



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 08:40 pm BST

PDB ID : 6YXR
EMDB ID : EMD-10995
Title : Dunaliella Minimal Photosystem I
Authors : Nelson, N.; Caspy, I.; Malavath, T.; Klaiman, D.; Shkolinsky, Y.
Deposited on : 2020-05-03
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

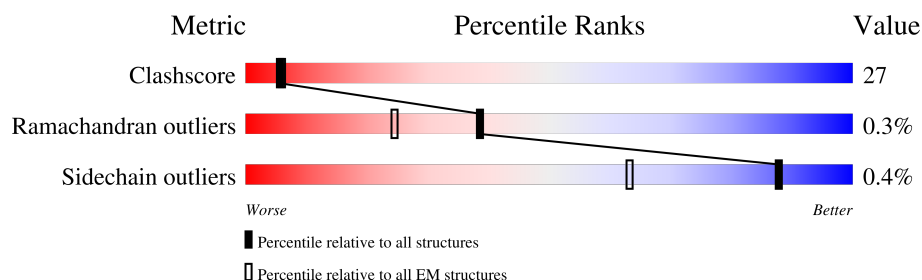
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	1	197	<div> <div>50%</div> <div> <div>73%</div> <div>27%</div> </div> </div>
2	2	208	<div> <div>20%</div> <div> <div>84%</div> <div>16%</div> </div> </div>
3	3	210	<div> <div>27%</div> <div> <div>79%</div> <div>21%</div> </div> </div>
4	4	211	<div> <div>30%</div> <div> <div>77%</div> <div>22%</div> </div> </div>
5	A	739	<div> <div>5%</div> <div> <div>74%</div> <div>25%</div> </div> </div>
6	B	730	<div> <div>10%</div> <div> <div>78%</div> <div>22%</div> </div> </div>
7	C	80	<div> <div>14%</div> <div> <div>71%</div> <div>28%</div> </div> </div>
8	D	141	<div> <div>28%</div> <div> <div>84%</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
9	E	64	
10	F	163	
11	J	40	

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
12	LUT	1	501	X	-	X	-
12	LUT	2	501	X	-	-	-
12	LUT	3	501	X	-	-	-
12	LUT	4	501	X	X	-	-
14	BCR	A	4003	-	-	X	-
14	BCR	F	4001	-	-	X	-
15	CLA	1	601	X	-	-	-
15	CLA	1	602	X	-	-	-
15	CLA	1	603	X	-	-	-
15	CLA	1	604	X	-	-	-
15	CLA	1	605	X	-	-	-
15	CLA	1	606	X	-	-	-
15	CLA	1	607	X	-	-	-
15	CLA	1	608	X	-	X	-
15	CLA	1	611	X	-	-	-
15	CLA	1	612	X	-	-	-
15	CLA	1	613	X	-	-	-
15	CLA	1	615	X	-	-	-
15	CLA	2	601	X	-	-	-
15	CLA	2	602	X	-	-	-
15	CLA	2	603	X	-	-	-
15	CLA	2	604	X	-	-	-
15	CLA	2	605	X	-	-	-
15	CLA	2	606	X	-	-	-
15	CLA	2	607	X	-	-	-
15	CLA	2	608	X	-	-	-
15	CLA	2	612	X	-	-	-
15	CLA	3	601	X	-	-	-
15	CLA	3	603	X	-	-	-
15	CLA	3	605	X	-	-	-
15	CLA	3	606	X	-	-	-
15	CLA	3	607	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	3	608	X	-	-	-
15	CLA	3	609	X	-	-	-
15	CLA	3	610	X	-	-	-
15	CLA	3	611	X	-	-	-
15	CLA	3	612	X	-	-	-
15	CLA	3	613	X	-	-	-
15	CLA	3	614	X	-	-	-
15	CLA	3	615	X	-	-	-
15	CLA	4	601	X	-	-	-
15	CLA	4	602	X	-	-	-
15	CLA	4	603	X	-	-	-
15	CLA	4	604	X	-	-	-
15	CLA	4	605	X	-	-	-
15	CLA	4	606	X	-	-	-
15	CLA	4	607	X	-	-	-
15	CLA	4	608	X	-	-	-
15	CLA	4	609	X	-	-	-
15	CLA	4	612	X	-	-	-
15	CLA	4	616	X	-	-	-
15	CLA	A	1012	X	-	X	-
15	CLA	A	1013	X	-	X	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	X	-	X	-
15	CLA	A	1104	X	-	-	-
15	CLA	A	1105	X	-	-	-
15	CLA	A	1106	X	-	-	-
15	CLA	A	1107	X	-	-	-
15	CLA	A	1108	X	-	-	-
15	CLA	A	1109	X	-	-	-
15	CLA	A	1110	X	-	-	-
15	CLA	A	1111	X	-	-	-
15	CLA	A	1112	X	-	X	-
15	CLA	A	1113	X	-	-	-
15	CLA	A	1114	X	-	-	-
15	CLA	A	1115	X	-	-	-
15	CLA	A	1116	X	-	-	-
15	CLA	A	1117	X	-	-	-
15	CLA	A	1118	X	-	-	-
15	CLA	A	1119	X	-	-	-
15	CLA	A	1120	X	-	-	-
15	CLA	A	1121	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	X	-
15	CLA	A	1124	X	-	X	-
15	CLA	A	1125	X	-	-	-
15	CLA	A	1126	X	-	X	-
15	CLA	A	1127	X	-	-	-
15	CLA	A	1128	X	-	-	-
15	CLA	A	1129	X	-	-	-
15	CLA	A	1130	X	-	-	-
15	CLA	A	1131	X	-	-	-
15	CLA	A	1132	X	-	-	-
15	CLA	A	1133	-	-	X	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	X	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1139	X	-	-	-
15	CLA	A	1141	X	-	-	-
15	CLA	B	1021	X	-	-	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1201	X	-	-	-
15	CLA	B	1202	X	-	-	-
15	CLA	B	1203	X	-	-	-
15	CLA	B	1204	X	-	-	-
15	CLA	B	1205	X	-	X	-
15	CLA	B	1206	X	-	-	-
15	CLA	B	1208	X	-	-	-
15	CLA	B	1209	X	-	-	-
15	CLA	B	1211	X	-	-	-
15	CLA	B	1212	X	-	-	-
15	CLA	B	1213	X	-	-	-
15	CLA	B	1214	X	-	-	-
15	CLA	B	1215	X	-	X	-
15	CLA	B	1216	X	-	-	-
15	CLA	B	1217	X	-	-	-
15	CLA	B	1218	X	-	-	-
15	CLA	B	1220	X	-	-	-
15	CLA	B	1221	X	-	-	-
15	CLA	B	1222	X	-	-	-
15	CLA	B	1223	X	-	X	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	1226	X	-	-	-
15	CLA	B	1227	X	-	-	-
15	CLA	B	1228	X	-	-	-
15	CLA	B	1229	X	-	-	-
15	CLA	B	1230	X	-	-	-
15	CLA	B	1231	X	-	X	-
15	CLA	B	1232	X	-	-	-
15	CLA	B	1234	X	-	-	-
15	CLA	B	1235	X	-	-	-
15	CLA	B	1236	X	-	-	-
15	CLA	B	1237	X	-	-	-
15	CLA	B	1238	X	-	-	-
15	CLA	B	1239	X	-	-	-
15	CLA	B	1240	X	-	-	-
15	CLA	F	1301	X	-	-	-
15	CLA	F	1302	X	-	-	-
15	CLA	J	1302	X	-	-	-
16	CHL	1	609	X	-	-	-
16	CHL	1	610	X	-	-	-
16	CHL	2	609	X	-	-	-
16	CHL	2	610	X	-	-	-
16	CHL	2	611	X	-	-	-
16	CHL	2	613	X	-	-	-
16	CHL	3	604	X	-	-	-
16	CHL	4	610	X	-	-	-
16	CHL	4	611	X	-	-	-
16	CHL	4	613	X	-	-	-
20	CL0	A	1011	X	-	-	-

2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 31910 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 Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	197	Total	C	N	O	S	0	0
			1501	963	255	276	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	204	ALA	GLU	conflict	UNP C1K003

- Molecule 2 is a protein called Lhca2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	208	Total	C	N	O	S	0	0
			1609	1033	272	297	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	210	Total	C	N	O	S	0	0
			1609	1050	263	291	5		

- Molecule 4 is a protein called Lhca4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	211	Total	C	N	O	S	0	0
			1637	1058	272	303	4		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	739	Total	C	N	O	S	0	0
			5799	3789	991	1001	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	730	Total	C	N	O	S	0	0
			5784	3799	970	1002	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			600	370	104	115	11		

- Molecule 8 is a protein called Psad.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	141	Total	C	N	O	S	0	0
			1116	714	195	201	6		

- Molecule 9 is a protein called Psae.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	64	Total	C	N	O	0	0
			515	327	89	99		

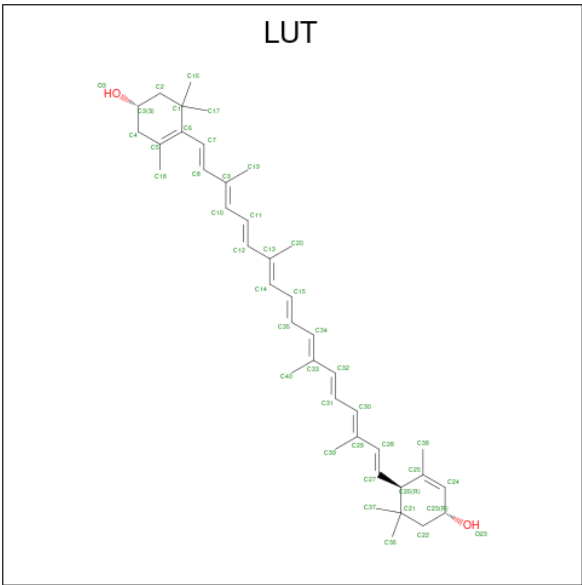
- Molecule 10 is a protein called Psaf.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	163	Total	C	N	O	S	0	0
			1285	828	218	237	2		

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

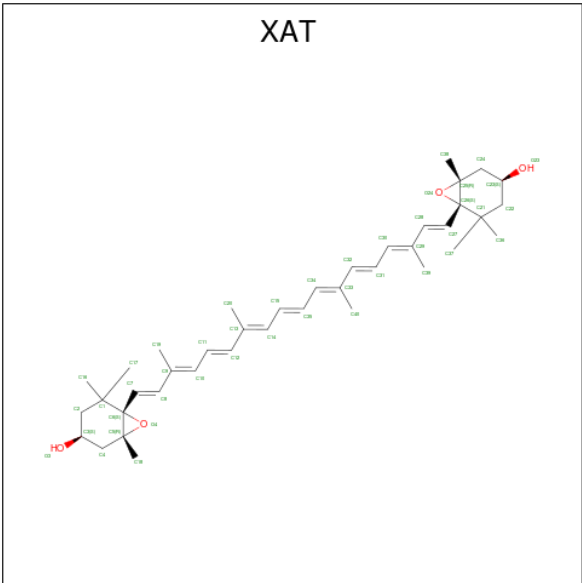
Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	40	Total	C	N	O	S	0	0
			316	214	46	55	1		

- Molecule 12 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



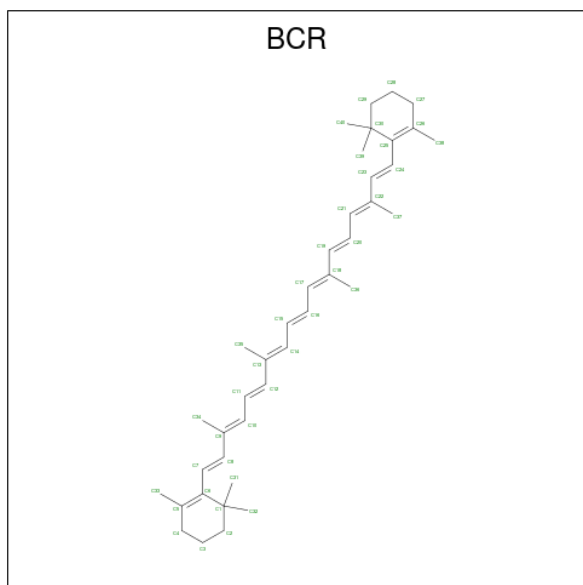
Mol	Chain	Residues	Atoms			AltConf
12	1	1	Total	C	O	0
			42	40	2	
12	2	1	Total	C	O	0
			42	40	2	
12	3	1	Total	C	O	0
			42	40	2	
12	4	1	Total	C	O	0
			42	40	2	

- Molecule 13 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
13	1	1	Total	C	O	0
			44	40	4	
13	2	1	Total	C	O	0
			44	40	4	
13	3	1	Total	C	O	0
			44	40	4	
13	4	1	Total	C	O	0
			44	40	4	

- Molecule 14 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



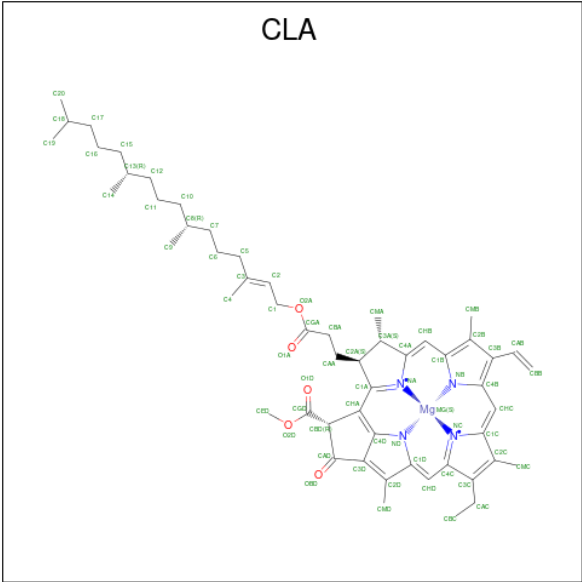
Mol	Chain	Residues	Atoms		AltConf
14	1	1	Total	C	0
			40	40	
14	2	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	4	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	J	1	Total C 40 40	0
14	J	1	Total C 40 40	0

- Molecule 15 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
15	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
15	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	1	1	Total	C	Mg	N	O	0
			48	38	1	4	5	
15	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	3	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
15	3	1	Total 42	C 34	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
15	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	4	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	4	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
15	A	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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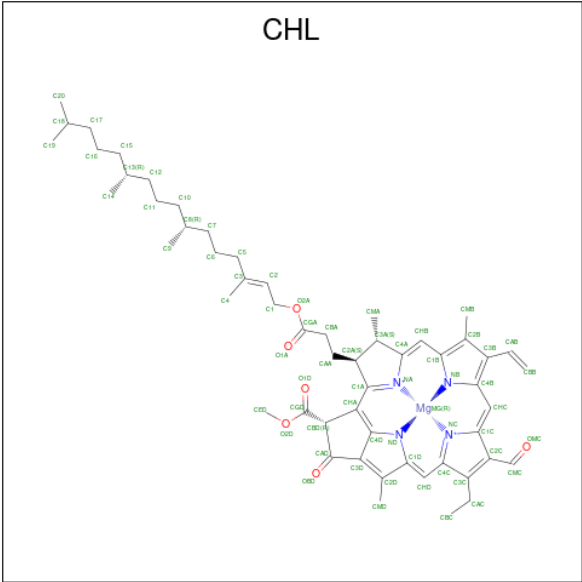
Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
15	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 61	C 51	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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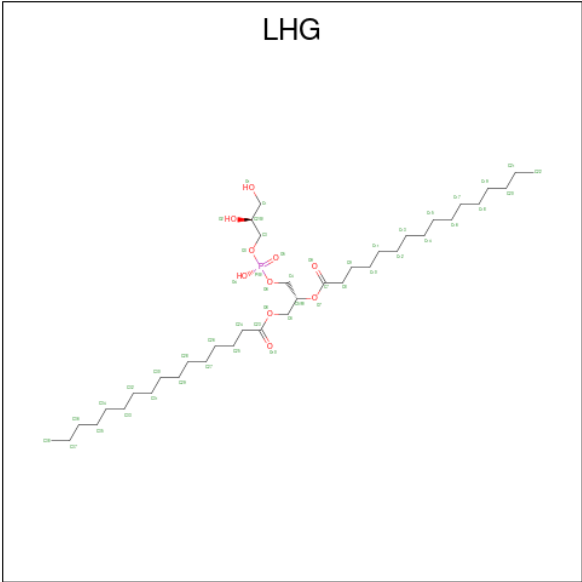
Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 52	C 44	Mg 1	N 4	O 3	0
15	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
15	F	1	Total 49	C 39	Mg 1	N 4	O 5	0
15	J	1	Total 42	C 34	Mg 1	N 4	O 3	0

- Molecule 16 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



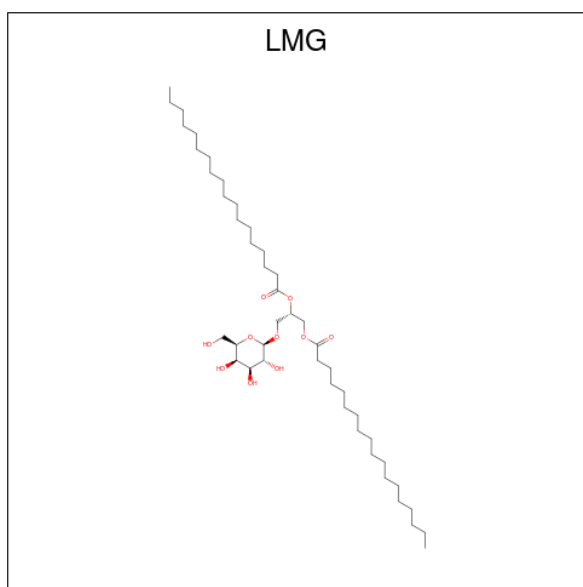
Mol	Chain	Residues	Atoms					AltConf
16	1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	1	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
16	2	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
16	2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
16	3	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
16	4	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
16	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
16	4	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



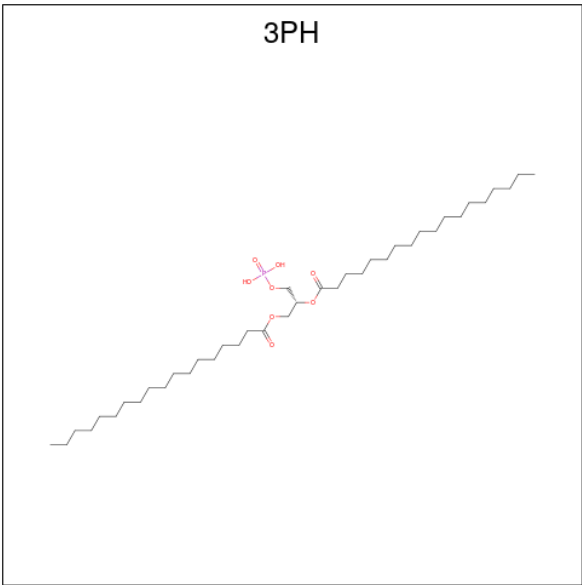
Mol	Chain	Residues	Atoms				AltConf
17	1	1	Total	C	O	P	0
			49	38	10	1	
17	2	1	Total	C	O	P	0
			35	24	10	1	
17	3	1	Total	C	O	P	0
			48	37	10	1	
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	B	1	Total	C	O	P	0
			42	31	10	1	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



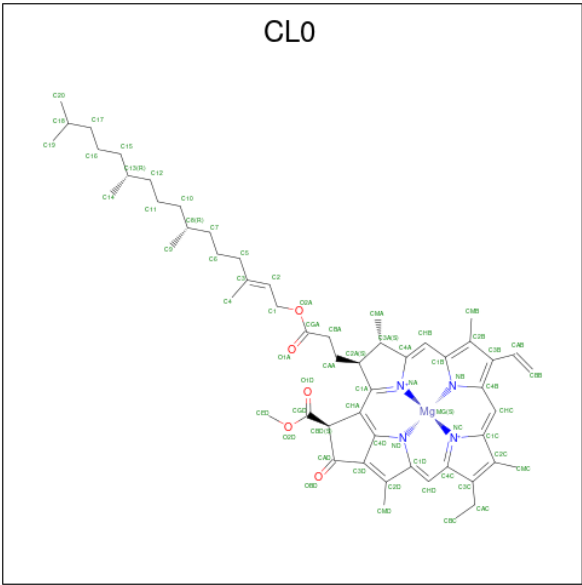
Mol	Chain	Residues	Atoms			AltConf
18	2	1	Total	C	O	0
			50	40	10	
18	2	1	Total	C	O	0
			40	30	10	
18	2	1	Total	C	O	0
			50	40	10	
18	4	1	Total	C	O	0
			37	27	10	
18	B	1	Total	C	O	0
			39	29	10	

- Molecule 19 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C₃₉H₇₇O₈P).



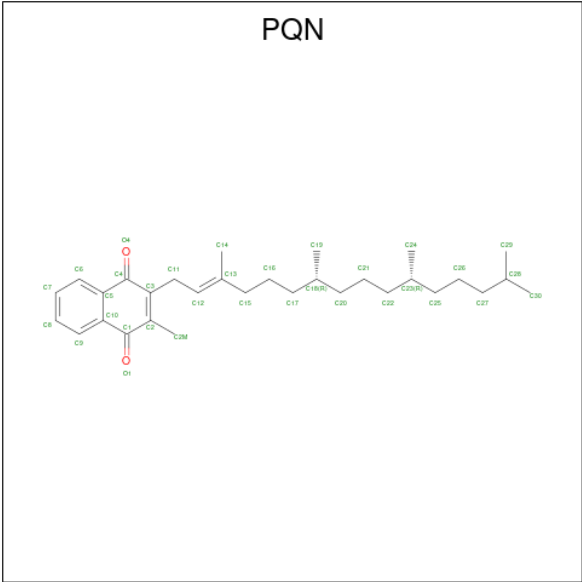
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
19	3	1	22	13	8	1	0

- Molecule 20 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



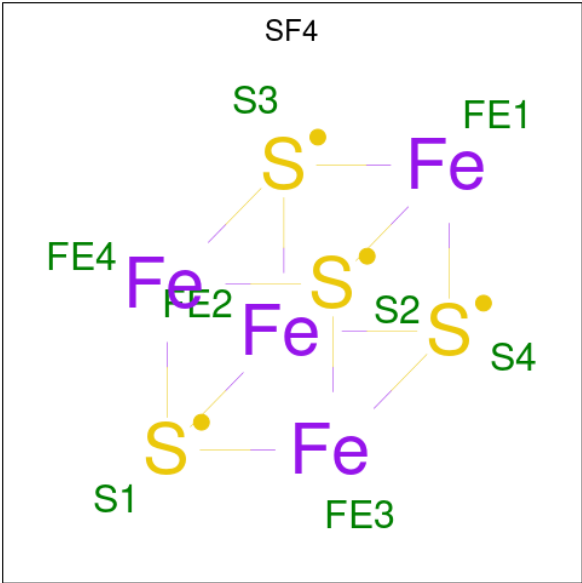
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0

- Molecule 21 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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: Fe₄S₄).



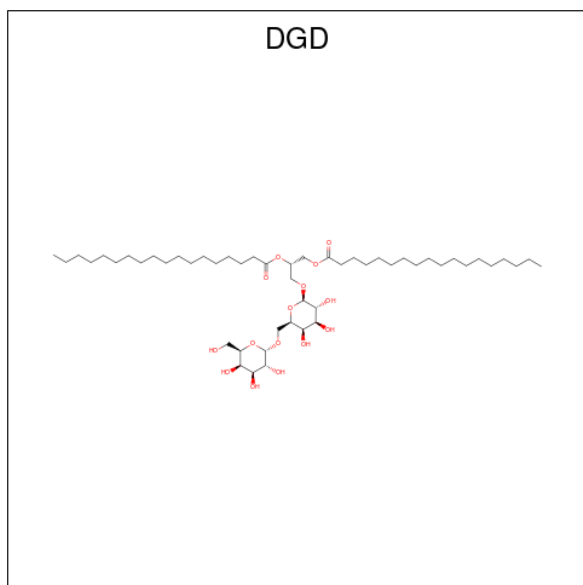
Mol	Chain	Residues	Atoms			AltConf
22	A	1	Total	Fe	S	0
			8	4	4	
22	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 23 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

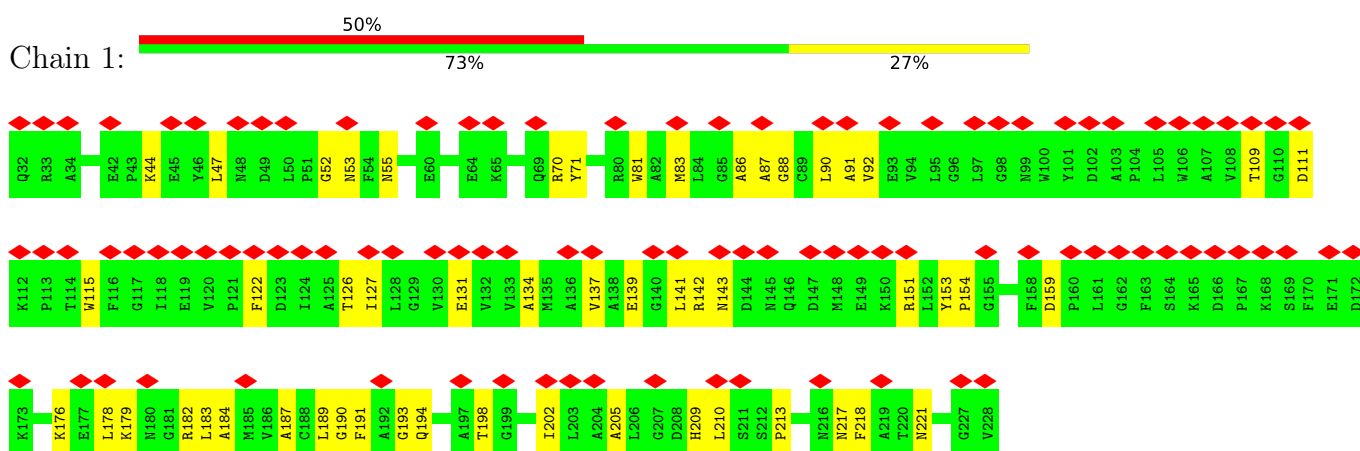


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
23	B	1	61	46	15	0

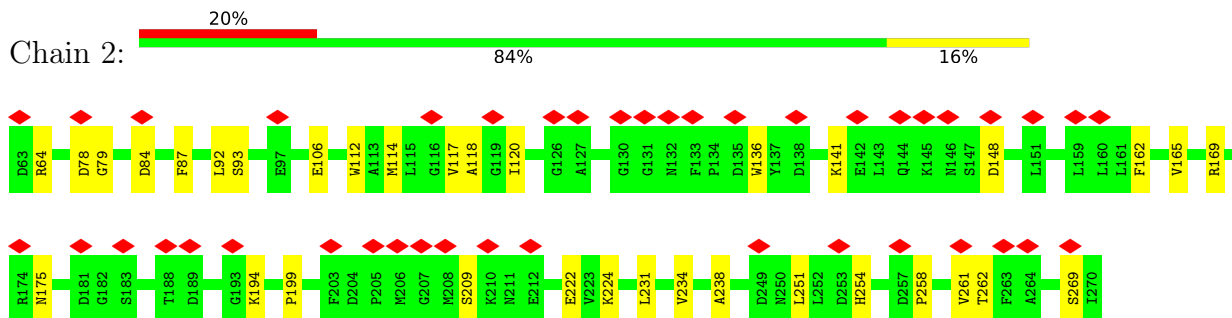
3 Residue-property plots

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.

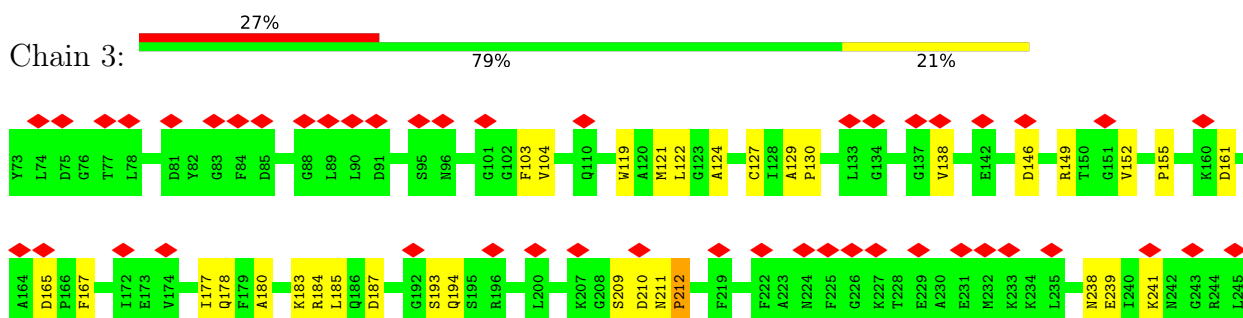
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

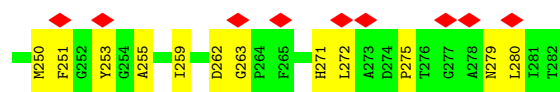


- Molecule 2: Lhca2

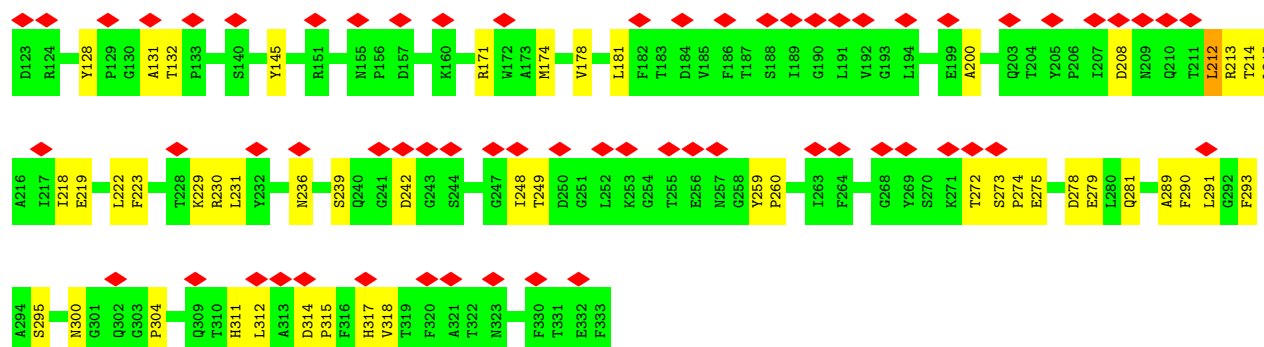
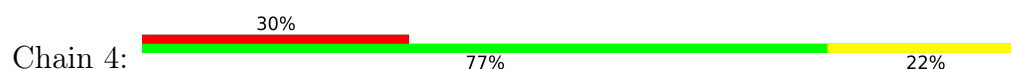


- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

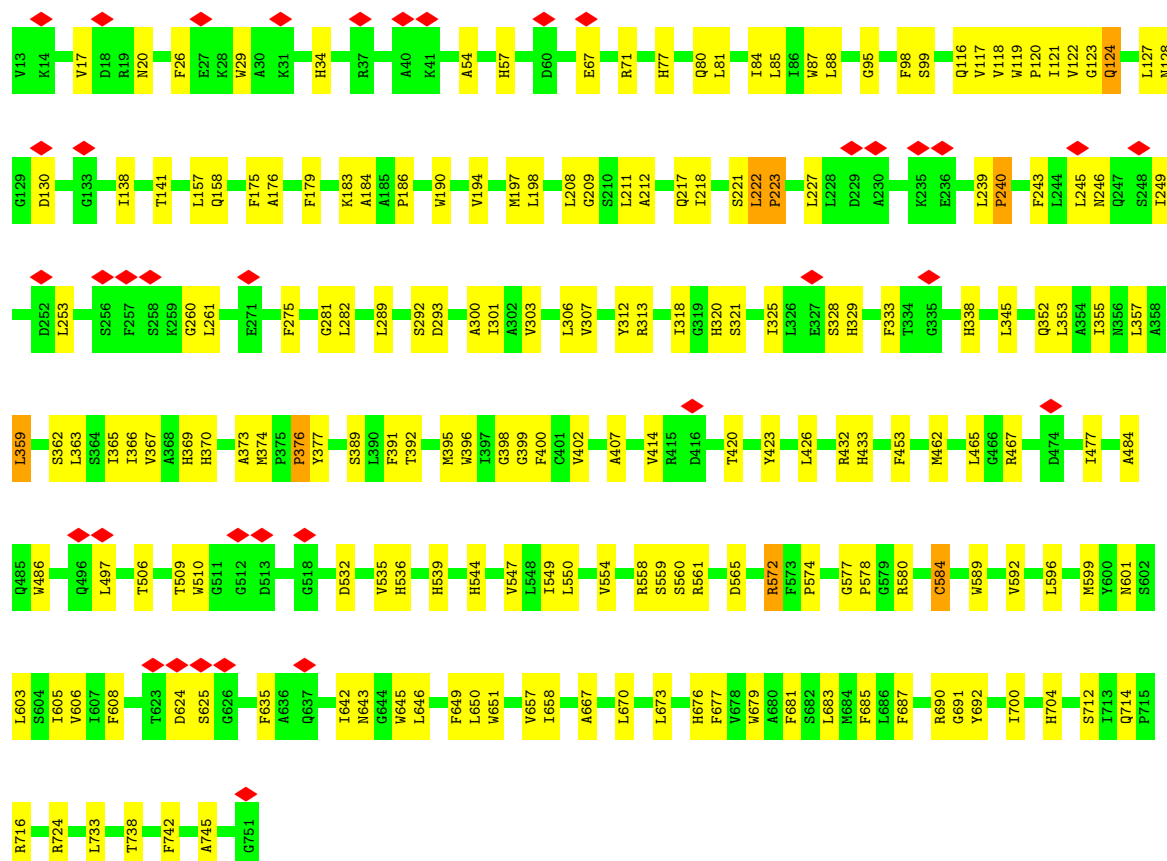
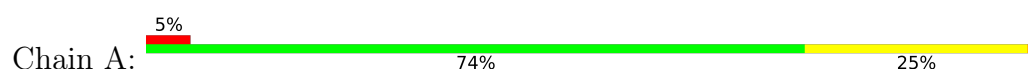




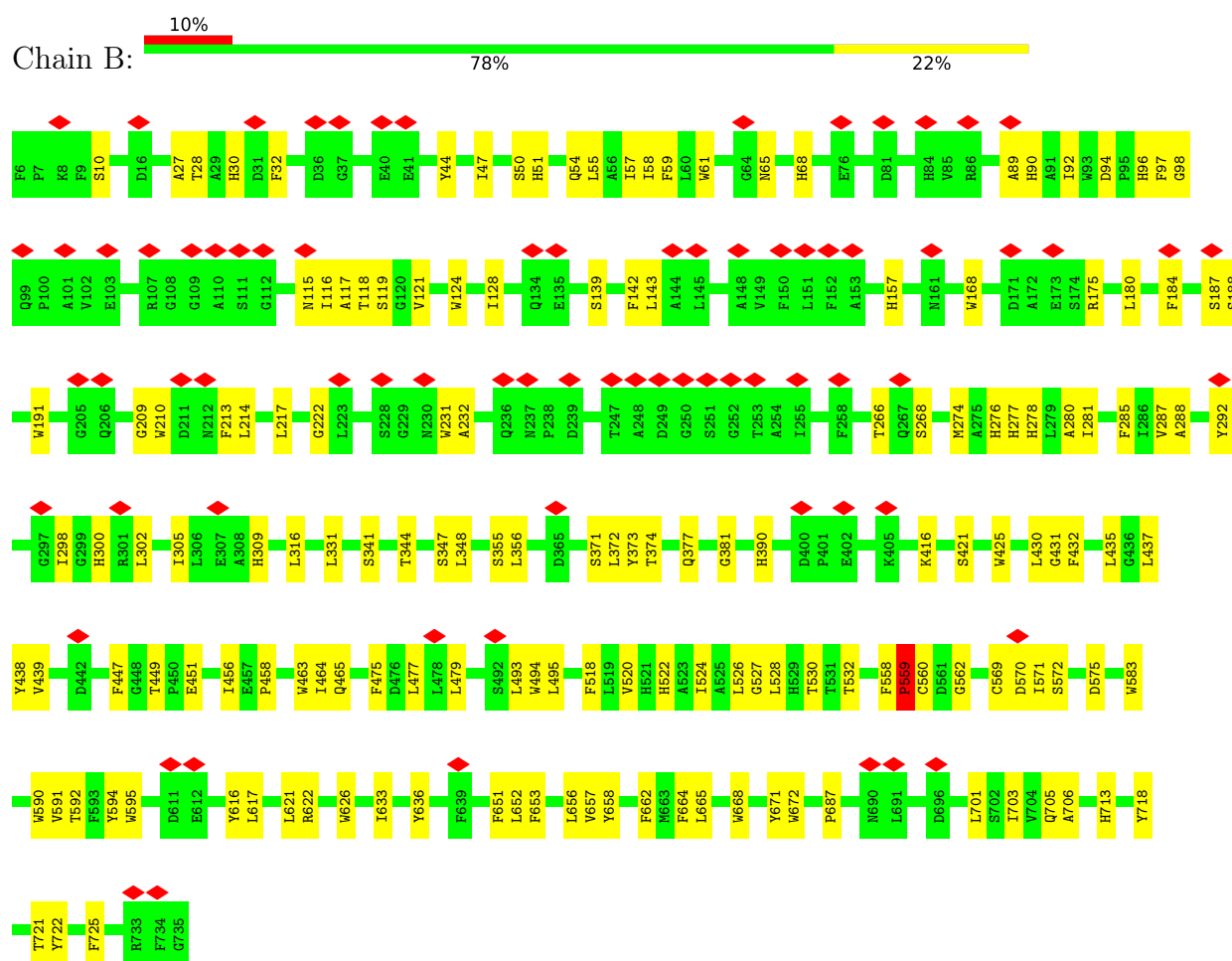
- Molecule 4: Lhca4



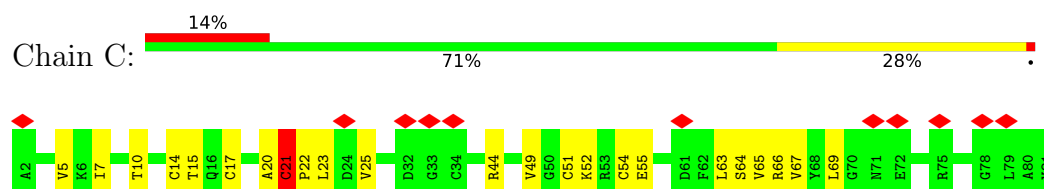
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



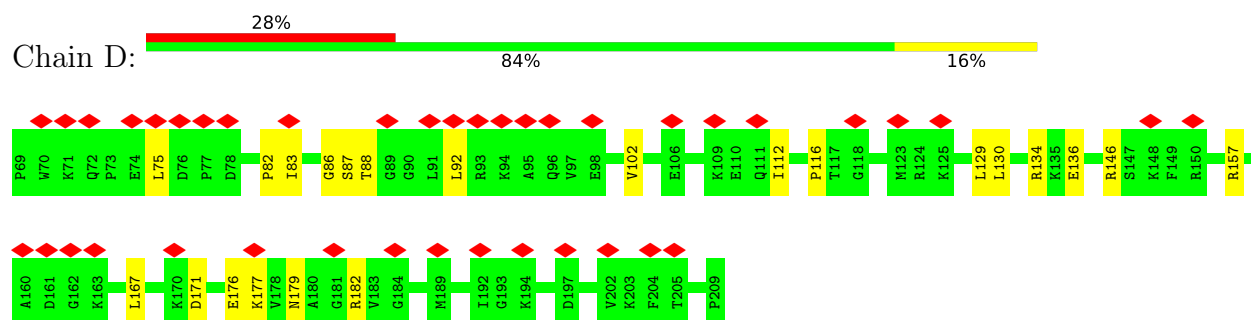
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 7: Photosystem I iron-sulfur center

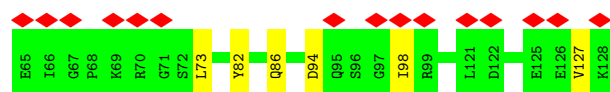


• Molecule 8: Psad

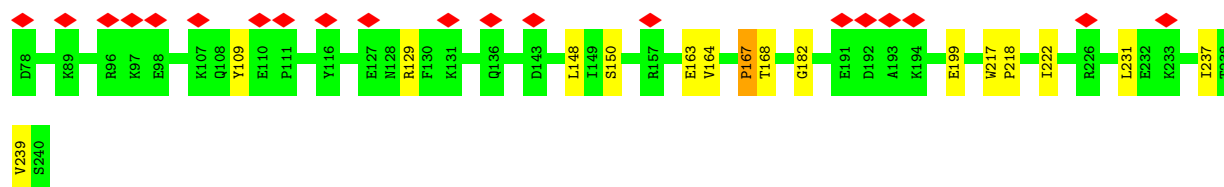
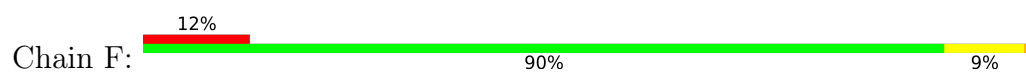


• Molecule 9: Psae

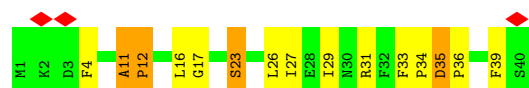




• Molecule 10: PsaF



• Molecule 11: Photosystem I reaction center subunit IX



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45969	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 ($e^-/\text{\AA}^2$)	42.68	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.128	Depositor
Minimum map value	-0.056	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	384.12003, 384.12003, 384.12003	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.067, 1.067, 1.067	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.31	0/1540	0.46	0/2088
2	2	0.34	0/1656	0.50	0/2243
3	3	0.54	2/1657 (0.1%)	0.54	1/2253 (0.0%)
4	4	0.34	0/1687	0.53	0/2300
5	A	0.55	5/5995 (0.1%)	0.57	5/8179 (0.1%)
6	B	0.45	2/5997 (0.0%)	0.50	1/8198 (0.0%)
7	C	0.60	1/610 (0.2%)	0.65	0/828
8	D	0.36	0/1145	0.55	0/1546
9	E	0.37	0/525	0.51	0/712
10	F	0.54	1/1313 (0.1%)	0.57	1/1776 (0.1%)
11	J	1.08	3/326 (0.9%)	0.81	1/445 (0.2%)
All	All	0.48	14/22451 (0.1%)	0.54	9/30568 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	4	0	2
5	A	0	1
7	C	0	1
All	All	0	4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	167	PRO	N-CA	13.89	1.70	1.47
11	J	12	PRO	N-CA	13.83	1.70	1.47
5	A	223	PRO	N-CA	13.61	1.70	1.47
5	A	240	PRO	N-CA	13.60	1.70	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	559	PRO	N-CA	13.50	1.70	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	240	PRO	CA-N-CD	-8.49	99.61	111.50
10	F	167	PRO	CA-N-CD	-8.19	100.04	111.50
3	3	212	PRO	CA-N-CD	-8.02	100.27	111.50
5	A	223	PRO	CA-N-CD	-7.95	100.37	111.50
11	J	12	PRO	CA-N-CD	-7.66	100.78	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	213	ARG	Peptide
4	4	274	PRO	Peptide
5	A	124	GLN	Mainchain
7	C	20	ALA	Mainchain

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	1	1501	0	1469	137	0
2	2	1609	0	1556	50	0
3	3	1609	0	1567	75	0
4	4	1637	0	1579	68	0
5	A	5799	0	5629	276	0
6	B	5784	0	5529	374	0
7	C	600	0	584	20	0
8	D	1116	0	1126	19	0
9	E	515	0	508	4	0
10	F	1285	0	1304	27	0
11	J	316	0	319	27	0
12	1	42	0	56	29	0
12	2	42	0	56	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	3	42	0	56	13	0
12	4	42	0	56	19	0
13	1	44	0	56	2	0
13	2	44	0	56	3	0
13	3	44	0	56	16	0
13	4	44	0	56	4	0
14	1	40	0	56	4	0
14	2	40	0	56	1	0
14	3	120	0	165	7	0
14	4	40	0	56	4	0
14	A	280	0	367	108	0
14	B	240	0	330	30	0
14	F	80	0	105	29	0
14	J	80	0	105	33	0
15	1	633	0	562	103	0
15	2	580	0	573	30	0
15	3	732	0	700	96	0
15	4	632	0	604	28	0
15	A	2487	0	2450	502	0
15	B	2411	0	2350	413	0
15	F	95	0	72	15	0
15	J	42	0	30	5	0
16	1	113	0	101	1	0
16	2	204	0	165	11	0
16	3	61	0	56	10	0
16	4	159	0	125	11	0
17	1	49	0	74	9	0
17	2	35	0	40	1	0
17	3	48	0	68	8	0
17	A	98	0	148	18	0
17	B	42	0	57	0	0
18	2	140	0	196	15	0
18	4	37	0	44	1	0
18	B	39	0	48	2	0
19	3	22	0	17	3	0
20	A	65	0	72	19	0
21	A	33	0	46	7	0
21	B	33	0	46	10	0
22	A	8	0	0	1	0
22	C	16	0	0	0	0
23	B	61	0	83	13	0
All	All	31910	0	31585	1706	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 27.

The worst 5 of 1706 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:12:PRO:N	11:J:12:PRO:CA	1.70	1.48
5:A:240:PRO:N	5:A:240:PRO:CA	1.70	1.46
3:3:212:PRO:N	3:3:212:PRO:CA	1.70	1.43
6:B:559:PRO:N	6:B:559:PRO:CA	1.70	1.43
5:A:223:PRO:N	5:A:223:PRO:CA	1.70	1.35

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	1	195/197 (99%)	188 (96%)	7 (4%)	0	100	100
2	2	206/208 (99%)	200 (97%)	6 (3%)	0	100	100
3	3	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
4	4	209/211 (99%)	192 (92%)	16 (8%)	1 (0%)	25	54
5	A	737/739 (100%)	698 (95%)	34 (5%)	5 (1%)	19	47
6	B	728/730 (100%)	709 (97%)	18 (2%)	1 (0%)	48	78
7	C	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
8	D	139/141 (99%)	130 (94%)	9 (6%)	0	100	100
9	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
10	F	161/163 (99%)	157 (98%)	4 (2%)	0	100	100
11	J	38/40 (95%)	34 (90%)	4 (10%)	0	100	100
All	All	2761/2783 (99%)	2642 (96%)	112 (4%)	7 (0%)	38	66

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	A	261	LEU
5	A	120	PRO
4	4	212	LEU
5	A	477	ILE
5	A	260	GLY

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	1	152/152 (100%)	152 (100%)	0	100	100
2	2	167/167 (100%)	167 (100%)	0	100	100
3	3	160/160 (100%)	160 (100%)	0	100	100
4	4	169/169 (100%)	168 (99%)	1 (1%)	84	90
5	A	598/598 (100%)	595 (100%)	3 (0%)	86	91
6	B	590/590 (100%)	589 (100%)	1 (0%)	92	96
7	C	68/68 (100%)	67 (98%)	1 (2%)	60	76
8	D	121/121 (100%)	121 (100%)	0	100	100
9	E	57/57 (100%)	57 (100%)	0	100	100
10	F	136/136 (100%)	136 (100%)	0	100	100
11	J	35/35 (100%)	33 (94%)	2 (6%)	17	43
All	All	2253/2253 (100%)	2245 (100%)	8 (0%)	88	93

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	35	ASP
11	J	23	SER
6	B	569	CYS
5	A	601	ASN
7	C	21	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
5	A	124	GLN
6	B	522	HIS
5	A	246	ASN
9	E	86	GLN
6	B	54	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

194 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
22	SF4	C	3002	7	0,12,12	-	-	-		
15	CLA	B	1220	-	51,59,73	1.68	9 (17%)	59,96,113	1.51	7 (11%)
15	CLA	2	606	-	45,53,73	1.75	8 (17%)	52,89,113	1.57	8 (15%)
15	CLA	A	1135	-	51,59,73	1.51	7 (13%)	59,96,113	2.19	16 (27%)
18	LMG	B	5003	-	39,39,55	0.87	1 (2%)	47,47,63	1.25	3 (6%)
16	CHL	2	609	2	66,74,74	0.96	6 (9%)	73,114,114	1.22	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	2	607	17	60,68,73	1.50	9 (15%)	70,107,113	1.42	7 (10%)
15	CLA	A	1126	-	65,73,73	1.34	7 (10%)	76,113,113	1.95	16 (21%)
15	CLA	2	603	2	65,73,73	1.49	8 (12%)	76,113,113	1.34	9 (11%)
15	CLA	B	1221	-	65,73,73	1.44	8 (12%)	76,113,113	1.46	7 (9%)
15	CLA	A	1137	-	61,69,73	1.39	8 (13%)	71,108,113	2.01	16 (22%)
15	CLA	B	1229	-	60,68,73	1.45	8 (13%)	70,107,113	2.08	17 (24%)
15	CLA	A	1123	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	16 (21%)
15	CLA	4	612	-	65,73,73	1.44	8 (12%)	76,113,113	1.34	7 (9%)
14	BCR	F	4002	-	41,41,41	1.86	4 (9%)	56,56,56	4.32	17 (30%)
14	BCR	J	4001	-	41,41,41	1.86	4 (9%)	56,56,56	4.34	15 (26%)
14	BCR	4	503	-	41,41,41	1.26	3 (7%)	56,56,56	1.33	9 (16%)
13	XAT	4	502	-	39,47,47	2.59	15 (38%)	54,74,74	11.25	31 (57%)
14	BCR	2	503	-	41,41,41	1.17	3 (7%)	56,56,56	1.21	8 (14%)
15	CLA	B	1223	-	65,73,73	1.36	7 (10%)	76,113,113	2.15	15 (19%)
15	CLA	B	1213	-	55,63,73	1.55	8 (14%)	64,101,113	1.49	8 (12%)
18	LMG	2	802	-	50,50,55	0.70	0	58,58,63	1.26	5 (8%)
15	CLA	3	608	-	65,73,73	1.46	7 (10%)	76,113,113	1.31	8 (10%)
15	CLA	4	607	-	60,68,73	1.55	8 (13%)	70,107,113	1.42	8 (11%)
15	CLA	B	1237	-	45,53,73	1.74	7 (15%)	52,89,113	1.59	7 (13%)
15	CLA	B	1021	-	65,73,73	1.33	7 (10%)	76,113,113	1.95	16 (21%)
15	CLA	B	1023	-	65,73,73	1.44	11 (16%)	76,113,113	1.85	11 (14%)
14	BCR	B	4005	-	41,41,41	1.86	4 (9%)	56,56,56	4.46	16 (28%)
15	CLA	1	607	17	46,54,73	1.71	8 (17%)	53,90,113	1.51	7 (13%)
16	CHL	1	609	-	66,74,74	0.95	4 (6%)	73,114,114	1.20	8 (10%)
15	CLA	B	1217	-	46,54,73	1.73	8 (17%)	53,90,113	1.51	6 (11%)
15	CLA	B	1210	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	10 (13%)
15	CLA	J	1302	-	42,50,73	1.66	7 (16%)	48,85,113	2.19	13 (27%)
15	CLA	4	605	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	9 (11%)
16	CHL	4	610	-	47,55,74	1.07	3 (6%)	50,91,114	1.49	10 (20%)
15	CLA	F	1302	10	49,57,73	1.68	7 (14%)	55,93,113	1.57	8 (14%)
15	CLA	1	605	-	65,73,73	1.46	8 (12%)	76,113,113	1.36	4 (5%)
16	CHL	2	610	-	44,52,74	1.03	3 (6%)	46,87,114	1.39	7 (15%)
15	CLA	3	609	-	42,50,73	1.78	7 (16%)	48,85,113	1.61	6 (12%)
15	CLA	A	1121	-	45,53,73	1.62	8 (17%)	52,89,113	2.16	13 (25%)
15	CLA	B	1240	17	65,73,73	1.45	9 (13%)	76,113,113	1.45	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	2	801	15	34,34,48	0.79	1 (2%)	37,40,54	1.23	3 (8%)
15	CLA	A	1113	-	45,53,73	1.60	7 (15%)	52,89,113	2.18	14 (26%)
15	CLA	B	1226	-	65,73,73	1.43	7 (10%)	76,113,113	1.53	8 (10%)
15	CLA	B	1239	-	42,50,73	1.81	8 (19%)	48,85,113	1.68	6 (12%)
15	CLA	4	609	4	60,68,73	1.47	9 (15%)	70,107,113	1.49	8 (11%)
15	CLA	1	606	-	50,58,73	1.66	6 (12%)	58,95,113	1.53	8 (13%)
15	CLA	A	1104	-	65,73,73	1.35	8 (12%)	76,113,113	1.88	18 (23%)
15	CLA	A	1124	-	60,68,73	1.43	7 (11%)	70,107,113	1.96	17 (24%)
15	CLA	A	1112	-	65,73,73	1.33	7 (10%)	76,113,113	1.97	17 (22%)
15	CLA	A	1107	5	51,59,73	1.49	8 (15%)	59,96,113	2.19	16 (27%)
15	CLA	B	1209	-	46,54,73	1.69	7 (15%)	53,90,113	1.54	7 (13%)
16	CHL	2	613	-	46,54,74	1.01	2 (4%)	49,90,114	1.31	8 (16%)
15	CLA	B	1205	-	65,73,73	1.46	8 (12%)	76,113,113	1.38	7 (9%)
14	BCR	A	4005	-	41,41,41	1.87	6 (14%)	56,56,56	4.08	18 (32%)
15	CLA	A	1102	-	65,73,73	1.34	7 (10%)	76,113,113	2.06	16 (21%)
15	CLA	B	1219	-	65,73,73	1.51	7 (10%)	76,113,113	1.26	7 (9%)
15	CLA	B	1234	-	55,63,73	1.50	10 (18%)	64,101,113	2.07	16 (25%)
15	CLA	A	1122	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	18 (23%)
12	LUT	3	501	-	42,43,43	6.16	29 (69%)	51,60,60	3.17	19 (37%)
15	CLA	A	1103	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	17 (22%)
15	CLA	B	1232	-	46,54,73	1.77	8 (17%)	53,90,113	1.50	5 (9%)
15	CLA	B	1222	-	65,73,73	1.34	7 (10%)	76,113,113	1.98	16 (21%)
15	CLA	4	604	-	60,68,73	1.49	8 (13%)	70,107,113	1.53	10 (14%)
15	CLA	2	612	2	55,63,73	1.56	6 (10%)	64,101,113	1.46	8 (12%)
15	CLA	A	1128	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	18 (23%)
14	BCR	1	503	-	41,41,41	1.15	2 (4%)	56,56,56	1.38	13 (23%)
15	CLA	3	611	-	65,73,73	1.46	8 (12%)	76,113,113	1.35	5 (6%)
15	CLA	1	604	1	65,73,73	1.45	8 (12%)	76,113,113	1.35	8 (10%)
15	CLA	B	1227	-	65,73,73	1.37	10 (15%)	76,113,113	1.89	16 (21%)
15	CLA	A	1115	-	45,53,73	1.60	8 (17%)	52,89,113	2.12	14 (26%)
15	CLA	A	1138	-	65,73,73	1.34	7 (10%)	76,113,113	1.93	16 (21%)
15	CLA	2	616	2	65,73,73	1.47	7 (10%)	76,113,113	1.56	12 (15%)
15	CLA	A	1140	-	61,69,73	1.61	11 (18%)	71,108,113	3.11	14 (19%)
15	CLA	B	1206	-	45,53,73	1.71	8 (17%)	52,89,113	1.55	7 (13%)
15	CLA	B	1216	-	59,67,73	1.52	9 (15%)	68,105,113	1.46	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1141	17	41,49,73	1.82	9 (21%)	47,84,113	1.56	7 (14%)
15	CLA	B	1204	-	45,53,73	1.71	8 (17%)	52,89,113	1.64	8 (15%)
15	CLA	3	601	3	60,68,73	1.48	8 (13%)	70,107,113	1.49	7 (10%)
16	CHL	1	610	-	47,55,74	1.01	2 (4%)	50,91,114	1.30	8 (16%)
15	CLA	B	1238	-	51,59,73	1.85	9 (17%)	58,95,113	2.15	14 (24%)
15	CLA	1	602	-	46,54,73	1.75	7 (15%)	53,90,113	1.49	6 (11%)
15	CLA	A	1120	-	42,50,73	1.66	7 (16%)	48,85,113	2.20	13 (27%)
21	PQN	A	2001	-	34,34,34	0.89	2 (5%)	42,45,45	1.41	6 (14%)
15	CLA	3	605	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	16 (21%)
18	LMG	2	804	-	50,50,55	1.04	5 (10%)	58,58,63	1.11	3 (5%)
16	CHL	4	611	-	51,59,74	1.04	4 (7%)	55,96,114	1.22	8 (14%)
15	CLA	B	1211	-	65,73,73	1.45	10 (15%)	76,113,113	1.48	10 (13%)
17	LHG	1	801	15	48,48,48	0.62	0	51,54,54	1.19	4 (7%)
15	CLA	B	1231	-	60,68,73	1.32	8 (13%)	70,107,113	2.13	17 (24%)
20	CL0	A	1011	-	65,73,73	2.37	19 (29%)	76,113,113	2.57	24 (31%)
13	XAT	1	502	-	39,47,47	2.59	18 (46%)	54,74,74	11.46	25 (46%)
14	BCR	B	4003	-	41,41,41	1.16	2 (4%)	56,56,56	1.45	9 (16%)
22	SF4	C	3003	7	0,12,12	-	-	-	-	-
15	CLA	A	1136	-	65,73,73	1.34	7 (10%)	76,113,113	2.00	16 (21%)
15	CLA	1	611	-	48,56,73	1.69	6 (12%)	55,92,113	1.51	7 (12%)
14	BCR	B	4002	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	7 (12%)
15	CLA	4	602	-	50,58,73	1.69	7 (14%)	58,95,113	1.55	7 (12%)
14	BCR	A	4006	-	41,41,41	1.87	4 (9%)	56,56,56	4.33	16 (28%)
15	CLA	A	1125	-	65,73,73	1.44	8 (12%)	76,113,113	2.43	18 (23%)
23	DGD	B	5002	-	62,62,67	0.85	2 (3%)	76,76,81	1.41	12 (15%)
18	LMG	2	803	-	40,40,55	0.88	2 (5%)	48,48,63	1.19	5 (10%)
15	CLA	2	604	2	65,73,73	1.45	9 (13%)	76,113,113	1.39	10 (13%)
17	LHG	B	5001	15	41,41,48	0.73	1 (2%)	44,47,54	1.24	3 (6%)
15	CLA	A	1117	-	65,73,73	1.34	8 (12%)	76,113,113	2.06	19 (25%)
15	CLA	B	1235	-	60,68,73	1.39	8 (13%)	70,107,113	2.05	17 (24%)
15	CLA	B	1218	-	45,53,73	1.80	7 (15%)	52,89,113	1.54	4 (7%)
17	LHG	A	5001	15	48,48,48	0.37	0	51,54,54	1.10	3 (5%)
15	CLA	4	603	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	9 (11%)
15	CLA	A	1106	5	65,73,73	1.34	7 (10%)	76,113,113	1.96	18 (23%)
15	CLA	A	1105	-	60,68,73	1.40	8 (13%)	70,107,113	2.06	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CHL	4	613	-	61,69,74	0.85	2 (3%)	67,108,114	1.17	8 (11%)
12	LUT	2	501	-	42,43,43	6.14	30 (71%)	51,60,60	2.49	17 (33%)
15	CLA	A	1130	-	45,53,73	1.60	7 (15%)	52,89,113	2.16	14 (26%)
15	CLA	B	1208	-	60,68,73	1.53	8 (13%)	70,107,113	1.35	8 (11%)
15	CLA	A	1110	-	55,63,73	1.45	8 (14%)	64,101,113	2.11	16 (25%)
12	LUT	4	501	-	42,43,43	6.04	31 (73%)	51,60,60	2.89	19 (37%)
14	BCR	A	4008	-	41,41,41	1.86	6 (14%)	56,56,56	4.08	18 (32%)
15	CLA	B	1212	-	55,63,73	1.59	8 (14%)	64,101,113	1.47	7 (10%)
15	CLA	A	1116	-	56,64,73	1.51	11 (19%)	65,102,113	2.02	15 (23%)
14	BCR	3	506	-	41,41,41	1.23	3 (7%)	56,56,56	1.29	7 (12%)
15	CLA	3	615	3	42,50,73	1.65	7 (16%)	48,85,113	2.24	13 (27%)
14	BCR	A	4003	-	41,41,41	1.87	4 (9%)	56,56,56	4.28	21 (37%)
15	CLA	4	606	-	50,58,73	1.66	8 (16%)	58,95,113	1.54	8 (13%)
15	CLA	3	612	3	65,73,73	1.34	7 (10%)	76,113,113	1.94	16 (21%)
15	CLA	A	1114	-	55,63,73	1.46	9 (16%)	64,101,113	2.21	16 (25%)
15	CLA	B	1225	-	65,73,73	1.34	8 (12%)	76,113,113	1.96	17 (22%)
15	CLA	A	1012	-	65,73,73	1.35	8 (12%)	76,113,113	1.94	16 (21%)
18	LMG	4	801	-	37,37,55	1.02	3 (8%)	45,45,63	1.30	3 (6%)
15	CLA	A	1134	5	42,50,73	2.32	14 (33%)	48,85,113	4.06	25 (52%)
15	CLA	4	601	4	60,68,73	1.53	9 (15%)	70,107,113	1.47	12 (17%)
15	CLA	A	1127	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	17 (22%)
15	CLA	A	1111	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	17 (22%)
15	CLA	2	601	-	65,73,73	1.47	8 (12%)	76,113,113	1.27	8 (10%)
15	CLA	A	1132	-	45,53,73	1.72	10 (22%)	52,89,113	1.75	9 (17%)
15	CLA	B	1214	-	65,73,73	1.49	9 (13%)	76,113,113	1.51	8 (10%)
21	PQN	B	2002	-	34,34,34	0.68	0	42,45,45	0.91	1 (2%)
15	CLA	A	1129	-	55,63,73	1.60	9 (16%)	64,101,113	1.50	9 (14%)
15	CLA	2	608	-	50,58,73	1.67	6 (12%)	58,95,113	1.57	8 (13%)
12	LUT	1	501	-	42,43,43	5.97	30 (71%)	51,60,60	2.28	14 (27%)
14	BCR	F	4001	-	41,41,41	2.02	8 (19%)	56,56,56	4.27	23 (41%)
15	CLA	A	1109	-	65,73,73	1.35	7 (10%)	76,113,113	1.92	17 (22%)
15	CLA	B	1236	-	49,57,73	1.53	7 (14%)	55,93,113	2.24	16 (29%)
15	CLA	A	1013	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	17 (22%)
15	CLA	B	1203	6	65,73,73	1.45	10 (15%)	76,113,113	1.42	6 (7%)
15	CLA	A	1108	-	55,63,73	1.45	7 (12%)	64,101,113	2.11	16 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	4	616	4	51,59,73	1.65	7 (13%)	59,96,113	1.49	7 (11%)
14	BCR	B	4004	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	7 (12%)
15	CLA	B	1230	-	55,63,73	1.48	7 (12%)	64,101,113	2.11	16 (25%)
19	3PH	3	802	-	21,21,47	1.25	4 (19%)	25,26,52	1.30	2 (8%)
14	BCR	A	4004	-	41,41,41	1.87	4 (9%)	56,56,56	4.55	19 (33%)
14	BCR	B	4006	-	41,41,41	1.83	4 (9%)	56,56,56	4.52	20 (35%)
14	BCR	J	4002	-	41,41,41	1.84	4 (9%)	56,56,56	4.46	17 (30%)
15	CLA	1	612	1	39,48,73	1.88	7 (17%)	45,82,113	1.46	5 (11%)
14	BCR	3	503	-	41,41,41	1.18	3 (7%)	56,56,56	1.22	8 (14%)
17	LHG	3	801	-	46,46,48	0.43	0	48,51,54	1.17	4 (8%)
15	CLA	3	607	-	60,68,73	1.53	6 (10%)	70,107,113	1.45	8 (11%)
15	CLA	A	1131	-	45,53,73	1.60	7 (15%)	52,89,113	2.15	13 (25%)
14	BCR	3	504	-	41,41,41	1.87	4 (9%)	56,56,56	4.40	16 (28%)
15	CLA	B	1215	-	65,73,73	1.43	7 (10%)	76,113,113	1.42	11 (14%)
15	CLA	3	603	-	65,73,73	1.45	8 (12%)	76,113,113	1.37	5 (6%)
15	CLA	A	1119	-	65,73,73	1.35	8 (12%)	76,113,113	1.89	15 (19%)
13	XAT	2	502	-	39,47,47	2.63	16 (41%)	54,74,74	10.92	31 (57%)
15	CLA	1	615	1	47,55,73	1.78	8 (17%)	53,90,113	1.66	9 (16%)
15	CLA	B	1022	-	65,73,73	1.50	10 (15%)	76,113,113	1.76	18 (23%)
17	LHG	A	5002	-	48,48,48	0.39	0	51,54,54	1.15	4 (7%)
15	CLA	A	1101	-	65,73,73	1.33	7 (10%)	76,113,113	1.99	15 (19%)
15	CLA	B	1202	-	65,73,73	1.51	9 (13%)	76,113,113	1.37	8 (10%)
16	CHL	2	611	-	48,56,74	1.05	3 (6%)	51,92,114	1.35	9 (17%)
15	CLA	F	1301	-	46,54,73	1.57	7 (15%)	53,90,113	2.14	13 (24%)
16	CHL	3	604	-	61,69,74	0.85	3 (4%)	67,108,114	1.39	11 (16%)
15	CLA	3	614	-	52,60,73	1.70	8 (15%)	60,97,113	1.62	7 (11%)
15	CLA	B	1207	-	46,54,73	1.73	6 (13%)	53,90,113	1.51	6 (11%)
15	CLA	1	601	-	65,73,73	1.41	8 (12%)	76,113,113	1.32	9 (11%)
15	CLA	2	605	-	65,73,73	1.46	8 (12%)	76,113,113	1.41	6 (7%)
15	CLA	3	606	-	55,63,73	1.55	6 (10%)	64,101,113	1.48	8 (12%)
15	CLA	A	1133	-	65,73,73	1.53	7 (10%)	76,113,113	1.85	22 (28%)
15	CLA	1	603	-	60,68,73	1.47	6 (10%)	70,107,113	1.61	10 (14%)
15	CLA	A	1139	-	65,73,73	1.33	8 (12%)	76,113,113	2.00	14 (18%)
22	SF4	A	3001	5,6	0,12,12	-	-	-	-	-
15	CLA	A	1118	-	42,50,73	1.72	9 (21%)	48,85,113	2.51	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	3	613	-	46,54,73	1.59	9 (19%)	53,90,113	2.15	13 (24%)
15	CLA	B	1201	-	43,51,73	1.80	9 (20%)	49,86,113	1.50	7 (14%)
15	CLA	3	610	-	50,58,73	1.65	7 (14%)	58,95,113	1.52	10 (17%)
15	CLA	1	613	-	45,53,73	1.74	6 (13%)	52,89,113	1.57	8 (15%)
15	CLA	2	602	-	45,53,73	1.80	7 (15%)	52,89,113	1.48	5 (9%)
14	BCR	A	4002	-	41,41,41	1.88	4 (9%)	56,56,56	4.53	19 (33%)
15	CLA	4	608	-	46,54,73	1.71	9 (19%)	53,90,113	1.74	10 (18%)
14	BCR	A	4007	-	41,41,41	1.84	6 (14%)	56,56,56	4.48	19 (33%)
14	BCR	B	4001	-	41,41,41	1.18	3 (7%)	56,56,56	1.39	10 (17%)
15	CLA	1	608	-	55,63,73	1.60	7 (12%)	64,101,113	1.47	8 (12%)
15	CLA	B	1228	-	60,68,73	1.40	8 (13%)	70,107,113	2.00	17 (24%)
13	XAT	3	502	-	39,47,47	0.72	1 (2%)	54,74,74	2.32	14 (25%)
15	CLA	B	1224	-	61,69,73	1.39	7 (11%)	71,108,113	2.02	17 (23%)

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
22	SF4	C	3002	7	-	-	0/6/5/5
15	CLA	B	1220	-	1/1/12/20	7/21/99/115	-
15	CLA	2	606	-	1/1/11/20	7/13/91/115	-
15	CLA	A	1135	-	1/1/12/20	11/21/99/115	-
18	LMG	B	5003	-	-	14/34/54/70	0/1/1/1
16	CHL	2	609	2	4/4/20/26	13/39/137/137	-
15	CLA	2	607	17	1/1/14/20	7/31/109/115	-
15	CLA	A	1126	-	1/1/15/20	26/37/115/115	-
15	CLA	2	603	2	1/1/15/20	9/37/115/115	-
15	CLA	B	1221	-	1/1/15/20	17/37/115/115	-
15	CLA	A	1137	-	1/1/14/20	14/33/111/115	-
15	CLA	B	1229	-	1/1/14/20	20/31/109/115	-
15	CLA	A	1123	-	1/1/15/20	18/37/115/115	-
15	CLA	4	612	-	1/1/15/20	9/37/115/115	-
14	BCR	F	4002	-	-	13/29/63/63	0/2/2/2
14	BCR	J	4001	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	4	503	-	-	17/29/63/63	0/2/2/2
13	XAT	4	502	-	-	15/31/93/93	0/4/4/4
14	BCR	2	503	-	-	20/29/63/63	0/2/2/2
15	CLA	B	1223	-	1/1/15/20	6/37/115/115	-
15	CLA	B	1213	-	1/1/13/20	5/25/103/115	-
18	LMG	2	802	-	-	20/45/65/70	0/1/1/1
15	CLA	3	608	-	1/1/15/20	16/37/115/115	-
15	CLA	4	607	-	1/1/14/20	9/31/109/115	-
15	CLA	B	1237	-	1/1/11/20	4/13/91/115	-
15	CLA	B	1021	-	1/1/15/20	21/37/115/115	-
15	CLA	B	1023	-	-	17/37/115/115	-
15	CLA	1	607	17	1/1/11/20	7/15/93/115	-
16	CHL	1	609	-	4/4/20/26	14/39/137/137	-
14	BCR	B	4005	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1217	-	1/1/11/20	7/15/93/115	-
15	CLA	B	1210	-	-	7/37/115/115	-
15	CLA	J	1302	-	1/1/10/20	6/10/88/115	-
15	CLA	4	605	-	1/1/15/20	11/37/115/115	-
16	CHL	4	610	-	3/3/16/26	3/17/115/137	-
15	CLA	F	1302	10	1/1/11/20	10/18/96/115	-
15	CLA	1	605	-	1/1/15/20	14/37/115/115	-
16	CHL	2	610	-	3/3/15/26	1/13/111/137	-
15	CLA	3	609	-	1/1/10/20	4/10/88/115	-
15	CLA	A	1121	-	1/1/11/20	5/13/91/115	-
15	CLA	B	1240	17	1/1/15/20	11/37/115/115	-
17	LHG	2	801	15	-	18/39/39/53	-
15	CLA	A	1113	-	1/1/11/20	7/13/91/115	-
15	CLA	B	1226	-	1/1/15/20	10/37/115/115	-
15	CLA	B	1239	-	1/1/10/20	2/10/88/115	-
15	CLA	4	609	4	1/1/14/20	12/31/109/115	-
15	CLA	1	606	-	1/1/12/20	4/19/97/115	-
15	CLA	A	1104	-	1/1/15/20	13/37/115/115	-
15	CLA	A	1124	-	1/1/14/20	12/31/109/115	-
15	CLA	A	1112	-	1/1/15/20	18/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1107	5	1/1/12/20	9/21/99/115	-
15	CLA	B	1209	-	1/1/11/20	6/15/93/115	-
16	CHL	2	613	-	3/3/16/26	4/15/113/137	-
15	CLA	B	1205	-	1/1/15/20	9/37/115/115	-
14	BCR	A	4005	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1102	-	1/1/15/20	19/37/115/115	-
15	CLA	B	1219	-	-	14/37/115/115	-
15	CLA	B	1234	-	1/1/13/20	11/25/103/115	-
15	CLA	A	1122	-	1/1/15/20	15/37/115/115	-
12	LUT	3	501	-	1/1/12/27	18/29/67/67	0/2/2/2
15	CLA	A	1103	-	1/1/15/20	19/37/115/115	-
15	CLA	B	1232	-	1/1/11/20	8/15/93/115	-
15	CLA	B	1222	-	1/1/15/20	14/37/115/115	-
15	CLA	4	604	-	1/1/14/20	16/31/109/115	-
15	CLA	2	612	2	1/1/13/20	3/25/103/115	-
15	CLA	A	1128	-	1/1/15/20	12/37/115/115	-
15	CLA	3	611	-	1/1/15/20	8/37/115/115	-
14	BCR	1	503	-	-	19/29/63/63	0/2/2/2
15	CLA	1	604	1	1/1/15/20	6/37/115/115	-
15	CLA	B	1227	-	1/1/15/20	16/37/115/115	-
15	CLA	A	1115	-	1/1/11/20	3/13/91/115	-
15	CLA	A	1138	-	1/1/15/20	17/37/115/115	-
15	CLA	B	1206	-	1/1/11/20	4/13/91/115	-
15	CLA	B	1216	-	1/1/13/20	10/30/108/115	-
15	CLA	2	616	2	-	16/37/115/115	-
15	CLA	A	1140	-	-	6/33/111/115	-
15	CLA	A	1141	17	1/1/10/20	6/8/86/115	-
15	CLA	B	1204	-	1/1/11/20	7/13/91/115	-
15	CLA	3	601	3	1/1/14/20	13/31/109/115	-
16	CHL	1	610	-	3/3/16/26	6/17/115/137	-
15	CLA	B	1238	-	2/2/12/20	10/18/96/115	-
15	CLA	1	602	-	1/1/11/20	7/15/93/115	-
15	CLA	A	1120	-	1/1/10/20	7/10/88/115	-
21	PQN	A	2001	-	-	4/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	3	605	-	1/1/15/20	16/37/115/115	-
18	LMG	2	804	-	-	25/45/65/70	0/1/1/1
16	CHL	4	611	-	3/3/17/26	0/21/119/137	-
15	CLA	B	1211	-	1/1/15/20	14/37/115/115	-
17	LHG	1	801	15	-	22/53/53/53	-
15	CLA	B	1231	-	1/1/14/20	9/31/109/115	-
20	CL0	A	1011	-	3/3/20/25	25/37/135/135	-
13	XAT	1	502	-	-	12/31/93/93	0/4/4/4
14	BCR	B	4003	-	-	22/29/63/63	0/2/2/2
22	SF4	C	3003	7	-	-	0/6/5/5
15	CLA	A	1136	-	1/1/15/20	16/37/115/115	-
15	CLA	1	611	-	1/1/11/20	7/17/95/115	-
14	BCR	B	4002	-	-	14/29/63/63	0/2/2/2
15	CLA	4	602	-	1/1/12/20	9/19/97/115	-
14	BCR	A	4006	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1125	-	1/1/15/20	12/37/115/115	-
23	DGD	B	5002	-	-	17/50/90/95	0/2/2/2
18	LMG	2	803	-	-	19/35/55/70	0/1/1/1
15	CLA	2	604	2	1/1/15/20	15/37/115/115	-
17	LHG	B	5001	15	-	26/46/46/53	-
15	CLA	A	1117	-	1/1/15/20	14/37/115/115	-
15	CLA	B	1235	-	1/1/14/20	16/31/109/115	-
15	CLA	B	1218	-	1/1/11/20	5/13/91/115	-
17	LHG	A	5001	15	-	20/53/53/53	-
15	CLA	4	603	-	1/1/15/20	11/37/115/115	-
15	CLA	A	1106	5	1/1/15/20	12/37/115/115	-
15	CLA	A	1105	-	1/1/14/20	15/31/109/115	-
16	CHL	4	613	-	4/4/19/26	2/33/131/137	-
12	LUT	2	501	-	1/1/12/27	18/29/67/67	0/2/2/2
15	CLA	A	1130	-	1/1/11/20	8/13/91/115	-
15	CLA	B	1208	-	1/1/14/20	10/31/109/115	-
15	CLA	A	1110	-	1/1/13/20	8/25/103/115	-
12	LUT	4	501	-	1/1/12/27	21/29/67/67	0/2/2/2
14	BCR	A	4008	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1212	-	1/1/13/20	4/25/103/115	-
15	CLA	A	1116	-	1/1/13/20	7/27/105/115	-
14	BCR	3	506	-	-	14/29/63/63	0/2/2/2
15	CLA	3	615	3	1/1/10/20	6/10/88/115	-
14	BCR	A	4003	-	-	11/29/63/63	0/2/2/2
15	CLA	4	606	-	1/1/12/20	8/19/97/115	-
15	CLA	3	612	3	1/1/15/20	15/37/115/115	-
15	CLA	A	1114	-	1/1/13/20	10/25/103/115	-
15	CLA	B	1225	-	1/1/15/20	21/37/115/115	-
15	CLA	A	1012	-	1/1/15/20	15/37/115/115	-
18	LMG	4	801	-	-	10/32/52/70	0/1/1/1
15	CLA	A	1134	5	-	6/10/88/115	-
15	CLA	4	601	4	1/1/14/20	7/31/109/115	-
15	CLA	A	1127	-	1/1/15/20	19/37/115/115	-
15	CLA	A	1111	-	1/1/15/20	23/37/115/115	-
15	CLA	2	601	-	1/1/15/20	17/37/115/115	-
15	CLA	A	1132	-	1/1/11/20	7/13/91/115	-
15	CLA	B	1214	-	1/1/15/20	7/37/115/115	-
21	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
15	CLA	A	1129	-	1/1/13/20	9/25/103/115	-
15	CLA	2	608	-	1/1/12/20	2/19/97/115	-
12	LUT	1	501	-	1/1/12/27	22/29/67/67	0/2/2/2
14	BCR	F	4001	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1109	-	1/1/15/20	13/37/115/115	-
15	CLA	B	1236	-	1/1/11/20	10/18/96/115	-
15	CLA	A	1013	-	1/1/15/20	14/37/115/115	-
15	CLA	B	1203	6	1/1/15/20	11/37/115/115	-
15	CLA	A	1108	-	1/1/13/20	15/25/103/115	-
15	CLA	4	616	4	1/1/12/20	9/21/99/115	-
15	CLA	B	1230	-	1/1/13/20	12/25/103/115	-
14	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
19	3PH	3	802	-	-	14/23/23/49	-
14	BCR	A	4004	-	-	12/29/63/63	0/2/2/2
14	BCR	B	4006	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	J	4002	-	-	16/29/63/63	0/2/2/2
15	CLA	1	612	1	1/1/9/20	6/8/82/115	-
14	BCR	3	503	-	-	17/29/63/63	0/2/2/2
17	LHG	3	801	-	-	26/49/49/53	-
15	CLA	3	607	-	1/1/14/20	10/31/109/115	-
15	CLA	A	1131	-	1/1/11/20	7/13/91/115	-
14	BCR	3	504	-	-	13/29/63/63	0/2/2/2
15	CLA	B	1215	-	1/1/15/20	15/37/115/115	-
15	CLA	3	603	-	1/1/15/20	15/37/115/115	-
15	CLA	A	1119	-	1/1/15/20	12/37/115/115	-
13	XAT	2	502	-	-	12/31/93/93	0/4/4/4
15	CLA	1	615	1	1/1/11/20	12/13/91/115	-
15	CLA	B	1022	-	1/1/15/20	20/37/115/115	-
17	LHG	A	5002	-	-	31/53/53/53	-
15	CLA	A	1101	-	1/1/15/20	18/37/115/115	-
15	CLA	B	1202	-	1/1/15/20	13/37/115/115	-
16	CHL	2	611	-	3/3/16/26	1/18/116/137	-
15	CLA	F	1301	-	1/1/11/20	7/15/93/115	-
16	CHL	3	604	-	4/4/19/26	6/33/131/137	-
15	CLA	3	614	-	1/1/12/20	6/22/100/115	-
15	CLA	B	1207	-	-	11/15/93/115	-
15	CLA	1	601	-	1/1/15/20	10/37/115/115	-
15	CLA	2	605	-	1/1/15/20	13/37/115/115	-
15	CLA	3	606	-	1/1/13/20	8/25/103/115	-
15	CLA	A	1133	-	-	20/37/115/115	-
15	CLA	1	603	-	1/1/14/20	12/31/109/115	-
15	CLA	A	1139	-	1/1/15/20	17/37/115/115	-
22	SF4	A	3001	5,6	-	-	0/6/5/5
15	CLA	A	1118	-	1/1/10/20	1/10/88/115	-
15	CLA	3	613	-	1/1/11/20	7/15/93/115	-
15	CLA	B	1201	-	1/1/10/20	3/11/89/115	-
15	CLA	3	610	-	1/1/12/20	9/19/97/115	-
15	CLA	1	613	-	1/1/11/20	8/13/91/115	-
15	CLA	2	602	-	1/1/11/20	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	4	608	-	1/1/11/20	6/15/93/115	-
14	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	8/29/63/63	0/2/2/2
14	BCR	B	4001	-	-	16/29/63/63	0/2/2/2
15	CLA	1	608	-	1/1/13/20	9/25/103/115	-
15	CLA	B	1228	-	1/1/14/20	12/31/109/115	-
13	XAT	3	502	-	-	15/31/93/93	0/4/4/4
15	CLA	B	1224	-	1/1/14/20	13/33/111/115	-

The worst 5 of 1382 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	2	501	LUT	C24-C25	21.34	1.59	1.33
12	3	501	LUT	C24-C25	21.04	1.59	1.33
12	1	501	LUT	C24-C25	20.96	1.59	1.33
12	4	501	LUT	C24-C25	20.76	1.59	1.33
12	3	501	LUT	C22-C21	-15.92	1.34	1.54

The worst 5 of 2219 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	502	XAT	O4-C5-C4	57.29	156.42	113.38
13	1	502	XAT	O24-C25-C24	55.15	154.81	113.38
13	2	502	XAT	O4-C5-C4	54.30	154.17	113.38
13	4	502	XAT	O4-C5-C4	54.21	154.10	113.38
13	4	502	XAT	O24-C25-C24	53.23	153.37	113.38

5 of 168 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	1	501	LUT	C26
12	2	501	LUT	C26
12	3	501	LUT	C26
12	4	501	LUT	C26
15	1	601	CLA	ND

5 of 2248 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	1	501	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
12	1	501	LUT	C11-C12-C13-C20
12	4	501	LUT	C11-C12-C13-C14
12	4	501	LUT	C11-C12-C13-C20
12	4	501	LUT	C21-C26-C27-C28

There are no ring outliers.

182 monomers are involved in 1482 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	1220	CLA	2	0
15	2	606	CLA	1	0
15	A	1135	CLA	13	0
18	B	5003	LMG	2	0
16	2	609	CHL	4	0
15	2	607	CLA	1	0
15	A	1126	CLA	23	0
15	2	603	CLA	2	0
15	B	1221	CLA	9	0
15	A	1137	CLA	25	0
15	B	1229	CLA	12	0
15	A	1123	CLA	22	0
15	4	612	CLA	1	0
14	F	4002	BCR	1	0
14	J	4001	BCR	17	0
14	4	503	BCR	4	0
13	4	502	XAT	4	0
14	2	503	BCR	1	0
15	B	1223	CLA	22	0
15	B	1213	CLA	9	0
15	3	608	CLA	19	0
15	4	607	CLA	2	0
15	B	1021	CLA	19	0
15	B	1023	CLA	10	0
14	B	4005	BCR	5	0
15	1	607	CLA	6	0
16	1	609	CHL	1	0
15	B	1210	CLA	7	0
15	J	1302	CLA	5	0
15	4	605	CLA	1	0
16	4	610	CHL	1	0
15	F	1302	CLA	11	0
15	1	605	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	610	CHL	2	0
15	3	609	CLA	1	0
15	A	1121	CLA	11	0
15	B	1240	CLA	10	0
17	2	801	LHG	1	0
15	A	1113	CLA	8	0
15	B	1226	CLA	8	0
15	B	1239	CLA	2	0
15	1	606	CLA	4	0
15	A	1104	CLA	7	0
15	A	1124	CLA	22	0
15	A	1112	CLA	24	0
15	A	1107	CLA	15	0
15	B	1209	CLA	1	0
15	B	1205	CLA	22	0
14	A	4005	BCR	17	0
15	A	1102	CLA	12	0
15	B	1219	CLA	6	0
15	B	1234	CLA	12	0
15	A	1122	CLA	17	0
12	3	501	LUT	13	0
15	A	1103	CLA	25	0
15	B	1232	CLA	5	0
15	B	1222	CLA	16	0
15	4	604	CLA	2	0
15	2	612	CLA	1	0
15	A	1128	CLA	12	0
14	1	503	BCR	4	0
15	3	611	CLA	8	0
15	1	604	CLA	3	0
15	B	1227	CLA	6	0
15	A	1115	CLA	3	0
15	A	1138	CLA	8	0
15	2	616	CLA	3	0
15	A	1140	CLA	10	0
15	B	1206	CLA	14	0
15	B	1216	CLA	20	0
15	A	1141	CLA	5	0
15	B	1204	CLA	7	0
15	3	601	CLA	8	0
15	B	1238	CLA	1	0
15	A	1120	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	2001	PQN	7	0
15	3	605	CLA	18	0
18	2	804	LMG	13	0
16	4	611	CHL	3	0
15	B	1211	CLA	14	0
17	1	801	LHG	9	0
15	B	1231	CLA	21	0
20	A	1011	CL0	19	0
13	1	502	XAT	2	0
14	B	4003	BCR	5	0
15	A	1136	CLA	12	0
15	1	611	CLA	6	0
14	B	4002	BCR	5	0
15	4	602	CLA	1	0
14	A	4006	BCR	8	0
15	A	1125	CLA	16	0
23	B	5002	DGD	13	0
18	2	803	LMG	2	0
15	2	604	CLA	2	0
15	A	1117	CLA	14	0
15	B	1235	CLA	17	0
15	B	1218	CLA	2	0
17	A	5001	LHG	6	0
15	4	603	CLA	1	0
15	A	1106	CLA	15	0
15	A	1105	CLA	13	0
16	4	613	CHL	7	0
12	2	501	LUT	9	0
15	A	1130	CLA	7	0
15	B	1208	CLA	3	0
15	A	1110	CLA	15	0
12	4	501	LUT	19	0
14	A	4008	BCR	14	0
15	B	1212	CLA	4	0
15	A	1116	CLA	20	0
14	3	506	BCR	2	0
15	3	615	CLA	9	0
14	A	4003	BCR	30	0
15	4	606	CLA	1	0
15	3	612	CLA	10	0
15	A	1114	CLA	15	0
15	B	1225	CLA	10	0

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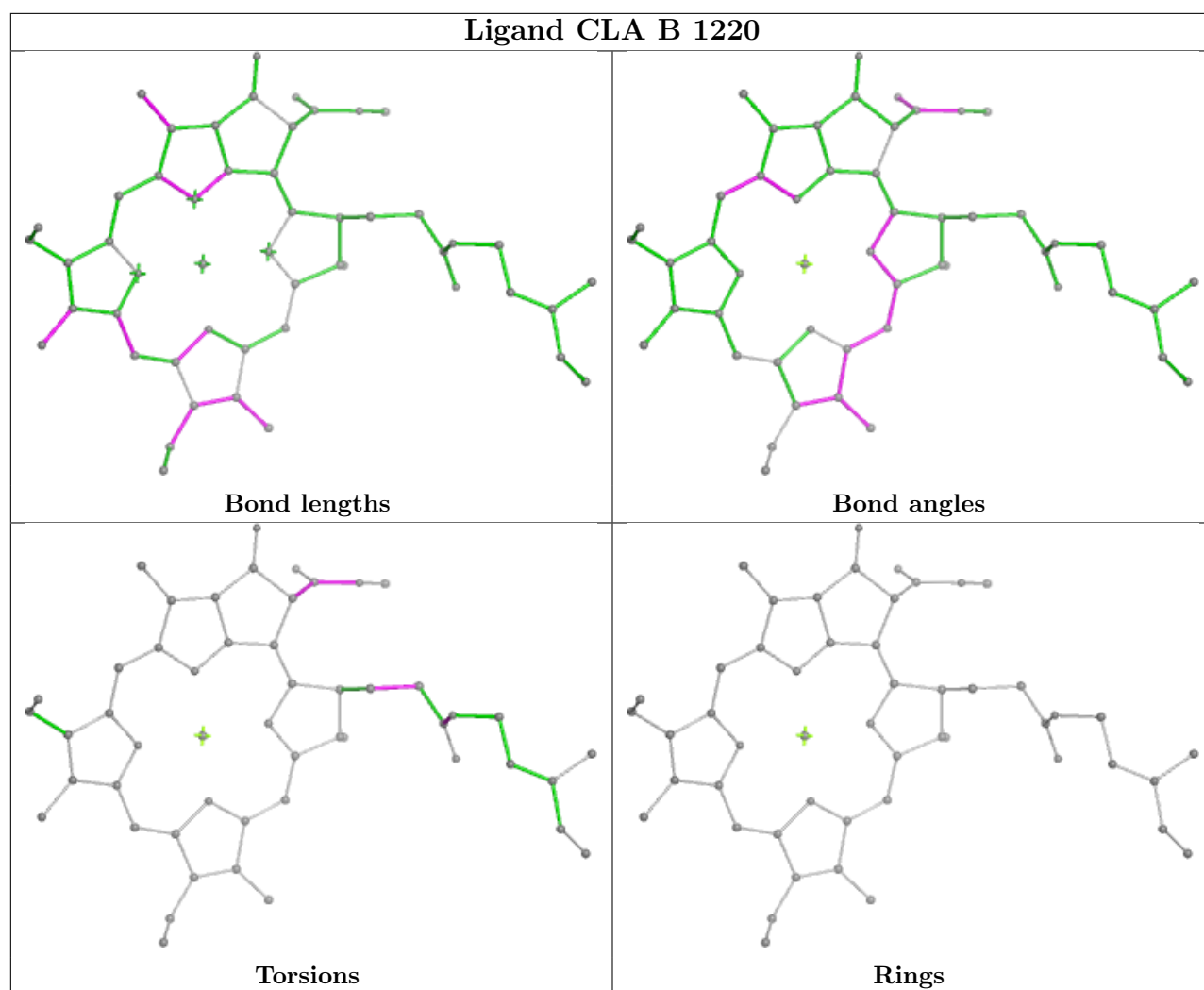
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	1012	CLA	25	0
18	4	801	LMG	1	0
15	A	1134	CLA	16	0
15	4	601	CLA	11	0
15	A	1127	CLA	7	0
15	A	1111	CLA	17	0
15	2	601	CLA	4	0
15	A	1132	CLA	5	0
15	B	1214	CLA	11	0
21	B	2002	PQN	10	0
15	A	1129	CLA	3	0
15	2	608	CLA	15	0
12	1	501	LUT	29	0
14	F	4001	BCR	28	0
15	A	1109	CLA	8	0
15	B	1236	CLA	18	0
15	A	1013	CLA	21	0
15	B	1203	CLA	14	0
15	A	1108	CLA	13	0
15	4	616	CLA	1	0
14	B	4004	BCR	2	0
15	B	1230	CLA	18	0
19	3	802	3PH	3	0
14	A	4004	BCR	7	0
14	B	4006	BCR	13	0
14	J	4002	BCR	16	0
15	1	612	CLA	3	0
14	3	503	BCR	1	0
17	3	801	LHG	8	0
15	3	607	CLA	2	0
15	A	1131	CLA	5	0
14	3	504	BCR	4	0
15	B	1215	CLA	37	0
15	3	603	CLA	11	0
15	A	1119	CLA	15	0
13	2	502	XAT	3	0
15	1	615	CLA	1	0
15	B	1022	CLA	16	0
17	A	5002	LHG	12	0
15	A	1101	CLA	6	0
15	B	1202	CLA	20	0
16	2	611	CHL	5	0

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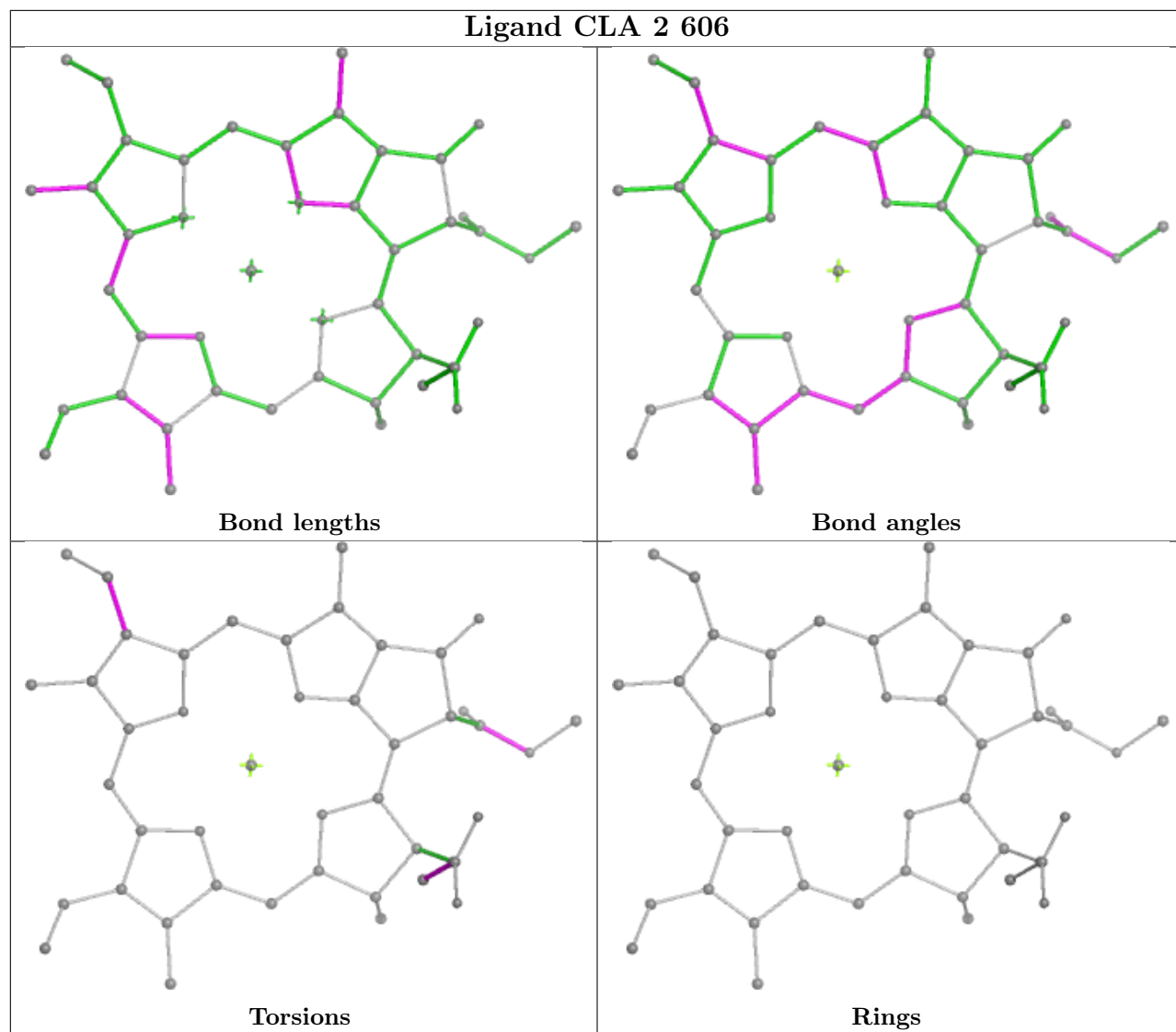
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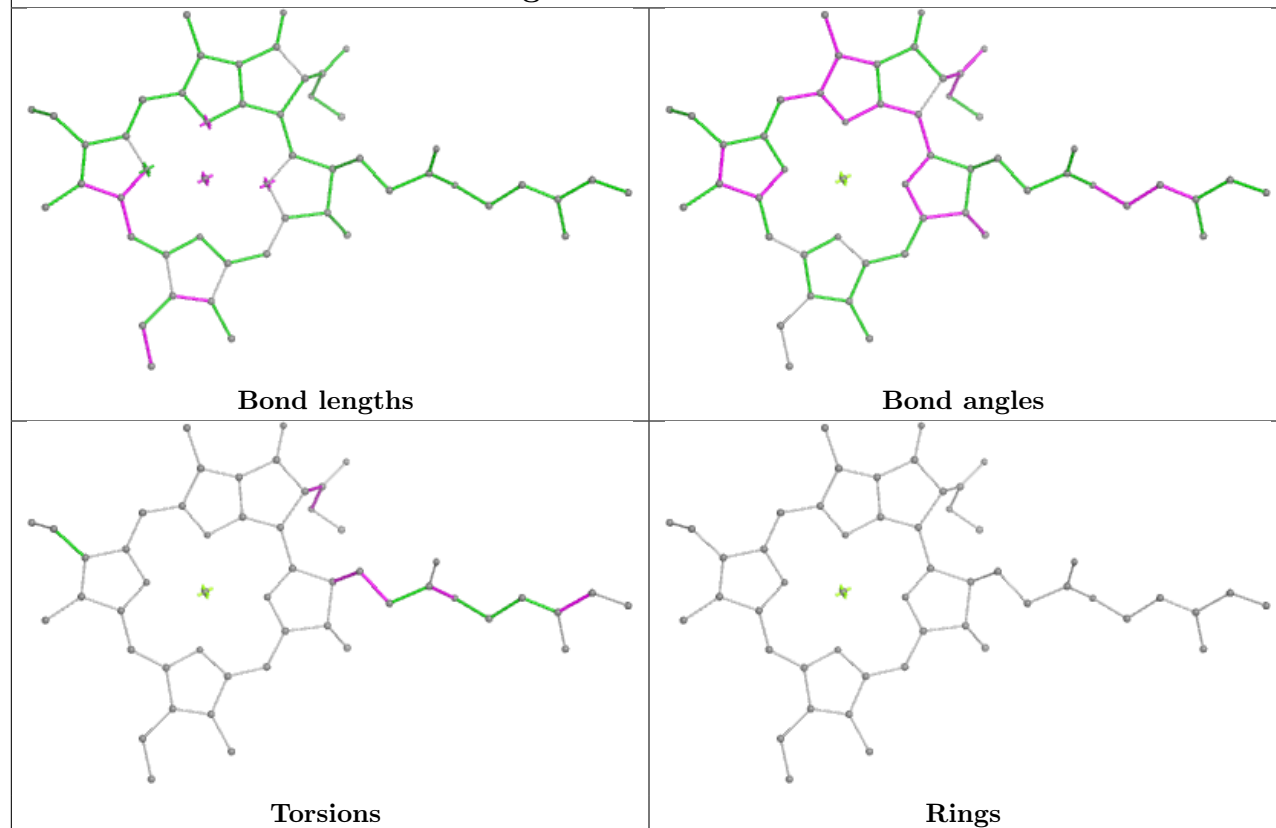
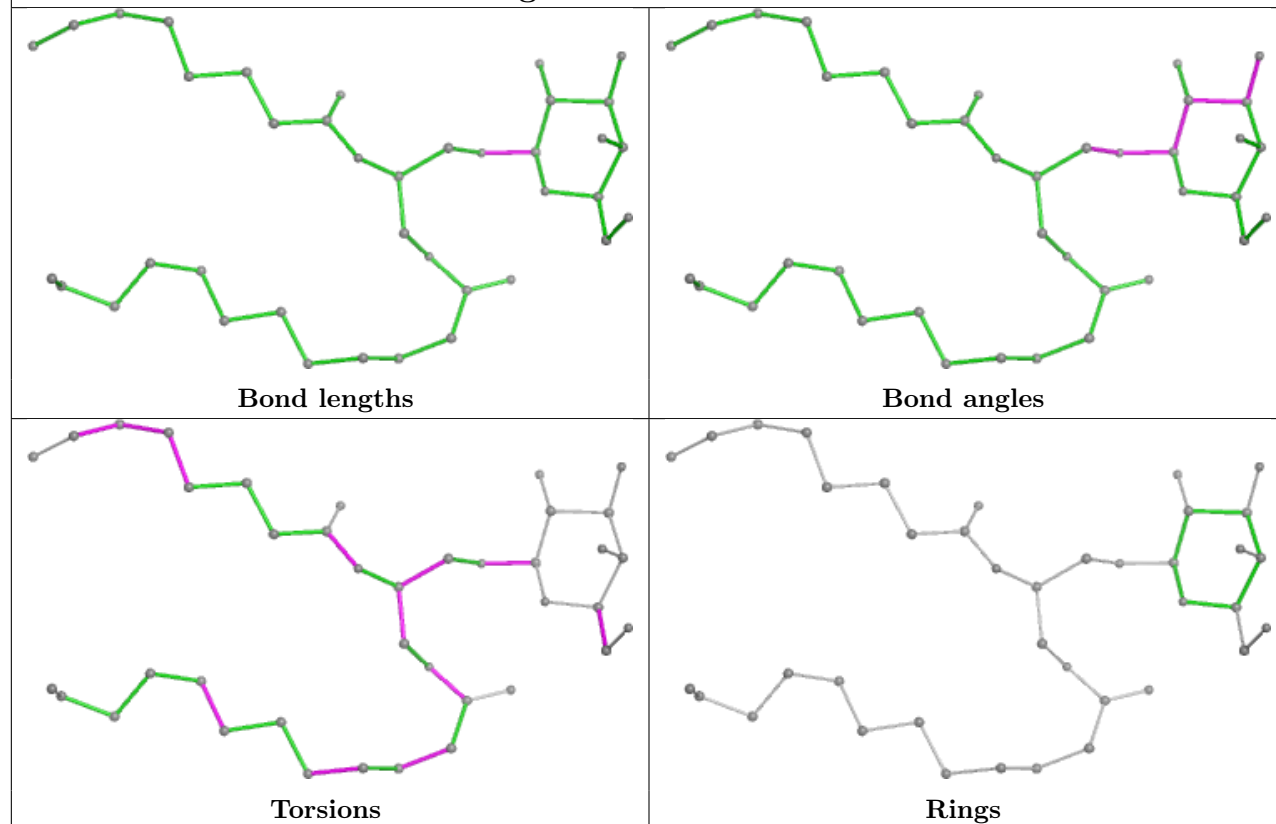
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	1301	CLA	4	0
16	3	604	CHL	10	0
15	3	614	CLA	2	0
15	B	1207	CLA	1	0
15	1	601	CLA	16	0
15	3	606	CLA	2	0
15	A	1133	CLA	24	0
15	1	603	CLA	16	0
15	A	1139	CLA	6	0
22	A	3001	SF4	1	0
15	A	1118	CLA	5	0
15	3	613	CLA	5	0
15	B	1201	CLA	2	0
15	3	610	CLA	5	0
15	1	613	CLA	18	0
15	2	602	CLA	1	0
14	A	4002	BCR	19	0
15	4	608	CLA	7	0
14	A	4007	BCR	20	0
15	1	608	CLA	26	0
15	B	1228	CLA	5	0
13	3	502	XAT	16	0
15	B	1224	CLA	17	0

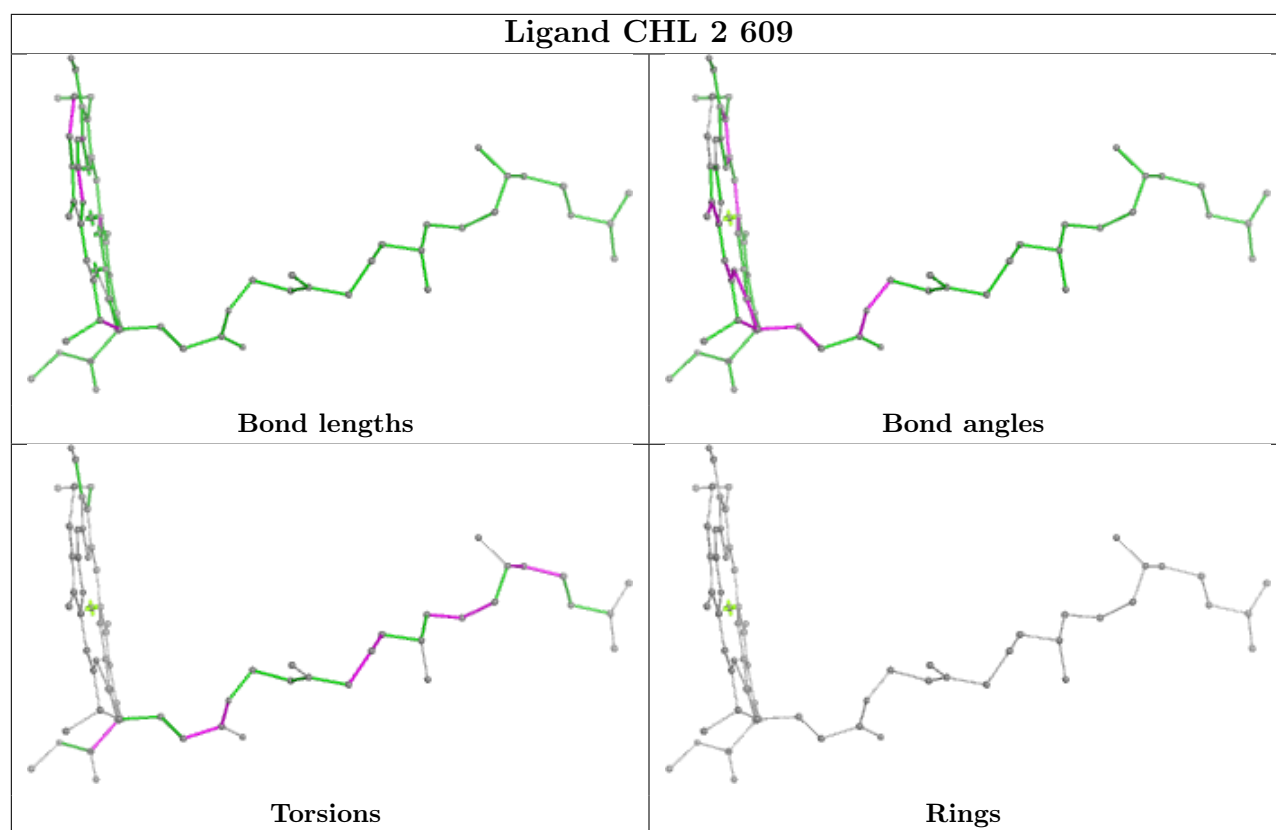
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



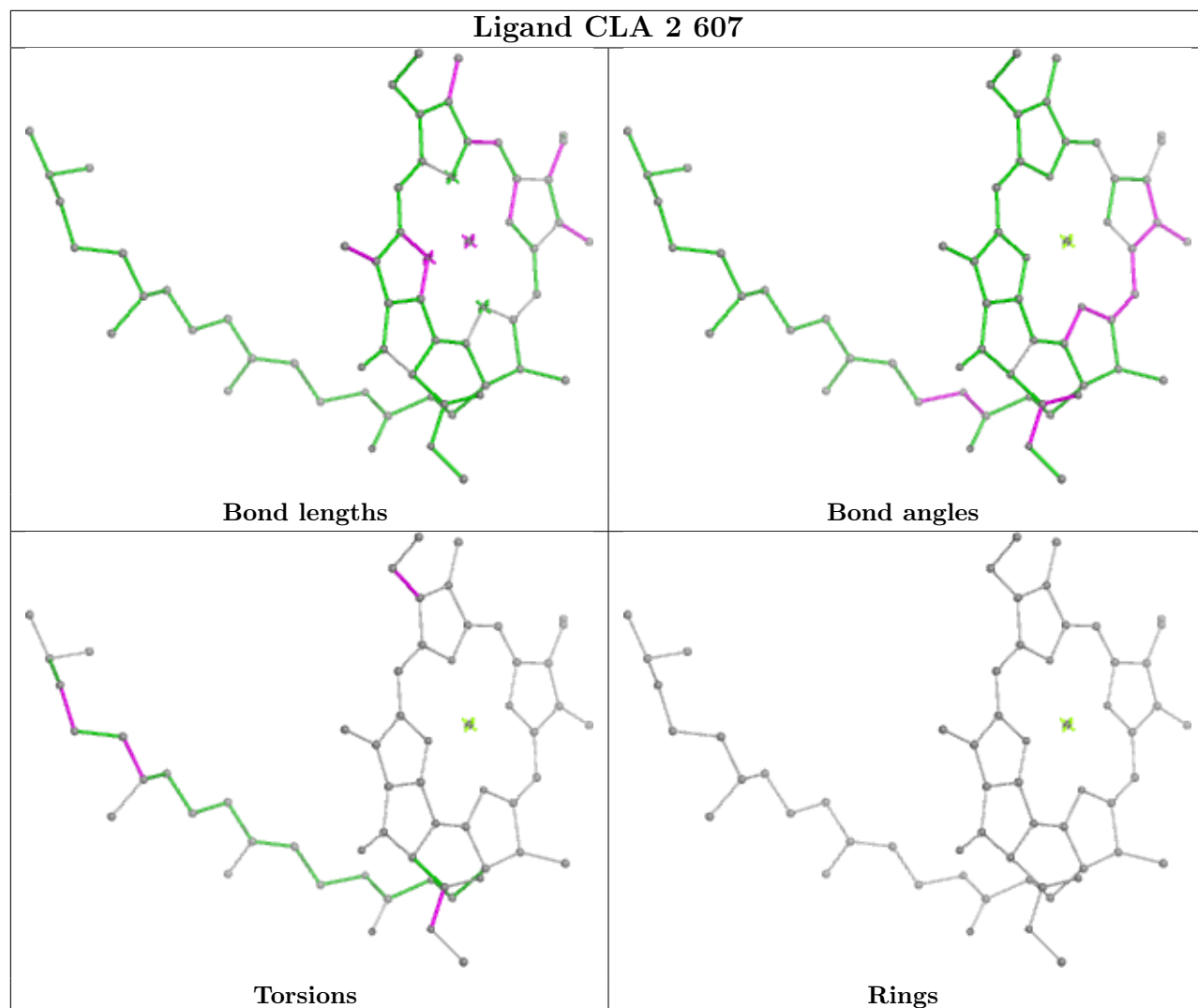
Ligand CLA 2 606

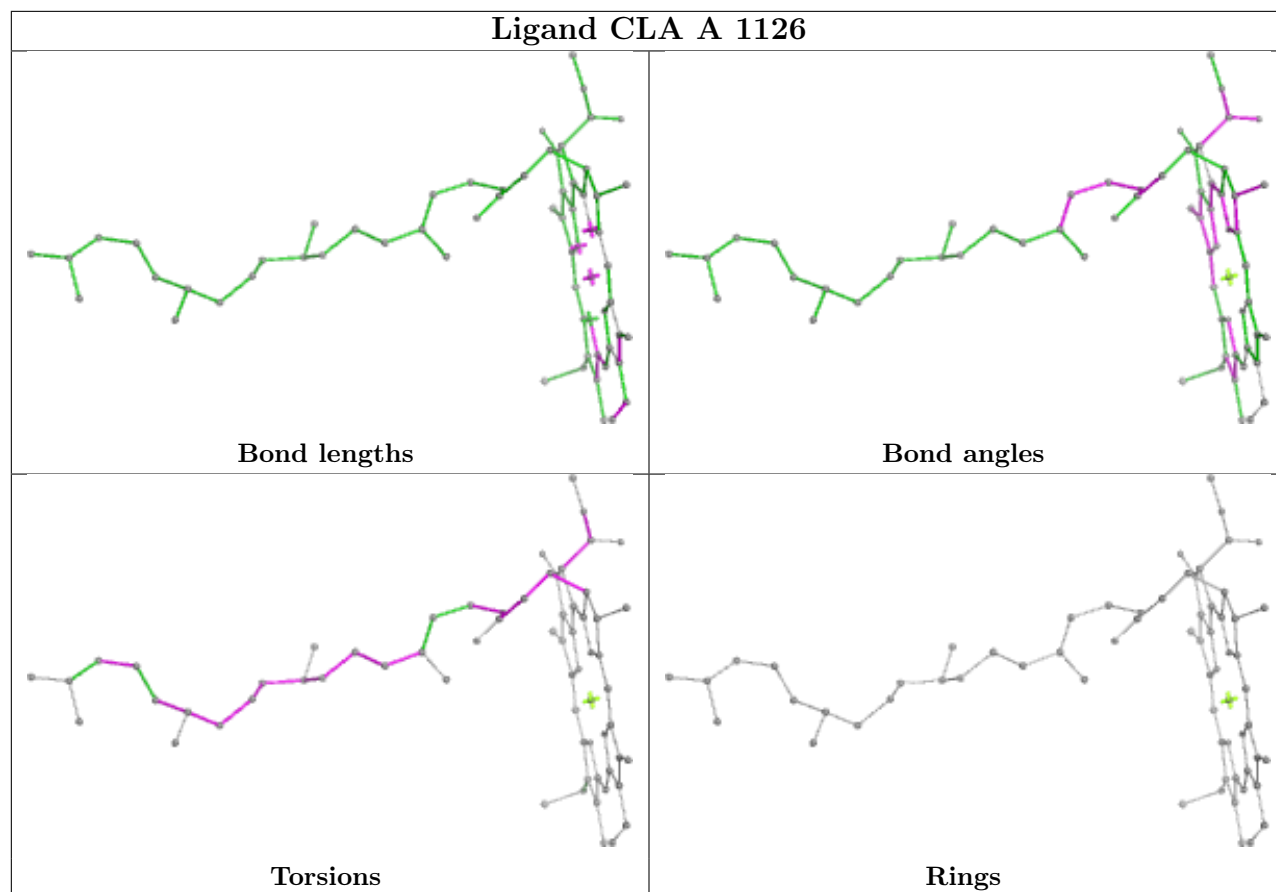


Ligand CLA A 1135**Ligand LMG B 5003**

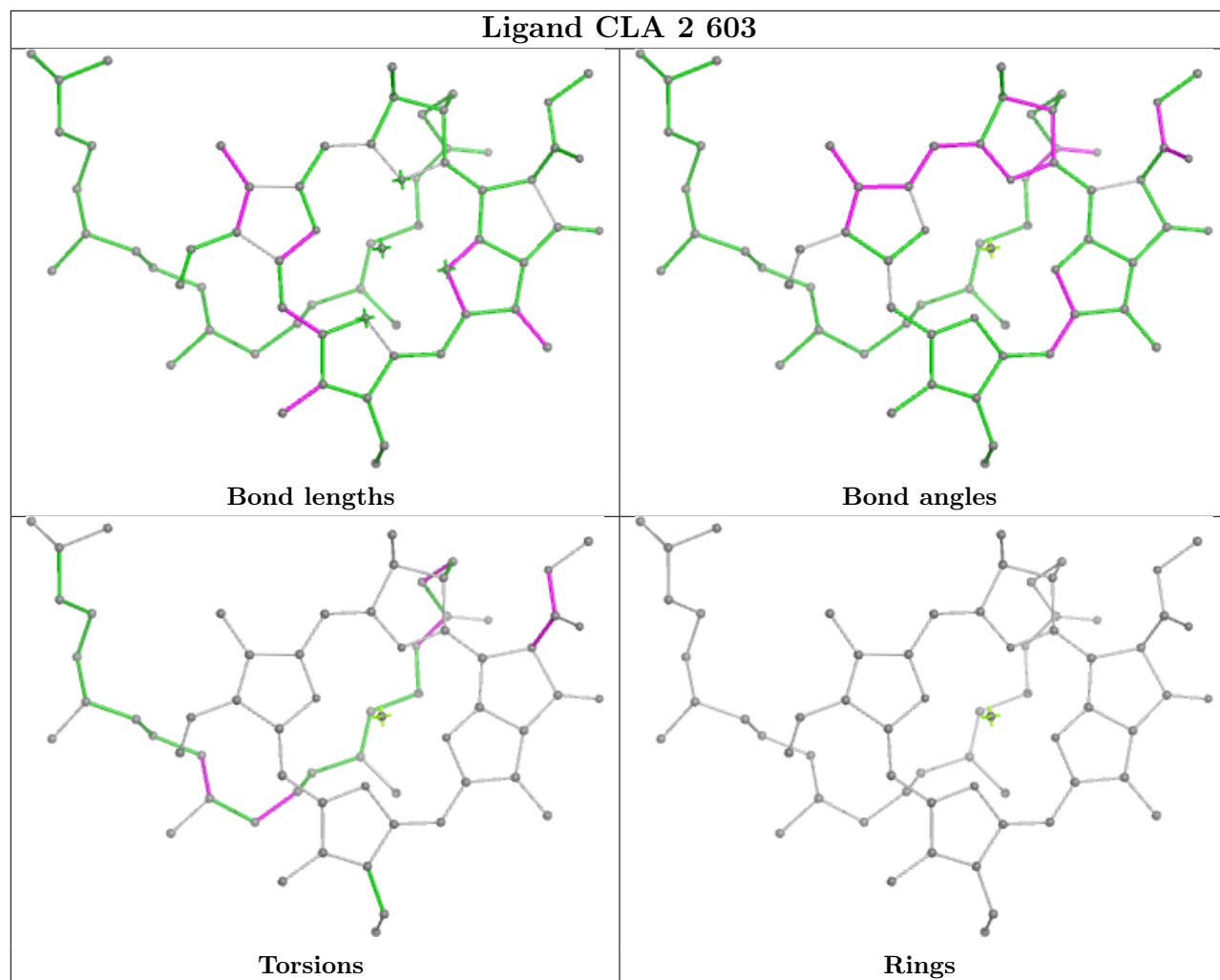


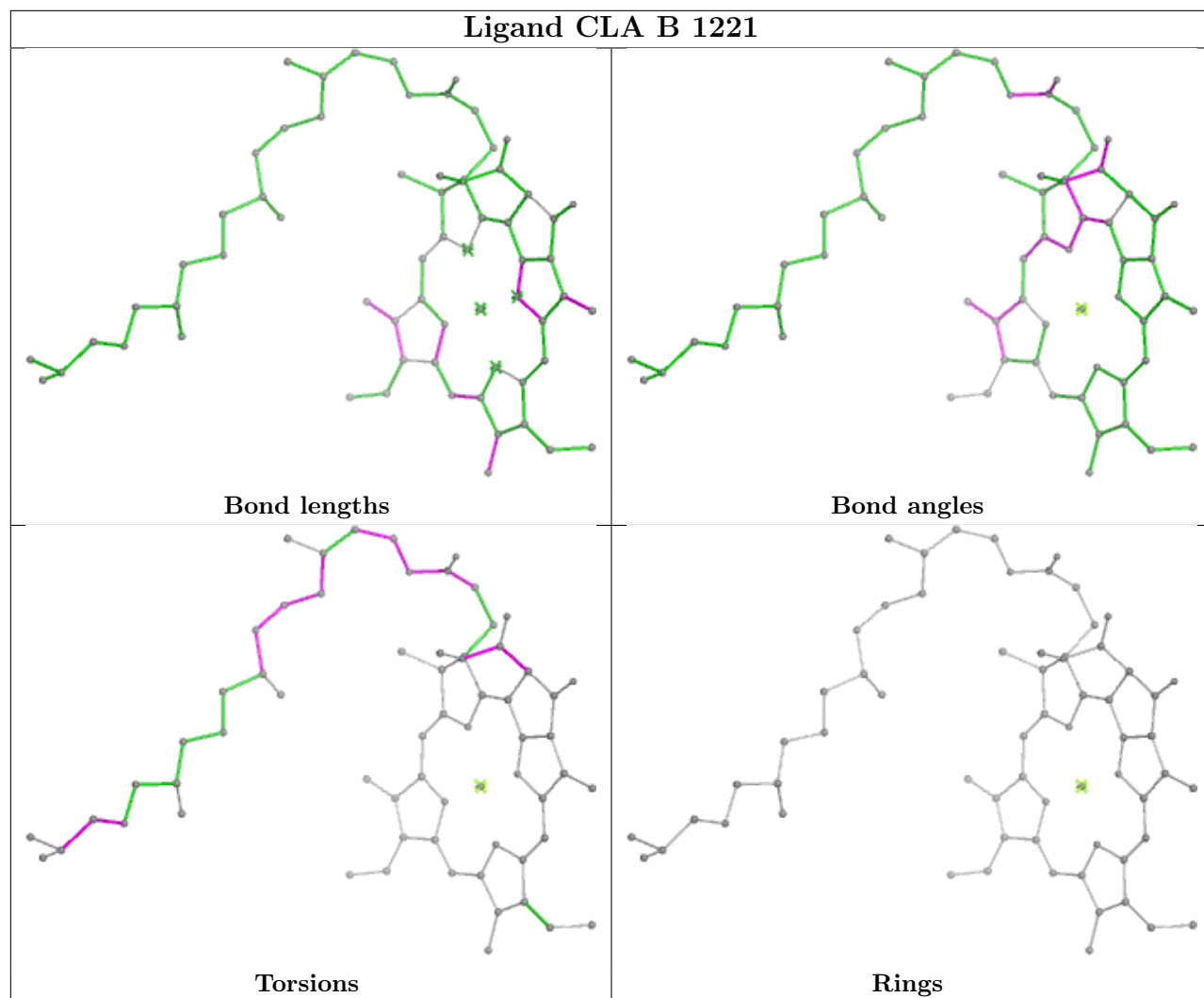
Ligand CLA 2 607

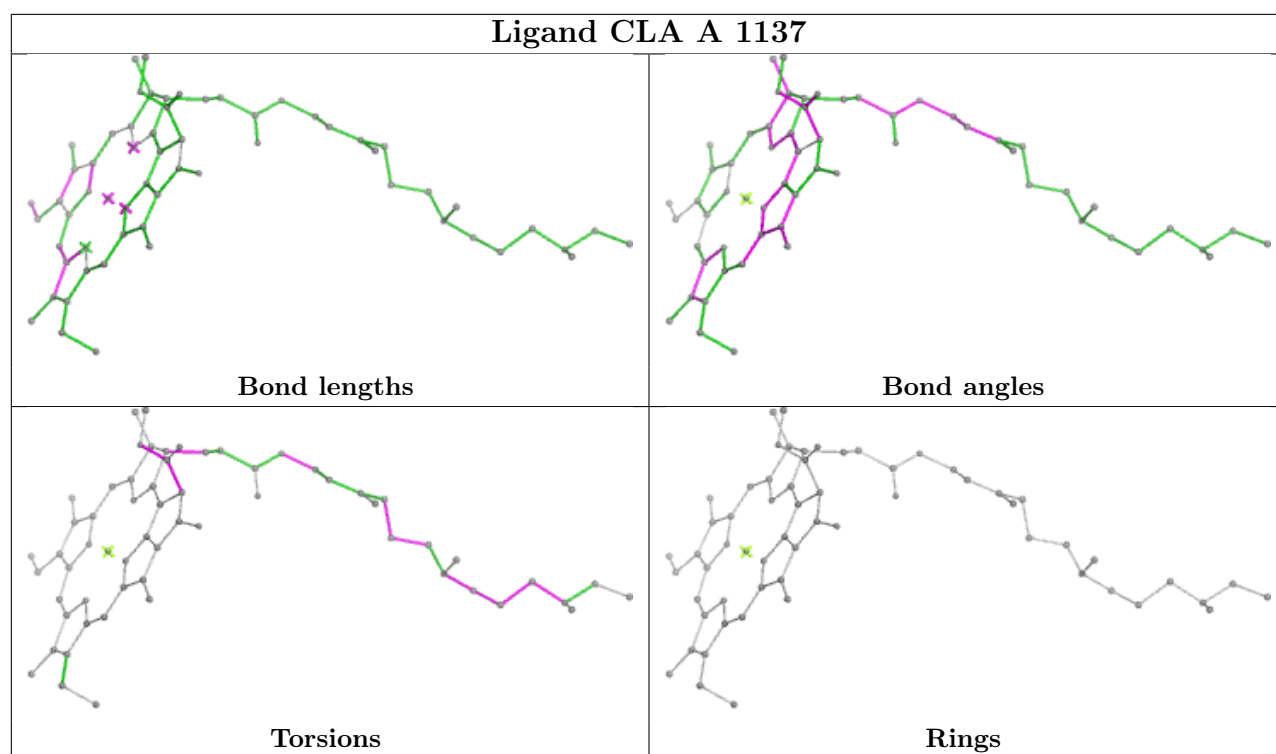


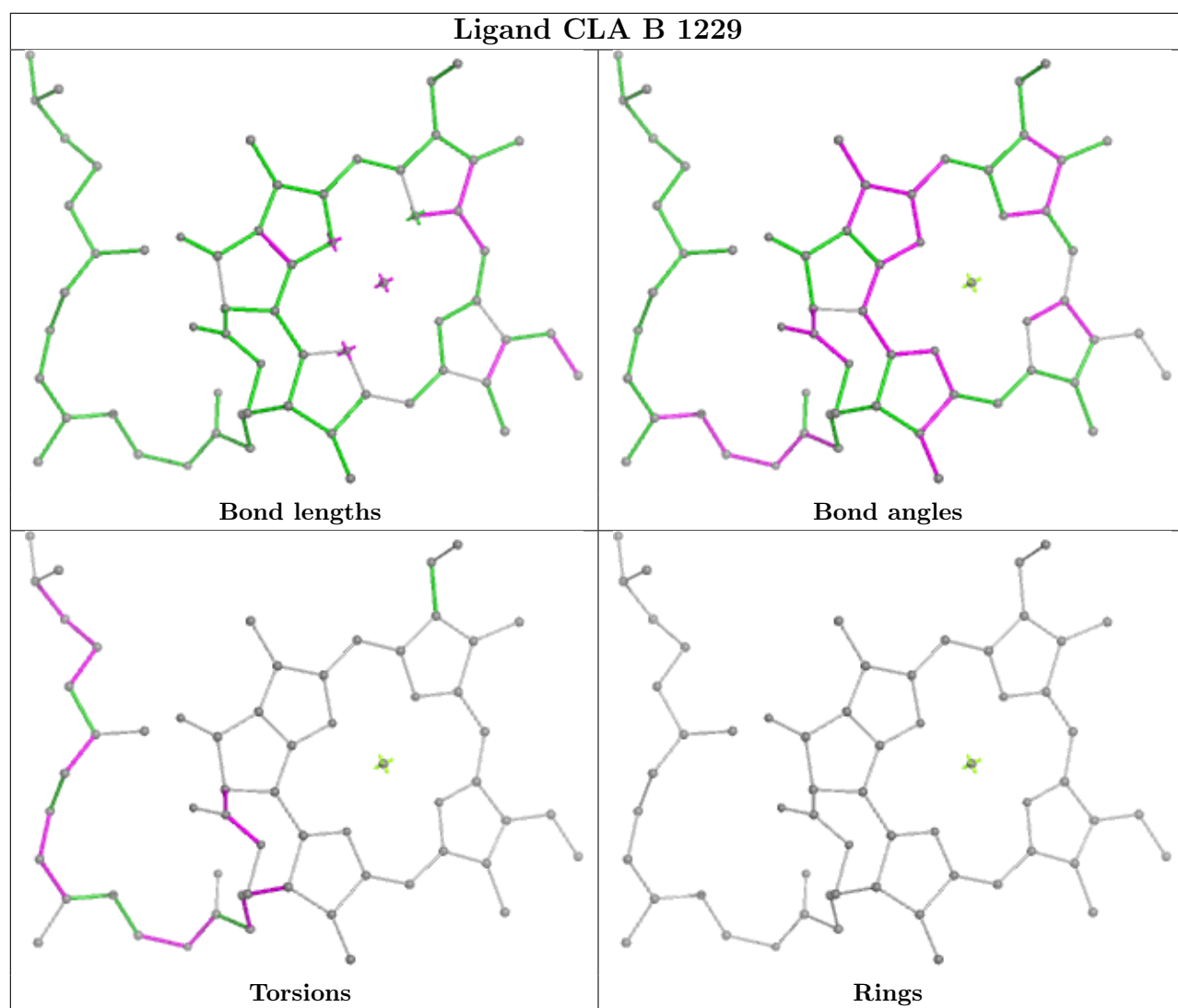


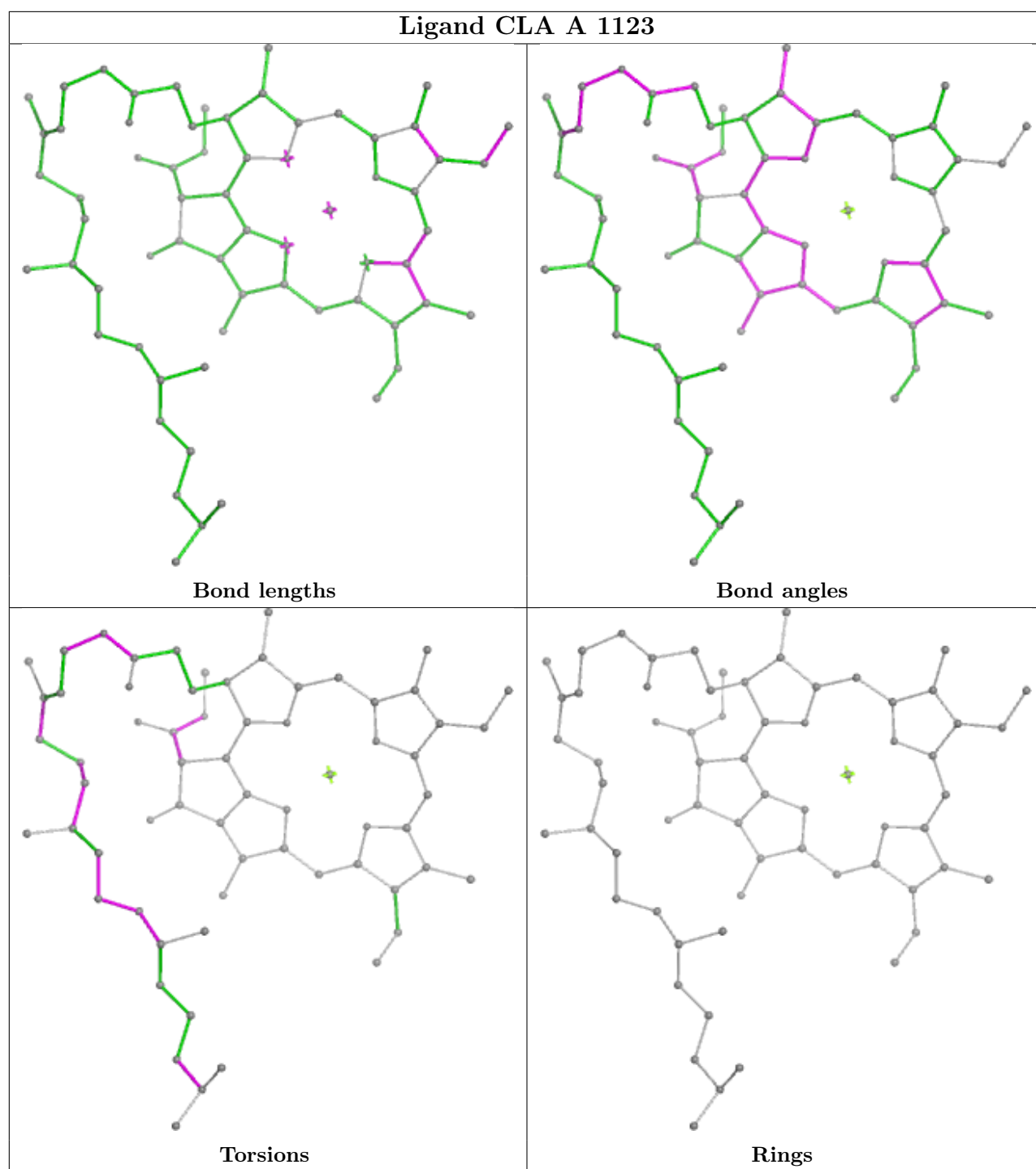
Ligand CLA 2 603

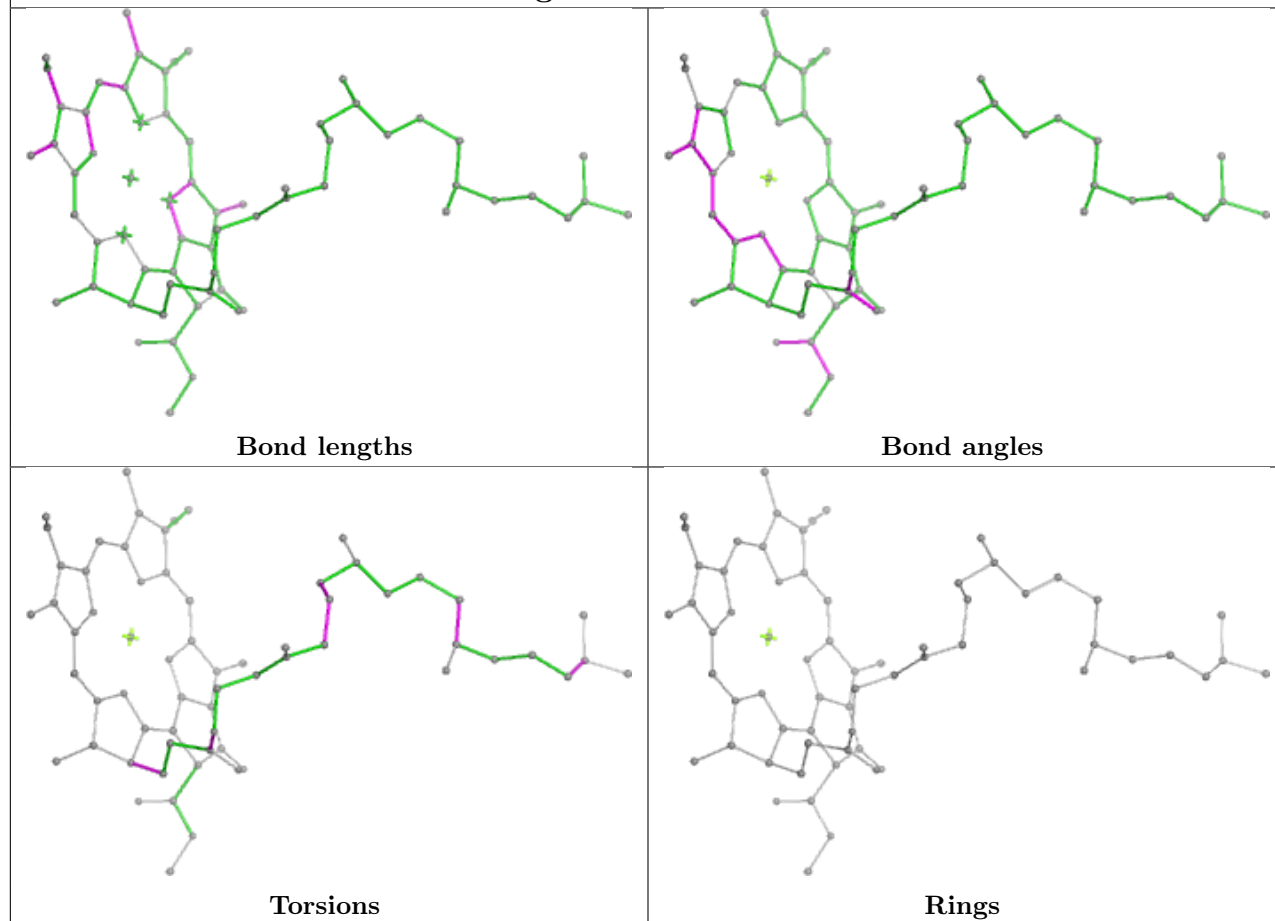
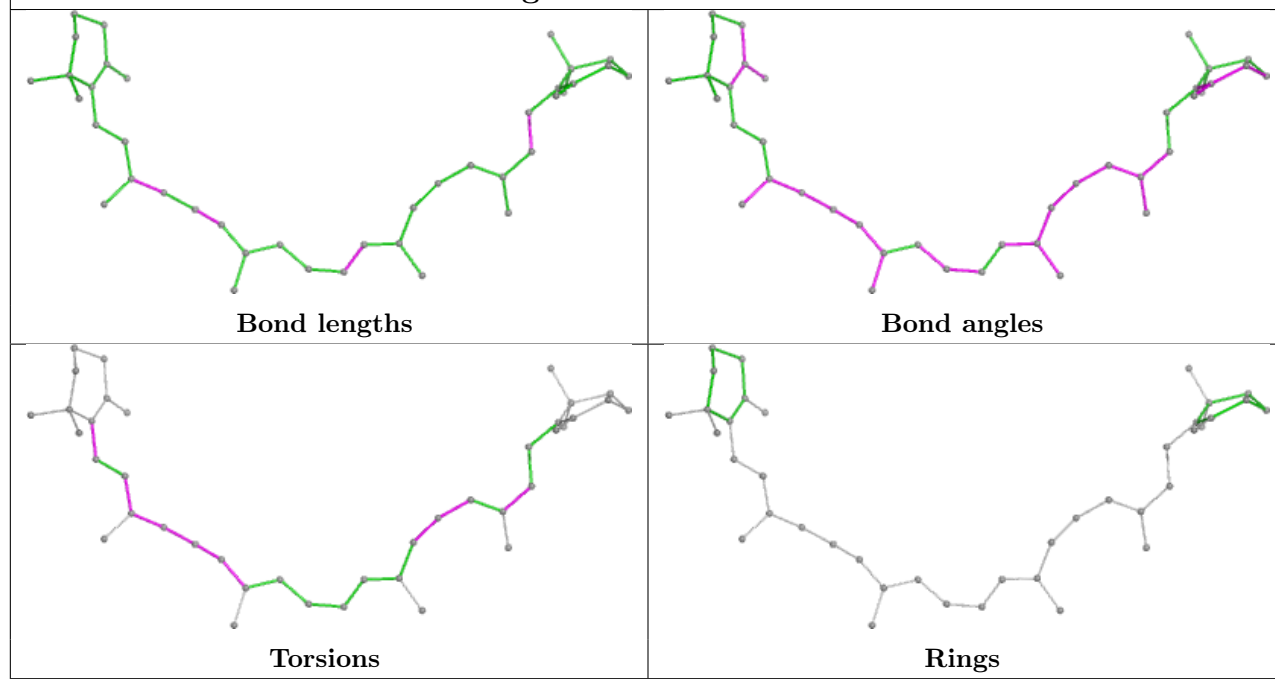


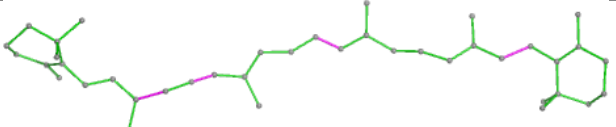
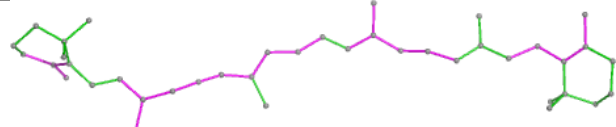
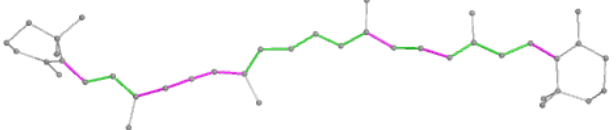
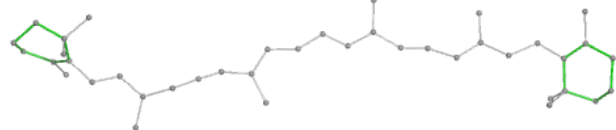


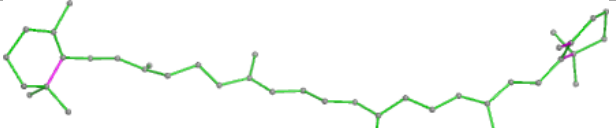
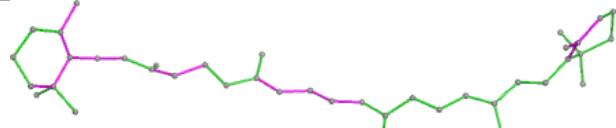
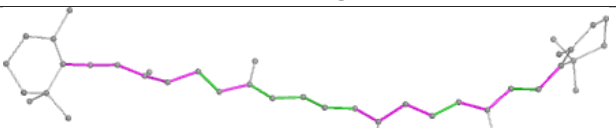
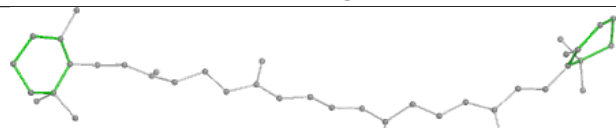


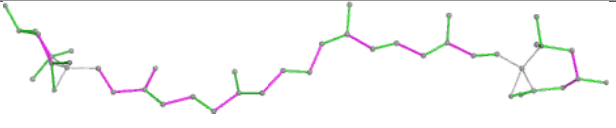
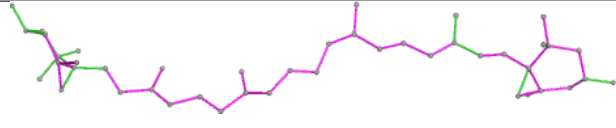
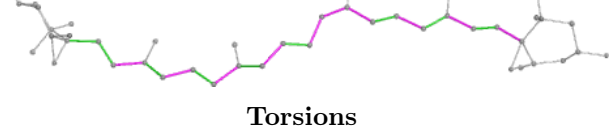




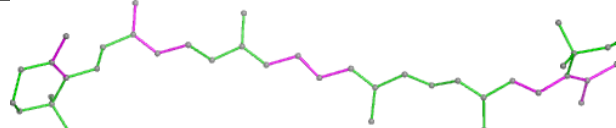
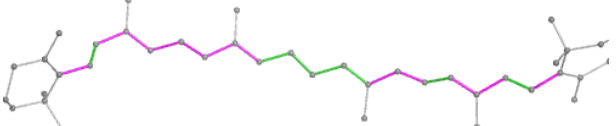
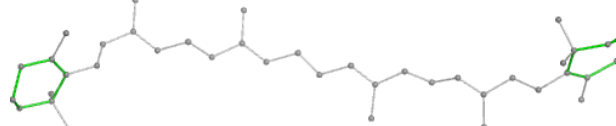


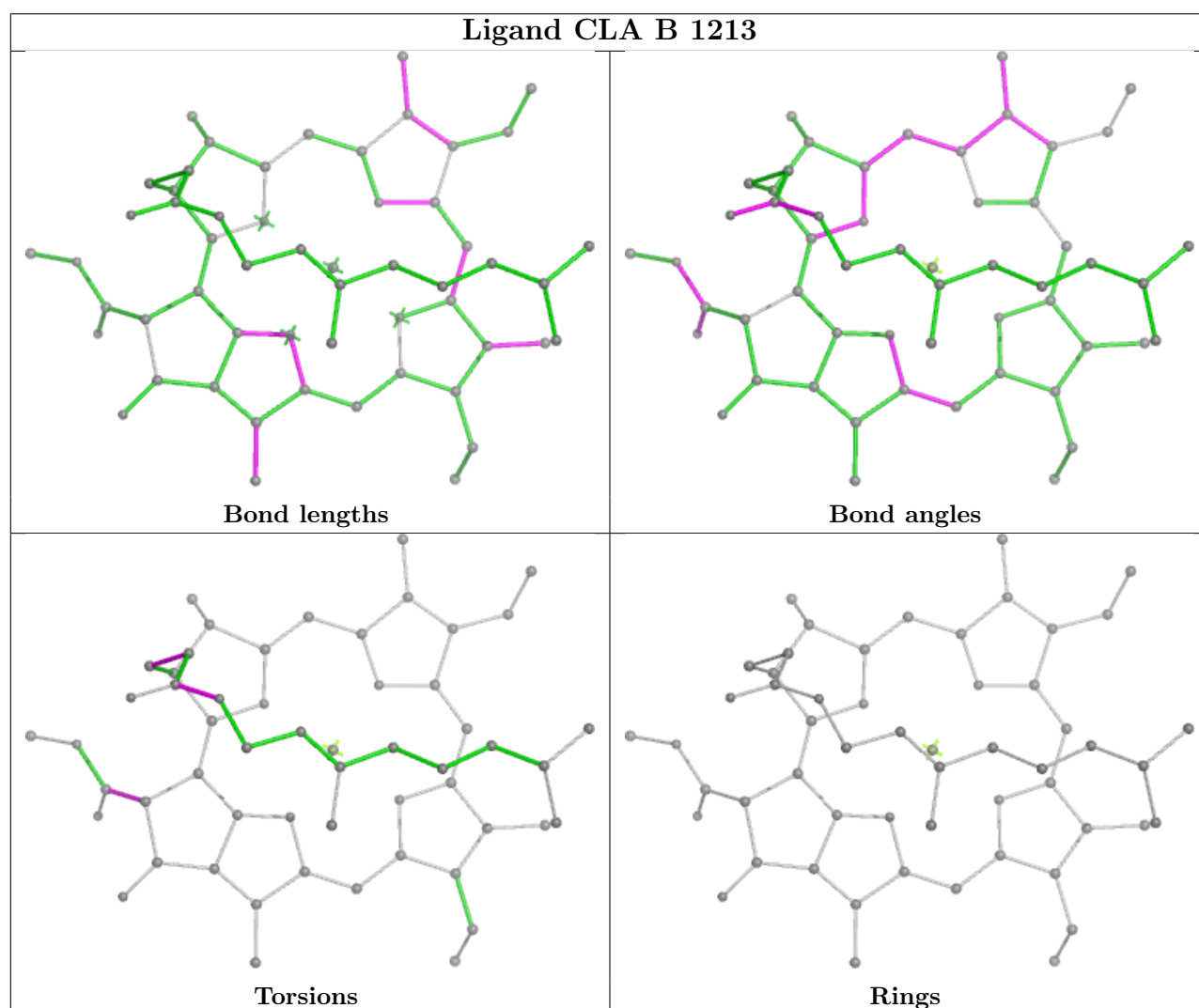
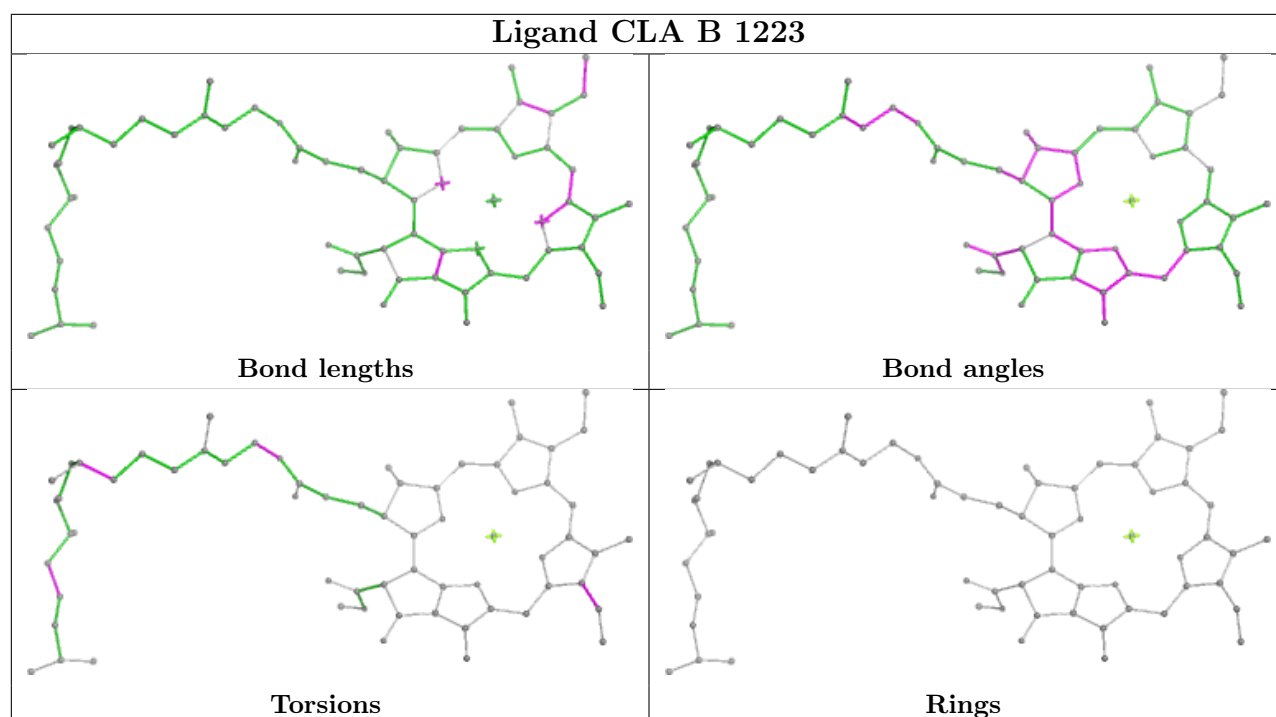
Ligand CLA 4 612**Ligand BCR F 4002**

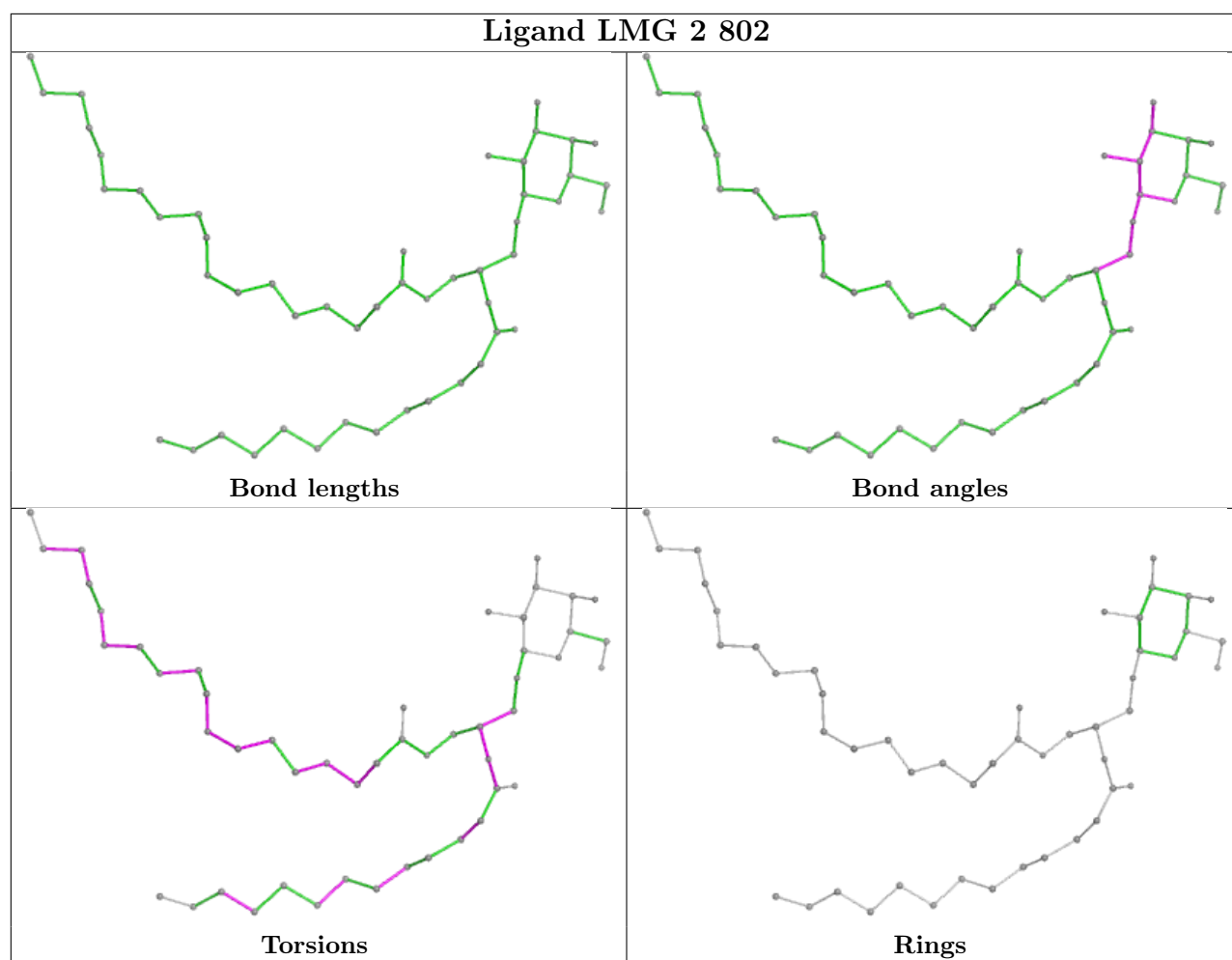
Ligand BCR J 4001	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 4 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

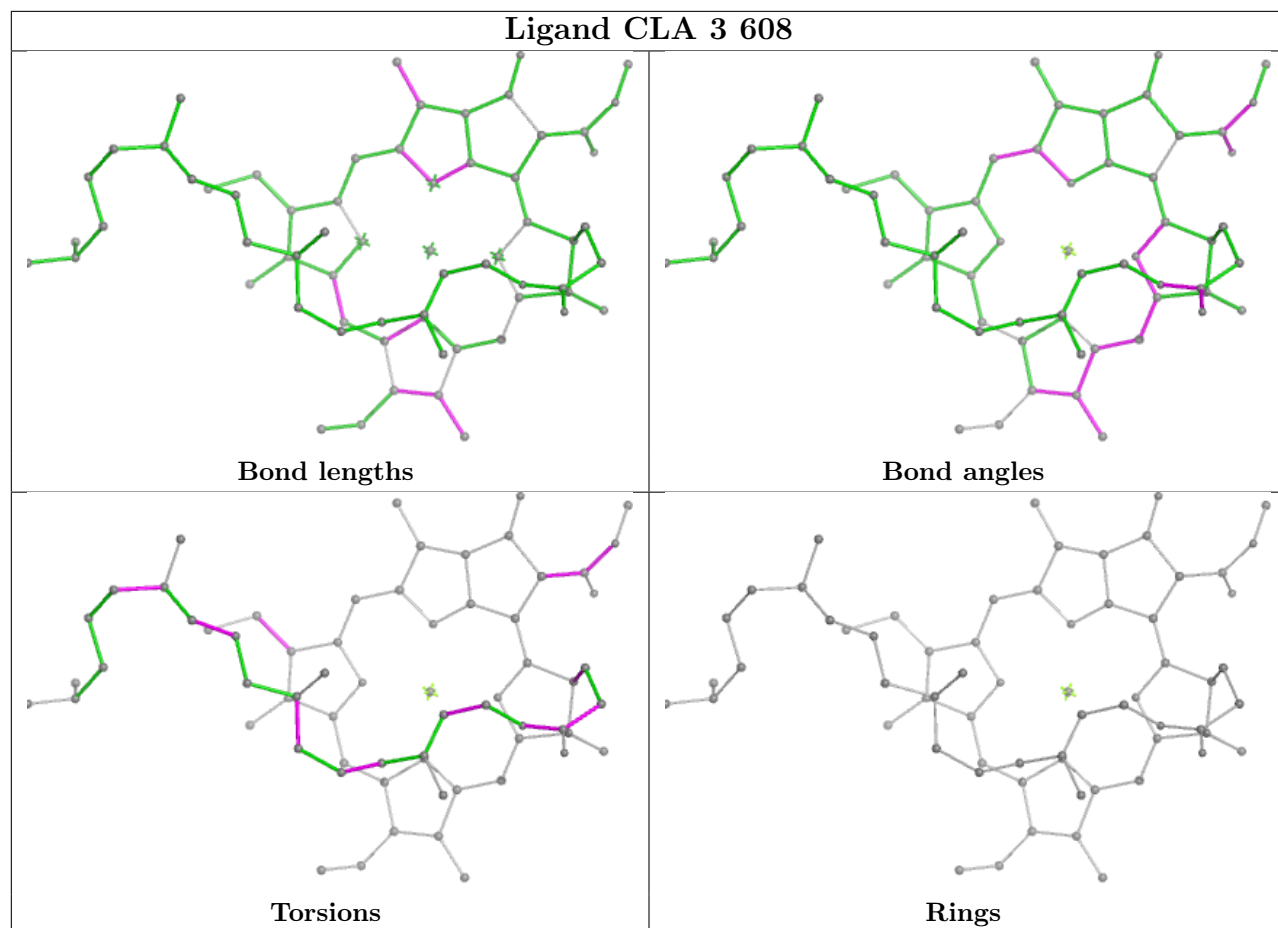
Ligand XAT 4 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

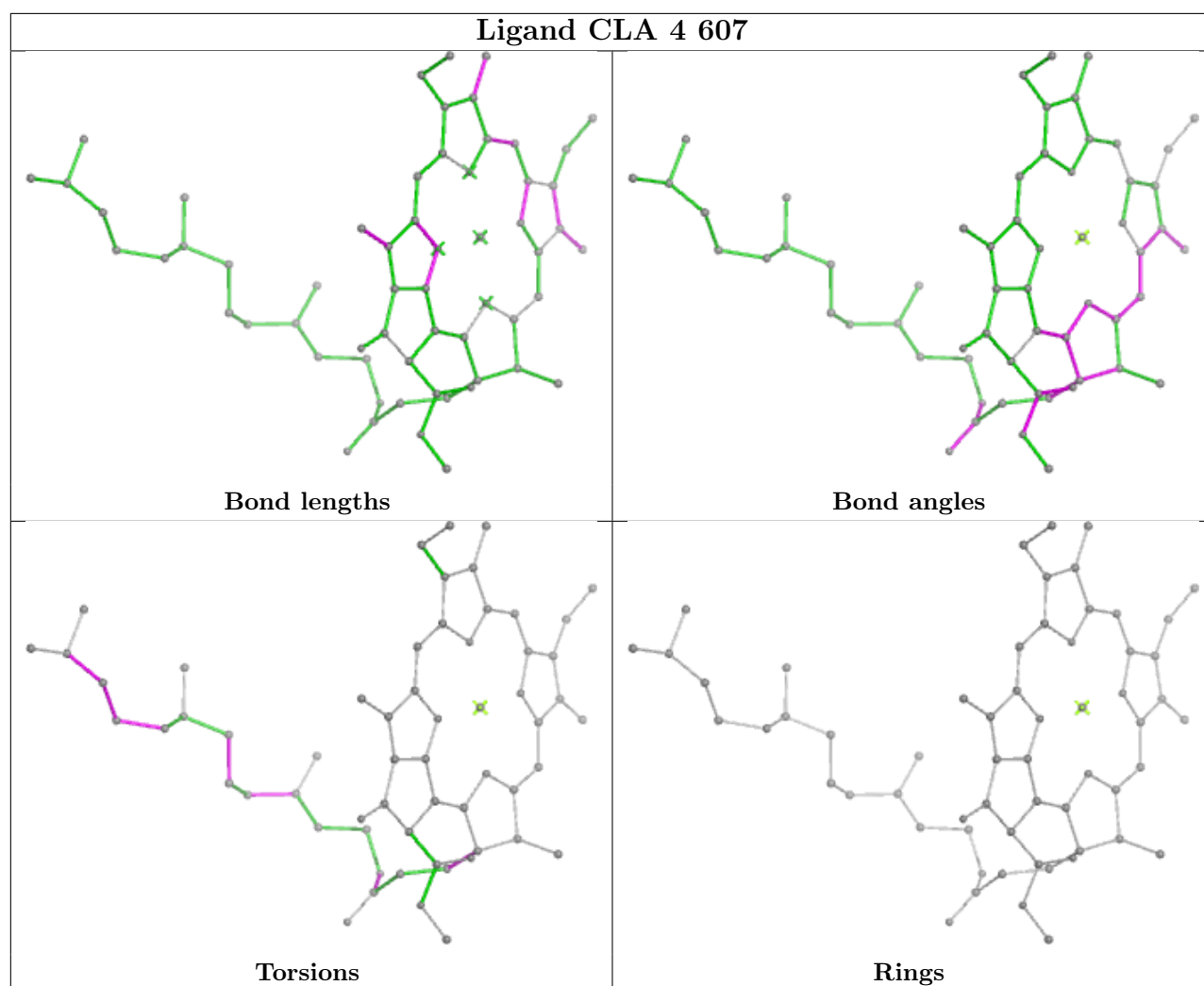
Ligand BCR 2 503	
	
Bond lengths	Bond angles
	
Torsions	Rings

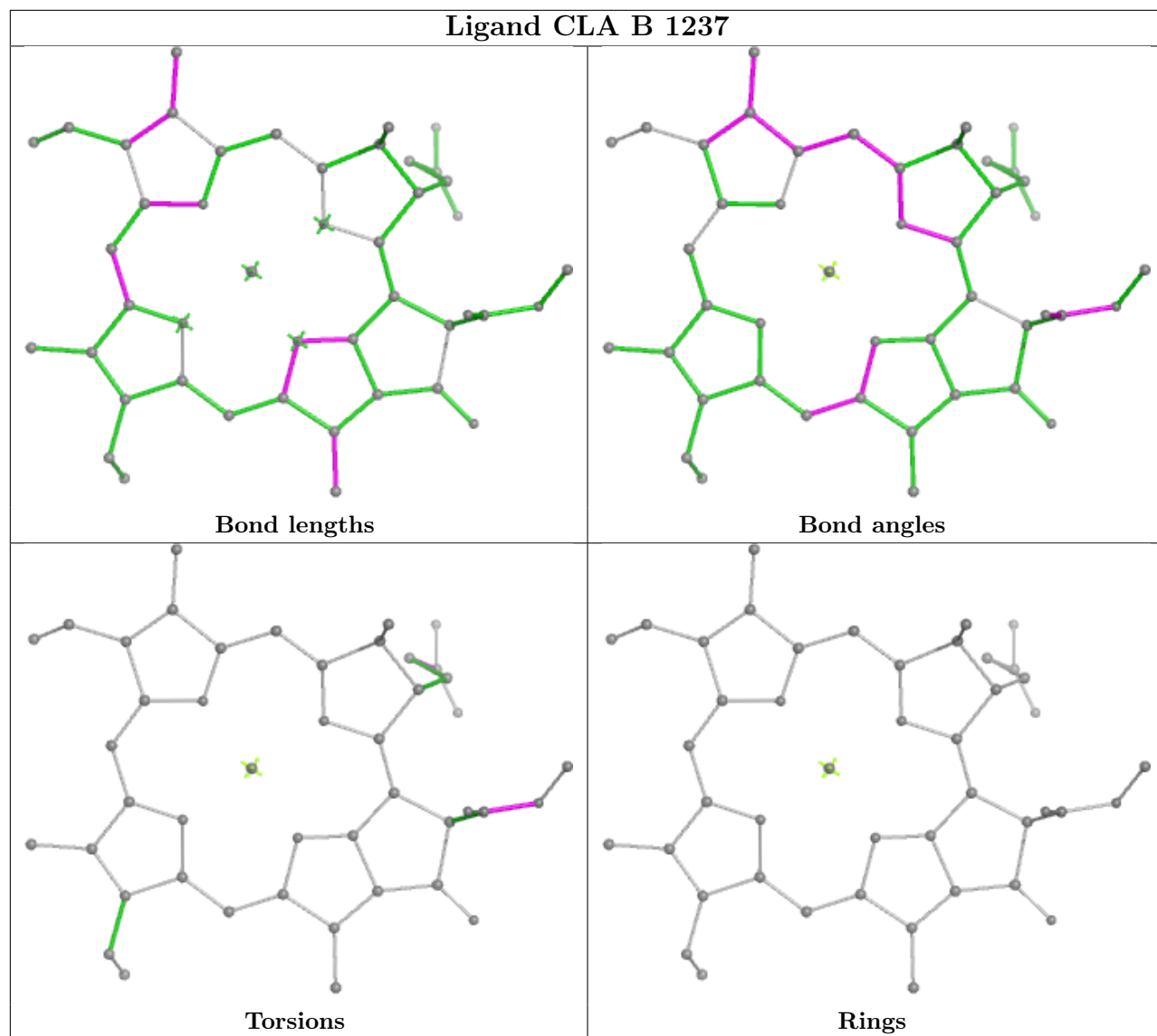


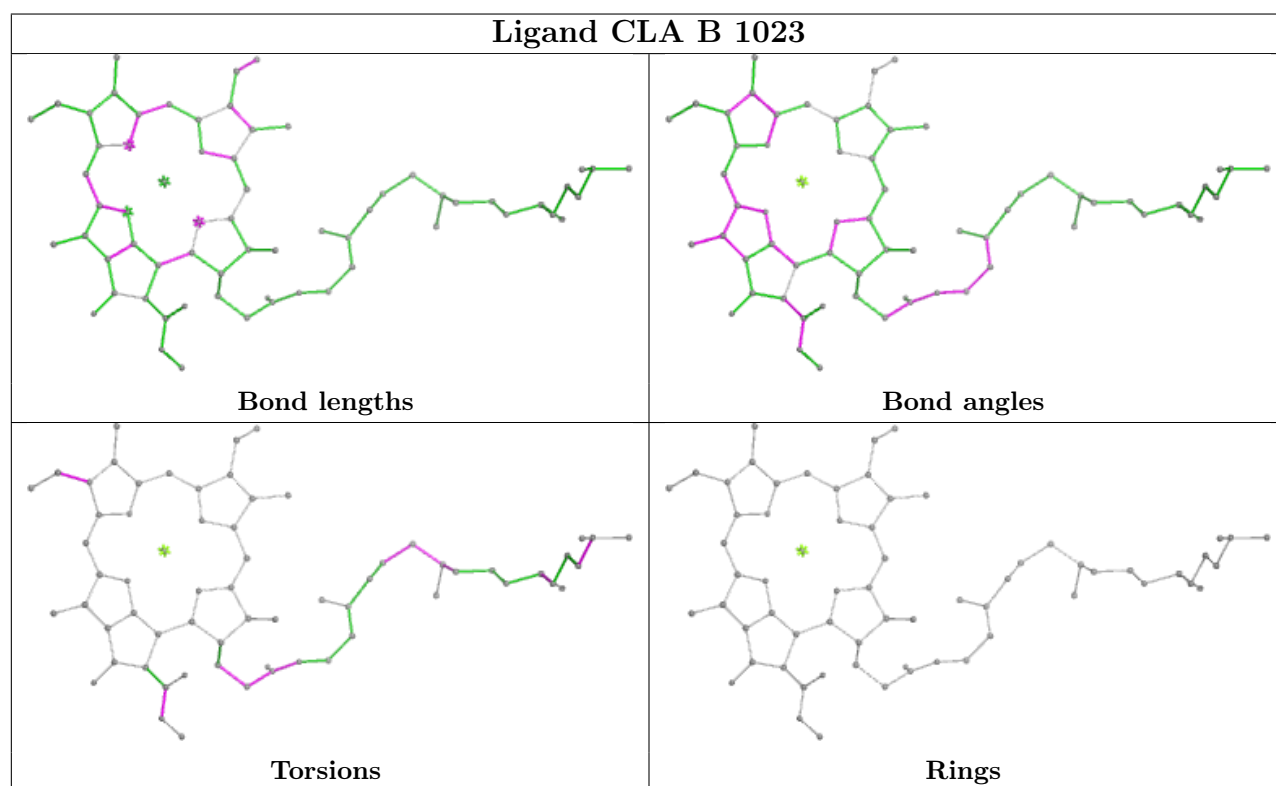
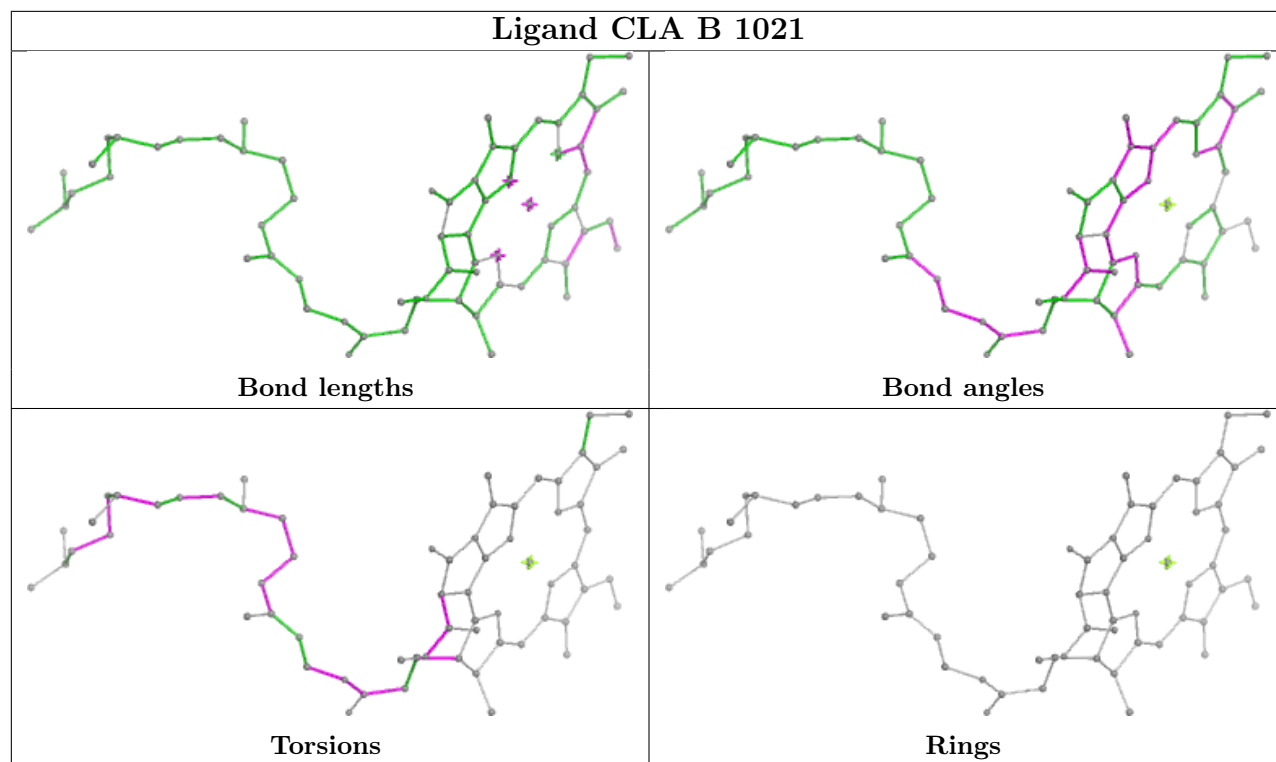


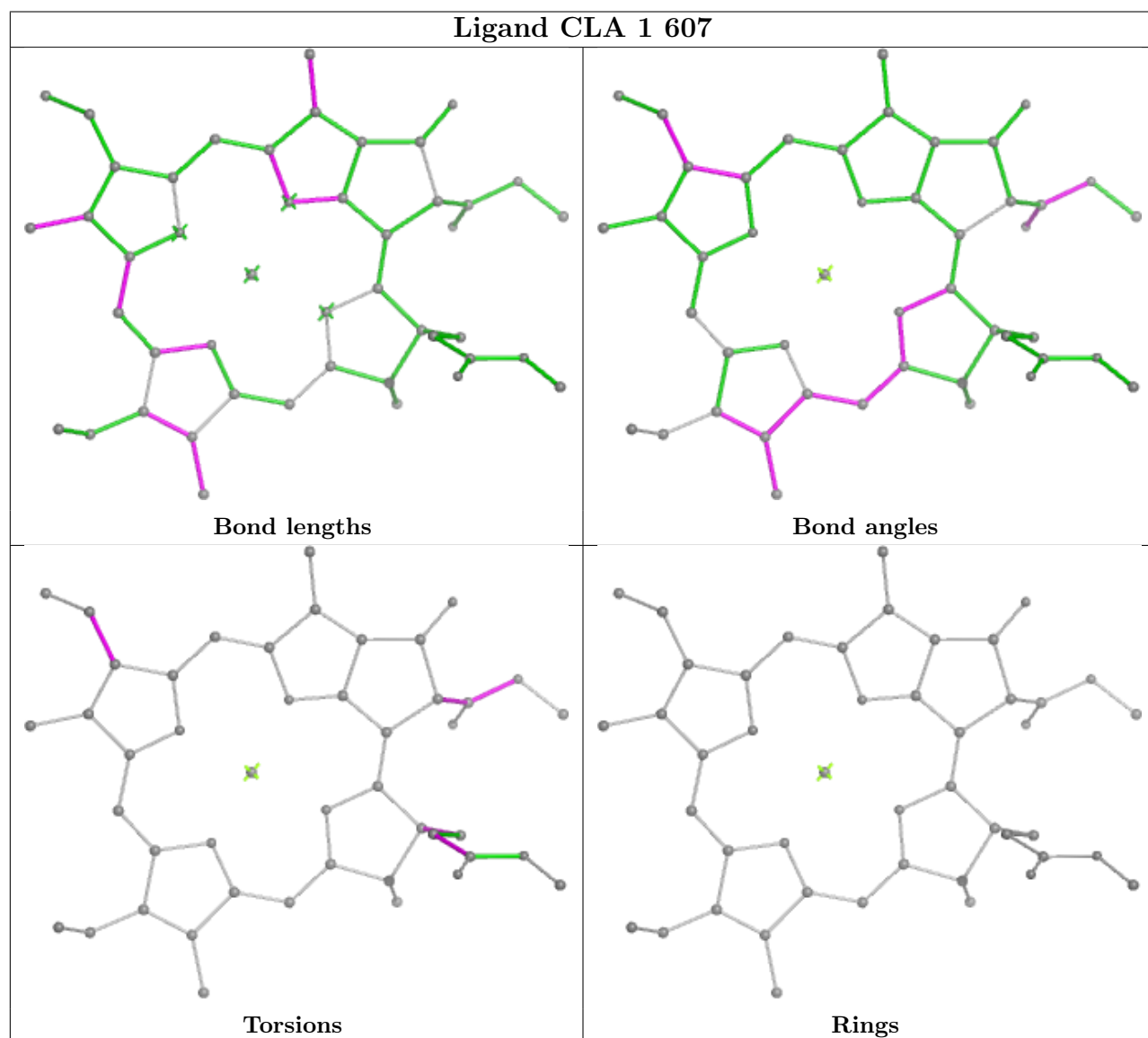
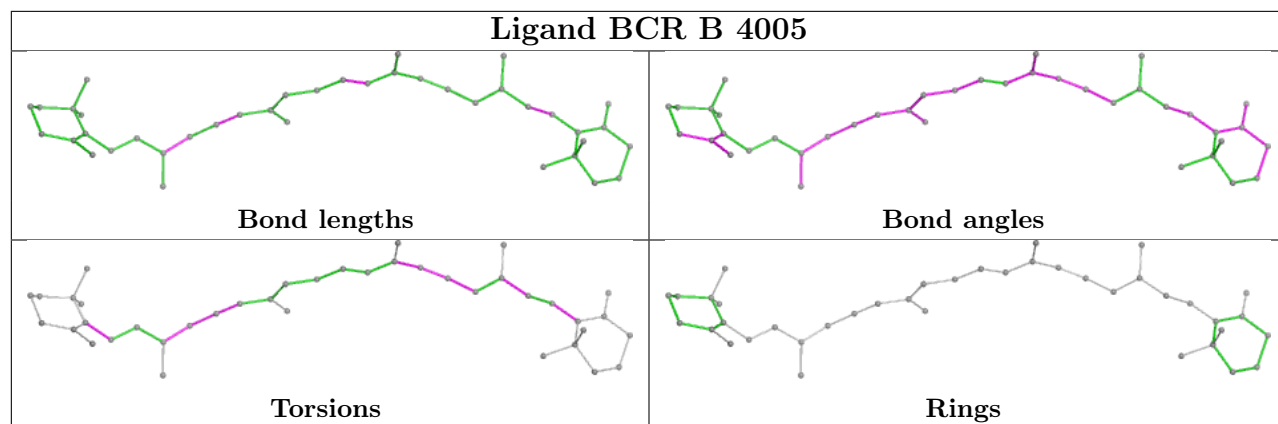
Ligand CLA 3 608

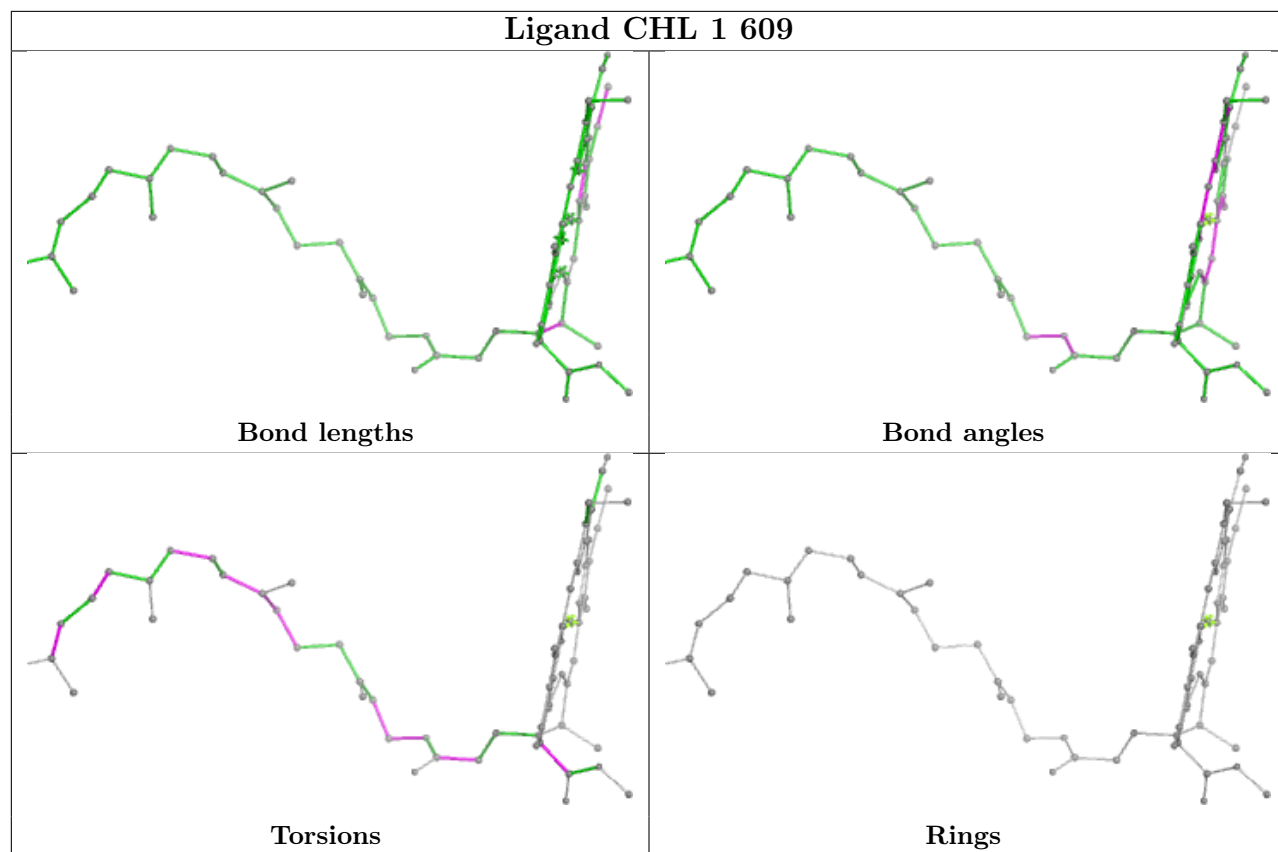


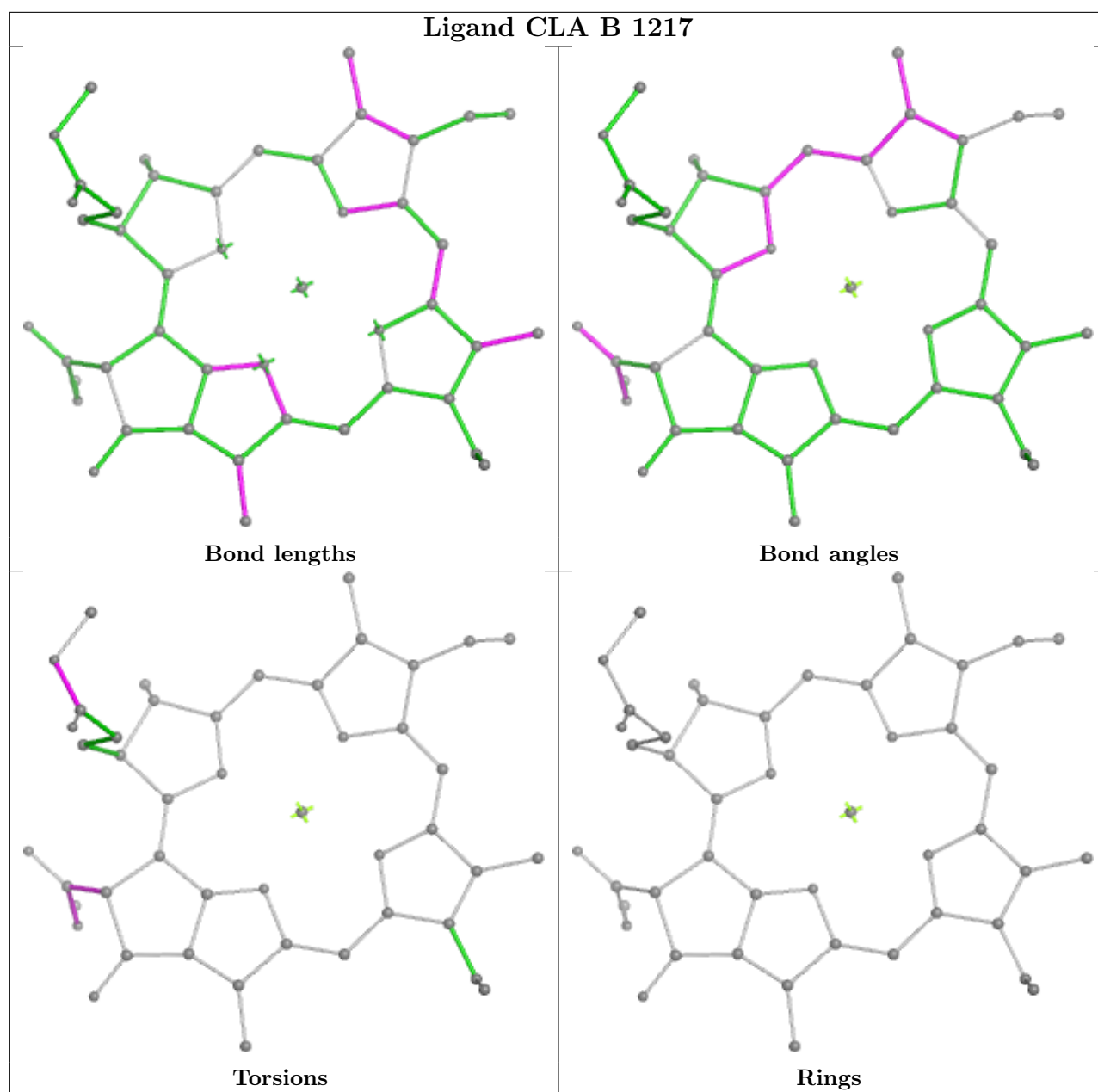


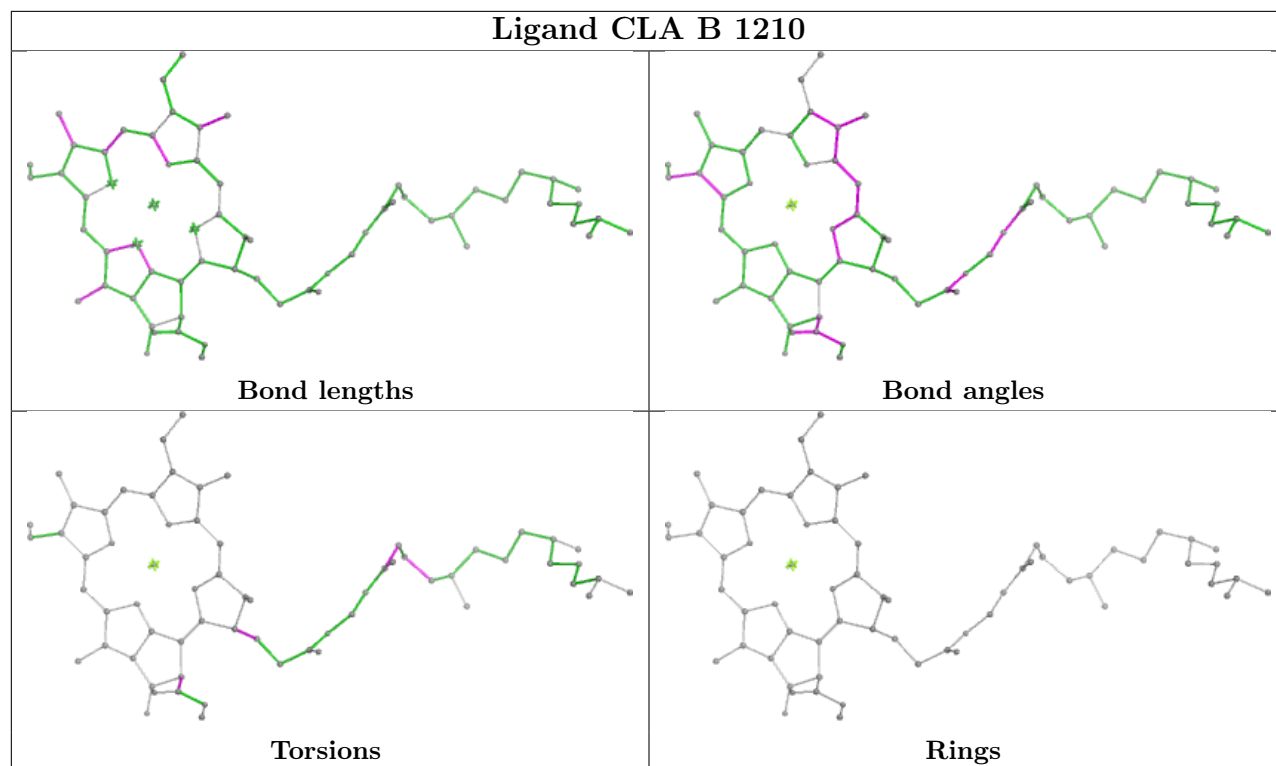


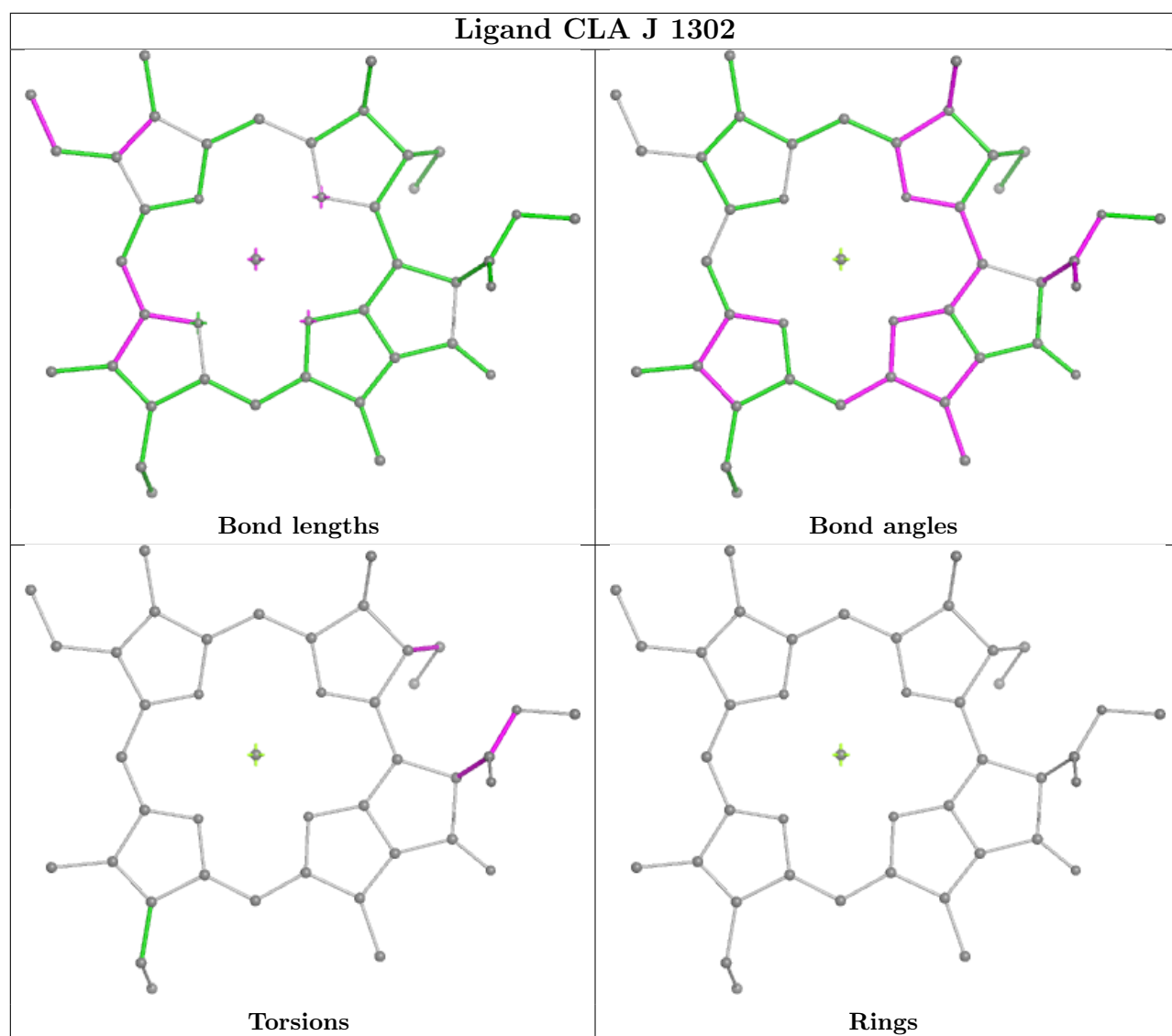




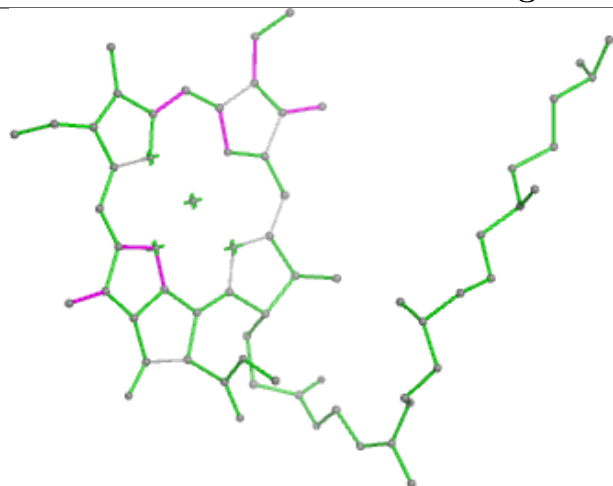




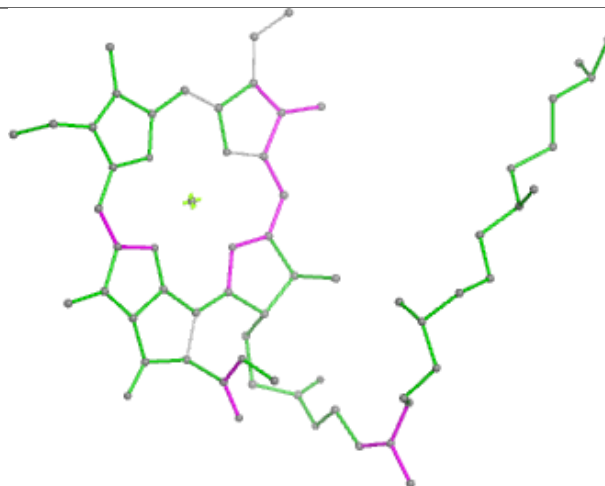




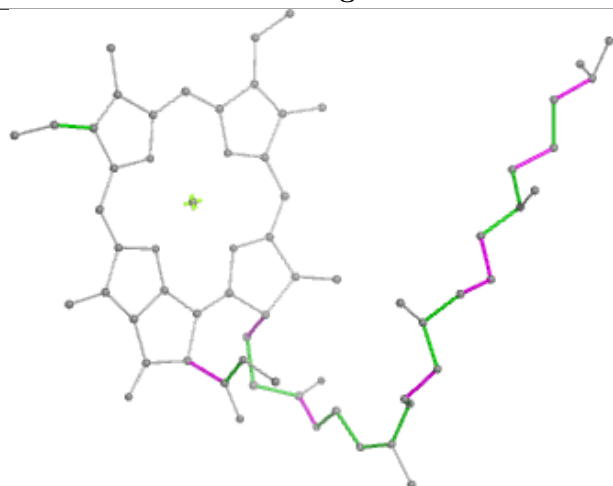
Ligand CLA 4 605



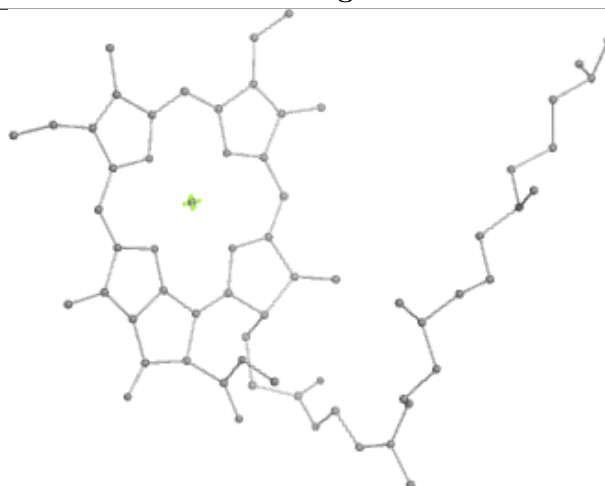
Bond lengths



Bond angles

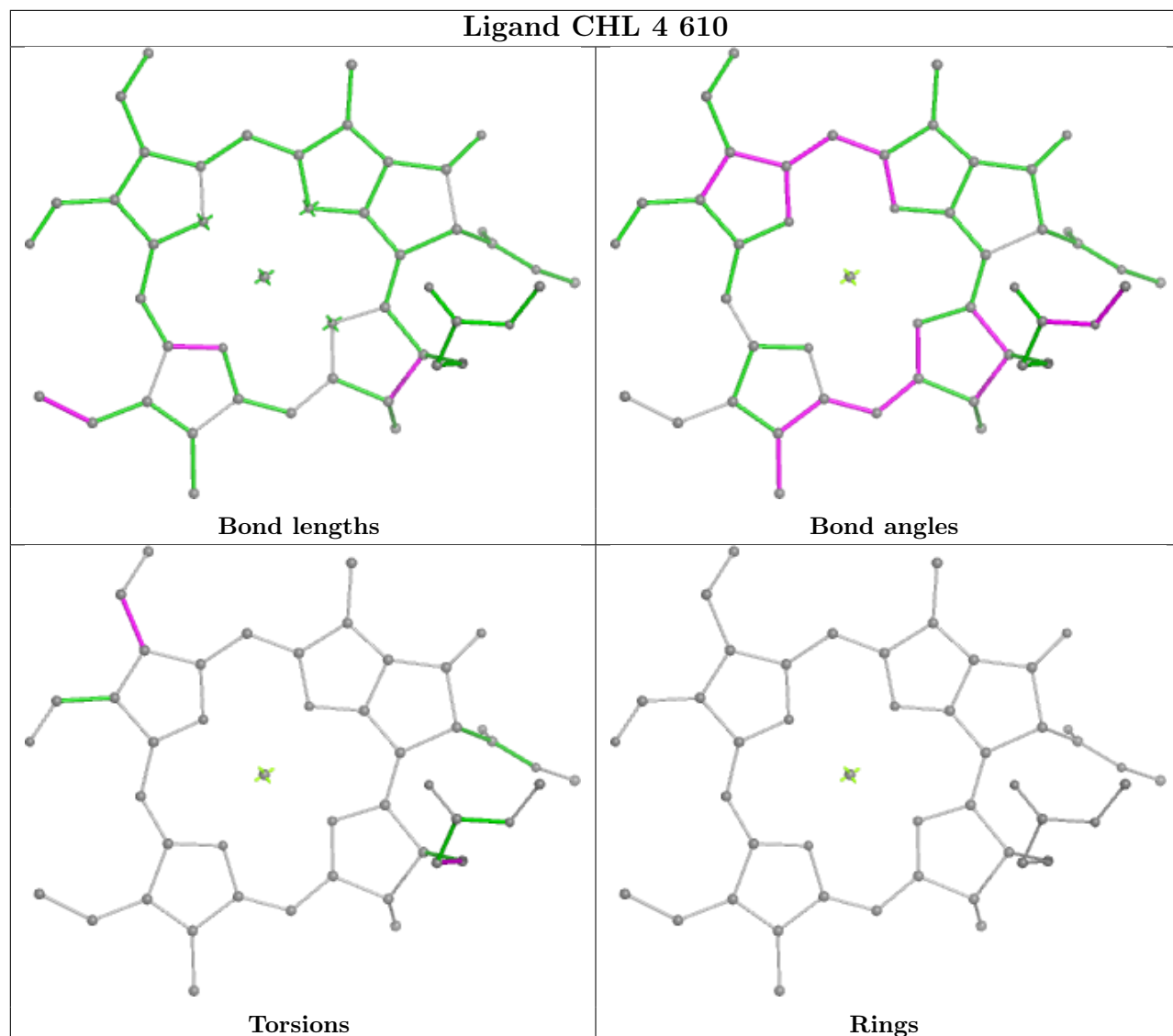


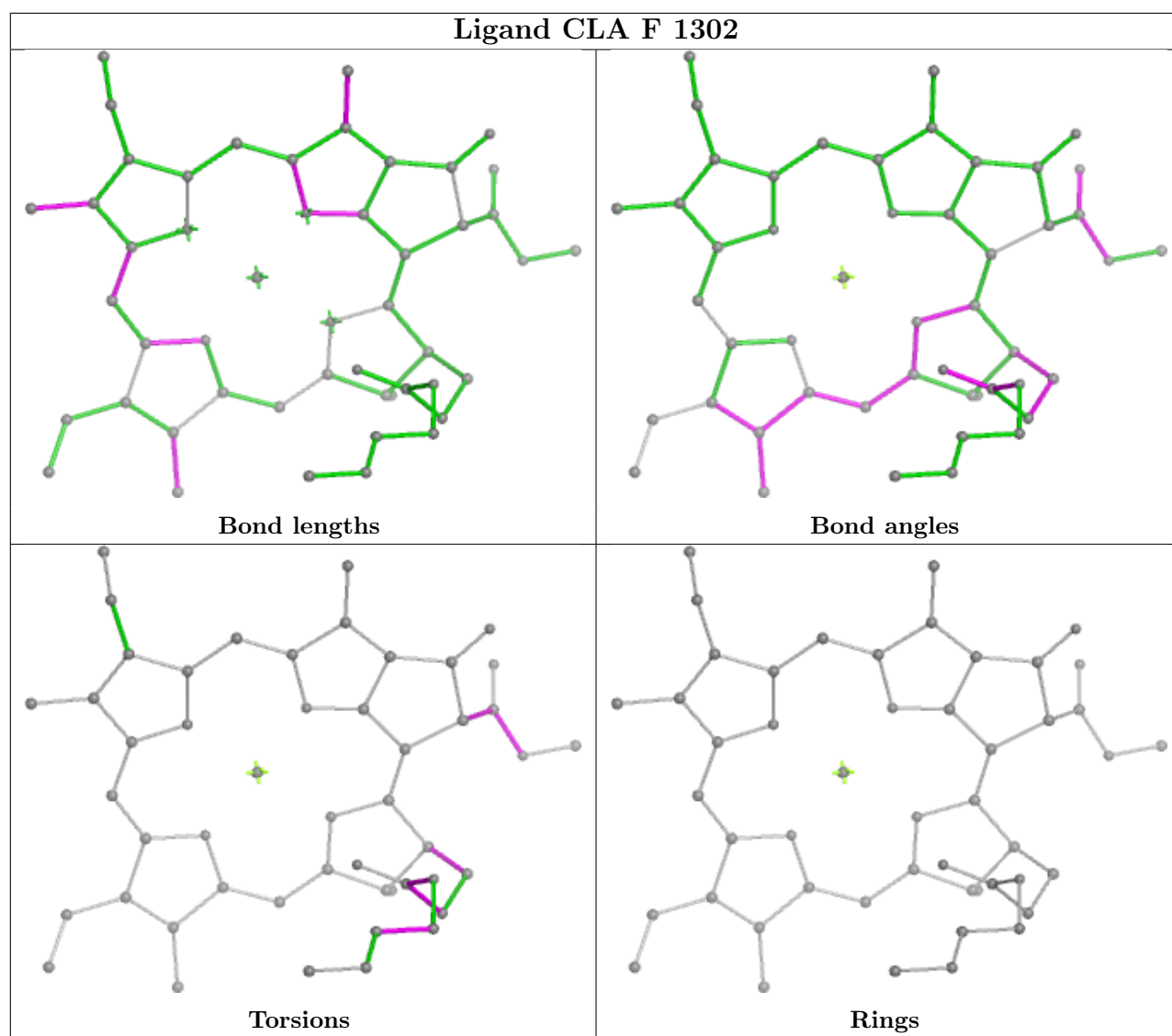
Torsions



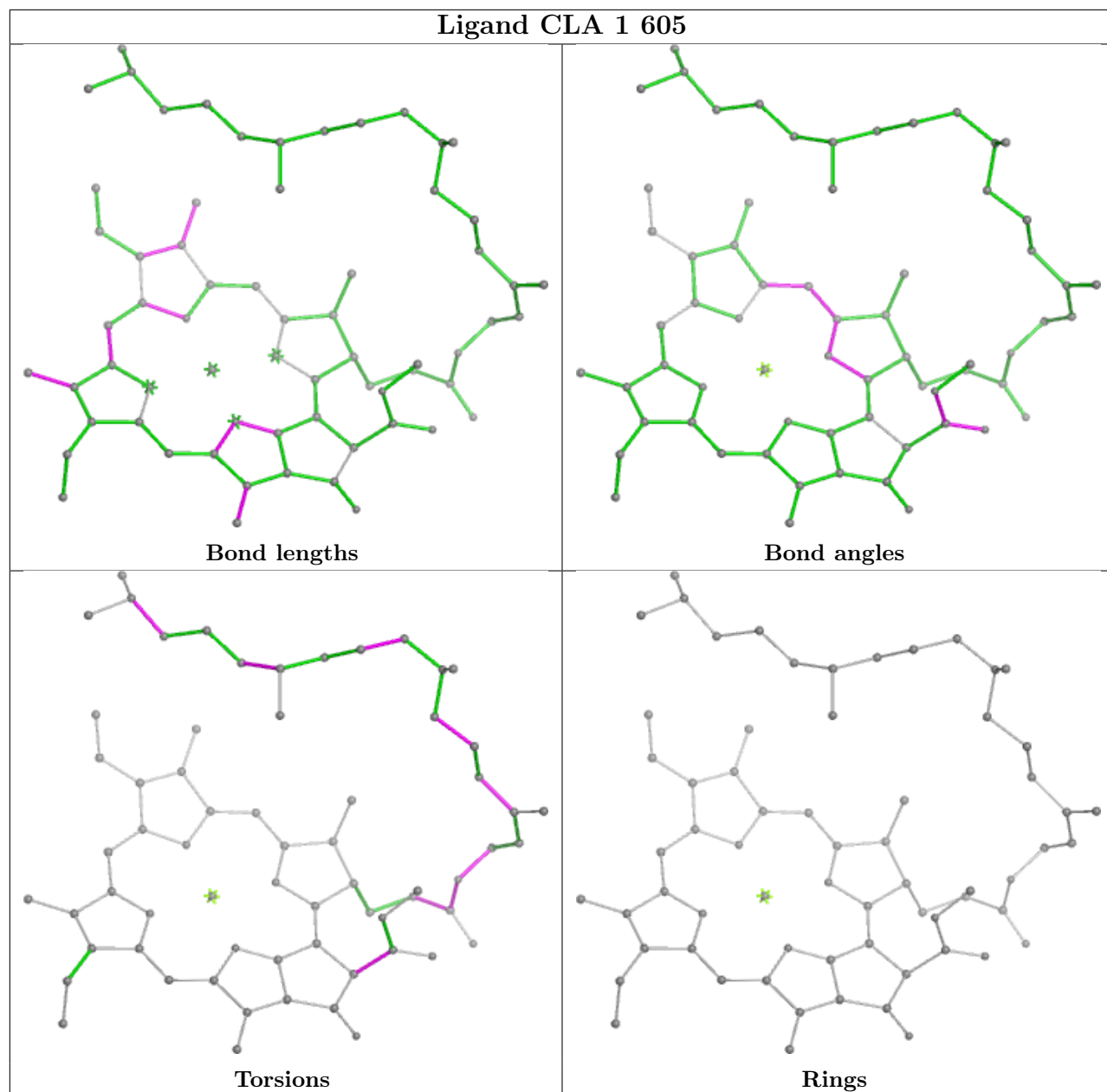
Rings

Ligand CHL 4 610

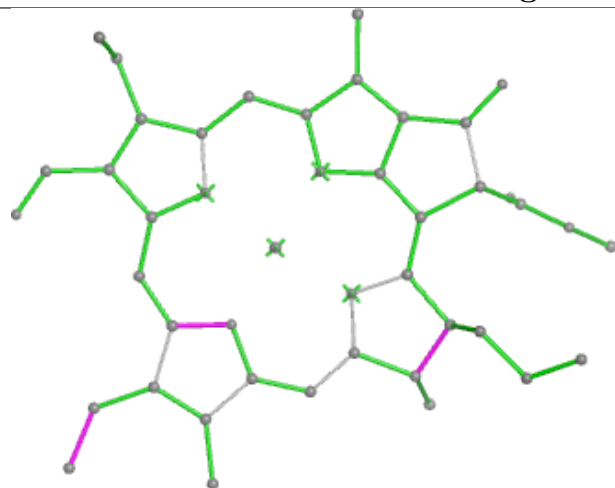




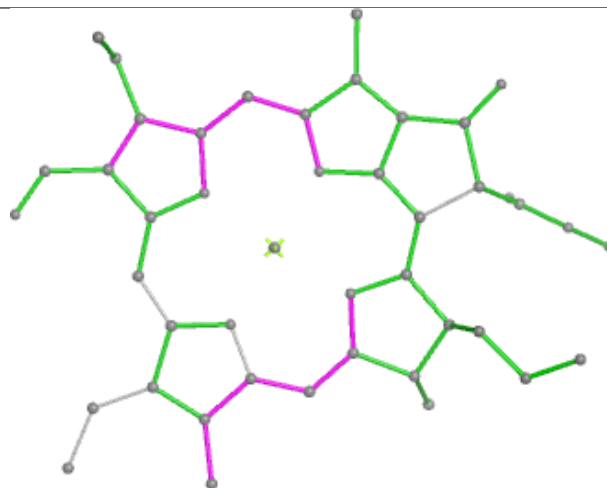
Ligand CLA 1 605



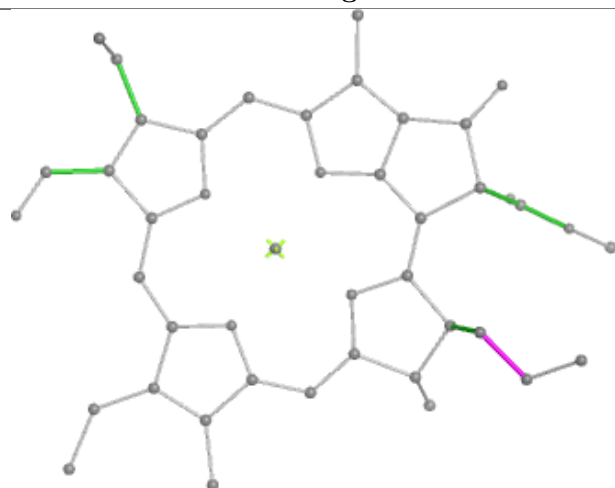
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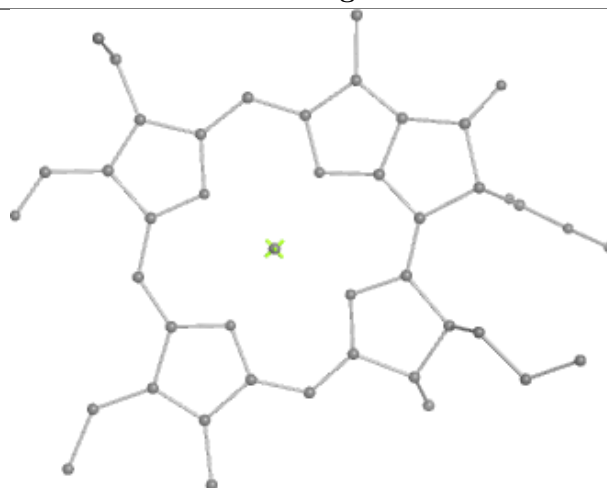
Bond lengths



Bond angles

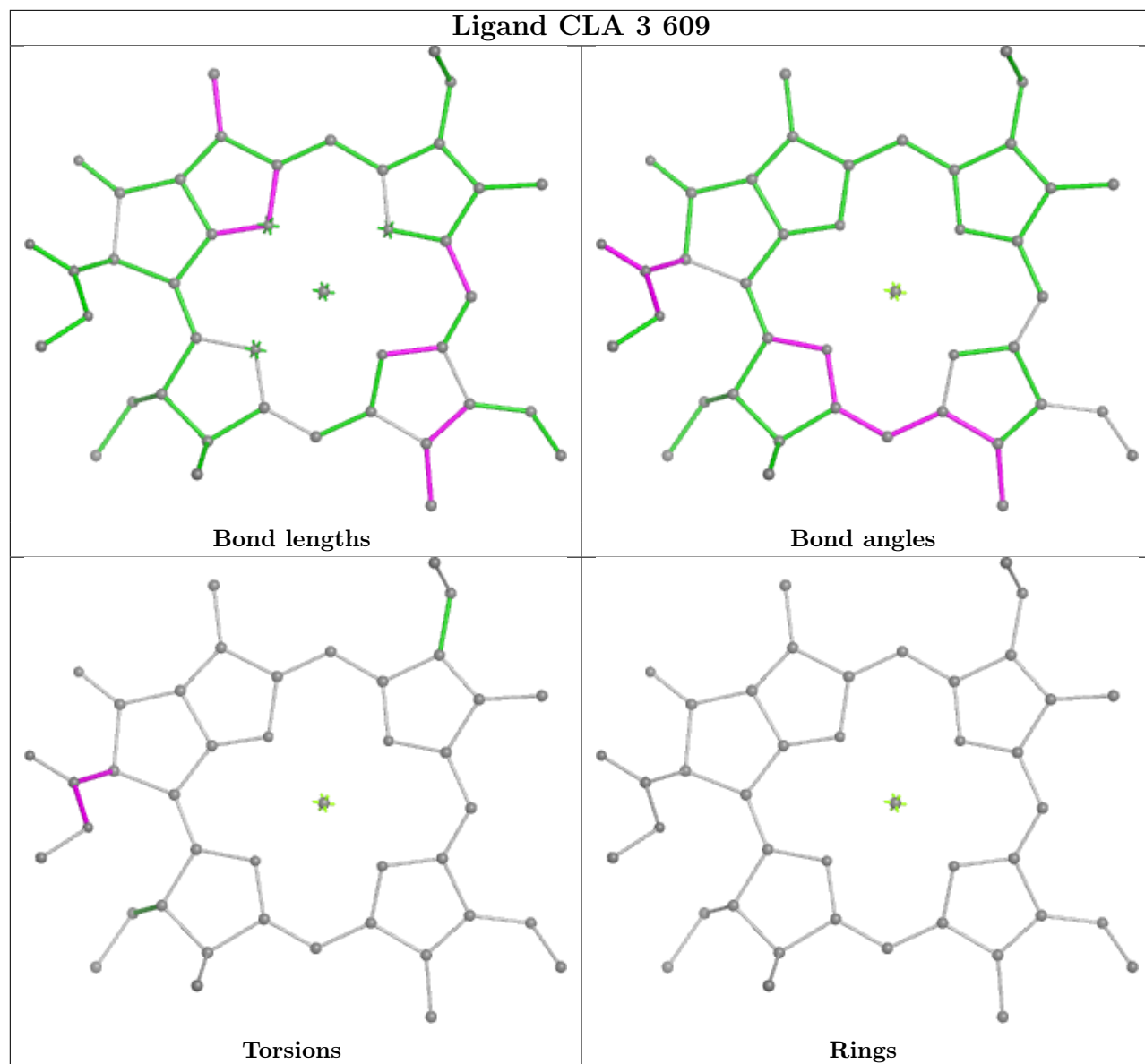


Torsions

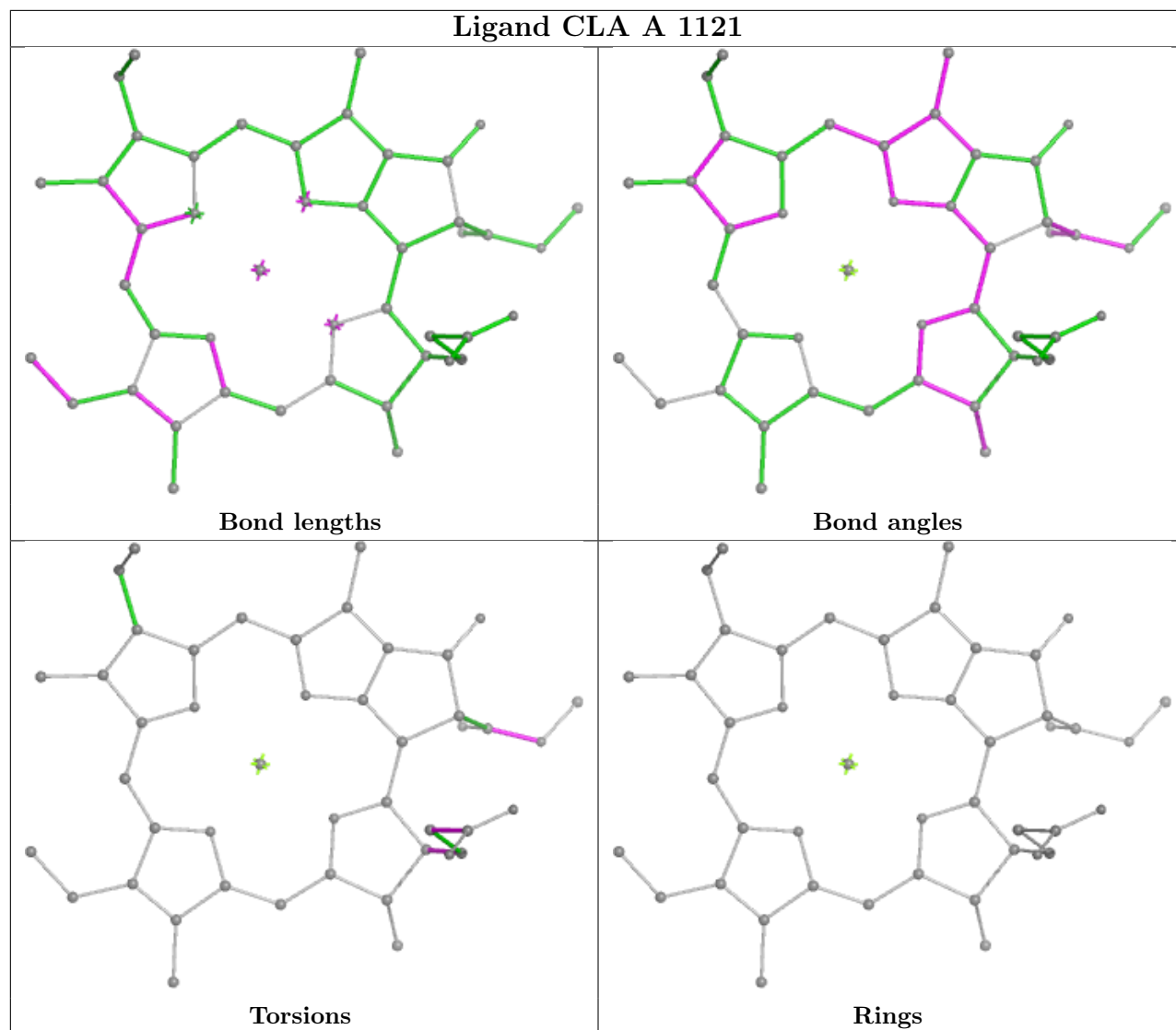


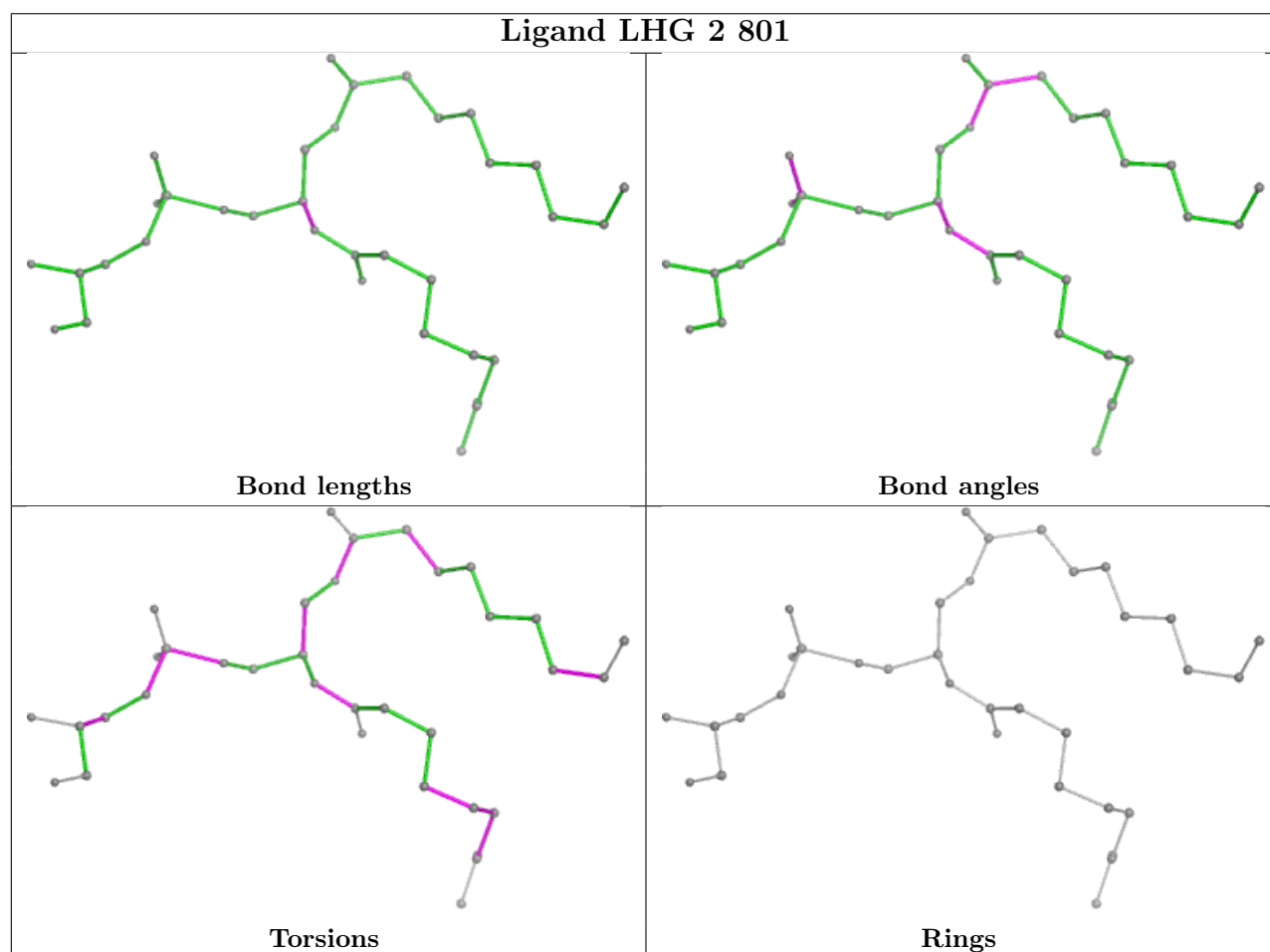
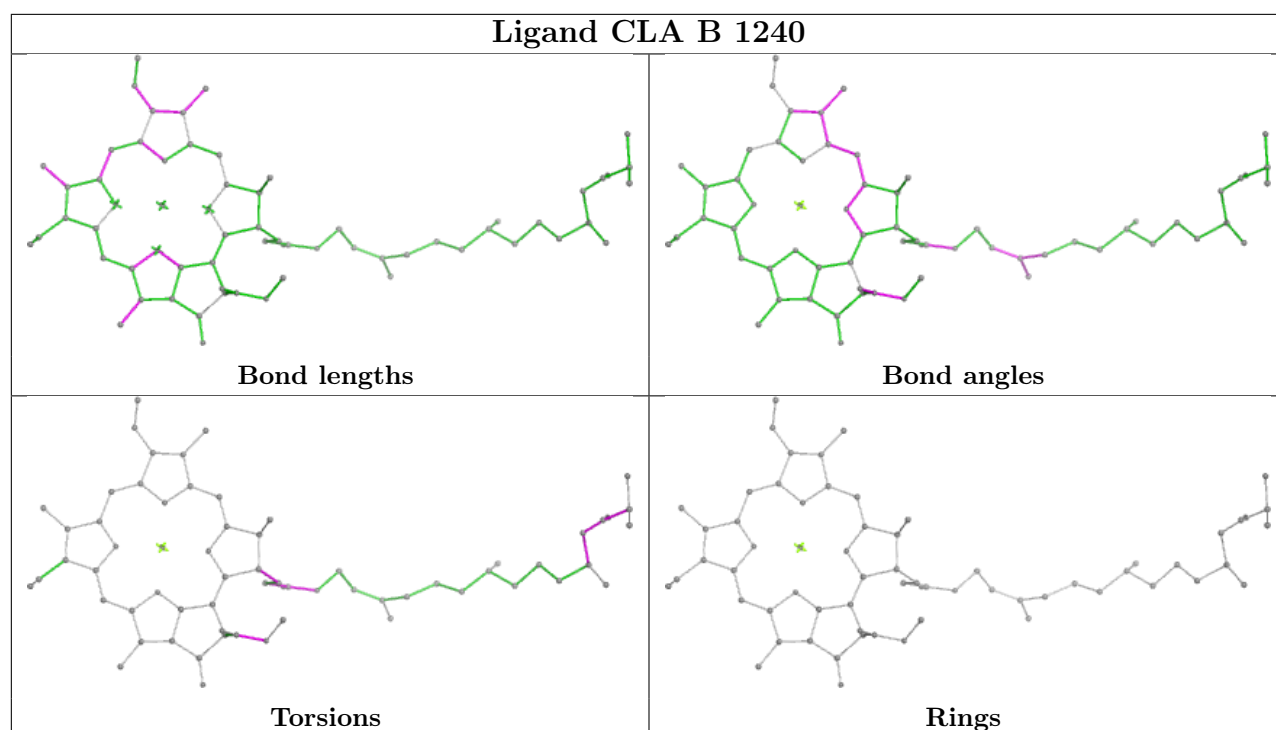
Rings

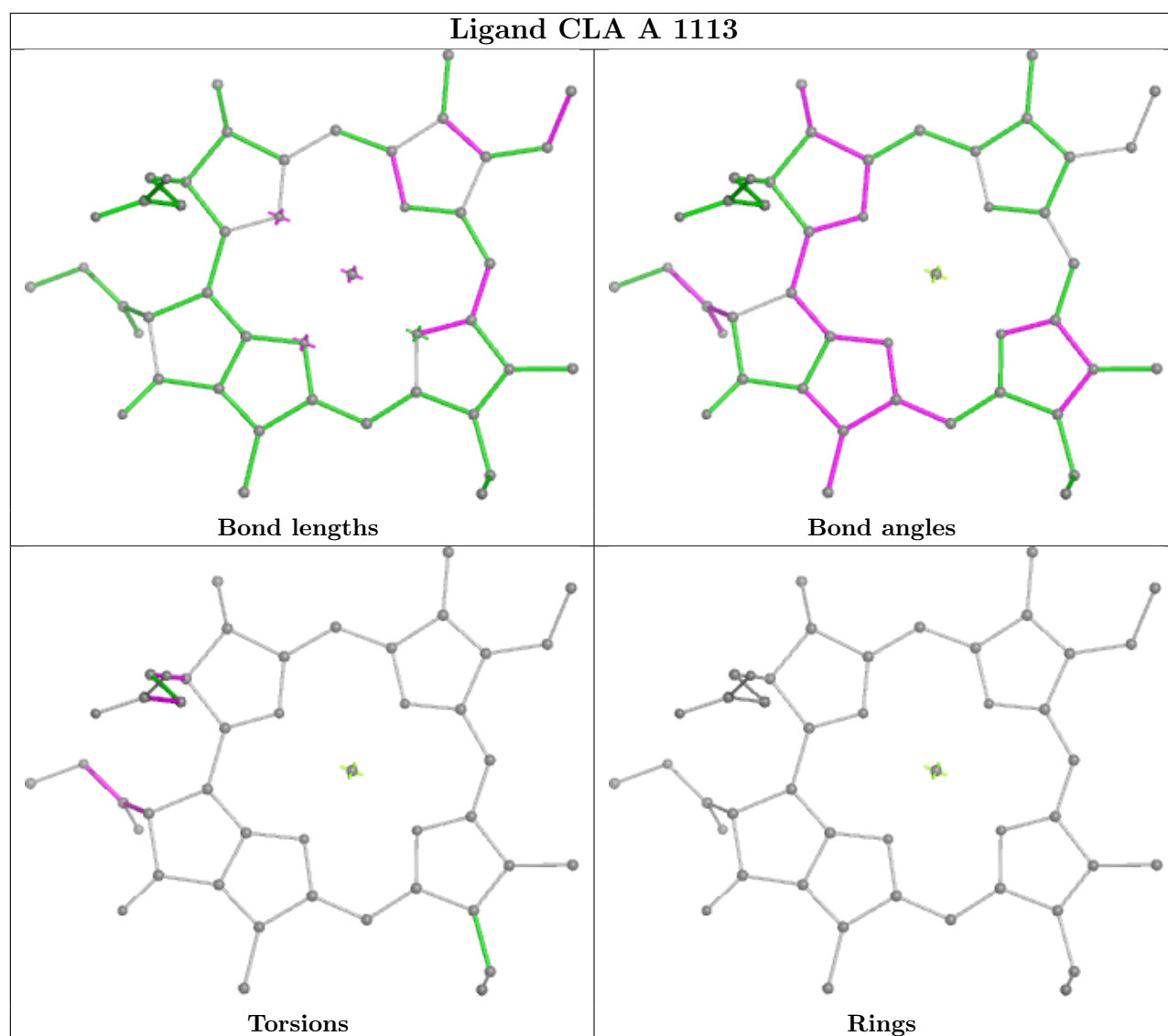
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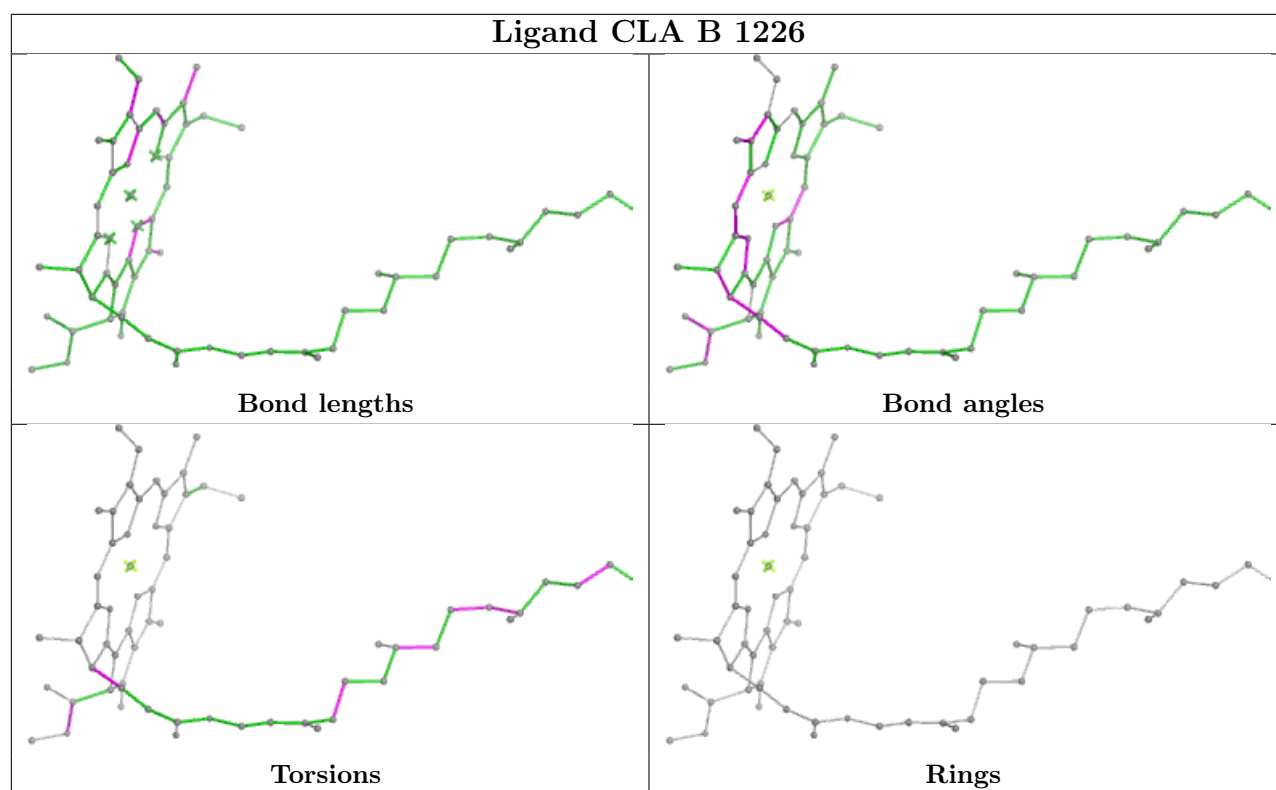


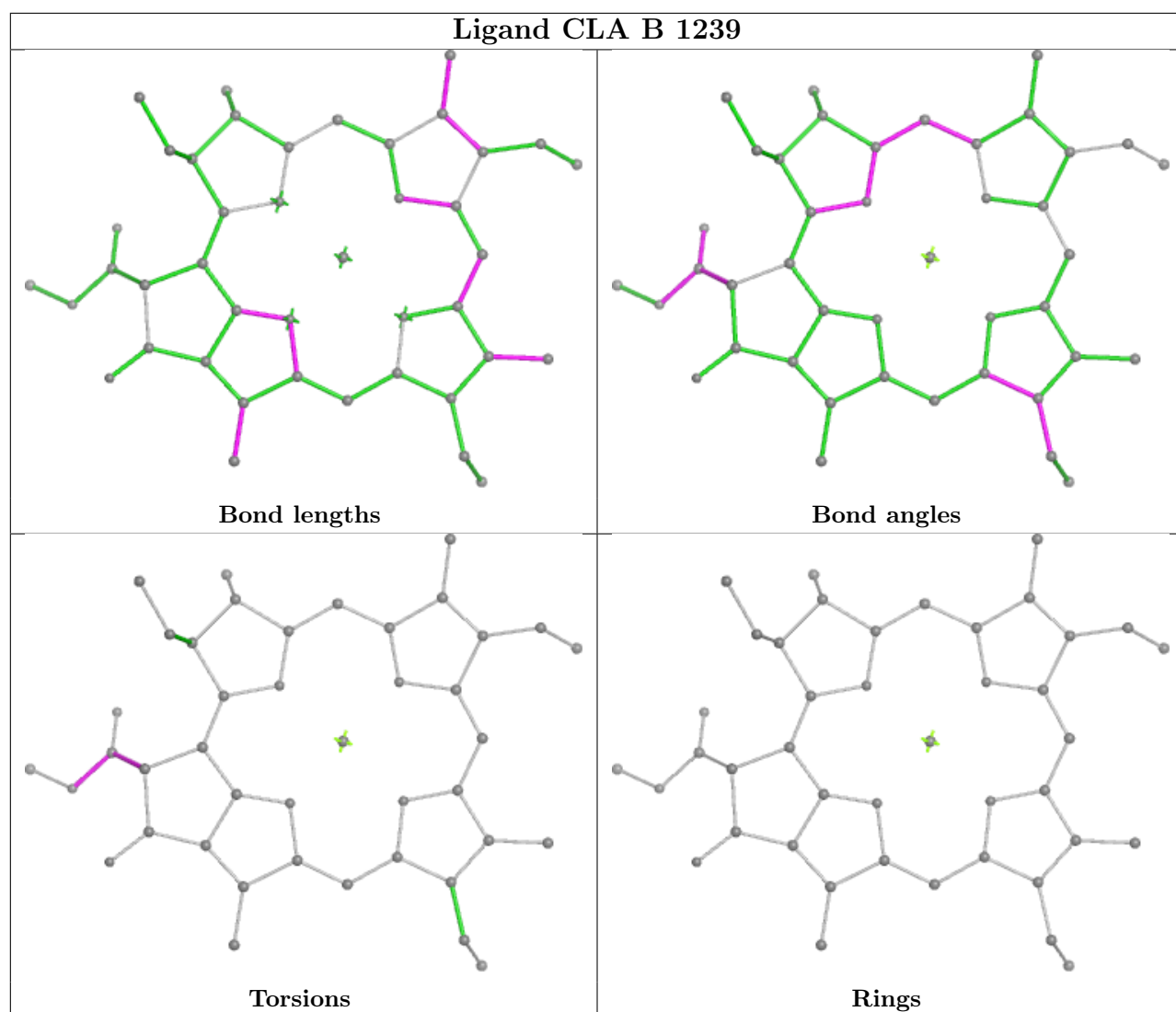
Ligand CLA A 1121

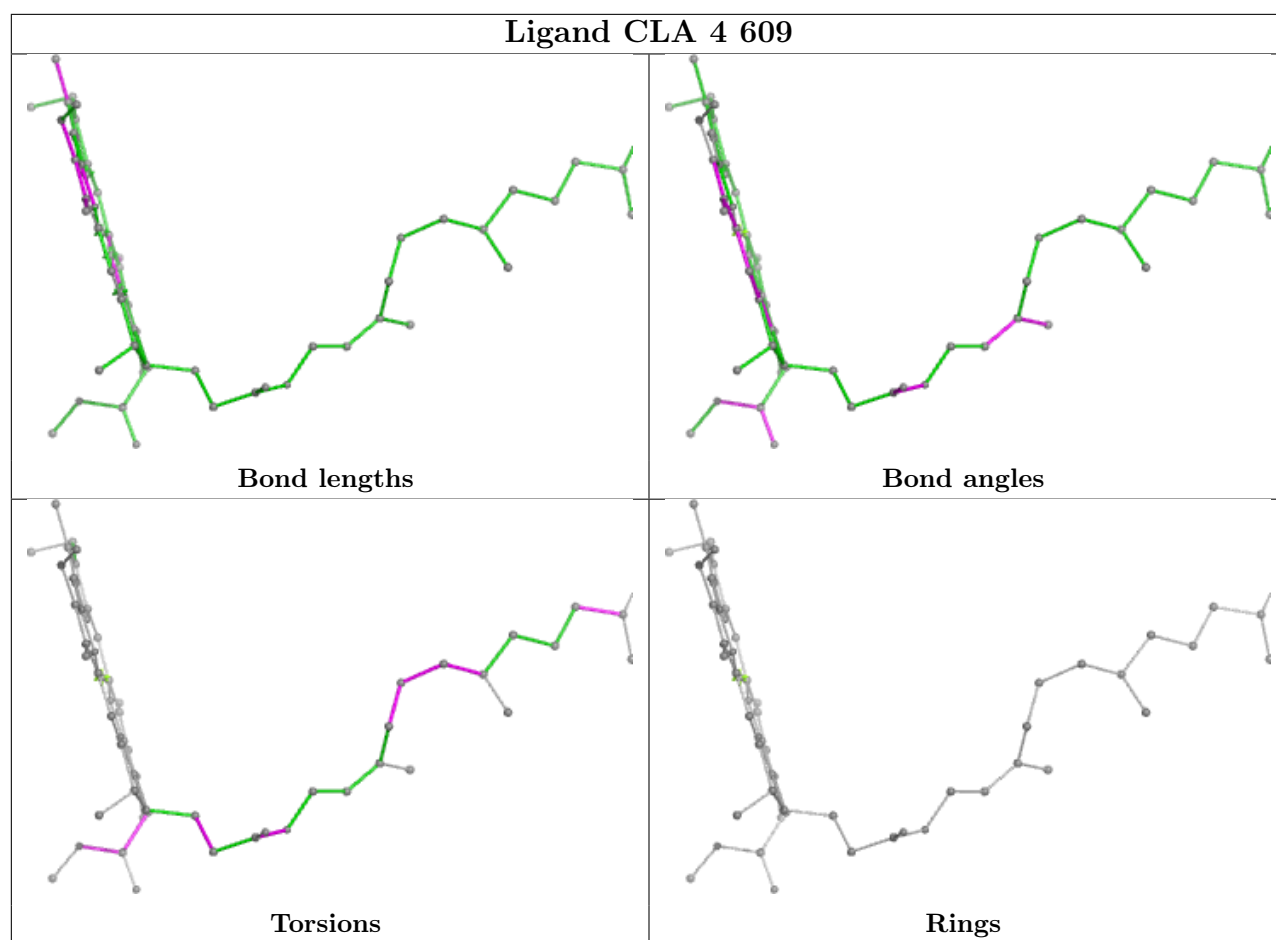




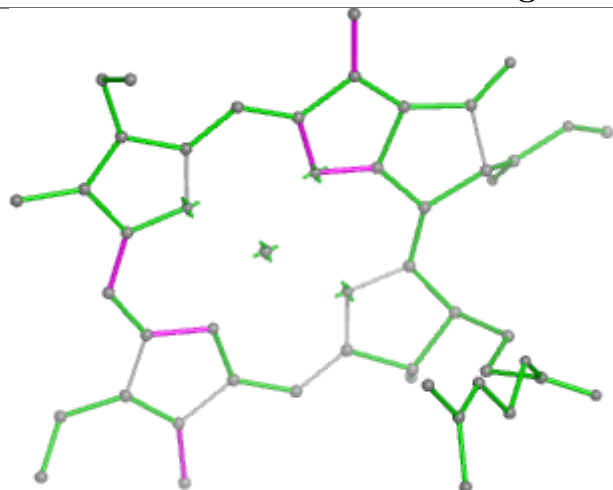




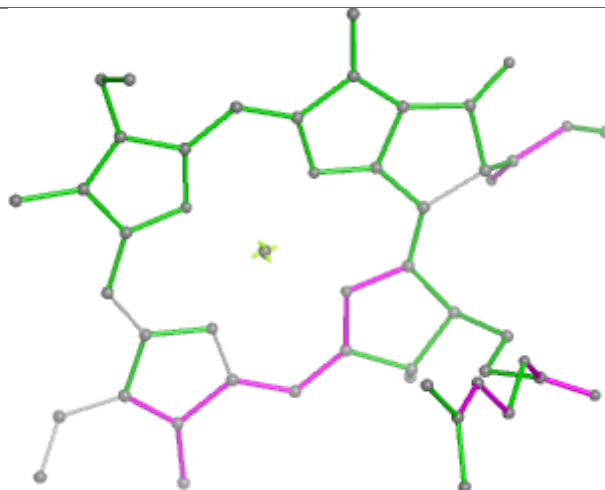




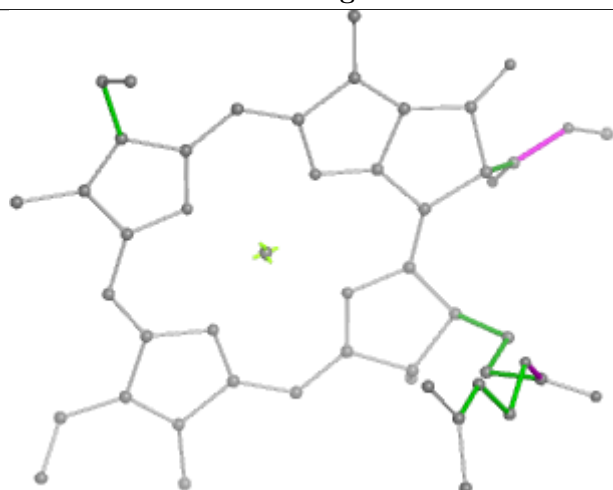
Ligand CLA 1 606



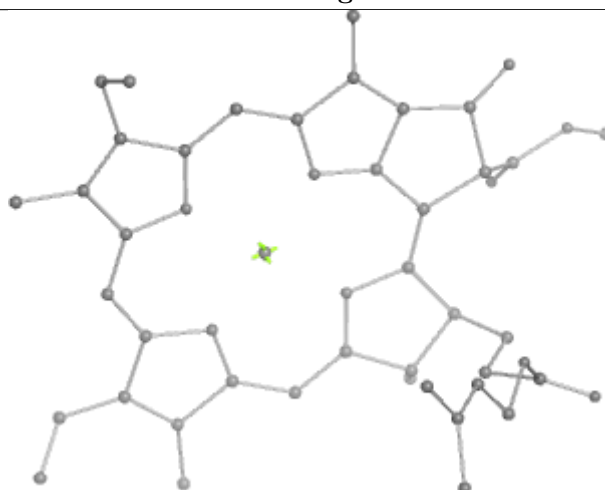
Bond lengths



Bond angles

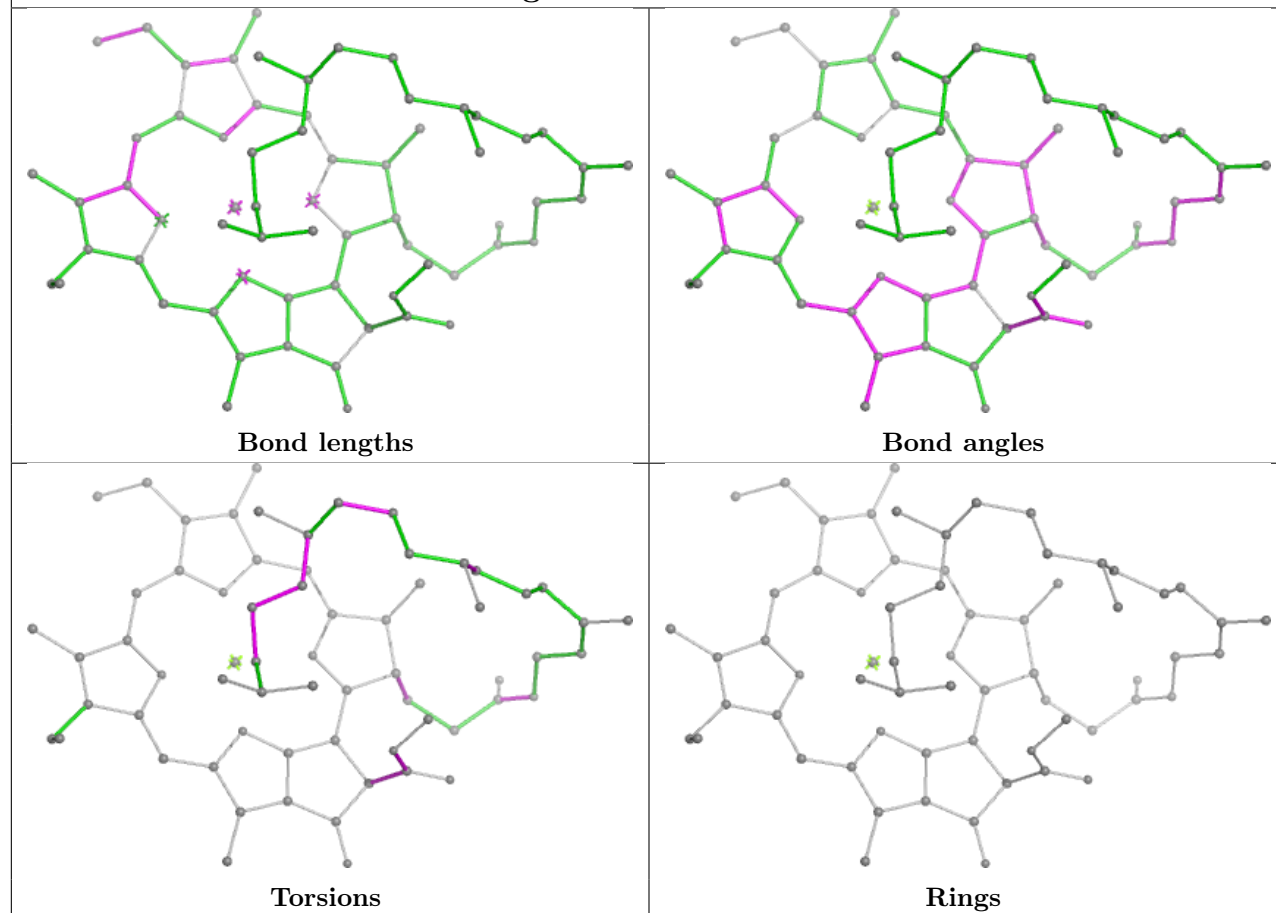


Torsions

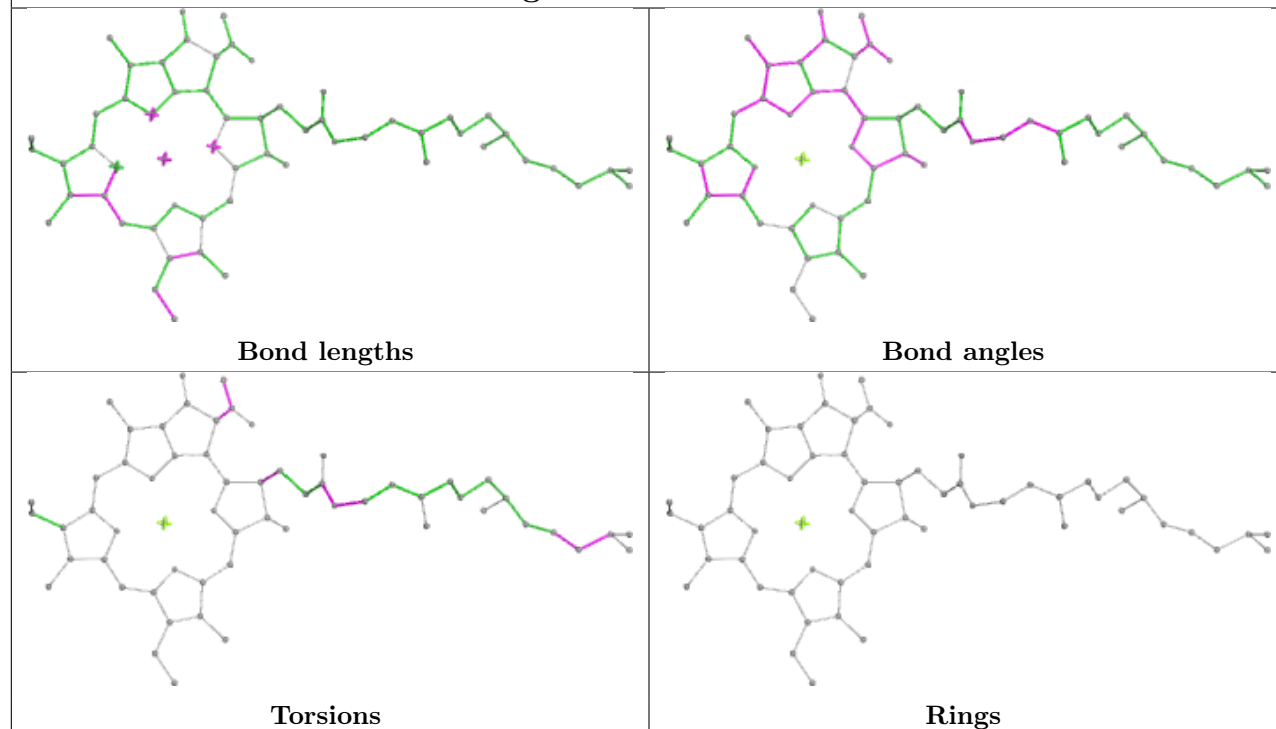


Rings

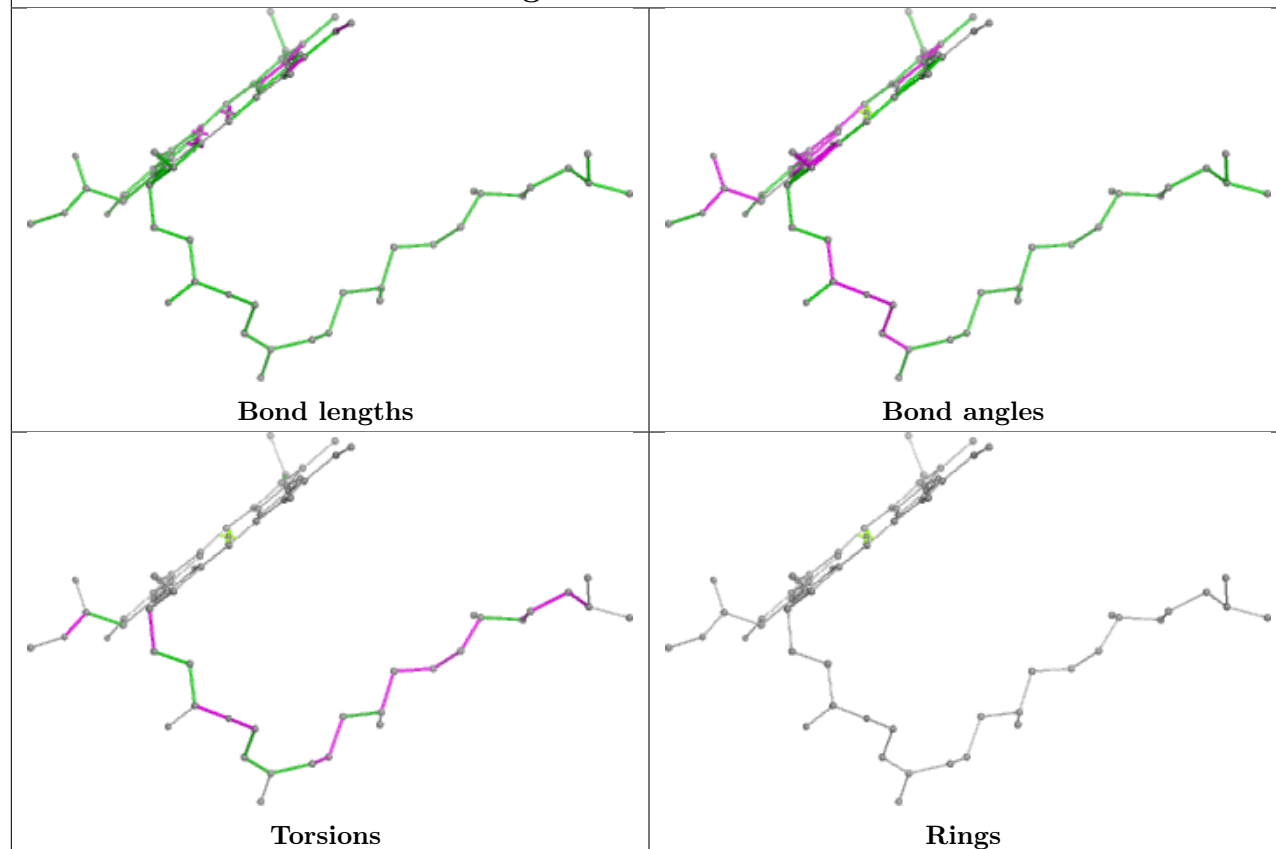
Ligand CLA A 1104



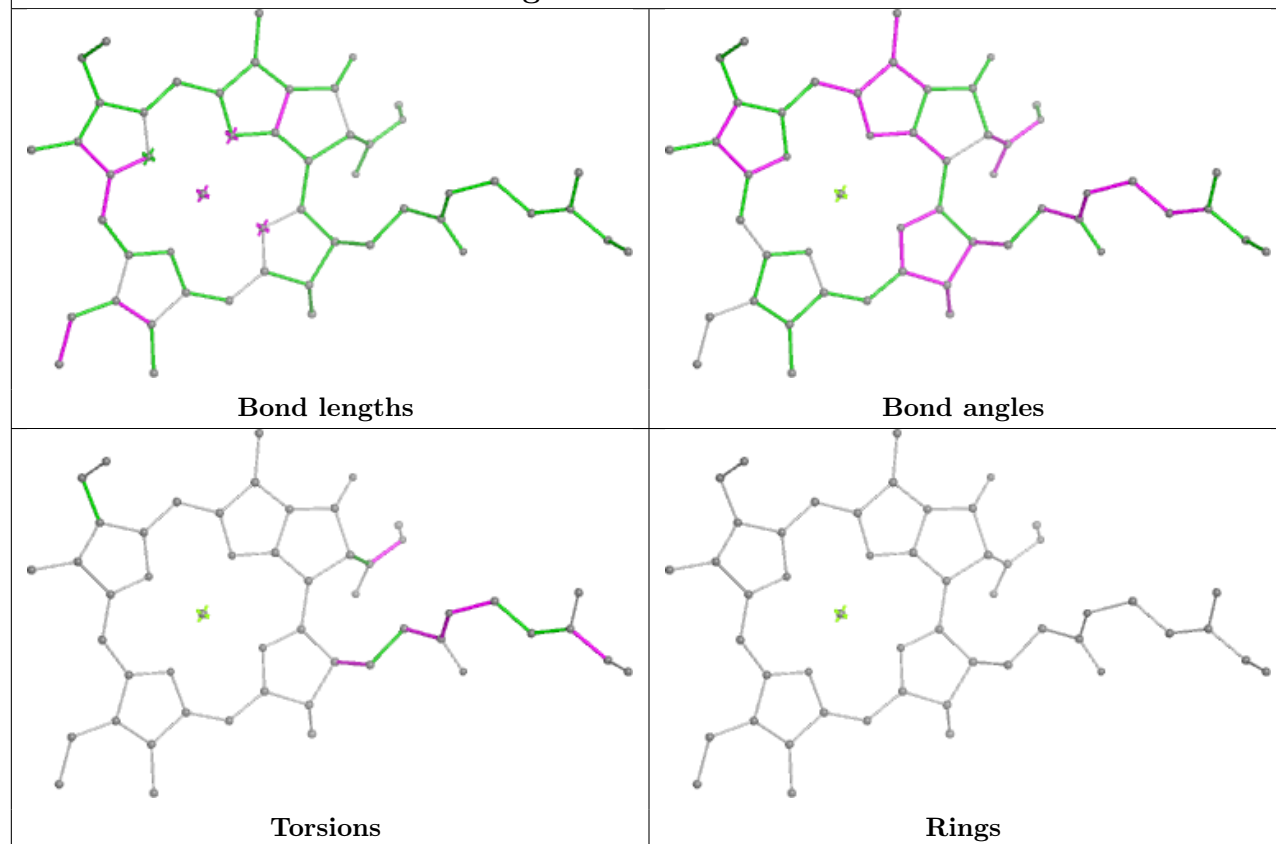
Ligand CLA A 1124

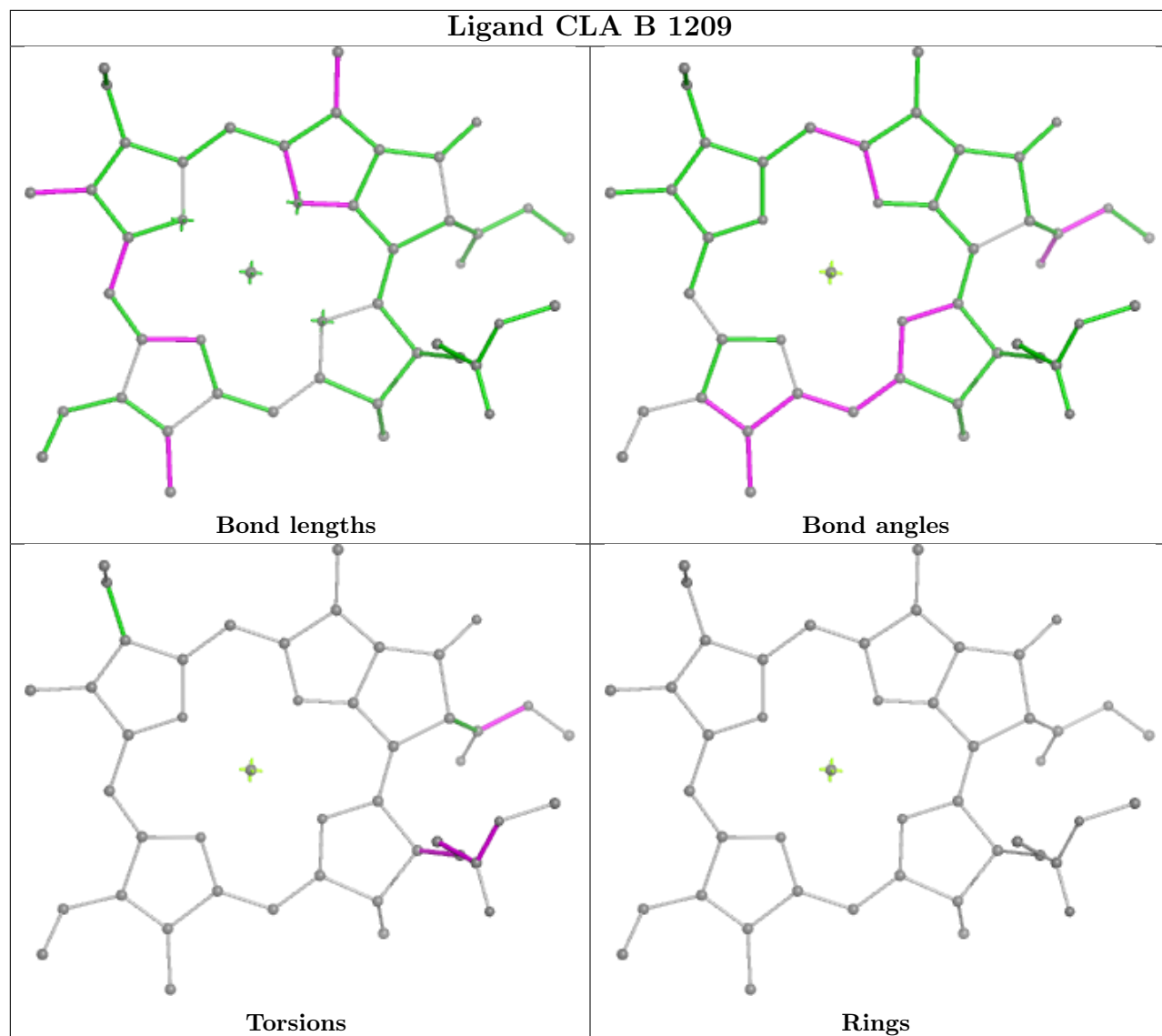


Ligand CLA A 1112

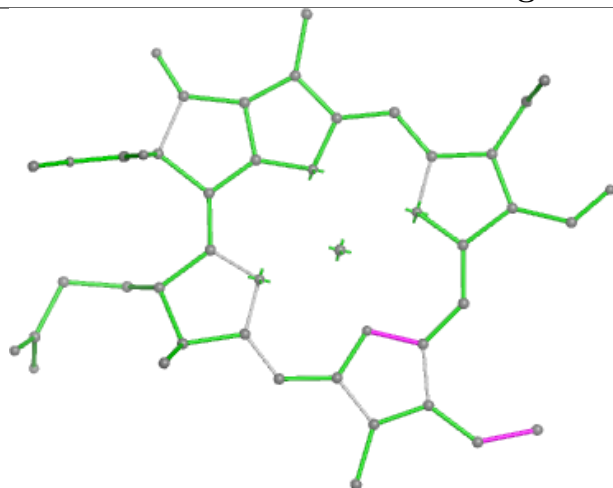


Ligand CLA A 1107

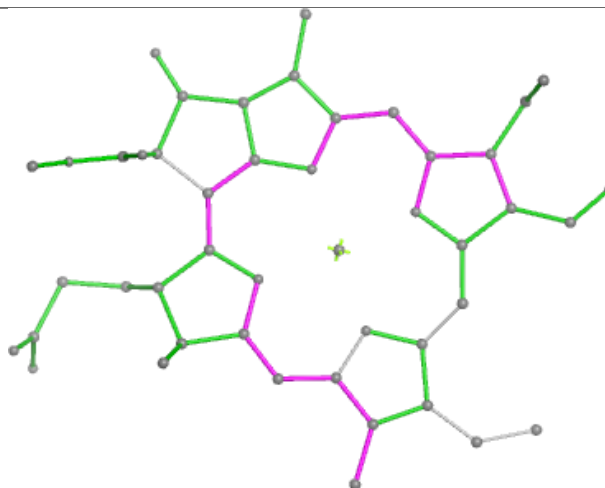




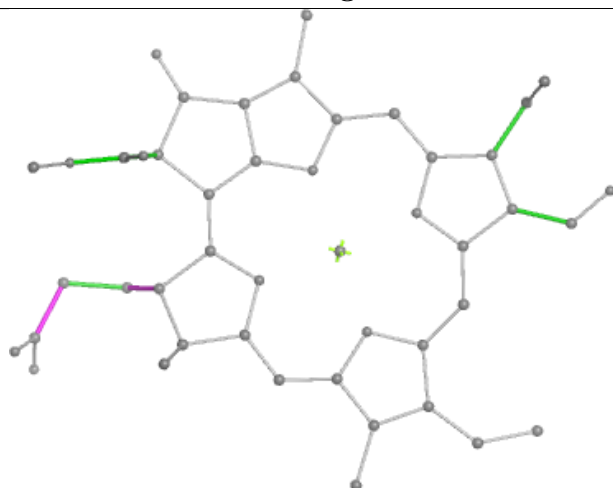
Ligand CHL 2 613



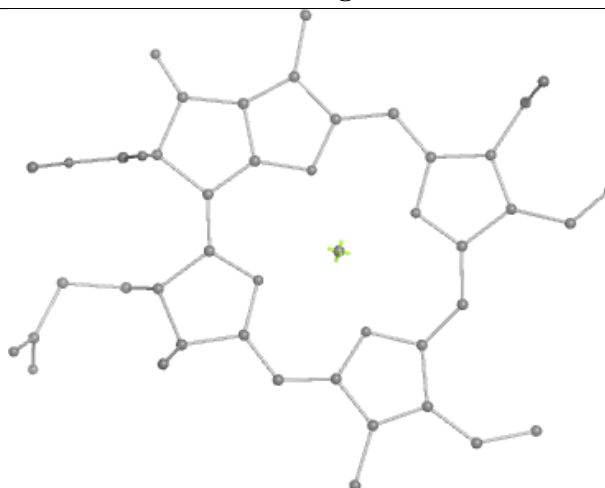
Bond lengths



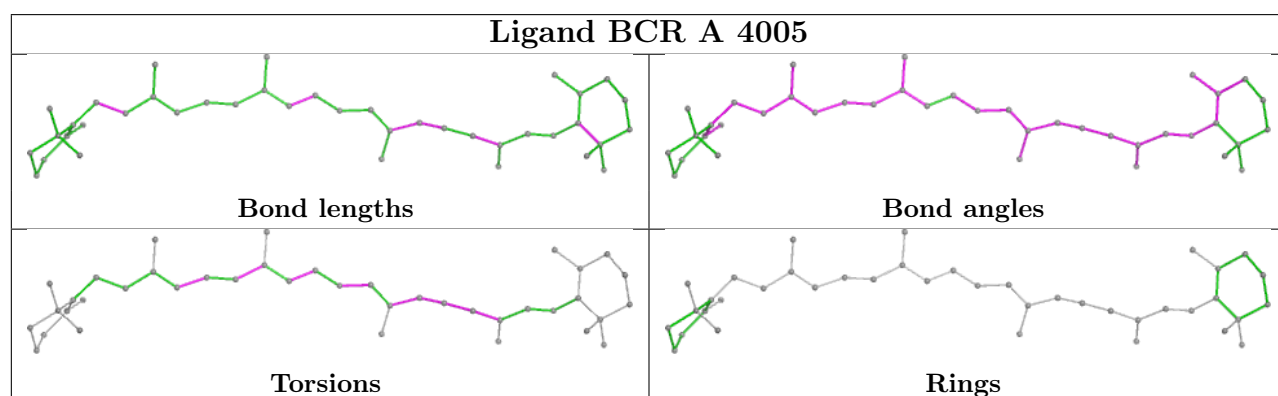
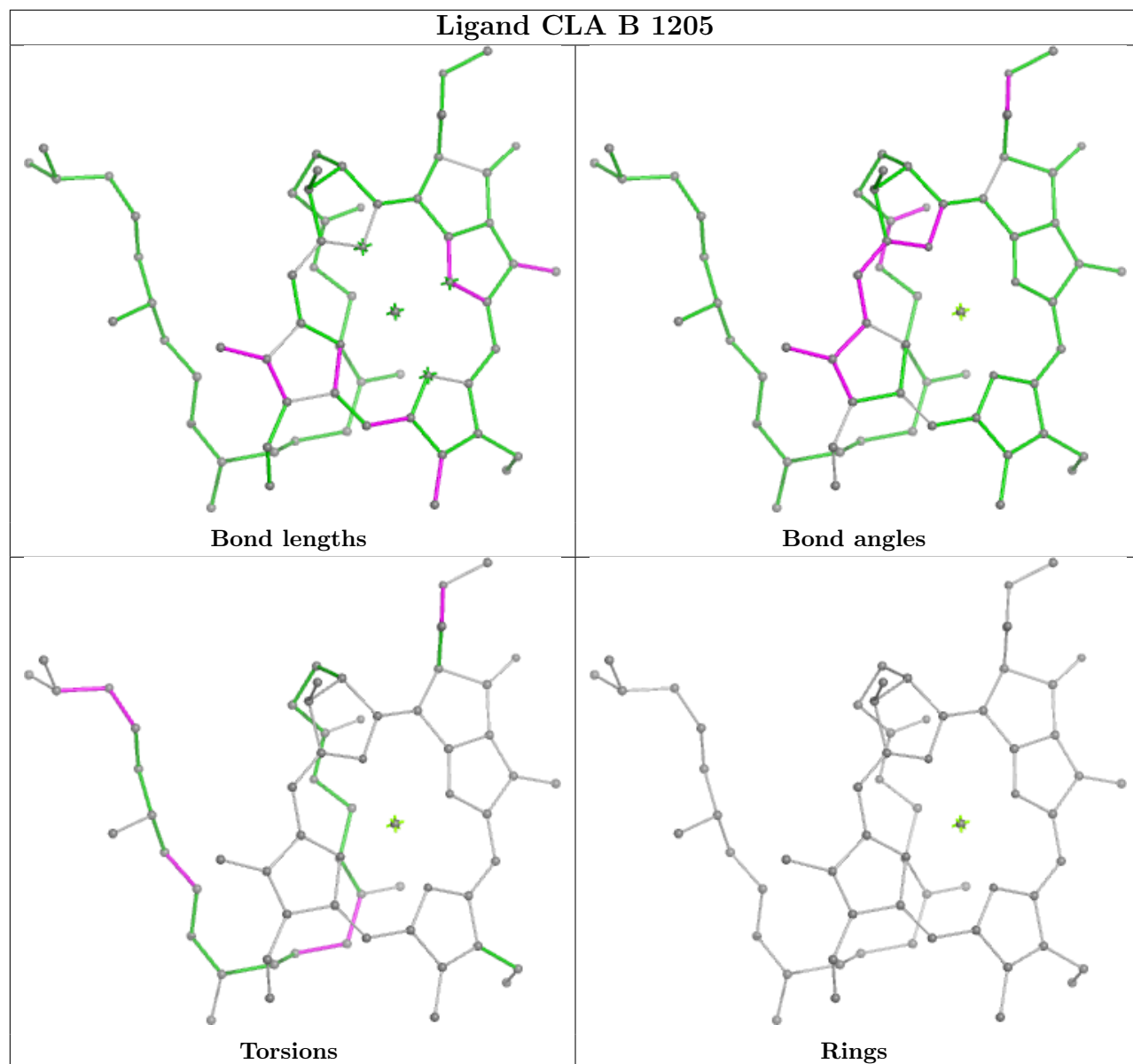
Bond angles

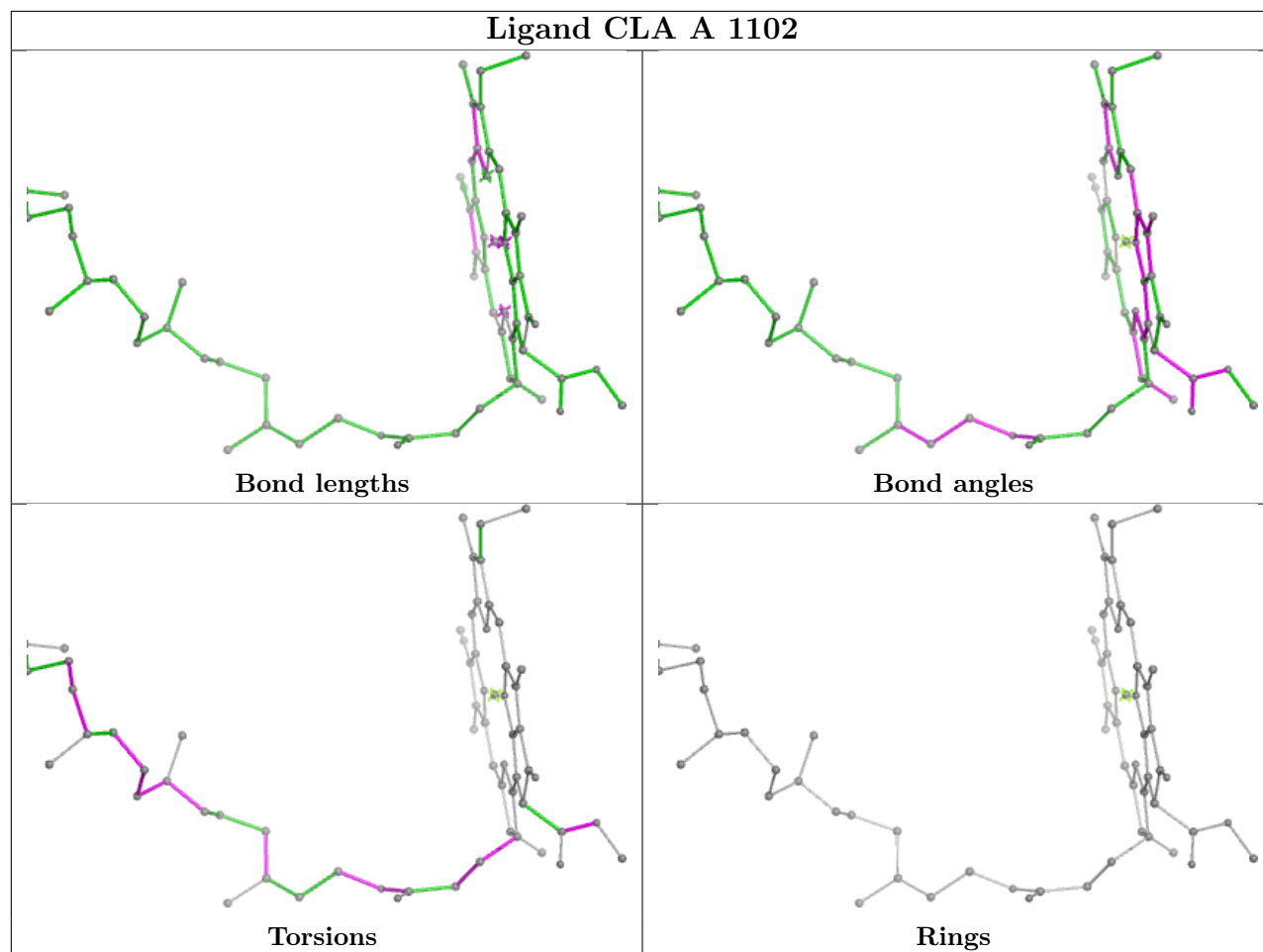


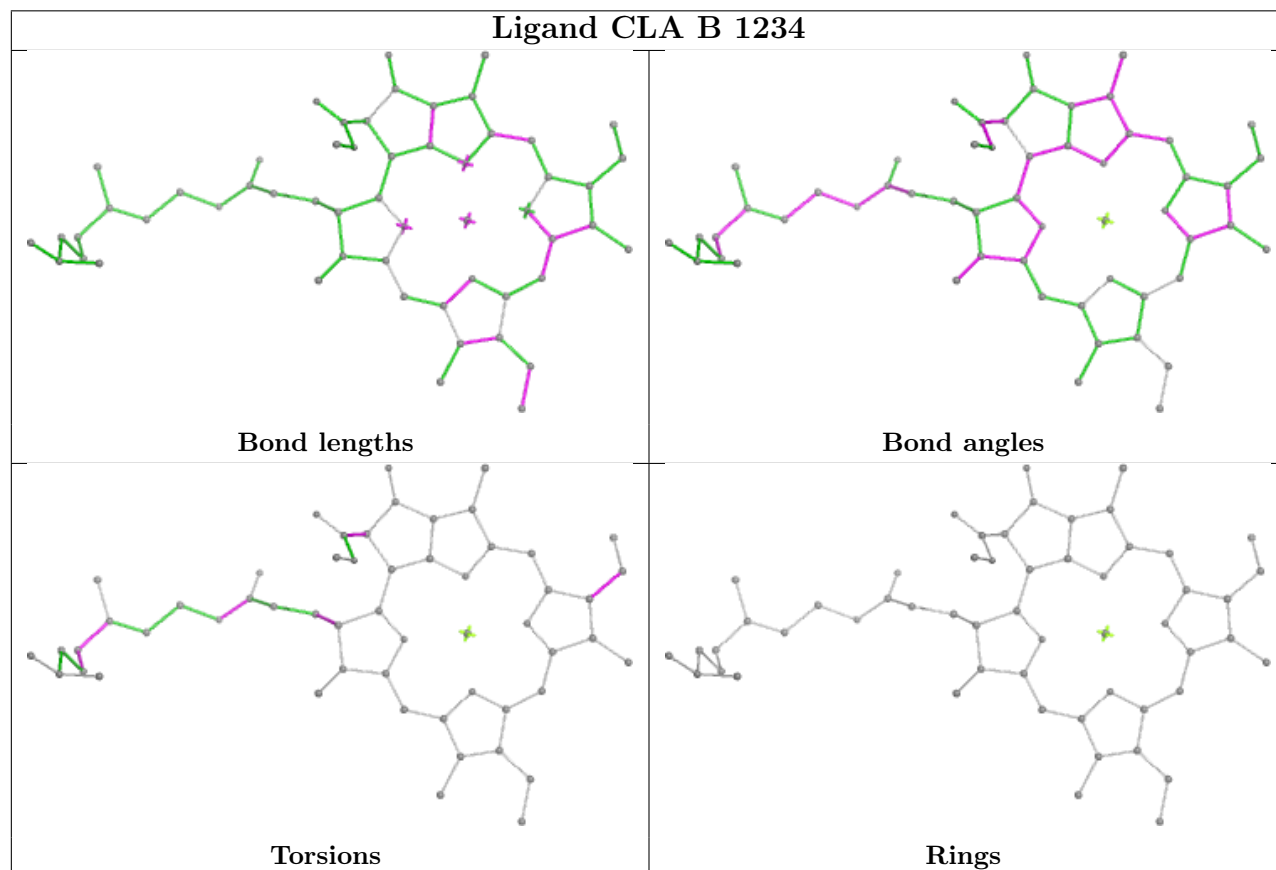
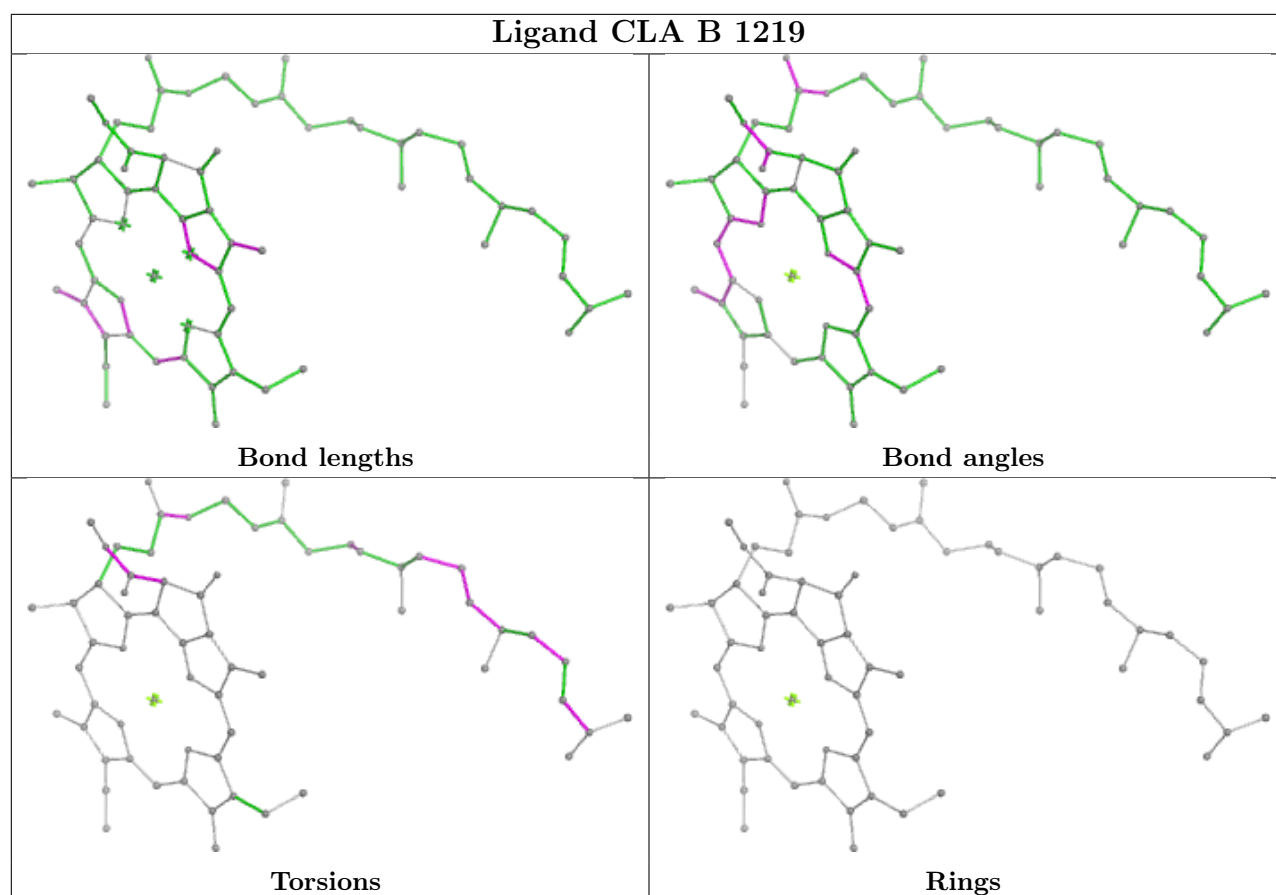
Torsions

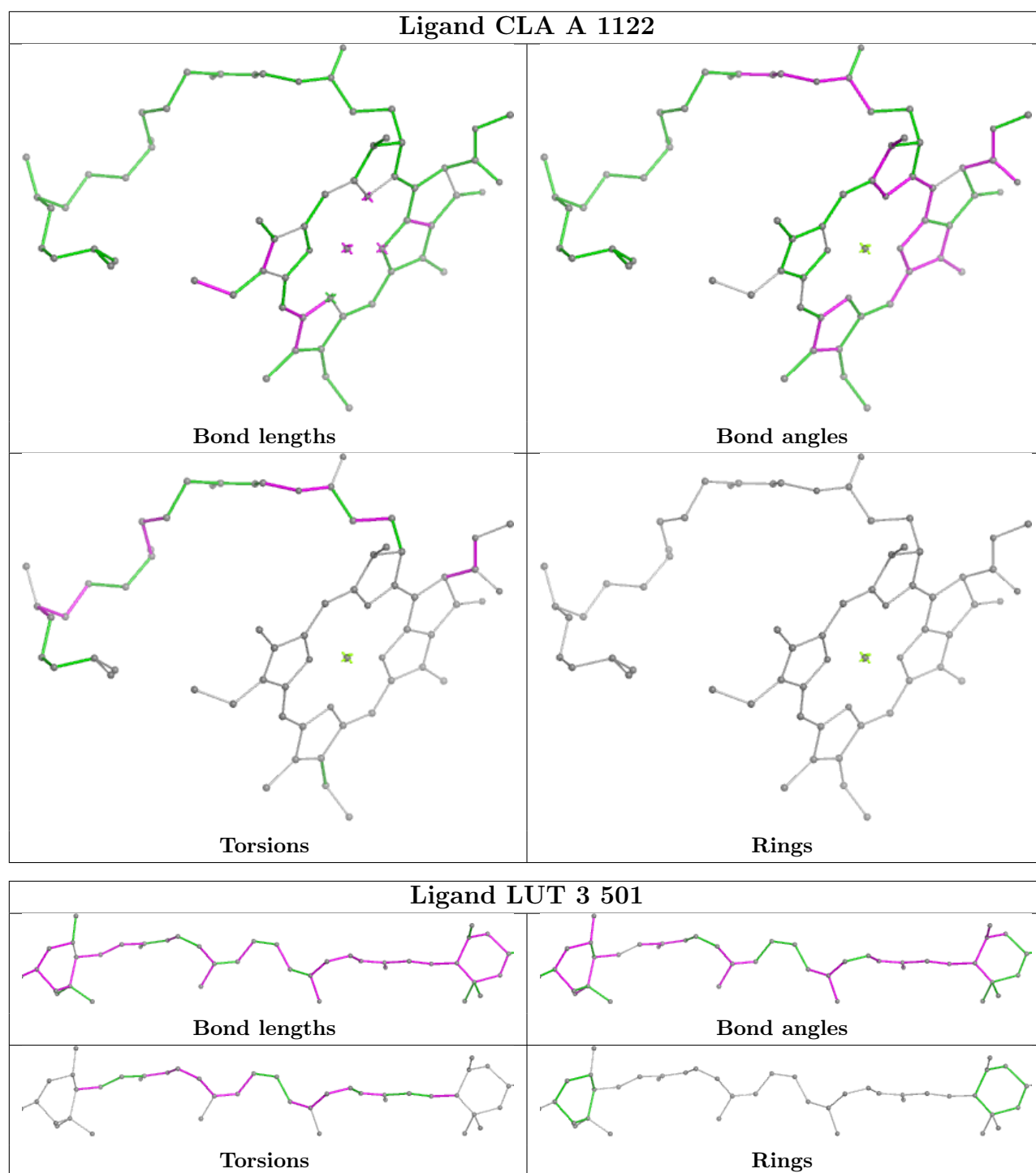


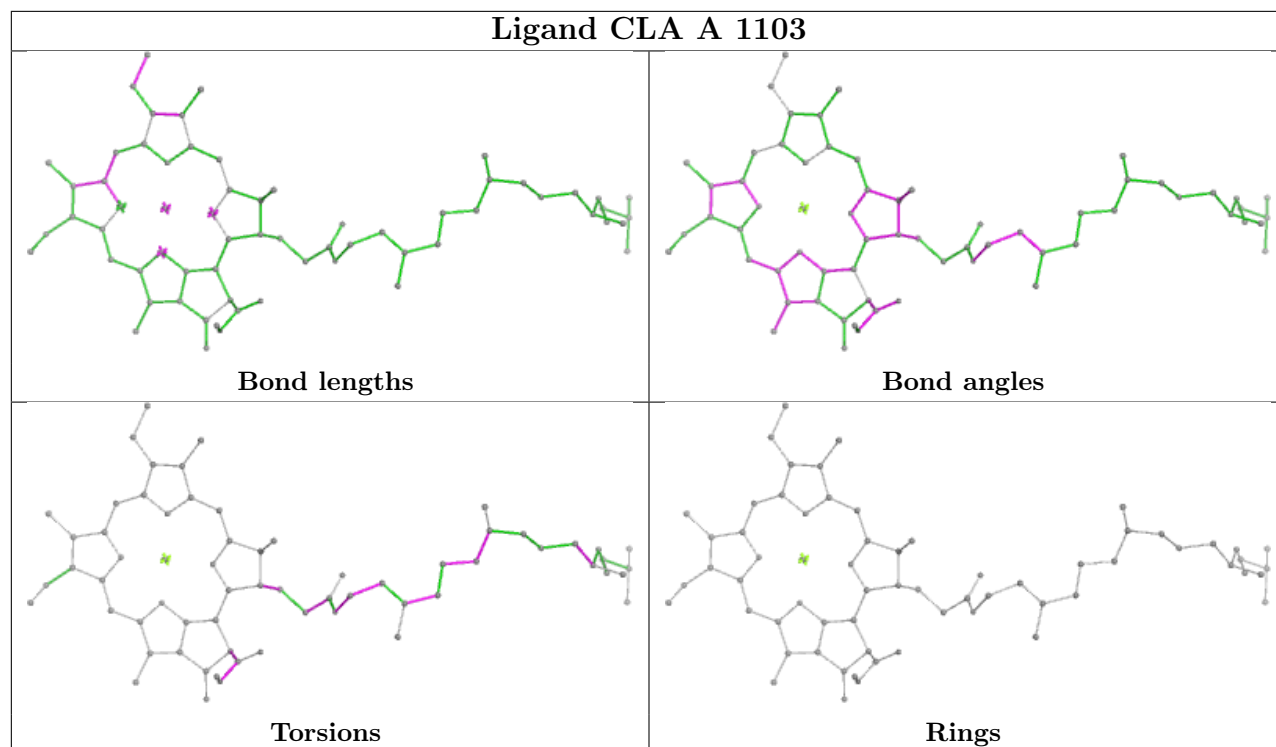
Rings



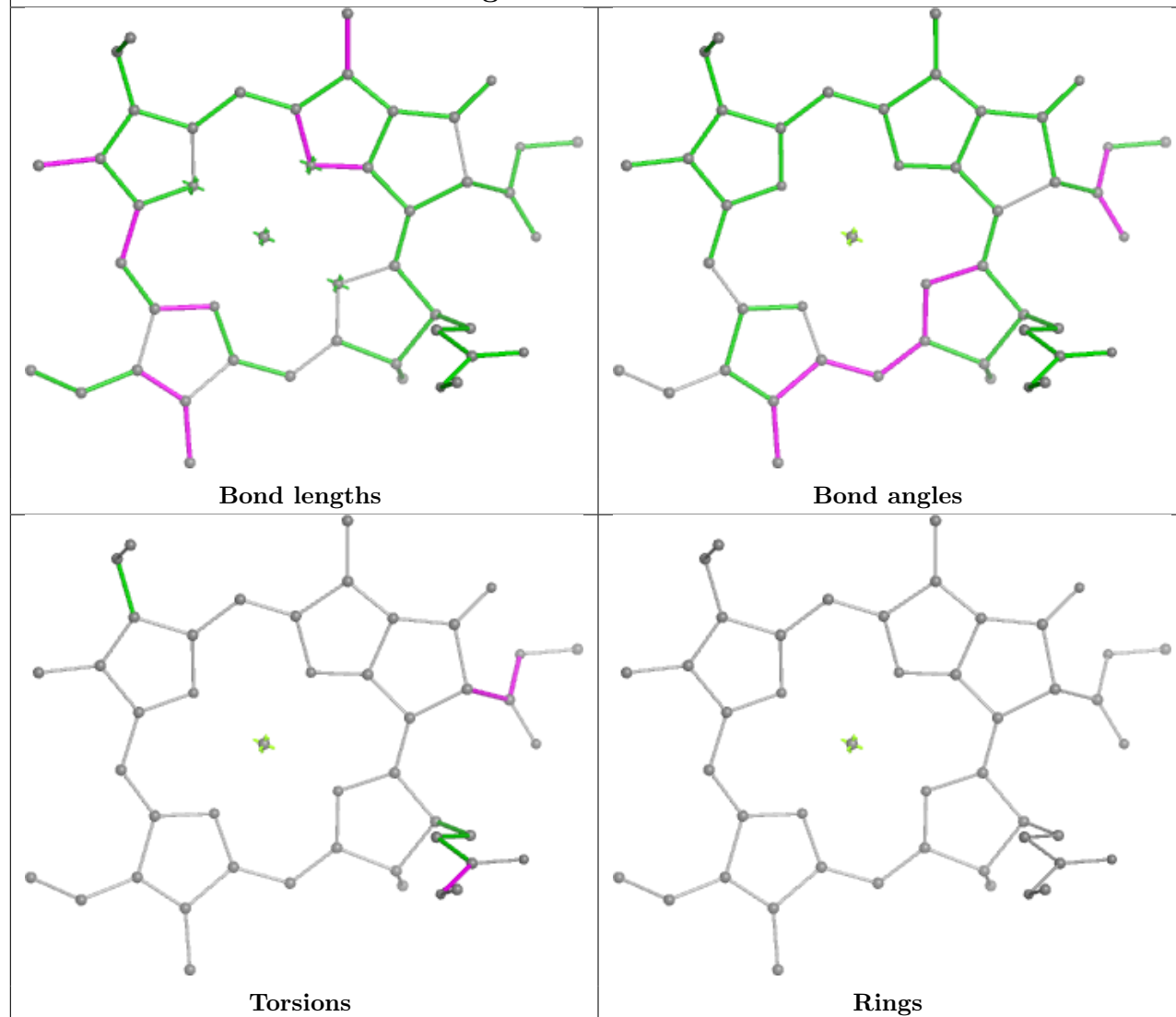


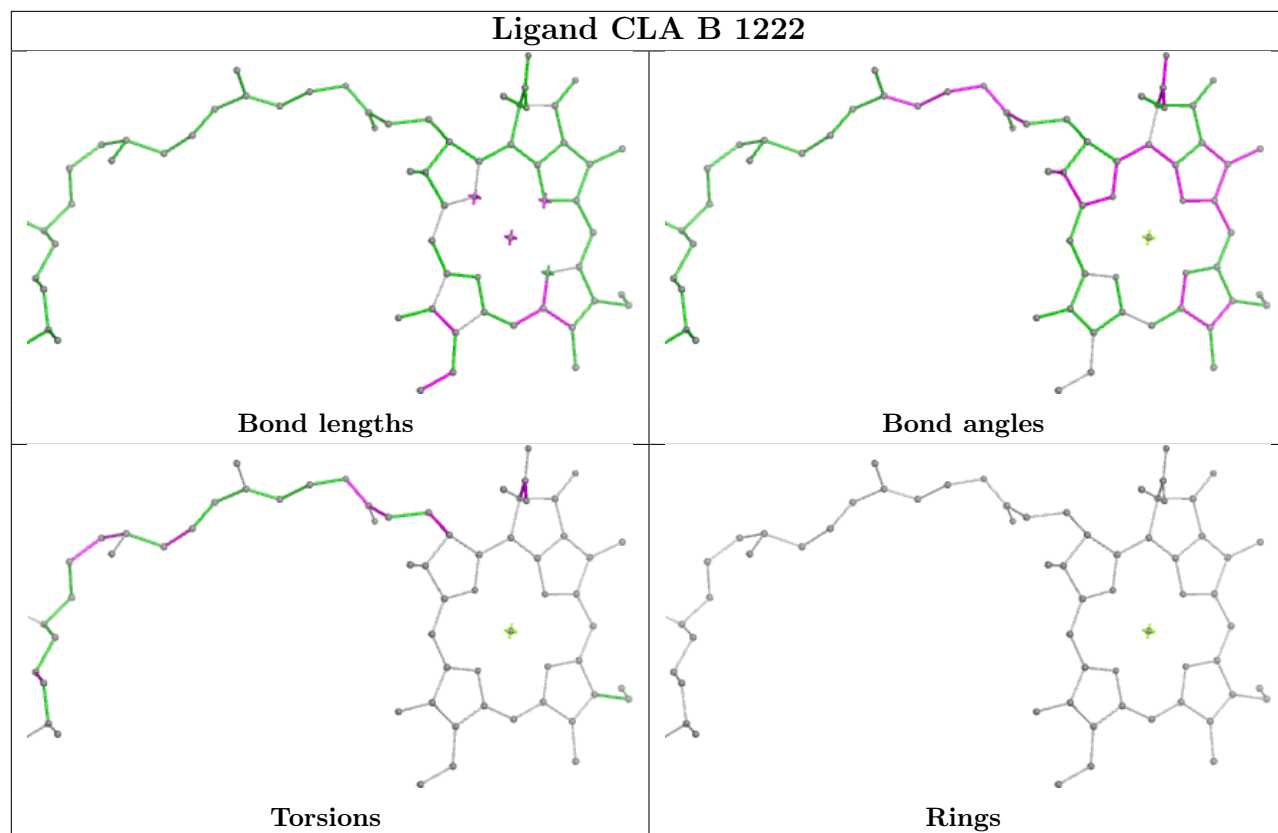




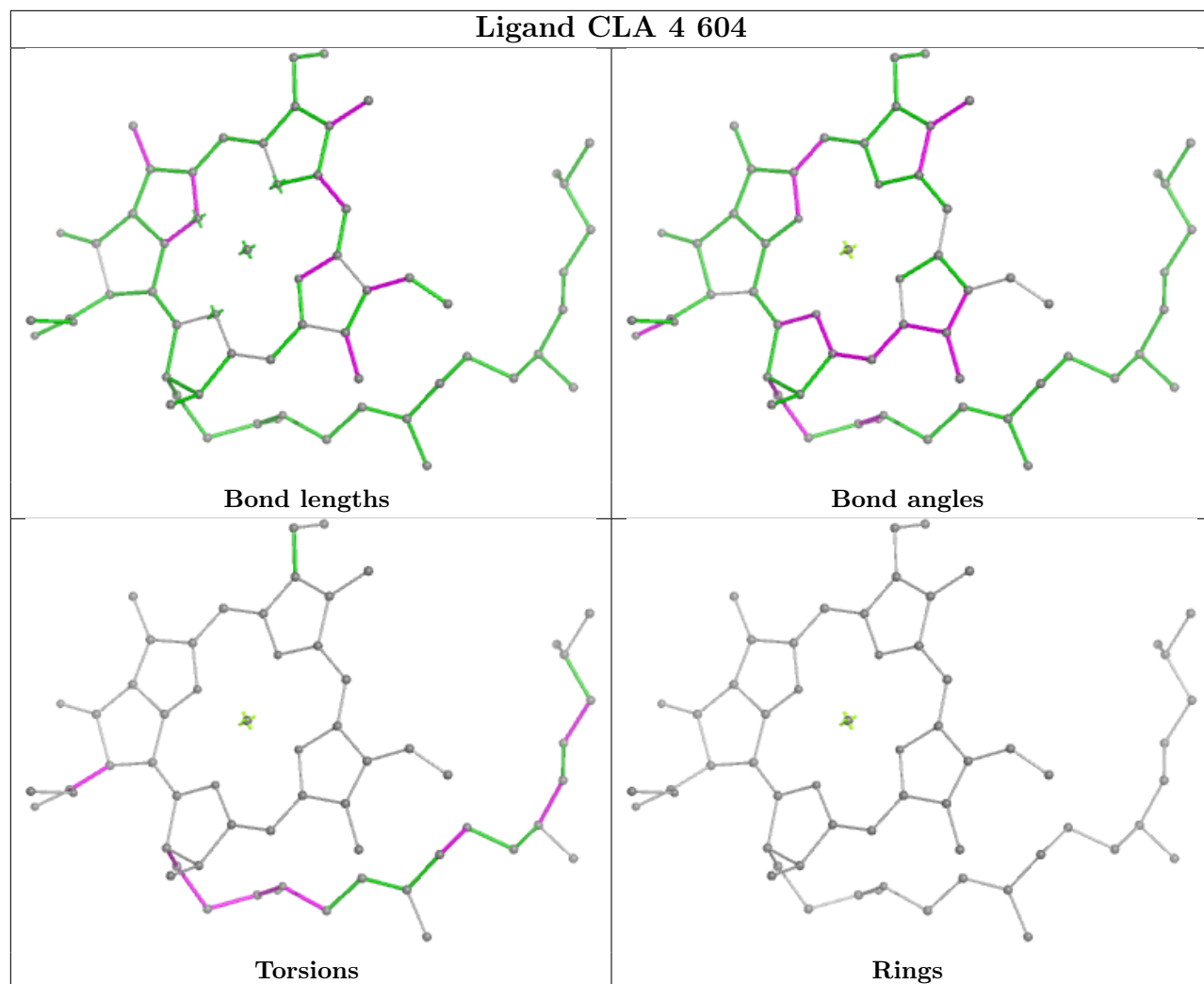


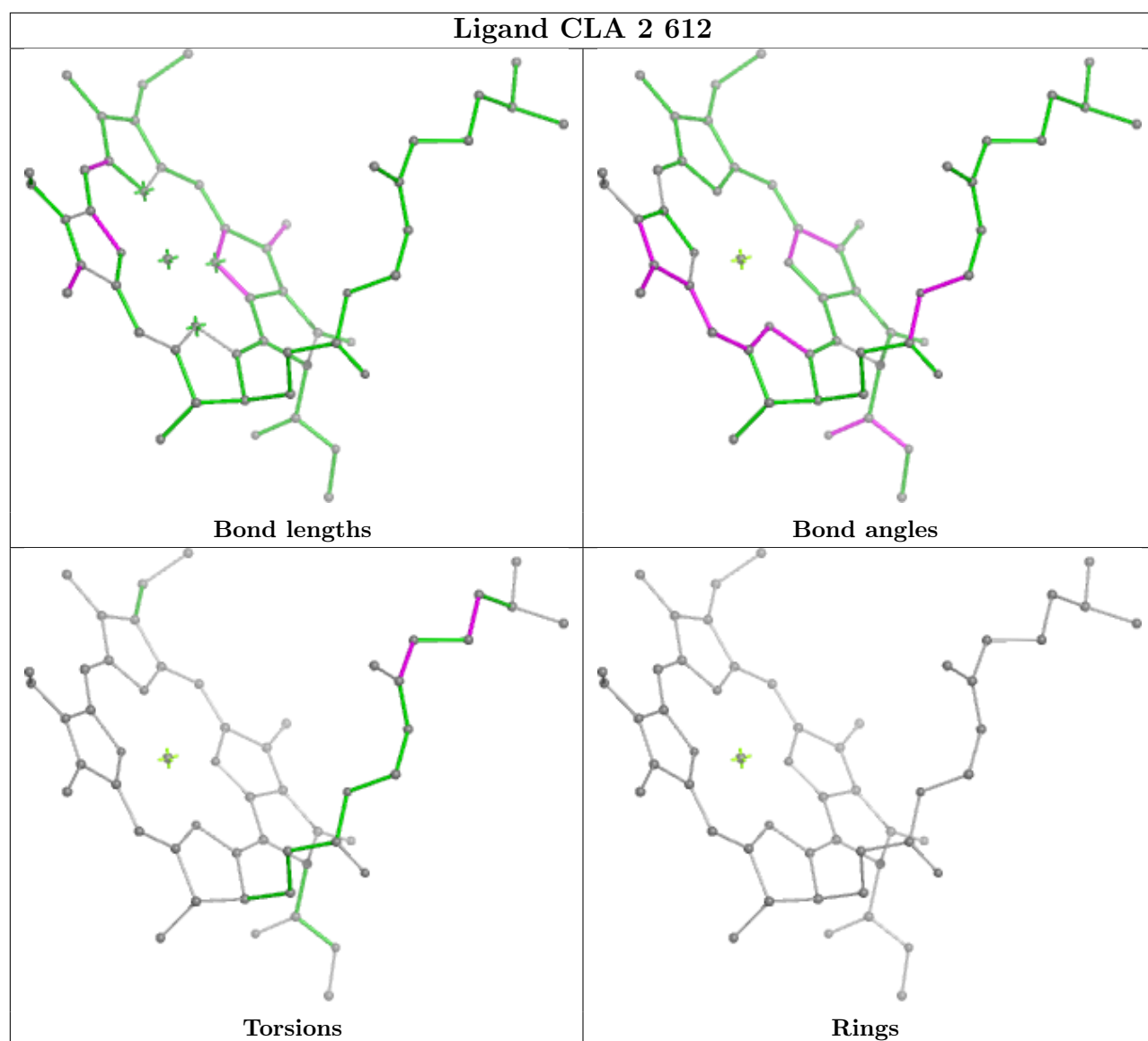
Ligand CLA B 1232

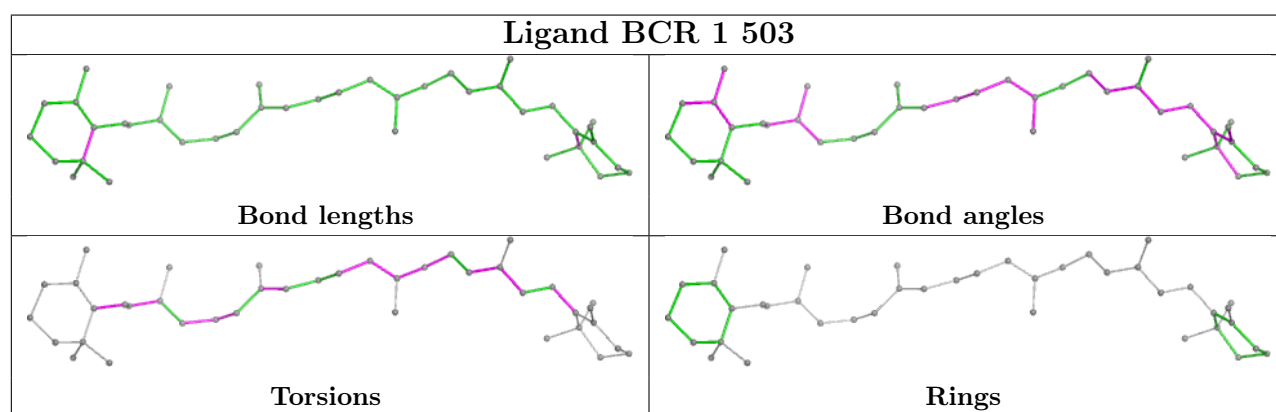
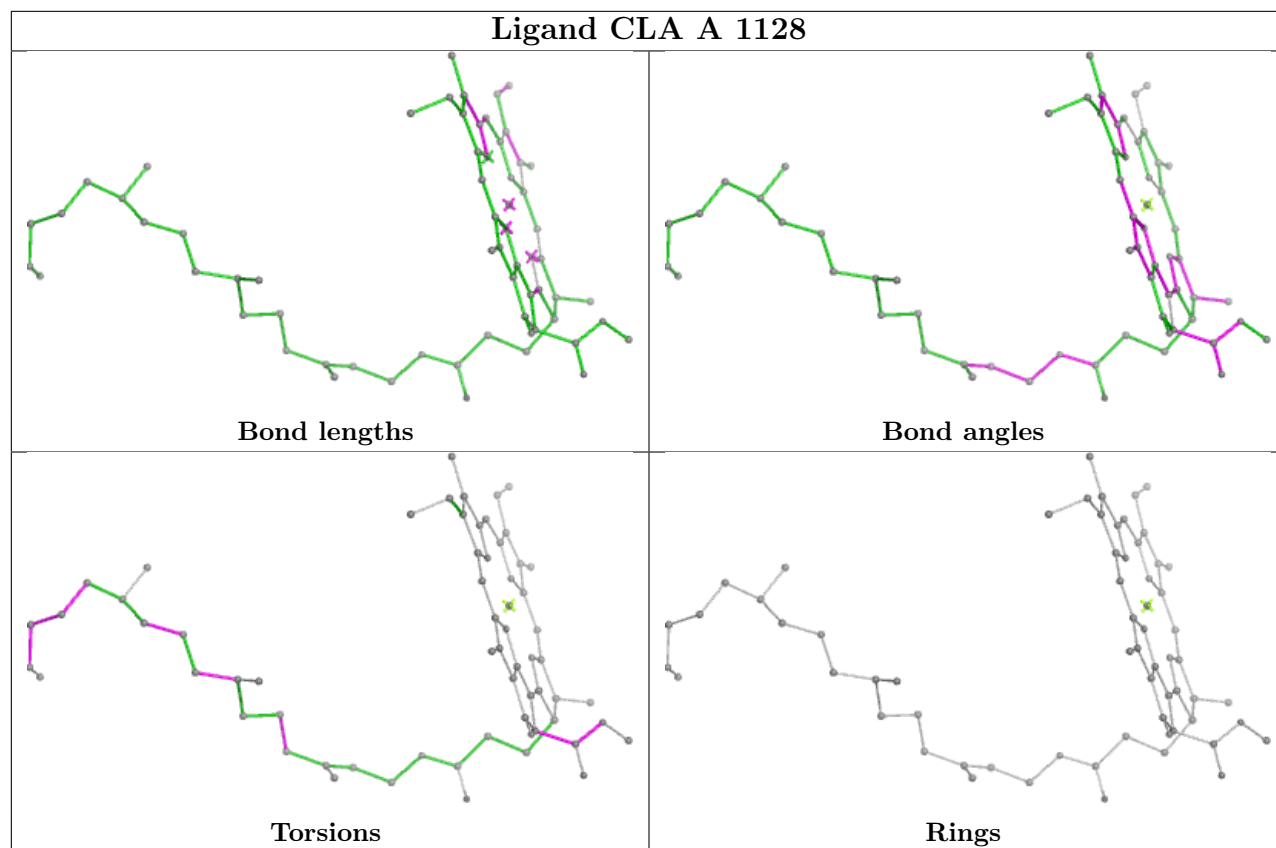




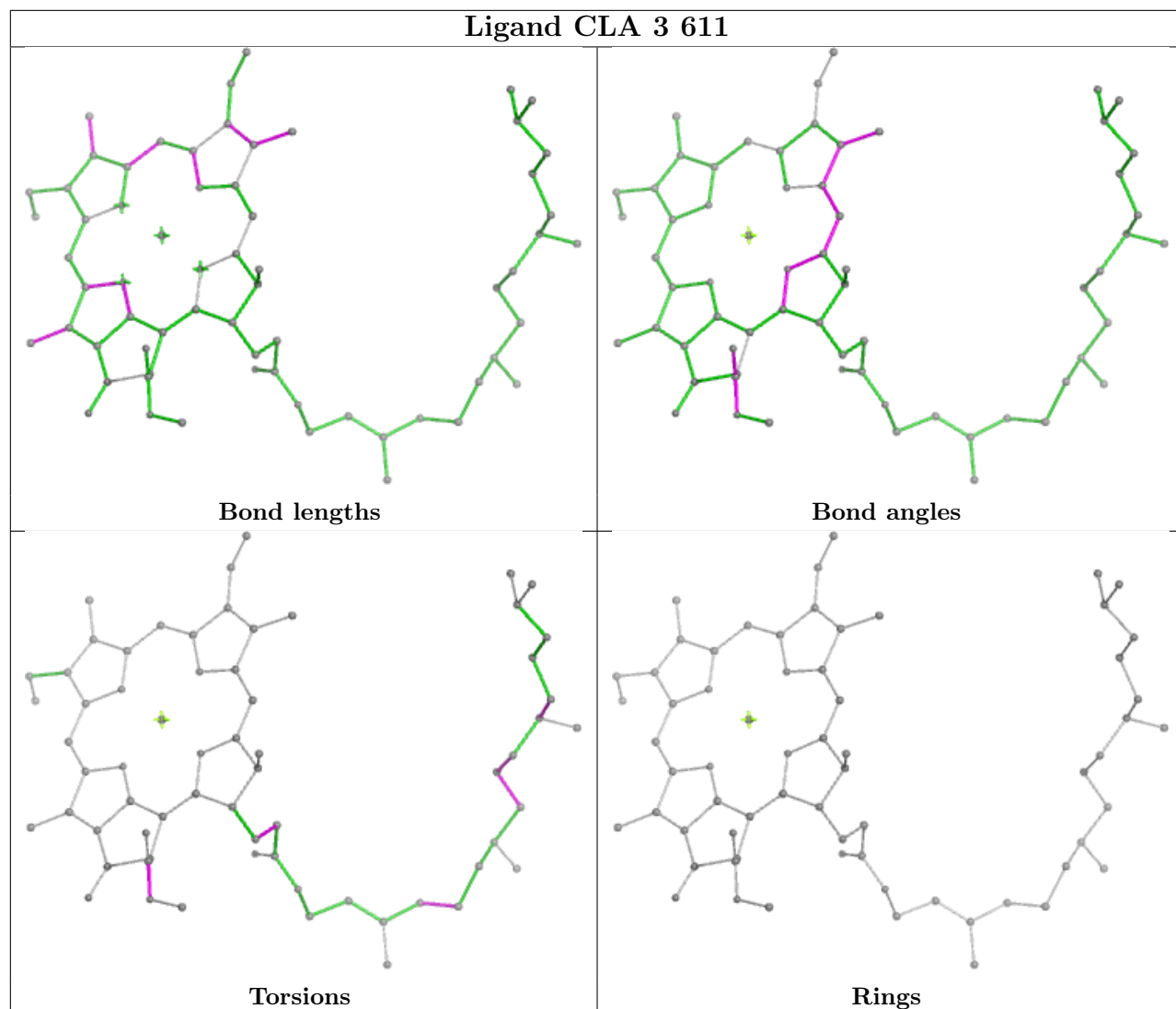
Ligand CLA 4 604



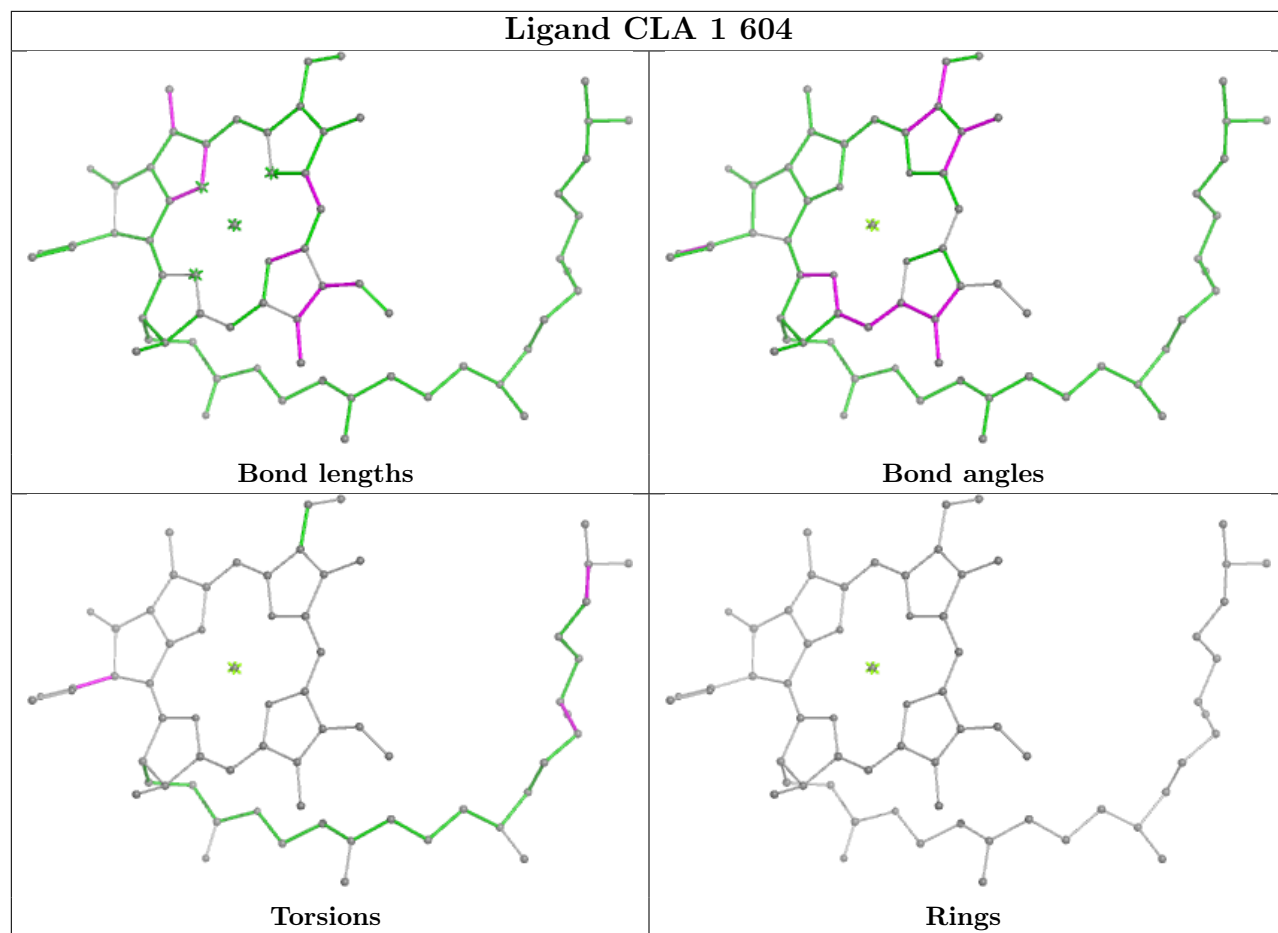


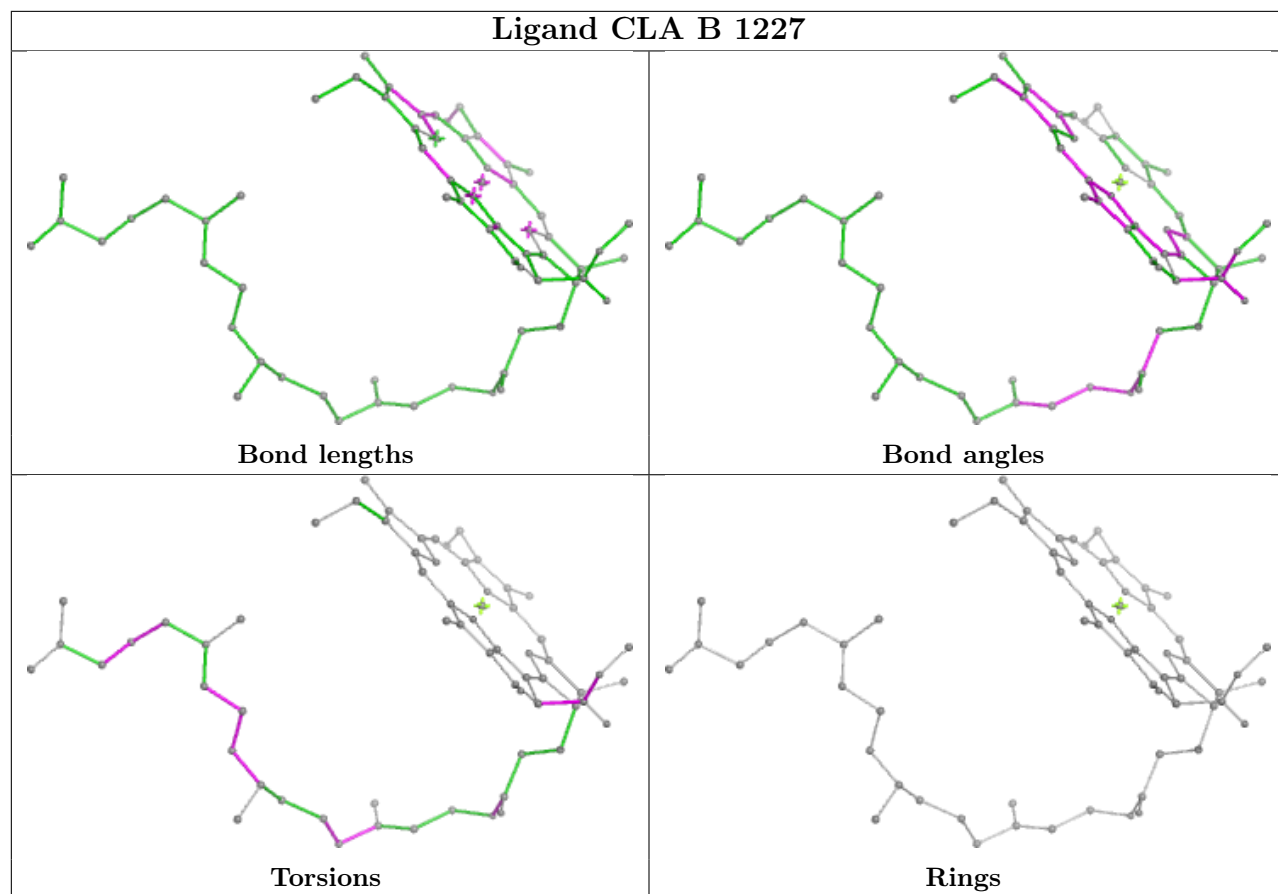


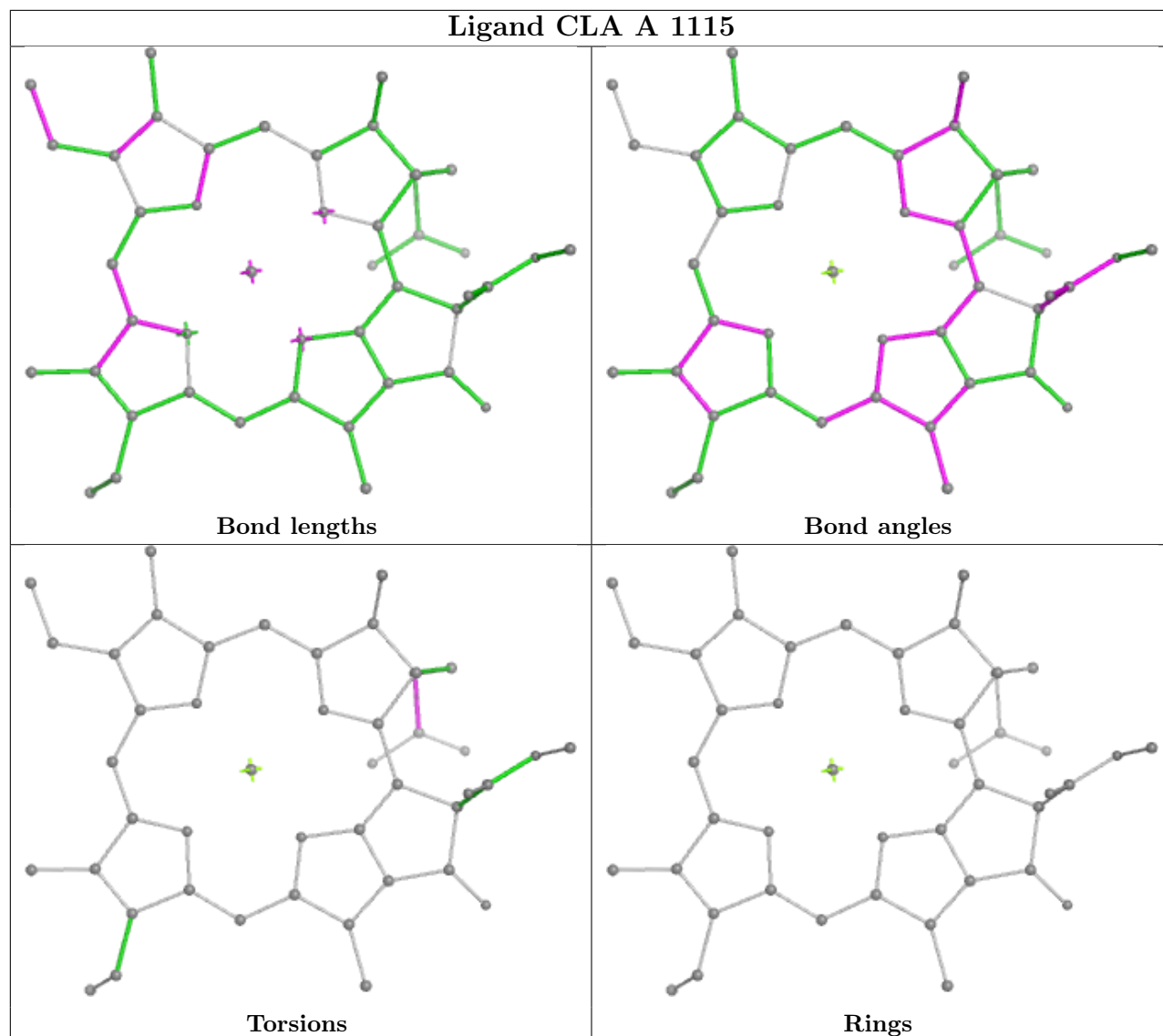
Ligand CLA 3 611



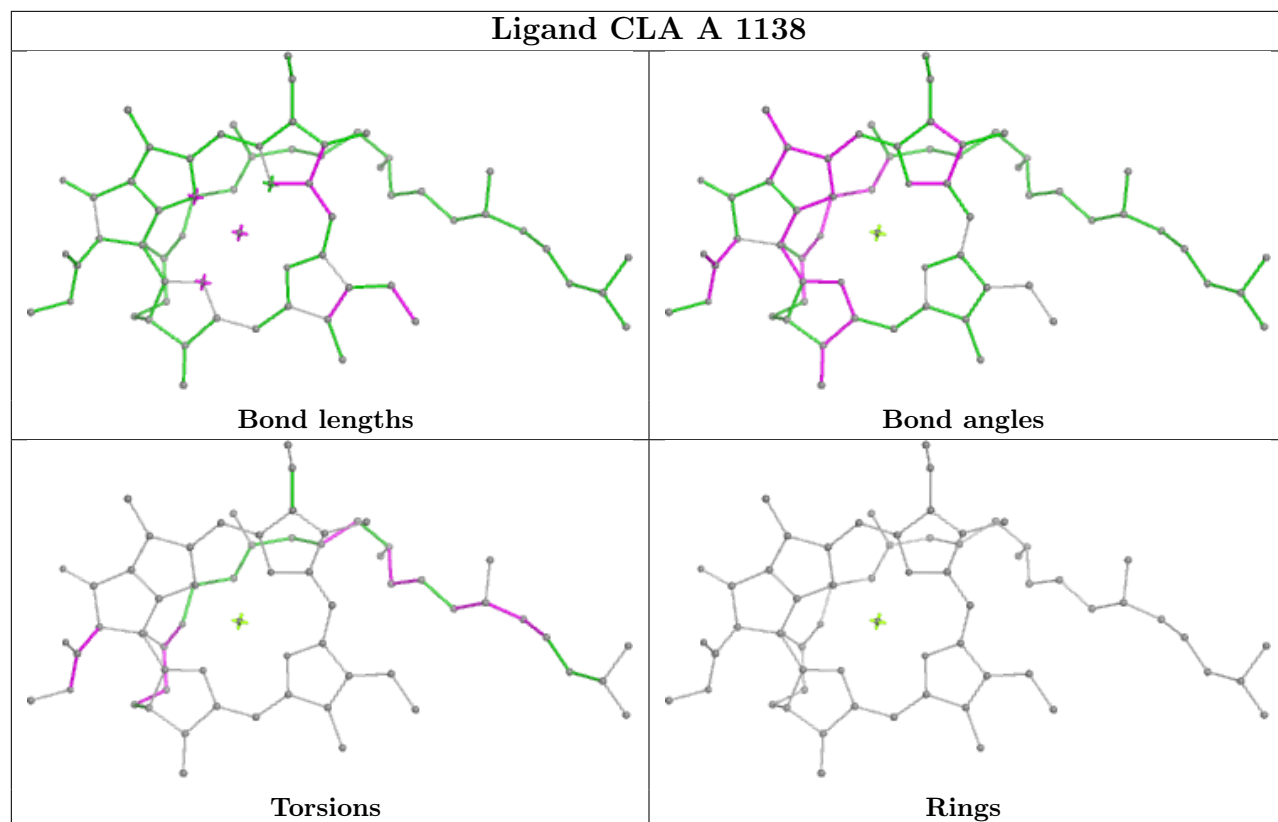
Ligand CLA 1 604



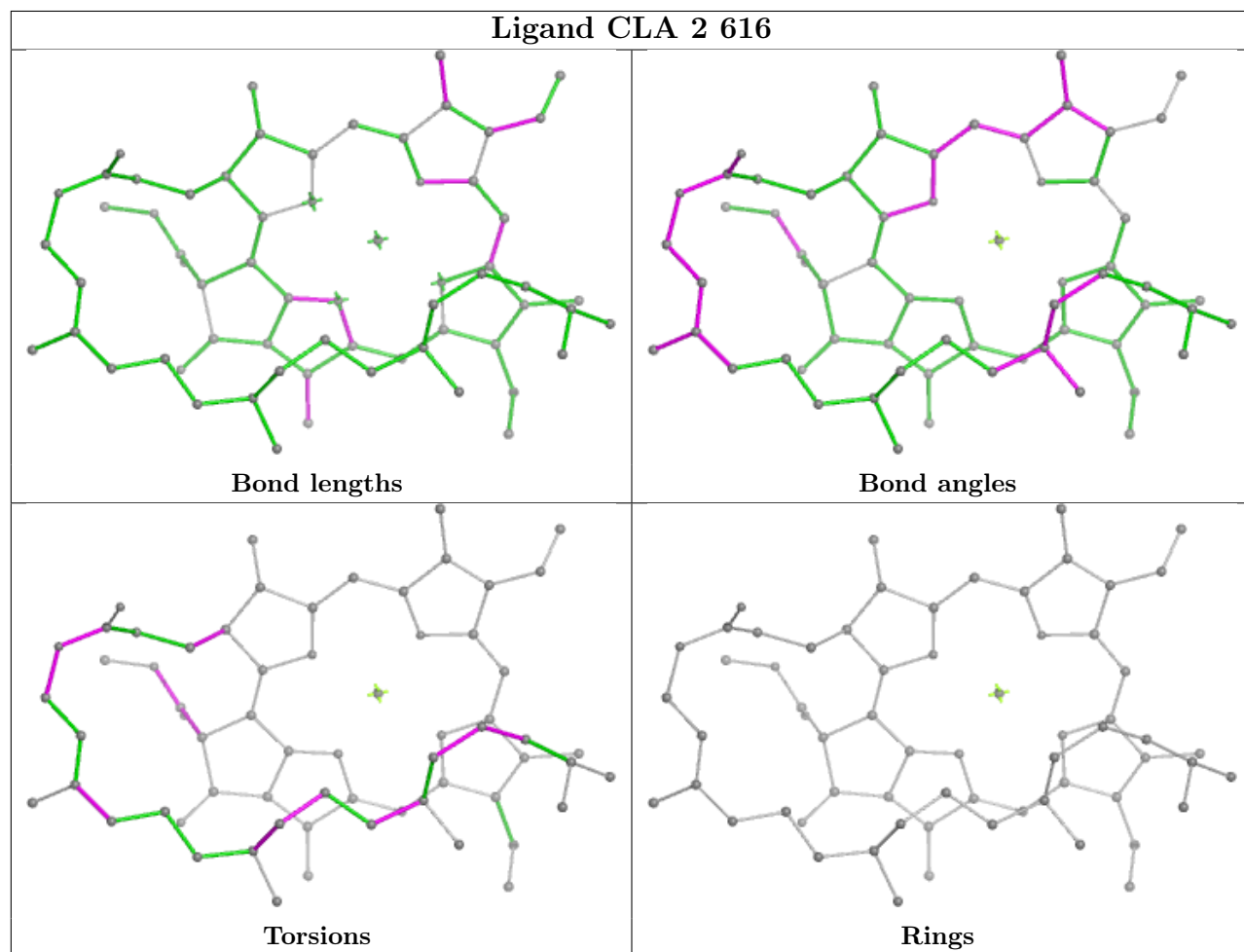


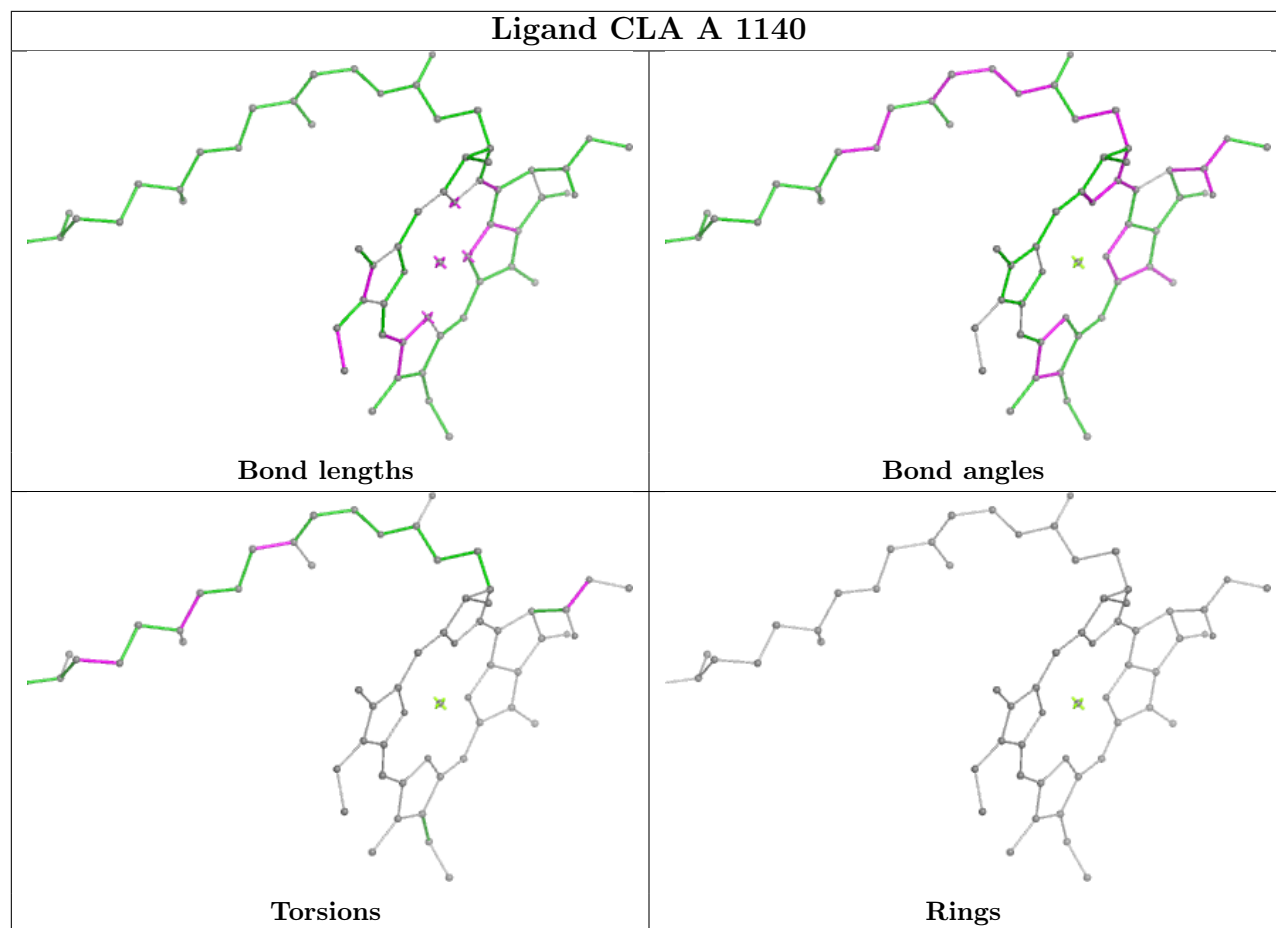


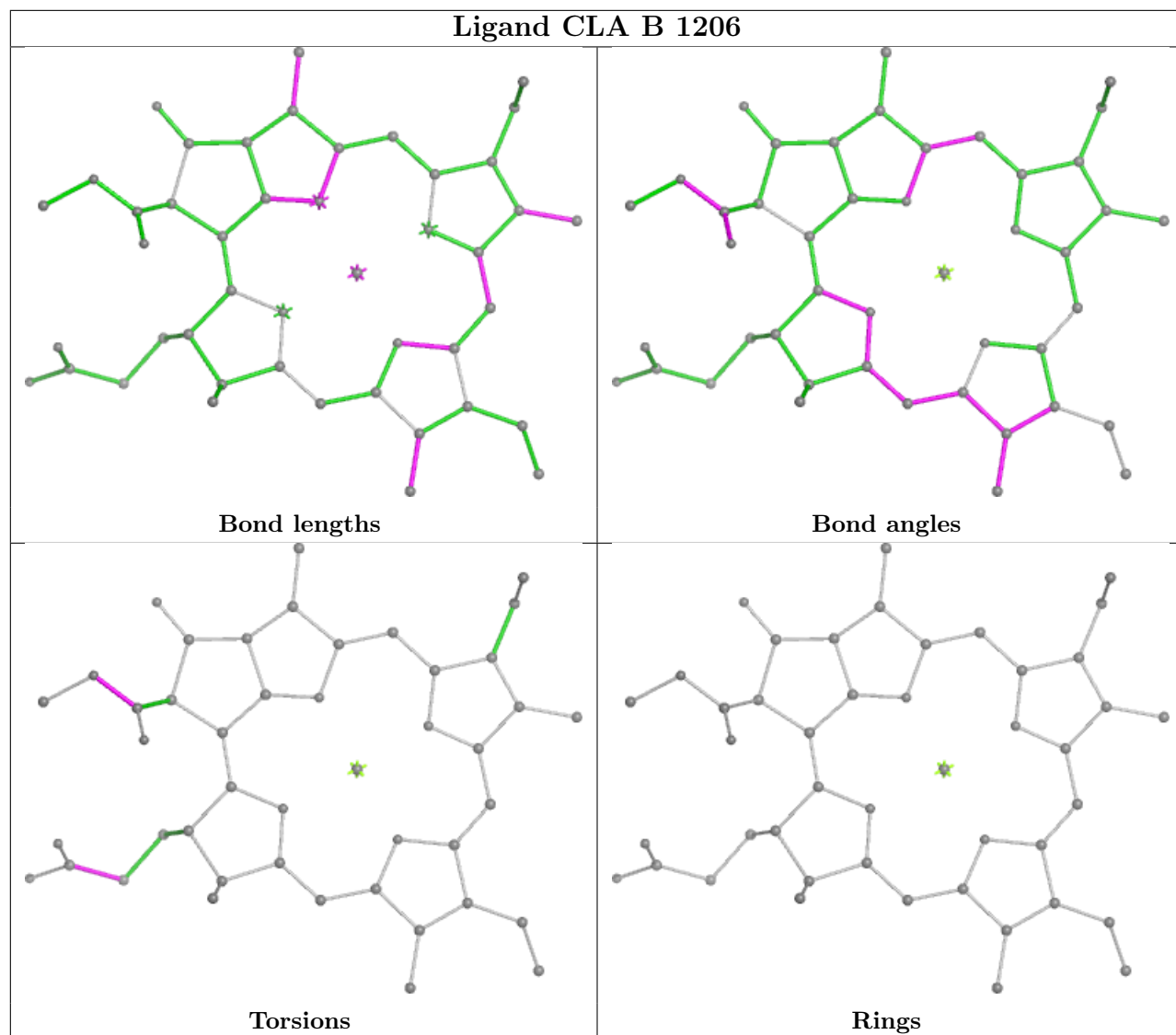
Ligand CLA A 1138

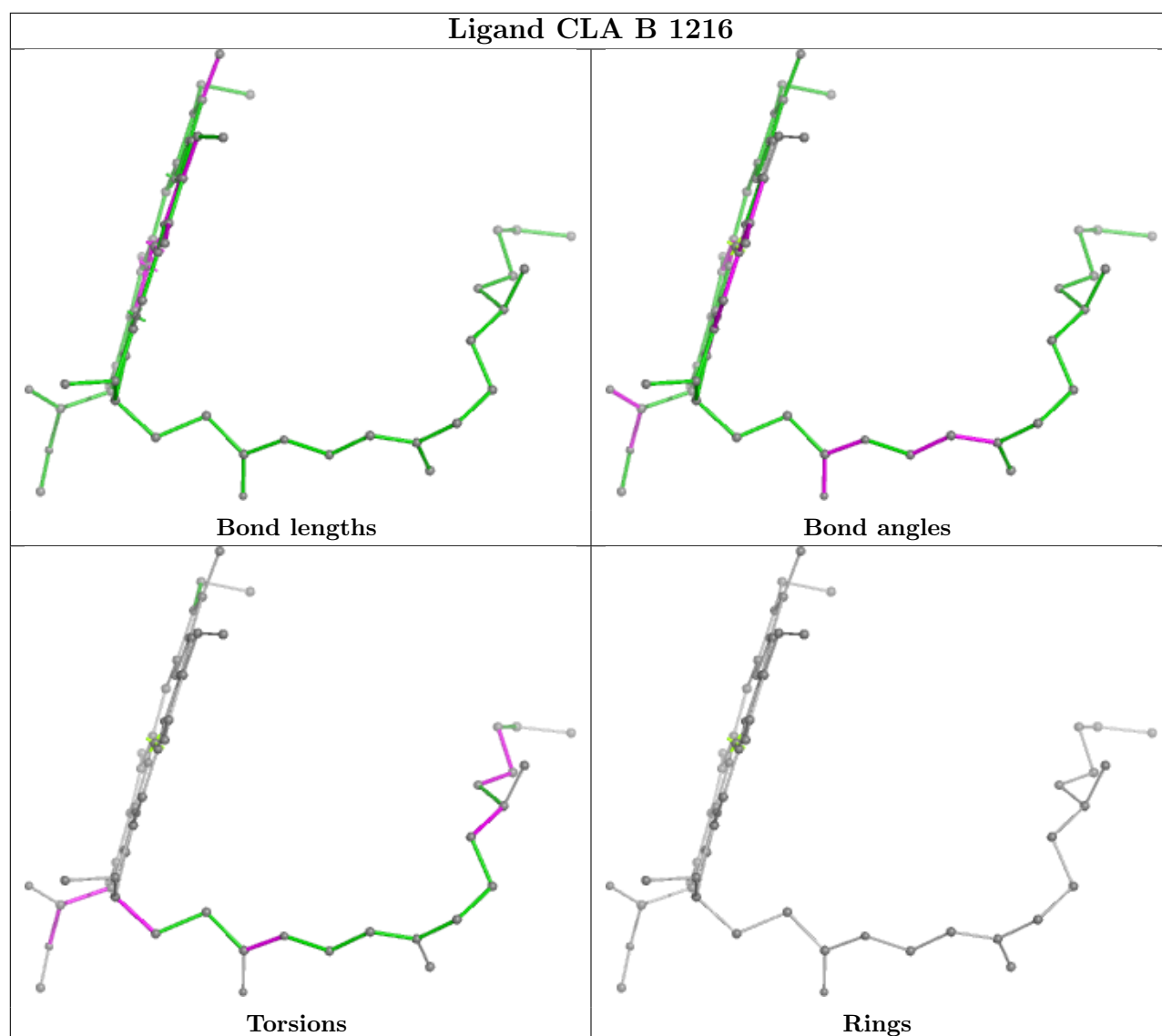


Ligand CLA 2 616

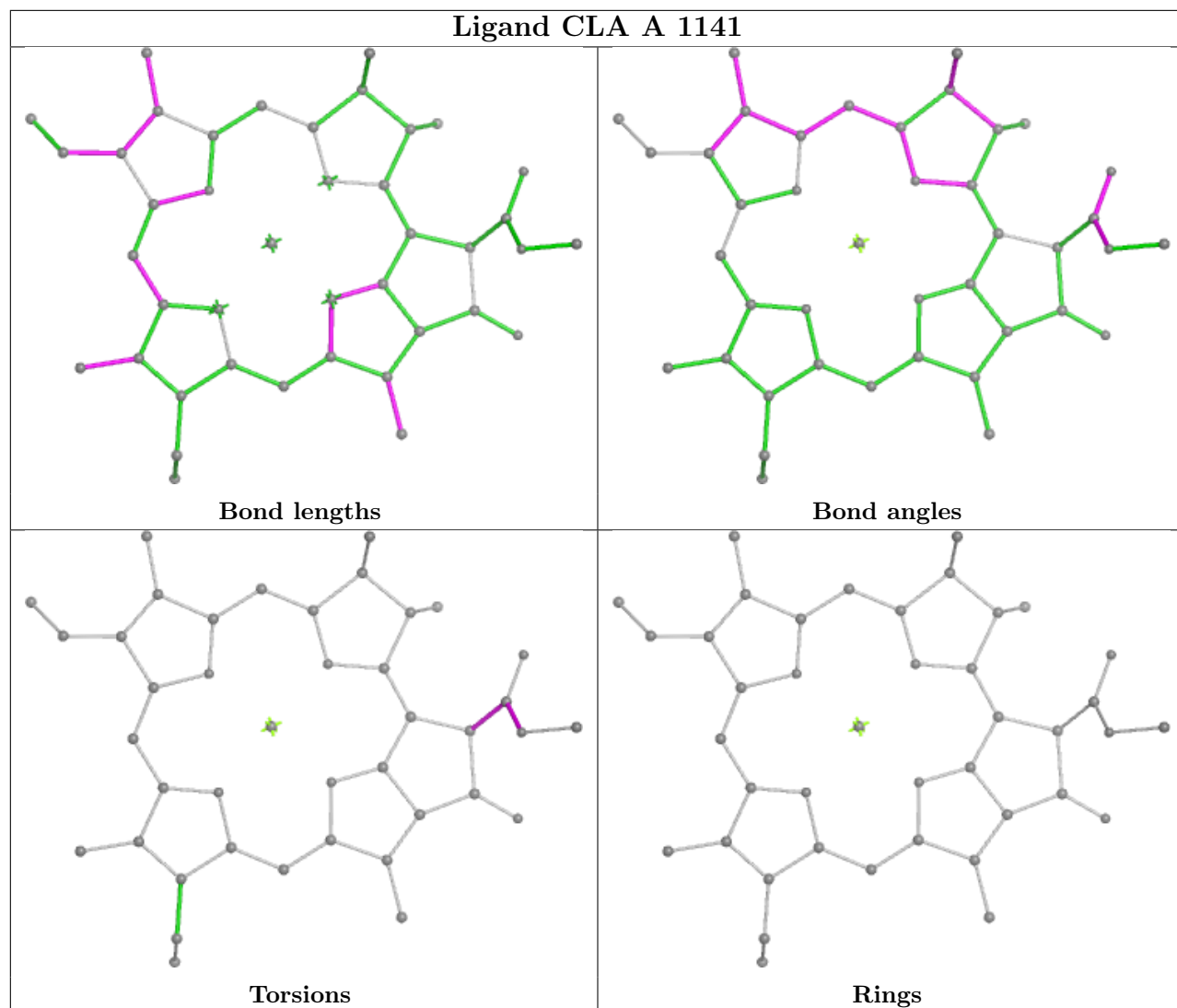




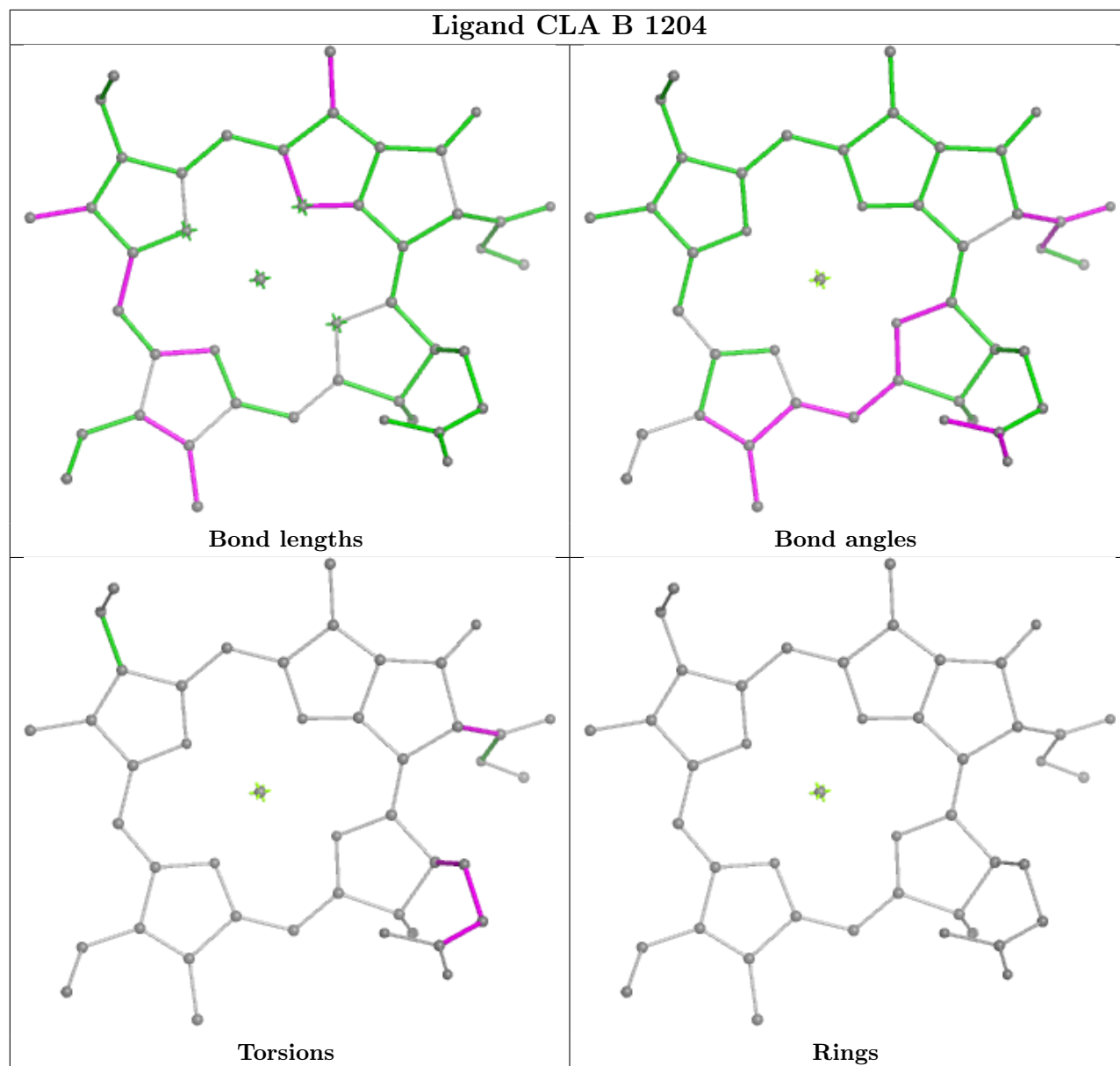




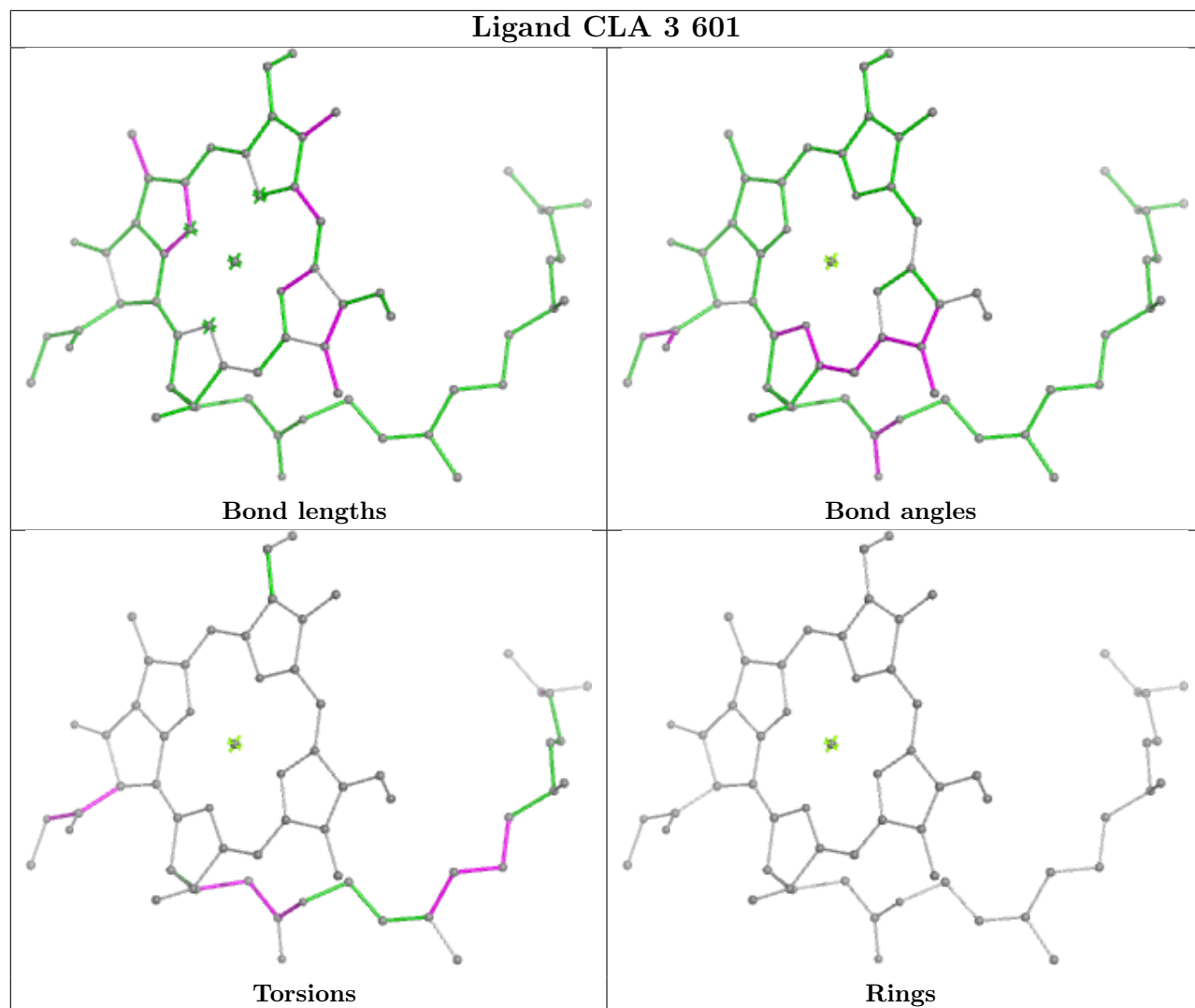
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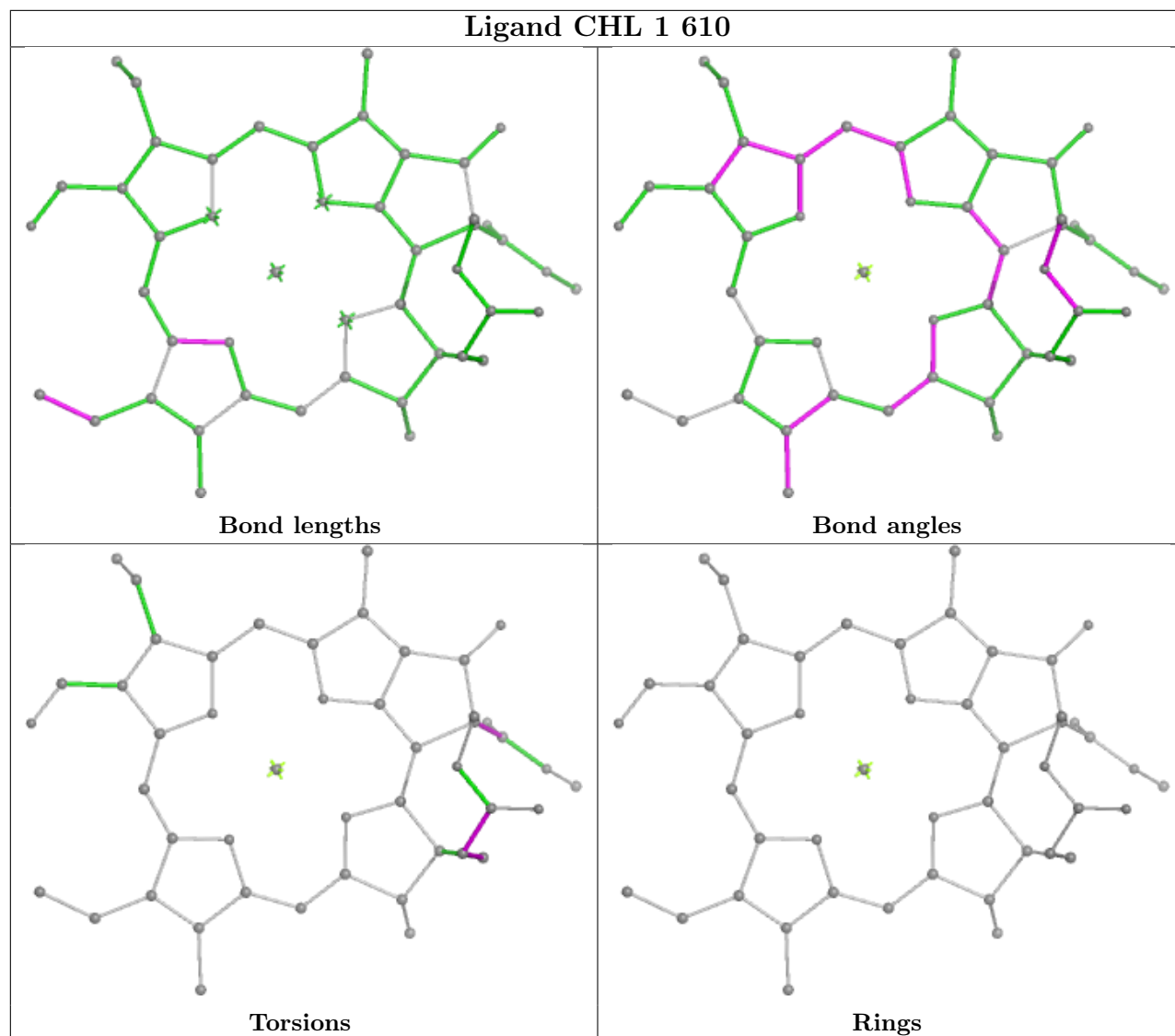
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Ligand CLA 3 601



Ligand CHL 1 610

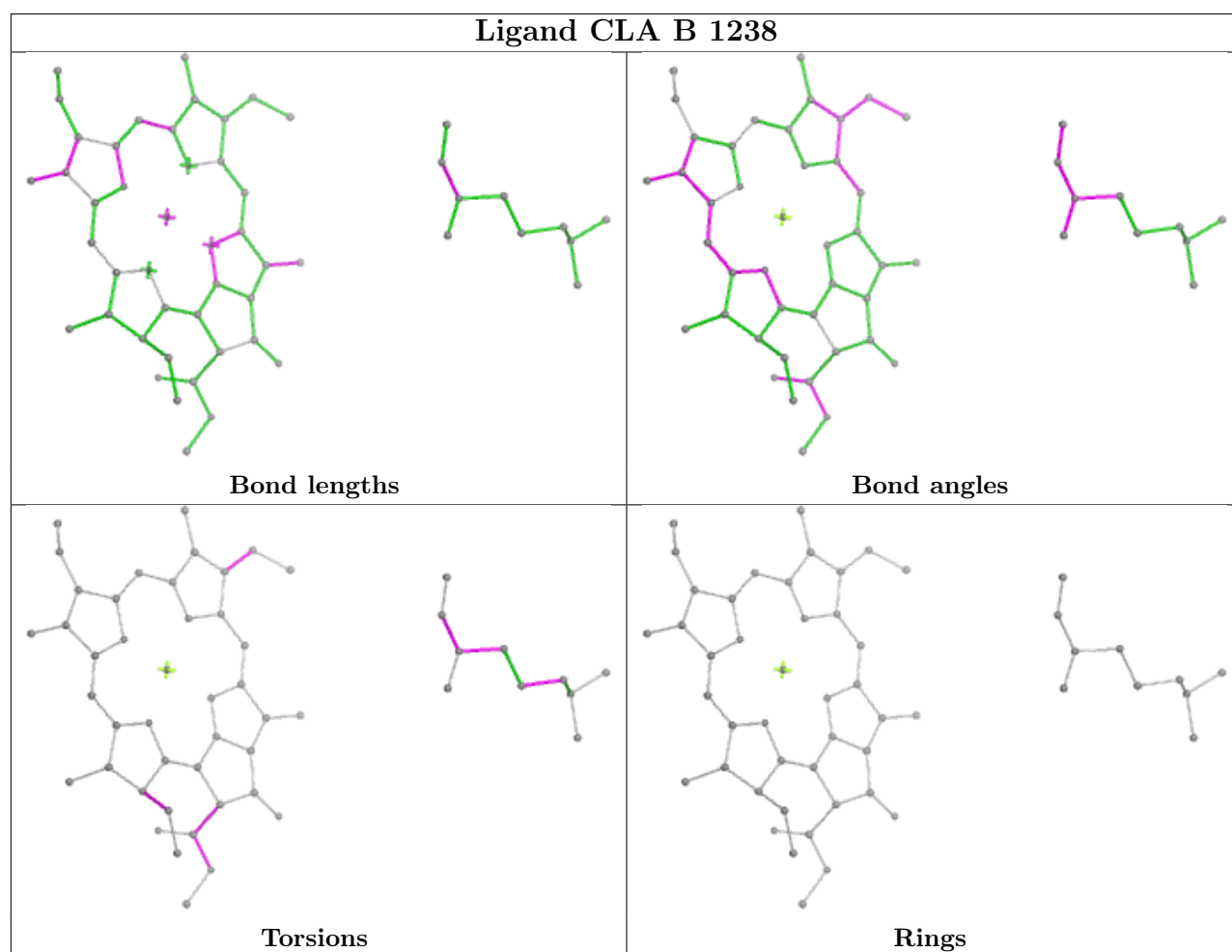


Bond lengths

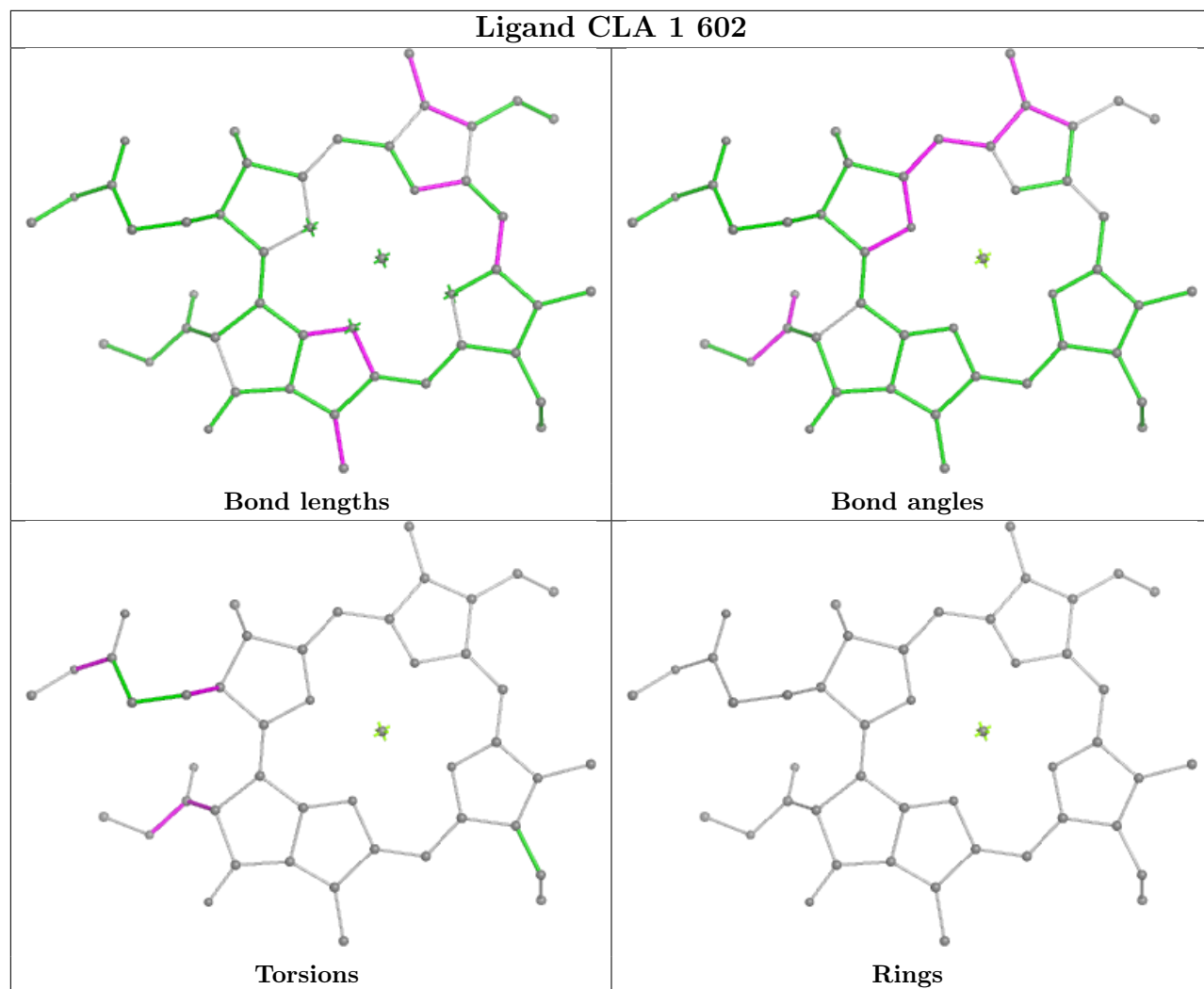
Bond angles

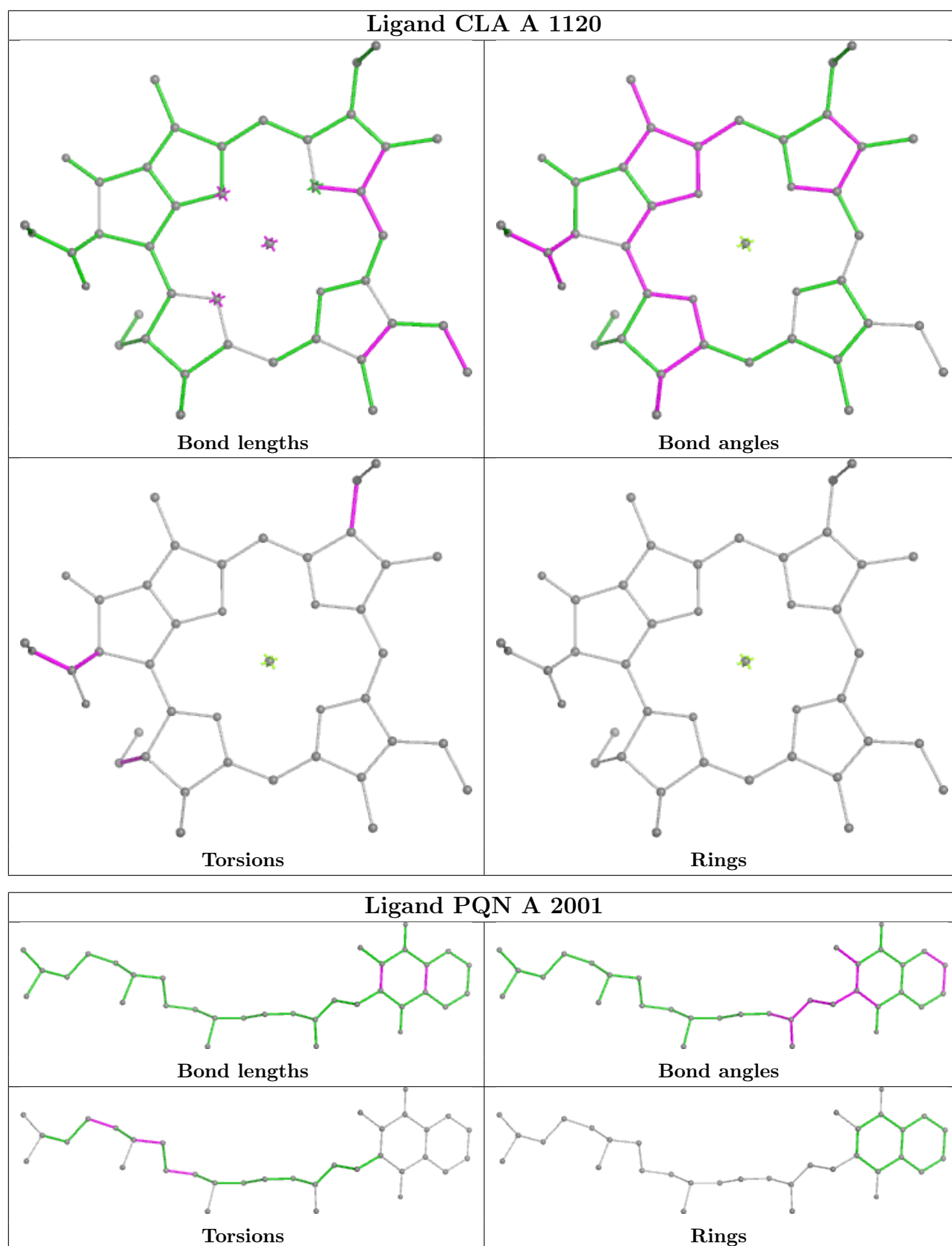
Torsions

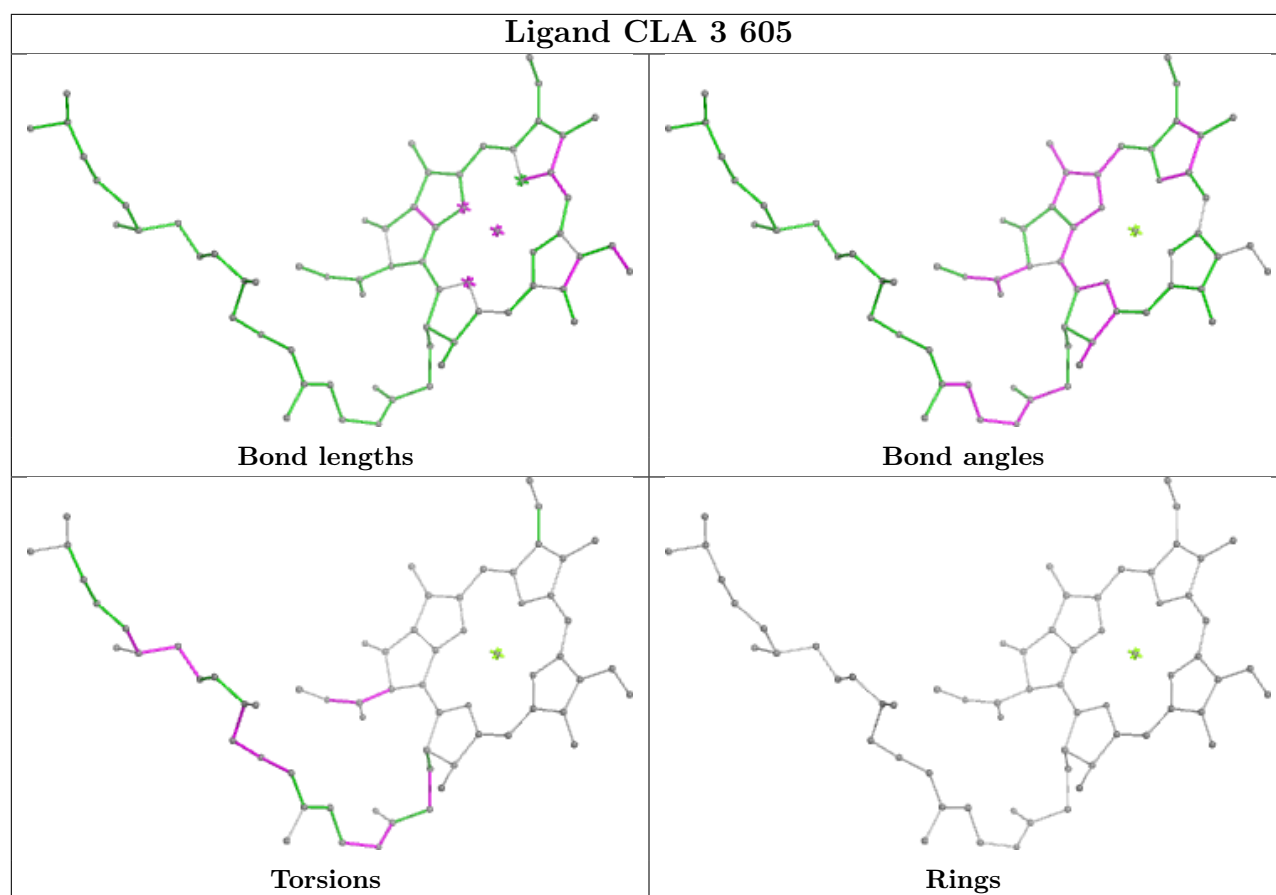
Rings

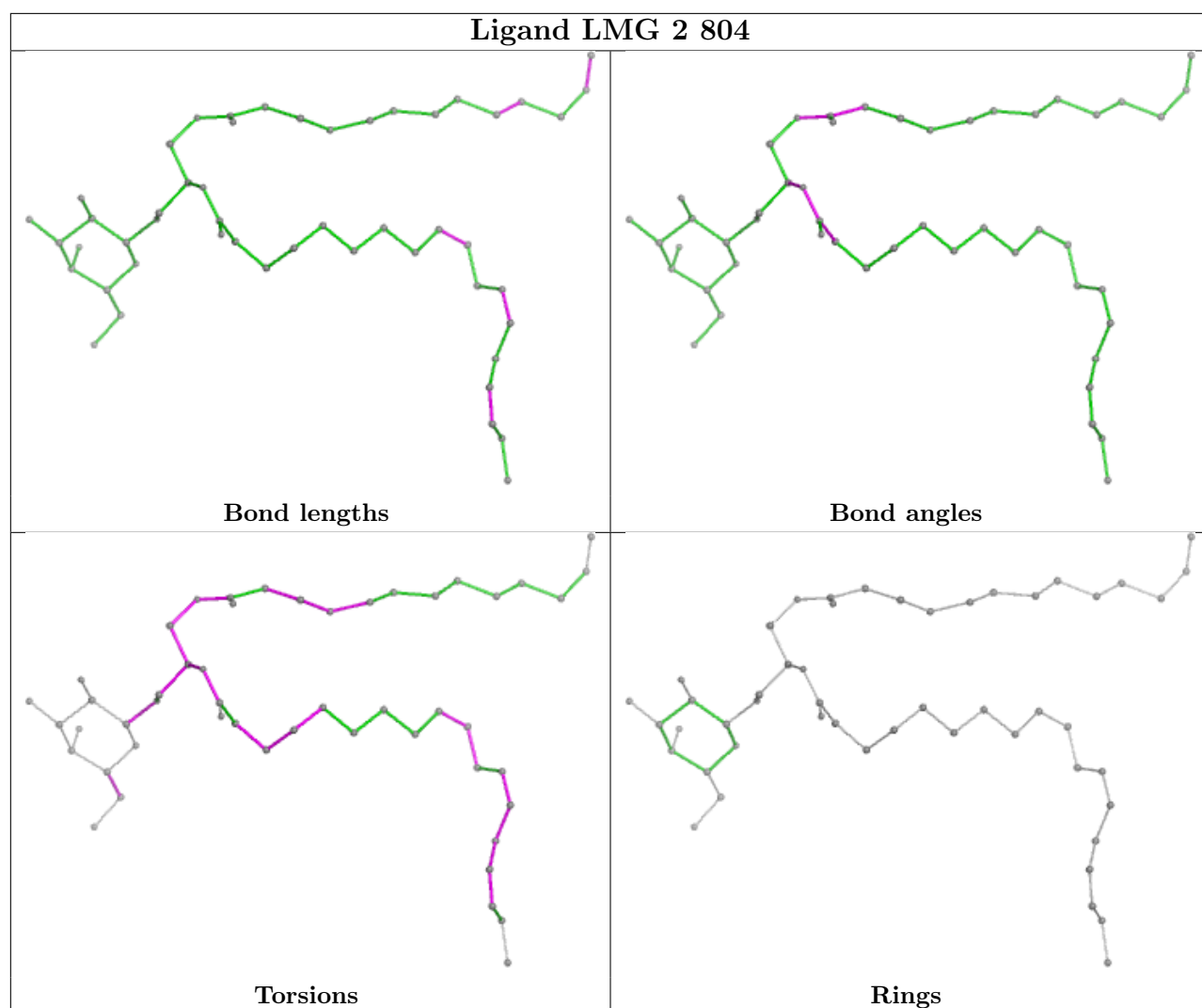


Ligand CLA 1 602

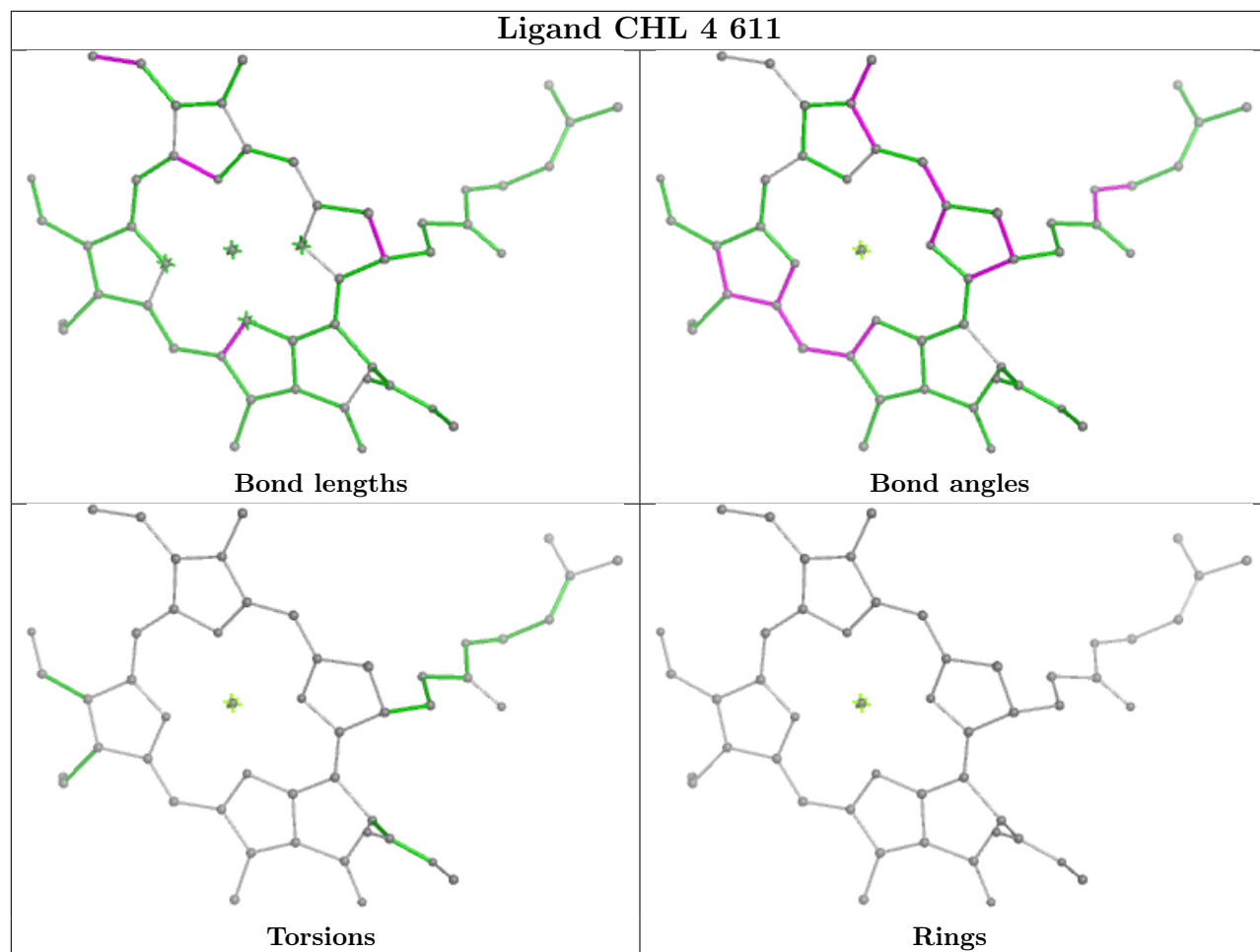


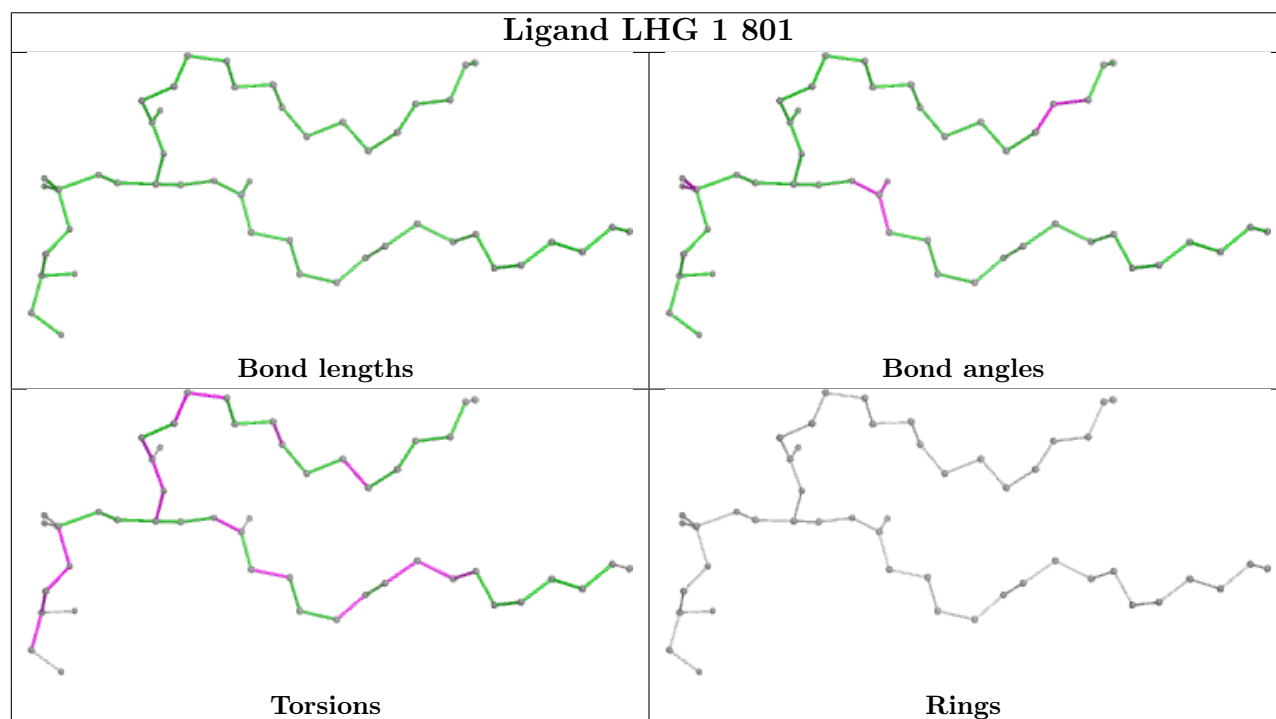
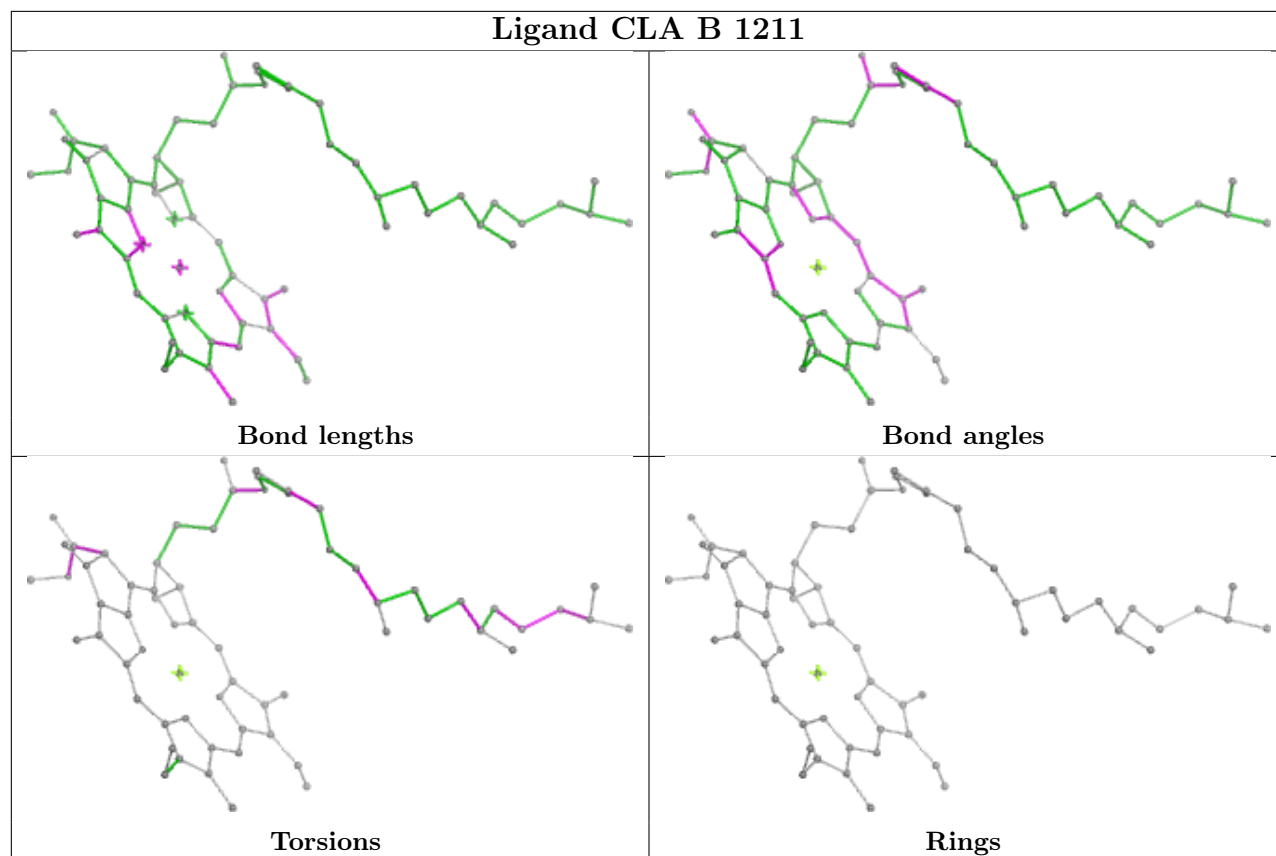




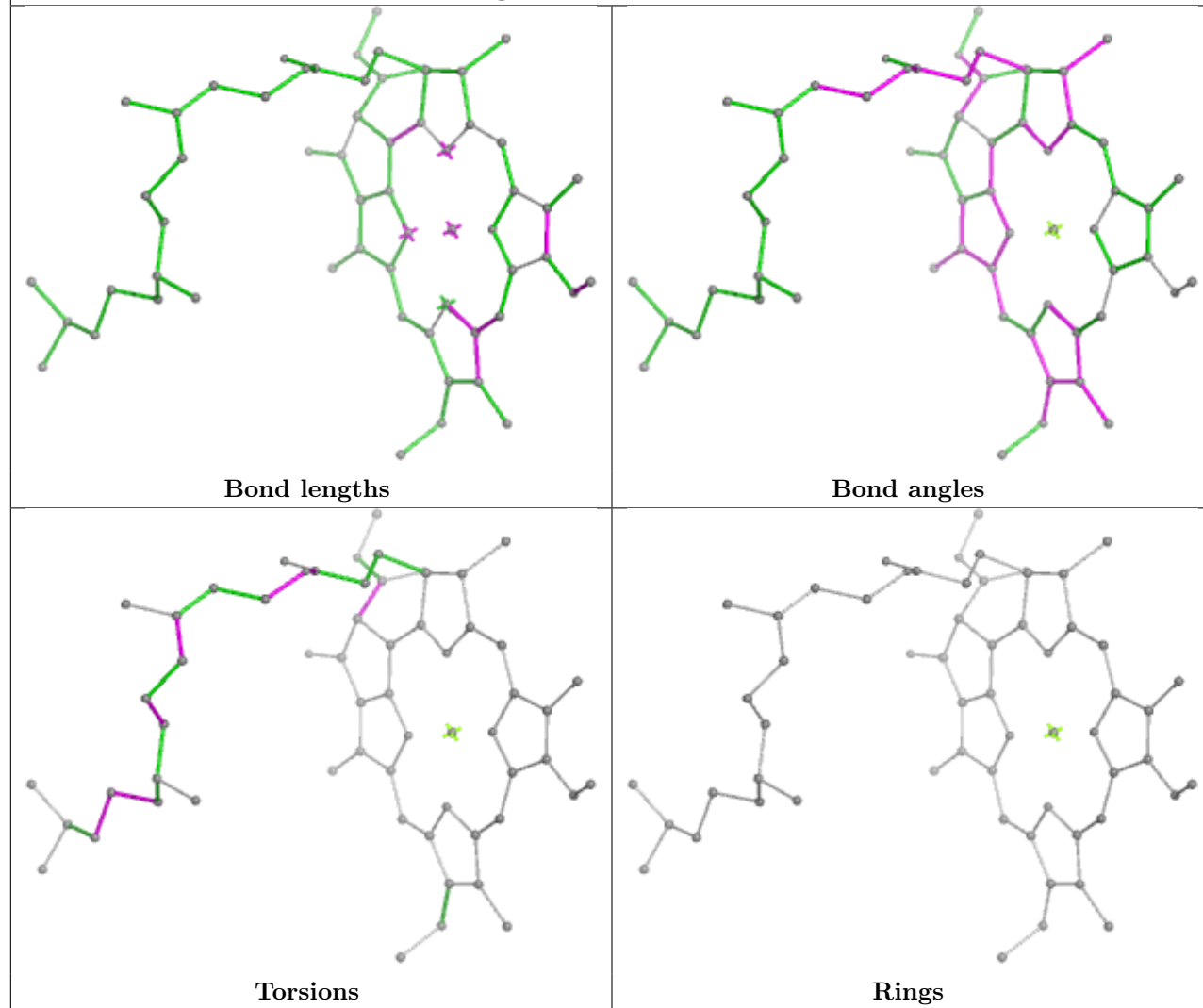


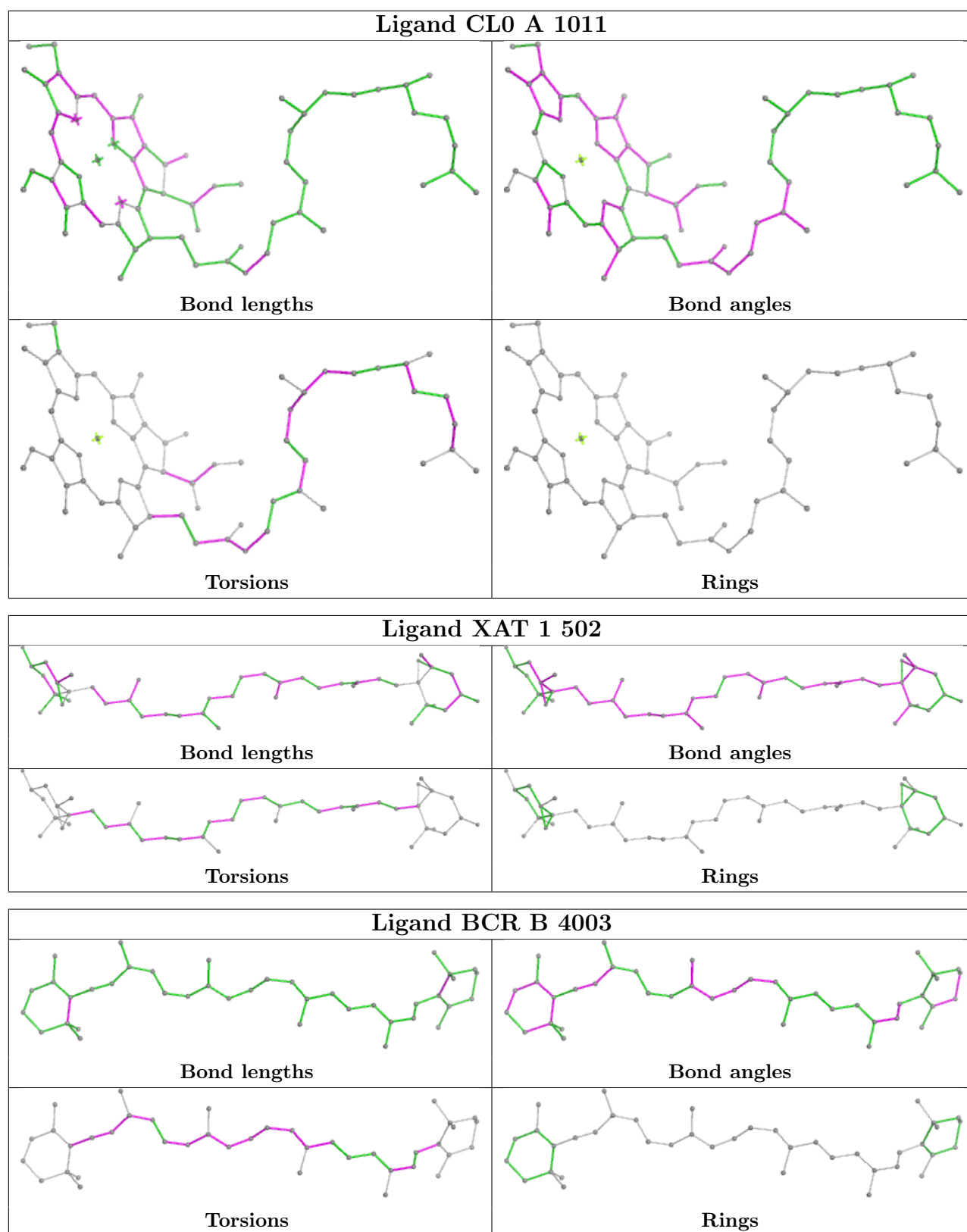
Ligand CHL 4 611

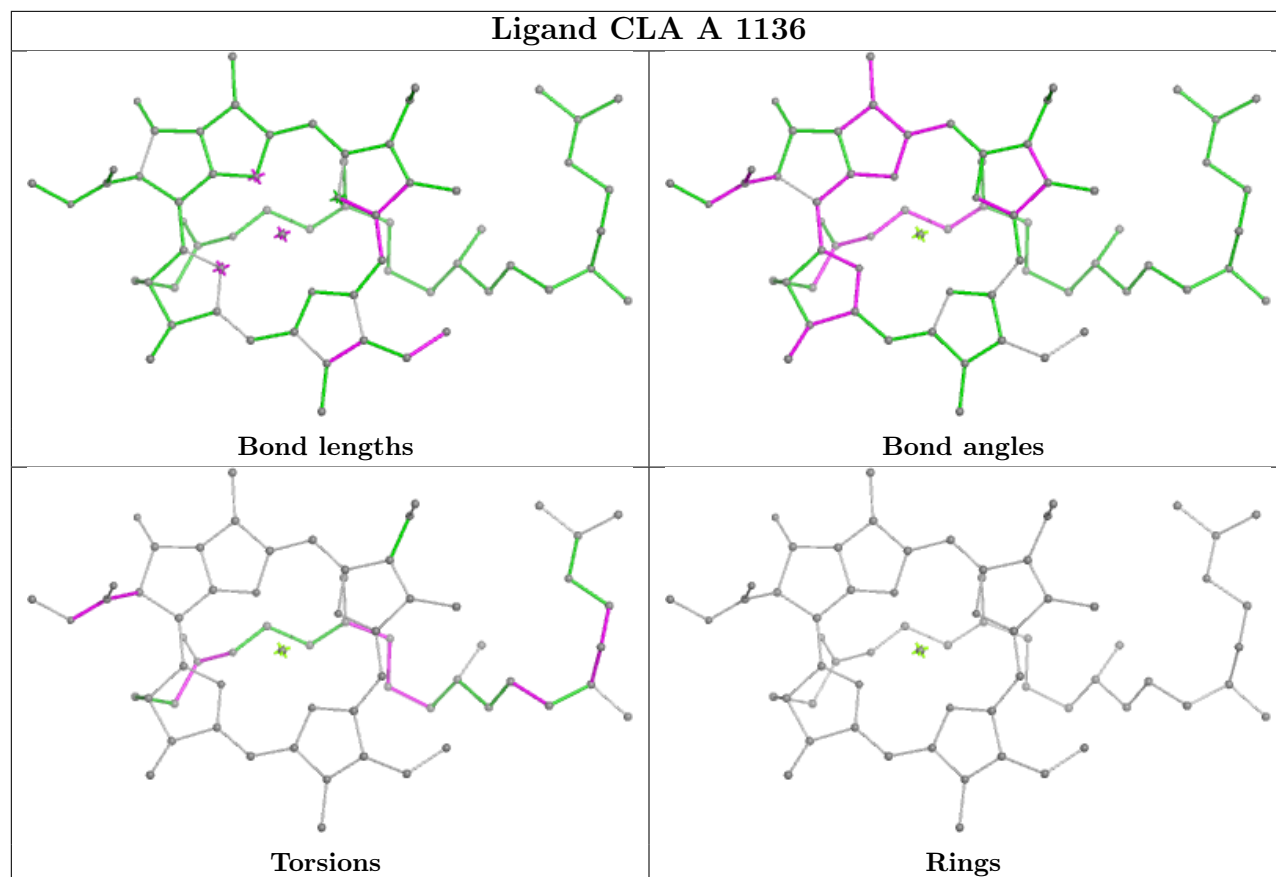


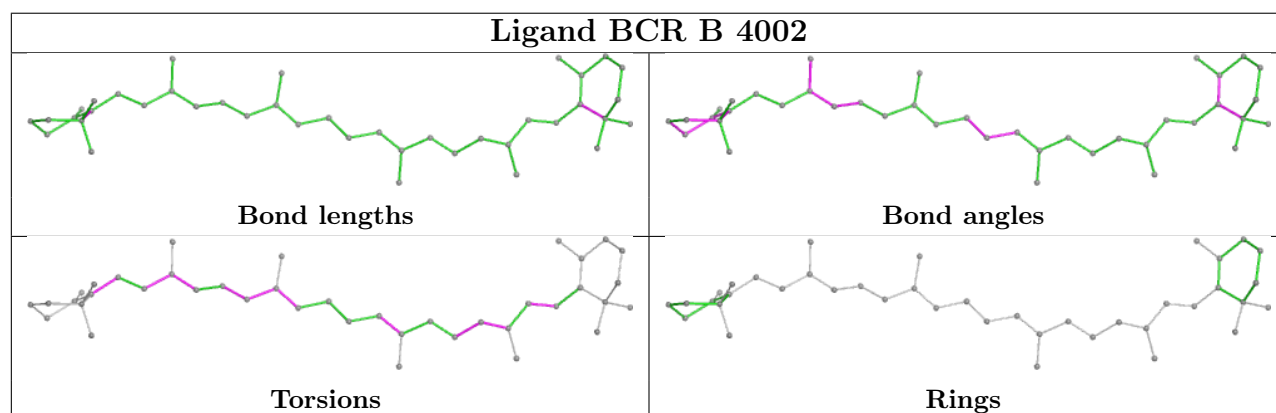
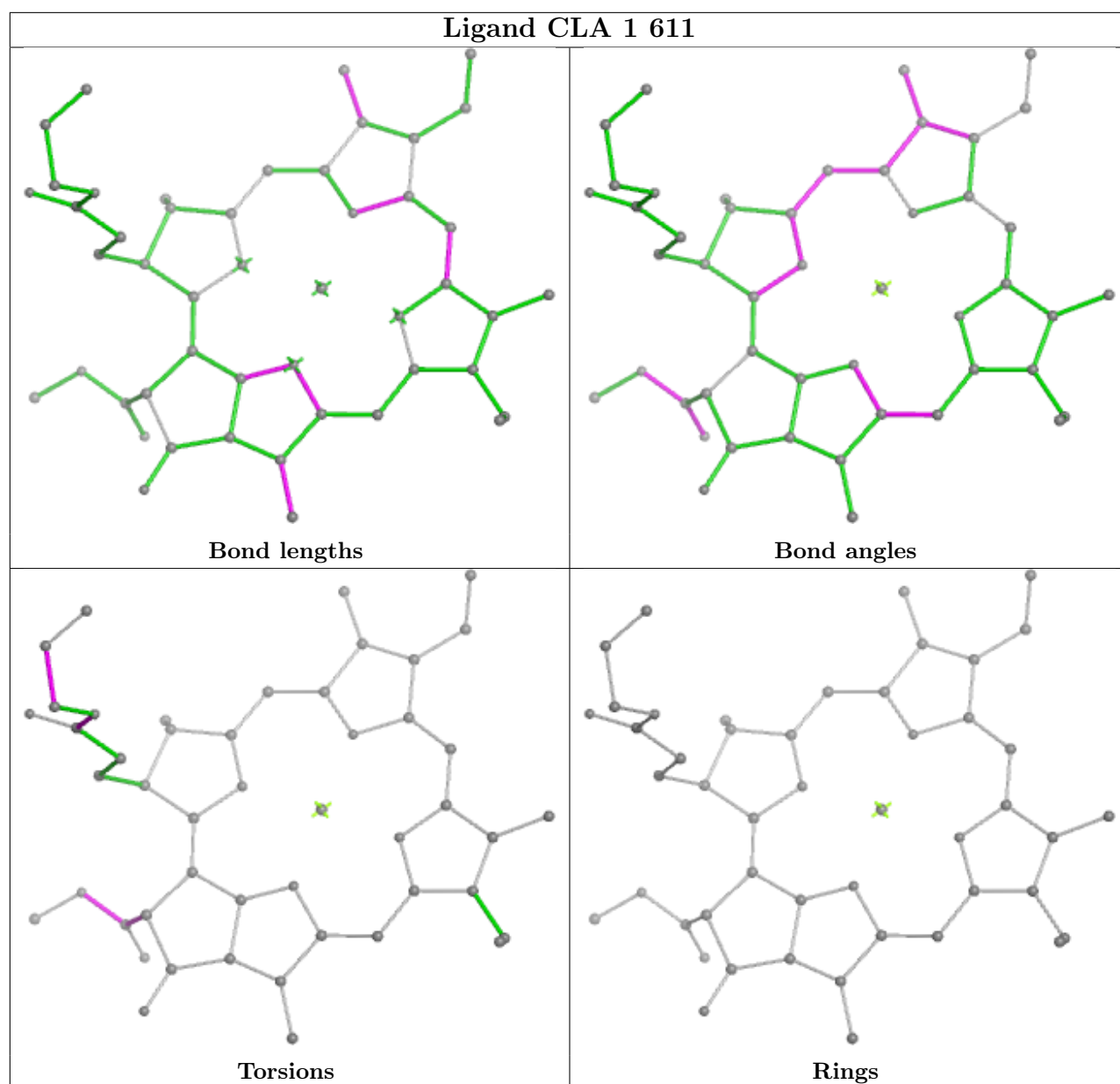


Ligand CLA B 1231

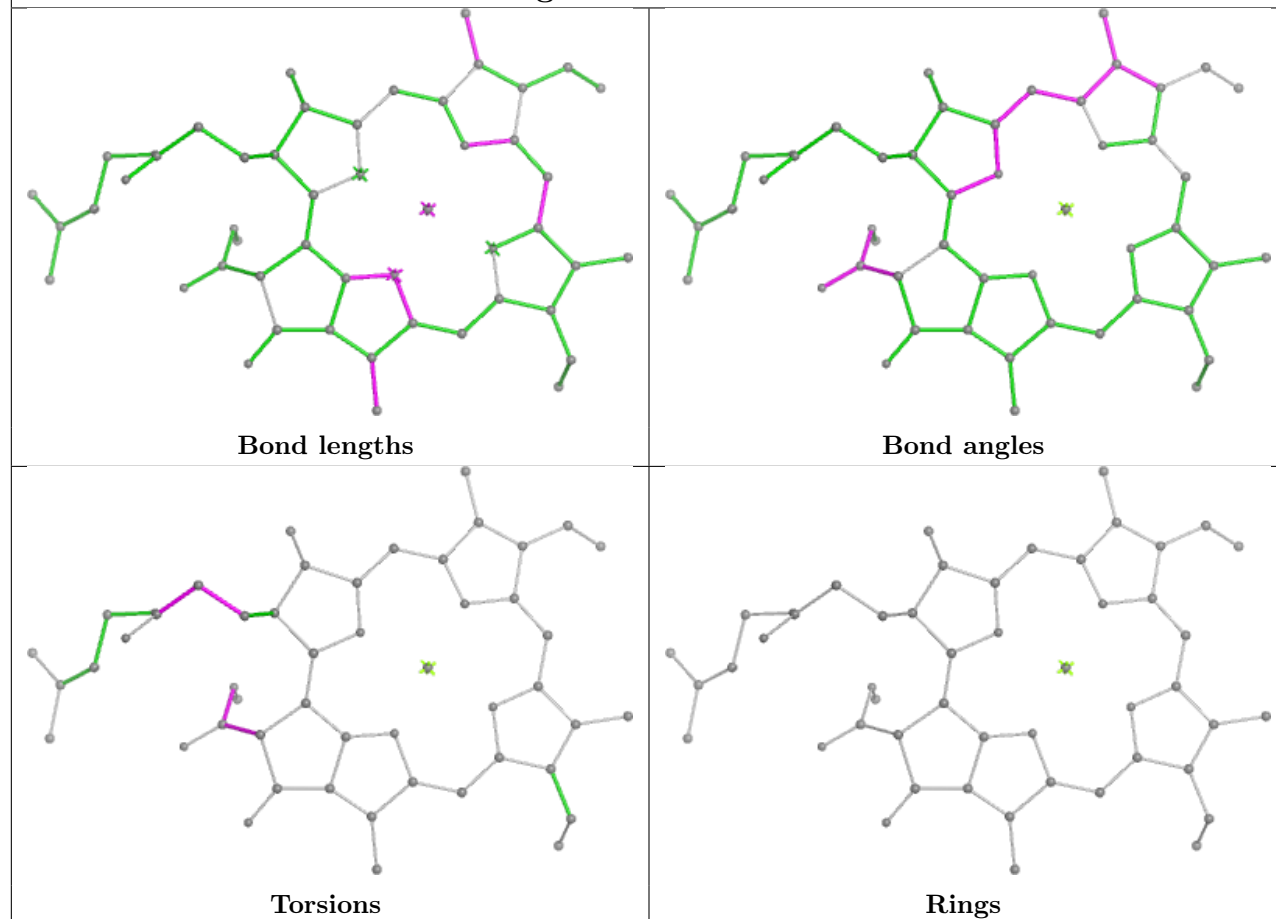




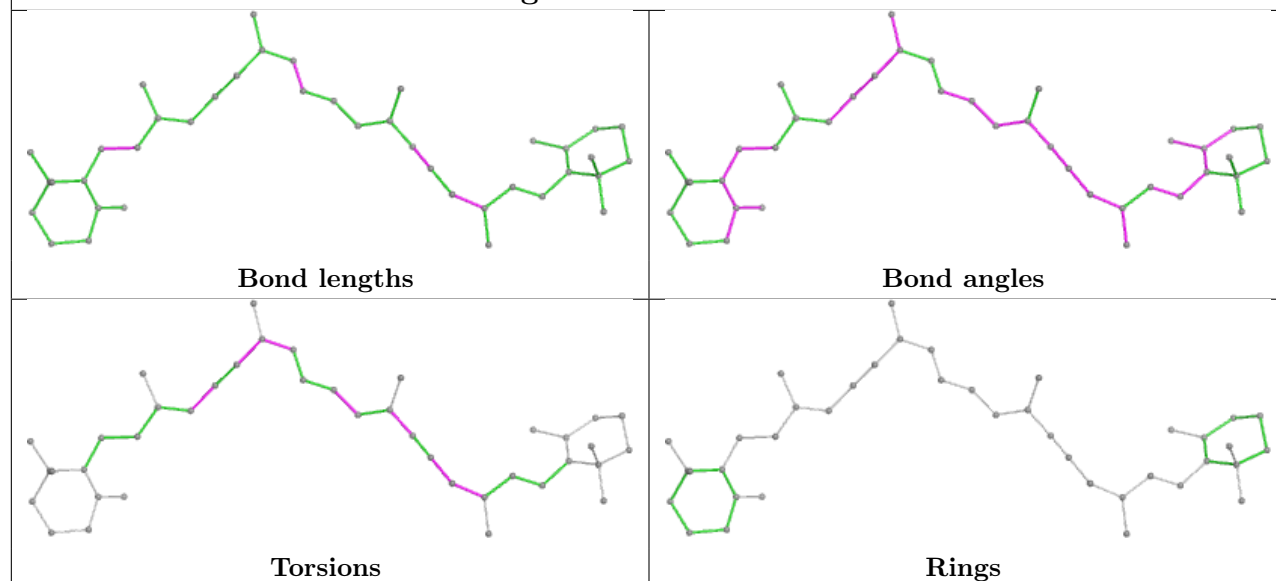


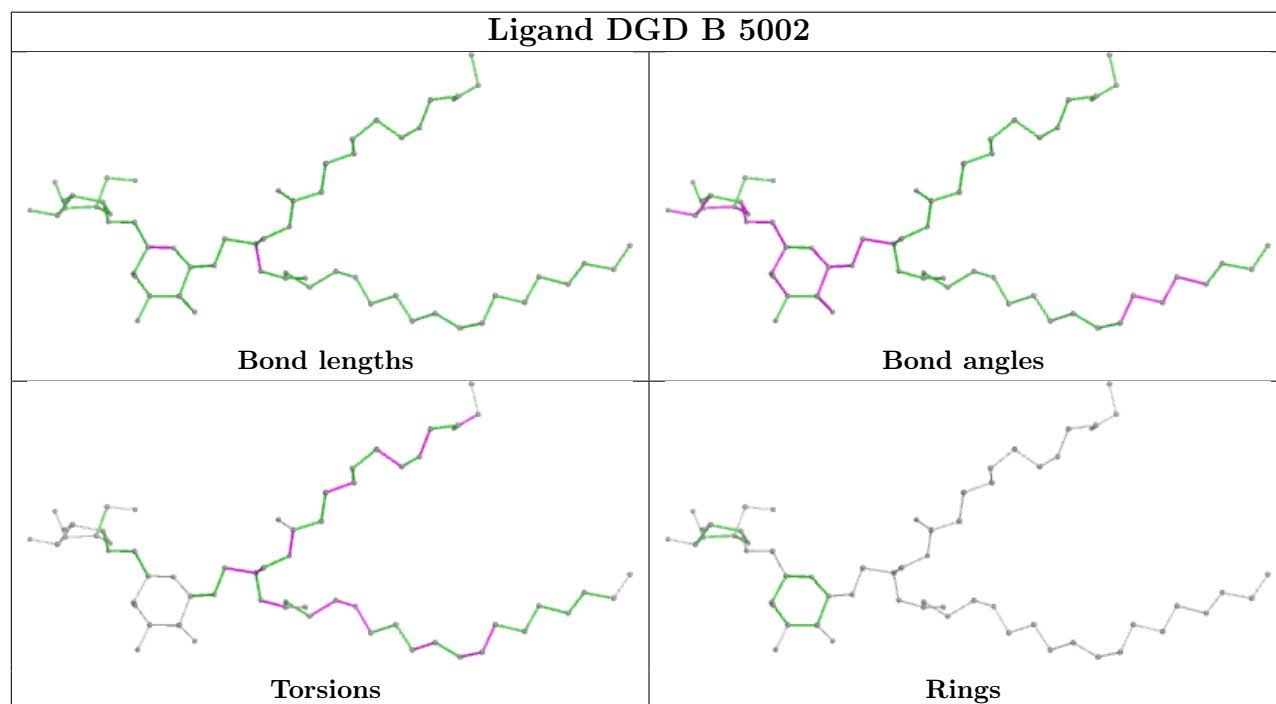
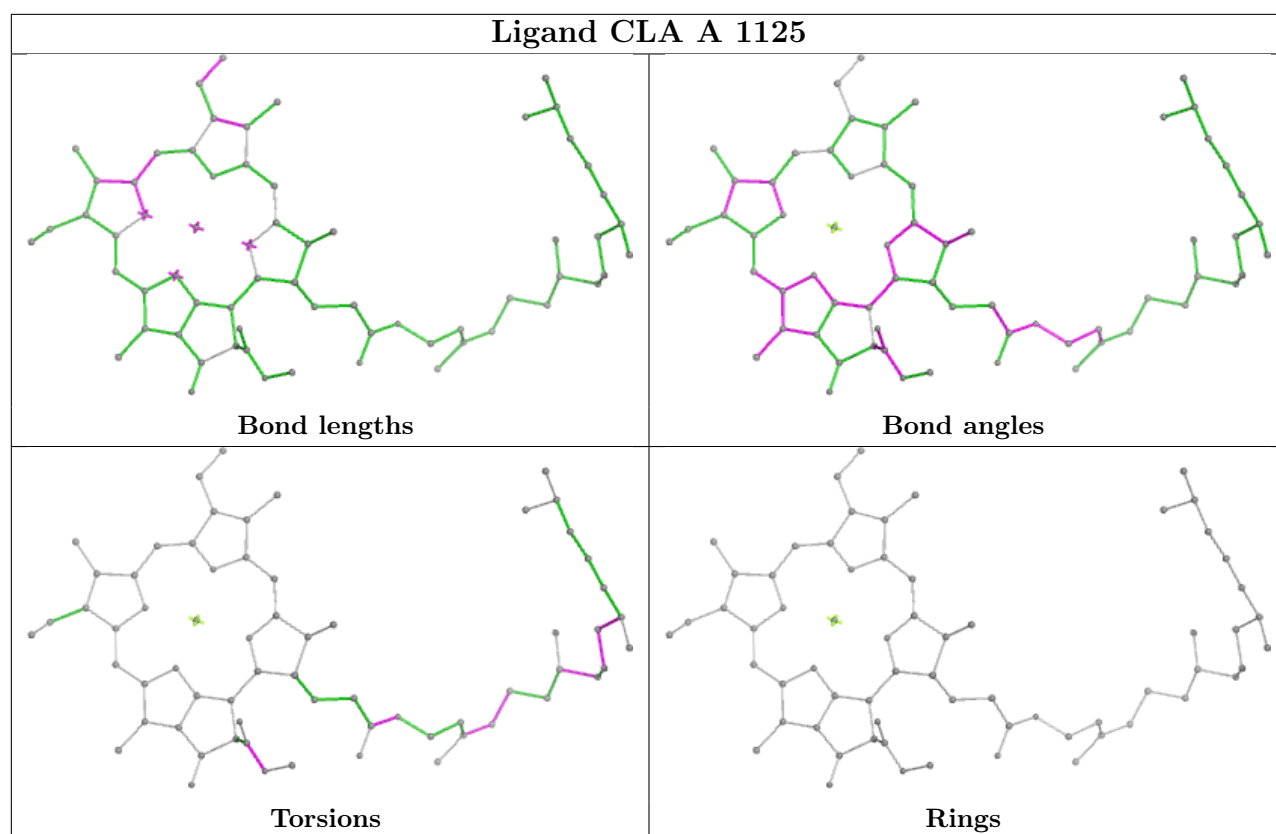


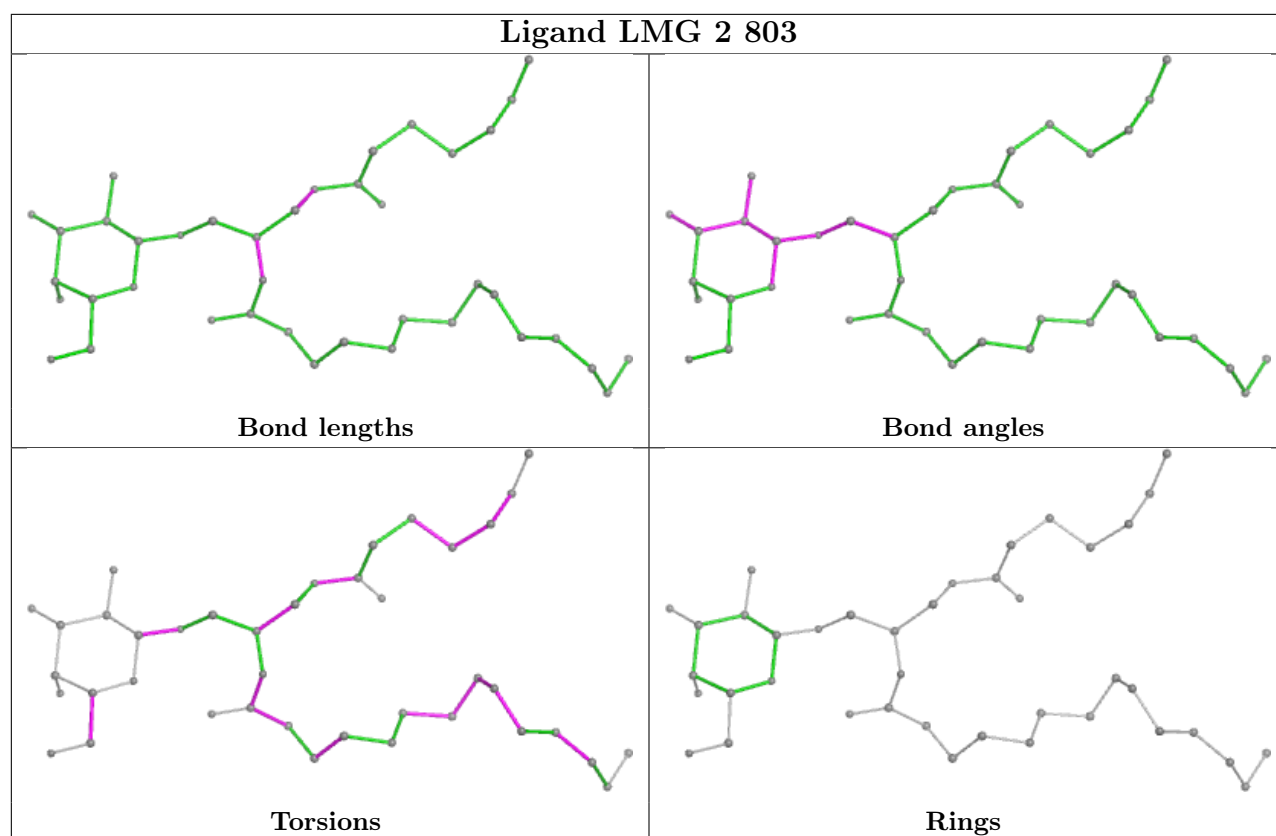
Ligand CLA 4 602



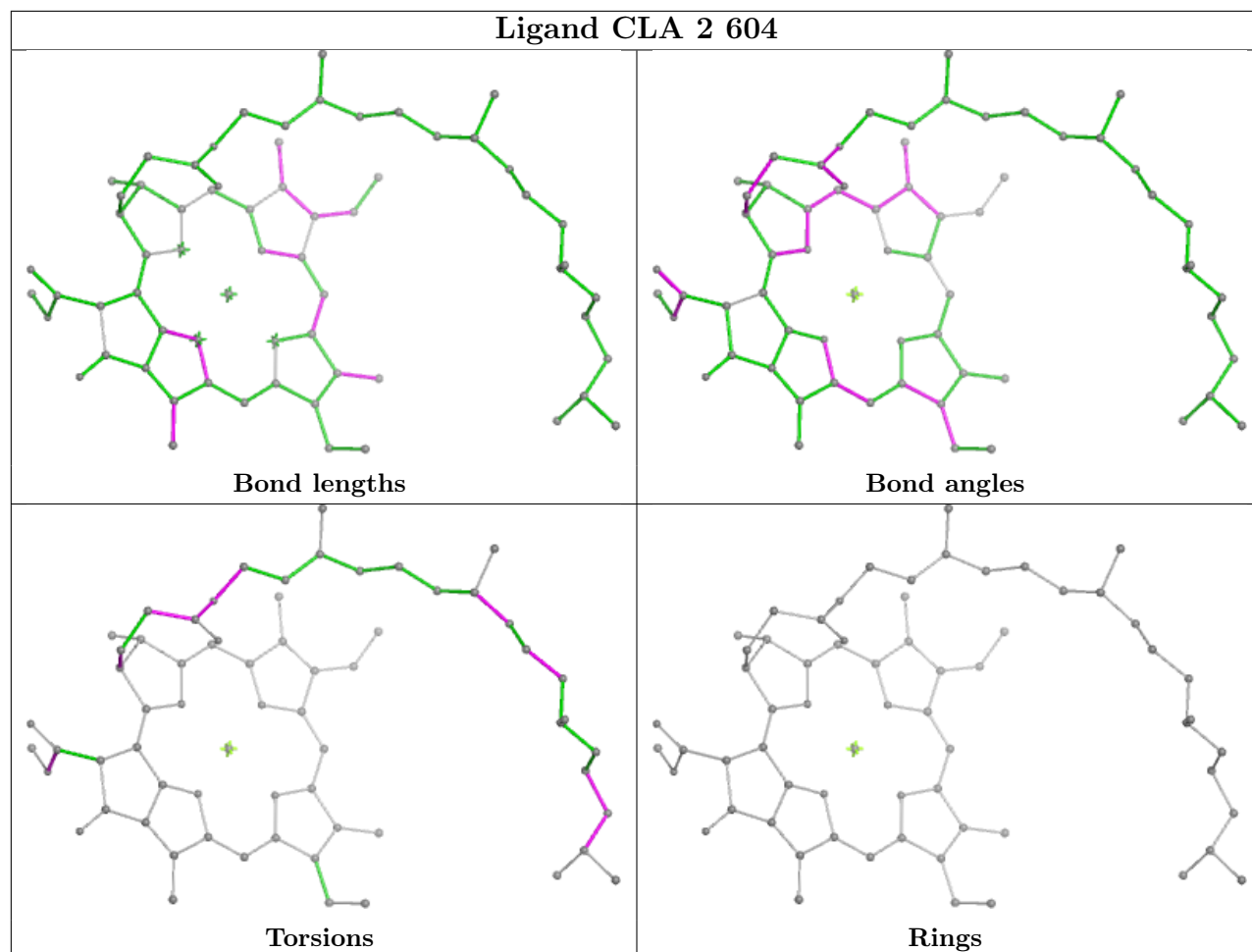
Ligand BCR A 4006

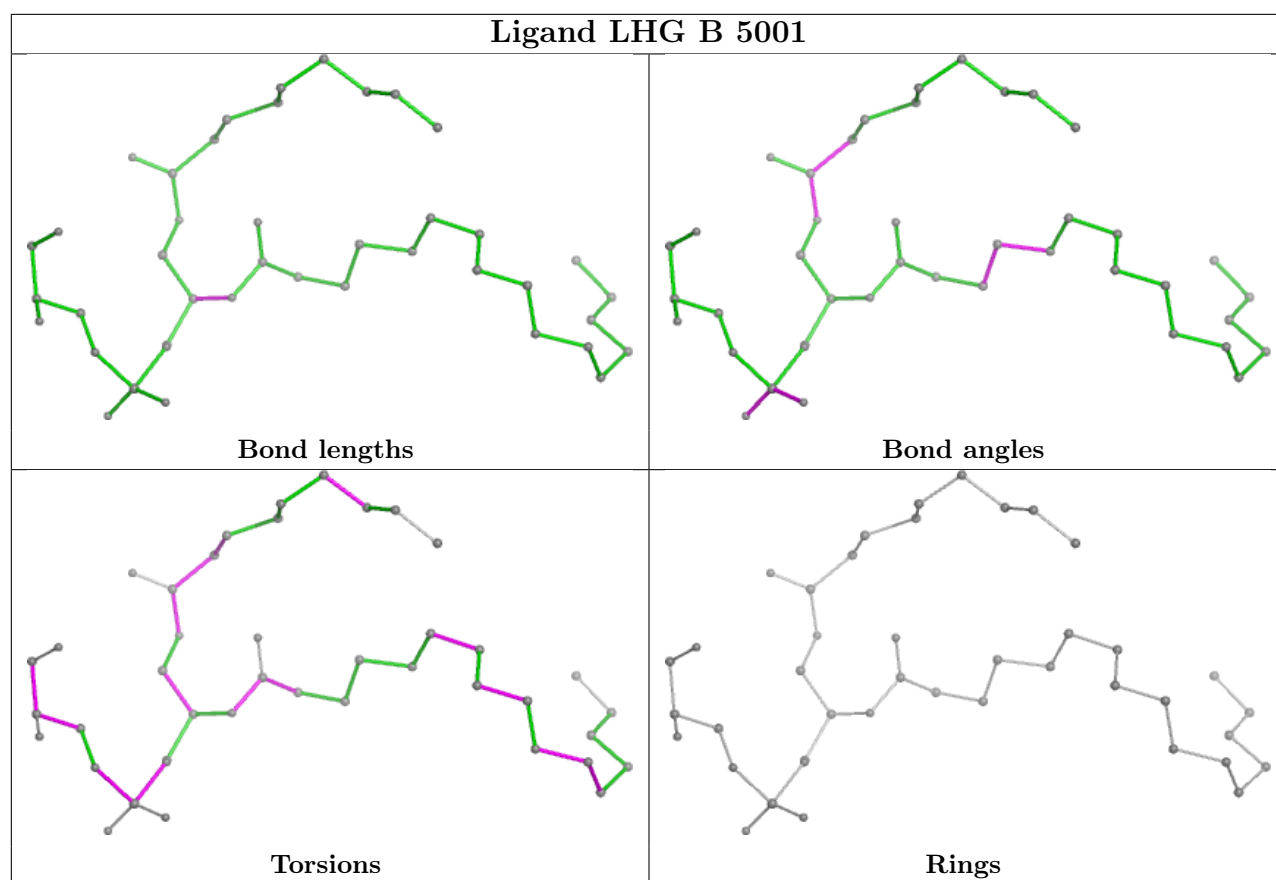




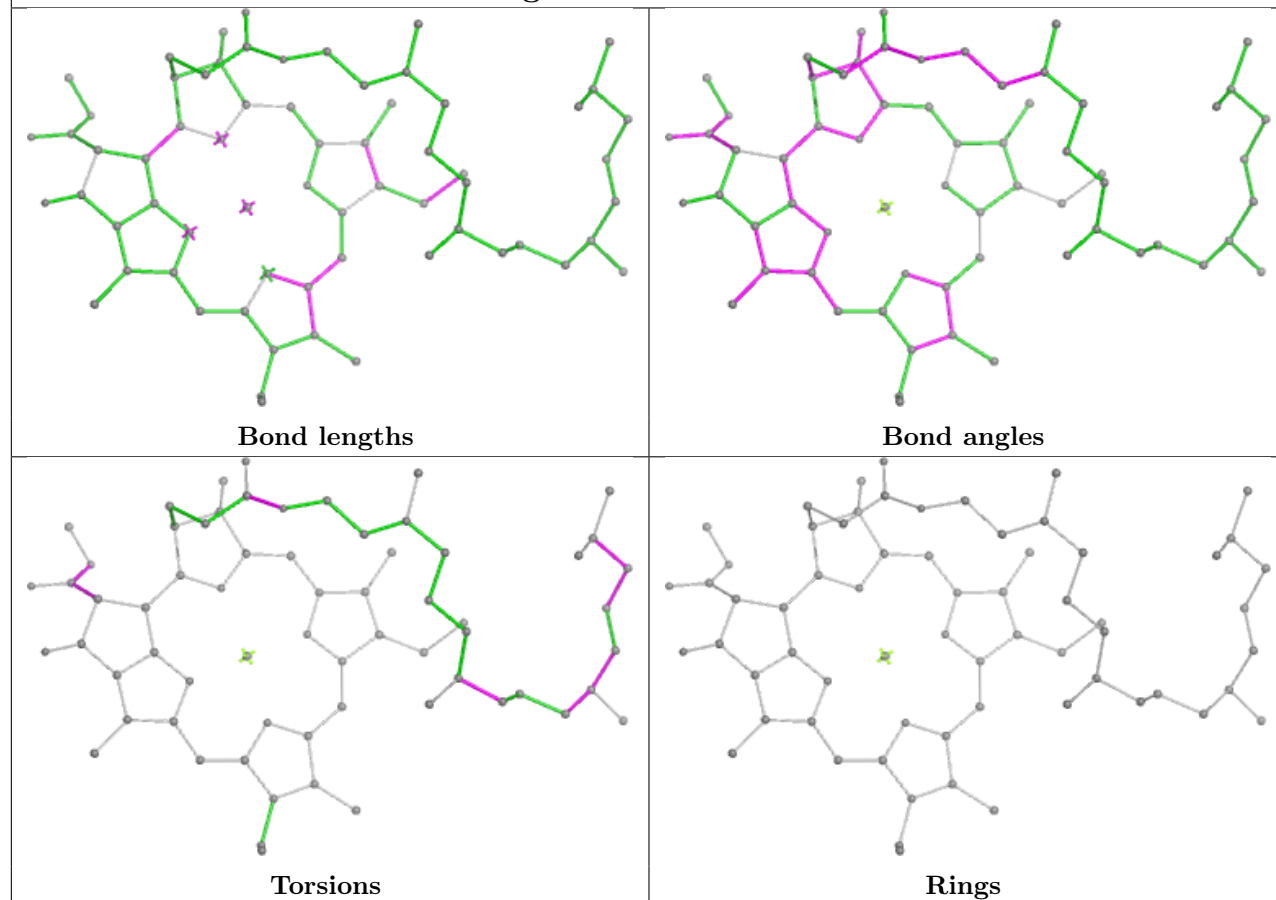


Ligand CLA 2 604

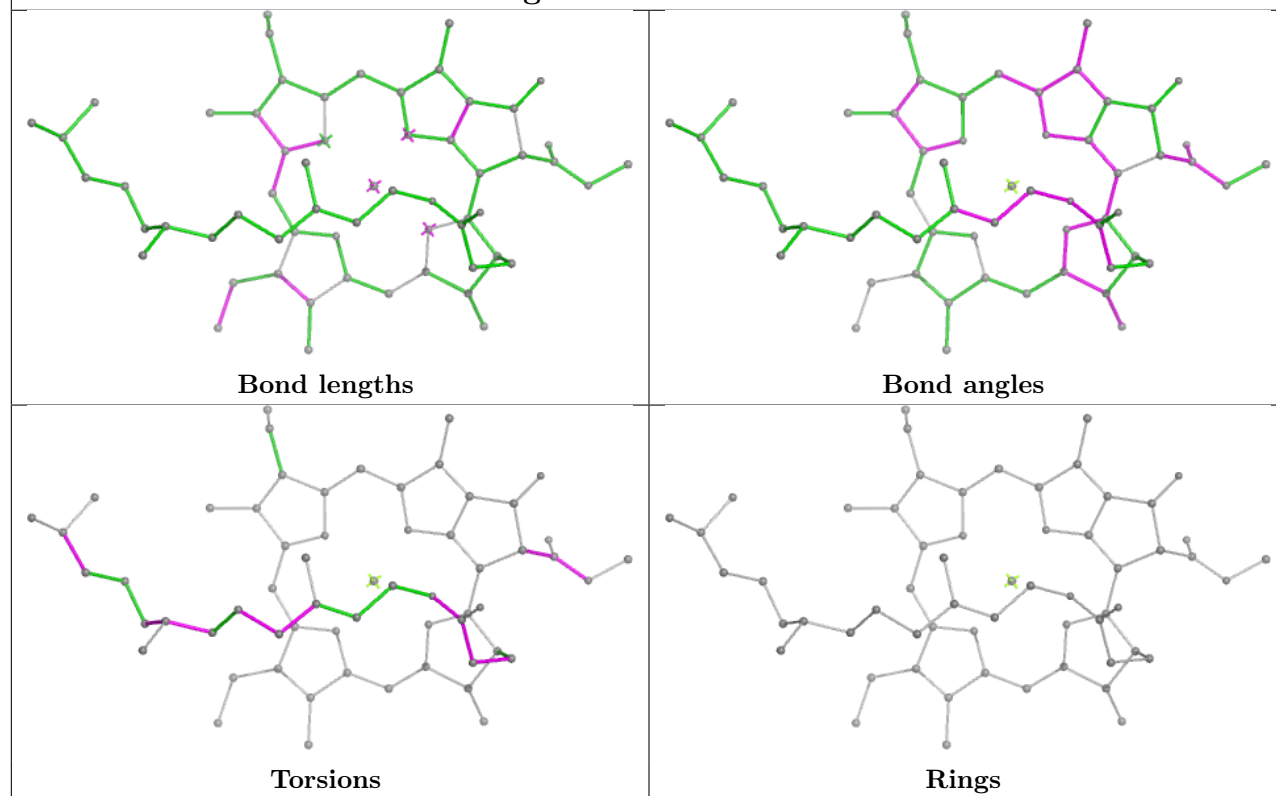




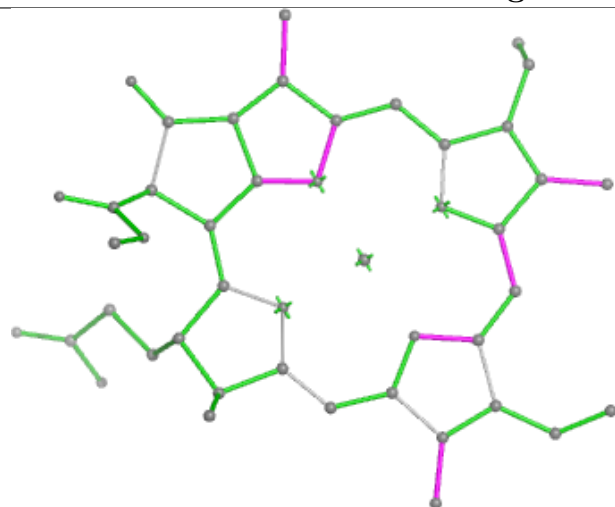
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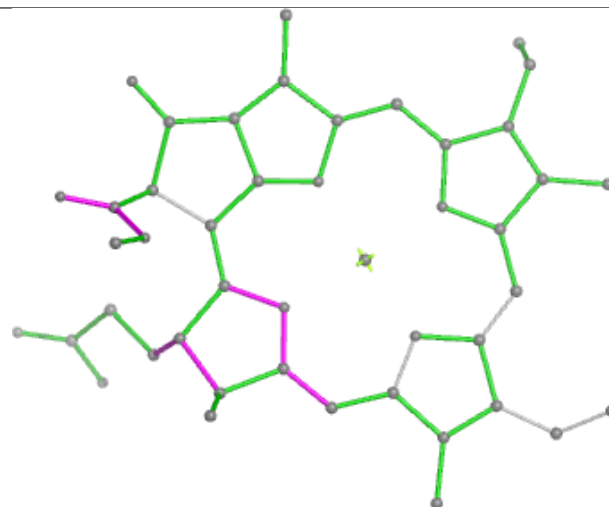
Ligand CLA B 1235



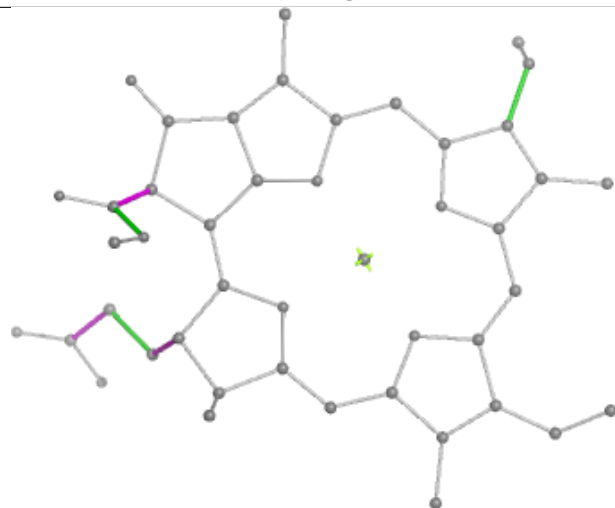
Ligand CLA B 1218



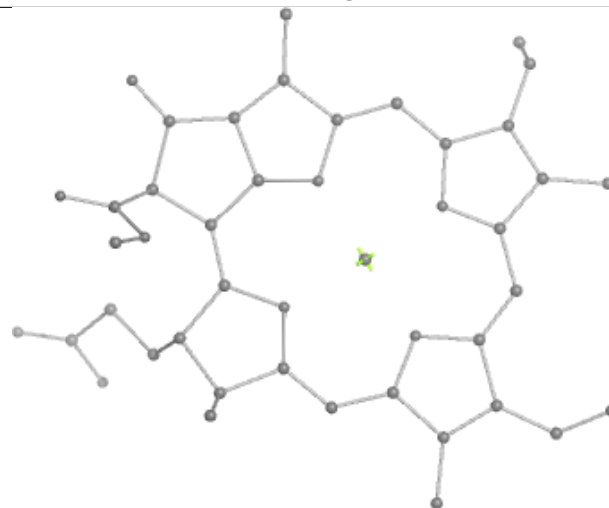
Bond lengths



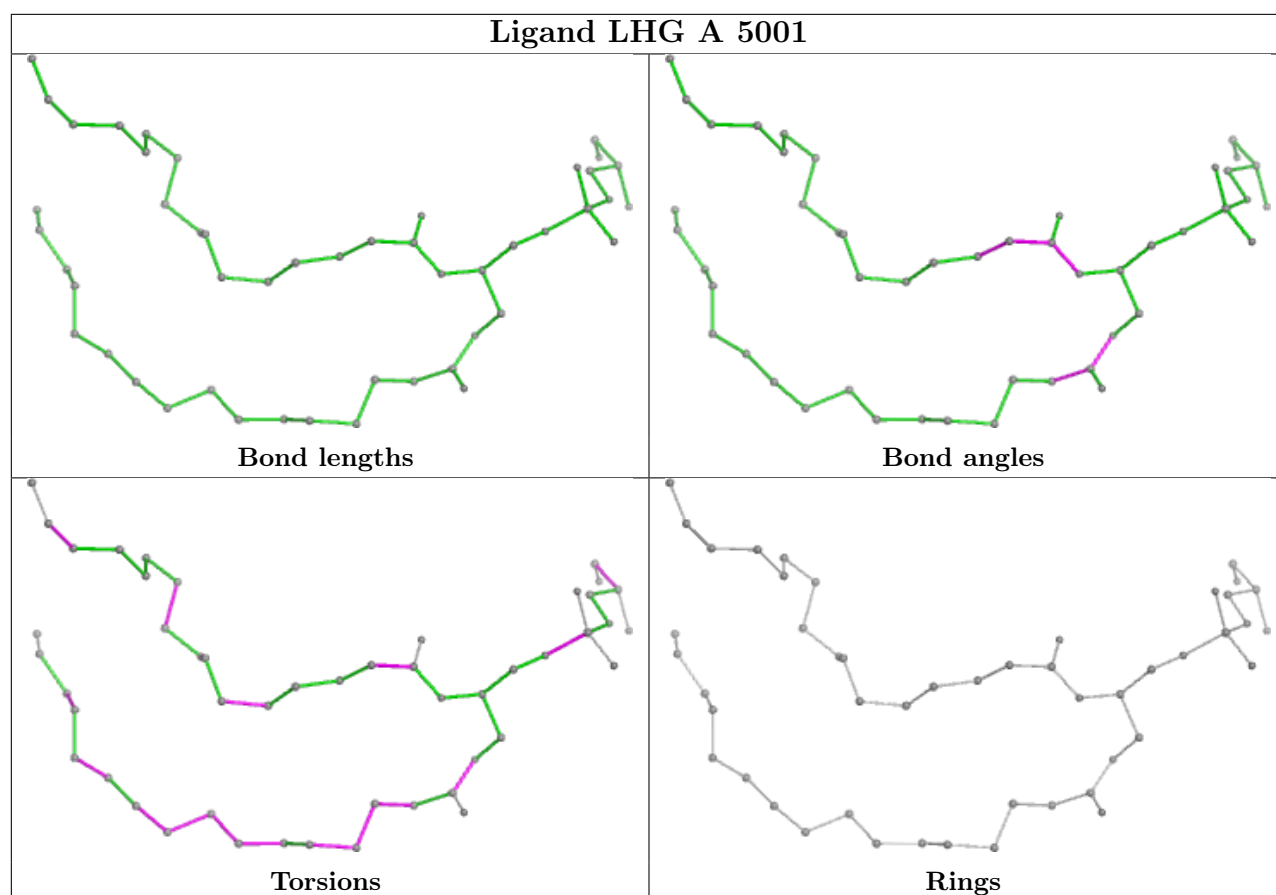
Bond angles



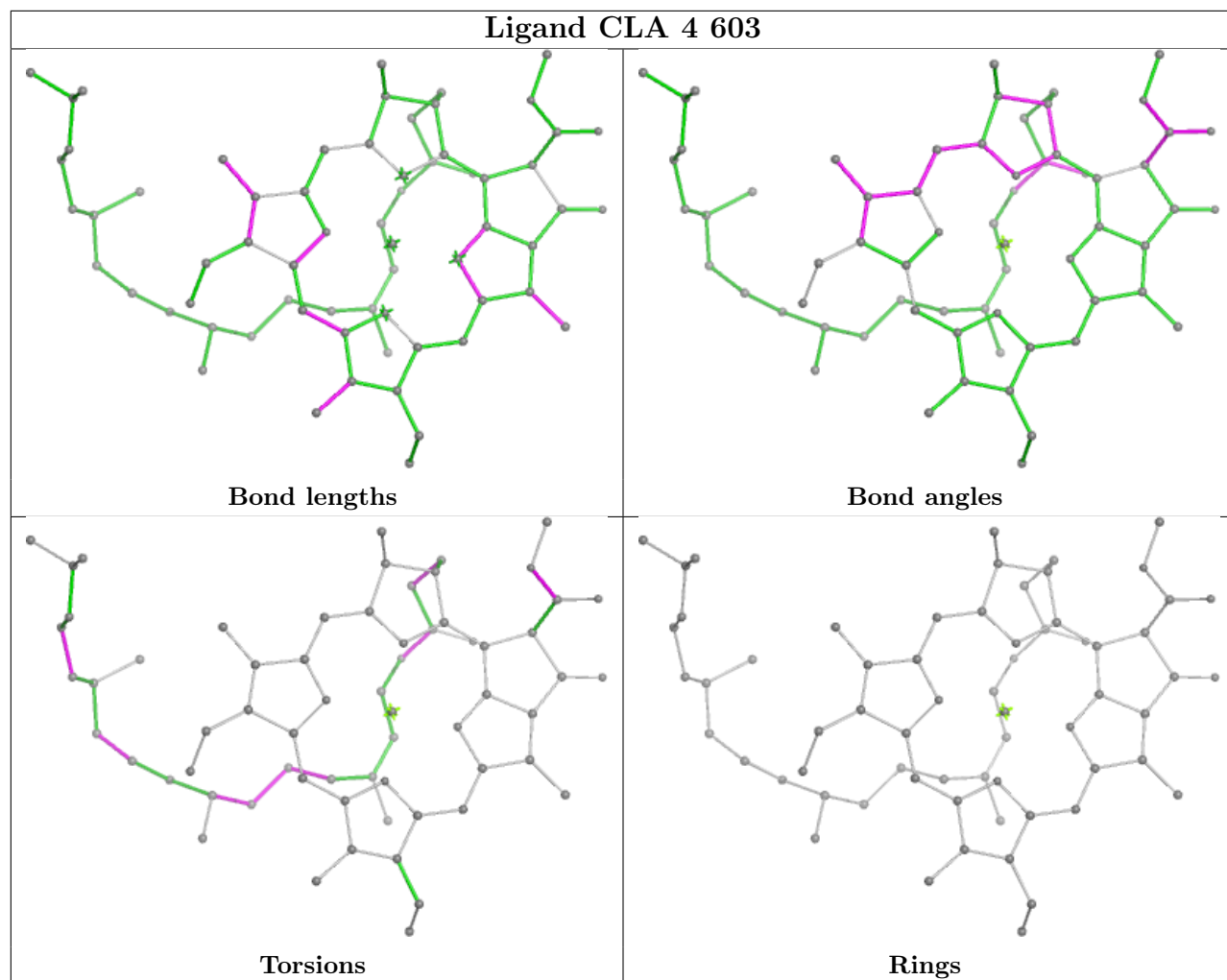
Torsions

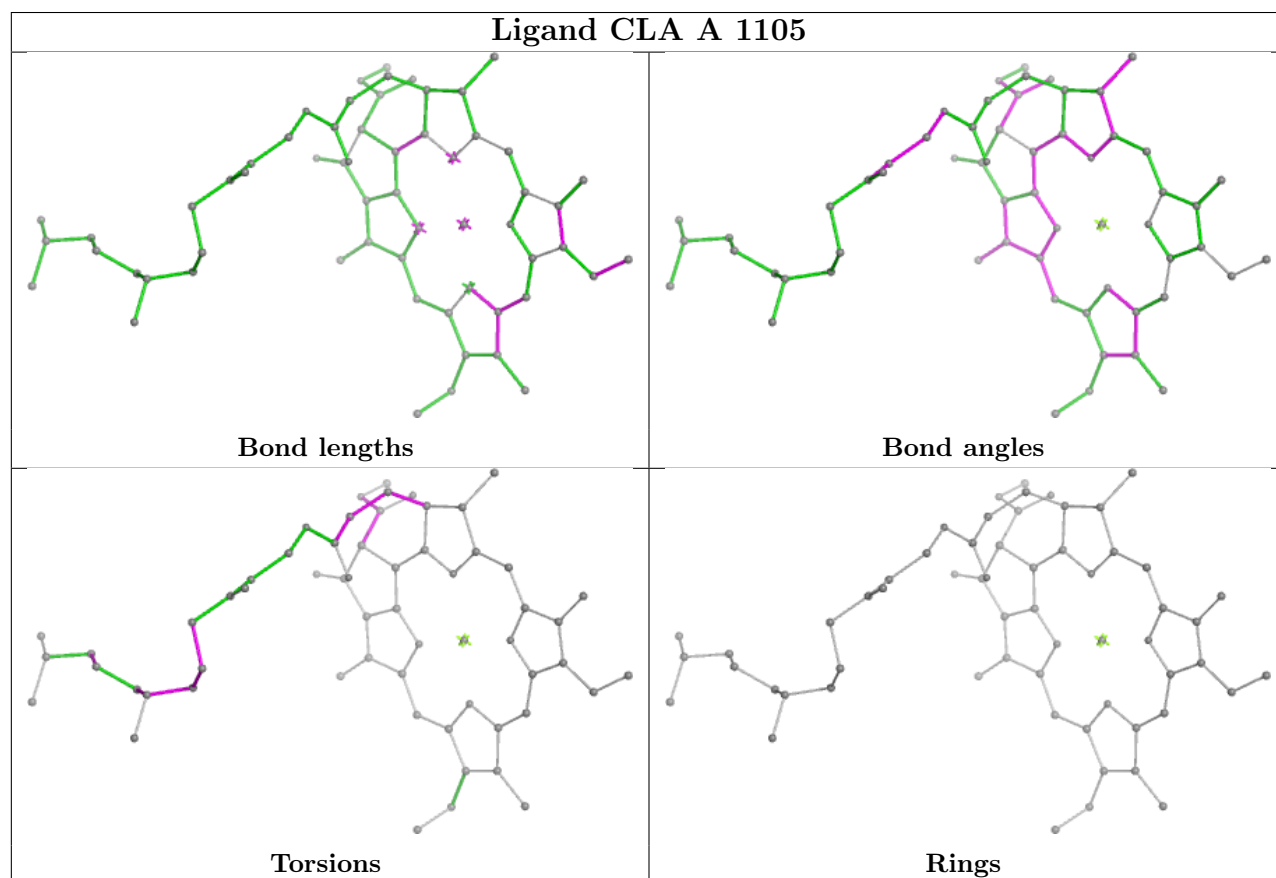
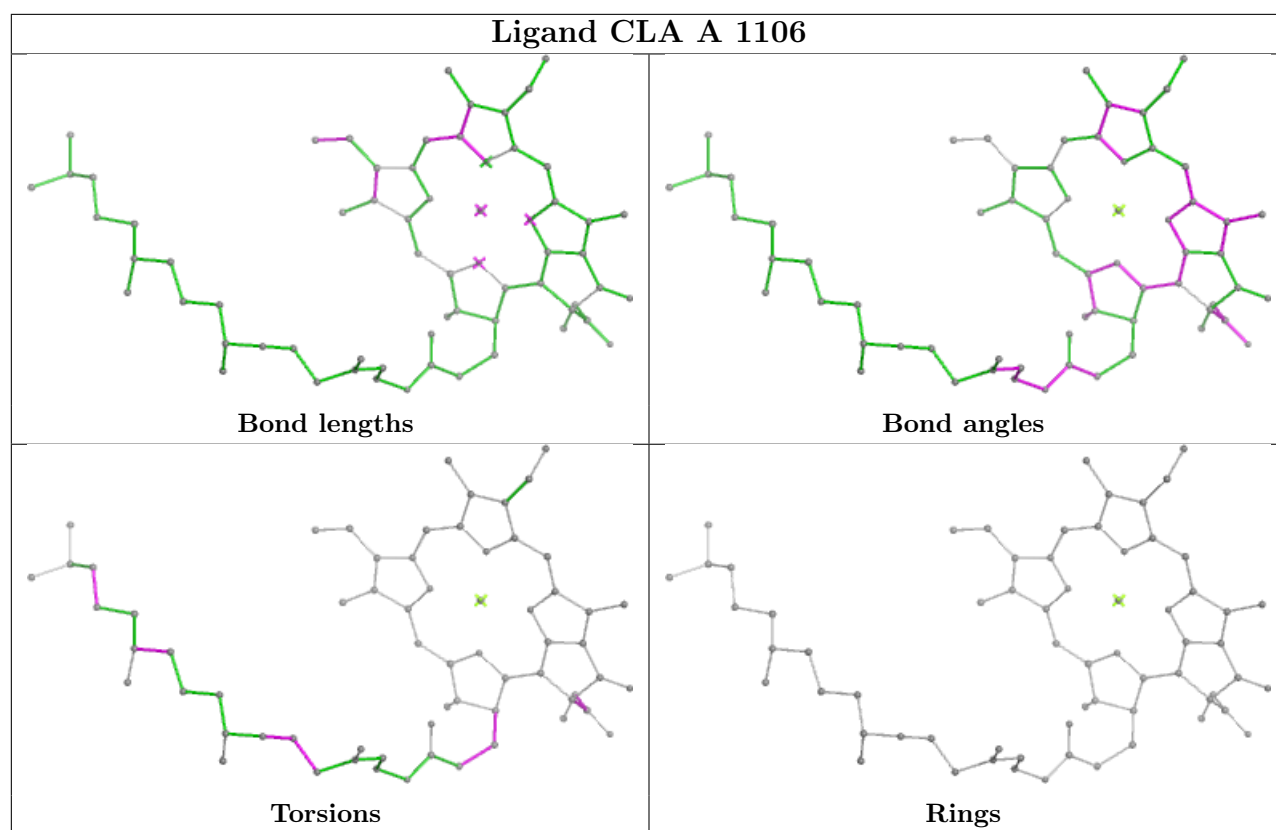


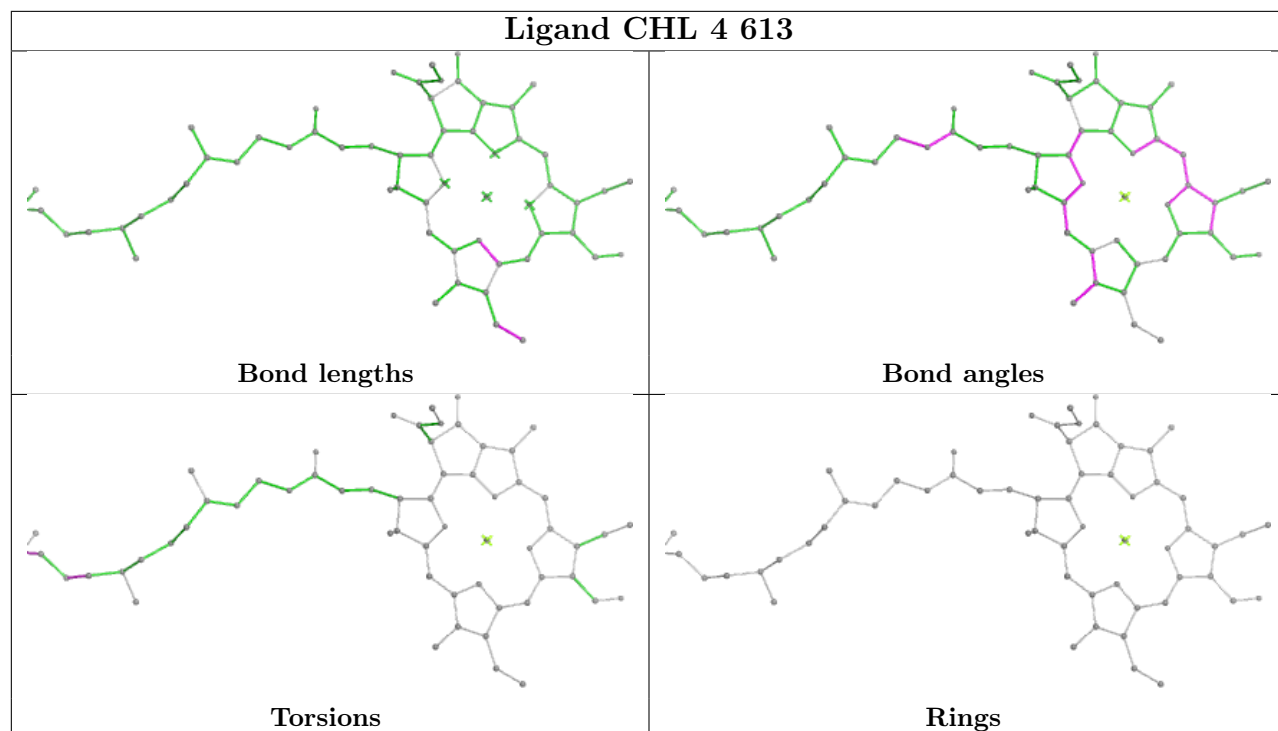
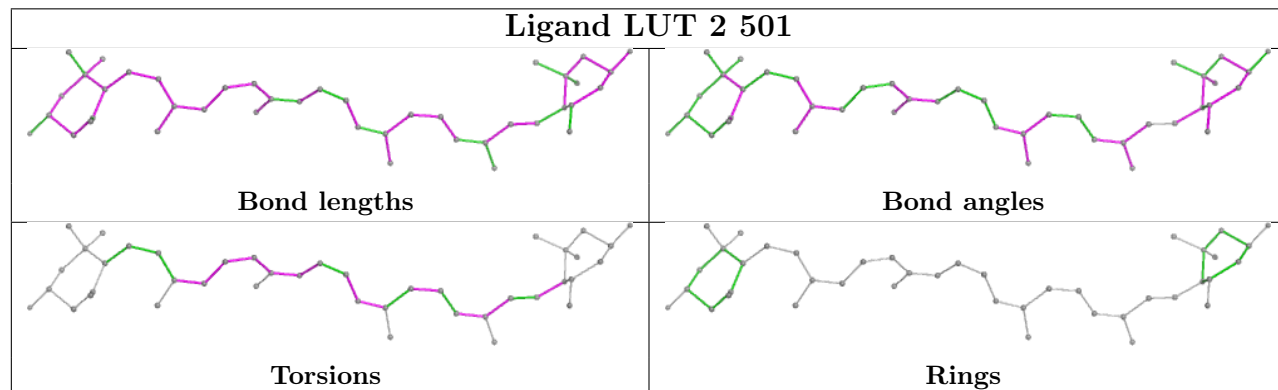
Rings



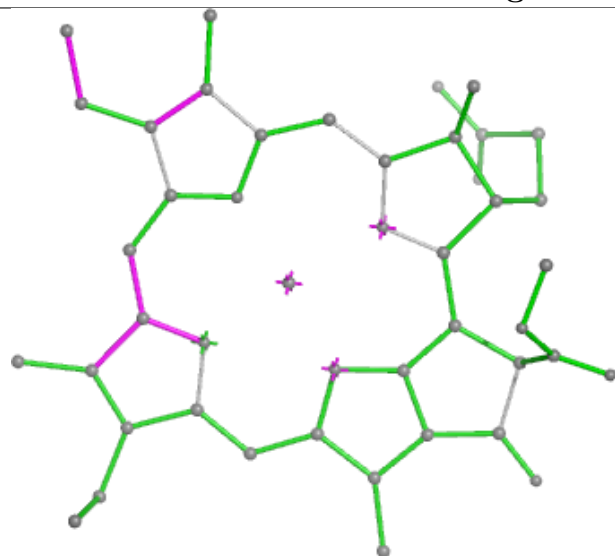
Ligand CLA 4 603



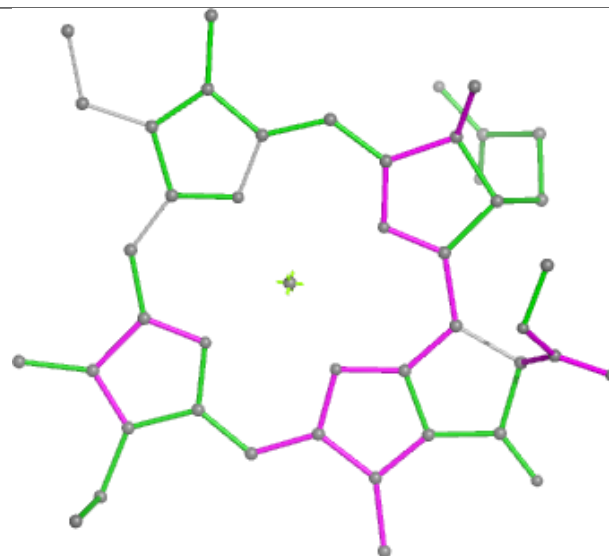


Ligand CHL 4 613**Ligand LUT 2 501**

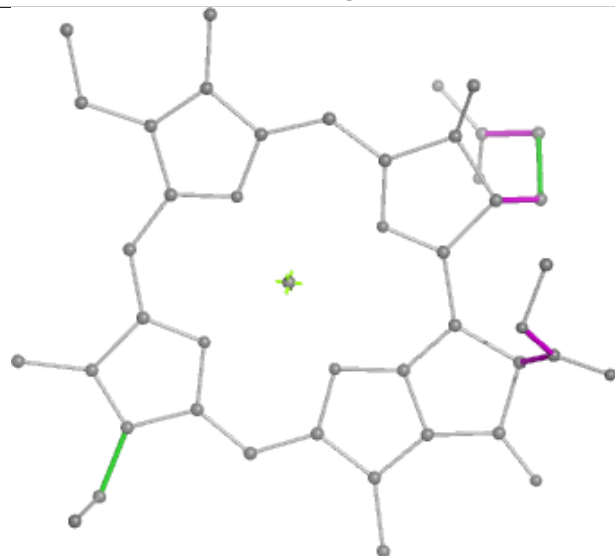
Ligand CLA A 1130



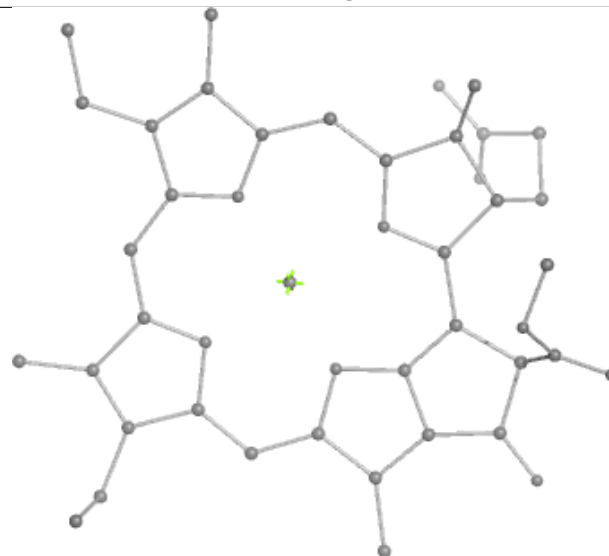
Bond lengths



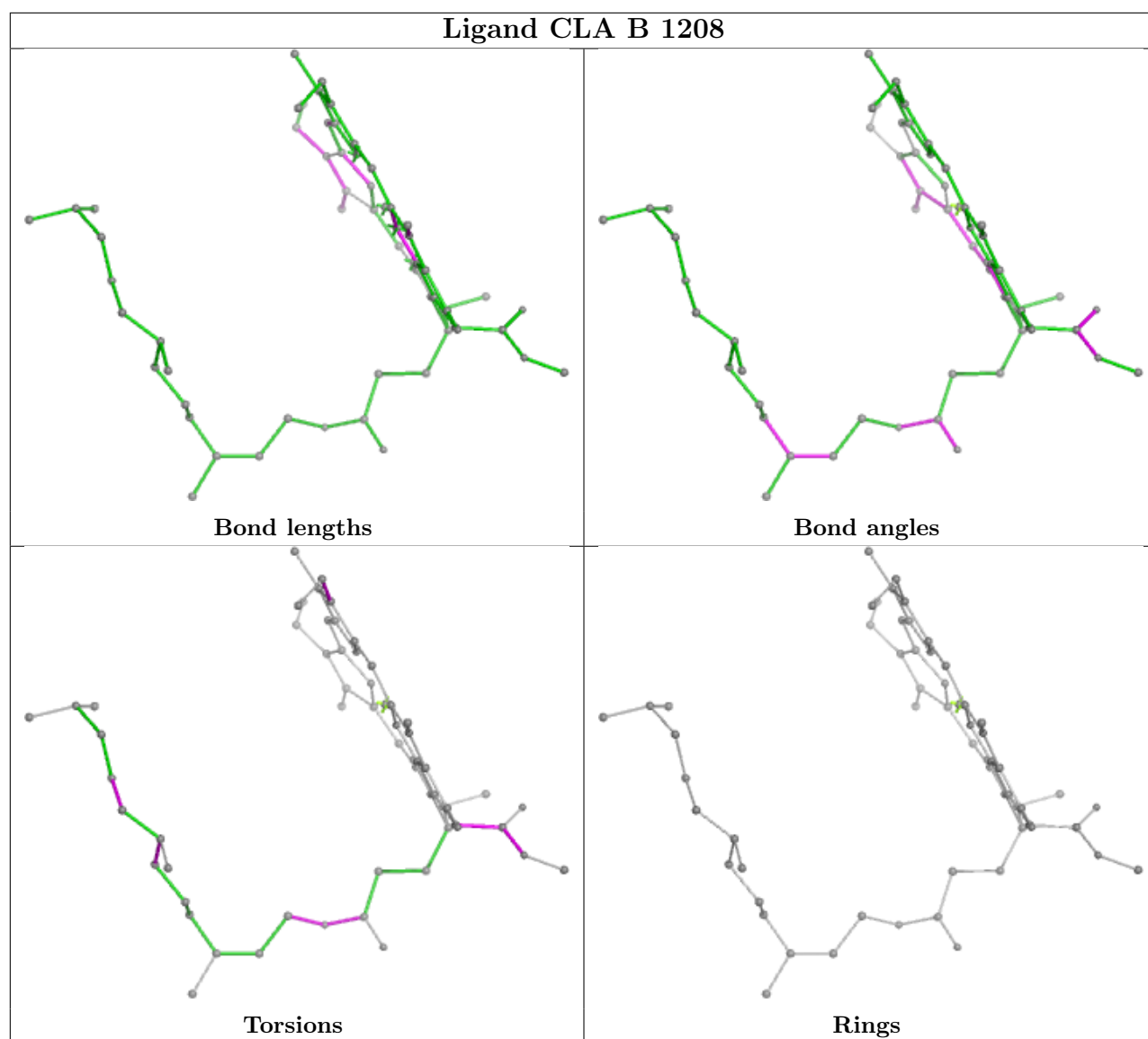
Bond angles



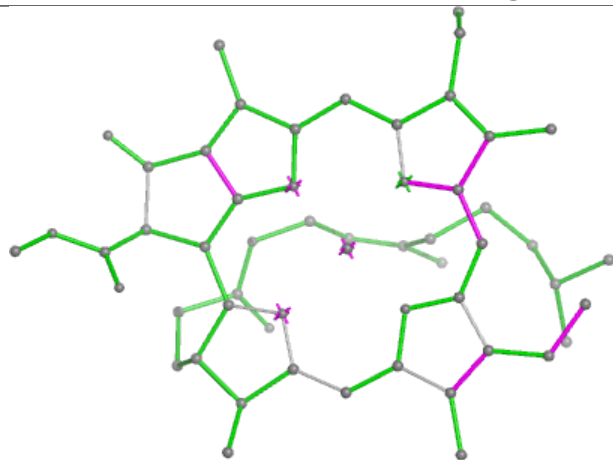
Torsions



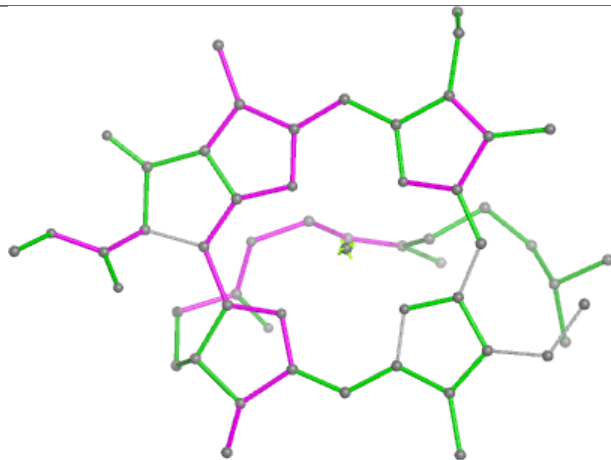
Rings



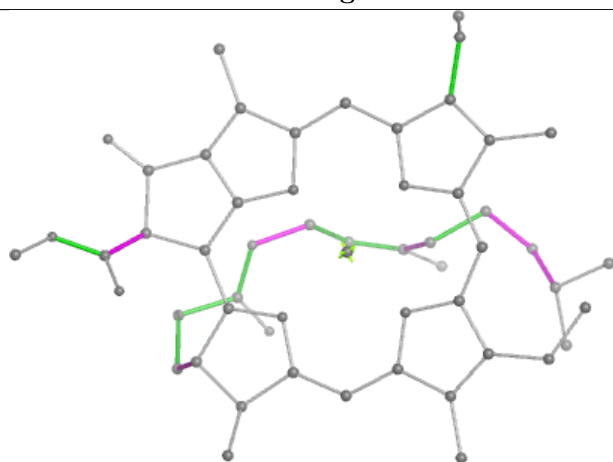
Ligand CLA A 1110



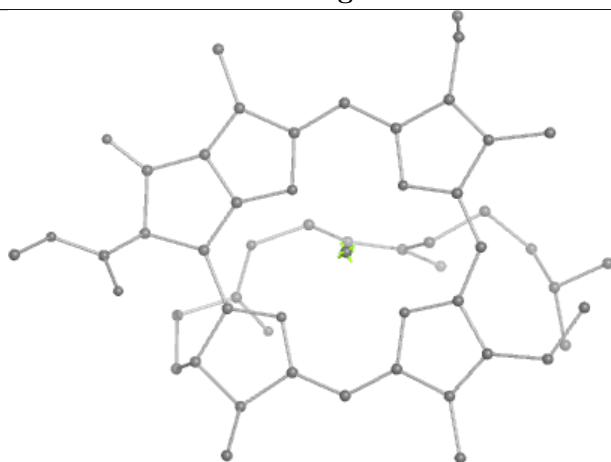
Bond lengths



Bond angles

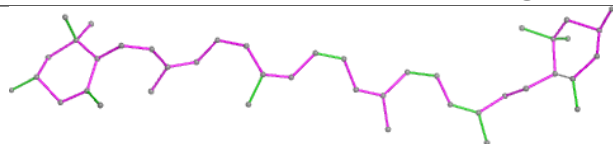


Torsions

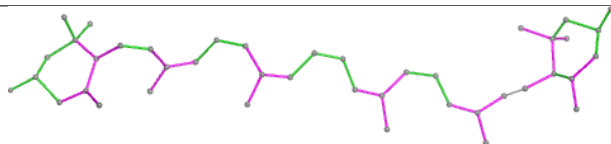


Rings

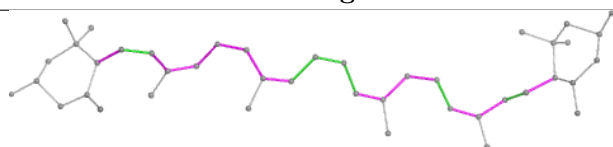
Ligand LUT 4 501



Bond lengths



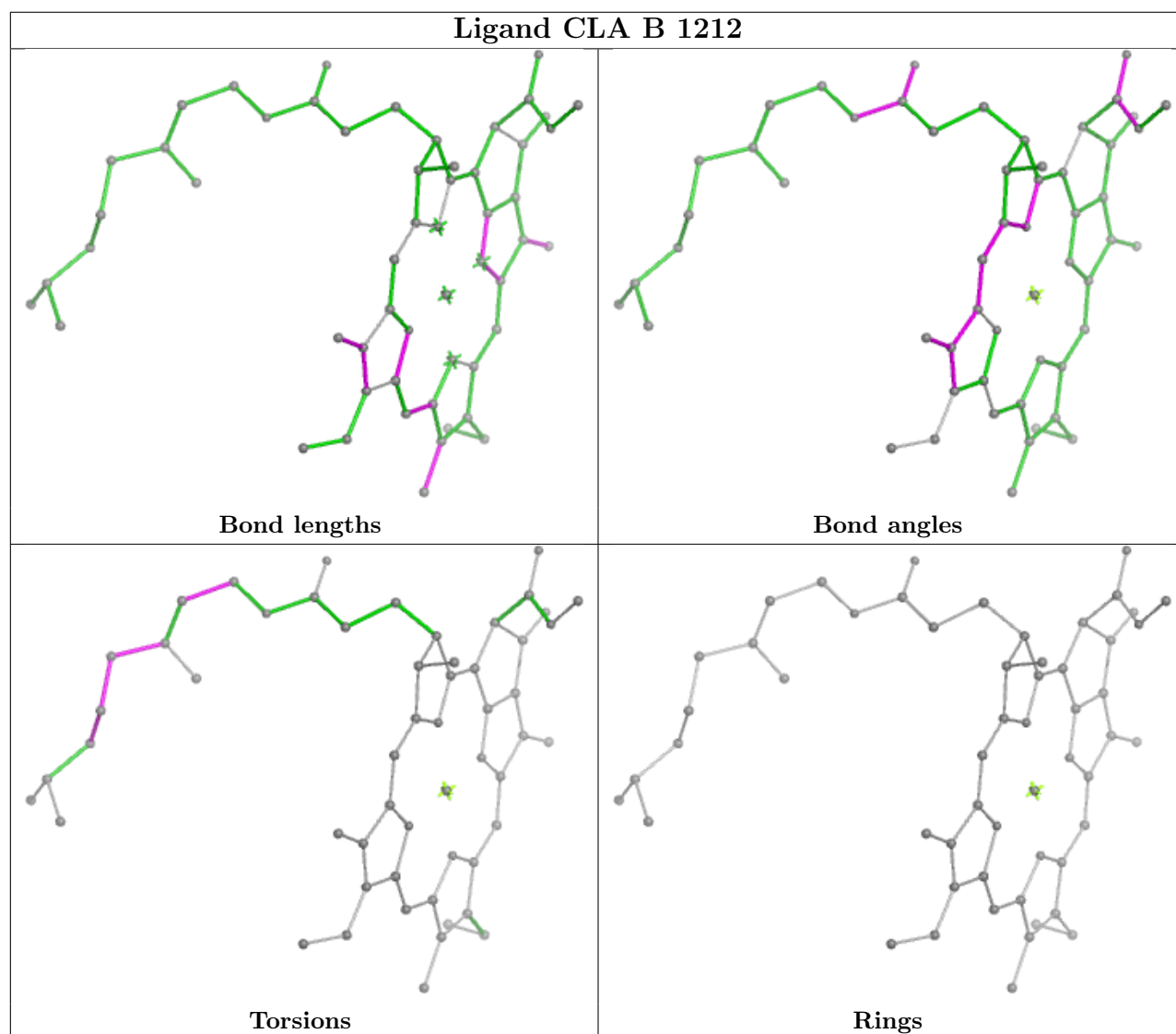
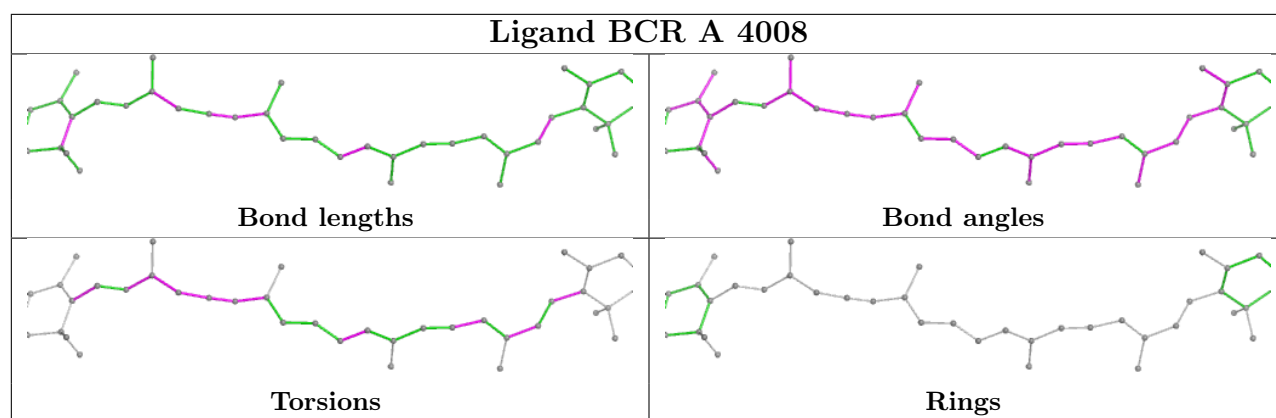
Bond angles

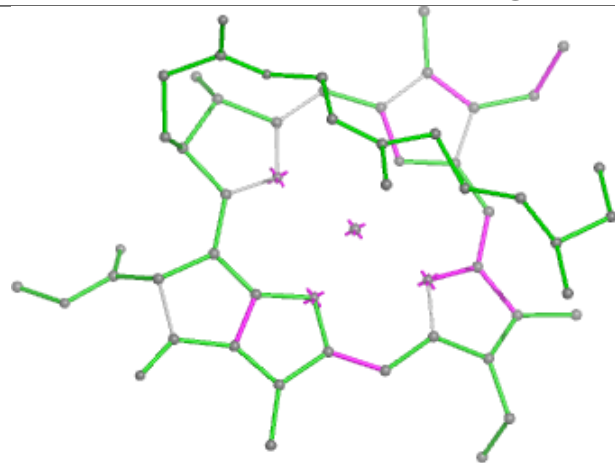
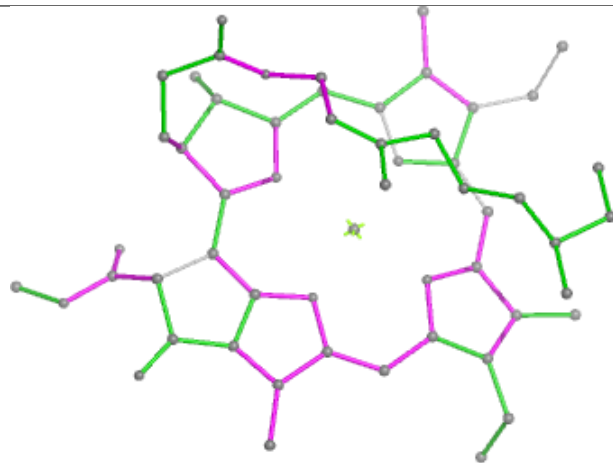
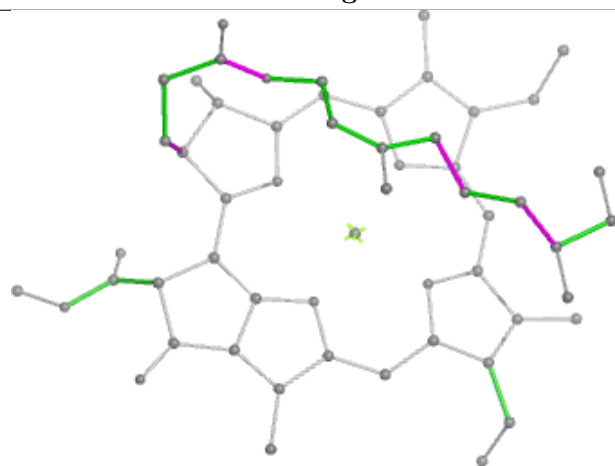
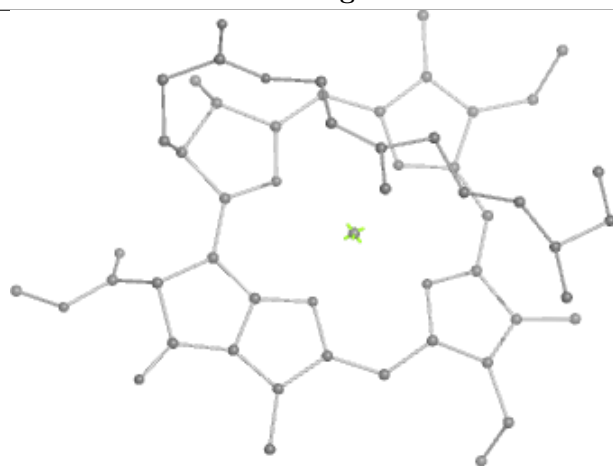
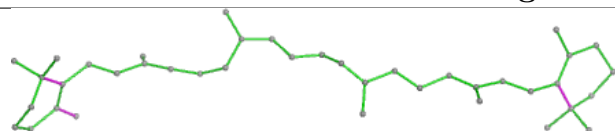
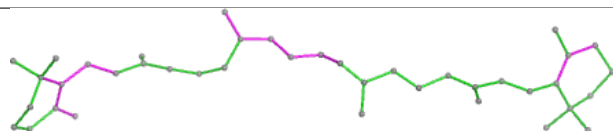
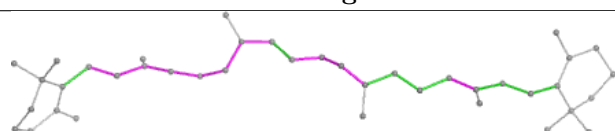
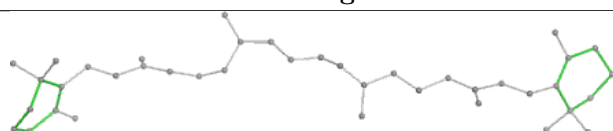


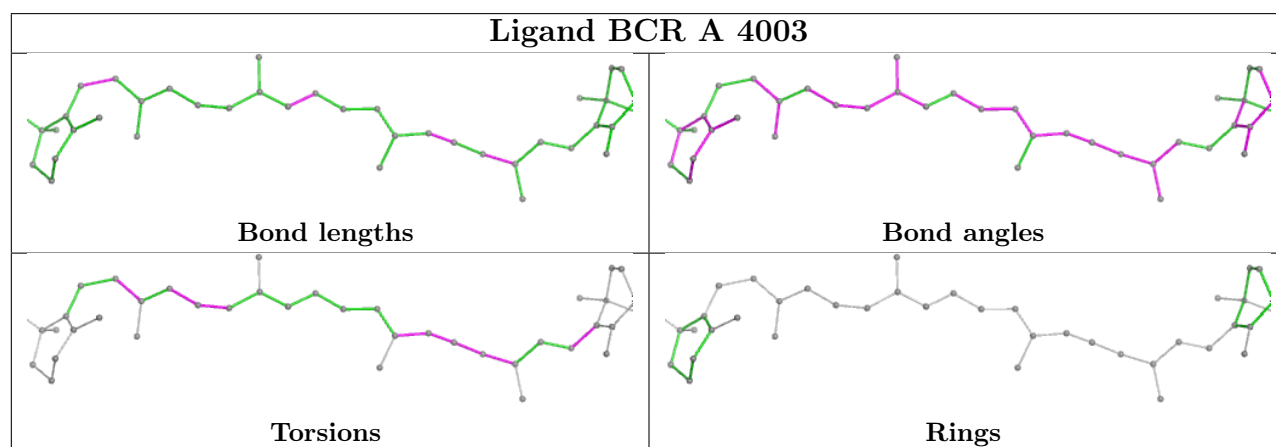
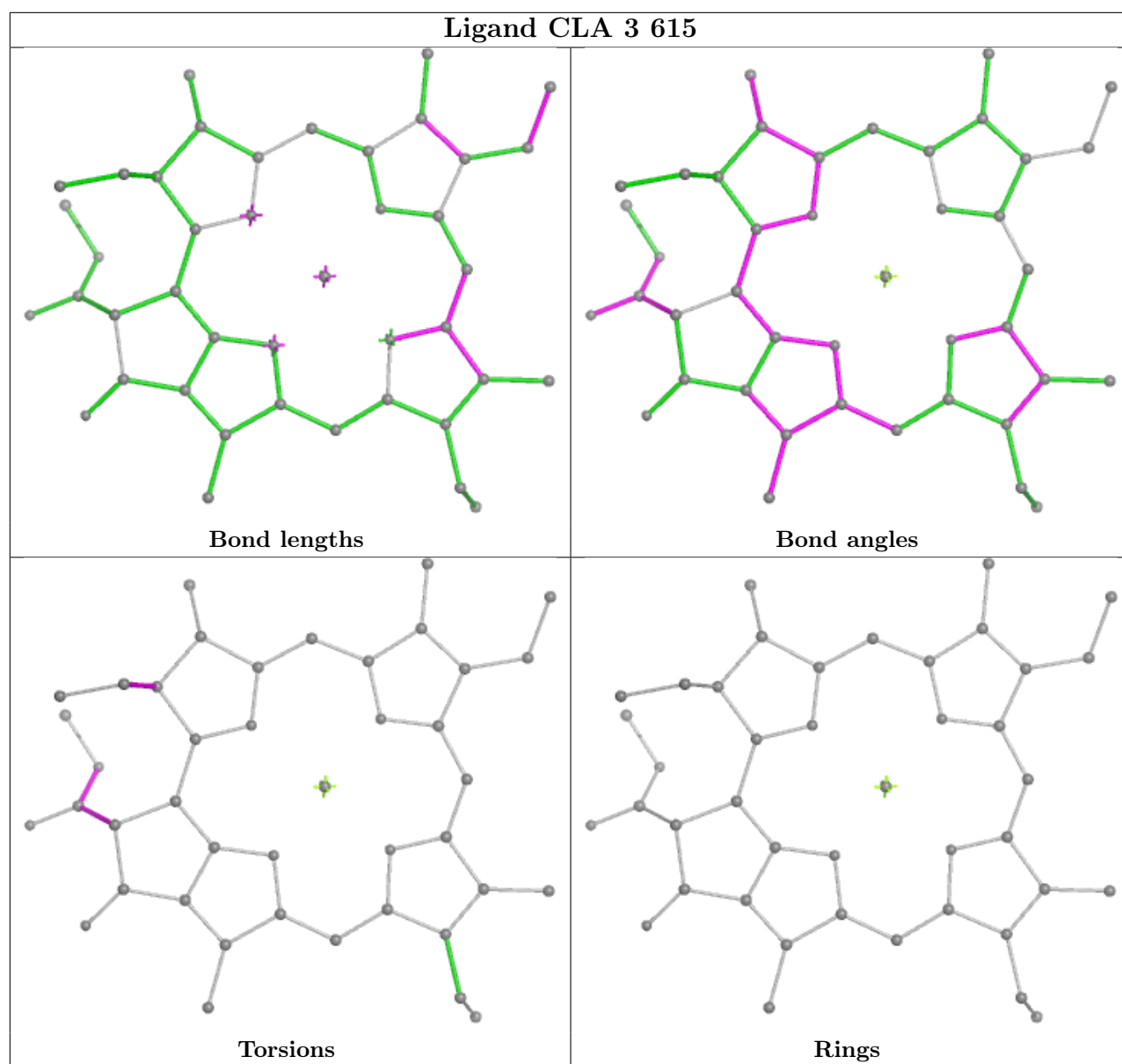
Torsions



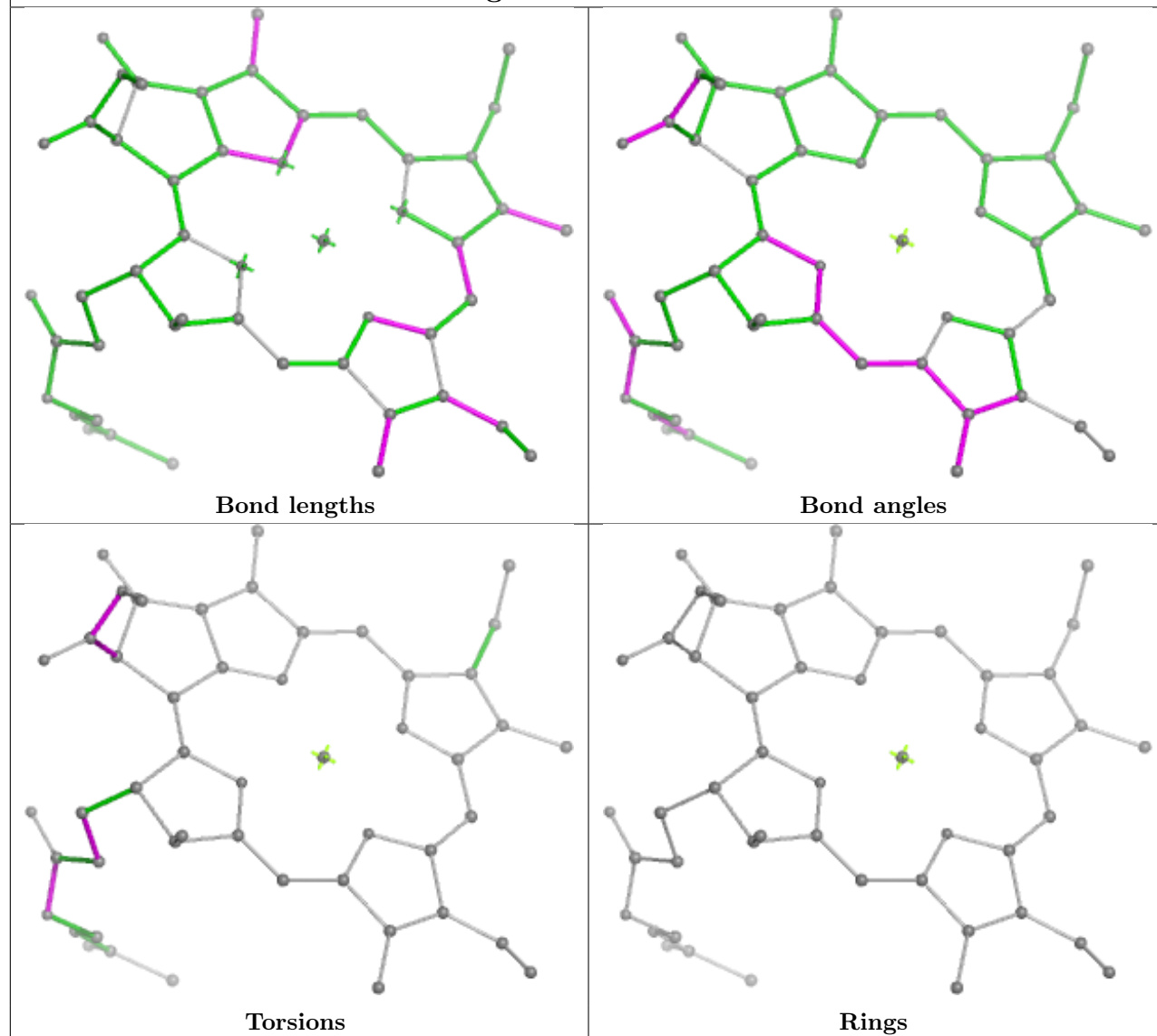
Rings

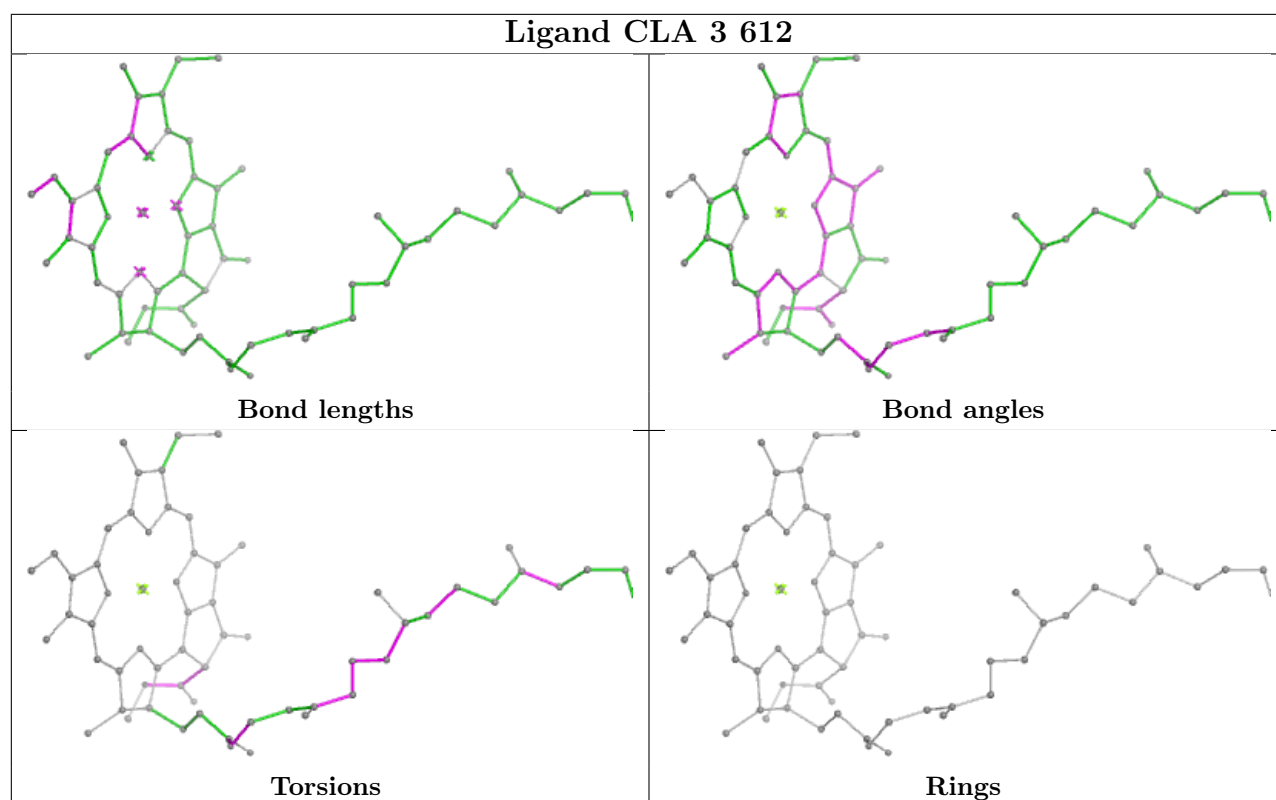


Ligand CLA A 1116**Bond lengths****Bond angles****Torsions****Rings****Ligand BCR 3 506****Bond lengths****Bond angles****Torsions****Rings**

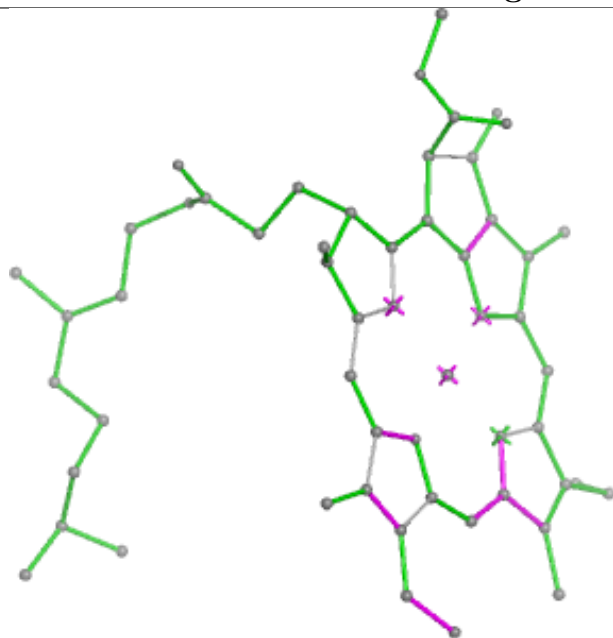


Ligand CLA 4 606

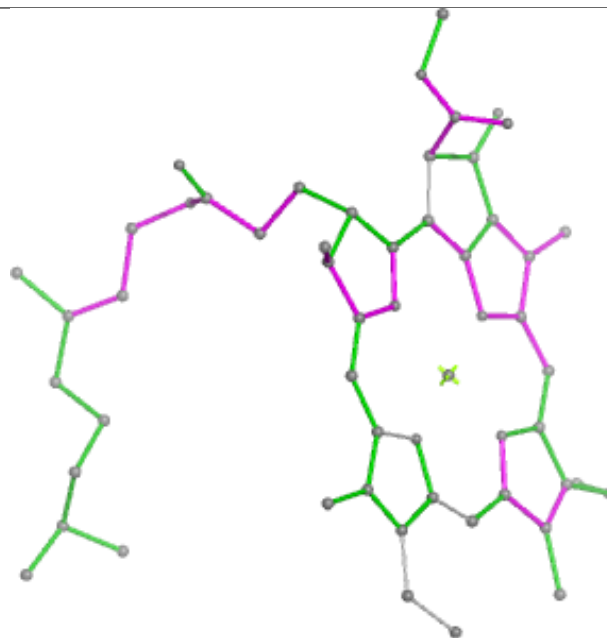




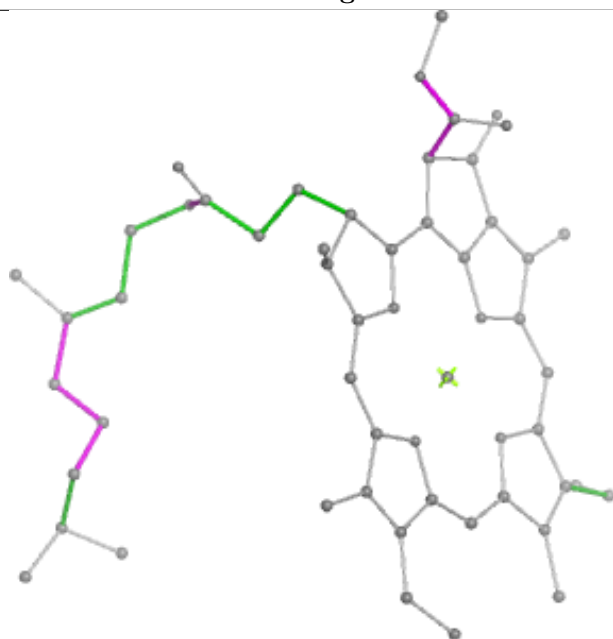
Ligand CLA A 1114



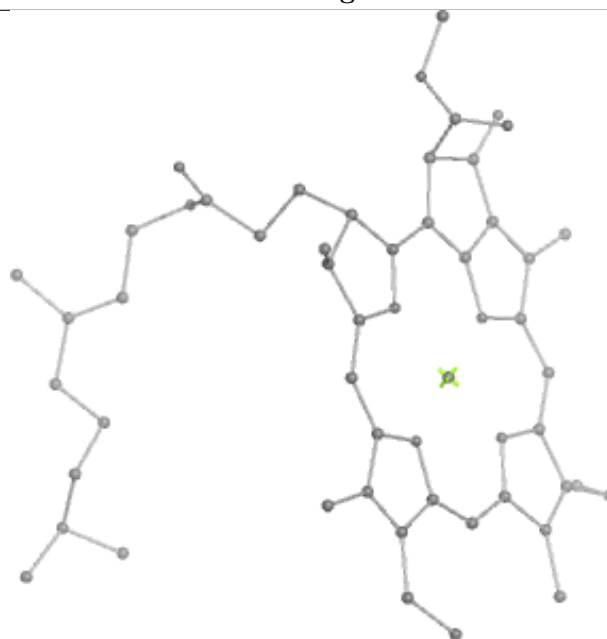
Bond lengths



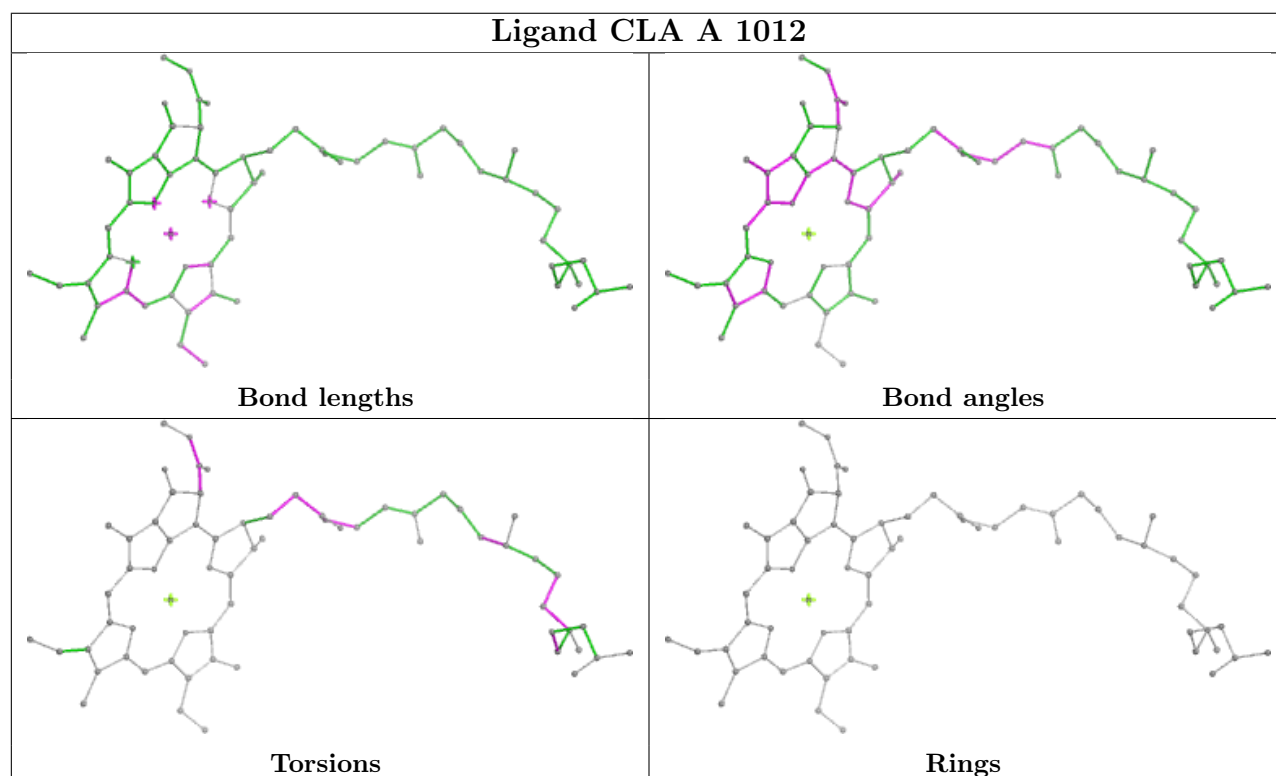
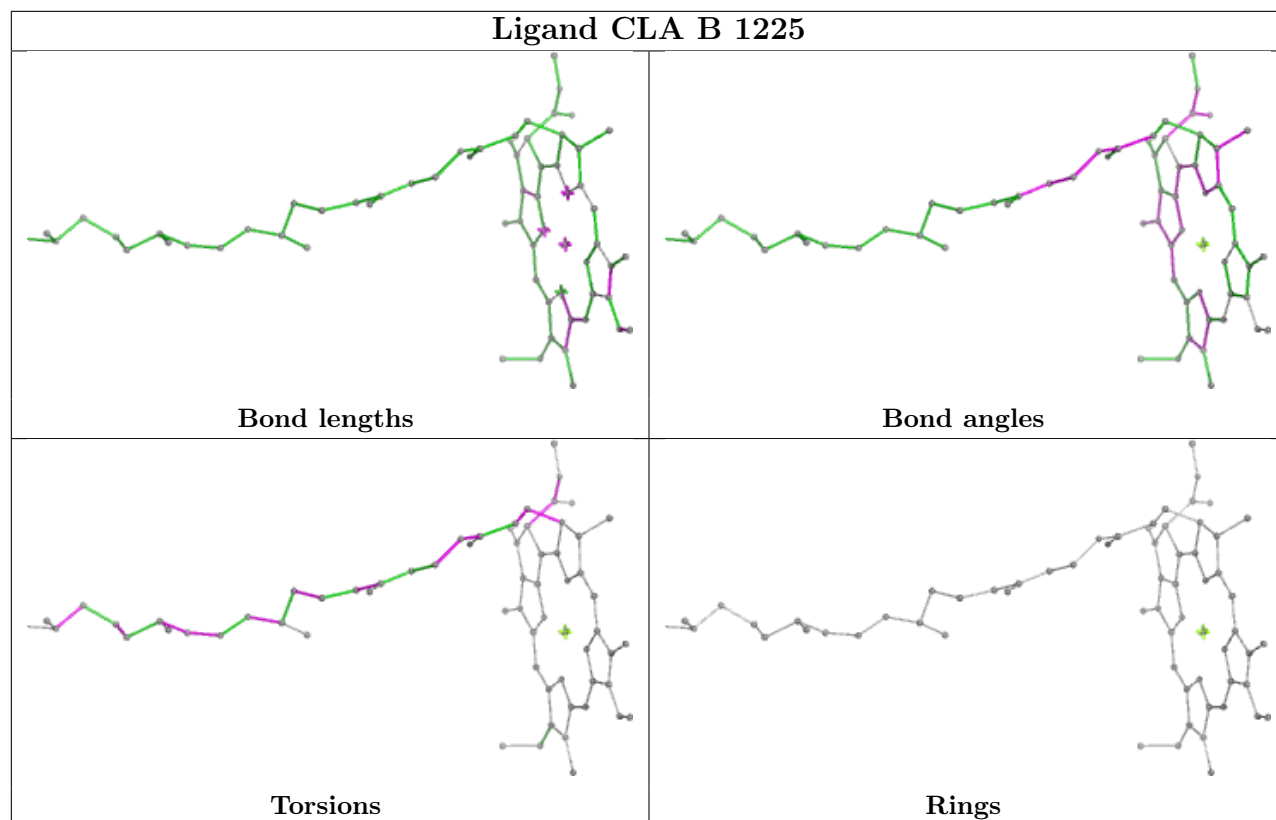
Bond angles

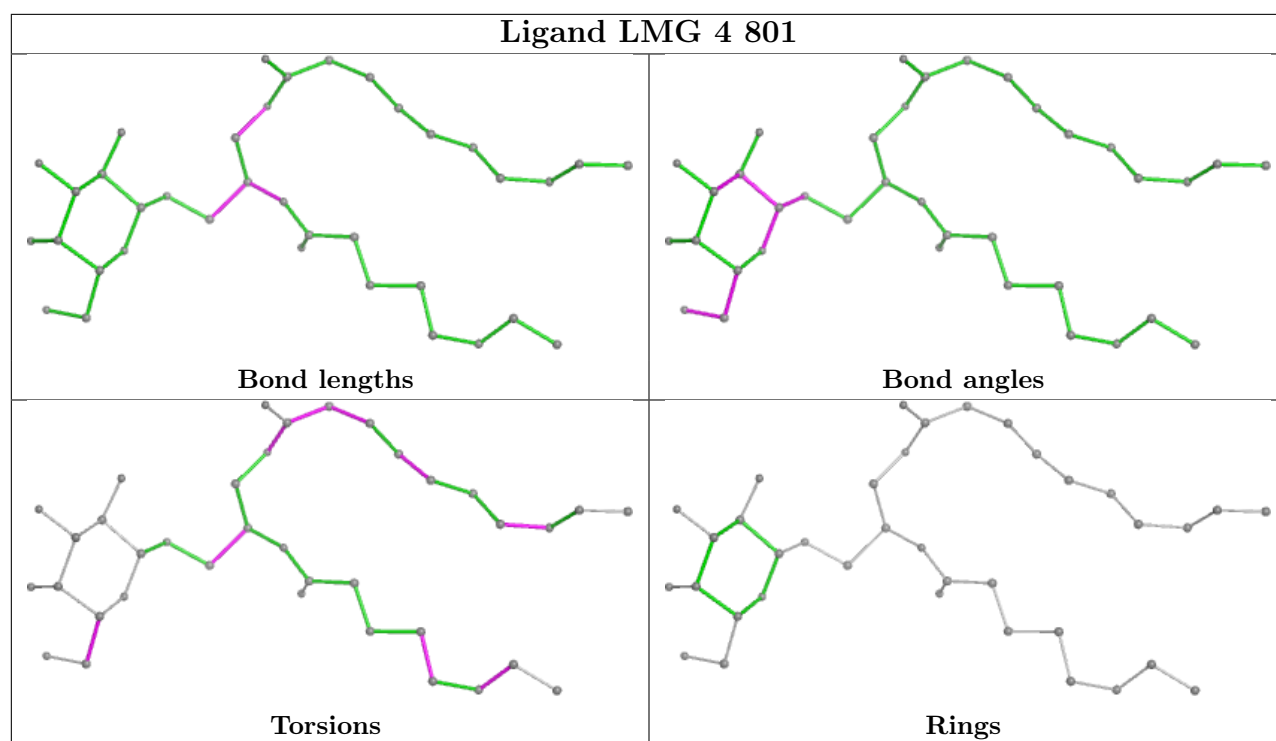


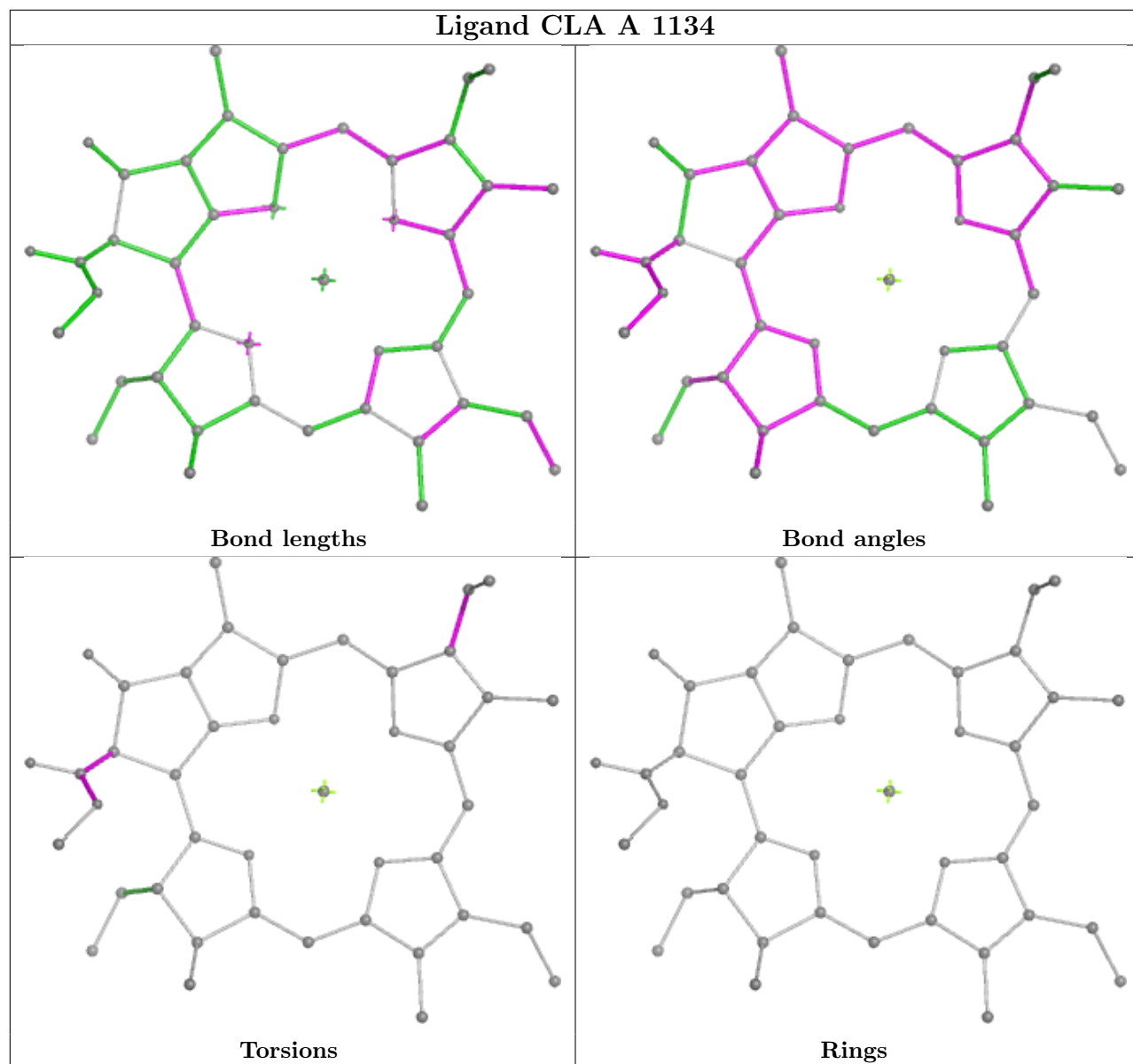
Torsions



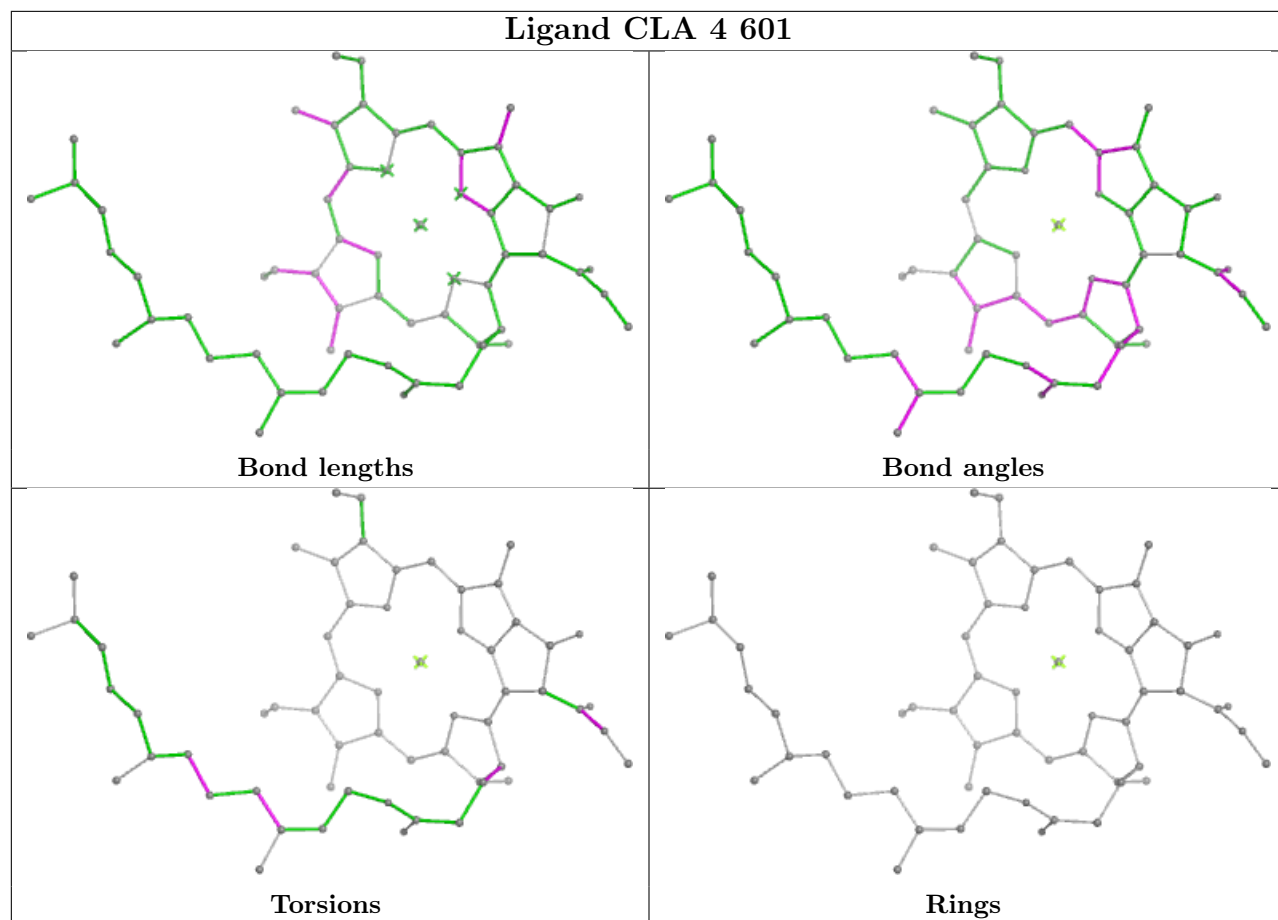
Rings



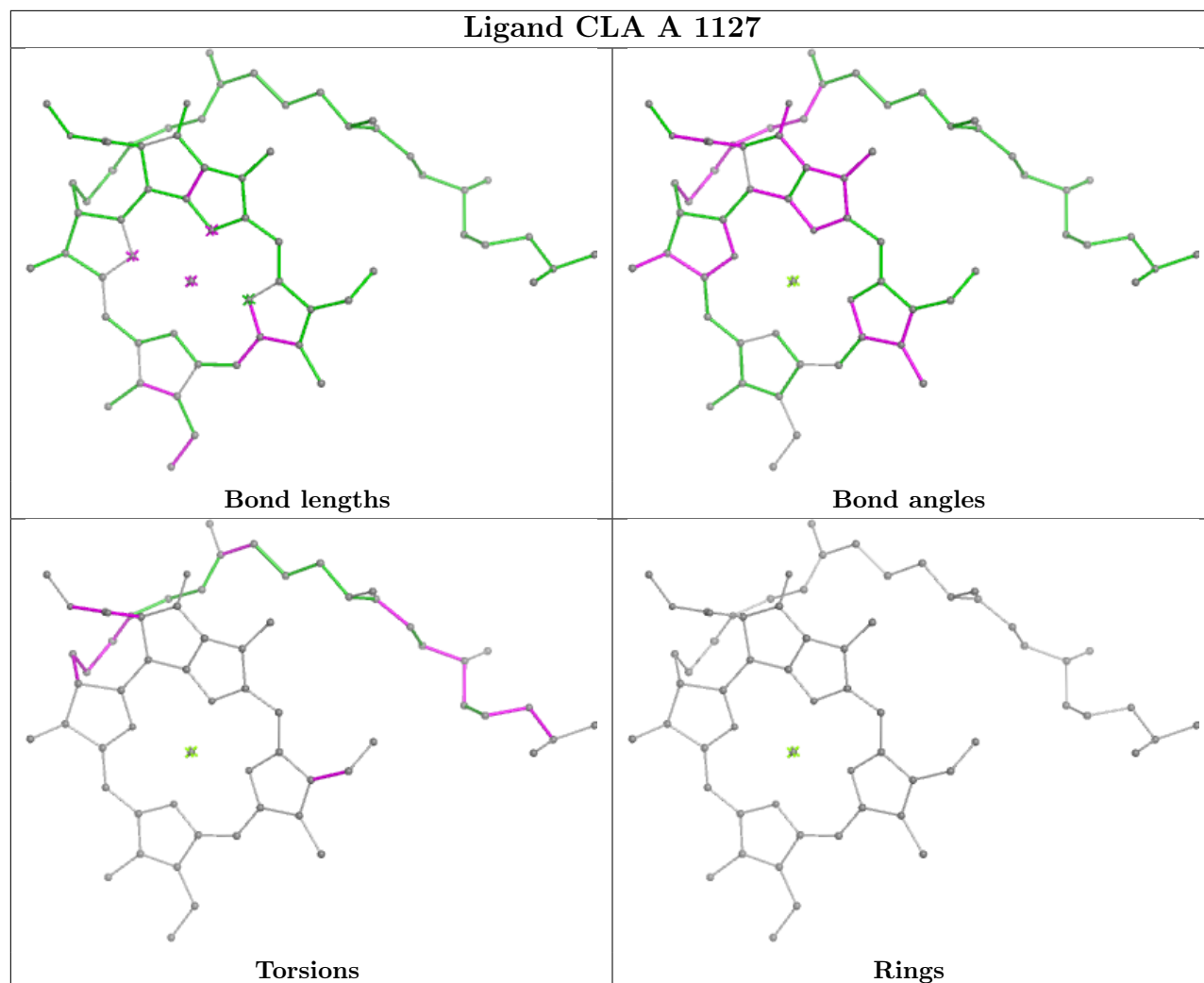


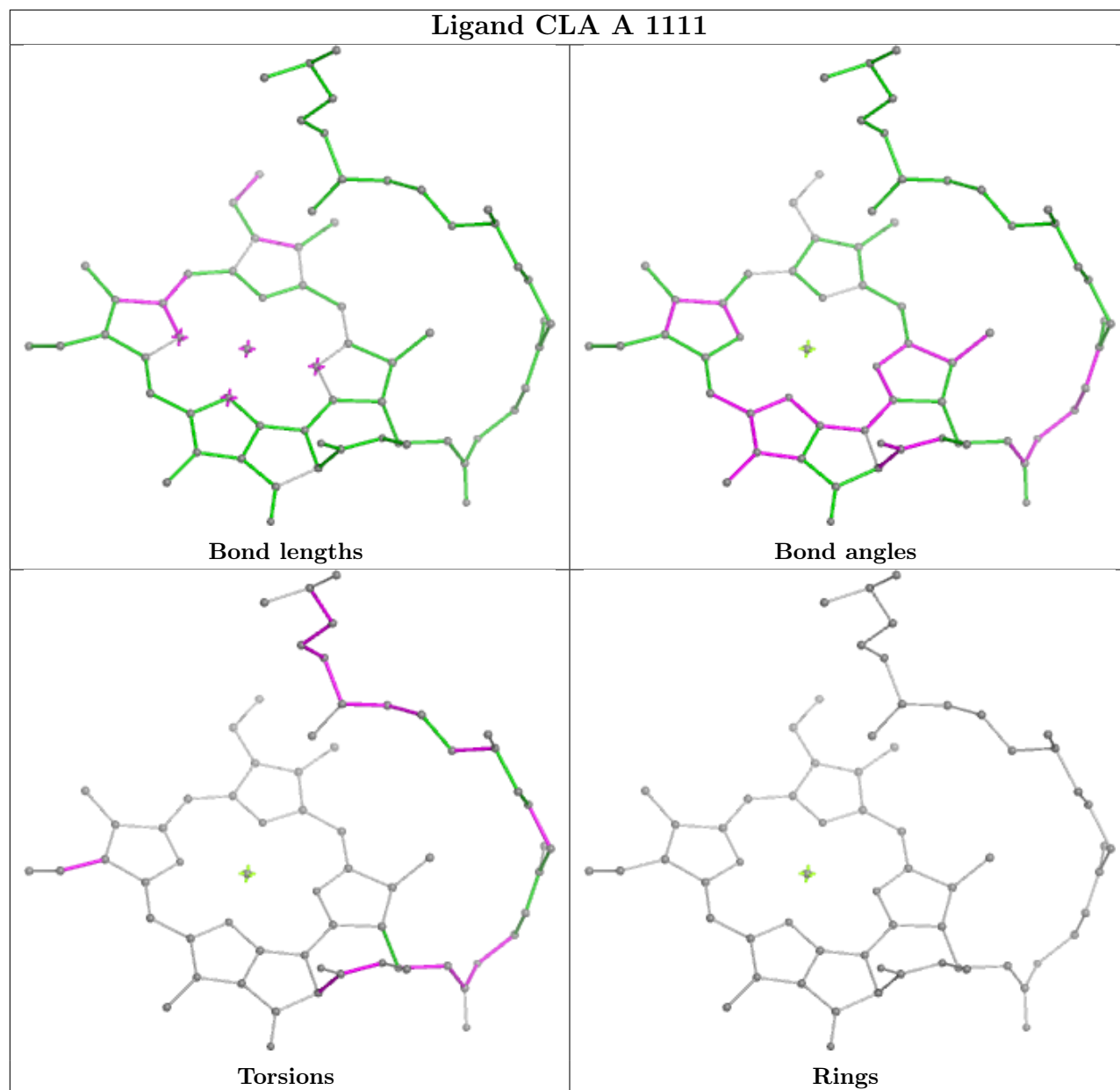


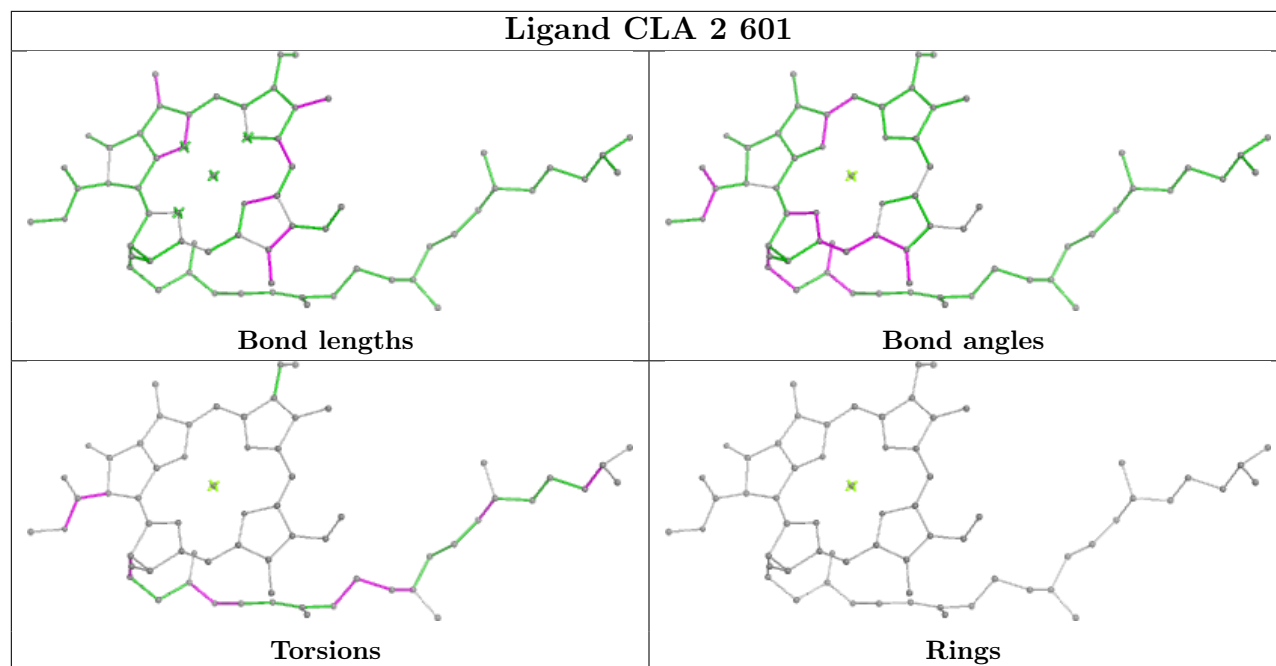
Ligand CLA 4 601



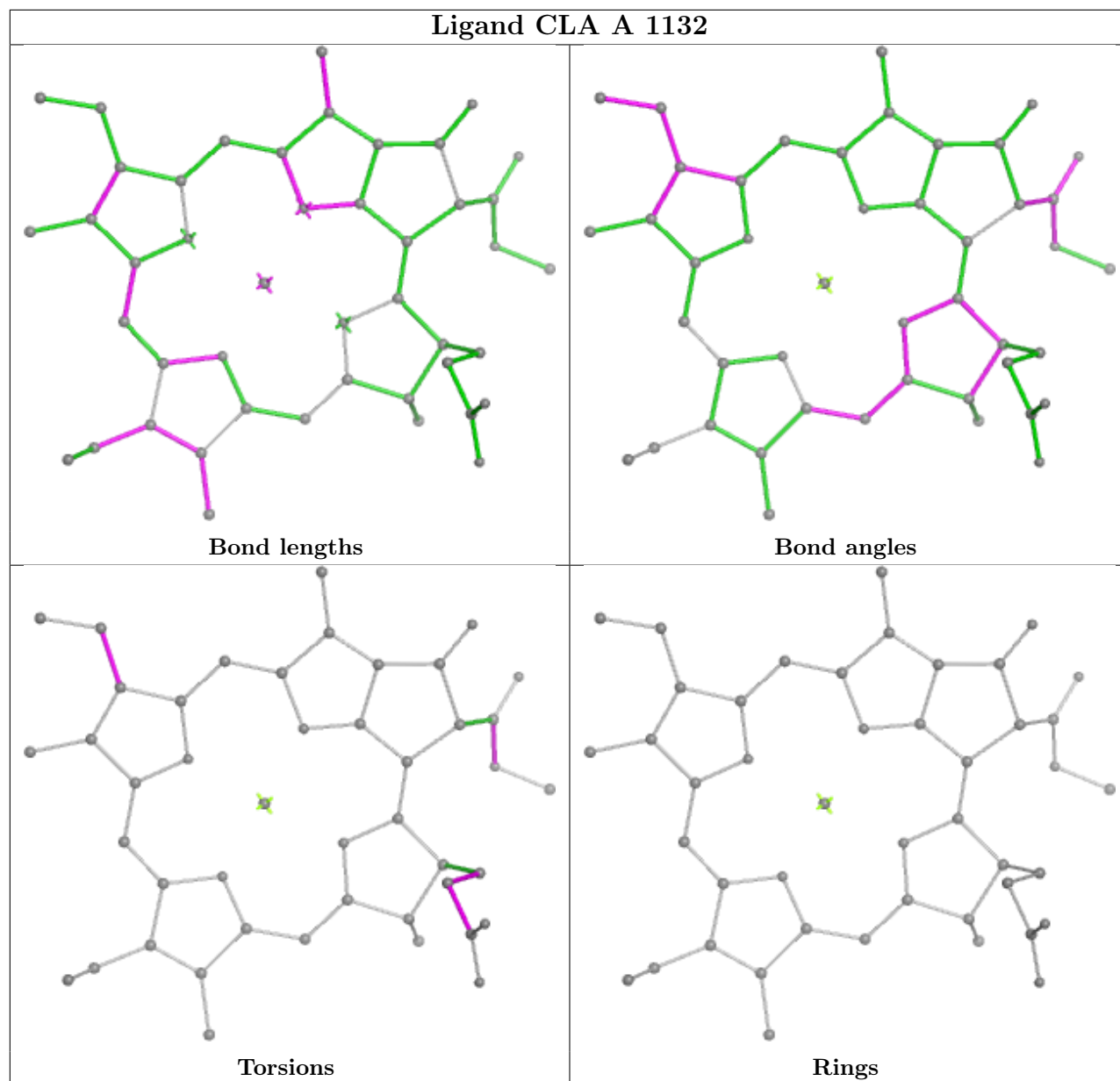
Ligand CLA A 1127

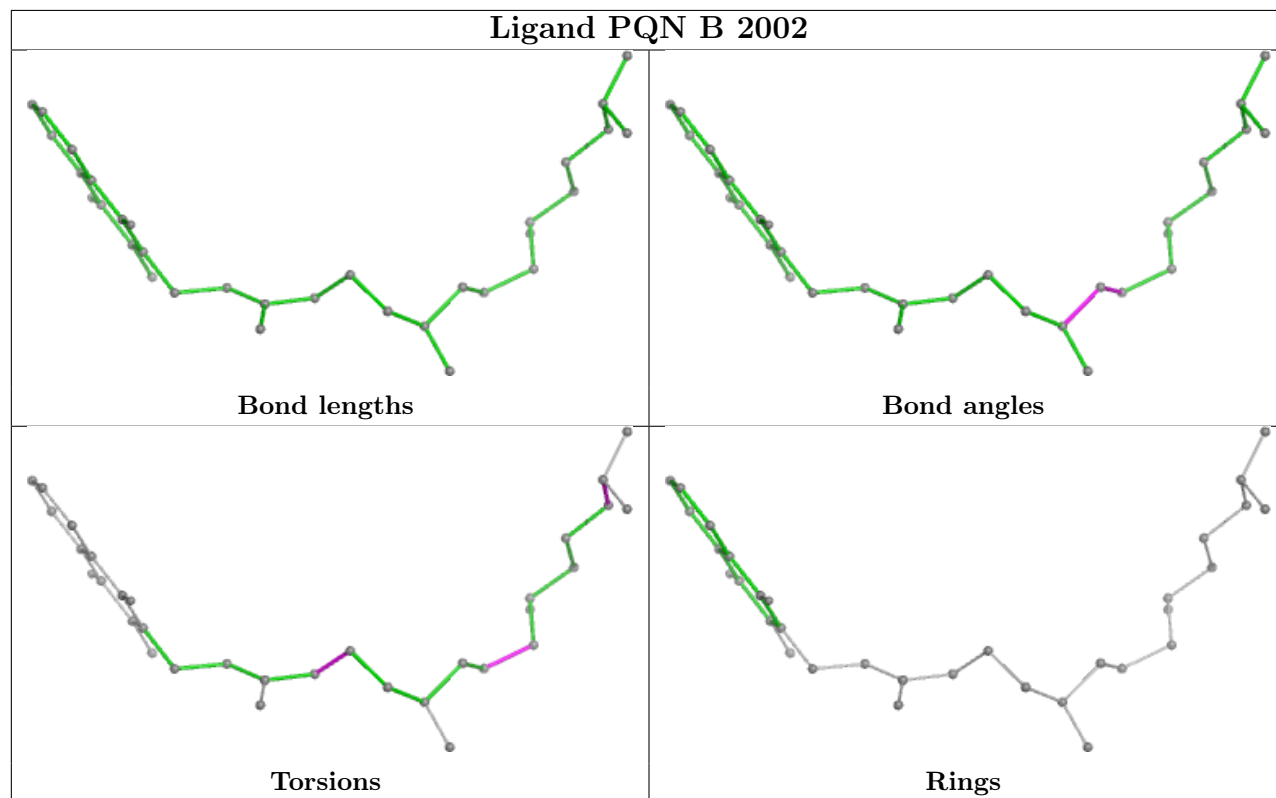
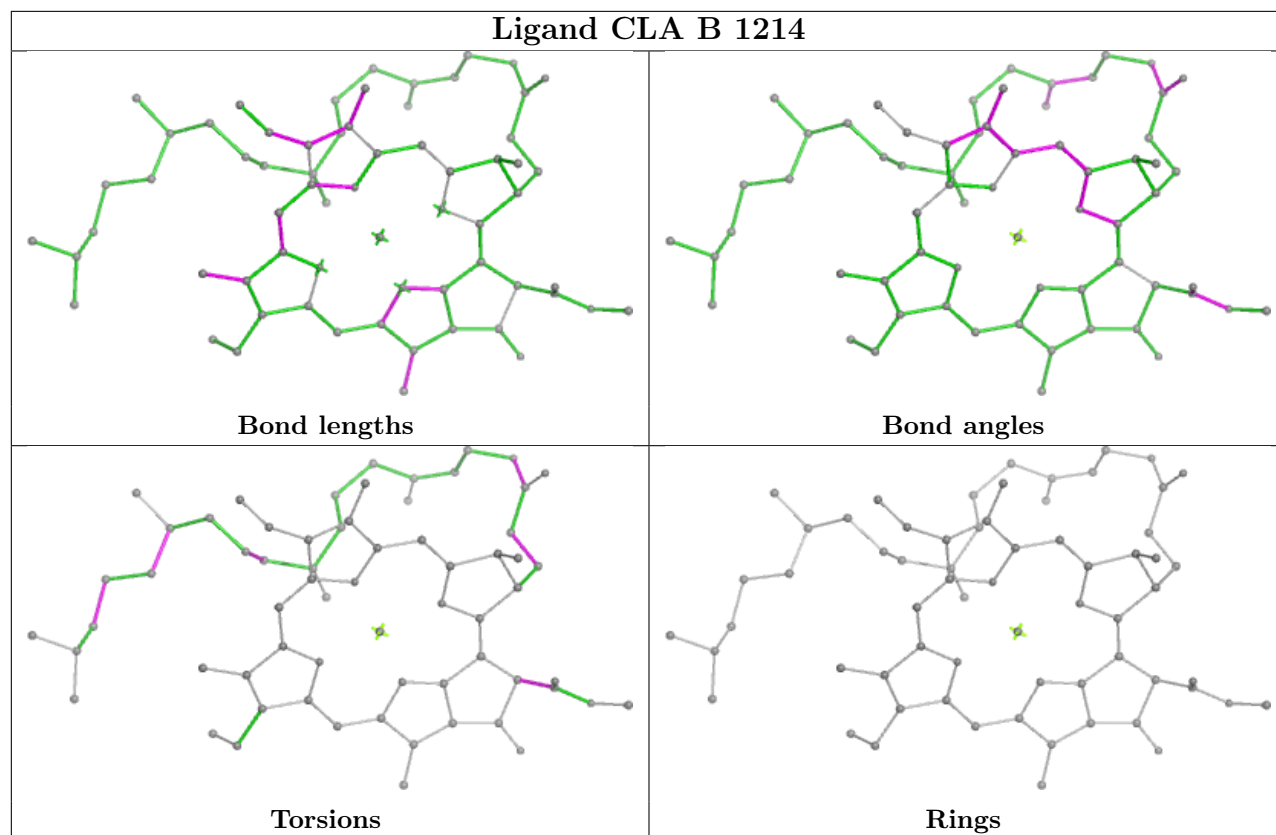


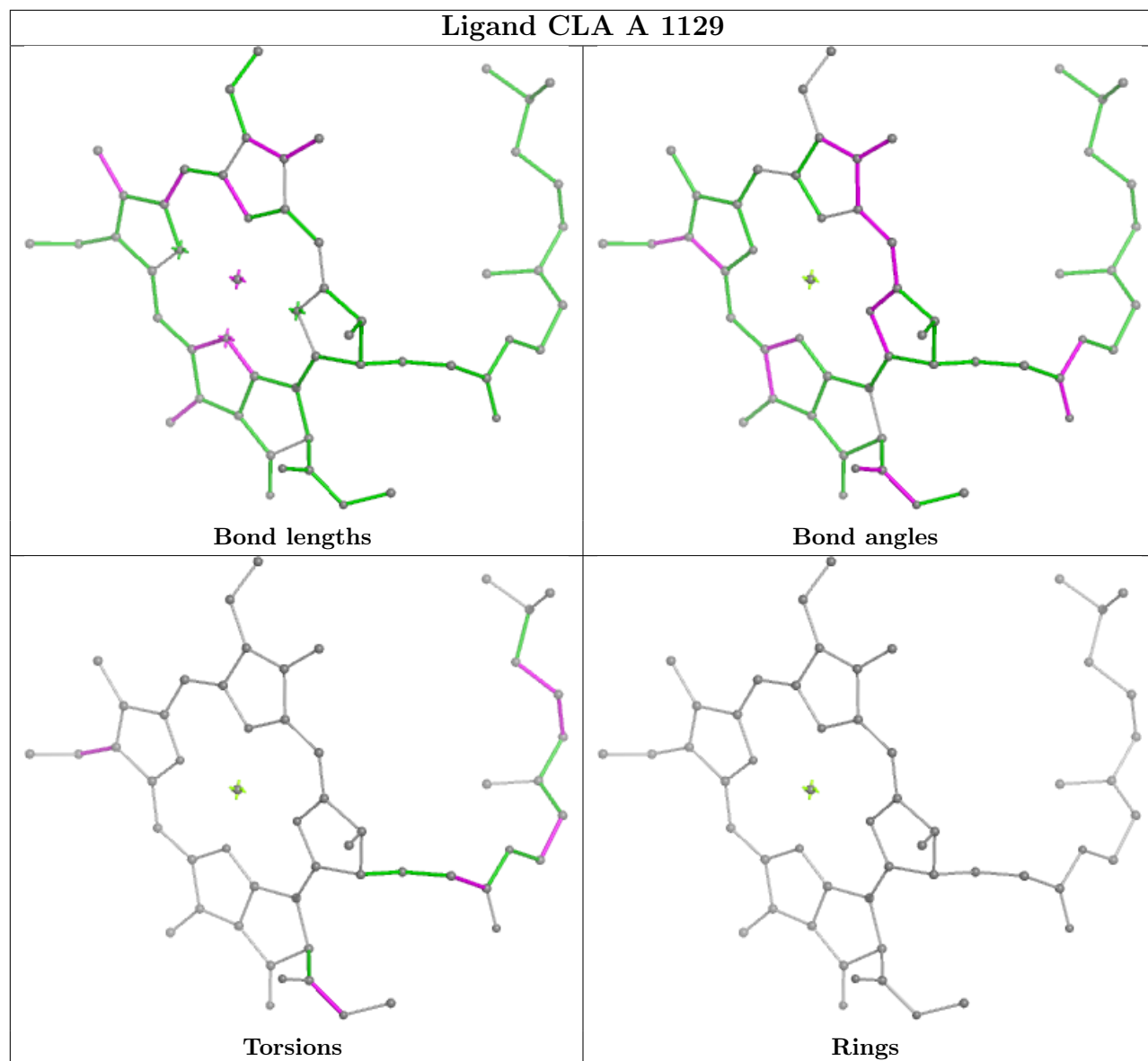




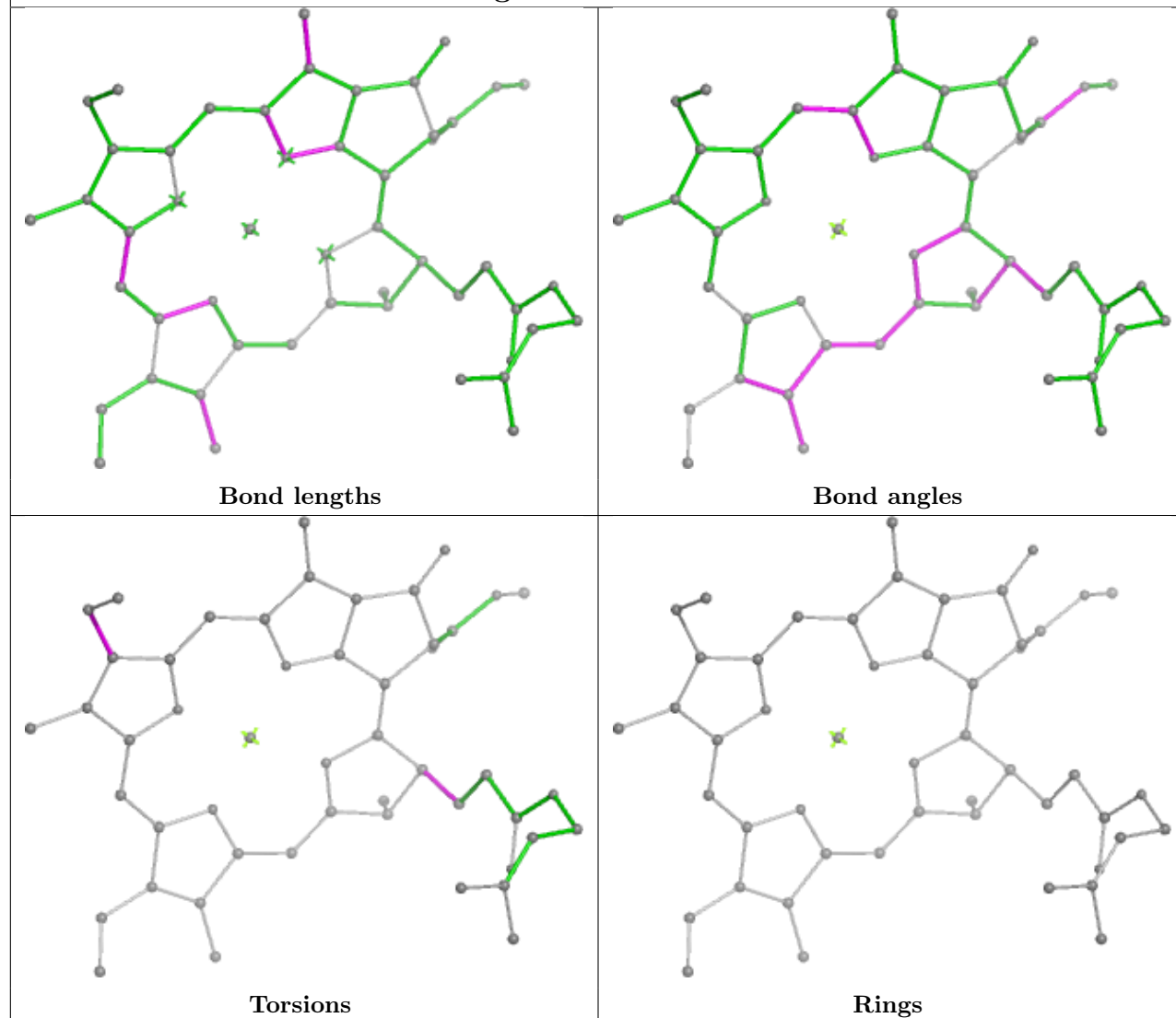
Ligand CLA A 1132



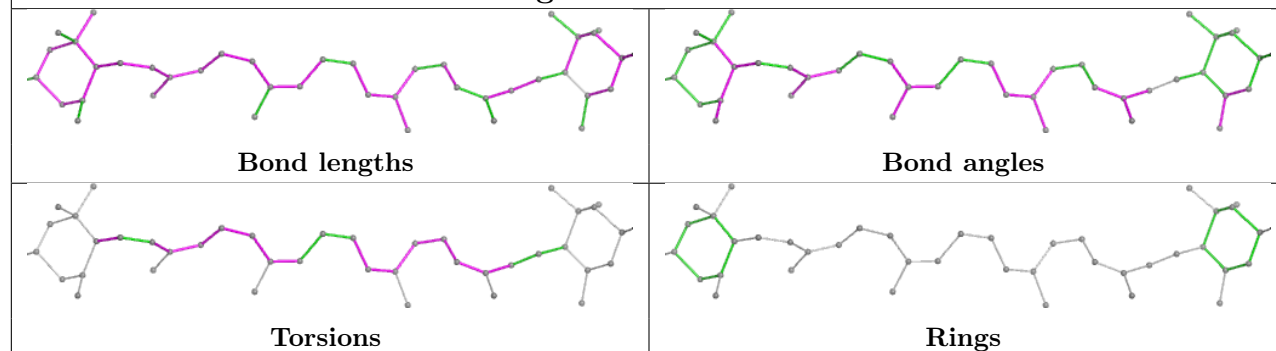


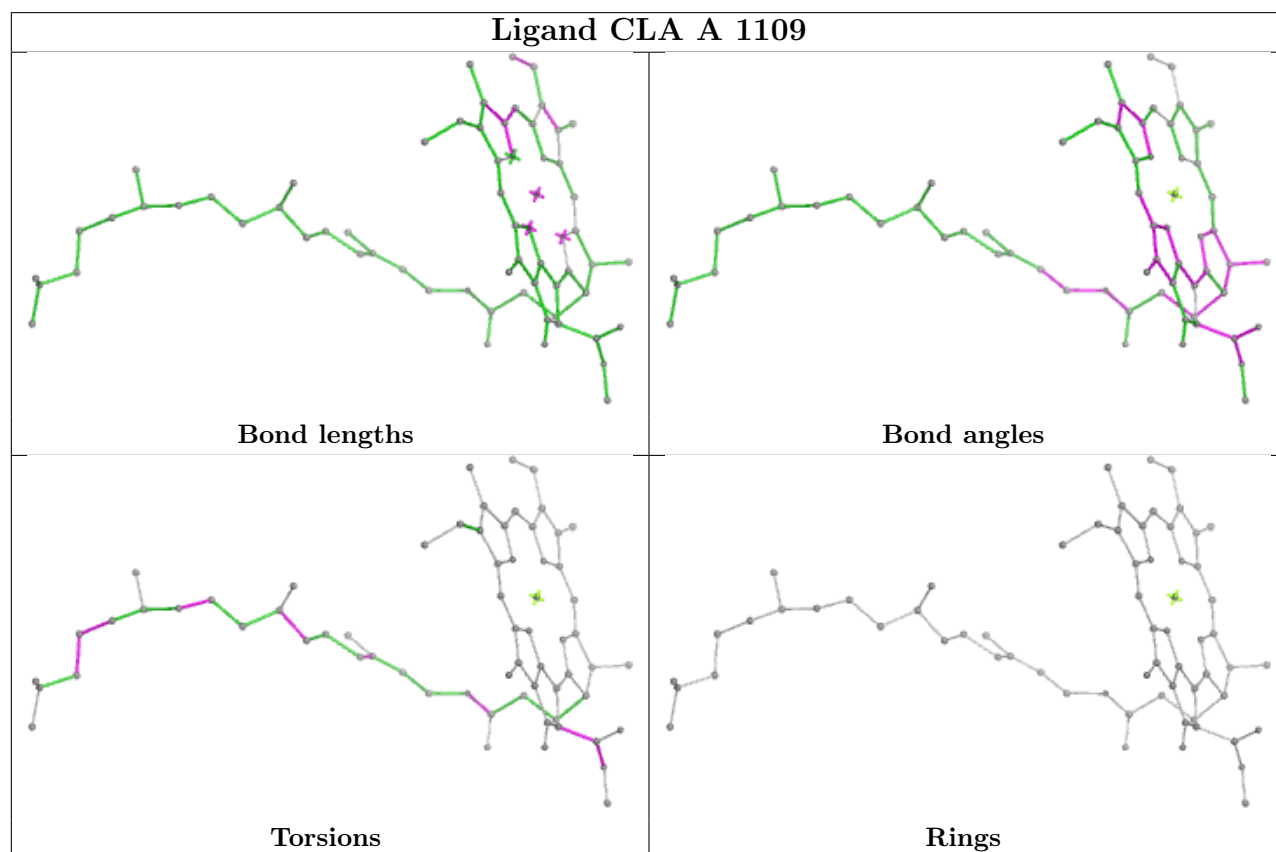
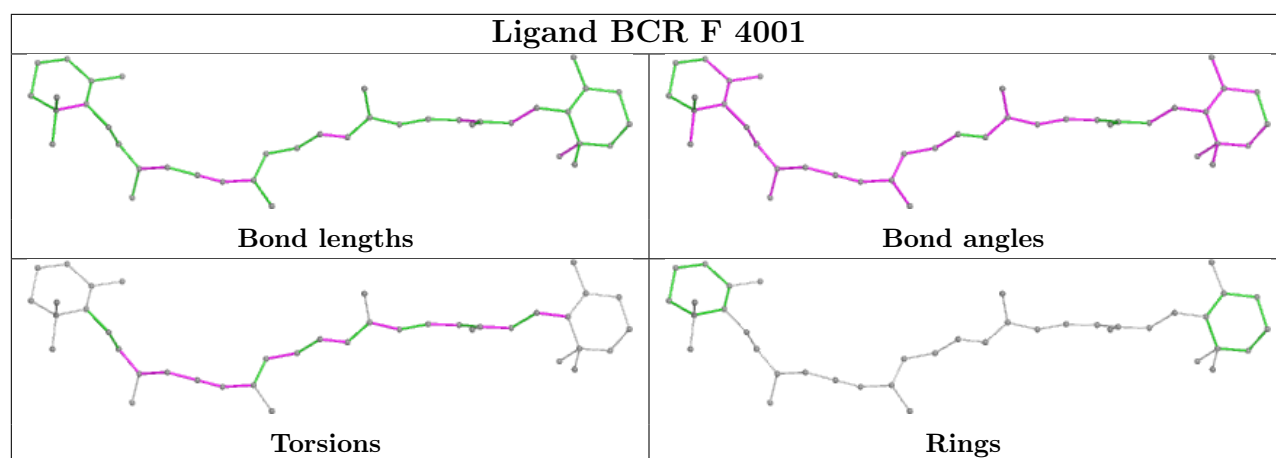


Ligand CLA 2 608

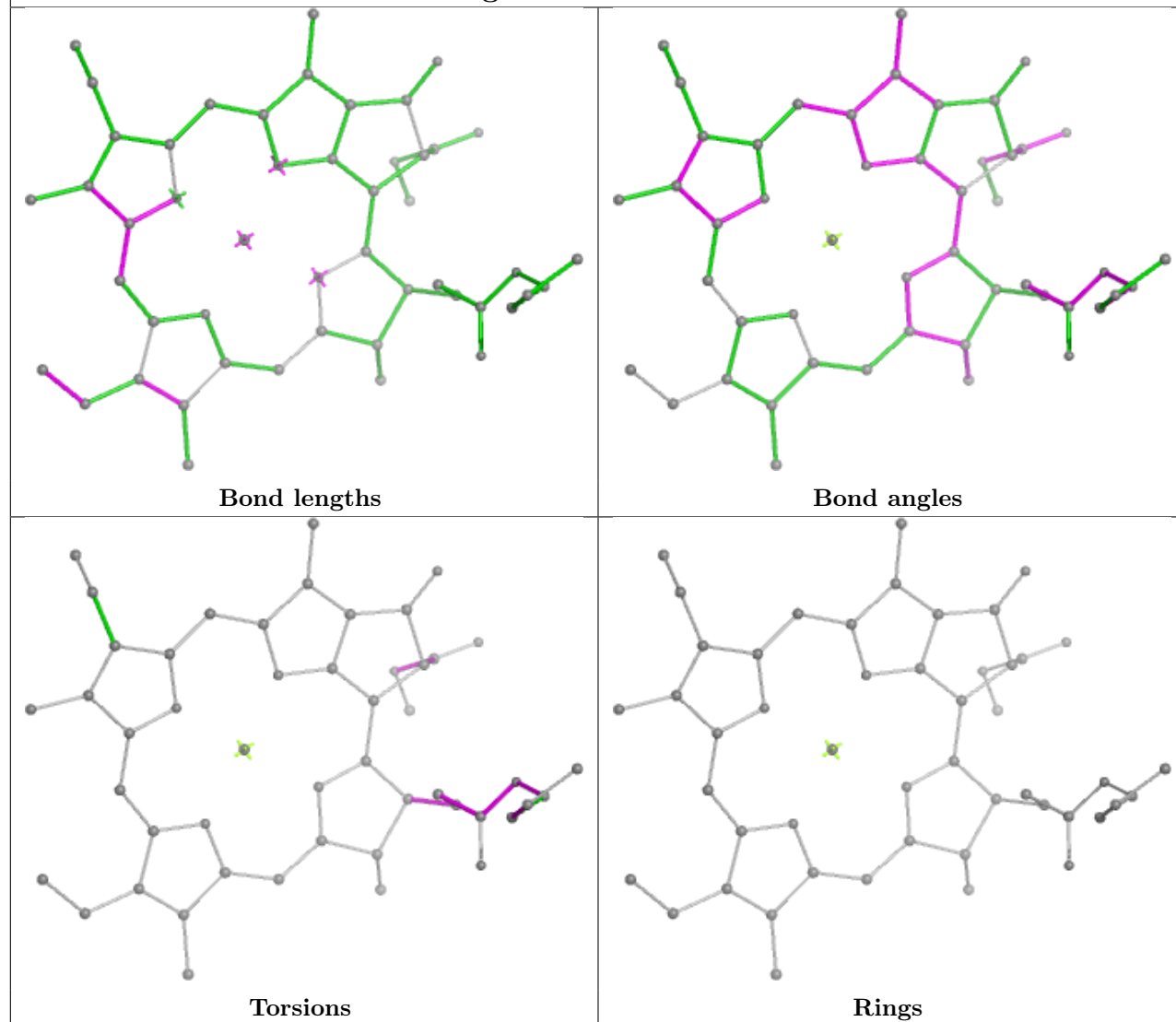


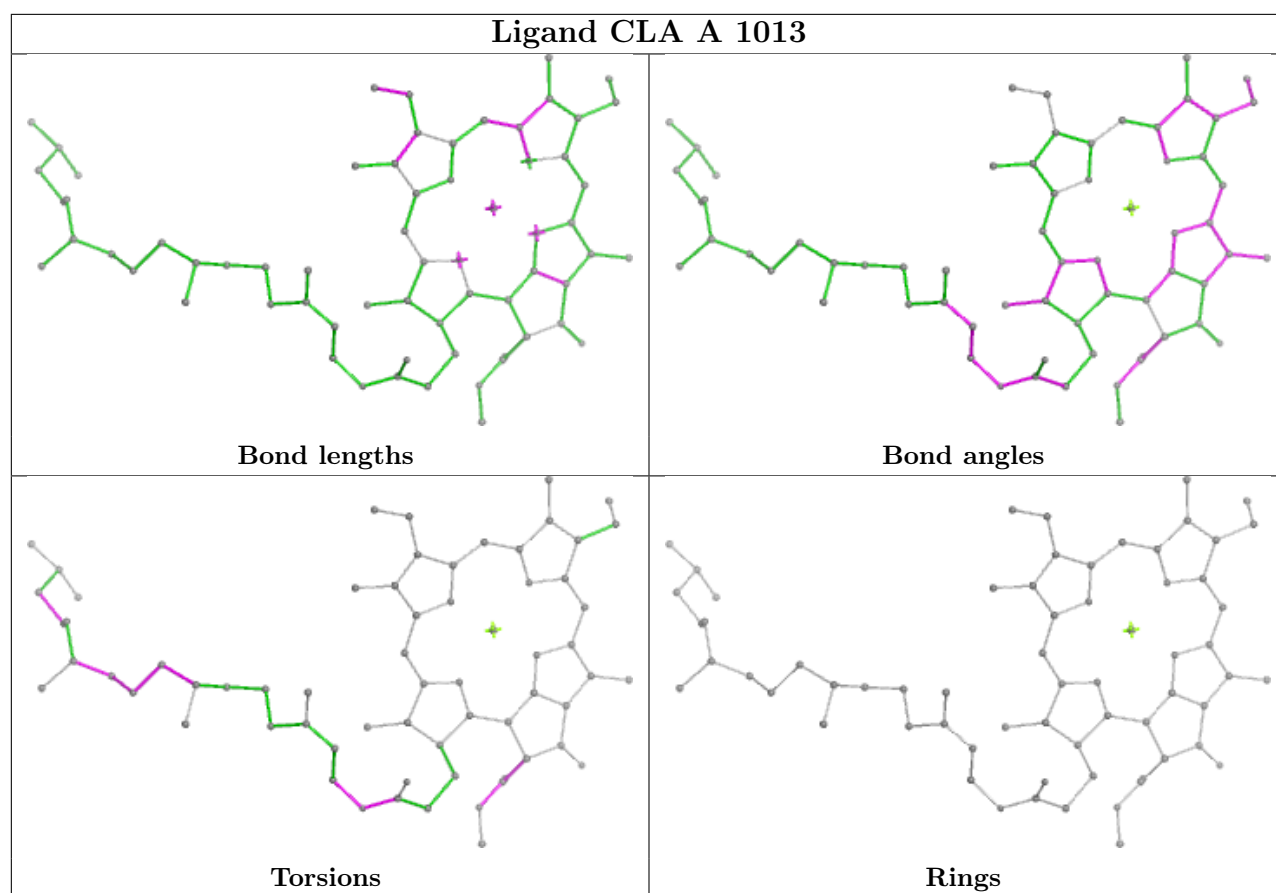
Ligand LUT 1 501



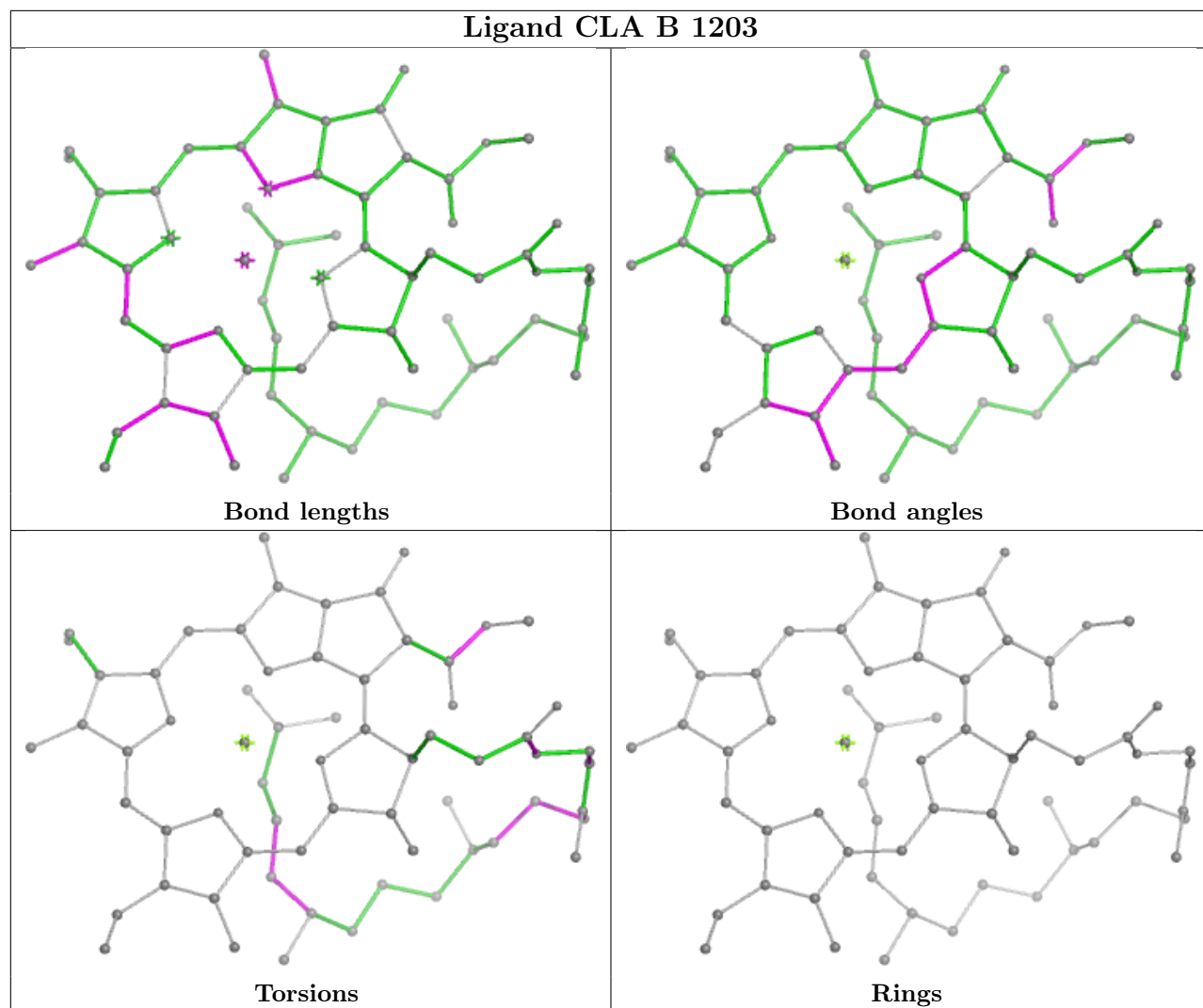


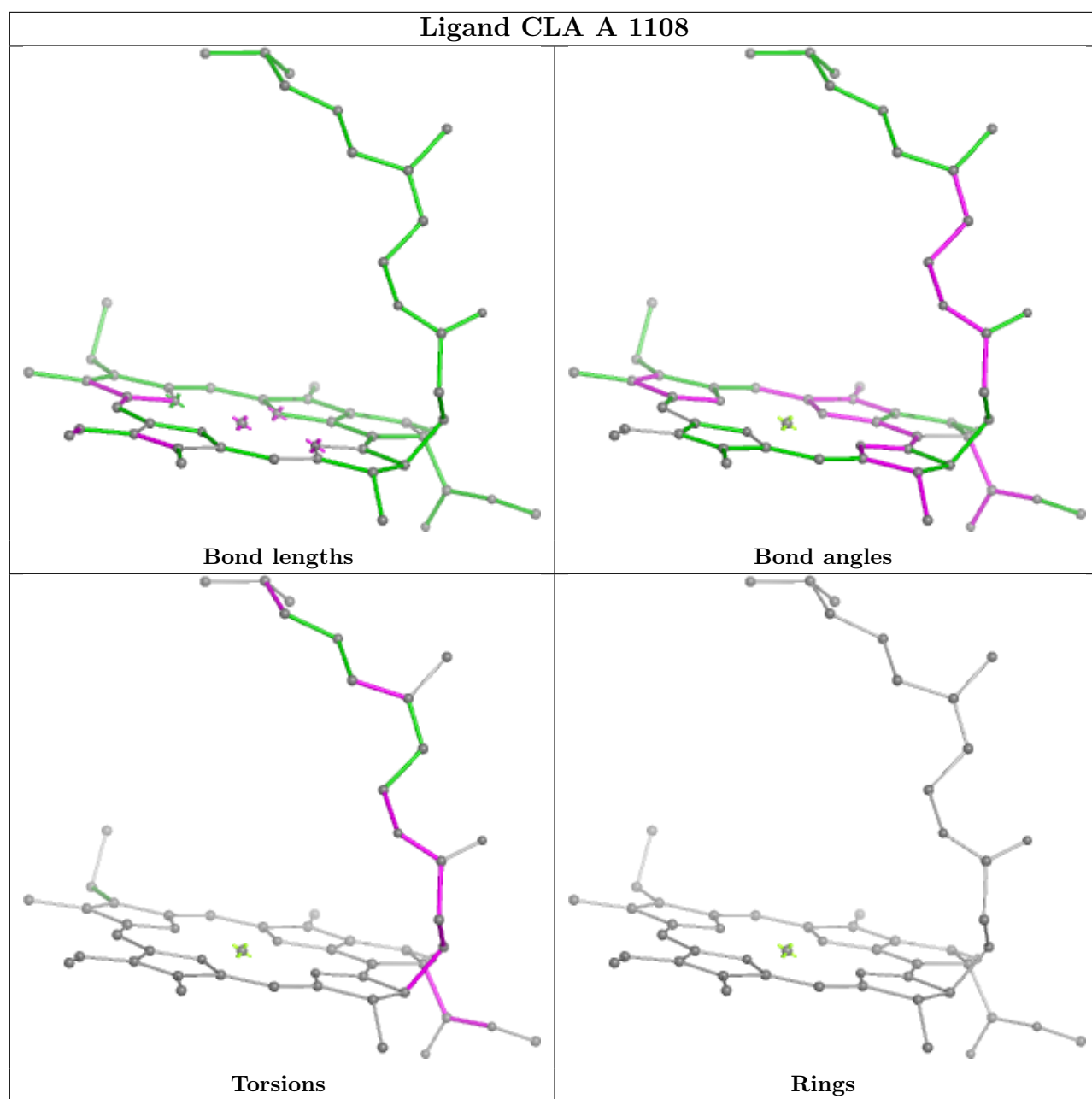
Ligand CLA B 1236



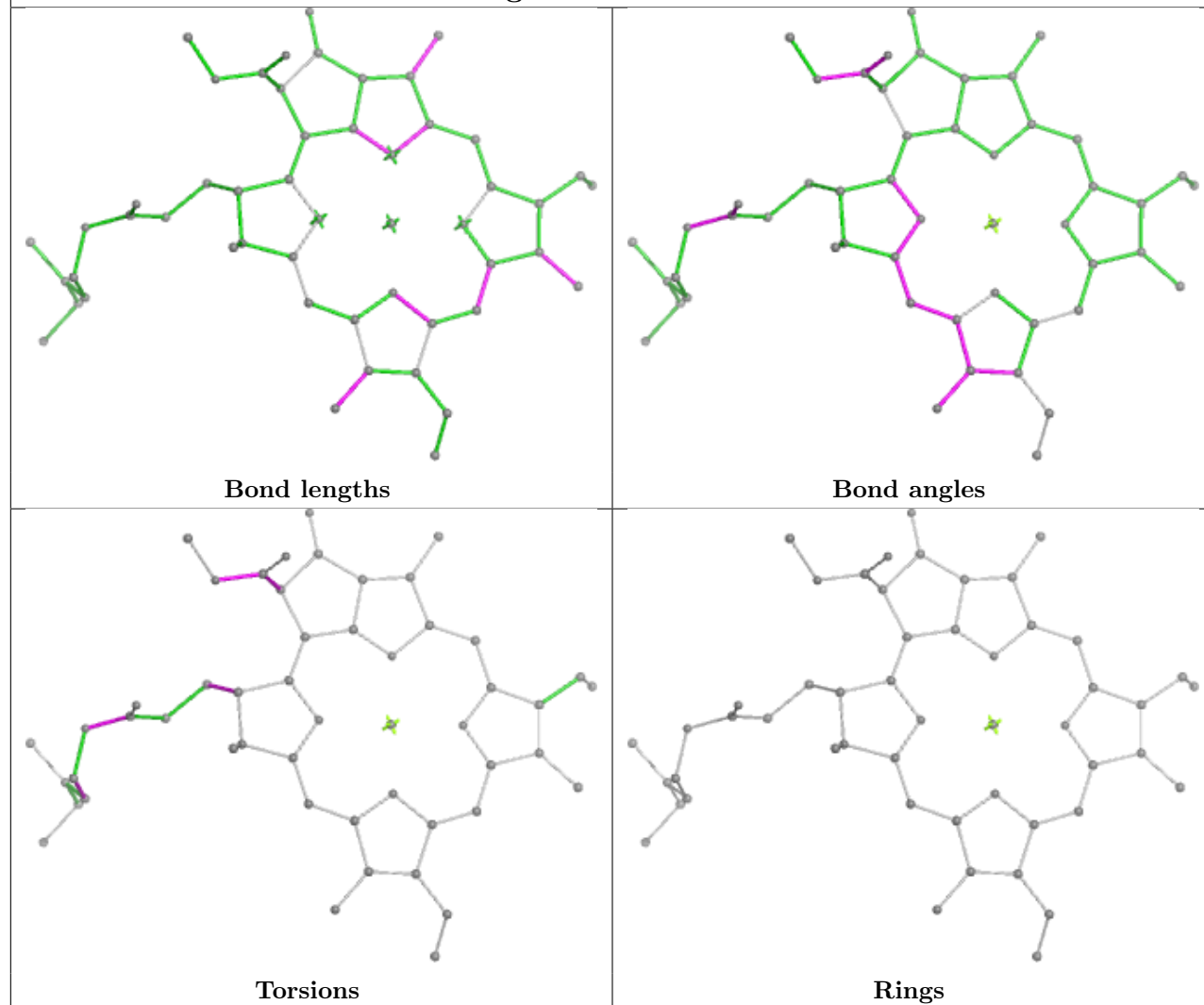


Ligand CLA B 1203

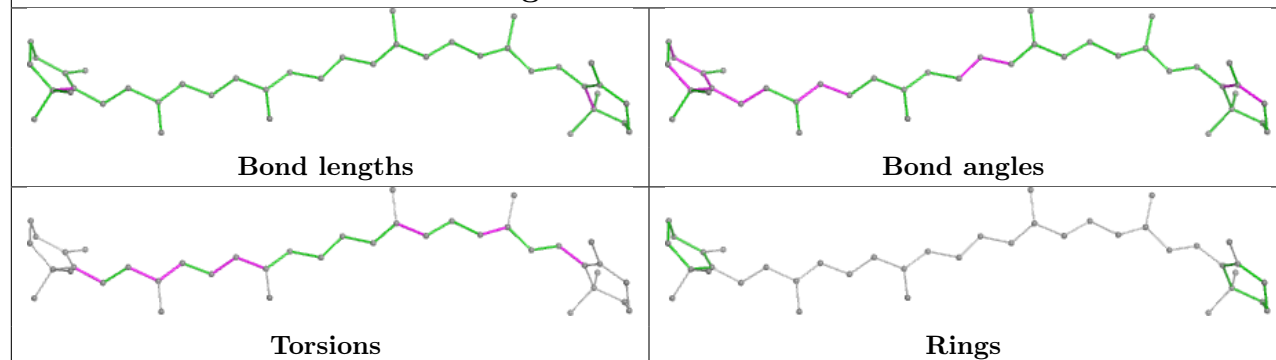


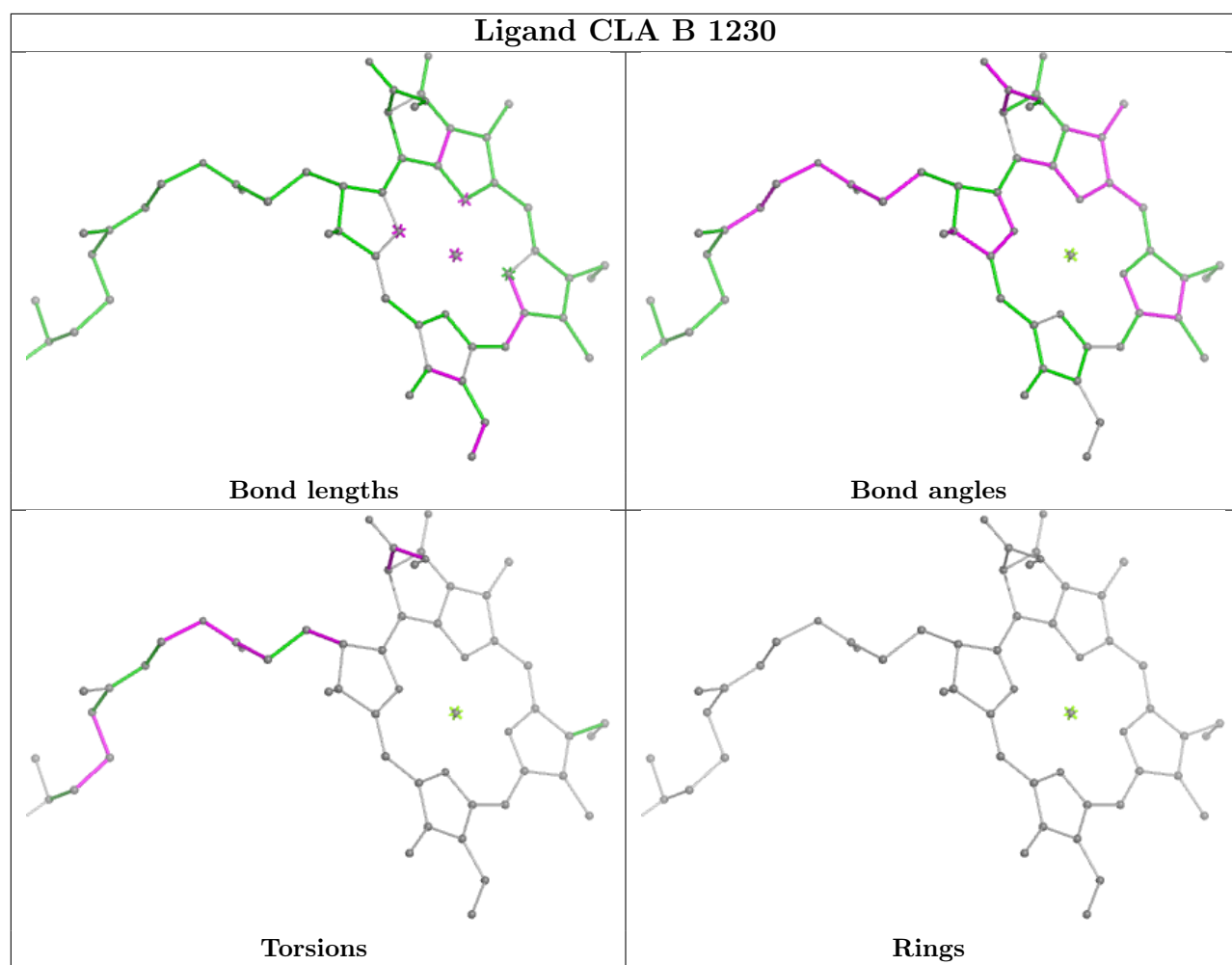


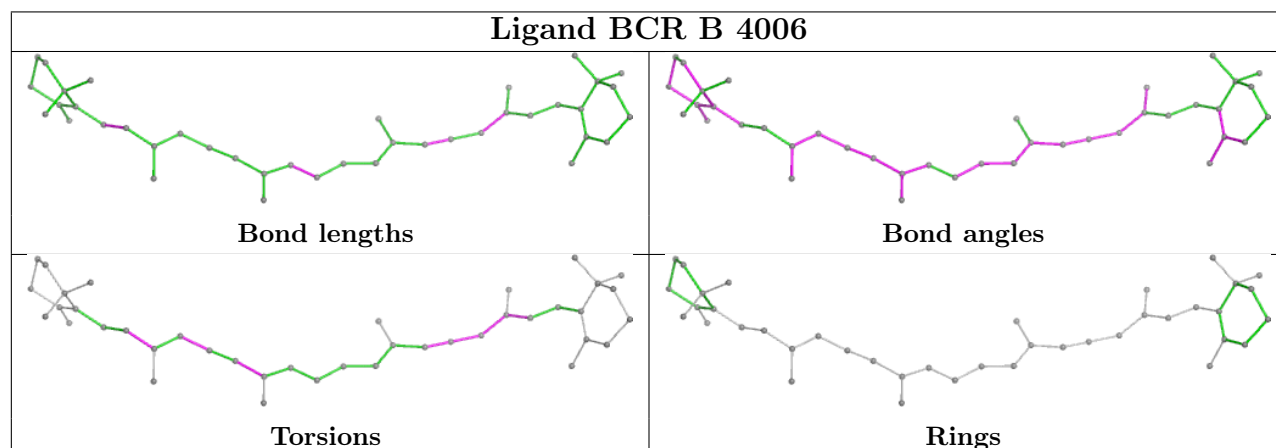
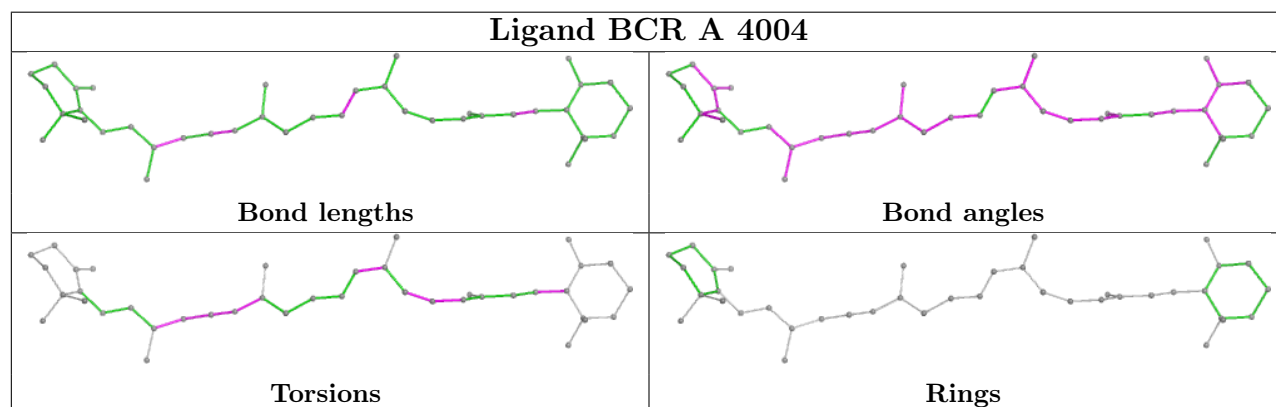
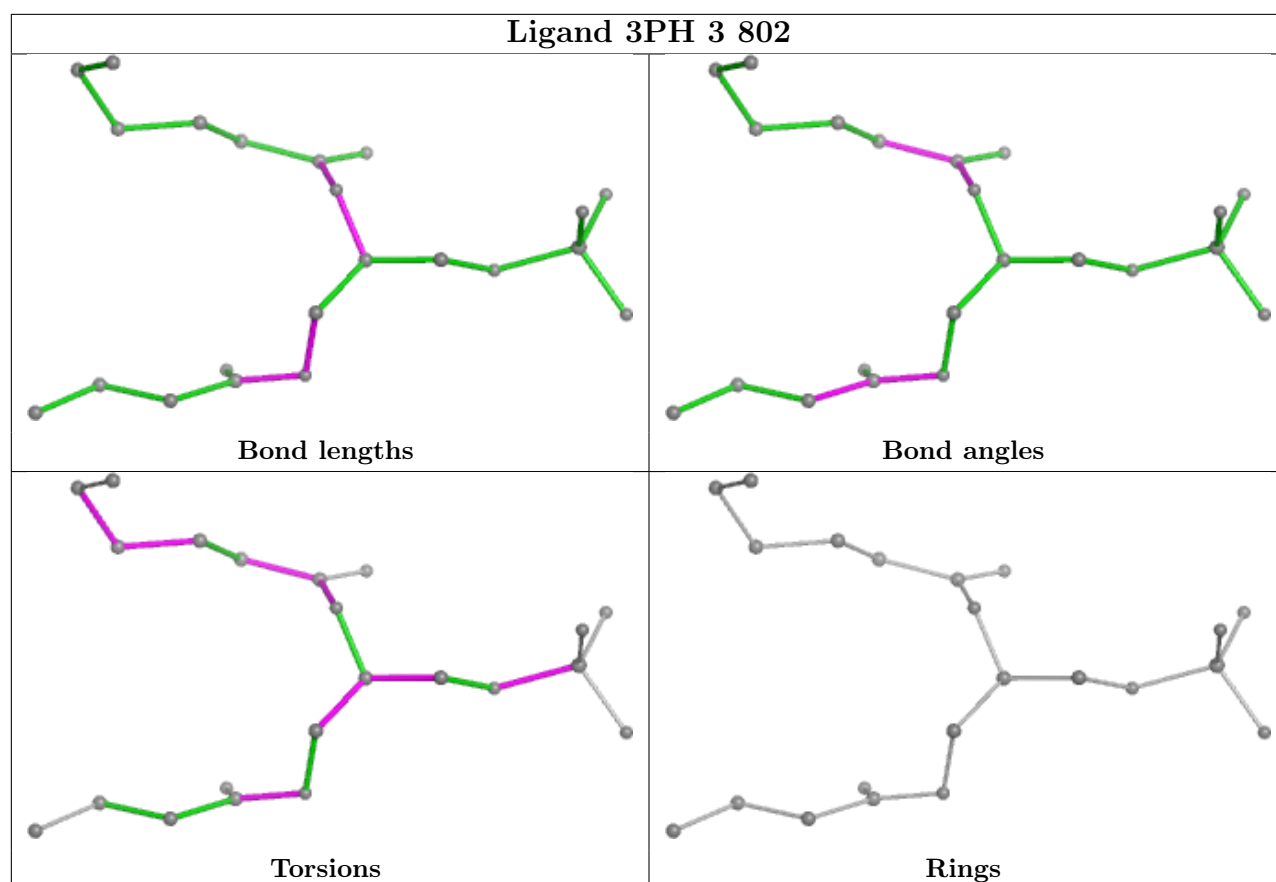
Ligand CLA 4 616

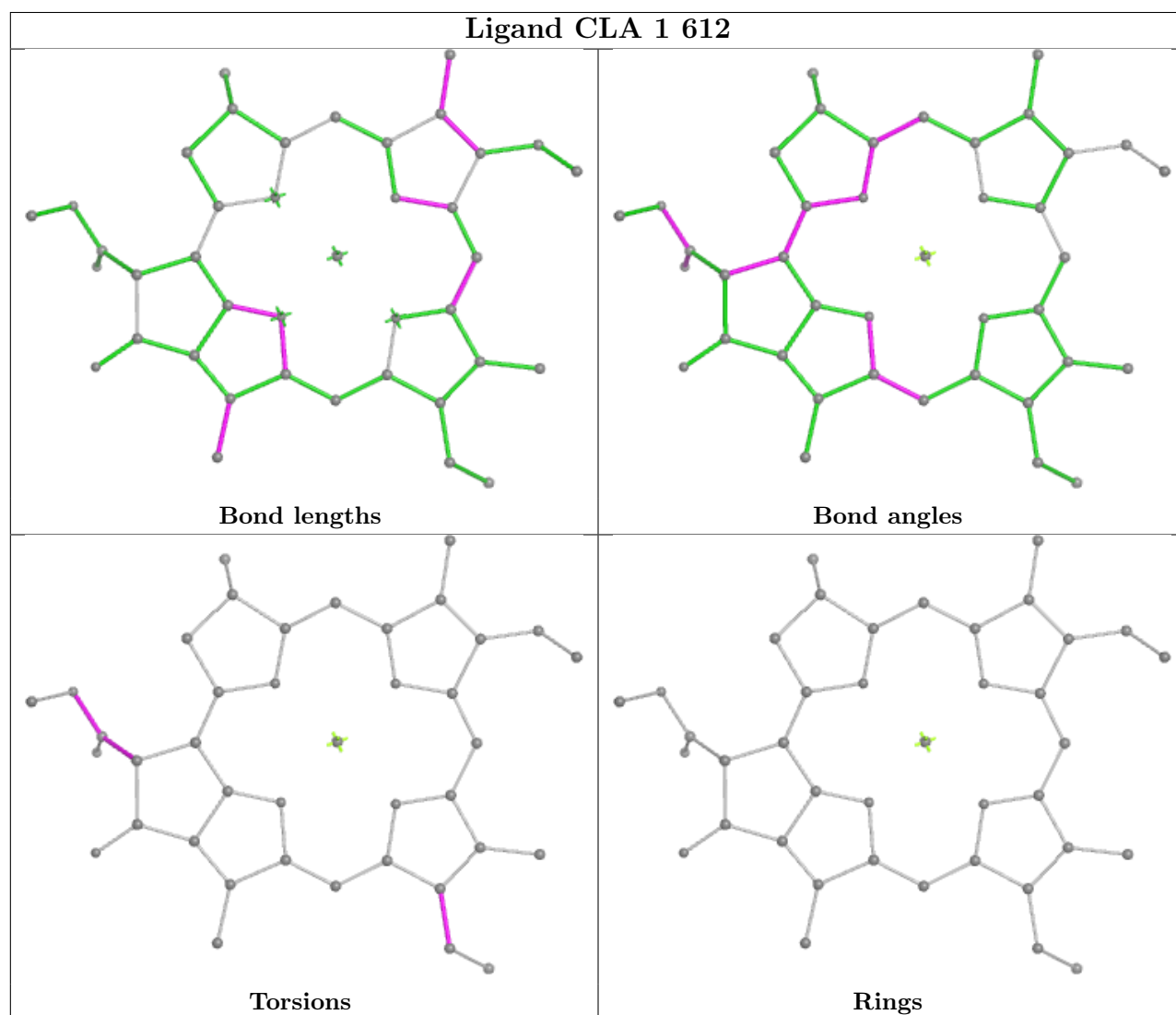
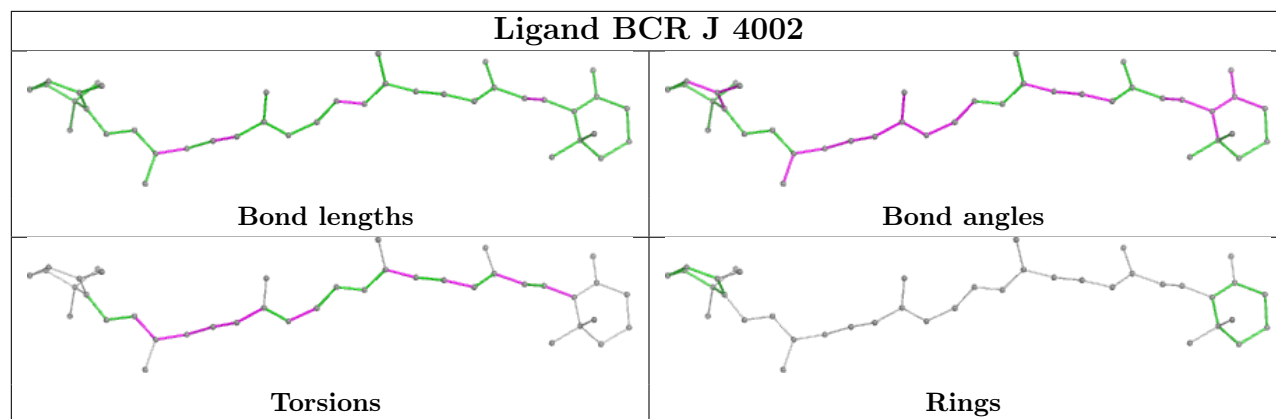


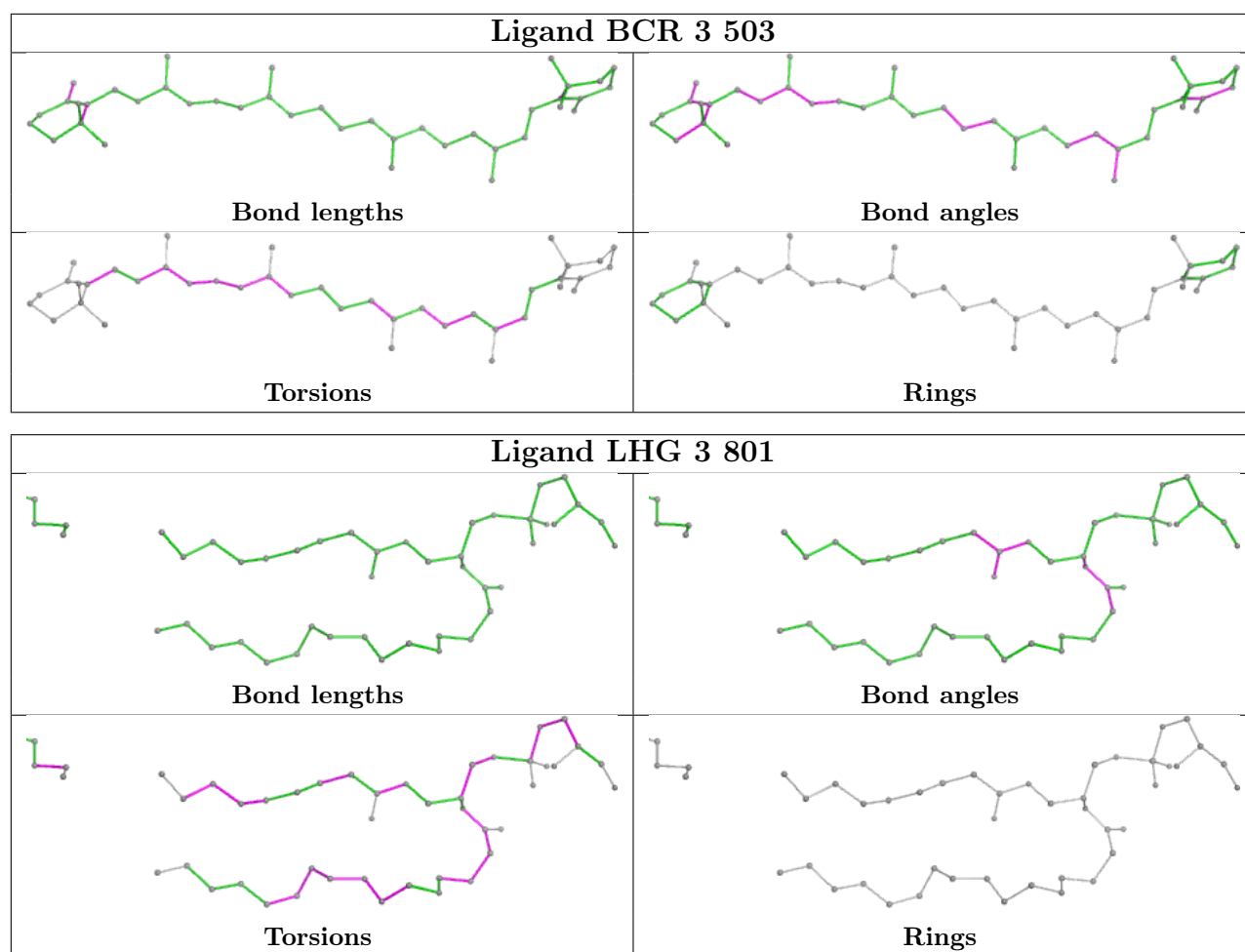
Ligand BCR B 4004

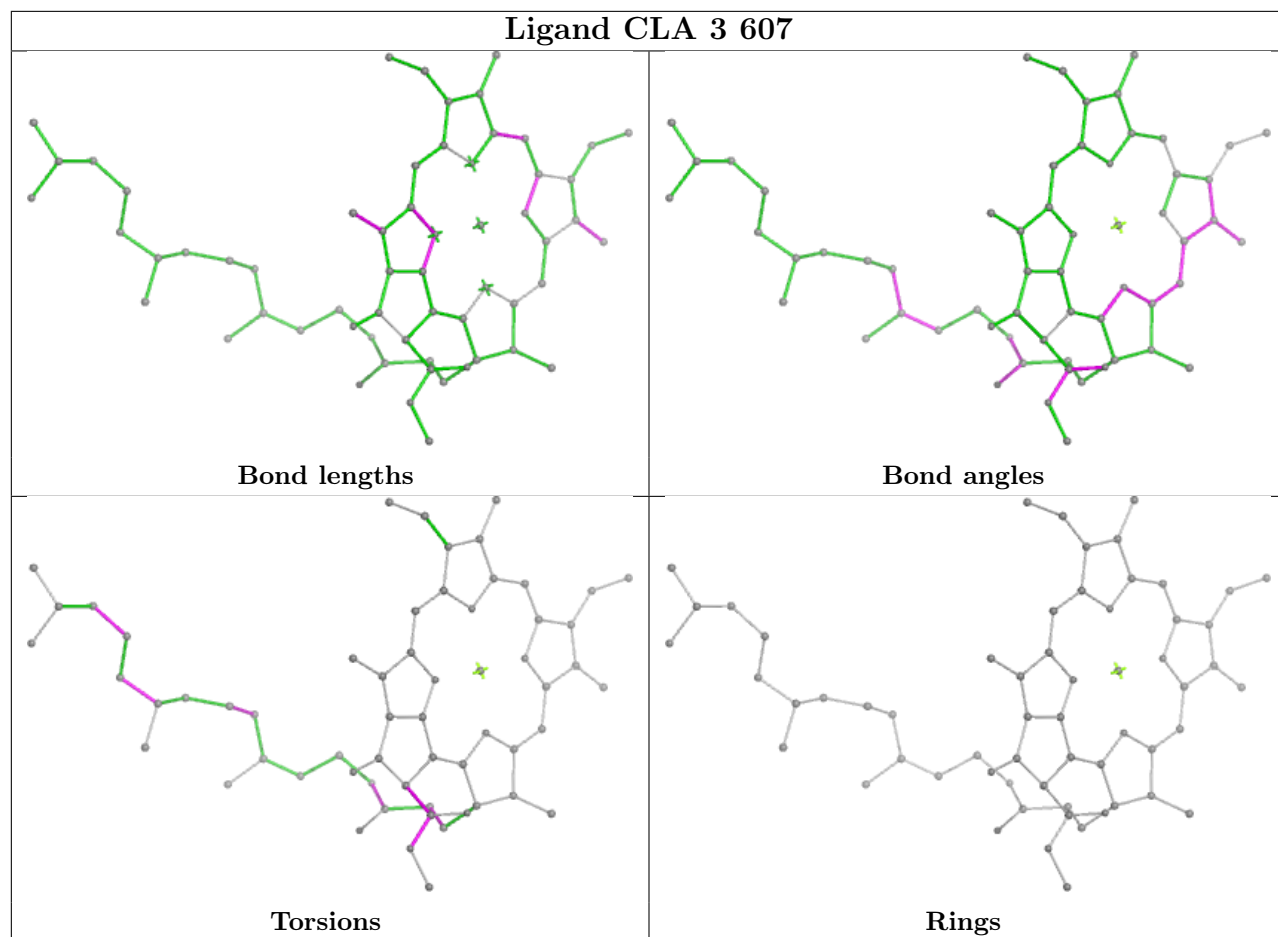




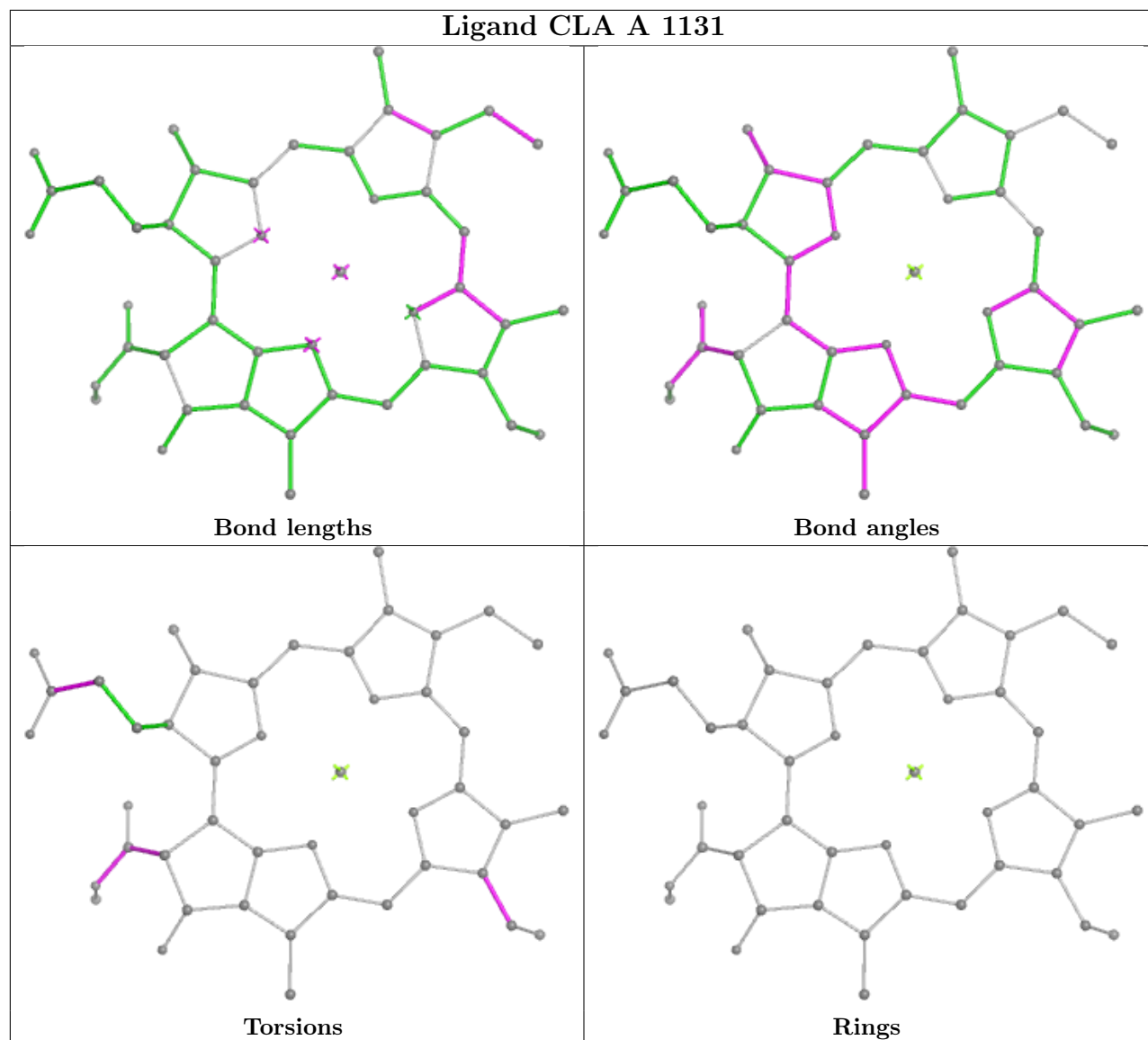




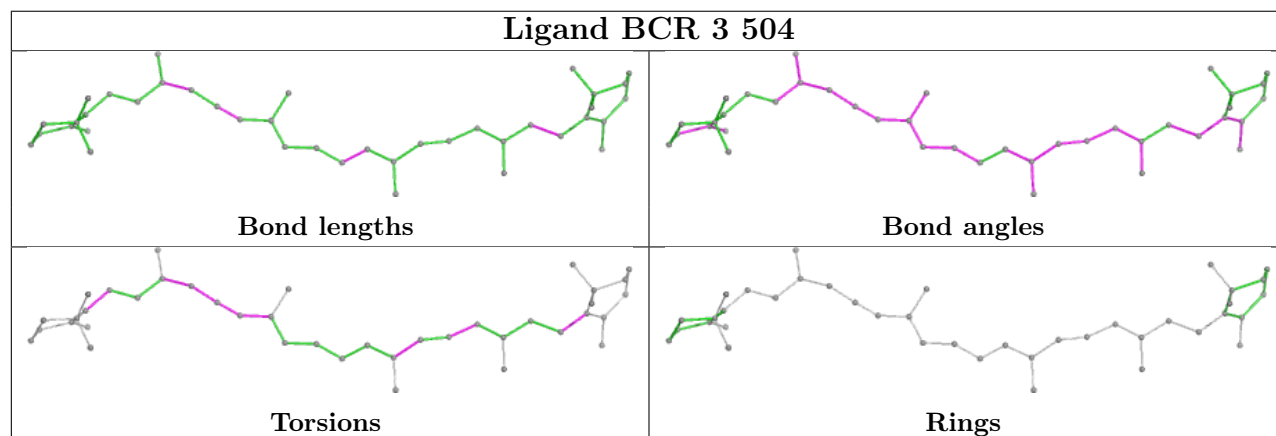


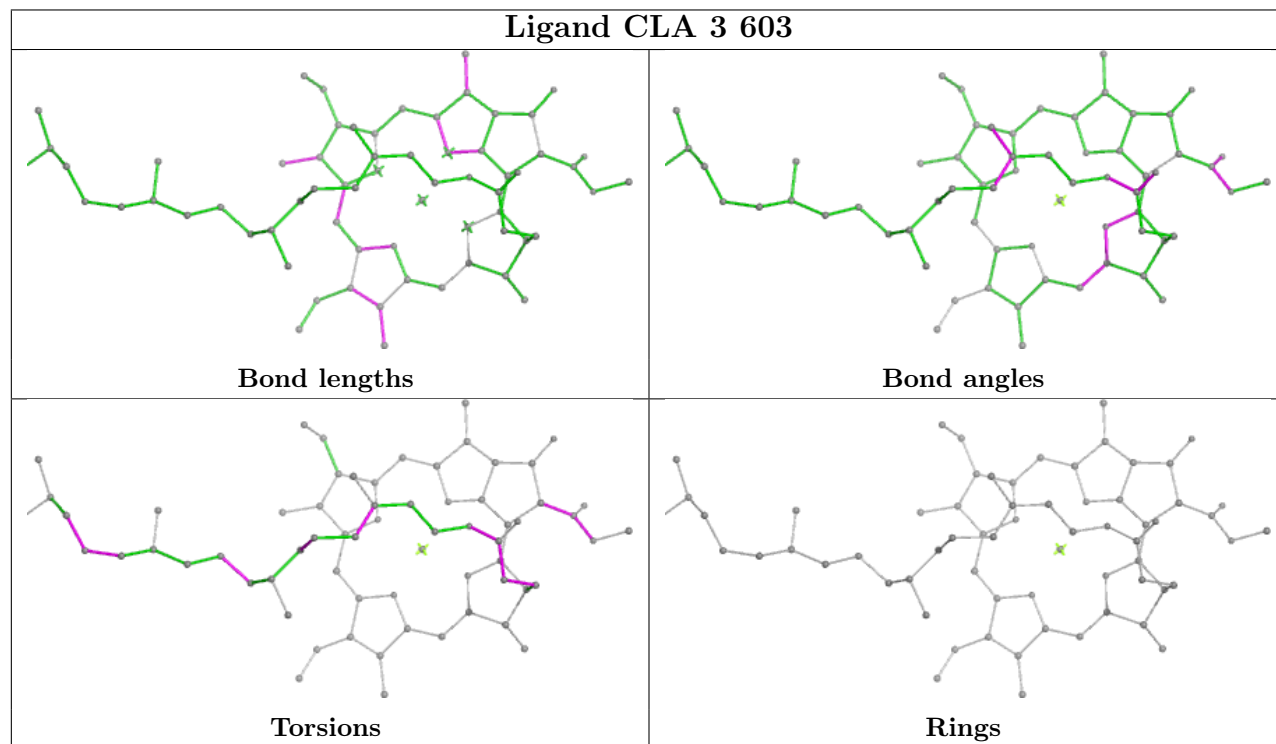
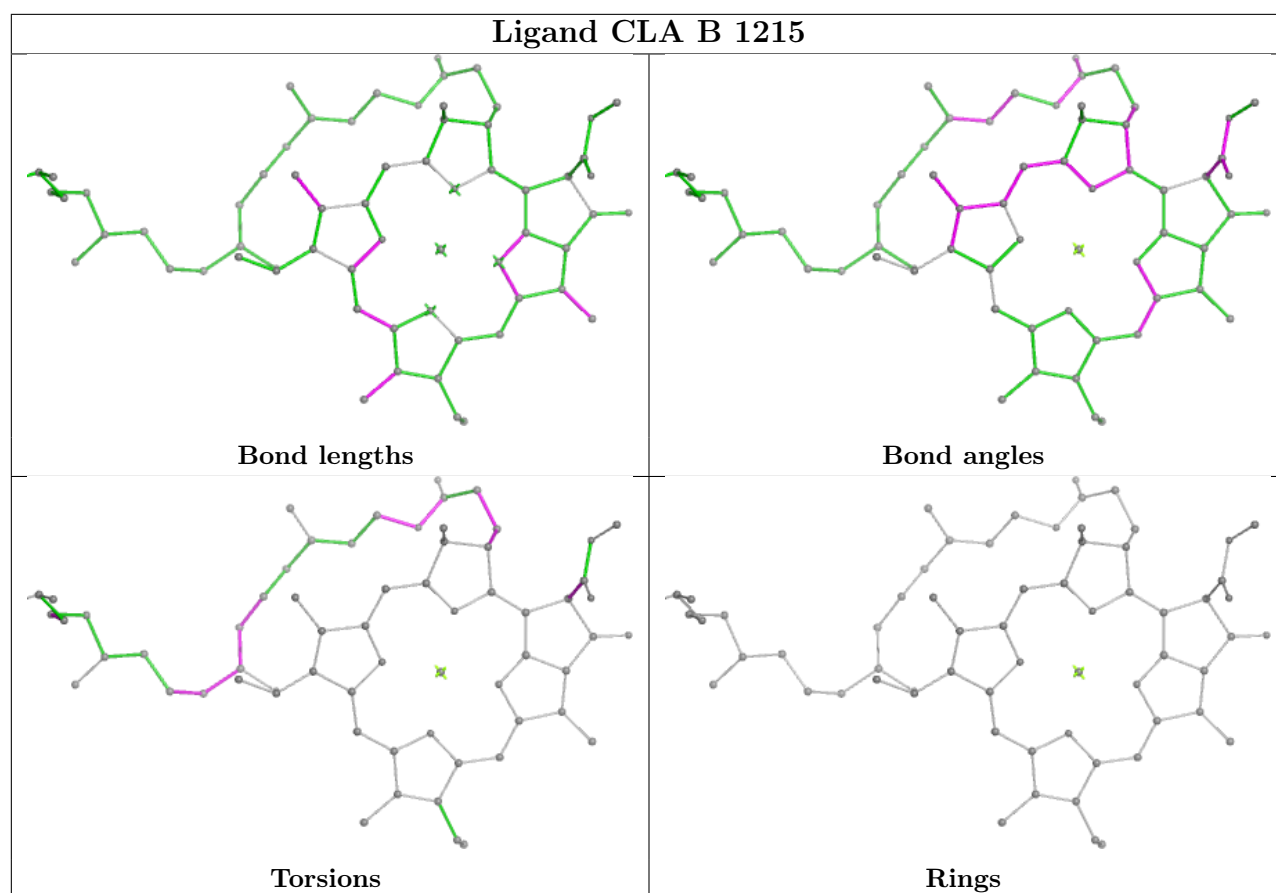


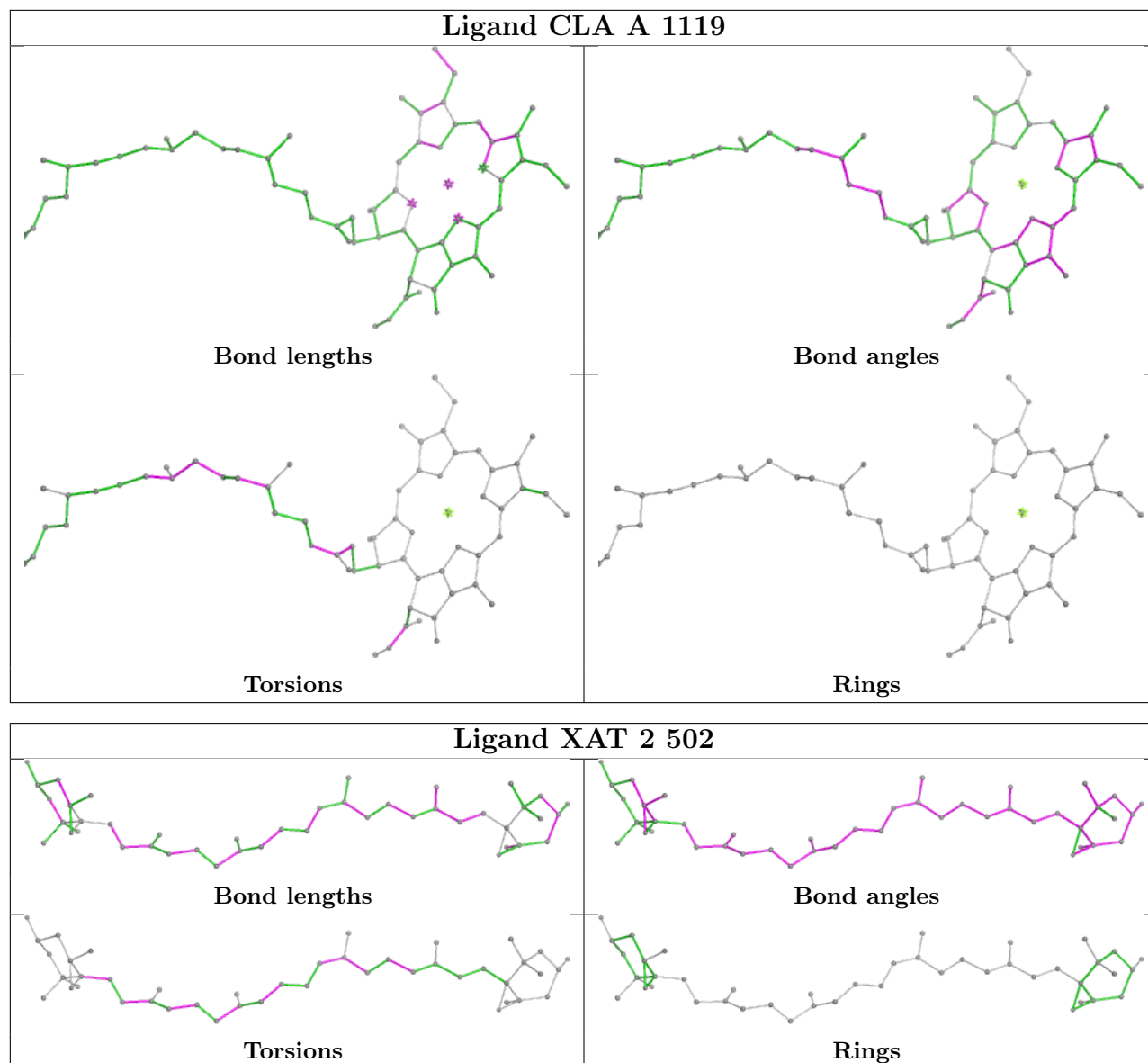
Ligand CLA A 1131



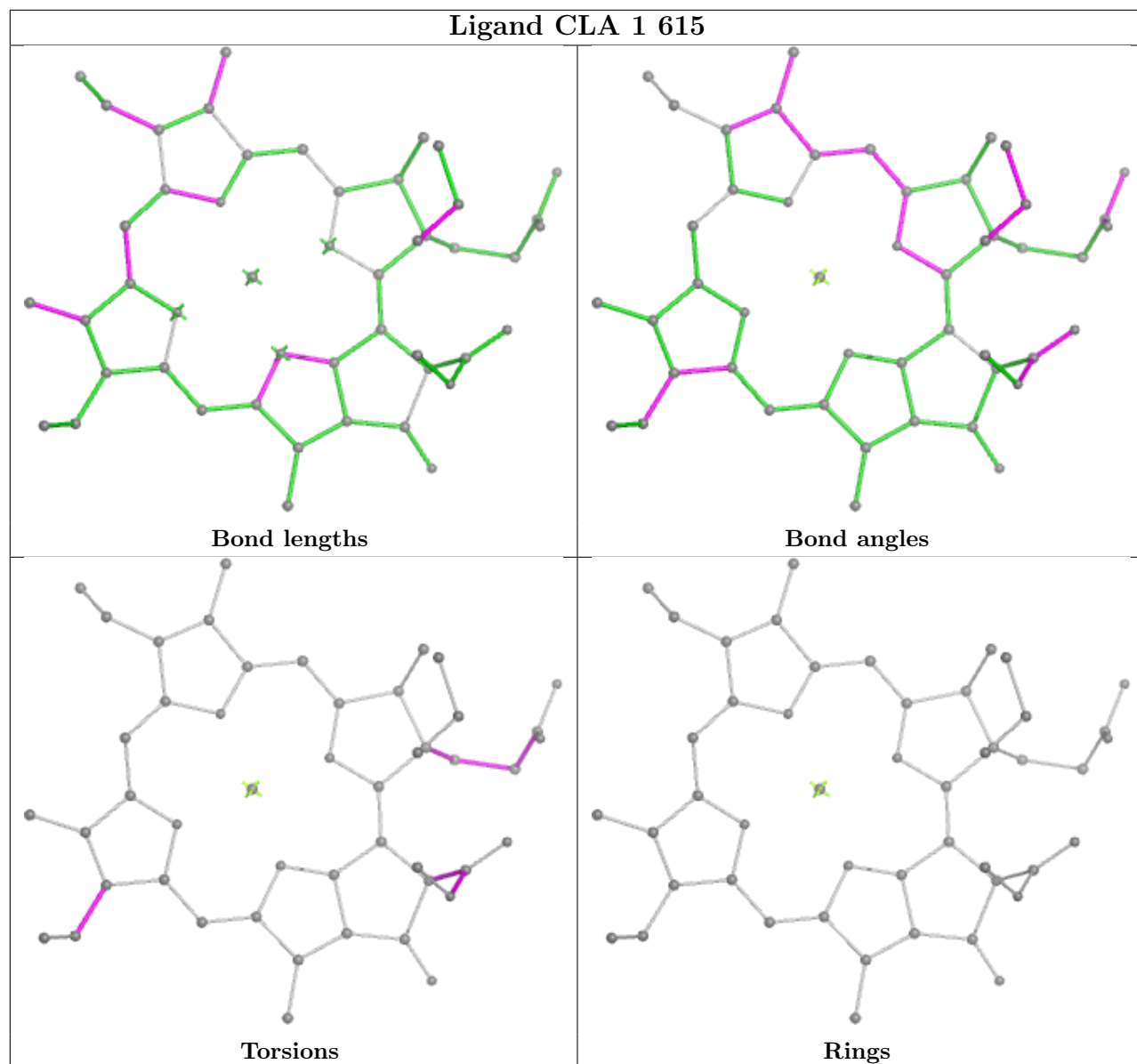
Ligand BCR 3 504

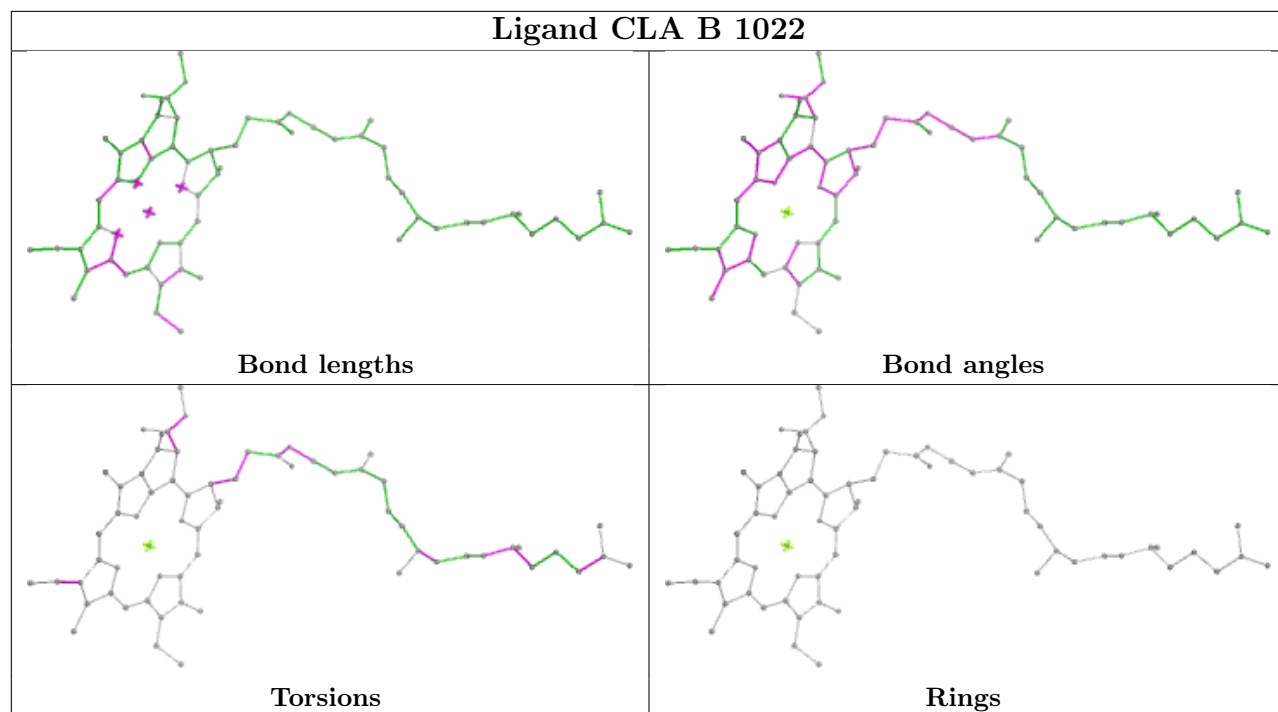


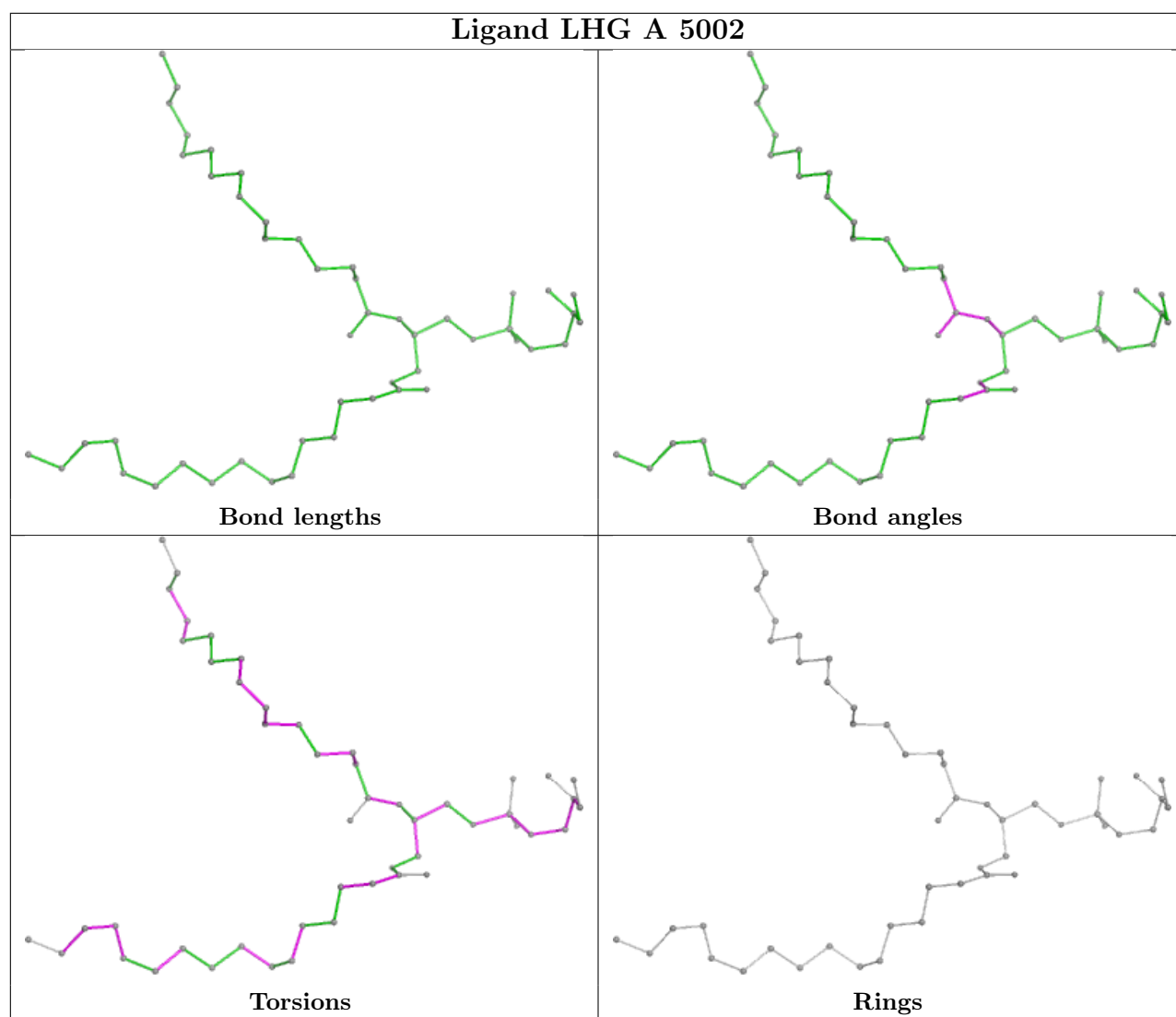




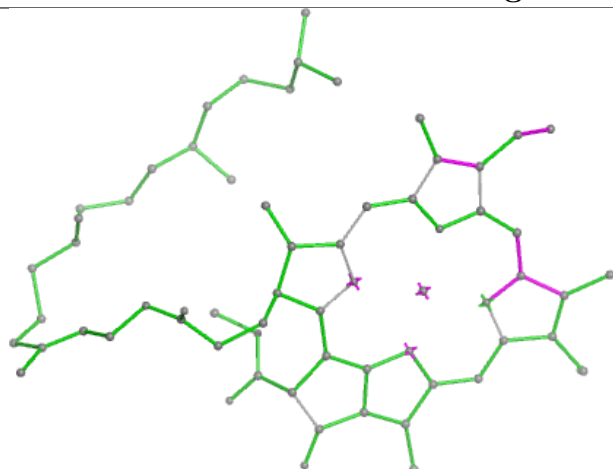
Ligand CLA 1 615



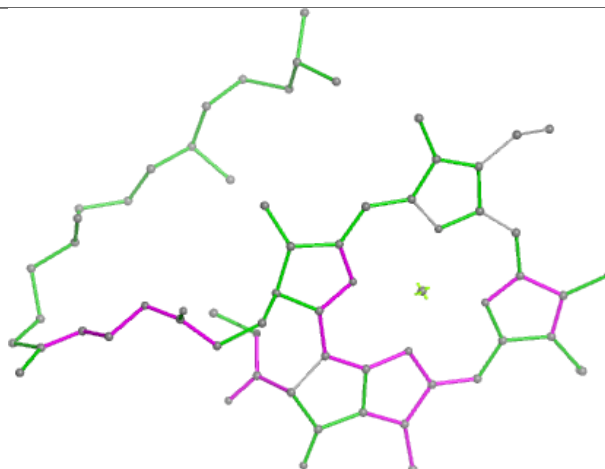




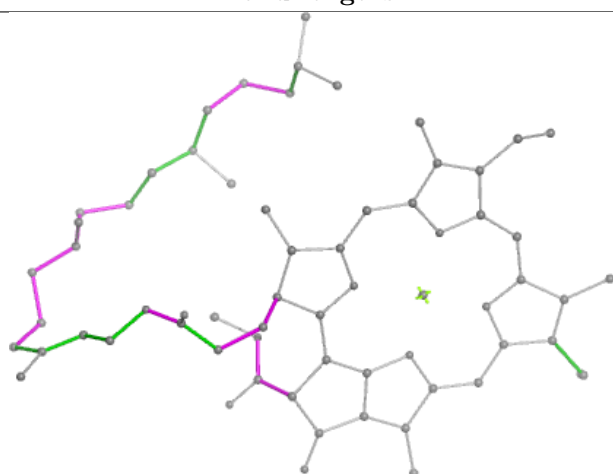
Ligand CLA A 1101



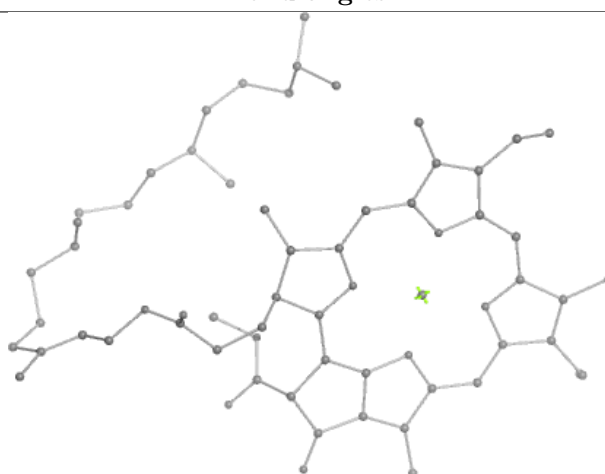
Bond lengths



Bond angles

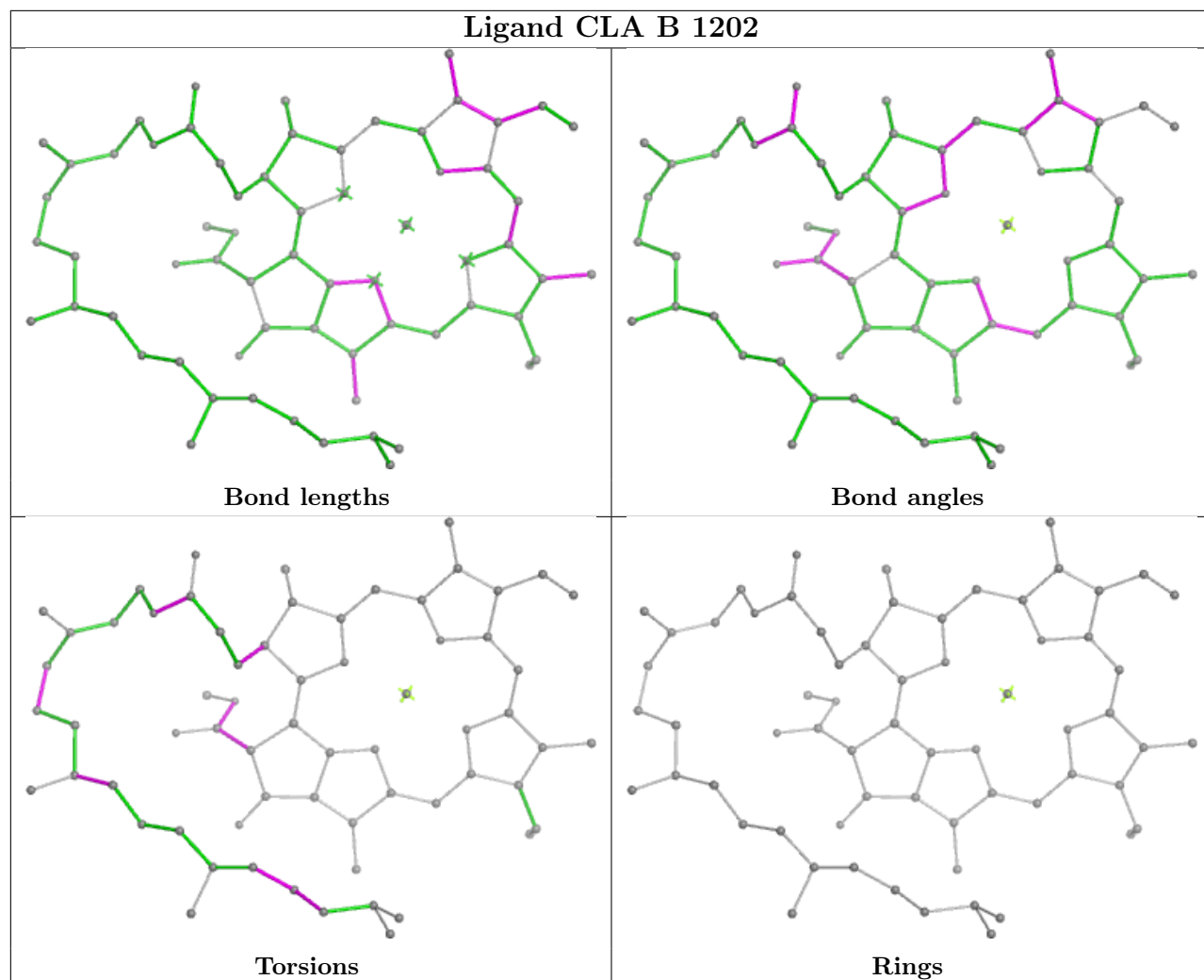


Torsions

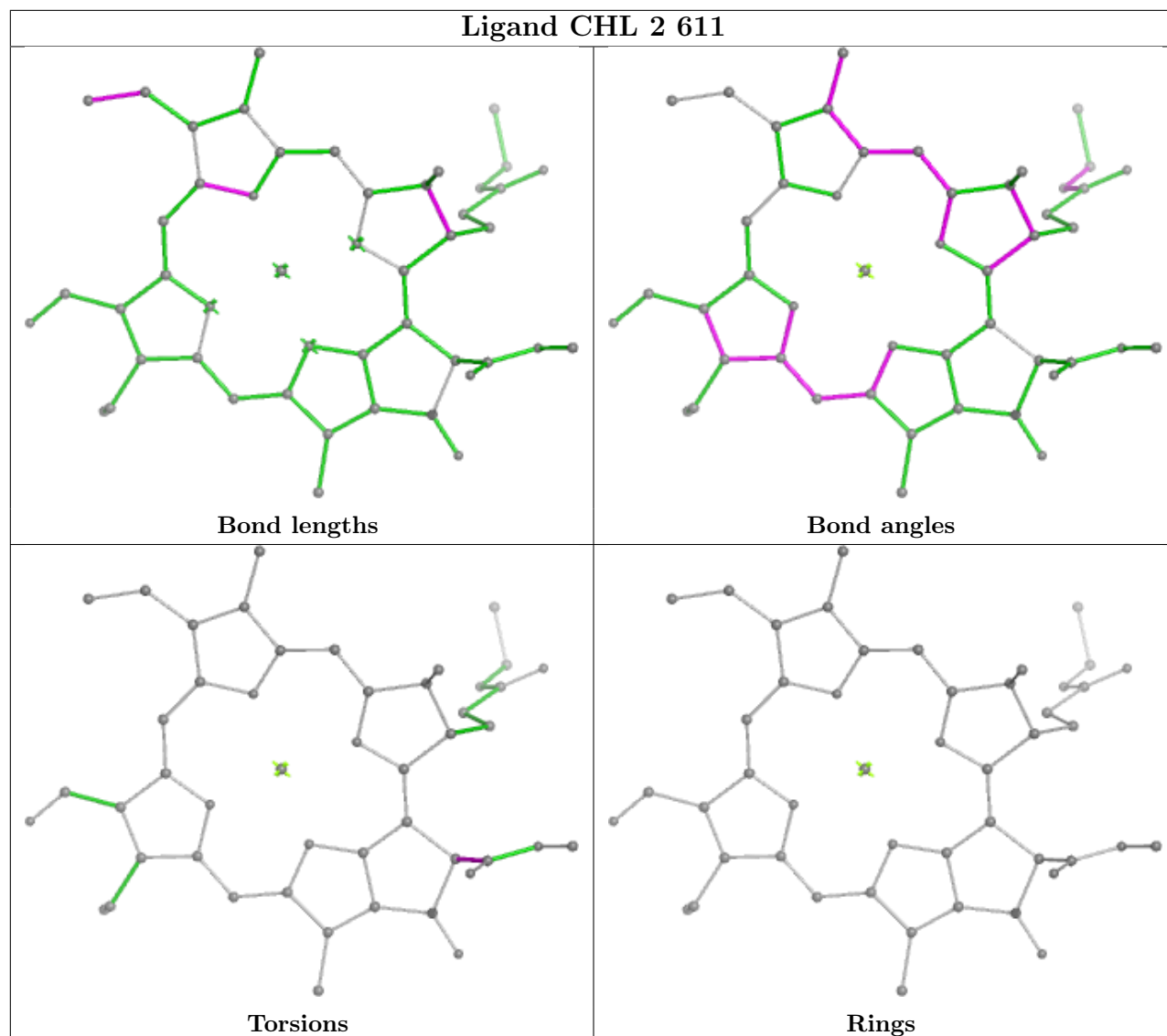


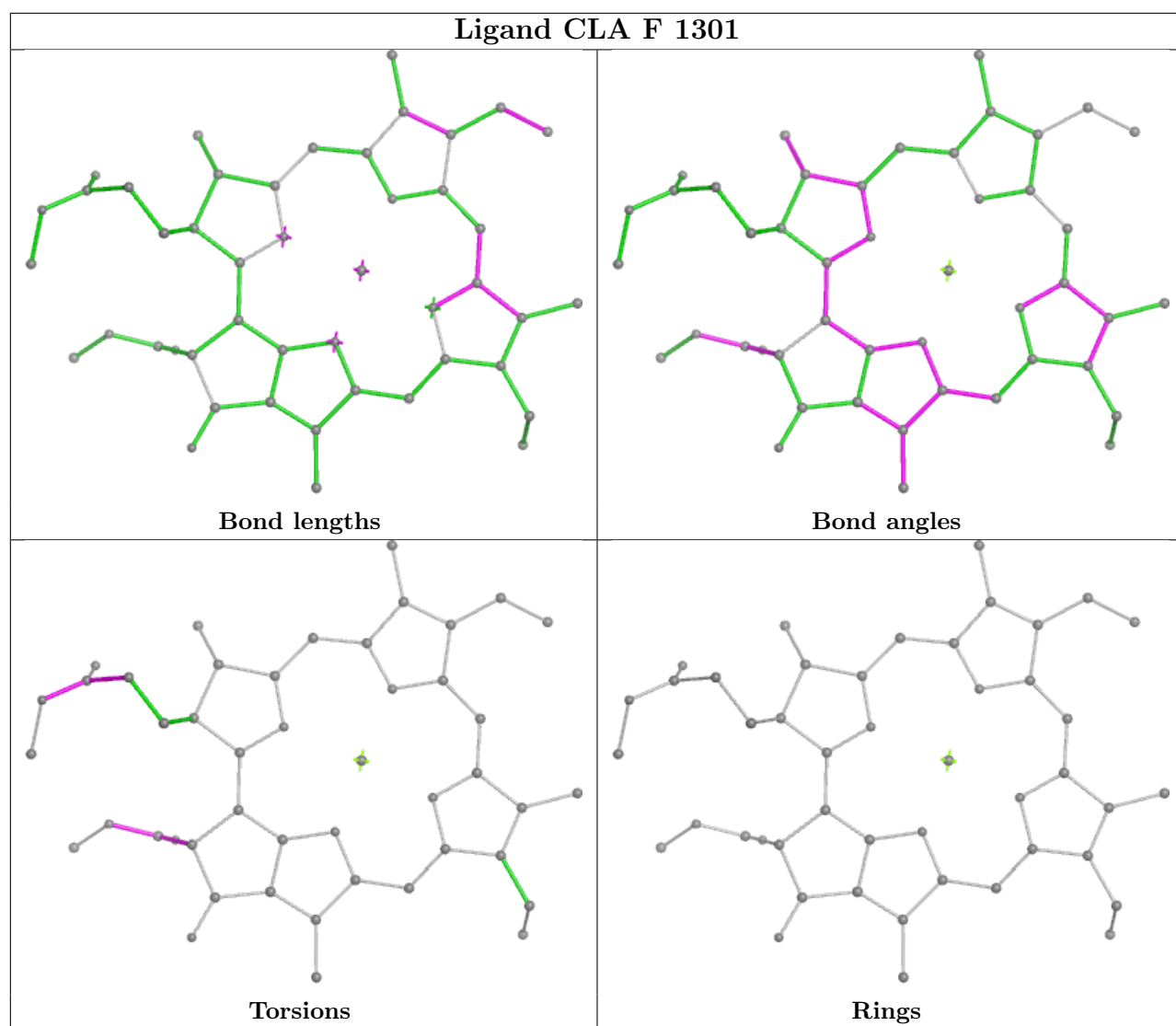
Rings

Ligand CLA B 1202

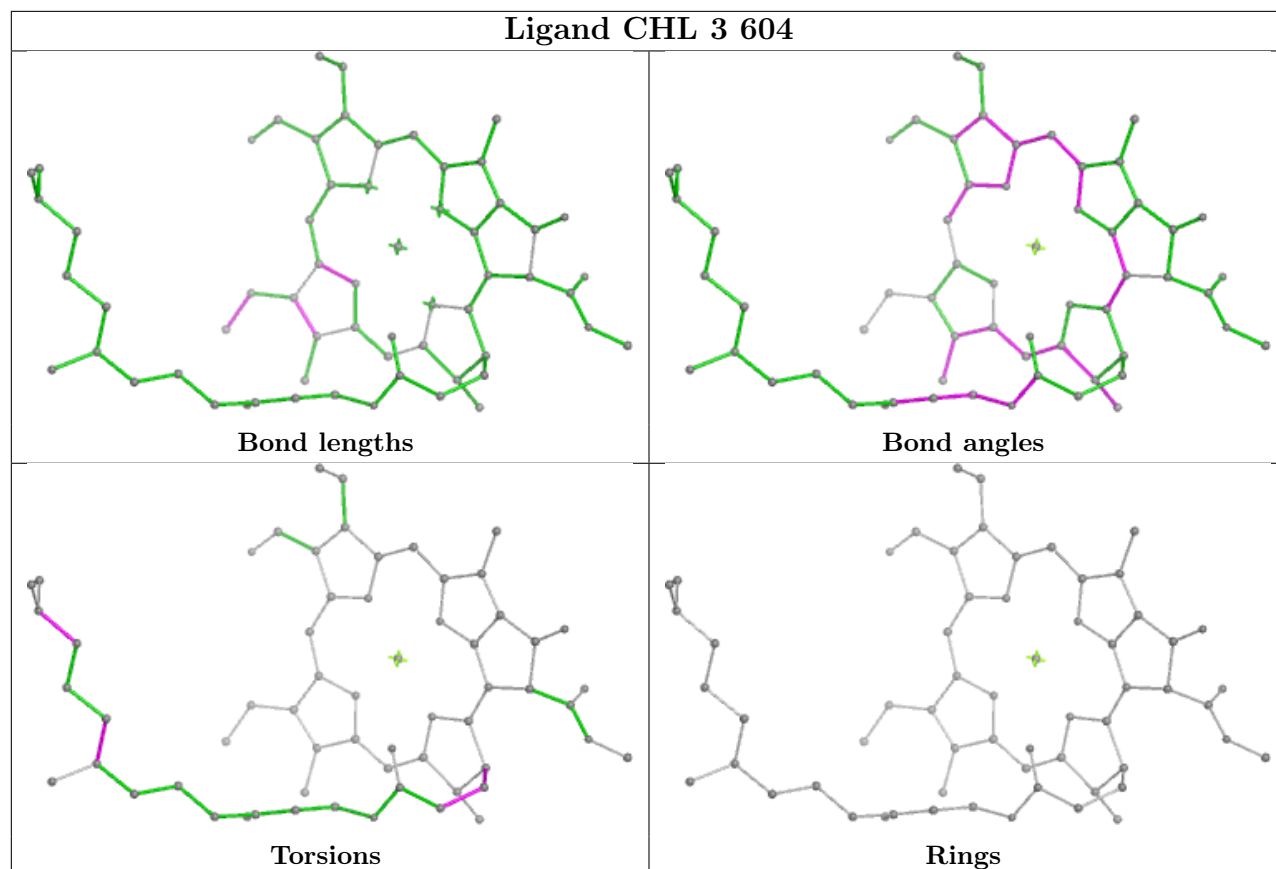


Ligand CHL 2 611

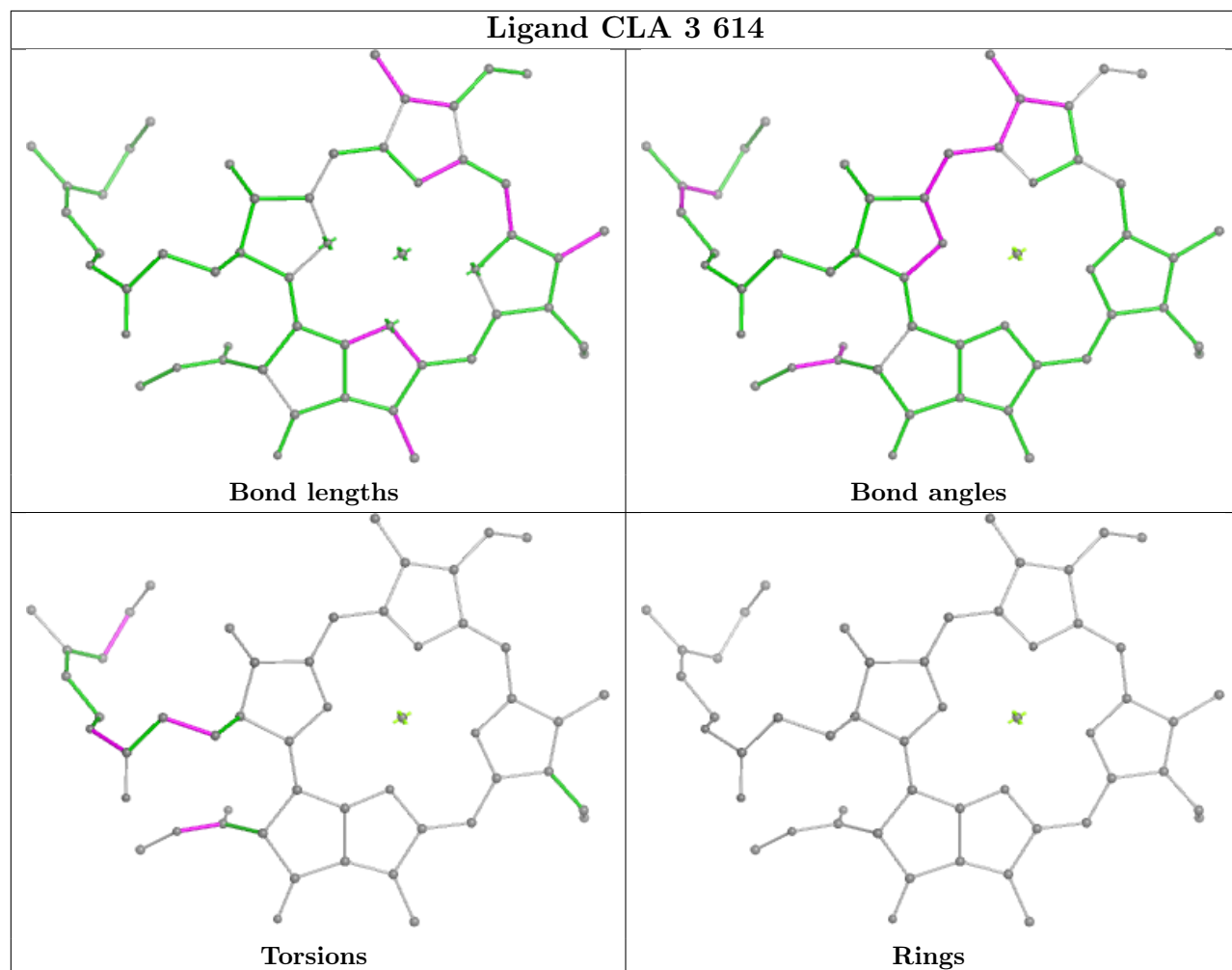


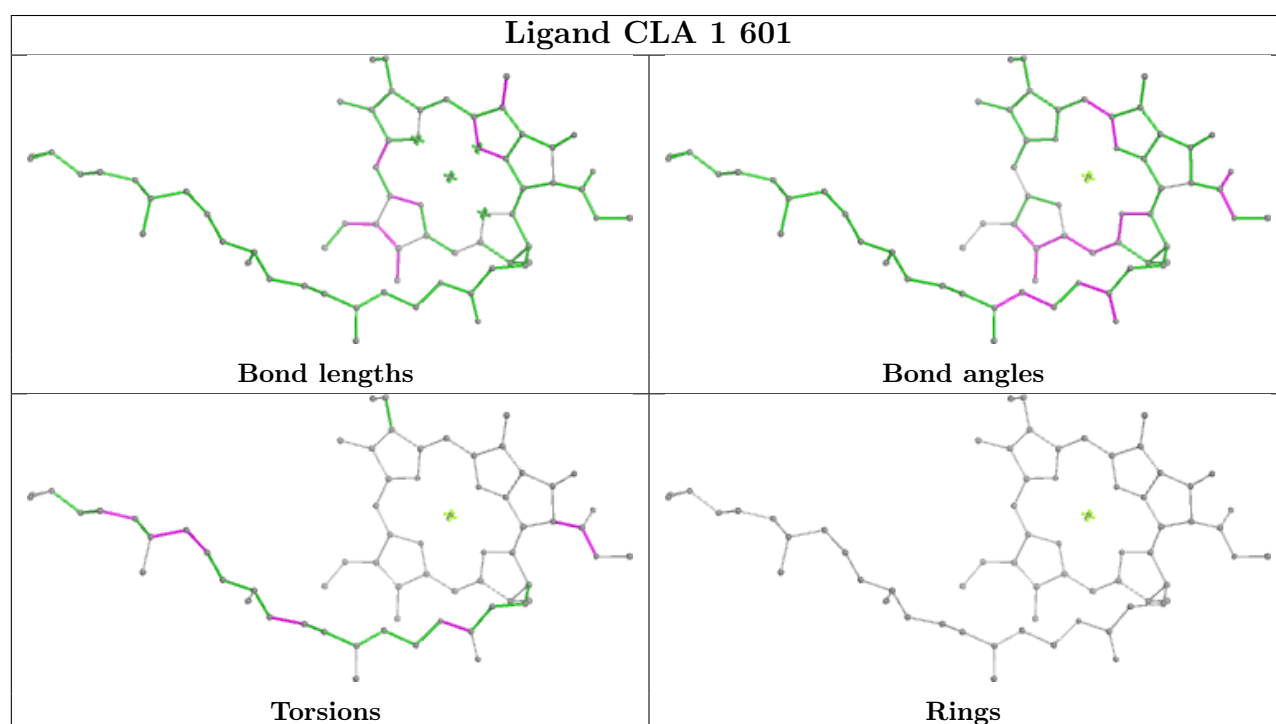
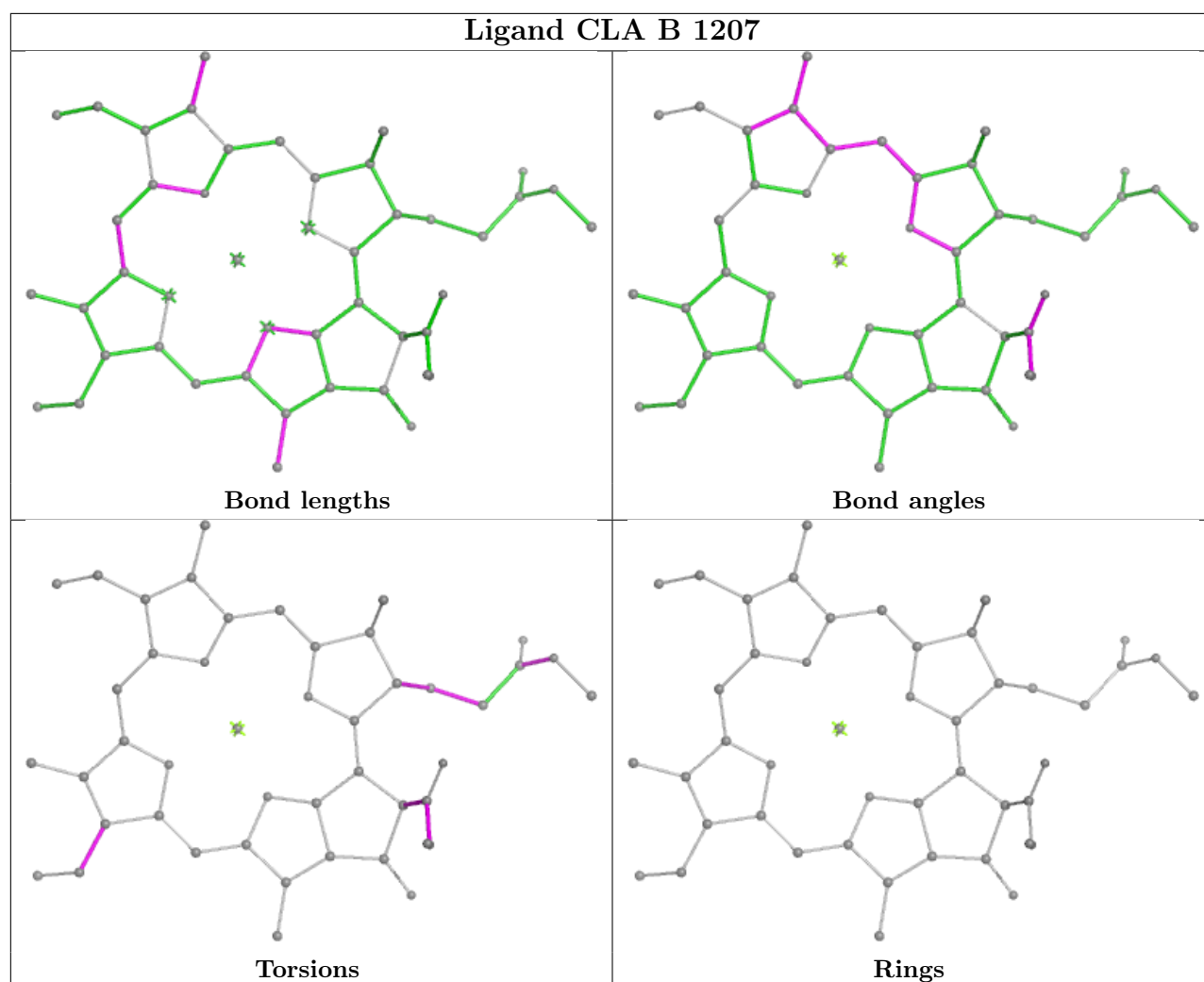


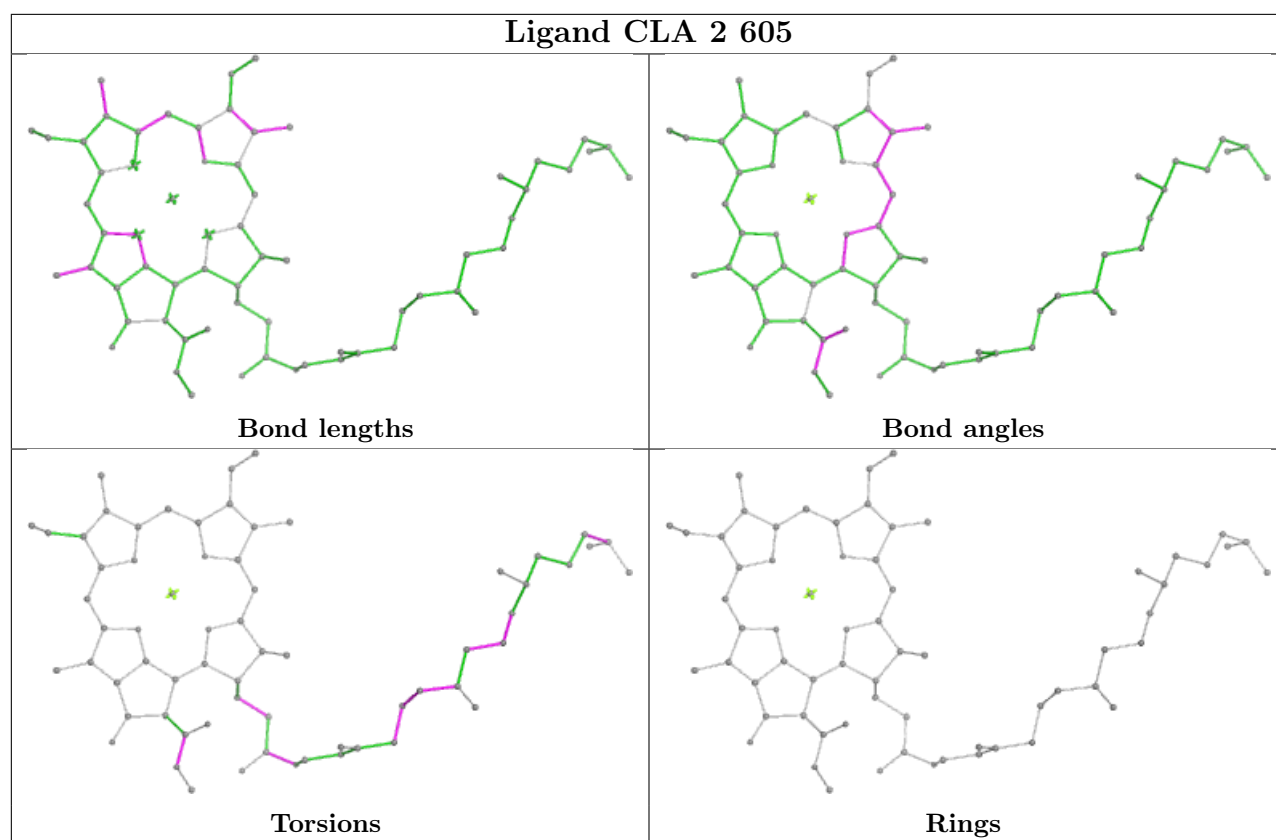
Ligand CHL 3 604



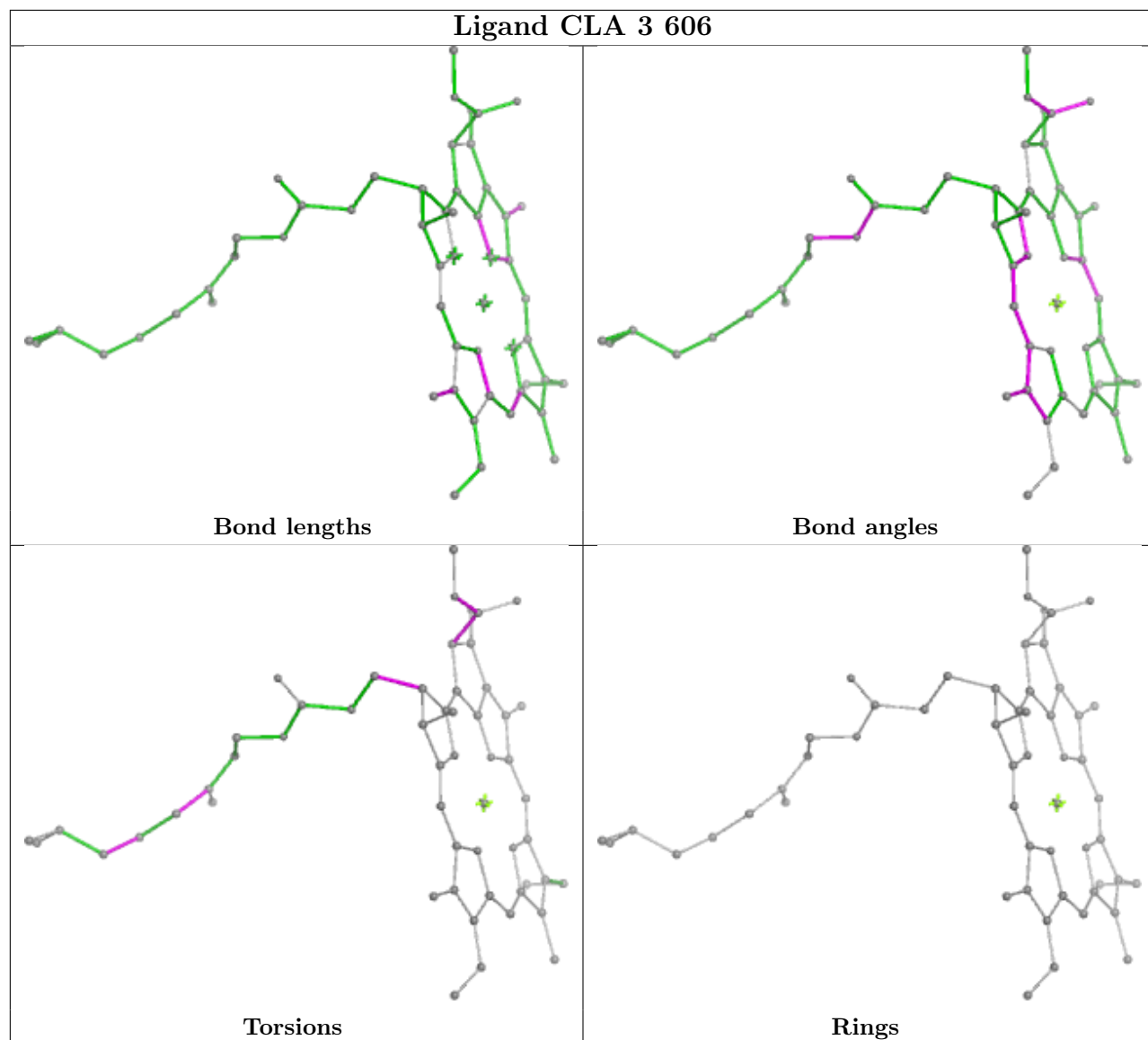
Ligand CLA 3 614

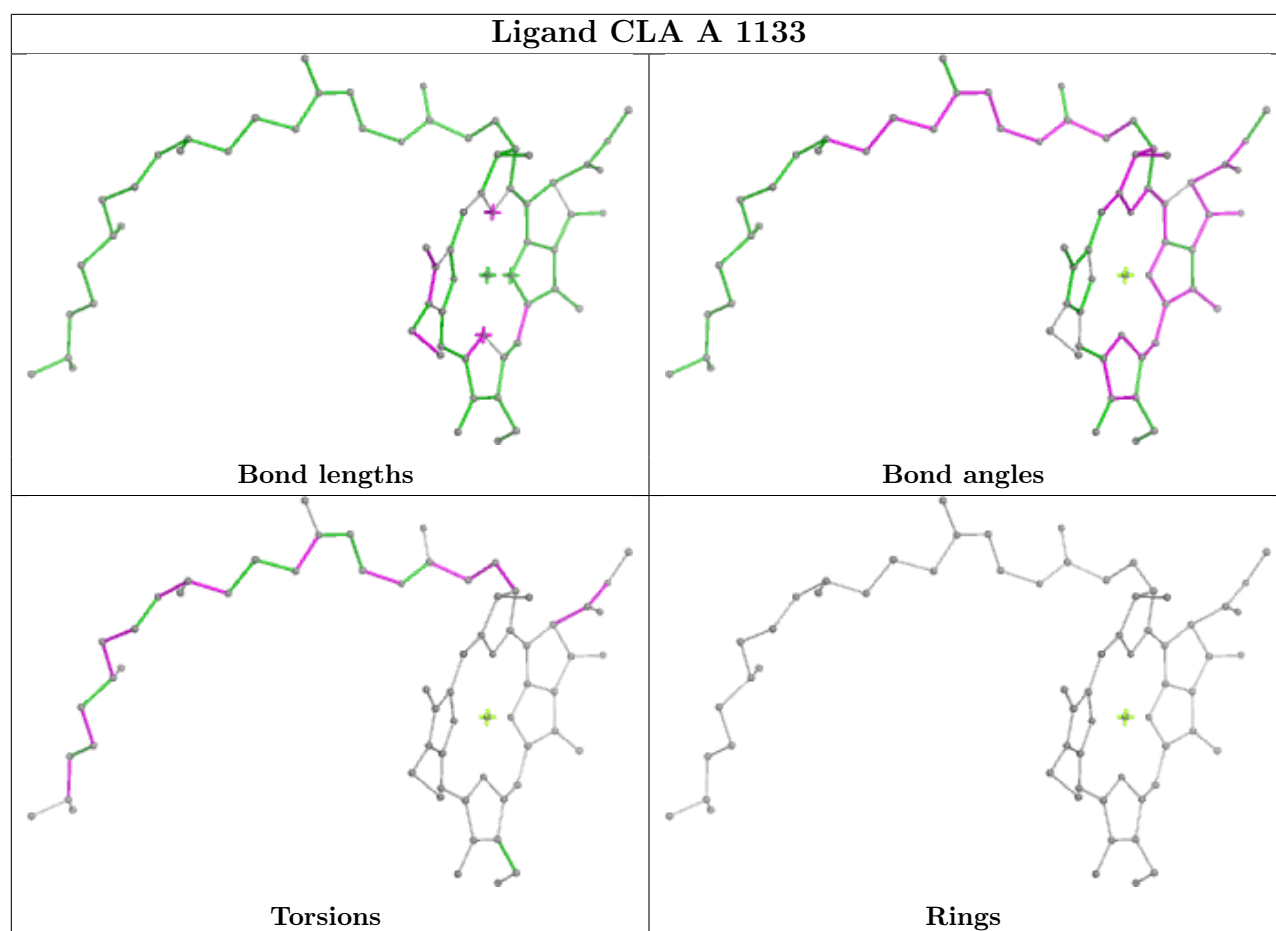


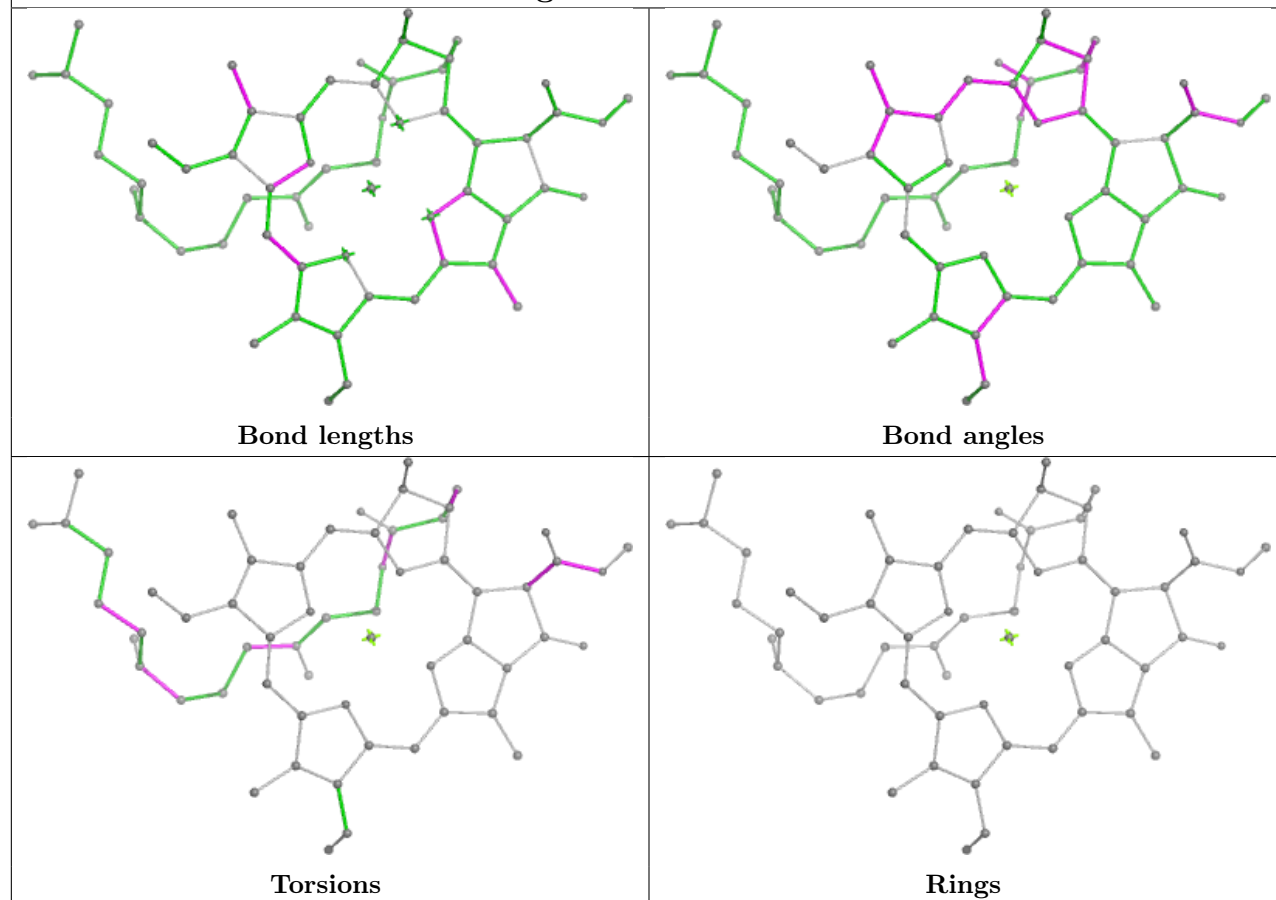
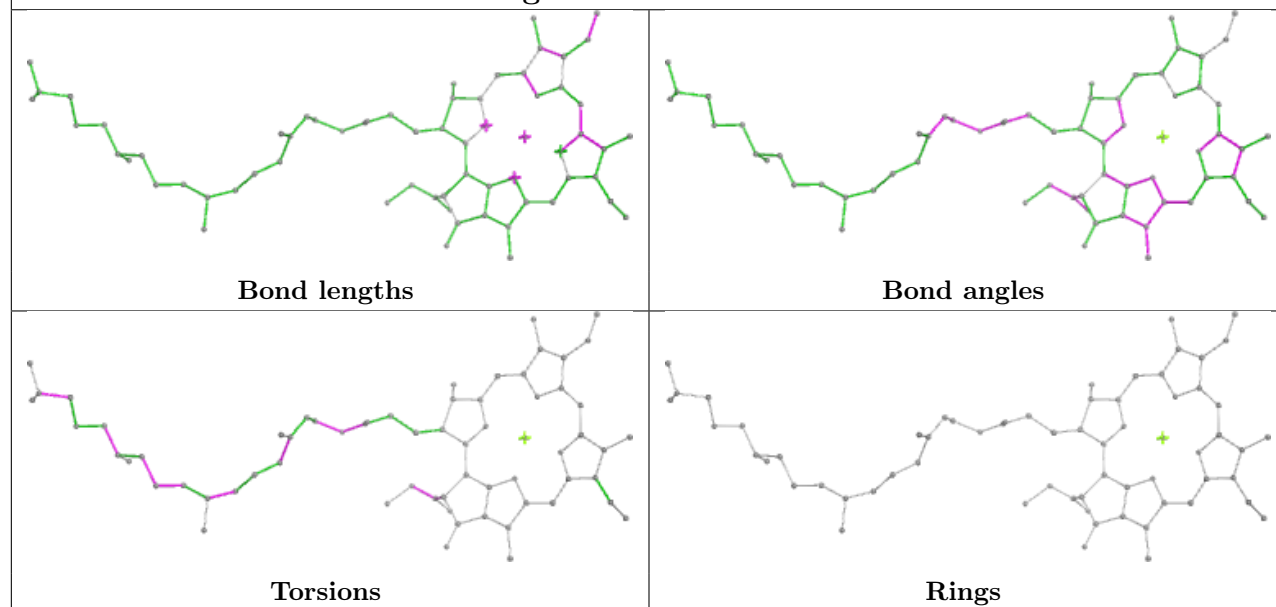




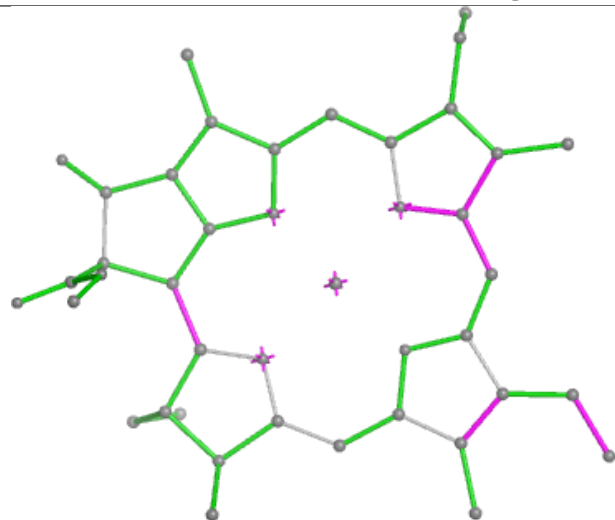
Ligand CLA 3 606



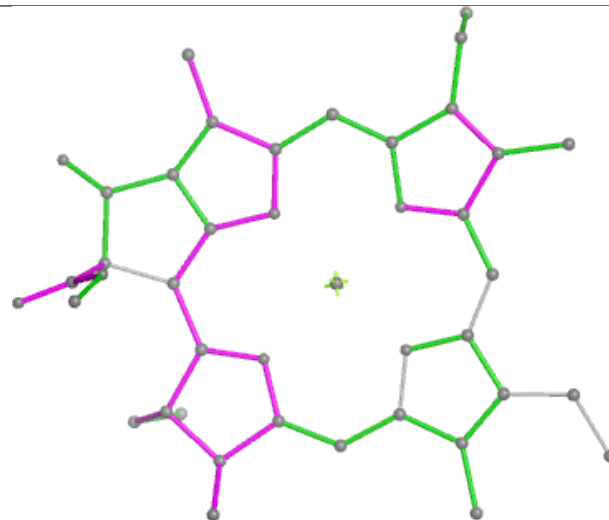


Ligand CLA 1 603**Ligand CLA A 1139**

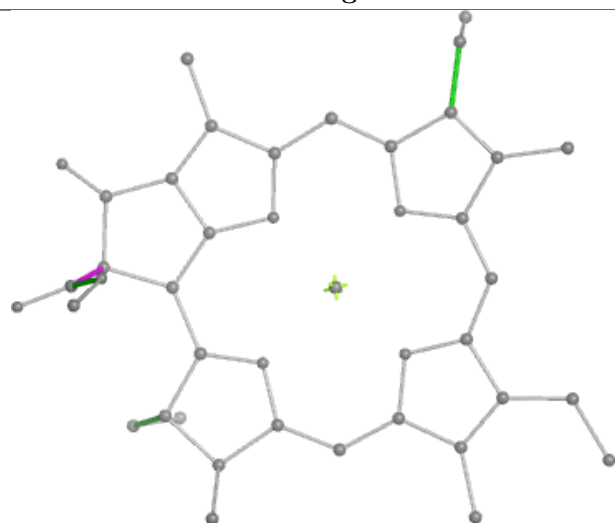
Ligand CLA A 1118



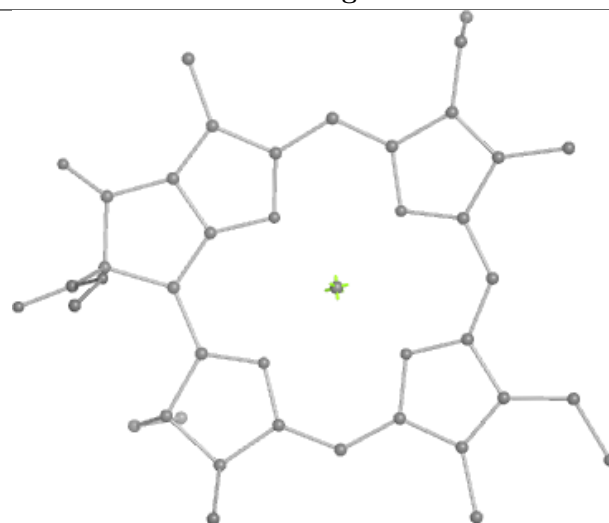
Bond lengths



Bond angles

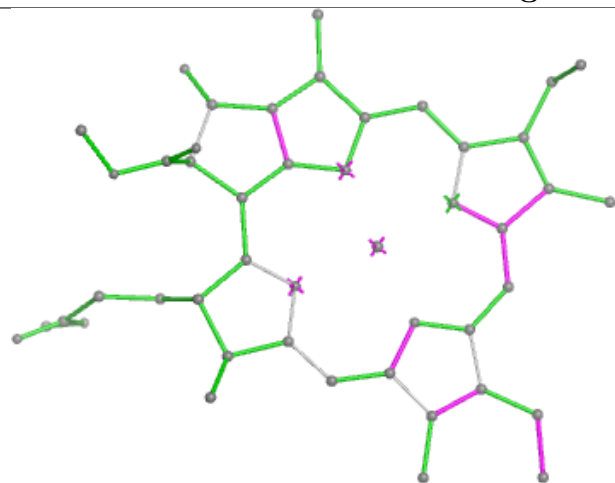


Torsions

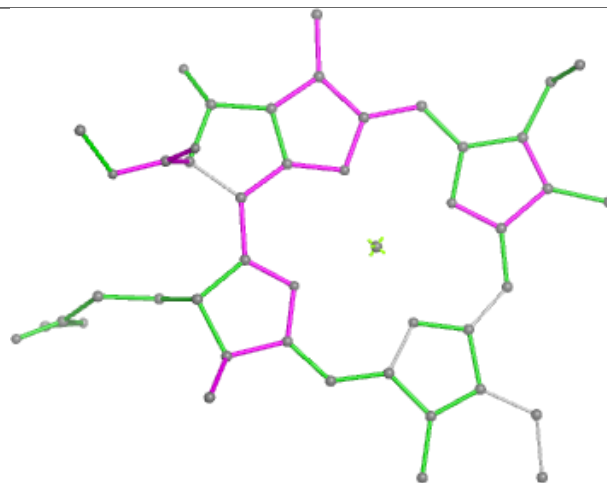


Rings

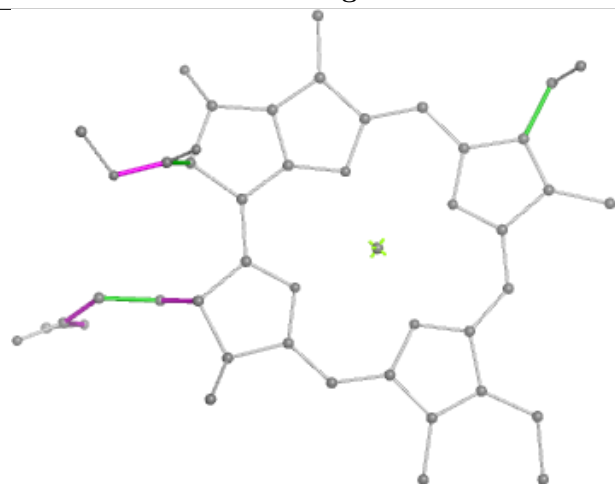
Ligand CLA 3 613



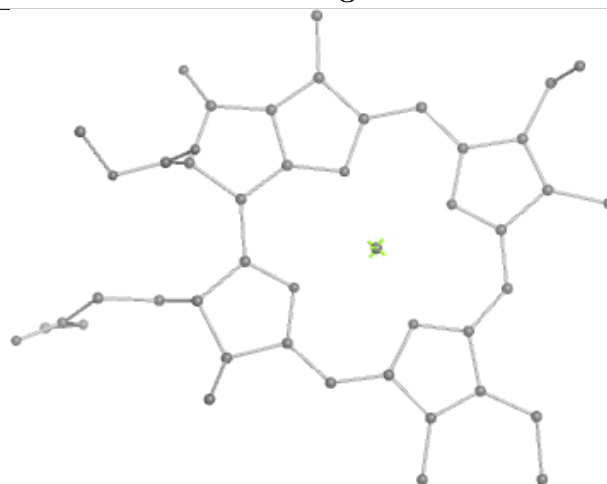
Bond lengths



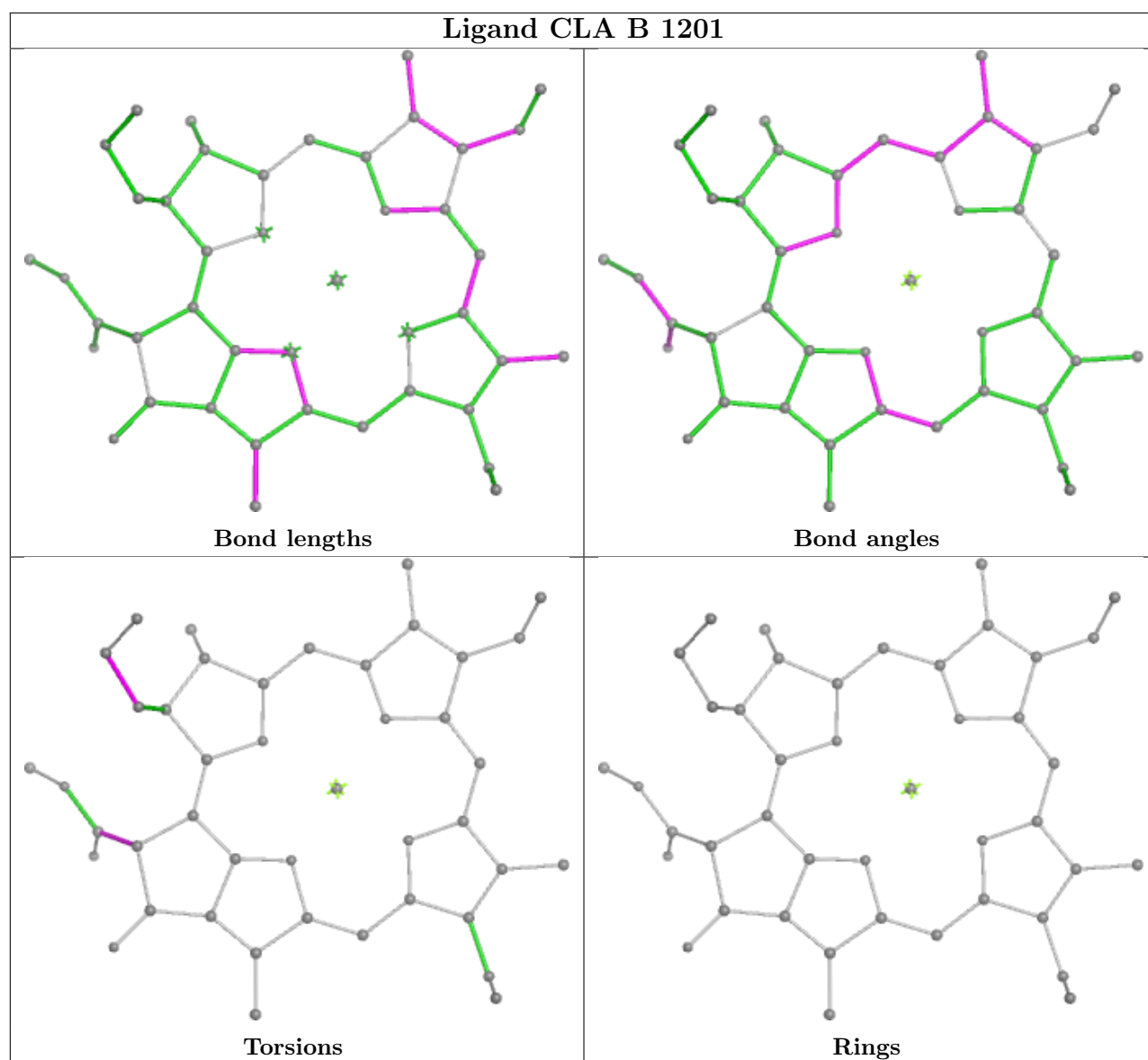
Bond angles



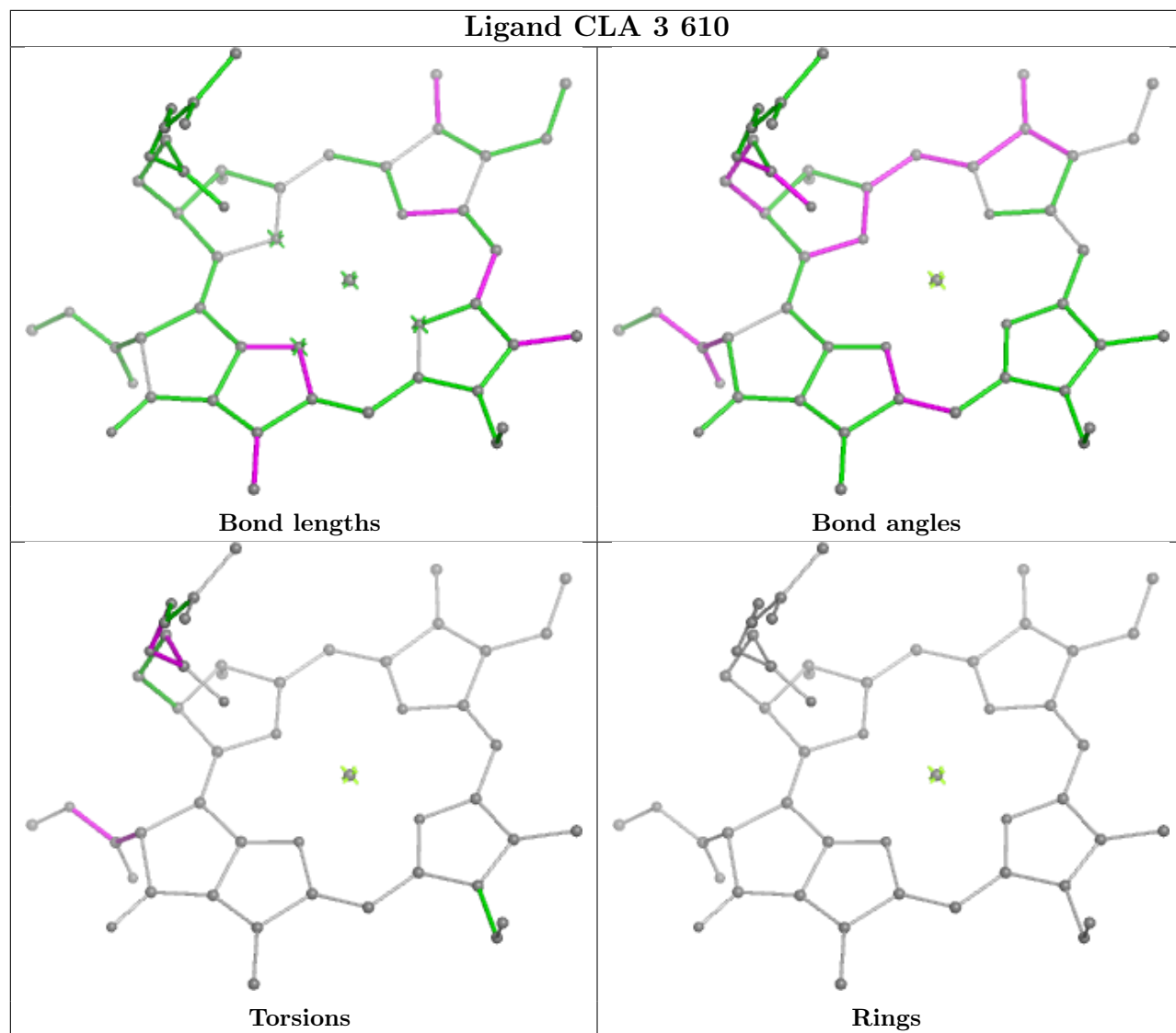
Torsions



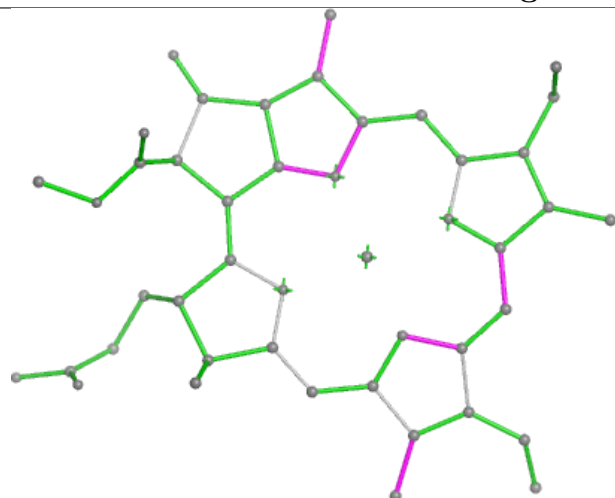
Rings



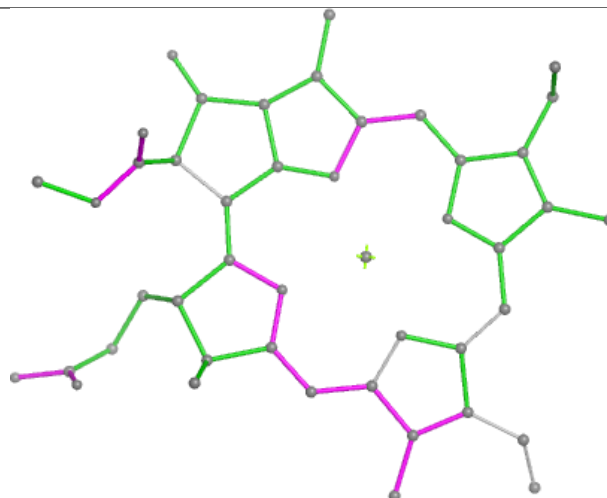
Ligand CLA 3 610



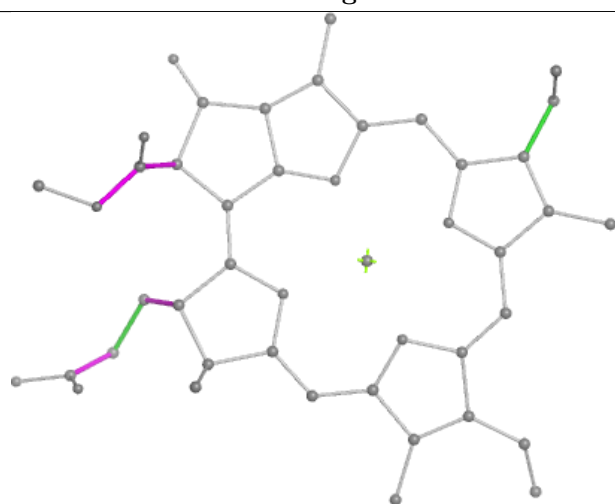
Ligand CLA 1 613



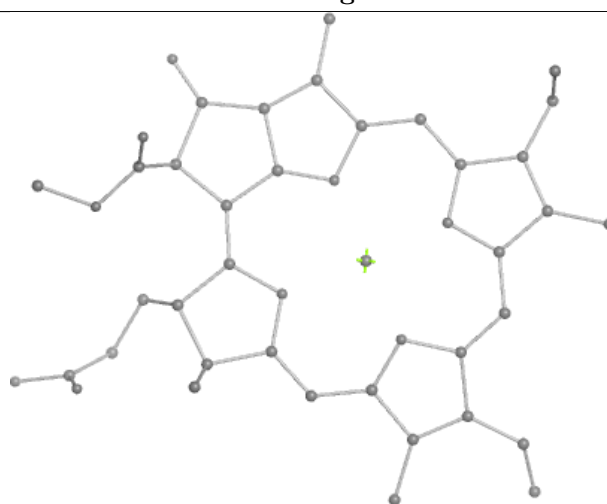
Bond lengths



Bond angles

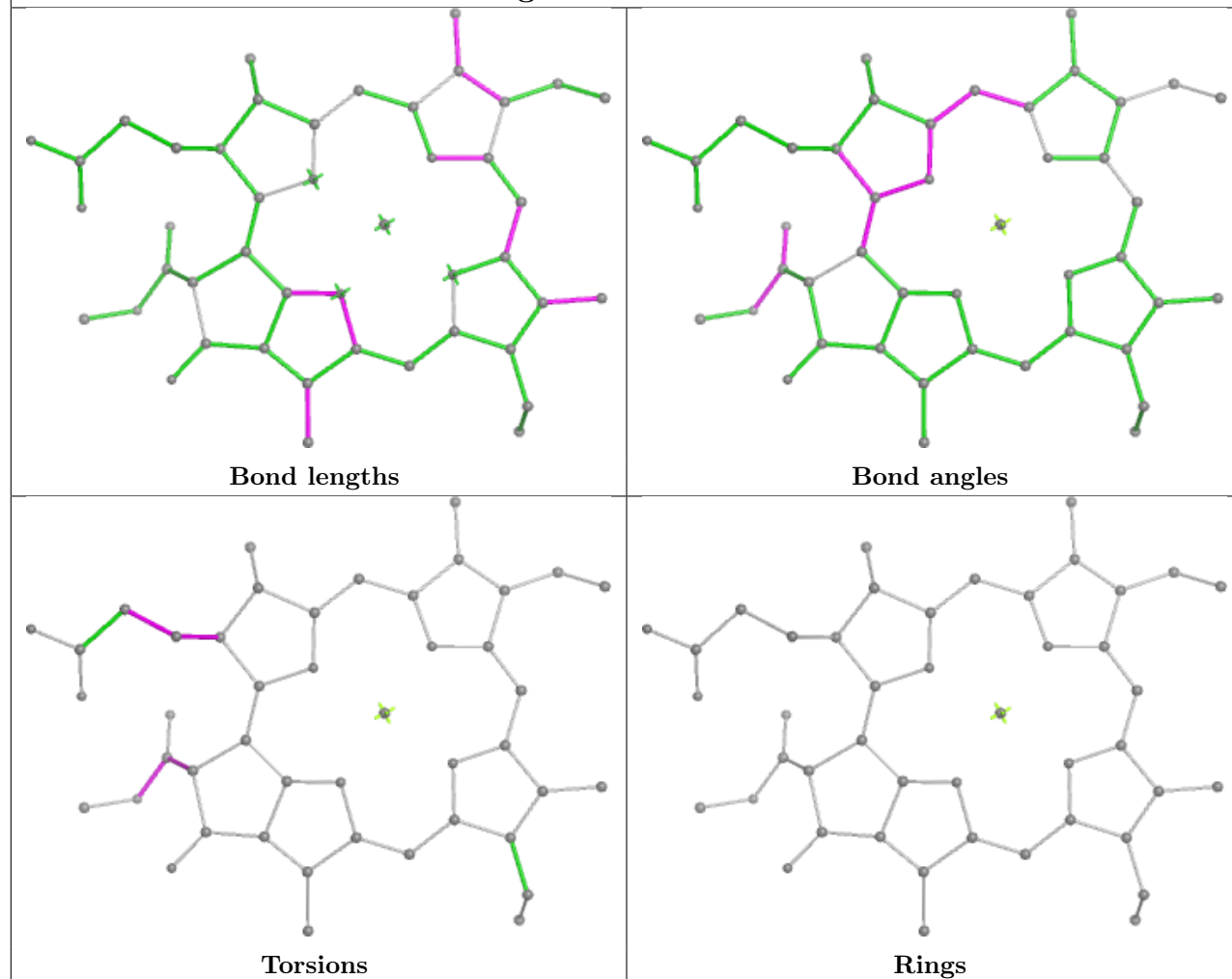


Torsions

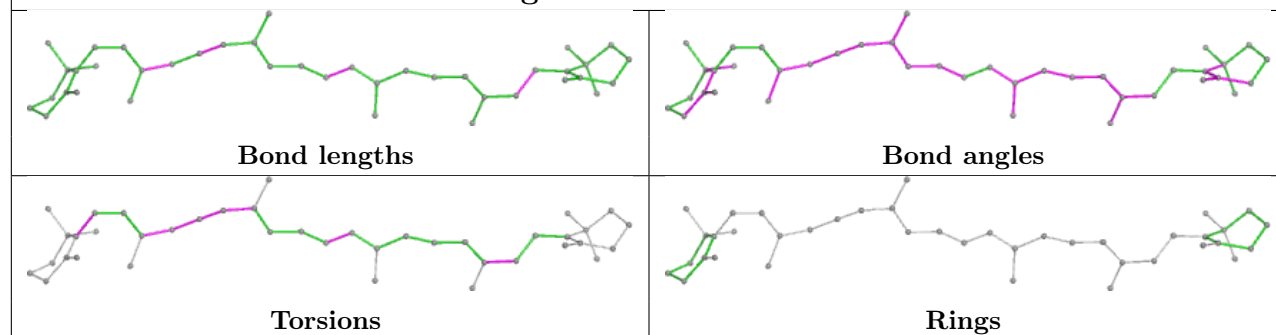


Rings

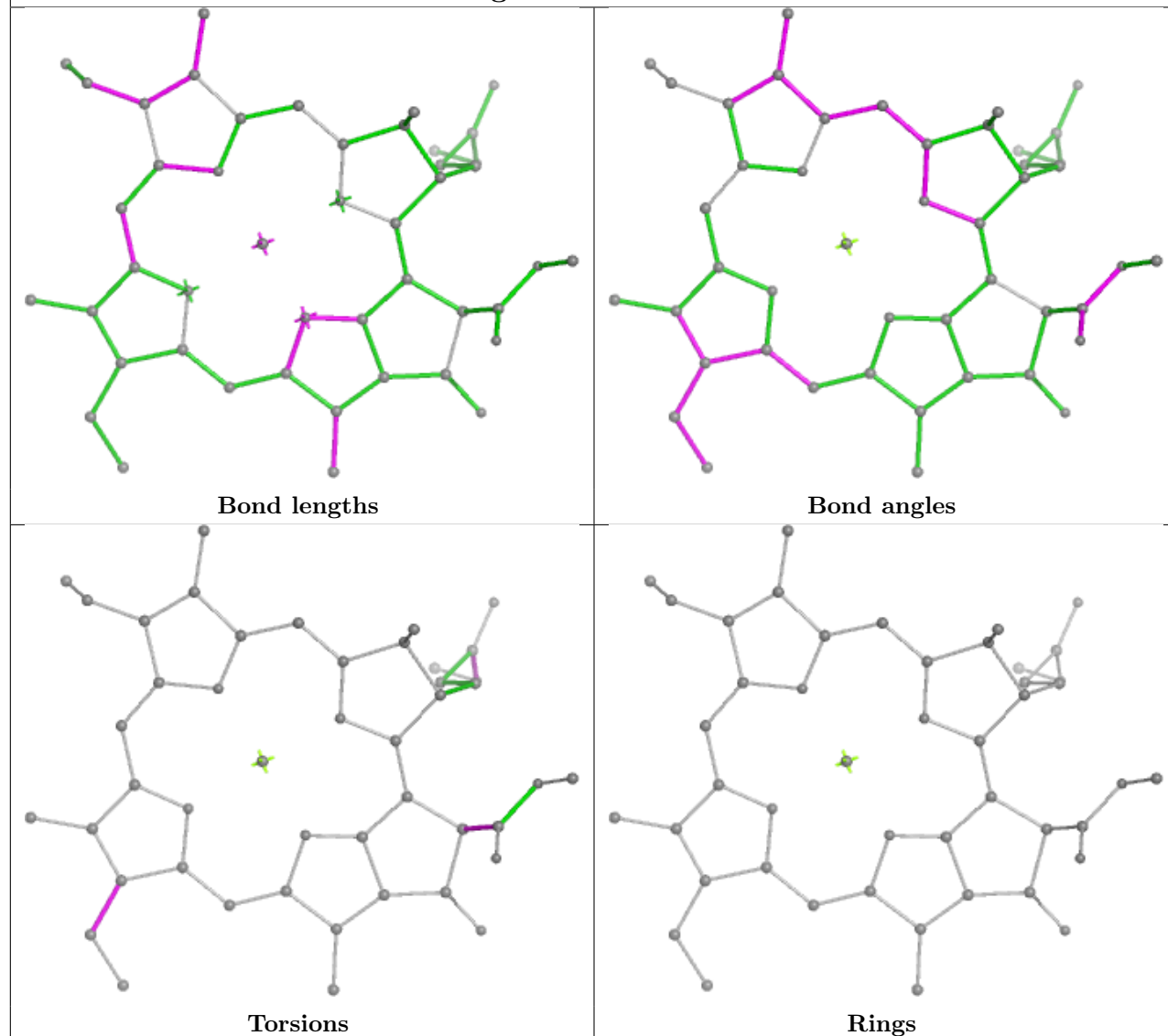
Ligand CLA 2 602



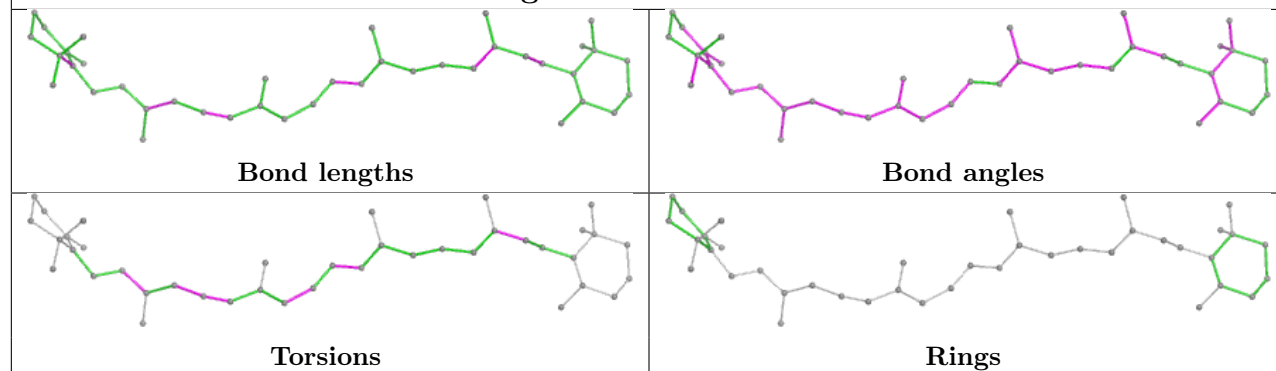
Ligand BCR A 4002

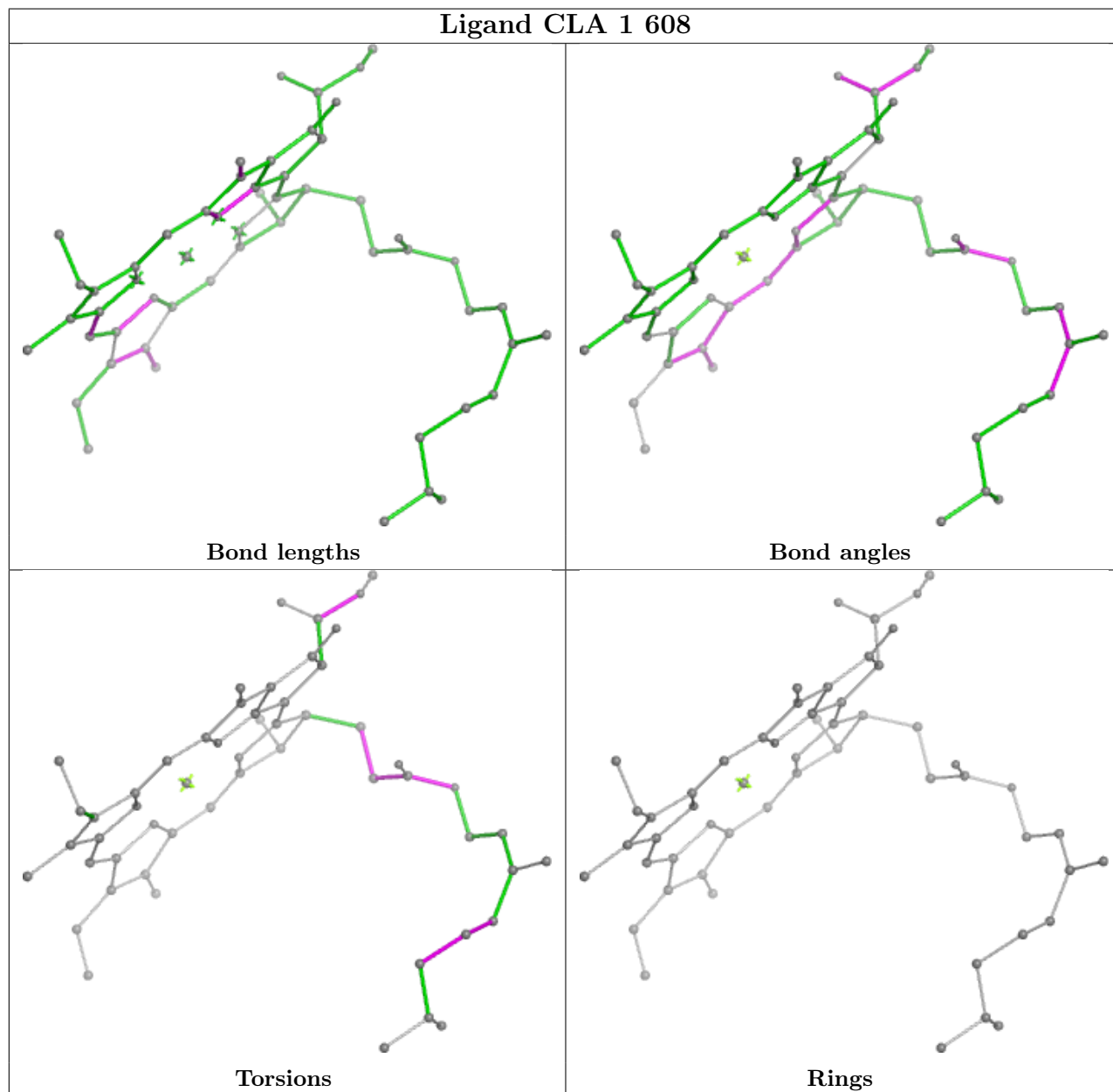
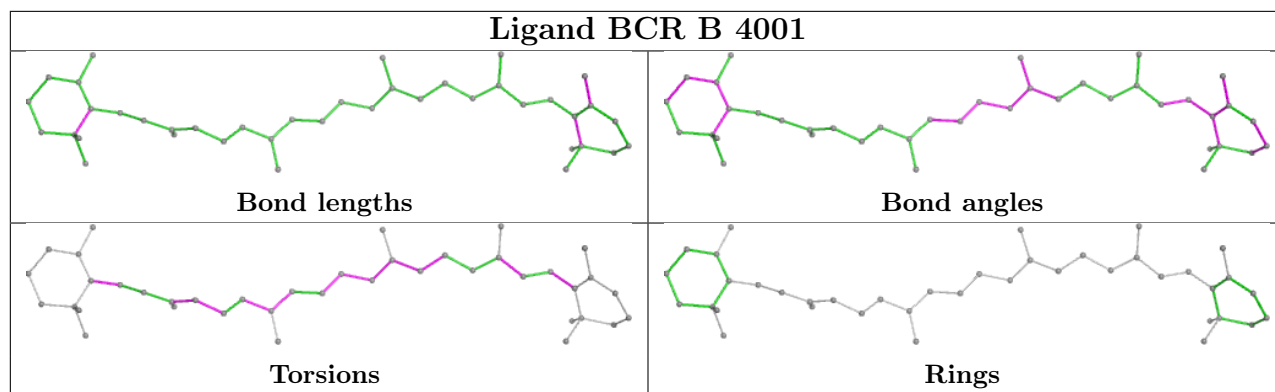


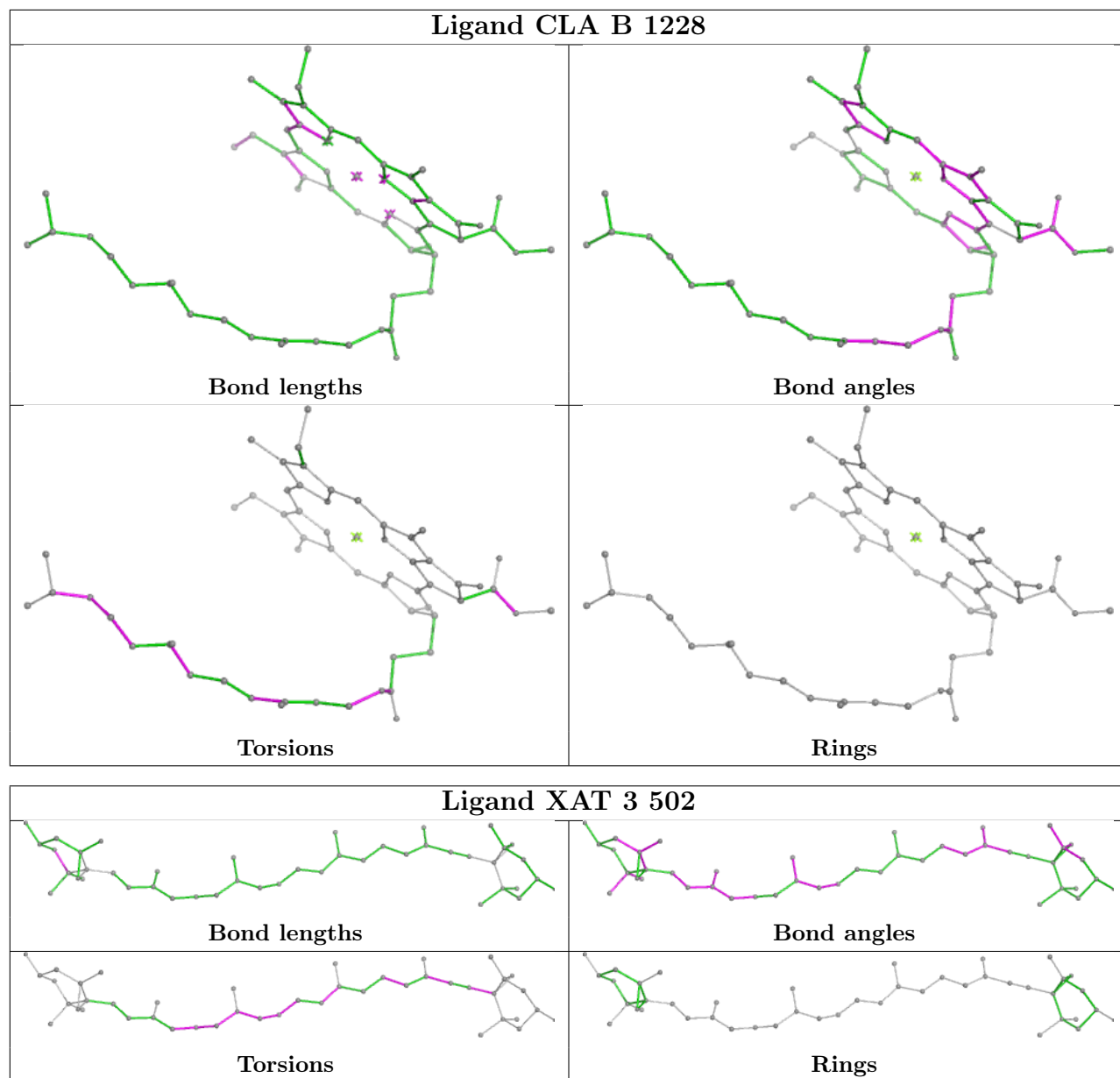
Ligand CLA 4 608

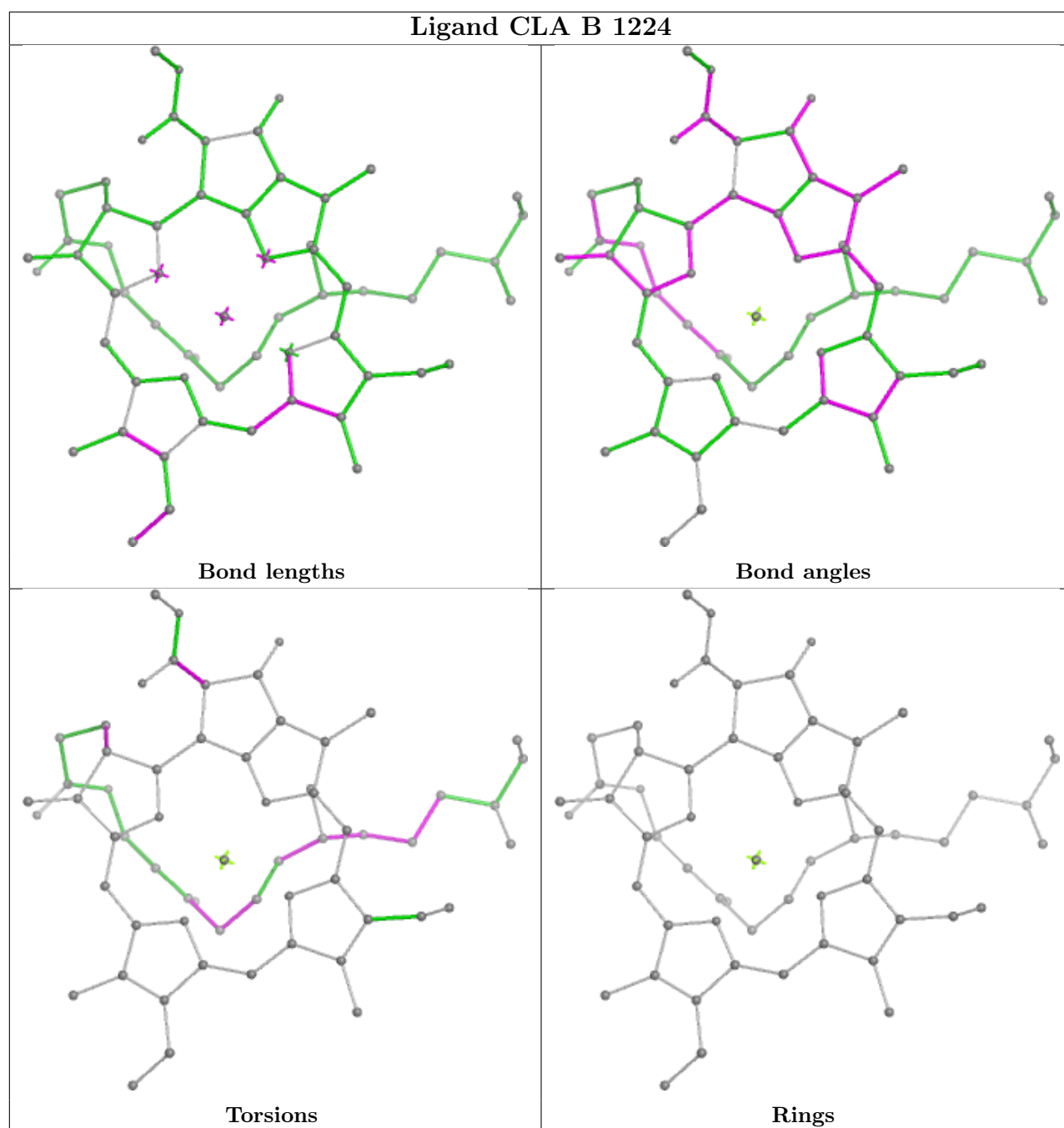


Ligand BCR A 4007









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

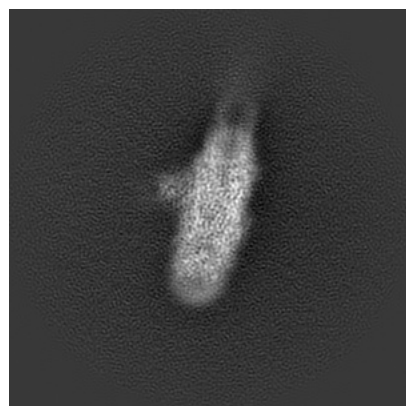
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10995. These allow visual inspection of the internal detail of the map and identification of artifacts.

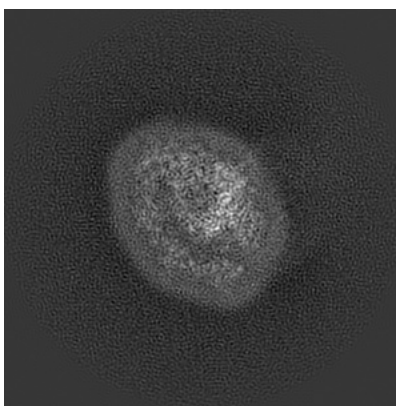
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

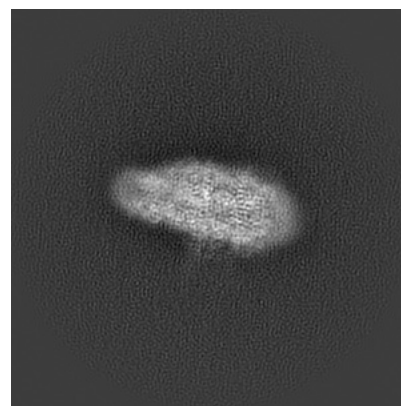
6.1.1 Primary map



X

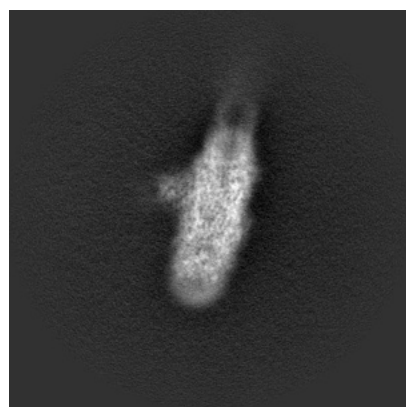


Y

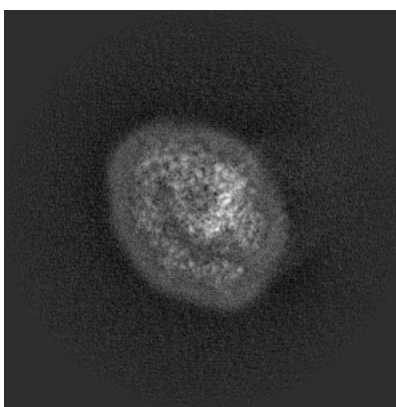


Z

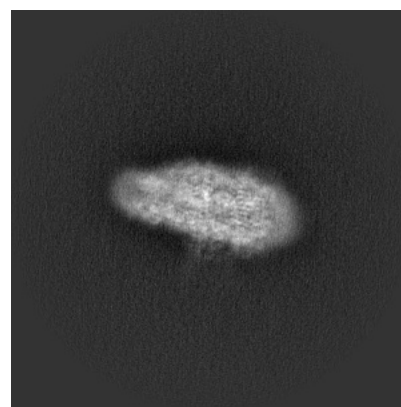
6.1.2 Raw map



X



Y

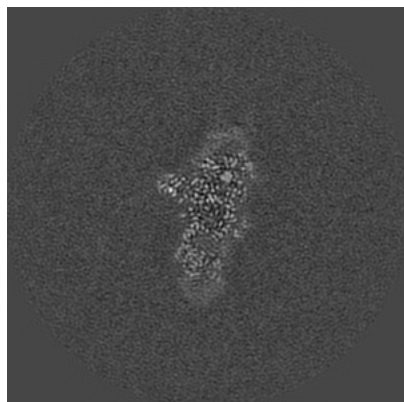


Z

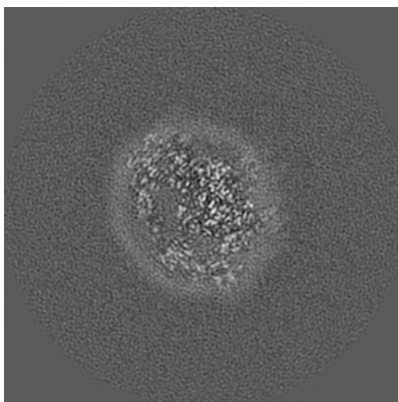
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

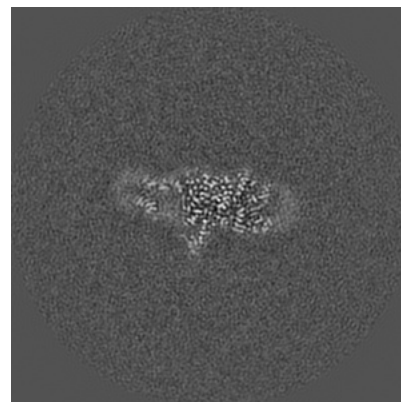
6.2.1 Primary map



X Index: 180

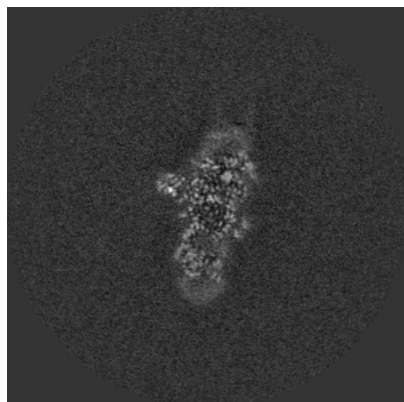


Y Index: 180

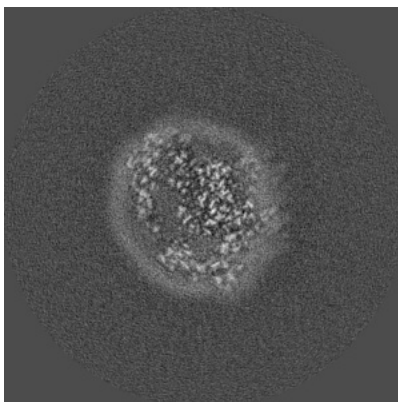


Z Index: 180

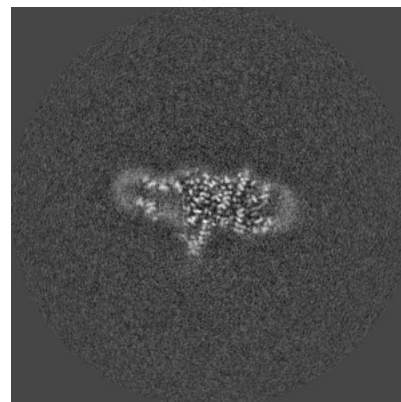
6.2.2 Raw map



X Index: 180



Y Index: 180

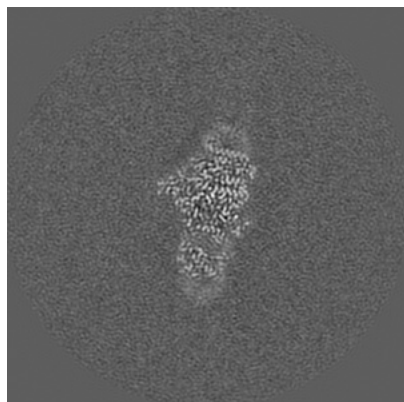


Z Index: 180

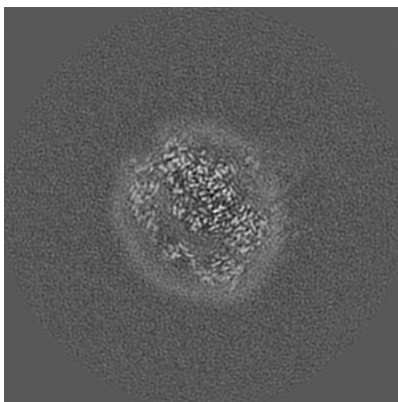
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

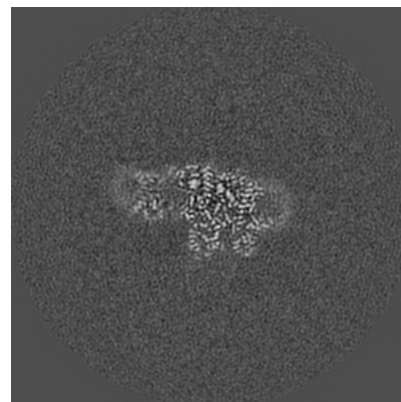
6.3.1 Primary map



X Index: 176

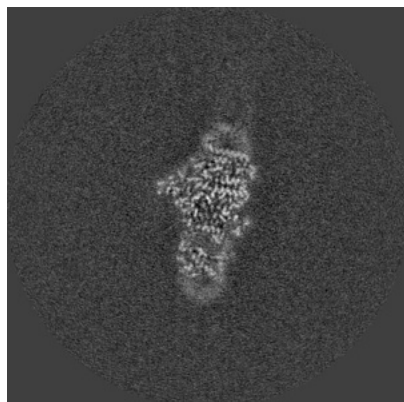


Y Index: 185

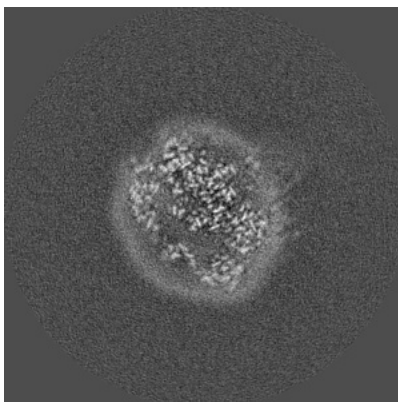


Z Index: 192

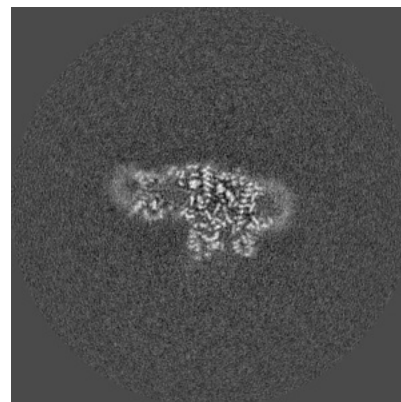
6.3.2 Raw map



X Index: 176



Y Index: 185

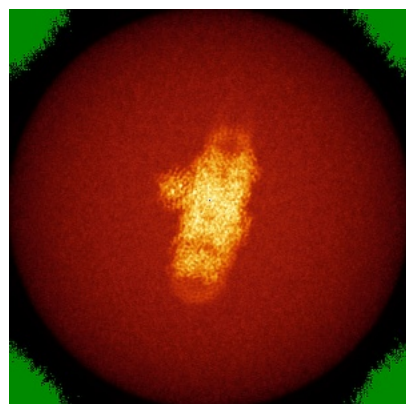


Z Index: 192

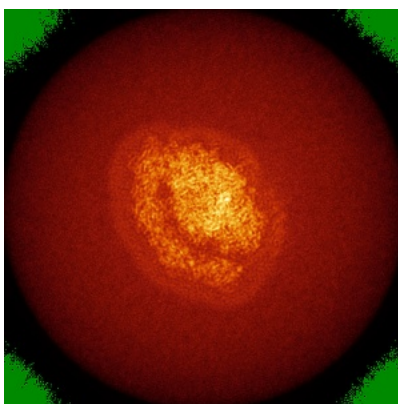
The images above show the largest variance slices of the map in three orthogonal directions.

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

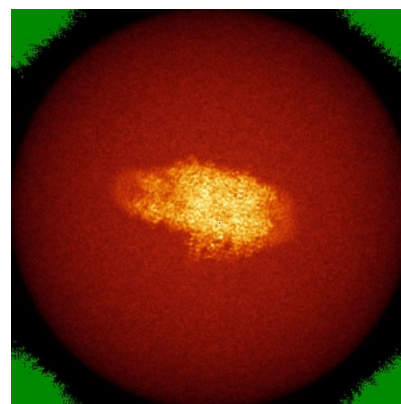
6.4.1 Primary map



X

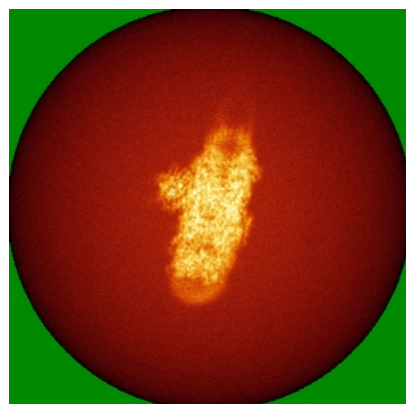


Y

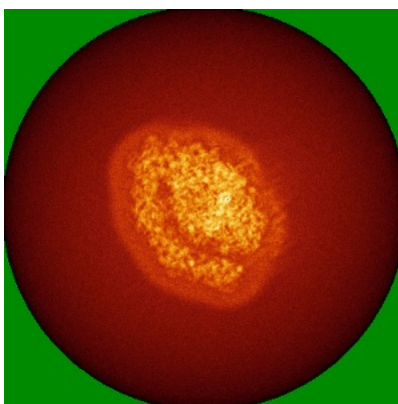


Z

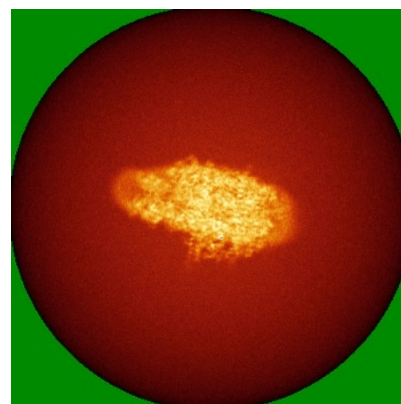
6.4.2 Raw map



X



Y

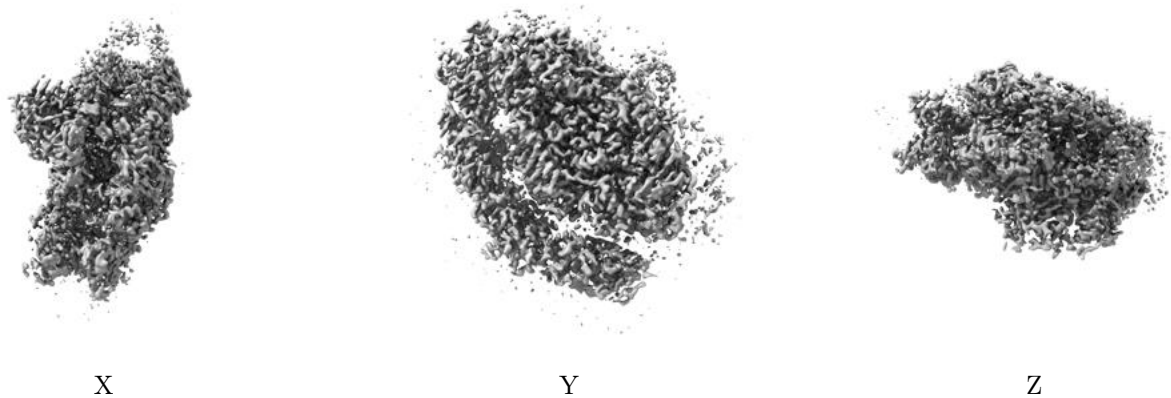


Z

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

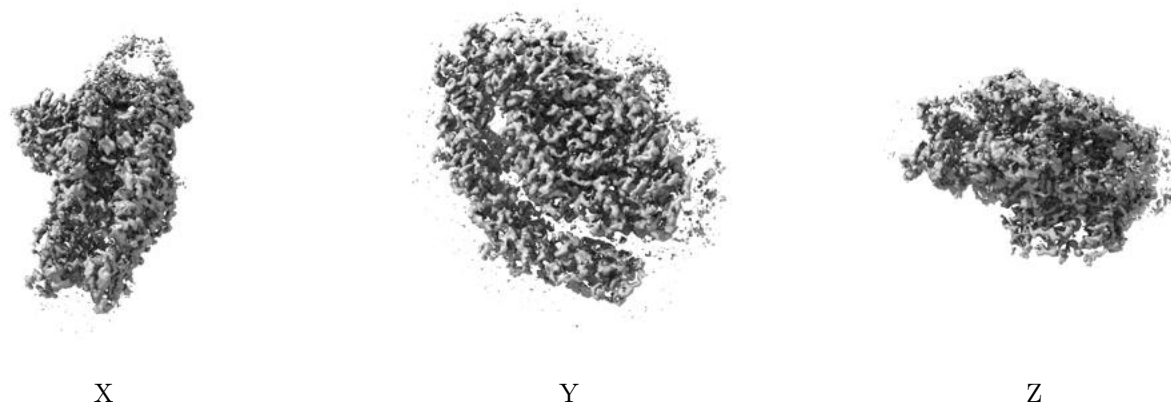
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

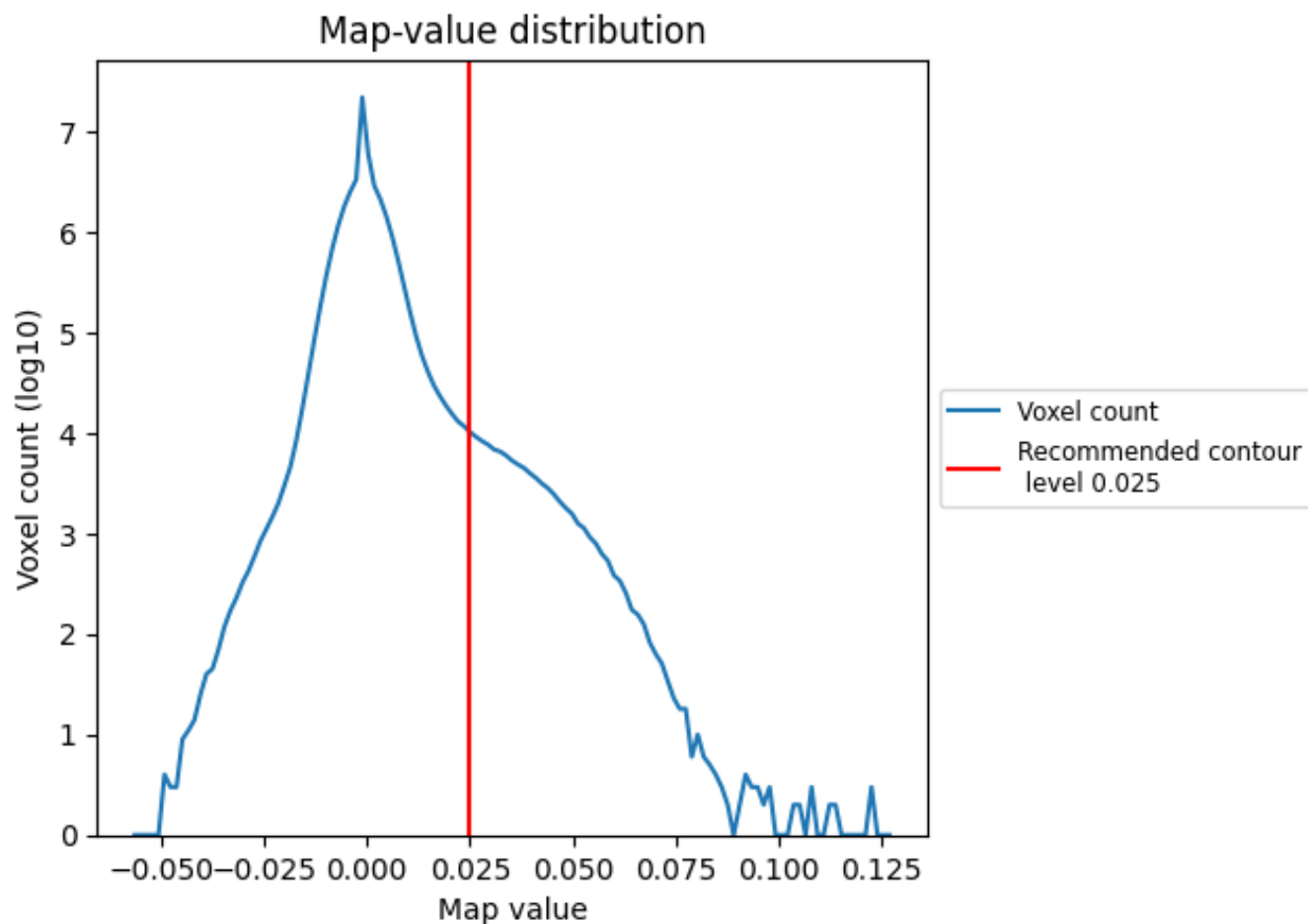
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

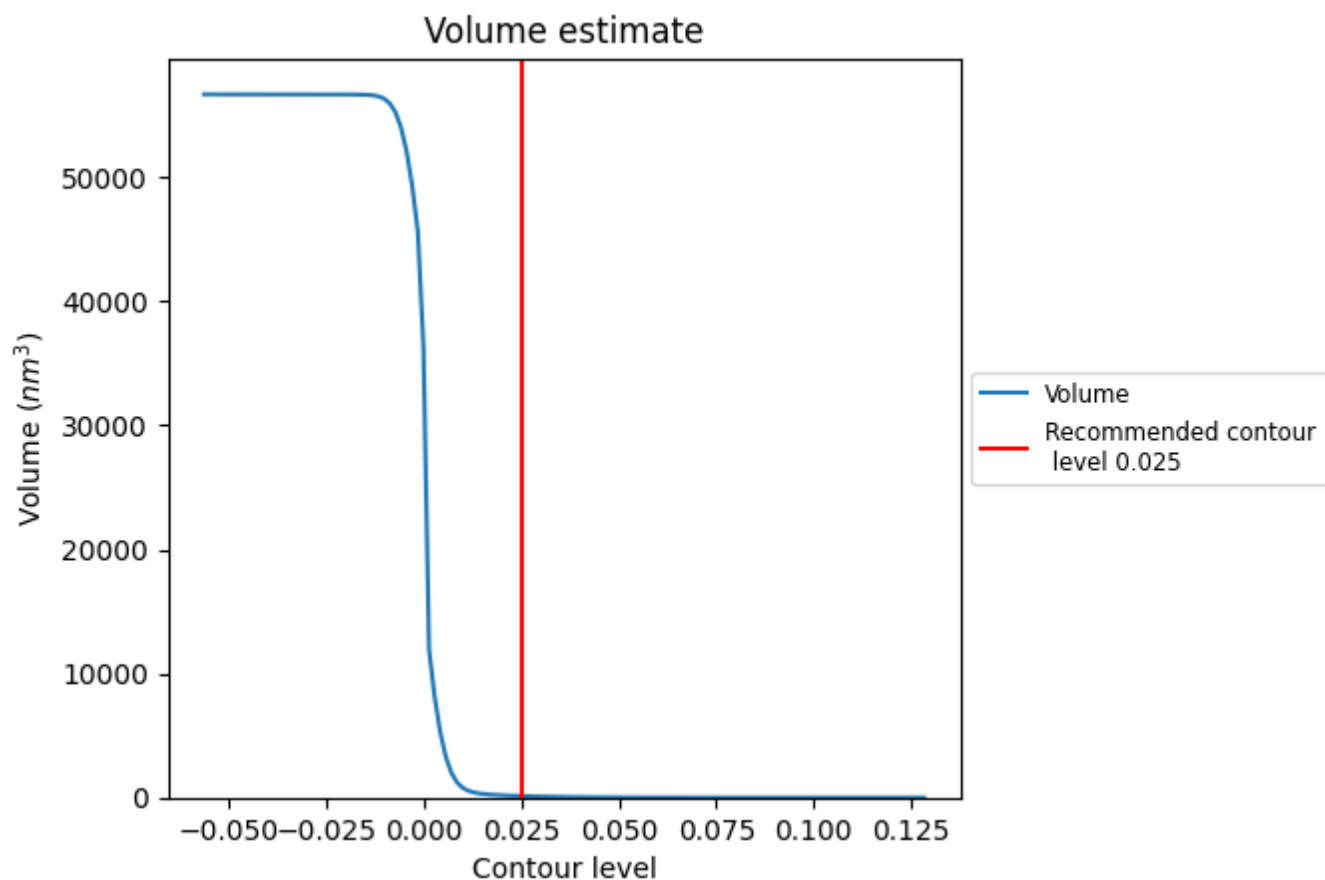
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

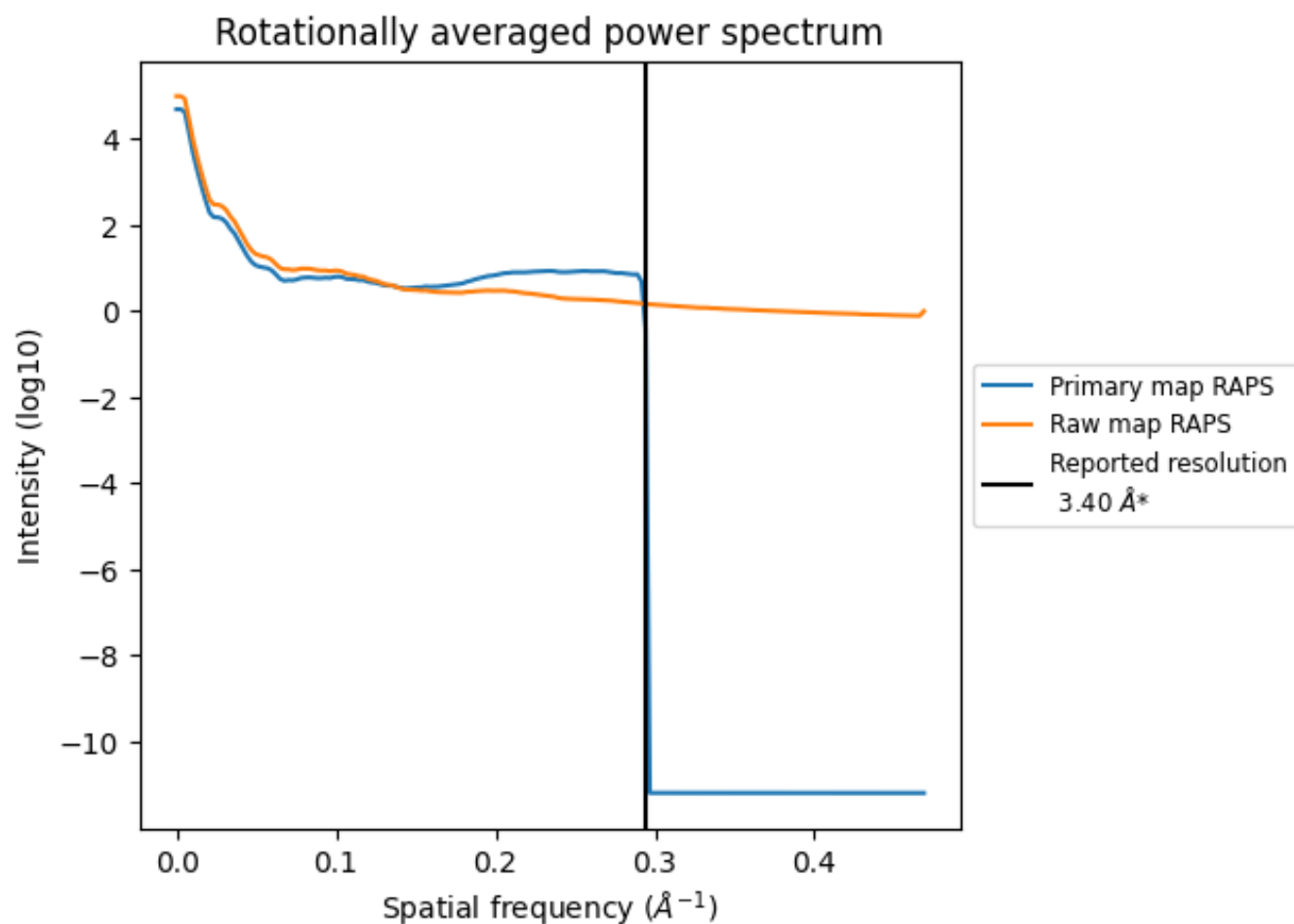
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm³; this corresponds to an approximate mass of 108 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 ⓘ

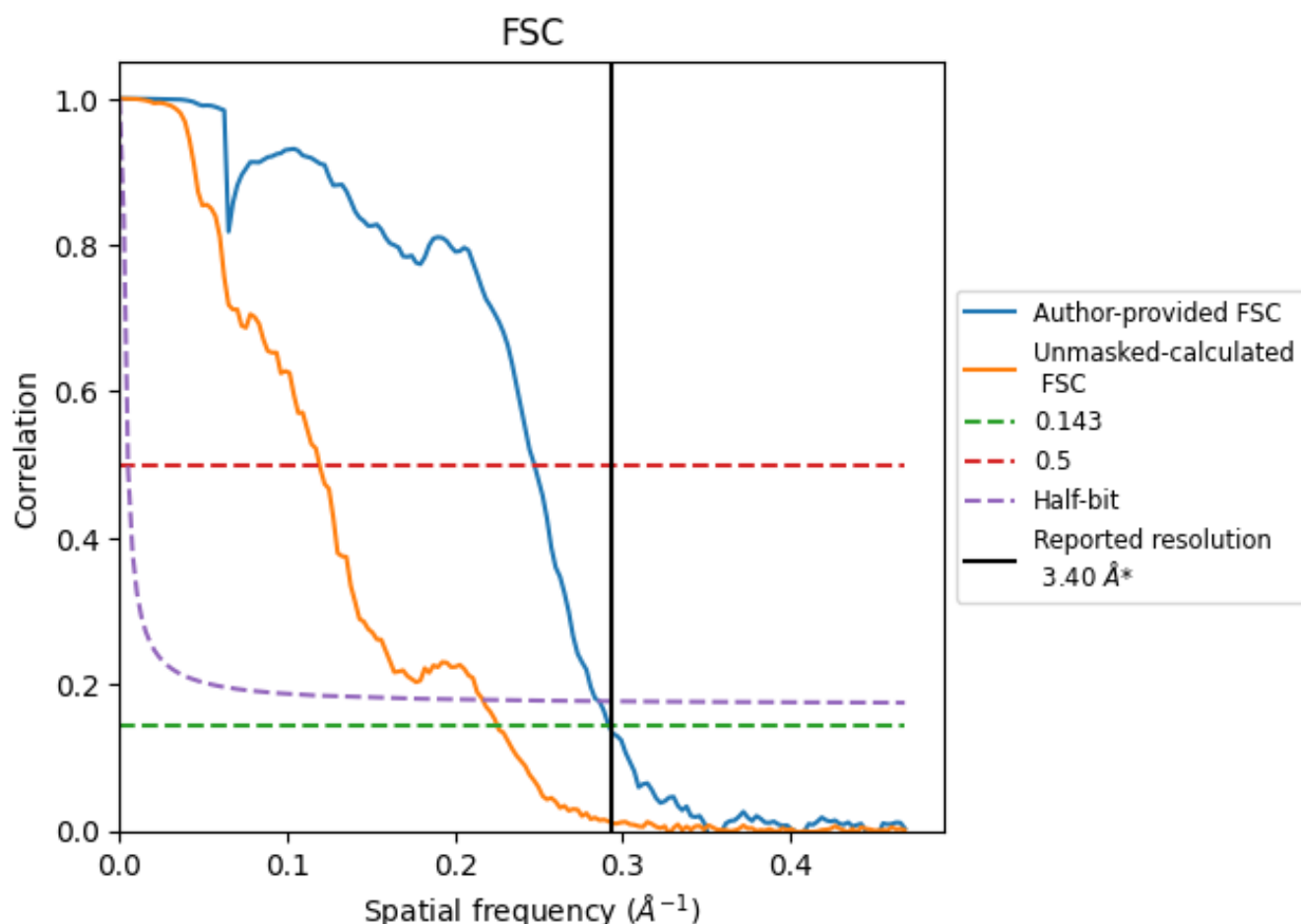


*Reported resolution corresponds to spatial frequency of 0.294 \AA^{-1}

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

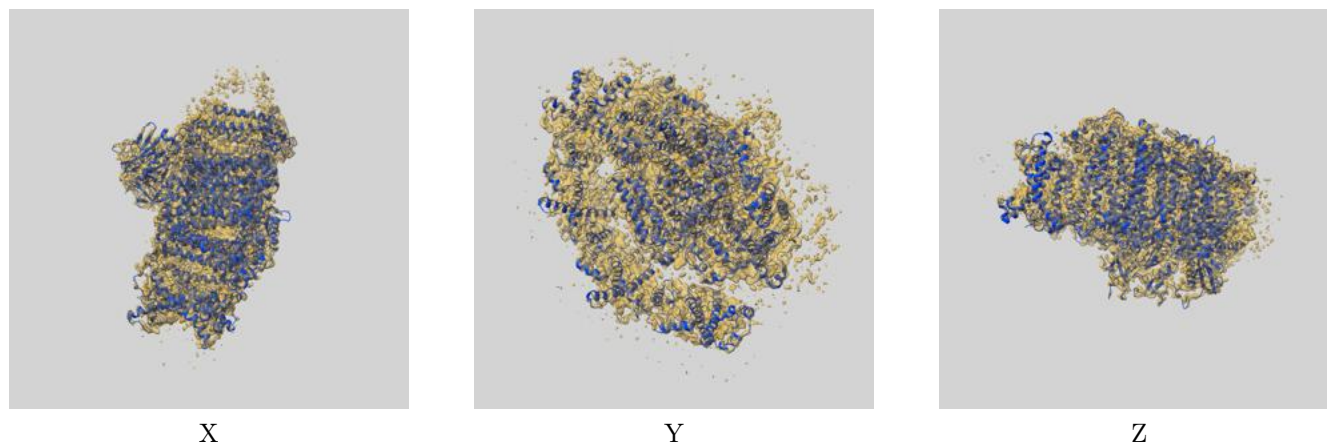
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.42	4.04	3.49
Unmasked-calculated*	4.43	8.38	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.43 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

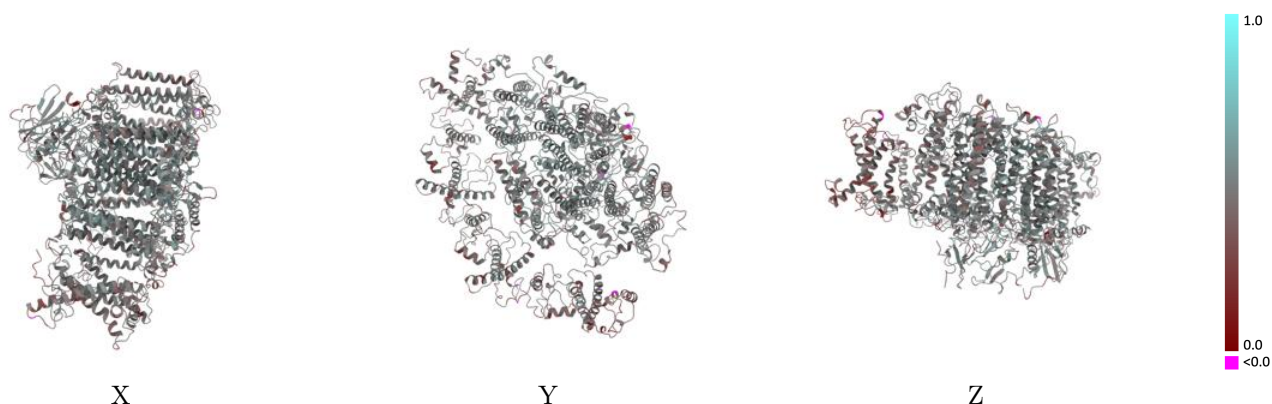
This section contains information regarding the fit between EMDB map EMD-10995 and PDB model 6YXR. Per-residue inclusion information can be found in [section 3](#) on [page 25](#).

9.1 Map-model overlay [i](#)



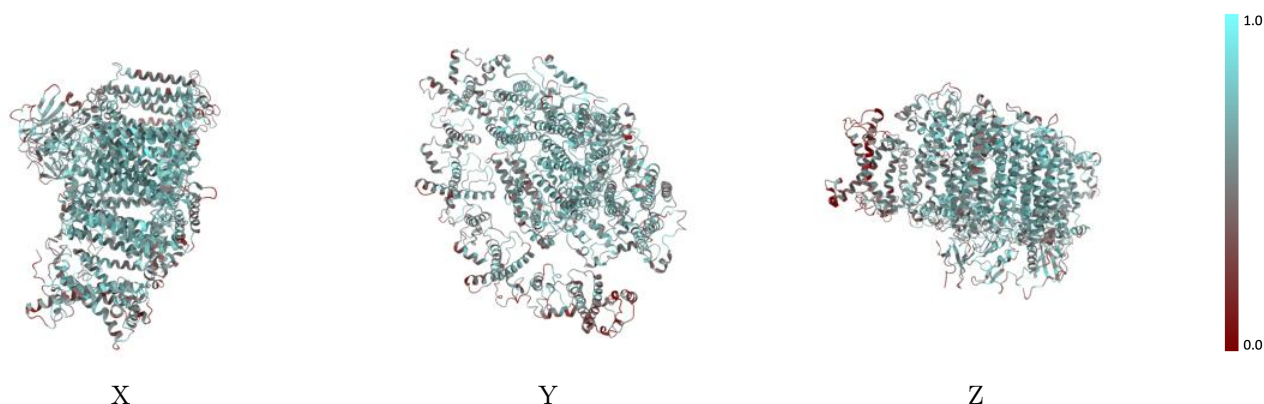
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



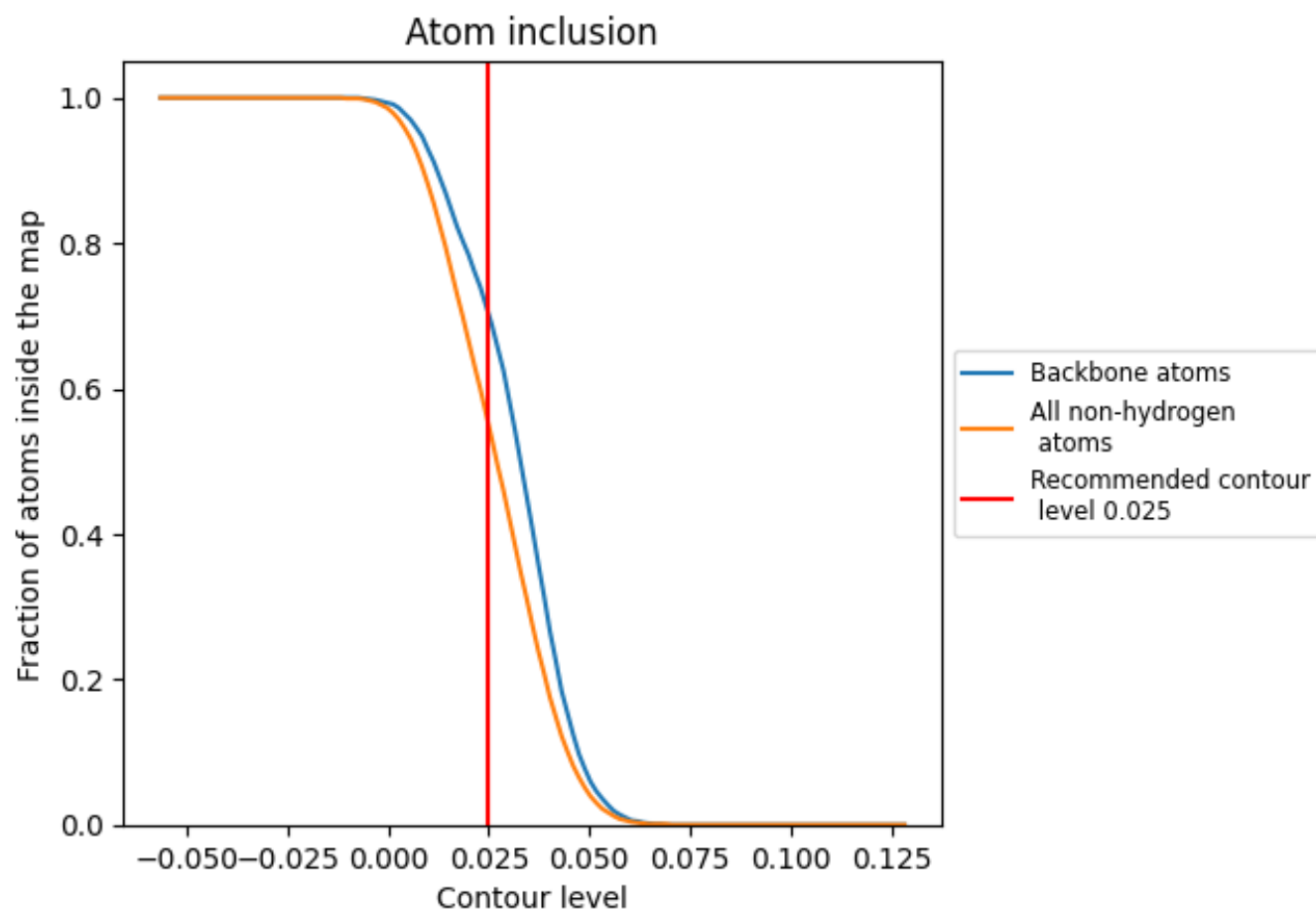
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 55% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5510	<div></div> 0.4530
1	<div></div> 0.3790	<div></div> 0.3630
2	<div></div> 0.4880	<div></div> 0.4320
3	<div></div> 0.4640	<div></div> 0.4200
4	<div></div> 0.4850	<div></div> 0.4160
A	<div></div> 0.6340	<div></div> 0.4970
B	<div></div> 0.5750	<div></div> 0.4530
C	<div></div> 0.6380	<div></div> 0.4890
D	<div></div> 0.5180	<div></div> 0.4550
E	<div></div> 0.5550	<div></div> 0.4630
F	<div></div> 0.5620	<div></div> 0.4680
J	<div></div> 0.6000	<div></div> 0.5000

