



wwPDB EM Validation Summary Report ⓘ

Apr 2, 2025 – 03:24 am BST

PDB ID : 6RHZ / pdb_00006rhz
EMDB ID : EMD-4883
Title : Structure of a minimal photosystem I from a green alga
Authors : Perez Boerema, A.; Klaiman, D.; Caspy, I.; Netzer-El, S.Y.; Amunts, A.;
Nelson, N.
Deposited on : 2019-04-23
Resolution : 3.20 Å(reported)
Based on initial model : 5L8R

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

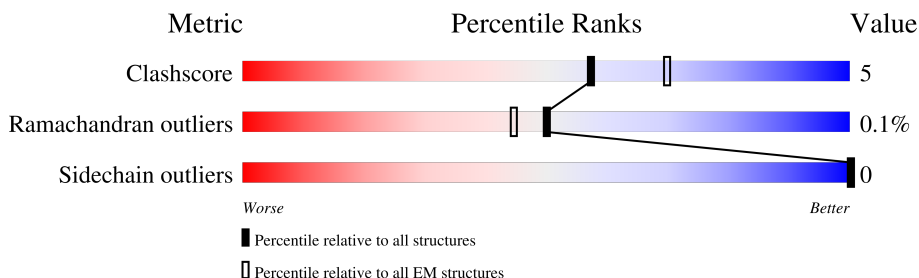
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.




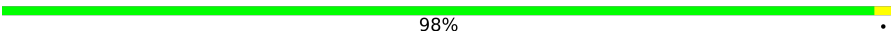
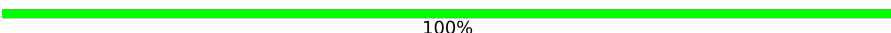
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	
2	2	208	
3	3	210	
4	4	211	
5	A	739	
6	B	730	
7	C	80	
8	D	141	

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Mol	Chain	Length	Quality of chain
9	E	64	 91% 9%
10	F	163	 98%
11	J	40	 100%

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	-	-	-
12	LUT	2	501	X	-	-	-
12	LUT	3	501	X	-	-	-
12	LUT	4	501	X	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	-	-	-
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	-	-	-
15	CLA	3	608	X	-	-	-
15	CLA	3	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
15	CLA	A	1013	X	-	-	-
15	CLA	A	1101	X	-	-	-
15	CLA	A	1102	X	-	-	-
15	CLA	A	1103	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	1112	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	-	-	-
15	CLA	A	1122	X	-	-	-
15	CLA	A	1123	X	-	-	-
15	CLA	A	1124	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	1126	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	1134	X	-	-	-
15	CLA	A	1135	X	-	-	-
15	CLA	A	1136	X	-	-	-
15	CLA	A	1137	X	-	-	-
15	CLA	A	1138	X	-	-	-
15	CLA	A	1139	X	-	-	-
15	CLA	A	1140	X	-	-	-
15	CLA	A	1141	X	-	-	-
15	CLA	B	1021	X	-	-	-
15	CLA	B	1022	X	-	-	-
15	CLA	B	1023	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	-	-	-
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	-	-	-
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	-	-	-
15	CLA	B	1224	X	-	-	-
15	CLA	B	1225	X	-	-	-
15	CLA	B	1226	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-
19	CLO	A	1011	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 63437 atoms, of which 31549 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	H	N	O	S	0	0
			2970	963	1469	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 Chlorophyll a-b binding protein, Lhca2.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	208	Total	C	H	N	O	S	0	0
			3164	1033	1555	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	H	N	O	S	0	0
			3176	1050	1567	263	291	5		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, Lhca4.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4	211	Total	C	H	N	O	S	0	0
			3216	1058	1579	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	H	N	O	S	0	0
			11429	3789	5630	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	H	N	O	S	0	0
			11312	3799	5528	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	H	N	O	S	0	0
			1184	370	584	104	115	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	D	141	Total	C	H	N	O	S	0	0
			2242	714	1126	195	201	6		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV, PsaE.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	E	64	Total	C	H	N	O	S	0	0
			1021	327	506	89	99			

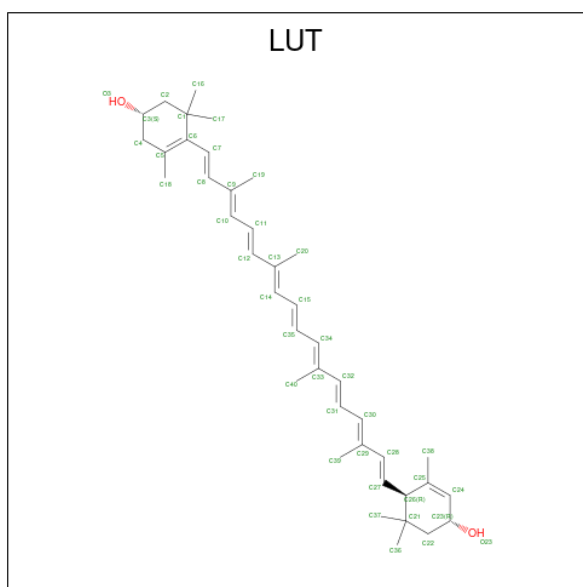
- Molecule 10 is a protein called Photosystem I reaction center subunit III, PsaF.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	F	163	Total	C	H	N	O	S	0	0
			2589	828	1304	218	237	2		

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

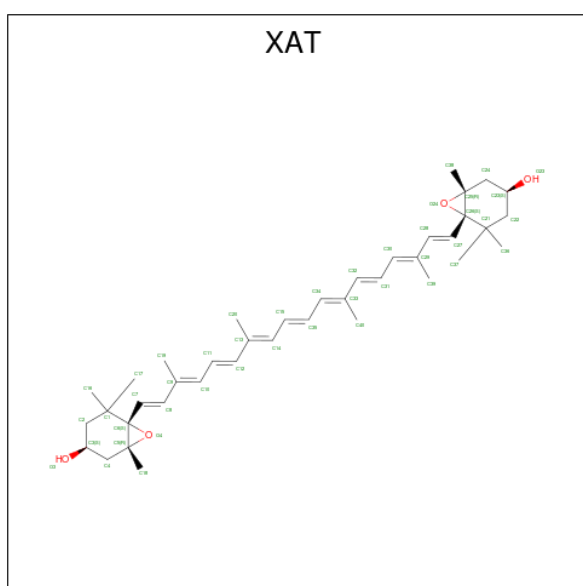
Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	40	Total	C	H	N	O	S	0	0
			635	214	319	46	55	1		

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



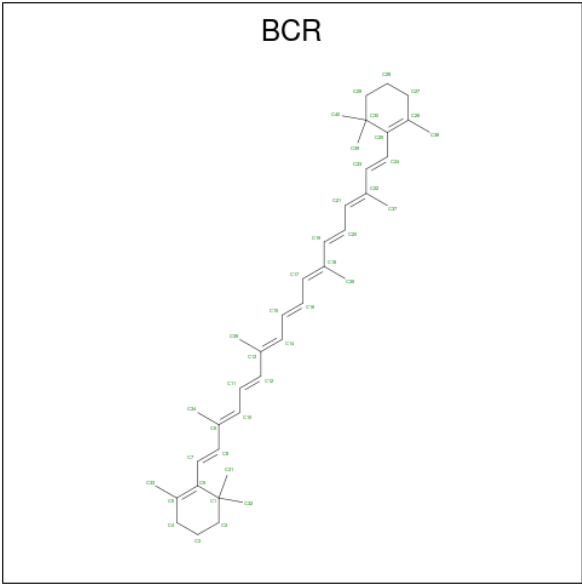
Mol	Chain	Residues	Atoms				AltConf
12	1	1	Total	C	H	O	0
			98	40	56	2	
12	2	1	Total	C	H	O	0
			98	40	56	2	
12	3	1	Total	C	H	O	0
			98	40	56	2	
12	4	1	Total	C	H	O	0
			98	40	56	2	

- 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 (CCD ID: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms				AltConf
13	1	1	Total	C	H	O	0
			100	40	56	4	
13	2	1	Total	C	H	O	0
			100	40	56	4	
13	3	1	Total	C	H	O	0
			100	40	56	4	
13	4	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



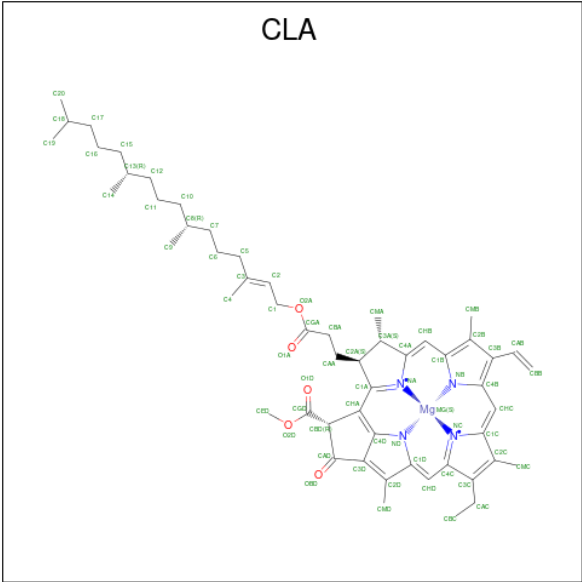
Mol	Chain	Residues	Atoms			AltConf
14	1	1	Total	C	H	0
			92	40	52	
14	2	1	Total	C	H	0
			93	40	53	
14	3	1	Total	C	H	0
			93	40	53	
14	3	1	Total	C	H	0
			92	40	52	
14	3	1	Total	C	H	0
			93	40	53	
14	4	1	Total	C	H	0
			93	40	53	
14	A	1	Total	C	H	0
			93	40	53	
14	A	1	Total	C	H	0
			93	40	53	

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Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	H	0
			92	40	52	
14	A	1	Total	C	H	0
			92	40	52	
14	A	1	Total	C	H	0
			92	40	52	
14	A	1	Total	C	H	0
			92	40	52	
14	A	1	Total	C	H	0
			93	40	53	
14	B	1	Total	C	H	0
			93	40	53	
14	B	1	Total	C	H	0
			92	40	52	
14	B	1	Total	C	H	0
			93	40	53	
14	B	1	Total	C	H	0
			92	40	52	
14	B	1	Total	C	H	0
			91	40	51	
14	B	1	Total	C	H	0
			92	40	52	
14	F	1	Total	C	H	0
			92	40	52	
14	F	1	Total	C	H	0
			90	40	50	
14	J	1	Total	C	H	0
			92	40	52	
14	J	1	Total	C	H	0
			92	40	52	

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



Mol	Chain	Residues	Atoms						AltConf
15	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			116	50	56	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			88	40	38	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			84	38	36	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			68	32	28	1	4	3	
15	1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	1	1	Total	C	H	Mg	N	O	0
			79	38	31	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
15	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			116	50	56	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			74	34	32	1	4	3	
15	3	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
15	3	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
15	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			77	36	31	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	4	1	Total	C	H	Mg	N	O	0
			91	41	40	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			91	41	40	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
15	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
15	A	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
15	B	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	

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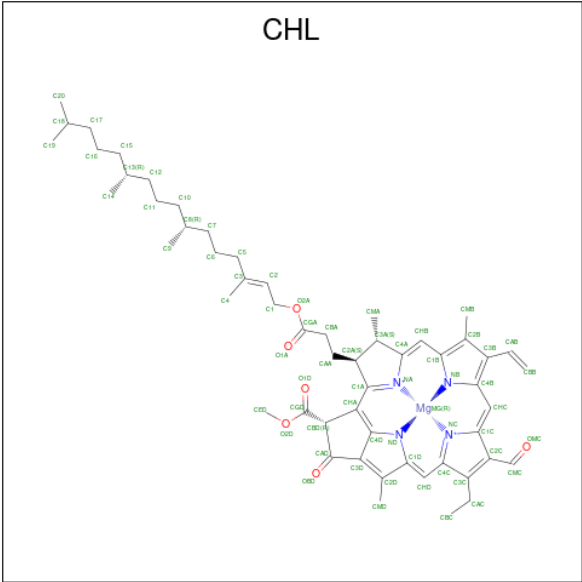
Mol	Chain	Residues	Atoms						AltConf
15	B	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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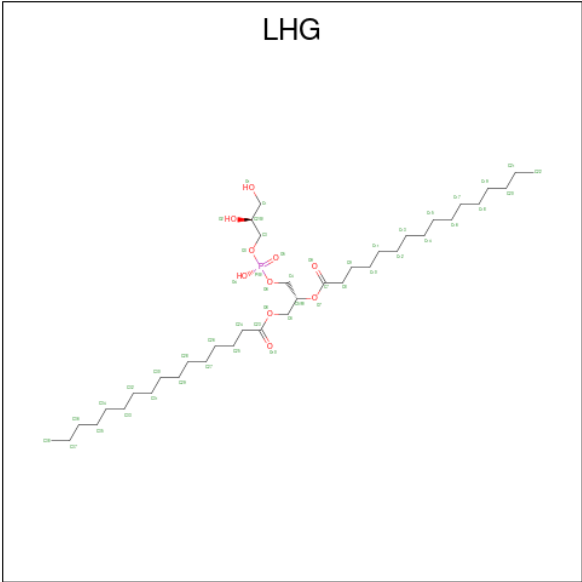
Mol	Chain	Residues	Atoms						AltConf
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
15	B	1	Total	C	H	Mg	N	O	0
			102	44	50	1	4	3	
15	B	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
15	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
15	F	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
15	F	1	Total	C	H	Mg	N	O	0
			88	39	39	1	4	5	
15	J	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	

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



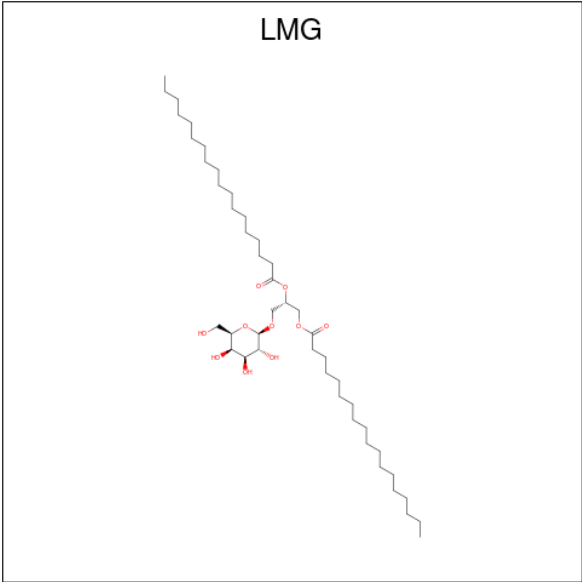
Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	Mg	N	O	
16	1	1	Total 136	55	70	1	4	6	0
16	1	1	Total 80	36	33	1	4	6	0
16	2	1	Total 136	55	70	1	4	6	0
16	2	1	Total 75	35	31	1	4	4	0
16	2	1	Total 82	37	34	1	4	6	0
16	2	1	Total 77	35	31	1	4	6	0
16	3	1	Total 120	50	59	1	4	6	0
16	4	1	Total 80	36	33	1	4	6	0
16	4	1	Total 90	40	39	1	4	6	0
16	4	1	Total 120	50	59	1	4	6	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



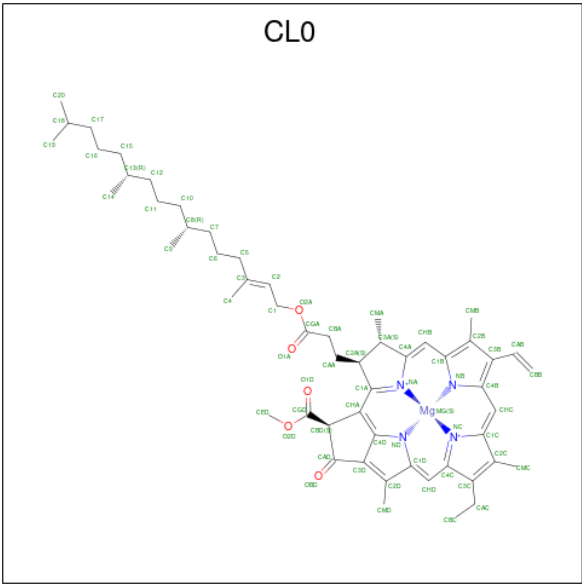
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	2	1	Total	C	H	O	P	0
			75	24	40	10	1	
17	3	1	Total	C	H	O	P	0
			116	37	68	10	1	
17	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
17	B	1	Total	C	H	O	P	0
			99	31	57	10	1	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



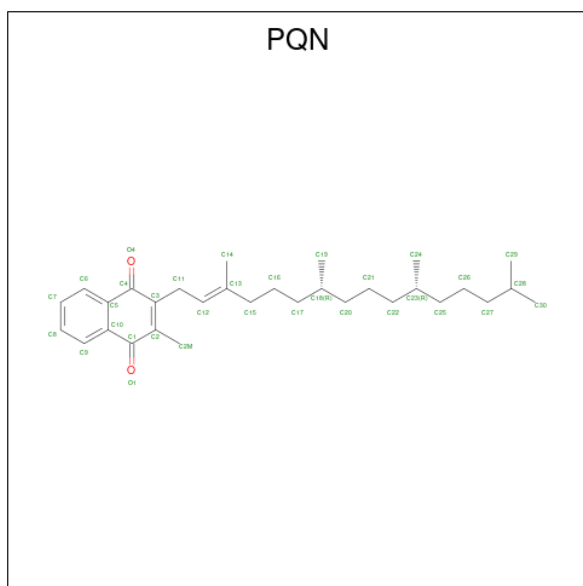
Mol	Chain	Residues	Atoms				AltConf
18	2	1	Total	C	H	O	0
			123	40	73	10	
18	2	1	Total	C	H	O	0
			90	30	50	10	
18	2	1	Total	C	H	O	0
			123	40	73	10	
18	4	1	Total	C	H	O	0
			80	27	43	10	
18	B	1	Total	C	H	O	0
			87	29	48	10	

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



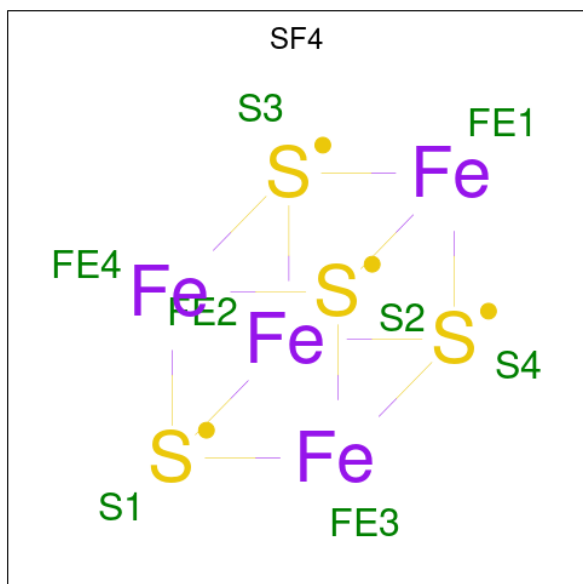
Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 20 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



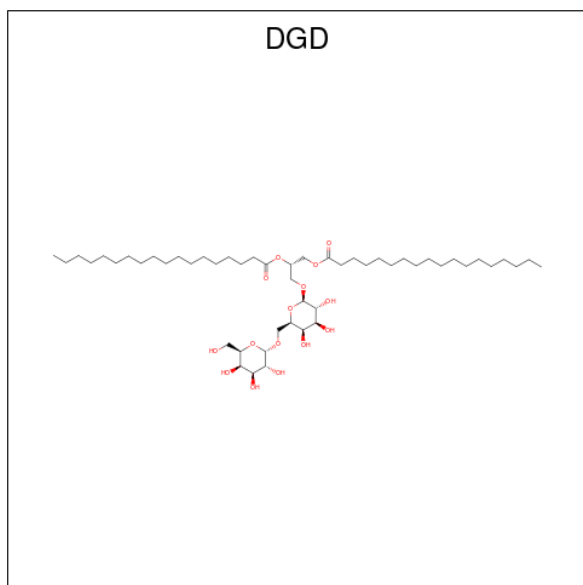
Mol	Chain	Residues	Atoms				AltConf
20	A	1	Total	C	H	O	0
			79	31	46	2	
20	B	1	Total	C	H	O	0
			79	31	46	2	

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



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

- Molecule 22 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).

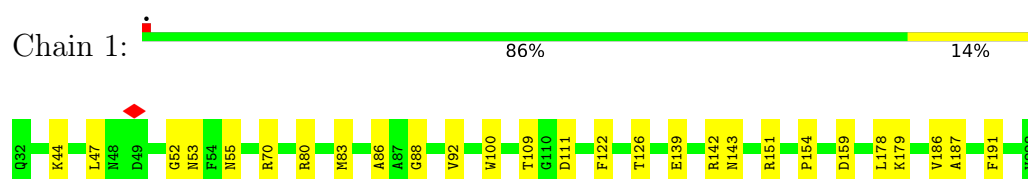


Mol	Chain	Residues	Atoms				AltConf
22	B	1	Total	C	H	O	0
			144	46	83	15	

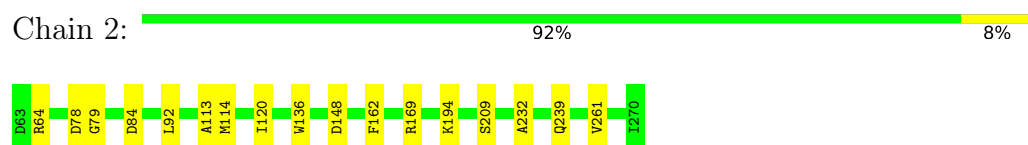
3 Residue-property plots

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.

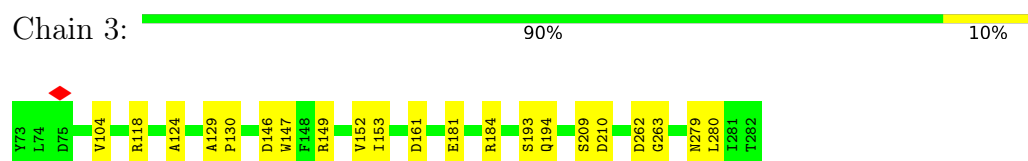
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



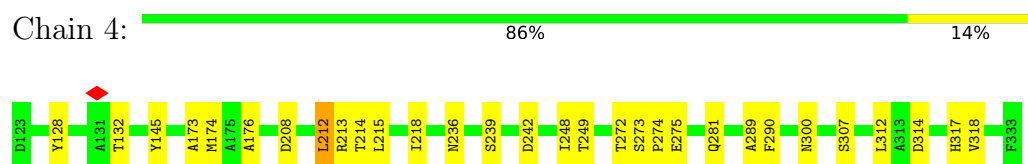
- Molecule 2: Chlorophyll a-b binding protein, Lhca2



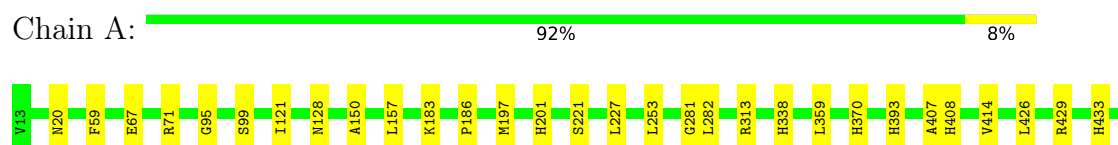
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



- Molecule 4: Chlorophyll a-b binding protein, Lhca4



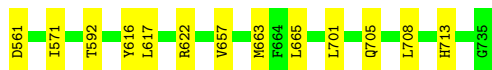
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1





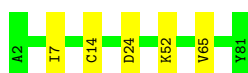
- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 94% 6%



- Molecule 7: Photosystem I iron-sulfur center

Chain C: 94% 6%



- Molecule 8: Photosystem I reaction center subunit II, PsaD

Chain D: 87% 13%



- Molecule 9: Photosystem I reaction center subunit IV, PsaE

Chain E: 91% 9%



- Molecule 10: Photosystem I reaction center subunit III, PsaF

Chain F: 98% 2%



- Molecule 11: Photosystem I reaction center subunit IX

Chain J: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	132017	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.299	Depositor
Minimum map value	-4.307	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.186	Depositor
Recommended contour level	1	Depositor
Map size (\AA)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.36	0/1657	0.48	0/2253
4	4	0.33	0/1687	0.53	0/2300
5	A	0.37	0/5995	0.46	0/8179
6	B	0.38	0/5997	0.46	0/8198
7	C	0.39	0/610	0.53	0/828
8	D	0.36	0/1145	0.55	0/1546
9	E	0.37	0/525	0.50	0/712
10	F	0.32	0/1313	0.48	0/1776
11	J	0.36	0/326	0.46	0/445
All	All	0.36	0/22451	0.48	0/30568

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
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	4	213	ARG	Peptide
4	4	274	PRO	Peptide
5	A	313	ARG	Peptide

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	1469	1469	24	0
2	2	1609	1555	1555	15	0
3	3	1609	1567	1566	13	0
4	4	1637	1579	1579	22	0
5	A	5799	5630	5628	46	0
6	B	5784	5528	5527	39	0
7	C	600	584	581	4	0
8	D	1116	1126	1126	12	0
9	E	515	506	508	4	0
10	F	1285	1304	1304	5	0
11	J	316	319	319	0	0
12	1	42	56	56	11	0
12	2	42	56	56	5	0
12	3	42	56	56	8	0
12	4	42	56	56	6	0
13	1	44	56	56	3	0
13	2	44	56	56	2	0
13	3	44	56	56	2	0
13	4	44	56	56	6	0
14	1	40	52	56	0	0
14	2	40	53	56	0	0
14	3	120	158	168	5	0
14	4	40	53	56	0	0
14	A	280	367	392	14	0
14	B	240	313	336	11	0
14	F	80	102	112	2	0
14	J	80	104	112	5	0
15	1	633	553	562	21	0
15	2	580	572	573	11	0
15	3	732	700	704	17	0
15	4	632	601	604	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	2487	2465	2473	50	0
15	B	2411	2358	2359	43	0
15	F	95	72	72	0	0
15	J	42	31	31	0	0
16	1	113	103	101	2	0
16	2	204	166	165	2	0
16	3	61	59	57	1	0
16	4	159	131	125	1	0
17	1	49	74	74	1	0
17	2	35	40	40	0	0
17	3	48	68	68	0	0
17	A	98	148	148	2	0
17	B	42	57	57	0	0
18	2	140	196	196	0	0
18	4	37	43	44	0	0
18	B	39	48	48	2	0
19	A	65	72	71	3	0
20	A	33	46	46	0	0
20	B	33	46	46	0	0
21	A	8	0	0	0	0
21	C	16	0	0	1	0
22	B	61	83	83	2	0
All	All	31888	31549	31645	293	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 5.

The worst 5 of 293 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)
15:B:1214:CLA:H43	15:B:1231:CLA:HED3	1.61	0.82
7:C:7:ILE:HG22	7:C:65:VAL:HG22	1.67	0.77
5:A:71:ARG:NH1	5:A:186:PRO:O	2.19	0.76
3:3:181:GLU:OE1	3:3:184:ARG:NH1	2.20	0.74
2:2:169:ARG:NH2	15:2:612:CLA:O1D	2.21	0.73

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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	60
5	A	737/739 (100%)	706 (96%)	30 (4%)	1 (0%)	48	80
6	B	728/730 (100%)	713 (98%)	15 (2%)	0	100	100
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%)	159 (99%)	2 (1%)	0	100	100
11	J	38/40 (95%)	34 (90%)	4 (10%)	0	100	100
All	All	2761/2783 (99%)	2656 (96%)	103 (4%)	2 (0%)	50	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4	212	LEU
5	A	477	ILE

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%)	169 (100%)	0	100	100
5	A	598/598 (100%)	598 (100%)	0	100	100
6	B	590/590 (100%)	590 (100%)	0	100	100
7	C	68/68 (100%)	68 (100%)	0	100	100
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%)	35 (100%)	0	100	100
All	All	2253/2253 (100%)	2253 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
6	B	713	HIS
9	E	86	GLN
10	F	223	GLN
9	E	117	ASN
4	4	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

193 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
17	LHG	A	5001	15	48,48,48	0.64	0	51,54,54	1.12	3 (5%)
15	CLA	1	605	-	65,73,73	1.47	8 (12%)	76,113,113	1.36	4 (5%)
15	CLA	3	614	-	52,60,73	1.69	8 (15%)	60,97,113	1.61	7 (11%)
14	BCR	3	506	-	41,41,41	1.21	3 (7%)	56,56,56	1.30	8 (14%)
15	CLA	B	1207	-	46,54,73	1.74	6 (13%)	53,90,113	1.50	6 (11%)
16	CHL	4	610	-	47,55,74	1.07	3 (6%)	50,91,114	1.49	10 (20%)
15	CLA	B	1238	-	51,59,73	1.85	9 (17%)	58,95,113	2.15	14 (24%)
15	CLA	F	1302	10	49,57,73	1.66	7 (14%)	55,93,113	1.58	8 (14%)
15	CLA	B	1217	-	46,54,73	1.71	8 (17%)	53,90,113	1.51	6 (11%)
15	CLA	B	1206	6	45,53,73	1.72	7 (15%)	52,89,113	1.57	7 (13%)
15	CLA	A	1140	-	61,69,73	1.52	8 (13%)	71,108,113	1.48	8 (11%)
15	CLA	A	1122	-	65,73,73	1.49	9 (13%)	76,113,113	1.54	12 (15%)
21	SF4	A	3001	5,6	0,12,12	-	-	-	-	-
16	CHL	2	613	-	46,54,74	1.01	2 (4%)	49,90,114	1.32	8 (16%)
14	BCR	3	504	-	41,41,41	1.28	4 (9%)	56,56,56	1.32	9 (16%)
15	CLA	B	1215	-	65,73,73	1.44	7 (10%)	76,113,113	1.42	11 (14%)
15	CLA	1	604	1	65,73,73	1.43	9 (13%)	76,113,113	1.35	8 (10%)
15	CLA	3	609	-	42,50,73	1.80	7 (16%)	48,85,113	1.61	6 (12%)
15	CLA	A	1102	-	65,73,73	1.45	9 (13%)	76,113,113	1.48	10 (13%)
13	XAT	1	502	-	39,47,47	2.59	17 (43%)	54,74,74	11.46	25 (46%)
15	CLA	B	1232	-	46,54,73	1.76	8 (17%)	53,90,113	1.51	5 (9%)
15	CLA	A	1124	-	60,68,73	1.50	8 (13%)	70,107,113	1.52	6 (8%)
14	BCR	B	4004	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	7 (12%)
15	CLA	B	1216	-	59,67,73	1.50	9 (15%)	68,105,113	1.45	9 (13%)
15	CLA	A	1118	-	42,50,73	1.76	7 (16%)	48,85,113	1.63	6 (12%)
15	CLA	2	607	17	60,68,73	1.51	9 (15%)	70,107,113	1.43	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LUT	1	501	-	42,43,43	5.97	30 (71%)	51,60,60	2.29	15 (29%)
15	CLA	A	1126	-	65,73,73	1.49	7 (10%)	76,113,113	1.35	10 (13%)
20	PQN	B	2002	-	34,34,34	0.69	0	42,45,45	0.90	1 (2%)
15	CLA	B	1203	-	65,73,73	1.45	9 (13%)	76,113,113	1.41	6 (7%)
15	CLA	1	615	1	47,55,73	1.76	8 (17%)	53,90,113	1.66	9 (16%)
15	CLA	4	605	-	65,73,73	1.44	6 (9%)	76,113,113	1.46	9 (11%)
13	XAT	2	502	-	39,47,47	2.63	15 (38%)	54,74,74	10.93	32 (59%)
14	BCR	J	4001	-	41,41,41	1.10	1 (2%)	56,56,56	1.37	8 (14%)
15	CLA	A	1113	-	45,53,73	1.72	7 (15%)	52,89,113	1.58	5 (9%)
15	CLA	B	1226	-	65,73,73	1.42	7 (10%)	76,113,113	1.52	8 (10%)
15	CLA	A	1104	-	65,73,73	1.47	9 (13%)	76,113,113	1.42	10 (13%)
15	CLA	4	612	4	65,73,73	1.45	8 (12%)	76,113,113	1.34	7 (9%)
18	LMG	4	801	-	37,37,55	1.02	3 (8%)	45,45,63	1.30	3 (6%)
15	CLA	3	615	3	42,50,73	1.77	6 (14%)	48,85,113	1.54	6 (12%)
15	CLA	F	1301	-	46,54,73	1.72	7 (15%)	53,90,113	1.55	6 (11%)
15	CLA	A	1129	-	55,63,73	1.60	10 (18%)	64,101,113	1.49	9 (14%)
21	SF4	C	3003	7	0,12,12	-	-	-	-	-
15	CLA	2	604	2	65,73,73	1.42	9 (13%)	76,113,113	1.38	10 (13%)
15	CLA	4	602	-	50,58,73	1.68	7 (14%)	58,95,113	1.56	7 (12%)
14	BCR	B	4002	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	7 (12%)
16	CHL	3	604	3	61,69,74	0.90	3 (4%)	67,108,114	1.33	12 (17%)
15	CLA	A	1136	-	65,73,73	1.46	8 (12%)	76,113,113	1.37	6 (7%)
15	CLA	A	1133	-	65,73,73	1.47	8 (12%)	76,113,113	1.44	7 (9%)
15	CLA	A	1119	-	65,73,73	1.44	8 (12%)	76,113,113	1.38	8 (10%)
14	BCR	A	4005	-	41,41,41	1.22	3 (7%)	56,56,56	1.25	8 (14%)
15	CLA	A	1110	-	55,63,73	1.63	8 (14%)	64,101,113	1.65	13 (20%)
15	CLA	B	1214	-	65,73,73	1.49	9 (13%)	76,113,113	1.52	10 (13%)
14	BCR	3	503	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	7 (12%)
14	BCR	A	4007	-	41,41,41	1.22	3 (7%)	56,56,56	1.30	9 (16%)
15	CLA	B	1208	-	60,68,73	1.54	8 (13%)	70,107,113	1.37	8 (11%)
14	BCR	F	4002	-	41,41,41	1.24	3 (7%)	56,56,56	1.34	7 (12%)
14	BCR	4	503	-	41,41,41	1.26	2 (4%)	56,56,56	1.34	9 (16%)
16	CHL	2	611	-	48,56,74	1.05	3 (6%)	51,92,114	1.33	10 (19%)
14	BCR	A	4006	-	41,41,41	1.25	3 (7%)	56,56,56	1.29	8 (14%)
14	BCR	A	4004	-	41,41,41	1.17	3 (7%)	56,56,56	1.43	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1240	17	65,73,73	1.46	9 (13%)	76,113,113	1.45	10 (13%)
15	CLA	2	602	-	45,53,73	1.80	8 (17%)	52,89,113	1.49	5 (9%)
15	CLA	A	1013	-	65,73,73	1.42	9 (13%)	76,113,113	1.41	9 (11%)
15	CLA	3	608	-	65,73,73	1.45	8 (12%)	76,113,113	1.32	8 (10%)
15	CLA	B	1201	-	43,51,73	1.78	9 (20%)	49,86,113	1.52	7 (14%)
15	CLA	B	1225	-	65,73,73	1.44	7 (10%)	76,113,113	1.41	8 (10%)
15	CLA	3	611	-	65,73,73	1.45	8 (12%)	76,113,113	1.34	6 (7%)
15	CLA	2	616	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	12 (15%)
15	CLA	A	1103	-	65,73,73	1.42	6 (9%)	76,113,113	1.45	8 (10%)
15	CLA	B	1210	-	65,73,73	1.47	8 (12%)	76,113,113	1.37	10 (13%)
15	CLA	1	611	-	48,56,73	1.70	6 (12%)	55,92,113	1.50	7 (12%)
16	CHL	4	611	-	51,59,74	1.04	3 (5%)	55,96,114	1.22	8 (14%)
15	CLA	A	1135	-	51,59,73	1.60	7 (13%)	59,96,113	1.62	6 (10%)
15	CLA	B	1234	-	55,63,73	1.55	7 (12%)	64,101,113	1.52	8 (12%)
14	BCR	B	4001	-	41,41,41	1.19	2 (4%)	56,56,56	1.39	10 (17%)
15	CLA	3	612	3	65,73,73	1.45	7 (10%)	76,113,113	1.39	7 (9%)
15	CLA	A	1130	-	45,53,73	1.74	8 (17%)	52,89,113	1.57	8 (15%)
15	CLA	A	1121	-	45,53,73	1.78	8 (17%)	52,89,113	1.58	6 (11%)
14	BCR	J	4002	-	41,41,41	1.22	4 (9%)	56,56,56	1.27	6 (10%)
15	CLA	B	1022	-	65,73,73	1.48	9 (13%)	76,113,113	1.37	7 (9%)
15	CLA	A	1114	-	55,63,73	1.62	8 (14%)	64,101,113	1.51	4 (6%)
15	CLA	1	603	-	60,68,73	1.48	6 (10%)	70,107,113	1.58	10 (14%)
15	CLA	A	1101	-	65,73,73	1.46	8 (12%)	76,113,113	1.38	7 (9%)
15	CLA	B	1209	-	46,54,73	1.70	7 (15%)	53,90,113	1.54	6 (11%)
16	CHL	1	609	1	66,74,74	0.95	5 (7%)	73,114,114	1.20	8 (10%)
15	CLA	4	601	4	60,68,73	1.54	10 (16%)	70,107,113	1.48	11 (15%)
15	CLA	A	1116	-	56,64,73	1.56	9 (16%)	65,102,113	1.58	10 (15%)
15	CLA	A	1138	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	10 (13%)
15	CLA	A	1125	-	65,73,73	1.44	9 (13%)	76,113,113	1.30	7 (9%)
14	BCR	B	4003	-	41,41,41	1.15	2 (4%)	56,56,56	1.46	9 (16%)
15	CLA	B	1222	-	65,73,73	1.44	8 (12%)	76,113,113	1.43	10 (13%)
15	CLA	A	1131	-	45,53,73	1.79	8 (17%)	52,89,113	1.49	7 (13%)
15	CLA	A	1120	-	42,50,73	1.77	7 (16%)	48,85,113	1.66	7 (14%)
14	BCR	2	503	-	41,41,41	1.18	3 (7%)	56,56,56	1.20	7 (12%)
16	CHL	2	610	-	44,52,74	1.04	3 (6%)	46,87,114	1.39	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CHL	1	610	-	47,55,74	1.01	2 (4%)	50,91,114	1.31	8 (16%)
15	CLA	B	1213	-	55,63,73	1.55	6 (10%)	64,101,113	1.49	8 (12%)
15	CLA	2	603	2	65,73,73	1.49	8 (12%)	76,113,113	1.35	8 (10%)
13	XAT	3	502	-	39,47,47	2.69	19 (48%)	54,74,74	11.58	28 (51%)
15	CLA	B	1205	-	65,73,73	1.46	8 (12%)	76,113,113	1.37	7 (9%)
15	CLA	A	1112	-	65,73,73	1.46	7 (10%)	76,113,113	1.34	6 (7%)
21	SF4	C	3002	7	0,12,12	-	-	-	-	-
14	BCR	F	4001	-	41,41,41	1.17	3 (7%)	56,56,56	1.32	7 (12%)
15	CLA	1	608	-	55,63,73	1.59	7 (12%)	64,101,113	1.48	8 (12%)
14	BCR	B	4006	-	41,41,41	1.24	3 (7%)	56,56,56	1.24	7 (12%)
15	CLA	3	606	-	55,63,73	1.57	7 (12%)	64,101,113	1.46	8 (12%)
15	CLA	B	1235	-	60,68,73	1.51	9 (15%)	70,107,113	1.48	7 (10%)
15	CLA	B	1219	-	65,73,73	1.52	7 (10%)	76,113,113	1.26	7 (9%)
15	CLA	B	1231	-	60,68,73	1.51	8 (13%)	70,107,113	1.51	10 (14%)
15	CLA	3	607	-	60,68,73	1.53	6 (10%)	70,107,113	1.45	8 (11%)
18	LMG	B	5003	-	39,39,55	0.86	1 (2%)	47,47,63	1.25	3 (6%)
15	CLA	1	601	-	65,73,73	1.43	9 (13%)	76,113,113	1.34	8 (10%)
15	CLA	3	610	-	50,58,73	1.64	7 (14%)	58,95,113	1.52	9 (15%)
17	LHG	1	801	15	48,48,48	0.61	0	51,54,54	1.18	4 (7%)
15	CLA	A	1127	-	65,73,73	1.43	7 (10%)	76,113,113	1.35	6 (7%)
15	CLA	A	1123	-	65,73,73	1.46	10 (15%)	76,113,113	1.47	9 (11%)
15	CLA	A	1108	-	55,63,73	1.59	8 (14%)	64,101,113	1.58	7 (10%)
15	CLA	A	1109	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	7 (9%)
14	BCR	A	4003	-	41,41,41	1.15	2 (4%)	56,56,56	1.43	10 (17%)
15	CLA	B	1236	-	49,57,73	1.71	8 (16%)	55,93,113	1.48	6 (10%)
15	CLA	A	1141	17	41,49,73	1.80	9 (21%)	47,84,113	1.57	7 (14%)
15	CLA	2	605	-	65,73,73	1.44	8 (12%)	76,113,113	1.41	8 (10%)
15	CLA	A	1107	5	51,59,73	1.64	8 (15%)	59,96,113	1.60	10 (16%)
16	CHL	2	609	2	66,74,74	0.96	5 (7%)	73,114,114	1.22	10 (13%)
15	CLA	B	1227	-	65,73,73	1.48	9 (13%)	76,113,113	1.38	7 (9%)
17	LHG	B	5001	15	41,41,48	0.72	1 (2%)	44,47,54	1.25	3 (6%)
15	CLA	3	613	-	46,54,73	1.71	7 (15%)	53,90,113	1.59	6 (11%)
15	CLA	A	1134	5	42,50,73	1.77	7 (16%)	48,85,113	1.72	8 (16%)
20	PQN	A	2001	-	34,34,34	0.64	0	42,45,45	0.89	1 (2%)
15	CLA	A	1139	-	65,73,73	1.44	7 (10%)	76,113,113	1.46	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	1220	-	51,59,73	1.68	9 (17%)	59,96,113	1.50	9 (15%)
17	LHG	2	801	15	34,34,48	0.80	1 (2%)	37,40,54	1.22	3 (8%)
15	CLA	B	1212	-	55,63,73	1.58	8 (14%)	64,101,113	1.46	7 (10%)
14	BCR	B	4005	-	41,41,41	1.24	3 (7%)	56,56,56	1.36	10 (17%)
15	CLA	4	606	-	50,58,73	1.65	8 (16%)	58,95,113	1.55	8 (13%)
15	CLA	4	616	4	51,59,73	1.64	6 (11%)	59,96,113	1.48	7 (11%)
15	CLA	B	1230	-	55,63,73	1.56	9 (16%)	64,101,113	1.51	9 (14%)
15	CLA	3	603	-	65,73,73	1.45	8 (12%)	76,113,113	1.37	5 (6%)
15	CLA	B	1239	-	42,50,73	1.80	8 (19%)	48,85,113	1.67	6 (12%)
15	CLA	B	1237	-	45,53,73	1.75	7 (15%)	52,89,113	1.58	6 (11%)
15	CLA	A	1111	-	65,73,73	1.44	8 (12%)	76,113,113	1.44	7 (9%)
15	CLA	B	1023	-	65,73,73	1.45	8 (12%)	76,113,113	1.44	7 (9%)
15	CLA	A	1012	-	65,73,73	1.45	9 (13%)	76,113,113	1.33	10 (13%)
15	CLA	1	613	-	45,53,73	1.74	6 (13%)	52,89,113	1.57	8 (15%)
15	CLA	B	1221	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	7 (9%)
14	BCR	A	4008	-	41,41,41	1.17	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	B	1021	-	65,73,73	1.38	8 (12%)	76,113,113	1.34	6 (7%)
15	CLA	2	608	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	8 (13%)
15	CLA	A	1106	5	65,73,73	1.44	8 (12%)	76,113,113	1.46	9 (11%)
15	CLA	3	605	-	65,73,73	1.43	9 (13%)	76,113,113	1.48	12 (15%)
15	CLA	B	1218	-	45,53,73	1.81	7 (15%)	52,89,113	1.54	4 (7%)
13	XAT	4	502	-	39,47,47	2.58	17 (43%)	54,74,74	11.25	31 (57%)
14	BCR	A	4002	-	41,41,41	1.25	4 (9%)	56,56,56	1.33	6 (10%)
15	CLA	B	1204	-	45,53,73	1.74	8 (17%)	52,89,113	1.65	9 (17%)
15	CLA	B	1211	-	65,73,73	1.46	10 (15%)	76,113,113	1.48	10 (13%)
18	LMG	2	803	-	40,40,55	0.87	1 (2%)	48,48,63	1.19	5 (10%)
15	CLA	4	603	-	65,73,73	1.49	8 (12%)	76,113,113	1.48	9 (11%)
15	CLA	1	607	17	46,54,73	1.72	7 (15%)	53,90,113	1.52	7 (13%)
15	CLA	2	601	-	65,73,73	1.47	8 (12%)	76,113,113	1.26	8 (10%)
15	CLA	J	1302	11	42,50,73	1.76	6 (14%)	48,85,113	1.70	6 (12%)
22	DGD	B	5002	-	62,62,67	0.86	2 (3%)	76,76,81	1.41	11 (14%)
15	CLA	B	1224	-	61,69,73	1.54	8 (13%)	71,108,113	1.35	8 (11%)
15	CLA	4	608	-	46,54,73	1.71	9 (19%)	53,90,113	1.74	10 (18%)
15	CLA	A	1105	-	60,68,73	1.52	9 (15%)	70,107,113	1.61	14 (20%)
18	LMG	2	802	-	50,50,55	0.71	0	58,58,63	1.26	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	1132	-	45,53,73	1.71	9 (20%)	52,89,113	1.75	9 (17%)
12	LUT	3	501	-	42,43,43	6.16	29 (69%)	51,60,60	3.18	20 (39%)
15	CLA	1	606	-	50,58,73	1.65	6 (12%)	58,95,113	1.53	8 (13%)
15	CLA	B	1228	-	60,68,73	1.54	8 (13%)	70,107,113	1.44	7 (10%)
15	CLA	A	1115	-	45,53,73	1.72	7 (15%)	52,89,113	1.63	7 (13%)
15	CLA	A	1137	-	61,69,73	1.48	7 (11%)	71,108,113	1.56	12 (16%)
18	LMG	2	804	-	50,50,55	0.72	1 (2%)	58,58,63	1.28	7 (12%)
12	LUT	2	501	-	42,43,43	6.13	31 (73%)	51,60,60	2.49	17 (33%)
15	CLA	3	601	3	60,68,73	1.49	9 (15%)	70,107,113	1.49	7 (10%)
16	CHL	4	613	-	61,69,74	0.87	2 (3%)	67,108,114	1.16	8 (11%)
17	LHG	3	801	-	46,46,48	0.66	1 (2%)	48,51,54	1.19	6 (12%)
19	CL0	A	1011	-	65,73,73	5.00	27 (41%)	76,113,113	6.07	36 (47%)
15	CLA	4	604	-	60,68,73	1.49	9 (15%)	70,107,113	1.53	10 (14%)
15	CLA	1	602	-	46,54,73	1.75	7 (15%)	53,90,113	1.48	6 (11%)
15	CLA	1	612	1	39,48,73	1.87	7 (17%)	45,82,113	1.46	5 (11%)
15	CLA	2	612	2	55,63,73	1.55	6 (10%)	64,101,113	1.48	7 (10%)
15	CLA	B	1229	-	60,68,73	1.48	6 (10%)	70,107,113	1.49	8 (11%)
15	CLA	4	609	4	60,68,73	1.49	9 (15%)	70,107,113	1.50	8 (11%)
15	CLA	A	1117	-	65,73,73	1.43	7 (10%)	76,113,113	1.47	10 (13%)
15	CLA	4	607	-	60,68,73	1.54	8 (13%)	70,107,113	1.41	8 (11%)
12	LUT	4	501	-	42,43,43	6.03	31 (73%)	51,60,60	2.90	19 (37%)
14	BCR	1	503	-	41,41,41	1.14	2 (4%)	56,56,56	1.37	13 (23%)
15	CLA	A	1128	-	65,73,73	1.45	8 (12%)	76,113,113	1.41	6 (7%)
15	CLA	B	1202	-	65,73,73	1.50	8 (12%)	76,113,113	1.37	8 (10%)
15	CLA	B	1223	-	65,73,73	1.47	8 (12%)	76,113,113	1.49	9 (11%)
17	LHG	A	5002	-	48,48,48	0.68	1 (2%)	51,54,54	1.18	4 (7%)
15	CLA	2	606	-	45,53,73	1.75	8 (17%)	52,89,113	1.57	7 (13%)

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
17	LHG	A	5001	15	-	17/53/53/53	-
15	CLA	1	605	-	1/1/20/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	3	614	-	1/1/17/20	6/22/100/115	-
14	BCR	3	506	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1207	-	-	11/15/93/115	-
16	CHL	4	610	-	3/3/21/26	3/17/115/137	-
15	CLA	B	1238	-	2/2/17/20	10/18/96/115	-
15	CLA	F	1302	10	1/1/16/20	10/18/96/115	-
15	CLA	B	1217	-	1/1/15/20	7/15/93/115	-
15	CLA	B	1206	6	1/1/15/20	4/13/91/115	-
15	CLA	A	1140	-	1/1/19/20	6/33/111/115	-
15	CLA	A	1122	-	1/1/20/20	14/37/115/115	-
21	SF4	A	3001	5,6	-	-	0/6/5/5
16	CHL	2	613	-	3/3/21/26	4/15/113/137	-
14	BCR	3	504	-	-	16/29/63/63	0/2/2/2
15	CLA	B	1215	-	1/1/20/20	15/37/115/115	-
15	CLA	1	604	1	1/1/20/20	6/37/115/115	-
15	CLA	3	609	-	1/1/14/20	4/10/88/115	-
15	CLA	A	1102	-	1/1/20/20	13/37/115/115	-
13	XAT	1	502	-	-	12/31/93/93	0/4/4/4
15	CLA	B	1232	-	1/1/15/20	8/15/93/115	-
15	CLA	A	1124	-	1/1/19/20	6/31/109/115	-
15	CLA	B	1216	-	1/1/18/20	10/30/108/115	-
14	BCR	B	4004	-	-	11/29/63/63	0/2/2/2
15	CLA	A	1118	-	1/1/14/20	3/10/88/115	-
15	CLA	2	607	17	1/1/19/20	7/31/109/115	-
12	LUT	1	501	-	1/1/27/27	22/29/67/67	0/2/2/2
15	CLA	A	1126	-	1/1/20/20	13/37/115/115	-
20	PQN	B	2002	-	-	4/23/43/43	0/2/2/2
15	CLA	B	1203	-	1/1/20/20	11/37/115/115	-
15	CLA	1	615	1	1/1/15/20	12/13/91/115	-
15	CLA	4	605	-	1/1/20/20	11/37/115/115	-
15	CLA	A	1113	-	1/1/15/20	5/13/91/115	-
15	CLA	B	1226	-	1/1/20/20	10/37/115/115	-
13	XAT	2	502	-	-	12/31/93/93	0/4/4/4
14	BCR	J	4001	-	-	19/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	1104	-	1/1/20/20	11/37/115/115	-
15	CLA	4	612	4	1/1/20/20	9/37/115/115	-
18	LMG	4	801	-	-	10/32/52/70	0/1/1/1
15	CLA	3	615	3	1/1/14/20	6/10/88/115	-
15	CLA	F	1301	-	1/1/15/20	7/15/93/115	-
15	CLA	A	1129	-	1/1/18/20	9/25/103/115	-
21	SF4	C	3003	7	-	-	0/6/5/5
15	CLA	2	604	2	1/1/20/20	15/37/115/115	-
15	CLA	4	602	-	1/1/17/20	9/19/97/115	-
14	BCR	B	4002	-	-	14/29/63/63	0/2/2/2
16	CHL	3	604	3	4/4/25/26	2/33/131/137	-
15	CLA	A	1136	-	1/1/20/20	14/37/115/115	-
15	CLA	A	1133	-	1/1/20/20	18/37/115/115	-
15	CLA	A	1119	-	1/1/20/20	8/37/115/115	-
15	CLA	B	1214	-	1/1/20/20	7/37/115/115	-
15	CLA	A	1110	-	1/1/18/20	9/25/103/115	-
14	BCR	A	4005	-	-	16/29/63/63	0/2/2/2
14	BCR	3	503	-	-	17/29/63/63	0/2/2/2
14	BCR	A	4007	-	-	14/29/63/63	0/2/2/2
15	CLA	B	1208	-	1/1/19/20	10/31/109/115	-
14	BCR	F	4002	-	-	17/29/63/63	0/2/2/2
14	BCR	4	503	-	-	16/29/63/63	0/2/2/2
16	CHL	2	611	-	3/3/21/26	1/18/116/137	-
15	CLA	B	1240	17	1/1/20/20	11/37/115/115	-
14	BCR	A	4004	-	-	16/29/63/63	0/2/2/2
14	BCR	A	4006	-	-	16/29/63/63	0/2/2/2
15	CLA	2	602	-	1/1/15/20	6/13/91/115	-
15	CLA	A	1013	-	1/1/20/20	13/37/115/115	-
15	CLA	3	608	-	1/1/20/20	16/37/115/115	-
15	CLA	B	1201	-	1/1/14/20	3/11/89/115	-
15	CLA	B	1225	-	1/1/20/20	18/37/115/115	-
15	CLA	3	611	-	1/1/20/20	8/37/115/115	-
15	CLA	A	1103	-	1/1/20/20	13/37/115/115	-
15	CLA	2	616	-	-	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	1210	-	-	8/37/115/115	-
15	CLA	1	611	-	1/1/16/20	7/17/95/115	-
16	CHL	4	611	-	3/3/23/26	0/21/119/137	-
15	CLA	A	1135	-	1/1/17/20	4/21/99/115	-
15	CLA	B	1234	-	1/1/18/20	12/25/103/115	-
15	CLA	3	612	3	1/1/20/20	8/37/115/115	-
14	BCR	B	4001	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1130	-	1/1/15/20	7/13/91/115	-
15	CLA	A	1121	-	1/1/15/20	4/13/91/115	-
14	BCR	J	4002	-	-	17/29/63/63	0/2/2/2
15	CLA	B	1022	-	1/1/20/20	12/37/115/115	-
15	CLA	A	1114	-	1/1/18/20	11/25/103/115	-
15	CLA	1	603	-	1/1/19/20	12/31/109/115	-
15	CLA	A	1101	-	1/1/20/20	16/37/115/115	-
15	CLA	B	1209	-	1/1/15/20	6/15/93/115	-
16	CHL	1	609	1	4/4/26/26	14/39/137/137	-
15	CLA	4	601	4	1/1/19/20	7/31/109/115	-
15	CLA	A	1116	-	1/1/18/20	8/27/105/115	-
15	CLA	A	1138	-	1/1/20/20	8/37/115/115	-
15	CLA	A	1125	-	-	14/37/115/115	-
14	BCR	B	4003	-	-	22/29/63/63	0/2/2/2
15	CLA	B	1222	-	1/1/20/20	11/37/115/115	-
15	CLA	A	1131	-	1/1/15/20	4/13/91/115	-
15	CLA	A	1120	-	1/1/14/20	5/10/88/115	-
16	CHL	2	610	-	3/3/20/26	2/13/111/137	-
14	BCR	2	503	-	-	20/29/63/63	0/2/2/2
16	CHL	1	610	-	3/3/21/26	5/17/115/137	-
15	CLA	B	1213	-	1/1/18/20	5/25/103/115	-
15	CLA	2	603	2	1/1/20/20	9/37/115/115	-
13	XAT	3	502	-	-	15/31/93/93	0/4/4/4
15	CLA	B	1205	-	1/1/20/20	9/37/115/115	-
15	CLA	A	1112	-	1/1/20/20	10/37/115/115	-
21	SF4	C	3002	7	-	-	0/6/5/5
15	CLA	1	608	-	1/1/18/20	9/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	F	4001	-	-	17/29/63/63	0/2/2/2
14	BCR	B	4006	-	-	15/29/63/63	0/2/2/2
15	CLA	3	606	-	1/1/18/20	8/25/103/115	-
15	CLA	B	1235	-	1/1/19/20	11/31/109/115	-
15	CLA	B	1219	-	-	15/37/115/115	-
15	CLA	B	1231	-	1/1/19/20	6/31/109/115	-
15	CLA	3	607	-	1/1/19/20	10/31/109/115	-
18	LMG	B	5003	-	-	14/34/54/70	0/1/1/1
15	CLA	1	601	-	1/1/20/20	9/37/115/115	-
15	CLA	3	610	-	1/1/17/20	9/19/97/115	-
17	LHG	1	801	15	-	22/53/53/53	-
15	CLA	A	1127	-	1/1/20/20	11/37/115/115	-
15	CLA	A	1123	-	1/1/20/20	16/37/115/115	-
15	CLA	A	1108	-	1/1/18/20	9/25/103/115	-
15	CLA	A	1109	-	1/1/20/20	13/37/115/115	-
15	CLA	B	1236	-	1/1/16/20	9/18/96/115	-
14	BCR	A	4003	-	-	16/29/63/63	0/2/2/2
15	CLA	A	1141	17	1/1/14/20	6/8/86/115	-
15	CLA	2	605	-	1/1/20/20	13/37/115/115	-
15	CLA	A	1107	5	1/1/17/20	4/21/99/115	-
16	CHL	2	609	2	4/4/26/26	13/39/137/137	-
15	CLA	B	1227	-	1/1/20/20	14/37/115/115	-
17	LHG	B	5001	15	-	26/46/46/53	-
15	CLA	3	613	-	1/1/15/20	2/15/93/115	-
15	CLA	A	1134	5	1/1/14/20	4/10/88/115	-
20	PQN	A	2001	-	-	1/23/43/43	0/2/2/2
15	CLA	A	1139	-	1/1/20/20	16/37/115/115	-
15	CLA	B	1220	-	1/1/17/20	7/21/99/115	-
17	LHG	2	801	15	-	18/39/39/53	-
15	CLA	B	1212	-	1/1/18/20	4/25/103/115	-
14	BCR	B	4005	-	-	17/29/63/63	0/2/2/2
15	CLA	4	606	-	1/1/17/20	8/19/97/115	-
15	CLA	4	616	4	1/1/17/20	9/21/99/115	-
15	CLA	B	1230	-	1/1/18/20	7/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	3	603	-	1/1/20/20	15/37/115/115	-
15	CLA	B	1239	-	1/1/14/20	2/10/88/115	-
15	CLA	B	1237	-	1/1/15/20	4/13/91/115	-
15	CLA	A	1111	-	-	13/37/115/115	-
15	CLA	B	1023	-	1/1/20/20	18/37/115/115	-
15	CLA	A	1012	-	1/1/20/20	19/37/115/115	-
15	CLA	1	613	-	1/1/15/20	8/13/91/115	-
15	CLA	B	1221	-	1/1/20/20	17/37/115/115	-
15	CLA	B	1021	-	1/1/20/20	16/37/115/115	-
14	BCR	A	4008	-	-	11/29/63/63	0/2/2/2
15	CLA	2	608	-	1/1/17/20	2/19/97/115	-
15	CLA	A	1106	5	1/1/20/20	10/37/115/115	-
15	CLA	3	605	-	1/1/20/20	16/37/115/115	-
15	CLA	B	1218	-	1/1/15/20	5/13/91/115	-
13	XAT	4	502	-	-	15/31/93/93	0/4/4/4
14	BCR	A	4002	-	-	18/29/63/63	0/2/2/2
15	CLA	B	1204	-	1/1/15/20	7/13/91/115	-
15	CLA	B	1211	-	1/1/20/20	14/37/115/115	-
18	LMG	2	803	-	-	19/35/55/70	0/1/1/1
15	CLA	4	603	-	1/1/20/20	11/37/115/115	-
15	CLA	1	607	17	1/1/15/20	7/15/93/115	-
15	CLA	2	601	-	1/1/20/20	17/37/115/115	-
15	CLA	J	1302	11	1/1/14/20	5/10/88/115	-
22	DGD	B	5002	-	-	17/50/90/95	0/2/2/2
15	CLA	B	1224	-	1/1/19/20	14/33/111/115	-
15	CLA	4	608	-	1/1/15/20	6/15/93/115	-
15	CLA	A	1105	-	1/1/19/20	16/31/109/115	-
18	LMG	2	802	-	-	20/45/65/70	0/1/1/1
15	CLA	A	1132	-	1/1/15/20	7/13/91/115	-
12	LUT	3	501	-	1/1/27/27	18/29/67/67	0/2/2/2
15	CLA	1	606	-	1/1/17/20	4/19/97/115	-
15	CLA	B	1228	-	1/1/19/20	7/31/109/115	-
15	CLA	A	1115	-	1/1/15/20	3/13/91/115	-
15	CLA	A	1137	-	1/1/19/20	11/33/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LMG	2	804	-	-	24/45/65/70	0/1/1/1
12	LUT	2	501	-	1/1/27/27	18/29/67/67	0/2/2/2
15	CLA	3	601	3	1/1/19/20	13/31/109/115	-
16	CHL	4	613	-	4/4/25/26	2/33/131/137	-
17	LHG	3	801	-	-	21/49/49/53	-
19	CL0	A	1011	-	3/3/25/25	21/37/135/135	-
15	CLA	4	604	-	1/1/19/20	16/31/109/115	-
15	CLA	1	602	-	1/1/15/20	7/15/93/115	-
15	CLA	1	612	1	1/1/14/20	6/8/82/115	-
15	CLA	2	612	2	1/1/18/20	3/25/103/115	-
15	CLA	B	1229	-	1/1/19/20	7/31/109/115	-
15	CLA	4	609	4	1/1/19/20	12/31/109/115	-
15	CLA	A	1117	-	1/1/20/20	13/37/115/115	-
15	CLA	4	607	-	1/1/19/20	9/31/109/115	-
12	LUT	4	501	-	1/1/27/27	21/29/67/67	0/2/2/2
15	CLA	A	1128	-	1/1/20/20	13/37/115/115	-
14	BCR	1	503	-	-	19/29/63/63	0/2/2/2
15	CLA	B	1202	-	1/1/20/20	13/37/115/115	-
15	CLA	B	1223	-	1/1/20/20	7/37/115/115	-
17	LHG	A	5002	-	-	25/53/53/53	-
15	CLA	2	606	-	1/1/15/20	7/13/91/115	-

The worst 5 of 1373 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	2	501	LUT	C24-C25	21.20	1.59	1.33
12	3	501	LUT	C24-C25	21.11	1.59	1.33
12	1	501	LUT	C24-C25	21.03	1.59	1.33
12	4	501	LUT	C24-C25	20.76	1.59	1.33
19	A	1011	CL0	C1D-ND	19.62	1.61	1.37

The worst 5 of 1617 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	502	XAT	O4-C5-C4	58.04	156.98	113.38
13	1	502	XAT	O4-C5-C4	57.31	156.43	113.38
13	1	502	XAT	O24-C25-C24	55.17	154.82	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	4	502	XAT	O4-C5-C4	54.25	154.14	113.38
13	2	502	XAT	O4-C5-C4	54.24	154.13	113.38

5 of 170 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 2090 torsion outliers are listed below:

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

115 monomers are involved in 201 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	A	5001	LHG	1	0
15	1	605	CLA	4	0
15	3	614	CLA	1	0
14	3	506	BCR	2	0
15	B	1207	CLA	1	0
16	4	610	CHL	1	0
15	B	1238	CLA	1	0
15	B	1206	CLA	2	0
15	A	1122	CLA	1	0
14	3	504	BCR	3	0
15	B	1215	CLA	1	0
13	1	502	XAT	3	0
14	B	4004	BCR	2	0
15	B	1216	CLA	1	0
12	1	501	LUT	11	0
15	A	1126	CLA	6	0
15	1	615	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	502	XAT	2	0
14	J	4001	BCR	3	0
15	B	1226	CLA	2	0
15	A	1104	CLA	2	0
15	3	615	CLA	1	0
15	A	1129	CLA	2	0
21	C	3003	SF4	1	0
15	2	604	CLA	1	0
14	B	4002	BCR	2	0
16	3	604	CHL	1	0
15	A	1133	CLA	1	0
15	A	1119	CLA	2	0
15	B	1214	CLA	2	0
14	A	4007	BCR	4	0
15	B	1208	CLA	2	0
14	A	4006	BCR	6	0
14	A	4004	BCR	1	0
15	B	1240	CLA	2	0
15	2	602	CLA	1	0
15	A	1013	CLA	4	0
15	3	608	CLA	3	0
15	B	1225	CLA	1	0
15	3	611	CLA	1	0
15	2	616	CLA	2	0
15	A	1103	CLA	1	0
15	B	1210	CLA	2	0
15	1	611	CLA	3	0
15	B	1234	CLA	2	0
14	B	4001	BCR	1	0
15	3	612	CLA	2	0
15	A	1121	CLA	1	0
14	J	4002	BCR	2	0
15	B	1022	CLA	2	0
15	A	1114	CLA	2	0
15	1	603	CLA	6	0
15	B	1209	CLA	1	0
16	1	609	CHL	1	0
15	4	601	CLA	1	0
15	A	1125	CLA	5	0
14	B	4003	BCR	1	0
16	2	610	CHL	1	0
16	1	610	CHL	1	0

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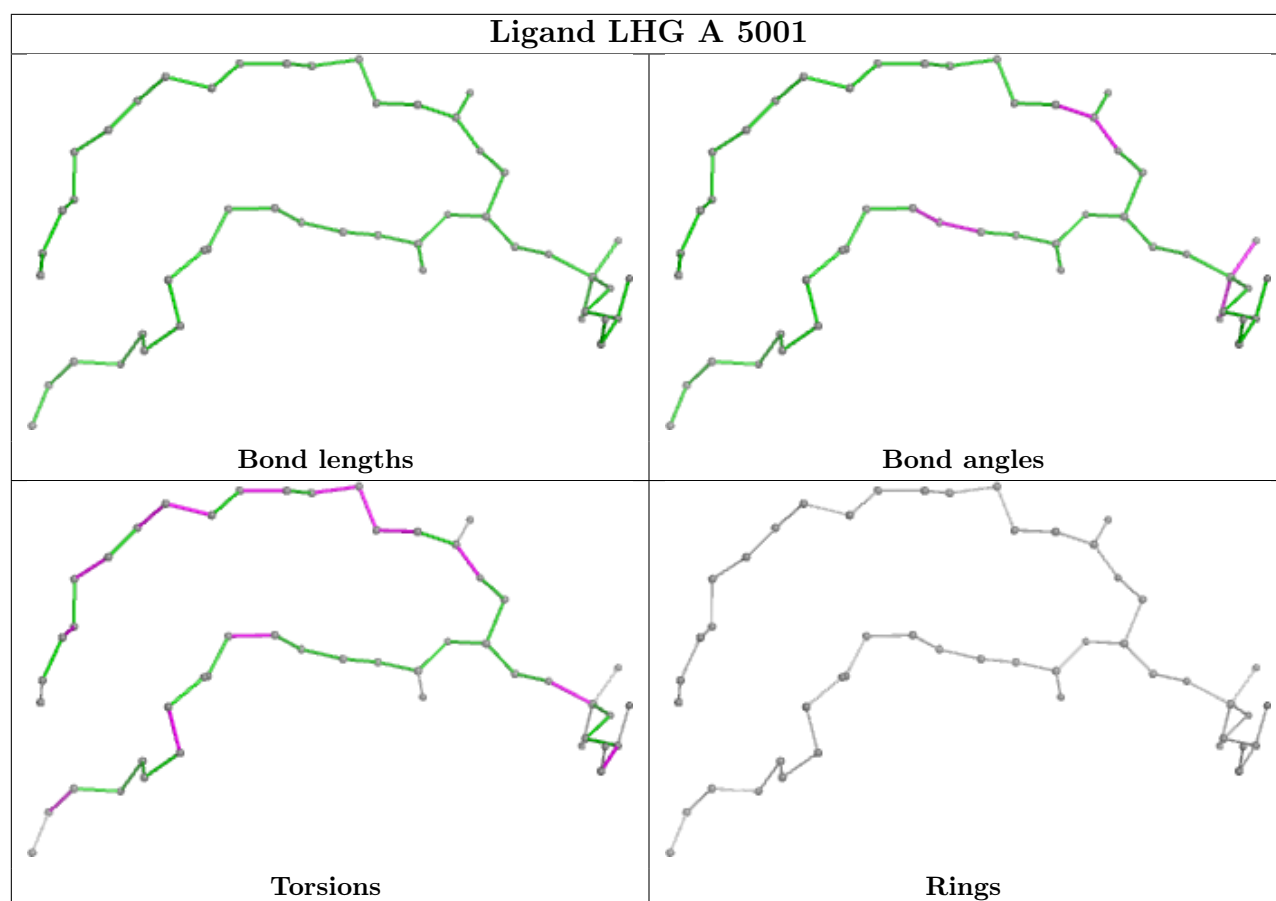
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13	3	502	XAT	2	0
15	A	1112	CLA	3	0
14	F	4001	BCR	2	0
14	B	4006	BCR	2	0
15	B	1231	CLA	4	0
18	B	5003	LMG	2	0
15	1	601	CLA	2	0
17	1	801	LHG	1	0
15	A	1127	CLA	2	0
15	A	1123	CLA	2	0
15	A	1108	CLA	1	0
15	B	1236	CLA	2	0
15	A	1141	CLA	2	0
16	2	609	CHL	1	0
15	B	1220	CLA	2	0
14	B	4005	BCR	3	0
15	B	1230	CLA	2	0
15	3	603	CLA	2	0
15	B	1239	CLA	3	0
15	A	1111	CLA	3	0
15	B	1023	CLA	2	0
15	A	1012	CLA	10	0
15	1	613	CLA	1	0
15	B	1221	CLA	2	0
14	A	4008	BCR	1	0
15	B	1021	CLA	3	0
15	2	608	CLA	1	0
15	3	605	CLA	5	0
13	4	502	XAT	6	0
14	A	4002	BCR	2	0
15	4	603	CLA	1	0
15	1	607	CLA	2	0
15	2	601	CLA	2	0
22	B	5002	DGD	2	0
15	B	1224	CLA	2	0
15	4	608	CLA	2	0
15	A	1105	CLA	2	0
15	A	1132	CLA	1	0
12	3	501	LUT	8	0
15	A	1137	CLA	1	0
12	2	501	LUT	5	0

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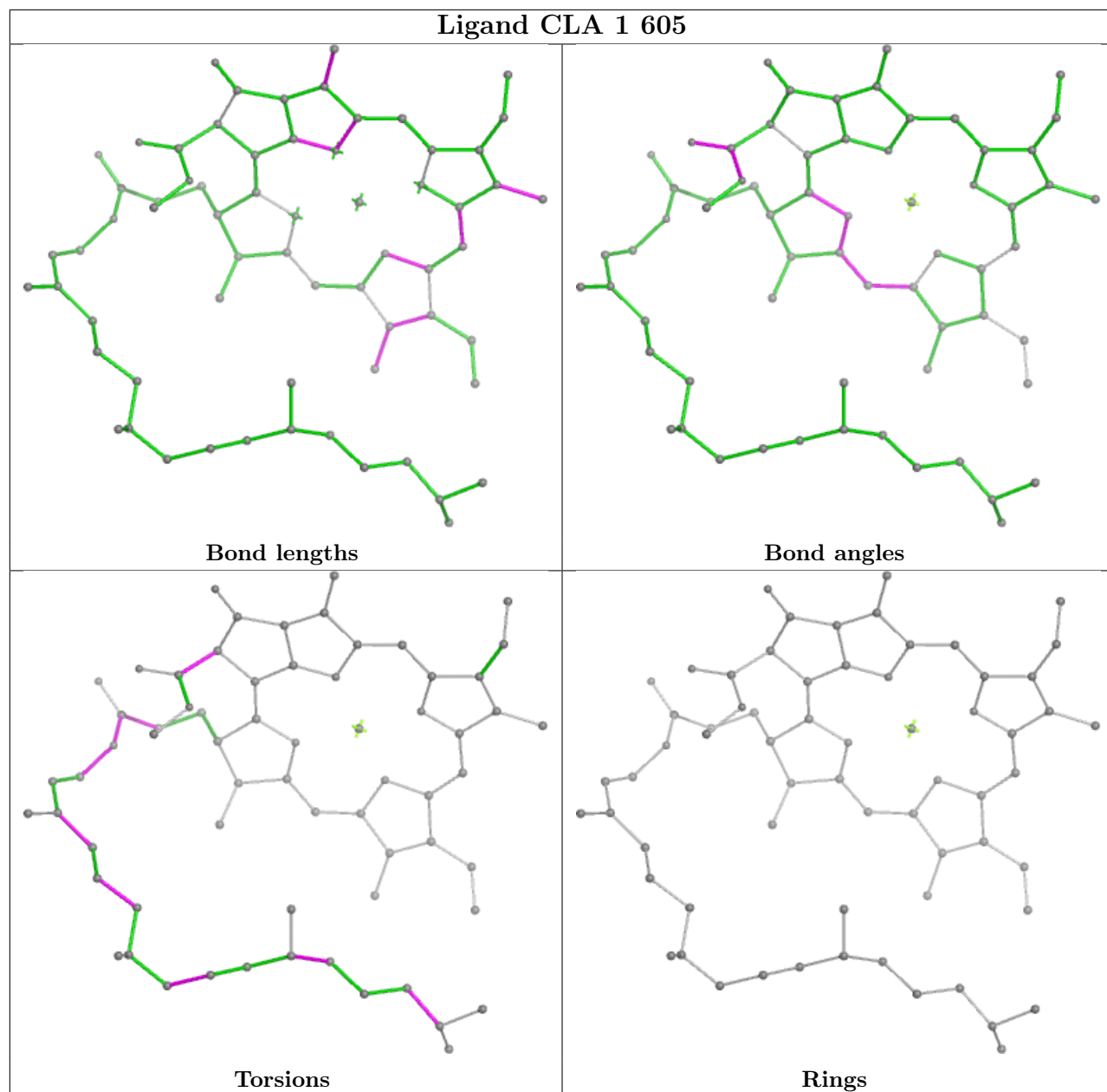
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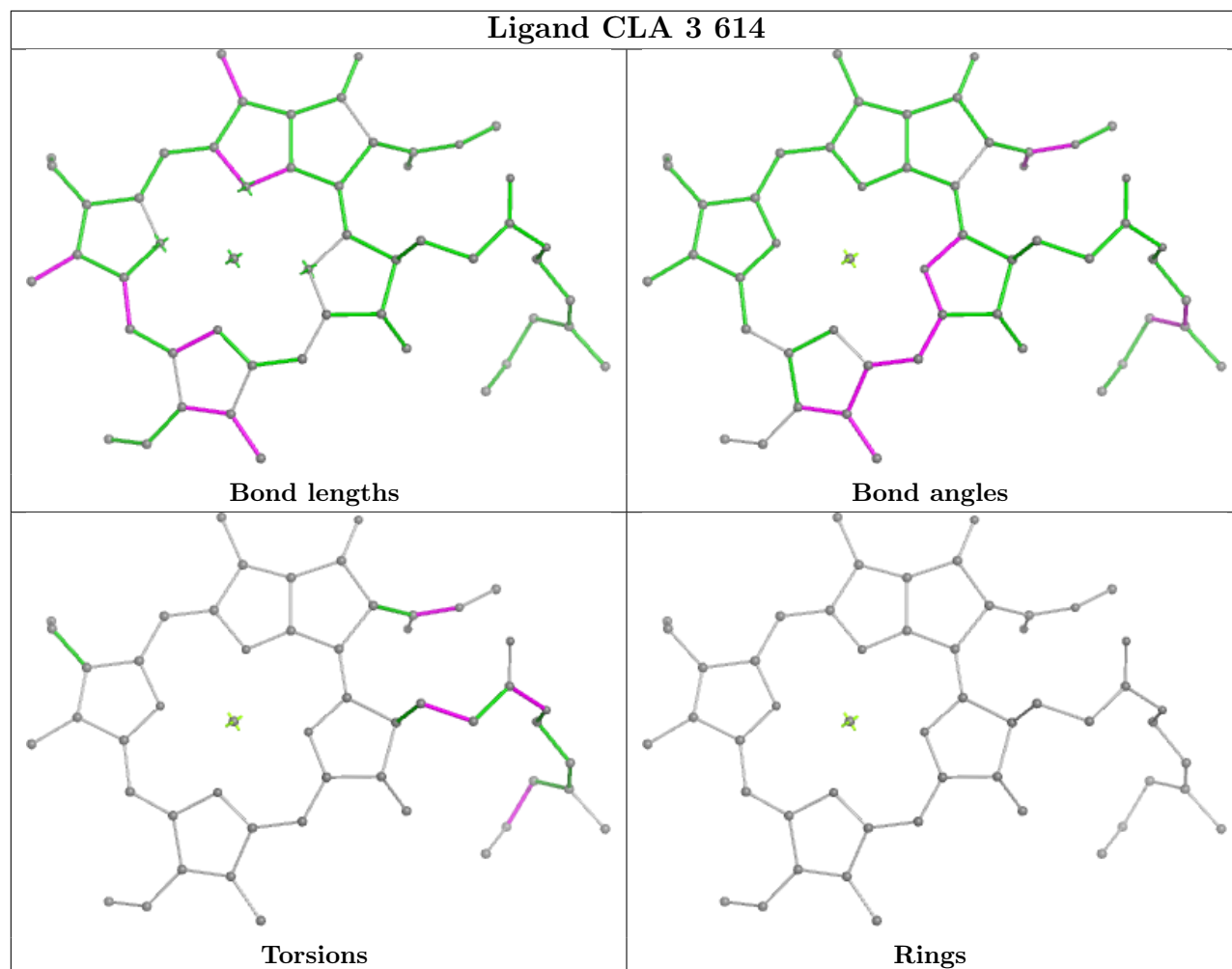
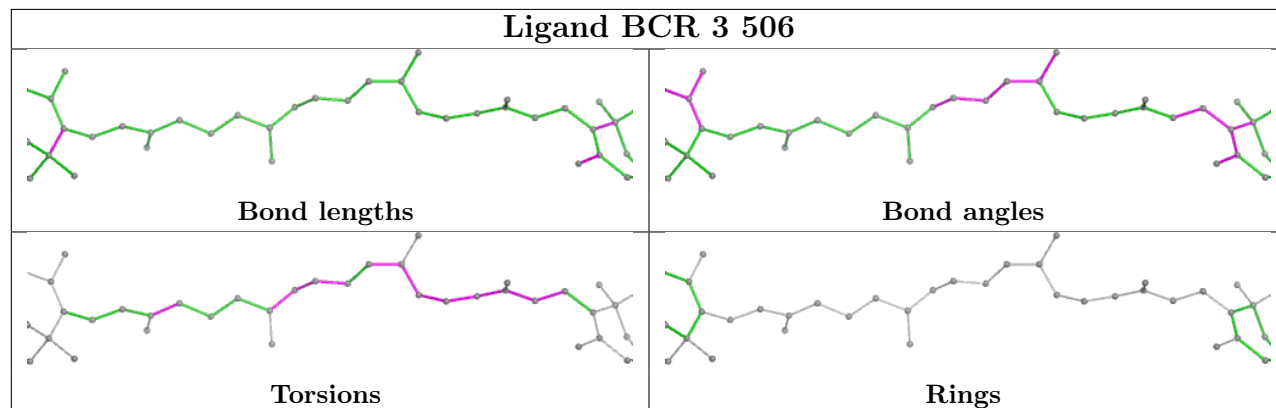
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3	601	CLA	4	0
19	A	1011	CL0	3	0
15	4	604	CLA	2	0
15	1	612	CLA	3	0
15	2	612	CLA	2	0
15	B	1229	CLA	2	0
15	4	609	CLA	1	0
15	A	1117	CLA	3	0
12	4	501	LUT	6	0
15	A	1128	CLA	1	0
15	B	1202	CLA	2	0
15	B	1223	CLA	2	0
17	A	5002	LHG	1	0
15	2	606	CLA	1	0

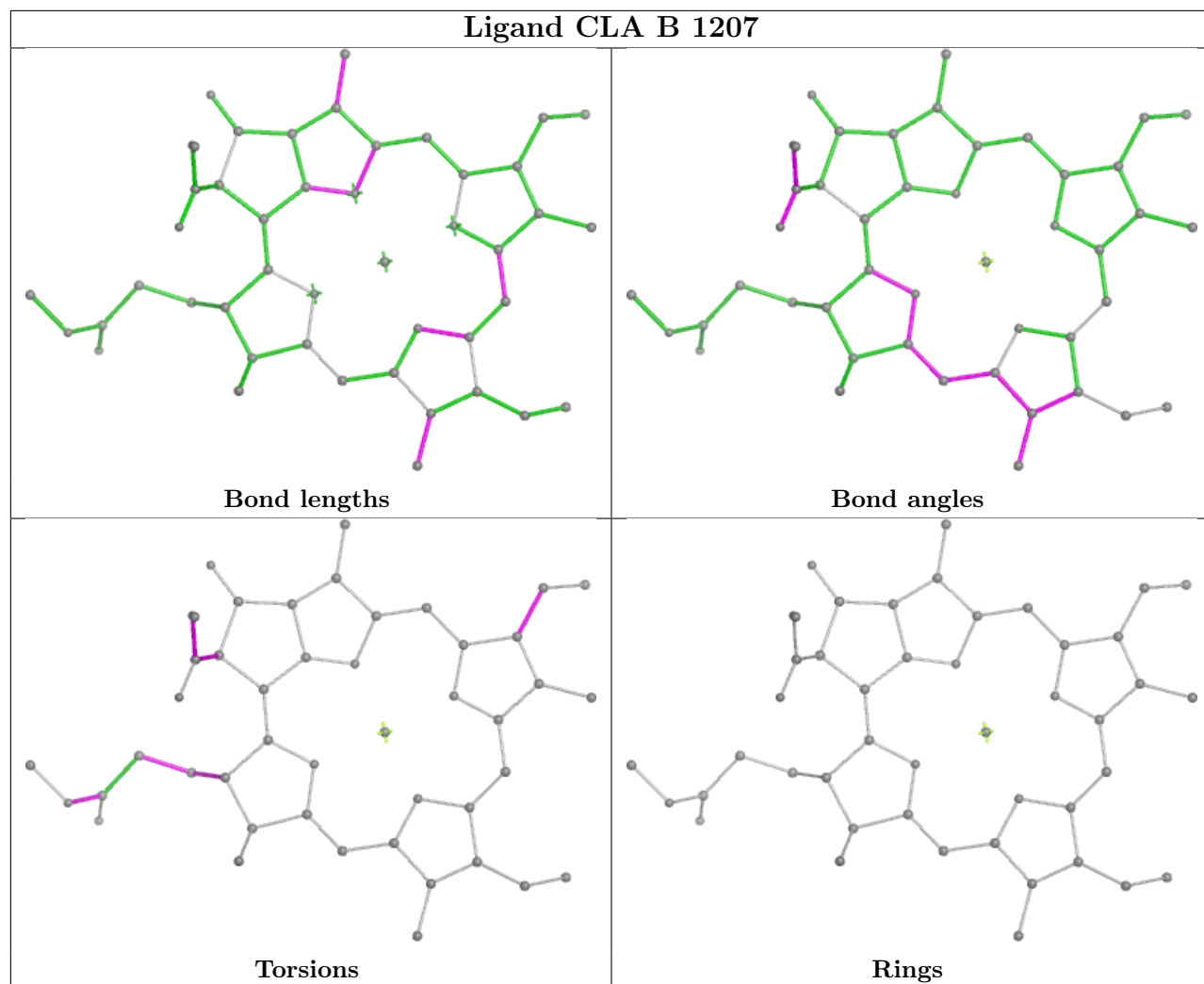
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



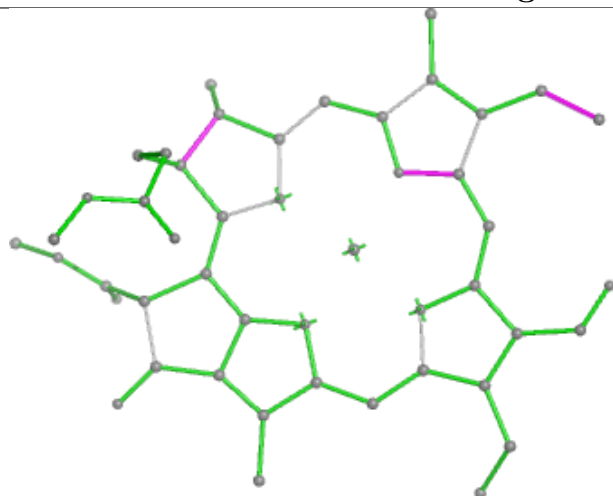
Ligand CLA 1 605



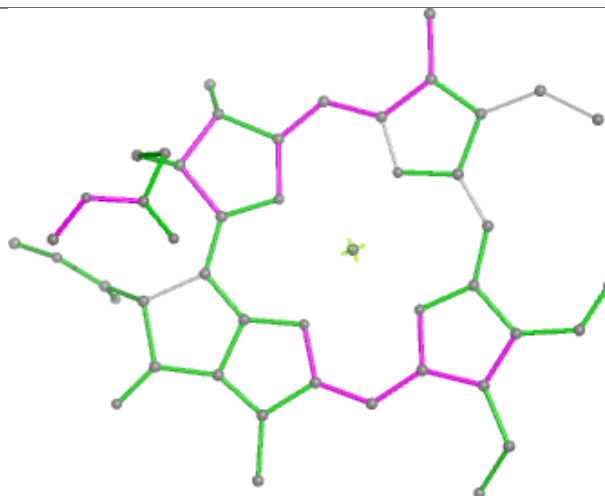
Ligand CLA 3 614**Ligand BCR 3 506**



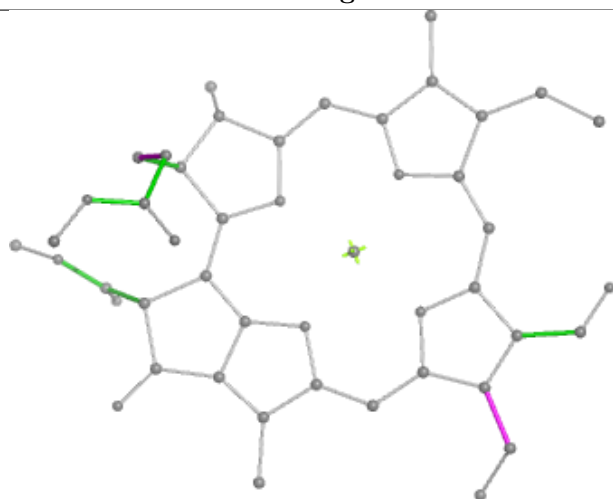
Ligand CHL 4 610



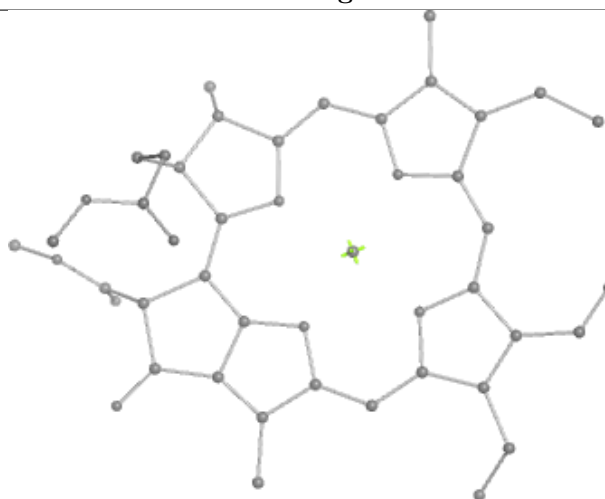
Bond lengths



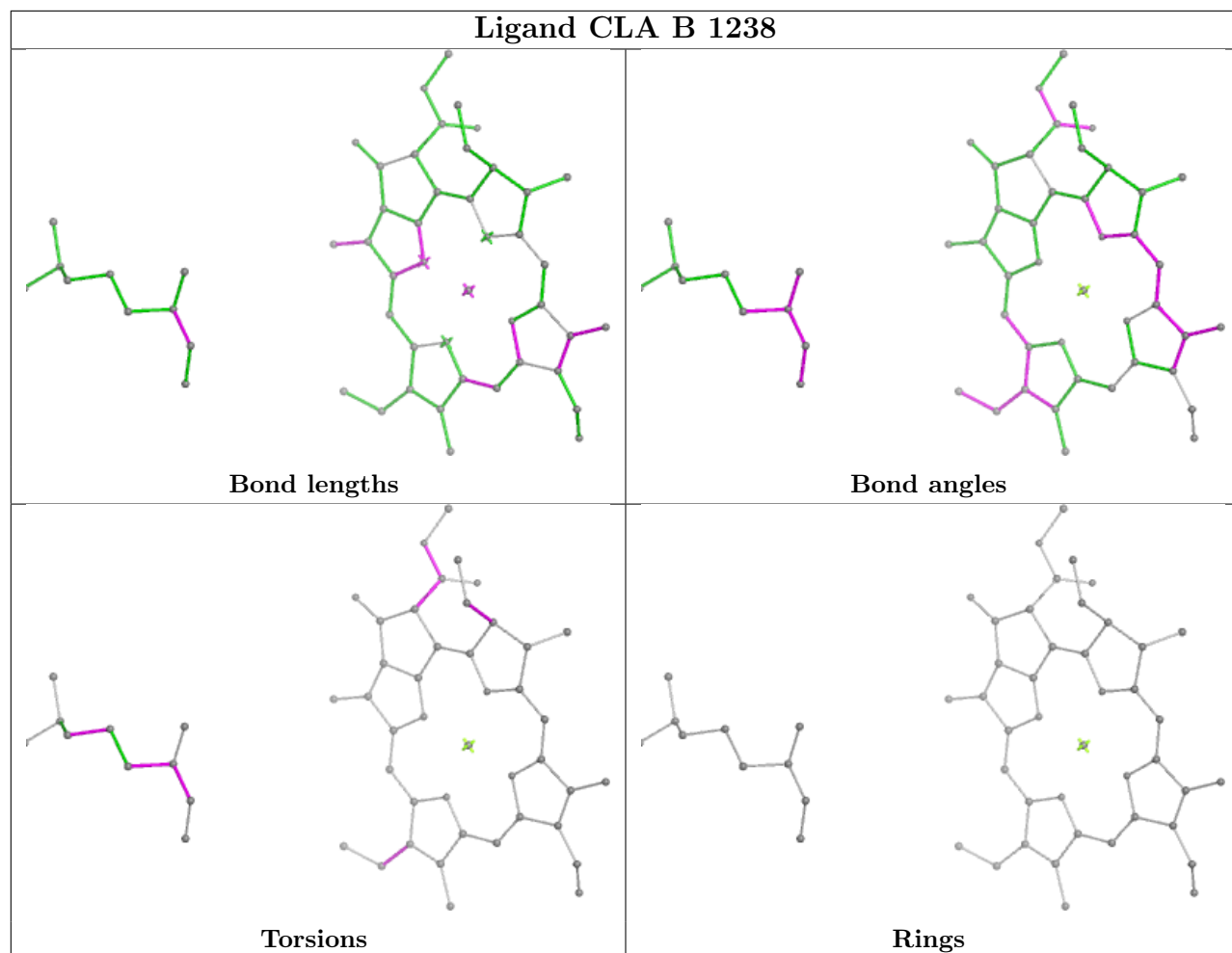
Bond angles

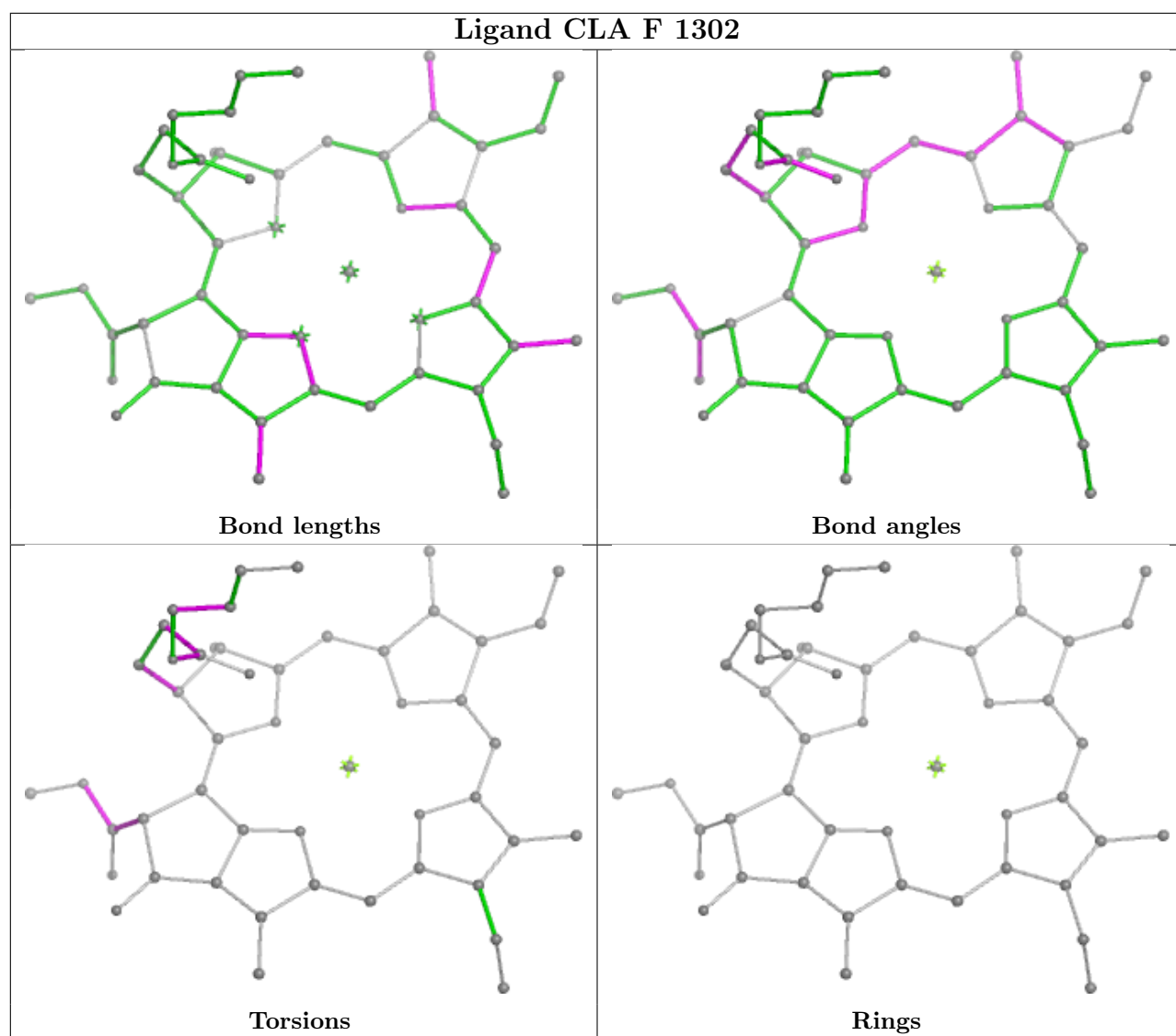


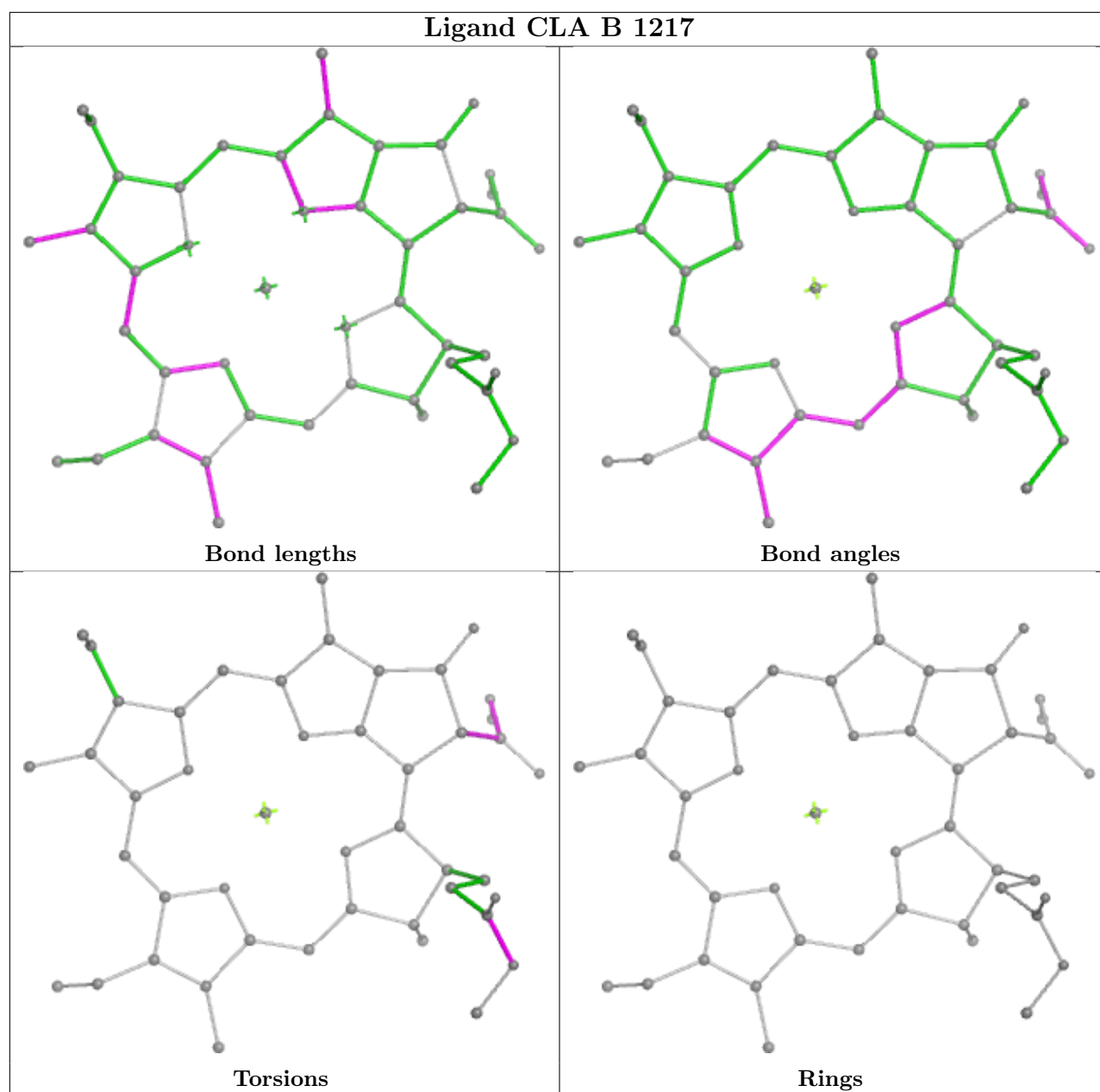
Torsions



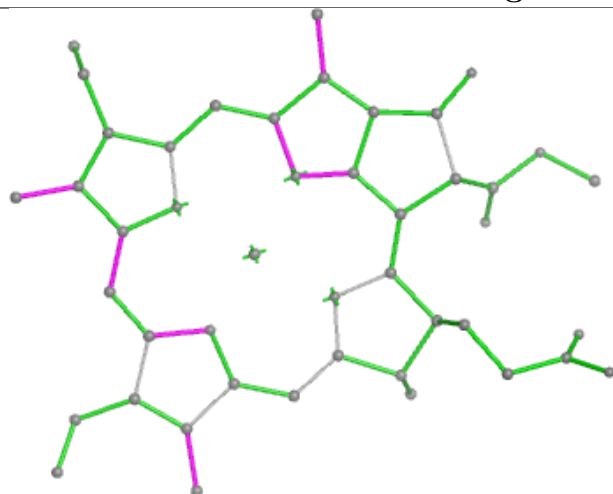
Rings



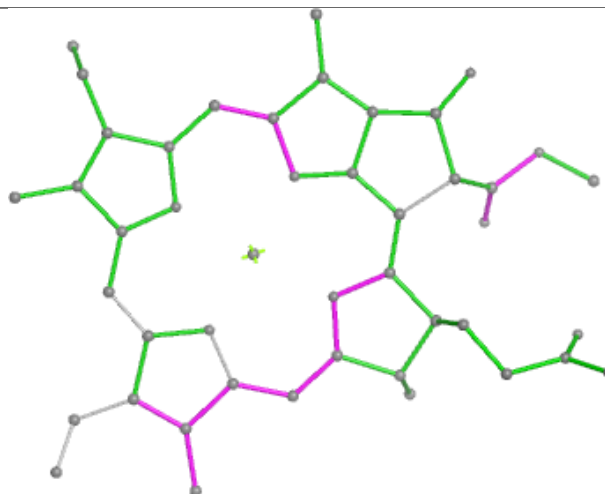




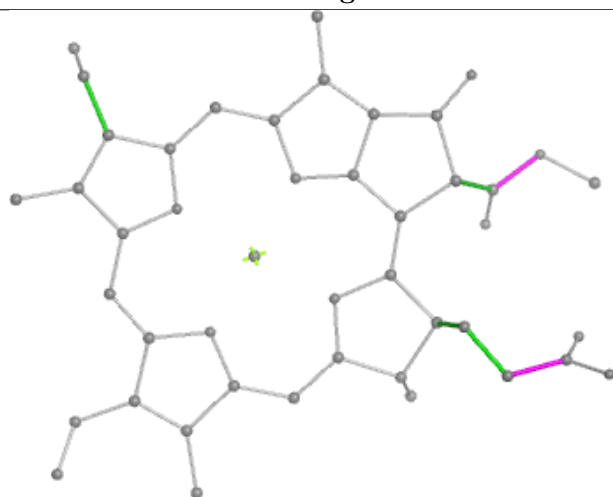
Ligand CLA B 1206



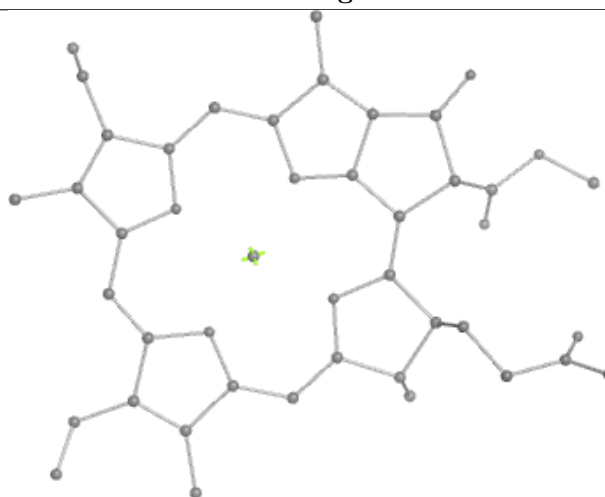
Bond lengths



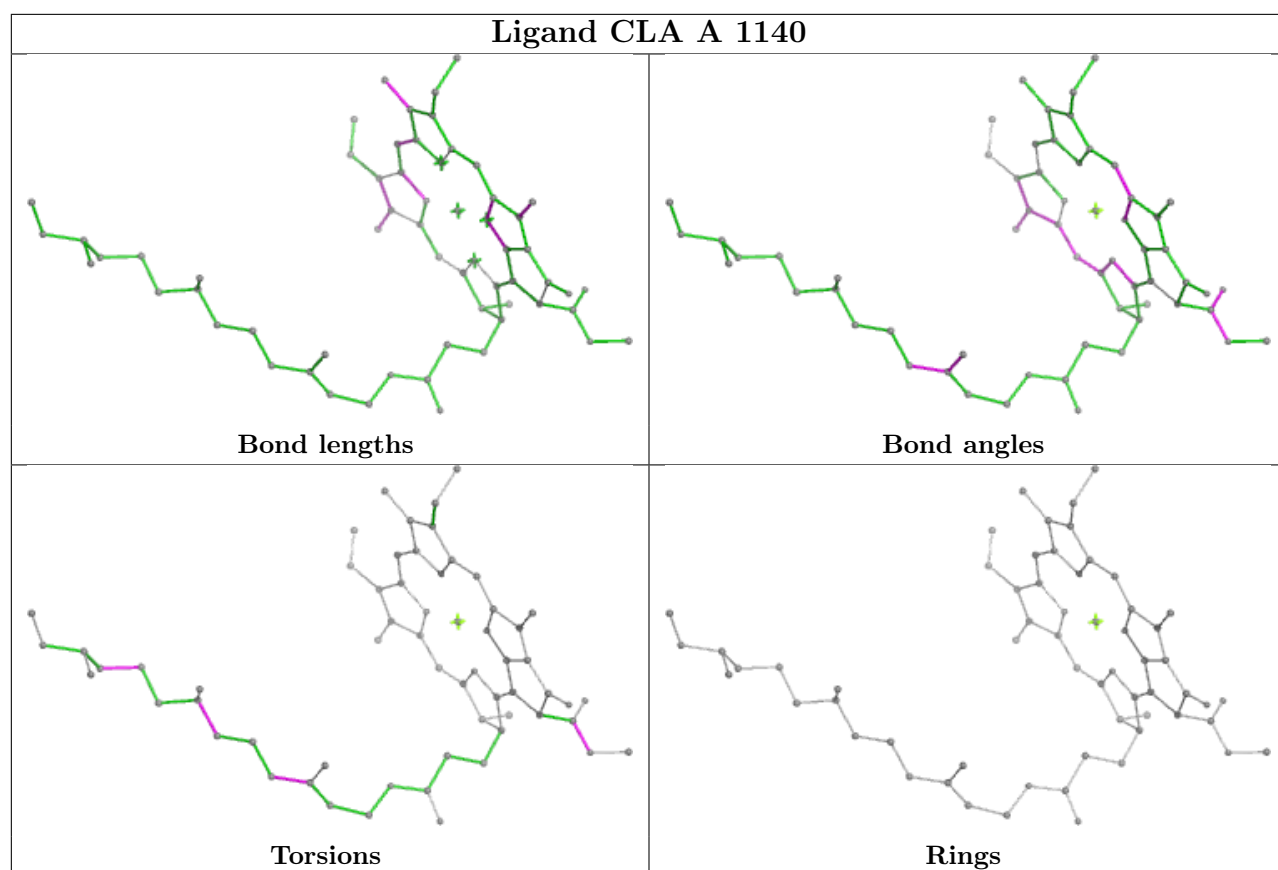
Bond angles

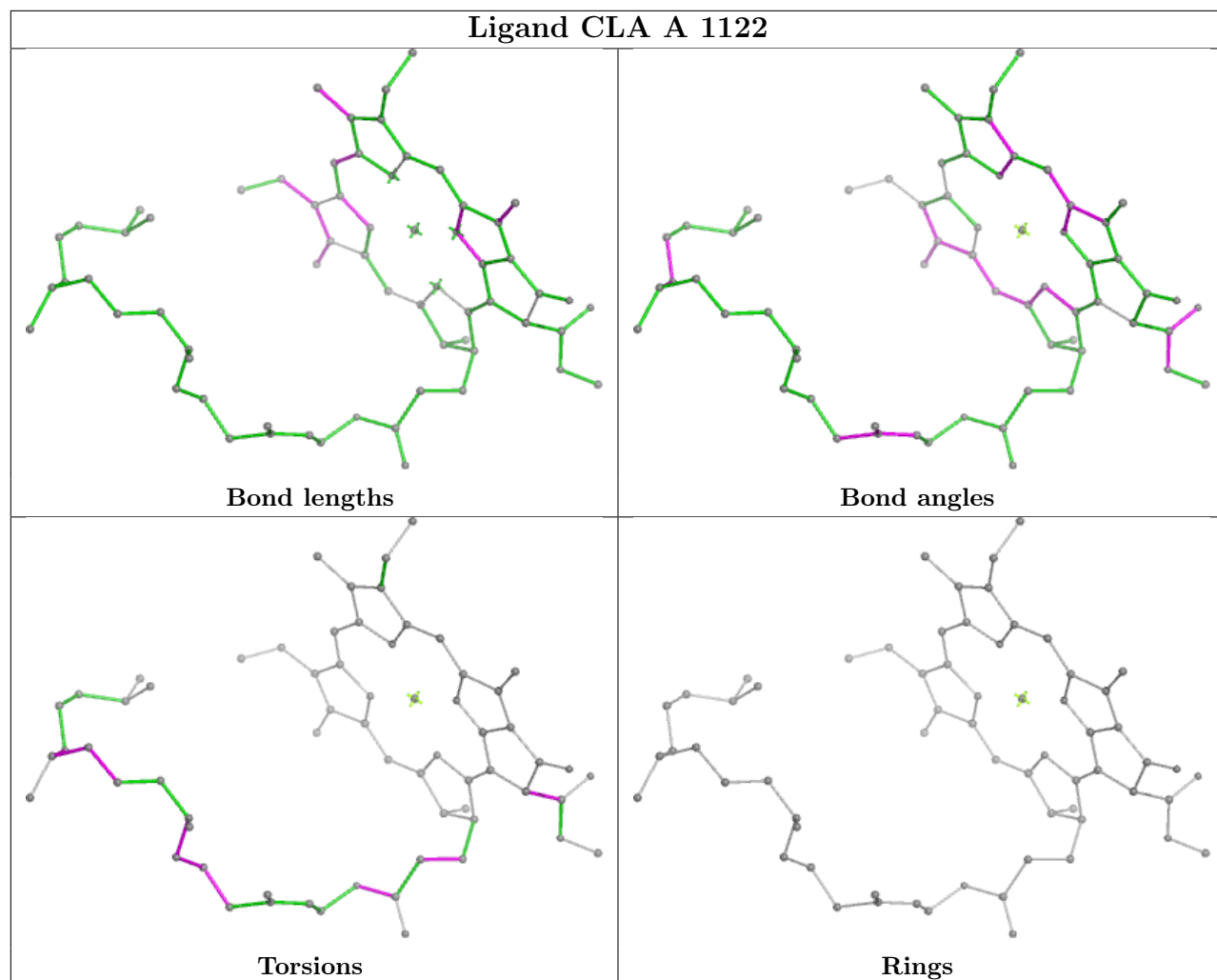


Torsions

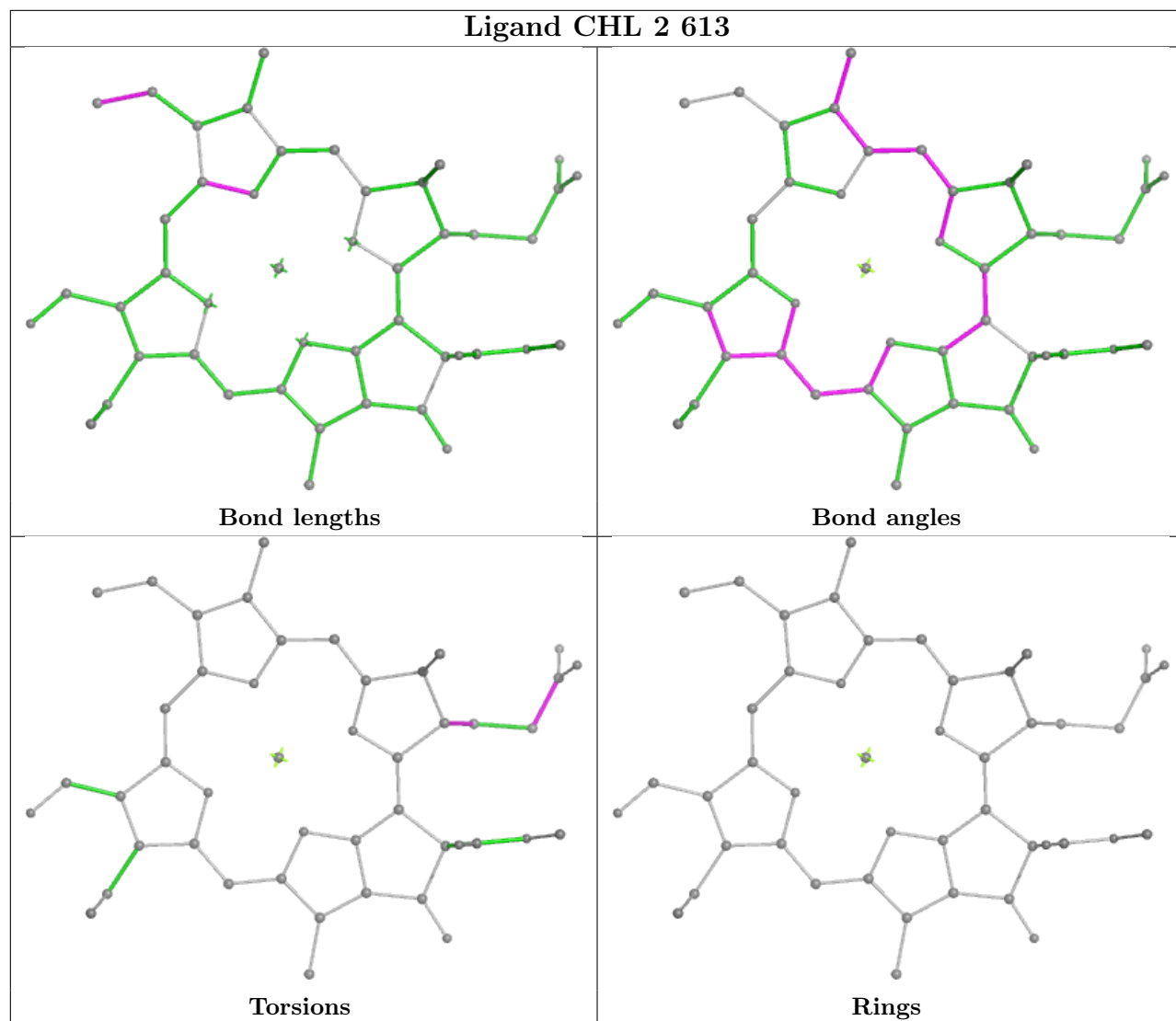


Rings

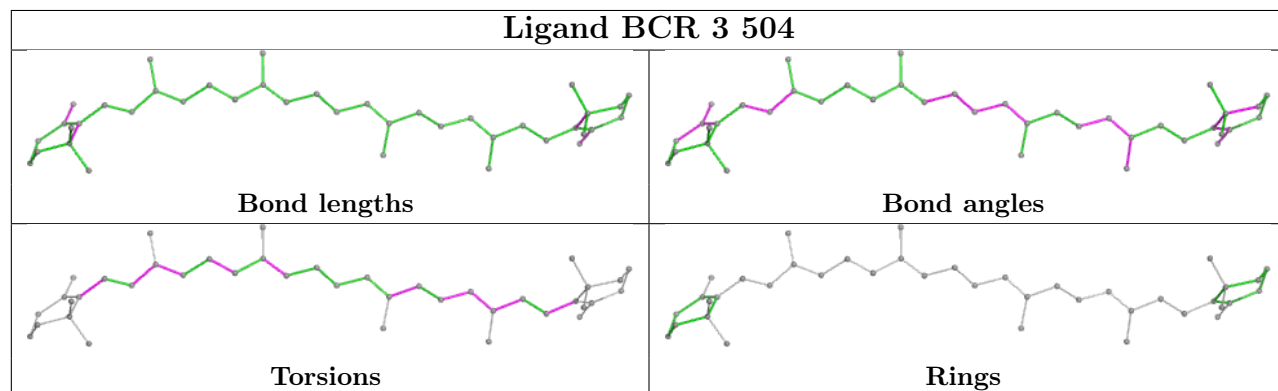


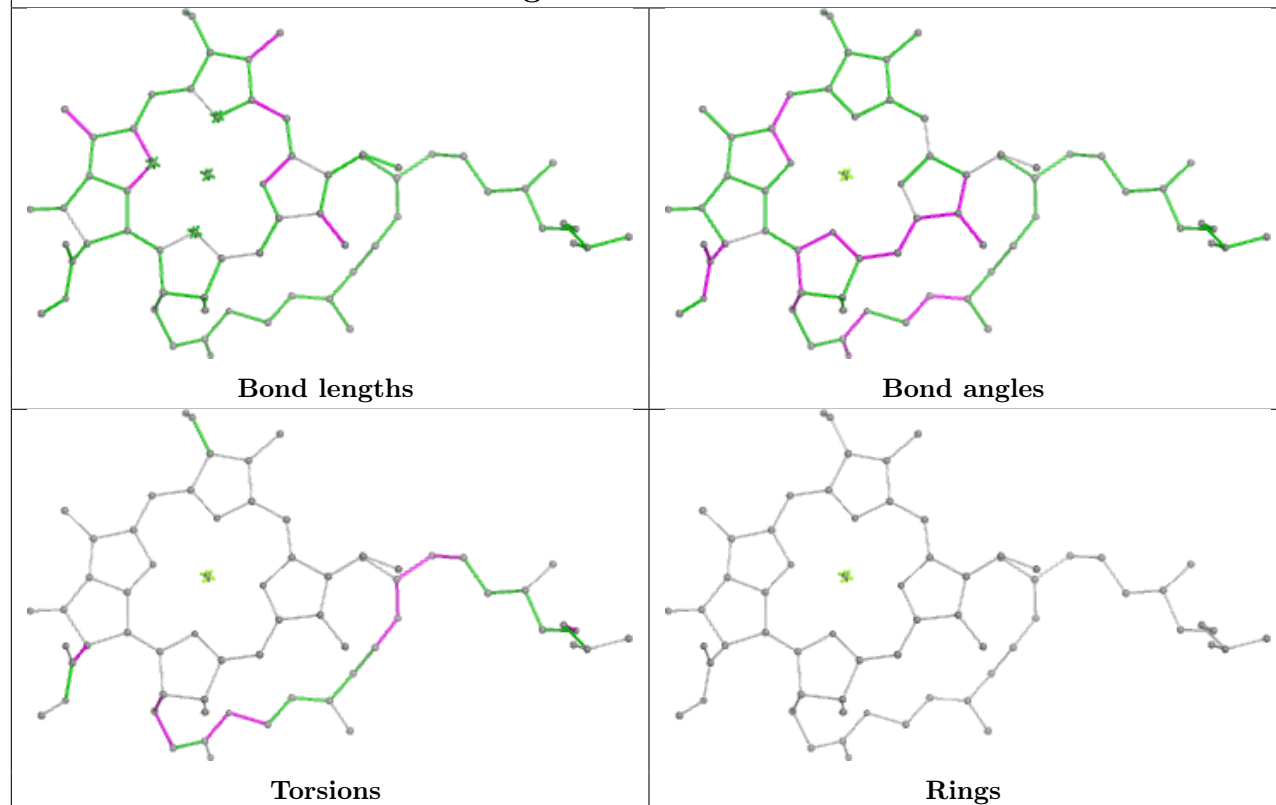
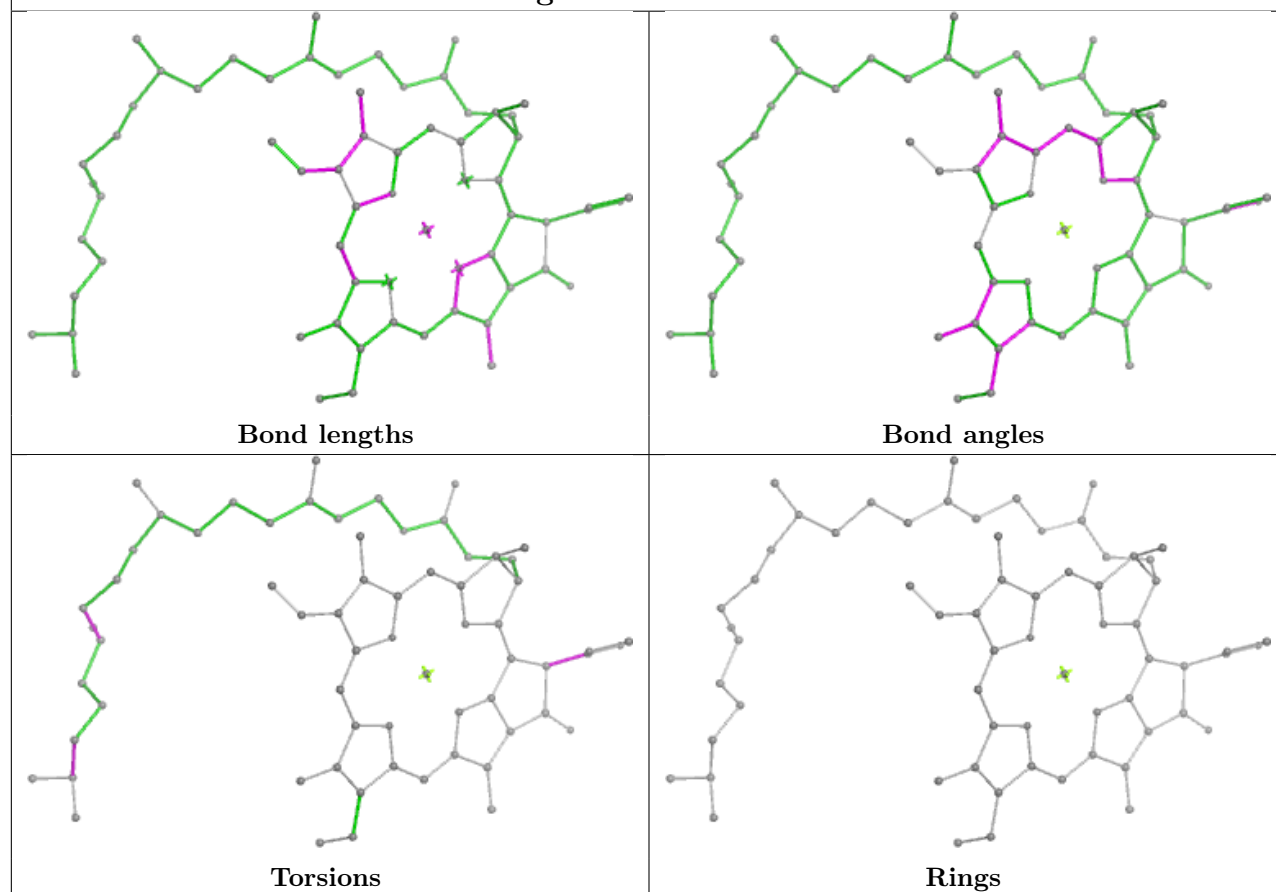


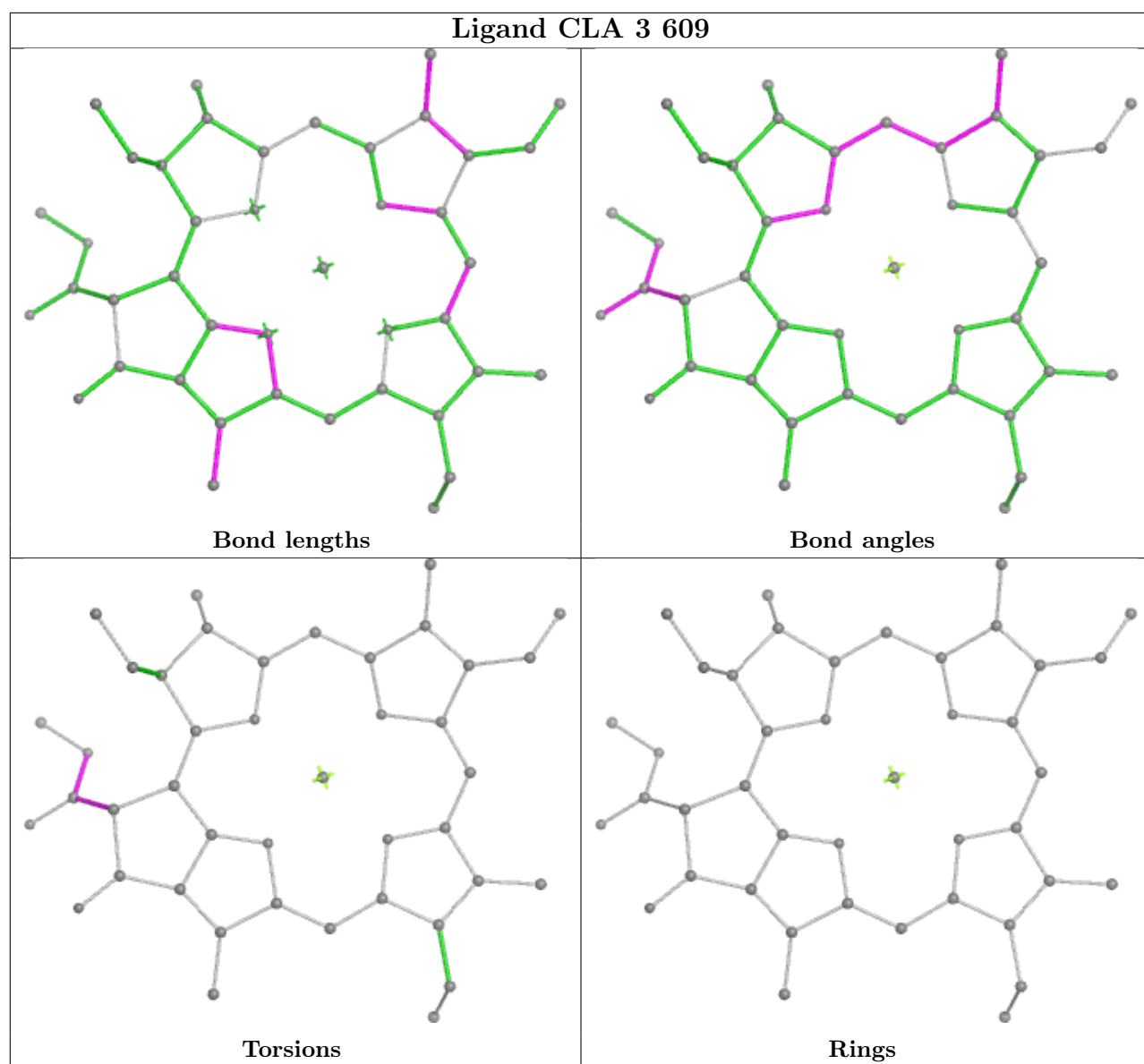
Ligand CHL 2 613

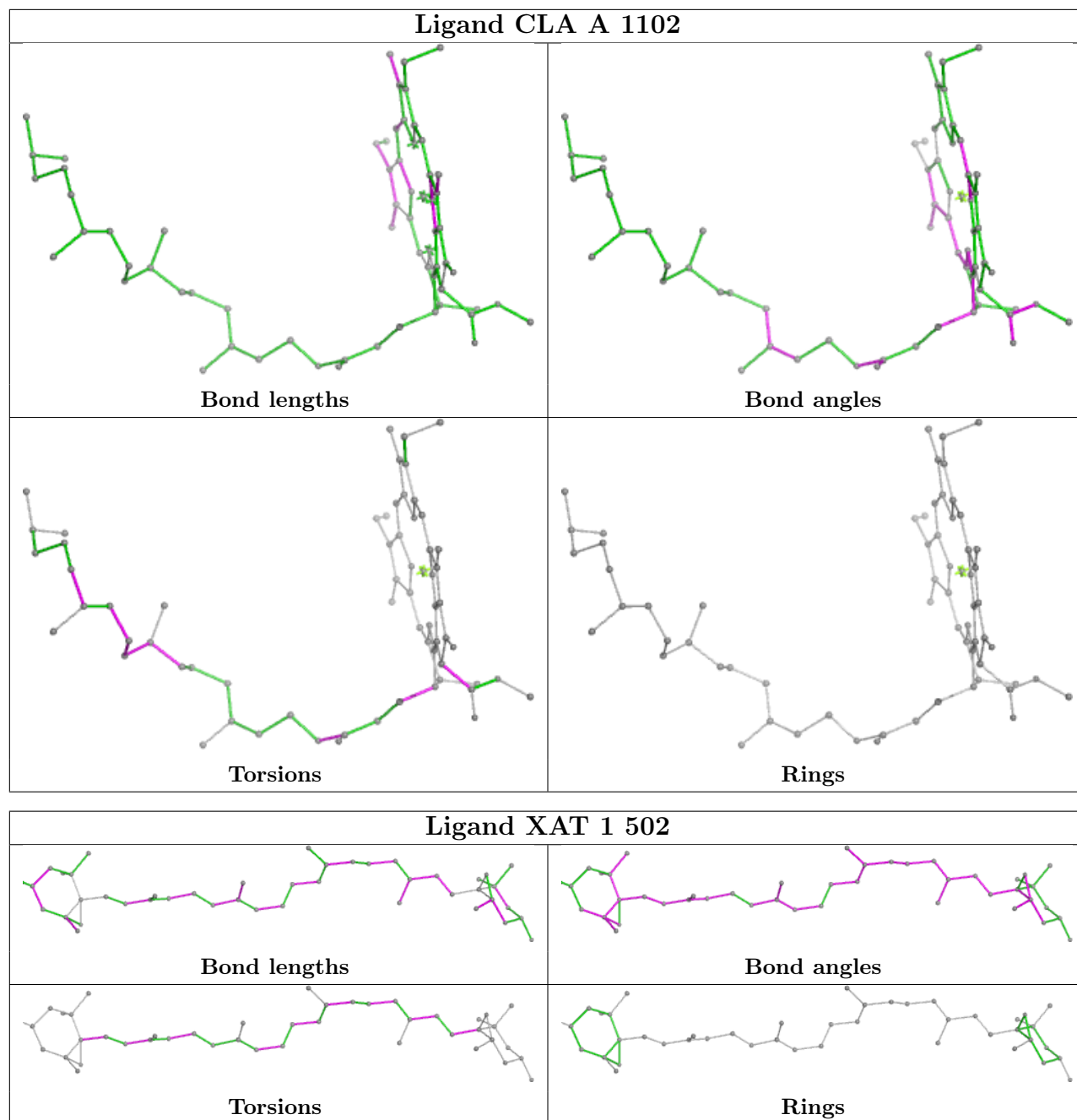


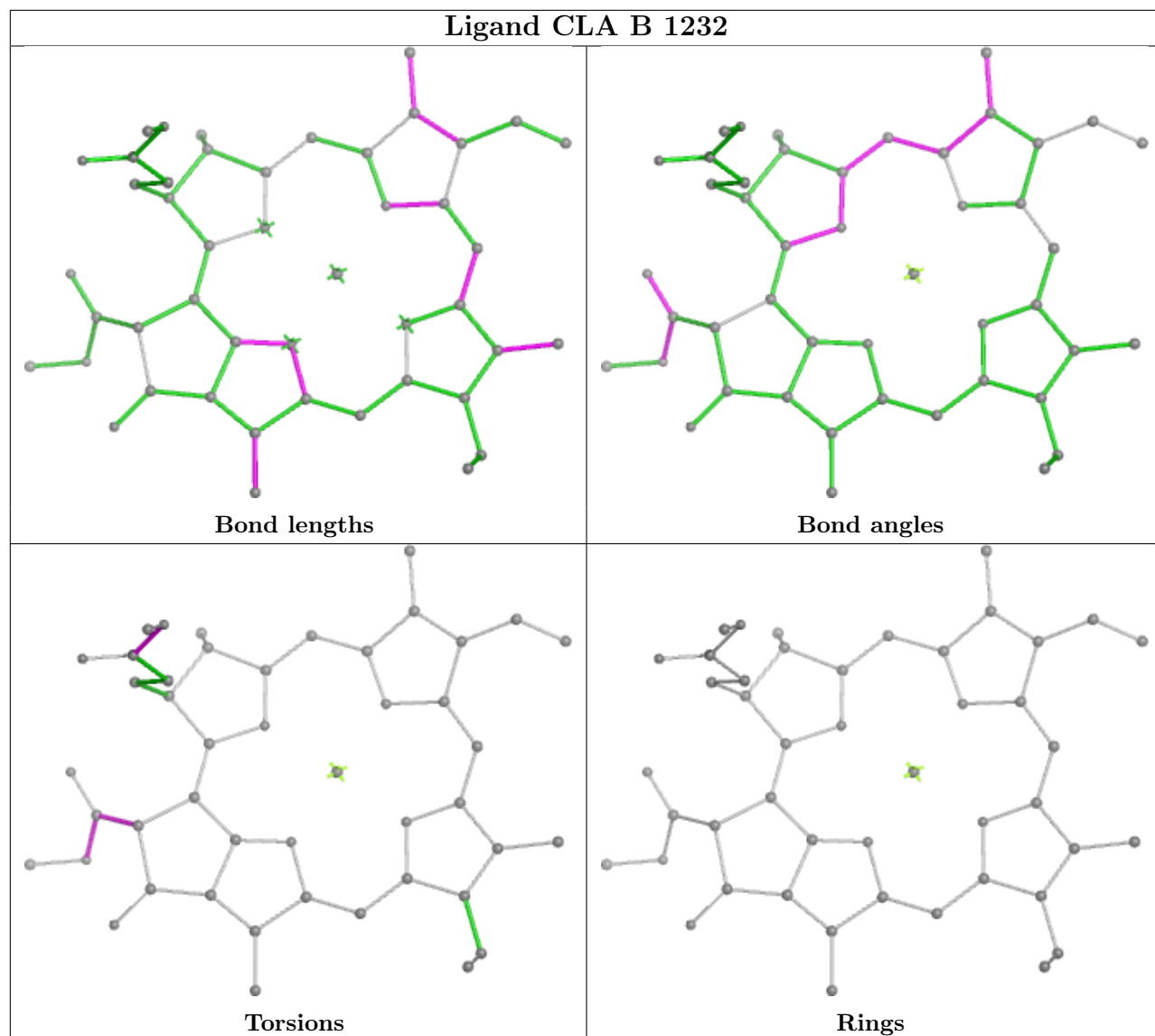
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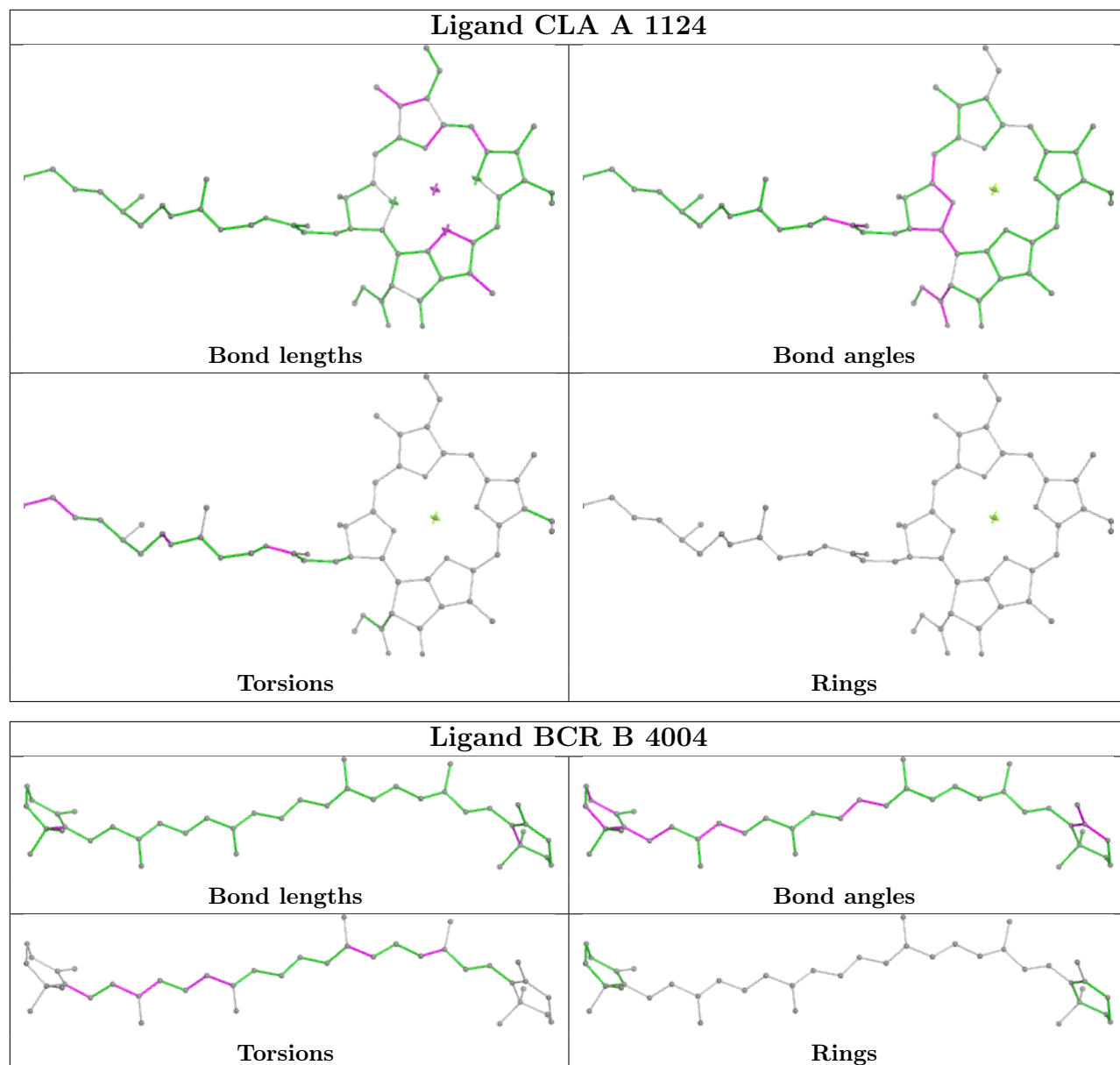


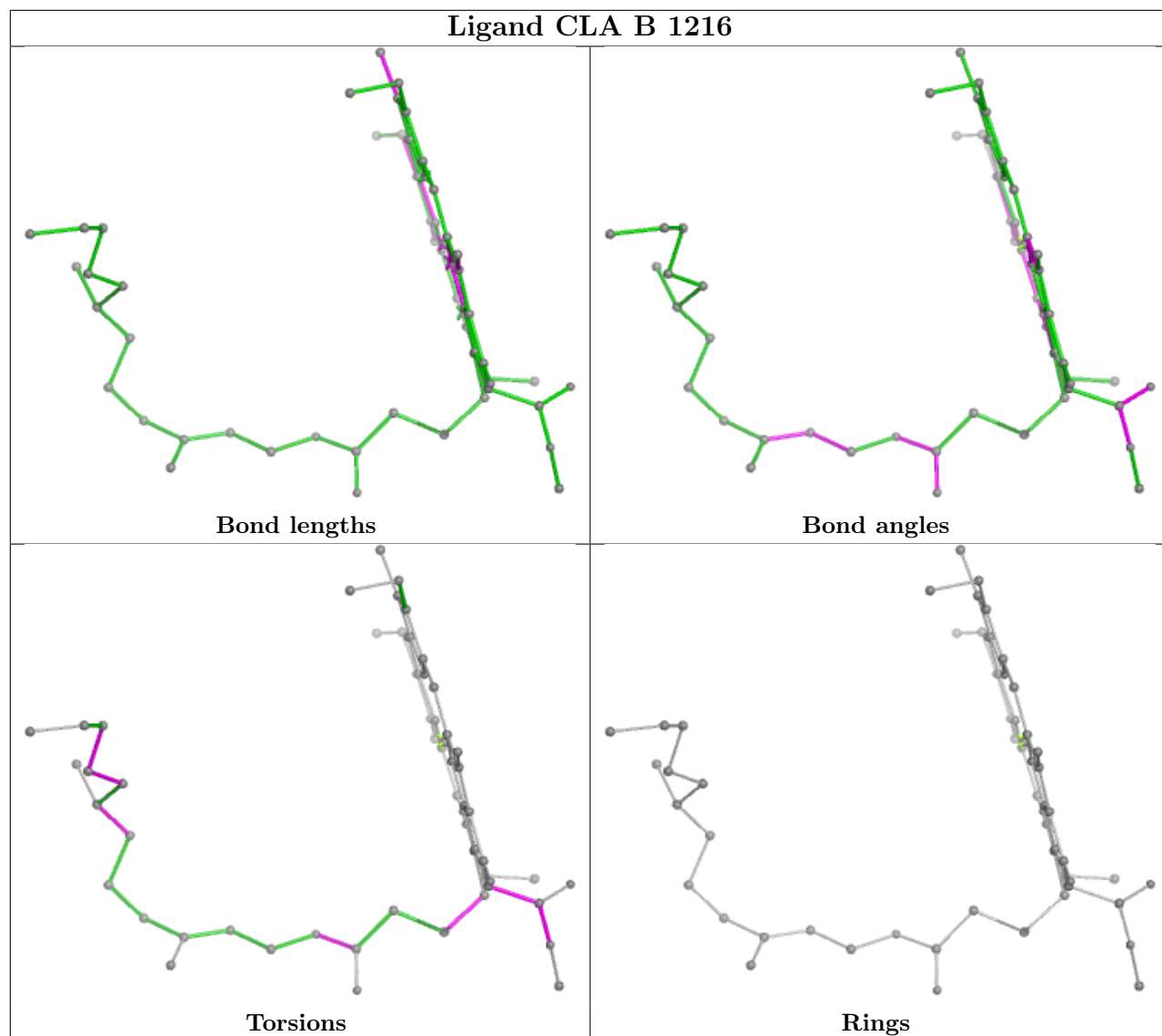
Ligand CLA B 1215**Ligand CLA 1 604**



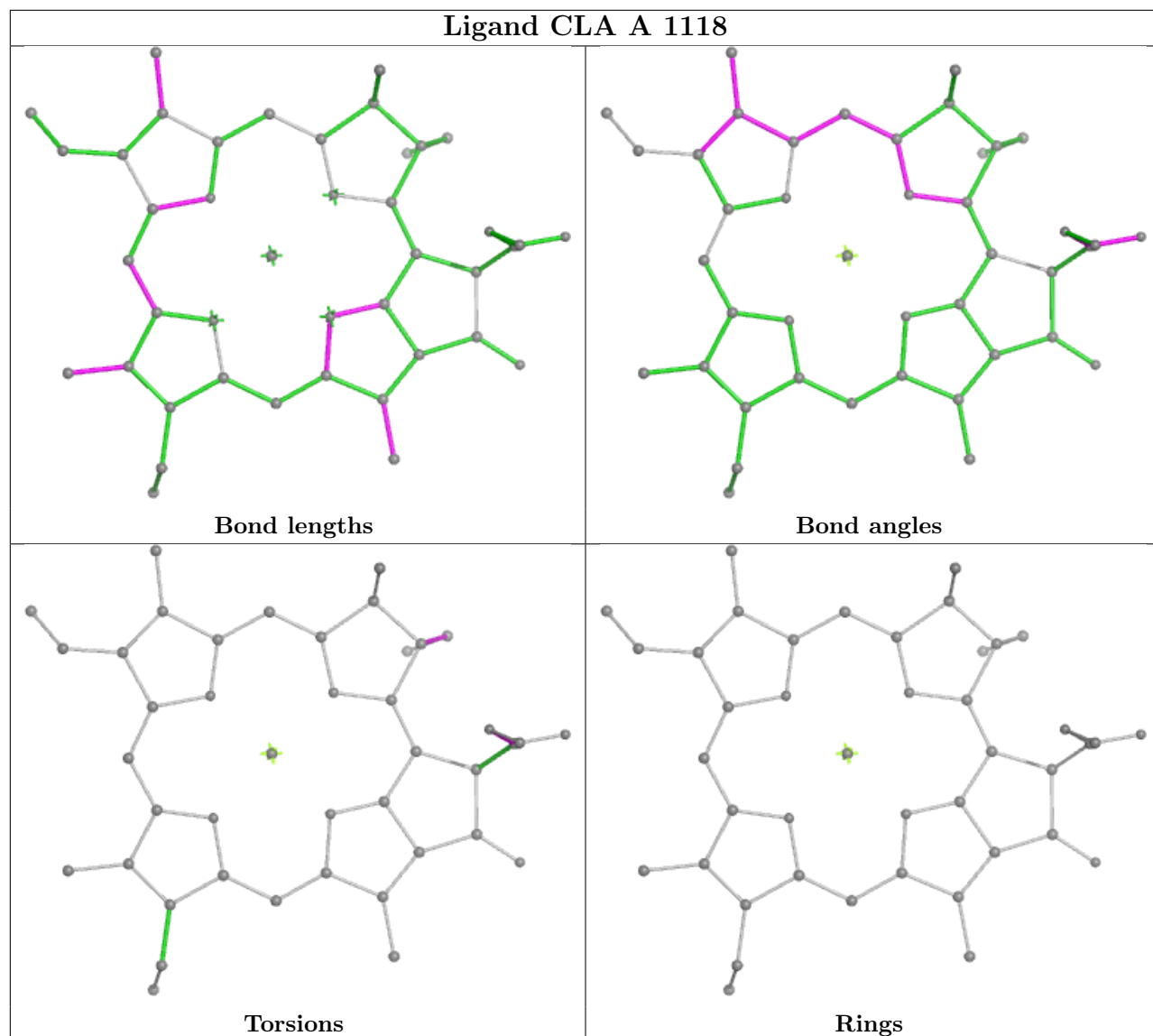




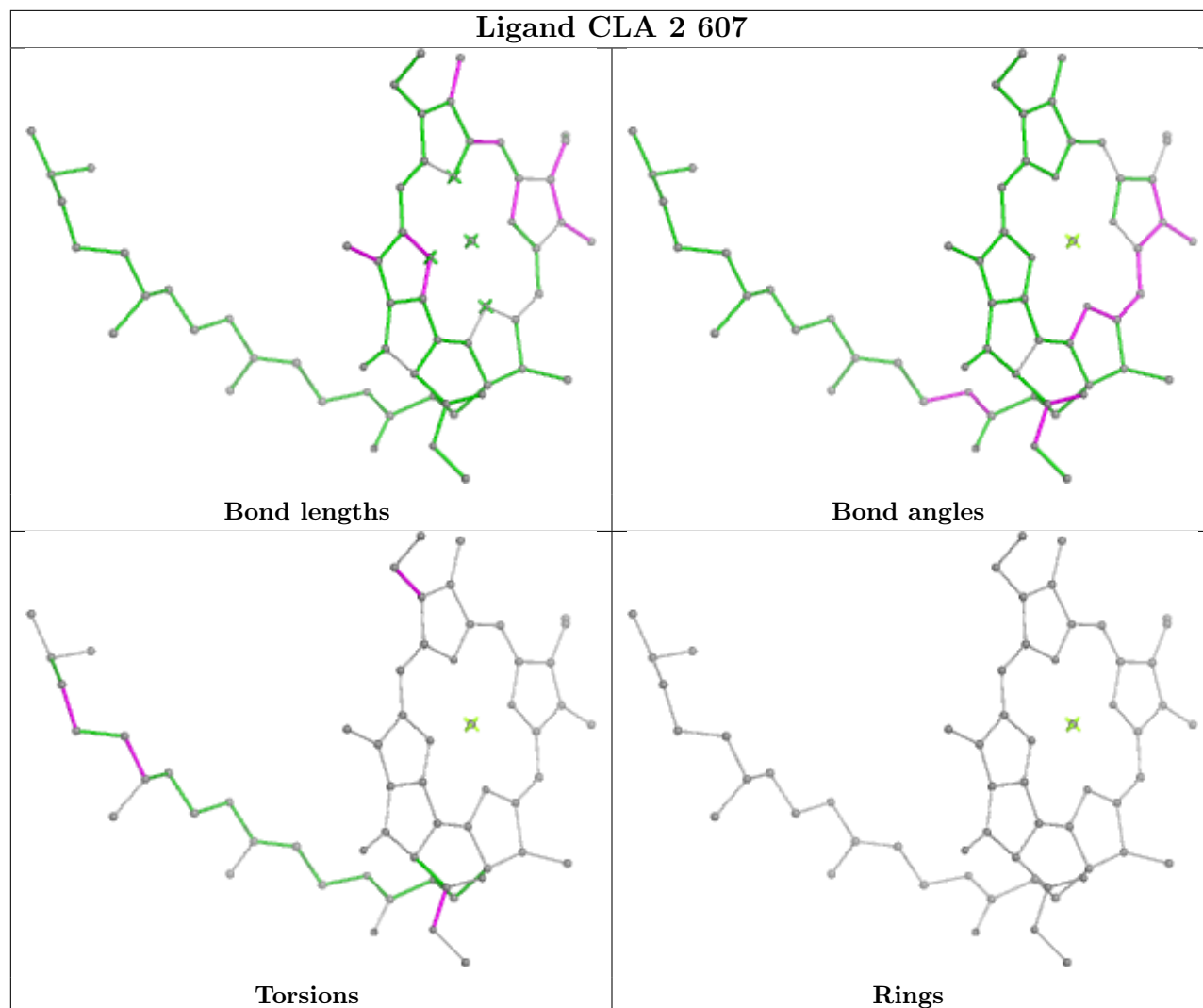




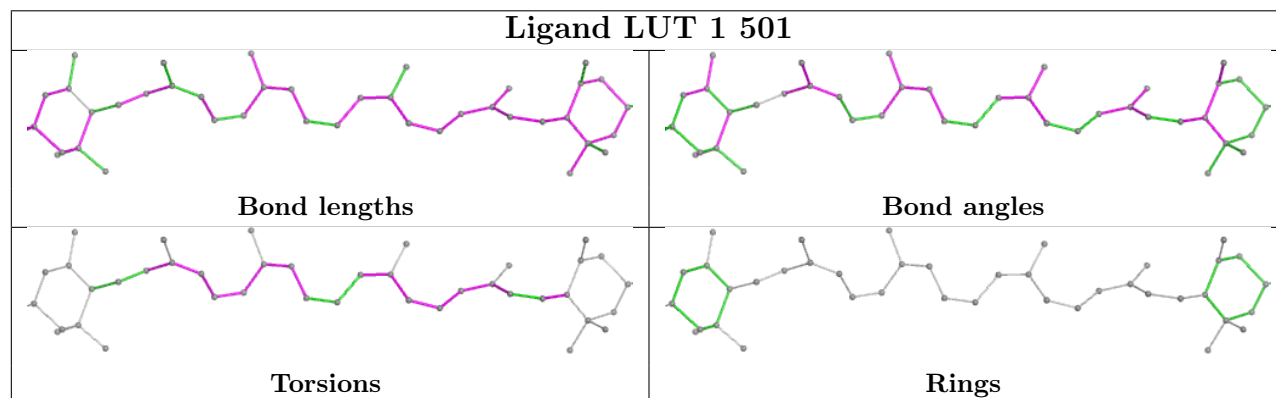
Ligand CLA A 1118

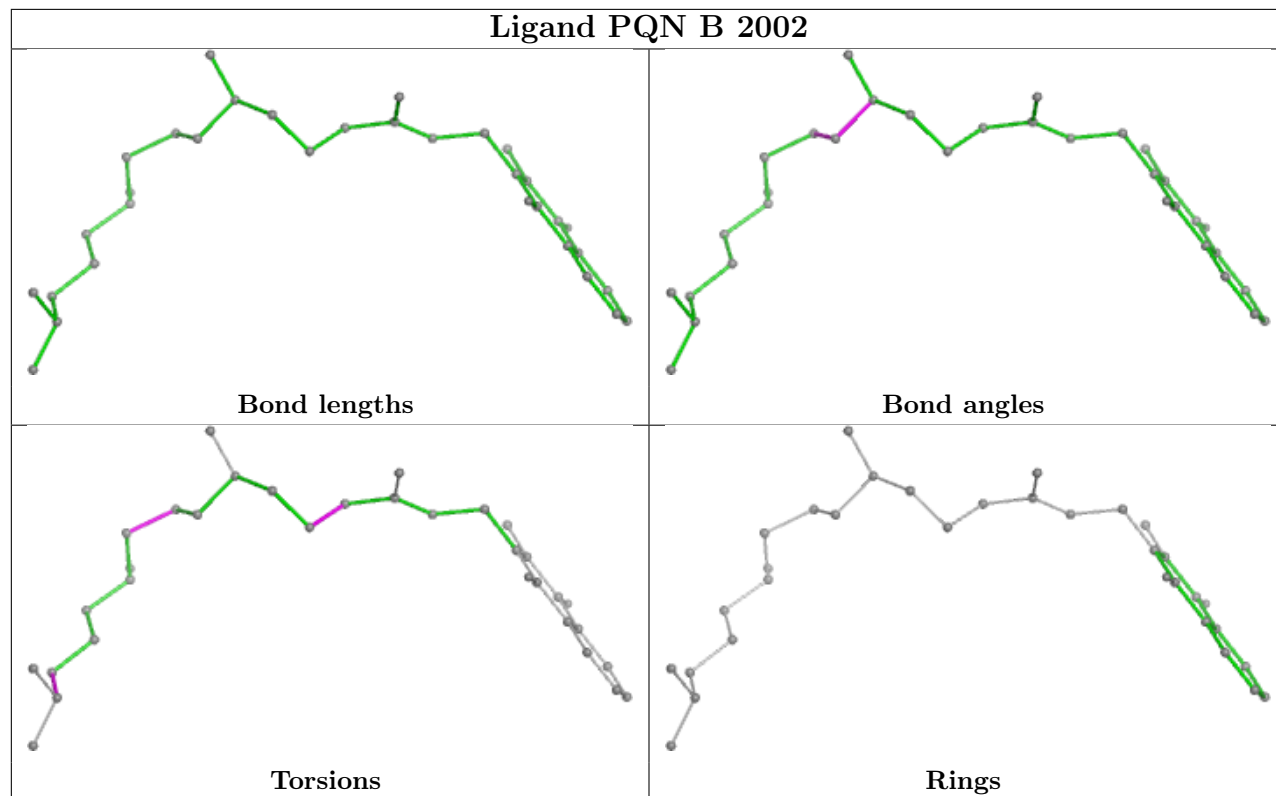
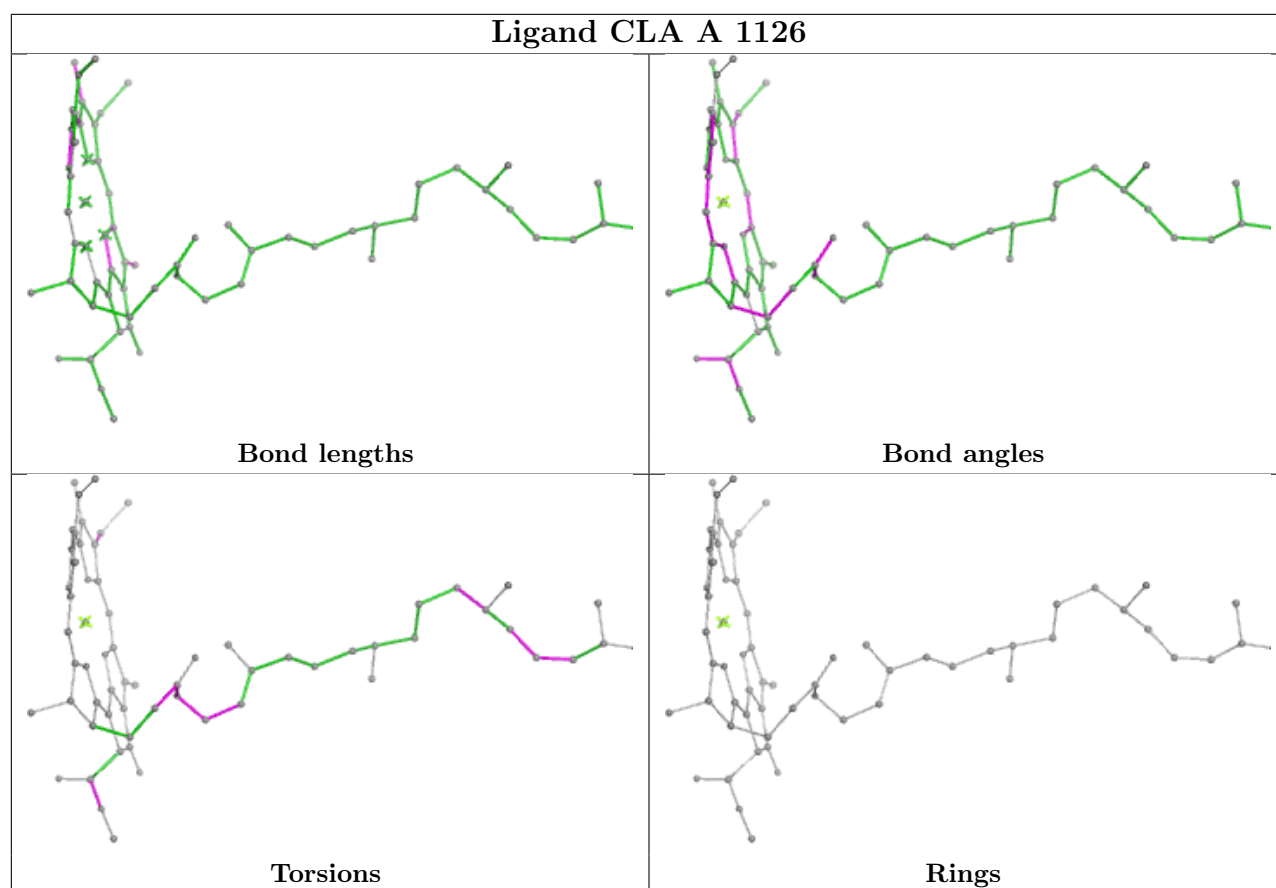


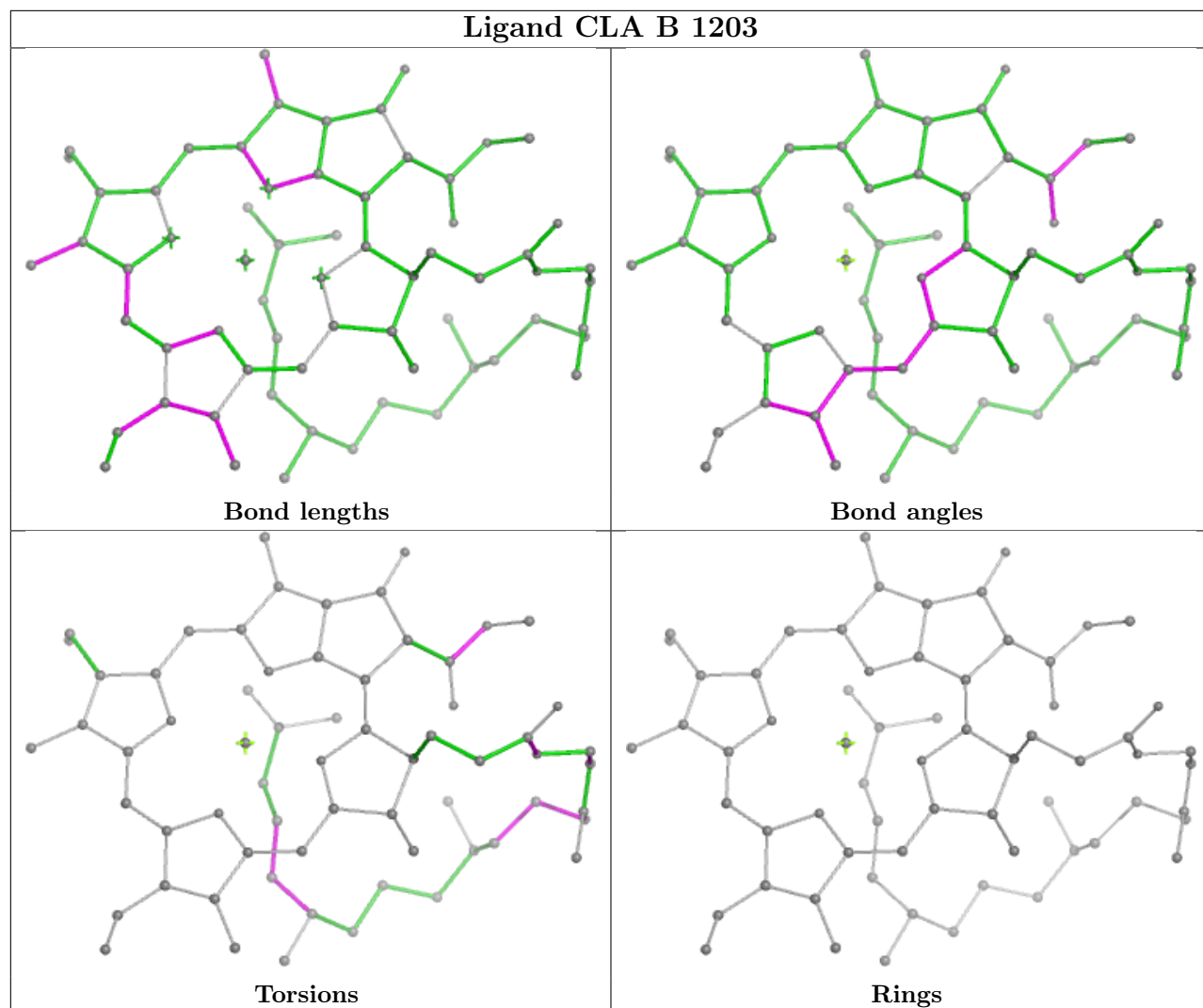
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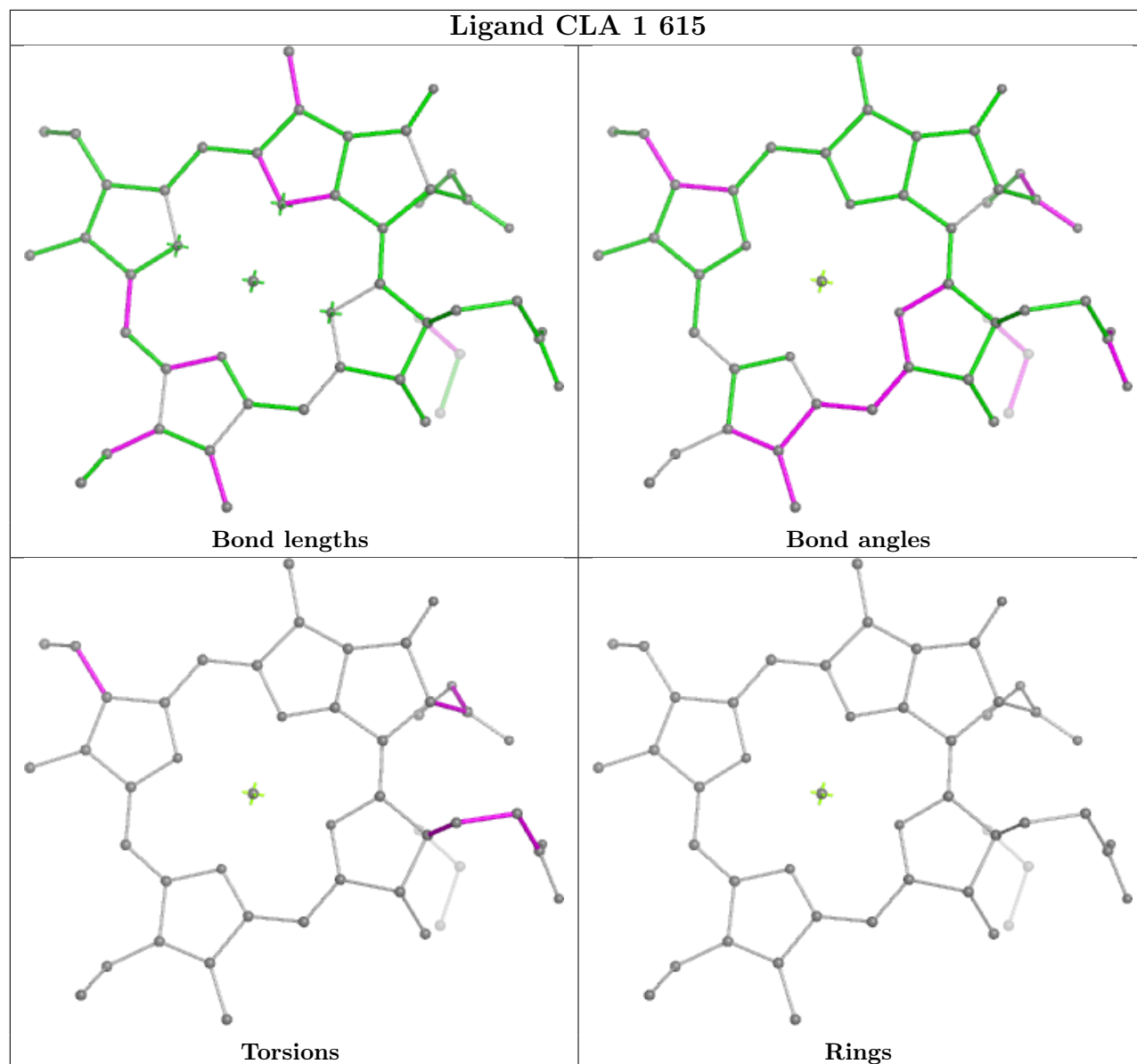
Ligand LUT 1 501



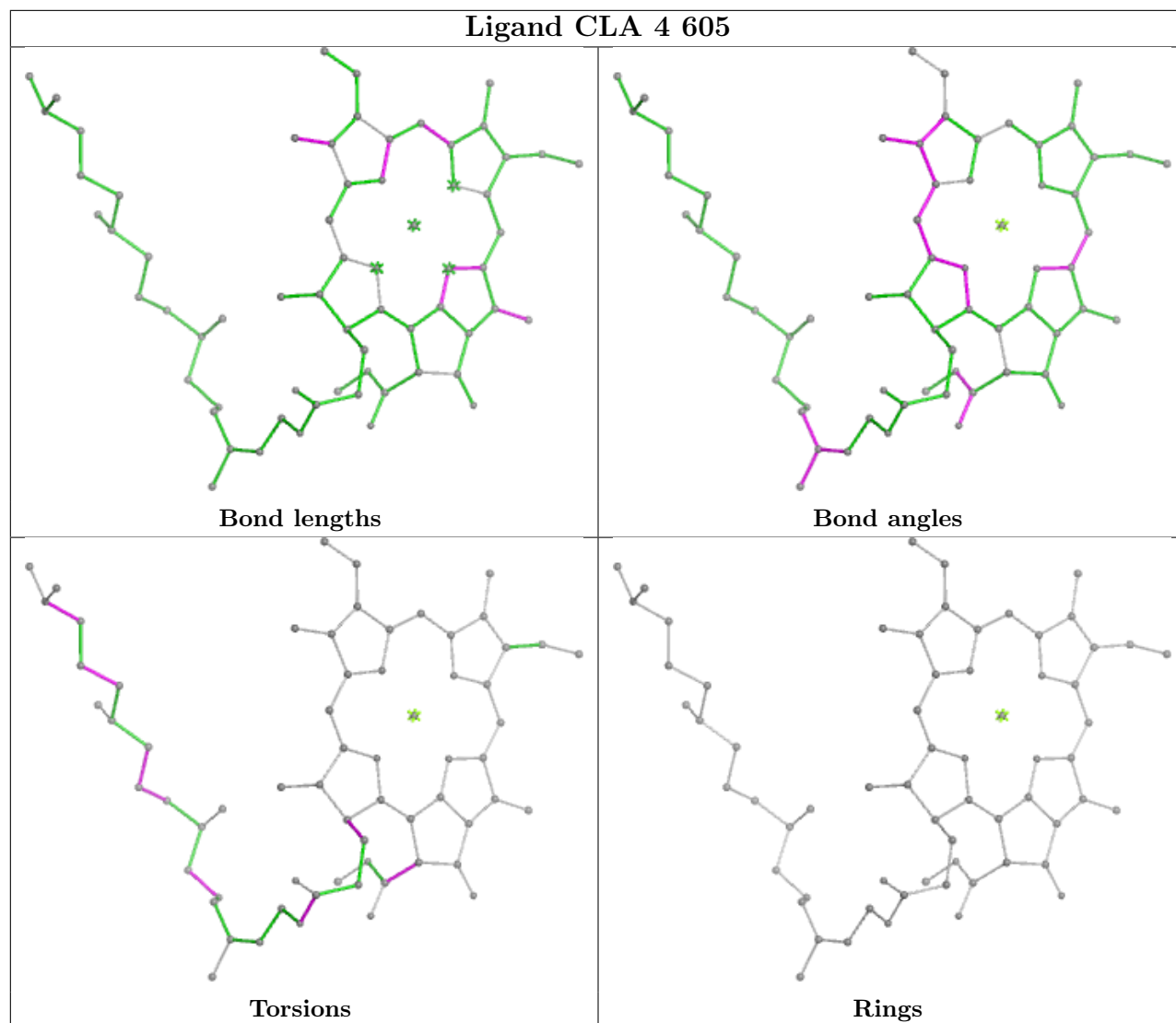




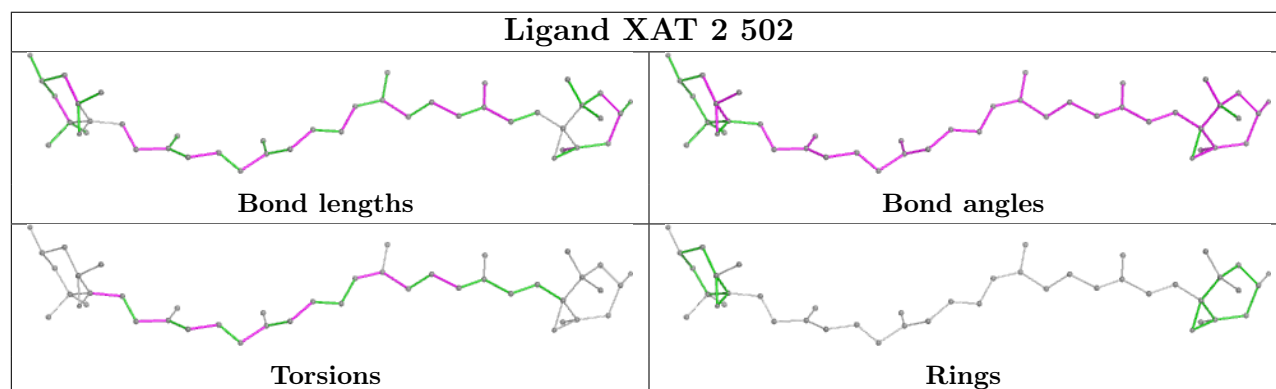
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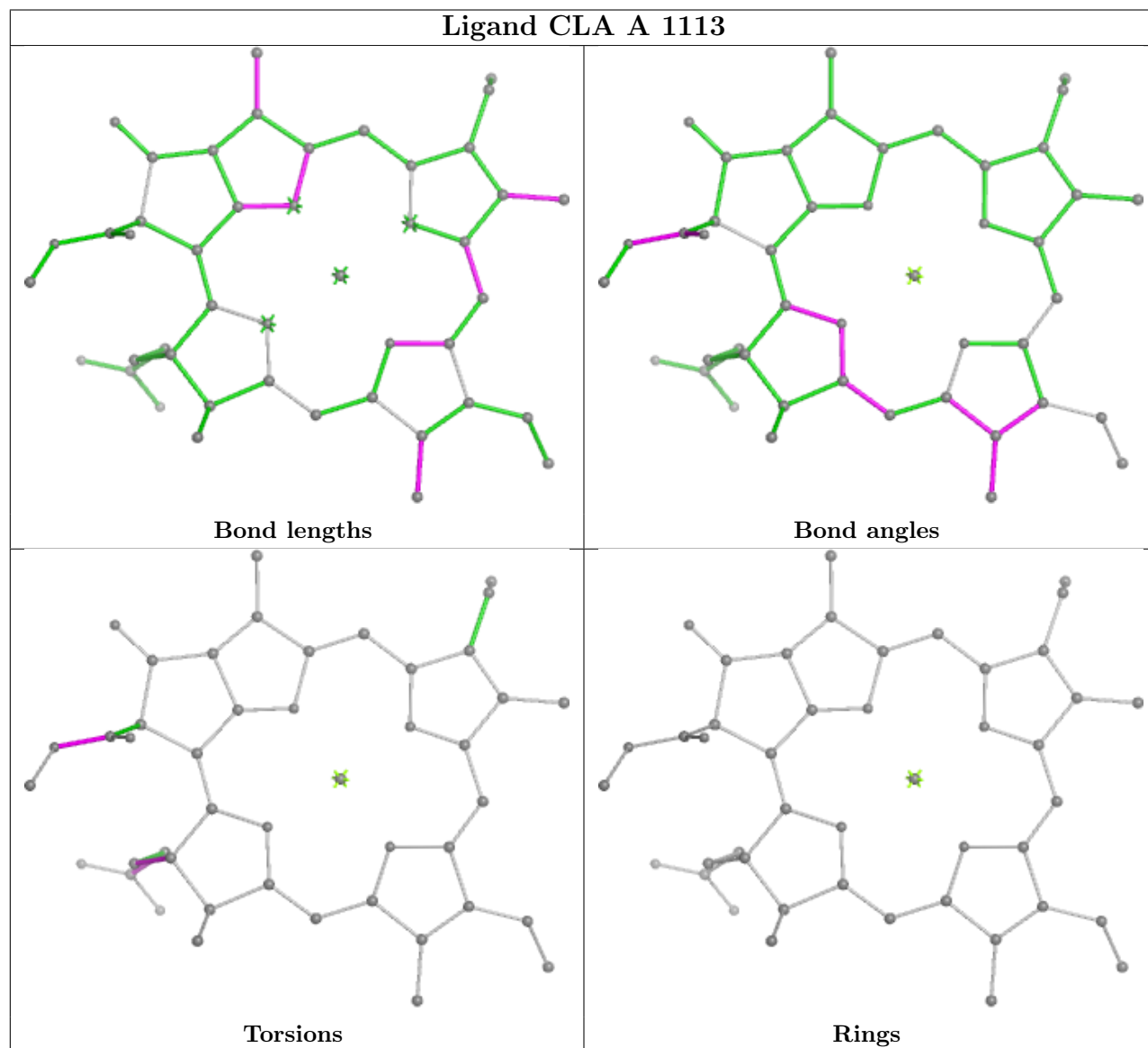
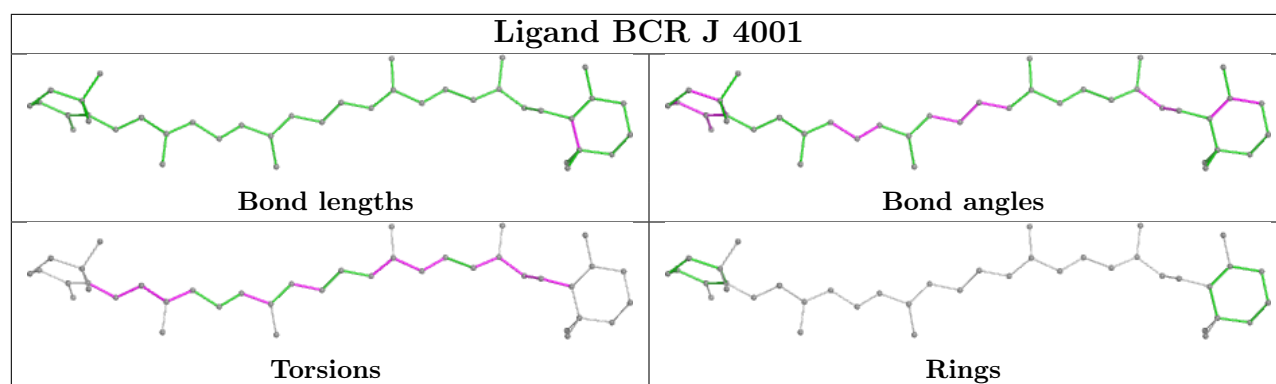


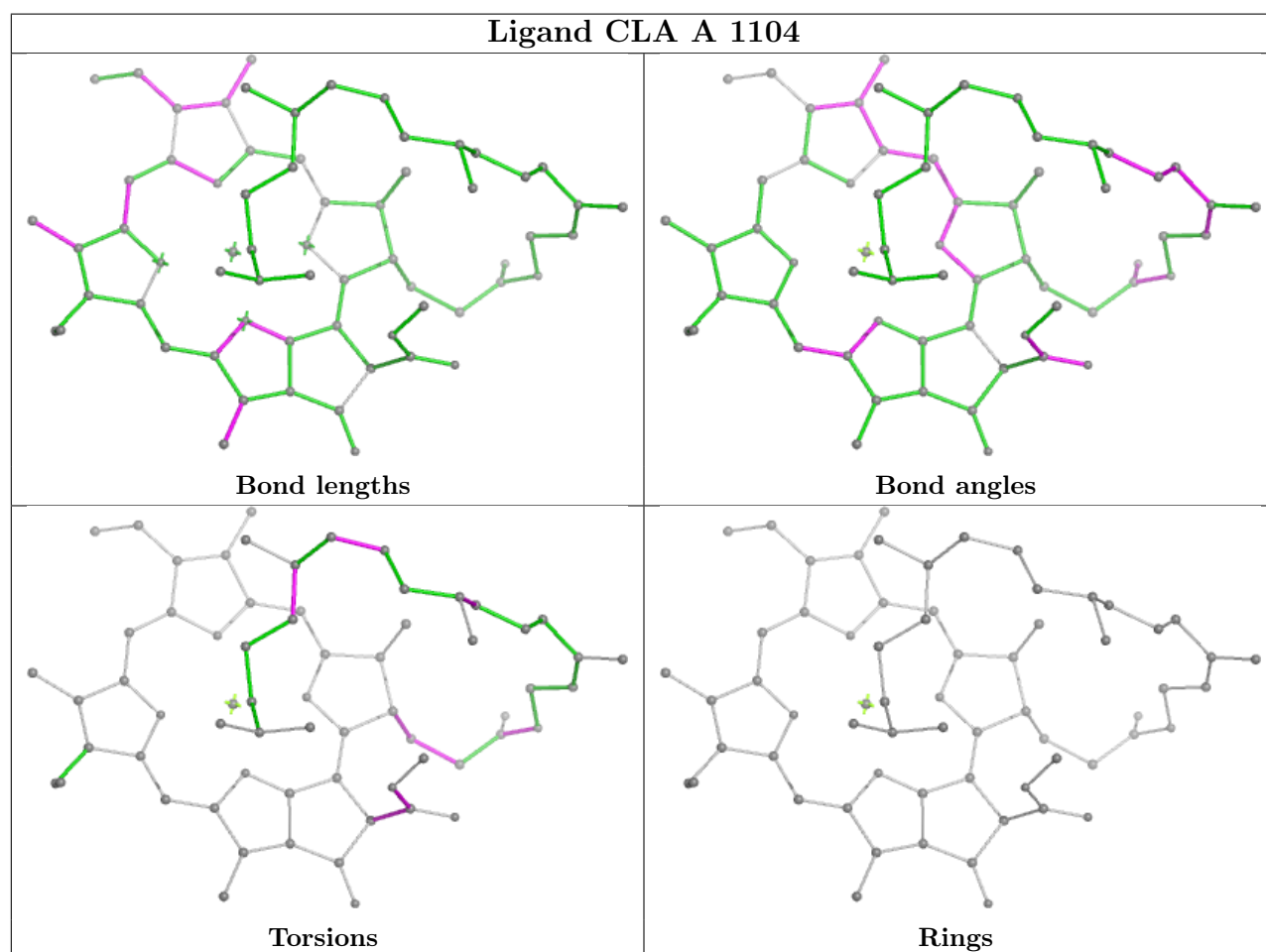
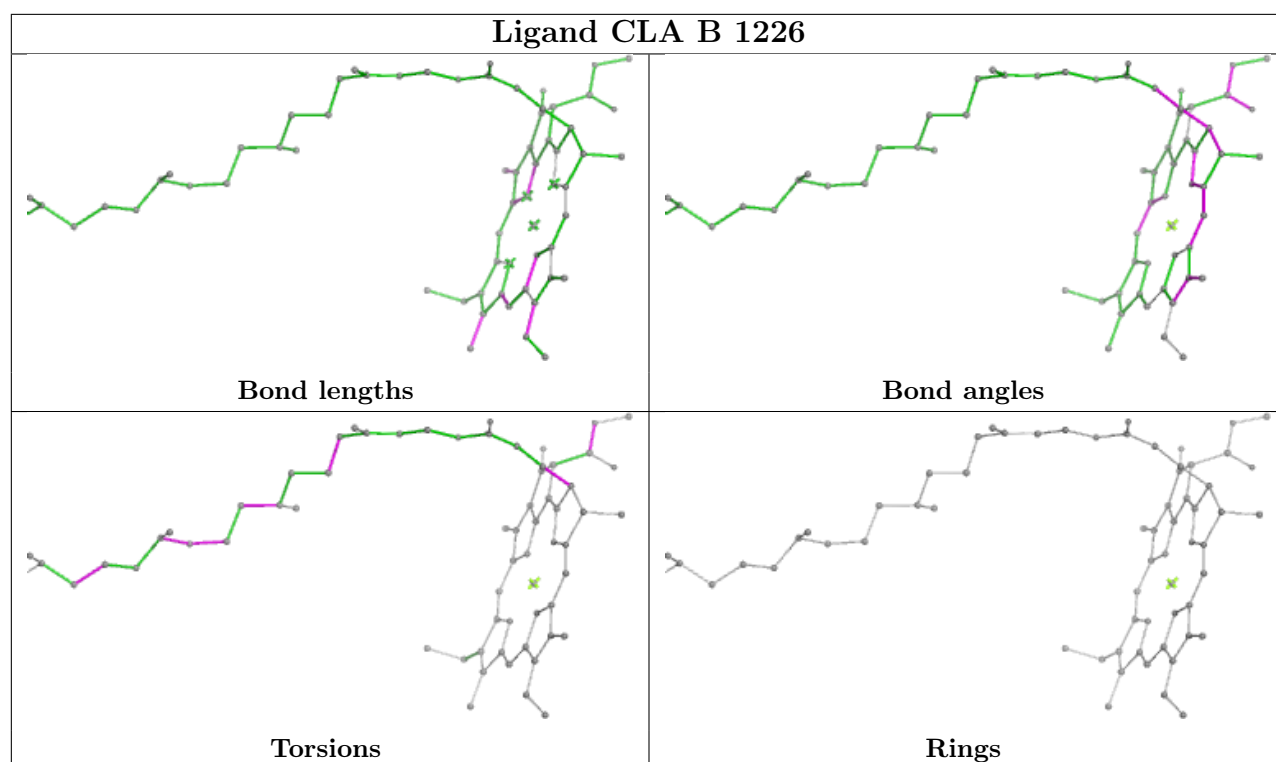
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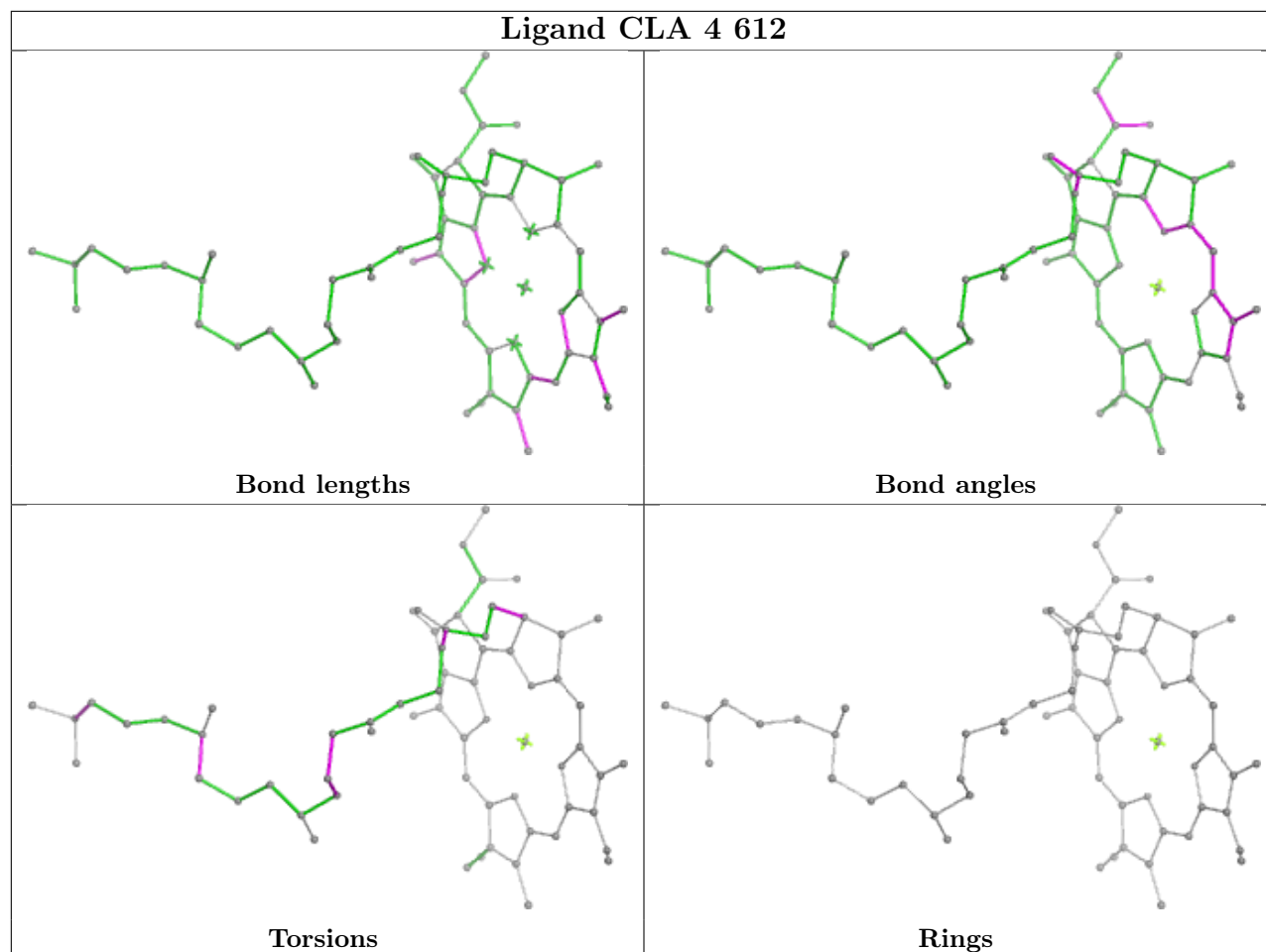
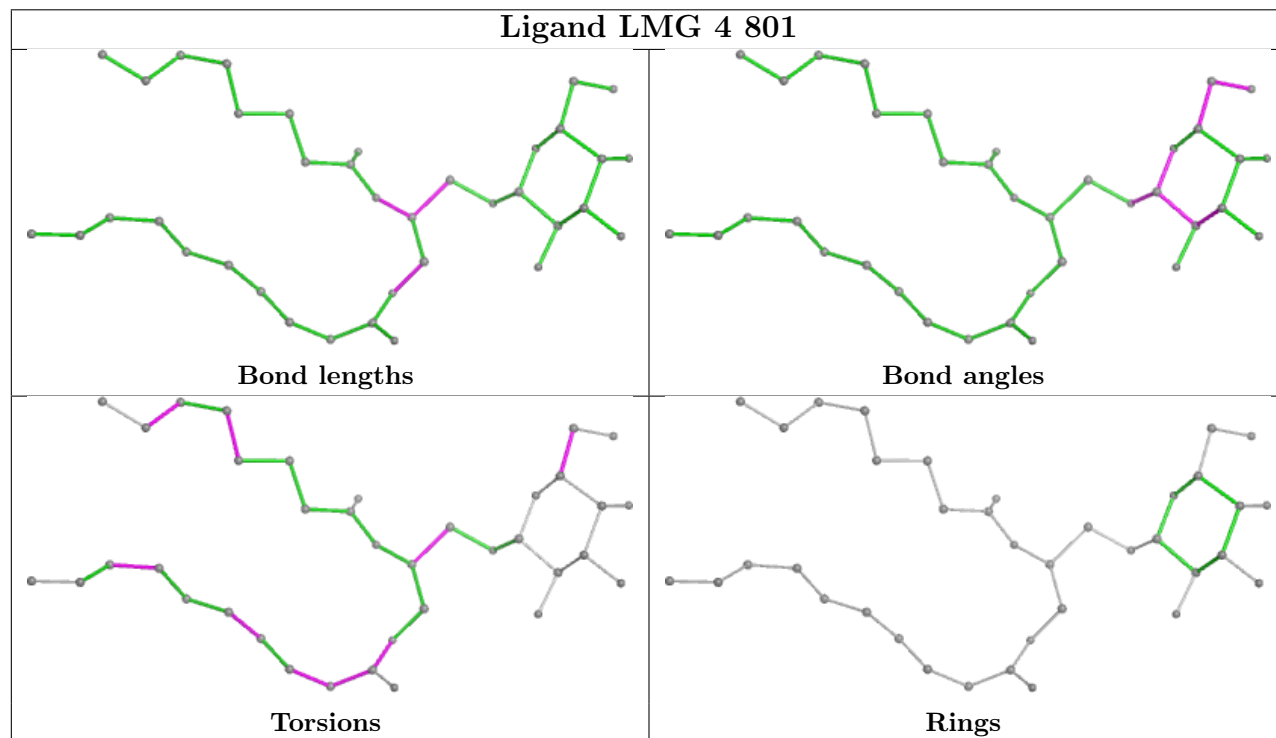


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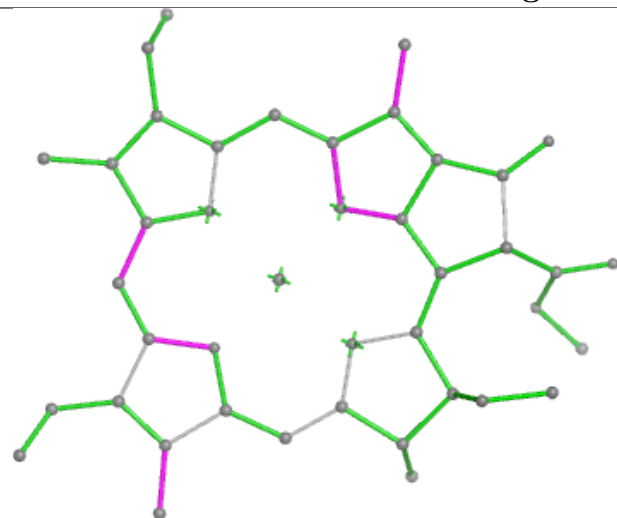




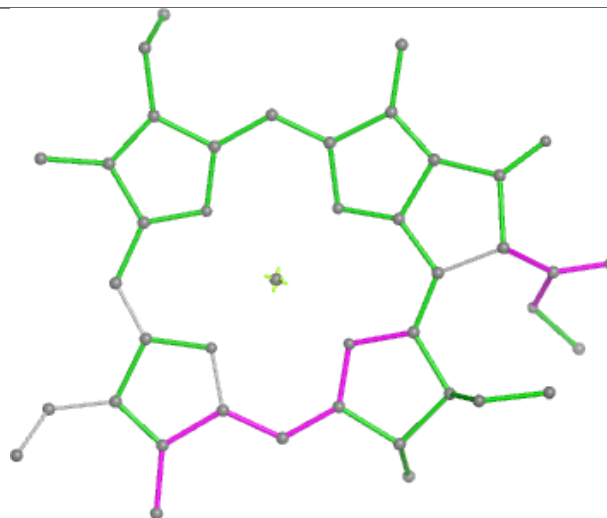


Ligand CLA 4 612**Ligand LMG 4 801**

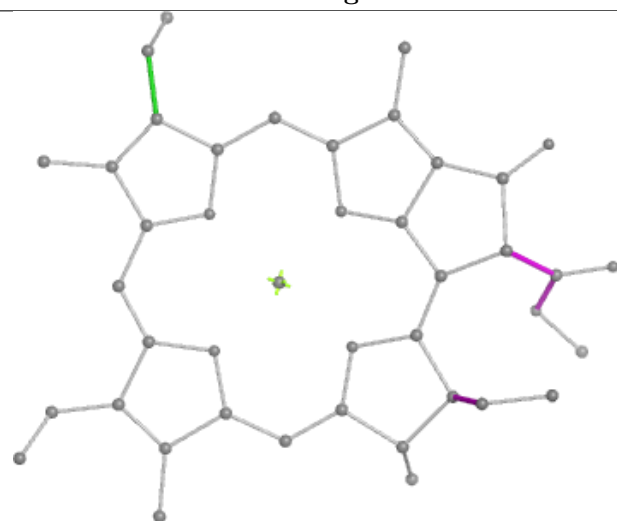
Ligand CLA 3 615



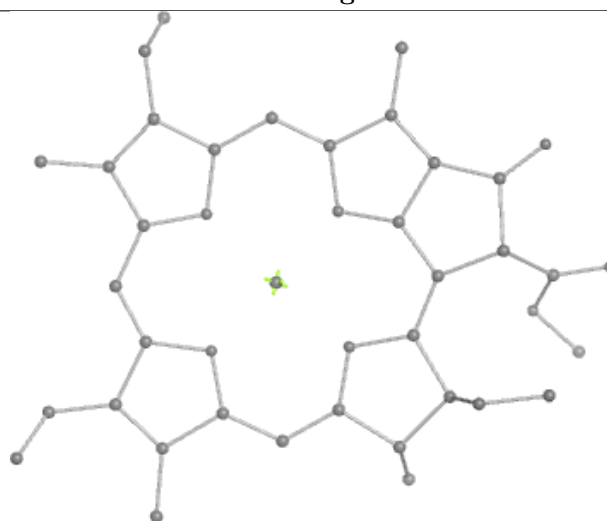
Bond lengths



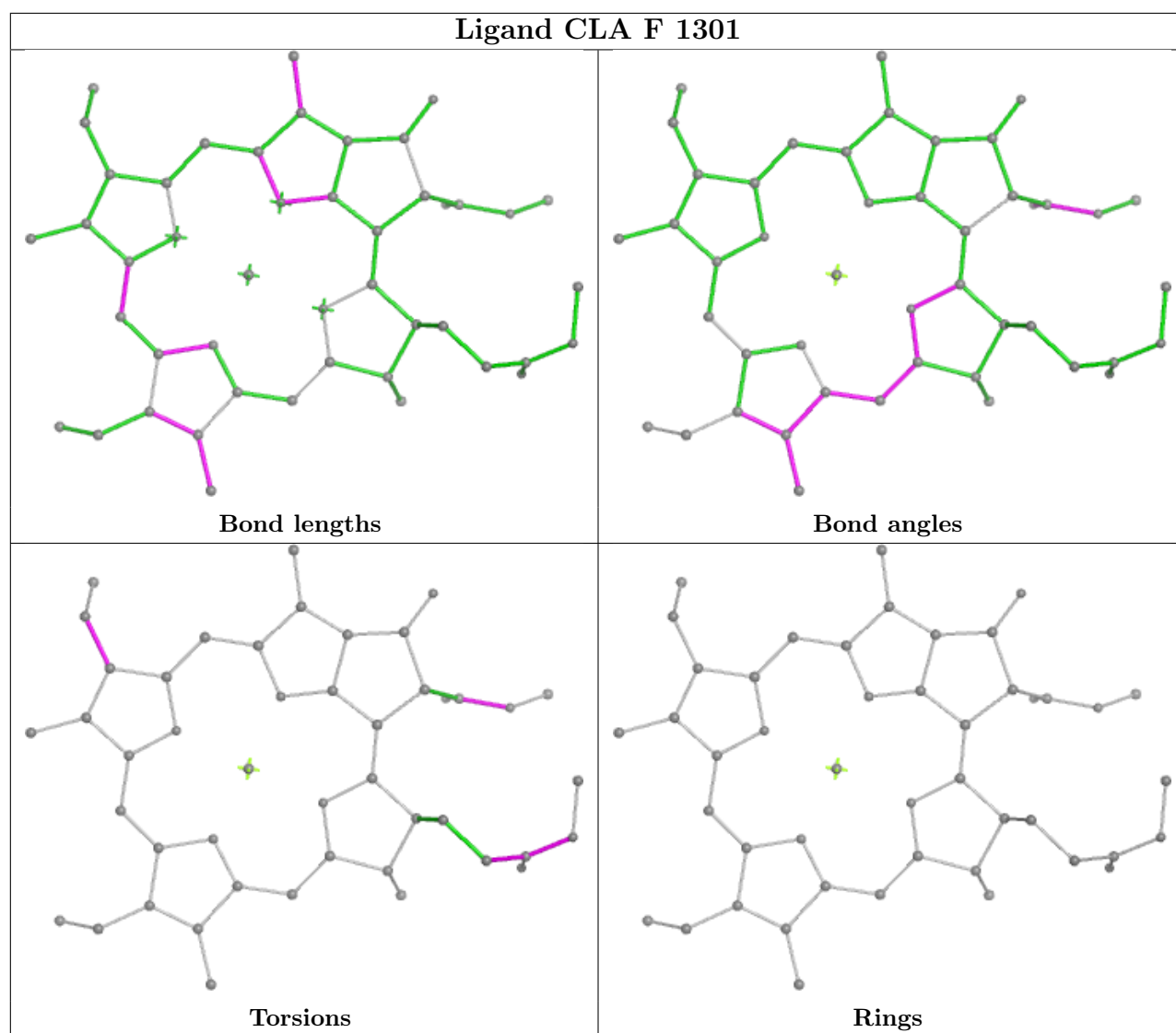
Bond angles

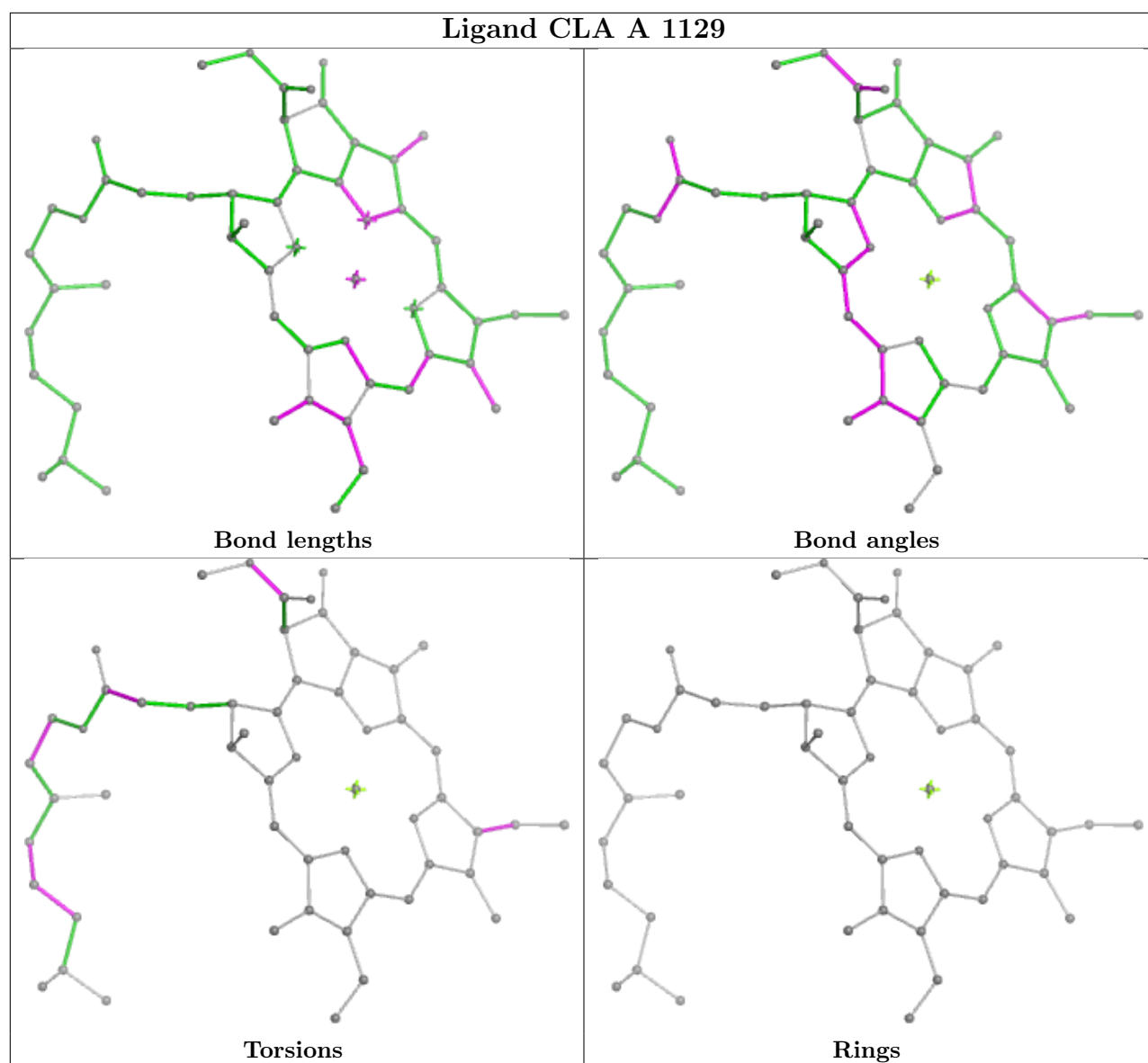


Torsions

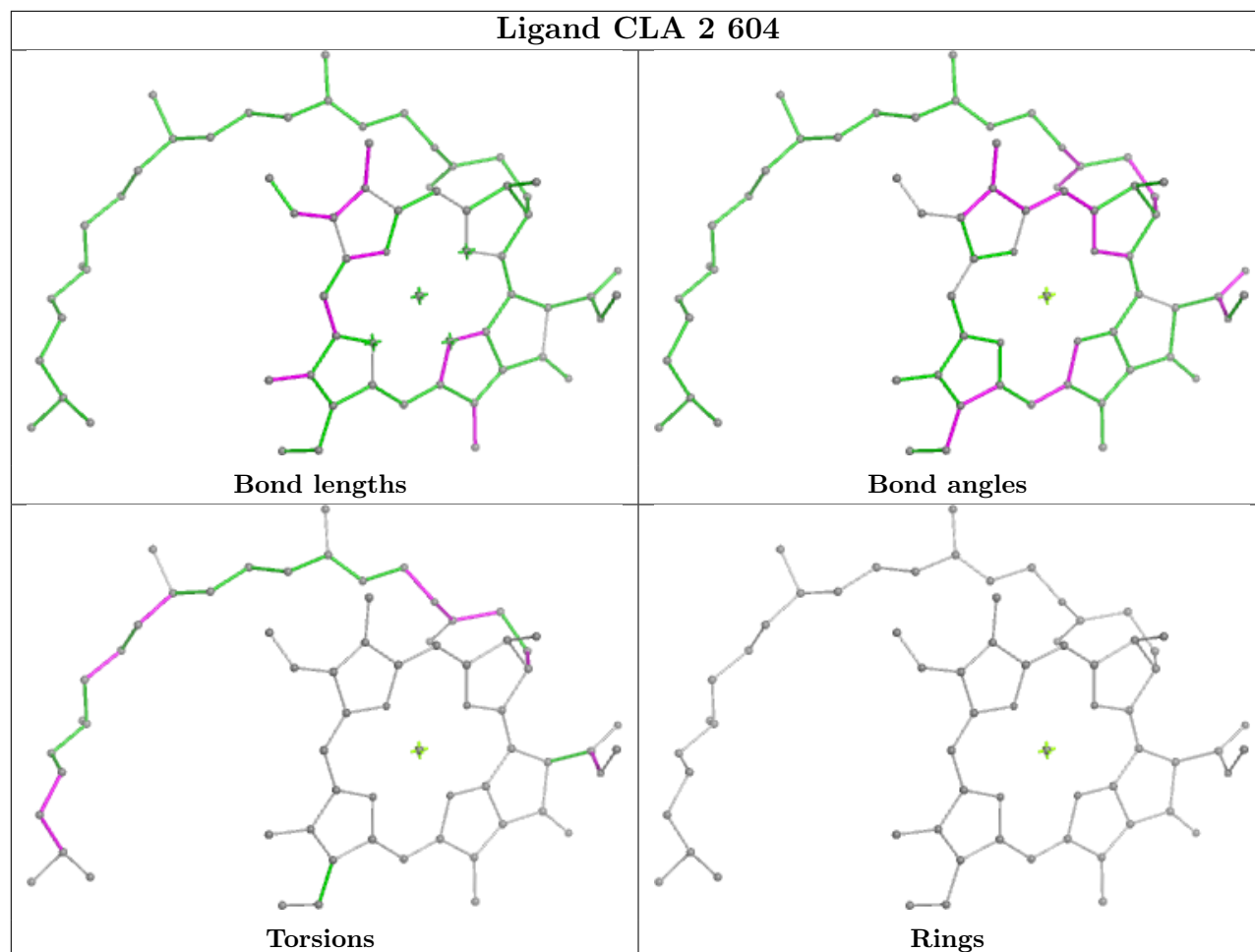


Rings

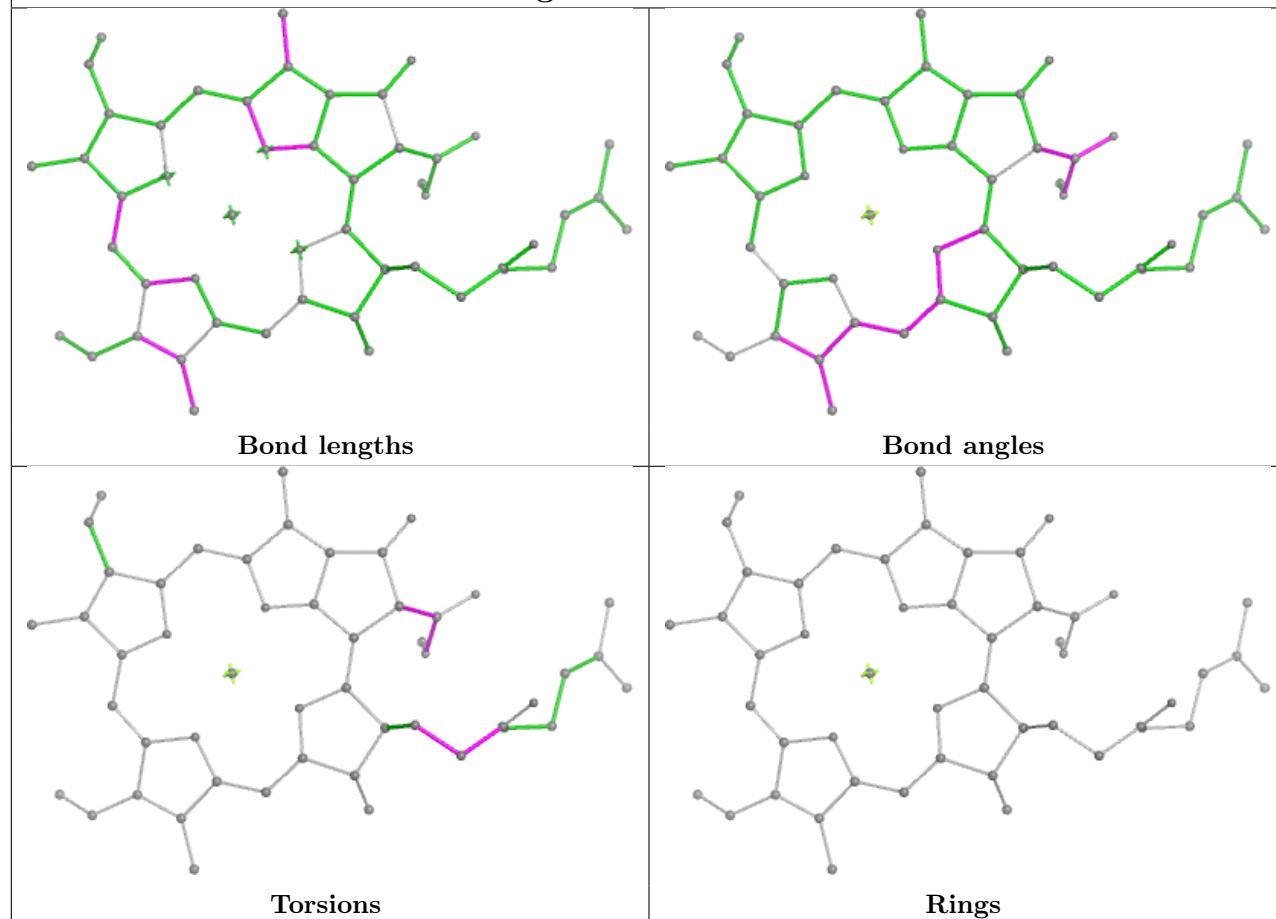




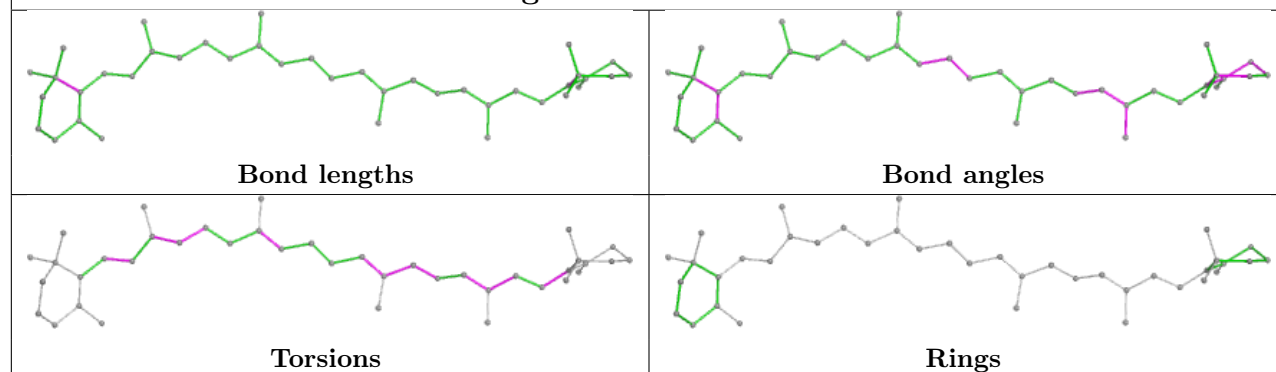
Ligand CLA 2 604



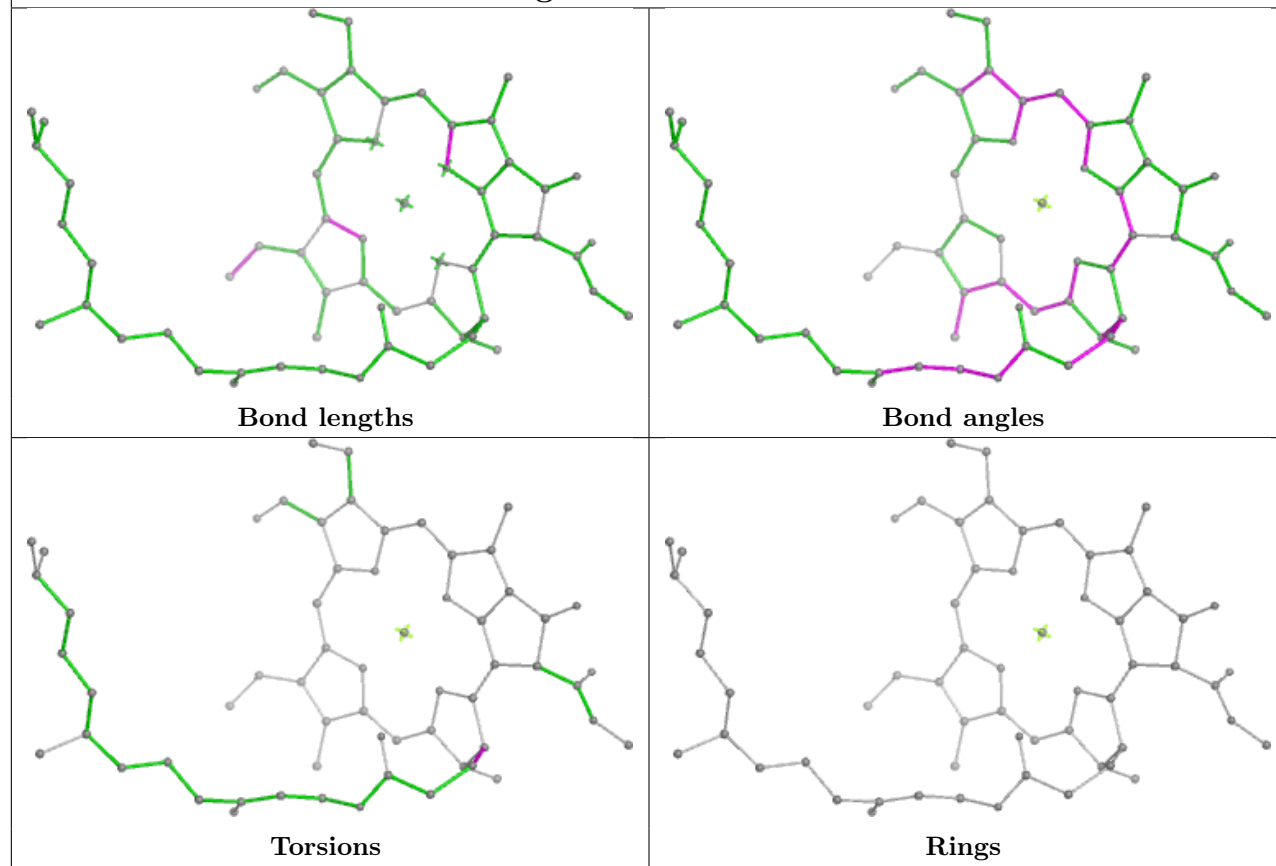
Ligand CLA 4 602



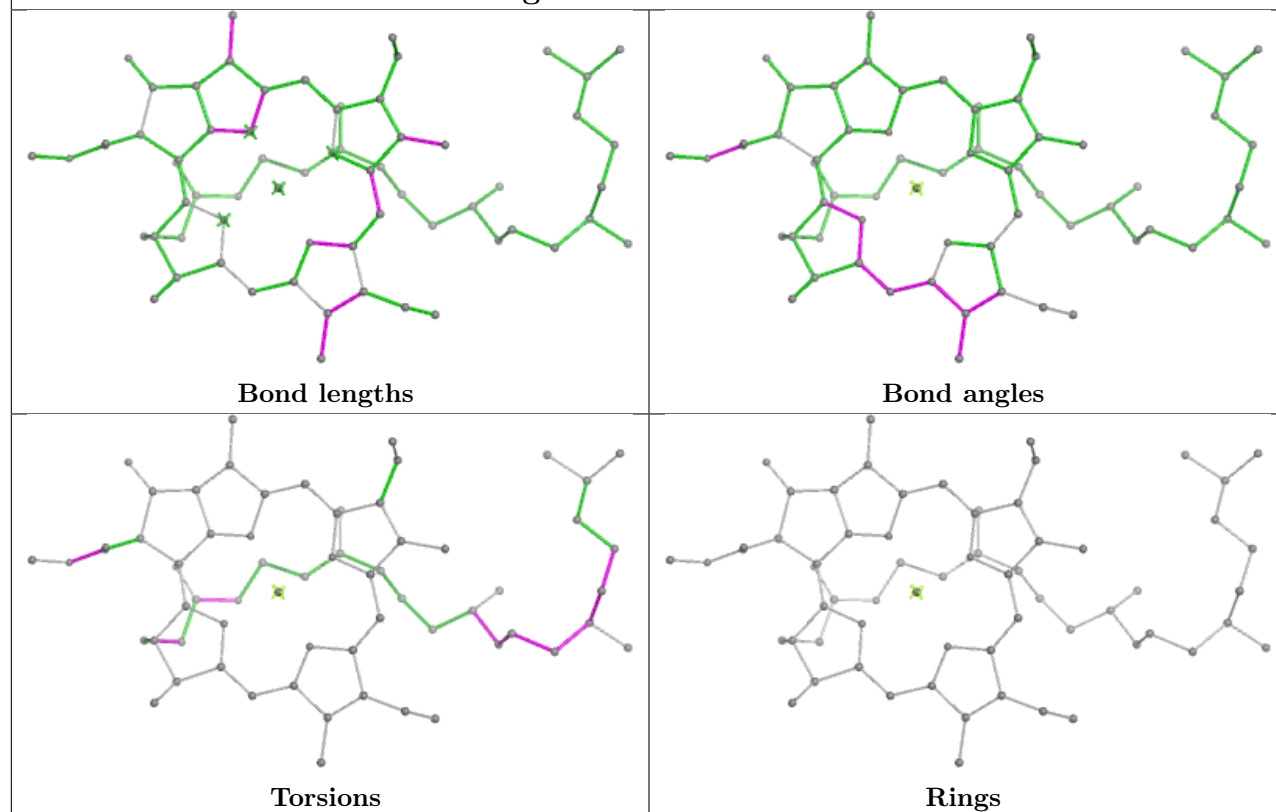
Ligand BCR B 4002

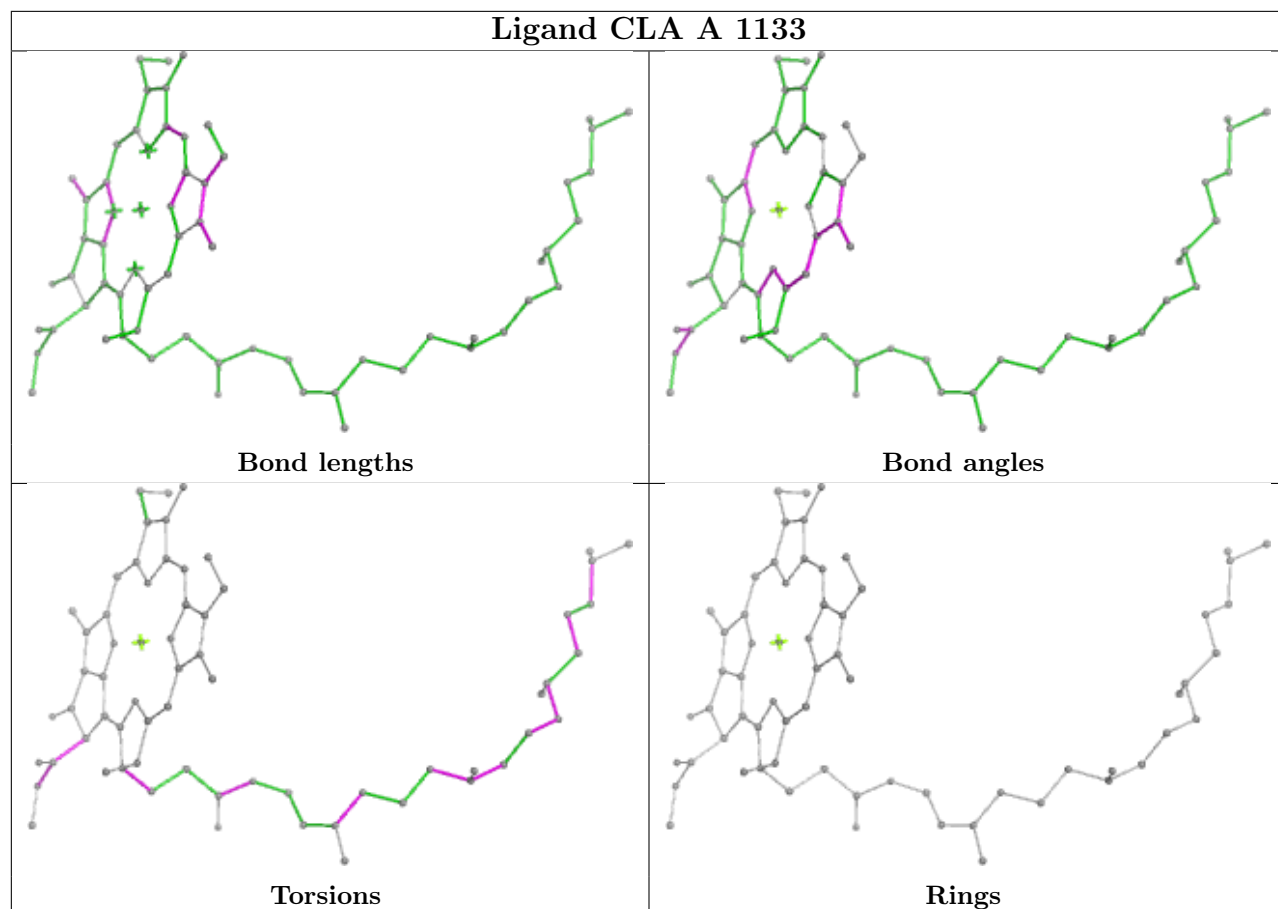
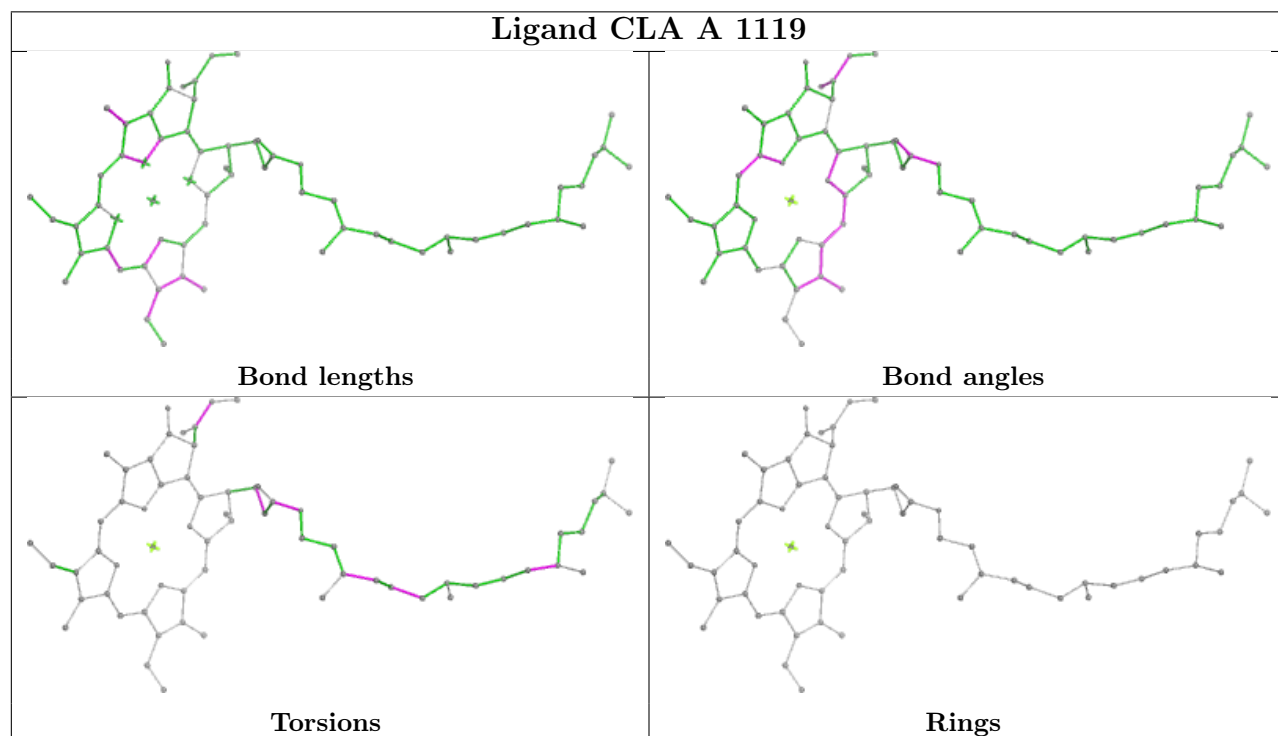


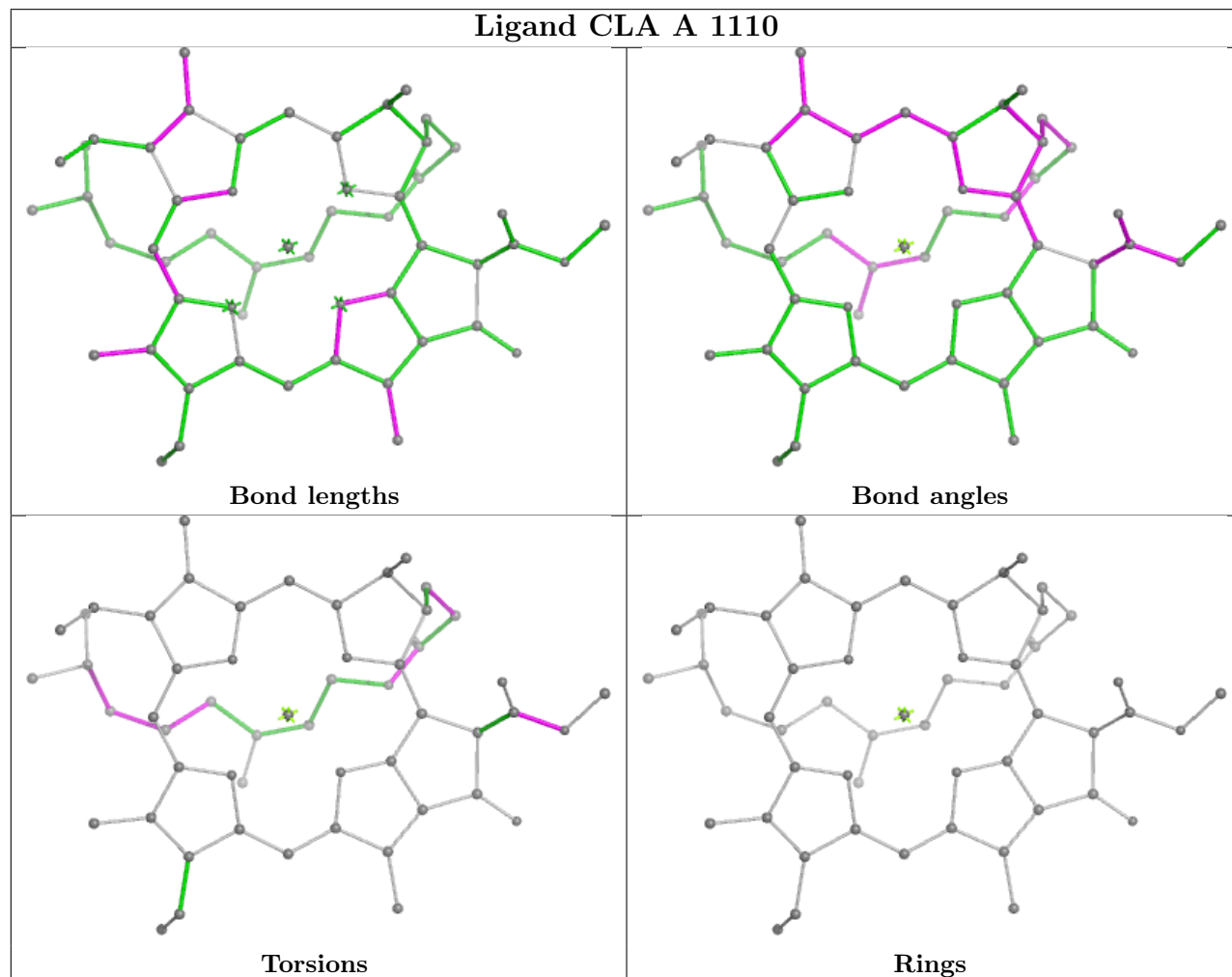
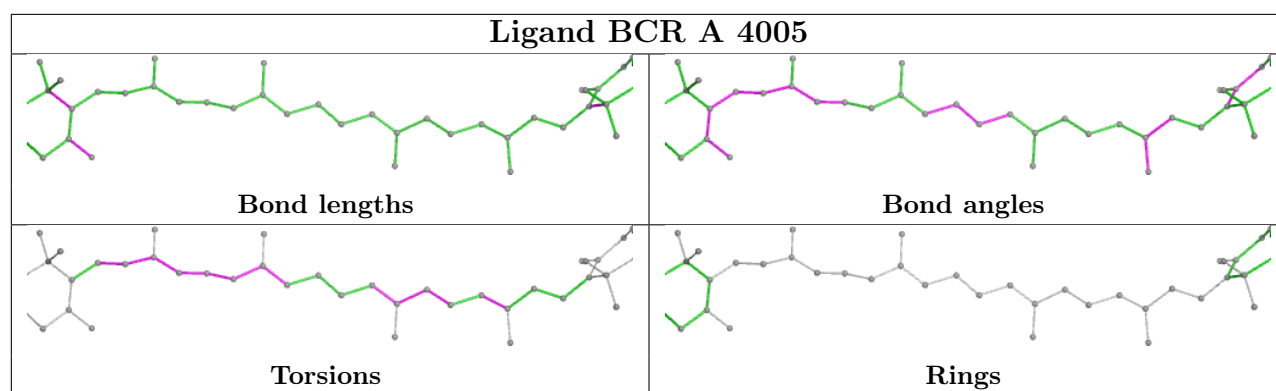
Ligand CHL 3 604

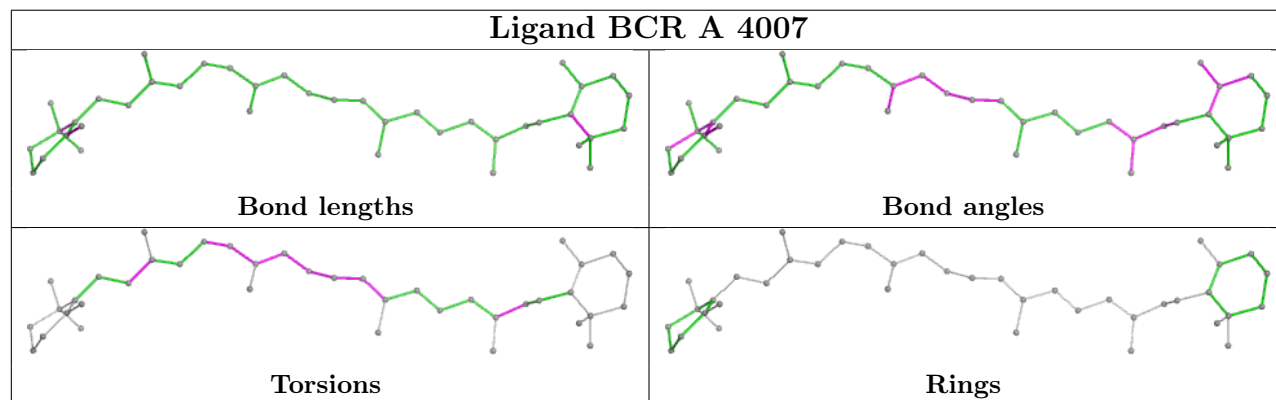
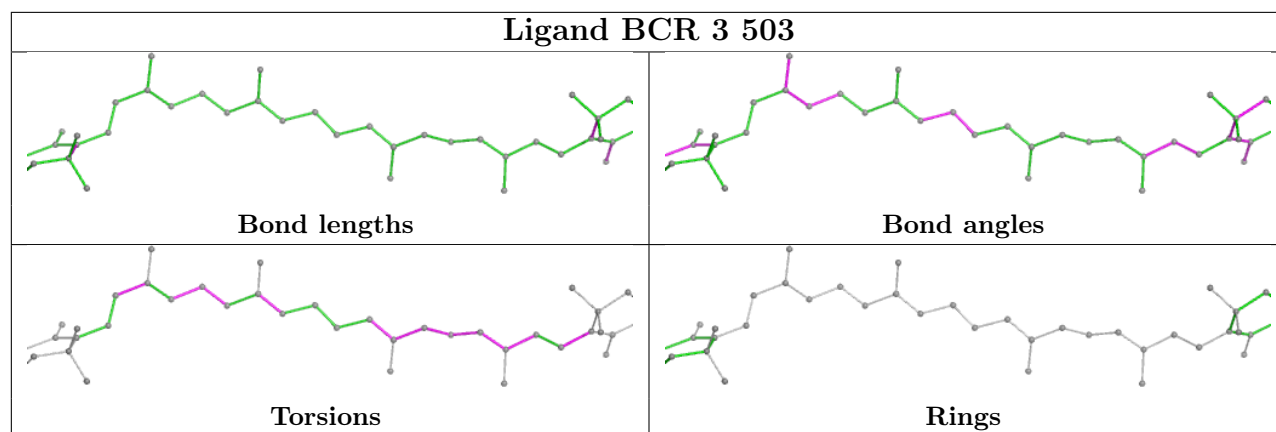
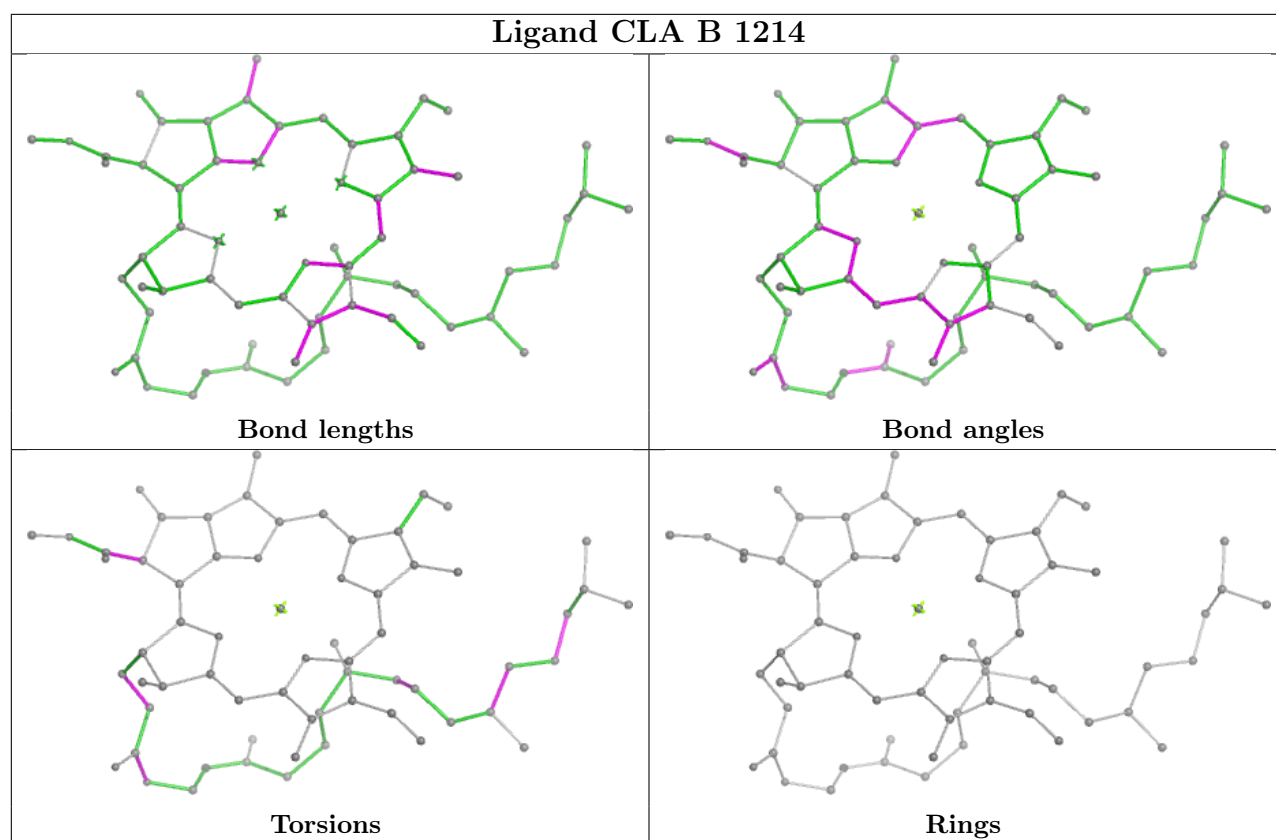


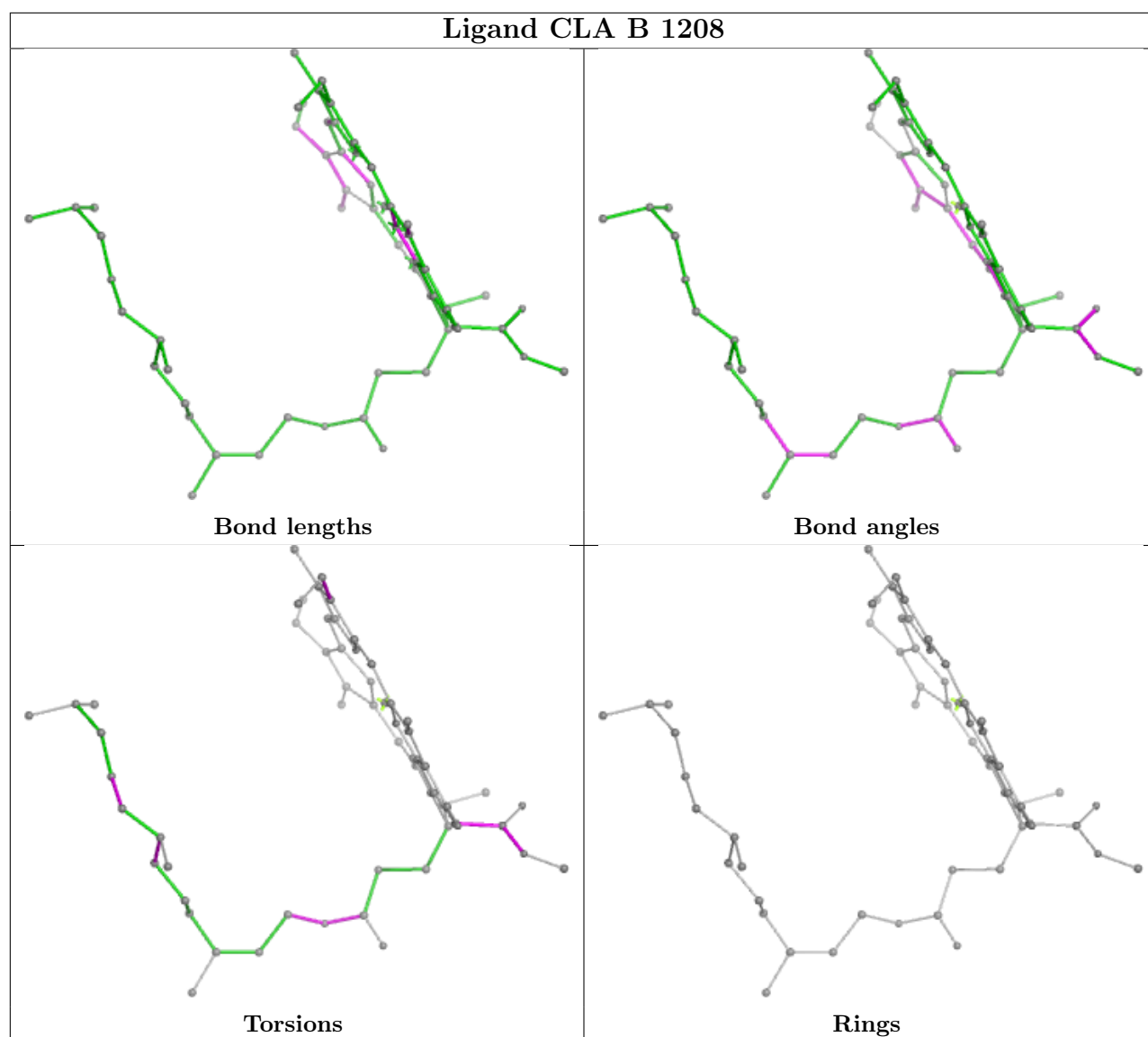
Ligand CLA A 1136

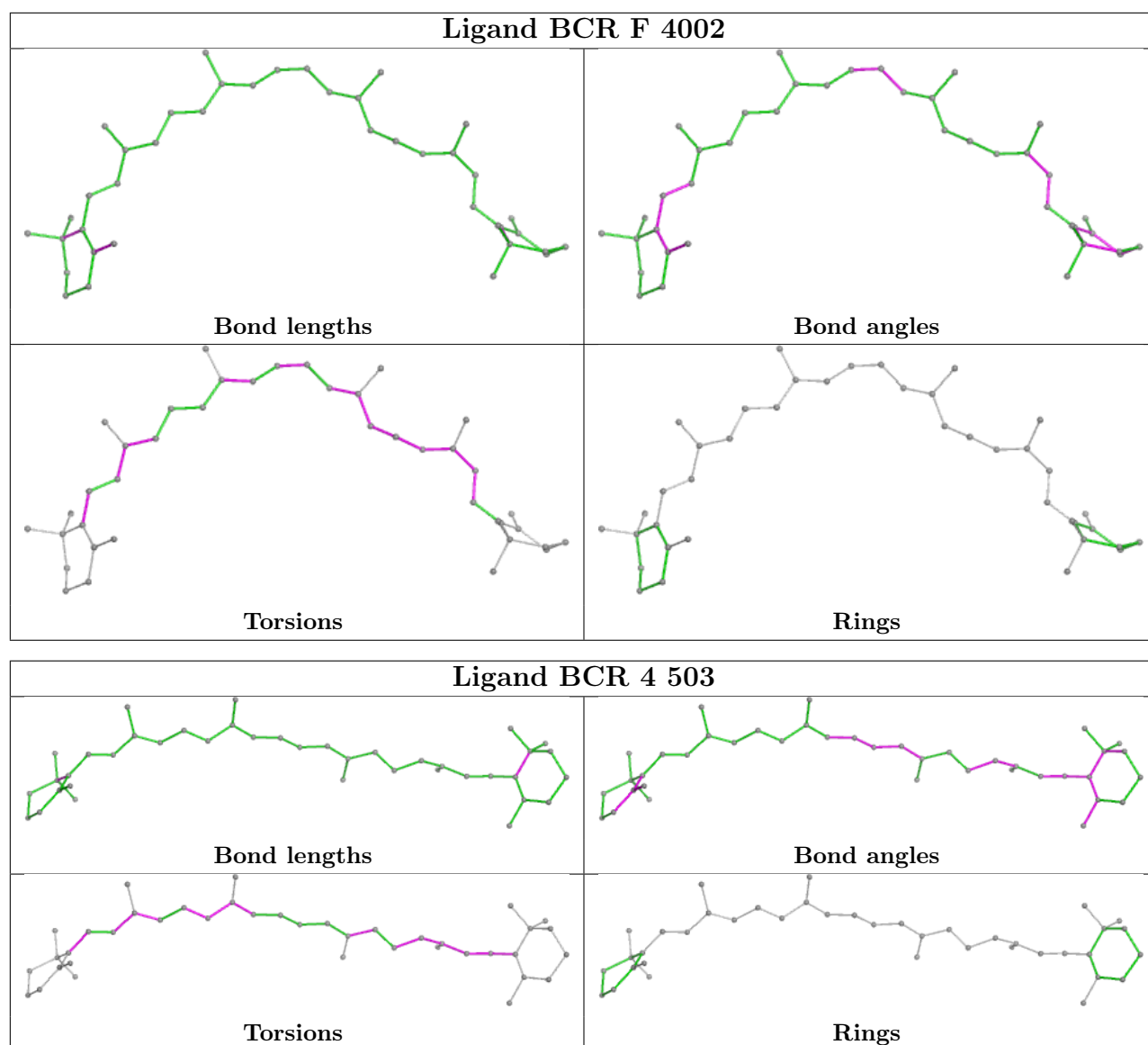


Ligand CLA A 1133**Ligand CLA A 1119**

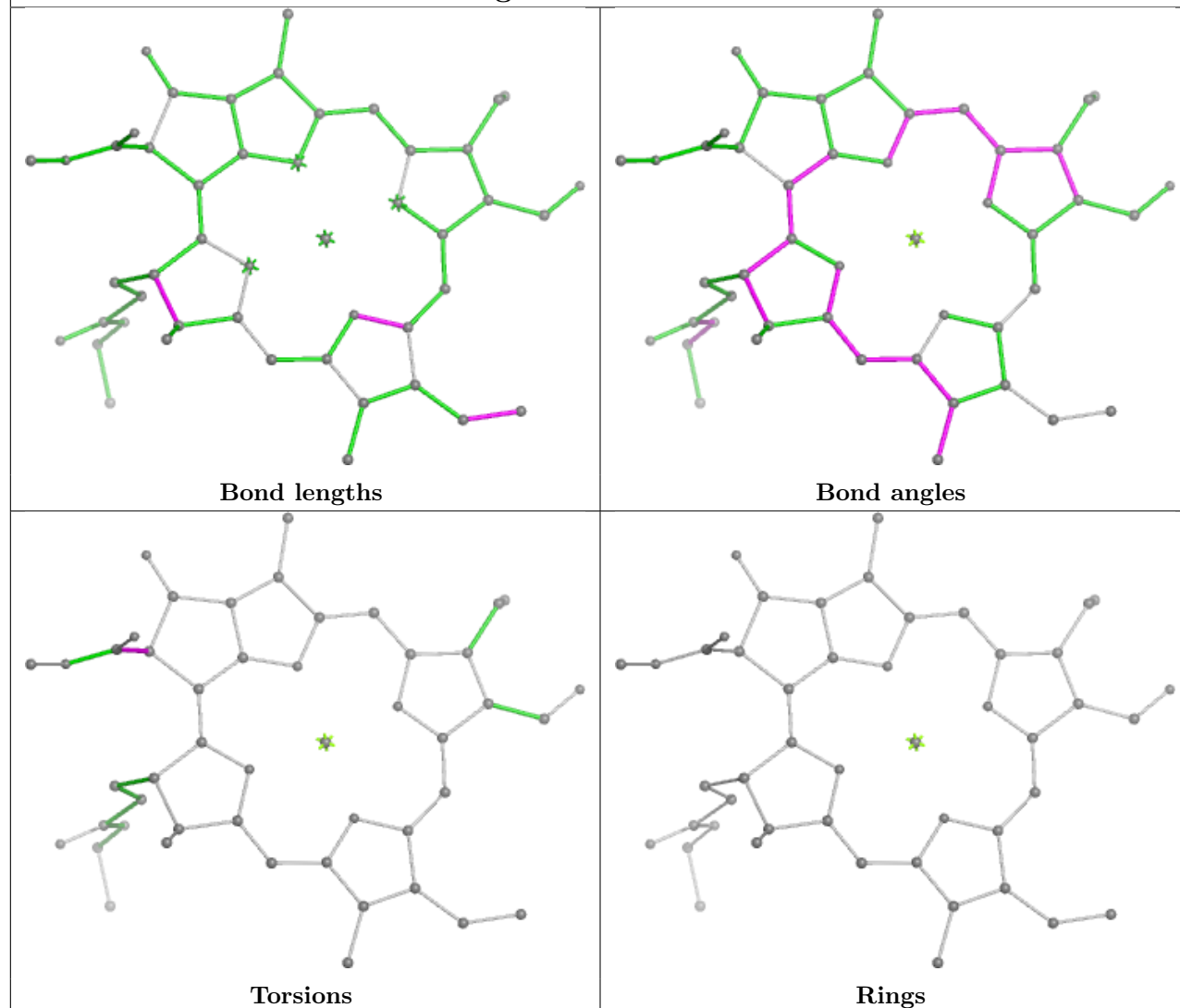




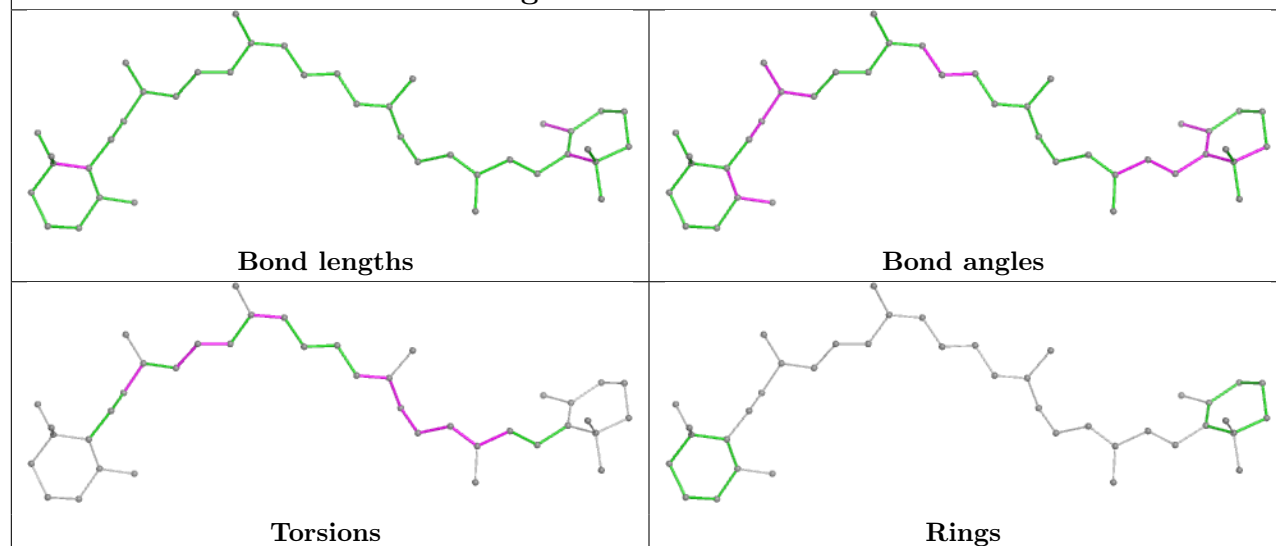


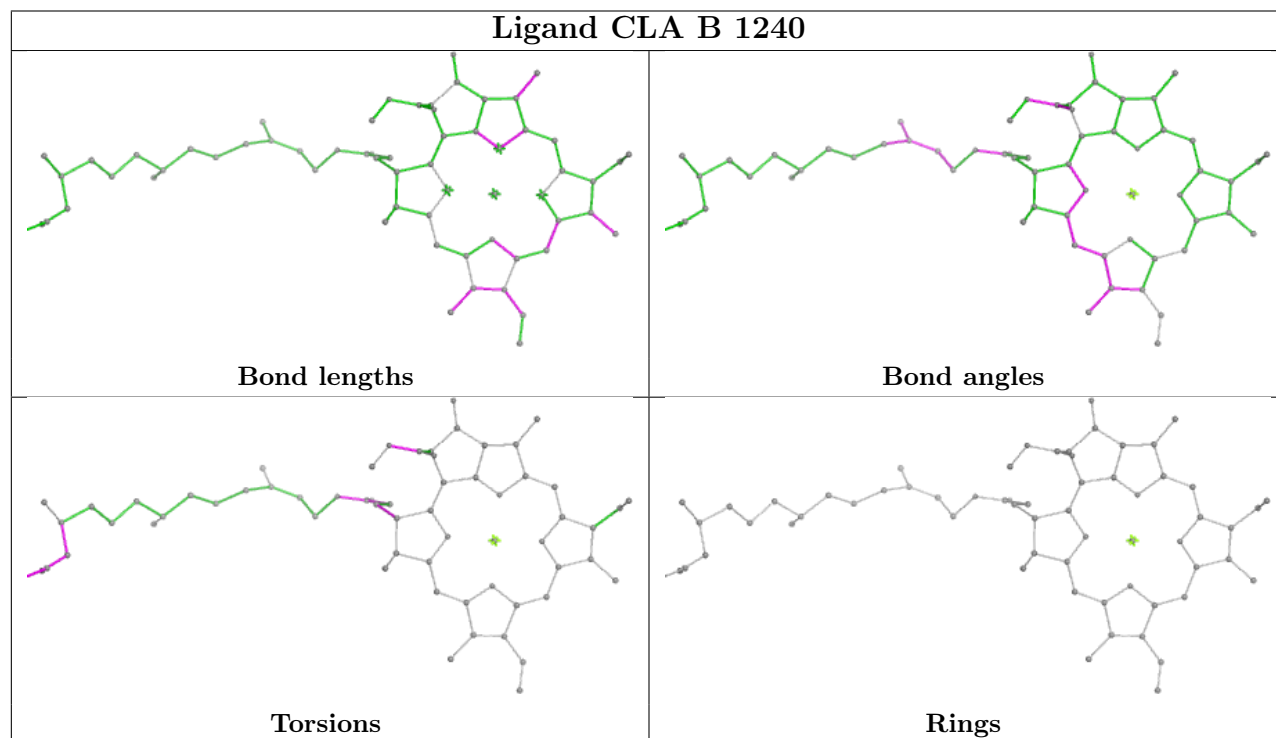
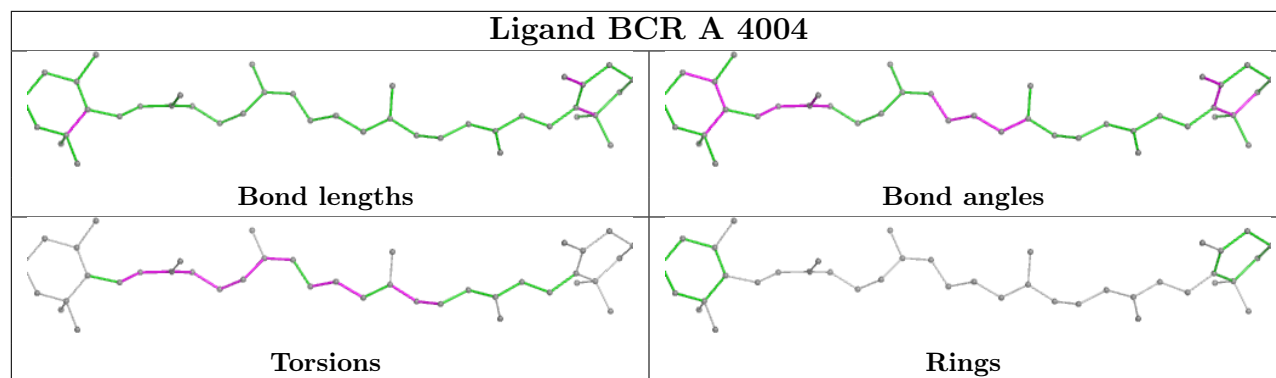


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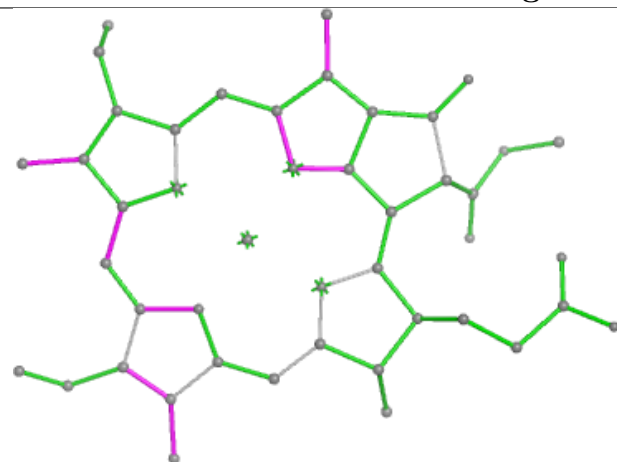


Ligand BCR A 4006

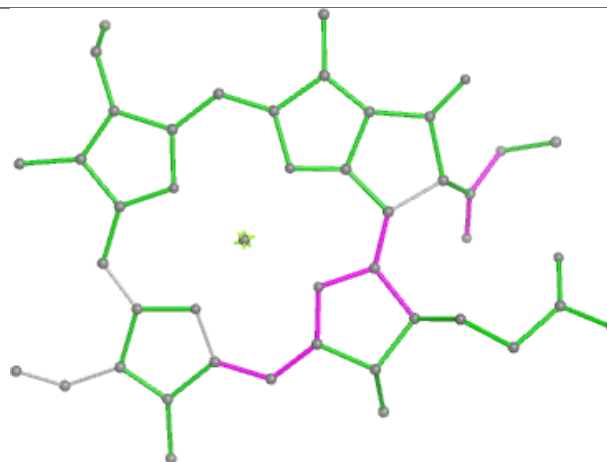




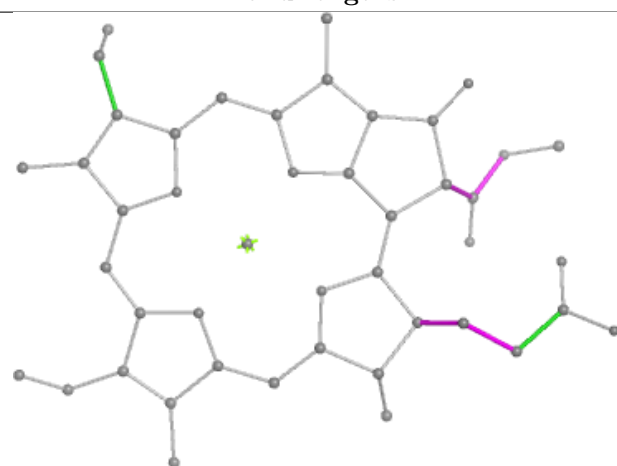
Ligand CLA 2 602



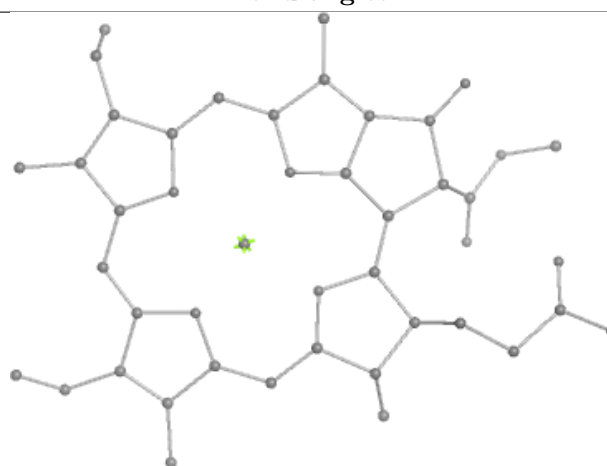
Bond lengths



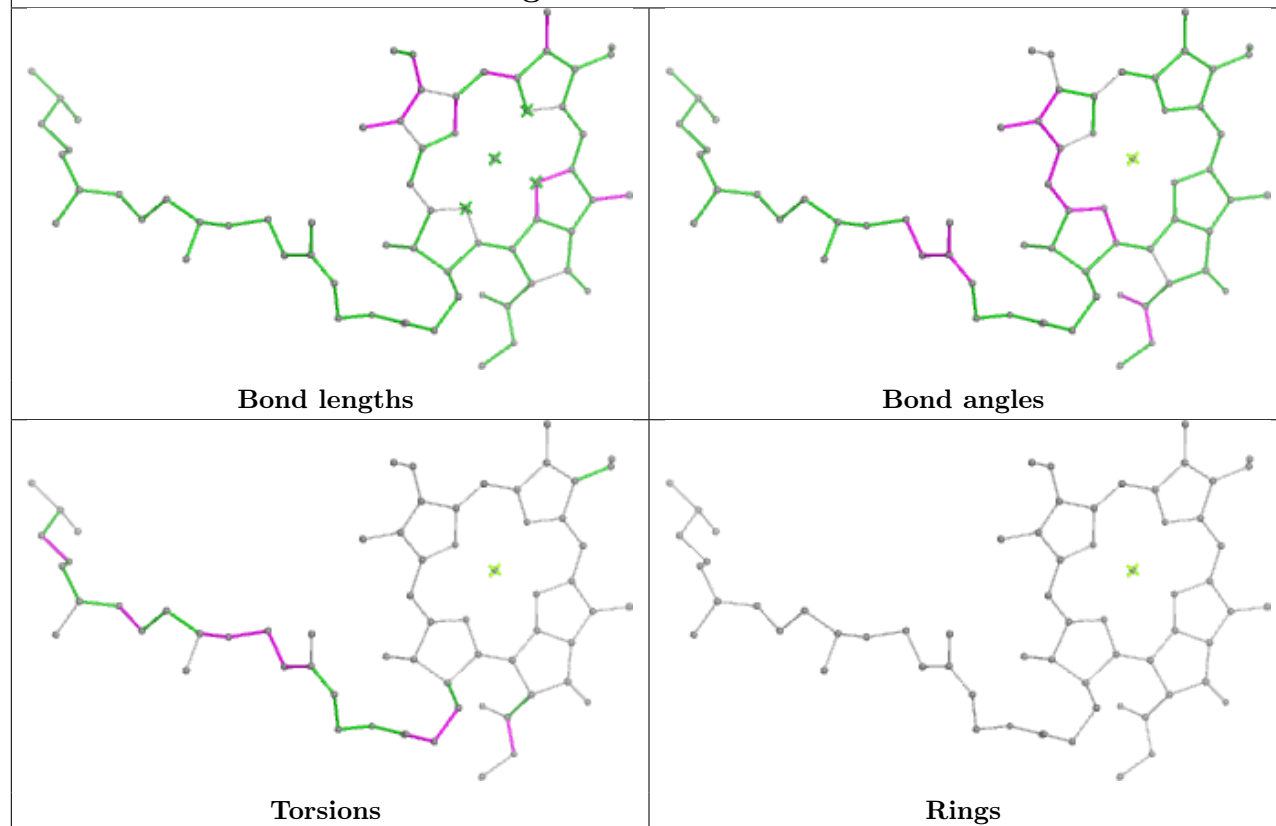
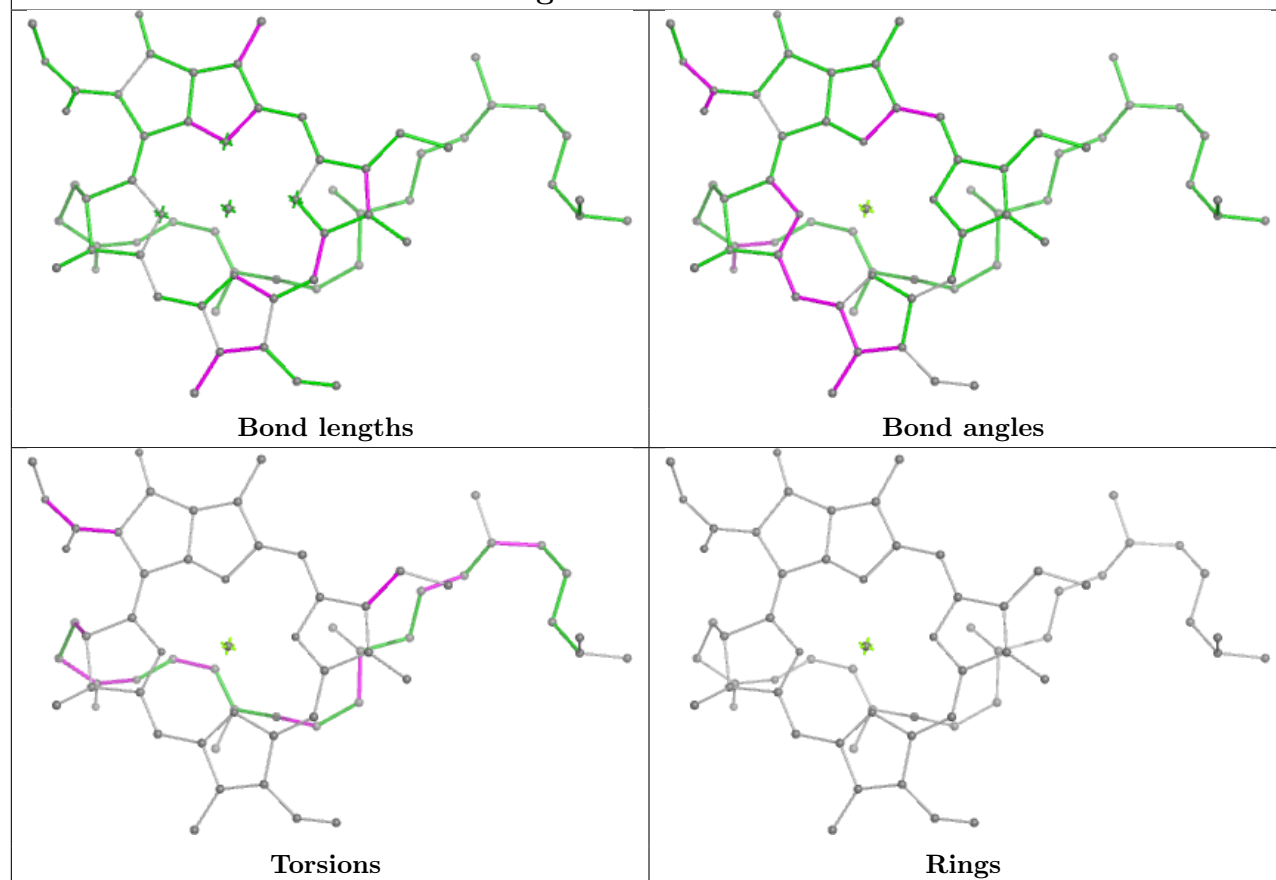
Bond angles



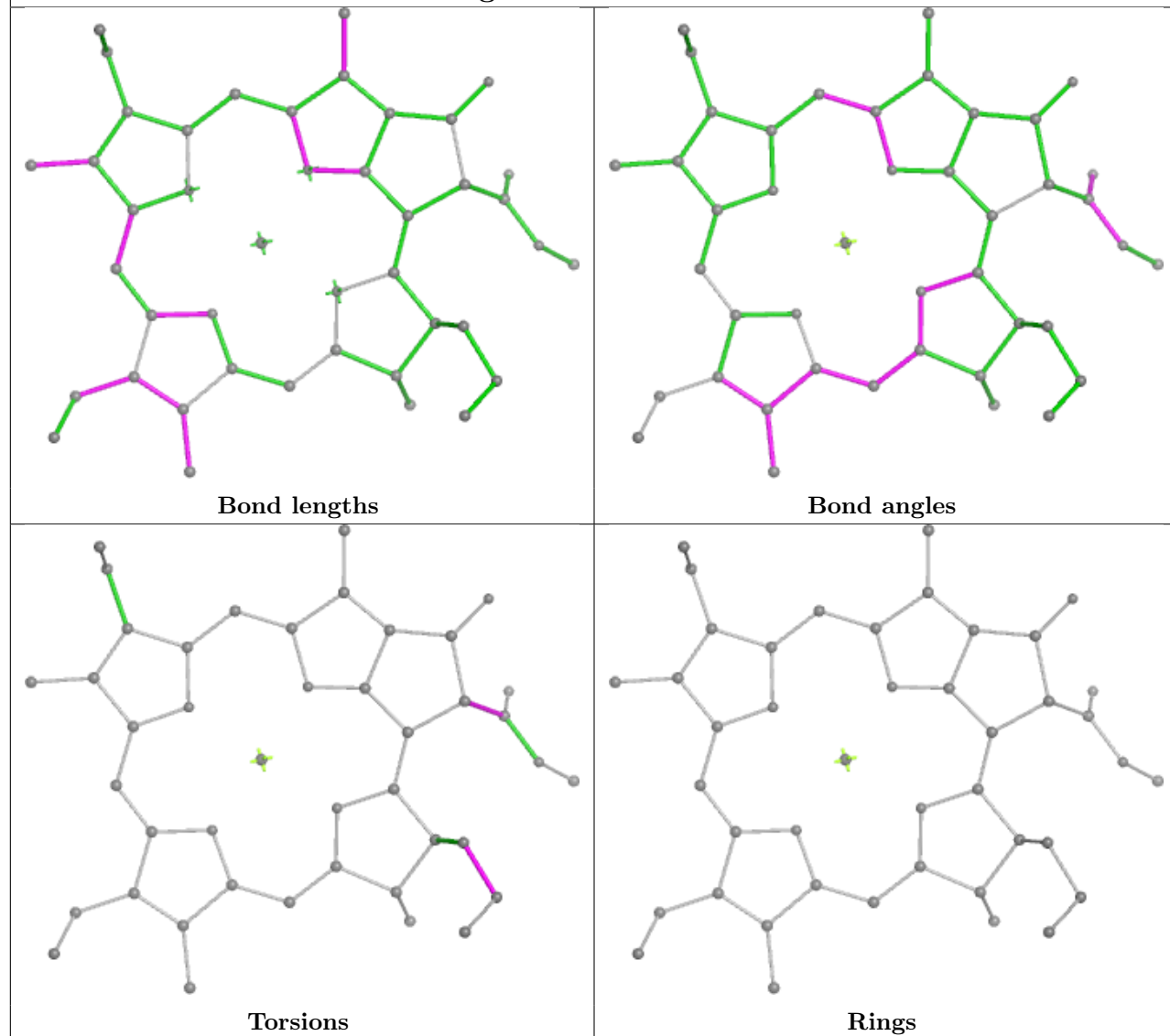
Torsions

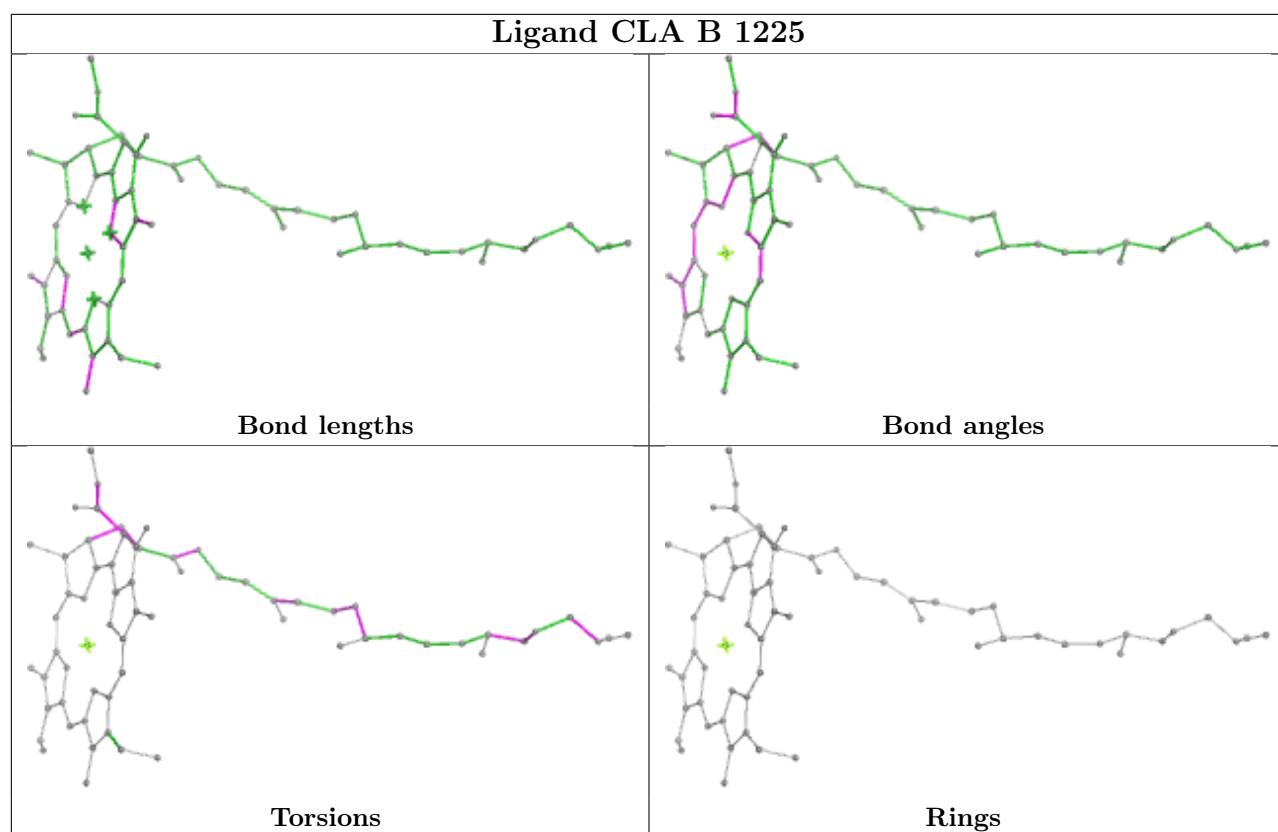


Rings

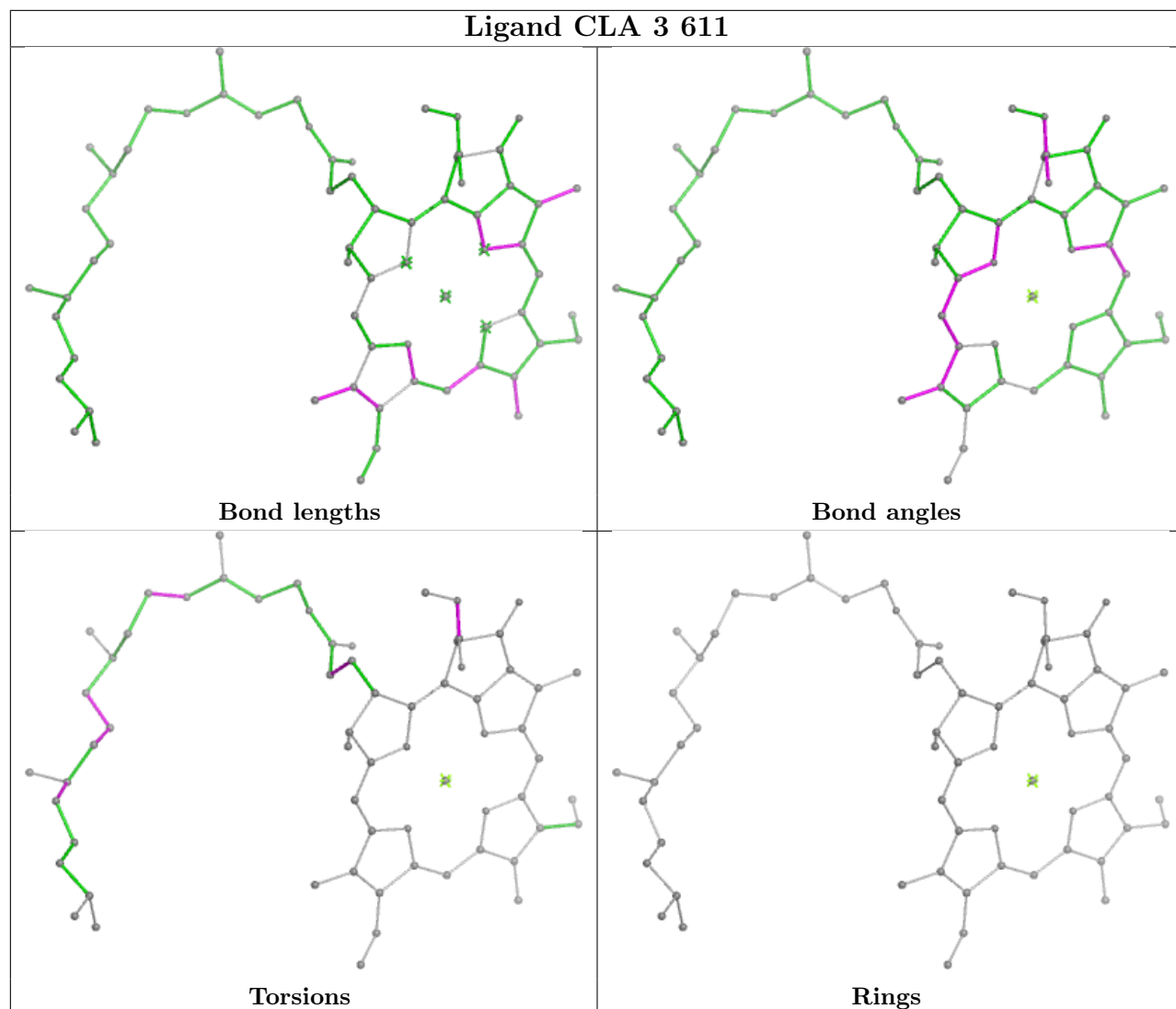
Ligand CLA A 1013**Ligand CLA 3 608**

Ligand CLA B 1201

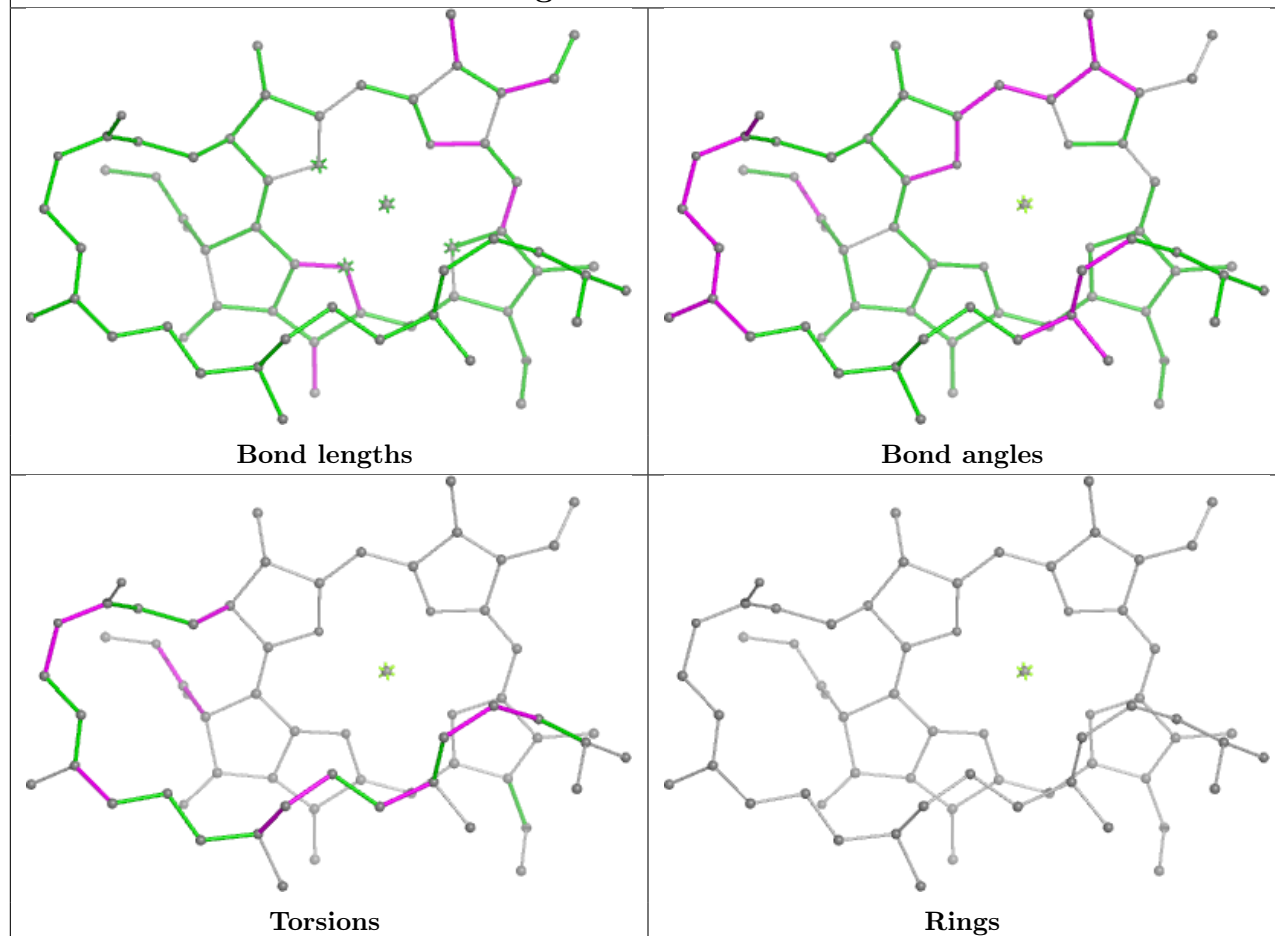




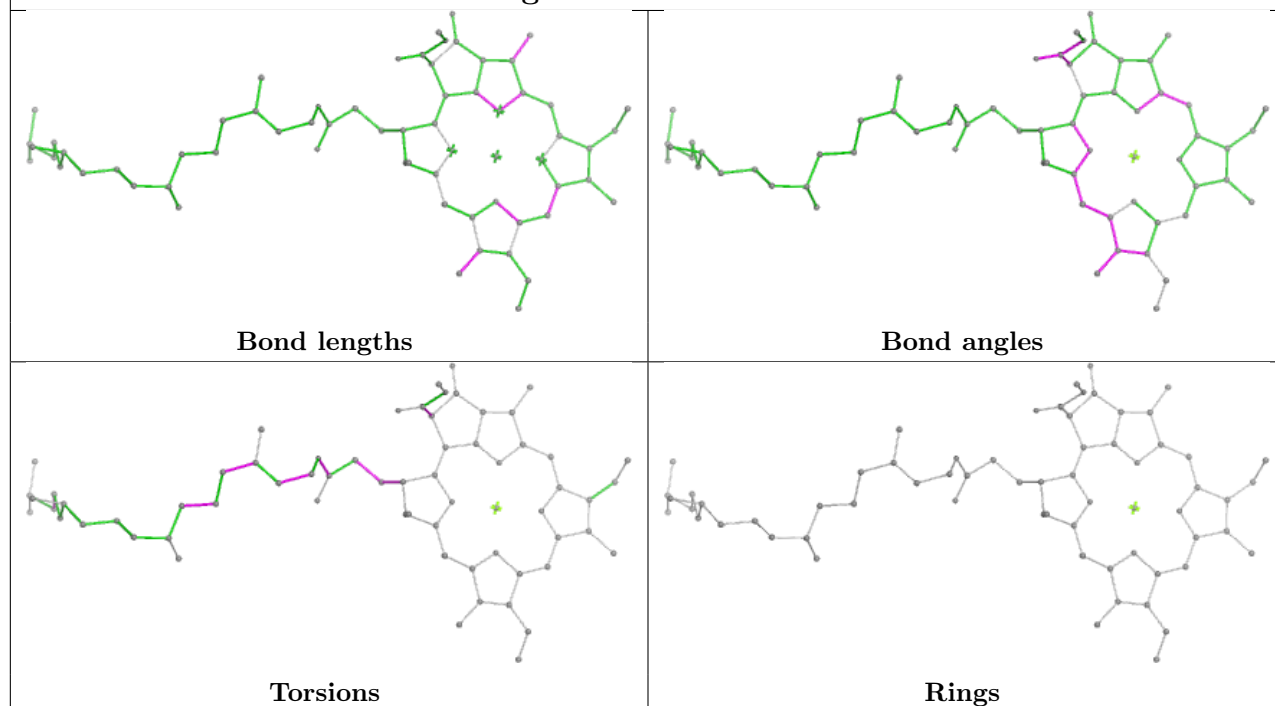
Ligand CLA 3 611

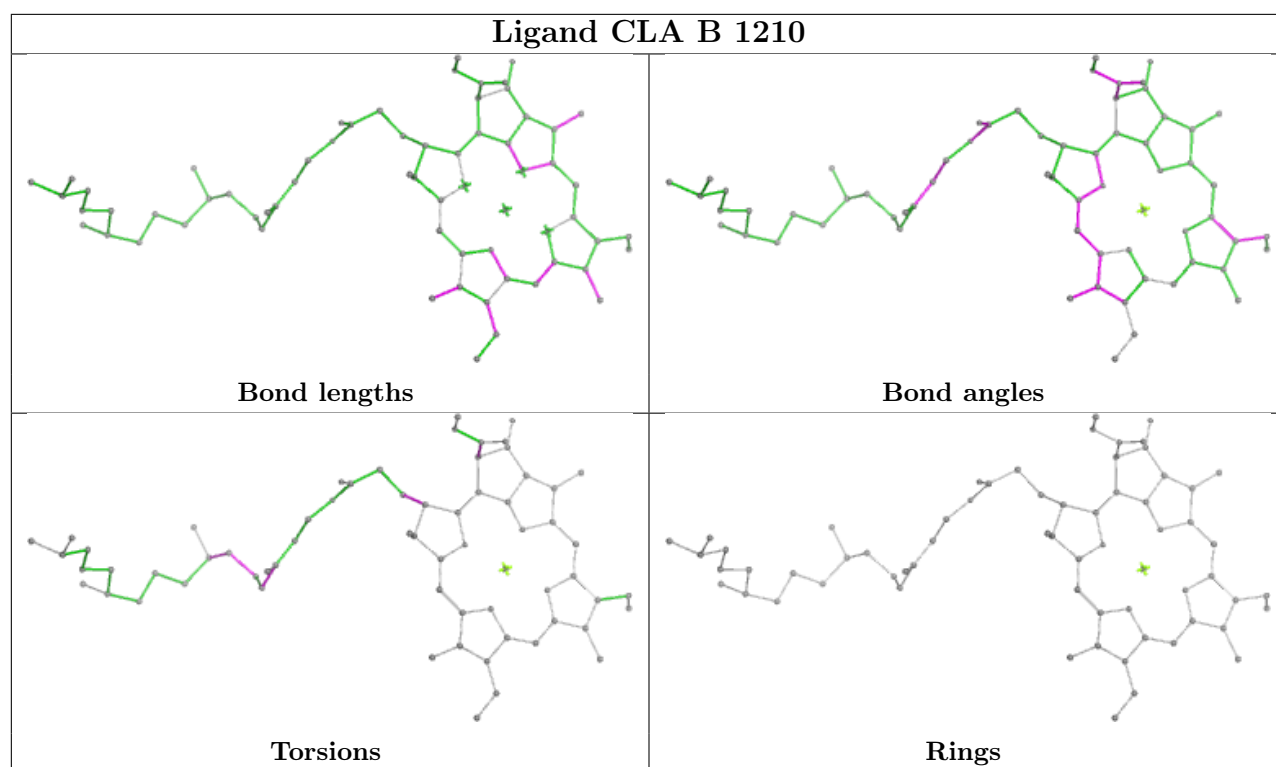


Ligand CLA 2 616

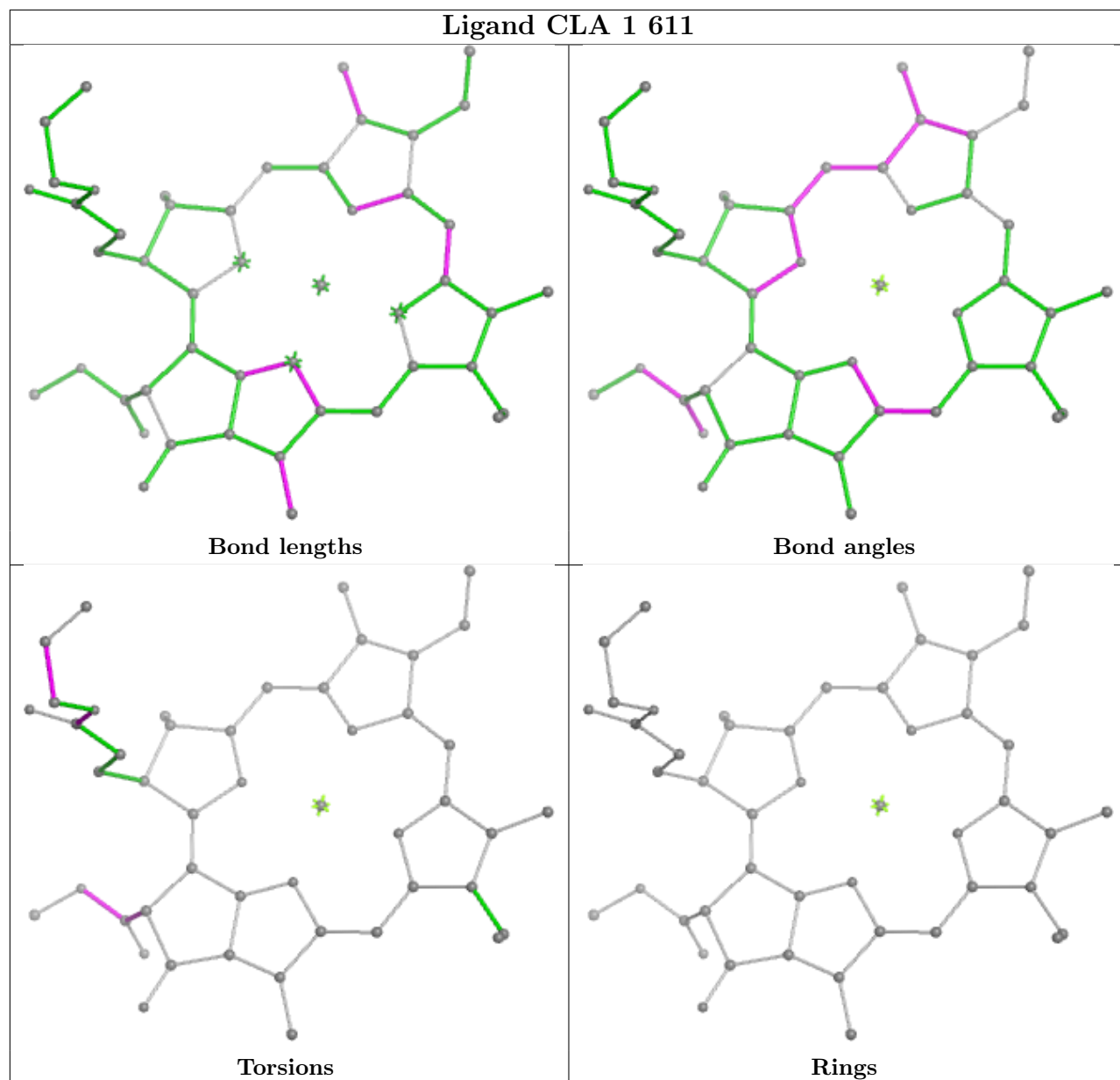


Ligand CLA A 1103

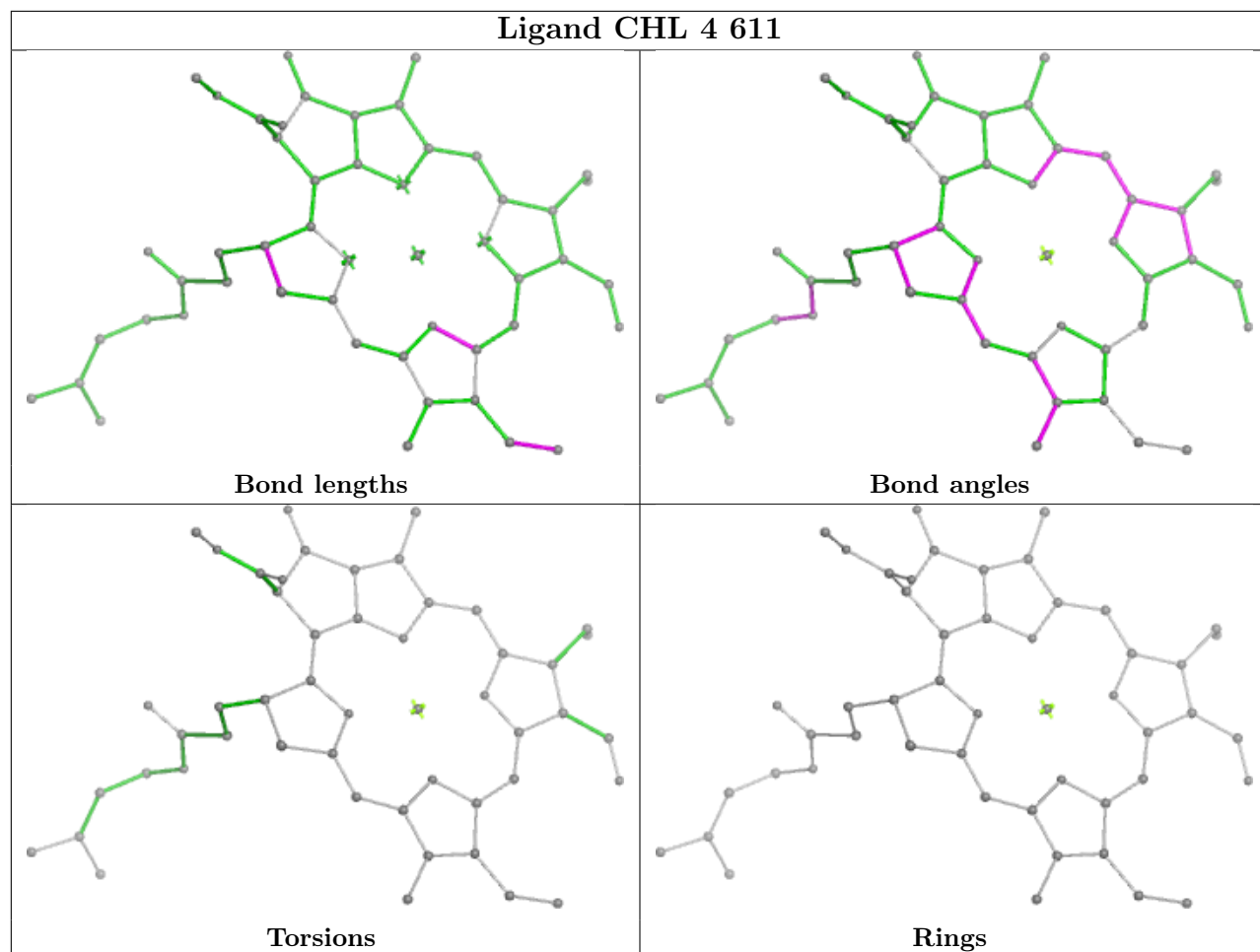




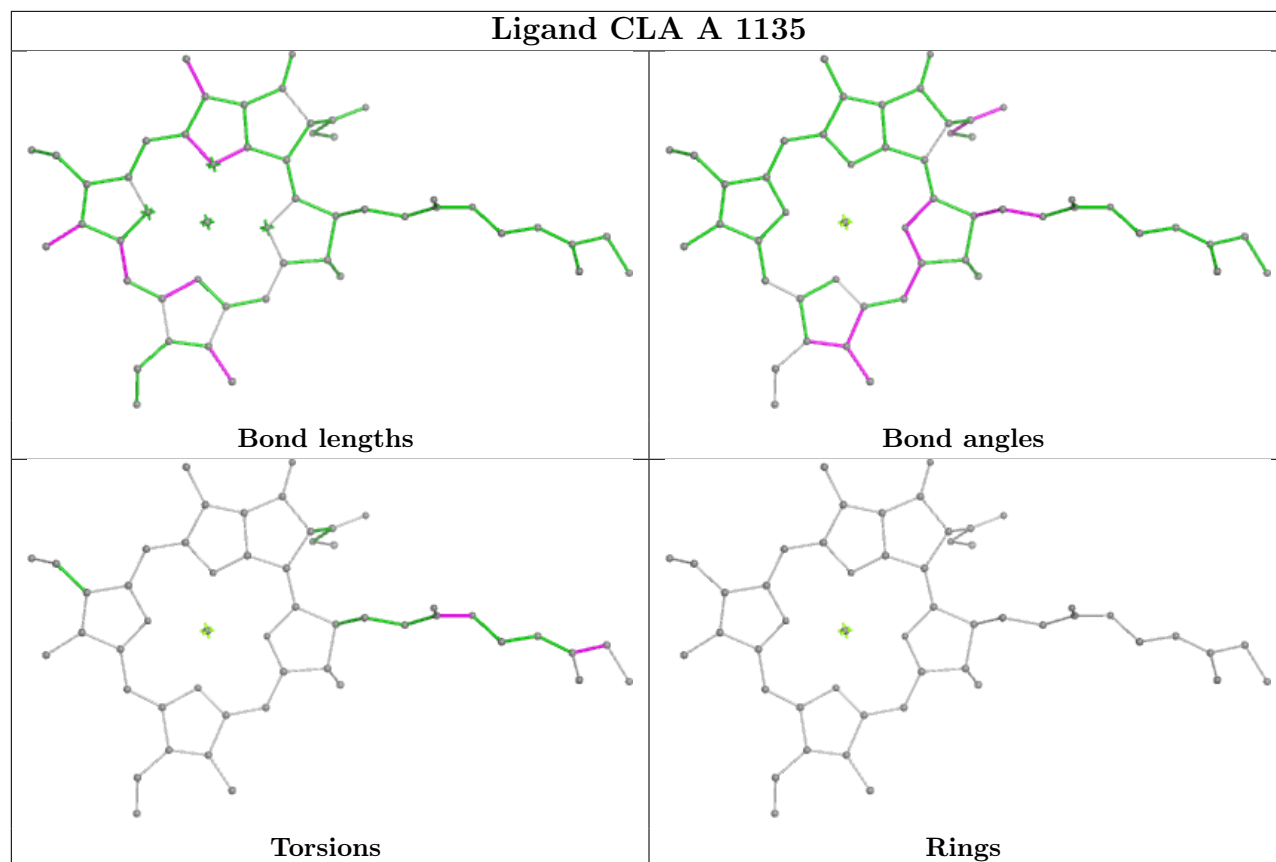
Ligand CLA 1 611



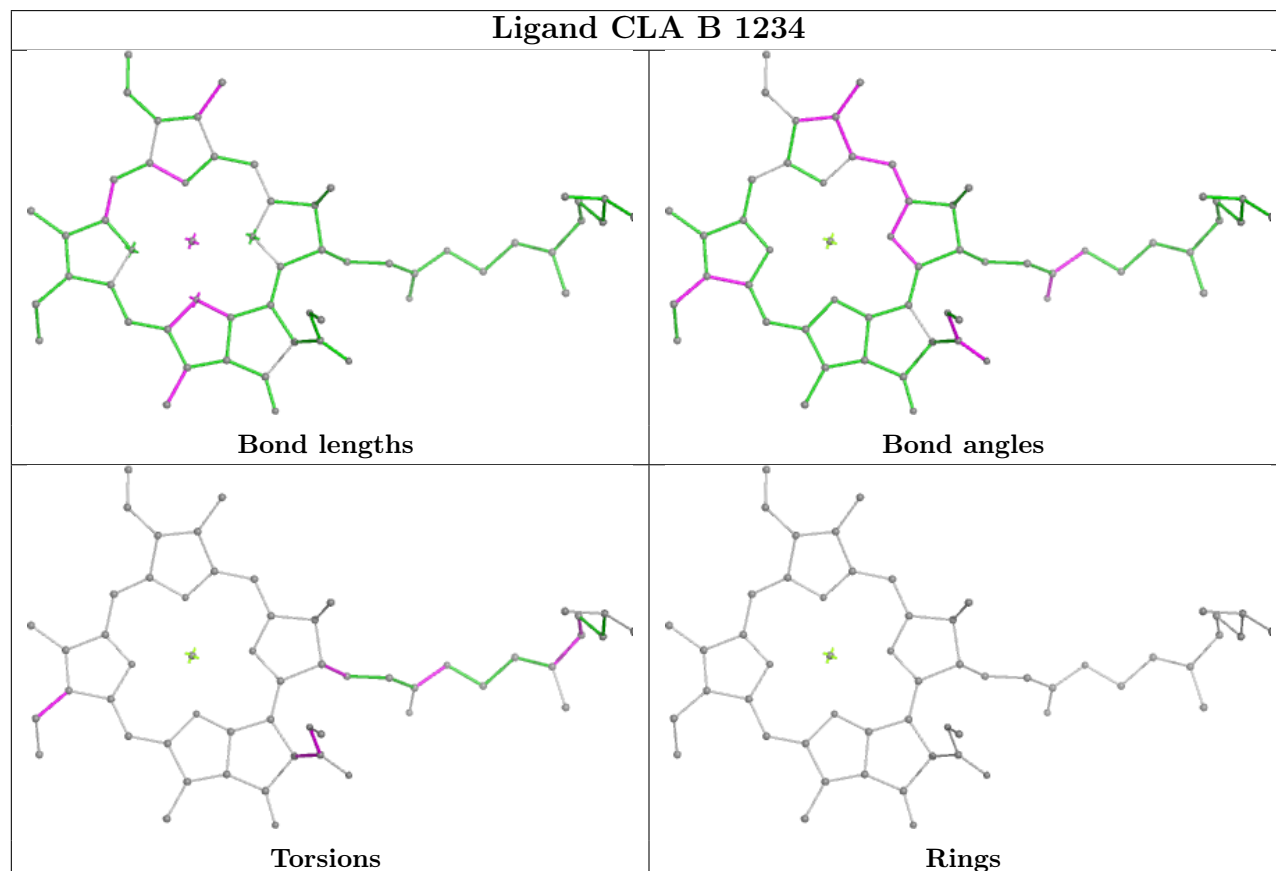
Ligand CHL 4 611

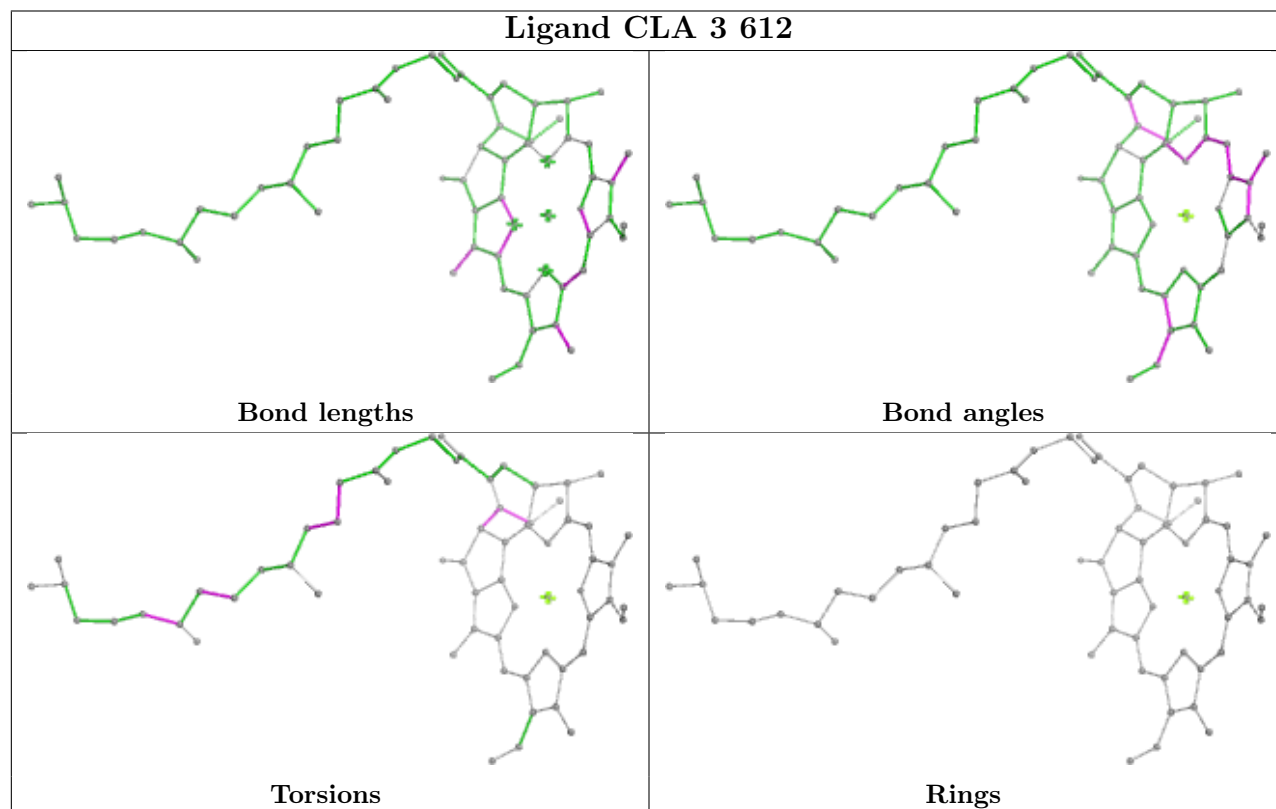
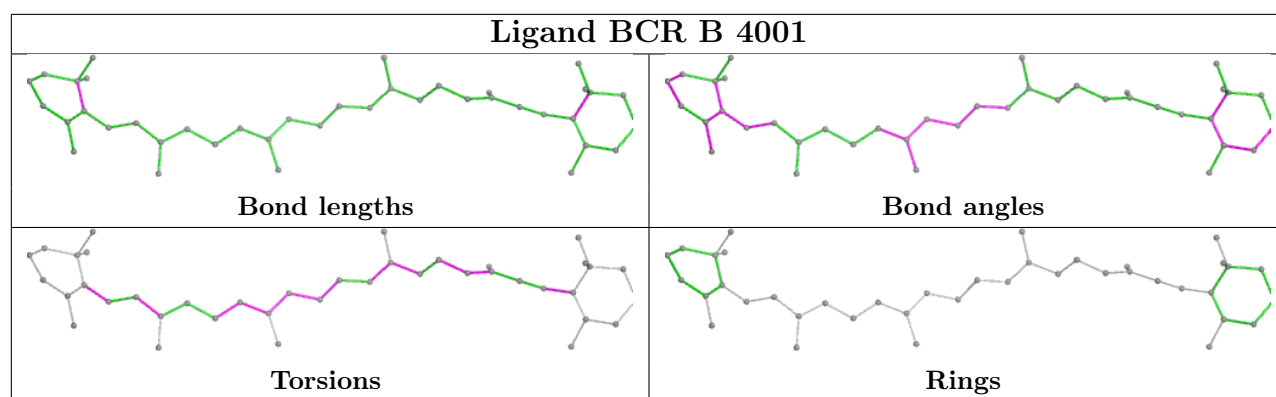


Ligand CLA A 1135

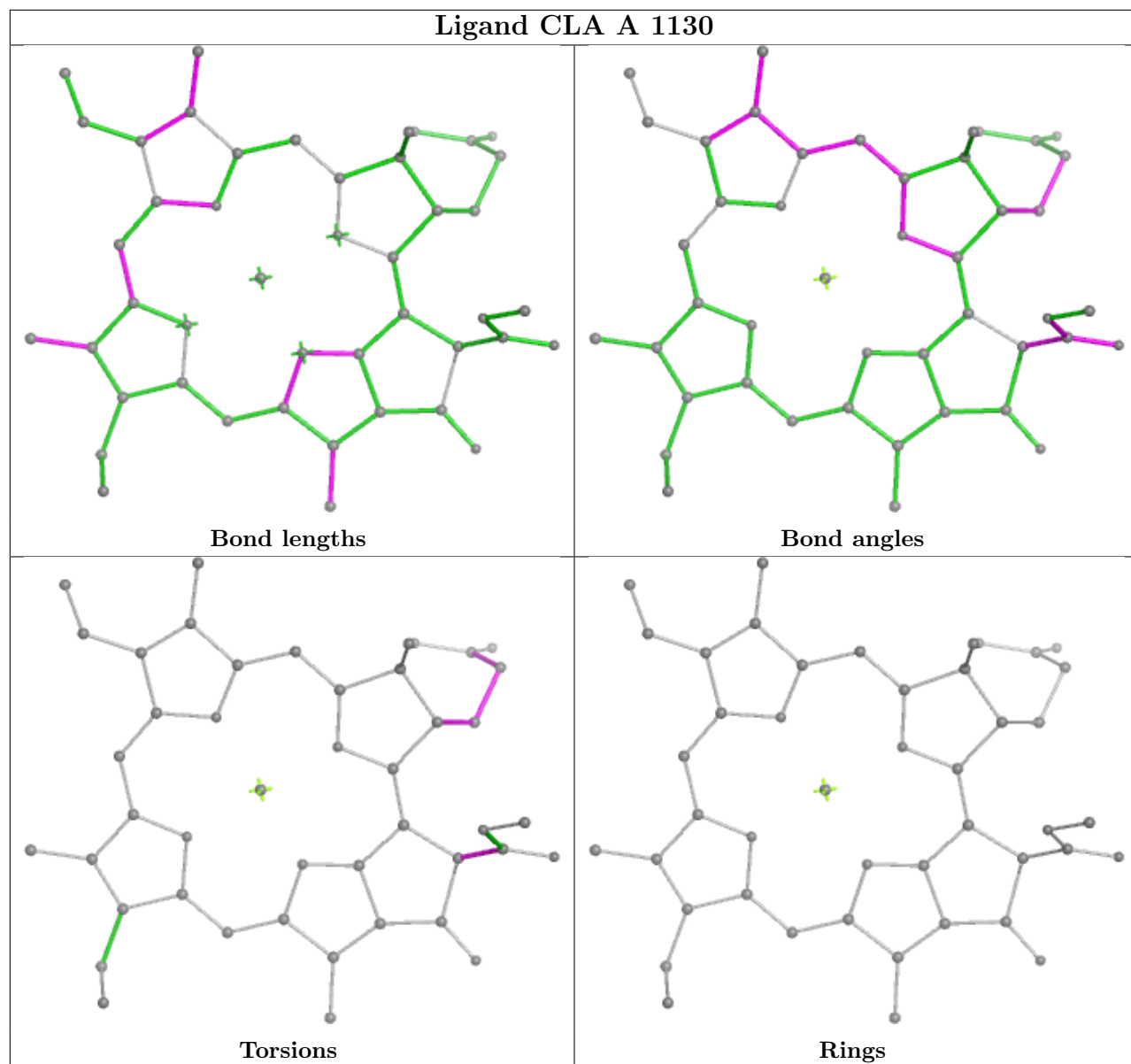


Ligand CLA B 1234

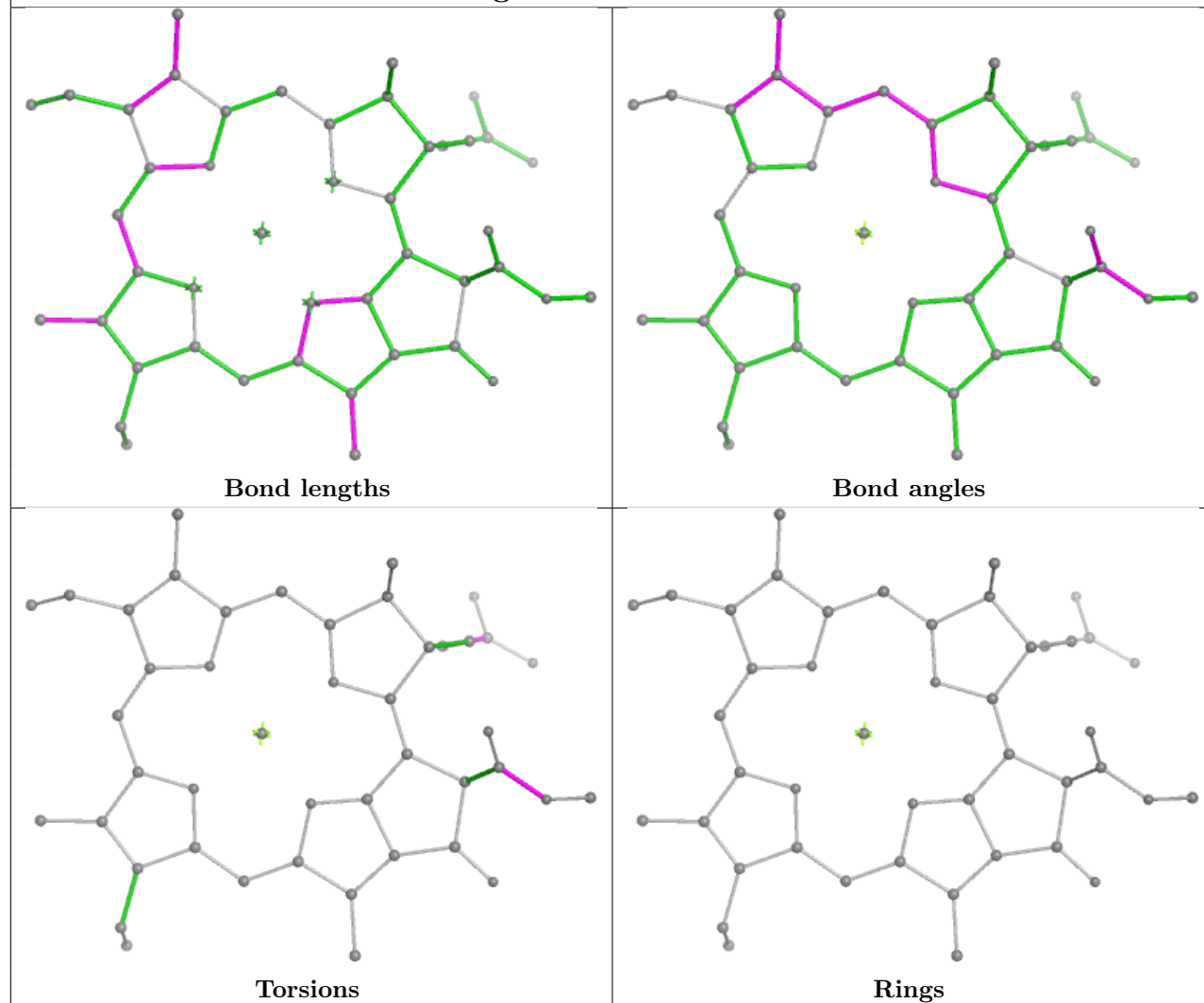




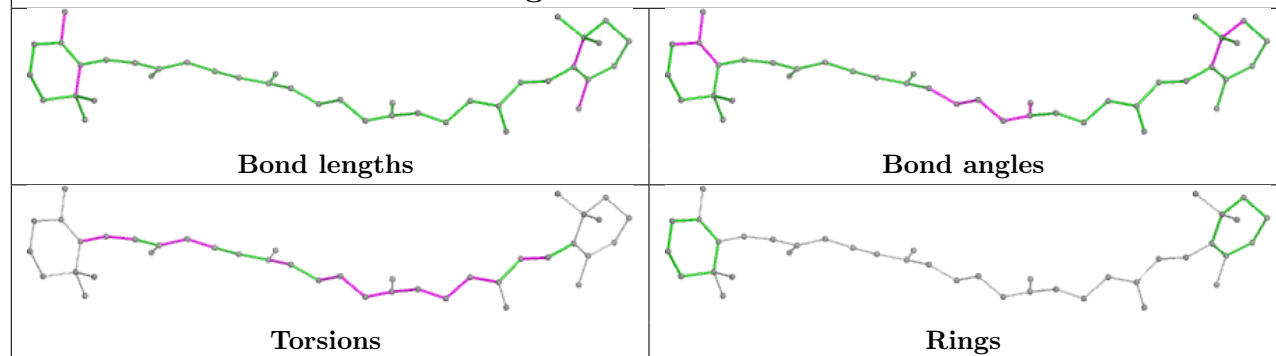
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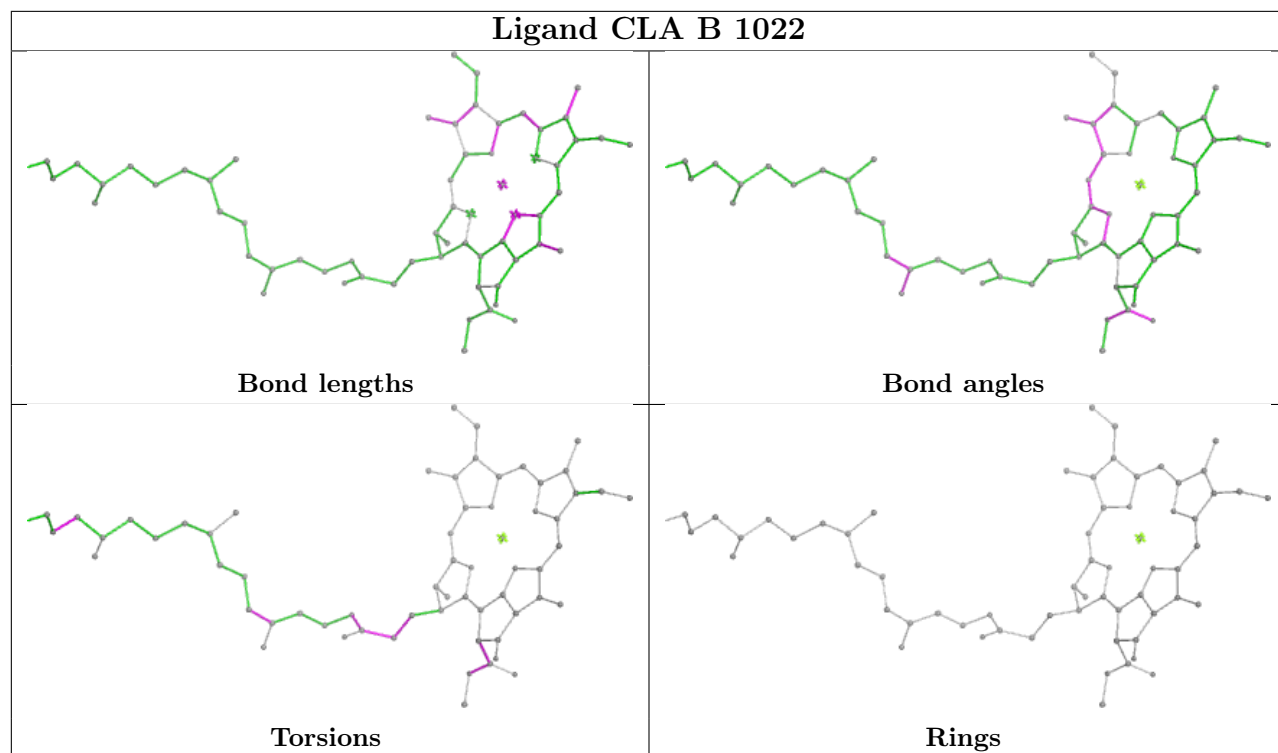


Ligand CLA A 1121

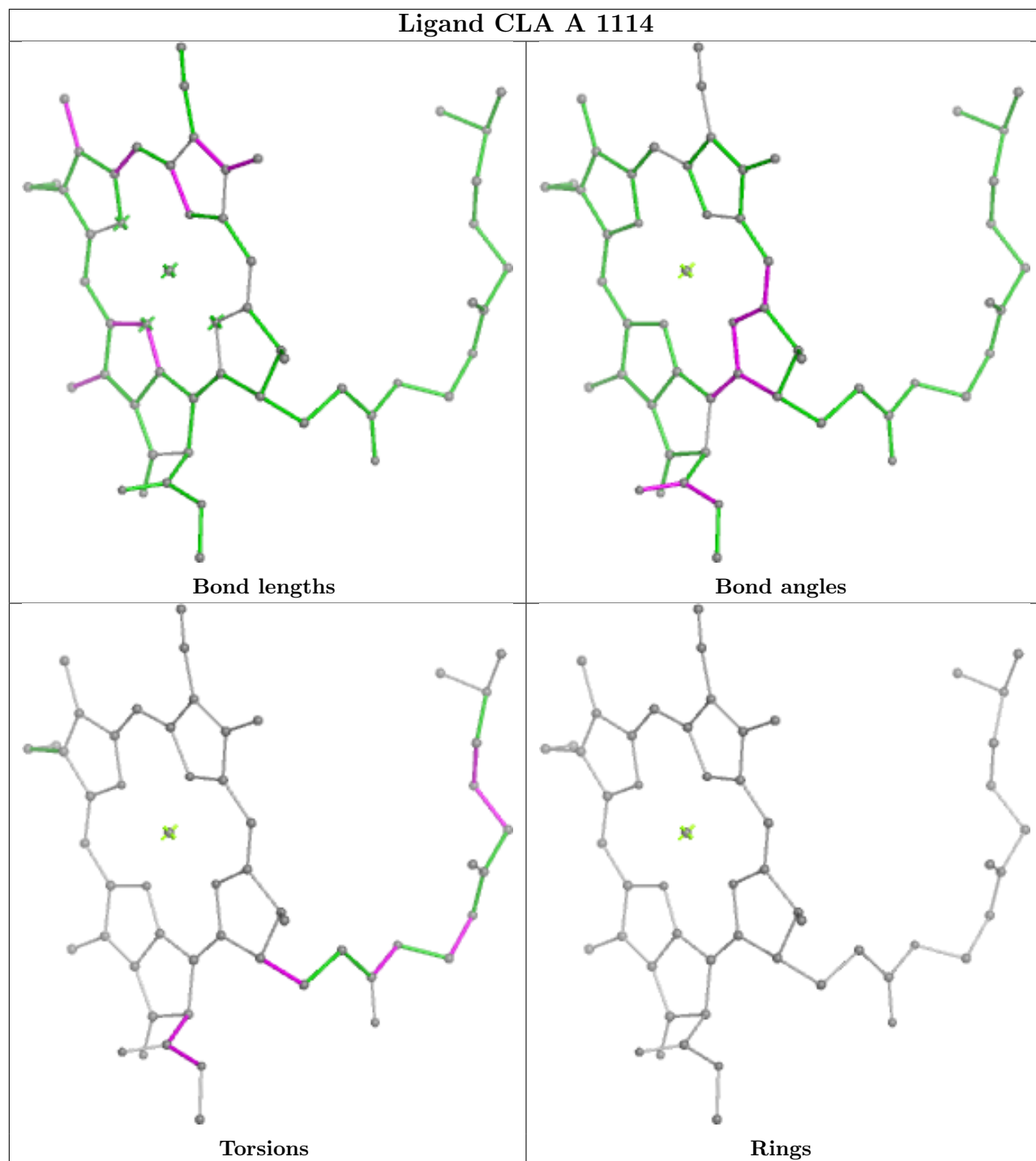


Ligand BCR J 4002

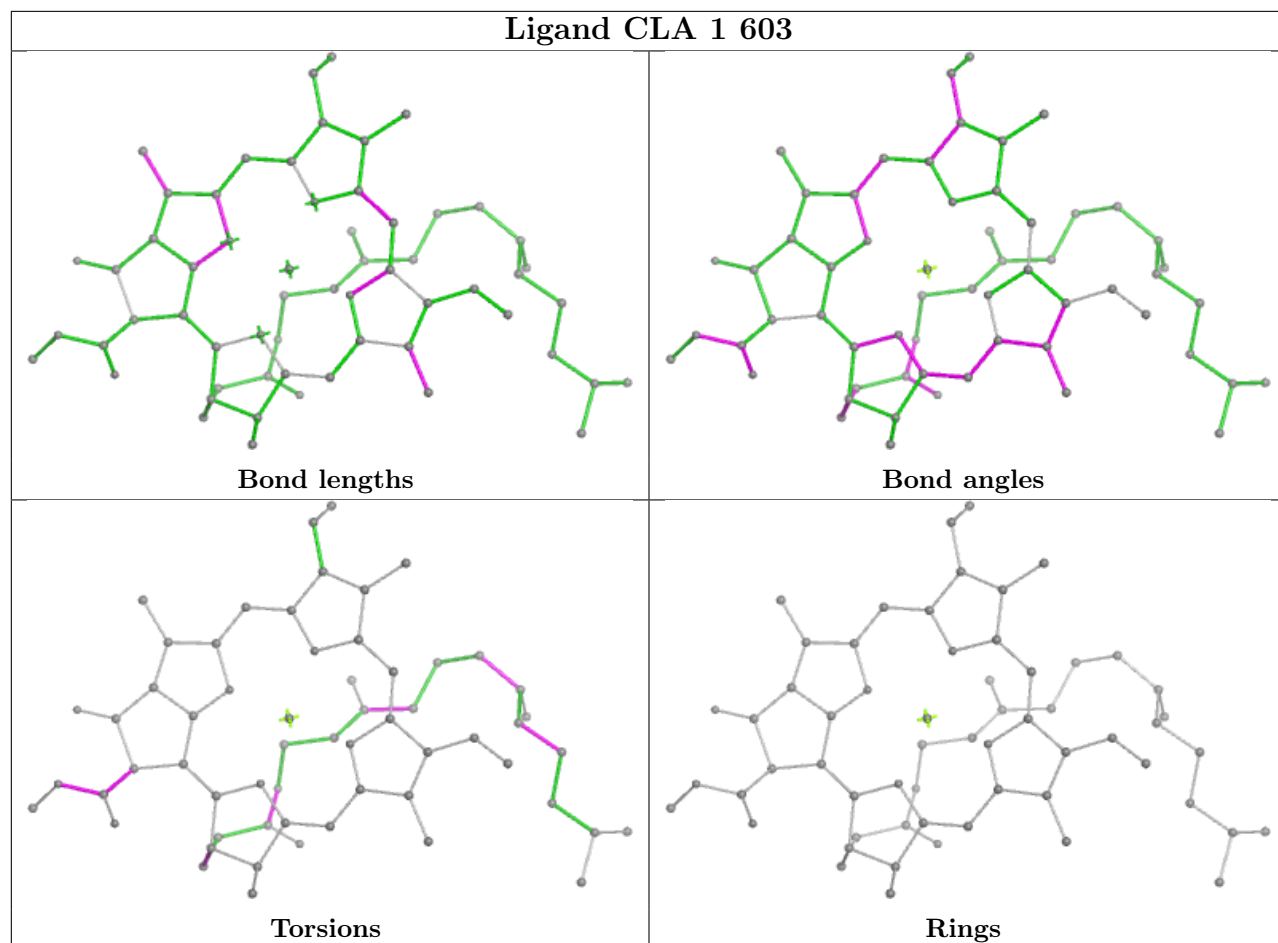


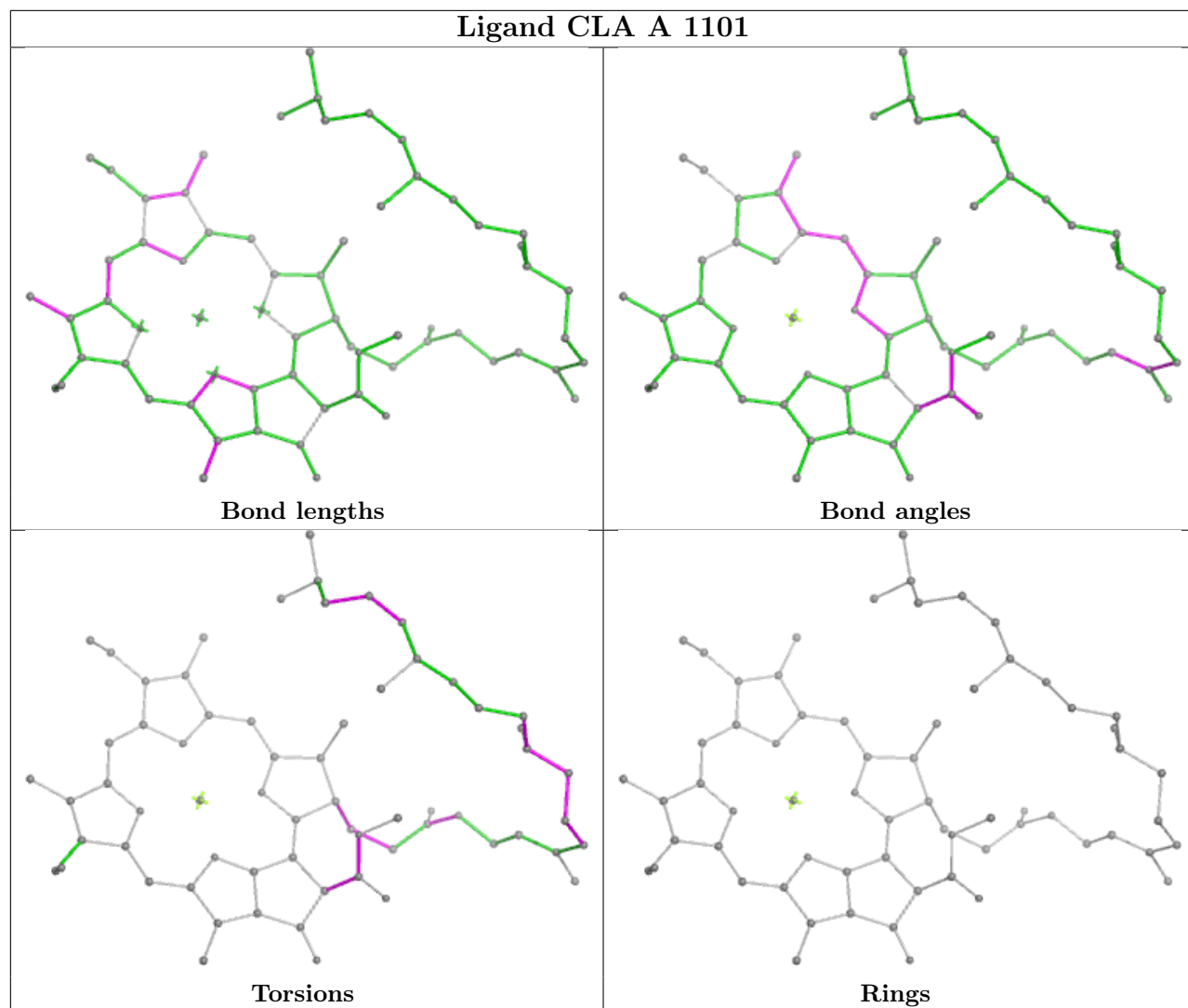


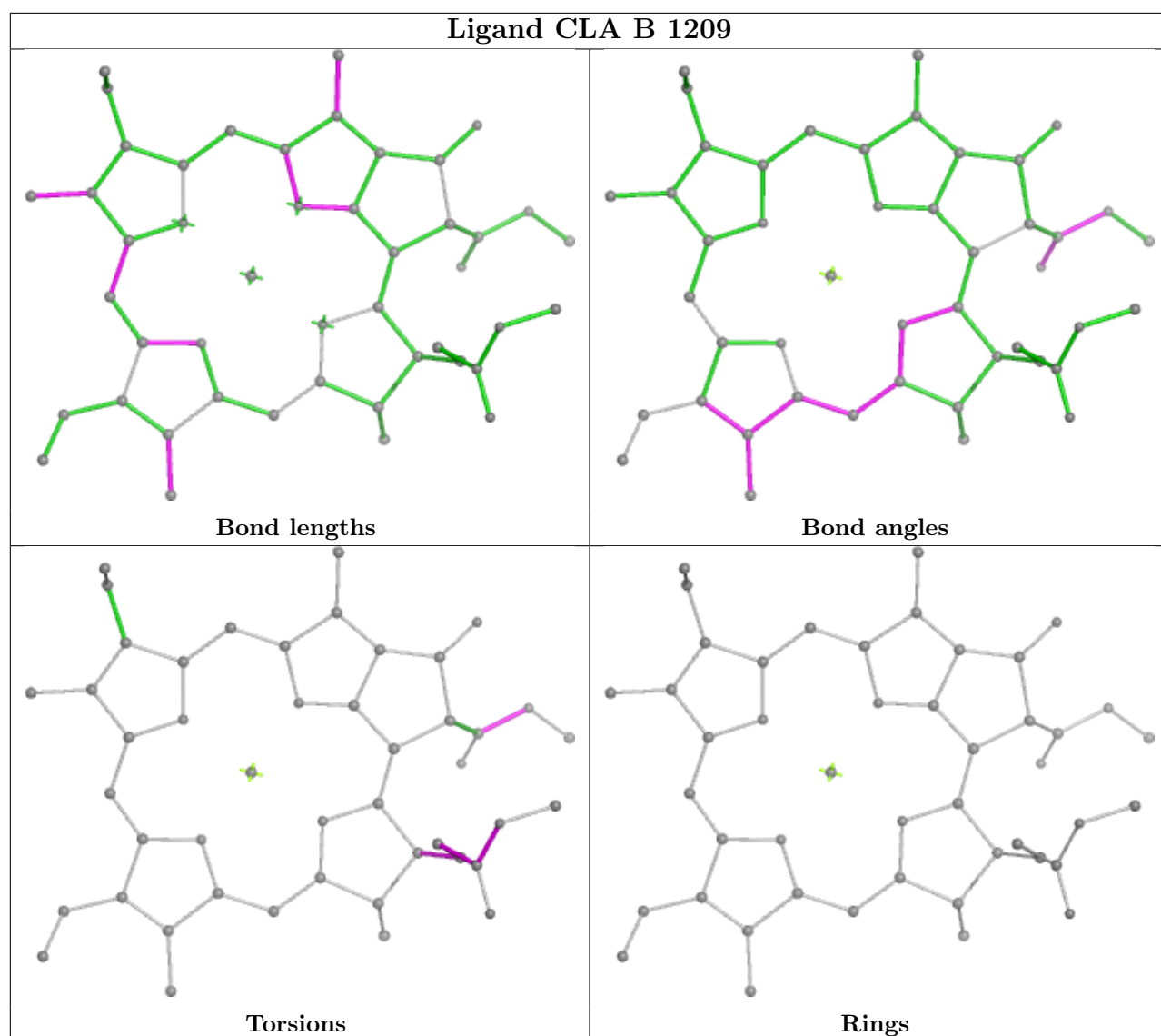
Ligand CLA A 1114



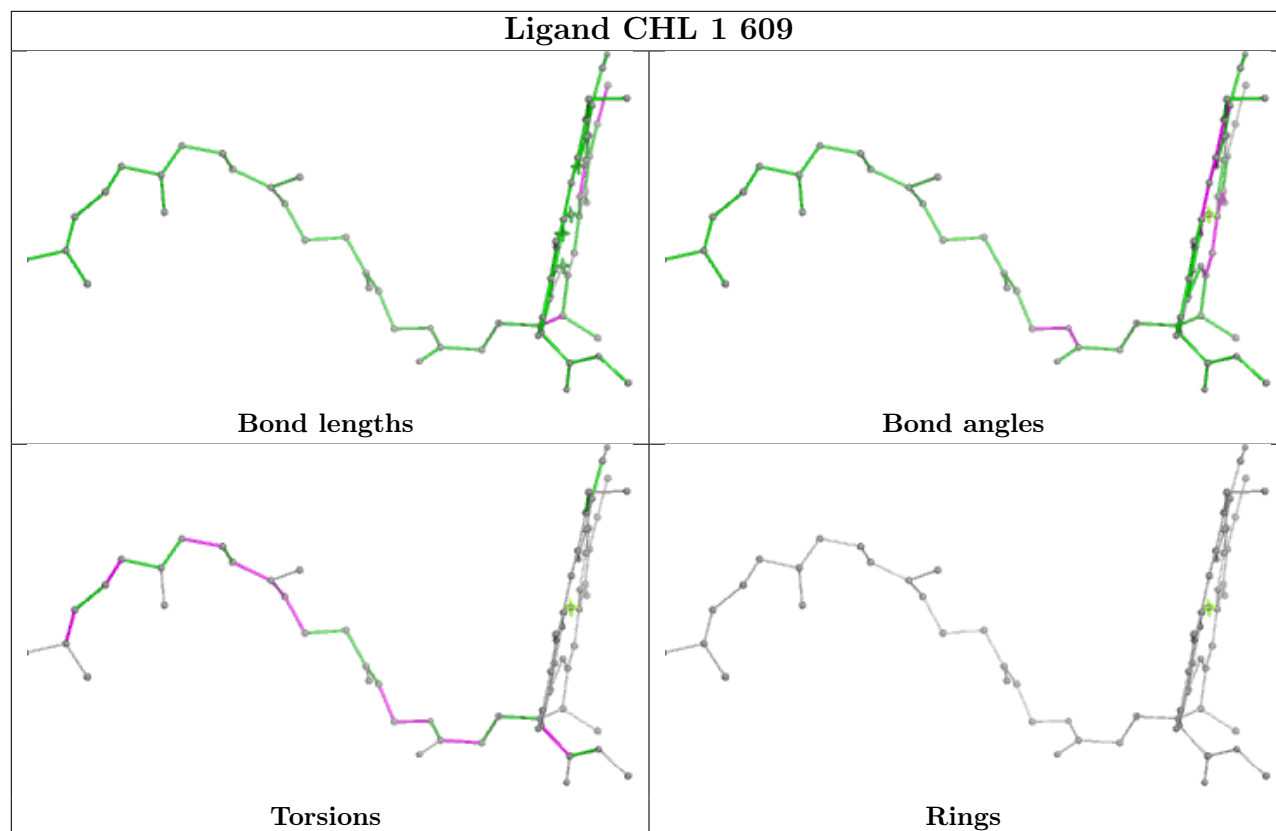
Ligand CLA 1 603



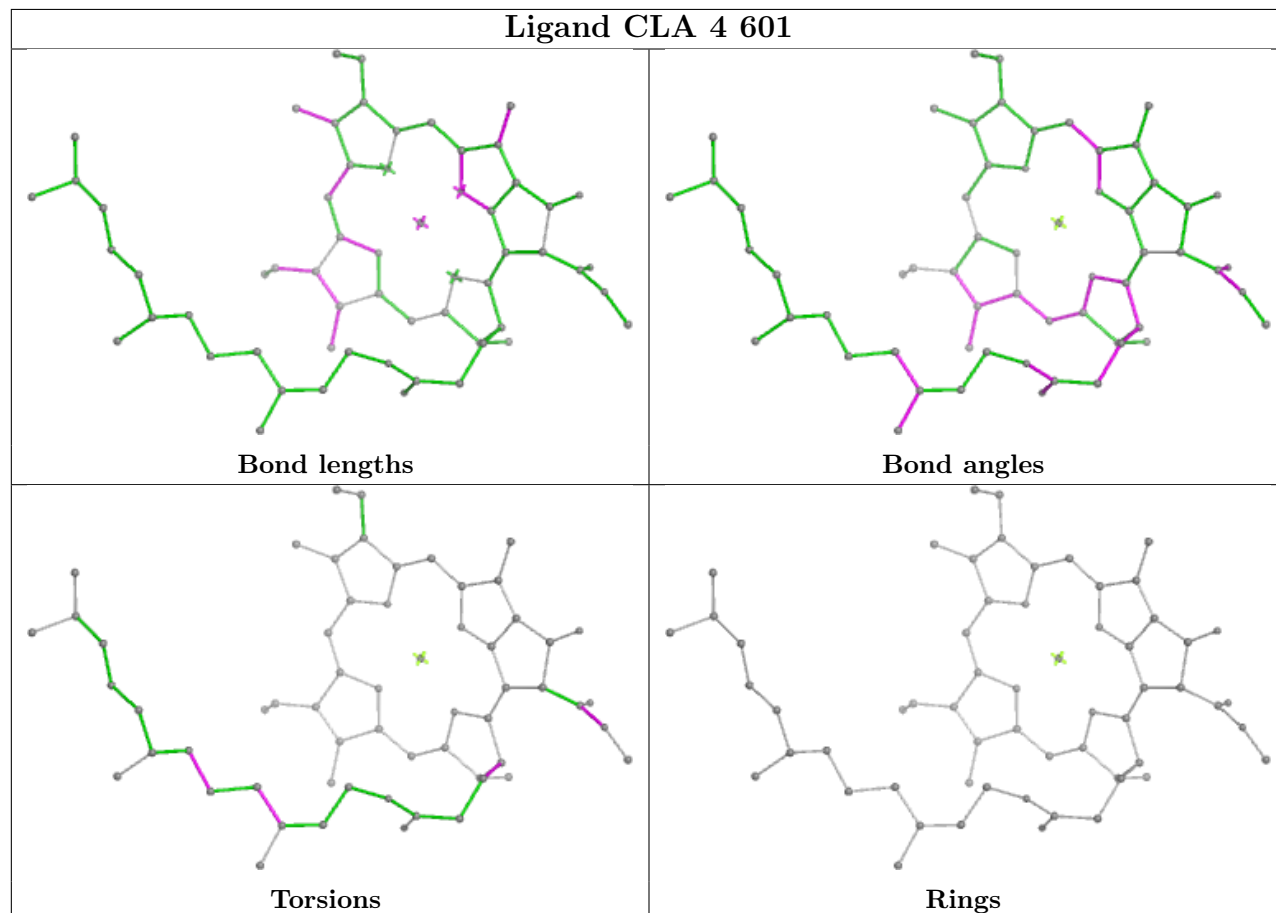


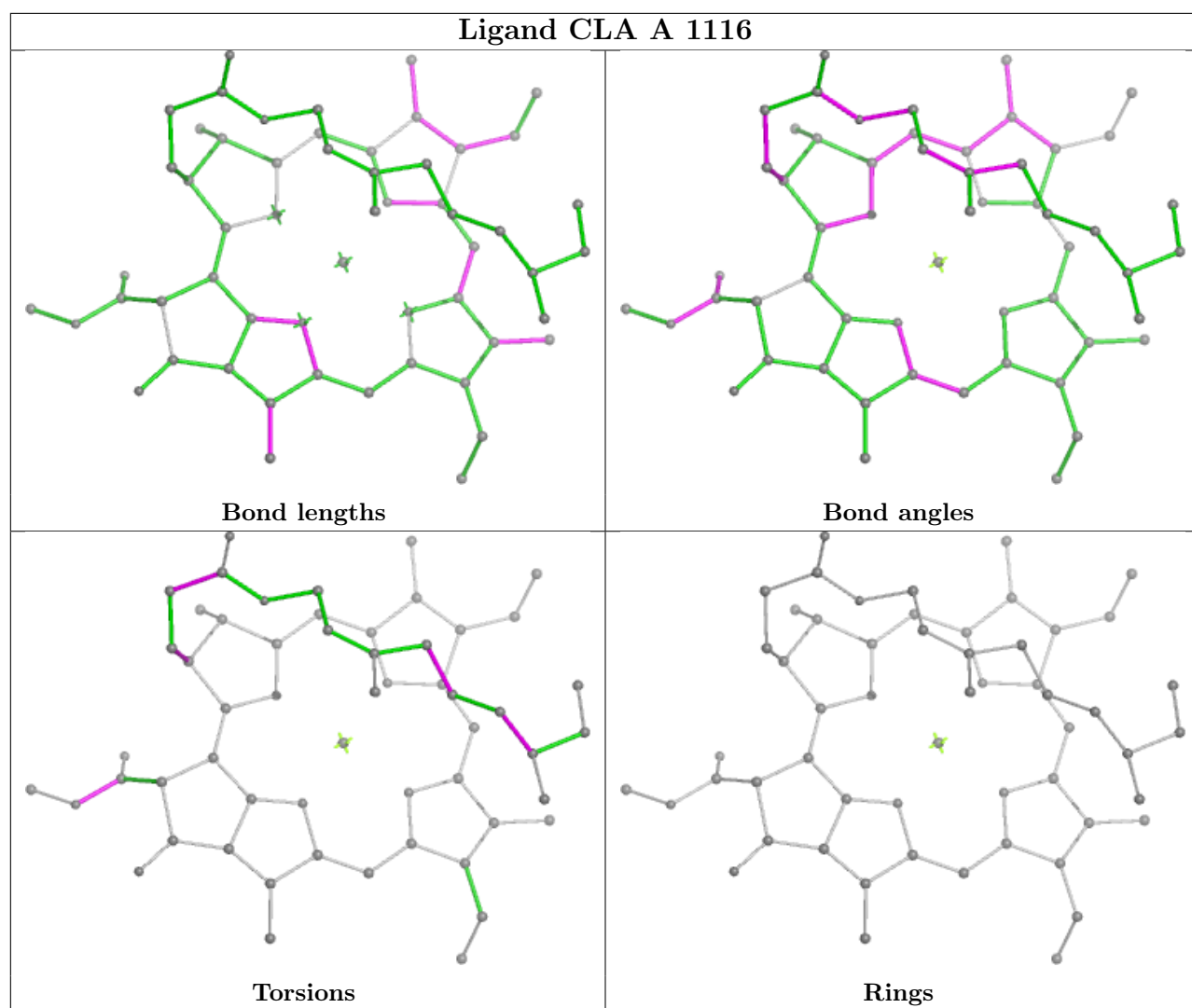


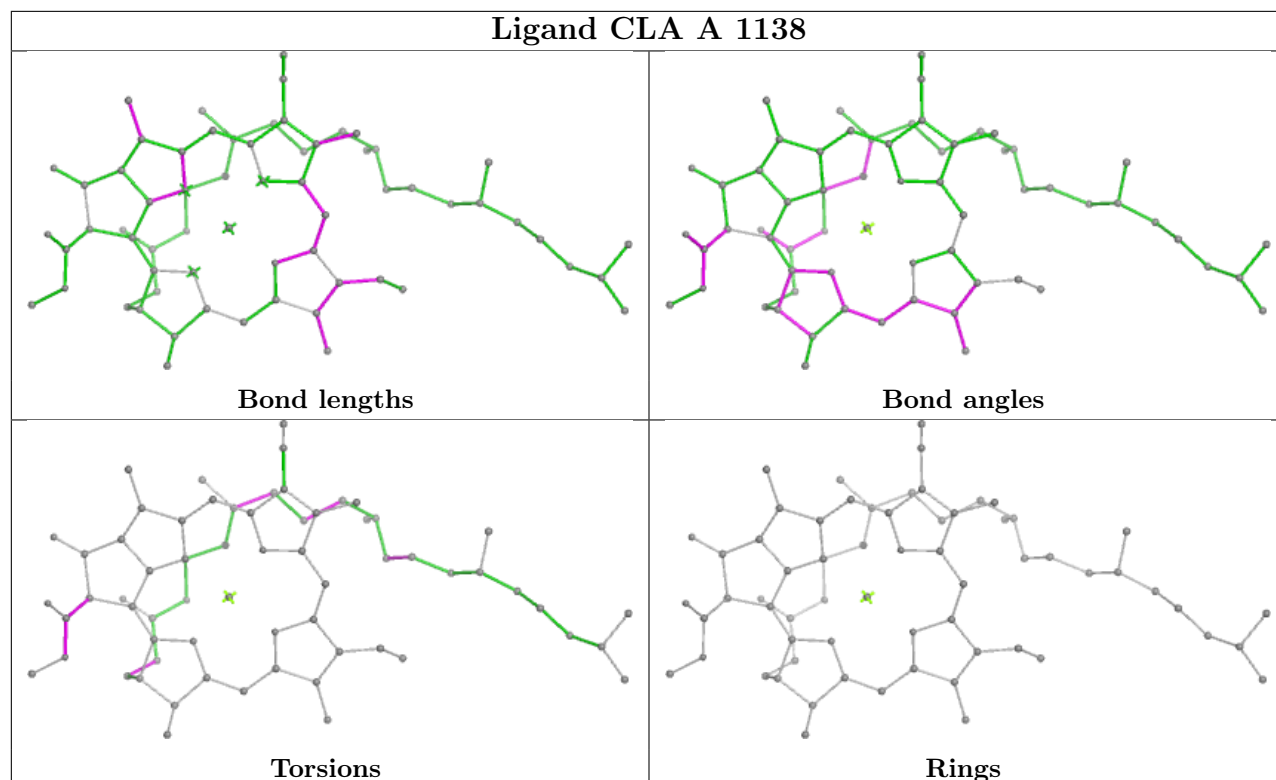
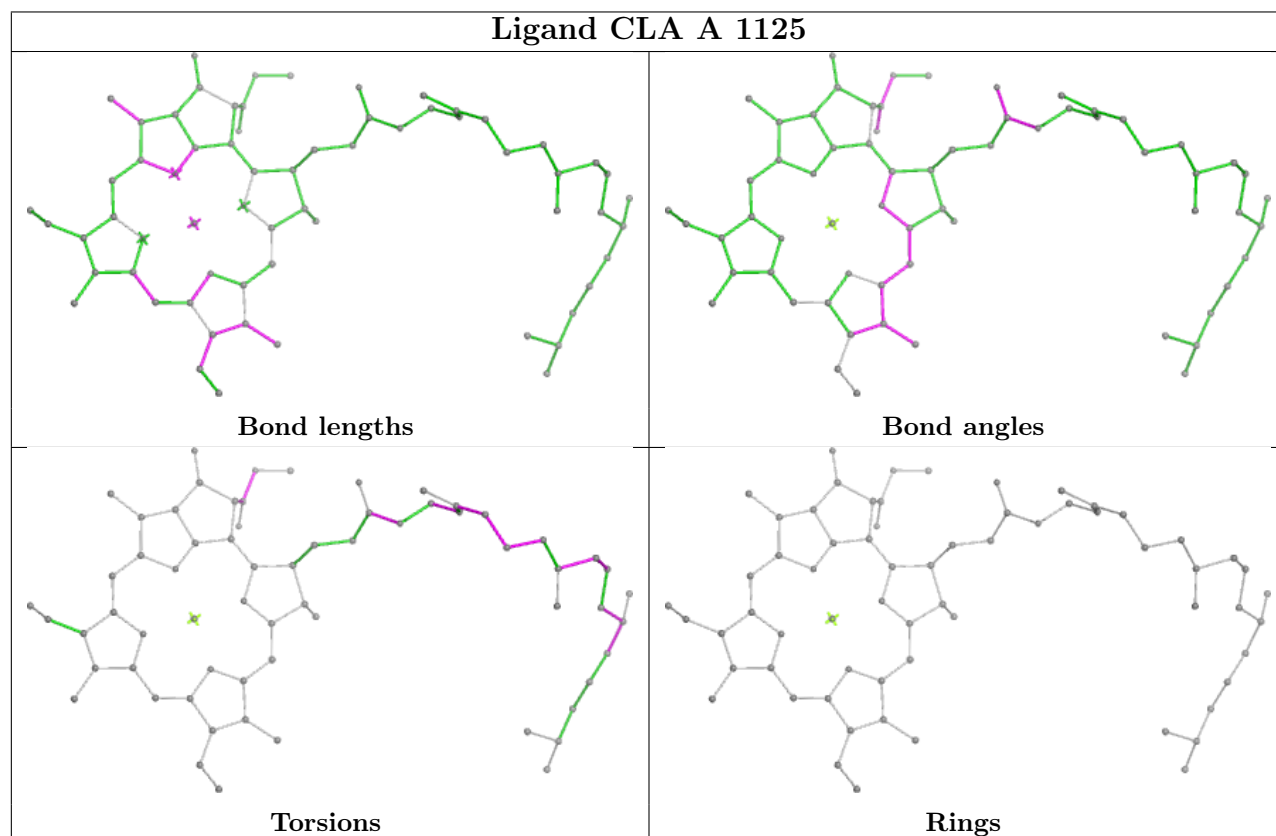
Ligand CHL 1 609

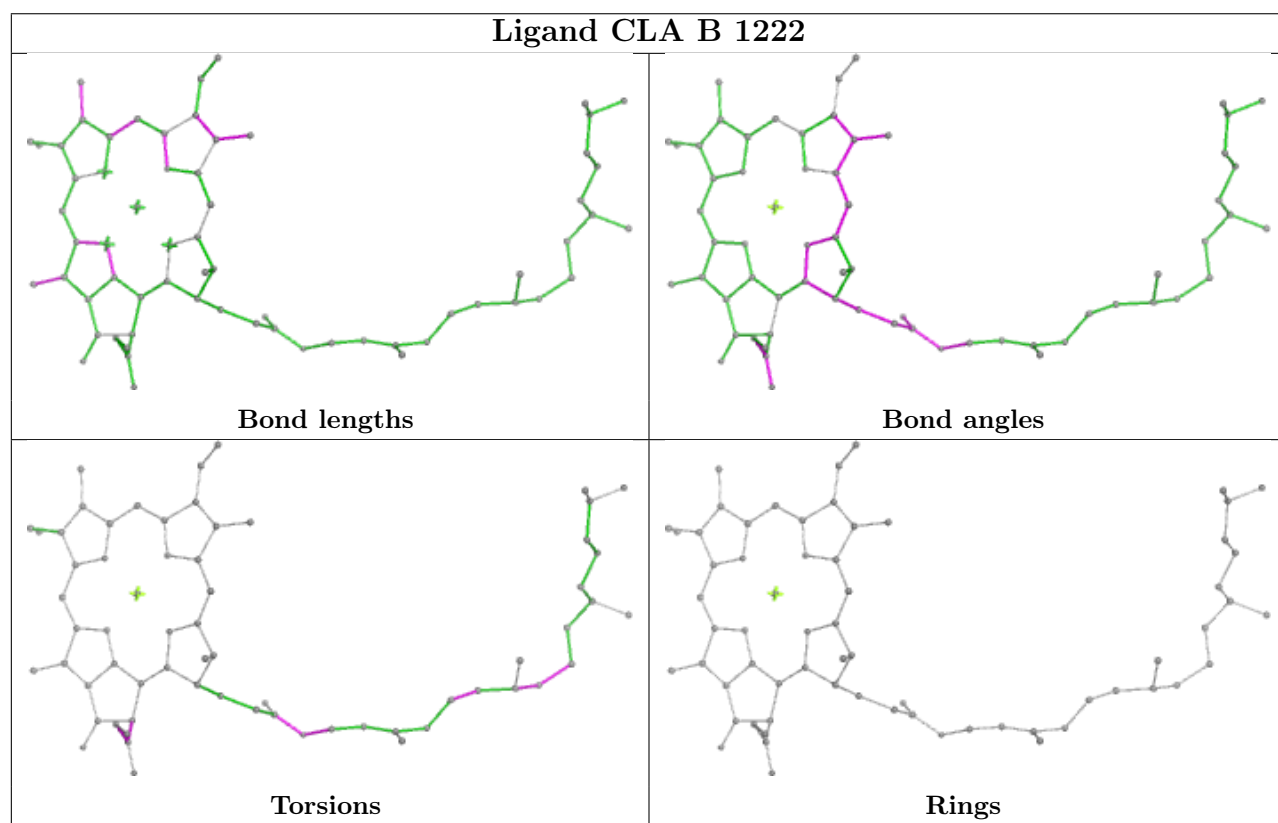
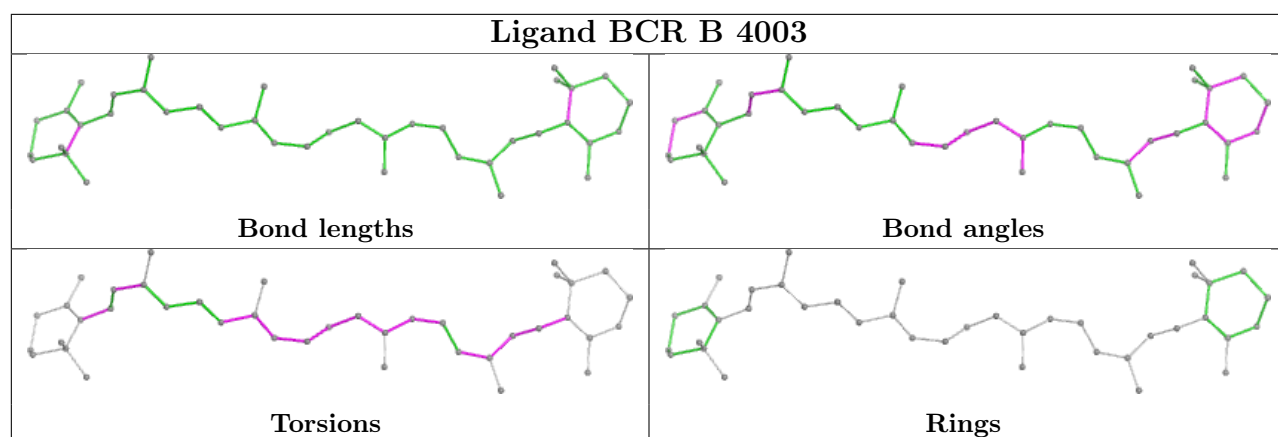


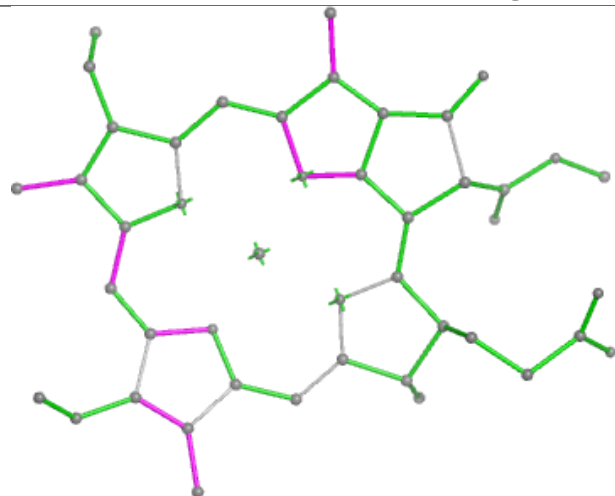
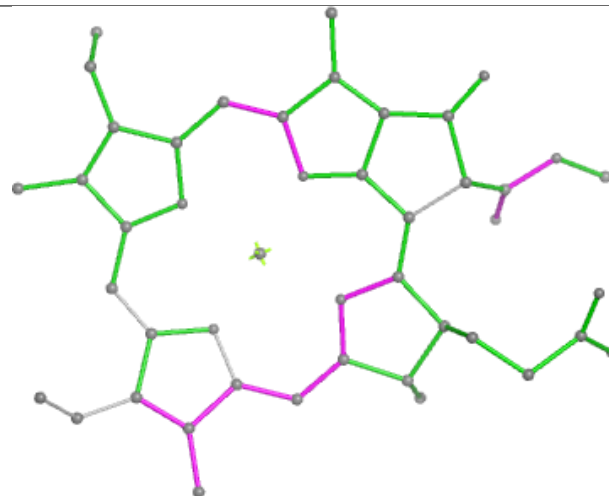
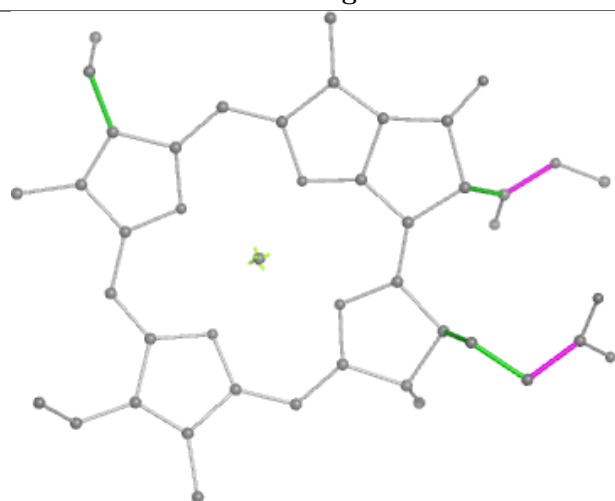
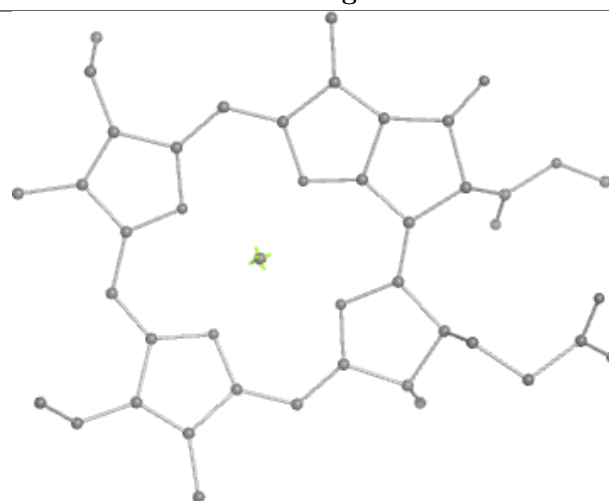
Ligand CLA 4 601

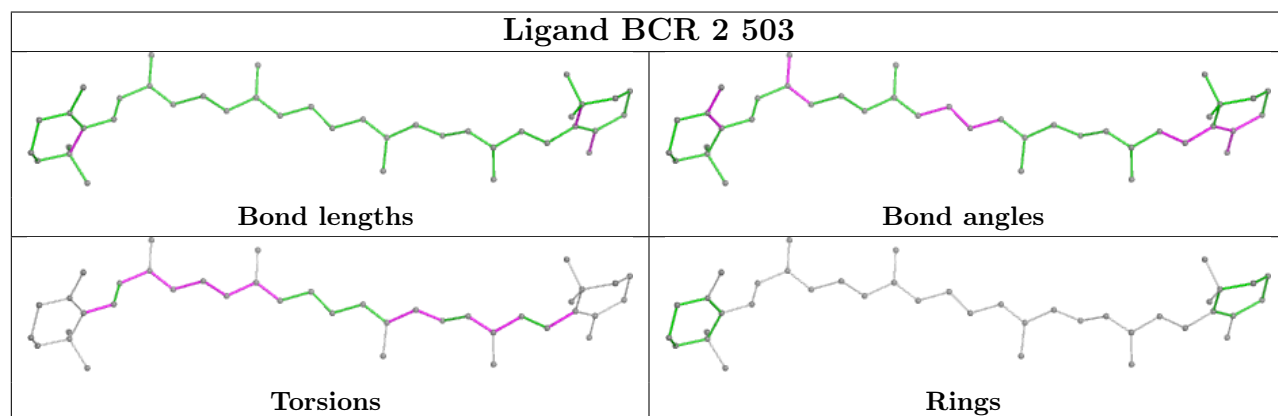
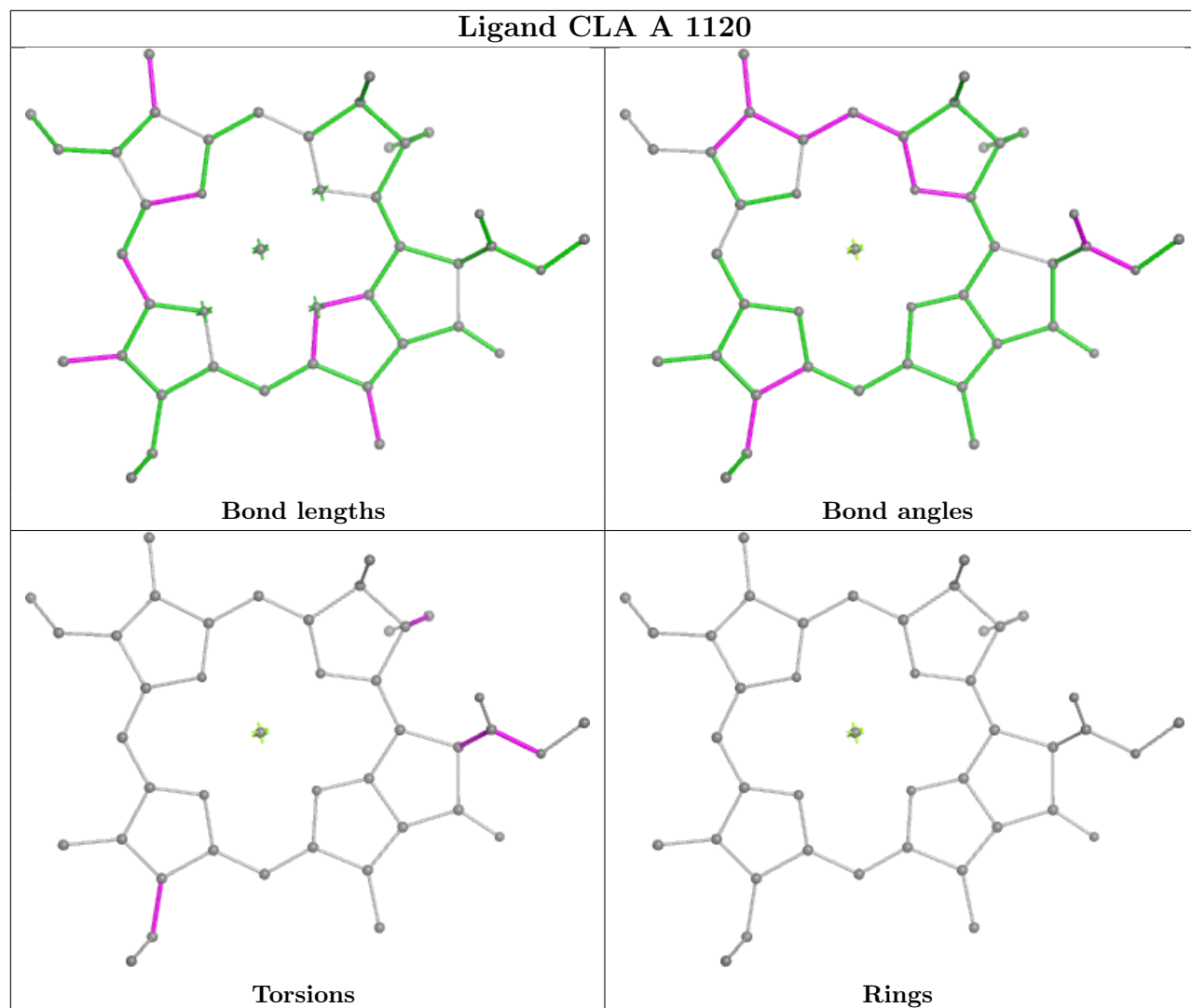




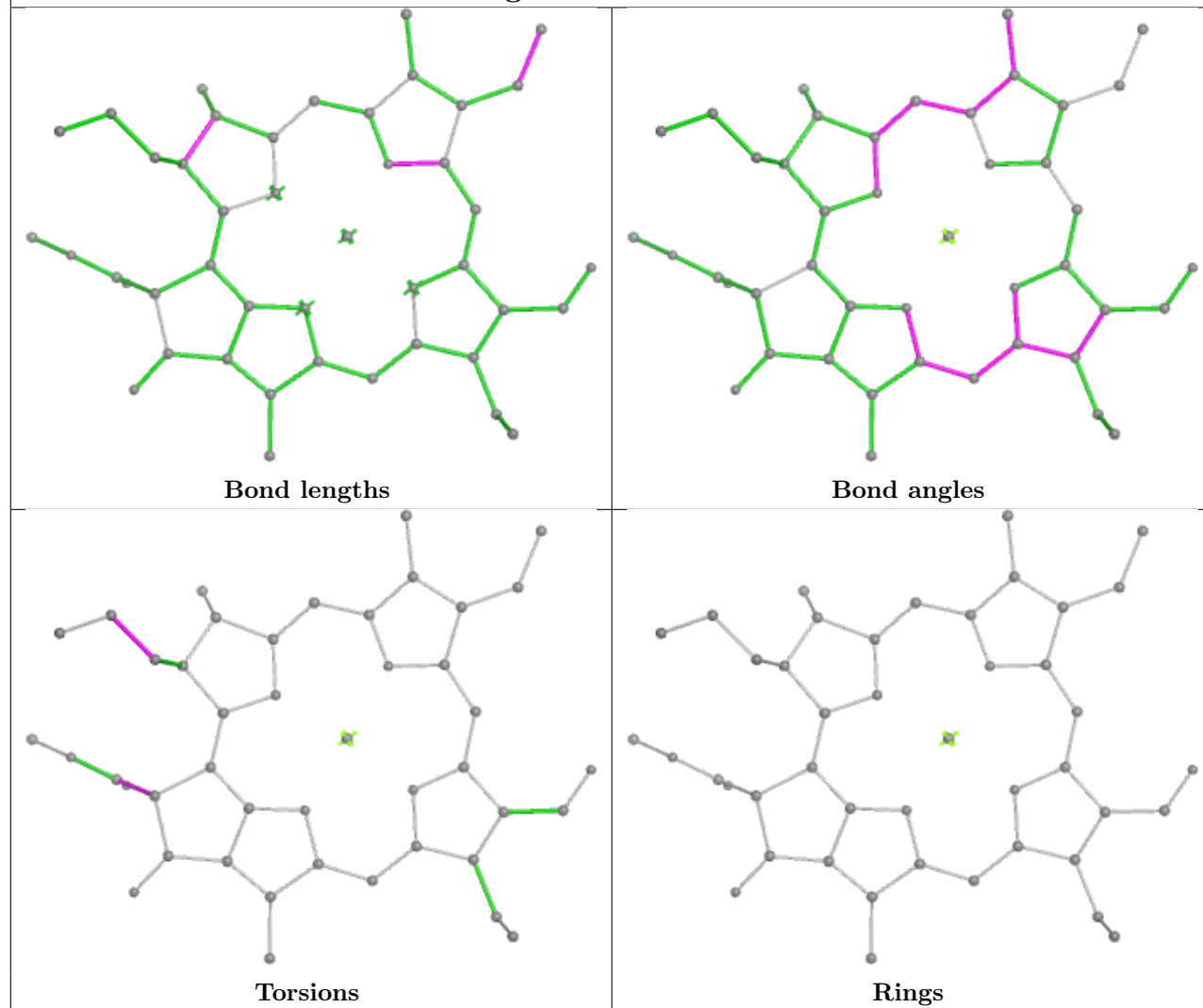
Ligand CLA A 1138**Ligand CLA A 1125**



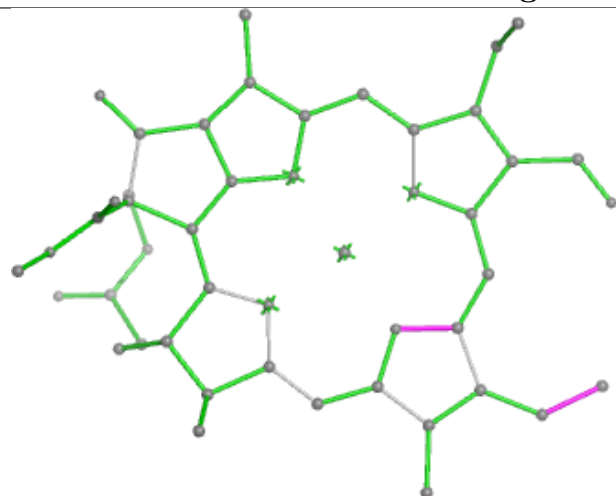
Ligand CLA A 1131**Bond lengths****Bond angles****Torsions****Rings**



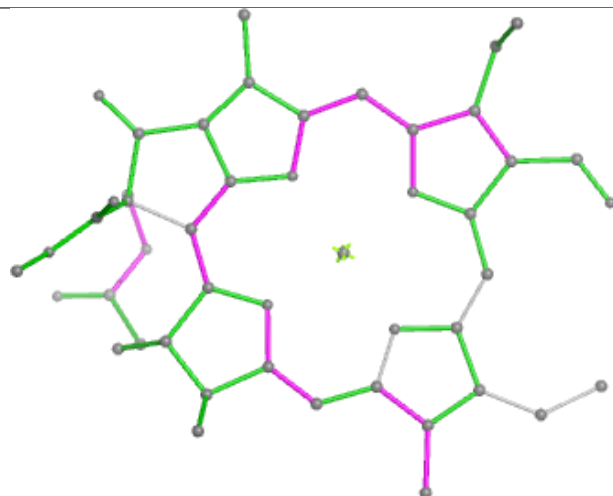
Ligand CHL 2 610



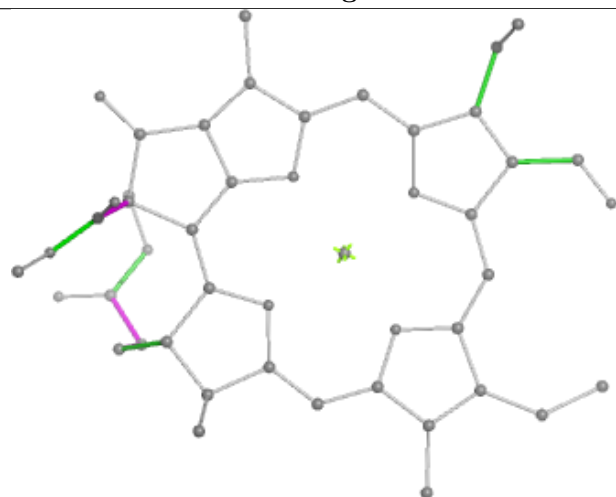
Ligand CHL 1 610



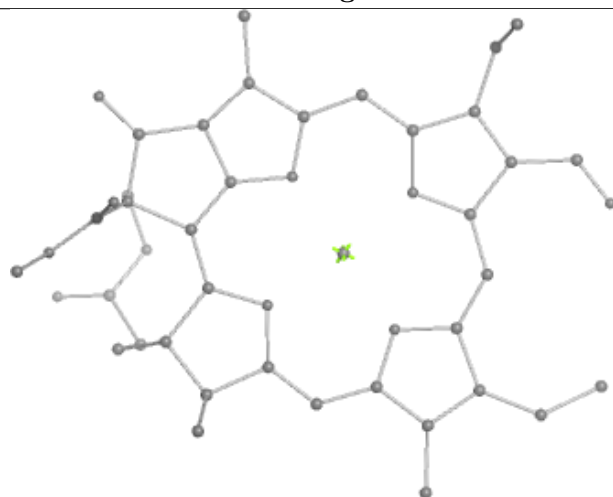
Bond lengths



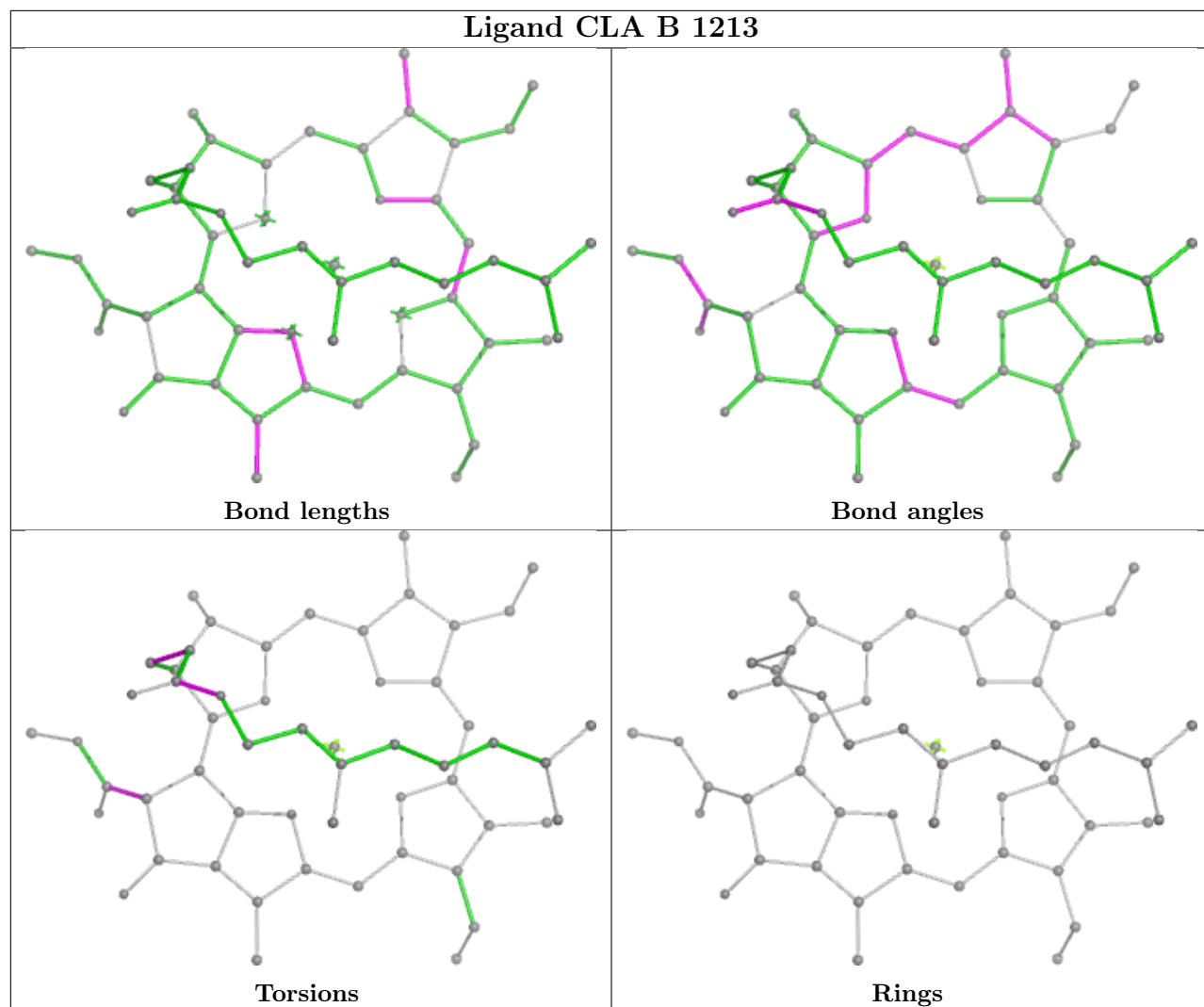
Bond angles

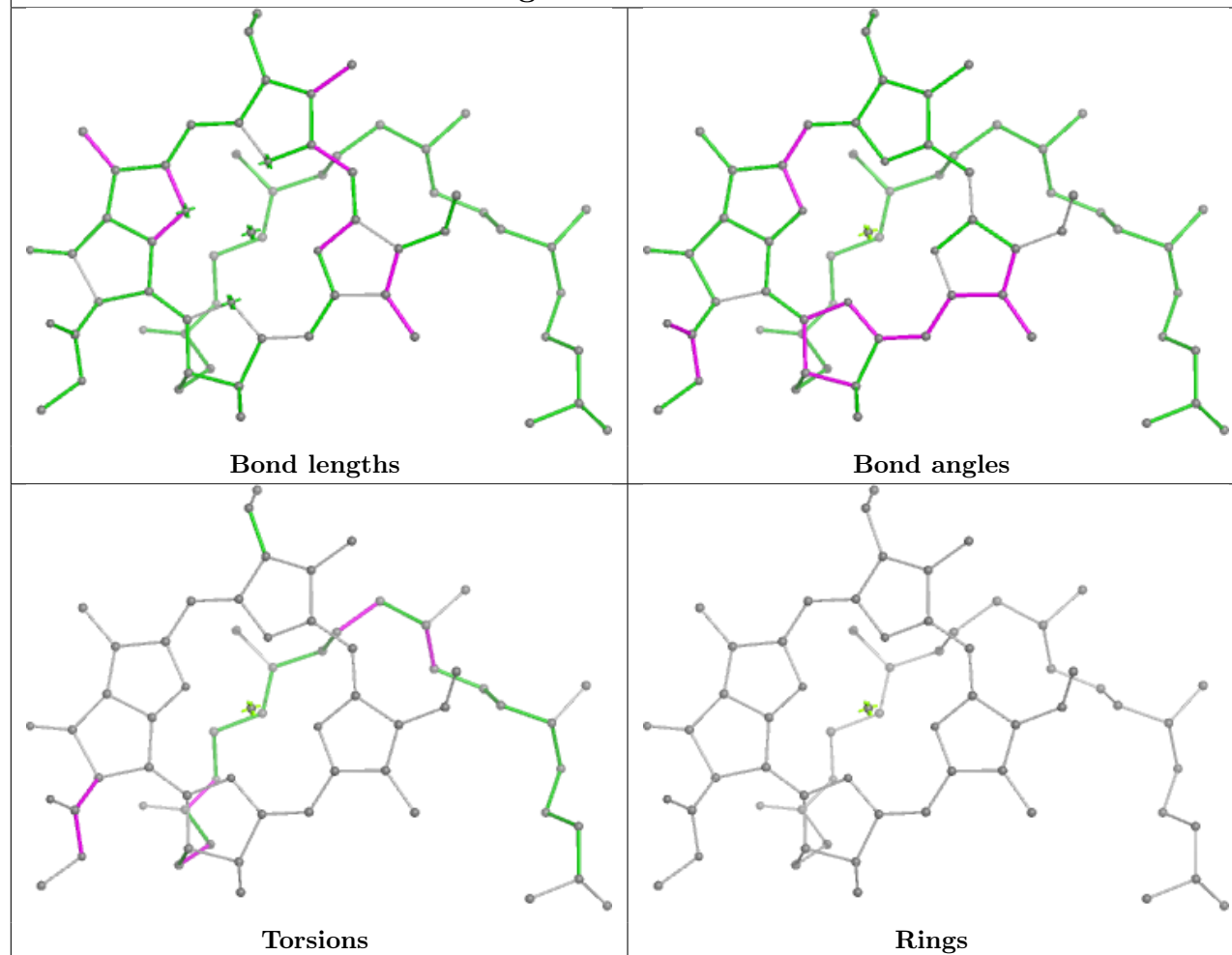
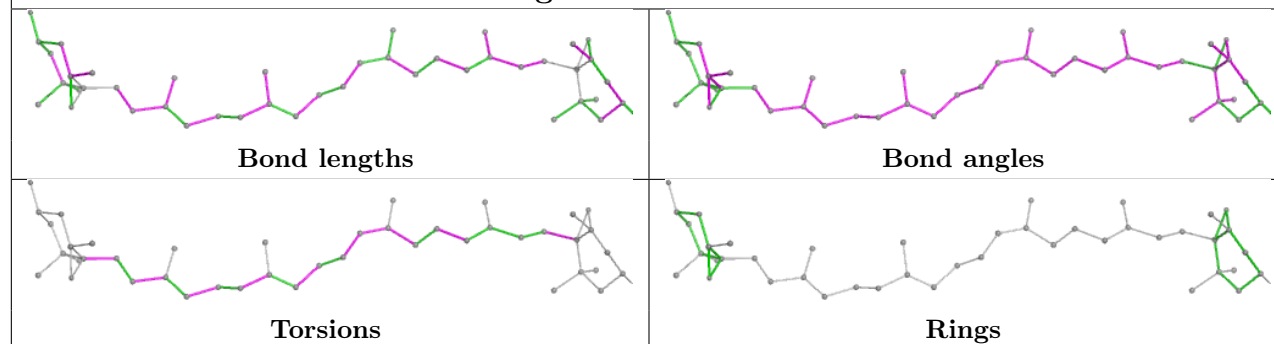


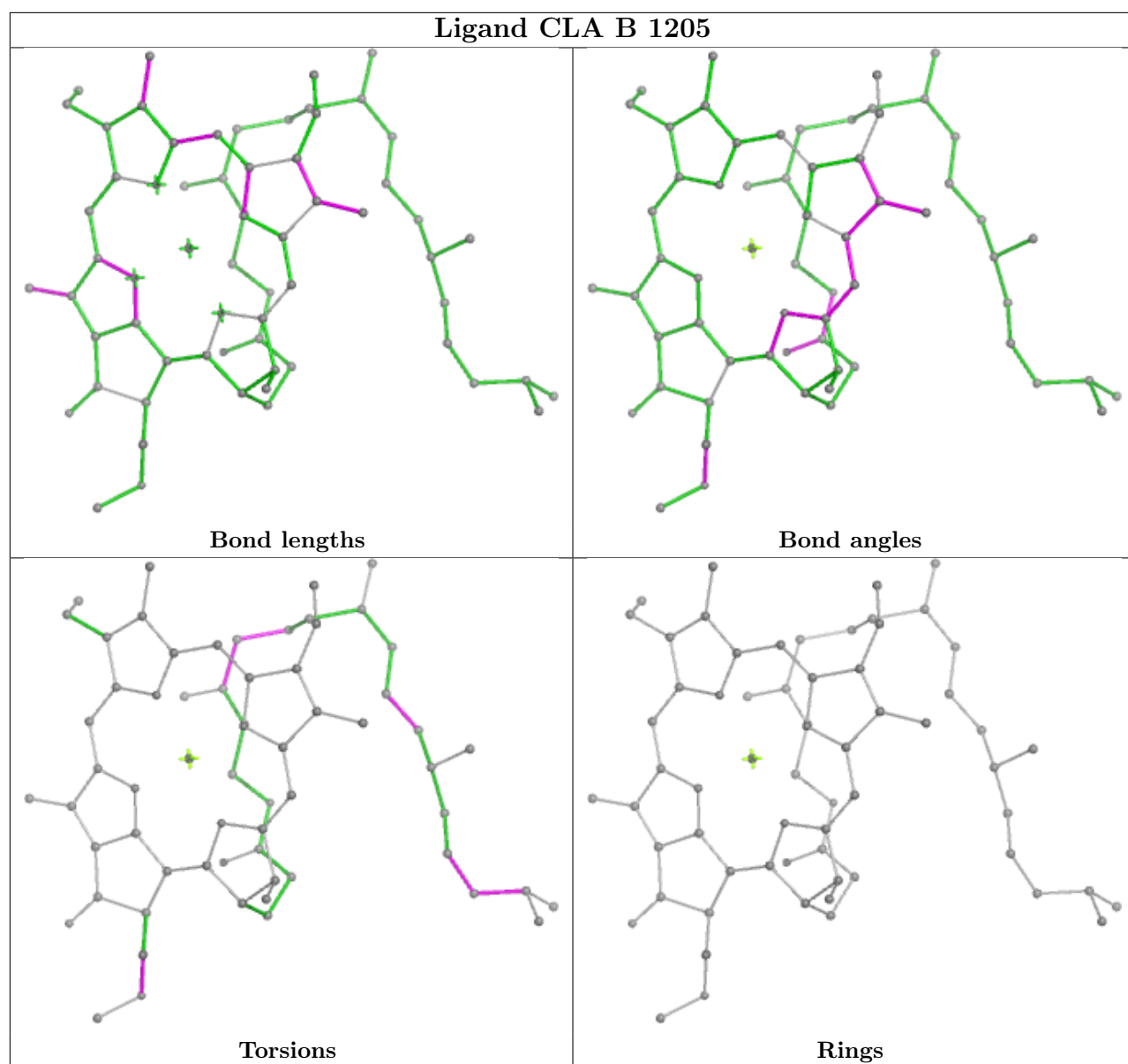
Torsions

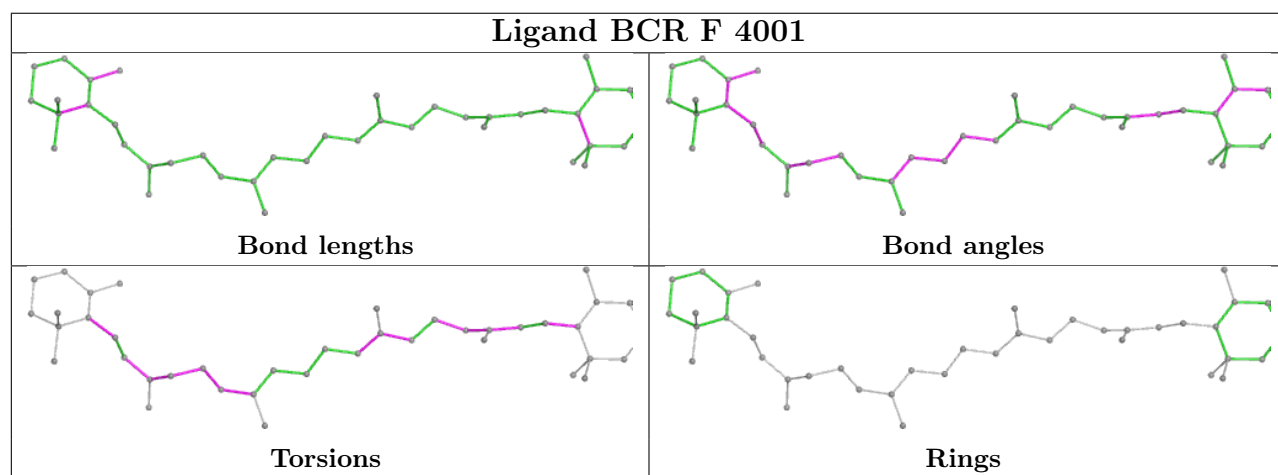
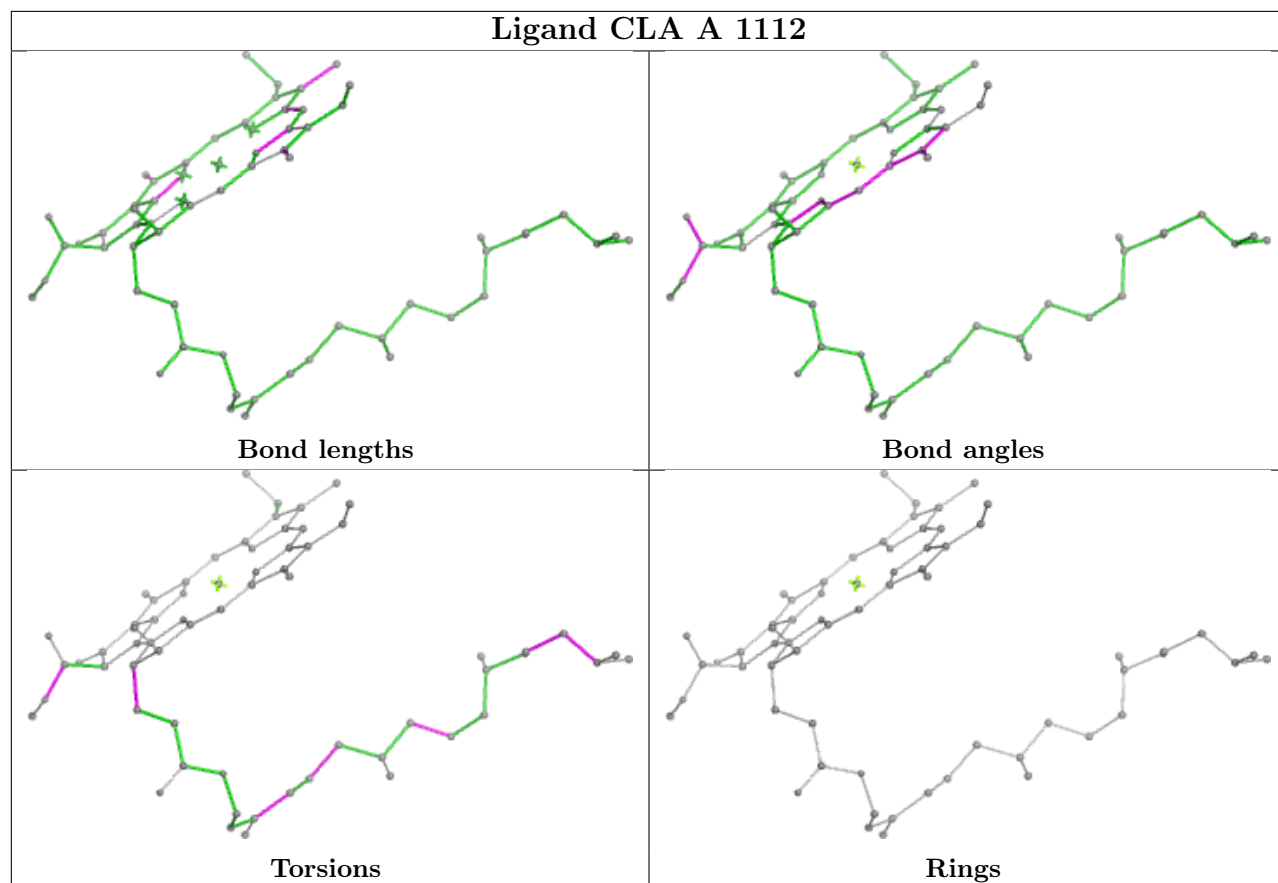


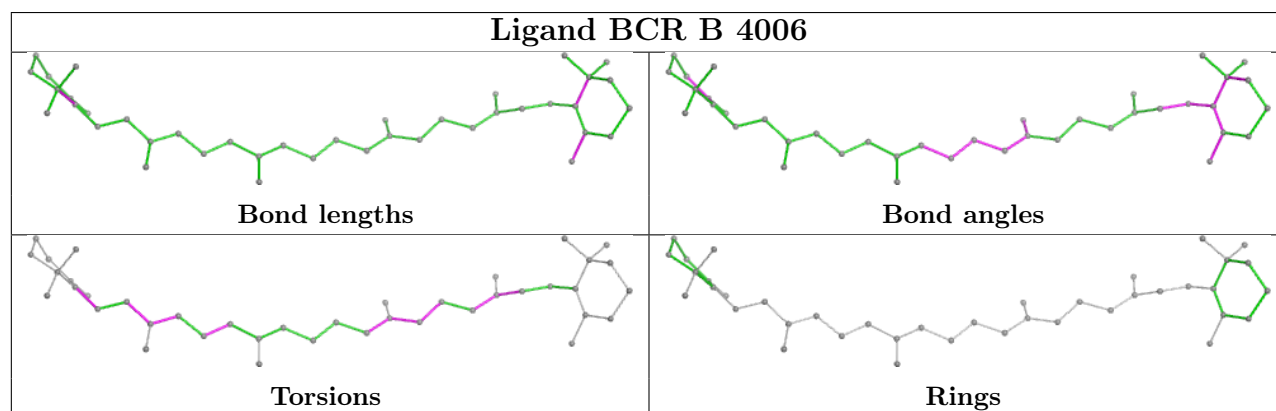
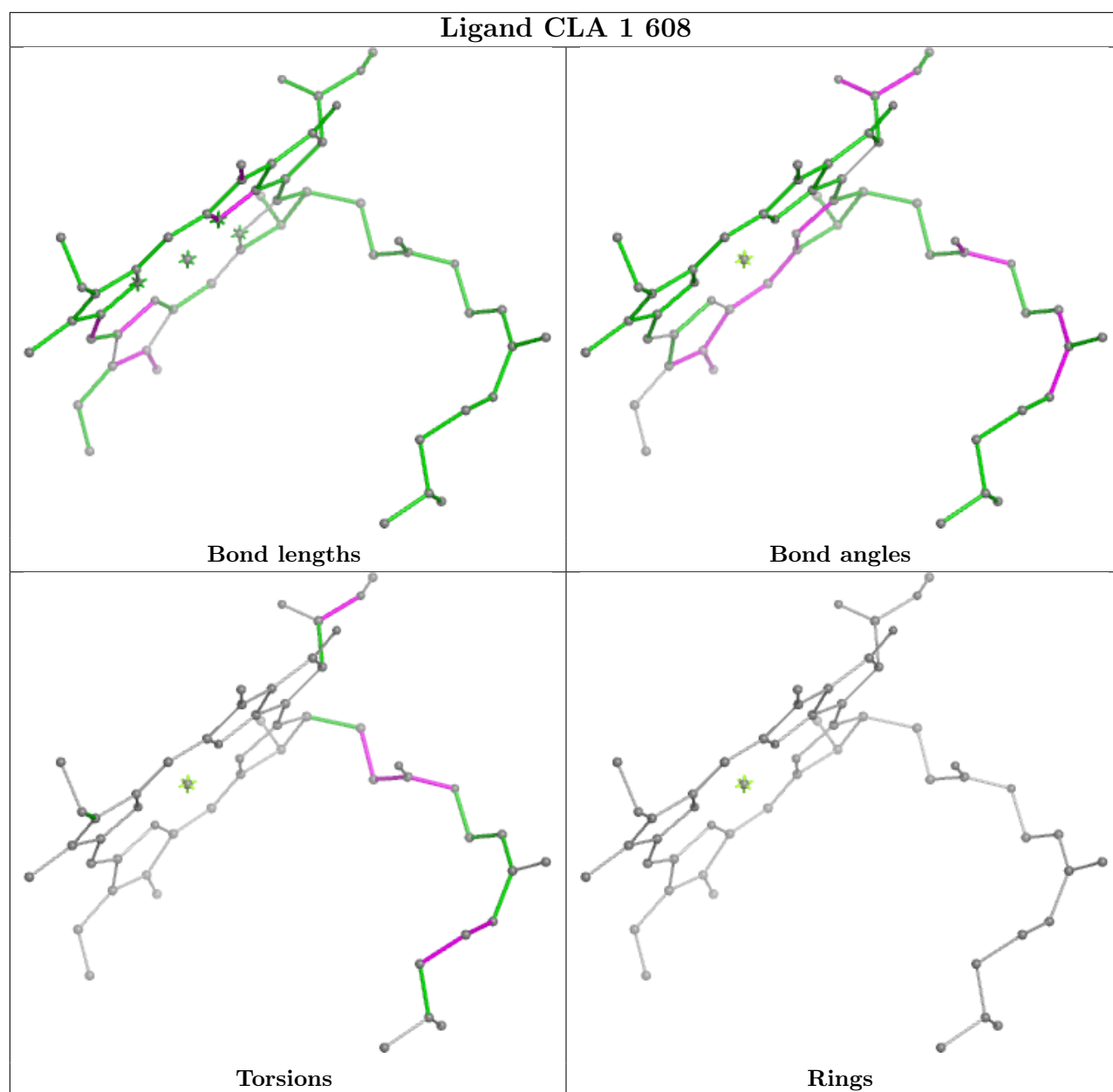
Rings



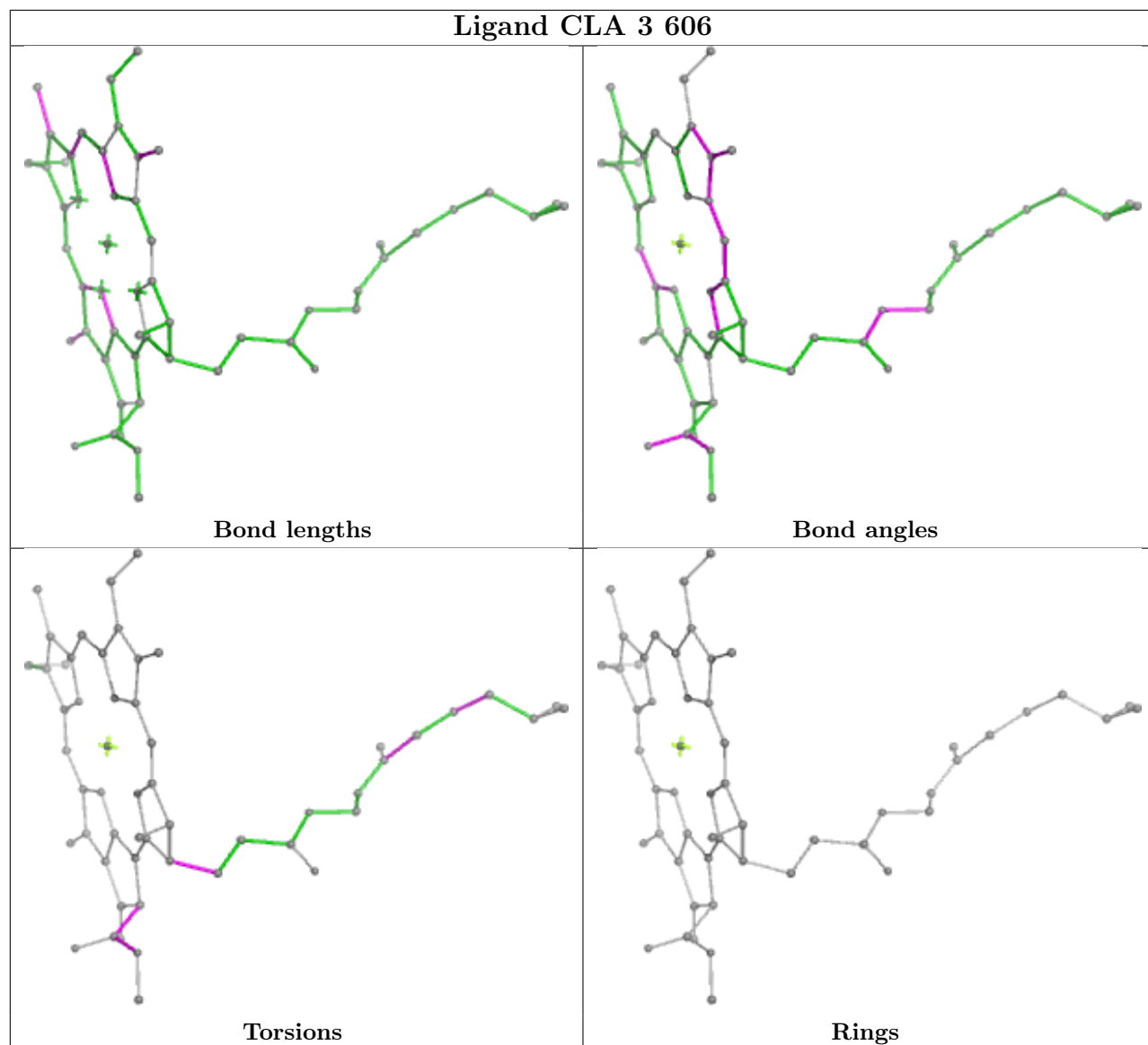
Ligand CLA 2 603**Ligand XAT 3 502**



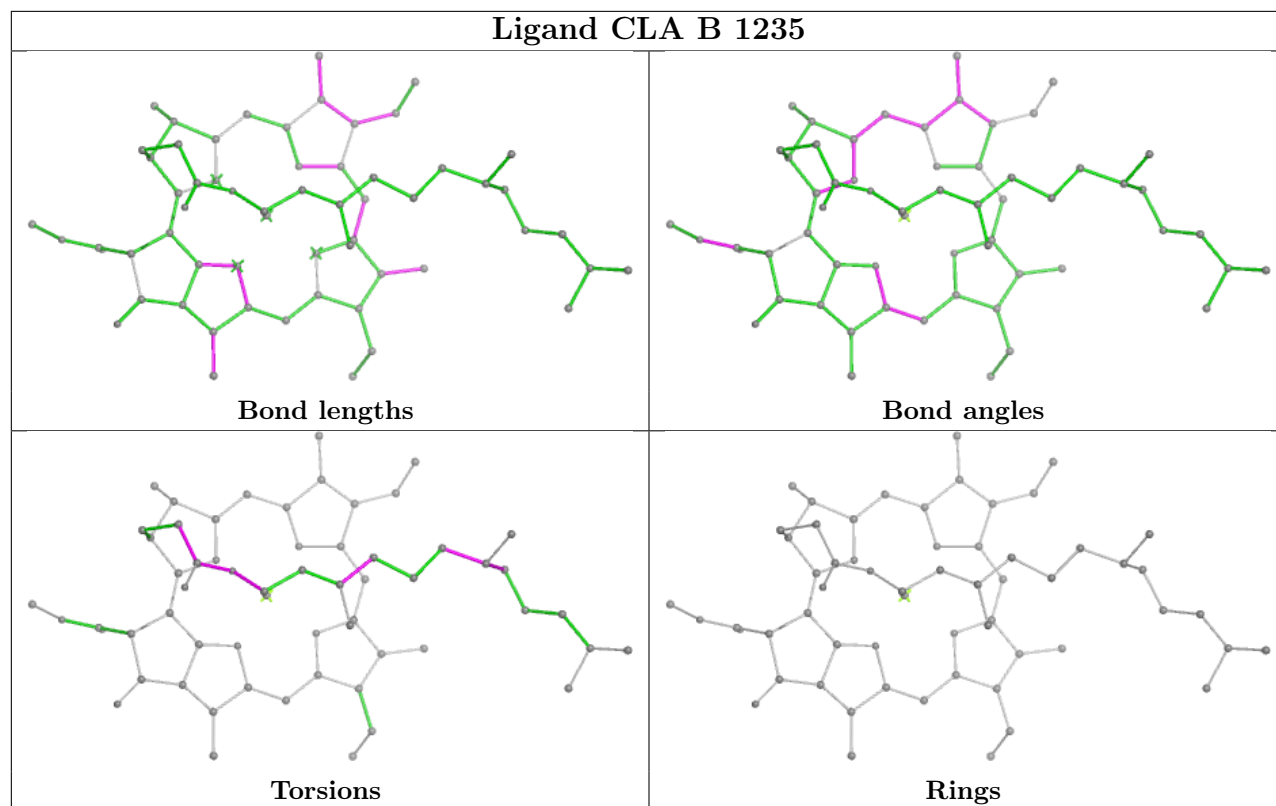




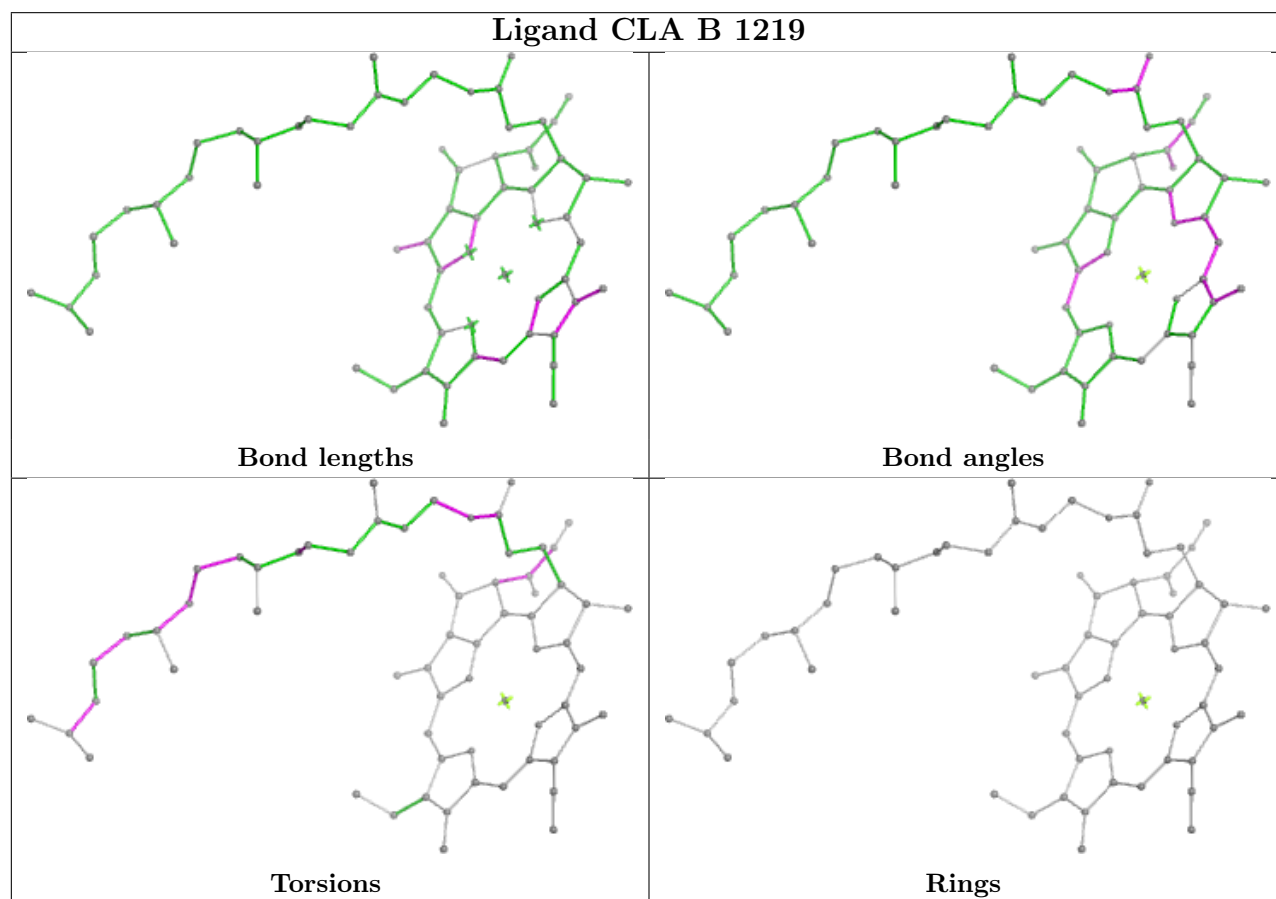
Ligand CLA 3 606

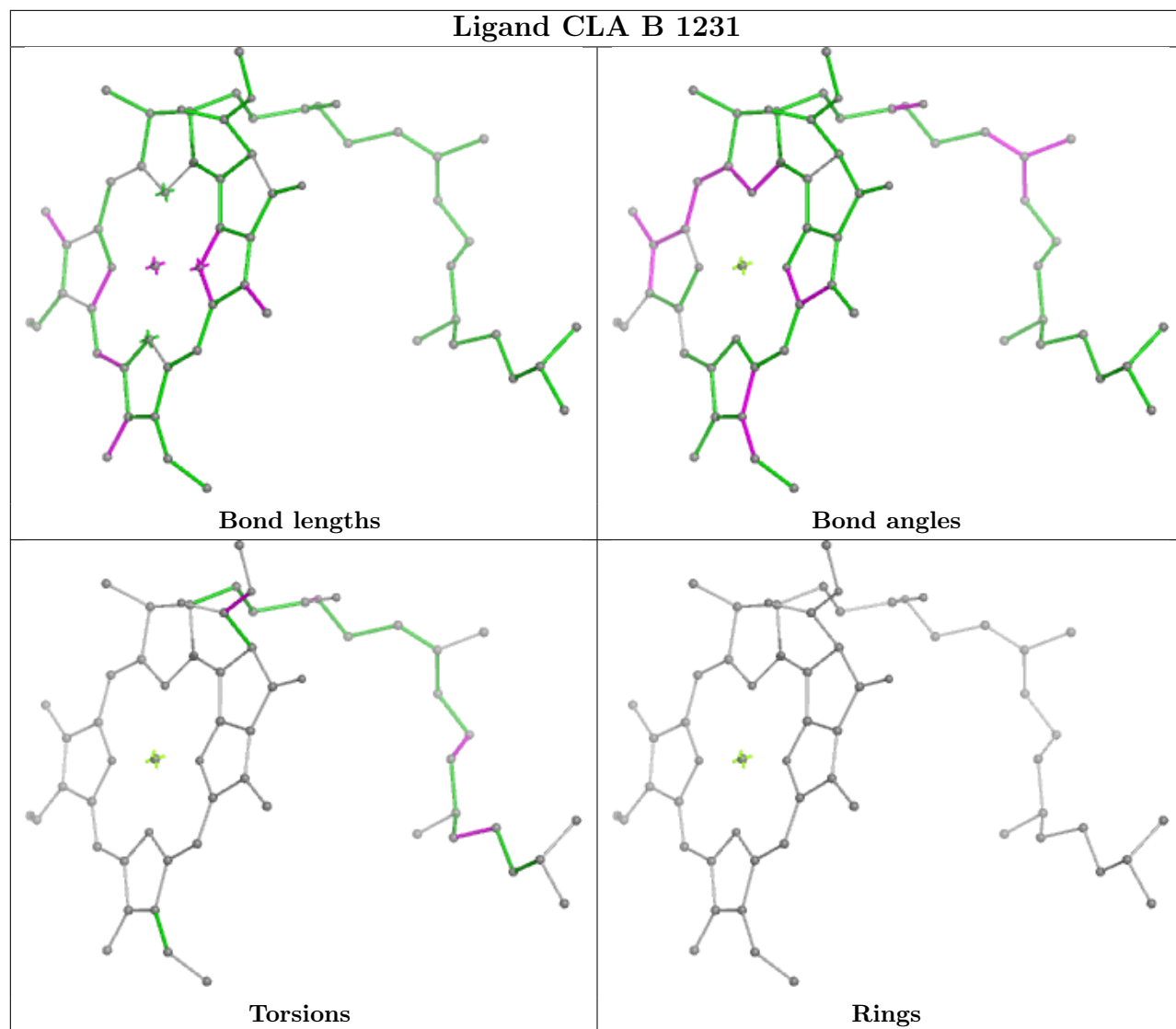


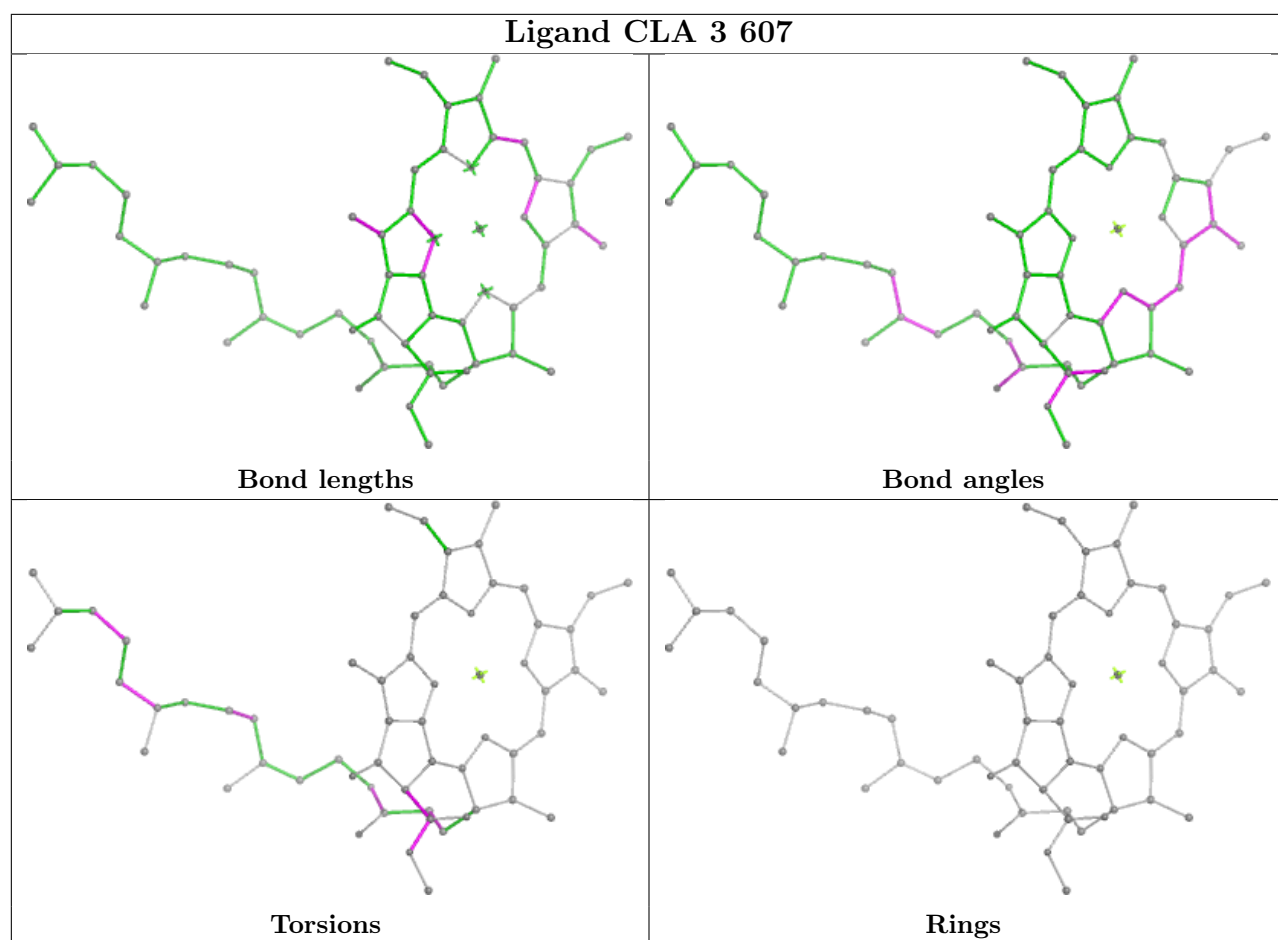
Ligand CLA B 1235

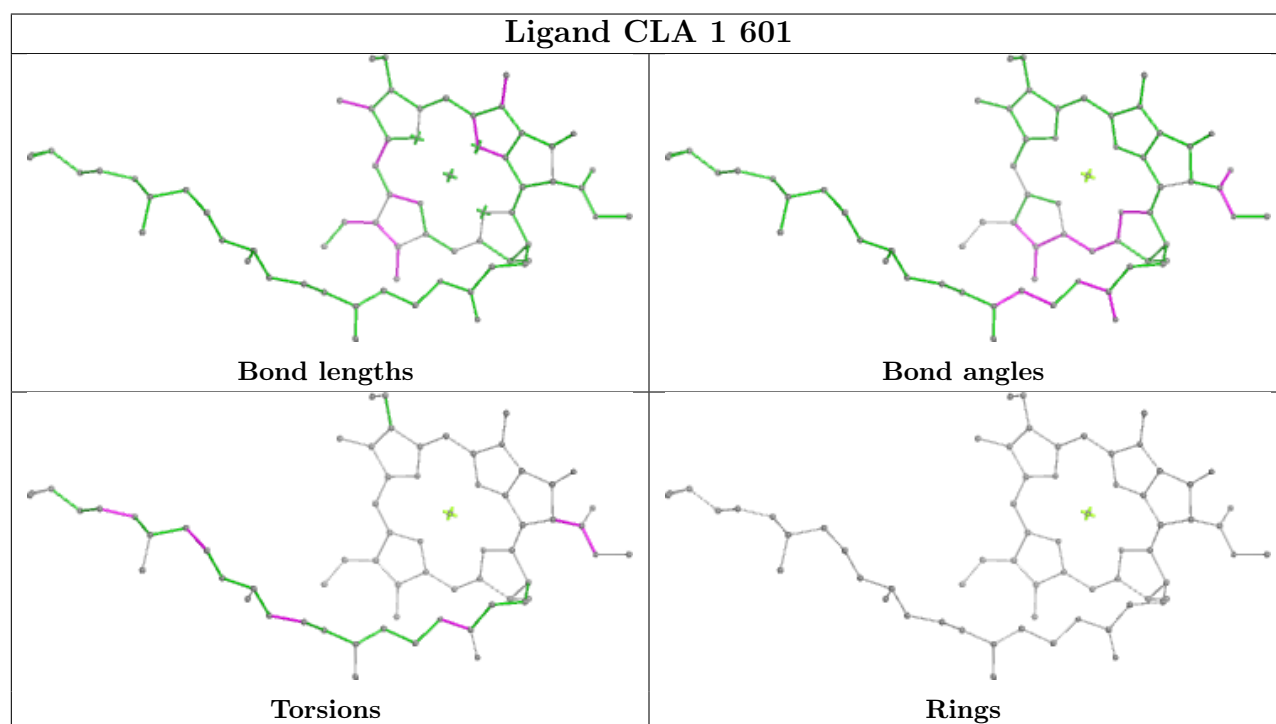
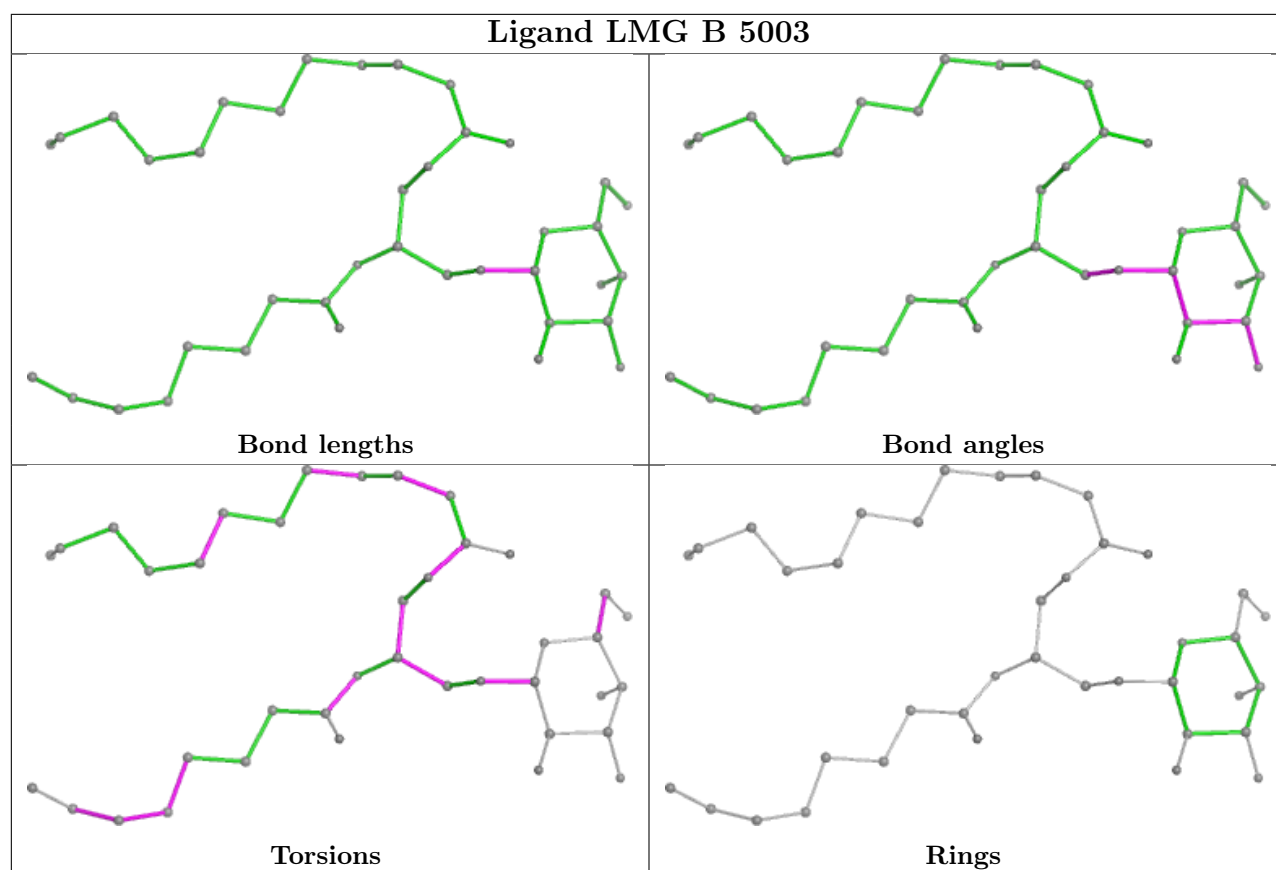


Ligand CLA B 1219

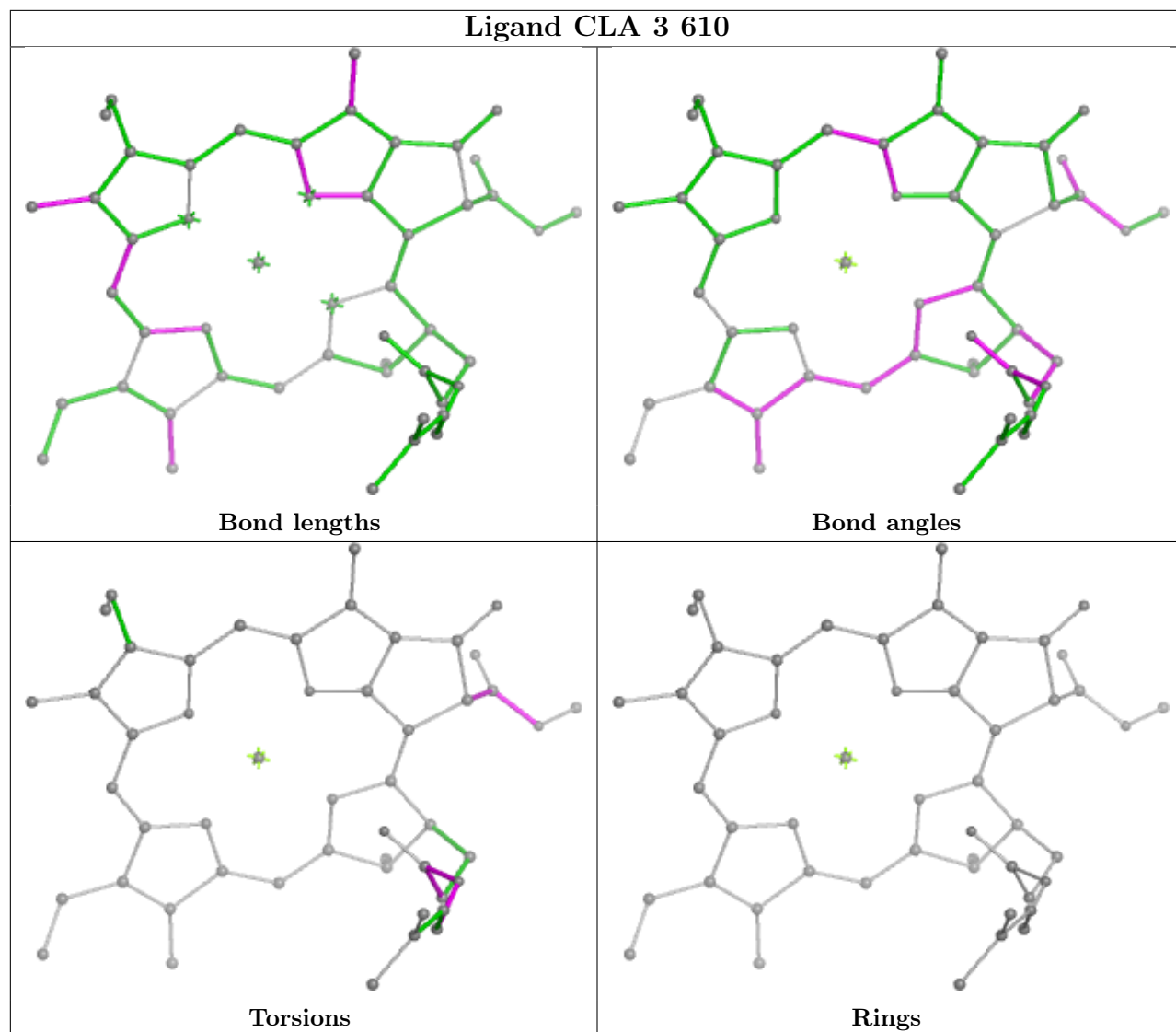


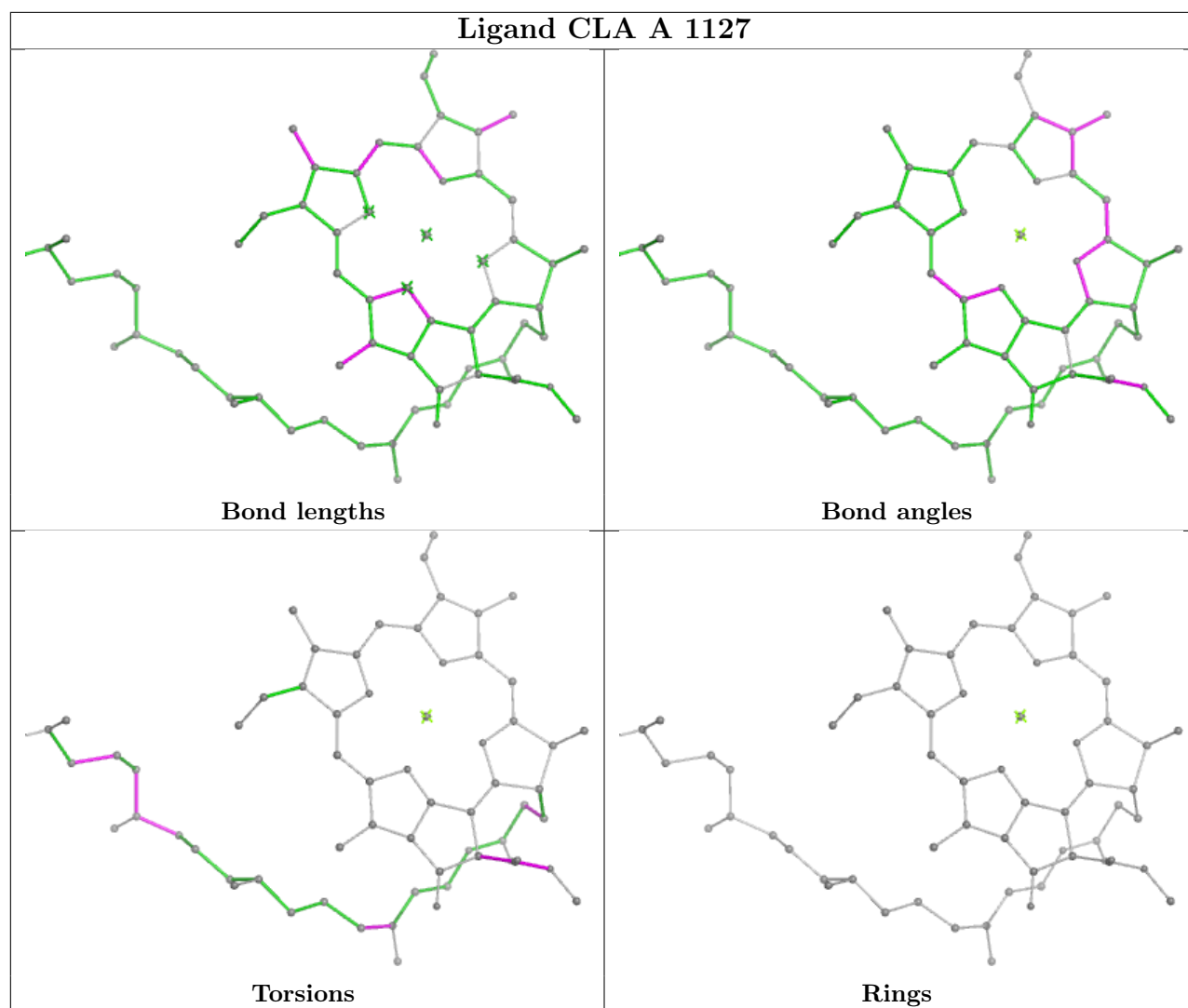
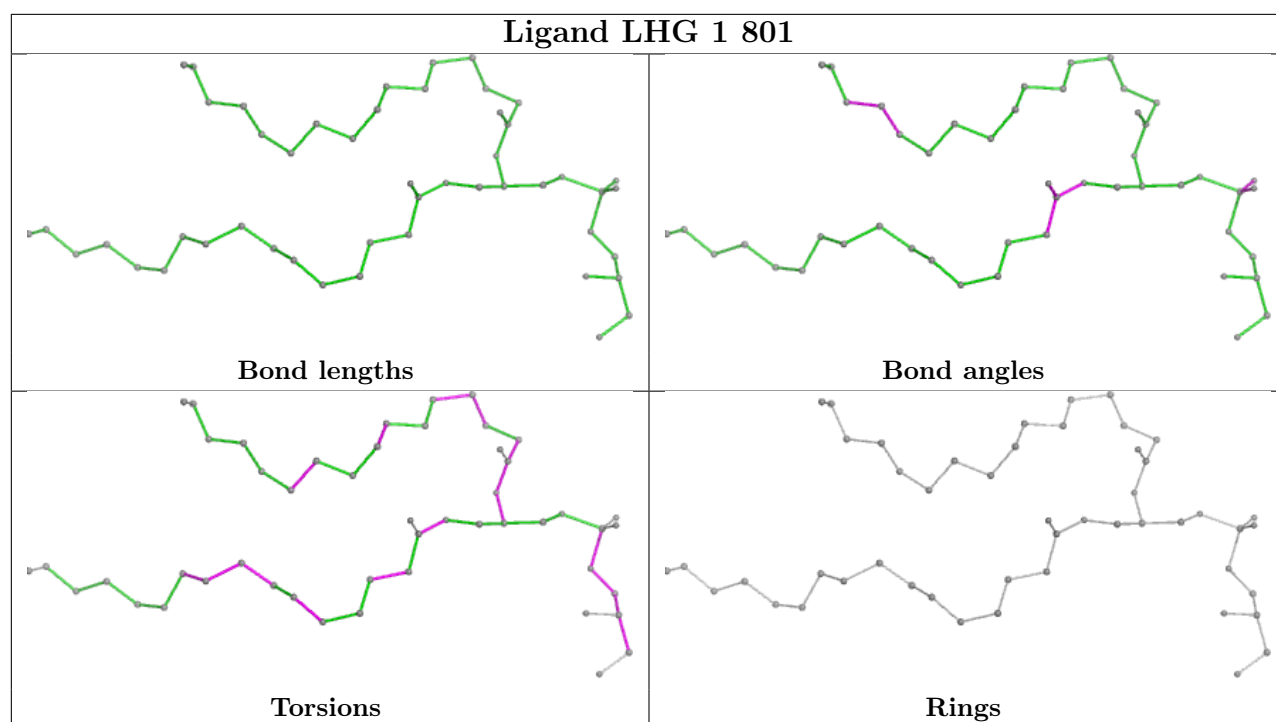




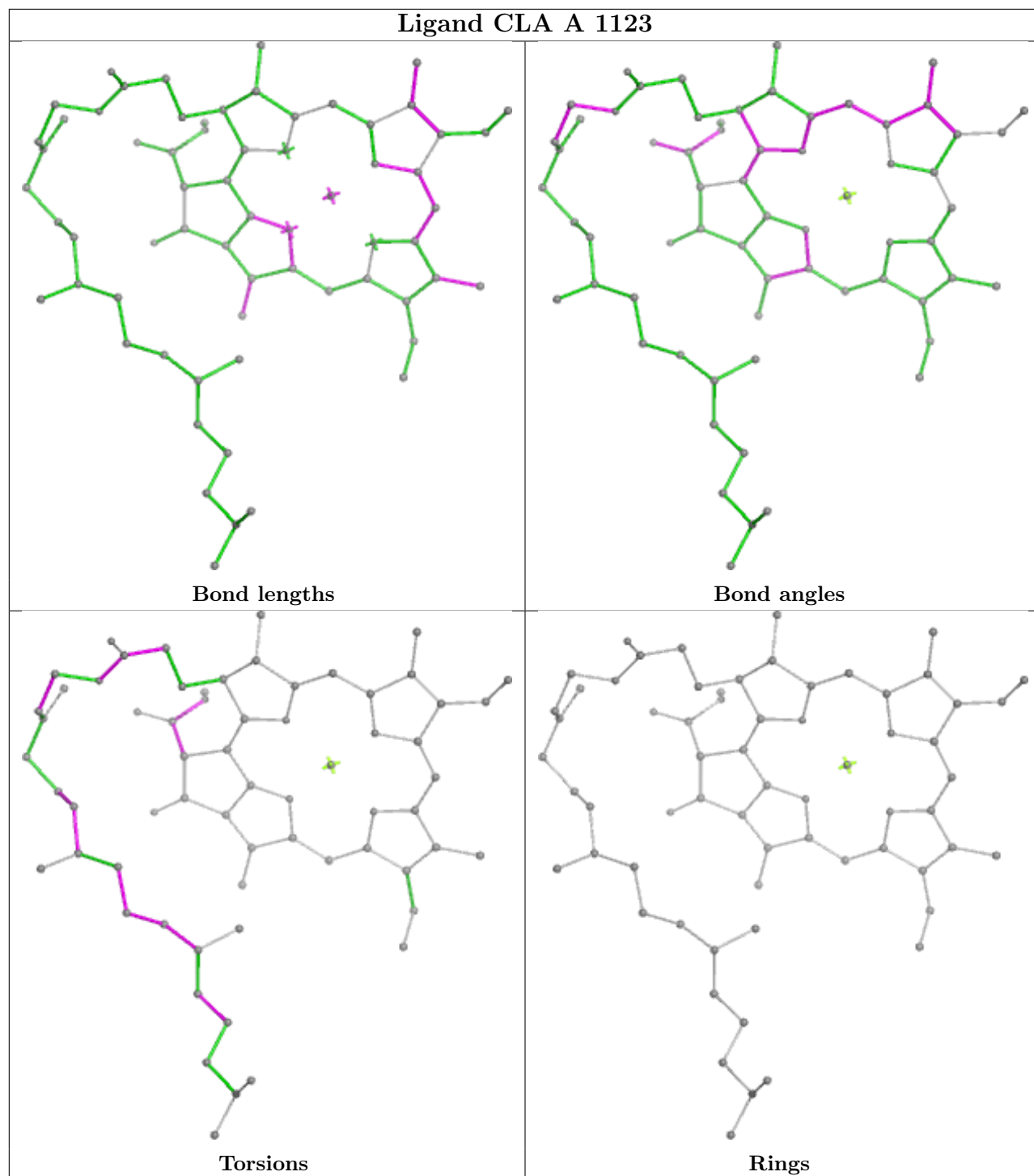


Ligand CLA 3 610

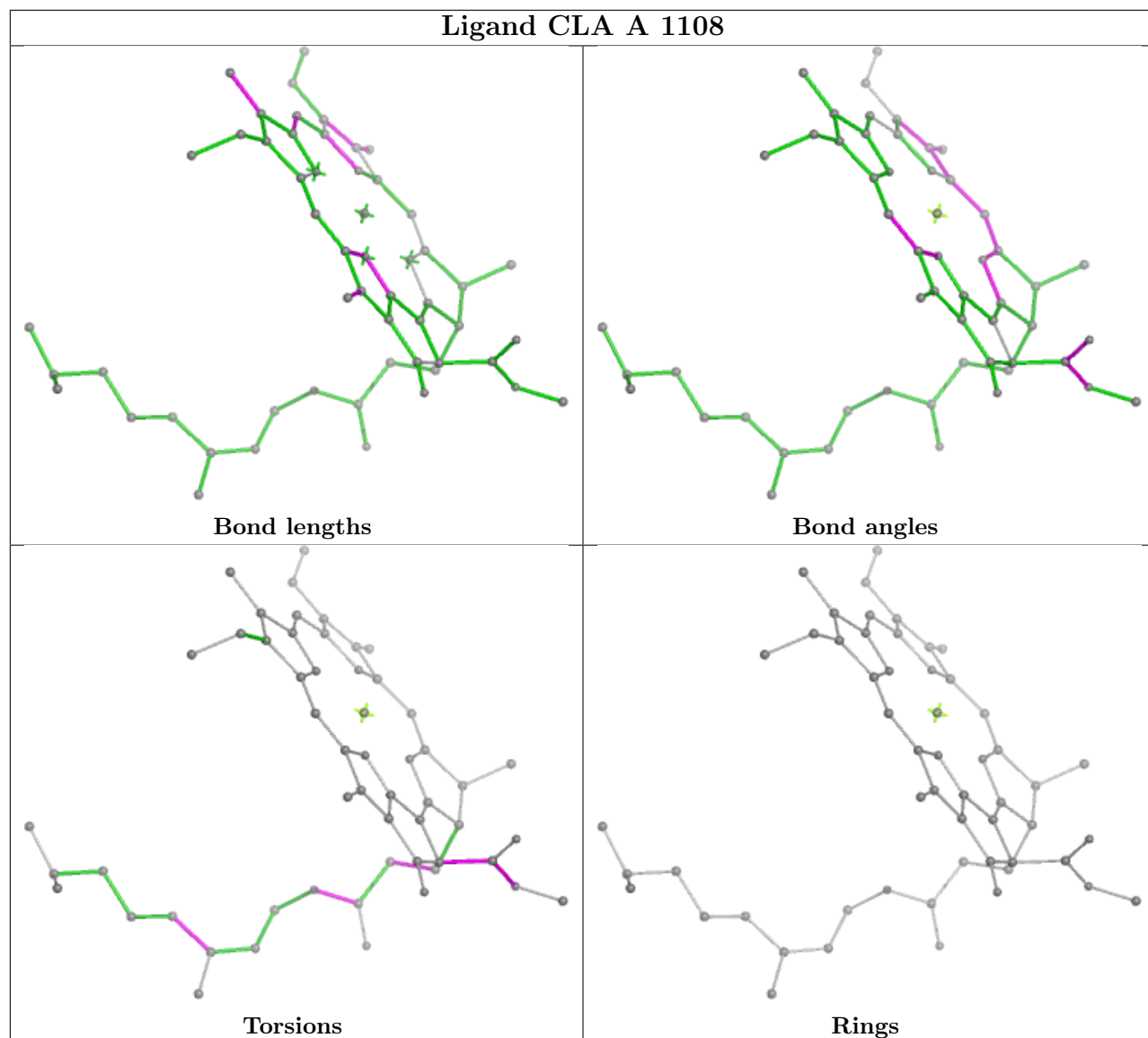


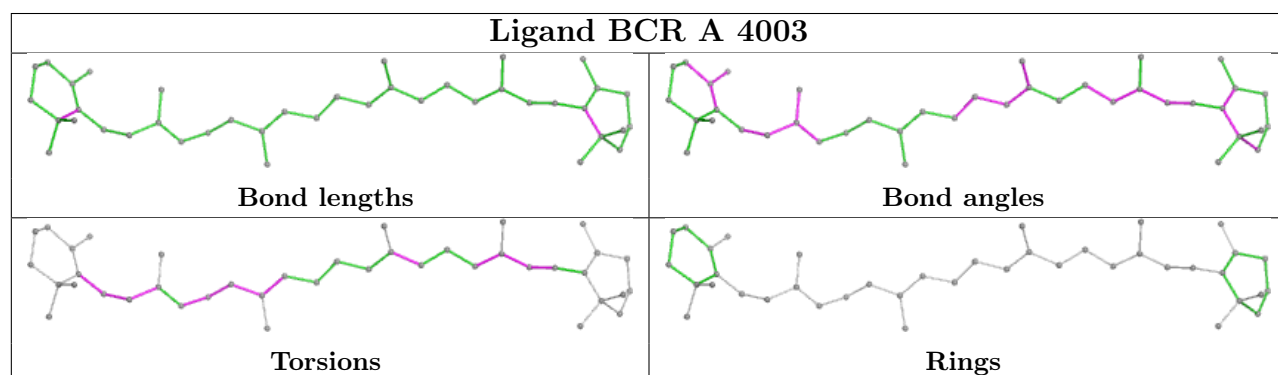
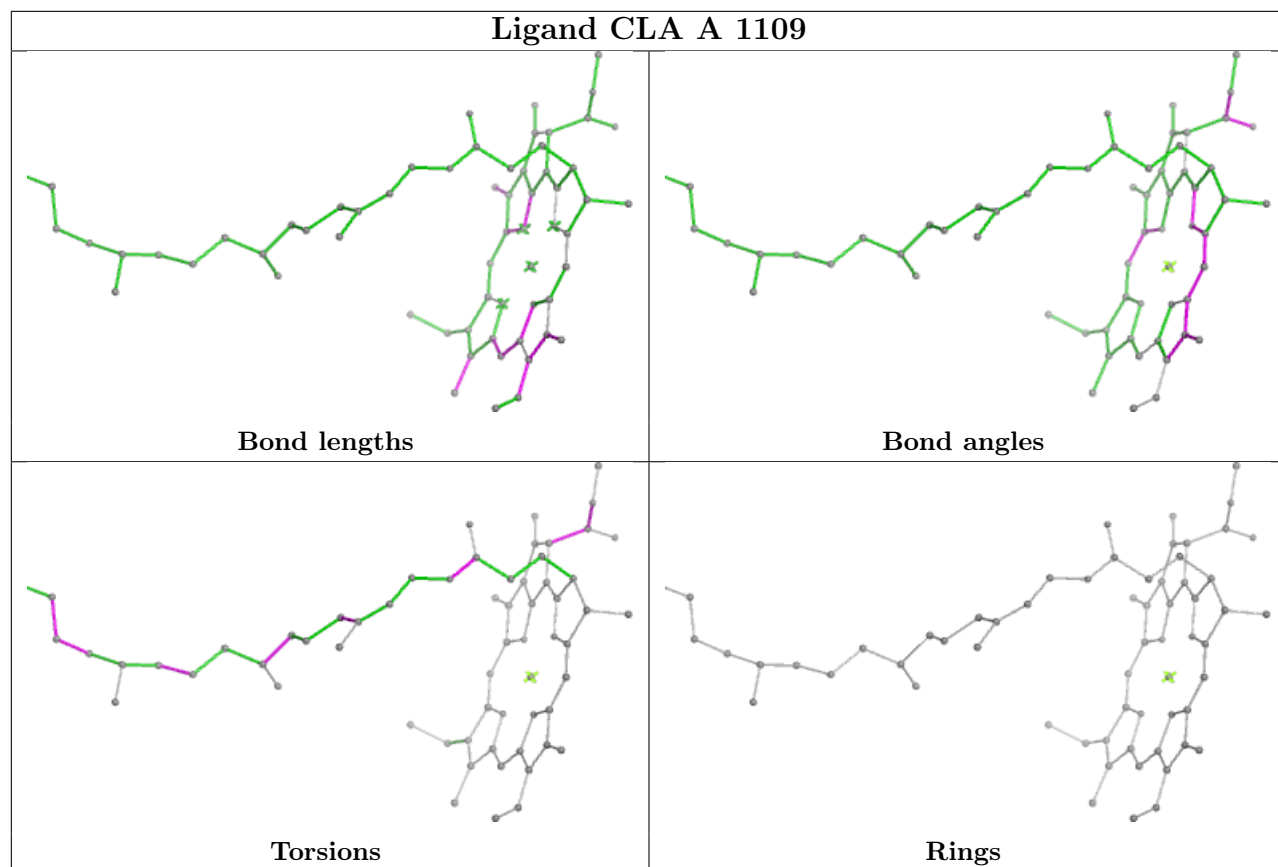


Ligand CLA A 1123

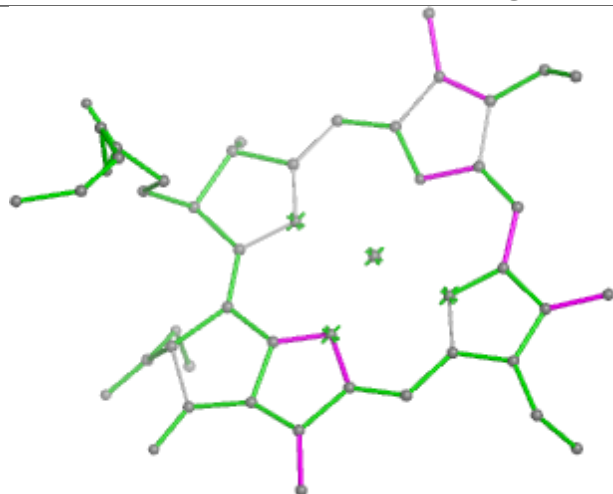


Ligand CLA A 1108

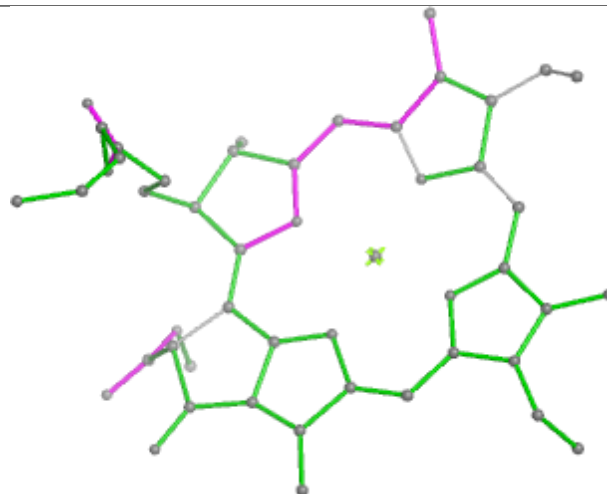




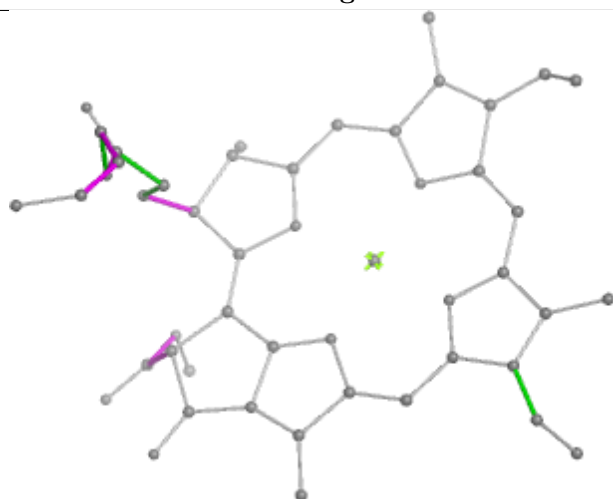
Ligand CLA B 1236



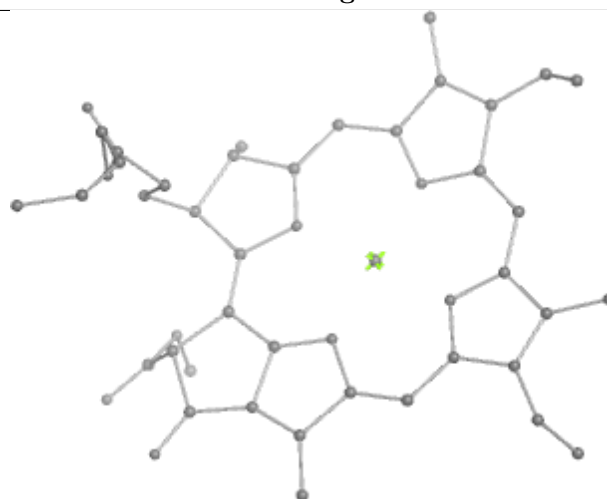
Bond lengths



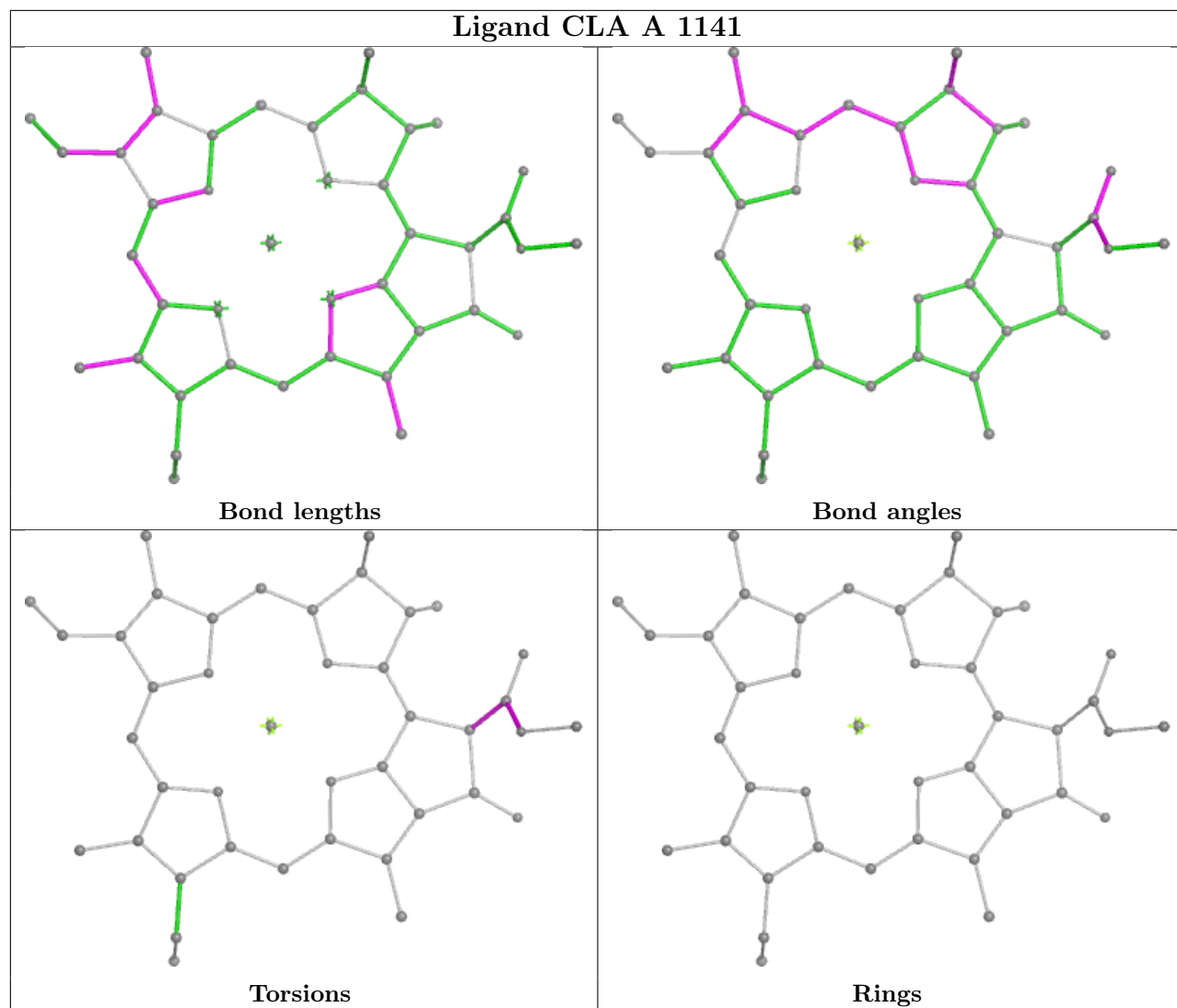
Bond angles

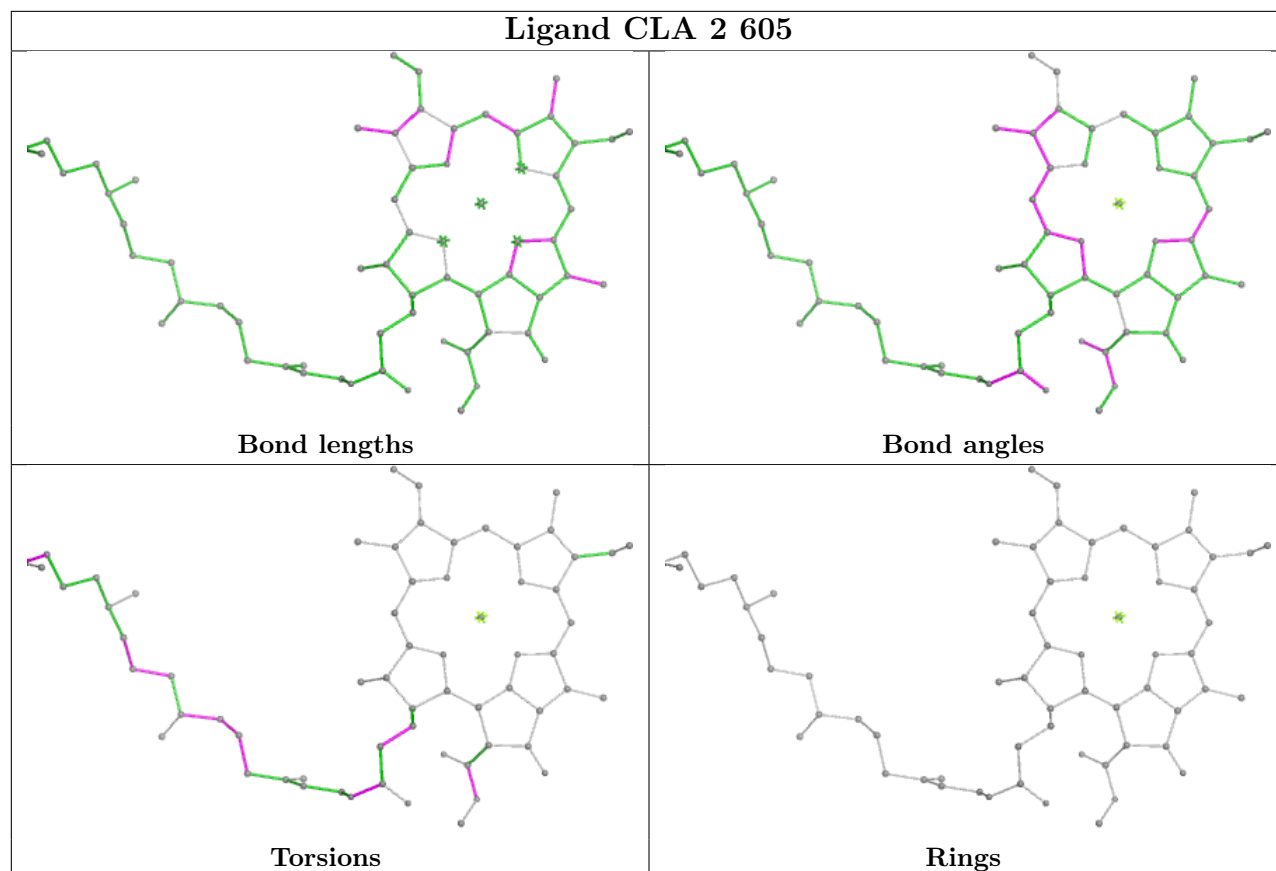
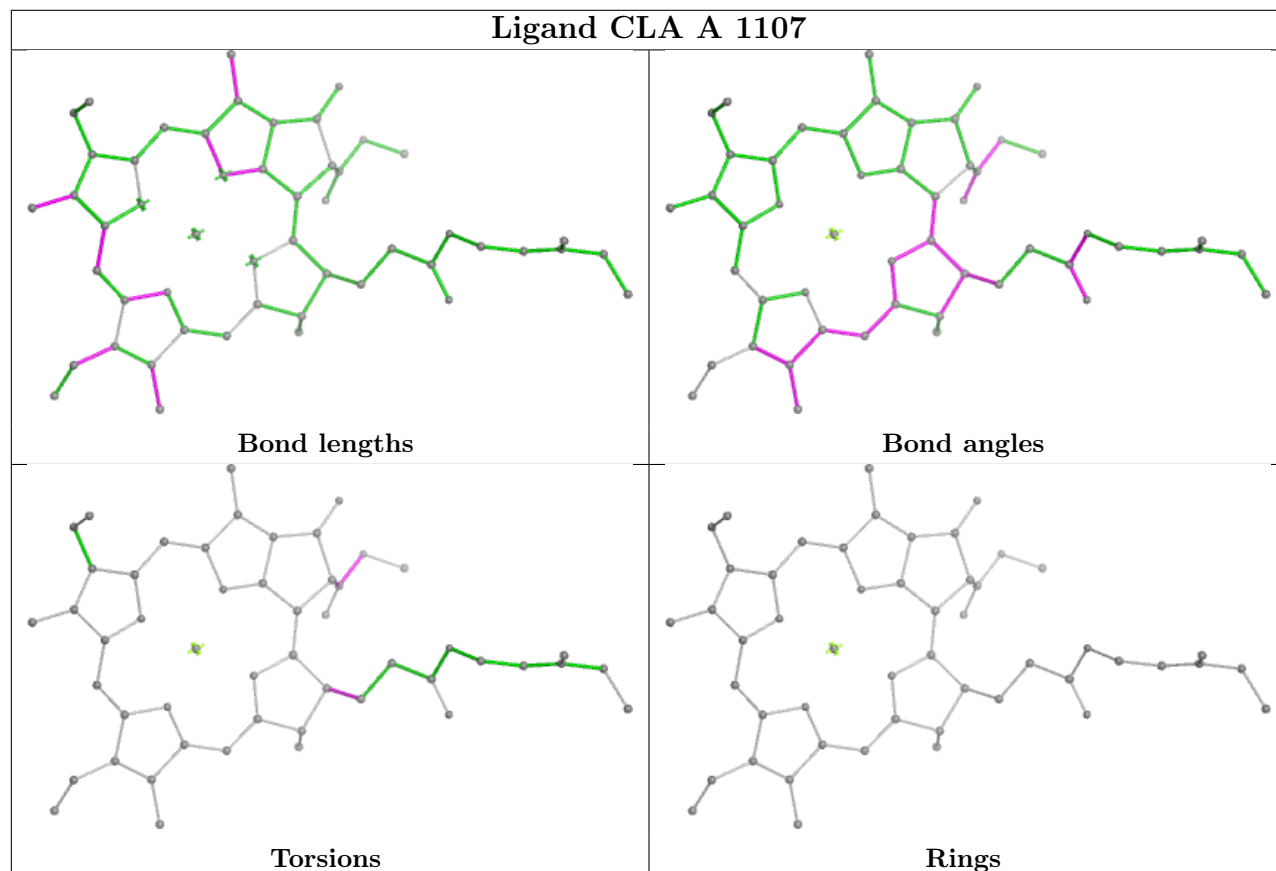


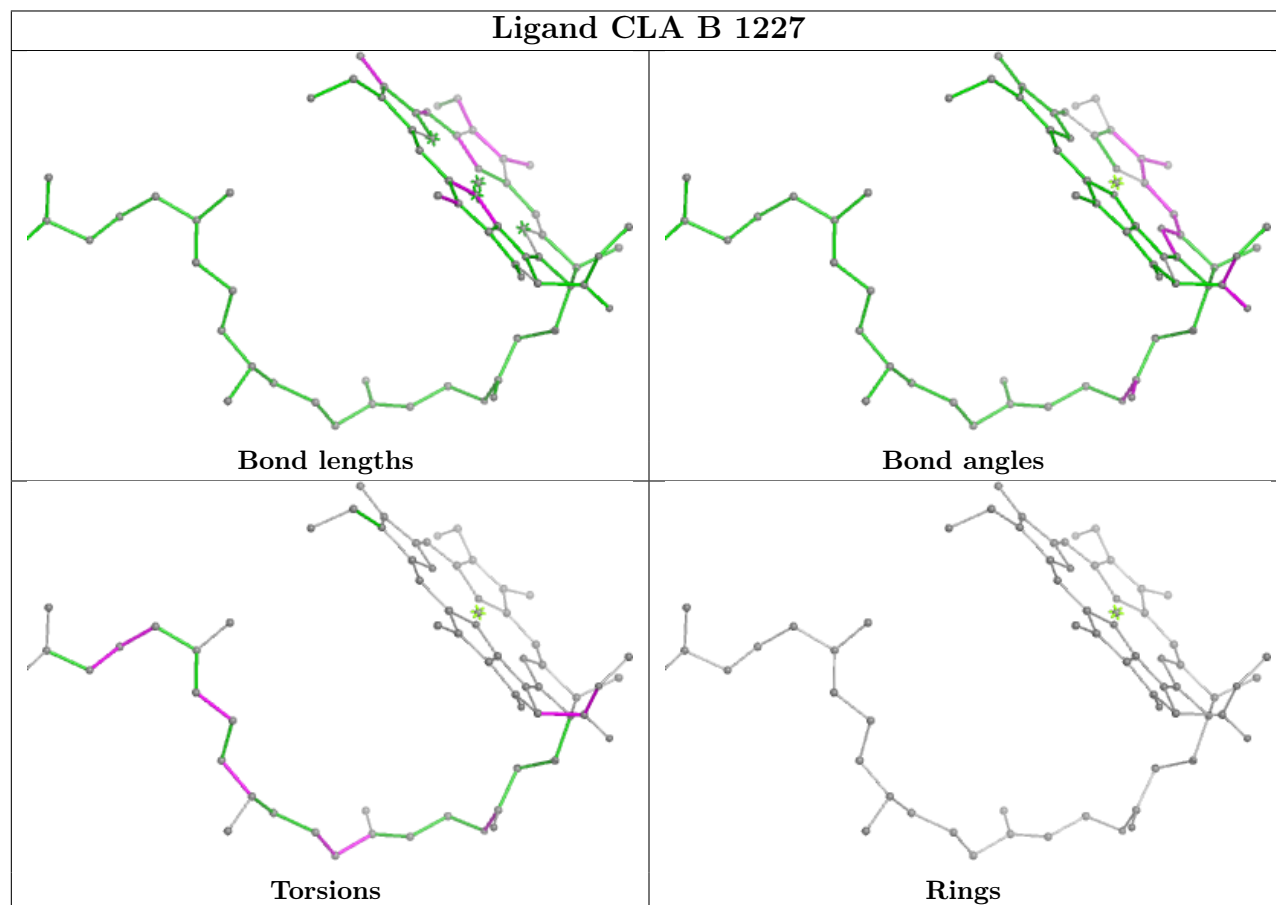
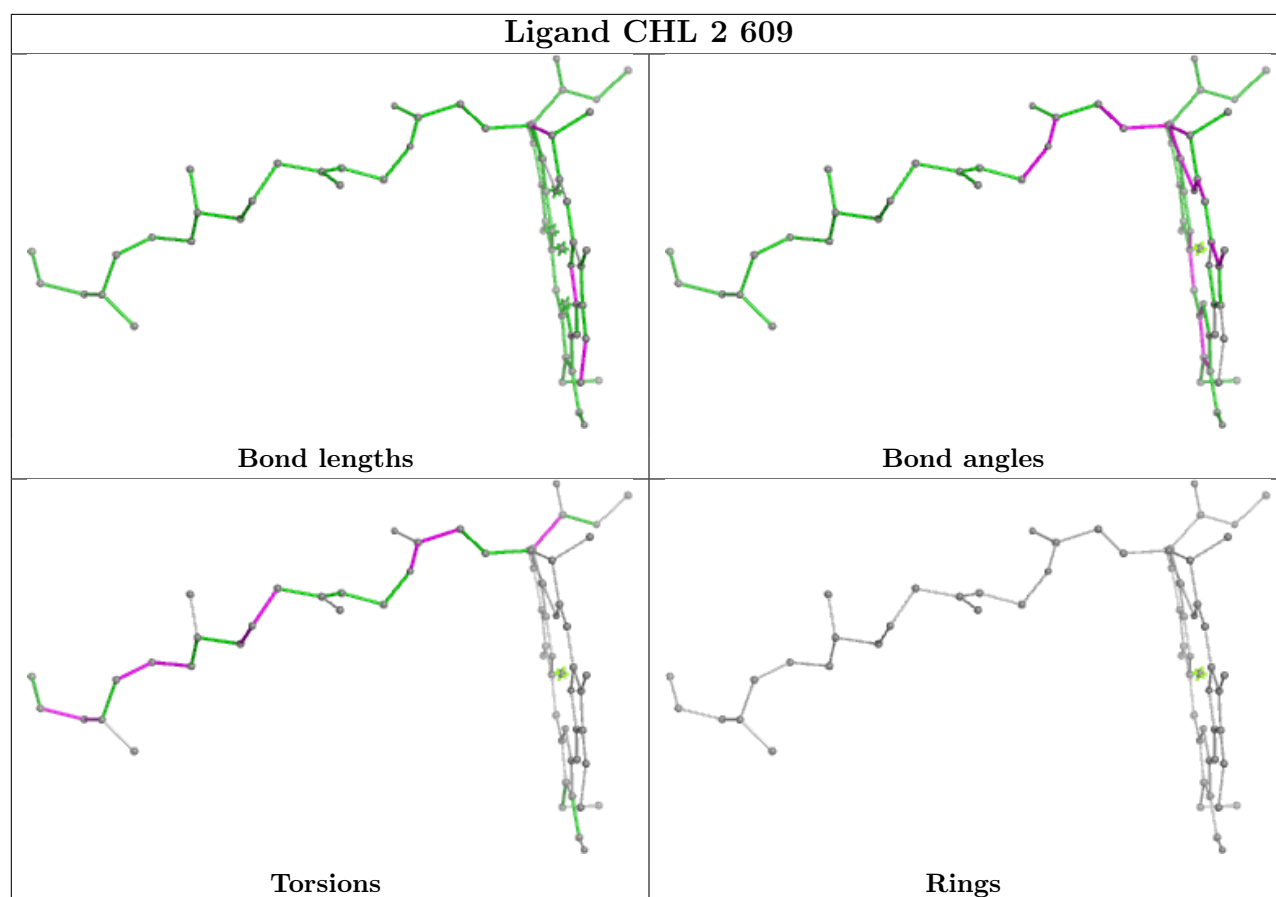
Torsions

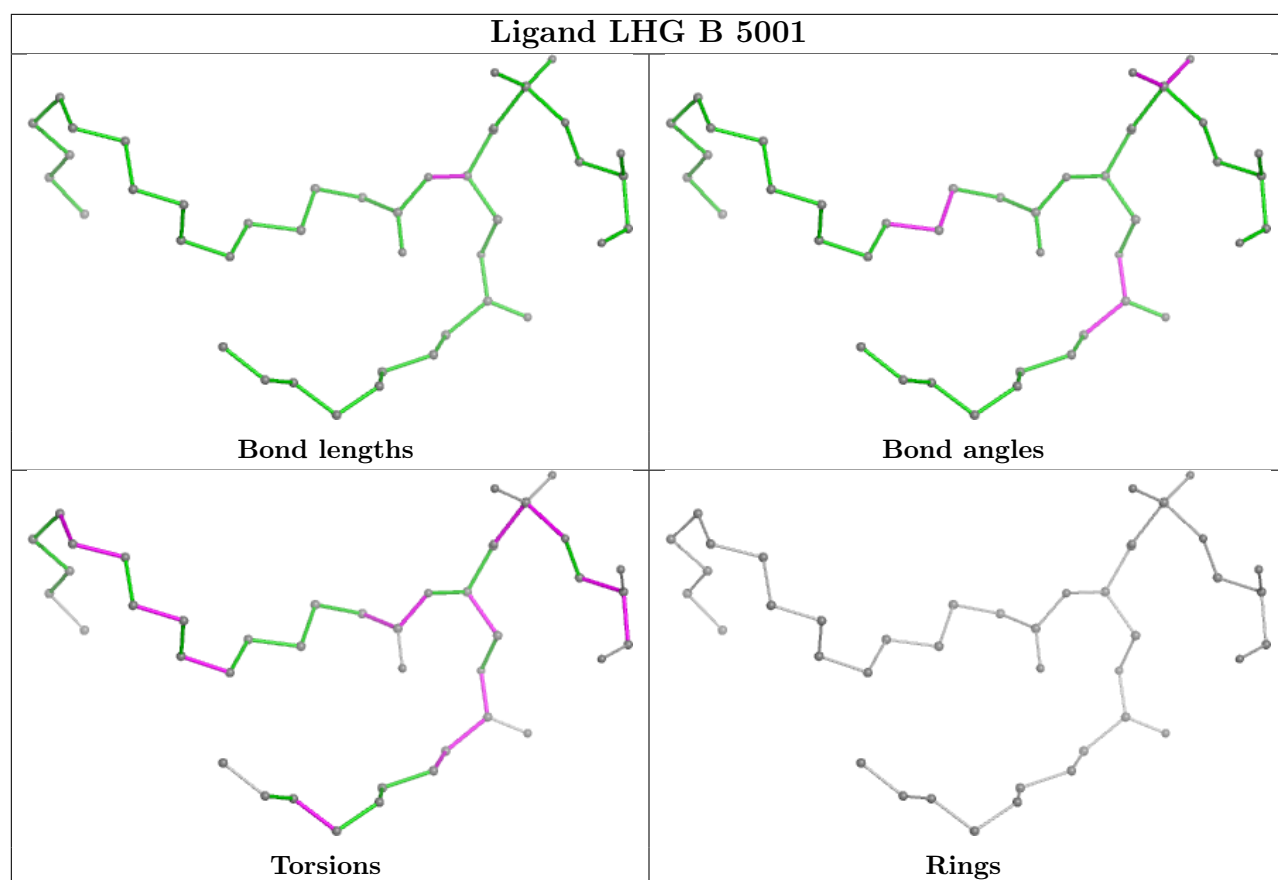


Rings

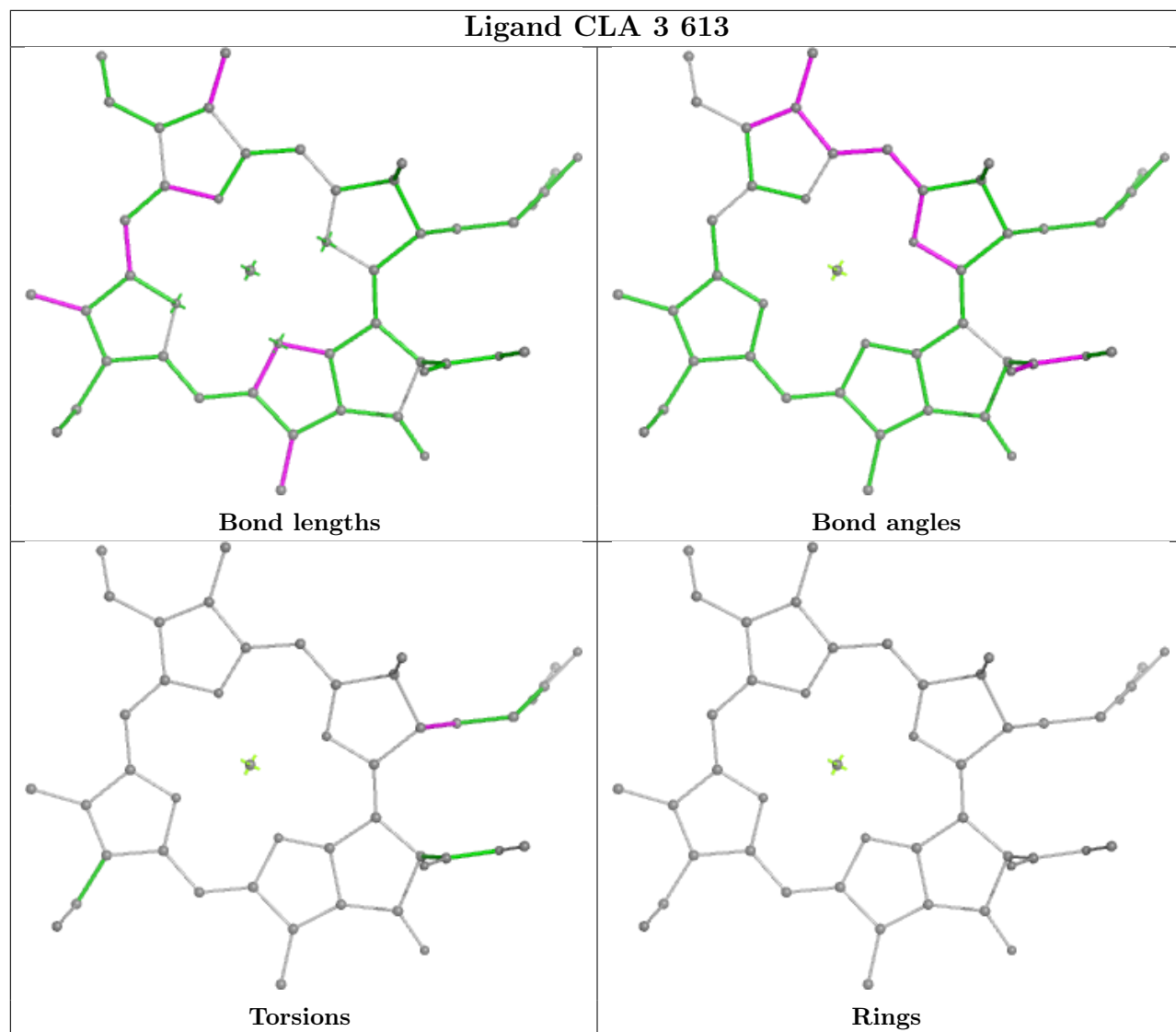


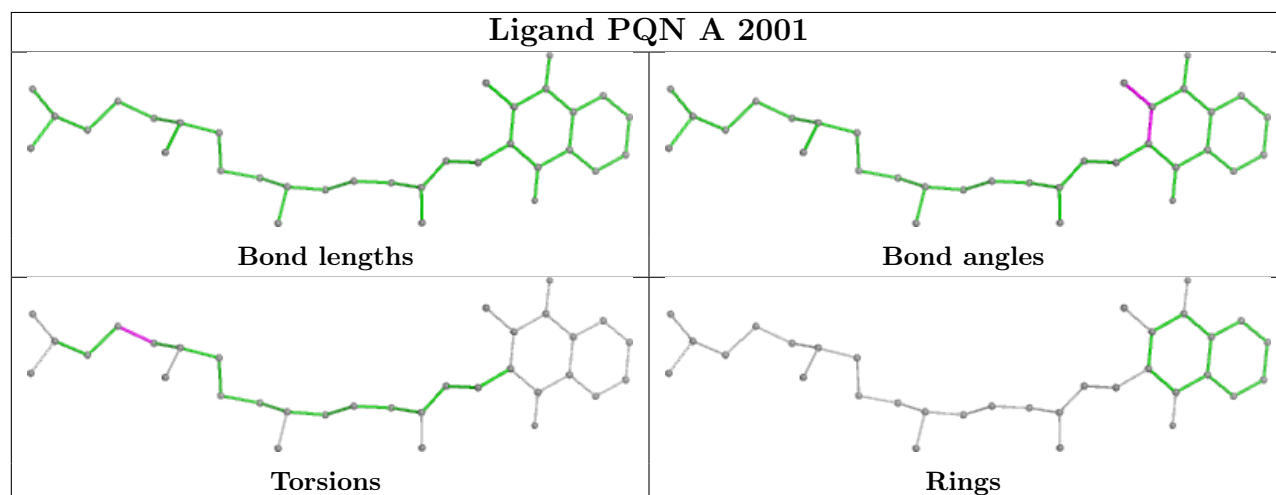
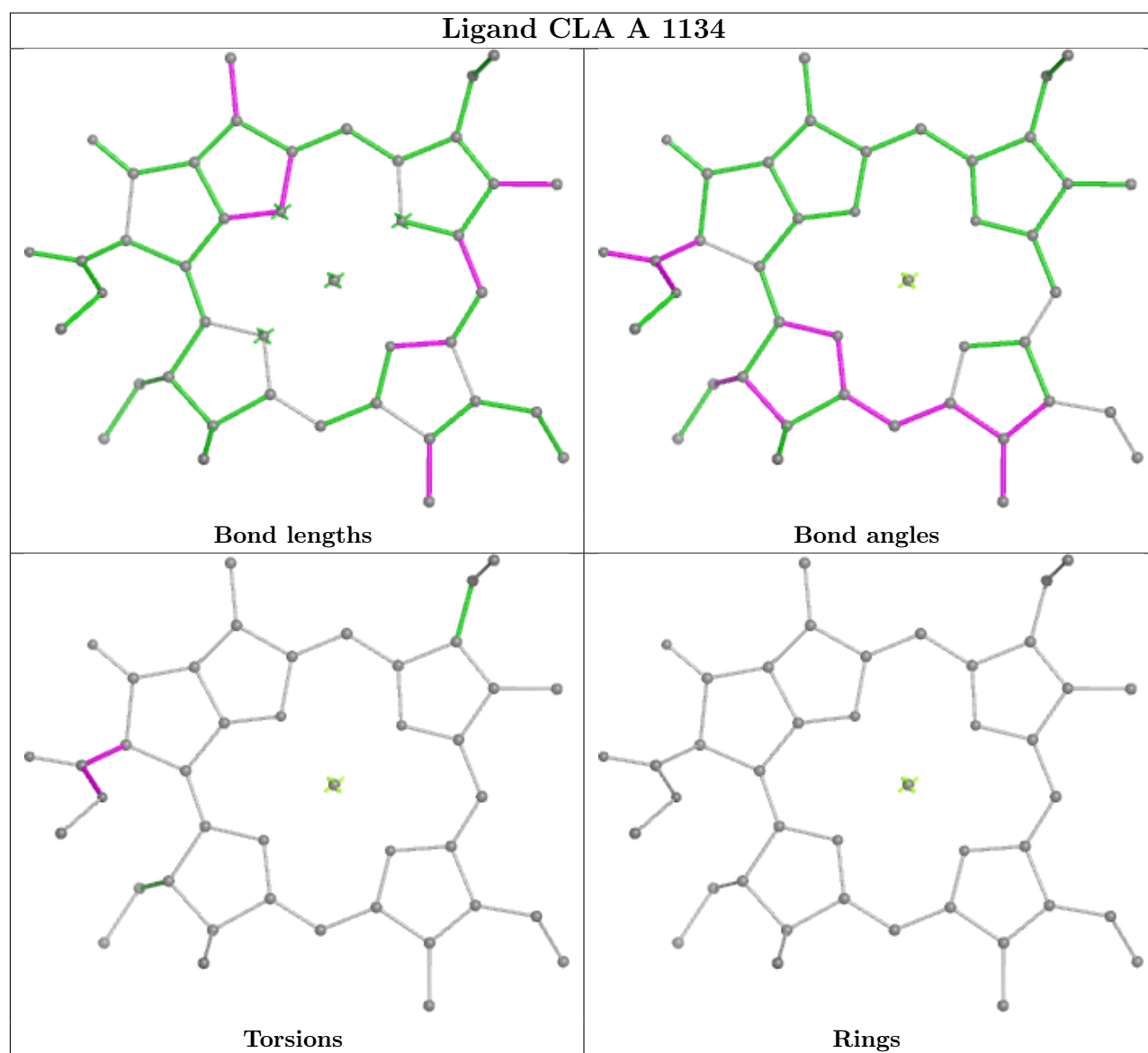
Ligand CLA 2 605**Ligand CLA A 1107**

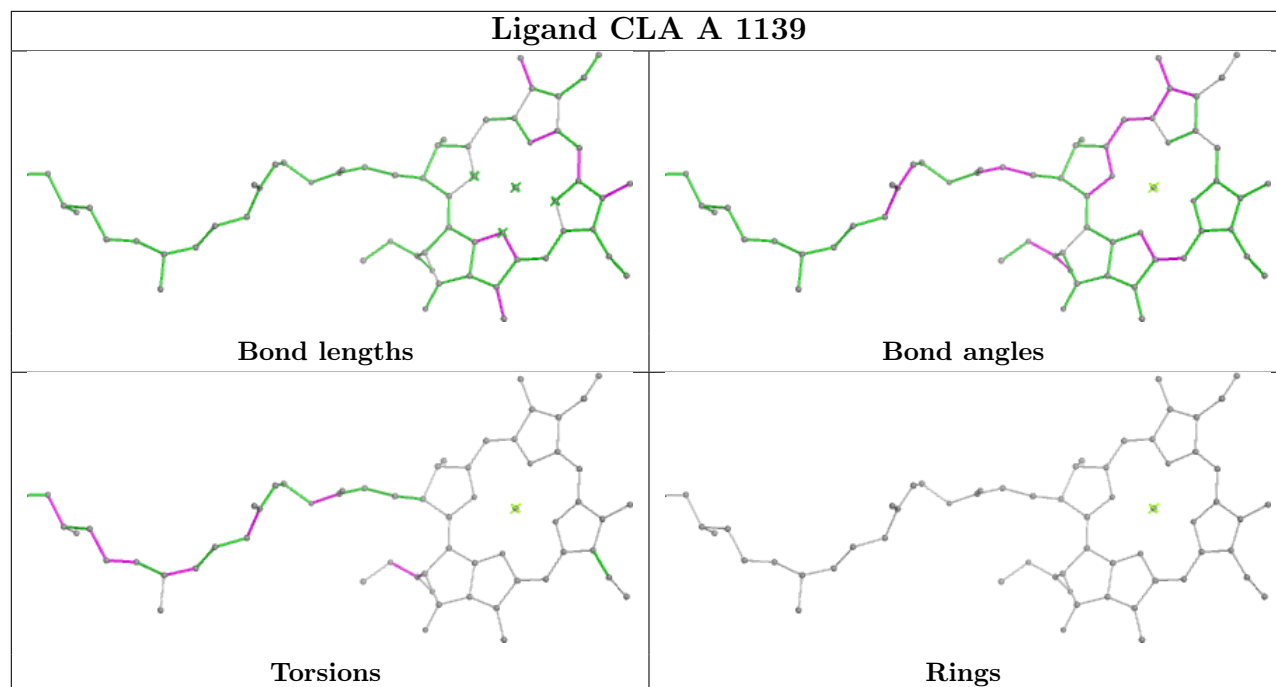
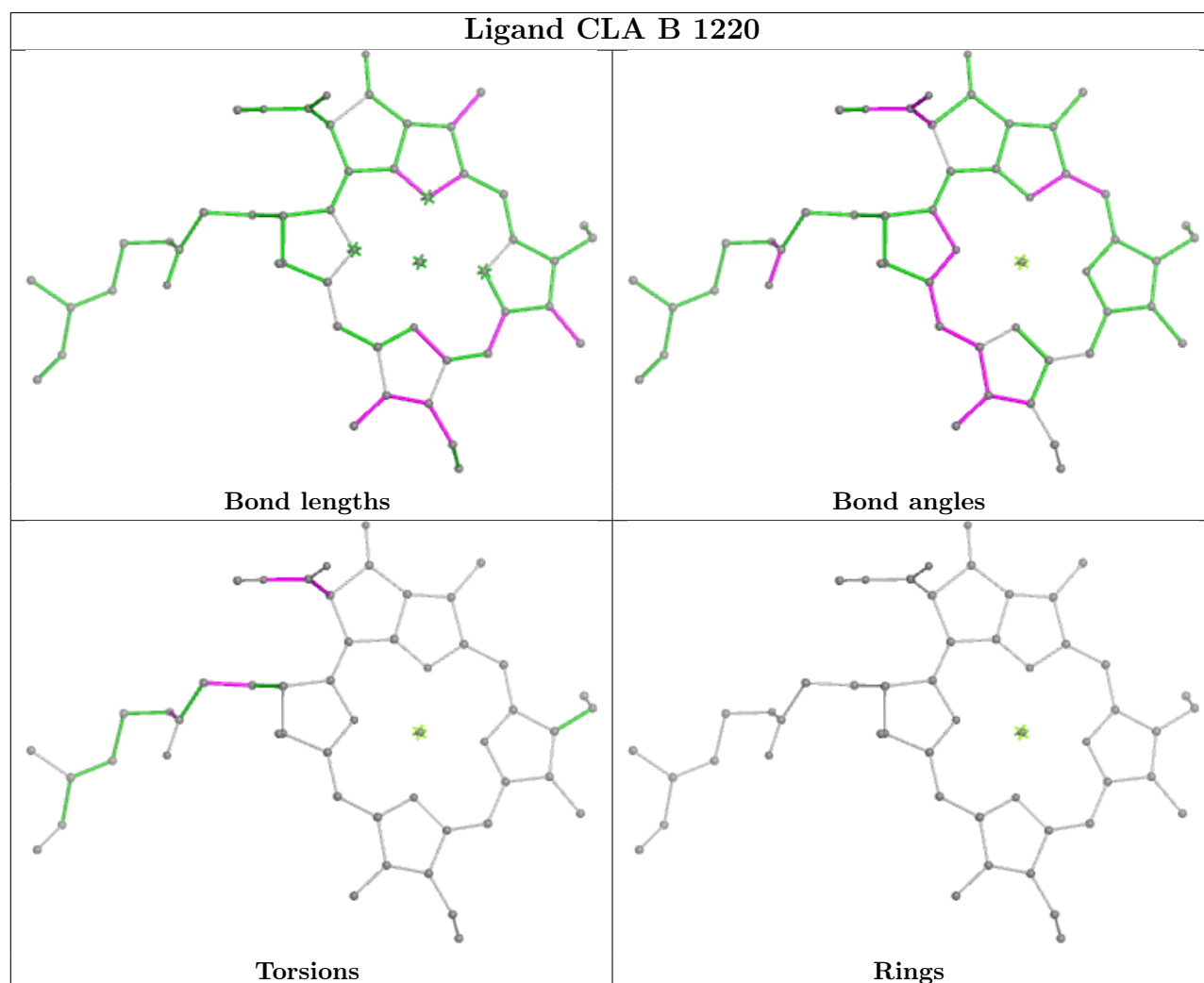


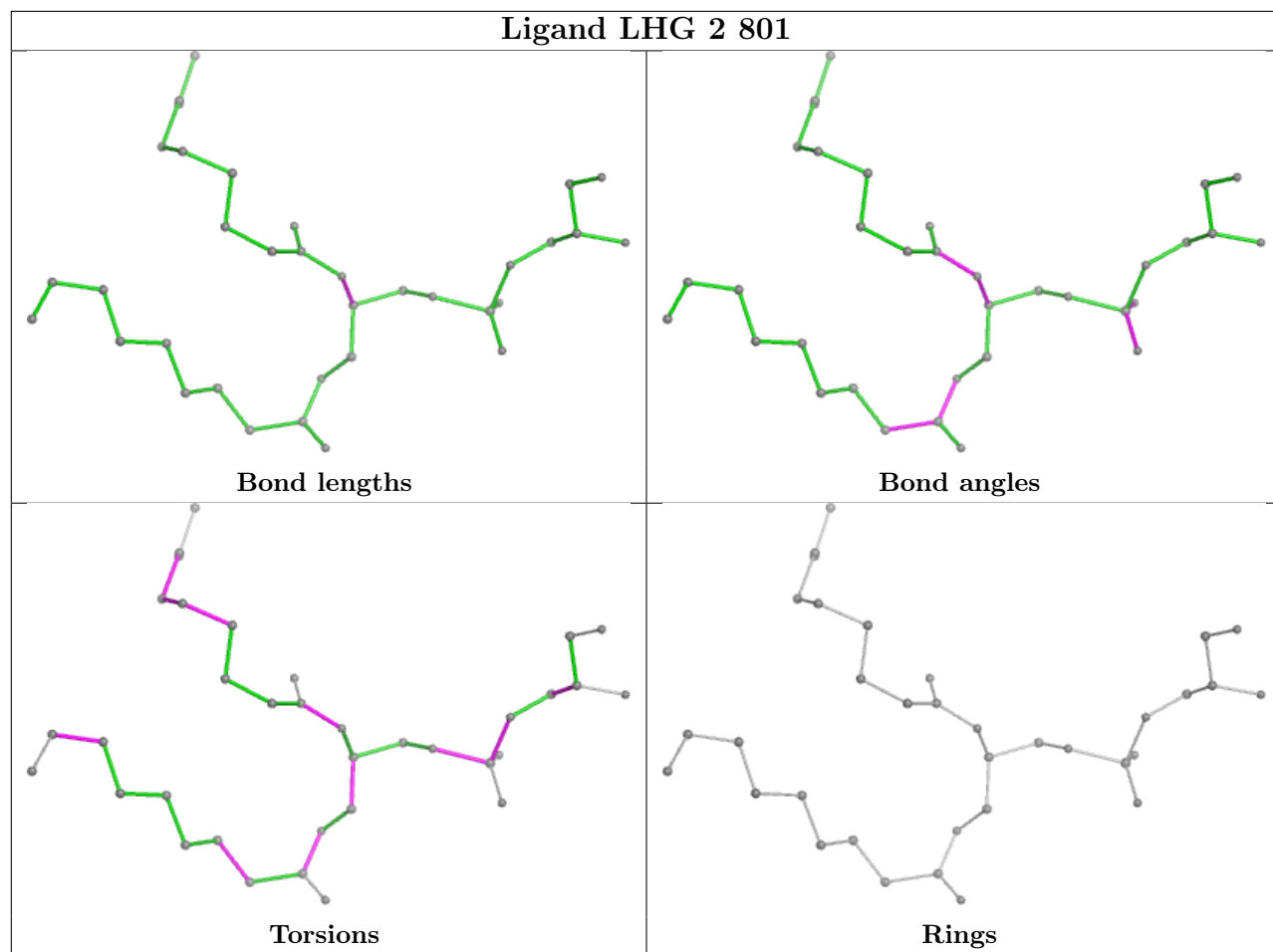


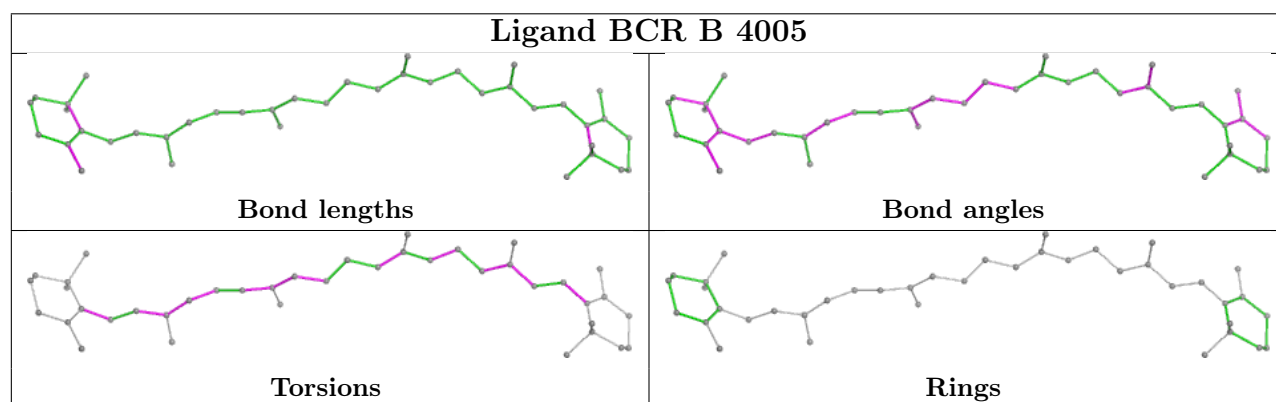
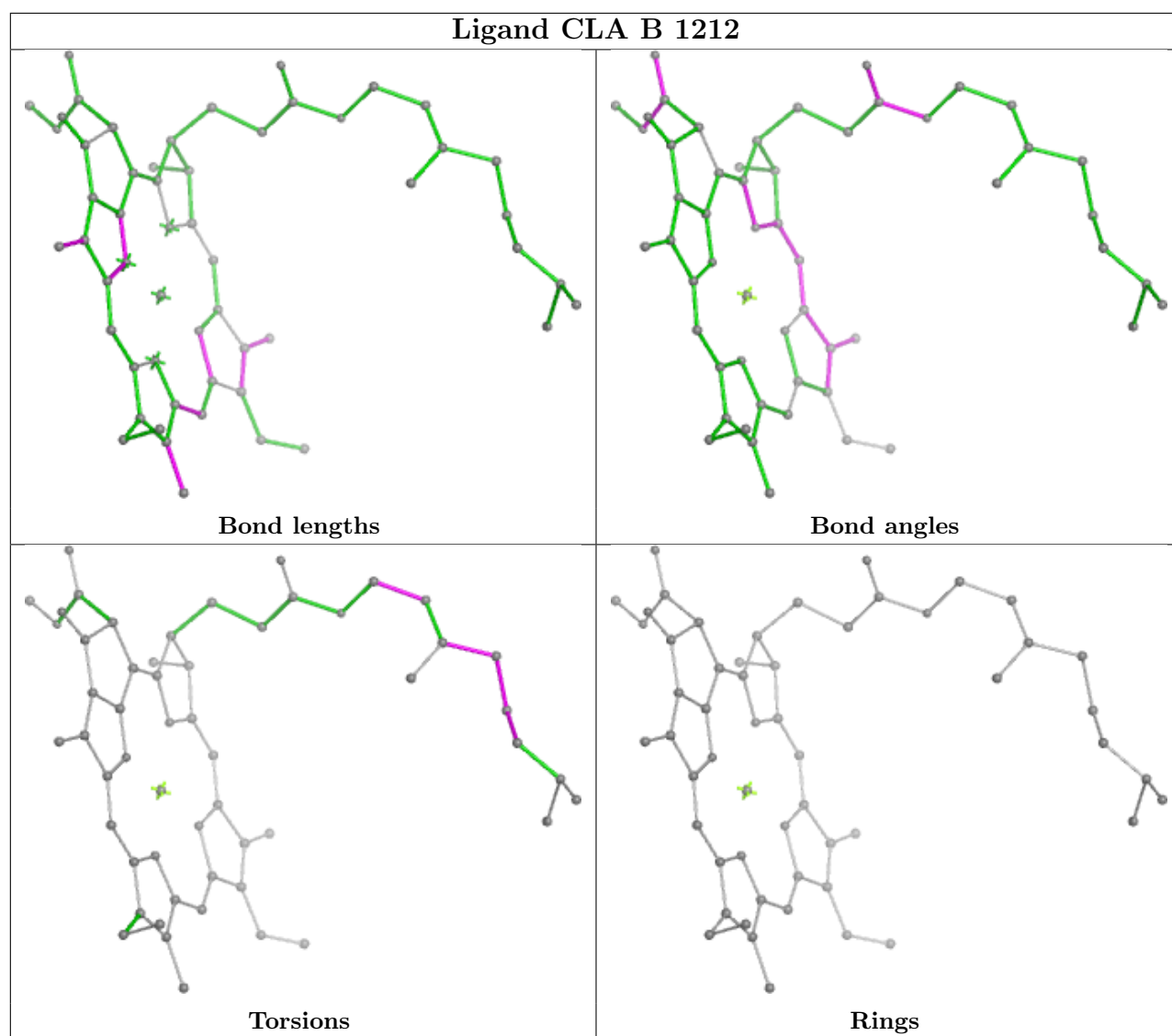
Ligand CLA 3 613



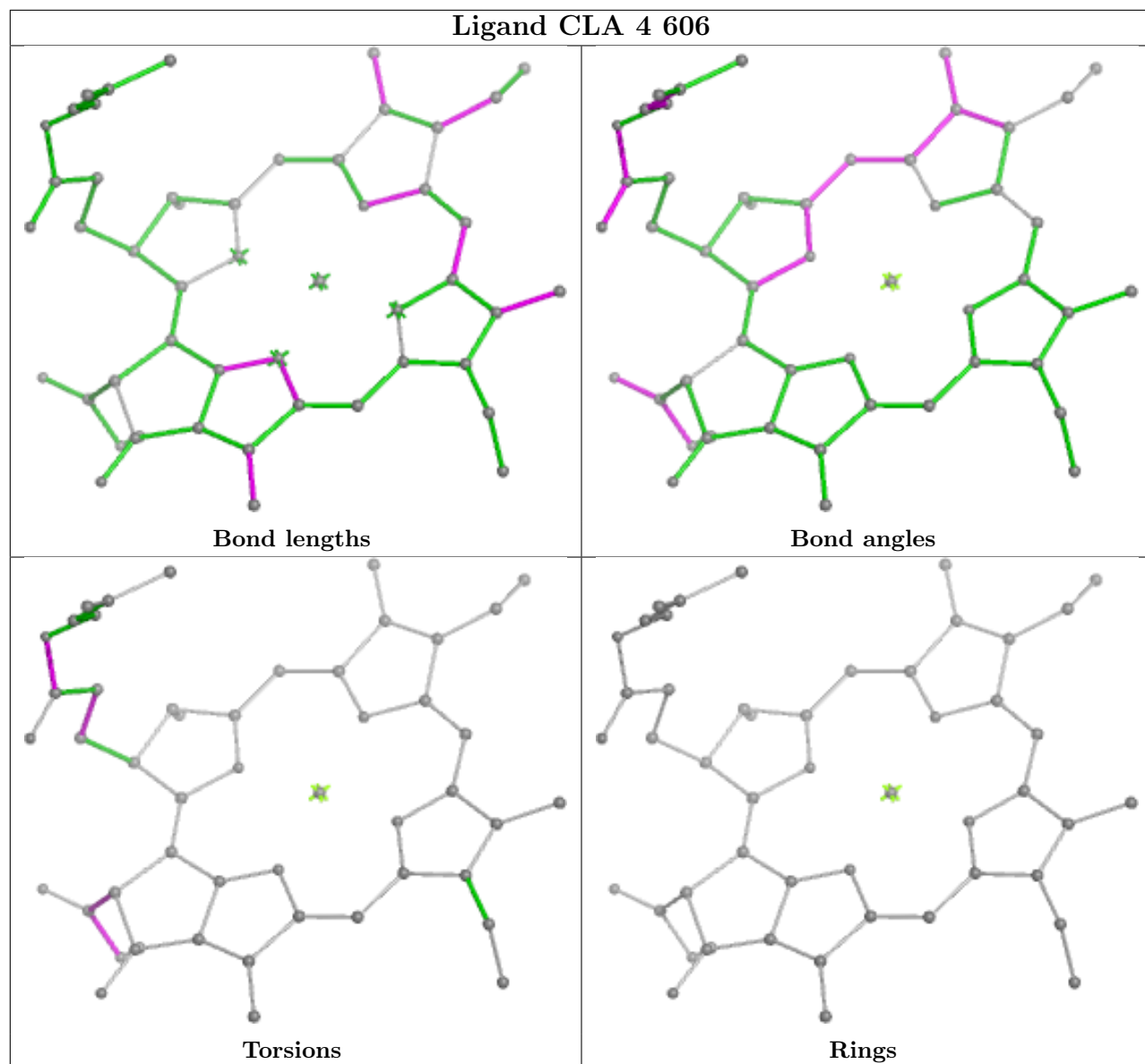


Ligand CLA A 1139**Ligand CLA B 1220**

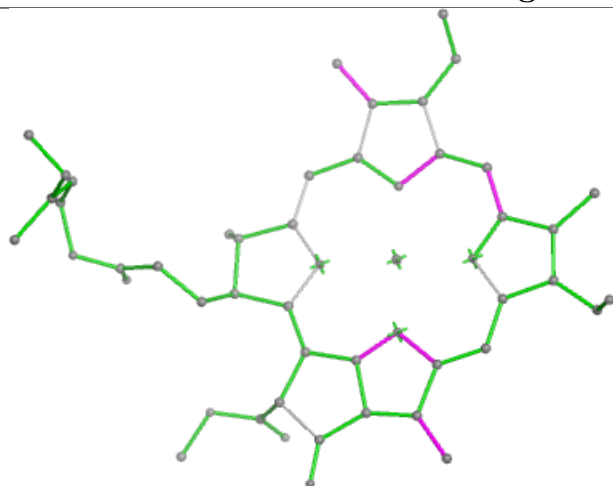




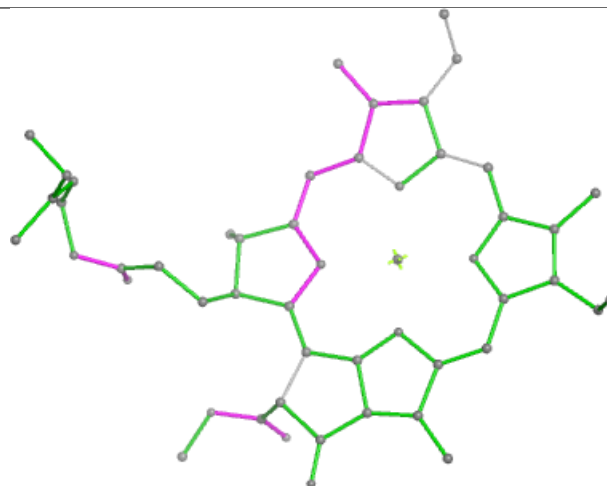
Ligand CLA 4 606



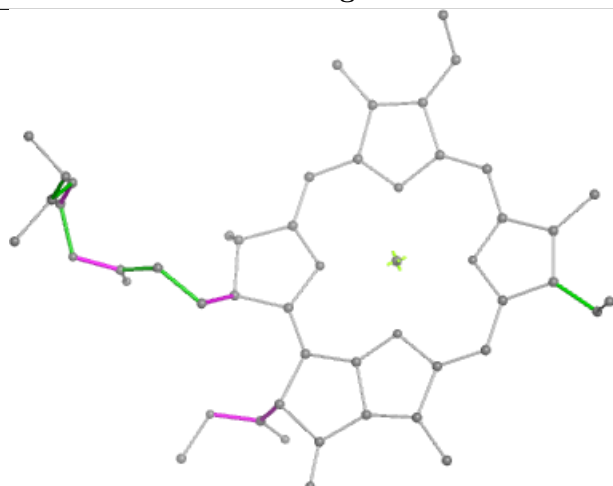
Ligand CLA 4 616



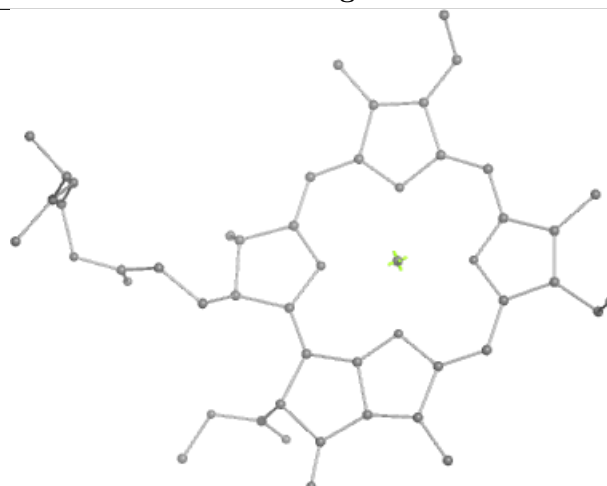
Bond lengths



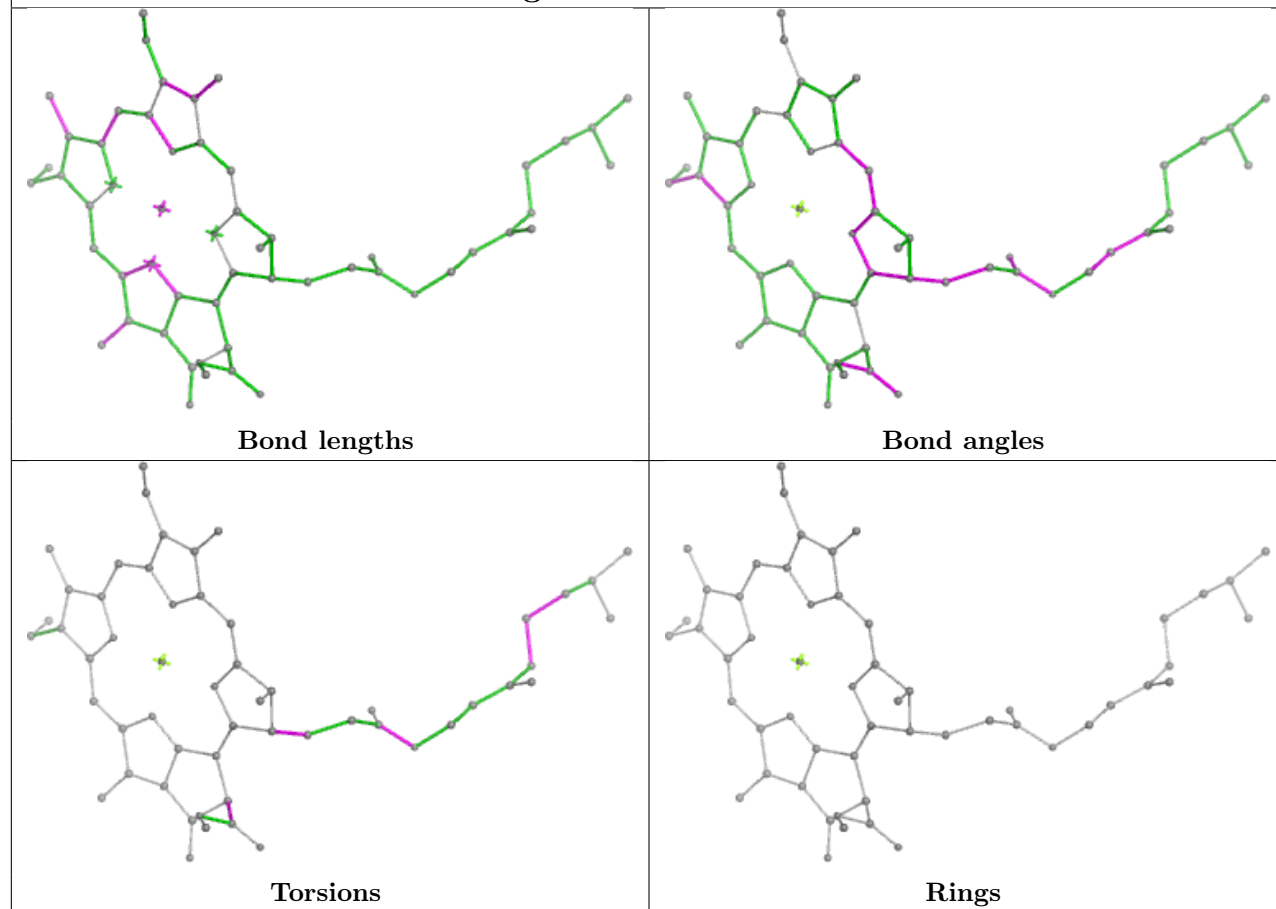
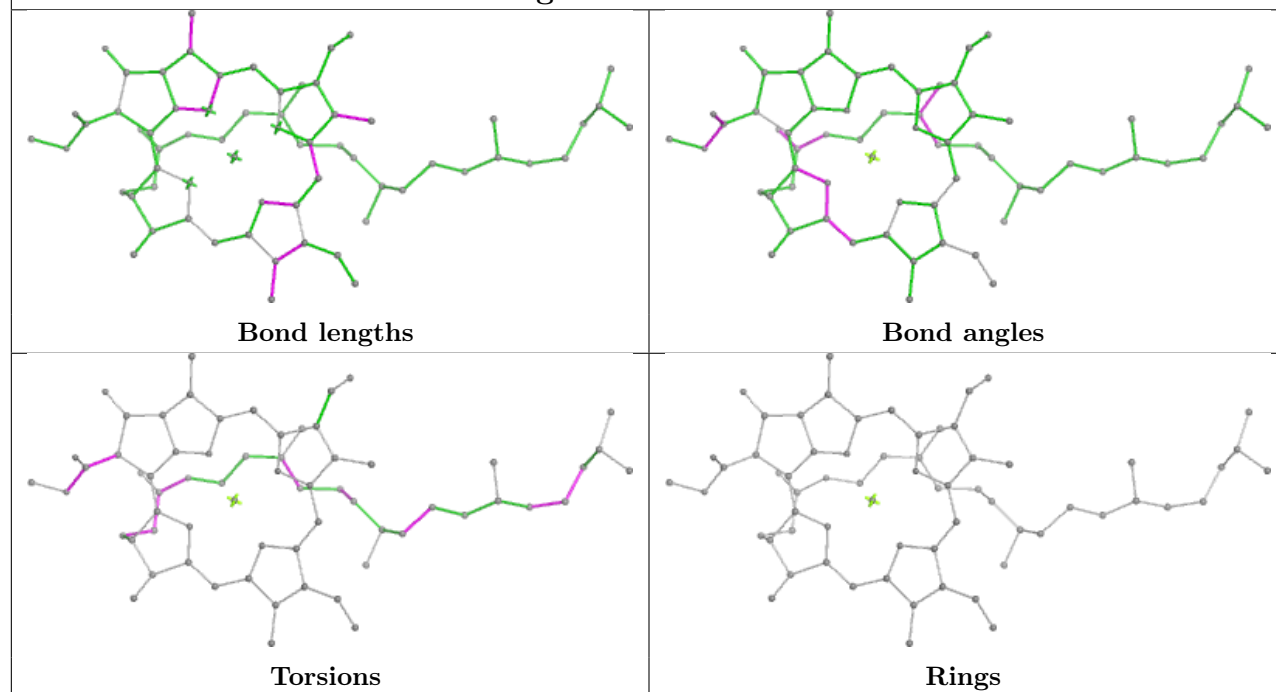
Bond angles



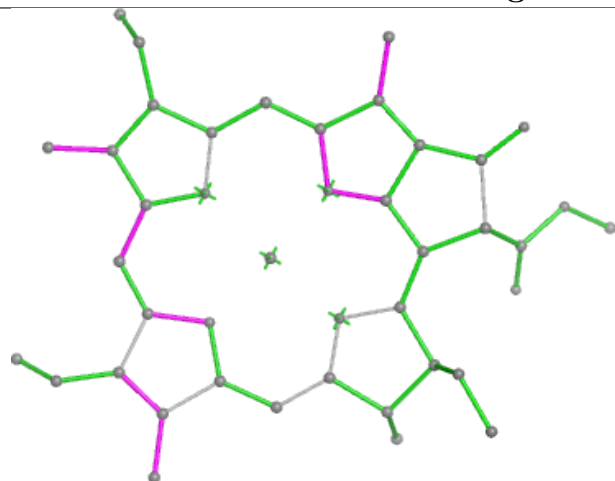
Torsions



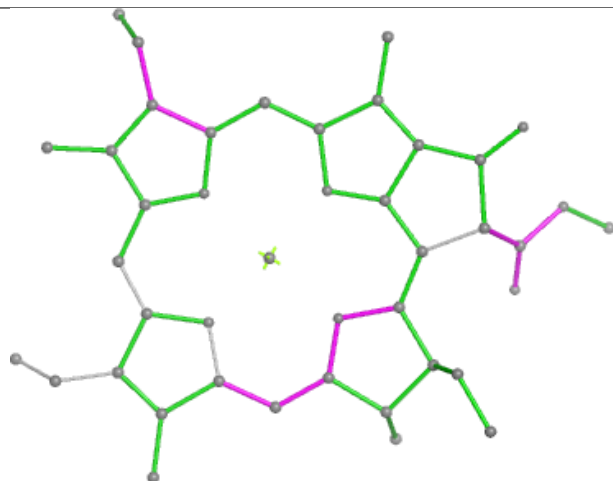
Rings

Ligand CLA B 1230**Ligand CLA 3 603**

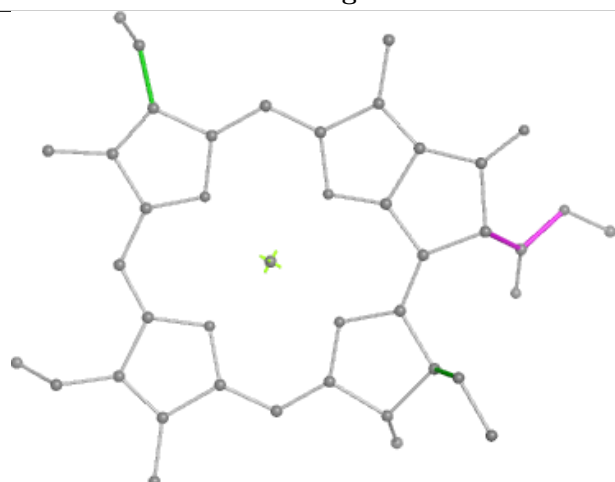
Ligand CLA B 1239



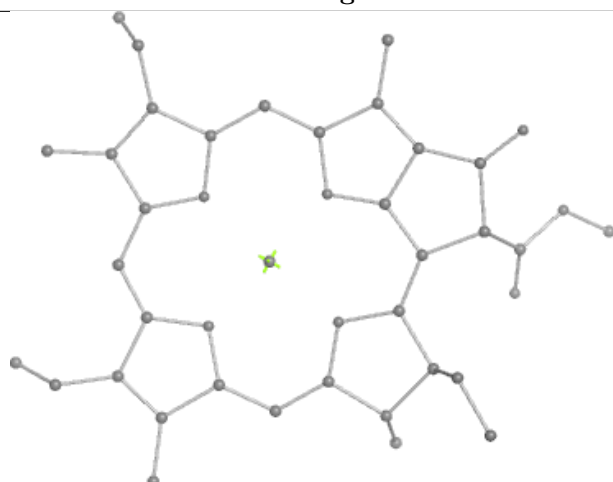
Bond lengths



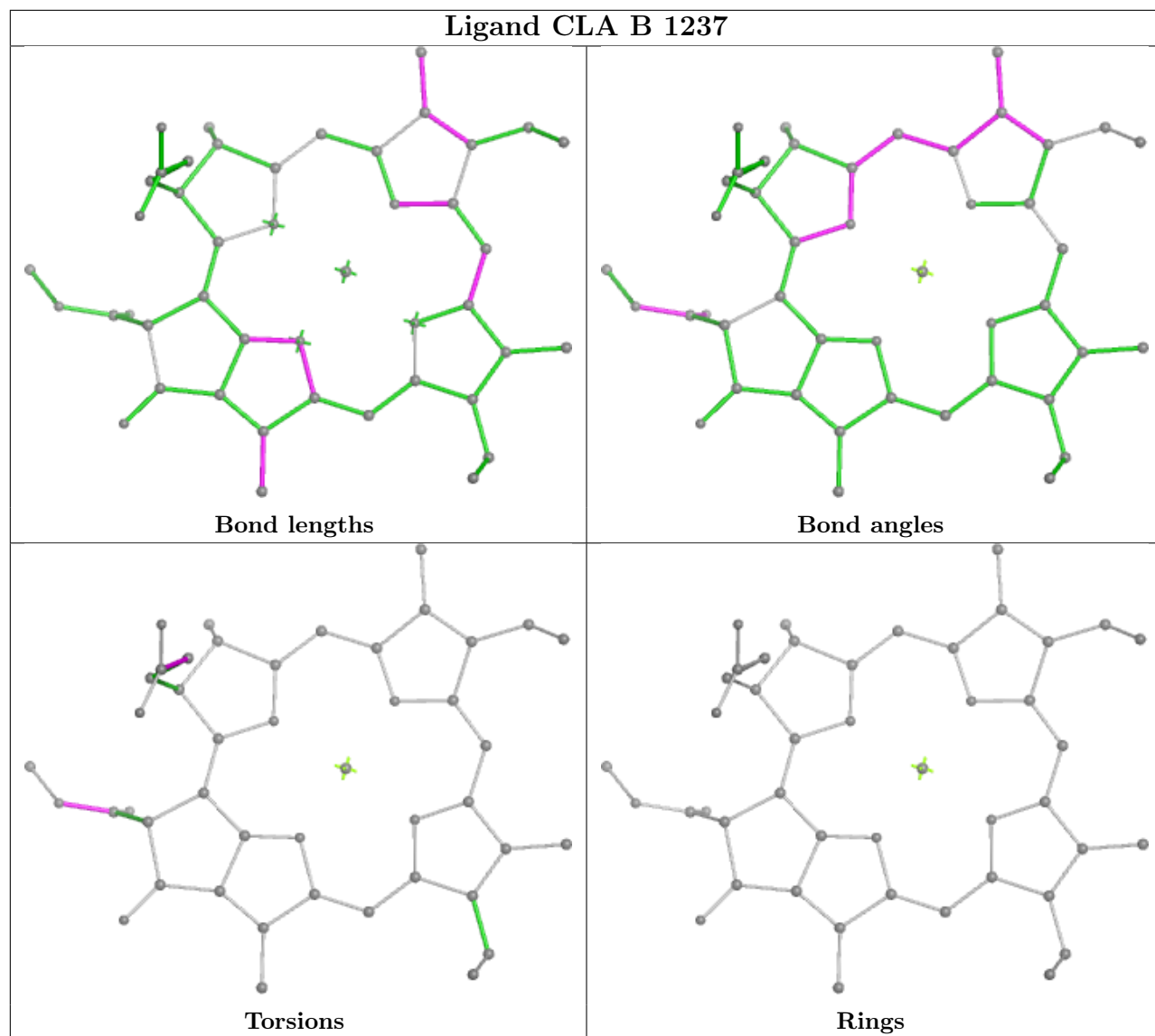
Bond angles



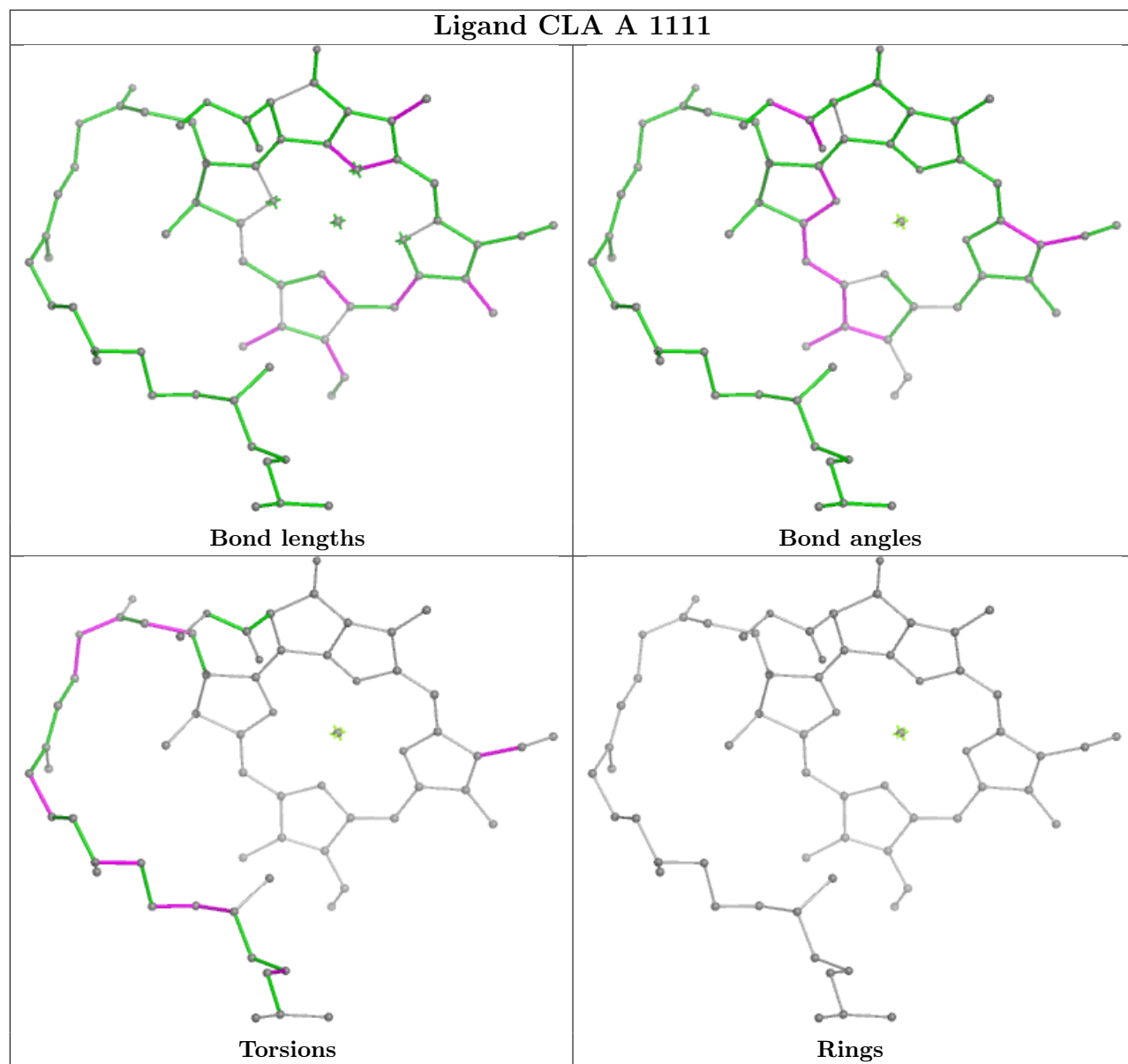
Torsions

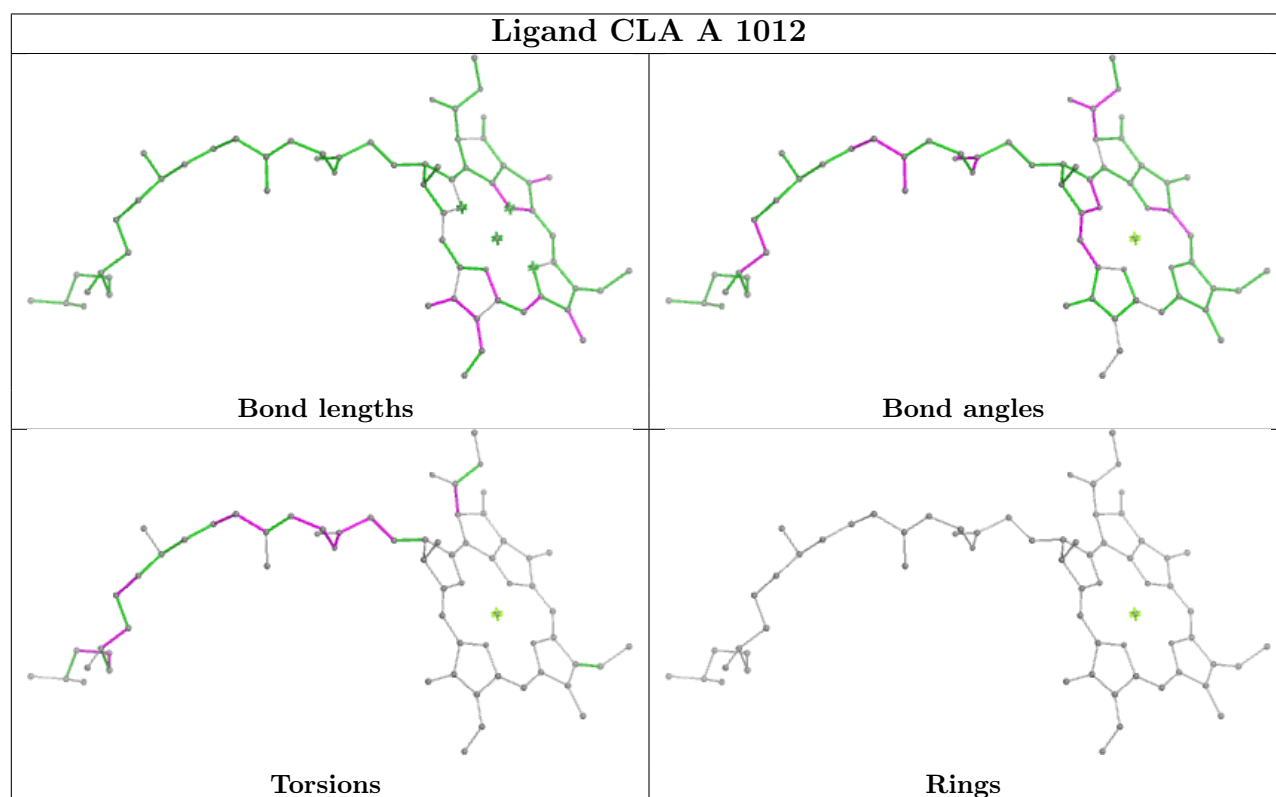
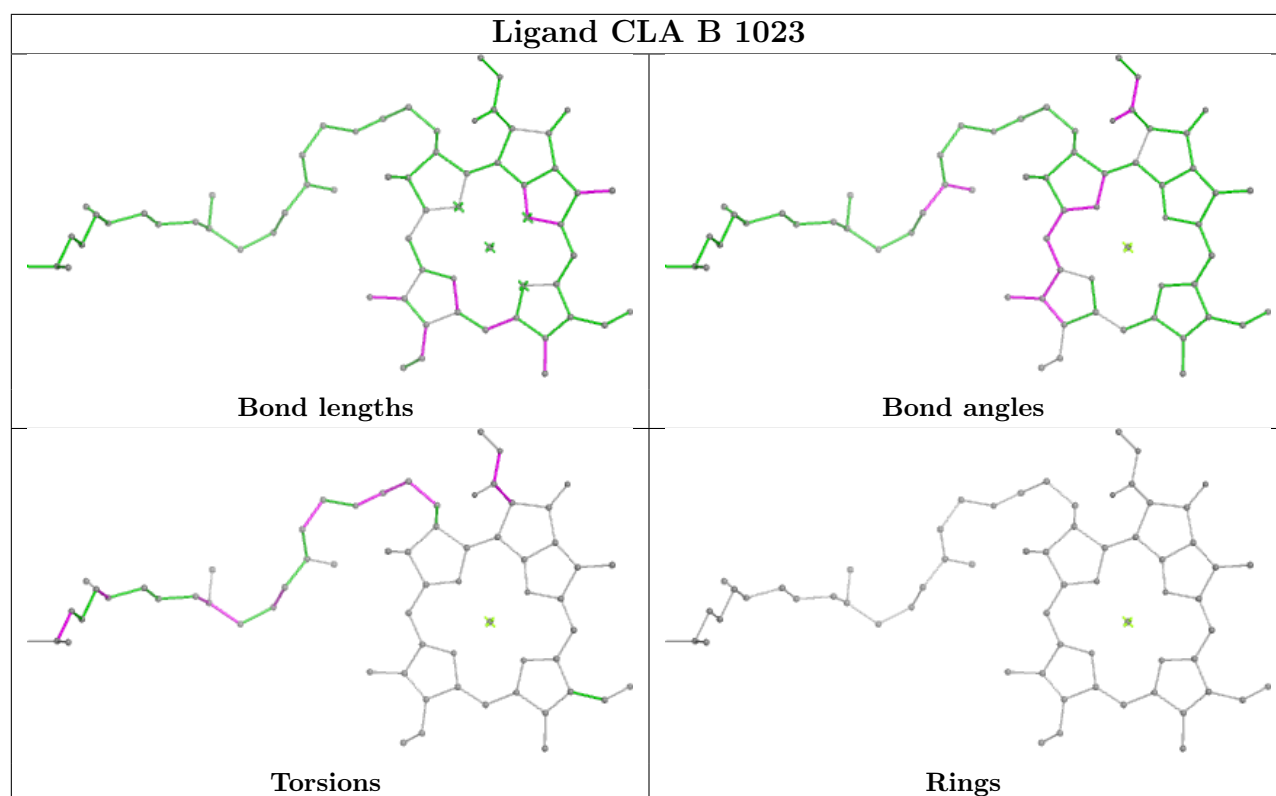


Rings

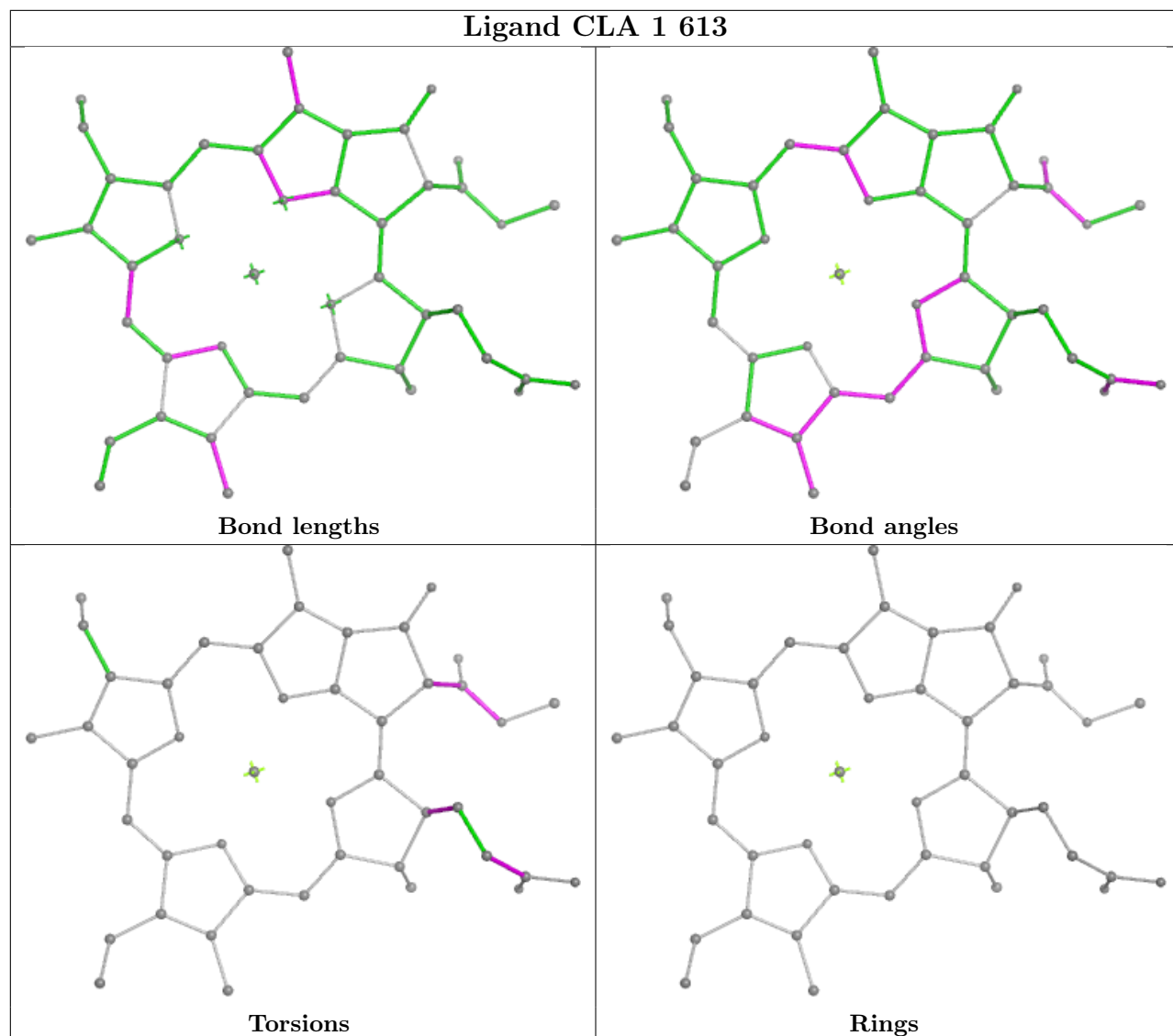


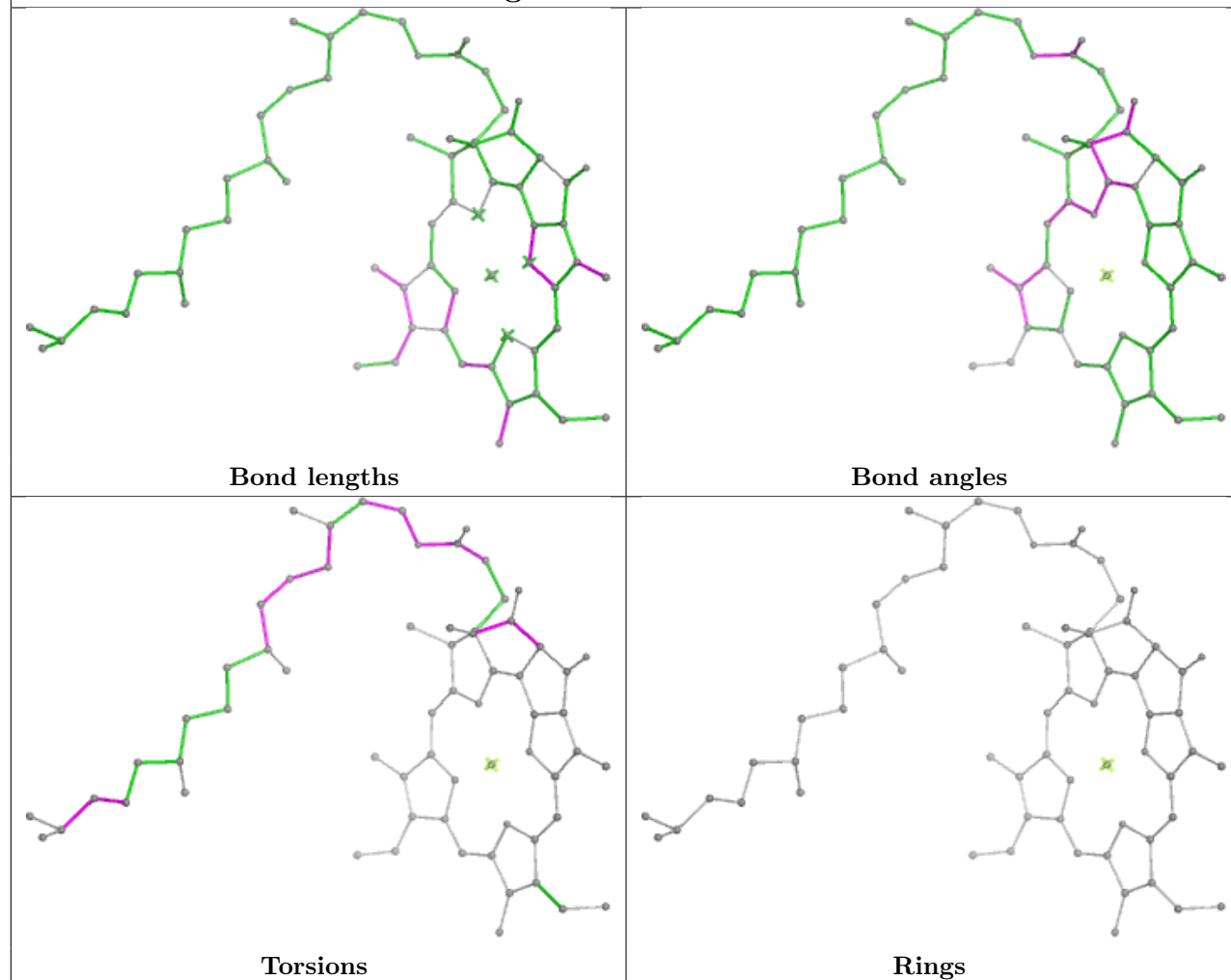
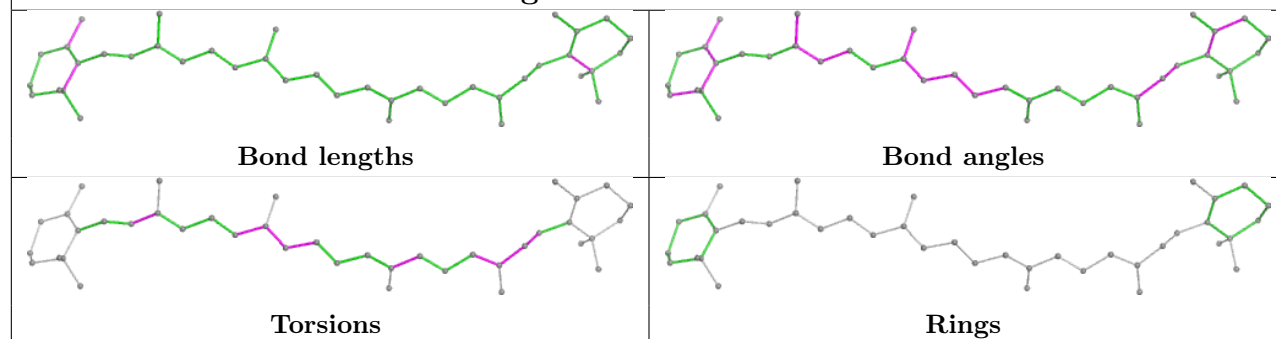
Ligand CLA A 1111

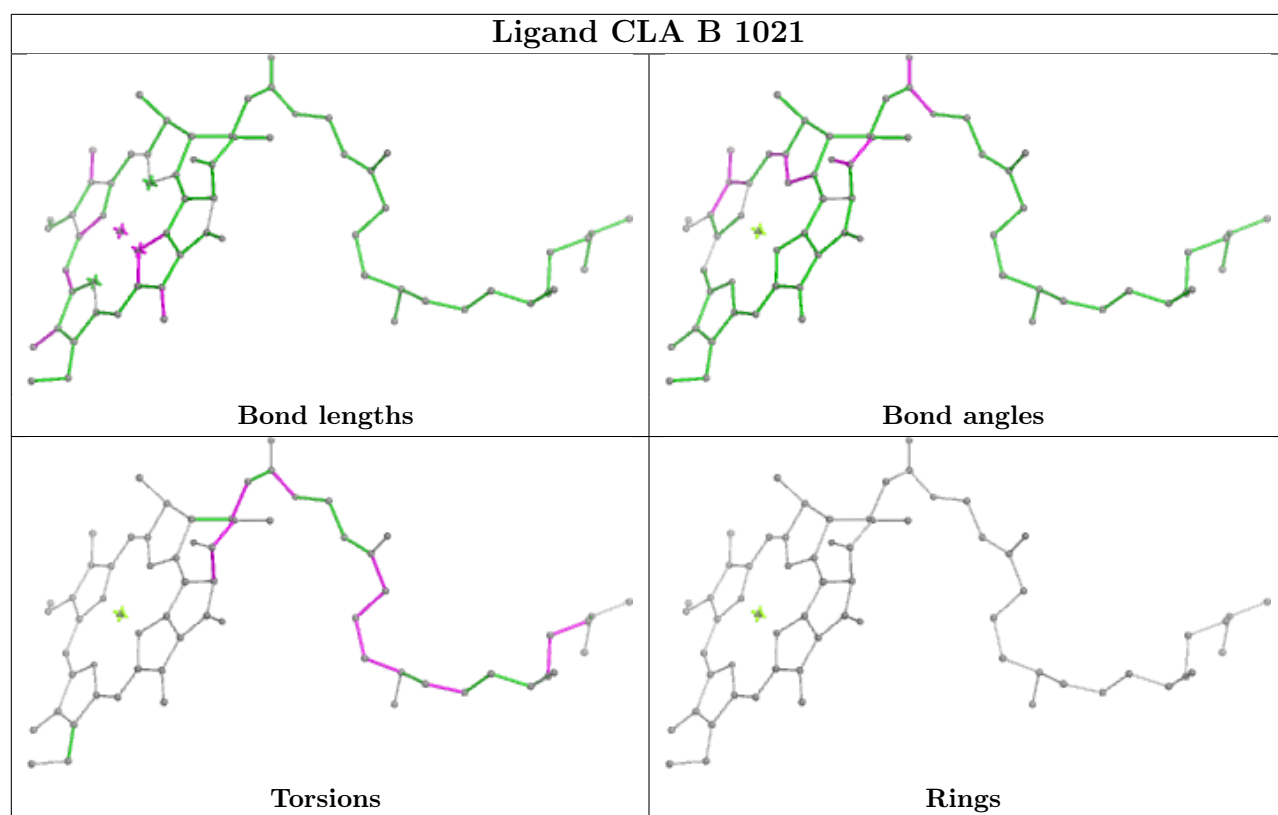




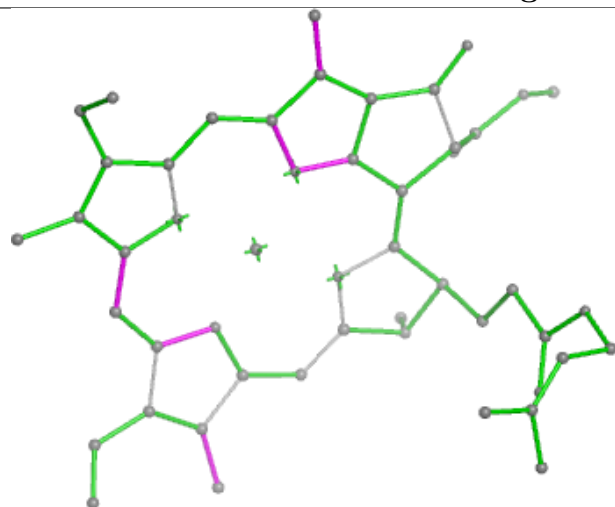
Ligand CLA 1 613



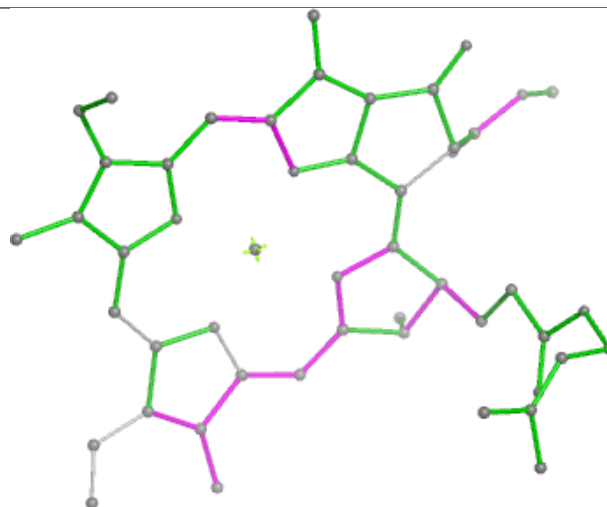
Ligand CLA B 1221**Ligand BCR A 4008**



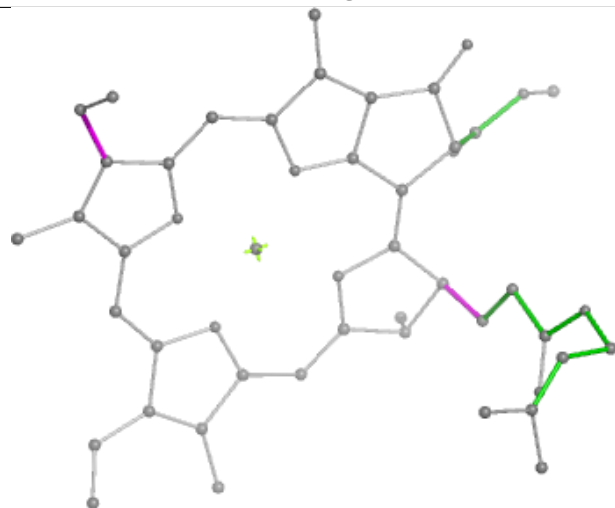
Ligand CLA 2 608



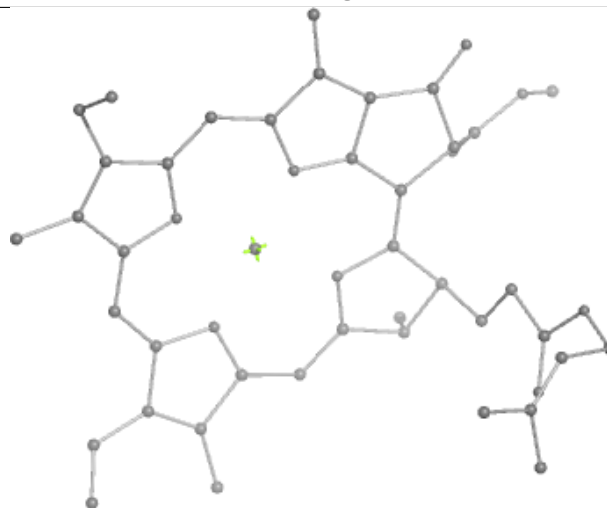
Bond lengths



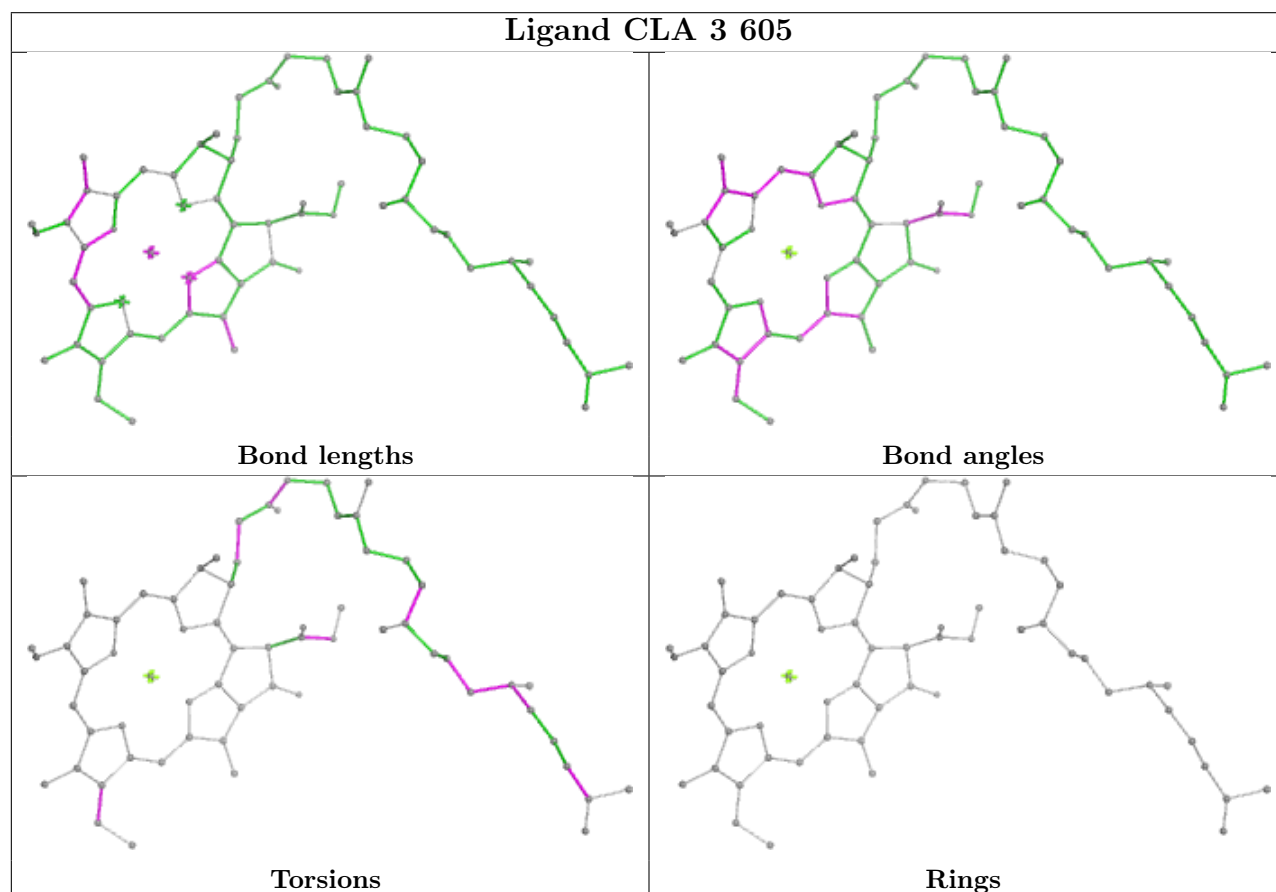
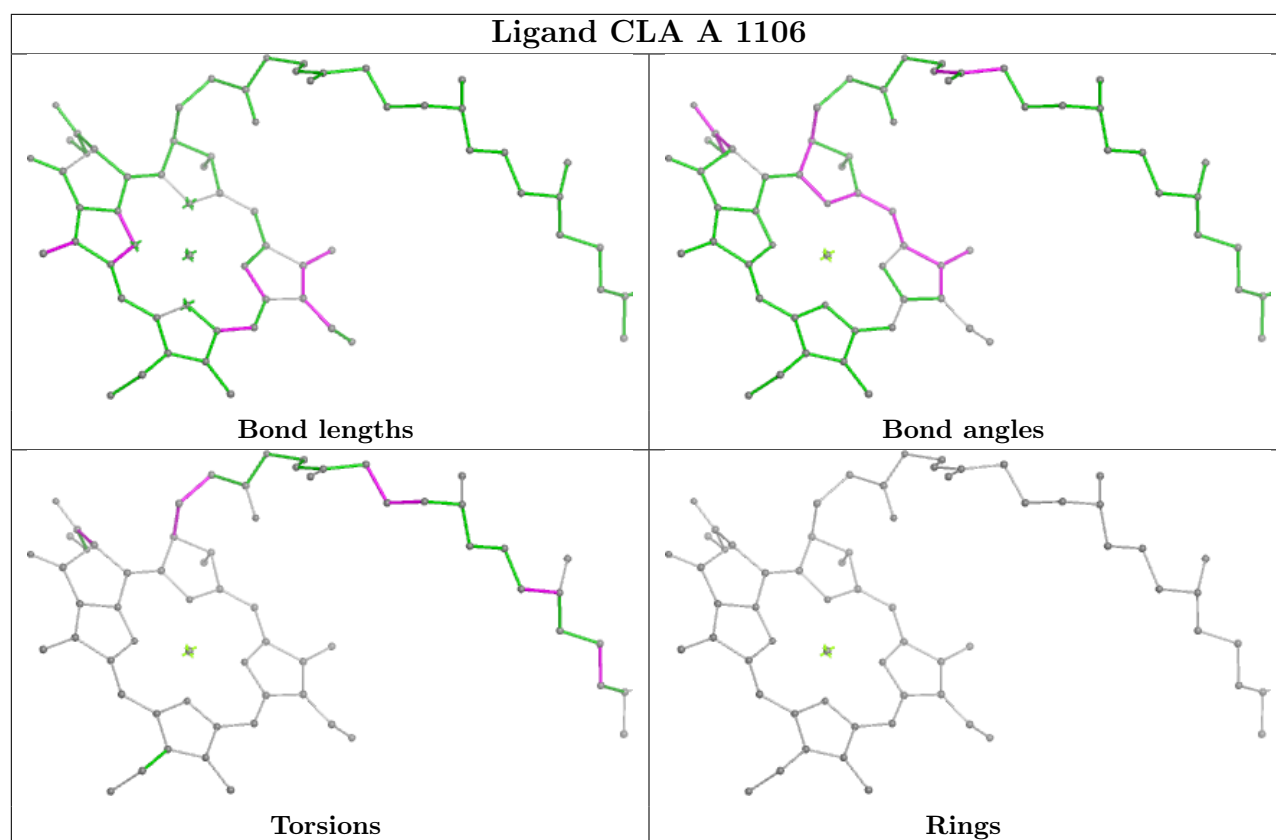
Bond angles



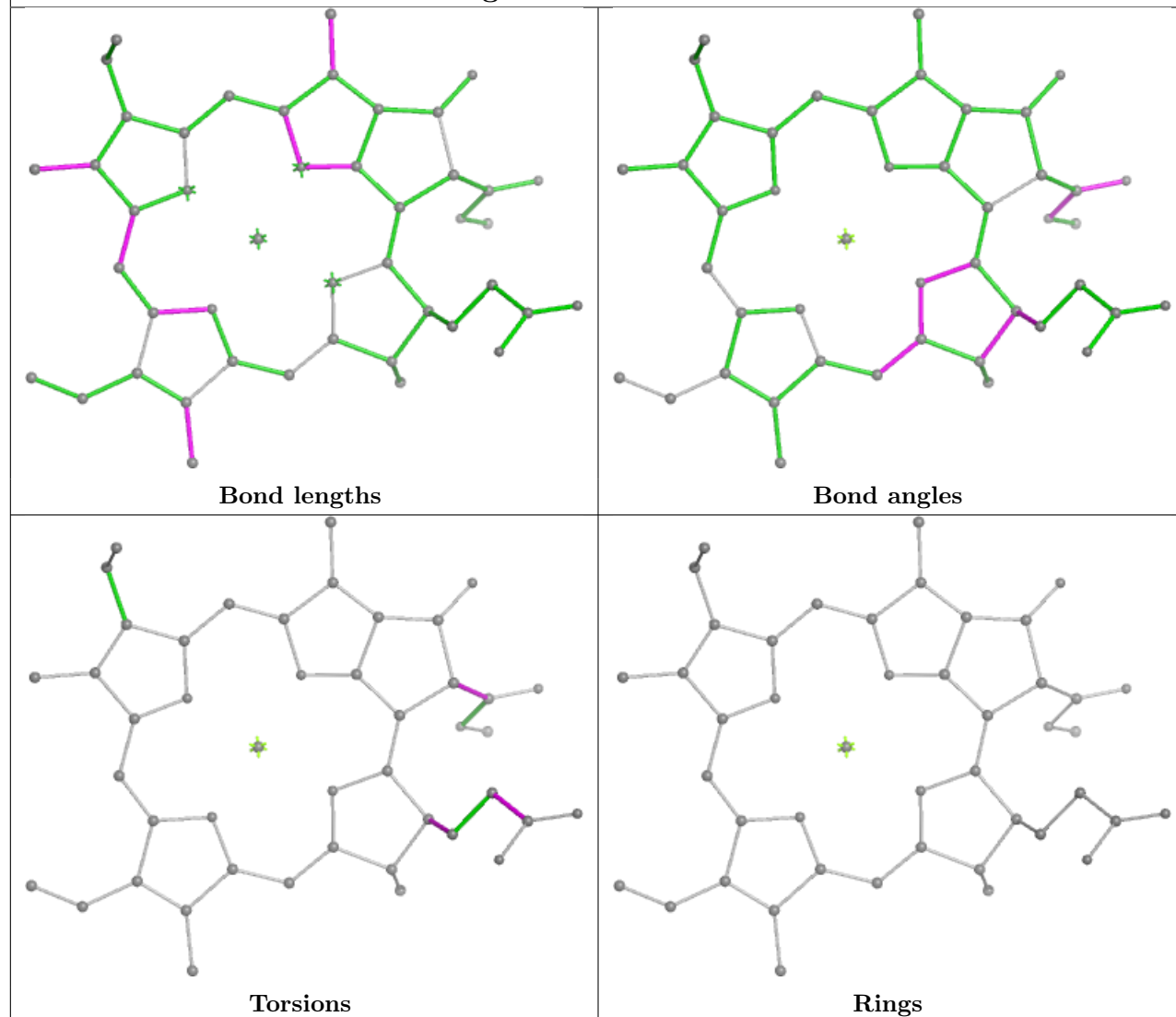
Torsions



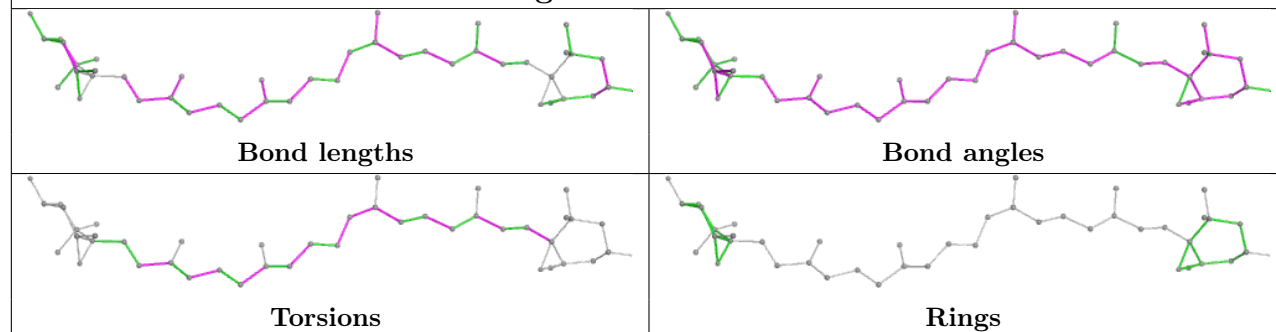
Rings

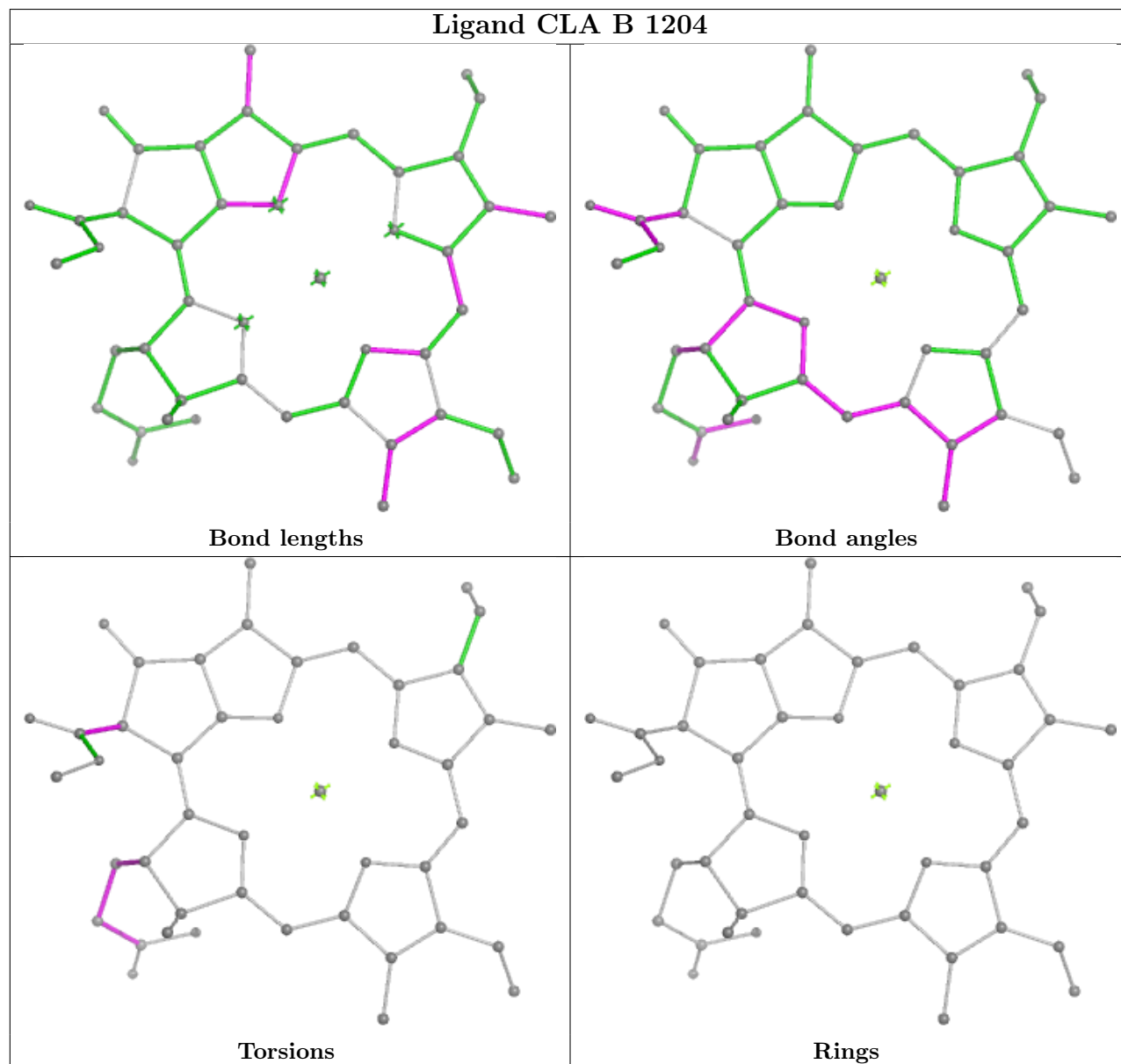
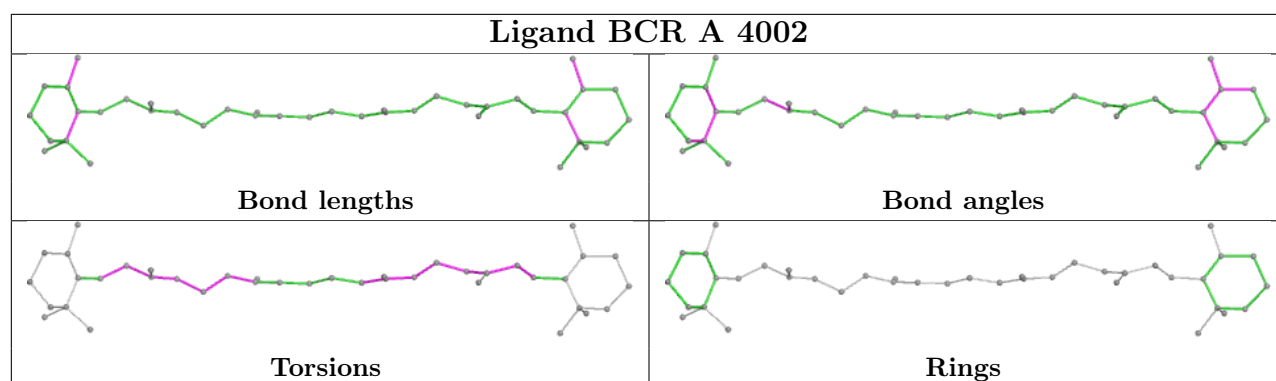


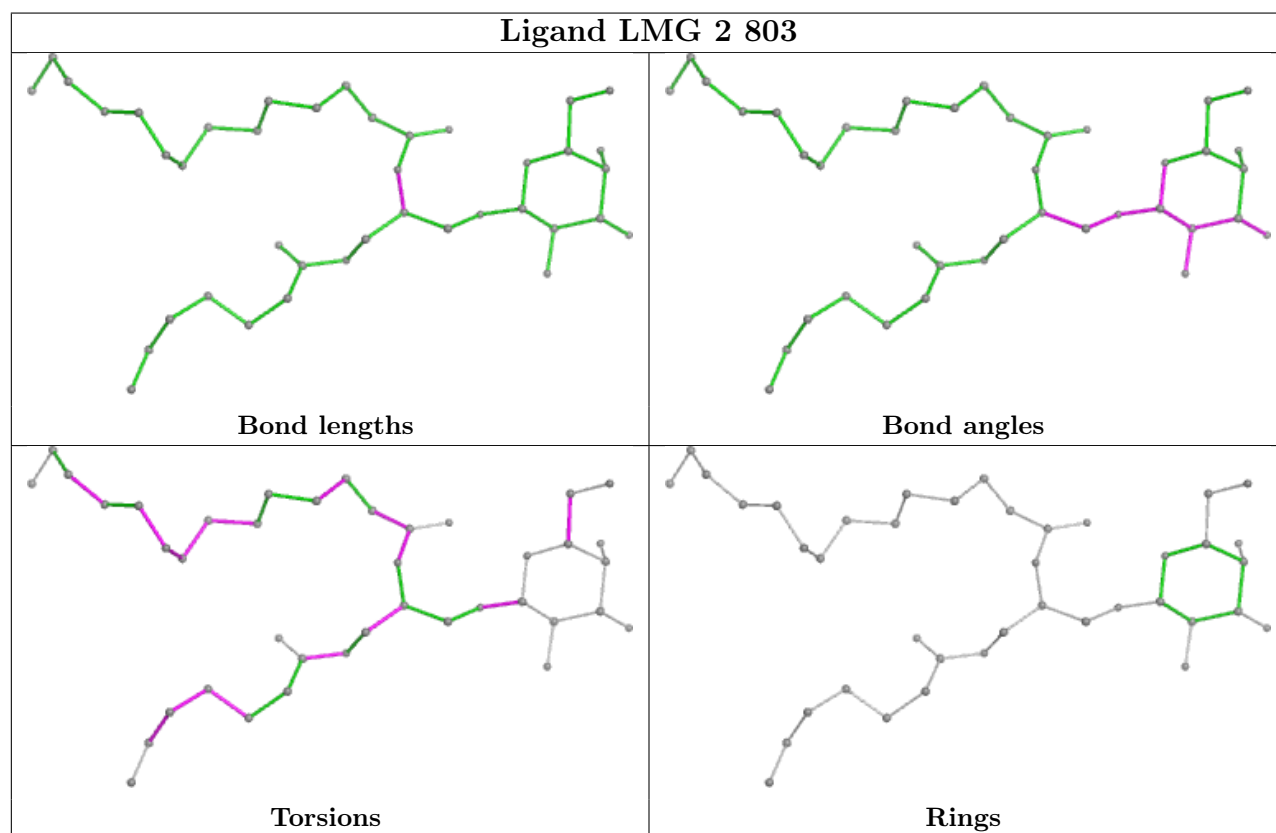
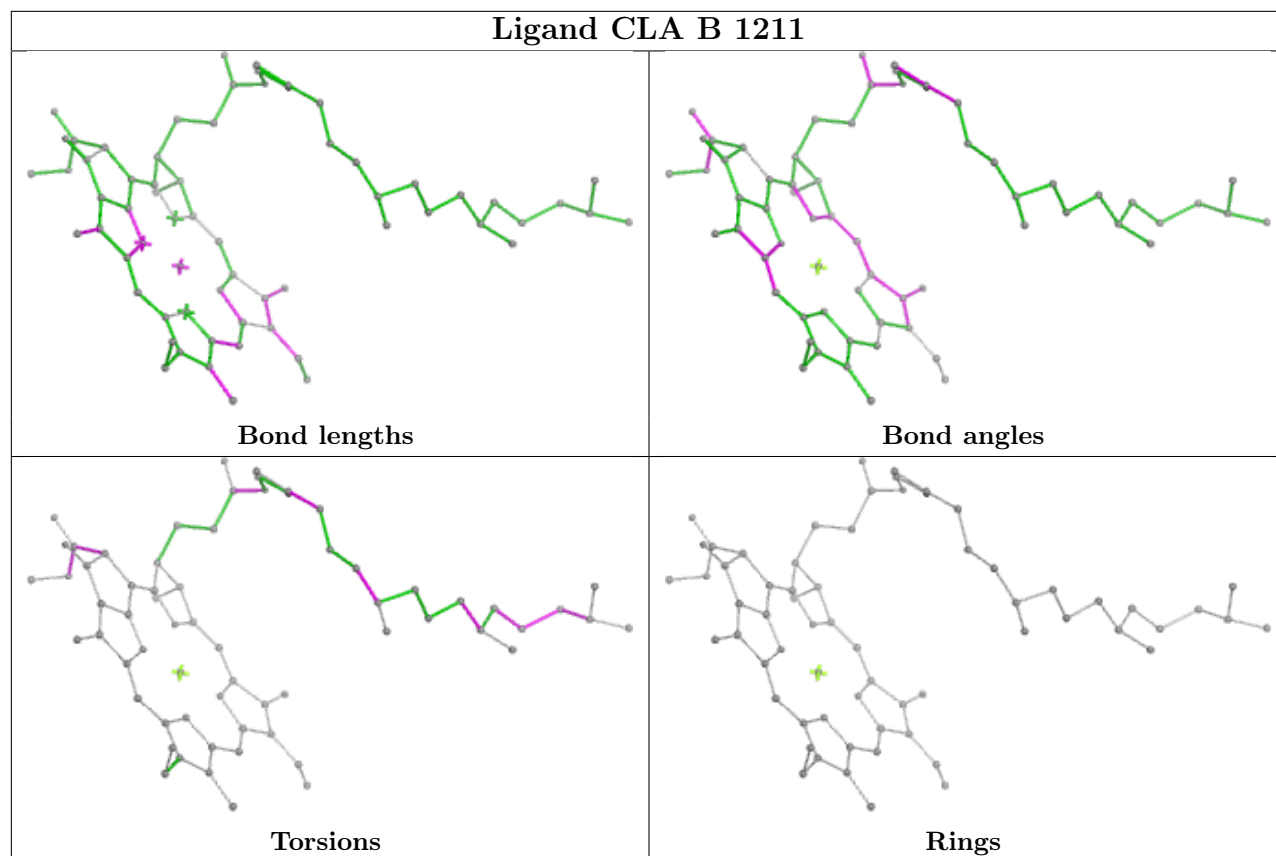
Ligand CLA B 1218



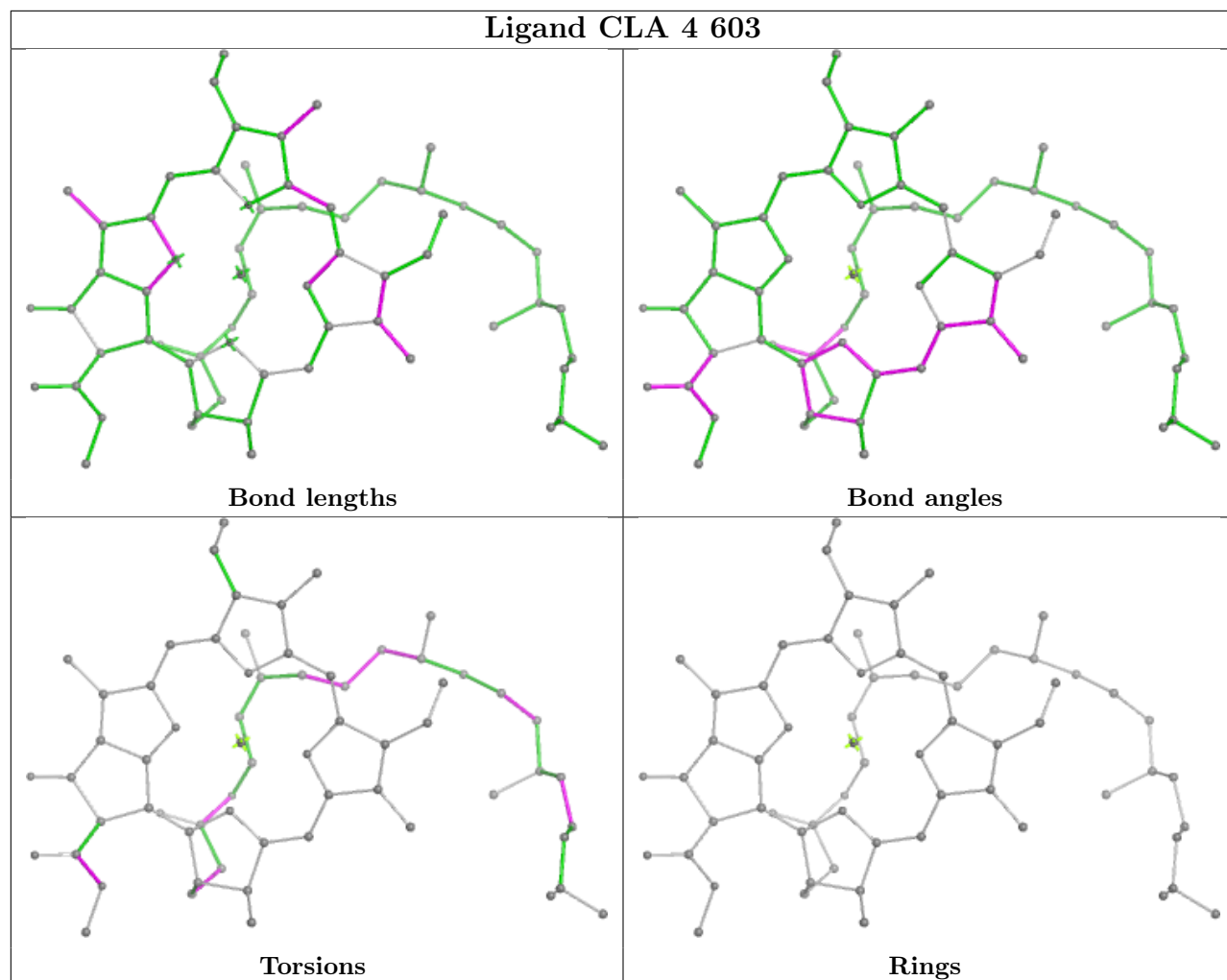
Ligand XAT 4 502



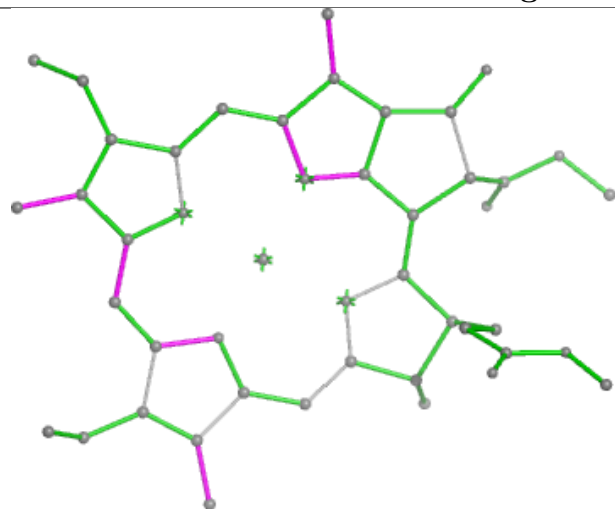




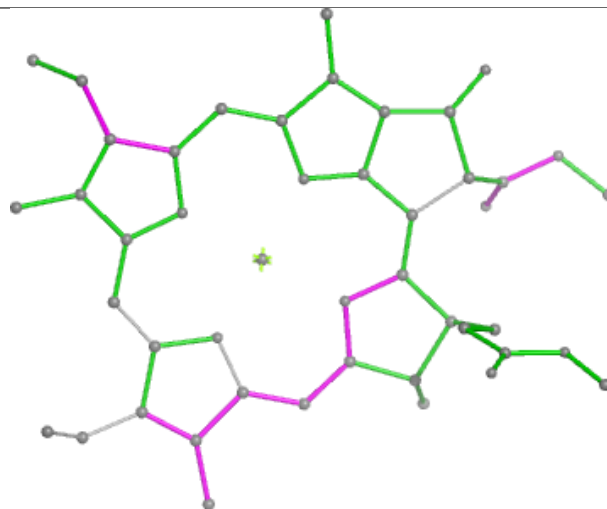
Ligand CLA 4 603



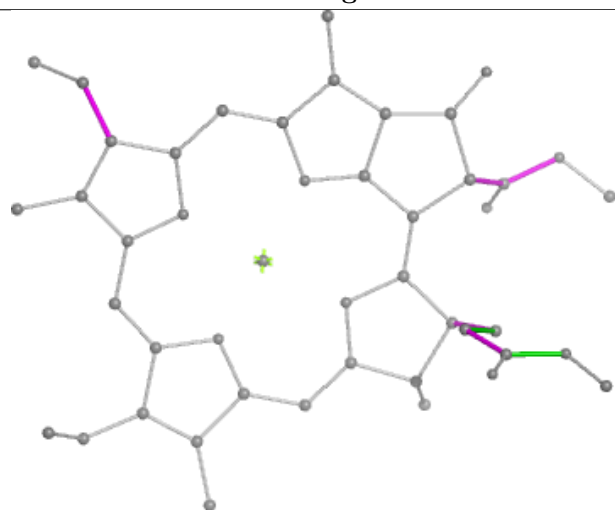
Ligand CLA 1 607



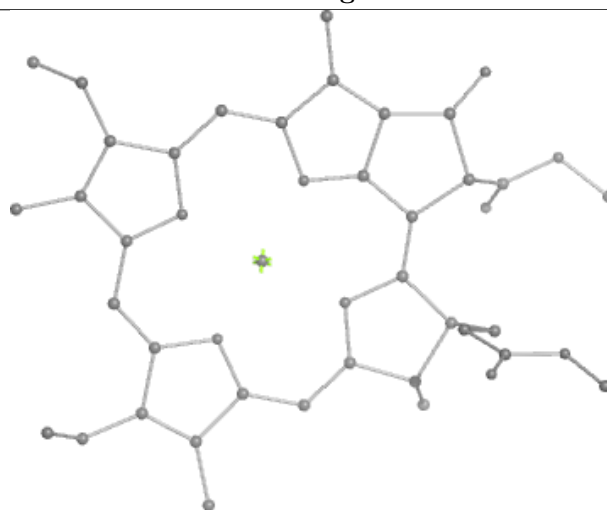
Bond lengths



Bond angles

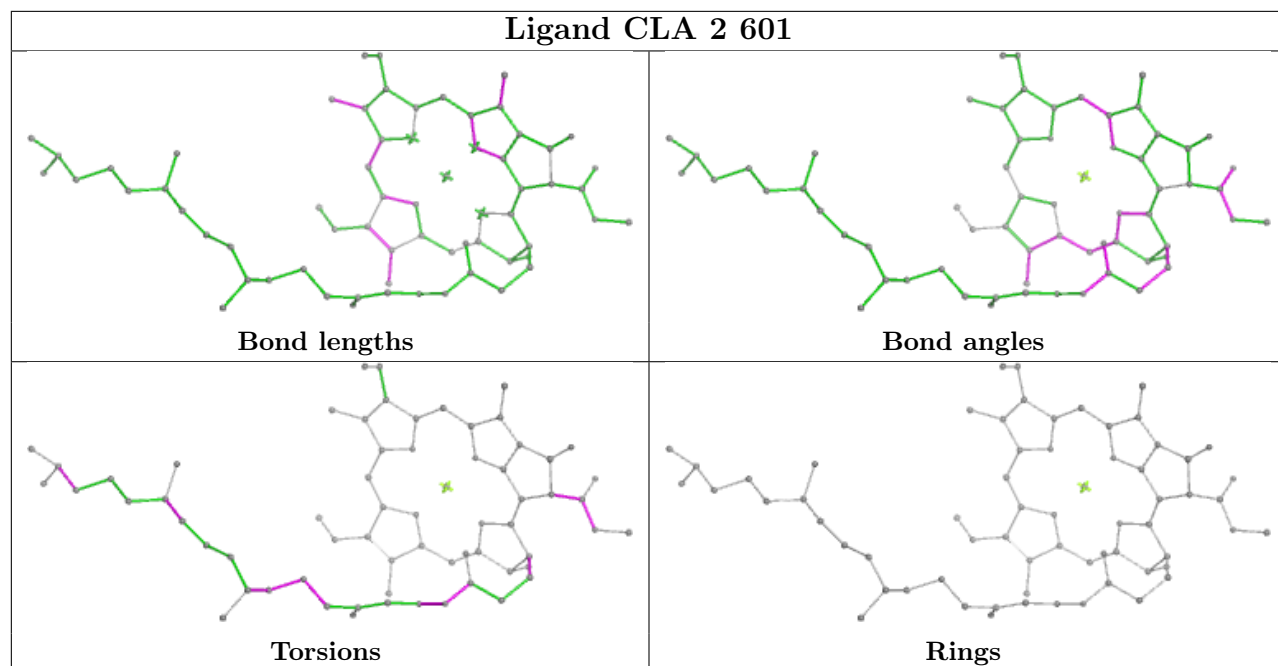


Torsions

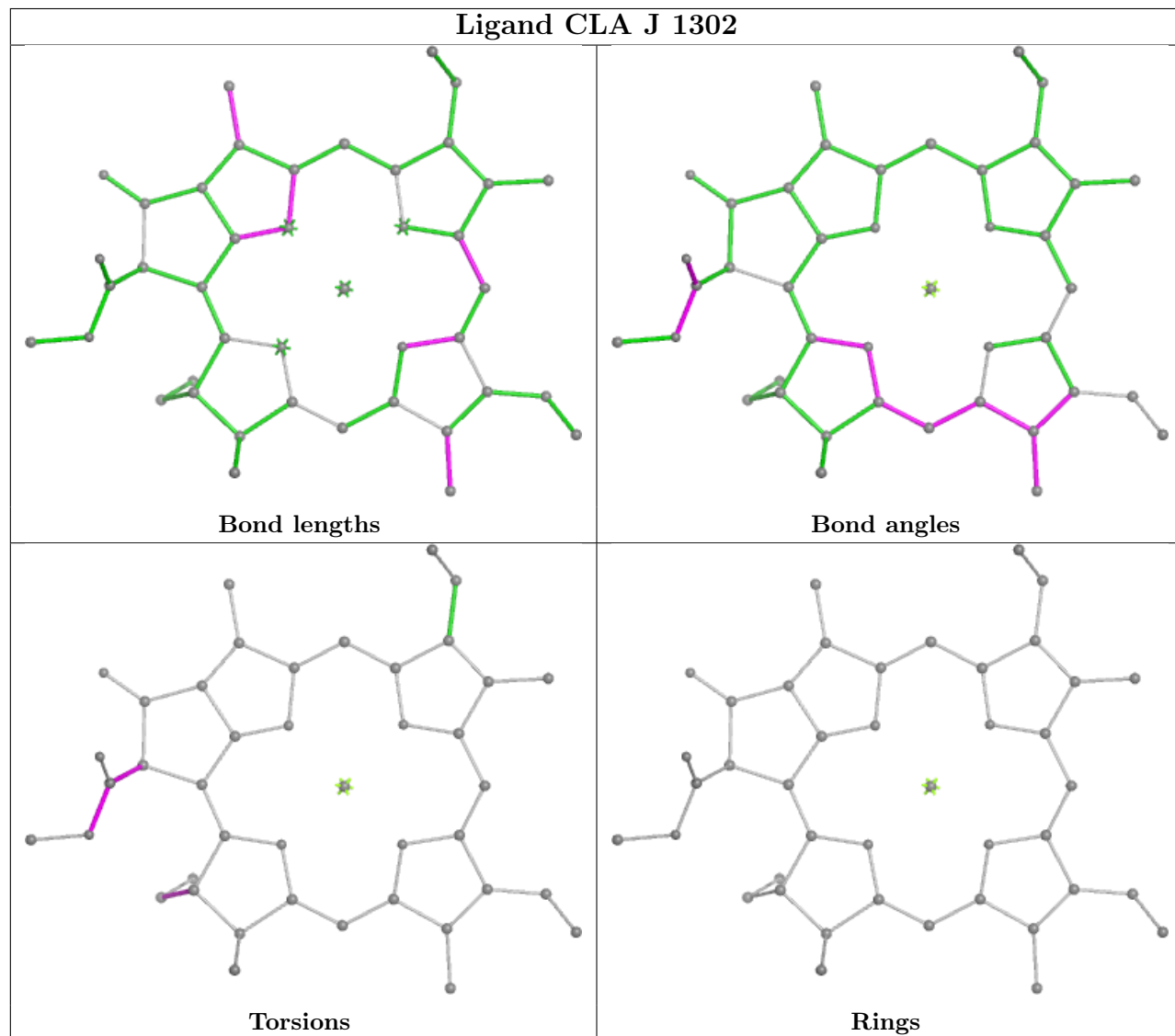


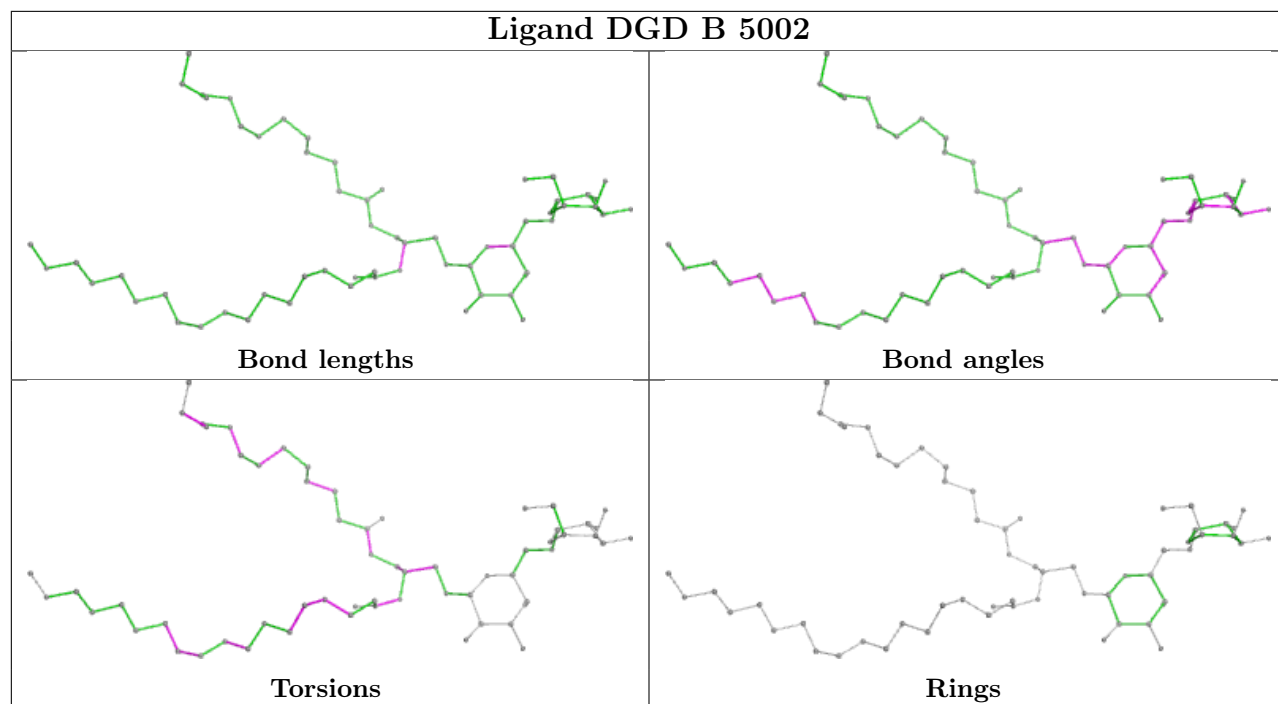
Rings

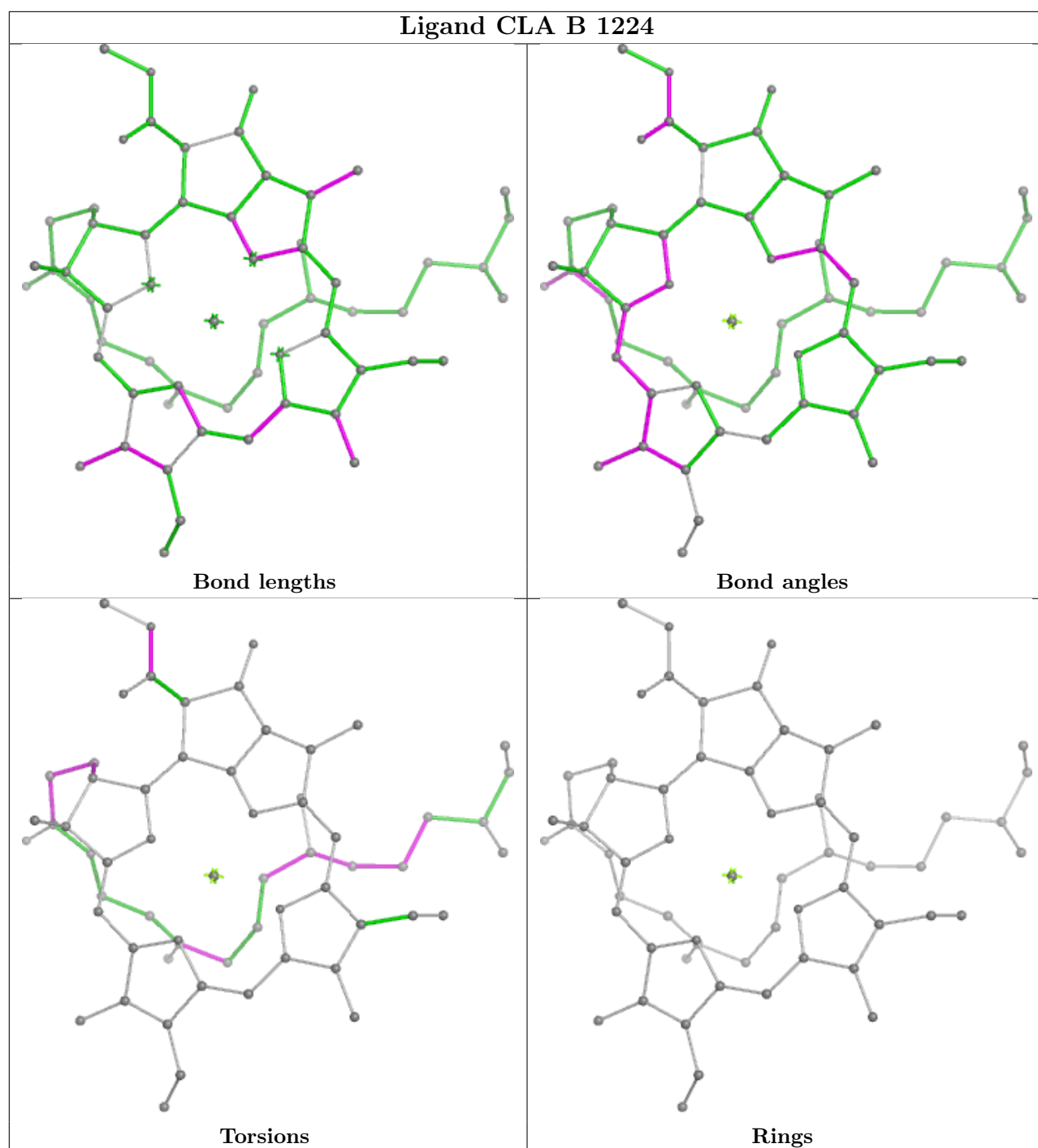
Ligand CLA 2 601



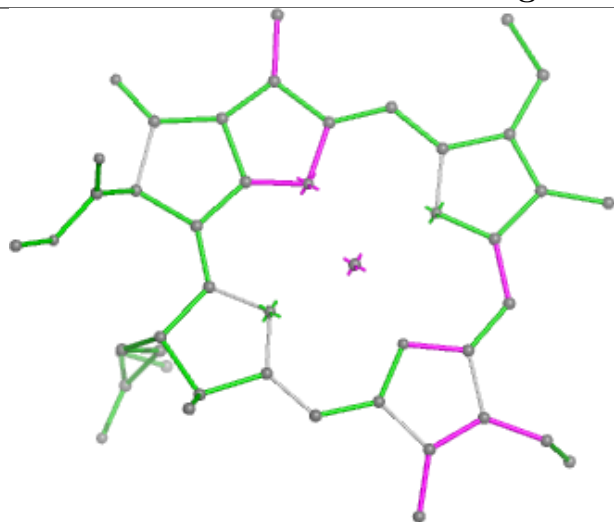
Ligand CLA J 1302



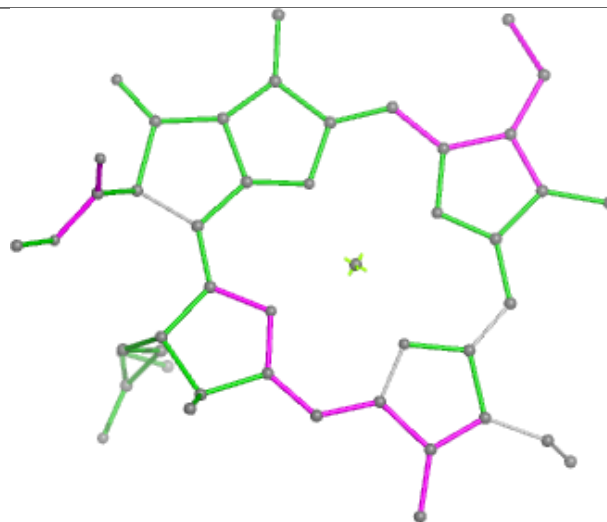




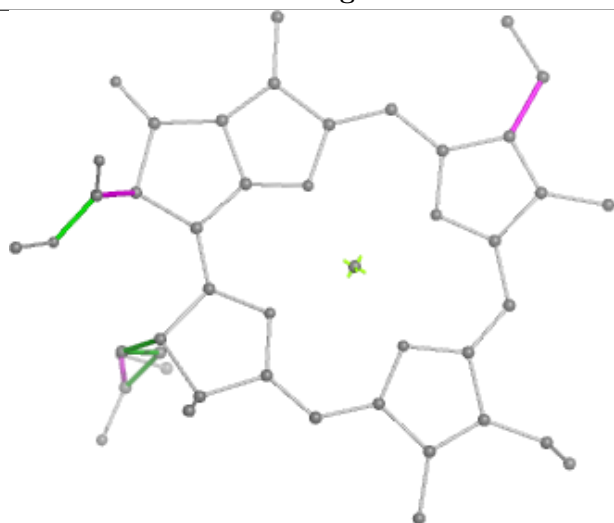
Ligand CLA 4 608



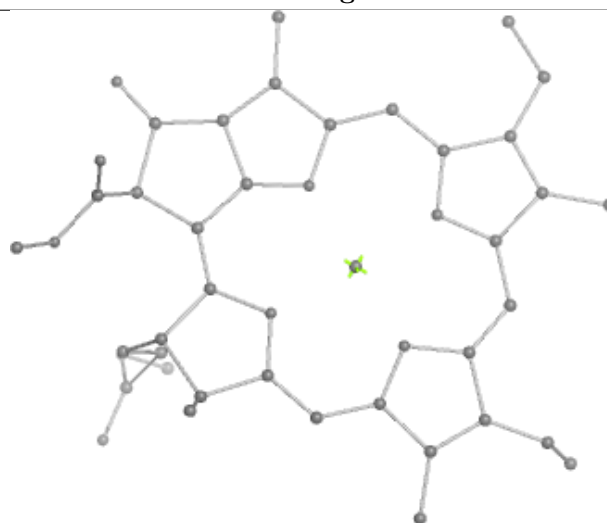
Bond lengths



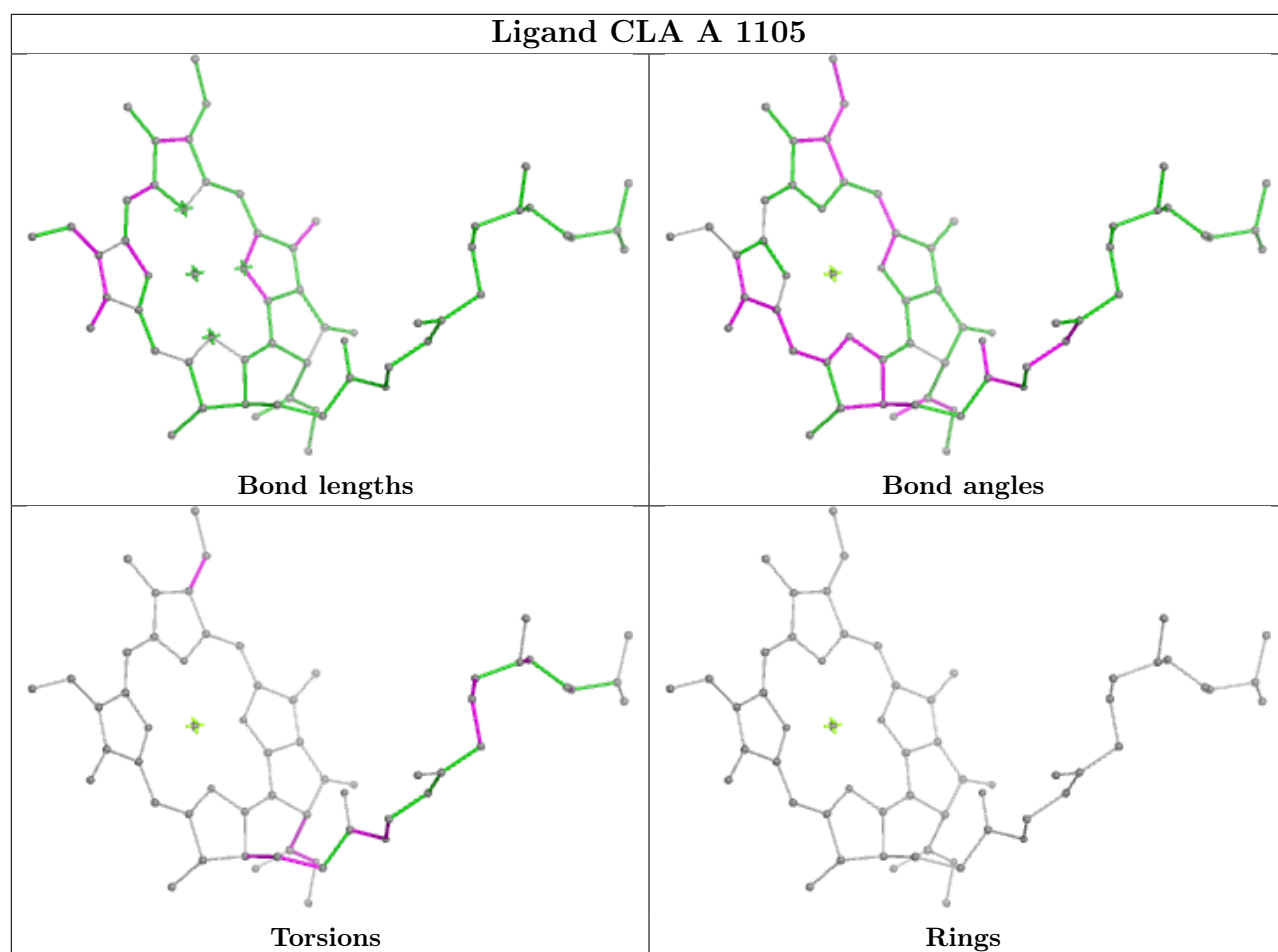
Bond angles

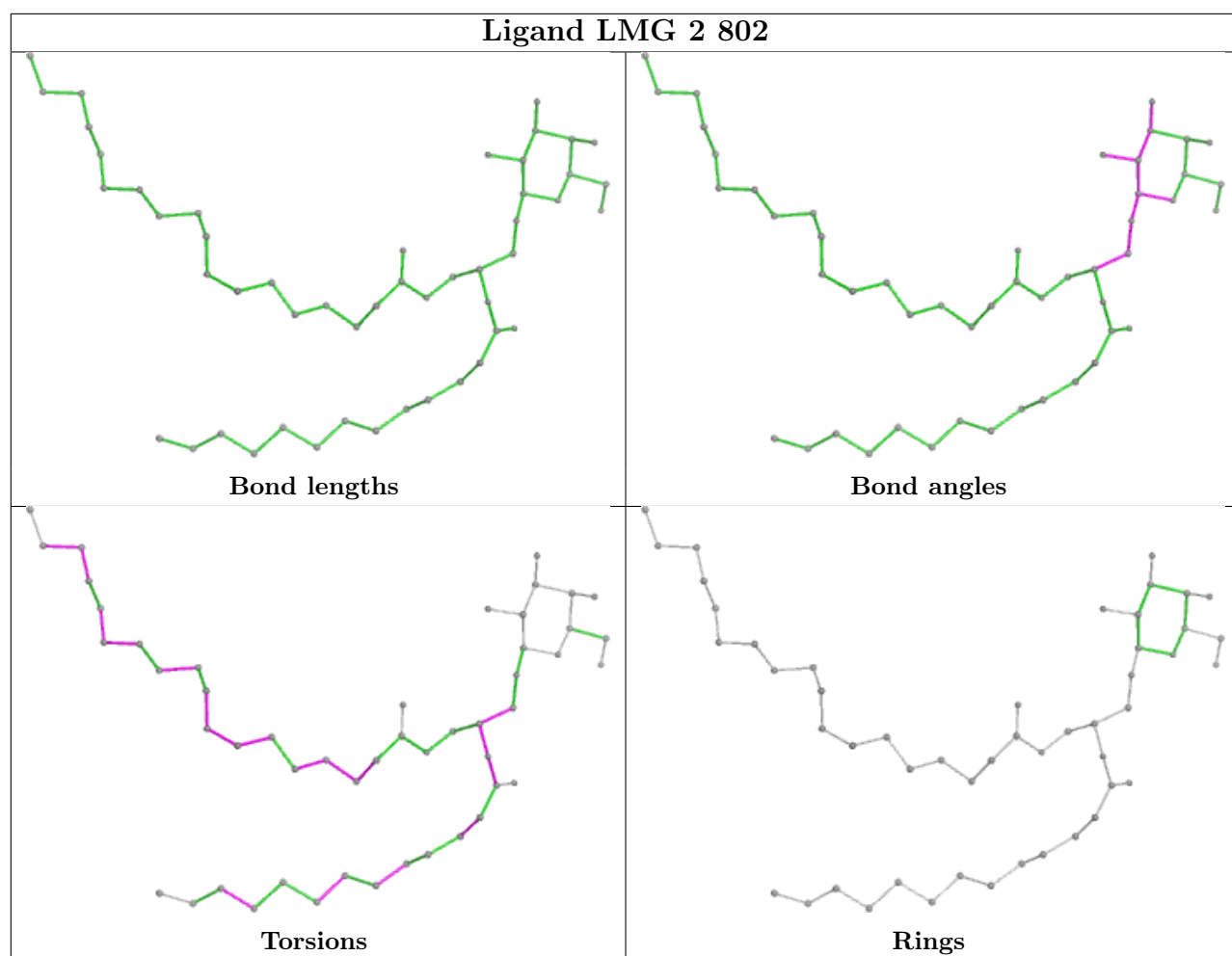


Torsions

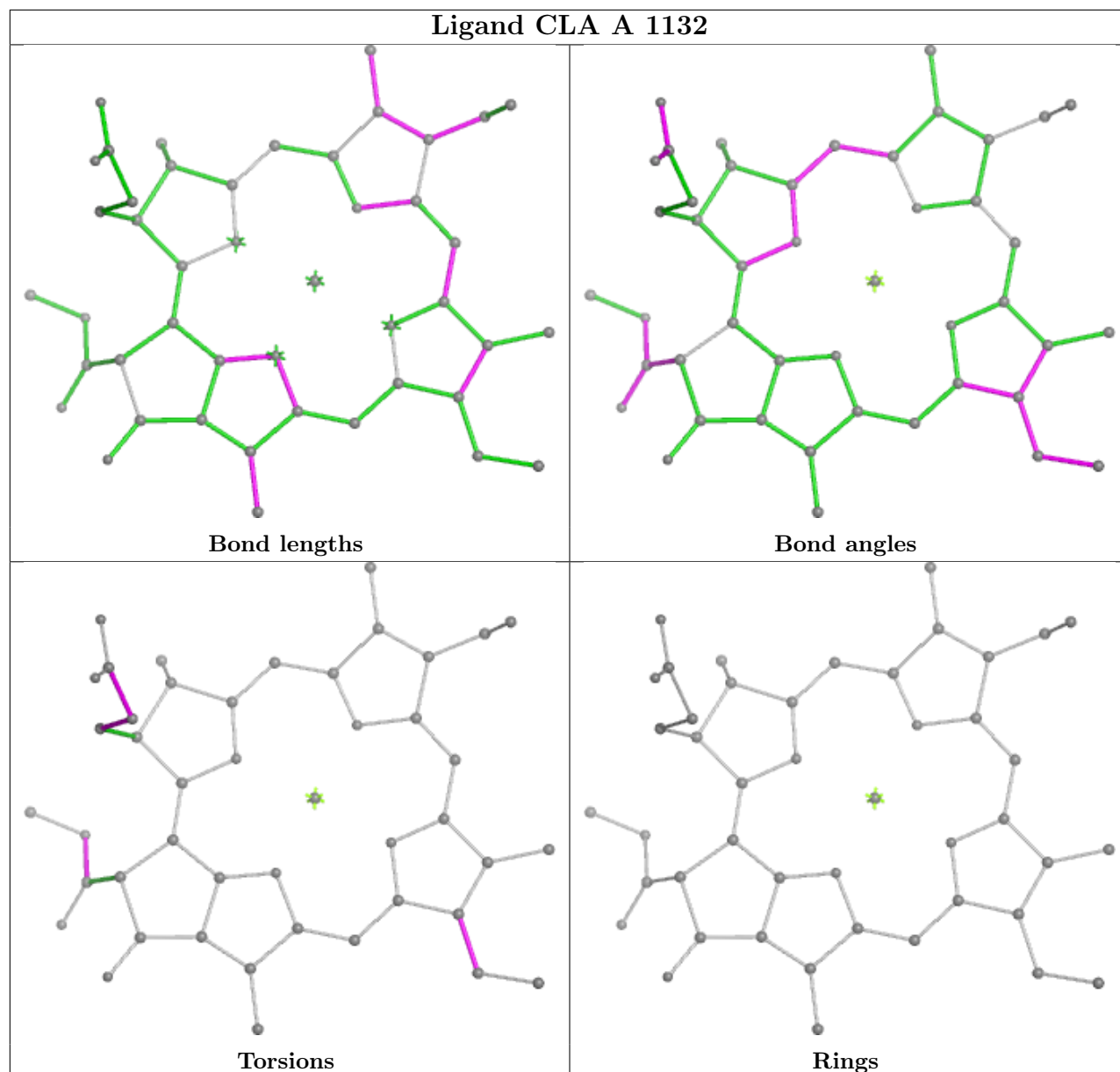


Rings

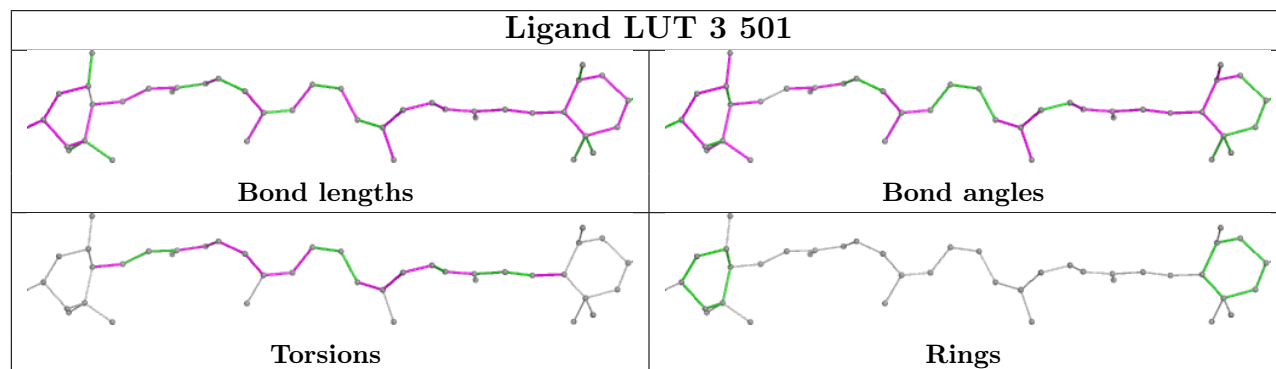


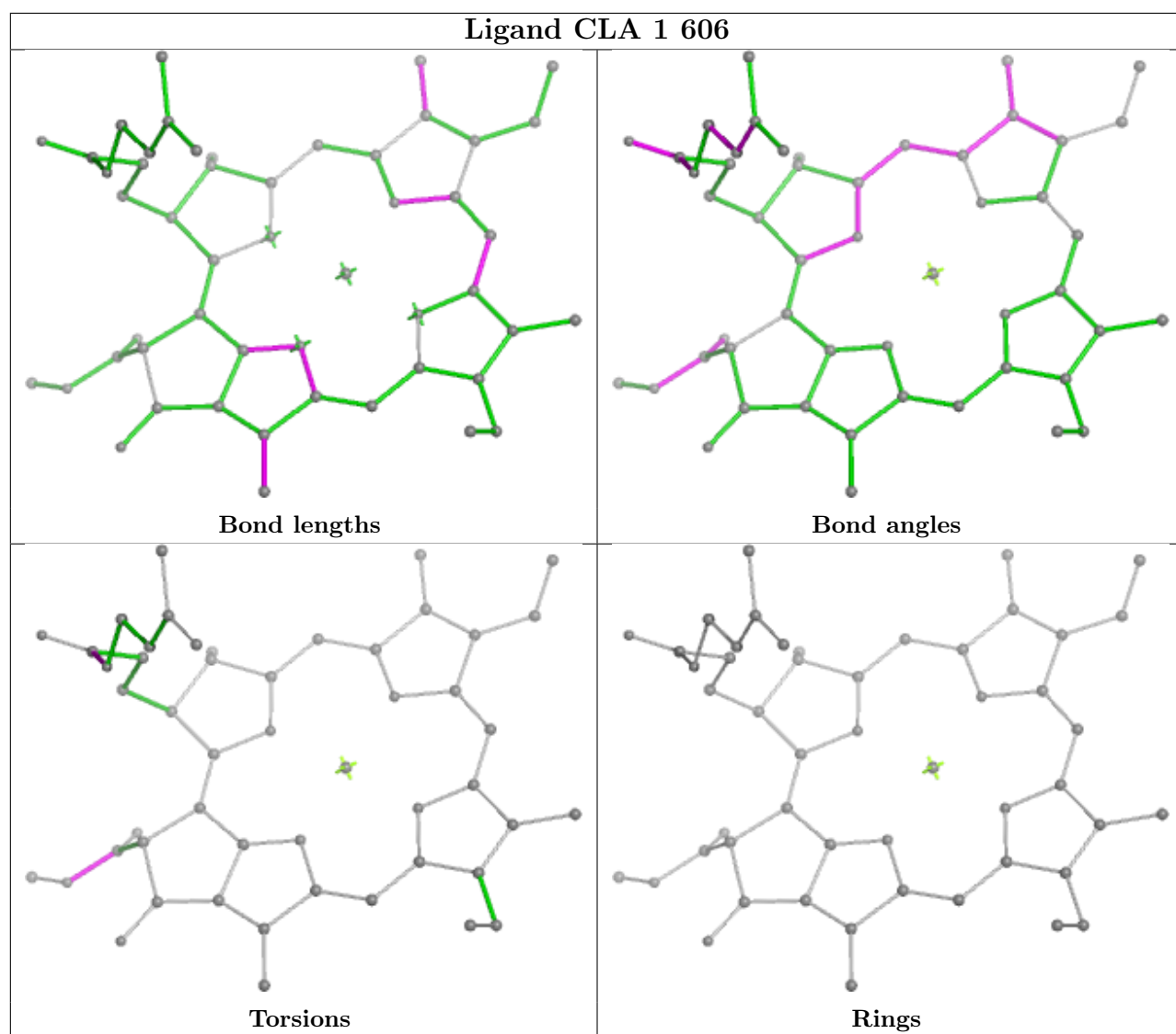


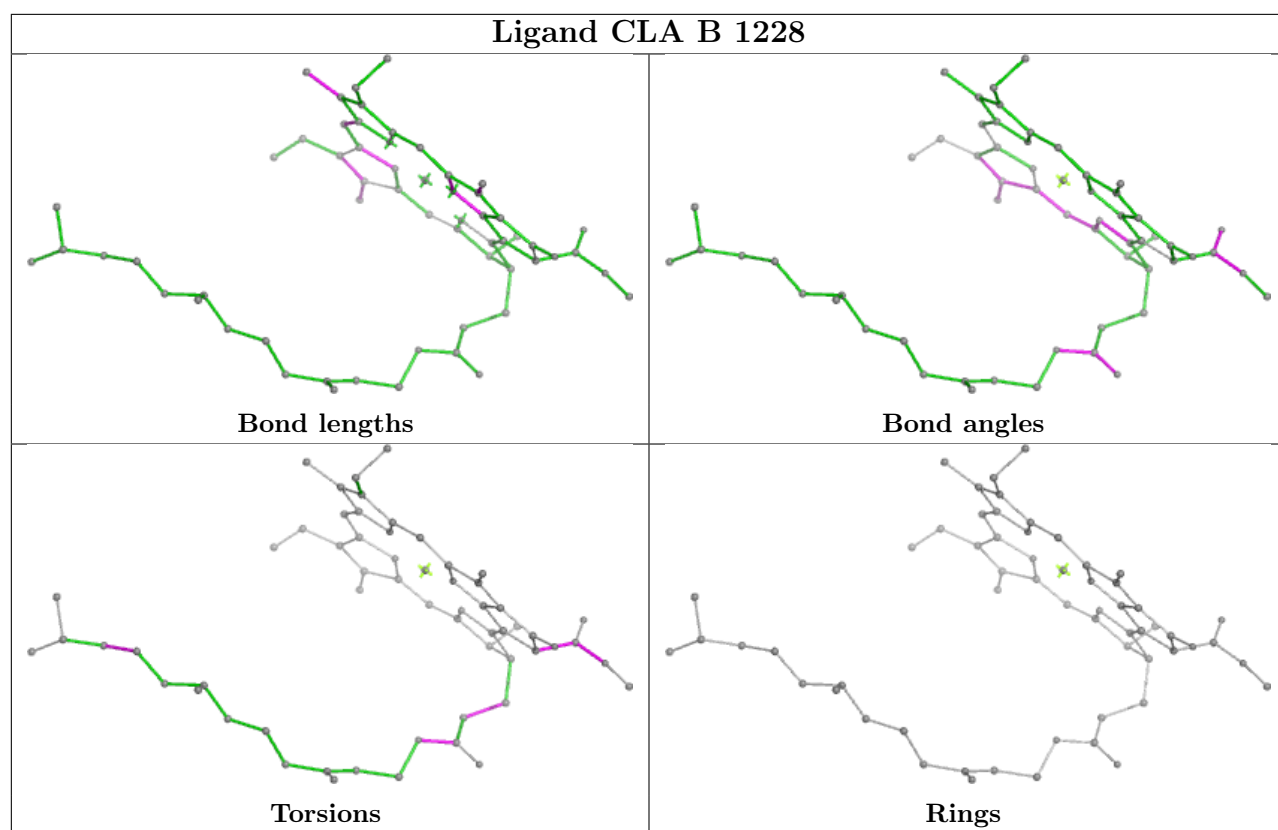
Ligand CLA A 1132



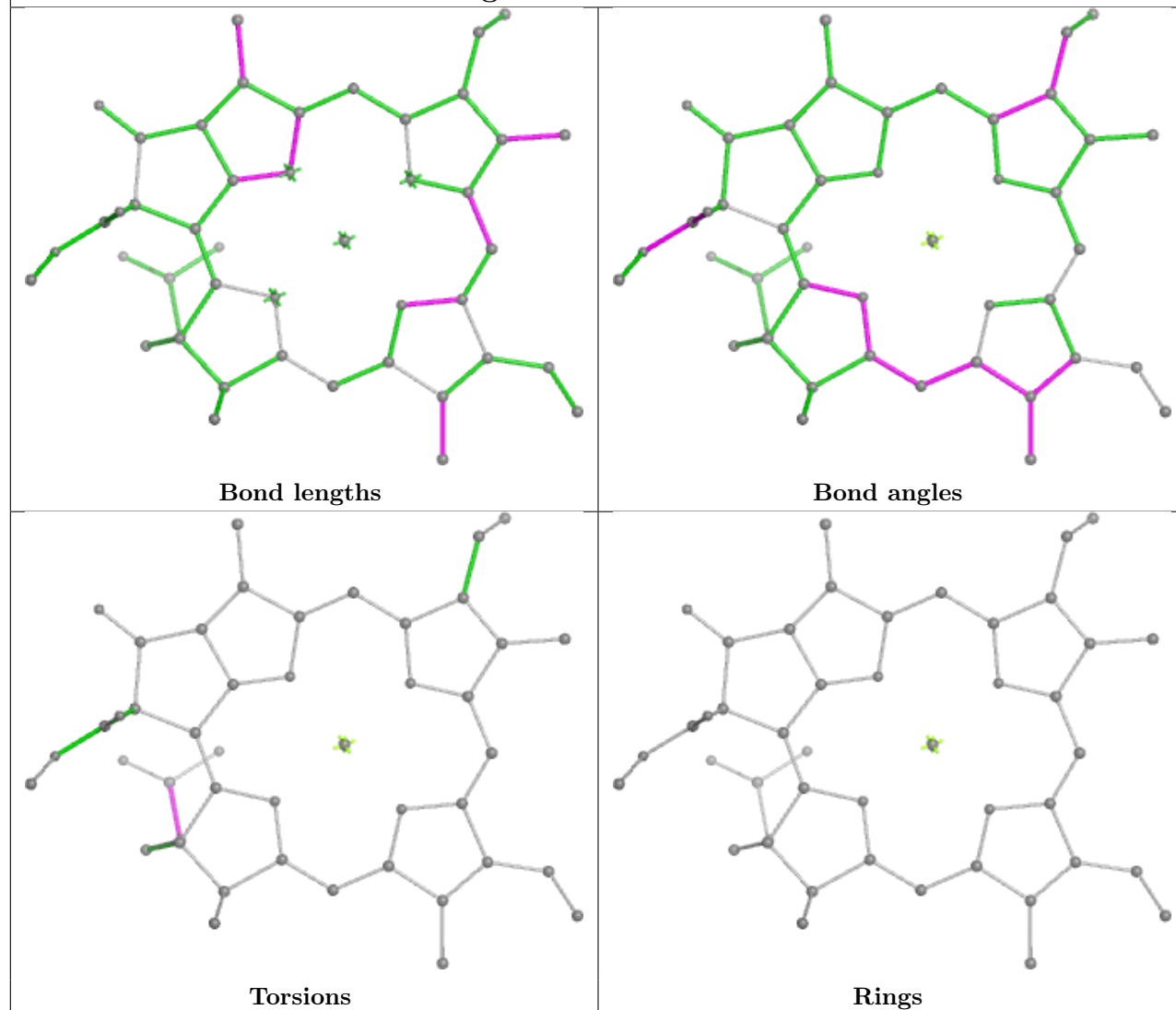
Ligand LUT 3 501

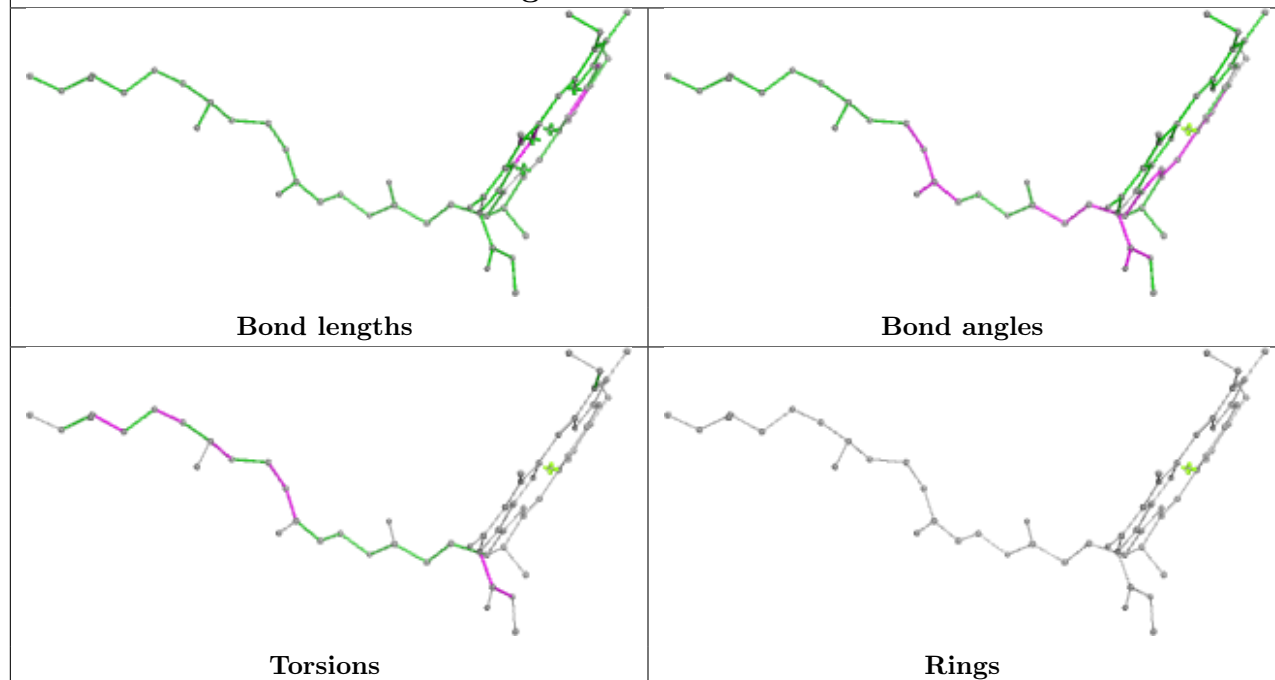
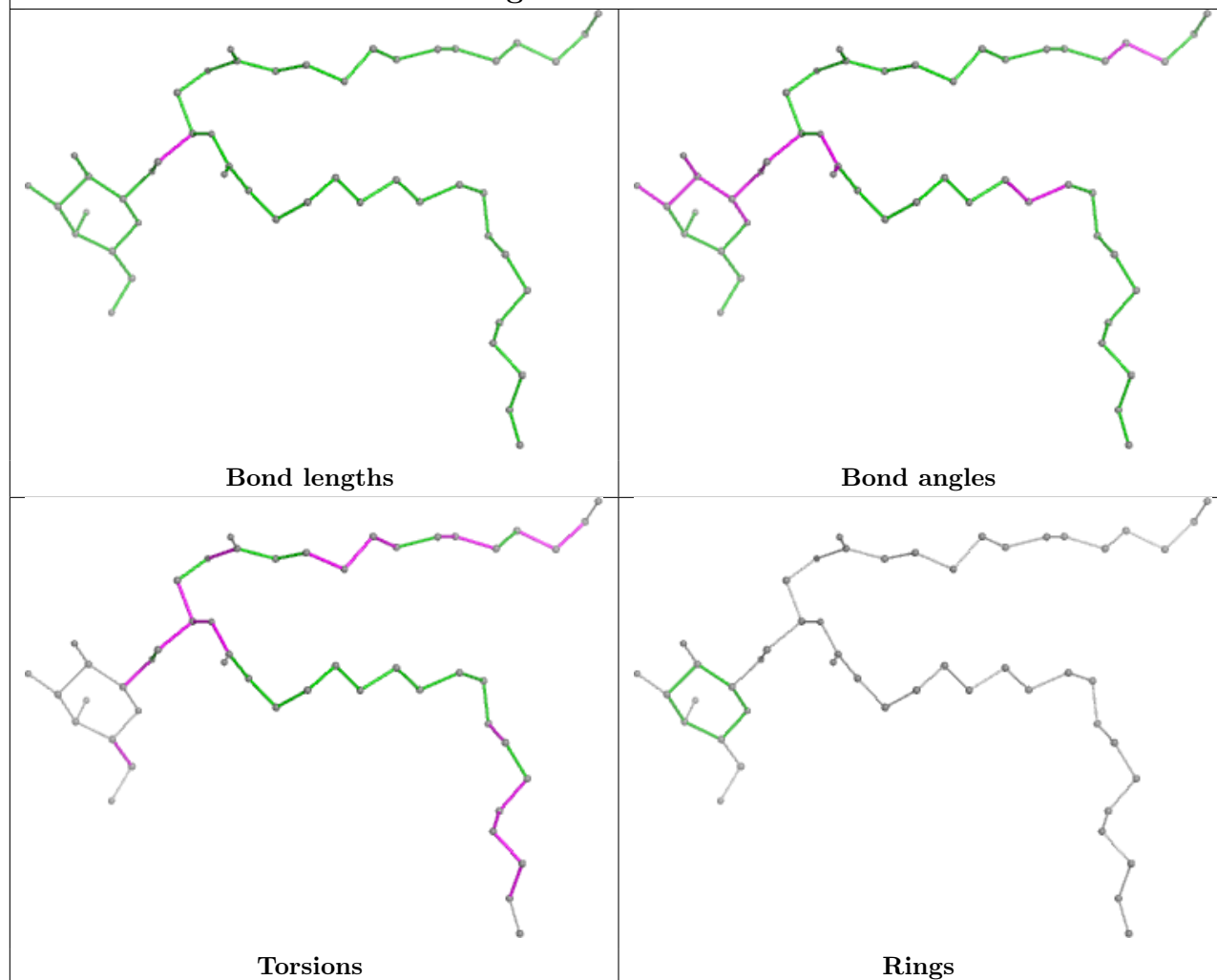


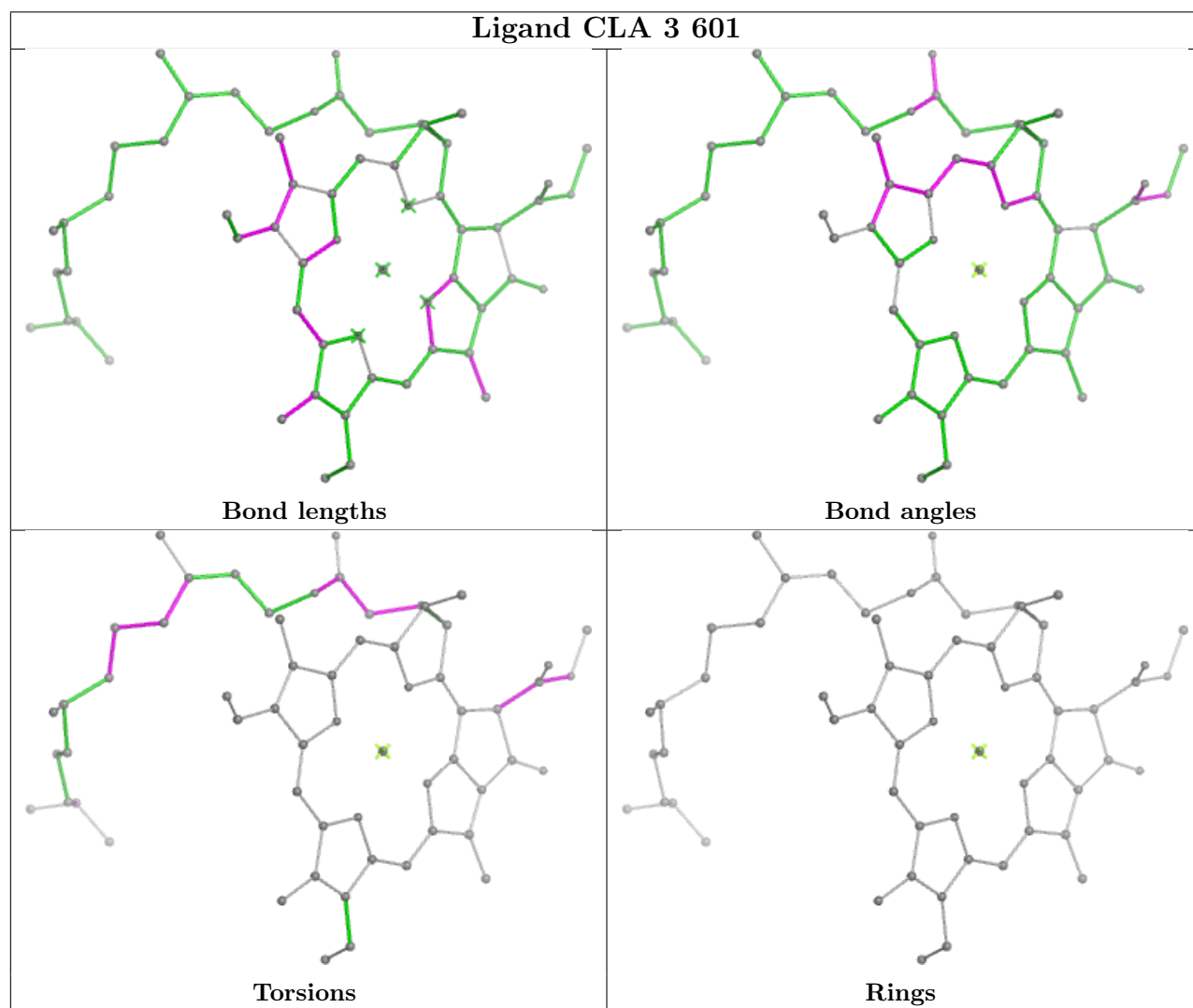
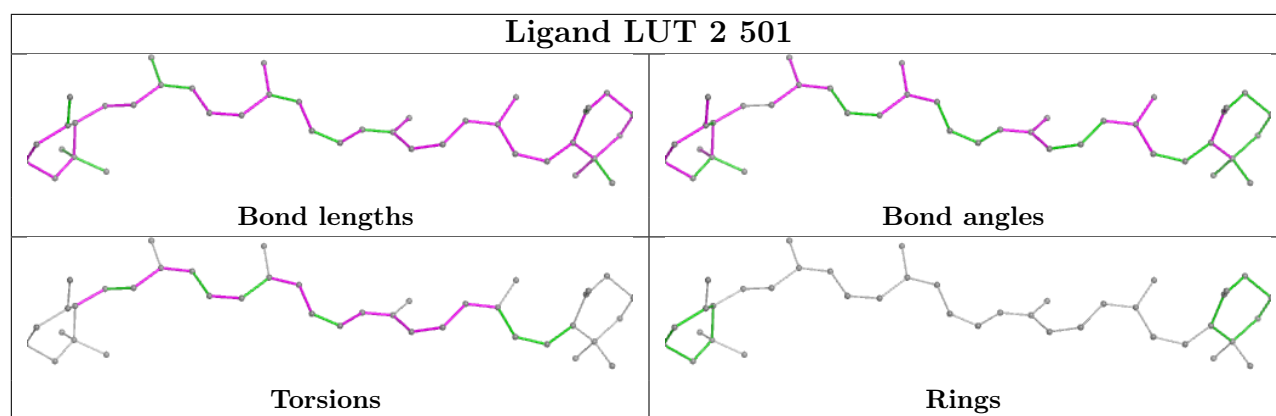


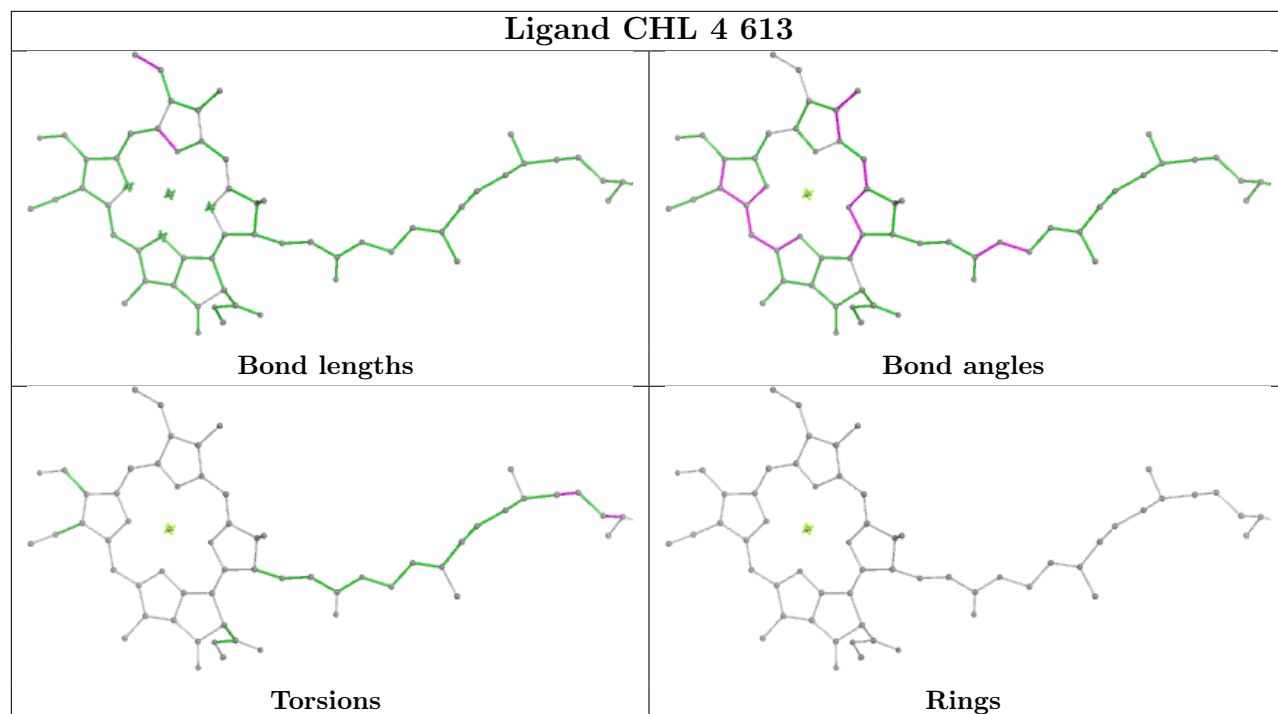
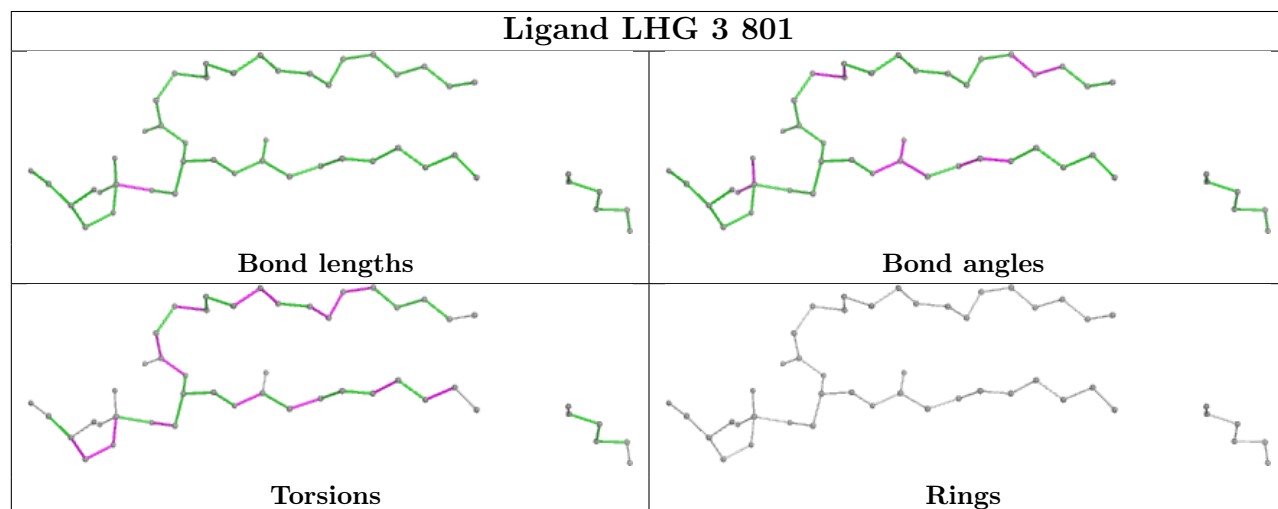


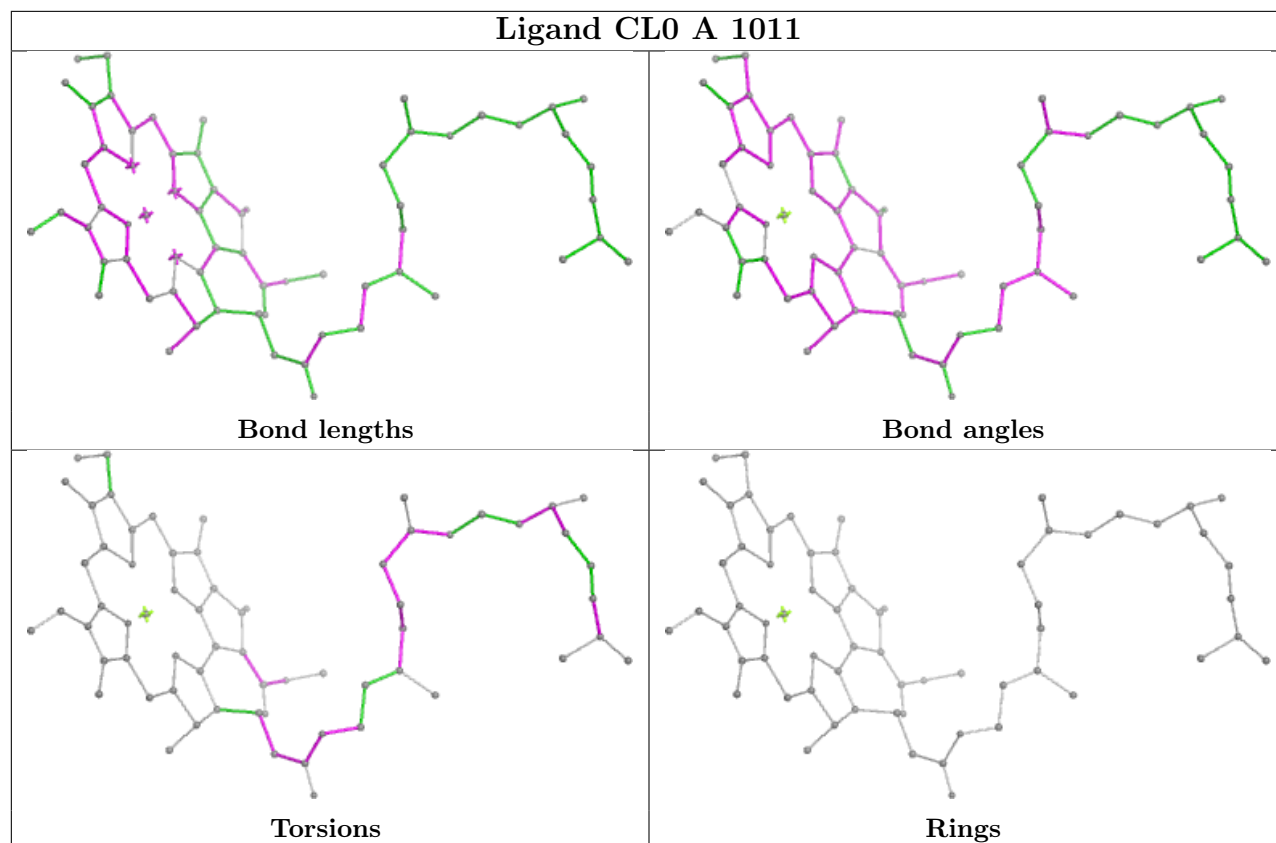
Ligand CLA A 1115



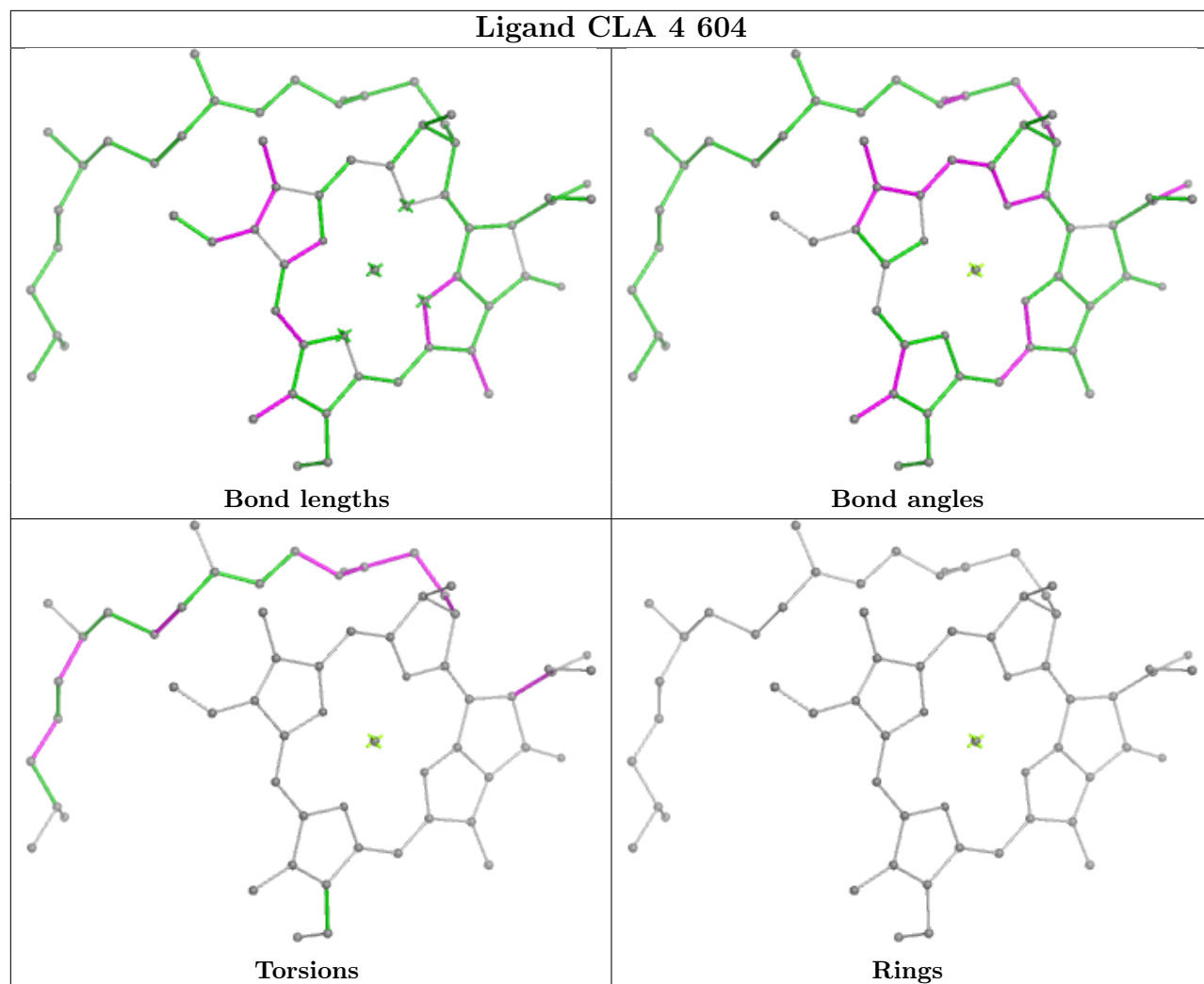
Ligand CLA A 1137**Ligand LMG 2 804**



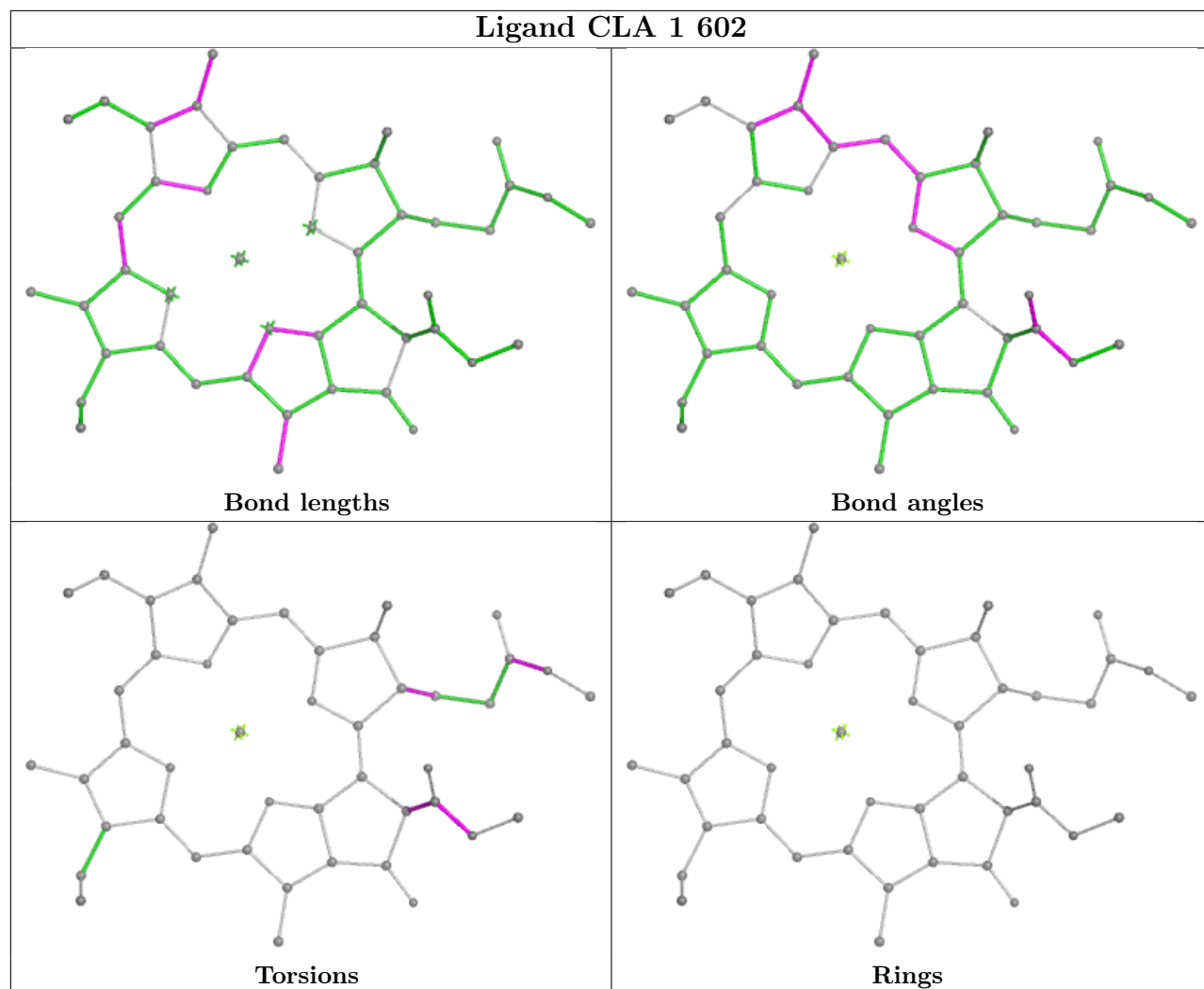
Ligand CHL 4 613**Ligand LHG 3 801**



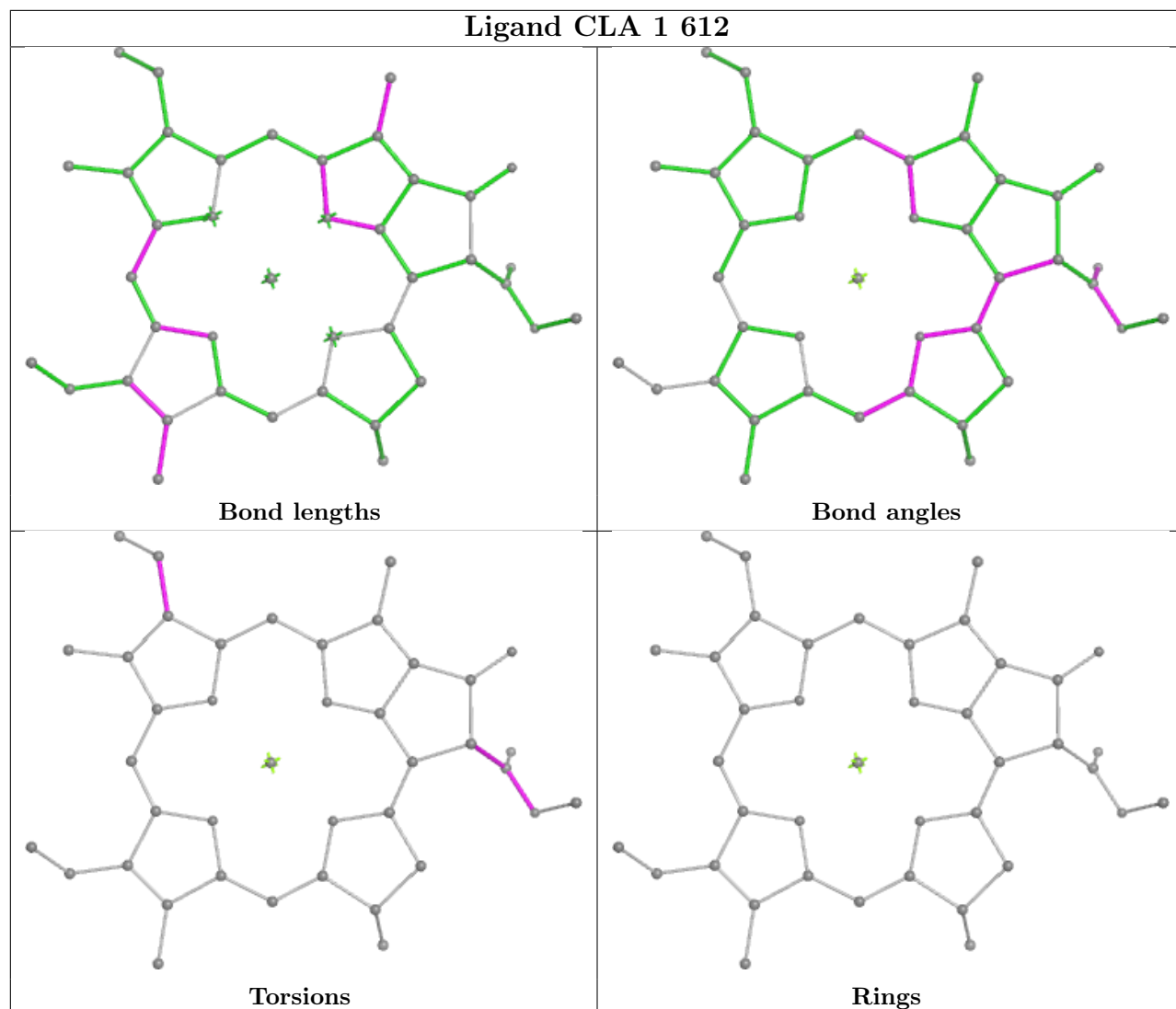
Ligand CLA 4 604



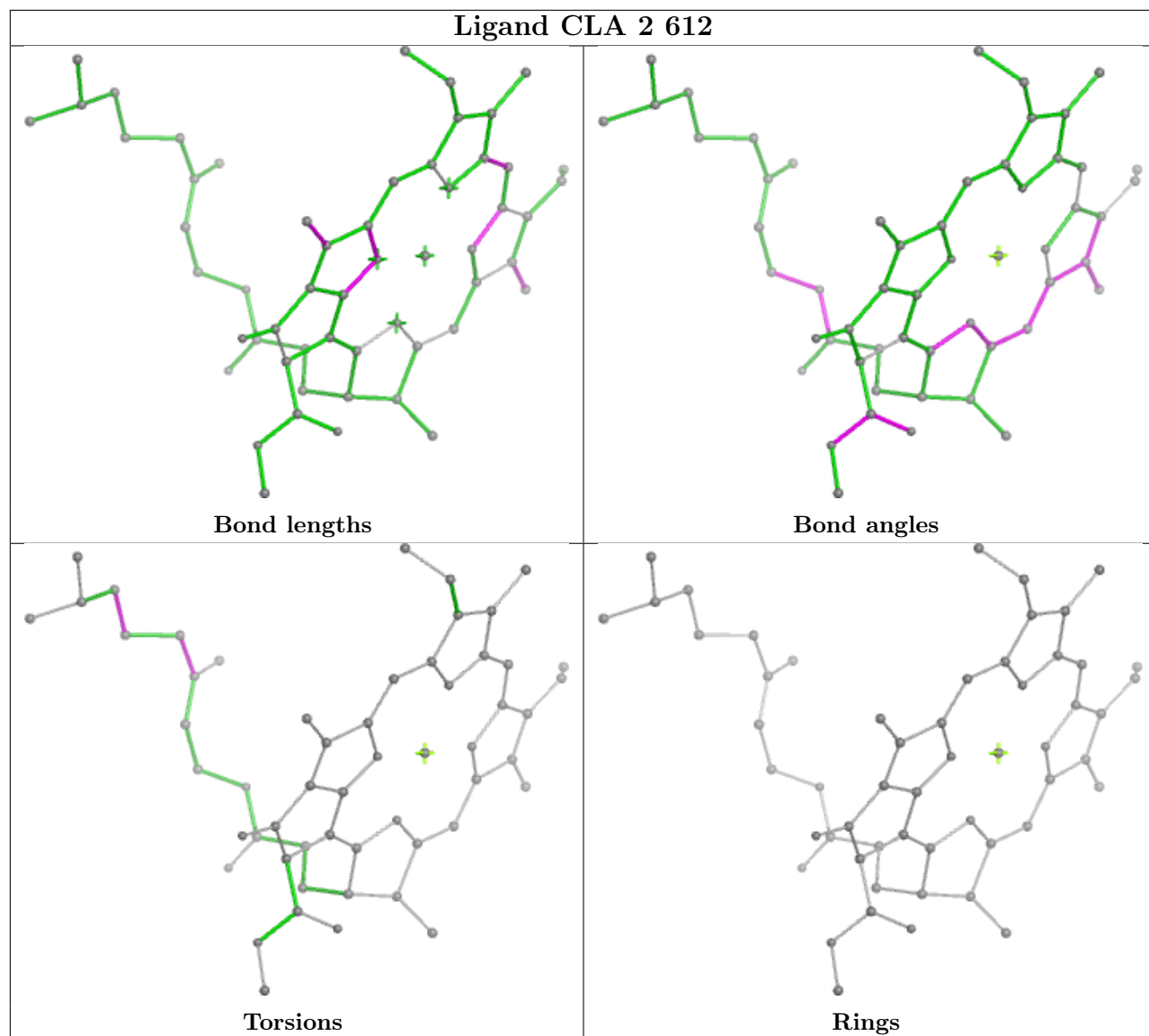
Ligand CLA 1 602

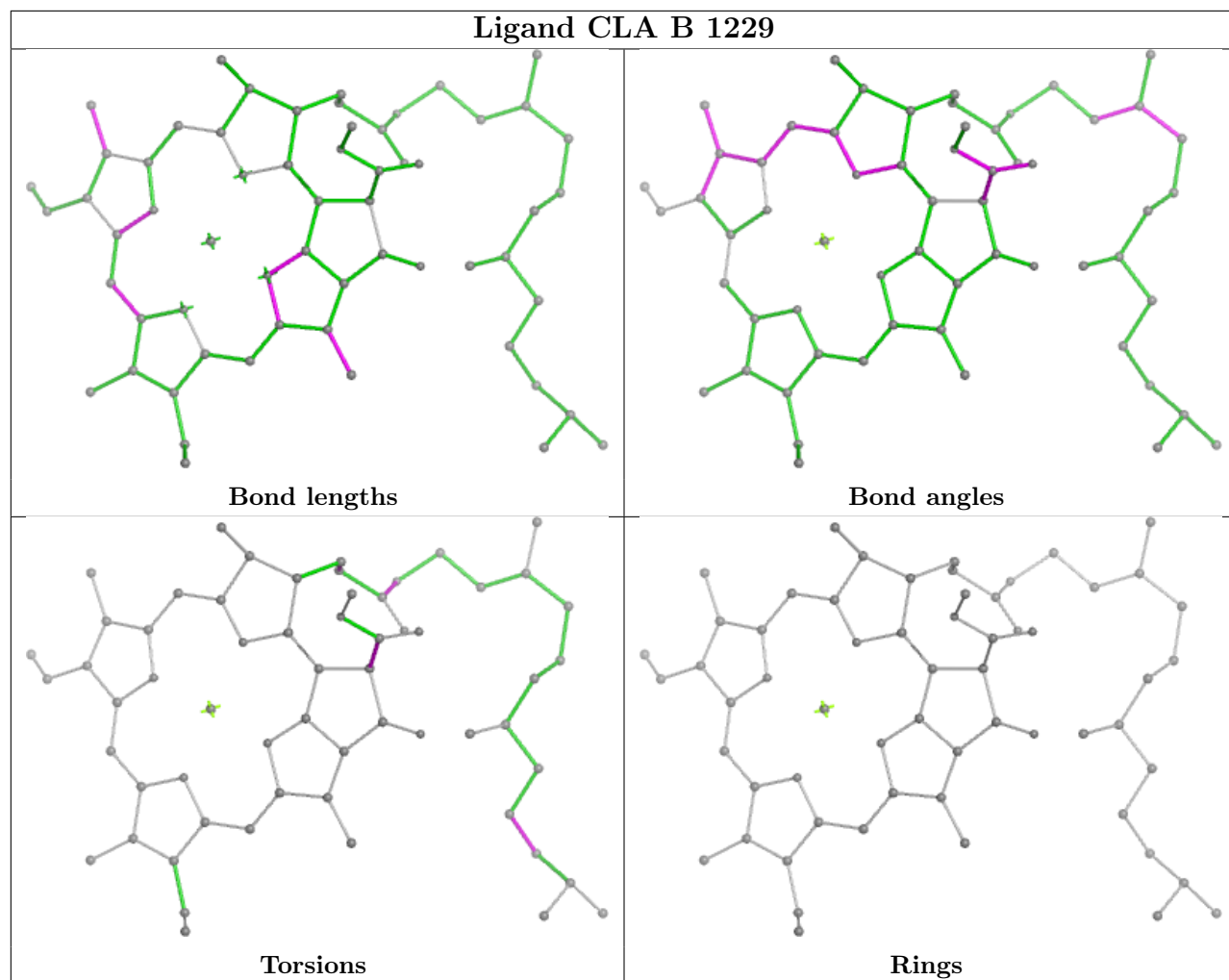


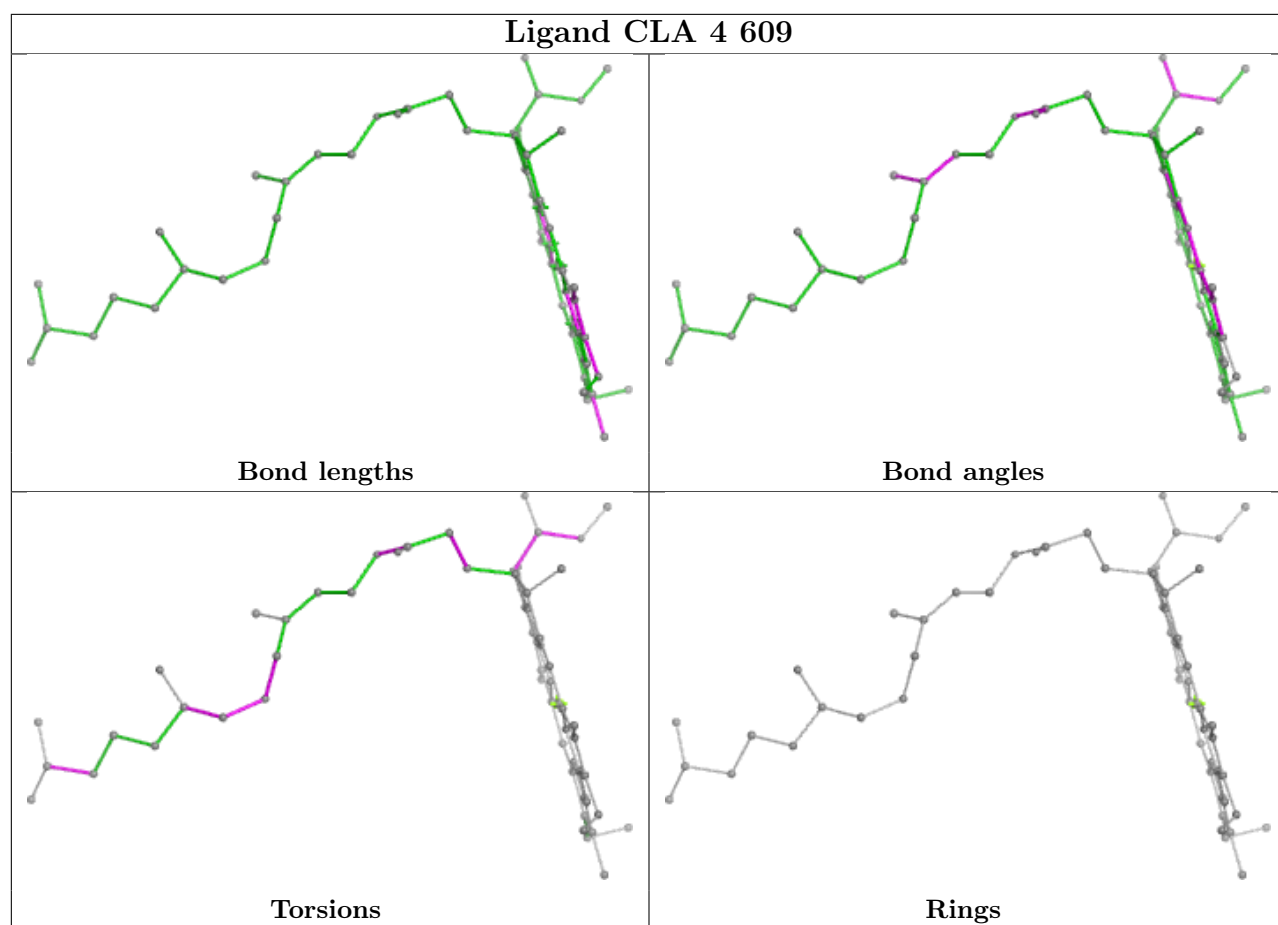
Ligand CLA 1 612

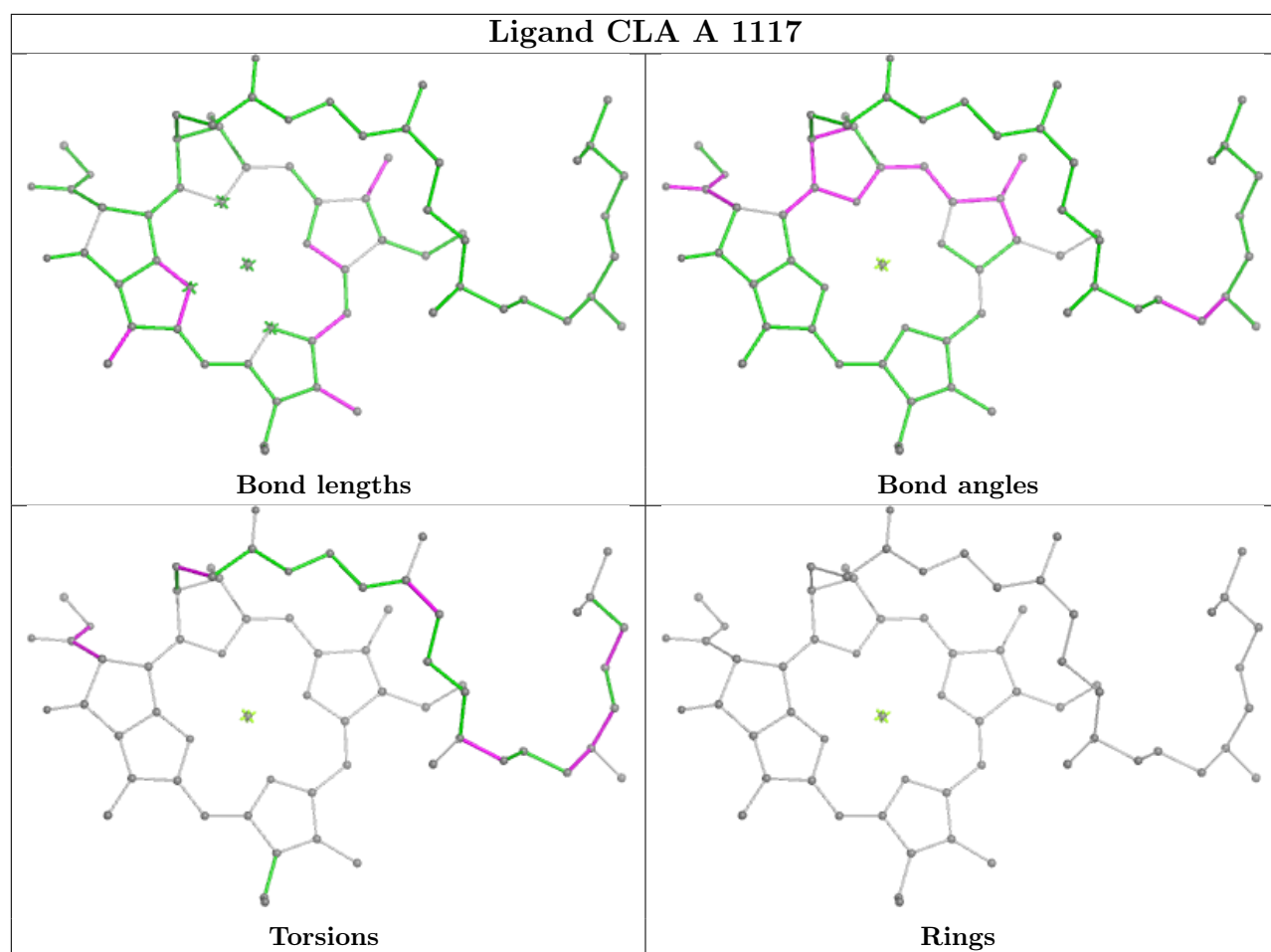


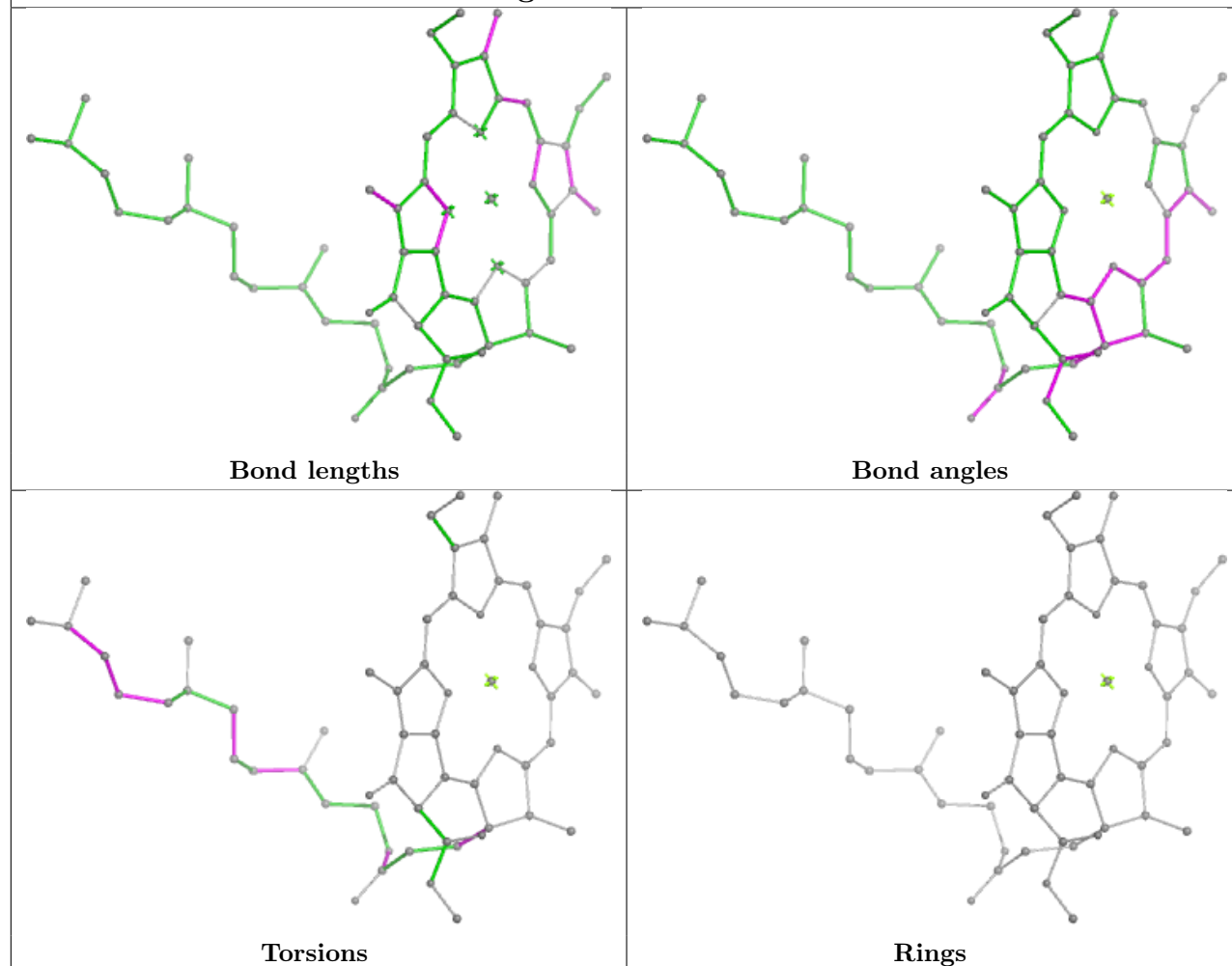
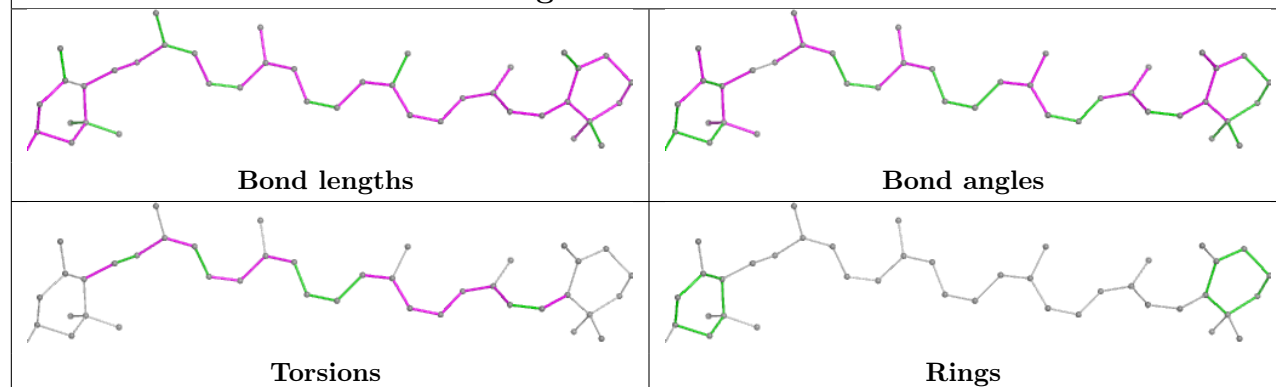
Ligand CLA 2 612

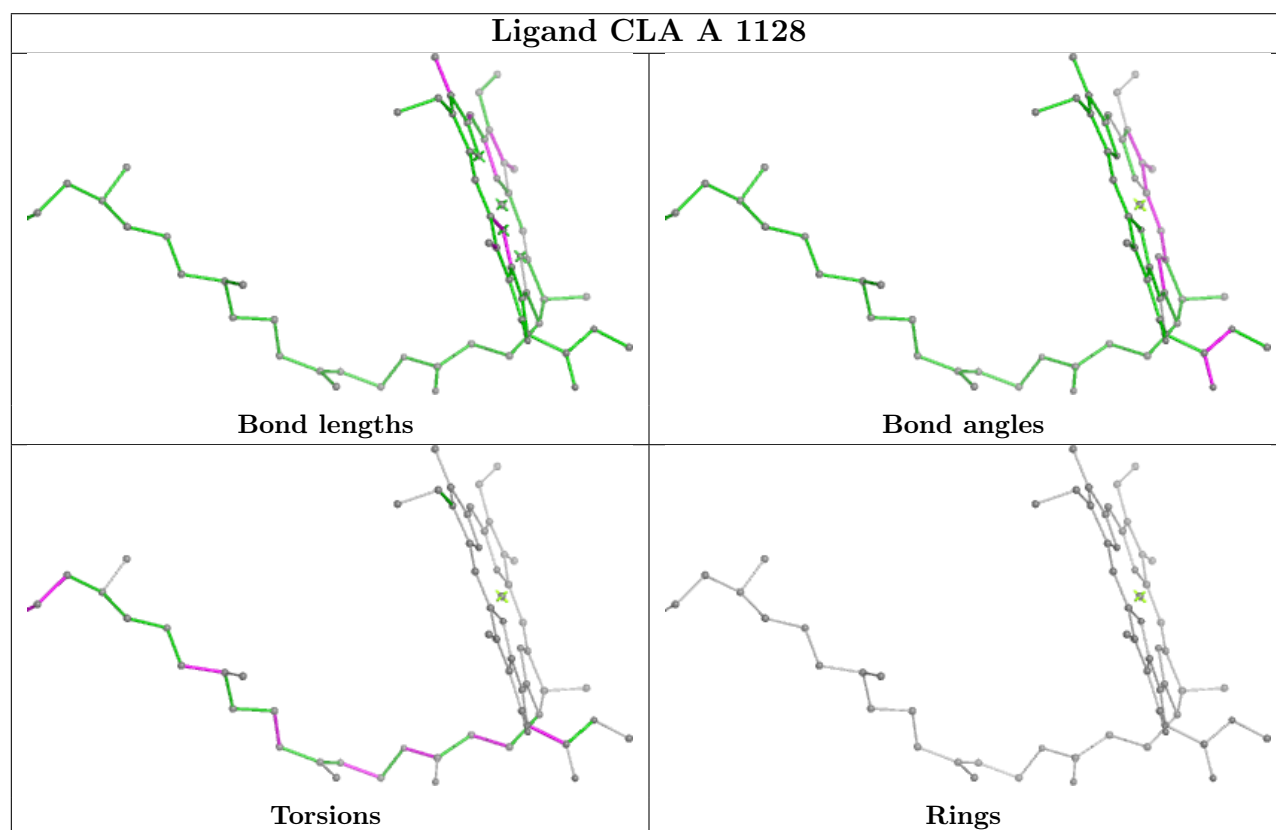
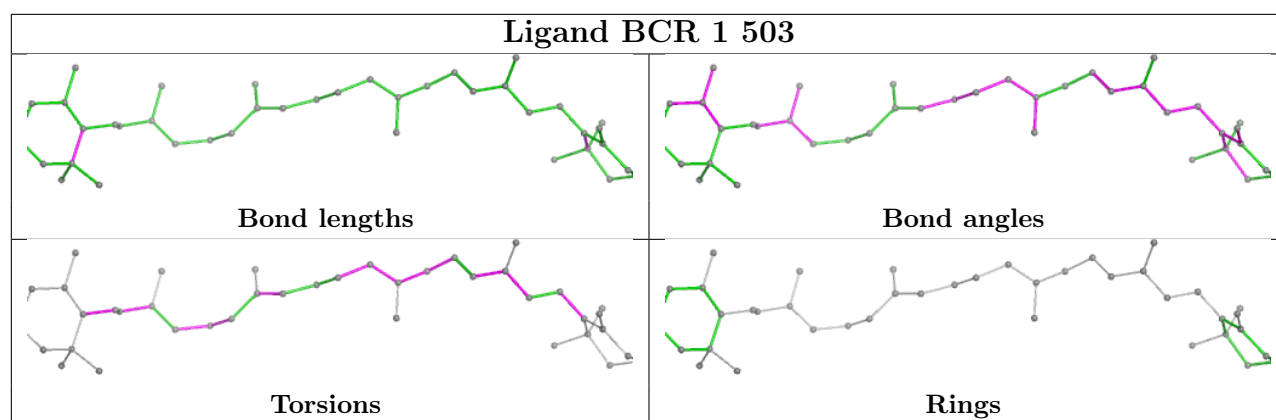




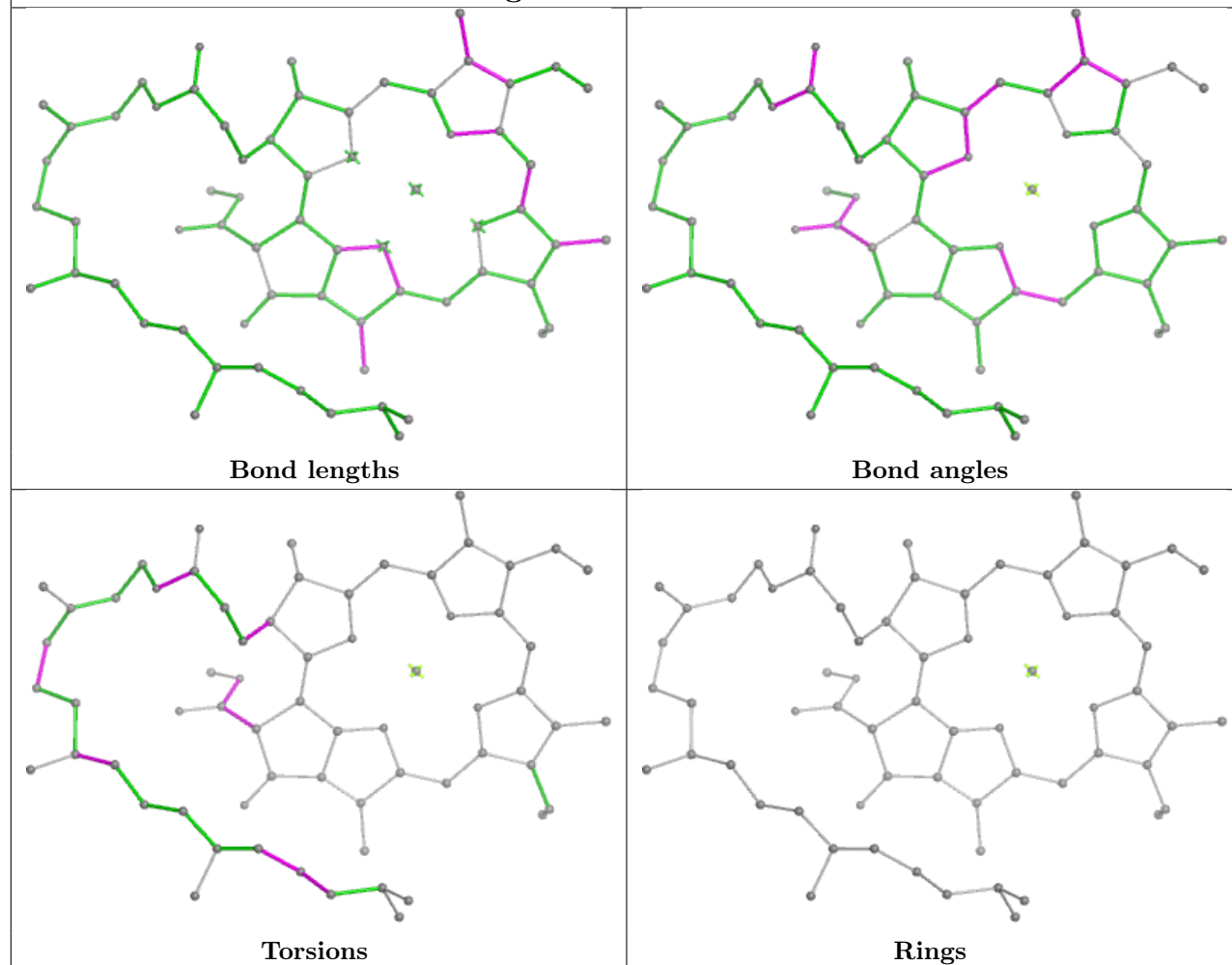




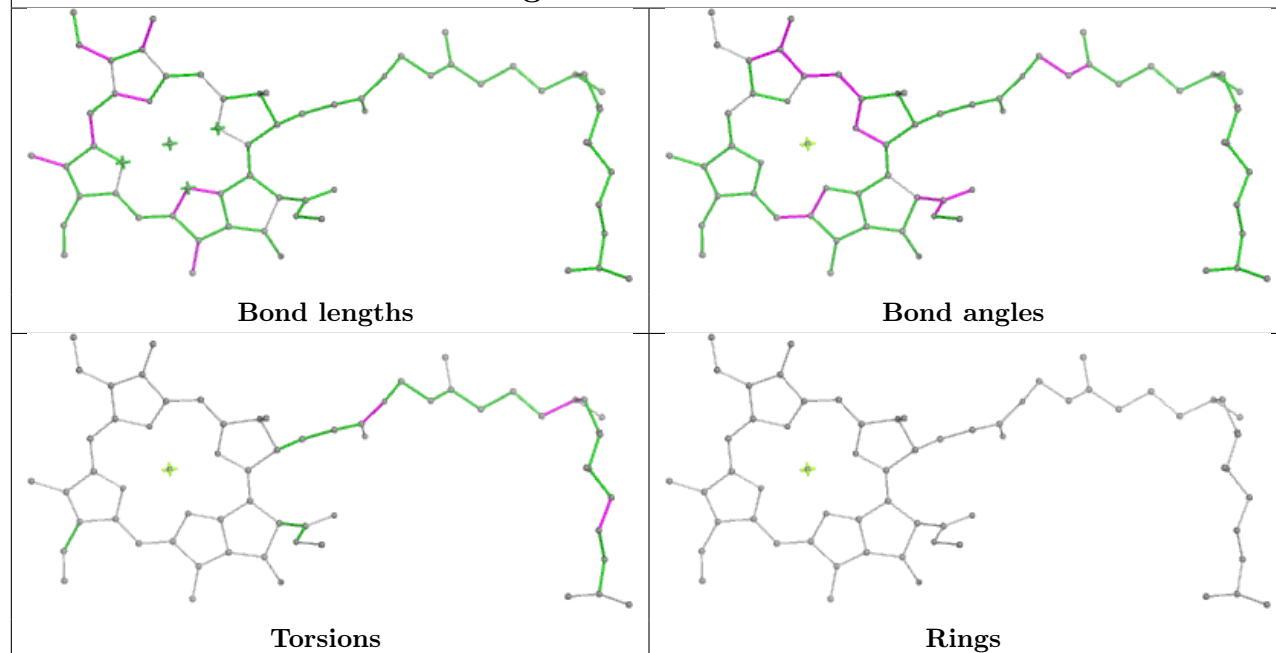
Ligand CLA 4 607**Ligand LUT 4 501**

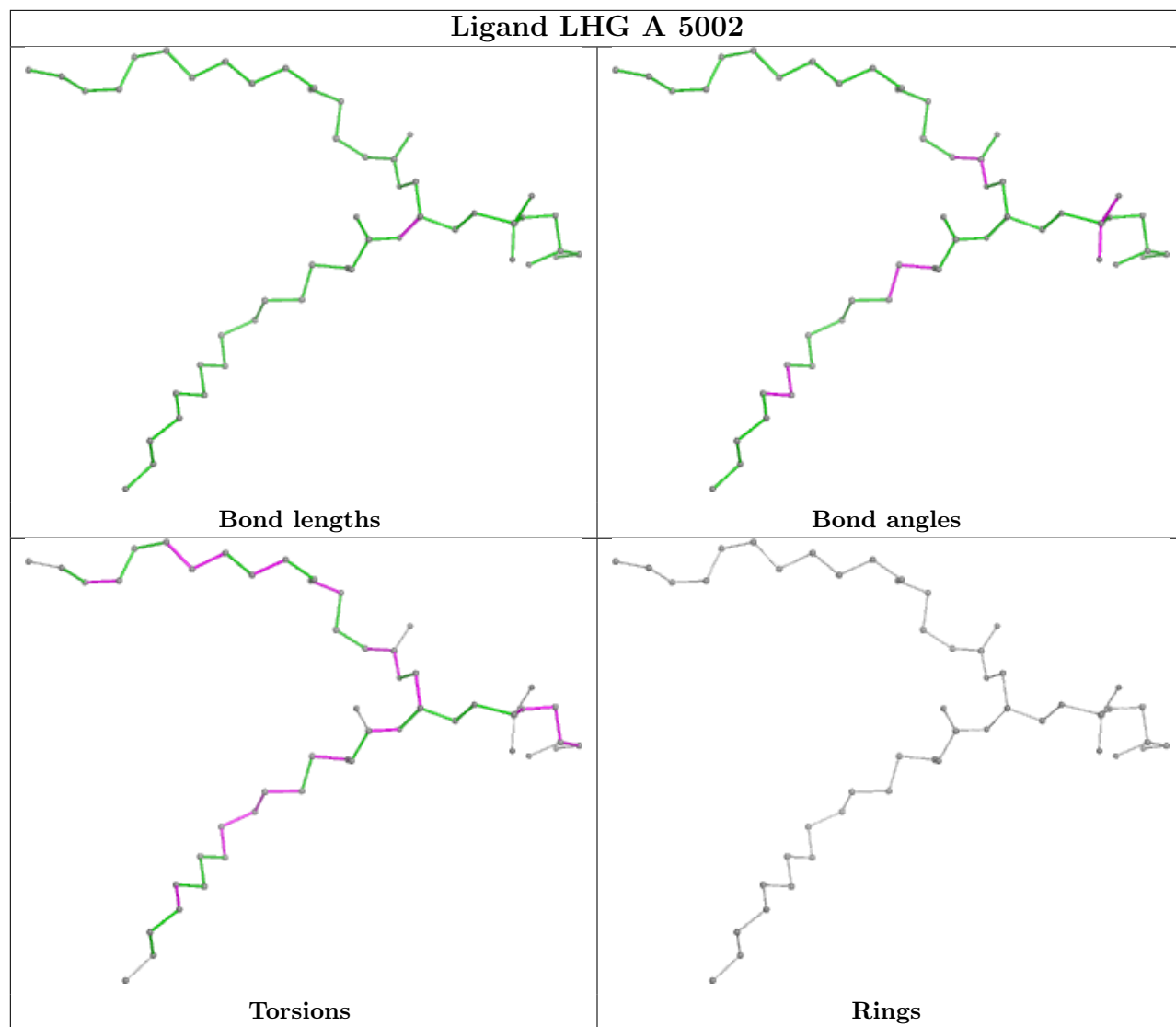


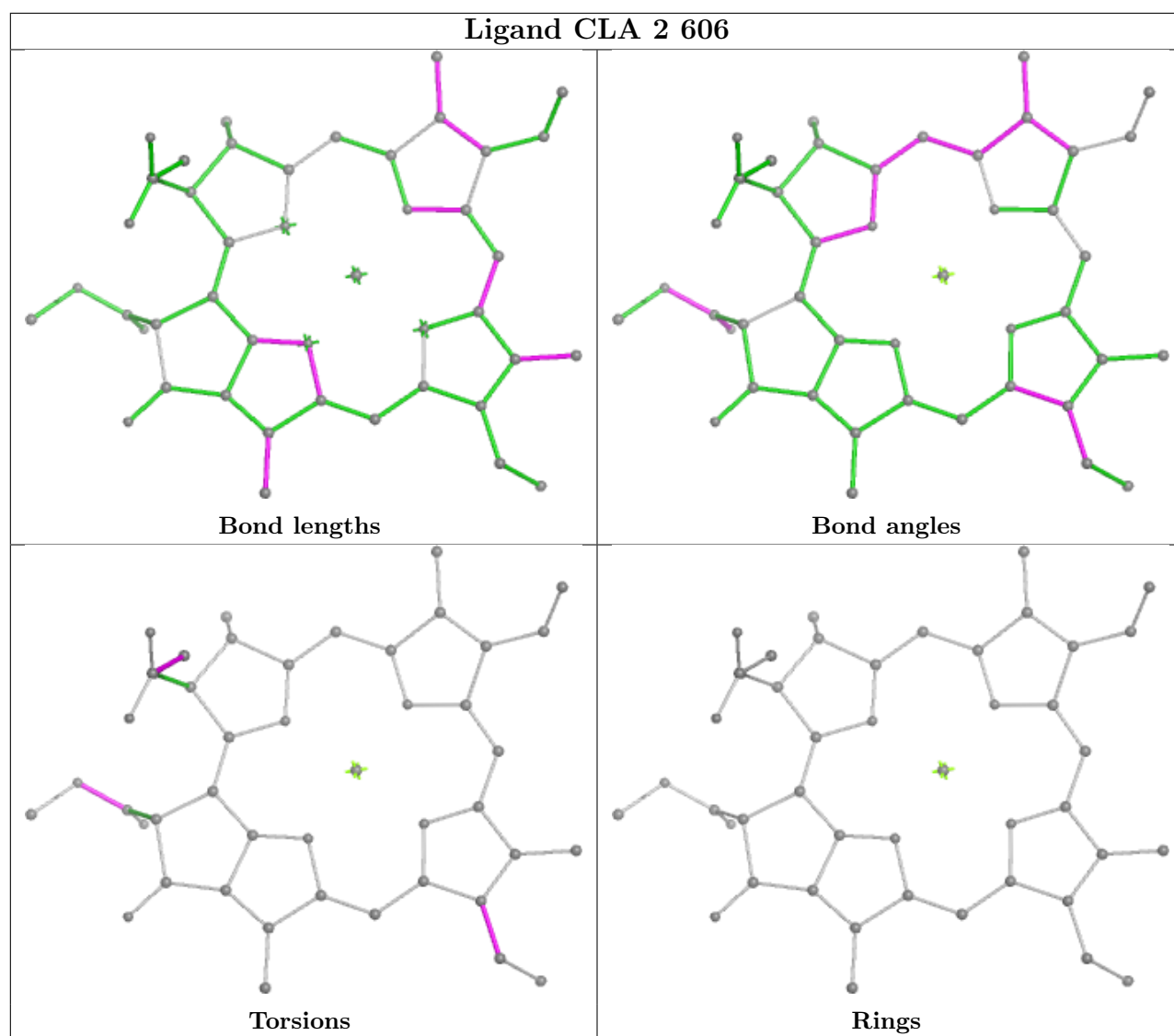
Ligand CLA B 1202



Ligand CLA B 1223







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.

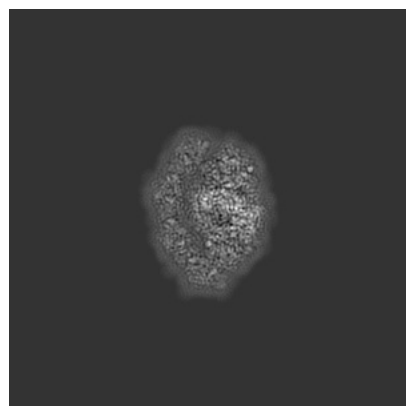
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4883. These allow visual inspection of the internal detail of the map and identification of artifacts.

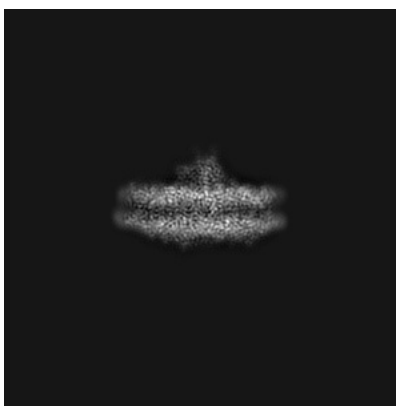
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

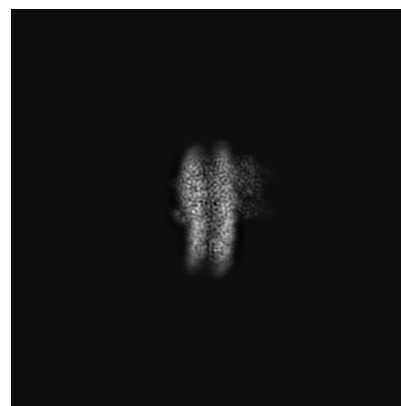
6.1.1 Primary map



X

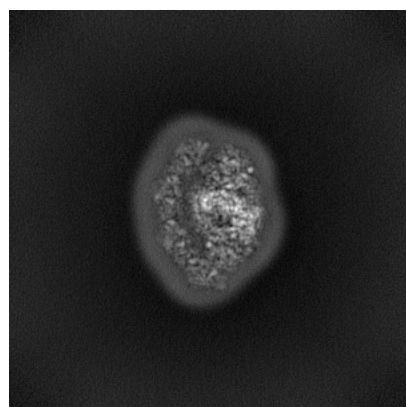


Y

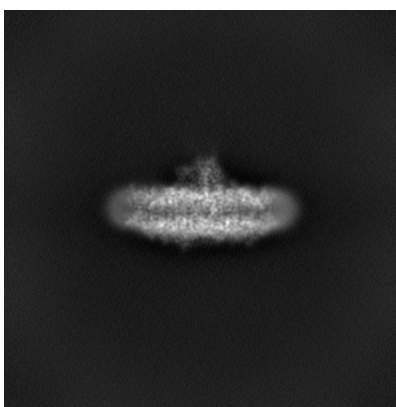


Z

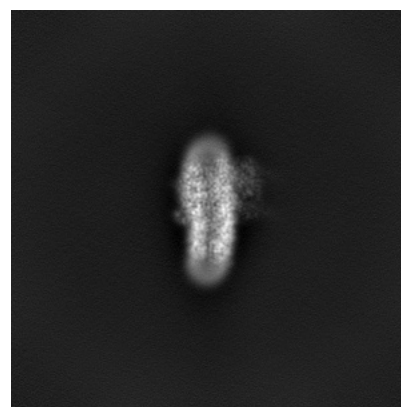
6.1.2 Raw map



X



Y

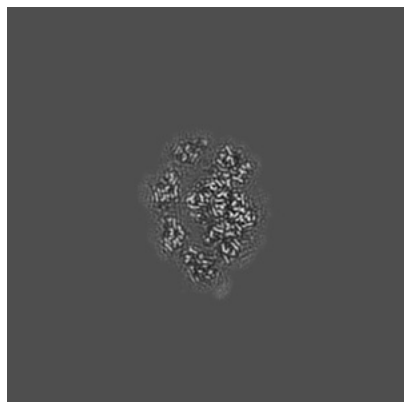


Z

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

6.2 Central slices [i](#)

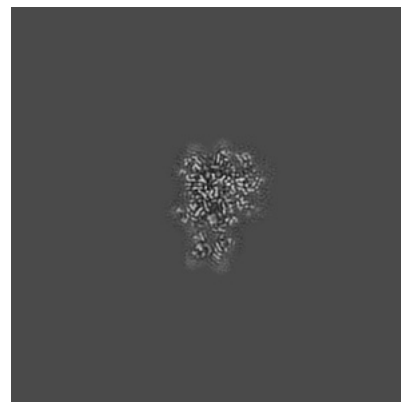
6.2.1 Primary map



X Index: 200

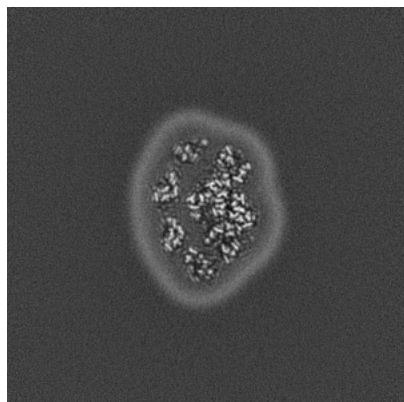


Y Index: 200

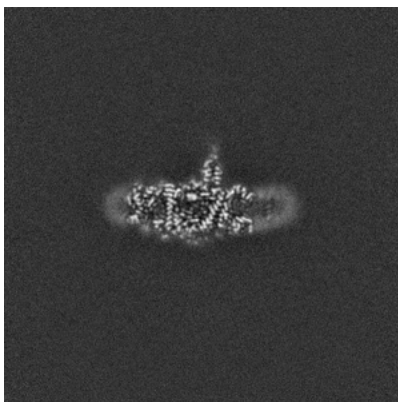


Z Index: 200

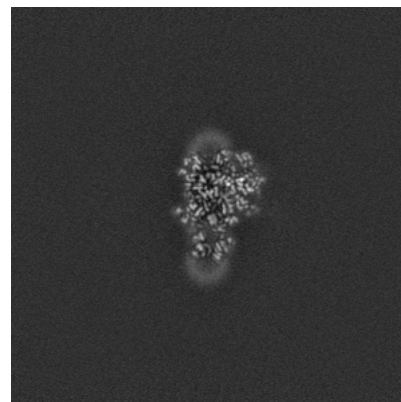
6.2.2 Raw map



X Index: 200



Y Index: 200

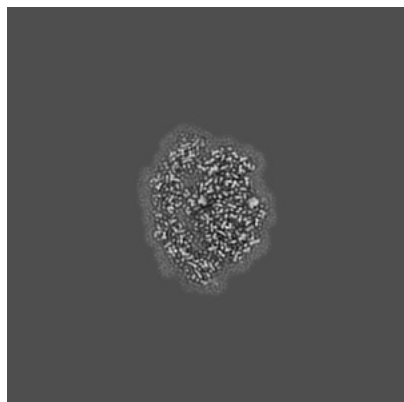


Z Index: 200

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

6.3 Largest variance slices [i](#)

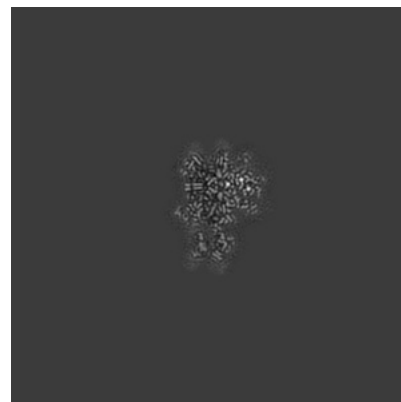
6.3.1 Primary map



X Index: 210

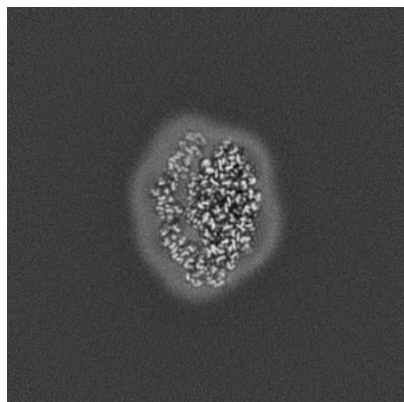


Y Index: 222

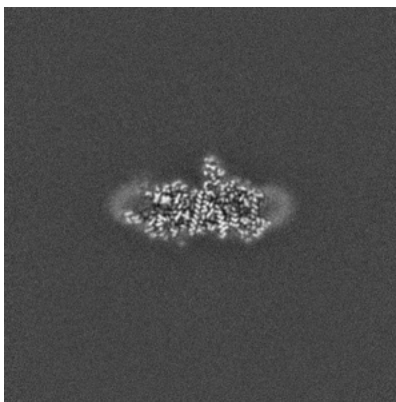


Z Index: 202

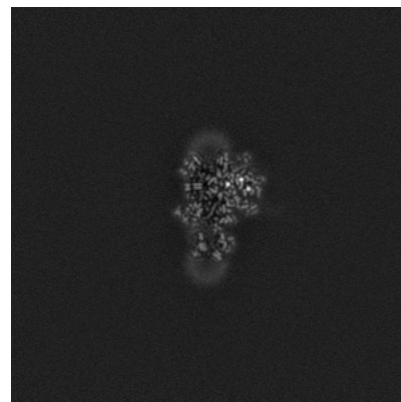
6.3.2 Raw map



X Index: 186



Y Index: 214

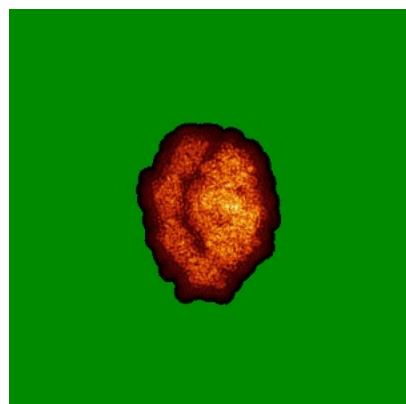


Z Index: 202

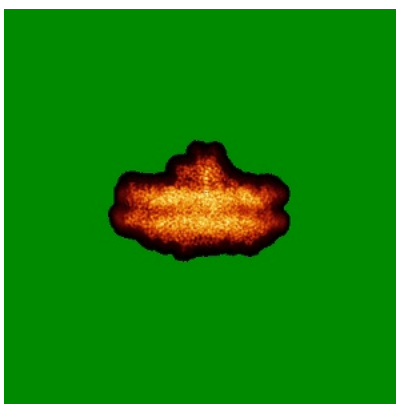
The images above show the largest variance slices of the map in three orthogonal directions.

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

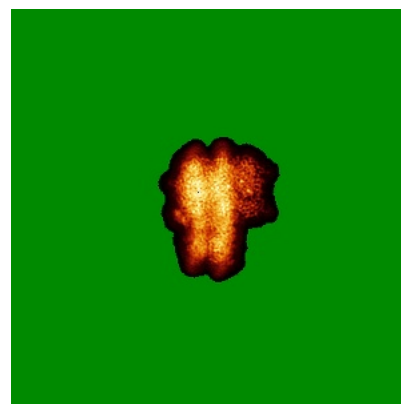
6.4.1 Primary map



X

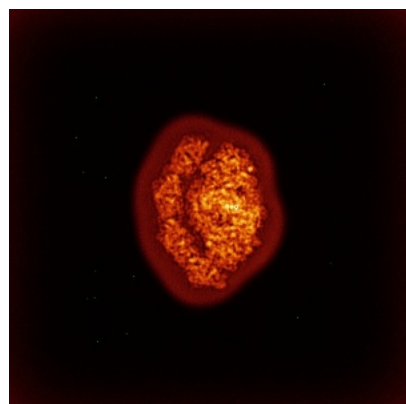


Y

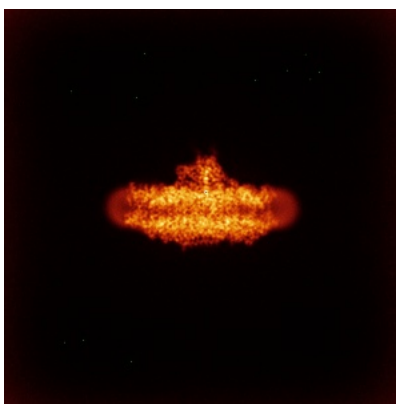


Z

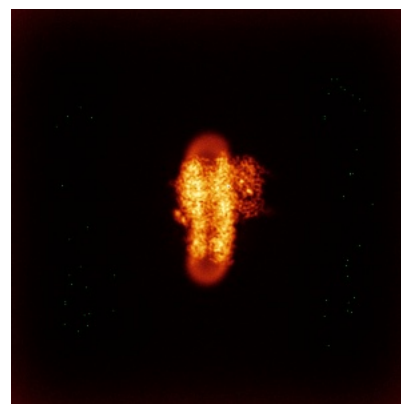
6.4.2 Raw map



X



Y

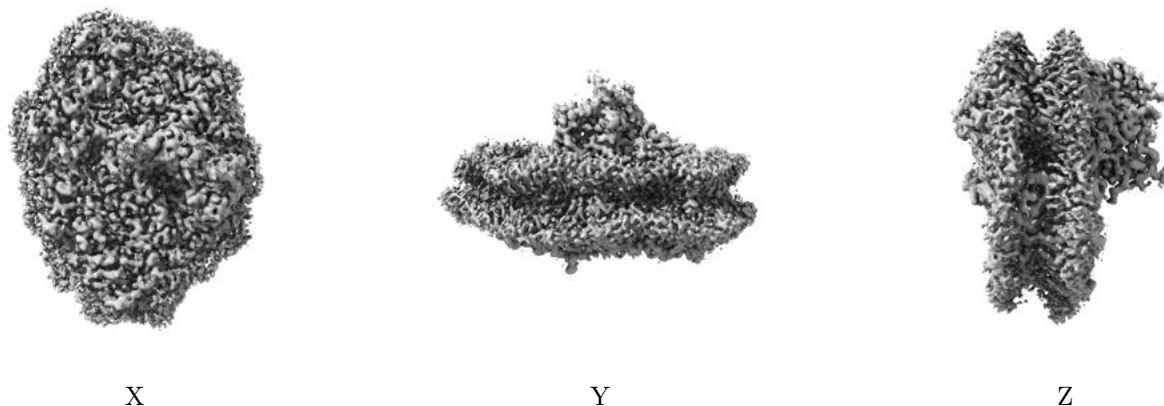


Z

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.

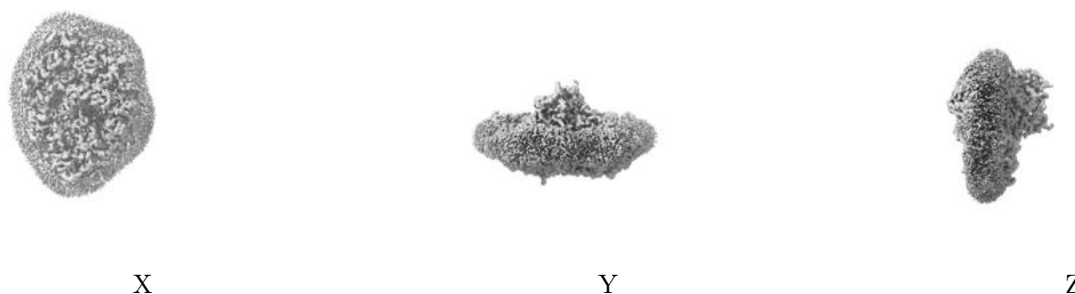
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. 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.

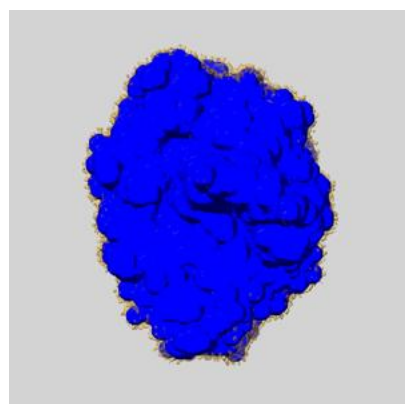
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

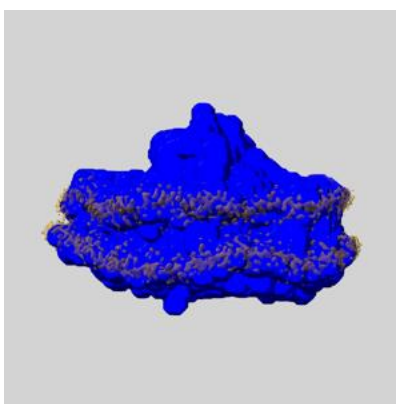
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

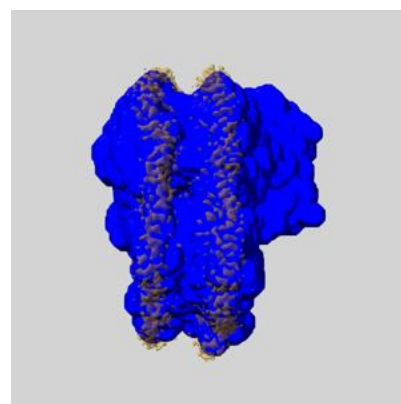
6.6.1 emd_4883_msk_1.map [i](#)



X



Y

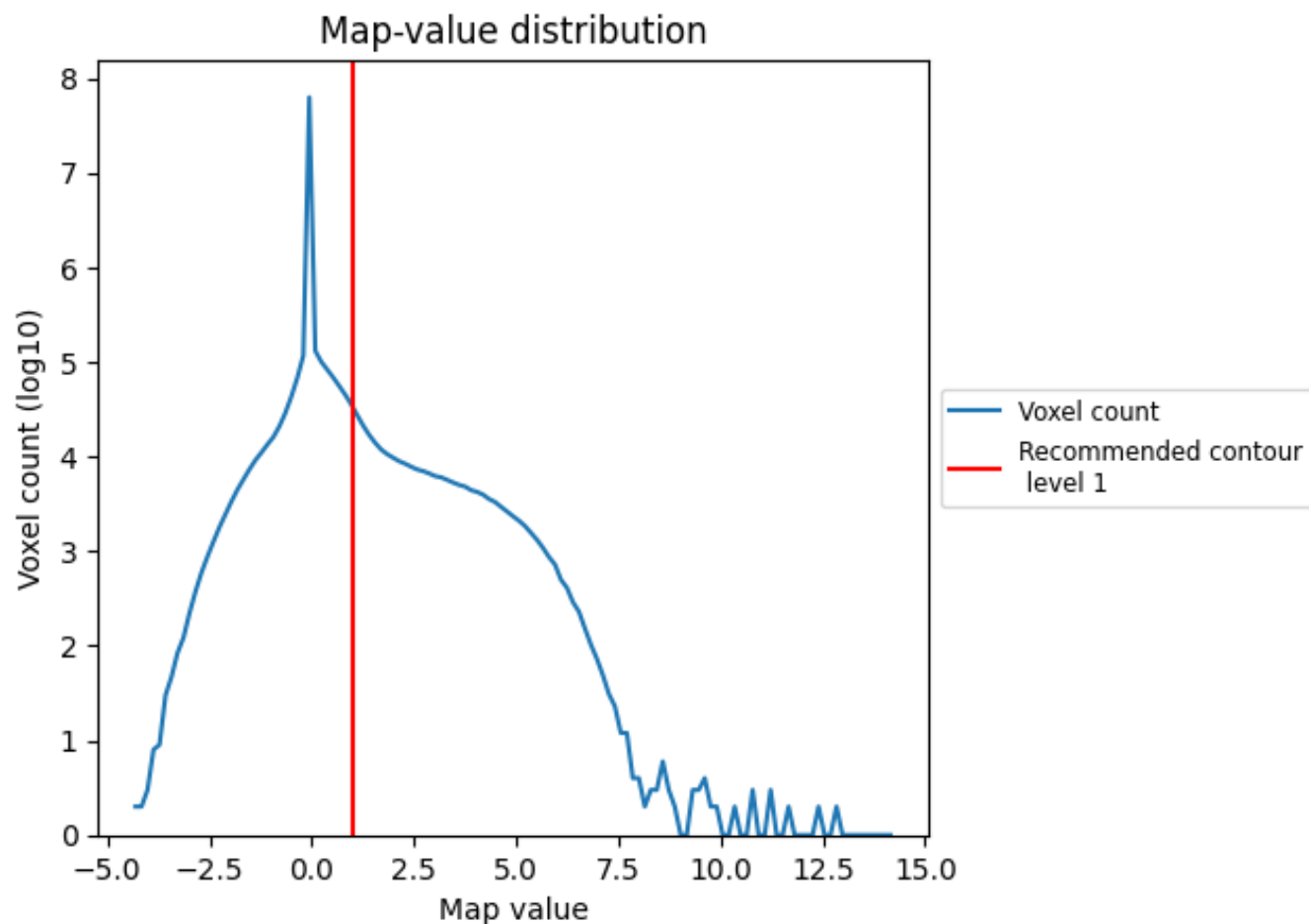


Z

7 Map analysis [i](#)

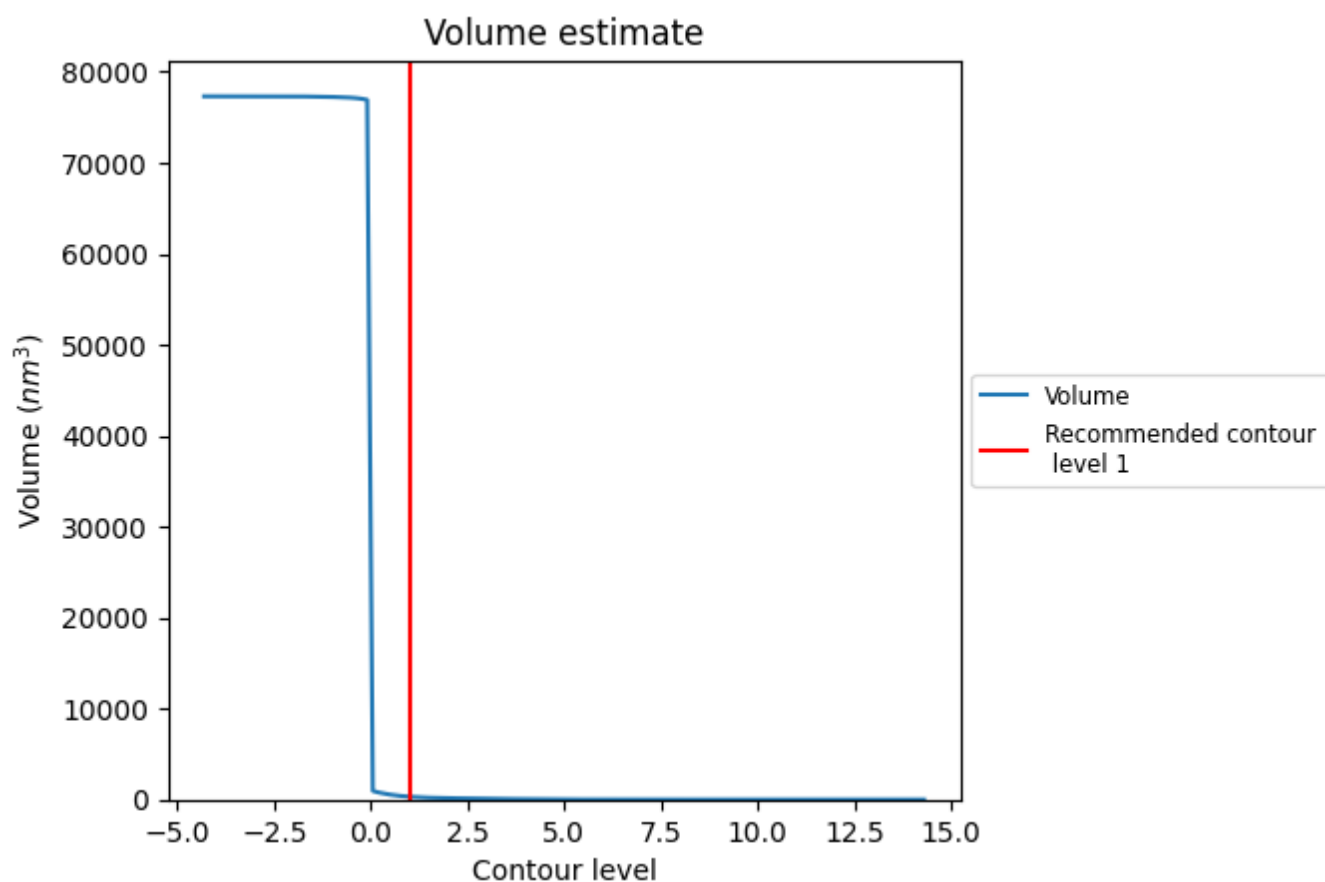
This section contains the results of statistical analysis of the map.

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.

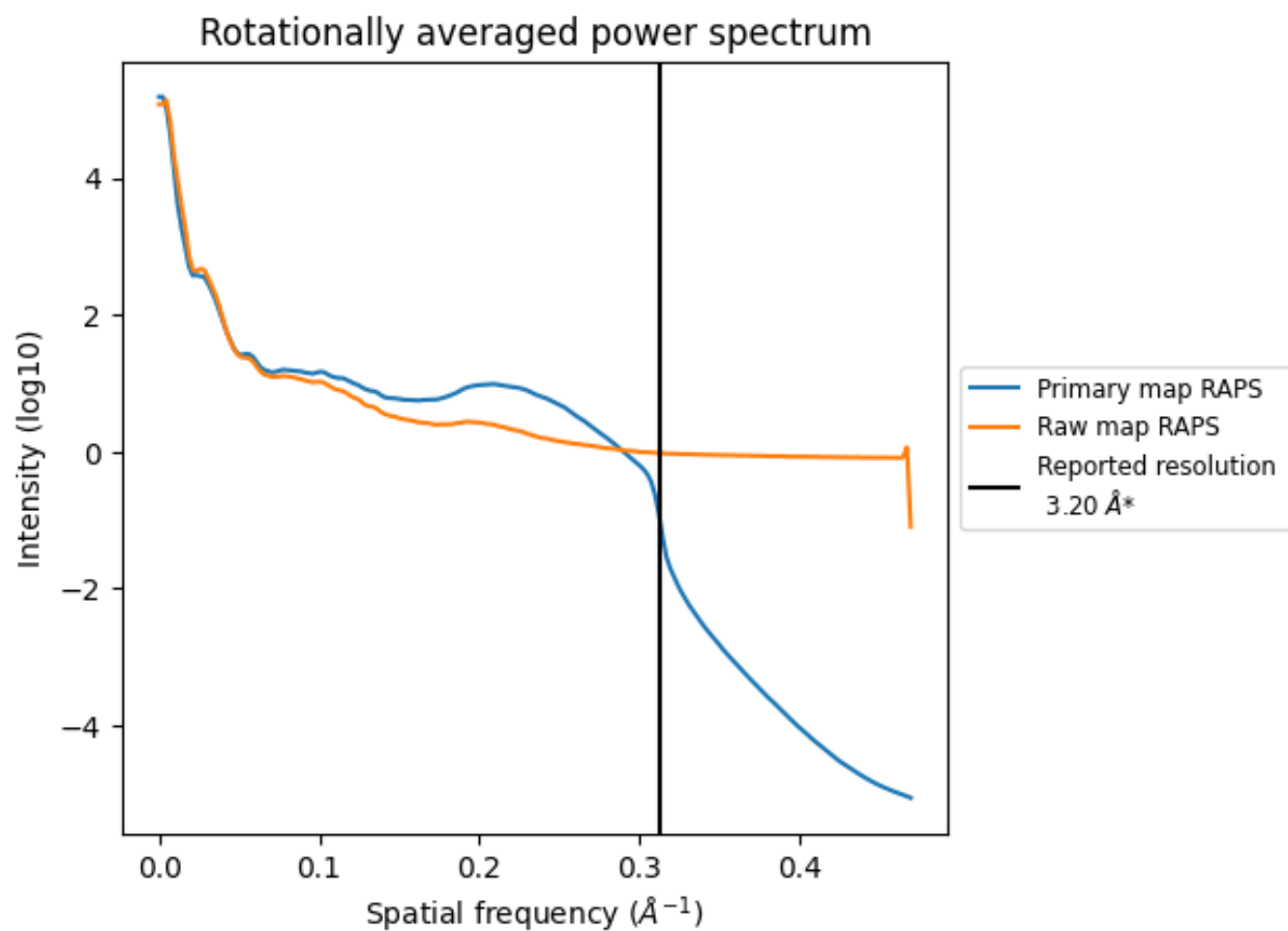
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 312 nm^3 ; this corresponds to an approximate mass of 282 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 ⓘ

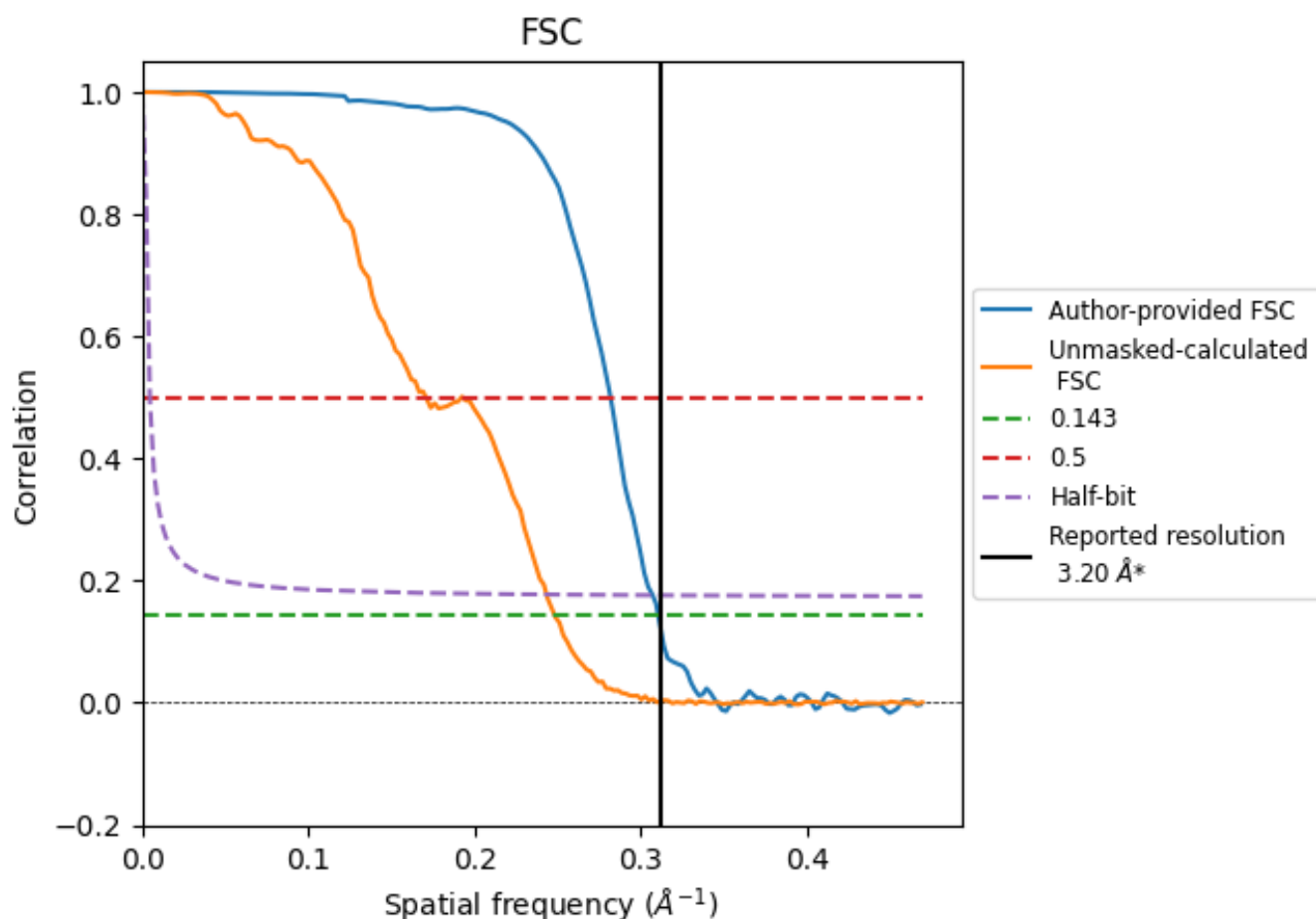


*Reported resolution corresponds to spatial frequency of 0.312 \AA^{-1}

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

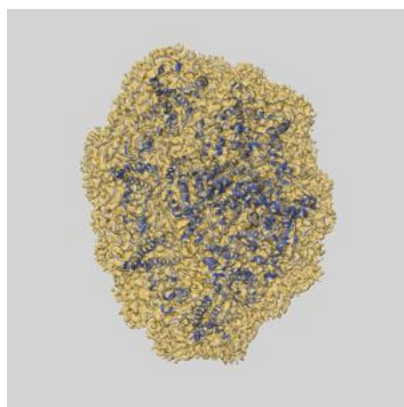
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.22	3.55	3.25
Unmasked-calculated*	4.03	5.85	4.11

*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 4.03 differs from the reported value 3.2 by more than 10 %

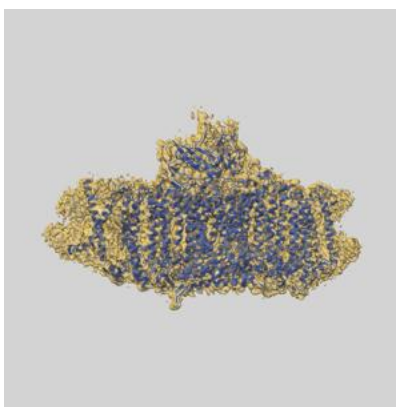
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4883 and PDB model 6RHZ. Per-residue inclusion information can be found in section 3 on page 24.

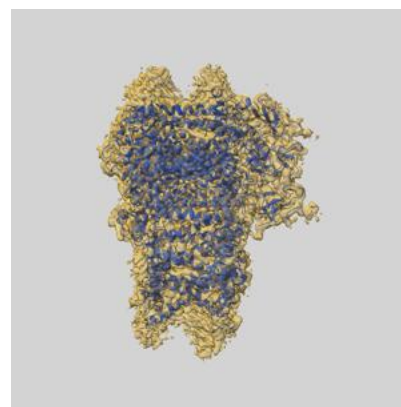
9.1 Map-model overlay [i](#)



X



Y



Z

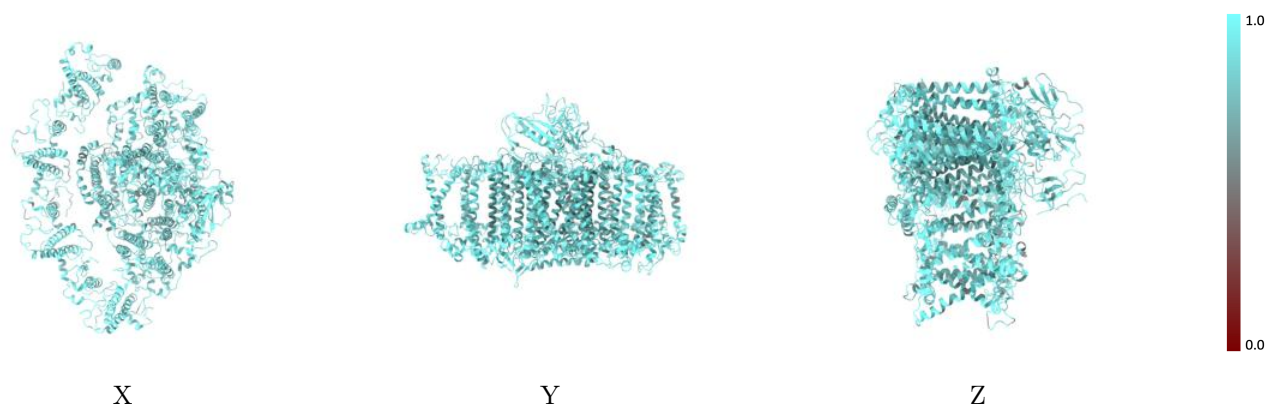
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



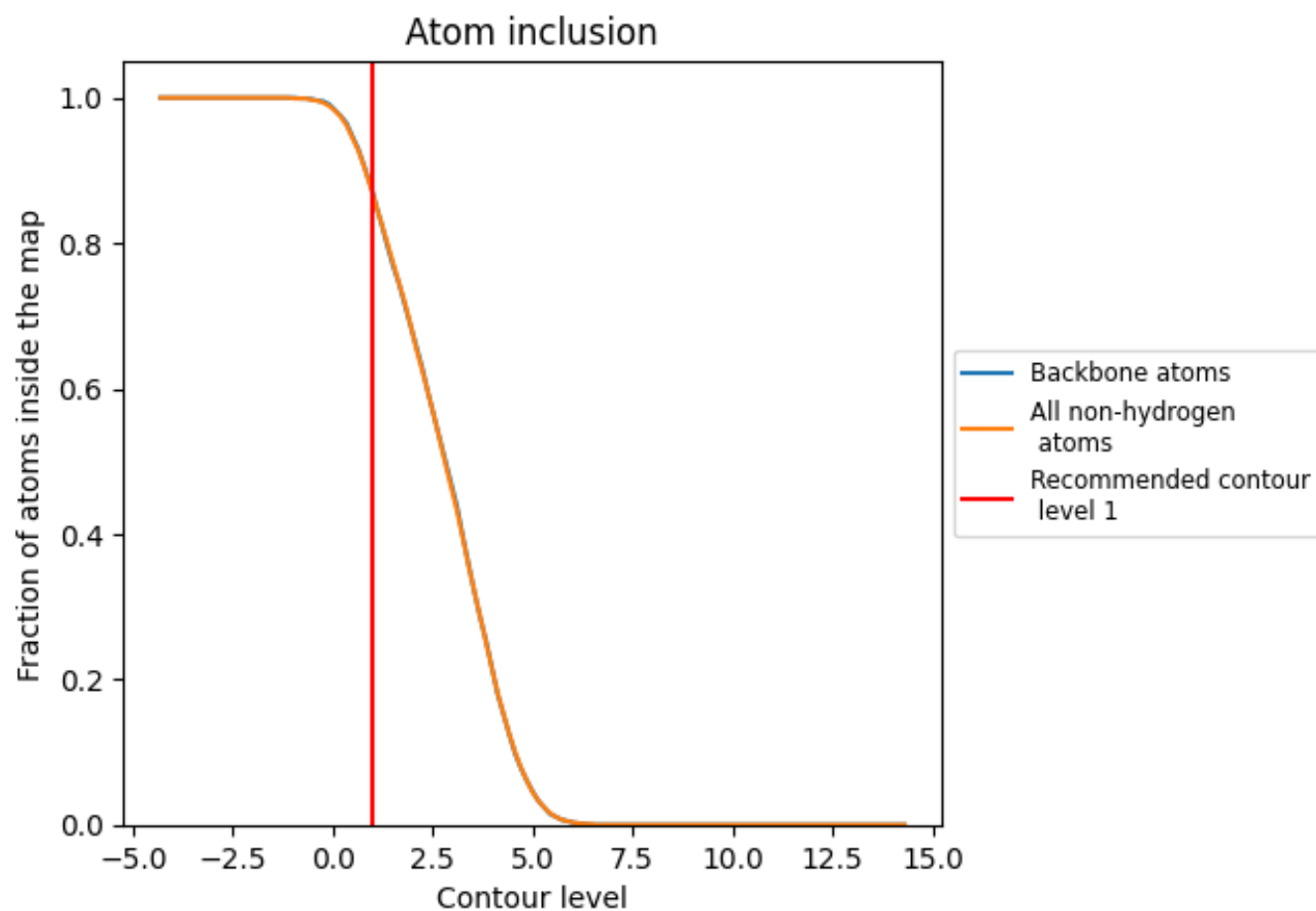
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8680	<div><div></div></div> 0.4670
1	<div><div></div></div> 0.8400	<div><div></div></div> 0.4240
2	<div><div></div></div> 0.8680	<div><div></div></div> 0.4760
3	<div><div></div></div> 0.8630	<div><div></div></div> 0.4740
4	<div><div></div></div> 0.8460	<div><div></div></div> 0.4470
A	<div><div></div></div> 0.8830	<div><div></div></div> 0.4870
B	<div><div></div></div> 0.8730	<div><div></div></div> 0.4650
C	<div><div></div></div> 0.8900	<div><div></div></div> 0.4440
D	<div><div></div></div> 0.8610	<div><div></div></div> 0.4330
E	<div><div></div></div> 0.8840	<div><div></div></div> 0.4690
F	<div><div></div></div> 0.8370	<div><div></div></div> 0.4540
J	<div><div></div></div> 0.8860	<div><div></div></div> 0.4880

1.0

0.0

<0.0