%)
20	CLA	1	604	-	60,68,73	1.41	7 (11%)	70,107,113	2.04	17 (24%)
20	CLA	B	1218	-	65,73,73	1.34	7 (10%)	76,113,113	2.09	22 (28%)
20	CLA	5	602	-	61,69,73	1.39	9 (14%)	71,108,113	1.96	14 (19%)
20	CLA	5	604	-	65,73,73	1.38	8 (12%)	76,113,113	1.99	18 (23%)
29	LMG	A	5003	-	29,29,55	0.55	0	37,37,63	1.26	4 (10%)
36	LUT	8	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.92	14 (27%)
23	BCR	3	505	-	41,41,41	1.85	4 (9%)	56,56,56	4.28	11 (19%)
20	CLA	7	606	-	56,64,73	1.47	7 (12%)	65,102,113	2.06	15 (23%)
20	CLA	A	1118	-	60,68,73	1.40	9 (15%)	70,107,113	2.07	17 (24%)
23	BCR	B	4002	-	41,41,41	1.86	4 (9%)	56,56,56	4.30	14 (25%)
20	CLA	8	604	-	62,70,73	1.40	7 (11%)	72,109,113	2.08	20 (27%)
37	CHL	7	610	-	54,62,74	1.00	3 (5%)	58,99,114	1.33	11 (18%)
23	BCR	8	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.24	14 (25%)
20	CLA	1	607	-	60,68,73	1.43	7 (11%)	70,107,113	2.07	18 (25%)
20	CLA	A	1133	-	65,73,73	1.36	8 (12%)	76,113,113	1.90	15 (19%)
20	CLA	3	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.06	17 (22%)
37	CHL	Z	609	12	66,74,74	0.91	3 (4%)	73,114,114	1.25	10 (13%)
20	CLA	Z	605	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	18 (23%)
35	SPH	7	804	-	19,20,20	0.69	0	18,21,21	1.06	1 (5%)
20	CLA	Z	606	-	57,65,73	1.46	10 (17%)	66,103,113	2.11	20 (30%)
20	CLA	B	1237	-	65,73,73	1.36	8 (12%)	76,113,113	1.92	15 (19%)
37	CHL	1	609	12	58,66,74	0.94	4 (6%)	63,104,114	1.27	11 (17%)
19	CL0	A	1011	-	65,73,73	2.34	17 (26%)	76,113,113	2.58	24 (31%)
23	BCR	5	503	-	41,41,41	1.84	4 (9%)	56,56,56	4.30	19 (33%)
37	CHL	5	617	-	43,51,74	1.06	3 (6%)	45,86,114	1.40	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	1	613	-	46,54,73	1.62	9 (19%)	53,90,113	2.18	14 (26%)
20	CLA	4	607	-	55,63,73	1.48	8 (14%)	64,101,113	2.09	16 (25%)
20	CLA	B	1221	-	65,73,73	1.34	7 (10%)	76,113,113	2.09	19 (25%)
23	BCR	B	4001	-	41,41,41	1.84	5 (12%)	56,56,56	4.19	13 (23%)
20	CLA	6	608	-	55,63,73	1.48	8 (14%)	64,101,113	2.19	16 (25%)
37	CHL	4	613	-	56,64,74	0.90	2 (3%)	61,102,114	1.38	11 (18%)
20	CLA	A	1106	-	65,73,73	1.36	8 (12%)	76,113,113	2.05	15 (19%)
20	CLA	B	1240	-	65,73,73	1.37	9 (13%)	76,113,113	1.93	18 (23%)
20	CLA	7	609	14	65,73,73	1.37	8 (12%)	76,113,113	2.03	19 (25%)
20	CLA	8	602	-	65,73,73	1.33	8 (12%)	76,113,113	2.07	19 (25%)
20	CLA	K	1402	-	55,63,73	1.49	10 (18%)	64,101,113	2.13	18 (28%)
20	CLA	A	1130	-	65,73,73	1.38	8 (12%)	76,113,113	1.93	16 (21%)
20	CLA	6	618	-	46,54,73	1.59	7 (15%)	53,90,113	2.21	14 (26%)
20	CLA	5	601	-	60,68,73	1.40	8 (13%)	70,107,113	2.11	19 (27%)
23	BCR	A	4002	-	41,41,41	1.85	4 (9%)	56,56,56	4.11	14 (25%)
40	3PH	6	802	-	28,28,47	1.11	4 (14%)	32,33,52	1.29	2 (6%)
20	CLA	A	1115	-	60,68,73	1.39	7 (11%)	70,107,113	2.10	19 (27%)
20	CLA	1	602	-	45,53,73	1.62	9 (20%)	52,89,113	2.19	15 (28%)
20	CLA	A	1139	-	65,73,73	1.38	8 (12%)	76,113,113	2.03	21 (27%)
20	CLA	B	1214	-	59,67,73	1.44	9 (15%)	68,105,113	2.20	22 (32%)
20	CLA	1	606	-	61,69,73	1.40	8 (13%)	71,108,113	2.03	15 (21%)
20	CLA	3	613	-	55,63,73	1.48	8 (14%)	64,101,113	2.12	15 (23%)
20	CLA	A	1013	-	65,73,73	1.34	8 (12%)	76,113,113	1.99	19 (25%)
20	CLA	5	605	-	55,63,73	1.47	8 (14%)	64,101,113	2.27	21 (32%)
20	CLA	B	1212	-	57,65,73	1.43	7 (12%)	66,103,113	2.17	19 (28%)
20	CLA	K	1404	-	55,63,73	1.48	8 (14%)	64,101,113	2.23	16 (25%)
20	CLA	B	1209	-	65,73,73	1.36	7 (10%)	76,113,113	1.92	16 (21%)
20	CLA	4	612	-	50,58,73	1.56	7 (14%)	58,95,113	2.32	19 (32%)
22	SF4	A	3001	2,1	0,12,12	-	-	-	-	-
26	LMT	4	803	-	36,36,36	1.21	6 (16%)	47,47,47	1.05	3 (6%)
20	CLA	A	1124	-	65,73,73	1.36	7 (10%)	76,113,113	1.92	17 (22%)
20	CLA	1	601	-	65,73,73	1.37	7 (10%)	76,113,113	2.00	19 (25%)
24	LHG	A	5001	20	34,34,48	0.45	0	37,40,54	1.16	3 (8%)
20	CLA	A	1132	-	65,73,73	1.37	9 (13%)	76,113,113	1.96	16 (21%)
20	CLA	3	607	-	60,68,73	1.42	9 (15%)	70,107,113	2.10	17 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	B	1222	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	21 (27%)
20	CLA	B	1201	-	45,53,73	1.58	8 (17%)	52,89,113	2.22	17 (32%)
20	CLA	5	618	-	65,73,73	1.33	8 (12%)	76,113,113	2.12	18 (23%)
24	LHG	8	801	-	37,37,48	0.43	0	40,43,54	1.14	4 (10%)
36	LUT	5	501	-	42,43,43	2.42	1 (2%)	51,60,60	1.94	11 (21%)
37	CHL	4	617	-	43,51,74	1.07	3 (6%)	45,86,114	1.42	8 (17%)
20	CLA	A	1137	-	65,73,73	1.34	8 (12%)	76,113,113	2.11	22 (28%)
20	CLA	3	605	-	65,73,73	1.37	8 (12%)	76,113,113	1.88	16 (21%)
20	CLA	6	602	-	52,60,73	1.51	6 (11%)	60,97,113	2.18	17 (28%)
33	RRX	F	4001	-	42,42,42	4.79	24 (57%)	57,58,58	2.53	23 (40%)
20	CLA	Z	612	-	65,73,73	1.36	7 (10%)	76,113,113	1.99	16 (21%)
20	CLA	J	1901	-	42,50,73	1.67	8 (19%)	48,85,113	2.31	17 (35%)
20	CLA	4	601	-	60,68,73	1.40	8 (13%)	70,107,113	2.11	17 (24%)
20	CLA	A	1135	-	51,59,73	1.57	9 (17%)	59,96,113	2.27	18 (30%)
20	CLA	5	608	-	45,53,73	1.64	9 (20%)	52,89,113	2.21	13 (25%)
20	CLA	A	1102	-	55,63,73	1.43	8 (14%)	64,101,113	2.27	20 (31%)
20	CLA	7	608	-	43,51,73	1.69	10 (23%)	49,86,113	2.24	13 (26%)
23	BCR	6	504	-	41,41,41	1.84	4 (9%)	56,56,56	4.10	17 (30%)
20	CLA	Z	615	-	46,54,73	1.61	7 (15%)	53,90,113	2.12	15 (28%)
36	LUT	4	502	-	42,43,43	2.31	1 (2%)	51,60,60	1.83	14 (27%)
20	CLA	B	1227	-	50,58,73	1.59	8 (16%)	58,95,113	2.19	16 (27%)
20	CLA	4	603	-	65,73,73	1.35	7 (10%)	76,113,113	2.15	20 (26%)
24	LHG	4	801	-	48,48,48	0.40	0	51,54,54	1.13	4 (7%)
37	CHL	5	610	-	66,74,74	0.90	3 (4%)	73,114,114	1.15	9 (12%)
20	CLA	A	1108	-	65,73,73	1.36	8 (12%)	76,113,113	1.98	16 (21%)
20	CLA	B	1203	-	65,73,73	1.34	9 (13%)	76,113,113	1.95	18 (23%)
20	CLA	B	1228	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	19 (25%)
42	LPX	8	803	-	29,29,29	1.02	2 (6%)	31,33,33	0.93	1 (3%)
27	OCA	A	5008	-	9,9,9	0.65	0	9,9,9	0.97	0
20	CLA	Z	601	-	60,68,73	1.41	8 (13%)	70,107,113	2.06	17 (24%)
20	CLA	A	1126	-	65,73,73	1.38	9 (13%)	76,113,113	1.99	17 (22%)
22	SF4	C	3002	3	0,12,12	-	-	-	-	-
20	CLA	B	1206	-	65,73,73	1.34	6 (9%)	76,113,113	2.00	18 (23%)
20	CLA	A	1134	1	55,63,73	1.48	7 (12%)	64,101,113	2.19	15 (23%)
20	CLA	1	608	-	60,68,73	1.40	7 (11%)	70,107,113	2.03	15 (21%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	F	1302	-	45,53,73	1.64	9 (20%)	52,89,113	2.07	13 (25%)
20	CLA	B	1205	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	16 (21%)
20	CLA	7	612	-	50,58,73	1.54	7 (14%)	58,95,113	2.20	17 (29%)
20	CLA	7	613	-	42,50,73	1.67	7 (16%)	48,85,113	2.27	15 (31%)
20	CLA	7	607	-	65,73,73	1.37	7 (10%)	76,113,113	2.00	16 (21%)
20	CLA	A	1128	-	65,73,73	1.40	8 (12%)	76,113,113	2.03	16 (21%)
28	DAO	A	5007	-	13,13,13	0.81	1 (7%)	13,13,13	0.92	0
25	NKP	A	5004	-	28,28,28	1.56	3 (10%)	31,32,32	1.23	3 (9%)
20	CLA	8	608	-	55,63,73	1.49	8 (14%)	64,101,113	2.04	15 (23%)
20	CLA	A	1122	-	65,73,73	1.36	7 (10%)	76,113,113	1.98	17 (22%)
20	CLA	B	1202	-	65,73,73	1.35	6 (9%)	76,113,113	2.10	21 (27%)
20	CLA	A	1111	-	65,73,73	1.34	8 (12%)	76,113,113	2.04	18 (23%)
20	CLA	6	603	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	17 (22%)
20	CLA	B	1225	-	65,73,73	1.37	8 (12%)	76,113,113	1.83	14 (18%)
20	CLA	3	612	-	60,68,73	1.41	9 (15%)	70,107,113	2.03	15 (21%)
37	CHL	6	617	-	43,51,74	1.02	3 (6%)	45,86,114	1.30	6 (13%)
22	SF4	C	3003	3	0,12,12	-	-	-	-	-
24	LHG	4	802	-	31,31,48	0.46	0	34,37,54	1.13	2 (5%)
20	CLA	K	1401	-	46,54,73	1.62	8 (17%)	53,90,113	2.07	13 (24%)
20	CLA	Z	602	-	46,54,73	1.58	6 (13%)	53,90,113	2.12	14 (26%)
20	CLA	8	609	15	65,73,73	1.38	7 (10%)	76,113,113	2.00	18 (23%)
20	CLA	B	1235	-	65,73,73	1.36	10 (15%)	76,113,113	2.03	16 (21%)
36	LUT	3	502	-	42,43,43	2.43	1 (2%)	51,60,60	2.02	16 (31%)
24	LHG	5	801	-	36,36,48	0.44	0	39,42,54	1.18	3 (7%)
36	LUT	5	502	-	42,43,43	2.27	1 (2%)	51,60,60	1.77	12 (23%)
20	CLA	A	1112	-	60,68,73	1.40	8 (13%)	70,107,113	2.04	18 (25%)
23	BCR	I	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.27	15 (26%)
20	CLA	G	1601	-	50,58,73	1.54	7 (14%)	58,95,113	2.24	16 (27%)
20	CLA	Z	608	-	56,64,73	1.47	10 (17%)	65,102,113	2.11	17 (26%)
20	CLA	B	1230	-	58,66,73	1.42	7 (12%)	67,104,113	2.14	18 (26%)
37	CHL	4	610	-	51,59,74	0.90	2 (3%)	55,96,114	1.57	13 (23%)
20	CLA	8	606	-	60,68,73	1.41	8 (13%)	70,107,113	2.00	16 (22%)
24	LHG	1	801	-	42,42,48	0.45	0	45,48,54	1.11	2 (4%)
24	LHG	B	5006	-	32,32,48	0.45	0	35,38,54	1.16	2 (5%)
36	LUT	1	502	-	42,43,43	2.31	1 (2%)	51,60,60	2.00	16 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CLA	5	622	-	46,54,73	1.64	8 (17%)	53,90,113	2.19	12 (22%)
37	CHL	4	611	-	51,59,74	0.94	2 (3%)	55,96,114	1.44	10 (18%)
20	CLA	A	1012	-	65,73,73	1.37	8 (12%)	76,113,113	2.06	17 (22%)
37	CHL	6	611	-	51,59,74	0.96	2 (3%)	55,96,114	1.34	7 (12%)
20	CLA	3	603	-	65,73,73	1.37	8 (12%)	76,113,113	2.09	17 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1226	-	1/1/15/20	17/37/115/115	-
20	CLA	7	601	-	1/1/14/20	12/31/109/115	-
20	CLA	B	1022	43	1/1/15/20	7/37/115/115	-
23	BCR	L	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	B	1229	-	1/1/15/20	13/37/115/115	-
20	CLA	7	603	-	1/1/15/20	13/37/115/115	-
20	CLA	B	1239	-	1/1/15/20	14/37/115/115	-
36	LUT	6	501	-	-	4/29/67/67	0/2/2/2
20	CLA	A	1104	-	1/1/15/20	19/37/115/115	-
20	CLA	7	616	-	1/1/14/20	11/31/109/115	-
20	CLA	8	615	15	1/1/11/20	7/15/93/115	-
23	BCR	4	503	-	-	16/29/63/63	0/2/2/2
20	CLA	3	608	-	1/1/11/20	6/13/91/115	-
23	BCR	B	4007	-	-	12/29/63/63	0/2/2/2
20	CLA	4	615	-	1/1/10/20	2/8/86/115	-
20	CLA	A	1131	-	1/1/15/20	15/37/115/115	-
20	CLA	K	1403	-	1/1/11/20	10/18/96/115	-
23	BCR	B	4003	-	-	9/29/63/63	0/2/2/2
20	CLA	L	1502	-	1/1/15/20	25/37/115/115	-
20	CLA	1	615	12	1/1/15/20	15/37/115/115	-
20	CLA	B	1217	-	1/1/13/20	16/27/105/115	-
20	CLA	4	606	-	1/1/12/20	9/19/97/115	-
20	CLA	B	1236	-	1/1/15/20	24/37/115/115	-
36	LUT	Z	501	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1107	1	1/1/15/20	17/37/115/115	-
24	LHG	7	801	-	-	26/41/41/53	-
34	C7Z	1	503	-	1/1/12/26	6/29/67/67	0/2/2/2
20	CLA	A	1120	-	1/1/13/20	13/25/103/115	-
37	CHL	3	611	-	4/4/20/26	7/39/137/137	-
20	CLA	A	1123	-	1/1/15/20	13/37/115/115	-
20	CLA	B	1021	-	1/1/15/20	15/37/115/115	-
20	CLA	B	1224	-	1/1/15/20	15/37/115/115	-
36	LUT	7	501	-	-	3/29/67/67	0/2/2/2
20	CLA	8	605	-	1/1/15/20	17/37/115/115	-
20	CLA	A	1116	-	1/1/14/20	12/31/109/115	-
20	CLA	Z	607	-	1/1/13/20	13/28/106/115	-
26	LMT	B	6101	-	-	10/21/61/61	0/2/2/2
20	CLA	5	609	-	1/1/15/20	11/37/115/115	-
20	CLA	6	604	-	1/1/15/20	10/37/115/115	-
36	LUT	Z	502	-	-	1/29/67/67	0/2/2/2
20	CLA	3	618	-	1/1/11/20	9/15/93/115	-
20	CLA	4	605	-	1/1/15/20	14/37/115/115	-
20	CLA	A	1114	-	1/1/14/20	9/33/111/115	-
20	CLA	A	1141	24	1/1/12/20	11/22/100/115	-
21	PQN	B	2002	-	-	11/23/43/43	0/2/2/2
26	LMT	8	805	-	-	5/21/61/61	0/2/2/2
20	CLA	F	1301	-	1/1/15/20	15/37/115/115	-
35	SPH	K	5001	-	-	14/21/21/21	-
37	CHL	Z	613	-	3/3/16/26	3/15/113/137	-
20	CLA	B	1204	-	1/1/15/20	13/37/115/115	-
20	CLA	A	1110	-	1/1/15/20	20/37/115/115	-
23	BCR	3	504	-	-	11/29/63/63	0/2/2/2
41	PLM	7	805	-	-	7/15/15/15	-
23	BCR	G	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	6	612	-	1/1/12/20	7/19/97/115	-
20	CLA	B	1023	-	1/1/15/20	15/37/115/115	-
26	LMT	B	5005	-	-	14/21/61/61	0/2/2/2
31	DGD	B	5003	-	-	17/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	7	611	-	1/1/12/20	4/19/97/115	-
36	LUT	8	501	-	-	2/29/67/67	0/2/2/2
20	CLA	A	1121	-	1/1/15/20	21/37/115/115	-
23	BCR	6	503	-	-	13/29/63/63	0/2/2/2
35	SPH	7	803	-	-	7/21/21/21	-
20	CLA	6	615	-	1/1/14/20	12/33/111/115	-
36	LUT	6	502	-	-	2/29/67/67	0/2/2/2
20	CLA	A	1103	-	1/1/15/20	17/37/115/115	-
20	CLA	8	611	-	1/1/12/20	7/19/97/115	-
36	LUT	1	501	-	-	5/29/67/67	0/2/2/2
20	CLA	A	1101	-	1/1/15/20	14/37/115/115	-
20	CLA	B	1207	-	1/1/15/20	16/37/115/115	-
20	CLA	3	602	-	1/1/11/20	4/15/93/115	-
20	CLA	B	1232	-	1/1/11/20	2/13/91/115	-
30	DGA	A	5005	-	-	21/45/45/45	-
20	CLA	7	602	-	1/1/12/20	5/19/97/115	-
34	C7Z	5	505	-	1/1/12/26	12/29/67/67	0/2/2/2
20	CLA	6	605	-	1/1/13/20	16/25/103/115	-
37	CHL	5	611	-	3/3/17/26	2/21/119/137	-
20	CLA	6	619	18	1/1/15/20	18/37/115/115	-
29	LMG	J	5001	-	-	10/30/50/70	0/1/1/1
23	BCR	3	503	-	-	10/29/63/63	0/2/2/2
20	CLA	1	611	-	1/1/15/20	14/37/115/115	-
20	CLA	A	1138	-	1/1/15/20	16/37/115/115	-
23	BCR	K	4002	-	-	8/29/63/63	0/2/2/2
26	LMT	1	803	-	-	6/21/61/61	0/2/2/2
24	LHG	B	5002	-	-	11/22/22/53	-
20	CLA	A	1109	-	1/1/15/20	11/37/115/115	-
20	CLA	8	601	15	1/1/14/20	11/31/109/115	-
40	3PH	5	802	-	-	9/24/24/49	-
20	CLA	1	605	-	1/1/13/20	9/25/103/115	-
20	CLA	7	615	14	1/1/13/20	15/29/107/115	-
36	LUT	7	502	-	-	2/29/67/67	0/2/2/2
20	CLA	B	1208	-	1/1/13/20	11/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	603	-	1/1/15/20	15/37/115/115	-
38	SQD	1	802	-	-	21/43/63/69	0/1/1/1
20	CLA	B	1219	-	1/1/13/20	15/30/108/115	-
20	CLA	4	604	-	1/1/14/20	9/31/109/115	-
39	QTB	Z	504	-	1/1/5/10	6/11/28/28	0/1/1/1
24	LHG	6	801	-	-	33/53/53/53	-
24	LHG	Z	801	-	-	29/47/47/53	-
20	CLA	4	602	-	1/1/12/20	6/22/100/115	-
37	CHL	8	610	-	4/4/18/26	5/27/125/137	-
20	CLA	6	607	-	1/1/13/20	6/25/103/115	-
20	CLA	B	1220	-	1/1/15/20	19/37/115/115	-
23	BCR	A	4005	-	-	15/29/63/63	0/2/2/2
23	BCR	B	4006	-	-	11/29/63/63	0/2/2/2
26	LMT	A	5006	-	-	12/21/61/61	0/2/2/2
20	CLA	Z	603	-	1/1/12/20	10/19/97/115	-
20	CLA	3	601	-	1/1/15/20	10/37/115/115	-
23	BCR	B	4004	-	-	9/29/63/63	0/2/2/2
37	CHL	6	613	-	4/4/18/26	2/27/125/137	-
20	CLA	5	606	-	1/1/12/20	12/19/97/115	-
37	CHL	Z	610	-	4/4/20/26	5/39/137/137	-
20	CLA	B	1238	-	1/1/15/20	13/37/115/115	-
23	BCR	L	4002	-	-	11/29/63/63	0/2/2/2
21	PQN	A	2001	-	-	7/23/43/43	0/2/2/2
20	CLA	8	612	-	1/1/11/20	8/15/93/115	-
20	CLA	B	1234	-	1/1/14/20	21/31/109/115	-
23	BCR	J	4001	-	-	17/29/63/63	0/2/2/2
20	CLA	B	1241	-	1/1/15/20	21/37/115/115	-
40	3PH	8	806	-	-	13/31/31/49	-
20	CLA	7	605	-	1/1/14/20	17/33/111/115	-
20	CLA	A	1113	-	1/1/15/20	12/37/115/115	-
20	CLA	B	1213	-	1/1/15/20	19/37/115/115	-
20	CLA	Z	611	-	1/1/13/20	8/25/103/115	-
34	C7Z	J	4002	-	1/1/12/26	11/29/67/67	0/2/2/2
23	BCR	5	504	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	7	504	-	-	13/29/63/63	0/2/2/2
20	CLA	G	1602	-	1/1/11/20	6/15/93/115	-
20	CLA	1	612	-	1/1/15/20	22/37/115/115	-
25	NKP	3	802	-	-	2/15/15/28	-
20	CLA	B	1223	-	1/1/15/20	18/37/115/115	-
36	LUT	Z	503	-	-	6/29/67/67	0/2/2/2
20	CLA	5	612	-	1/1/15/20	8/37/115/115	-
24	LHG	A	5002	-	-	29/53/53/53	-
37	CHL	6	610	-	4/4/18/26	8/27/125/137	-
20	CLA	6	609	18	1/1/15/20	13/37/115/115	-
20	CLA	3	616	-	1/1/13/20	10/27/105/115	-
23	BCR	K	4001	-	-	14/29/63/63	0/2/2/2
20	CLA	7	604	-	1/1/15/20	13/37/115/115	-
20	CLA	A	1136	-	1/1/15/20	16/37/115/115	-
20	CLA	A	1105	-	1/1/15/20	14/37/115/115	-
23	BCR	B	4005	-	-	13/29/63/63	0/2/2/2
20	CLA	Z	604	-	1/1/15/20	17/37/115/115	-
20	CLA	A	1125	-	1/1/15/20	22/37/115/115	-
24	LHG	B	5001	-	-	15/26/26/53	-
20	CLA	A	1119	-	1/1/15/20	17/37/115/115	-
20	CLA	B	1215	-	1/1/14/20	15/31/109/115	-
20	CLA	5	607	-	1/1/14/20	13/33/111/115	-
20	CLA	B	1211	-	1/1/14/20	16/31/109/115	-
24	LHG	3	801	-	-	12/22/22/53	-
20	CLA	L	1503	-	1/1/12/20	10/19/97/115	-
23	BCR	7	503	-	-	10/29/63/63	0/2/2/2
23	BCR	A	4003	-	-	14/29/63/63	0/2/2/2
20	CLA	A	1127	-	1/1/15/20	14/37/115/115	-
20	CLA	5	615	17	1/1/12/20	5/19/97/115	-
20	CLA	6	606	-	1/1/15/20	16/37/115/115	-
20	CLA	A	1140	-	1/1/15/20	19/37/115/115	-
20	CLA	B	1210	-	1/1/15/20	20/37/115/115	-
20	CLA	8	607	-	1/1/13/20	14/25/103/115	-
40	3PH	7	802	-	-	21/40/40/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	CHL	1	610	-	3/3/16/26	4/18/116/137	-
20	CLA	4	608	-	1/1/13/20	8/25/103/115	-
25	NKP	8	802	-	-	15/28/28/28	-
20	CLA	5	603	-	1/1/13/20	8/27/105/115	-
36	LUT	3	501	-	-	1/29/67/67	0/2/2/2
20	CLA	4	609	16	1/1/14/20	13/31/109/115	-
20	CLA	B	1231	-	1/1/15/20	10/37/115/115	-
20	CLA	6	601	-	1/1/14/20	13/31/109/115	-
20	CLA	3	610	13	1/1/14/20	14/31/109/115	-
20	CLA	A	1117	-	1/1/15/20	19/37/115/115	-
20	CLA	3	604	-	1/1/14/20	8/31/109/115	-
20	CLA	5	613	-	1/1/13/20	12/25/103/115	-
23	BCR	A	4004	-	-	15/29/63/63	0/2/2/2
23	BCR	A	4001	-	-	10/29/63/63	0/2/2/2
20	CLA	8	603	-	1/1/15/20	6/37/115/115	-
37	CHL	8	613	-	5/5/20/26	10/39/137/137	-
20	CLA	B	1216	-	1/1/15/20	20/37/115/115	-
23	BCR	3	506	-	-	15/29/63/63	0/2/2/2
20	CLA	A	1129	-	1/1/12/20	7/19/97/115	-
36	LUT	4	501	-	-	5/29/67/67	0/2/2/2
26	LMT	F	5001	-	-	8/21/61/61	0/2/2/2
20	CLA	1	604	-	1/1/14/20	11/31/109/115	-
20	CLA	B	1218	-	1/1/15/20	16/37/115/115	-
20	CLA	5	602	-	1/1/14/20	14/33/111/115	-
20	CLA	5	604	-	1/1/15/20	13/37/115/115	-
29	LMG	A	5003	-	-	8/24/44/70	0/1/1/1
36	LUT	8	502	-	-	2/29/67/67	0/2/2/2
23	BCR	3	505	-	-	10/29/63/63	0/2/2/2
20	CLA	7	606	-	1/1/13/20	13/27/105/115	-
20	CLA	A	1118	-	1/1/14/20	14/31/109/115	-
23	BCR	B	4002	-	-	12/29/63/63	0/2/2/2
20	CLA	8	604	-	1/1/14/20	11/34/112/115	-
37	CHL	7	610	-	3/3/17/26	5/25/123/137	-
23	BCR	8	503	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	607	-	1/1/14/20	12/31/109/115	-
20	CLA	A	1133	-	1/1/15/20	15/37/115/115	-
20	CLA	3	606	-	1/1/15/20	18/37/115/115	-
37	CHL	Z	609	12	4/4/20/26	12/39/137/137	-
20	CLA	Z	605	-	1/1/15/20	10/37/115/115	-
35	SPH	7	804	-	-	11/21/21/21	-
20	CLA	Z	606	-	1/1/13/20	9/28/106/115	-
20	CLA	B	1237	-	1/1/15/20	18/37/115/115	-
37	CHL	1	609	12	4/4/18/26	5/30/128/137	-
19	CL0	A	1011	-	3/3/20/25	11/37/135/135	-
23	BCR	5	503	-	-	12/29/63/63	0/2/2/2
37	CHL	5	617	-	3/3/15/26	3/12/110/137	-
20	CLA	1	613	-	1/1/11/20	8/15/93/115	-
20	CLA	4	607	-	1/1/13/20	8/25/103/115	-
20	CLA	B	1221	-	1/1/15/20	16/37/115/115	-
23	BCR	B	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	6	608	-	1/1/13/20	12/25/103/115	-
37	CHL	4	613	-	4/4/18/26	3/27/125/137	-
20	CLA	A	1106	-	1/1/15/20	18/37/115/115	-
20	CLA	B	1240	-	1/1/15/20	21/37/115/115	-
20	CLA	7	609	14	1/1/15/20	19/37/115/115	-
20	CLA	8	602	-	1/1/15/20	15/37/115/115	-
20	CLA	K	1402	-	1/1/13/20	14/25/103/115	-
20	CLA	A	1130	-	1/1/15/20	15/37/115/115	-
20	CLA	6	618	-	1/1/11/20	8/15/93/115	-
20	CLA	5	601	-	1/1/14/20	15/31/109/115	-
23	BCR	A	4002	-	-	8/29/63/63	0/2/2/2
40	3PH	6	802	-	-	15/30/30/49	-
20	CLA	A	1115	-	1/1/14/20	15/31/109/115	-
20	CLA	1	602	-	1/1/11/20	5/13/91/115	-
20	CLA	A	1139	-	1/1/15/20	13/37/115/115	-
20	CLA	B	1214	-	1/1/13/20	13/30/108/115	-
20	CLA	1	606	-	1/1/14/20	13/33/111/115	-
20	CLA	3	613	-	1/1/13/20	5/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	1013	-	1/1/15/20	18/37/115/115	-
20	CLA	5	605	-	1/1/13/20	14/25/103/115	-
20	CLA	B	1212	-	1/1/13/20	9/28/106/115	-
20	CLA	K	1404	-	1/1/13/20	11/25/103/115	-
20	CLA	B	1209	-	1/1/15/20	25/37/115/115	-
20	CLA	4	612	-	1/1/12/20	7/19/97/115	-
22	SF4	A	3001	2,1	-	-	0/6/5/5
26	LMT	4	803	-	-	11/21/61/61	0/2/2/2
20	CLA	A	1124	-	1/1/15/20	14/37/115/115	-
20	CLA	1	601	-	1/1/15/20	15/37/115/115	-
24	LHG	A	5001	20	-	22/39/39/53	-
20	CLA	A	1132	-	1/1/15/20	18/37/115/115	-
20	CLA	3	607	-	1/1/14/20	21/31/109/115	-
20	CLA	B	1222	-	1/1/15/20	15/37/115/115	-
20	CLA	B	1201	-	1/1/11/20	4/13/91/115	-
20	CLA	5	618	-	1/1/15/20	16/37/115/115	-
24	LHG	8	801	-	-	20/42/42/53	-
36	LUT	5	501	-	-	3/29/67/67	0/2/2/2
37	CHL	4	617	-	3/3/15/26	1/12/110/137	-
20	CLA	A	1137	-	1/1/15/20	13/37/115/115	-
20	CLA	3	605	-	1/1/15/20	11/37/115/115	-
20	CLA	6	602	-	1/1/12/20	6/22/100/115	-
33	RRX	F	4001	-	1/1/11/25	9/29/65/65	0/2/2/2
20	CLA	Z	612	-	1/1/15/20	16/37/115/115	-
20	CLA	J	1901	-	1/1/10/20	4/10/88/115	-
20	CLA	4	601	-	1/1/14/20	8/31/109/115	-
20	CLA	A	1135	-	1/1/12/20	9/21/99/115	-
20	CLA	5	608	-	1/1/11/20	5/13/91/115	-
20	CLA	A	1102	-	1/1/13/20	15/25/103/115	-
20	CLA	7	608	-	1/1/10/20	6/11/89/115	-
23	BCR	6	504	-	-	11/29/63/63	0/2/2/2
20	CLA	Z	615	-	1/1/11/20	7/15/93/115	-
36	LUT	4	502	-	-	4/29/67/67	0/2/2/2
20	CLA	B	1227	-	1/1/12/20	9/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	603	-	1/1/15/20	14/37/115/115	-
24	LHG	4	801	-	-	33/53/53/53	-
37	CHL	5	610	-	4/4/20/26	9/39/137/137	-
20	CLA	A	1108	-	1/1/15/20	23/37/115/115	-
20	CLA	B	1203	-	1/1/15/20	17/37/115/115	-
20	CLA	B	1228	-	1/1/15/20	18/37/115/115	-
42	LPX	8	803	-	-	11/31/31/31	-
27	OCA	A	5008	-	-	2/7/7/7	-
20	CLA	Z	601	-	1/1/14/20	10/31/109/115	-
20	CLA	A	1126	-	1/1/15/20	20/37/115/115	-
22	SF4	C	3002	3	-	-	0/6/5/5
20	CLA	B	1206	-	1/1/15/20	18/37/115/115	-
20	CLA	A	1134	1	1/1/13/20	10/25/103/115	-
20	CLA	1	608	-	1/1/14/20	12/31/109/115	-
20	CLA	F	1302	-	1/1/11/20	4/13/91/115	-
20	CLA	B	1205	-	1/1/15/20	16/37/115/115	-
20	CLA	7	612	-	1/1/12/20	10/19/97/115	-
20	CLA	7	613	-	1/1/10/20	6/10/88/115	-
20	CLA	7	607	-	1/1/15/20	21/37/115/115	-
20	CLA	A	1128	-	1/1/15/20	19/37/115/115	-
28	DAO	A	5007	-	-	1/11/11/11	-
25	NKP	A	5004	-	-	14/28/28/28	-
20	CLA	8	608	-	1/1/13/20	11/25/103/115	-
20	CLA	A	1122	-	1/1/15/20	19/37/115/115	-
20	CLA	B	1202	-	1/1/15/20	17/37/115/115	-
20	CLA	A	1111	-	1/1/15/20	17/37/115/115	-
20	CLA	6	603	-	1/1/15/20	19/37/115/115	-
20	CLA	B	1225	-	1/1/15/20	11/37/115/115	-
20	CLA	3	612	-	1/1/14/20	9/31/109/115	-
37	CHL	6	617	-	3/3/15/26	2/12/110/137	-
22	SF4	C	3003	3	-	-	0/6/5/5
24	LHG	4	802	-	-	20/36/36/53	-
20	CLA	K	1401	-	1/1/11/20	6/15/93/115	-
20	CLA	Z	602	-	1/1/11/20	4/15/93/115	-
20	CLA	8	609	15	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	B	1235	-	1/1/15/20	15/37/115/115	-
36	LUT	3	502	-	-	1/29/67/67	0/2/2/2
24	LHG	5	801	-	-	27/41/41/53	-
36	LUT	5	502	-	-	2/29/67/67	0/2/2/2
20	CLA	A	1112	-	1/1/14/20	13/31/109/115	-
23	BCR	I	4001	-	-	13/29/63/63	0/2/2/2
20	CLA	G	1601	-	1/1/12/20	8/19/97/115	-
20	CLA	Z	608	-	1/1/13/20	11/27/105/115	-
20	CLA	B	1230	-	1/1/13/20	12/29/107/115	-
37	CHL	4	610	-	4/4/17/26	4/21/119/137	-
20	CLA	8	606	-	1/1/14/20	12/31/109/115	-
24	LHG	1	801	-	-	24/47/47/53	-
24	LHG	B	5006	-	-	24/37/37/53	-
36	LUT	1	502	-	-	1/29/67/67	0/2/2/2
20	CLA	5	622	-	1/1/11/20	5/15/93/115	-
37	CHL	4	611	-	3/3/17/26	5/21/119/137	-
20	CLA	A	1012	-	1/1/15/20	17/37/115/115	-
37	CHL	6	611	-	3/3/17/26	6/21/119/137	-
20	CLA	3	603	-	1/1/15/20	16/37/115/115	-

The worst 5 of 1947 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	J	4002	C7Z	C25-C26	15.76	1.61	1.34
34	5	505	C7Z	C5-C6	15.72	1.61	1.34
34	1	503	C7Z	C25-C26	15.70	1.61	1.34
34	5	505	C7Z	C25-C26	15.69	1.61	1.34
34	1	503	C7Z	C5-C6	15.12	1.60	1.34

The worst 5 of 4441 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	5	504	BCR	C10-C11-C12	18.18	179.94	123.22
23	5	504	BCR	C16-C15-C14	17.70	159.73	123.47
23	K	4001	BCR	C10-C11-C12	17.63	178.24	123.22
23	A	4003	BCR	C10-C11-C12	17.47	177.75	123.22
23	B	4007	BCR	C10-C11-C12	17.47	177.72	123.22

5 of 277 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	A	1011	CL0	ND
19	A	1011	CL0	NC
19	A	1011	CL0	NA
20	A	1012	CLA	ND
20	A	1102	CLA	ND

5 of 3749 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	1012	CLA	CHA-CBD-CGD-O1D
20	A	1012	CLA	CBD-CGD-O2D-CED
20	A	1012	CLA	C2-C3-C5-C6
20	A	1102	CLA	CBD-CGD-O2D-CED
20	A	1104	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

274 monomers are involved in 647 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	1226	CLA	7	0
20	7	601	CLA	4	0
20	B	1022	CLA	2	0
23	L	4001	BCR	4	0
20	B	1229	CLA	2	0
20	7	603	CLA	2	0
20	B	1239	CLA	3	0
36	6	501	LUT	4	0
20	A	1104	CLA	3	0
20	7	616	CLA	7	0
23	4	503	BCR	1	0
20	3	608	CLA	2	0
23	B	4007	BCR	1	0
20	K	1403	CLA	1	0
23	B	4003	BCR	2	0
20	L	1502	CLA	4	0
20	1	615	CLA	3	0
20	B	1217	CLA	1	0
20	B	1236	CLA	4	0
36	Z	501	LUT	1	0
20	A	1107	CLA	5	0
24	7	801	LHG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	1120	CLA	3	0
37	3	611	CHL	5	0
20	A	1123	CLA	3	0
20	B	1021	CLA	7	0
20	B	1224	CLA	8	0
20	8	605	CLA	2	0
20	A	1116	CLA	5	0
26	B	6101	LMT	1	0
20	5	609	CLA	4	0
20	6	604	CLA	3	0
36	Z	502	LUT	1	0
20	3	618	CLA	1	0
20	4	605	CLA	2	0
20	A	1114	CLA	6	0
20	A	1141	CLA	1	0
26	8	805	LMT	1	0
20	F	1301	CLA	4	0
35	K	5001	SPH	2	0
37	Z	613	CHL	4	0
20	B	1204	CLA	1	0
20	A	1110	CLA	3	0
23	3	504	BCR	4	0
23	G	4001	BCR	3	0
20	6	612	CLA	3	0
20	B	1023	CLA	4	0
26	B	5005	LMT	1	0
31	B	5003	DGD	5	0
20	7	611	CLA	1	0
36	8	501	LUT	4	0
20	A	1121	CLA	2	0
23	6	503	BCR	4	0
35	7	803	SPH	1	0
20	6	615	CLA	4	0
36	6	502	LUT	1	0
20	A	1103	CLA	5	0
20	8	611	CLA	2	0
36	1	501	LUT	2	0
20	A	1101	CLA	3	0
20	B	1207	CLA	5	0
20	3	602	CLA	1	0
20	B	1232	CLA	1	0
30	A	5005	DGA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	7	602	CLA	1	0
20	6	605	CLA	2	0
37	5	611	CHL	3	0
20	6	619	CLA	5	0
23	3	503	BCR	2	0
20	1	611	CLA	4	0
20	A	1138	CLA	3	0
23	K	4002	BCR	3	0
26	1	803	LMT	1	0
20	A	1109	CLA	5	0
20	8	601	CLA	4	0
20	1	605	CLA	3	0
20	7	615	CLA	5	0
36	7	502	LUT	1	0
20	B	1208	CLA	1	0
20	1	603	CLA	2	0
38	1	802	SQD	1	0
20	4	604	CLA	4	0
24	6	801	LHG	4	0
20	4	602	CLA	2	0
37	8	610	CHL	2	0
20	B	1220	CLA	3	0
23	A	4005	BCR	6	0
23	B	4006	BCR	4	0
26	A	5006	LMT	2	0
20	Z	603	CLA	1	0
20	3	601	CLA	5	0
23	B	4004	BCR	3	0
37	6	613	CHL	4	0
20	5	606	CLA	1	0
37	Z	610	CHL	4	0
20	B	1238	CLA	5	0
23	L	4002	BCR	2	0
20	8	612	CLA	1	0
20	B	1234	CLA	4	0
23	J	4001	BCR	3	0
20	B	1241	CLA	5	0
20	7	605	CLA	1	0
20	A	1113	CLA	4	0
20	B	1213	CLA	2	0
20	Z	611	CLA	1	0
23	5	504	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	7	504	BCR	3	0
20	G	1602	CLA	2	0
20	1	612	CLA	4	0
25	3	802	NKP	1	0
20	B	1223	CLA	2	0
36	Z	503	LUT	2	0
20	5	612	CLA	6	0
24	A	5002	LHG	3	0
37	6	610	CHL	2	0
20	6	609	CLA	9	0
23	K	4001	BCR	2	0
20	7	604	CLA	1	0
20	A	1136	CLA	3	0
20	A	1105	CLA	3	0
23	B	4005	BCR	2	0
20	Z	604	CLA	5	0
20	A	1125	CLA	4	0
20	A	1119	CLA	5	0
20	B	1215	CLA	3	0
20	5	607	CLA	2	0
20	B	1211	CLA	2	0
23	7	503	BCR	2	0
23	A	4003	BCR	4	0
20	A	1127	CLA	5	0
20	5	615	CLA	2	0
20	6	606	CLA	3	0
20	A	1140	CLA	3	0
20	B	1210	CLA	5	0
20	8	607	CLA	3	0
40	7	802	3PH	5	0
37	1	610	CHL	2	0
20	4	608	CLA	2	0
20	5	603	CLA	1	0
36	3	501	LUT	6	0
20	4	609	CLA	5	0
20	B	1231	CLA	1	0
20	6	601	CLA	5	0
20	3	610	CLA	3	0
20	A	1117	CLA	4	0
20	3	604	CLA	3	0
20	5	613	CLA	3	0
23	A	4004	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	4001	BCR	2	0
20	8	603	CLA	3	0
23	3	506	BCR	3	0
20	B	1216	CLA	4	0
37	8	613	CHL	4	0
20	A	1129	CLA	3	0
36	4	501	LUT	5	0
20	1	604	CLA	3	0
20	B	1218	CLA	5	0
20	5	604	CLA	7	0
36	8	502	LUT	1	0
23	3	505	BCR	2	0
20	7	606	CLA	2	0
20	A	1118	CLA	2	0
23	B	4002	BCR	5	0
20	8	604	CLA	2	0
37	7	610	CHL	3	0
23	8	503	BCR	2	0
20	1	607	CLA	1	0
20	A	1133	CLA	3	0
20	3	606	CLA	2	0
37	Z	609	CHL	4	0
20	Z	605	CLA	6	0
35	7	804	SPH	2	0
20	Z	606	CLA	2	0
20	B	1237	CLA	2	0
37	1	609	CHL	3	0
19	A	1011	CL0	3	0
23	5	503	BCR	2	0
37	5	617	CHL	1	0
20	1	613	CLA	4	0
20	4	607	CLA	1	0
20	B	1221	CLA	6	0
23	B	4001	BCR	5	0
20	6	608	CLA	6	0
37	4	613	CHL	2	0
20	A	1106	CLA	7	0
20	B	1240	CLA	5	0
20	7	609	CLA	2	0
20	8	602	CLA	3	0
20	K	1402	CLA	2	0
20	A	1130	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	6	618	CLA	1	0
20	5	601	CLA	5	0
23	A	4002	BCR	4	0
20	A	1115	CLA	2	0
20	A	1139	CLA	6	0
20	B	1214	CLA	6	0
20	1	606	CLA	2	0
20	3	613	CLA	3	0
20	A	1013	CLA	6	0
20	5	605	CLA	3	0
20	B	1212	CLA	1	0
20	K	1404	CLA	1	0
20	B	1209	CLA	3	0
20	4	612	CLA	1	0
26	4	803	LMT	2	0
20	A	1124	CLA	6	0
20	1	601	CLA	5	0
24	A	5001	LHG	1	0
20	A	1132	CLA	1	0
20	3	607	CLA	2	0
20	B	1222	CLA	4	0
20	B	1201	CLA	1	0
20	5	618	CLA	5	0
24	8	801	LHG	2	0
36	5	501	LUT	3	0
37	4	617	CHL	1	0
20	A	1137	CLA	2	0
20	3	605	CLA	2	0
33	F	4001	RRX	4	0
20	Z	612	CLA	1	0
20	4	601	CLA	5	0
20	A	1135	CLA	1	0
20	A	1102	CLA	2	0
20	7	608	CLA	1	0
23	6	504	BCR	2	0
20	Z	615	CLA	2	0
36	4	502	LUT	4	0
20	B	1227	CLA	3	0
20	4	603	CLA	4	0
24	4	801	LHG	2	0
37	5	610	CHL	5	0
20	A	1108	CLA	2	0

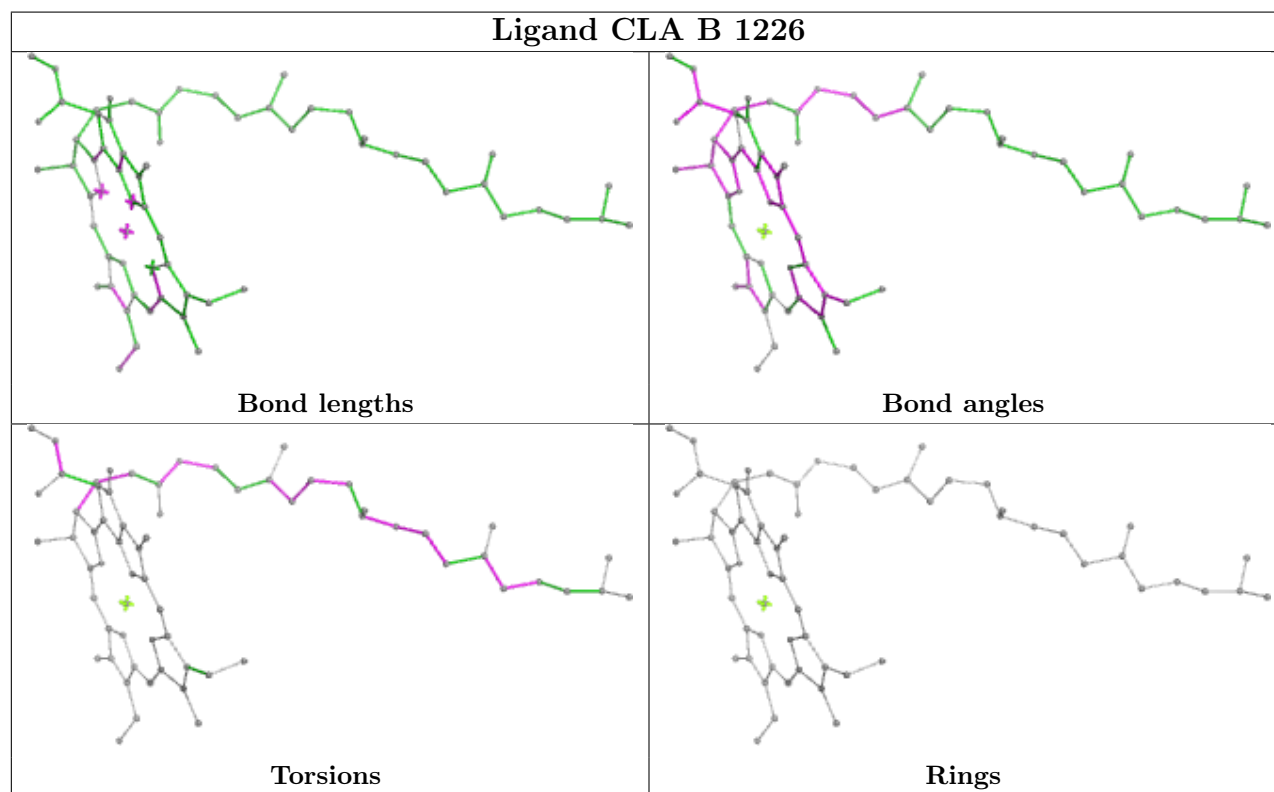
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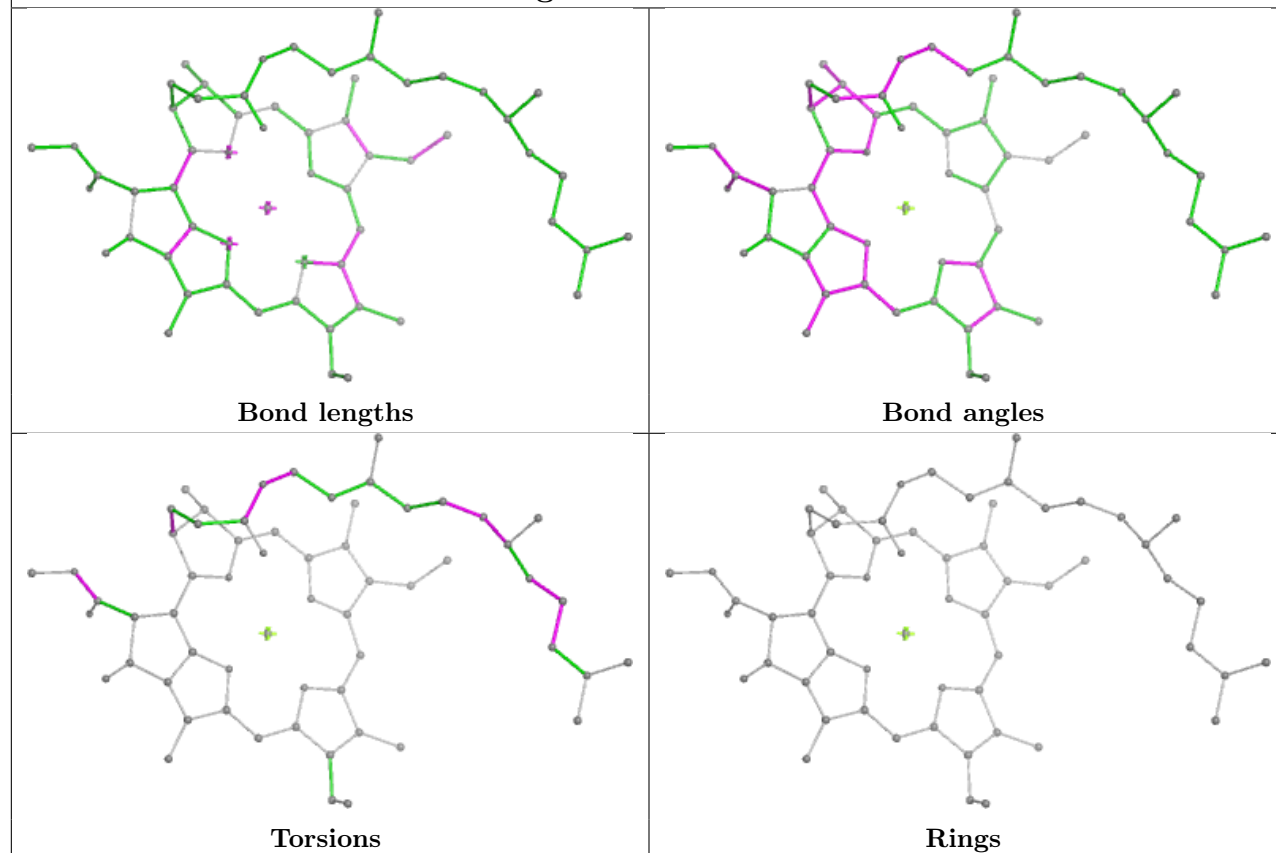
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20	B	1203	CLA	6	0
20	Z	601	CLA	3	0
20	A	1126	CLA	14	0
20	B	1206	CLA	4	0
20	A	1134	CLA	2	0
20	1	608	CLA	2	0
20	F	1302	CLA	4	0
20	B	1205	CLA	3	0
20	7	612	CLA	1	0
20	7	613	CLA	3	0
20	7	607	CLA	3	0
20	A	1128	CLA	4	0
20	8	608	CLA	1	0
20	A	1122	CLA	3	0
20	B	1202	CLA	2	0
20	A	1111	CLA	7	0
20	6	603	CLA	3	0
20	B	1225	CLA	8	0
20	3	612	CLA	3	0
37	6	617	CHL	1	0
22	C	3003	SF4	1	0
24	4	802	LHG	1	0
20	K	1401	CLA	5	0
20	8	609	CLA	1	0
20	B	1235	CLA	5	0
36	3	502	LUT	5	0
24	5	801	LHG	2	0
36	5	502	LUT	8	0
20	A	1112	CLA	5	0
23	I	4001	BCR	2	0
20	Z	608	CLA	2	0
20	B	1230	CLA	4	0
37	4	610	CHL	3	0
20	8	606	CLA	1	0
24	1	801	LHG	2	0
24	B	5006	LHG	2	0
36	1	502	LUT	2	0
20	5	622	CLA	1	0
37	4	611	CHL	1	0
20	A	1012	CLA	9	0
37	6	611	CHL	1	0
20	3	603	CLA	2	0



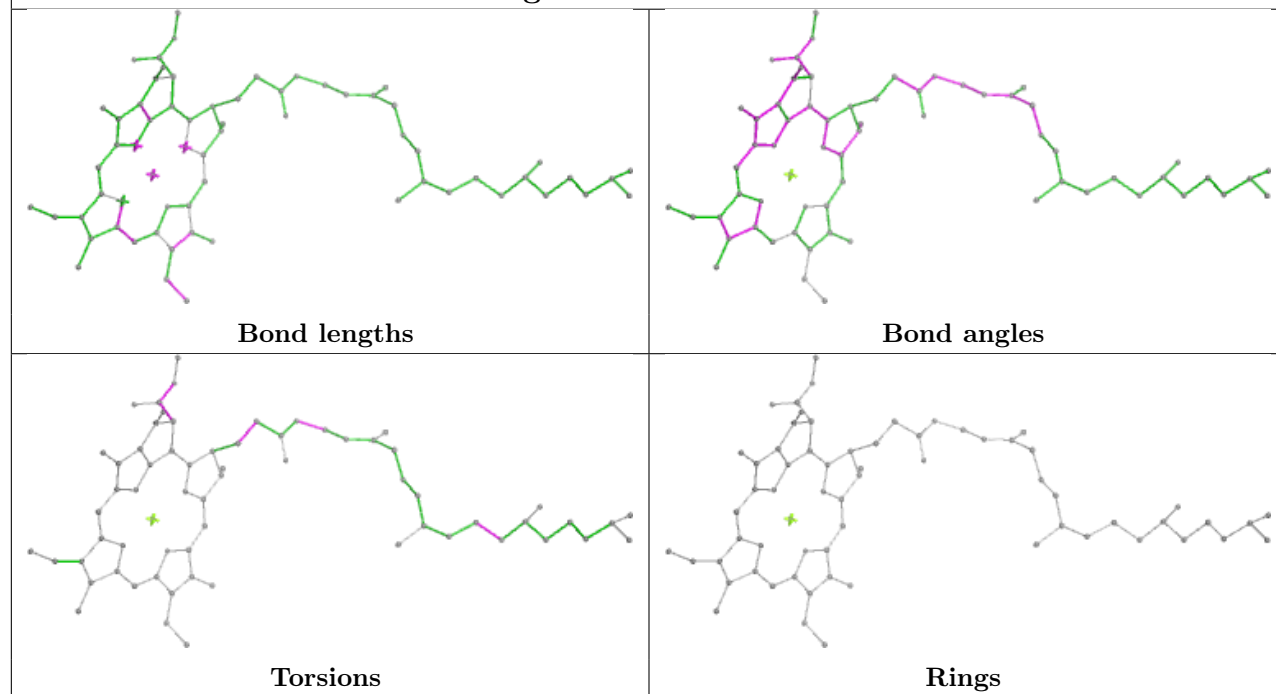
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

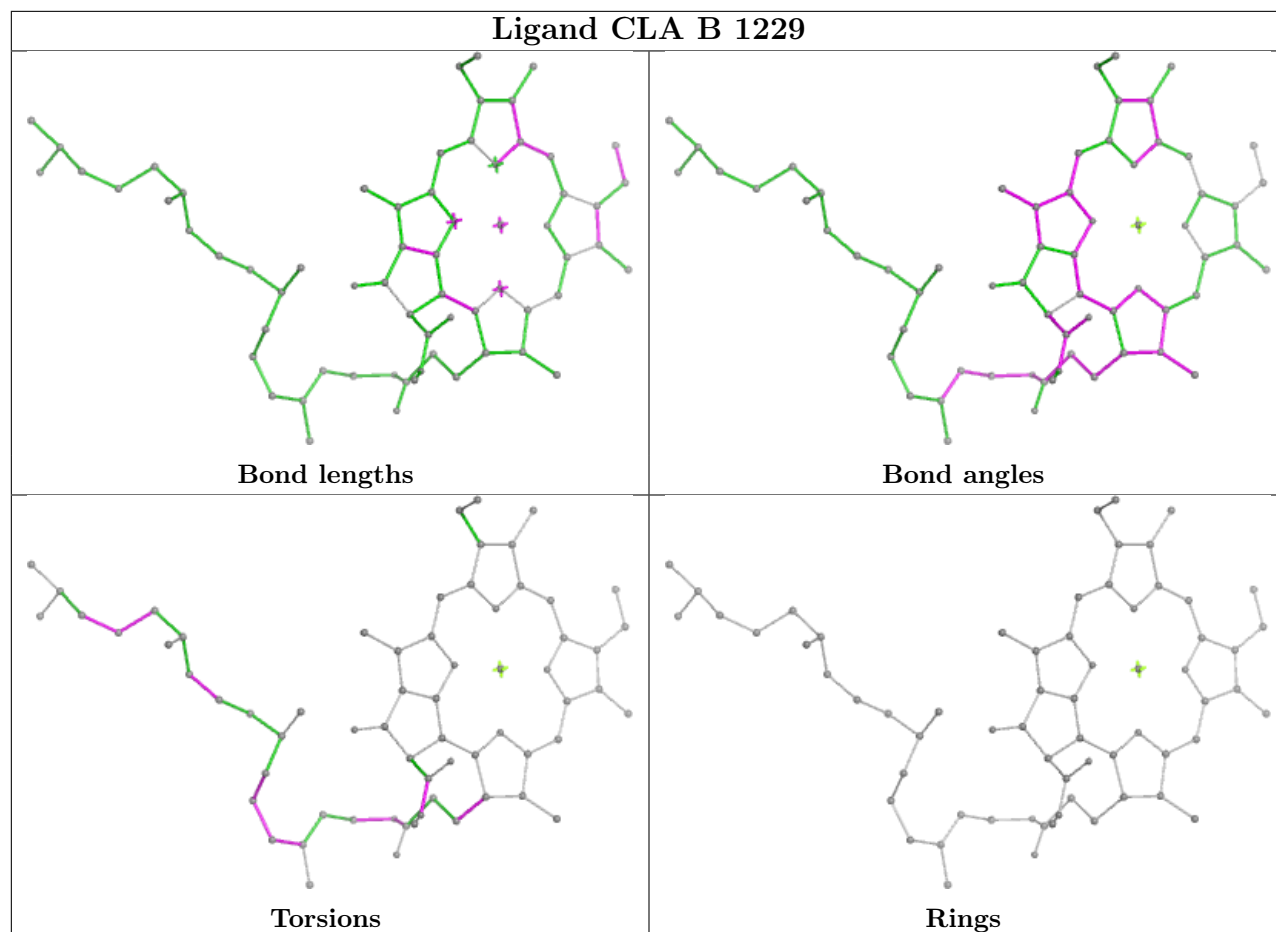
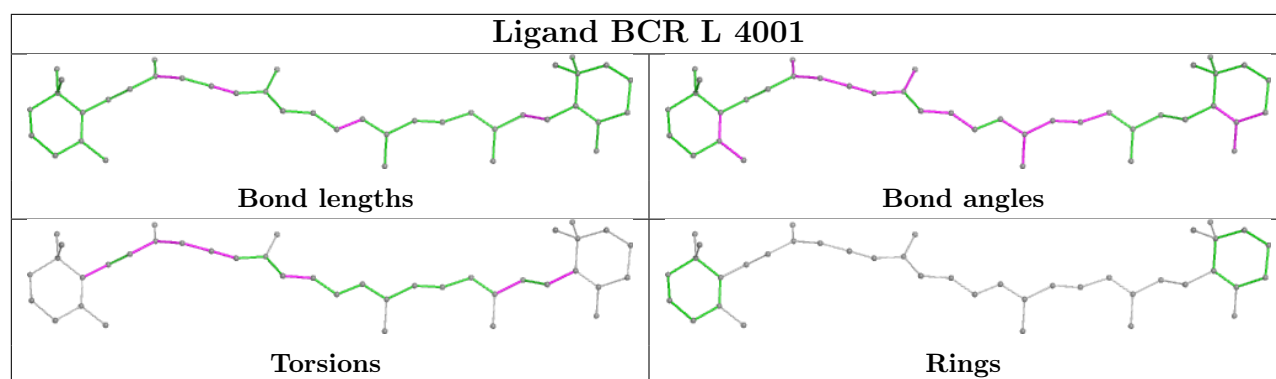


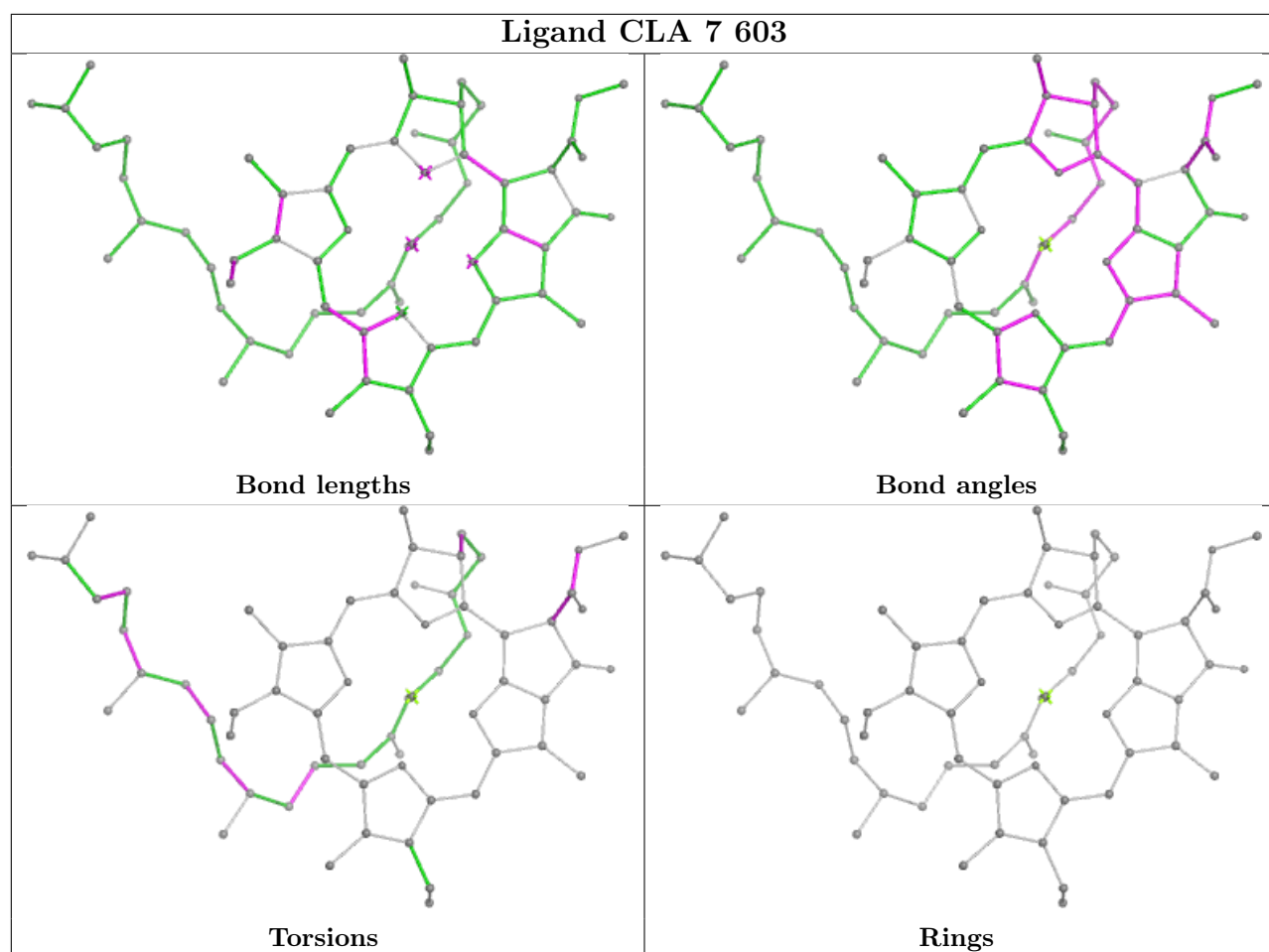
## Ligand CLA 7 601

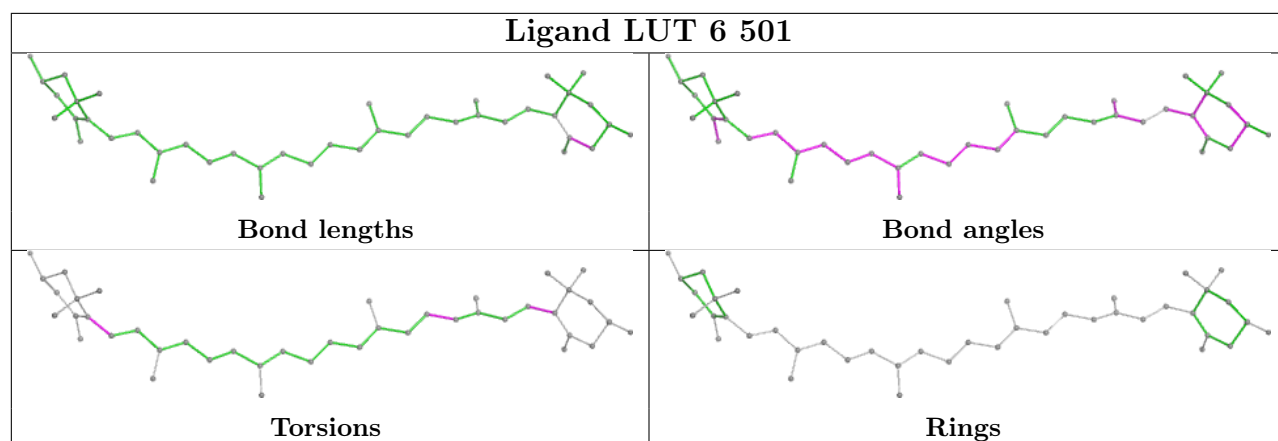
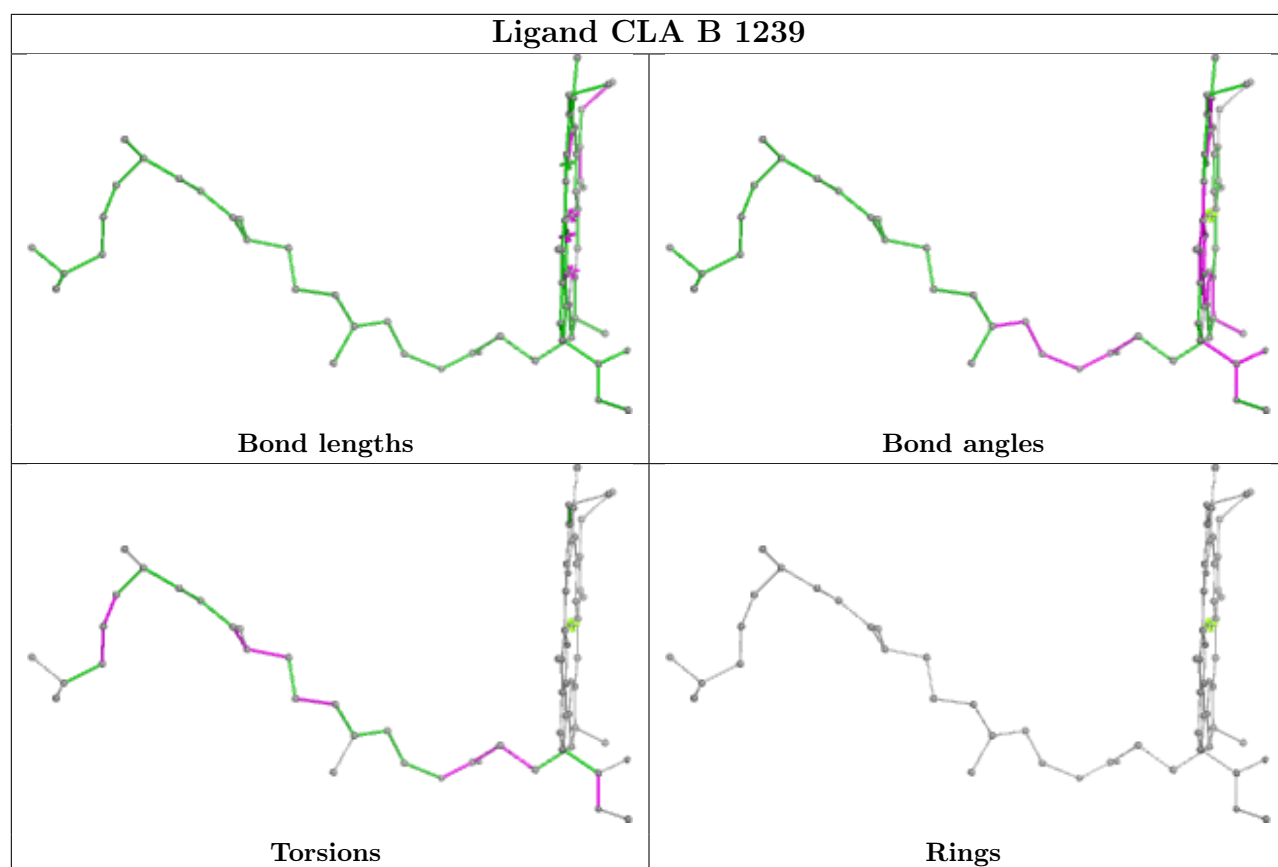


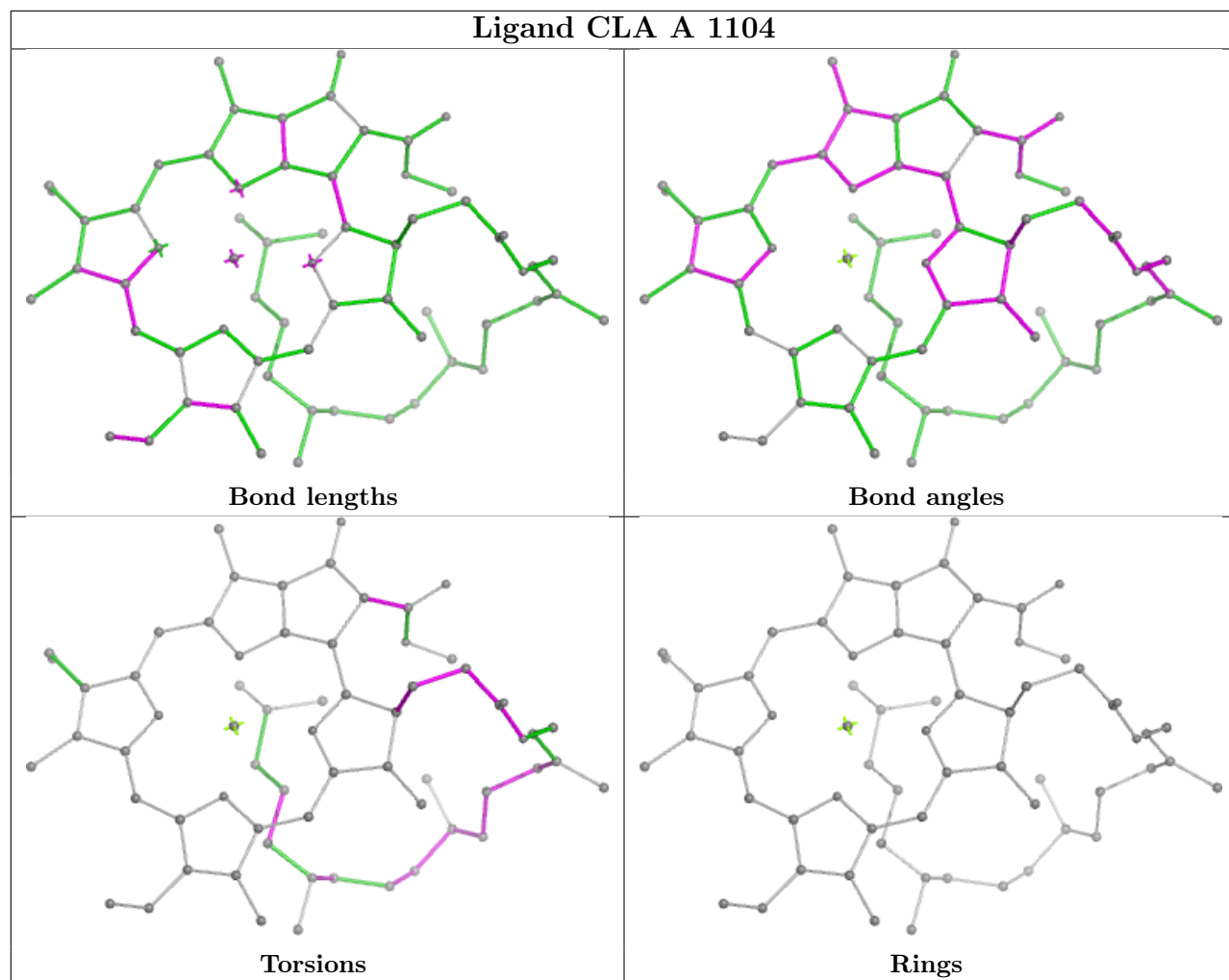
## Ligand CLA B 1022

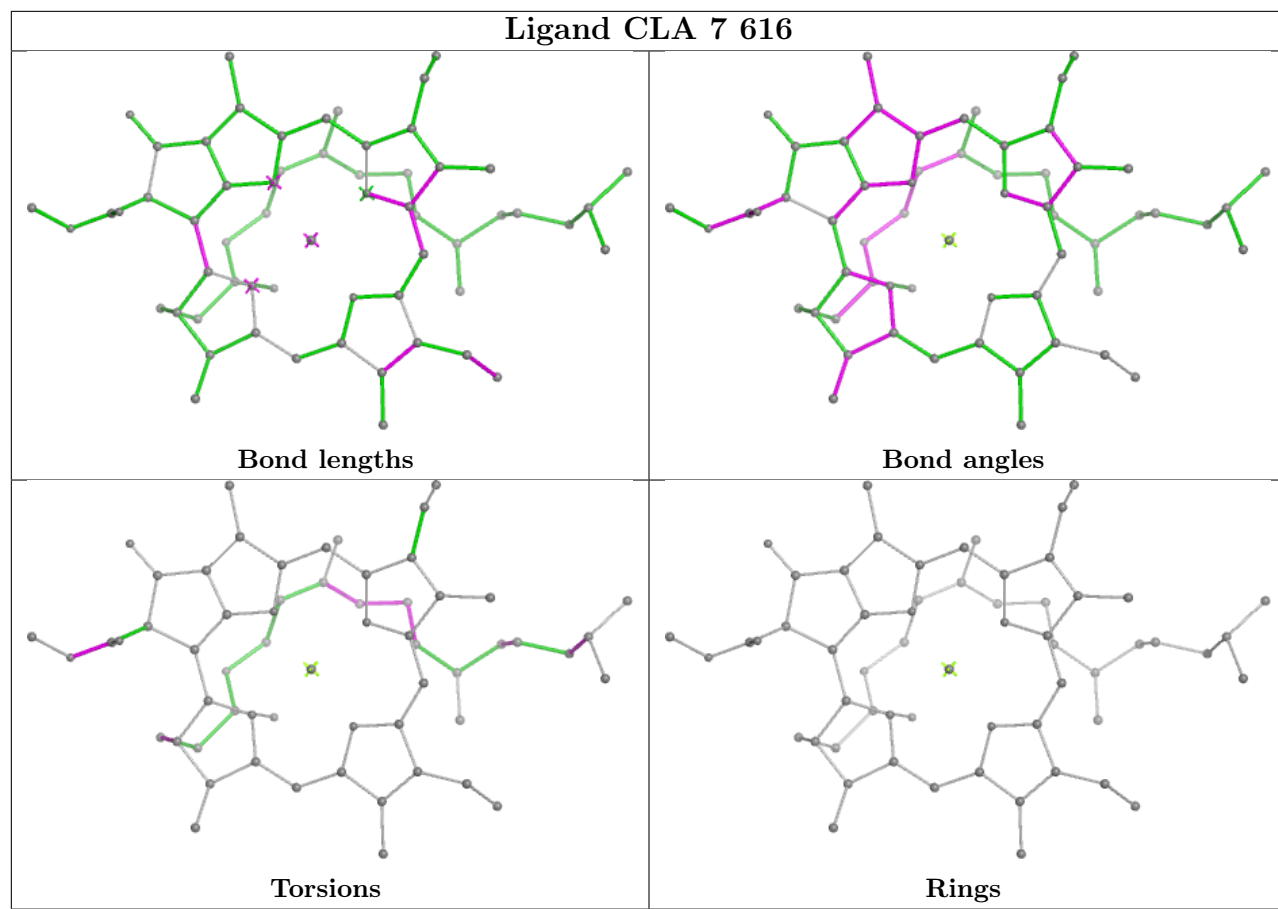




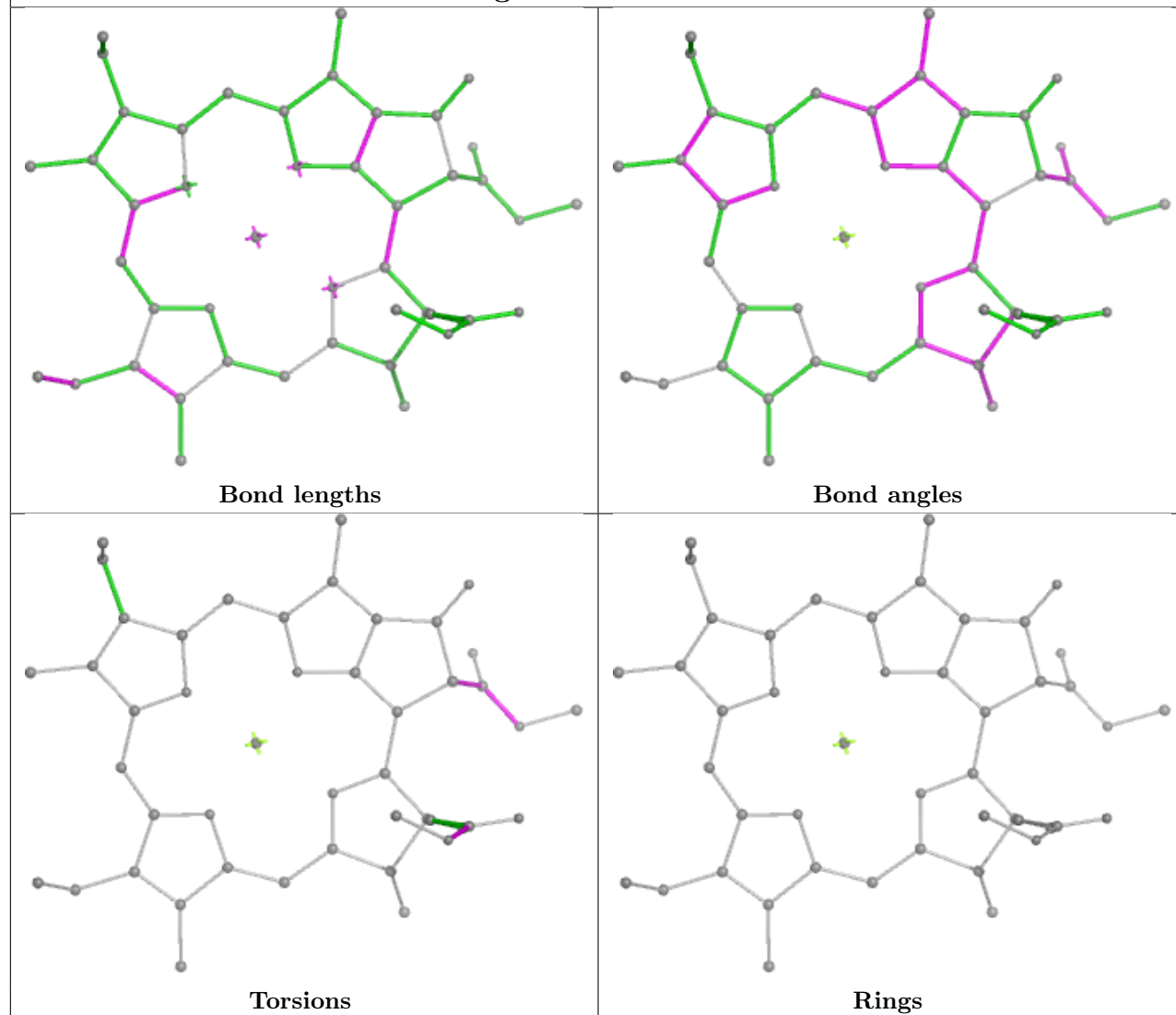




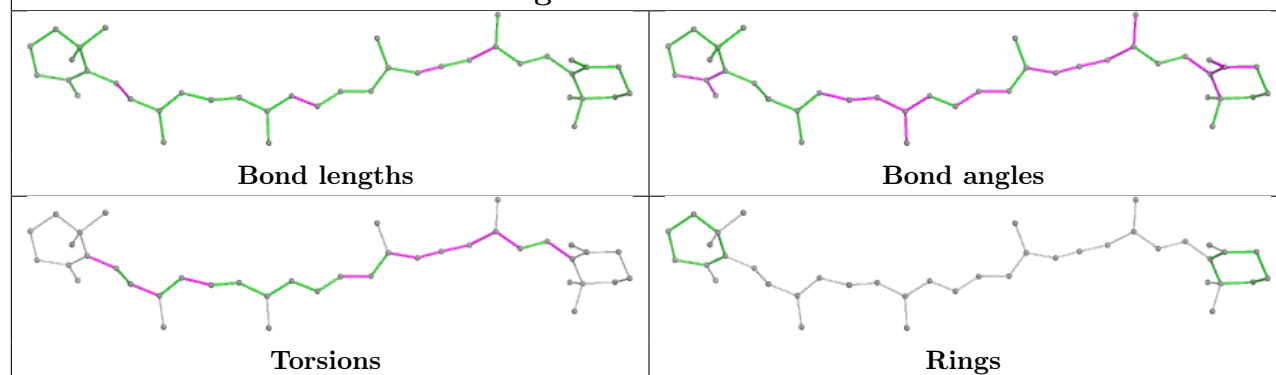




## Ligand CLA 8 615

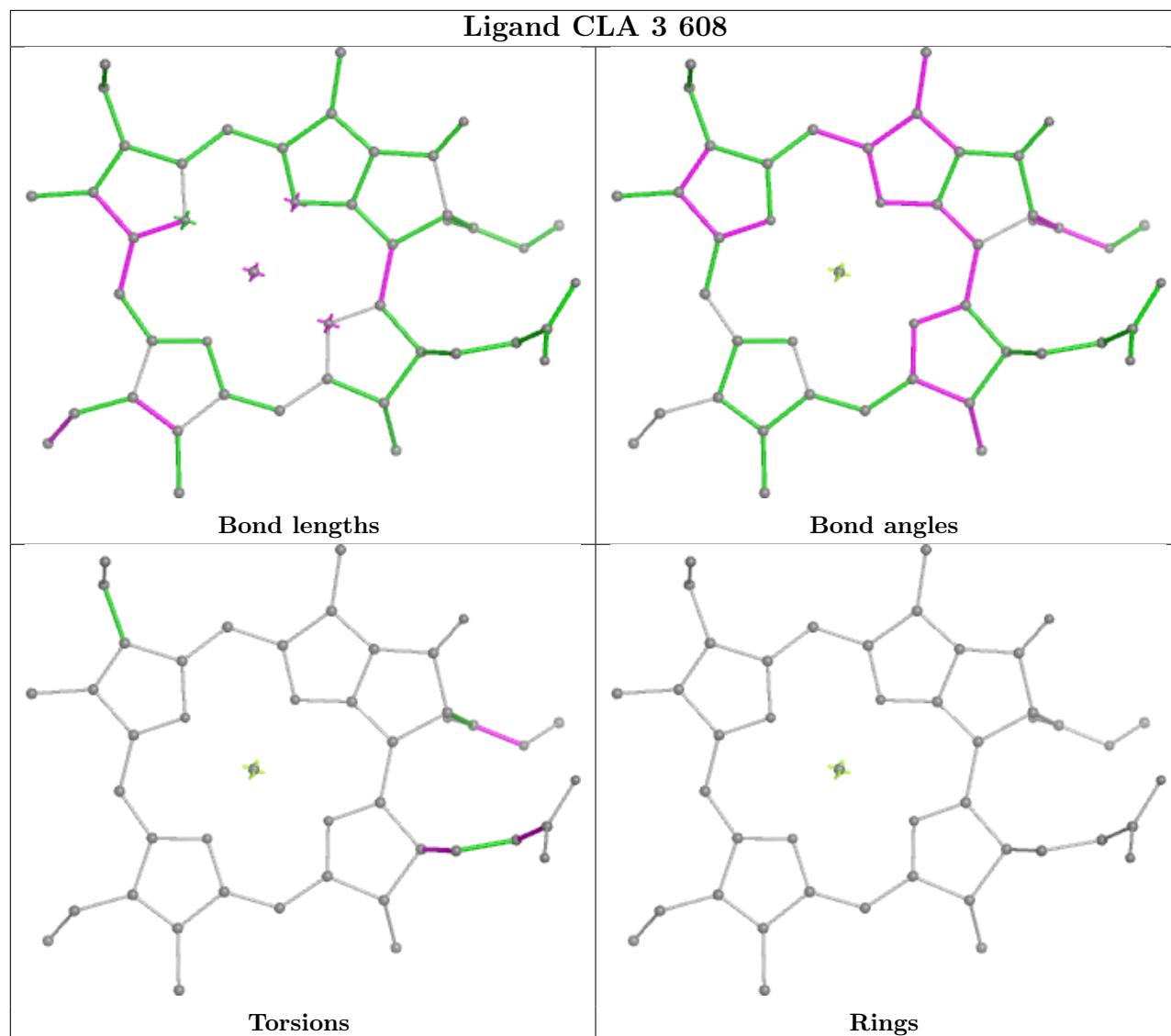


## Ligand BCR 4 503

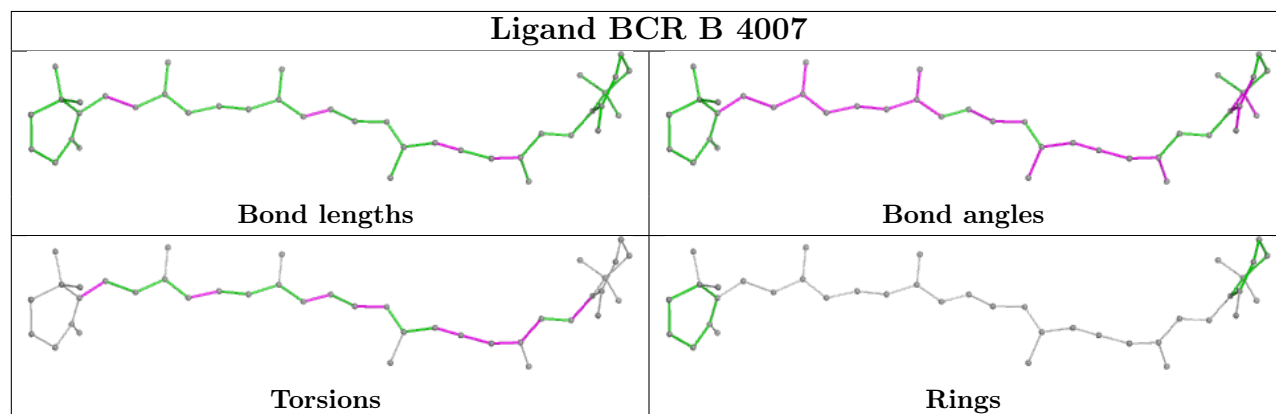




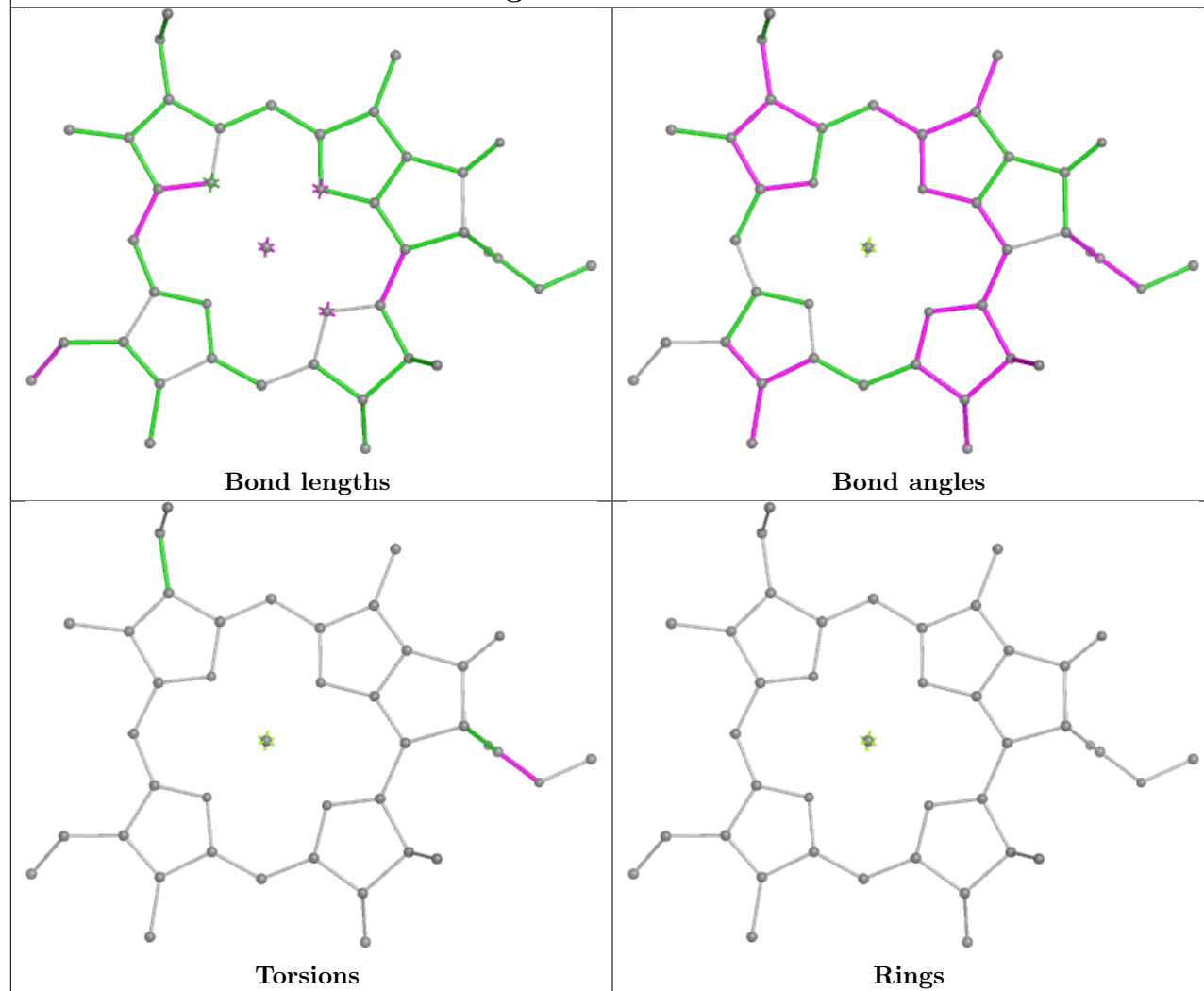
## Ligand CLA 3 608



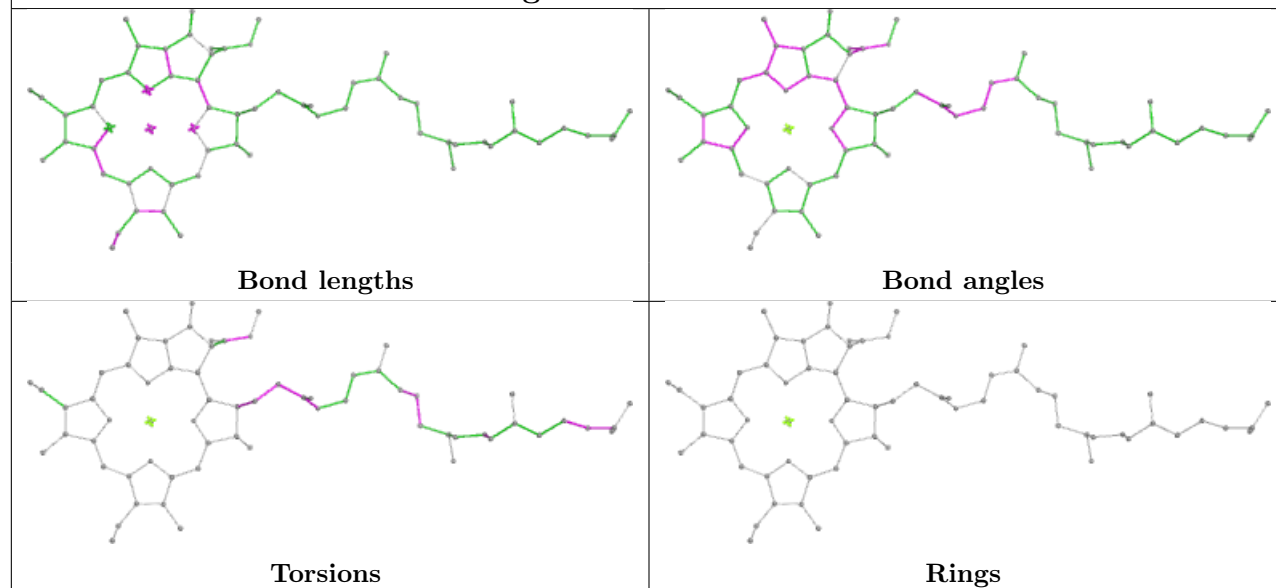
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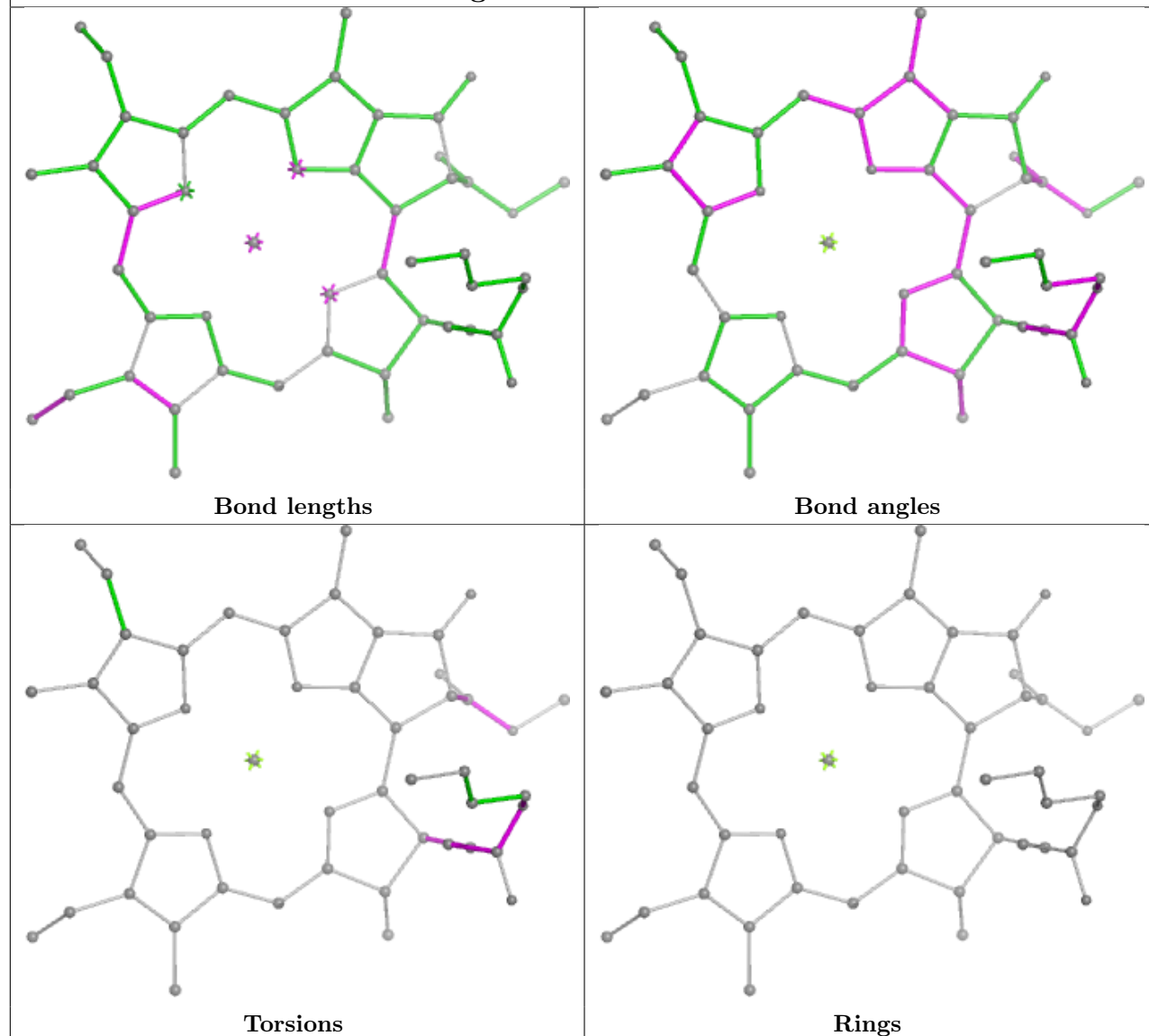
## Ligand CLA 4 615



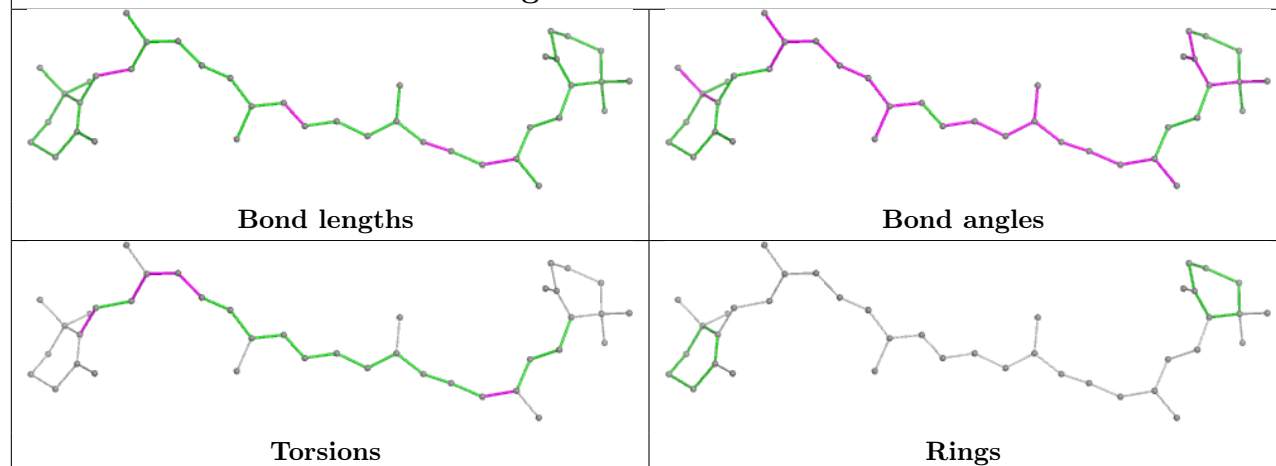
## Ligand CLA A 1131

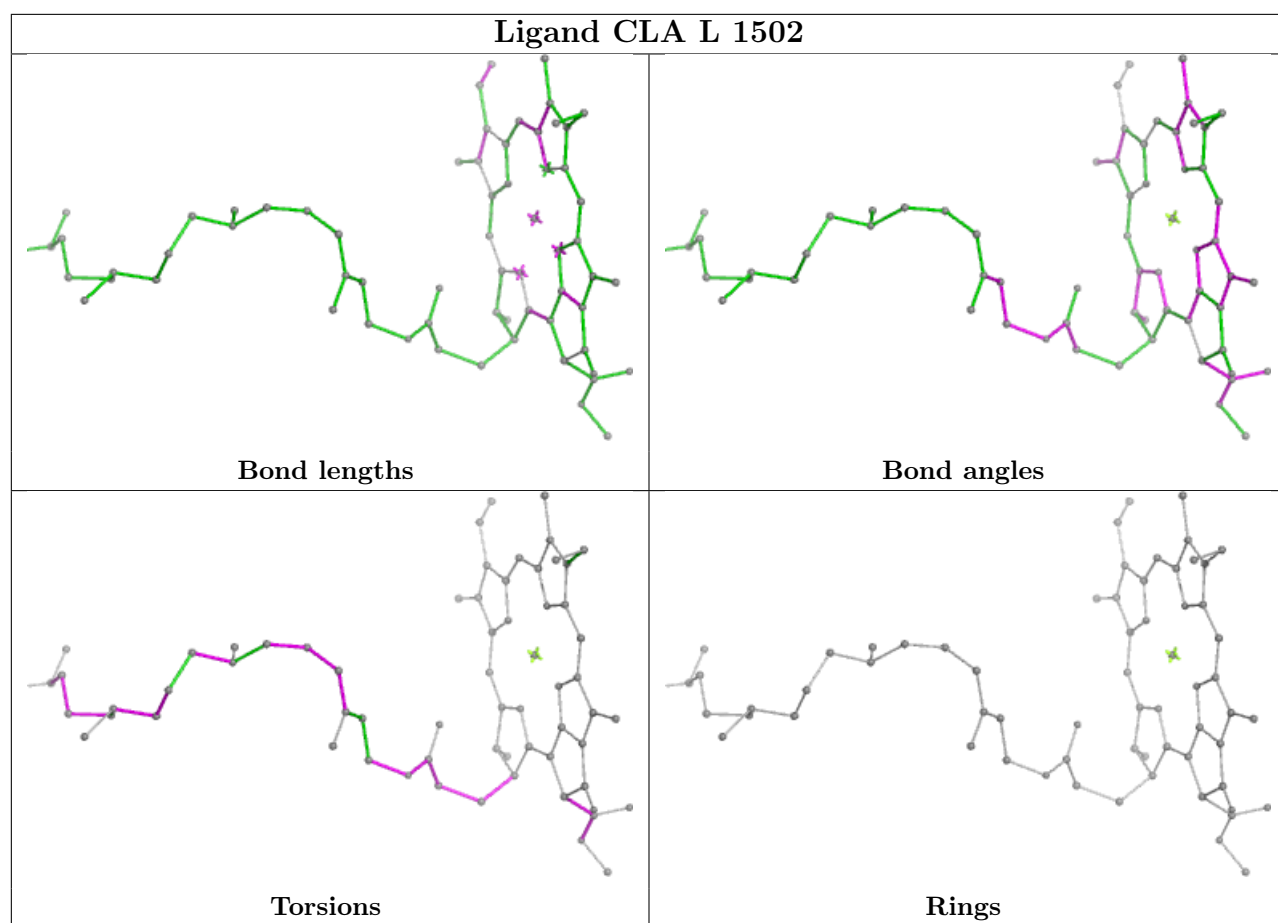


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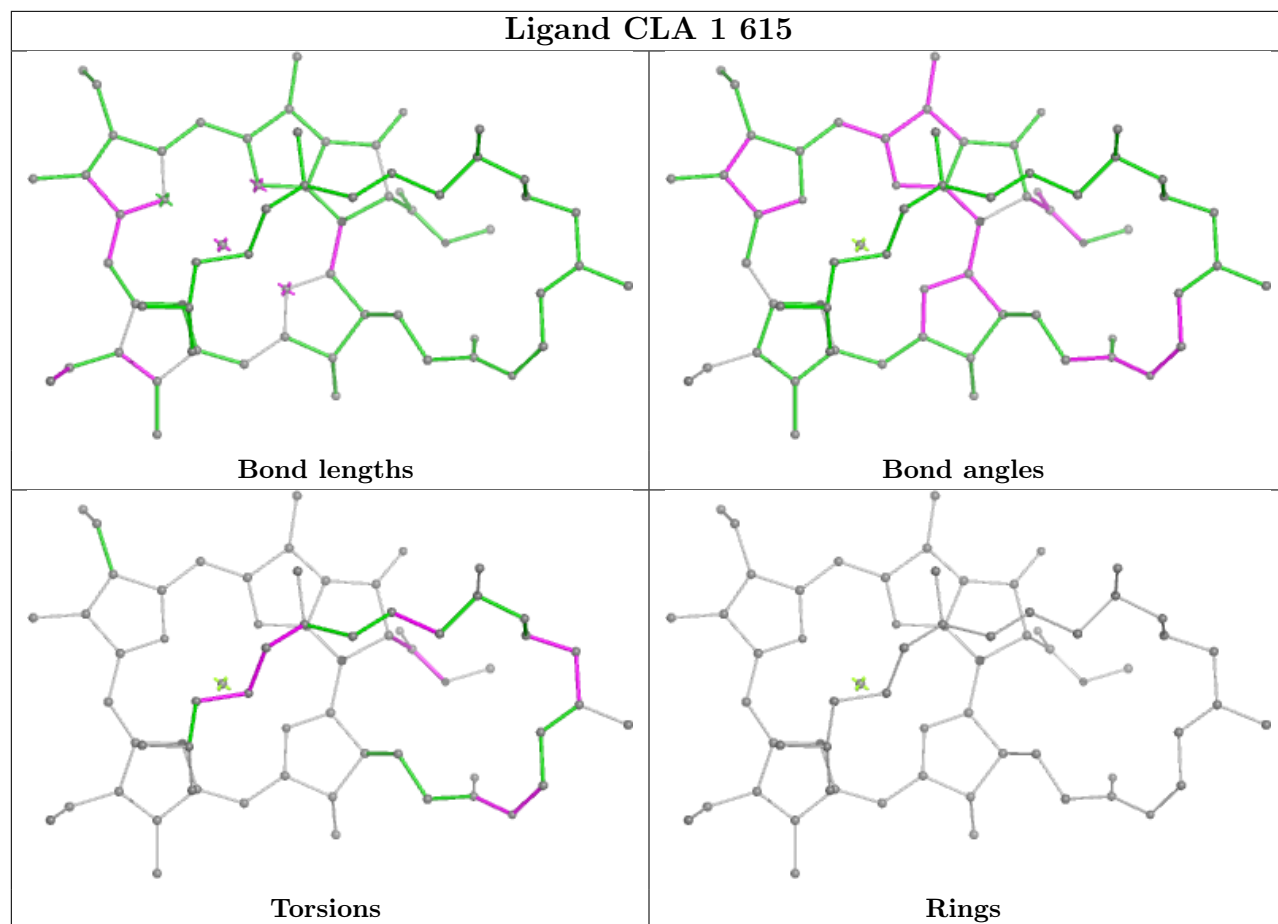


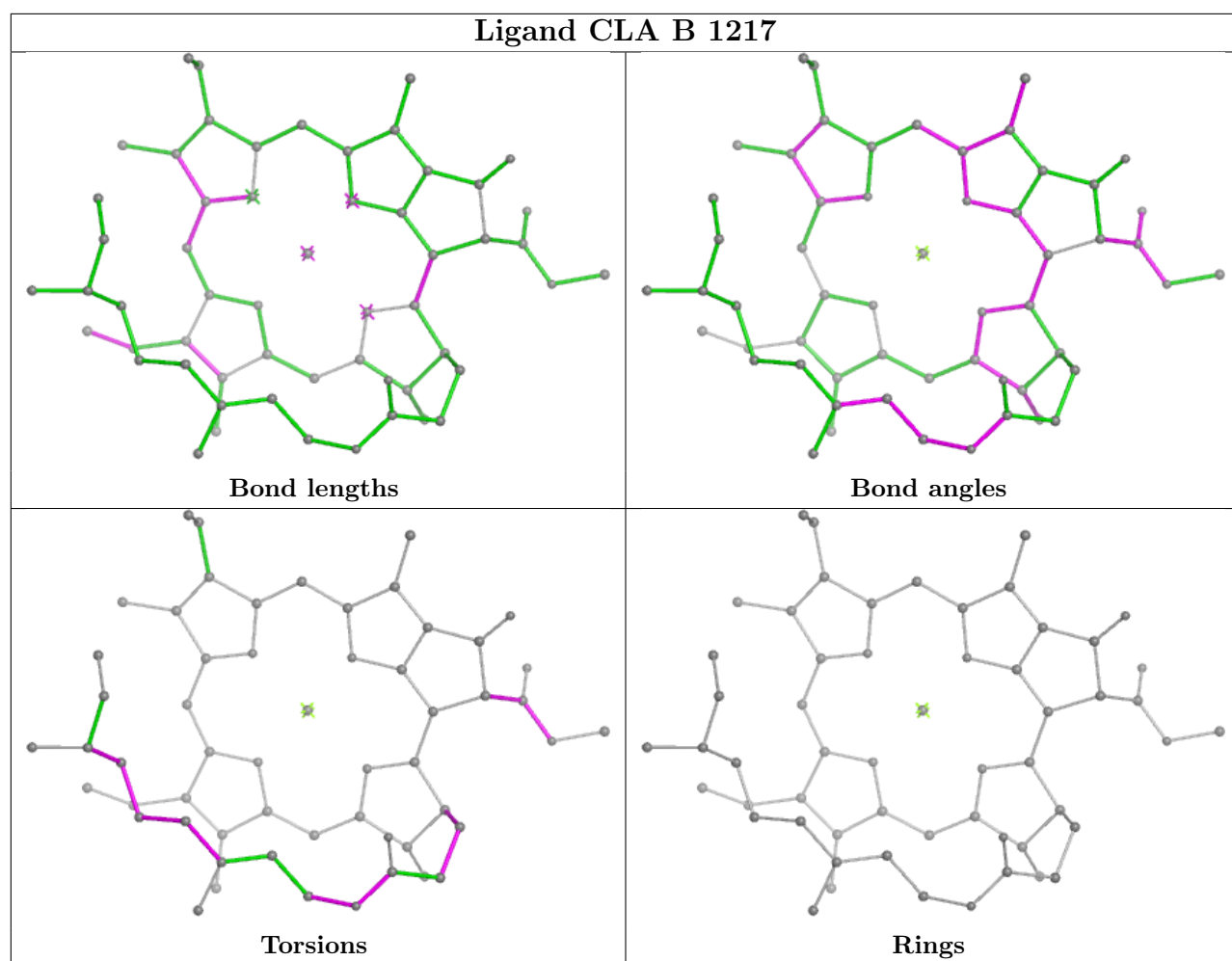
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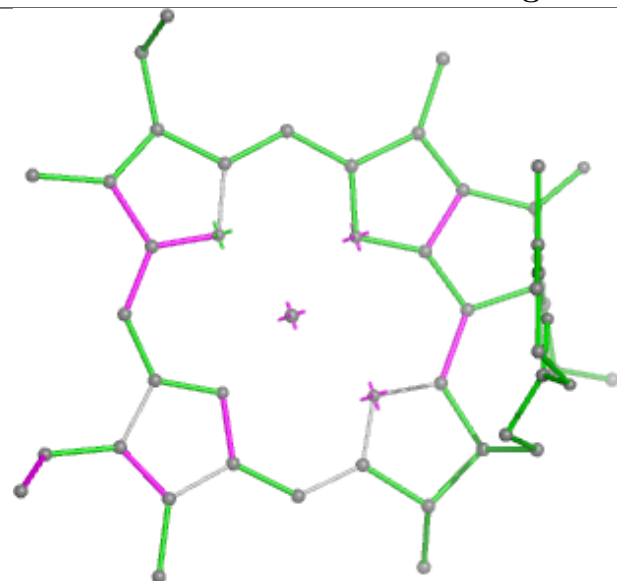


## Ligand CLA 1 615

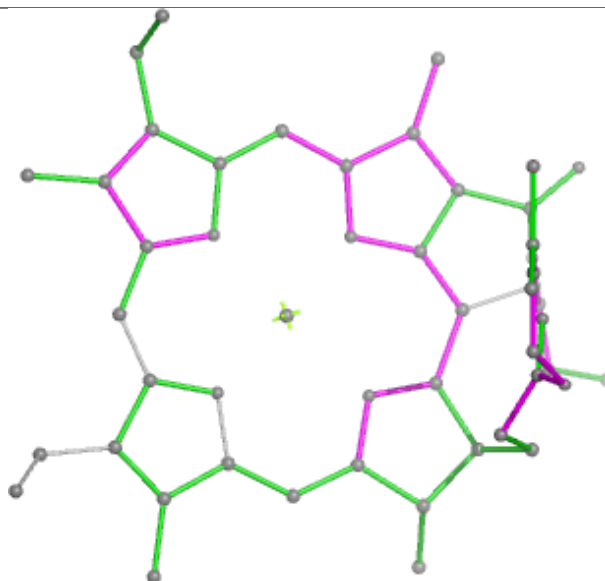




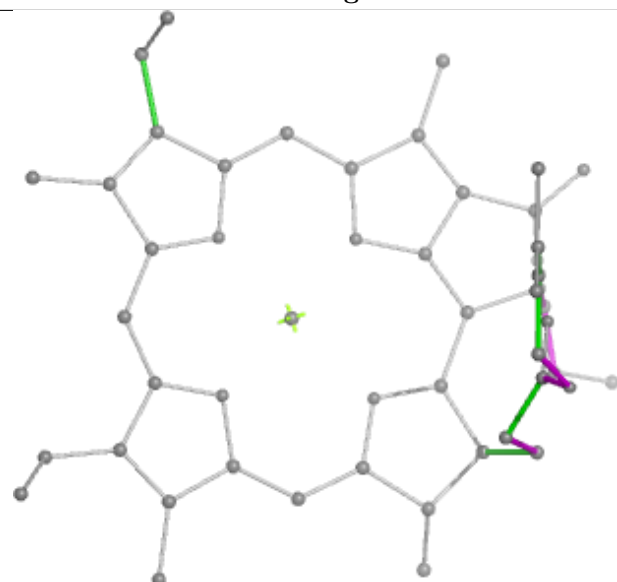
## Ligand CLA 4 606



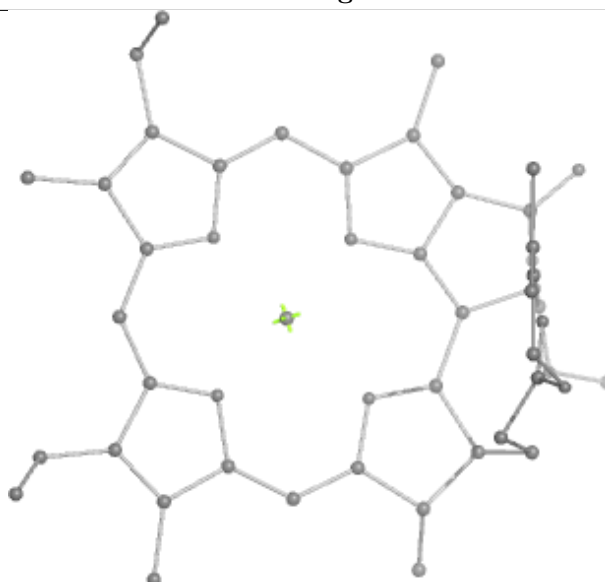
Bond lengths



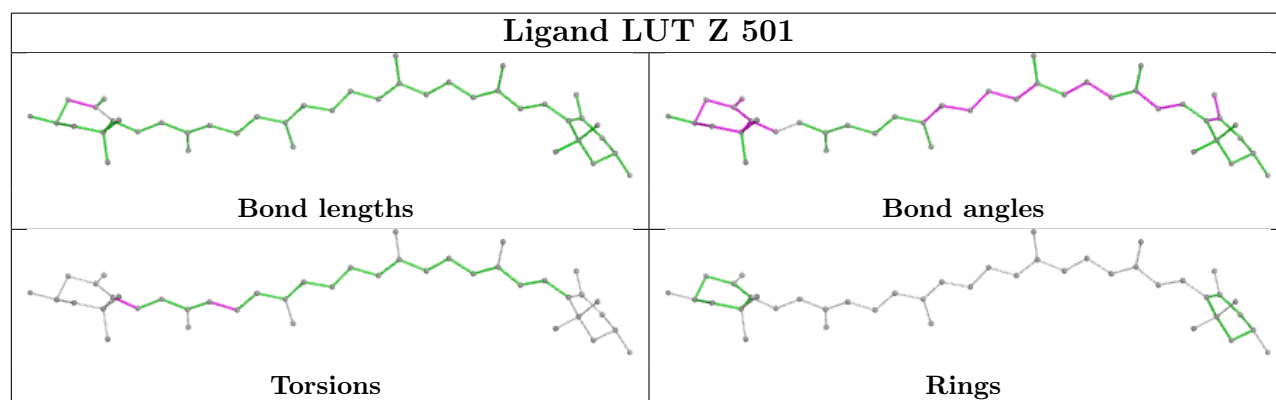
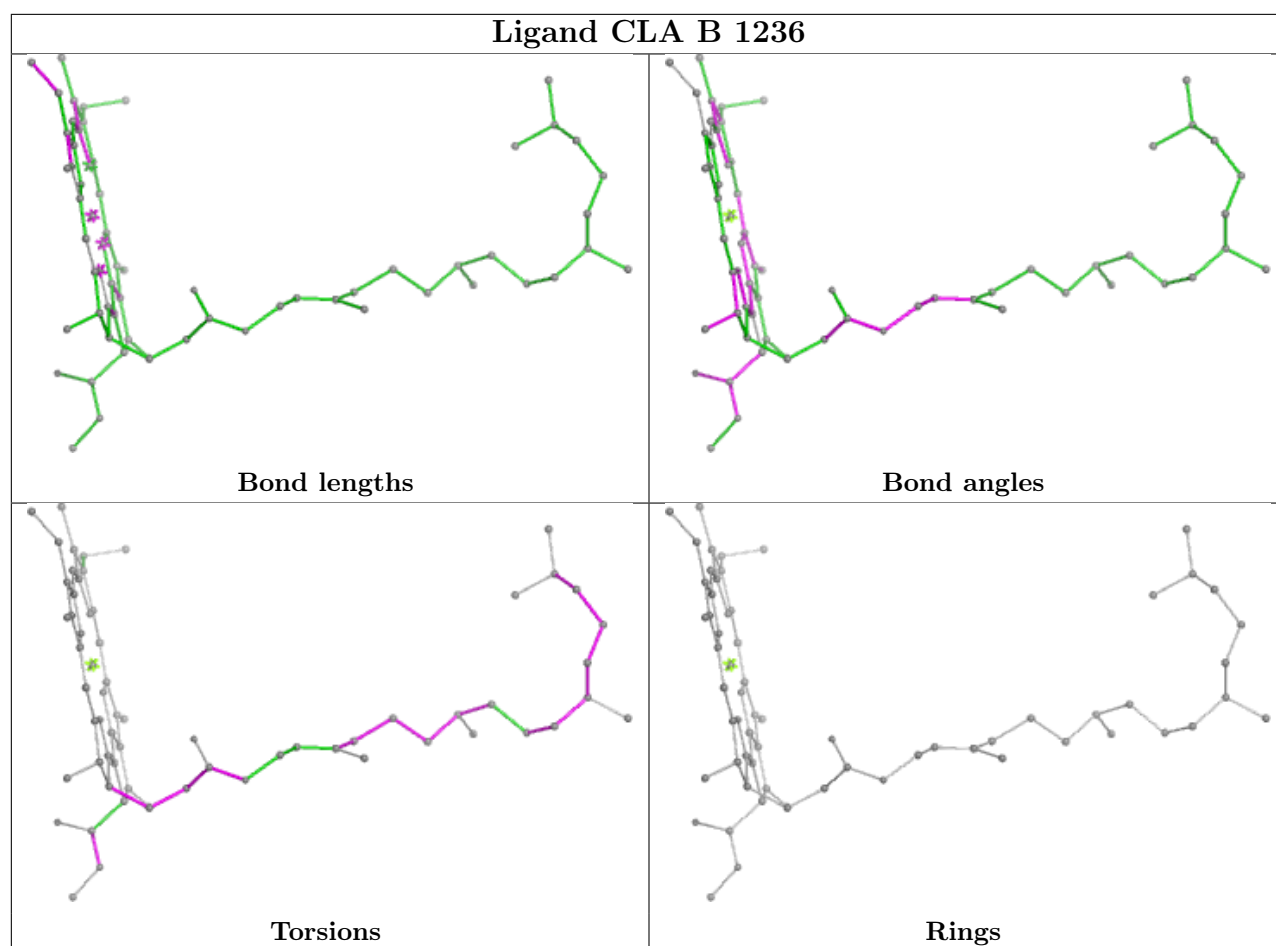
Bond angles



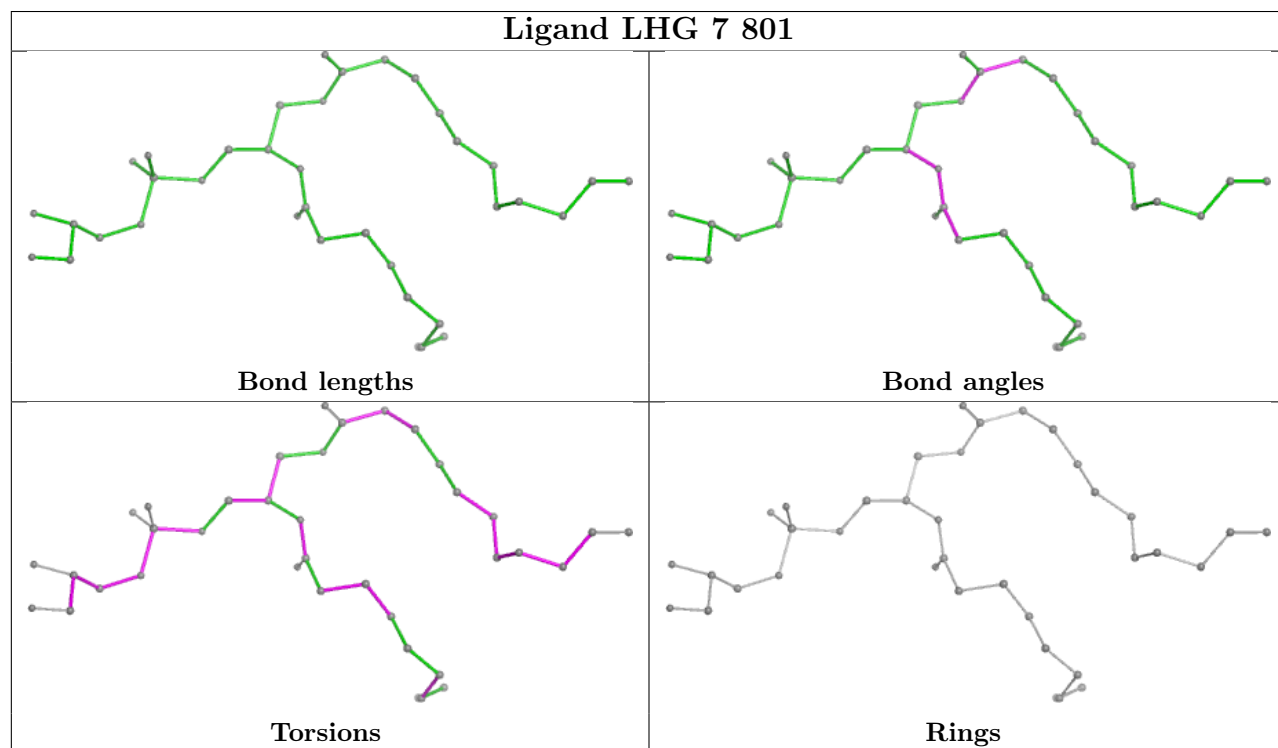
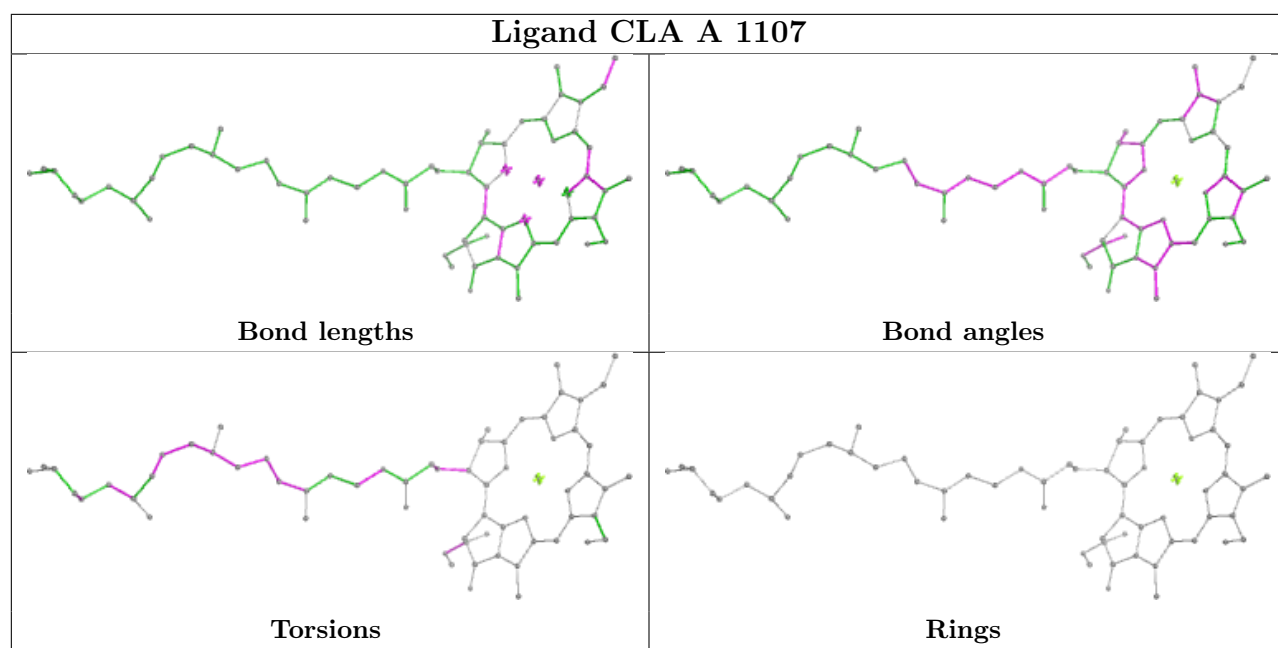
Torsions

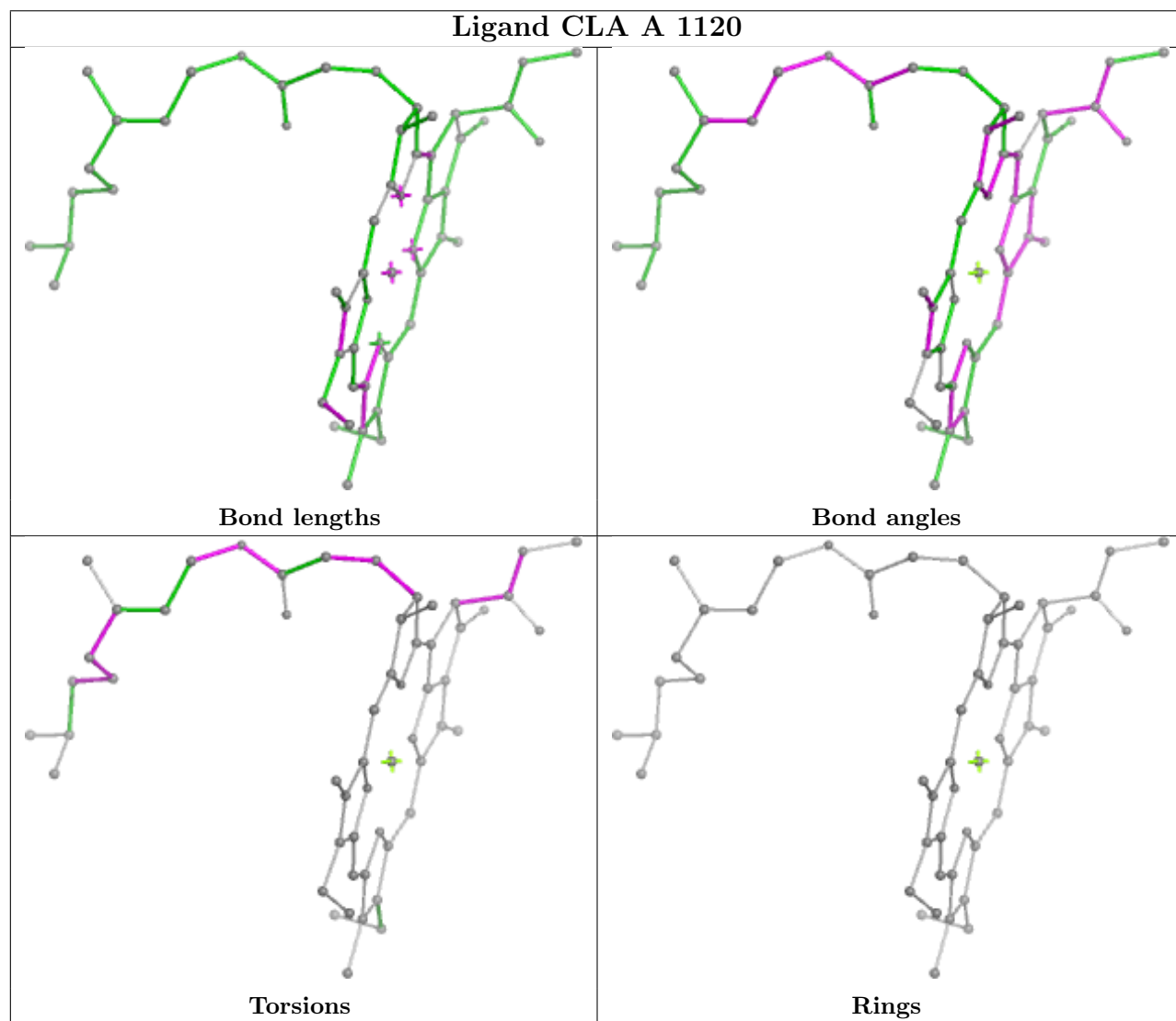
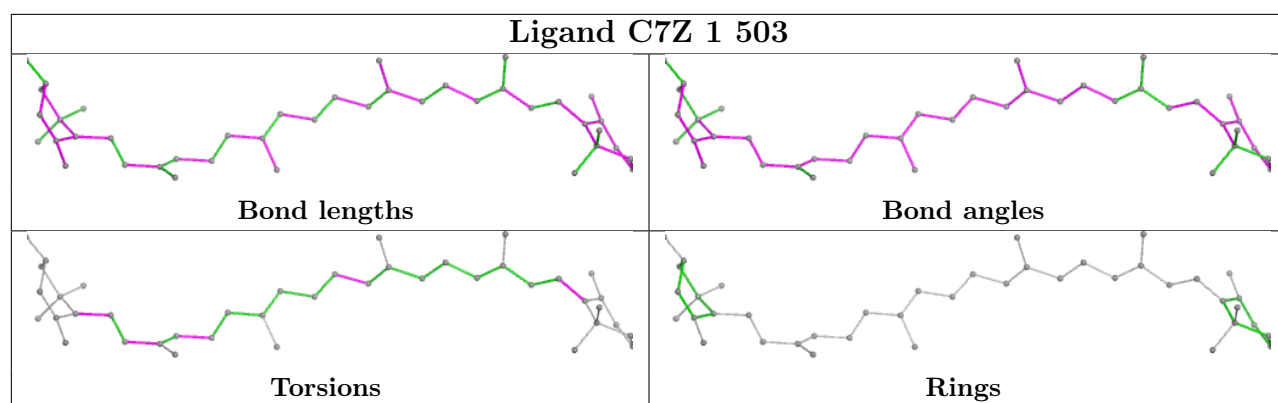


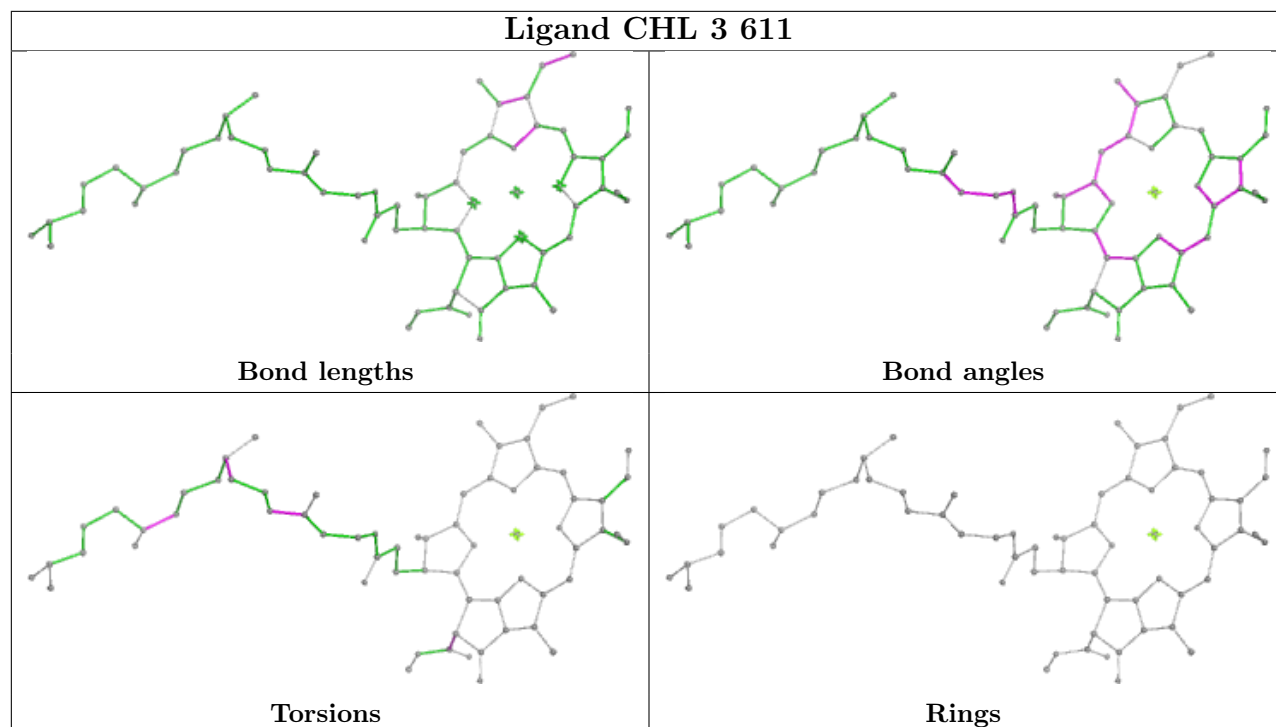
Rings

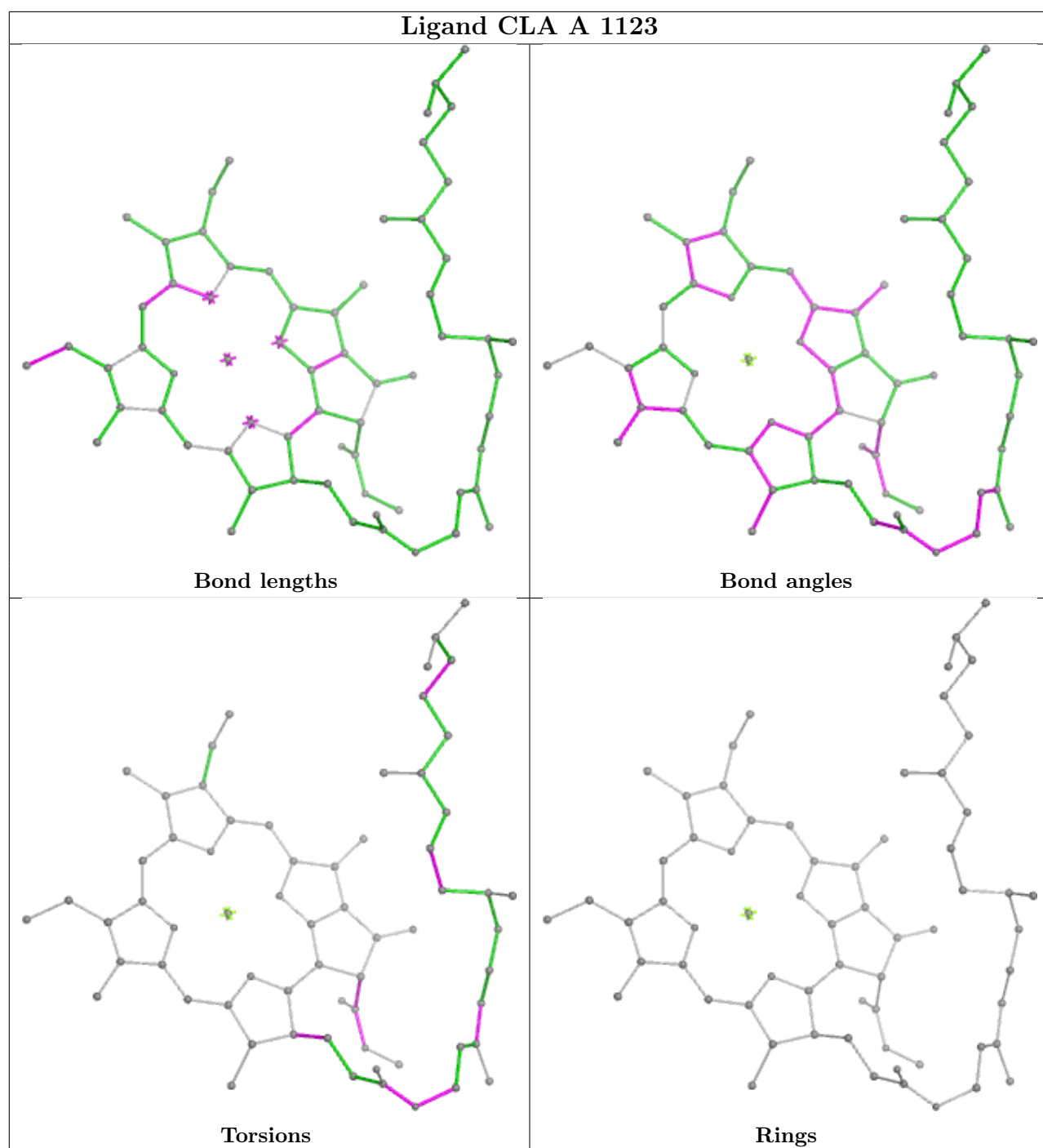


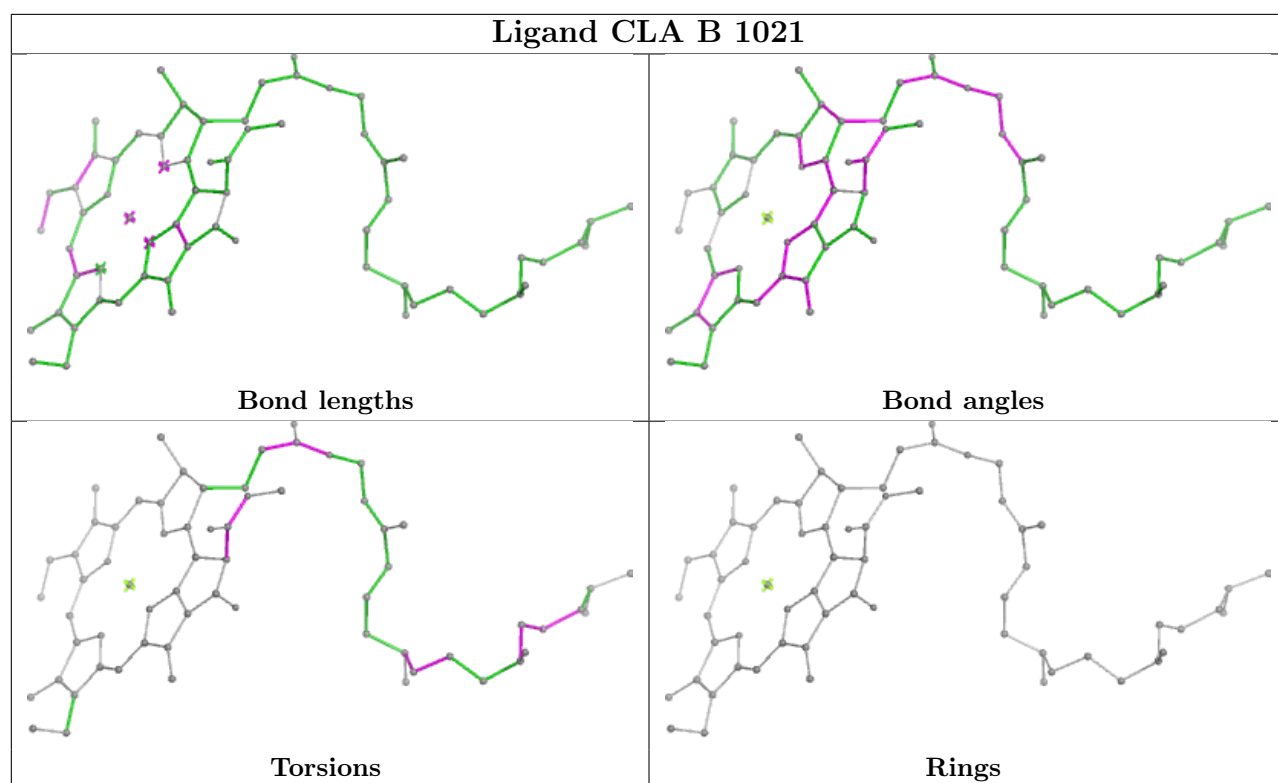


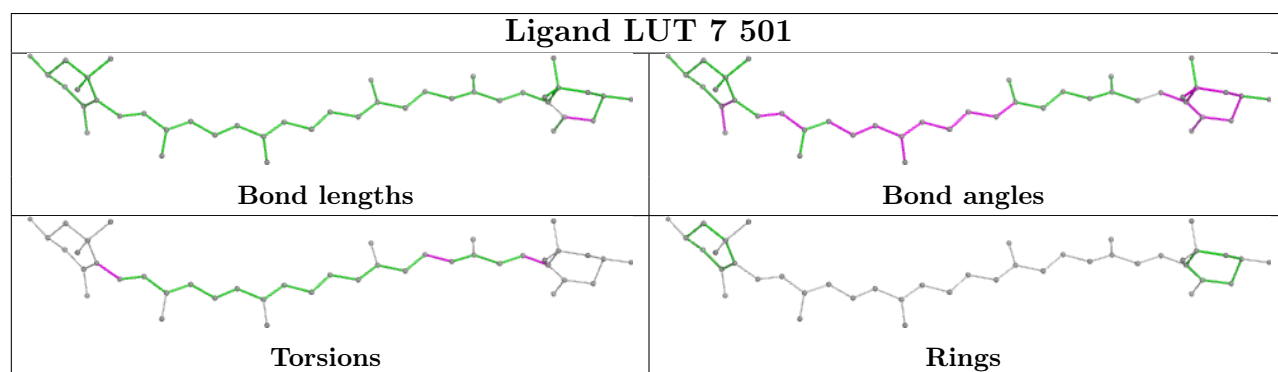
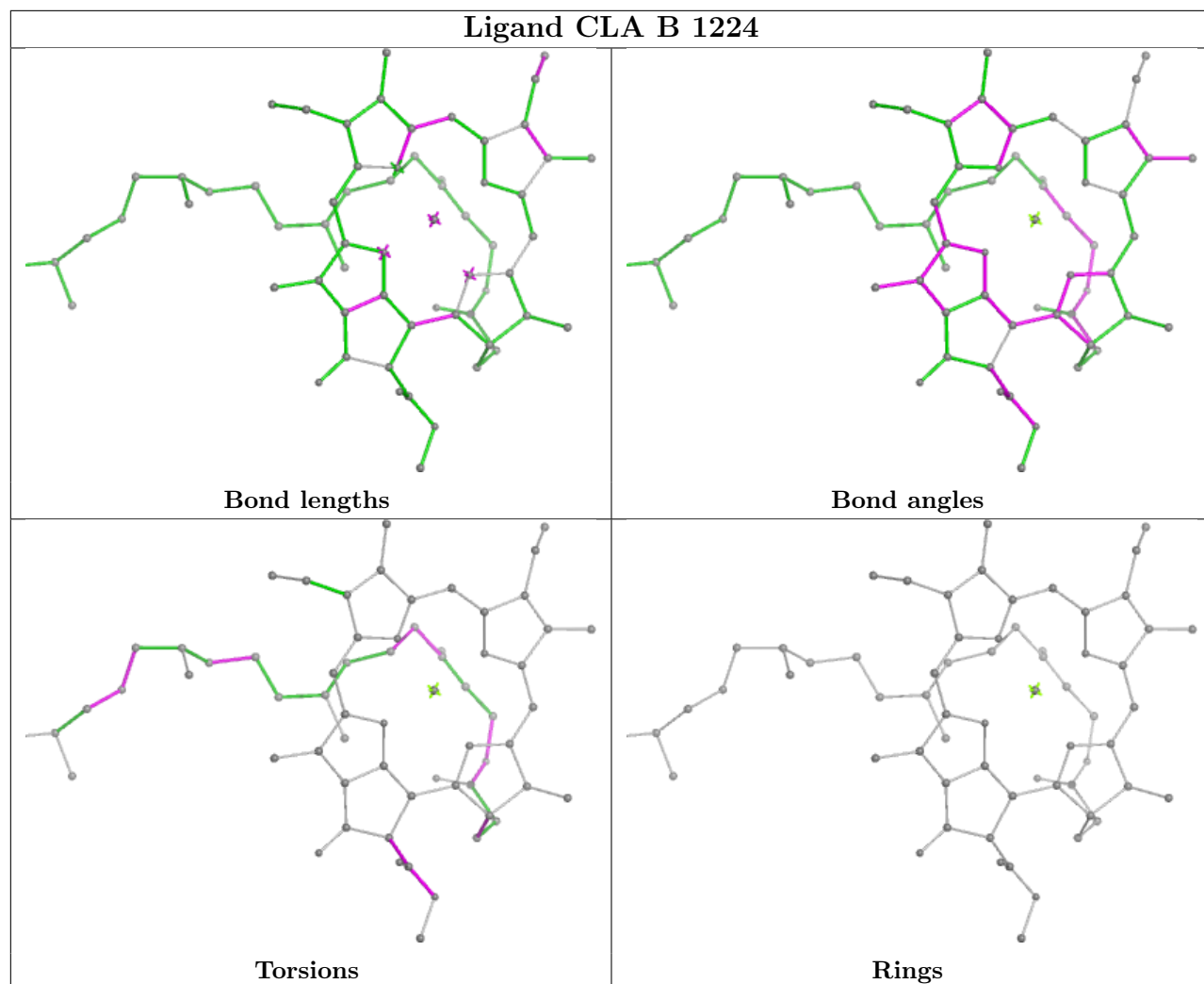




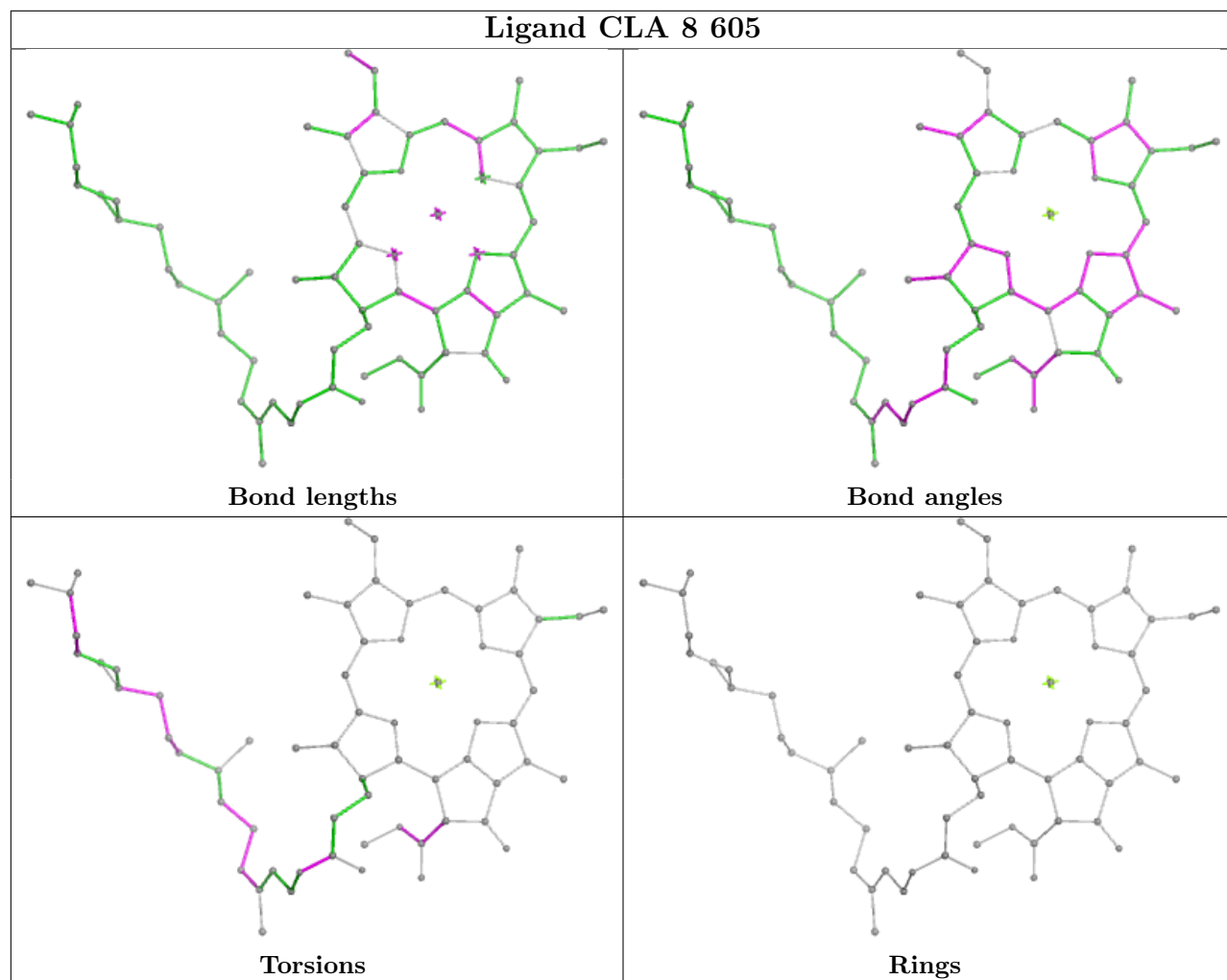


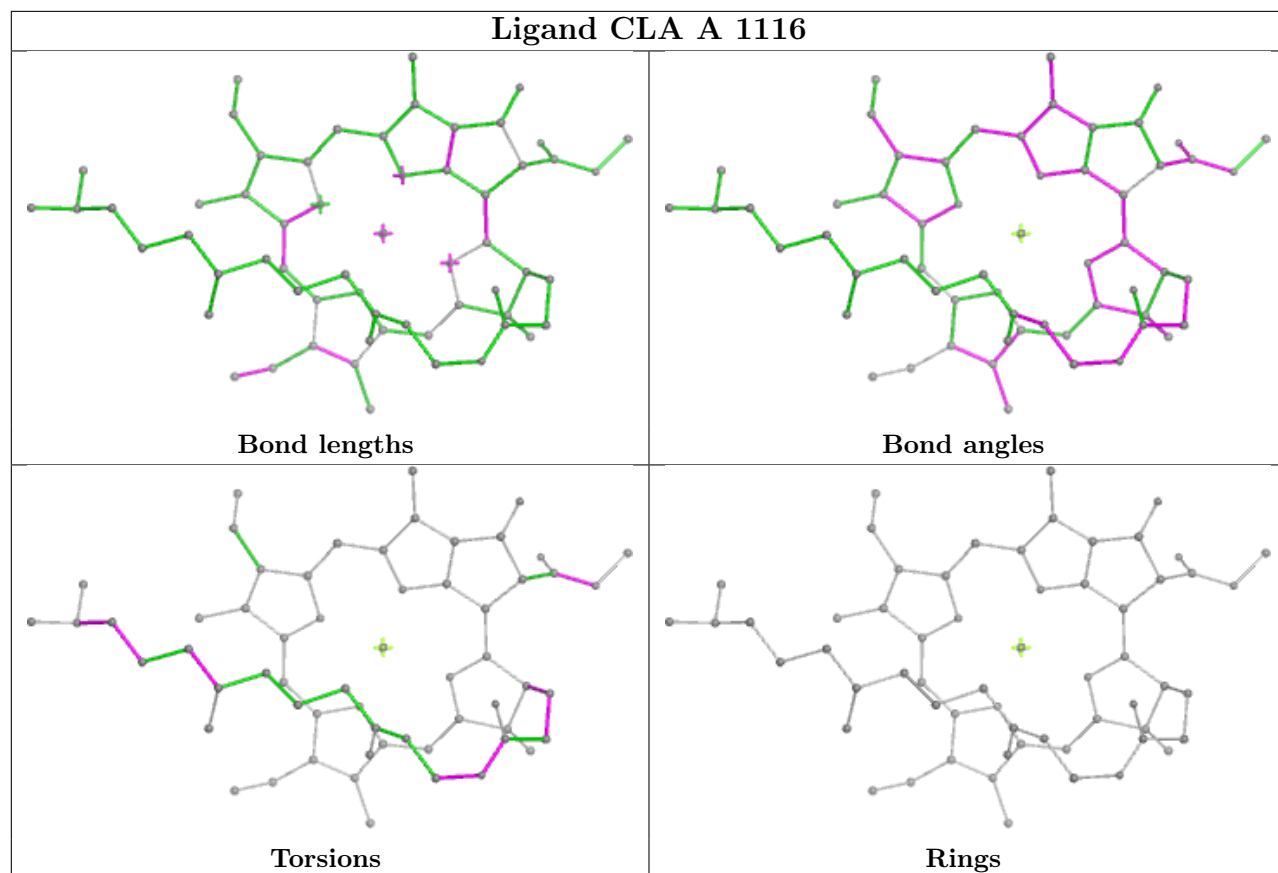






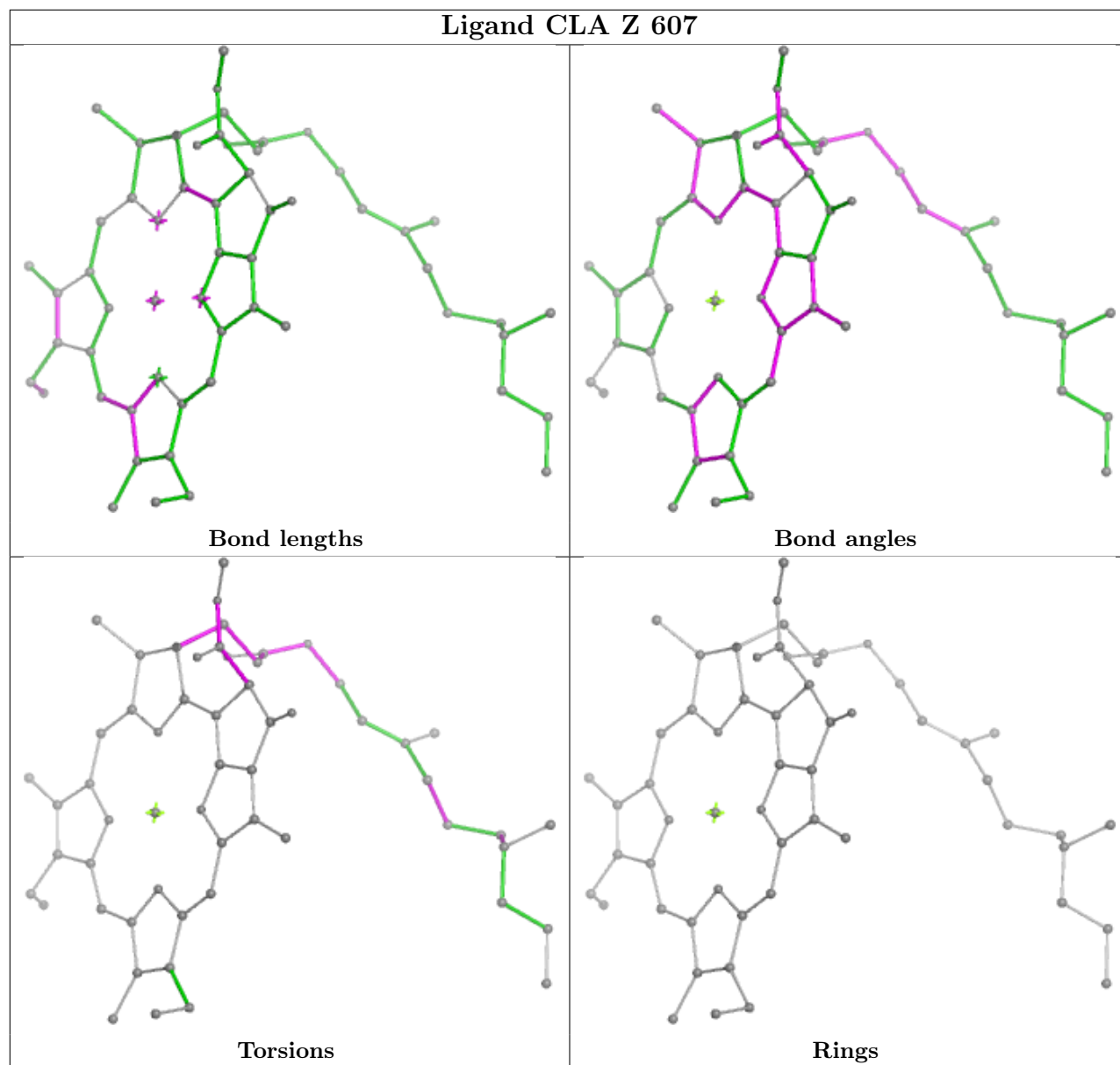
## Ligand CLA 8 605

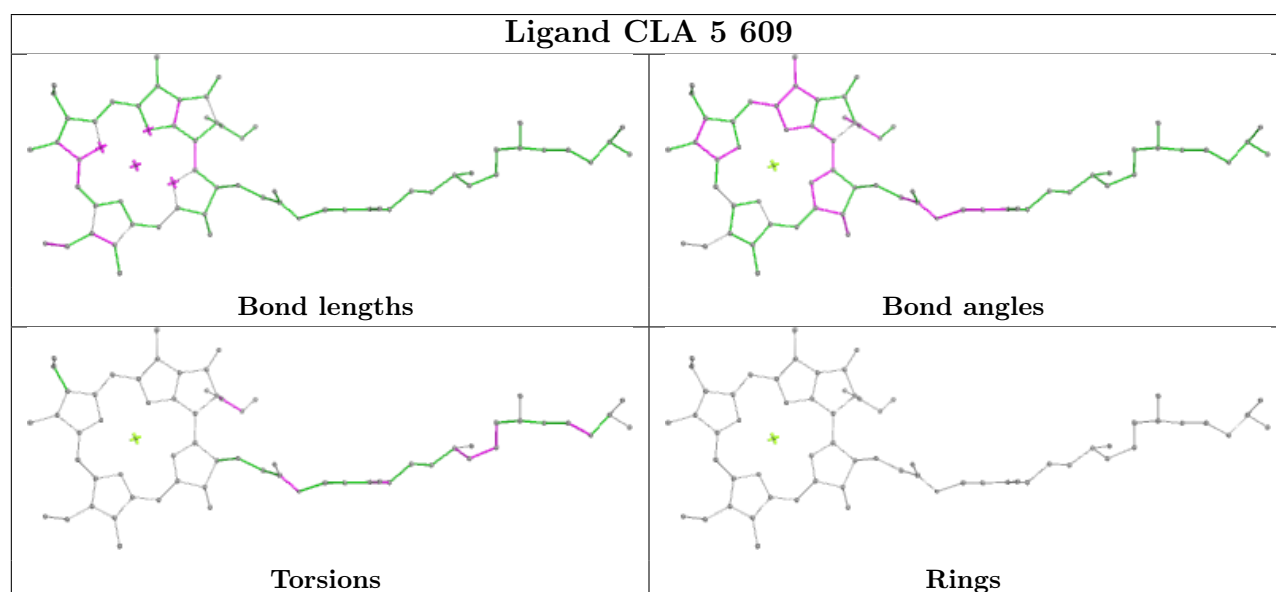
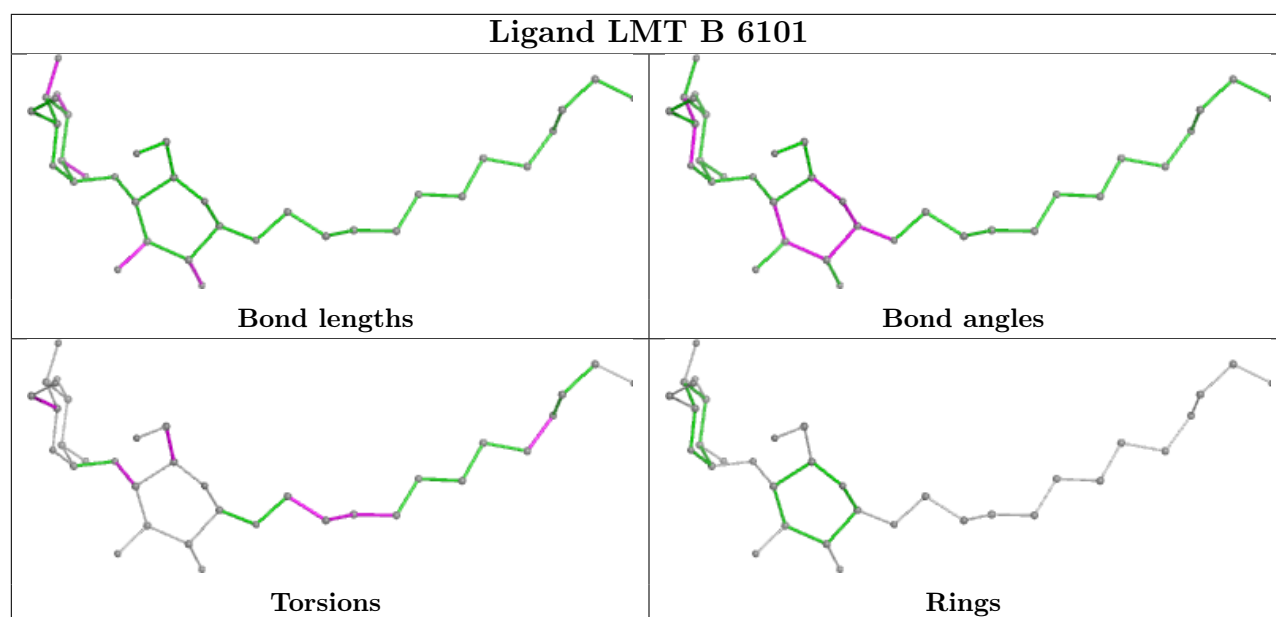




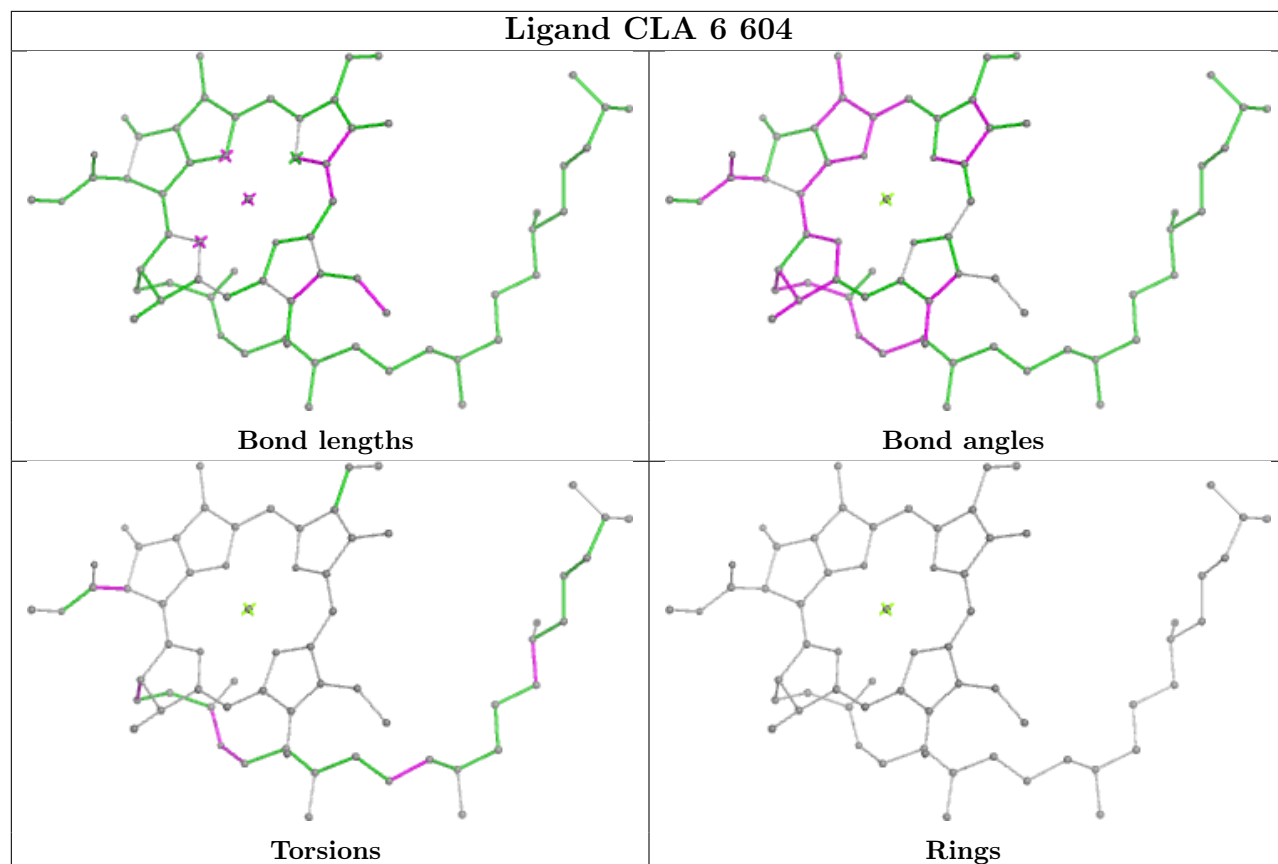


## Ligand CLA Z 607

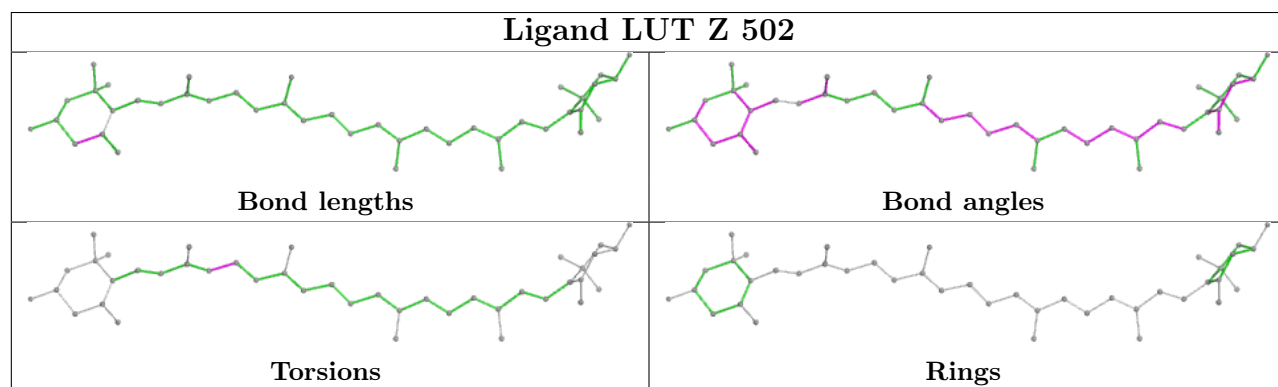




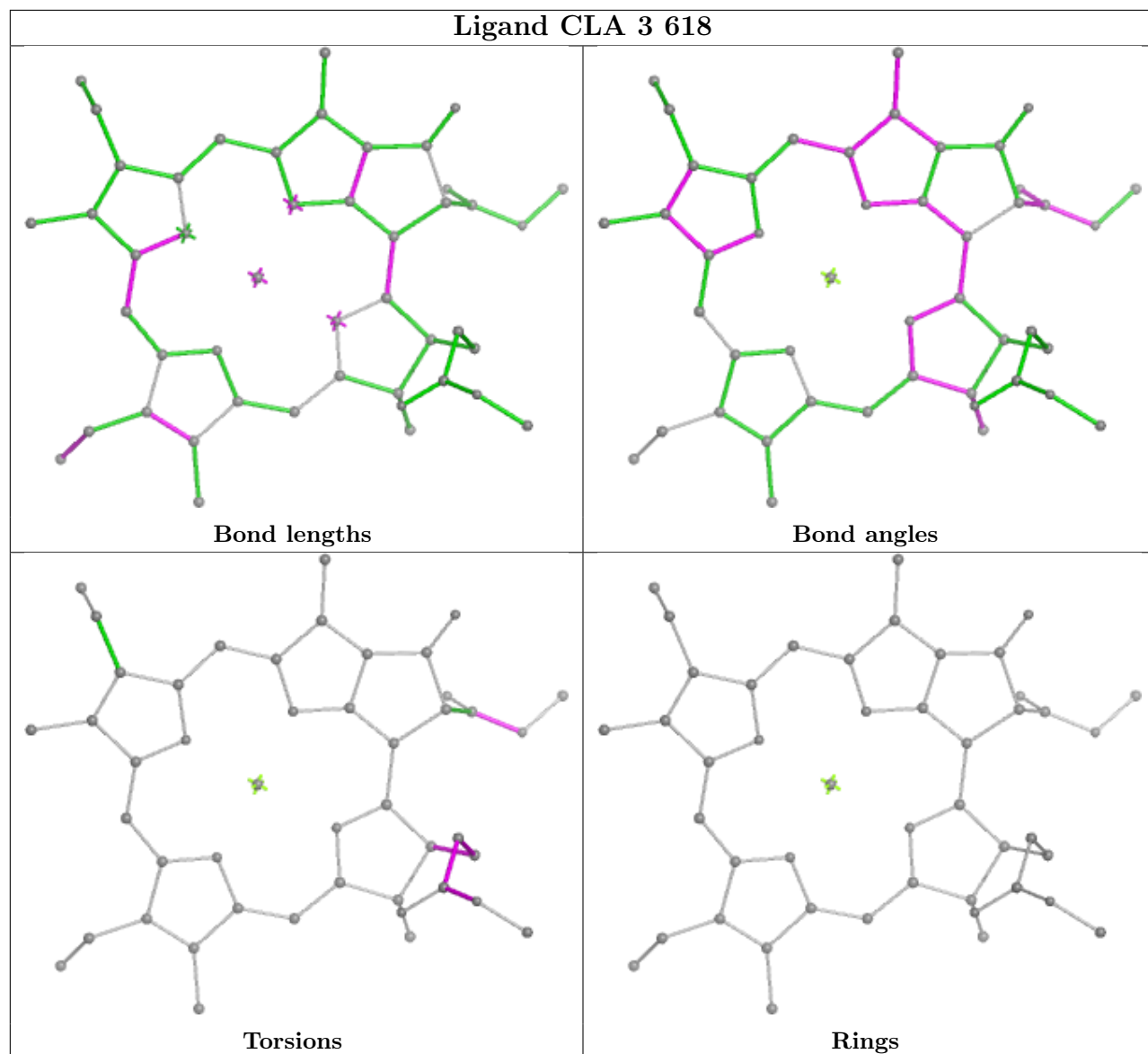
## Ligand CLA 6 604



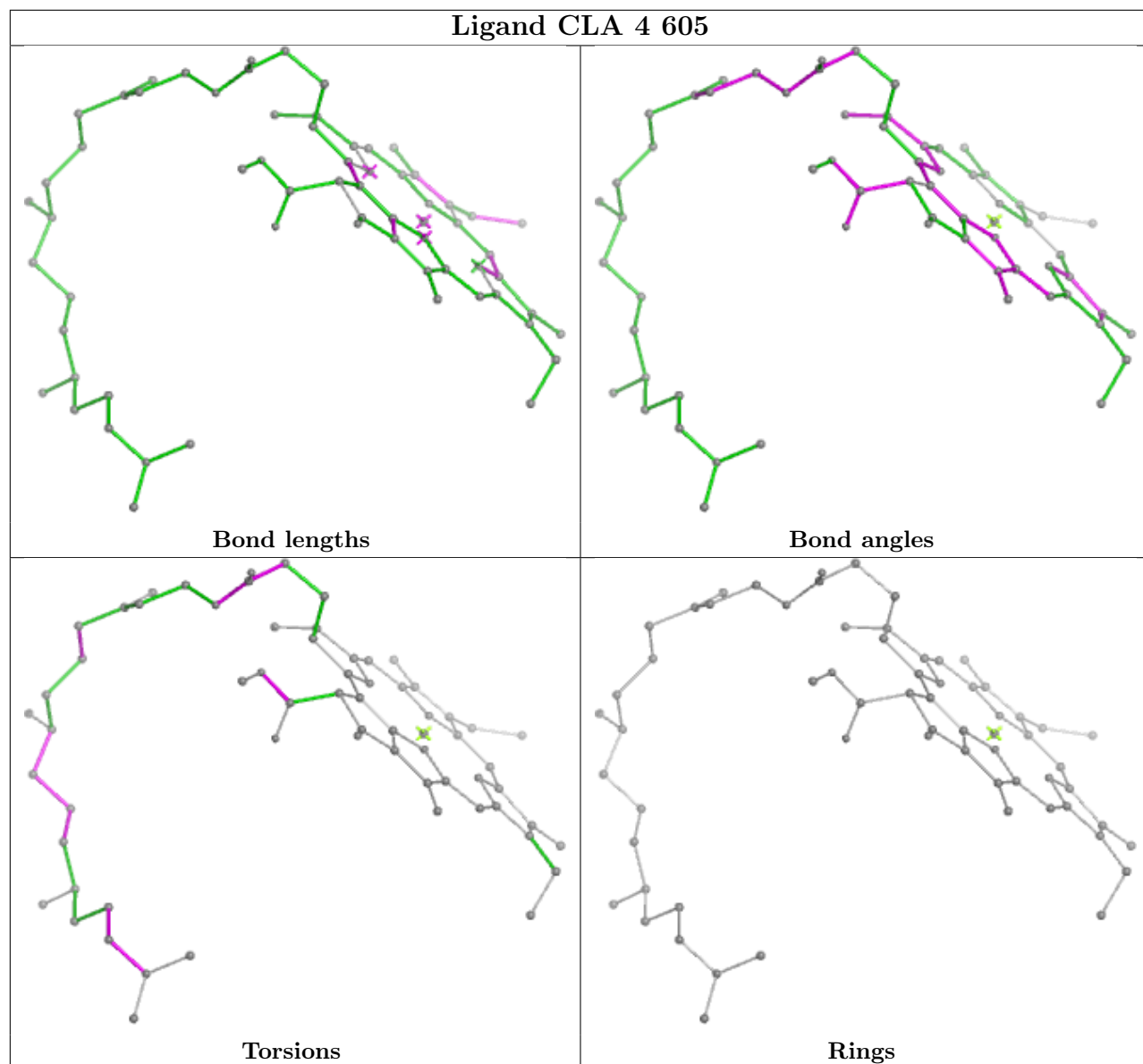
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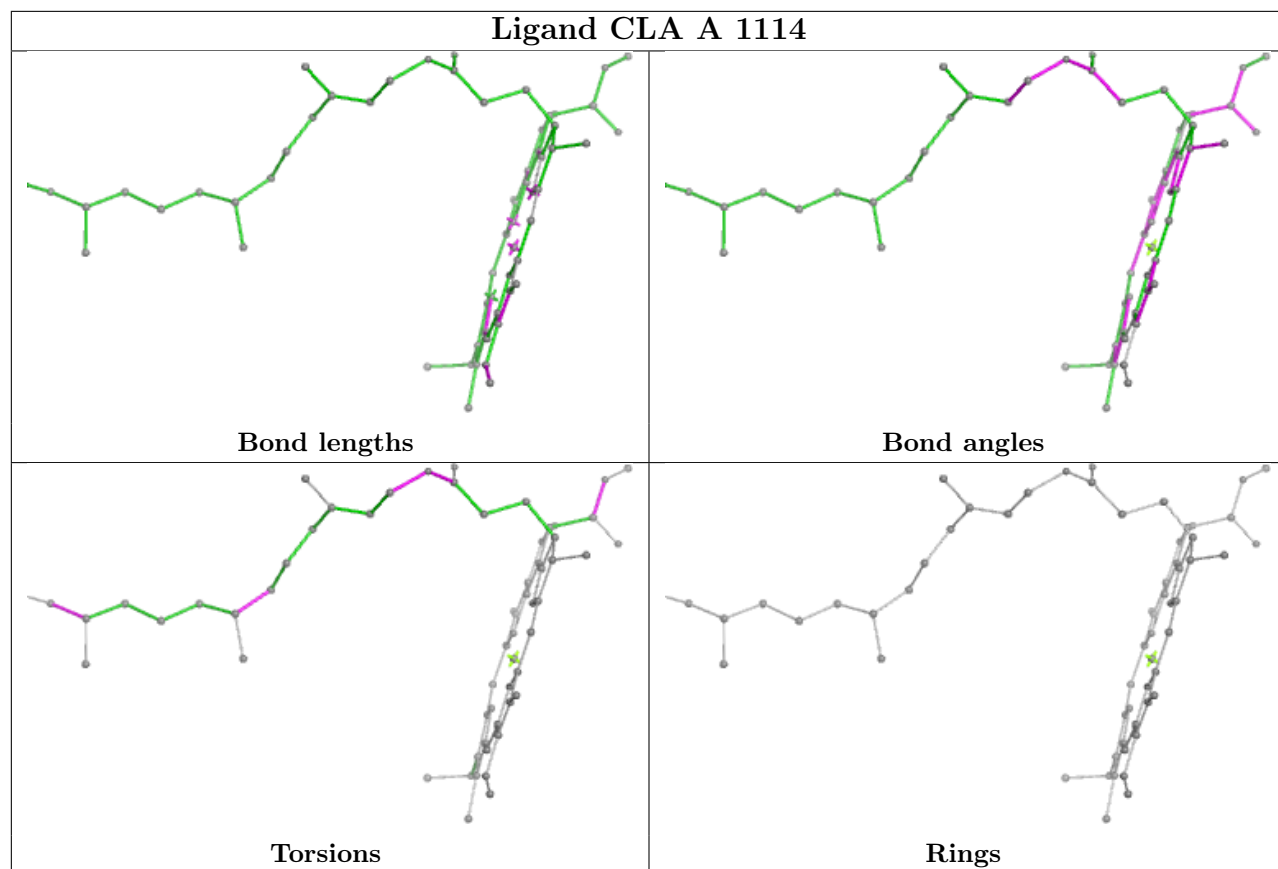


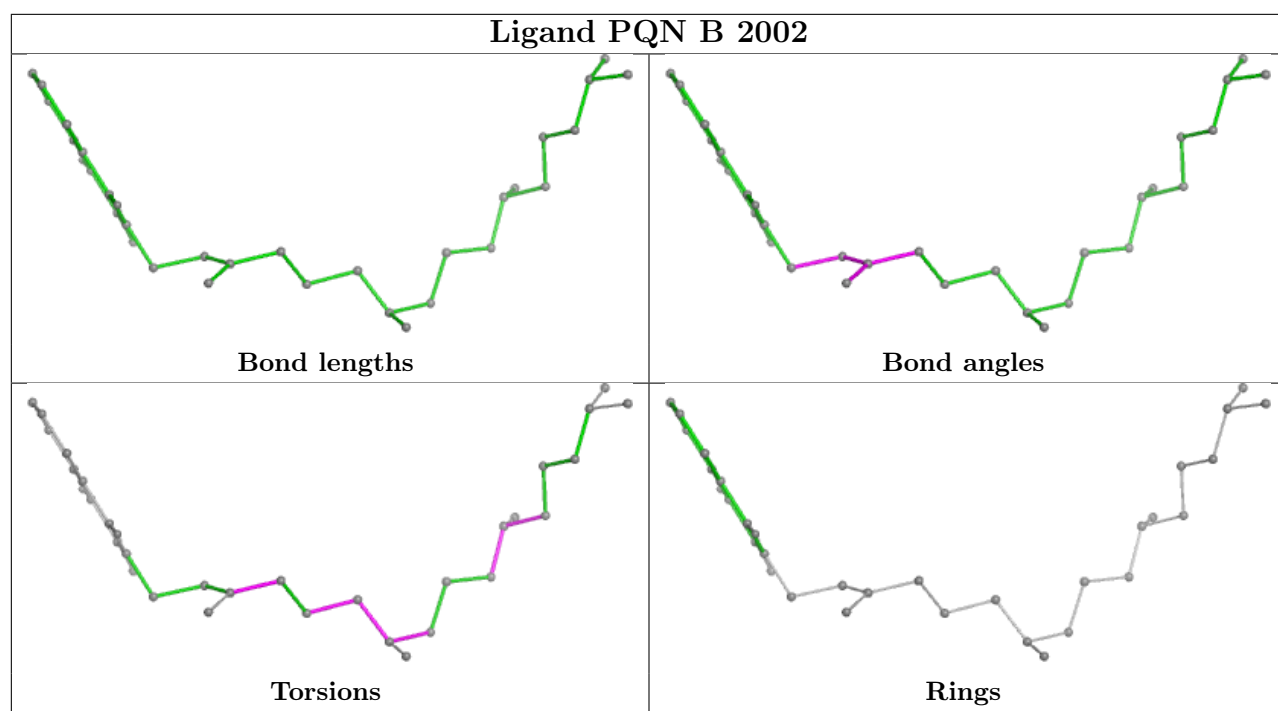
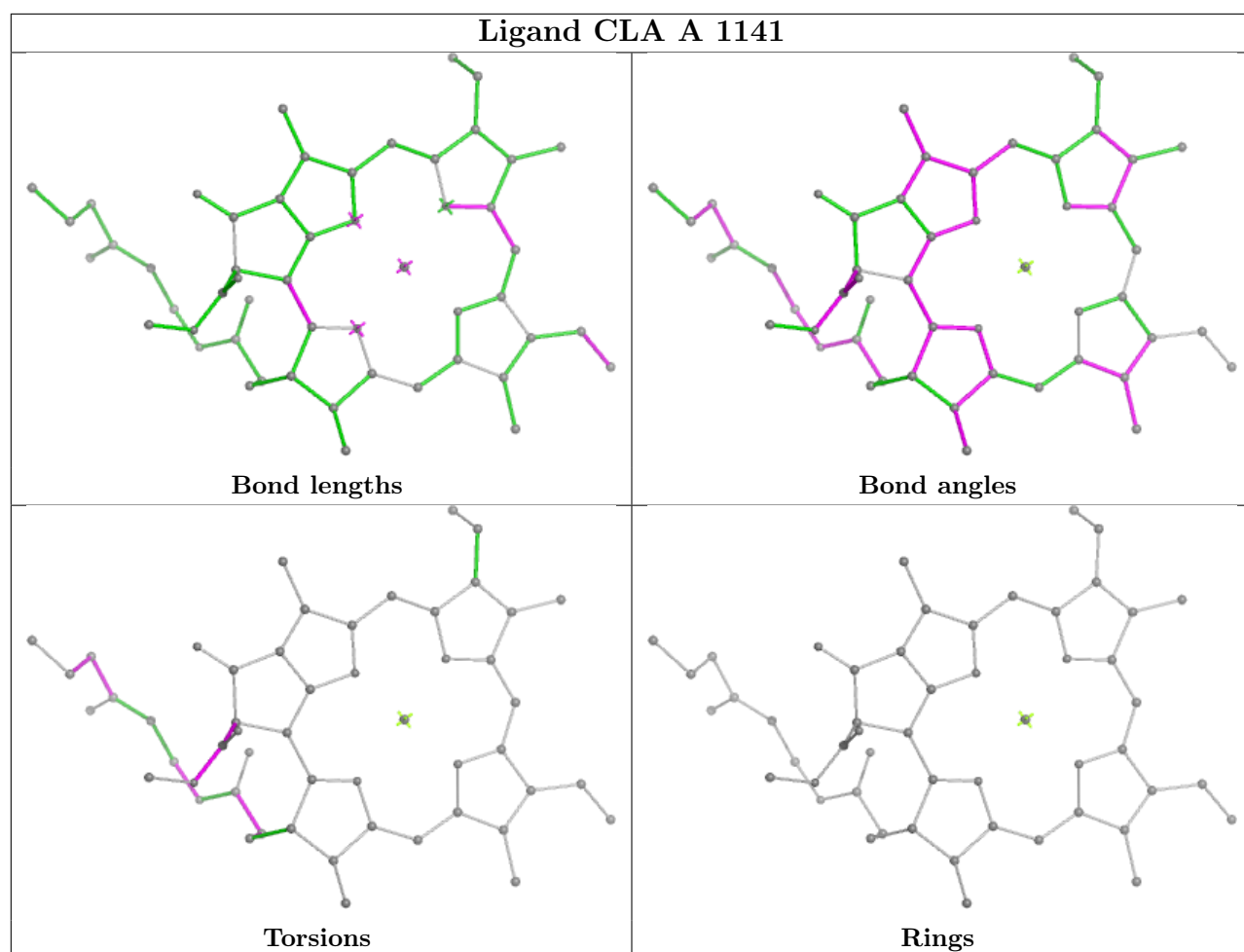
## Ligand CLA 3 618

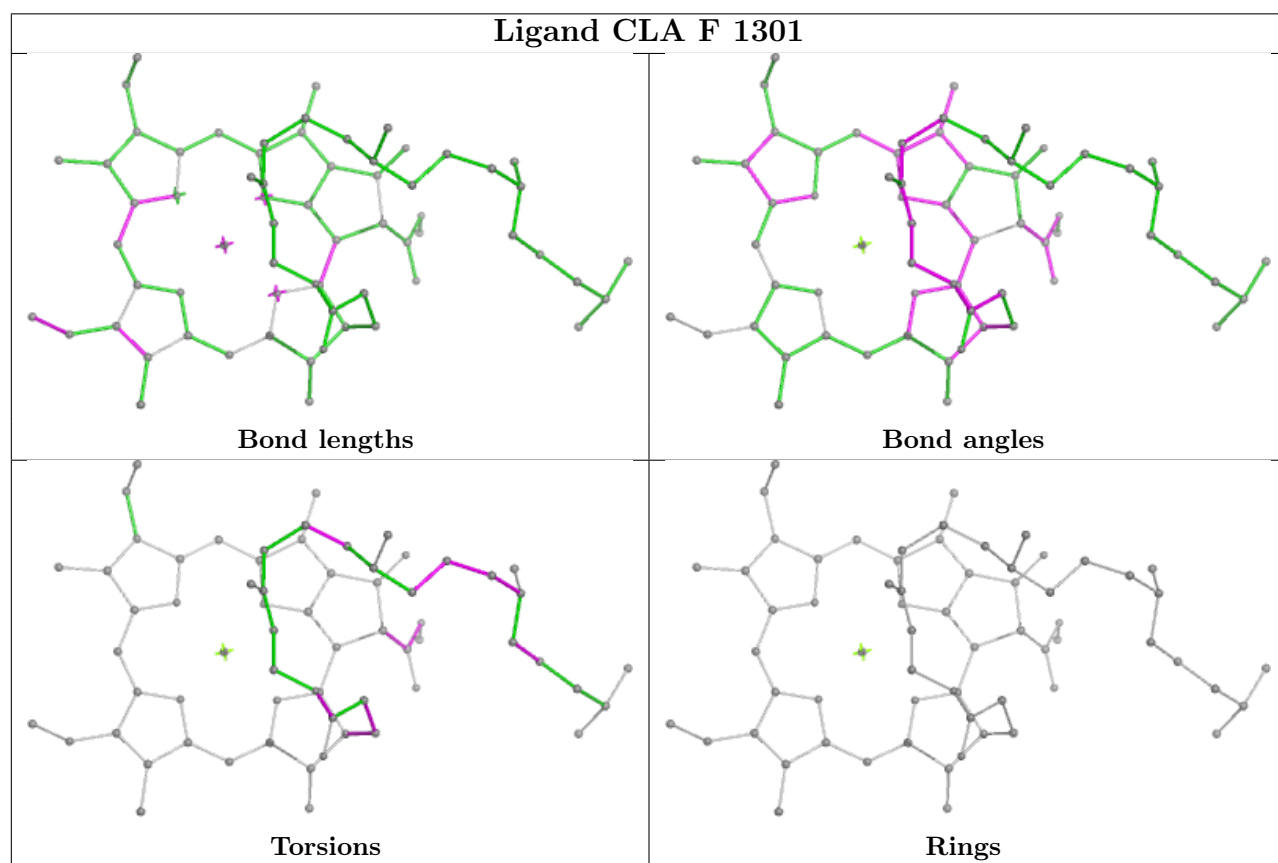
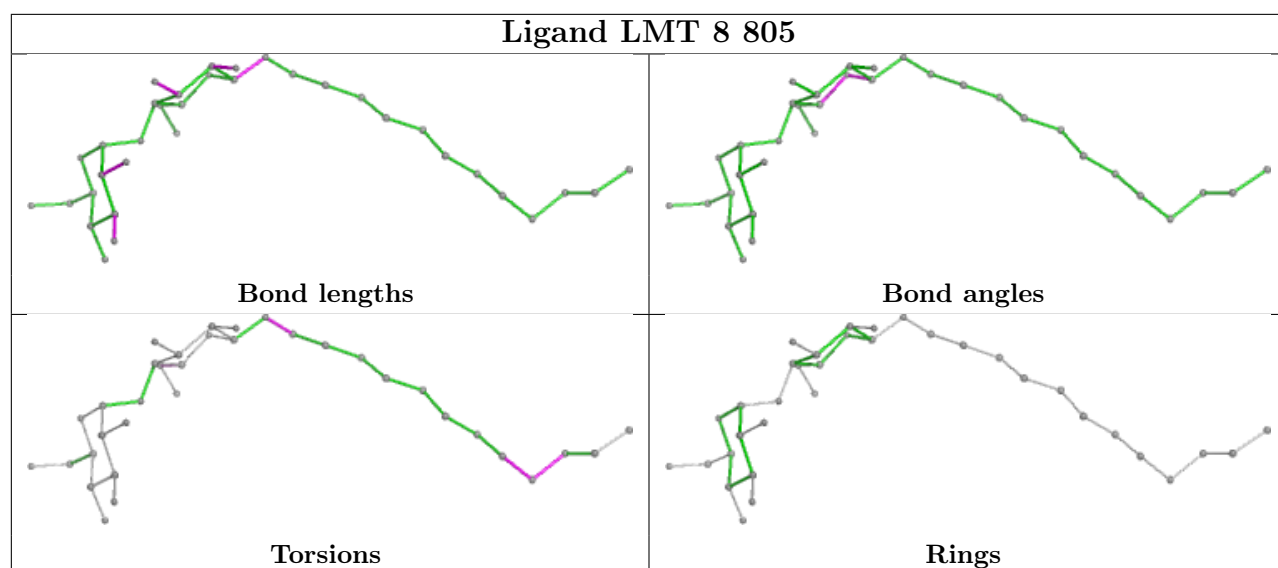


## Ligand CLA 4 605

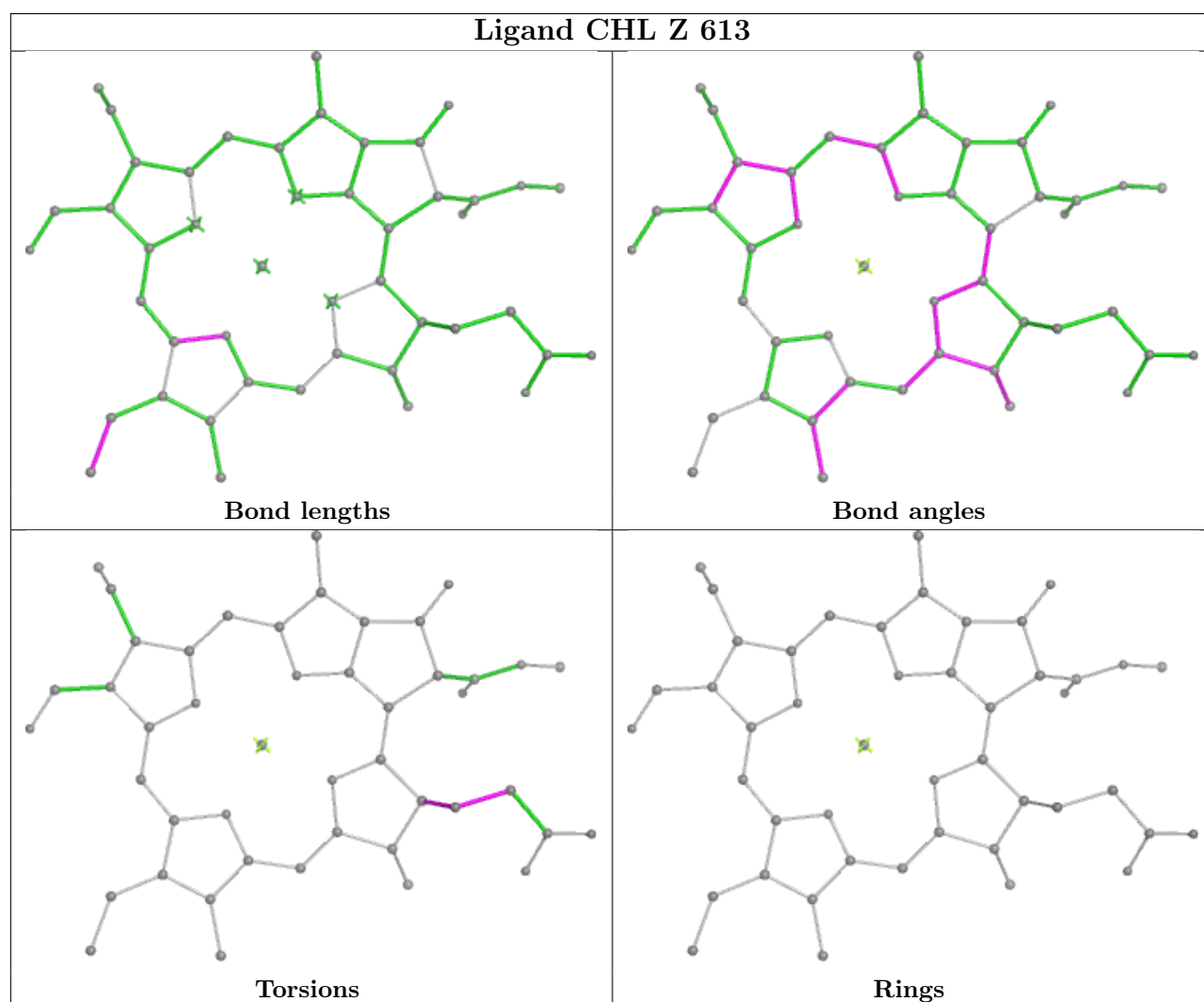
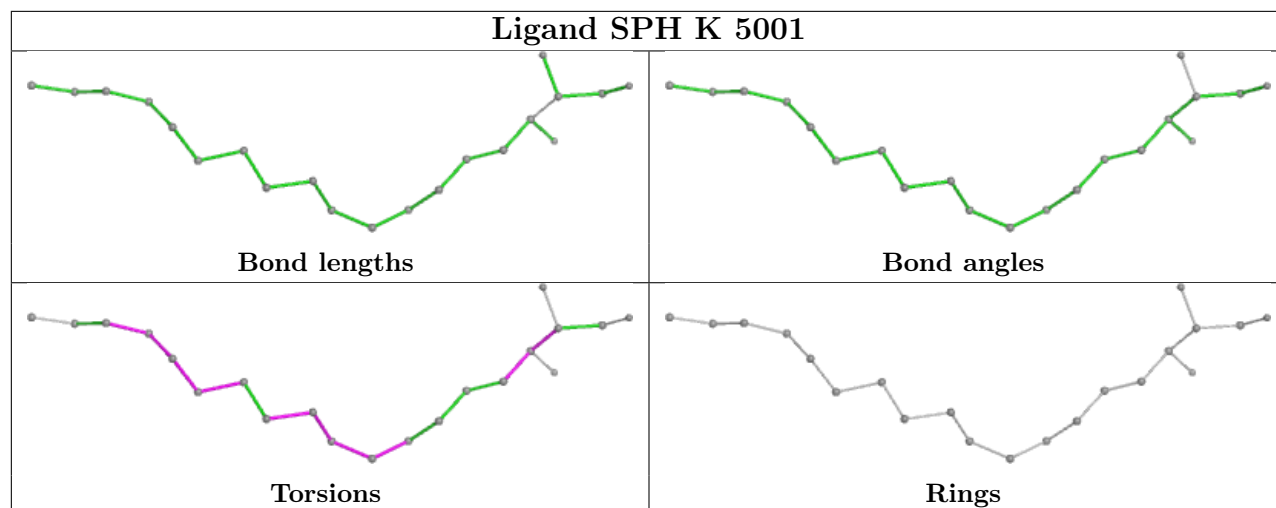


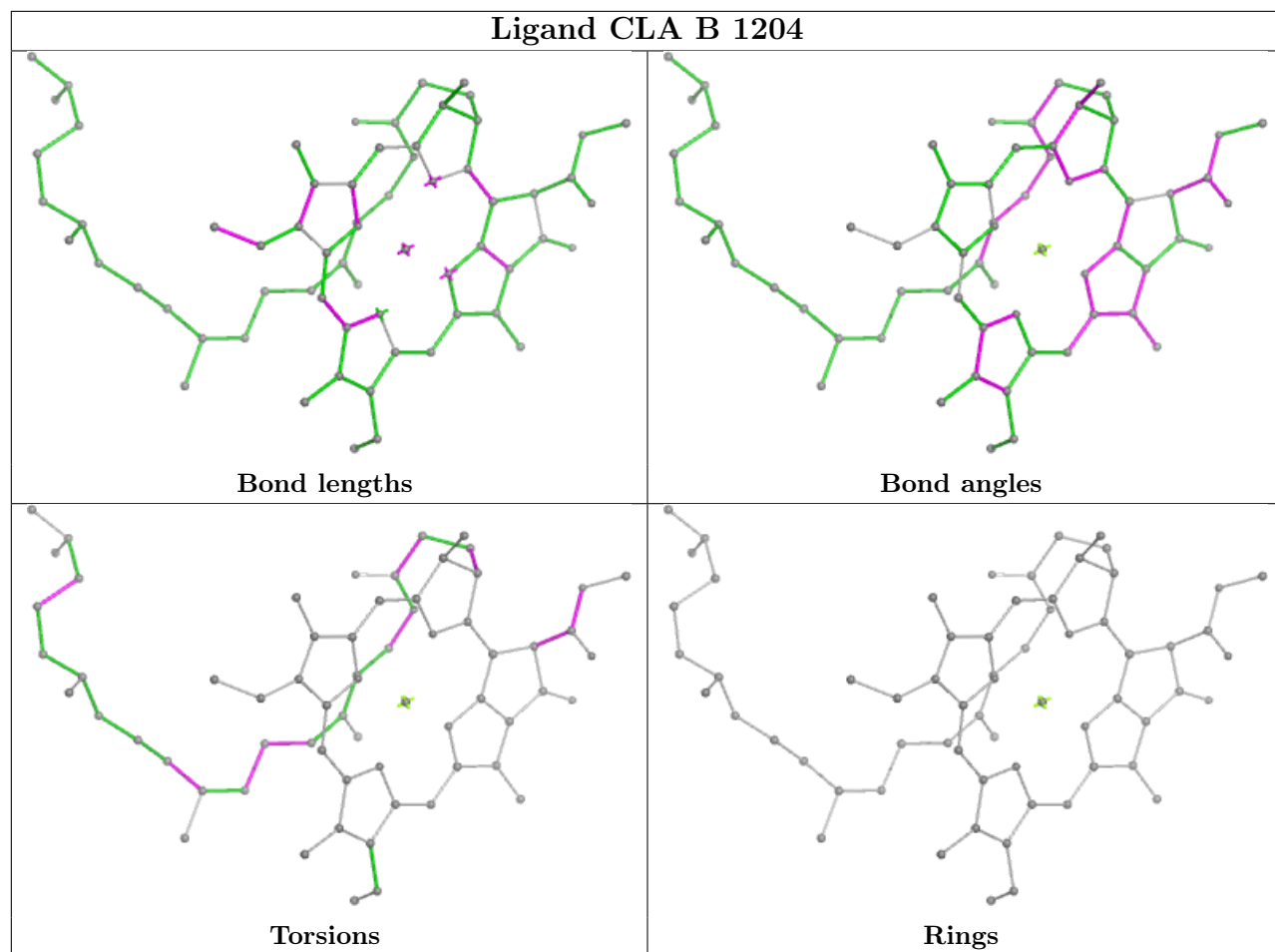


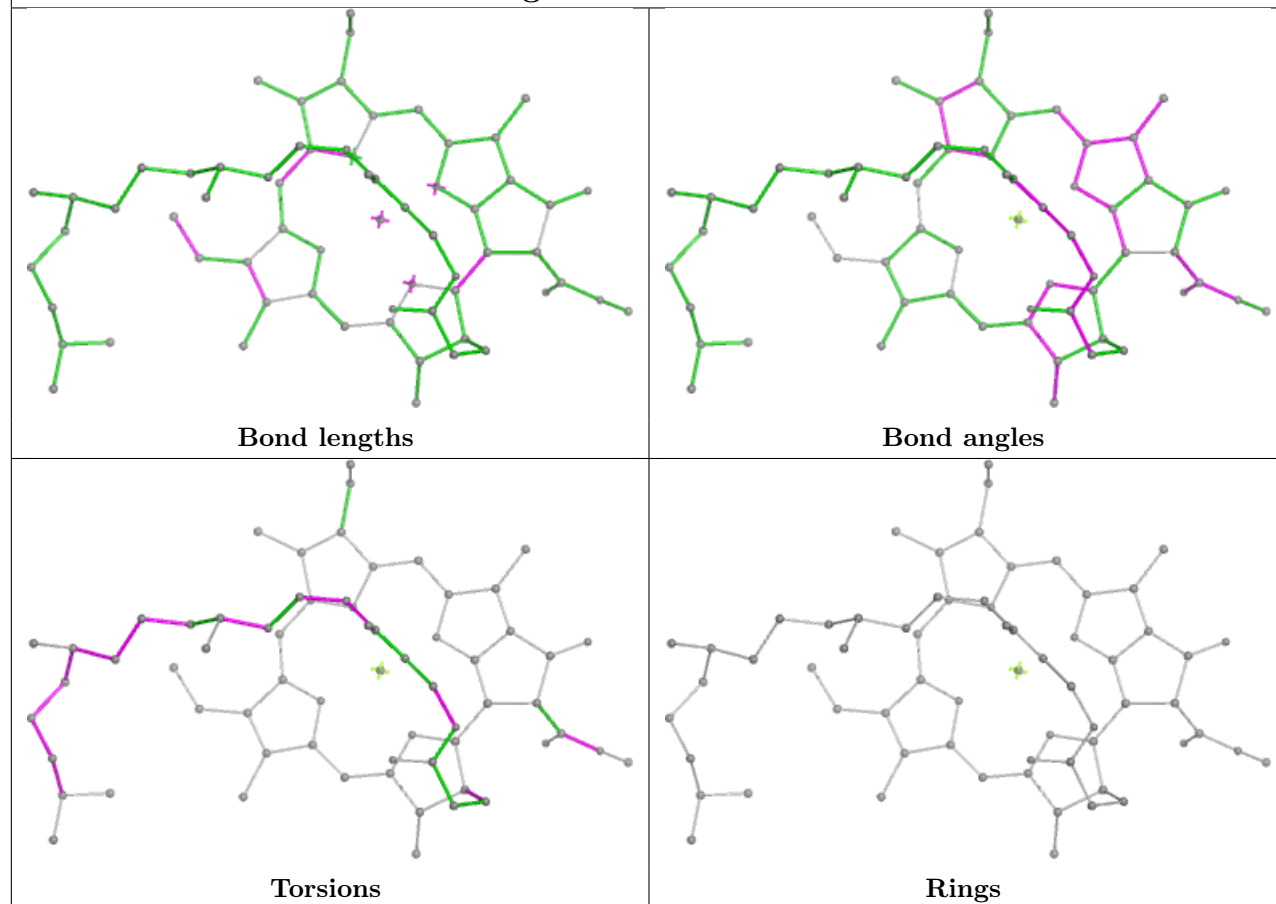
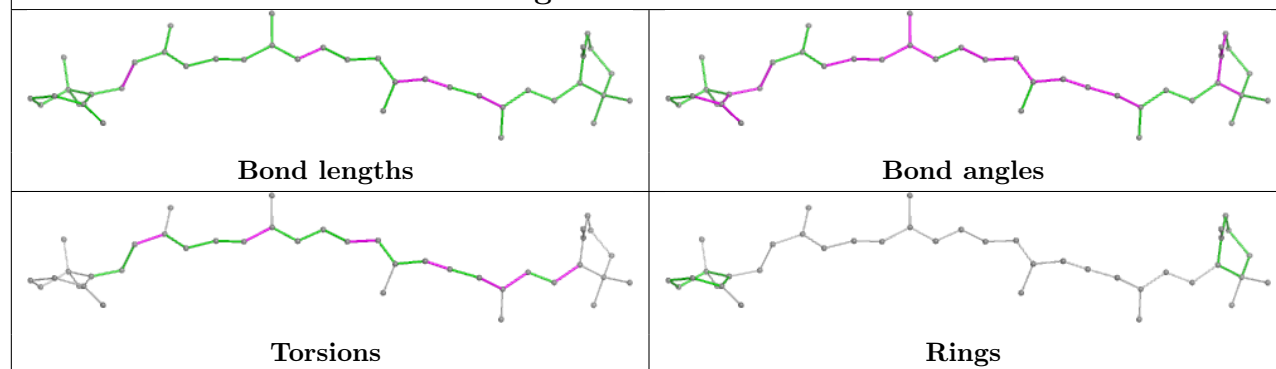


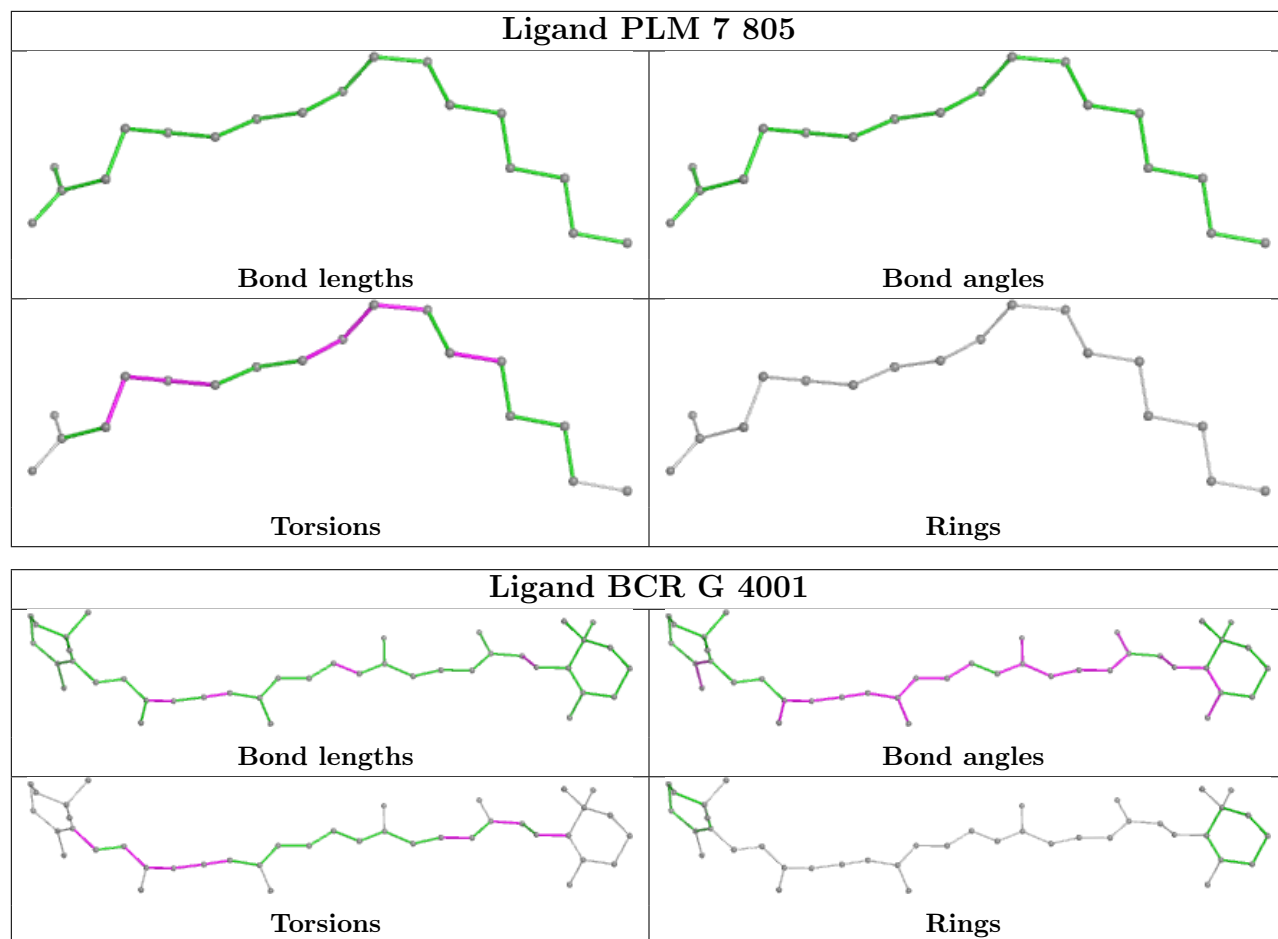




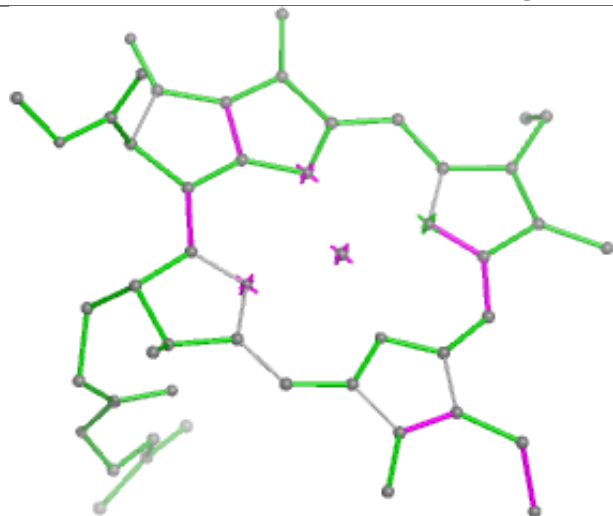




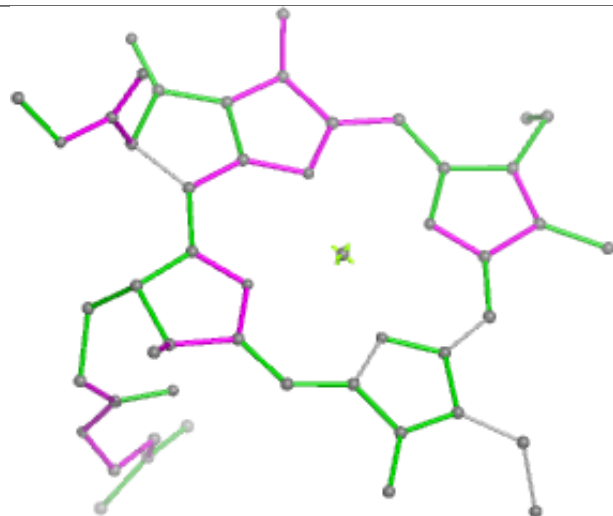
**Ligand CLA A 1110****Ligand BCR 3 504**



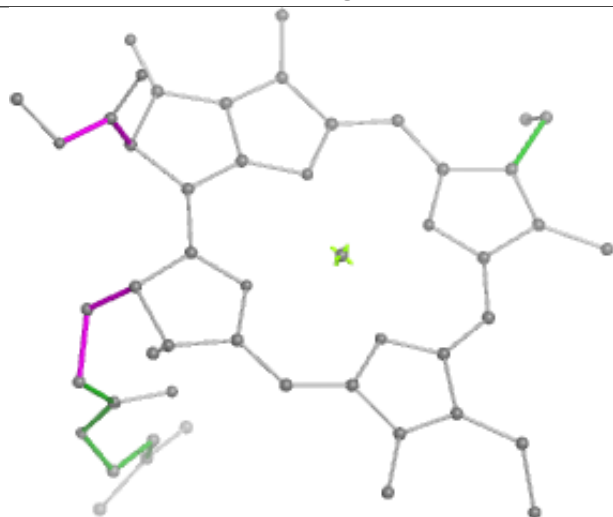
## Ligand CLA 6 612



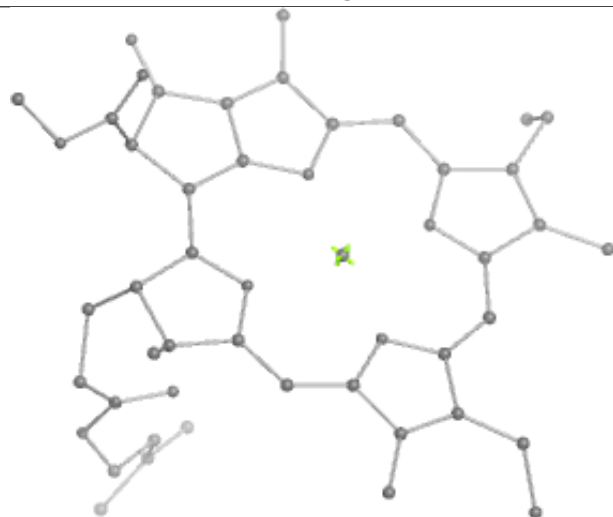
Bond lengths



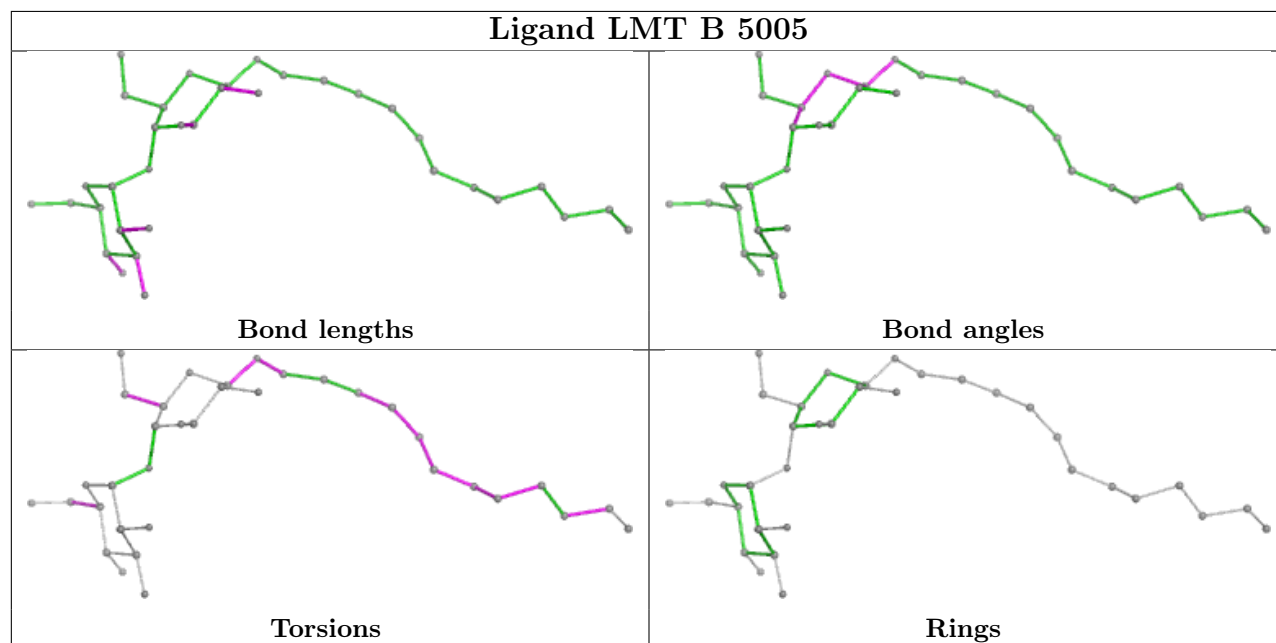
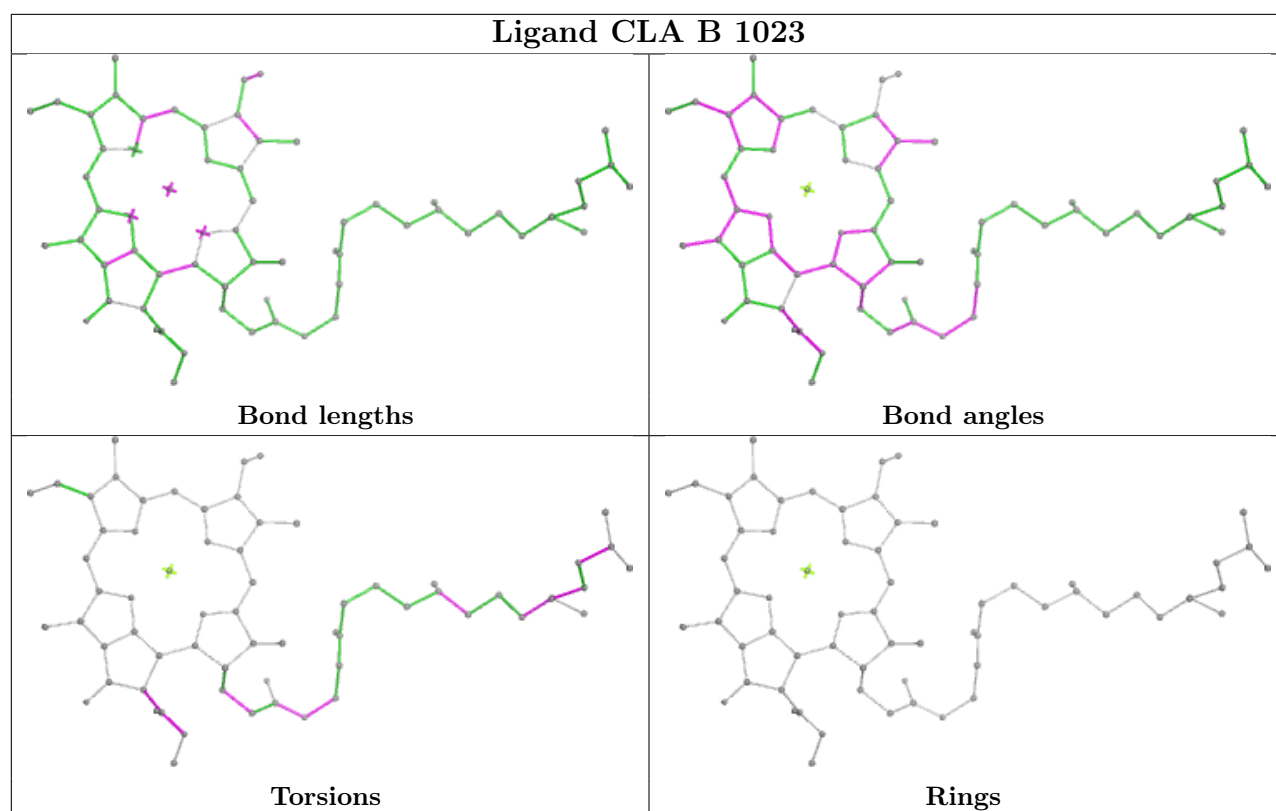
Bond angles

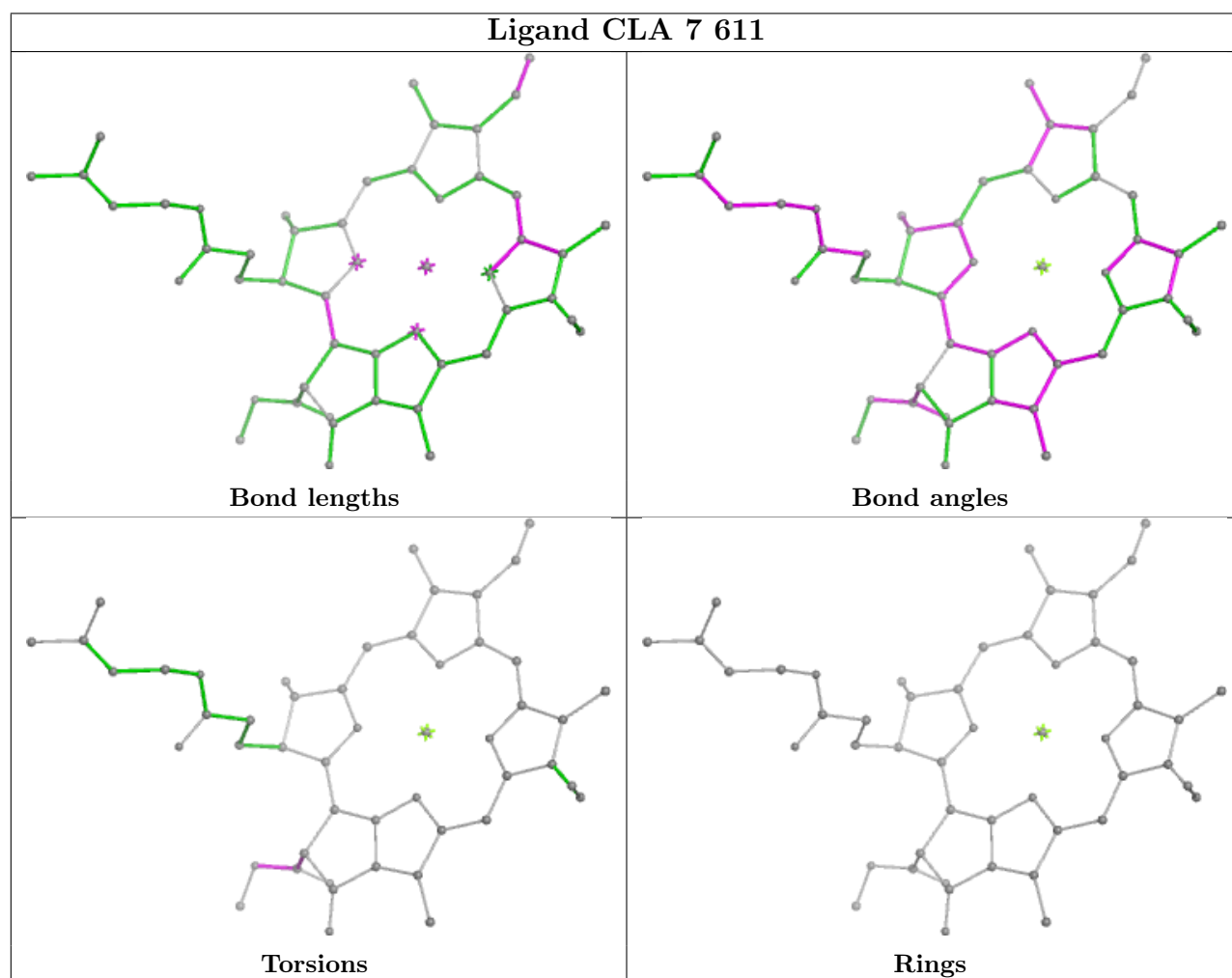
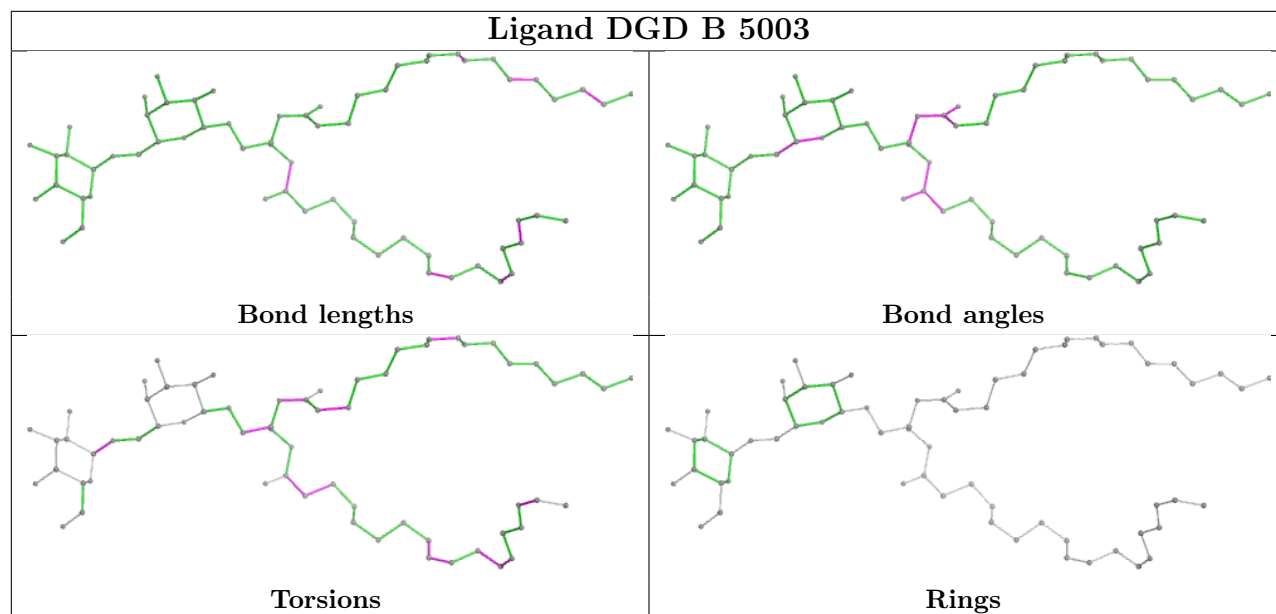


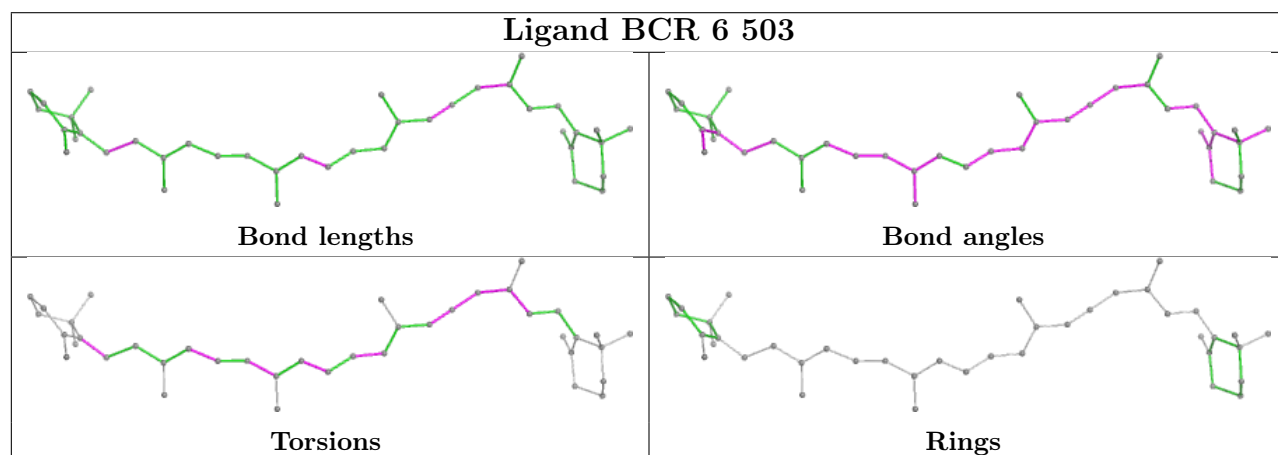
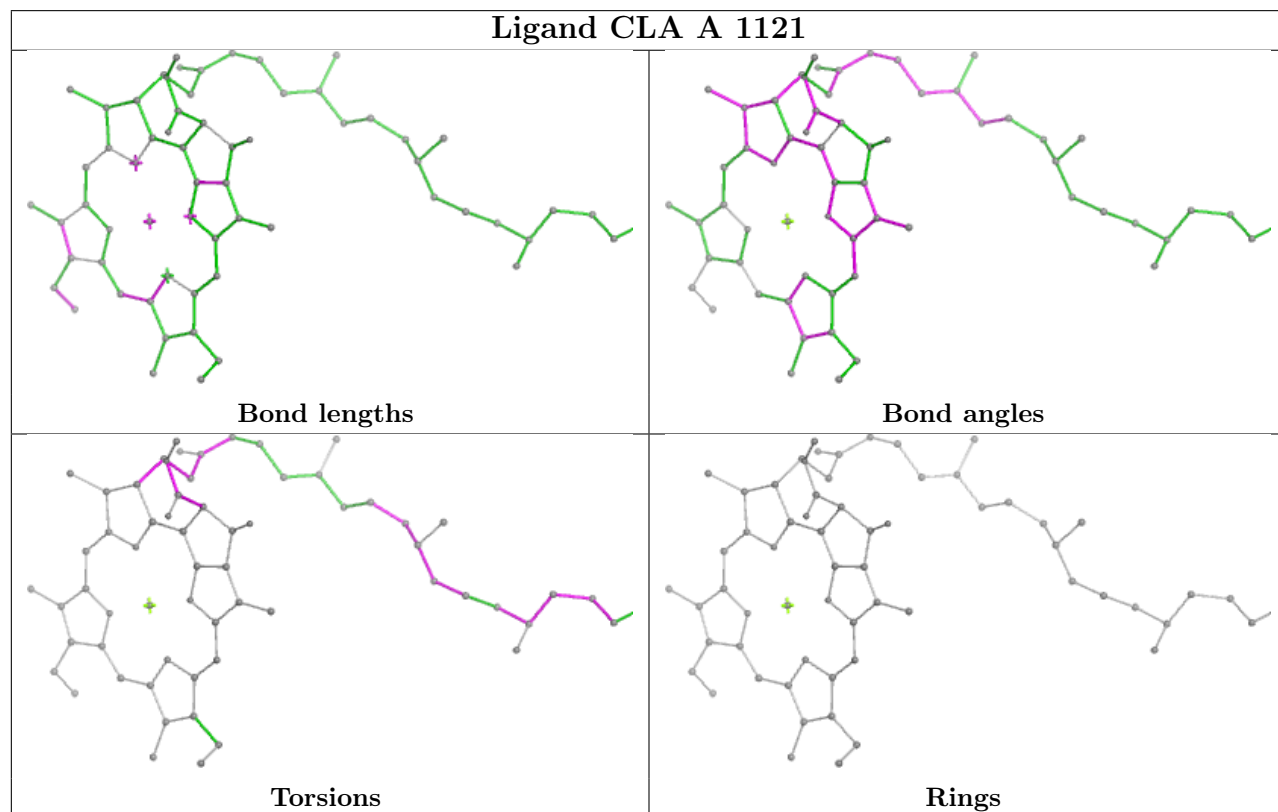
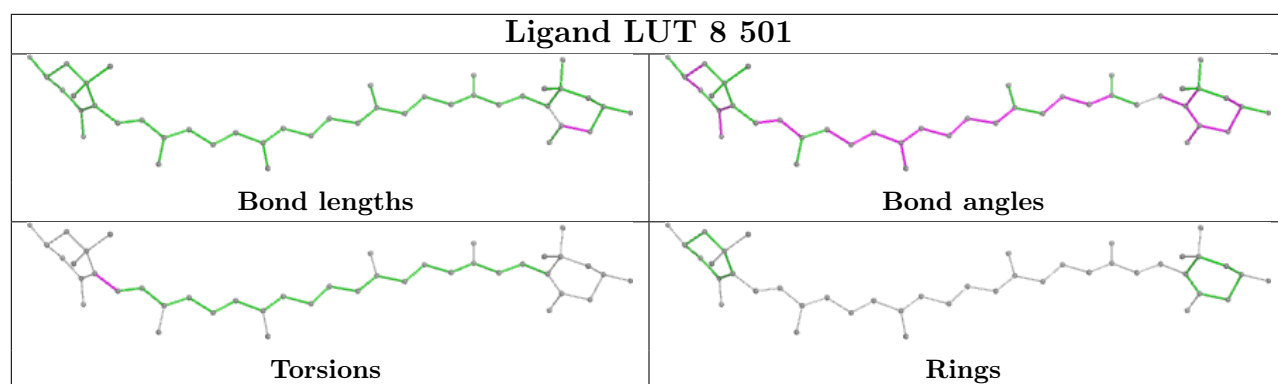
Torsions



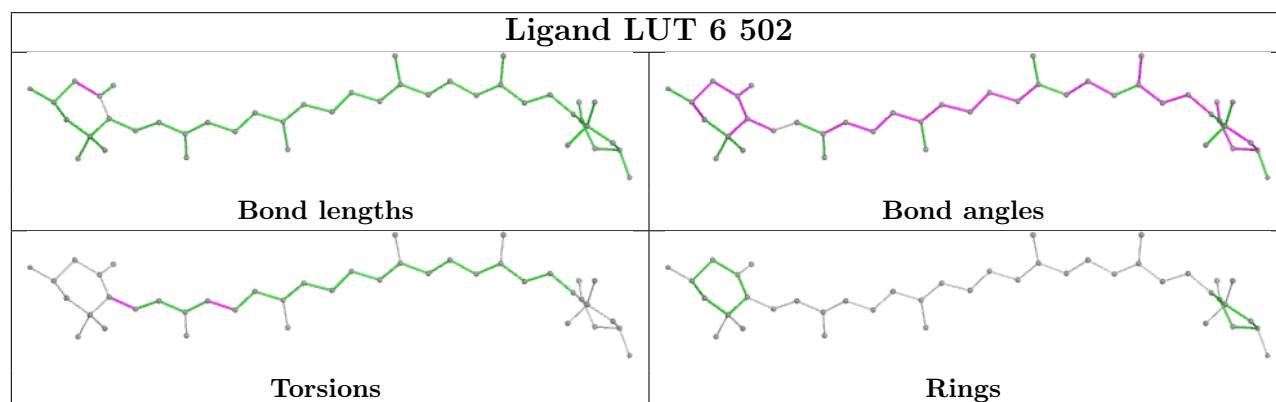
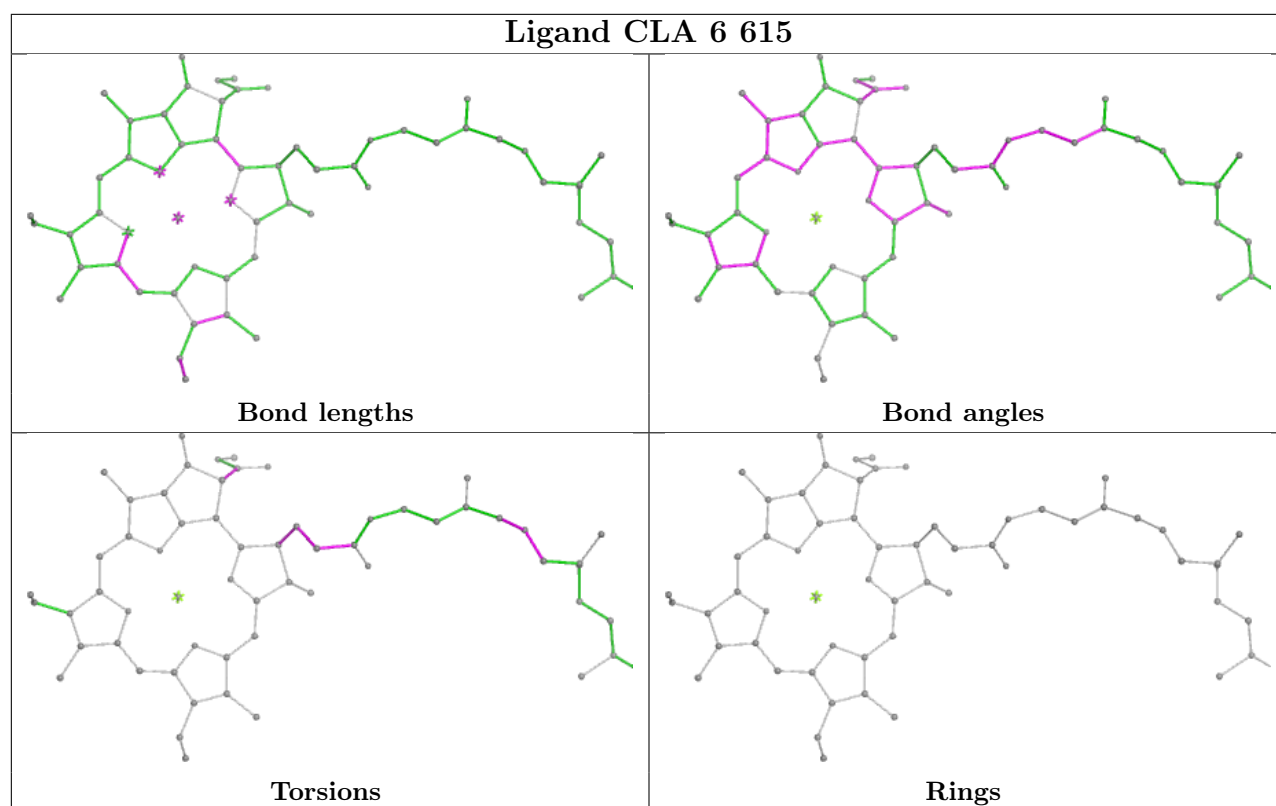
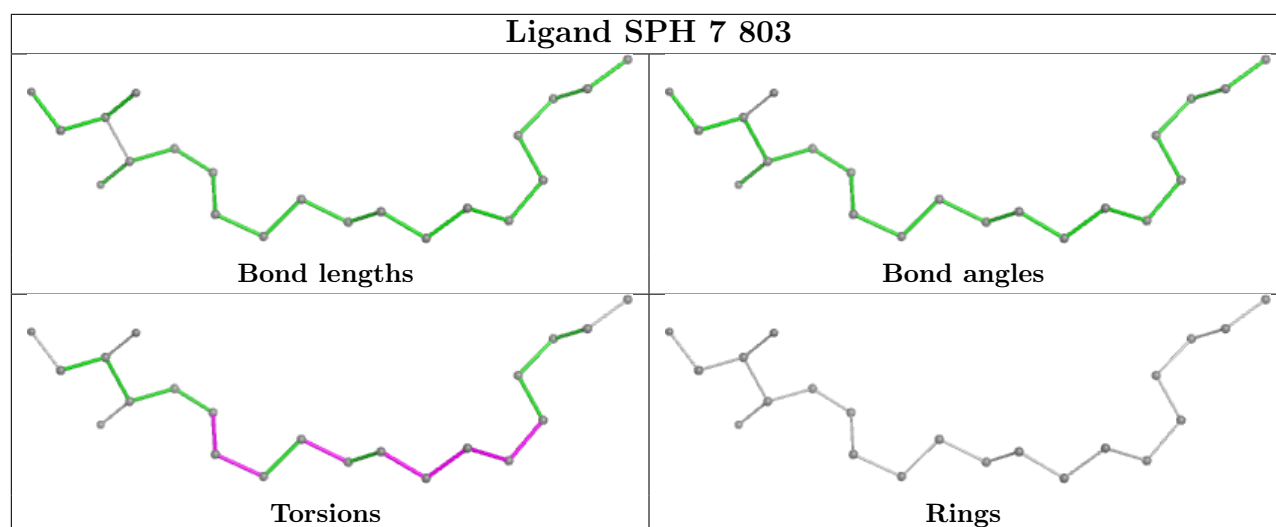
Rings

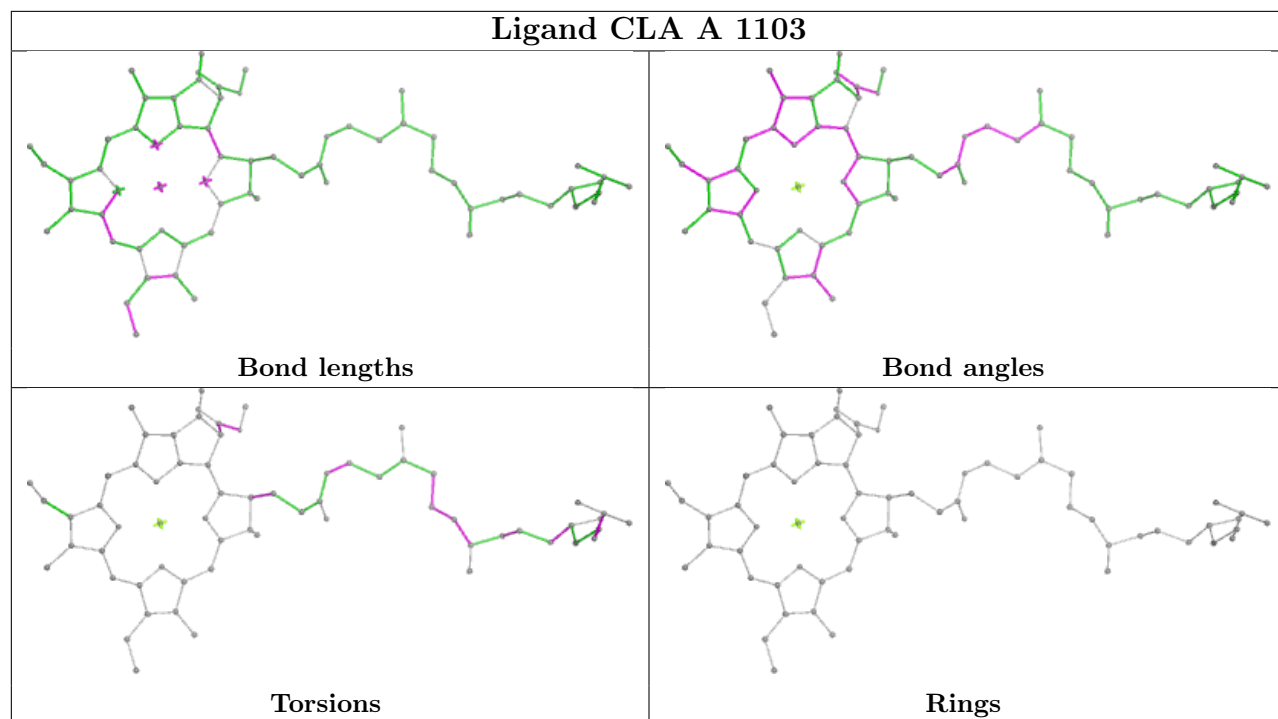




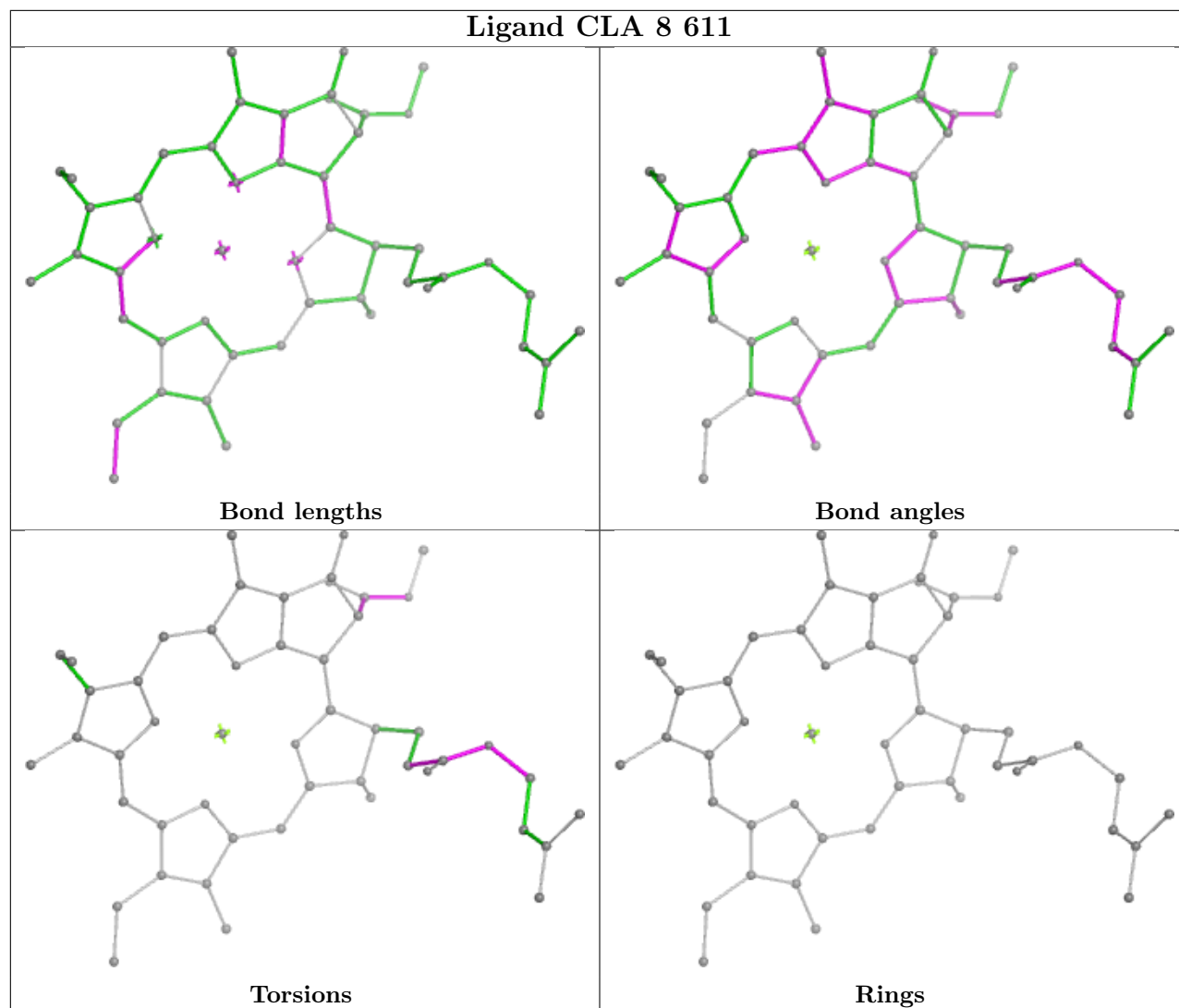




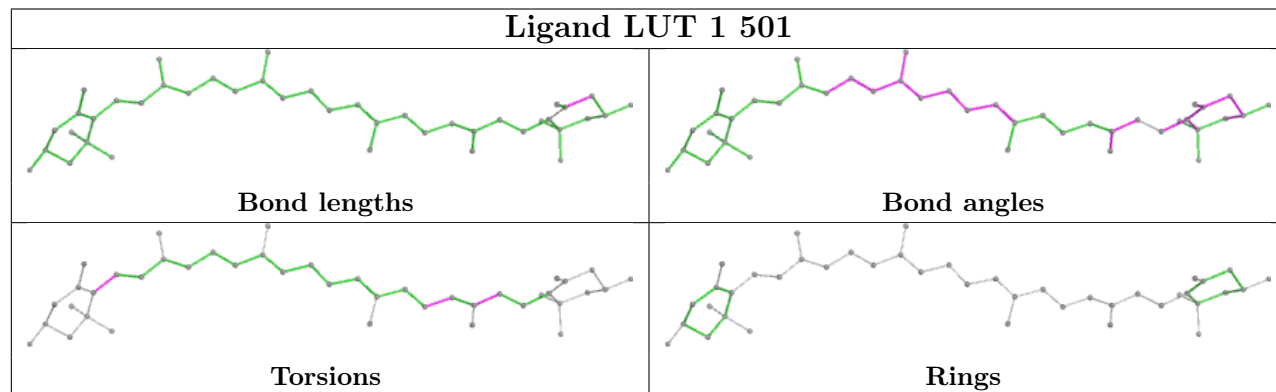


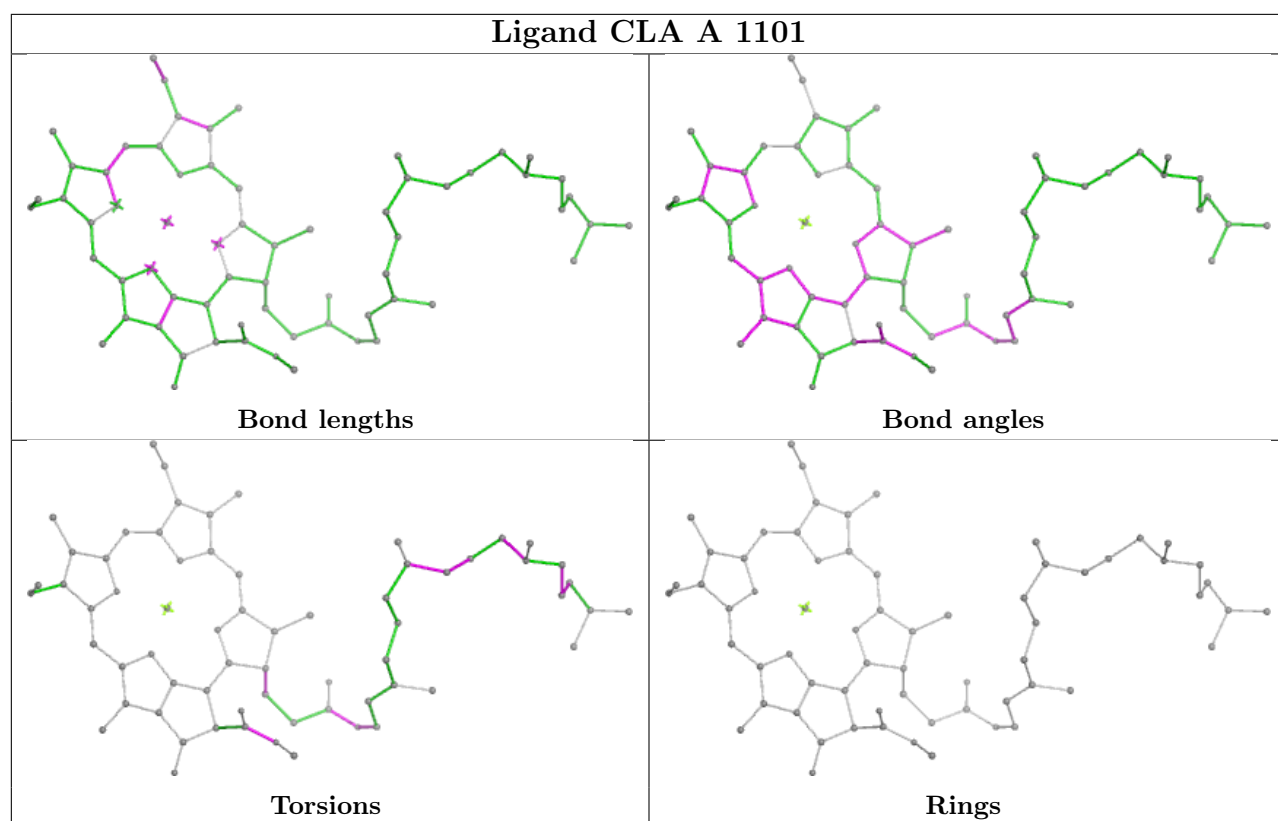


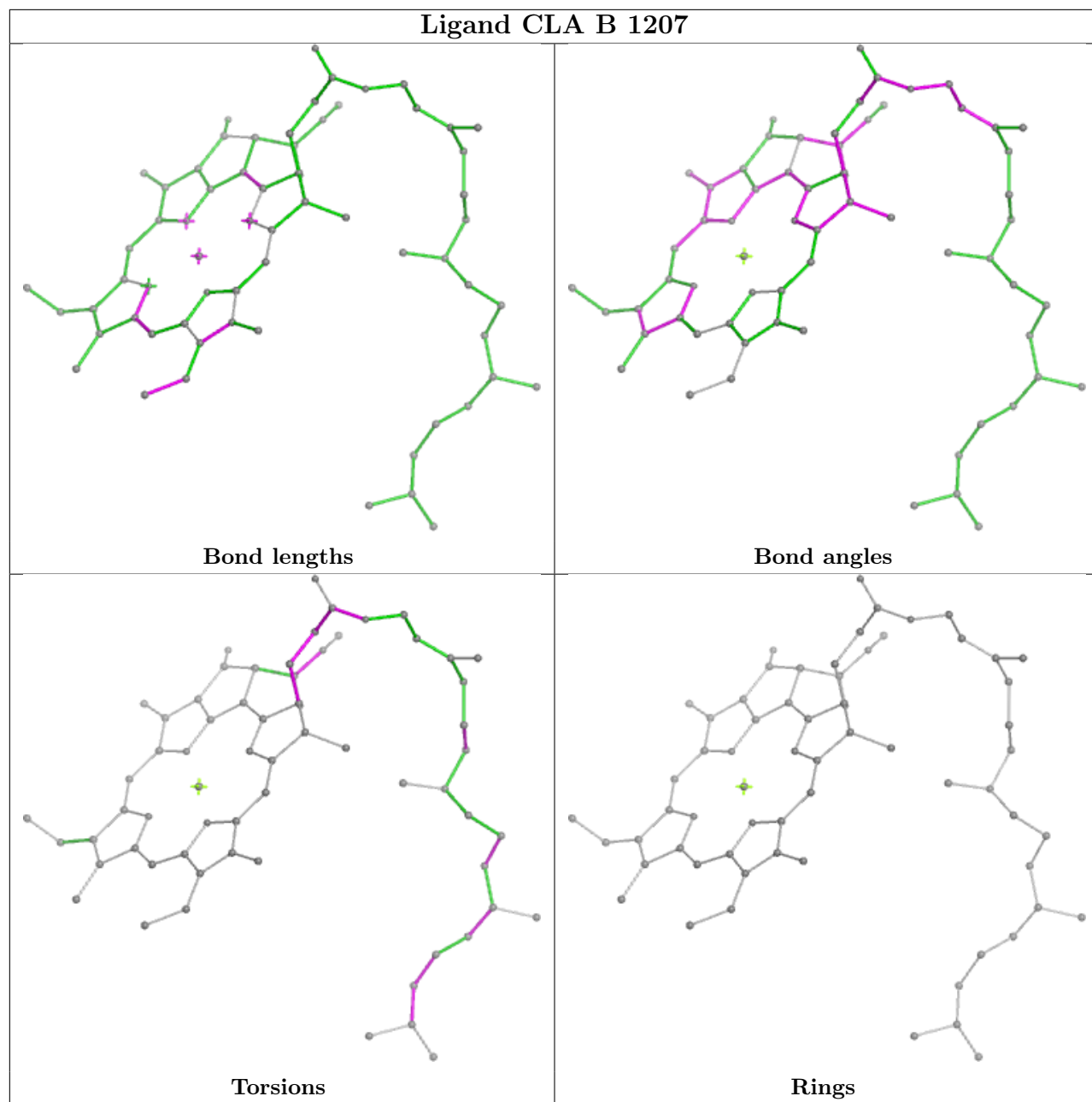
## Ligand CLA 8 611



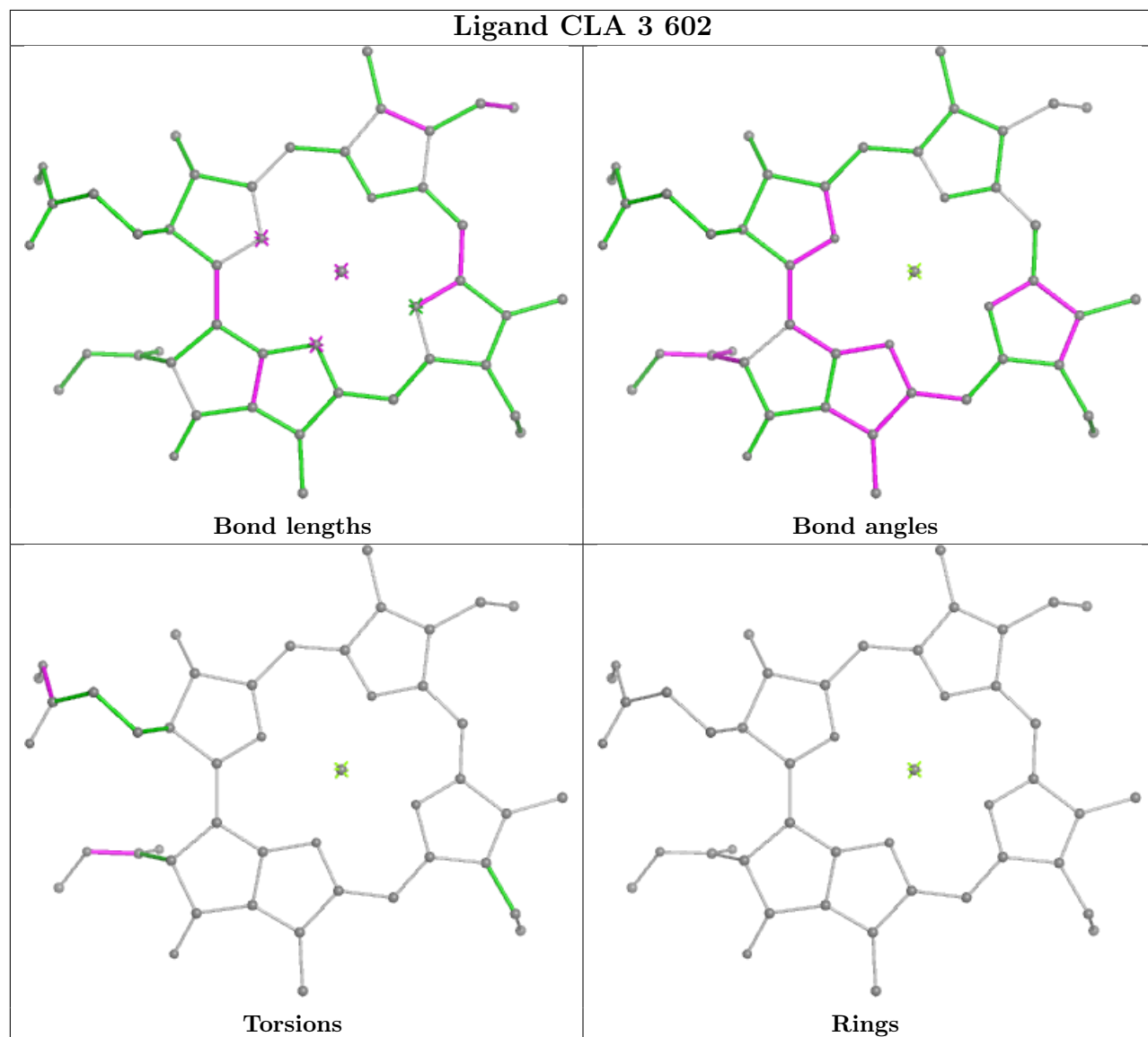
## Ligand LUT 1 501

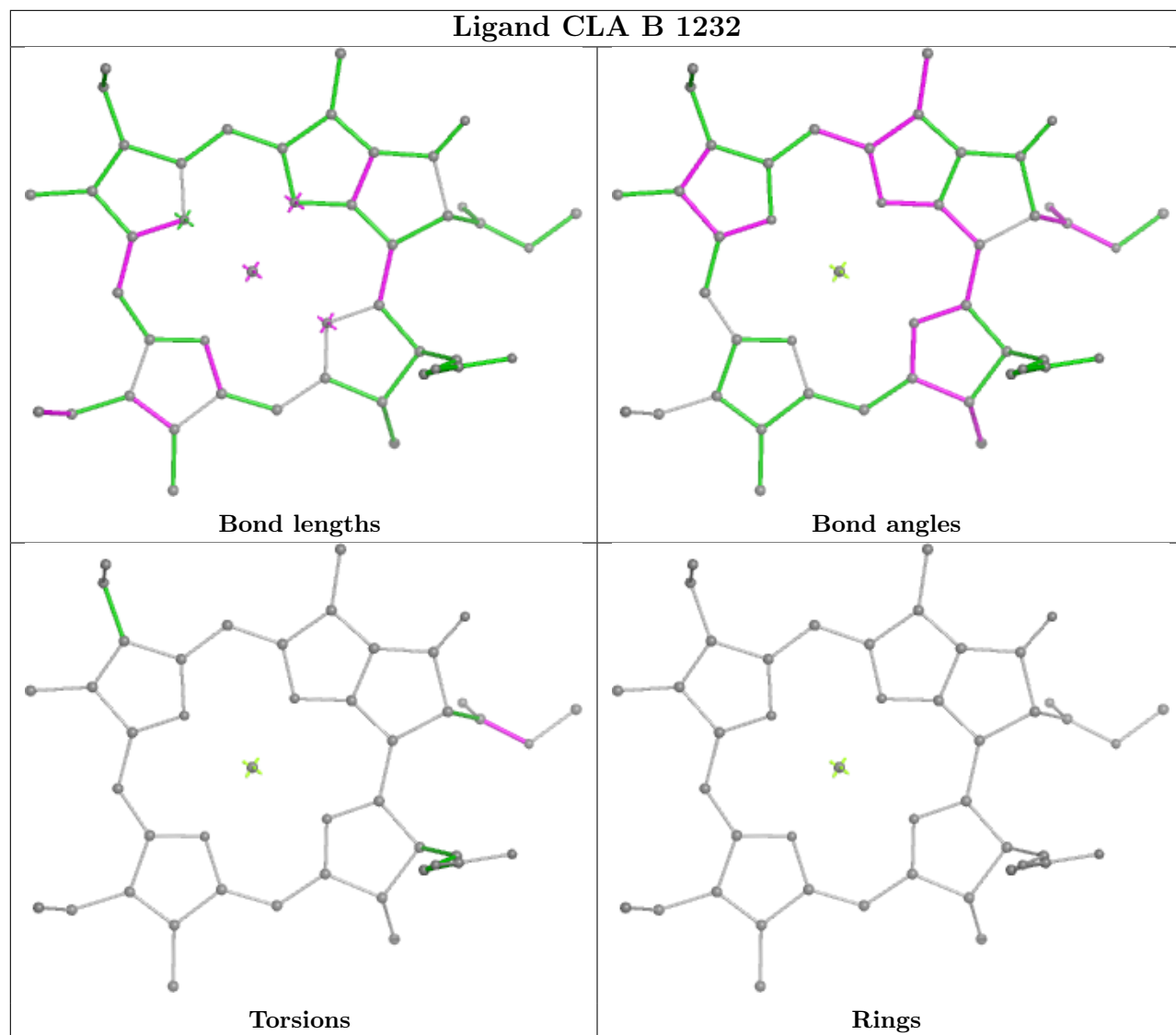


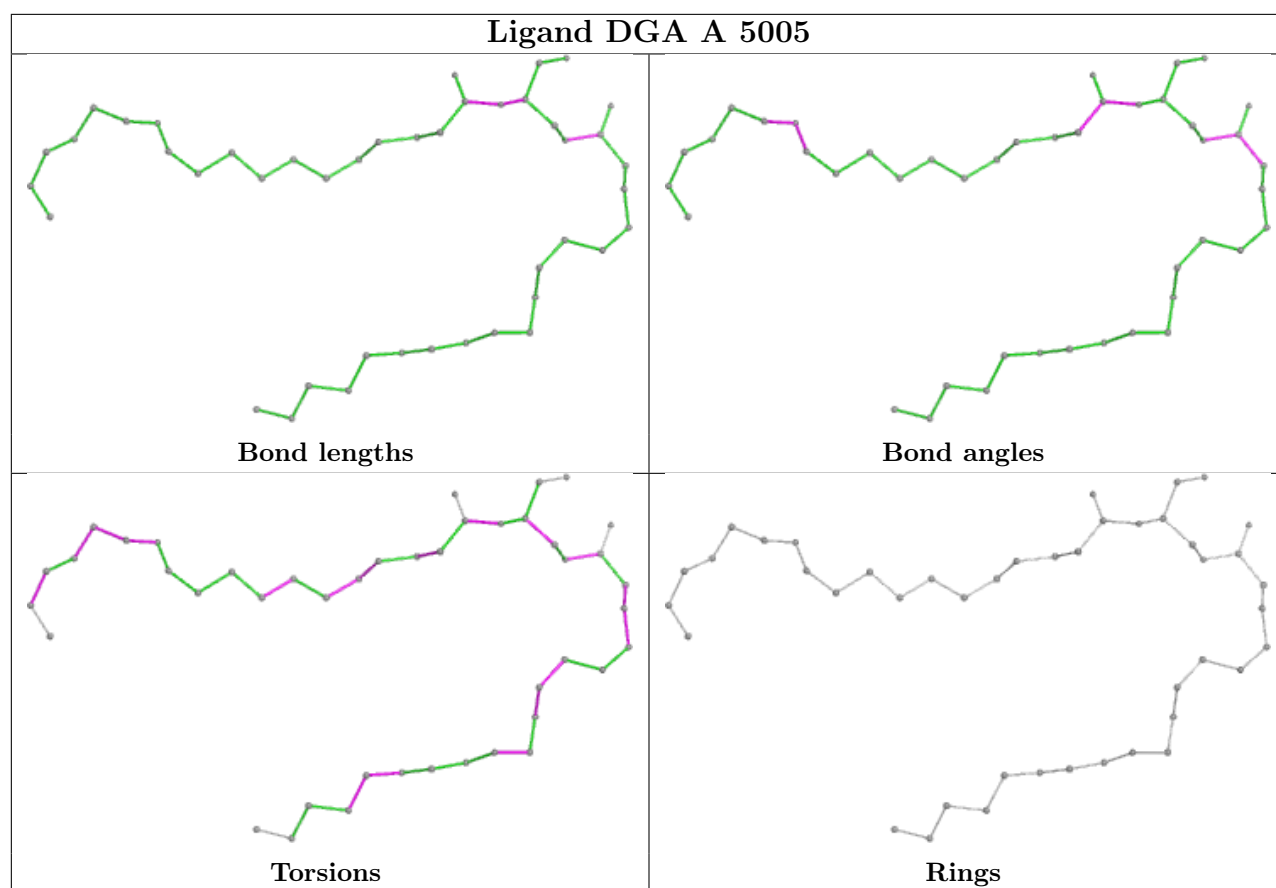




## Ligand CLA 3 602

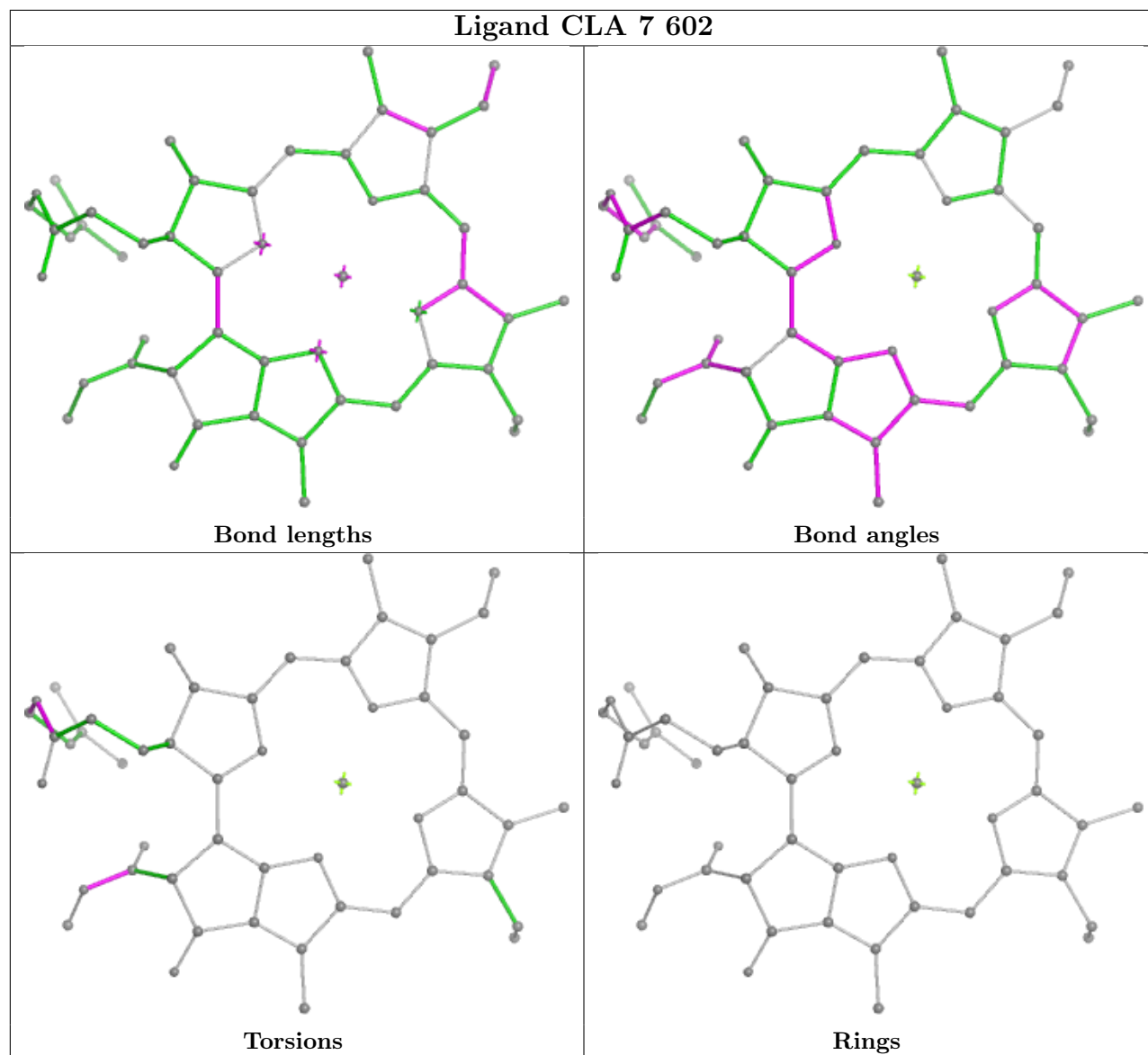




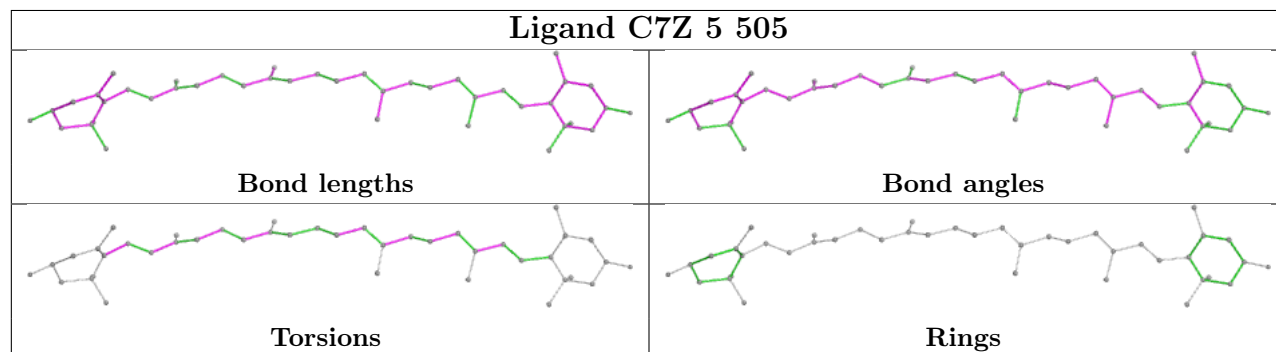




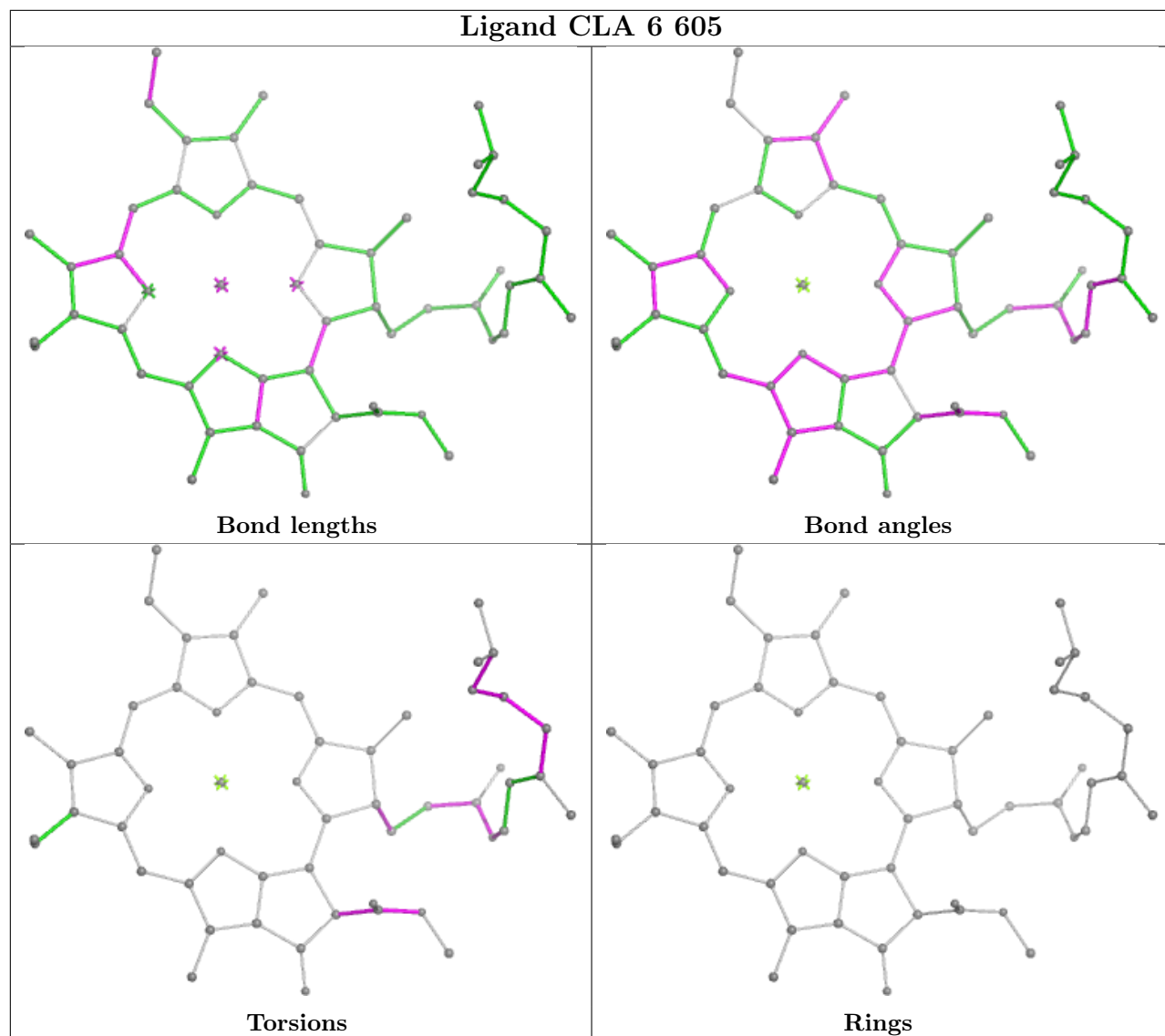
## Ligand CLA 7 602



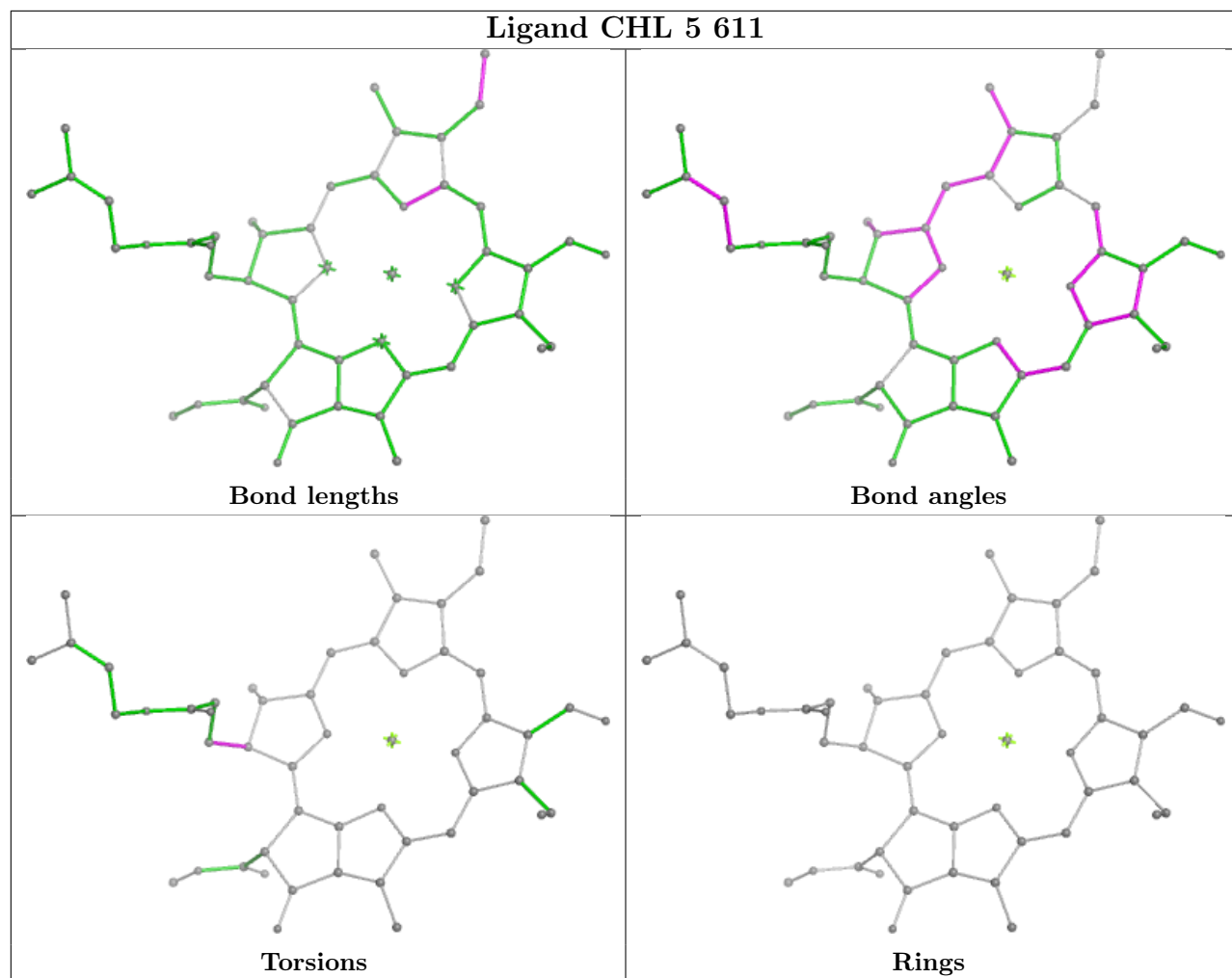
## Ligand C7Z 5 505



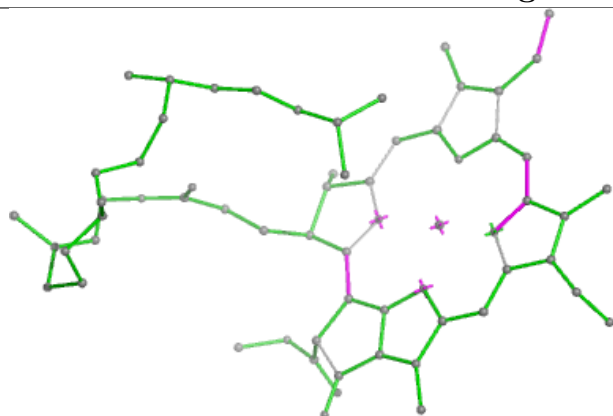
## Ligand CLA 6 605



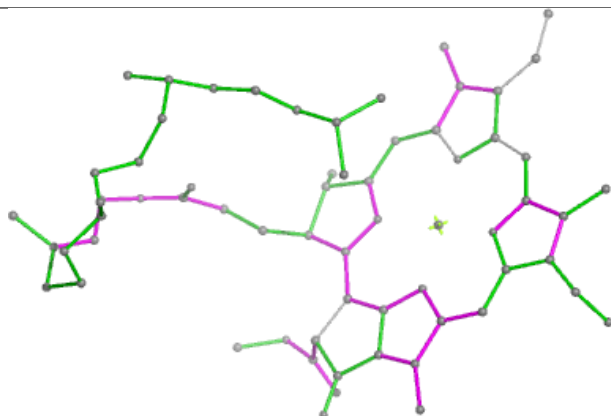
## Ligand CHL 5 611



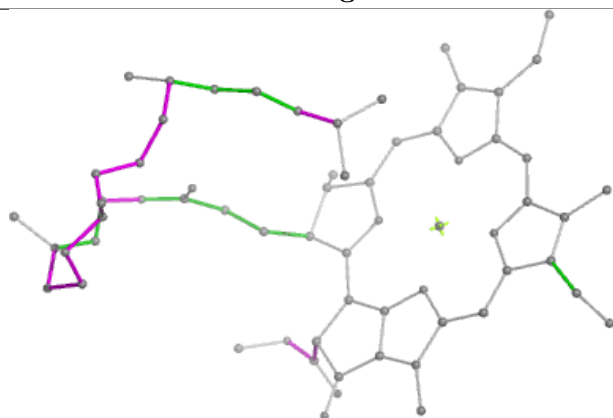
## Ligand CLA 6 619



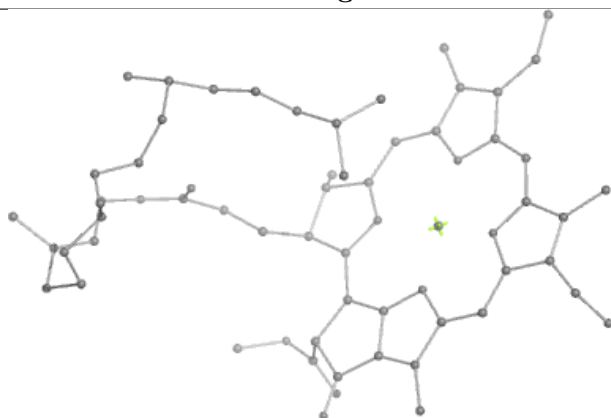
Bond lengths



Bond angles

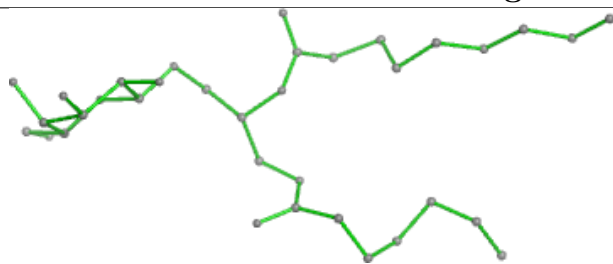


Torsions

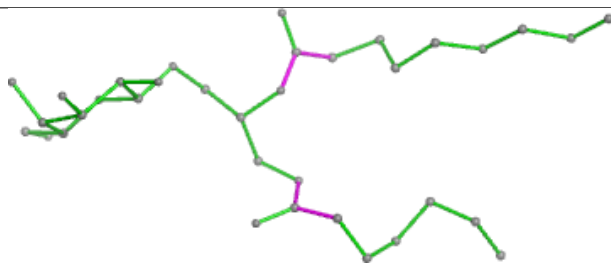


Rings

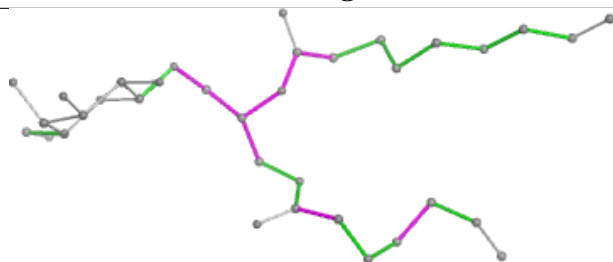
## Ligand LMG J 5001



Bond lengths



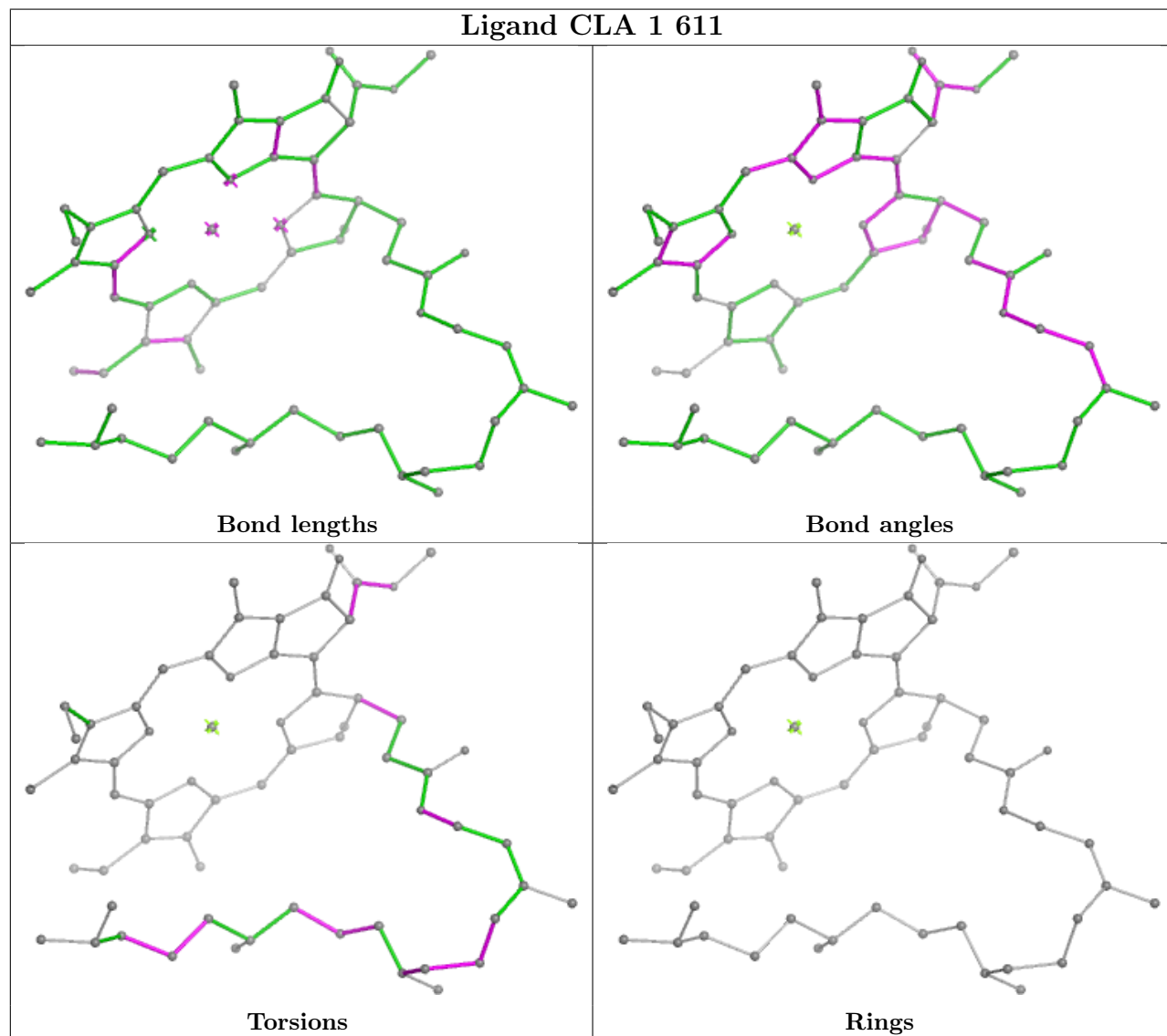
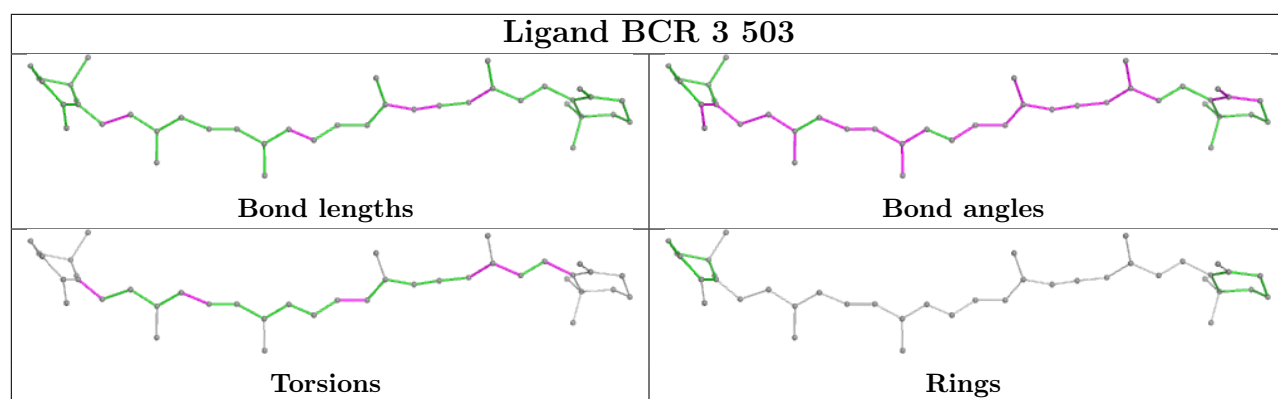
Bond angles

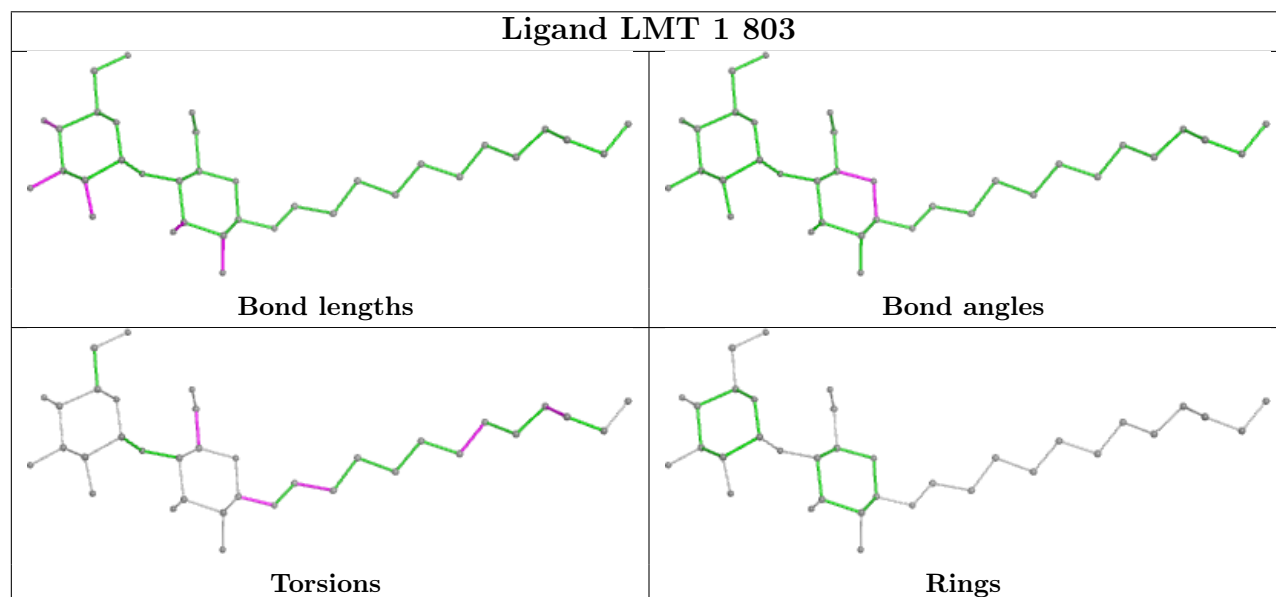
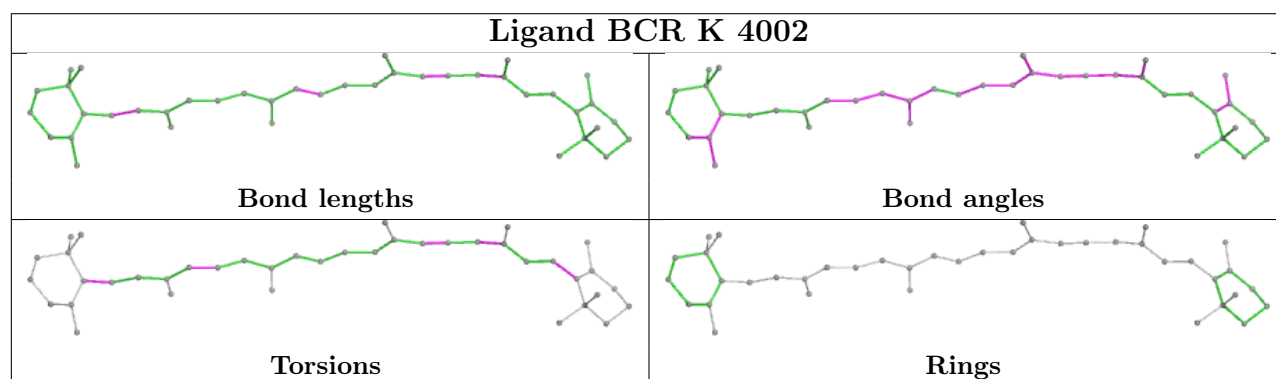
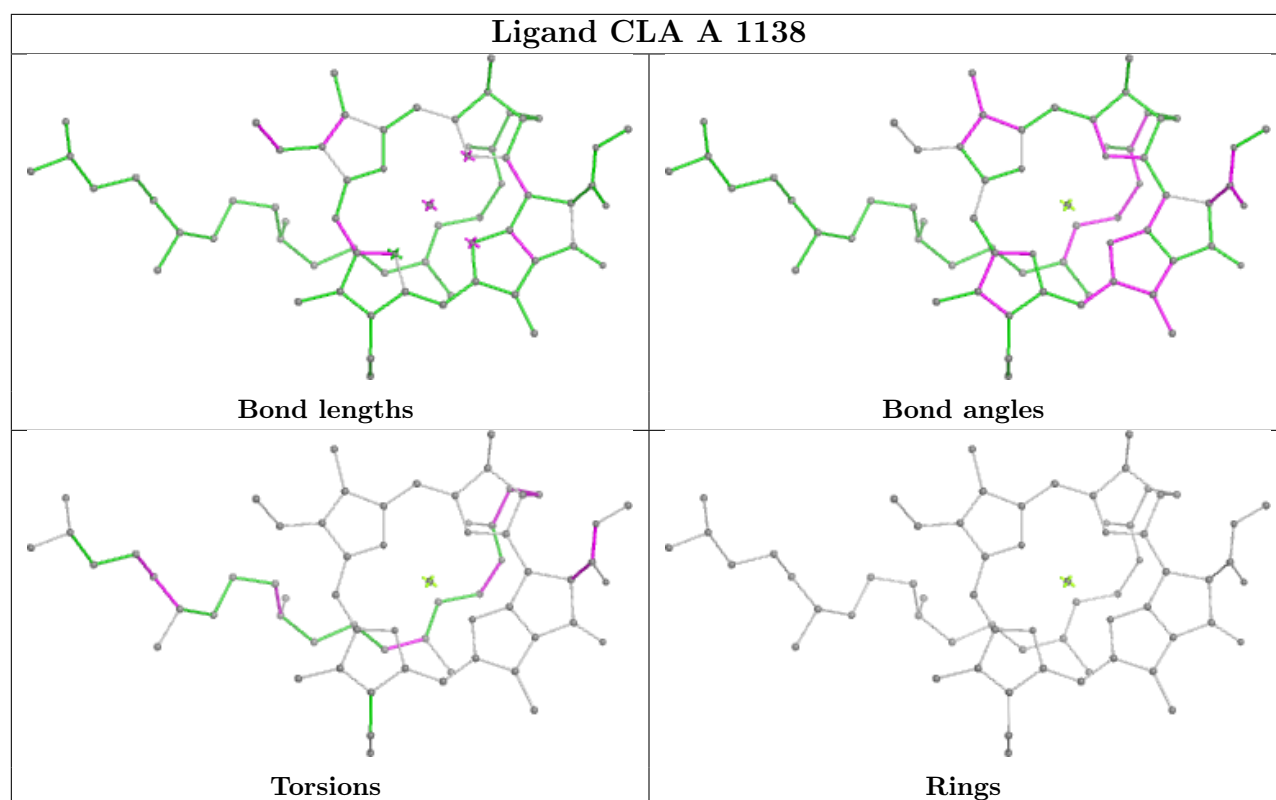


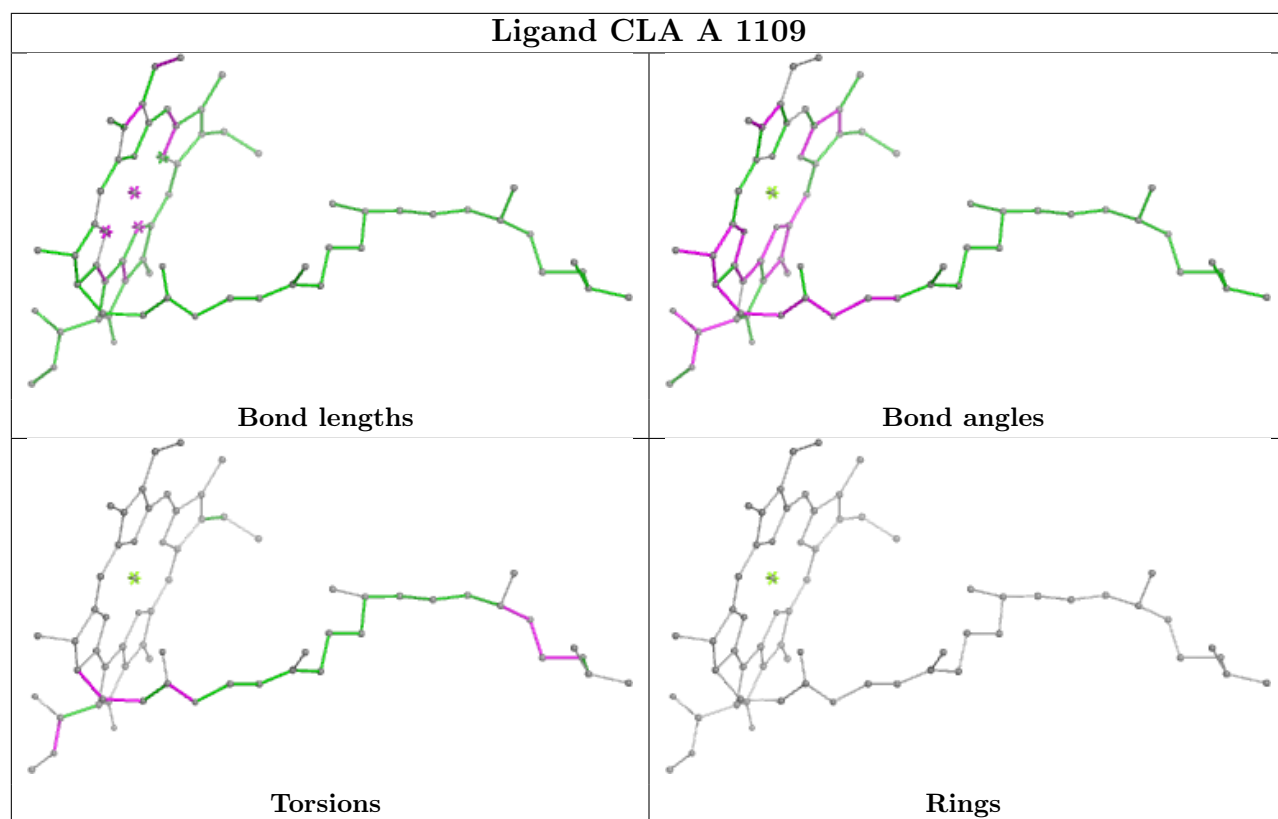
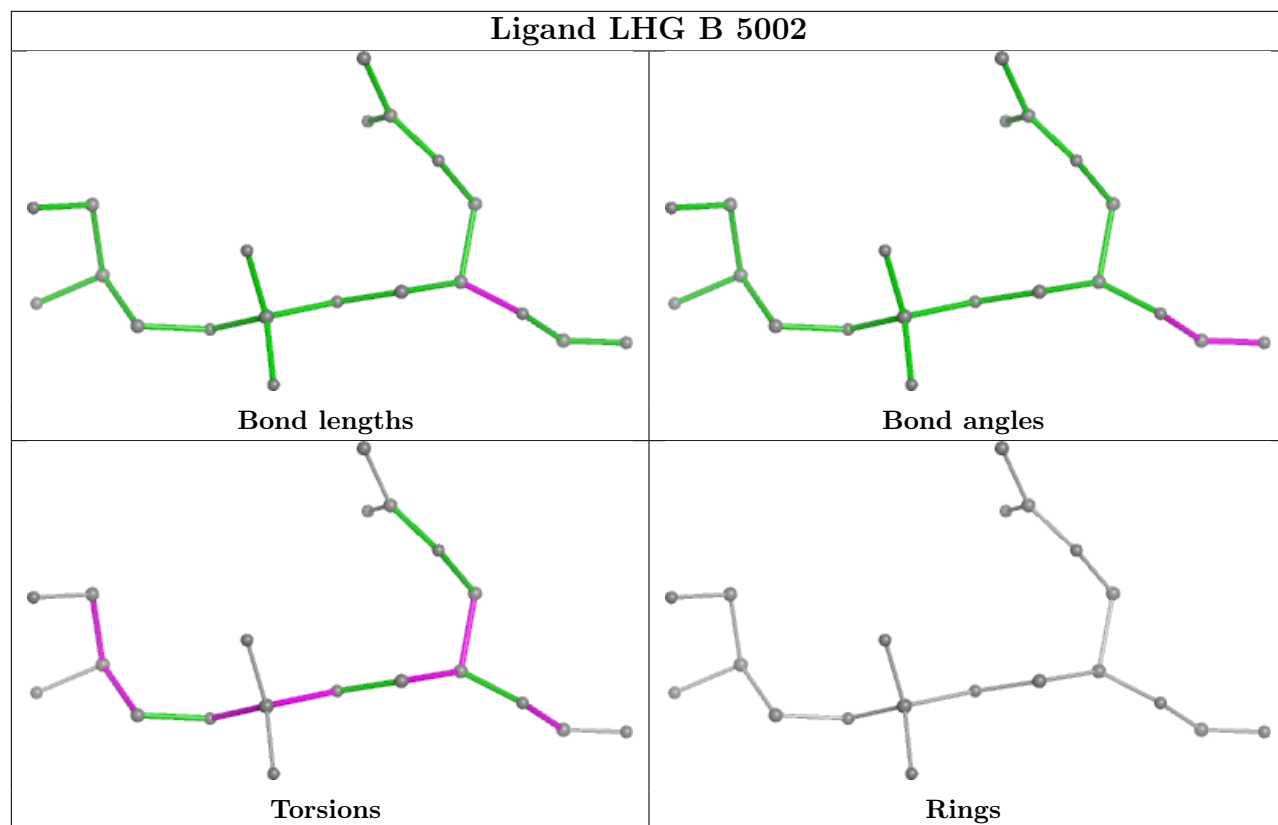
Torsions



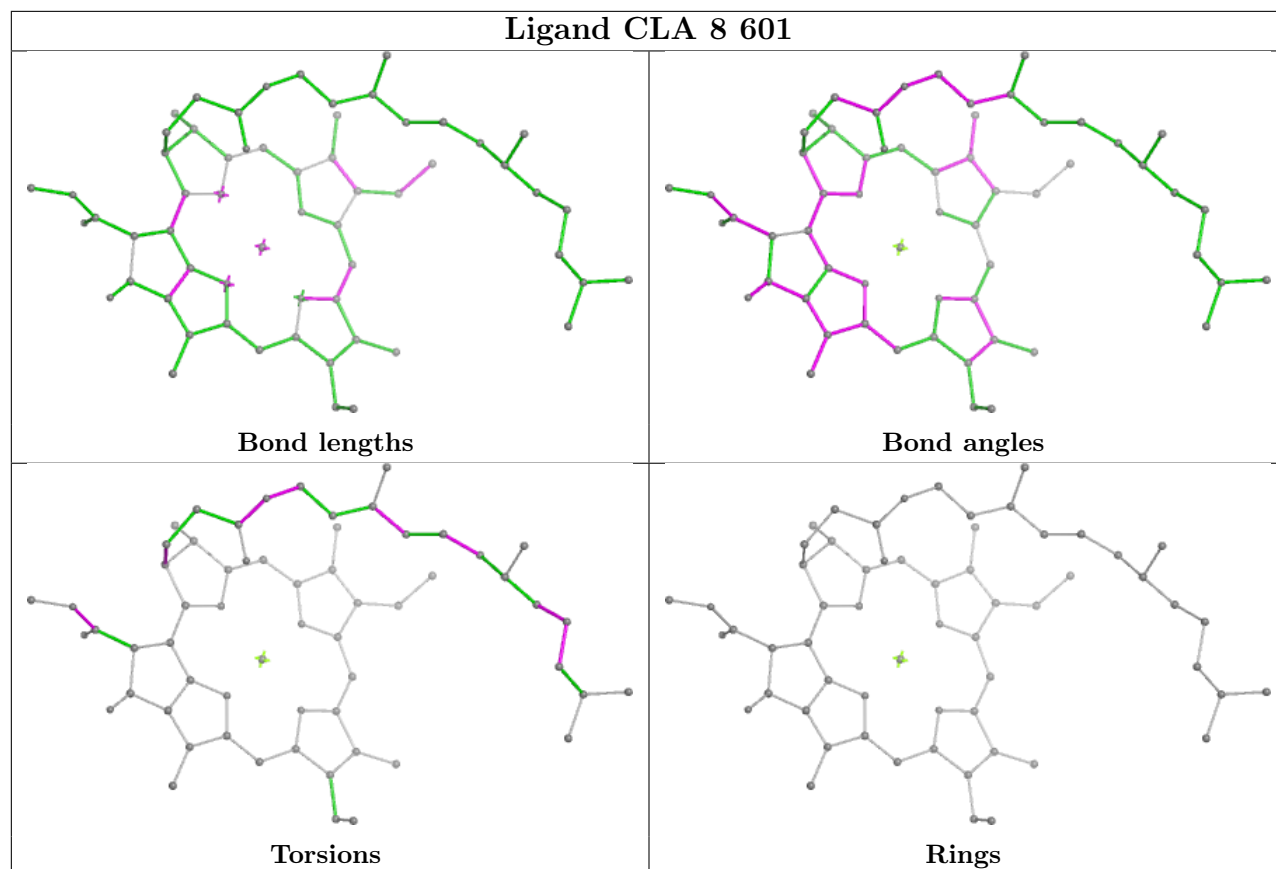
Rings



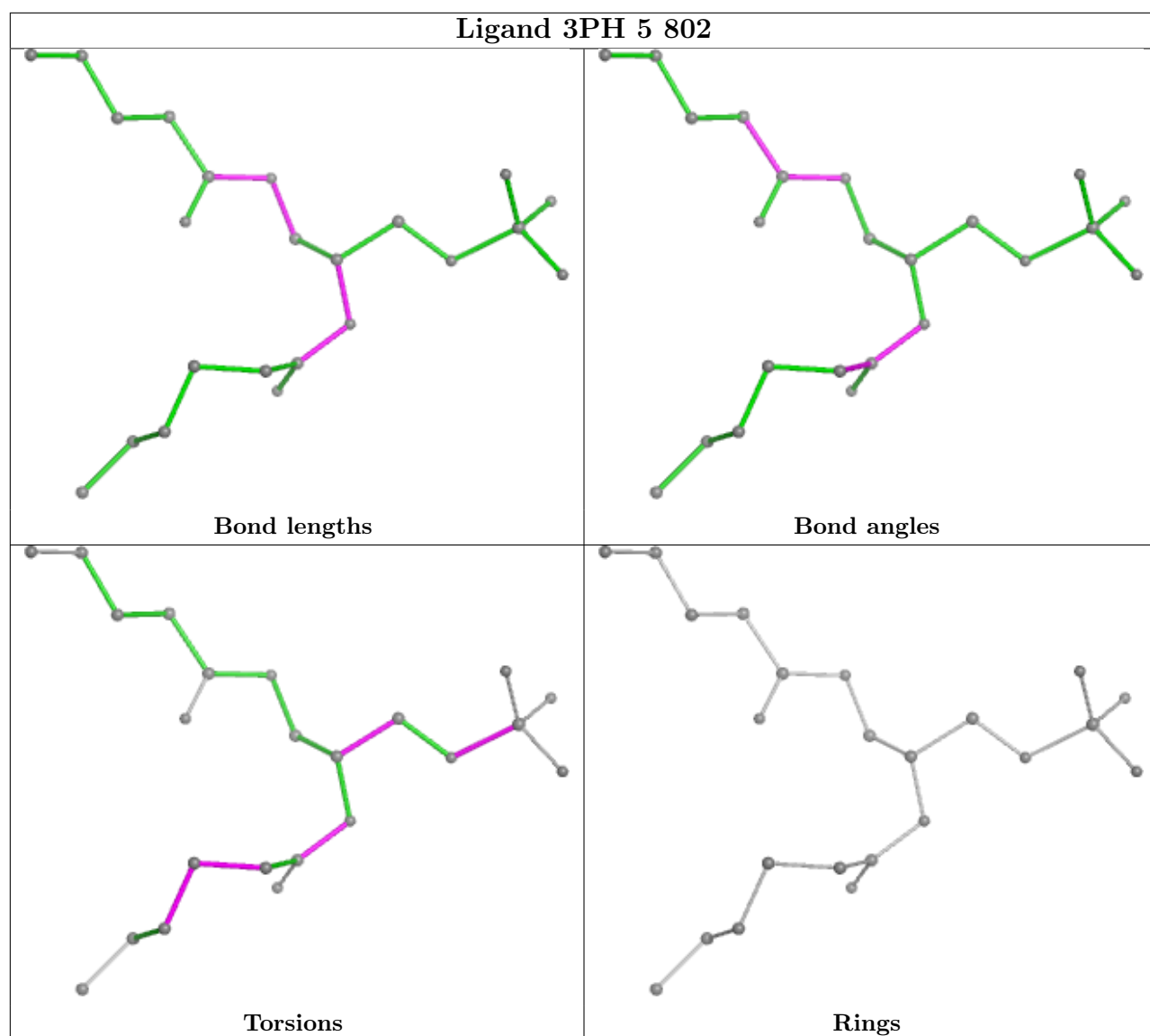




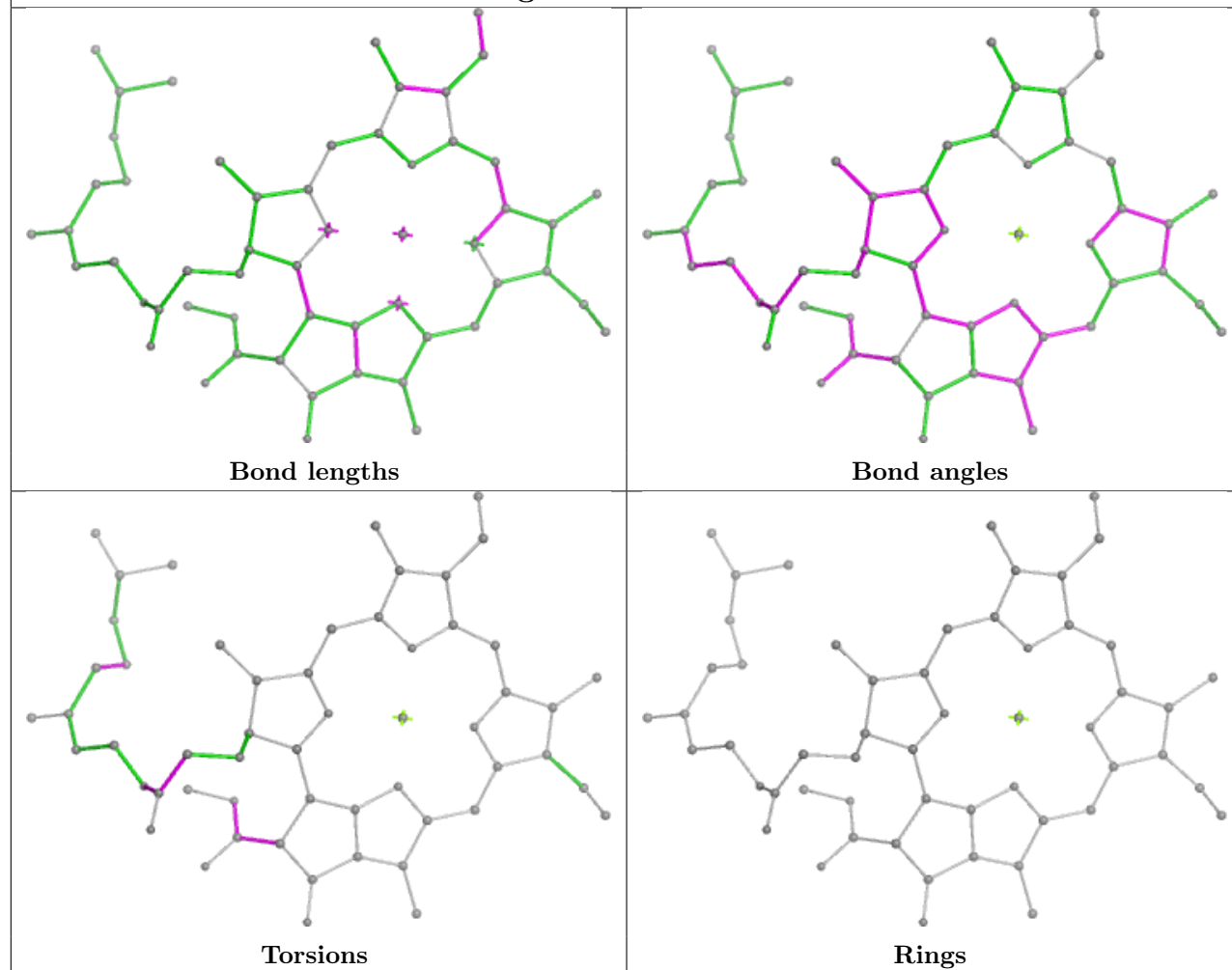
## Ligand CLA 8 601



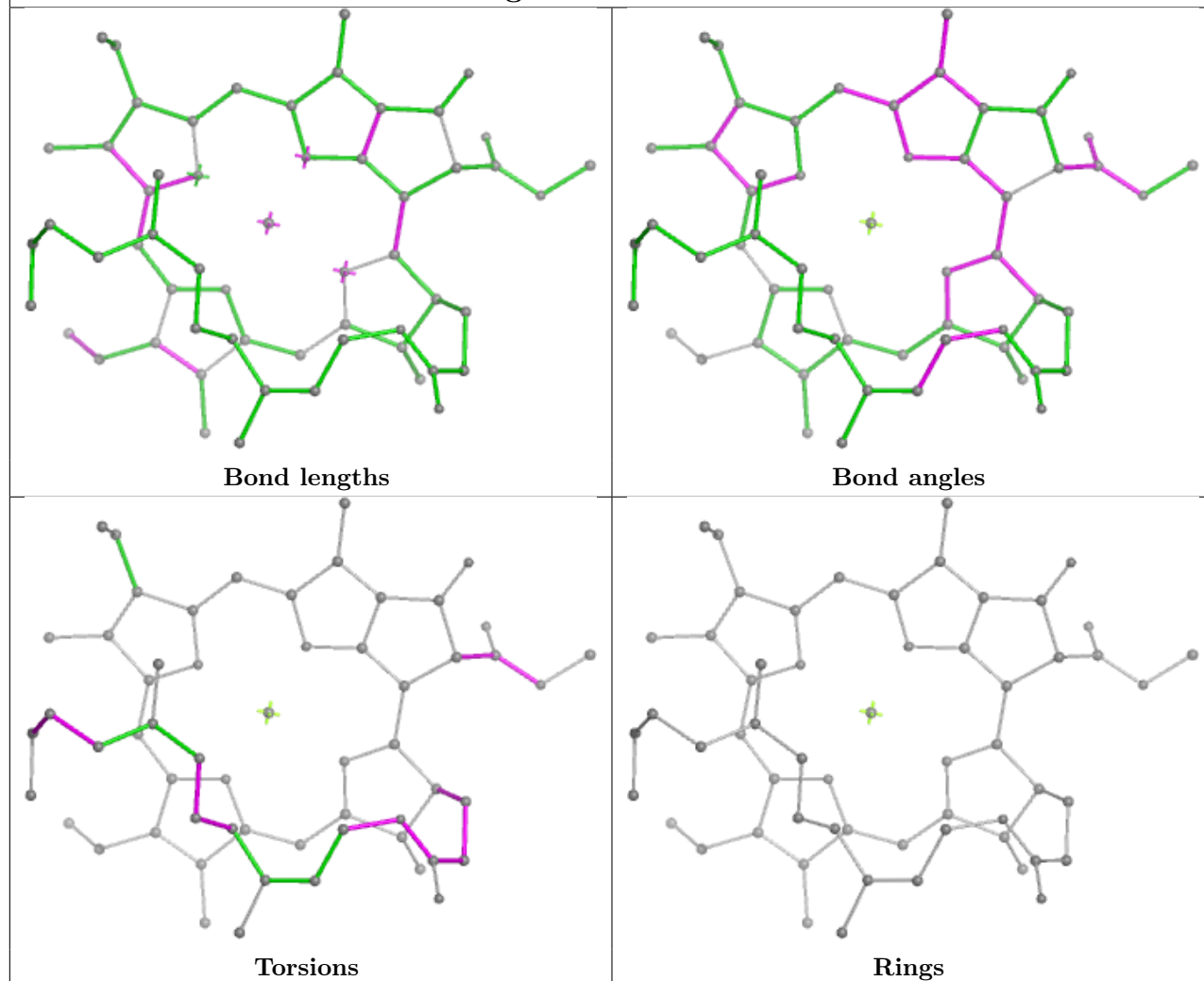




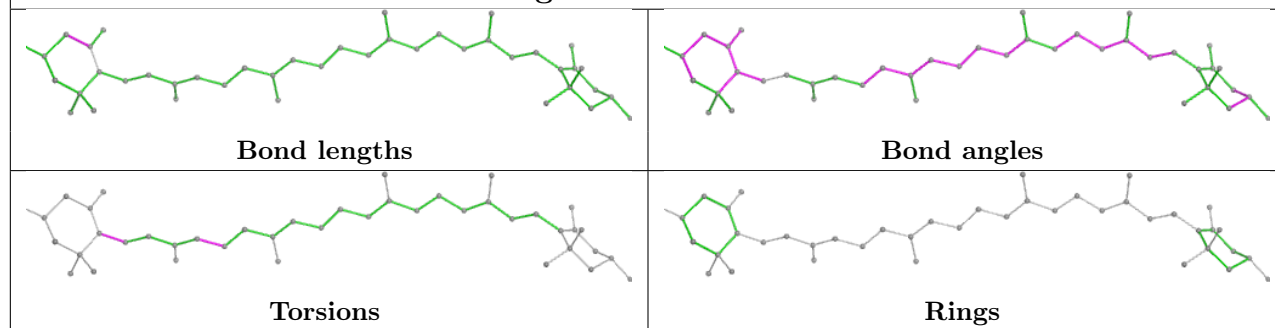
## Ligand CLA 1 605

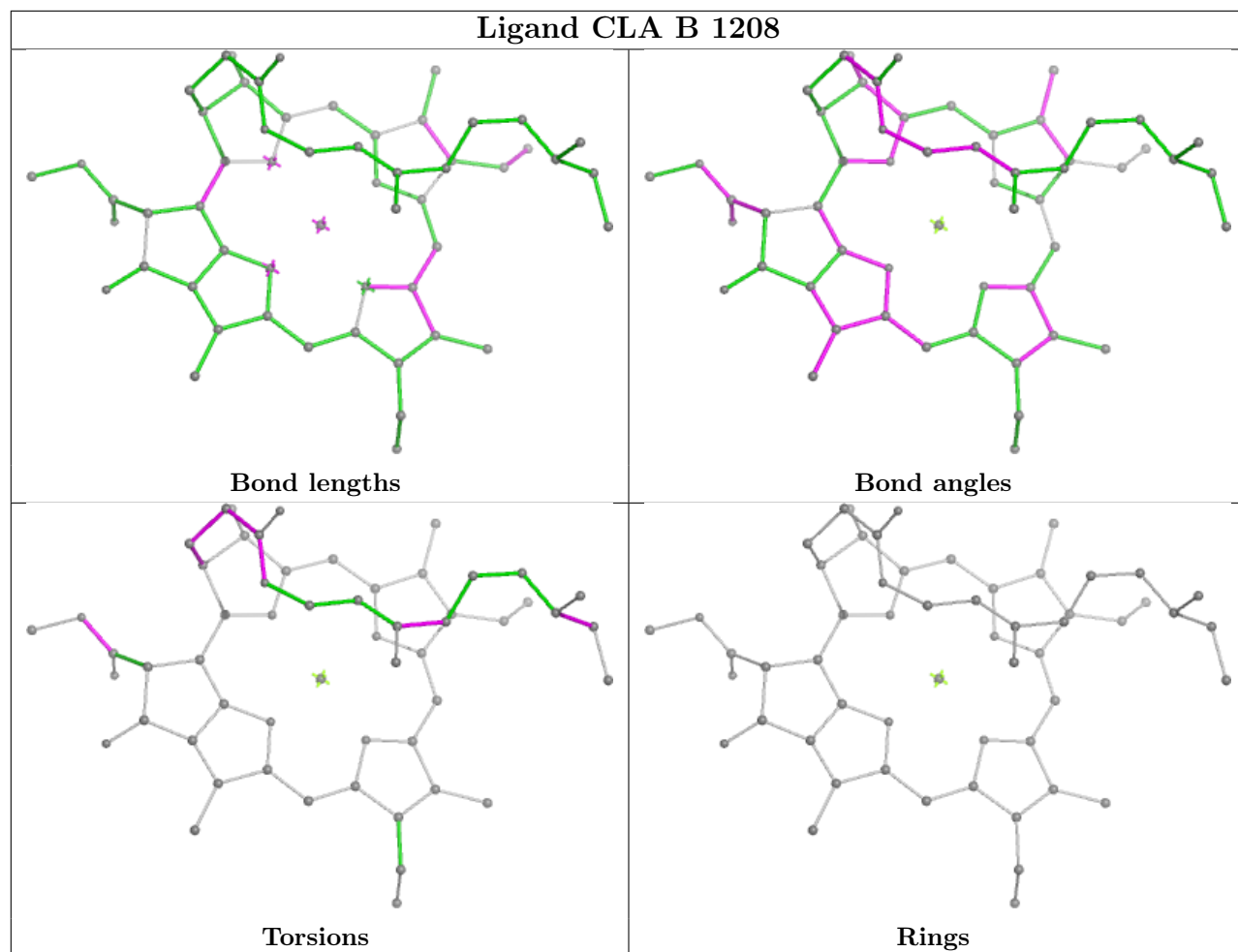


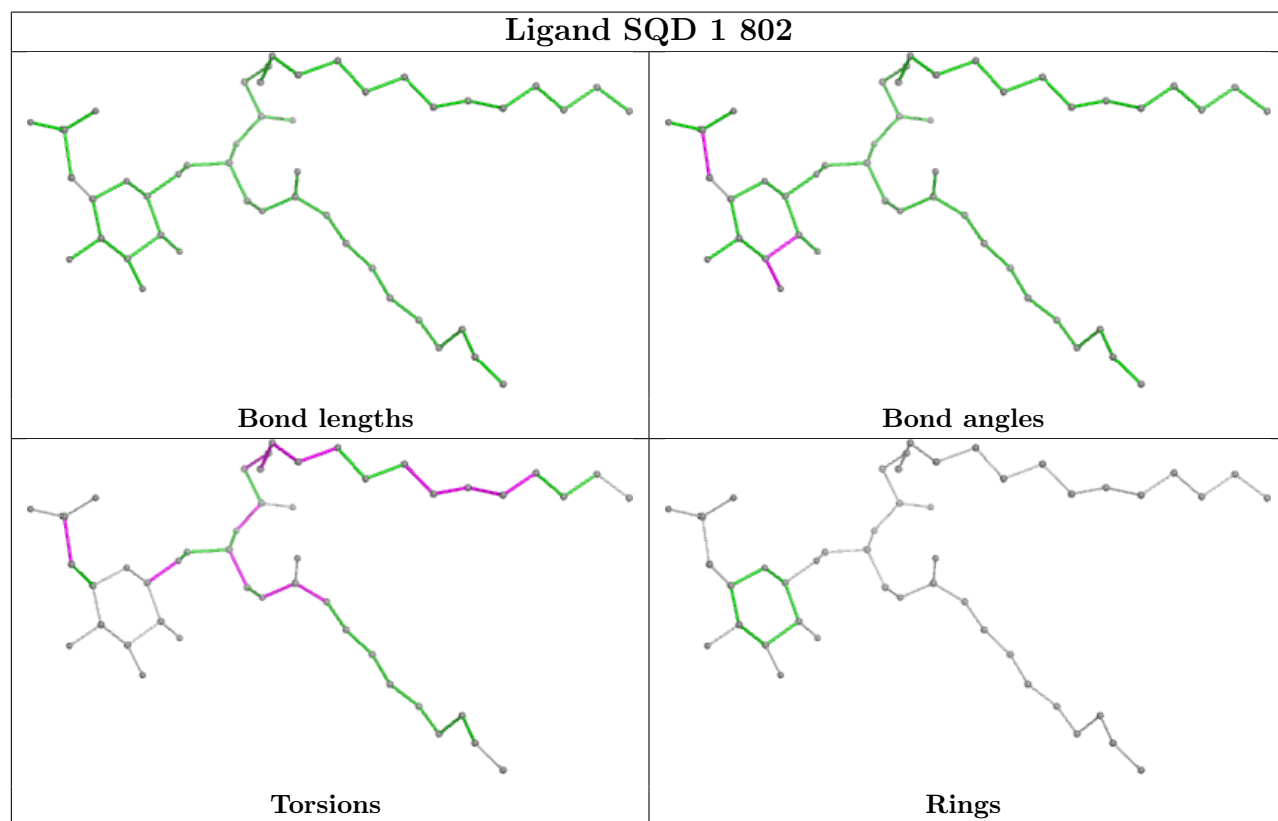
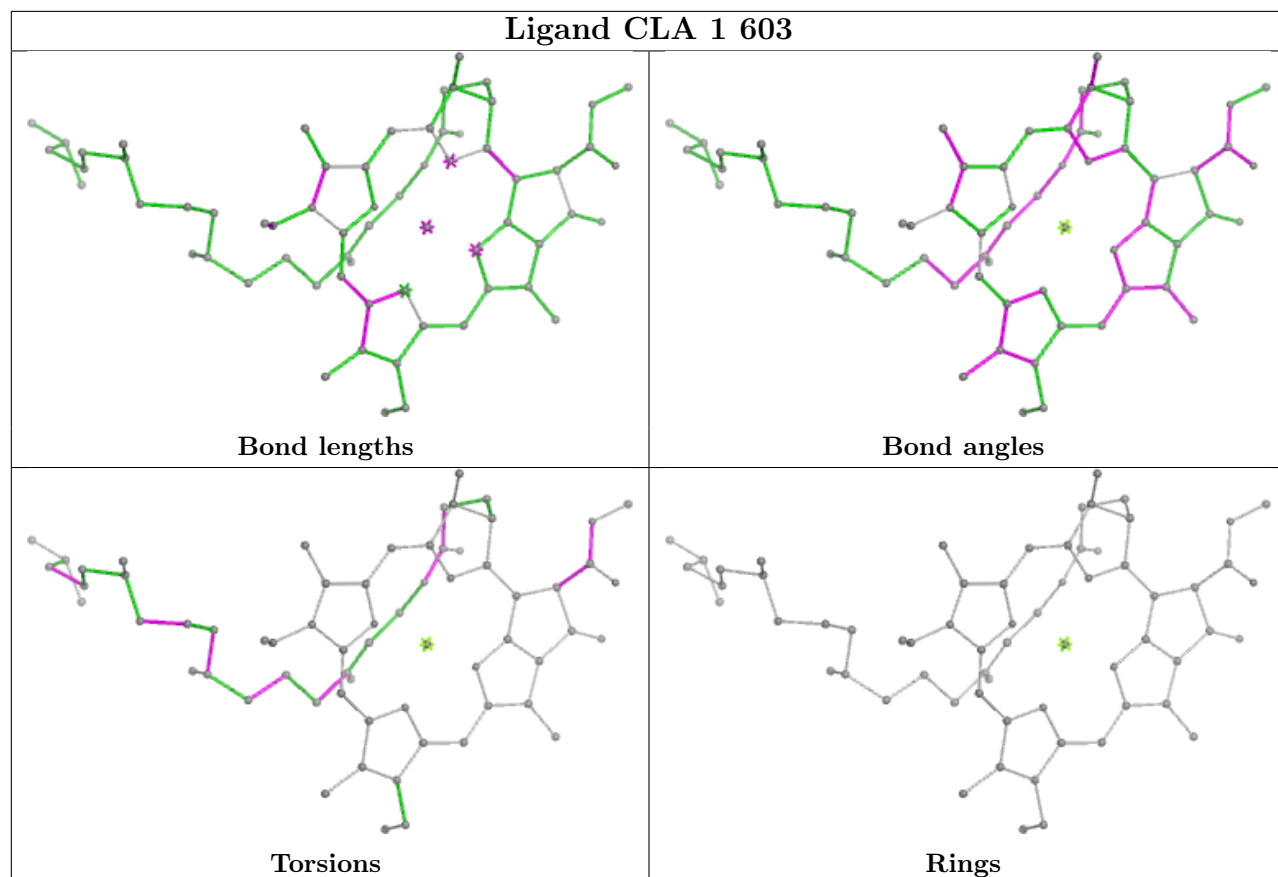
## Ligand CLA 7 615

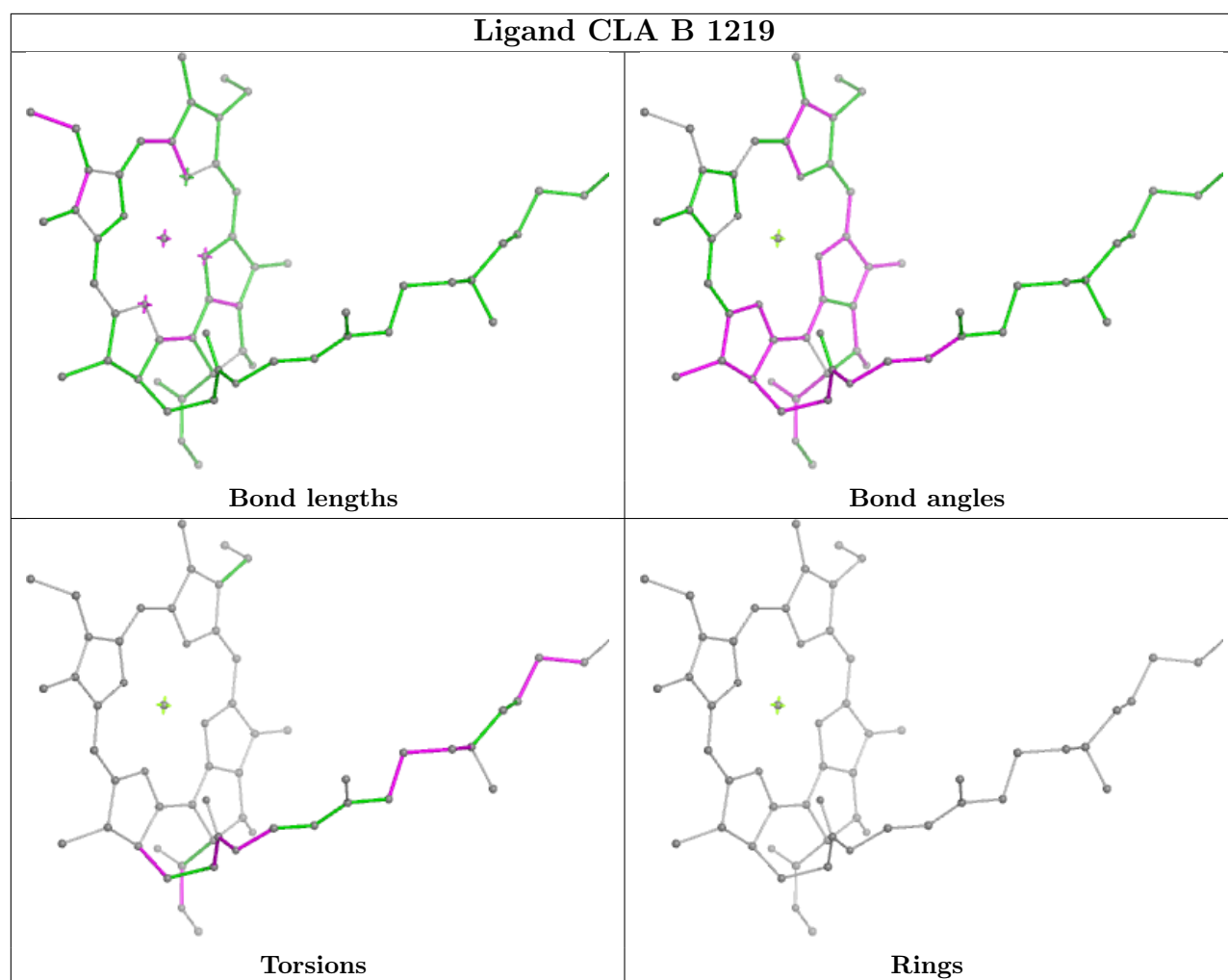


## Ligand LUT 7 502

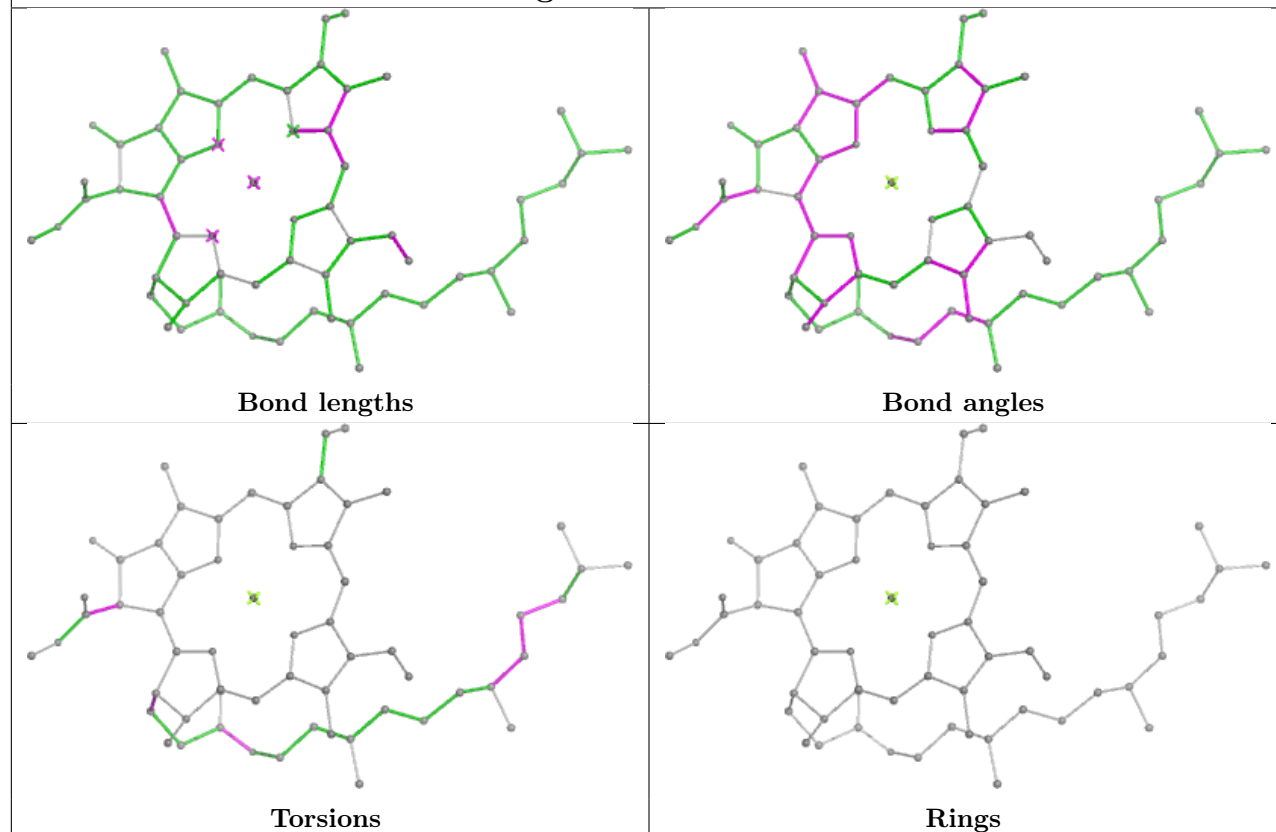




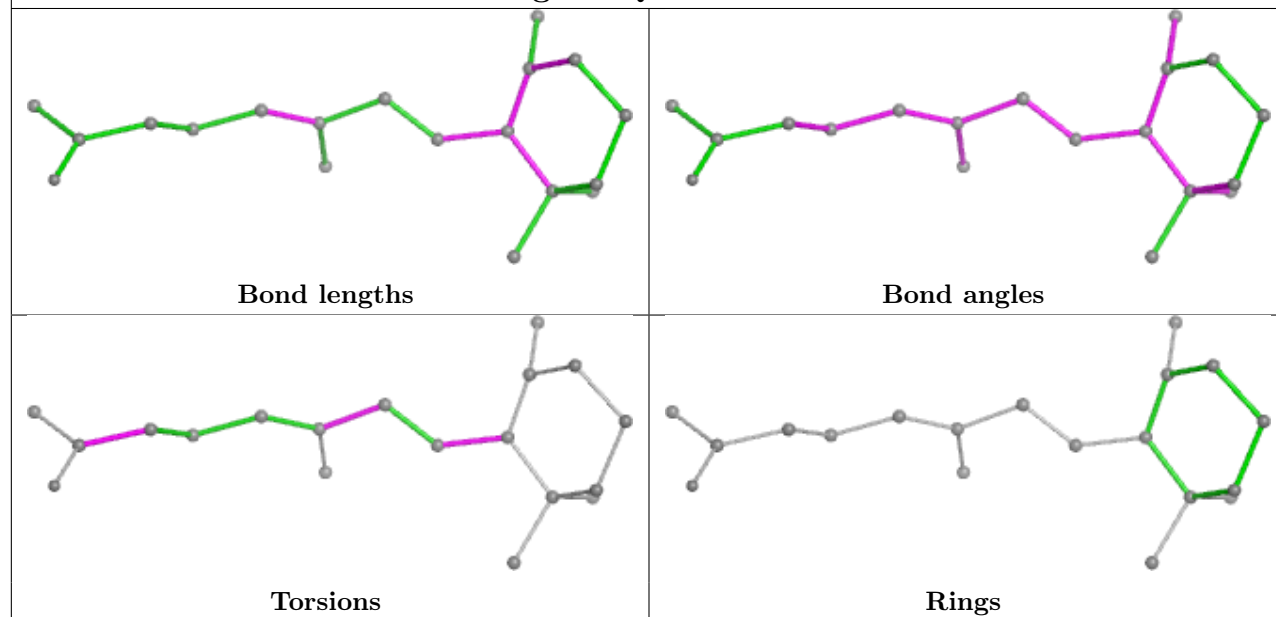


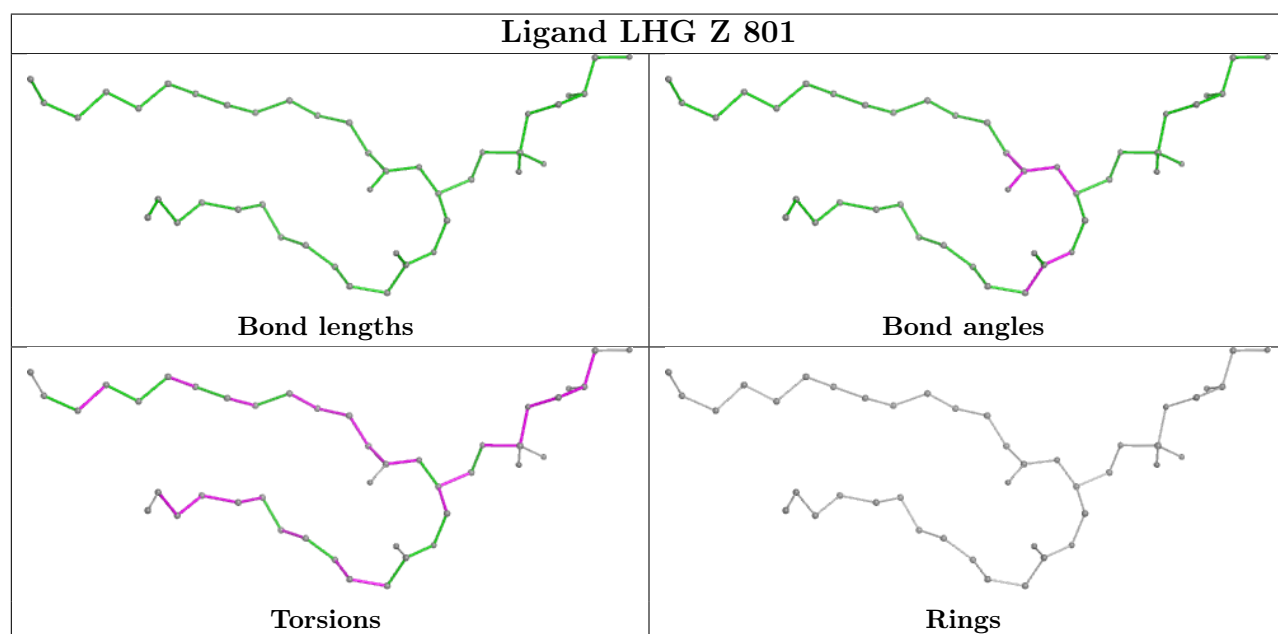
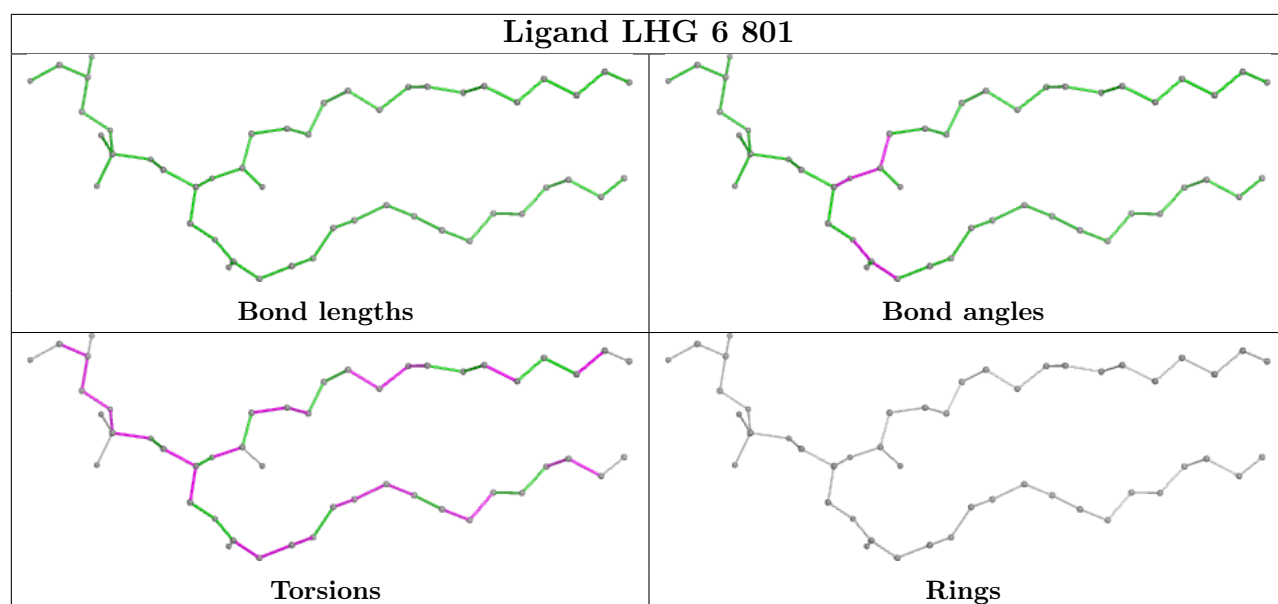


## Ligand CLA 4 604



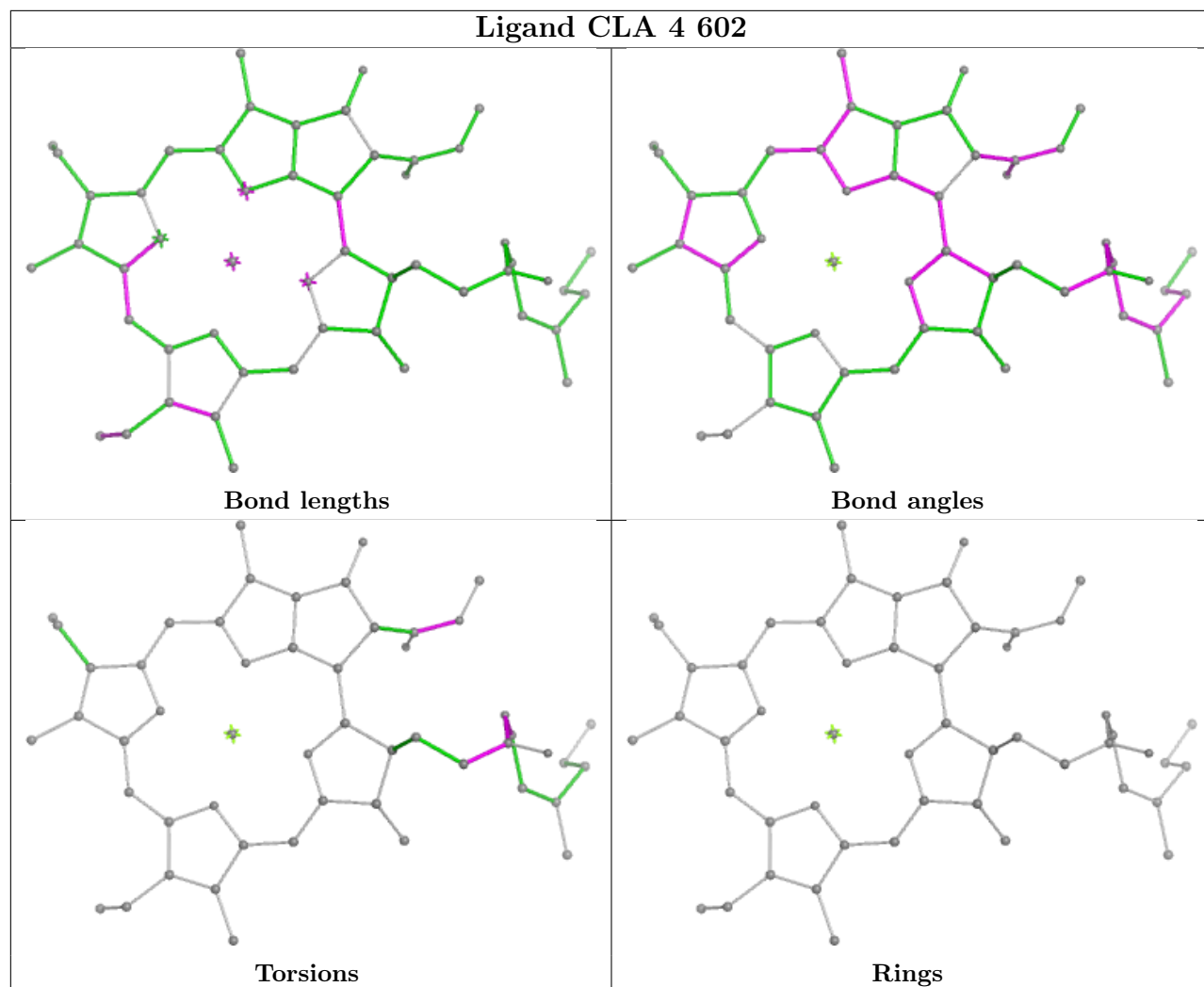
## Ligand QTB Z 504



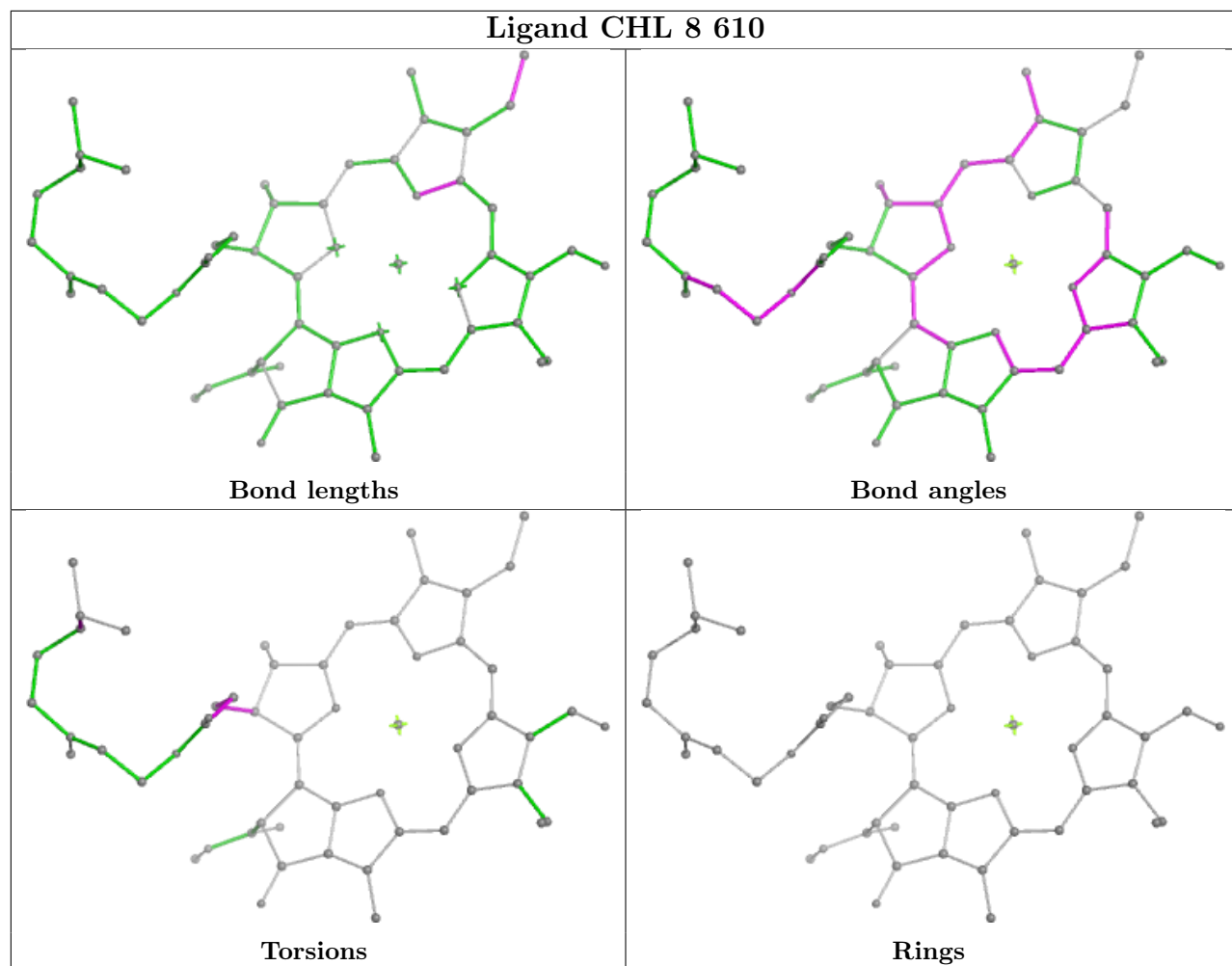




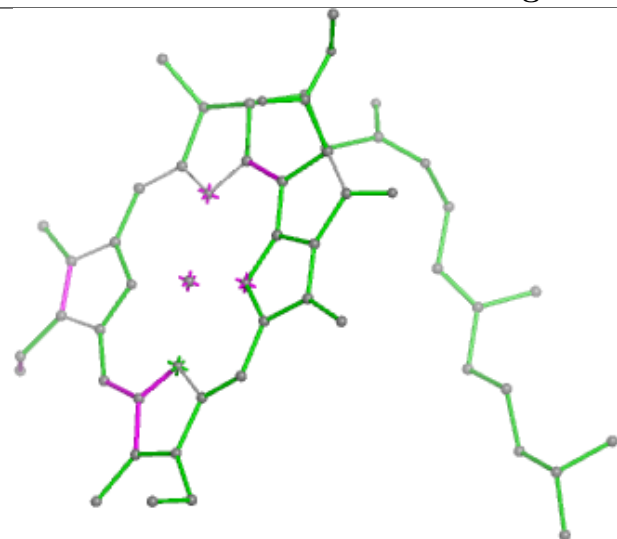
## Ligand CLA 4 602



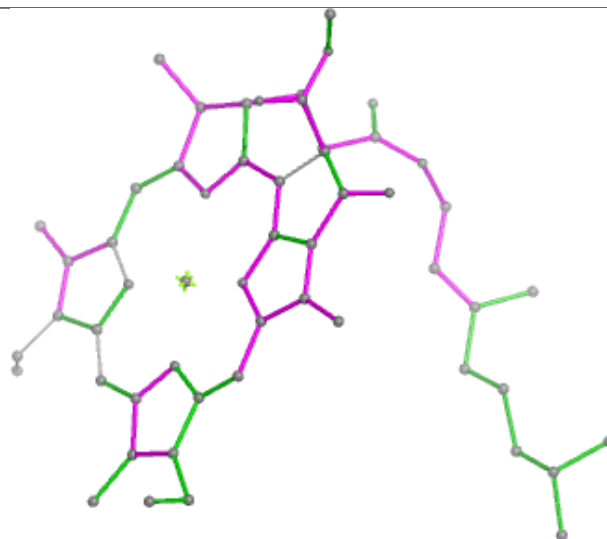
## Ligand CHL 8 610



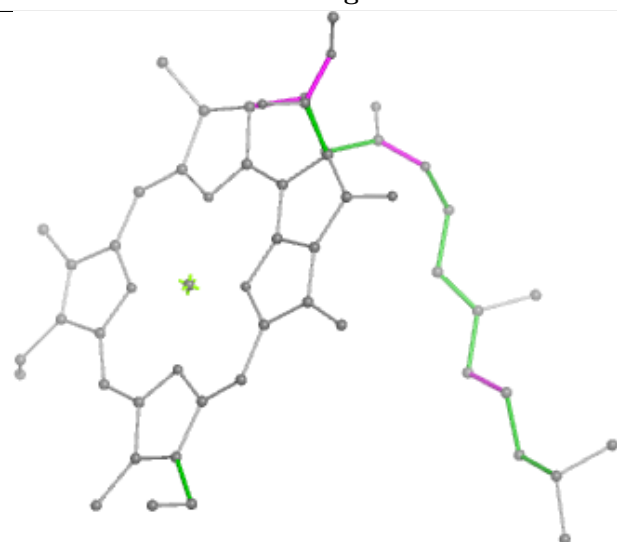
## Ligand CLA 6 607



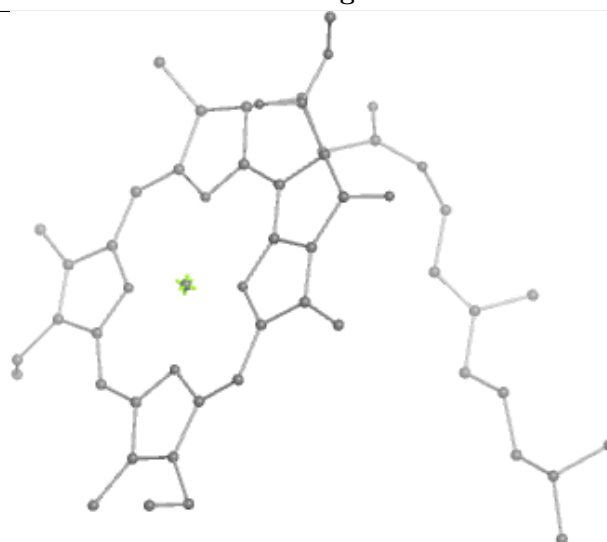
Bond lengths



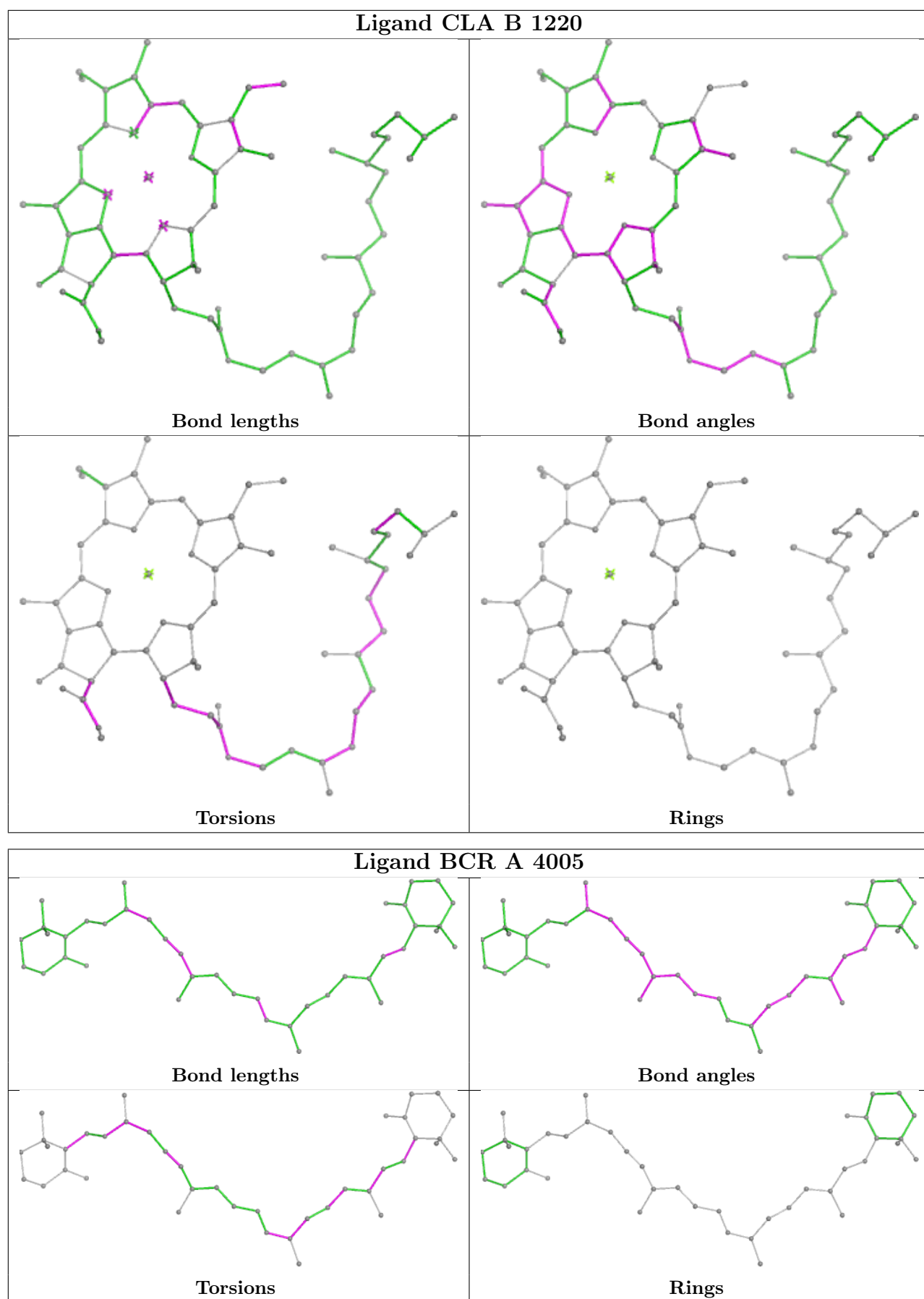
Bond angles

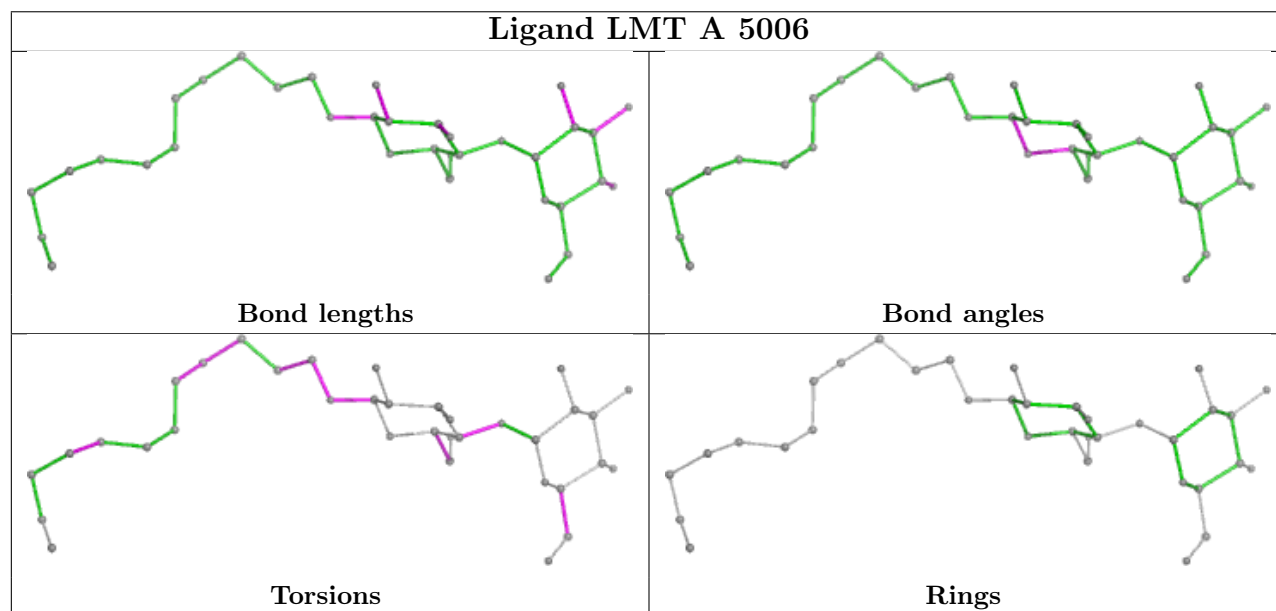
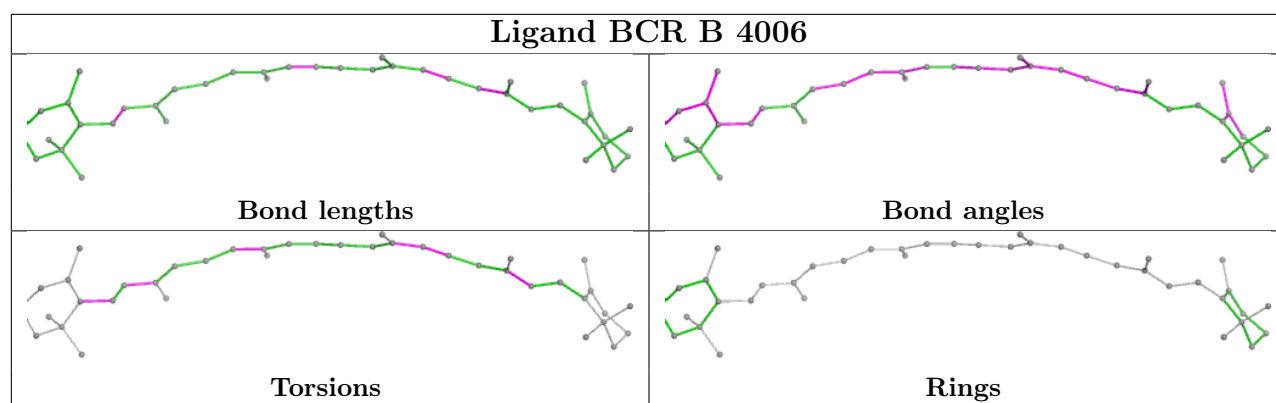


Torsions

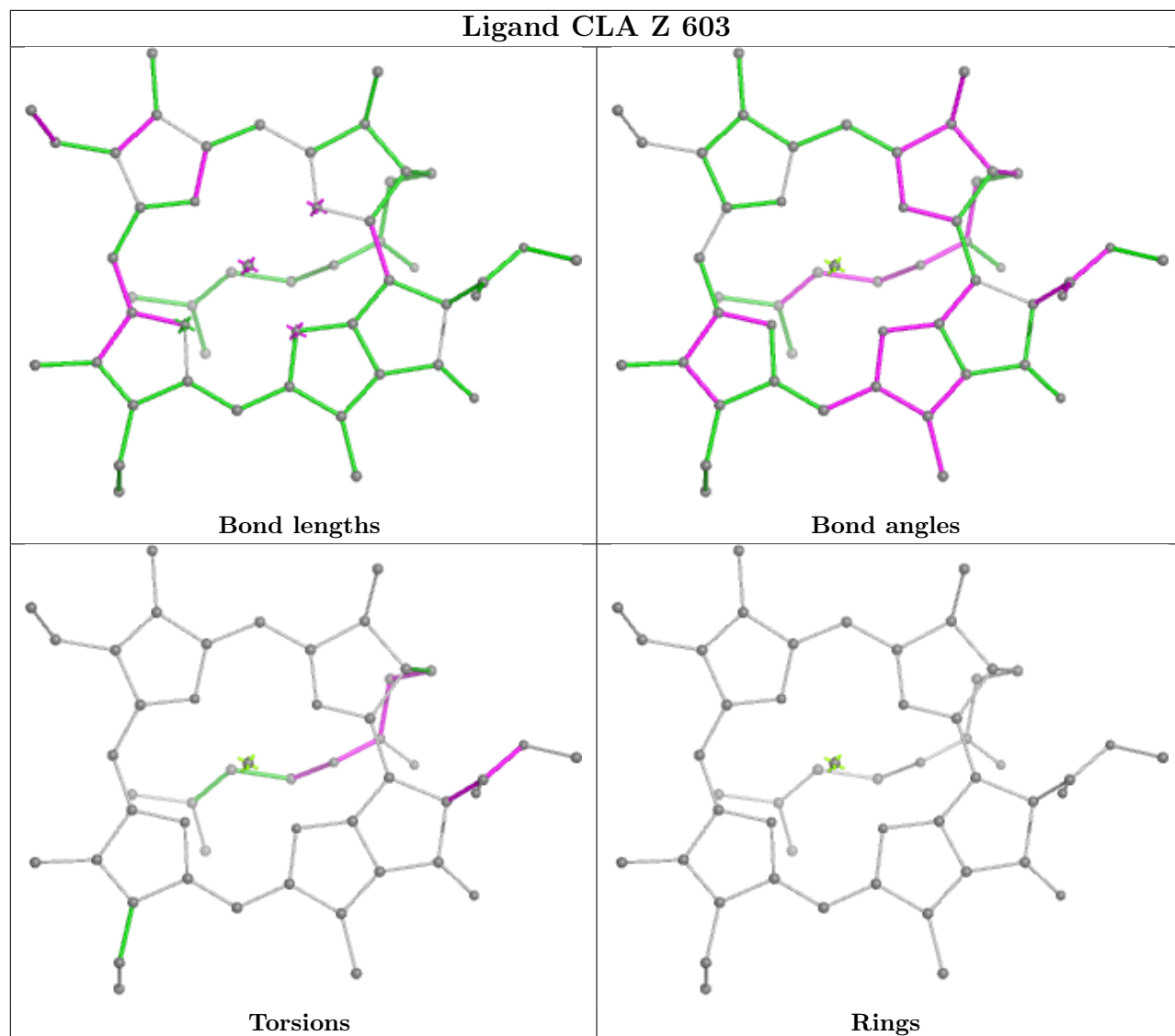


Rings

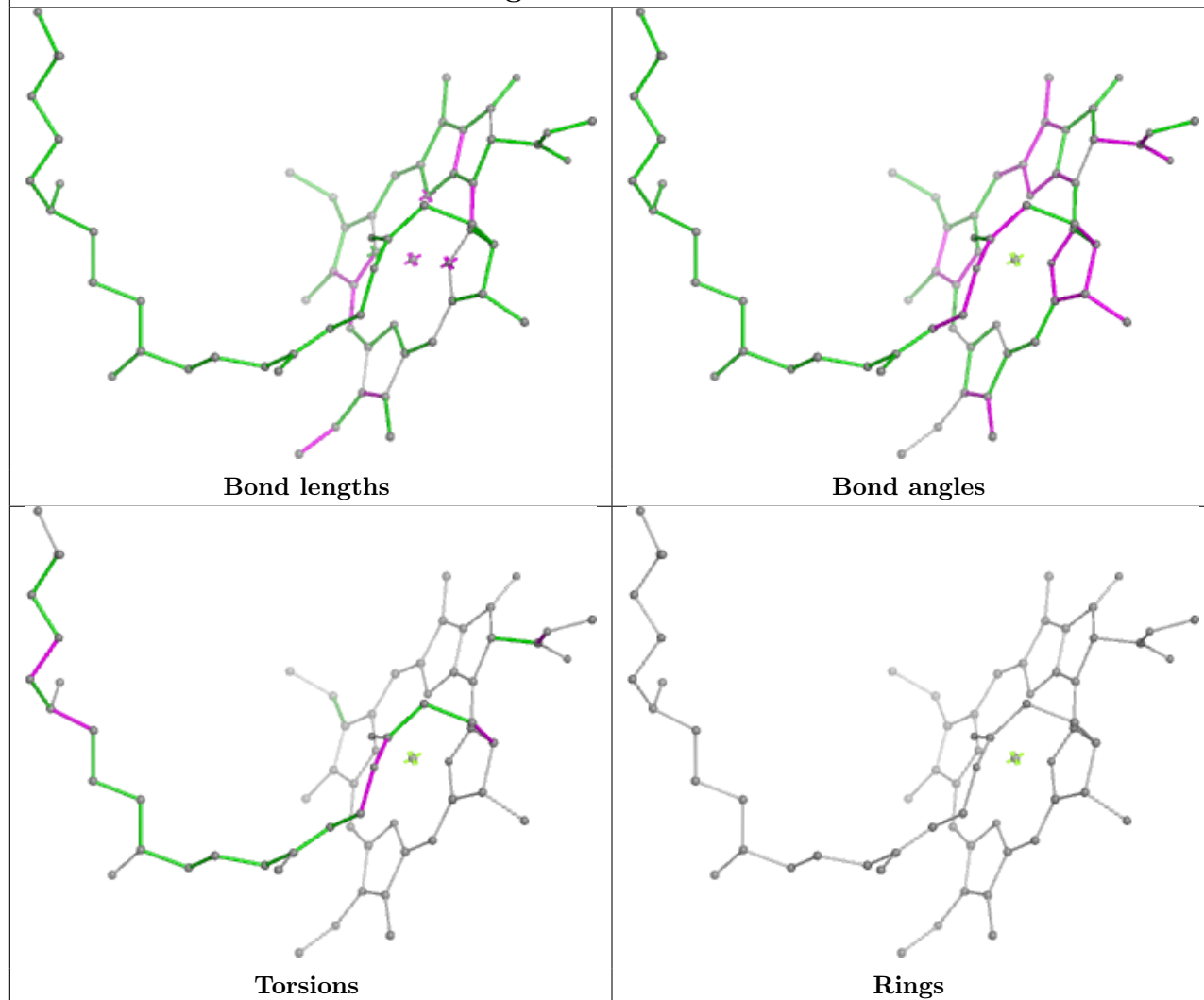




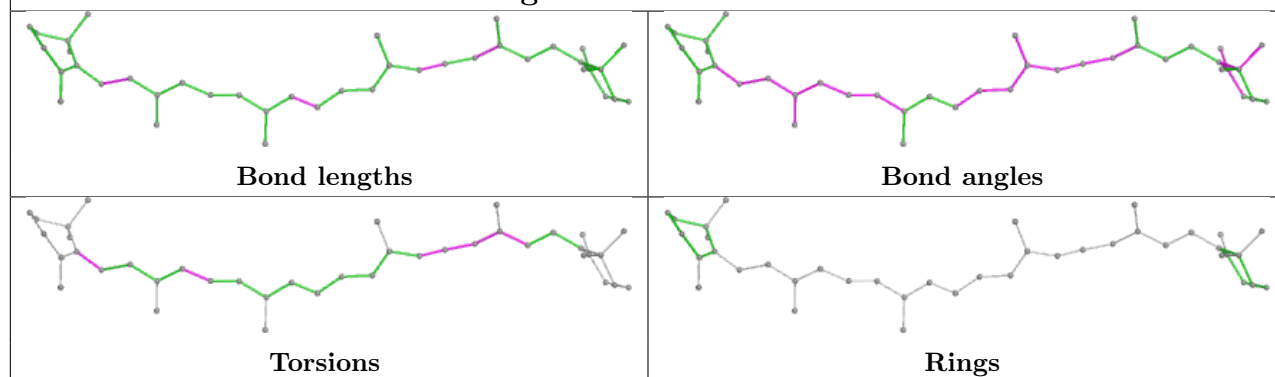
## Ligand CLA Z 603

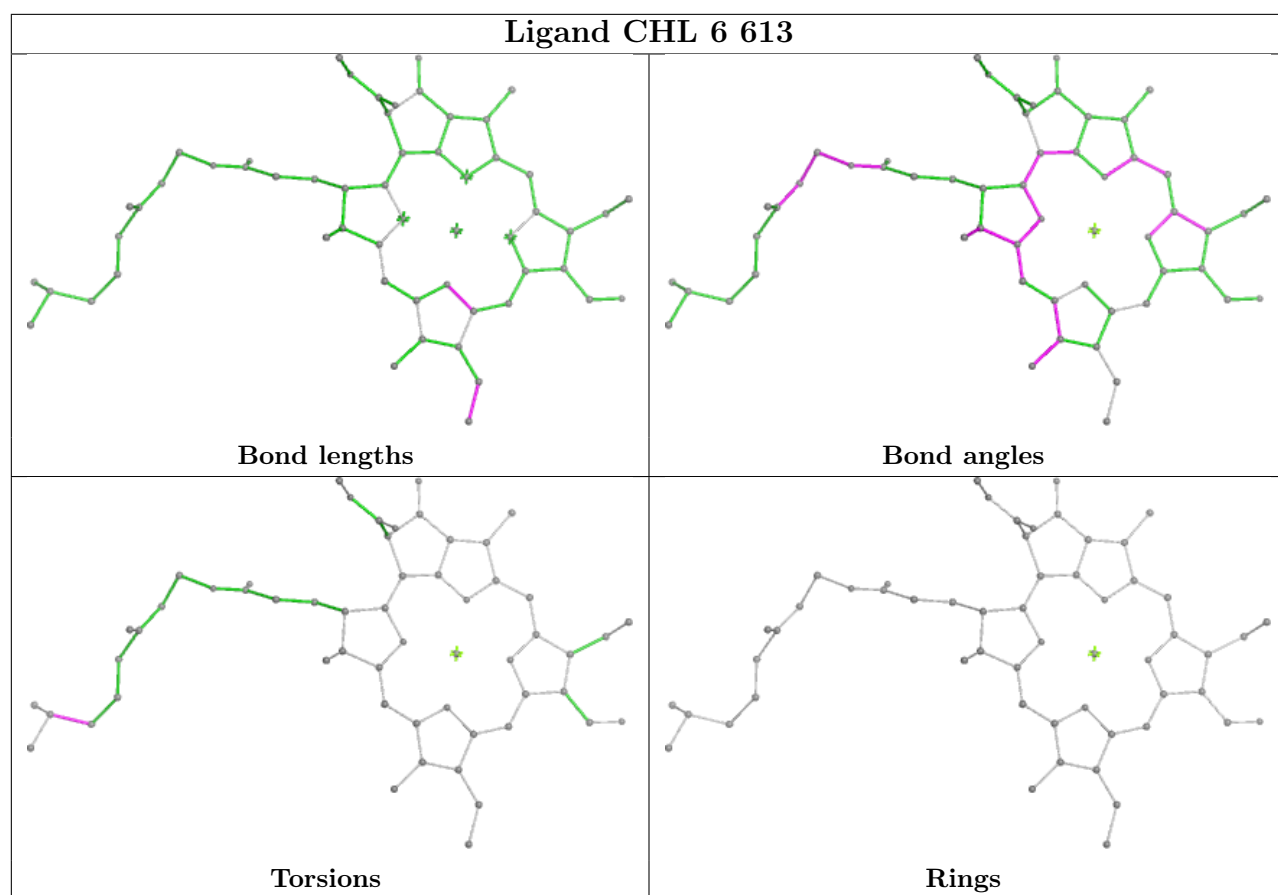


## Ligand CLA 3 601



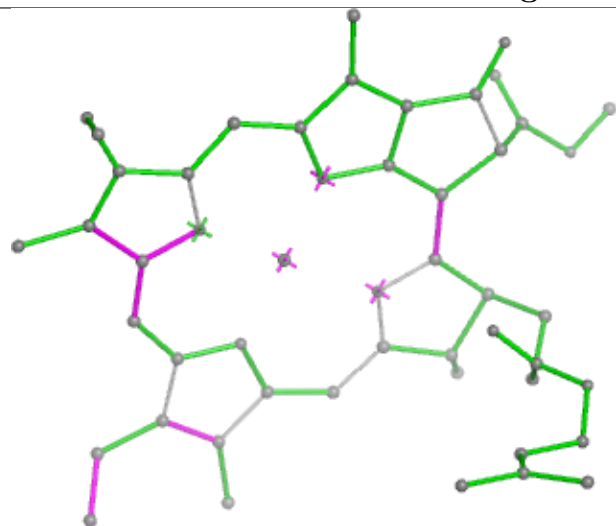
## Ligand BCR B 4004



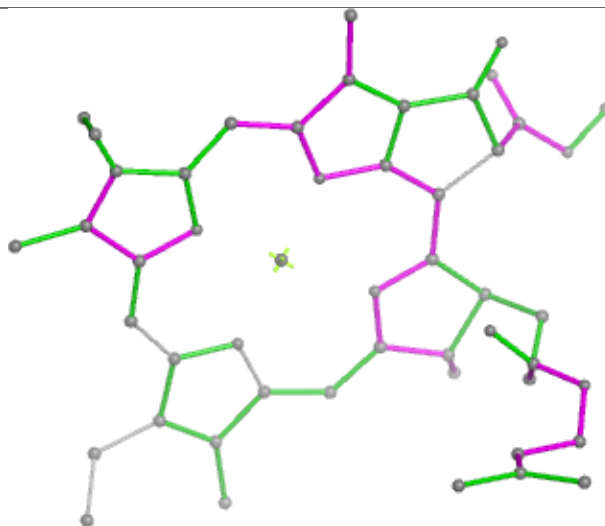




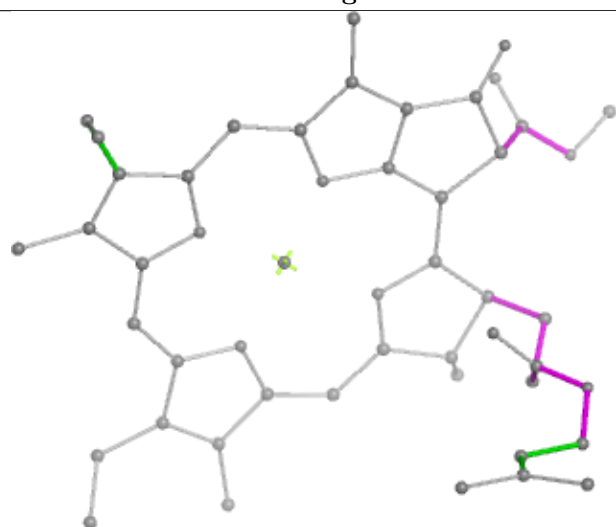
## Ligand CLA 5 606



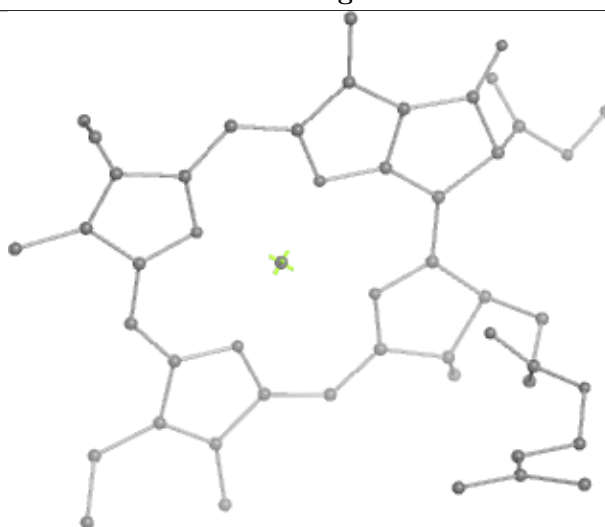
Bond lengths



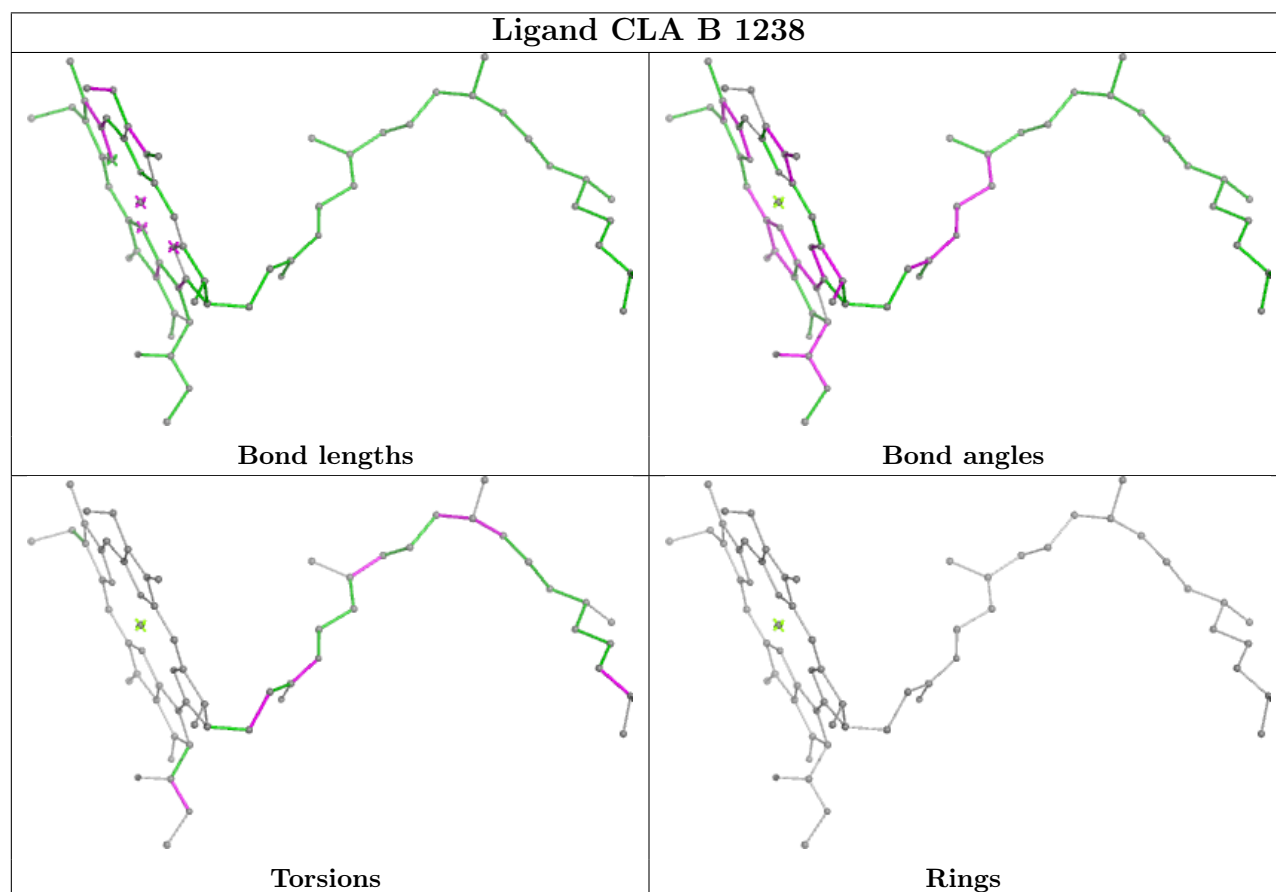
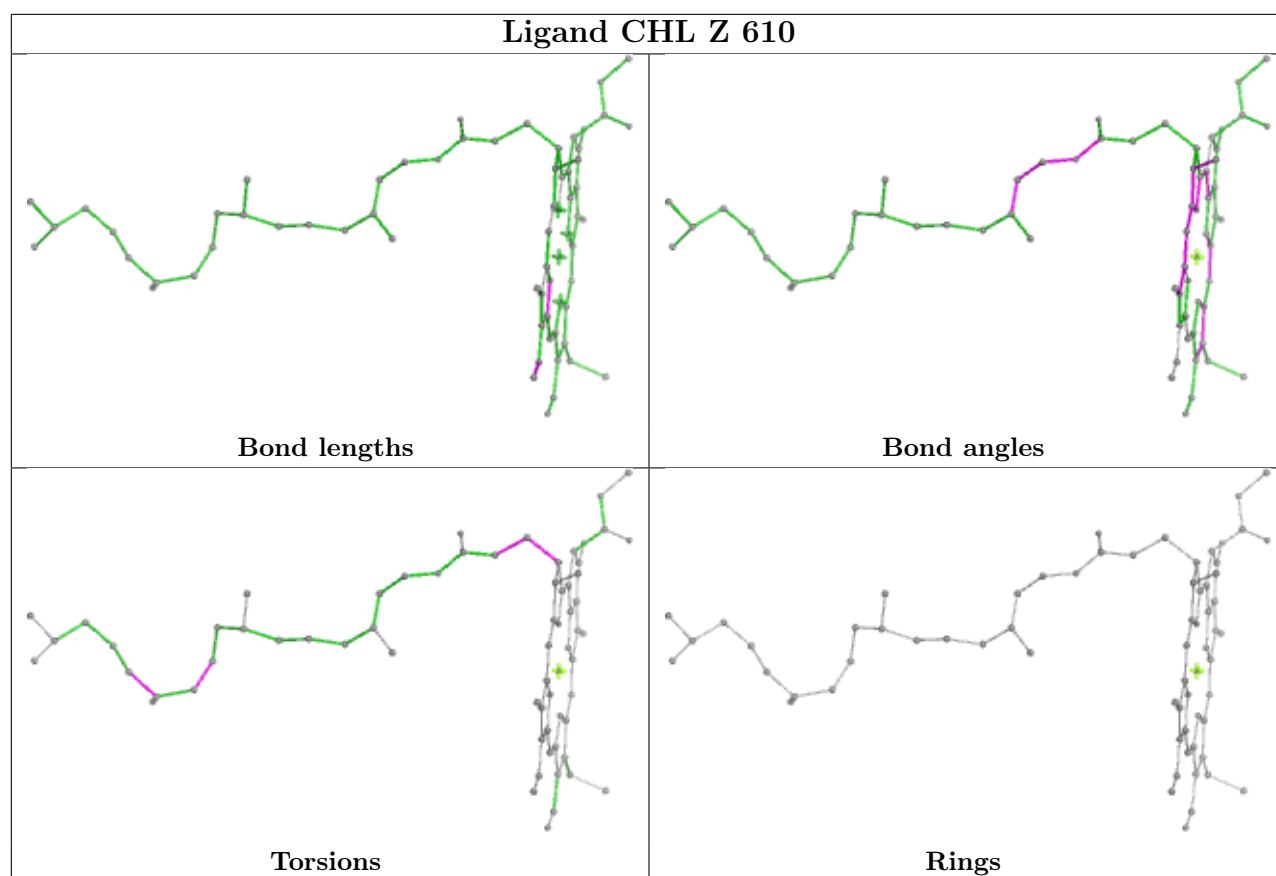
Bond angles

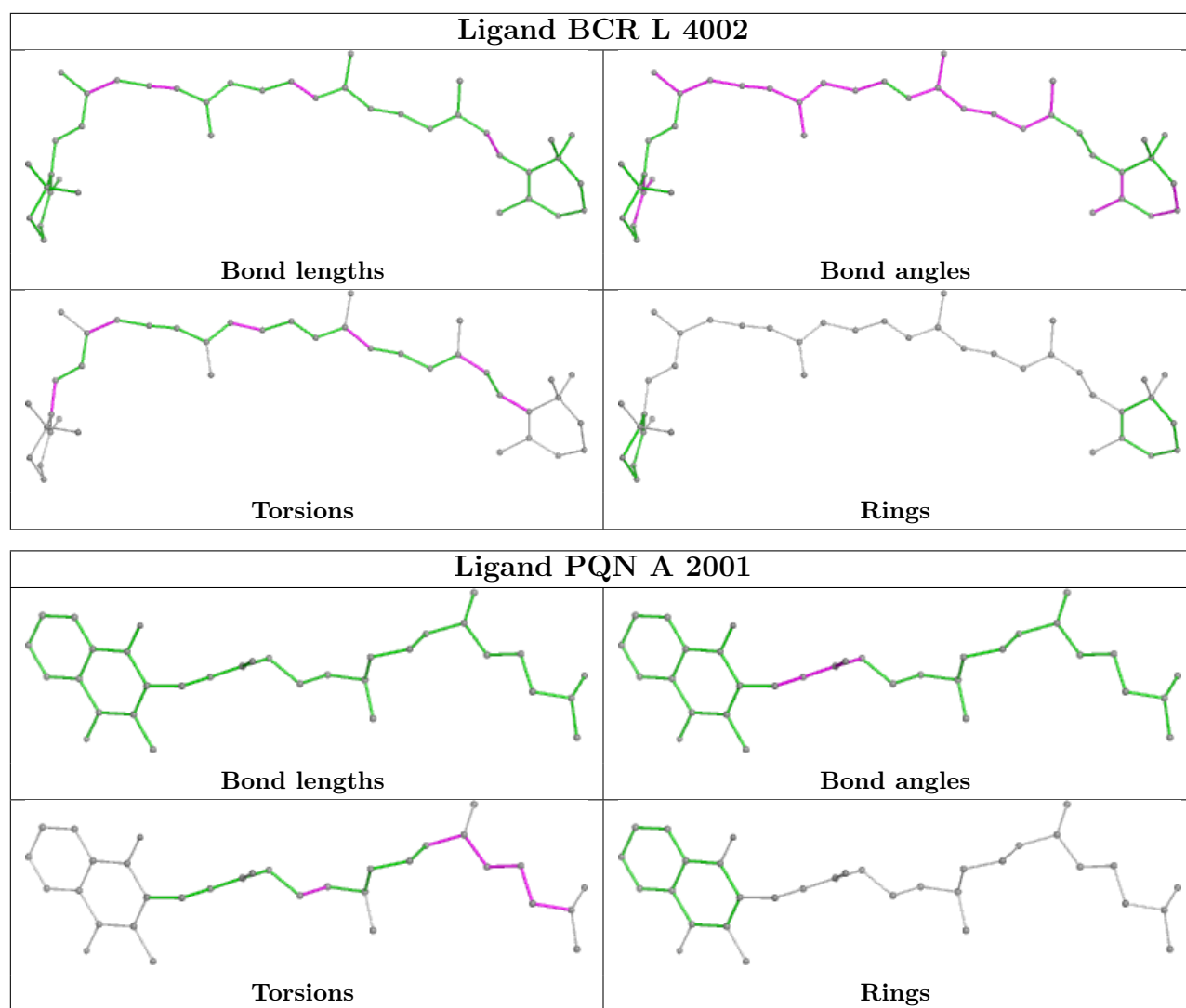


Torsions

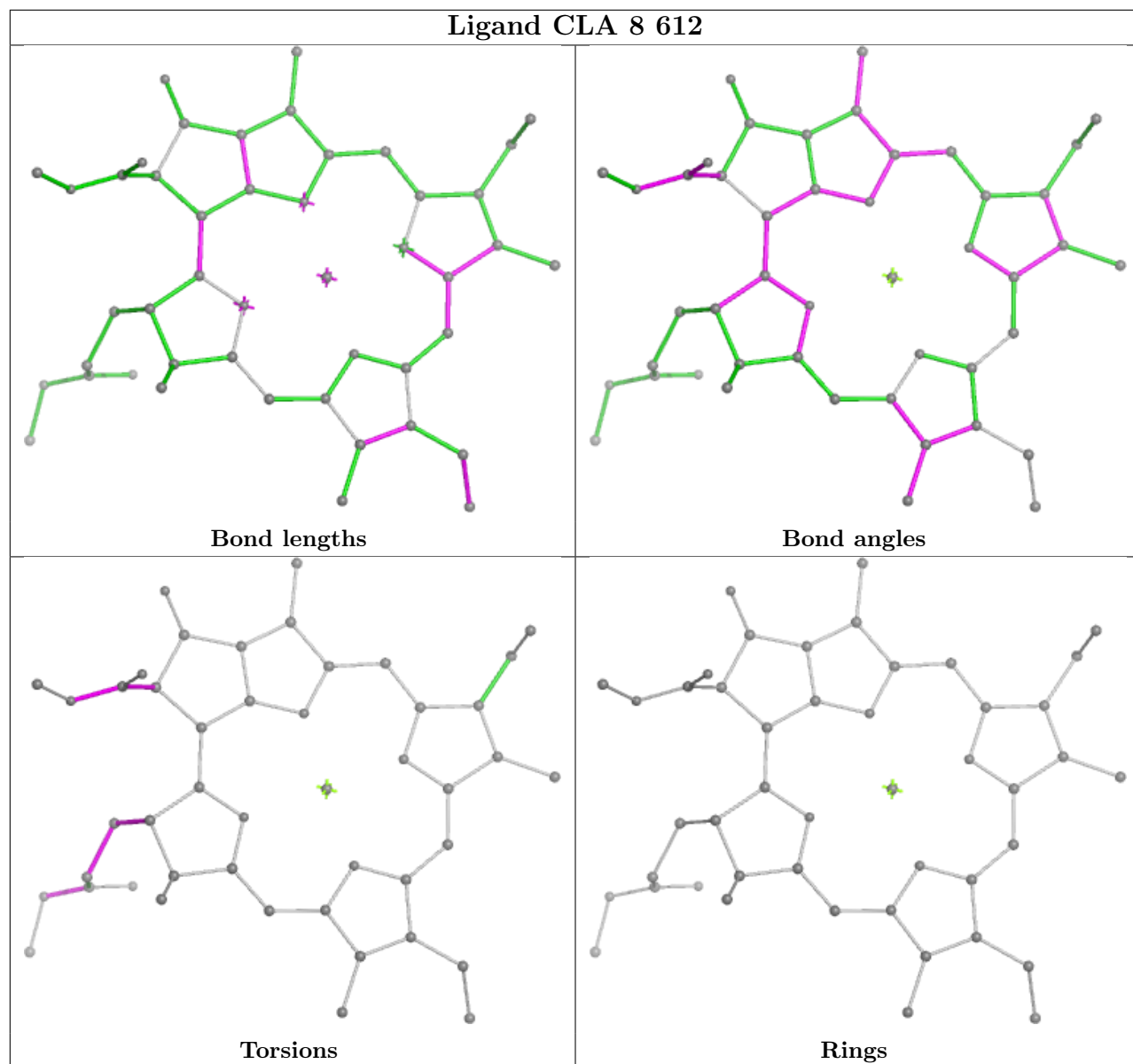


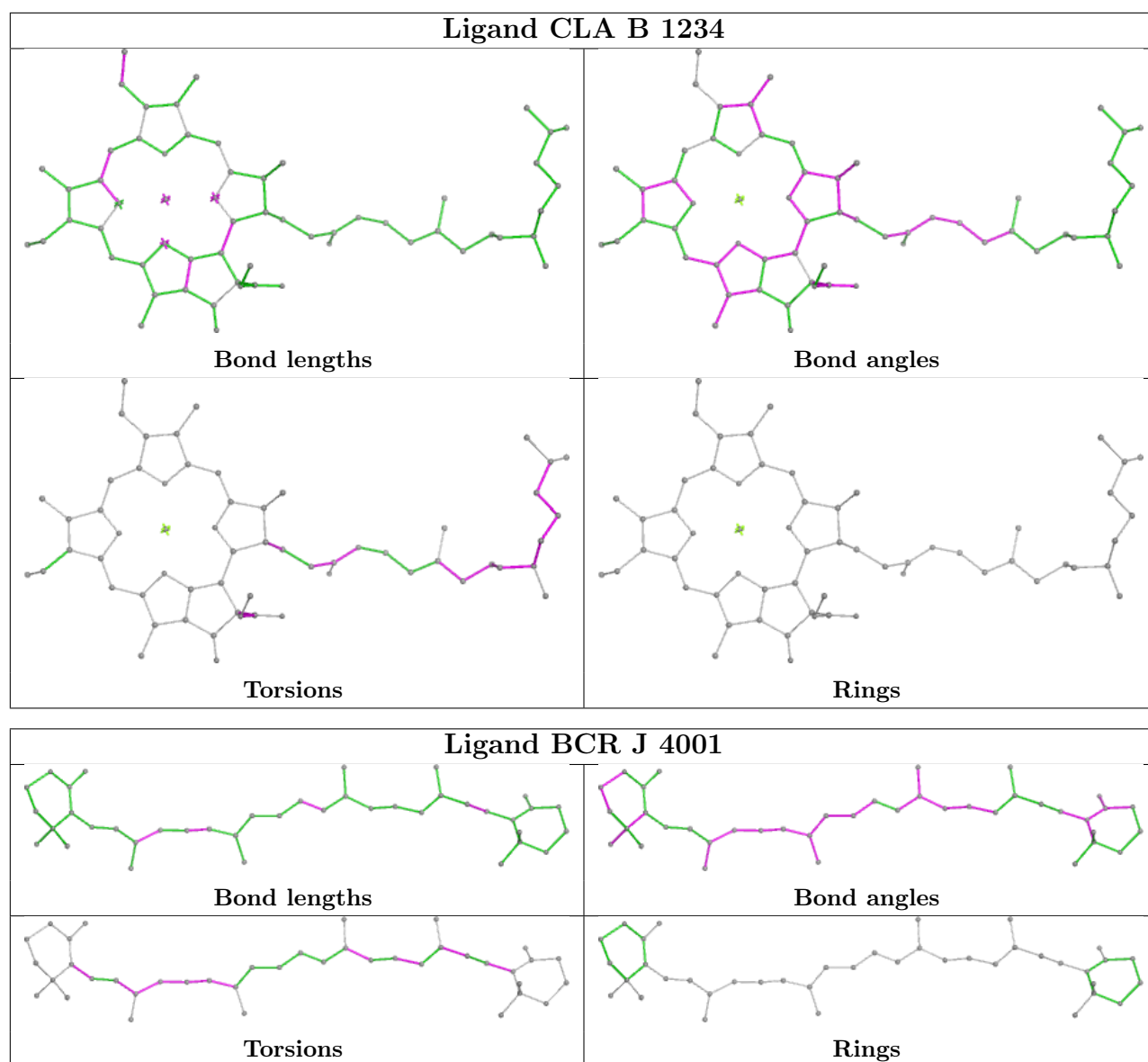
Rings

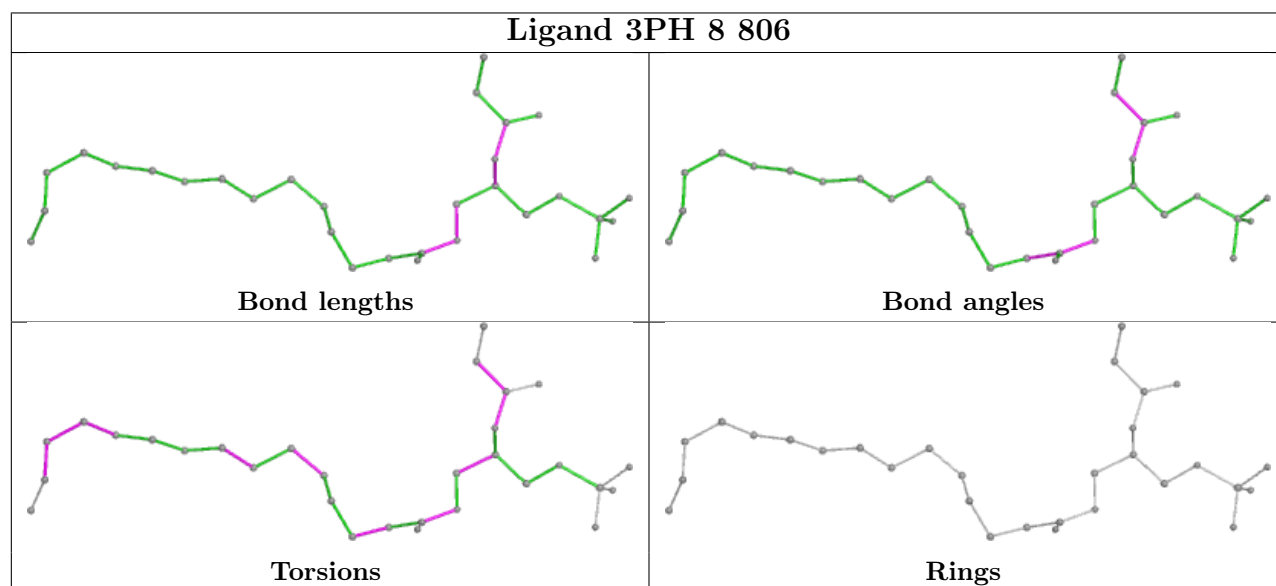
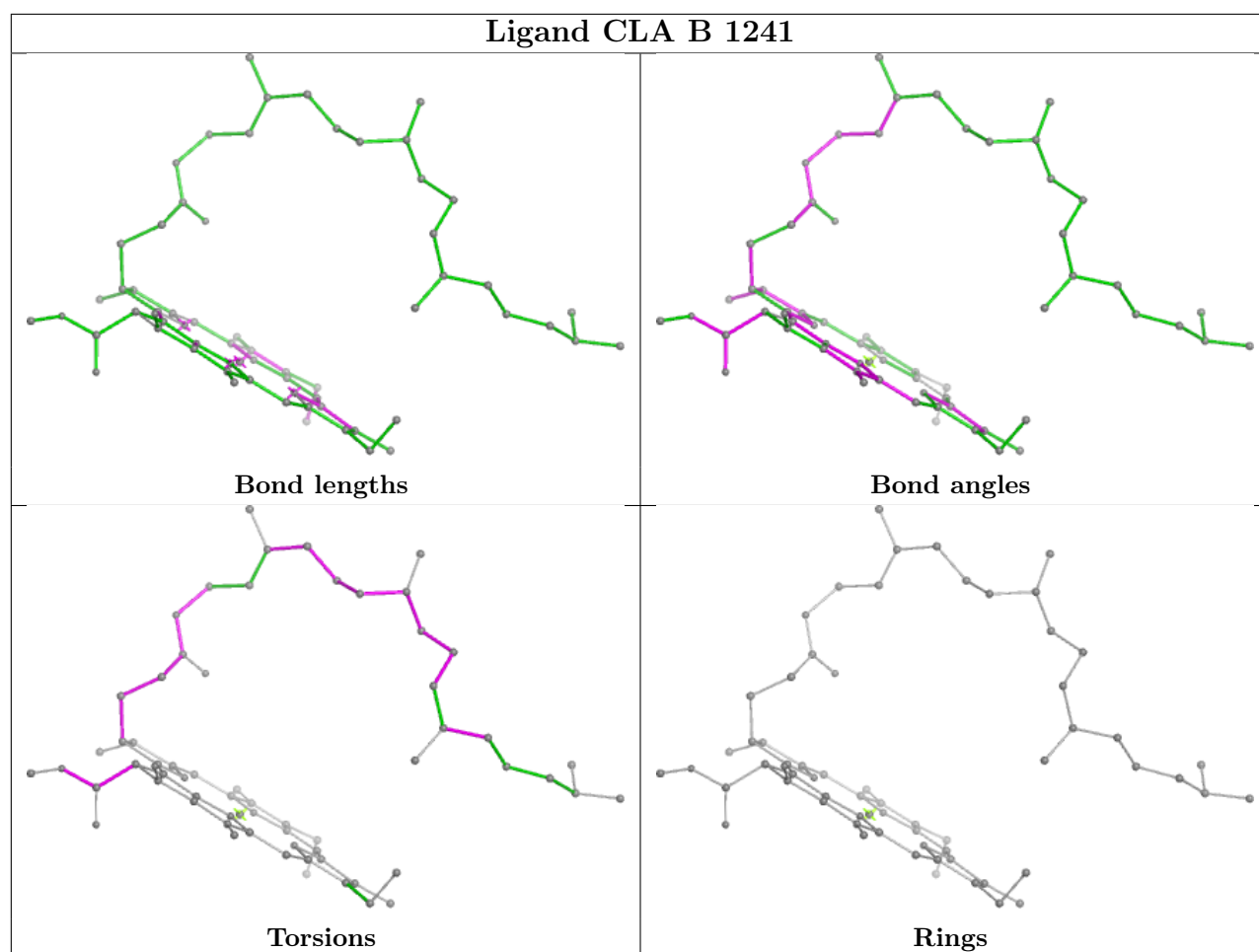


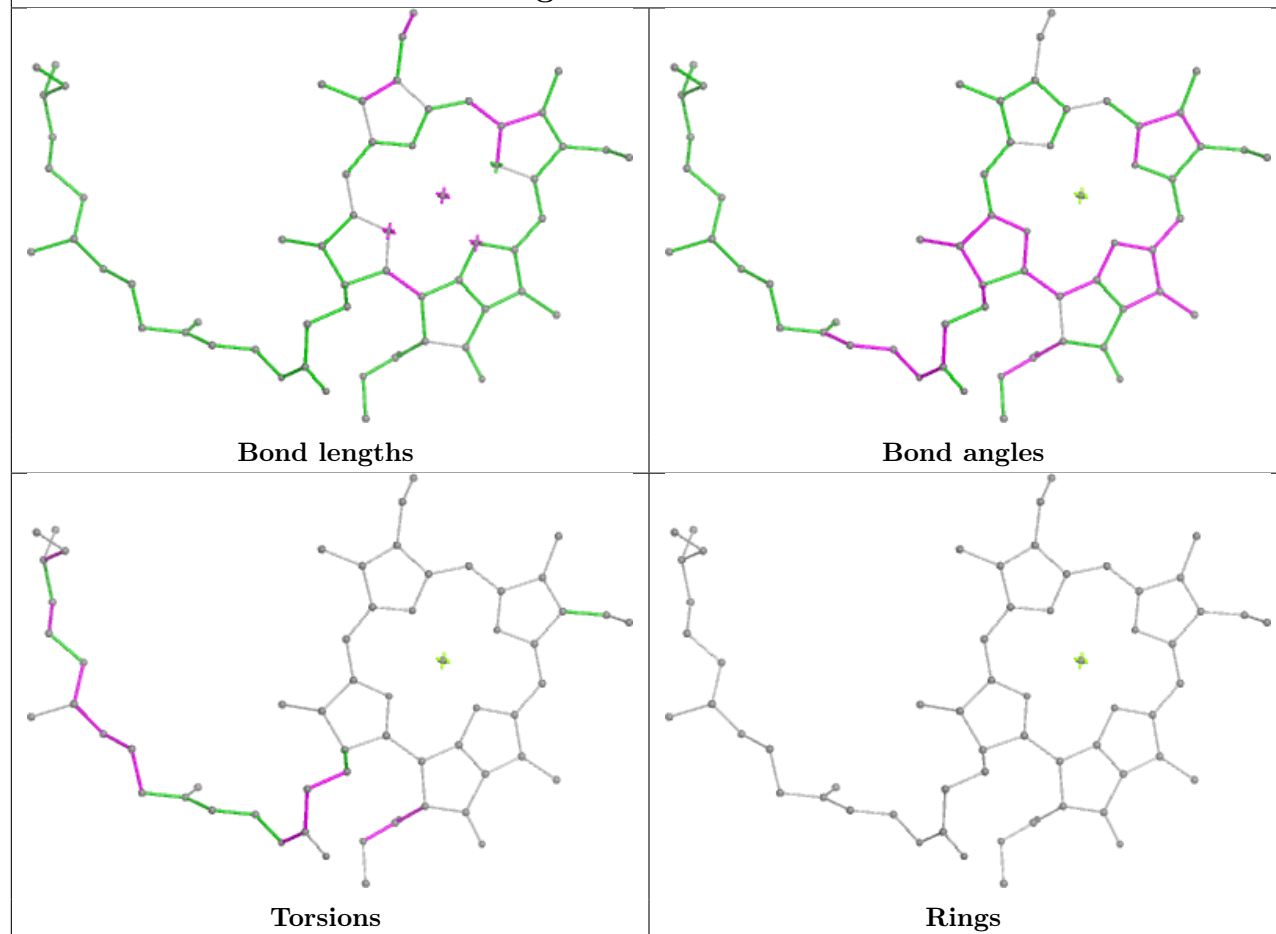
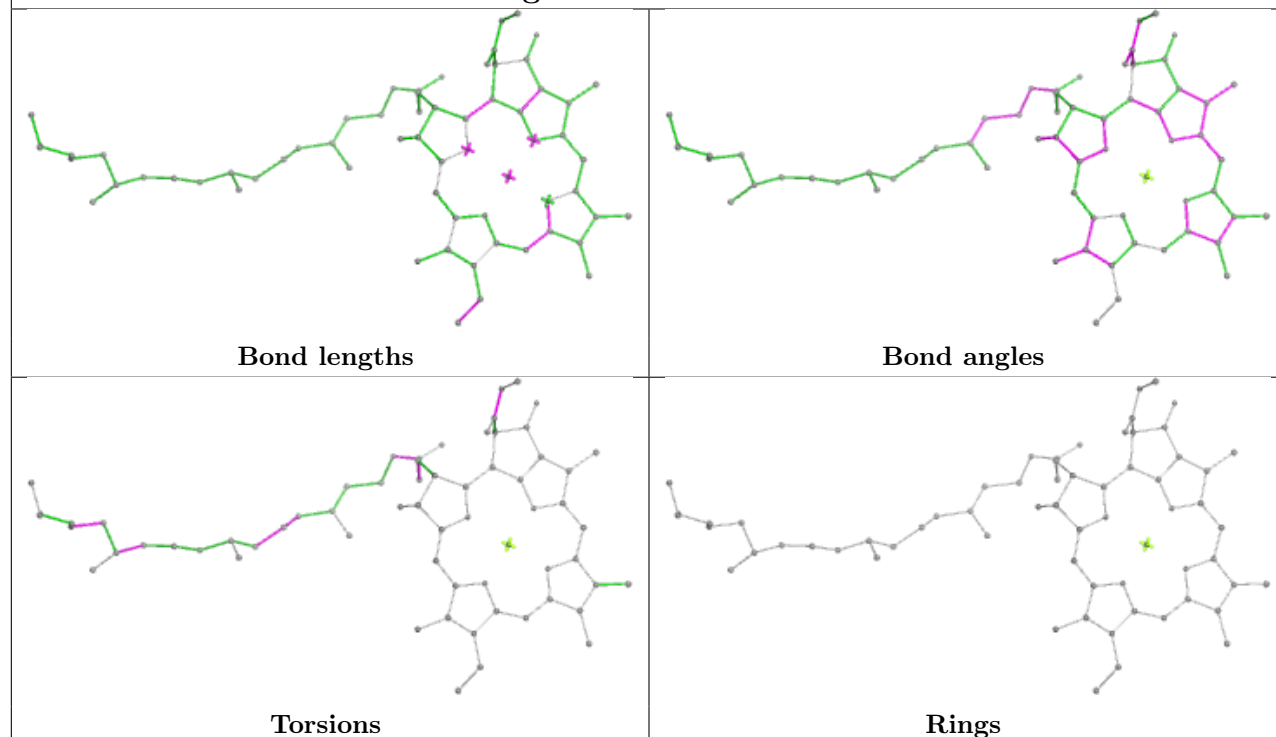


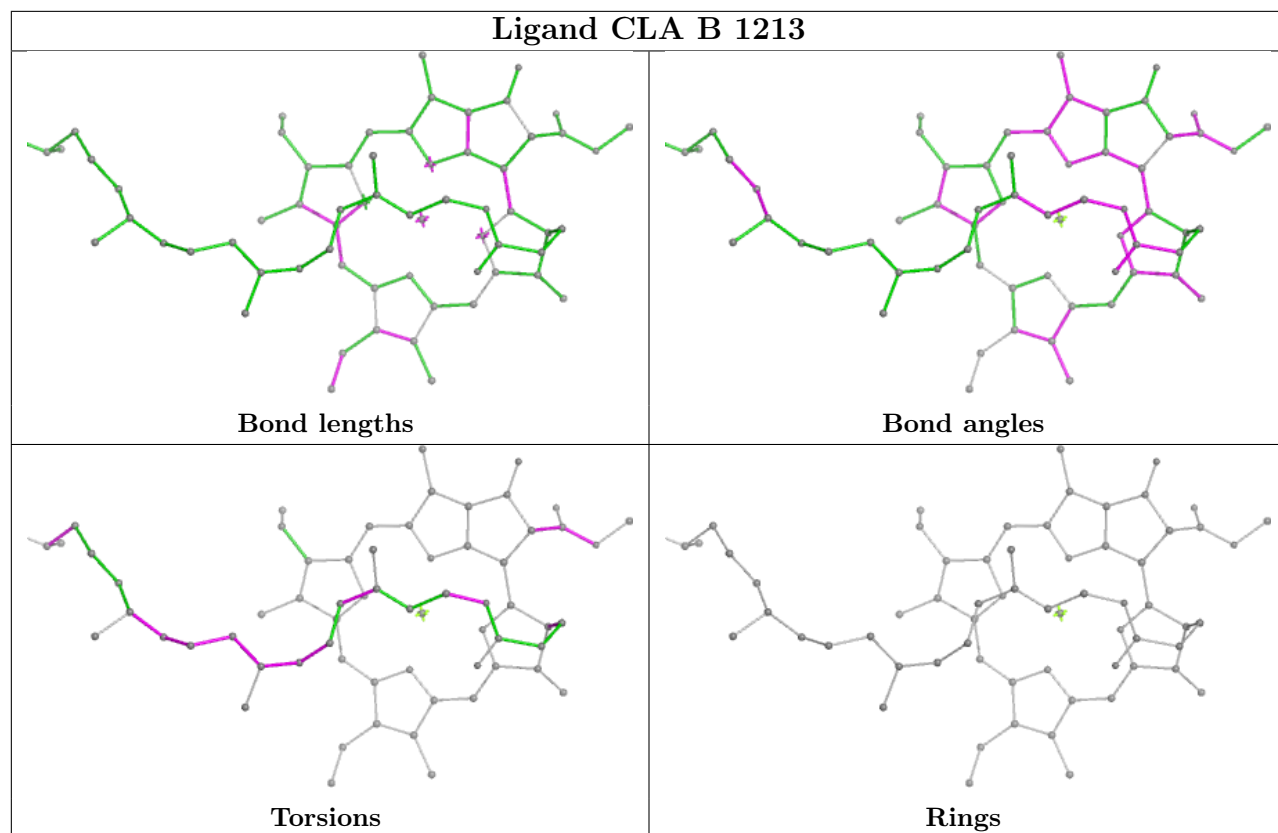
## Ligand CLA 8 612





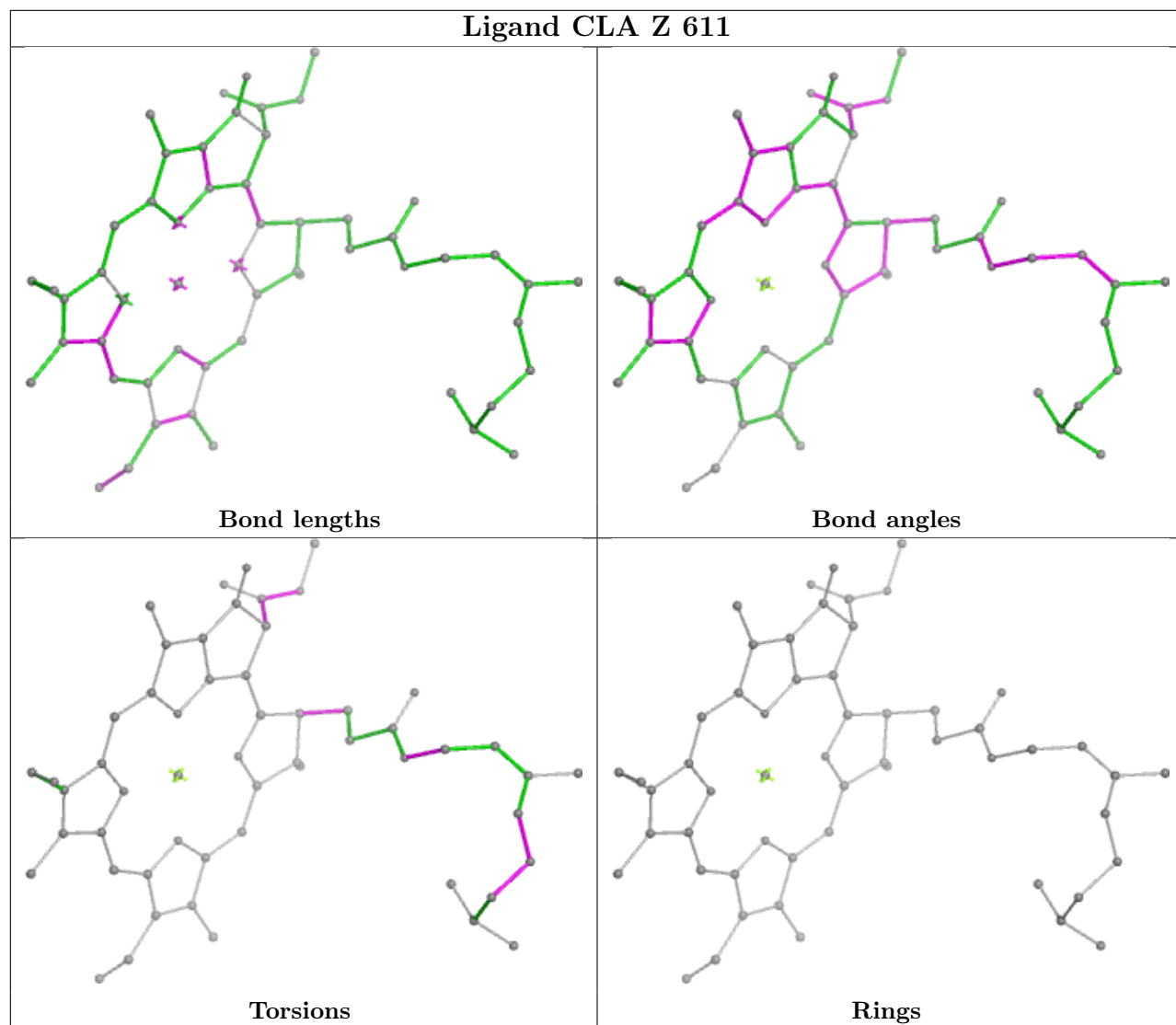


**Ligand CLA 7 605****Ligand CLA A 1113**

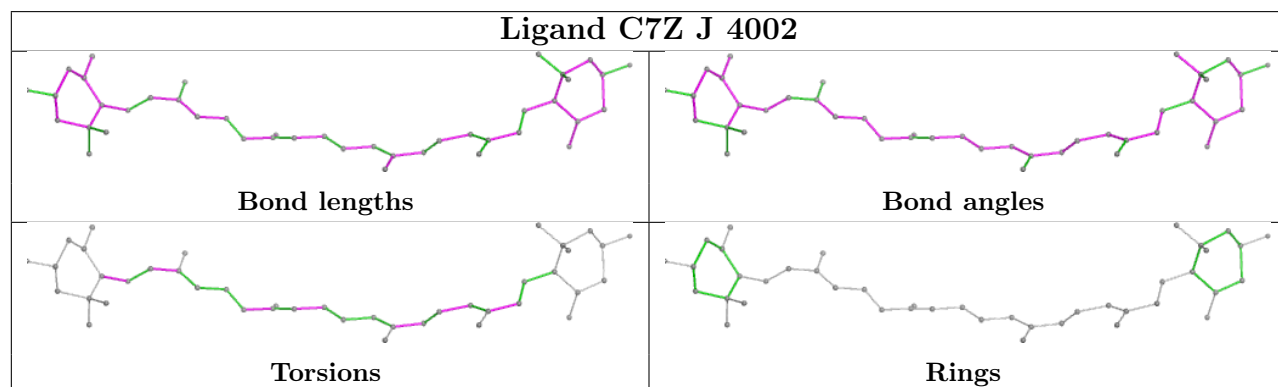


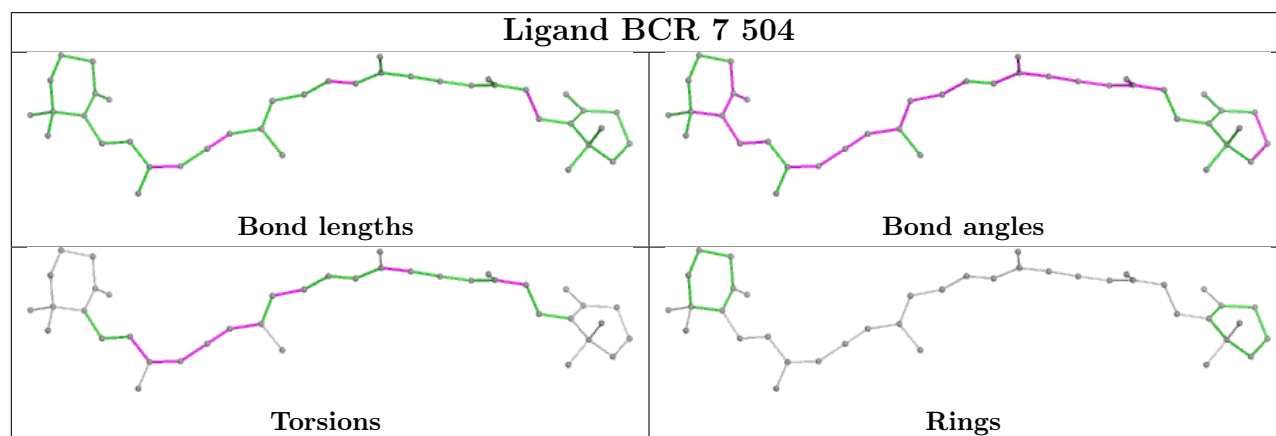
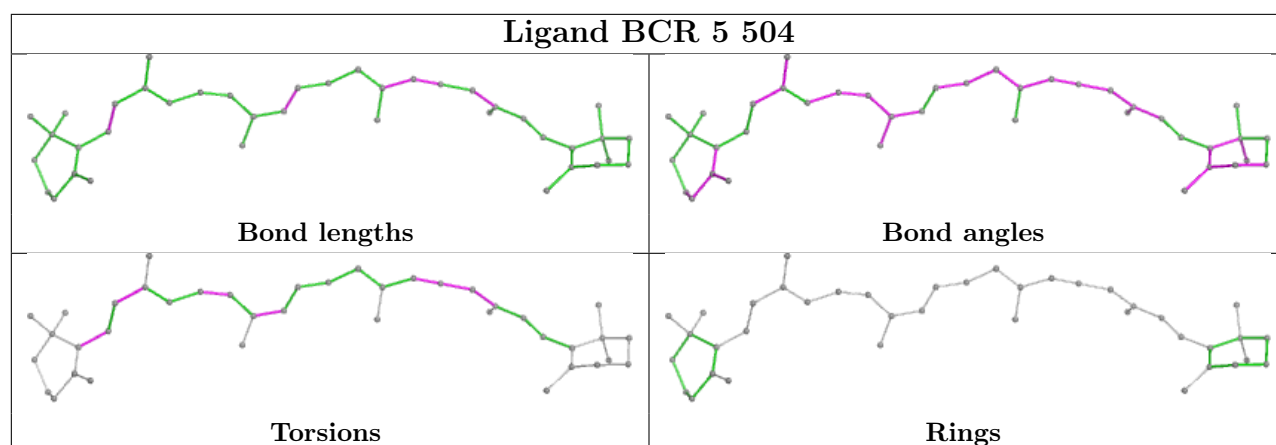


## Ligand CLA Z 611

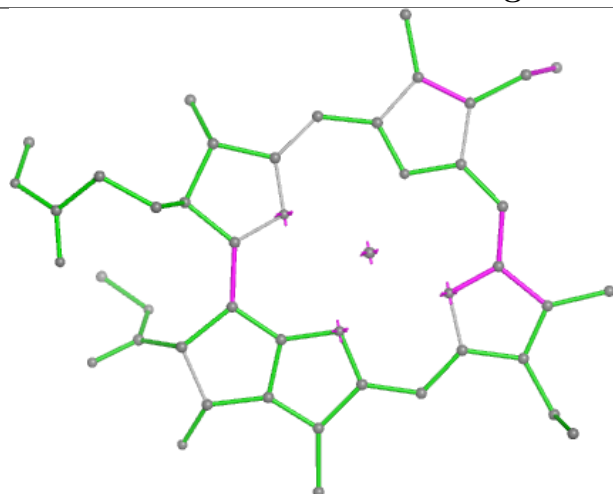


## Ligand C7Z J 4002

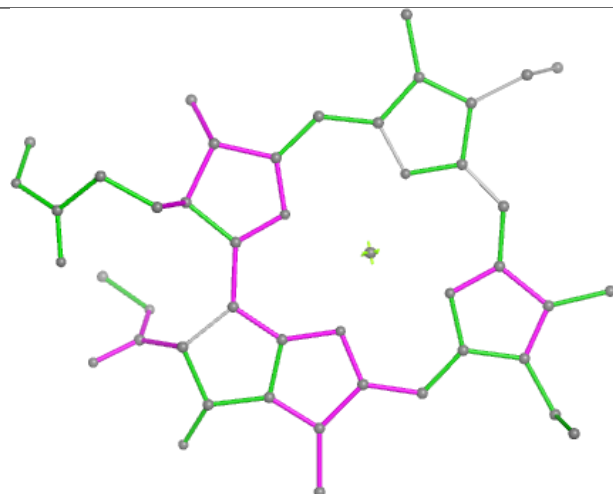




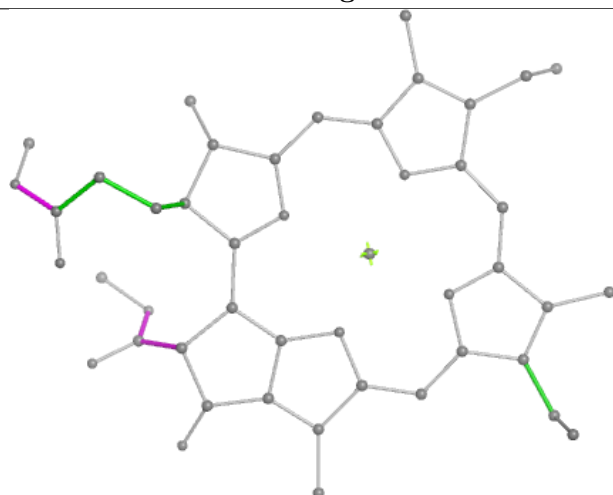
## Ligand CLA G 1602



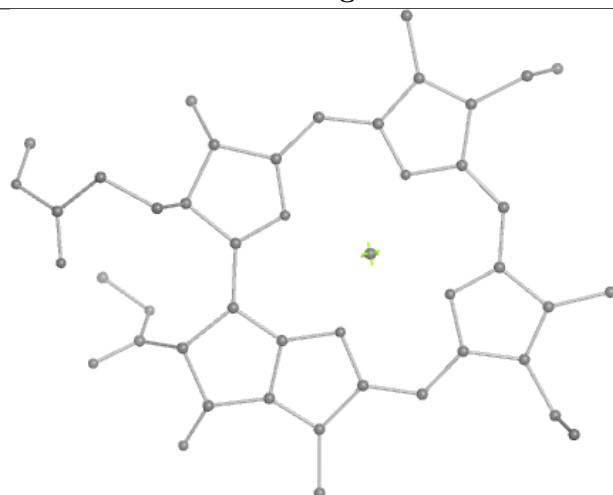
Bond lengths



Bond angles

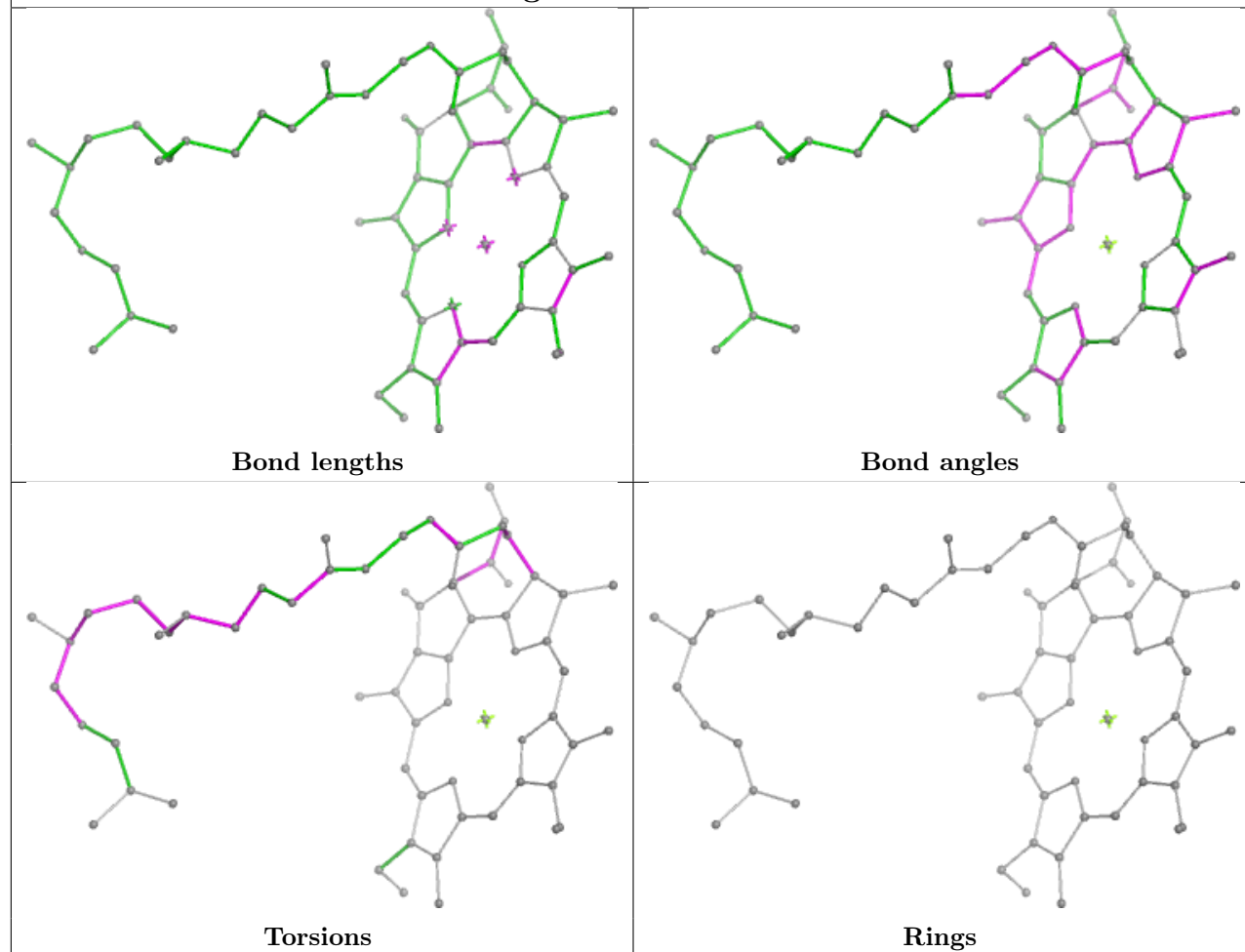


Torsions

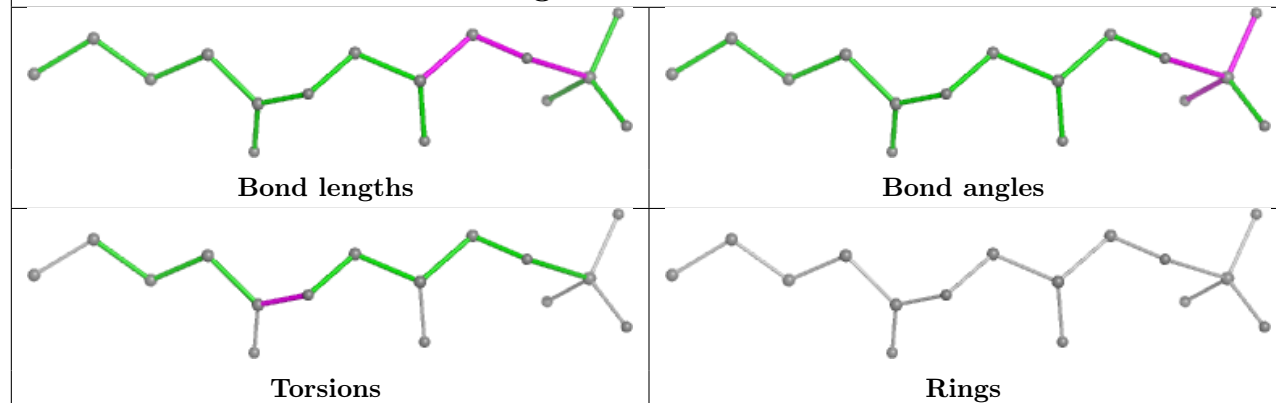


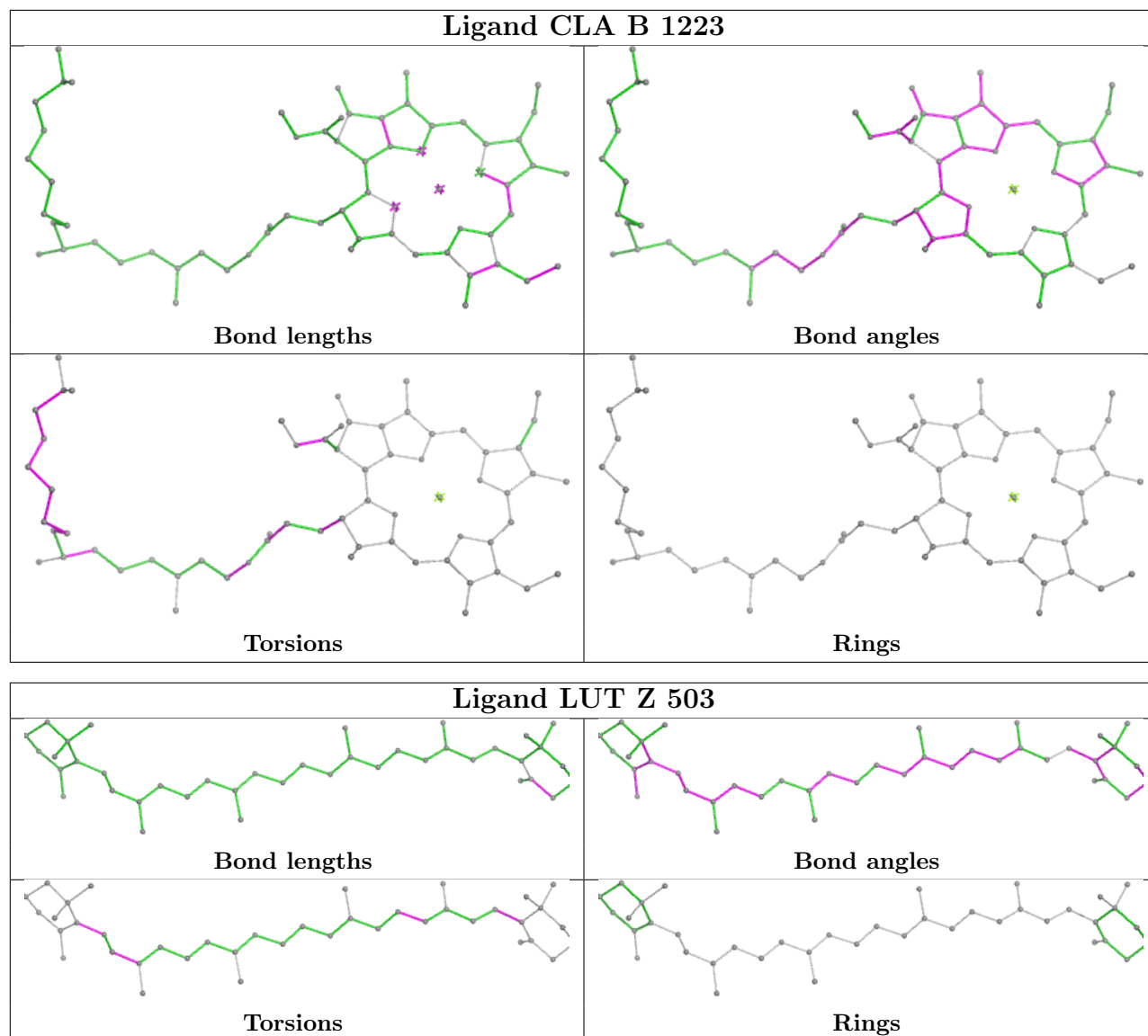
Rings

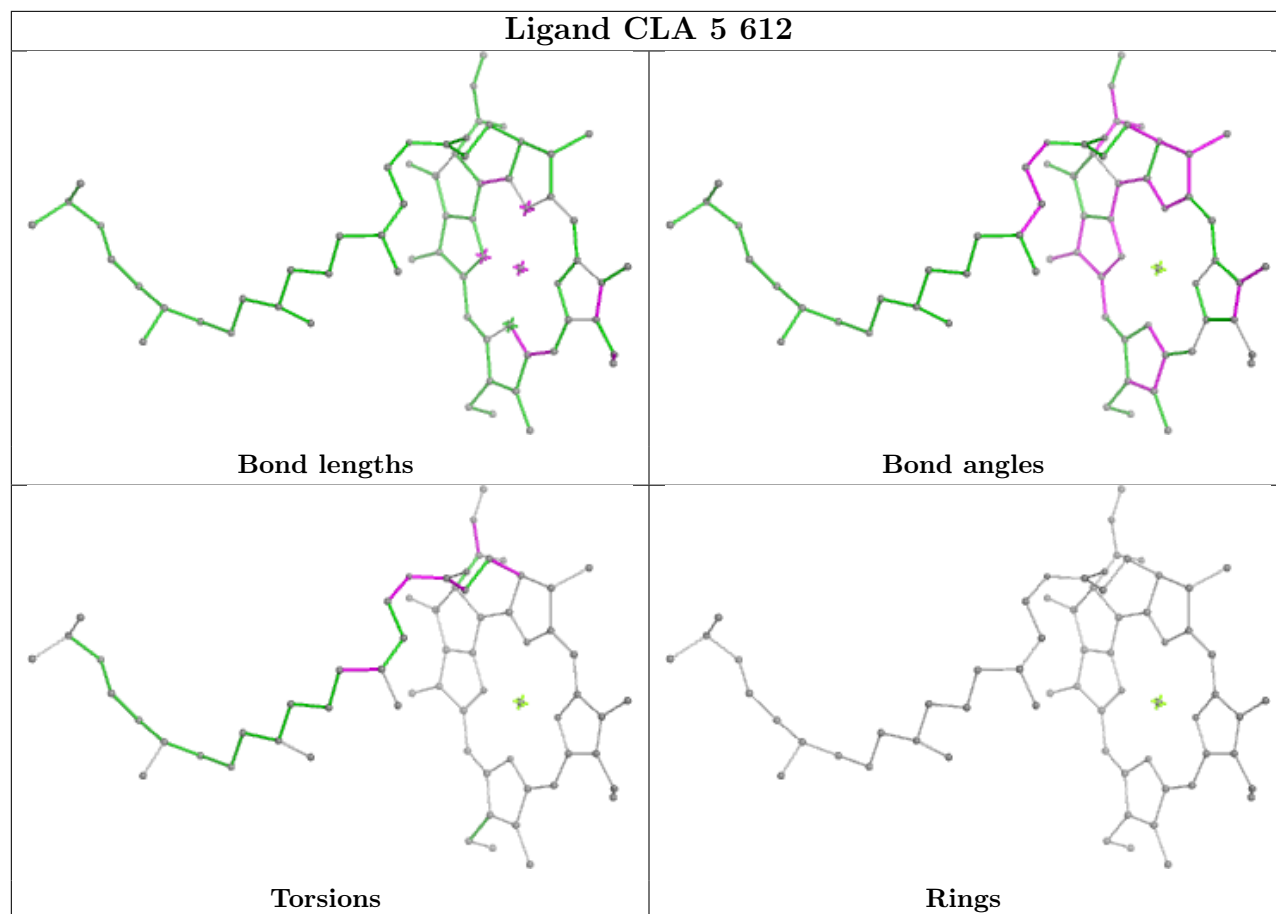
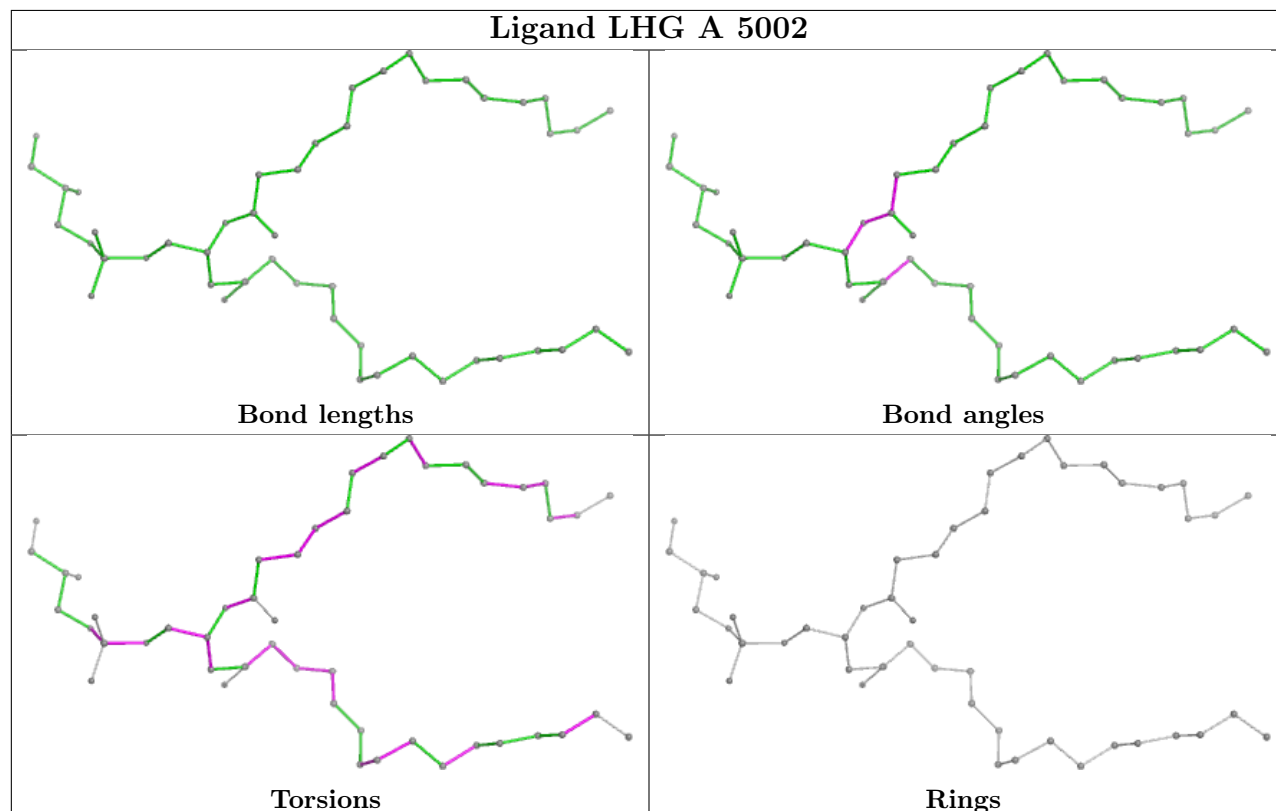
## Ligand CLA 1 612



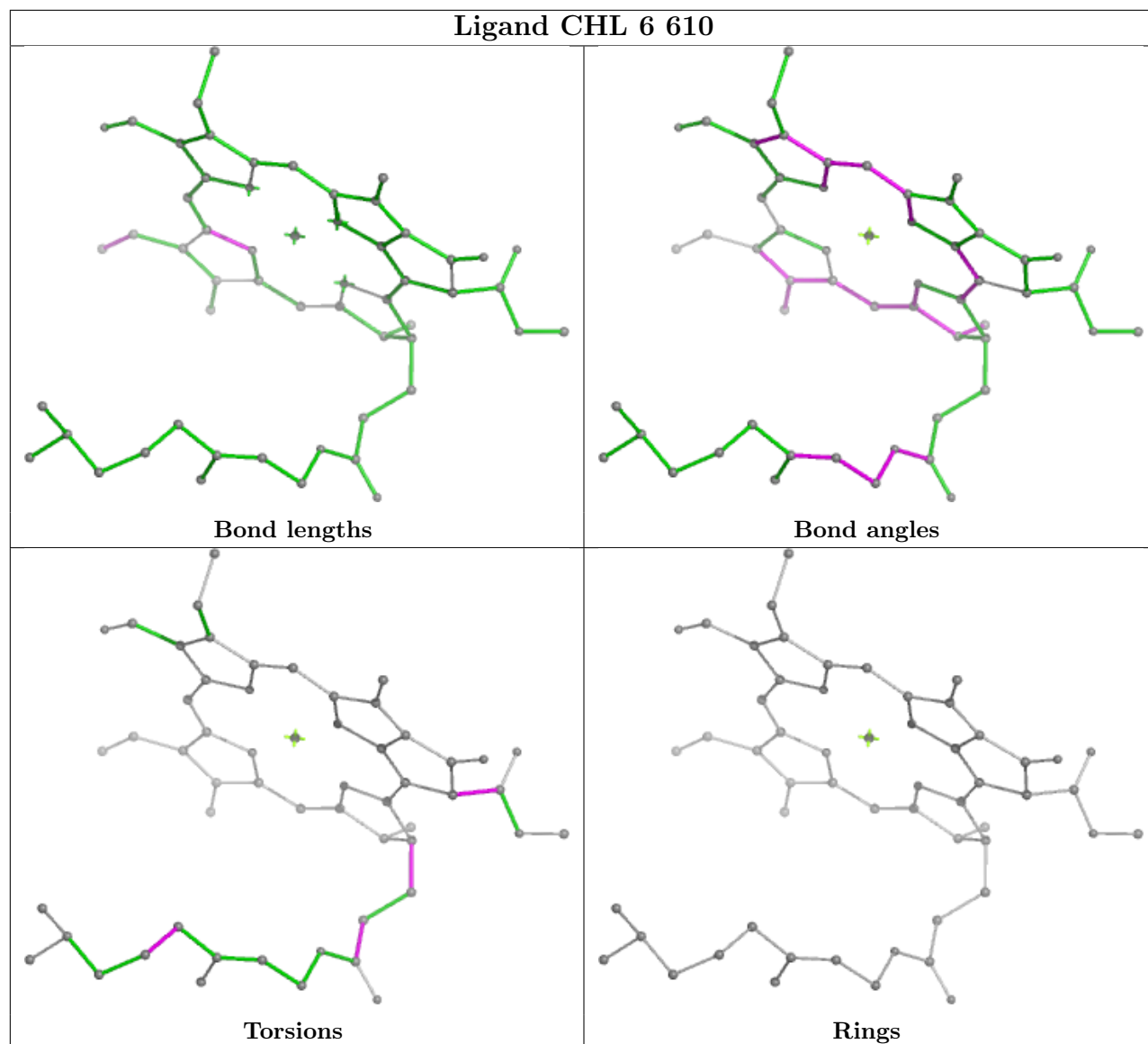
## Ligand NKP 3 802



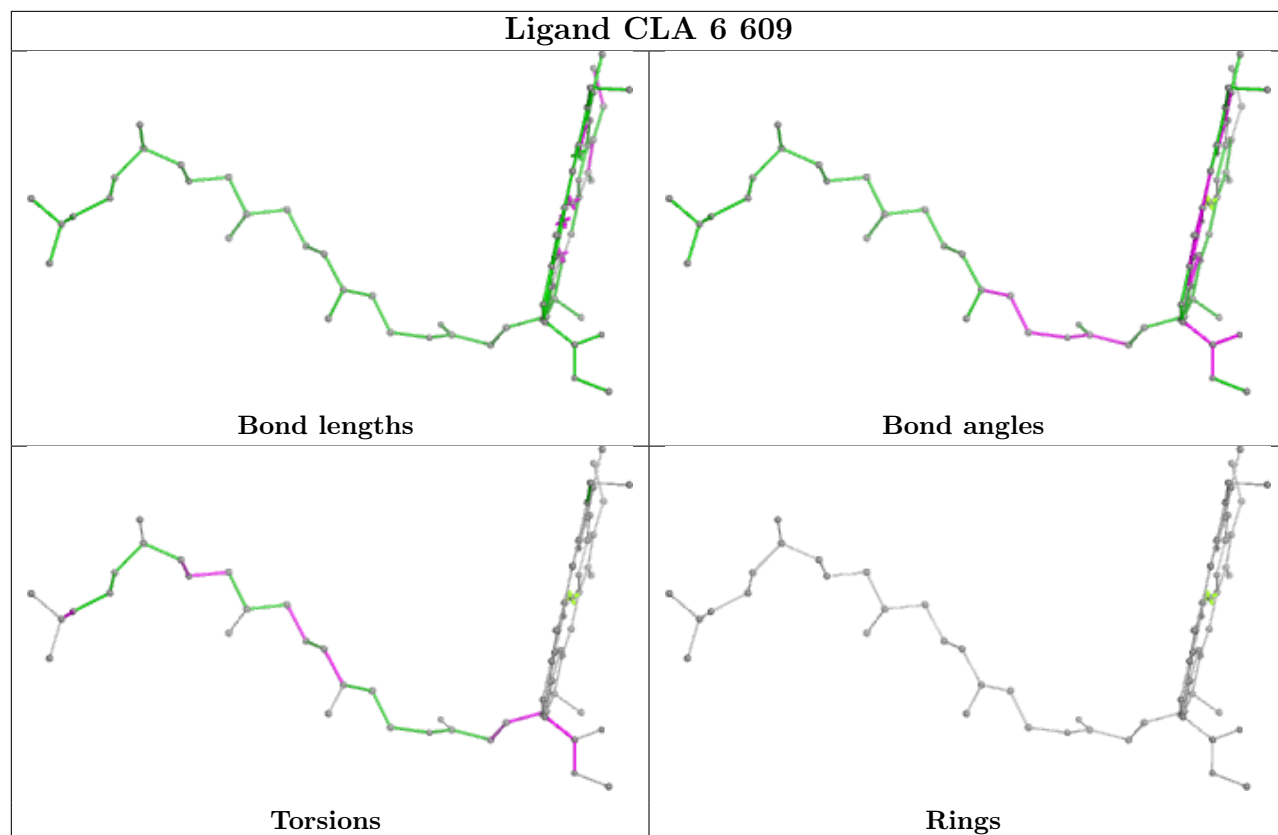


**Ligand CLA 5 612****Ligand LHG A 5002**

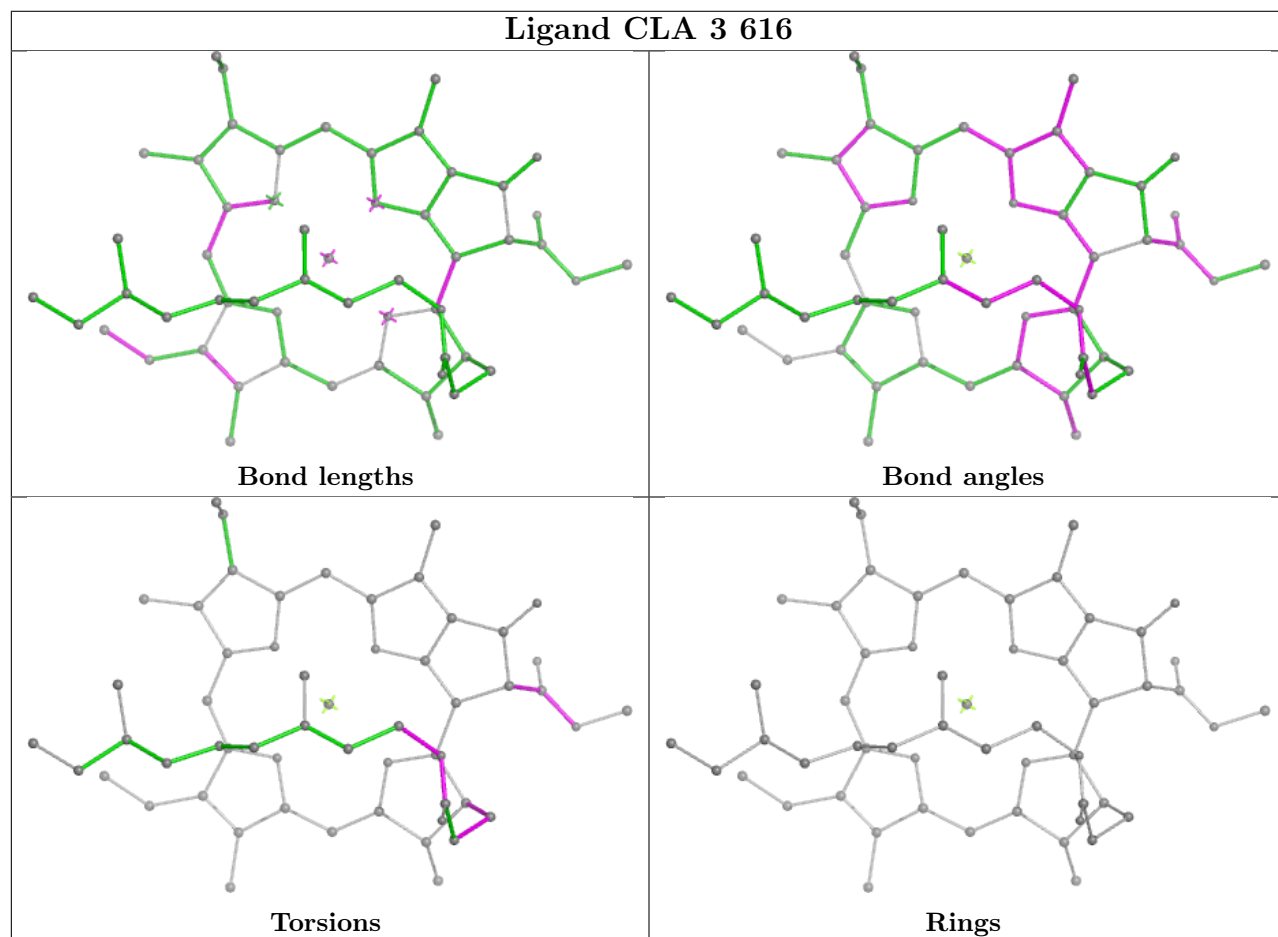
## Ligand CHL 6 610



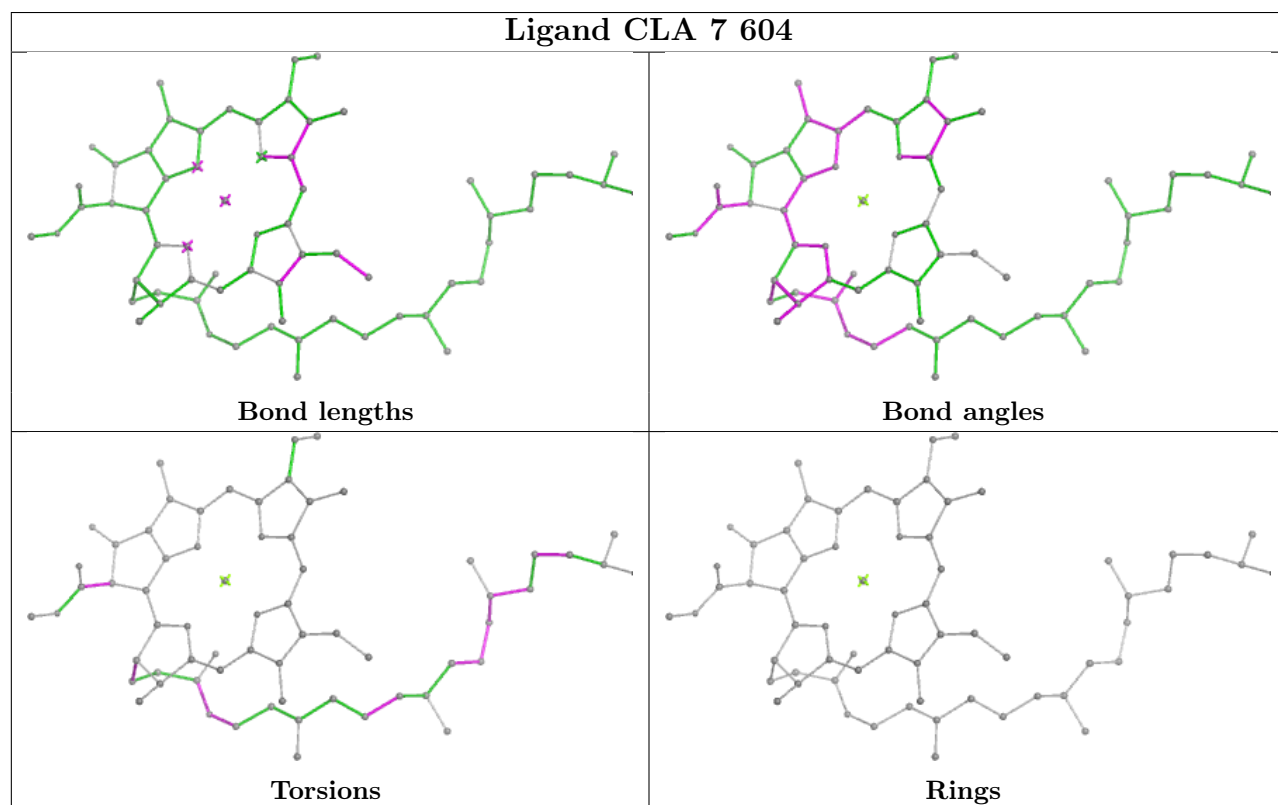
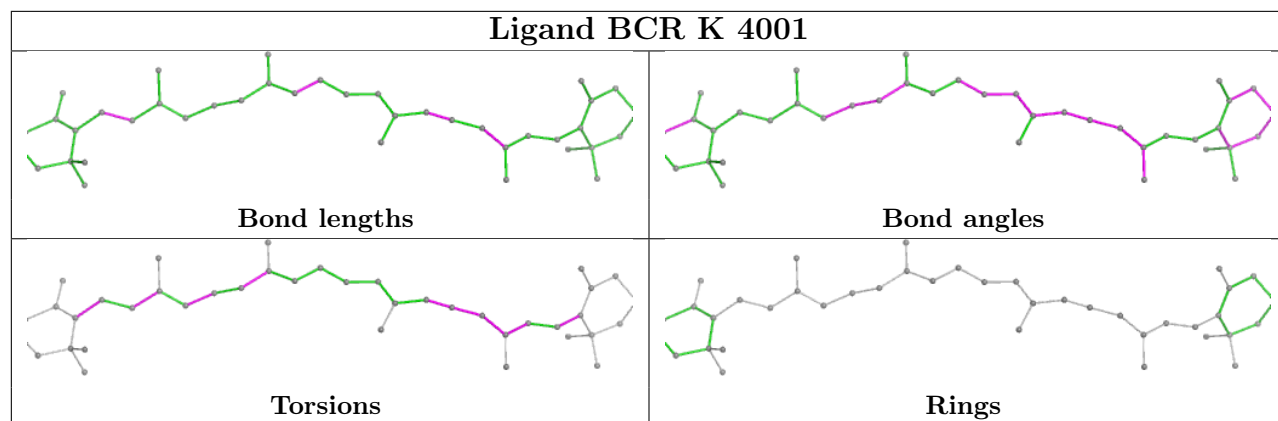
## Ligand CLA 6 609

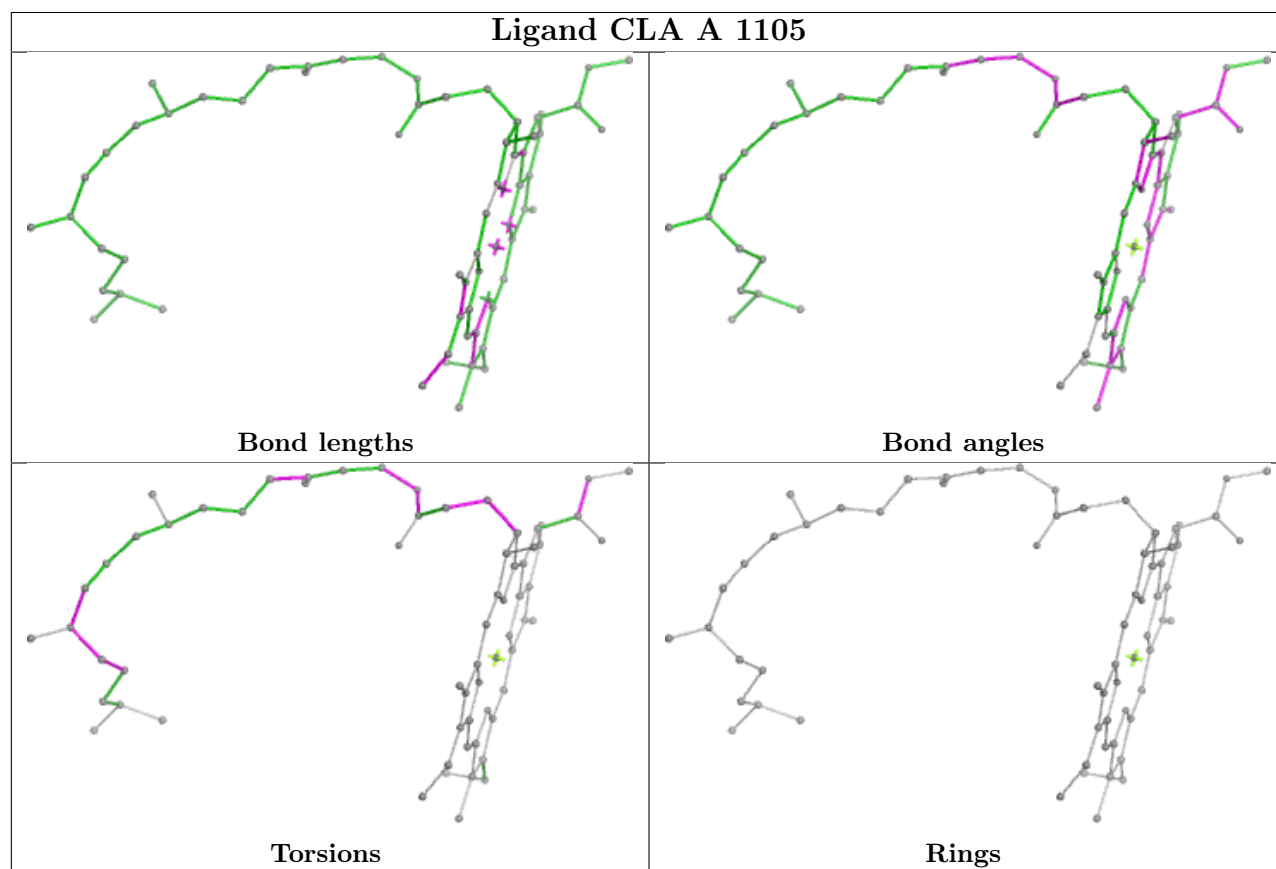
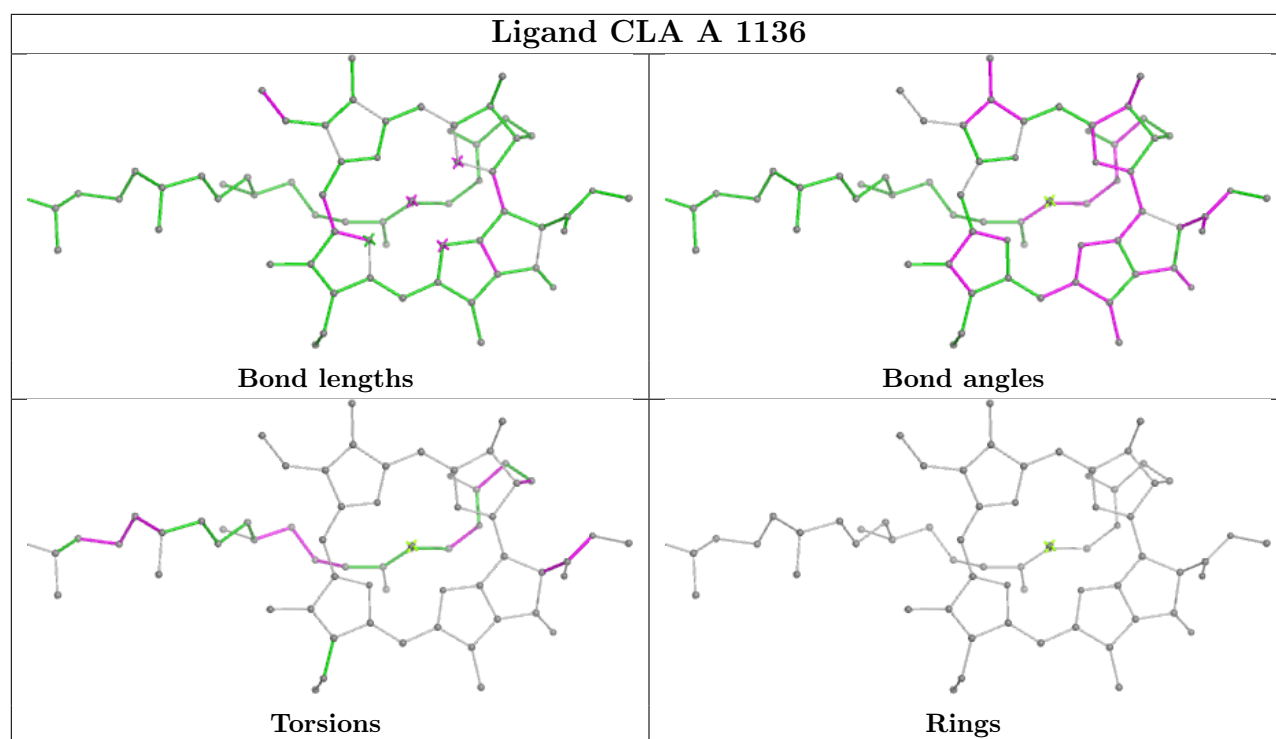


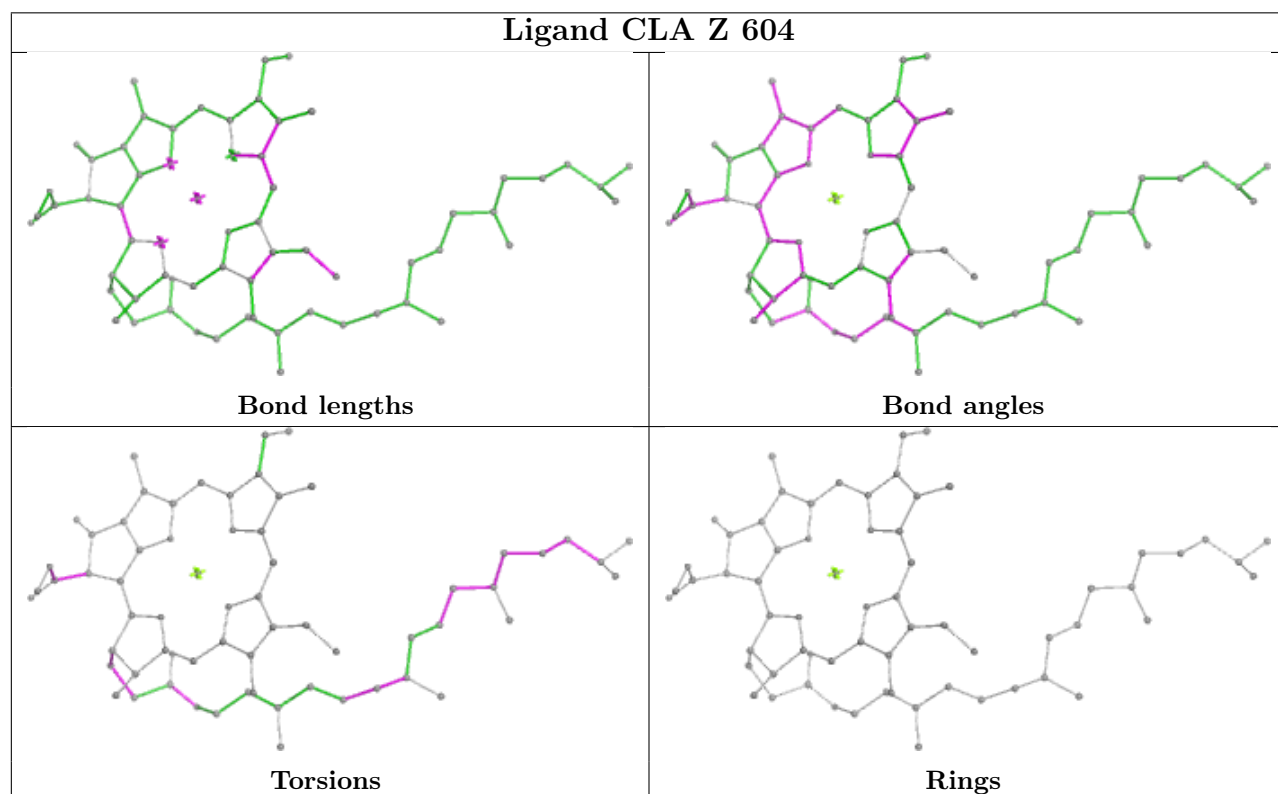
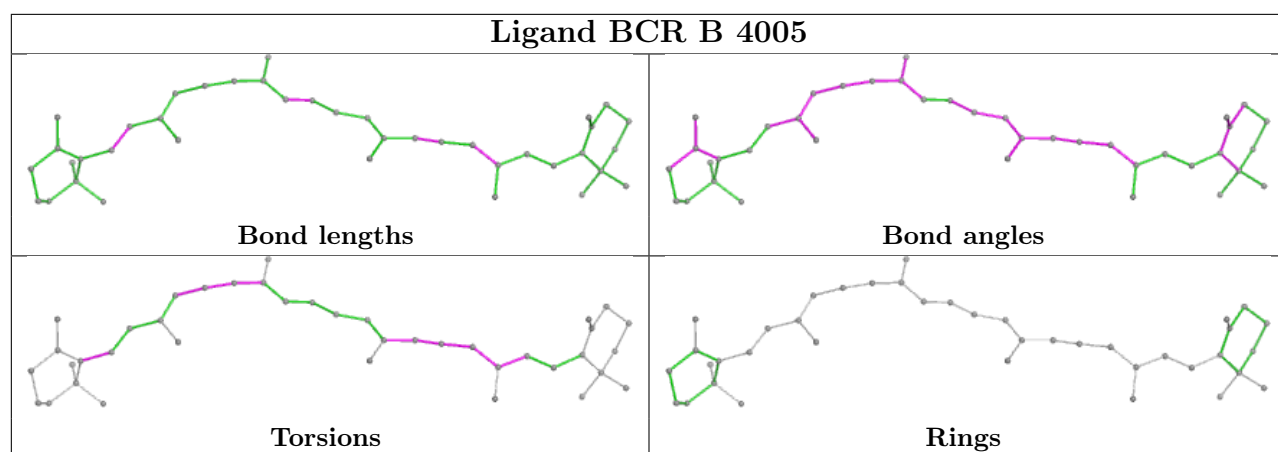
## Ligand CLA 3 616

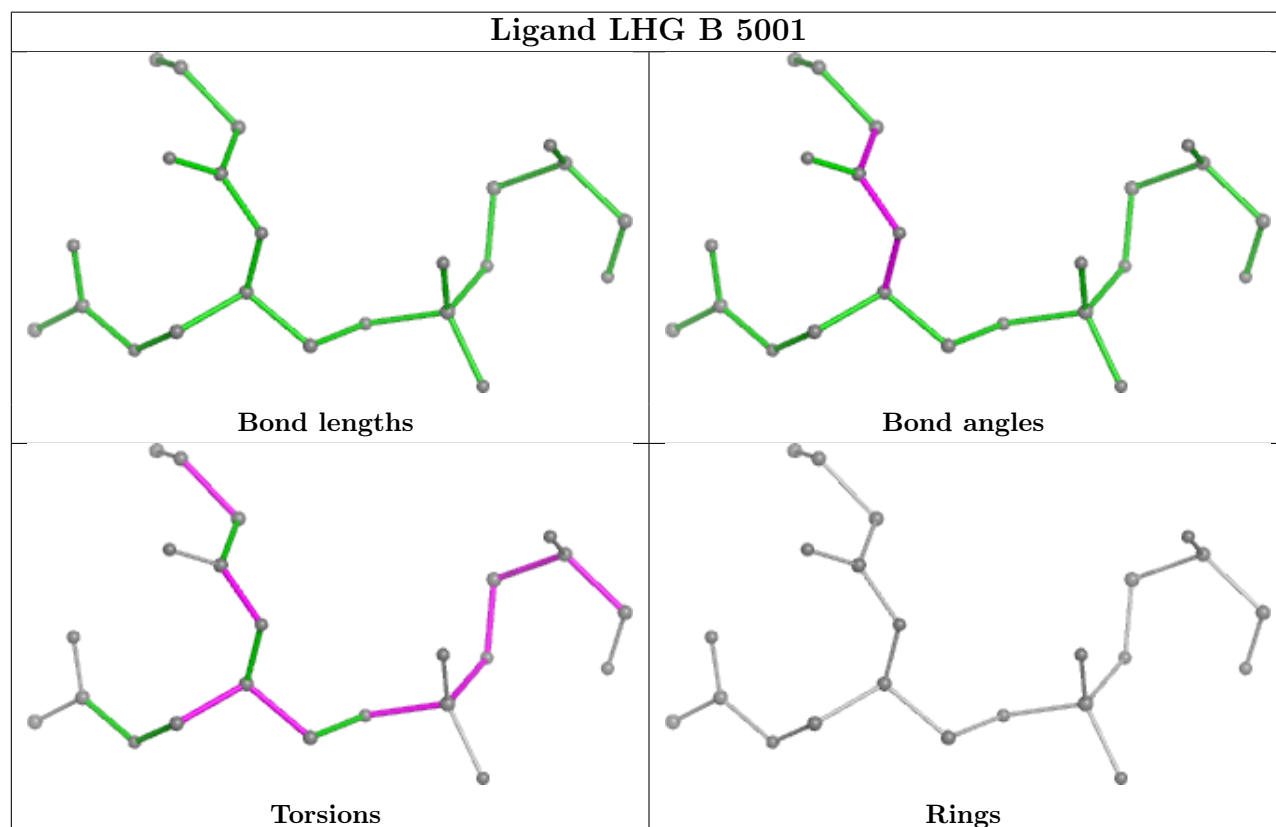
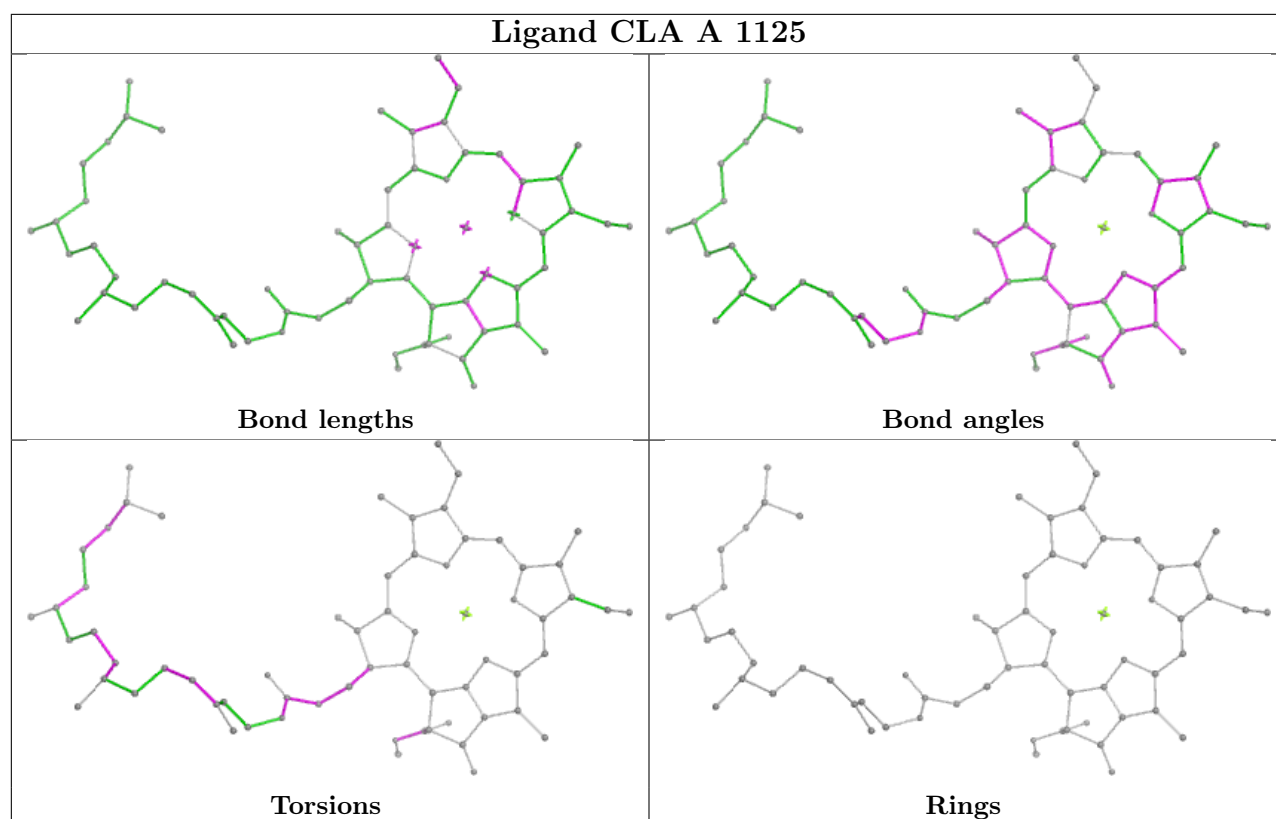


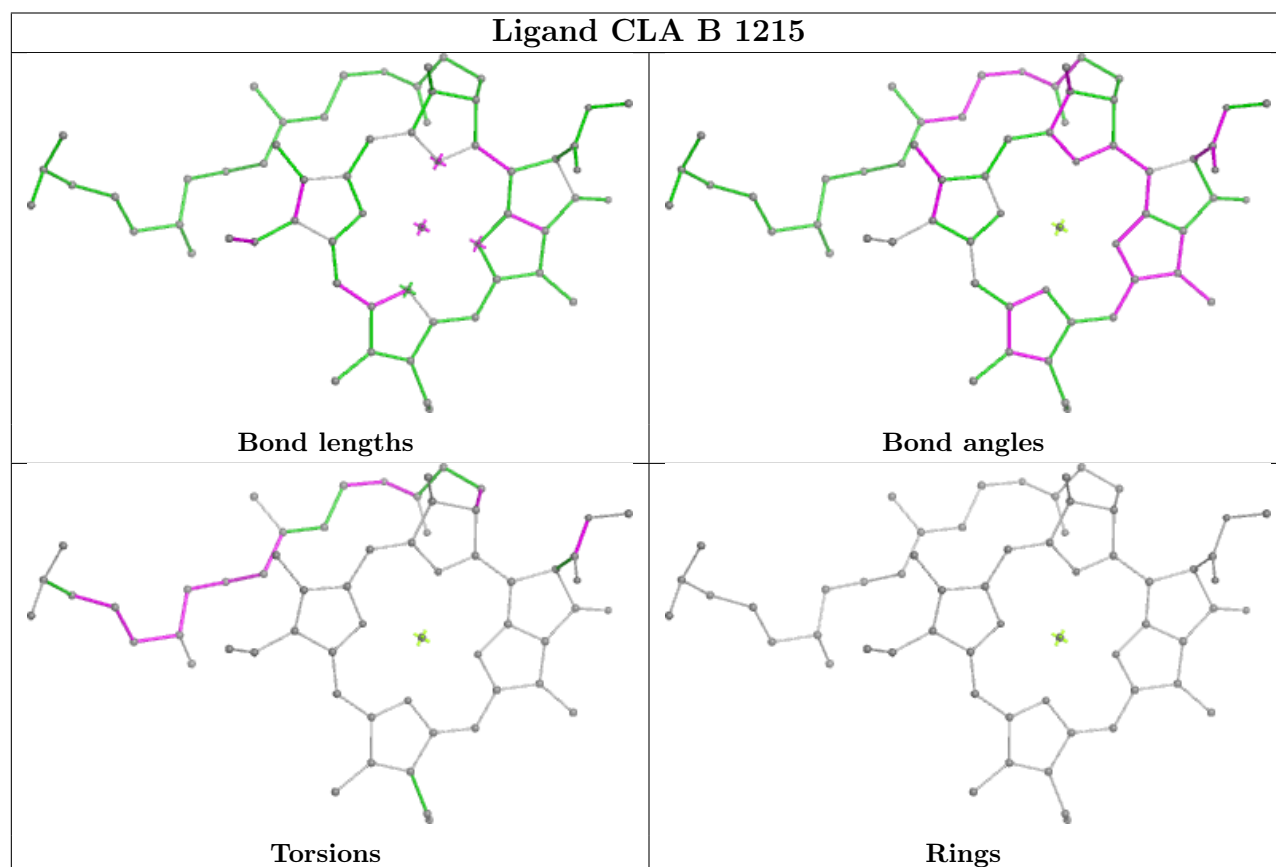
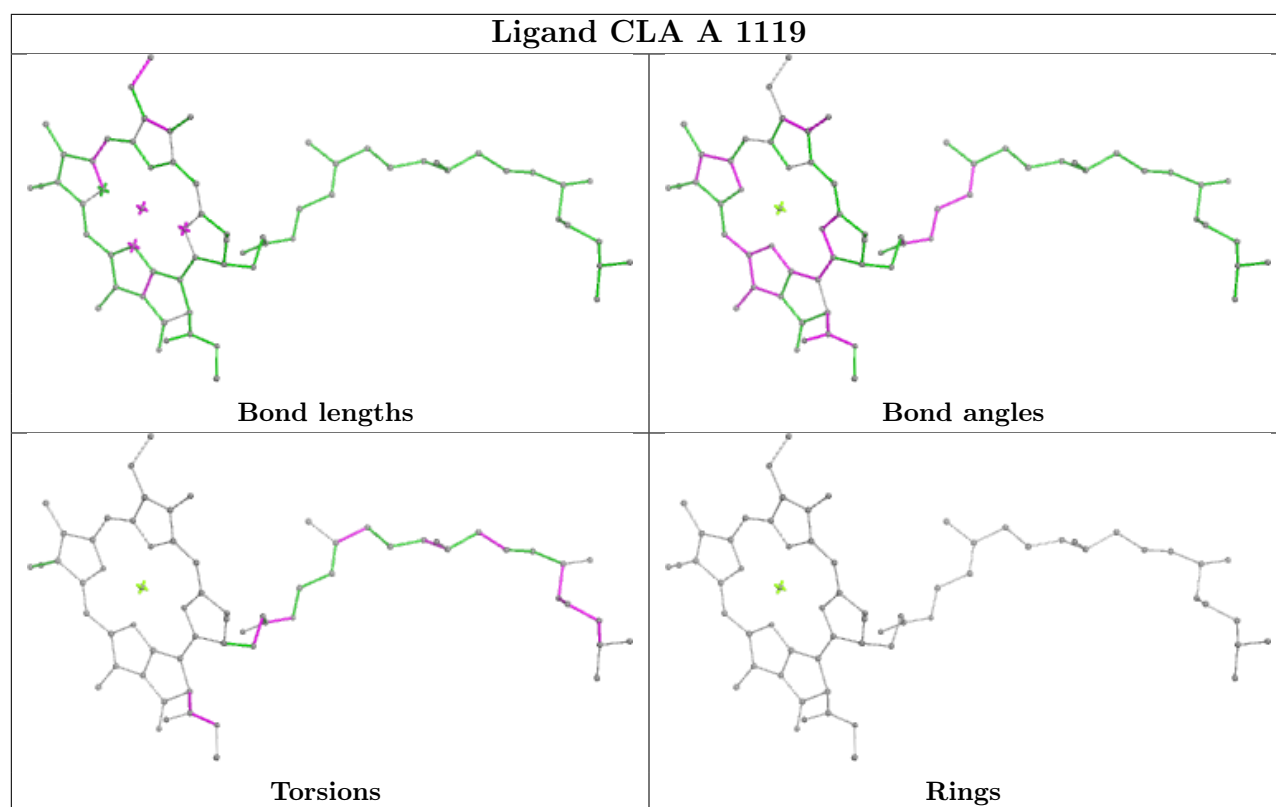




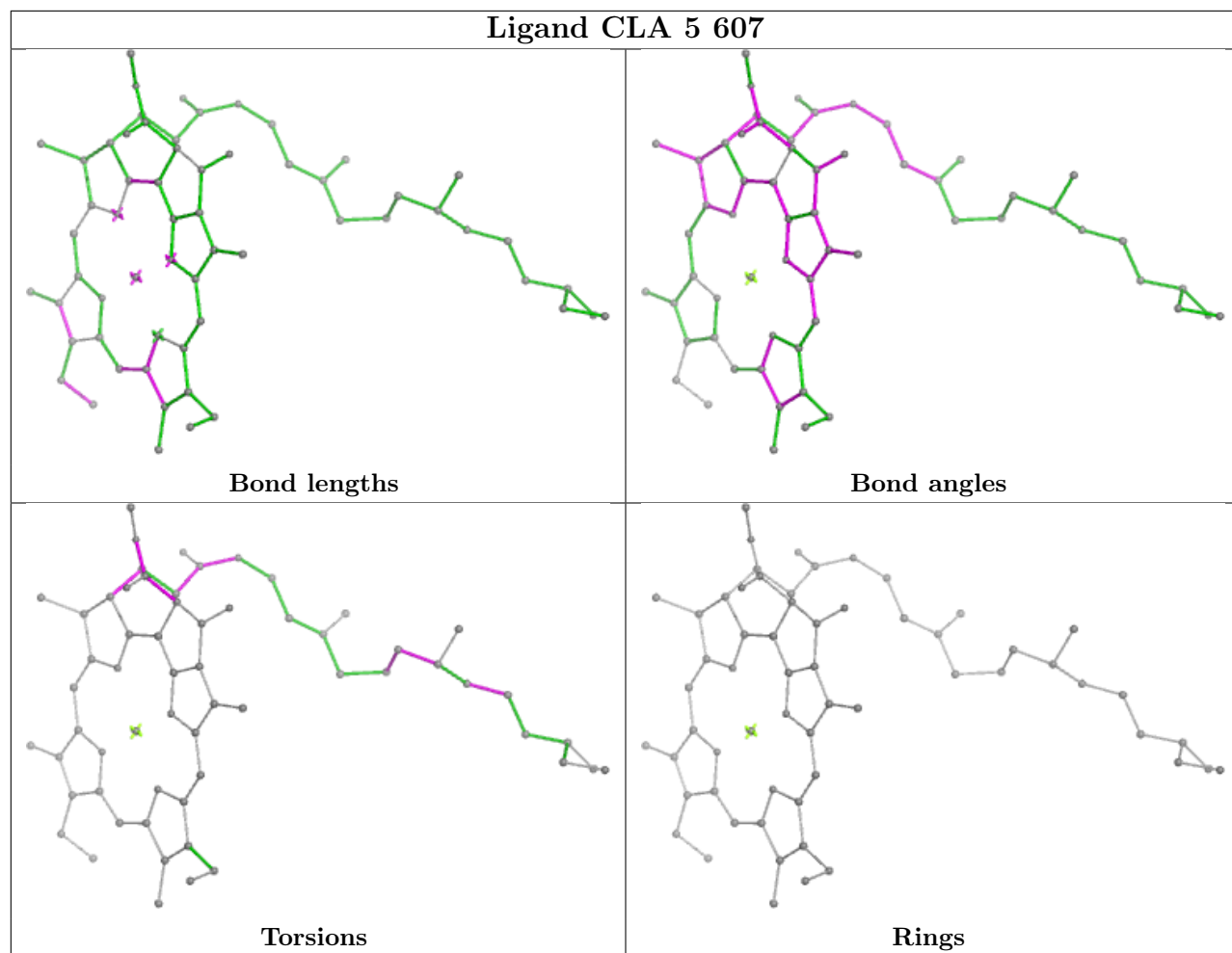


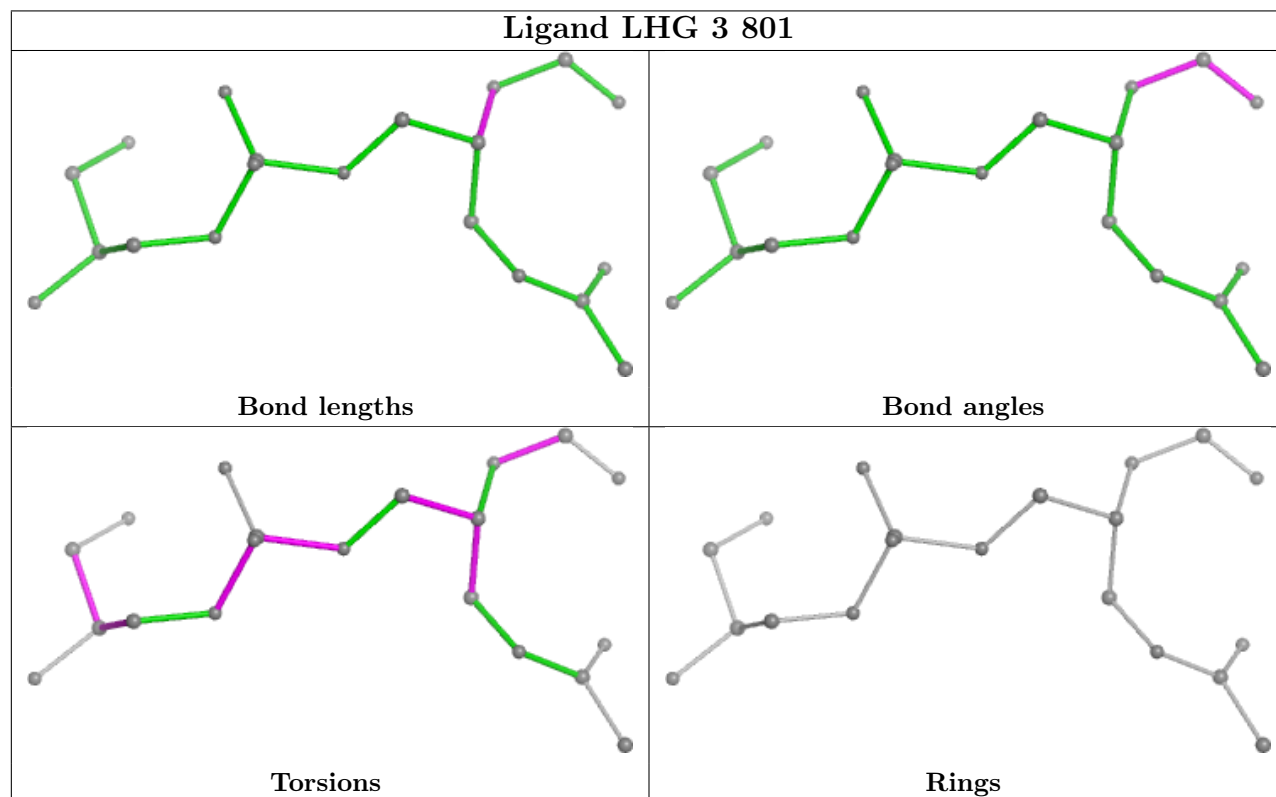
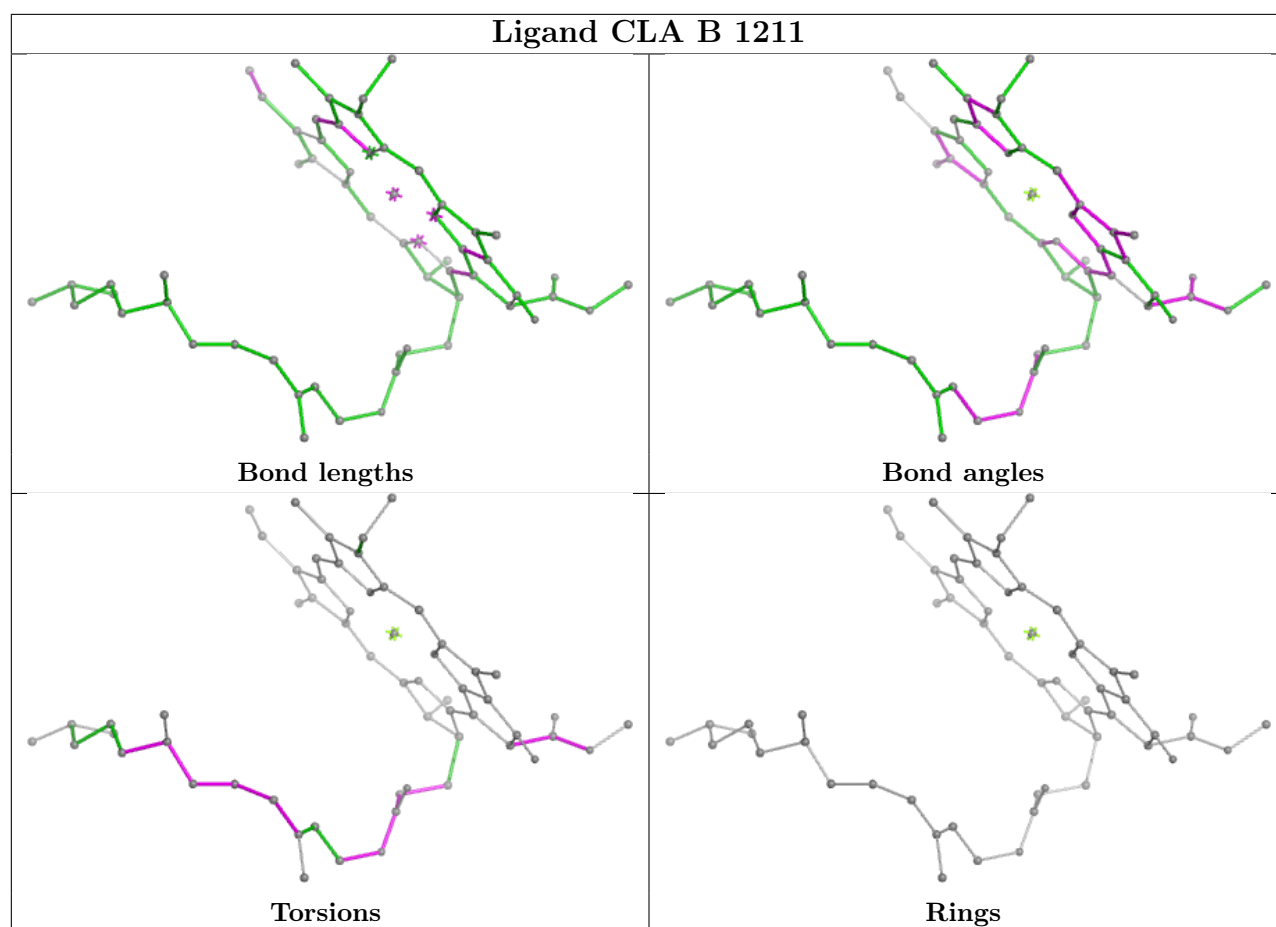


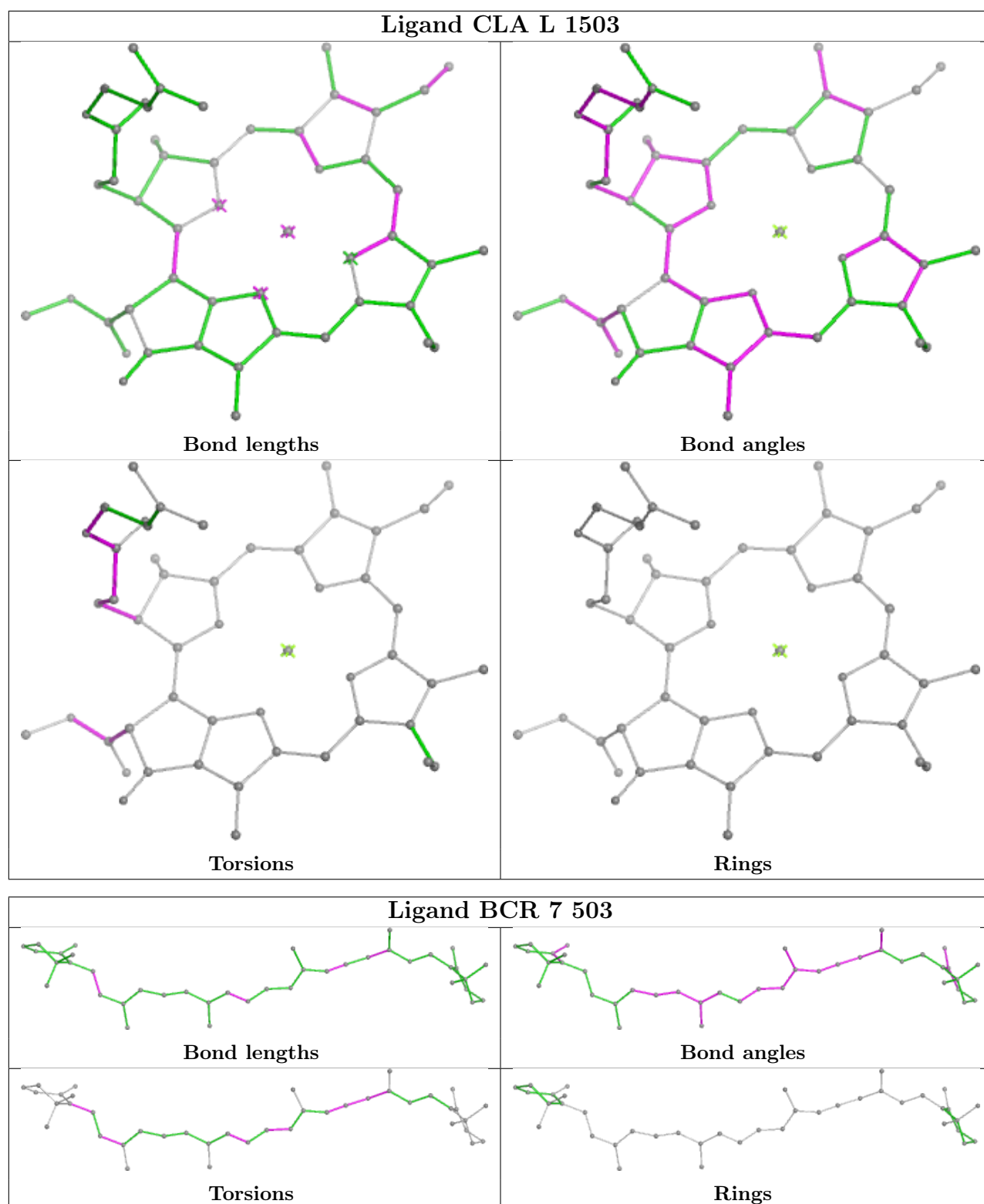




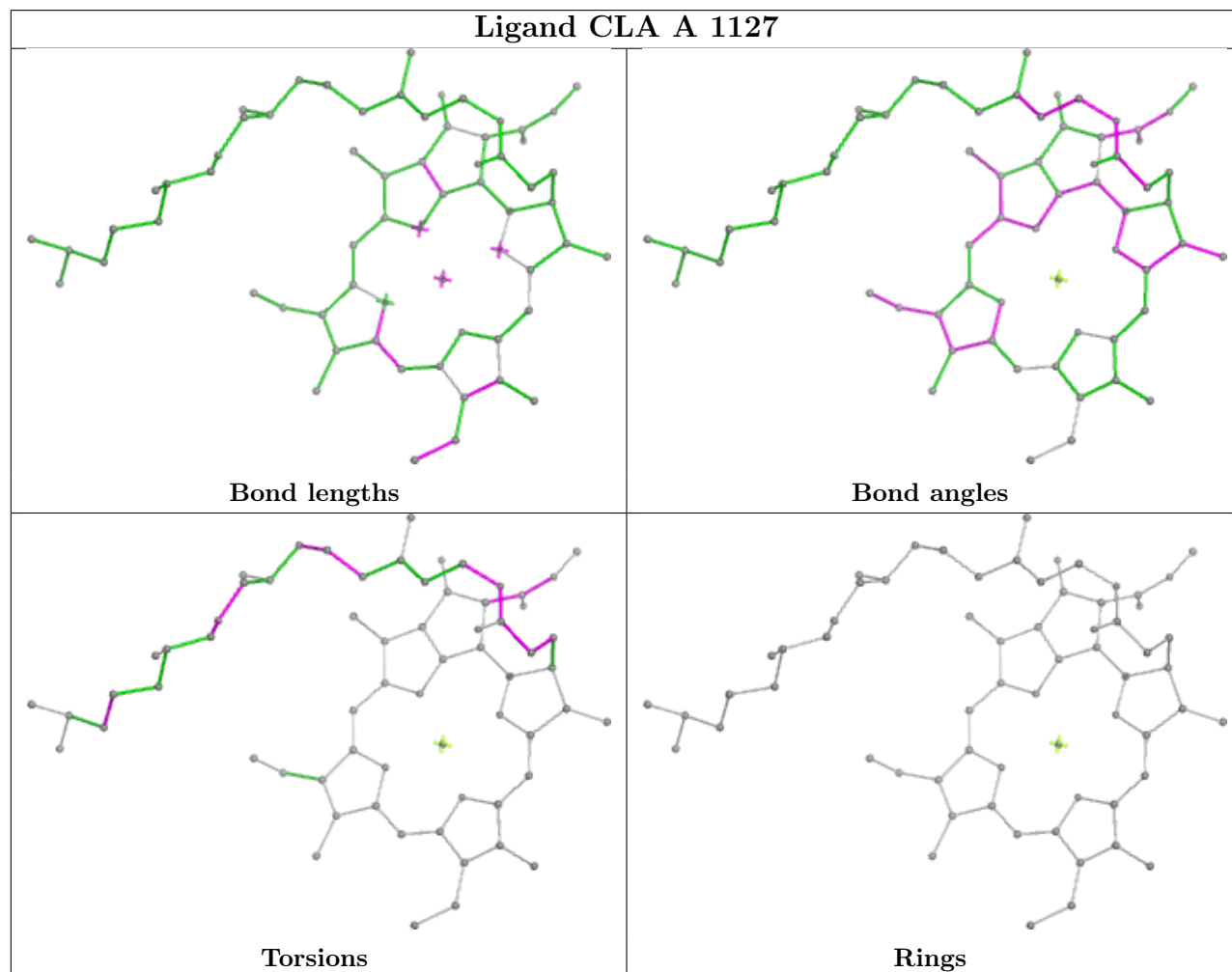
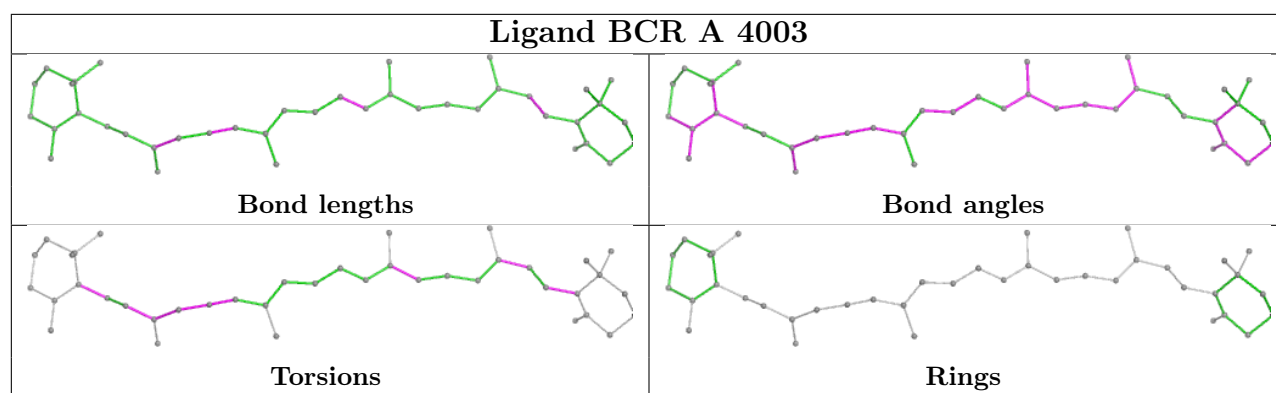
## Ligand CLA 5 607



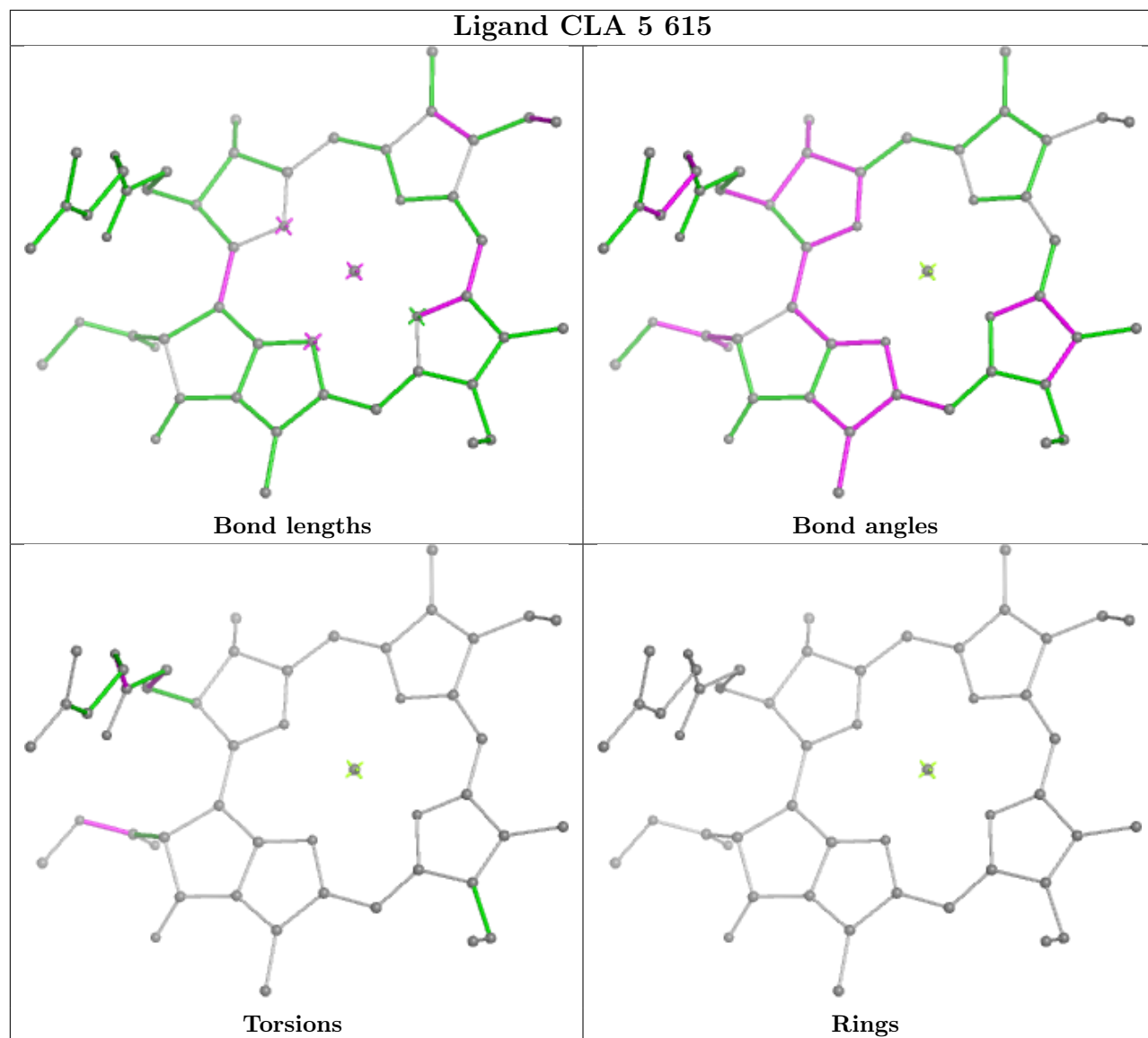




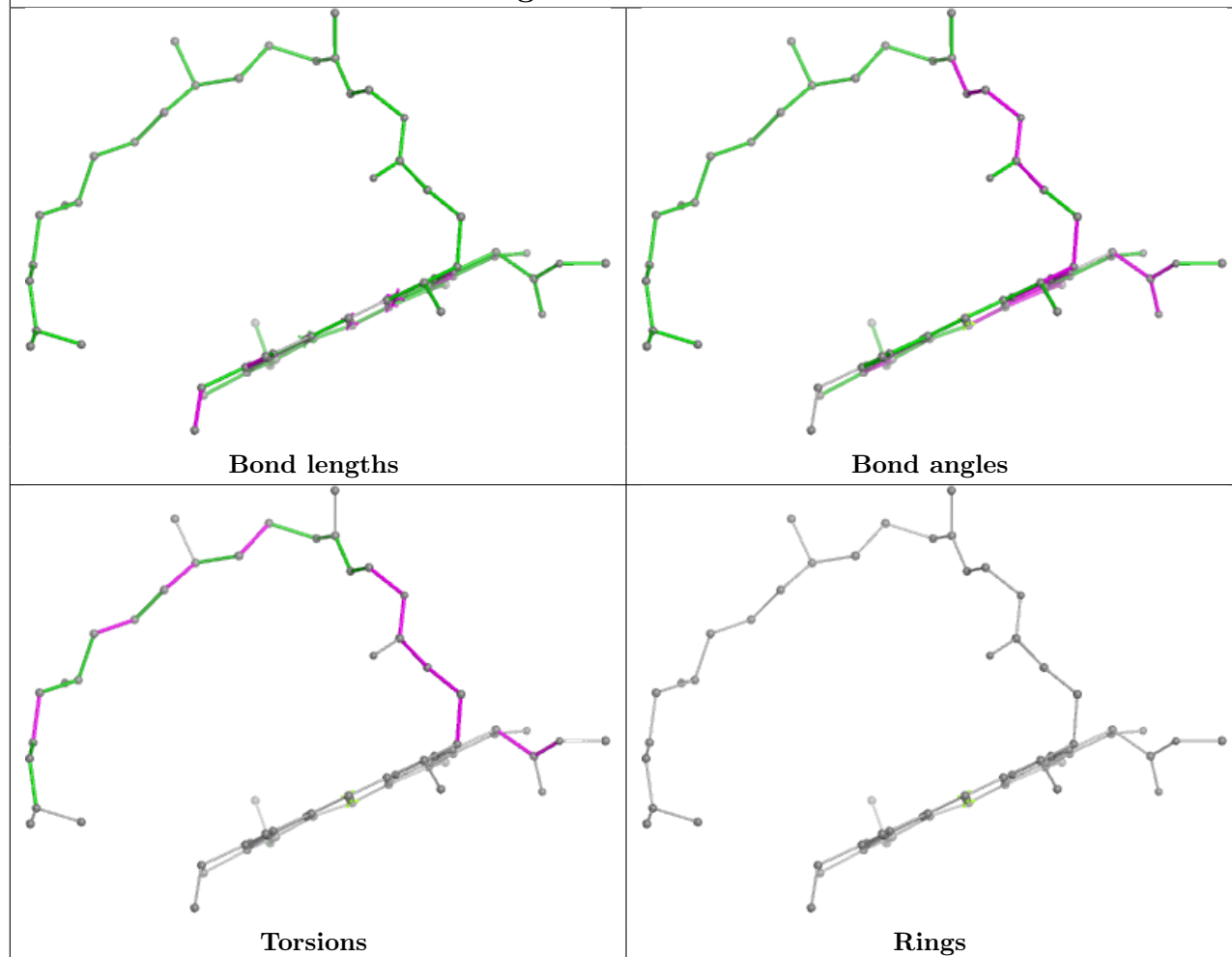




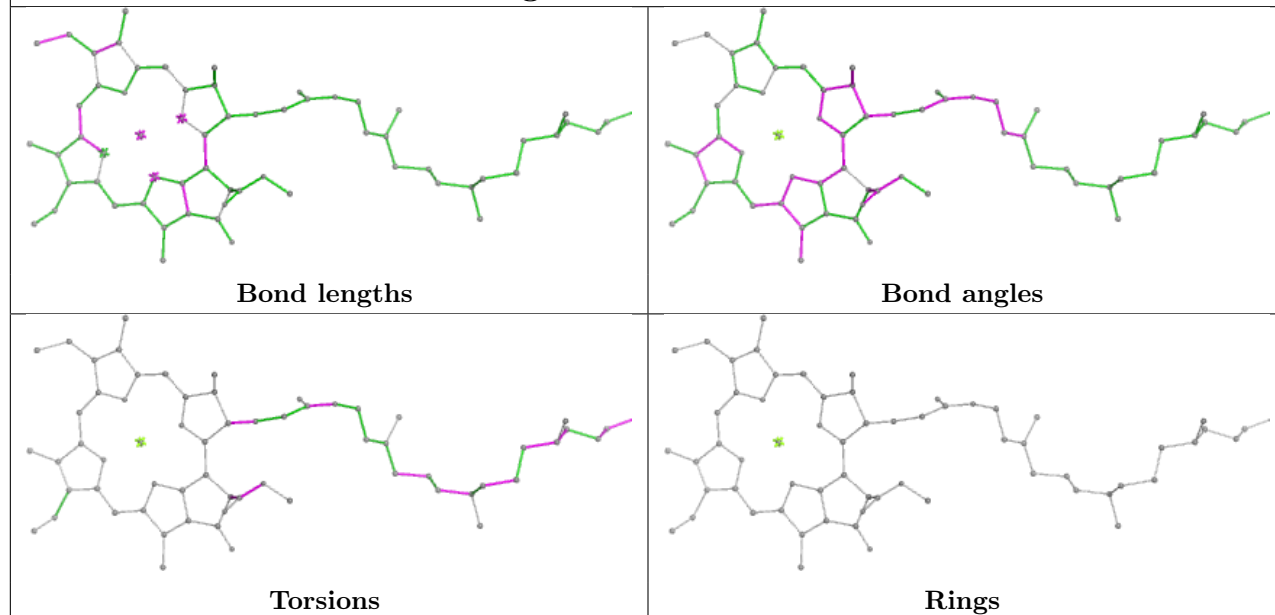
## Ligand CLA 5 615

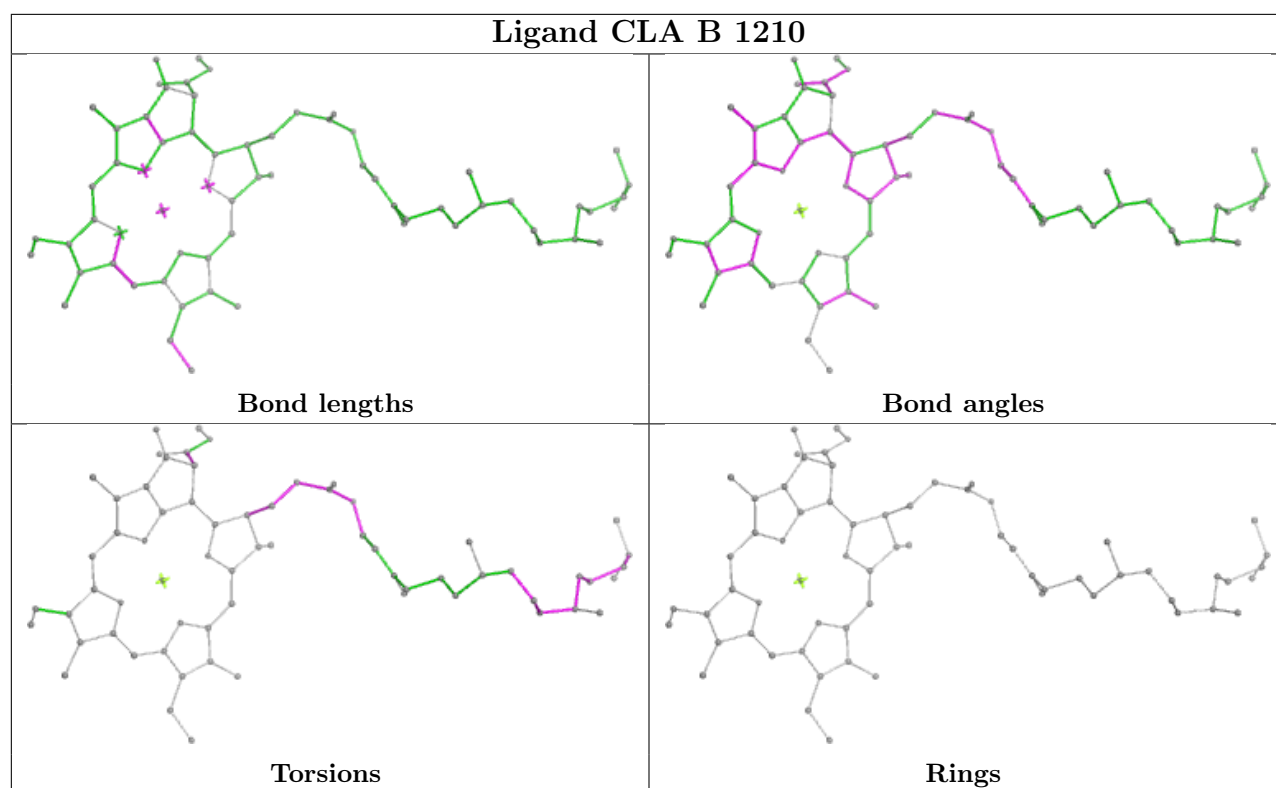


## Ligand CLA 6 606

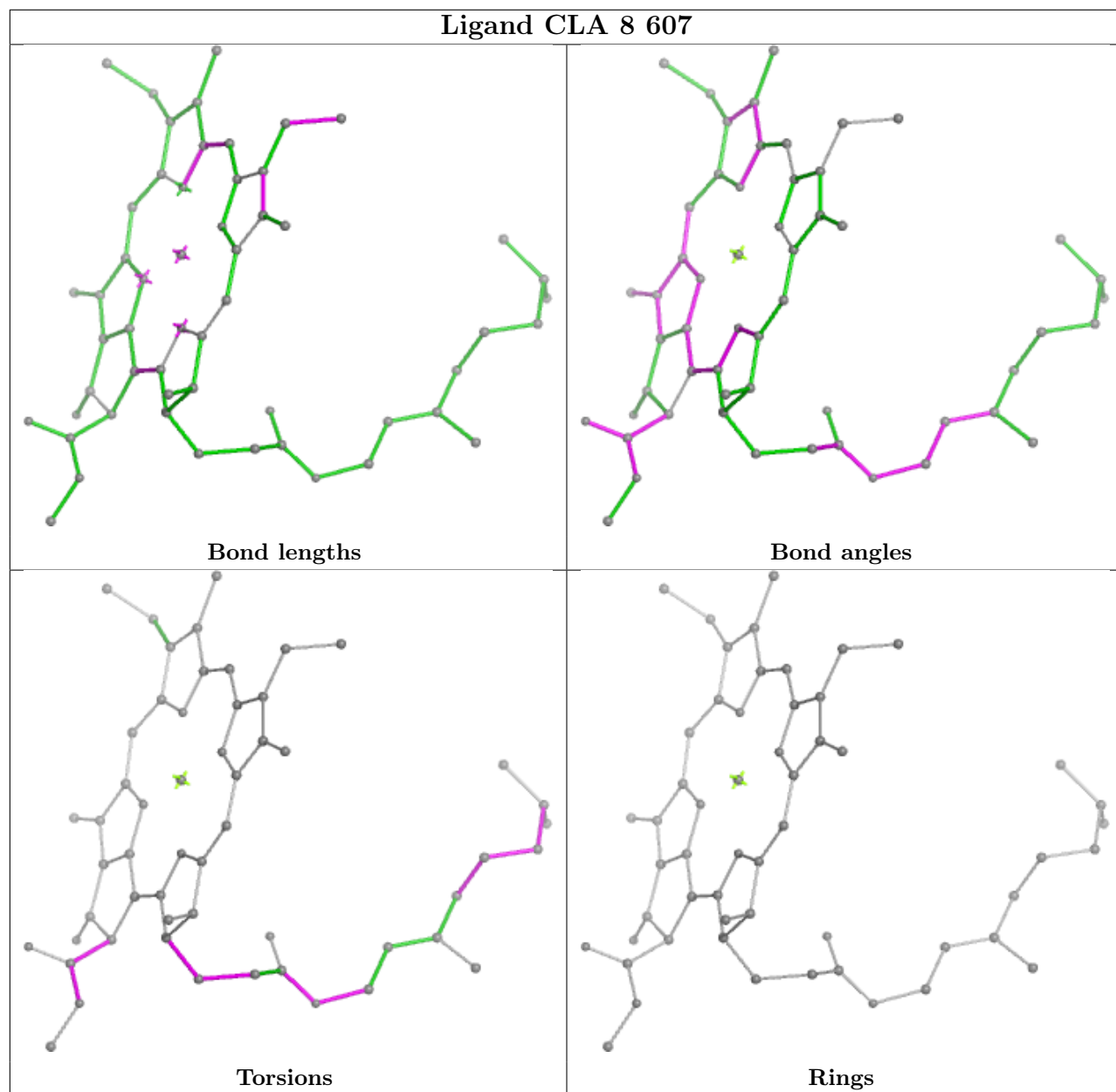


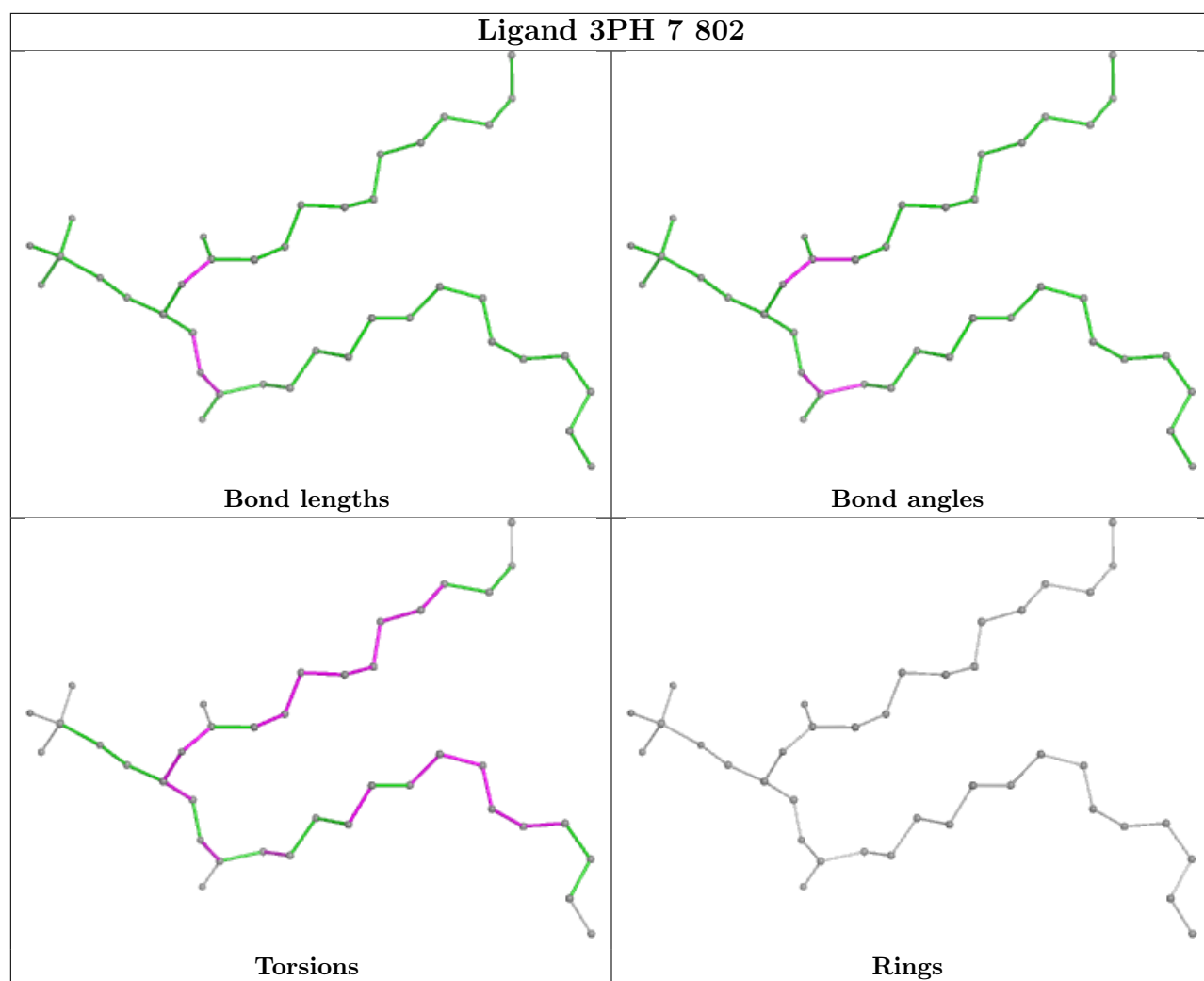
## Ligand CLA A 1140



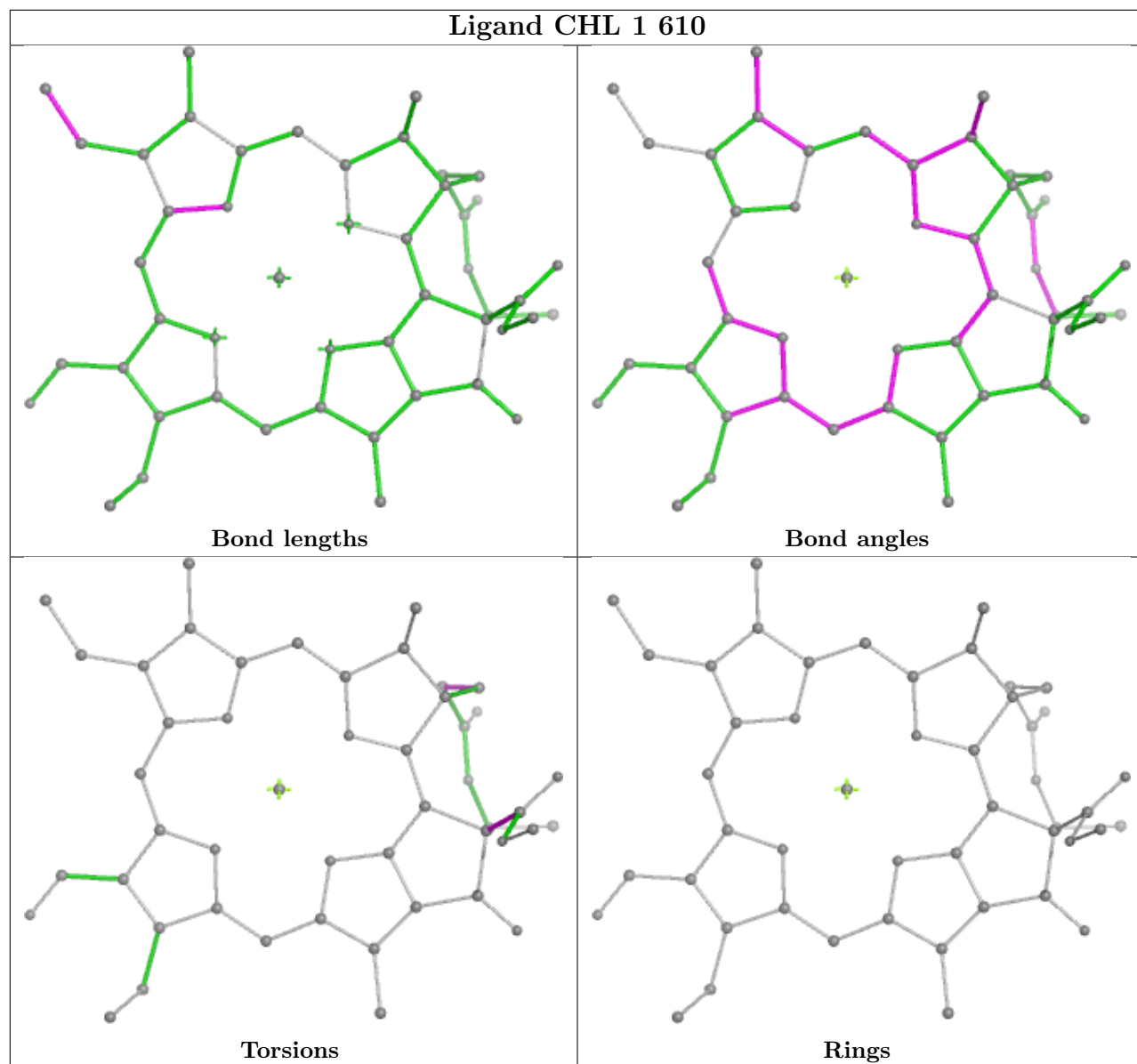


## Ligand CLA 8 607

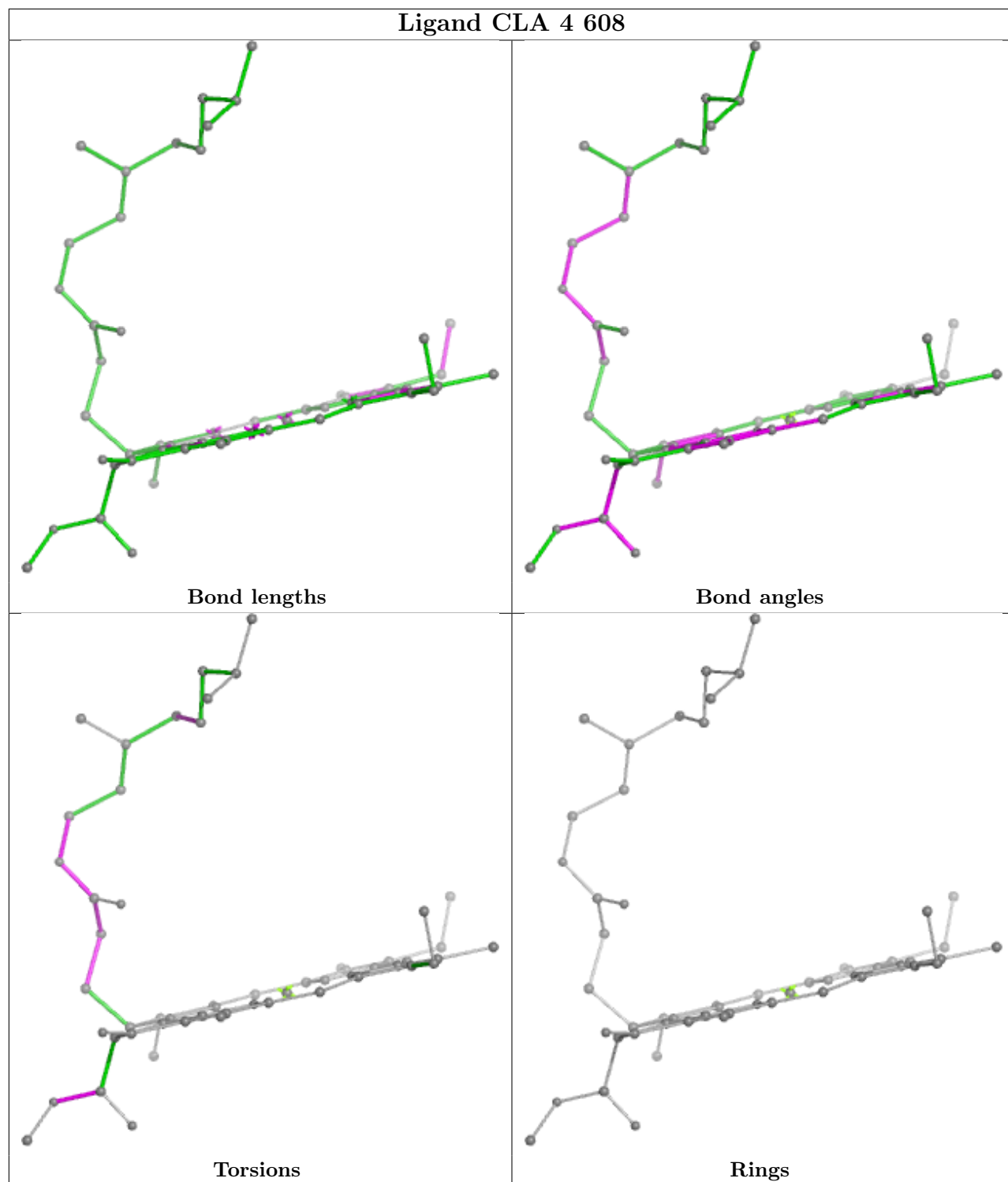




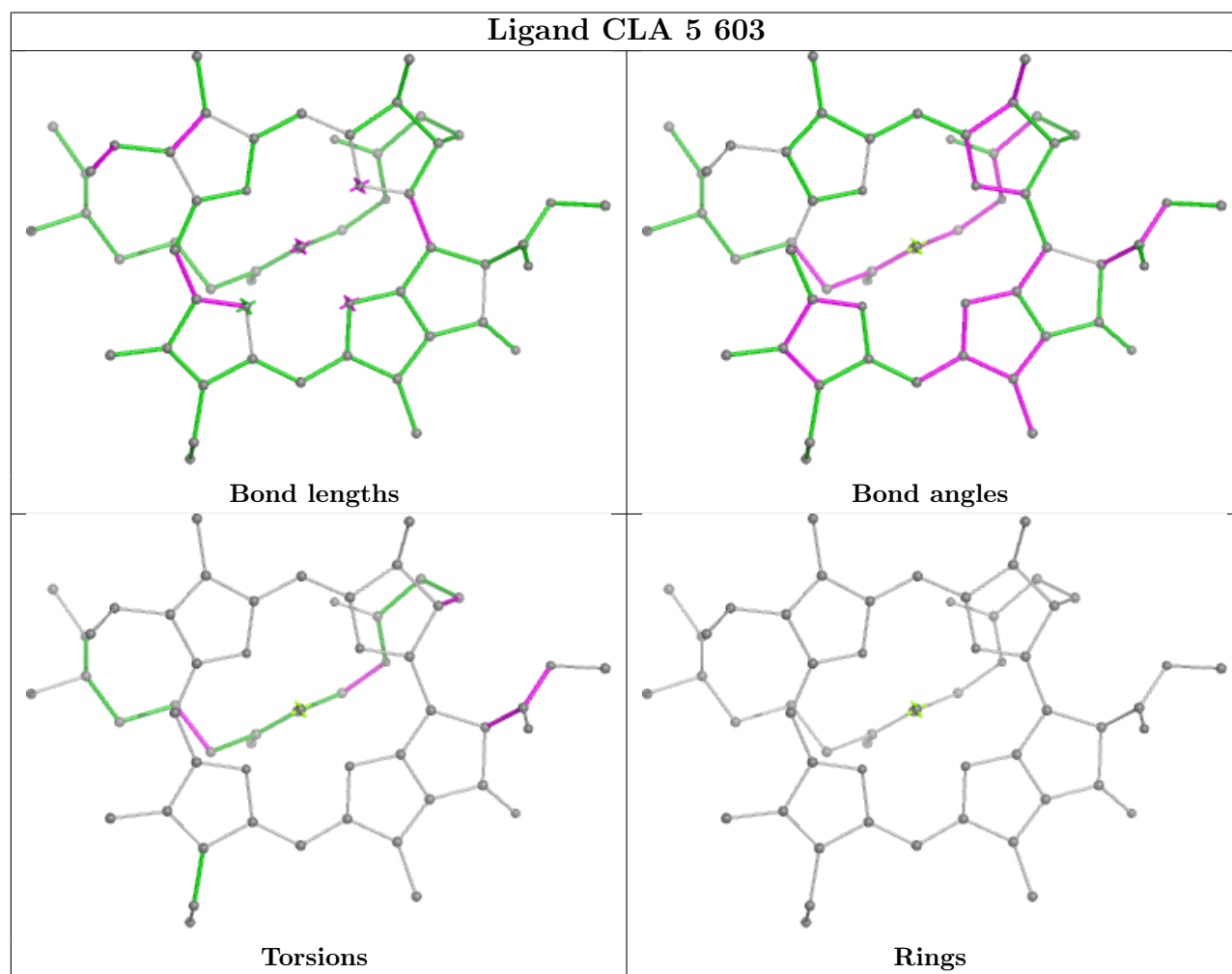
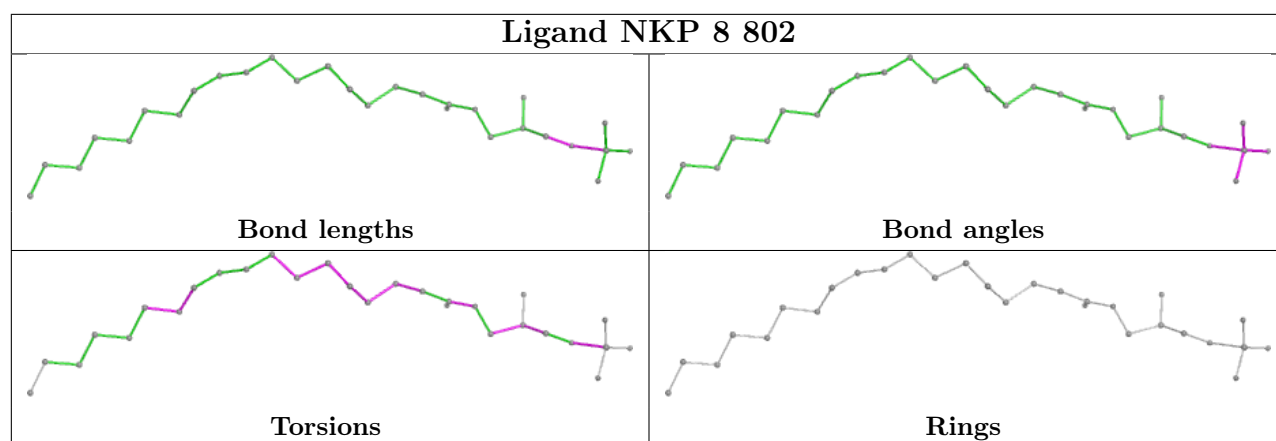
## Ligand CHL 1 610

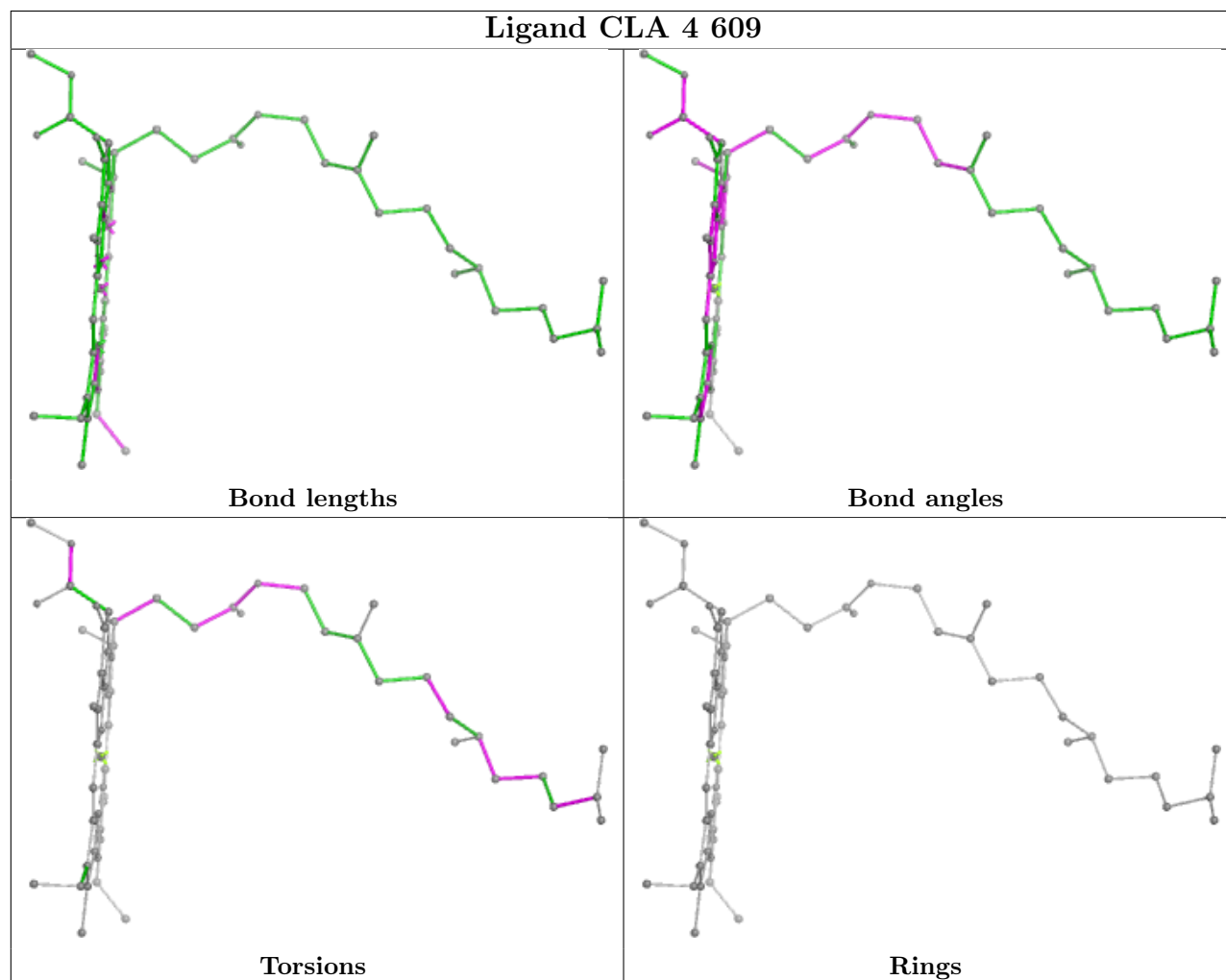
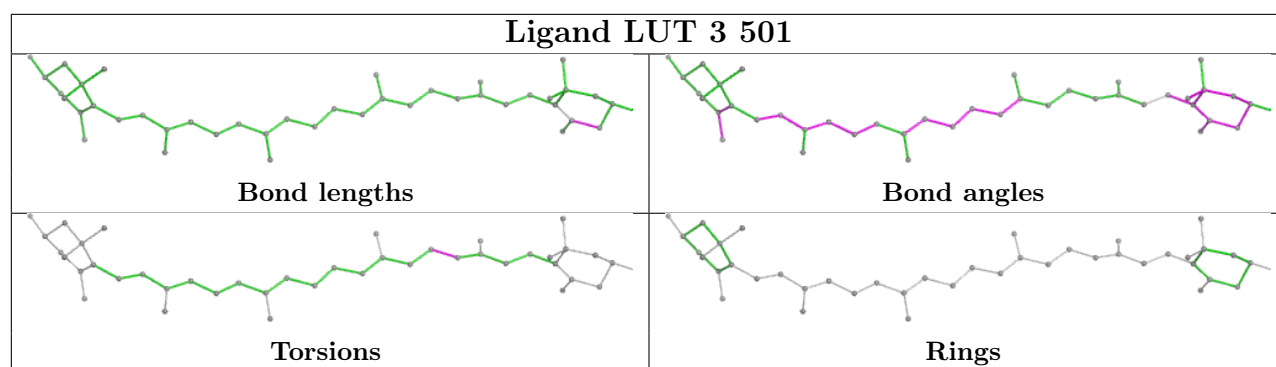


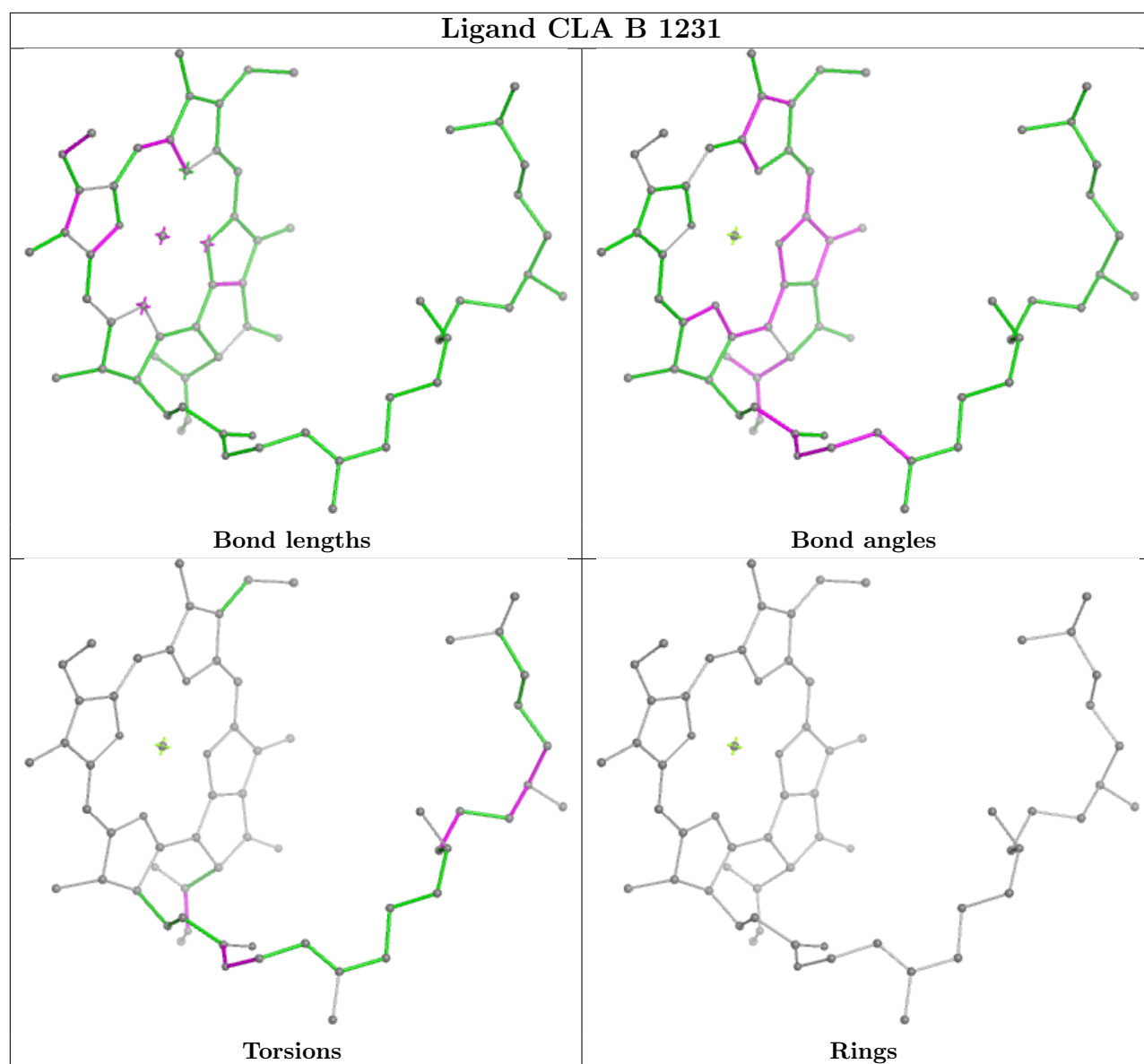
## Ligand CLA 4 608

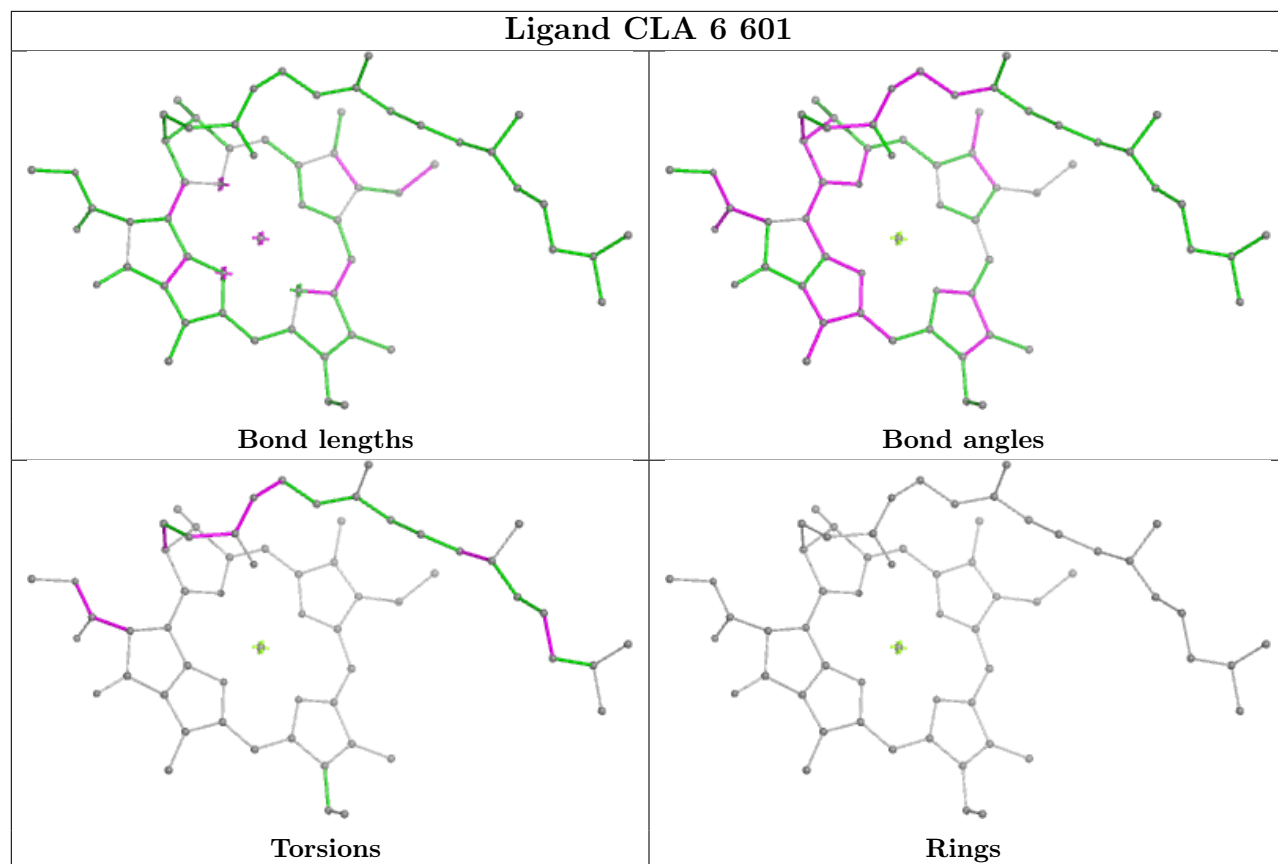


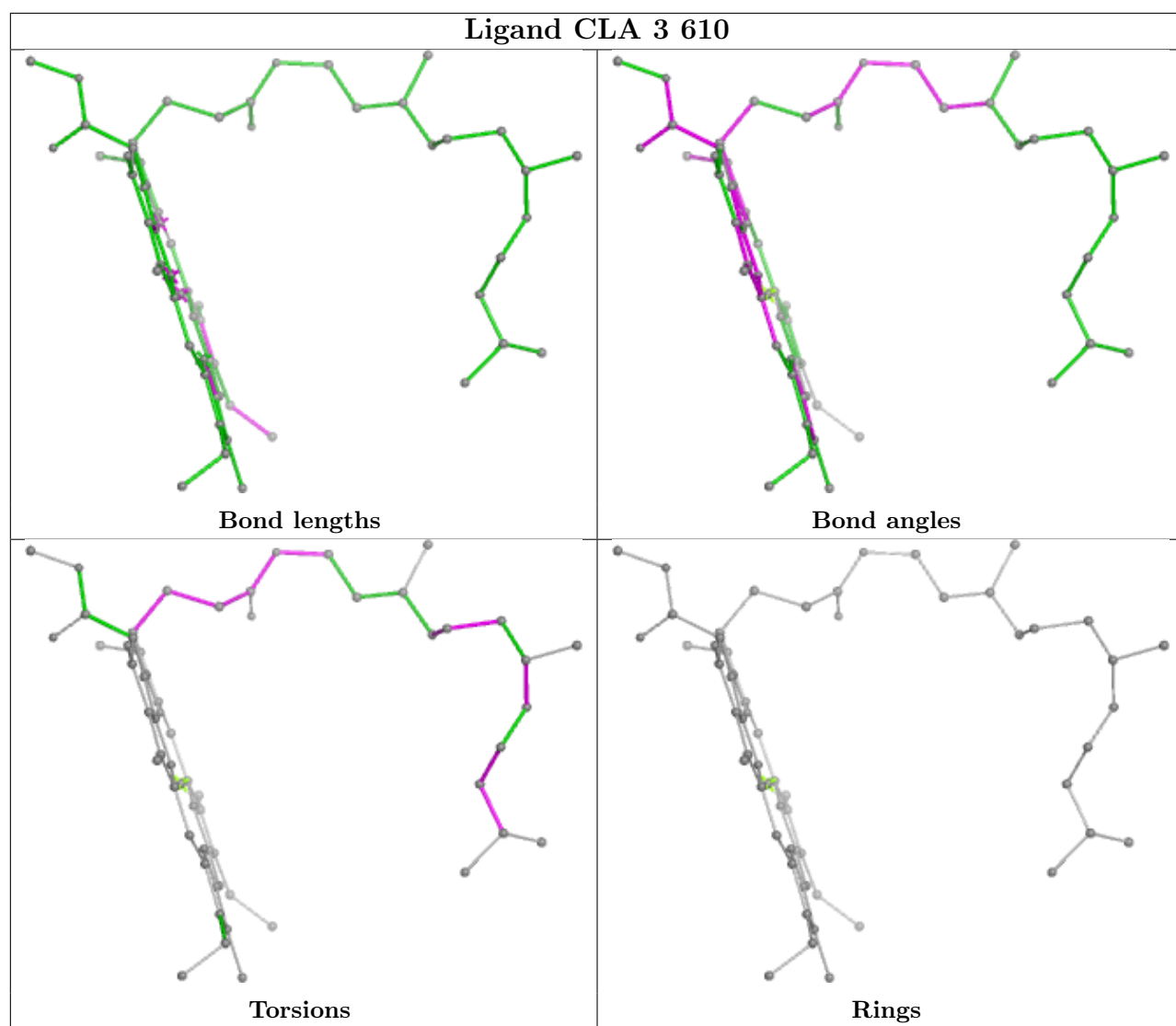


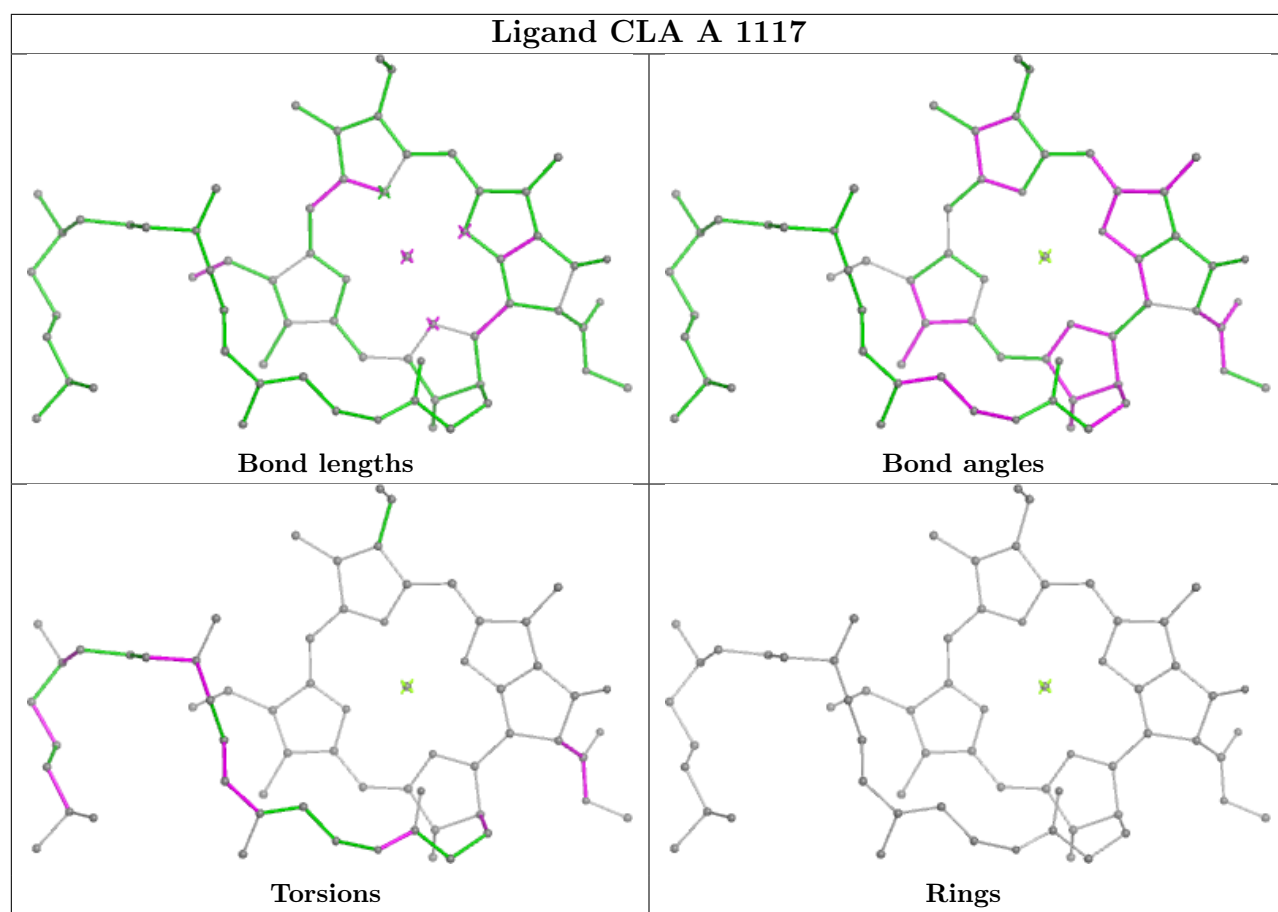




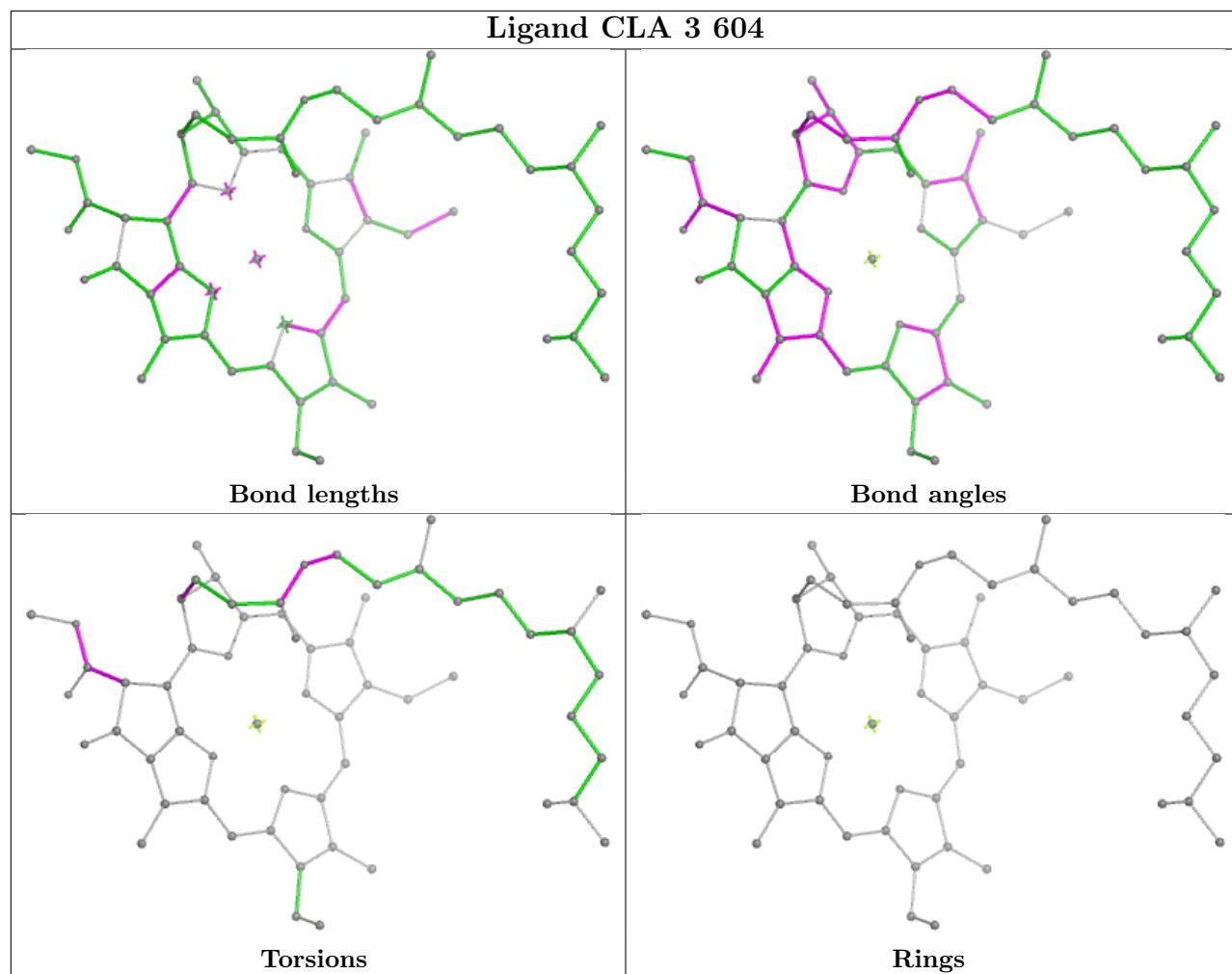


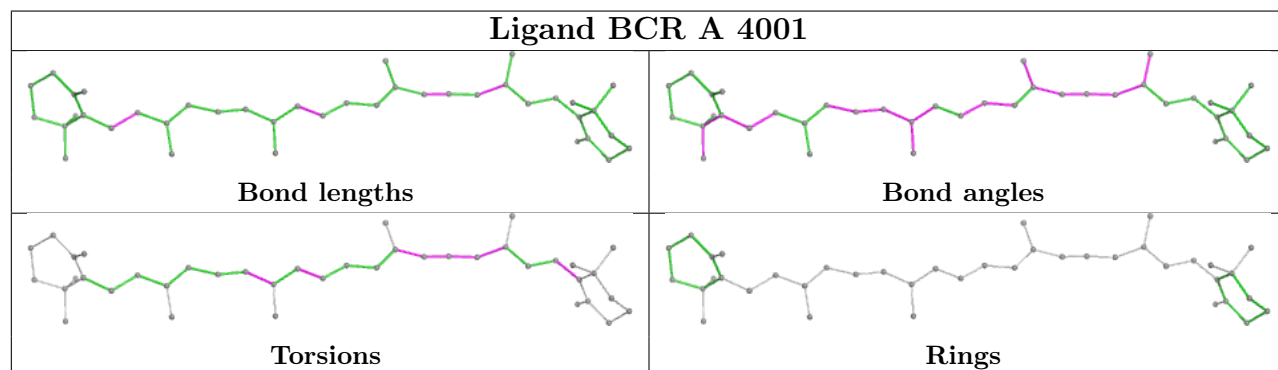
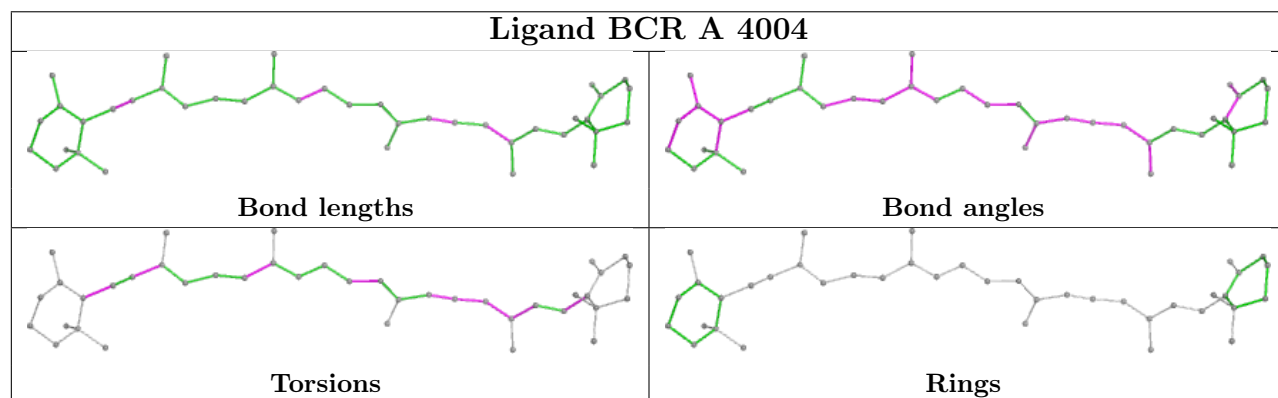
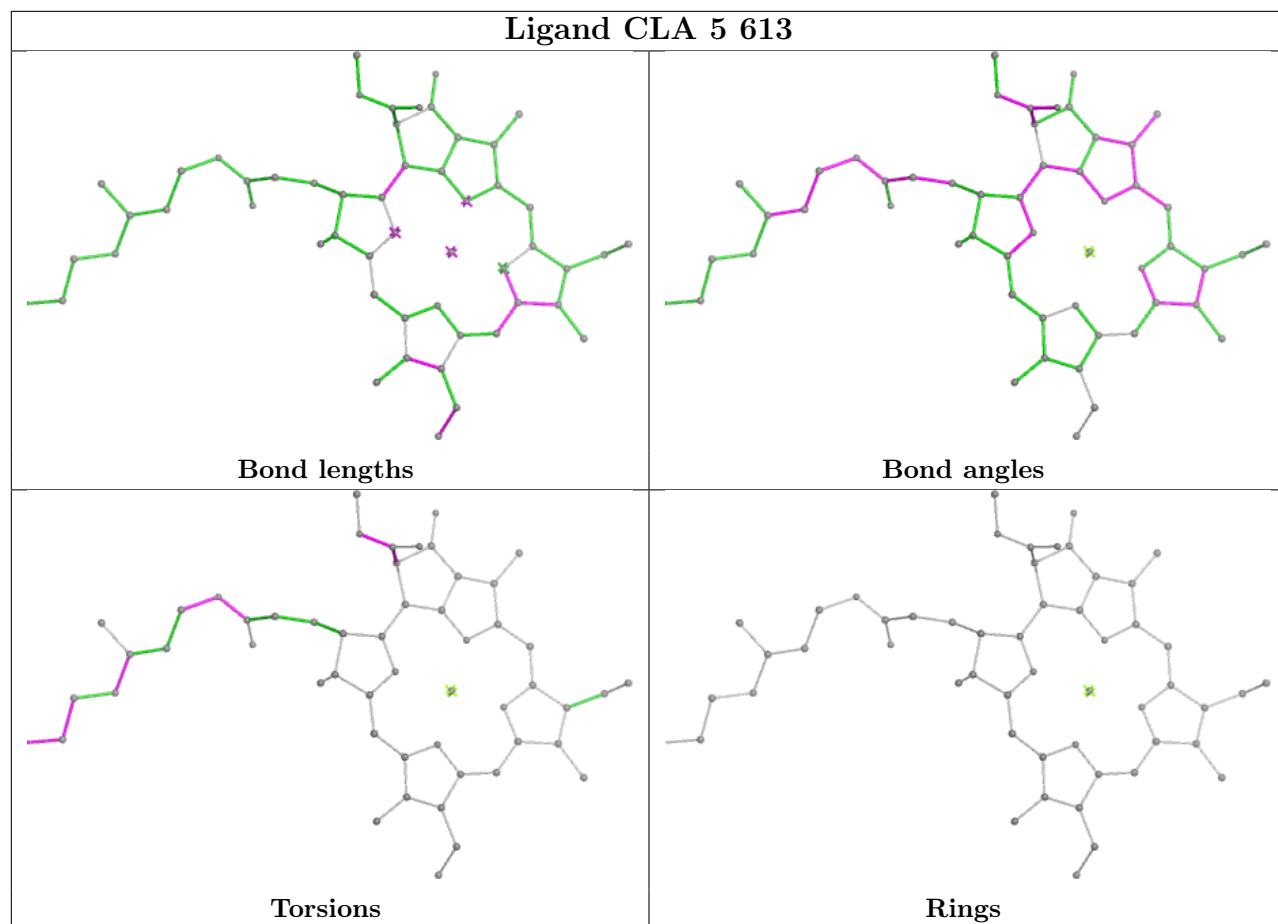






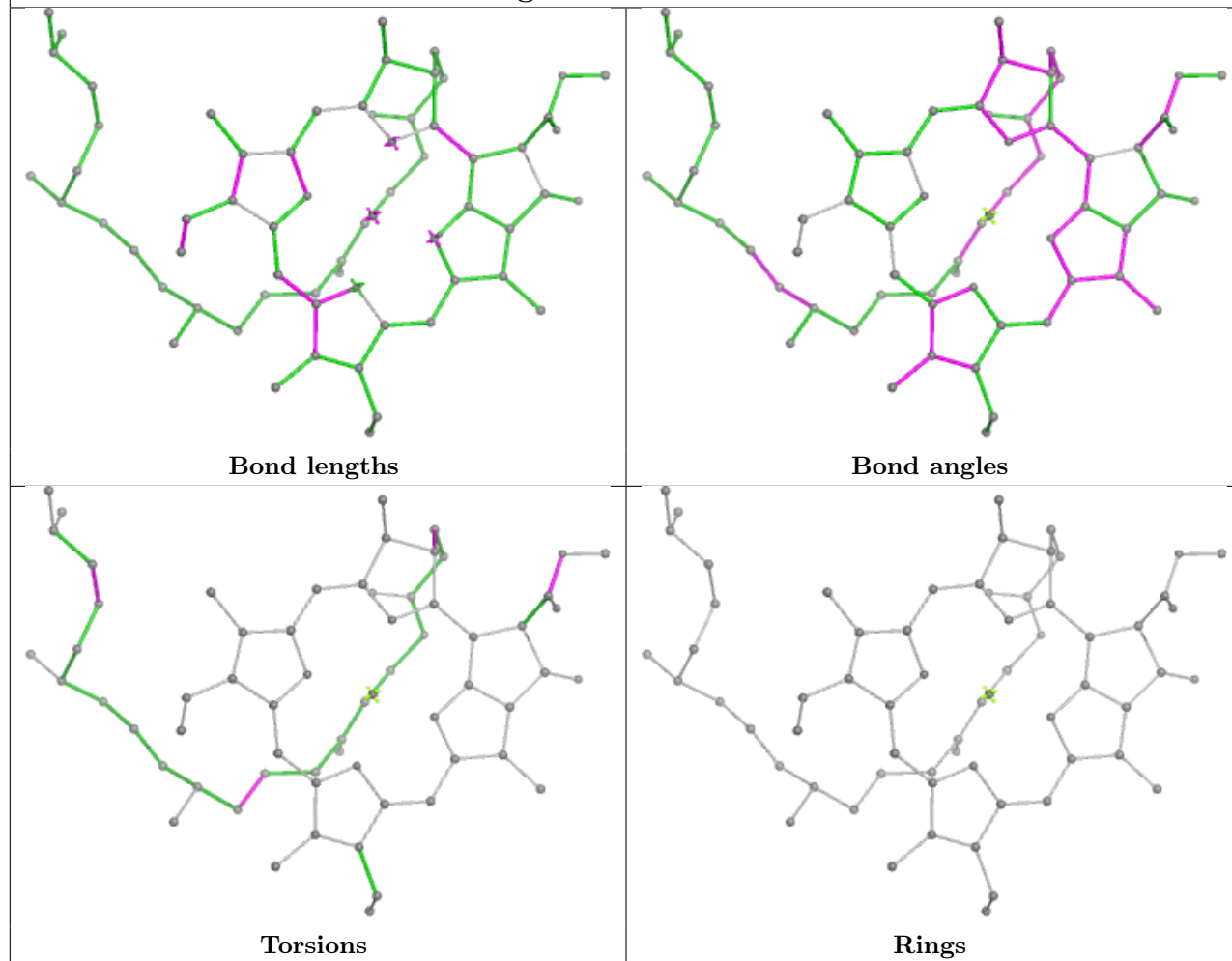
## Ligand CLA 3 604



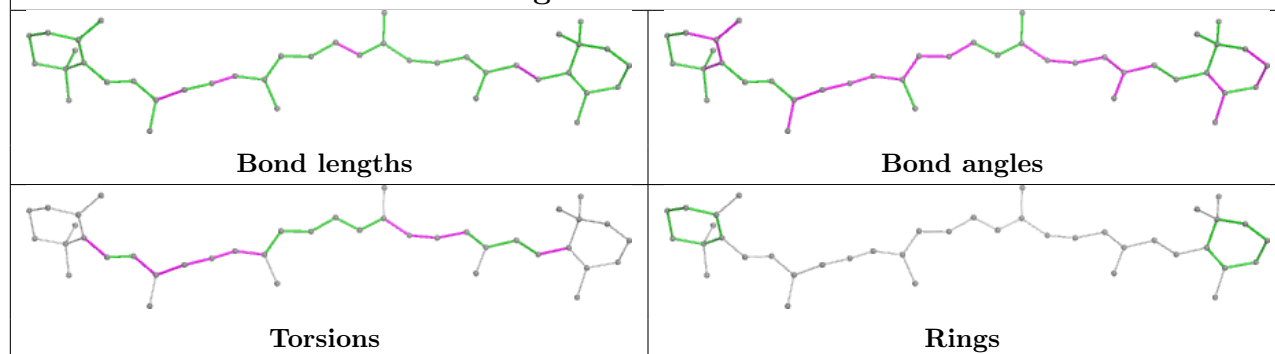


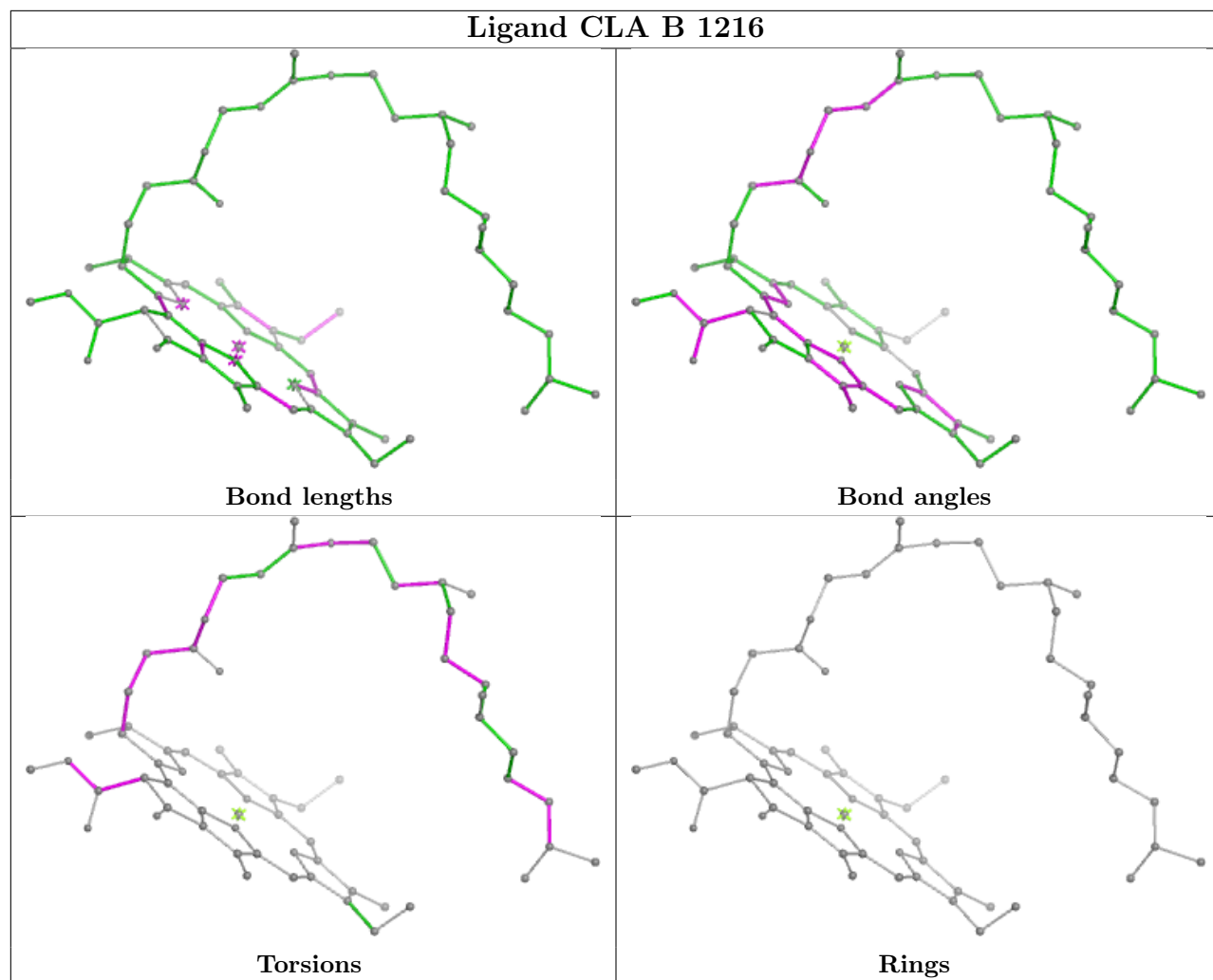


## Ligand CLA 8 603

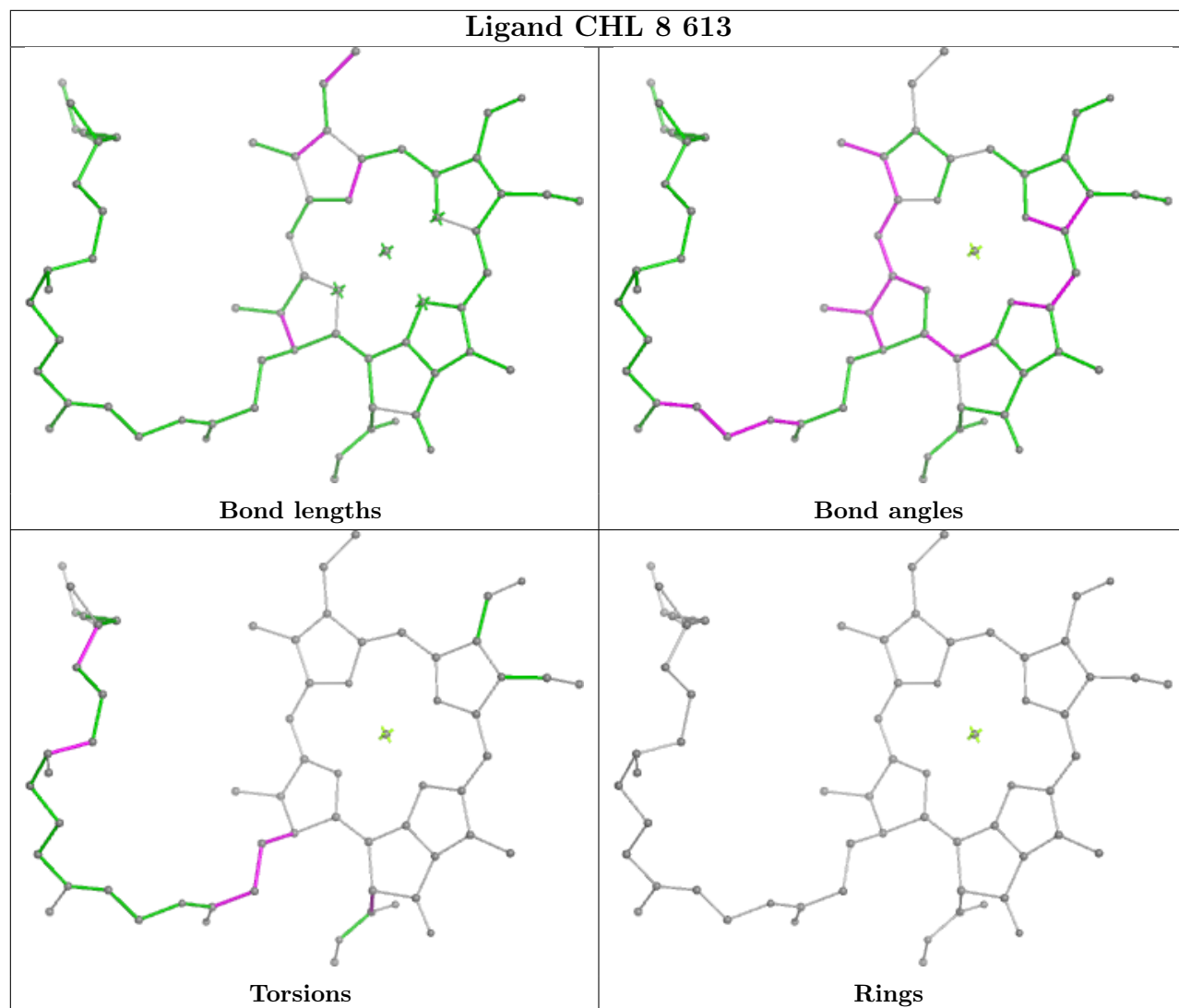


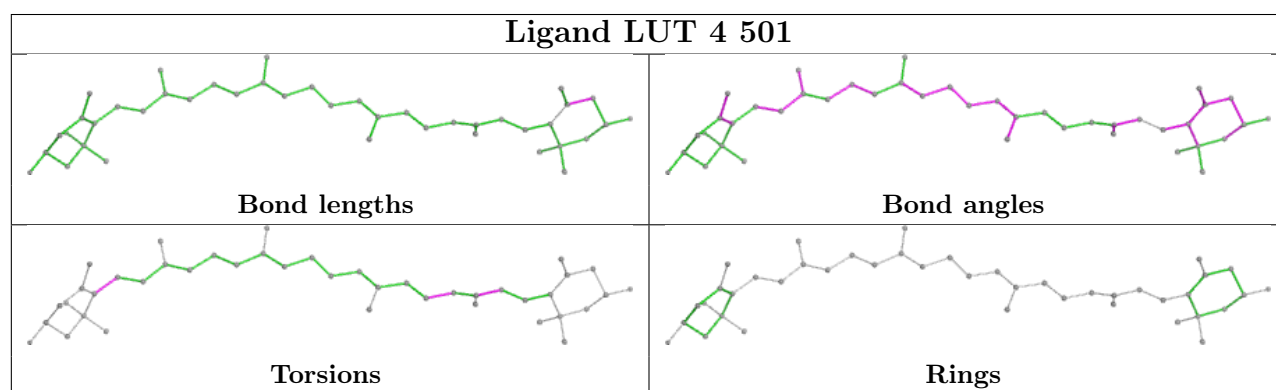
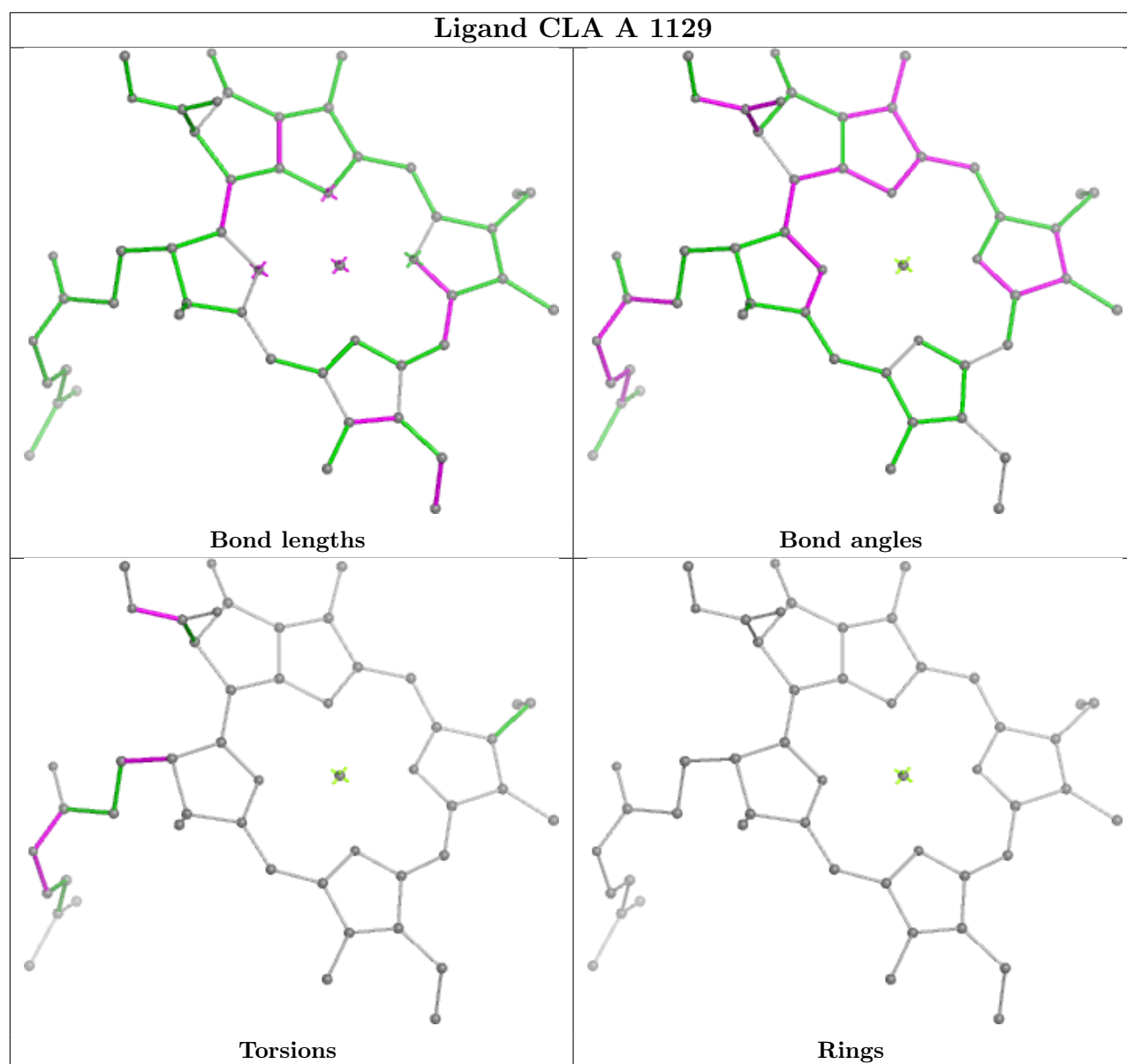
## Ligand BCR 3 506

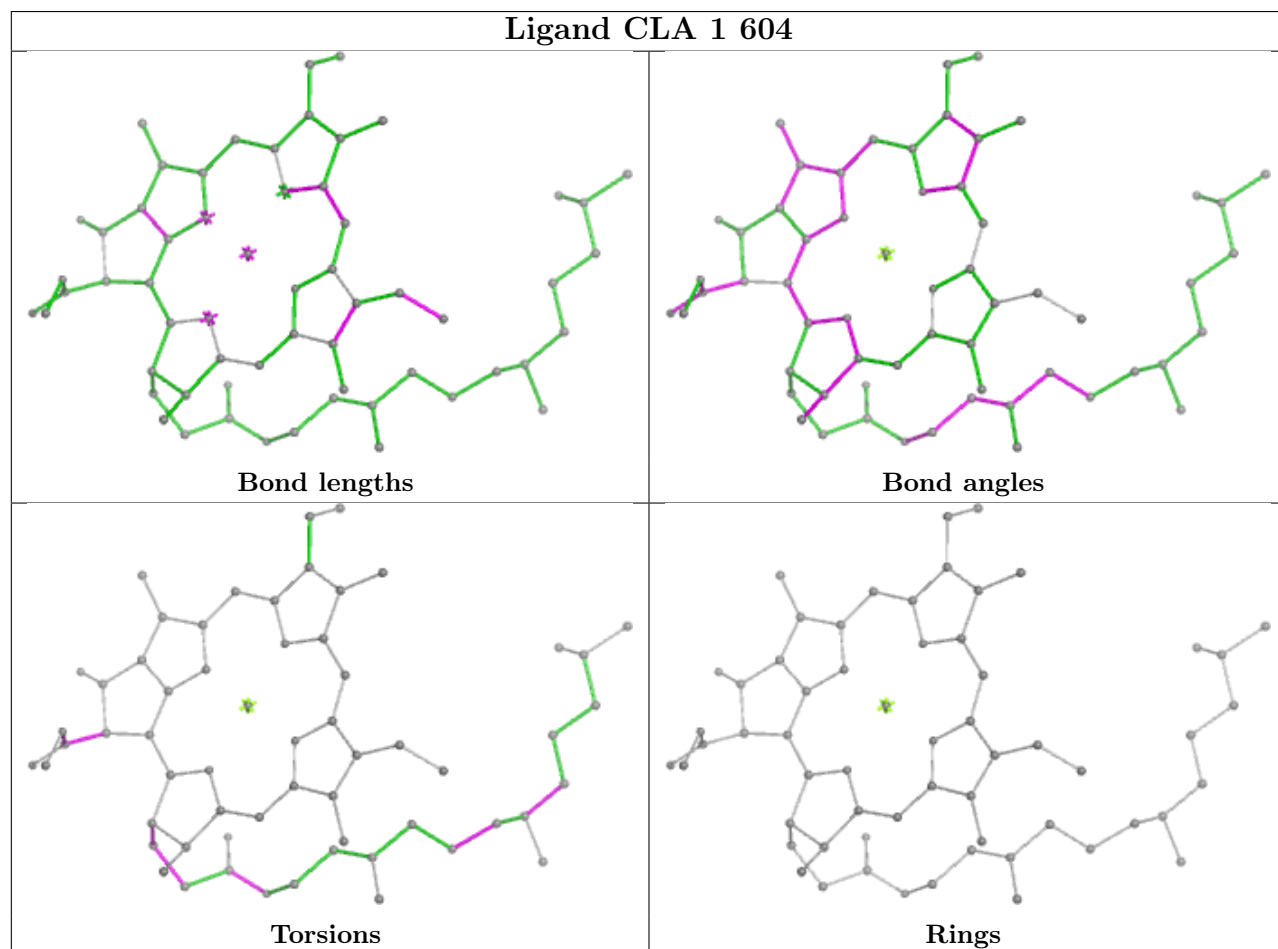
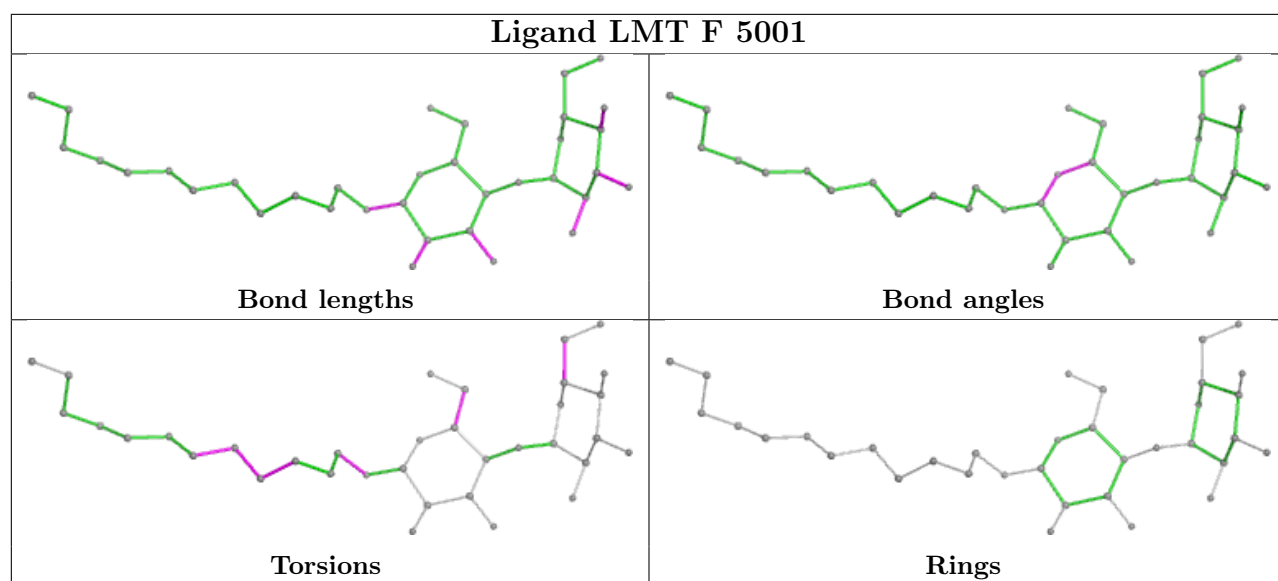


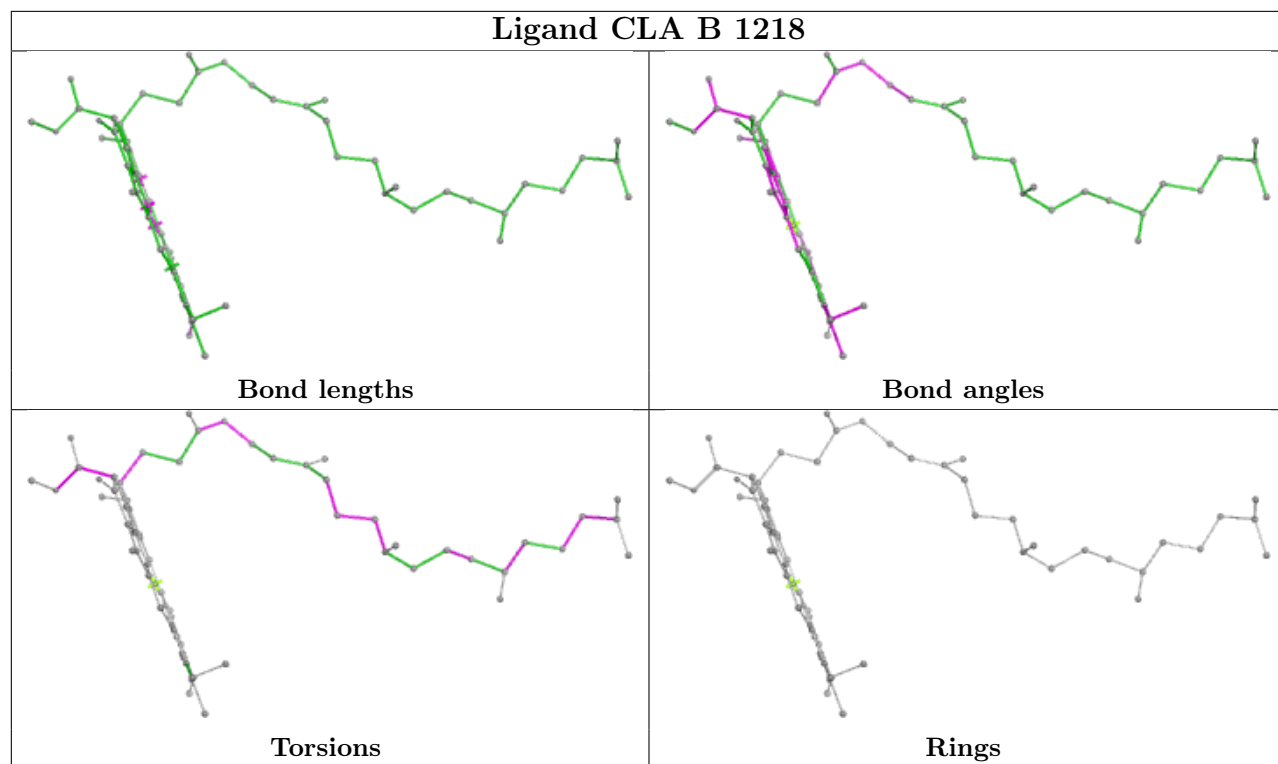


## Ligand CHL 8 613

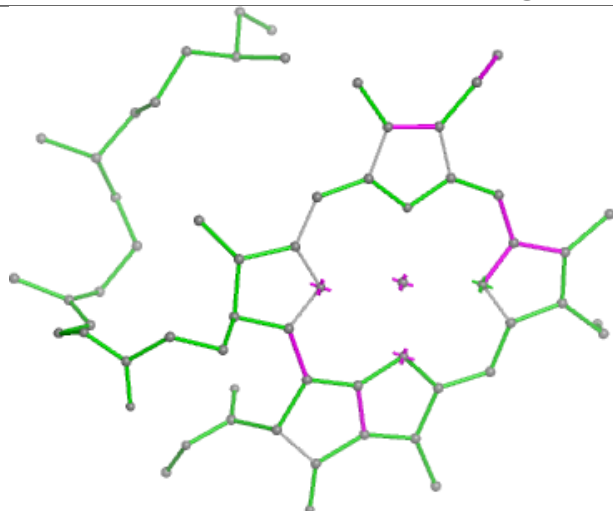




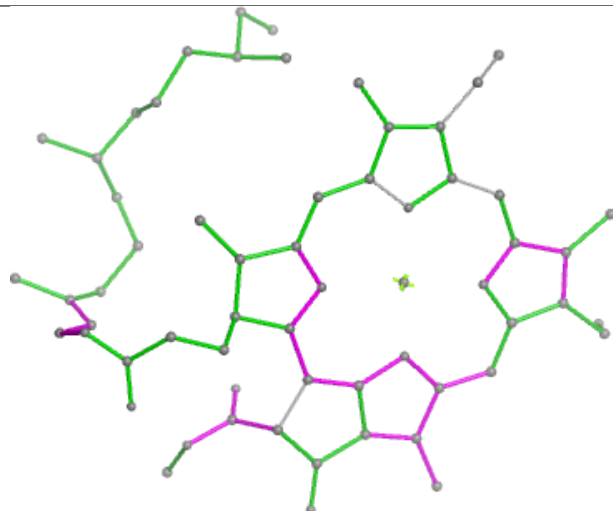




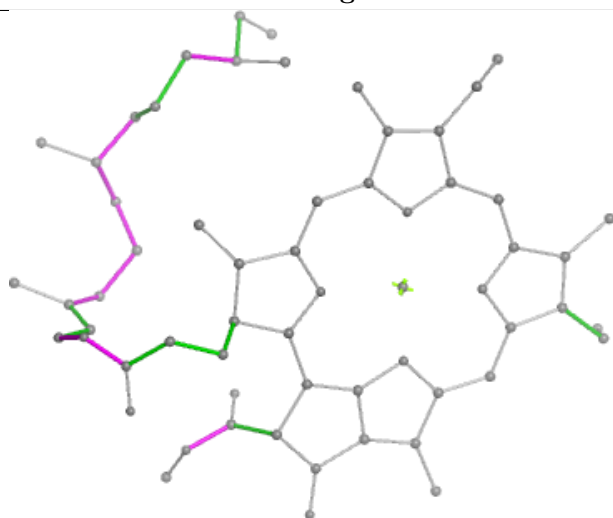
## Ligand CLA 5 602



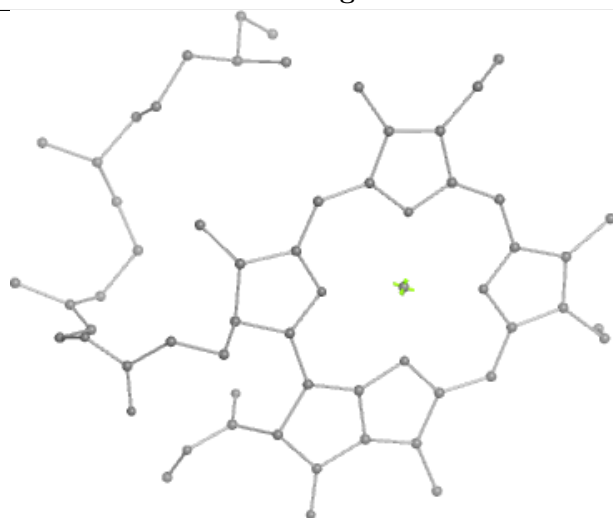
Bond lengths



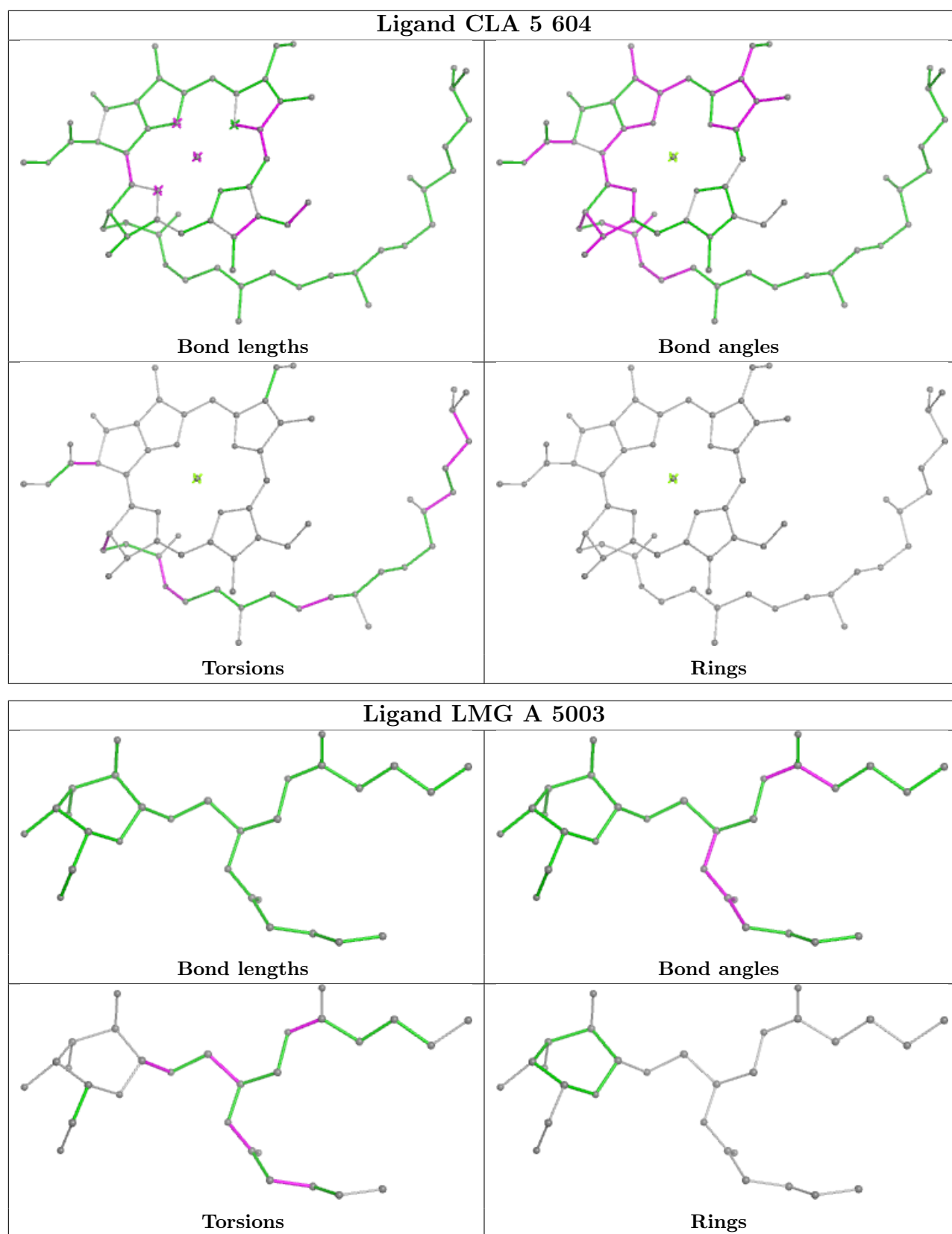
Bond angles



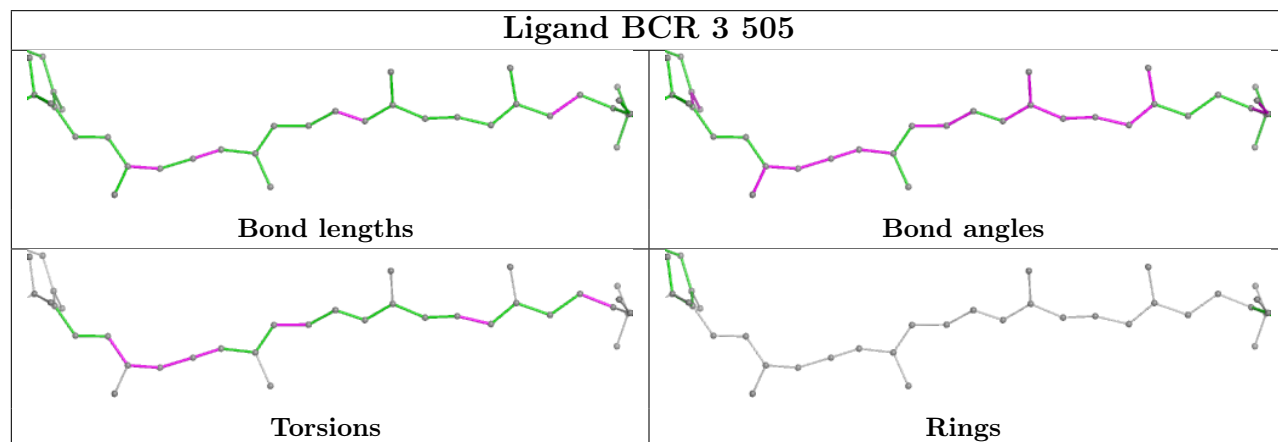
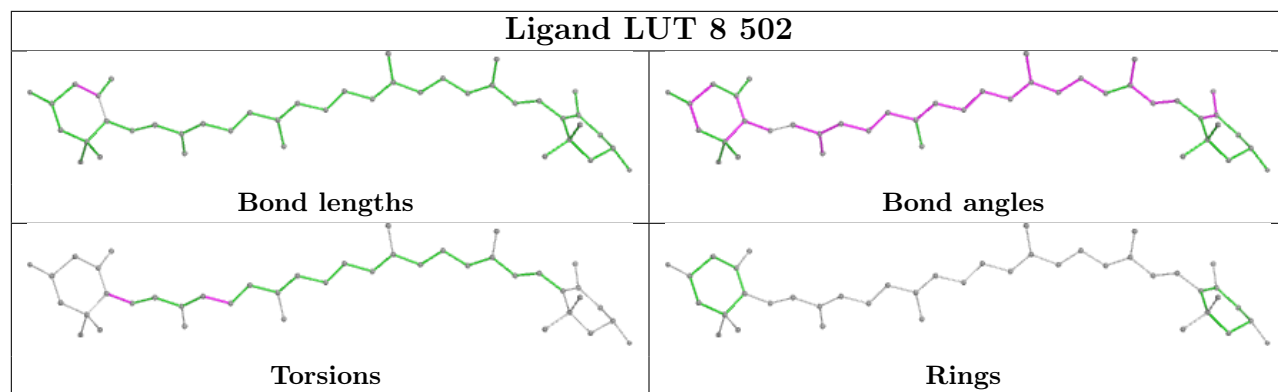
Torsions

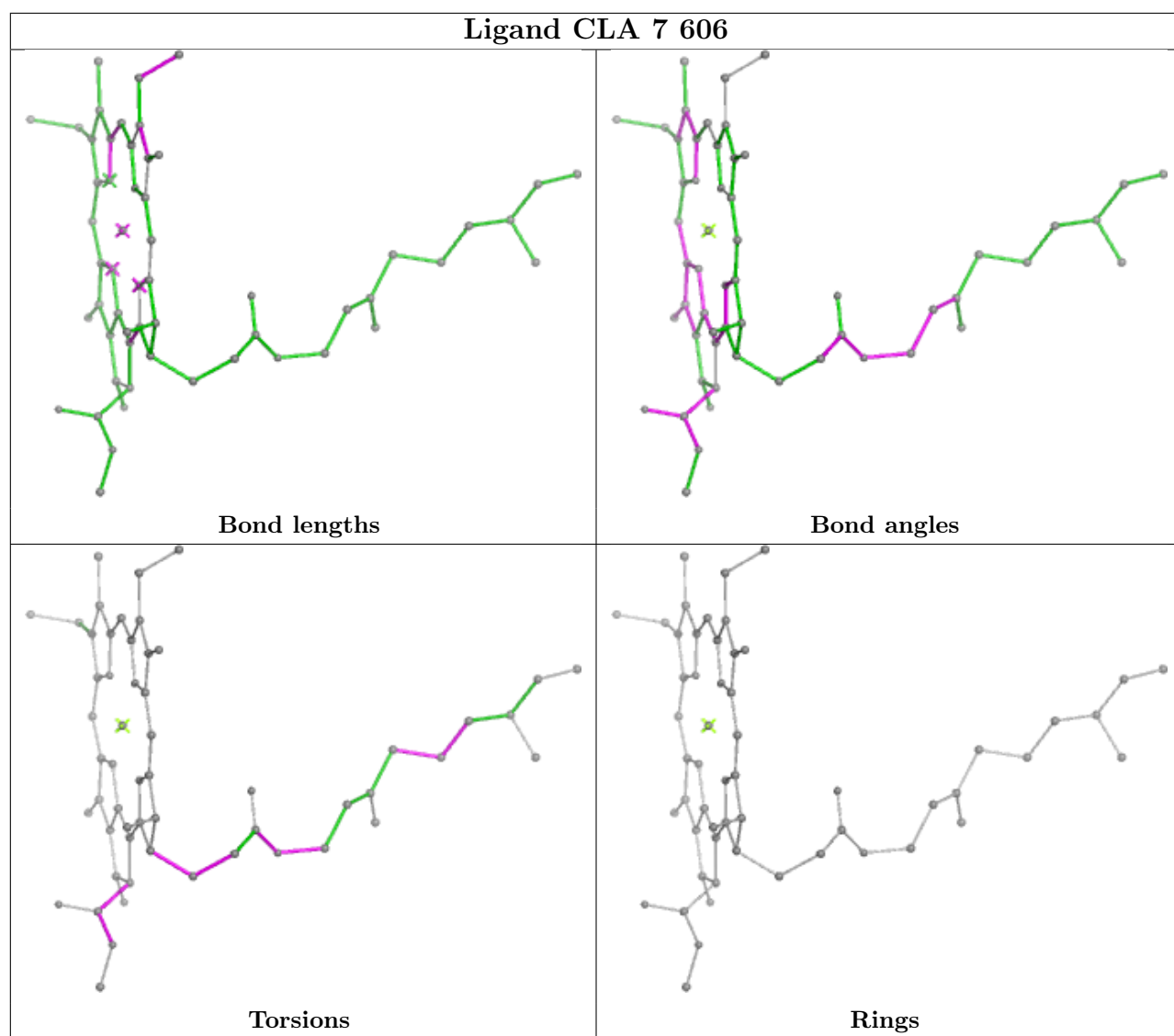


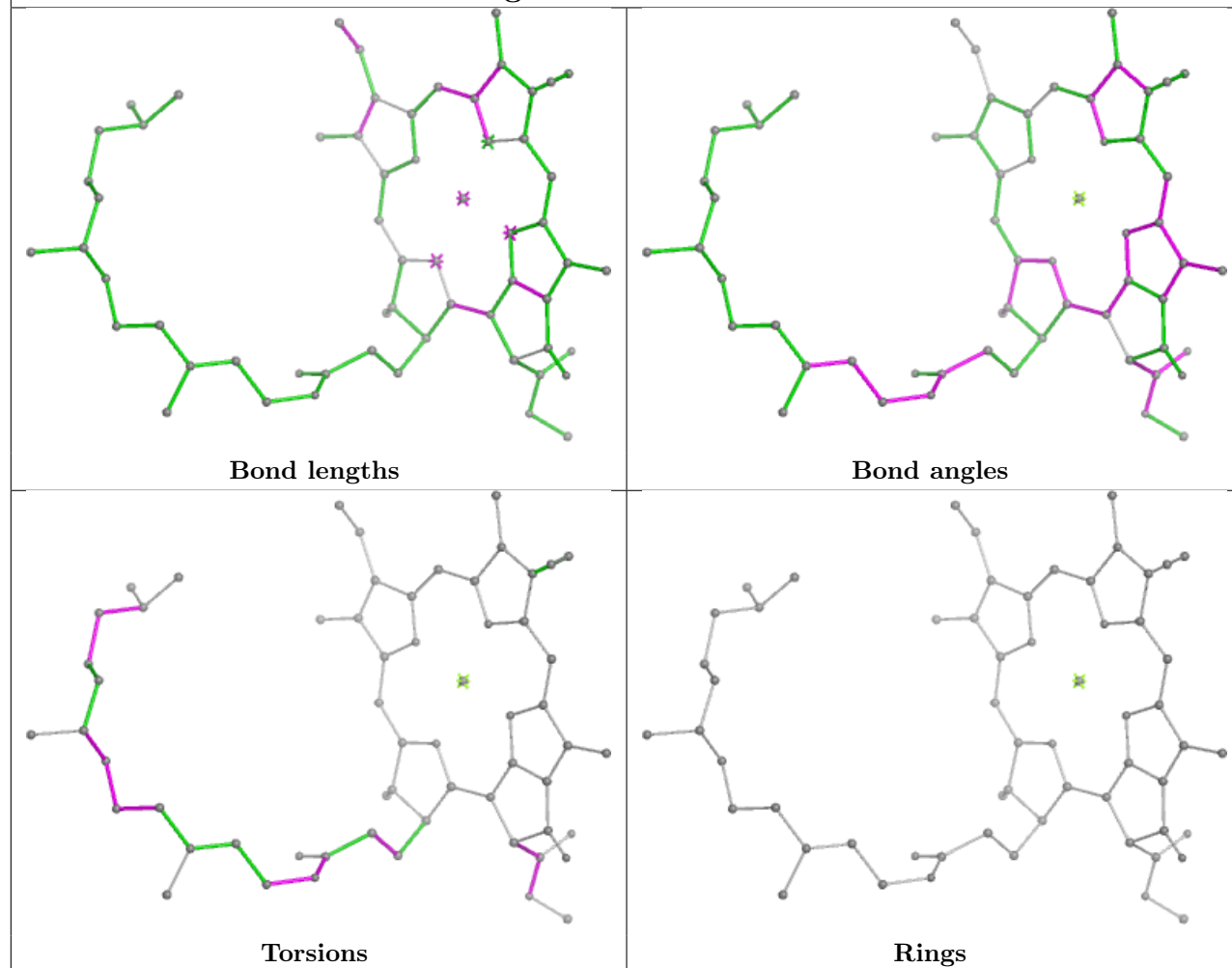
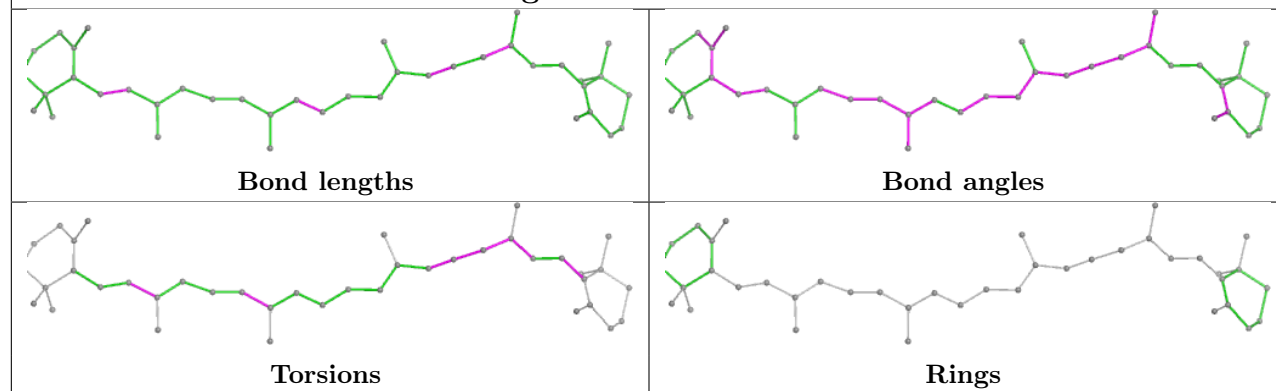
Rings

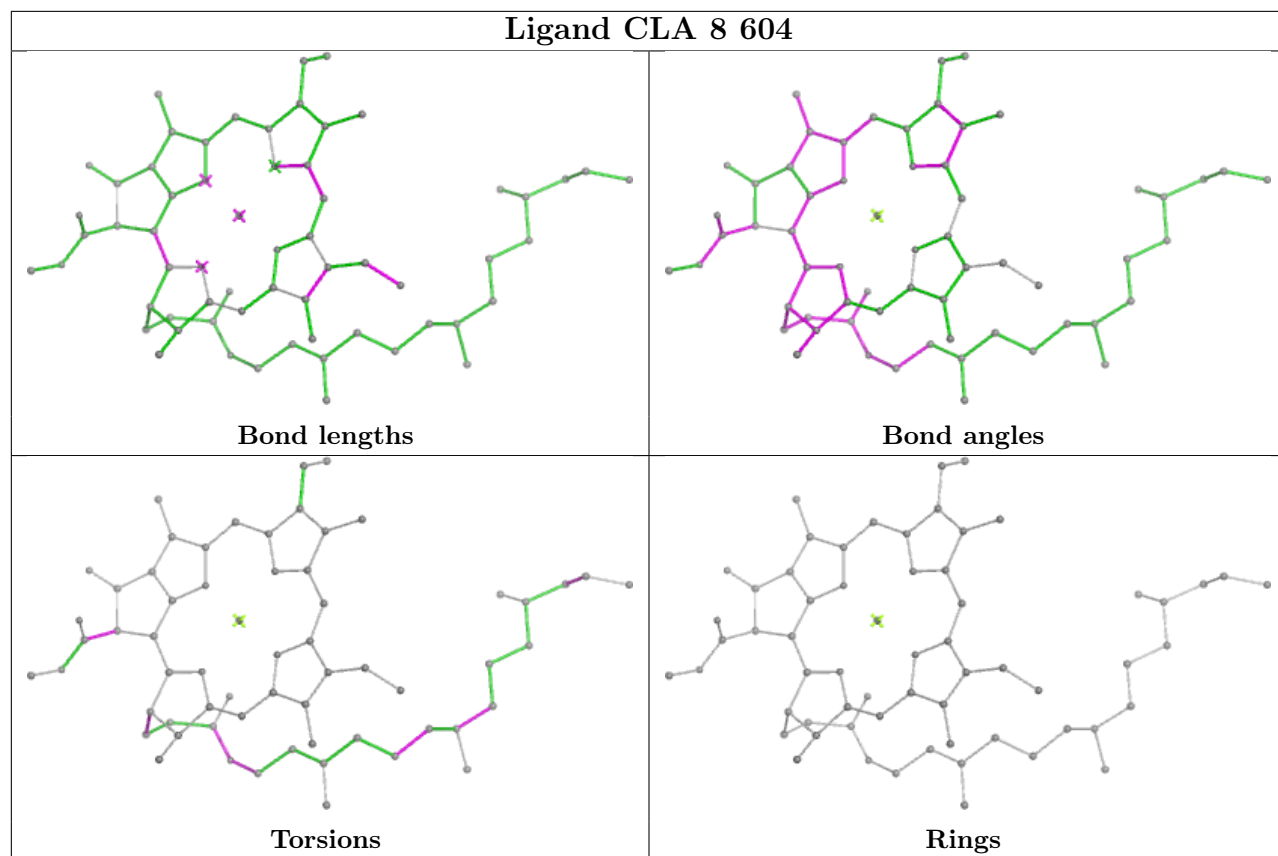




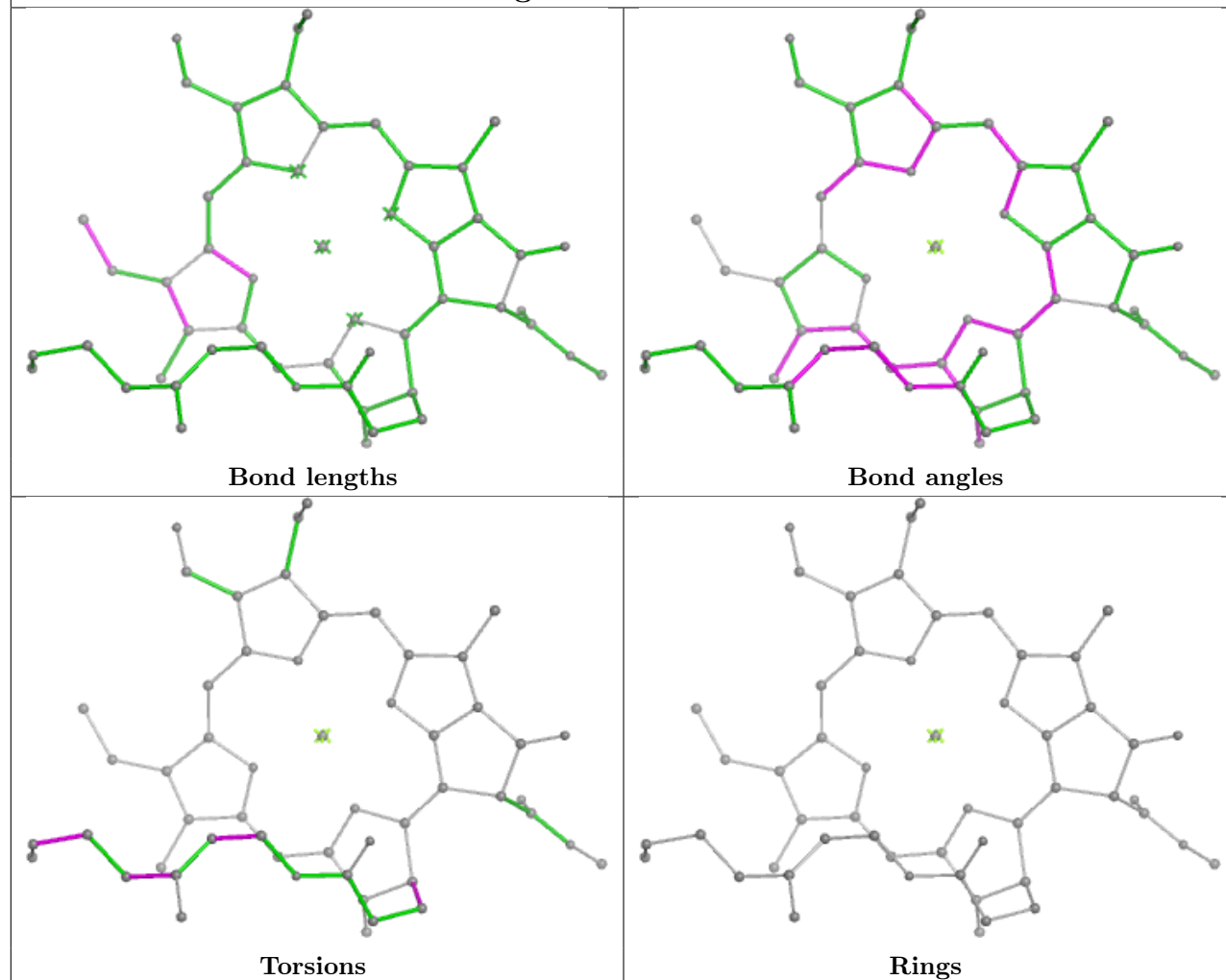




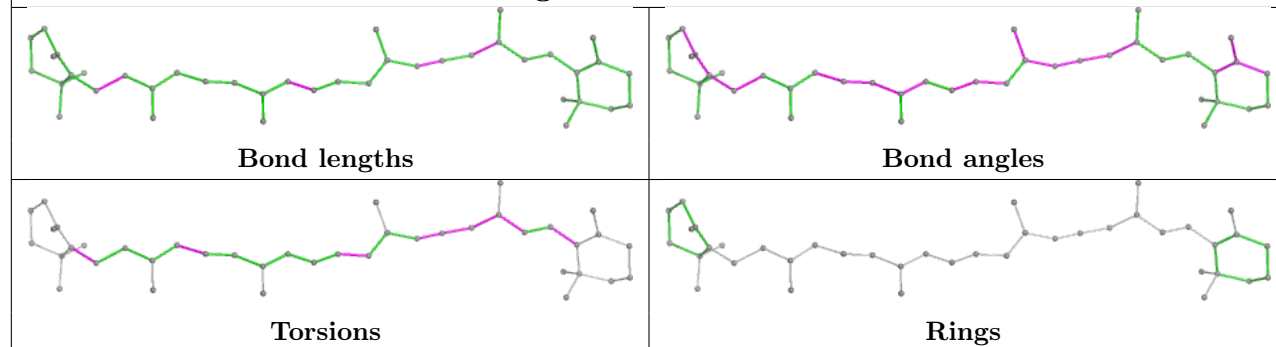
**Ligand CLA A 1118****Ligand BCR B 4002**



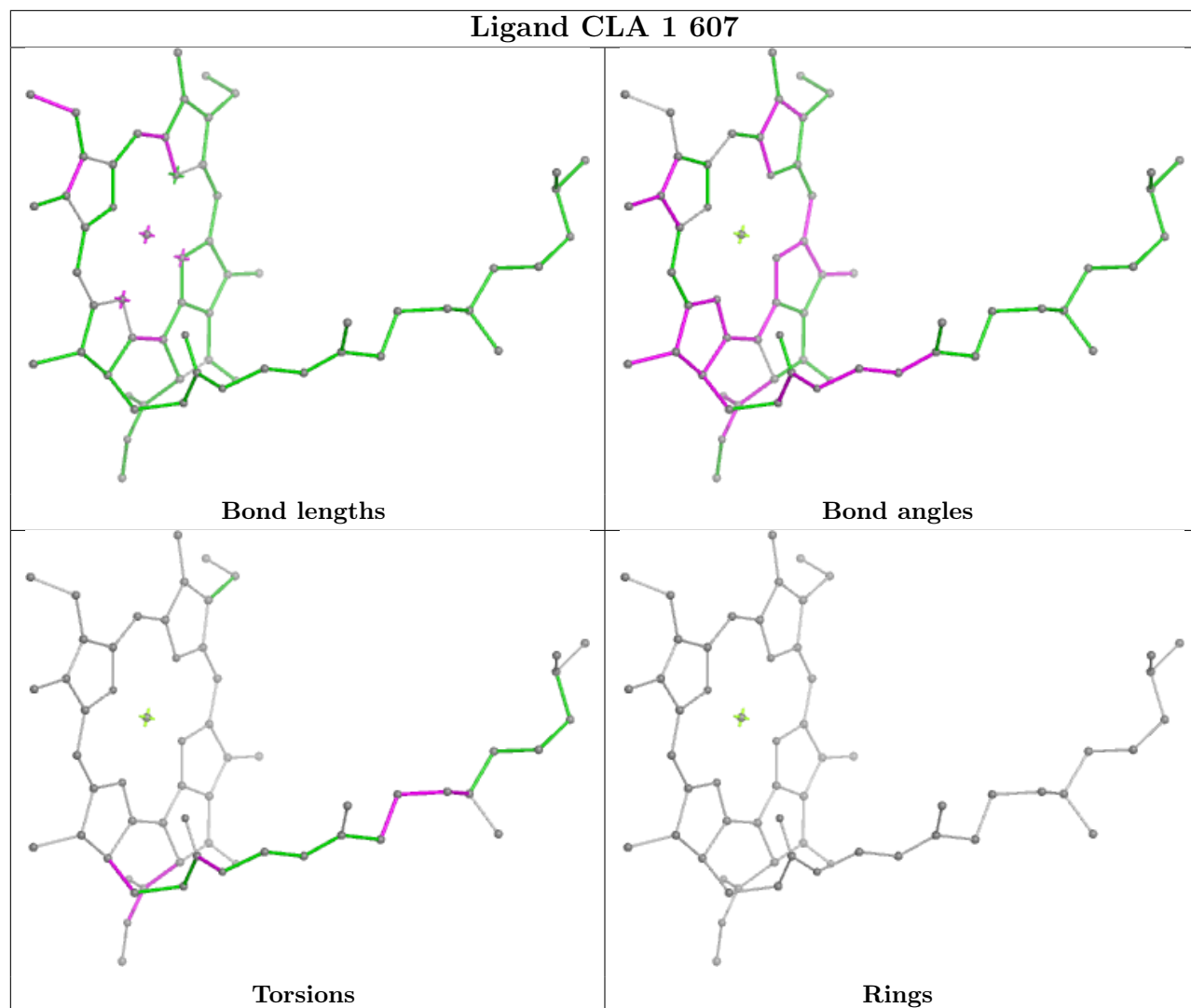
## Ligand CHL 7 610

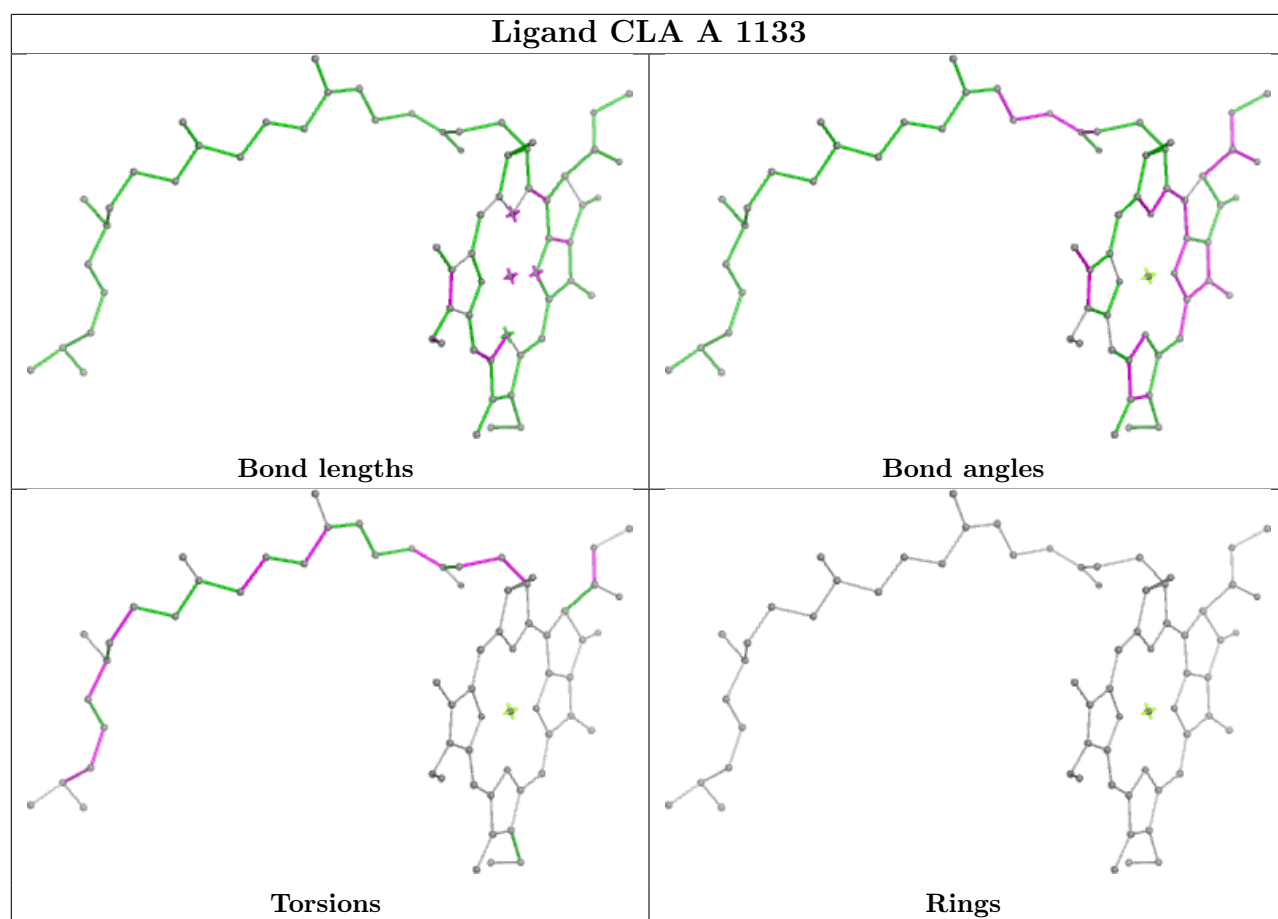


## Ligand BCR 8 503

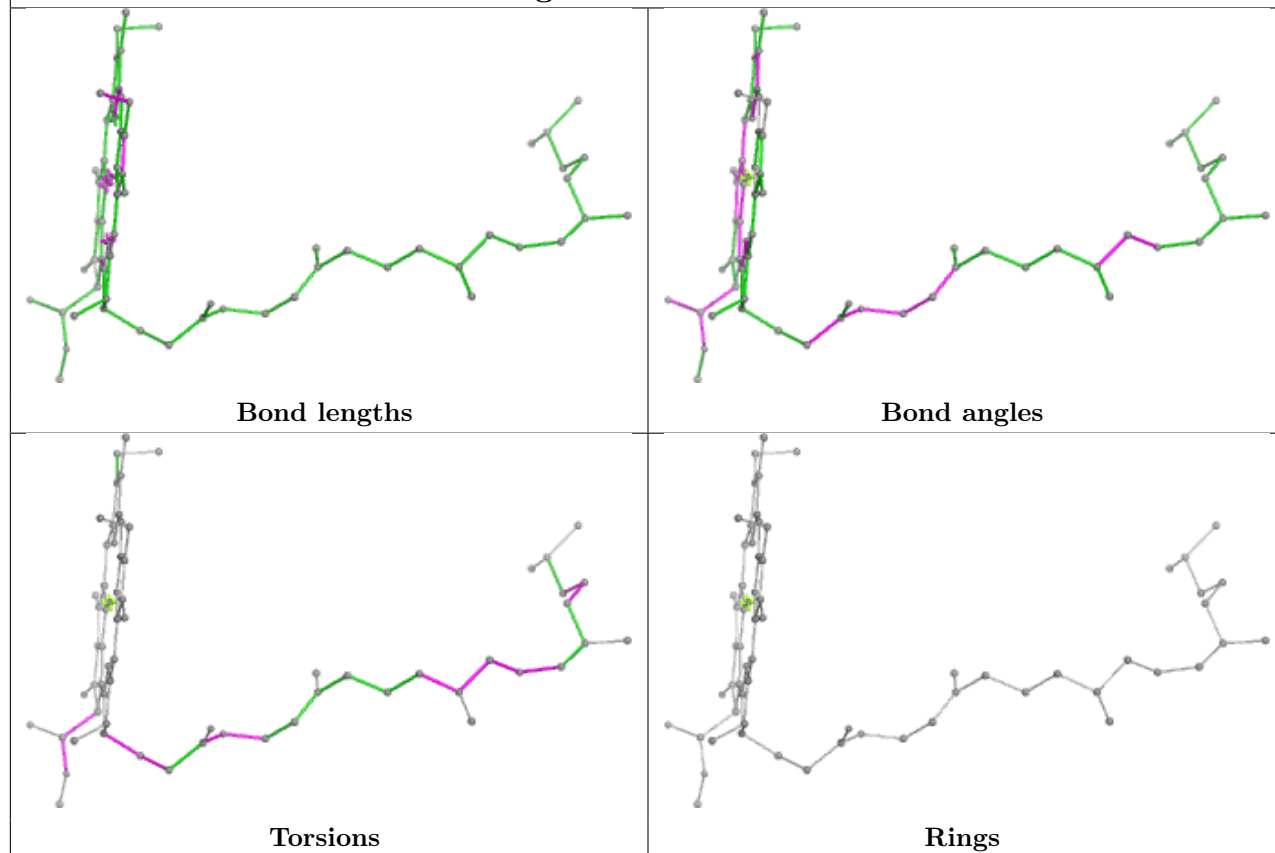


## Ligand CLA 1 607

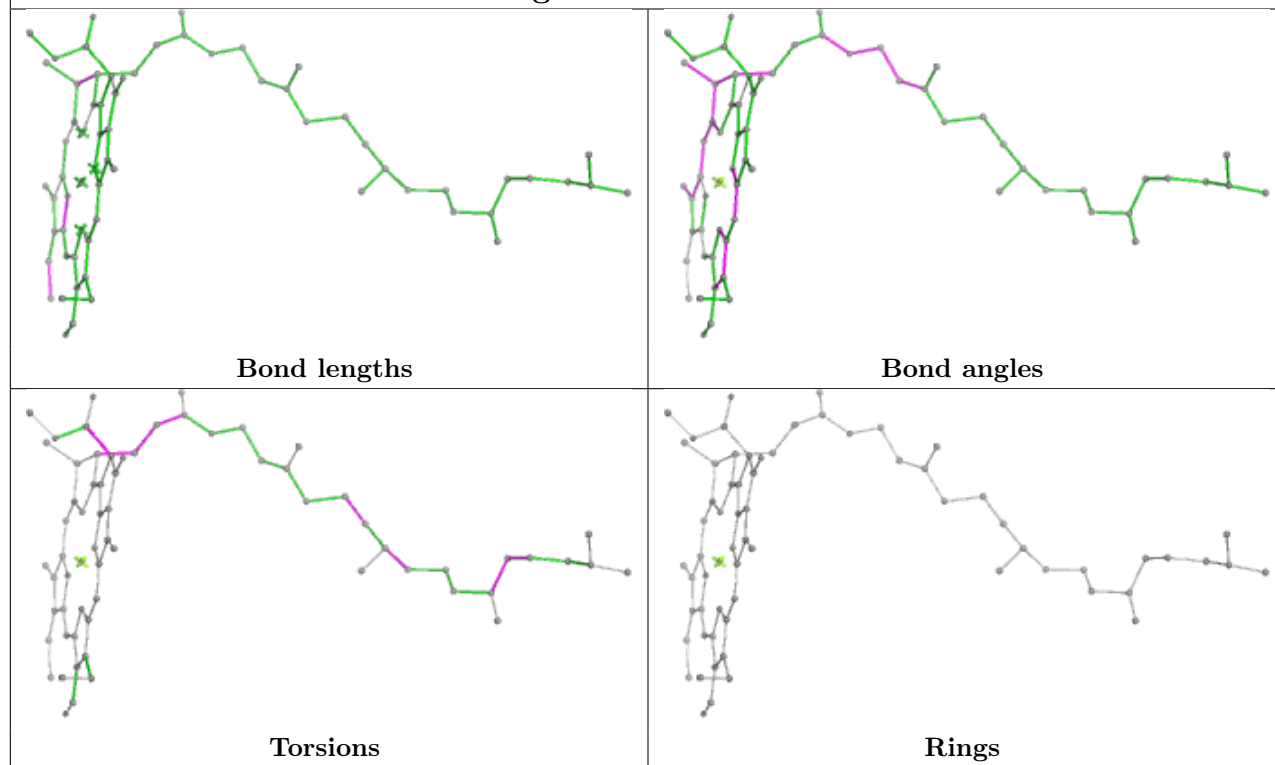




## Ligand CLA 3 606

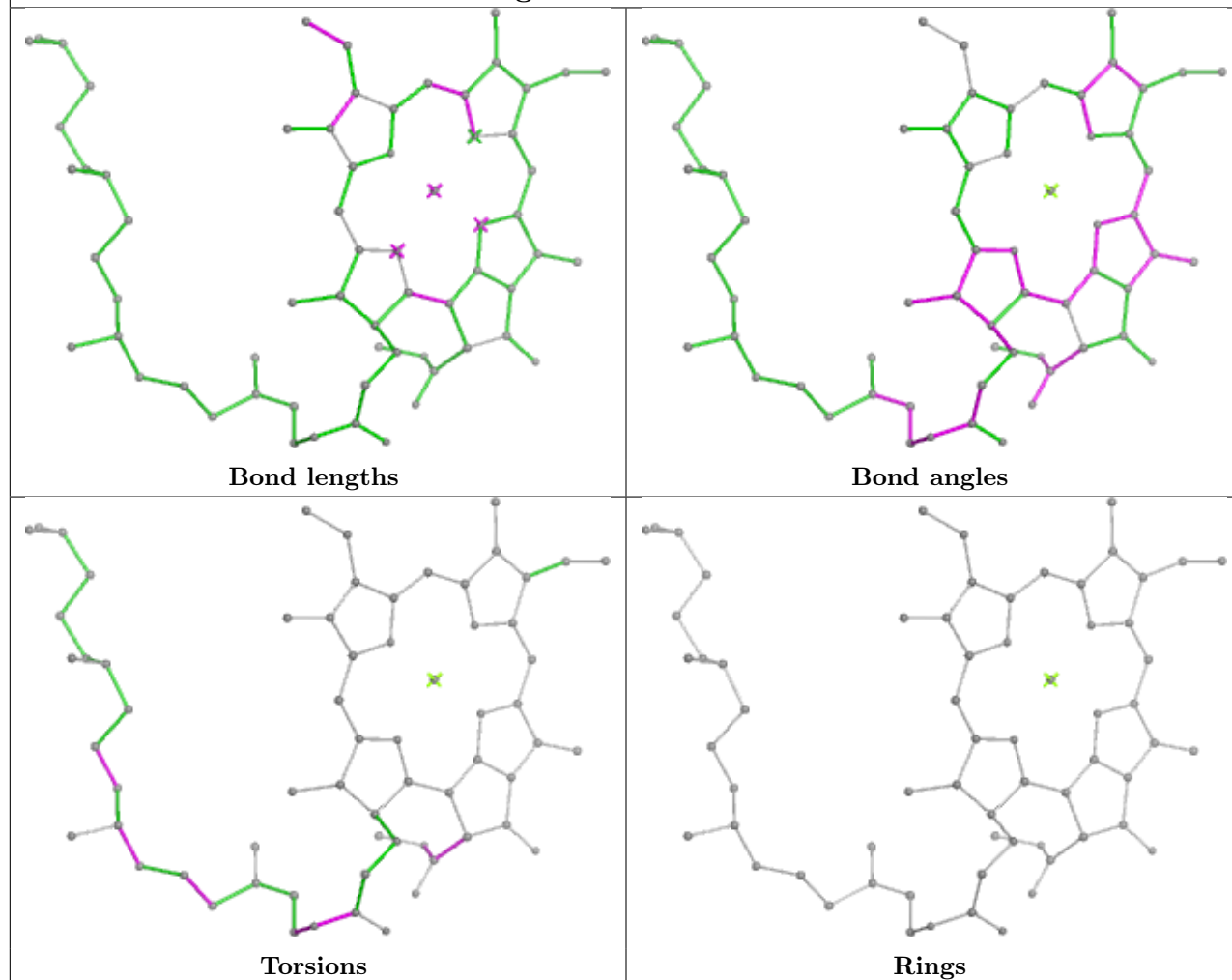


## Ligand CHL Z 609

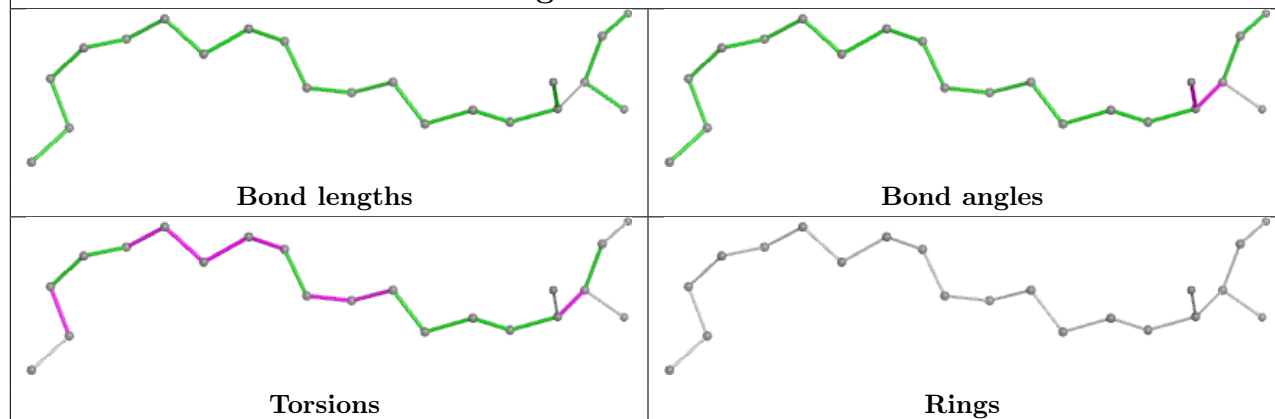


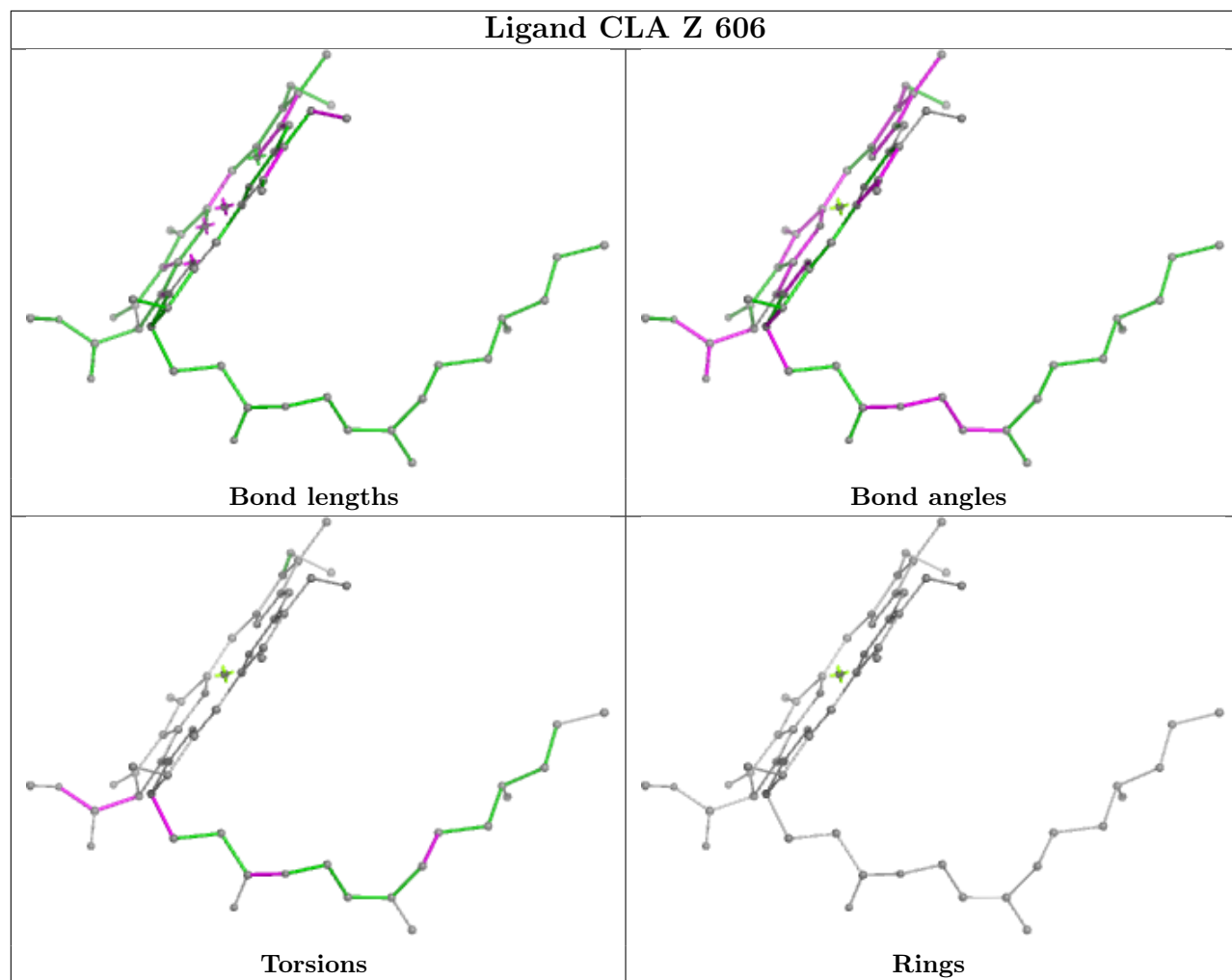


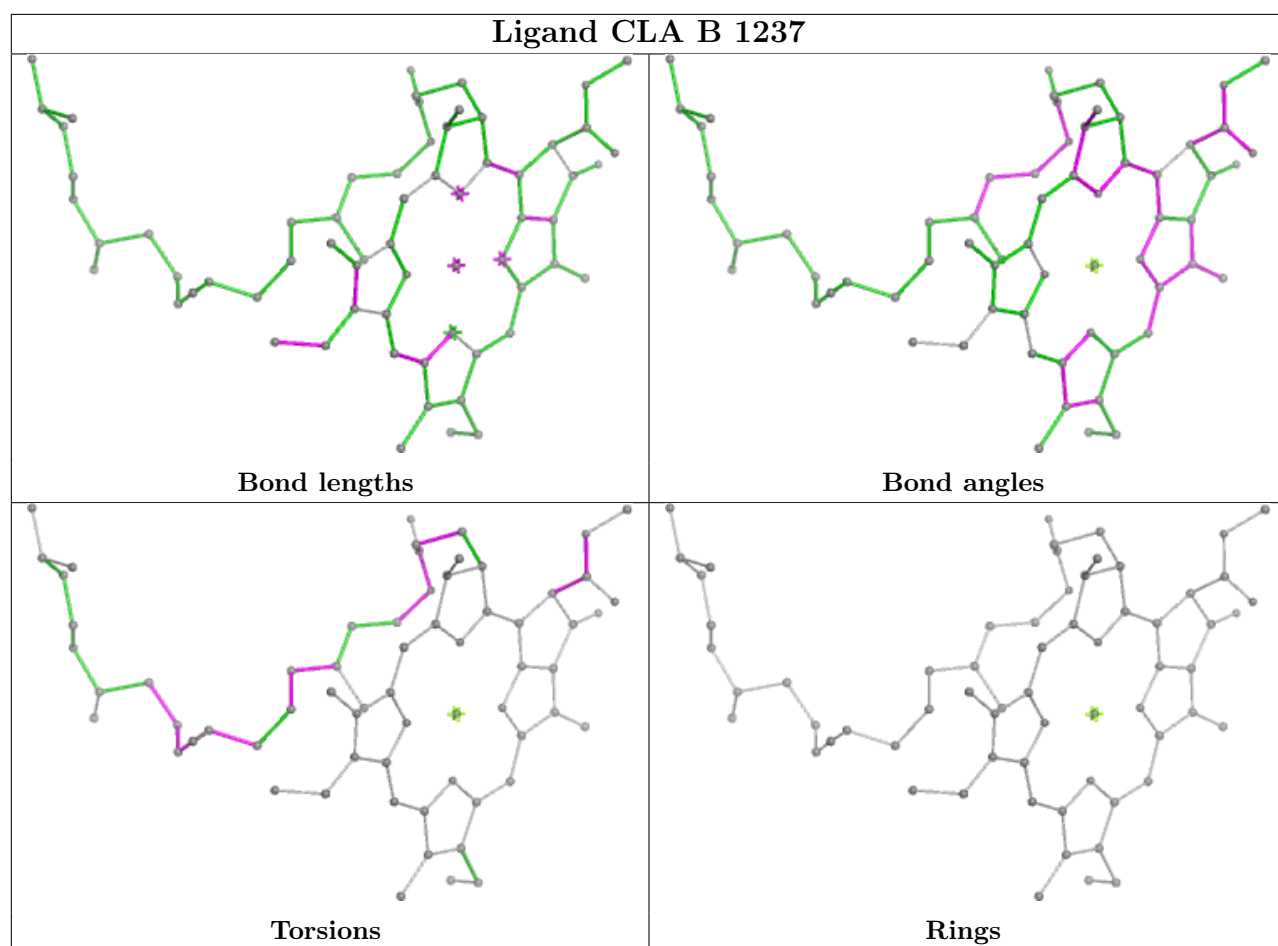
## Ligand CLA Z 605



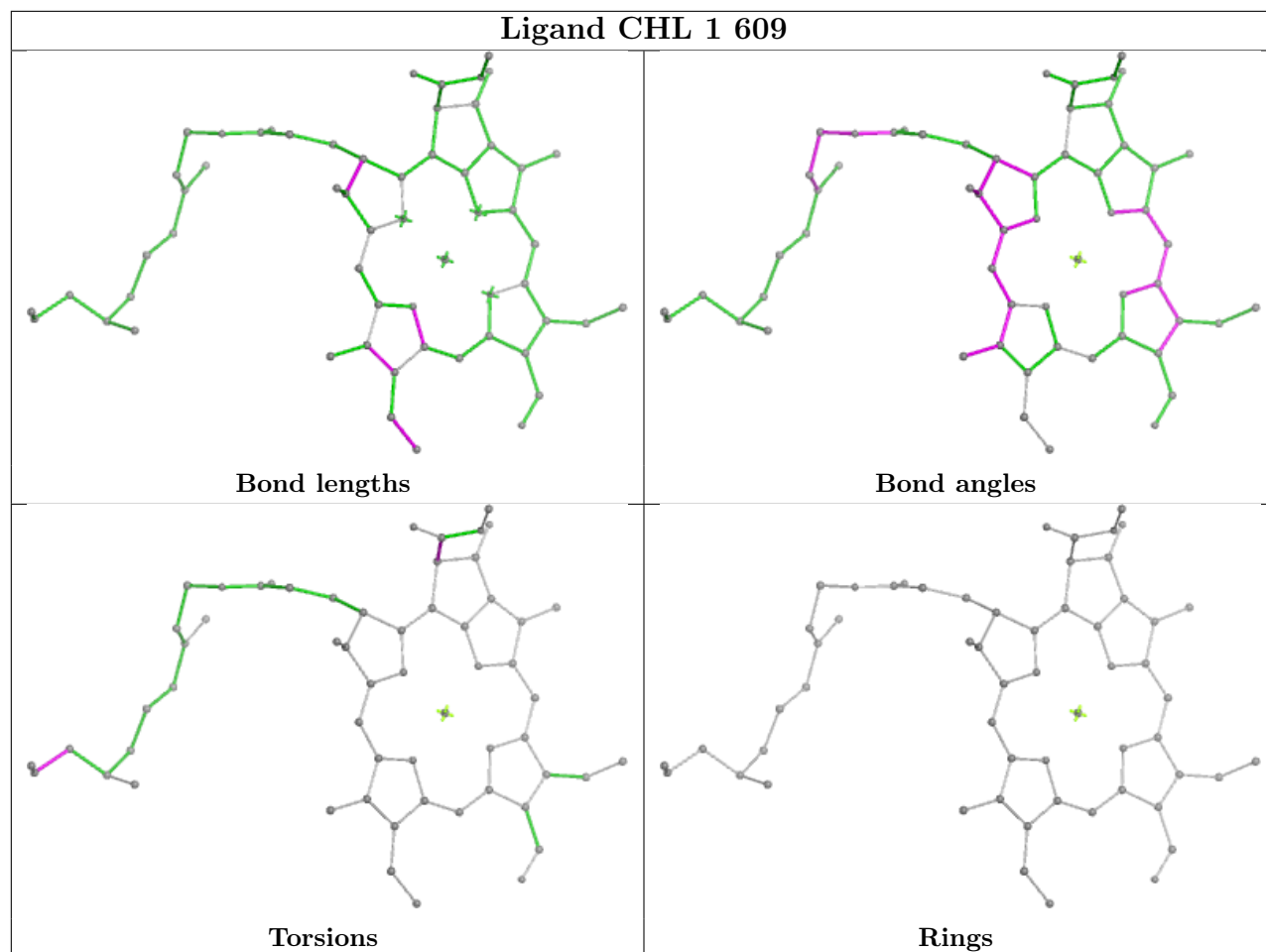
## Ligand SPH 7 804



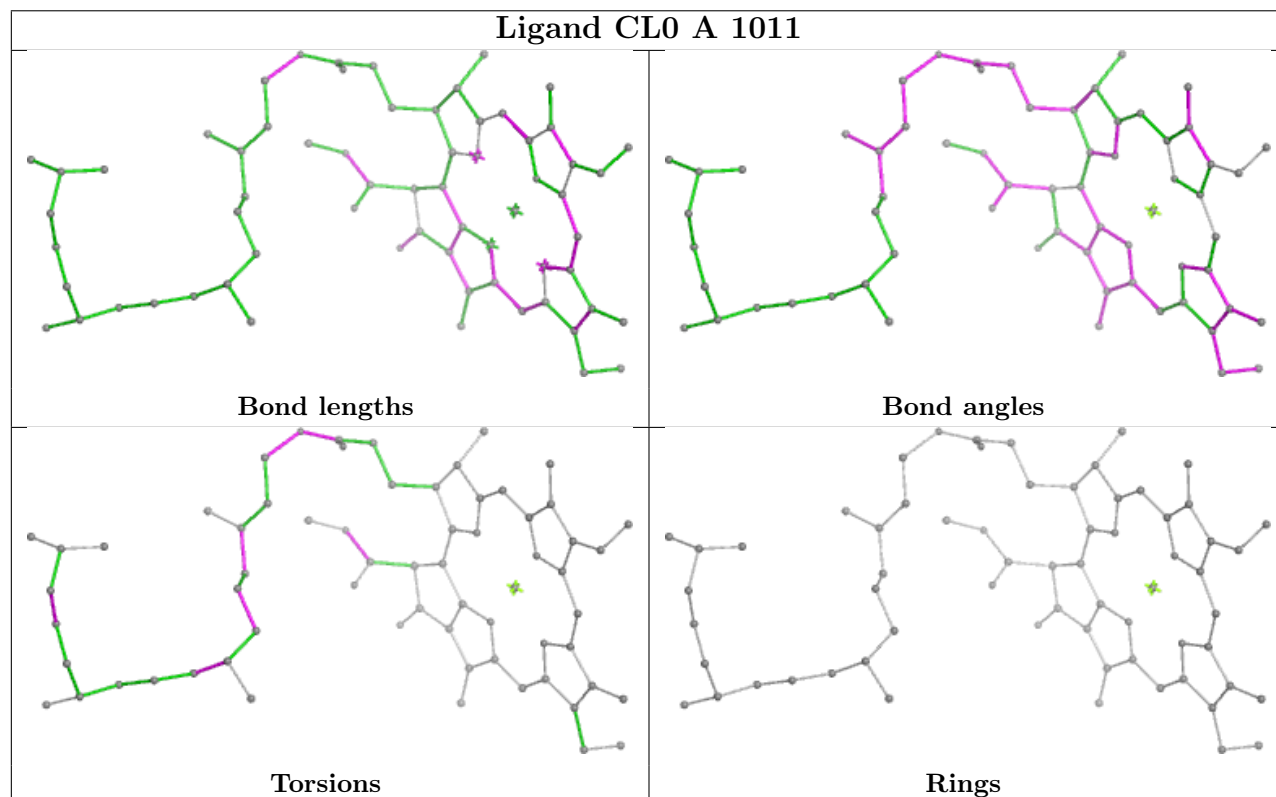


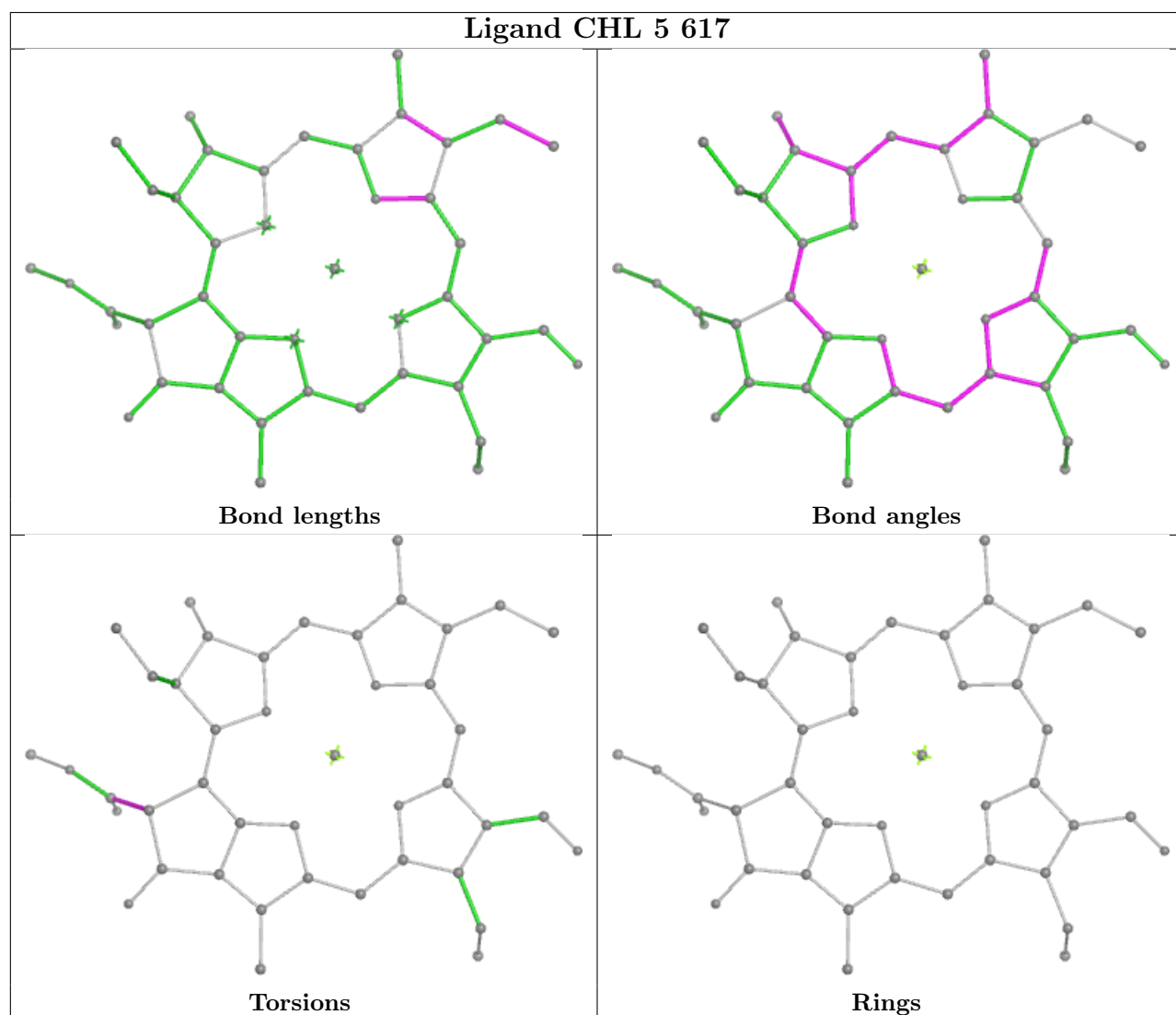
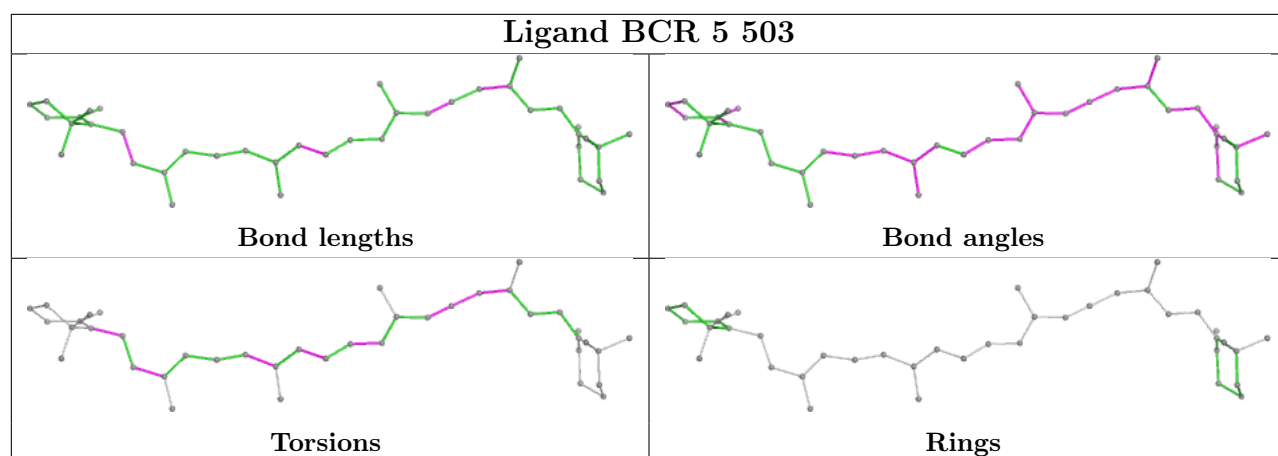


## Ligand CHL 1 609

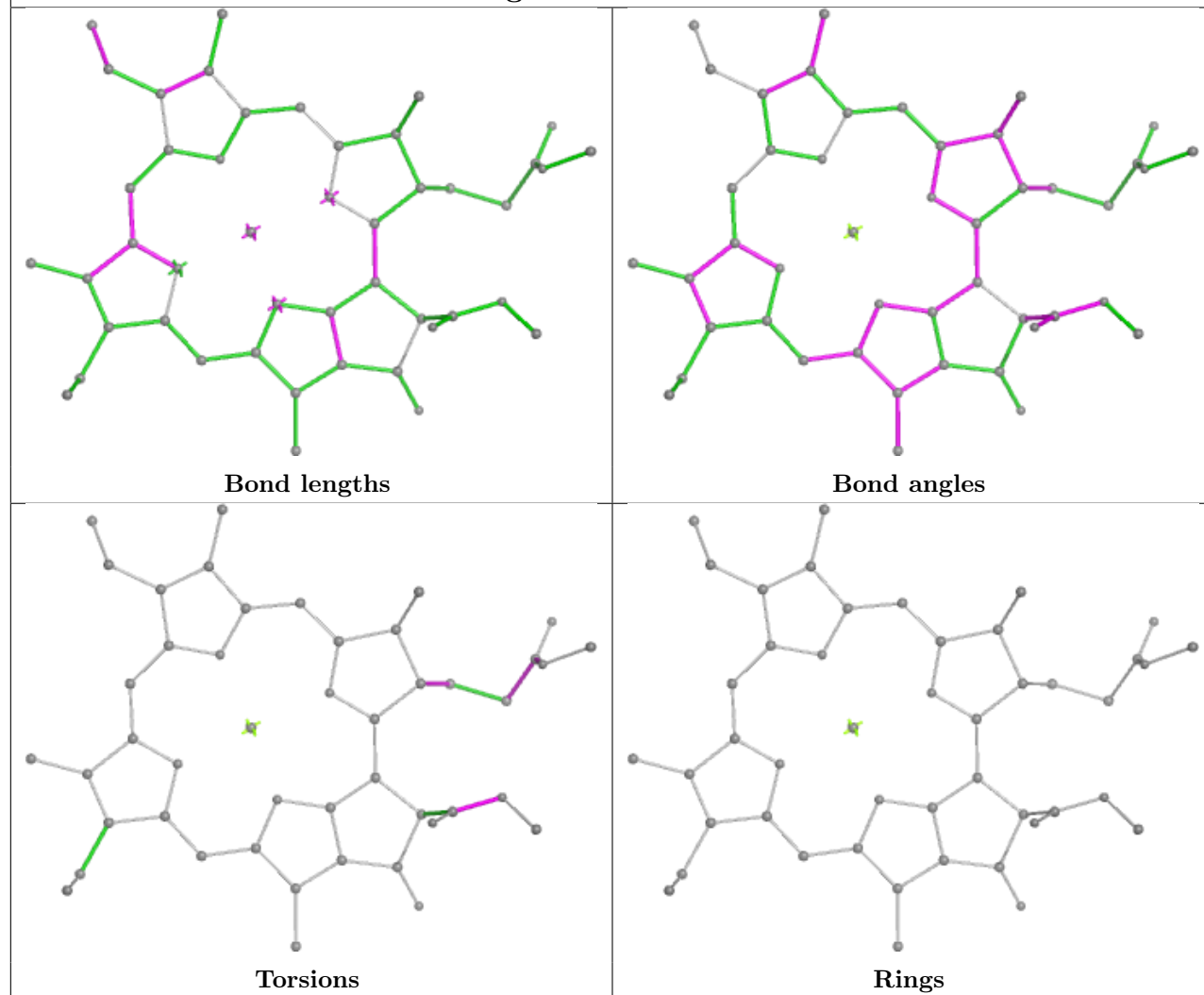


## Ligand CL0 A 1011

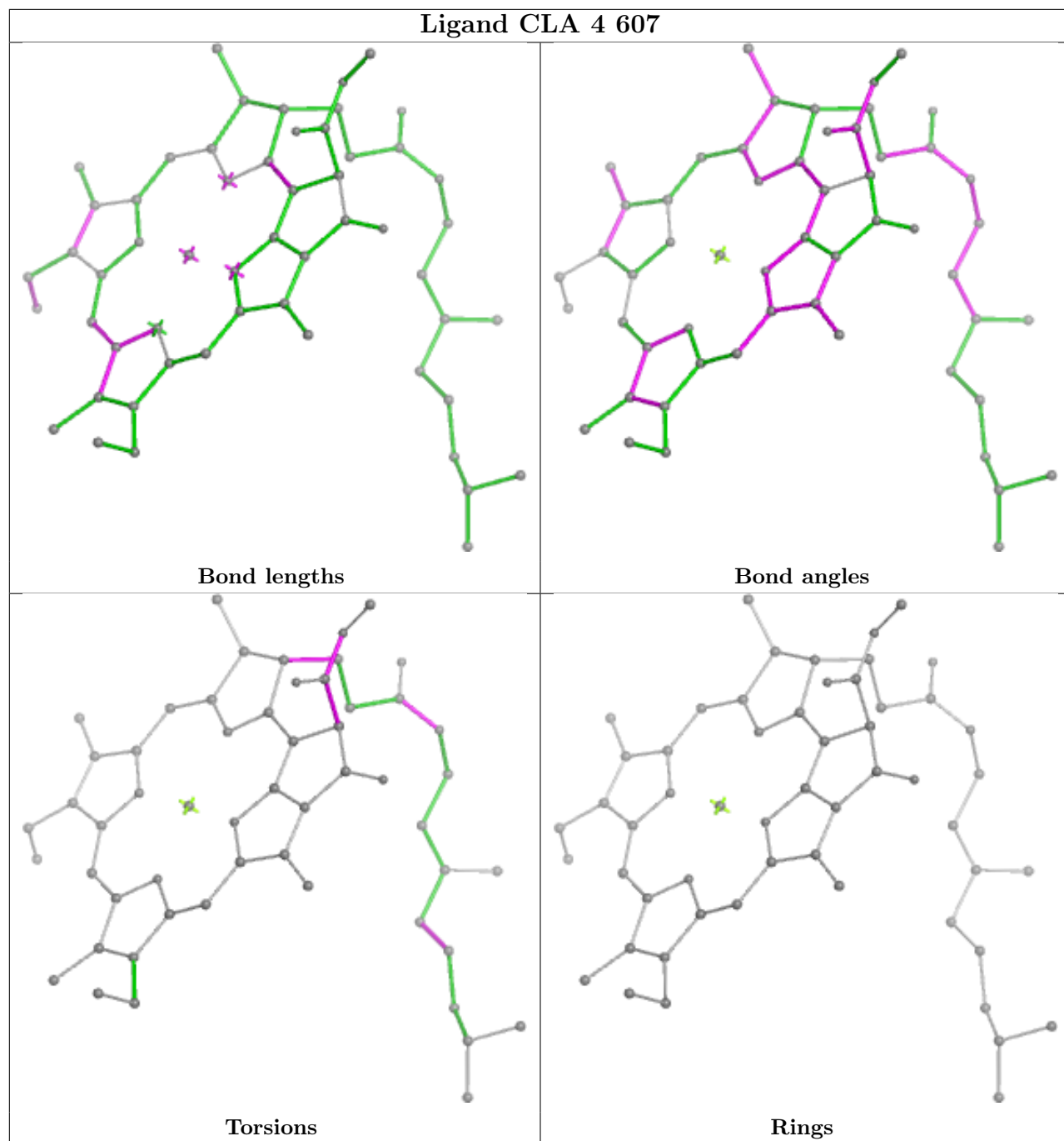


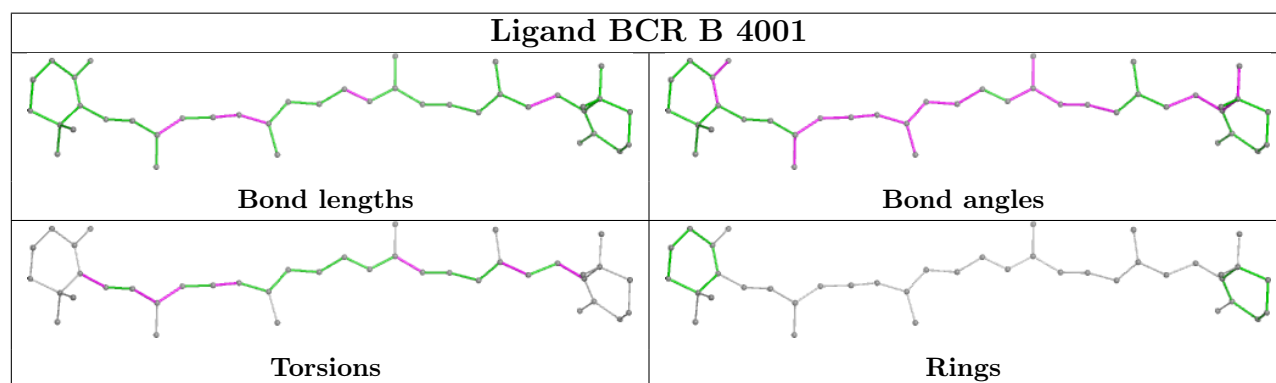
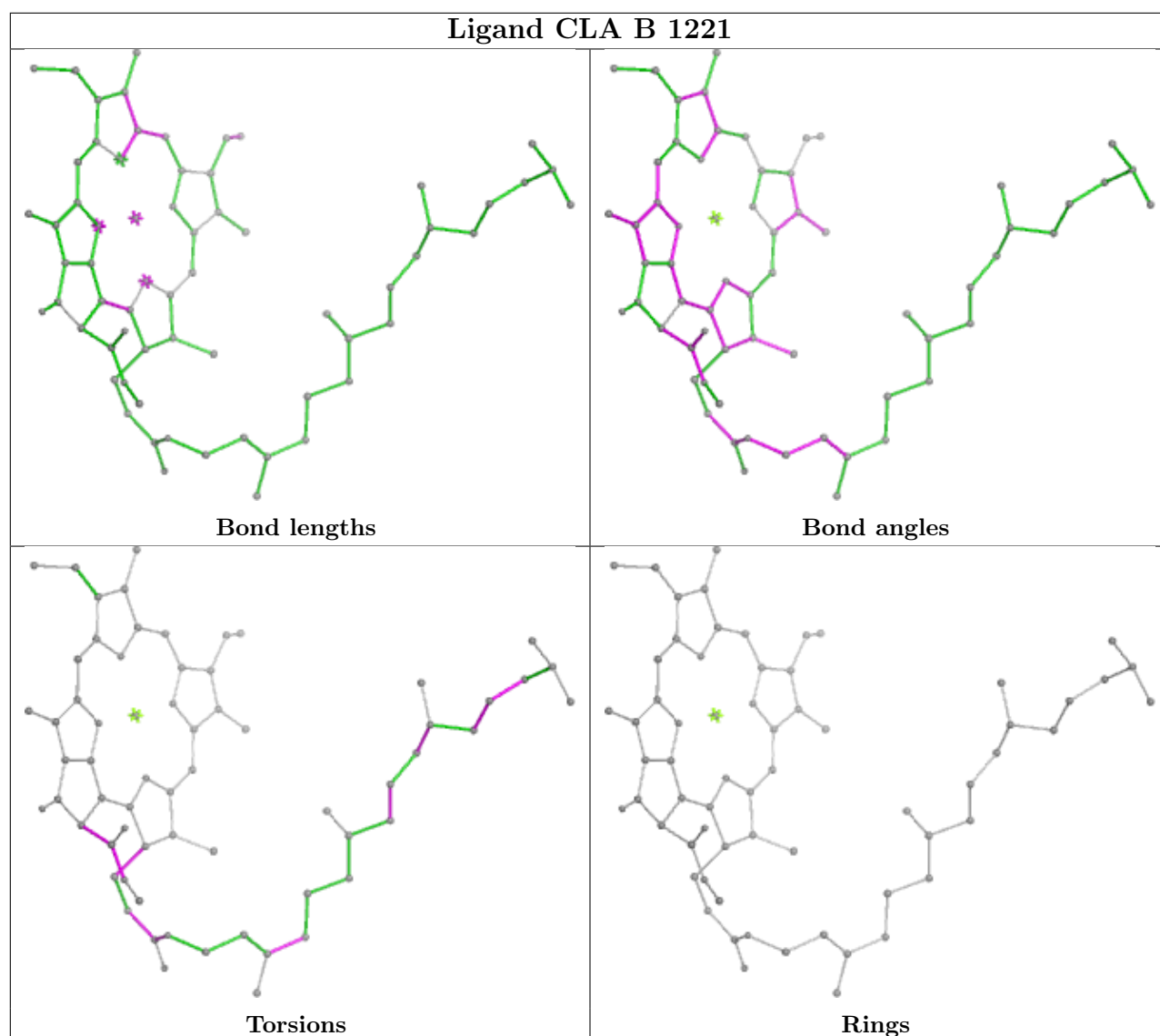


## Ligand CLA 1 613



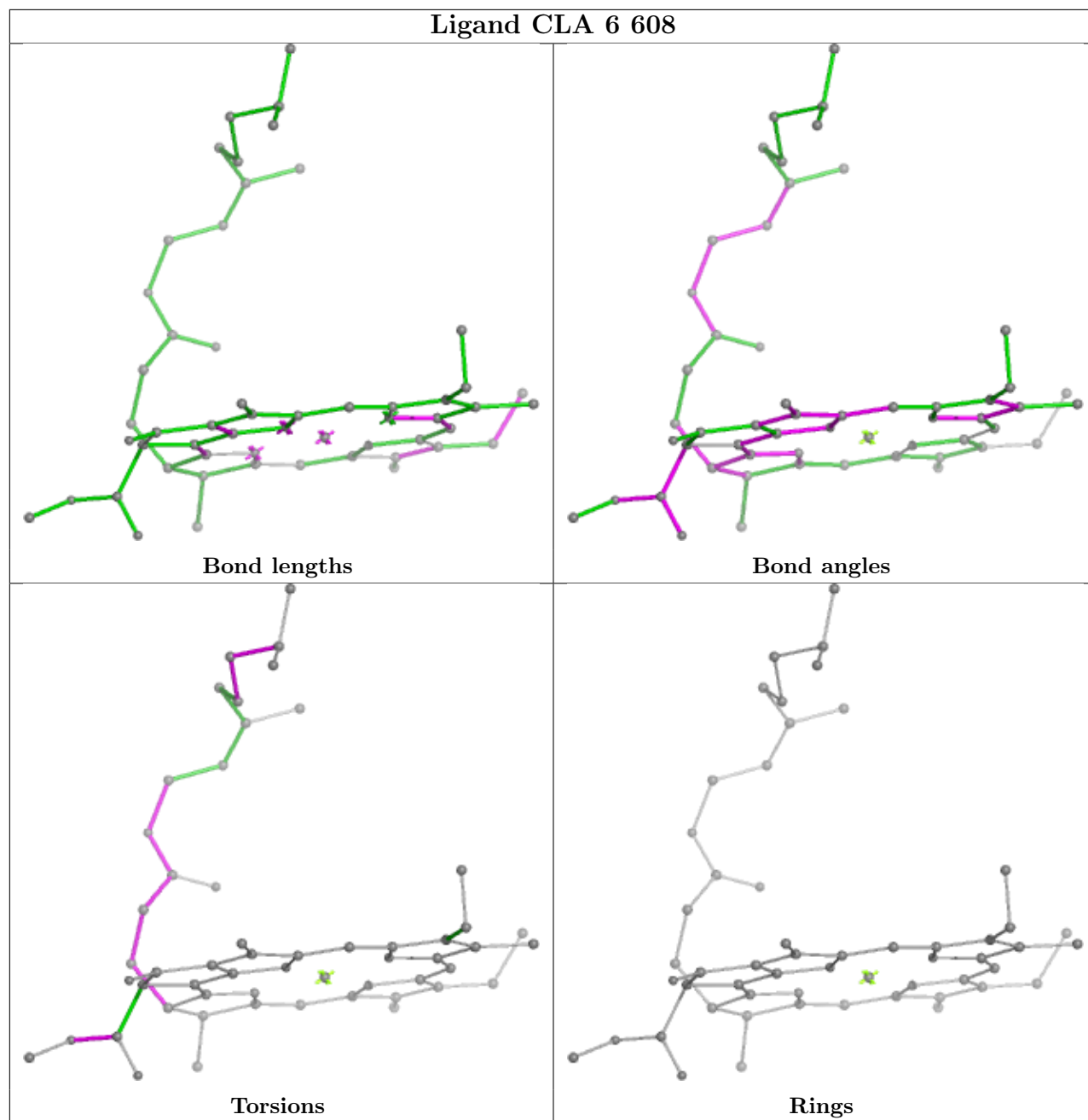
## Ligand CLA 4 607

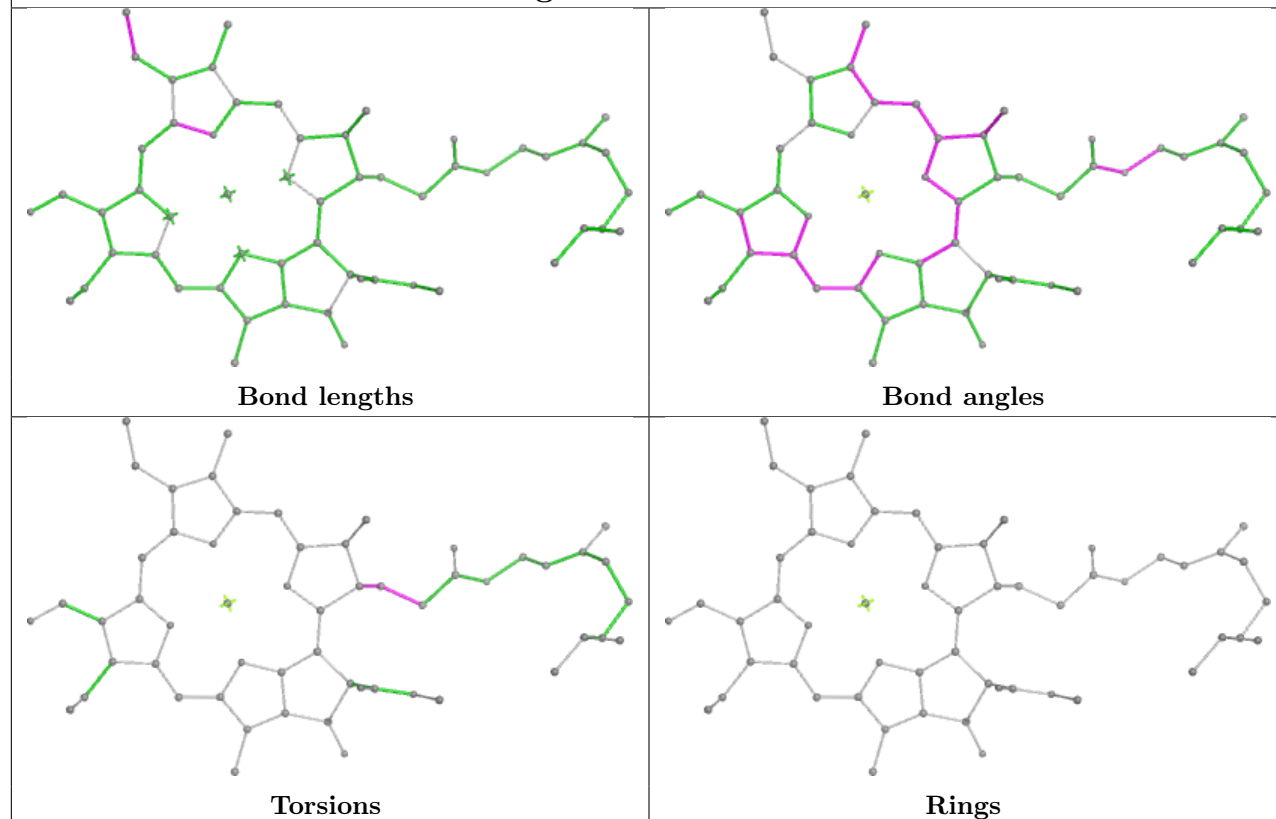
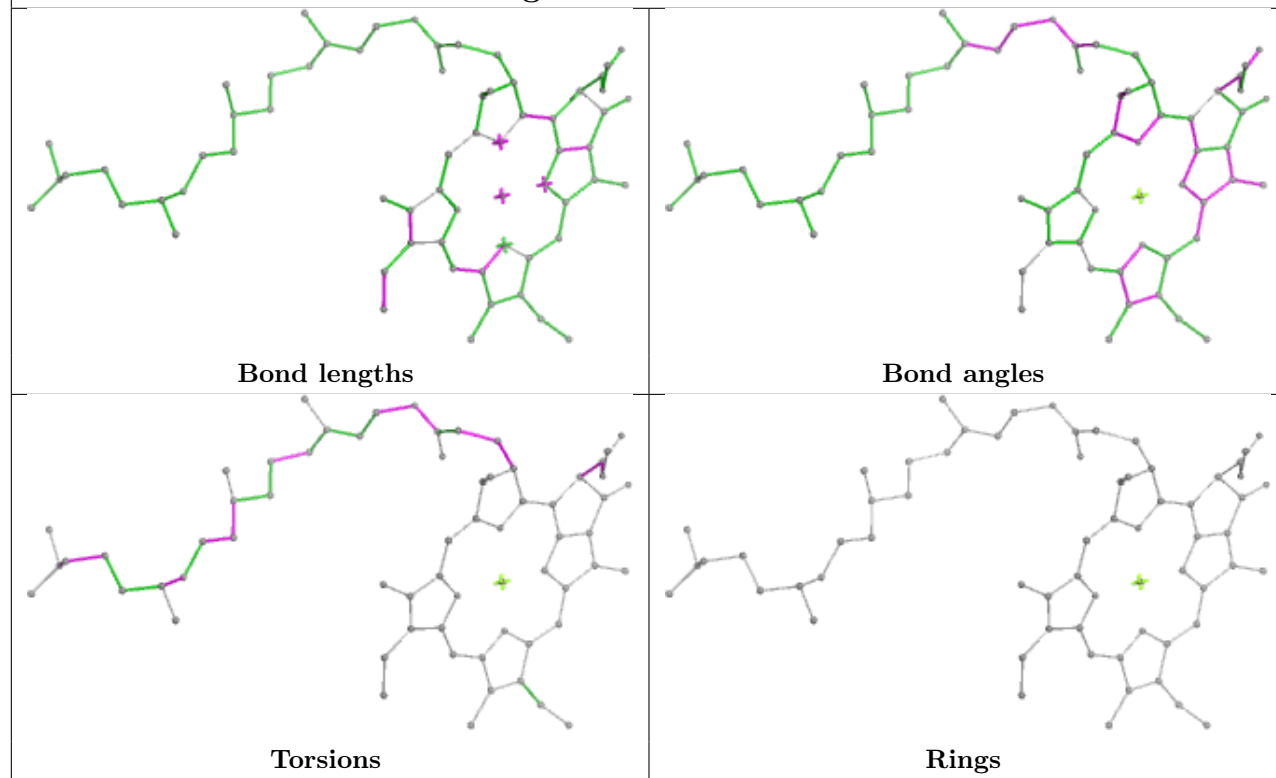


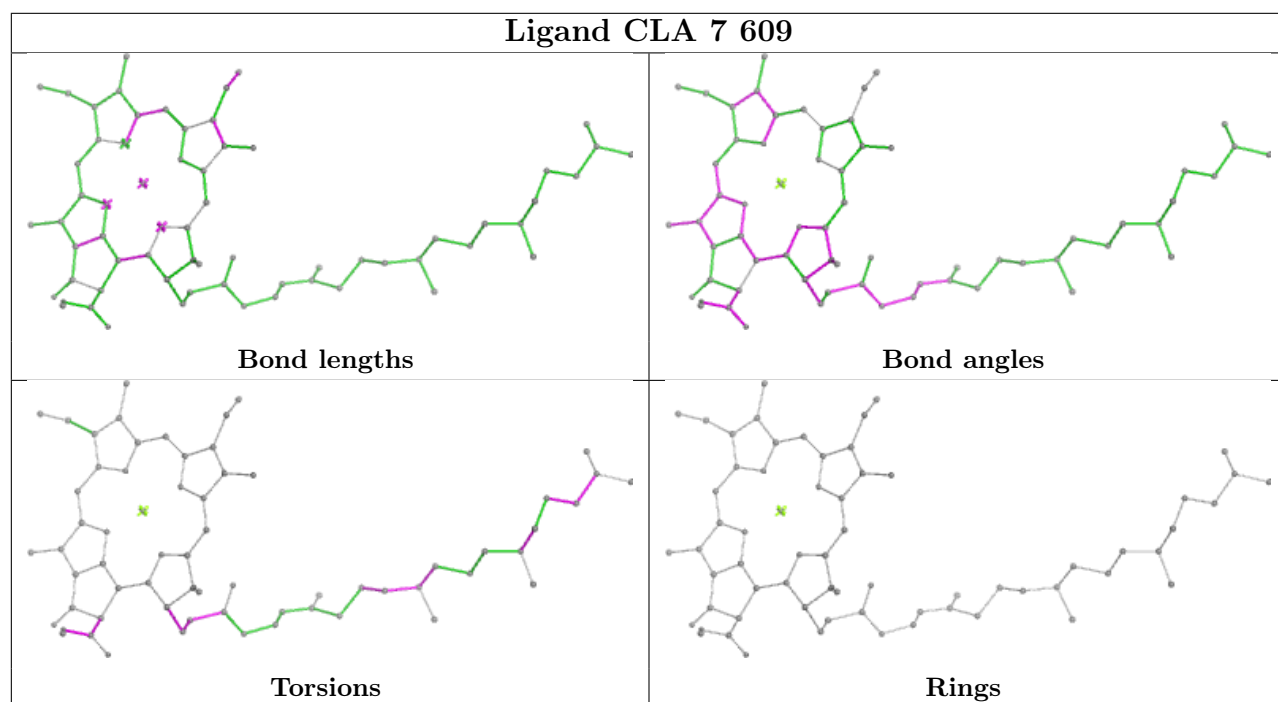
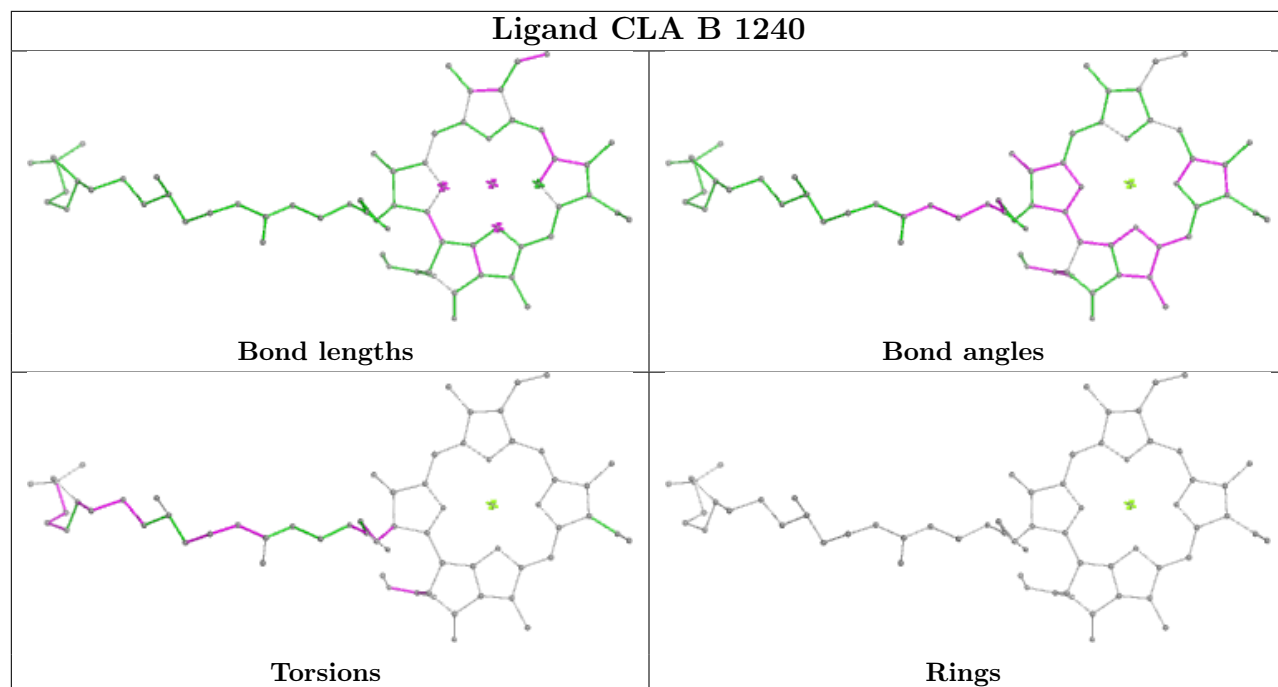


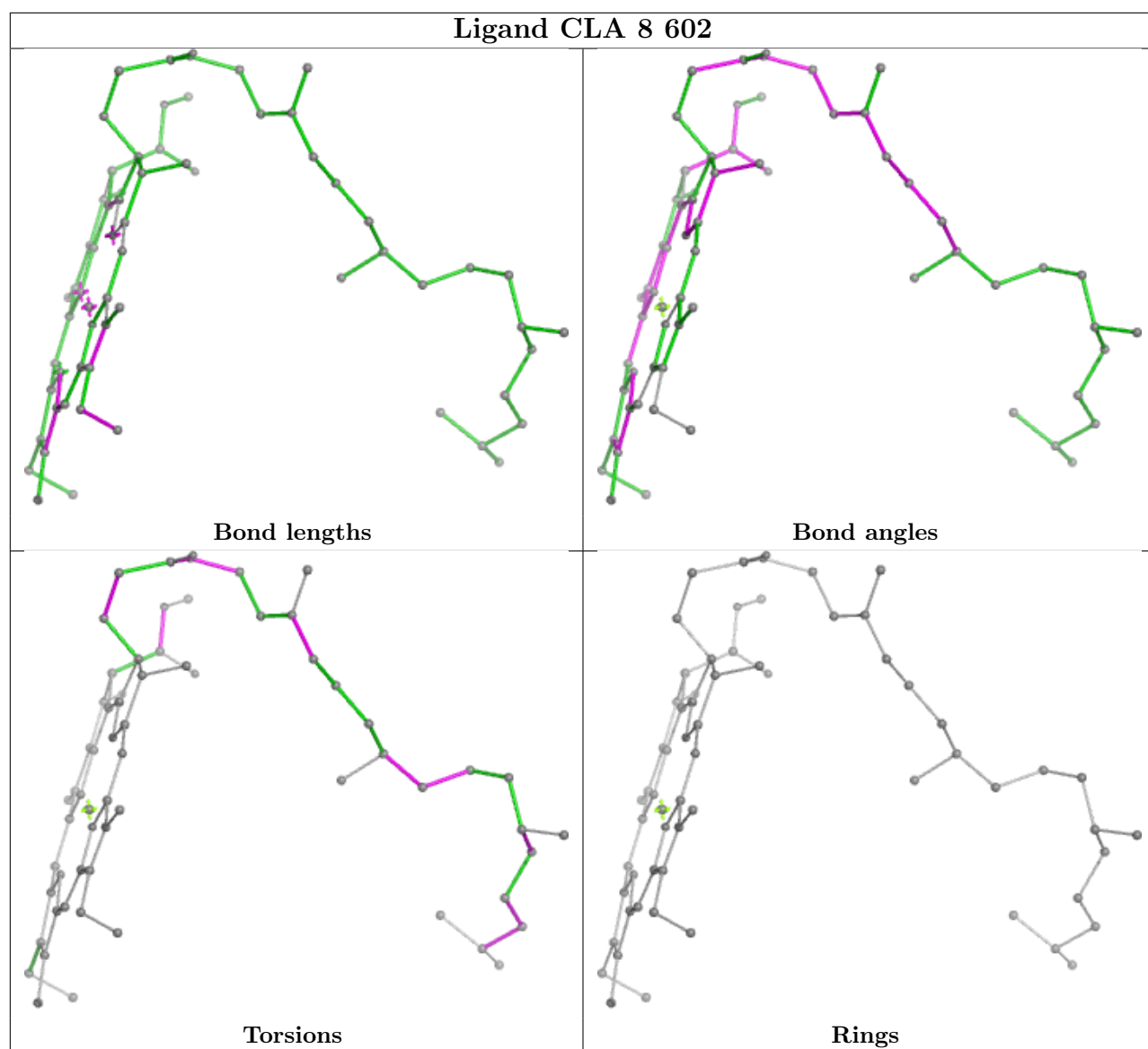


## Ligand CLA 6 608

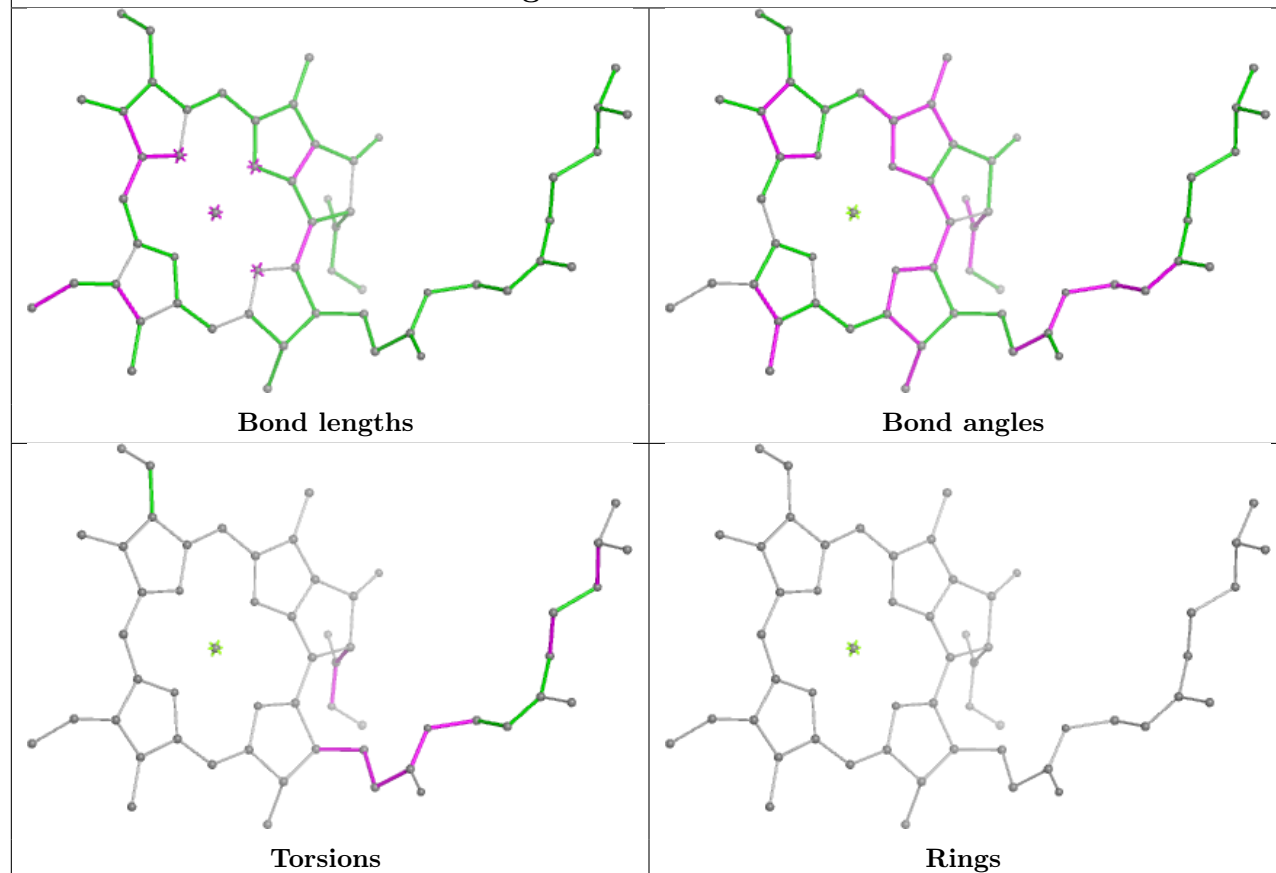


**Ligand CHL 4 613****Ligand CLA A 1106**

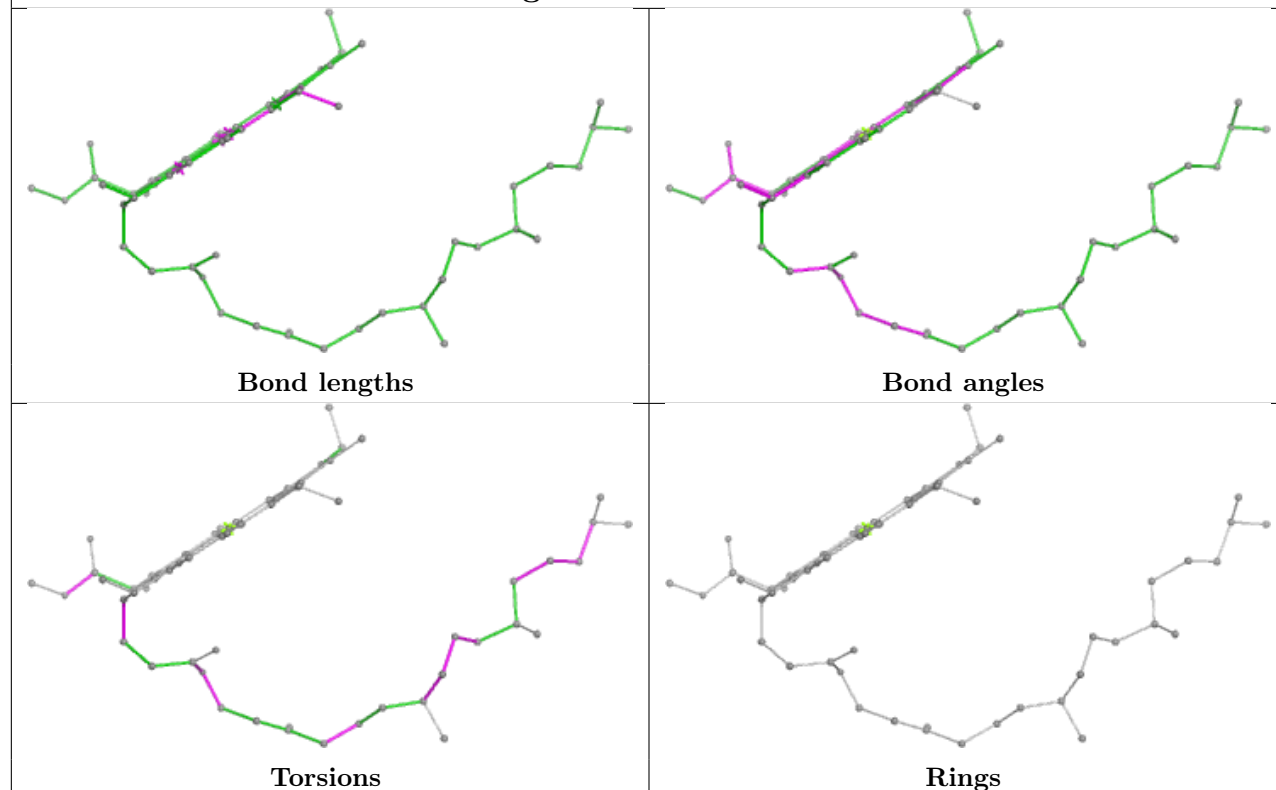




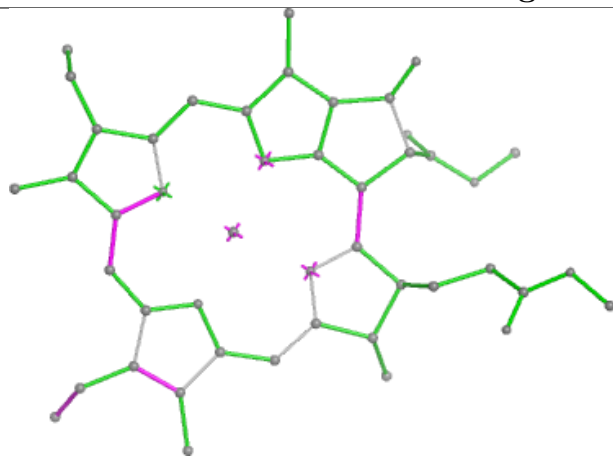
## Ligand CLA K 1402



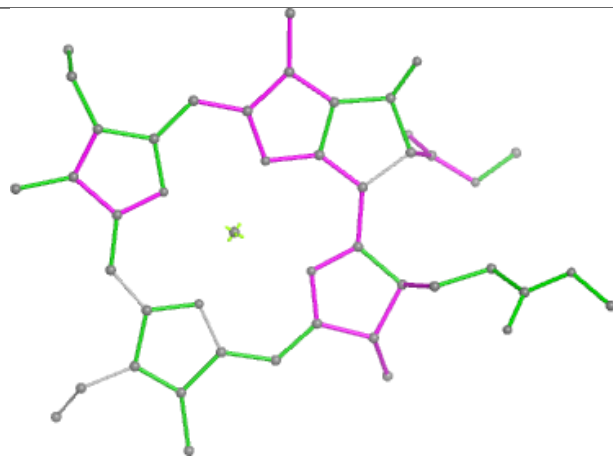
## Ligand CLA A 1130



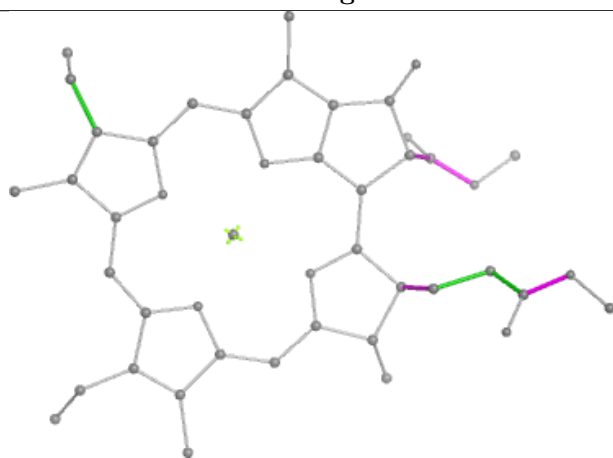
## Ligand CLA 6 618



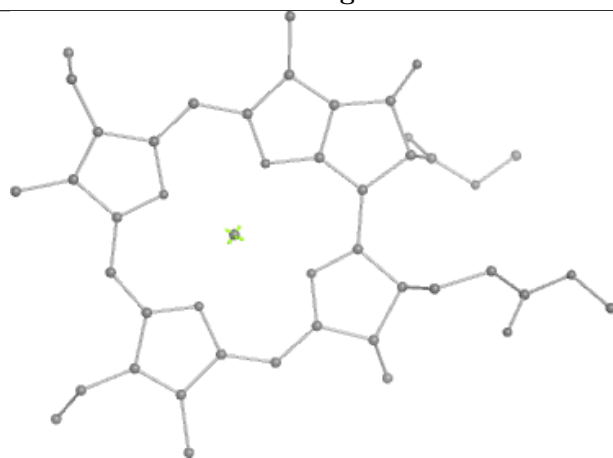
Bond lengths



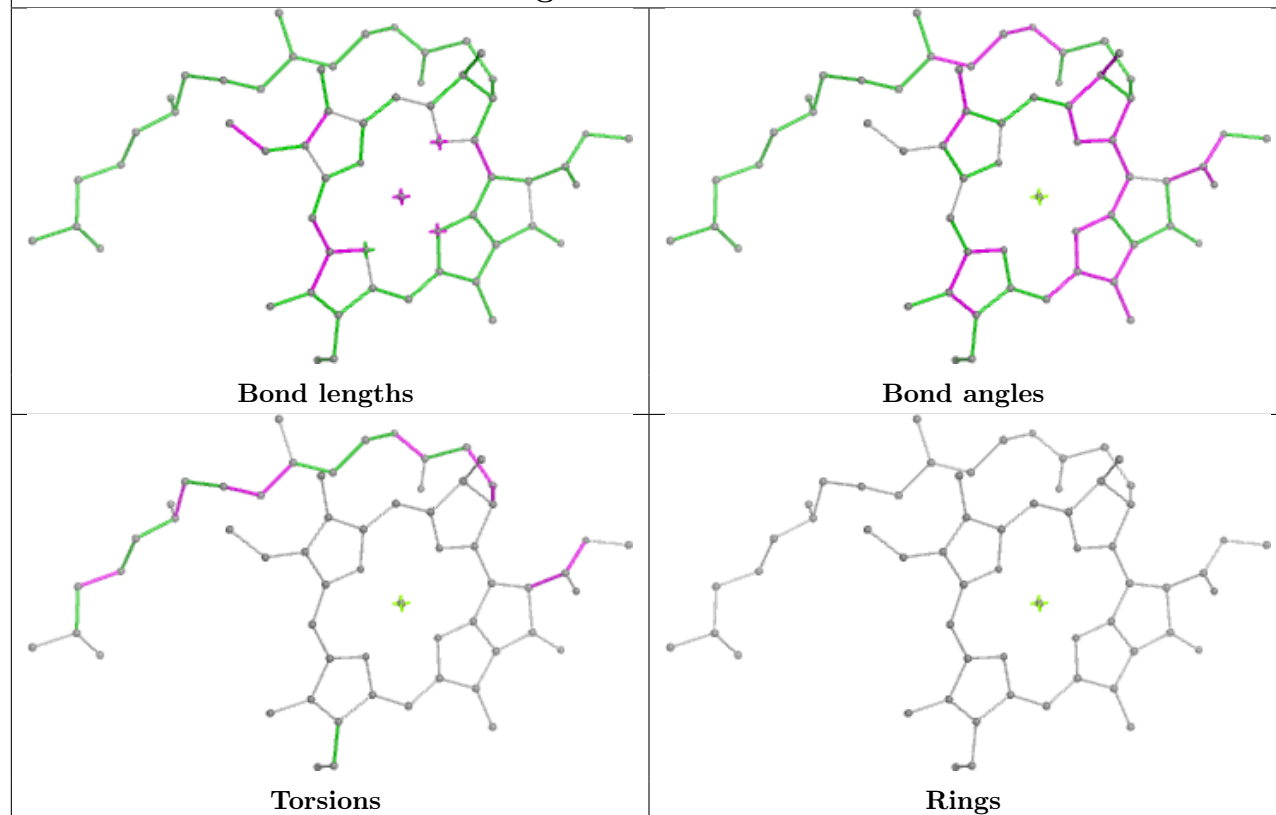
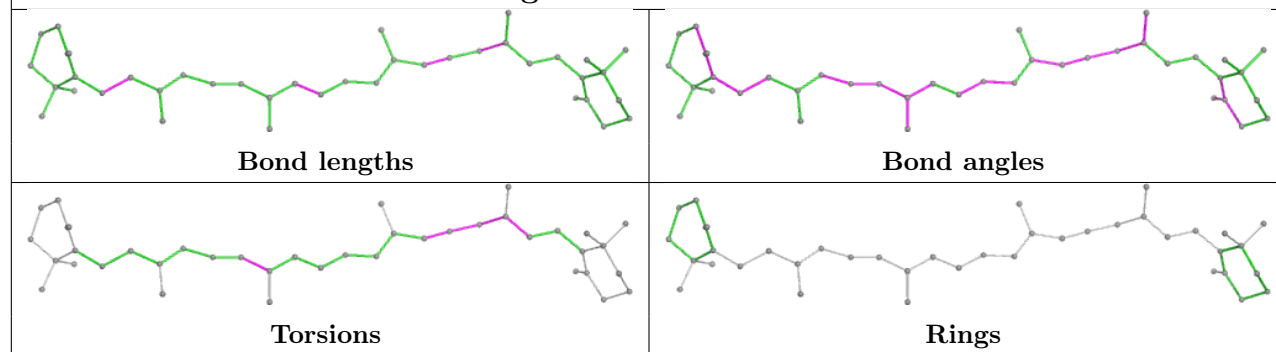
Bond angles

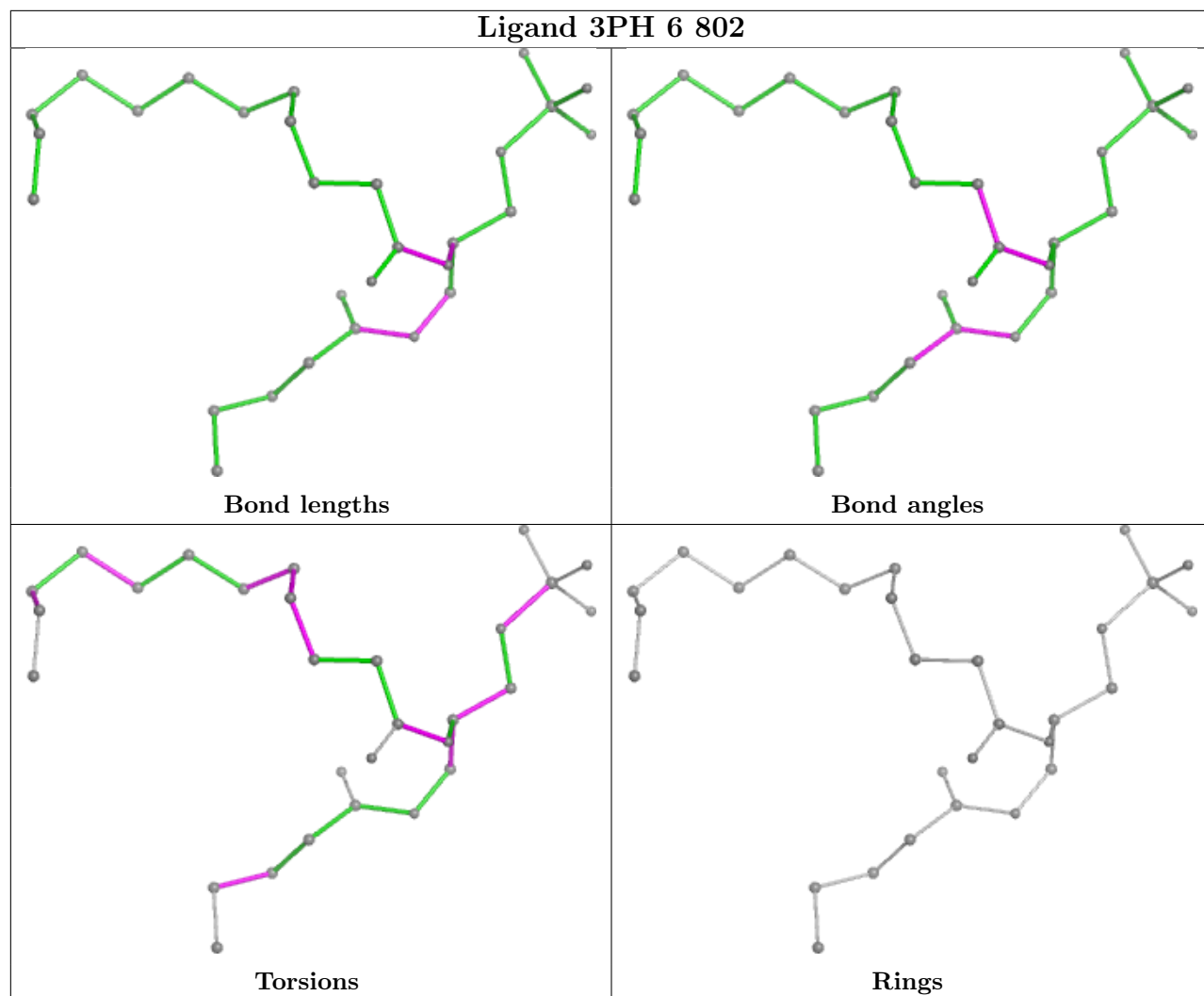


Torsions

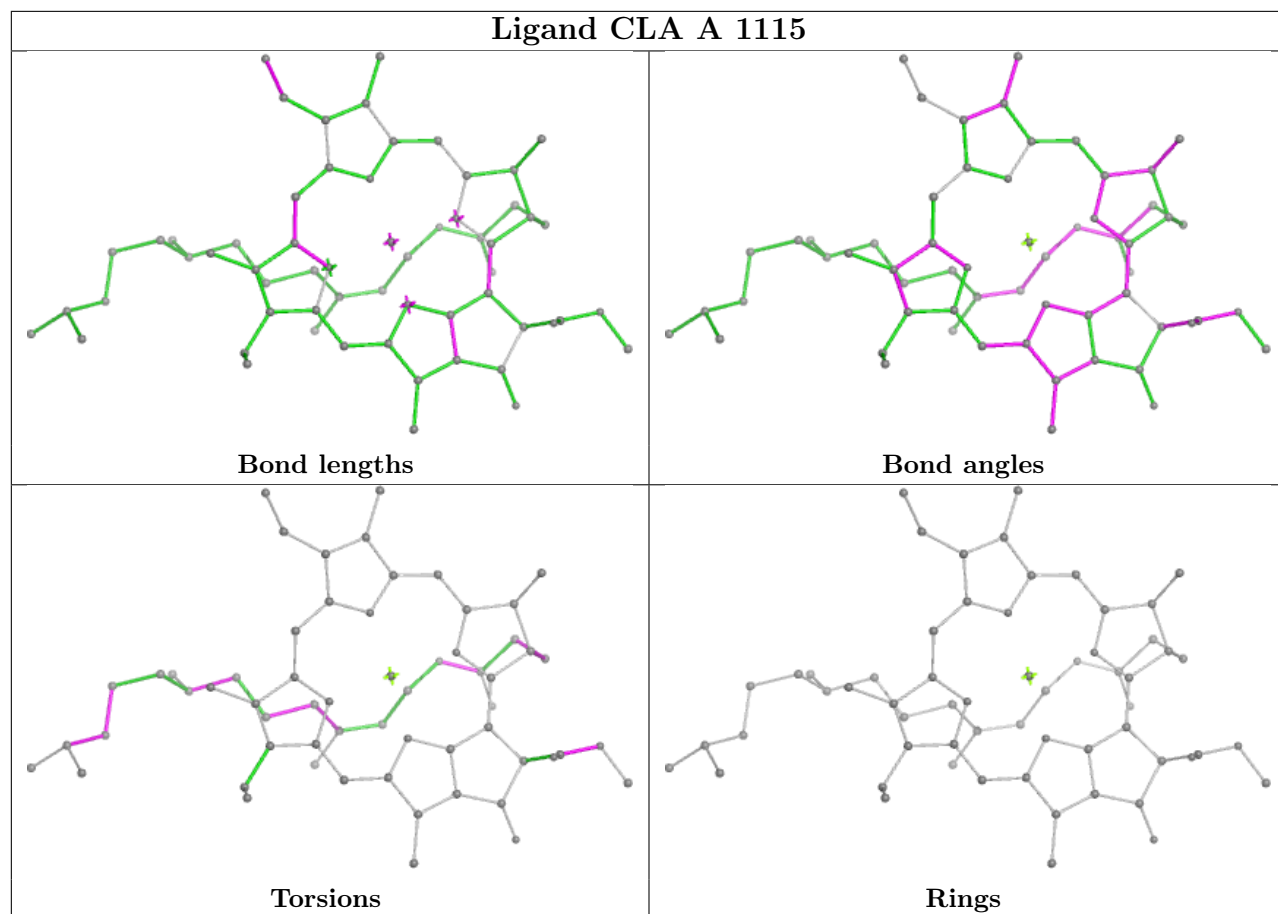


Rings

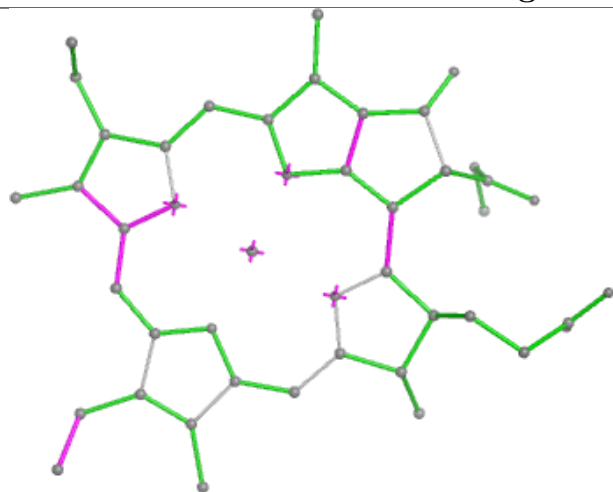
**Ligand CLA 5 601****Ligand BCR A 4002**



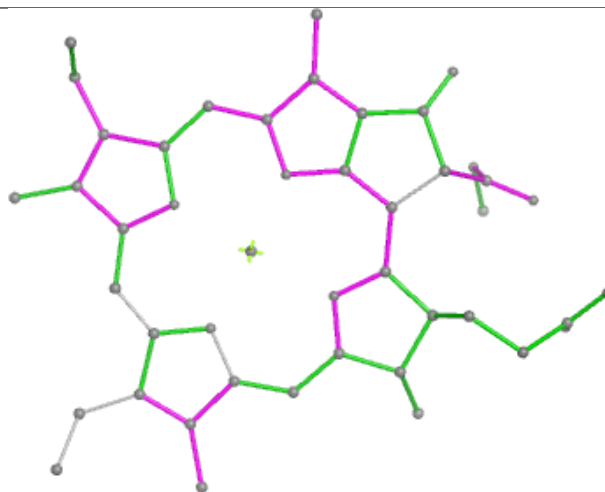




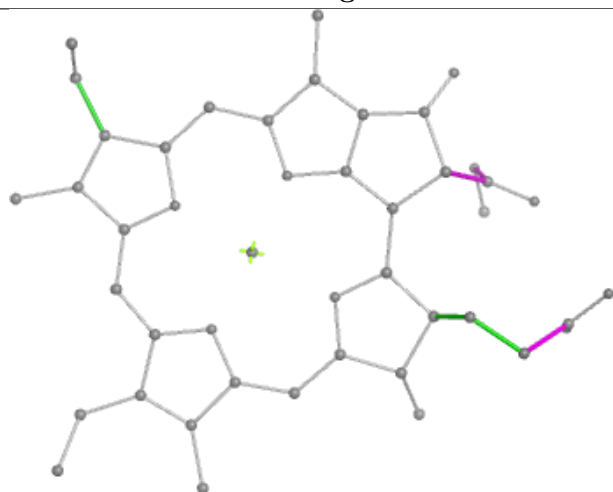
## Ligand CLA 1 602



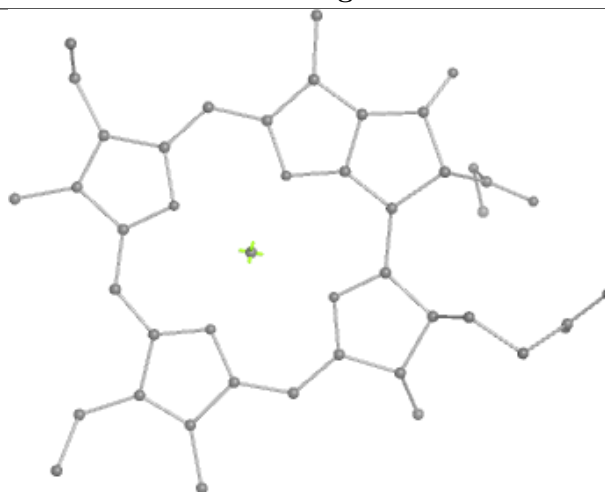
Bond lengths



Bond angles

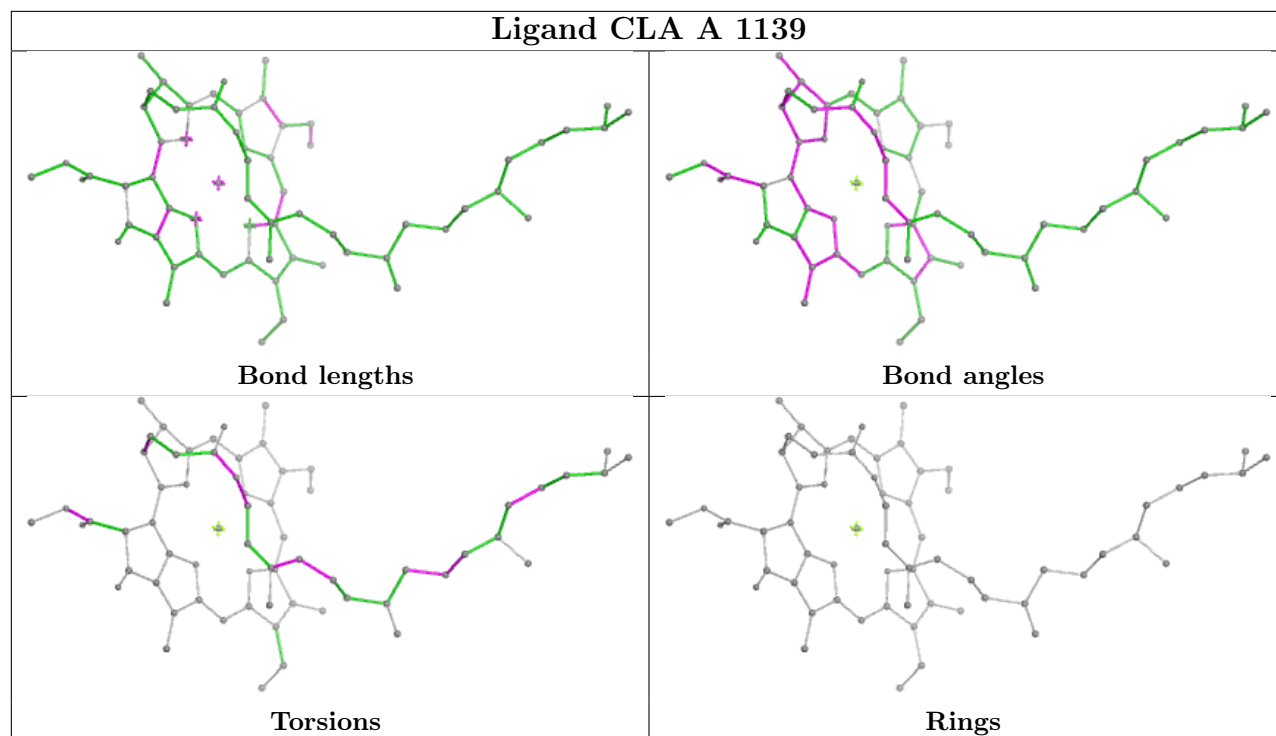


Torsions

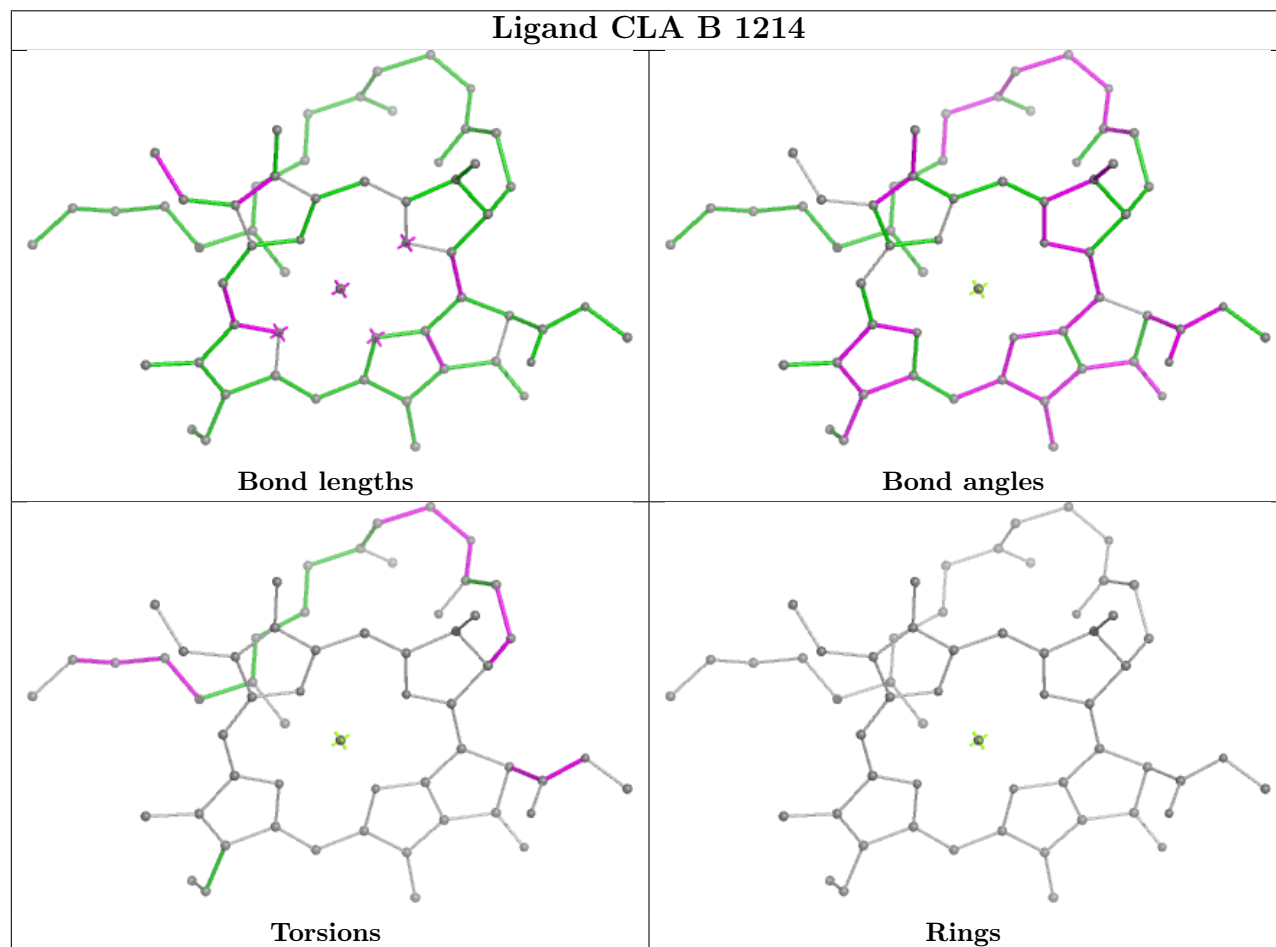


Rings

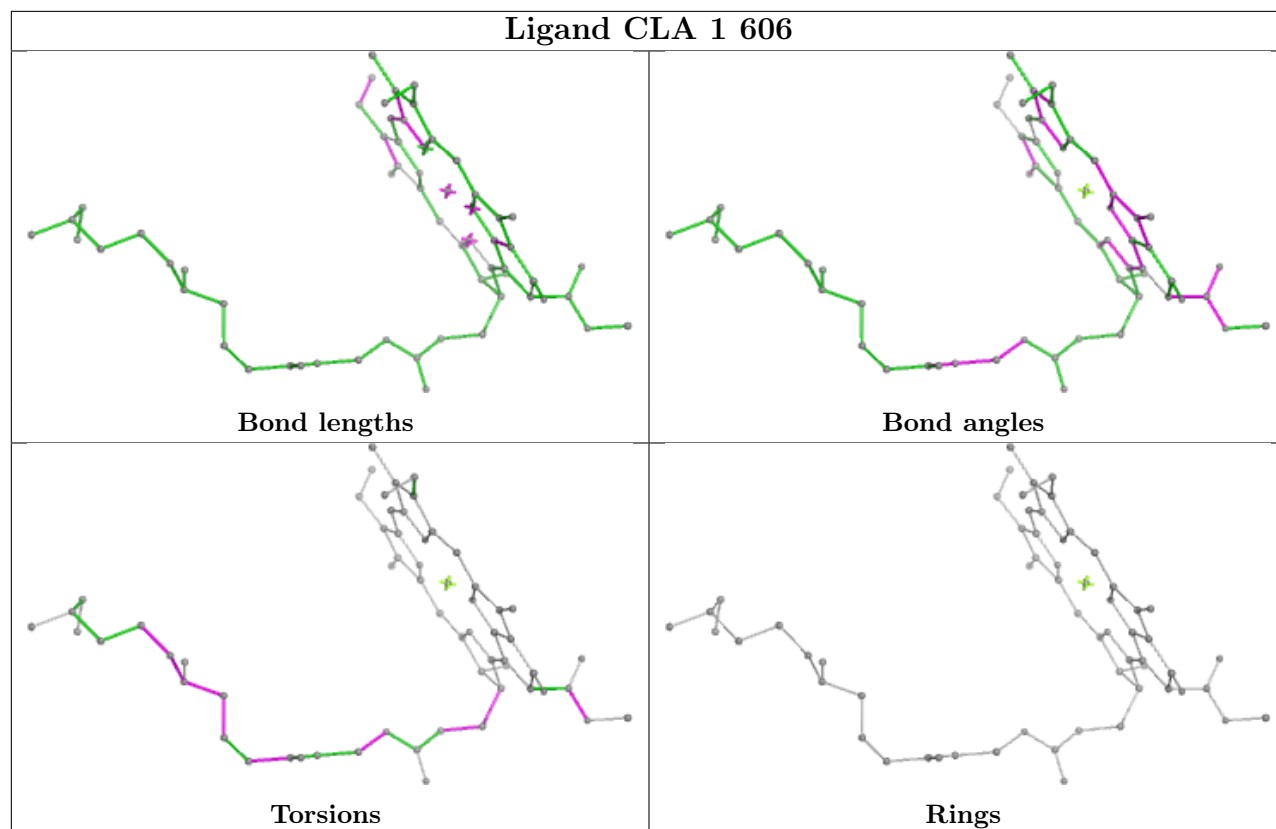
## Ligand CLA A 1139



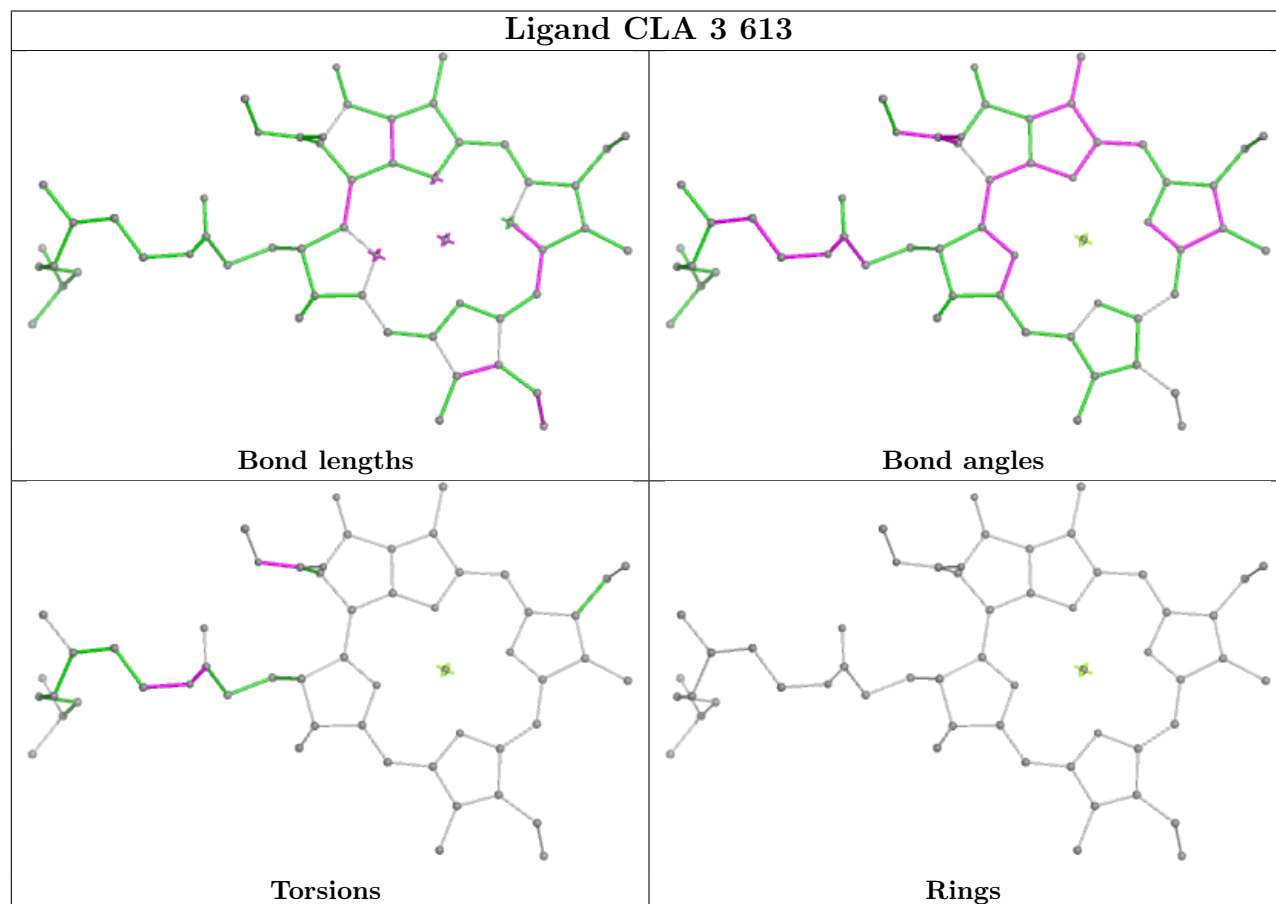
## Ligand CLA B 1214

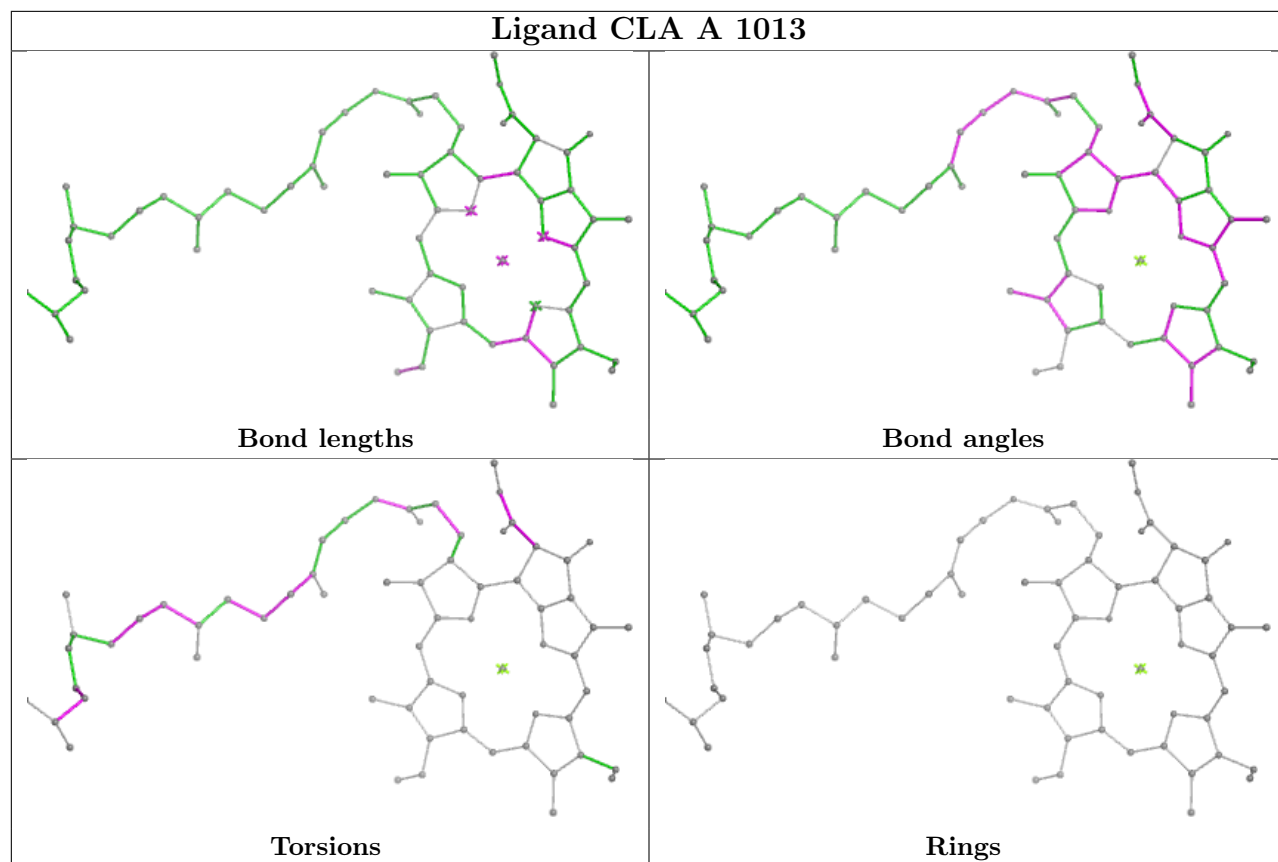


## Ligand CLA 1 606

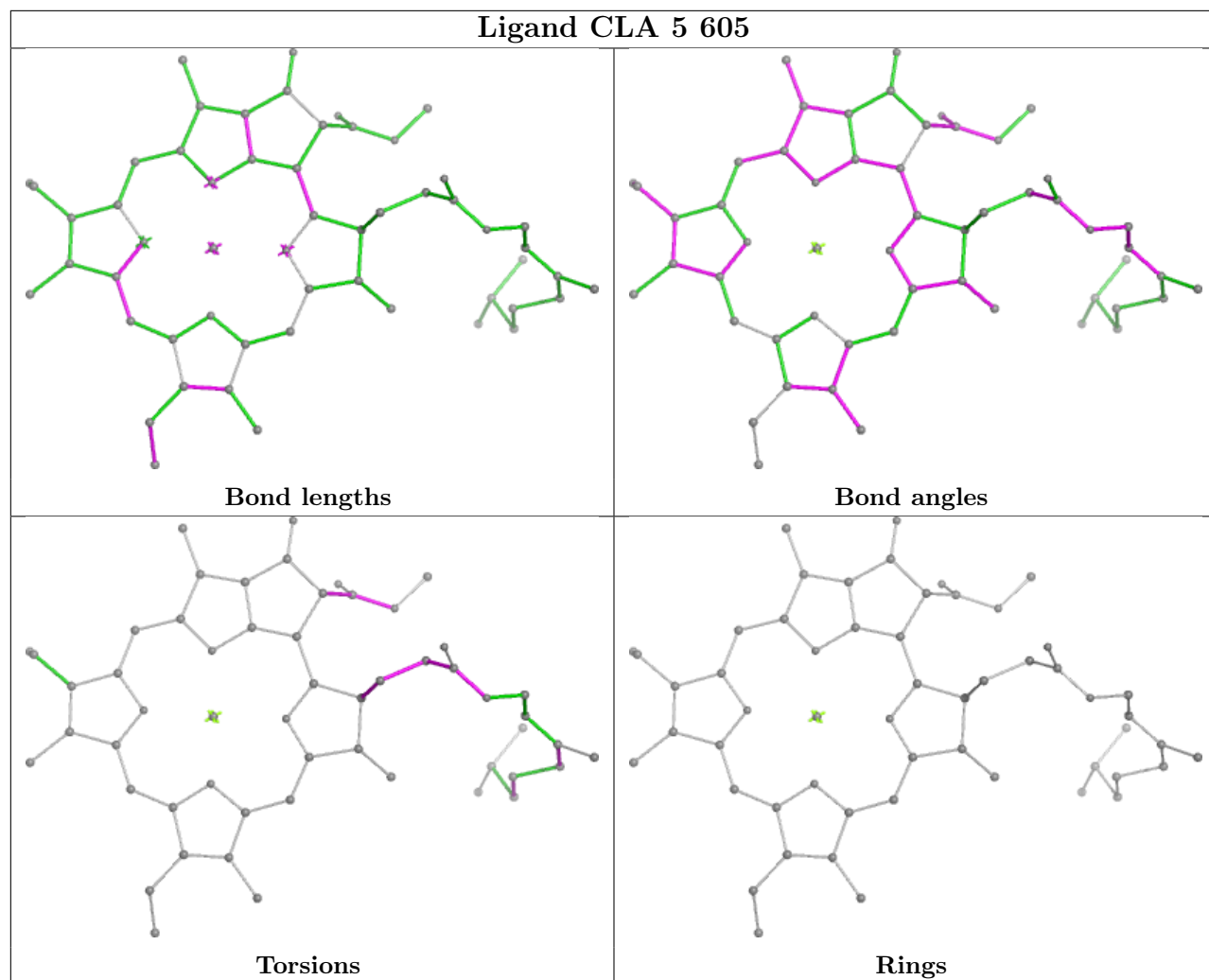


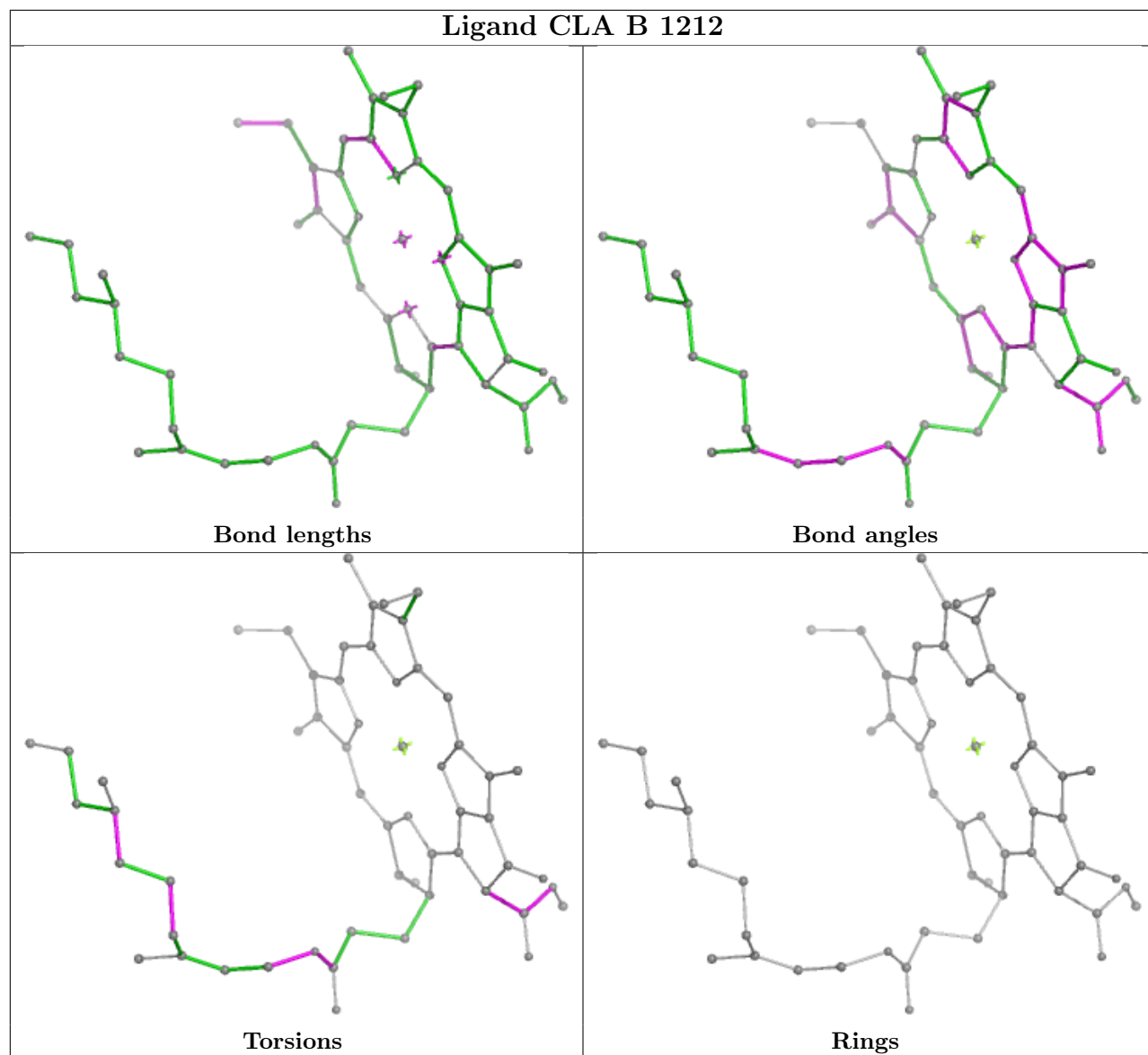
## Ligand CLA 3 613



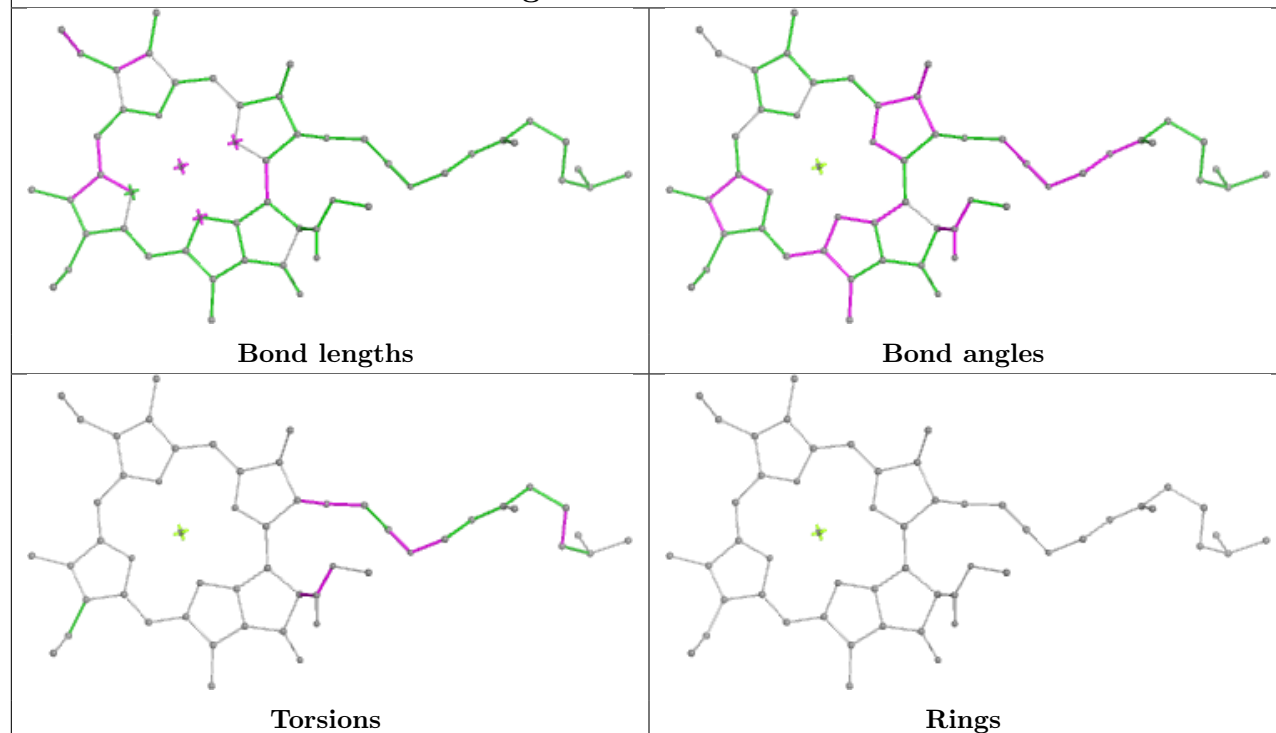


## Ligand CLA 5 605

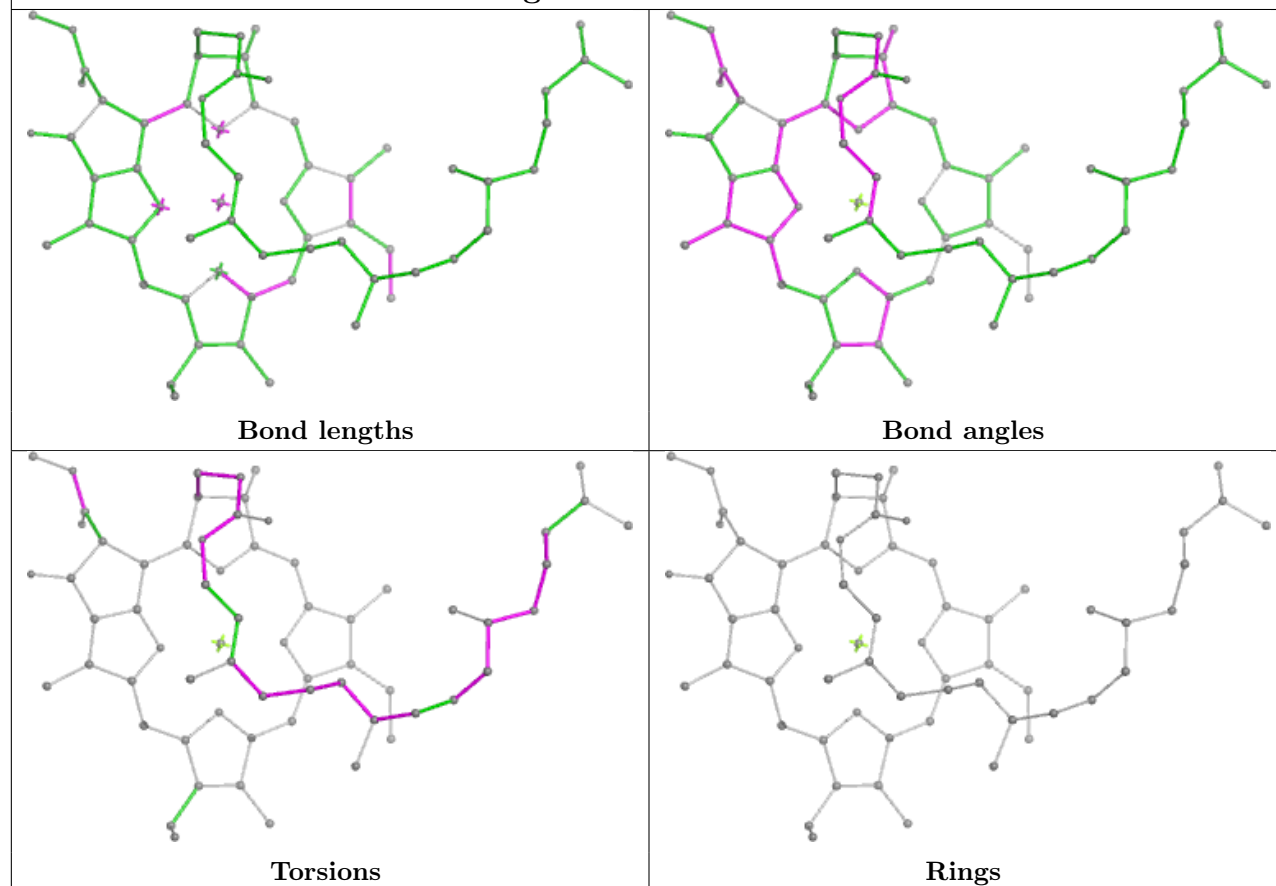




## Ligand CLA K 1404

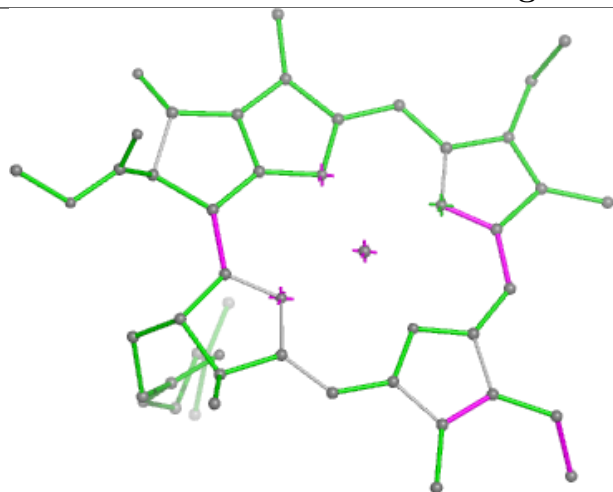


## Ligand CLA B 1209

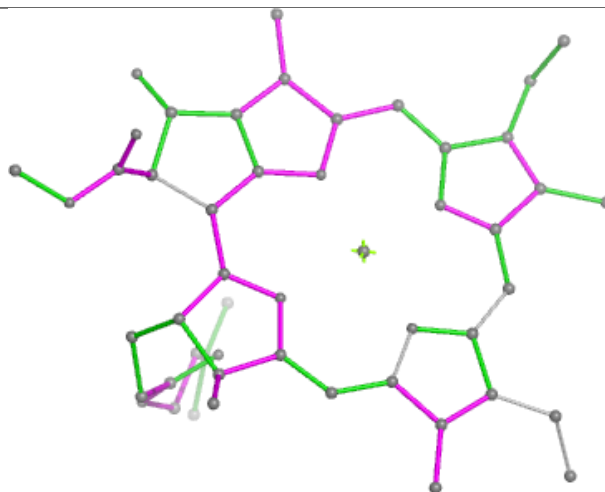




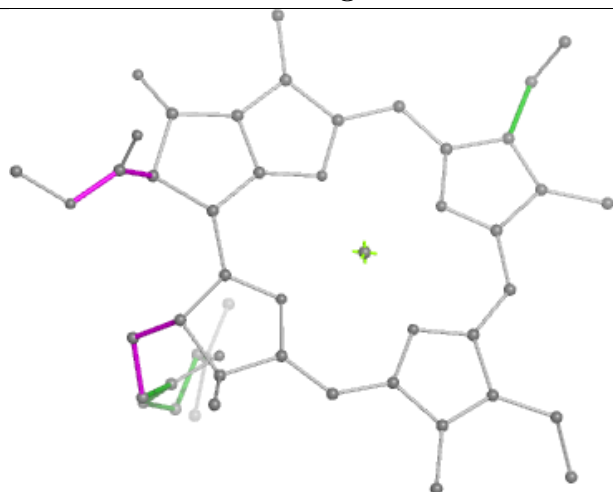
## Ligand CLA 4 612



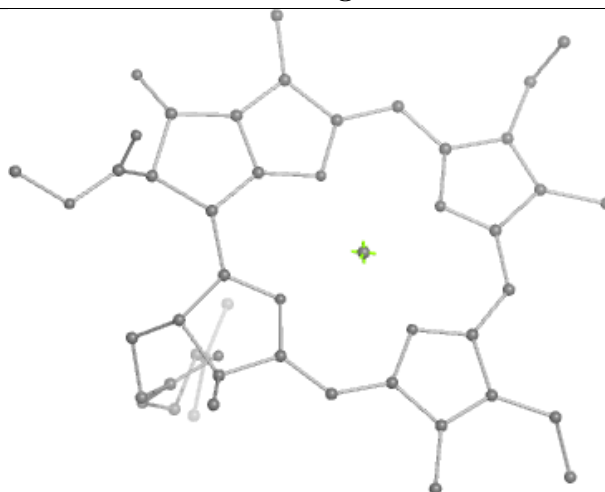
Bond lengths



Bond angles

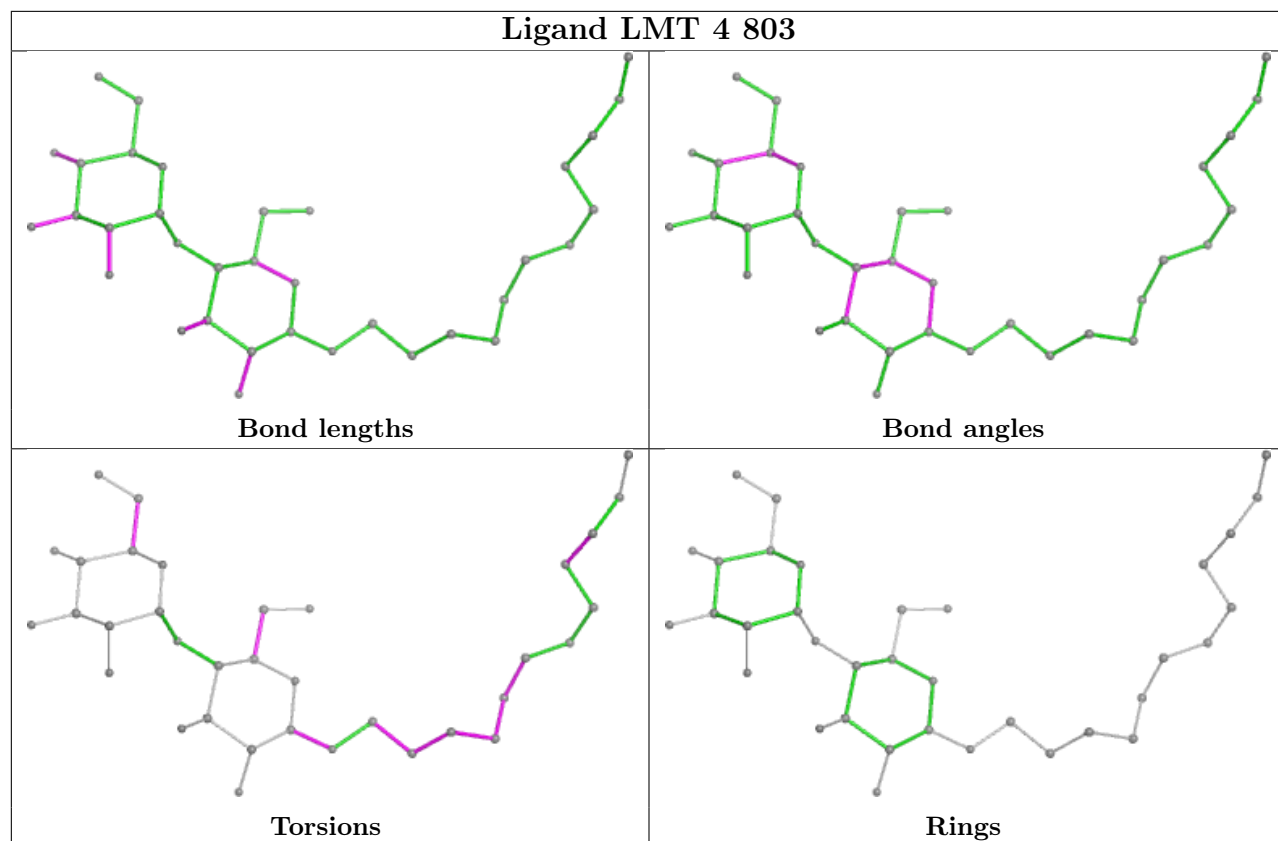


Torsions

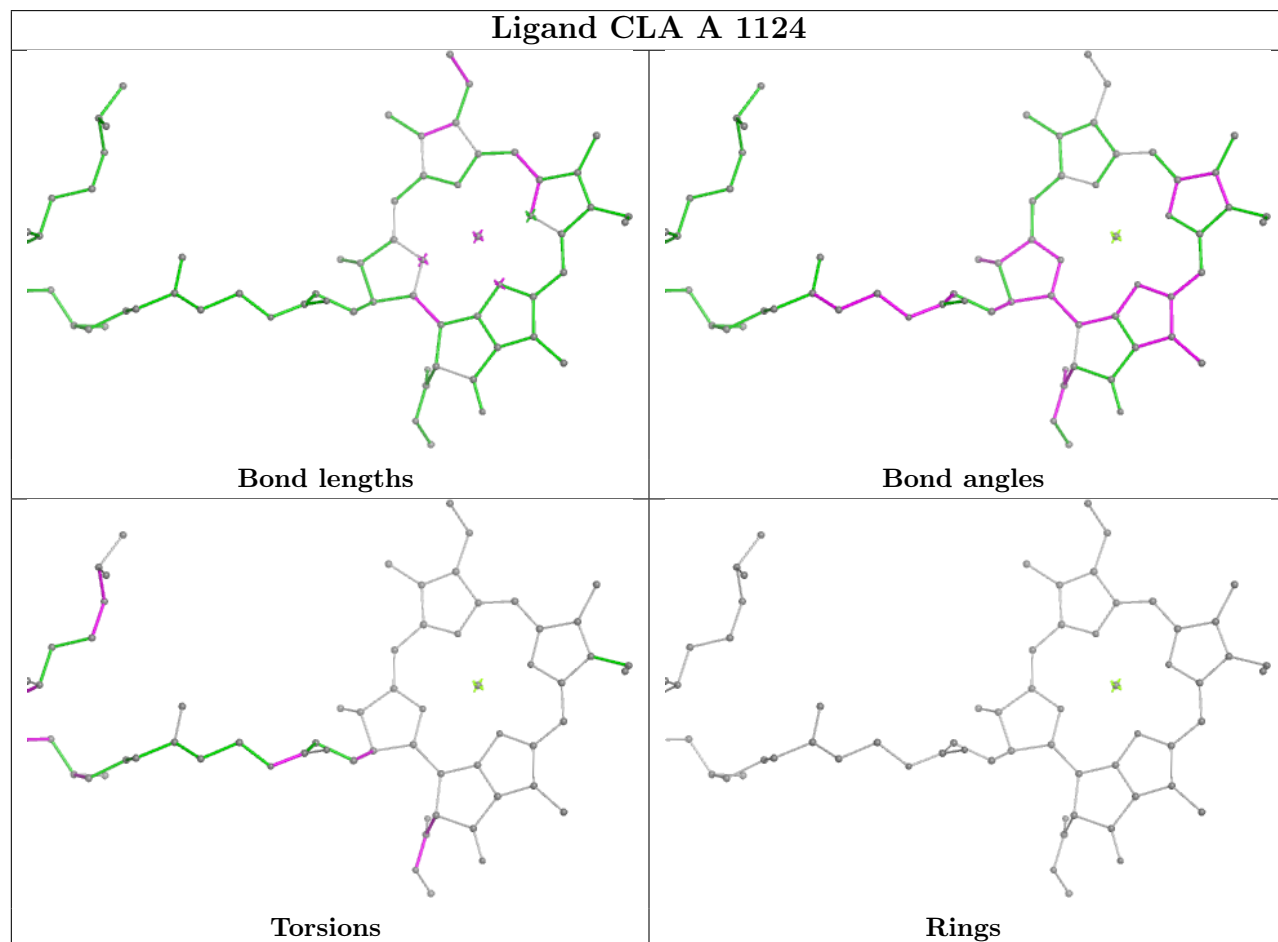


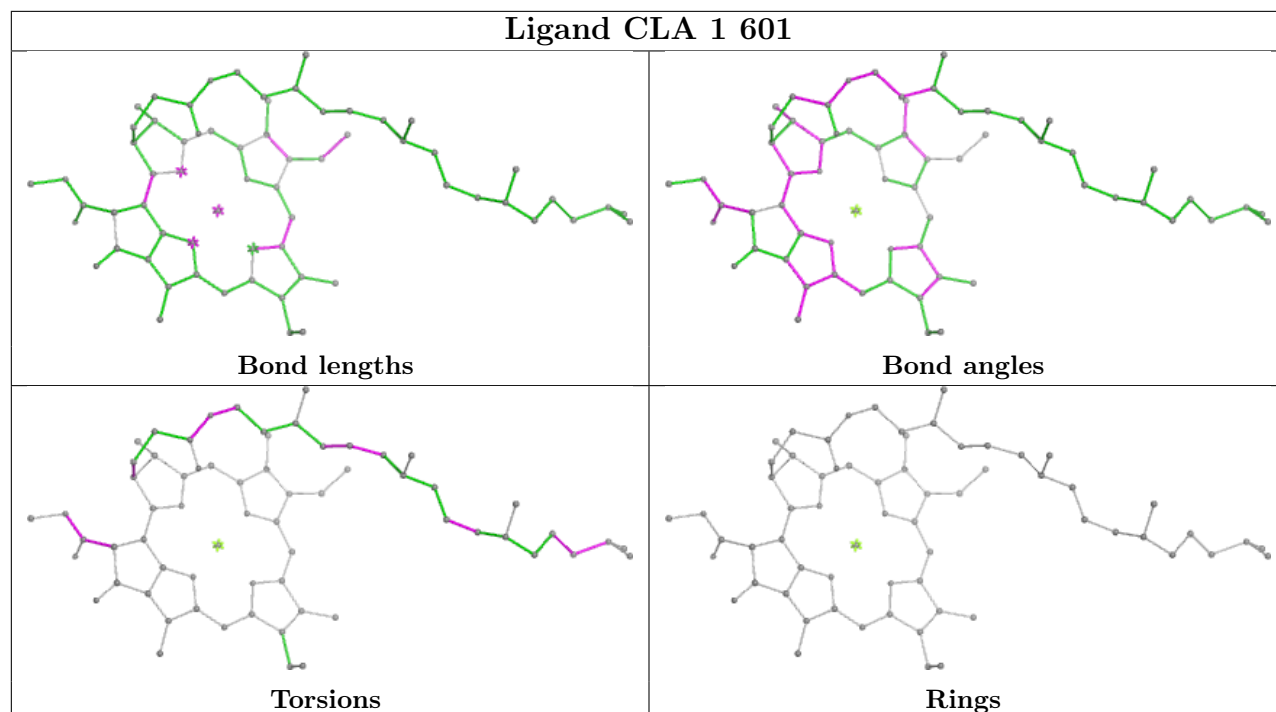
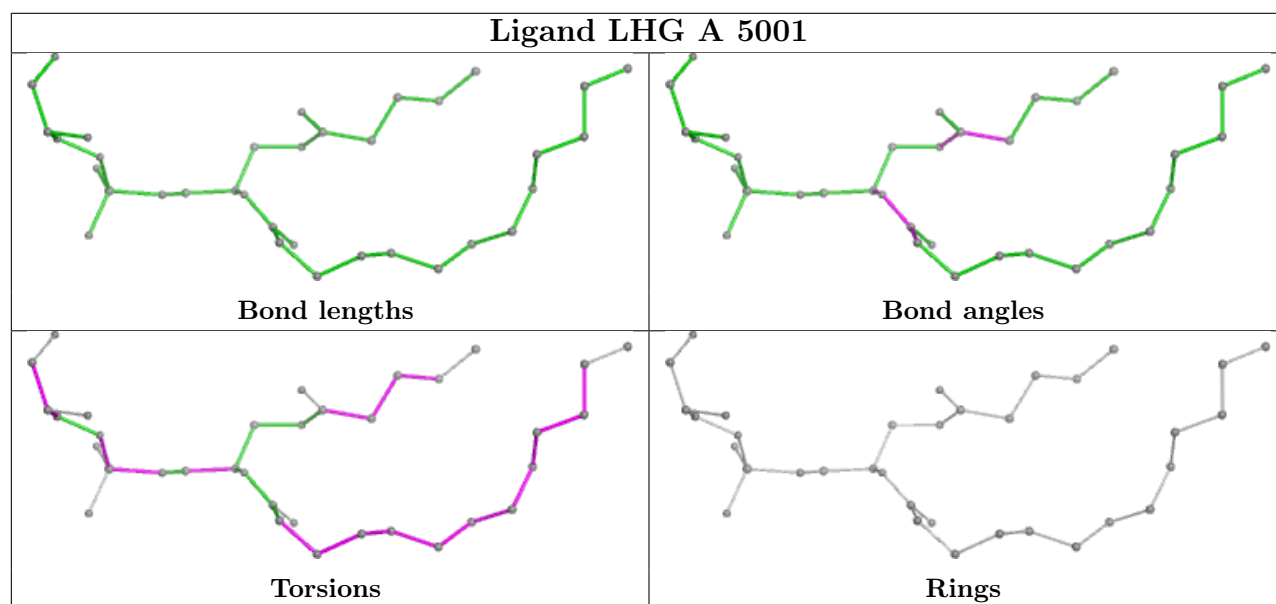
Rings

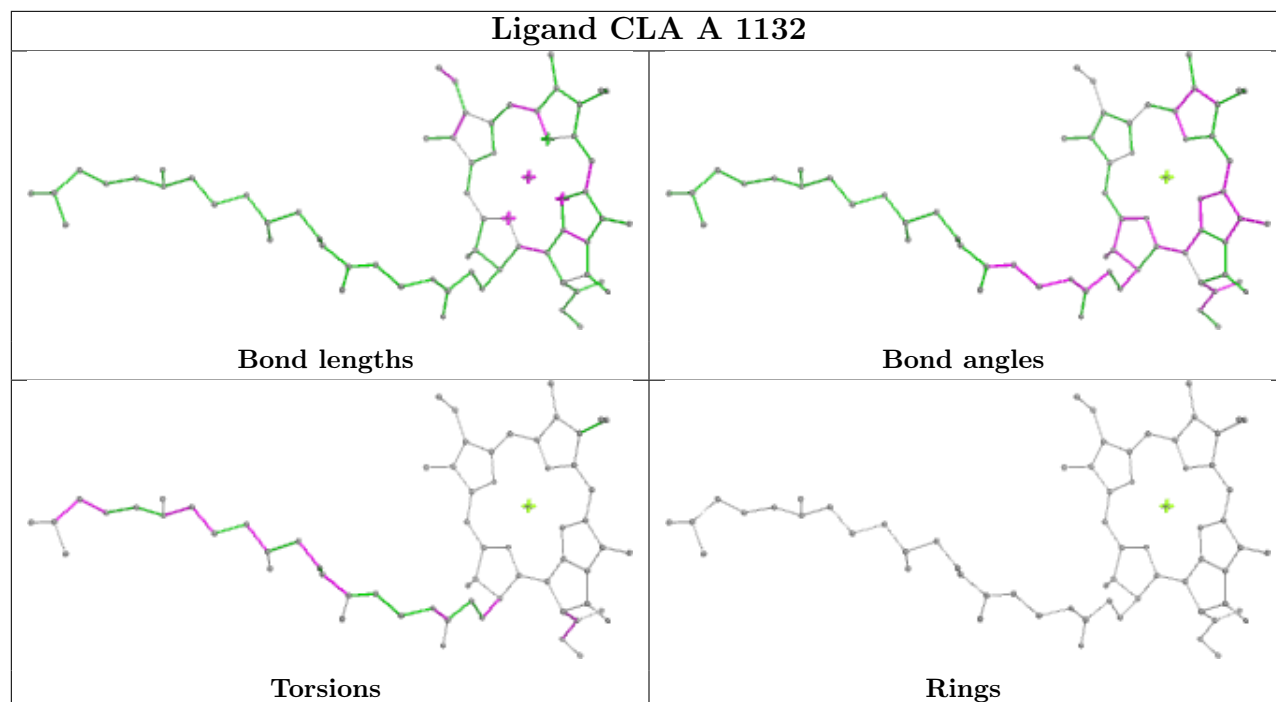
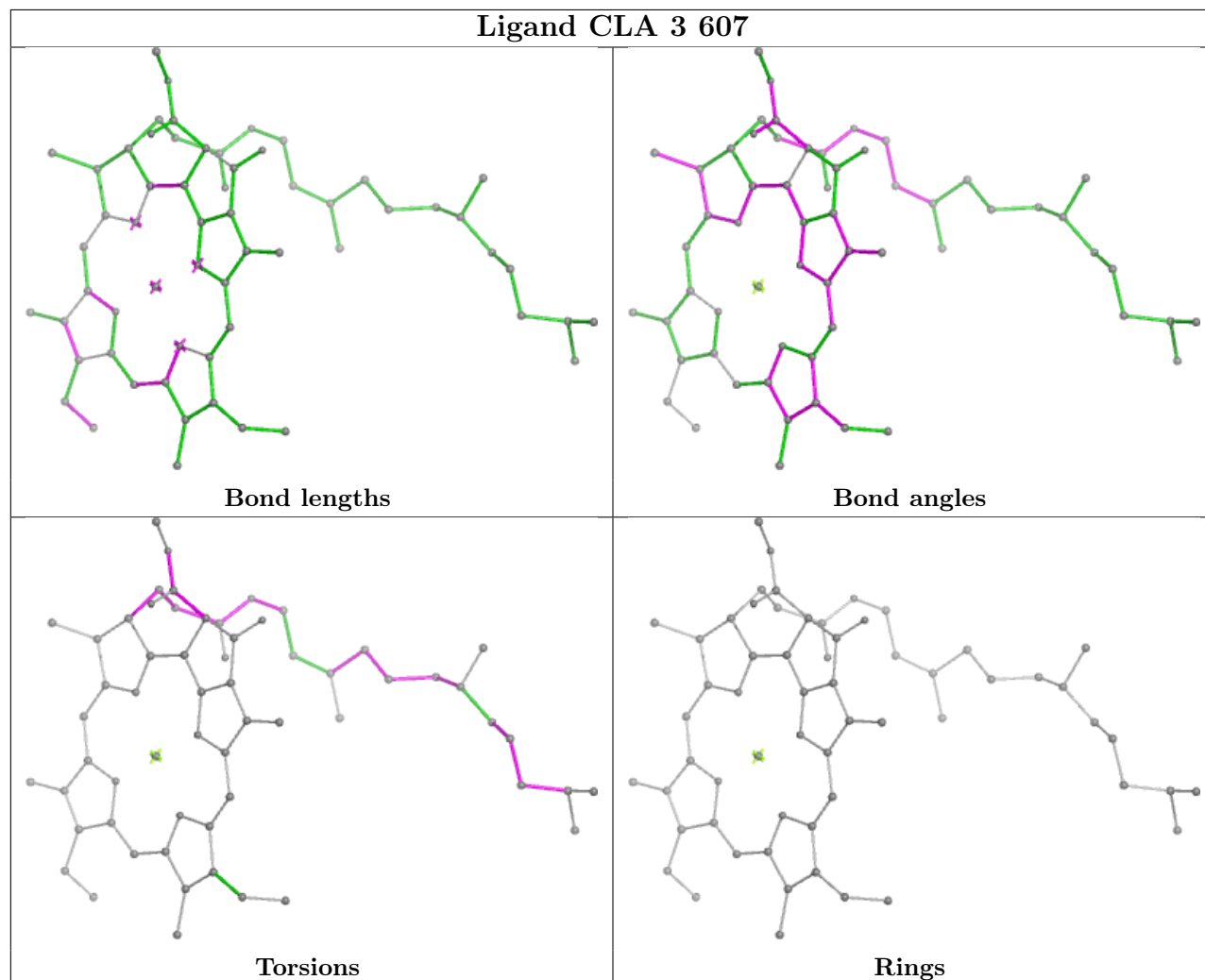
## Ligand LMT 4 803

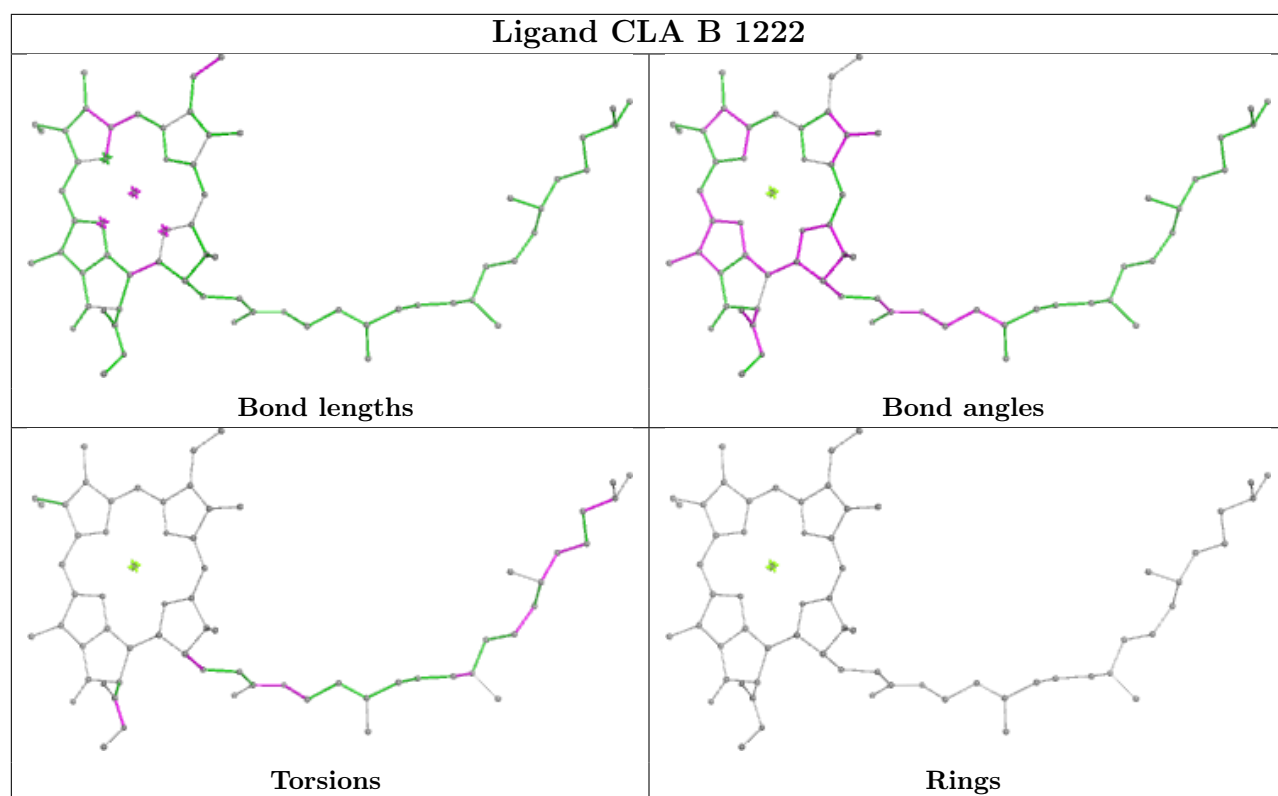


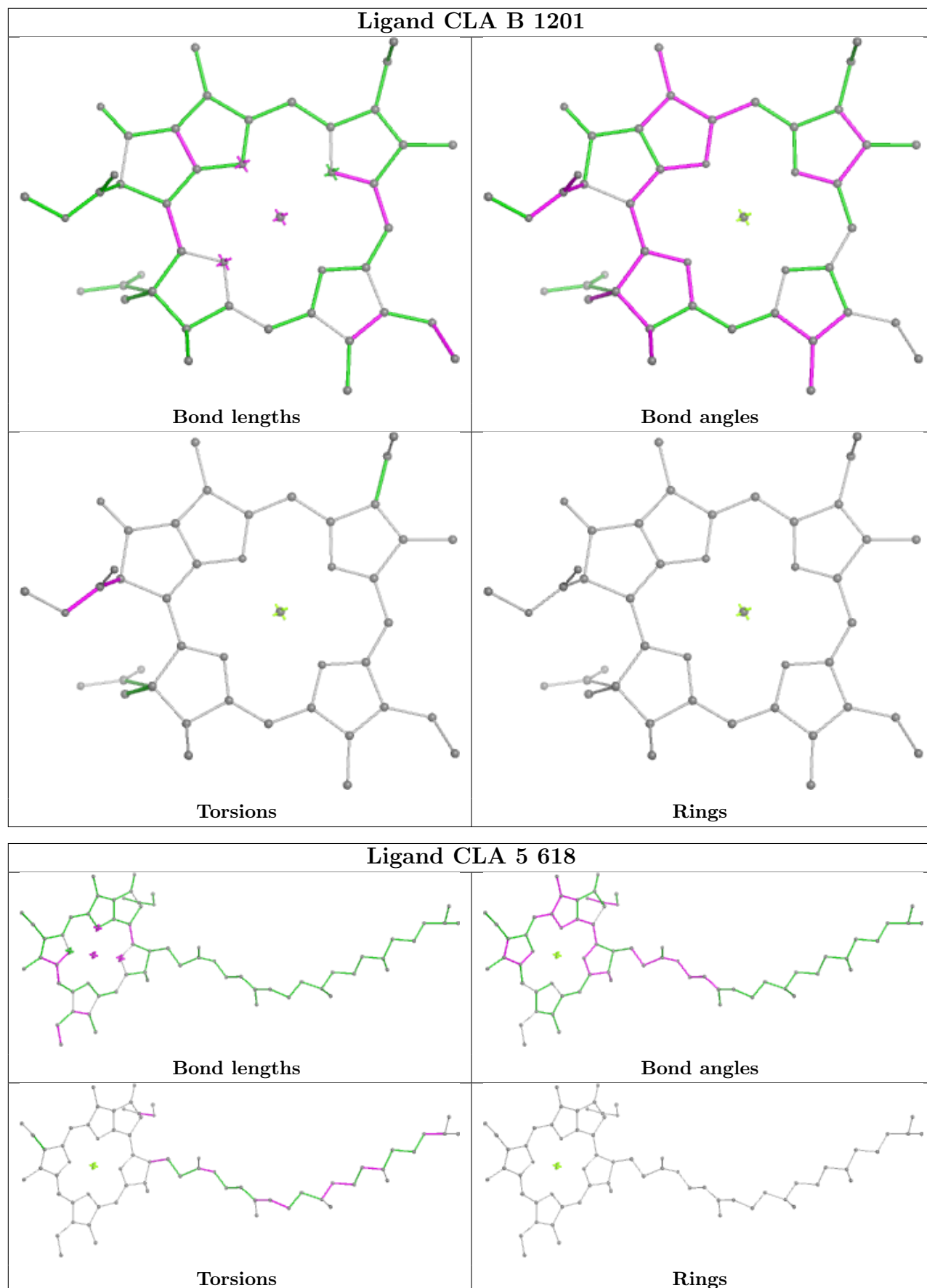
## Ligand CLA A 1124

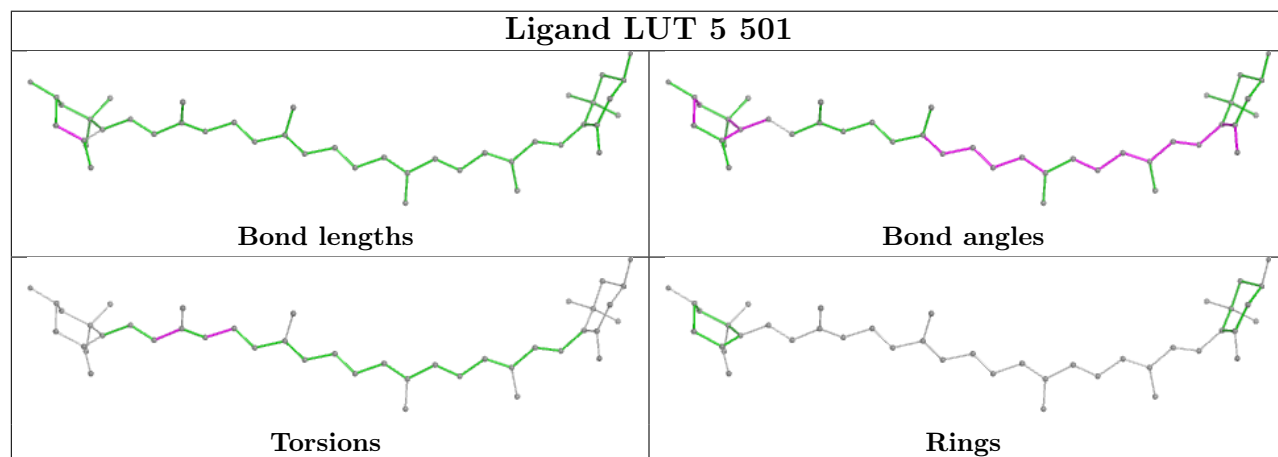
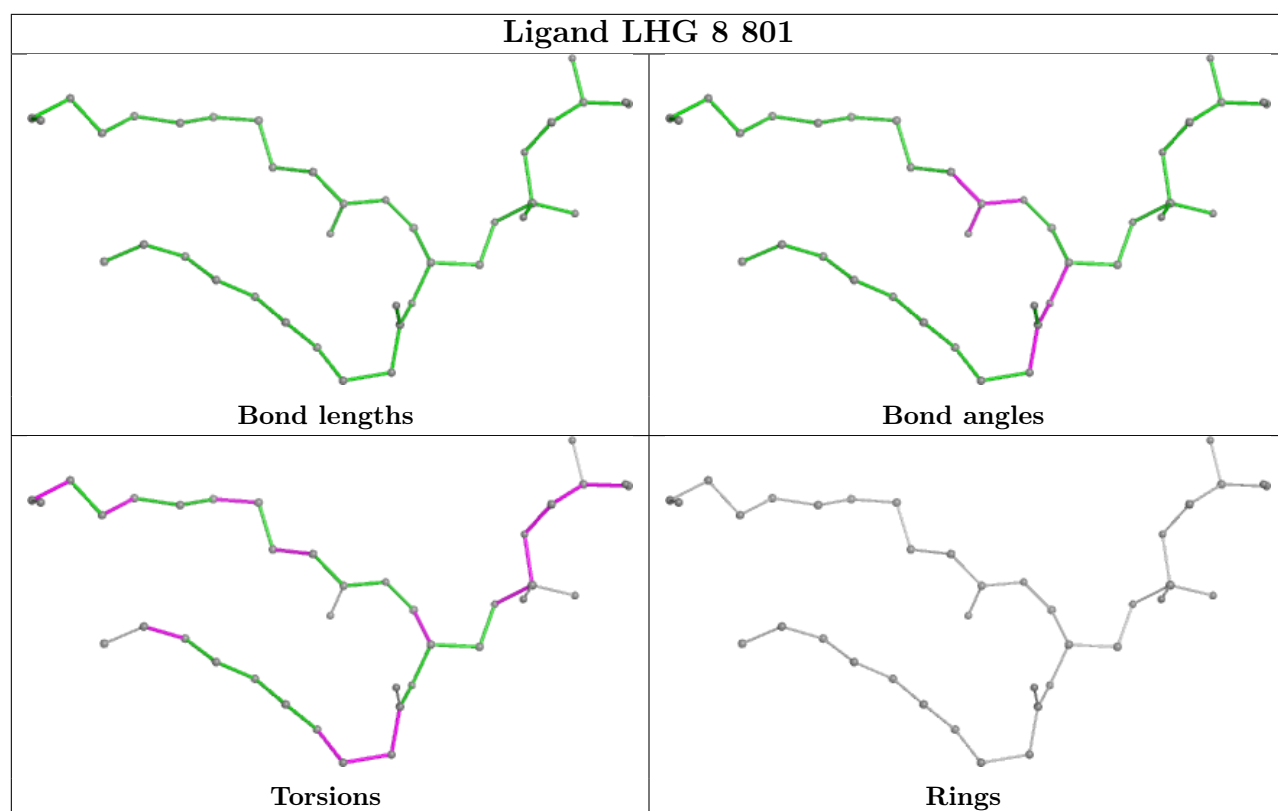


**Ligand CLA 1 601****Ligand LHG A 5001**

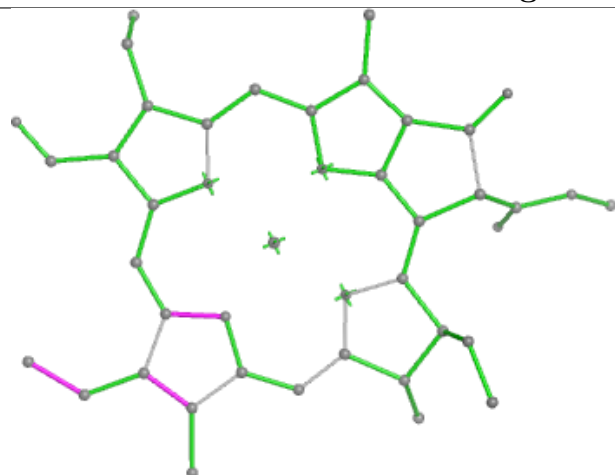
**Ligand CLA A 1132****Ligand CLA 3 607**



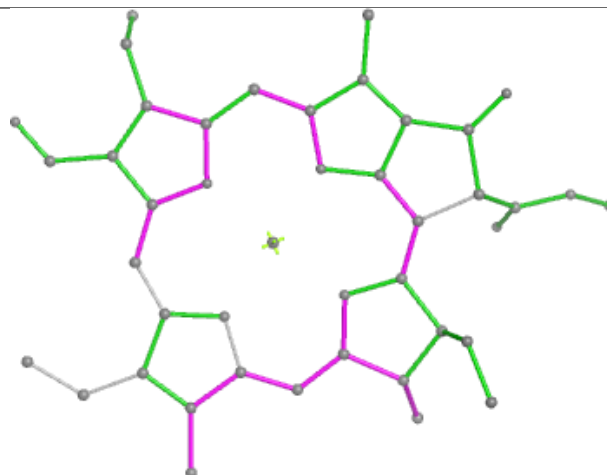




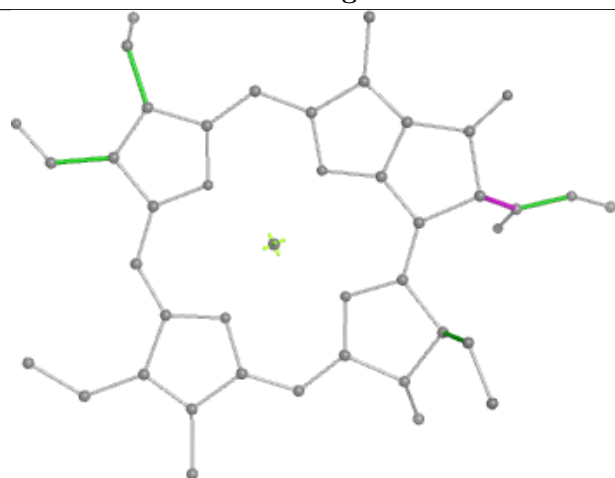
## Ligand CHL 4 617



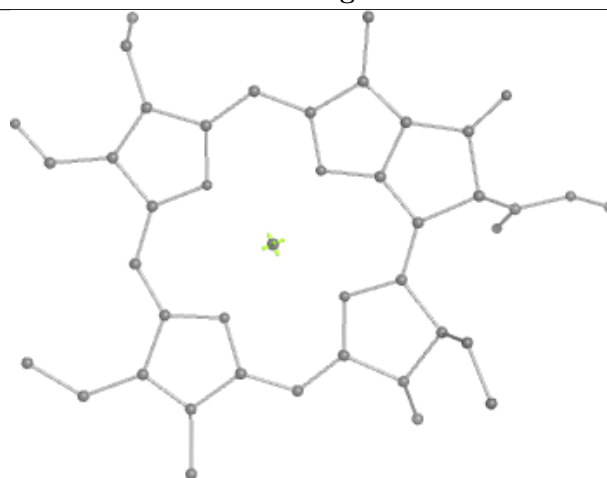
Bond lengths



Bond angles

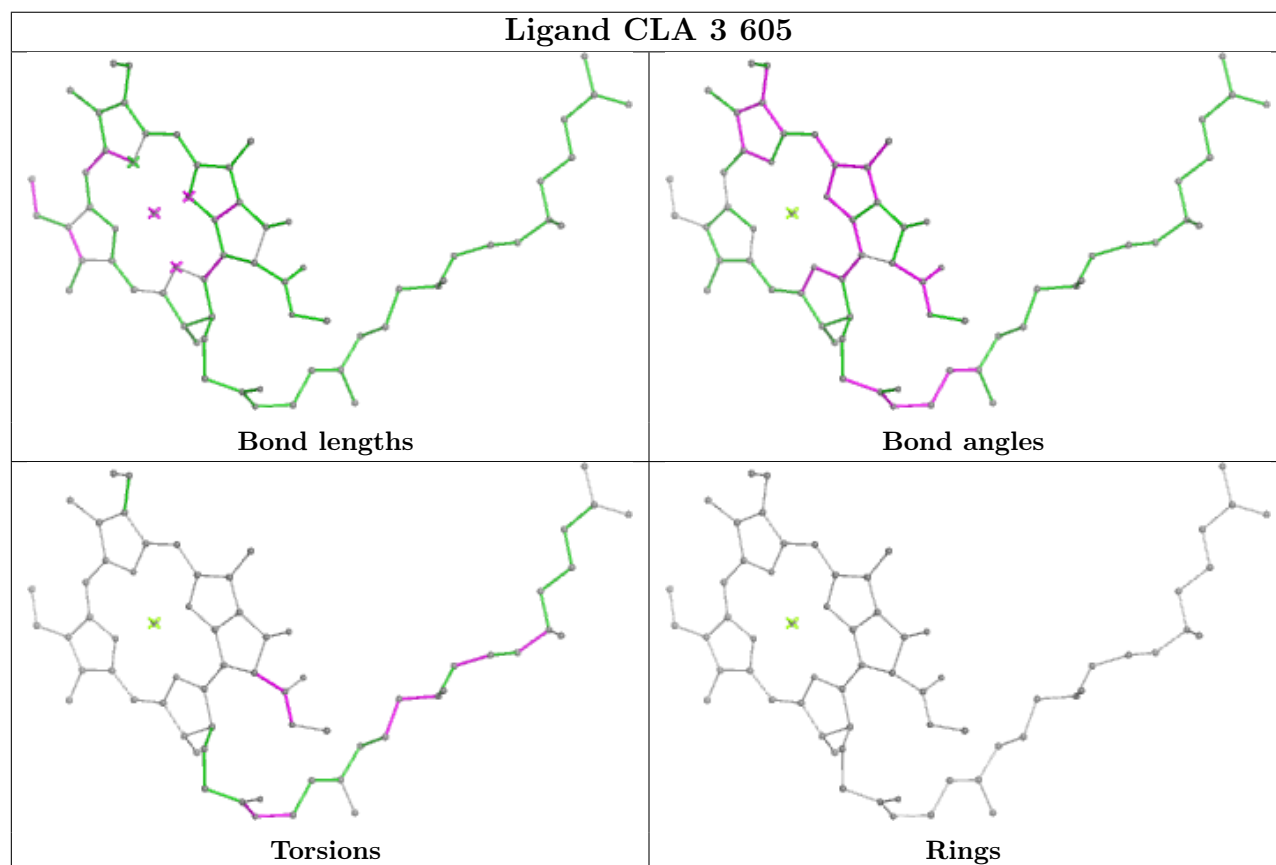
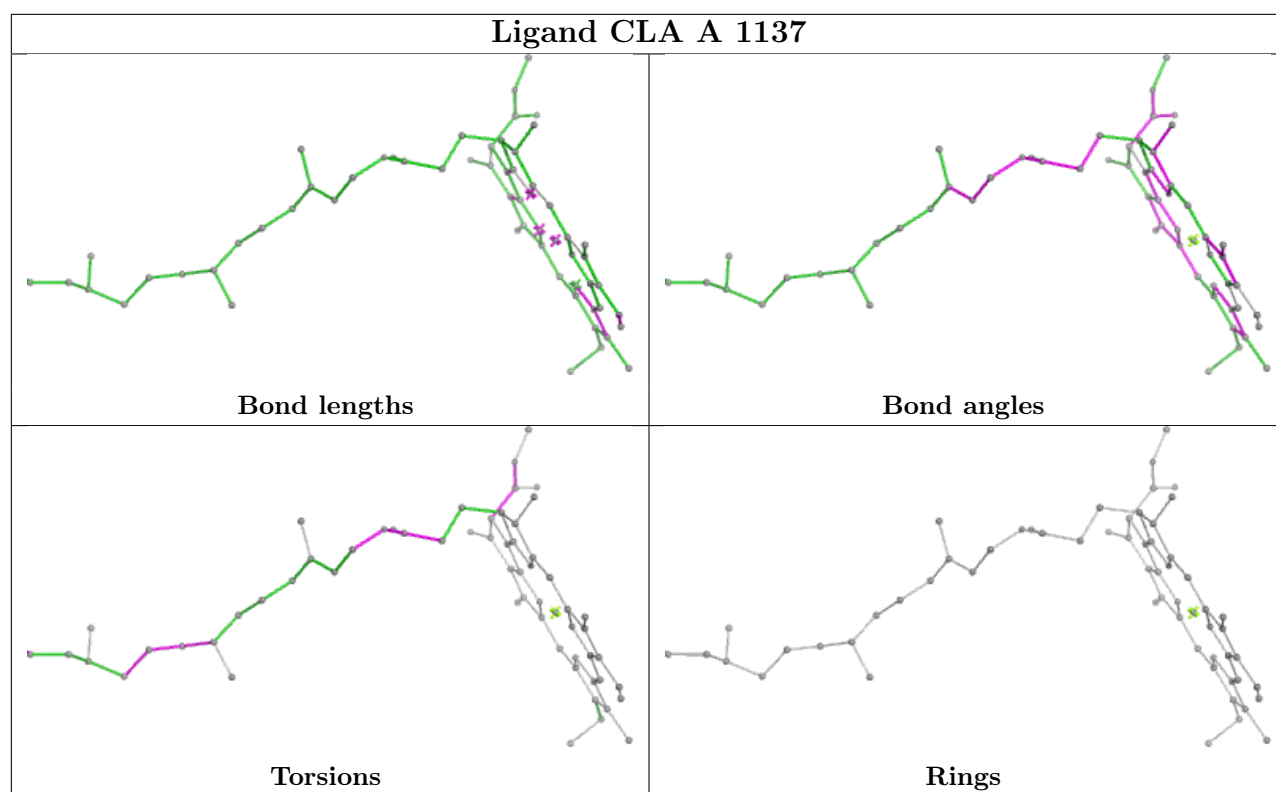


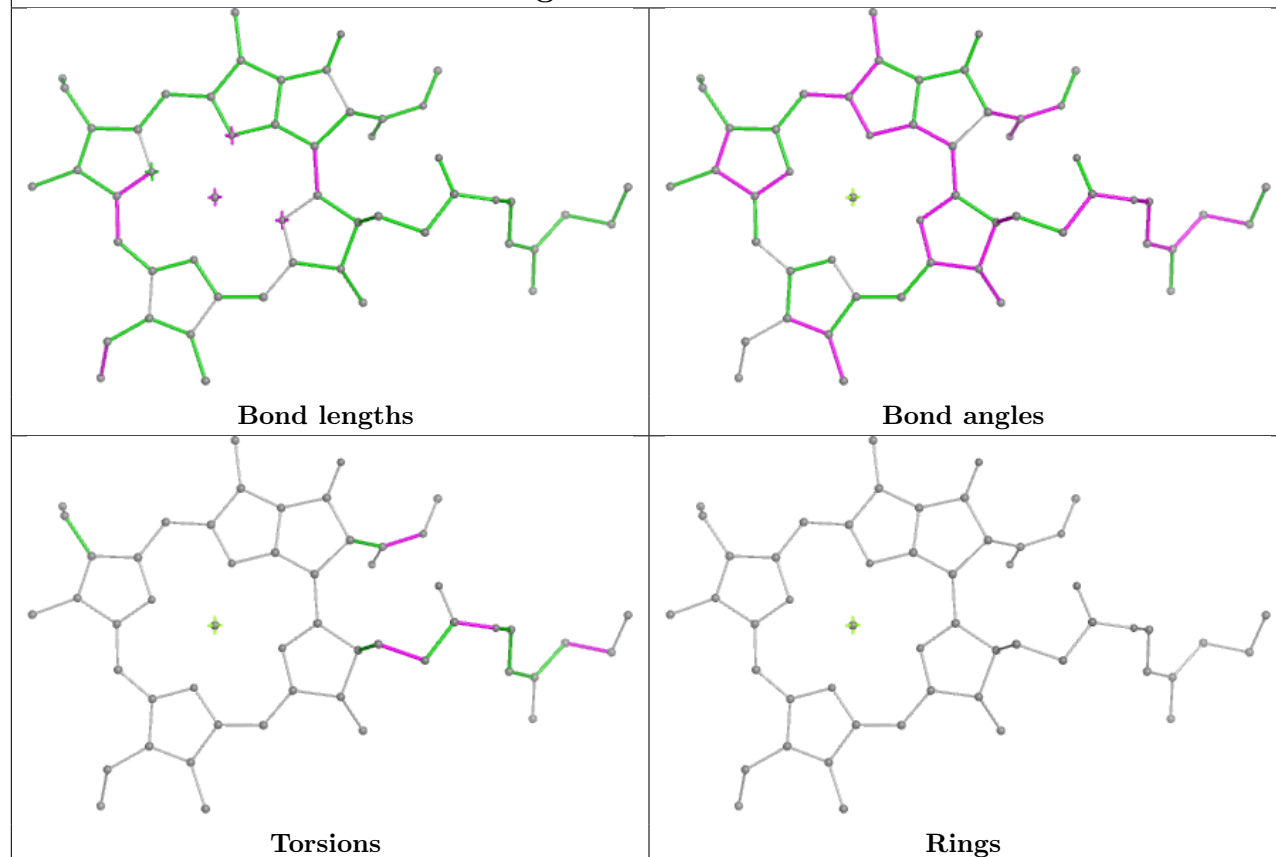
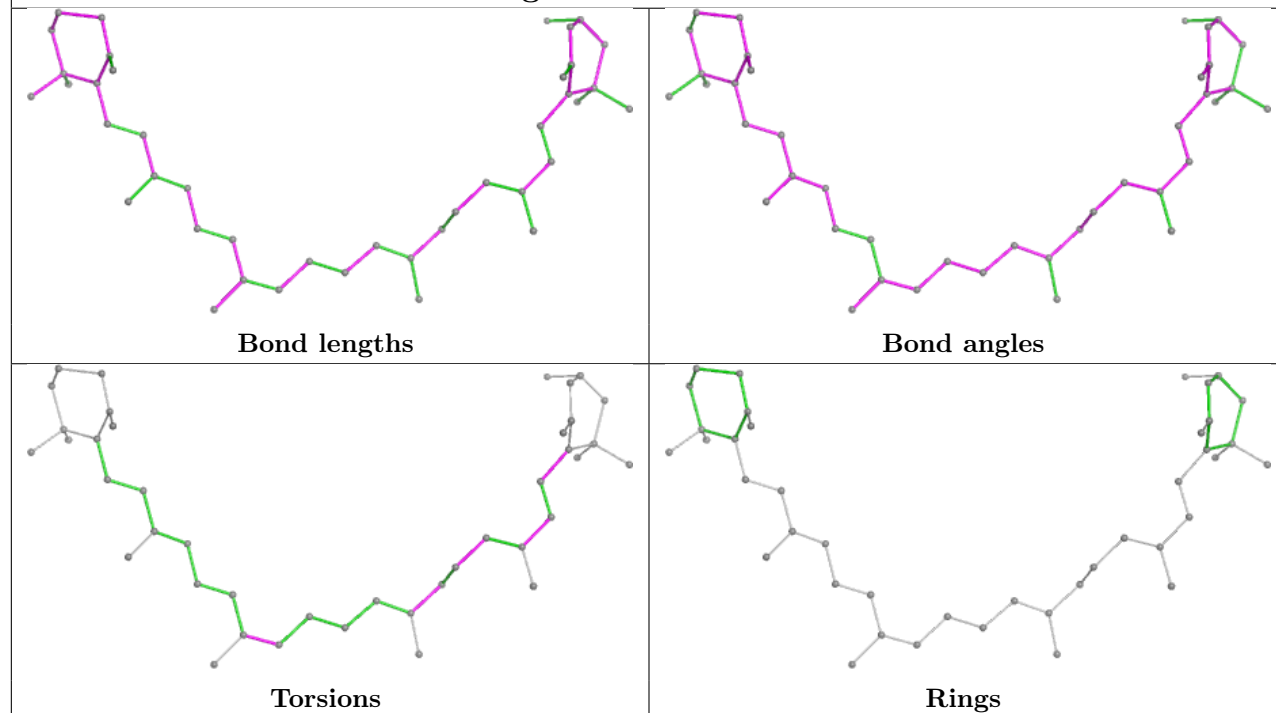
Torsions

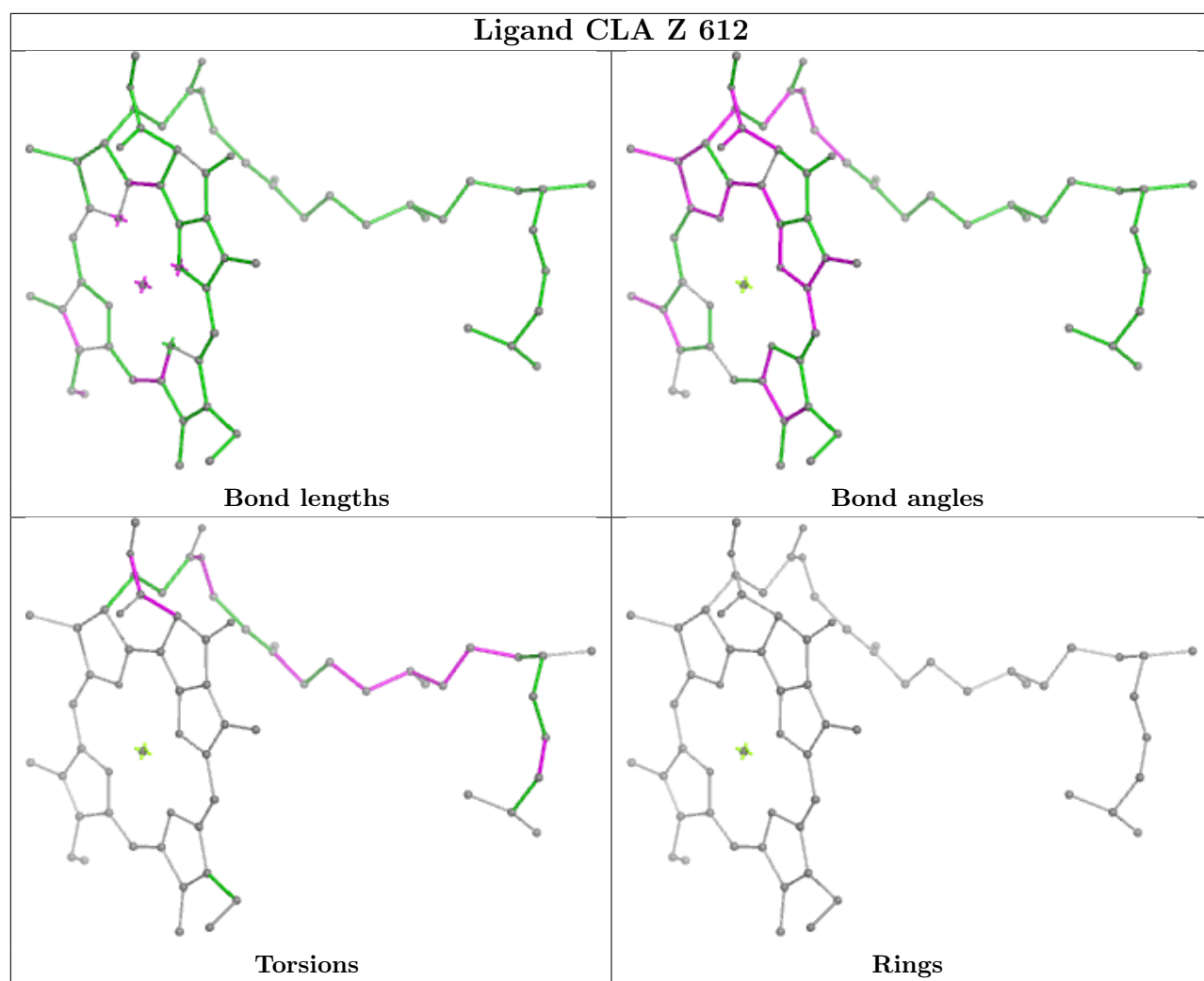


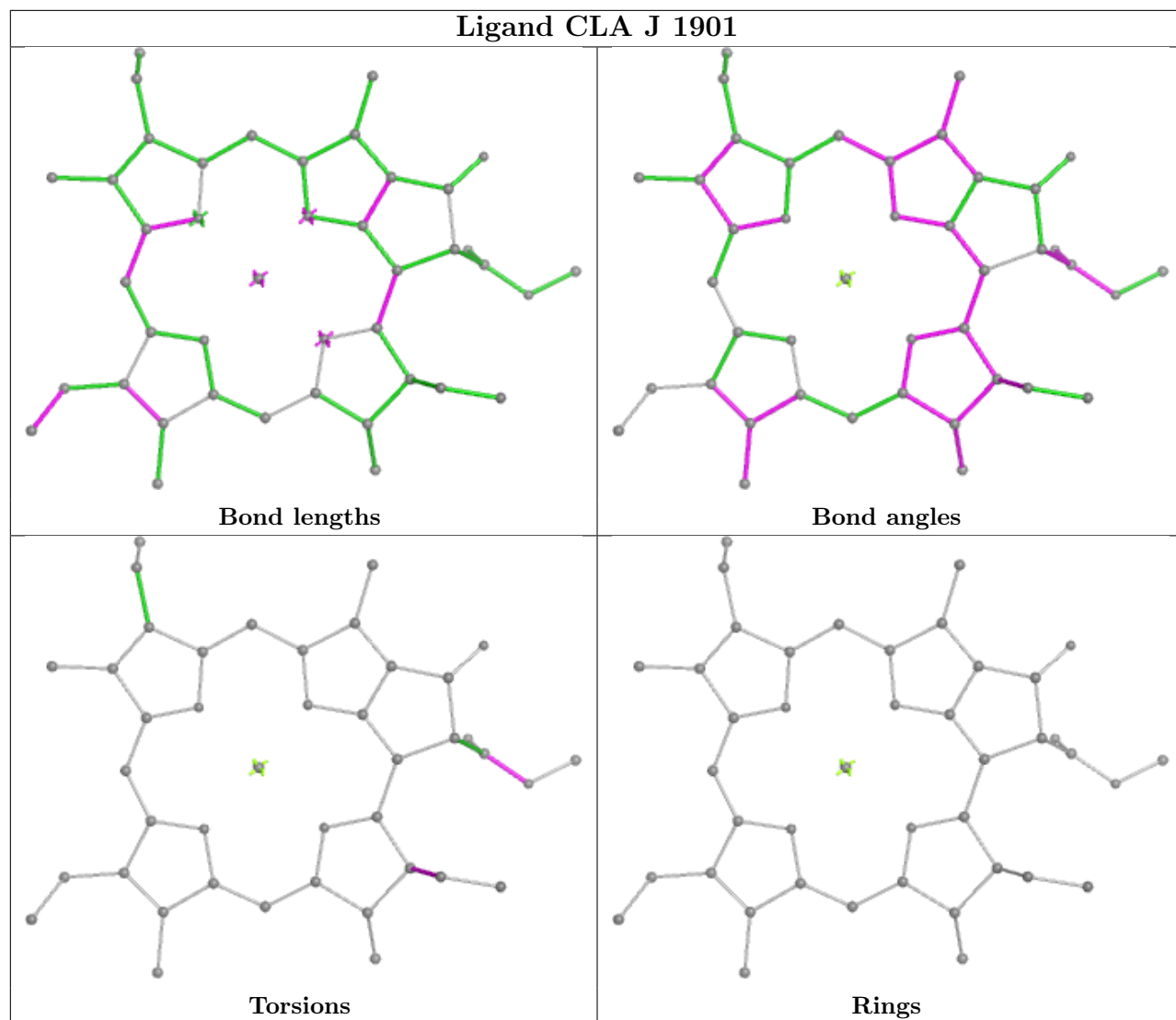
Rings

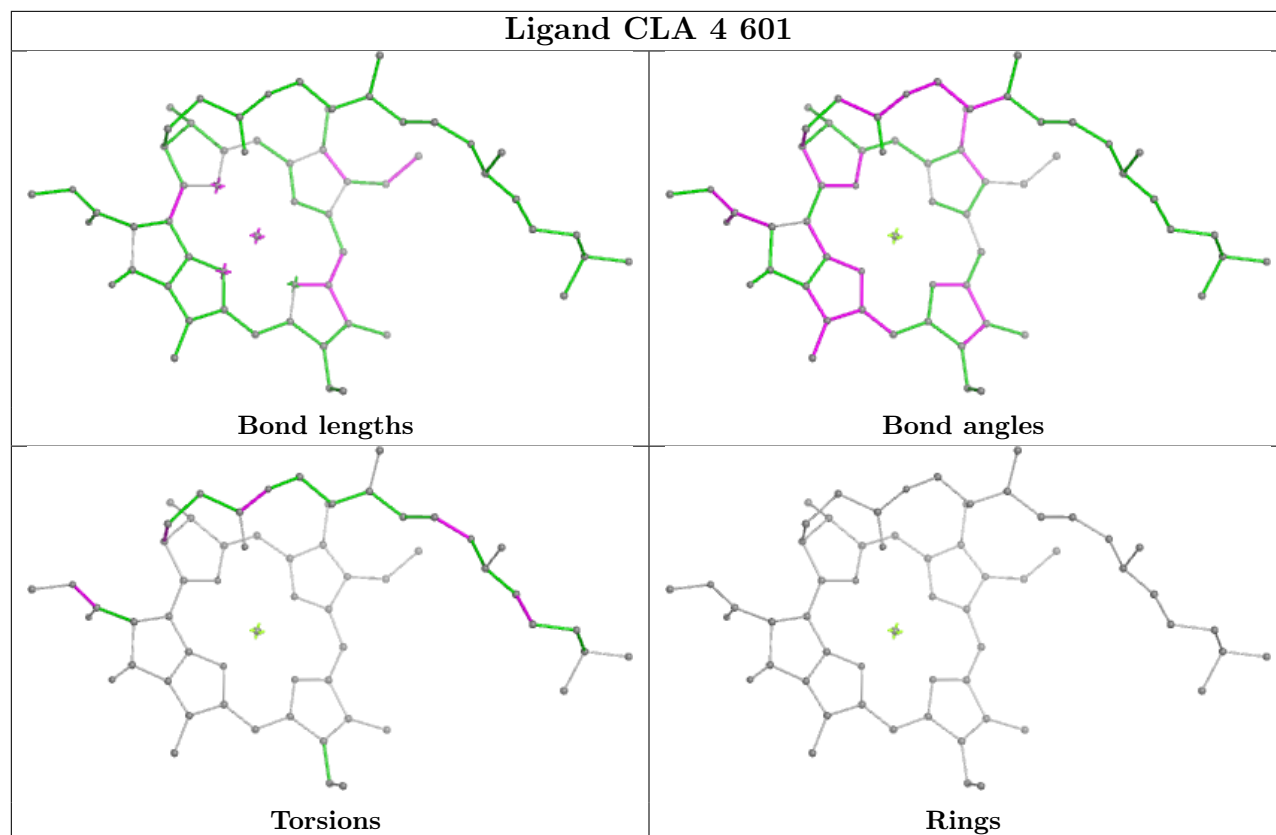
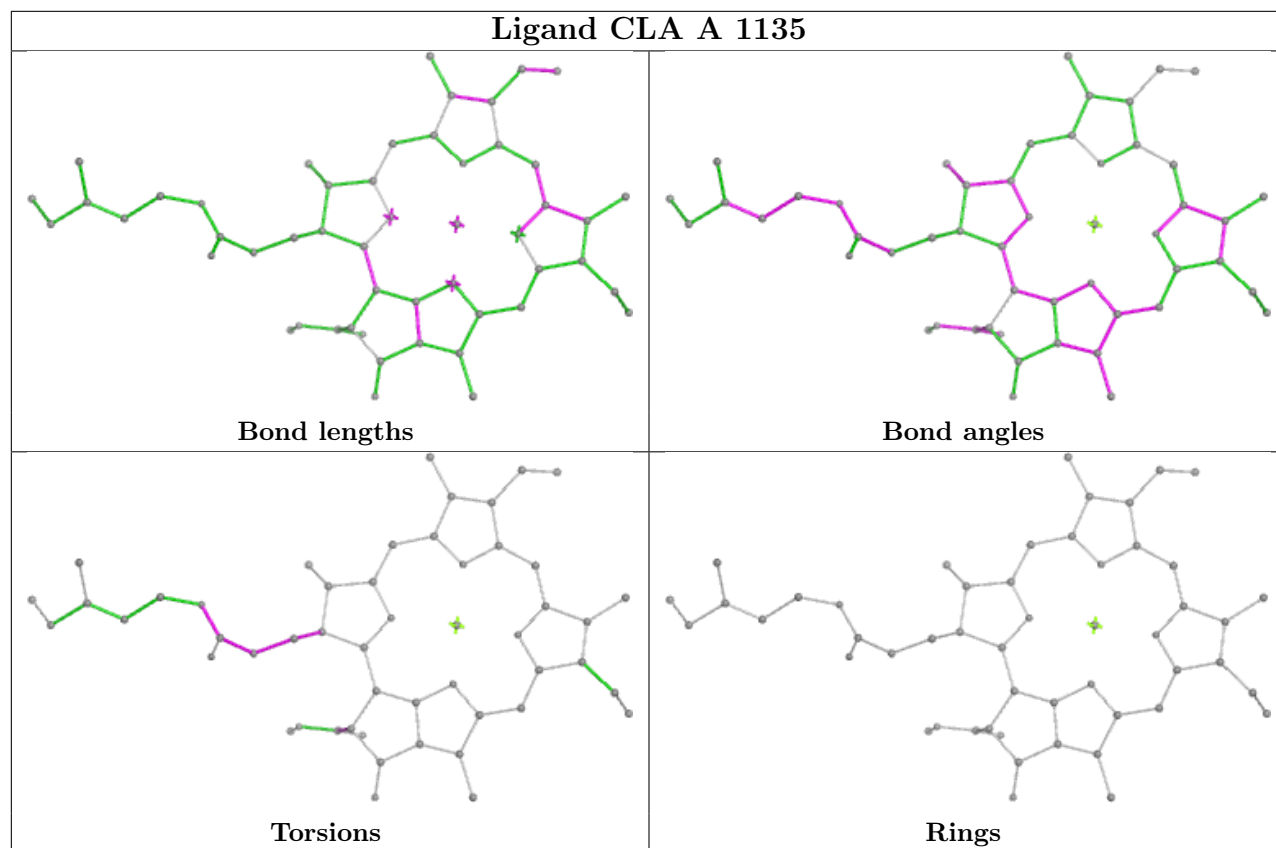




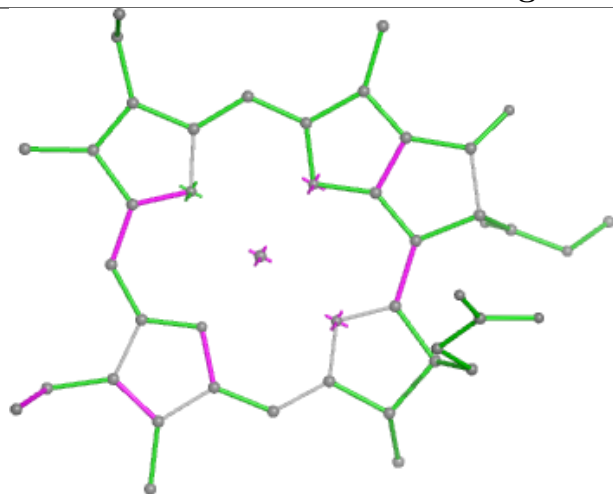
**Ligand CLA 6 602****Ligand RRX F 4001**



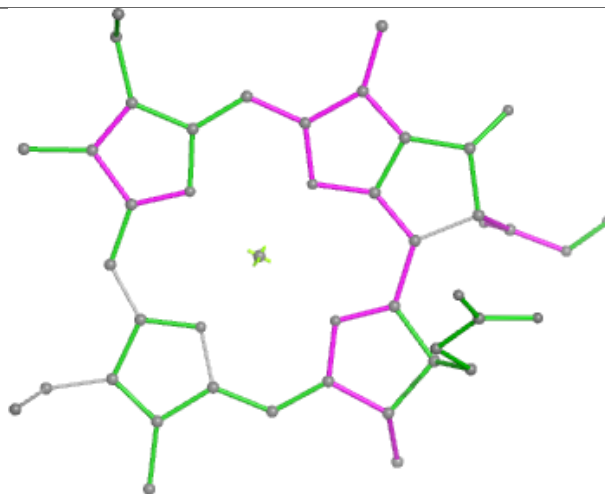


**Ligand CLA 4 601****Ligand CLA A 1135**

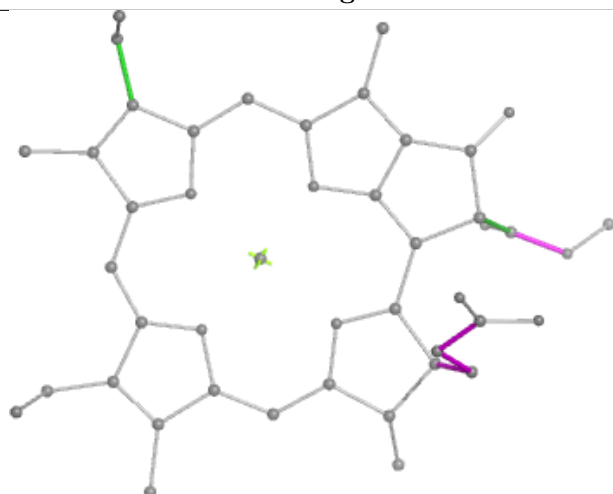
## Ligand CLA 5 608



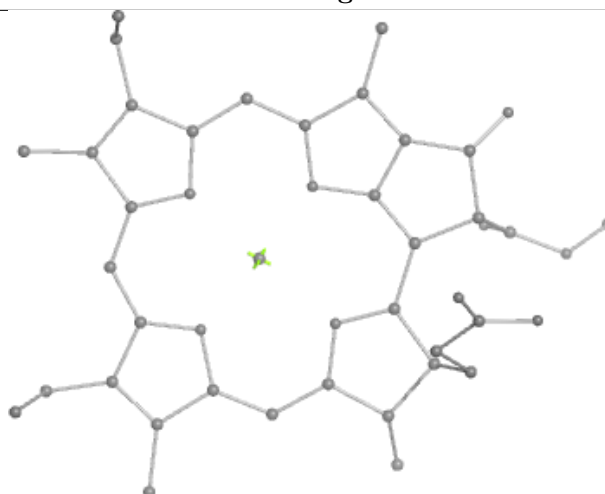
Bond lengths



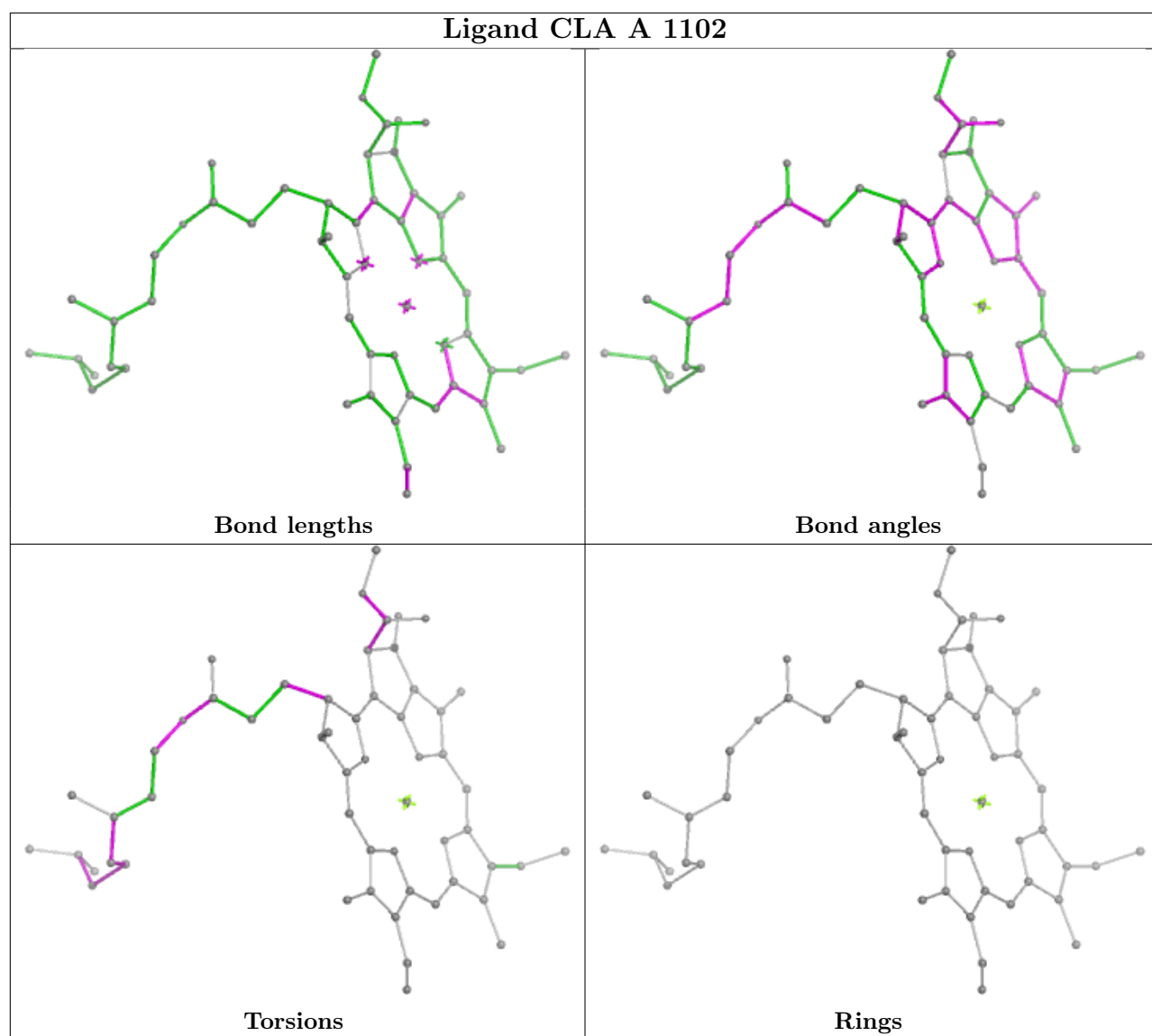
Bond angles



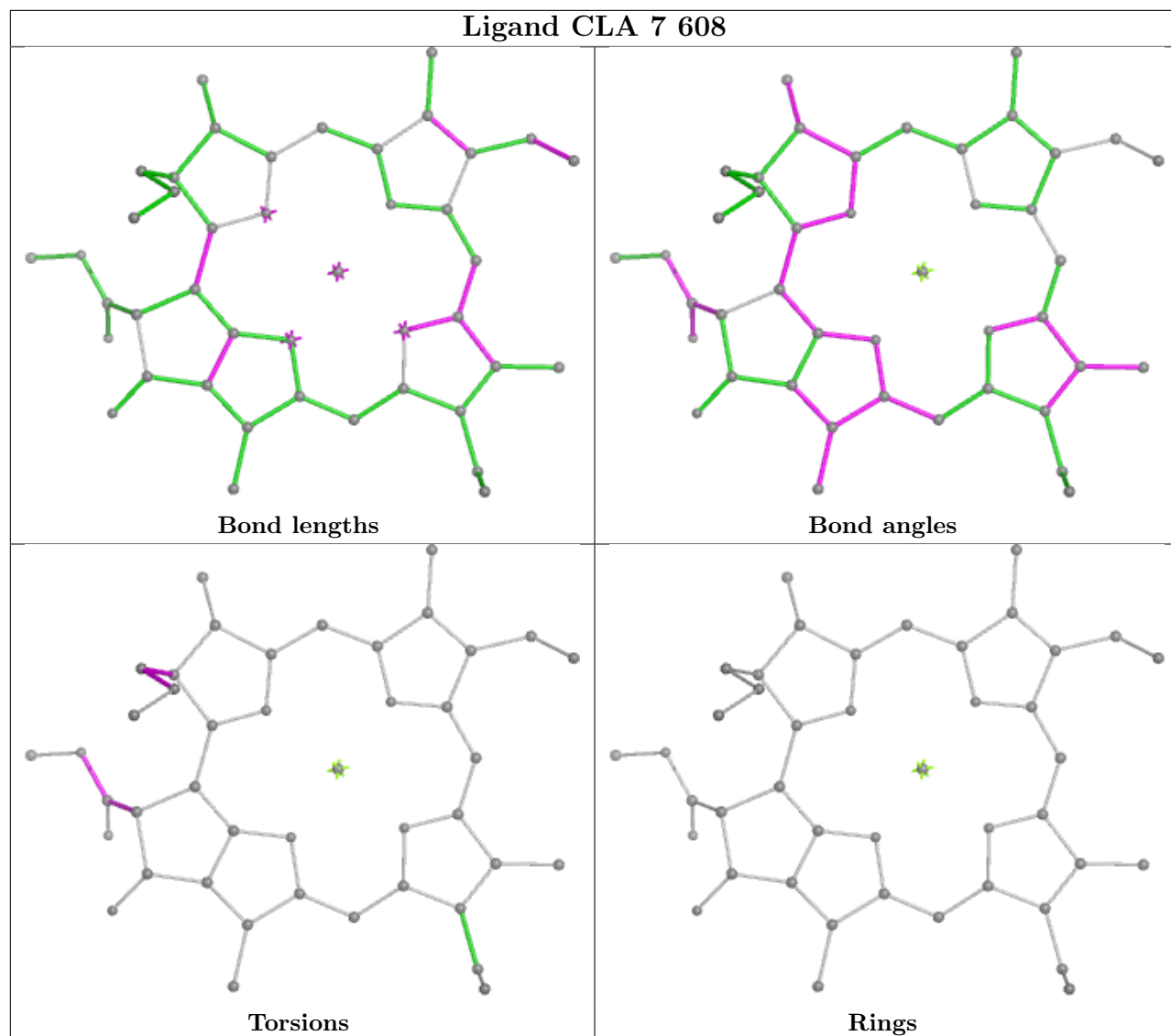
Torsions



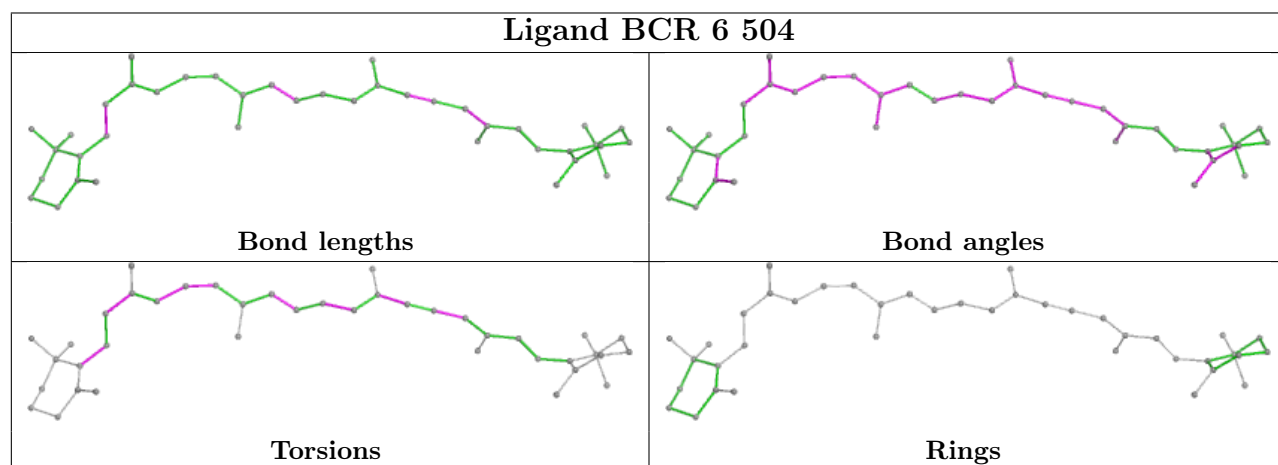
Rings



## Ligand CLA 7 608

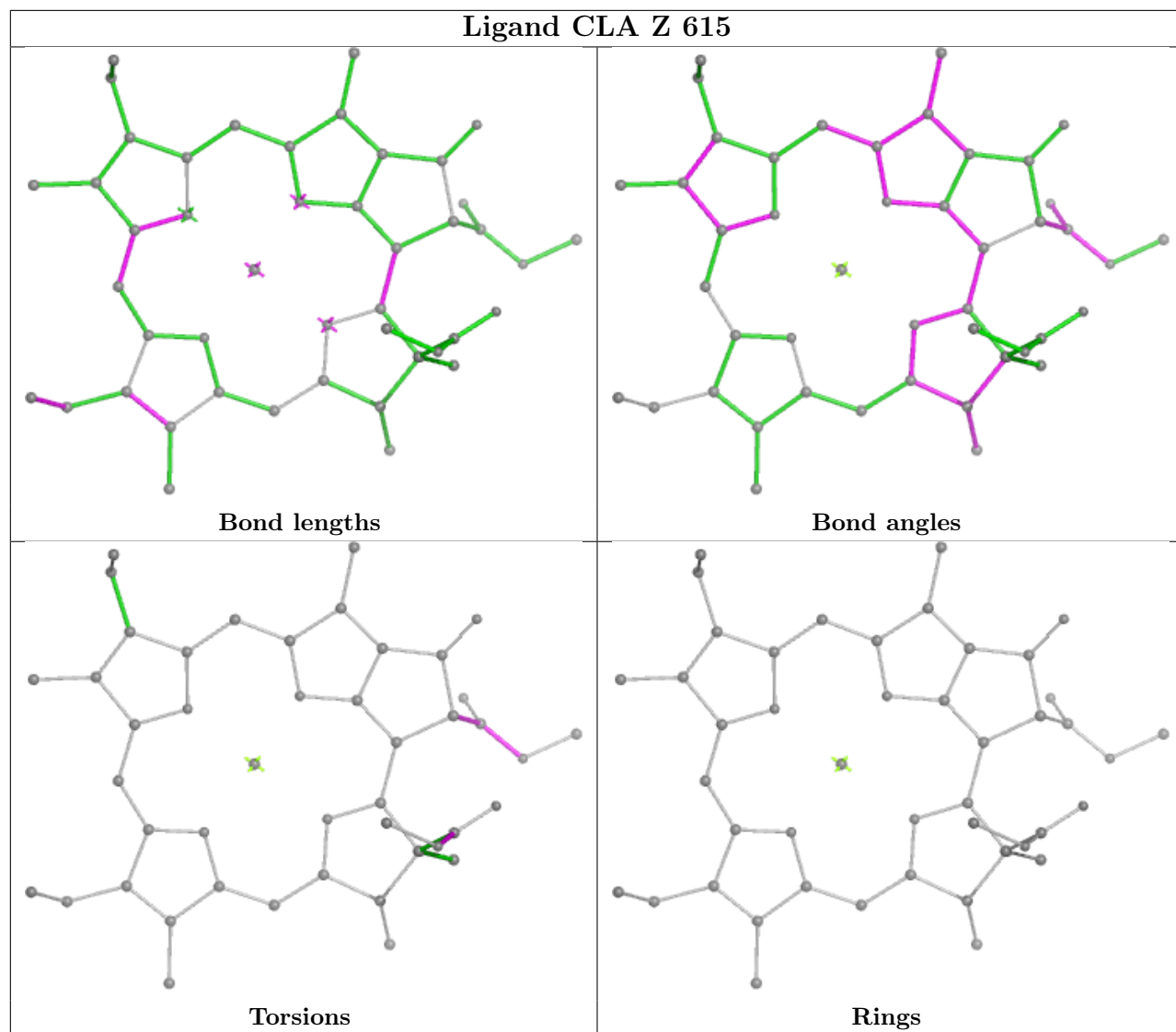


## Ligand BCR 6 504

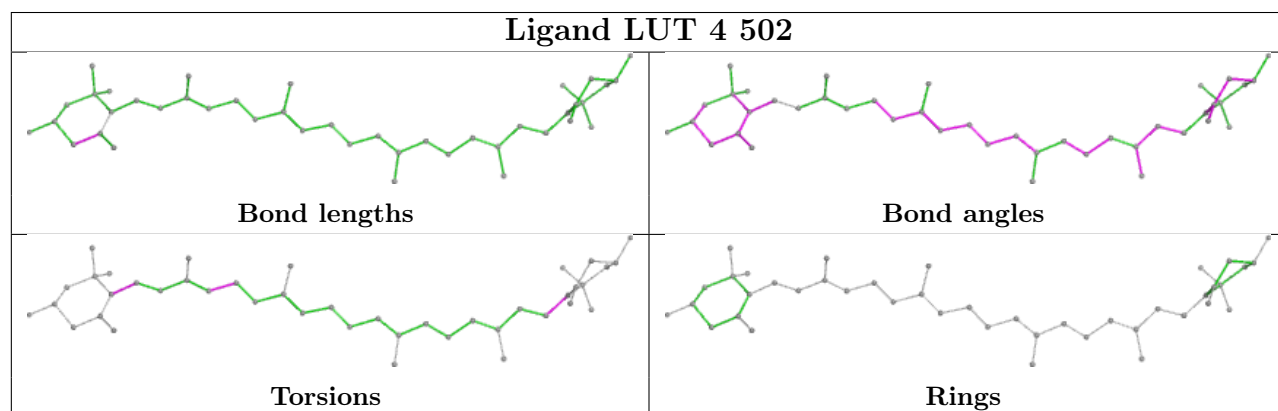


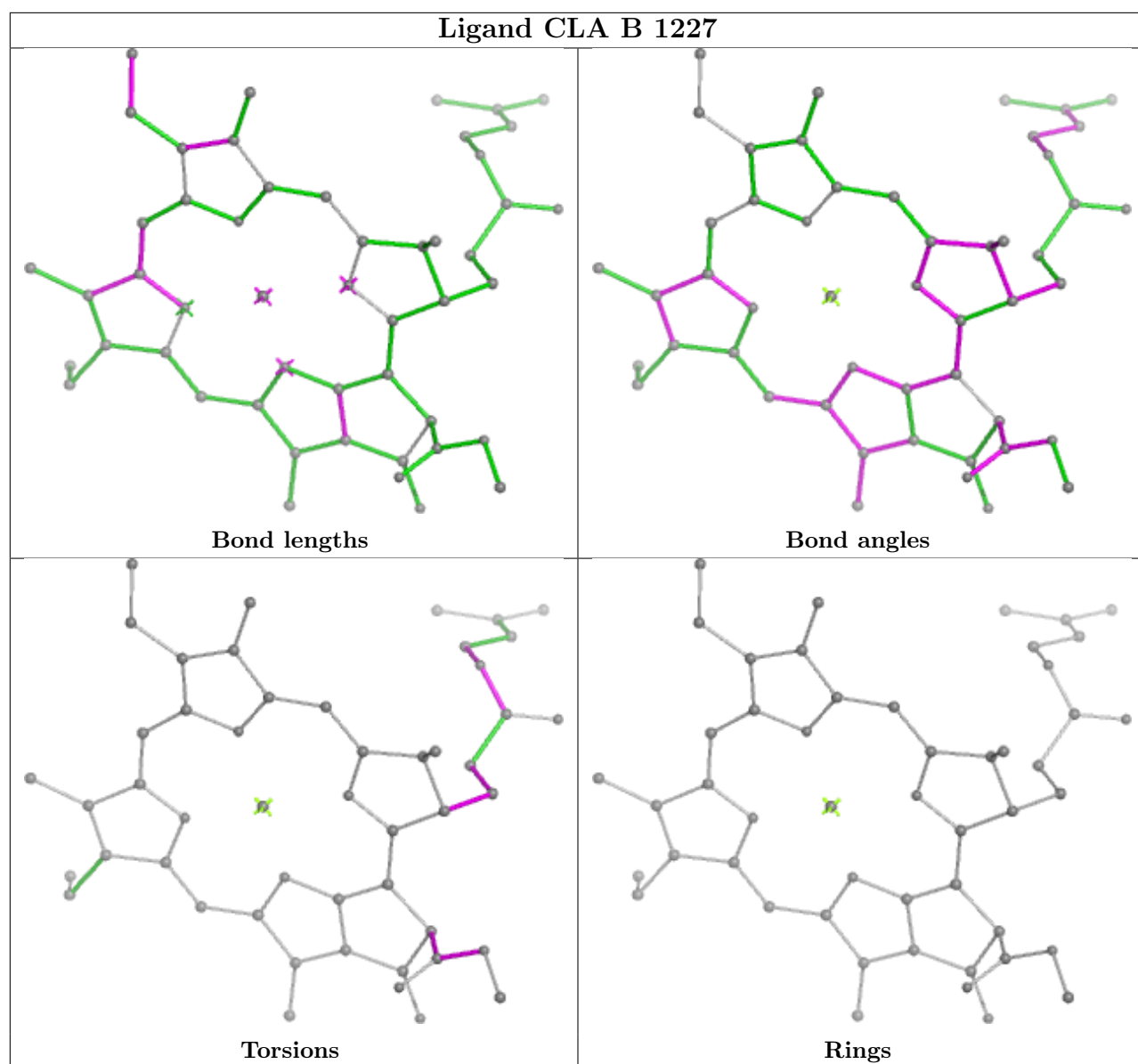


## Ligand CLA Z 615

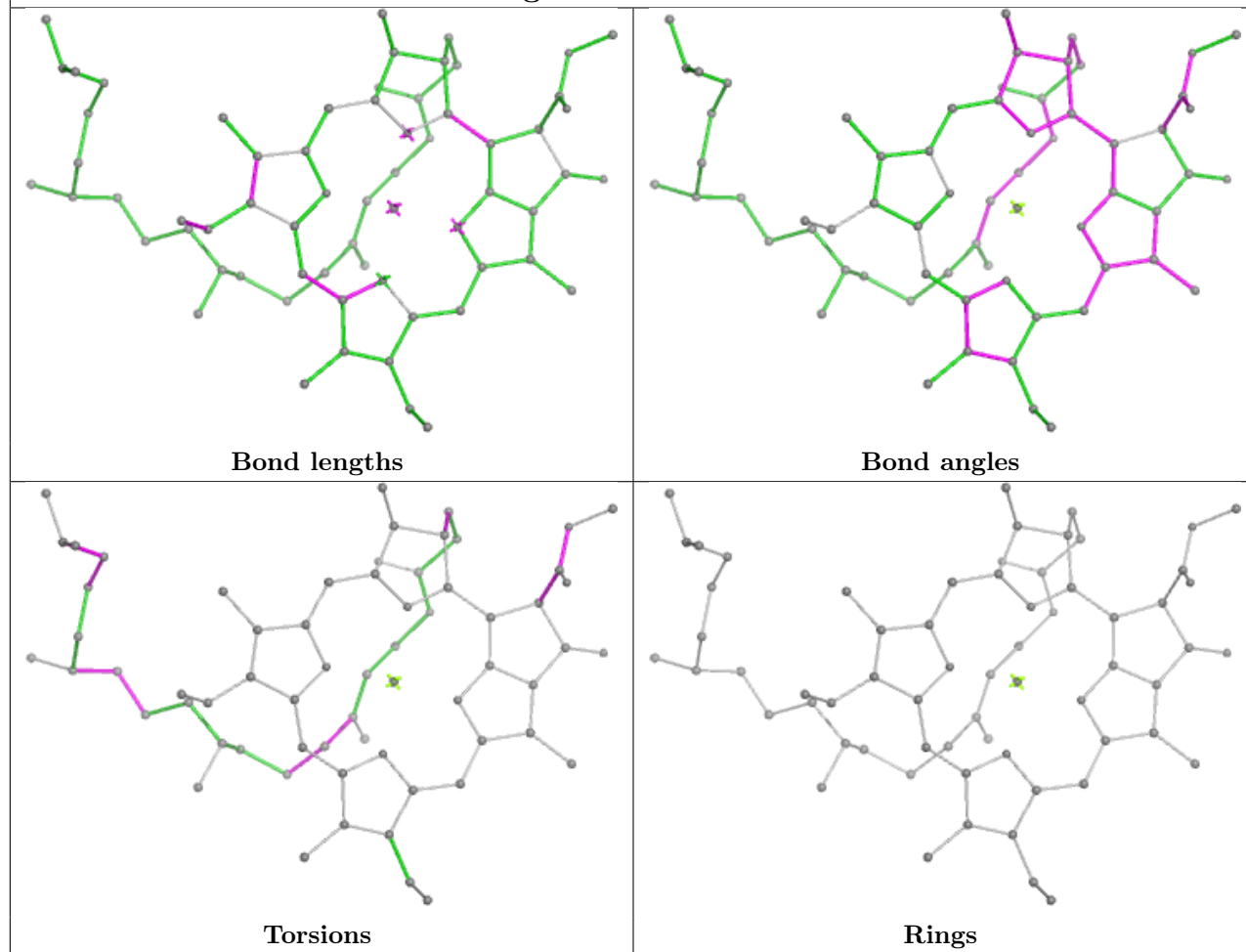


## Ligand LUT 4 502

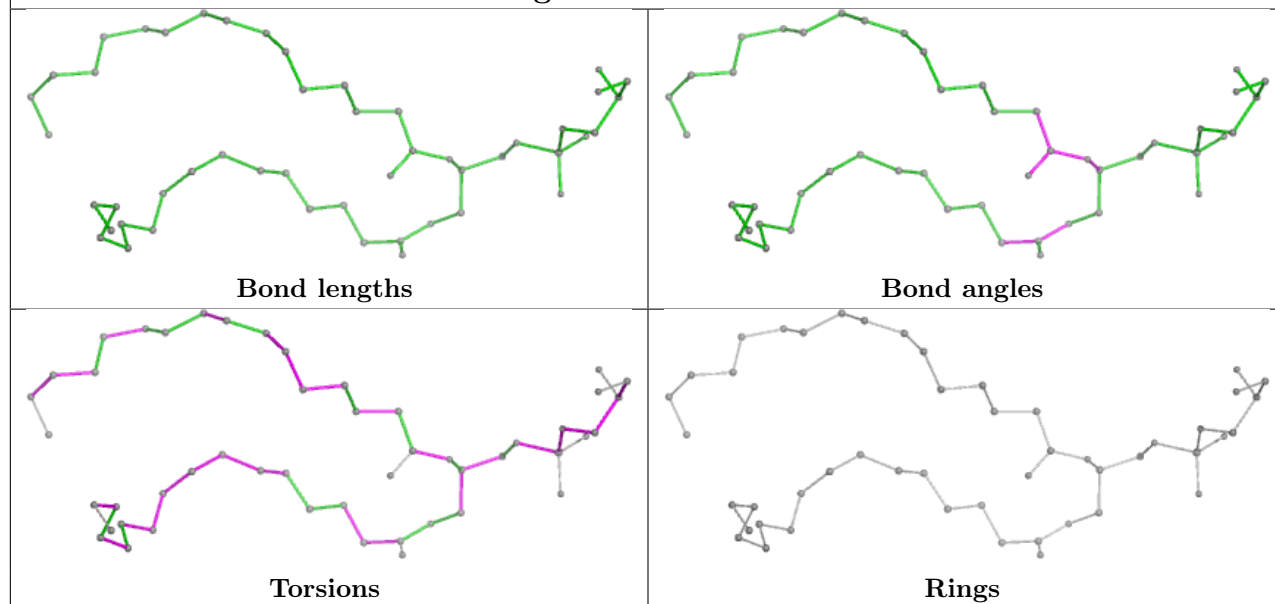


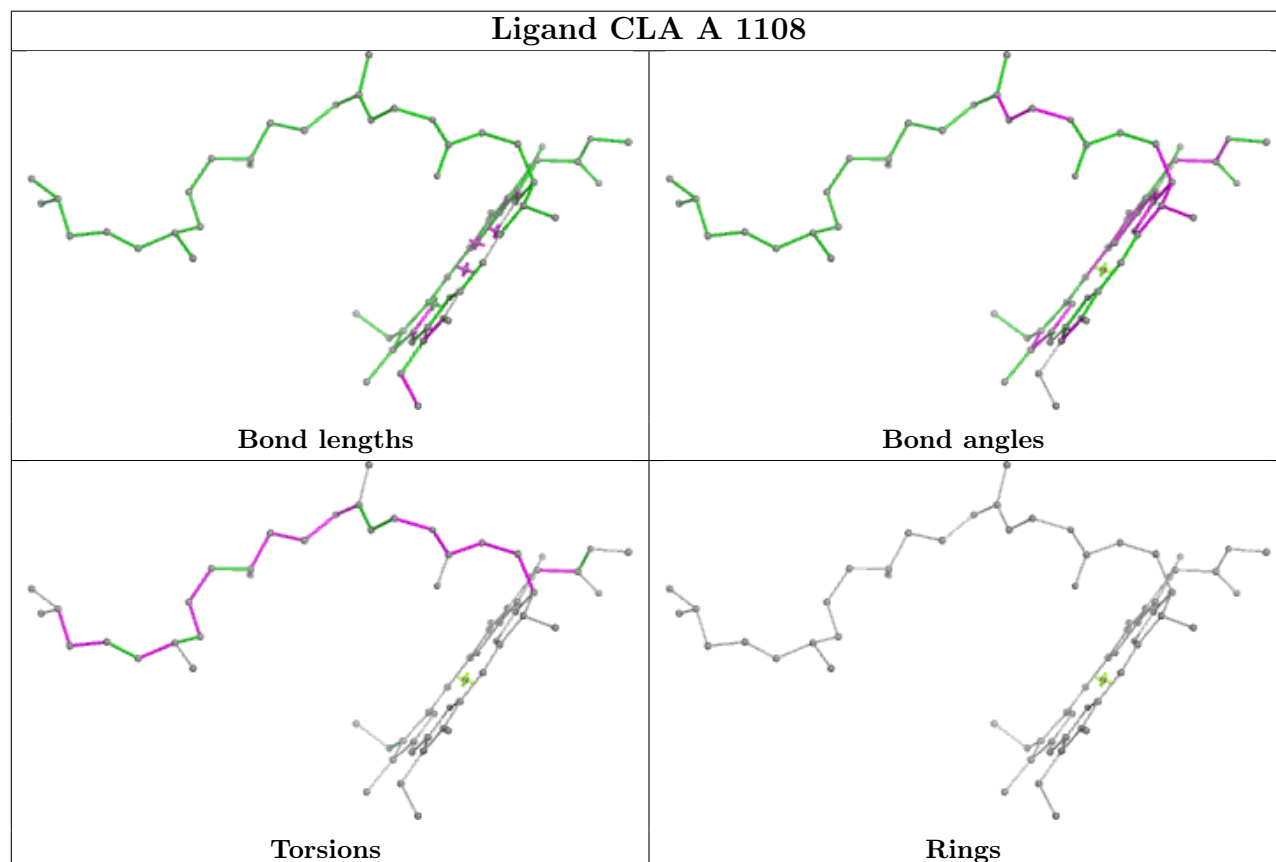
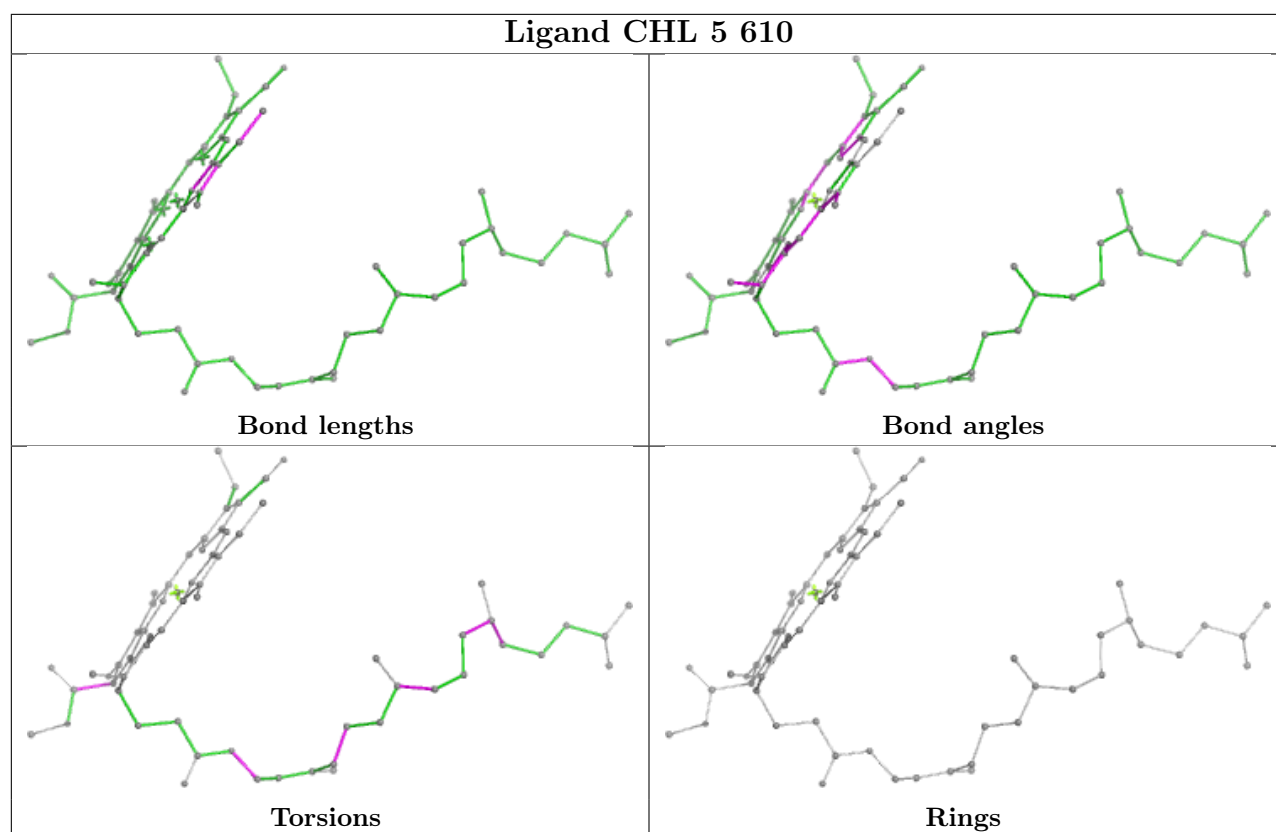


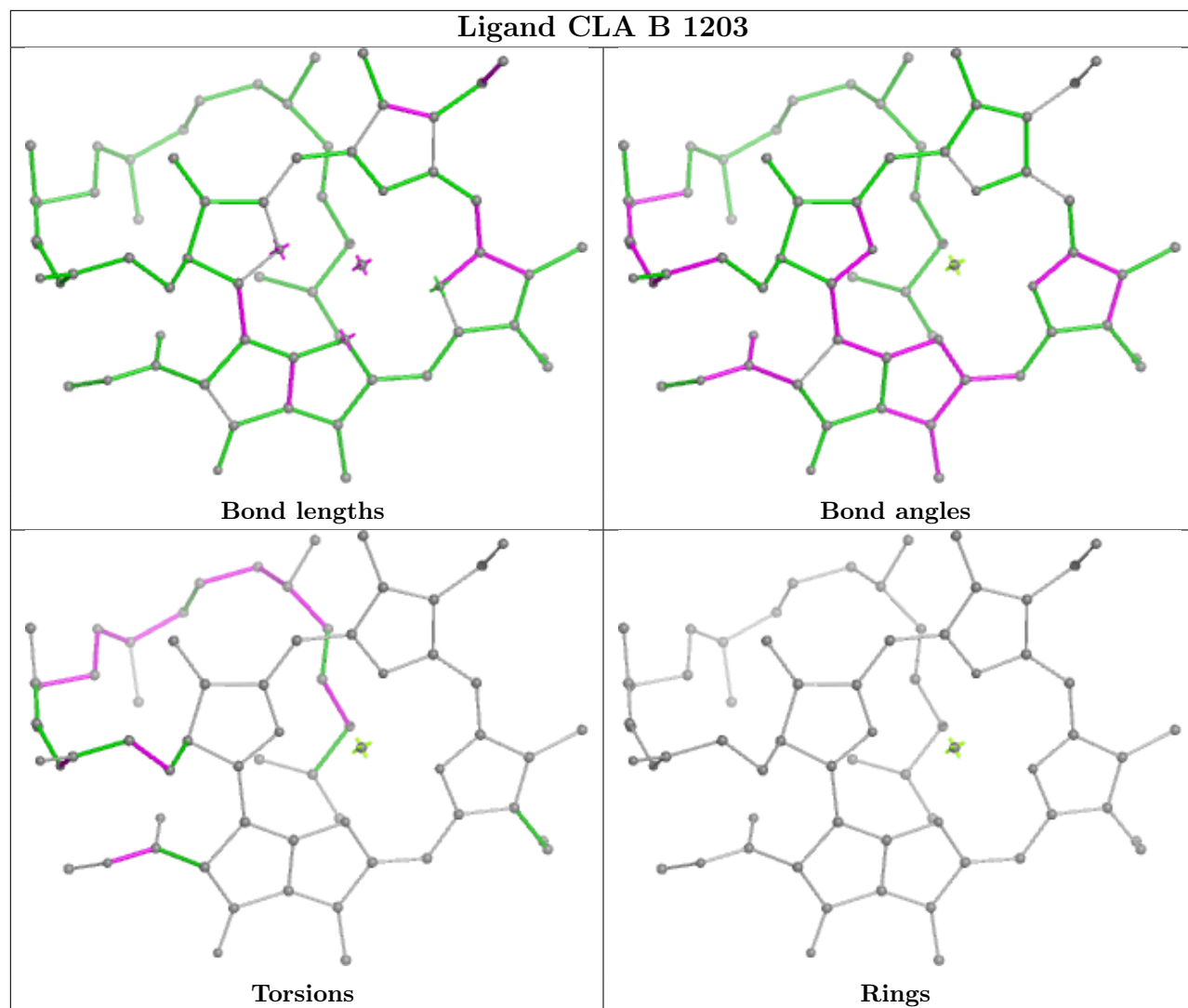
## Ligand CLA 4 603

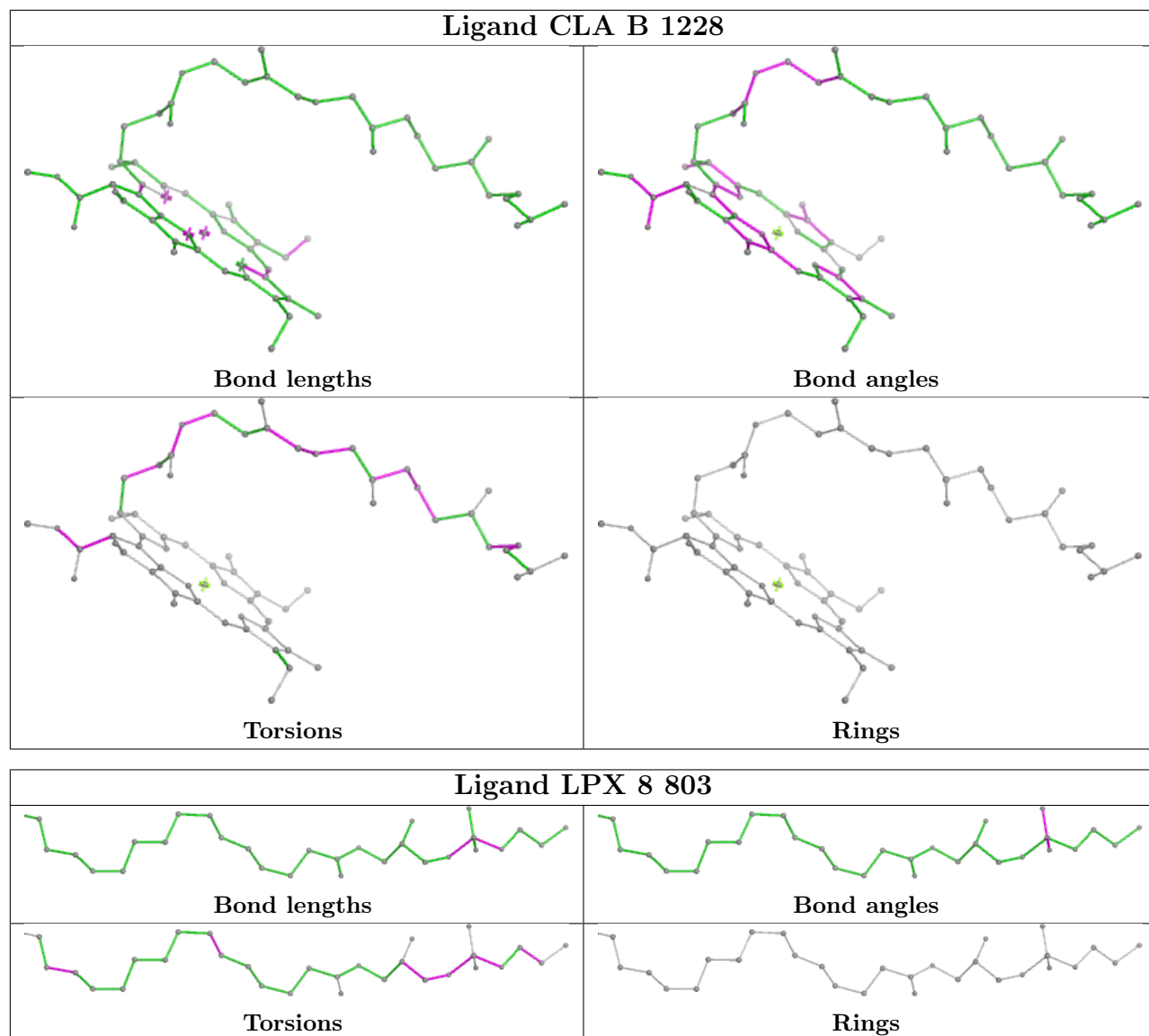


## Ligand LHG 4 801

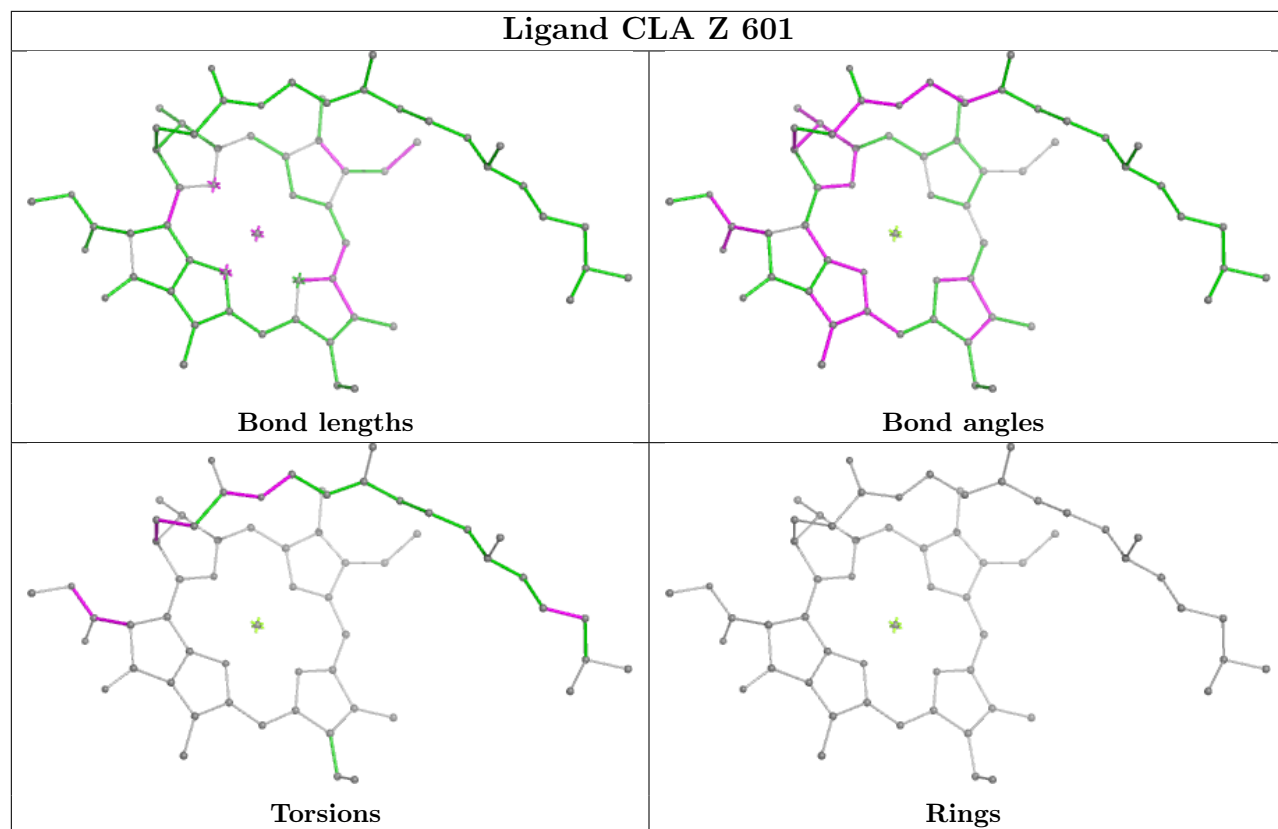




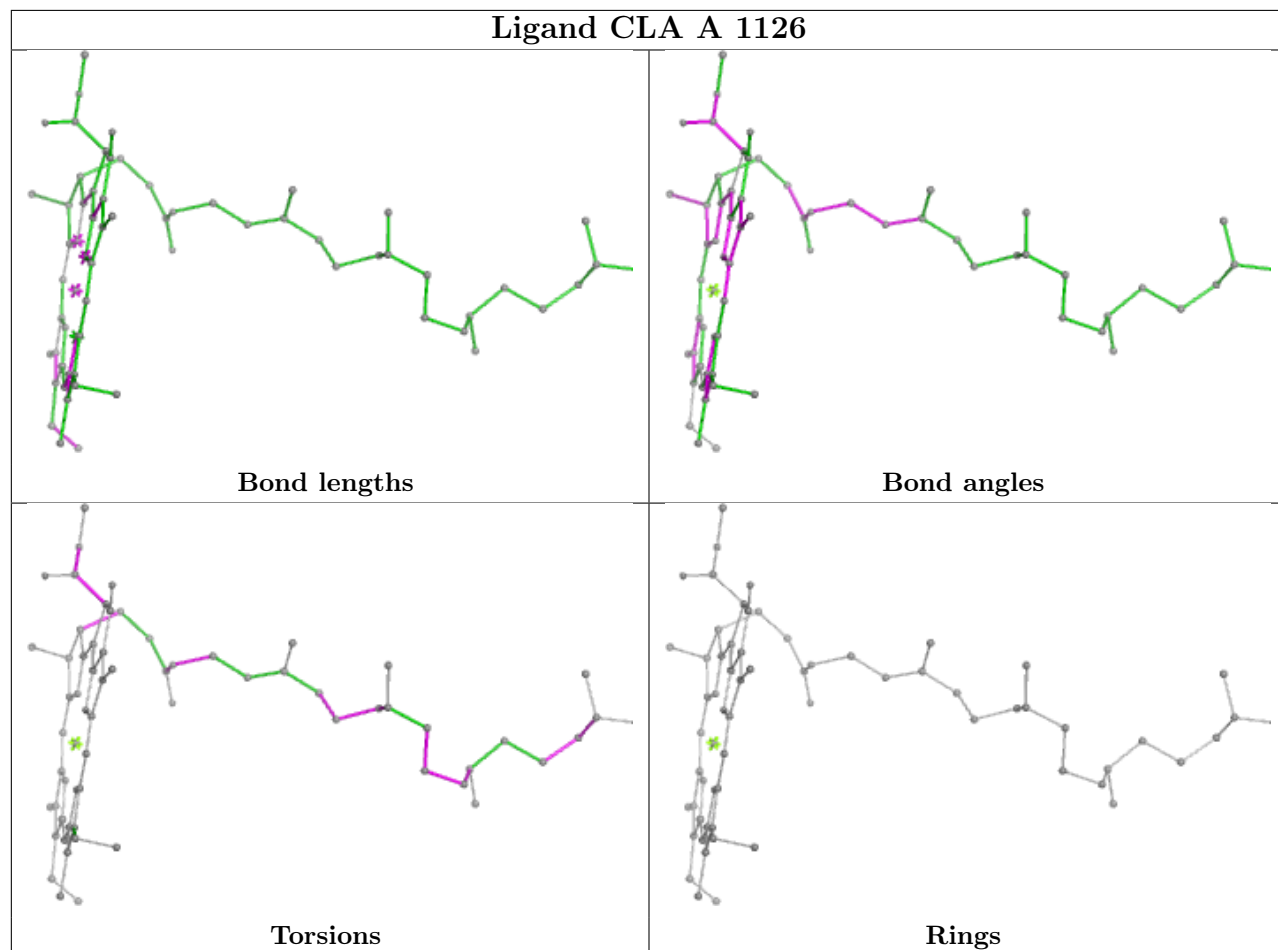


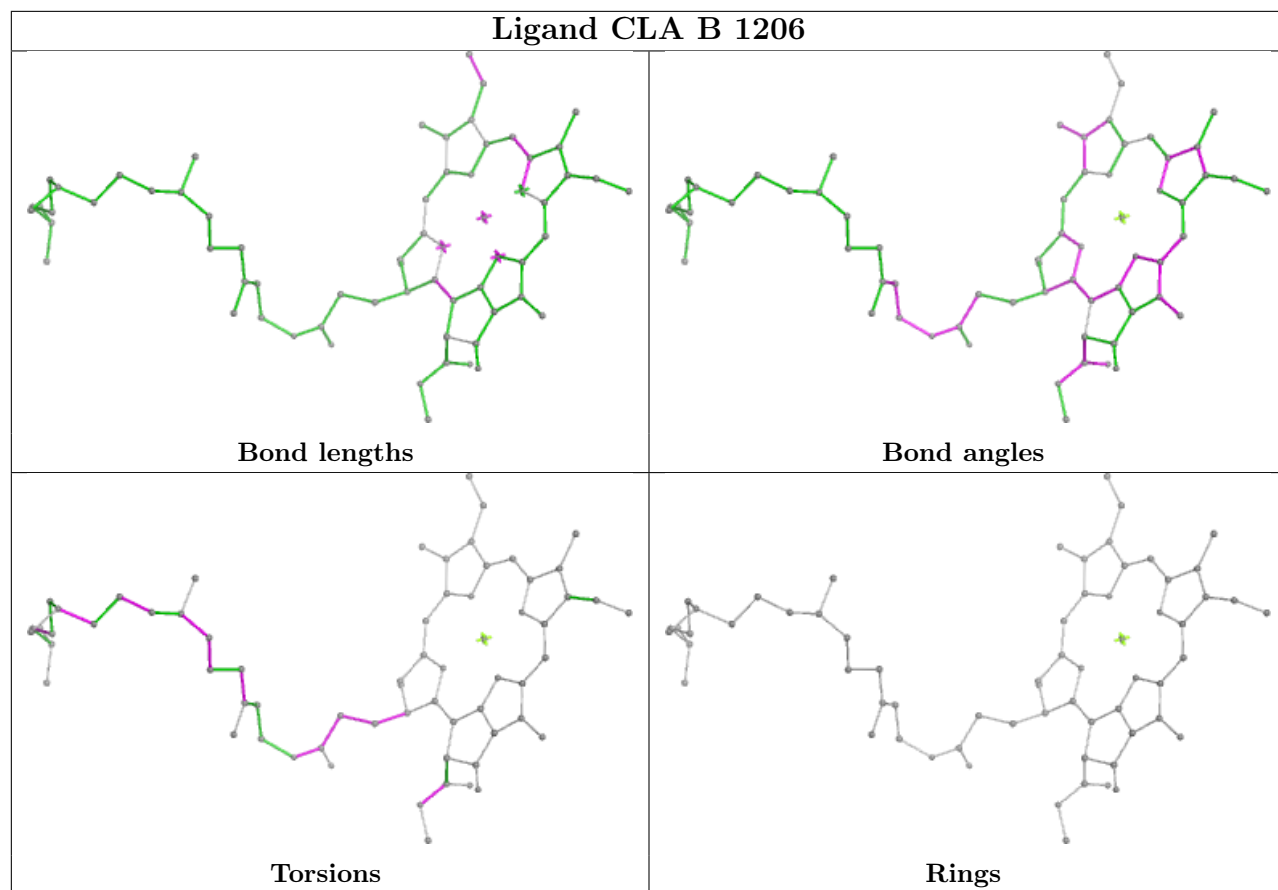


## Ligand CLA Z 601

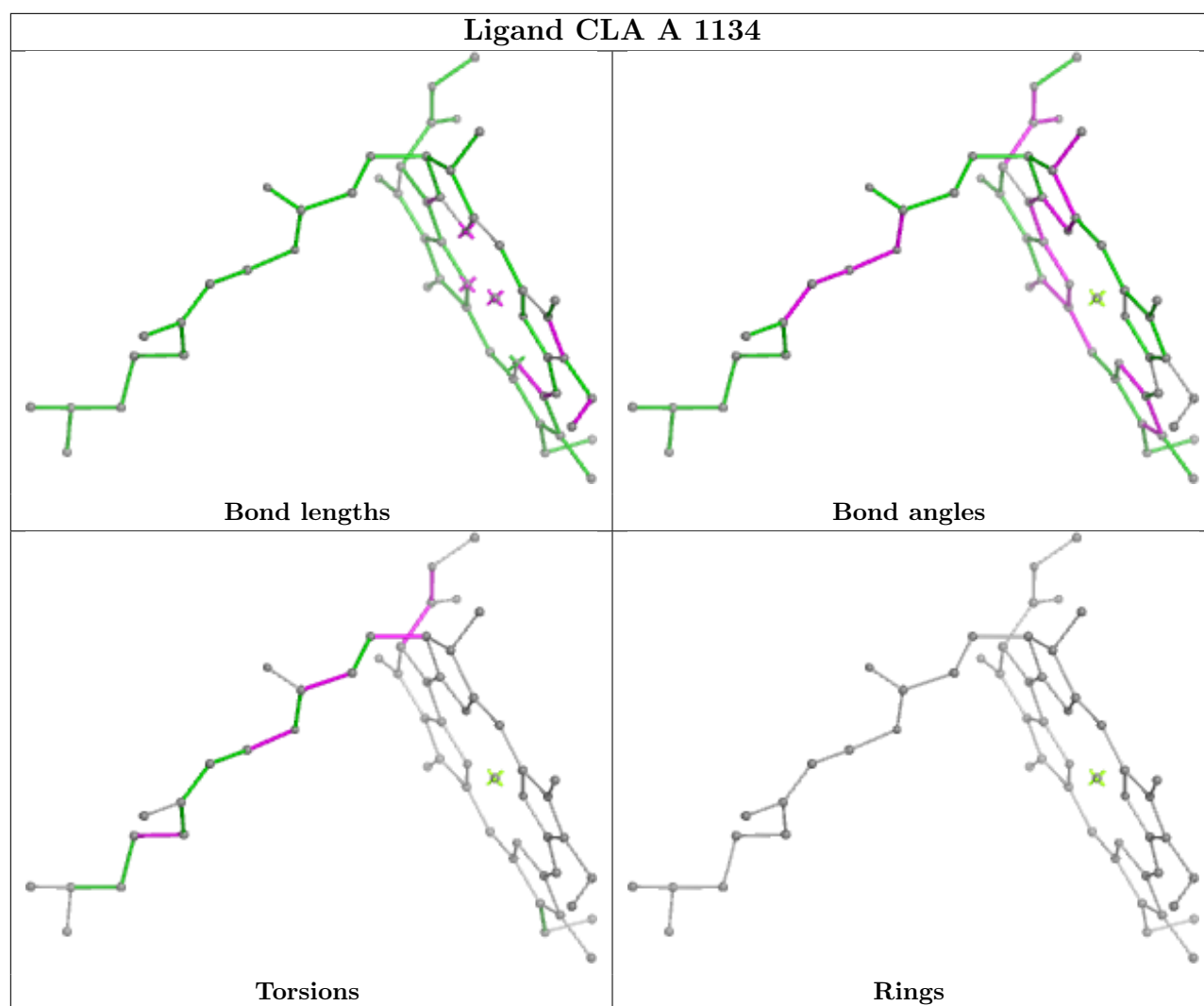


## Ligand CLA A 1126

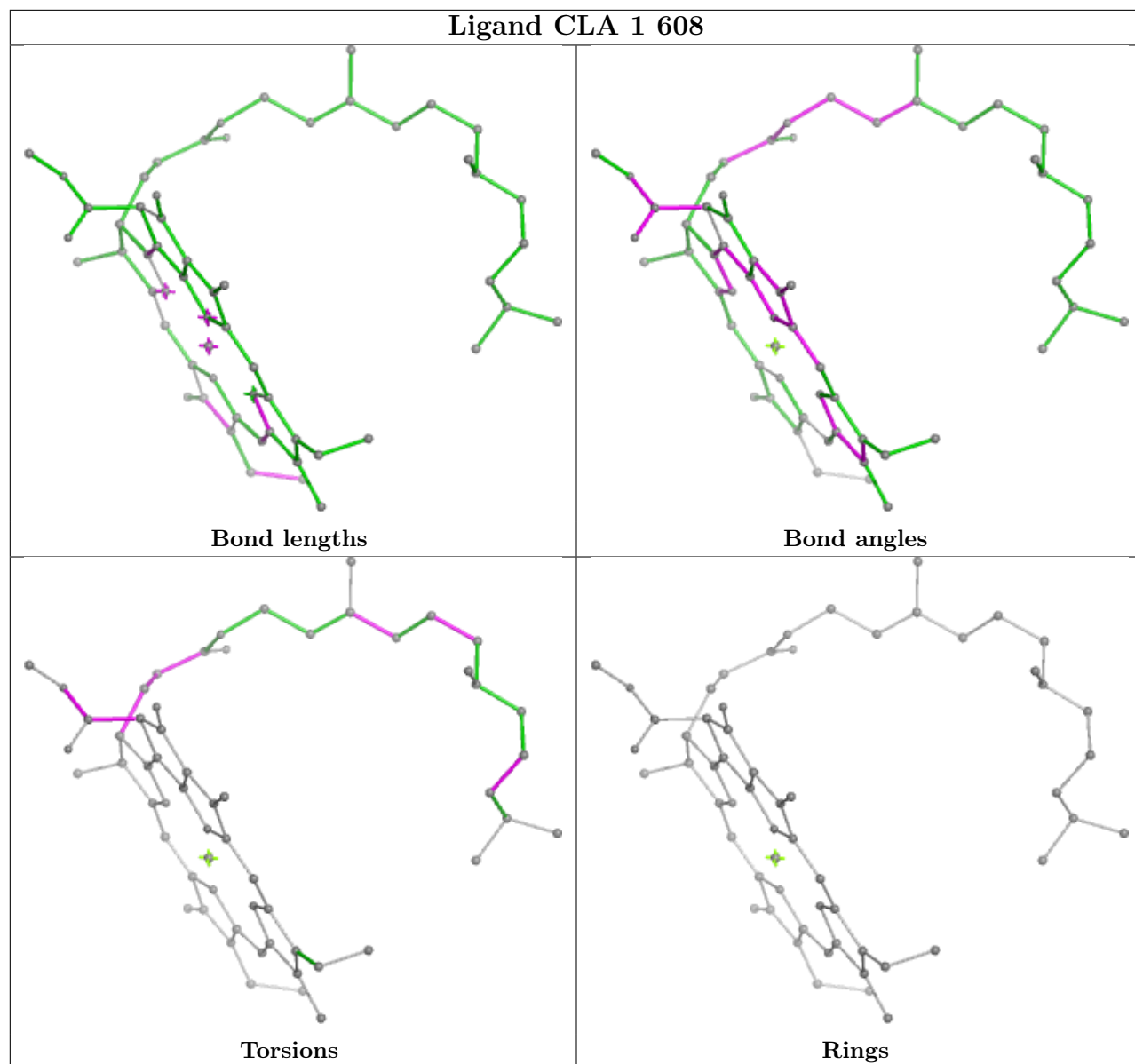


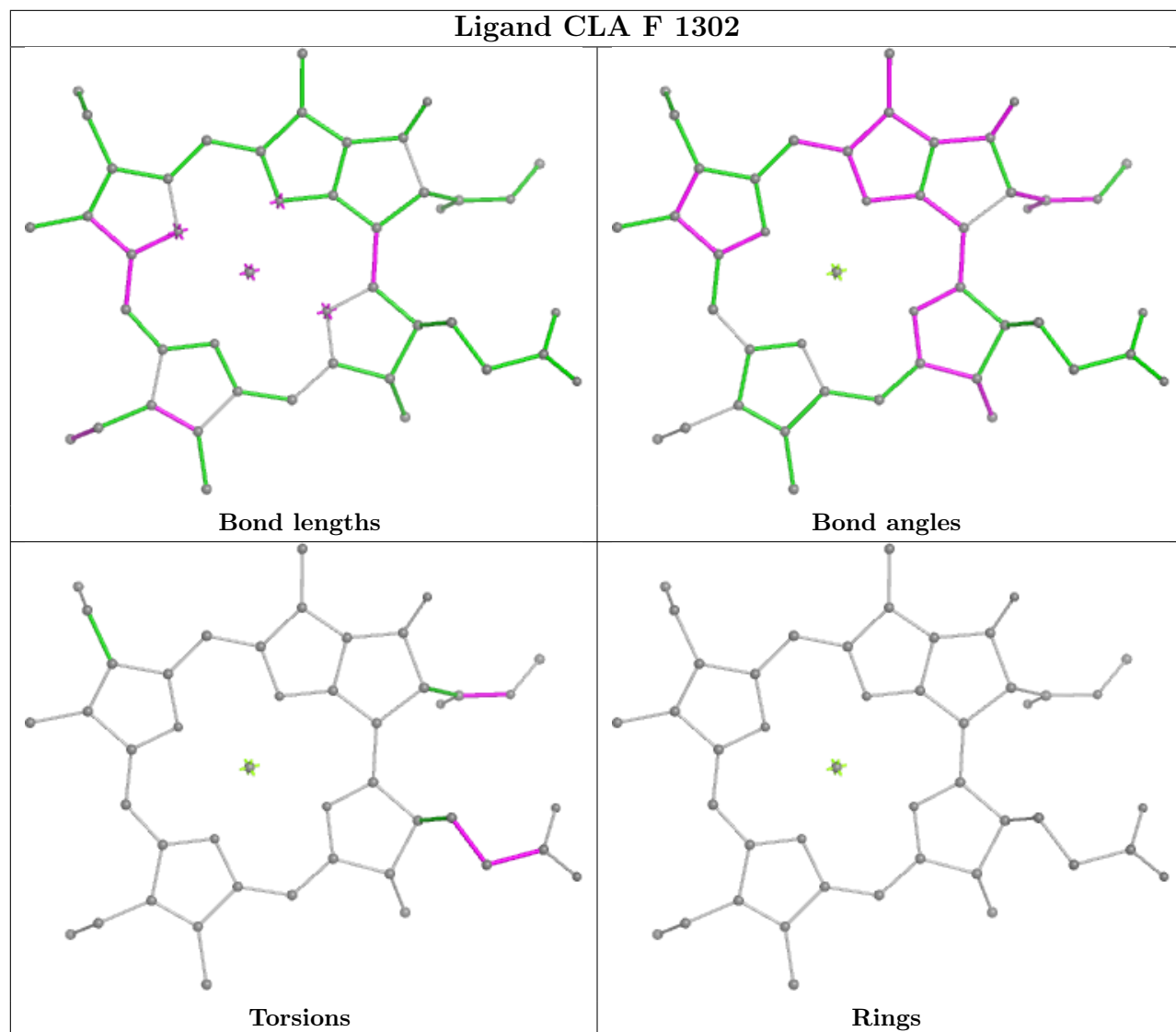


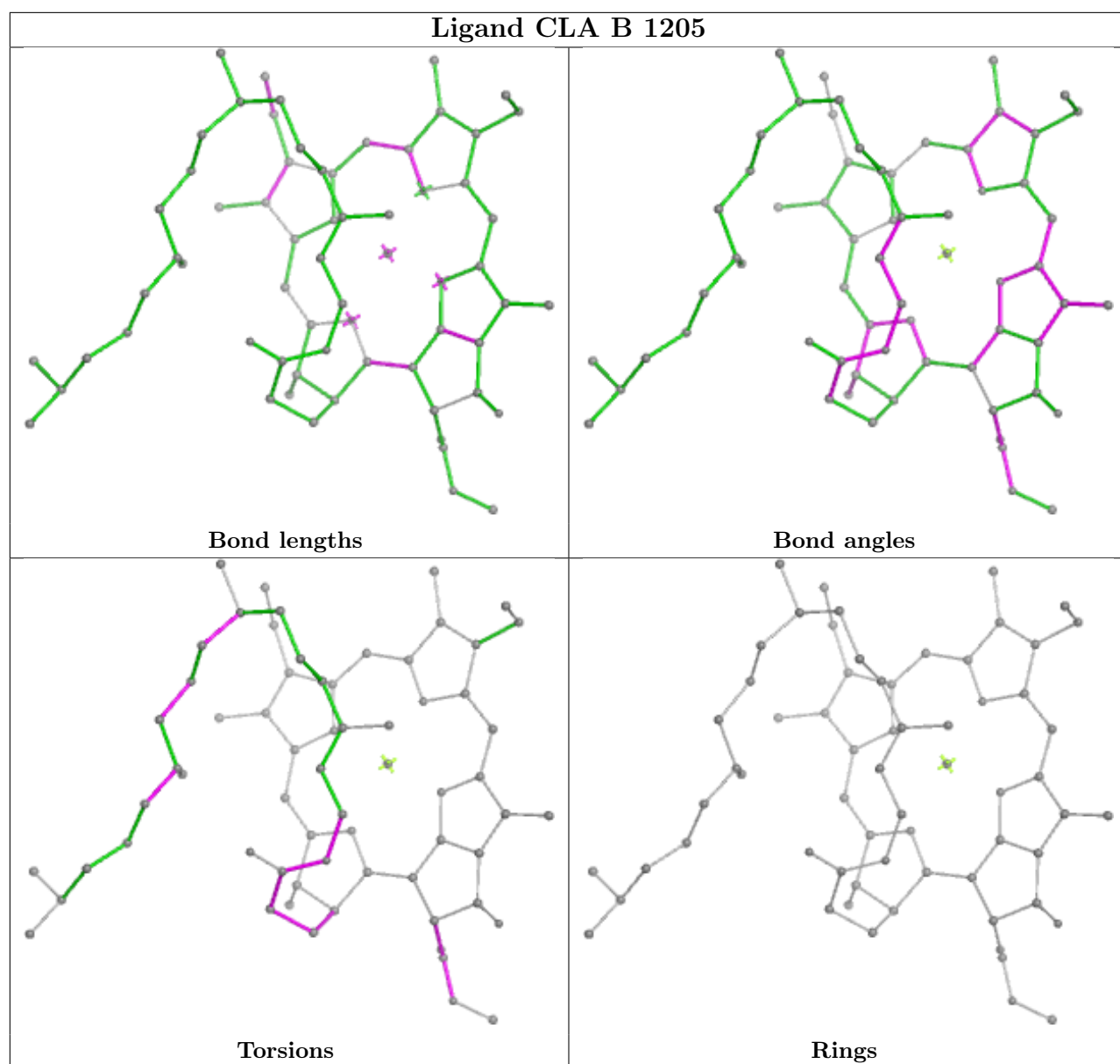




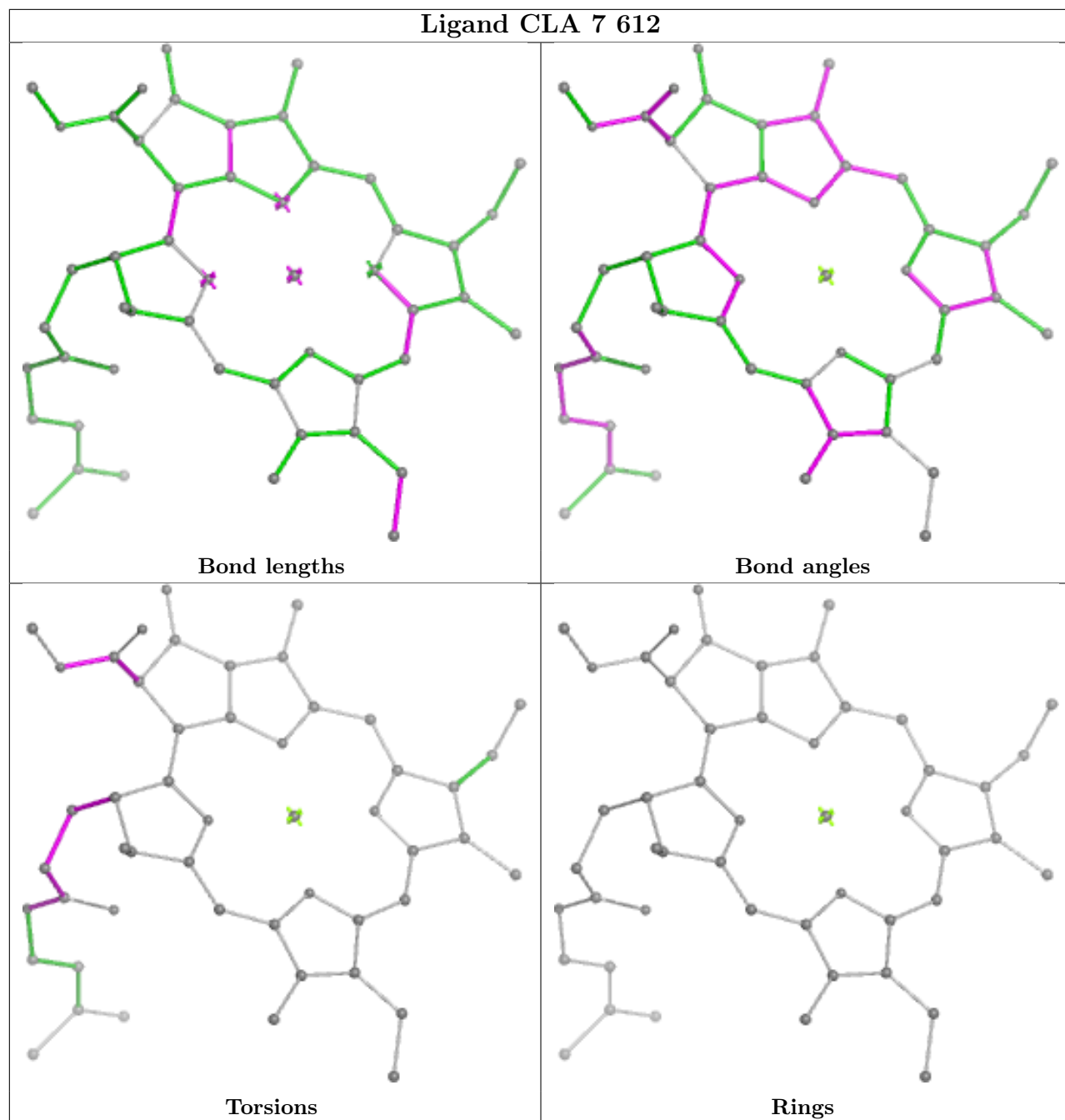
## Ligand CLA 1 608



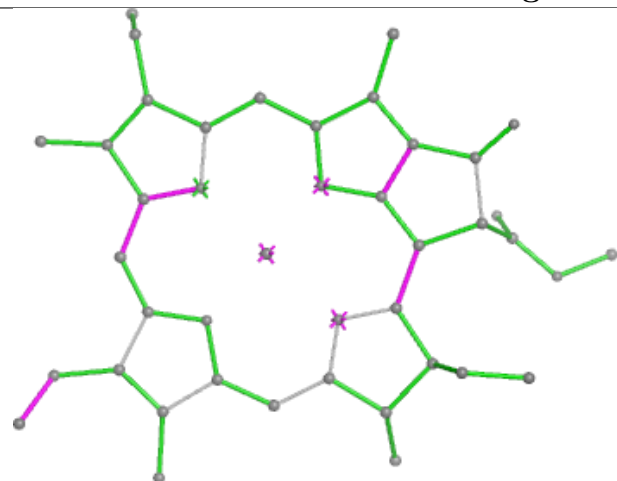




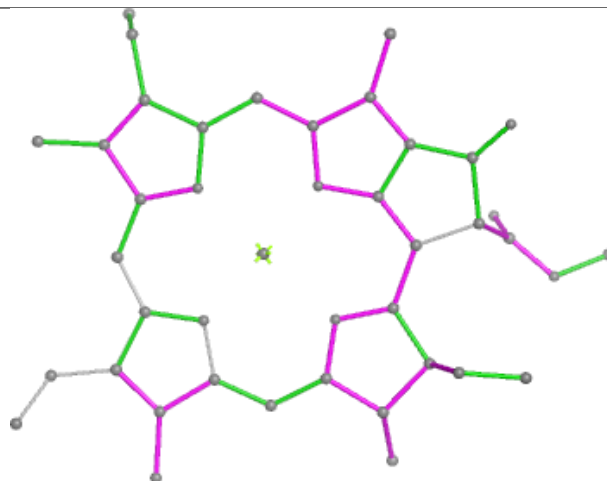
## Ligand CLA 7 612



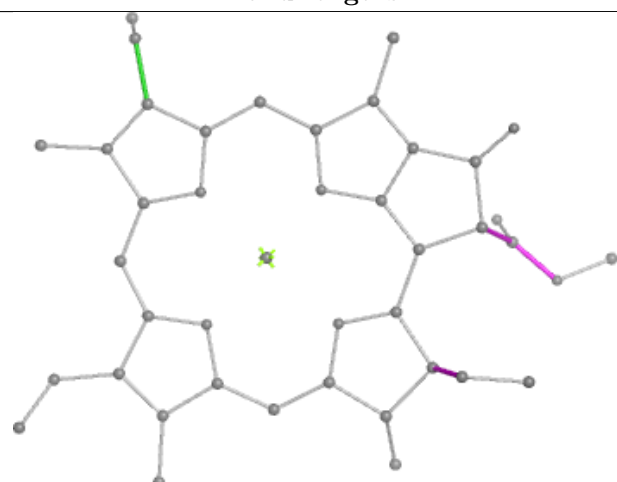
## Ligand CLA 7 613



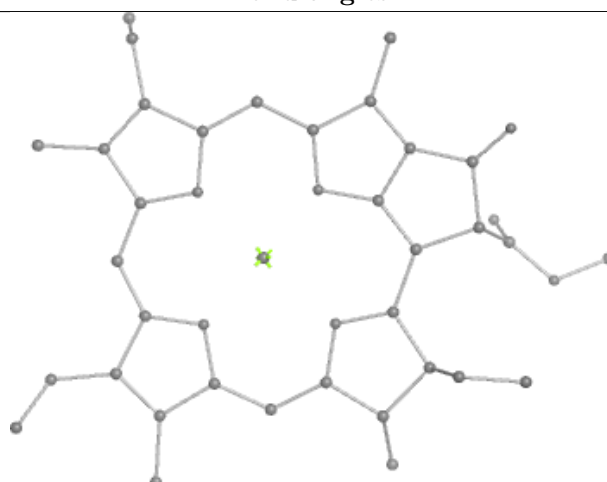
Bond lengths



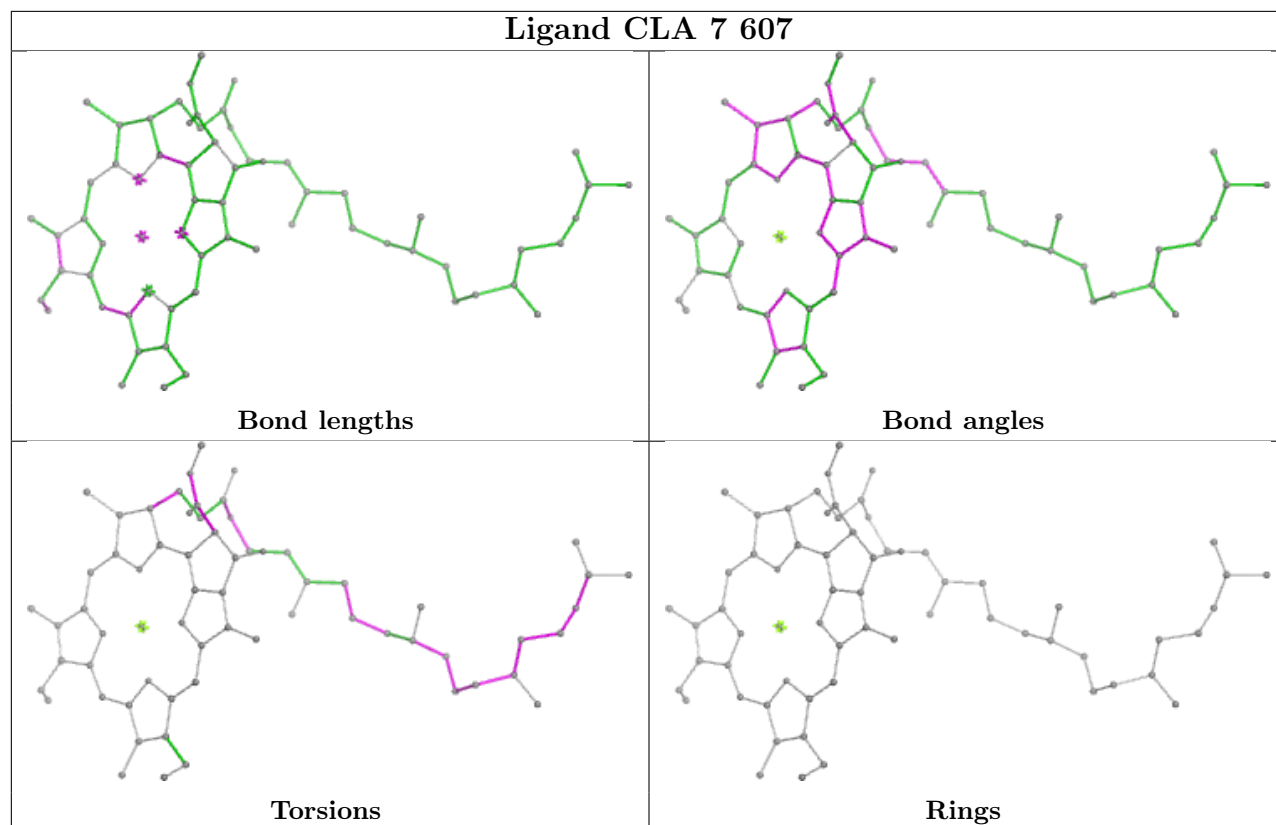
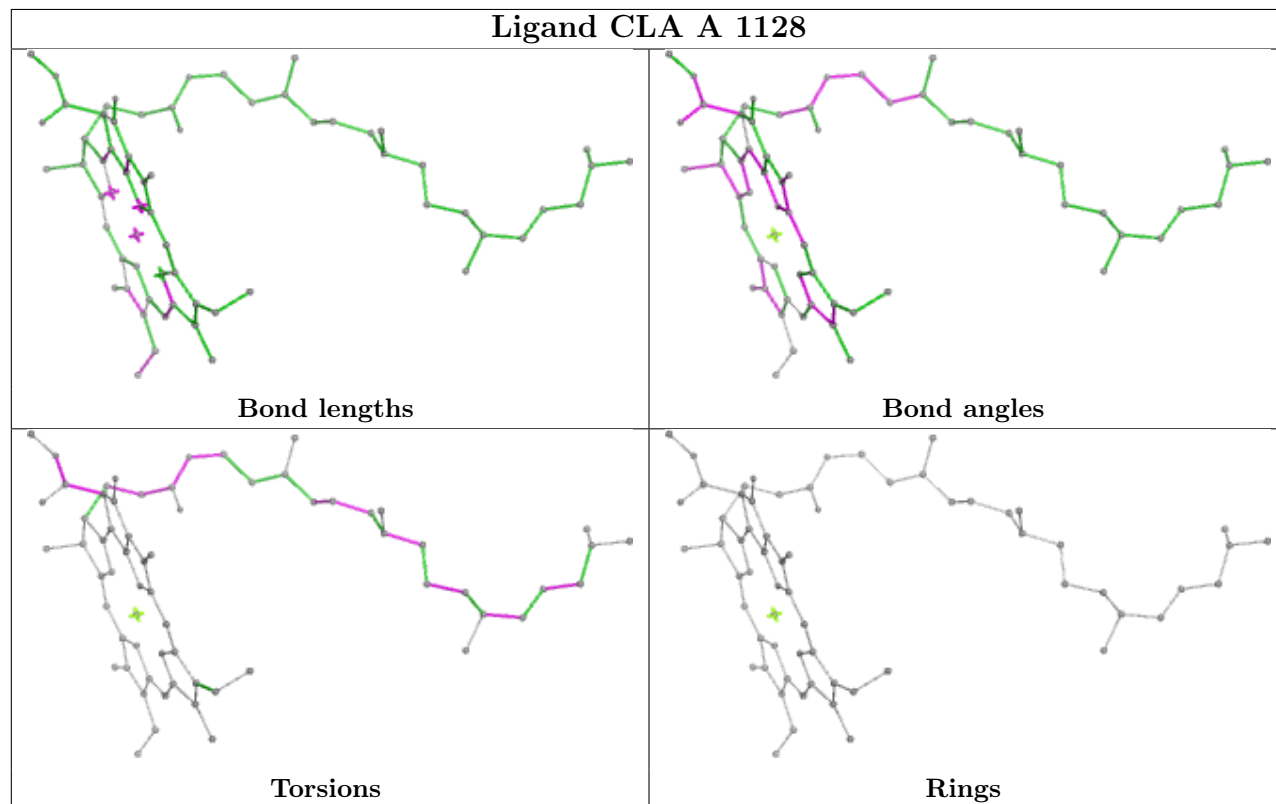
Bond angles

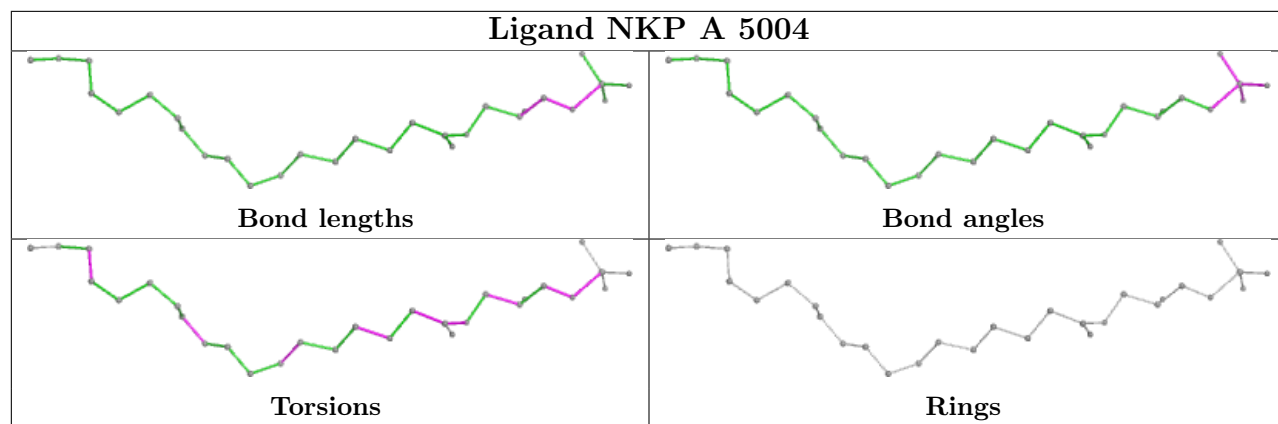


Torsions



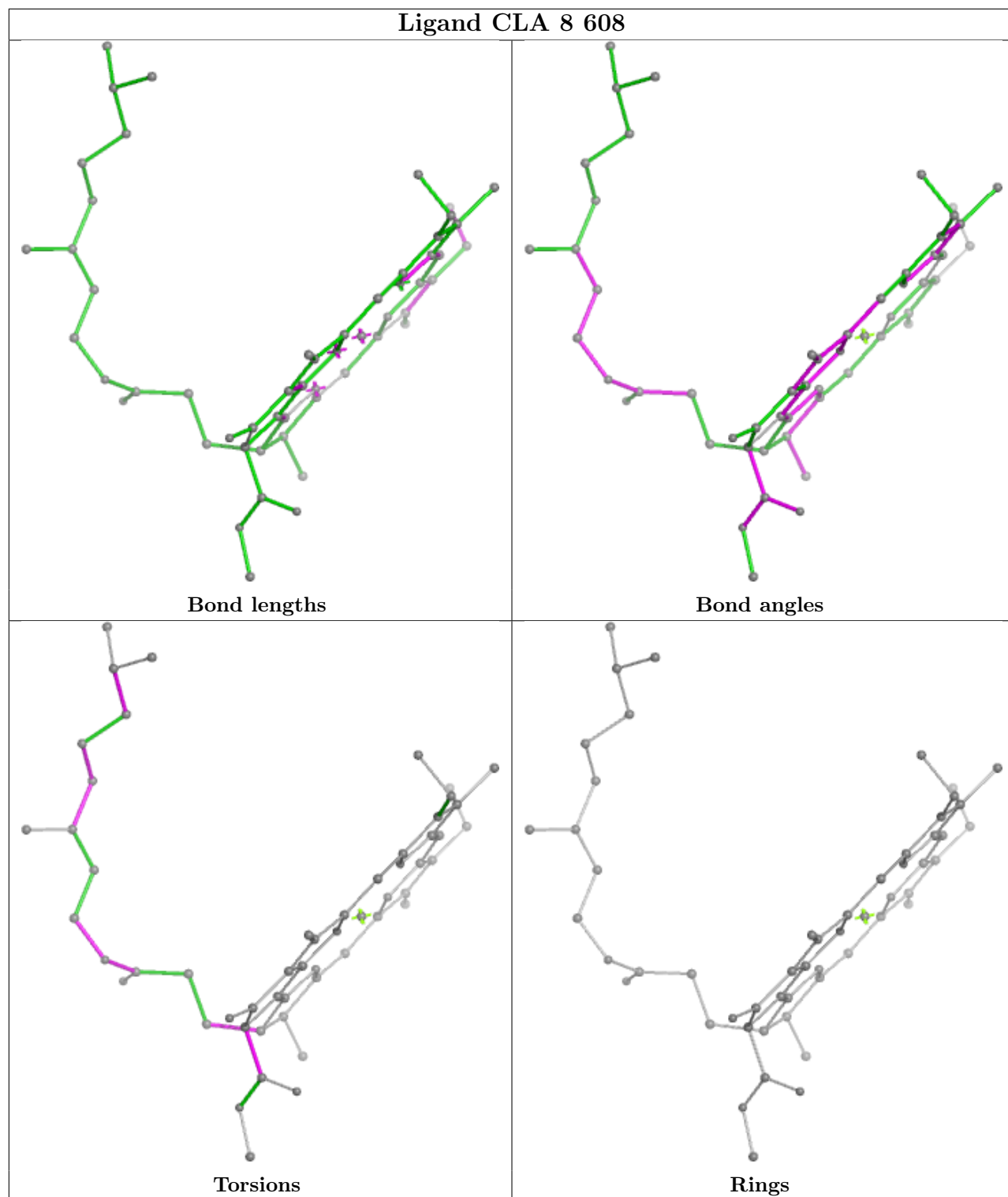
Rings

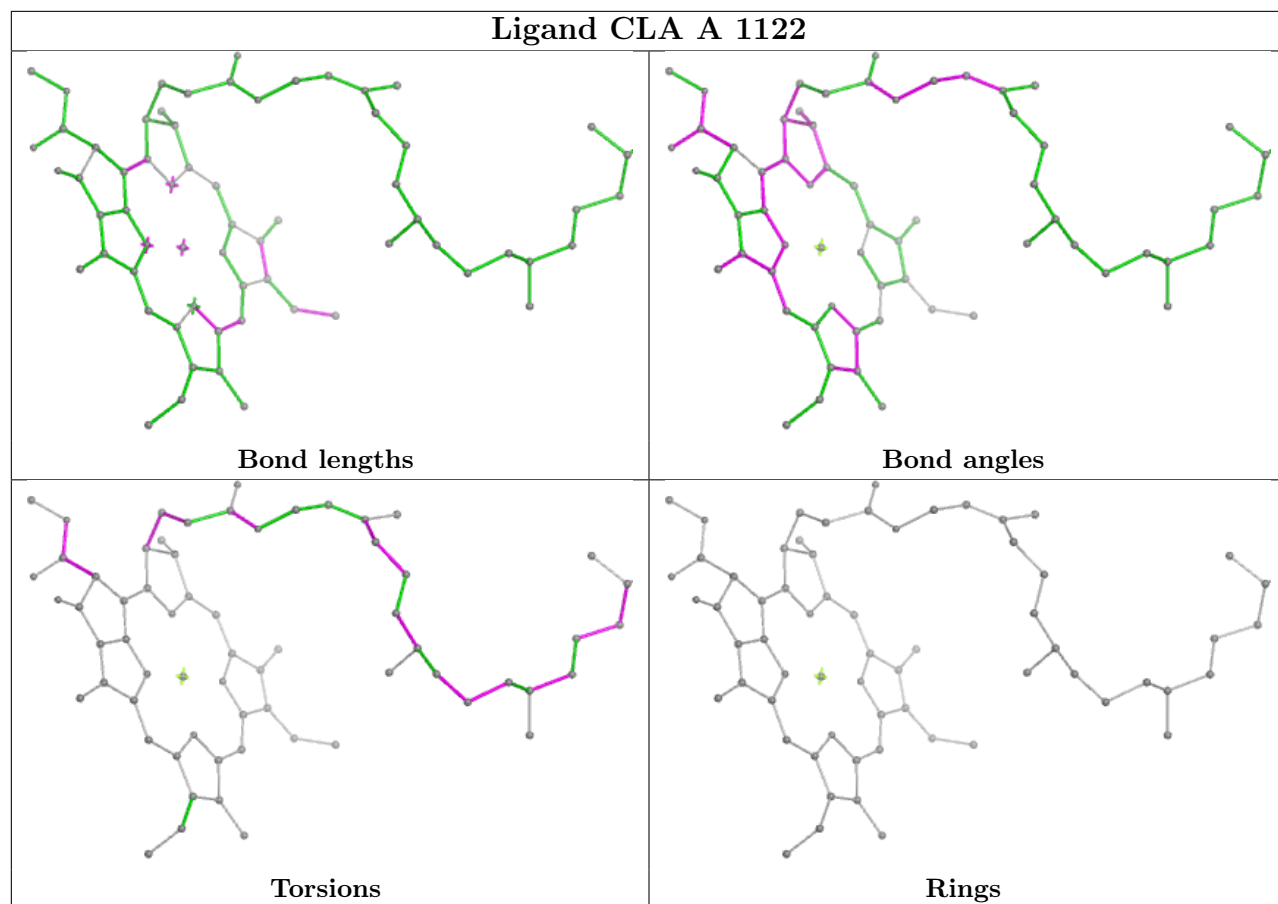
**Ligand CLA 7 607****Ligand CLA A 1128**



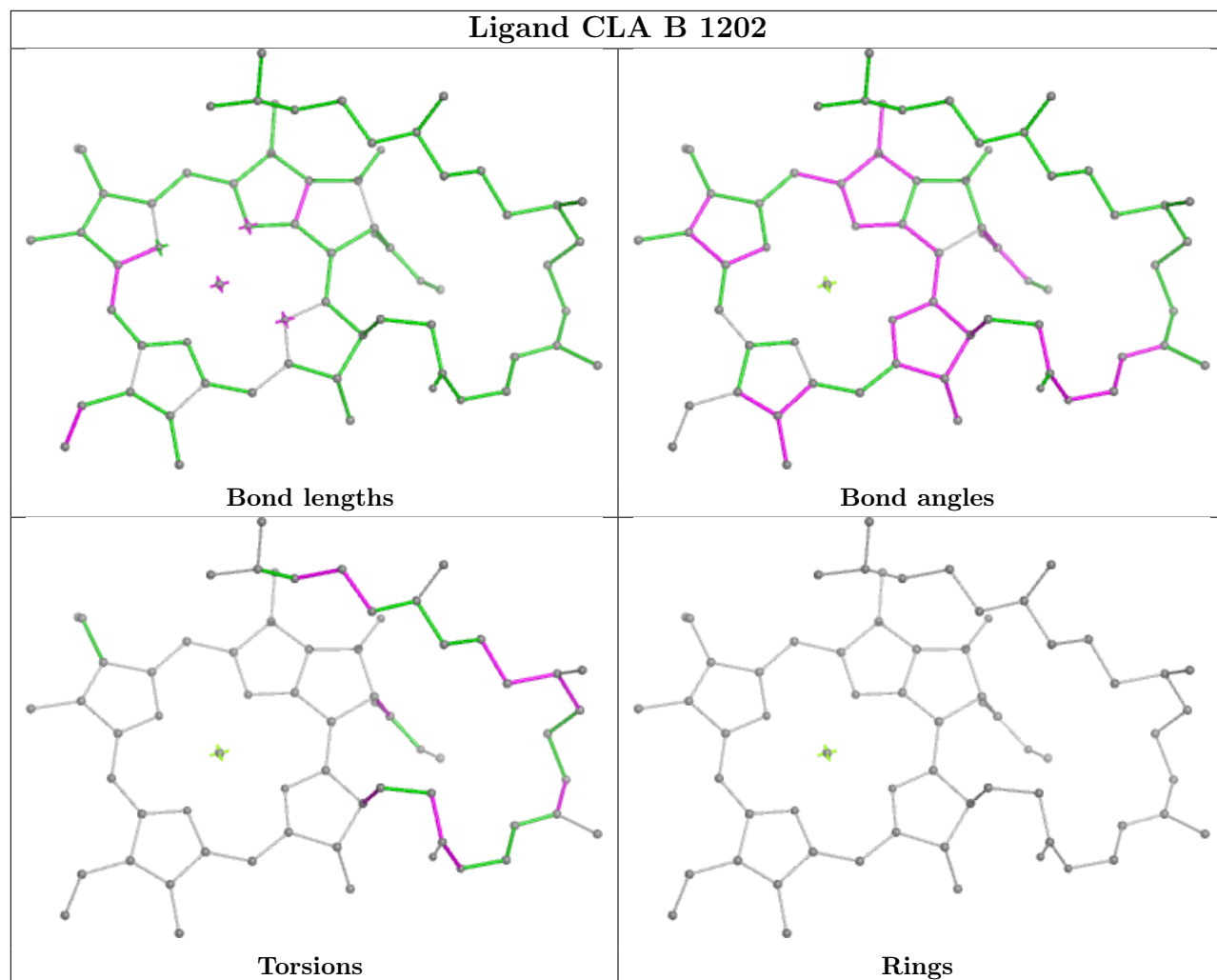


## Ligand CLA 8 608

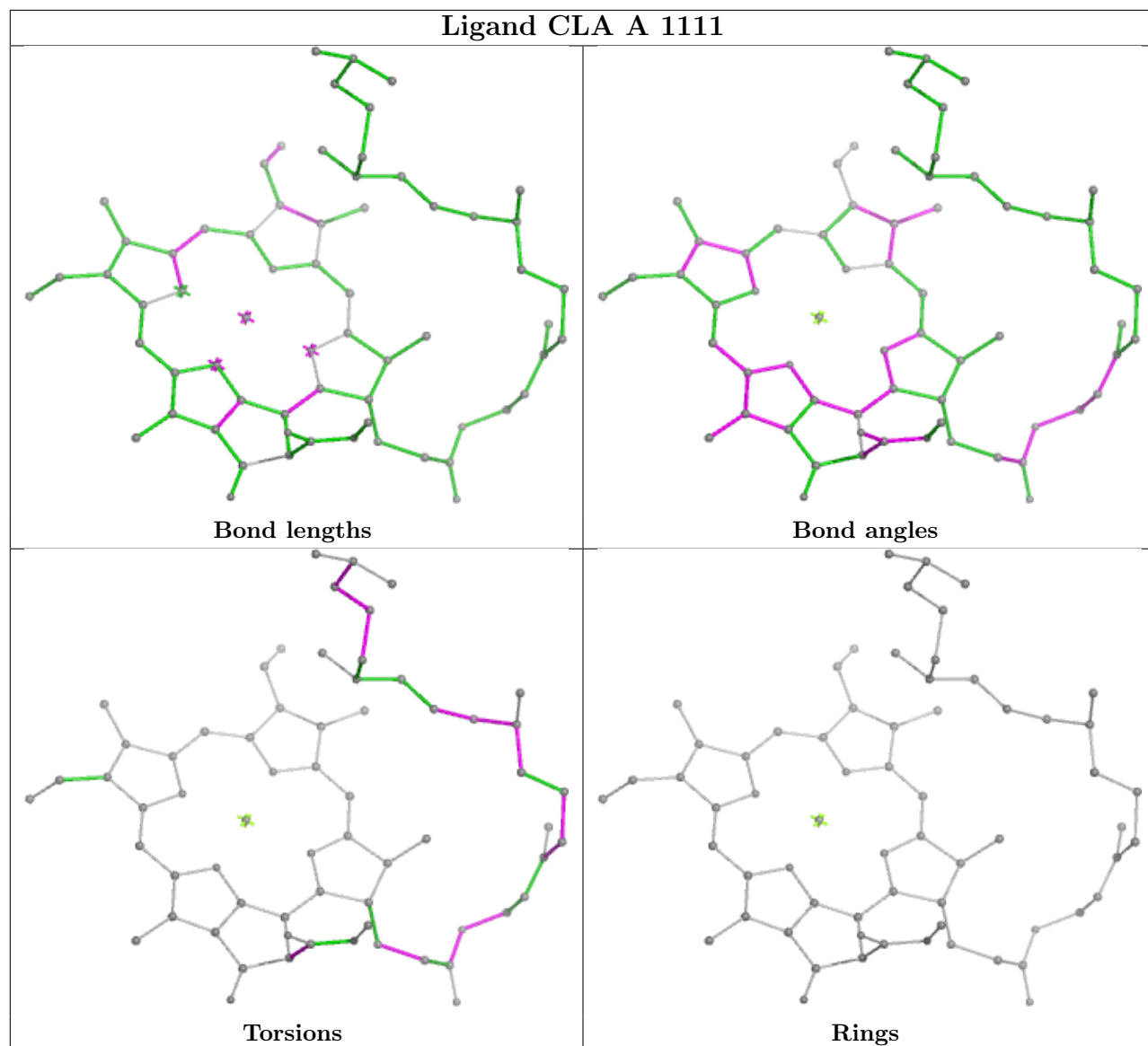




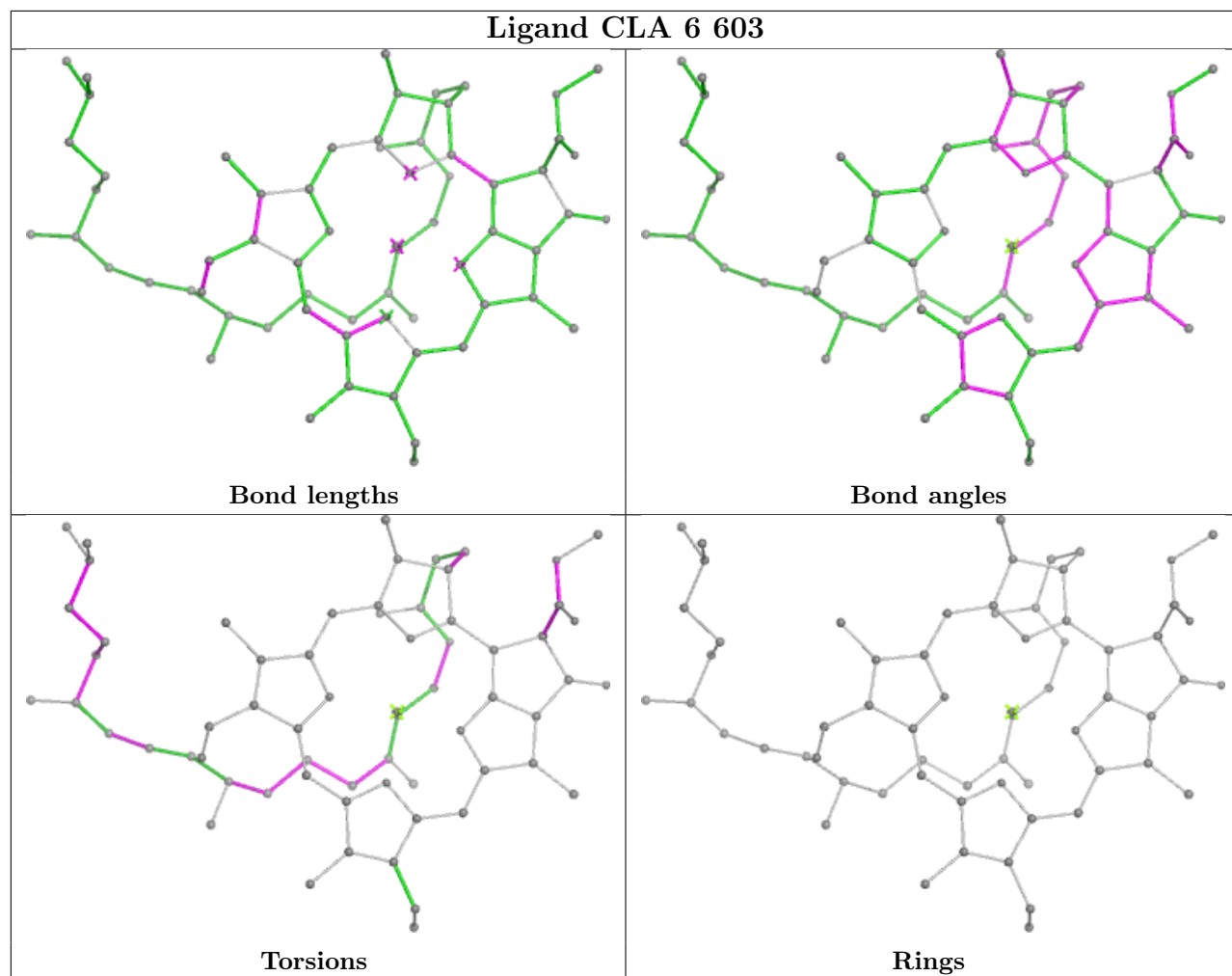
## Ligand CLA B 1202

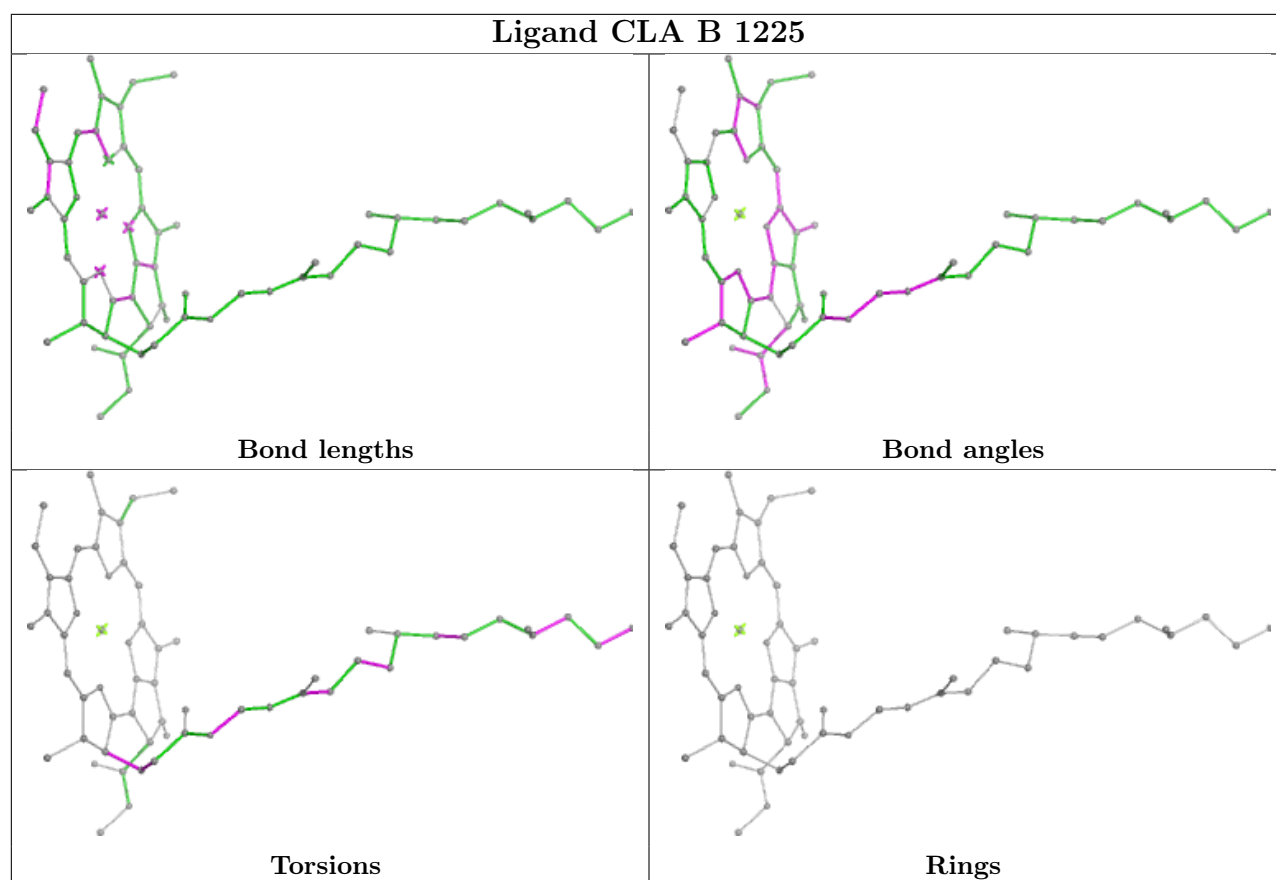


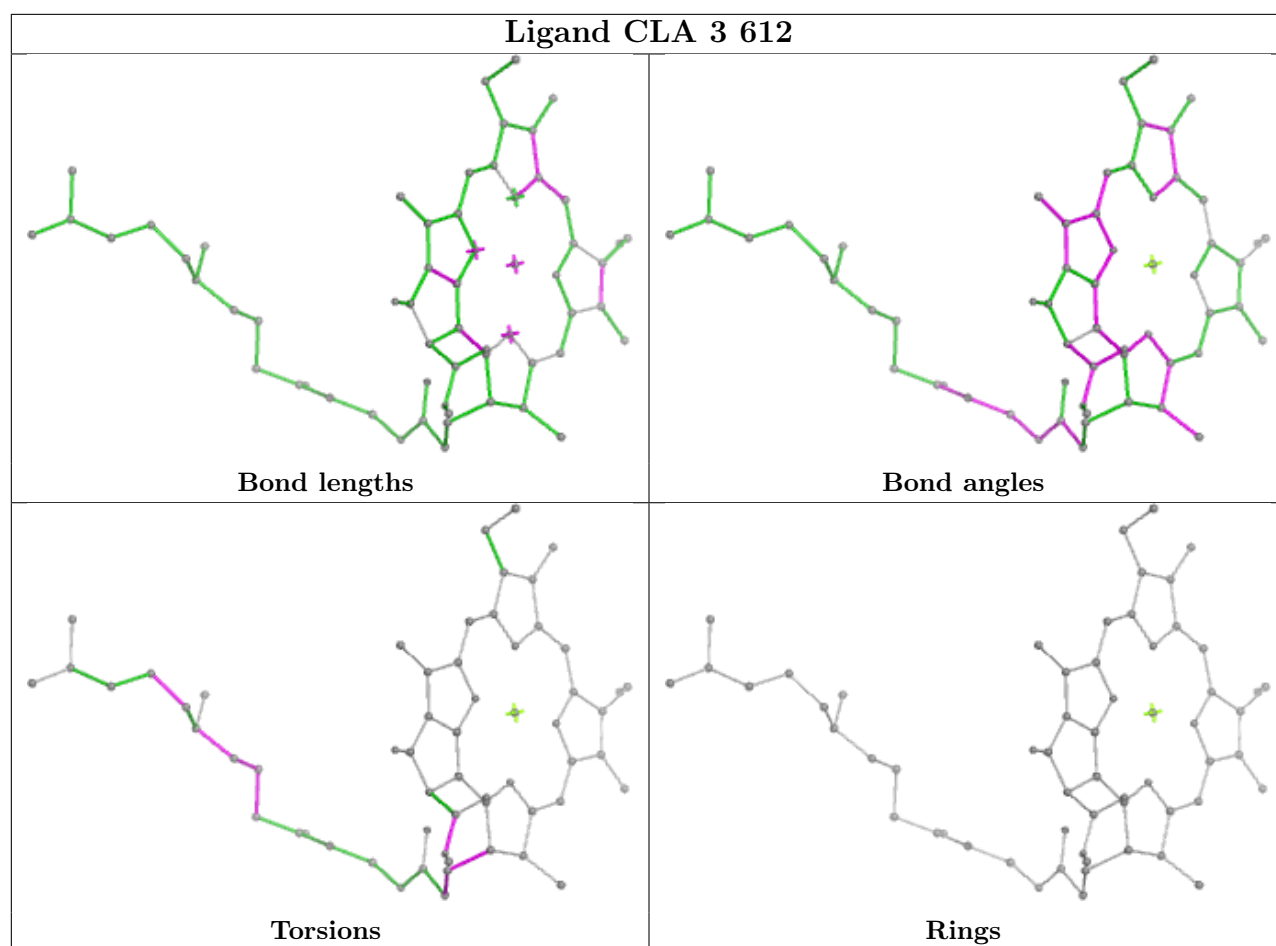
## Ligand CLA A 1111



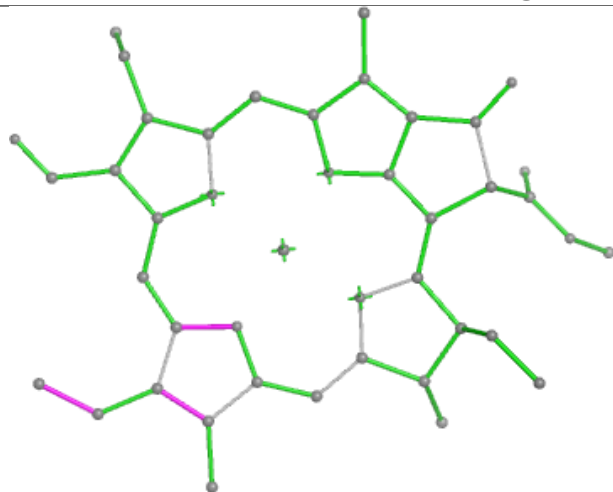
## Ligand CLA 6 603



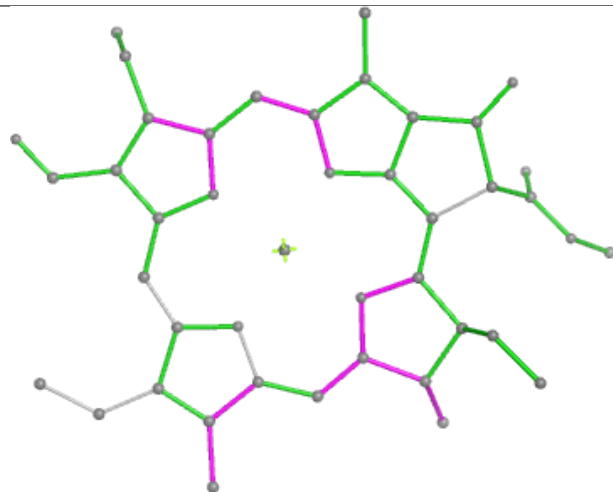




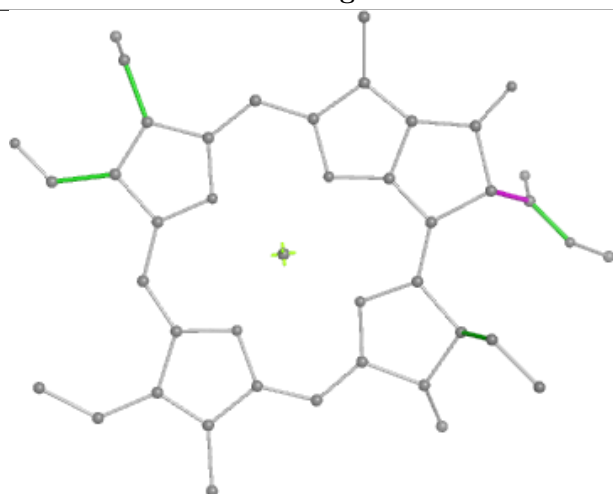
## Ligand CHL 6 617



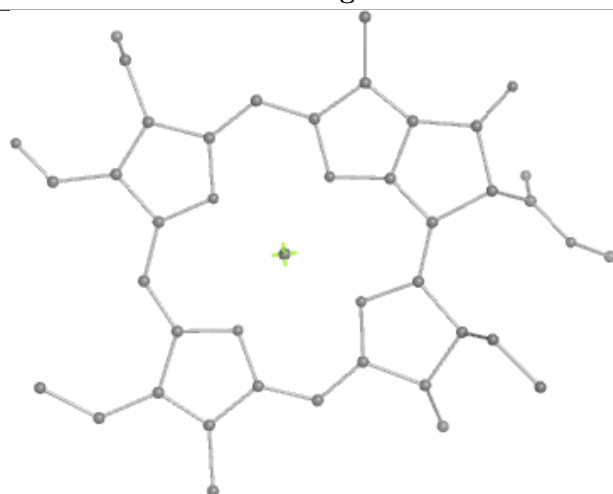
Bond lengths



Bond angles



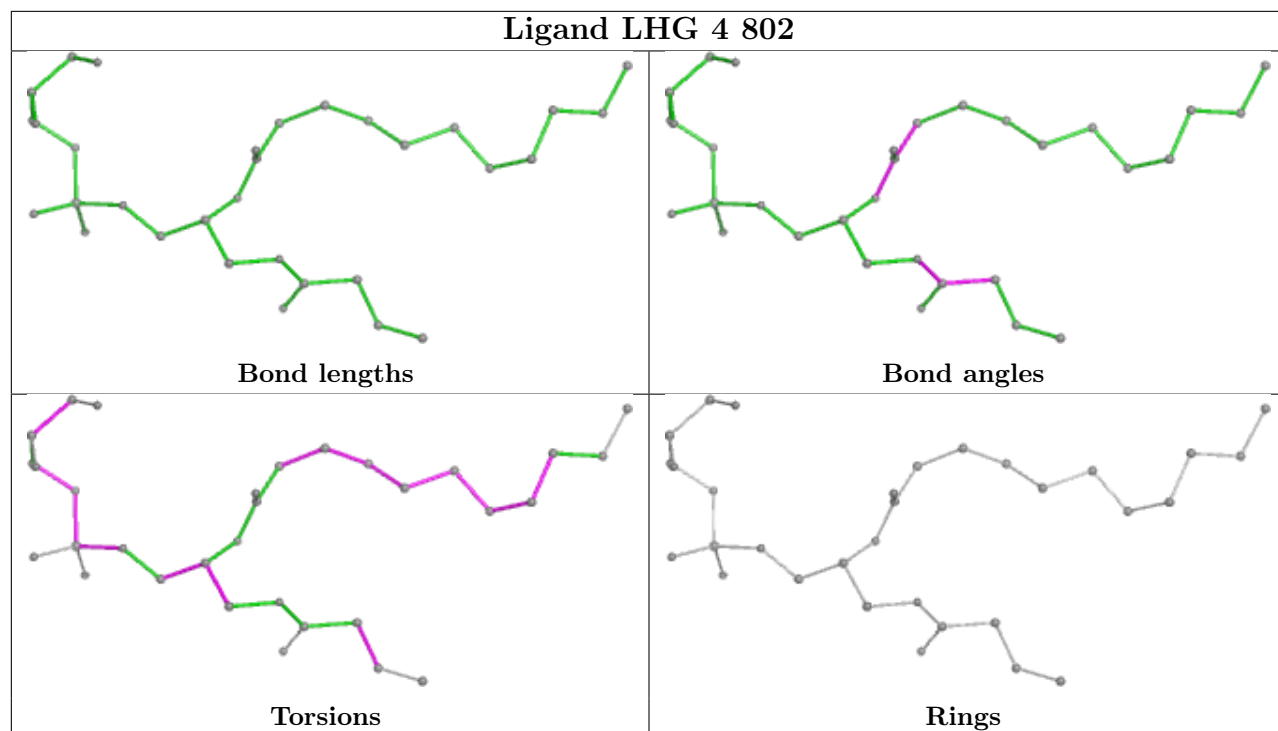
Torsions



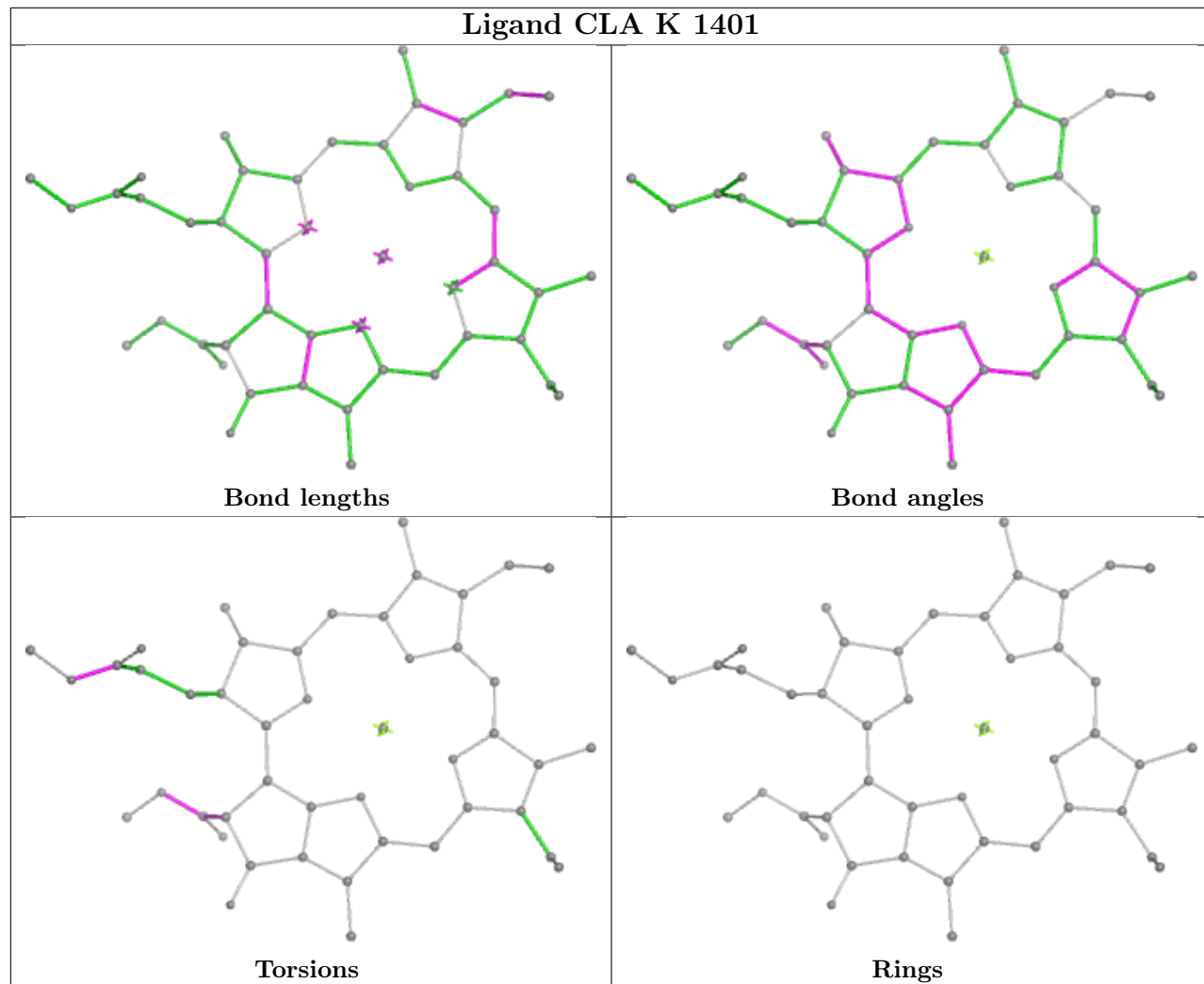
Rings



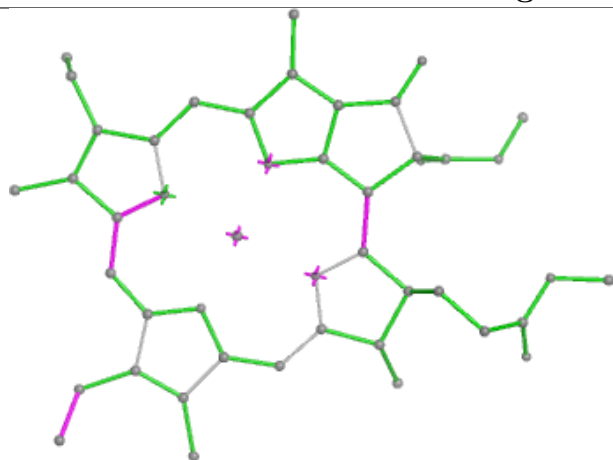
## Ligand LHG 4 802



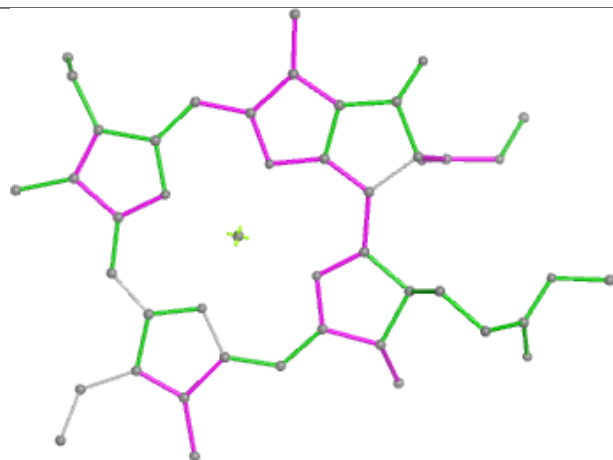
## Ligand CLA K 1401



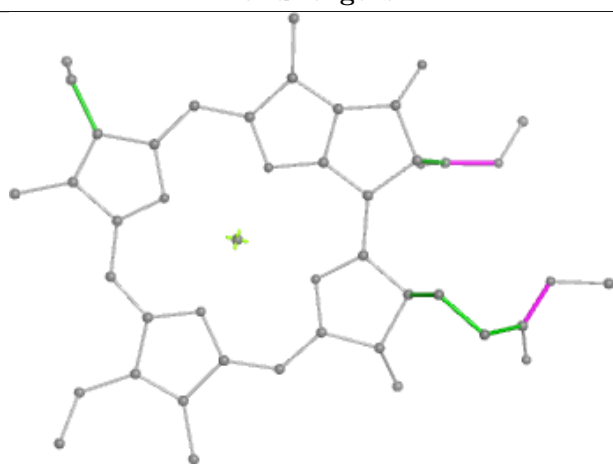
## Ligand CLA Z 602



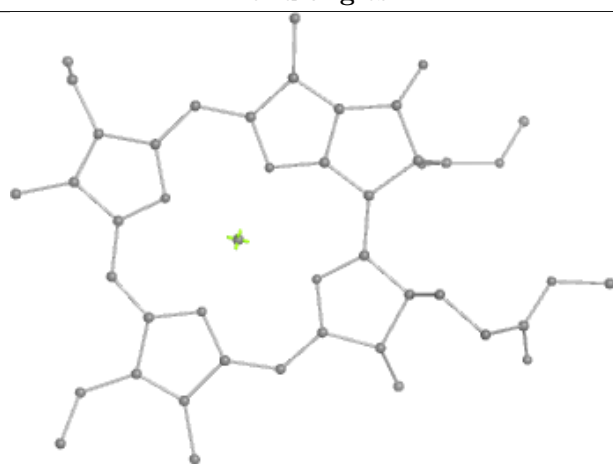
Bond lengths



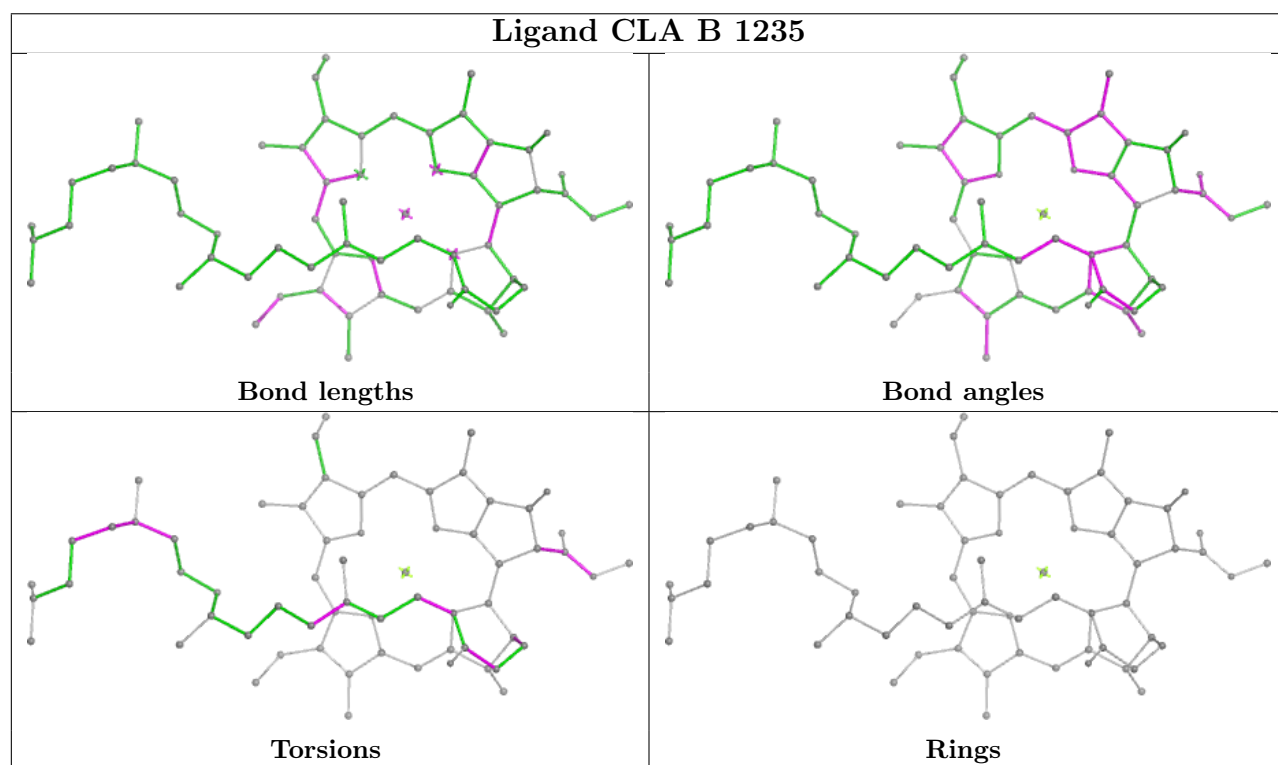
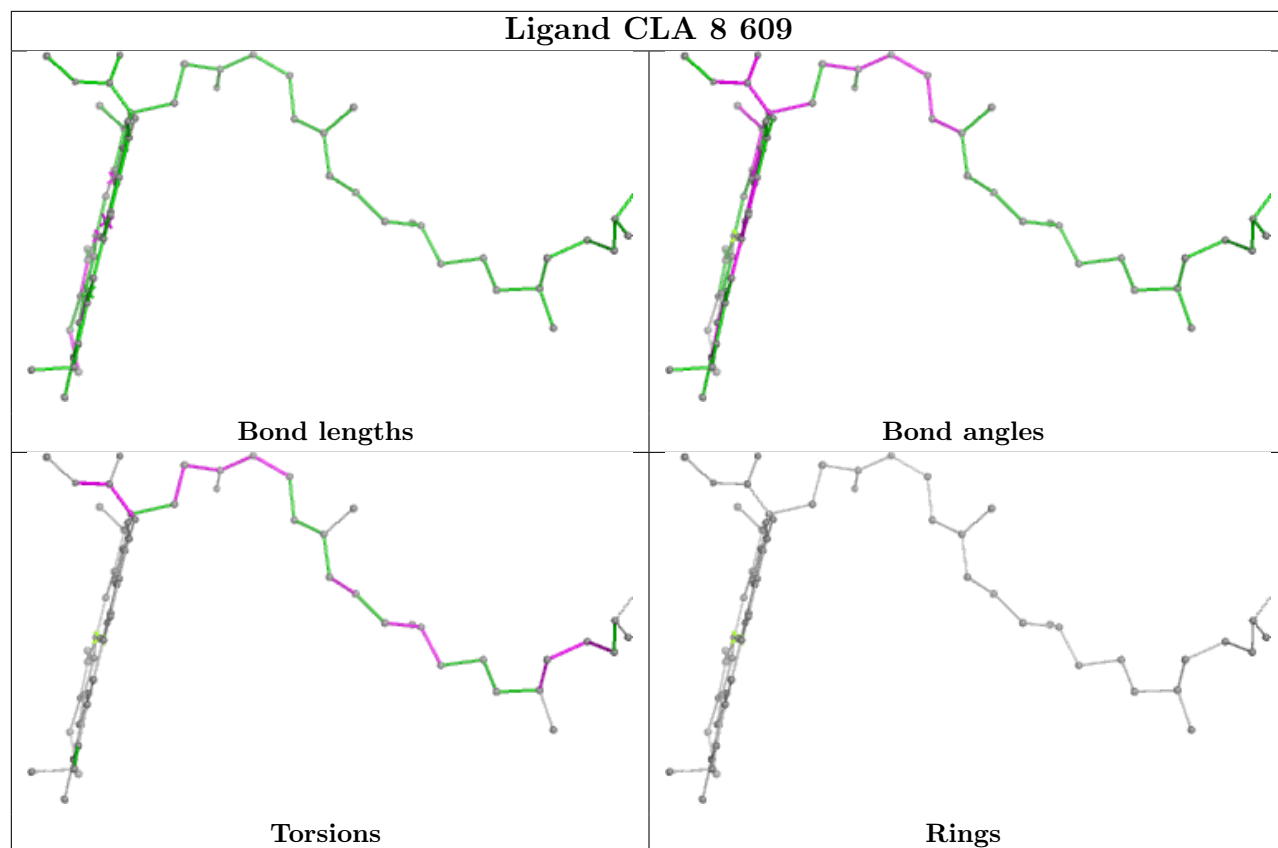
Bond angles

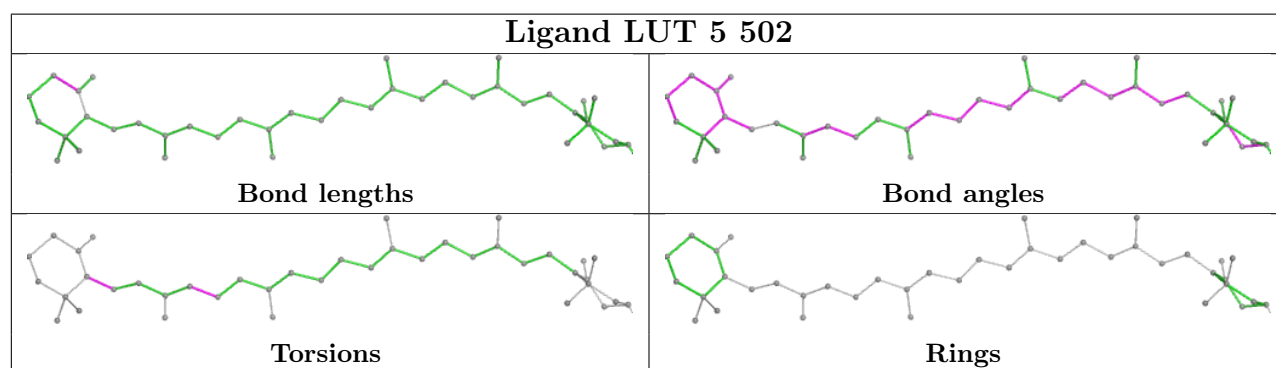
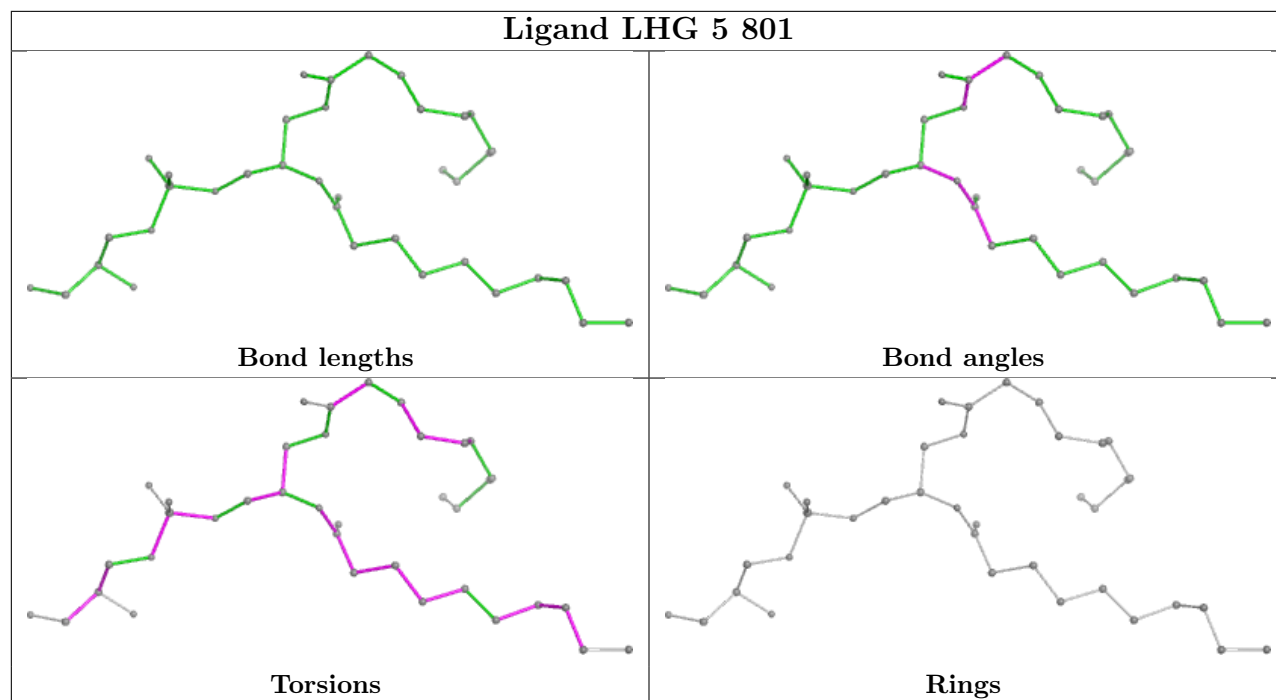
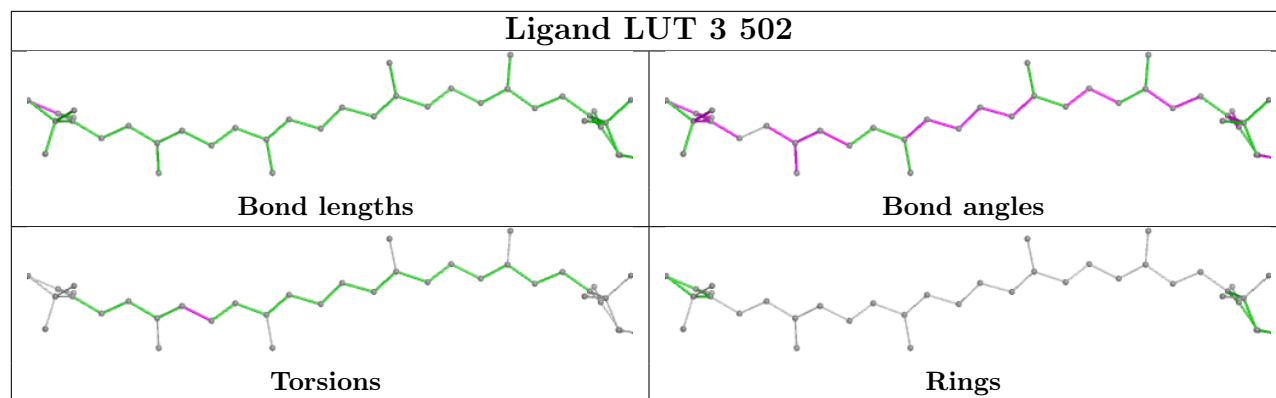


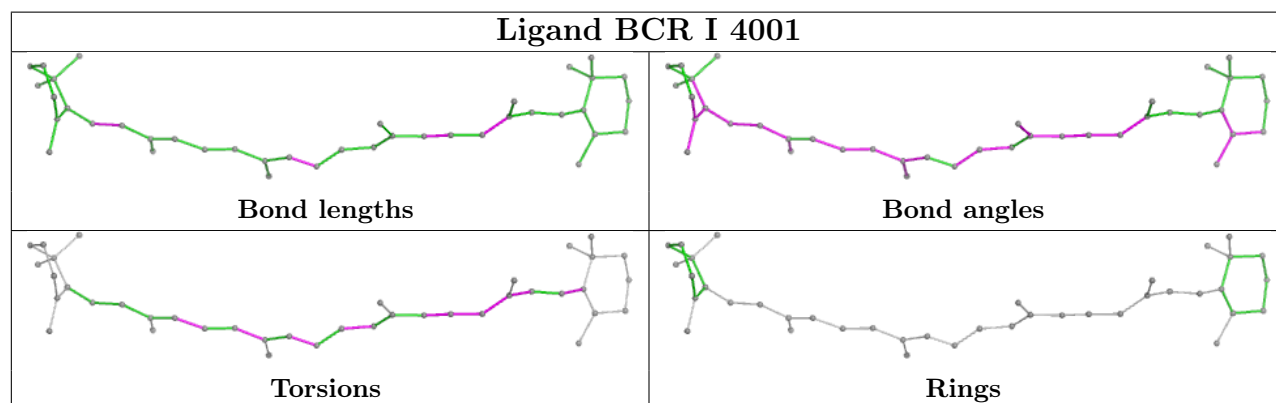
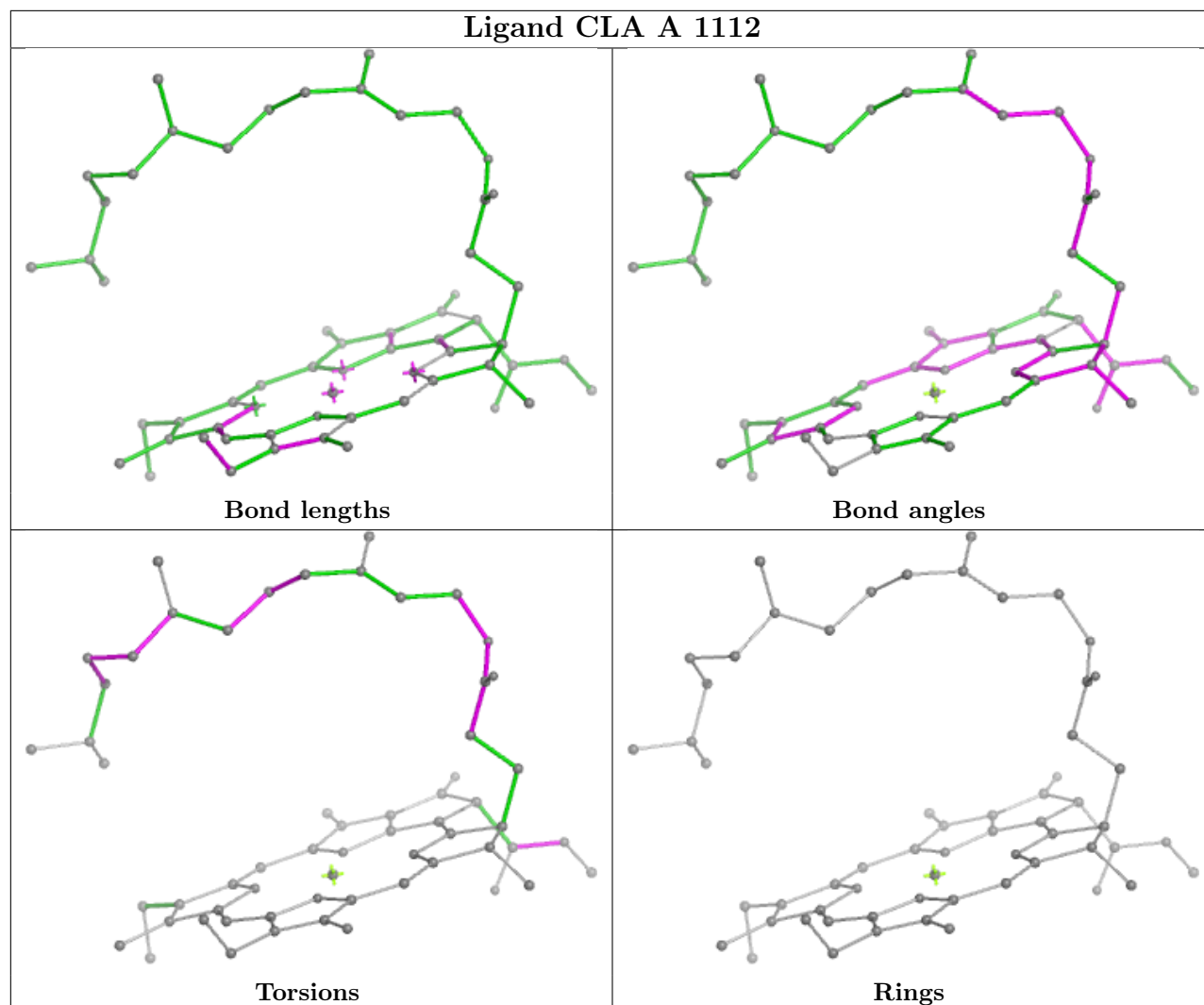
Torsions

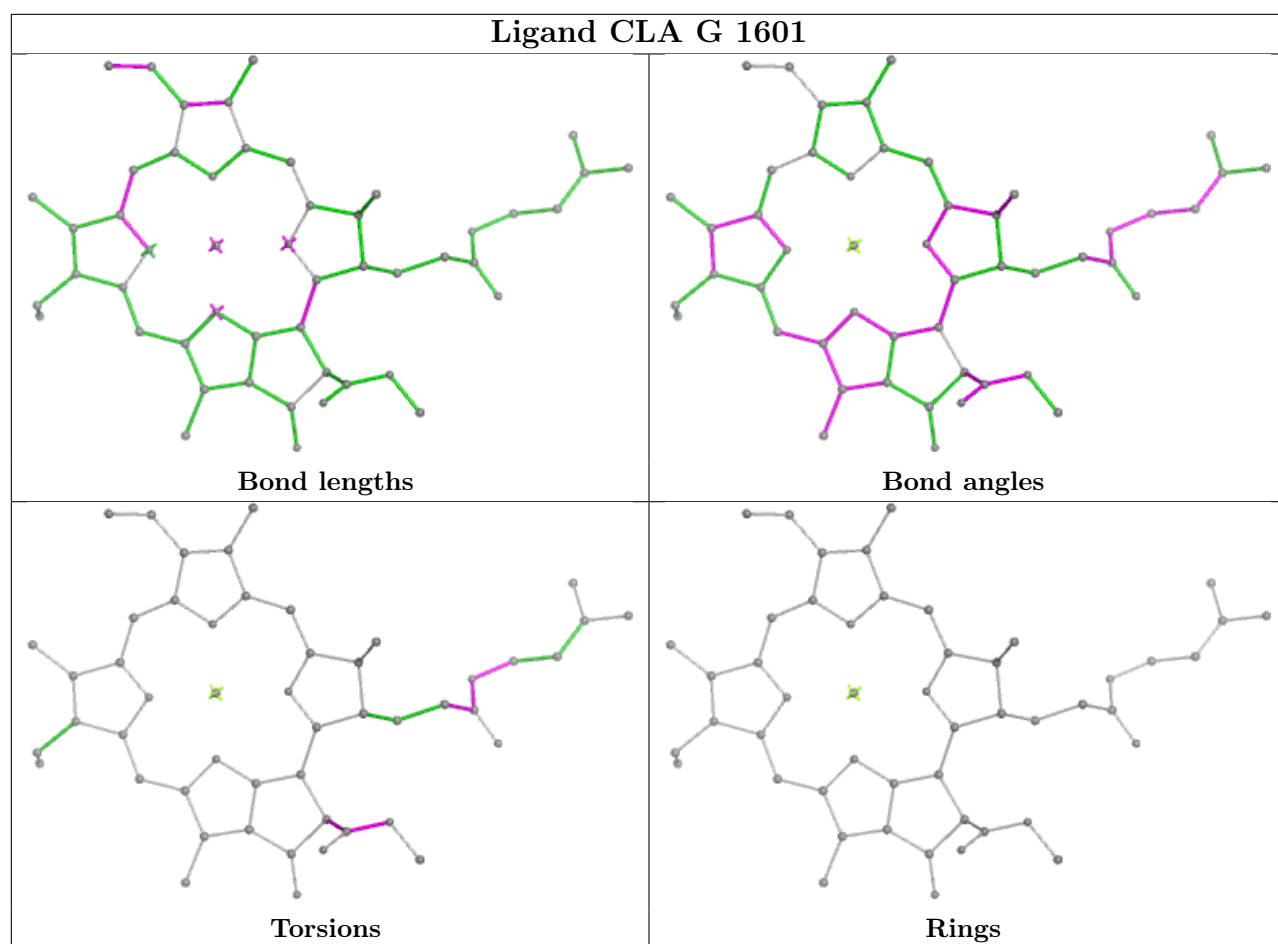


Rings

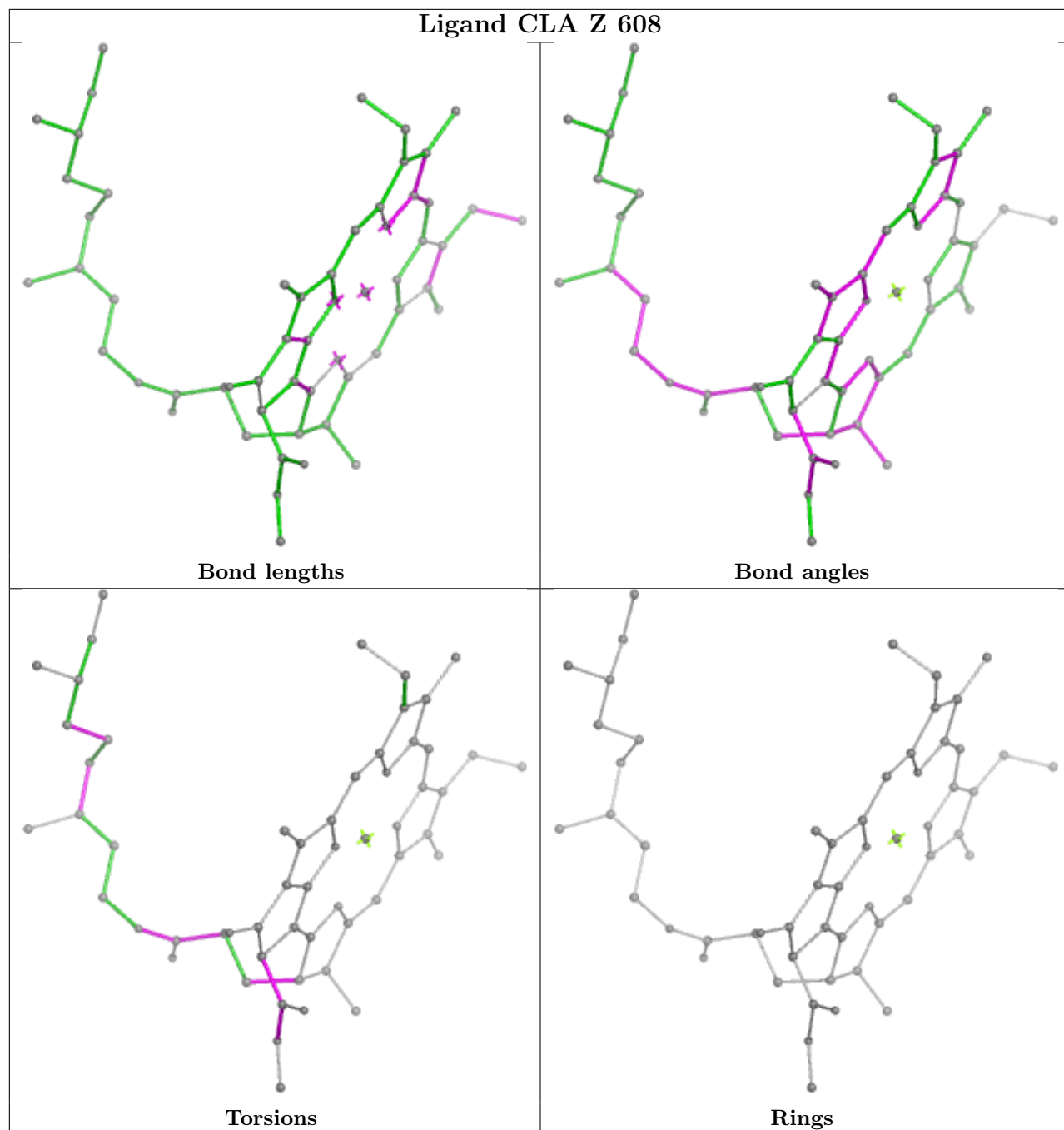


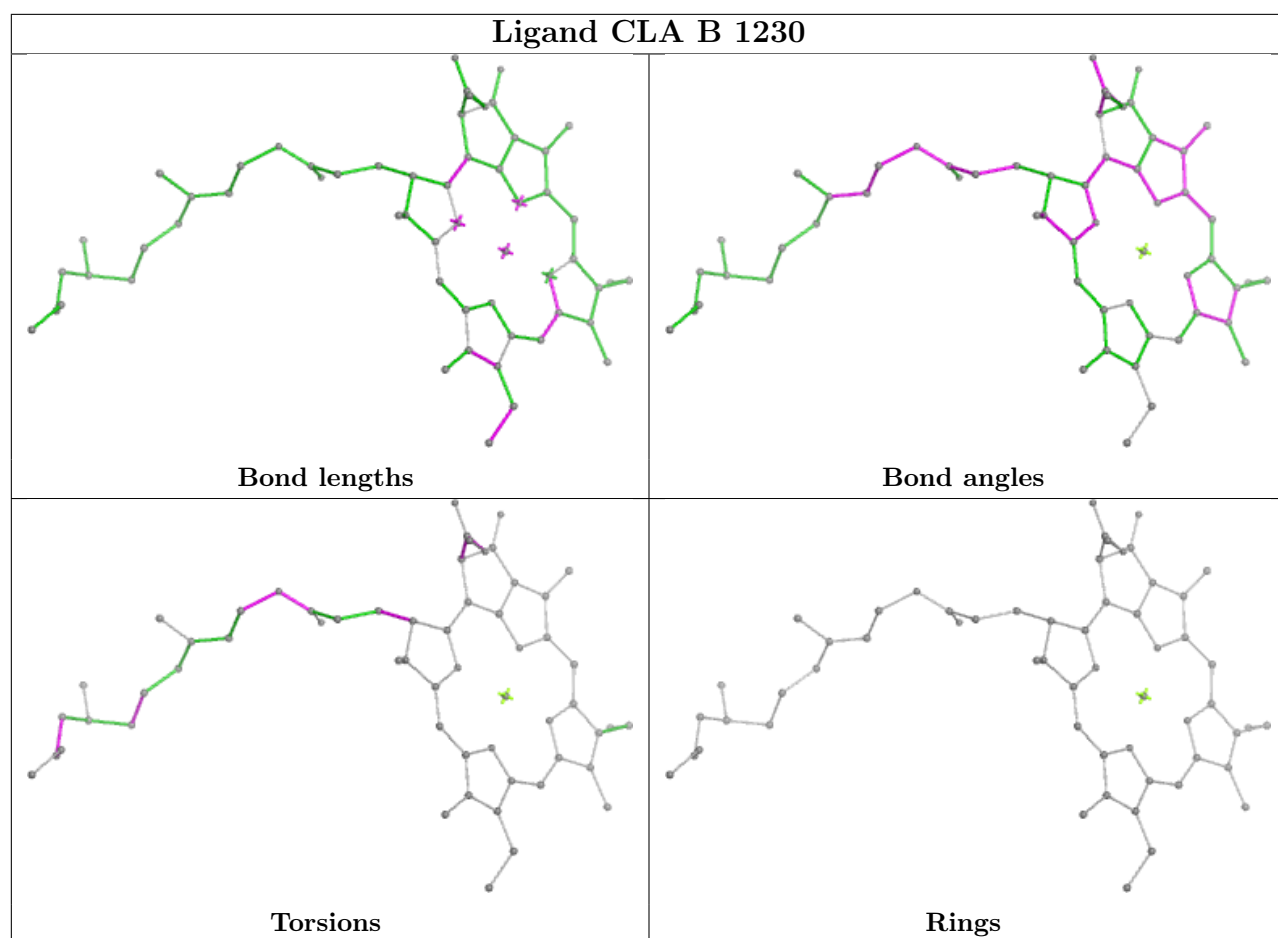






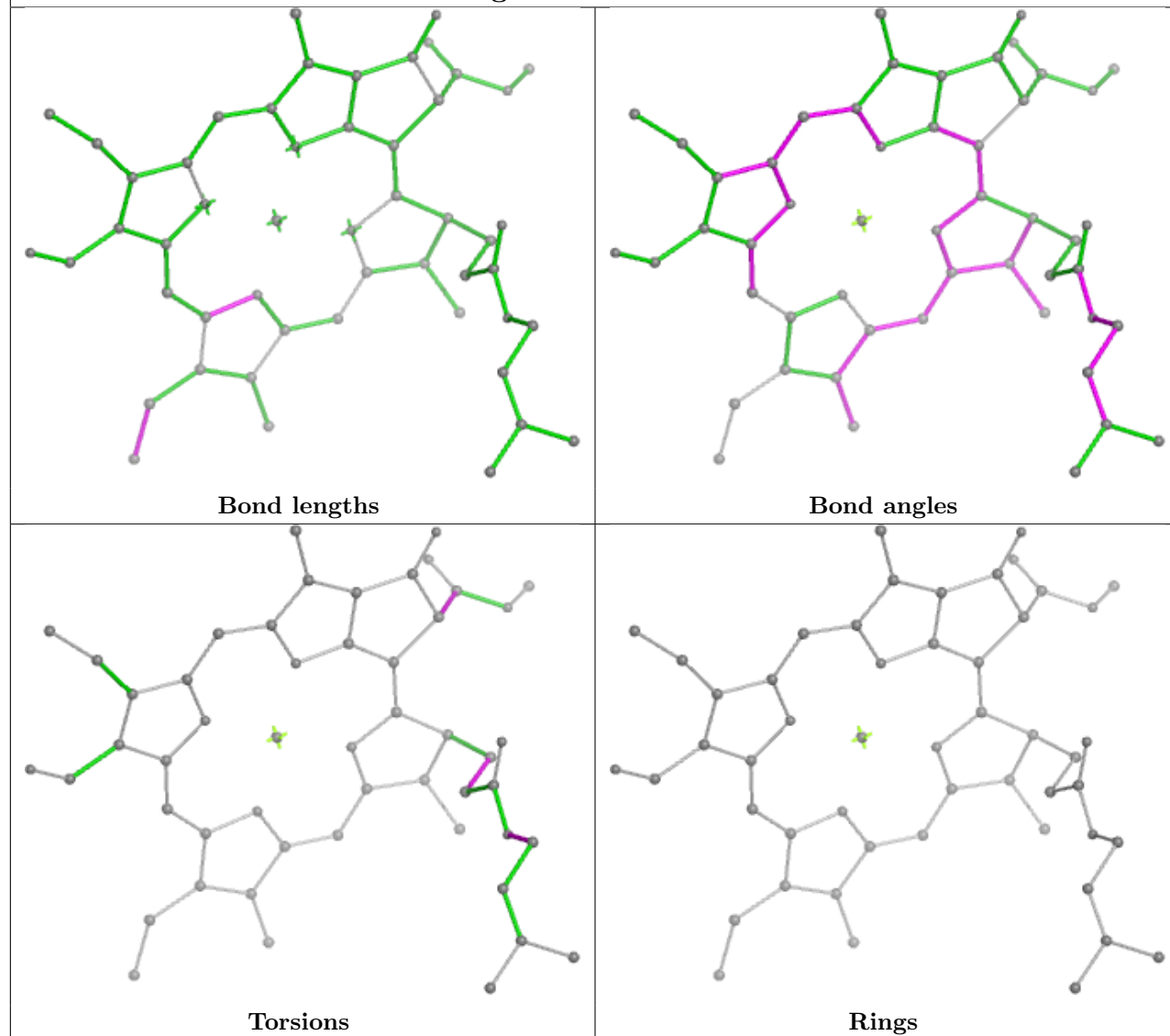
## Ligand CLA Z 608



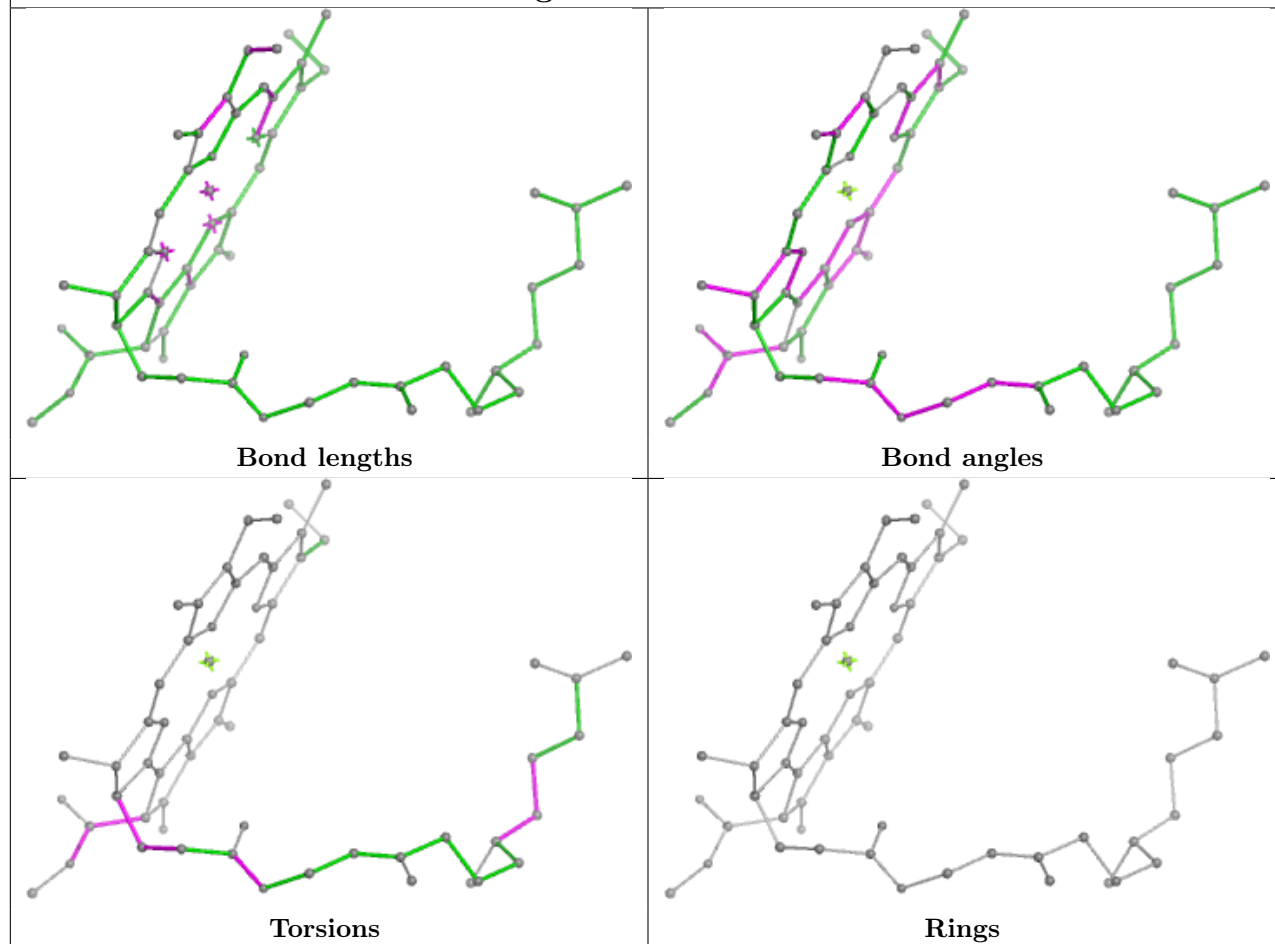




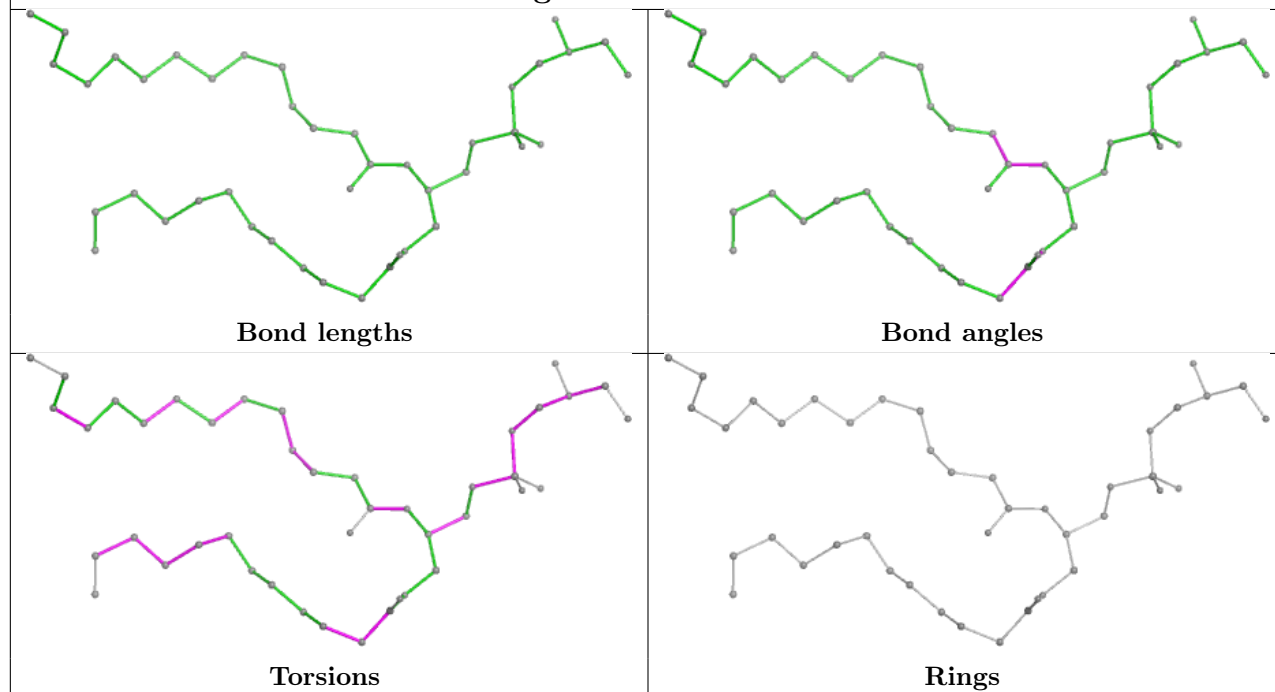
## Ligand CHL 4 610



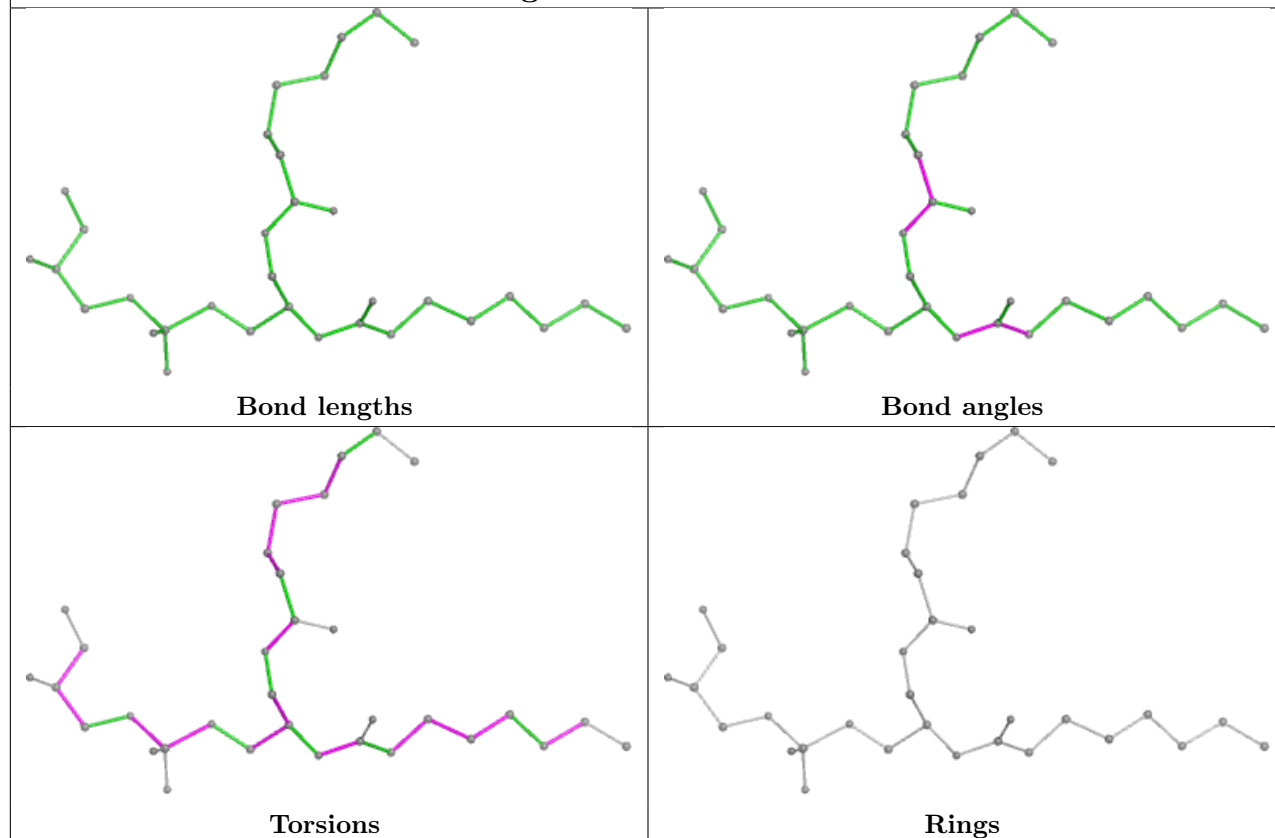
## Ligand CLA 8 606



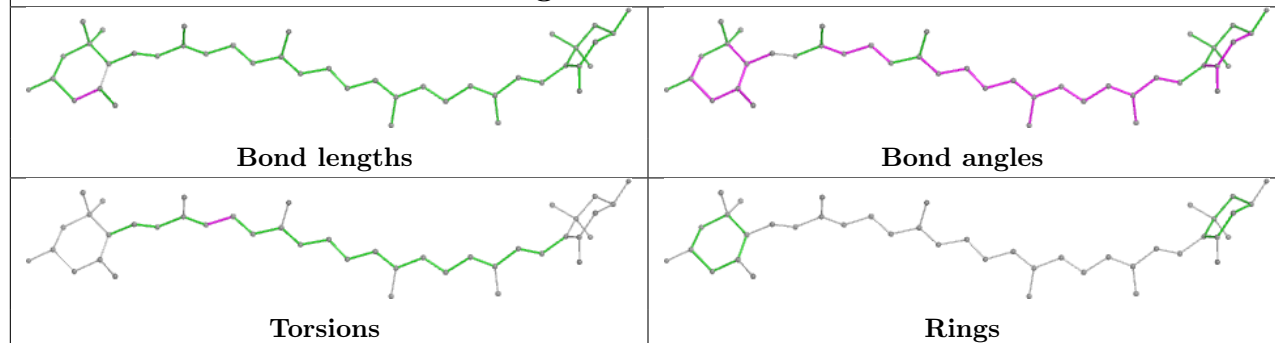
## Ligand LHG 1 801



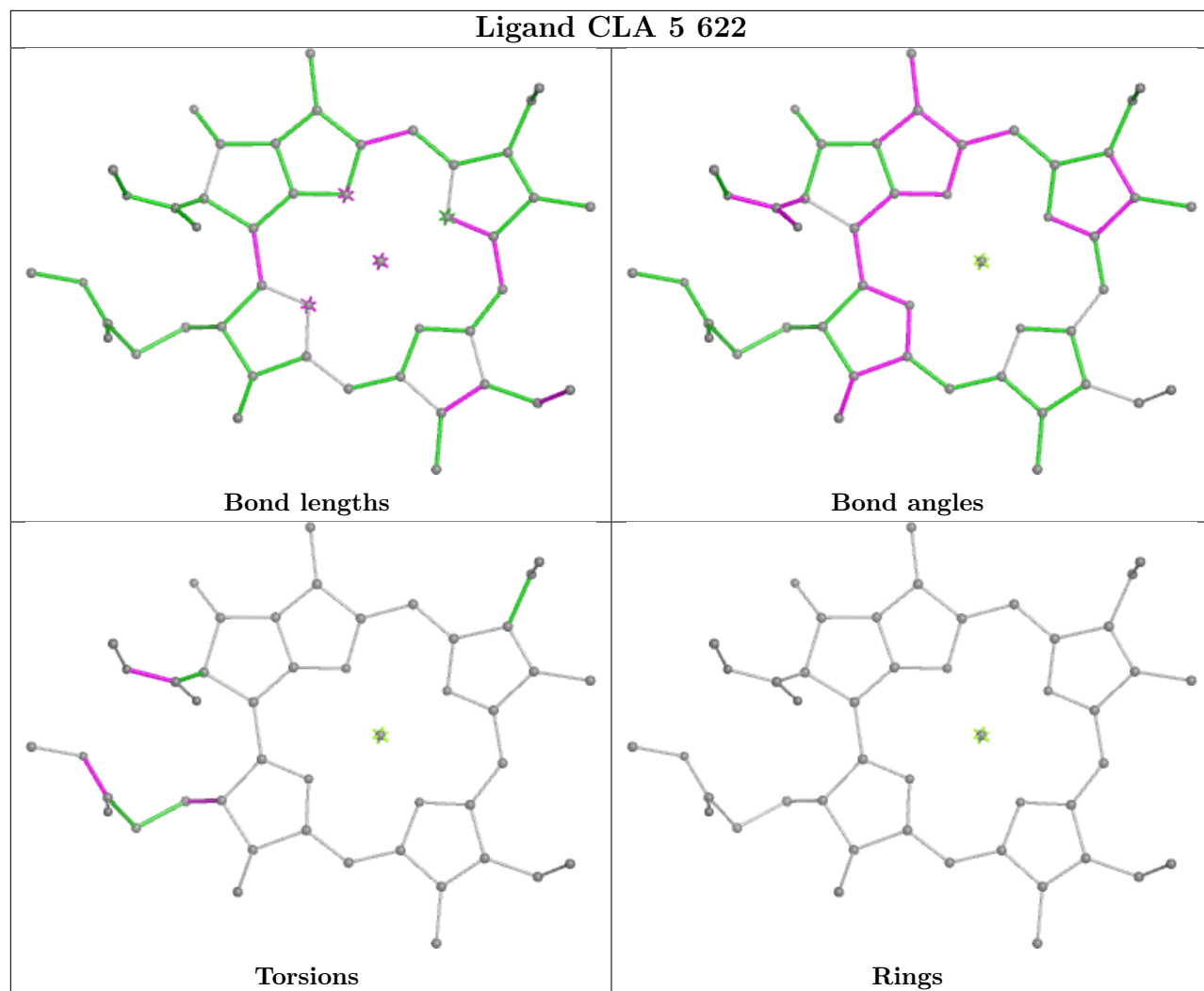
## Ligand LHG B 5006



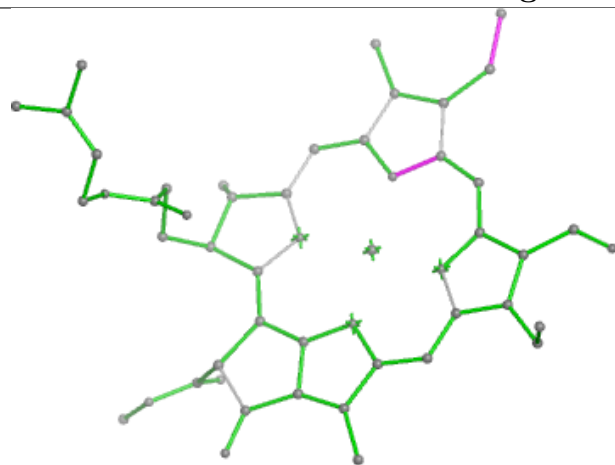
## Ligand LUT 1 502



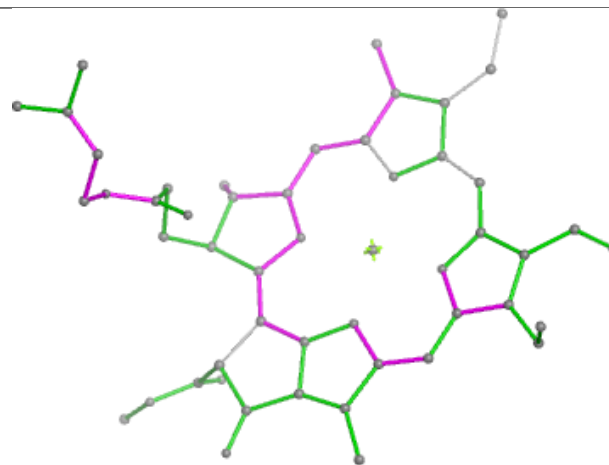
## Ligand CLA 5 622



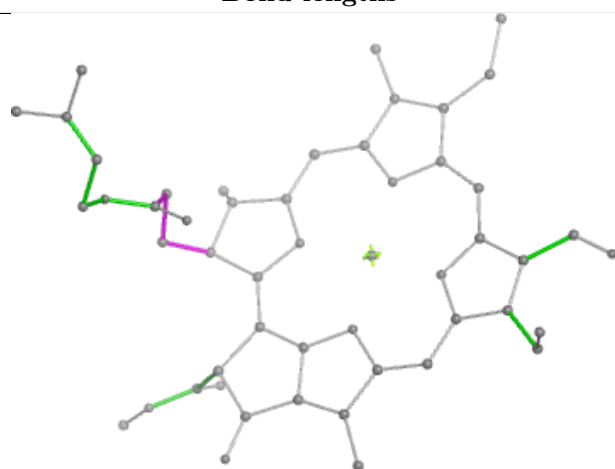
## Ligand CHL 4 611



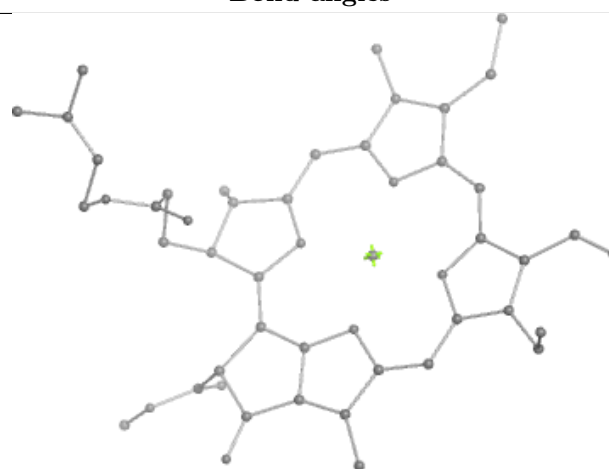
Bond lengths



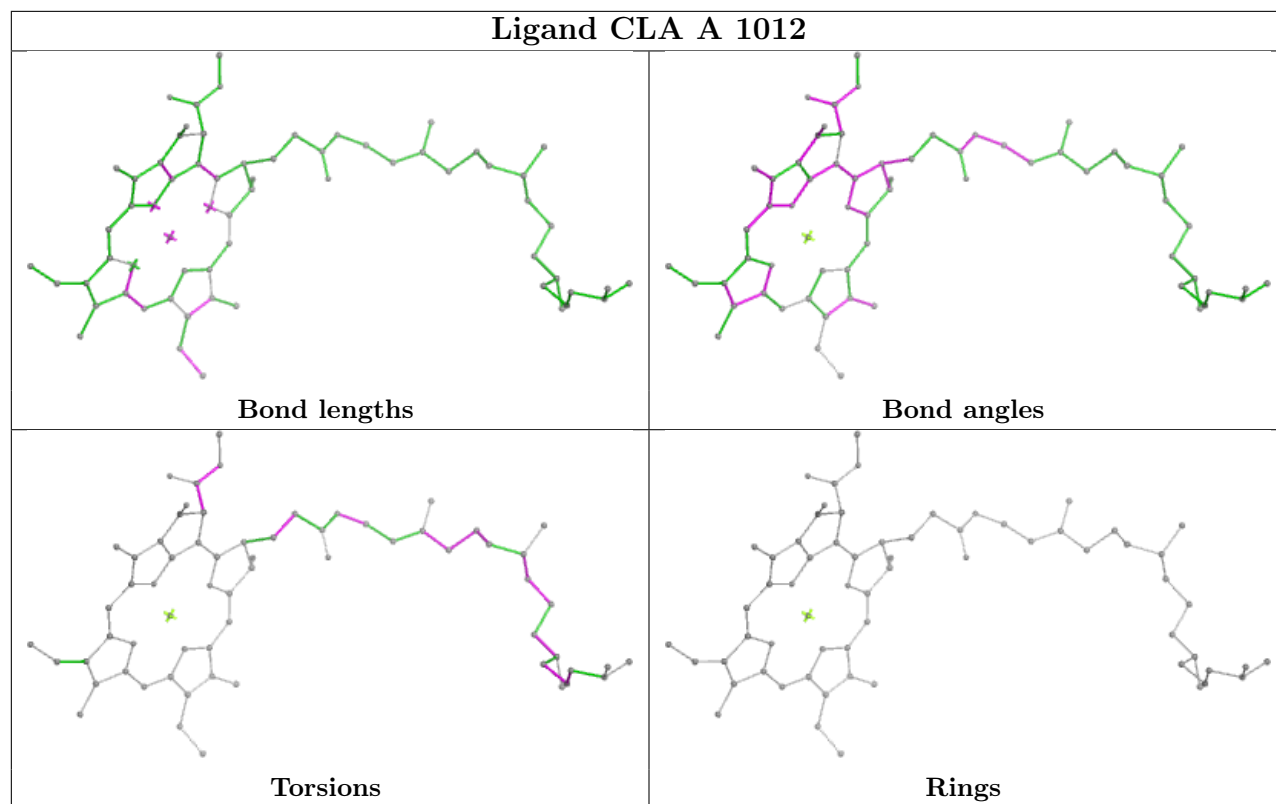
Bond angles



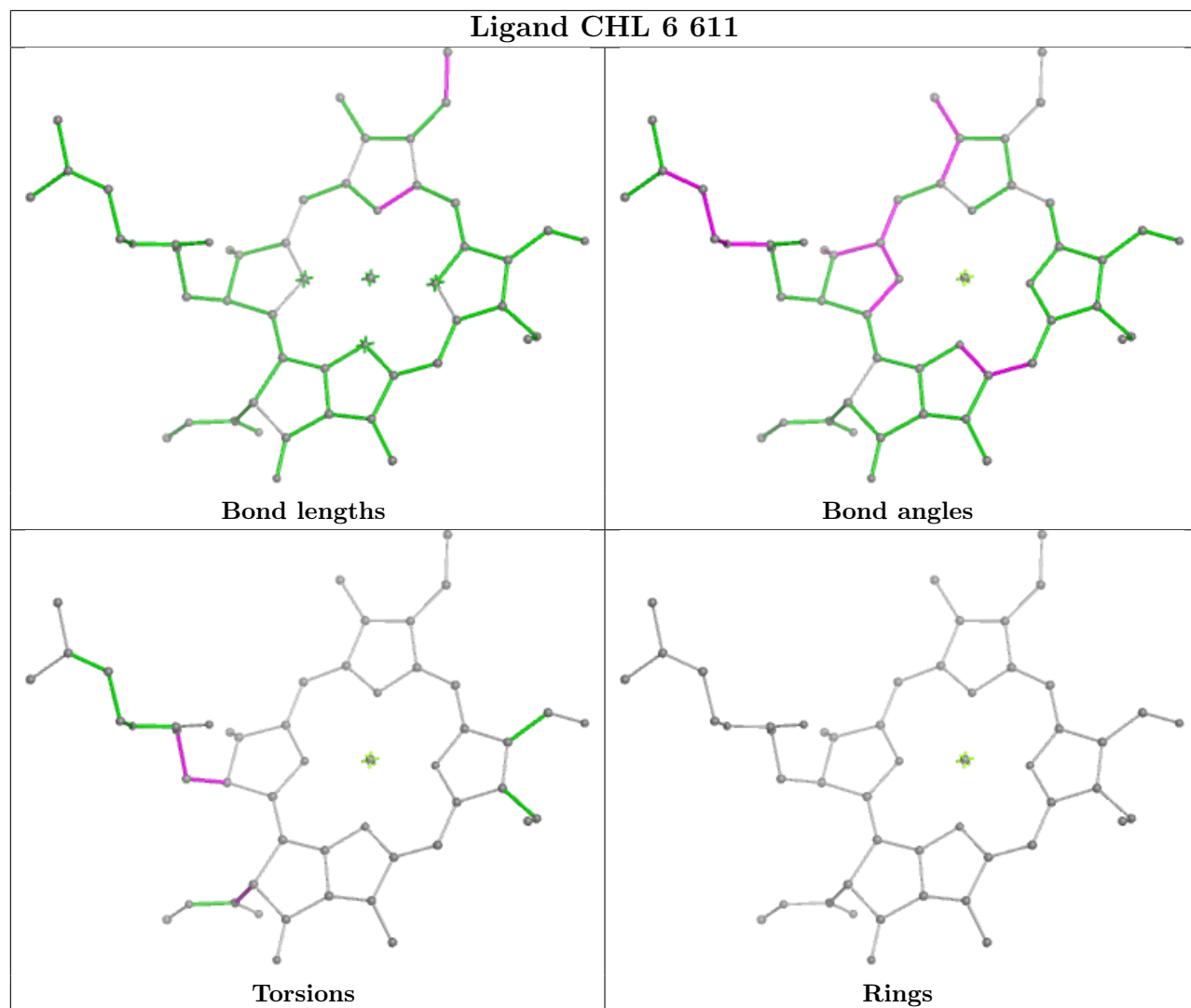
Torsions

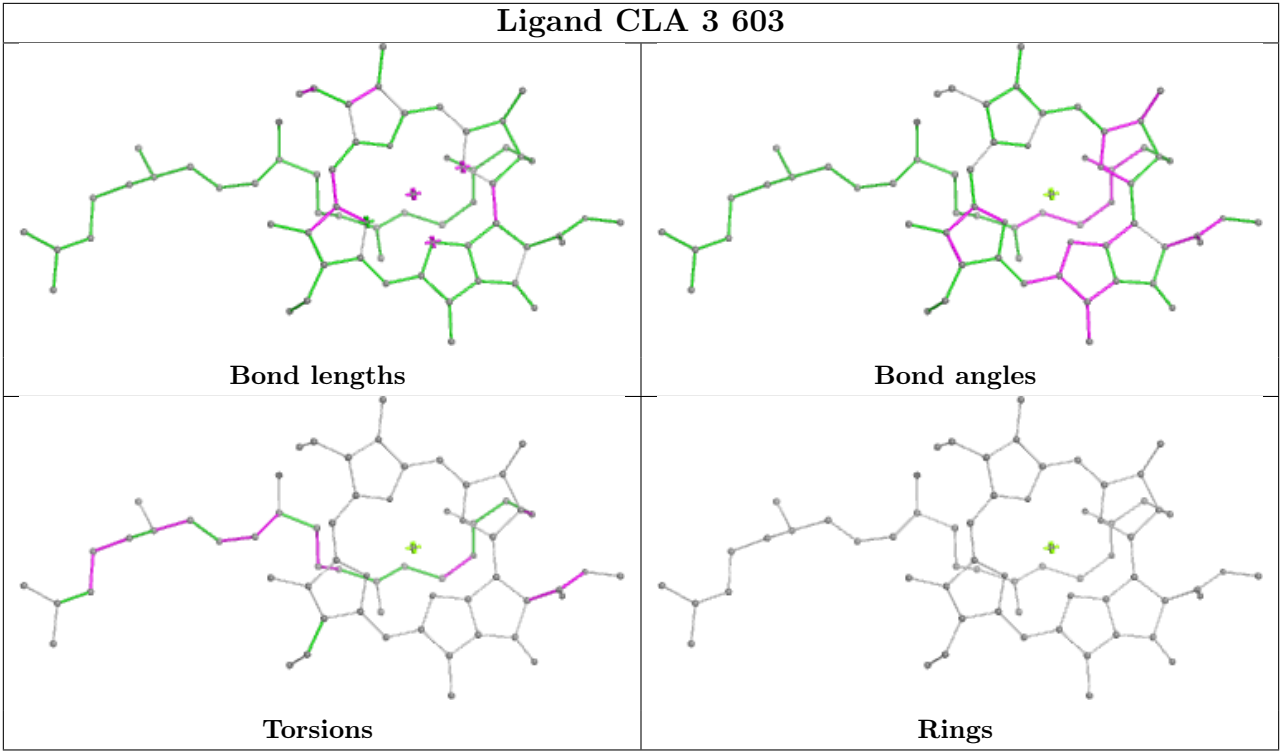


Rings



## Ligand CHL 6 611





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	143:THR	C	156:VAL	N	16.29



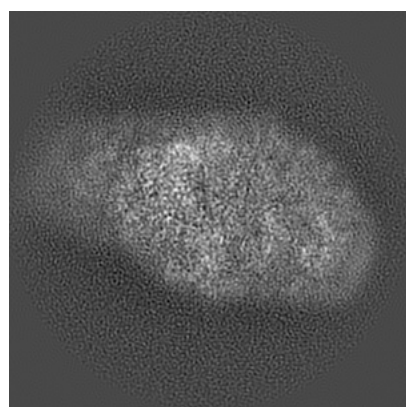
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12227. These allow visual inspection of the internal detail of the map and identification of artifacts.

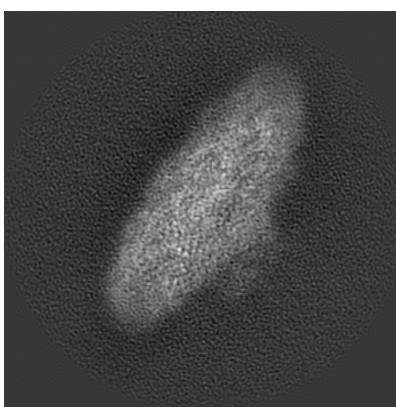
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

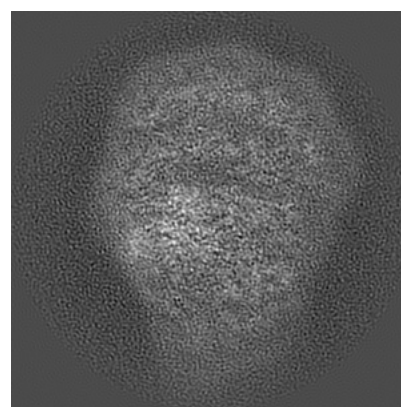
#### 6.1.1 Primary map



X



Y

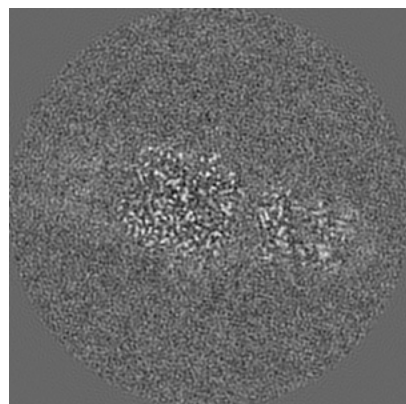


Z

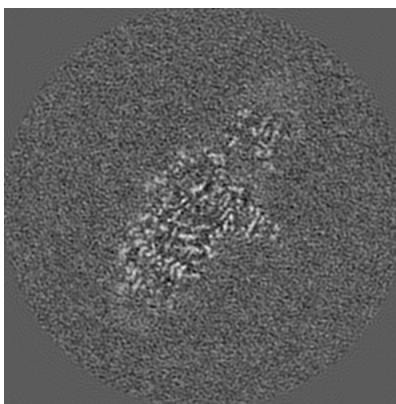
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

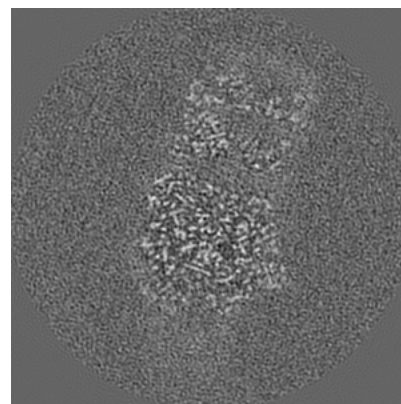
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

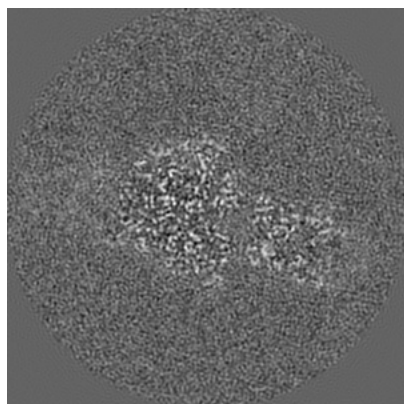


Z Index: 160

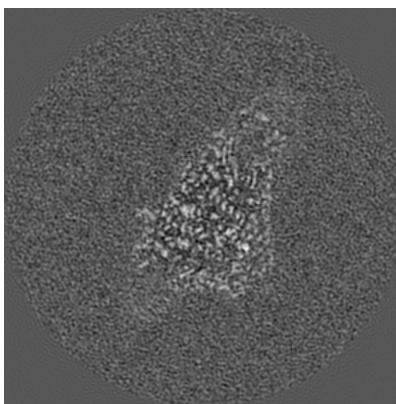
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

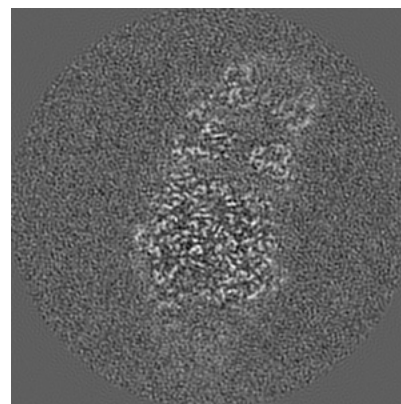
### 6.3.1 Primary map



X Index: 147



Y Index: 135

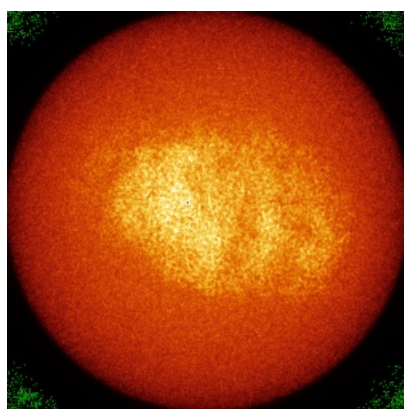


Z Index: 163

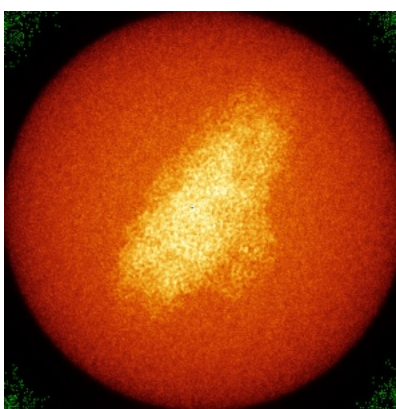
The images above show the largest variance slices of the map in three orthogonal directions.

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

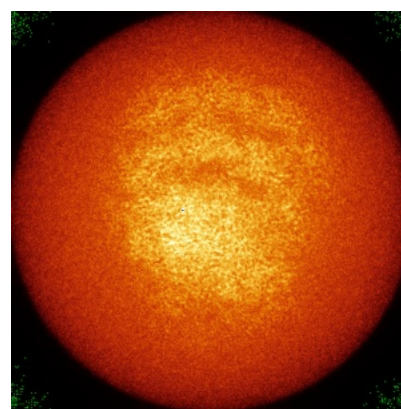
### 6.4.1 Primary map



X



Y

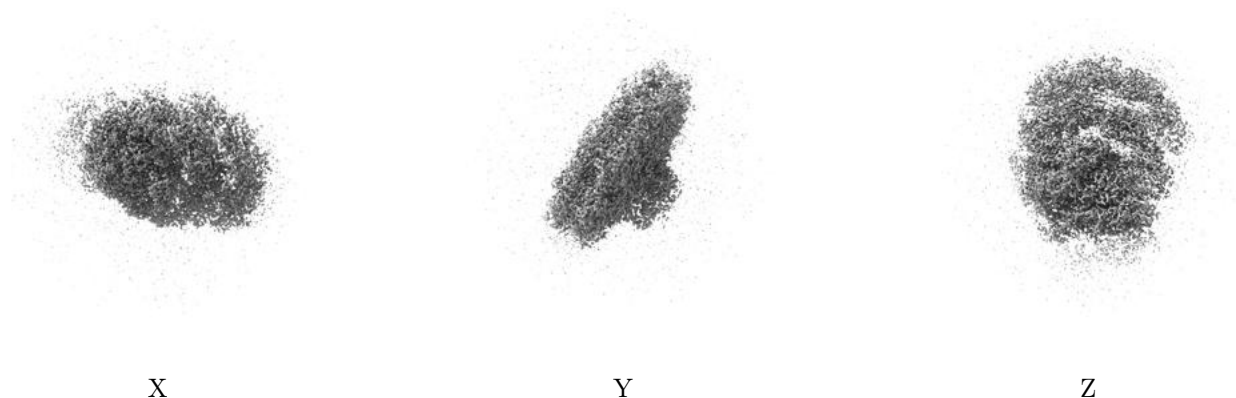


Z

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 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

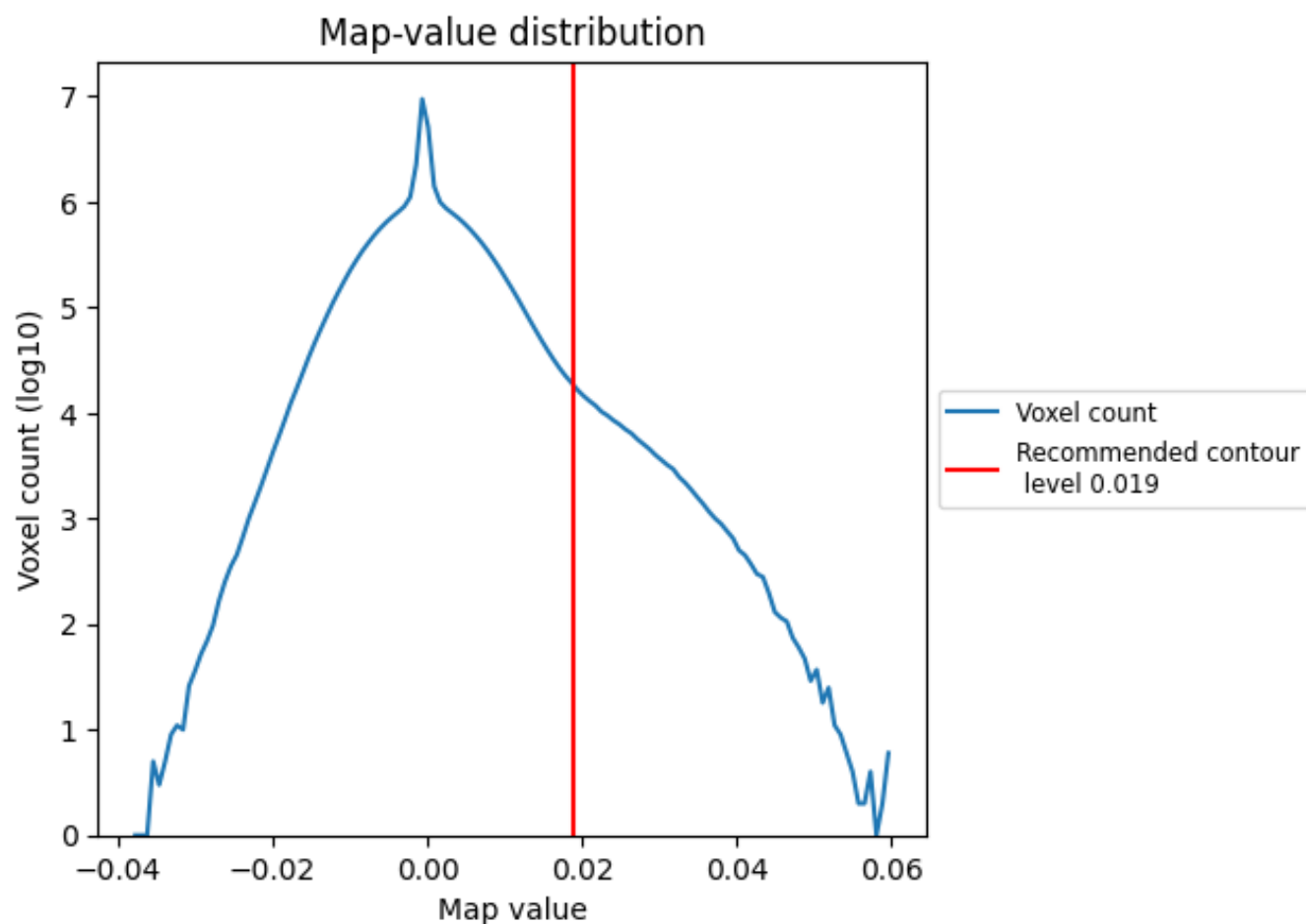
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

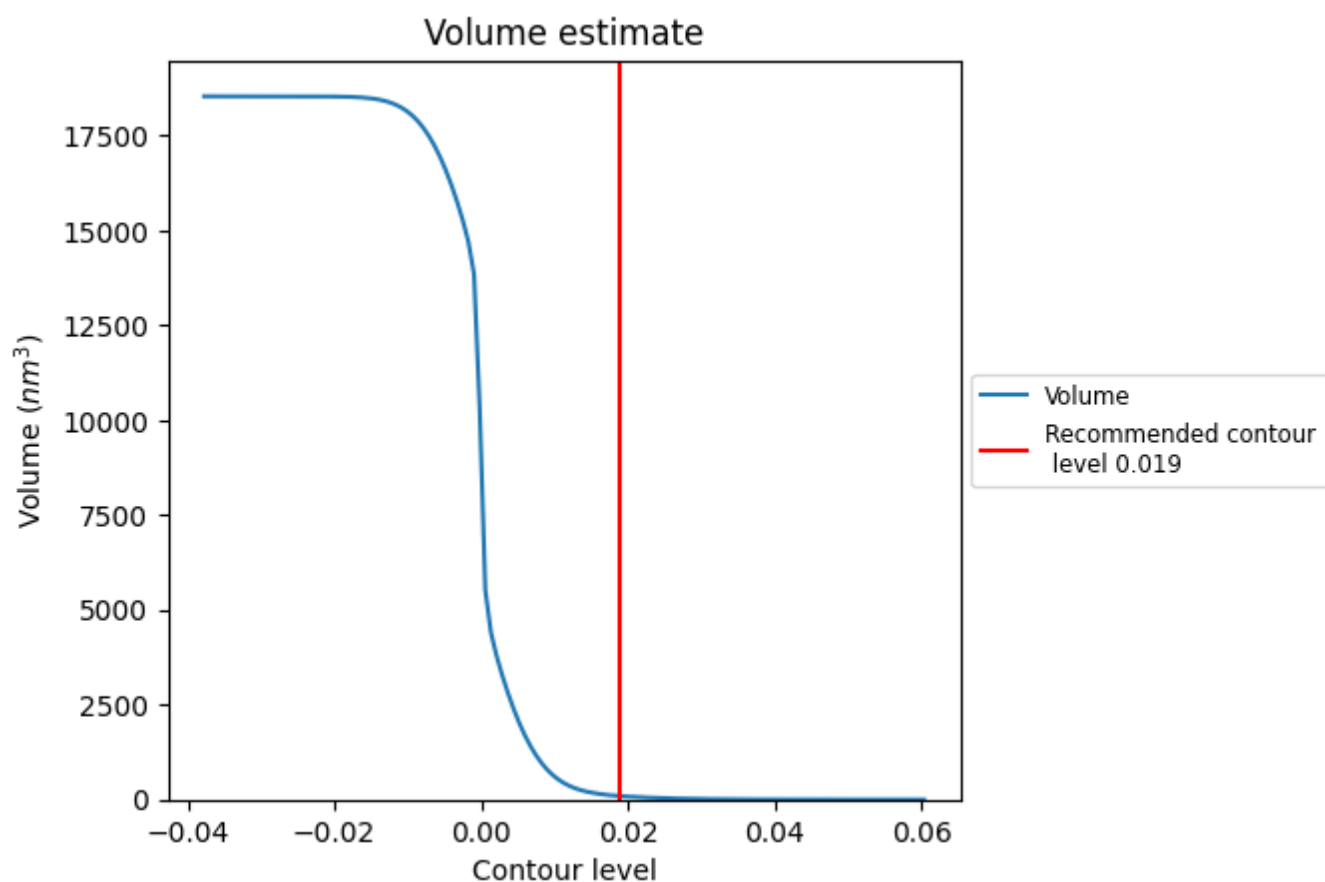
This section contains the results of statistical analysis of the map.

### 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.

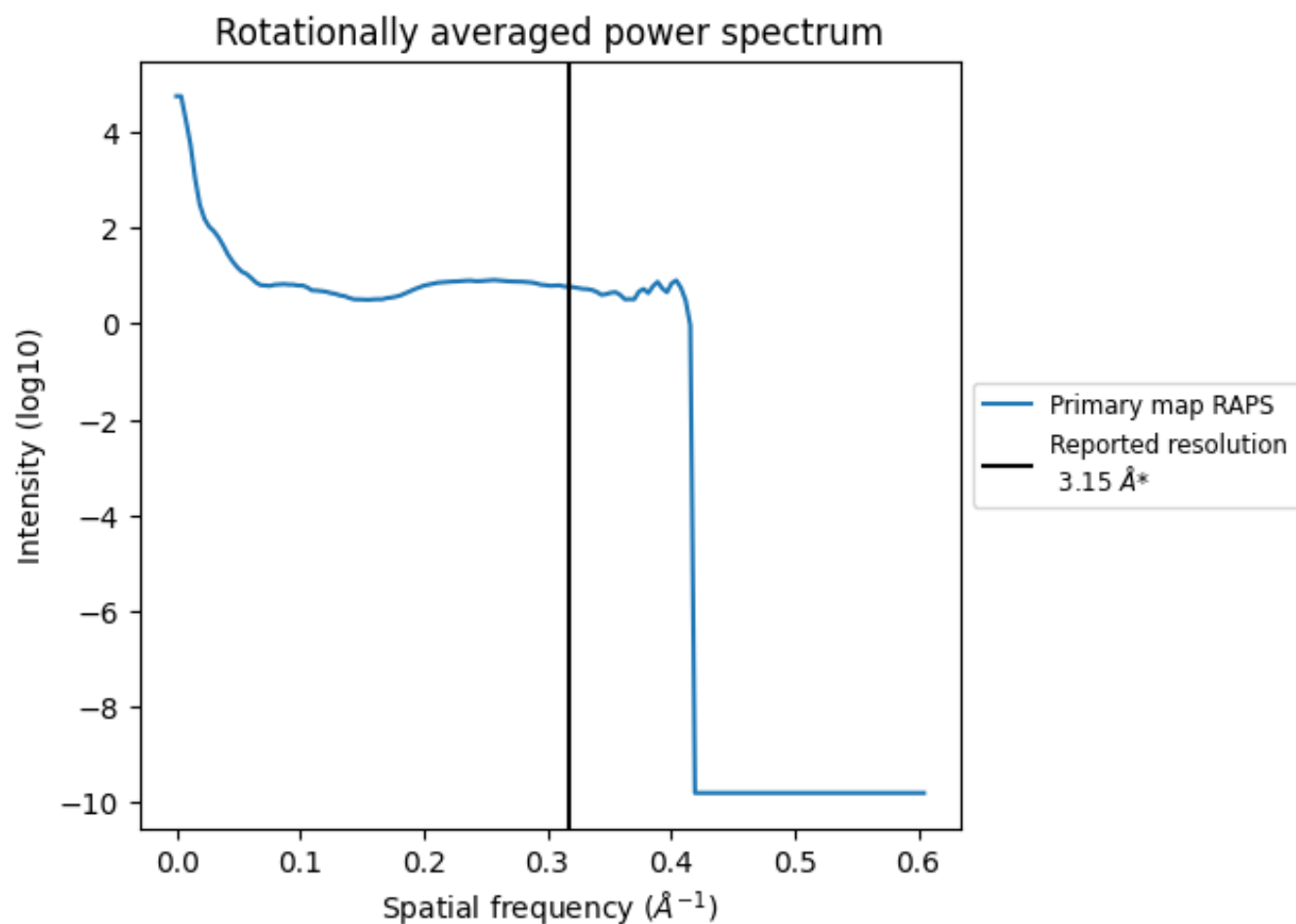
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 91 nm<sup>3</sup>; this corresponds to an approximate mass of 83 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 ⓘ

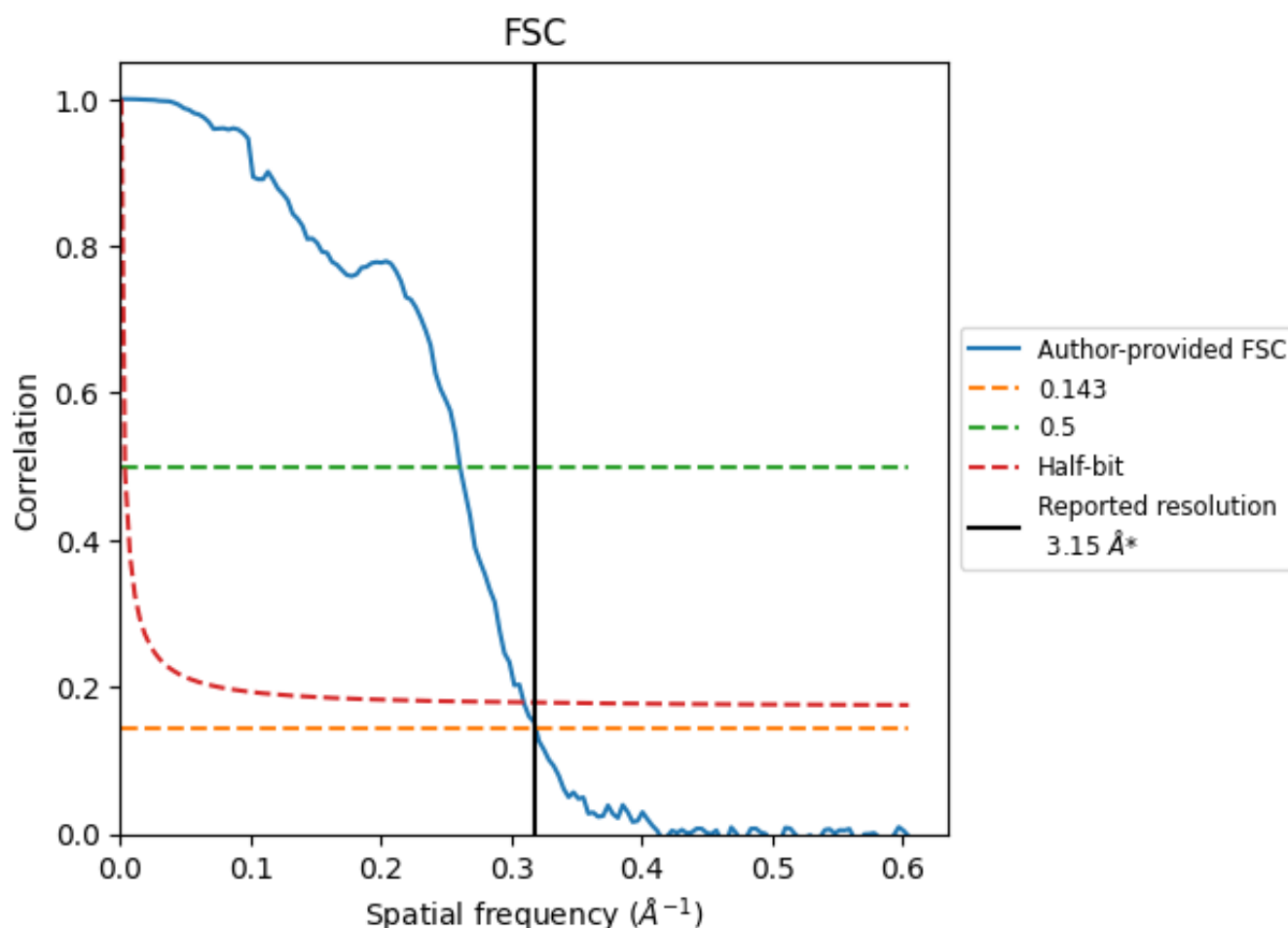


\*Reported resolution corresponds to spatial frequency of 0.317  $\text{\AA}^{-1}$

## 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 0.317 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.15	-	-
Author-provided FSC curve	3.14	3.84	3.23
Unmasked-calculated*	-	-	-

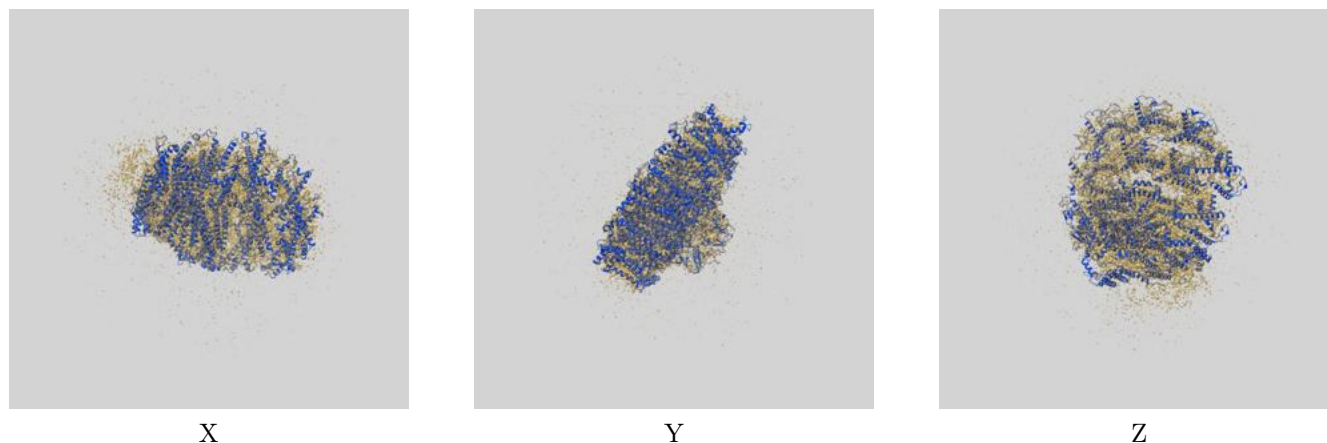
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.



## 9 Map-model fit [i](#)

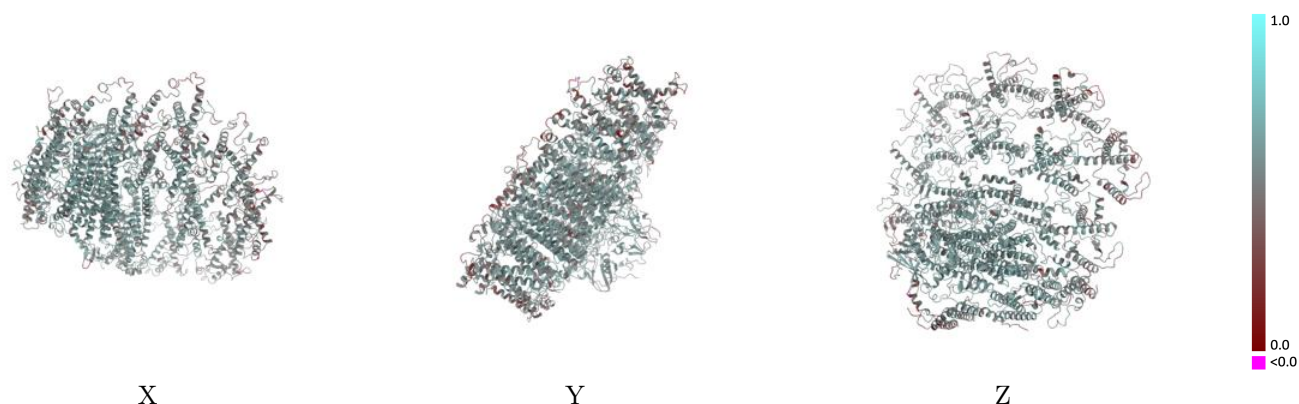
This section contains information regarding the fit between EMDB map EMD-12227 and PDB model 7BLX. Per-residue inclusion information can be found in section 3 on page 43.

### 9.1 Map-model overlay [i](#)



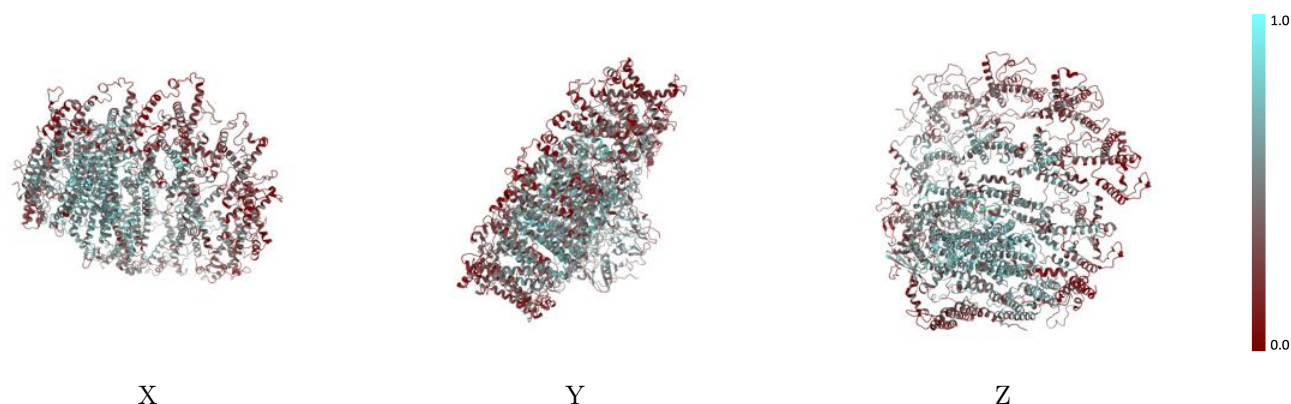
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



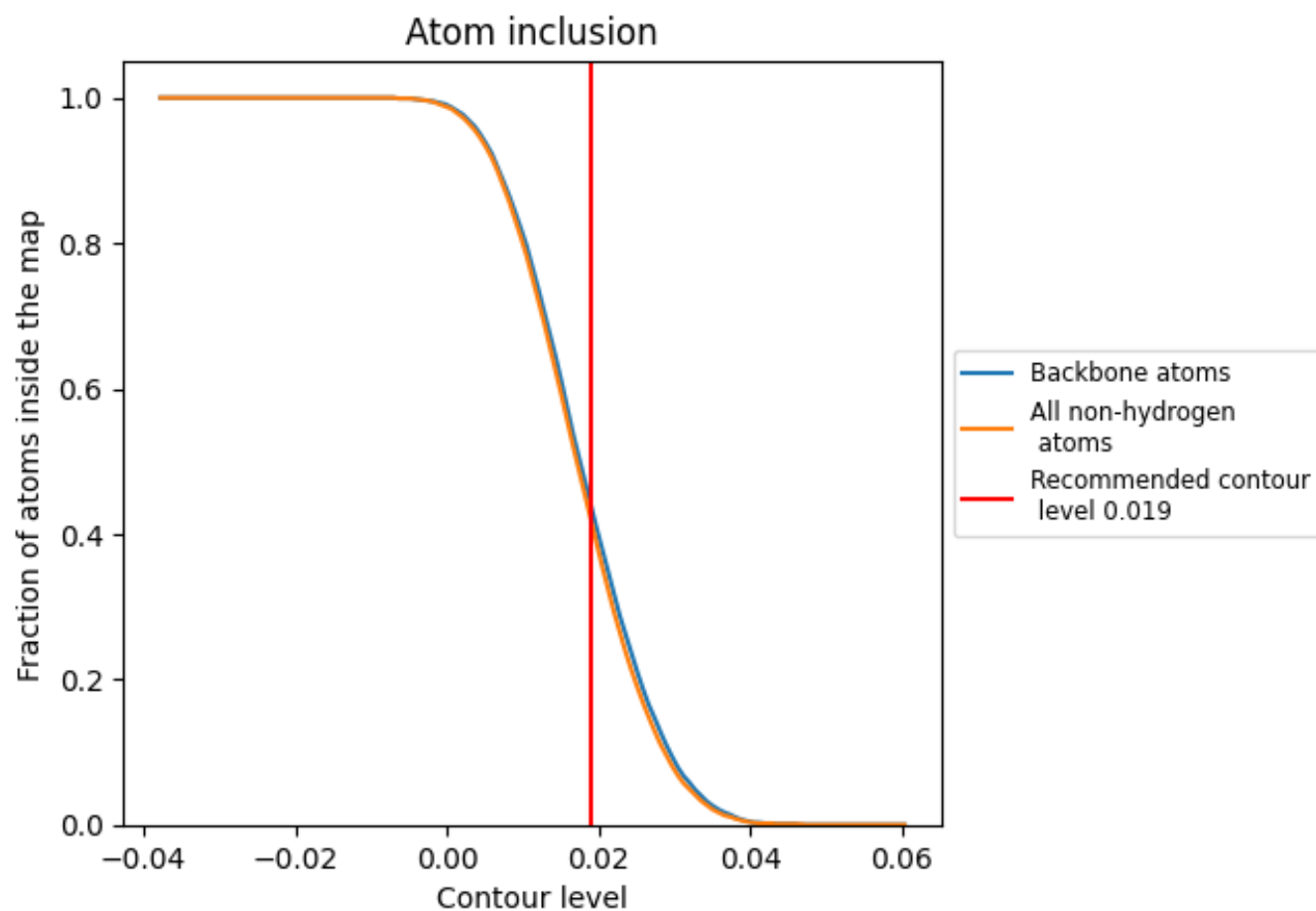
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.019).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 44% of all backbone atoms, 42% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.4190	<div></div> 0.5360
1	<div></div> 0.3530	<div></div> 0.5190
3	<div></div> 0.3980	<div></div> 0.5260
4	<div></div> 0.2400	<div></div> 0.4710
5	<div></div> 0.2730	<div></div> 0.4920
6	<div></div> 0.2620	<div></div> 0.4830
7	<div></div> 0.4720	<div></div> 0.5520
8	<div></div> 0.4530	<div></div> 0.5500
A	<div></div> 0.5670	<div></div> 0.5860
B	<div></div> 0.5320	<div></div> 0.5780
C	<div></div> 0.5820	<div></div> 0.5690
D	<div></div> 0.4130	<div></div> 0.5350
E	<div></div> 0.4900	<div></div> 0.5270
F	<div></div> 0.4540	<div></div> 0.5500
G	<div></div> 0.1450	<div></div> 0.4470
I	<div></div> 0.2720	<div></div> 0.5160
J	<div></div> 0.4710	<div></div> 0.5680
K	<div></div> 0.1890	<div></div> 0.4500
L	<div></div> 0.1900	<div></div> 0.4460
Z	<div></div> 0.1980	<div></div> 0.4510

1.0

0.0

<0.0