



wwPDB EM Validation Summary Report ⓘ

Sep 9, 2026 – 12:51 pm BST

PDB ID : 7BLZ / pdb_00007blz
EMDB ID : EMD-12228
Title : Red alga C.merolae Photosystem I
Authors : Nelson, N.; Klaiman, D.; Hippler, M.
Deposited on : 2021-01-19
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

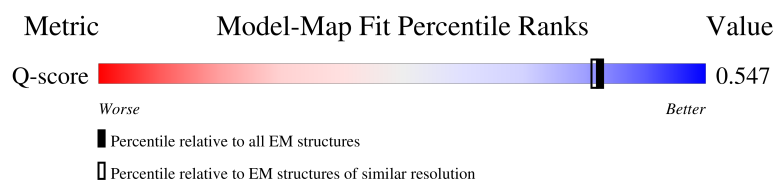
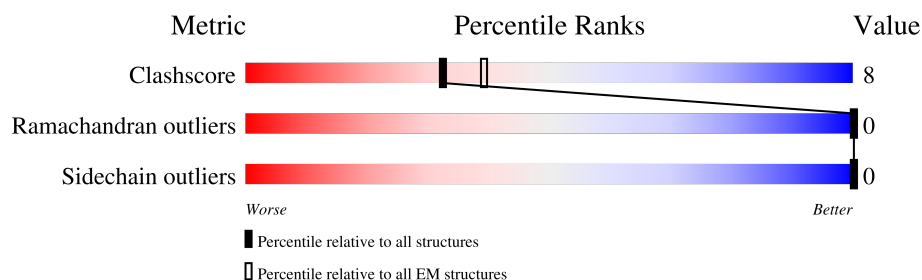
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



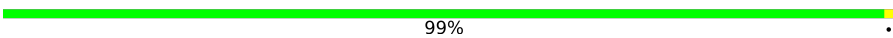
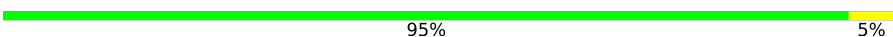
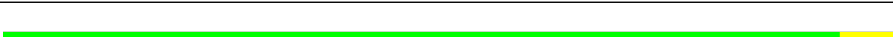
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	173	 87% 13%
2	2	179	 91% 9%
3	3	174	 83% 17%
4	A	743	 89% 11%

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Mol	Chain	Length	Quality of chain
5	B	731	
6	C	80	
7	D	138	
8	E	61	
9	F	155	
10	I	31	
11	J	38	
12	K	54	
13	L	136	
14	M	27	
15	O	97	

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
16	CLA	B	821	X	-	-	-
16	CLA	F	202	X	-	-	-
16	CLA	J	102	X	-	-	-
17	C7Z	1	612	X	-	-	-
17	C7Z	1	614	X	-	-	-
17	C7Z	1	615	X	-	-	-
17	C7Z	1	616	X	-	-	-
17	C7Z	2	614	X	-	-	-
17	C7Z	2	615	X	-	-	-
17	C7Z	3	201	X	-	-	-
17	C7Z	3	215	X	-	-	-
17	C7Z	3	216	X	-	-	-
17	C7Z	3	217	X	-	-	-
17	C7Z	3	218	X	-	-	-
17	C7Z	A	843	X	-	-	-
17	C7Z	J	104	X	-	-	-
18	RRX	1	613	X	-	-	-
18	RRX	2	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	RRX	A	847	X	-	-	-
18	RRX	J	103	X	X	-	-
18	RRX	K	103	X	-	-	-
20	ERG	1	618	X	-	-	-
20	ERG	2	618	X	-	-	-
20	ERG	2	621	X	-	-	-
22	PGT	2	619	X	-	-	-
22	PGT	B	848	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 68571 atoms, of which 34687 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 Similar to light harvesting protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	173	Total	C	H	N	O	S	0	0
			2734	906	1353	232	235	8		

- Molecule 2 is a protein called Similar to chlorophyll a/b-binding protein, CP24.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	179	Total	C	H	N	O	S	0	0
			2780	906	1385	237	244	8		

- Molecule 3 is a protein called Lhcr3.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	3	174	Total	C	H	N	O	S	0	0
			2689	871	1348	226	237	7		

- Molecule 4 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	A	743	Total	C	H	N	O	S	0	0
			11555	3802	5740	999	987	27		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	B	731	Total	C	H	N	O	S	0	0
			11464	3827	5645	982	991	19		

- Molecule 6 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	80	Total	C	H	N	O	S	0	0
			1173	367	576	104	114	12		

- Molecule 7 is a protein called Photosystem I p700 chlorophyll A apoprotein A2.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	138	Total	C	H	N	O	S	0	0
			2187	694	1093	192	203	5		

- Molecule 8 is a protein called Photosystem I iron-sulfur center subunit VII.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	E	61	Total	C	H	N	O		0	0
			1002	322	509	79	92			

- Molecule 9 is a protein called PSI-F.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	F	155	Total	C	H	N	O	S	0	0
			2513	816	1243	215	235	4		

- Molecule 10 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	I	31	Total	C	H	N	O	S	0	0
			483	158	253	32	39	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	J	38	Total	C	H	N	O	S	0	0
			639	214	327	46	51	1		

- Molecule 12 is a protein called PSI-K.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	K	54	Total	C	H	N	O	S	0	0
			809	253	419	65	68	4		

- Molecule 13 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	L	136	Total	C	H	N	O	S	0	0
			2096	682	1057	170	185	2		

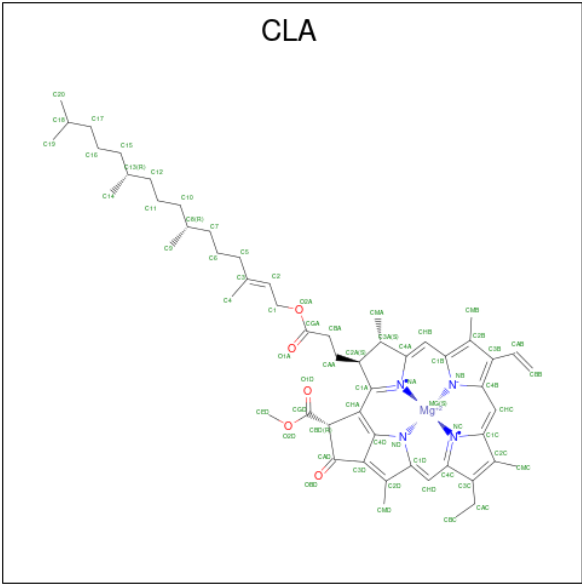
- Molecule 14 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	M	27	Total	C	H	N	O	S	0	0
			430	136	226	32	34	2		

- Molecule 15 is a protein called PsaO.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	97	Total	C	H	N	O	0	0
			1489	505	742	113	129		

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						AltConf
16	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			118	49	59	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			120	50	60	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
16	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	1	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			131	53	68	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	3	1	Total	C	H	Mg	N	O	0
			129	53	66	1	4	5	
16	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	3	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	3	1	Total	C	H	Mg	N	O	0
			126	52	64	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
16	3	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	3	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	3	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	3	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	3	1	Total 113	C 48	H 55	Mg 1	N 4	O 5	0
16	3	1	Total 79	C 36	H 33	Mg 1	N 4	O 5	0
16	3	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
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16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	A	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
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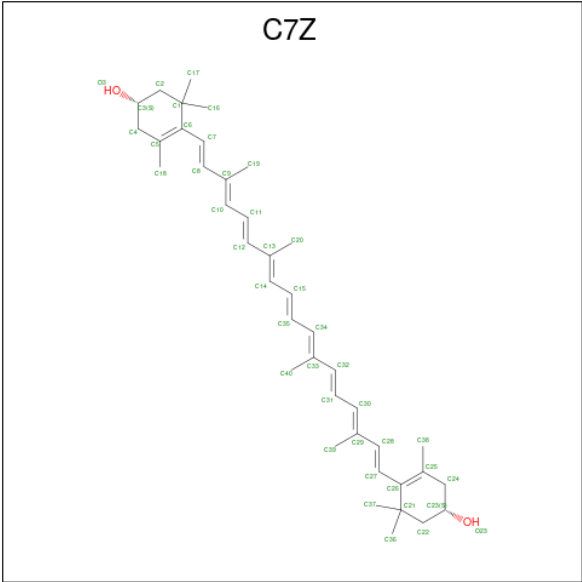
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16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
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16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 138	C 55	H 73	Mg 1	N 4	O 5	0
16	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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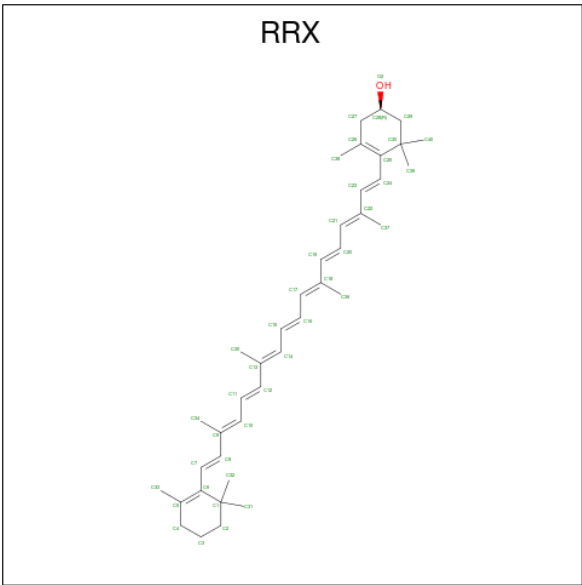
Mol	Chain	Residues	Atoms						AltConf
16	B	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	B	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	F	1	Total	C	H	Mg	N	O	0
			123	51	62	1	4	5	
16	F	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	F	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	I	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	I	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	J	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	K	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	K	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	L	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	L	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	L	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	
16	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	O	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	O	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
16	O	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 17 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: C₄₀H₅₆O₂).



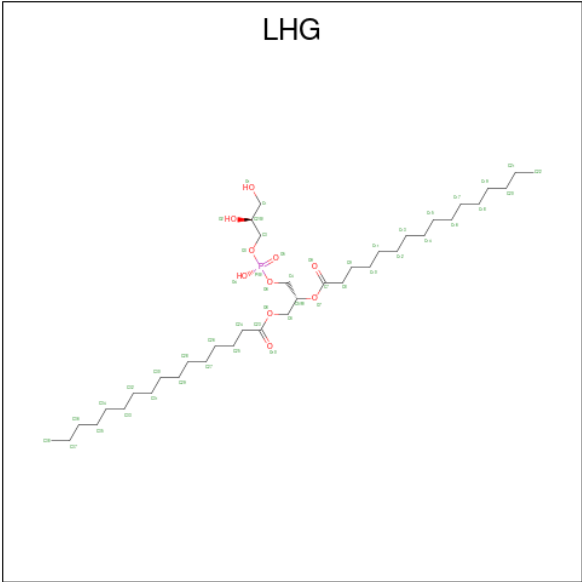
Mol	Chain	Residues	Atoms			AltConf
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			42	40	2	
17	1	1	Total	C	O	0
			42	40	2	
17	1	1	Total	C	O	0
			42	40	2	
17	1	1	Total	C	O	0
			42	40	2	
17	2	1	Total	C	O	0
			42	40	2	
17	2	1	Total	C	O	0
			42	40	2	
17	3	1	Total	C	O	0
			42	40	2	
17	3	1	Total	C	O	0
			42	40	2	
17	3	1	Total	C	O	0
			42	40	2	
17	3	1	Total	C	O	0
			42	40	2	
17	A	1	Total	C	O	0
			42	40	2	
17	J	1	Total	C	O	0
			42	40	2	

- Molecule 18 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: C₄₀H₅₆O).



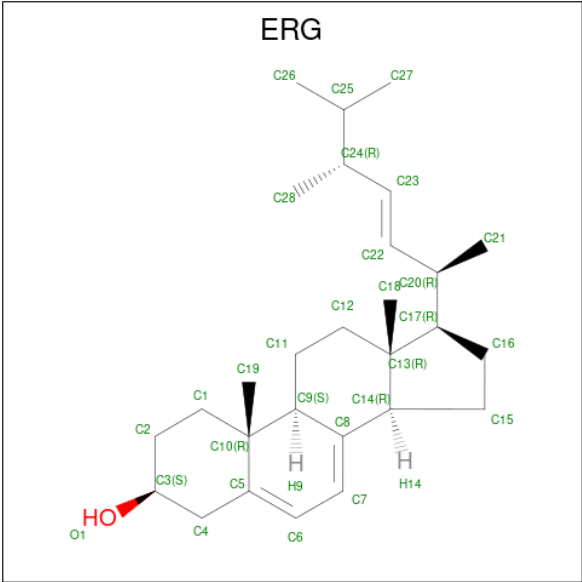
Mol	Chain	Residues	Atoms				AltConf
18	1	1	Total	C	H	O	0
			97	40	56	1	
18	2	1	Total	C	H	O	0
			97	40	56	1	
18	A	1	Total	C	H	O	0
			96	40	55	1	
18	J	1	Total	C	H	O	0
			97	40	56	1	
18	K	1	Total	C	H	O	0
			97	40	56	1	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



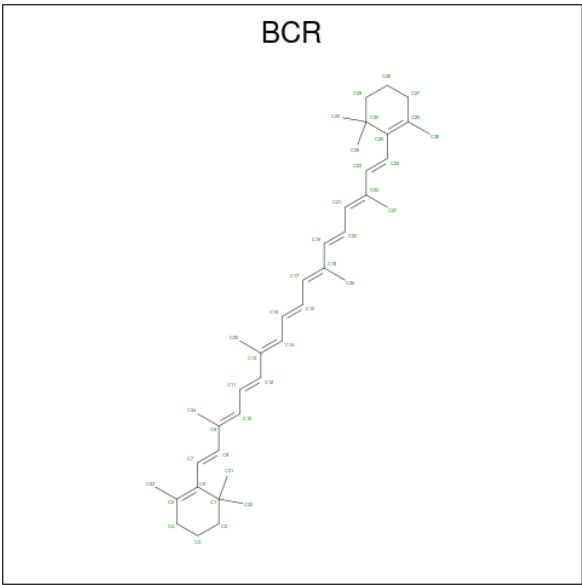
Mol	Chain	Residues	Atoms					AltConf
19	1	1	Total	C	H	O	P	0
			123	38	74	10	1	
19	2	1	Total	C	H	O	P	0
			123	38	74	10	1	
19	3	1	Total	C	H	O	P	0
			123	38	74	10	1	
19	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
19	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
19	B	1	Total	C	H	O	P	0
			108	34	63	10	1	

- Molecule 20 is ERGOSTEROL (CCD ID: ERG) (formula: C₂₈H₄₄O).



Mol	Chain	Residues	Atoms				AltConf
20	1	1	Total	C	H	O	0
			67	28	38	1	
20	2	1	Total	C	H	O	0
			67	28	38	1	
20	2	1	Total	C	H	O	0
			67	28	38	1	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



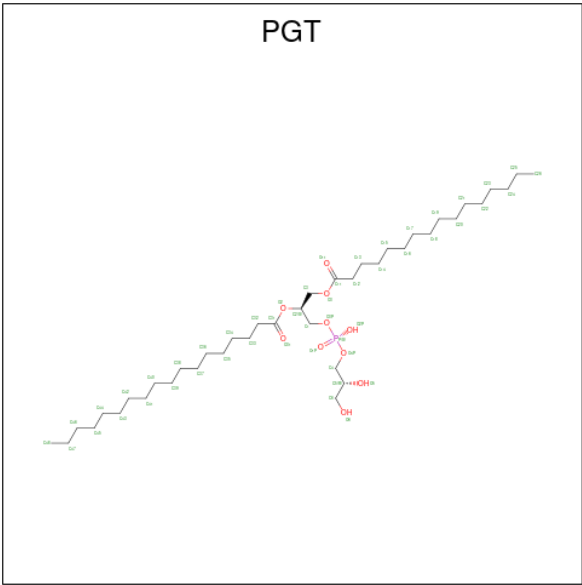
Mol	Chain	Residues	Atoms				AltConf
21	2	1	Total	C	H		0
			93	40	53		

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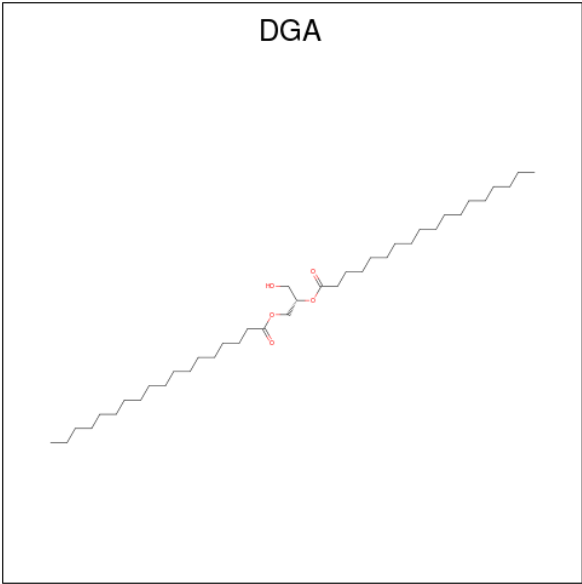
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total 92	C 40	H 52	0
21	A	1	Total 92	C 40	H 52	0
21	A	1	Total 92	C 40	H 52	0
21	A	1	Total 92	C 40	H 52	0
21	A	1	Total 92	C 40	H 52	0
21	B	1	Total 92	C 40	H 52	0
21	B	1	Total 92	C 40	H 52	0
21	B	1	Total 91	C 40	H 51	0
21	B	1	Total 91	C 40	H 51	0
21	B	1	Total 92	C 40	H 52	0
21	B	1	Total 92	C 40	H 52	0
21	B	1	Total 92	C 40	H 52	0
21	B	1	Total 91	C 40	H 51	0
21	F	1	Total 92	C 40	H 52	0
21	F	1	Total 92	C 40	H 52	0
21	I	1	Total 91	C 40	H 51	0
21	K	1	Total 91	C 40	H 51	0
21	L	1	Total 92	C 40	H 52	0
21	L	1	Total 92	C 40	H 52	0
21	L	1	Total 92	C 40	H 52	0
21	O	1	Total 92	C 40	H 52	0

- Molecule 22 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



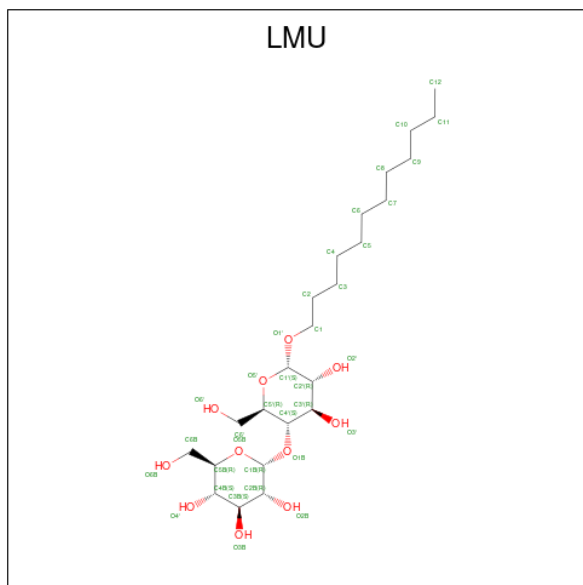
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
22	2	1	81	24	46	10	1	0
			Total	C	H	O	P	
22	B	1	81	24	46	10	1	0
			Total	C	H	O	P	

- Molecule 23 is DIACYL GLYCEROL (CCD ID: DGA) (formula: C₃₉H₇₆O₅).



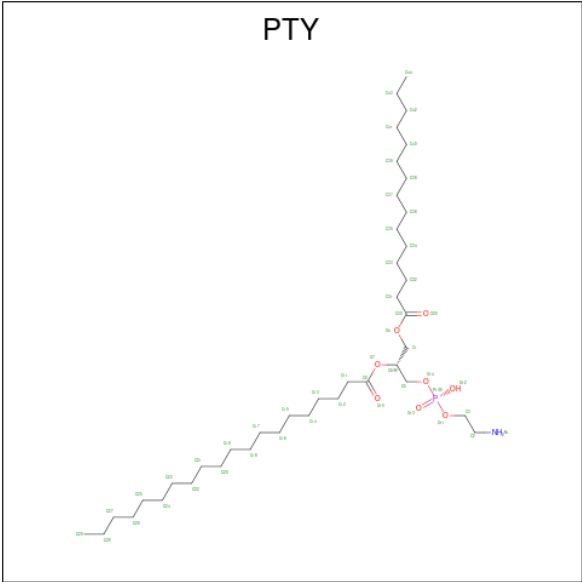
Mol	Chain	Residues	Atoms				AltConf
23	2	1	Total	C	H	O	0
			120	39	76	5	
23	J	1	Total	C	H	O	0
			120	39	76	5	

- Molecule 24 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



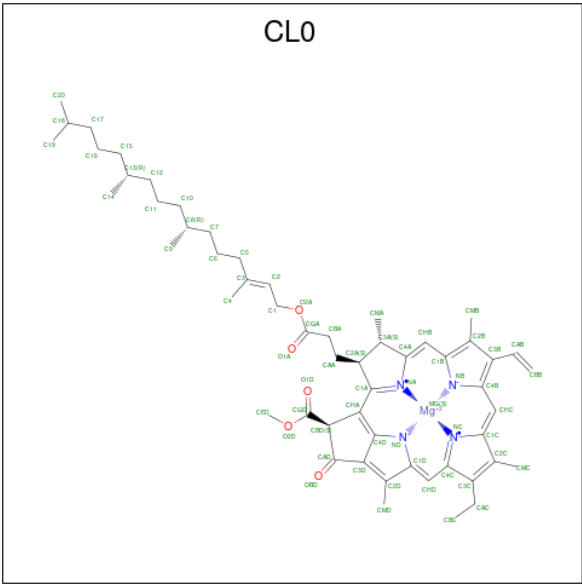
Mol	Chain	Residues	Atoms				AltConf
24	3	1	Total	C	H	O	0
			81	24	46	11	
24	A	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 25 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



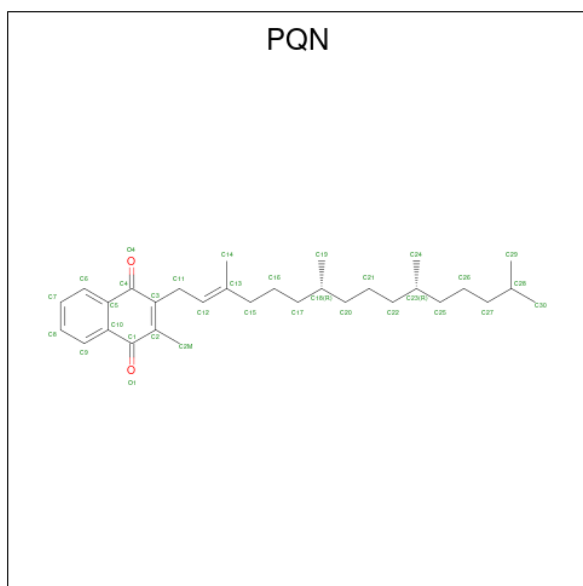
Mol	Chain	Residues	Atoms						AltConf
25	3	1	Total	C	H	N	O	P	0
			129	40	79	1	8	1	
25	3	1	Total	C	H	N	O	P	0
			129	40	79	1	8	1	
25	A	1	Total	C	H	N	O	P	0
			113	37	66	1	8	1	
25	L	1	Total	C	H	N	O	P	0
			129	40	79	1	8	1	

- Molecule 26 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



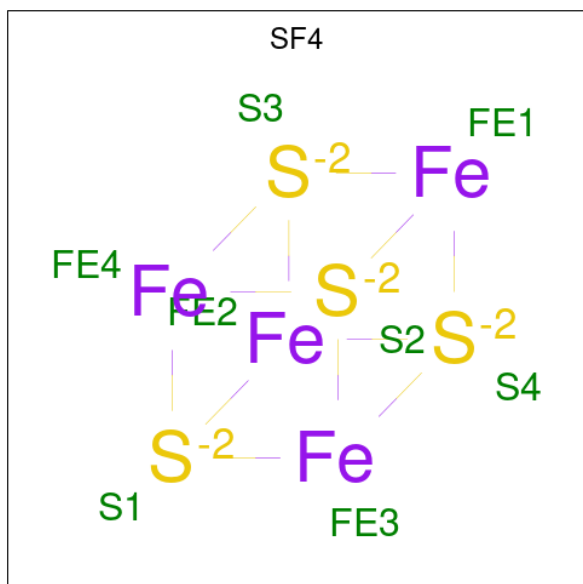
Mol	Chain	Residues	Atoms						AltConf
26	A	1	Total	C	H	Mg	N	O	0
			138	55	73	1	4	5	

- Molecule 27 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



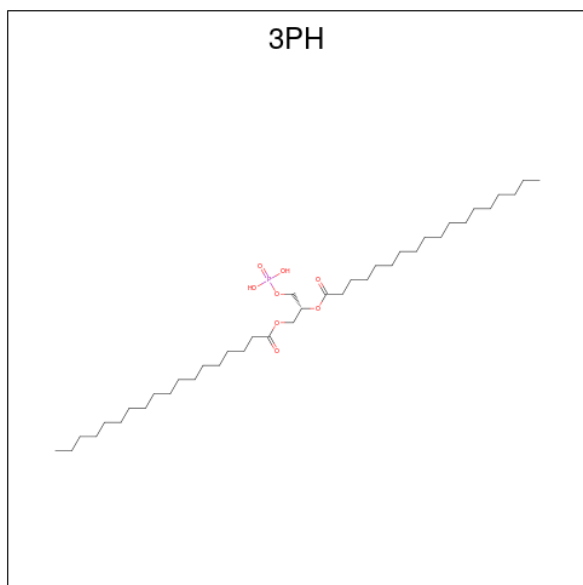
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	H	O	0
			79	31	46	2	
27	B	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



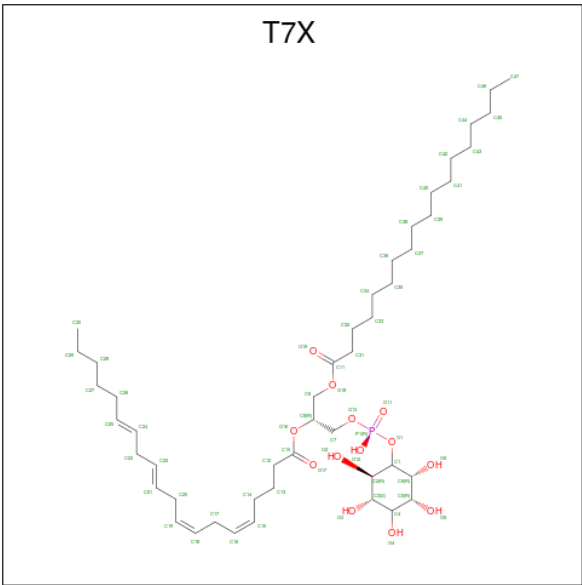
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 29 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula: $C_{39}H_{77}O_8P$).



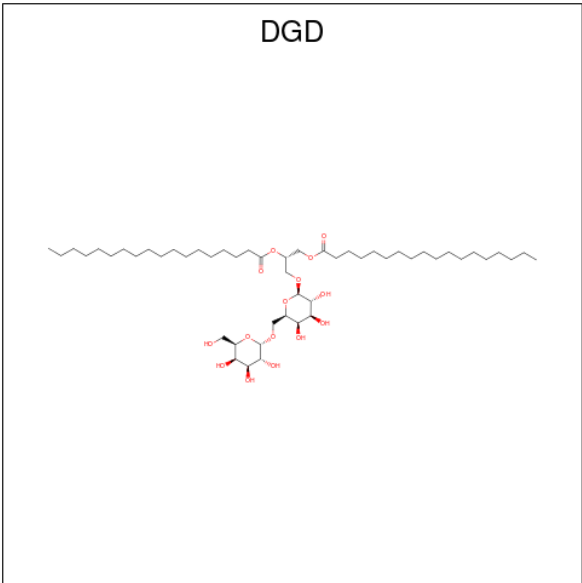
Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	H	O	P	0
			123	39	75	8	1	
29	B	1	Total	C	H	O	P	0
			123	39	75	8	1	
29	J	1	Total	C	H	O	P	0
			123	39	75	8	1	

- Molecule 30 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).



Mol	Chain	Residues	Atoms					AltConf
30	A	1	Total	C	H	O	P	0
			123	40	69	13	1	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms					AltConf
31	B	1	Total	C	H	O		0
			150	51	84	15		
31	B	1	Total	C	H	O		0
			150	51	84	15		

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Mol	Chain	Residues	Atoms				AltConf
31	B	1	Total	C	H	O	0
			150	51	84	15	

- Molecule 32 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
32	B	2	Total	Ca	0
			2	2	

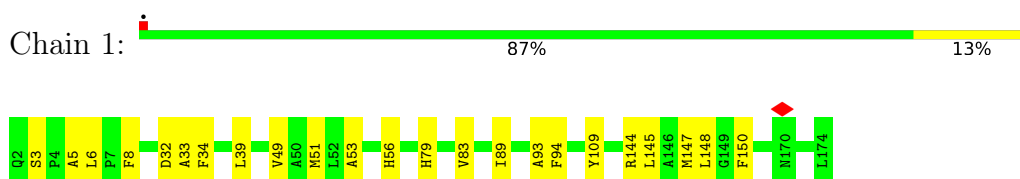
- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	1	15	Total	O	0
			15	15	
33	2	8	Total	O	0
			8	8	
33	3	6	Total	O	0
			6	6	
33	A	79	Total	O	0
			79	79	
33	B	68	Total	O	0
			68	68	
33	C	24	Total	O	0
			24	24	
33	D	14	Total	O	0
			14	14	
33	E	11	Total	O	0
			11	11	
33	F	11	Total	O	0
			11	11	
33	J	2	Total	O	0
			2	2	
33	K	2	Total	O	0
			2	2	
33	L	2	Total	O	0
			2	2	
33	M	2	Total	O	0
			2	2	
33	O	5	Total	O	0
			5	5	

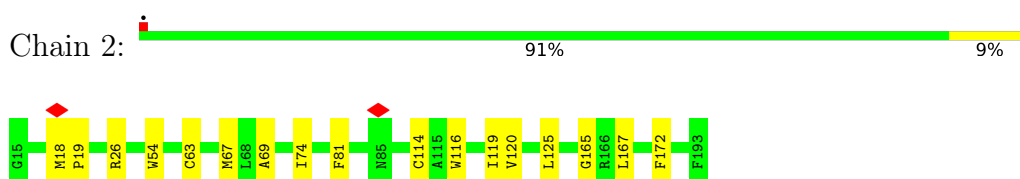
3 Residue-property plots

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.

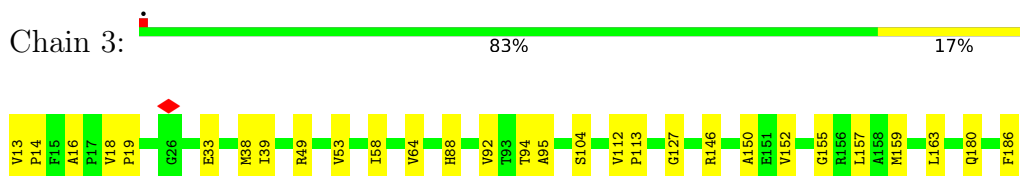
- Molecule 1: Similar to light harvesting protein



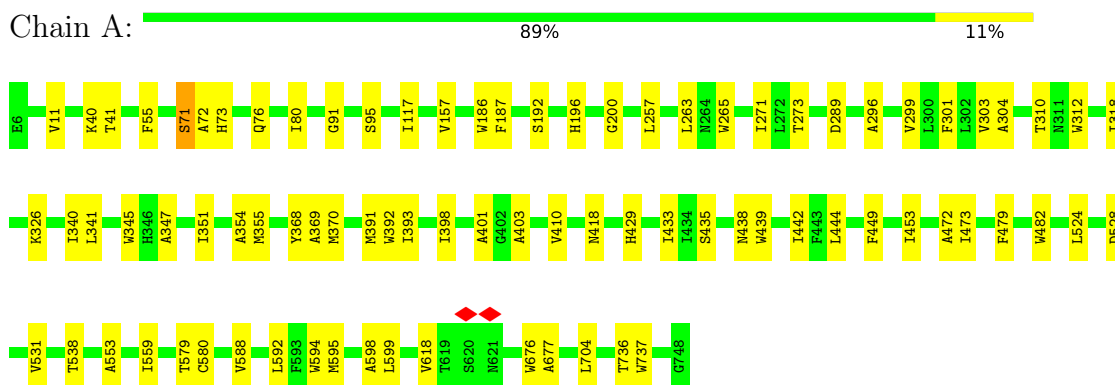
- Molecule 2: Similar to chlorophyll a/b-binding protein, CP24



- Molecule 3: Lhcr3

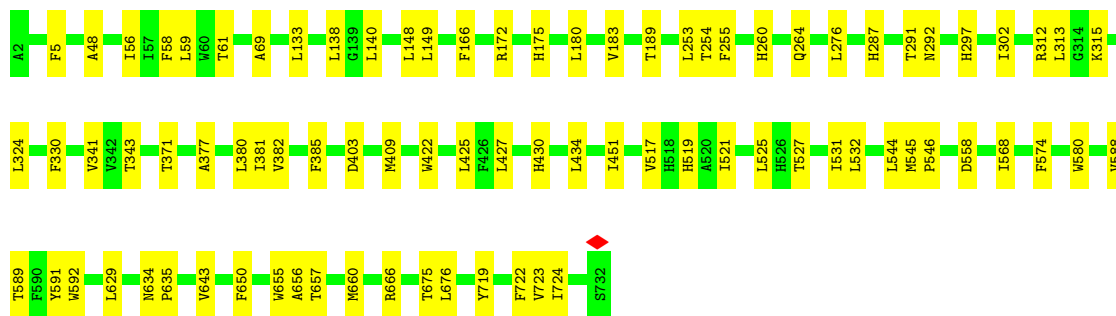


- Molecule 4: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A2

Chain B:  89% 11%

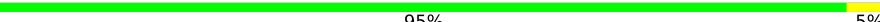


- Molecule 6: Photosystem I iron-sulfur center

Chain C:  99% .



- Molecule 7: Photosystem I p700 chlorophyll A apoprotein A2

Chain D:  95% 5%



- Molecule 8: Photosystem I iron-sulfur center subunit VII

Chain E:  87% 13%



- Molecule 9: PSI-F

Chain F:  93% 7%



- Molecule 10: Photosystem I reaction center subunit VIII

Chain I:  87% 13%



- Molecule 11: Photosystem I reaction center subunit IX

Chain J:  89% 11%



- Molecule 12: PSI-K

Chain K:  85% 15%



- Molecule 13: Photosystem I reaction center subunit XI

Chain L:  87% 12%



- Molecule 14: Photosystem I reaction center subunit XII

Chain M:  85% 15%



- Molecule 15: PsaO

Chain O:  94% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	128943	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.0	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.163	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0186	Depositor
Map size ($\text{\AA}$)	315.59998, 315.59998, 315.59998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0519999, 1.0519999, 1.0519999	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LMU, T7X, ERG, DGD, CL0, BCR, DGA, CA, PQN, RRX, 3PH, LHG, PTY, CLA, SF4, PGT, C7Z

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	0.16	0/1426	0.49	0/1927
2	2	0.17	0/1431	0.47	0/1931
3	3	0.14	0/1376	0.49	0/1867
4	A	0.15	0/6002	0.42	2/8179 (0.0%)
5	B	0.14	0/6028	0.42	0/8236
6	C	0.11	0/607	0.39	0/822
7	D	0.13	0/1118	0.36	0/1509
8	E	0.10	0/502	0.36	0/680
9	F	0.14	0/1304	0.46	0/1772
10	I	0.13	0/235	0.38	0/321
11	J	0.15	0/321	0.41	0/437
12	K	0.14	0/394	0.35	0/534
13	L	0.20	0/1064	0.43	1/1448 (0.1%)
14	M	0.10	0/205	0.47	1/277 (0.4%)
15	O	0.18	0/773	0.41	0/1061
All	All	0.15	0/22786	0.43	4/31001 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	71	SER	N-CA-C	-5.86	102.64	110.55
14	M	22	VAL	N-CA-C	-5.60	105.65	111.58
4	A	73	HIS	N-CA-C	-5.24	105.64	111.36
13	L	93	MET	CG-SD-CE	-5.21	89.44	100.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1381	1353	1353	19	0
2	2	1395	1385	1385	17	0
3	3	1341	1348	1348	30	0
4	A	5815	5740	5740	81	0
5	B	5819	5645	5645	75	0
6	C	597	576	576	1	0
7	D	1094	1093	1093	6	0
8	E	493	509	509	6	0
9	F	1270	1243	1243	10	0
10	I	230	253	253	4	0
11	J	312	327	327	3	0
12	K	390	419	419	7	0
13	L	1039	1057	1057	13	0
14	M	204	226	226	3	0
15	O	747	742	742	8	0
16	1	704	770	759	20	0
16	2	843	938	928	29	0
16	3	749	798	786	28	0
16	A	2665	2984	2944	115	0
16	B	2460	2742	2705	93	0
16	F	256	280	276	9	0
16	I	130	146	144	6	0
16	J	65	73	71	2	0
16	K	130	145	144	4	0
16	L	260	291	287	9	0
16	O	260	288	284	10	0
17	1	168	0	0	6	0
17	2	84	0	0	0	0
17	3	210	0	0	6	0
17	A	42	0	0	0	0
17	J	42	0	0	0	0
18	1	41	56	56	9	0
18	2	41	56	56	2	0
18	A	41	55	56	2	0
18	J	41	56	56	2	0
18	K	41	56	56	3	0
19	1	49	74	74	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	2	49	74	74	1	0
19	3	49	74	74	0	0
19	A	98	148	148	1	0
19	B	45	63	63	0	0
20	1	29	38	38	4	0
20	2	58	76	76	9	0
21	2	40	53	54	9	0
21	A	200	260	260	43	0
21	B	320	413	415	45	0
21	F	80	104	105	8	0
21	I	40	51	53	3	0
21	K	40	51	54	5	0
21	L	120	156	156	19	0
21	O	40	52	52	8	0
22	2	35	46	40	0	0
22	B	35	46	40	0	0
23	2	44	76	76	0	0
23	J	44	76	76	0	0
24	3	35	46	46	1	0
24	A	35	46	46	0	0
25	3	100	158	158	0	0
25	A	47	66	66	3	0
25	L	50	79	79	0	0
26	A	65	73	72	4	0
27	A	33	46	46	0	0
27	B	33	46	46	4	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	A	48	75	75	0	0
29	B	48	75	75	0	0
29	J	48	75	75	0	0
30	A	54	69	0	1	0
31	B	198	252	288	9	0
32	B	2	0	0	0	0
33	1	15	0	0	0	0
33	2	8	0	0	0	0
33	3	6	0	0	0	0
33	A	79	0	0	0	0
33	B	68	0	0	0	0
33	C	24	0	0	0	0
33	D	14	0	0	0	0
33	E	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	F	11	0	0	0	0
33	J	2	0	0	0	0
33	K	2	0	0	0	0
33	L	2	0	0	0	0
33	M	2	0	0	0	0
33	O	5	0	0	0	0
All	All	33884	34687	34524	577	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 8.

The worst 5 of 577 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)
20:2:621:ERG:C3	20:2:621:ERG:O1	1.70	1.39
20:2:618:ERG:O1	20:2:618:ERG:C3	1.70	1.37
20:1:618:ERG:C3	20:1:618:ERG:O1	1.70	1.36
16:A:802:CLA:HHC	16:A:802:CLA:HBB1	1.47	0.94
16:B:811:CLA:HHC	16:B:811:CLA:HBB1	1.51	0.92

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	171/173 (99%)	163 (95%)	8 (5%)	0	100	100
2	2	177/179 (99%)	167 (94%)	10 (6%)	0	100	100
3	3	172/174 (99%)	160 (93%)	12 (7%)	0	100	100
4	A	741/743 (100%)	714 (96%)	27 (4%)	0	100	100
5	B	729/731 (100%)	703 (96%)	26 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
7	D	136/138 (99%)	128 (94%)	8 (6%)	0	100	100
8	E	59/61 (97%)	56 (95%)	3 (5%)	0	100	100
9	F	153/155 (99%)	144 (94%)	9 (6%)	0	100	100
10	I	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	J	36/38 (95%)	36 (100%)	0	0	100	100
12	K	52/54 (96%)	52 (100%)	0	0	100	100
13	L	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
14	M	25/27 (93%)	25 (100%)	0	0	100	100
15	O	95/97 (98%)	92 (97%)	3 (3%)	0	100	100
All	All	2787/2817 (99%)	2668 (96%)	119 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	143/143 (100%)	143 (100%)	0	100	100
2	2	144/144 (100%)	144 (100%)	0	100	100
3	3	136/136 (100%)	136 (100%)	0	100	100
4	A	600/600 (100%)	600 (100%)	0	100	100
5	B	598/598 (100%)	598 (100%)	0	100	100
6	C	66/66 (100%)	66 (100%)	0	100	100
7	D	117/117 (100%)	117 (100%)	0	100	100
8	E	58/58 (100%)	58 (100%)	0	100	100
9	F	137/137 (100%)	137 (100%)	0	100	100
10	I	26/26 (100%)	26 (100%)	0	100	100
11	J	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	K	43/43 (100%)	43 (100%)	0	100	100
13	L	109/109 (100%)	109 (100%)	0	100	100
14	M	22/22 (100%)	22 (100%)	0	100	100
15	O	75/75 (100%)	75 (100%)	0	100	100
All	All	2308/2308 (100%)	2308 (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 33 such sidechains are listed below:

Mol	Chain	Res	Type
13	L	16	HIS
13	L	22	ASN
14	M	6	GLN
4	A	533	HIS
4	A	383	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 206 ligands modelled in this entry, 2 are monoatomic - leaving 204 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	CLA	A	808	4	69,73,73	1.36	7 (10%)	83,113,113	1.92	21 (25%)
16	CLA	3	209	3	69,73,73	1.36	8 (11%)	83,113,113	1.89	17 (20%)
16	CLA	A	817	-	69,73,73	1.36	7 (10%)	83,113,113	1.84	17 (20%)
21	BCR	K	104	-	41,41,41	1.82	4 (9%)	56,56,56	4.15	26 (46%)
16	CLA	L	201	4	69,73,73	1.38	7 (10%)	83,113,113	1.83	18 (21%)
16	CLA	3	210	3	69,73,73	1.36	6 (8%)	83,113,113	2.12	19 (22%)
16	CLA	B	801	-	69,73,73	1.37	7 (10%)	83,113,113	1.81	15 (18%)
21	BCR	2	617	-	41,41,41	1.90	5 (12%)	56,56,56	4.54	20 (35%)
16	CLA	3	214	3	69,73,73	1.38	7 (10%)	83,113,113	1.89	17 (20%)
21	BCR	B	840	-	41,41,41	1.83	4 (9%)	56,56,56	4.56	18 (32%)
16	CLA	A	805	-	69,73,73	1.35	6 (8%)	83,113,113	1.88	16 (19%)
31	DGD	B	849	-	67,67,67	1.20	8 (11%)	81,81,81	1.04	5 (6%)
16	CLA	A	812	4	69,73,73	1.36	6 (8%)	83,113,113	1.86	15 (18%)
16	CLA	3	213	-	50,54,73	1.59	7 (14%)	60,90,113	2.11	15 (25%)
16	CLA	B	806	5	69,73,73	1.36	7 (10%)	83,113,113	1.84	17 (20%)
16	CLA	A	836	4	69,73,73	1.36	7 (10%)	83,113,113	1.91	18 (21%)
16	CLA	2	603	2	69,73,73	1.37	9 (13%)	83,113,113	1.83	17 (20%)
16	CLA	A	832	4	69,73,73	1.36	8 (11%)	83,113,113	1.86	16 (19%)
16	CLA	B	821	5	69,73,73	1.37	7 (10%)	83,113,113	2.07	19 (22%)
16	CLA	B	811	5	69,73,73	1.37	7 (10%)	83,113,113	1.82	15 (18%)
16	CLA	J	102	11	69,73,73	1.35	7 (10%)	83,113,113	2.02	18 (21%)
16	CLA	A	806	-	69,73,73	1.36	6 (8%)	83,113,113	1.91	16 (19%)
16	CLA	B	805	-	69,73,73	1.36	7 (10%)	83,113,113	1.87	16 (19%)
17	C7Z	1	612	-	43,43,43	5.41	25 (58%)	58,60,60	2.10	16 (27%)
17	C7Z	J	104	-	43,43,43	5.40	26 (60%)	58,60,60	2.55	23 (39%)
21	BCR	A	846	-	41,41,41	1.80	4 (9%)	56,56,56	4.48	25 (44%)
21	BCR	B	844	-	41,41,41	1.82	4 (9%)	56,56,56	4.48	21 (37%)
21	BCR	O	205	-	41,41,41	1.83	4 (9%)	56,56,56	4.44	16 (28%)
16	CLA	3	211	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	17 (20%)
30	T7X	A	851	-	54,54,61	0.88	4 (7%)	64,66,73	1.00	3 (4%)
16	CLA	2	609	-	69,73,73	1.36	7 (10%)	83,113,113	1.88	17 (20%)
16	CLA	A	839	33	69,73,73	1.37	7 (10%)	83,113,113	1.84	14 (16%)
21	BCR	F	206	-	41,41,41	1.86	4 (9%)	56,56,56	4.22	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	826	-	69,73,73	1.36	7 (10%)	83,113,113	1.85	16 (19%)
16	CLA	A	831	4	69,73,73	1.38	7 (10%)	83,113,113	1.82	16 (19%)
16	CLA	B	834	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	18 (21%)
16	CLA	O	204	-	69,73,73	1.36	7 (10%)	83,113,113	1.91	18 (21%)
16	CLA	A	810	16	69,73,73	1.37	7 (10%)	83,113,113	1.97	19 (22%)
18	RRX	J	103	-	42,42,42	4.92	24 (57%)	57,58,58	3.14	30 (52%)
16	CLA	2	605	-	69,73,73	1.36	6 (8%)	83,113,113	1.86	17 (20%)
16	CLA	A	809	-	69,73,73	1.36	7 (10%)	83,113,113	1.79	15 (18%)
16	CLA	B	829	5	69,73,73	1.36	8 (11%)	83,113,113	1.86	16 (19%)
21	BCR	F	203	-	41,41,41	1.83	4 (9%)	56,56,56	4.72	22 (39%)
16	CLA	B	814	-	69,73,73	1.36	8 (11%)	83,113,113	1.85	16 (19%)
26	CL0	A	801	-	69,73,73	2.35	22 (31%)	83,113,113	2.51	26 (31%)
16	CLA	A	823	-	69,73,73	1.36	6 (8%)	83,113,113	1.81	17 (20%)
16	CLA	F	201	-	65,69,73	1.40	7 (10%)	78,108,113	1.80	15 (19%)
17	C7Z	3	201	-	43,43,43	5.42	26 (60%)	58,60,60	2.37	20 (34%)
16	CLA	B	822	5	69,73,73	1.37	6 (8%)	83,113,113	1.84	18 (21%)
16	CLA	B	831	33	69,73,73	1.36	6 (8%)	83,113,113	1.88	16 (19%)
16	CLA	A	829	4	69,73,73	1.36	6 (8%)	83,113,113	1.80	14 (16%)
17	C7Z	2	615	-	43,43,43	5.41	26 (60%)	58,60,60	2.57	22 (37%)
16	CLA	B	807	5	69,73,73	1.34	6 (8%)	83,113,113	1.84	15 (18%)
17	C7Z	A	843	-	43,43,43	5.41	26 (60%)	58,60,60	2.24	18 (31%)
16	CLA	A	837	4	69,73,73	1.37	7 (10%)	83,113,113	1.85	17 (20%)
16	CLA	B	824	-	69,73,73	1.35	6 (8%)	83,113,113	1.86	17 (20%)
20	ERG	2	621	-	31,32,32	8.27	19 (61%)	47,50,50	2.95	18 (38%)
16	CLA	B	816	5	69,73,73	1.38	8 (11%)	83,113,113	1.84	19 (22%)
21	BCR	B	842	-	41,41,41	1.87	4 (9%)	56,56,56	4.46	21 (37%)
21	BCR	I	103	-	41,41,41	1.81	4 (9%)	56,56,56	5.34	25 (44%)
16	CLA	1	601	-	69,73,73	1.37	6 (8%)	83,113,113	1.83	16 (19%)
16	CLA	2	611	2	69,73,73	1.37	7 (10%)	83,113,113	1.89	18 (21%)
16	CLA	A	825	-	69,73,73	1.38	7 (10%)	83,113,113	1.86	17 (20%)
16	CLA	1	605	-	69,73,73	1.36	7 (10%)	83,113,113	1.86	17 (20%)
16	CLA	B	838	22	69,73,73	1.37	7 (10%)	83,113,113	1.88	18 (21%)
17	C7Z	1	615	-	43,43,43	5.38	26 (60%)	58,60,60	2.45	19 (32%)
16	CLA	1	606	-	69,73,73	1.35	7 (10%)	83,113,113	2.06	20 (24%)
16	CLA	B	809	5	69,73,73	1.36	7 (10%)	83,113,113	2.01	20 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	827	-	69,73,73	1.36	7 (10%)	83,113,113	1.84	14 (16%)
21	BCR	A	850	-	41,41,41	1.88	4 (9%)	56,56,56	4.87	23 (41%)
16	CLA	B	835	5	69,73,73	1.36	8 (11%)	83,113,113	1.85	17 (20%)
31	DGD	B	850	-	67,67,67	1.18	7 (10%)	81,81,81	1.04	3 (3%)
16	CLA	2	613	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	18 (21%)
16	CLA	2	607	-	69,73,73	1.37	7 (10%)	83,113,113	1.82	14 (16%)
16	CLA	2	608	-	69,73,73	1.39	6 (8%)	83,113,113	1.95	20 (24%)
19	LHG	1	617	16	48,48,48	0.42	0	51,54,54	0.94	3 (5%)
28	SF4	C	102	6	0,12,12	-	-	-	-	-
16	CLA	1	607	1	64,68,73	1.41	7 (10%)	77,107,113	1.92	16 (20%)
22	PGT	B	848	16	34,34,50	1.54	7 (20%)	37,40,56	1.06	2 (5%)
16	CLA	A	815	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	19 (22%)
16	CLA	2	604	-	69,73,73	1.35	7 (10%)	83,113,113	1.95	19 (22%)
16	CLA	B	819	5	69,73,73	1.37	7 (10%)	83,113,113	1.91	16 (19%)
16	CLA	2	606	2	69,73,73	1.36	7 (10%)	83,113,113	1.93	16 (19%)
20	ERG	1	618	-	31,32,32	8.17	18 (58%)	47,50,50	4.76	19 (40%)
16	CLA	F	202	5	69,73,73	1.36	7 (10%)	83,113,113	2.10	21 (25%)
21	BCR	L	207	-	41,41,41	1.85	4 (9%)	56,56,56	4.57	23 (41%)
29	3PH	B	854	-	47,47,47	0.87	4 (8%)	51,52,52	1.02	2 (3%)
21	BCR	L	202	-	41,41,41	1.75	4 (9%)	56,56,56	4.40	19 (33%)
16	CLA	A	830	4	69,73,73	1.39	7 (10%)	83,113,113	1.83	16 (19%)
29	3PH	A	849	-	47,47,47	0.86	4 (8%)	51,52,52	1.07	2 (3%)
16	CLA	B	836	-	69,73,73	1.38	7 (10%)	83,113,113	1.86	15 (18%)
25	PTY	3	221	-	49,49,49	0.89	4 (8%)	52,54,54	0.98	2 (3%)
17	C7Z	3	218	-	43,43,43	5.38	26 (60%)	58,60,60	2.50	25 (43%)
16	CLA	A	813	-	69,73,73	1.37	7 (10%)	83,113,113	1.85	16 (19%)
18	RRX	A	847	-	42,42,42	4.98	25 (59%)	57,58,58	2.92	26 (45%)
21	BCR	B	843	-	41,41,41	1.84	4 (9%)	56,56,56	4.82	27 (48%)
28	SF4	A	848	5,4	0,12,12	-	-	-	-	-
21	BCR	B	845	-	41,41,41	1.84	4 (9%)	56,56,56	4.44	19 (33%)
16	CLA	I	102	-	69,73,73	1.36	6 (8%)	83,113,113	1.80	15 (18%)
23	DGA	2	620	-	43,43,43	1.17	3 (6%)	45,45,45	1.16	3 (6%)
16	CLA	O	203	15	69,73,73	1.38	7 (10%)	83,113,113	1.89	16 (19%)
22	PGT	2	619	-	34,34,50	1.45	6 (17%)	37,40,56	1.03	2 (5%)
29	3PH	J	105	-	47,47,47	0.88	3 (6%)	51,52,52	0.96	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	A	855	33	69,73,73	1.38	7 (10%)	83,113,113	1.76	15 (18%)
16	CLA	B	804	-	69,73,73	1.35	6 (8%)	83,113,113	1.91	19 (22%)
16	CLA	L	203	13	69,73,73	1.37	7 (10%)	83,113,113	1.82	16 (19%)
16	CLA	A	811	4	69,73,73	1.37	7 (10%)	83,113,113	1.83	16 (19%)
16	CLA	A	835	4	69,73,73	1.36	6 (8%)	83,113,113	1.99	18 (21%)
16	CLA	L	204	-	69,73,73	1.36	7 (10%)	83,113,113	1.83	17 (20%)
19	LHG	B	851	-	44,44,48	0.42	0	47,50,54	0.95	3 (6%)
17	C7Z	3	215	-	43,43,43	5.42	26 (60%)	58,60,60	2.20	14 (24%)
16	CLA	B	833	5	69,73,73	1.37	7 (10%)	83,113,113	1.83	20 (24%)
31	DGD	B	846	-	67,67,67	1.19	7 (10%)	81,81,81	1.03	3 (3%)
16	CLA	A	804	4	69,73,73	1.39	9 (13%)	83,113,113	1.87	19 (22%)
16	CLA	B	823	-	69,73,73	1.37	7 (10%)	83,113,113	1.78	13 (15%)
16	CLA	A	854	-	69,73,73	1.34	7 (10%)	83,113,113	1.77	13 (15%)
16	CLA	B	802	5	69,73,73	1.37	7 (10%)	83,113,113	1.89	15 (18%)
19	LHG	A	841	-	48,48,48	0.41	0	51,54,54	0.90	2 (3%)
16	CLA	3	212	-	62,66,73	1.44	7 (11%)	74,104,113	2.02	18 (24%)
16	CLA	3	208	-	69,73,73	1.36	6 (8%)	83,113,113	1.88	17 (20%)
16	CLA	A	828	-	69,73,73	1.37	7 (10%)	83,113,113	1.78	15 (18%)
16	CLA	A	802	-	69,73,73	1.37	7 (10%)	83,113,113	1.97	15 (18%)
16	CLA	B	828	5	69,73,73	1.38	7 (10%)	83,113,113	1.80	15 (18%)
16	CLA	A	856	4	69,73,73	1.36	7 (10%)	83,113,113	1.87	15 (18%)
20	ERG	2	618	-	31,32,32	8.30	18 (58%)	47,50,50	3.52	22 (46%)
28	SF4	C	101	6	0,12,12	-	-	-	-	-
16	CLA	1	610	-	69,73,73	1.35	7 (10%)	83,113,113	1.96	17 (20%)
17	C7Z	1	616	-	43,43,43	5.38	26 (60%)	58,60,60	2.79	22 (37%)
16	CLA	A	814	-	69,73,73	1.36	7 (10%)	83,113,113	1.92	17 (20%)
16	CLA	3	206	-	69,73,73	1.35	7 (10%)	83,113,113	1.85	18 (21%)
16	CLA	3	207	-	66,70,73	1.39	6 (9%)	79,109,113	1.89	16 (20%)
17	C7Z	1	614	-	43,43,43	5.41	26 (60%)	58,60,60	2.32	17 (29%)
16	CLA	1	609	-	69,73,73	1.38	6 (8%)	83,113,113	1.80	15 (18%)
16	CLA	I	101	5	69,73,73	1.34	6 (8%)	83,113,113	1.89	15 (18%)
17	C7Z	3	217	-	43,43,43	5.36	25 (58%)	58,60,60	2.58	22 (37%)
16	CLA	A	834	4	69,73,73	1.36	7 (10%)	83,113,113	1.83	15 (18%)
16	CLA	O	202	-	69,73,73	1.35	6 (8%)	83,113,113	1.85	14 (16%)
16	CLA	B	812	5	69,73,73	1.38	7 (10%)	83,113,113	1.90	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	K	101	-	69,73,73	1.37	8 (11%)	83,113,113	1.87	18 (21%)
16	CLA	F	205	9	69,73,73	1.36	6 (8%)	83,113,113	1.92	17 (20%)
16	CLA	A	816	-	69,73,73	1.38	6 (8%)	83,113,113	1.88	18 (21%)
16	CLA	B	825	5	69,73,73	1.38	7 (10%)	83,113,113	1.89	15 (18%)
18	RRX	K	103	-	42,42,42	4.99	26 (61%)	57,58,58	2.35	22 (38%)
16	CLA	3	204	3	67,71,73	1.39	7 (10%)	80,110,113	1.86	13 (16%)
16	CLA	B	832	-	69,73,73	1.36	7 (10%)	83,113,113	1.90	17 (20%)
16	CLA	B	815	-	59,63,73	1.48	7 (11%)	71,101,113	1.94	16 (22%)
16	CLA	O	201	-	69,73,73	1.34	6 (8%)	83,113,113	1.96	18 (21%)
17	C7Z	2	614	-	43,43,43	5.39	26 (60%)	58,60,60	2.31	17 (29%)
19	LHG	3	219	-	48,48,48	0.41	0	51,54,54	0.93	3 (5%)
23	DGA	J	101	-	43,43,43	1.15	3 (6%)	45,45,45	1.16	3 (6%)
16	CLA	B	818	33	69,73,73	1.36	7 (10%)	83,113,113	1.96	16 (19%)
16	CLA	F	204	-	69,73,73	1.37	7 (10%)	83,113,113	1.80	16 (19%)
18	RRX	2	616	-	42,42,42	5.00	25 (59%)	57,58,58	2.37	24 (42%)
17	C7Z	3	216	-	43,43,43	5.39	27 (62%)	58,60,60	3.47	24 (41%)
16	CLA	A	833	4	69,73,73	1.37	7 (10%)	83,113,113	1.87	16 (19%)
16	CLA	B	813	5	69,73,73	1.36	6 (8%)	83,113,113	1.84	16 (19%)
21	BCR	B	847	-	41,41,41	1.88	4 (9%)	56,56,56	4.87	26 (46%)
21	BCR	B	855	-	41,41,41	1.85	4 (9%)	56,56,56	4.67	28 (50%)
16	CLA	A	818	4	69,73,73	1.35	7 (10%)	83,113,113	2.10	19 (22%)
16	CLA	A	807	-	69,73,73	1.36	6 (8%)	83,113,113	1.88	16 (19%)
16	CLA	B	817	5	69,73,73	1.36	7 (10%)	83,113,113	1.80	15 (18%)
16	CLA	L	205	-	69,73,73	1.35	7 (10%)	83,113,113	1.93	16 (19%)
16	CLA	B	810	-	69,73,73	1.36	6 (8%)	83,113,113	1.86	17 (20%)
24	LMU	A	853	-	36,36,36	0.44	0	47,47,47	0.75	0
16	CLA	2	612	-	69,73,73	1.37	7 (10%)	83,113,113	1.82	16 (19%)
16	CLA	A	820	33	69,73,73	1.36	8 (11%)	83,113,113	1.85	16 (19%)
16	CLA	A	824	33	69,73,73	1.37	8 (11%)	83,113,113	1.88	16 (19%)
16	CLA	3	203	-	69,73,73	1.37	7 (10%)	83,113,113	1.98	18 (21%)
16	CLA	2	601	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	15 (18%)
16	CLA	1	611	-	69,73,73	1.37	7 (10%)	83,113,113	1.84	16 (19%)
16	CLA	K	102	-	69,73,73	1.36	6 (8%)	83,113,113	1.85	15 (18%)
16	CLA	B	837	5	69,73,73	1.36	6 (8%)	83,113,113	2.03	18 (21%)
16	CLA	A	826	4	69,73,73	1.36	7 (10%)	83,113,113	1.86	13 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	CLA	B	820	-	69,73,73	1.36	7 (10%)	83,113,113	1.93	17 (20%)
16	CLA	B	830	5	69,73,73	1.35	7 (10%)	83,113,113	1.80	15 (18%)
16	CLA	A	838	4	69,73,73	1.35	6 (8%)	83,113,113	1.88	19 (22%)
16	CLA	1	608	19	69,73,73	1.36	6 (8%)	83,113,113	1.83	17 (20%)
16	CLA	A	821	4	69,73,73	1.37	7 (10%)	83,113,113	1.95	21 (25%)
16	CLA	A	803	4,16	69,73,73	1.35	6 (8%)	83,113,113	1.93	16 (19%)
16	CLA	B	803	33	69,73,73	1.38	7 (10%)	83,113,113	1.81	18 (21%)
24	LMU	3	202	-	36,36,36	0.46	0	47,47,47	0.74	0
25	PTY	L	208	-	49,49,49	0.89	4 (8%)	52,54,54	1.03	2 (3%)
25	PTY	A	852	-	45,45,49	0.92	4 (8%)	47,49,54	1.01	2 (4%)
27	PQN	B	839	-	34,34,34	0.46	0	42,45,45	1.00	2 (4%)
16	CLA	2	602	2	68,71,73	1.49	8 (11%)	81,110,113	1.86	17 (20%)
19	LHG	A	842	-	48,48,48	0.40	0	51,54,54	0.93	3 (5%)
16	CLA	A	822	4	69,73,73	1.36	6 (8%)	83,113,113	1.86	18 (21%)
18	RRX	1	613	-	42,42,42	4.96	25 (59%)	57,58,58	2.41	20 (35%)
25	PTY	3	220	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
16	CLA	2	610	19	69,73,73	1.36	7 (10%)	83,113,113	1.98	19 (22%)
16	CLA	1	602	1	63,67,73	1.42	6 (9%)	75,105,113	2.03	18 (24%)
16	CLA	B	827	-	69,73,73	1.37	8 (11%)	83,113,113	1.77	17 (20%)
19	LHG	2	622	16	48,48,48	0.40	0	51,54,54	1.06	4 (7%)
21	BCR	B	841	-	41,41,41	1.79	4 (9%)	56,56,56	4.44	26 (46%)
16	CLA	1	603	-	69,73,73	1.37	7 (10%)	83,113,113	1.92	21 (25%)
27	PQN	A	840	-	34,34,34	0.44	0	42,45,45	1.30	4 (9%)
21	BCR	A	845	-	41,41,41	1.82	4 (9%)	56,56,56	5.62	29 (51%)
16	CLA	3	205	3	69,73,73	1.37	6 (8%)	83,113,113	2.12	21 (25%)
16	CLA	B	808	-	69,73,73	1.36	8 (11%)	83,113,113	1.92	17 (20%)
21	BCR	L	206	-	41,41,41	1.82	5 (12%)	56,56,56	4.49	19 (33%)
21	BCR	A	857	-	41,41,41	1.85	4 (9%)	56,56,56	4.85	26 (46%)
21	BCR	A	844	-	41,41,41	1.86	4 (9%)	56,56,56	4.26	21 (37%)
16	CLA	1	604	1	69,73,73	1.36	6 (8%)	83,113,113	1.88	16 (19%)
16	CLA	A	819	4	69,73,73	1.37	8 (11%)	83,113,113	1.93	18 (21%)

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
16	CLA	A	808	4	-	16/39/115/115	-
16	CLA	3	209	3	-	19/39/115/115	-
16	CLA	A	817	-	-	15/39/115/115	-
21	BCR	K	104	-	-	14/29/63/63	0/2/2/2
16	CLA	L	201	4	-	8/39/115/115	-
16	CLA	3	210	3	-	15/39/115/115	-
16	CLA	B	801	-	-	16/39/115/115	-
21	BCR	2	617	-	-	8/29/63/63	0/2/2/2
16	CLA	3	214	3	-	18/39/115/115	-
21	BCR	B	840	-	-	8/29/63/63	0/2/2/2
16	CLA	A	805	-	-	18/39/115/115	-
31	DGD	B	849	-	-	16/55/95/95	0/2/2/2
16	CLA	A	812	4	-	14/39/115/115	-
16	CLA	3	213	-	-	9/17/93/115	-
16	CLA	B	806	5	-	11/39/115/115	-
16	CLA	A	836	4	-	9/39/115/115	-
16	CLA	2	603	2	-	10/39/115/115	-
16	CLA	A	832	4	-	12/39/115/115	-
16	CLA	B	821	5	1/1/19/20	13/39/115/115	-
16	CLA	B	811	5	-	8/39/115/115	-
16	CLA	J	102	11	1/1/19/20	18/39/115/115	-
16	CLA	A	806	-	-	13/39/115/115	-
16	CLA	B	805	-	-	15/39/115/115	-
17	C7Z	J	104	-	1/1/12/26	6/29/67/67	0/2/2/2
17	C7Z	1	612	-	1/1/12/26	11/29/67/67	0/2/2/2
21	BCR	A	846	-	-	6/29/63/63	0/2/2/2
21	BCR	B	844	-	-	7/29/63/63	0/2/2/2
21	BCR	O	205	-	-	11/29/63/63	0/2/2/2
16	CLA	3	211	-	-	19/39/115/115	-
30	T7X	A	851	-	-	19/49/73/80	0/1/1/1
16	CLA	2	609	-	-	17/39/115/115	-
16	CLA	A	839	33	-	14/39/115/115	-
21	BCR	F	206	-	-	10/29/63/63	0/2/2/2
16	CLA	B	826	-	-	18/39/115/115	-
16	CLA	A	831	4	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	834	-	-	14/39/115/115	-
16	CLA	O	204	-	-	12/39/115/115	-
16	CLA	A	810	16	-	13/39/115/115	-
18	RRX	J	103	-	1/1/25/25	16/29/65/65	0/2/2/2
16	CLA	2	605	-	-	16/39/115/115	-
16	CLA	A	809	-	-	17/39/115/115	-
16	CLA	B	829	5	-	14/39/115/115	-
21	BCR	F	203	-	-	8/29/63/63	0/2/2/2
16	CLA	B	814	-	-	13/39/115/115	-
26	CL0	A	801	-	-	15/39/115/115	-
16	CLA	A	823	-	-	11/39/115/115	-
16	CLA	F	201	-	-	15/35/111/115	-
17	C7Z	3	201	-	1/1/12/26	10/29/67/67	0/2/2/2
16	CLA	B	822	5	-	8/39/115/115	-
16	CLA	B	831	33	-	15/39/115/115	-
16	CLA	A	829	4	-	13/39/115/115	-
17	C7Z	2	615	-	1/1/12/26	8/29/67/67	0/2/2/2
17	C7Z	A	843	-	1/1/12/26	12/29/67/67	0/2/2/2
16	CLA	B	807	5	-	13/39/115/115	-
20	ERG	2	621	-	5/5/15/15	4/13/71/71	0/4/4/4
16	CLA	A	837	4	-	17/39/115/115	-
16	CLA	B	824	-	-	15/39/115/115	-
16	CLA	B	816	5	-	13/39/115/115	-
21	BCR	B	842	-	-	6/29/63/63	0/2/2/2
21	BCR	I	103	-	-	10/29/63/63	0/2/2/2
16	CLA	1	601	-	-	16/39/115/115	-
16	CLA	2	611	2	-	15/39/115/115	-
16	CLA	A	825	-	-	17/39/115/115	-
16	CLA	1	605	-	-	16/39/115/115	-
16	CLA	B	838	22	-	13/39/115/115	-
17	C7Z	1	615	-	1/1/12/26	11/29/67/67	0/2/2/2
16	CLA	1	606	-	-	19/39/115/115	-
16	CLA	B	809	5	-	17/39/115/115	-
16	CLA	A	827	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	A	850	-	-	14/29/63/63	0/2/2/2
16	CLA	B	835	5	-	14/39/115/115	-
31	DGD	B	850	-	-	18/55/95/95	0/2/2/2
16	CLA	2	613	-	-	20/39/115/115	-
16	CLA	2	607	-	-	14/39/115/115	-
16	CLA	2	608	-	-	21/39/115/115	-
19	LHG	1	617	16	-	29/53/53/53	-
28	SF4	C	102	6	-	-	0/6/5/5
16	CLA	1	607	1	-	12/33/109/115	-
22	PGT	B	848	16	1/1/5/5	21/38/38/55	-
20	ERG	1	618	-	6/6/15/15	3/13/71/71	0/4/4/4
16	CLA	2	604	-	-	12/39/115/115	-
16	CLA	A	815	-	-	21/39/115/115	-
16	CLA	2	606	2	-	15/39/115/115	-
16	CLA	B	819	5	-	14/39/115/115	-
16	CLA	F	202	5	1/1/19/20	15/39/115/115	-
21	BCR	L	207	-	-	8/29/63/63	0/2/2/2
29	3PH	B	854	-	-	28/49/49/49	-
21	BCR	L	202	-	-	8/29/63/63	0/2/2/2
16	CLA	A	830	4	-	13/39/115/115	-
29	3PH	A	849	-	-	19/49/49/49	-
16	CLA	B	836	-	-	13/39/115/115	-
25	PTY	3	221	-	-	18/53/53/53	-
17	C7Z	3	218	-	1/1/12/26	8/29/67/67	0/2/2/2
16	CLA	A	813	-	-	18/39/115/115	-
18	RRX	A	847	-	1/1/24/25	13/29/65/65	0/2/2/2
21	BCR	B	843	-	-	9/29/63/63	0/2/2/2
28	SF4	A	848	5,4	-	-	0/6/5/5
21	BCR	B	845	-	-	12/29/63/63	0/2/2/2
16	CLA	I	102	-	-	14/39/115/115	-
23	DGA	2	620	-	-	21/45/45/45	-
16	CLA	O	203	15	-	19/39/115/115	-
22	PGT	2	619	-	1/1/5/5	20/38/38/55	-
29	3PH	J	105	-	-	20/49/49/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	A	855	33	-	12/39/115/115	-
16	CLA	B	804	-	-	13/39/115/115	-
16	CLA	L	203	13	-	12/39/115/115	-
16	CLA	A	811	4	-	10/39/115/115	-
16	CLA	A	835	4	-	13/39/115/115	-
16	CLA	L	204	-	-	21/39/115/115	-
19	LHG	B	851	-	-	24/49/49/53	-
17	C7Z	3	215	-	1/1/12/26	9/29/67/67	0/2/2/2
16	CLA	B	833	5	-	15/39/115/115	-
31	DGD	B	846	-	-	20/55/95/95	0/2/2/2
16	CLA	A	804	4	-	14/39/115/115	-
16	CLA	B	823	-	-	15/39/115/115	-
16	CLA	A	854	-	-	12/39/115/115	-
16	CLA	B	802	5	-	12/39/115/115	-
19	LHG	A	841	-	-	35/53/53/53	-
16	CLA	3	212	-	-	12/31/107/115	-
16	CLA	3	208	-	-	14/39/115/115	-
16	CLA	A	828	-	-	8/39/115/115	-
16	CLA	A	802	-	-	17/39/115/115	-
16	CLA	B	828	5	-	7/39/115/115	-
16	CLA	A	856	4	-	13/39/115/115	-
20	ERG	2	618	-	4/4/15/15	10/13/71/71	0/4/4/4
28	SF4	C	101	6	-	-	0/6/5/5
16	CLA	1	610	-	-	13/39/115/115	-
17	C7Z	1	616	-	1/1/12/26	7/29/67/67	0/2/2/2
16	CLA	A	814	-	-	20/39/115/115	-
16	CLA	3	206	-	-	11/39/115/115	-
16	CLA	3	207	-	-	14/36/112/115	-
17	C7Z	1	614	-	1/1/12/26	13/29/67/67	0/2/2/2
16	CLA	1	609	-	-	13/39/115/115	-
16	CLA	I	101	5	-	12/39/115/115	-
17	C7Z	3	217	-	1/1/12/26	11/29/67/67	0/2/2/2
16	CLA	A	834	4	-	14/39/115/115	-
16	CLA	O	202	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	812	5	-	20/39/115/115	-
16	CLA	K	101	-	-	18/39/115/115	-
16	CLA	F	205	9	-	19/39/115/115	-
16	CLA	A	816	-	-	16/39/115/115	-
16	CLA	B	825	5	-	12/39/115/115	-
18	RRX	K	103	-	1/1/25/25	16/29/65/65	0/2/2/2
16	CLA	3	204	3	-	8/37/113/115	-
16	CLA	B	832	-	-	17/39/115/115	-
16	CLA	B	815	-	-	11/27/103/115	-
16	CLA	O	201	-	-	12/39/115/115	-
17	C7Z	2	614	-	1/1/12/26	10/29/67/67	0/2/2/2
19	LHG	3	219	-	-	32/53/53/53	-
23	DGA	J	101	-	-	17/45/45/45	-
16	CLA	B	818	33	-	17/39/115/115	-
16	CLA	F	204	-	-	11/39/115/115	-
18	RRX	2	616	-	1/1/25/25	13/29/65/65	0/2/2/2
17	C7Z	3	216	-	1/1/12/26	9/29/67/67	0/2/2/2
16	CLA	A	833	4	-	17/39/115/115	-
16	CLA	B	813	5	-	12/39/115/115	-
21	BCR	B	847	-	-	15/29/63/63	0/2/2/2
21	BCR	B	855	-	-	9/29/63/63	0/2/2/2
16	CLA	A	818	4	-	14/39/115/115	-
16	CLA	A	807	-	-	14/39/115/115	-
16	CLA	B	817	5	-	7/39/115/115	-
16	CLA	L	205	-	-	13/39/115/115	-
16	CLA	B	810	-	-	11/39/115/115	-
24	LMU	A	853	-	-	7/21/61/61	0/2/2/2
16	CLA	2	612	-	-	14/39/115/115	-
16	CLA	A	820	33	-	13/39/115/115	-
16	CLA	A	824	33	-	14/39/115/115	-
16	CLA	3	203	-	-	17/39/115/115	-
16	CLA	2	601	-	-	20/39/115/115	-
16	CLA	1	611	-	-	15/39/115/115	-
16	CLA	K	102	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	CLA	B	837	5	-	15/39/115/115	-
16	CLA	A	826	4	-	13/39/115/115	-
16	CLA	B	820	-	-	16/39/115/115	-
16	CLA	B	830	5	-	16/39/115/115	-
16	CLA	A	838	4	-	8/39/115/115	-
16	CLA	1	608	19	-	16/39/115/115	-
16	CLA	A	821	4	-	13/39/115/115	-
16	CLA	A	803	4,16	-	13/39/115/115	-
16	CLA	B	803	33	-	9/39/115/115	-
24	LMU	3	202	-	-	13/21/61/61	0/2/2/2
25	PTY	L	208	-	-	23/53/53/53	-
25	PTY	A	852	-	-	23/48/48/53	-
27	PQN	B	839	-	-	9/23/43/43	0/2/2/2
16	CLA	2	602	2	-	13/37/113/115	-
19	LHG	A	842	-	-	28/53/53/53	-
18	RRX	1	613	-	1/1/25/25	20/29/65/65	0/2/2/2
16	CLA	A	822	4	-	13/39/115/115	-
25	PTY	3	220	-	-	19/53/53/53	-
16	CLA	2	610	19	-	16/39/115/115	-
16	CLA	1	602	1	-	8/32/108/115	-
16	CLA	B	827	-	-	12/39/115/115	-
19	LHG	2	622	16	-	30/53/53/53	-
21	BCR	B	841	-	-	10/29/63/63	0/2/2/2
16	CLA	1	603	-	-	13/39/115/115	-
27	PQN	A	840	-	-	10/23/43/43	0/2/2/2
21	BCR	A	845	-	-	11/29/63/63	0/2/2/2
16	CLA	3	205	3	-	11/39/115/115	-
16	CLA	B	808	-	-	13/39/115/115	-
21	BCR	L	206	-	-	8/29/63/63	0/2/2/2
21	BCR	A	857	-	-	9/29/63/63	0/2/2/2
21	BCR	A	844	-	-	6/29/63/63	0/2/2/2
16	CLA	1	604	1	-	13/39/115/115	-
16	CLA	A	819	4	-	17/39/115/115	-

The worst 5 of 1606 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	621	ERG	C1-C10	-24.95	1.06	1.54
20	2	618	ERG	C1-C10	-24.94	1.06	1.54
20	1	618	ERG	C1-C10	-24.51	1.07	1.54
20	2	618	ERG	C10-C9	-22.33	1.26	1.55
20	2	621	ERG	C10-C9	-21.86	1.26	1.55

The worst 5 of 3243 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	K	104	BCR	C10-C11-C12	18.18	179.96	123.22
20	1	618	ERG	C18-C13-C12	-18.17	81.89	110.59
21	B	842	BCR	C10-C11-C12	17.98	179.32	123.22
21	O	205	BCR	C10-C11-C12	17.86	178.94	123.22
21	L	202	BCR	C10-C11-C12	17.78	178.71	123.22

5 of 38 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	B	821	CLA	C3A
16	F	202	CLA	C3A
16	J	102	CLA	C3A
17	1	612	C7Z	C3
17	1	614	C7Z	C3

5 of 2818 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	1	601	CLA	CHA-CBD-CGD-O1D
16	1	601	CLA	CHA-CBD-CGD-O2D
16	1	601	CLA	CBD-CGD-O2D-CED
16	1	603	CLA	C4B-C3B-CAB-CBB
16	1	604	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

169 monomers are involved in 454 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	808	CLA	1	0
16	3	209	CLA	8	0
16	A	817	CLA	4	0
21	K	104	BCR	5	0
16	L	201	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	801	CLA	4	0
21	2	617	BCR	9	0
16	3	214	CLA	2	0
21	B	840	BCR	5	0
16	A	805	CLA	3	0
31	B	849	DGD	2	0
16	A	812	CLA	2	0
16	3	213	CLA	4	0
16	A	836	CLA	1	0
16	2	603	CLA	1	0
16	A	832	CLA	5	0
16	B	821	CLA	6	0
16	B	811	CLA	4	0
16	J	102	CLA	2	0
16	A	806	CLA	1	0
16	B	805	CLA	2	0
17	1	612	C7Z	2	0
21	A	846	BCR	14	0
21	B	844	BCR	8	0
21	O	205	BCR	8	0
16	3	211	CLA	1	0
30	A	851	T7X	1	0
16	2	609	CLA	1	0
16	A	839	CLA	2	0
21	F	206	BCR	4	0
16	B	826	CLA	3	0
16	B	834	CLA	6	0
16	O	204	CLA	1	0
18	J	103	RRX	2	0
16	2	605	CLA	4	0
16	A	809	CLA	4	0
16	B	829	CLA	4	0
21	F	203	BCR	4	0
16	B	814	CLA	2	0
26	A	801	CL0	4	0
16	A	823	CLA	4	0
16	F	201	CLA	3	0
17	3	201	C7Z	2	0
16	B	822	CLA	2	0
16	B	831	CLA	6	0
16	A	829	CLA	3	0
16	A	837	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	824	CLA	1	0
20	2	621	ERG	5	0
16	B	816	CLA	3	0
21	B	842	BCR	3	0
21	I	103	BCR	3	0
16	1	601	CLA	4	0
16	2	611	CLA	2	0
16	A	825	CLA	7	0
16	1	605	CLA	1	0
16	B	838	CLA	2	0
17	1	615	C7Z	1	0
16	1	606	CLA	1	0
16	B	809	CLA	4	0
16	A	827	CLA	5	0
21	A	850	BCR	5	0
16	B	835	CLA	5	0
31	B	850	DGD	3	0
16	2	613	CLA	2	0
16	2	607	CLA	4	0
16	2	608	CLA	4	0
19	1	617	LHG	1	0
16	1	607	CLA	2	0
16	A	815	CLA	2	0
16	2	604	CLA	1	0
16	B	819	CLA	3	0
16	2	606	CLA	3	0
20	1	618	ERG	4	0
16	F	202	CLA	5	0
21	L	207	BCR	4	0
21	L	202	BCR	9	0
16	A	830	CLA	3	0
16	B	836	CLA	2	0
16	A	813	CLA	1	0
18	A	847	RRX	2	0
21	B	843	BCR	6	0
21	B	845	BCR	7	0
16	I	102	CLA	3	0
16	O	203	CLA	4	0
16	A	855	CLA	4	0
16	B	804	CLA	4	0
16	L	203	CLA	4	0
16	A	811	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	835	CLA	1	0
16	L	204	CLA	1	0
17	3	215	C7Z	2	0
16	B	833	CLA	4	0
31	B	846	DGD	4	0
16	A	804	CLA	1	0
16	A	854	CLA	12	0
16	B	802	CLA	4	0
16	3	212	CLA	2	0
16	3	208	CLA	1	0
16	A	828	CLA	7	0
16	A	802	CLA	2	0
16	B	828	CLA	3	0
16	A	856	CLA	2	0
20	2	618	ERG	4	0
16	1	610	CLA	1	0
17	1	616	C7Z	1	0
16	A	814	CLA	2	0
16	3	206	CLA	1	0
16	3	207	CLA	5	0
17	1	614	C7Z	2	0
16	1	609	CLA	3	0
16	I	101	CLA	3	0
17	3	217	C7Z	1	0
16	A	834	CLA	1	0
16	O	202	CLA	3	0
16	B	812	CLA	2	0
16	K	101	CLA	2	0
16	A	816	CLA	4	0
16	B	825	CLA	5	0
18	K	103	RRX	3	0
16	3	204	CLA	2	0
16	B	832	CLA	4	0
16	B	815	CLA	1	0
16	O	201	CLA	2	0
16	F	204	CLA	1	0
18	2	616	RRX	2	0
17	3	216	C7Z	1	0
16	A	833	CLA	2	0
21	B	847	BCR	4	0
21	B	855	BCR	9	0
16	A	818	CLA	3	0

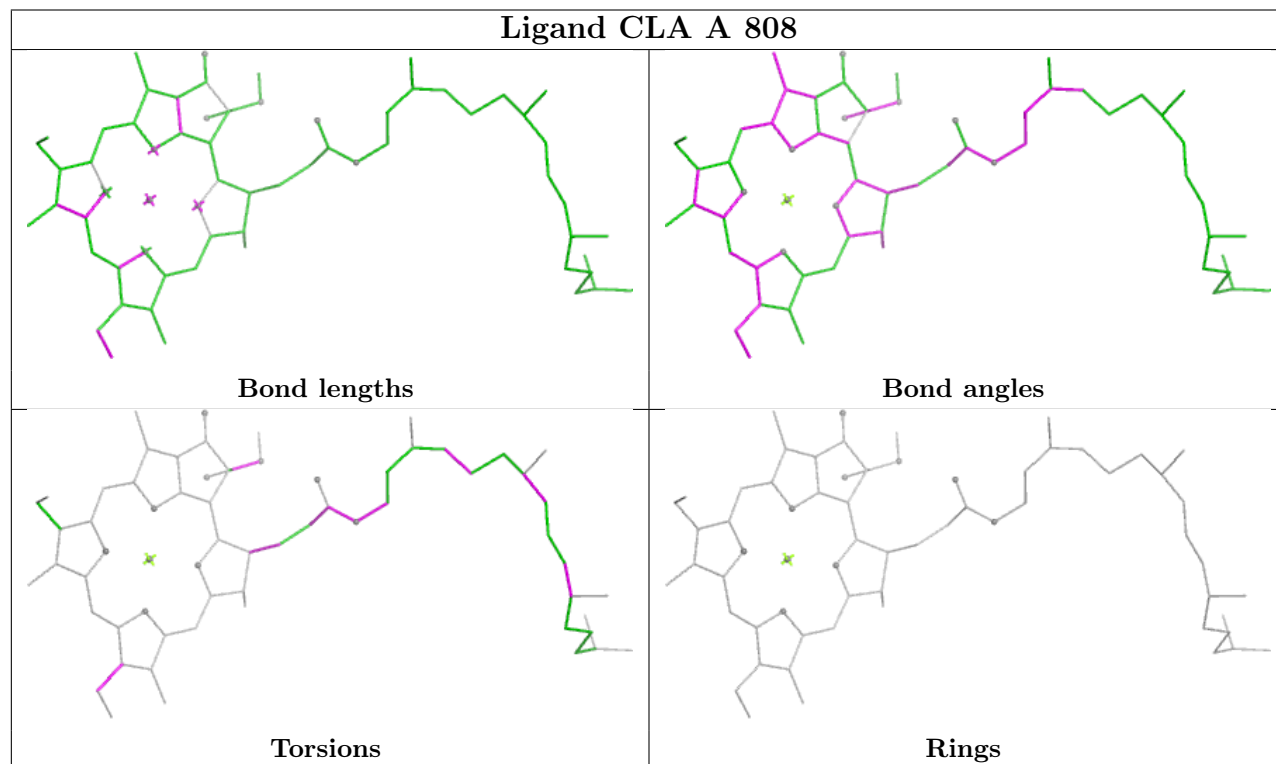
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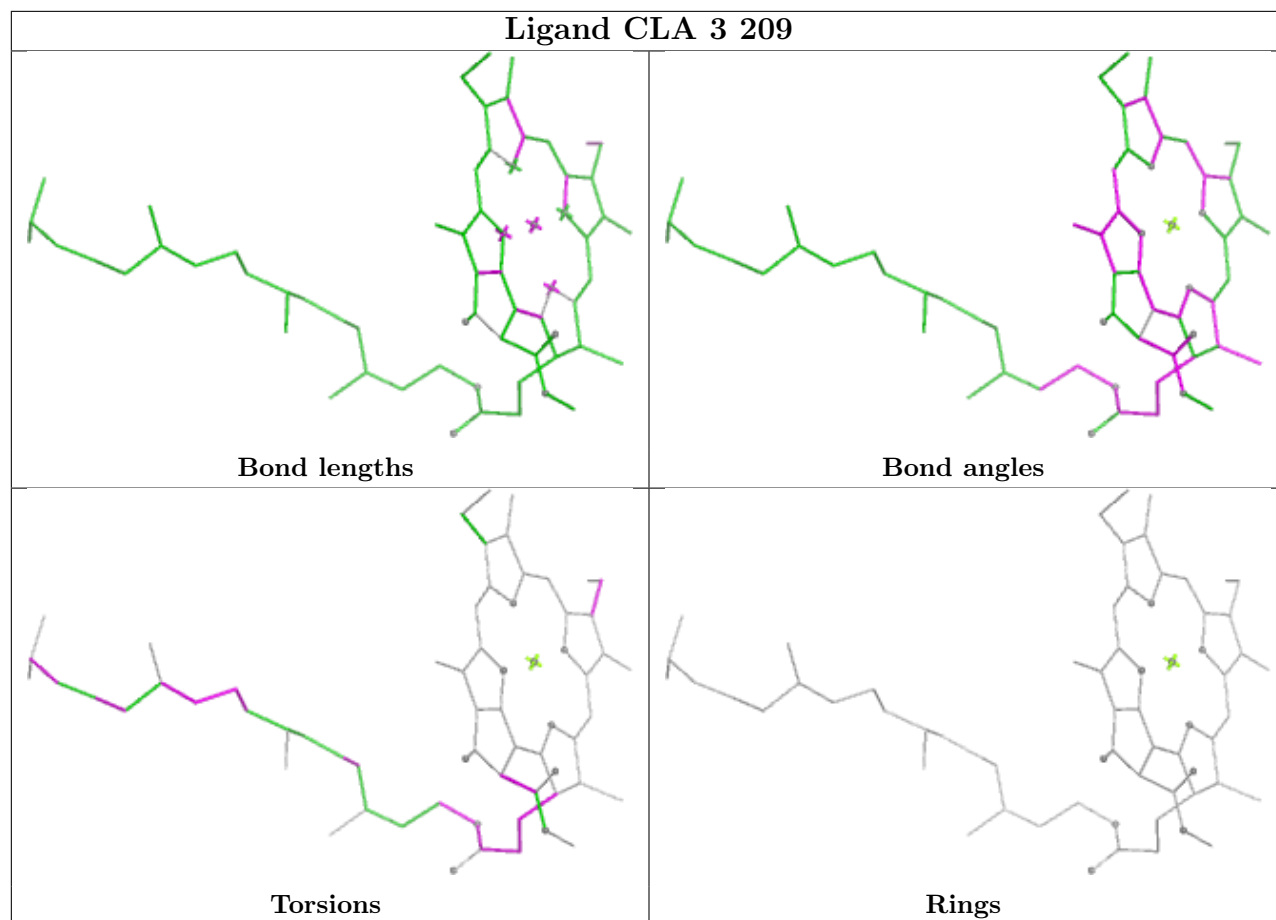
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	807	CLA	3	0
16	B	817	CLA	3	0
16	B	810	CLA	2	0
16	2	612	CLA	4	0
16	A	820	CLA	2	0
16	A	824	CLA	4	0
16	3	203	CLA	1	0
16	2	601	CLA	3	0
16	1	611	CLA	2	0
16	K	102	CLA	2	0
16	B	837	CLA	3	0
16	A	826	CLA	6	0
16	B	830	CLA	1	0
16	A	838	CLA	1	0
16	1	608	CLA	2	0
16	A	821	CLA	5	0
16	A	803	CLA	2	0
16	B	803	CLA	4	0
24	3	202	LMU	1	0
25	A	852	PTY	3	0
27	B	839	PQN	4	0
16	2	602	CLA	2	0
19	A	842	LHG	1	0
16	A	822	CLA	2	0
18	1	613	RRX	9	0
16	1	602	CLA	1	0
16	B	827	CLA	4	0
19	2	622	LHG	1	0
21	B	841	BCR	3	0
16	1	603	CLA	2	0
21	A	845	BCR	9	0
16	3	205	CLA	3	0
16	B	808	CLA	5	0
21	L	206	BCR	6	0
21	A	857	BCR	7	0
21	A	844	BCR	8	0
16	1	604	CLA	2	0
16	A	819	CLA	5	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

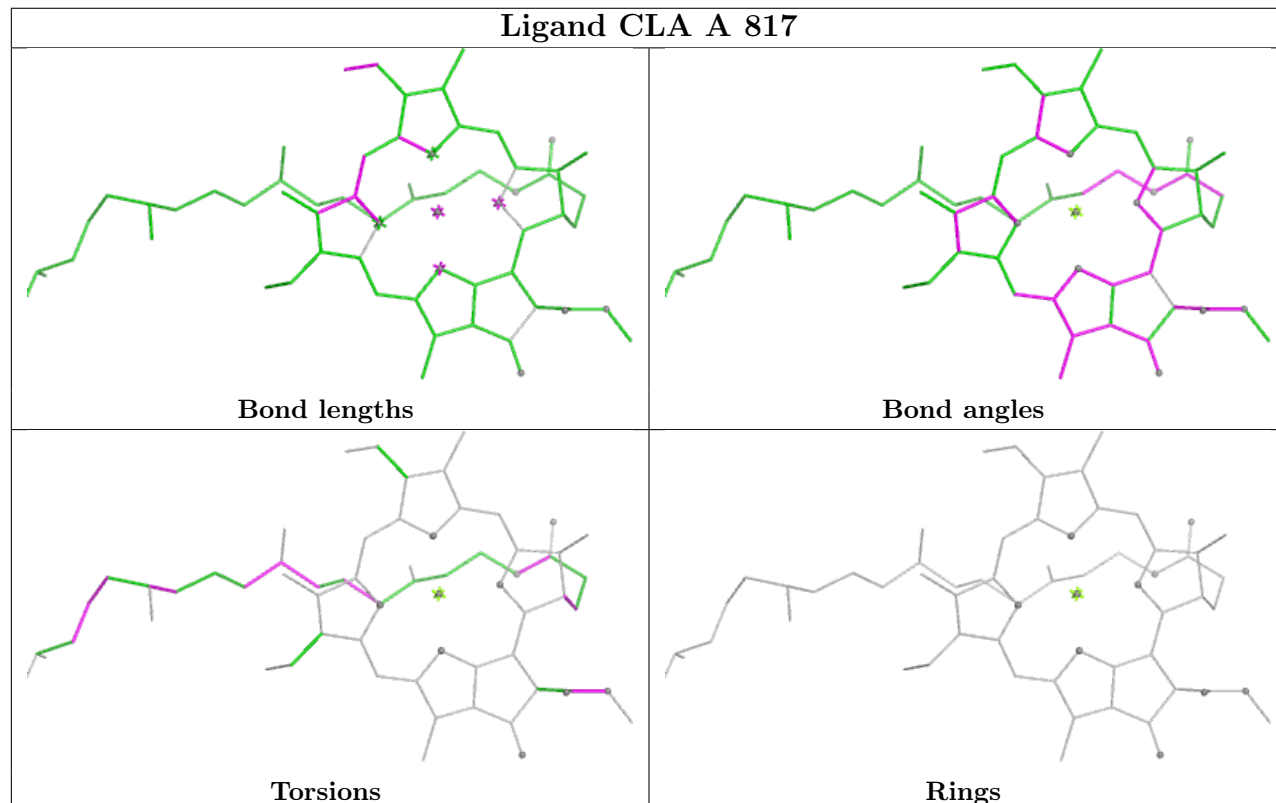
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

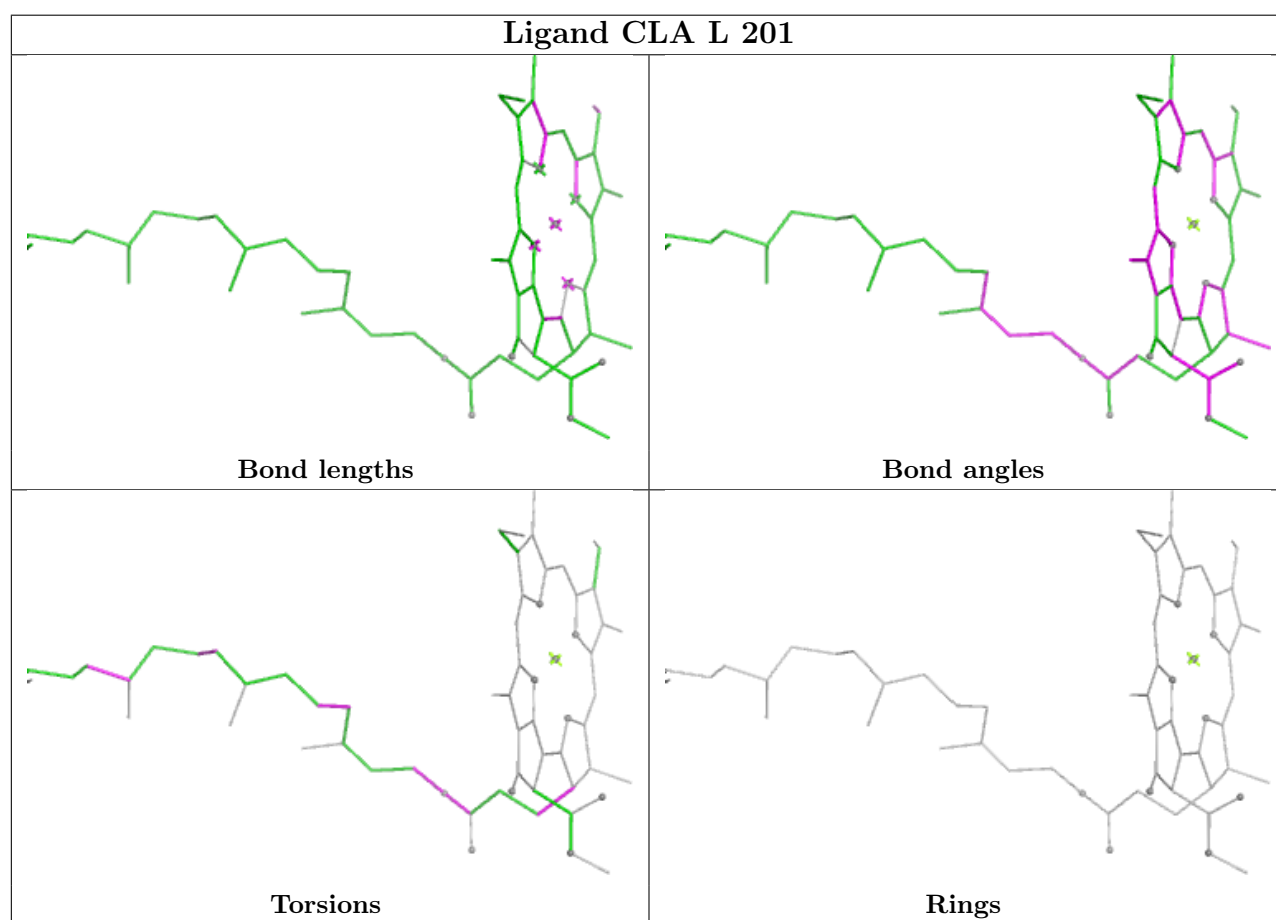
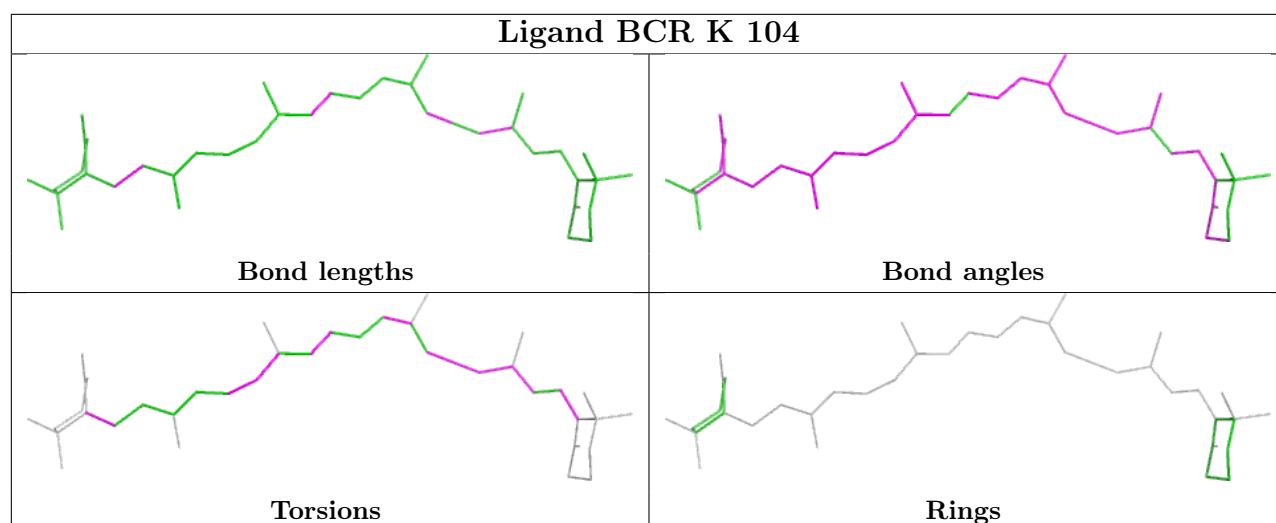


Ligand CLA 3 209

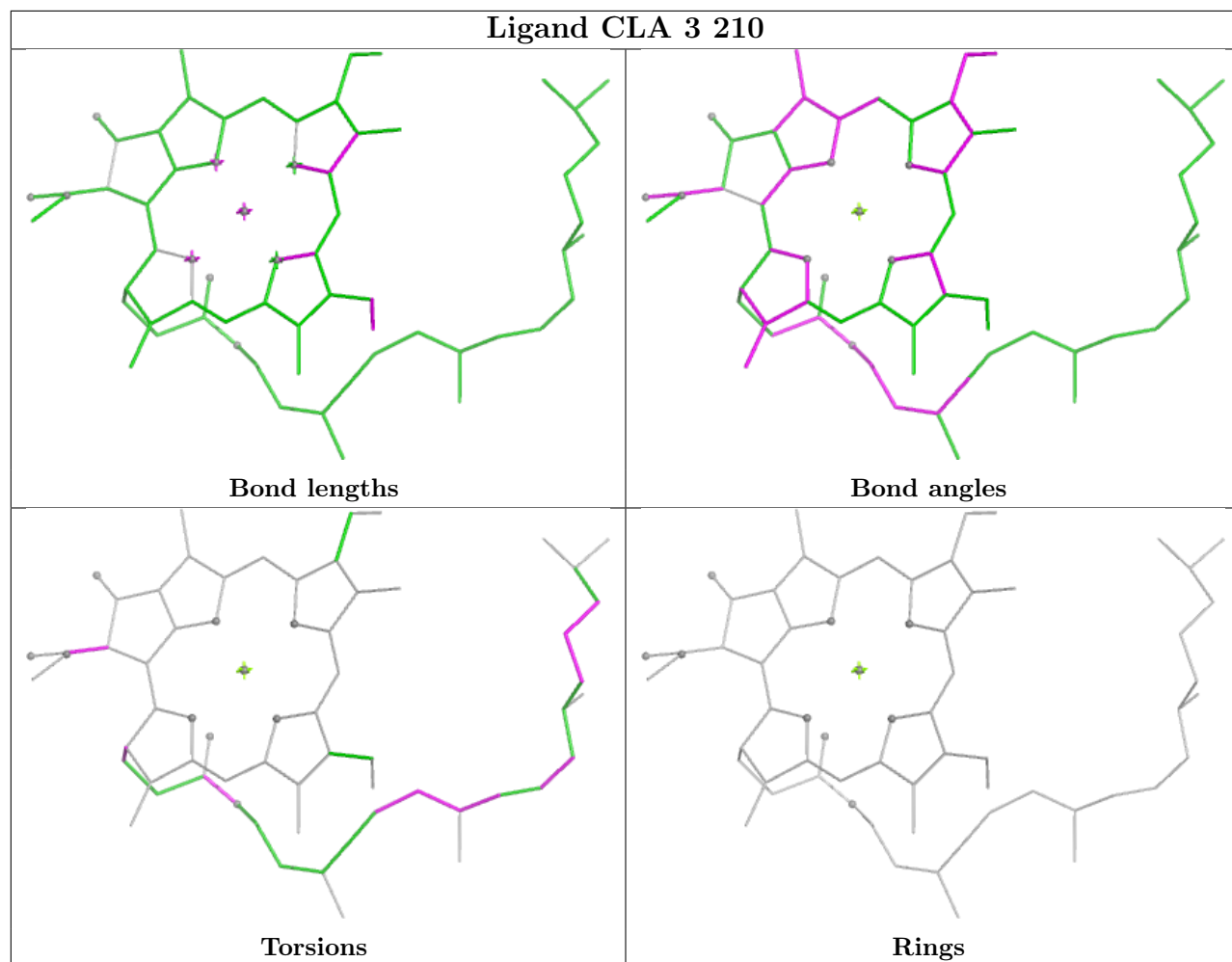


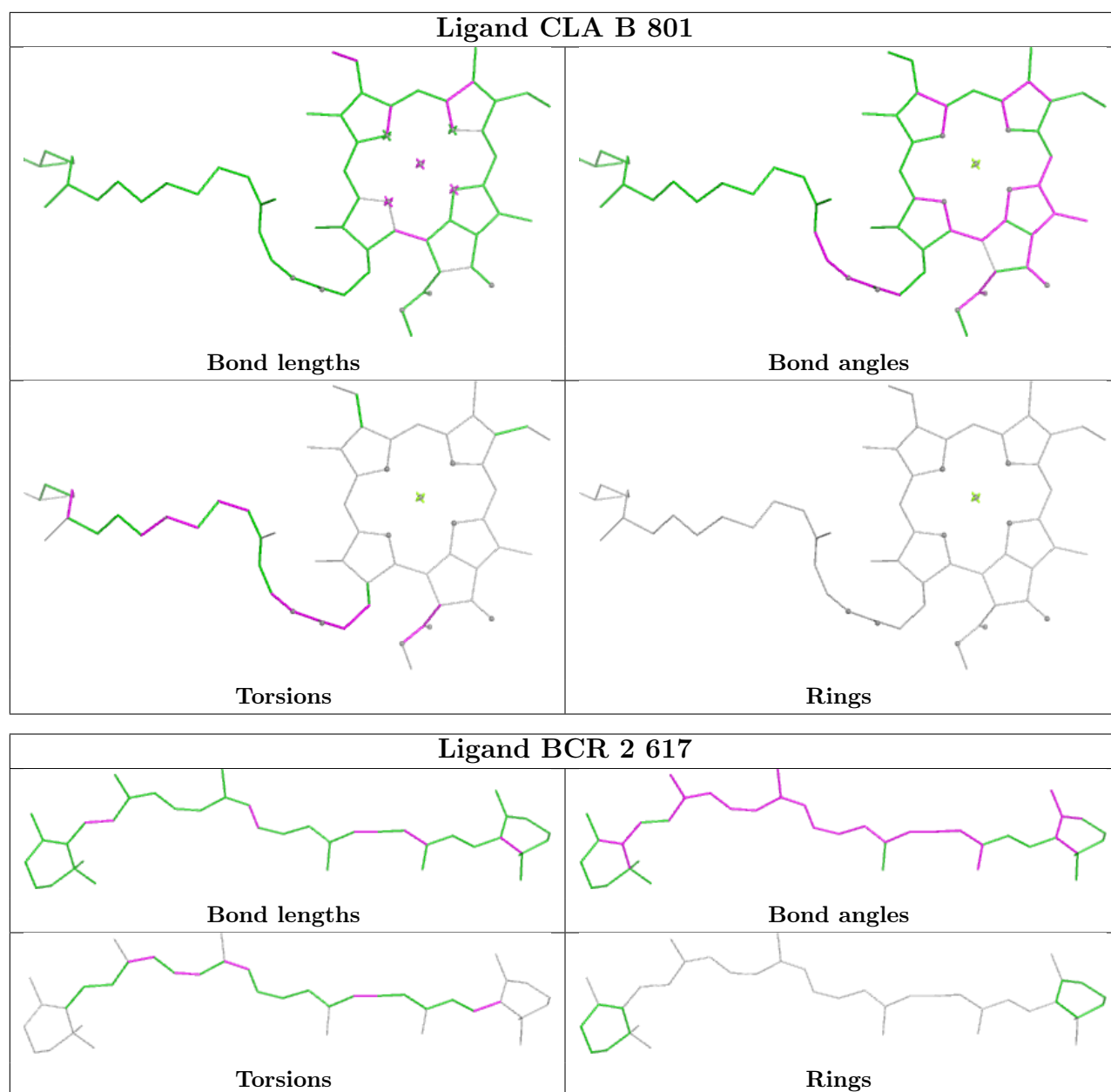
Ligand CLA A 817

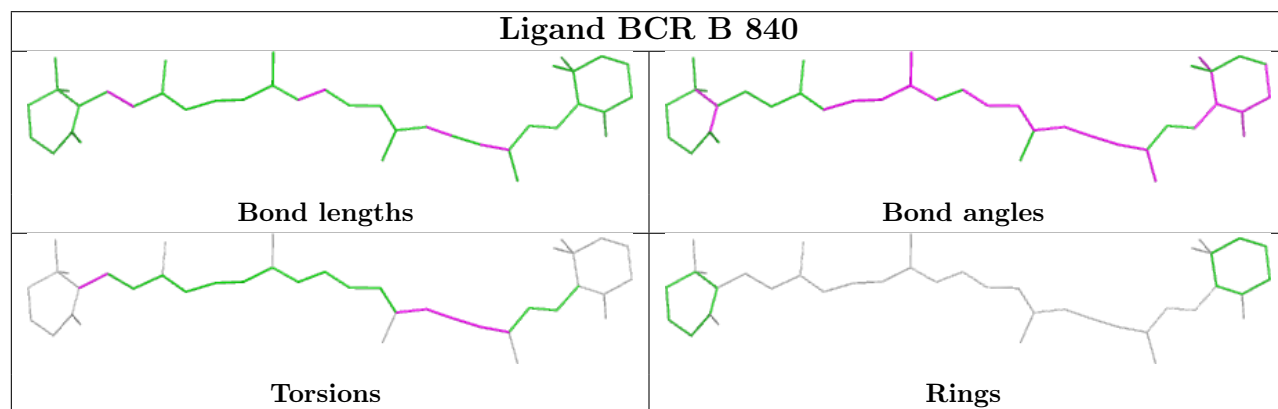
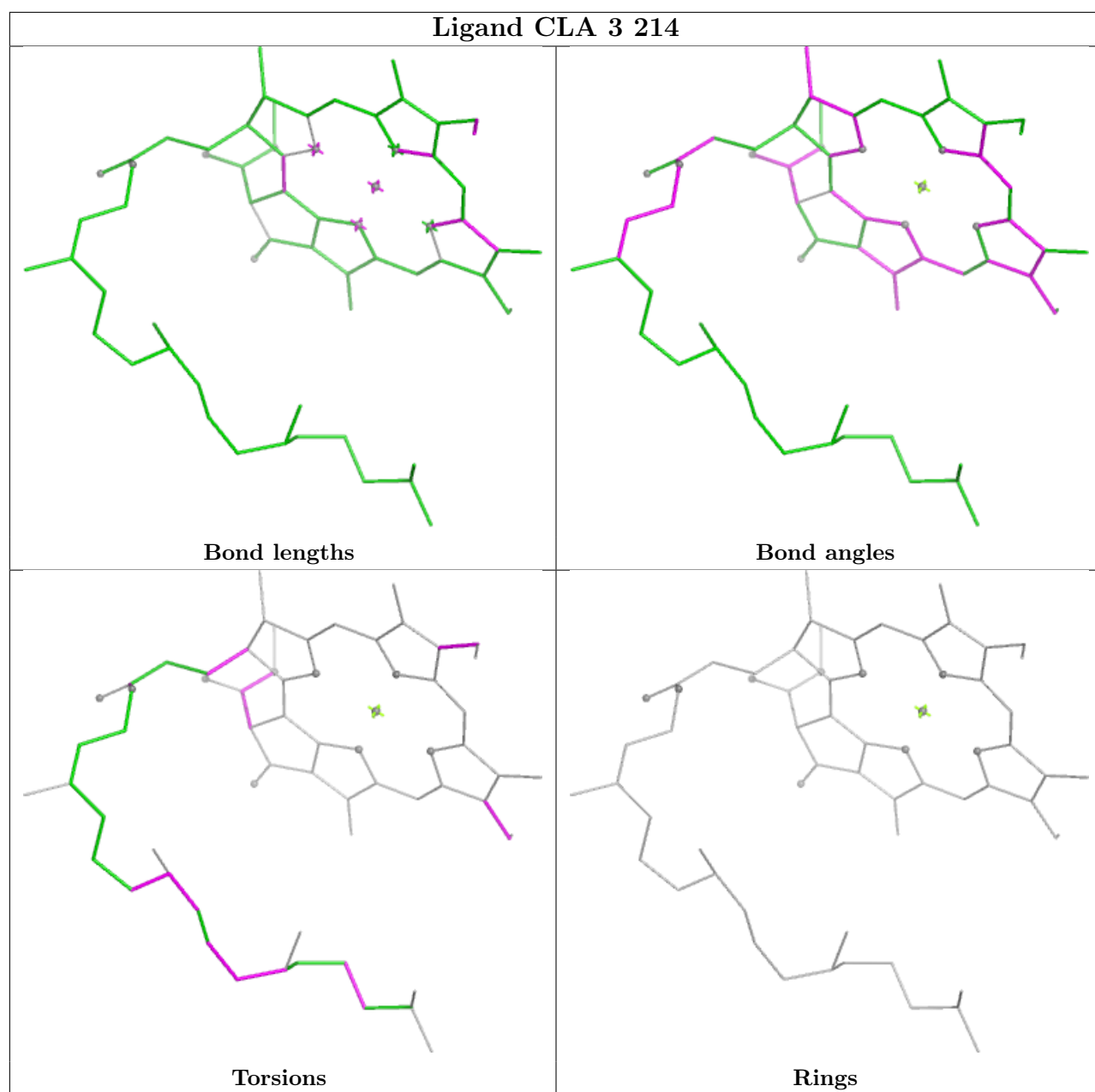




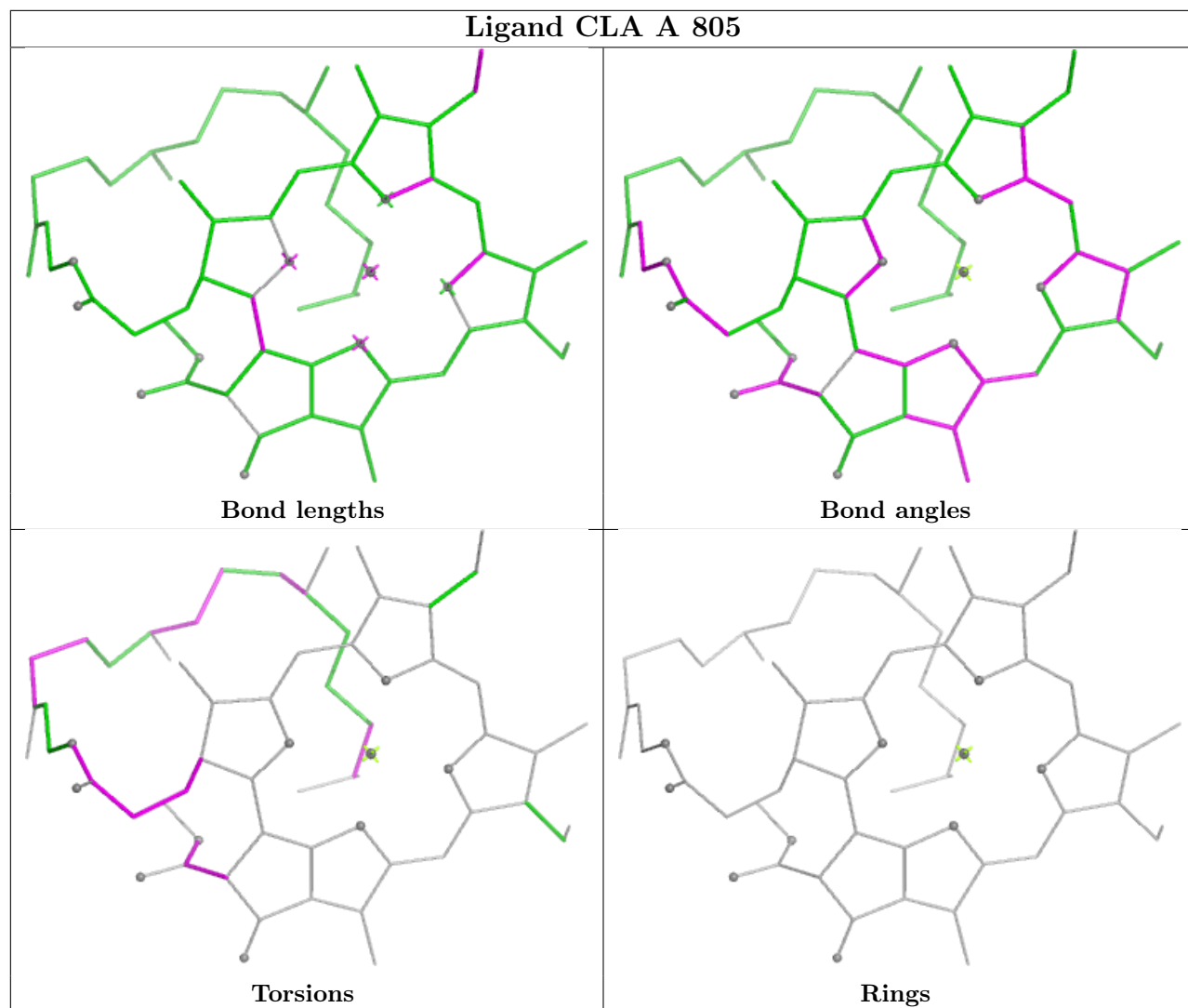
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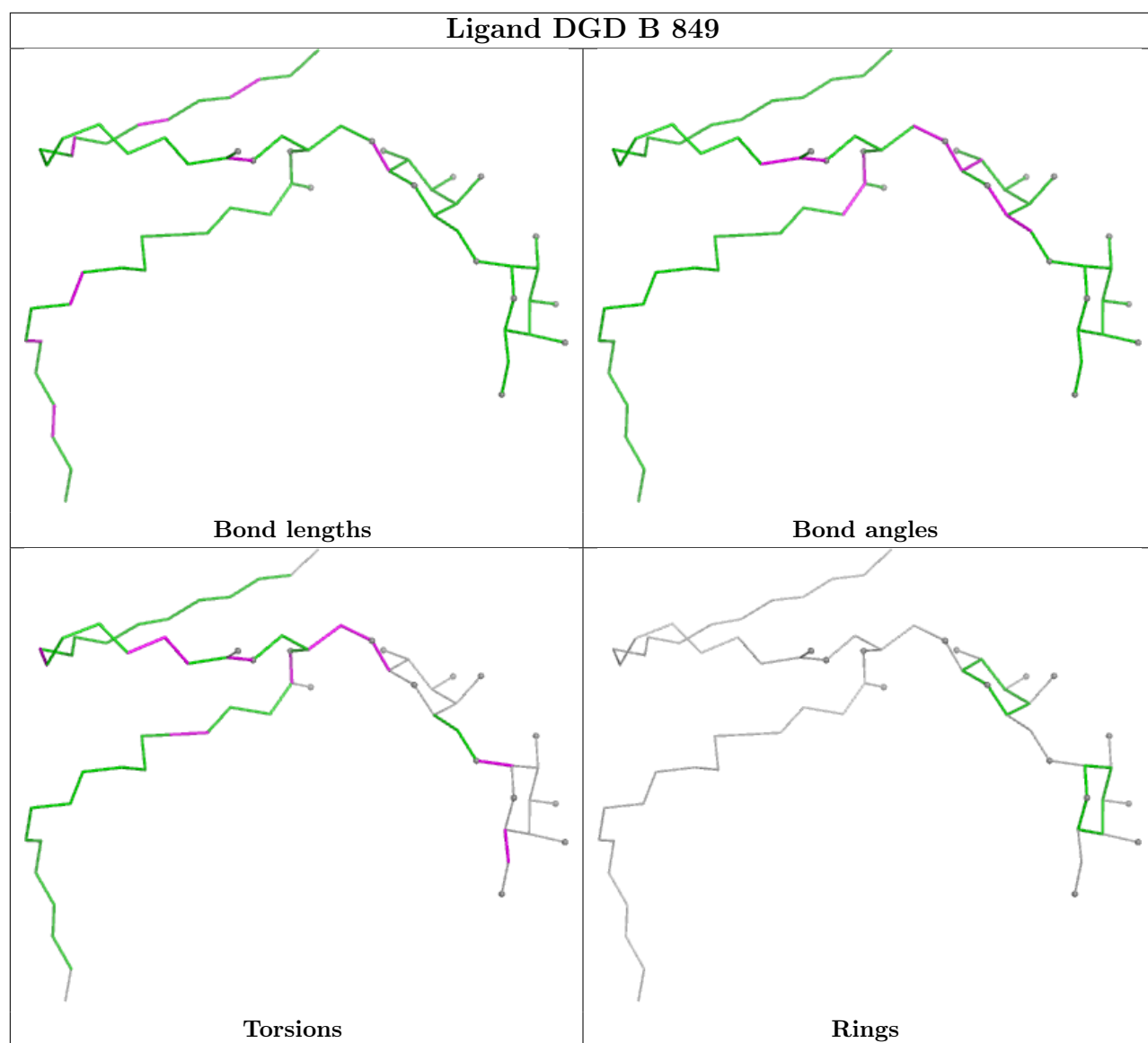




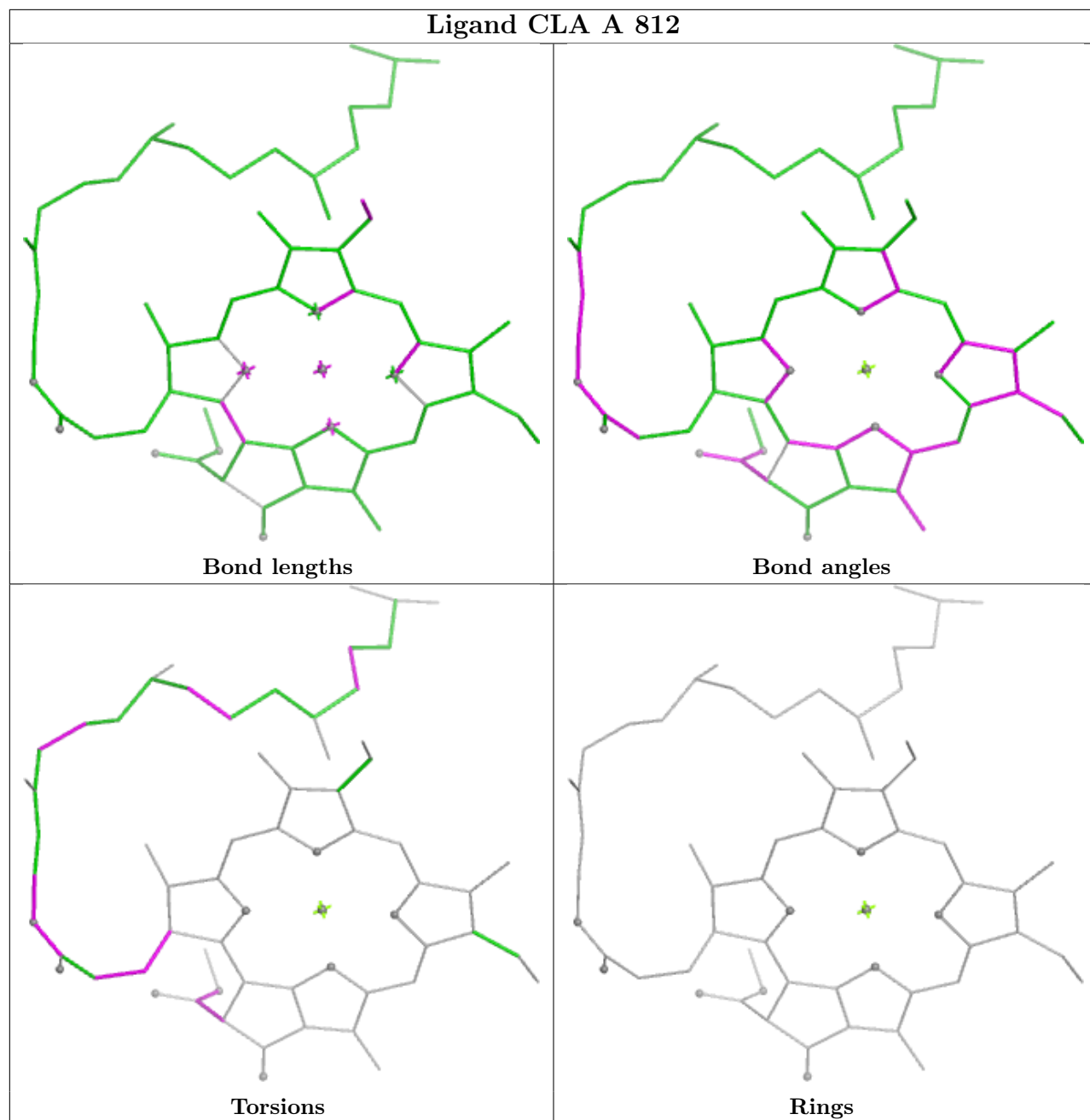


Ligand CLA A 805

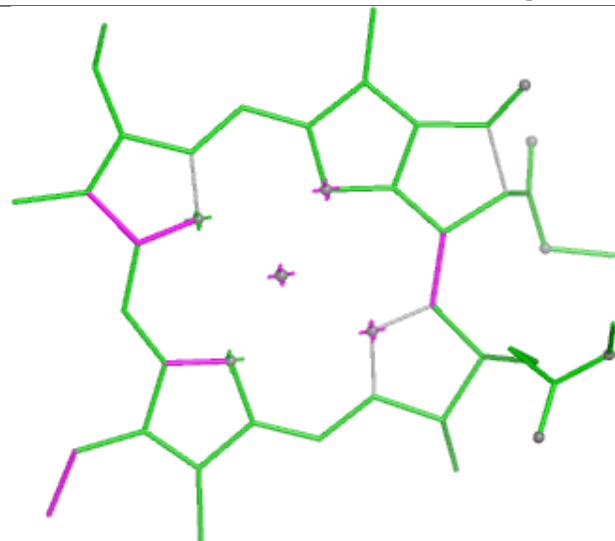




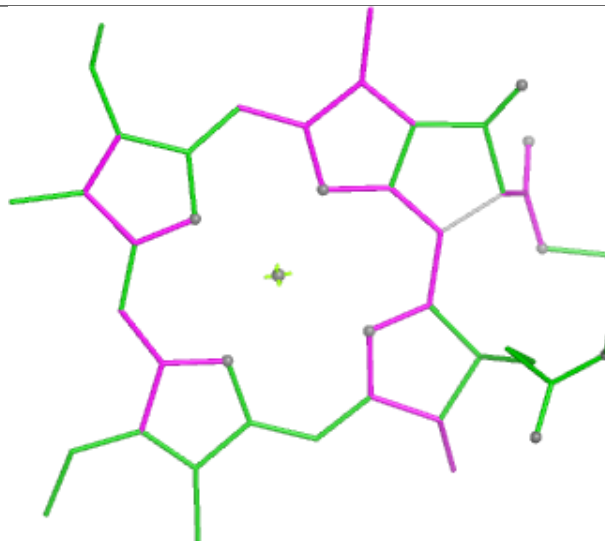
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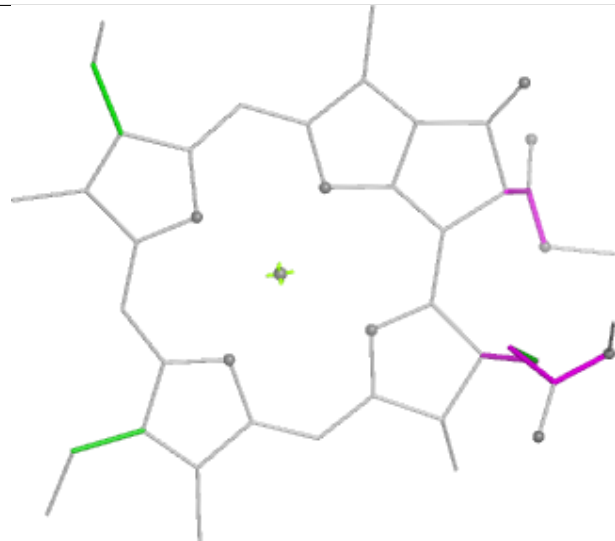
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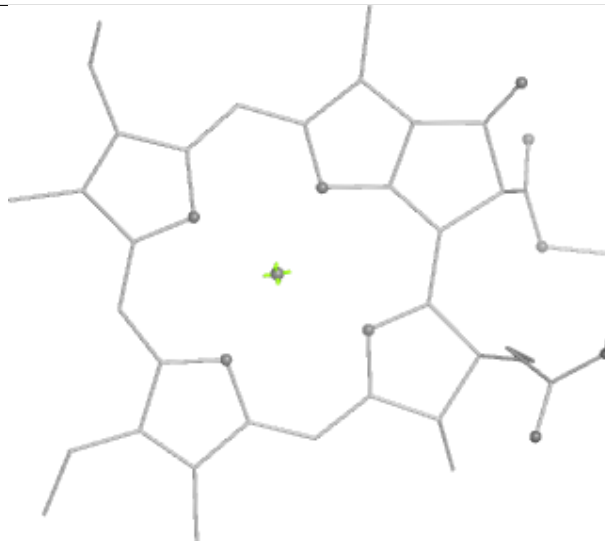
Bond lengths



Bond angles

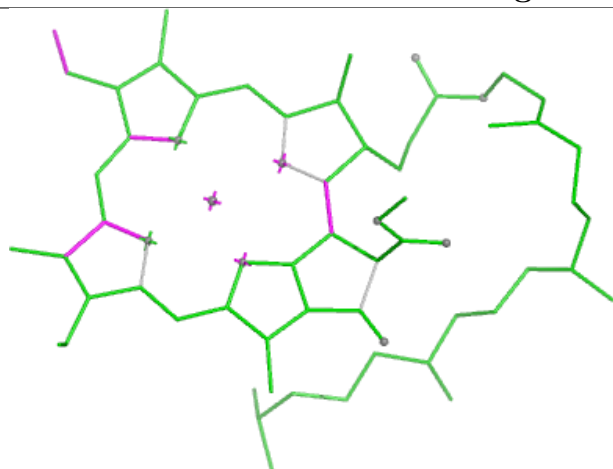


Torsions

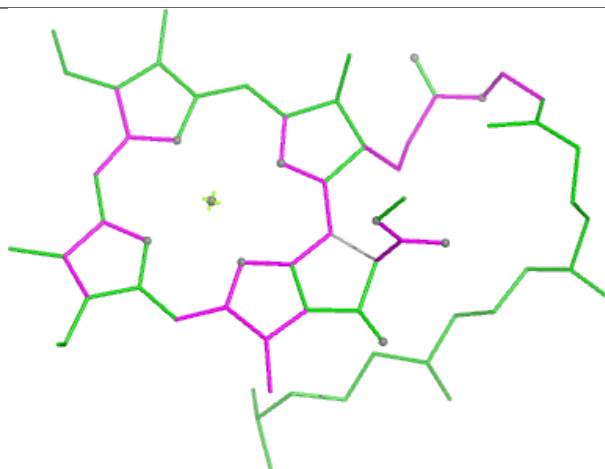


Rings

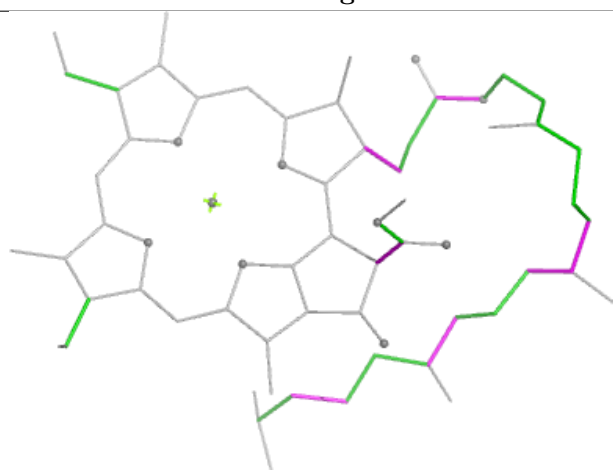
Ligand CLA B 806



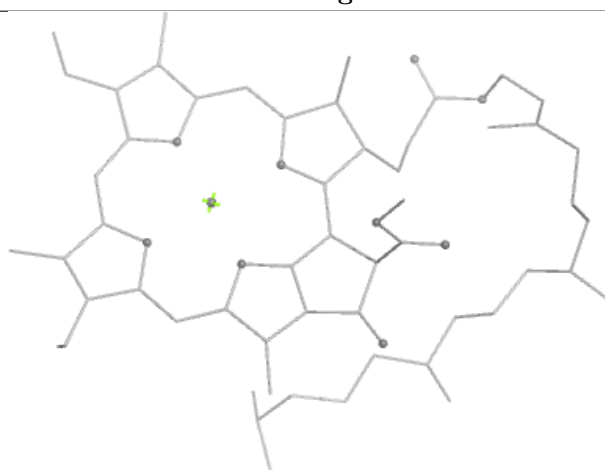
Bond lengths



Bond angles

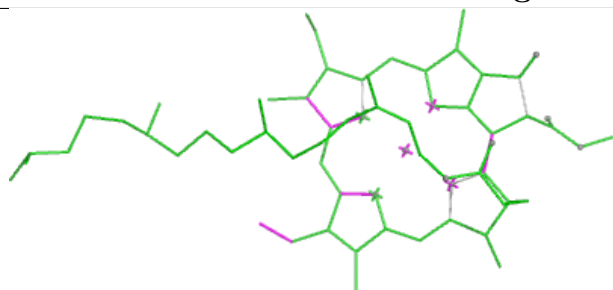


Torsions

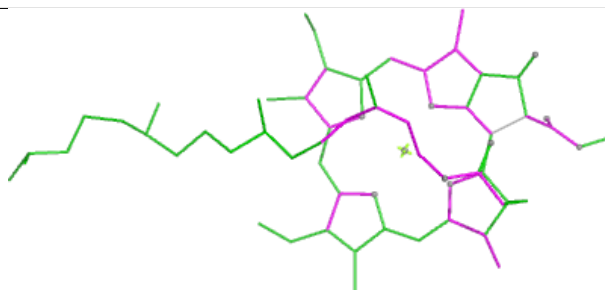


Rings

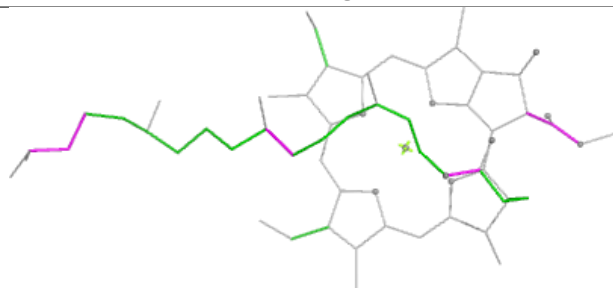
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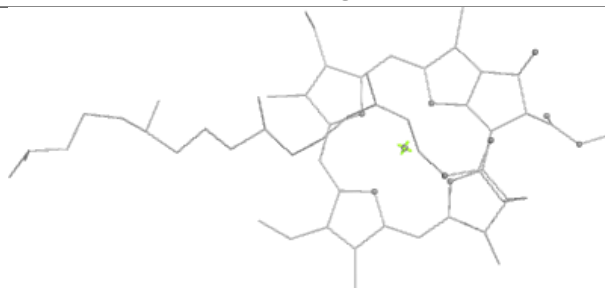
Bond lengths



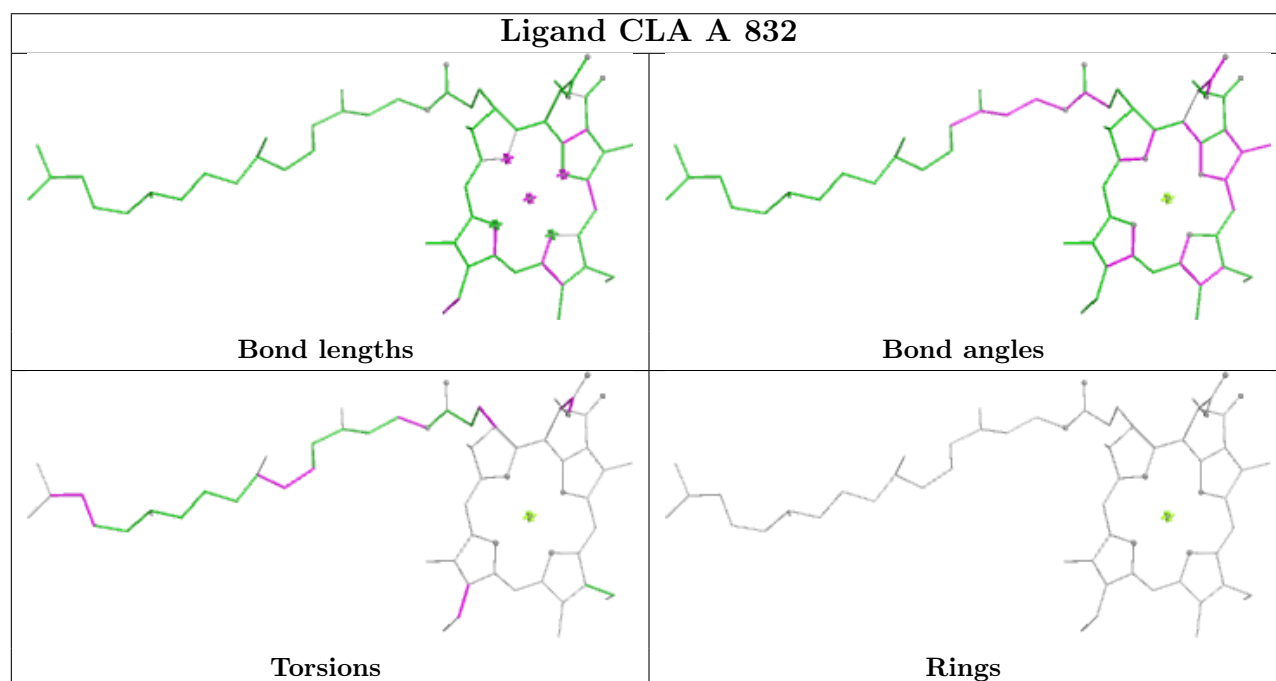
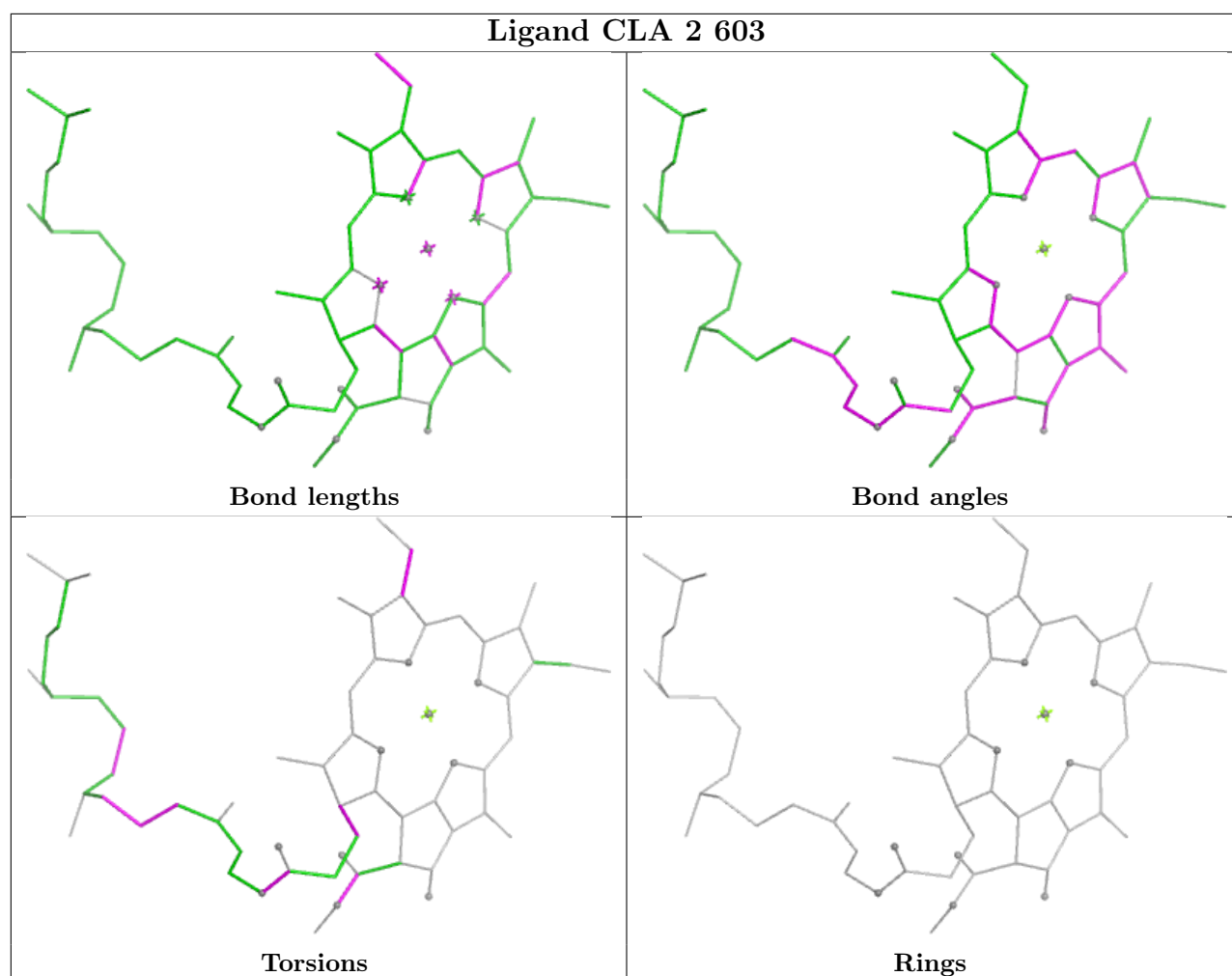
Bond angles

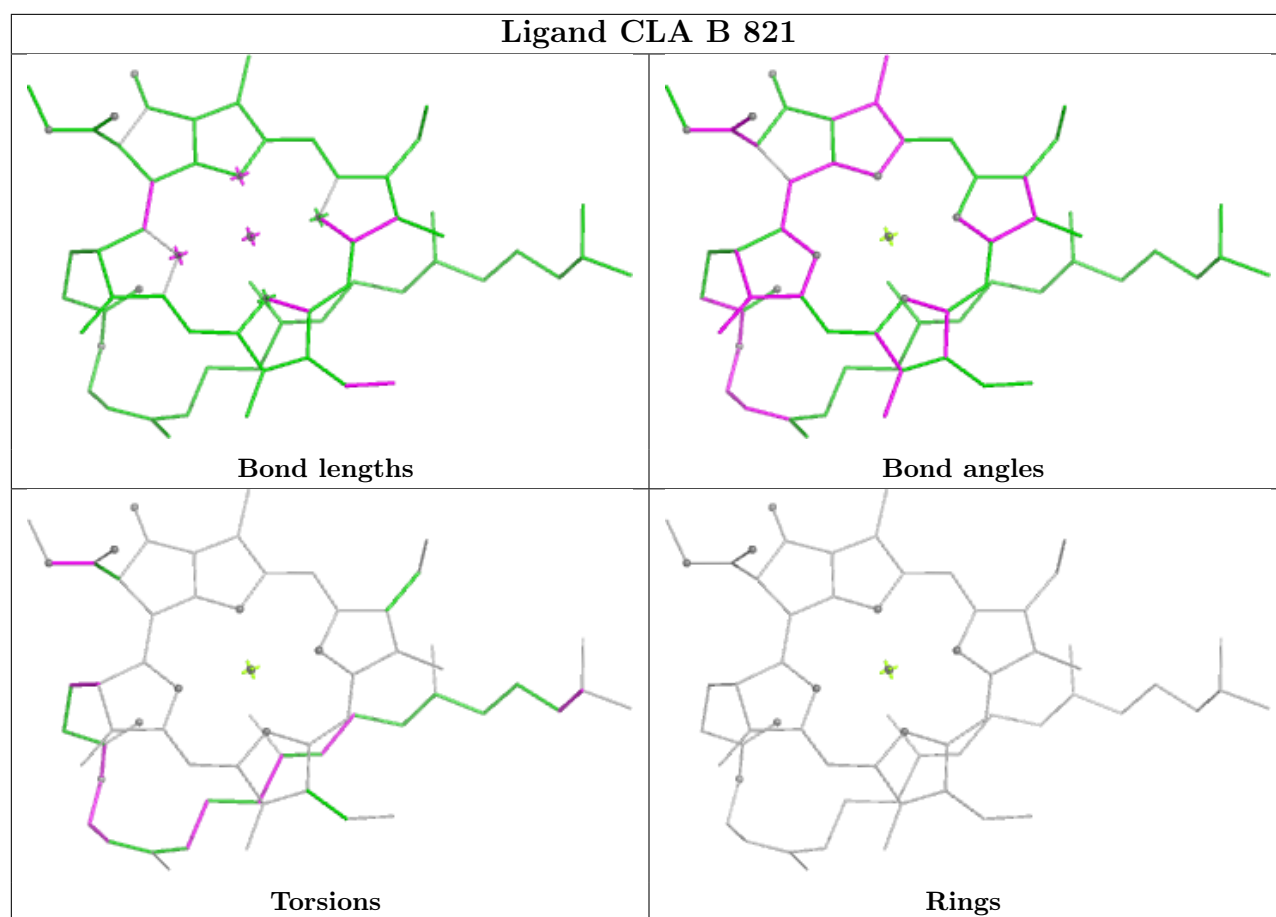


Torsions

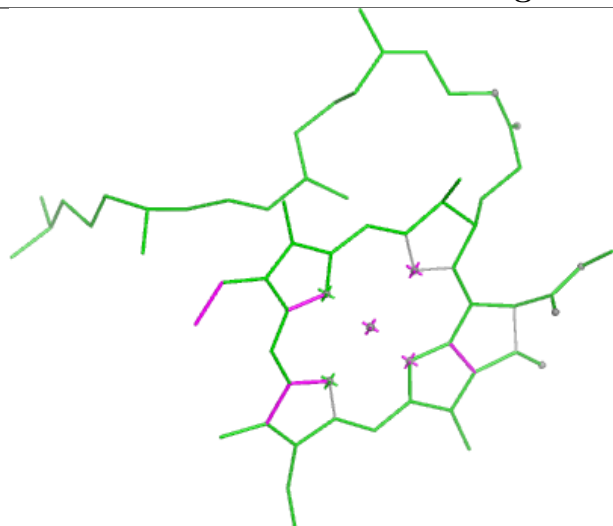


Rings

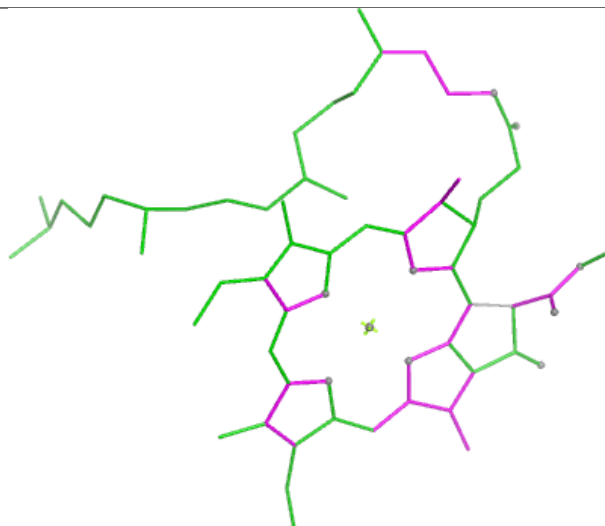




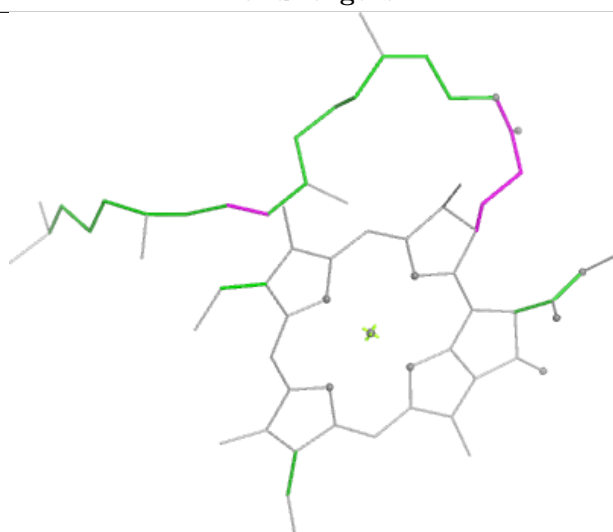
Ligand CLA B 811



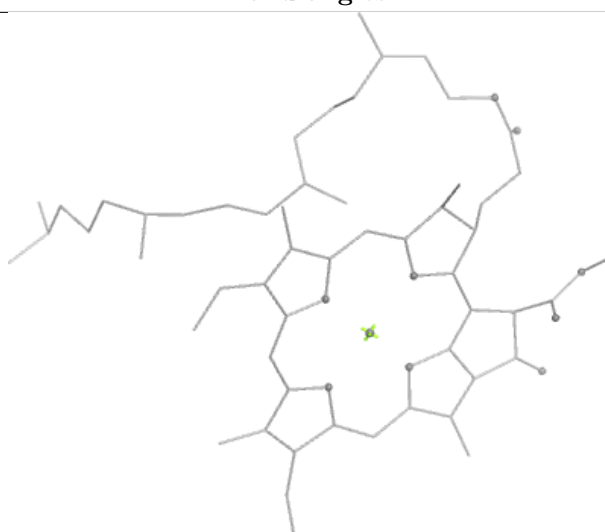
Bond lengths



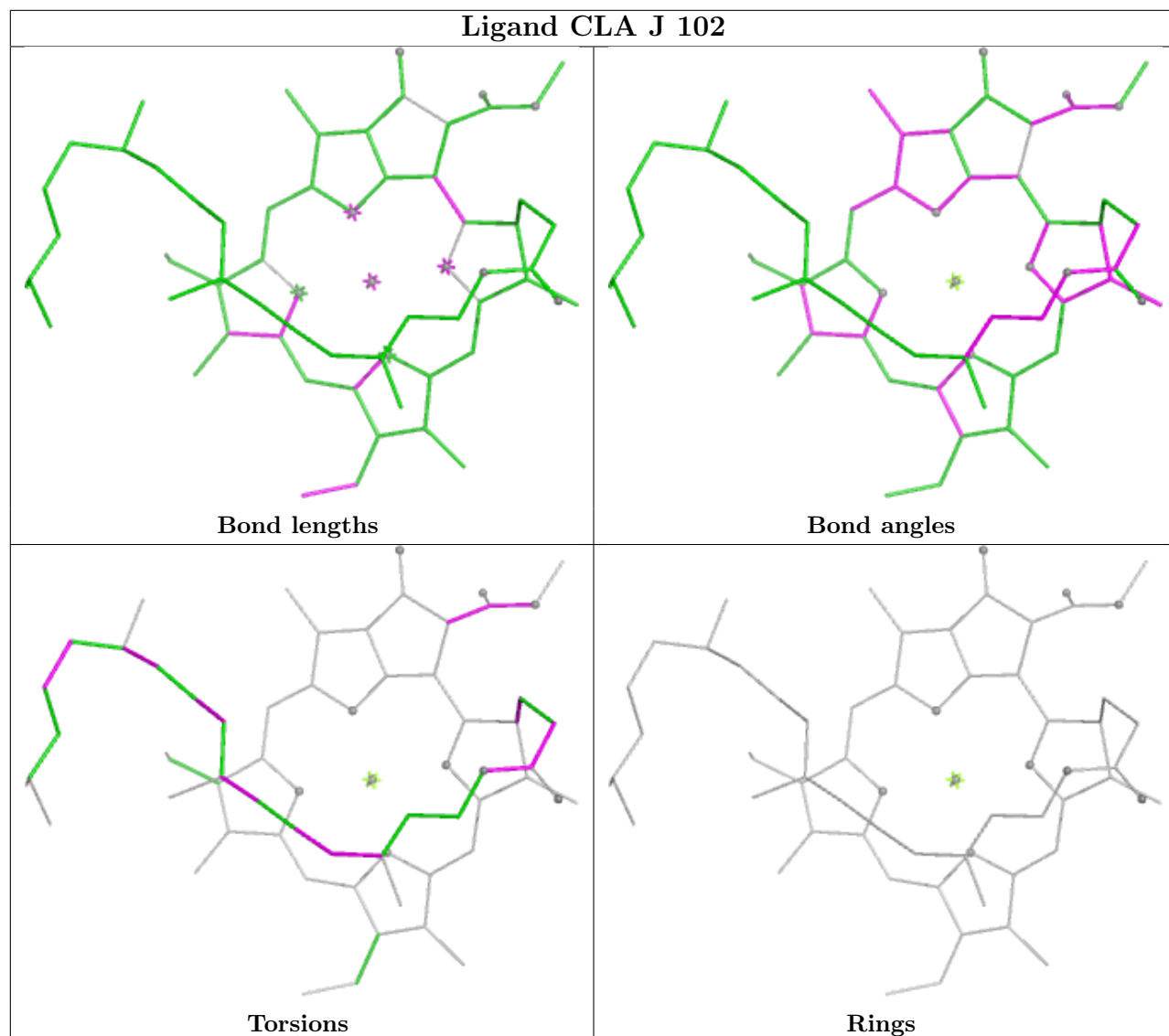
Bond angles

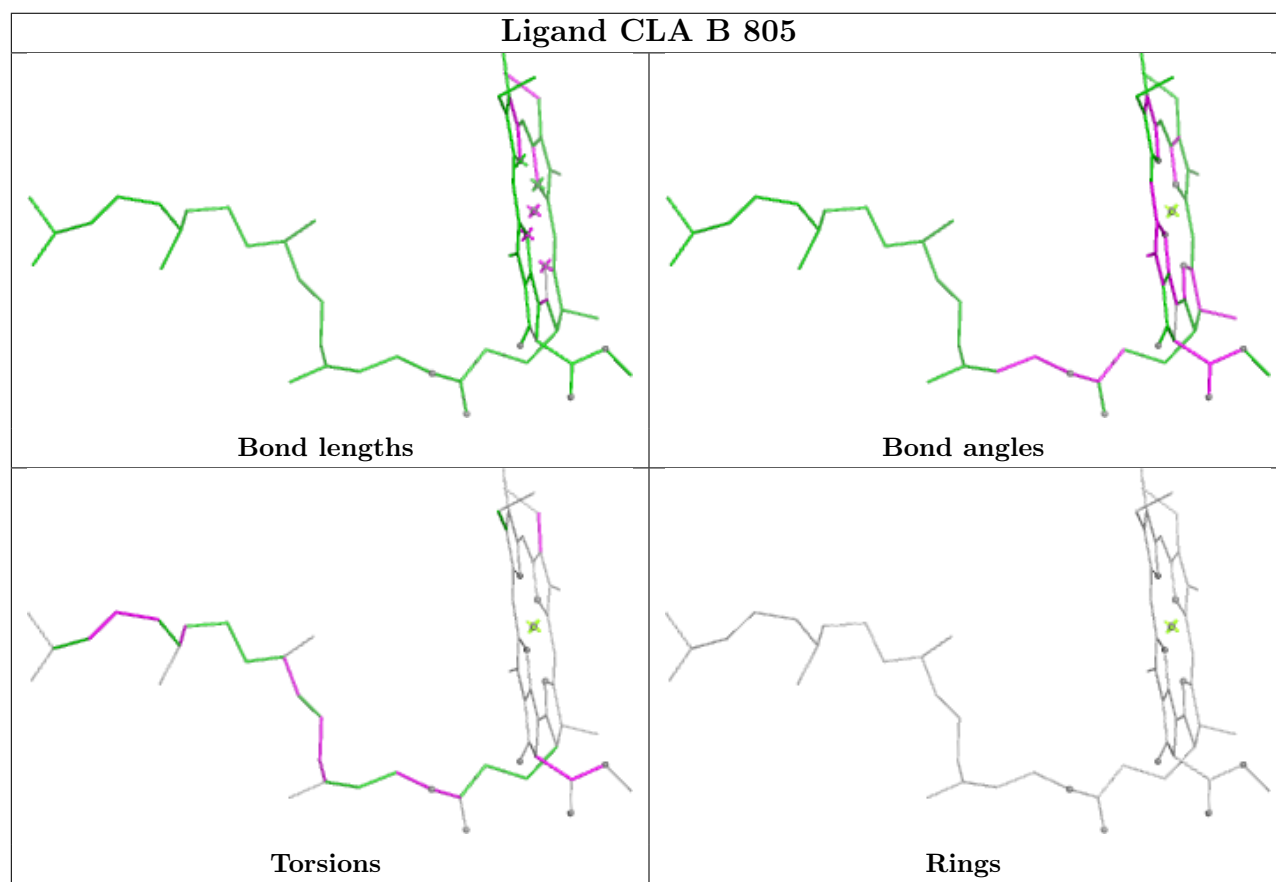
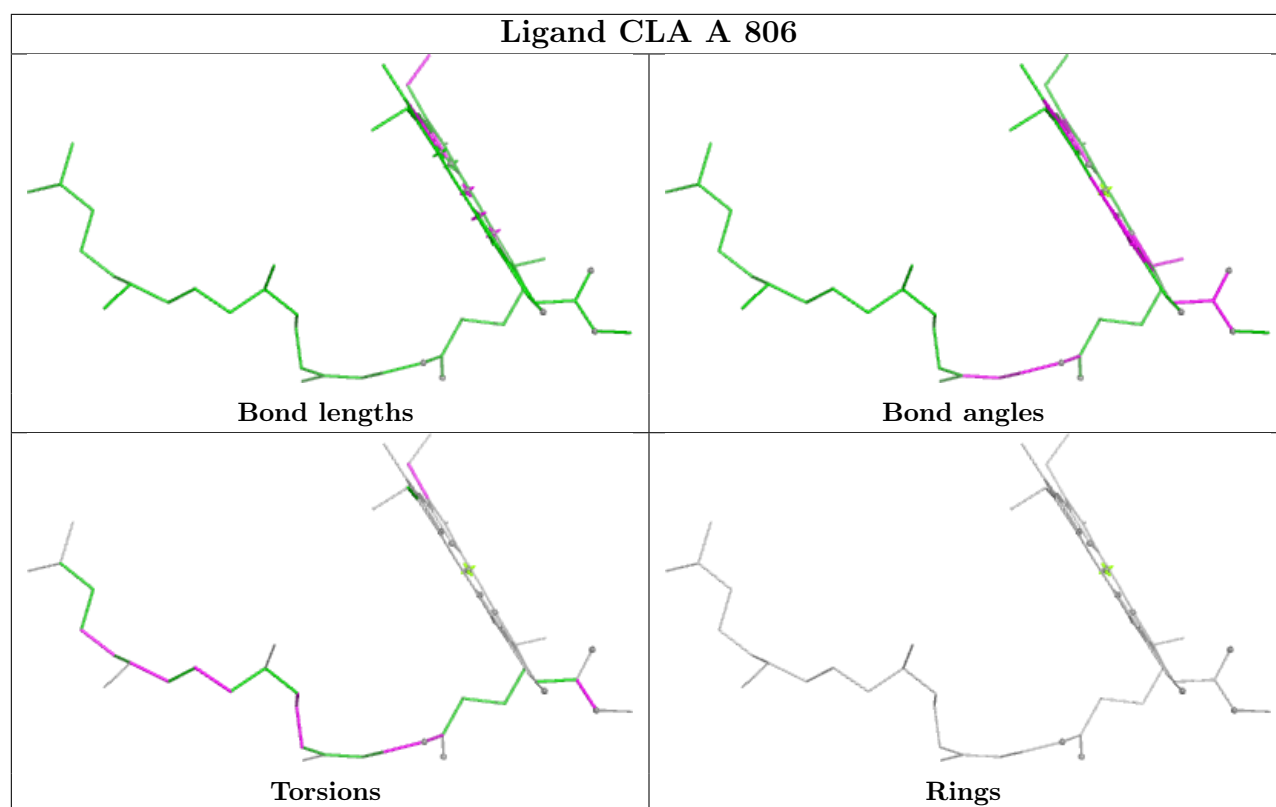


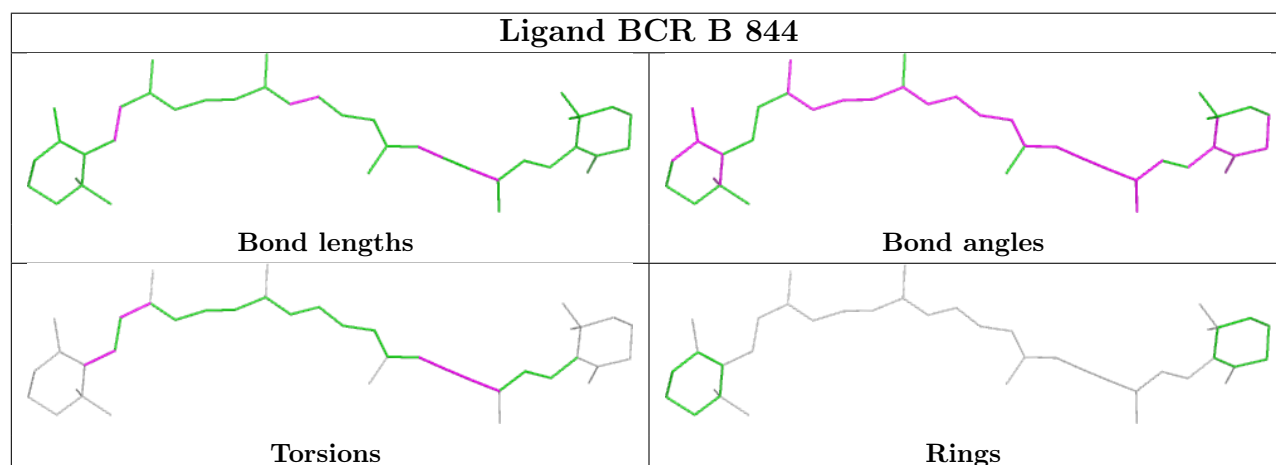
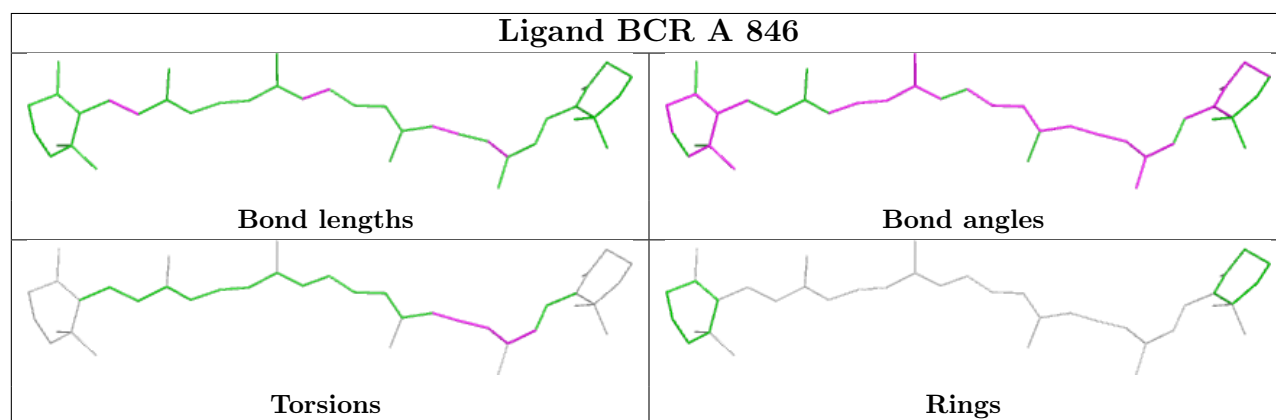
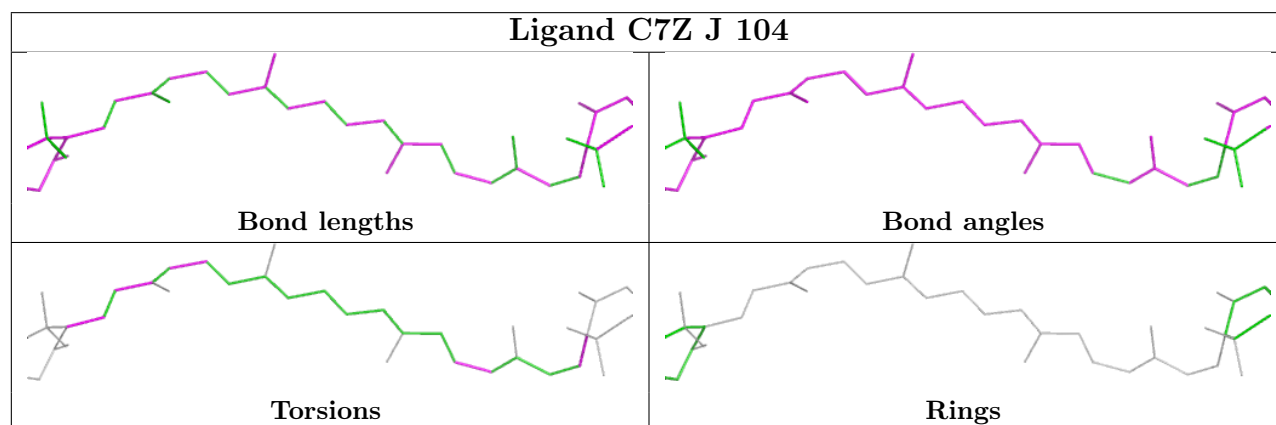
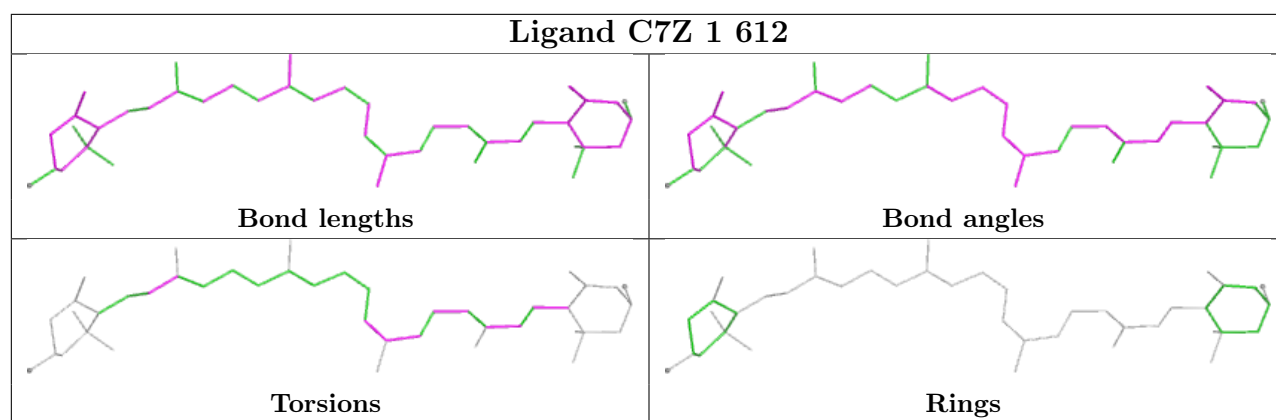
Torsions

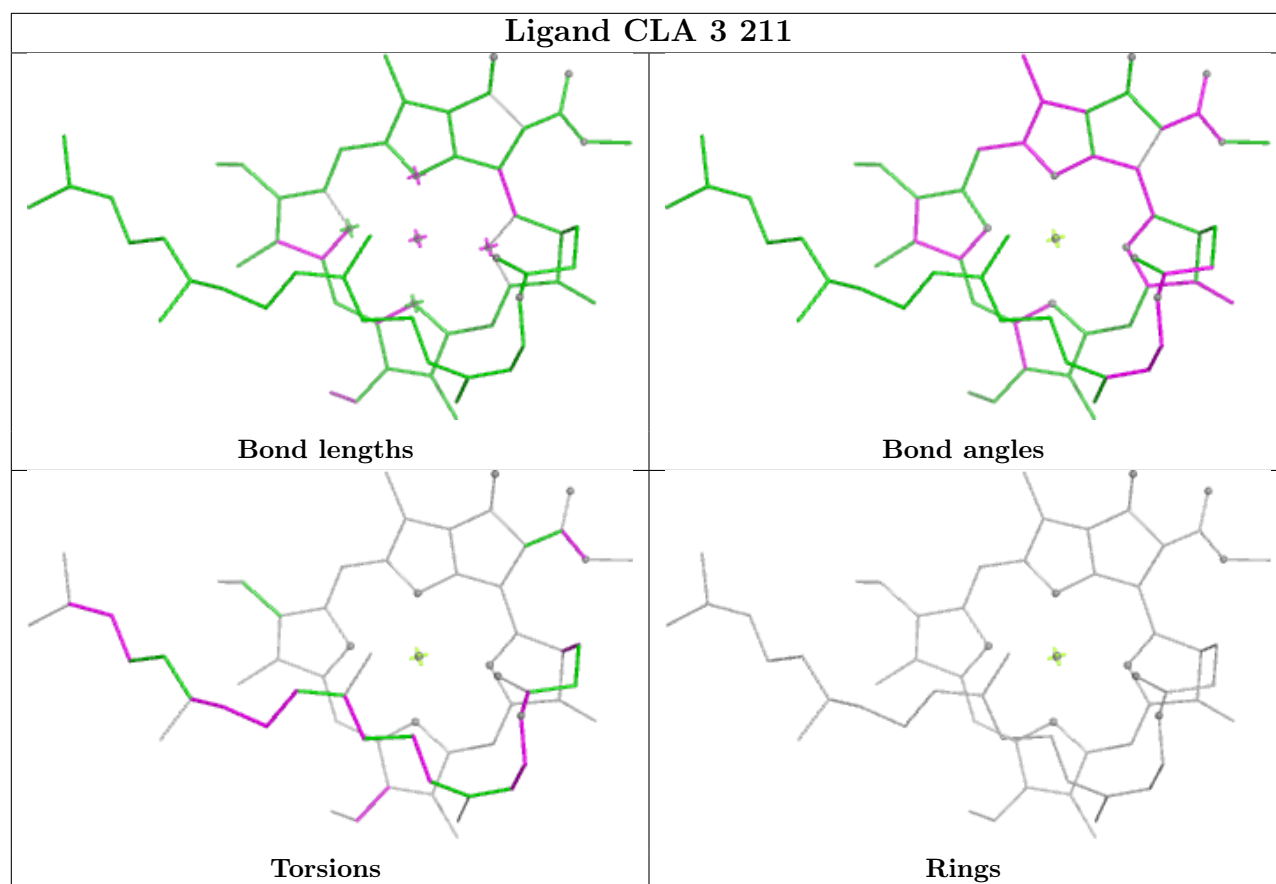
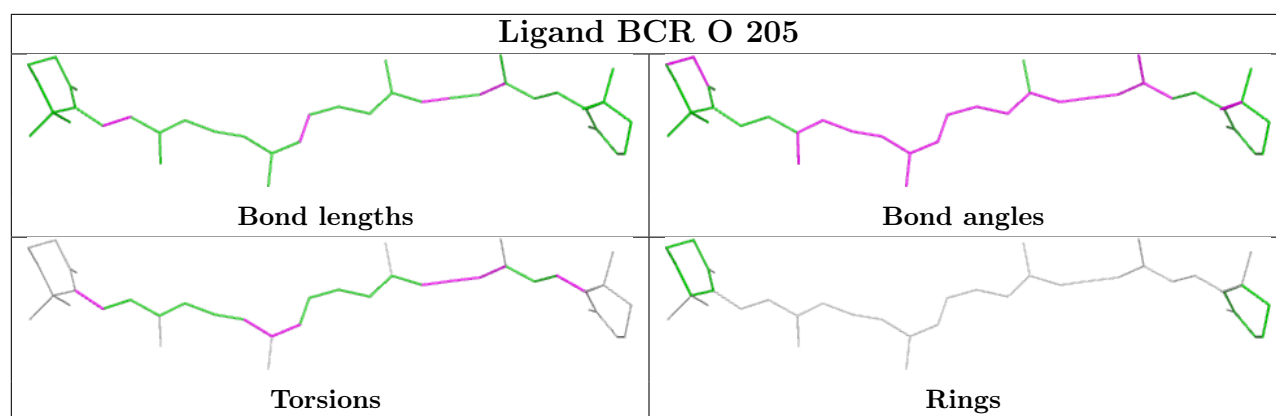


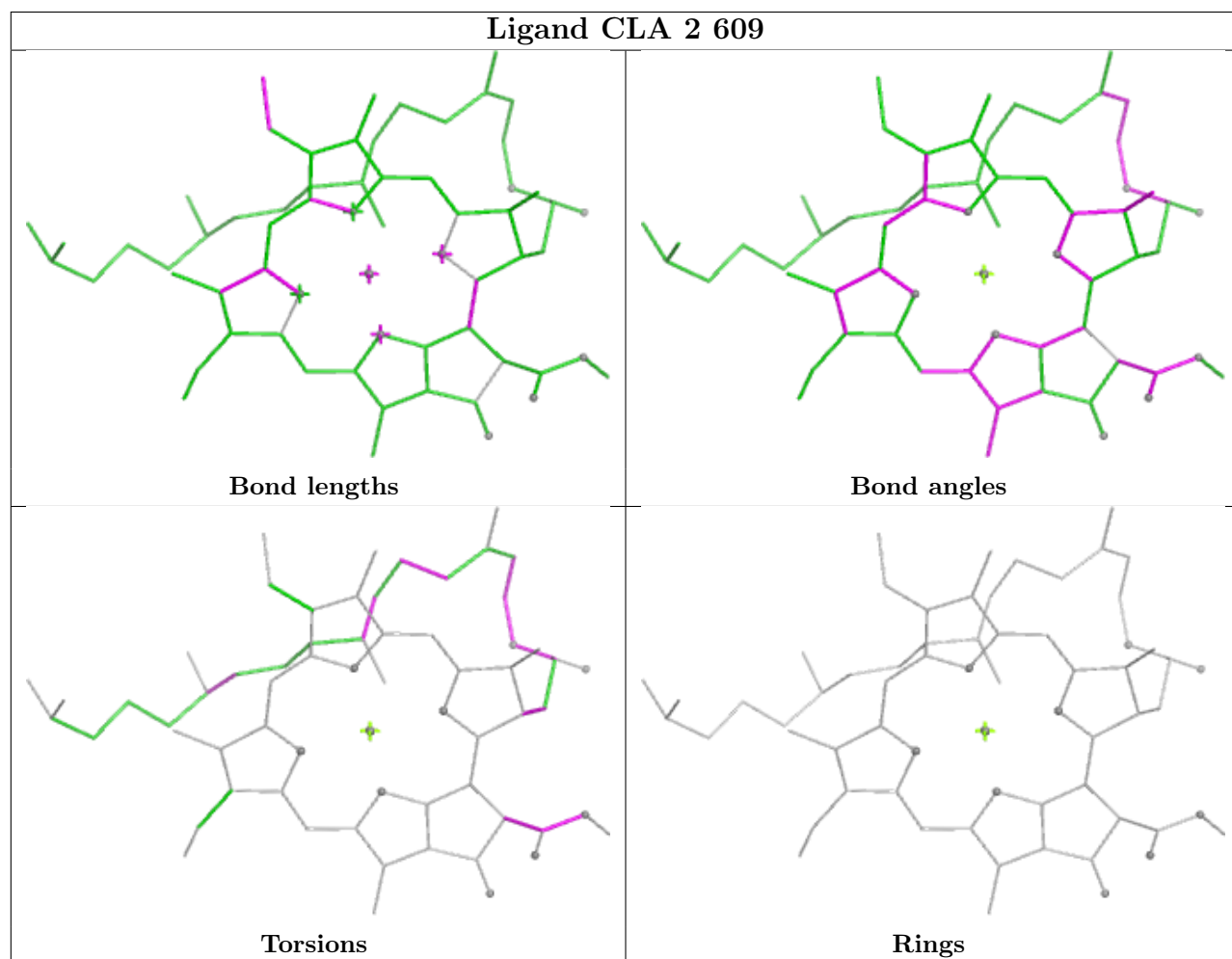
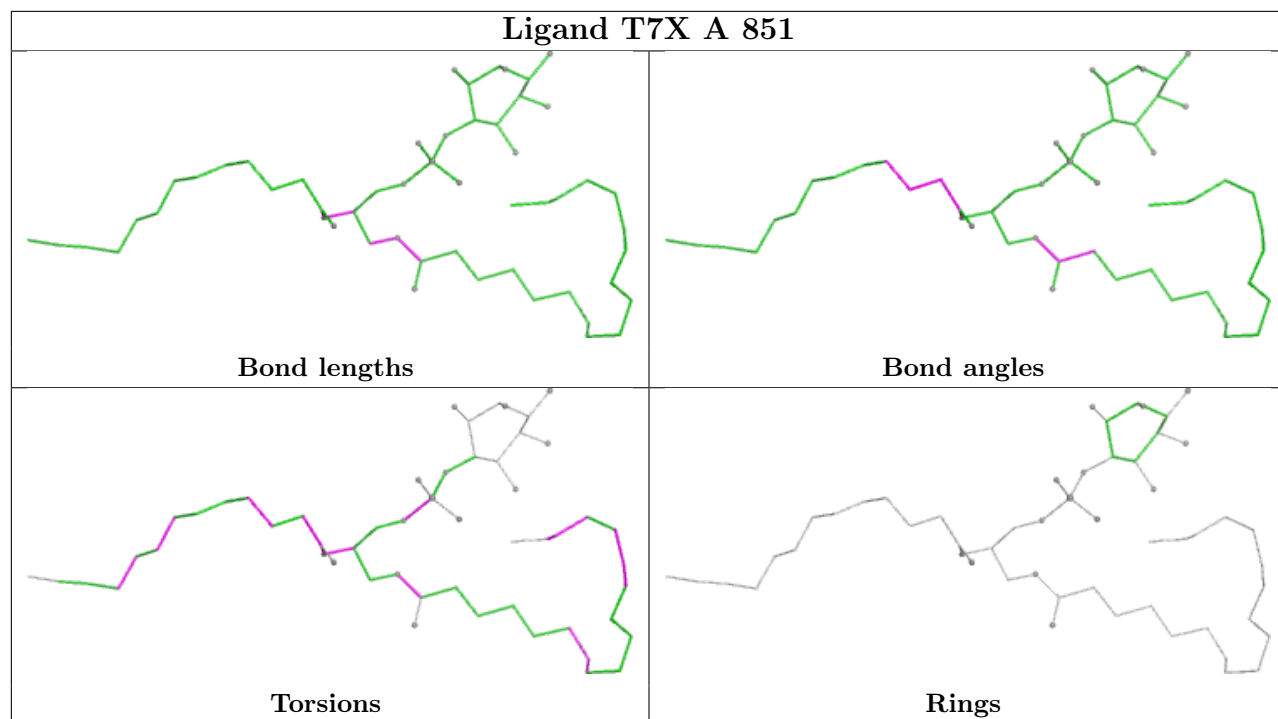
Rings

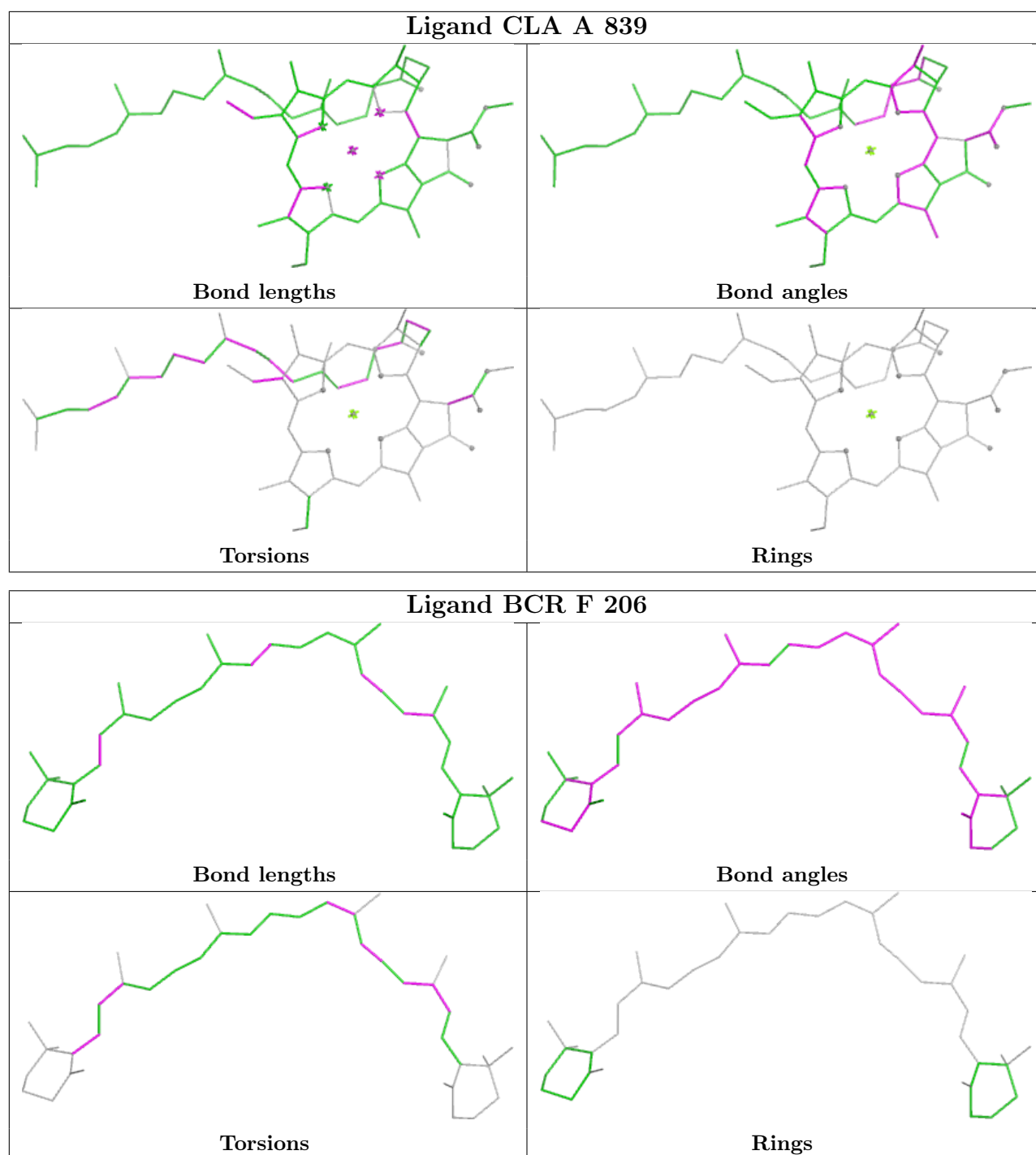




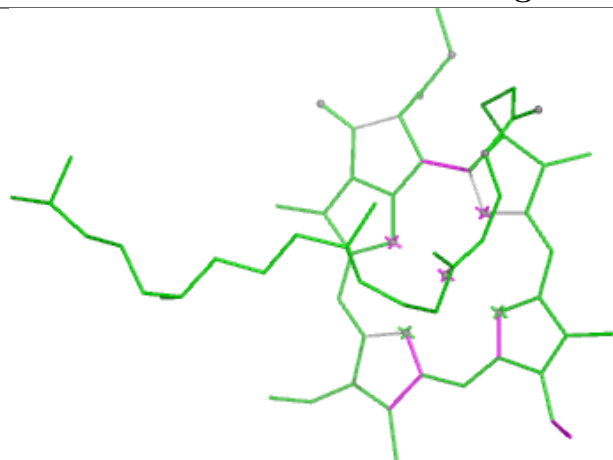




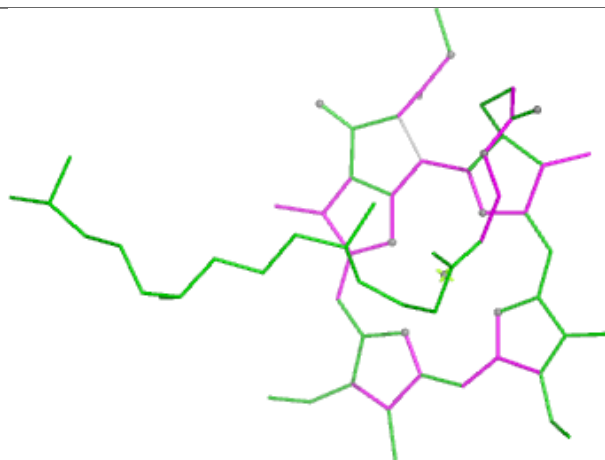




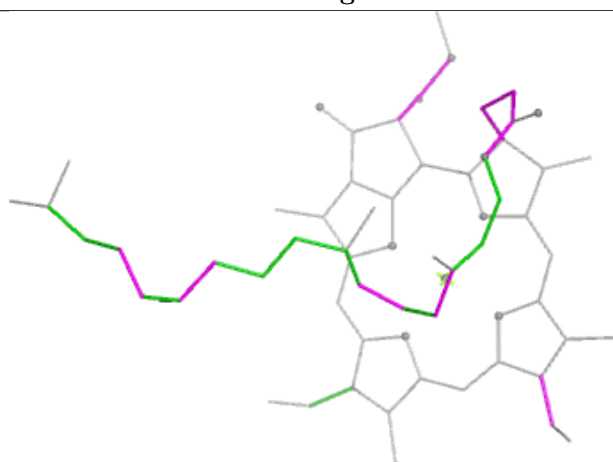
Ligand CLA B 826



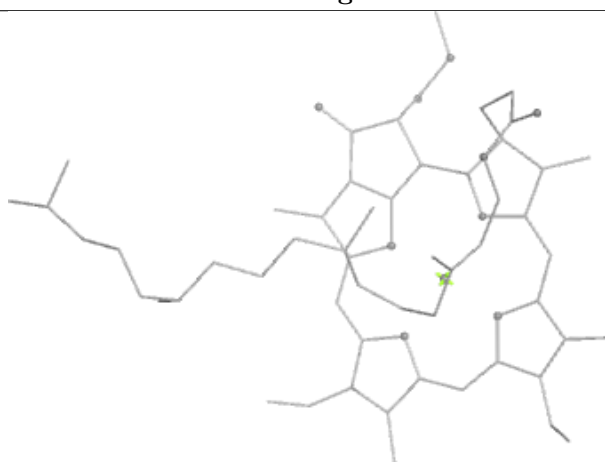
Bond lengths



Bond angles

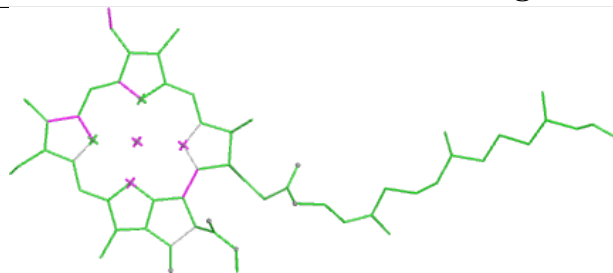


Torsions

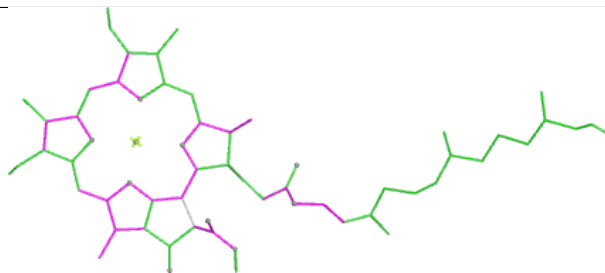


Rings

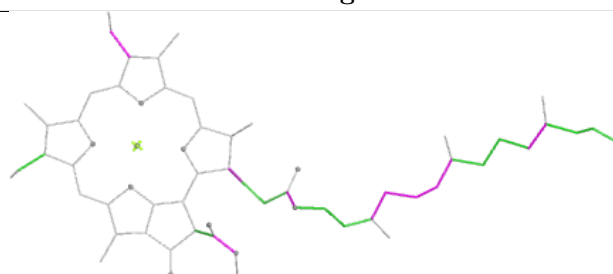
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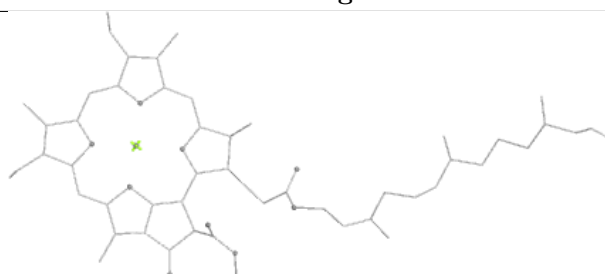
Bond lengths



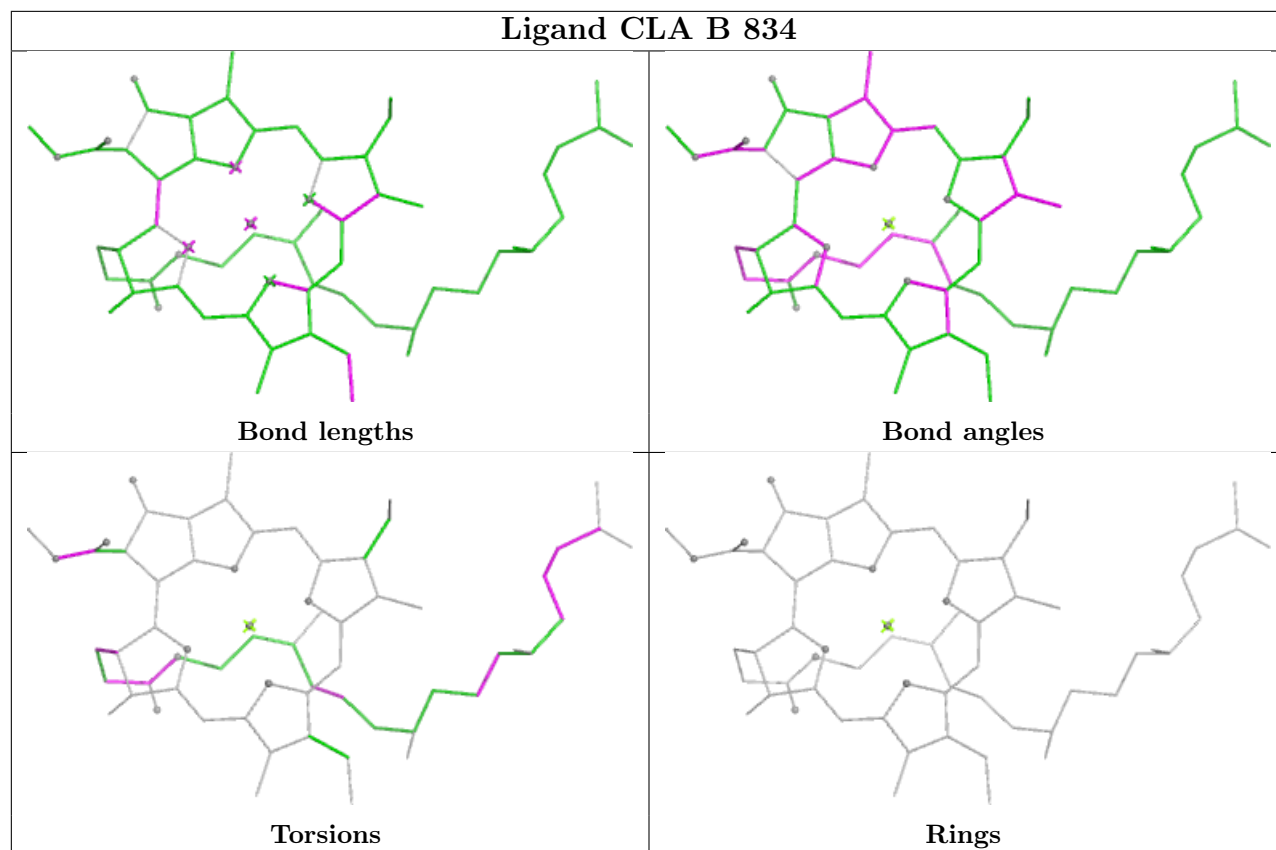
Bond angles

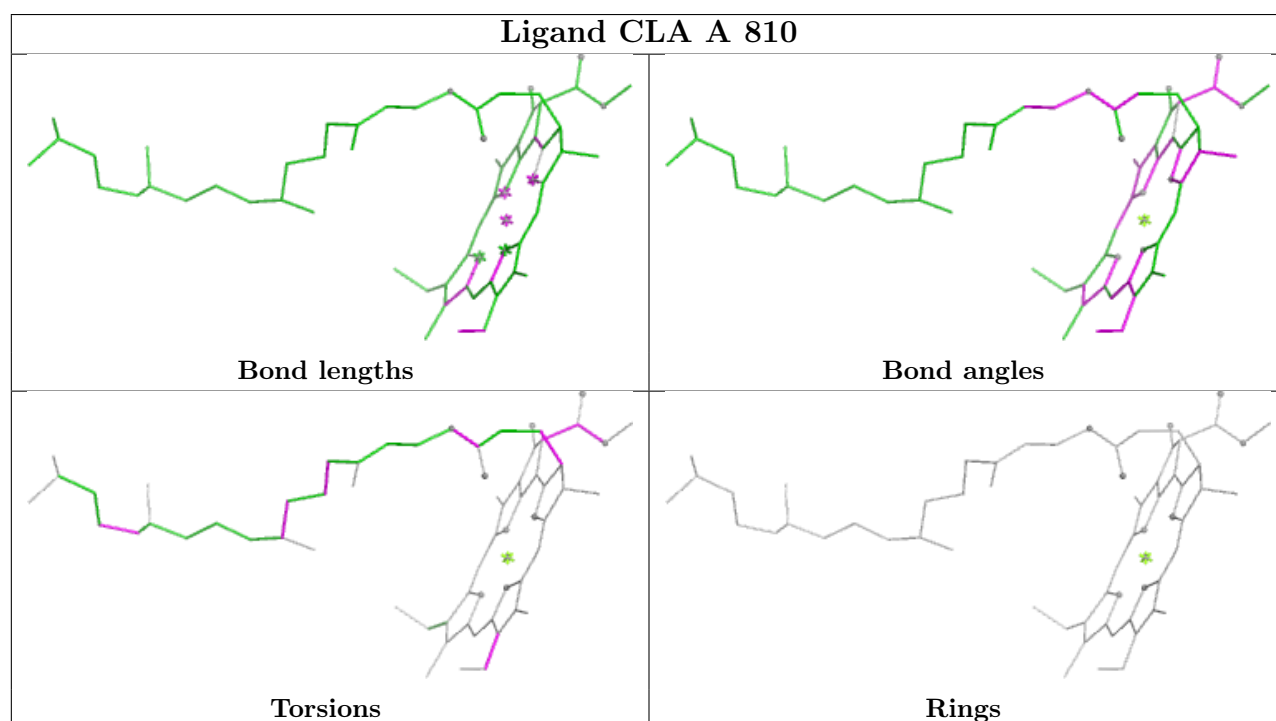
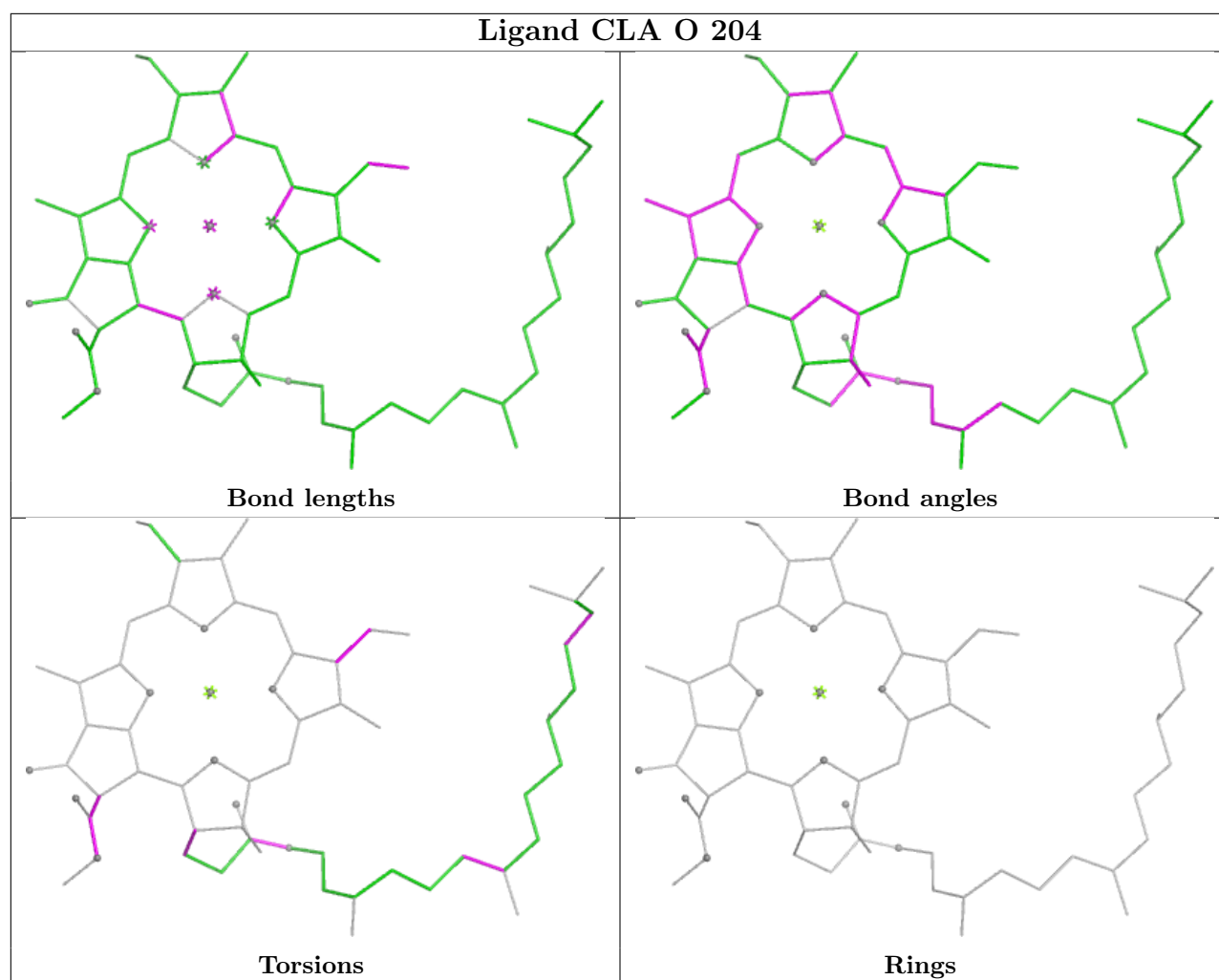


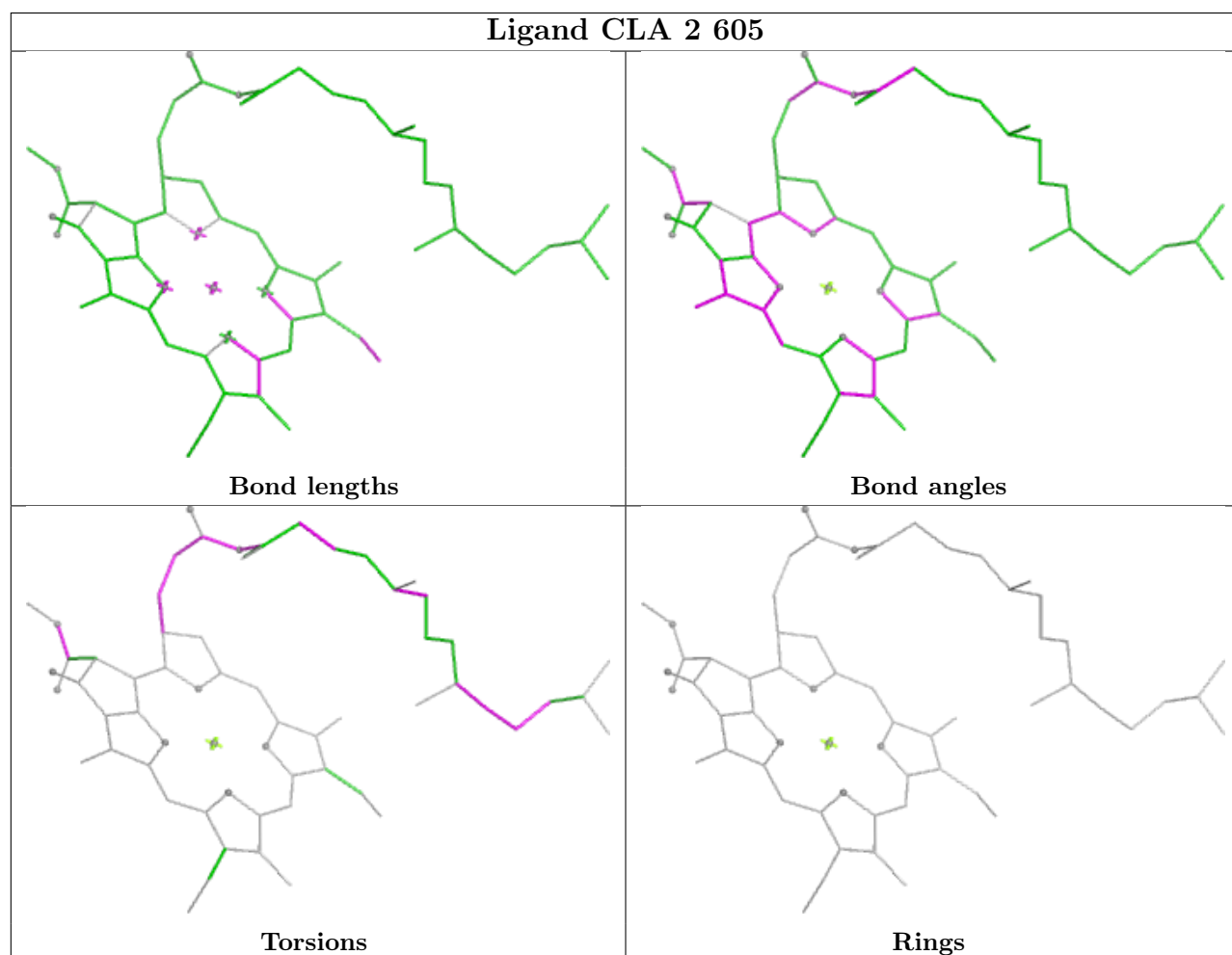
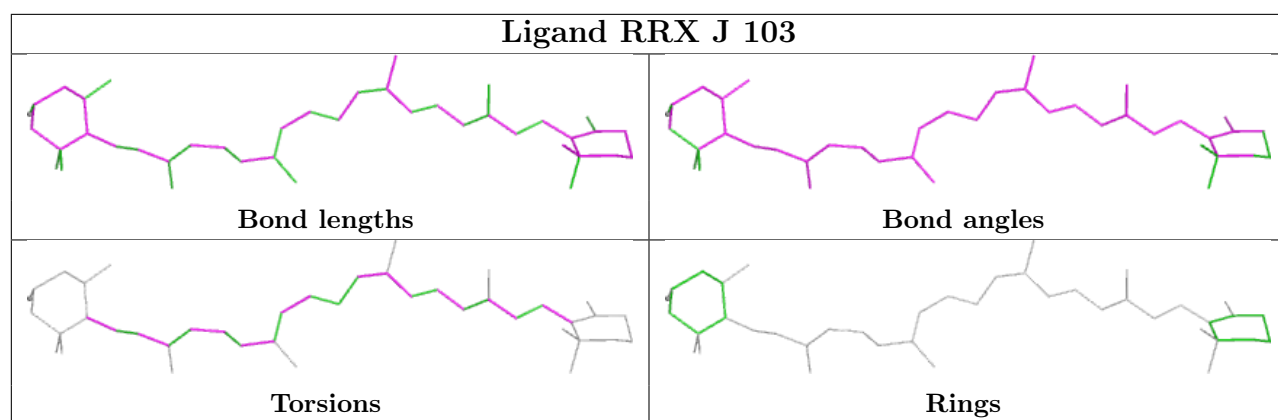
Torsions

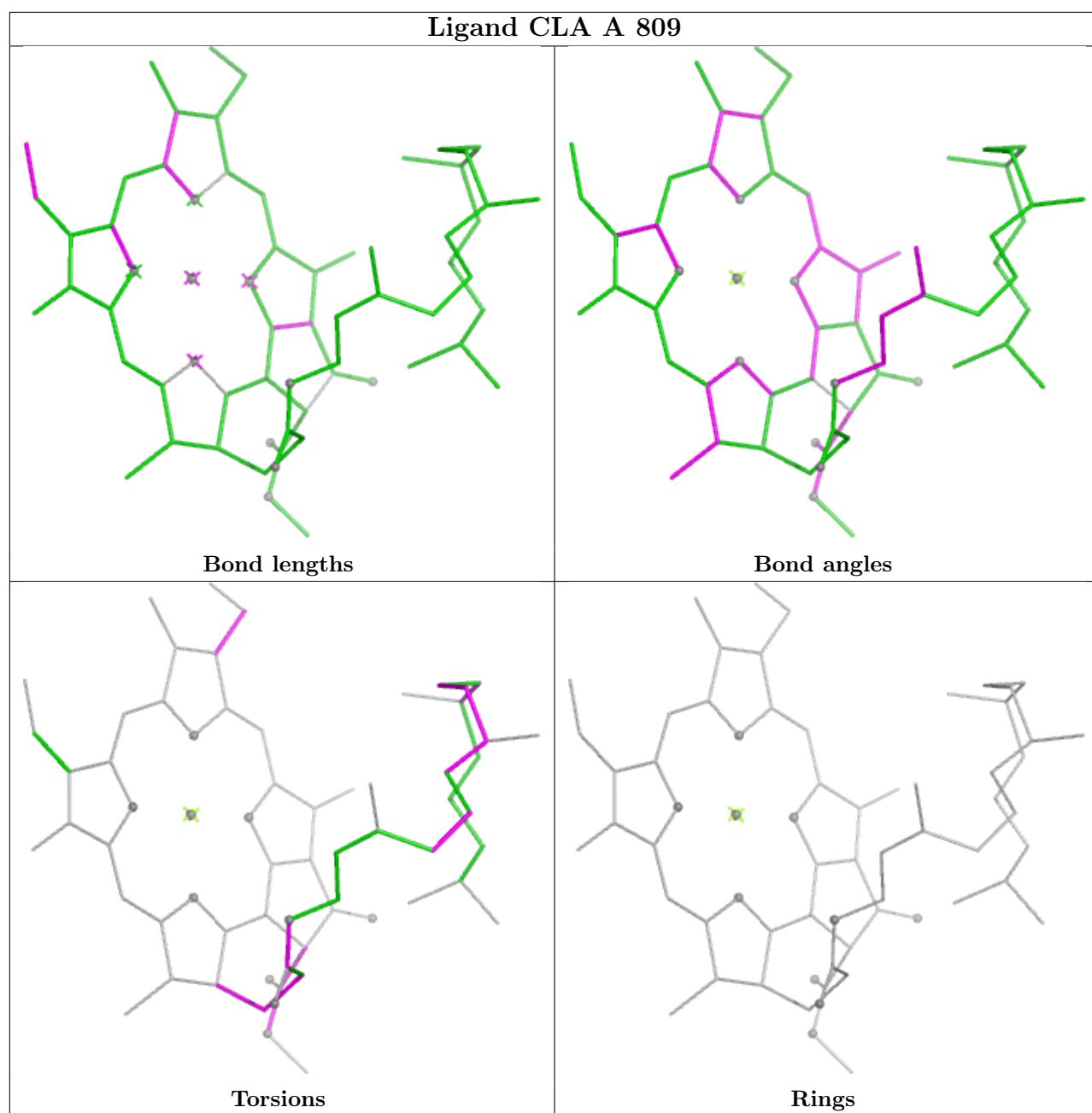


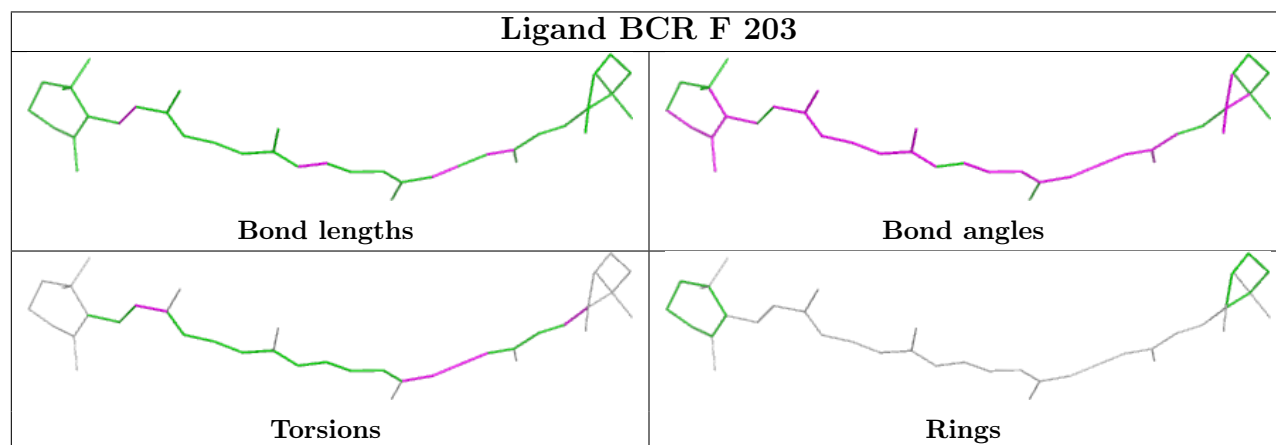
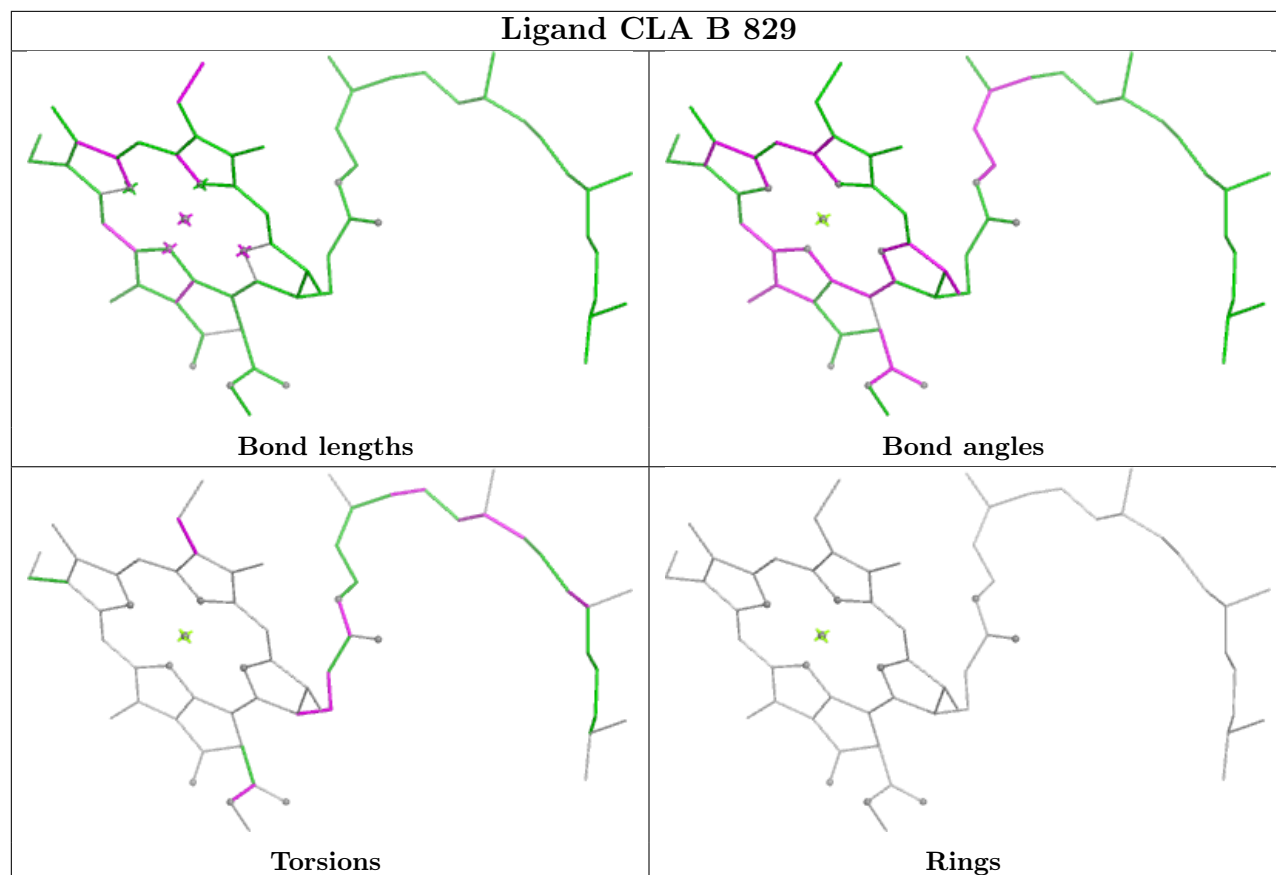
Rings

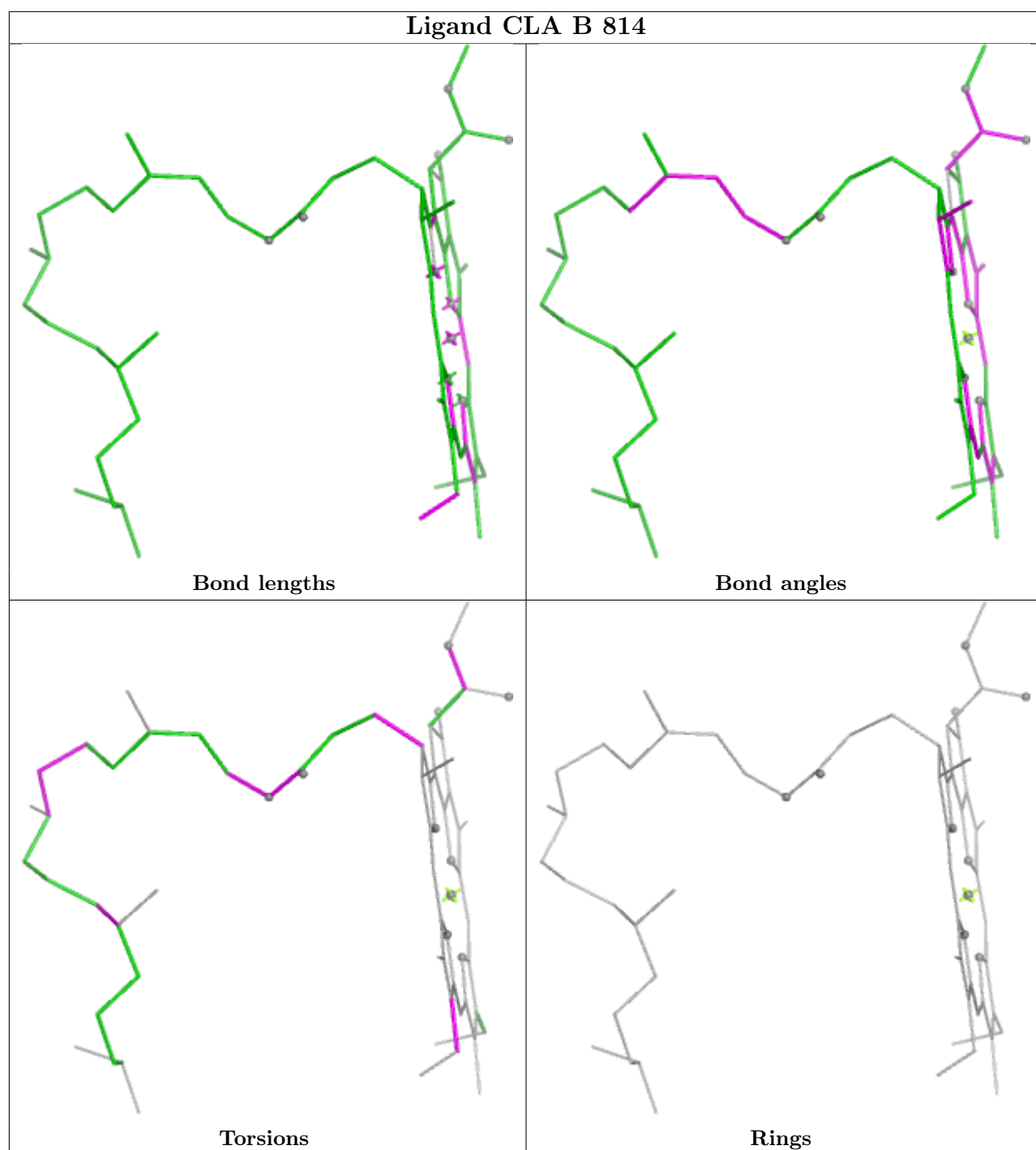


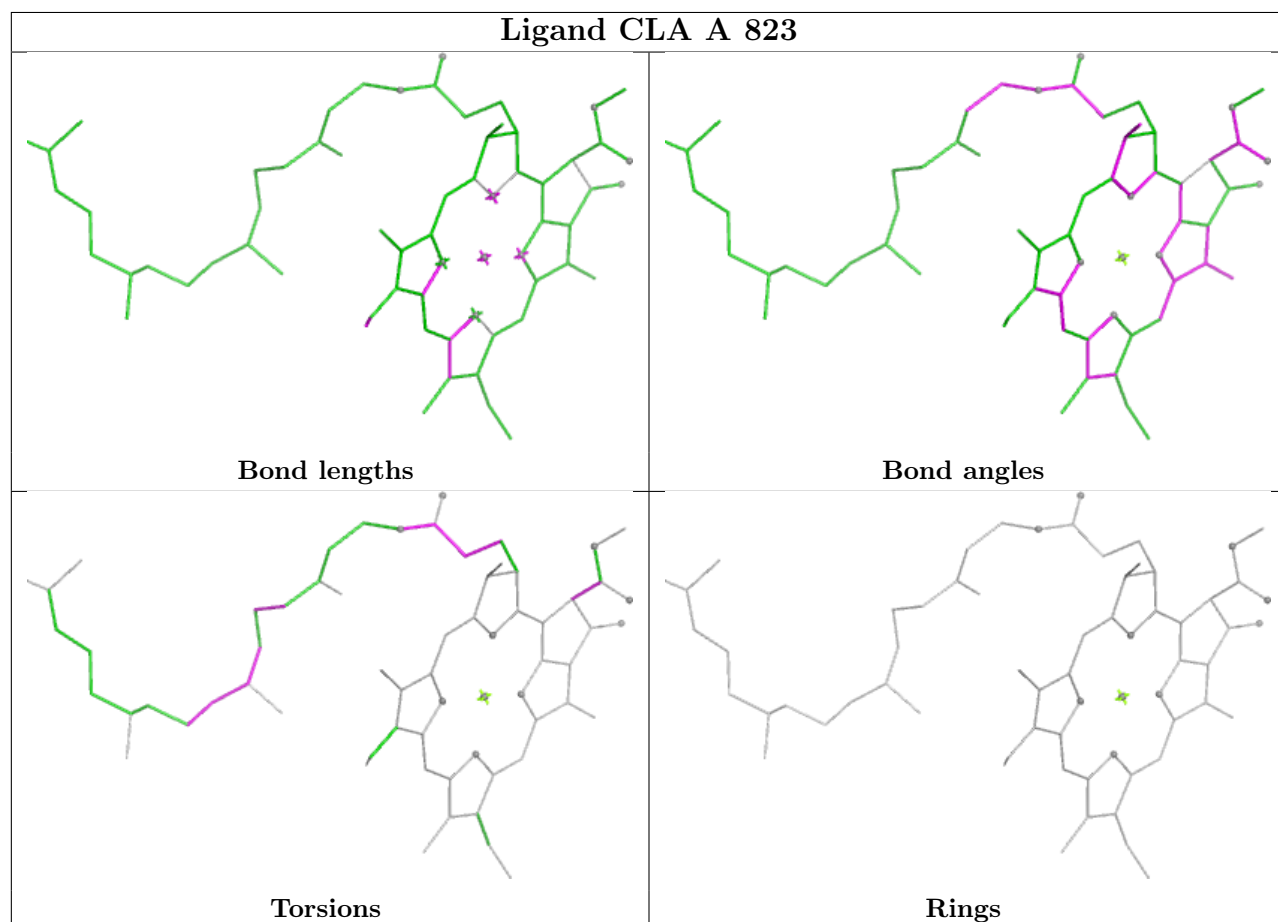
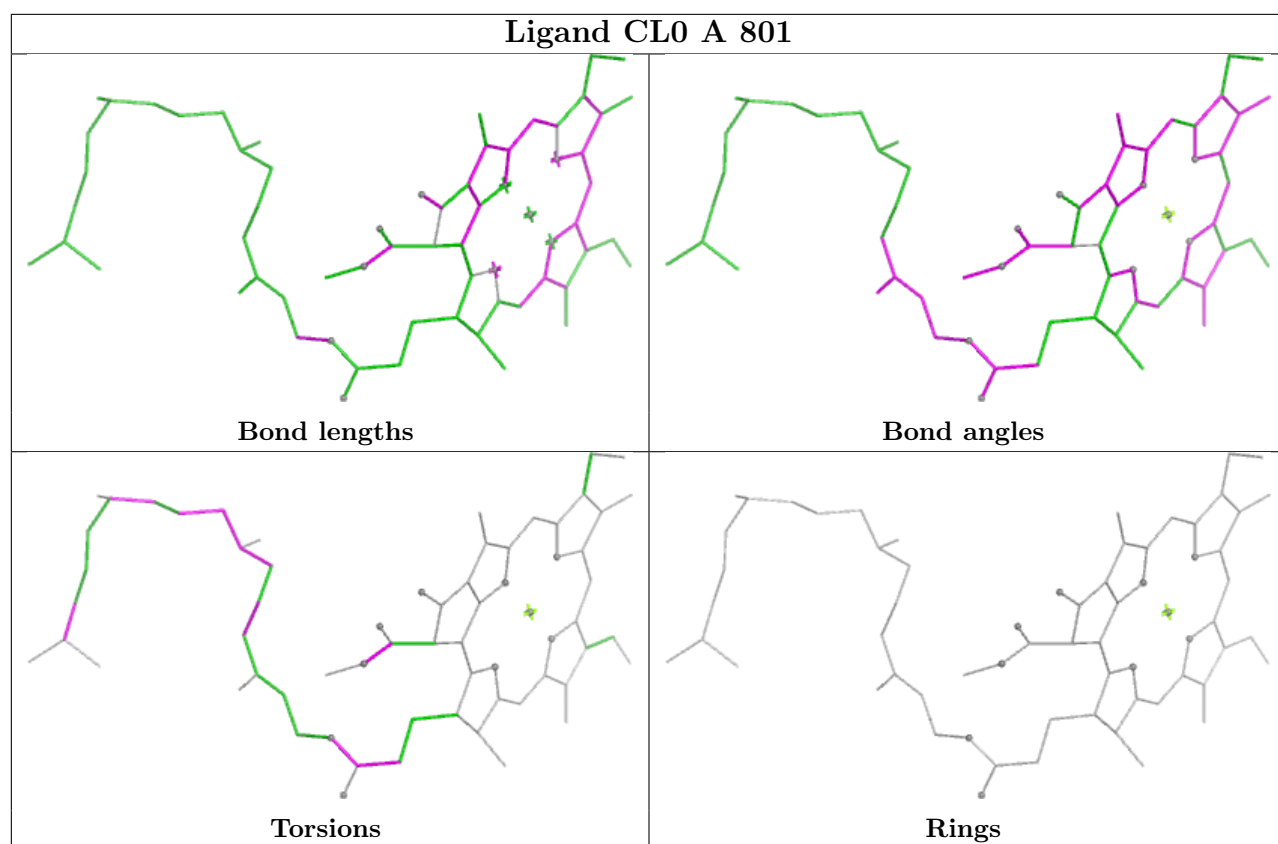


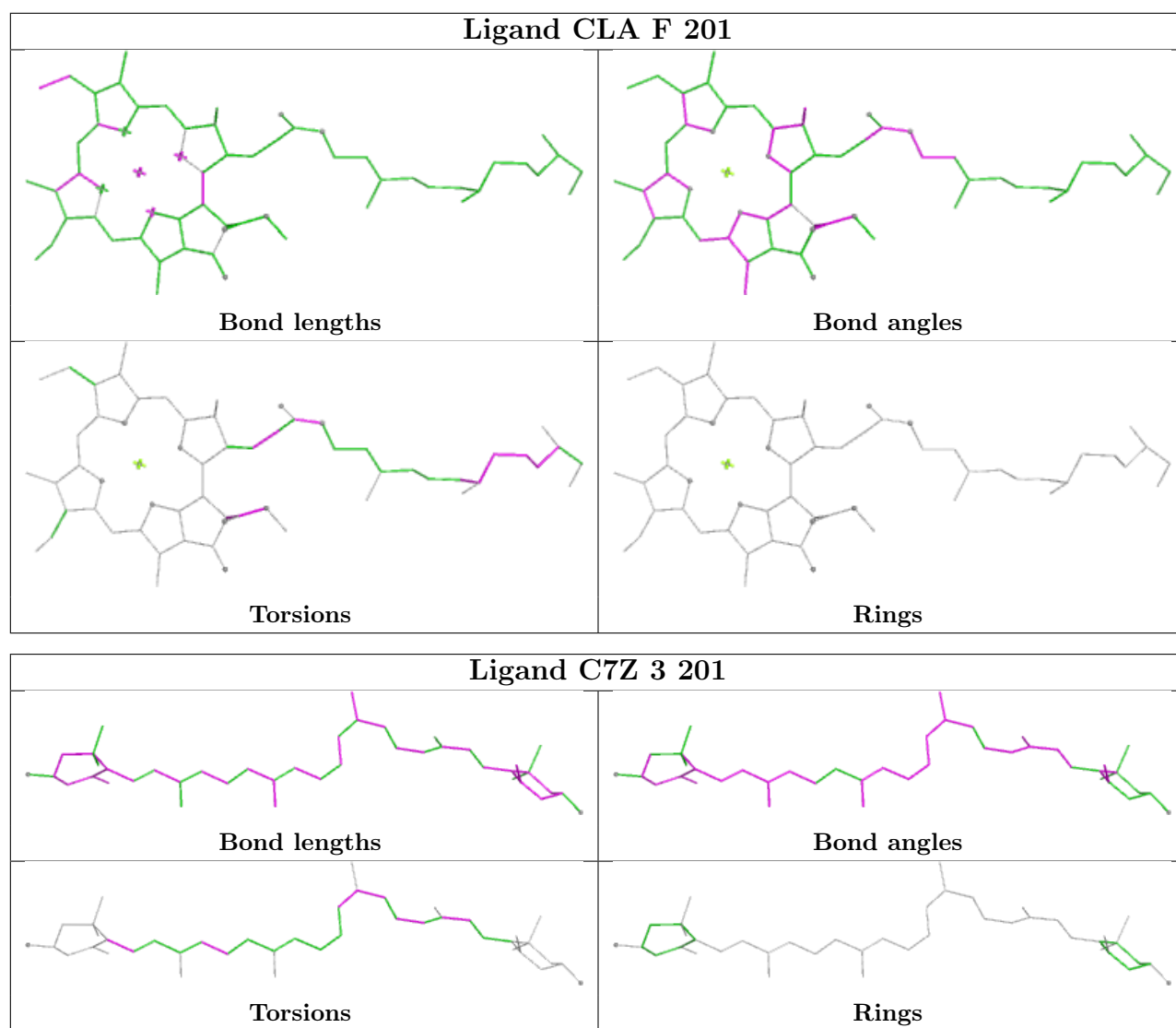


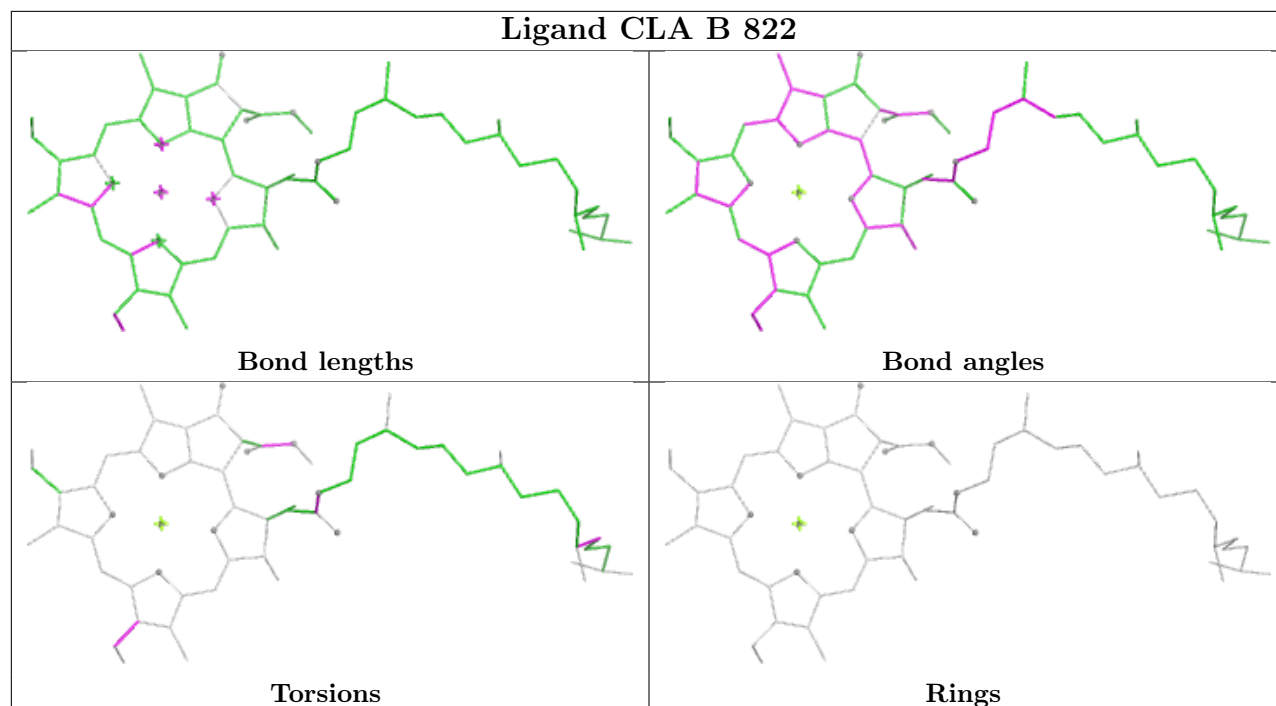
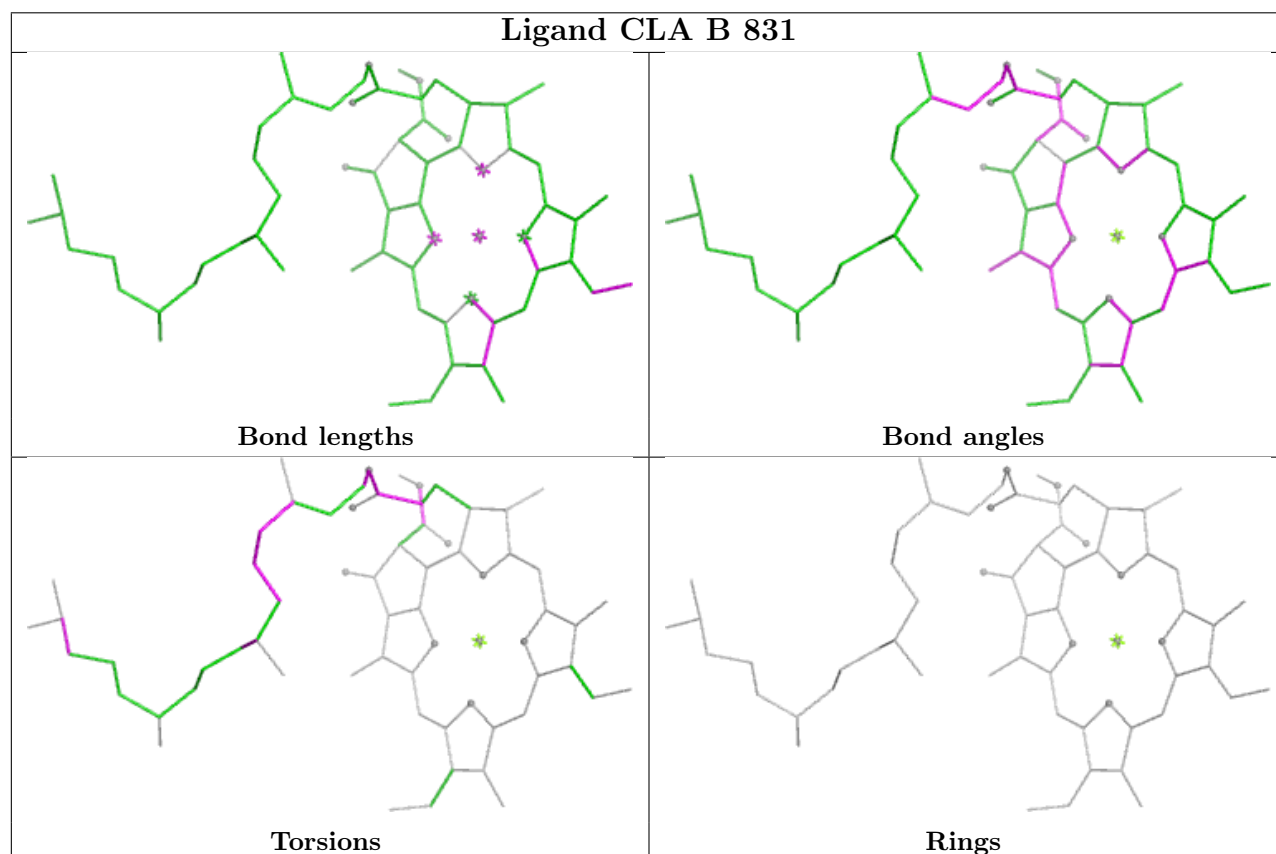


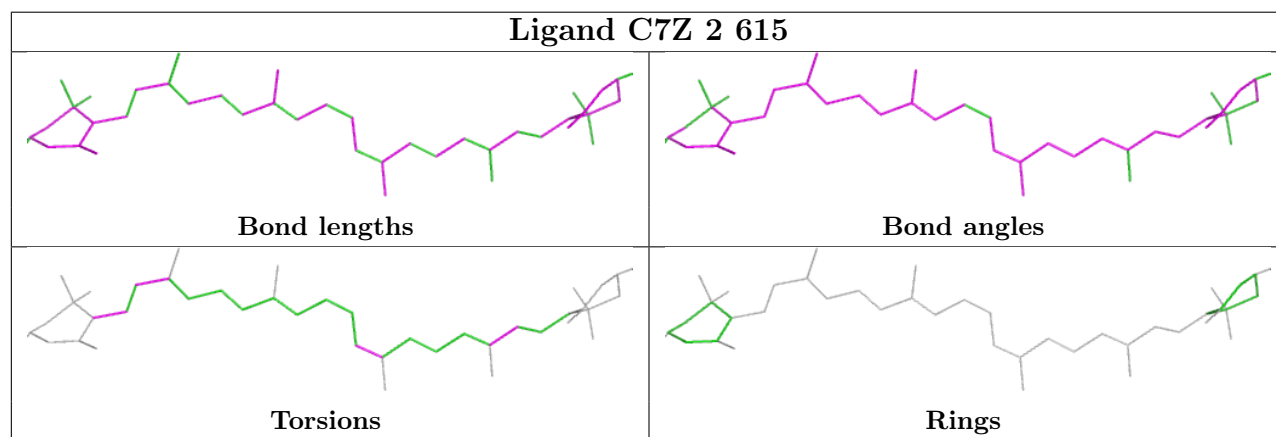
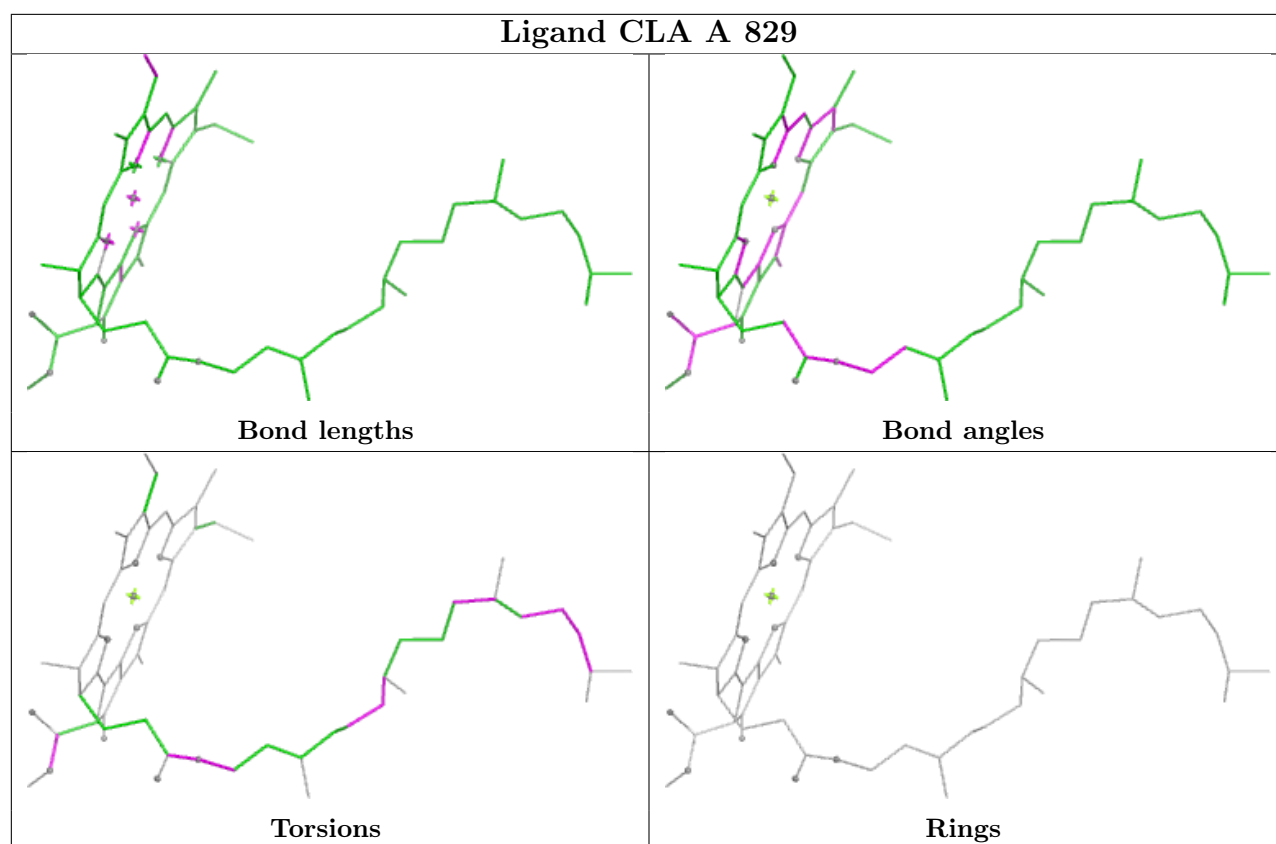




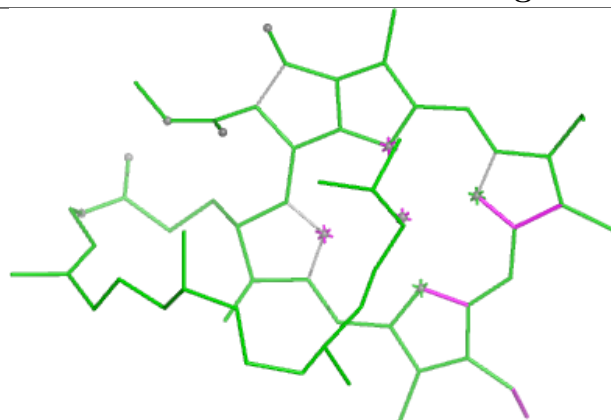




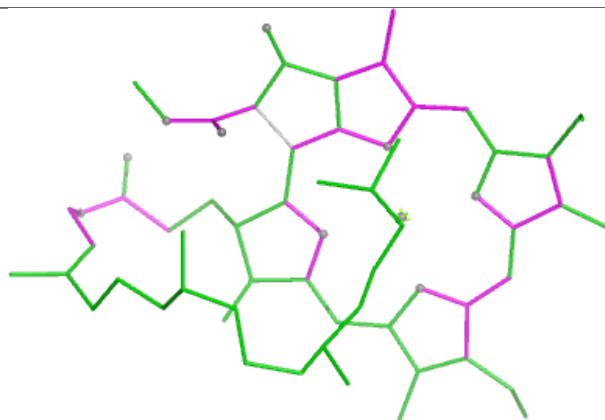
Ligand CLA B 822**Ligand CLA B 831**



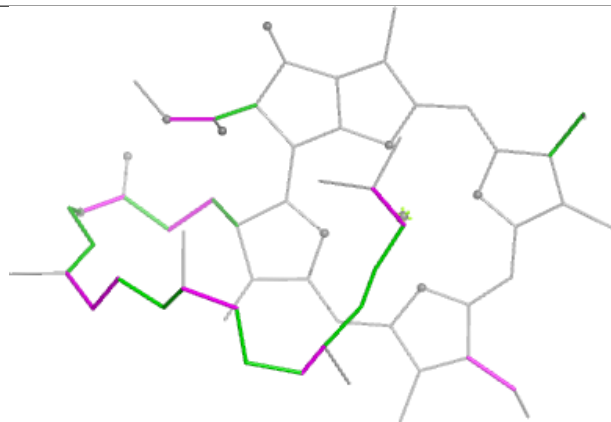
Ligand CLA B 807



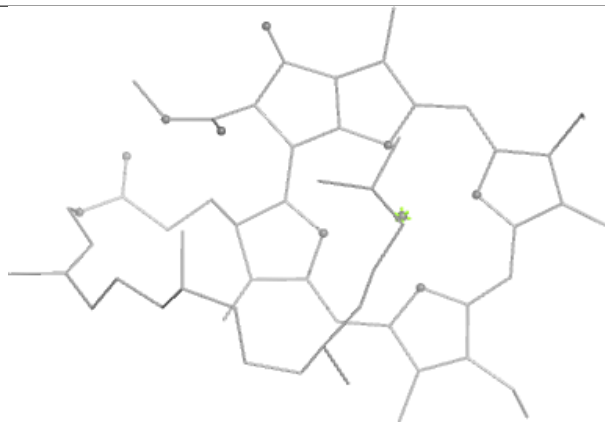
Bond lengths



Bond angles

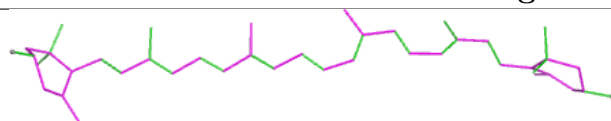


Torsions

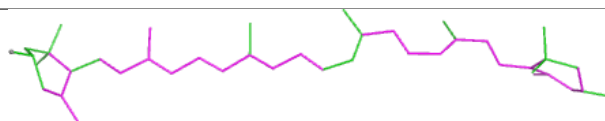


Rings

Ligand C7Z A 843



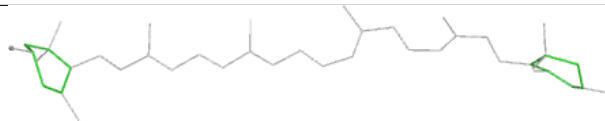
Bond lengths



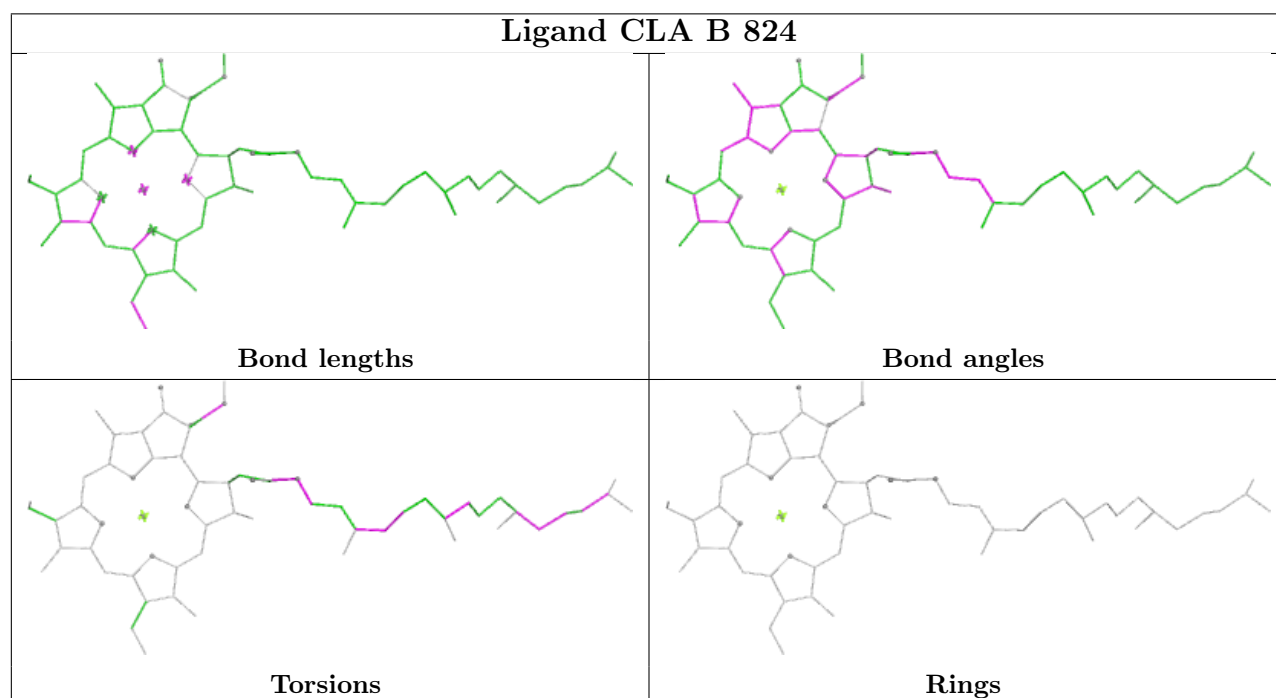
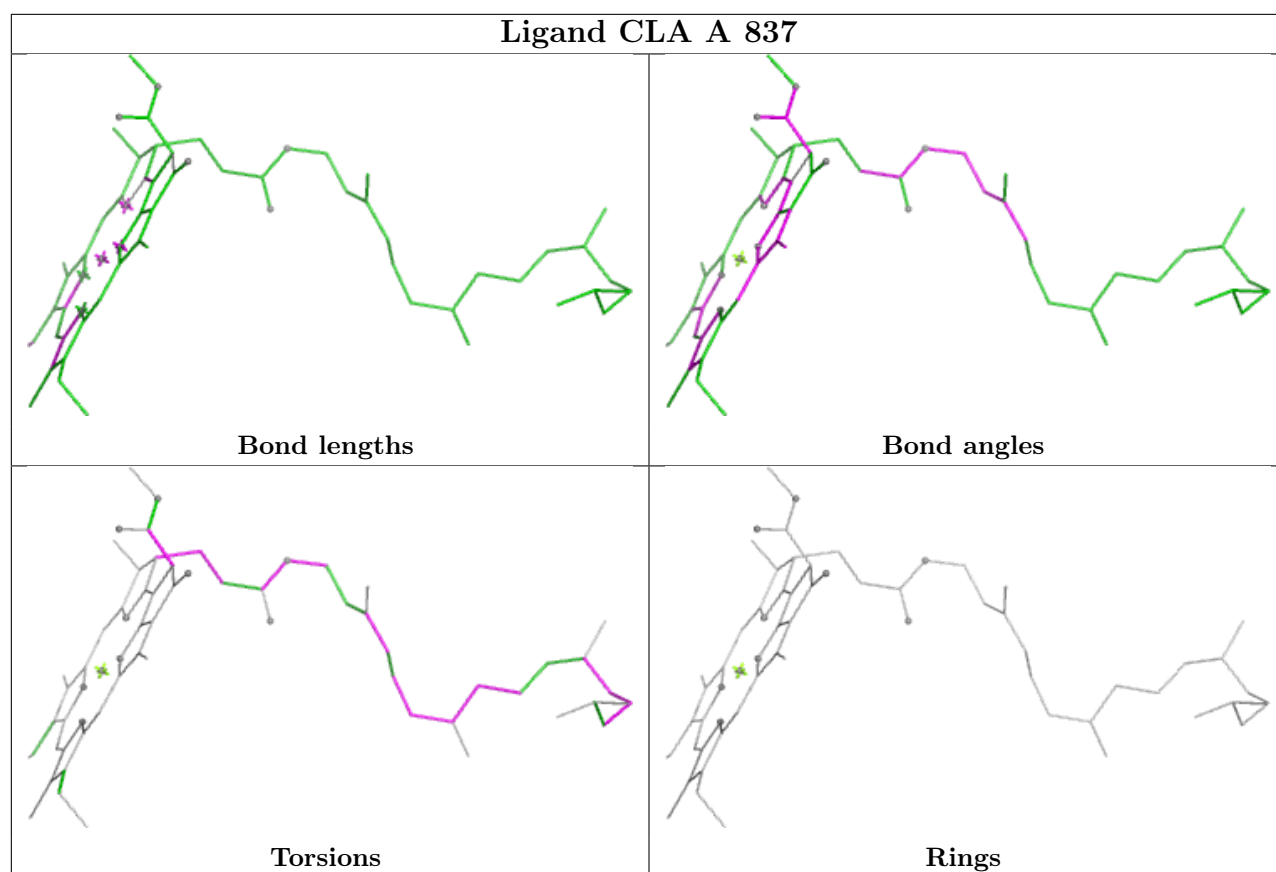
Bond angles



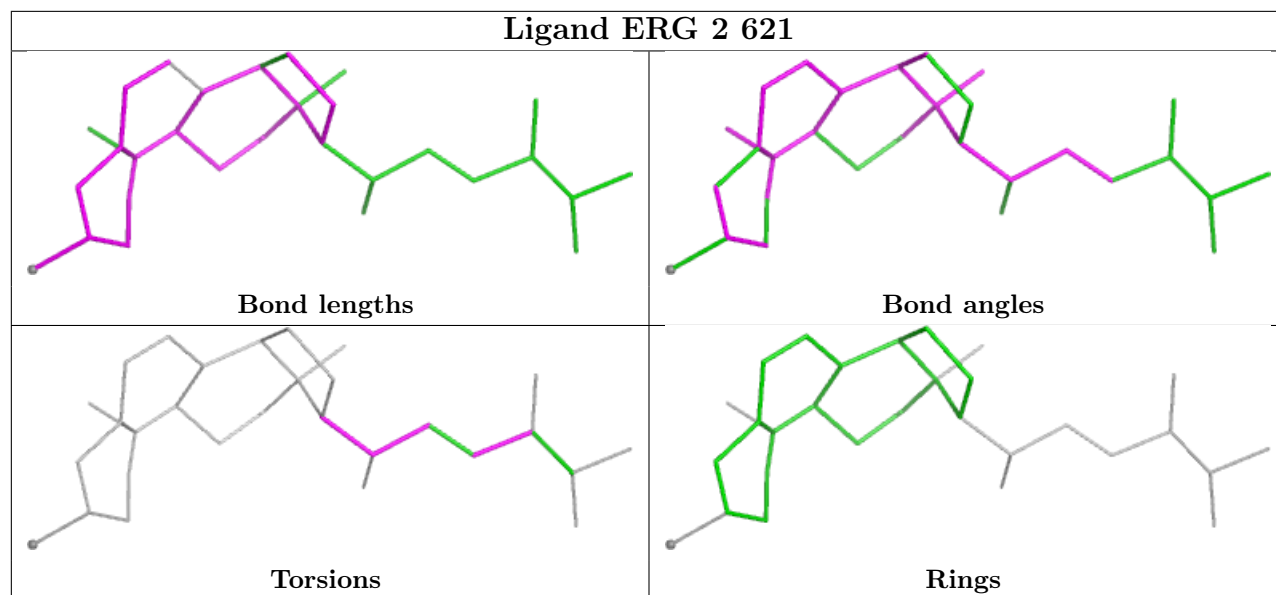
Torsions



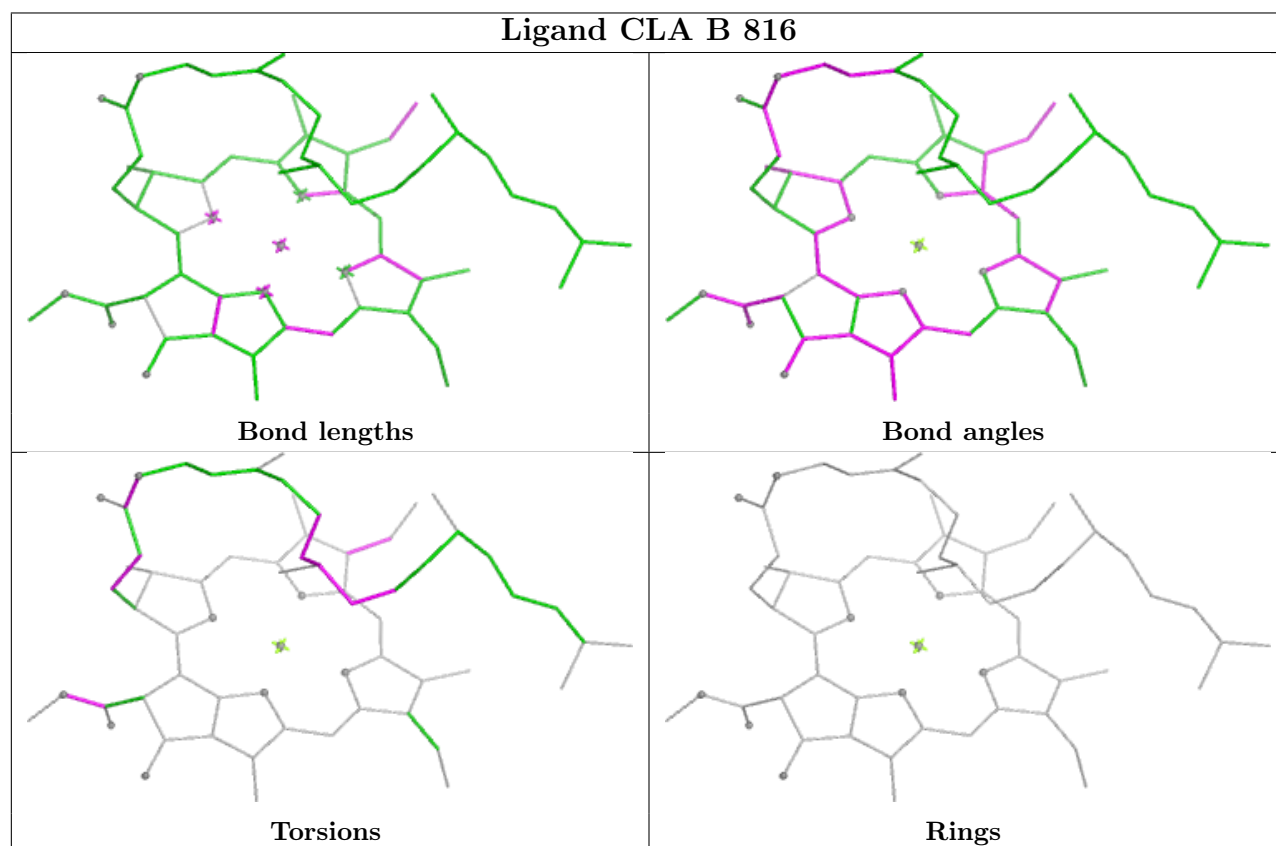
Rings

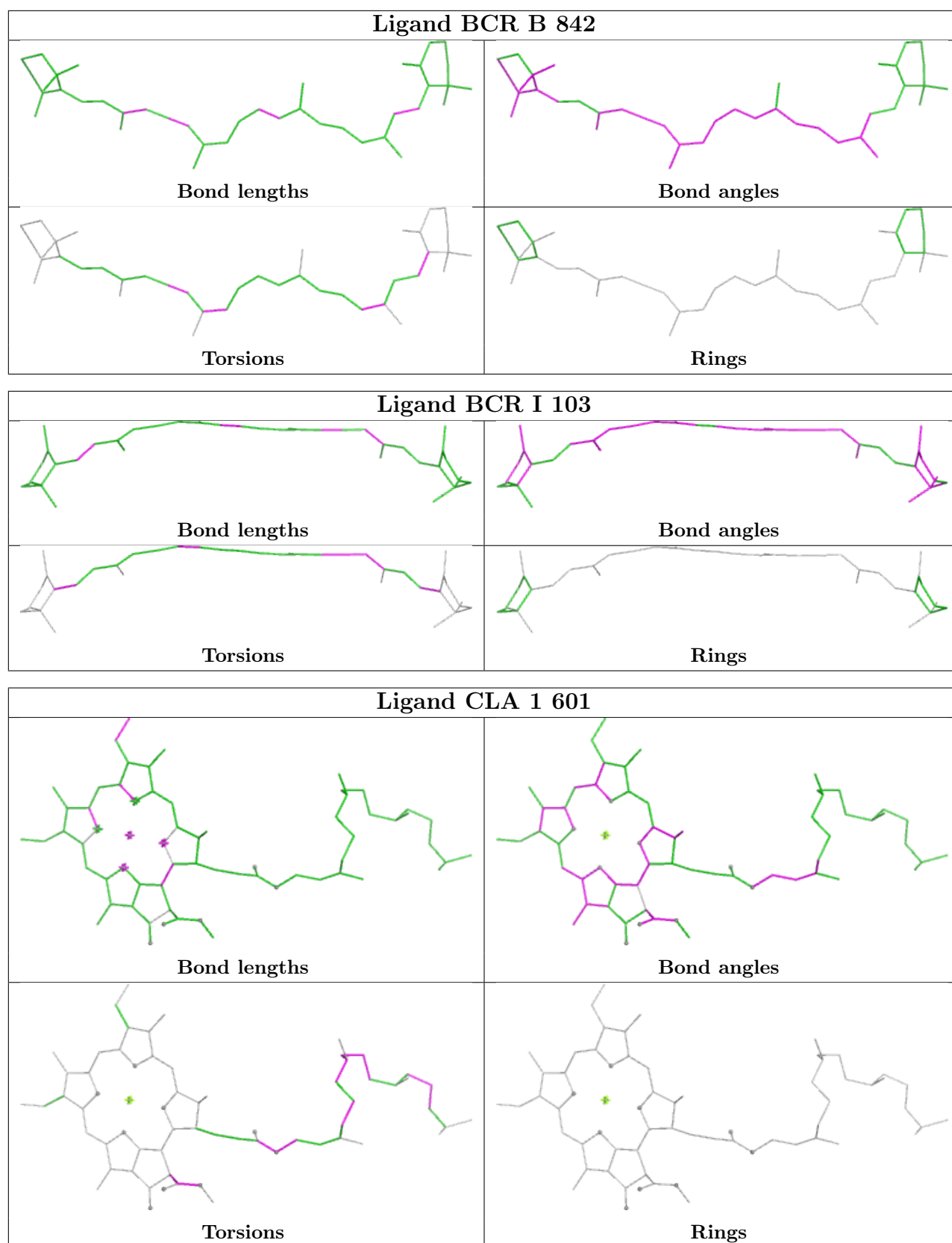


Ligand ERG 2 621



Ligand CLA B 816

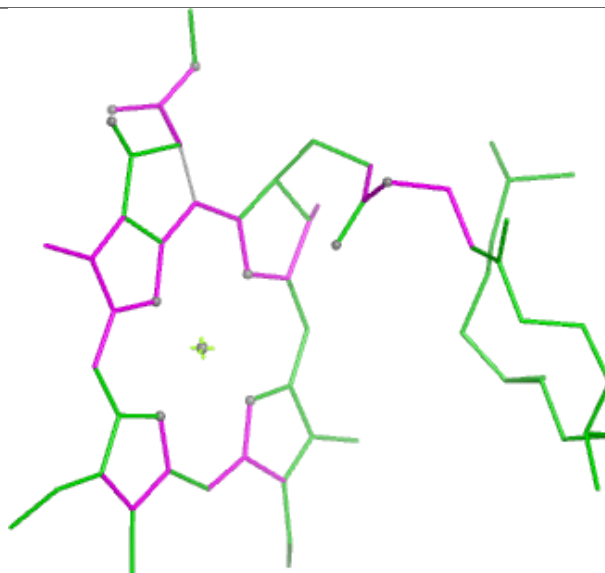




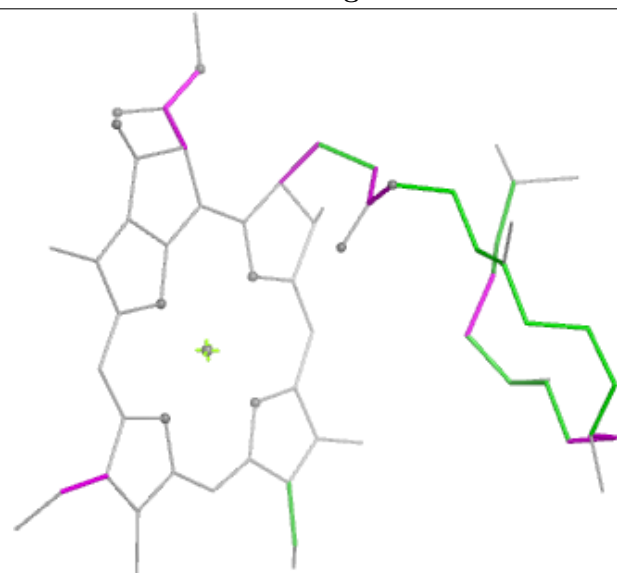
Ligand CLA 2 611



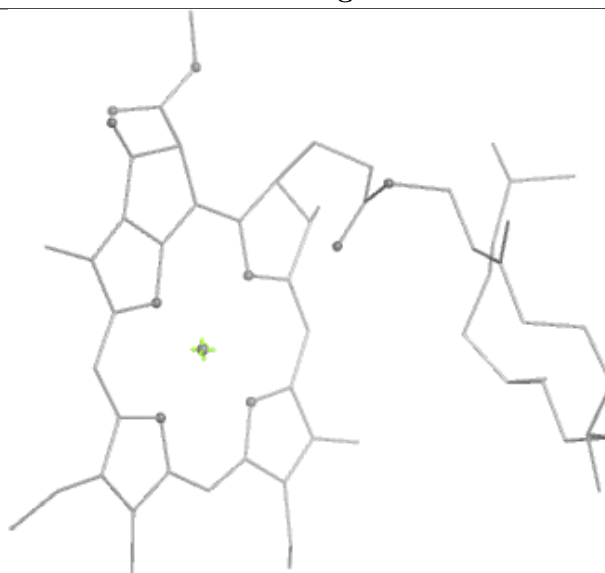
Bond lengths



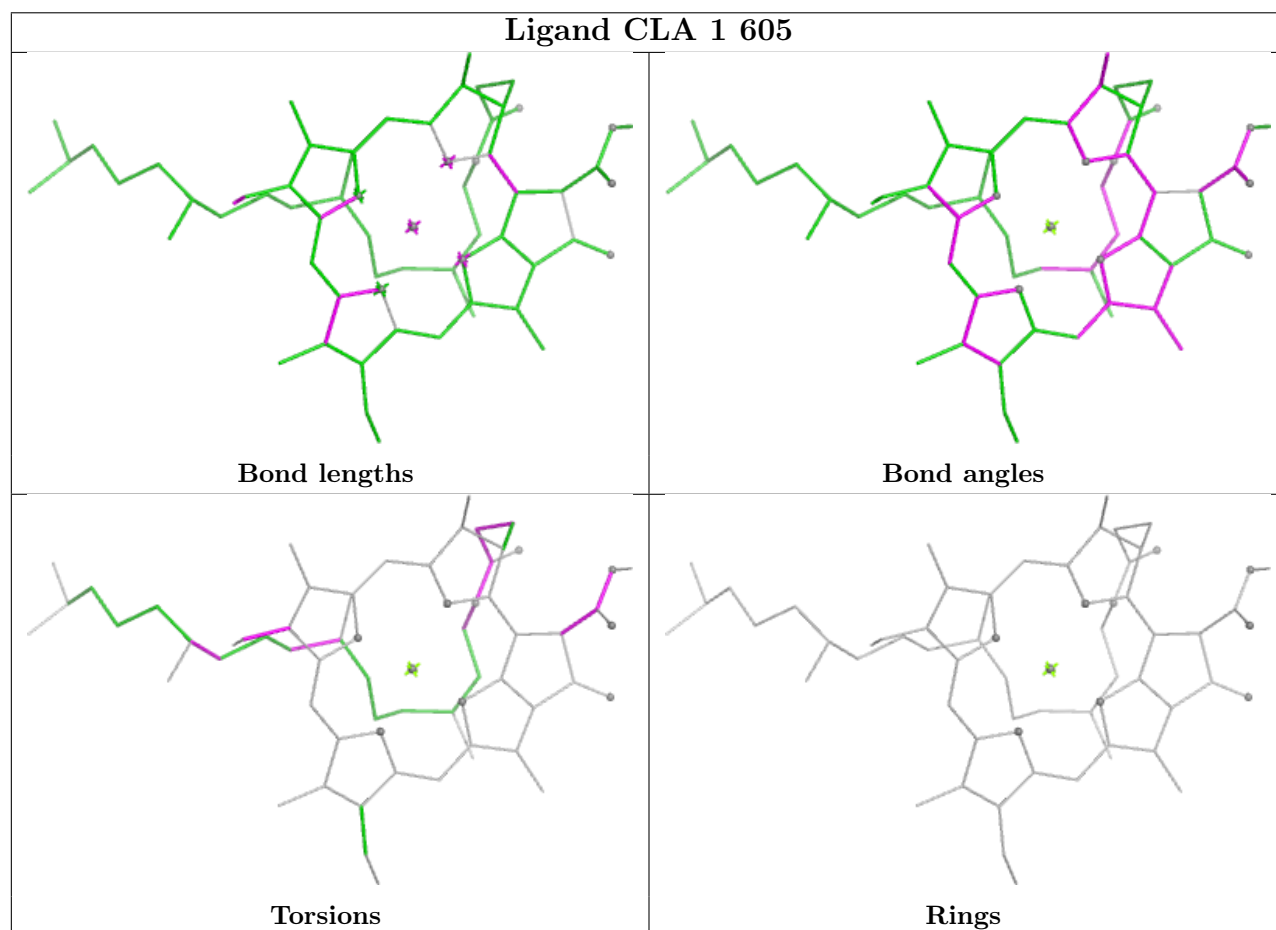
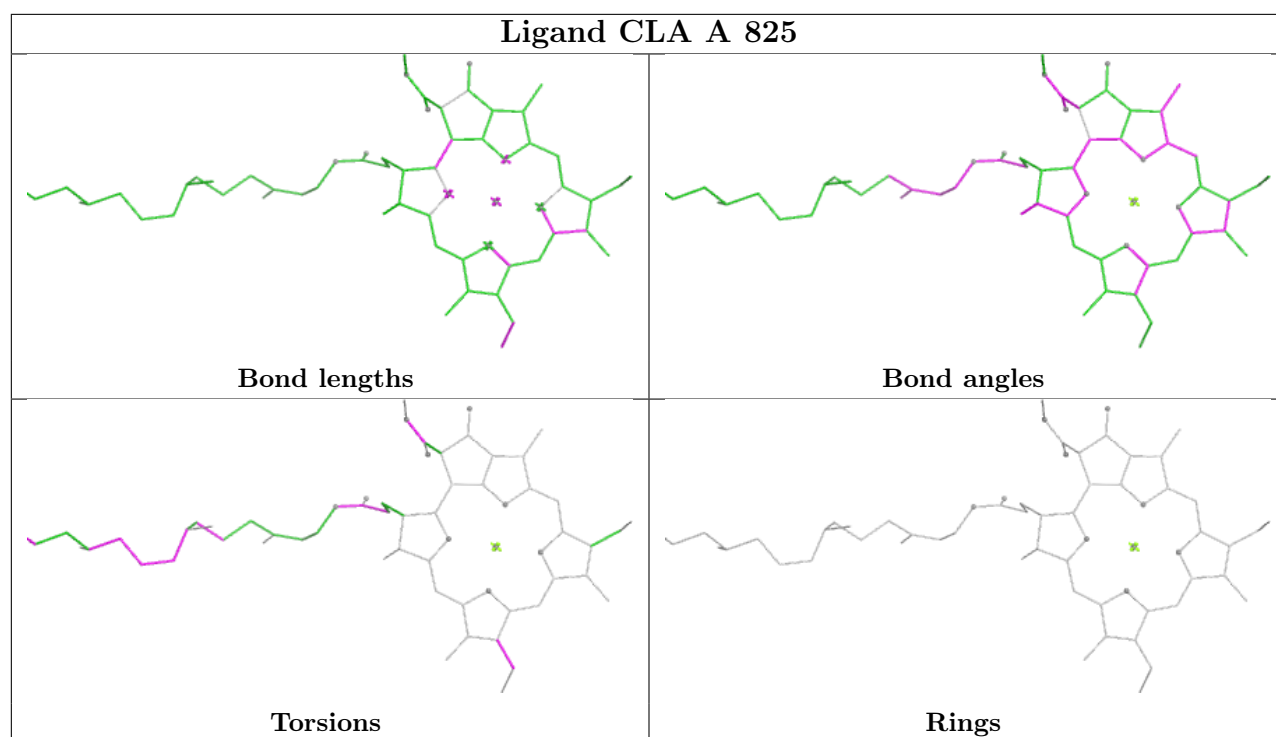
Bond angles

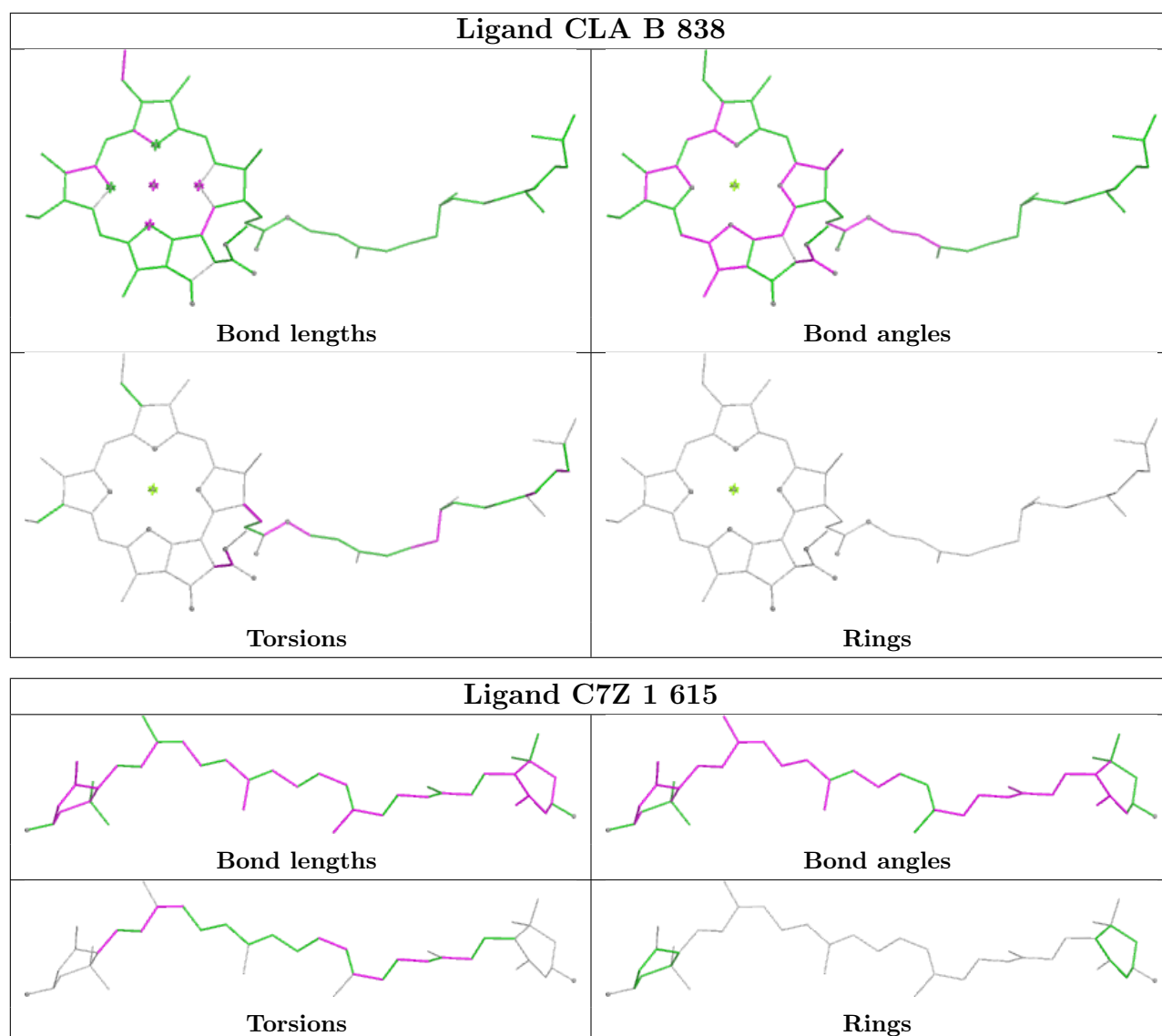


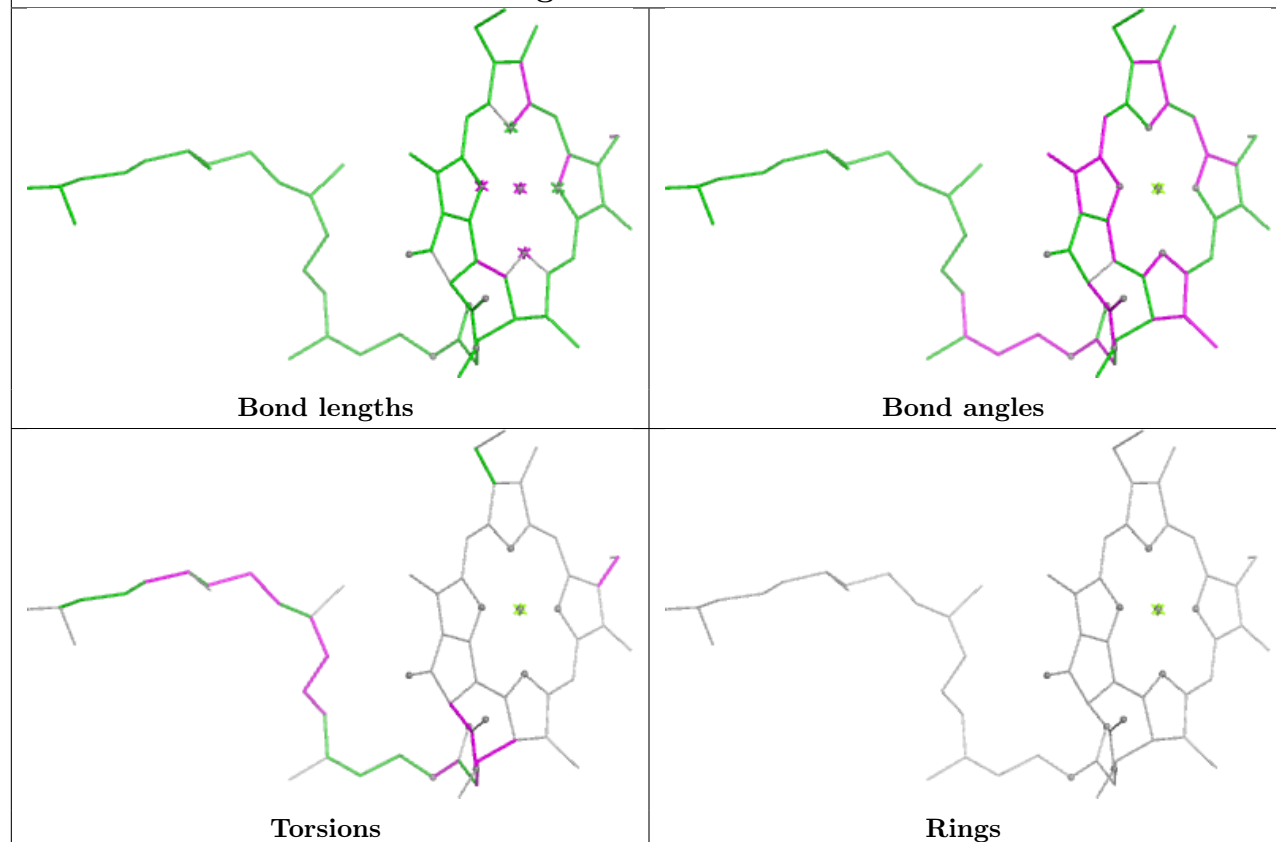
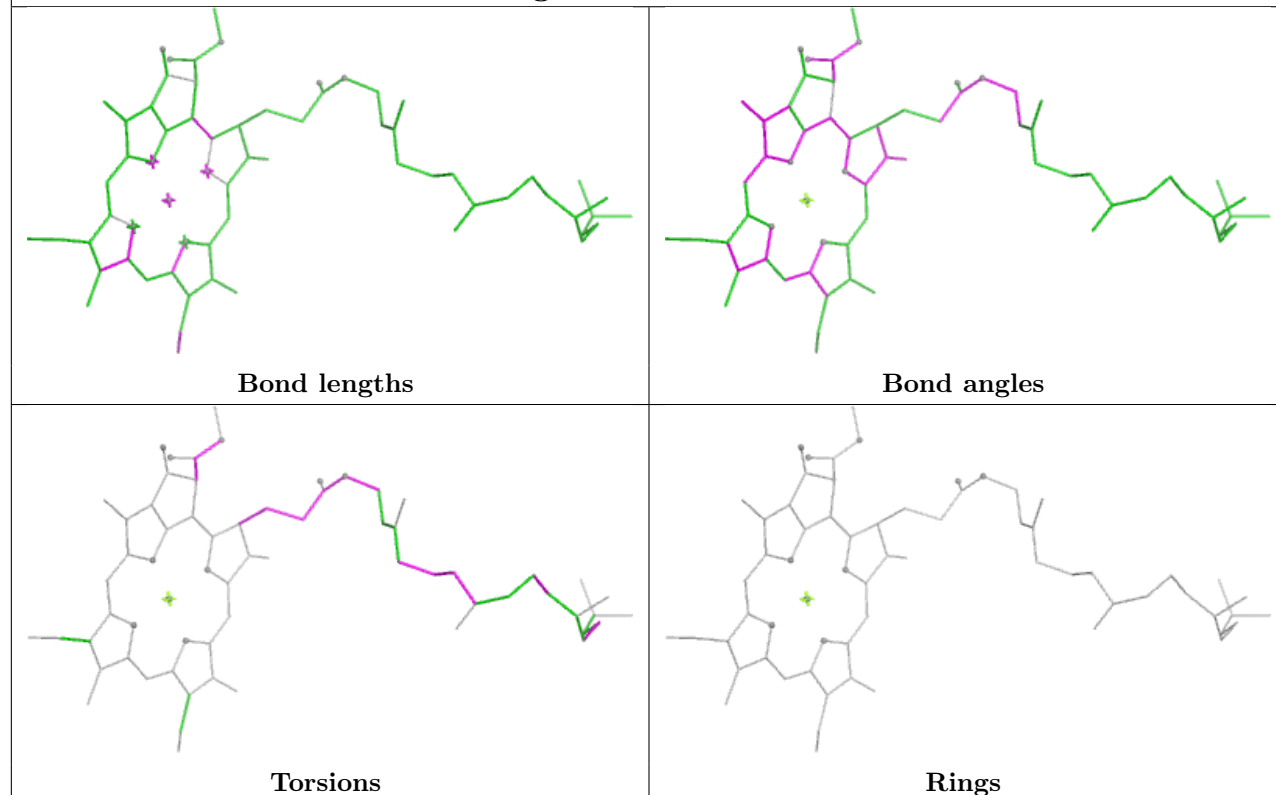
Torsions

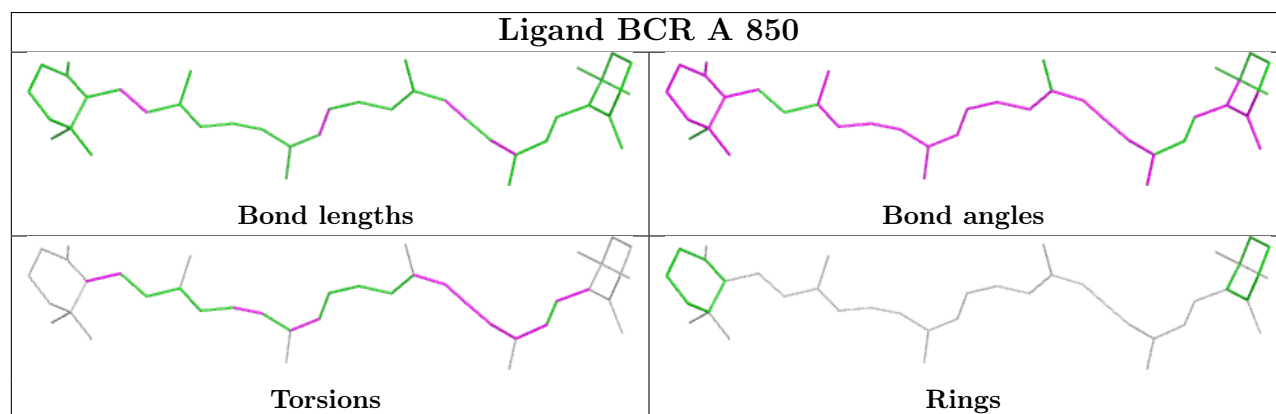
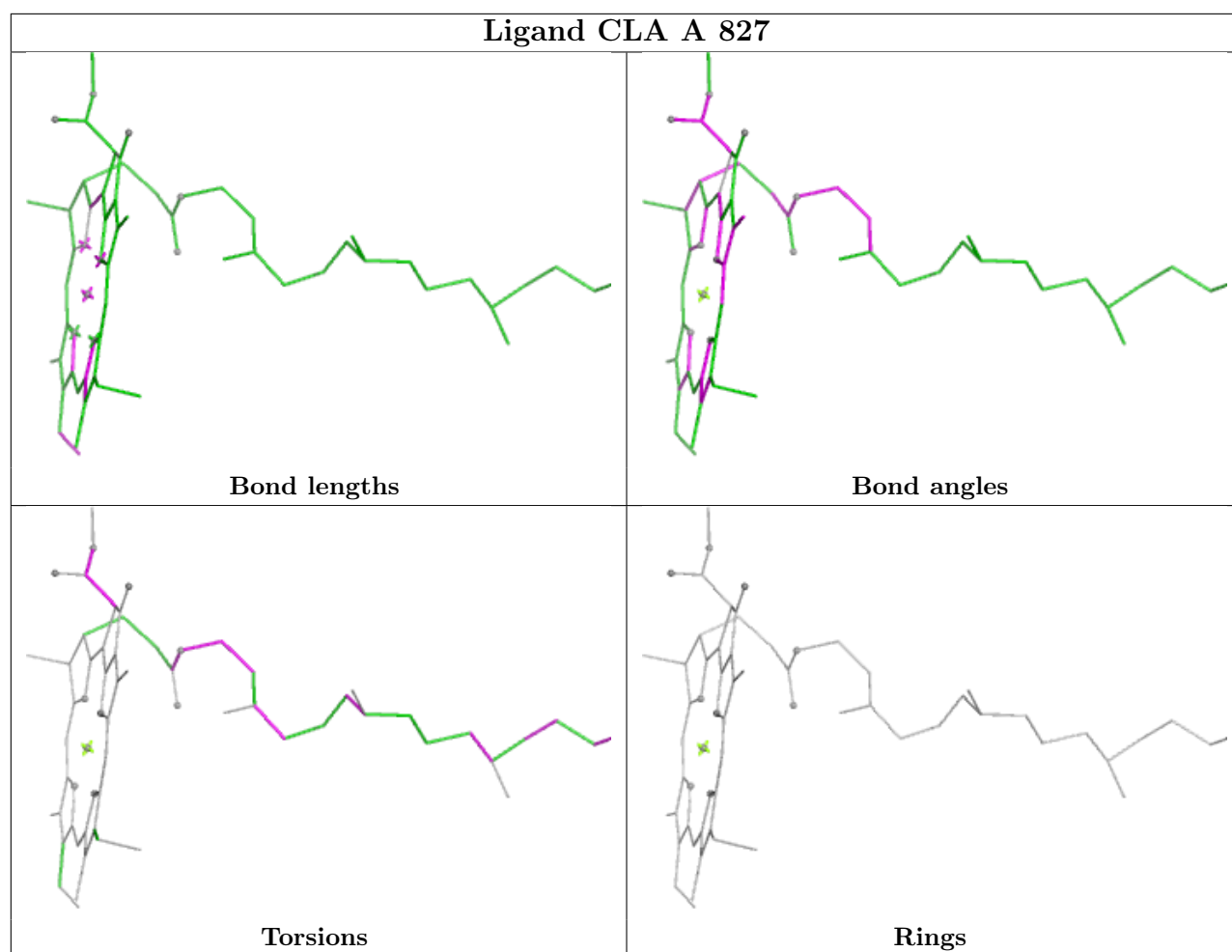


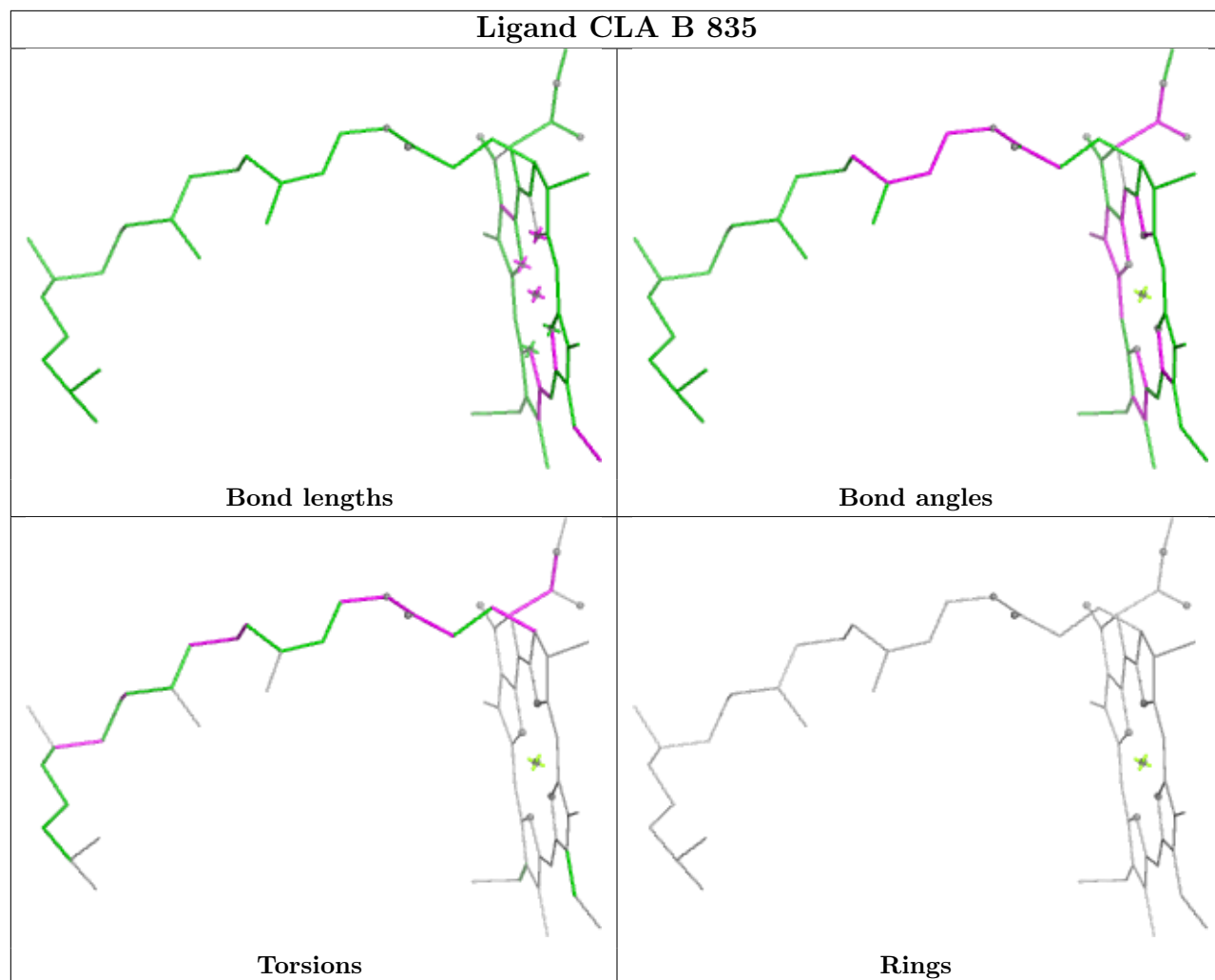
Rings

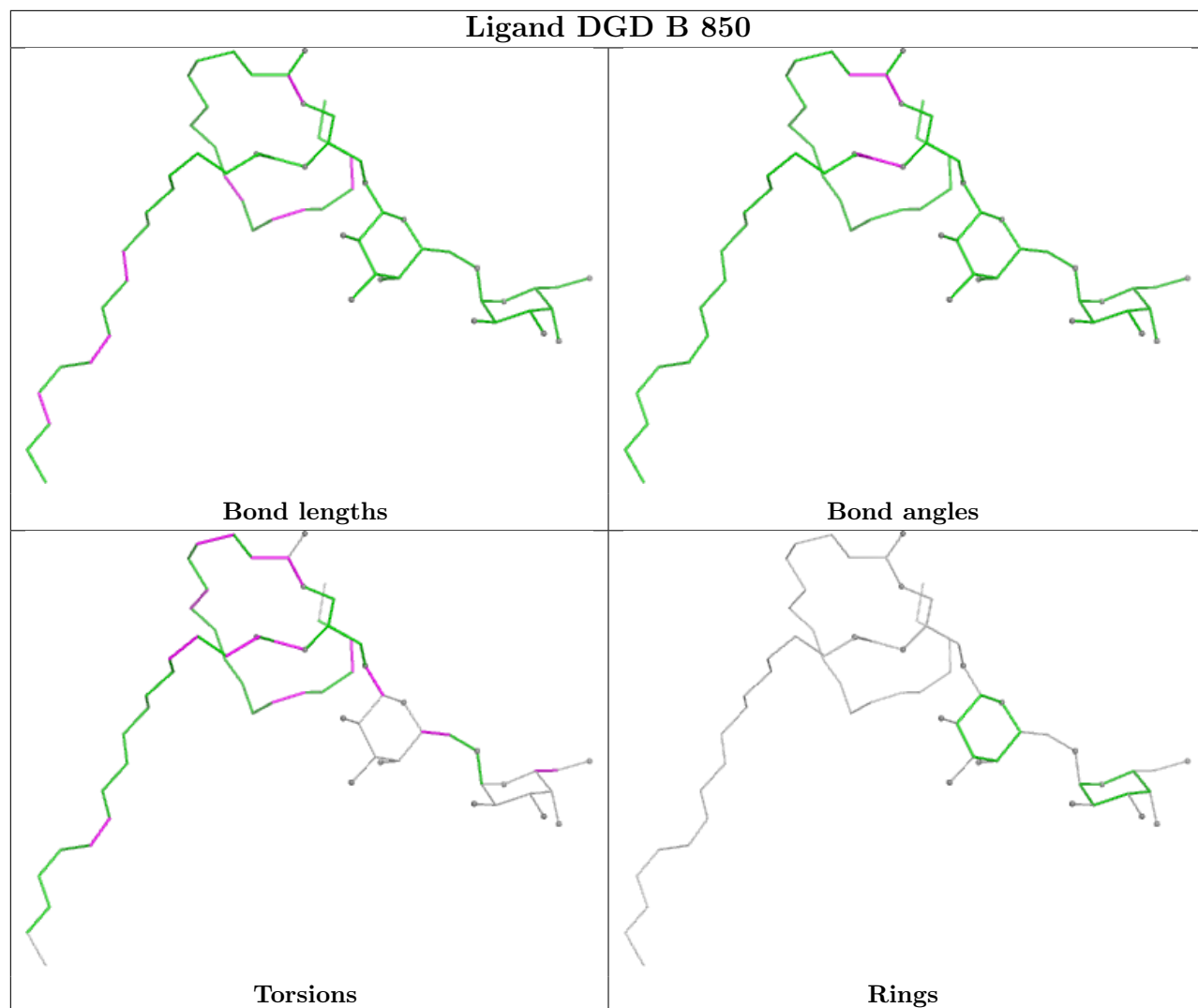




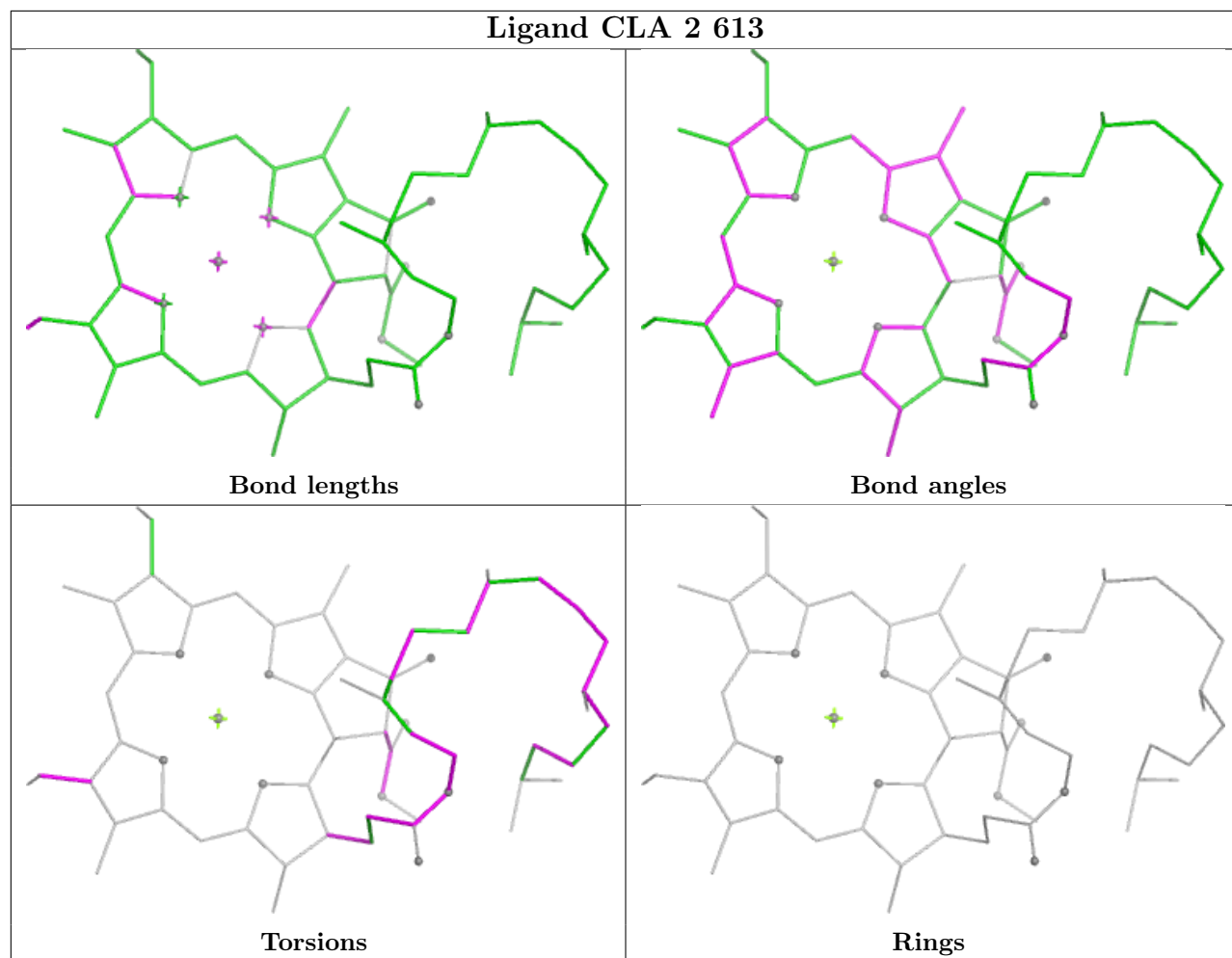
Ligand CLA 1 606**Ligand CLA B 809**

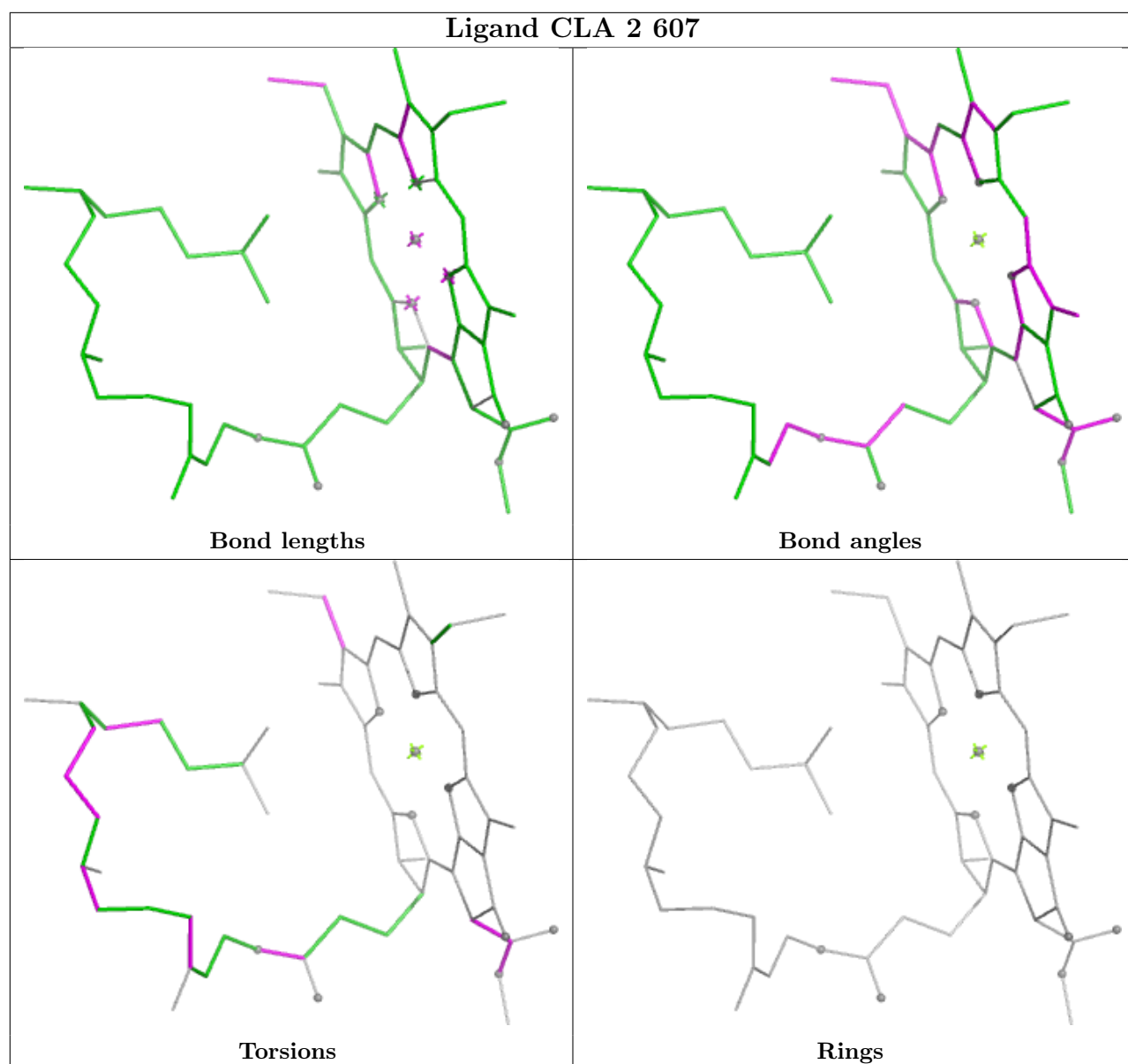


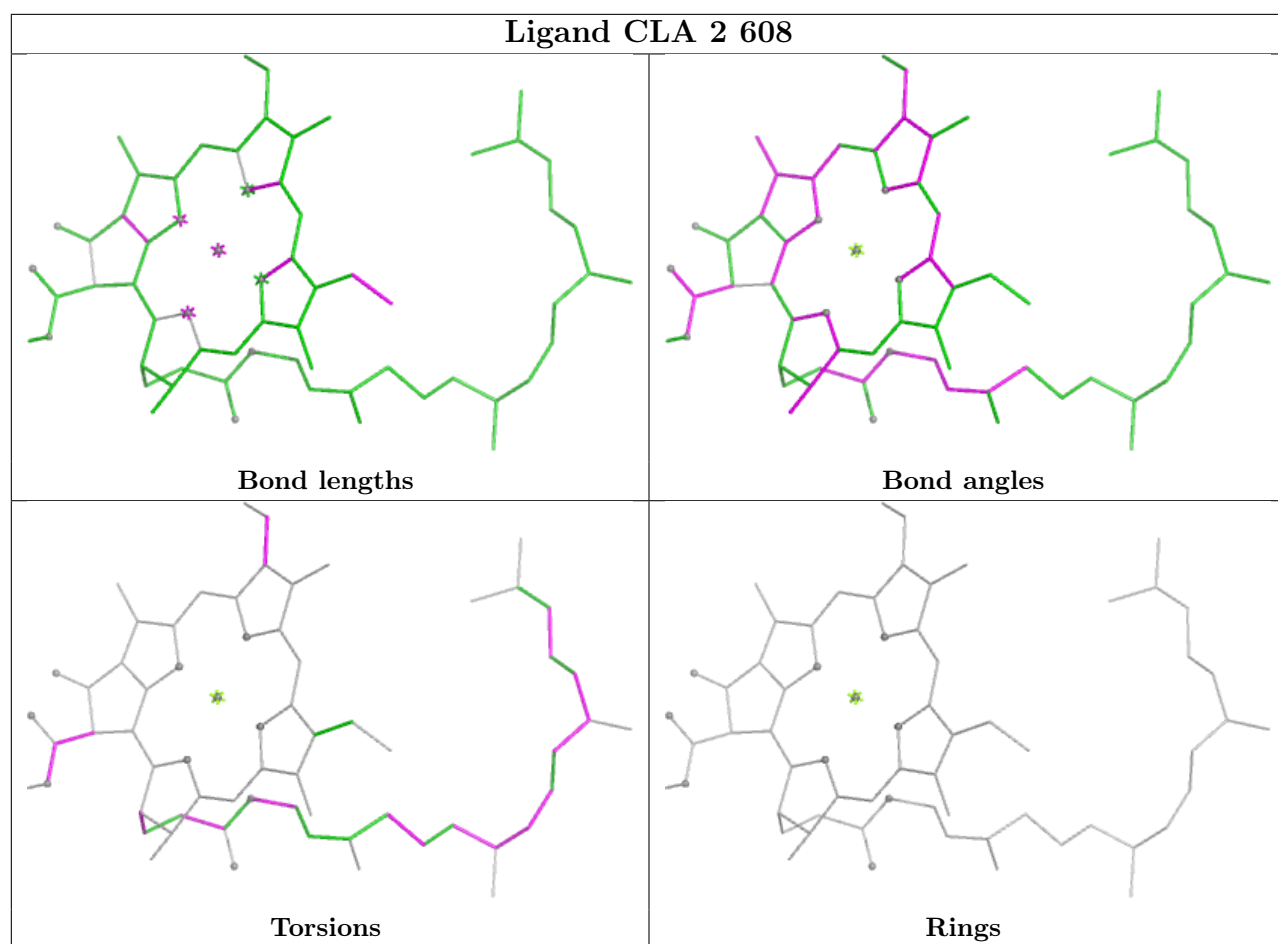


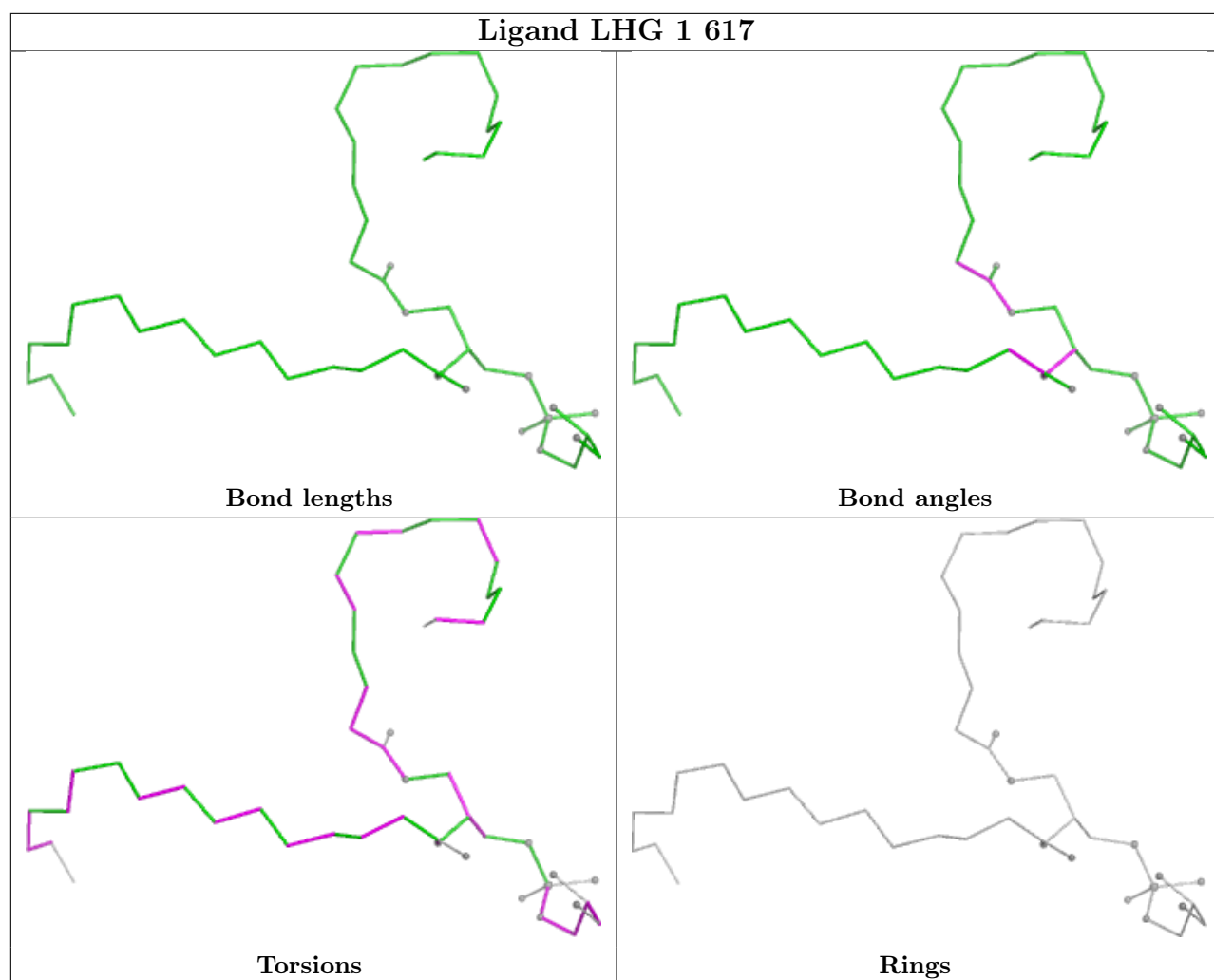


Ligand CLA 2 613

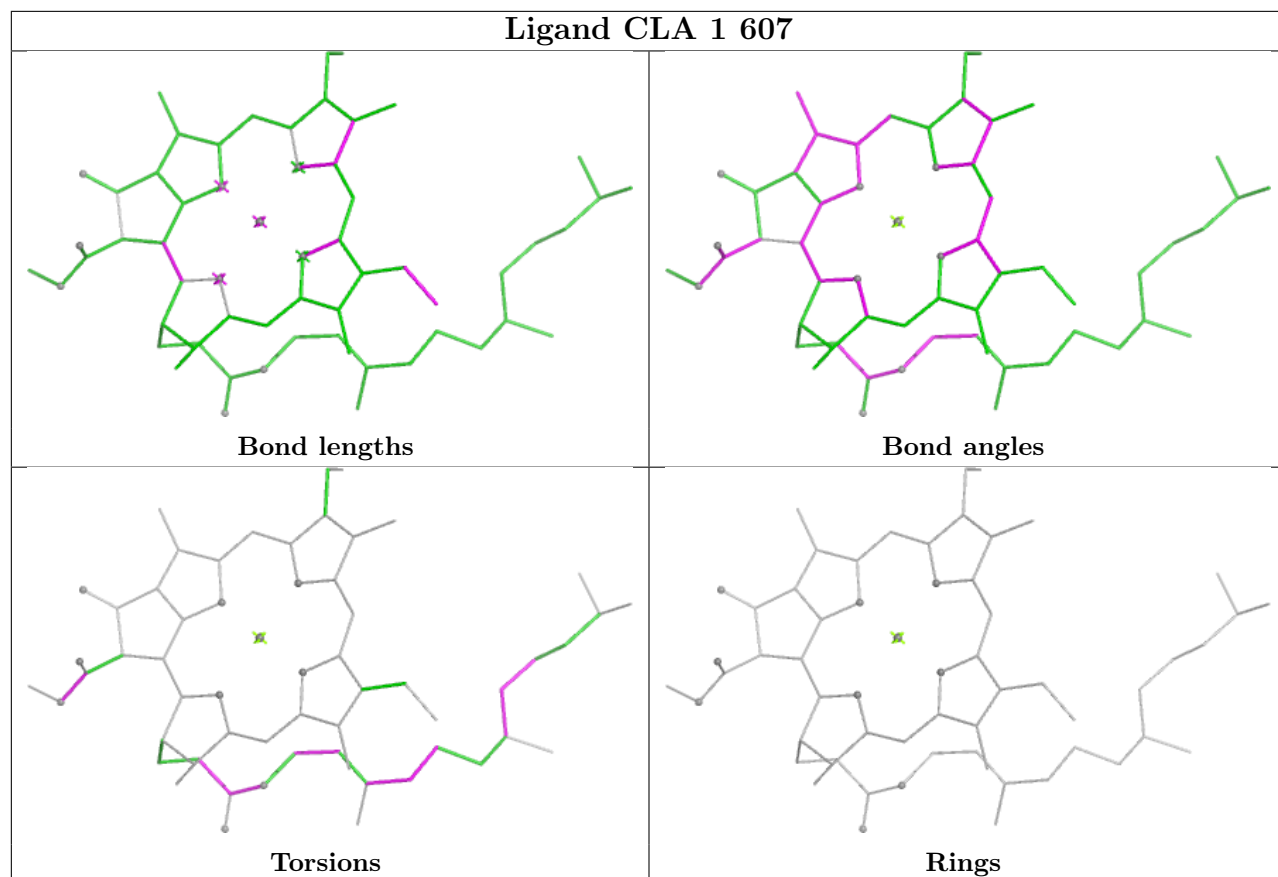




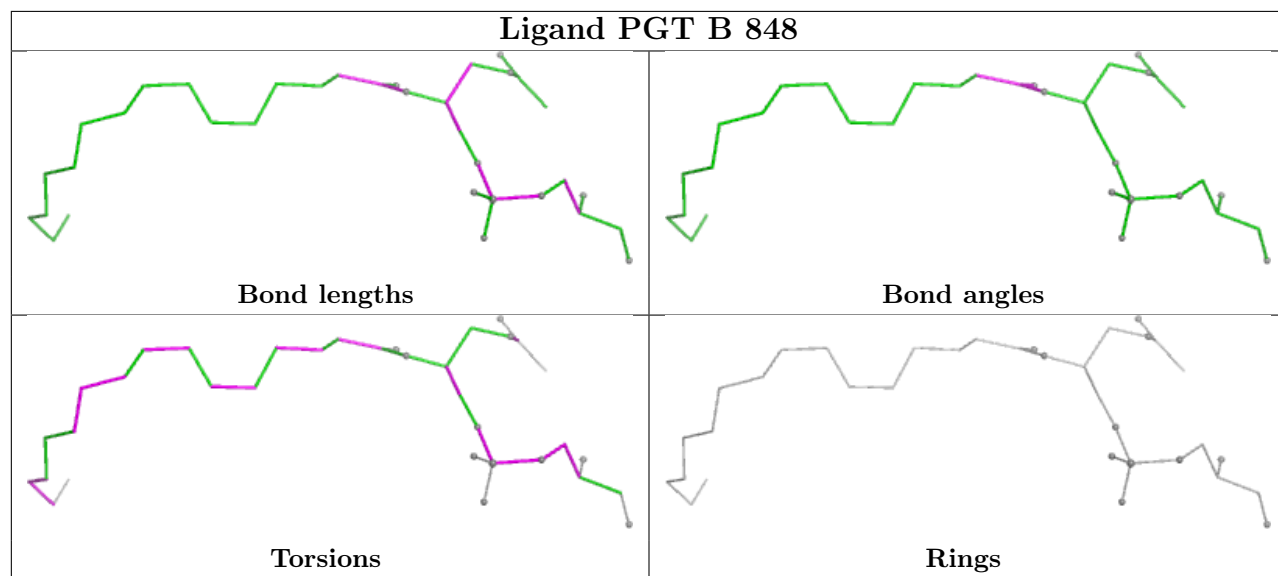


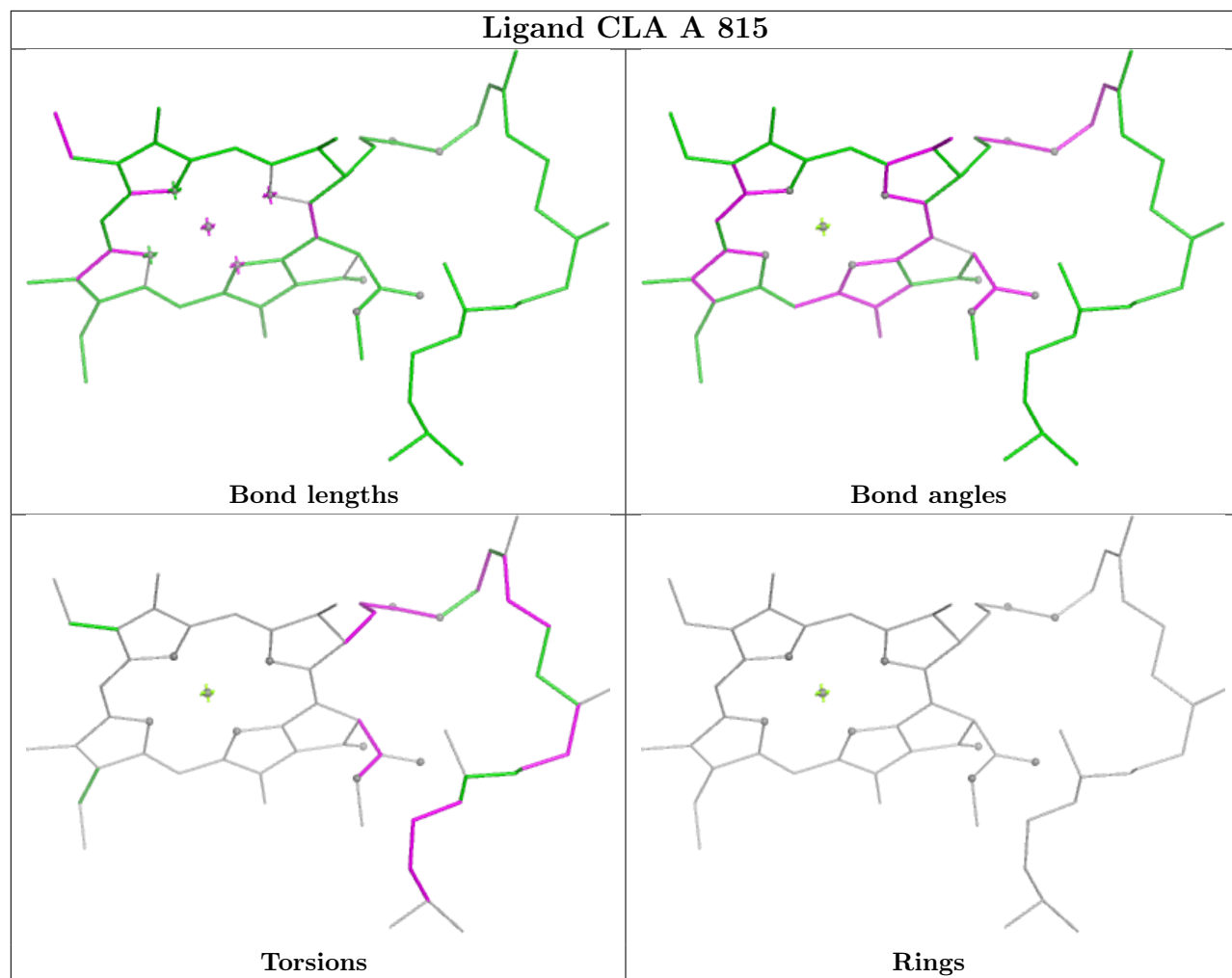


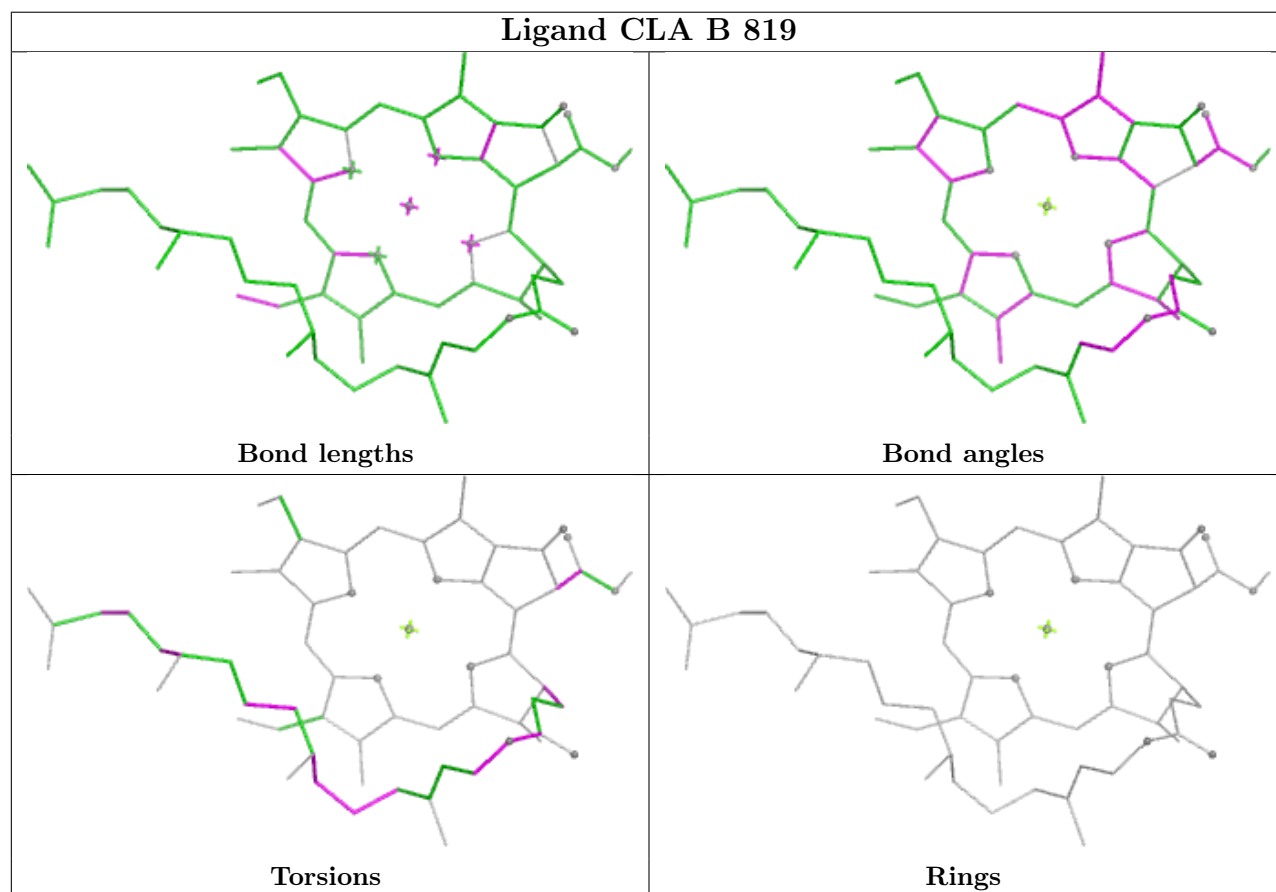
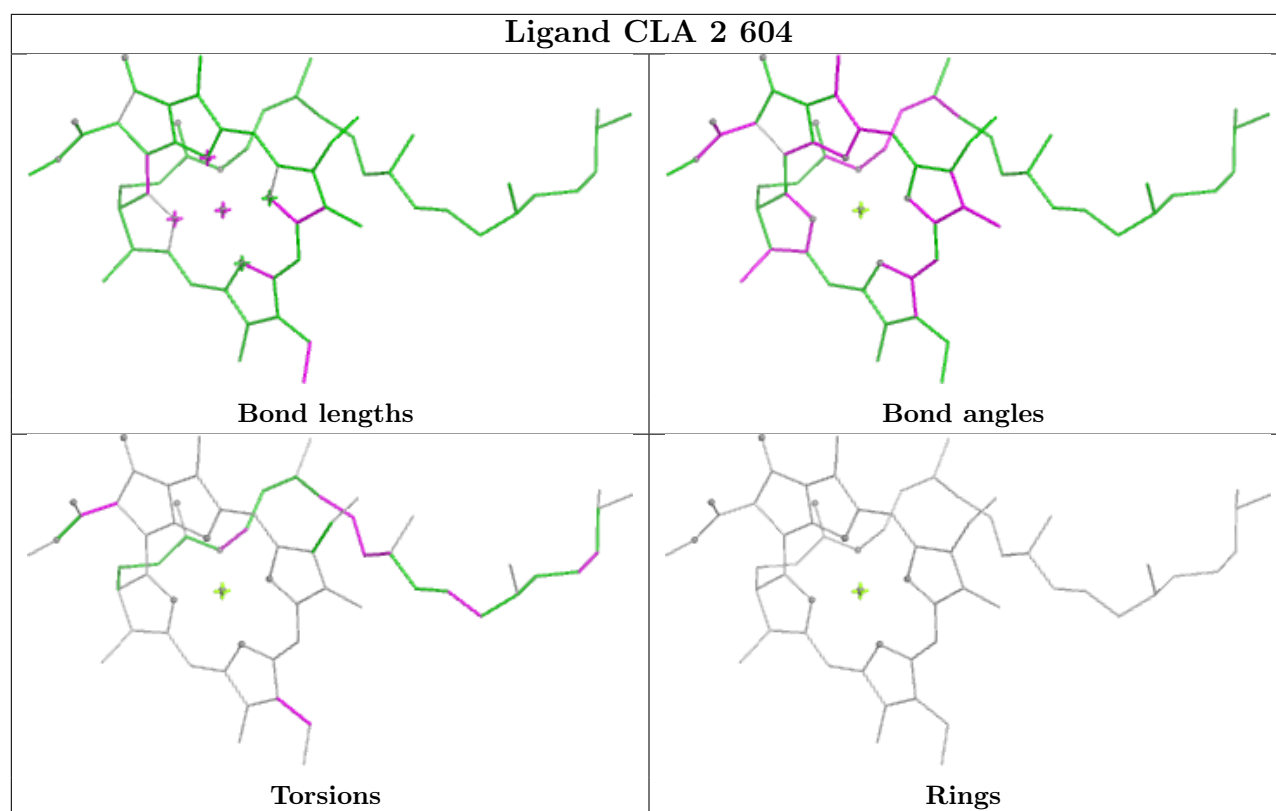
Ligand CLA 1 607



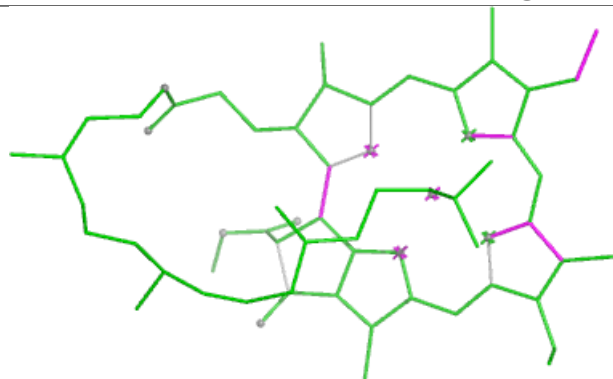
Ligand PGT B 848



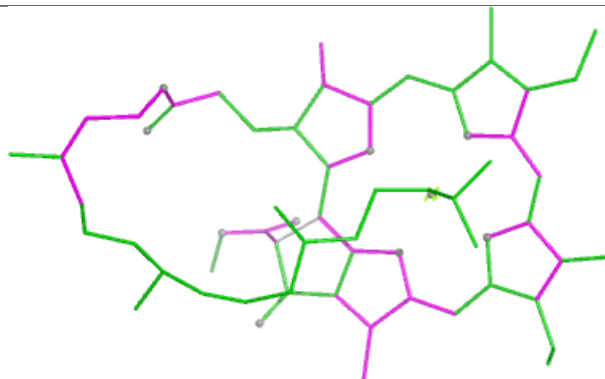




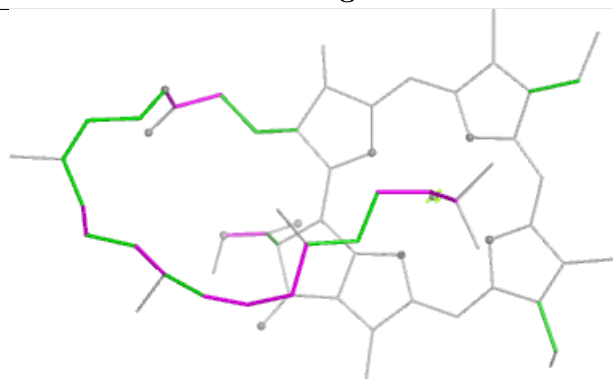
Ligand CLA 2 606



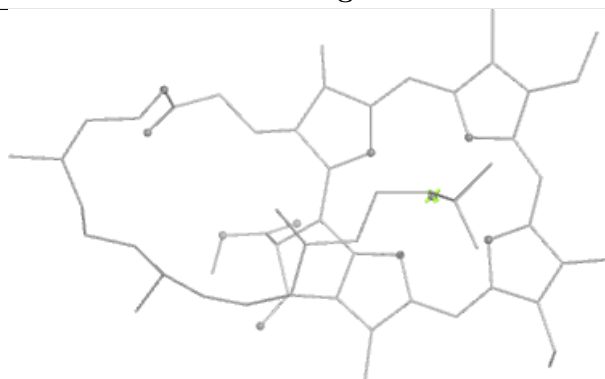
Bond lengths



Bond angles

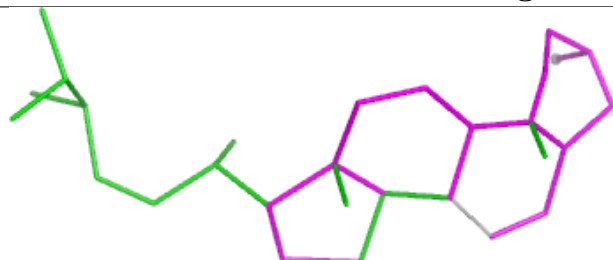


Torsions

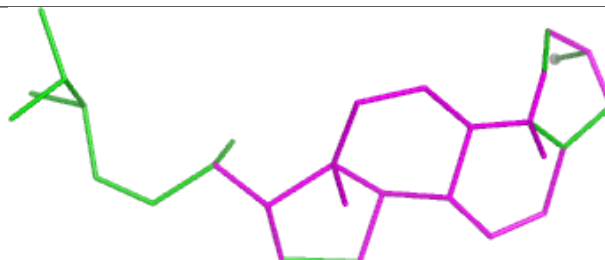


Rings

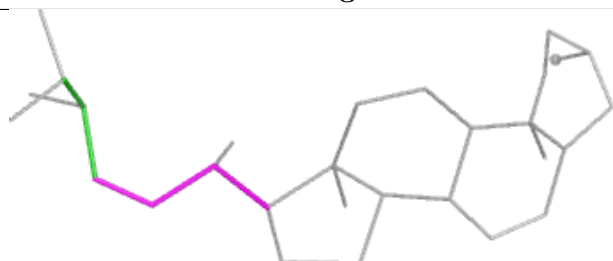
Ligand ERG 1 618



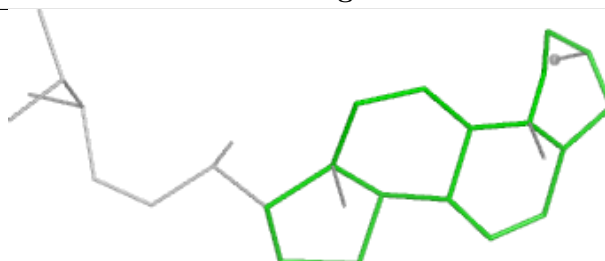
Bond lengths



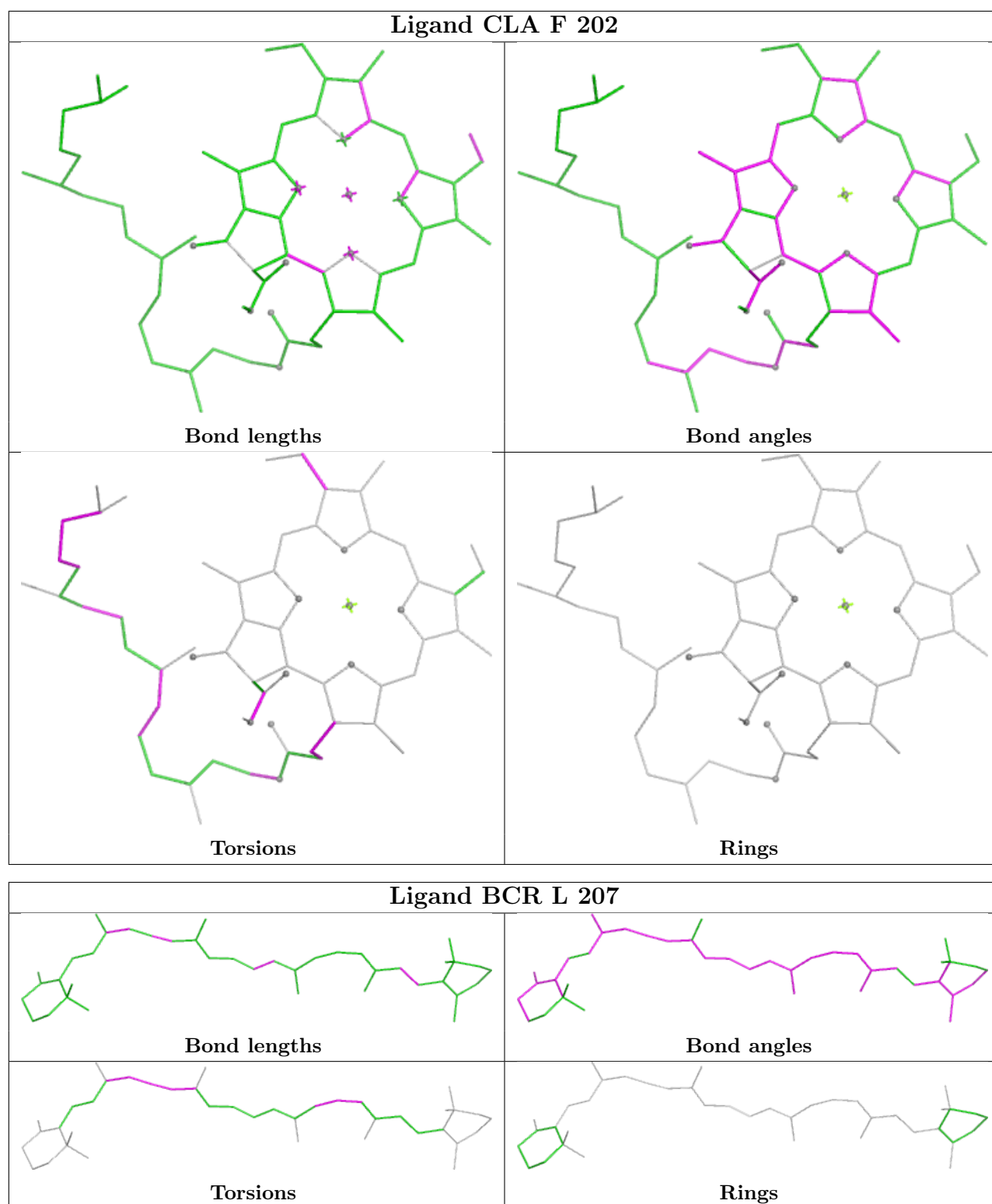
Bond angles

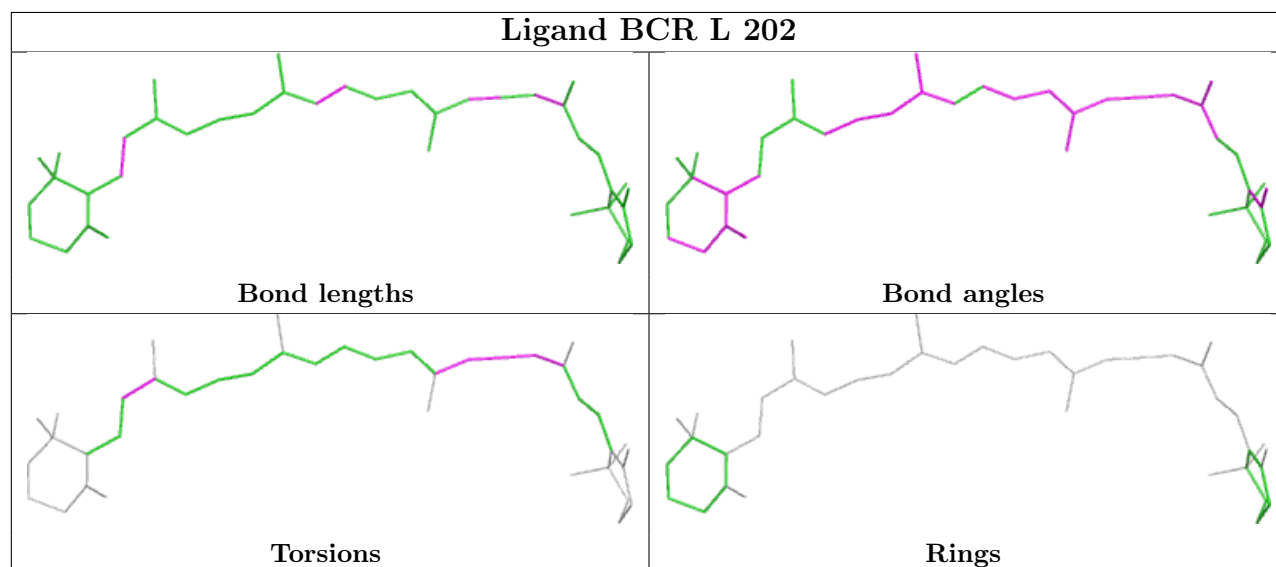
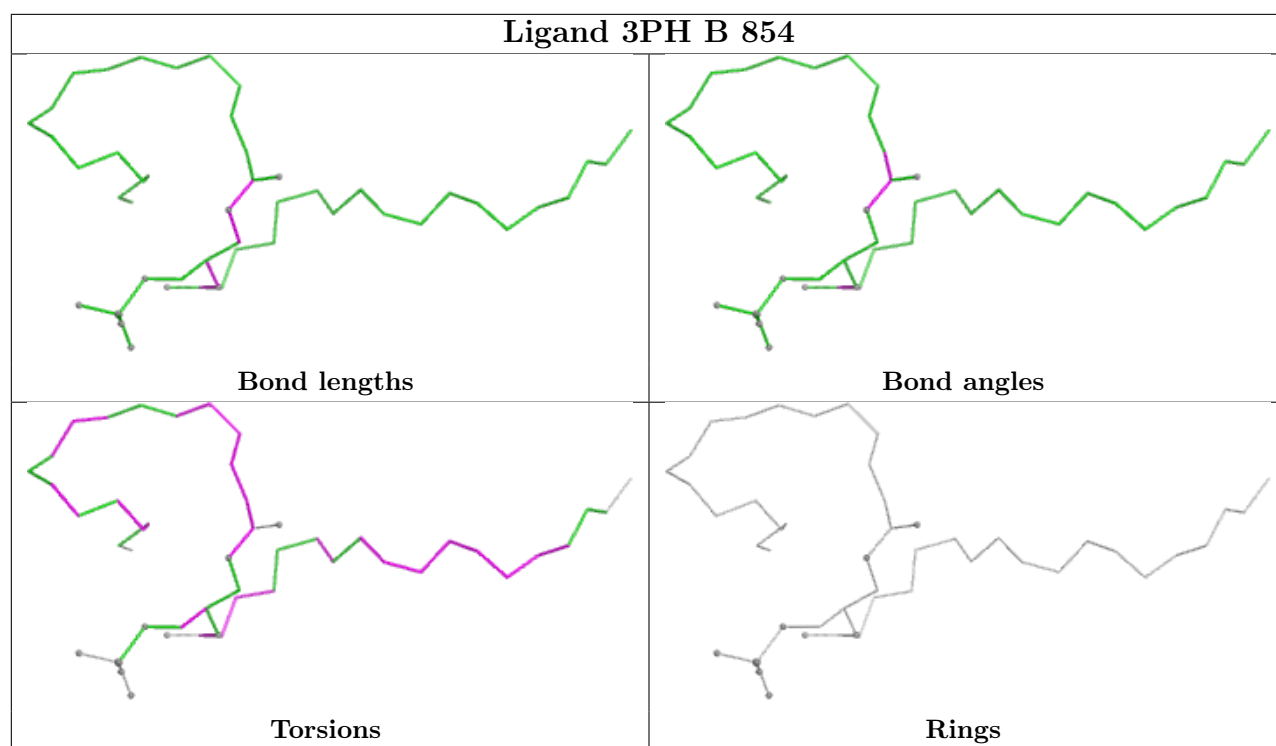


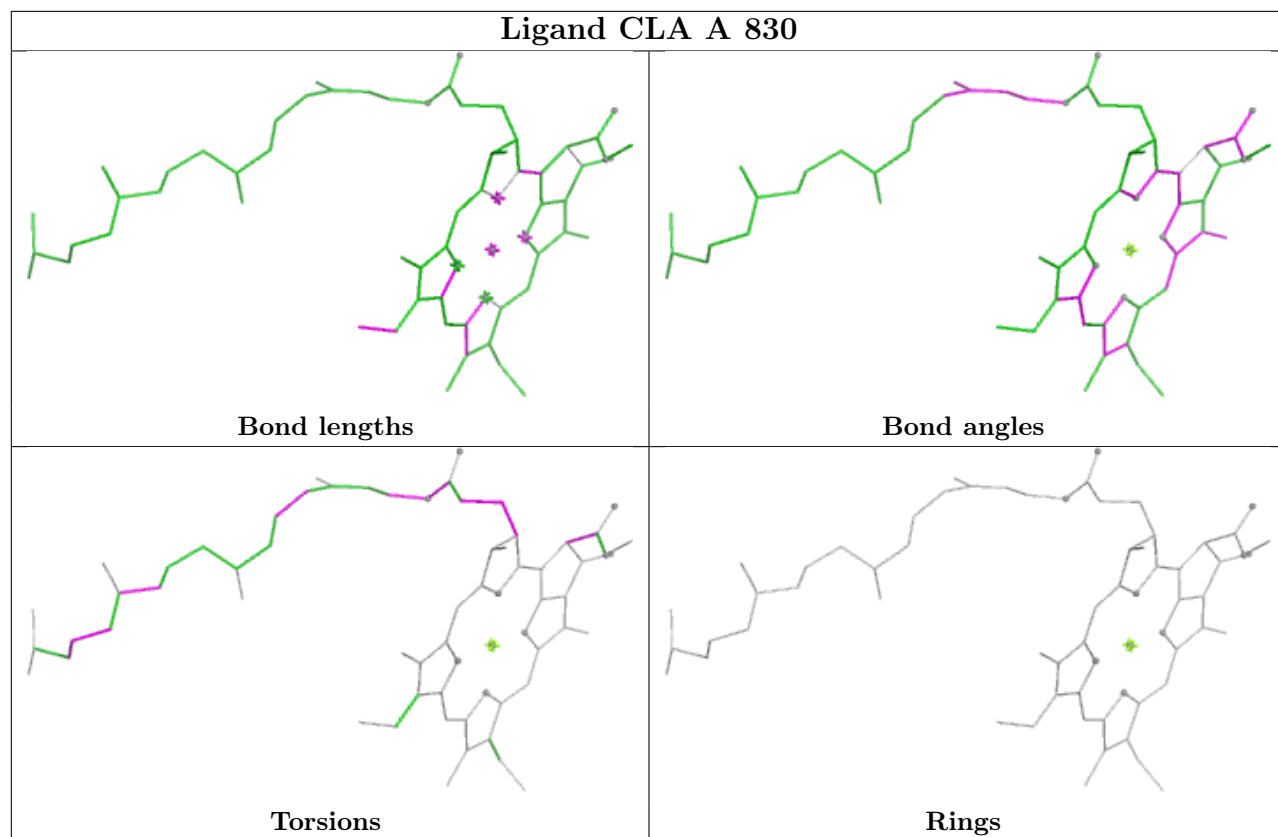
Torsions

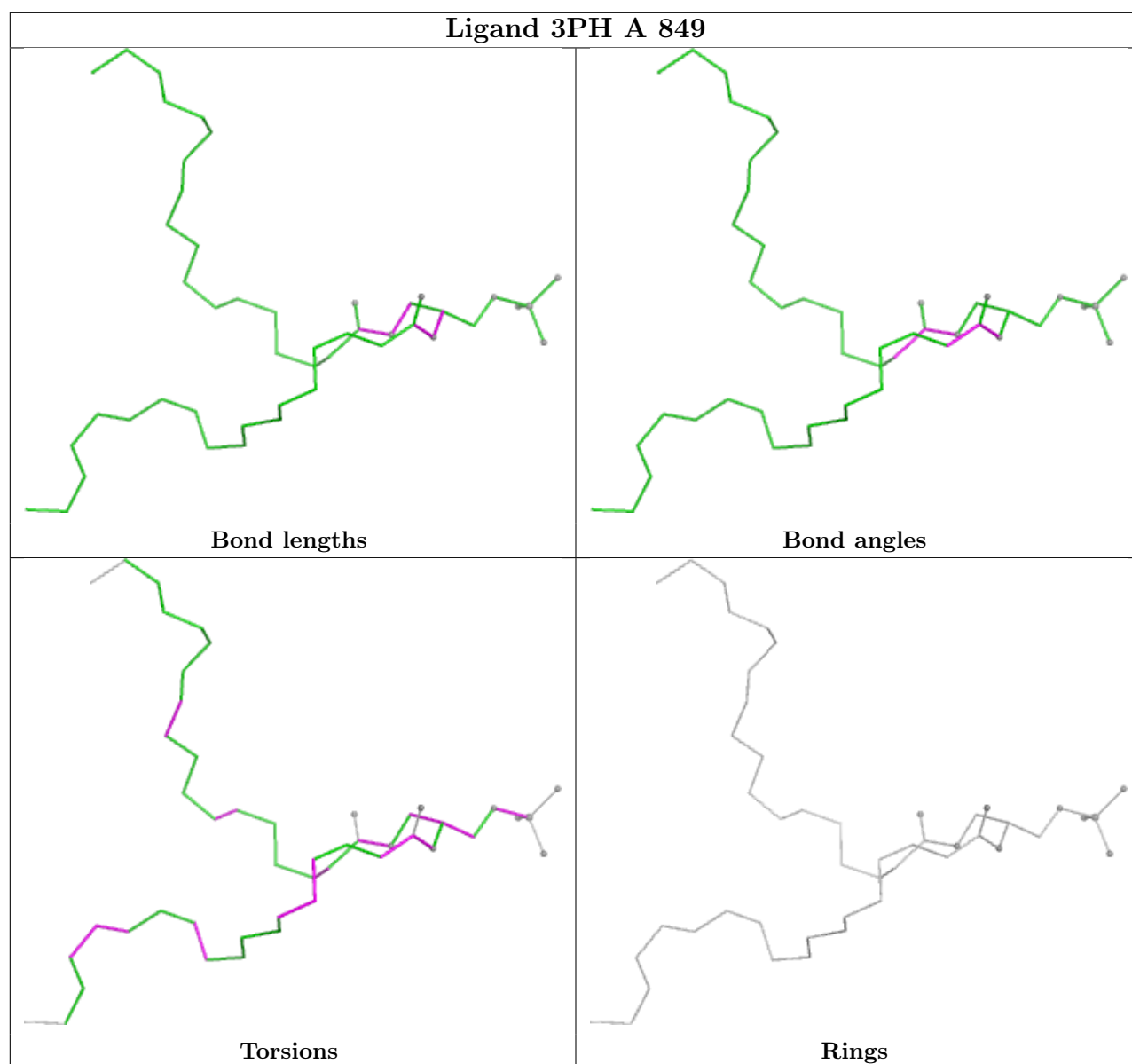


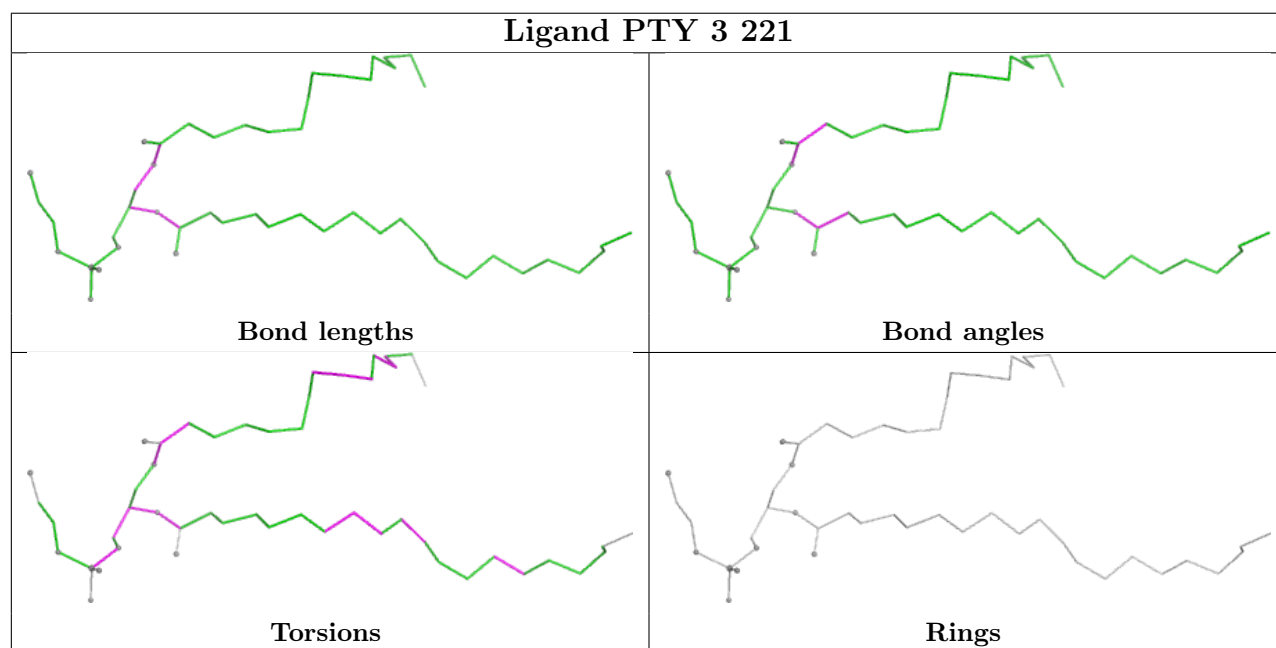
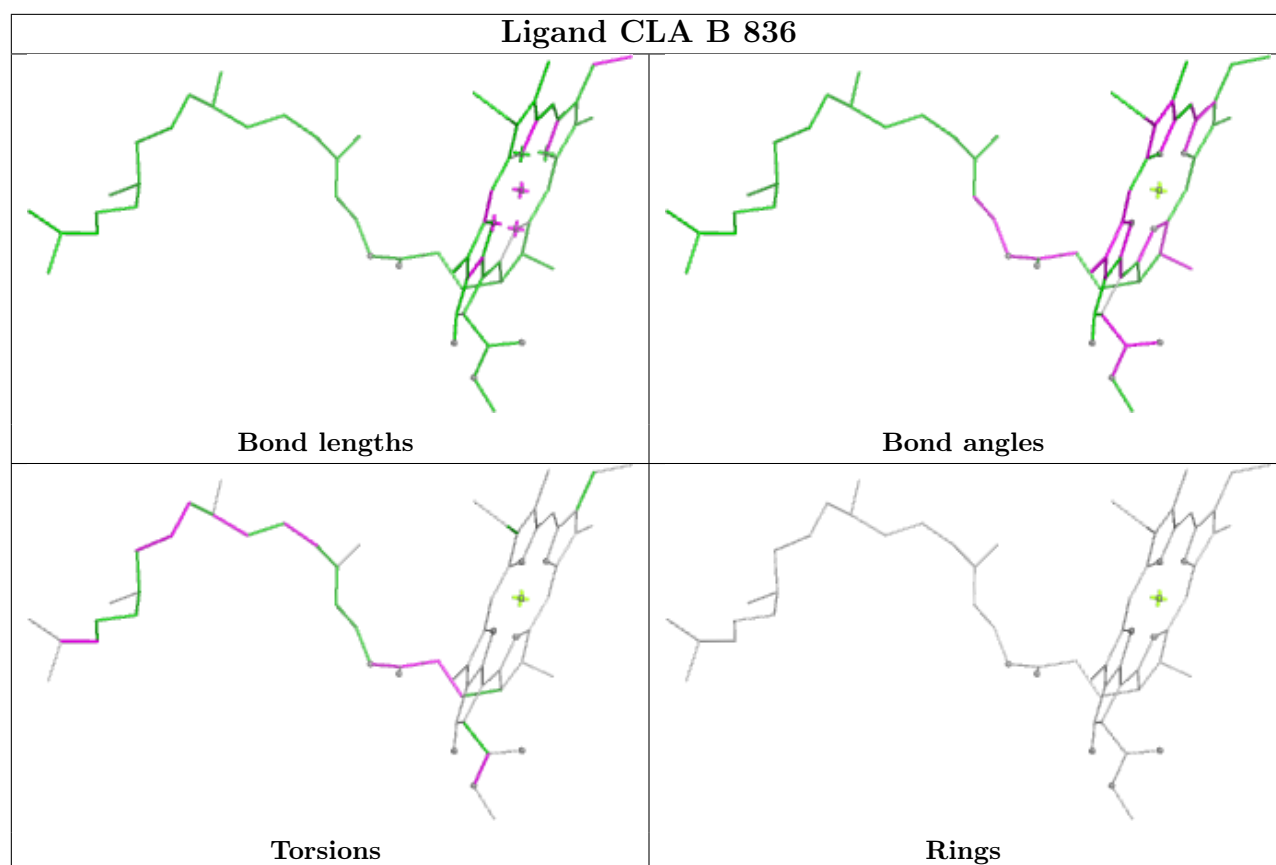
Rings

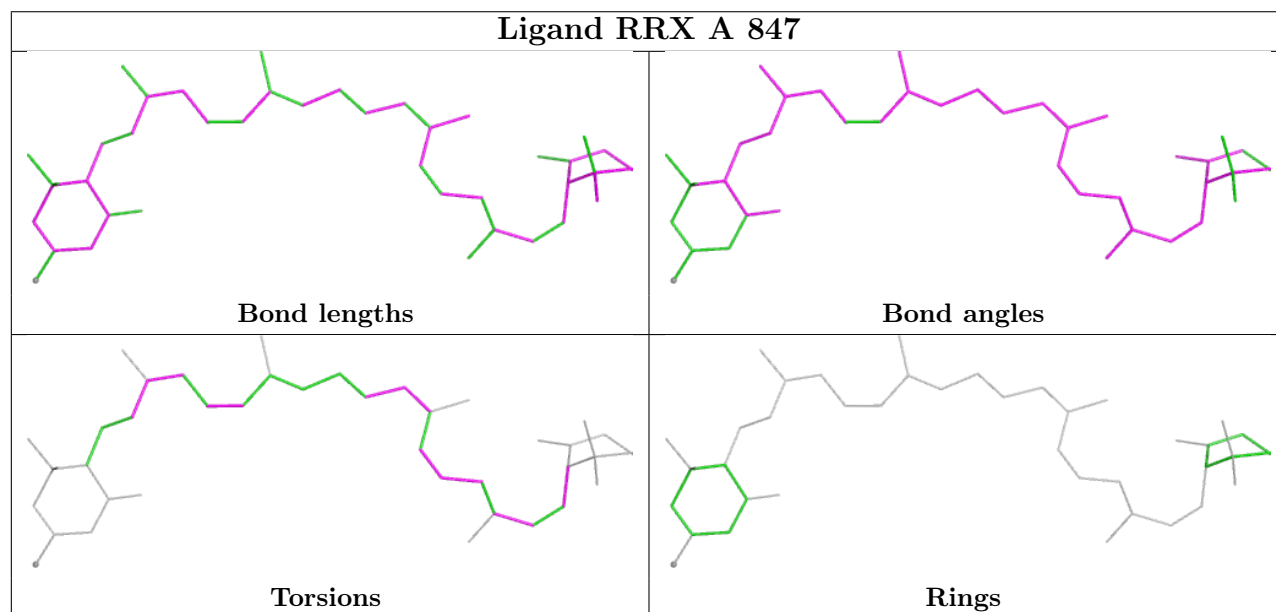
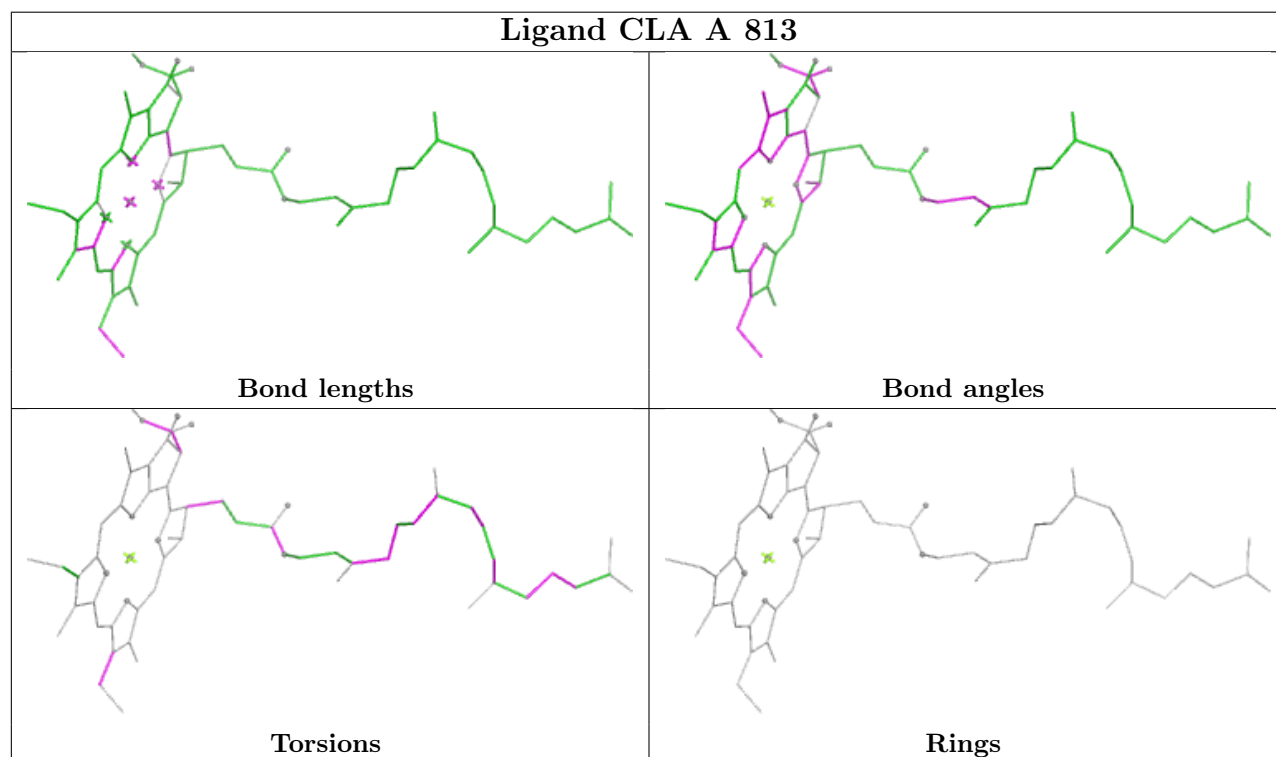
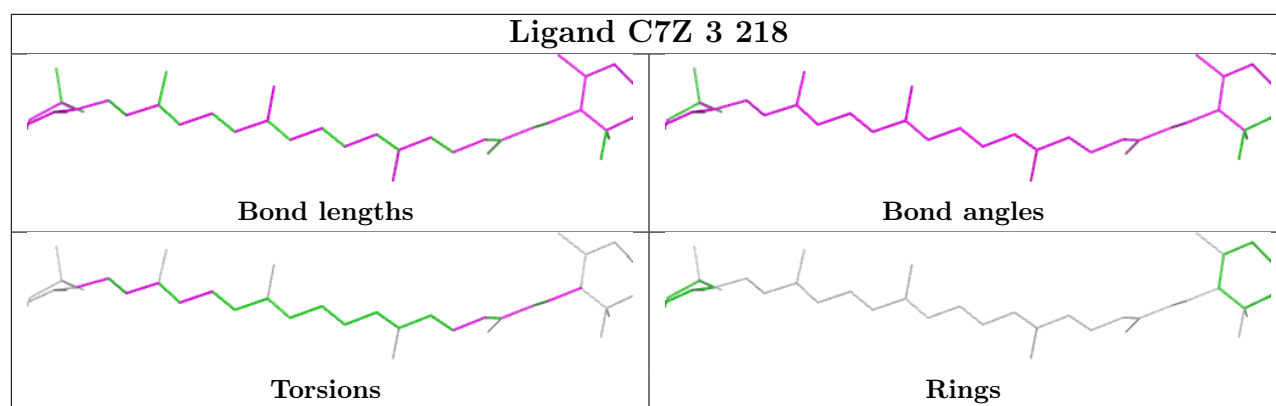


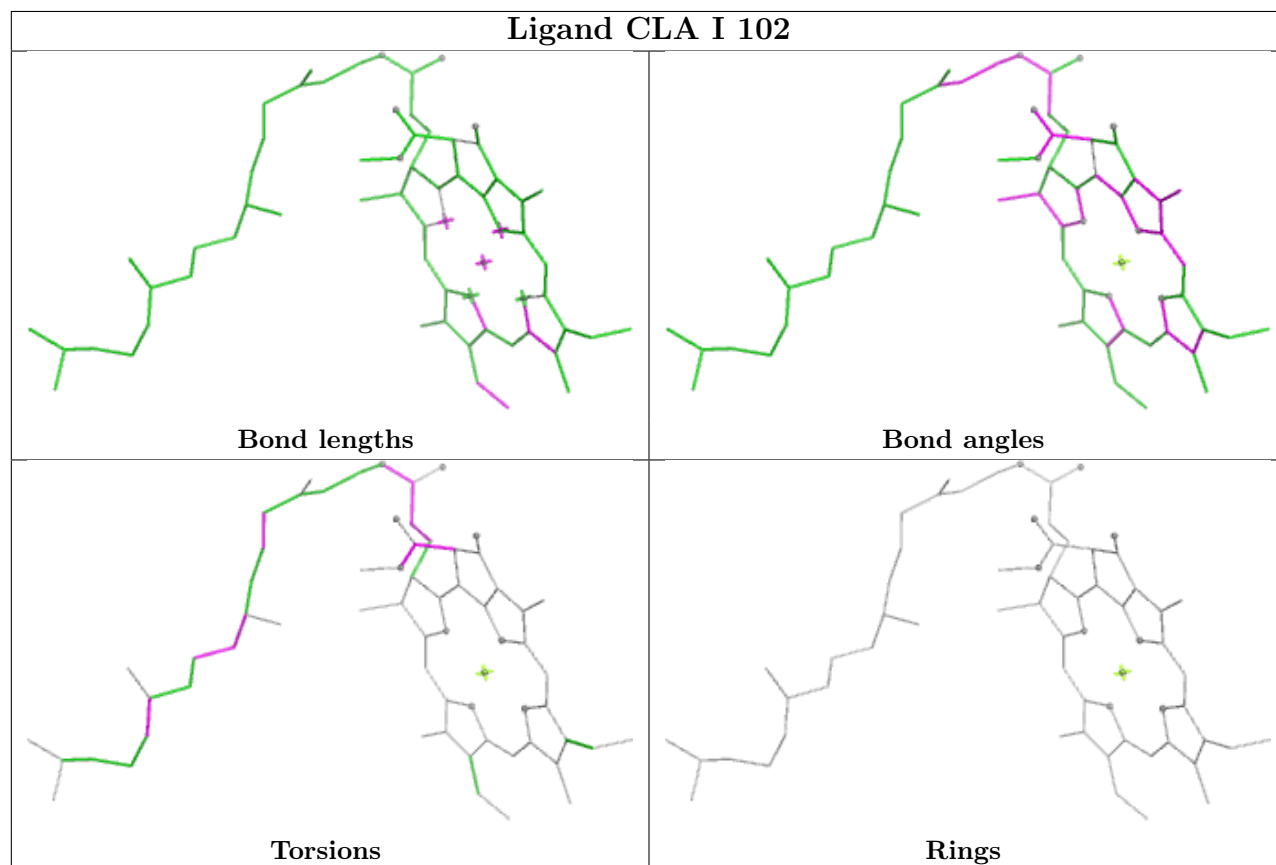
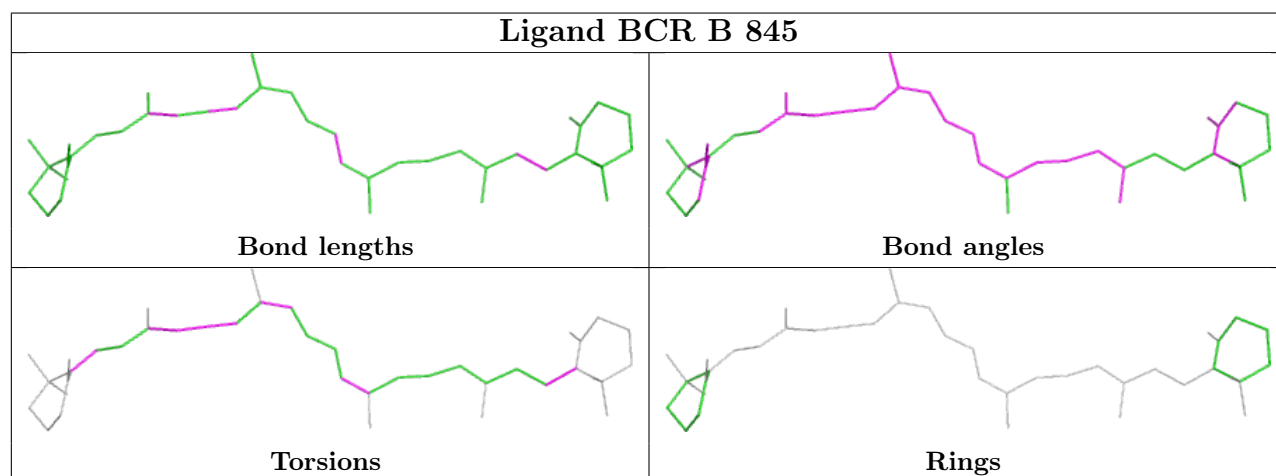
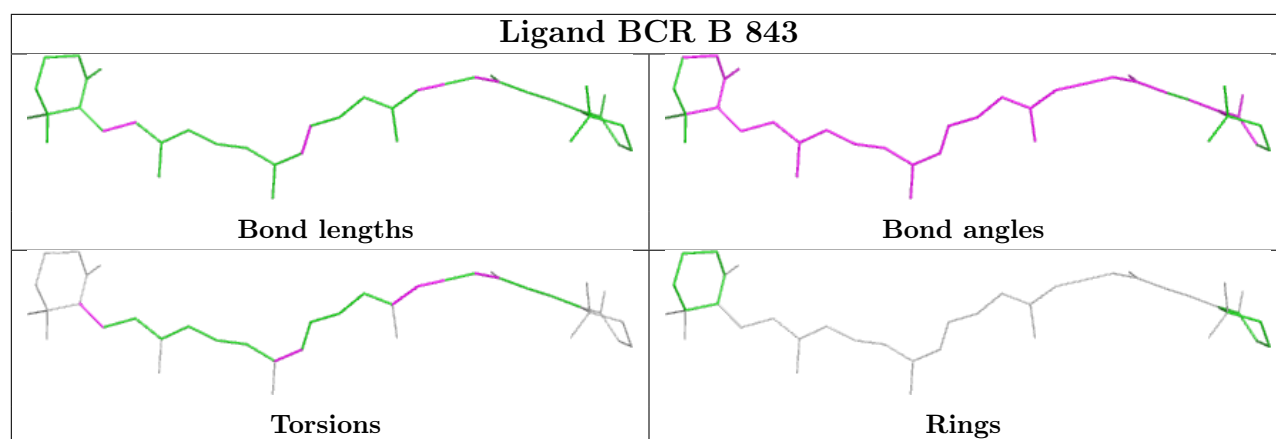


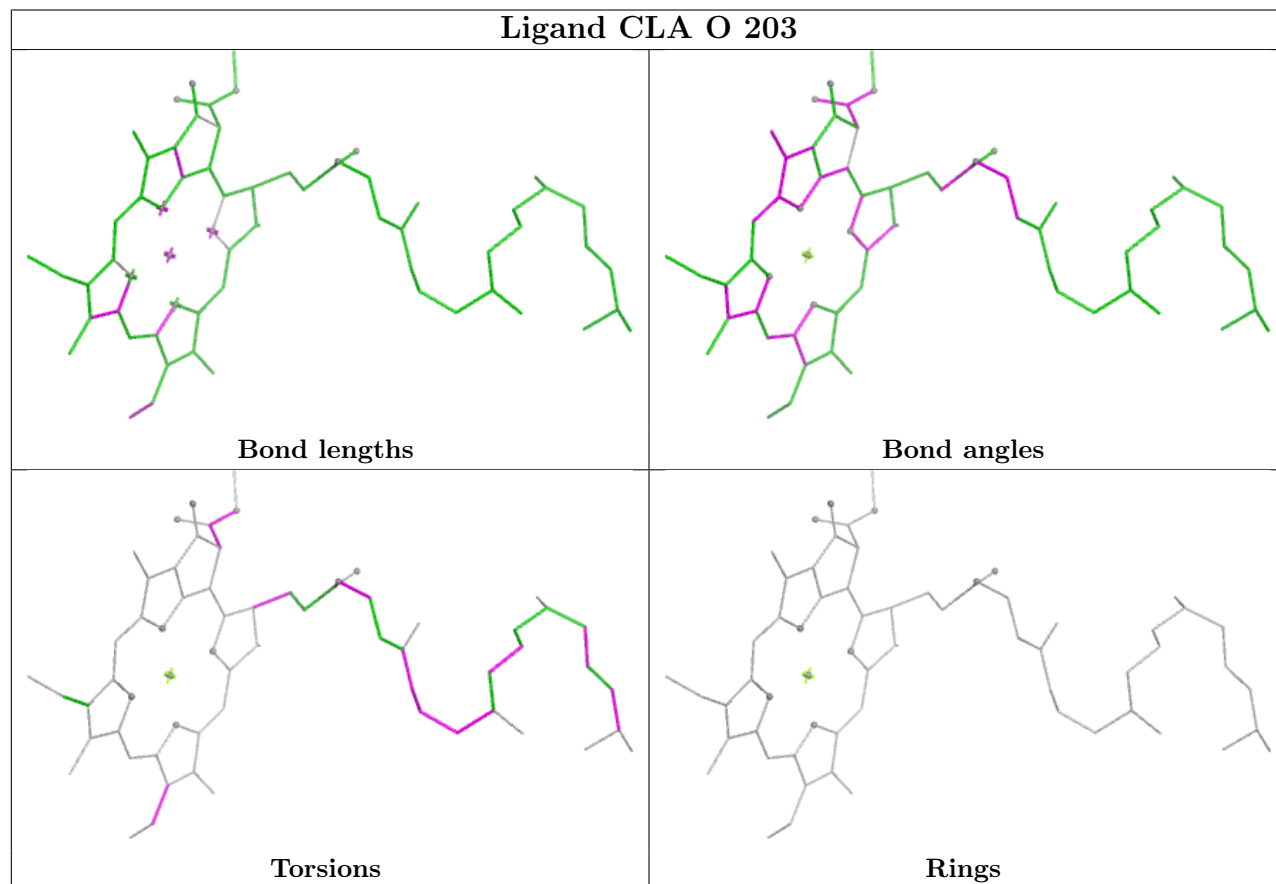
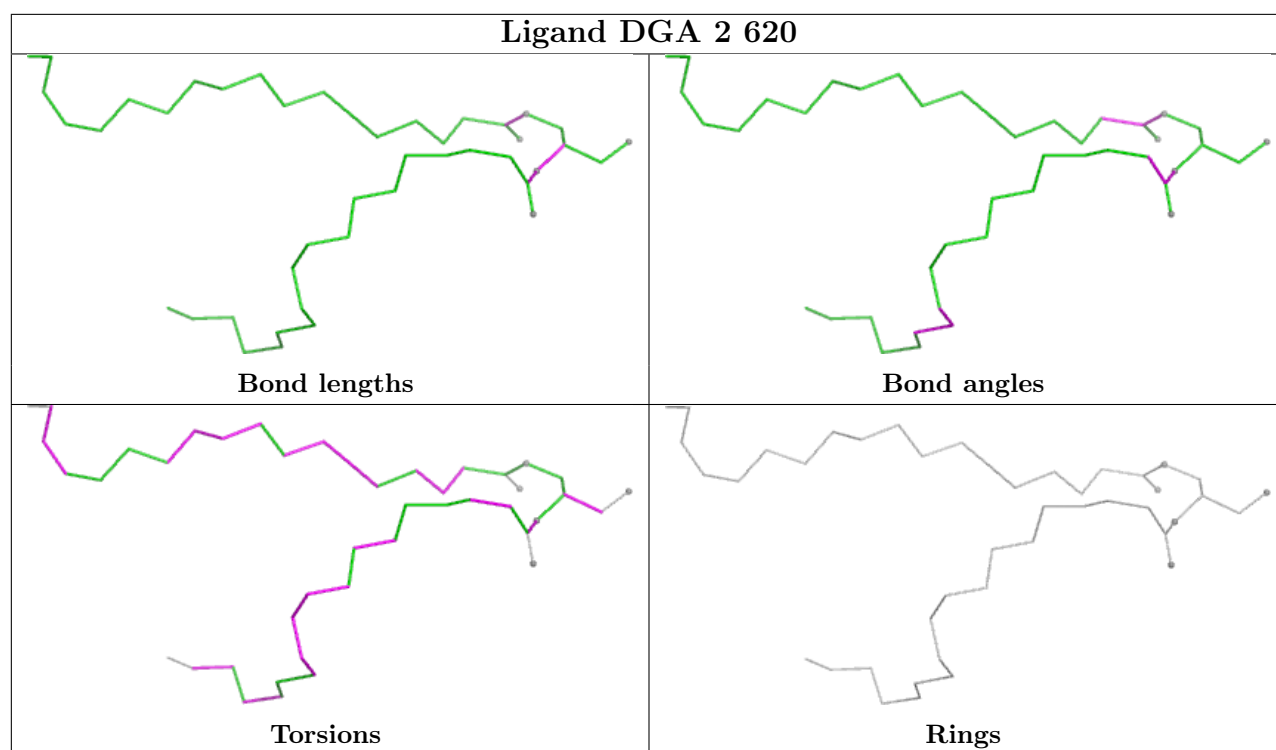


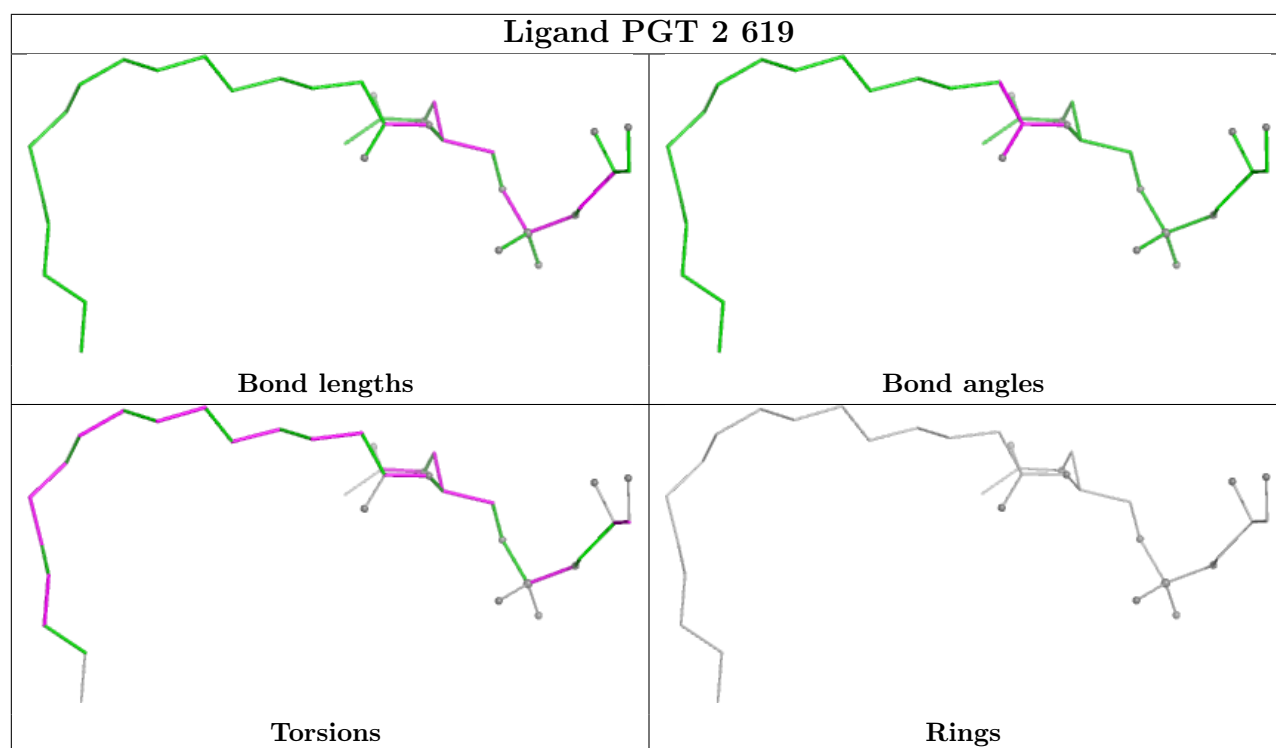


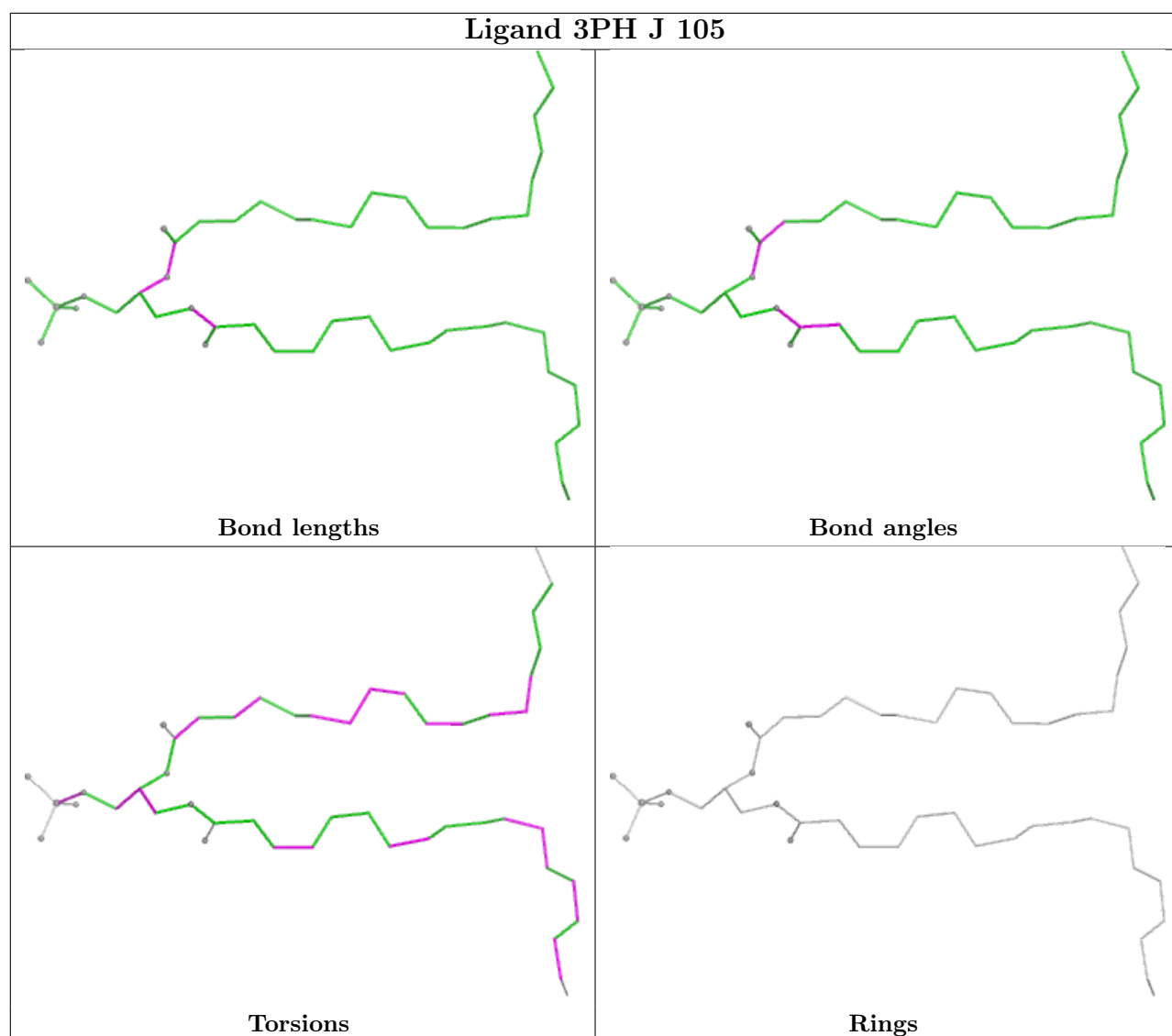


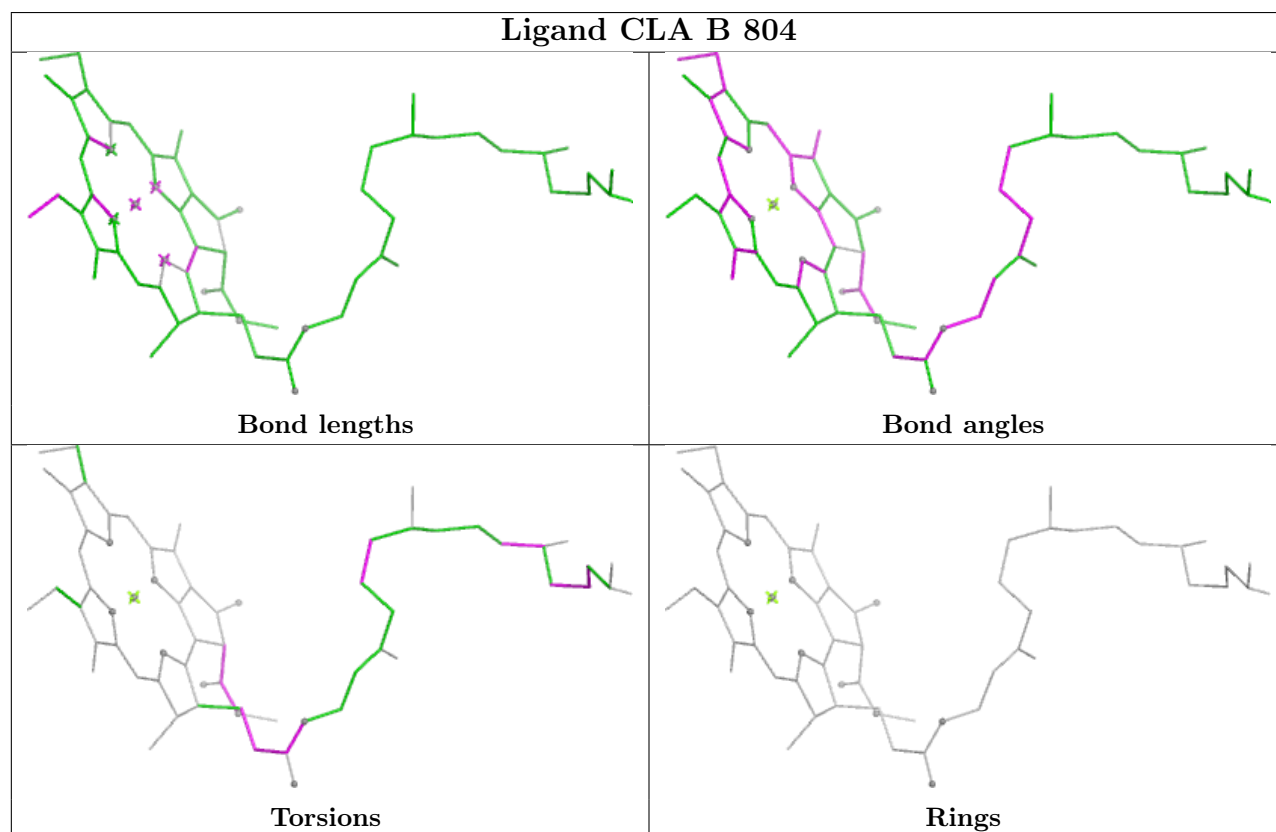
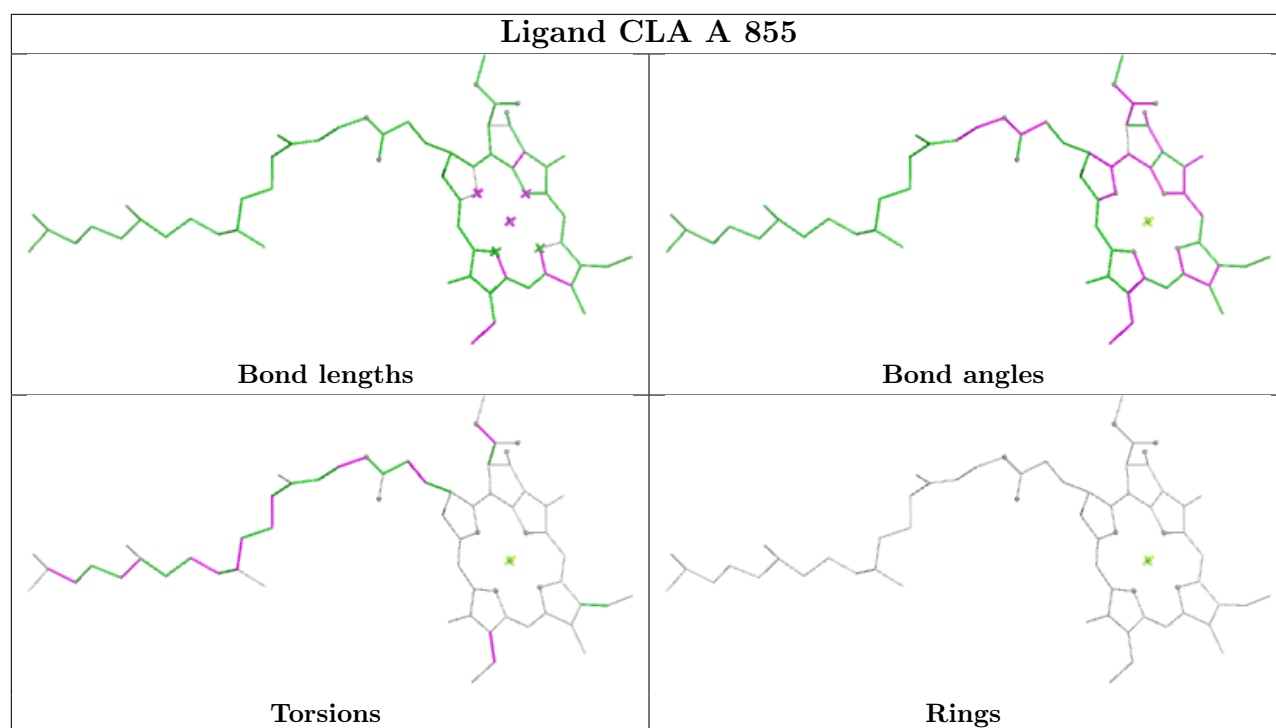




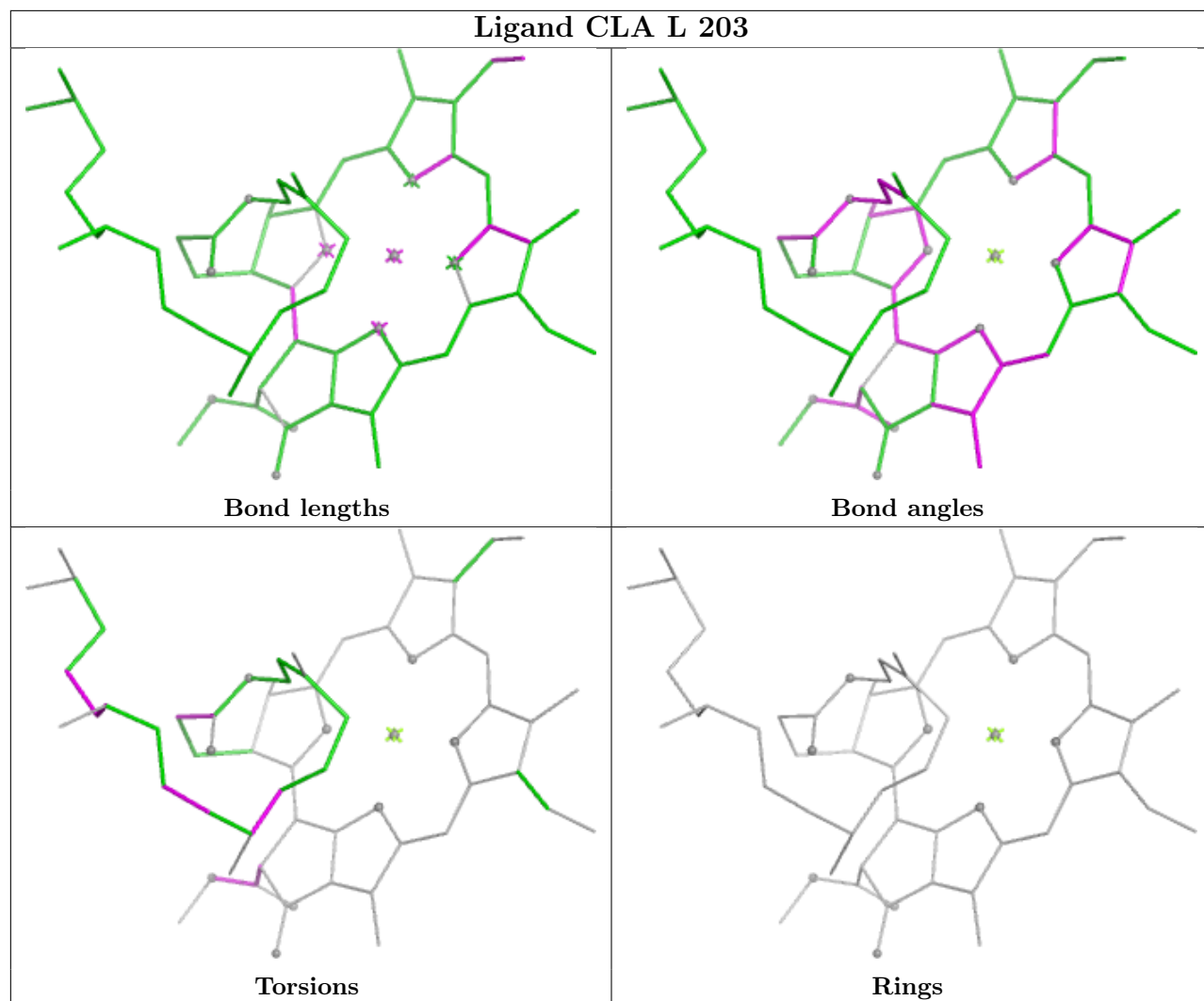


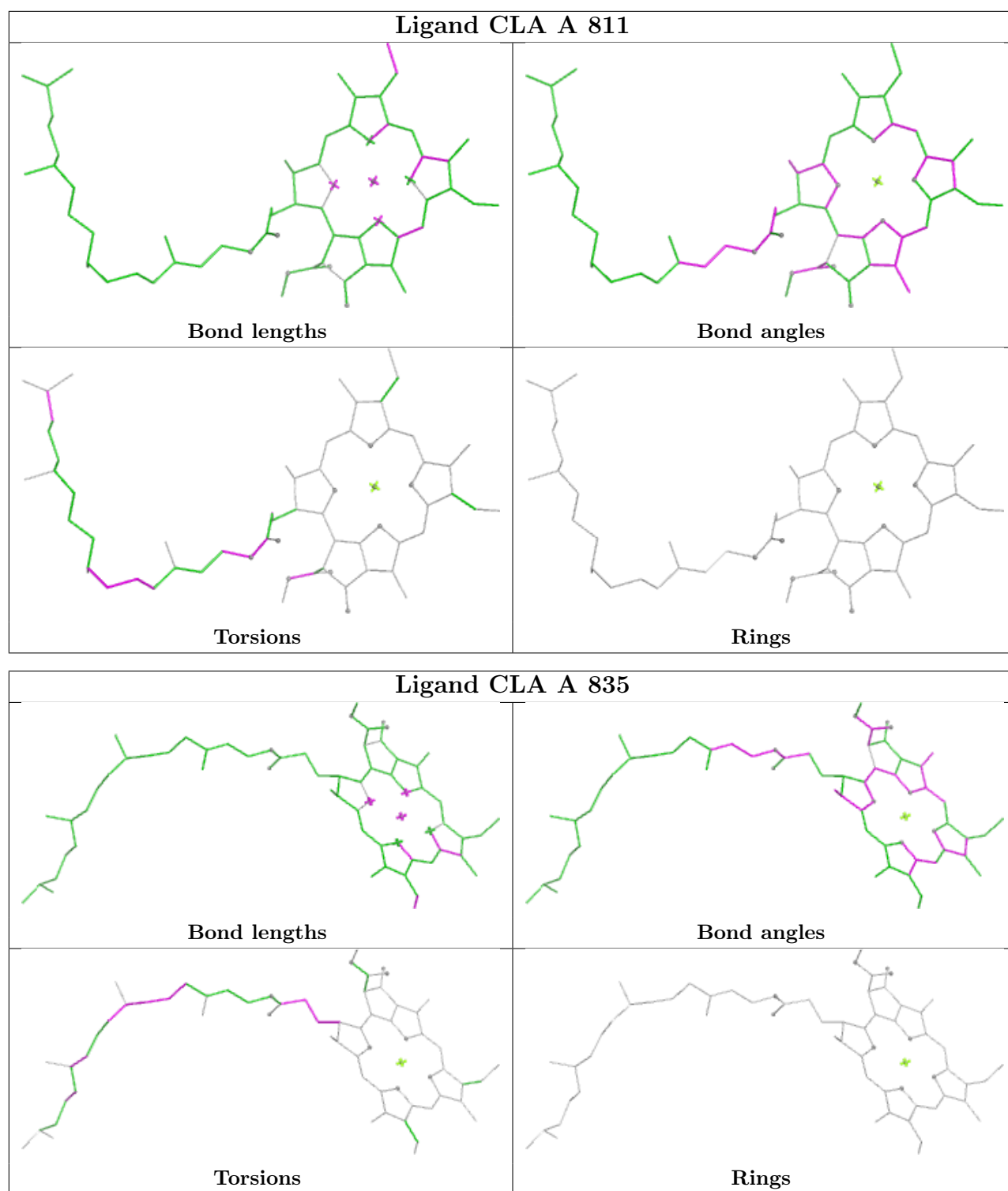


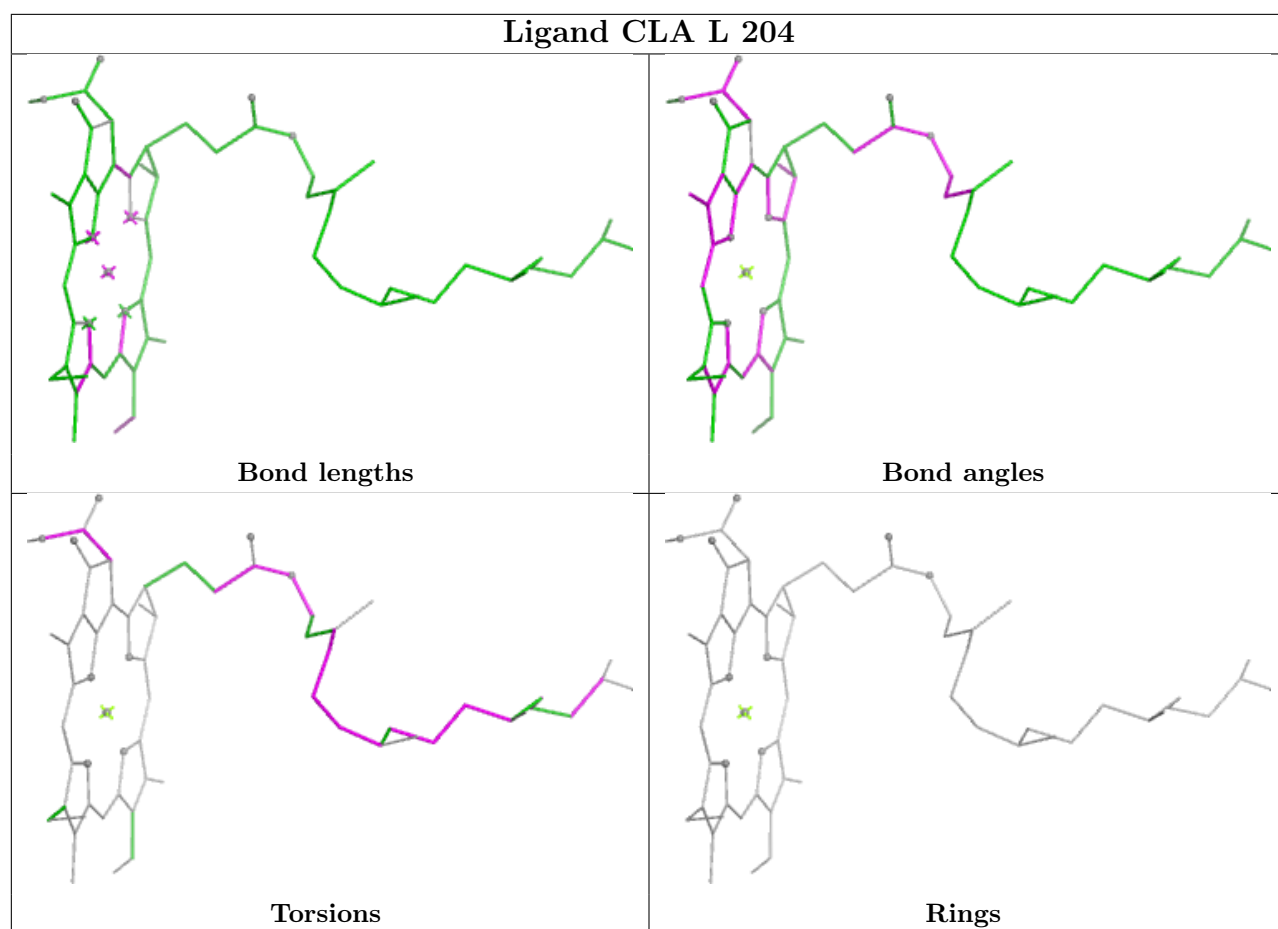


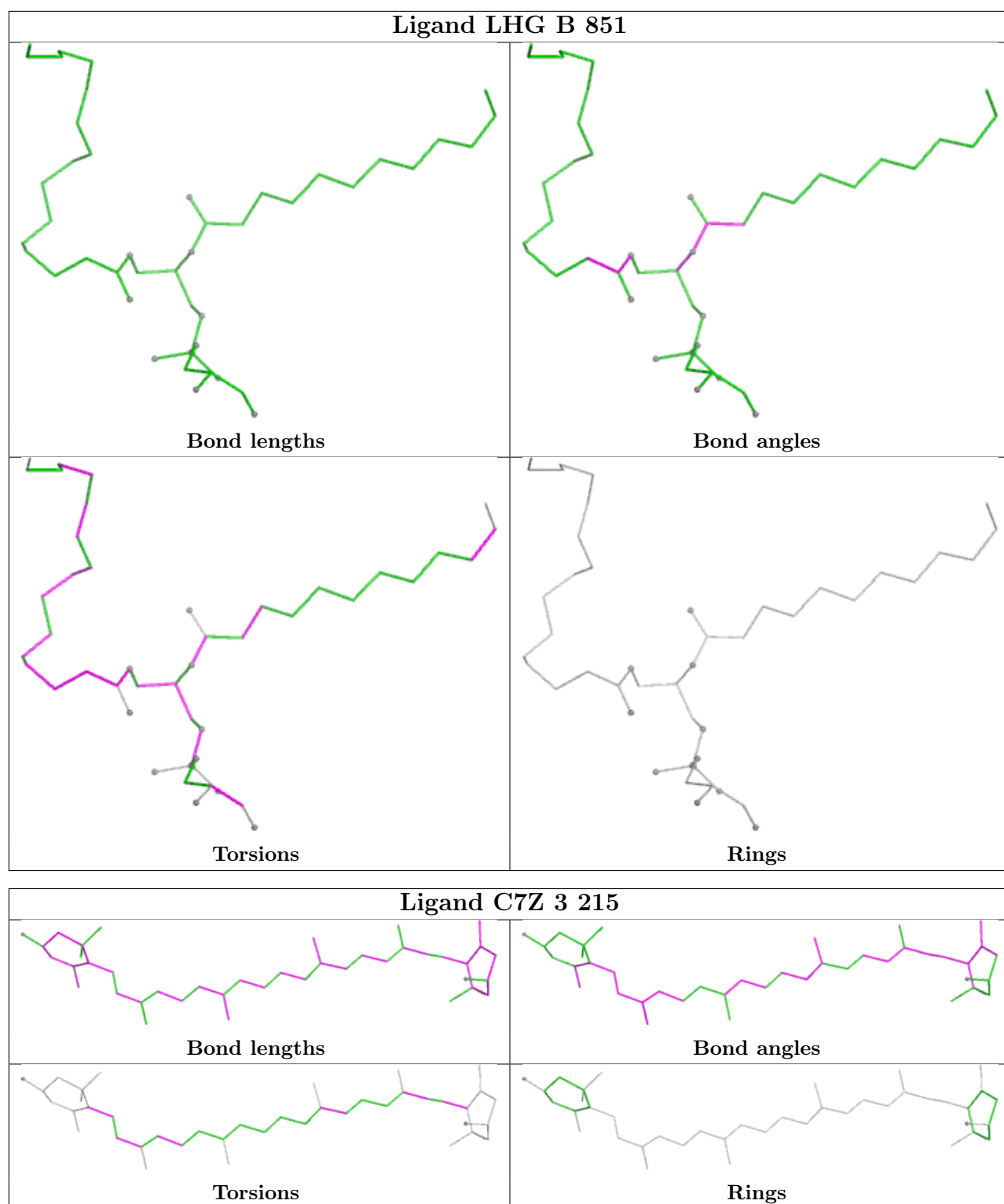


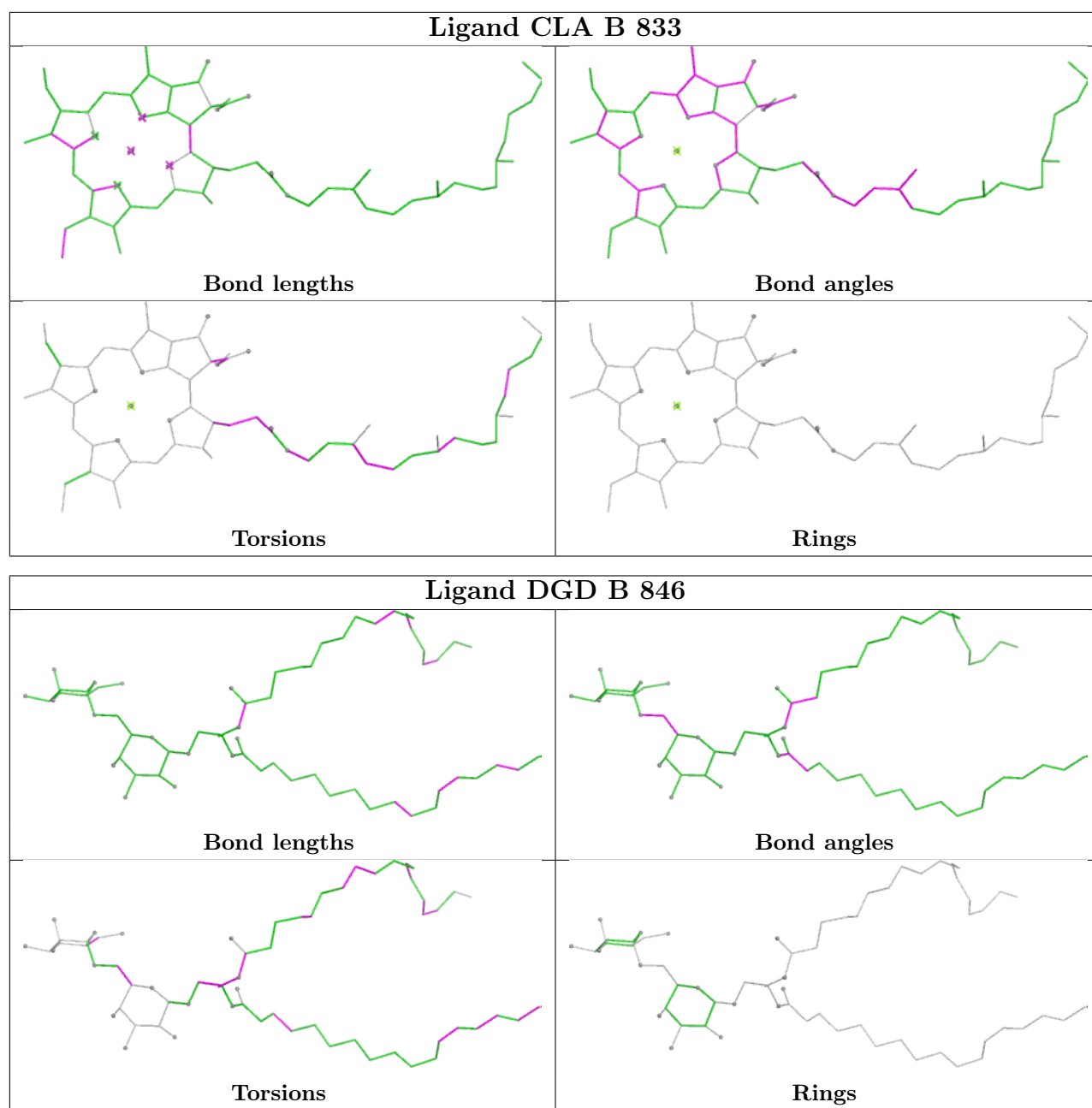
Ligand CLA L 203

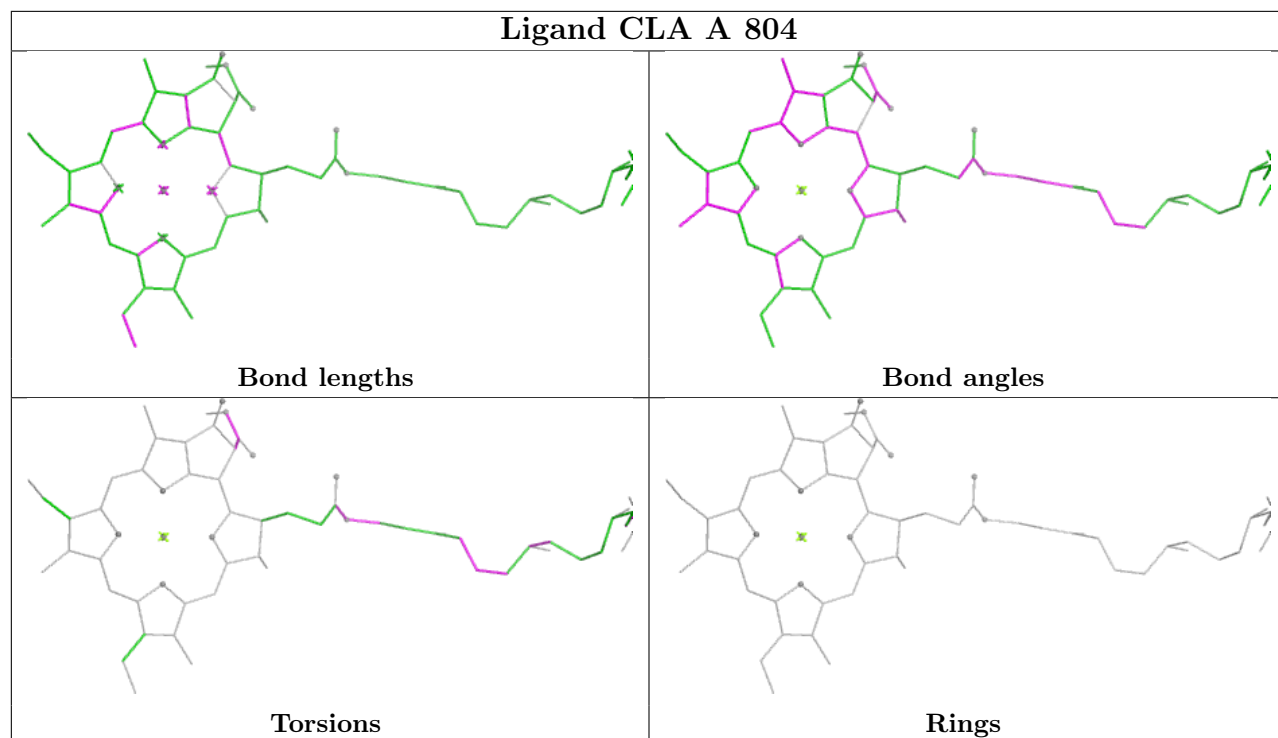
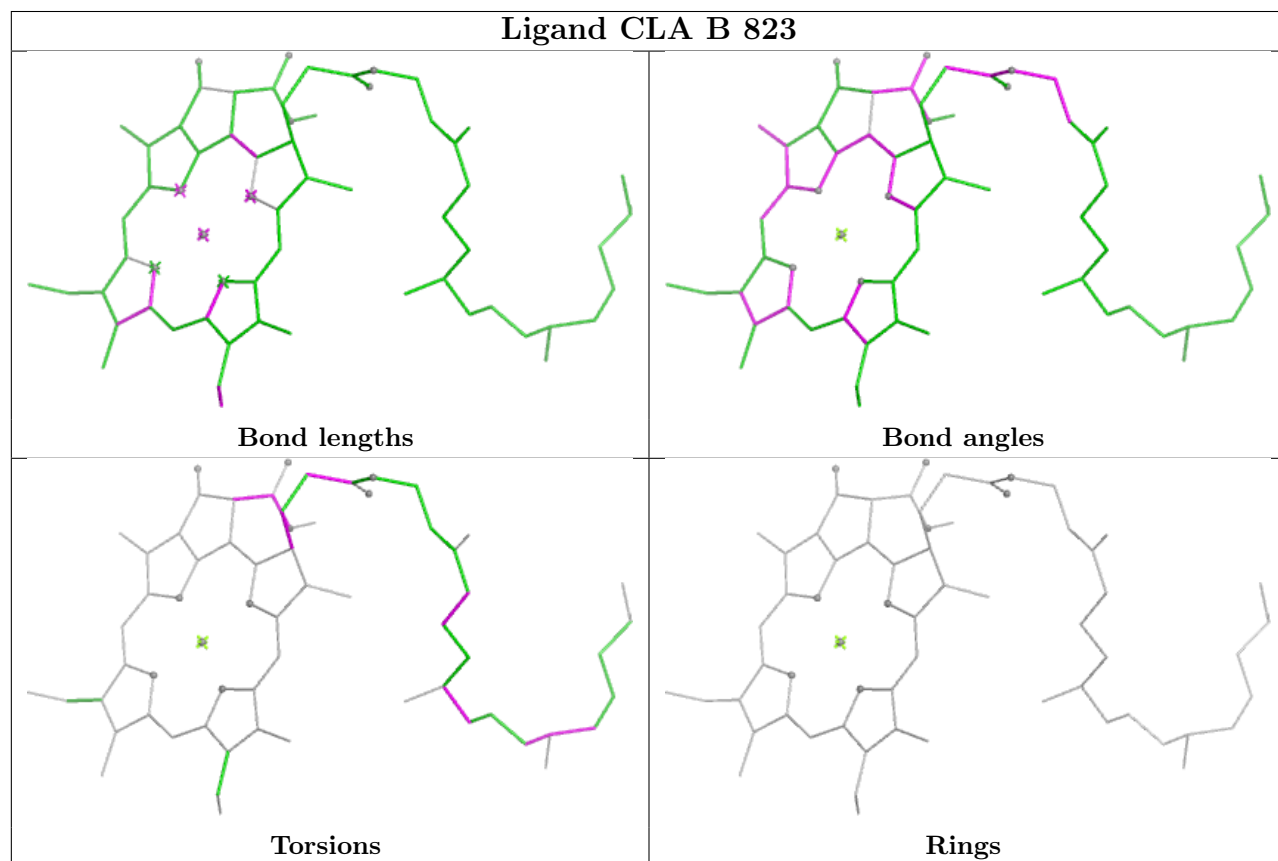


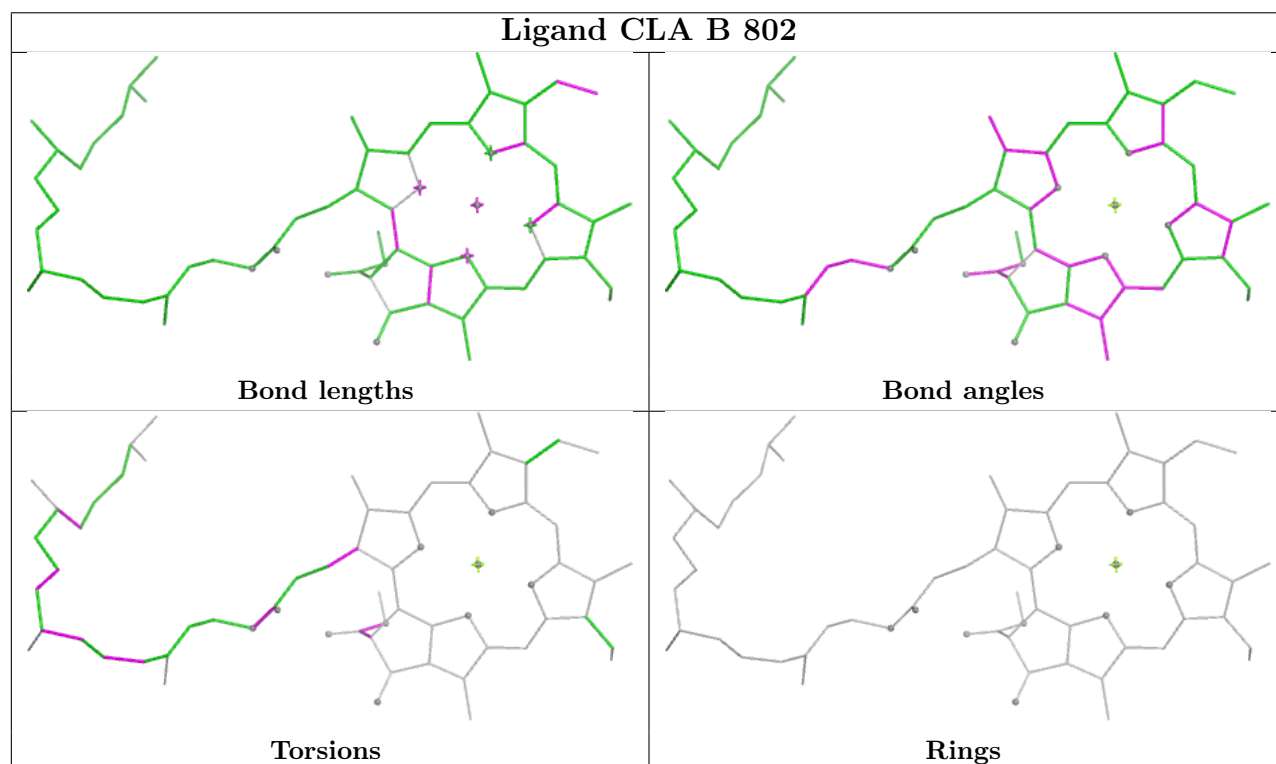
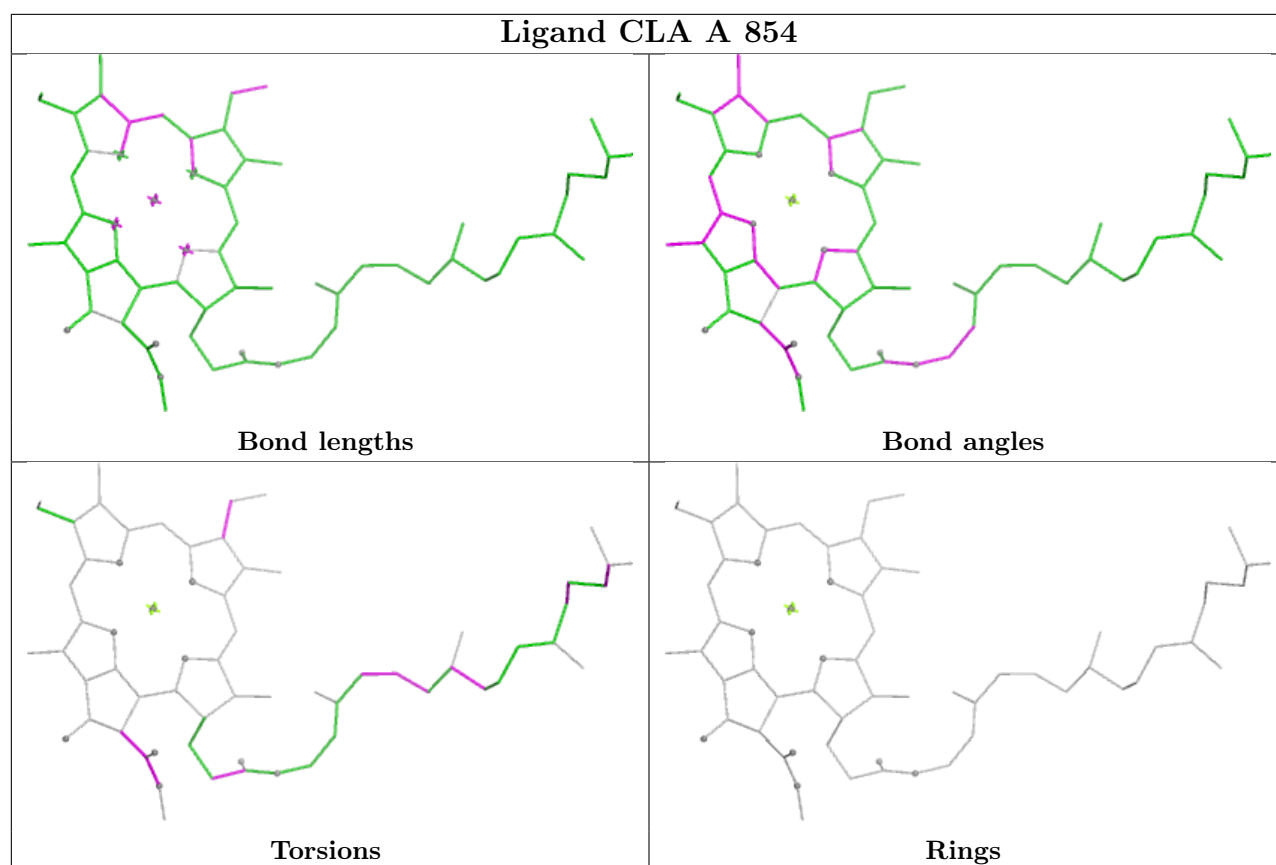


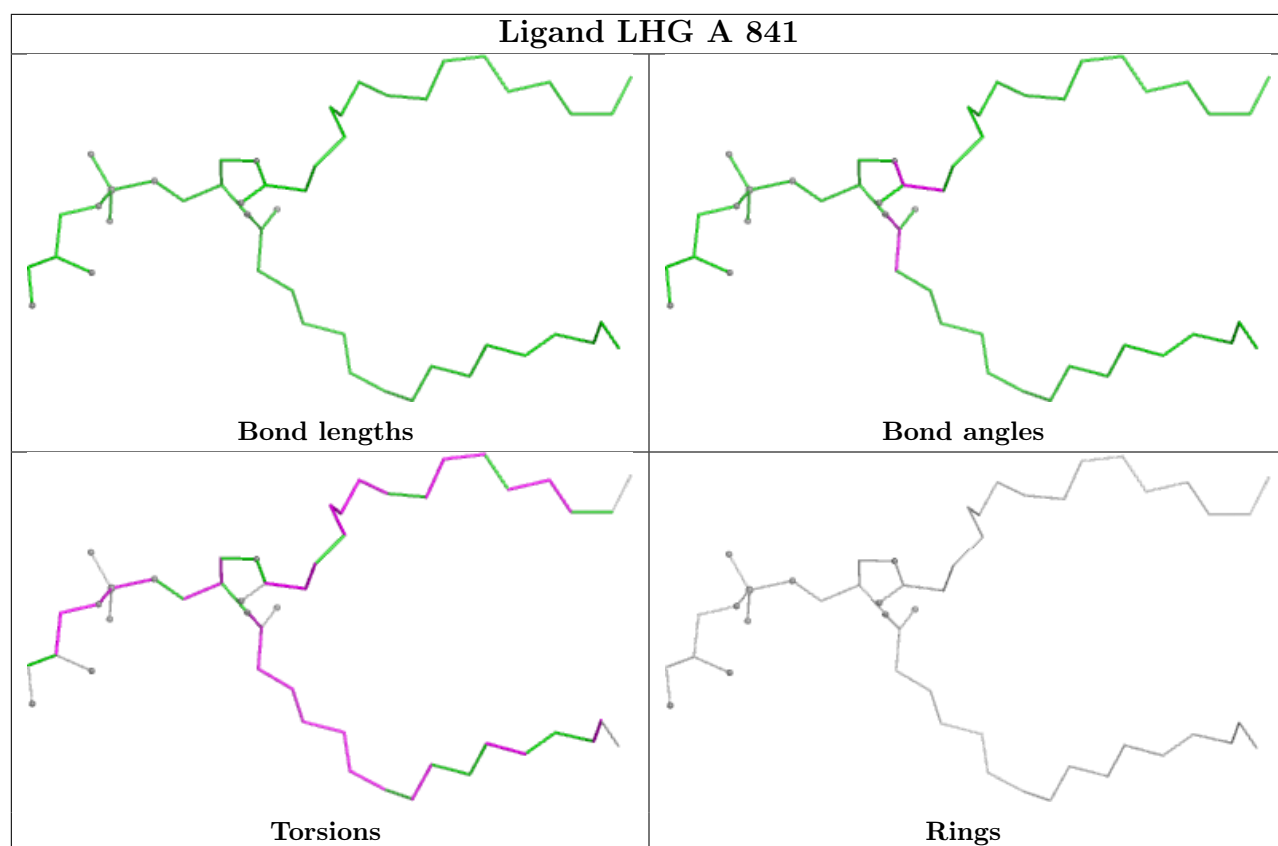




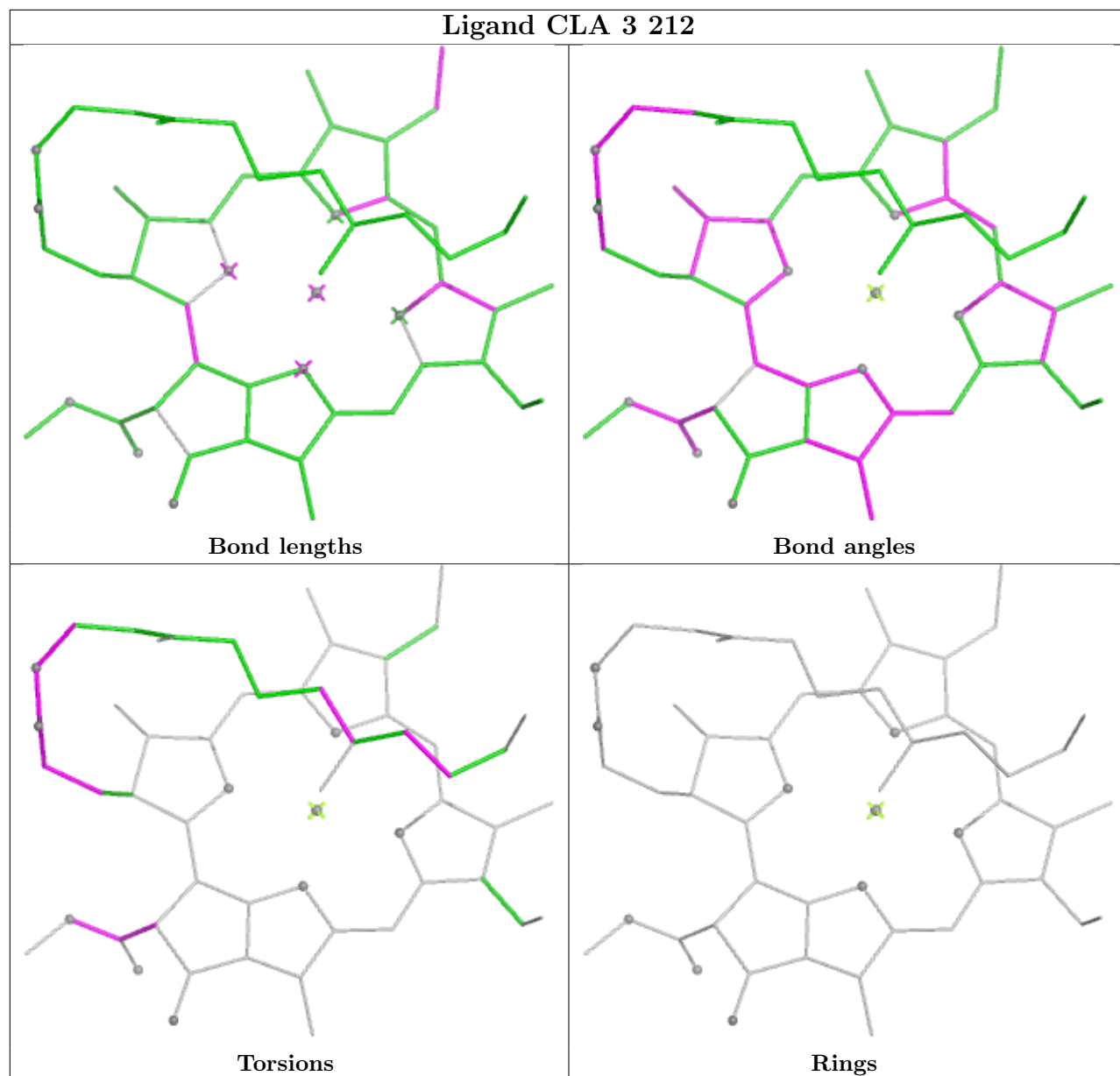


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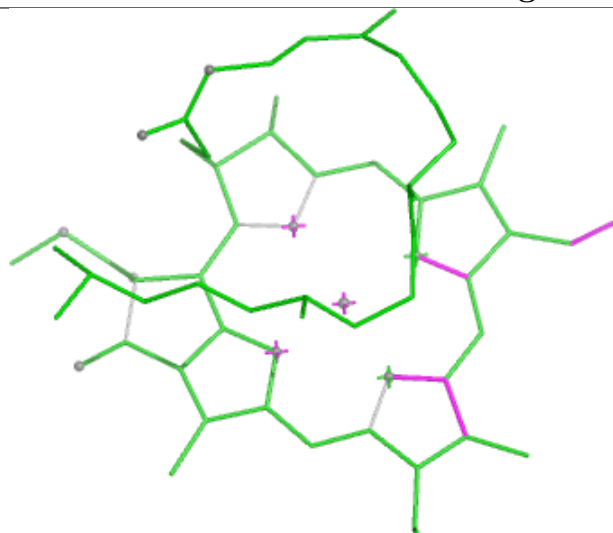




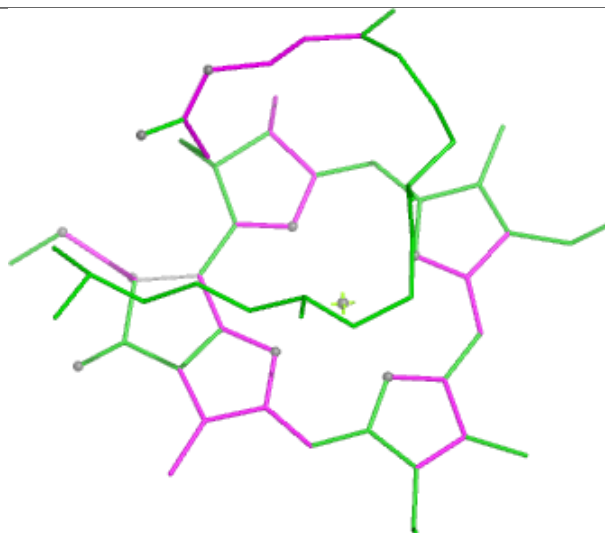
Ligand CLA 3 212



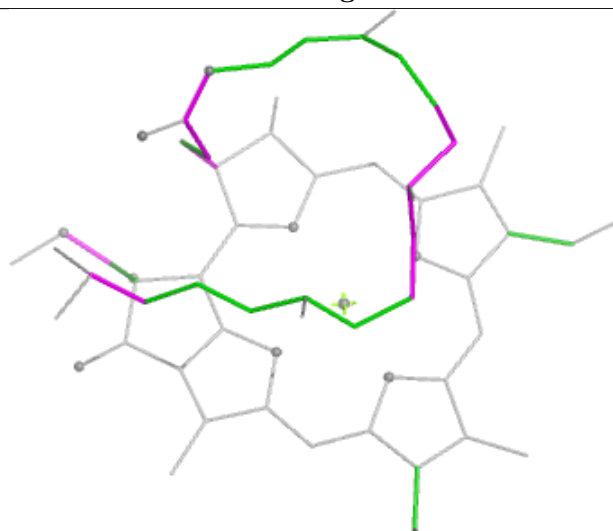
Ligand CLA 3 208



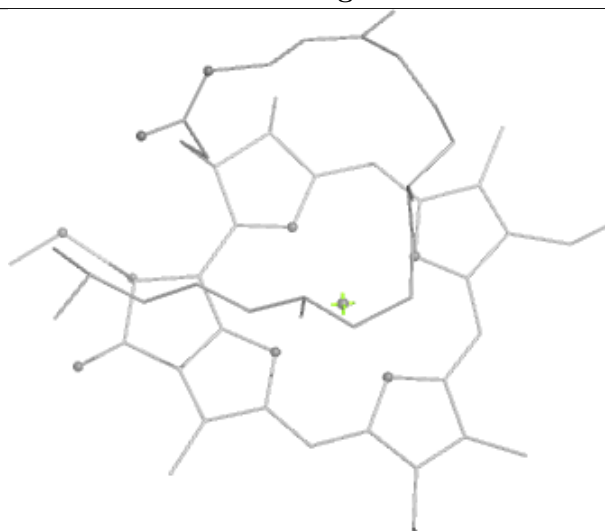
Bond lengths



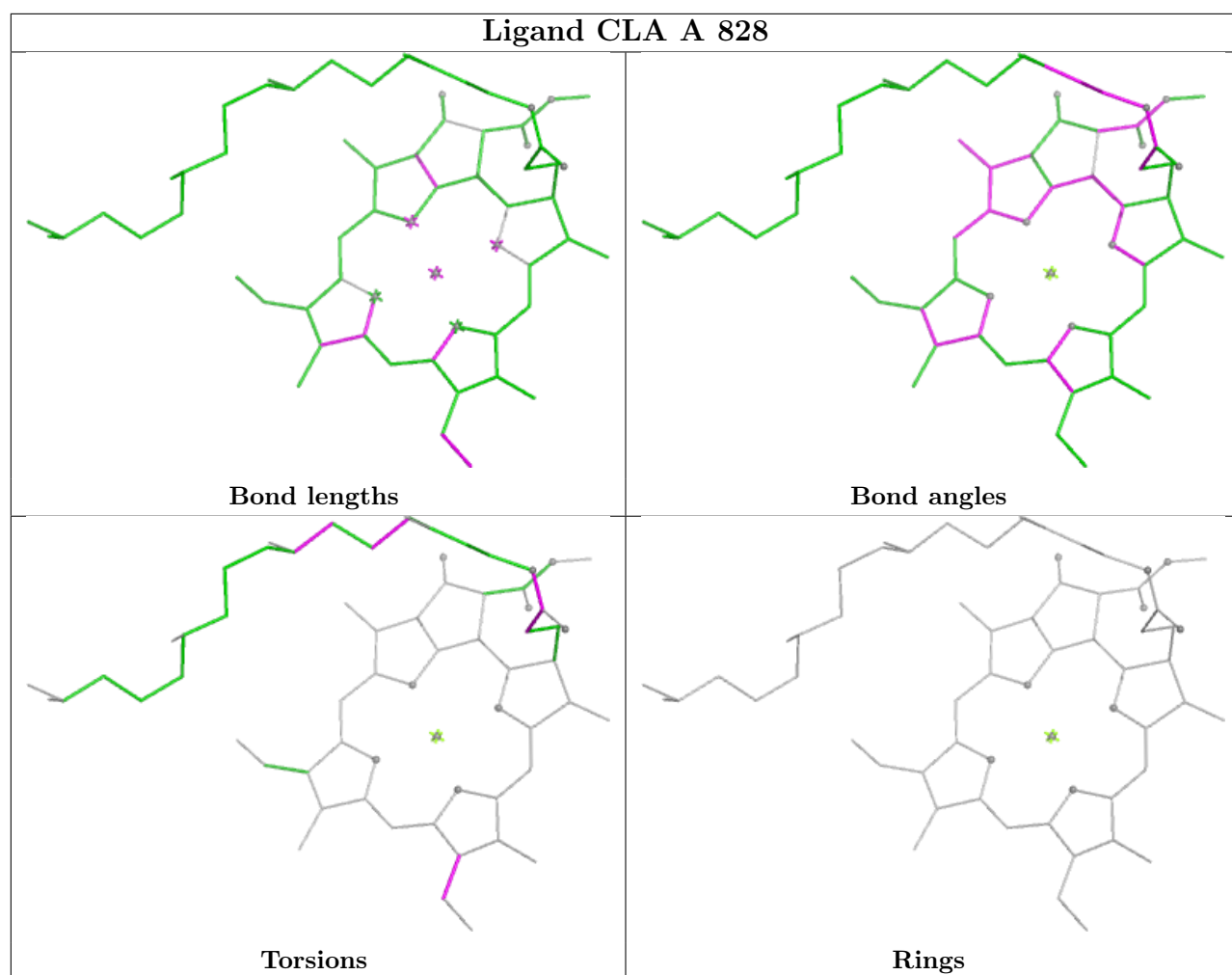
Bond angles

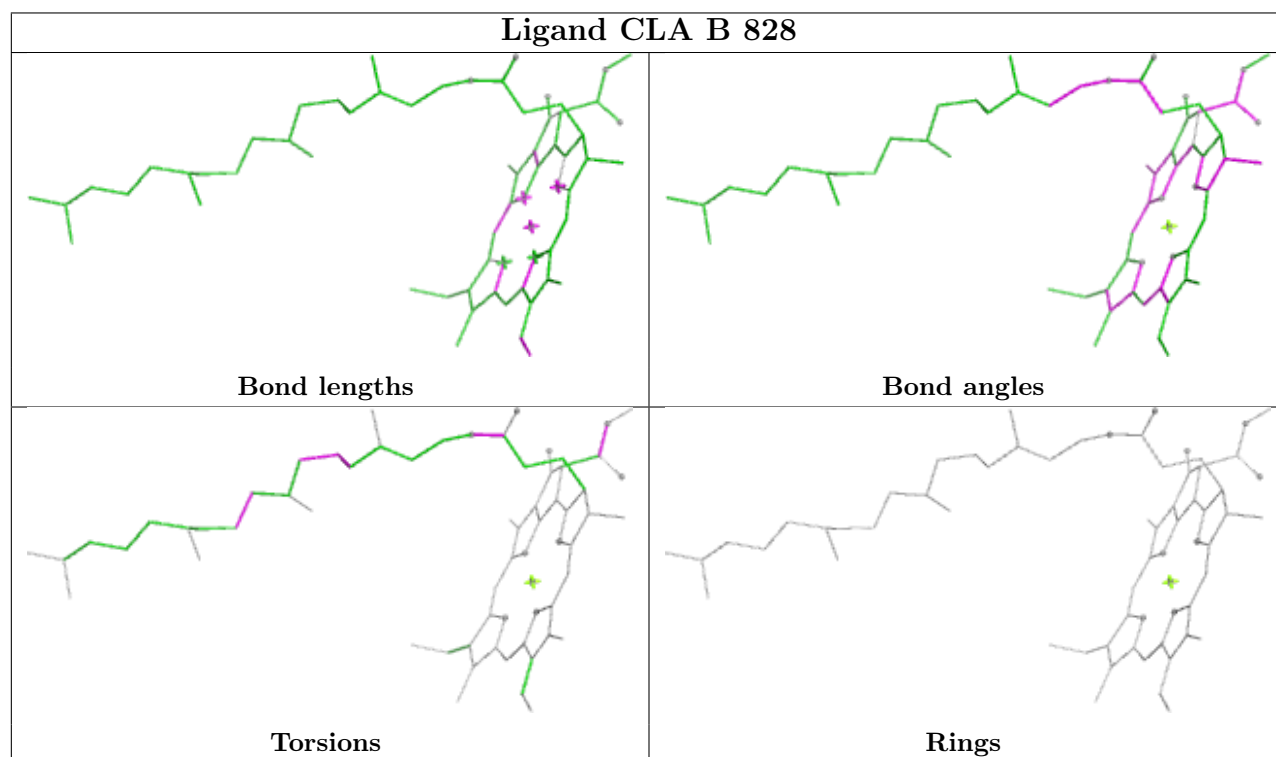
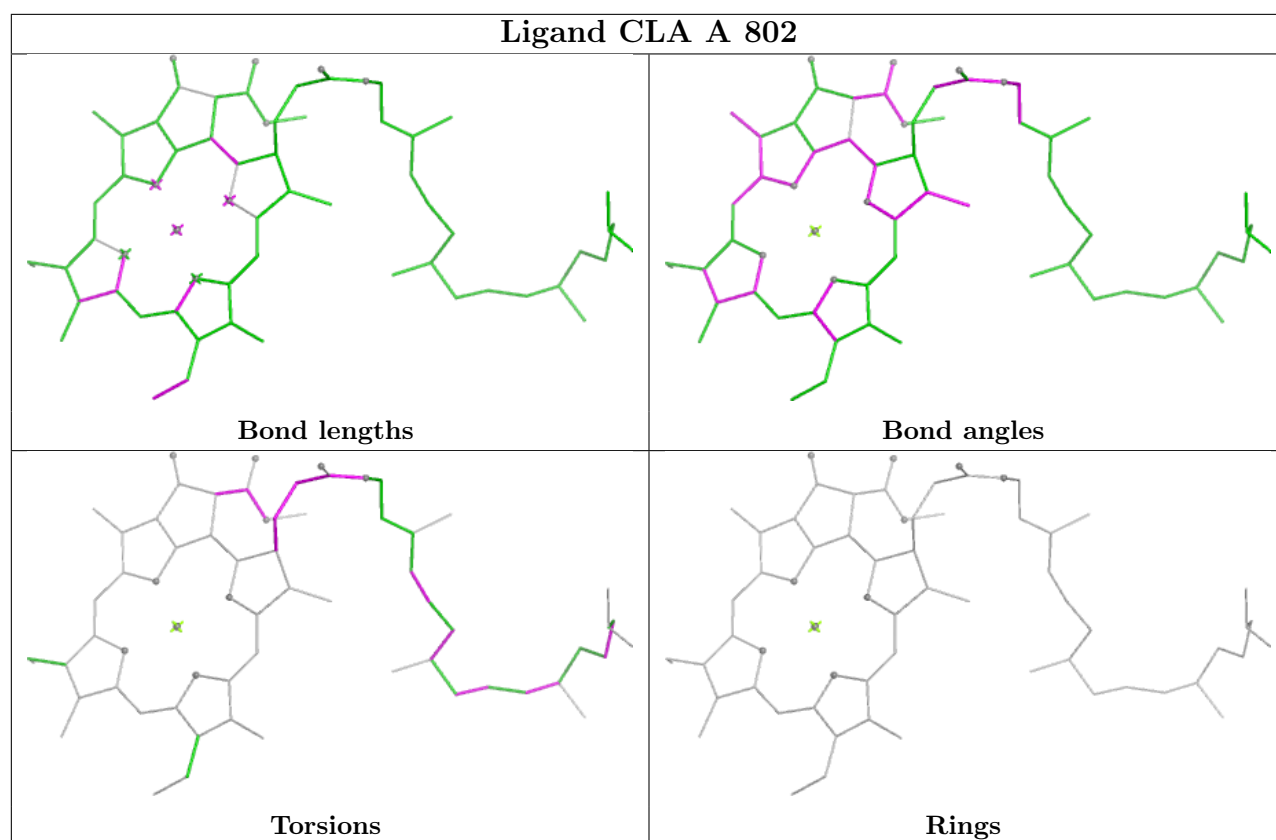


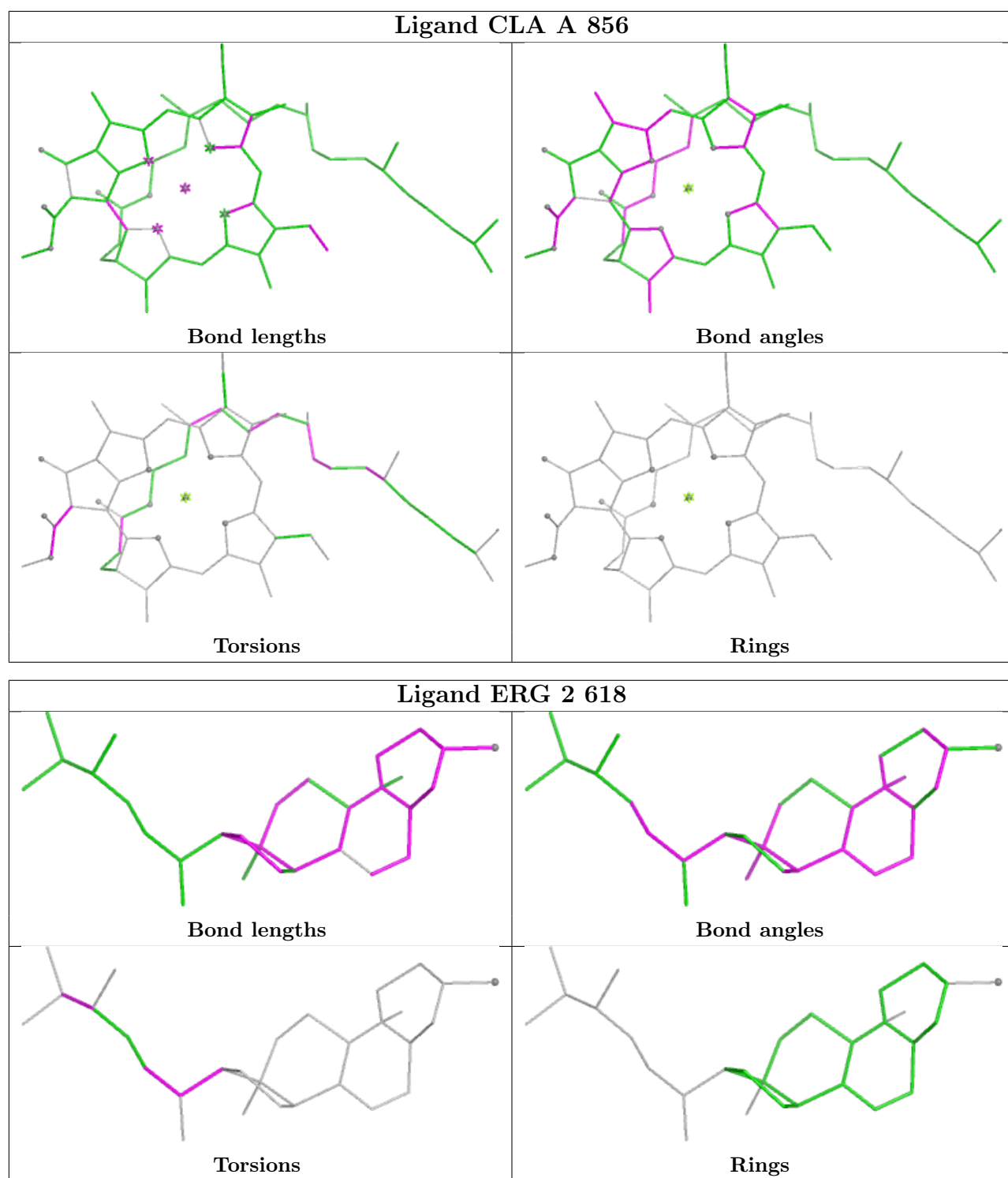
Torsions

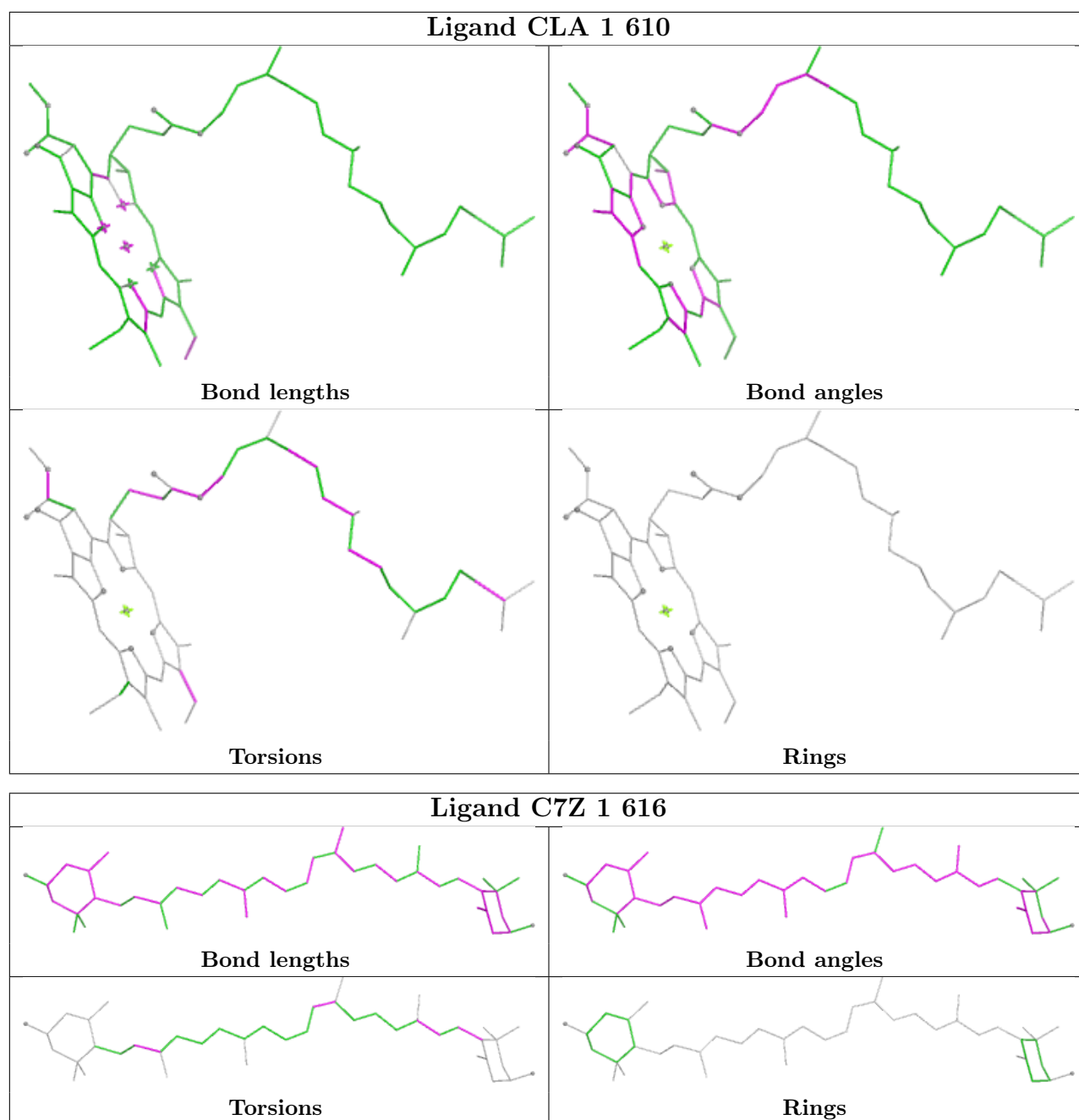


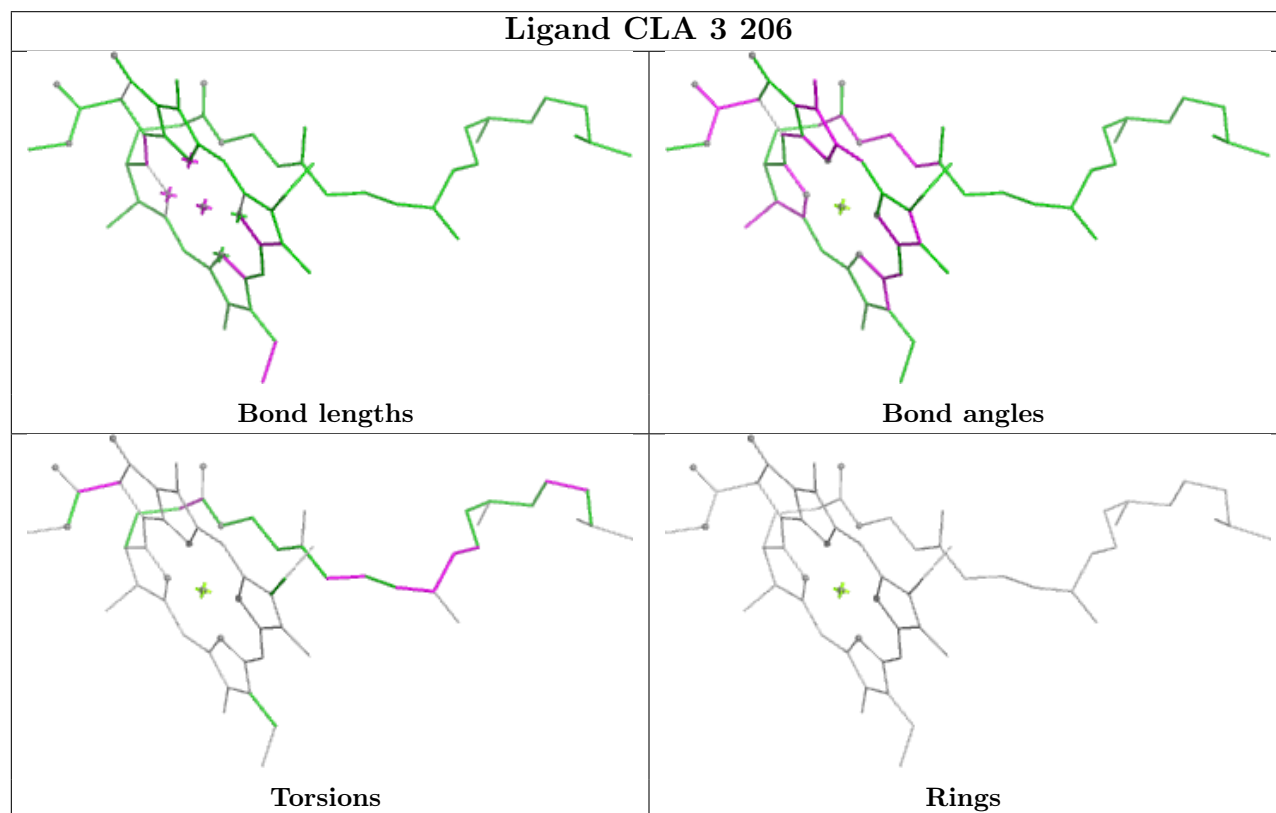
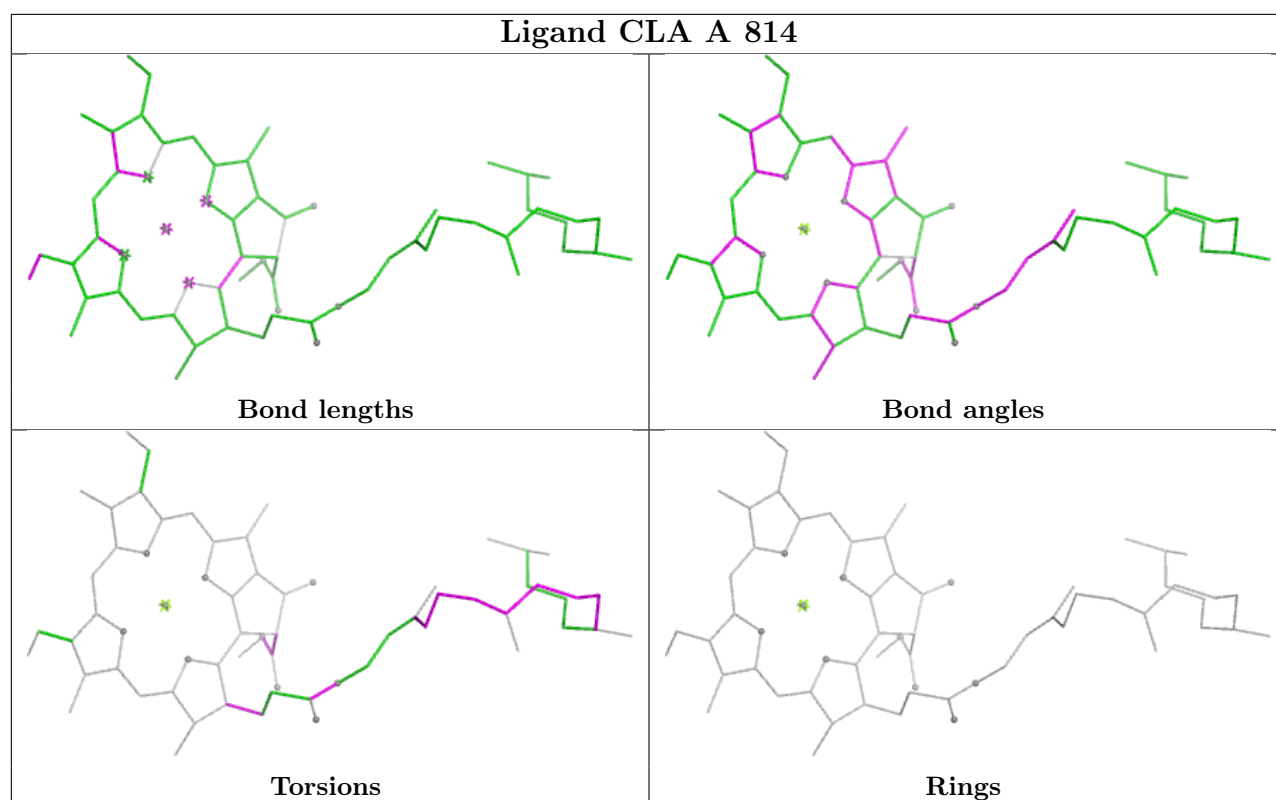
Rings



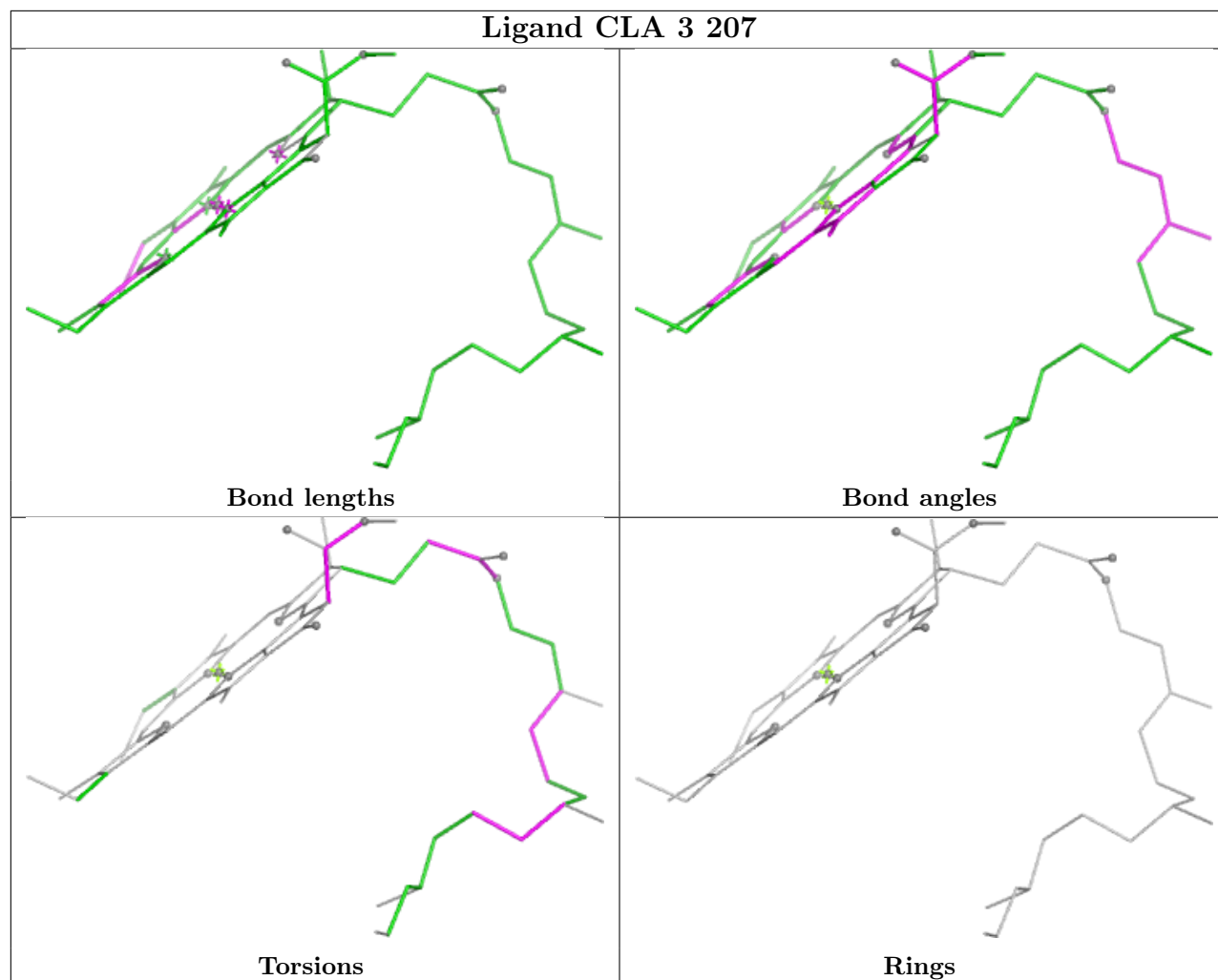




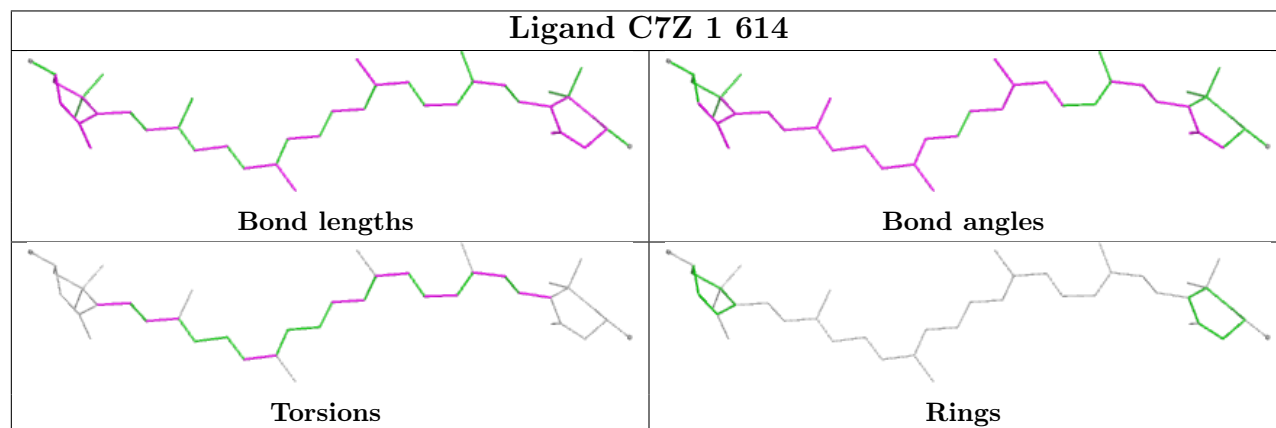


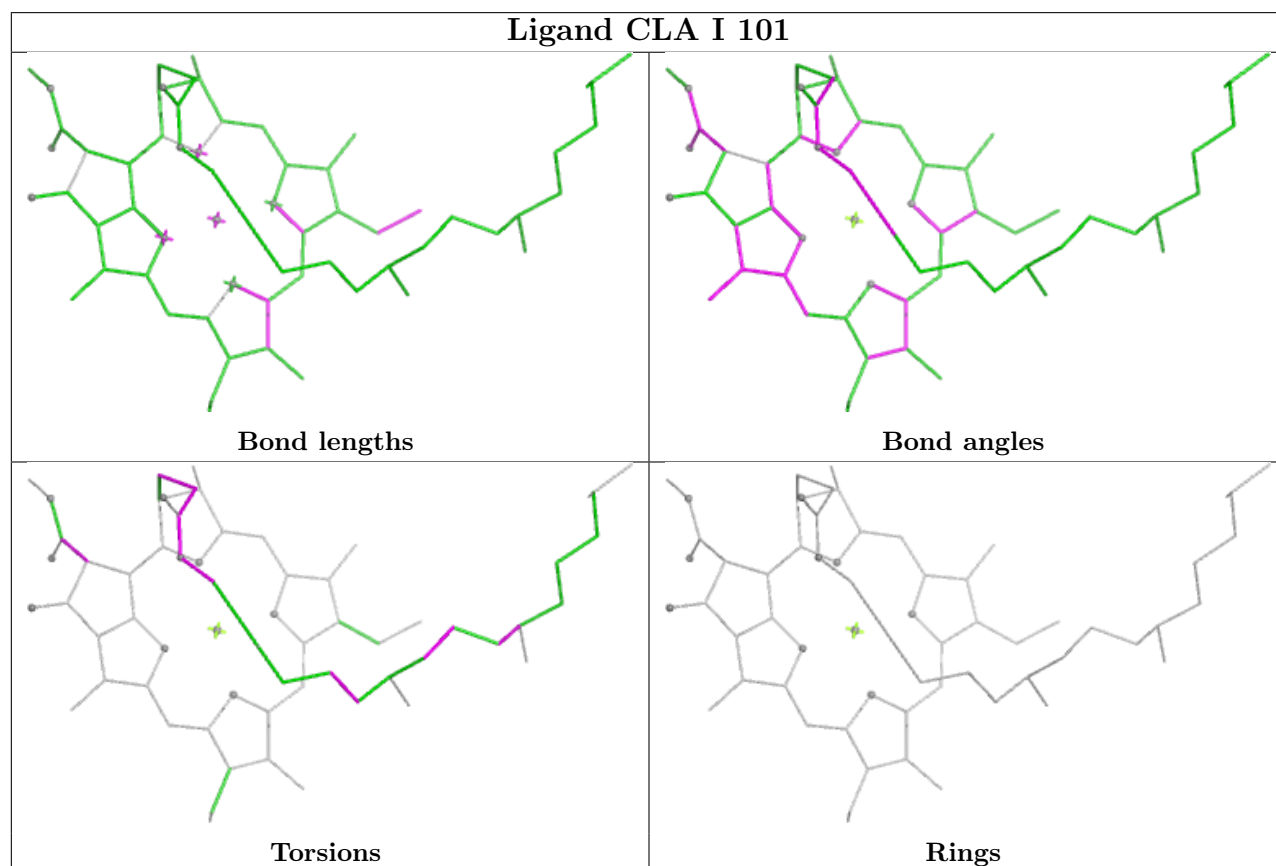
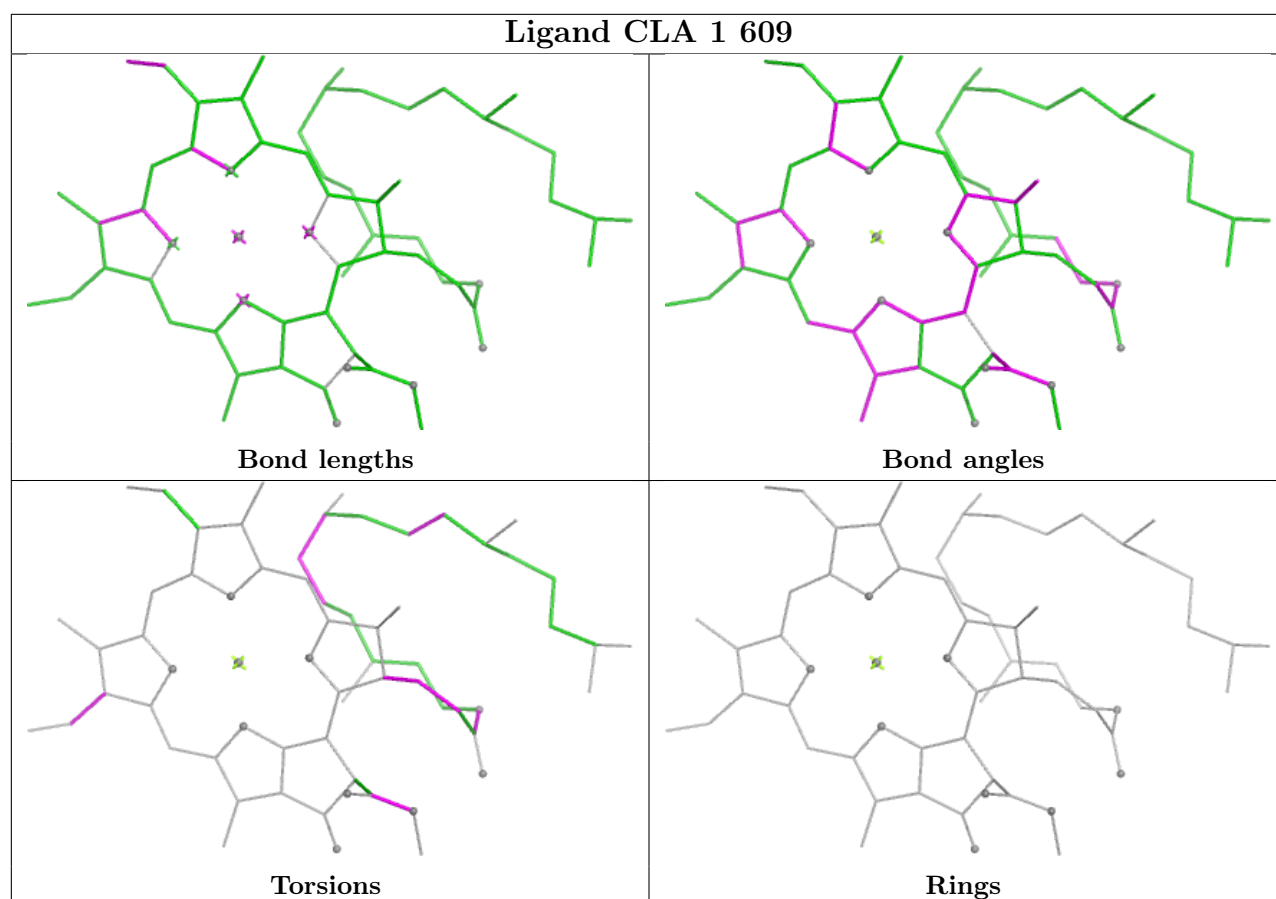


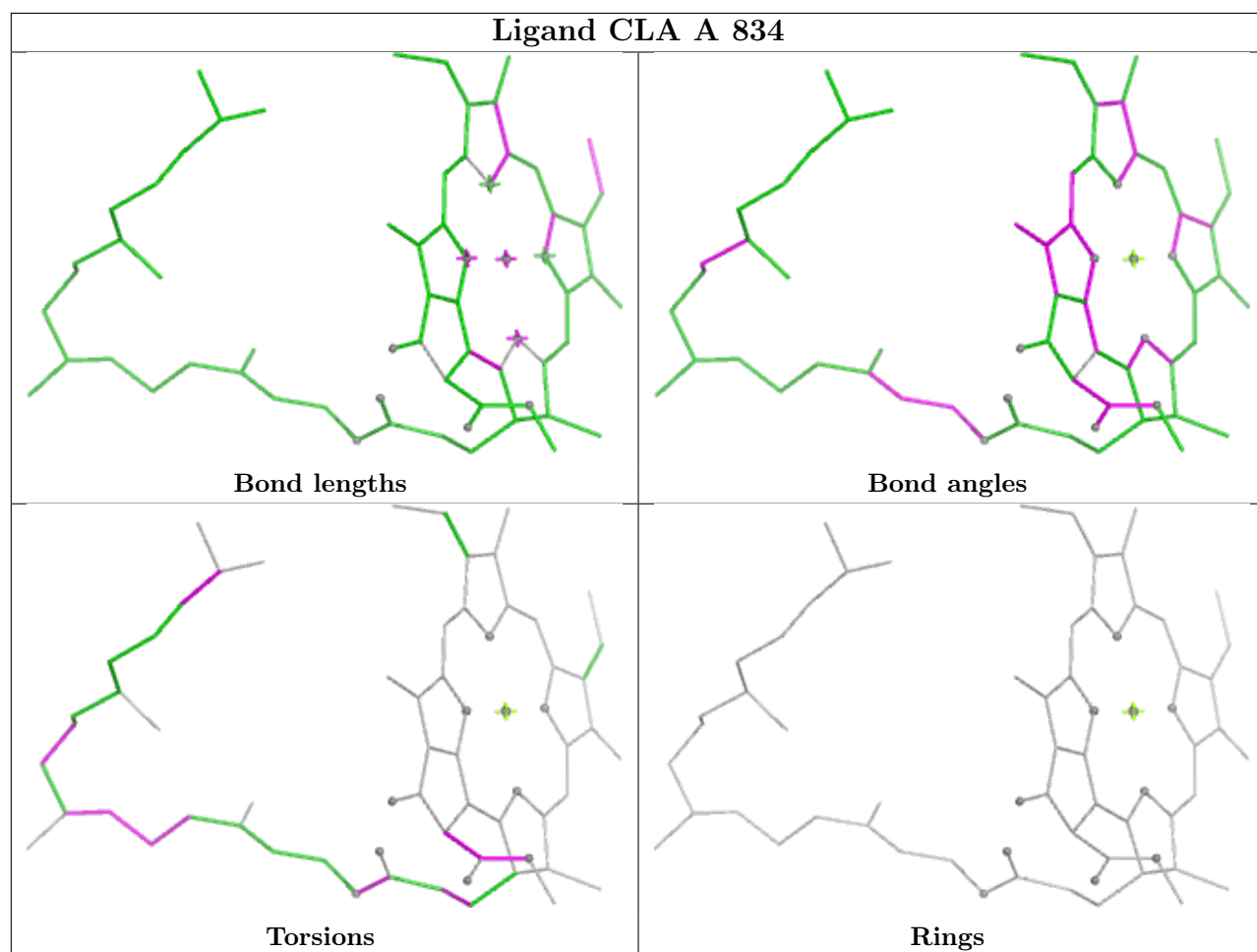
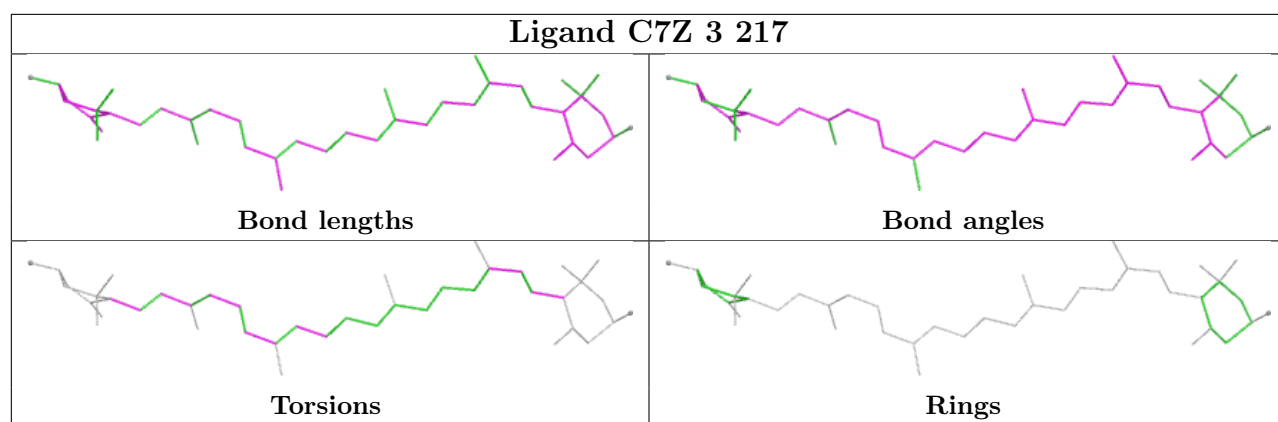
Ligand CLA 3 207

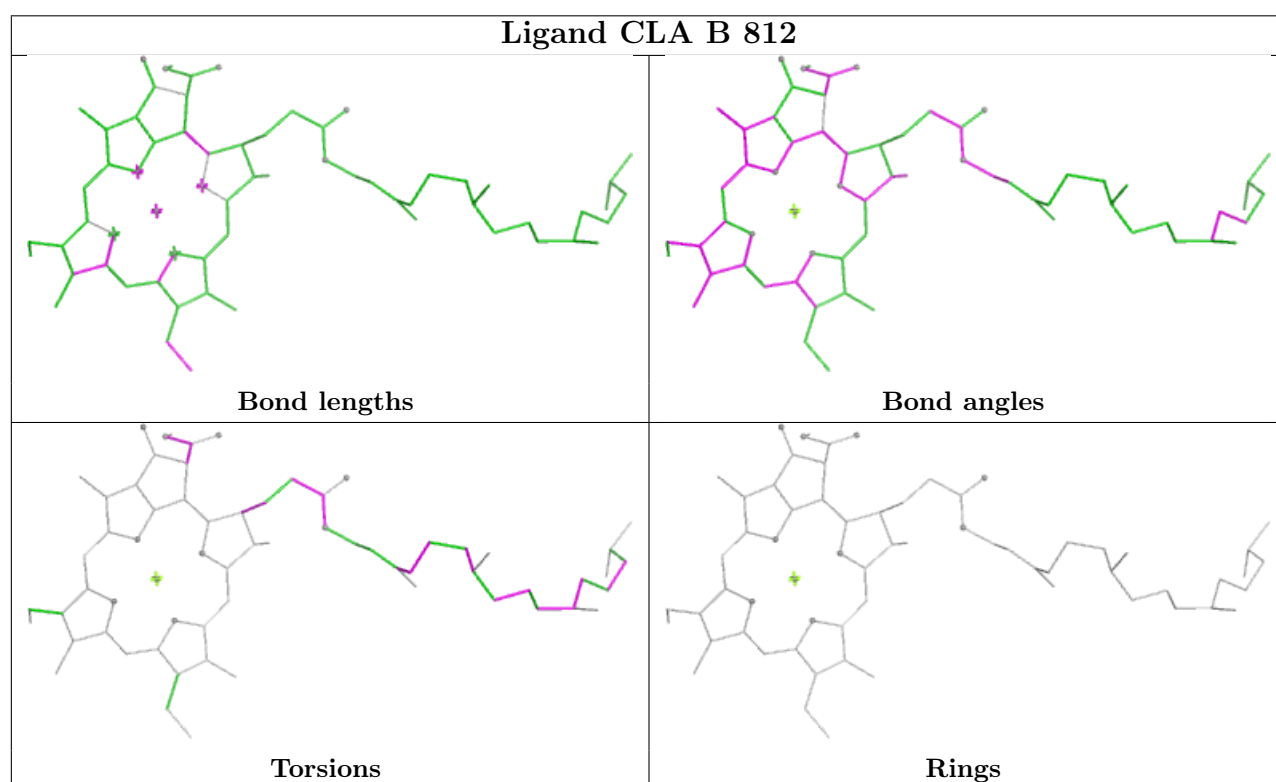
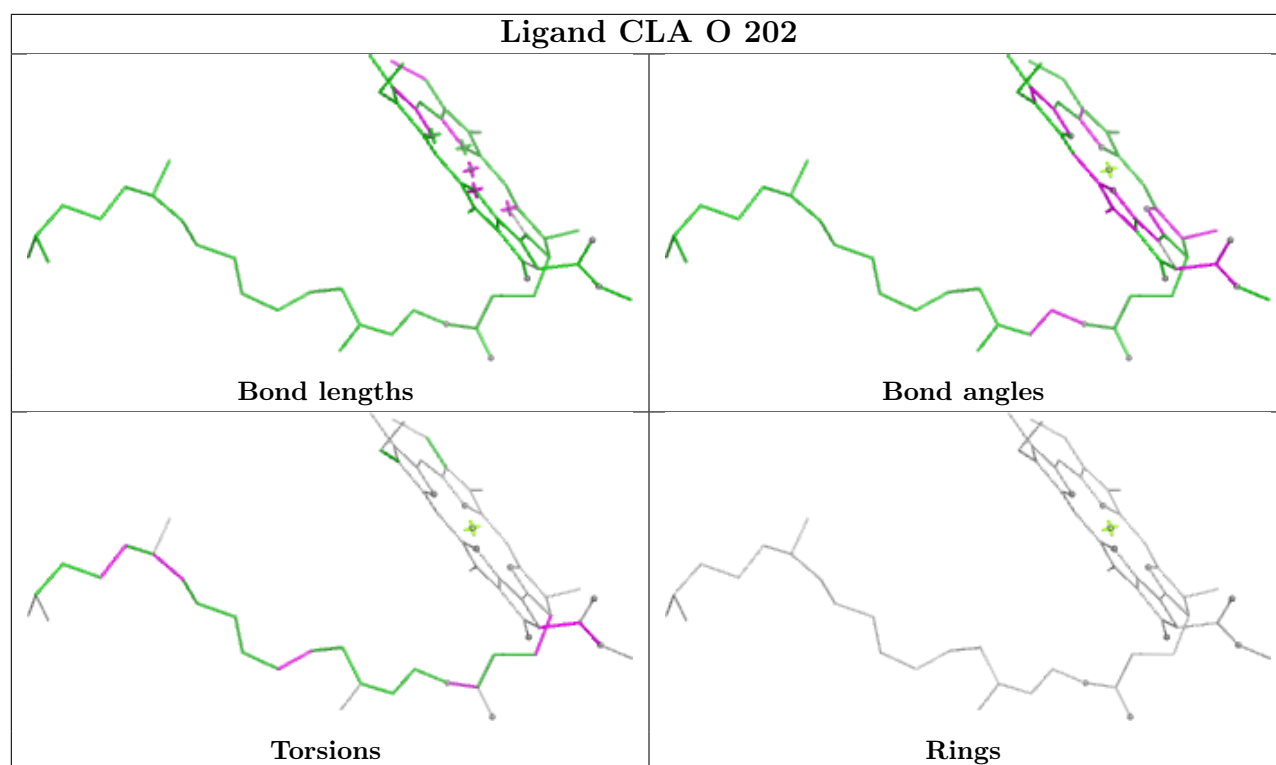


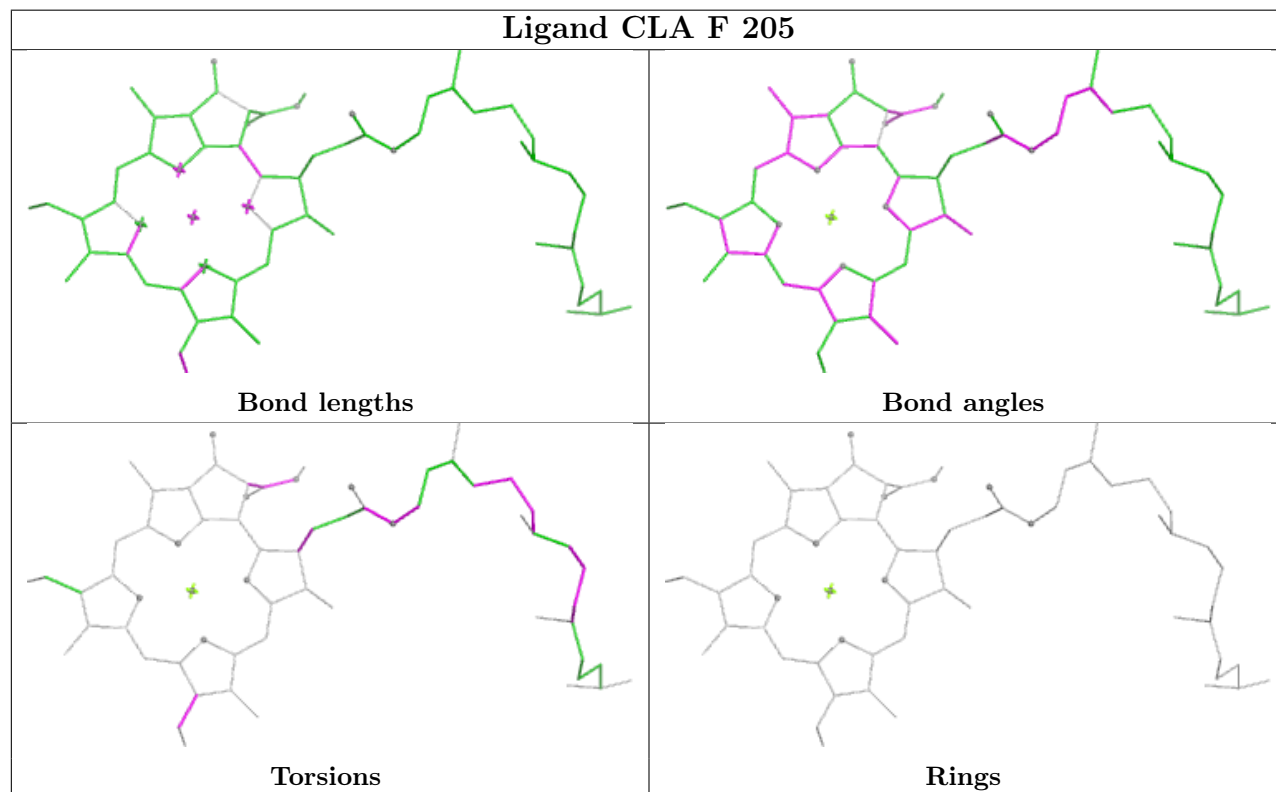
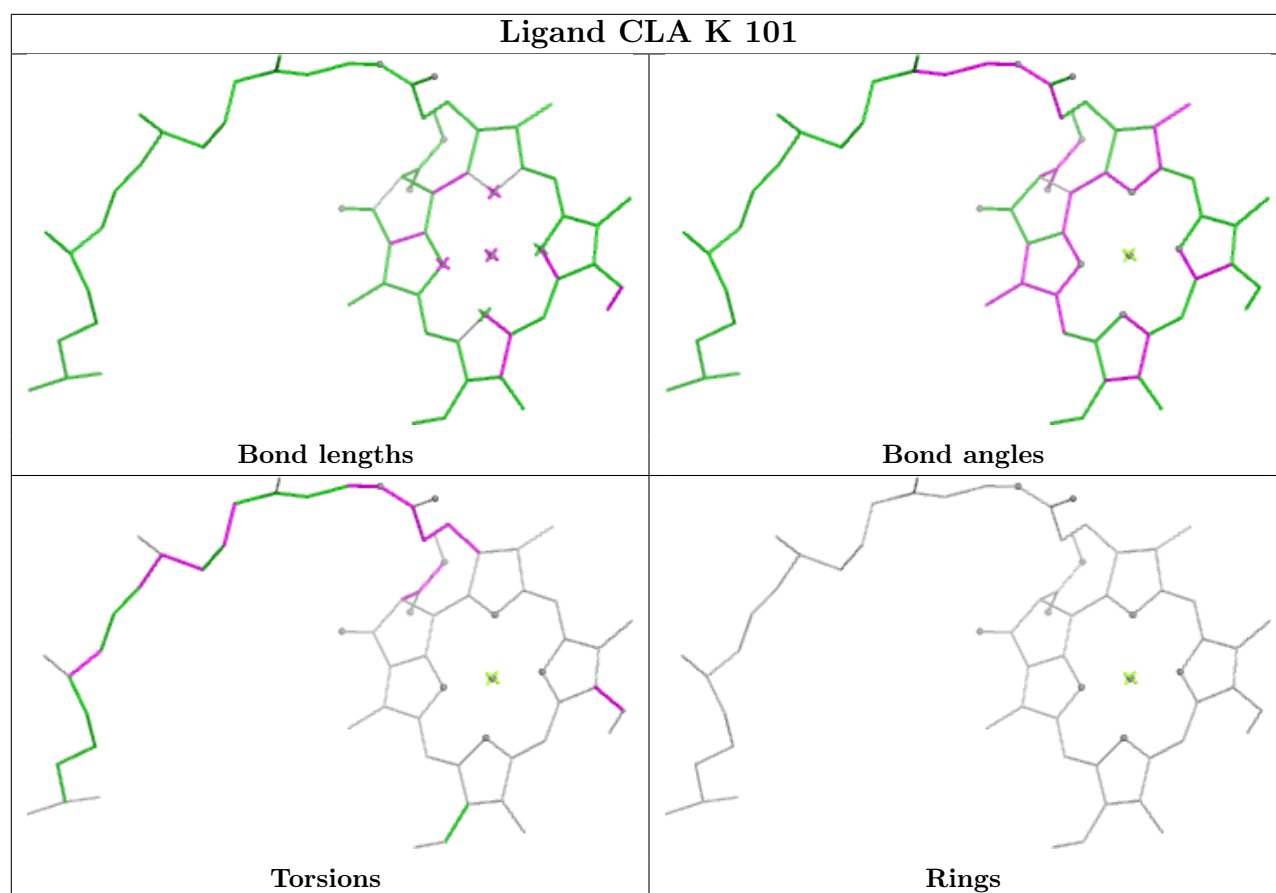
Ligand C7Z 1 614

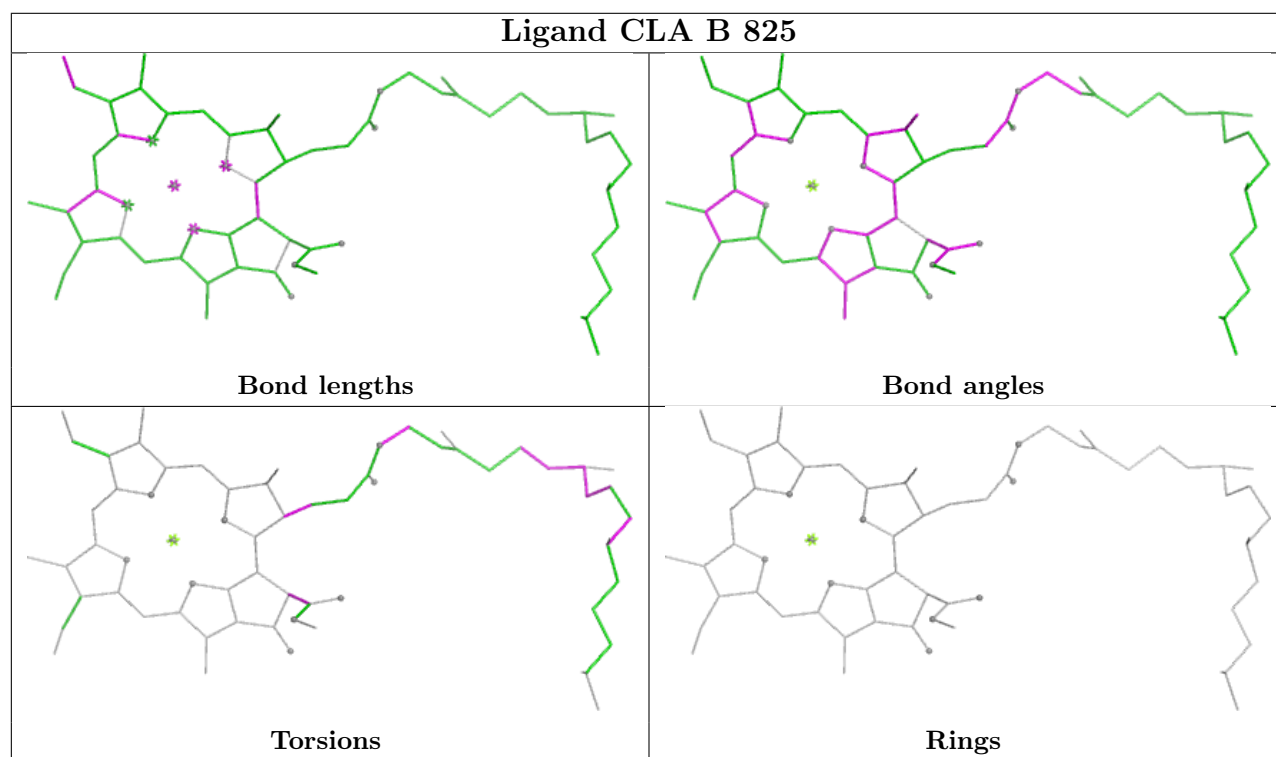
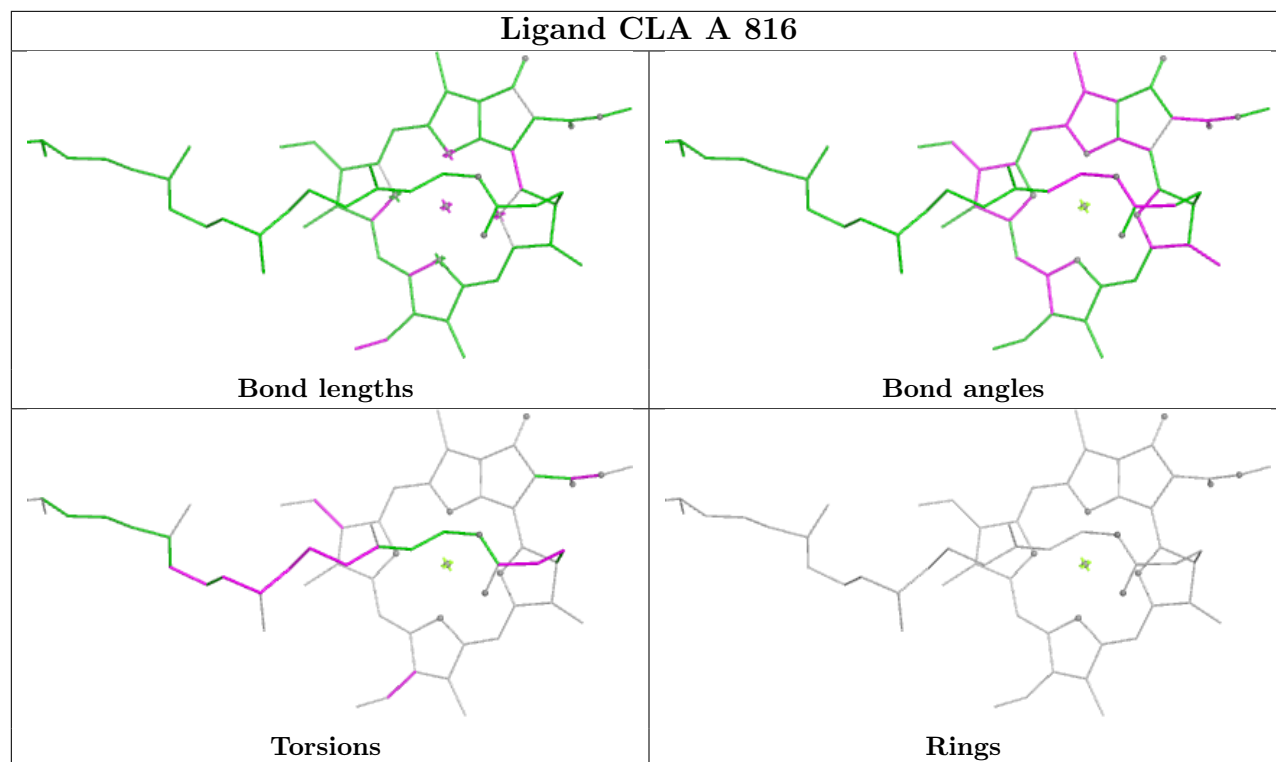


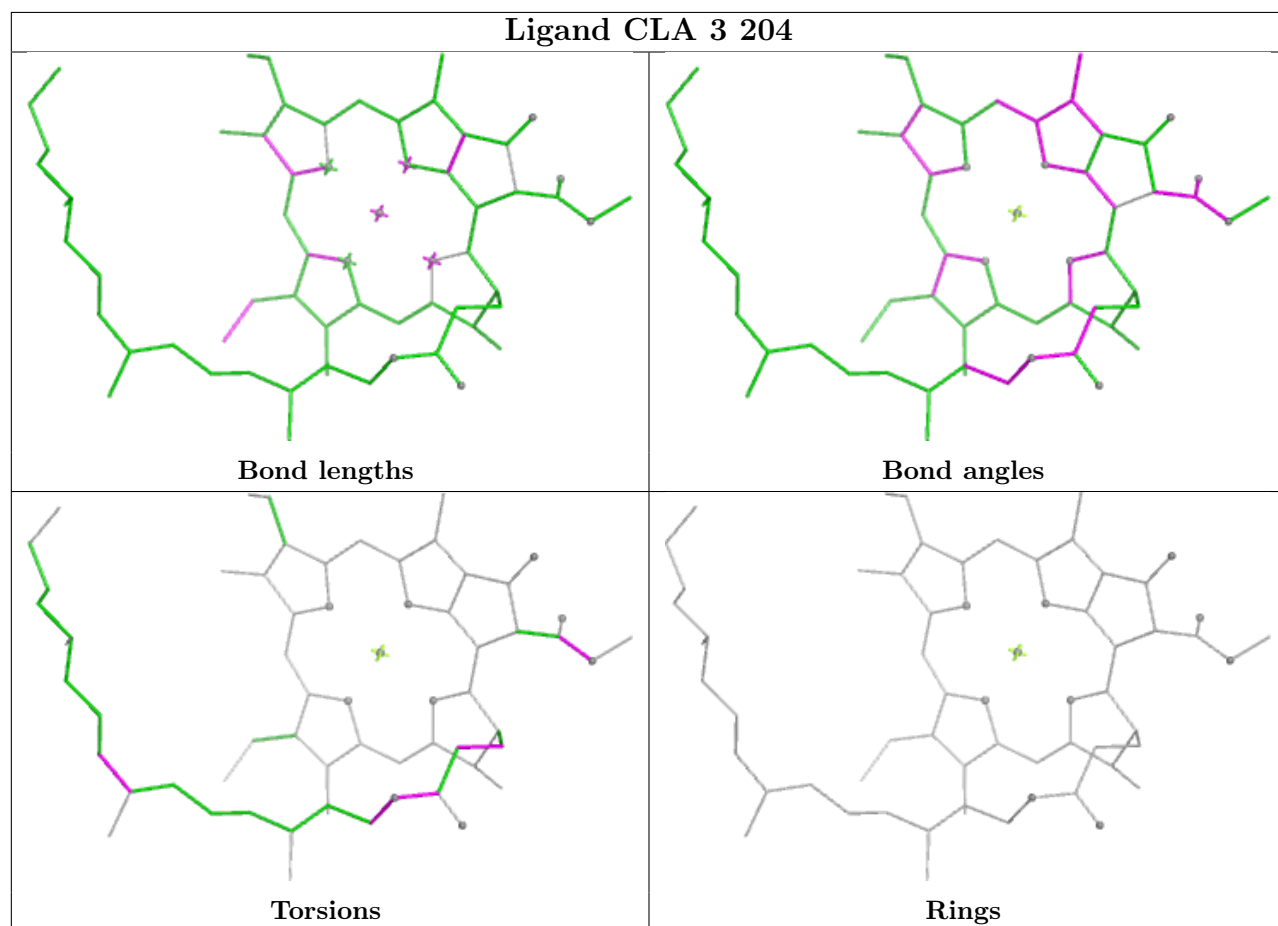
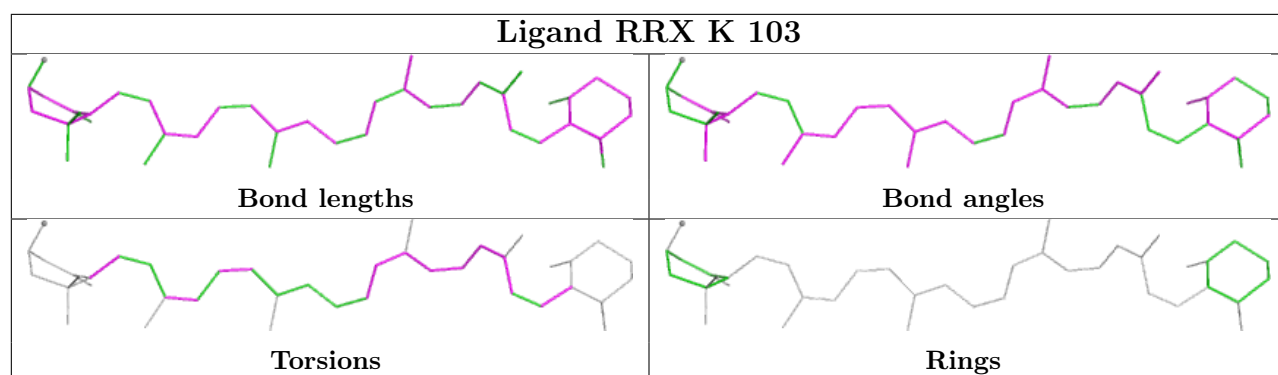


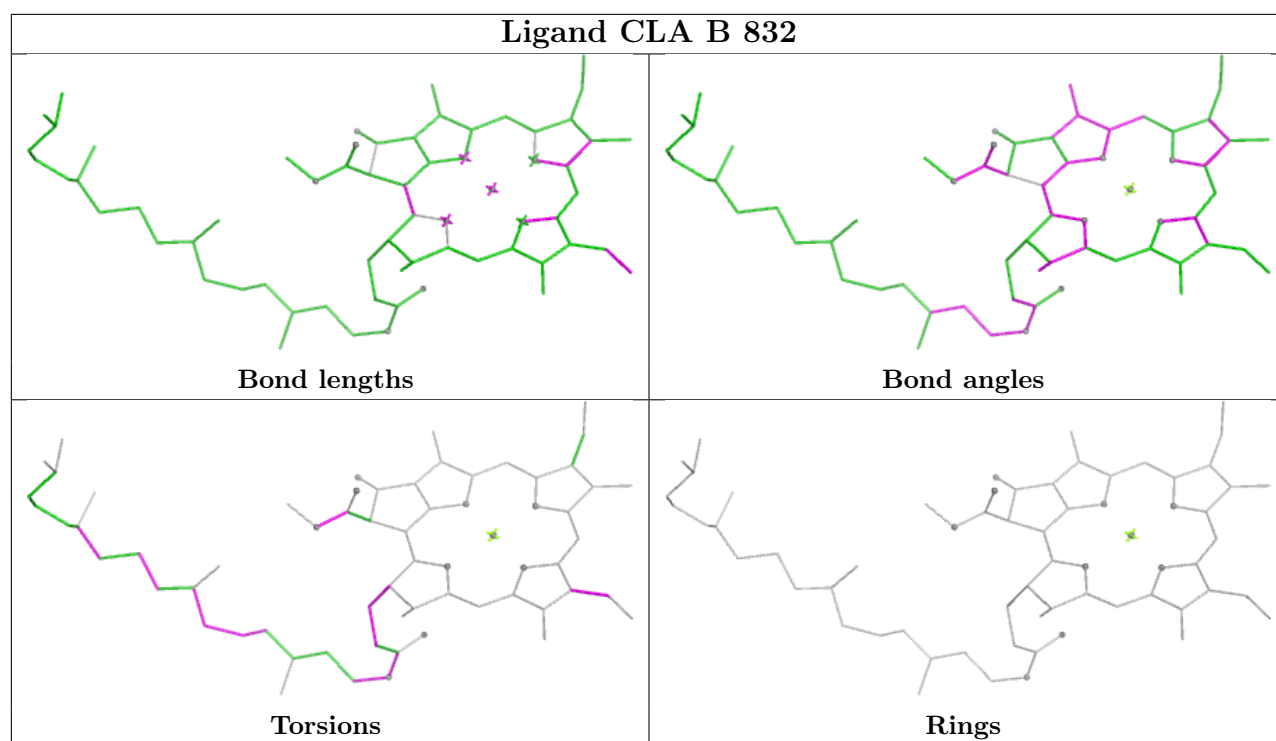




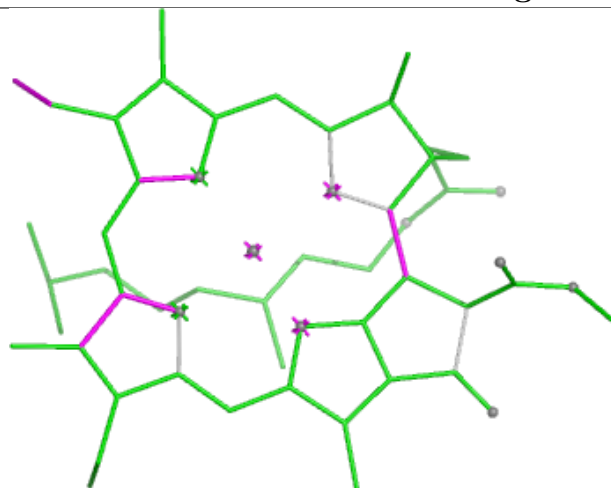




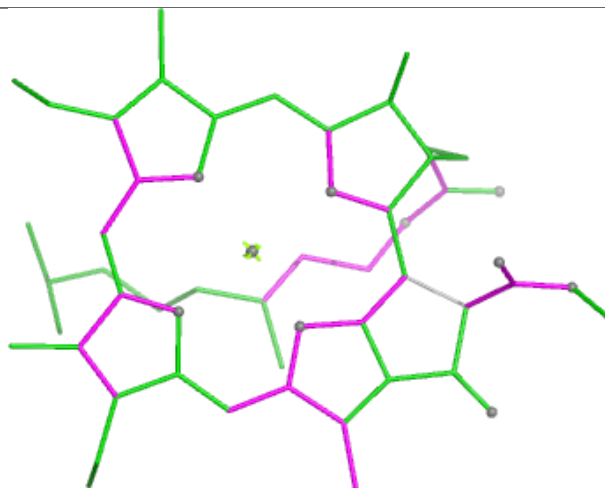




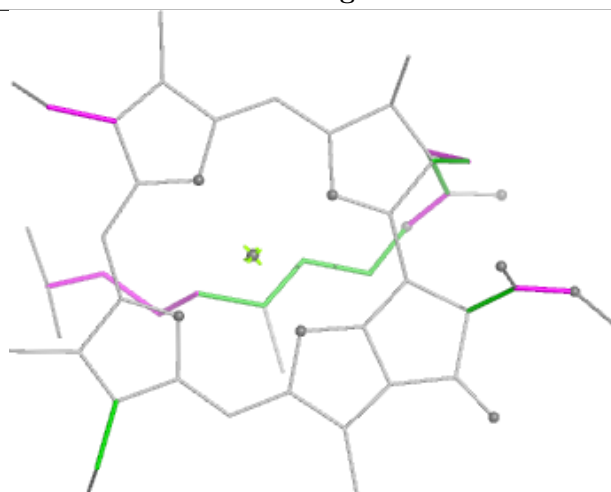
Ligand CLA B 815



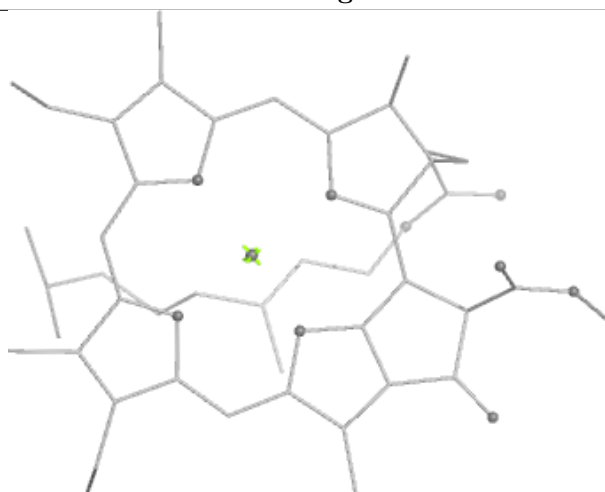
Bond lengths



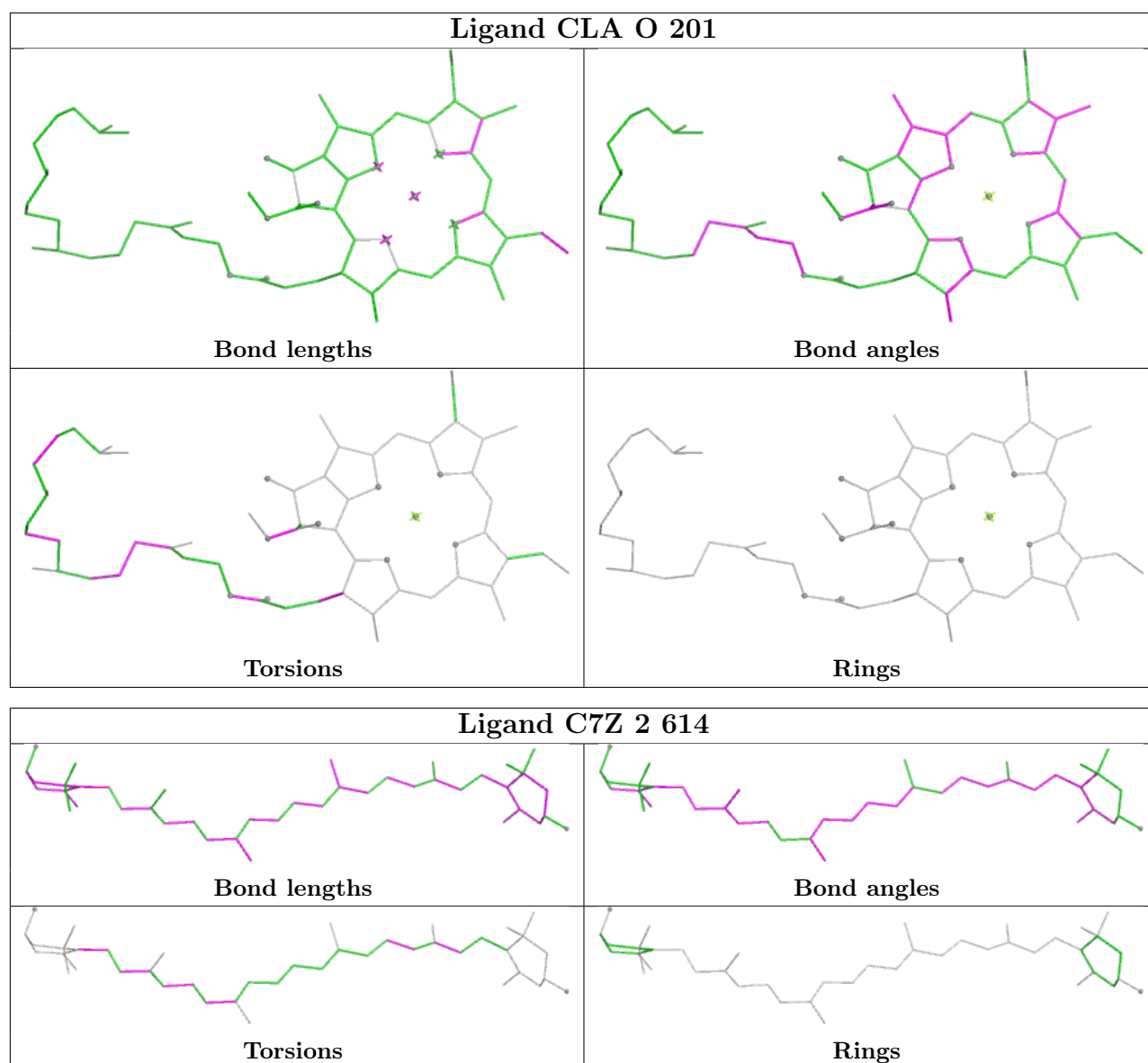
Bond angles

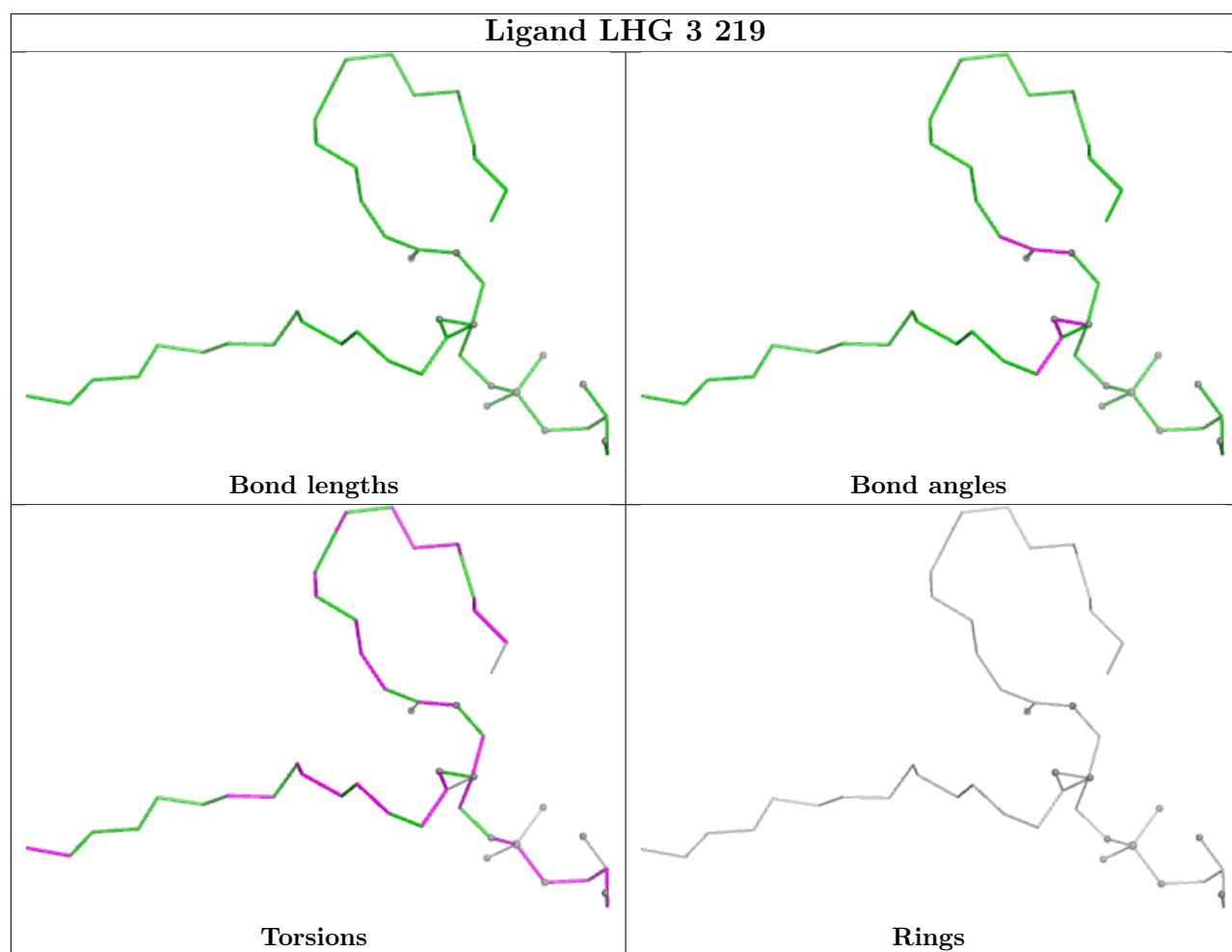


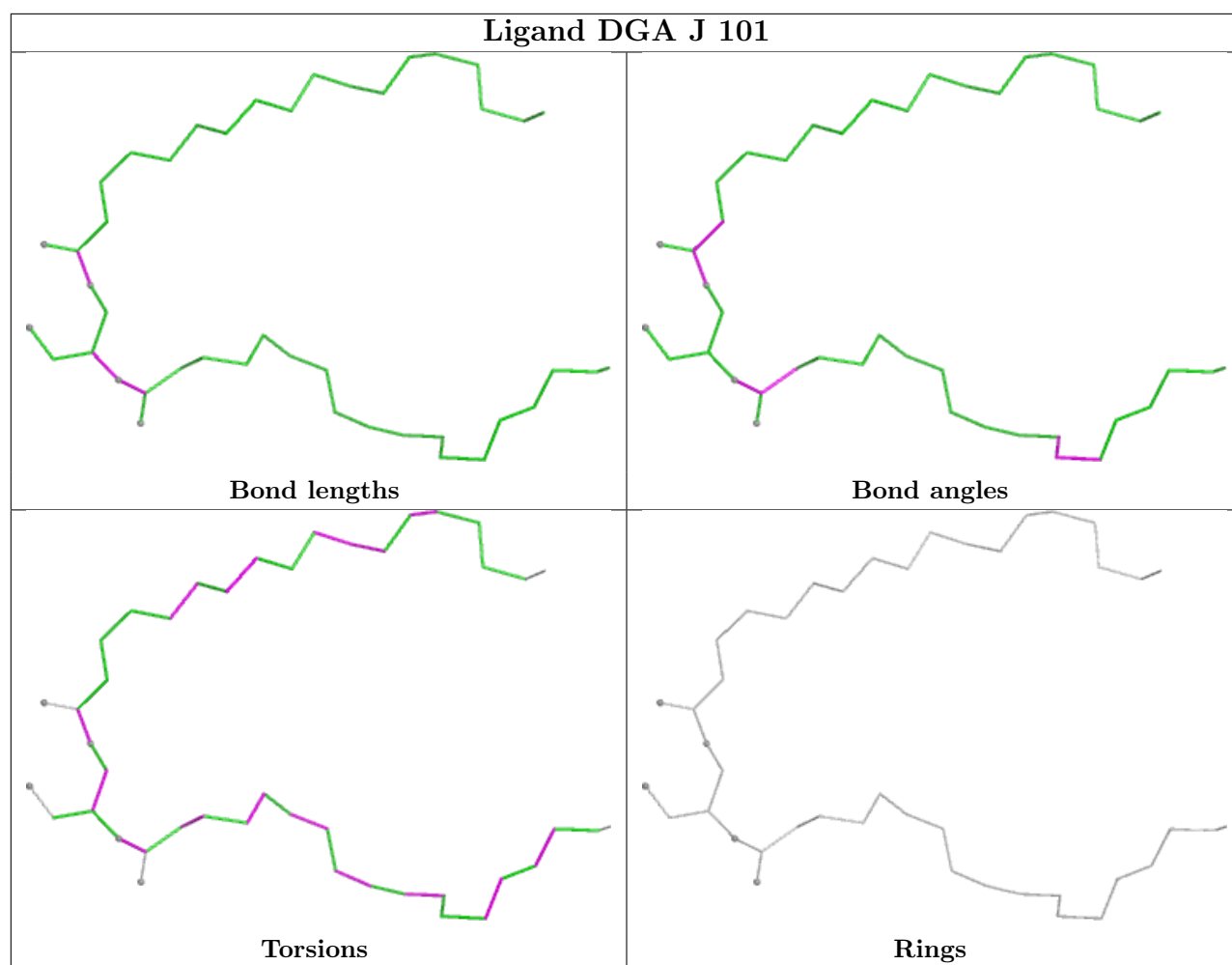
Torsions



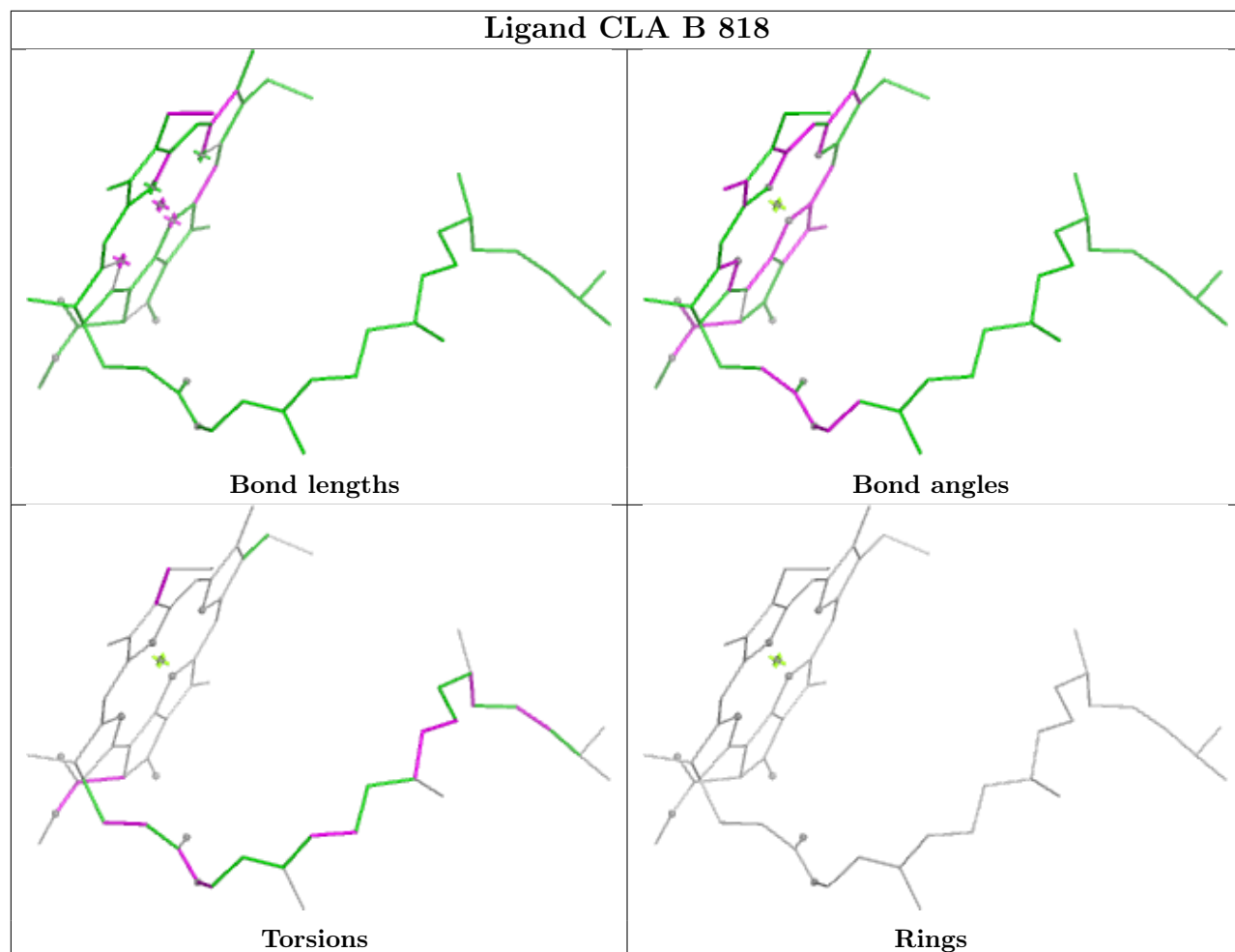
Rings



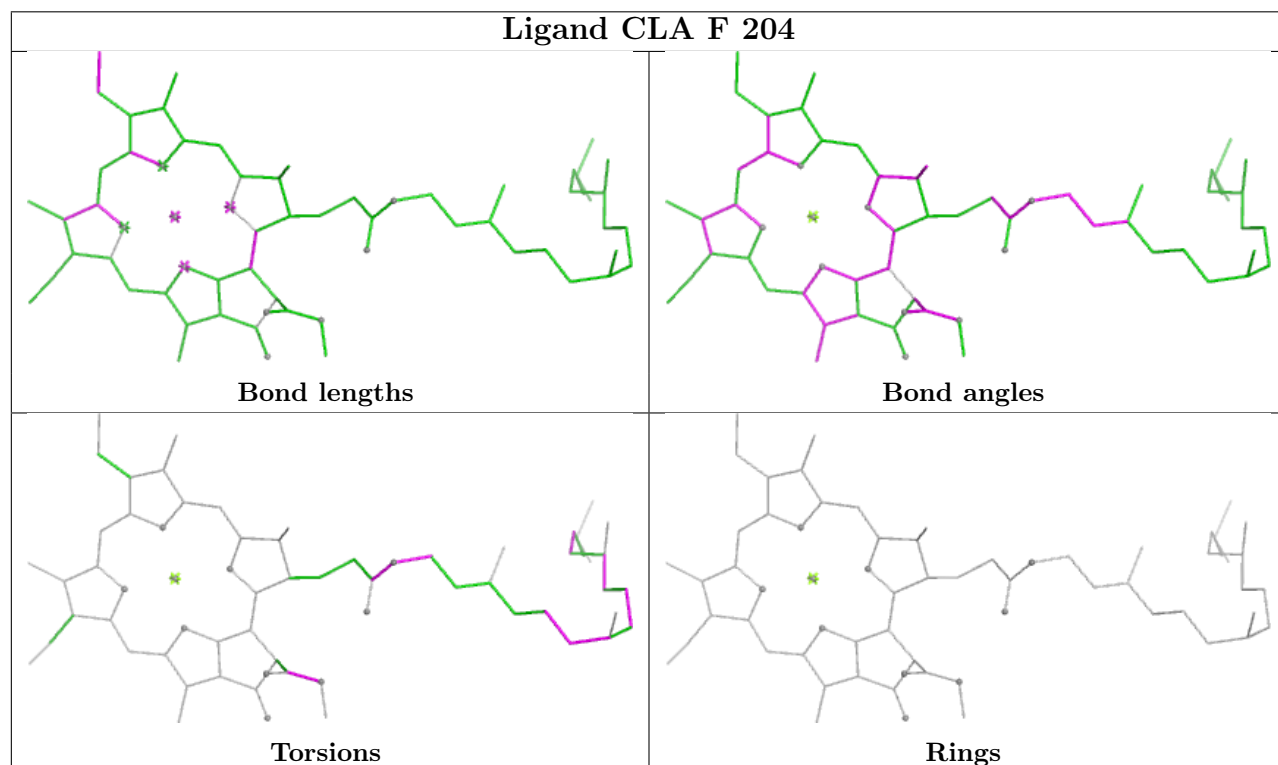


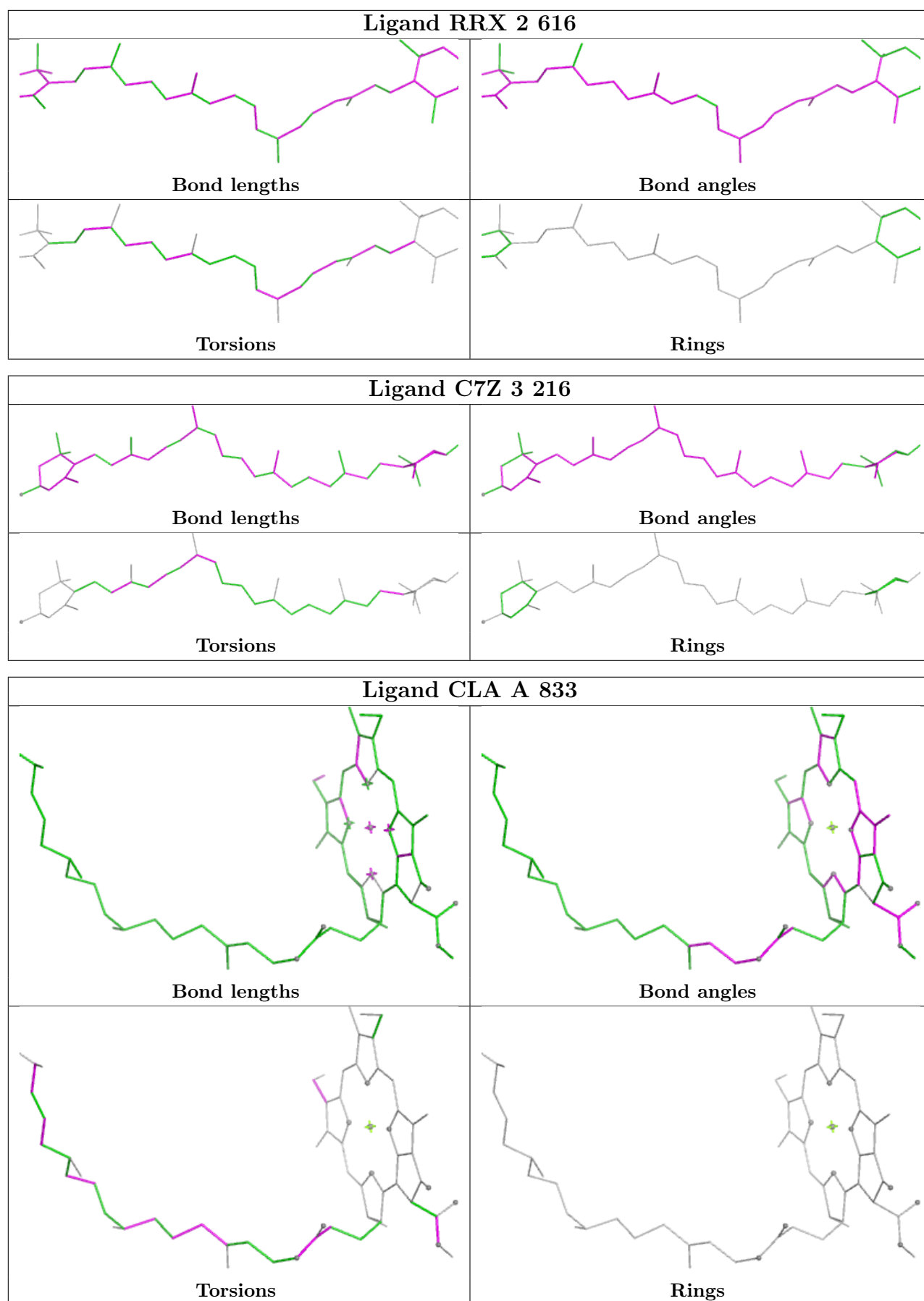


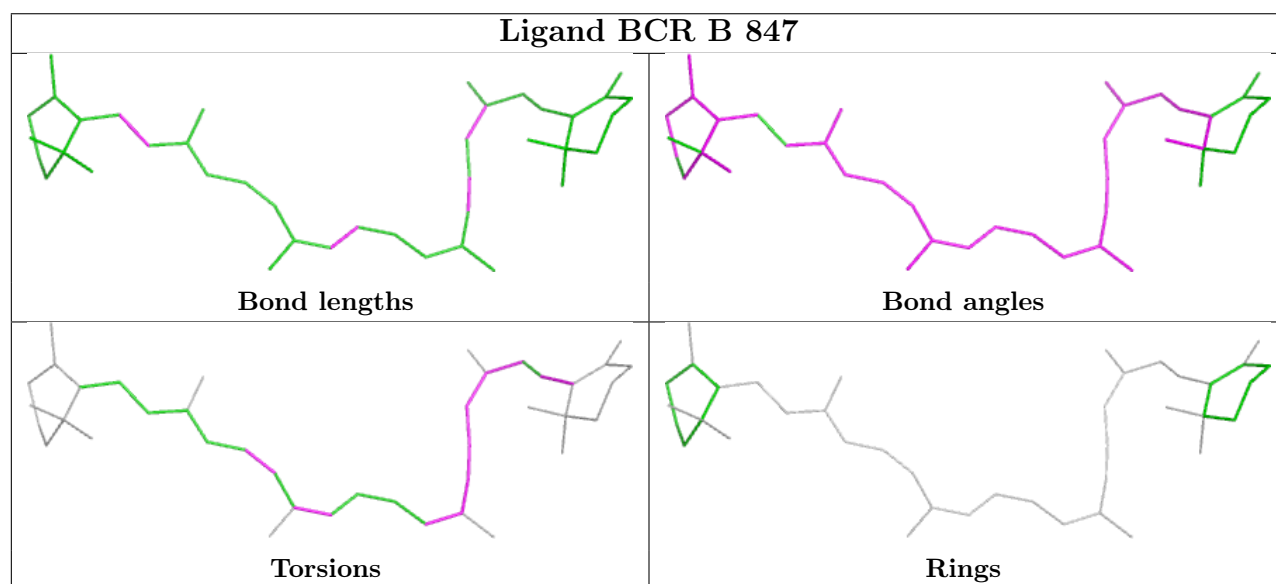
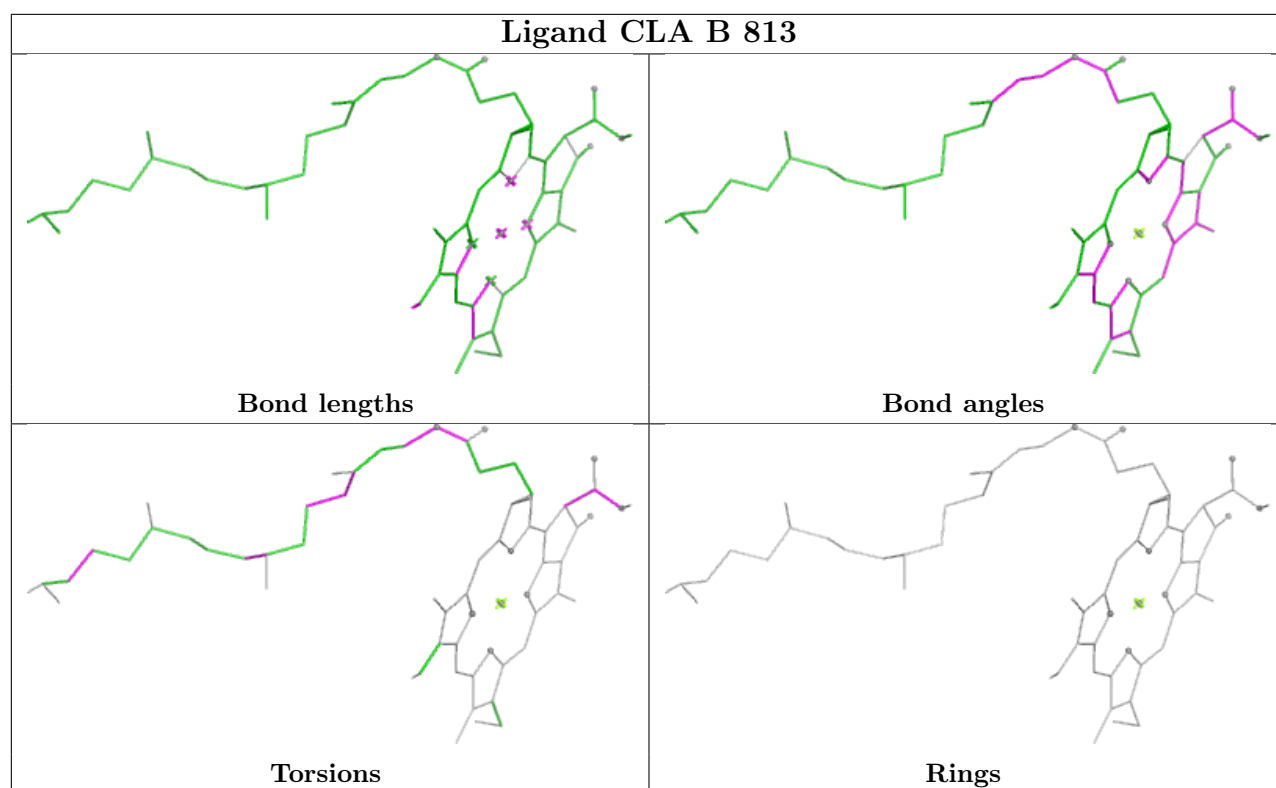
Ligand CLA B 818

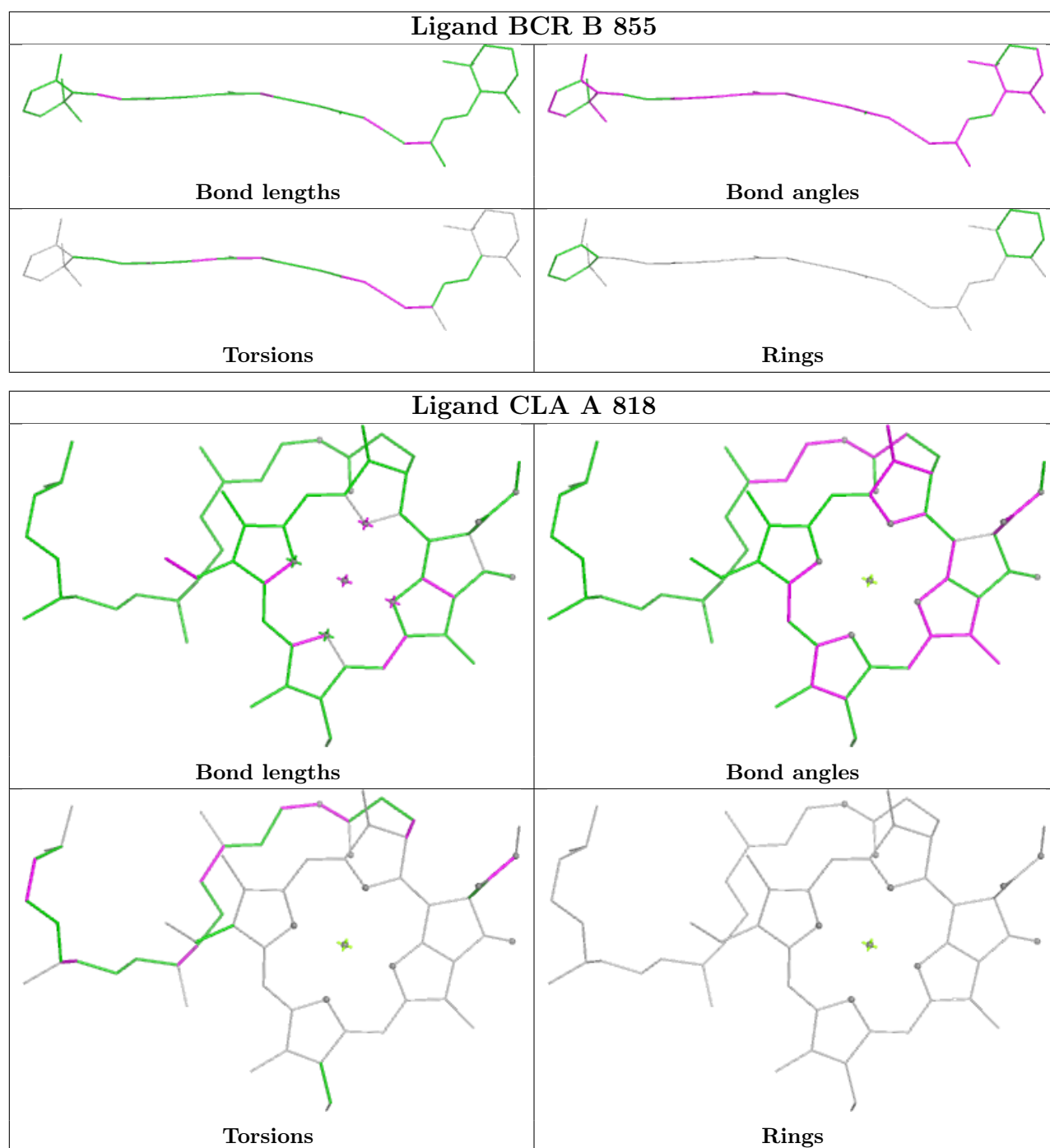


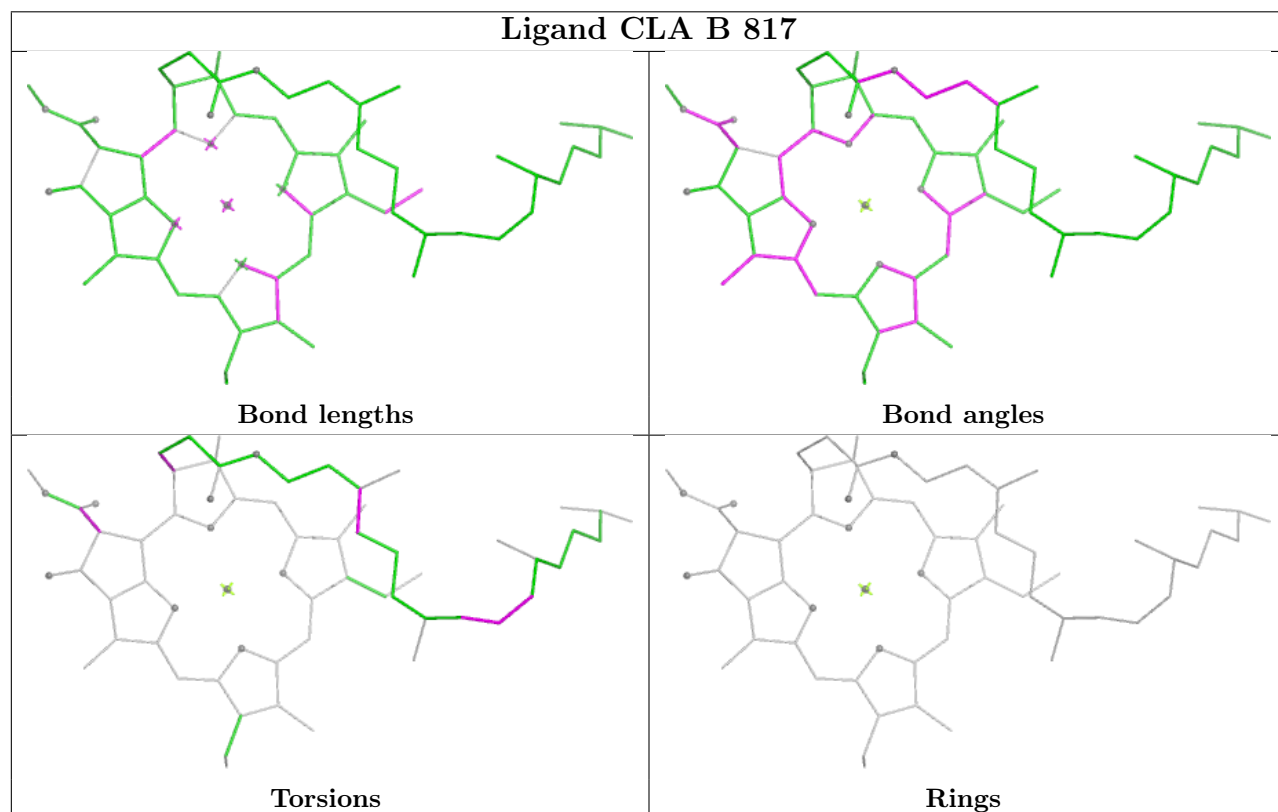
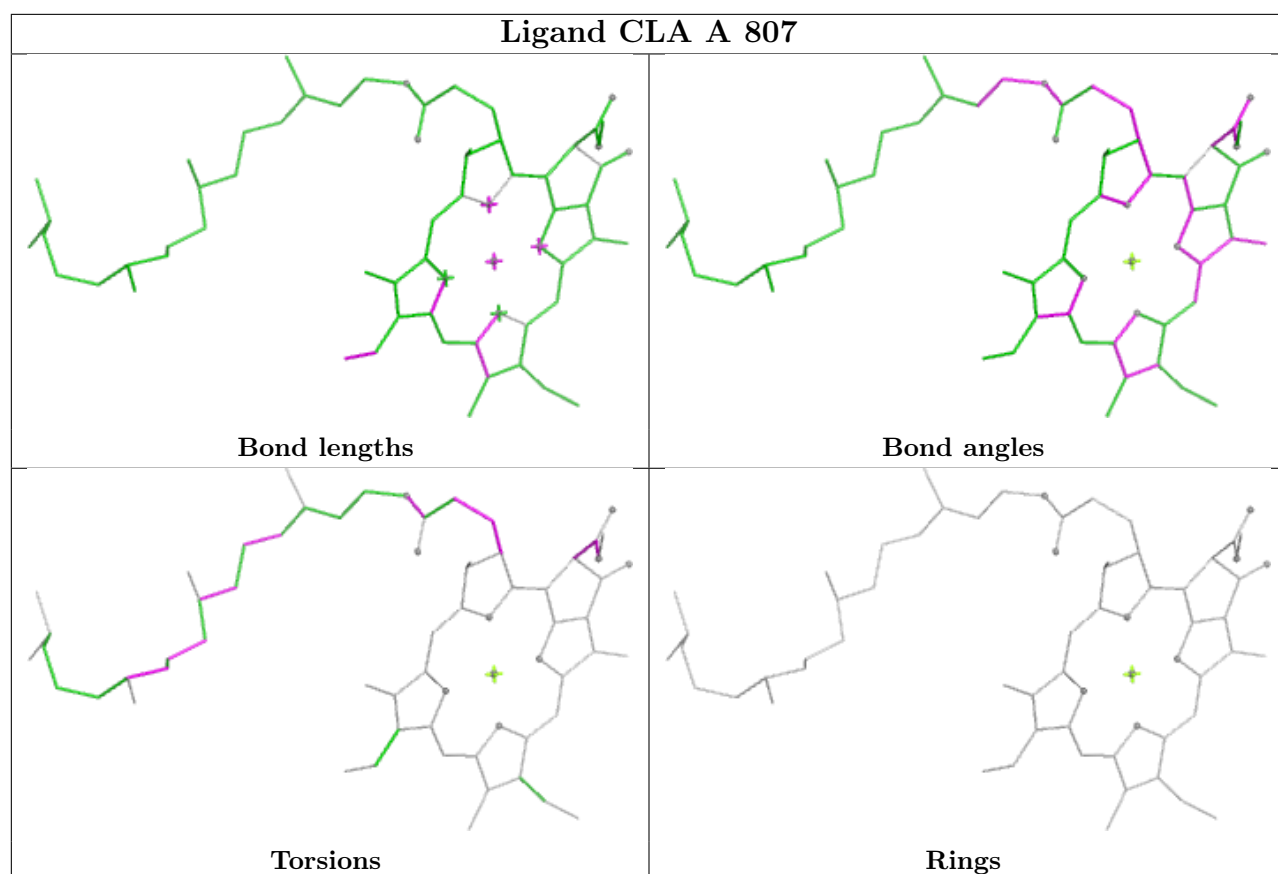
Ligand CLA F 204

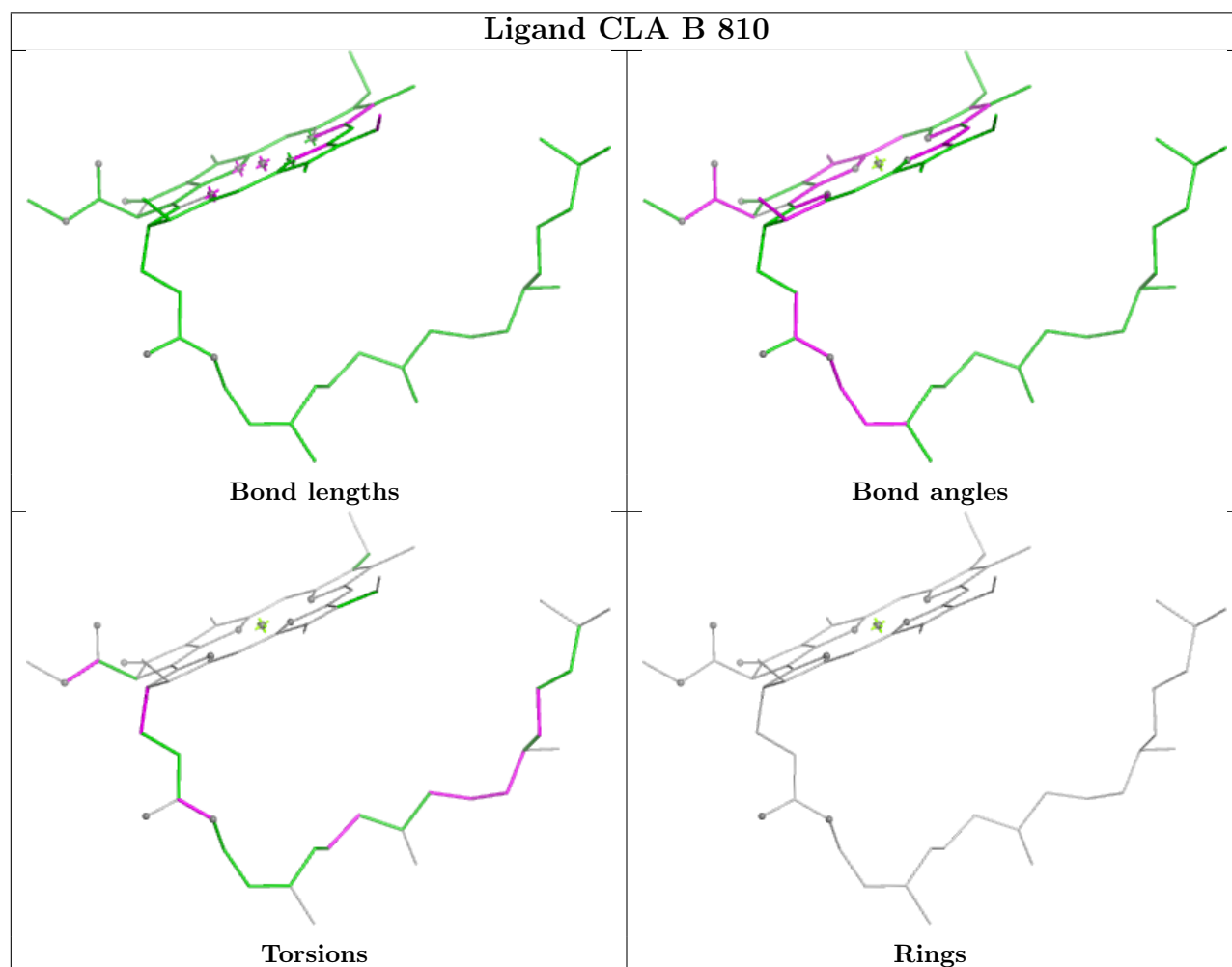
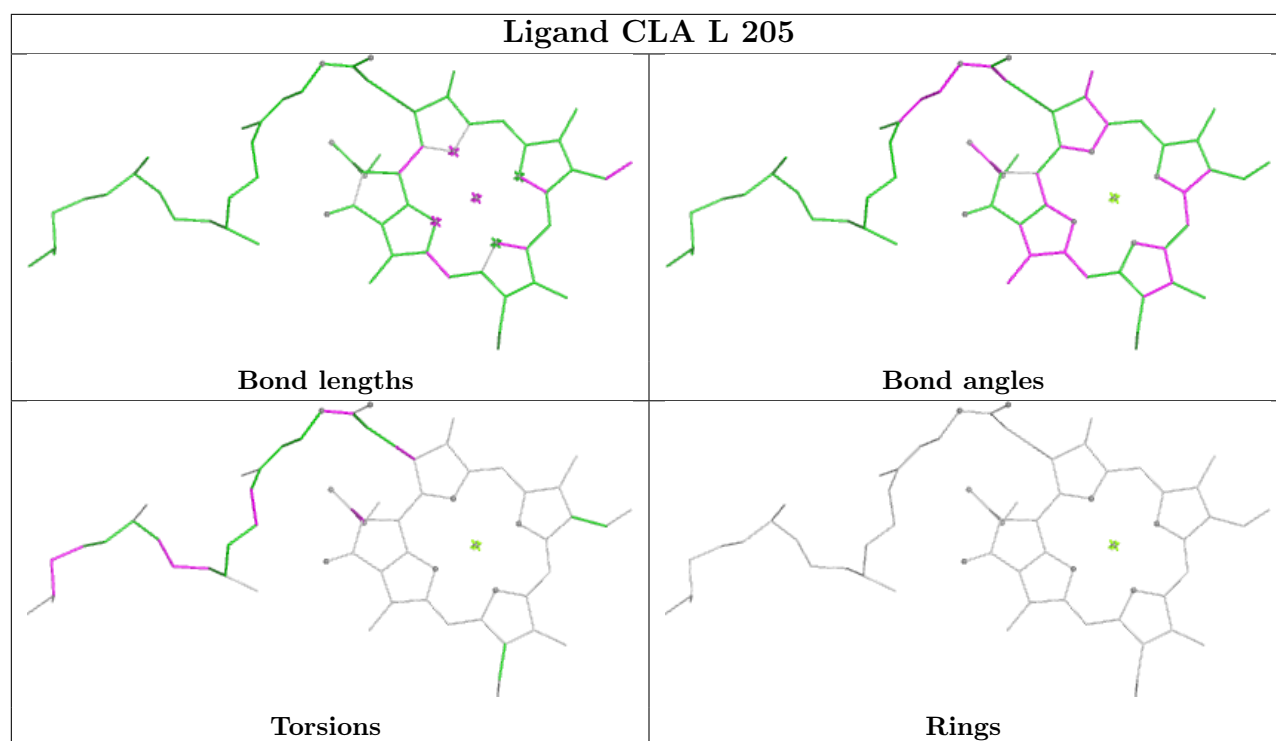


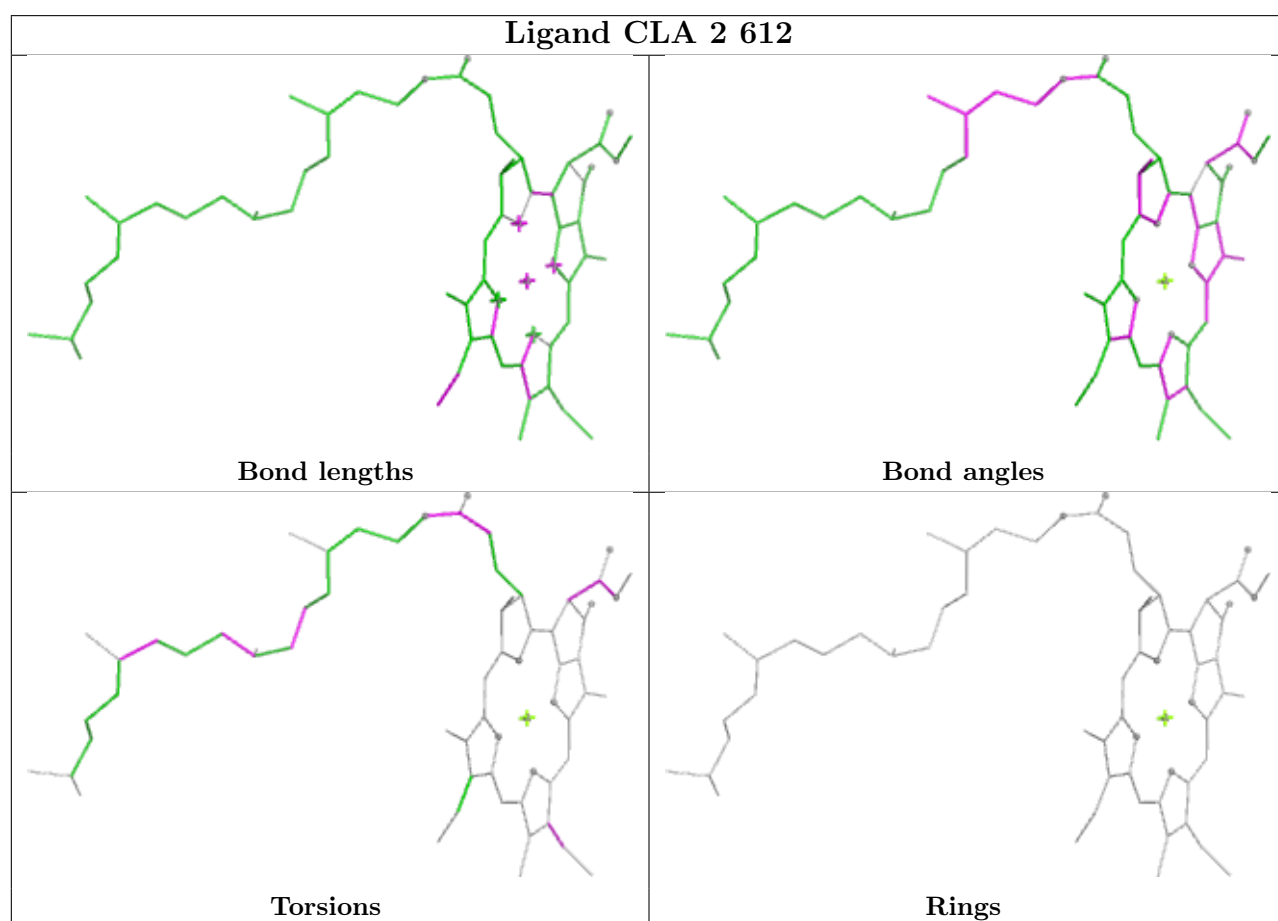
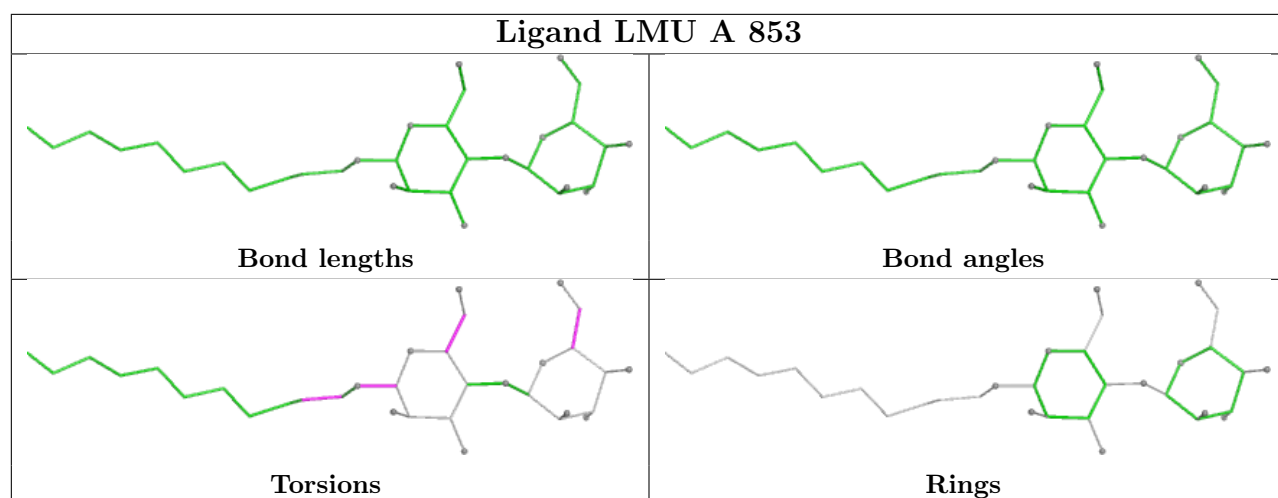


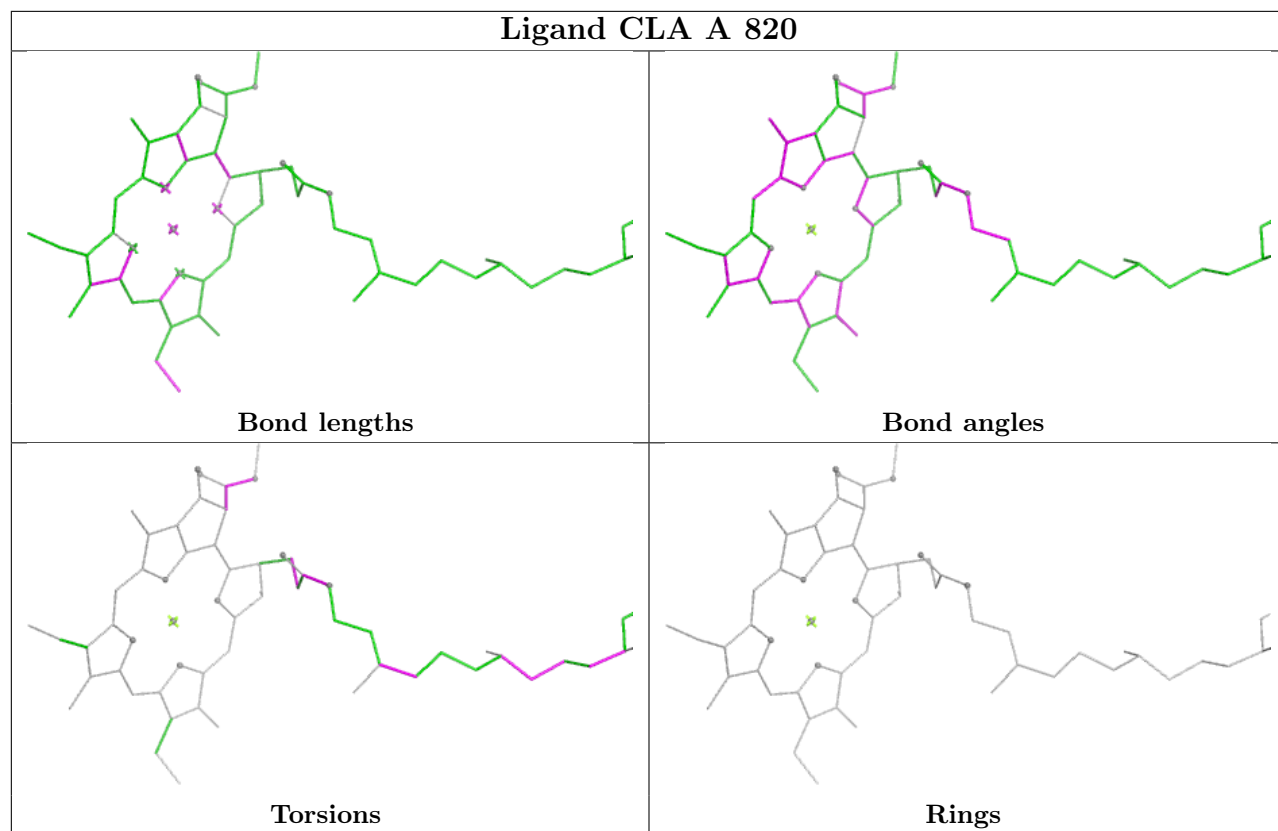


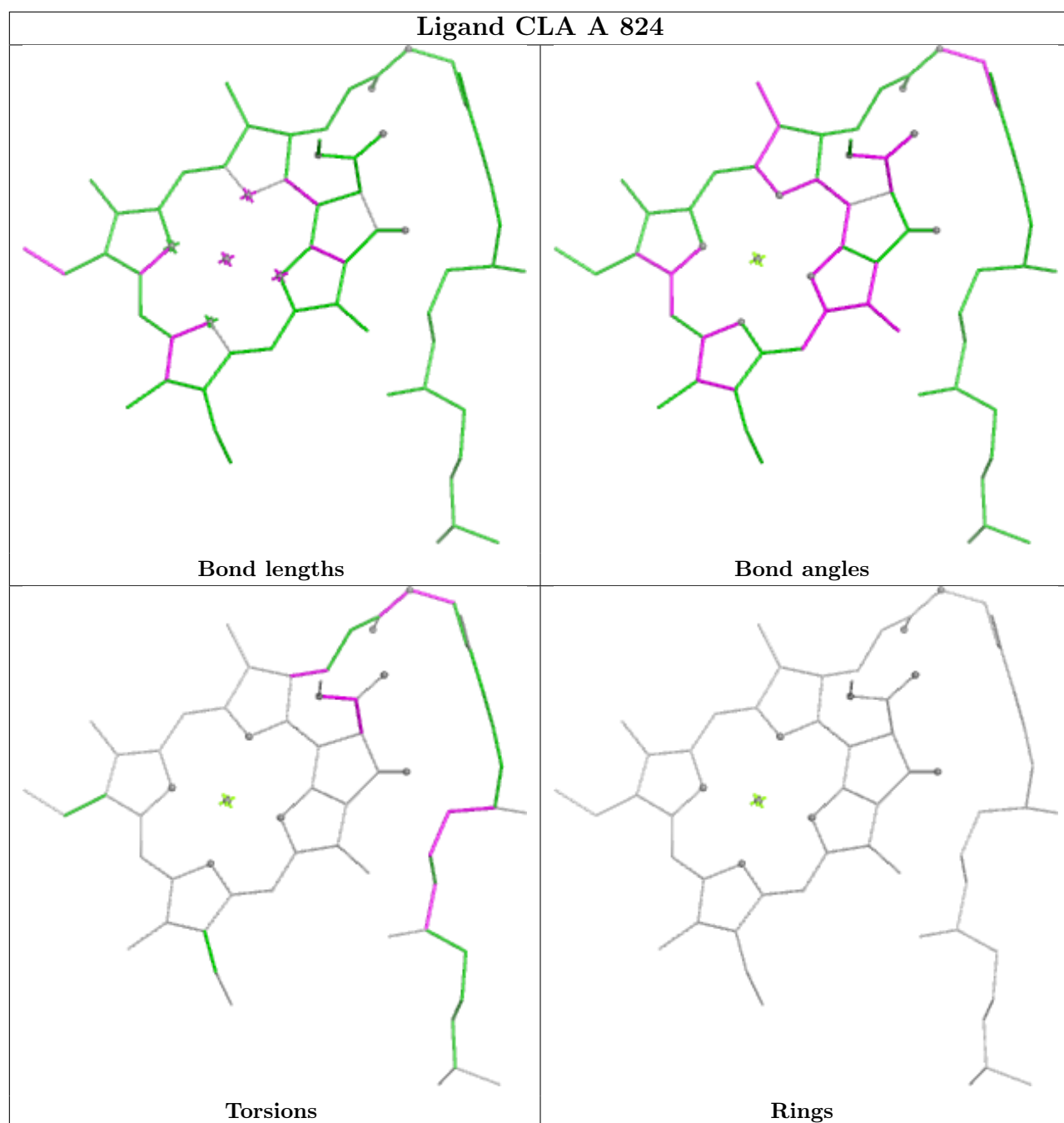




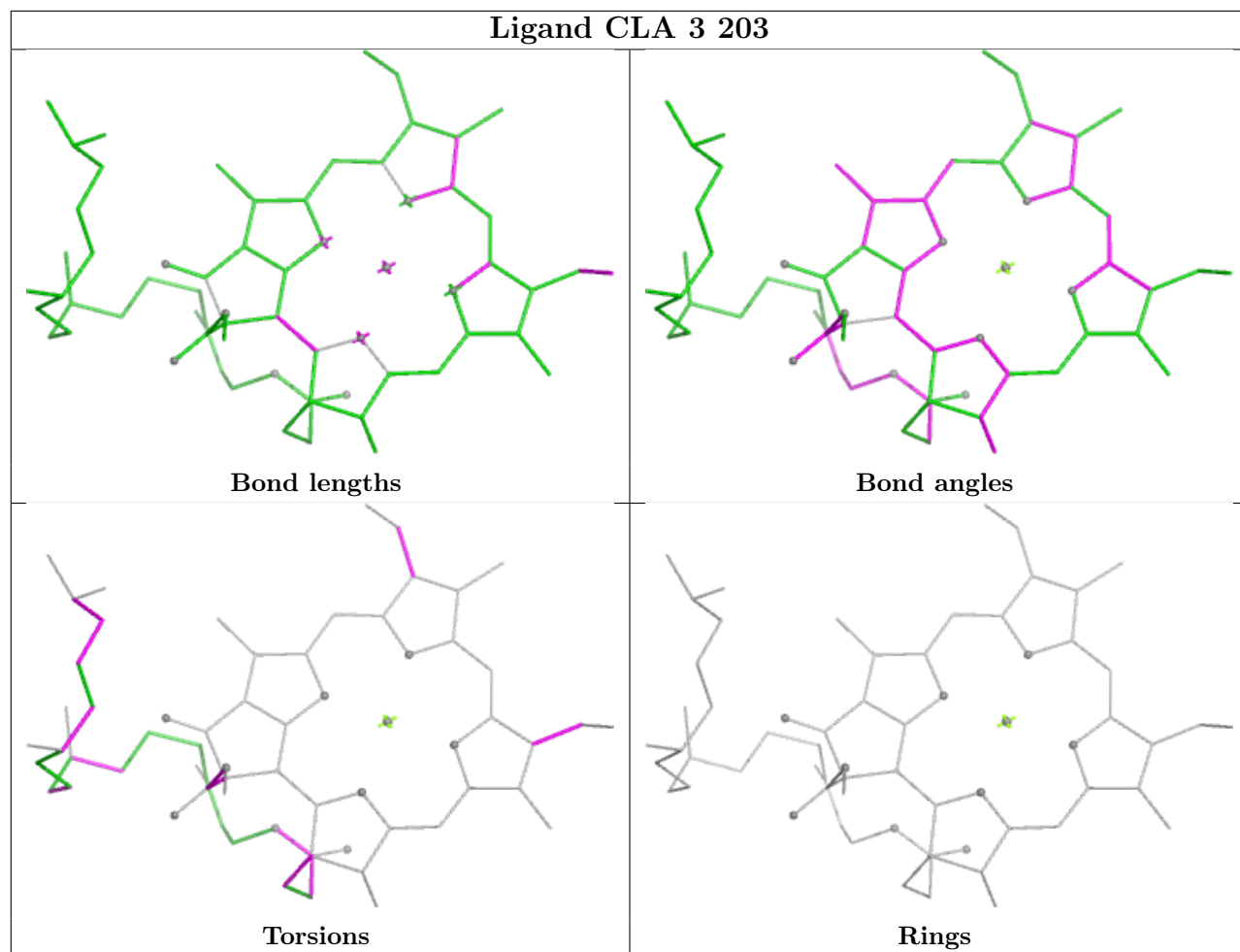




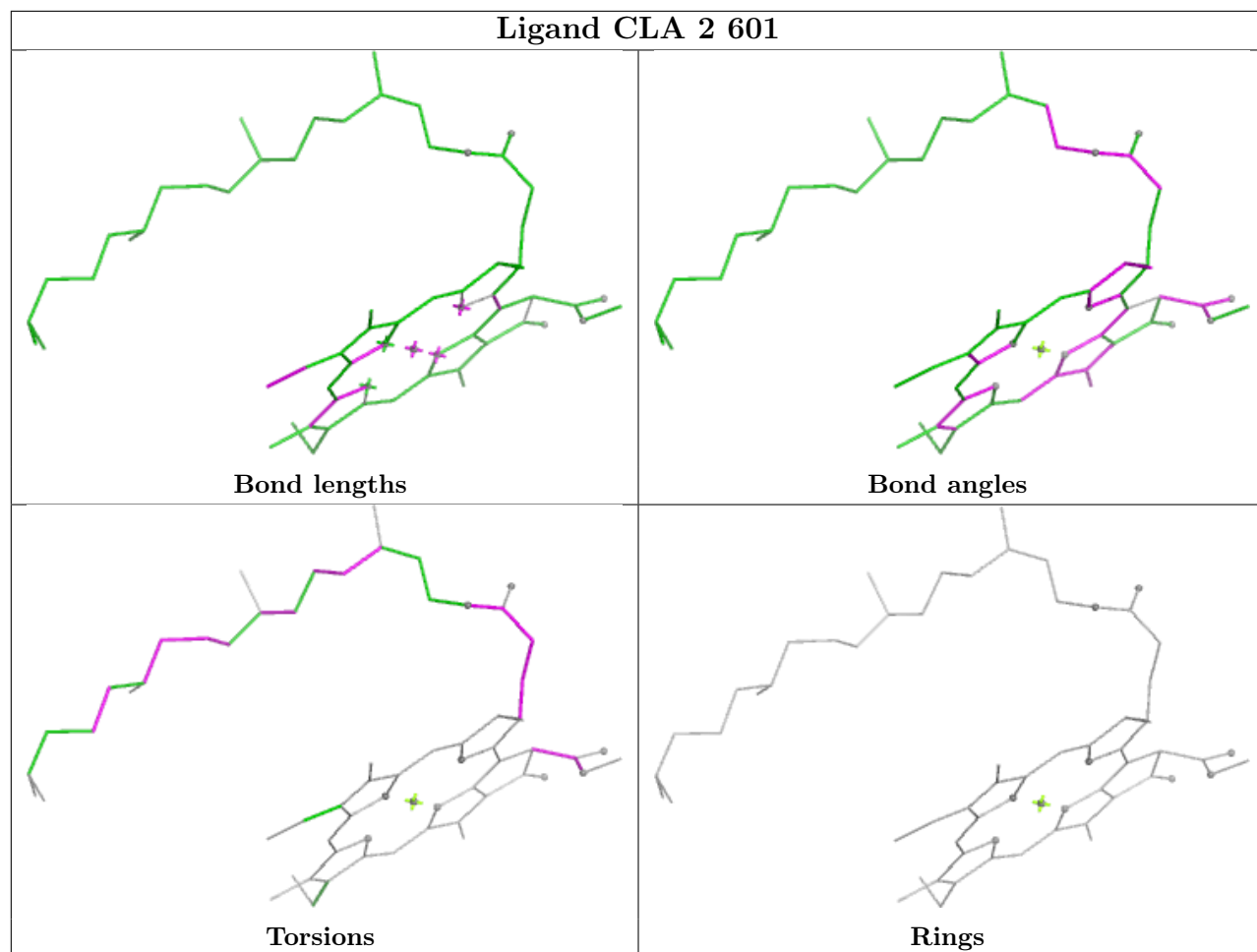


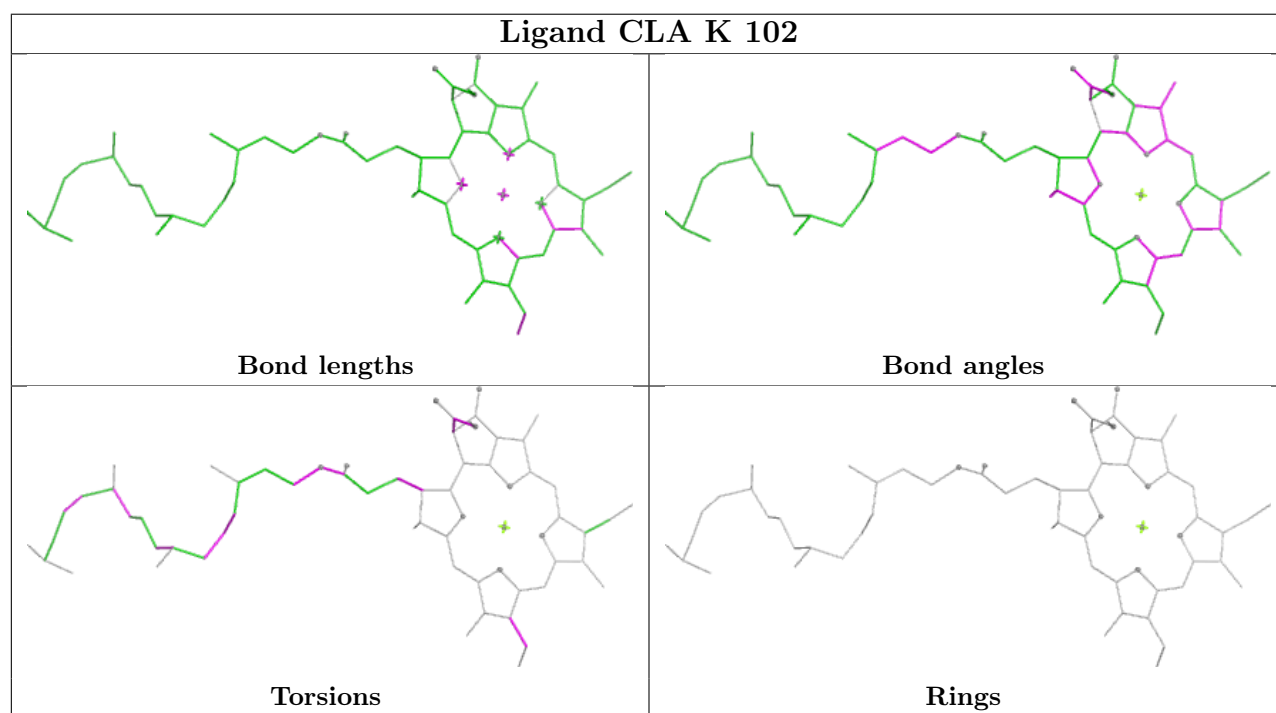
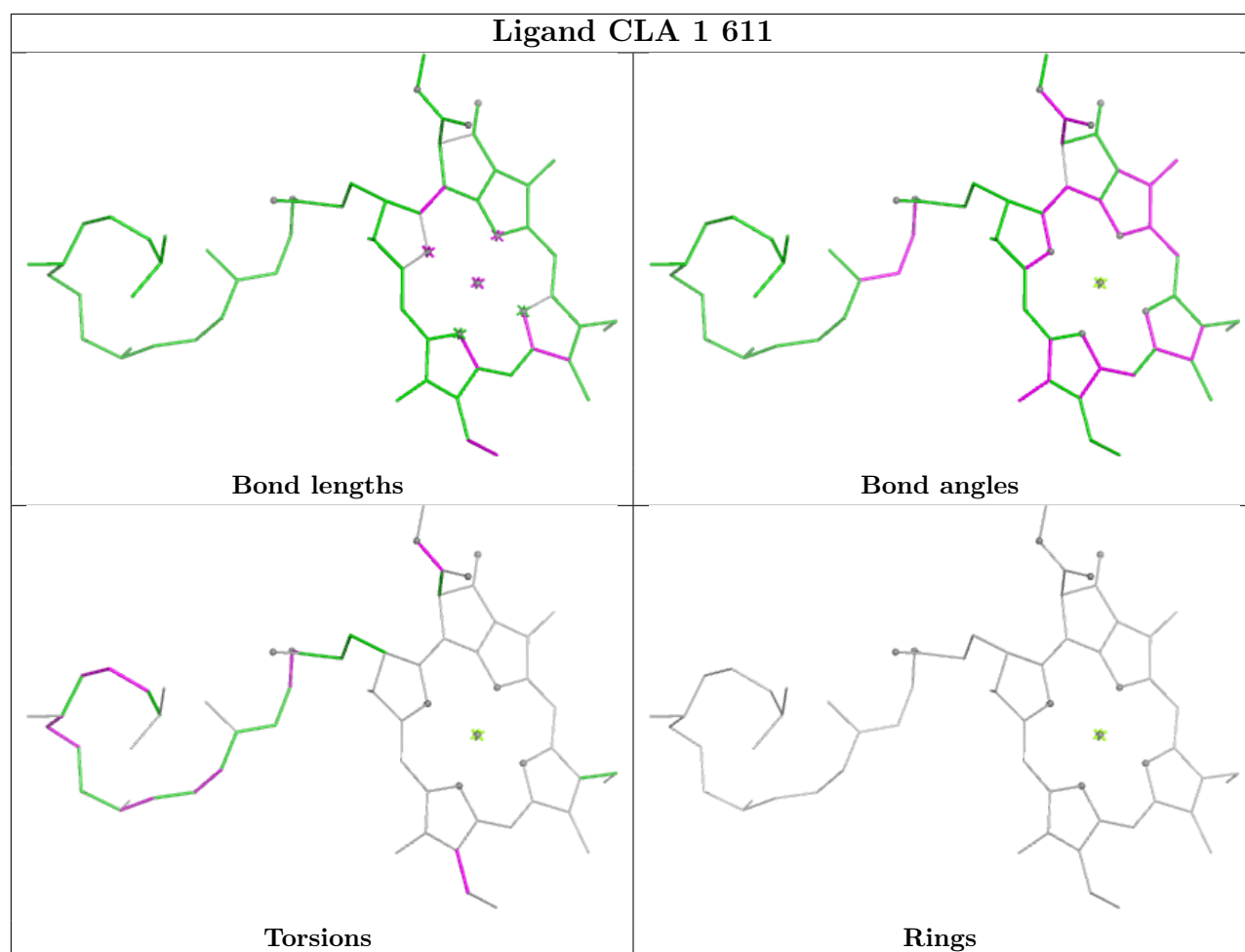


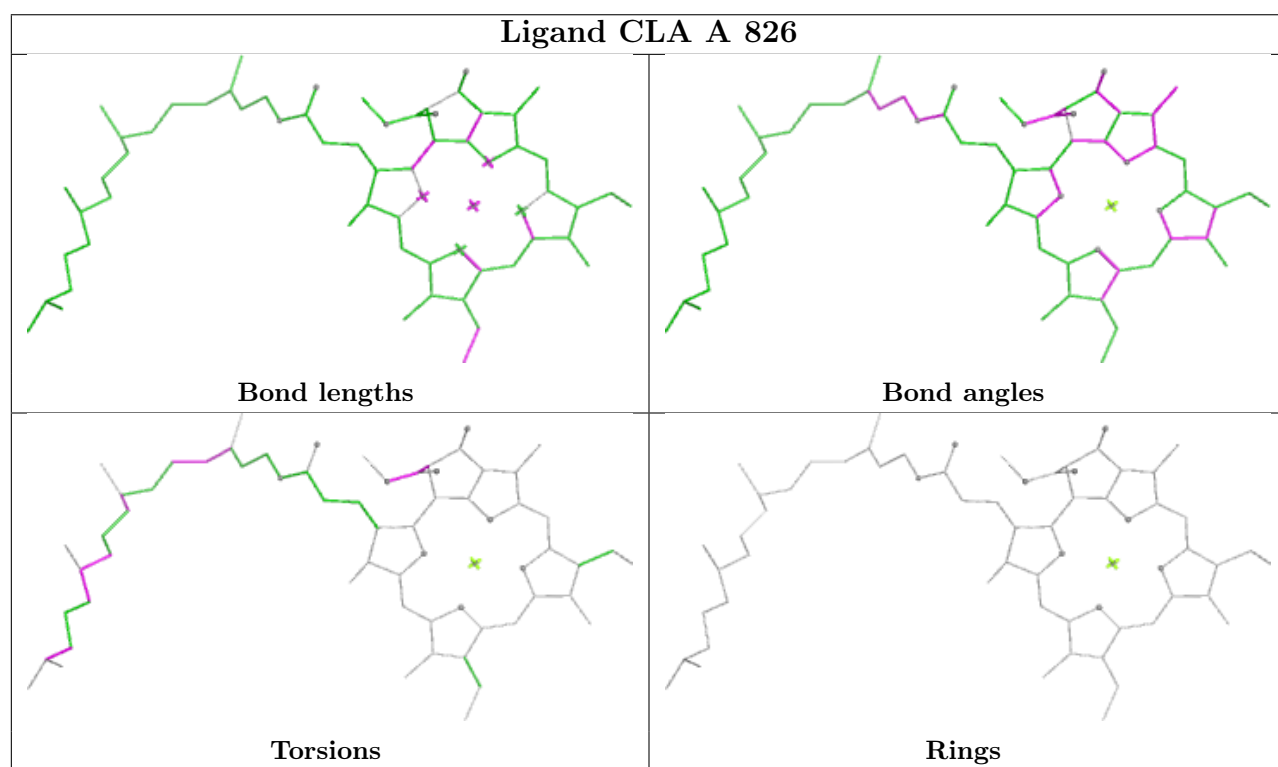
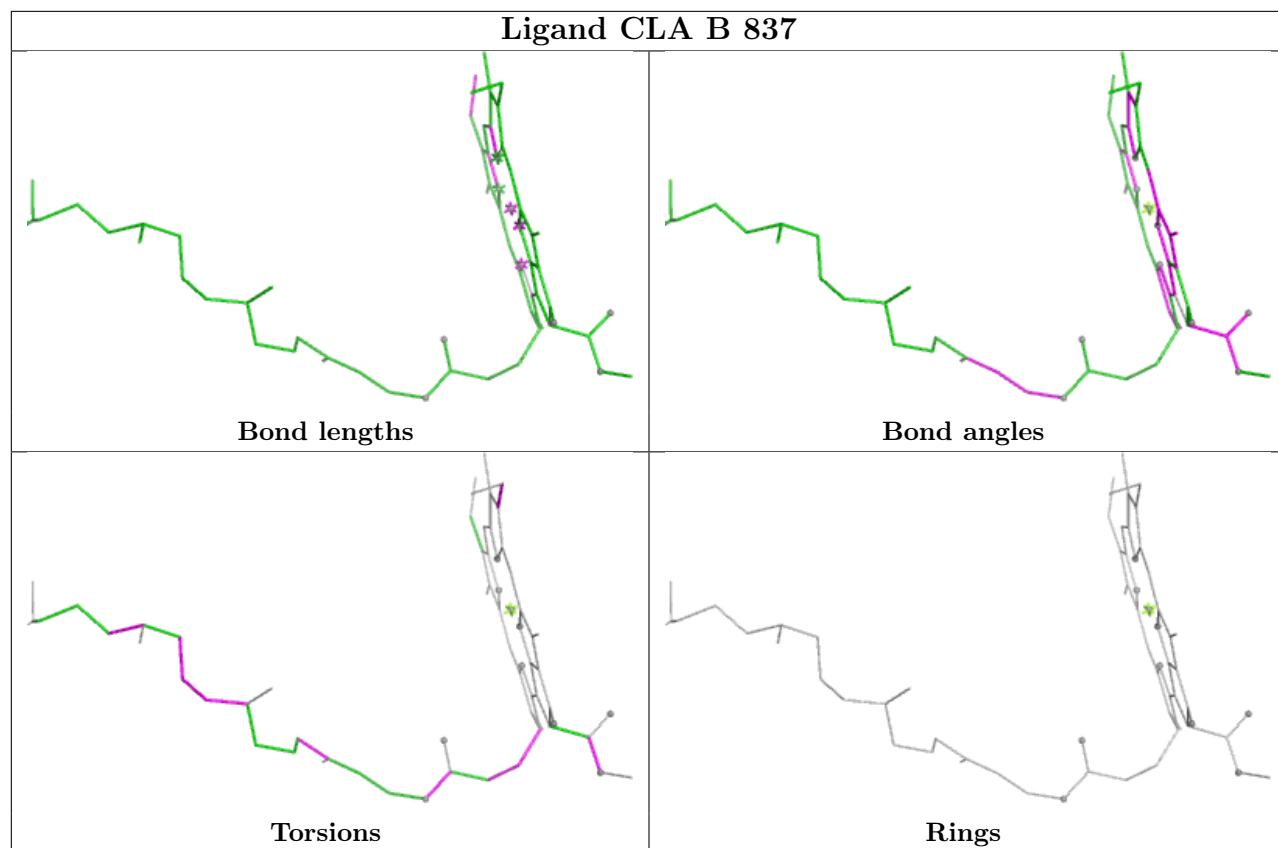
Ligand CLA 3 203



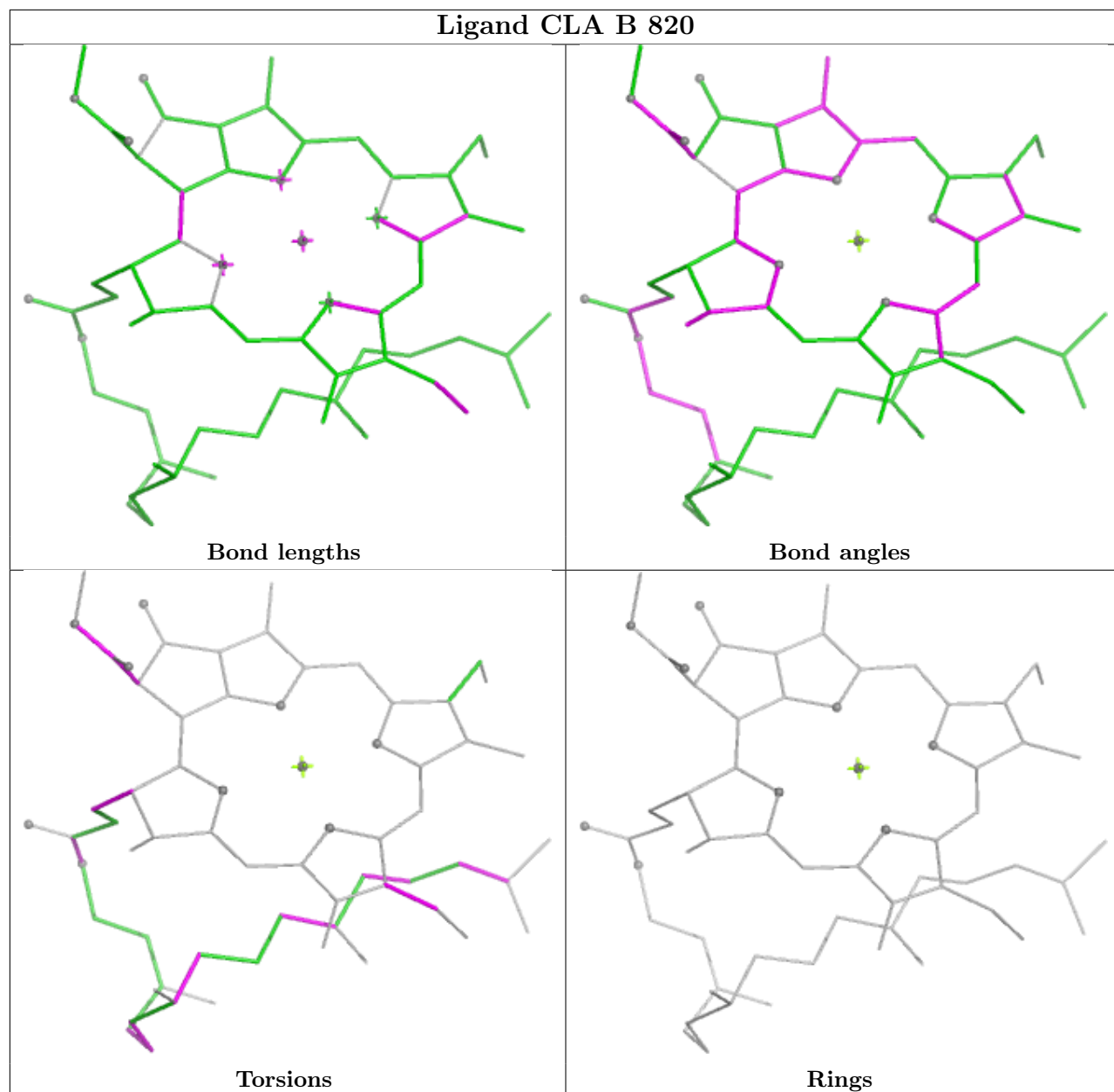
Ligand CLA 2 601

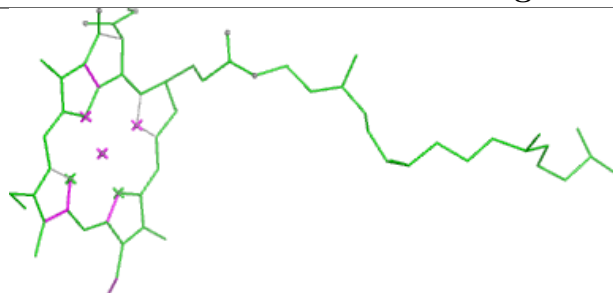




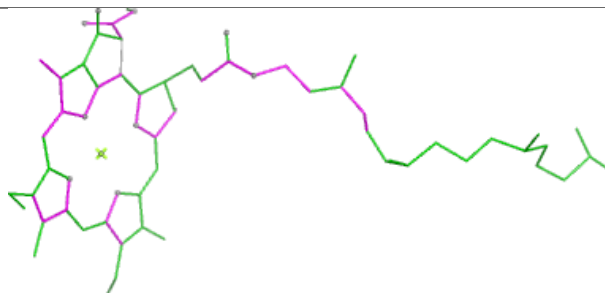


Ligand CLA B 820

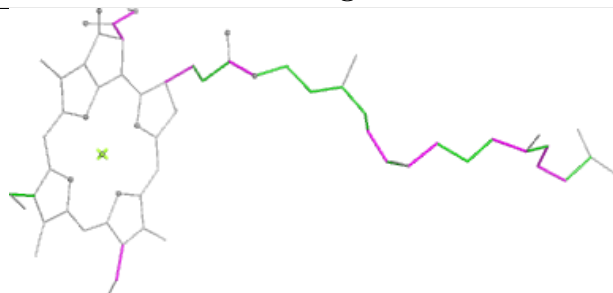


Ligand CLA B 830

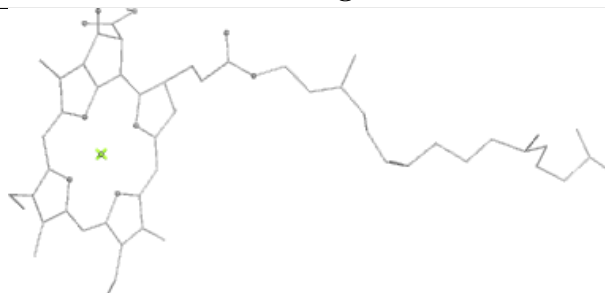
Bond lengths



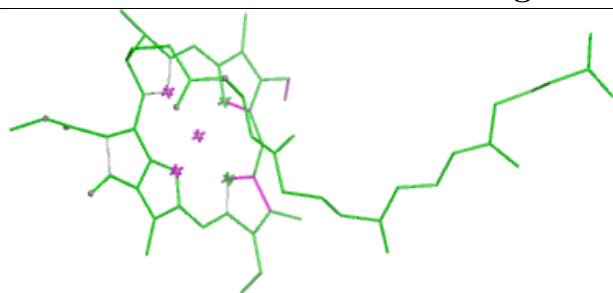
Bond angles



Torsions



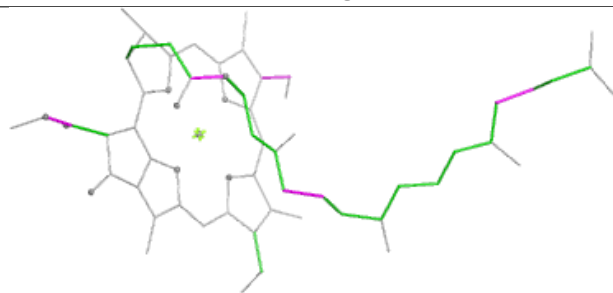
Rings

Ligand CLA A 838

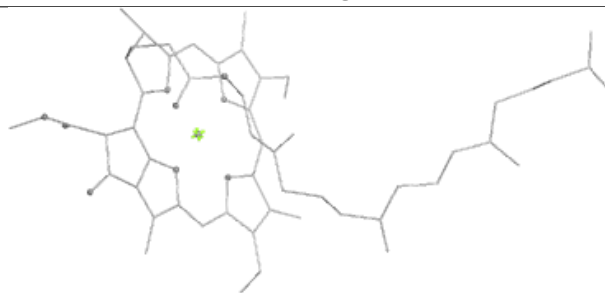
Bond lengths



Bond angles

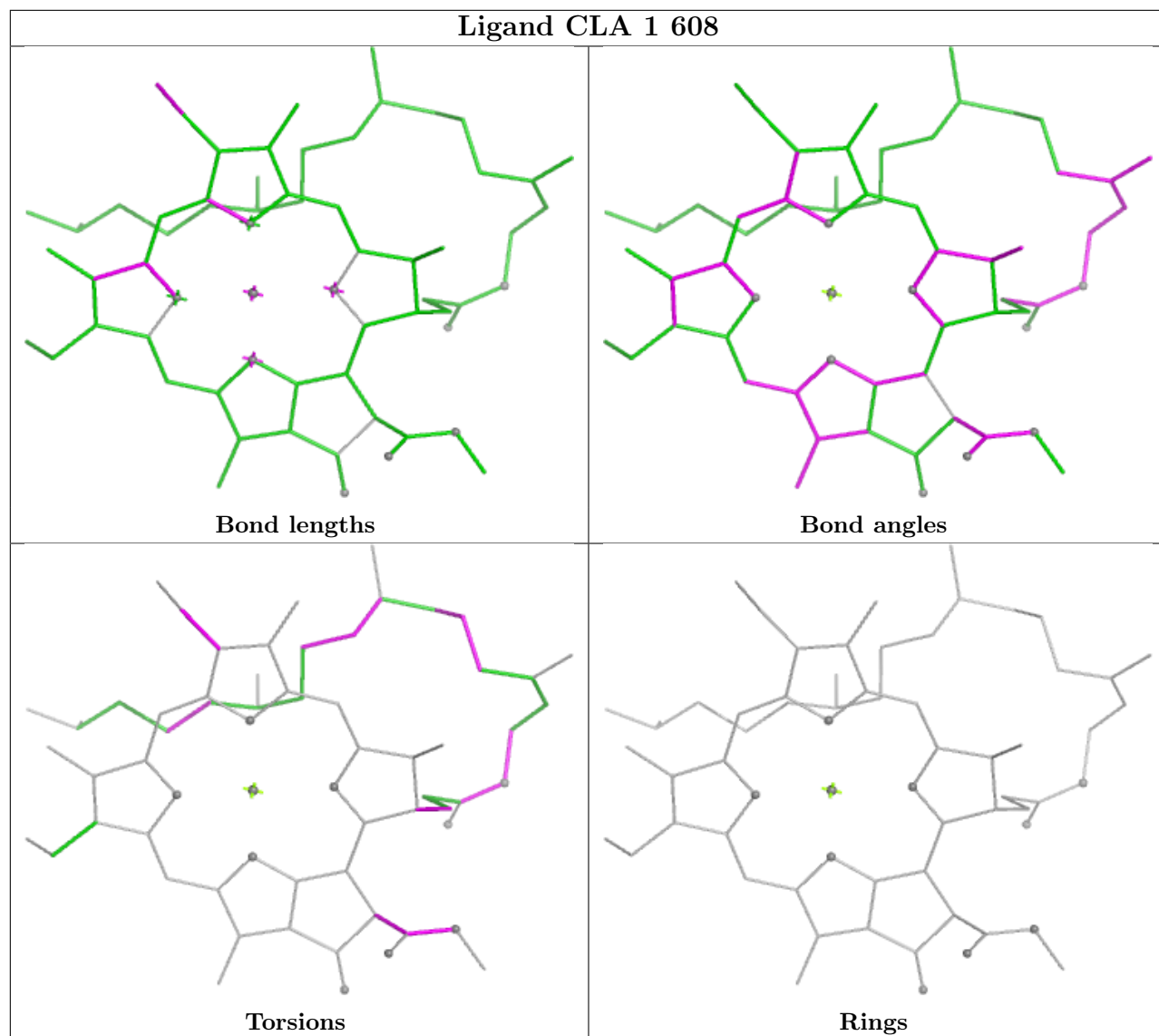


Torsions

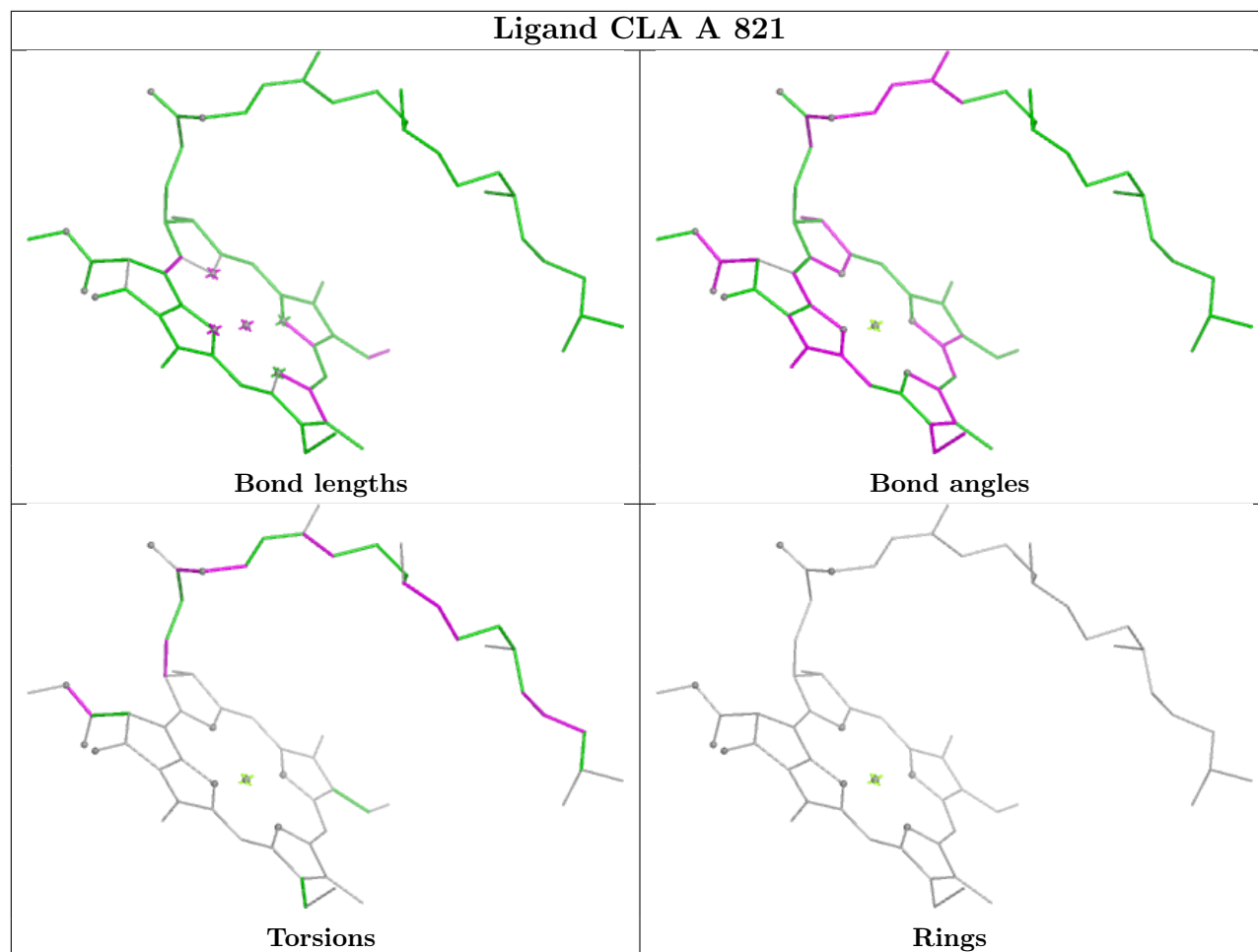


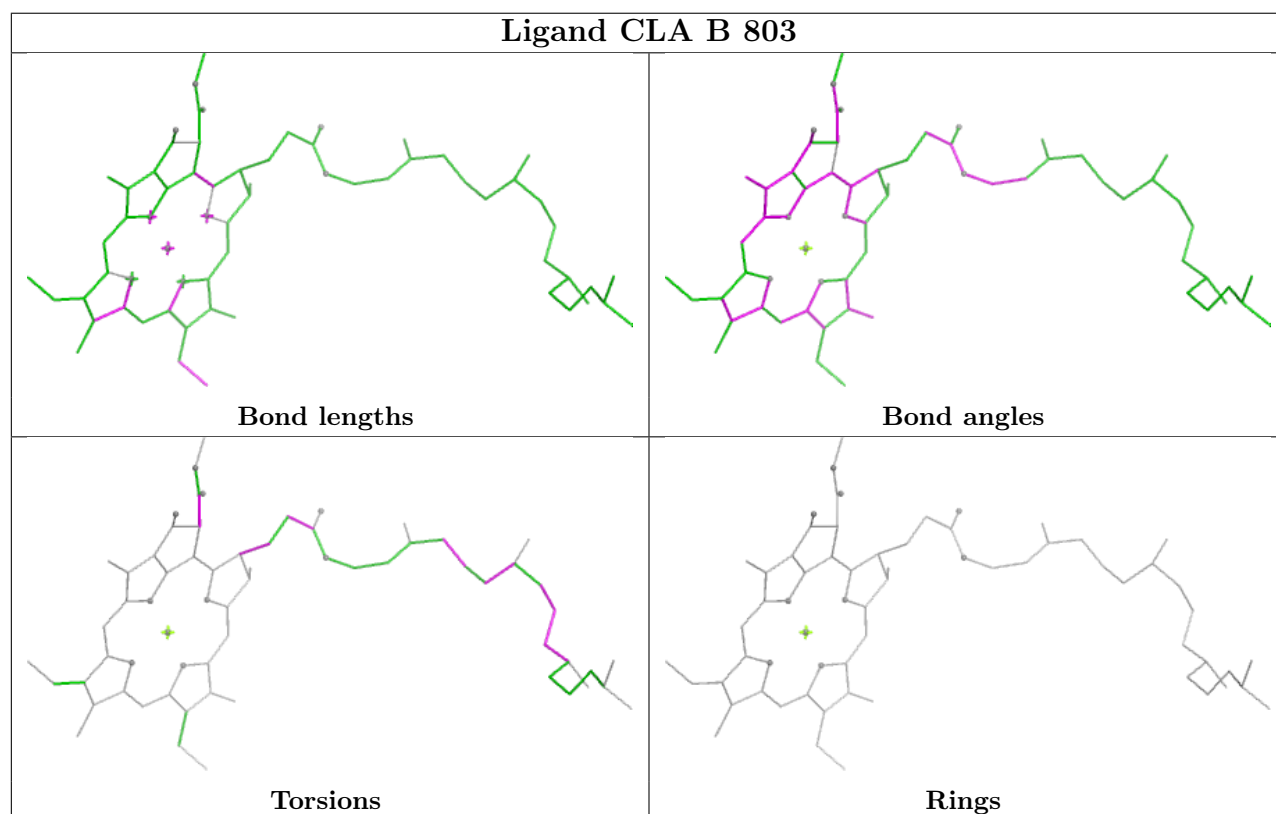
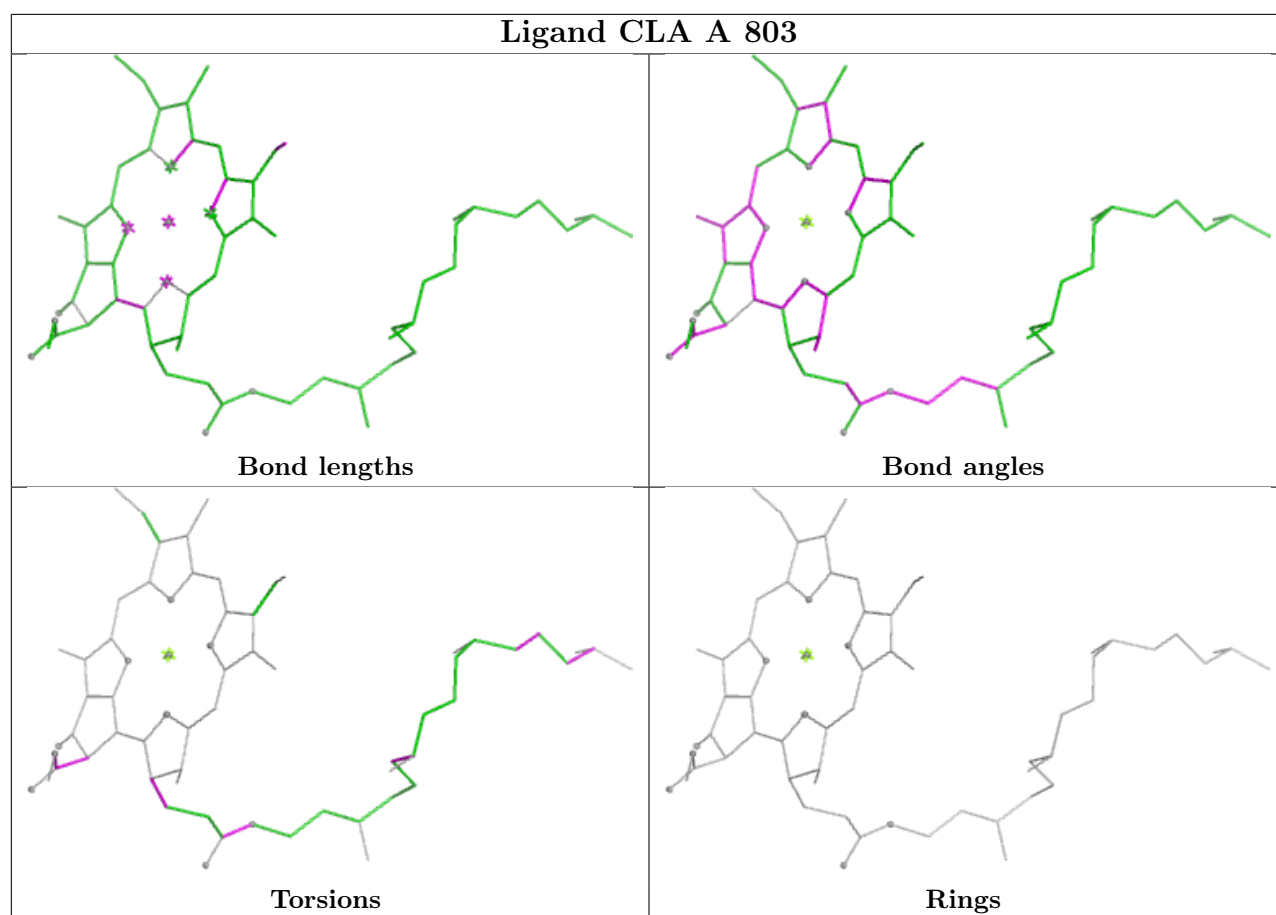
Rings

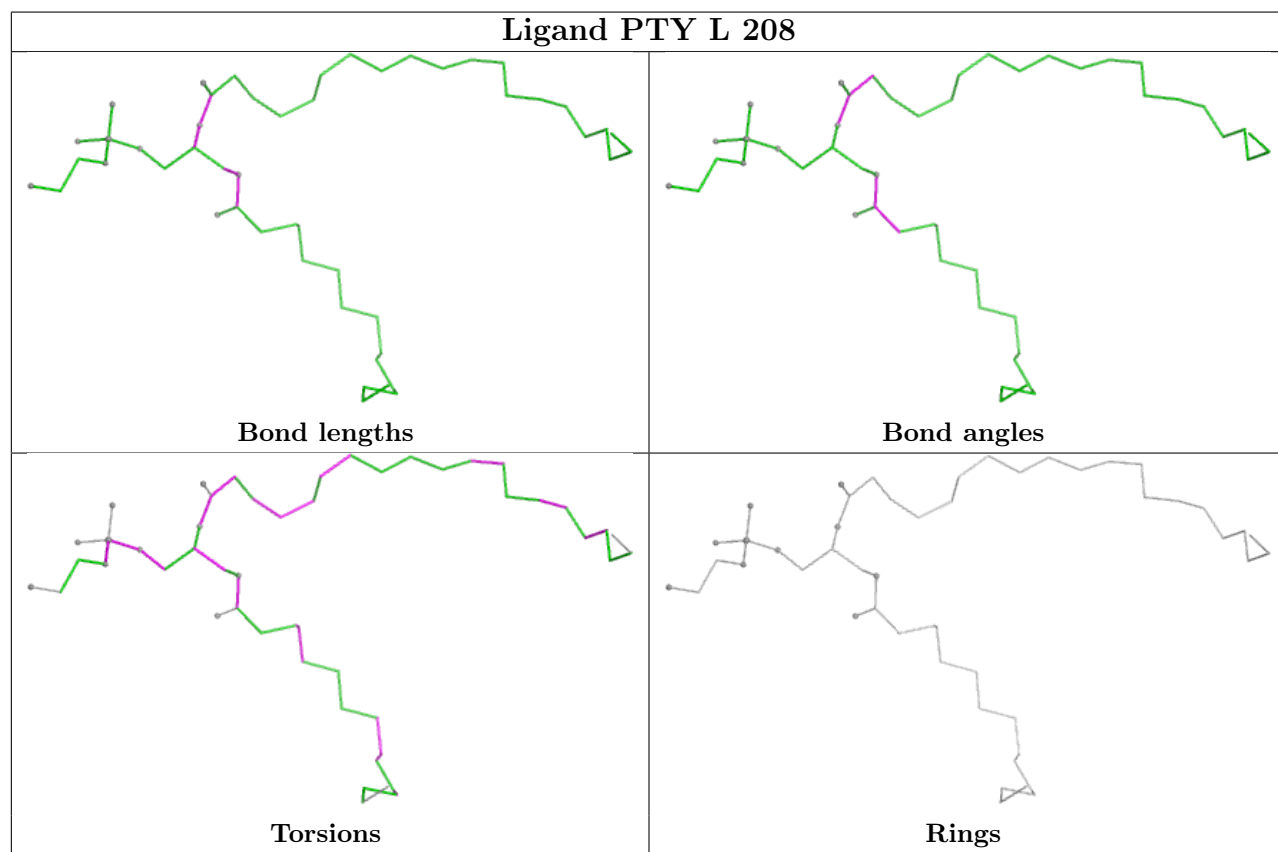
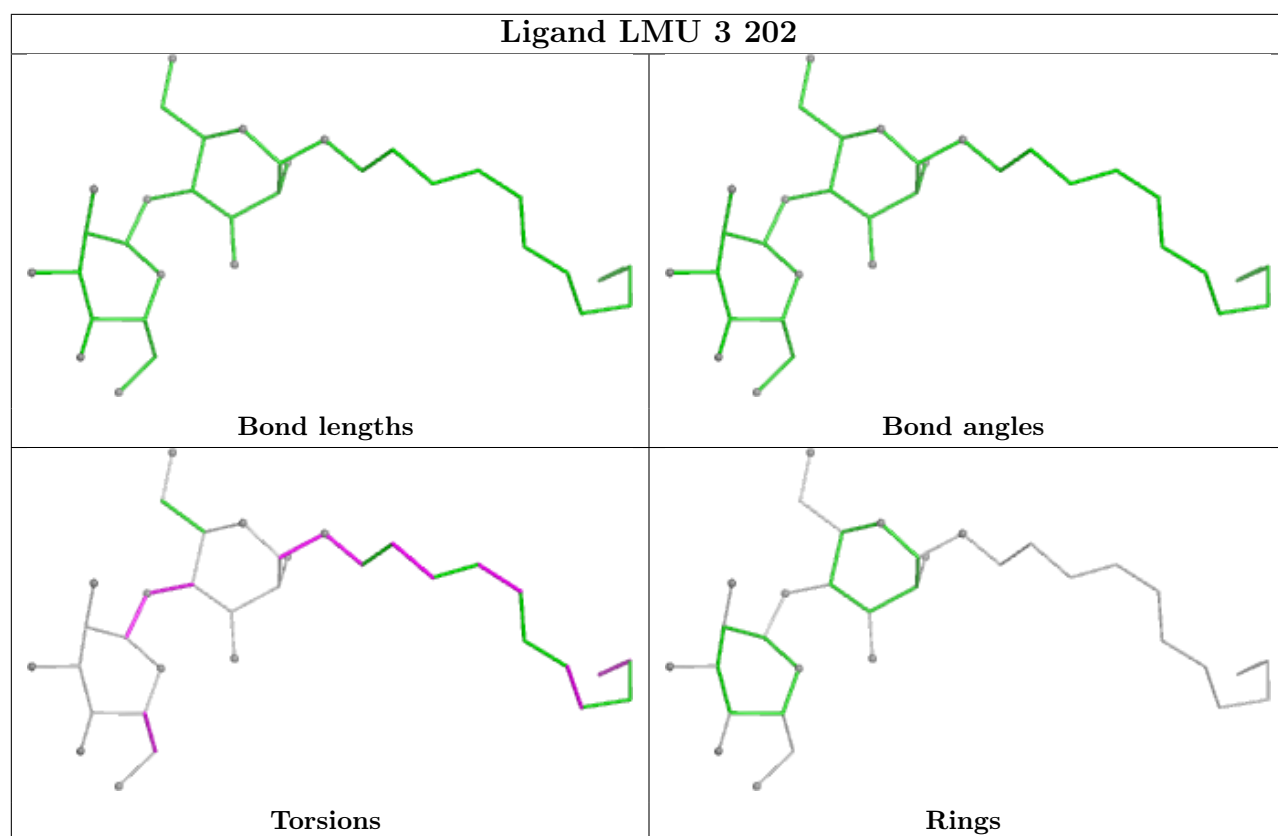
Ligand CLA 1 608

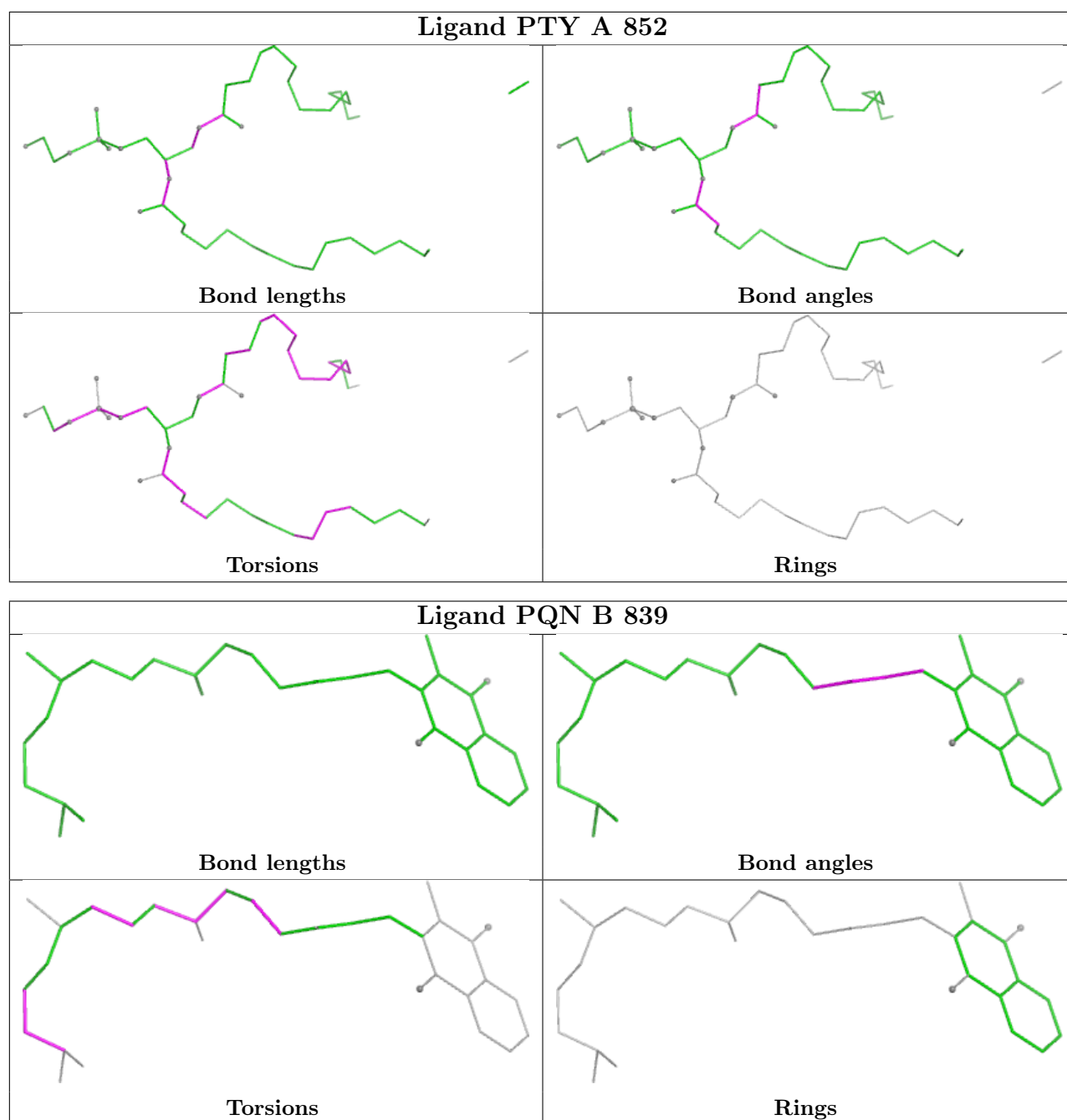


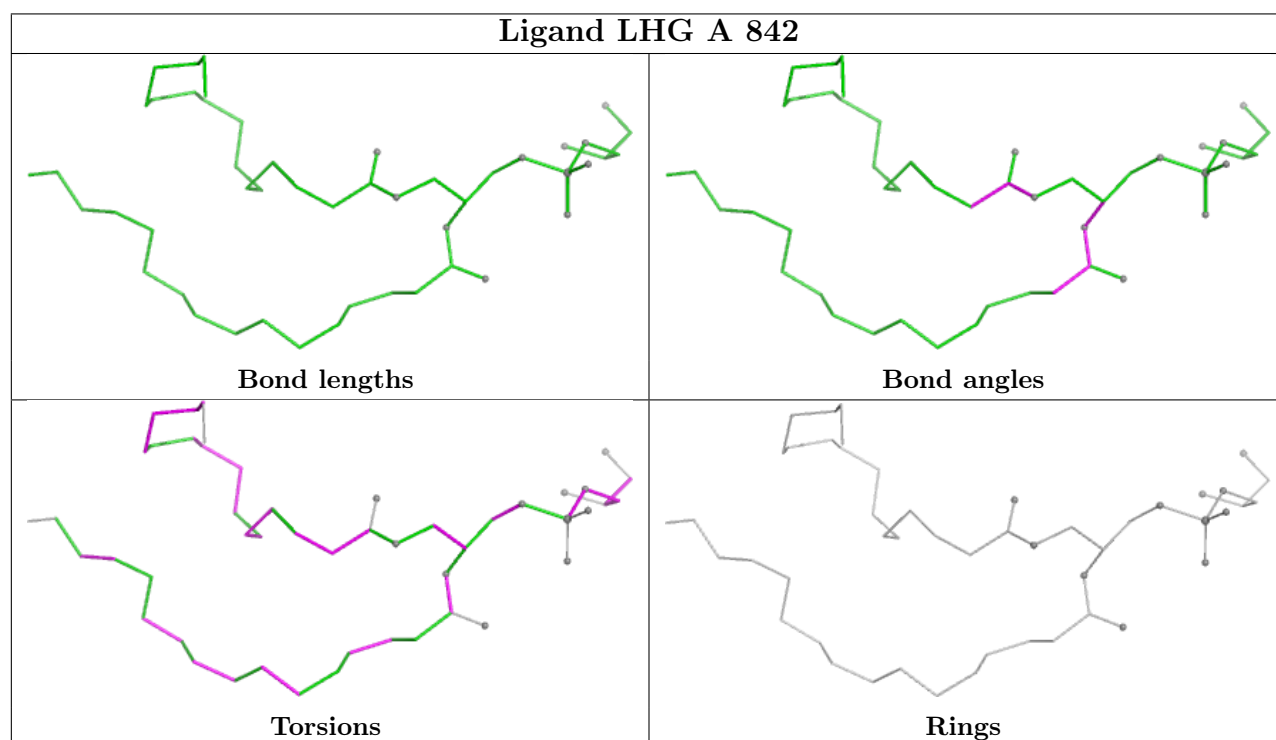
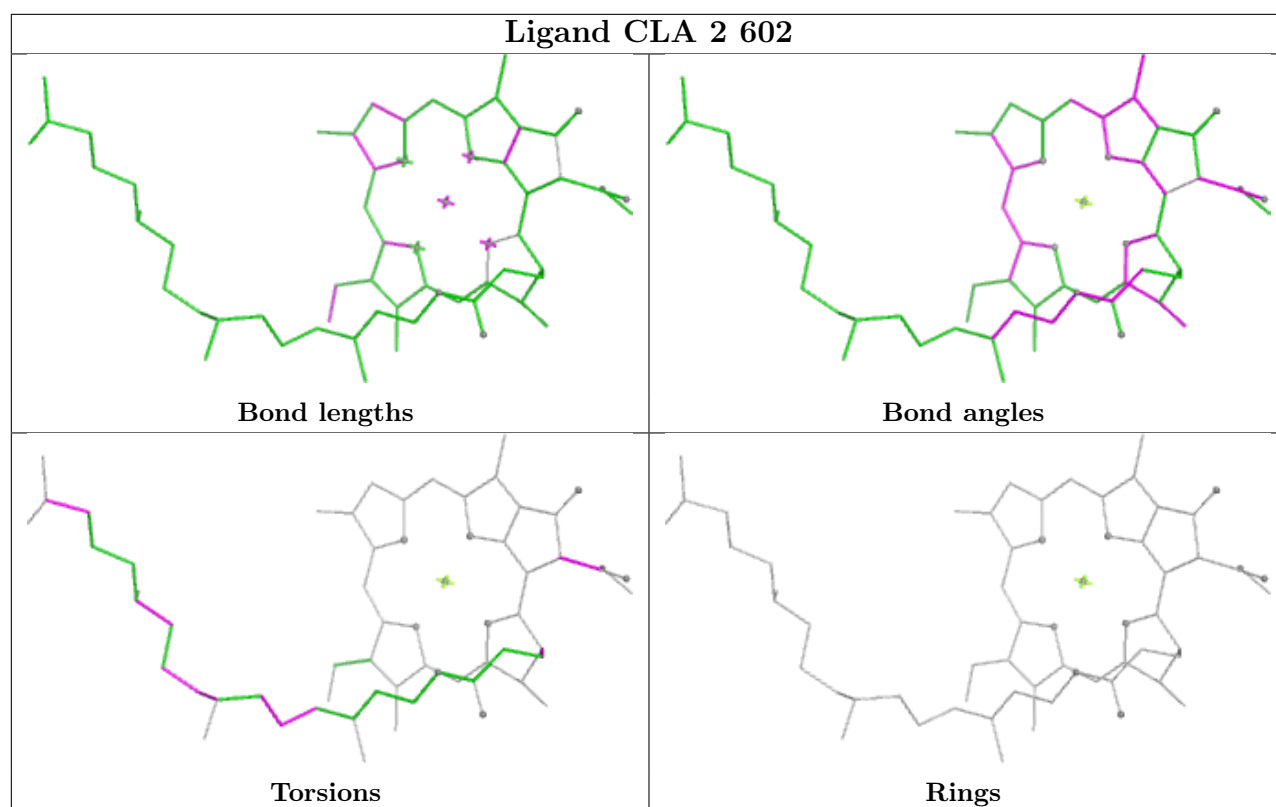
Ligand CLA A 821



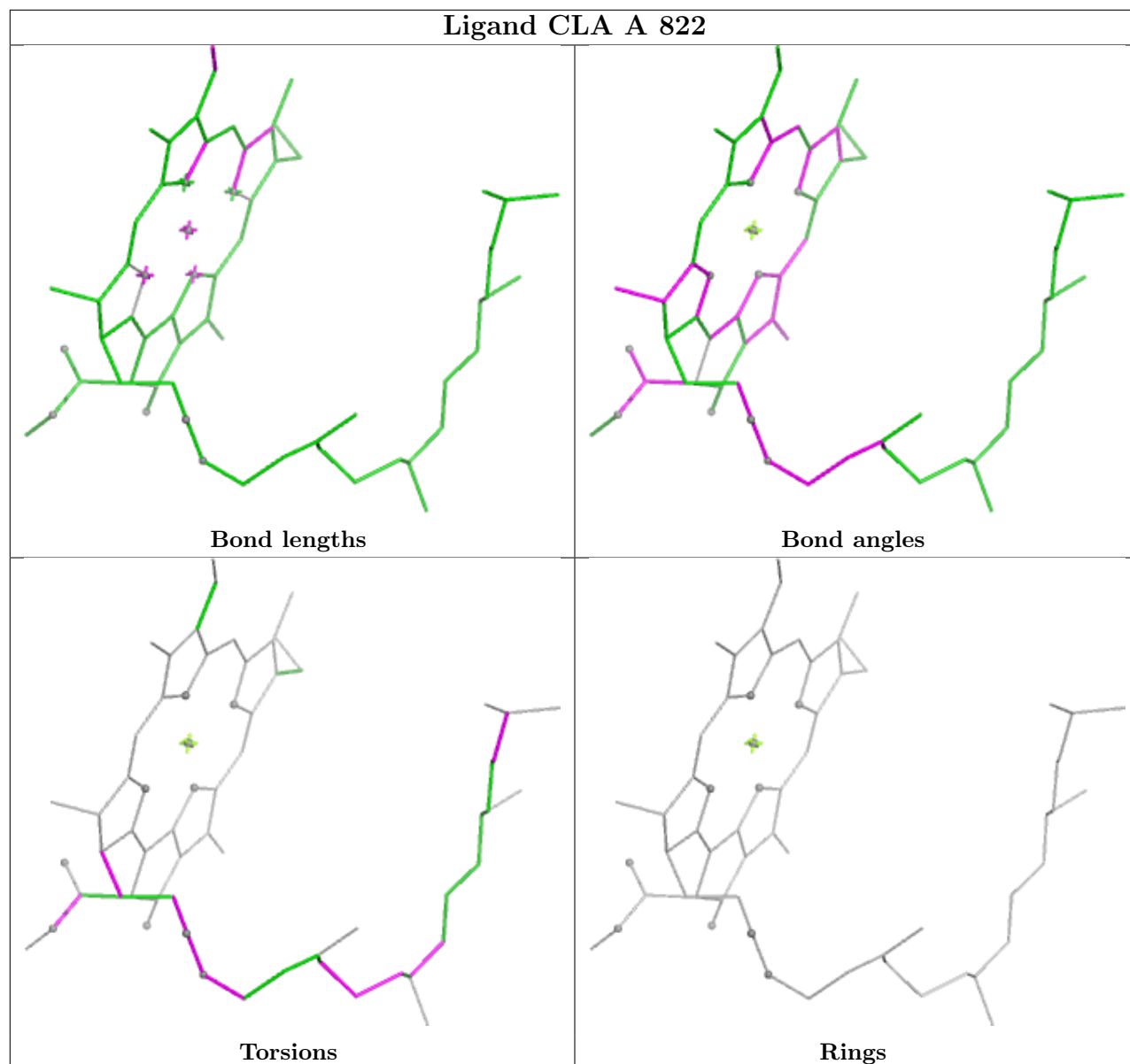




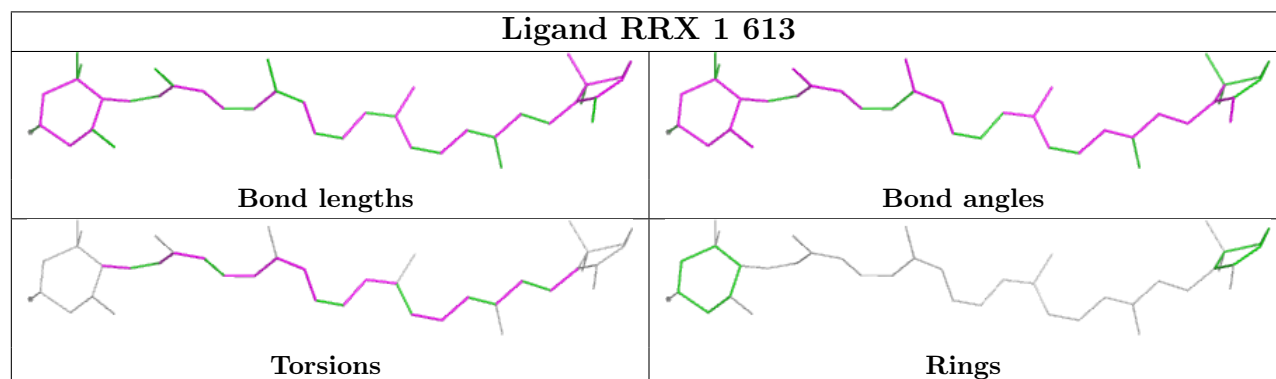


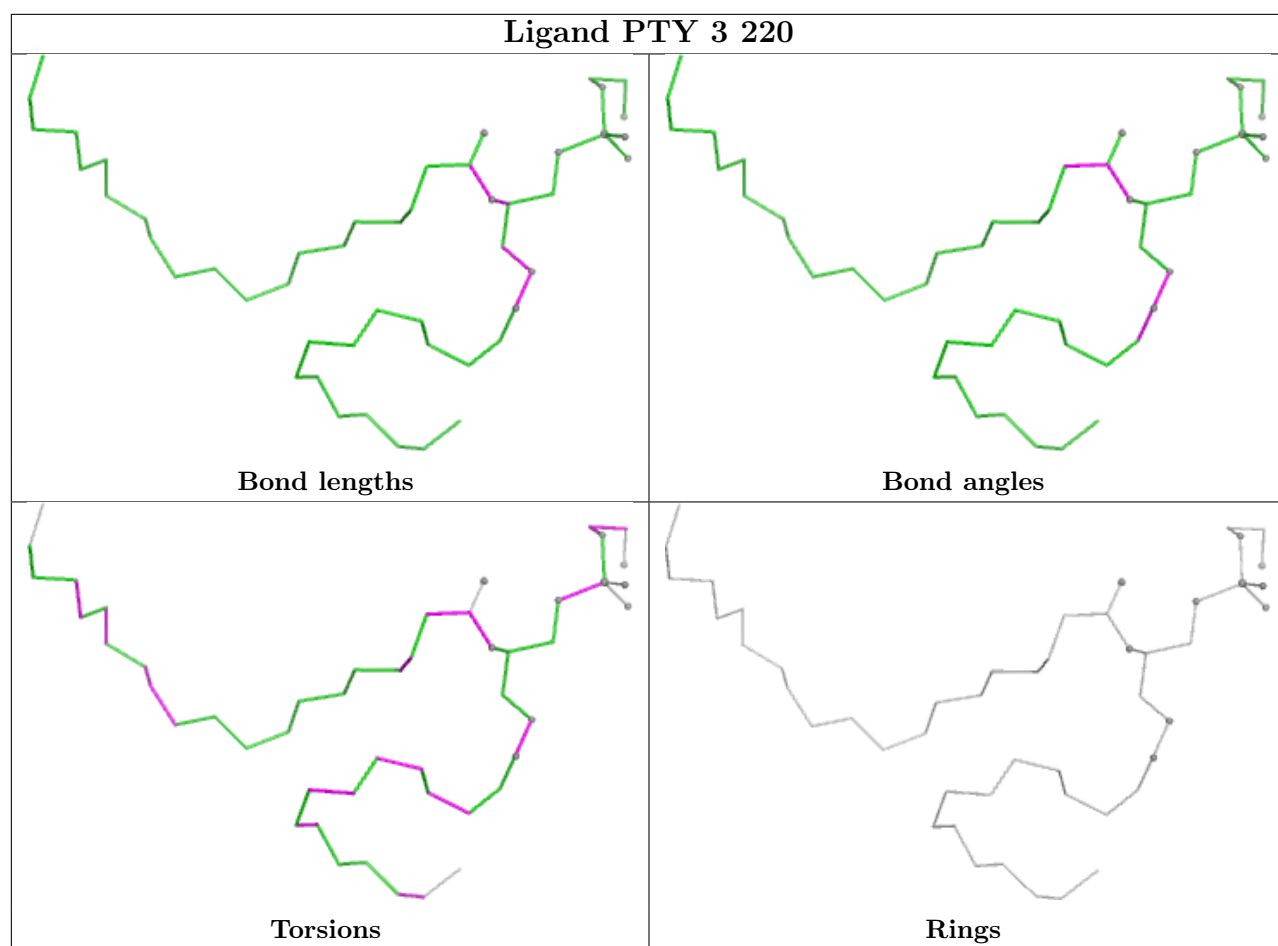


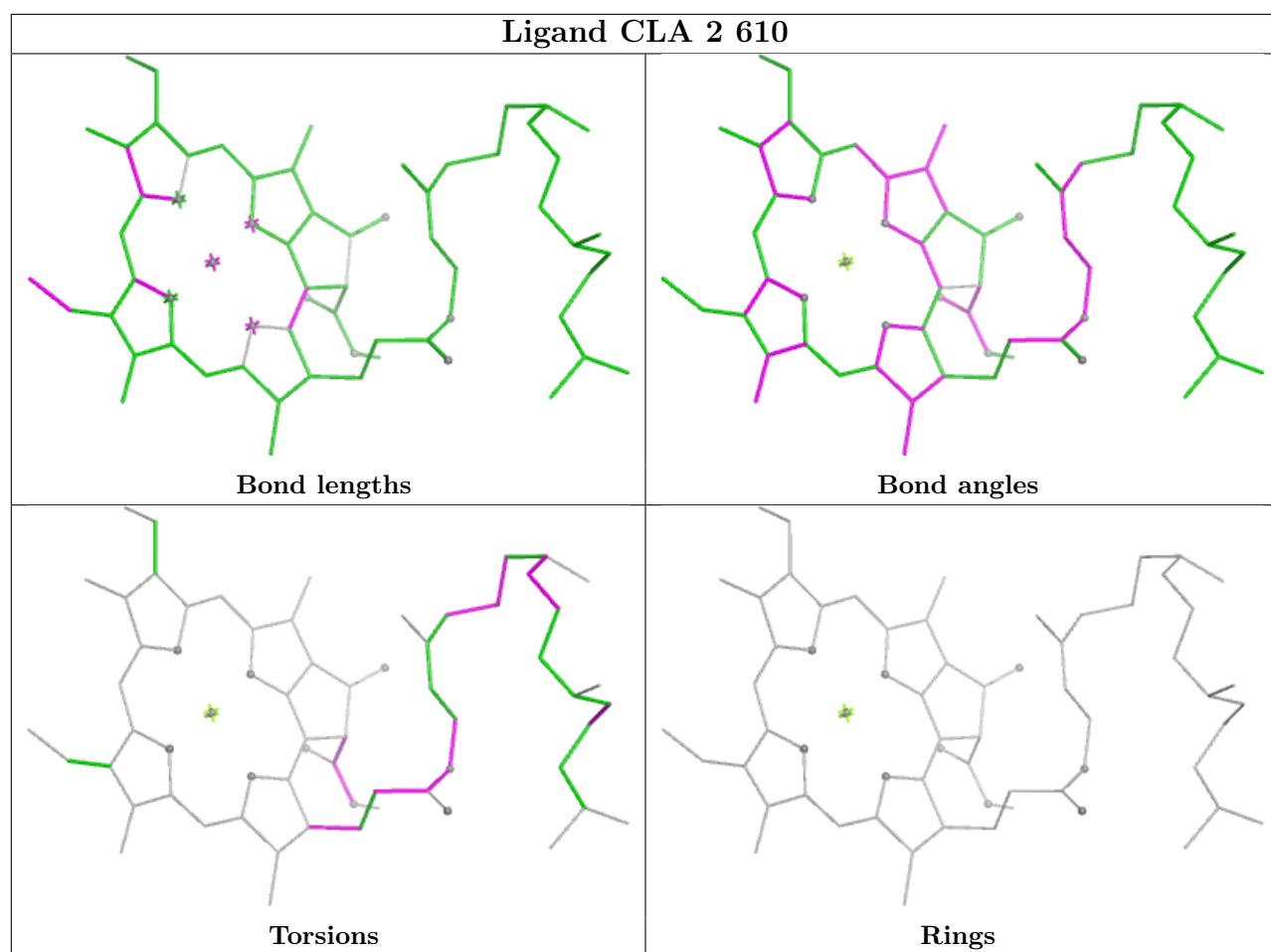
Ligand CLA A 822



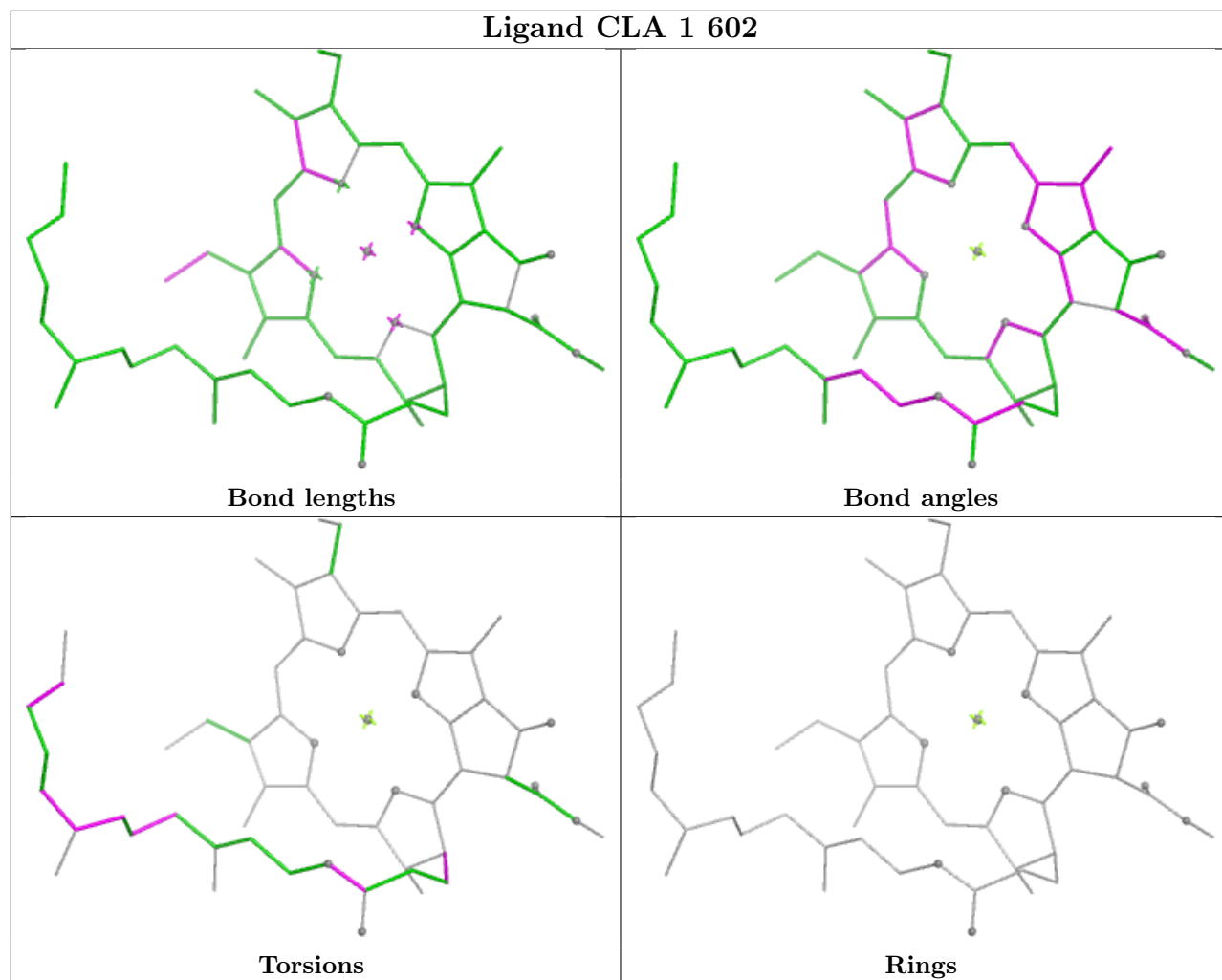
Ligand RRX 1 613

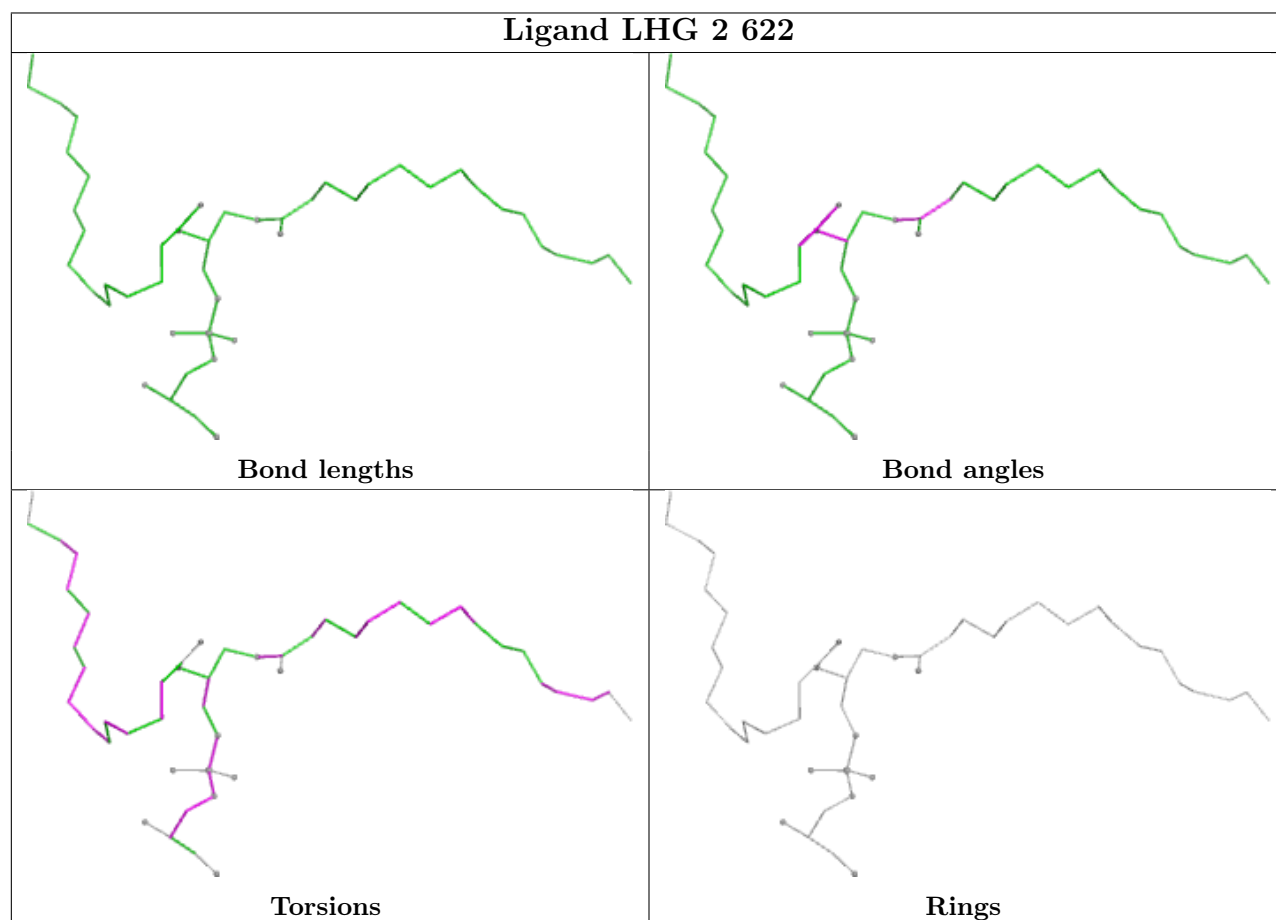
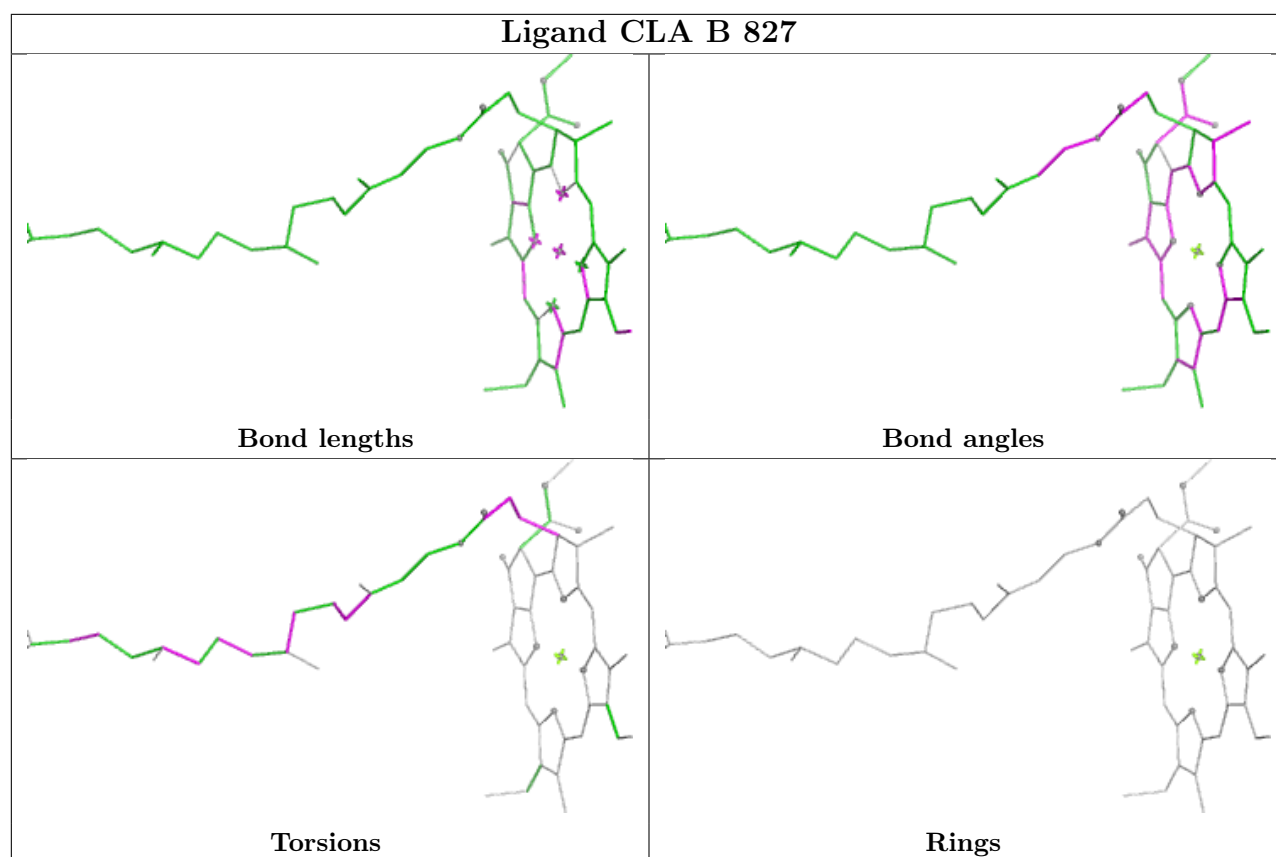


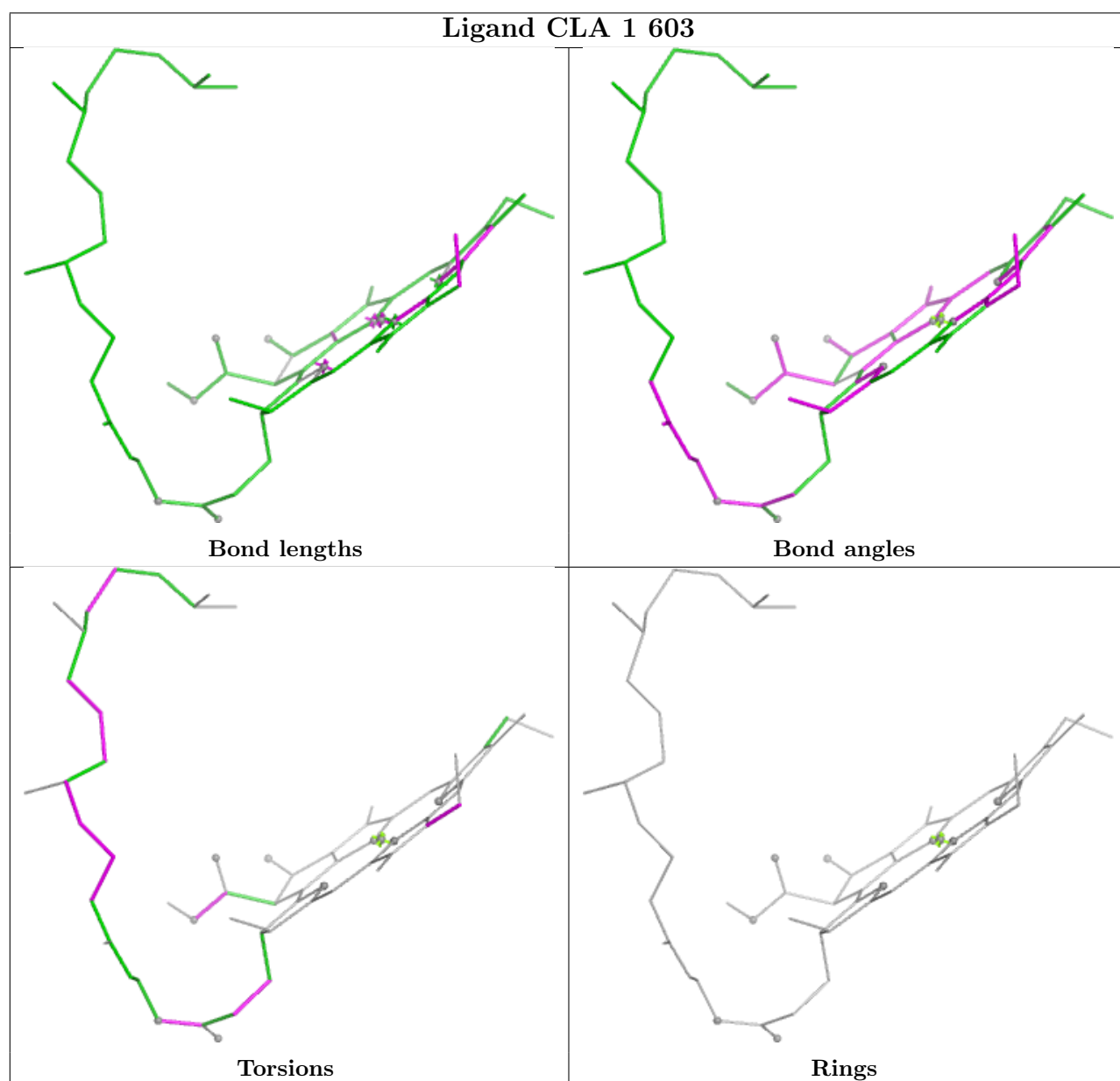
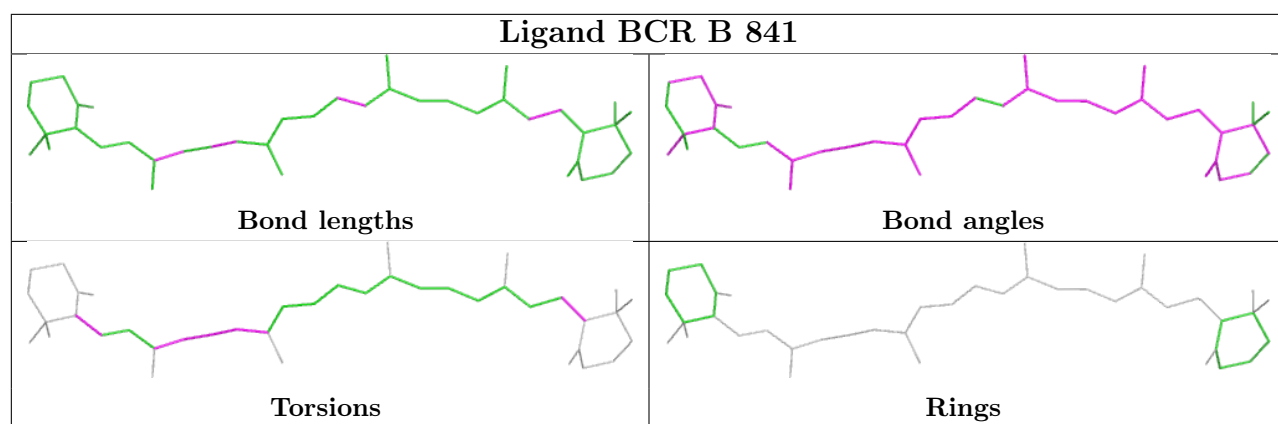


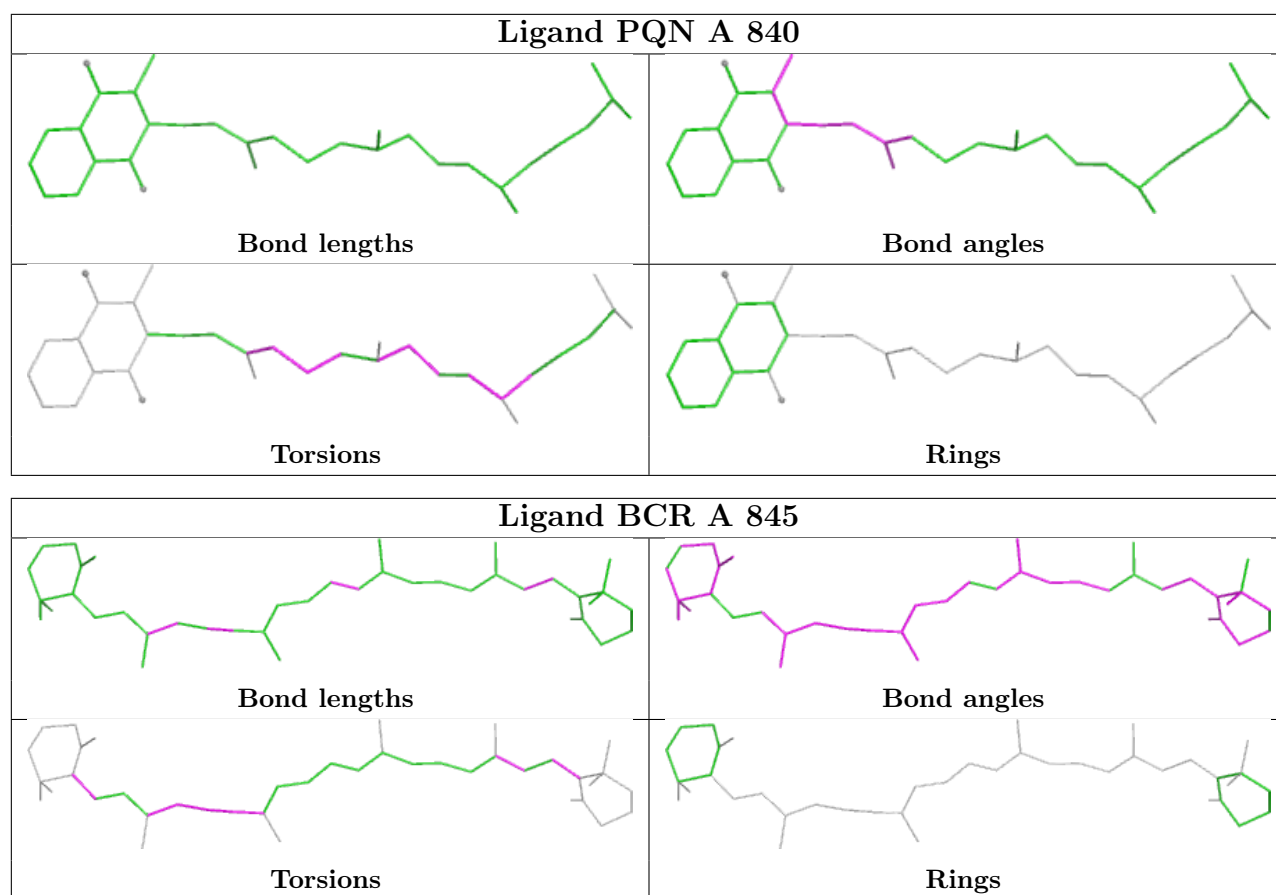


Ligand CLA 1 602

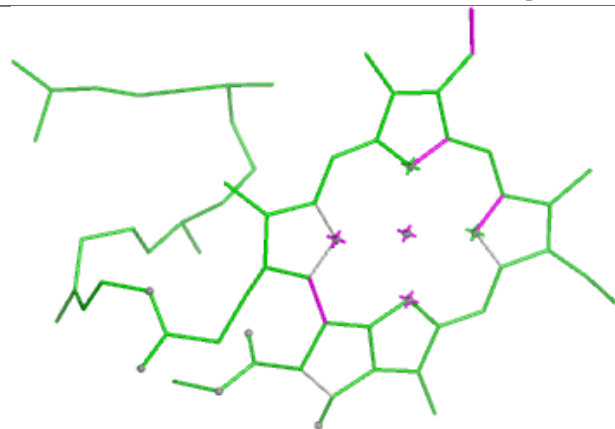




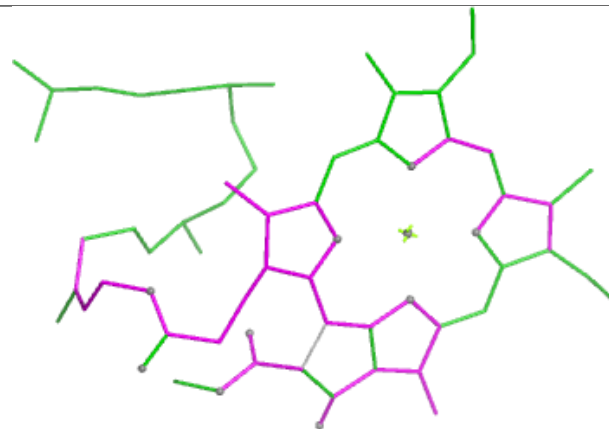




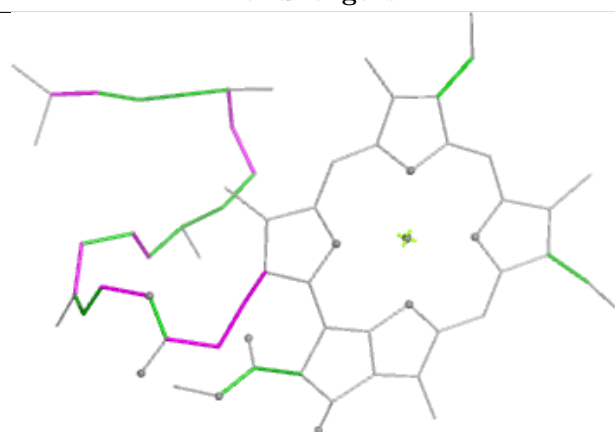
Ligand CLA 3 205



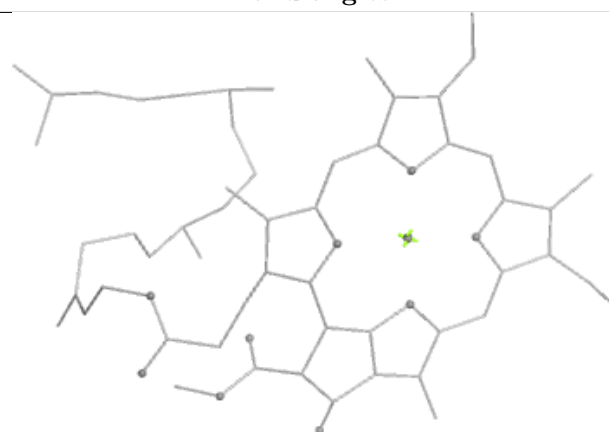
Bond lengths



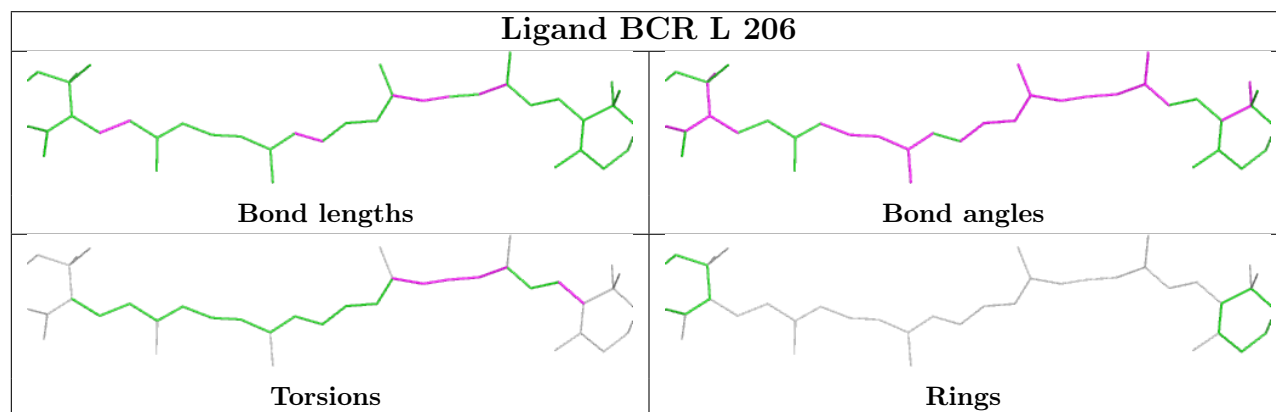
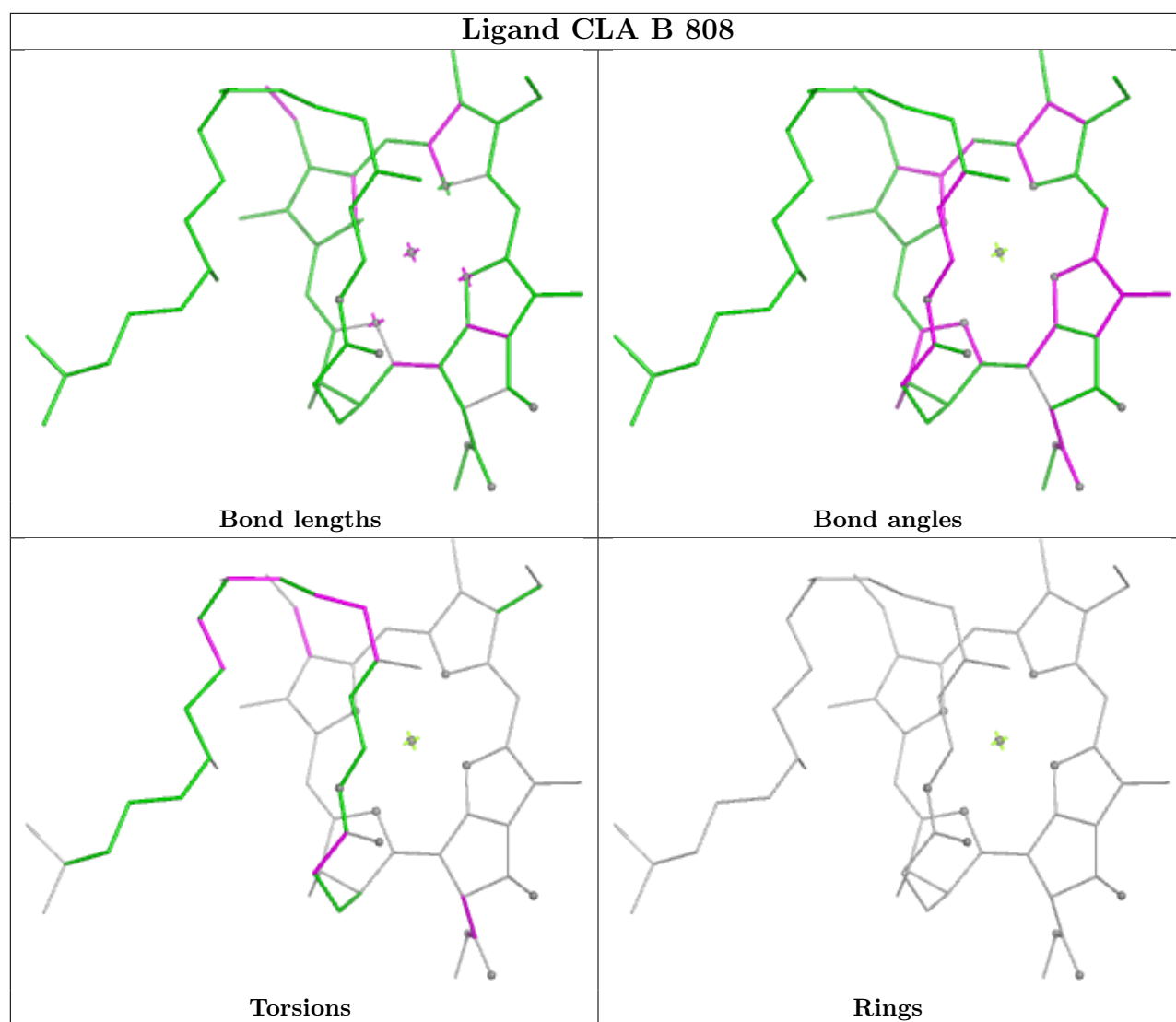
Bond angles

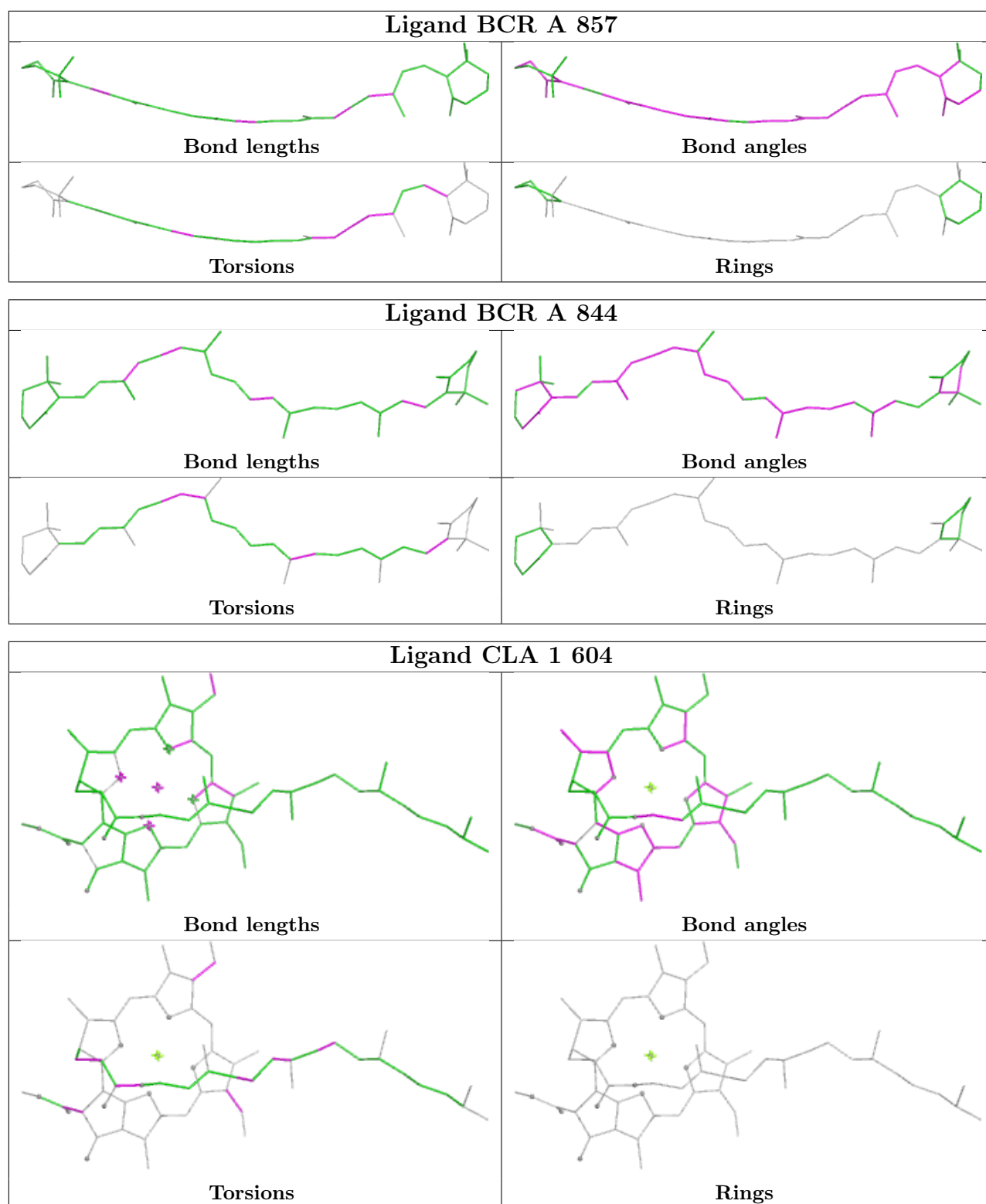


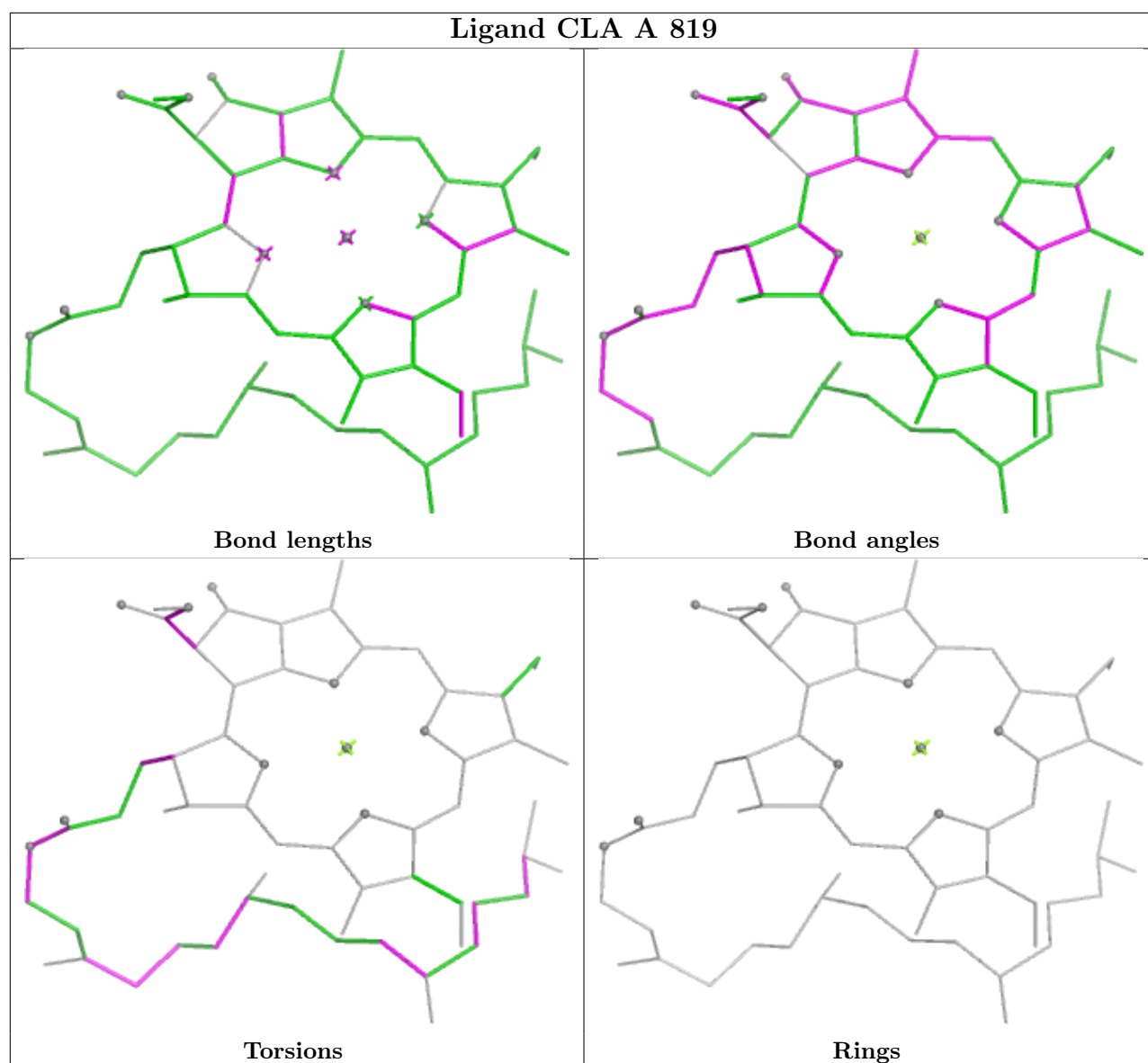
Torsions



Rings







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

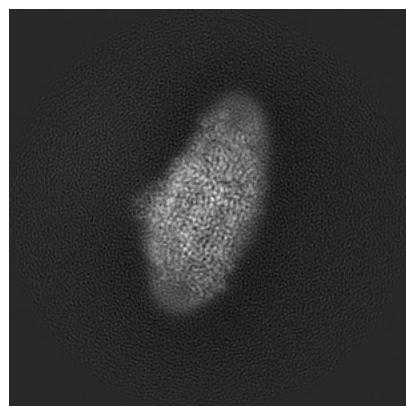
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12228. These allow visual inspection of the internal detail of the map and identification of artifacts.

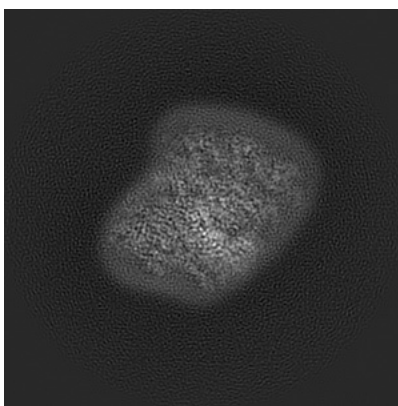
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

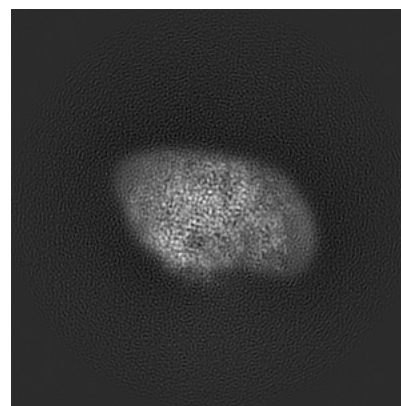
6.1.1 Primary map



X

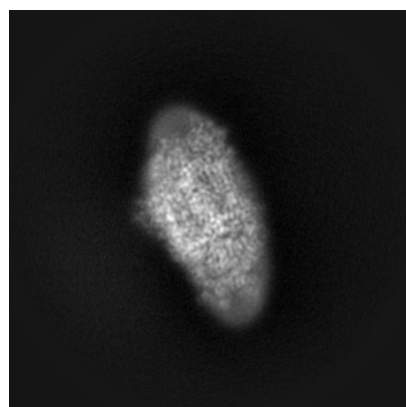


Y

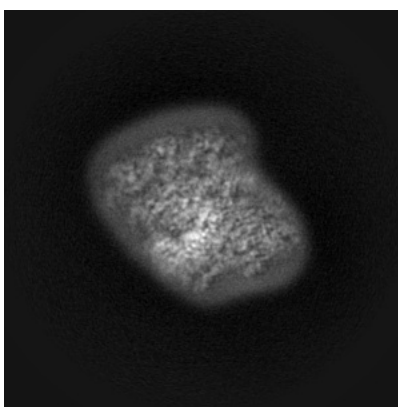


Z

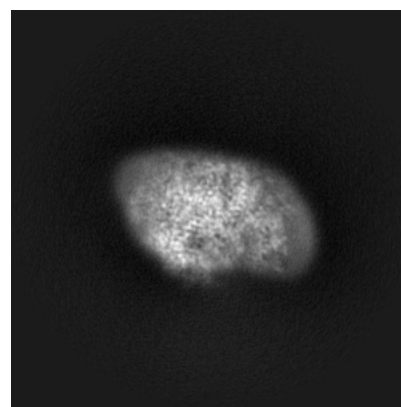
6.1.2 Raw map



X



Y

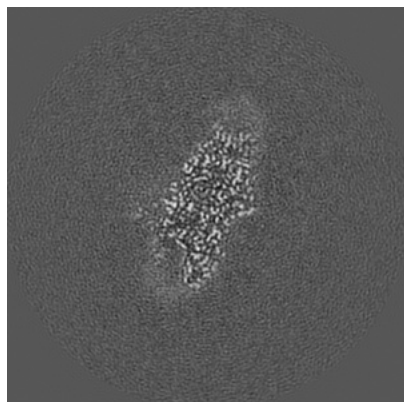


Z

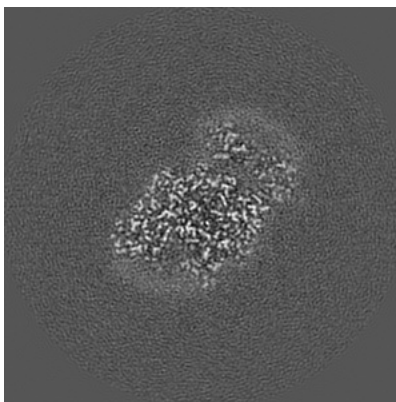
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

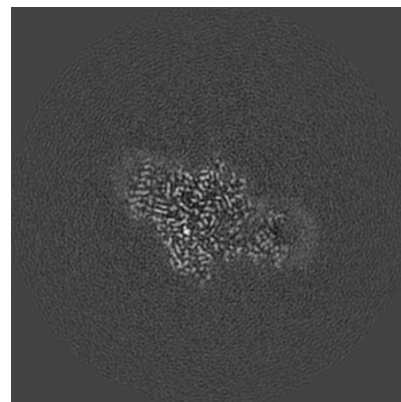
6.2.1 Primary map



X Index: 150

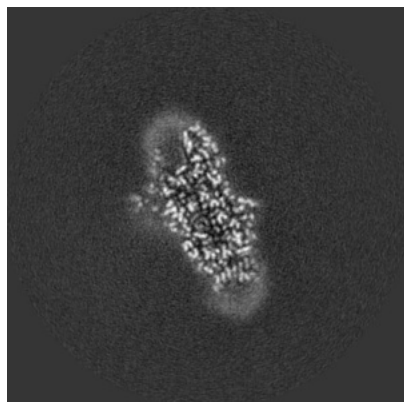


Y Index: 150

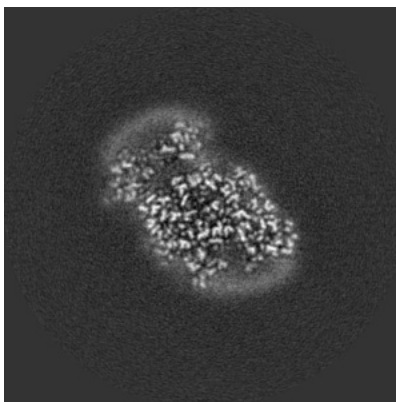


Z Index: 150

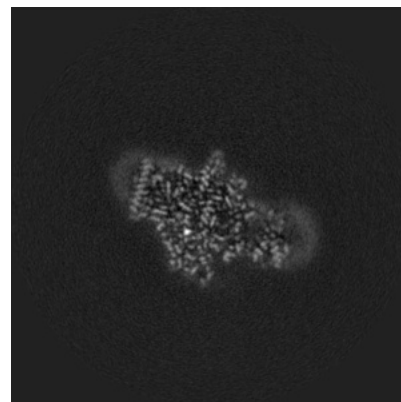
6.2.2 Raw map



X Index: 150



Y Index: 150

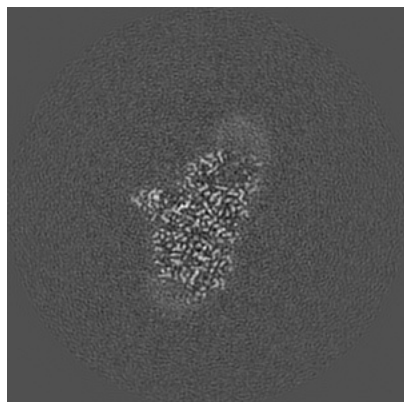


Z Index: 150

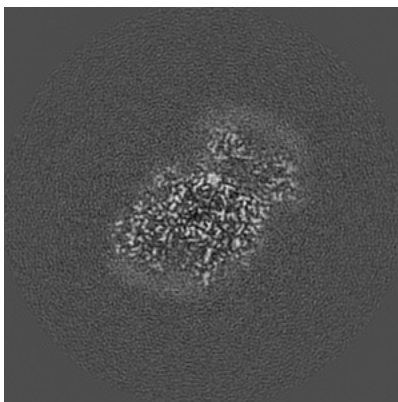
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

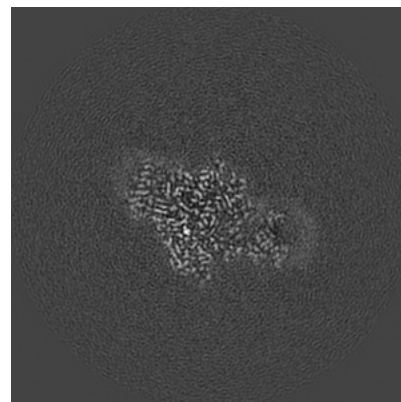
6.3.1 Primary map



X Index: 130

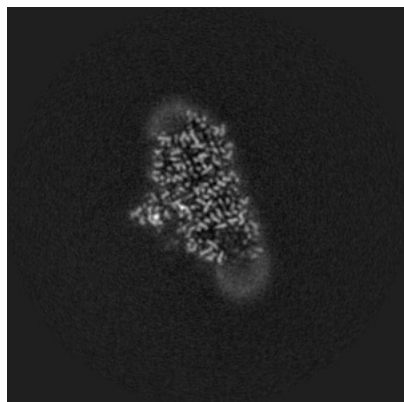


Y Index: 151

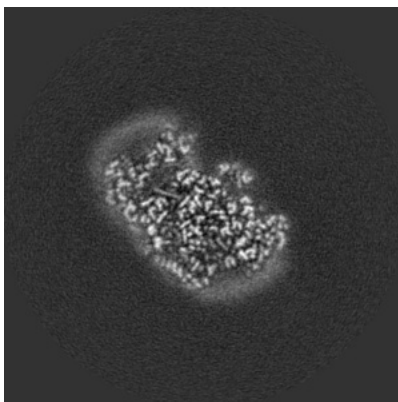


Z Index: 150

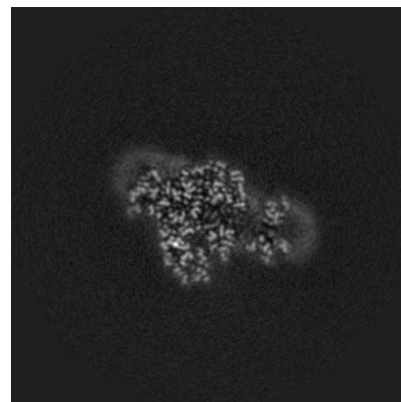
6.3.2 Raw map



X Index: 130



Y Index: 158

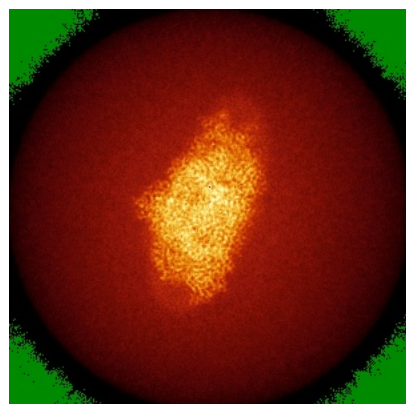


Z Index: 144

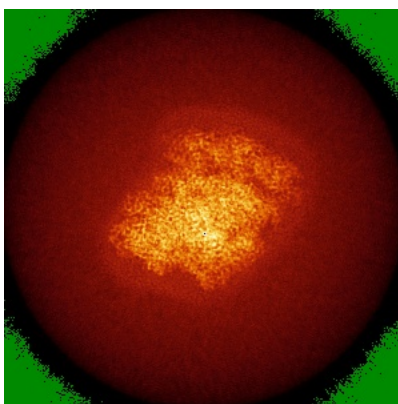
The images above show the largest variance slices of the map in three orthogonal directions.

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

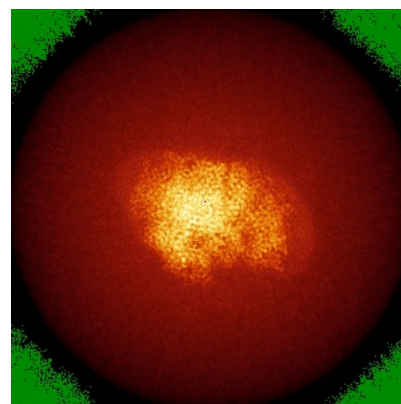
6.4.1 Primary map



X

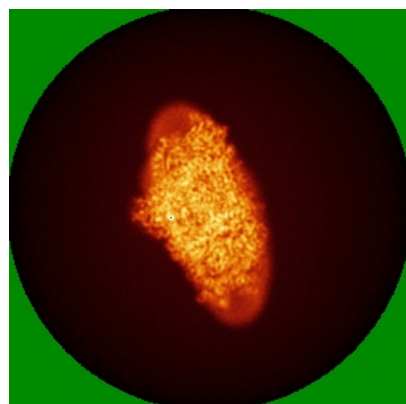


Y

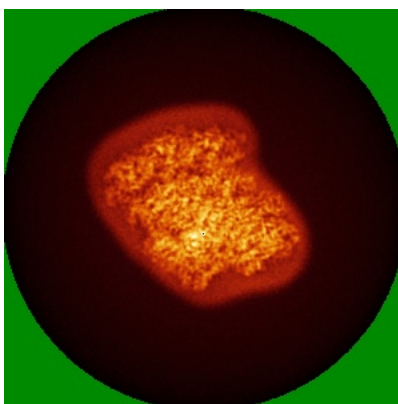


Z

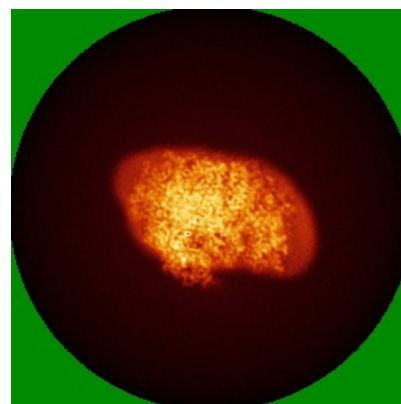
6.4.2 Raw map



X



Y

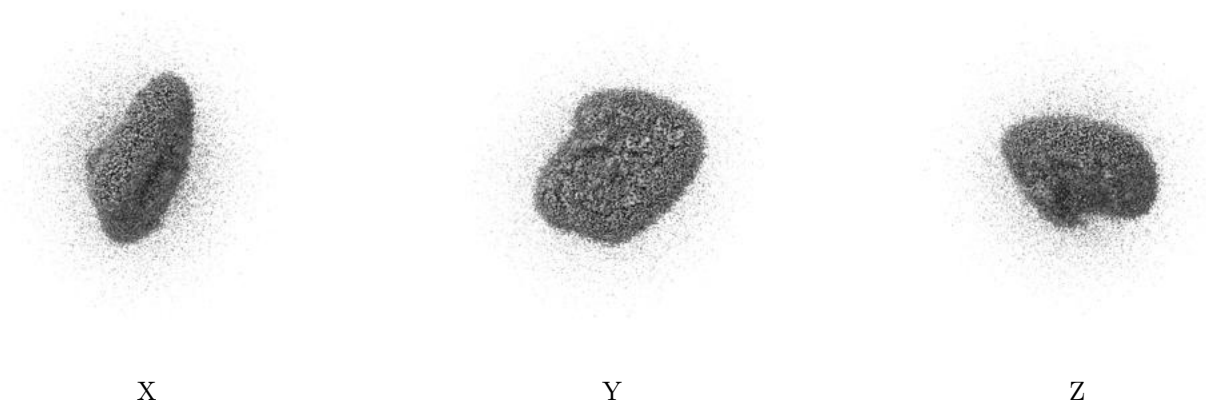


Z

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

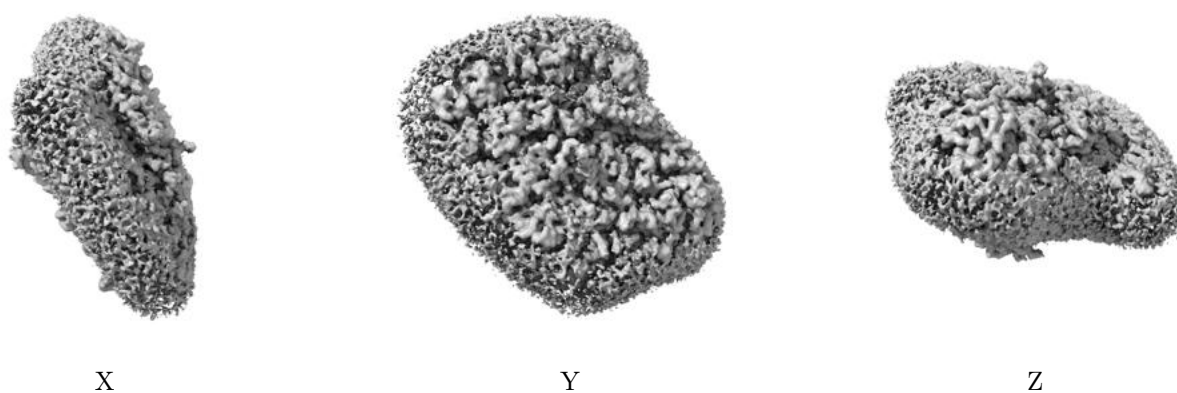
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0186. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

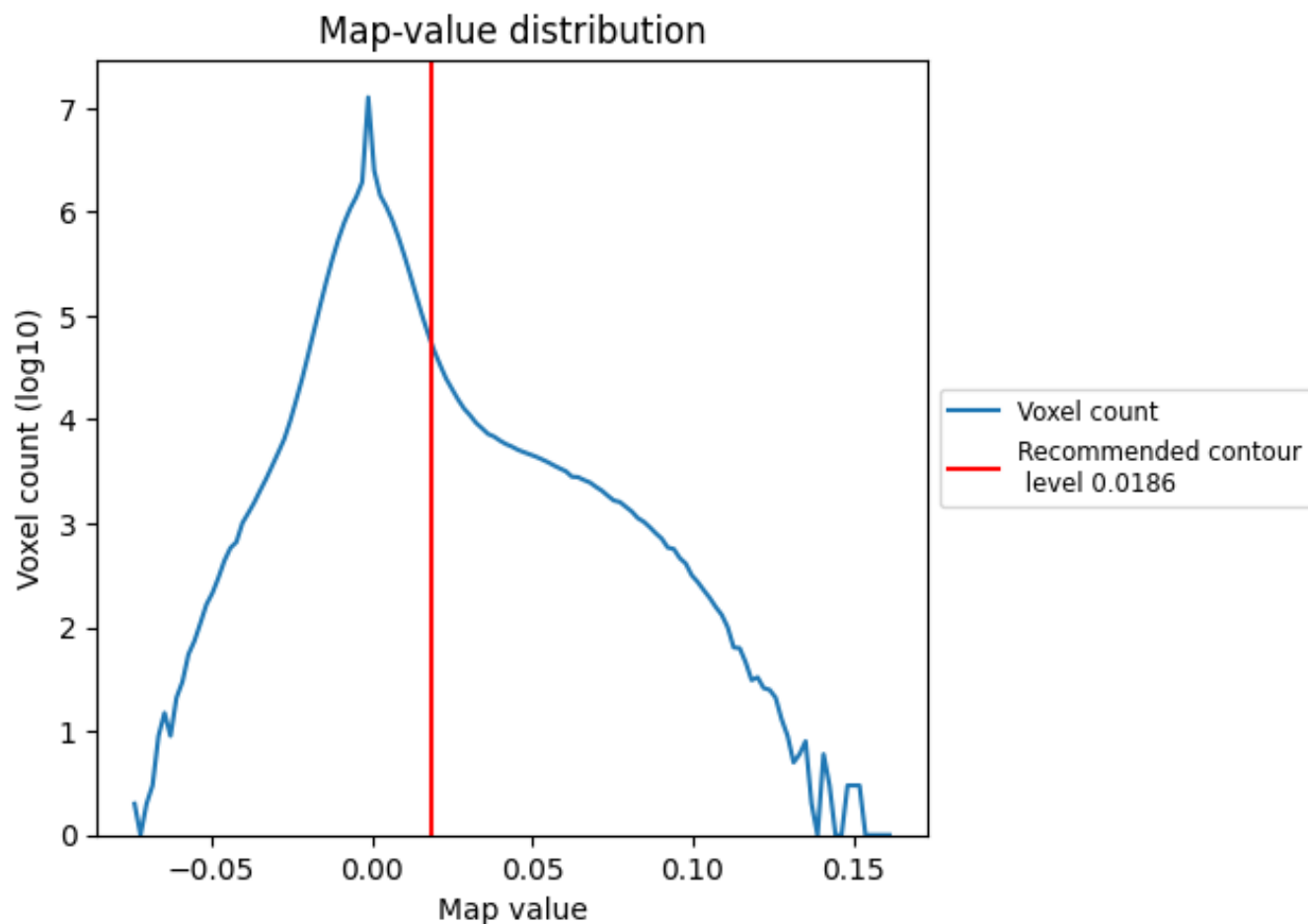
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

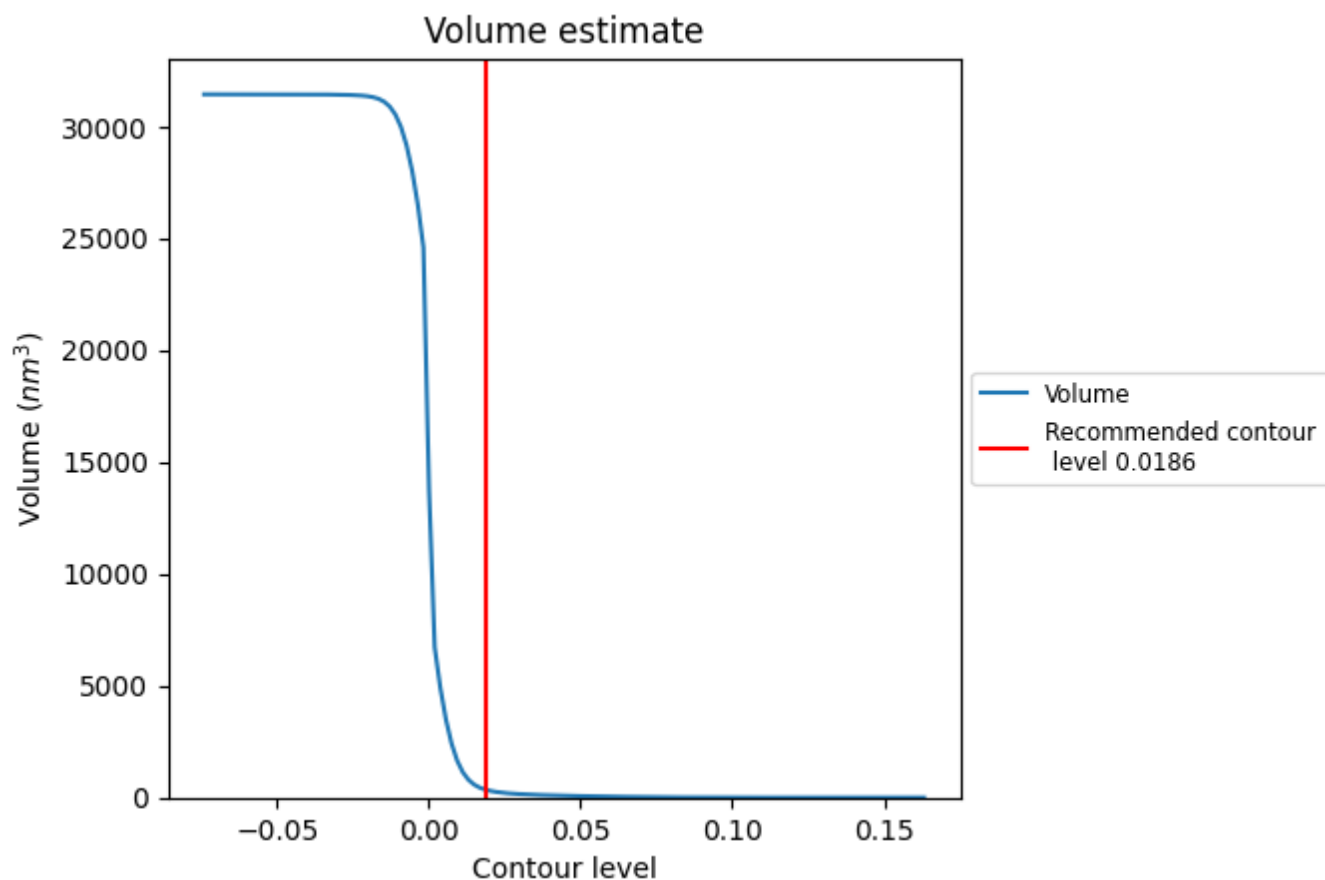
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

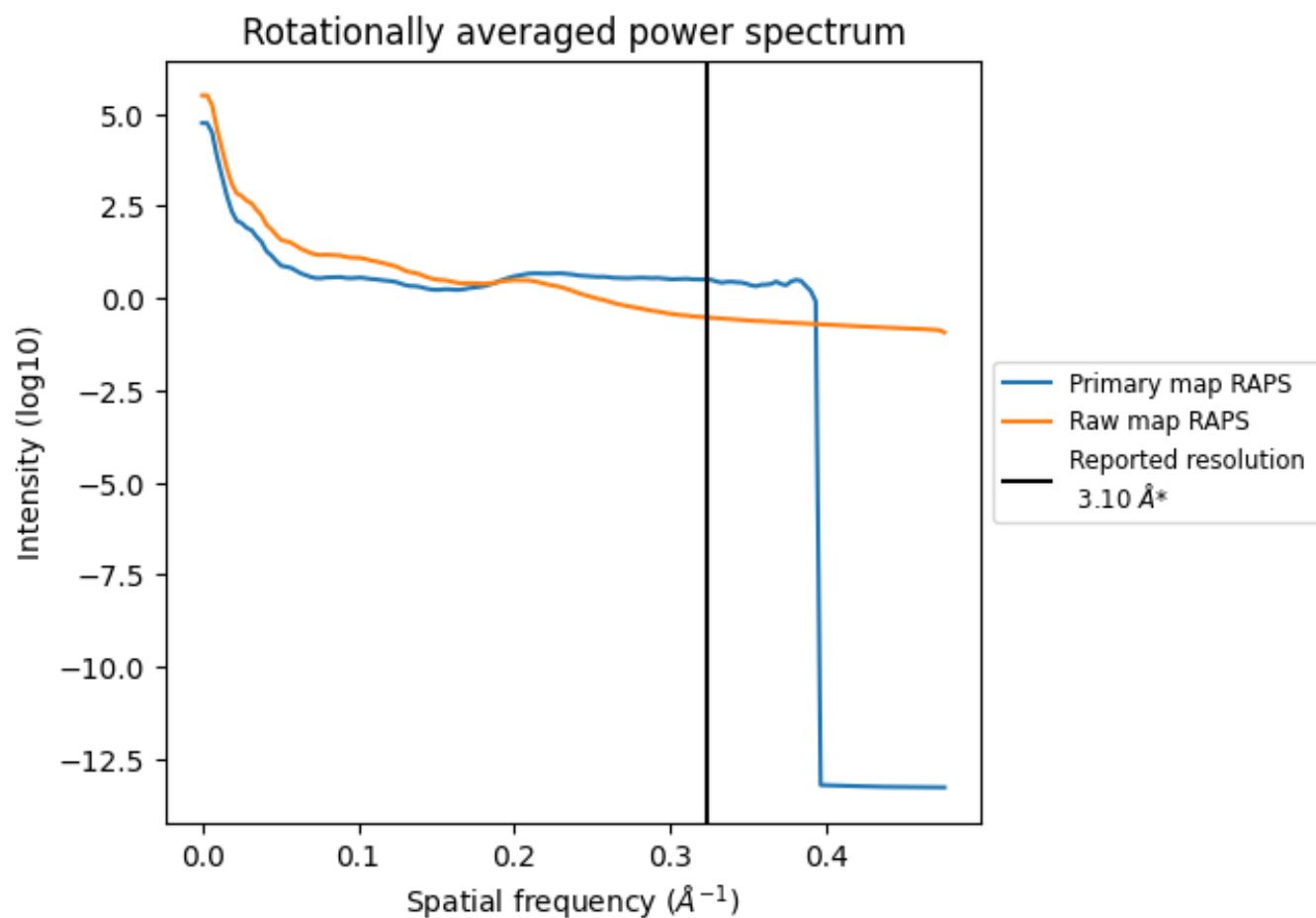
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 355 nm³; this corresponds to an approximate mass of 321 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 ⓘ

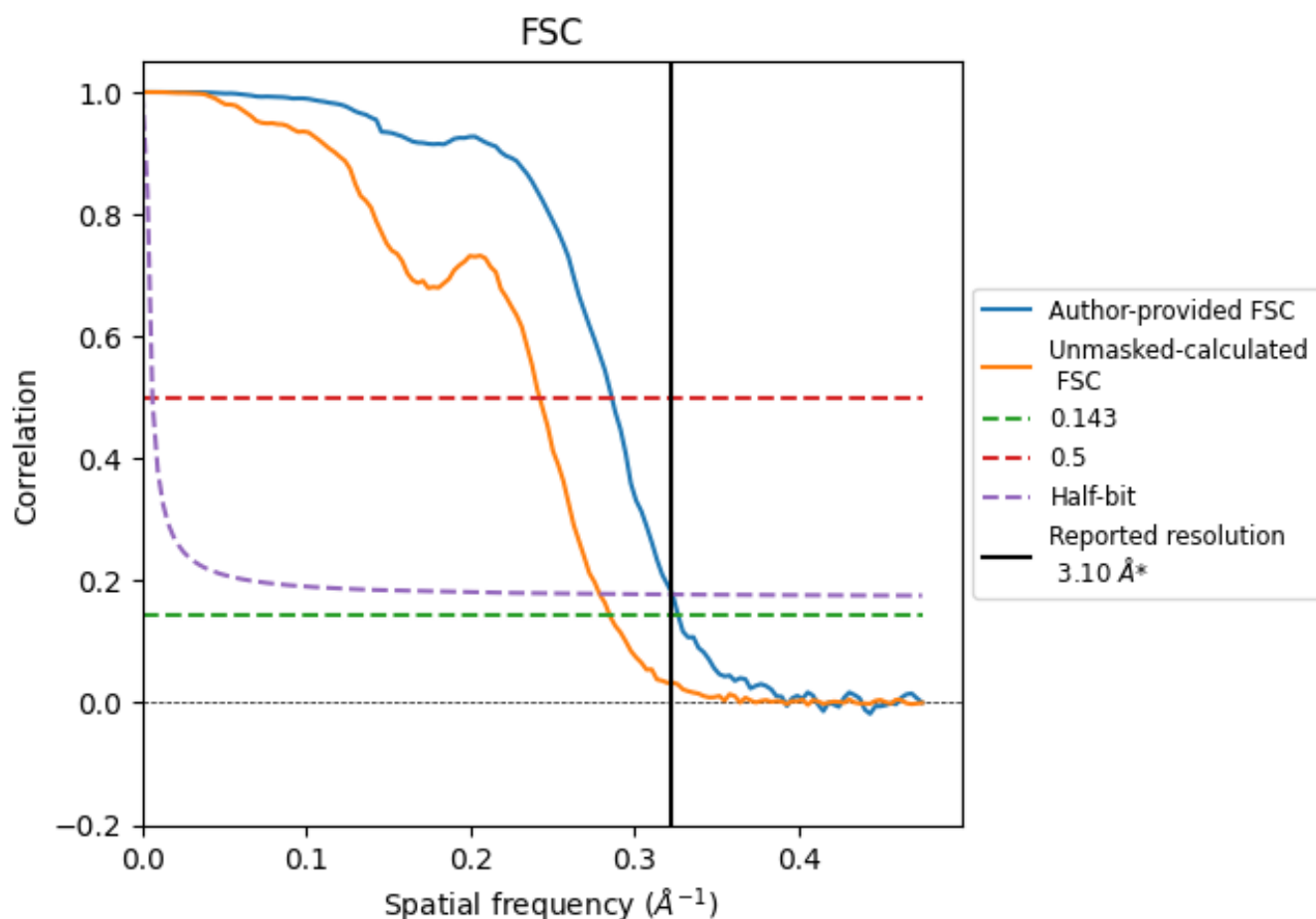


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

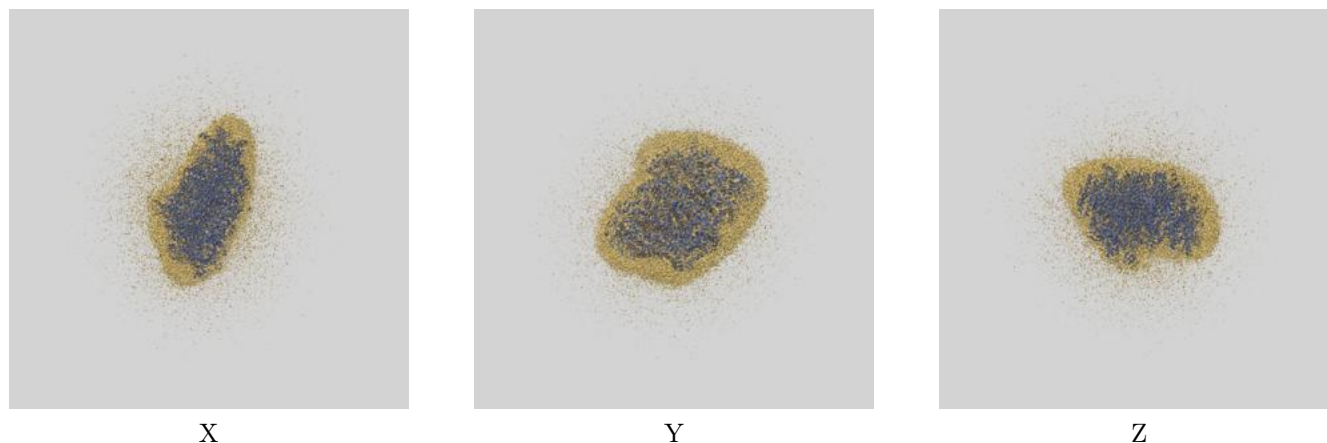
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.50	3.09
Unmasked-calculated*	3.51	4.13	3.59

*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 3.51 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

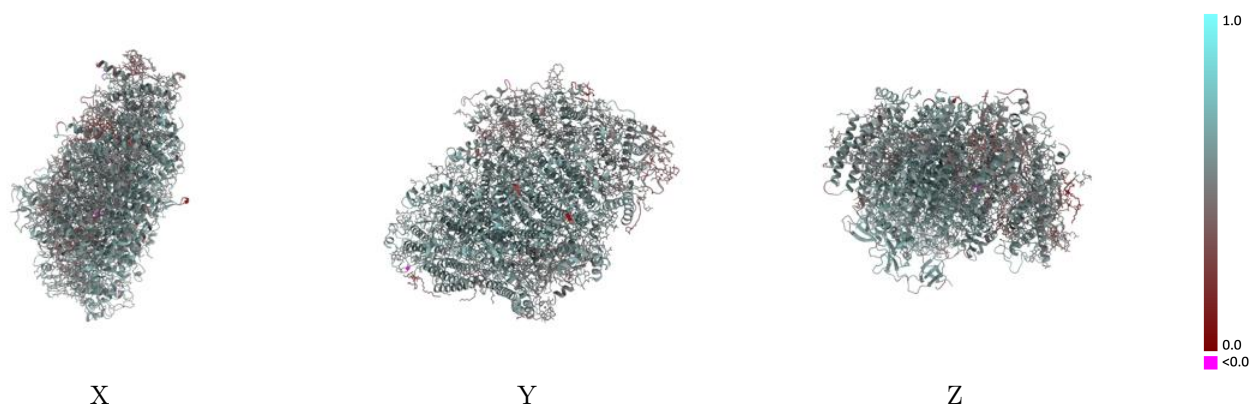
This section contains information regarding the fit between EMDB map EMD-12228 and PDB model 7BLZ. Per-residue inclusion information can be found in [section 3](#) on [page 26](#).

9.1 Map-model overlay [i](#)



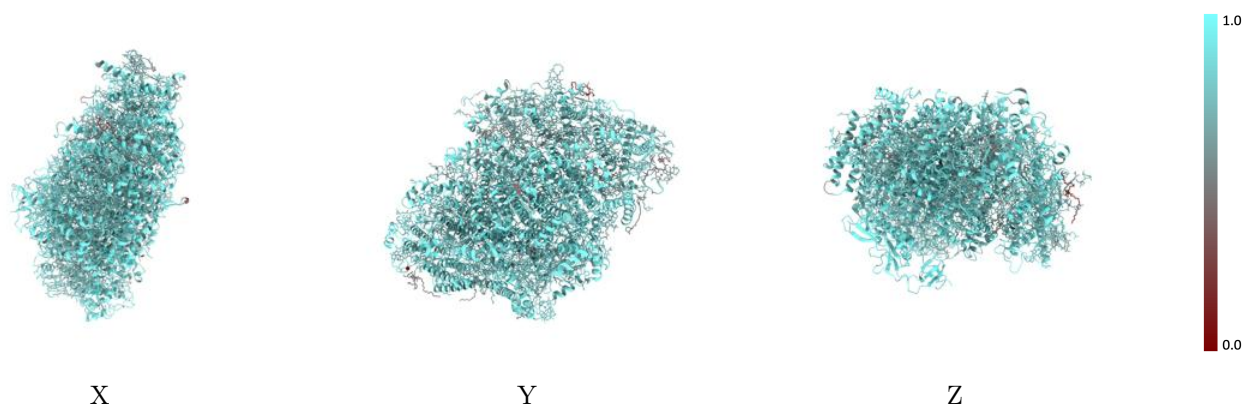
The images above show the 3D surface view of the map at the recommended contour level 0.0186 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



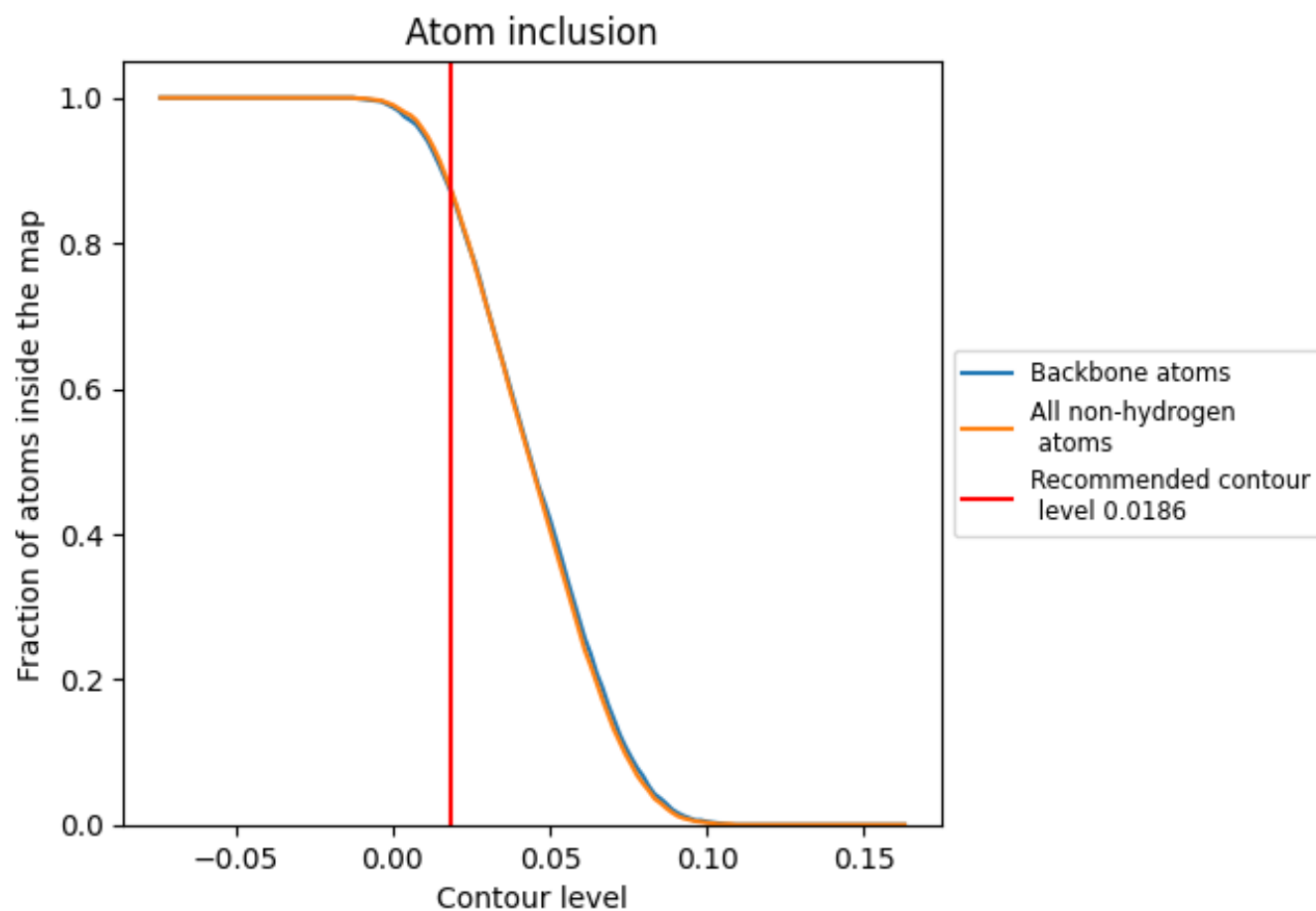
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0186).

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 (0.0186) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.5470
1	0.8140	0.4800
2	0.8130	0.4930
3	0.7950	0.4820
A	0.9140	0.5800
B	0.9070	0.5710
C	0.9570	0.5860
D	0.9220	0.5680
E	0.9130	0.5640
F	0.8730	0.5450
I	0.8770	0.5500
J	0.8240	0.5150
K	0.8230	0.5260
L	0.8480	0.5200
M	0.8720	0.5430
O	0.8450	0.5130

1.0

0.0

<0.0