



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 03:48 am BST

PDB ID : 6TRA
EMDB ID : EMD-10557
Title : Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6
Authors : Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Miehke, T.; Lisdat, F.; Zouni, A.; Wendler, P.
Deposited on : 2019-12-18
Resolution : 2.85 Å(reported)
Based on initial model : 1JB0

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

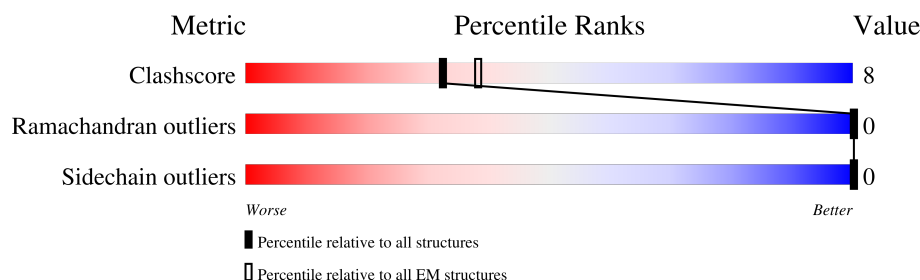
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.85 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	755	<div> <div>9%</div> <div>82%</div> <div>17%</div> <div>.</div> </div>
2	B	741	<div> <div>11%</div> <div>84%</div> <div>16%</div> </div>
3	C	81	<div> <div>11%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
4	D	139	<div> <div>26%</div> <div>88%</div> <div>12%</div> <div>.</div> </div>
5	E	76	<div> <div>30%</div> <div>82%</div> <div>11%</div> <div>8%</div> </div>
6	F	141	<div> <div>65%</div> <div>86%</div> <div>14%</div> </div>
7	I	38	<div> <div>21%</div> <div>68%</div> <div>32%</div> </div>
8	J	41	<div> <div>61%</div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain
9	K	83	
10	L	155	
11	M	31	
12	X	36	

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
13	CL0	A	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	854	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	B	842	X	-	-	-
14	CLA	F	201	X	-	-	-
14	CLA	F	203	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	M	102	X	-	-	-
14	CLA	X	1701	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 25197 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		

- Molecule 3 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	70	Total	C	N	O	0	0
			546	347	94	105		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			303	209	40	49	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	79	Total	C	N	O	S	0	0
			571	377	92	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	27	Total	C	N	O	0	0
			228	163	33	32		

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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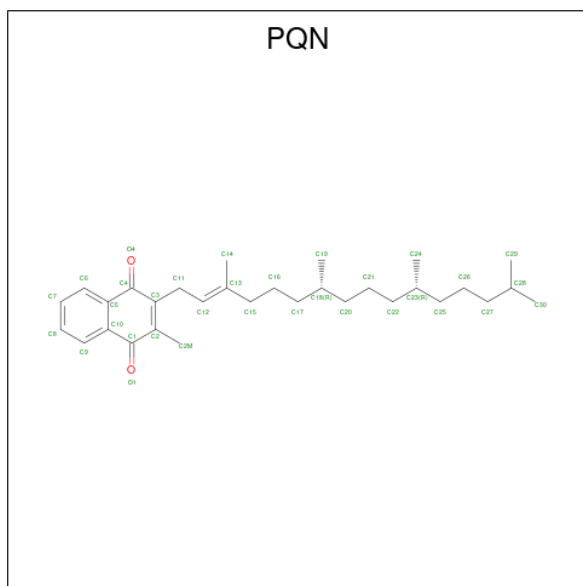
Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	F	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0

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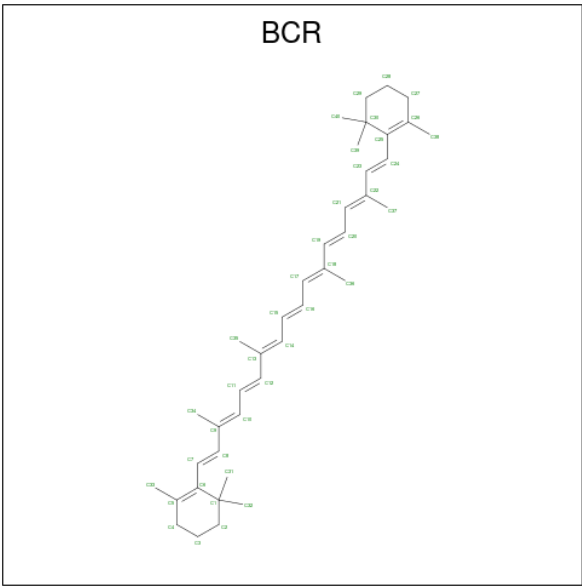
Mol	Chain	Residues	Atoms					AltConf
14	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	K	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	M	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	X	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



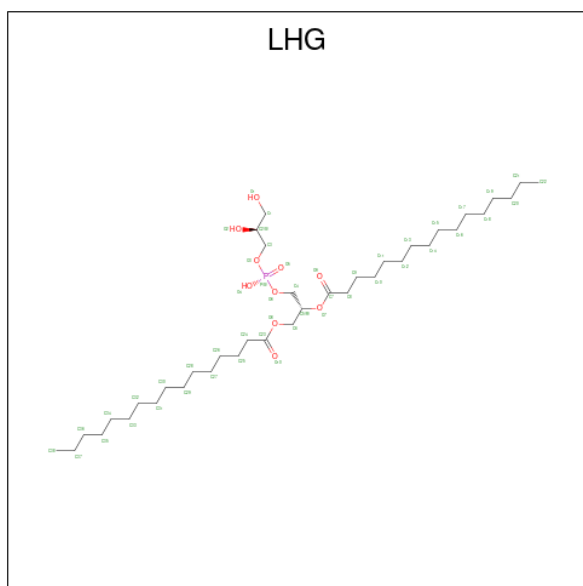
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40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

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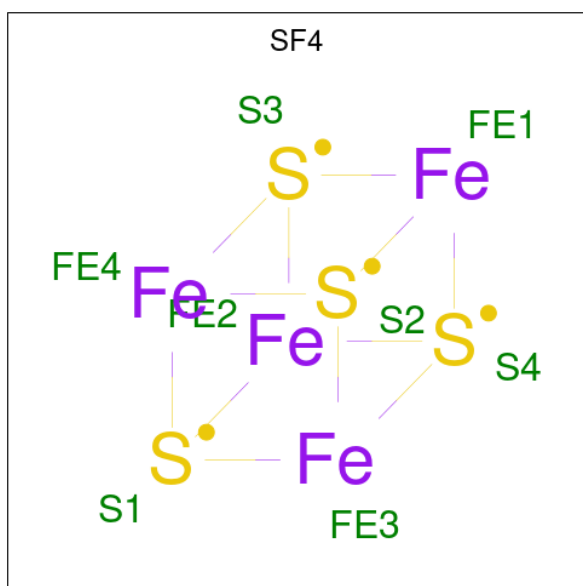
Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 25 25	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	B	1	Total	C	O	P	0
			49	38	10	1	
17	I	1	Total	C	O	P	0
			39	28	10	1	
17	M	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

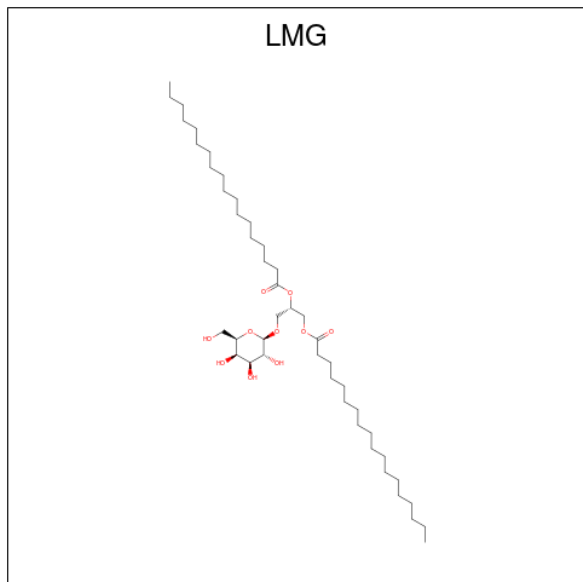


Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Ca	0
			1	1	
19	L	1	Total	Ca	0
			1	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			55	45	10	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	65	Total	O	0
			65	65	
21	B	77	Total	O	0
			77	77	
21	C	25	Total	O	0
			25	25	
21	D	23	Total	O	0
			23	23	
21	E	9	Total	O	0
			9	9	
21	F	4	Total	O	0
			4	4	
21	I	1	Total	O	0
			1	1	
21	J	1	Total	O	0
			1	1	
21	K	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
21	L	10	Total 10	O 10	0
21	M	1	Total 1	O 1	0

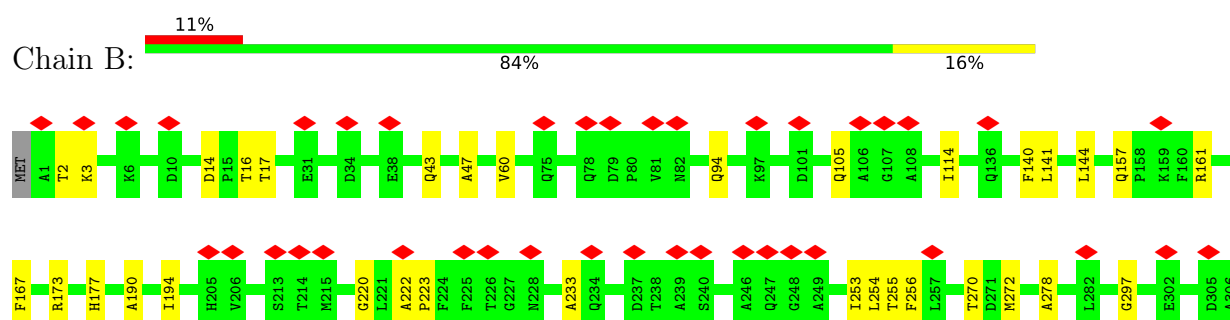
3 Residue-property plots

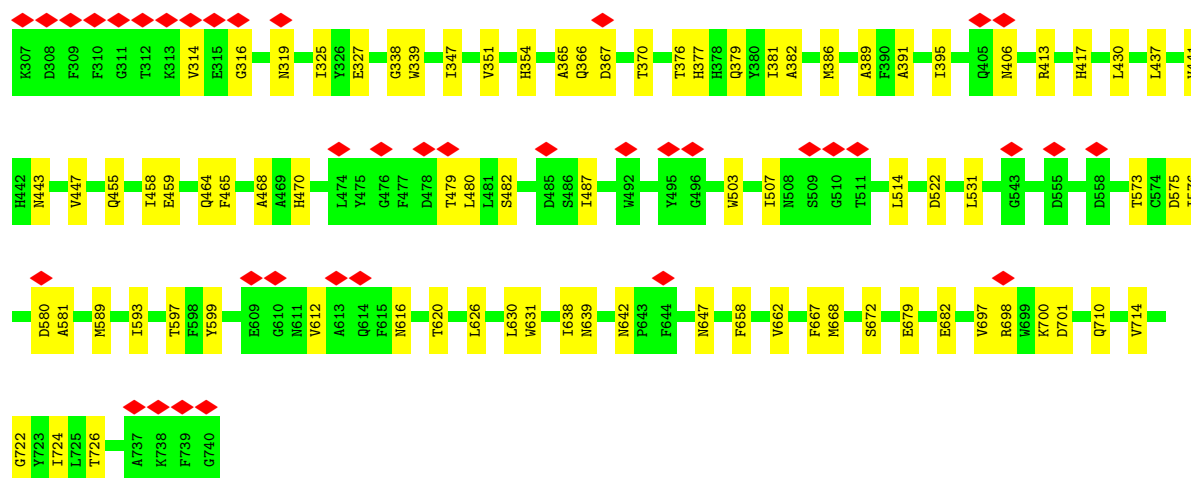
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

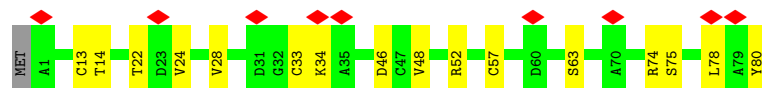


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

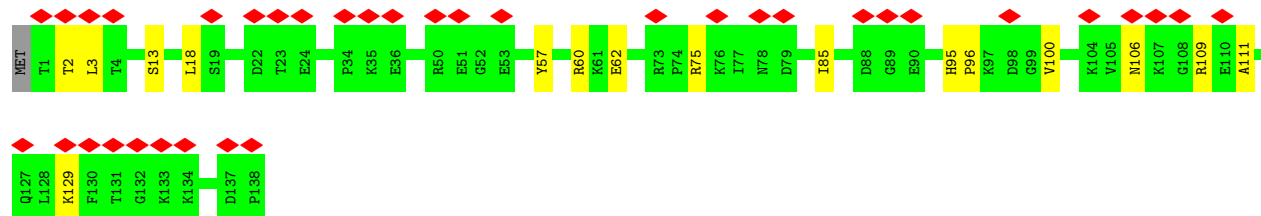
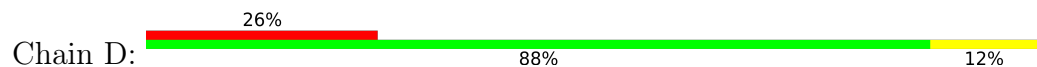




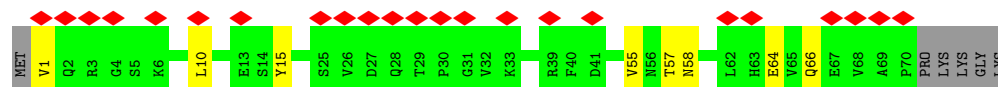
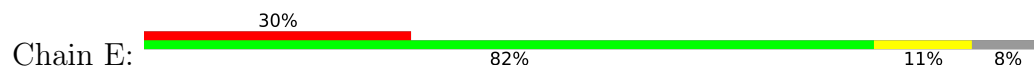
- Molecule 3: Photosystem I iron-sulfur center



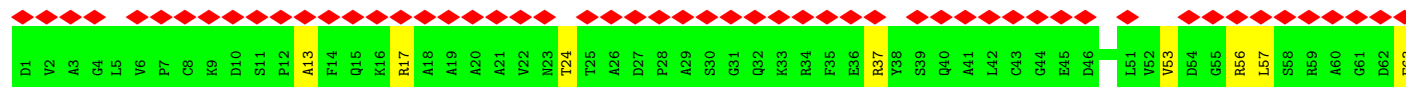
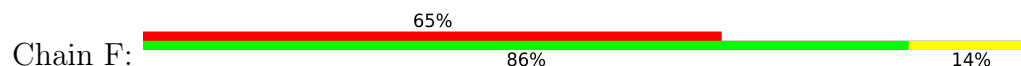
- Molecule 4: Photosystem I reaction center subunit II

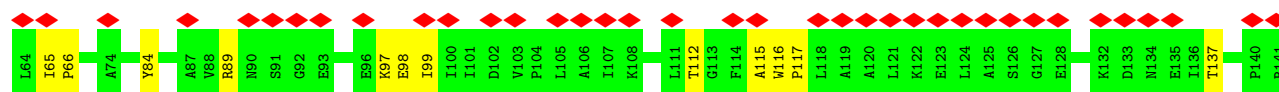


- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit III





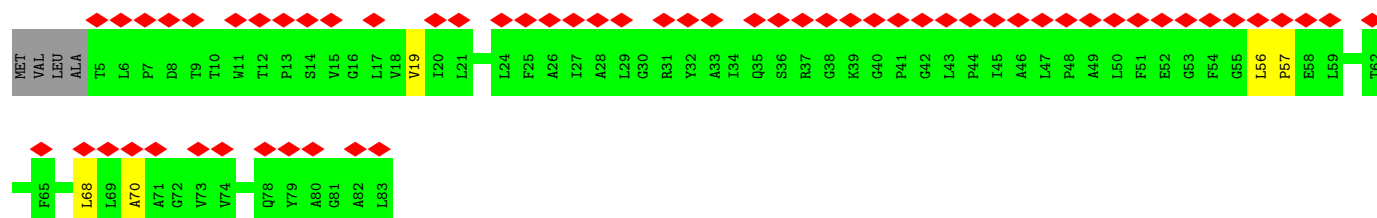
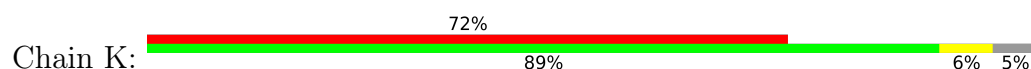
• Molecule 7: Photosystem I reaction center subunit VIII



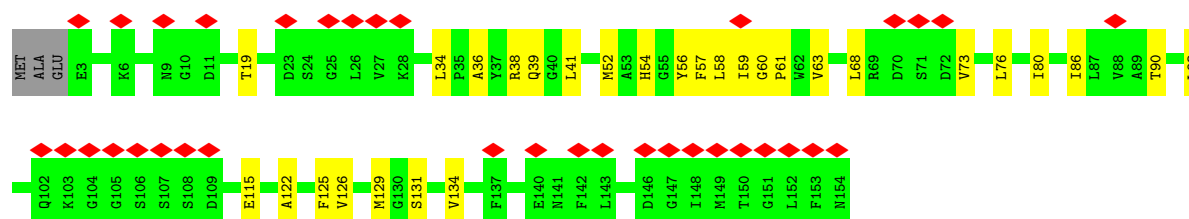
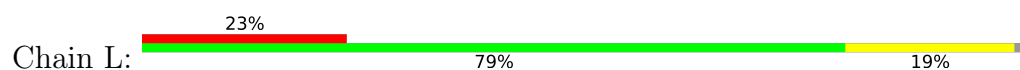
• Molecule 8: Photosystem I reaction center subunit IX



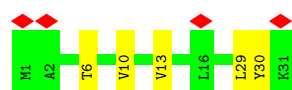
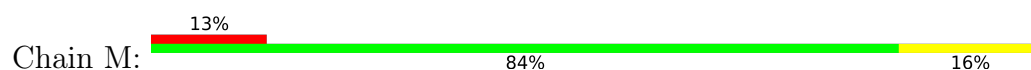
• Molecule 9: Photosystem I reaction center subunit PsaK



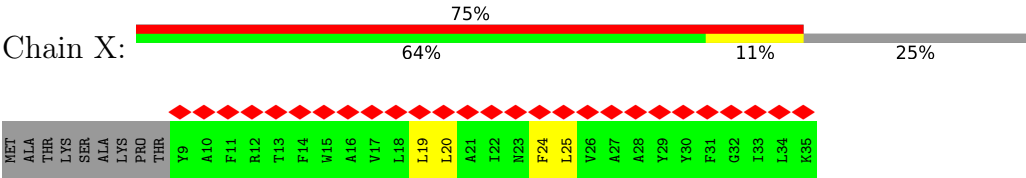
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 12: Photosystem I 4.8K protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.017	Depositor
Map size (\AA)	351.68002, 351.68002, 351.68002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.628, 0.628, 0.628	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: CA, CLA, SF4, LMG, BCR, LHG, PQN, CL0, FME

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/6027	0.43	0/8220
2	B	0.31	0/6112	0.43	0/8350
3	C	0.32	0/608	0.45	0/824
4	D	0.30	0/1101	0.47	0/1492
5	E	0.31	0/559	0.42	0/762
6	F	0.27	0/1087	0.44	0/1476
7	I	0.31	0/304	0.45	0/415
8	J	0.27	0/342	0.40	0/467
9	K	0.27	0/585	0.45	0/800
10	L	0.30	0/1153	0.42	0/1565
11	M	0.31	0/244	0.43	0/332
12	X	0.27	0/236	0.38	0/321
All	All	0.30	0/18358	0.44	0/25024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5826	0	5692	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5894	0	5653	99	0
3	C	598	0	580	13	0
4	D	1075	0	1077	18	0
5	E	546	0	535	7	0
6	F	1065	0	1077	15	0
7	I	303	0	305	9	0
8	J	340	0	346	1	0
9	K	571	0	593	3	0
10	L	1124	0	1127	22	0
11	M	241	0	264	5	0
12	X	228	0	234	4	0
13	A	65	0	72	1	0
14	A	2674	0	2849	82	0
14	B	2446	0	2562	64	0
14	F	153	0	127	4	0
14	J	82	0	58	2	0
14	K	104	0	88	4	0
14	L	260	0	288	7	0
14	M	36	0	24	0	0
14	X	45	0	33	1	0
15	A	33	0	46	2	0
15	B	33	0	46	0	0
16	A	265	0	369	18	0
16	B	320	0	448	13	0
16	F	80	0	112	1	0
16	I	80	0	112	3	0
16	J	80	0	112	6	0
16	K	25	0	33	4	0
16	L	80	0	112	1	0
17	A	90	0	129	4	0
17	B	49	0	74	1	0
17	I	39	0	51	2	0
17	M	49	0	74	1	0
18	B	8	0	0	0	0
18	C	16	0	0	0	0
19	B	1	0	0	0	0
19	L	1	0	0	0	0
20	B	55	0	86	3	0
21	A	65	0	0	21	0
21	B	77	0	0	10	0
21	C	25	0	0	5	0
21	D	23	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	E	9	0	0	5	0
21	F	4	0	0	1	0
21	I	1	0	0	1	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	10	0	0	6	0
21	M	1	0	0	0	0
All	All	25197	0	25388	419	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 419 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:OD1	1:A:183:ARG:NH1	2.08	0.87
4:D:95:HIS:O	21:D:201:HOH:O	1.96	0.84
7:I:33:TYR:OH	11:M:30:TYR:OH	1.92	0.84
4:D:60:ARG:NH2	4:D:62:GLU:OE1	2.11	0.82
7:I:33:TYR:HH	11:M:30:TYR:HH	1.18	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	744/755 (98%)	712 (96%)	32 (4%)	0	100	100
2	B	738/741 (100%)	706 (96%)	32 (4%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	136/139 (98%)	124 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	68/76 (90%)	68 (100%)	0	0	100	100
6	F	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	K	77/83 (93%)	72 (94%)	5 (6%)	0	100	100
10	L	150/155 (97%)	145 (97%)	5 (3%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	X	25/36 (69%)	25 (100%)	0	0	100	100
All	All	2259/2317 (98%)	2154 (95%)	105 (5%)	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	A	594/603 (98%)	594 (100%)	0	100	100
2	B	597/598 (100%)	597 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/116 (99%)	115 (100%)	0	100	100
5	E	60/65 (92%)	60 (100%)	0	100	100
6	F	109/109 (100%)	109 (100%)	0	100	100
7	I	31/31 (100%)	31 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
9	K	58/61 (95%)	58 (100%)	0	100	100
10	L	117/120 (98%)	117 (100%)	0	100	100
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	21/28 (75%)	21 (100%)	0	100	100
All	All	1830/1860 (98%)	1830 (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 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	647	ASN
5	E	58	ASN
4	D	106	ASN
9	K	23	ASN
2	B	195	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	J	1	8	8,9,10	0.93	0	7,9,11	0.90	0
7	FME	I	1	7	8,9,10	0.97	0	7,9,11	0.82	0

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
8	FME	J	1	8	-	1/7/9/11	-
7	FME	I	1	7	-	0/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 134 ligands modelled in this entry, 2 are monoatomic - leaving 132 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	$\# Z > 2$
14	CLA	B	832	-	49,57,73	1.69	6 (12%)	55,93,113	1.52	7 (12%)
16	BCR	B	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	8 (14%)
16	BCR	A	849	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	5 (8%)
14	CLA	B	827	-	65,73,73	1.46	7 (10%)	76,113,113	1.34	7 (9%)
16	BCR	B	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.19	6 (10%)
16	BCR	B	852	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	9 (16%)
14	CLA	A	811	-	49,57,73	1.72	7 (14%)	55,93,113	1.41	7 (12%)
14	CLA	A	843	17	45,53,73	1.77	7 (15%)	52,89,113	1.55	7 (13%)
14	CLA	A	819	-	65,73,73	1.50	9 (13%)	76,113,113	1.32	8 (10%)
17	LHG	I	102	-	38,38,48	0.70	0	41,44,54	1.26	4 (9%)
16	BCR	A	845	-	41,41,41	1.13	2 (4%)	56,56,56	1.29	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	B	845	-	41,41,41	1.12	3 (7%)	56,56,56	1.17	4 (7%)
14	CLA	A	816	-	65,73,73	1.45	7 (10%)	76,113,113	1.36	6 (7%)
14	CLA	L	204	10	65,73,73	1.51	7 (10%)	76,113,113	1.51	11 (14%)
14	CLA	B	834	-	65,73,73	1.48	7 (10%)	76,113,113	1.31	7 (9%)
14	CLA	L	205	-	65,73,73	1.45	6 (9%)	76,113,113	1.38	9 (11%)
14	CLA	K	102	21	58,66,73	1.58	5 (8%)	67,104,113	1.39	8 (11%)
14	CLA	A	805	14	59,67,73	1.53	6 (10%)	68,105,113	1.42	9 (13%)
14	CLA	A	837	1	45,53,73	1.77	6 (13%)	52,89,113	1.60	8 (15%)
14	CLA	B	813	-	45,53,73	1.77	7 (15%)	52,89,113	1.55	6 (11%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	A	818	-	65,73,73	1.46	7 (10%)	76,113,113	1.38	8 (10%)
14	CLA	A	838	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	8 (10%)
14	CLA	A	824	-	65,73,73	1.53	7 (10%)	76,113,113	1.26	6 (7%)
14	CLA	A	841	-	65,73,73	1.47	6 (9%)	76,113,113	1.32	7 (9%)
14	CLA	A	812	14	65,73,73	1.47	7 (10%)	76,113,113	1.32	6 (7%)
14	CLA	A	833	-	65,73,73	1.45	7 (10%)	76,113,113	1.31	6 (7%)
14	CLA	B	820	21	65,73,73	1.49	7 (10%)	76,113,113	1.42	8 (10%)
14	CLA	B	824	-	45,53,73	1.80	5 (11%)	52,89,113	1.54	8 (15%)
14	CLA	A	821	-	65,73,73	1.45	6 (9%)	76,113,113	1.37	7 (9%)
14	CLA	A	826	21	65,73,73	1.46	6 (9%)	76,113,113	1.34	6 (7%)
14	CLA	A	832	-	60,68,73	1.53	9 (15%)	70,107,113	1.39	7 (10%)
14	CLA	X	1701	12	45,53,73	1.79	6 (13%)	52,89,113	1.56	7 (13%)
14	CLA	A	806	-	65,73,73	1.44	8 (12%)	76,113,113	1.37	8 (10%)
15	PQN	A	844	-	34,34,34	0.40	0	42,45,45	0.37	0
14	CLA	B	816	-	65,73,73	1.45	7 (10%)	76,113,113	1.35	7 (9%)
16	BCR	I	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.24	7 (12%)
14	CLA	B	841	21	65,73,73	1.48	6 (9%)	76,113,113	1.31	8 (10%)
14	CLA	B	837	21	45,53,73	1.81	6 (13%)	52,89,113	1.52	6 (11%)
14	CLA	A	809	1	65,73,73	1.44	6 (9%)	76,113,113	1.38	7 (9%)
14	CLA	B	842	-	65,73,73	1.50	8 (12%)	76,113,113	1.35	7 (9%)
14	CLA	B	807	-	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
14	CLA	B	809	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	7 (9%)
14	CLA	A	810	1	65,73,73	1.47	7 (10%)	76,113,113	1.37	7 (9%)
16	BCR	A	850	-	41,41,41	1.19	2 (4%)	56,56,56	1.45	12 (21%)
16	BCR	L	207	-	41,41,41	1.13	2 (4%)	56,56,56	1.19	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	803	21	65,73,73	1.54	8 (12%)	76,113,113	1.24	6 (7%)
14	CLA	A	804	-	65,73,73	1.44	6 (9%)	76,113,113	1.36	7 (9%)
14	CLA	A	817	21	65,73,73	1.50	6 (9%)	76,113,113	1.35	8 (10%)
14	CLA	B	810	-	65,73,73	1.50	8 (12%)	76,113,113	1.41	8 (10%)
14	CLA	A	830	-	65,73,73	1.47	8 (12%)	76,113,113	1.31	6 (7%)
16	BCR	F	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
16	BCR	A	847	-	41,41,41	1.16	4 (9%)	56,56,56	1.38	8 (14%)
14	CLA	A	802	-	65,73,73	1.45	6 (9%)	76,113,113	1.35	9 (11%)
14	CLA	J	101	8	45,53,73	1.79	6 (13%)	52,89,113	1.52	7 (13%)
14	CLA	A	807	-	65,73,73	1.45	6 (9%)	76,113,113	1.31	7 (9%)
14	CLA	B	822	-	45,53,73	1.76	6 (13%)	52,89,113	1.58	7 (13%)
16	BCR	B	853	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	4 (7%)
14	CLA	A	829	-	65,73,73	1.45	7 (10%)	76,113,113	1.38	6 (7%)
14	CLA	A	840	-	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
14	CLA	B	826	21	65,73,73	1.49	8 (12%)	76,113,113	1.43	10 (13%)
14	CLA	L	206	21	65,73,73	1.47	7 (10%)	76,113,113	1.41	9 (11%)
14	CLA	A	827	21	65,73,73	1.46	6 (9%)	76,113,113	1.40	11 (14%)
14	CLA	B	823	21	55,63,73	1.61	6 (10%)	64,101,113	1.39	6 (9%)
17	LHG	A	852	-	48,48,48	0.65	1 (2%)	51,54,54	1.21	5 (9%)
16	BCR	B	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.28	8 (14%)
14	CLA	B	830	-	65,73,73	1.48	6 (9%)	76,113,113	1.42	8 (10%)
16	BCR	L	202	-	41,41,41	1.20	2 (4%)	56,56,56	1.30	8 (14%)
14	CLA	B	828	-	65,73,73	1.51	7 (10%)	76,113,113	1.27	8 (10%)
14	CLA	F	203	21	45,53,73	1.76	7 (15%)	52,89,113	1.58	7 (13%)
14	CLA	M	102	-	36,44,73	1.96	7 (19%)	40,76,113	1.59	6 (15%)
14	CLA	A	831	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	8 (10%)
14	CLA	B	817	-	65,73,73	1.49	6 (9%)	76,113,113	1.32	8 (10%)
14	CLA	J	102	-	38,45,73	1.92	6 (15%)	43,78,113	1.58	6 (13%)
14	CLA	A	815	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	6 (7%)
14	CLA	B	815	-	65,73,73	1.46	6 (9%)	76,113,113	1.34	8 (10%)
14	CLA	A	825	-	65,73,73	1.48	6 (9%)	76,113,113	1.30	8 (10%)
14	CLA	L	201	2	65,73,73	1.45	7 (10%)	76,113,113	1.39	7 (9%)
14	CLA	F	204	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	8 (13%)
14	CLA	B	839	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	8 (10%)
18	SF4	B	802	1,2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	819	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	8 (10%)
14	CLA	B	818	-	65,73,73	1.45	6 (9%)	76,113,113	1.47	8 (10%)
14	CLA	B	836	21	50,58,73	1.71	7 (14%)	58,95,113	1.51	8 (13%)
14	CLA	B	821	-	65,73,73	1.51	6 (9%)	76,113,113	1.29	7 (9%)
14	CLA	A	834	-	65,73,73	1.45	6 (9%)	76,113,113	1.44	8 (10%)
16	BCR	I	103	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	7 (12%)
14	CLA	A	839	-	65,73,73	1.45	7 (10%)	76,113,113	1.36	8 (10%)
16	BCR	J	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	7 (12%)
14	CLA	A	820	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	9 (11%)
14	CLA	A	828	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	8 (10%)
14	CLA	A	842	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	7 (9%)
16	BCR	K	103	-	25,25,41	1.14	1 (4%)	33,33,56	1.34	5 (15%)
14	CLA	A	808	-	51,59,73	1.65	7 (13%)	59,96,113	1.43	7 (11%)
16	BCR	A	851	-	25,25,41	1.16	1 (4%)	33,33,56	1.46	5 (15%)
17	LHG	M	101	-	48,48,48	0.60	0	51,54,54	1.17	5 (9%)
15	PQN	B	843	-	34,34,34	0.41	0	42,45,45	0.38	0
14	CLA	A	814	-	65,73,73	1.47	7 (10%)	76,113,113	1.34	6 (7%)
14	CLA	K	101	-	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
14	CLA	B	814	-	65,73,73	1.44	7 (10%)	76,113,113	1.50	11 (14%)
16	BCR	F	202	-	41,41,41	1.19	2 (4%)	56,56,56	1.25	8 (14%)
14	CLA	B	801	21	65,73,73	1.48	7 (10%)	76,113,113	1.32	6 (7%)
14	CLA	A	822	21	65,73,73	1.46	7 (10%)	76,113,113	1.34	6 (7%)
14	CLA	B	805	-	65,73,73	1.43	7 (10%)	76,113,113	1.42	7 (9%)
17	LHG	A	853	14	40,40,48	0.71	1 (2%)	43,46,54	1.19	4 (9%)
14	CLA	A	836	-	65,73,73	1.49	9 (13%)	76,113,113	1.34	8 (10%)
14	CLA	B	829	-	65,73,73	1.50	8 (12%)	76,113,113	1.34	9 (11%)
14	CLA	B	808	-	65,73,73	1.47	7 (10%)	76,113,113	1.34	7 (9%)
14	CLA	B	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	7 (9%)
14	CLA	A	854	21	65,73,73	1.44	7 (10%)	76,113,113	1.43	9 (11%)
16	BCR	A	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	9 (16%)
14	CLA	A	835	-	65,73,73	1.44	7 (10%)	76,113,113	1.40	7 (9%)
16	BCR	J	104	-	41,41,41	1.21	2 (4%)	56,56,56	1.38	10 (17%)
14	CLA	B	835	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	6 (7%)
16	BCR	B	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.26	6 (10%)
13	CL0	A	801	-	65,73,73	1.44	6 (9%)	76,113,113	1.32	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	838	-	60,68,73	1.57	8 (13%)	70,107,113	1.36	7 (10%)
14	CLA	B	806	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	8 (10%)
16	BCR	B	844	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
14	CLA	A	813	-	45,53,73	1.82	8 (17%)	52,89,113	1.47	7 (13%)
20	LMG	B	850	-	55,55,55	0.70	0	63,63,63	1.33	7 (11%)
14	CLA	F	201	21	58,66,73	1.58	6 (10%)	67,104,113	1.36	8 (11%)
14	CLA	B	825	2	65,73,73	1.47	7 (10%)	76,113,113	1.28	7 (9%)
14	CLA	B	804	-	65,73,73	1.44	8 (12%)	76,113,113	1.31	6 (7%)
14	CLA	B	840	-	47,55,73	1.75	8 (17%)	54,91,113	1.51	9 (16%)
17	LHG	B	851	-	48,48,48	0.66	1 (2%)	51,54,54	1.19	5 (9%)
14	CLA	B	811	2	65,73,73	1.47	7 (10%)	76,113,113	1.36	8 (10%)
14	CLA	B	833	-	65,73,73	1.50	7 (10%)	76,113,113	1.33	8 (10%)
14	CLA	A	823	-	45,53,73	1.76	6 (13%)	52,89,113	1.57	8 (15%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	B	831	-	55,63,73	1.60	6 (10%)	64,101,113	1.42	7 (10%)
16	BCR	A	848	-	41,41,41	1.11	2 (4%)	56,56,56	1.16	5 (8%)

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
14	CLA	B	832	-	1/1/11/20	5/18/96/115	-
16	BCR	B	847	-	-	10/29/63/63	0/2/2/2
16	BCR	A	849	-	-	5/29/63/63	0/2/2/2
14	CLA	B	827	-	1/1/15/20	10/37/115/115	-
16	BCR	B	849	-	-	4/29/63/63	0/2/2/2
16	BCR	B	852	-	-	12/29/63/63	0/2/2/2
14	CLA	A	811	-	1/1/11/20	7/18/96/115	-
14	CLA	A	843	17	1/1/11/20	5/13/91/115	-
14	CLA	A	819	-	1/1/15/20	12/37/115/115	-
17	LHG	I	102	-	-	23/43/43/53	-
16	BCR	A	845	-	-	4/29/63/63	0/2/2/2
16	BCR	B	845	-	-	15/29/63/63	0/2/2/2
14	CLA	A	816	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	L	204	10	1/1/15/20	16/37/115/115	-
14	CLA	B	834	-	1/1/15/20	9/37/115/115	-
14	CLA	L	205	-	1/1/15/20	14/37/115/115	-
14	CLA	K	102	21	1/1/13/20	12/29/107/115	-
14	CLA	A	805	14	1/1/13/20	9/30/108/115	-
14	CLA	A	837	1	1/1/11/20	5/13/91/115	-
14	CLA	B	813	-	1/1/11/20	5/13/91/115	-
18	SF4	C	101	3	-	-	0/6/5/5
14	CLA	A	818	-	1/1/15/20	12/37/115/115	-
14	CLA	A	838	-	1/1/15/20	14/37/115/115	-
14	CLA	A	824	-	1/1/15/20	7/37/115/115	-
14	CLA	A	841	-	1/1/15/20	12/37/115/115	-
14	CLA	A	812	14	1/1/15/20	13/37/115/115	-
14	CLA	A	833	-	1/1/15/20	13/37/115/115	-
14	CLA	B	820	21	1/1/15/20	16/37/115/115	-
14	CLA	B	824	-	1/1/11/20	6/13/91/115	-
14	CLA	A	821	-	1/1/15/20	12/37/115/115	-
14	CLA	A	826	21	1/1/15/20	15/37/115/115	-
14	CLA	A	832	-	1/1/14/20	9/31/109/115	-
14	CLA	X	1701	12	1/1/11/20	7/13/91/115	-
14	CLA	A	806	-	1/1/15/20	25/37/115/115	-
15	PQN	A	844	-	-	1/23/43/43	0/2/2/2
14	CLA	B	816	-	1/1/15/20	13/37/115/115	-
16	BCR	I	101	-	-	11/29/63/63	0/2/2/2
14	CLA	B	841	21	1/1/15/20	9/37/115/115	-
14	CLA	B	837	21	1/1/11/20	5/13/91/115	-
14	CLA	A	809	1	1/1/15/20	7/37/115/115	-
14	CLA	B	842	-	1/1/15/20	8/37/115/115	-
14	CLA	B	807	-	1/1/15/20	19/37/115/115	-
14	CLA	B	809	-	1/1/15/20	10/37/115/115	-
14	CLA	A	810	1	1/1/15/20	13/37/115/115	-
16	BCR	A	850	-	-	18/29/63/63	0/2/2/2
16	BCR	L	207	-	-	17/29/63/63	0/2/2/2
14	CLA	A	803	21	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	804	-	1/1/15/20	11/37/115/115	-
14	CLA	A	817	21	1/1/15/20	9/37/115/115	-
14	CLA	B	810	-	1/1/15/20	6/37/115/115	-
14	CLA	A	830	-	1/1/15/20	10/37/115/115	-
16	BCR	F	205	-	-	10/29/63/63	0/2/2/2
16	BCR	A	847	-	-	13/29/63/63	0/2/2/2
14	CLA	A	802	-	1/1/15/20	13/37/115/115	-
14	CLA	J	101	8	1/1/11/20	2/13/91/115	-
14	CLA	A	807	-	1/1/15/20	14/37/115/115	-
14	CLA	B	822	-	1/1/11/20	7/13/91/115	-
16	BCR	B	853	-	-	13/29/63/63	0/2/2/2
14	CLA	A	829	-	1/1/15/20	14/37/115/115	-
14	CLA	A	840	-	1/1/15/20	8/37/115/115	-
14	CLA	B	826	21	1/1/15/20	15/37/115/115	-
14	CLA	L	206	21	1/1/15/20	7/37/115/115	-
14	CLA	A	827	21	1/1/15/20	12/37/115/115	-
14	CLA	B	823	21	1/1/13/20	6/25/103/115	-
17	LHG	A	852	-	-	23/53/53/53	-
16	BCR	B	846	-	-	8/29/63/63	0/2/2/2
14	CLA	B	830	-	1/1/15/20	8/37/115/115	-
16	BCR	L	202	-	-	12/29/63/63	0/2/2/2
14	CLA	B	828	-	1/1/15/20	20/37/115/115	-
14	CLA	F	203	21	1/1/11/20	4/13/91/115	-
14	CLA	M	102	-	1/1/7/20	0/2/72/115	-
14	CLA	A	831	-	1/1/15/20	7/37/115/115	-
14	CLA	B	817	-	1/1/15/20	17/37/115/115	-
14	CLA	J	102	-	1/1/8/20	0/2/76/115	-
14	CLA	A	815	-	1/1/15/20	14/37/115/115	-
14	CLA	B	815	-	1/1/15/20	20/37/115/115	-
14	CLA	A	825	-	1/1/15/20	13/37/115/115	-
14	CLA	L	201	2	1/1/15/20	15/37/115/115	-
14	CLA	F	204	-	1/1/12/20	8/19/97/115	-
14	CLA	B	839	-	1/1/15/20	10/37/115/115	-
18	SF4	B	802	1,2	-	-	0/6/5/5
14	CLA	B	819	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	818	-	1/1/15/20	12/37/115/115	-
14	CLA	B	836	21	1/1/12/20	5/19/97/115	-
14	CLA	B	821	-	1/1/15/20	14/37/115/115	-
14	CLA	A	834	-	1/1/15/20	14/37/115/115	-
16	BCR	I	103	-	-	10/29/63/63	0/2/2/2
14	CLA	A	839	-	1/1/15/20	16/37/115/115	-
16	BCR	J	103	-	-	13/29/63/63	0/2/2/2
14	CLA	A	820	-	1/1/15/20	8/37/115/115	-
14	CLA	A	828	-	1/1/15/20	6/37/115/115	-
14	CLA	A	842	-	1/1/15/20	6/37/115/115	-
16	BCR	K	103	-	-	5/18/35/63	0/1/1/2
14	CLA	A	808	-	1/1/12/20	4/21/99/115	-
16	BCR	A	851	-	-	13/18/35/63	0/1/1/2
17	LHG	M	101	-	-	19/53/53/53	-
15	PQN	B	843	-	-	2/23/43/43	0/2/2/2
14	CLA	A	814	-	1/1/15/20	14/37/115/115	-
14	CLA	K	101	-	1/1/11/20	6/15/93/115	-
14	CLA	B	814	-	1/1/15/20	19/37/115/115	-
16	BCR	F	202	-	-	8/29/63/63	0/2/2/2
14	CLA	B	801	21	1/1/15/20	16/37/115/115	-
14	CLA	A	822	21	1/1/15/20	8/37/115/115	-
14	CLA	B	805	-	1/1/15/20	14/37/115/115	-
17	LHG	A	853	14	-	13/45/45/53	-
14	CLA	A	836	-	1/1/15/20	14/37/115/115	-
14	CLA	B	829	-	1/1/15/20	14/37/115/115	-
14	CLA	B	808	-	1/1/15/20	8/37/115/115	-
14	CLA	B	812	-	1/1/15/20	8/37/115/115	-
14	CLA	A	854	21	1/1/15/20	17/37/115/115	-
16	BCR	A	846	-	-	11/29/63/63	0/2/2/2
14	CLA	A	835	-	1/1/15/20	7/37/115/115	-
16	BCR	J	104	-	-	10/29/63/63	0/2/2/2
14	CLA	B	835	-	1/1/15/20	11/37/115/115	-
16	BCR	B	848	-	-	6/29/63/63	0/2/2/2
13	CL0	A	801	-	3/3/20/25	9/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	838	-	1/1/14/20	7/31/109/115	-
14	CLA	B	806	-	1/1/15/20	10/37/115/115	-
16	BCR	B	844	-	-	12/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/11/20	3/13/91/115	-
20	LMG	B	850	-	-	23/50/70/70	0/1/1/1
14	CLA	F	201	21	1/1/13/20	12/29/107/115	-
14	CLA	B	825	2	1/1/15/20	13/37/115/115	-
14	CLA	B	804	-	1/1/15/20	13/37/115/115	-
14	CLA	B	840	-	1/1/11/20	3/16/94/115	-
17	LHG	B	851	-	-	28/53/53/53	-
14	CLA	B	811	2	1/1/15/20	8/37/115/115	-
14	CLA	B	833	-	1/1/15/20	12/37/115/115	-
14	CLA	A	823	-	1/1/11/20	6/13/91/115	-
18	SF4	C	102	3	-	-	0/6/5/5
14	CLA	B	831	-	1/1/13/20	10/25/103/115	-
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2

The worst 5 of 711 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	824	CLA	C4B-NB	7.81	1.42	1.35
14	A	811	CLA	C4B-NB	7.72	1.42	1.35
14	B	828	CLA	C4B-NB	7.71	1.42	1.35
14	L	204	CLA	C4B-NB	7.70	1.42	1.35
14	A	803	CLA	C4B-NB	7.64	1.42	1.35

The worst 5 of 923 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	835	CLA	C4A-NA-C1A	7.46	110.06	106.71
14	L	201	CLA	C4A-NA-C1A	7.34	110.01	106.71
14	B	805	CLA	C4A-NA-C1A	7.06	109.88	106.71
14	A	837	CLA	C4A-NA-C1A	6.98	109.85	106.71
14	B	839	CLA	C4A-NA-C1A	6.97	109.84	106.71

5 of 99 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	ND
13	A	801	CL0	NC
13	A	801	CL0	NA
14	A	802	CLA	ND
14	A	803	CLA	ND

5 of 1391 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

107 monomers are involved in 201 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	832	CLA	1	0
16	B	847	BCR	3	0
16	A	849	BCR	2	0
14	B	827	CLA	2	0
16	B	849	BCR	1	0
16	B	852	BCR	2	0
14	A	811	CLA	1	0
14	A	843	CLA	1	0
14	A	819	CLA	3	0
17	I	102	LHG	2	0
16	A	845	BCR	1	0
14	A	816	CLA	3	0
14	L	204	CLA	3	0
14	B	834	CLA	1	0
14	L	205	CLA	1	0
14	A	805	CLA	2	0
14	A	837	CLA	2	0
14	A	838	CLA	2	0
14	A	824	CLA	1	0
14	A	841	CLA	2	0
14	A	812	CLA	2	0
14	A	833	CLA	3	0
14	B	824	CLA	2	0
14	A	821	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	826	CLA	3	0
14	A	832	CLA	1	0
14	X	1701	CLA	1	0
15	A	844	PQN	2	0
14	B	816	CLA	2	0
16	I	101	BCR	2	0
14	B	841	CLA	1	0
14	A	809	CLA	2	0
14	B	842	CLA	1	0
14	B	807	CLA	1	0
14	B	809	CLA	1	0
14	A	810	CLA	2	0
16	A	850	BCR	6	0
14	A	803	CLA	1	0
14	A	804	CLA	2	0
14	B	810	CLA	2	0
14	A	830	CLA	6	0
16	F	205	BCR	1	0
16	A	847	BCR	3	0
14	A	802	CLA	6	0
14	J	101	CLA	1	0
14	A	807	CLA	3	0
14	B	822	CLA	1	0
16	B	853	BCR	3	0
14	A	829	CLA	6	0
14	A	840	CLA	2	0
14	B	826	CLA	4	0
14	A	827	CLA	1	0
14	B	823	CLA	1	0
17	A	852	LHG	2	0
16	B	846	BCR	1	0
14	B	830	CLA	2	0
16	L	202	BCR	1	0
14	B	828	CLA	6	0
14	F	203	CLA	1	0
14	B	817	CLA	1	0
14	J	102	CLA	1	0
14	B	815	CLA	2	0
14	A	825	CLA	7	0
14	L	201	CLA	3	0
14	F	204	CLA	1	0
14	B	839	CLA	2	0

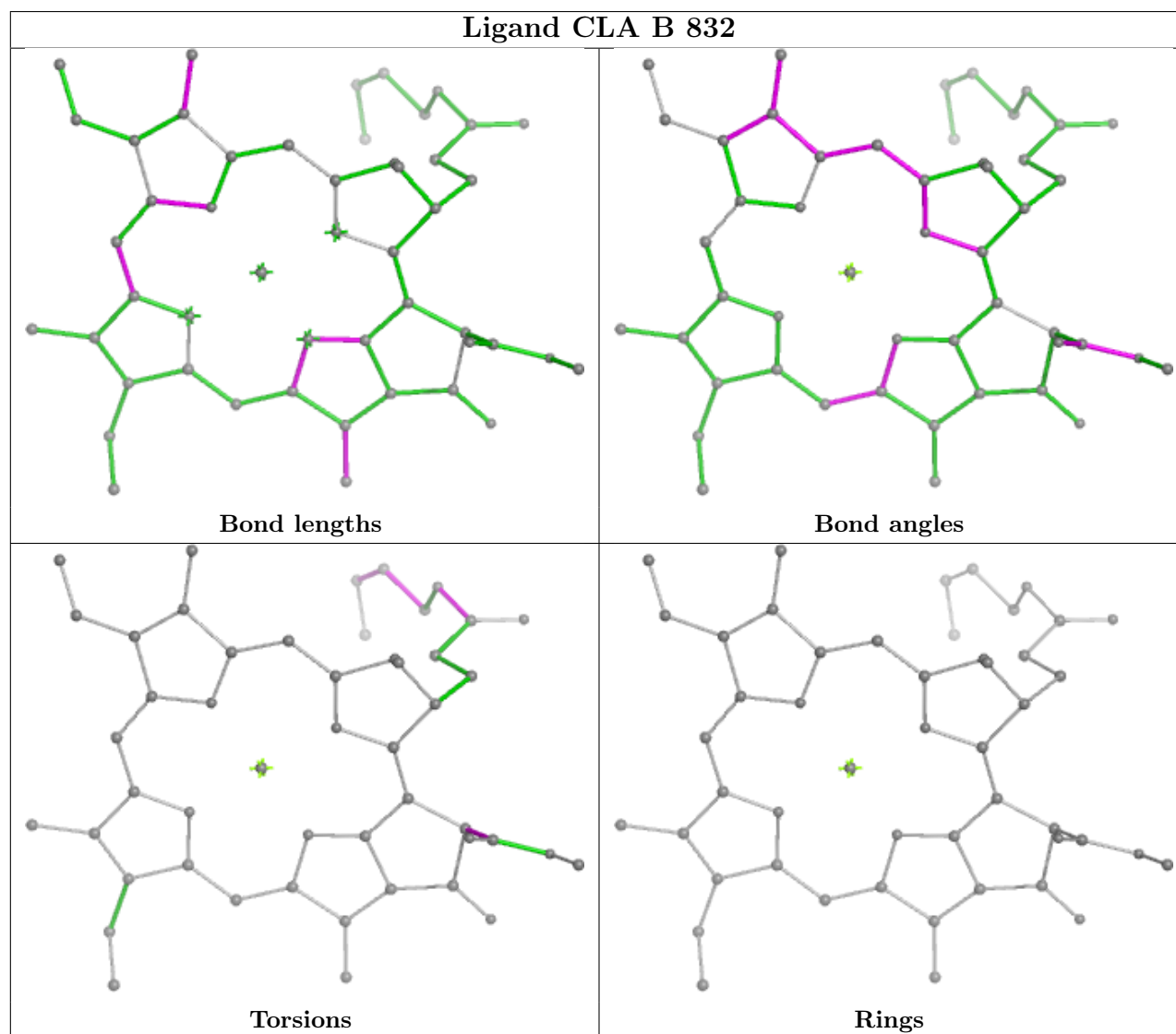
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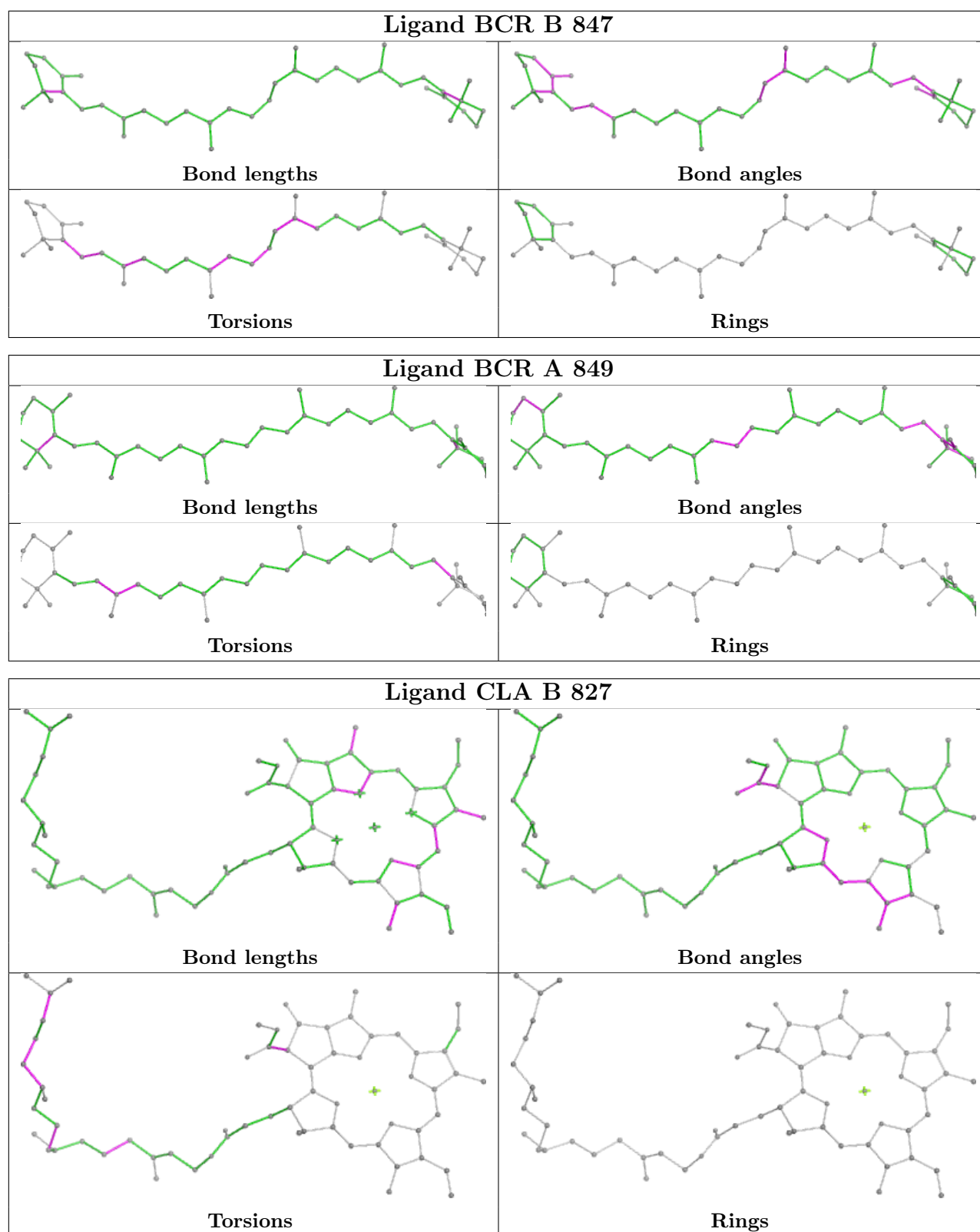
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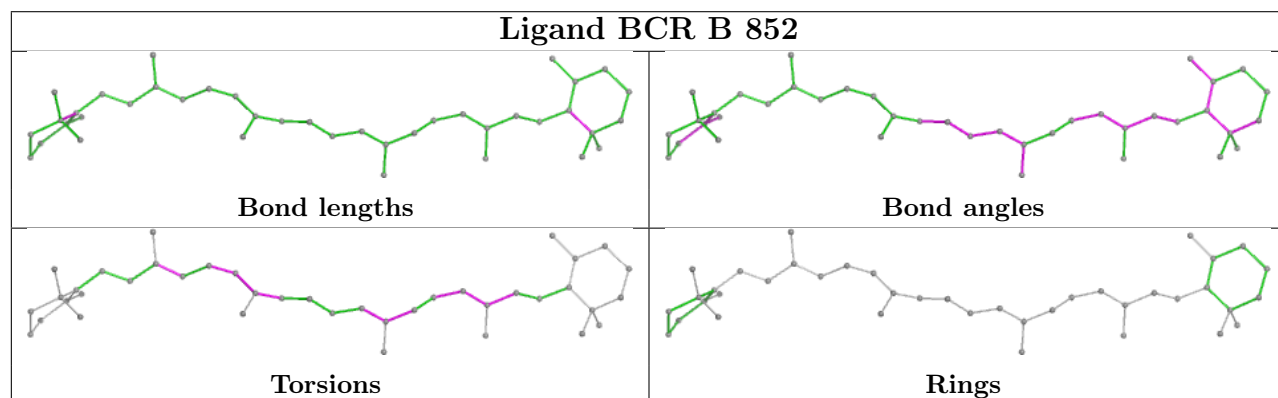
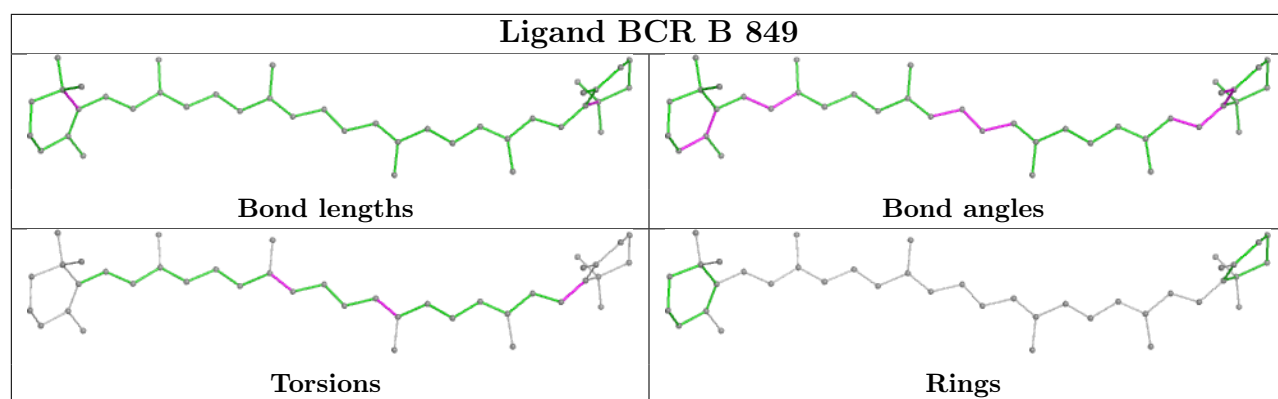
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	819	CLA	1	0
14	B	818	CLA	4	0
14	B	836	CLA	3	0
14	B	821	CLA	1	0
16	I	103	BCR	1	0
16	J	103	BCR	3	0
14	A	820	CLA	4	0
14	A	828	CLA	2	0
14	A	842	CLA	2	0
16	K	103	BCR	4	0
16	A	851	BCR	2	0
17	M	101	LHG	1	0
14	A	814	CLA	1	0
14	K	101	CLA	4	0
14	B	814	CLA	3	0
14	B	801	CLA	2	0
14	A	822	CLA	5	0
14	B	805	CLA	3	0
17	A	853	LHG	2	0
14	A	836	CLA	4	0
14	B	829	CLA	2	0
14	B	808	CLA	2	0
14	A	854	CLA	5	0
16	A	846	BCR	5	0
14	A	835	CLA	4	0
16	J	104	BCR	3	0
14	B	835	CLA	3	0
16	B	848	BCR	2	0
13	A	801	CL0	1	0
14	B	838	CLA	1	0
14	B	806	CLA	1	0
16	B	844	BCR	1	0
14	A	813	CLA	1	0
20	B	850	LMG	3	0
14	F	201	CLA	2	0
14	B	825	CLA	4	0
14	B	804	CLA	2	0
17	B	851	LHG	1	0
14	B	833	CLA	1	0
14	B	831	CLA	1	0
16	A	848	BCR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

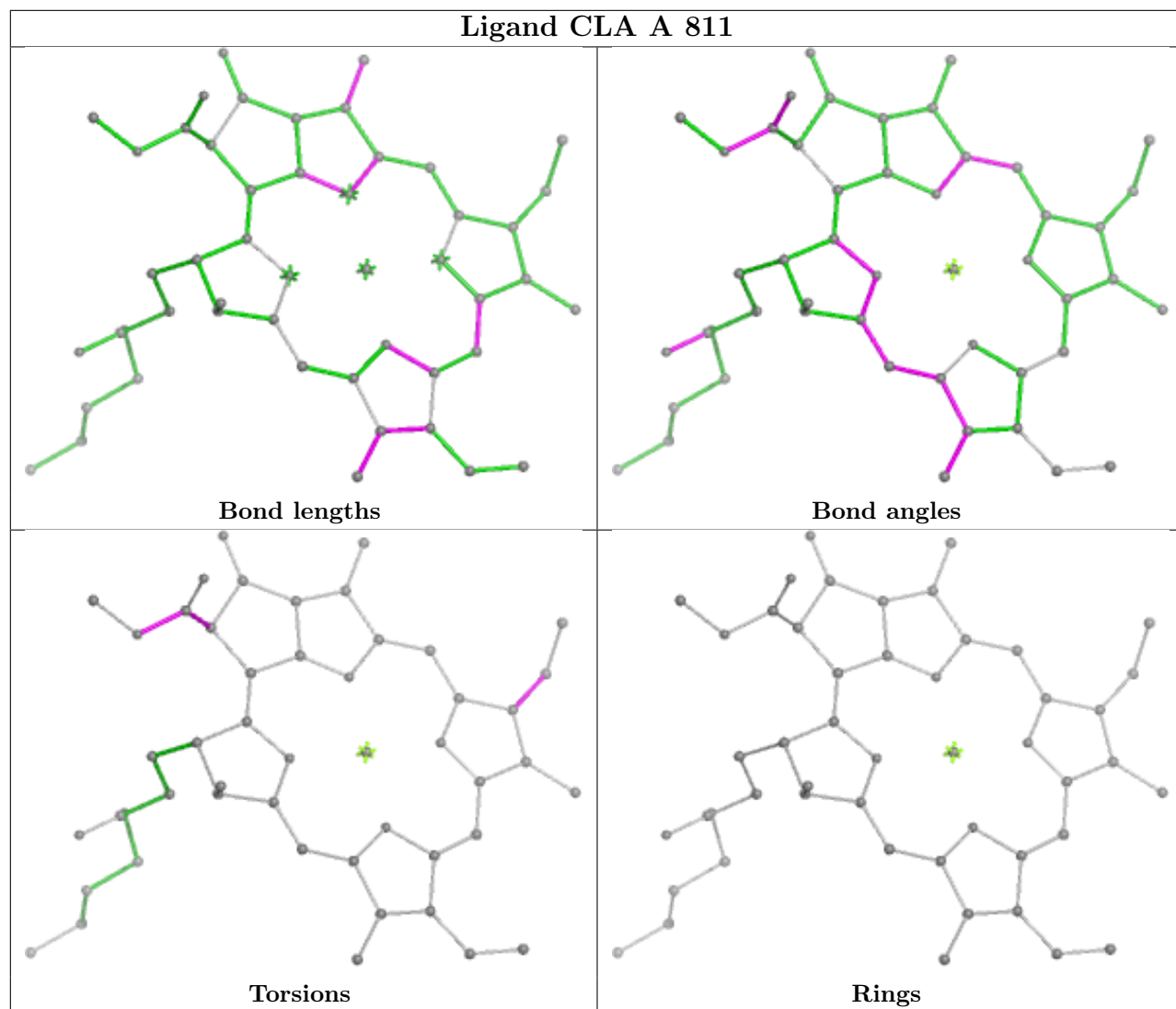
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

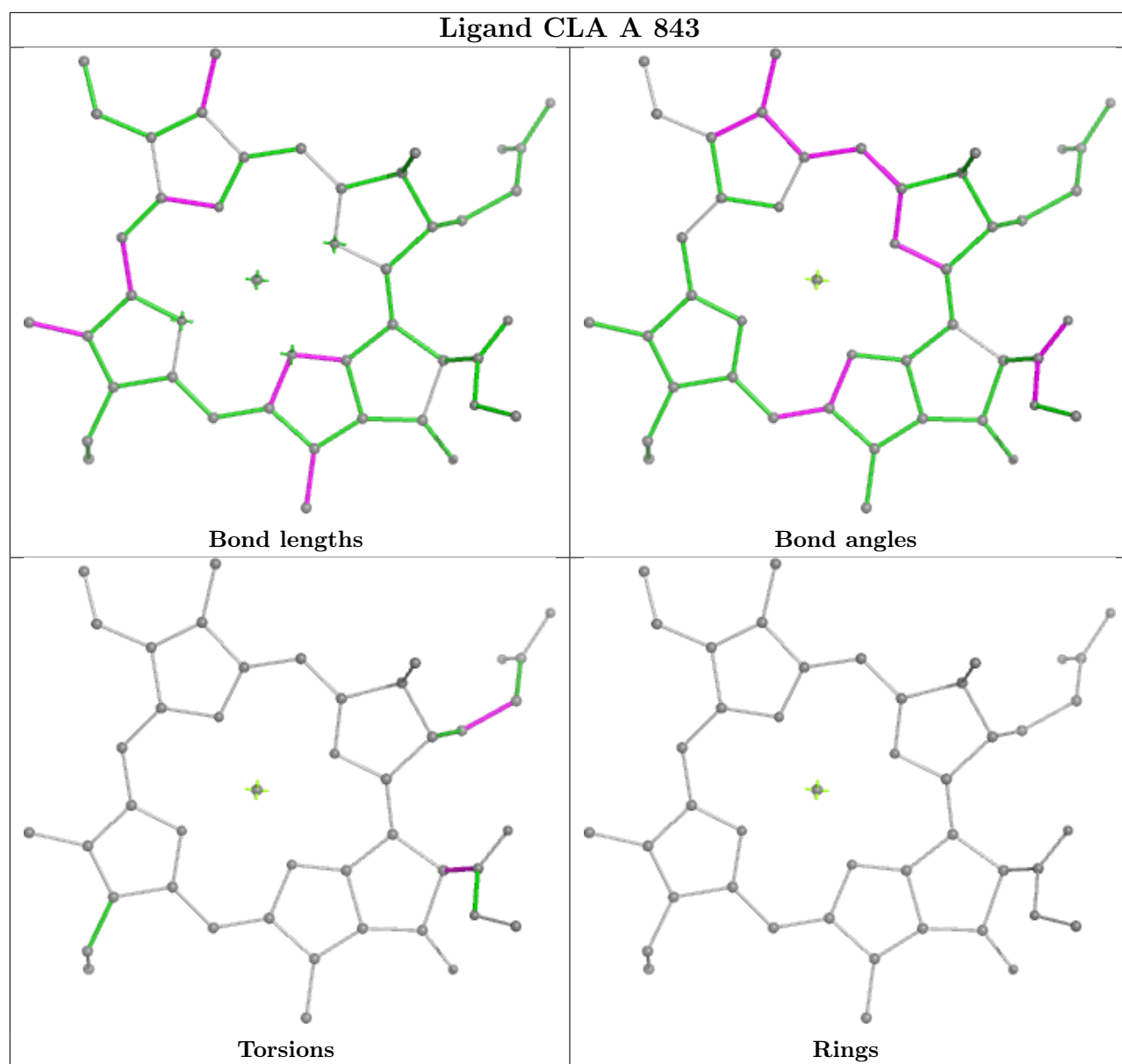


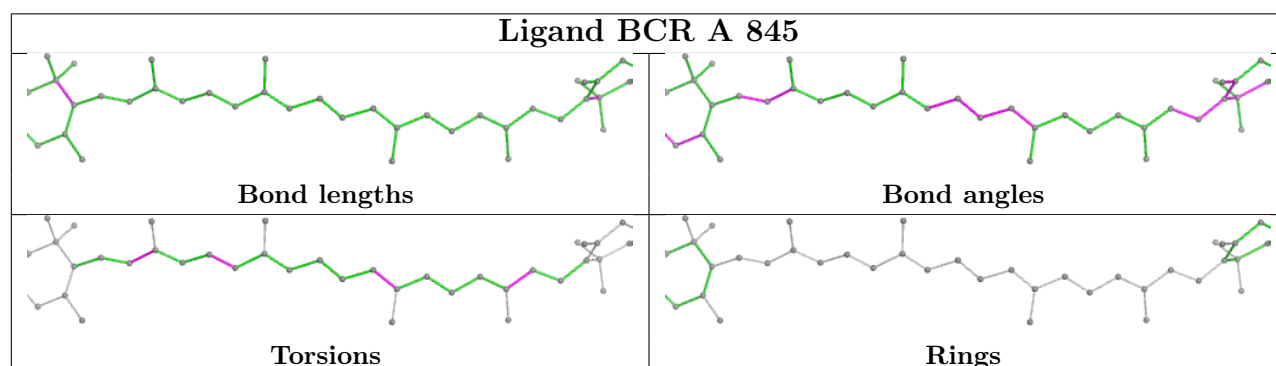
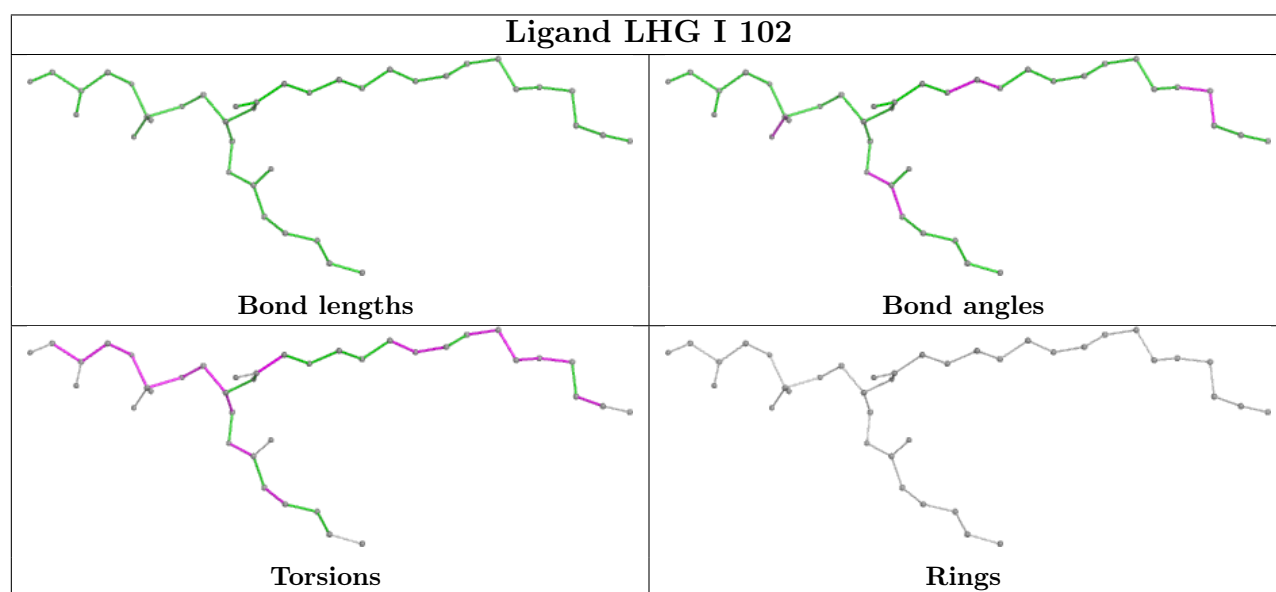
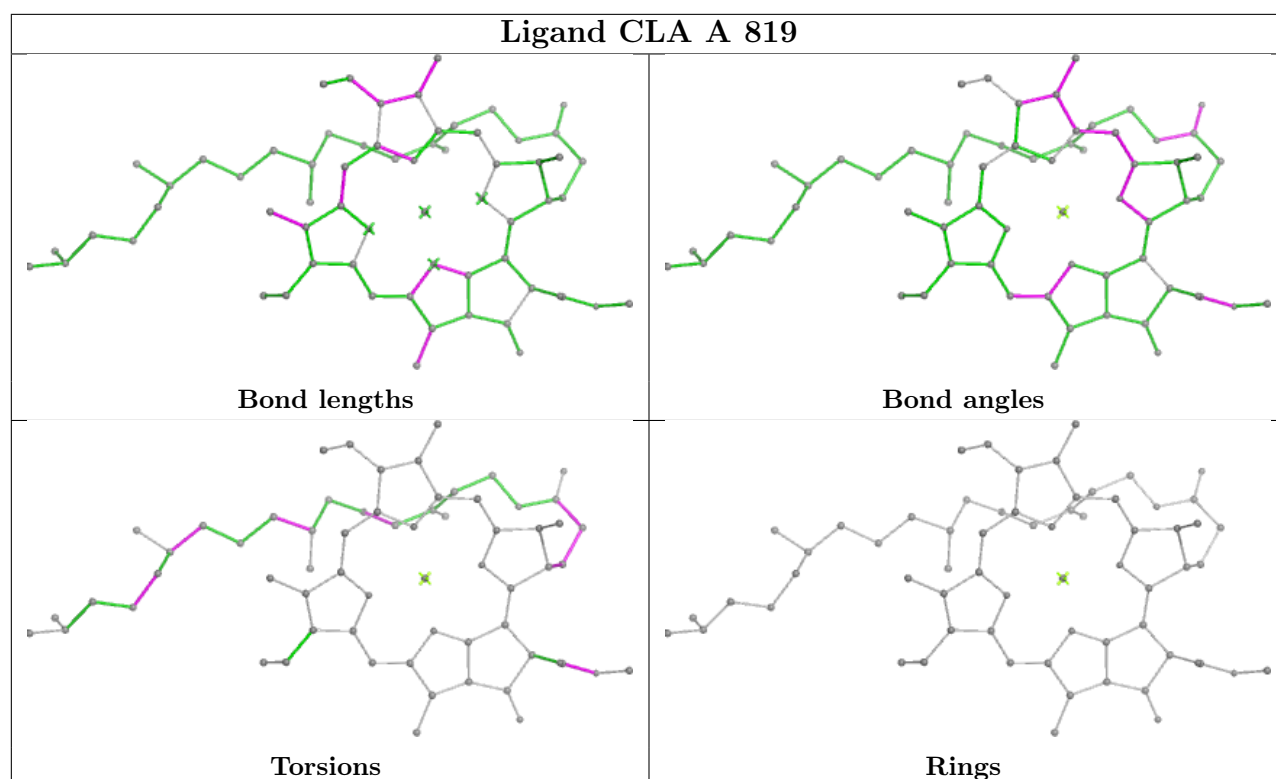


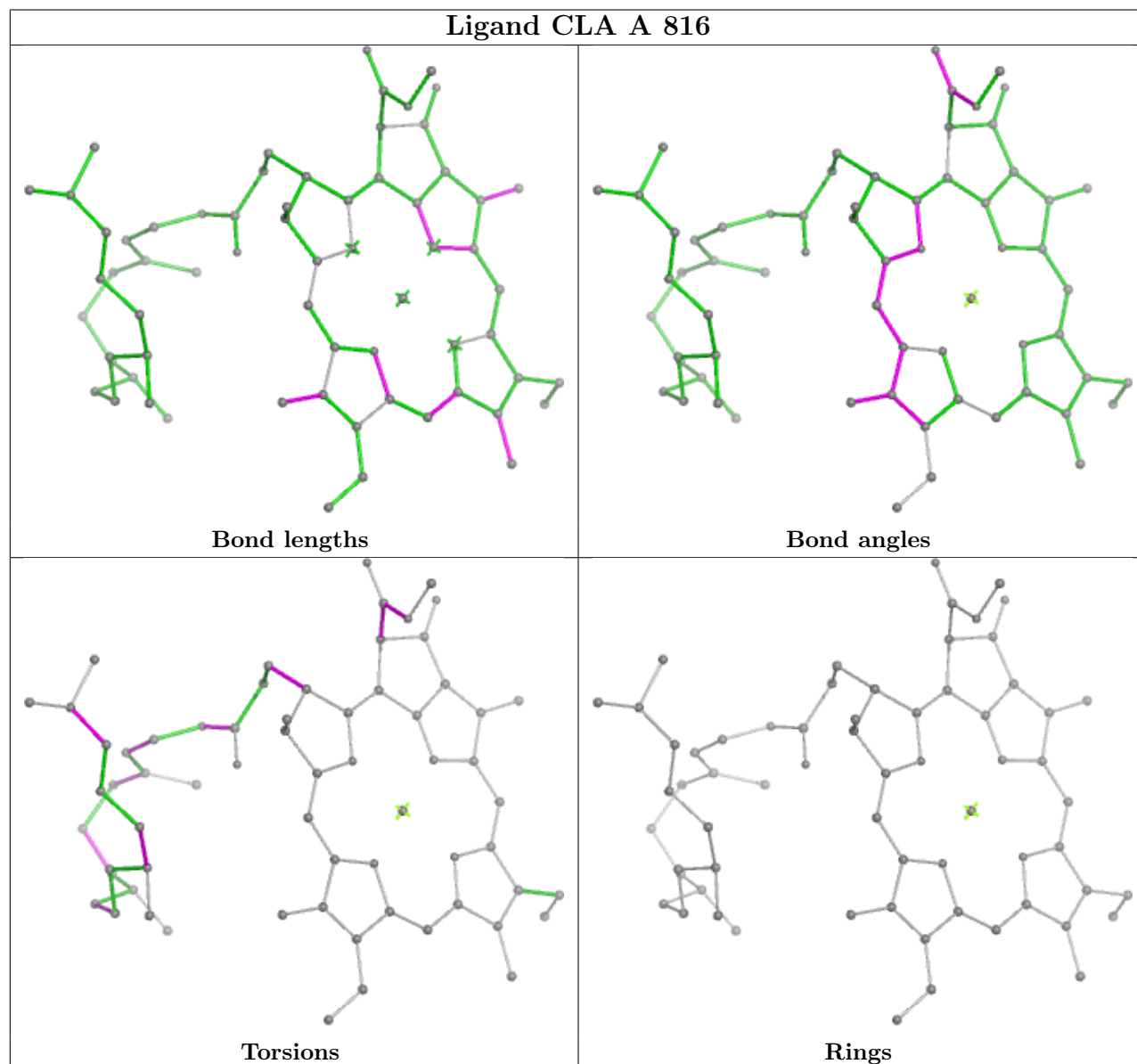
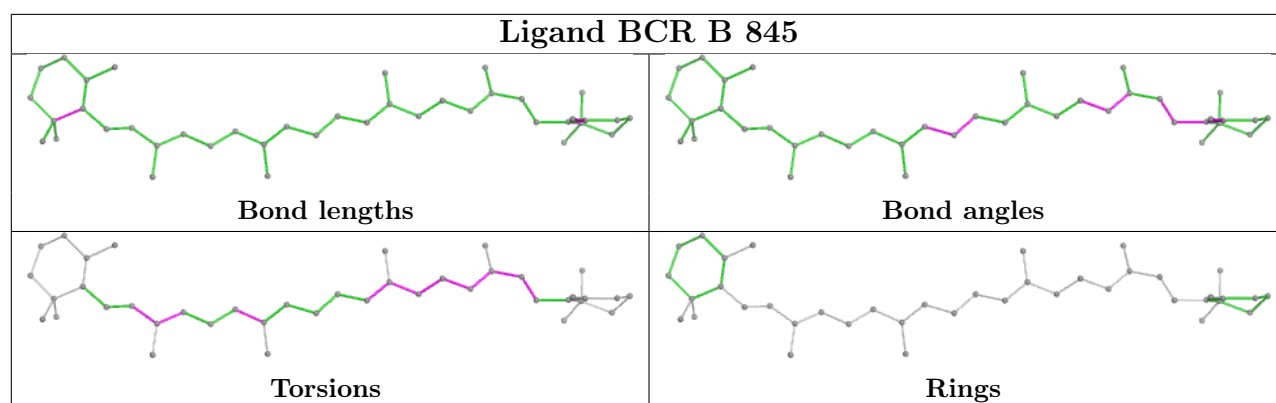


Ligand CLA A 811

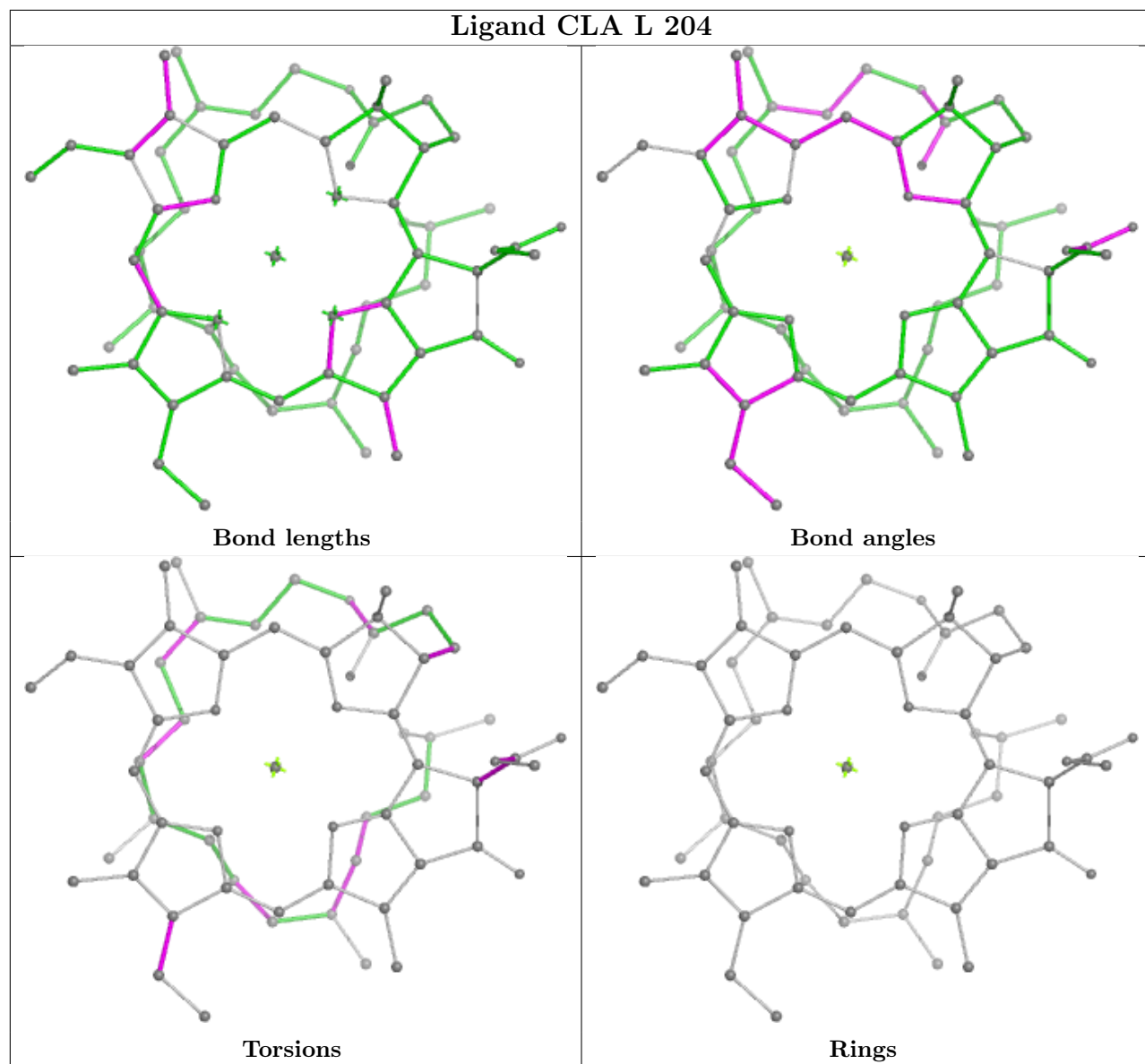


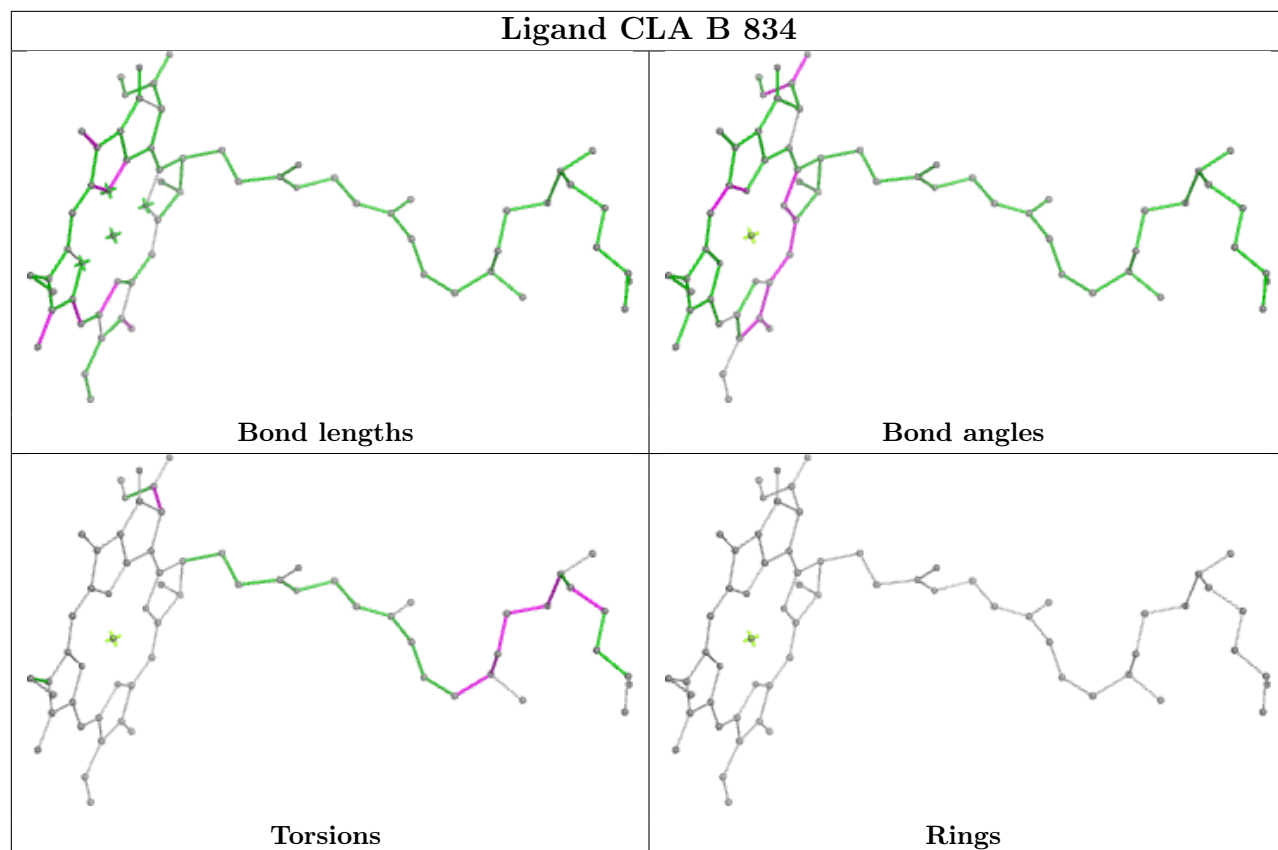
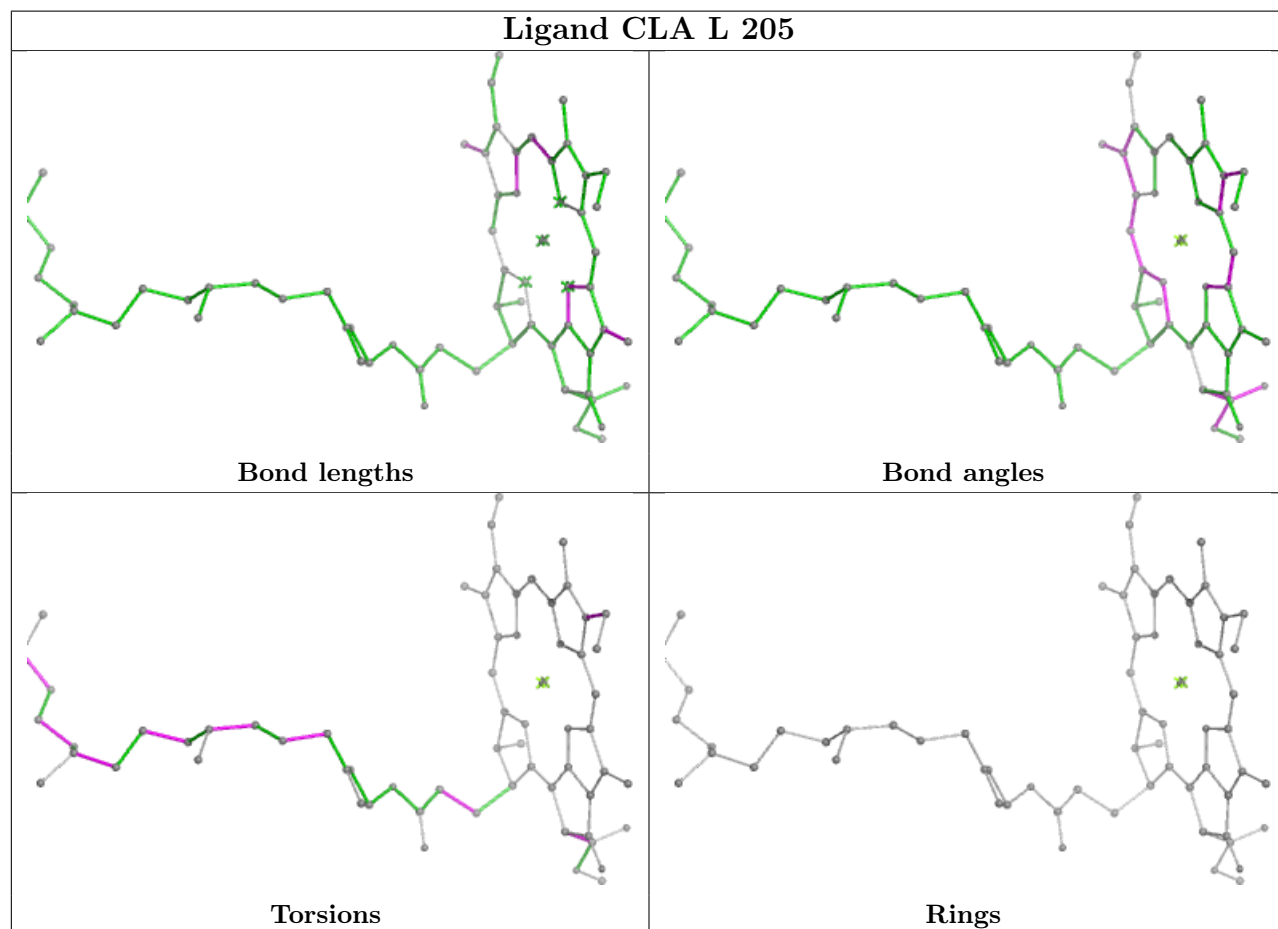


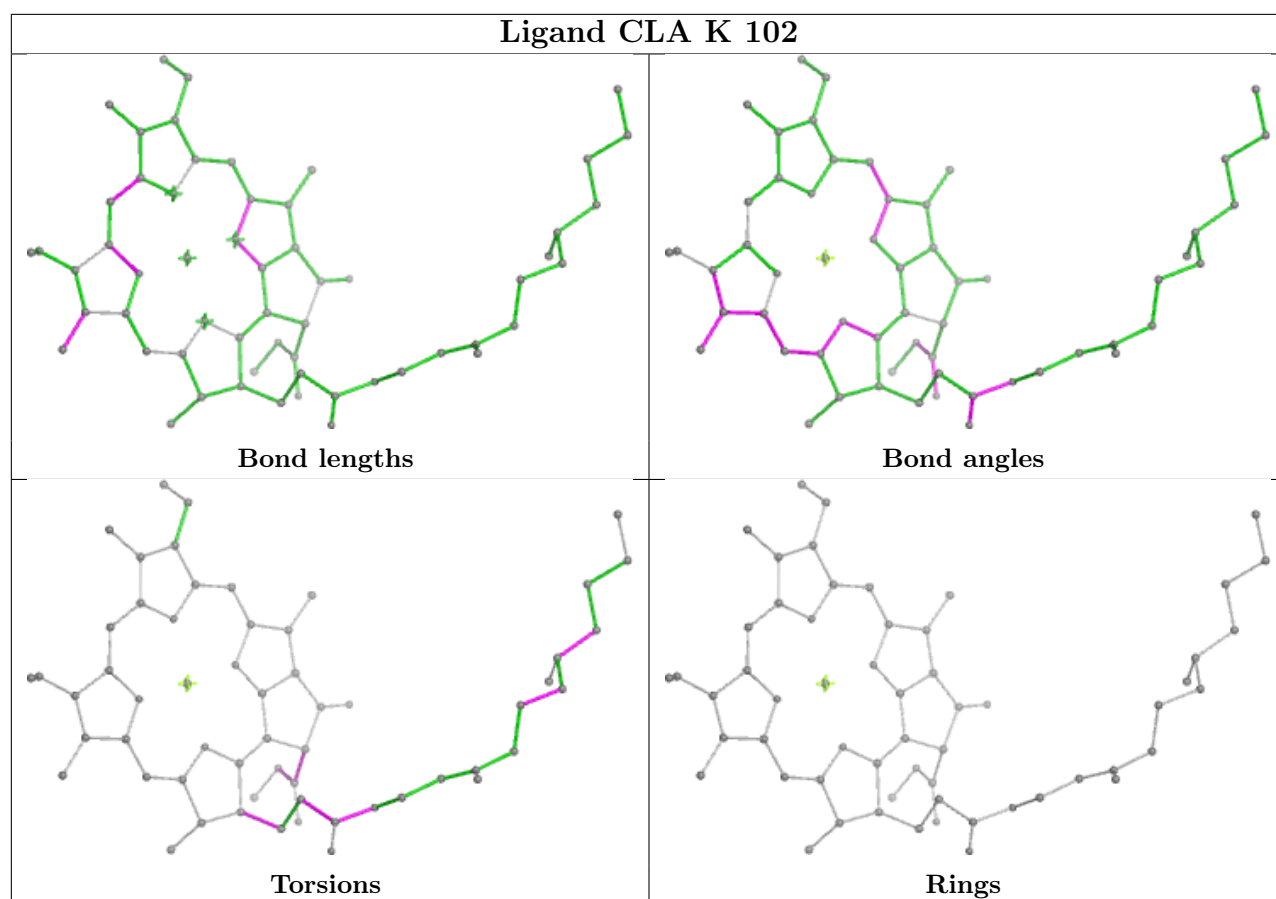


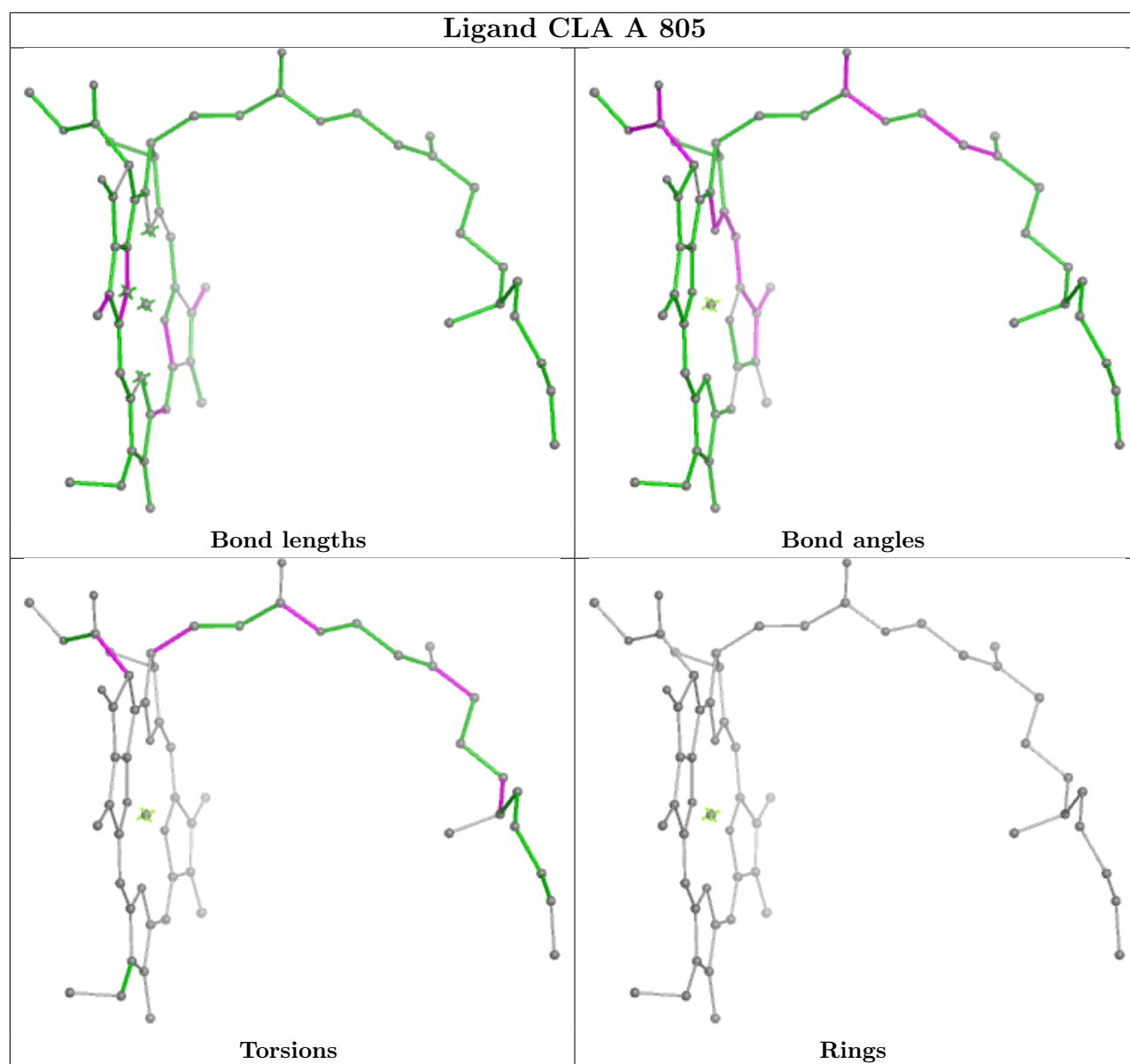


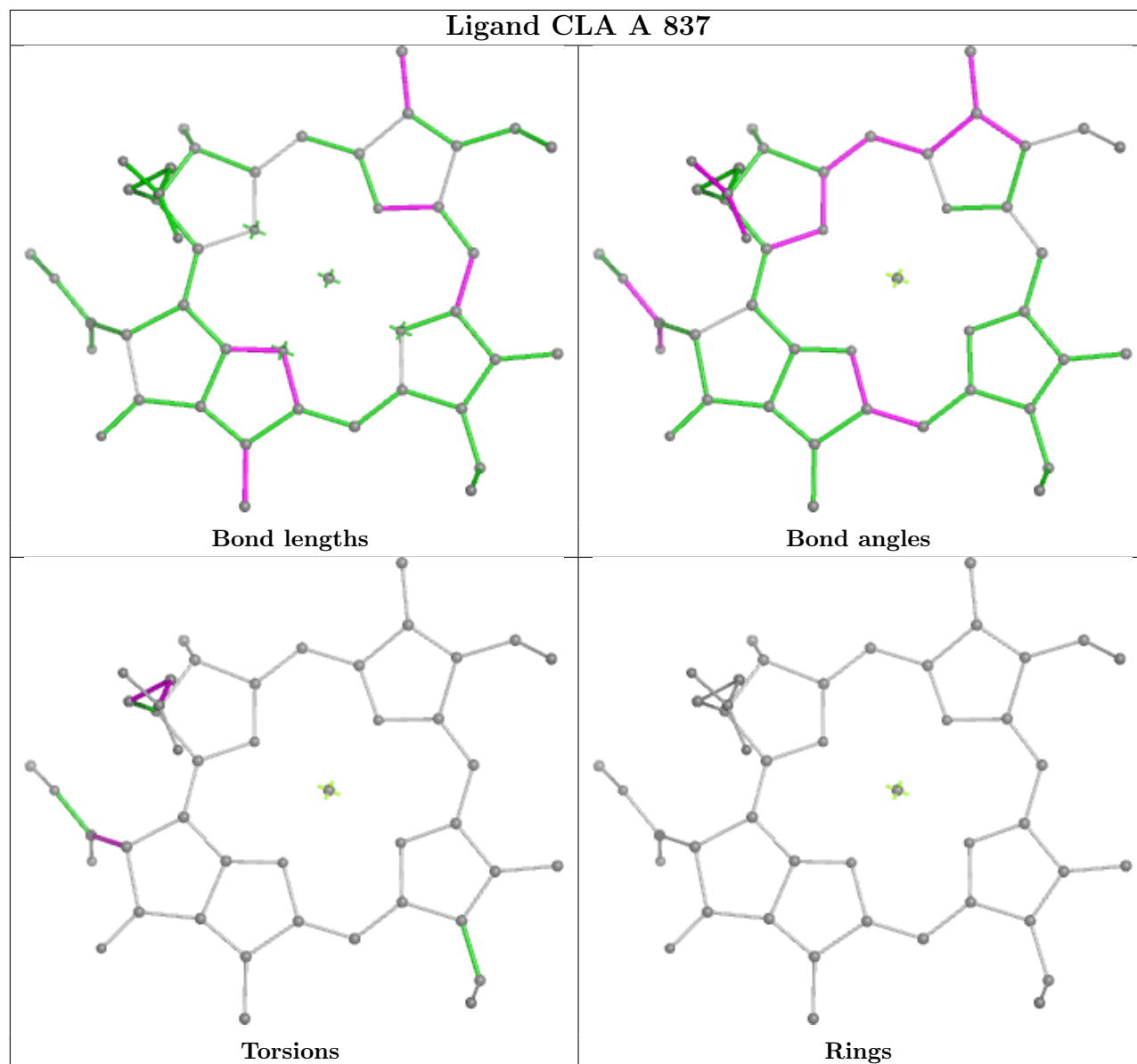
Ligand CLA L 204

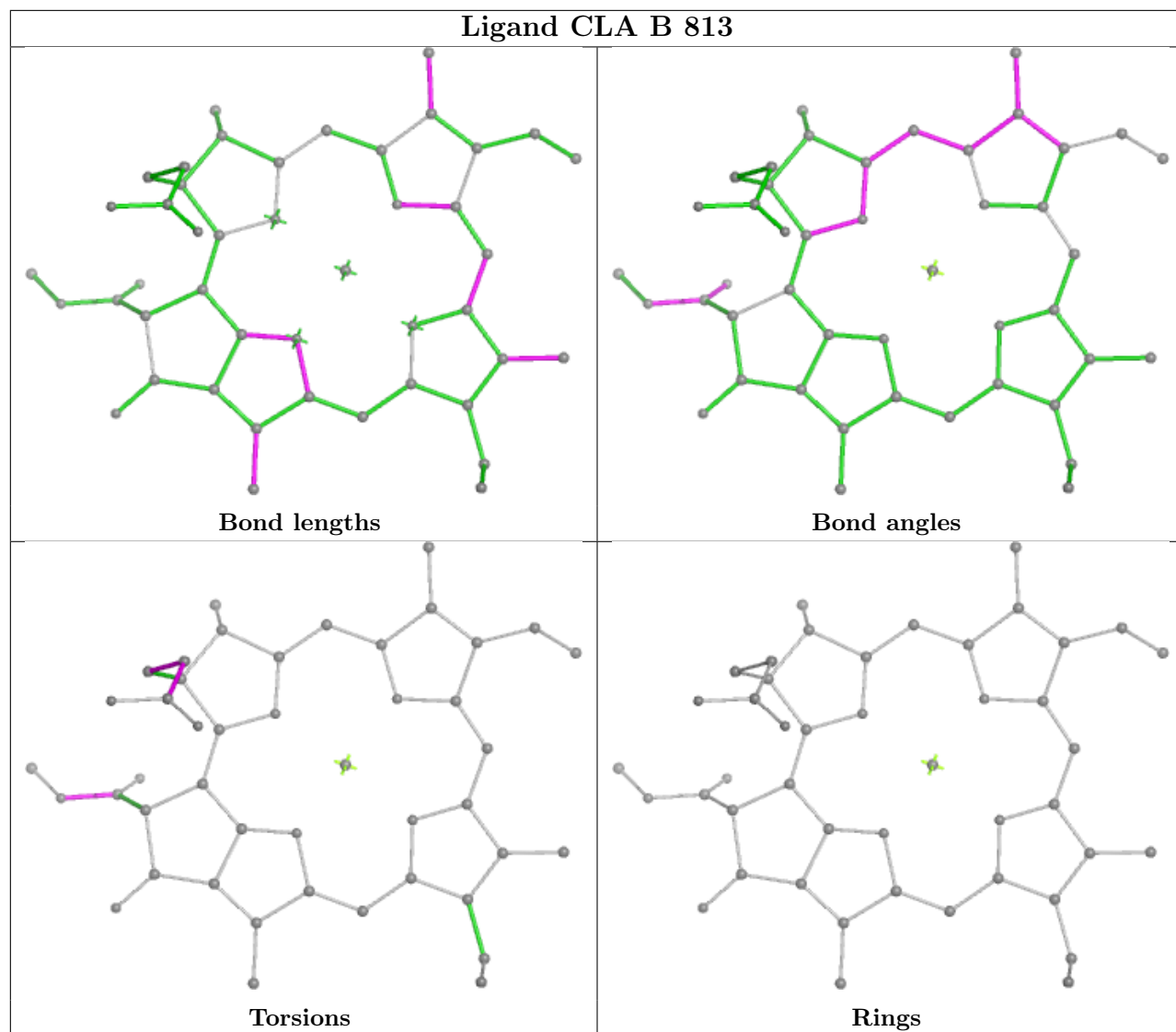


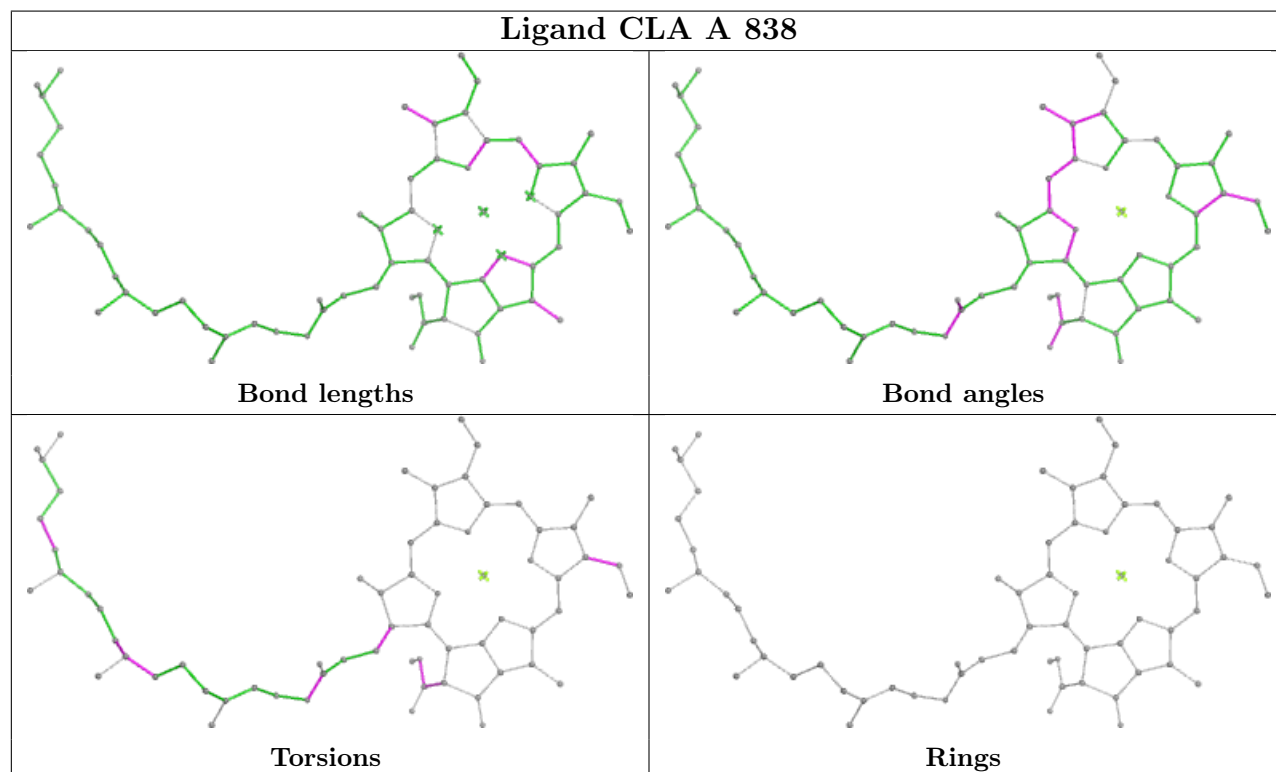
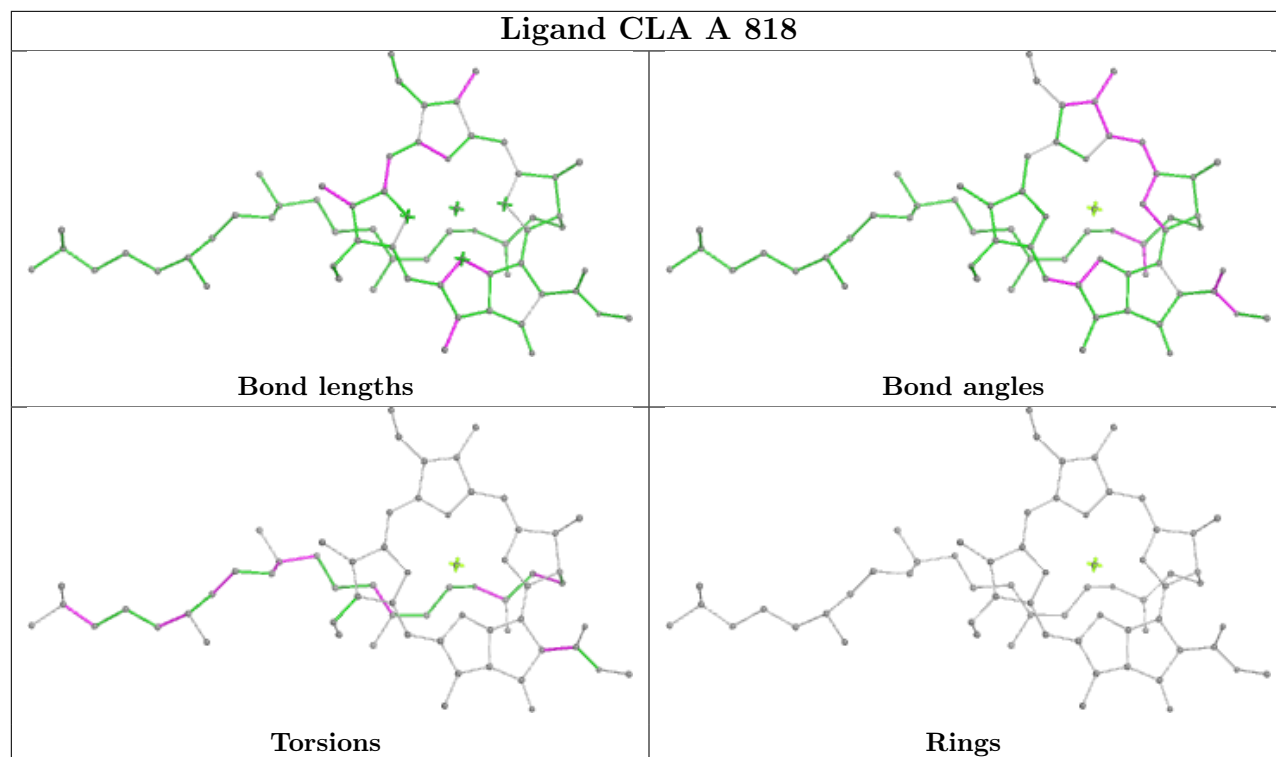
Ligand CLA B 834**Ligand CLA L 205**



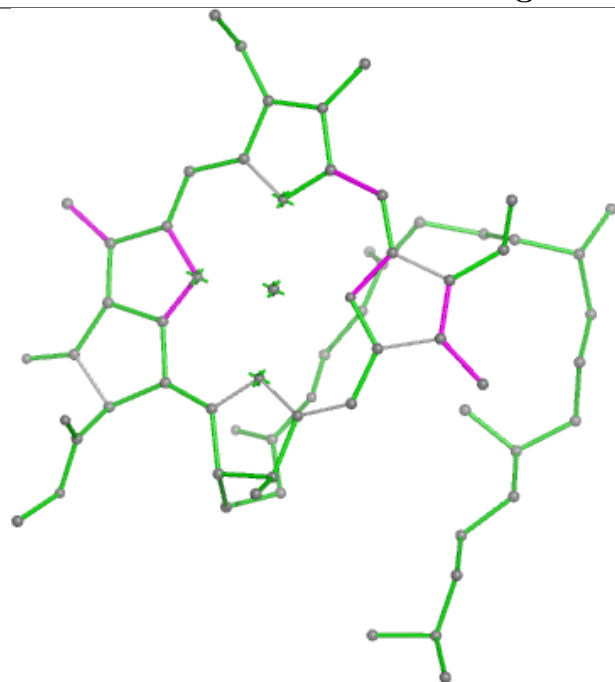




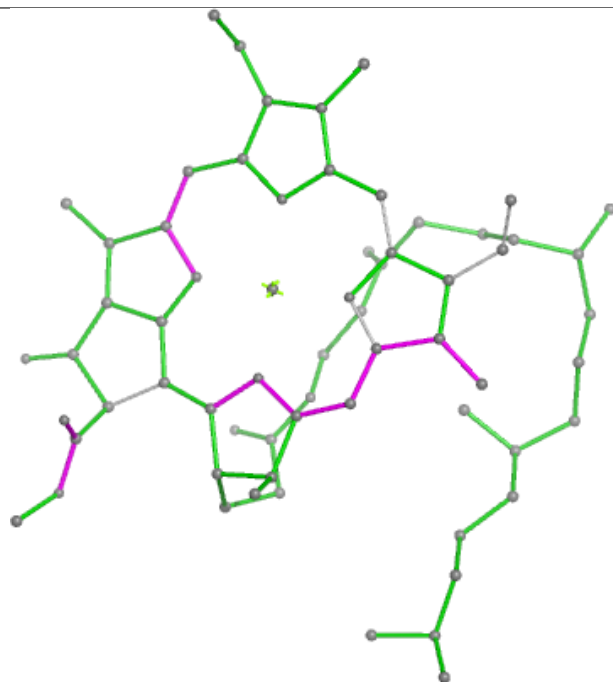




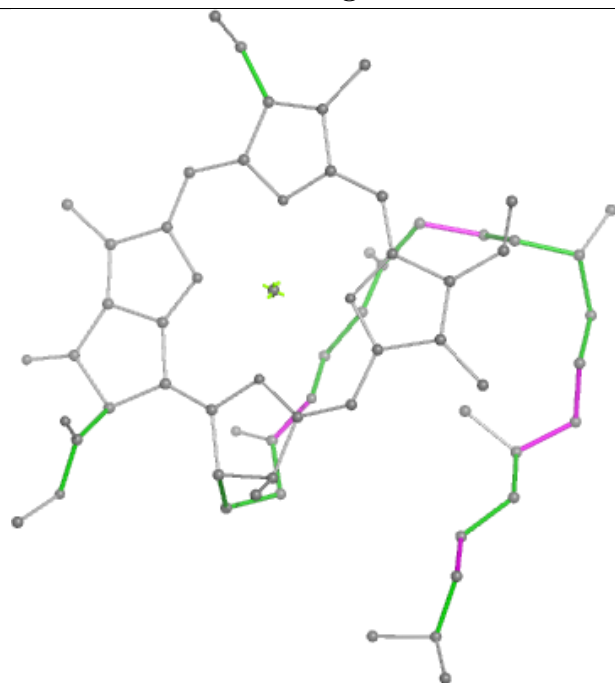
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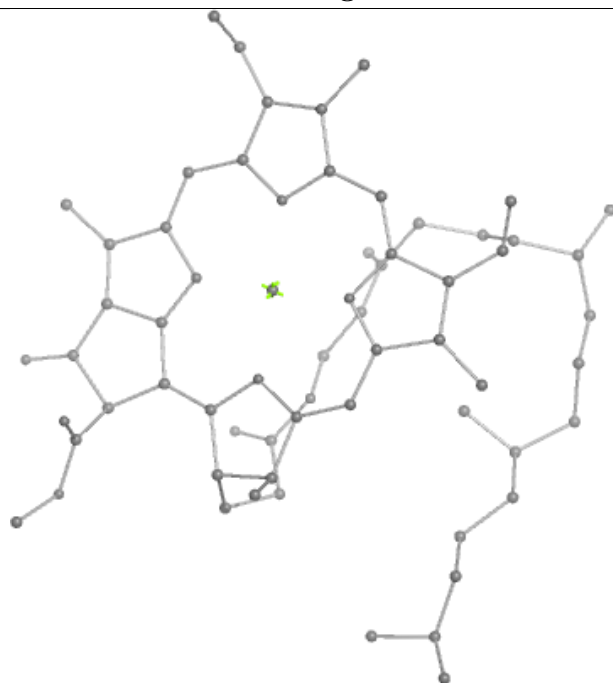
Bond lengths



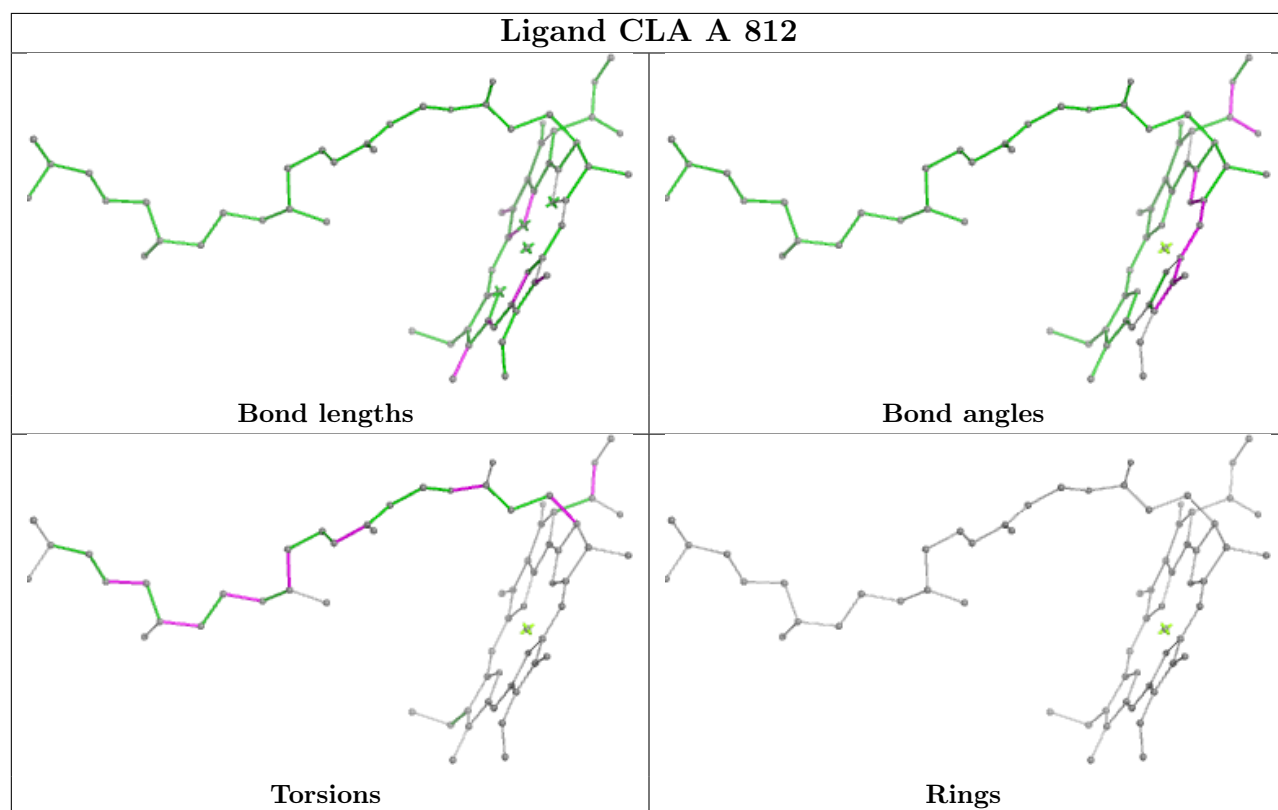
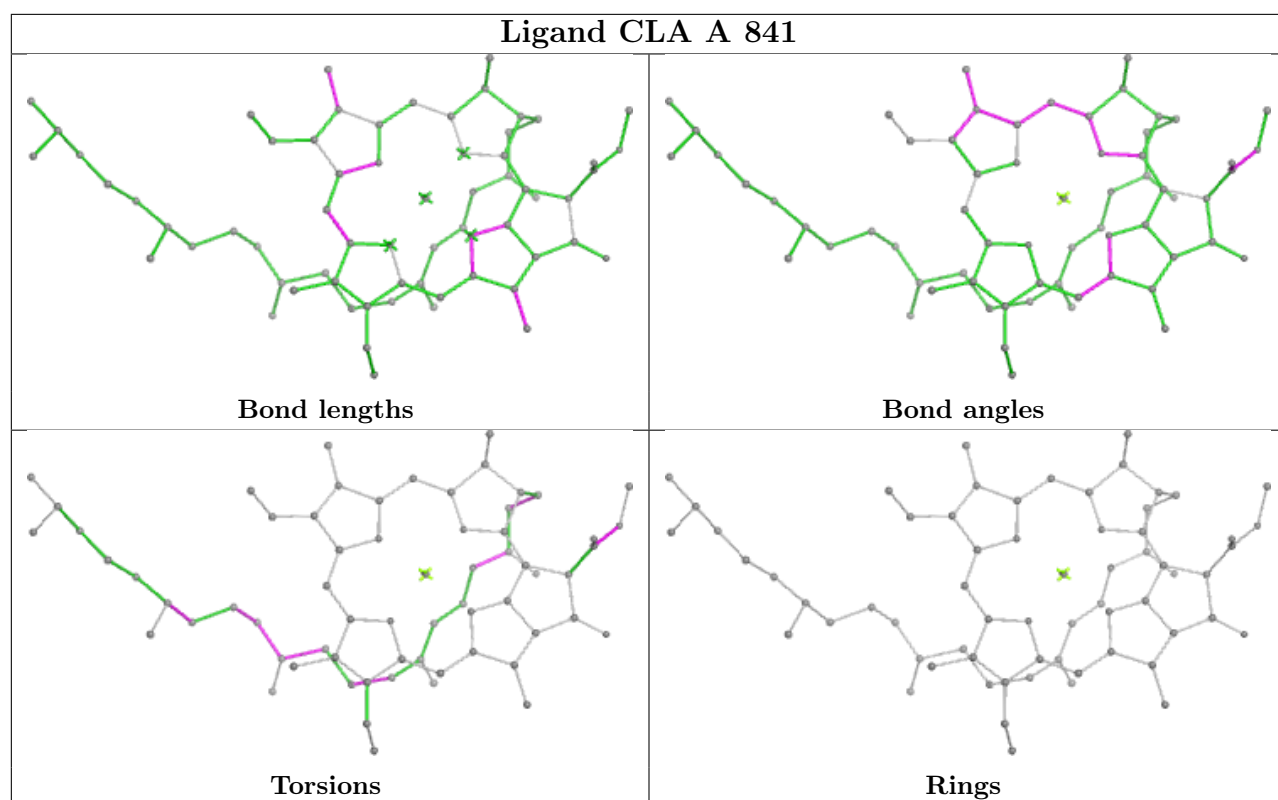
Bond angles

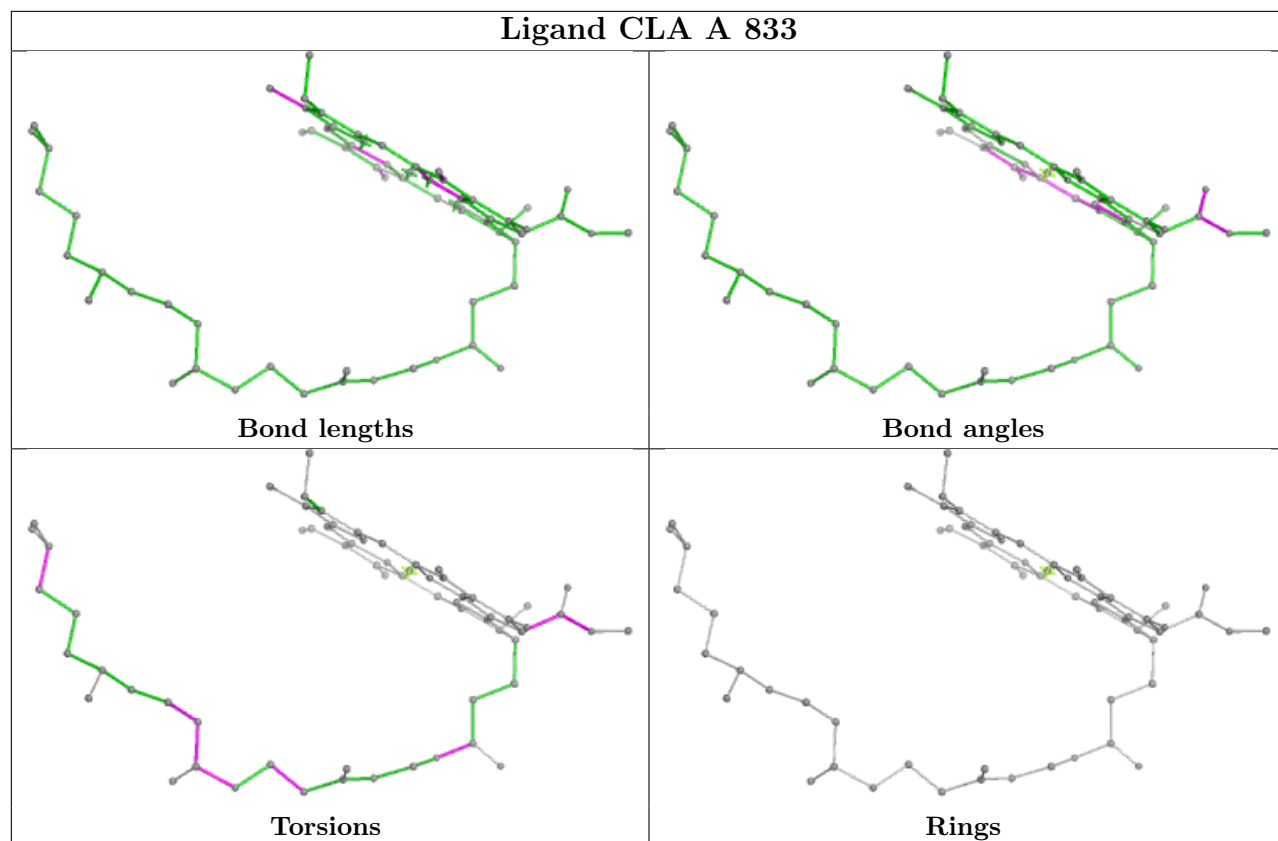


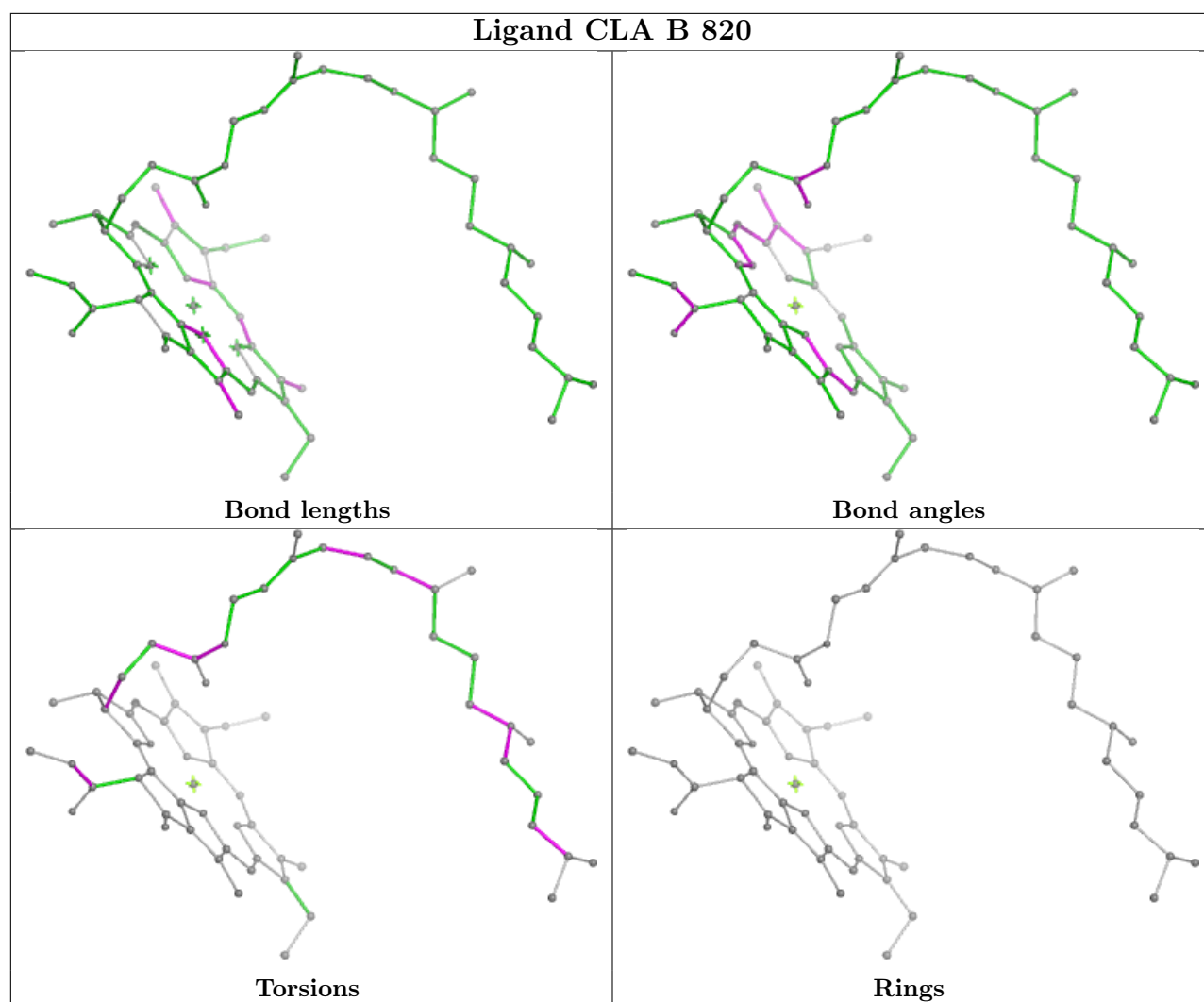
Torsions



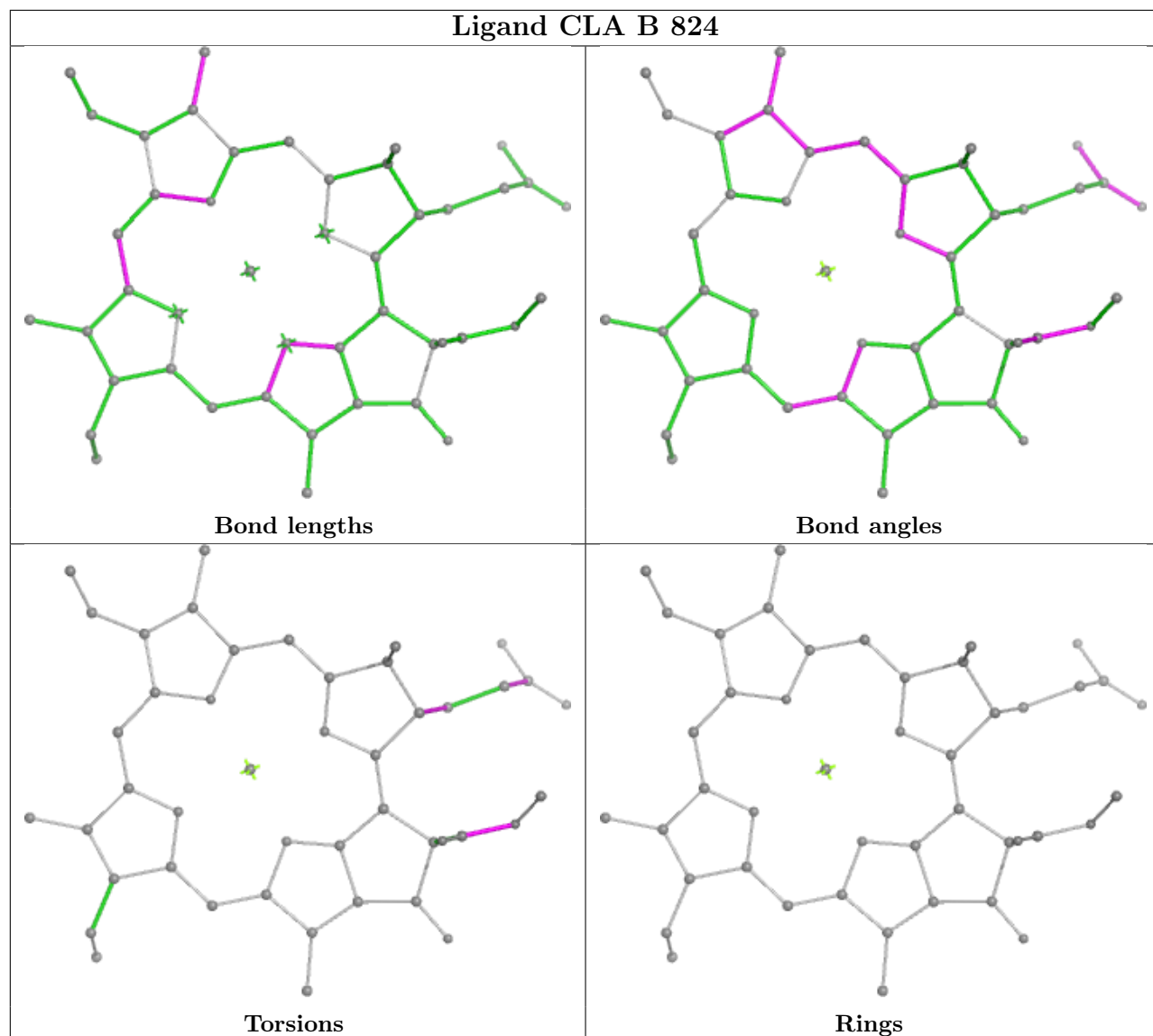
Rings

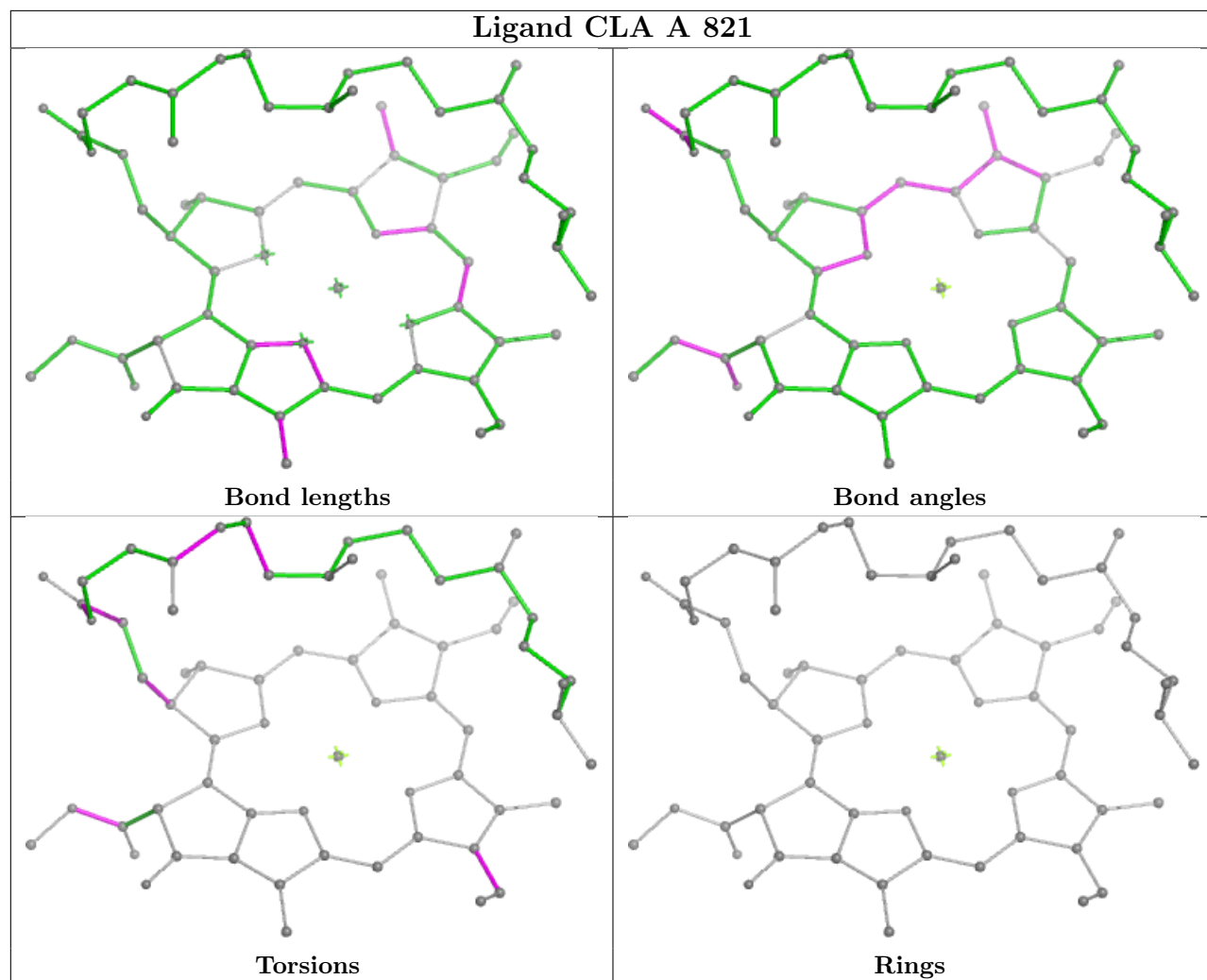


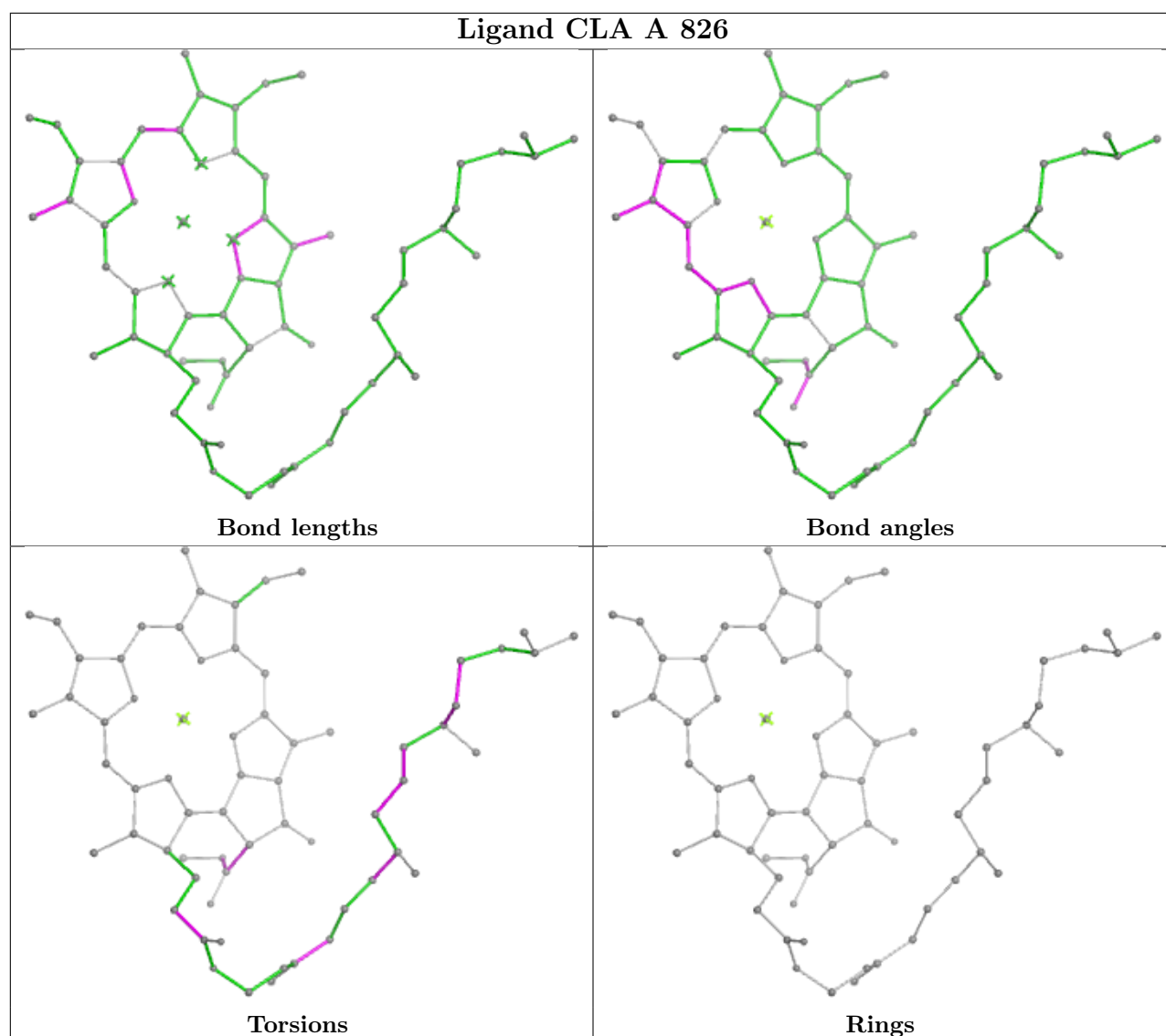


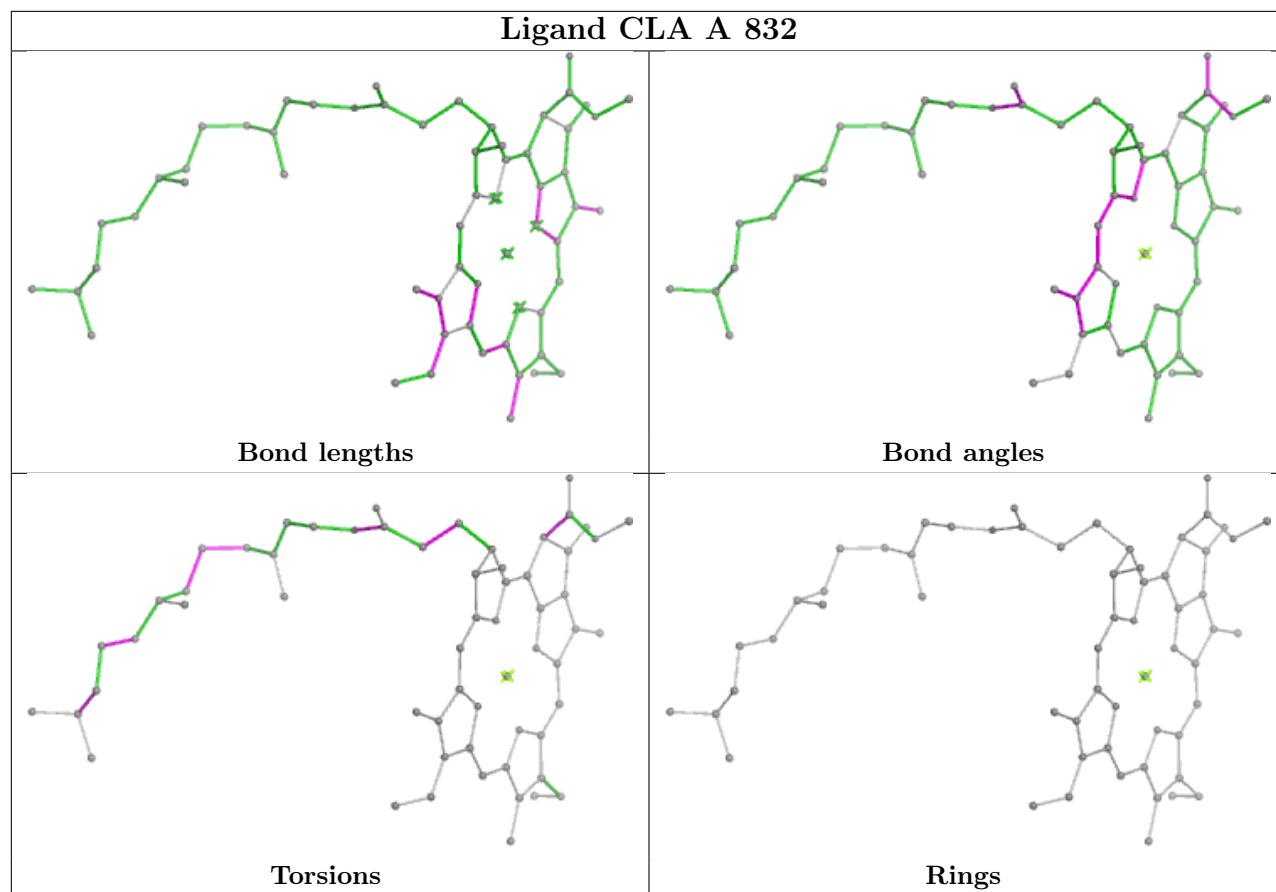


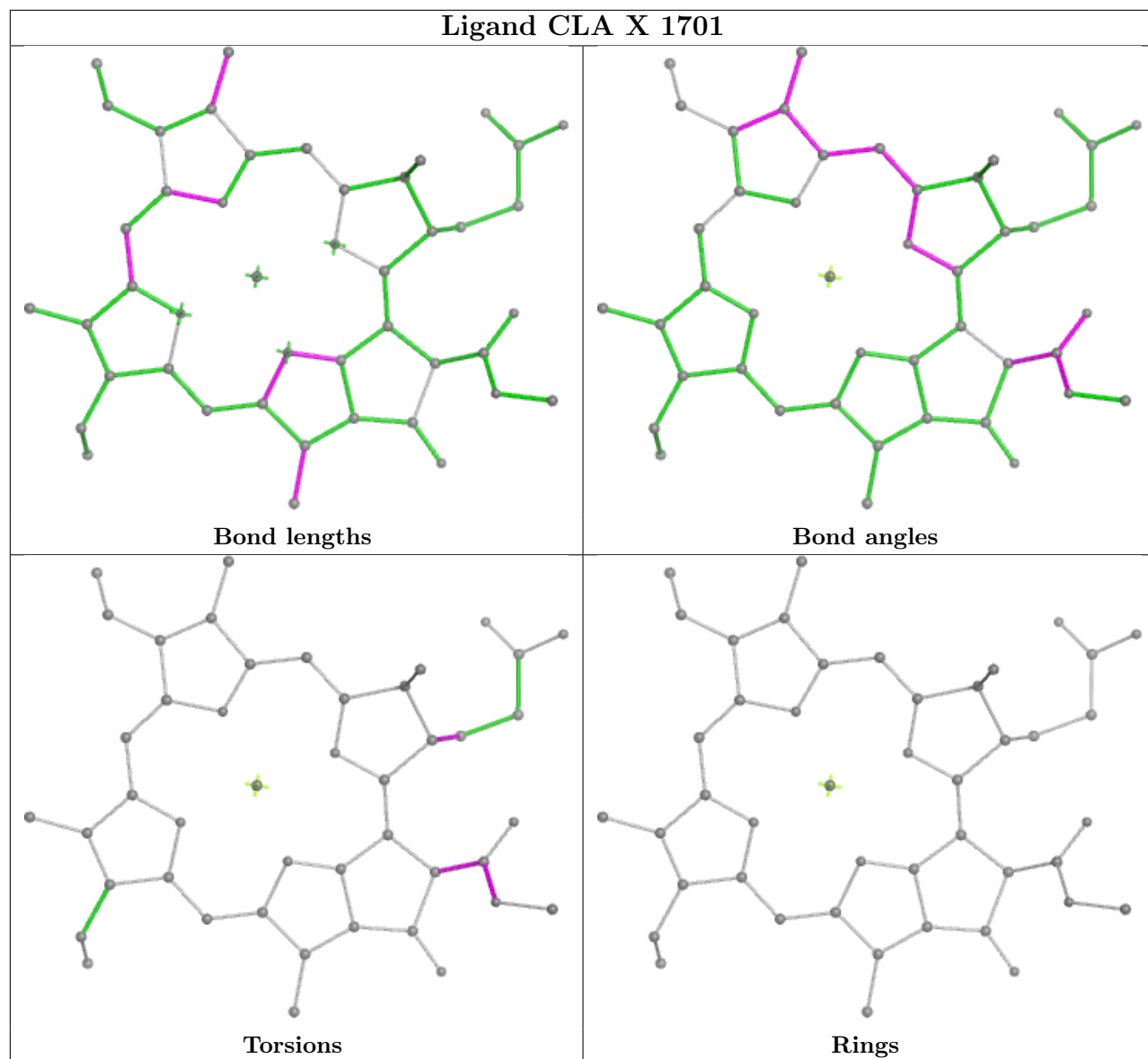
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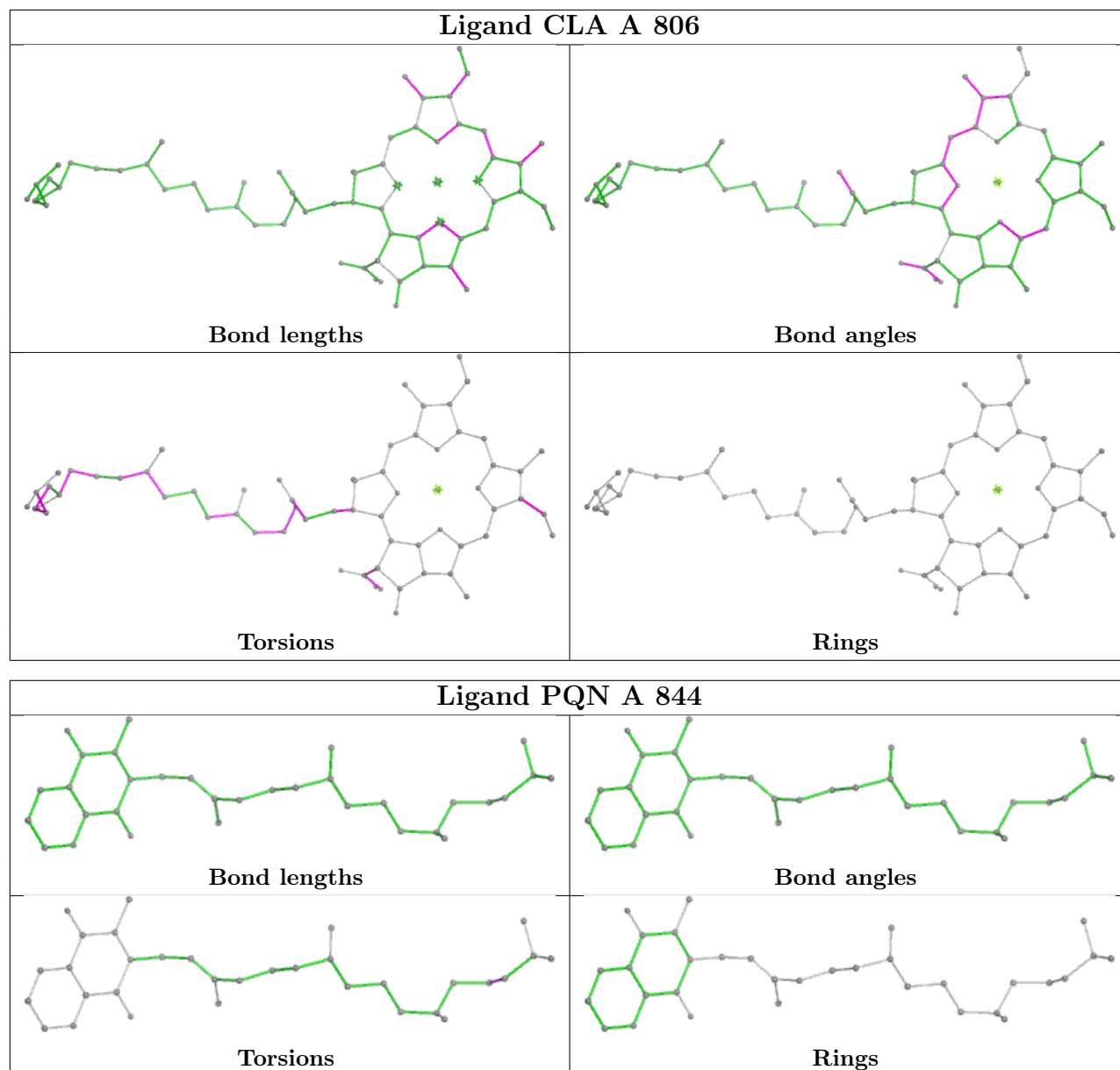


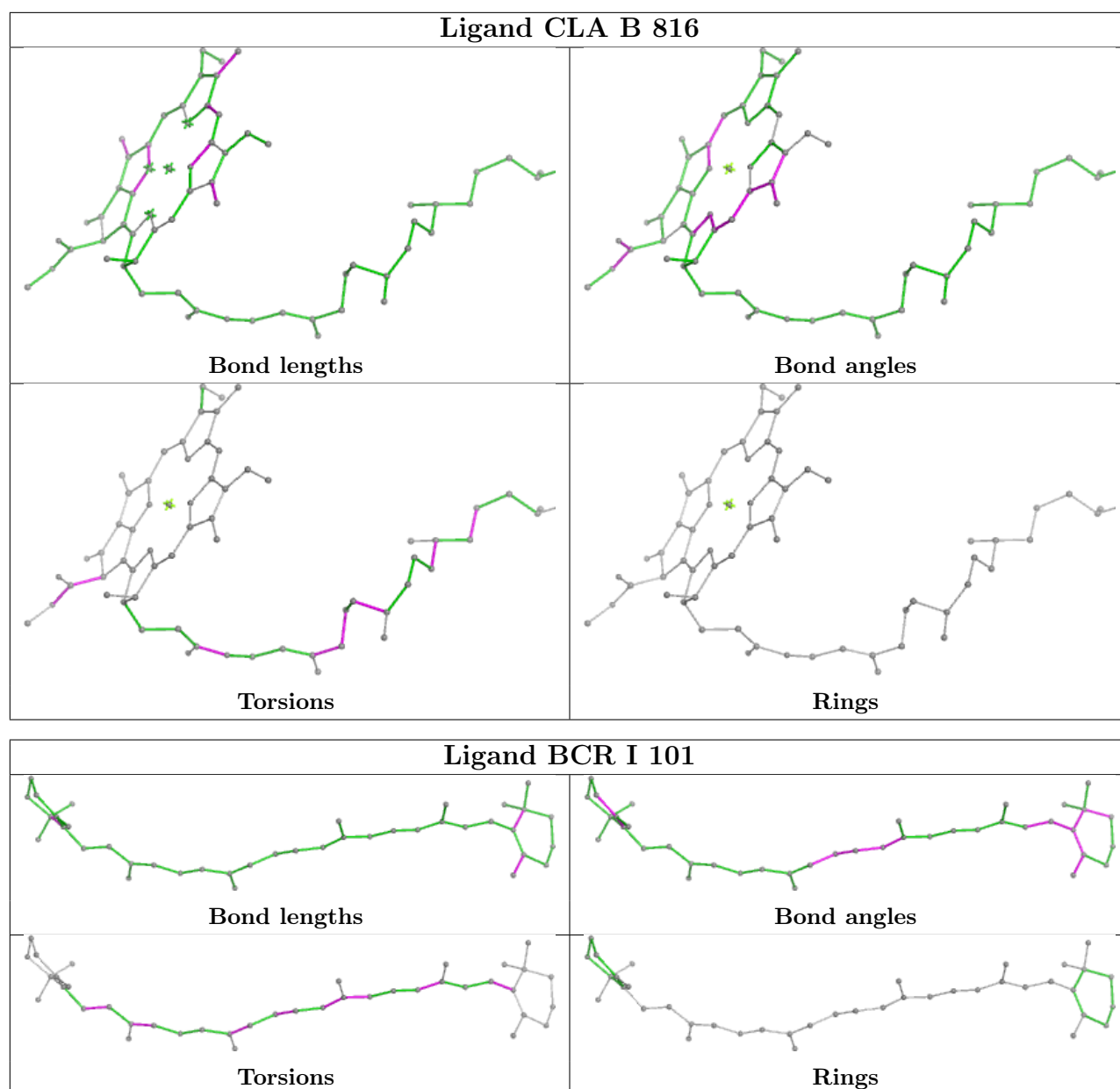


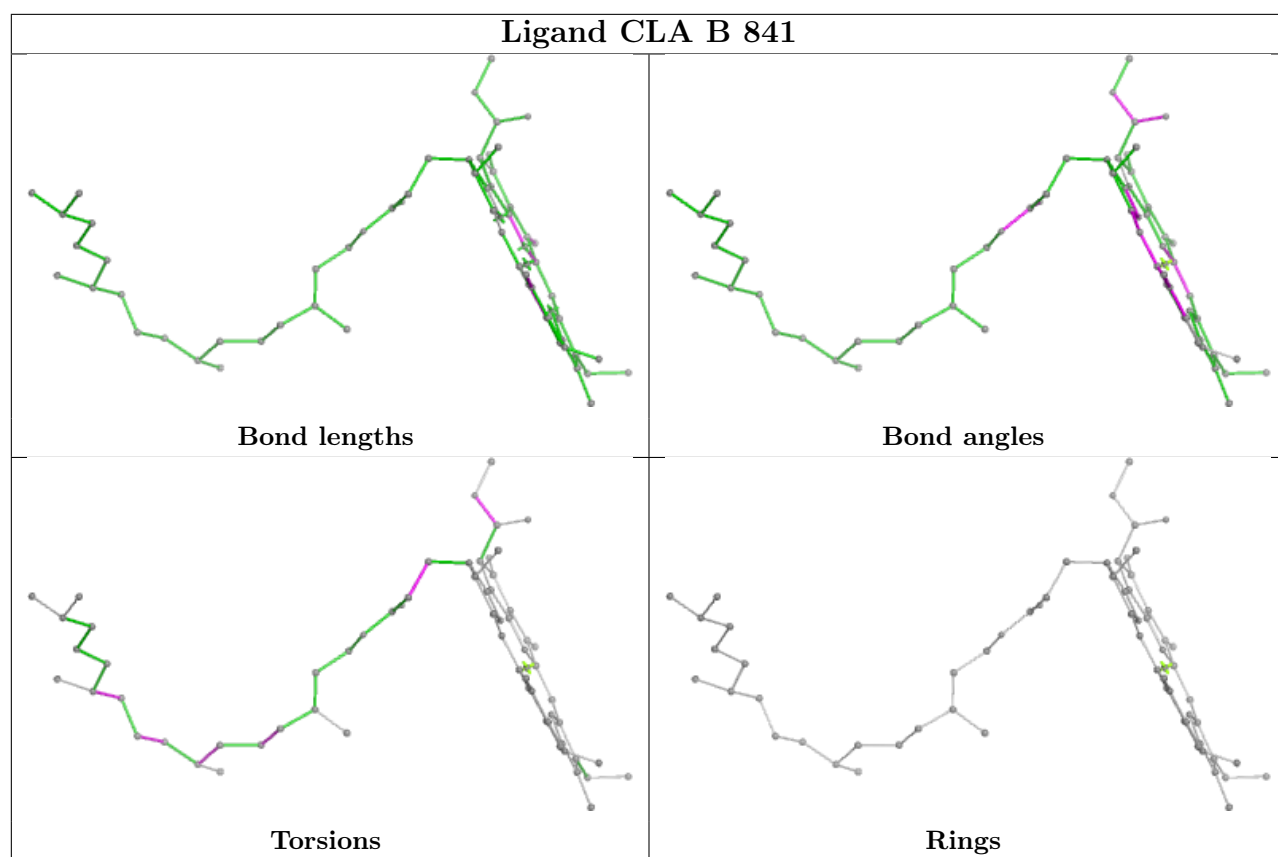




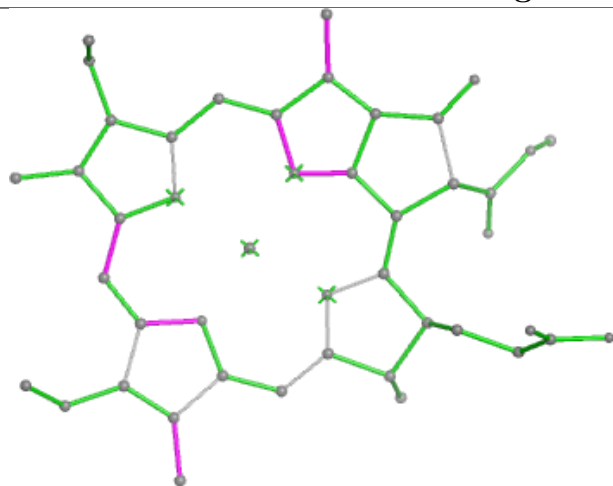




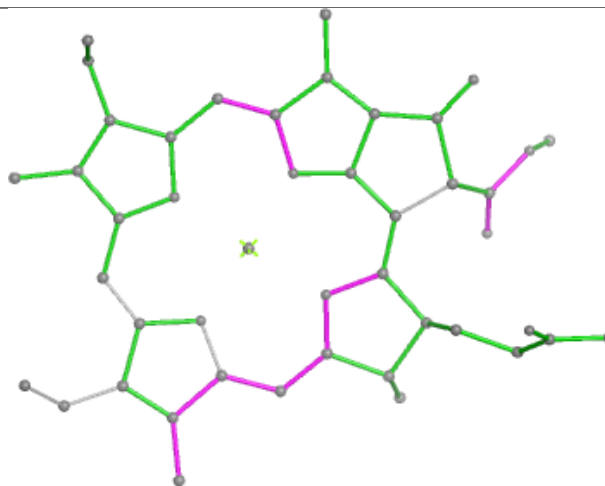




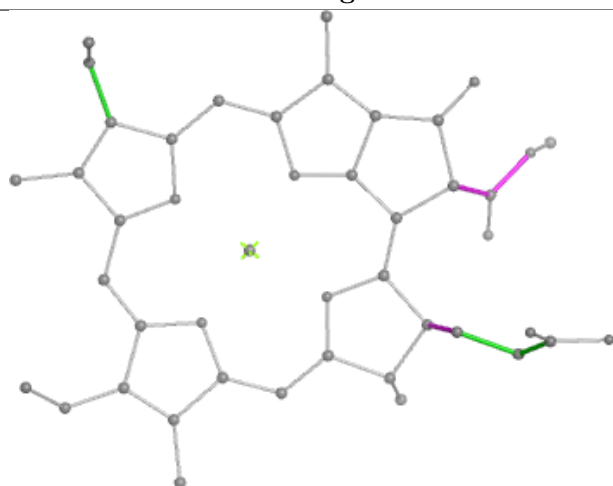
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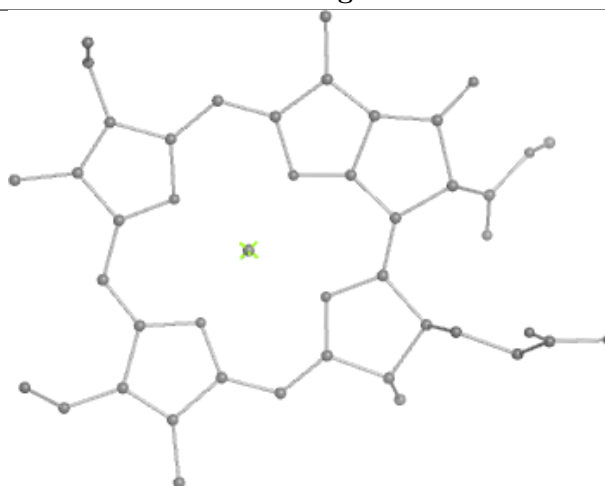
Bond lengths



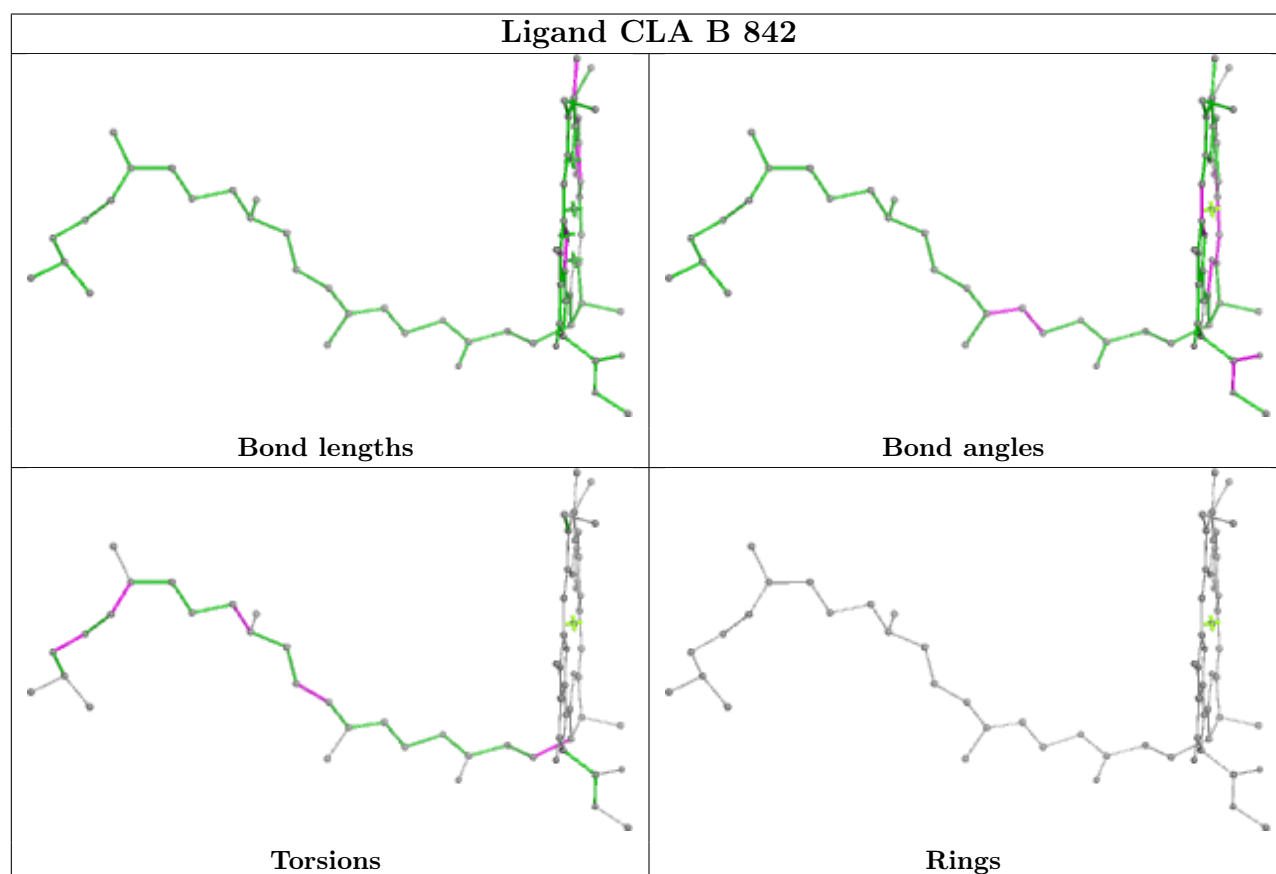
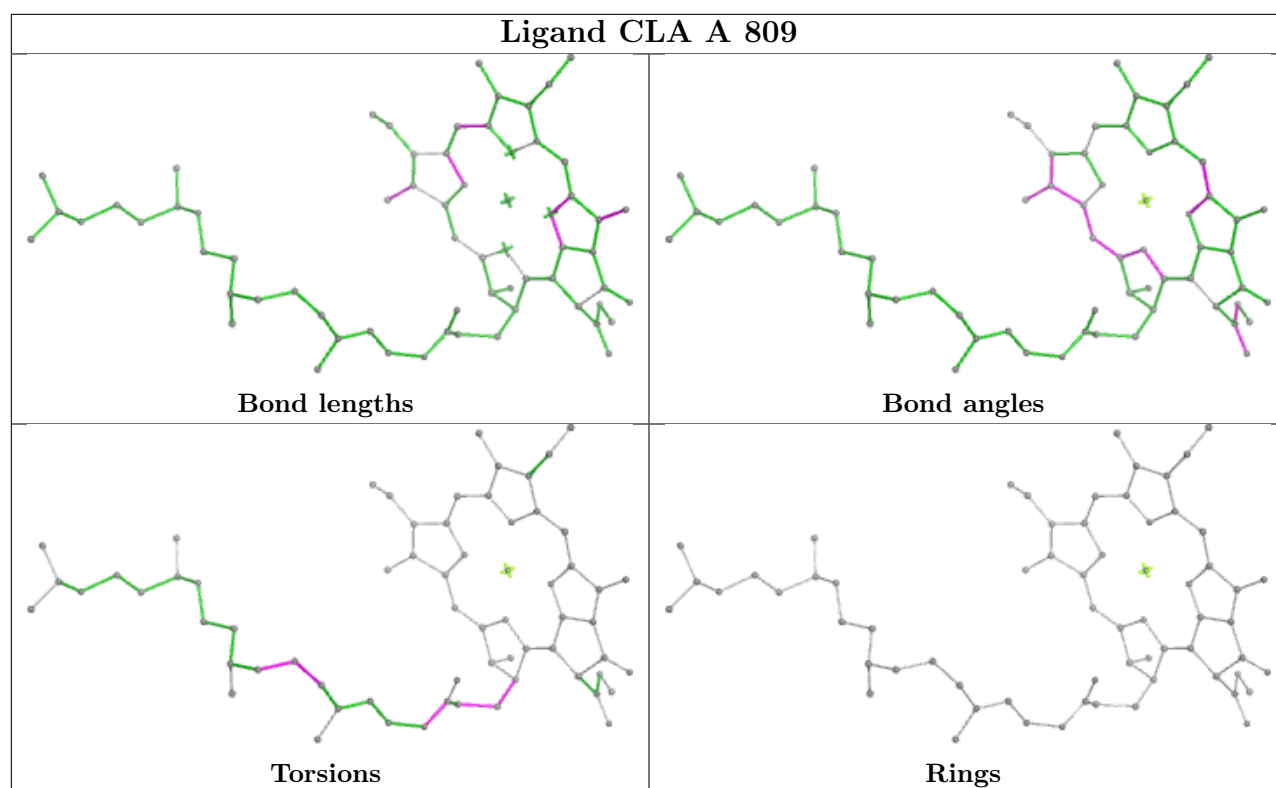
Bond angles



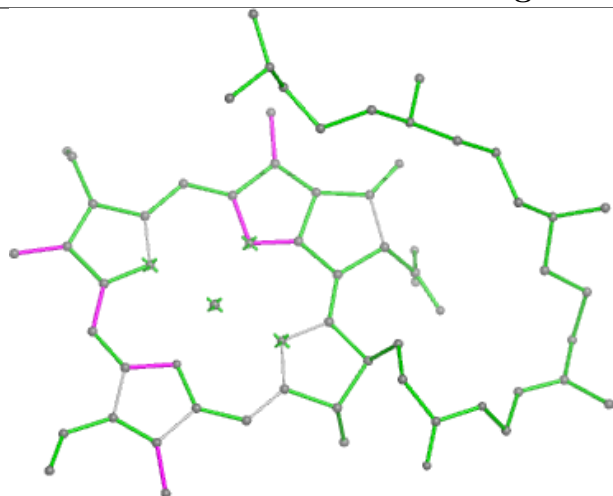
Torsions



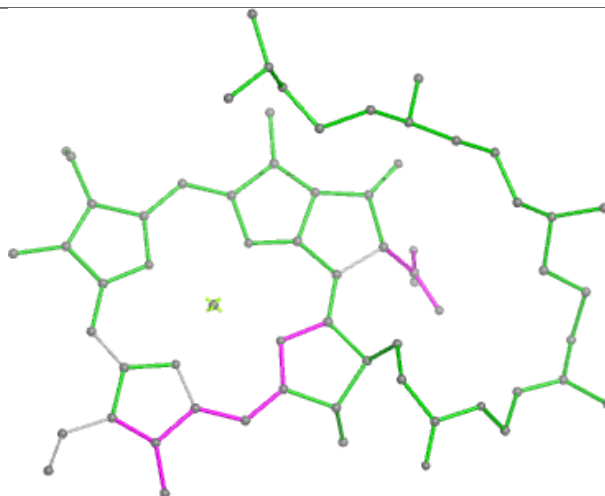
Rings



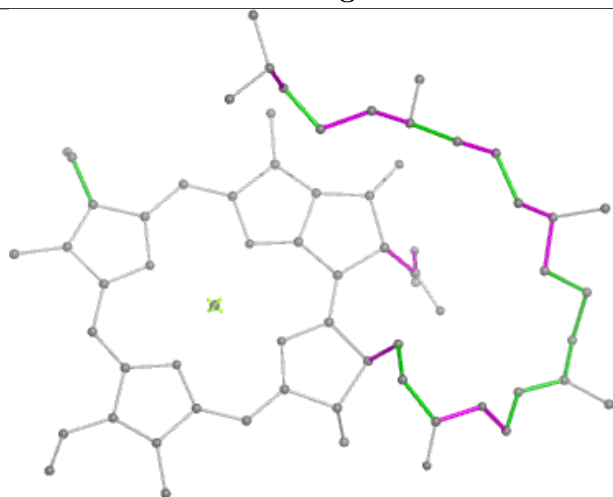
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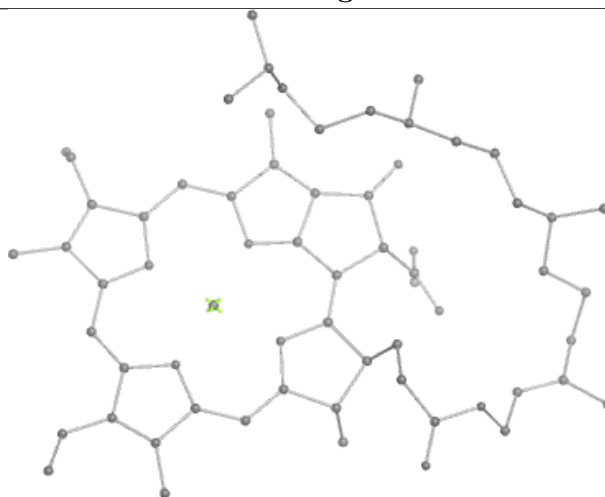
Bond lengths



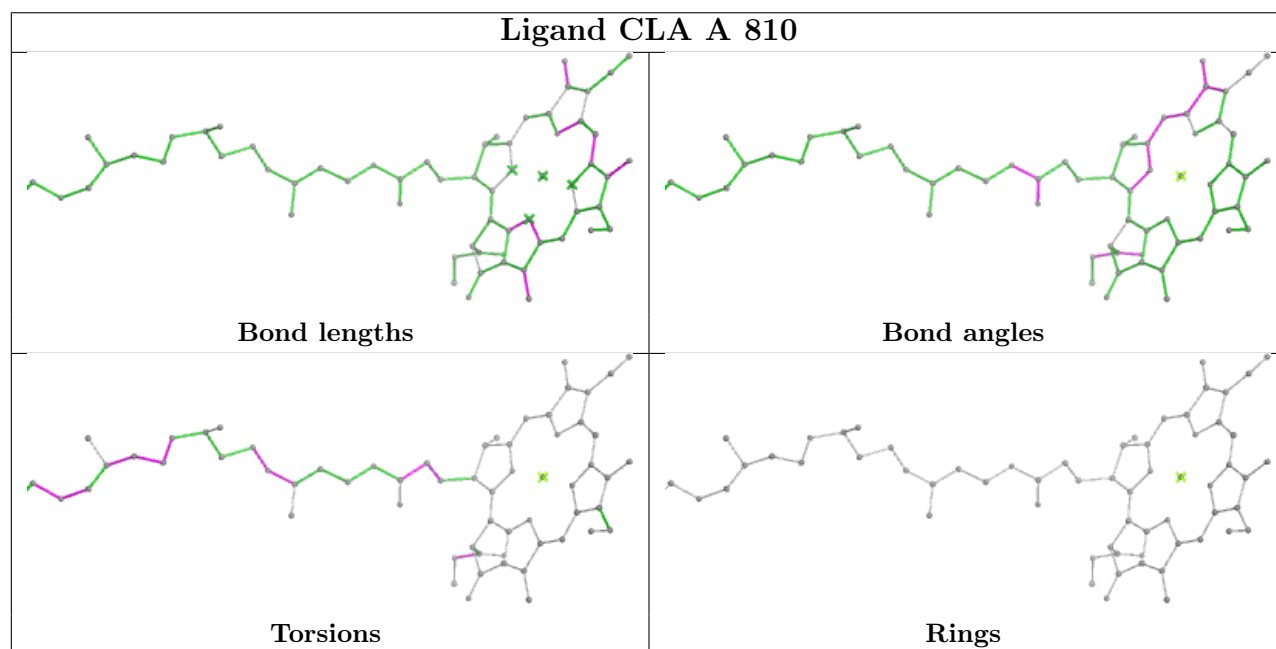
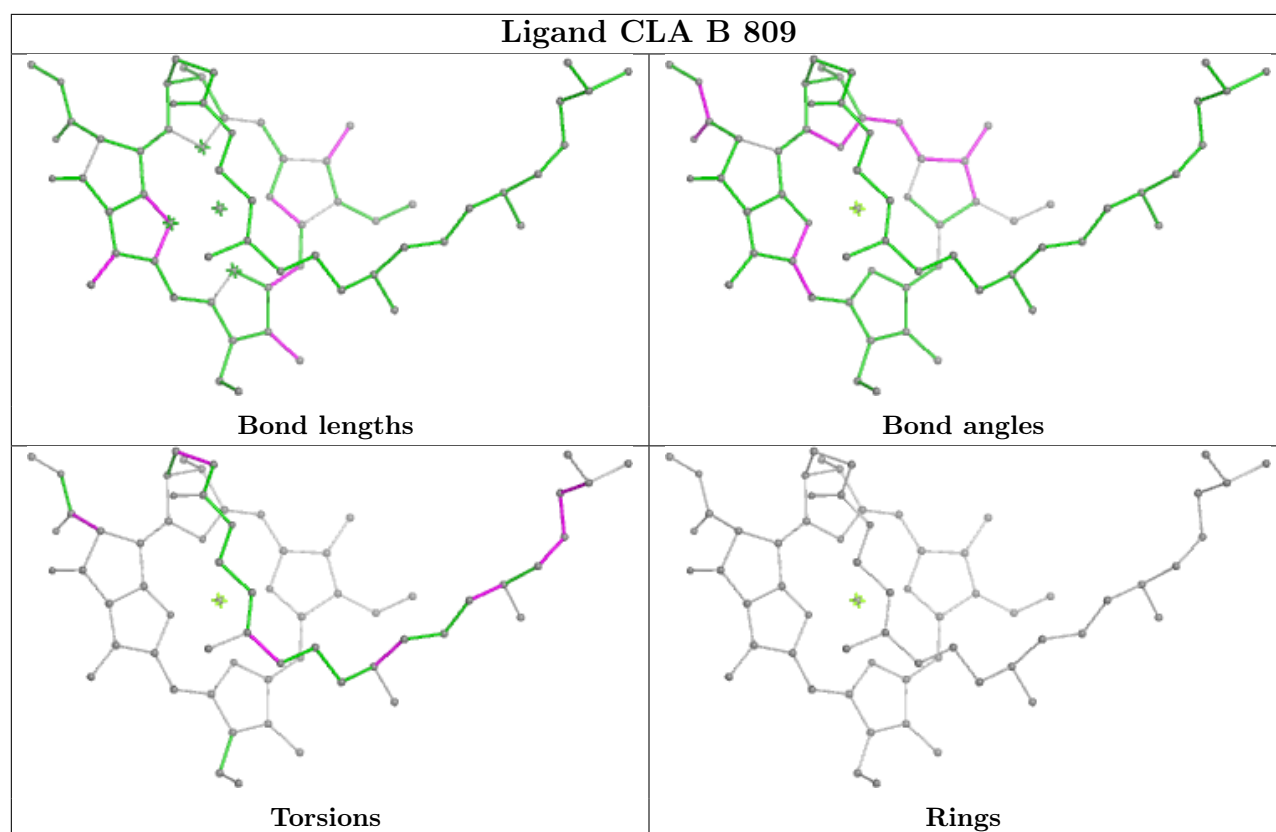
Bond angles

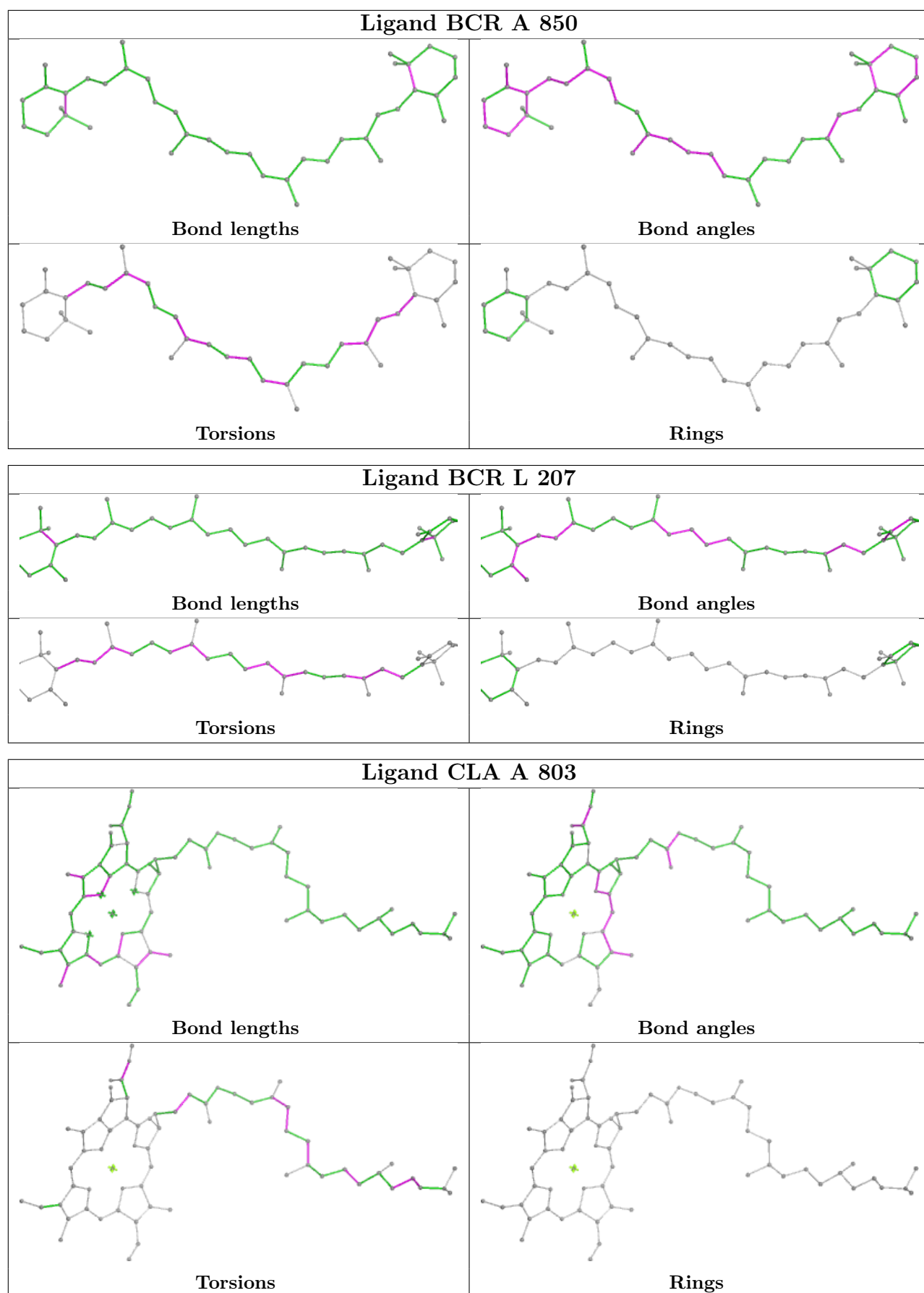


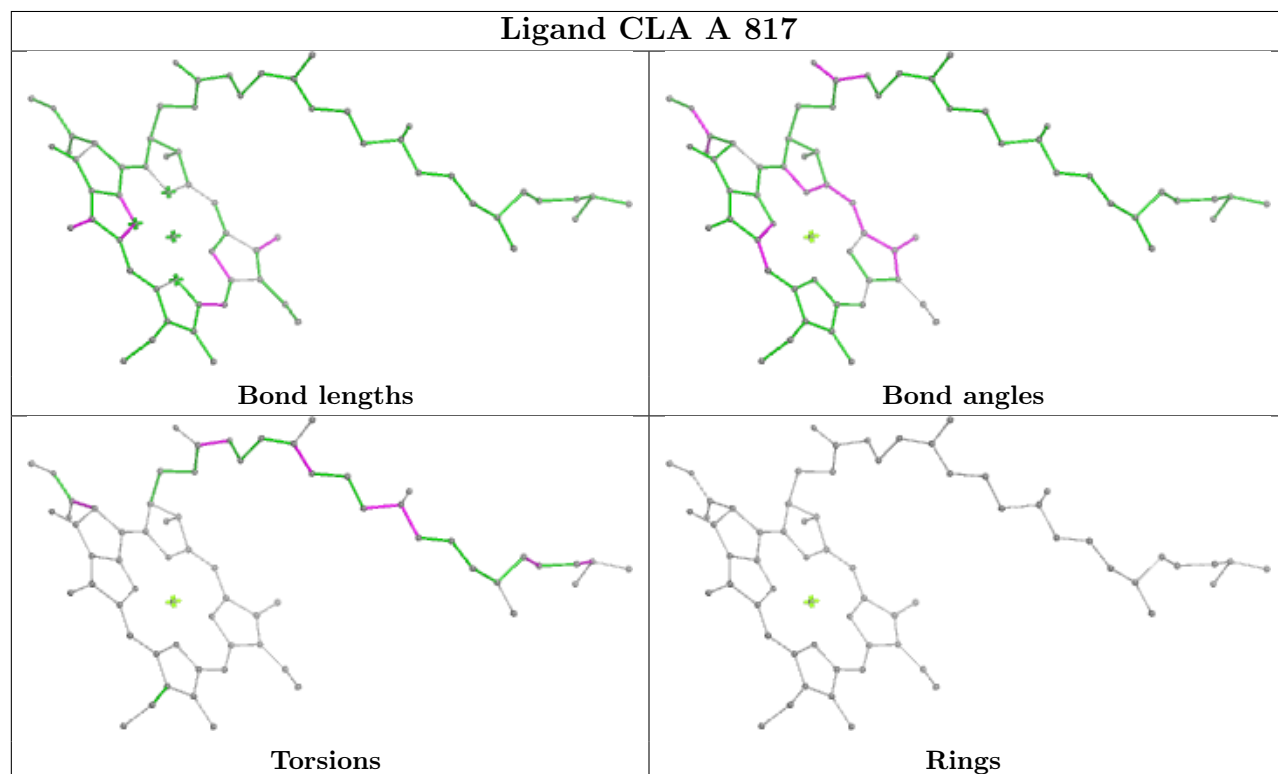
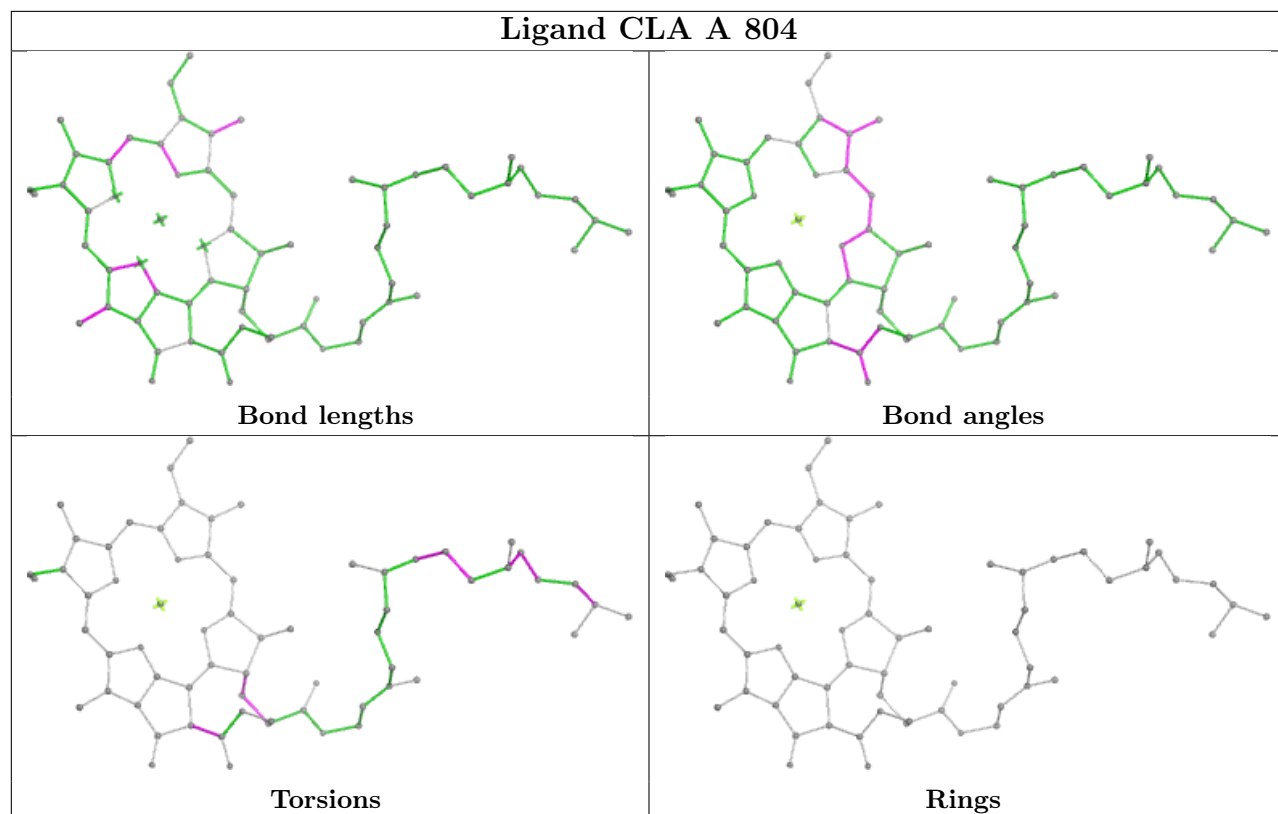
Torsions

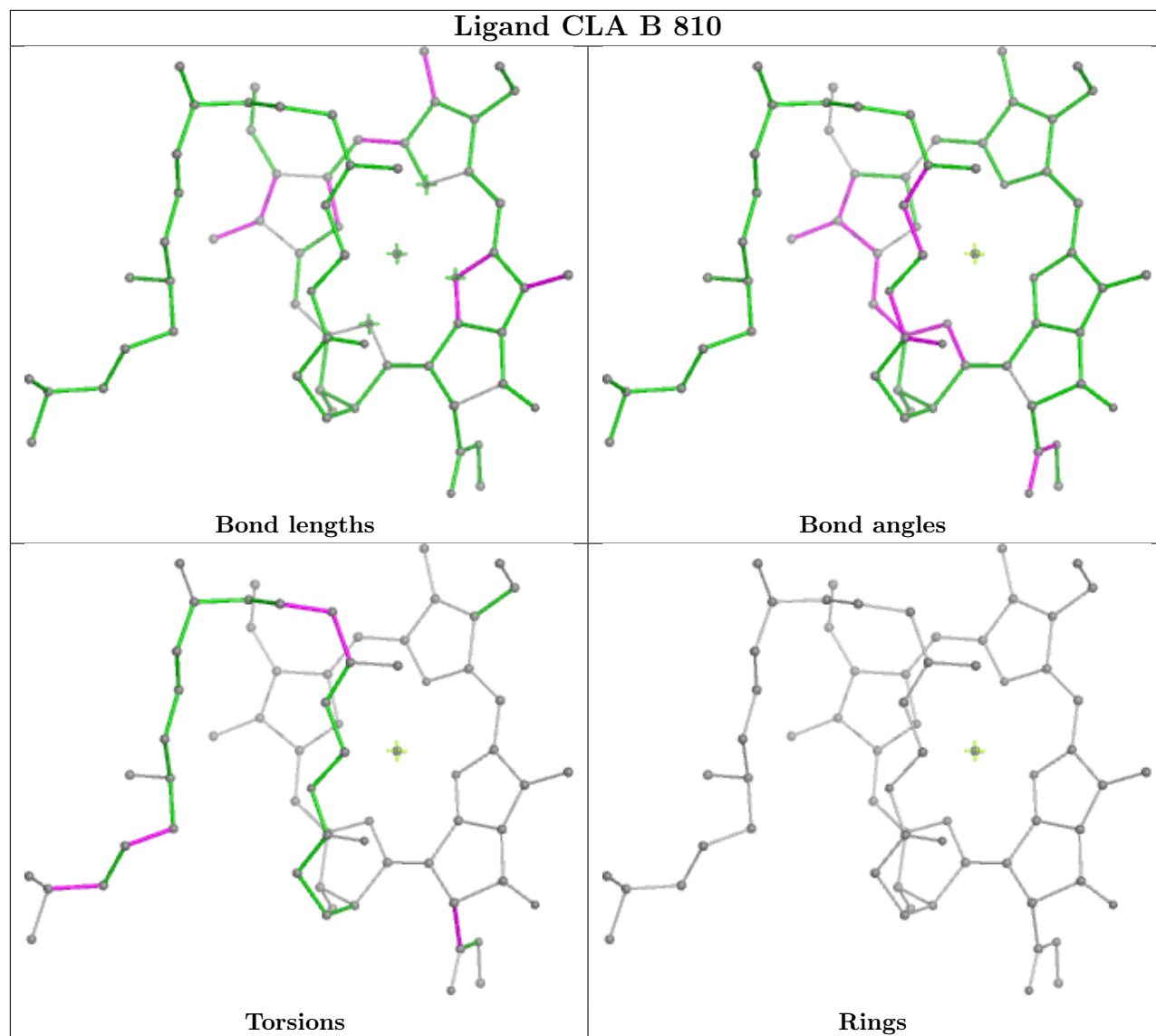


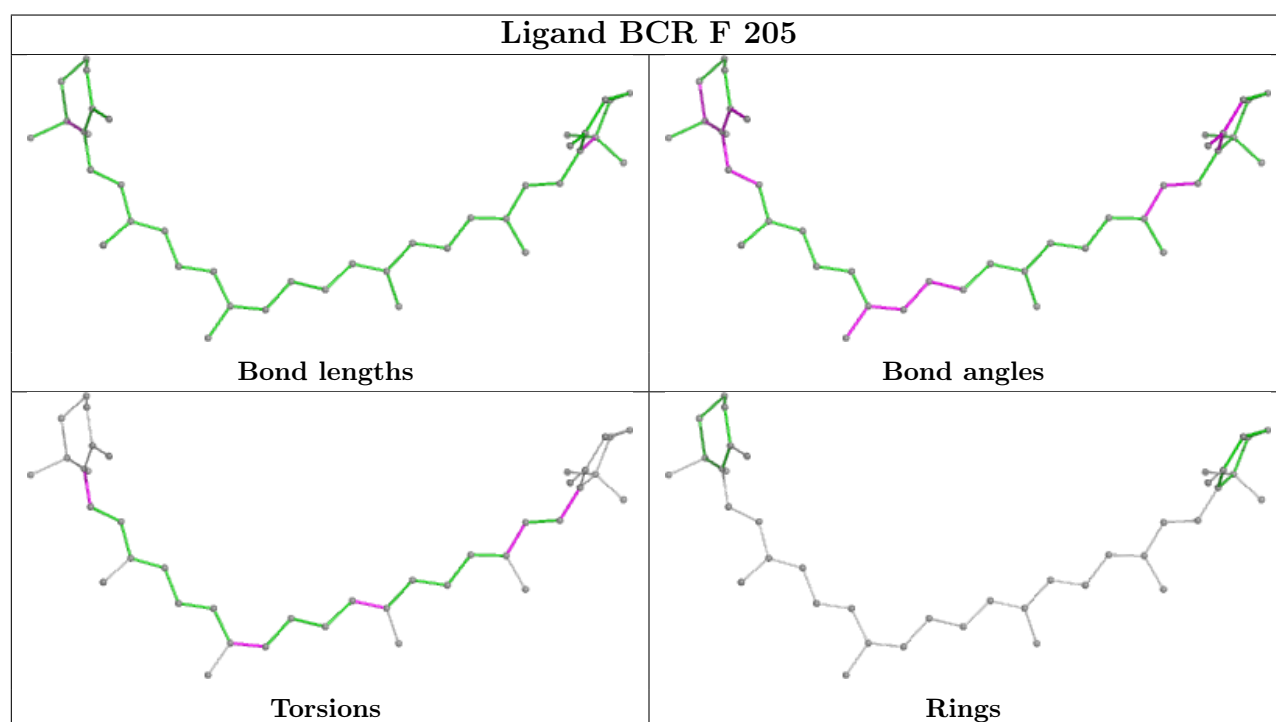
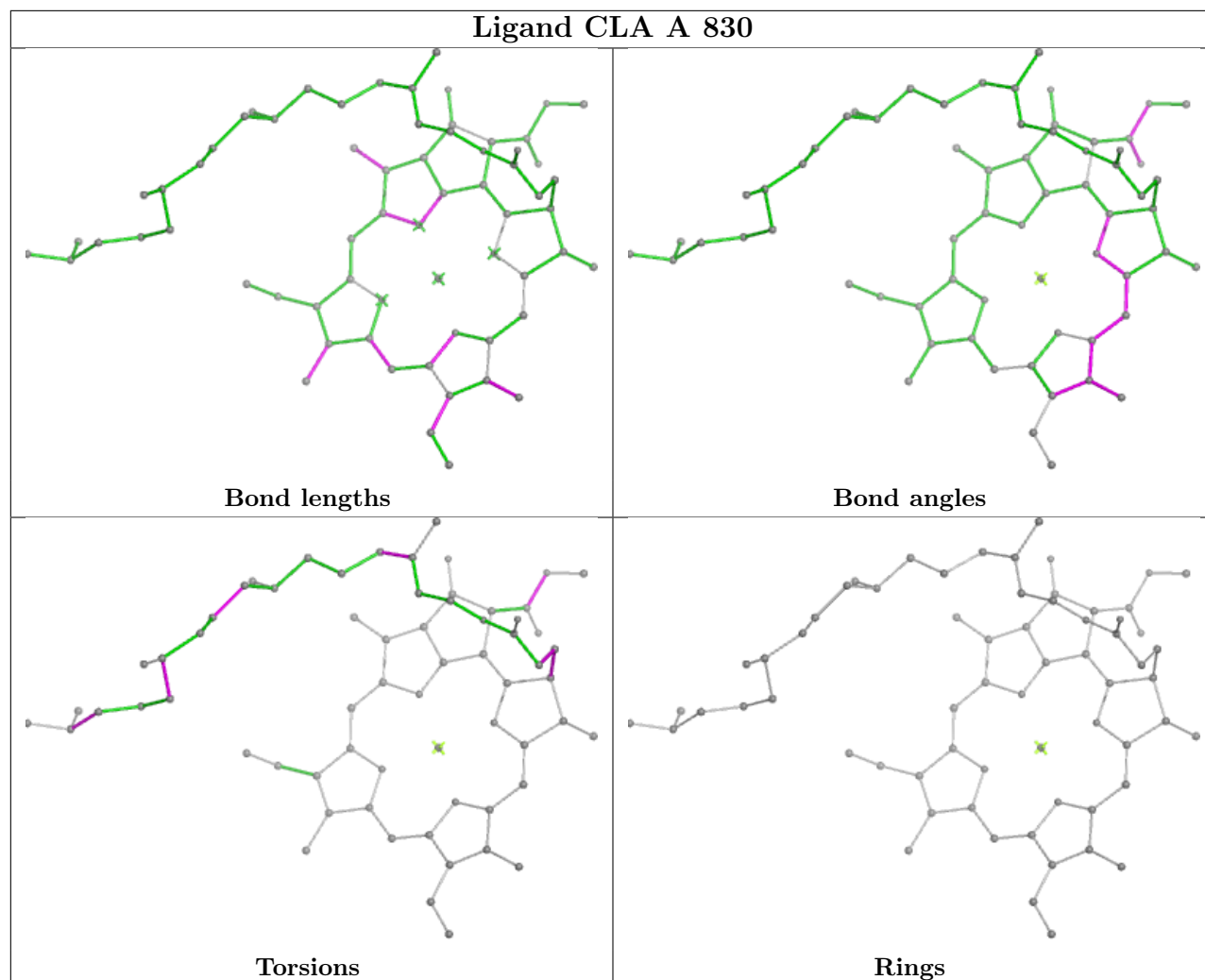
Rings

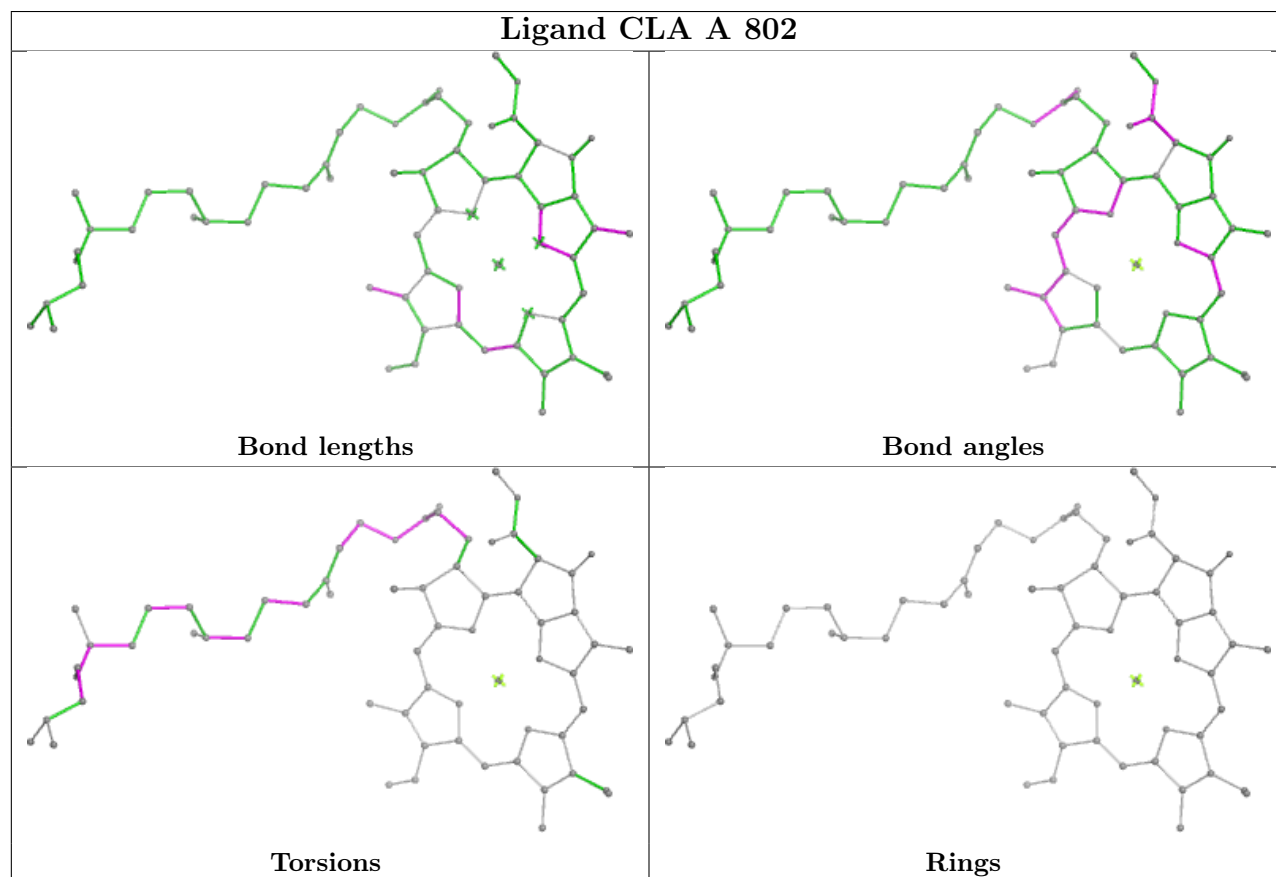
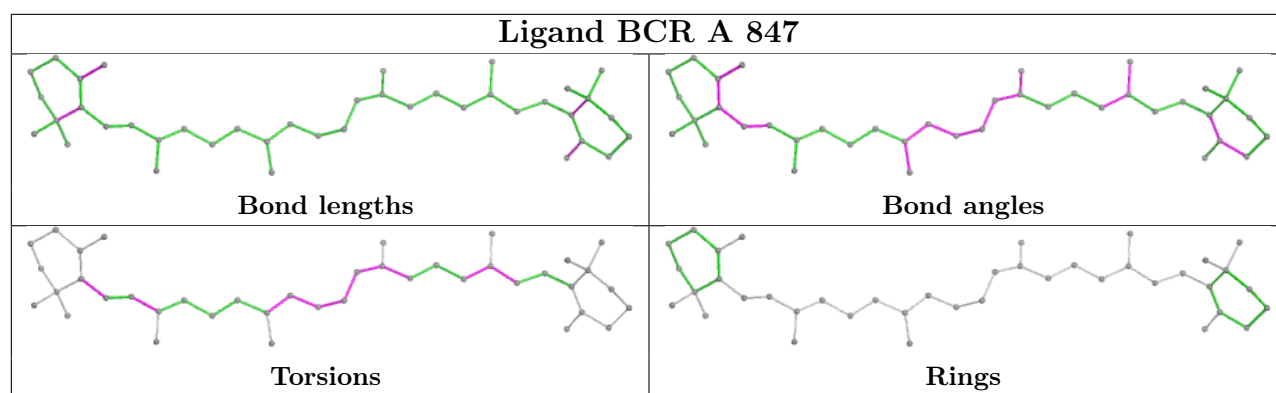


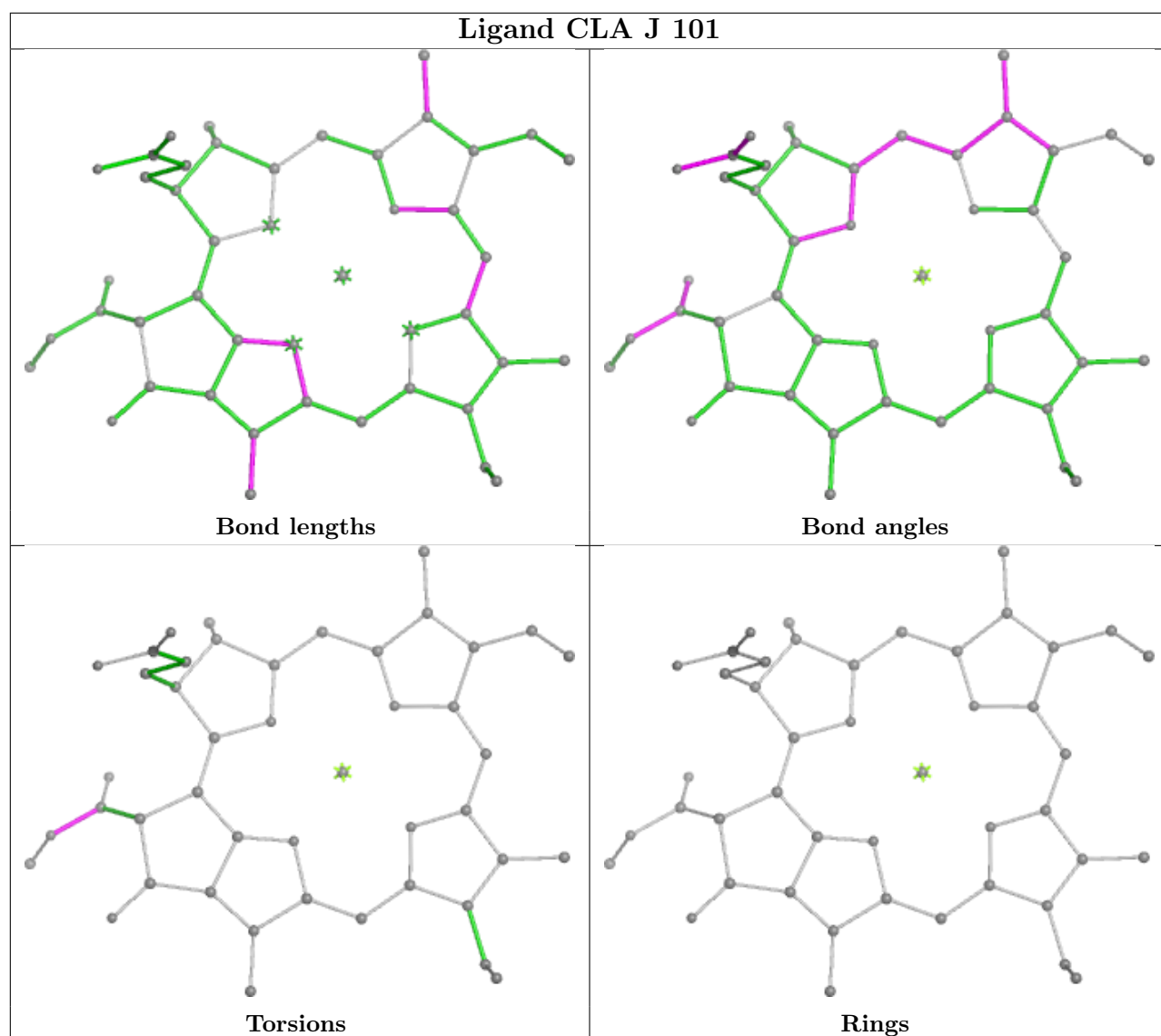




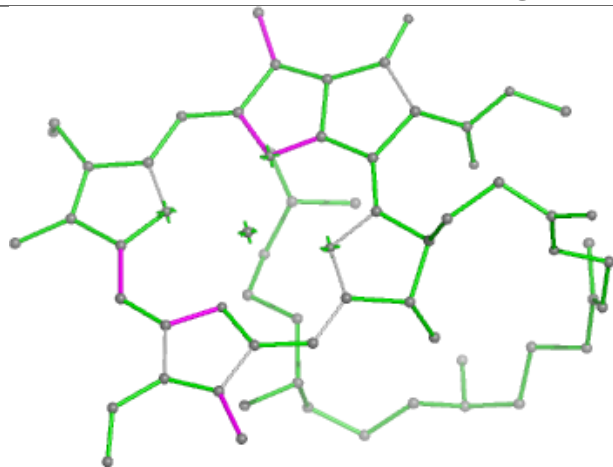




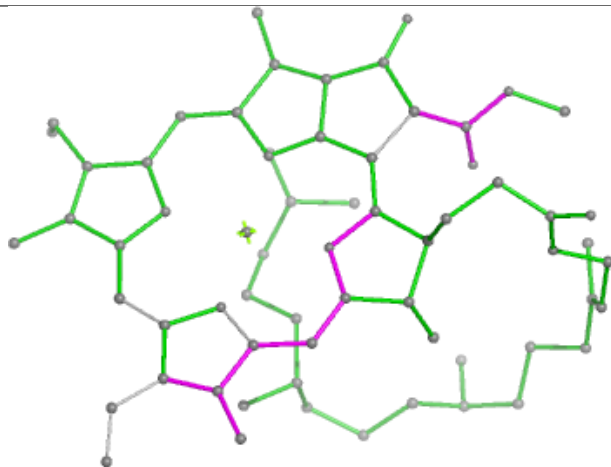




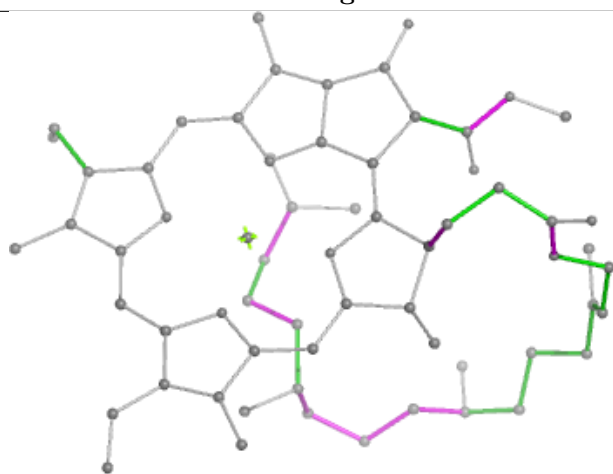
Ligand CLA A 807



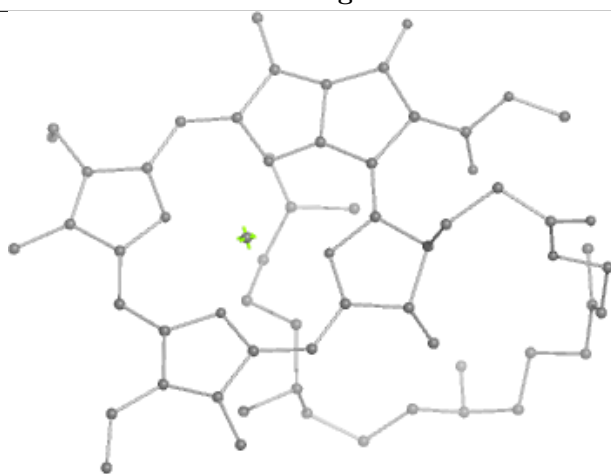
Bond lengths



Bond angles

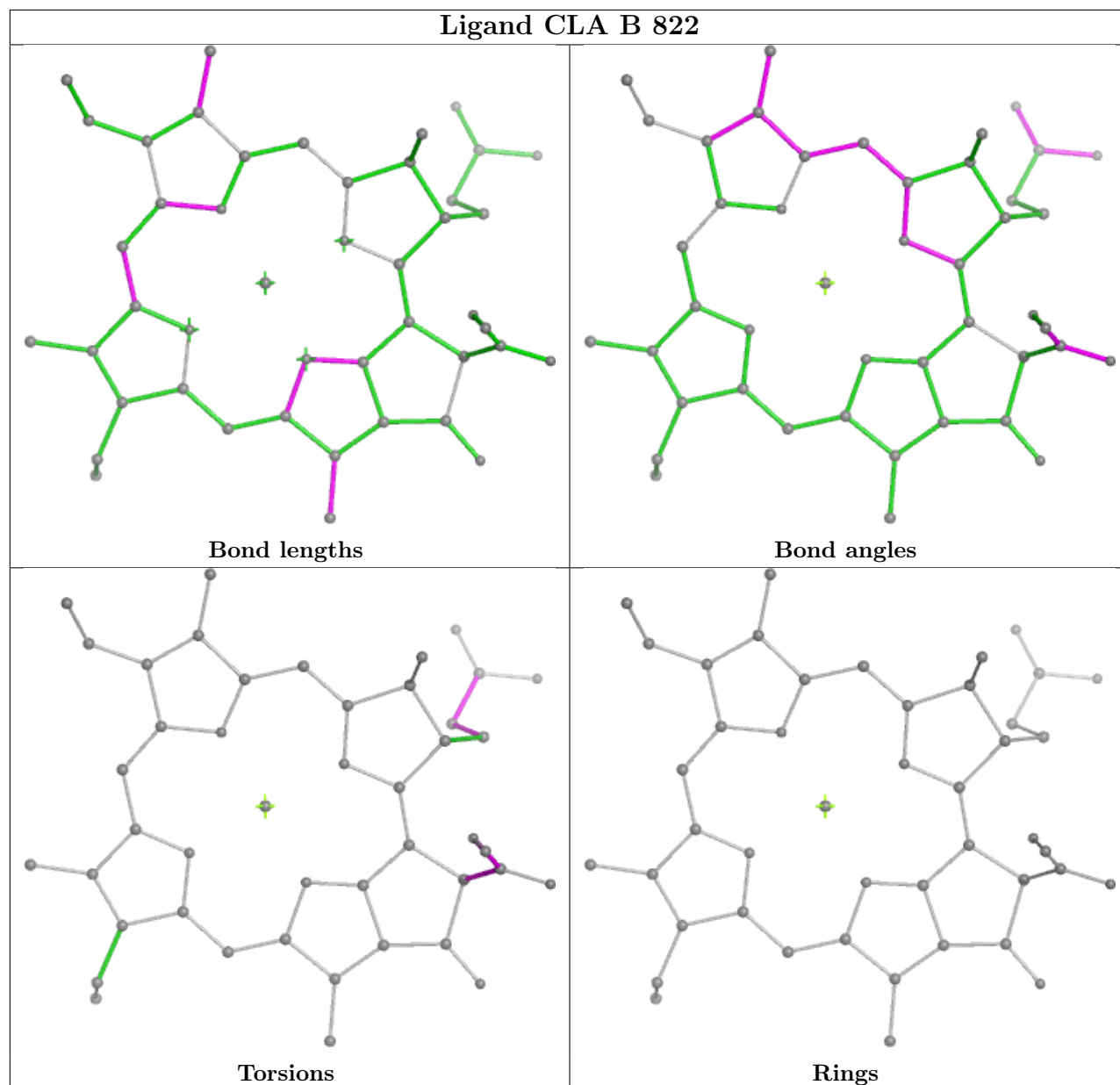


Torsions

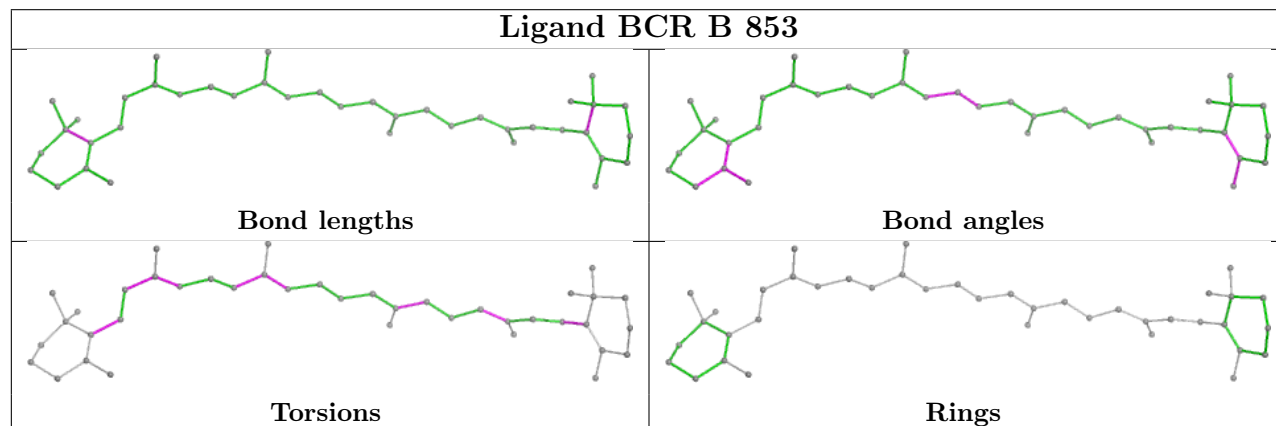


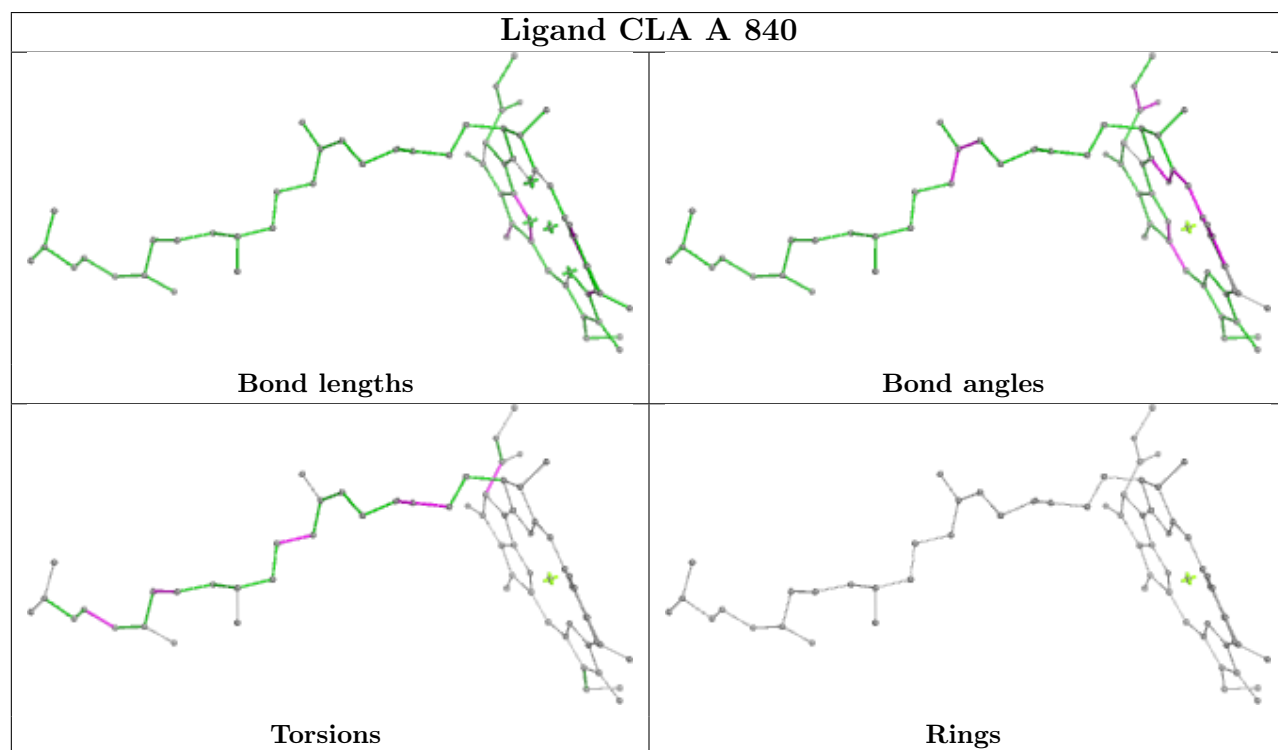
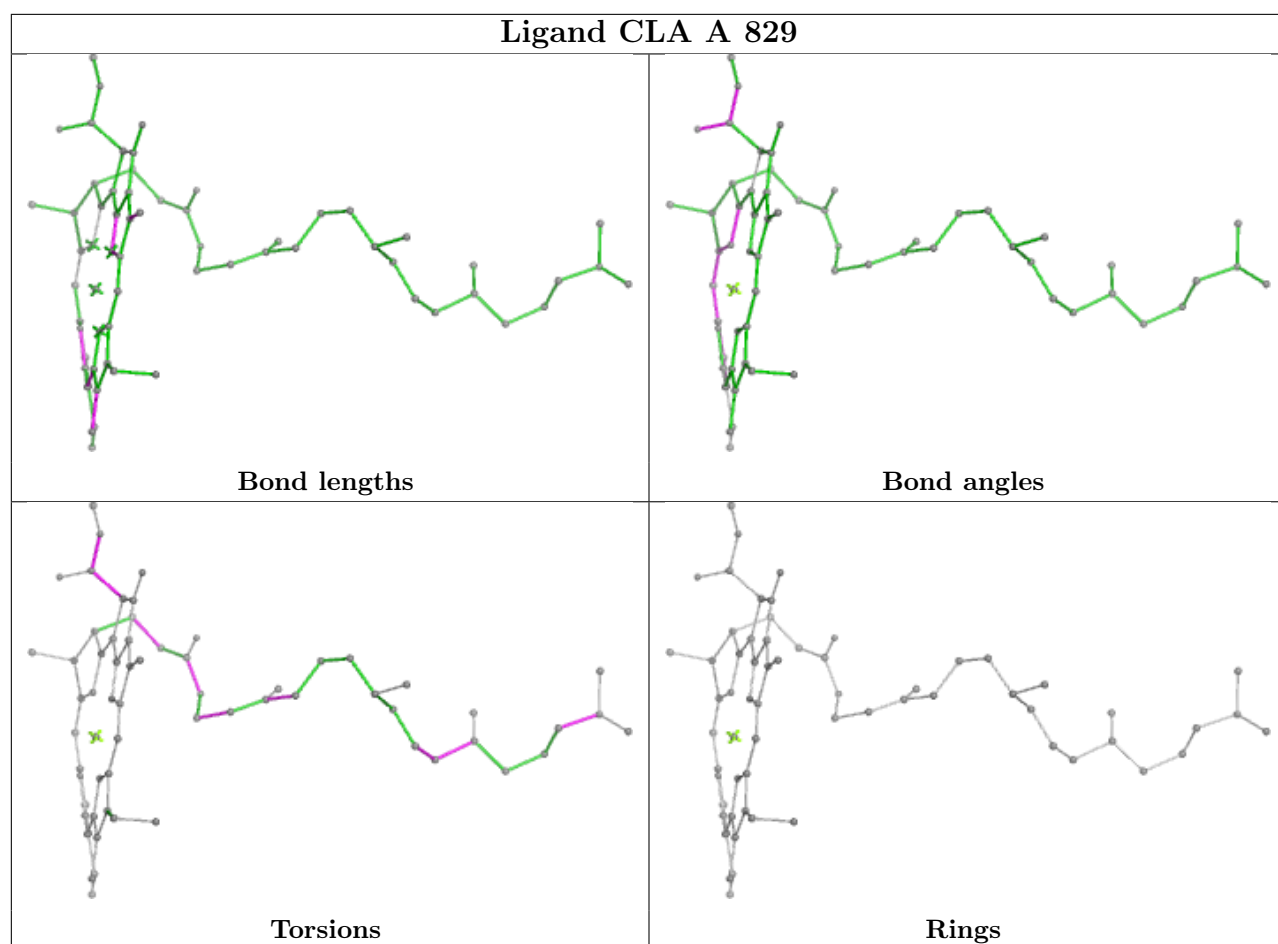
Rings

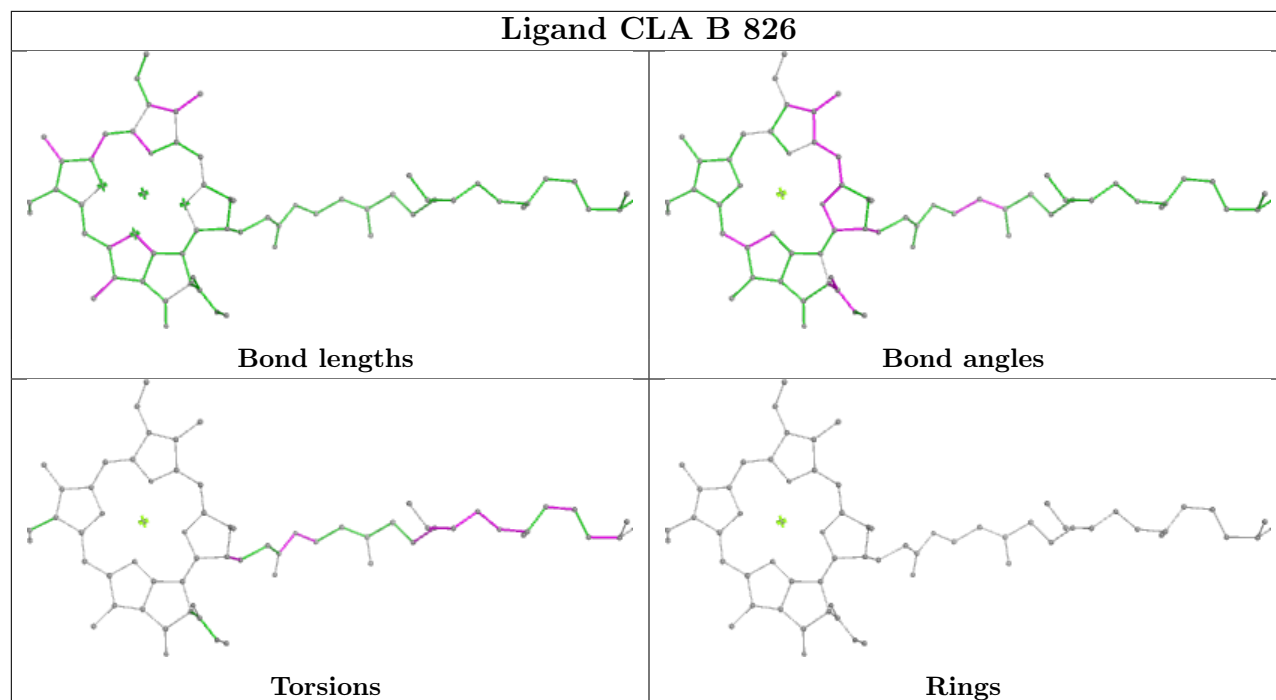
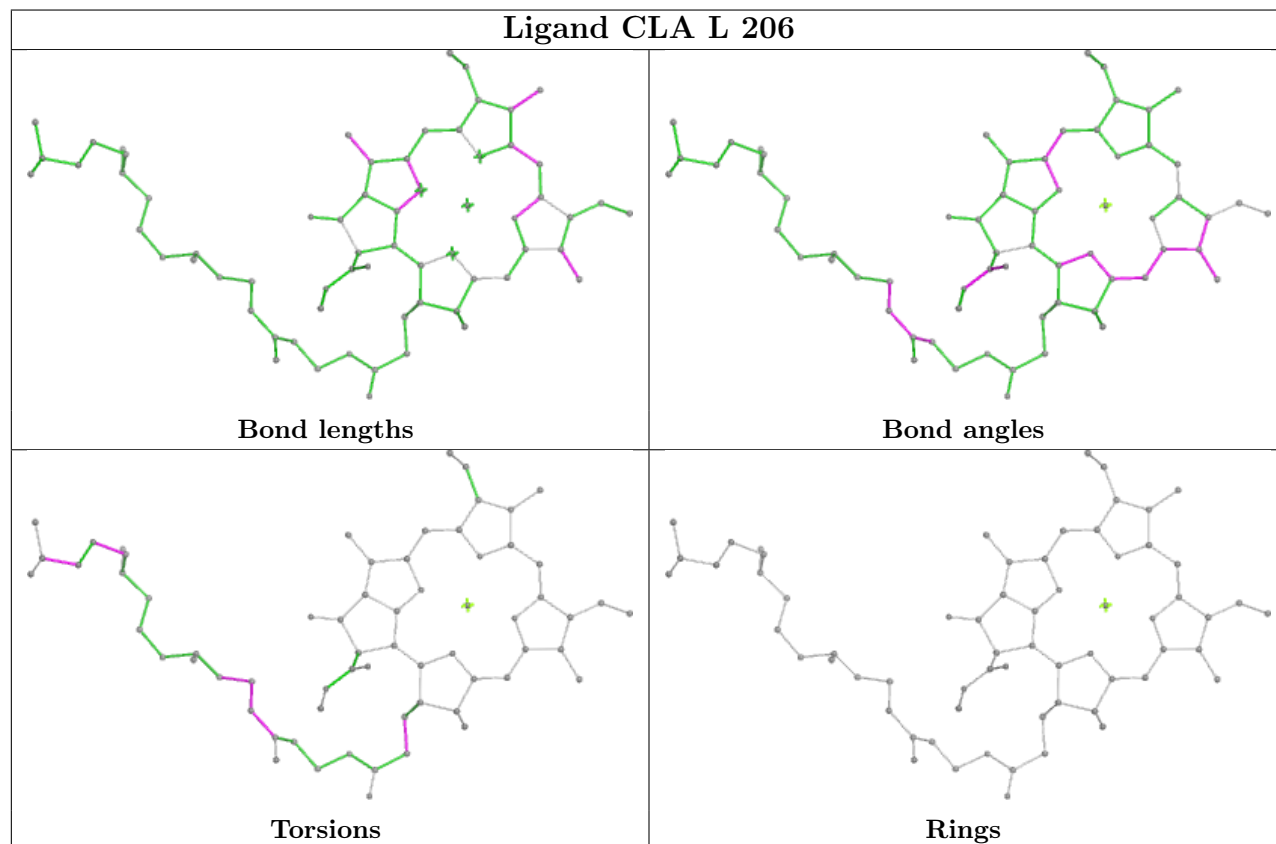
Ligand CLA B 822

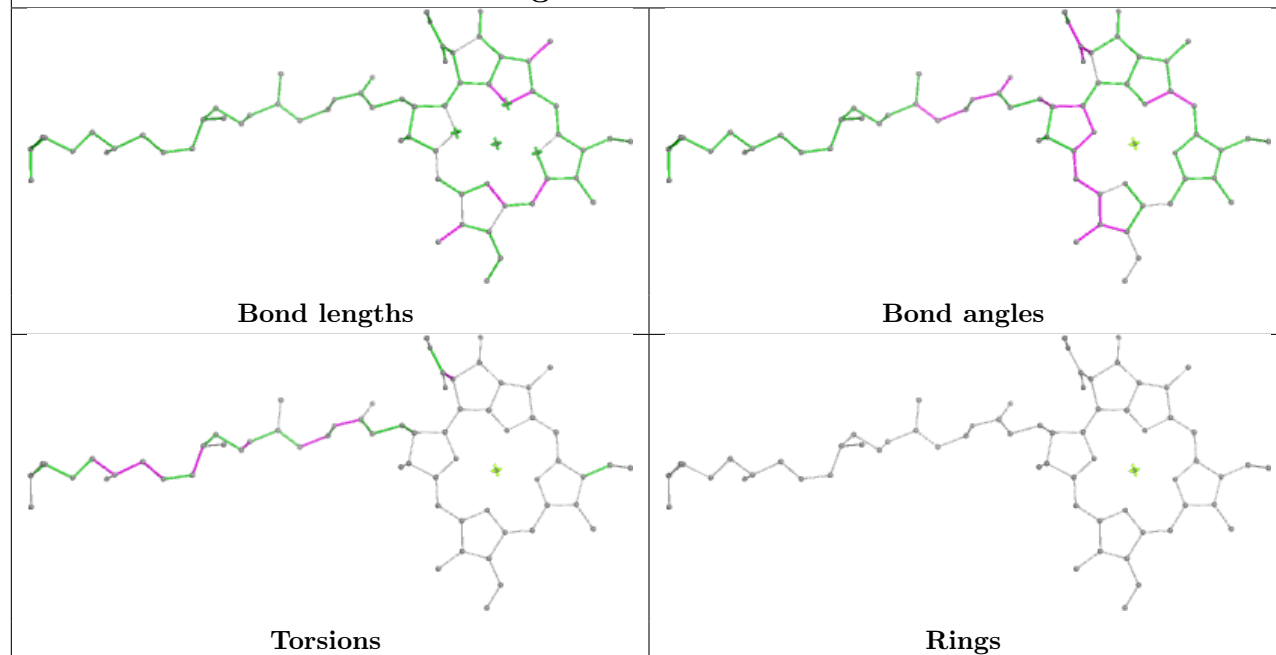
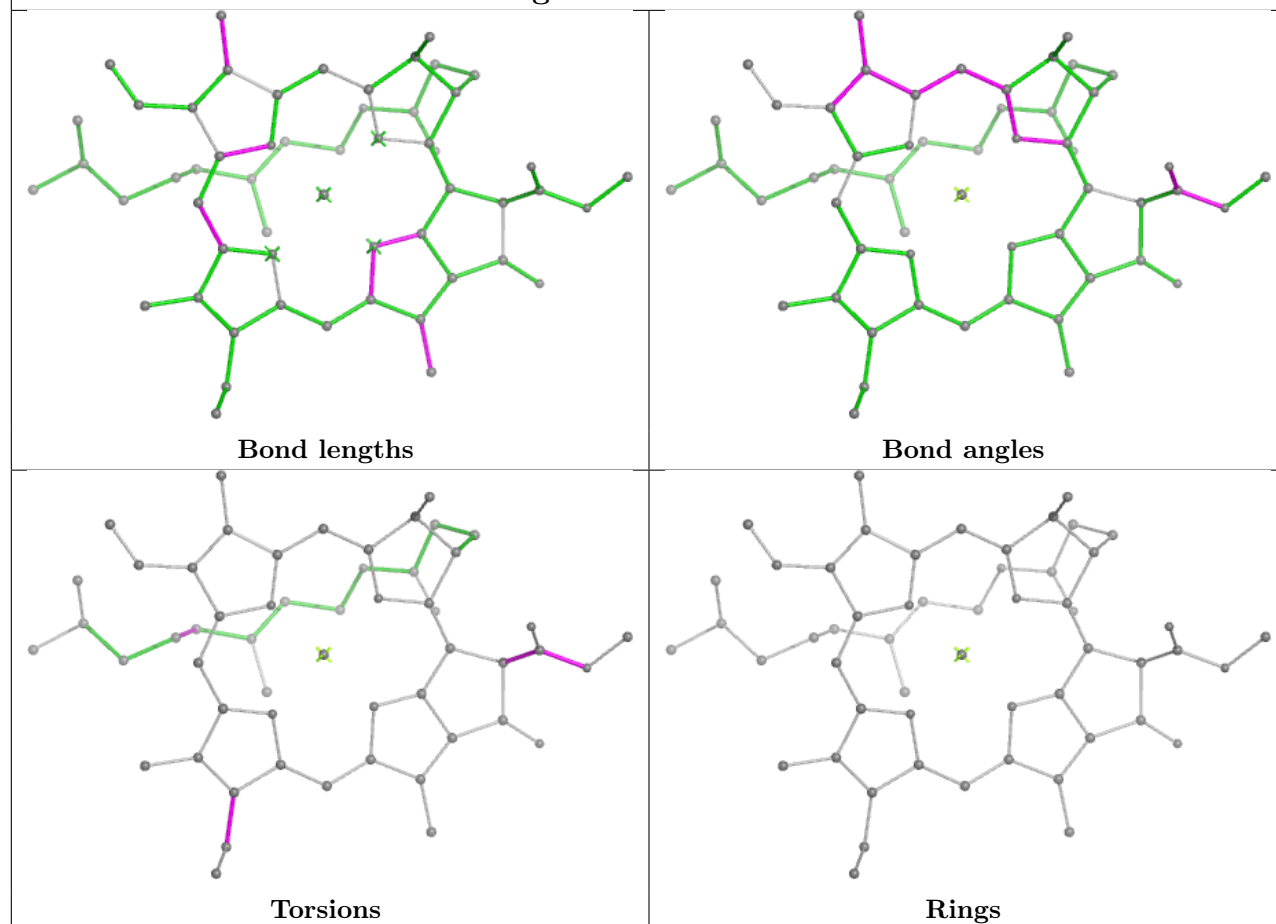


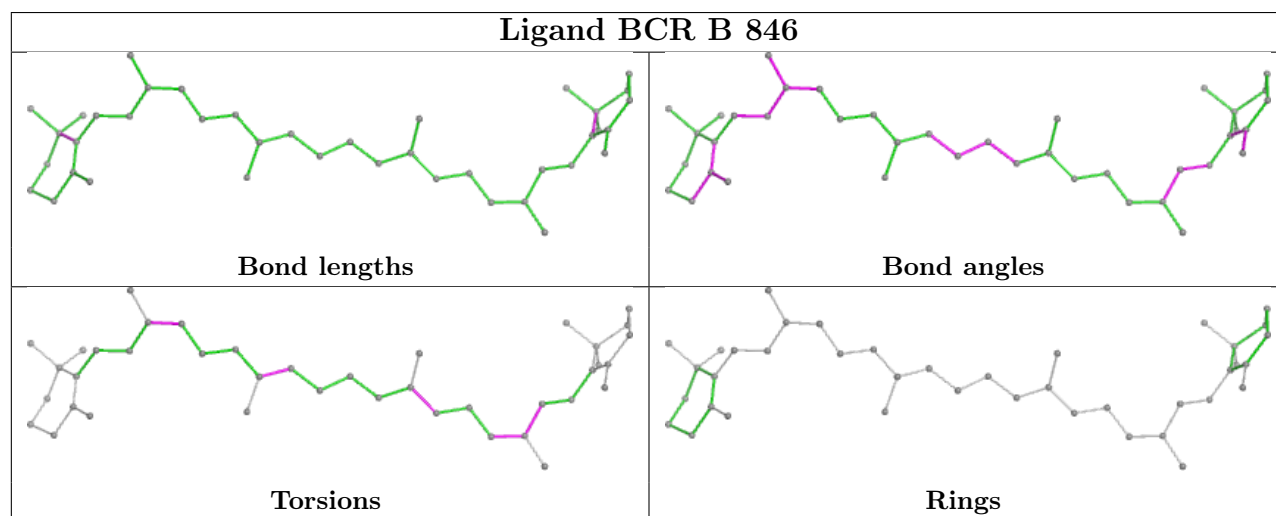
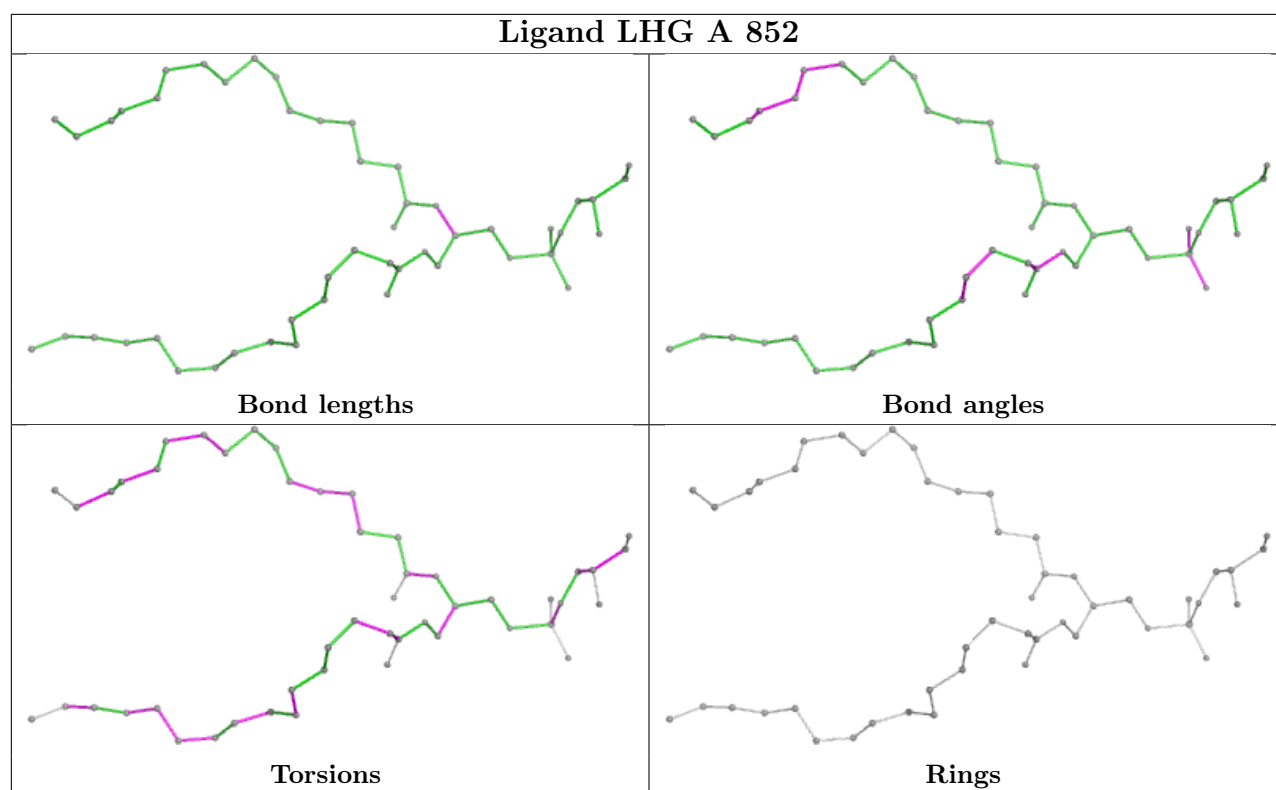
Ligand BCR B 853

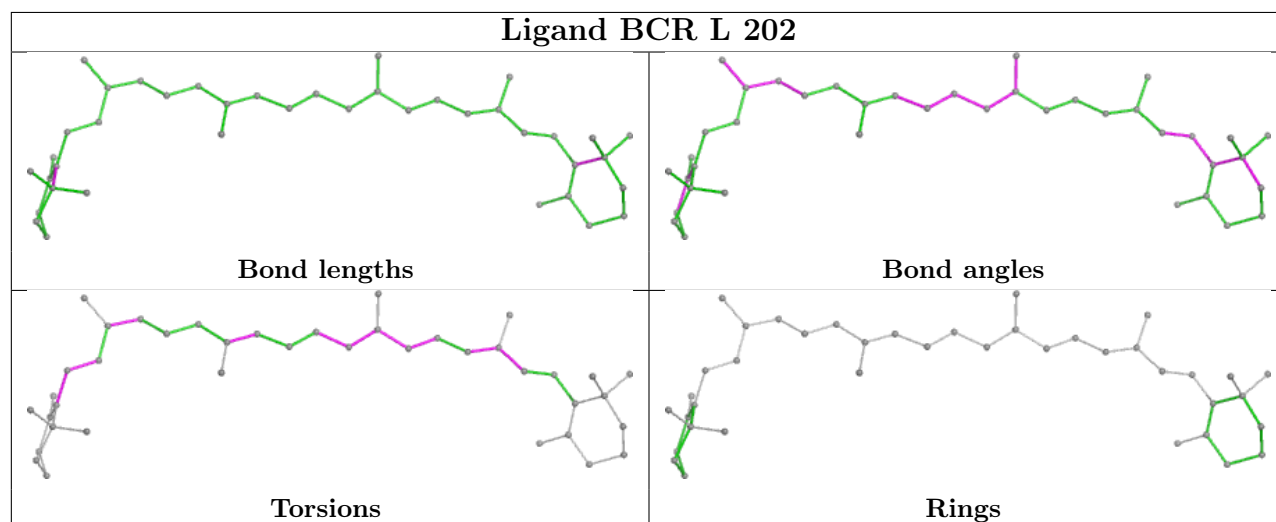
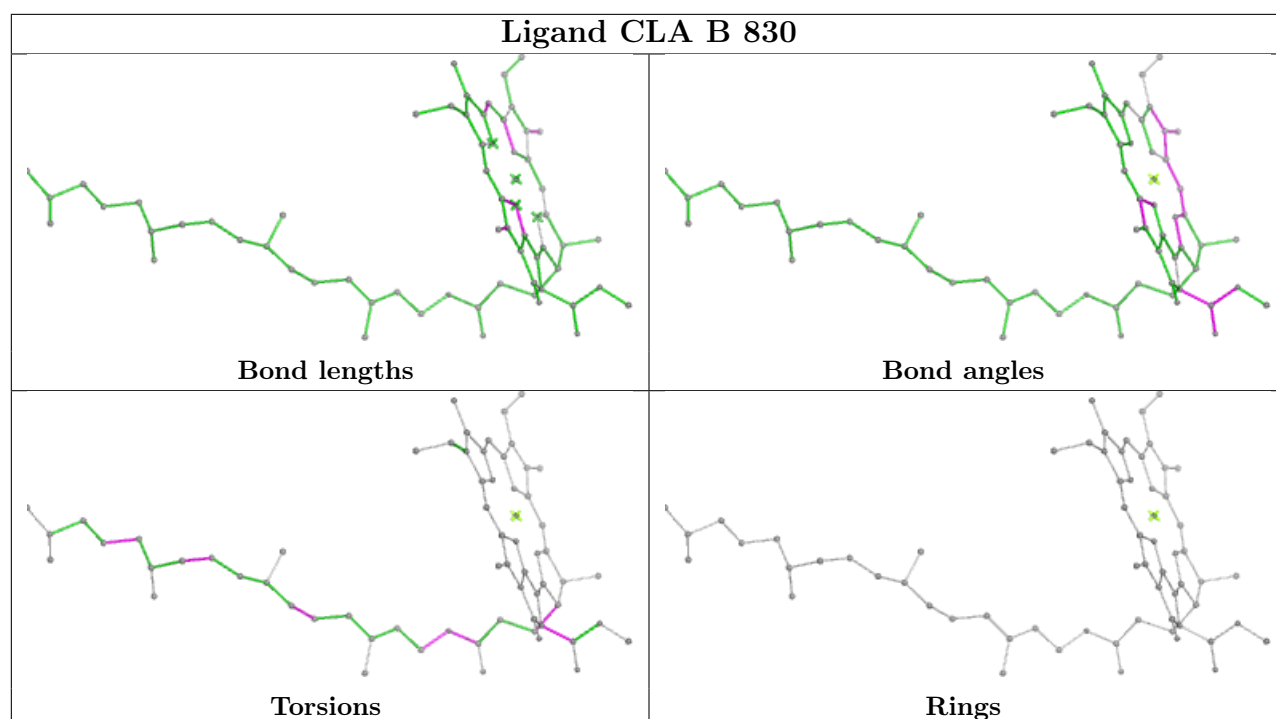


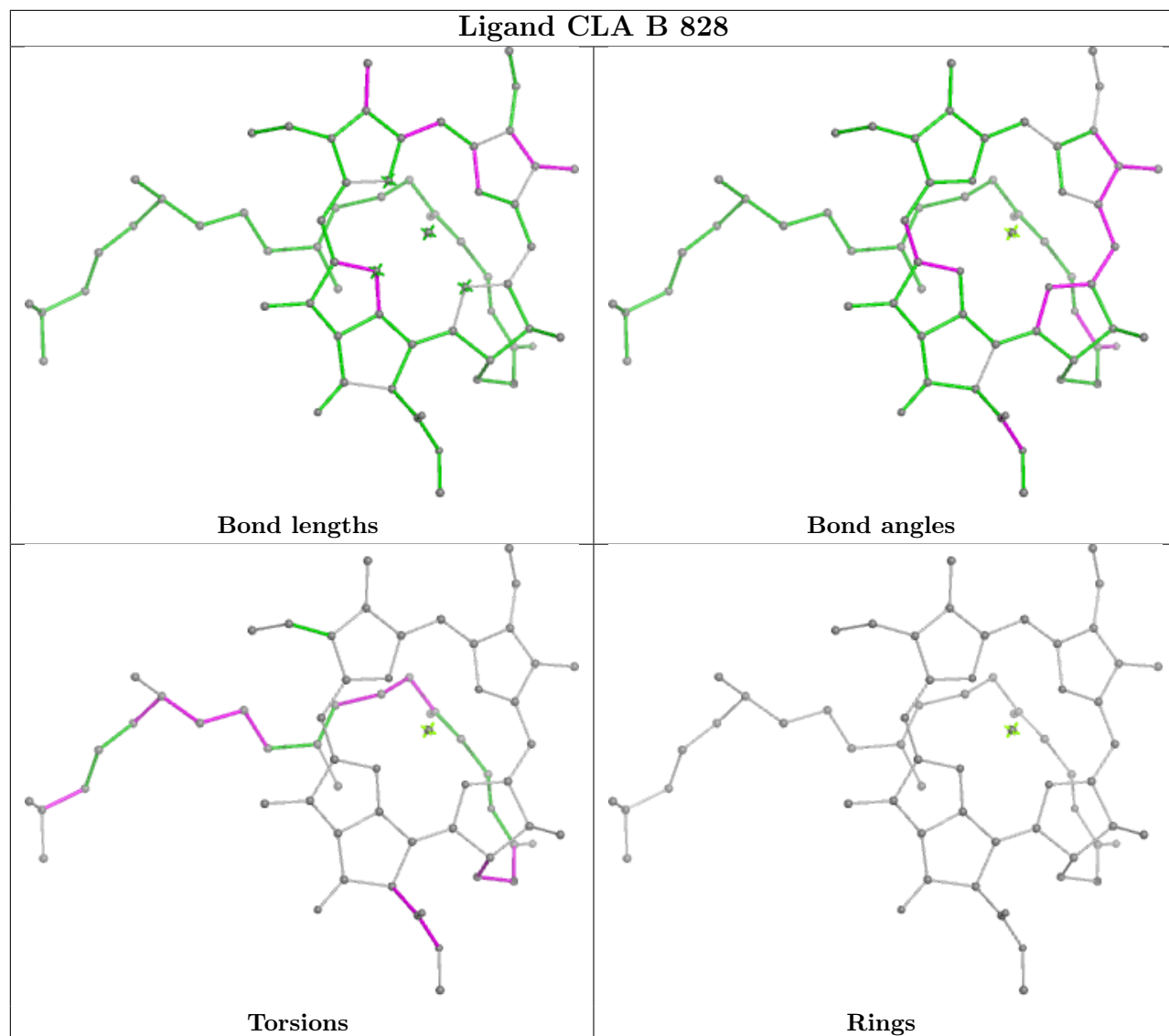


Ligand CLA B 826**Ligand CLA L 206**

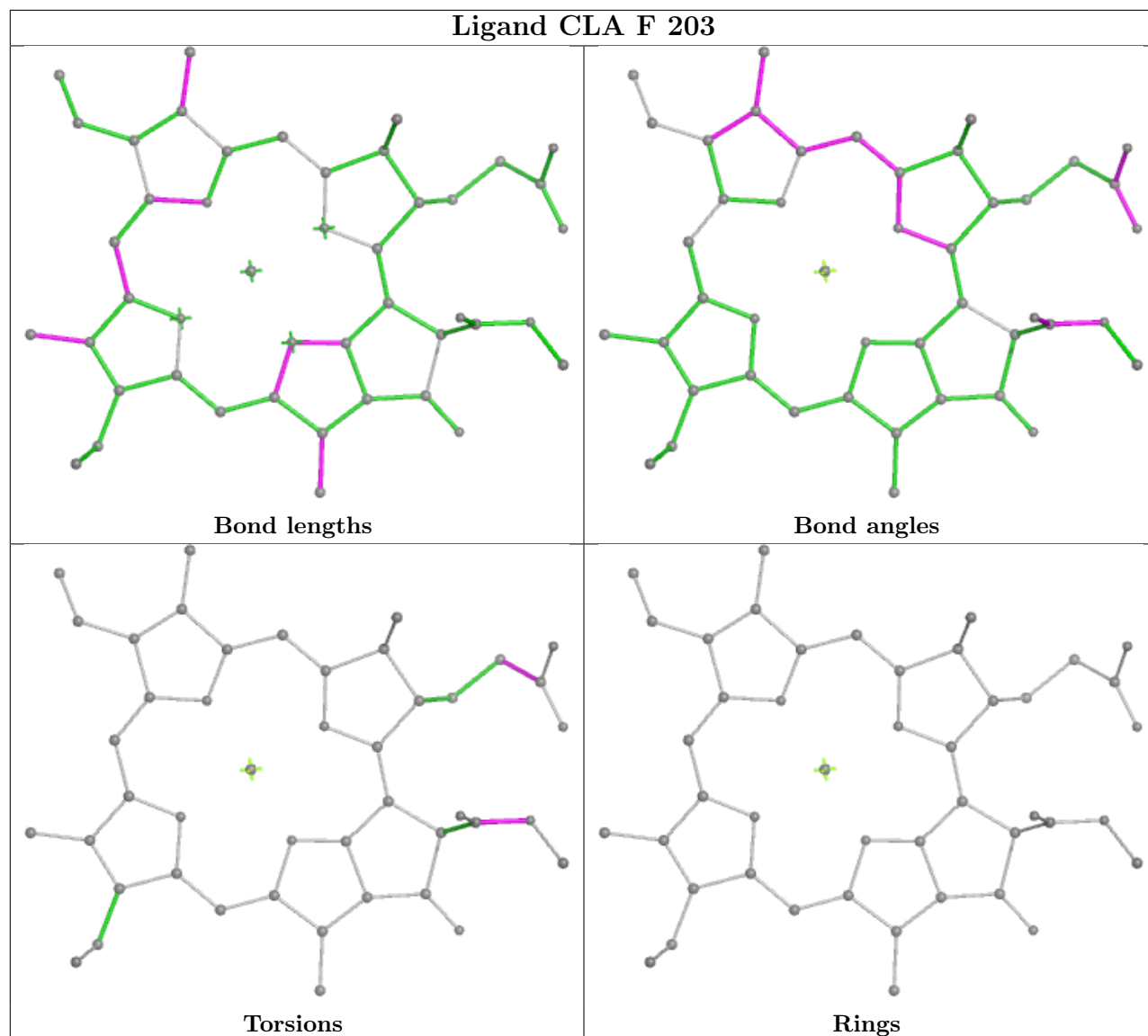
Ligand CLA A 827**Ligand CLA B 823**

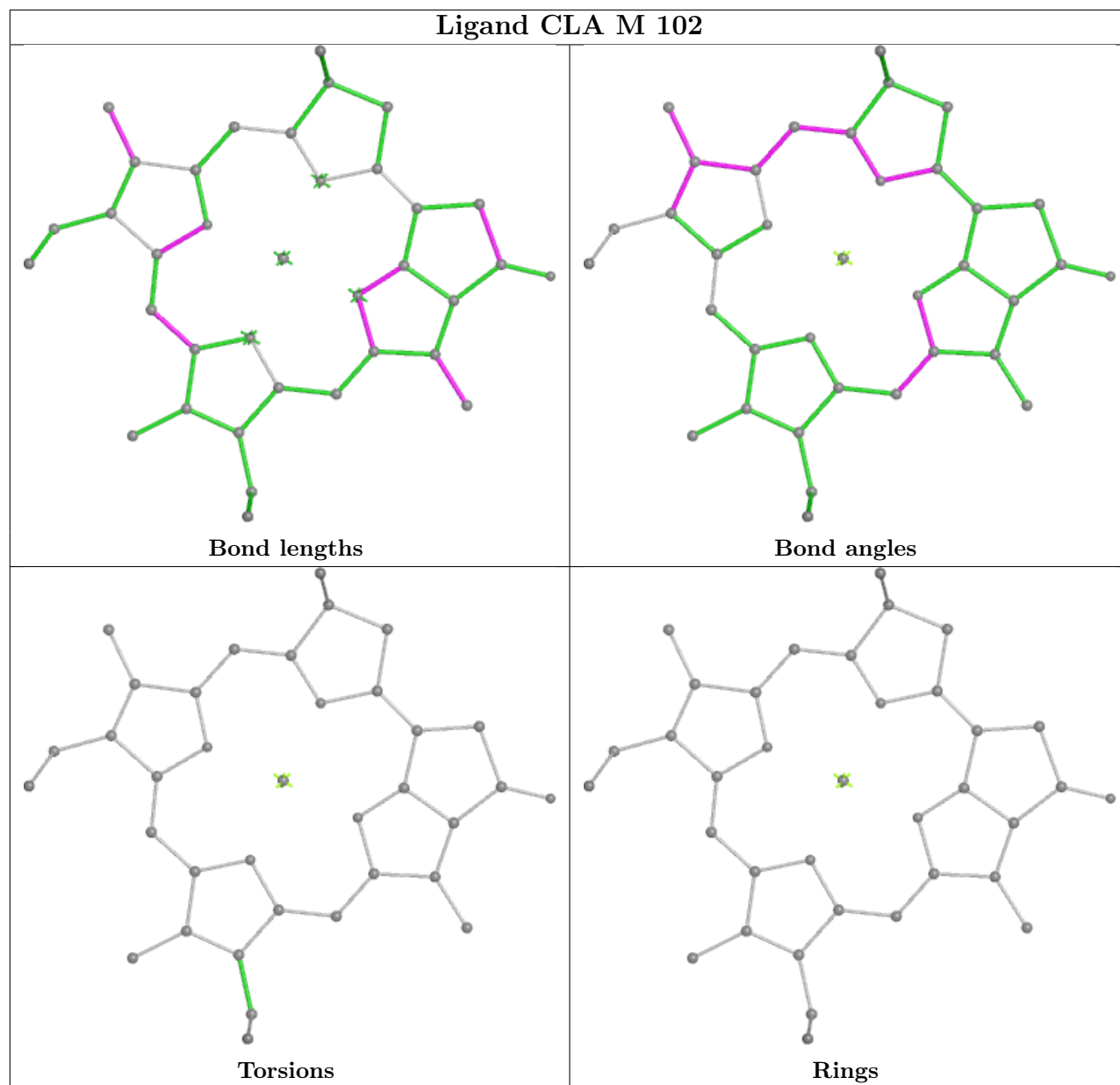




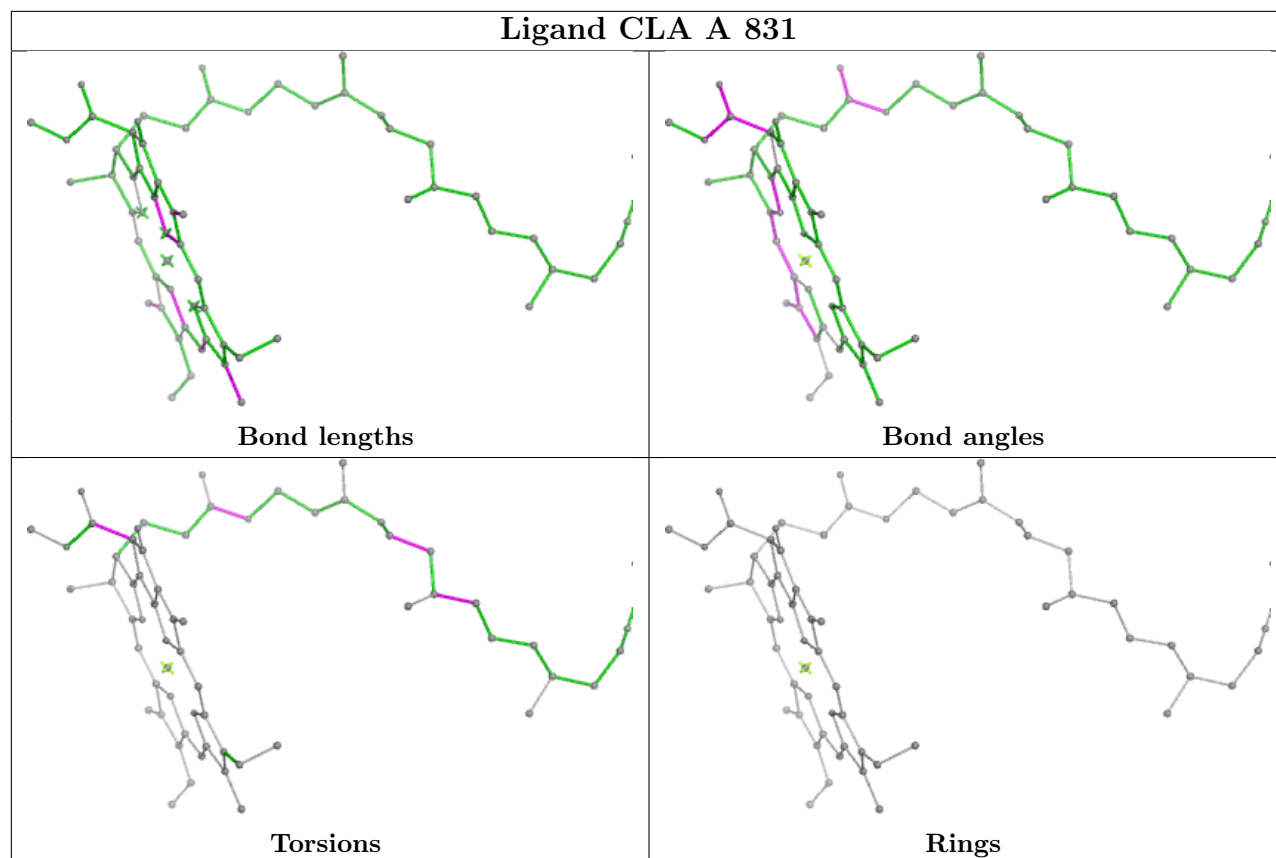


Ligand CLA F 203

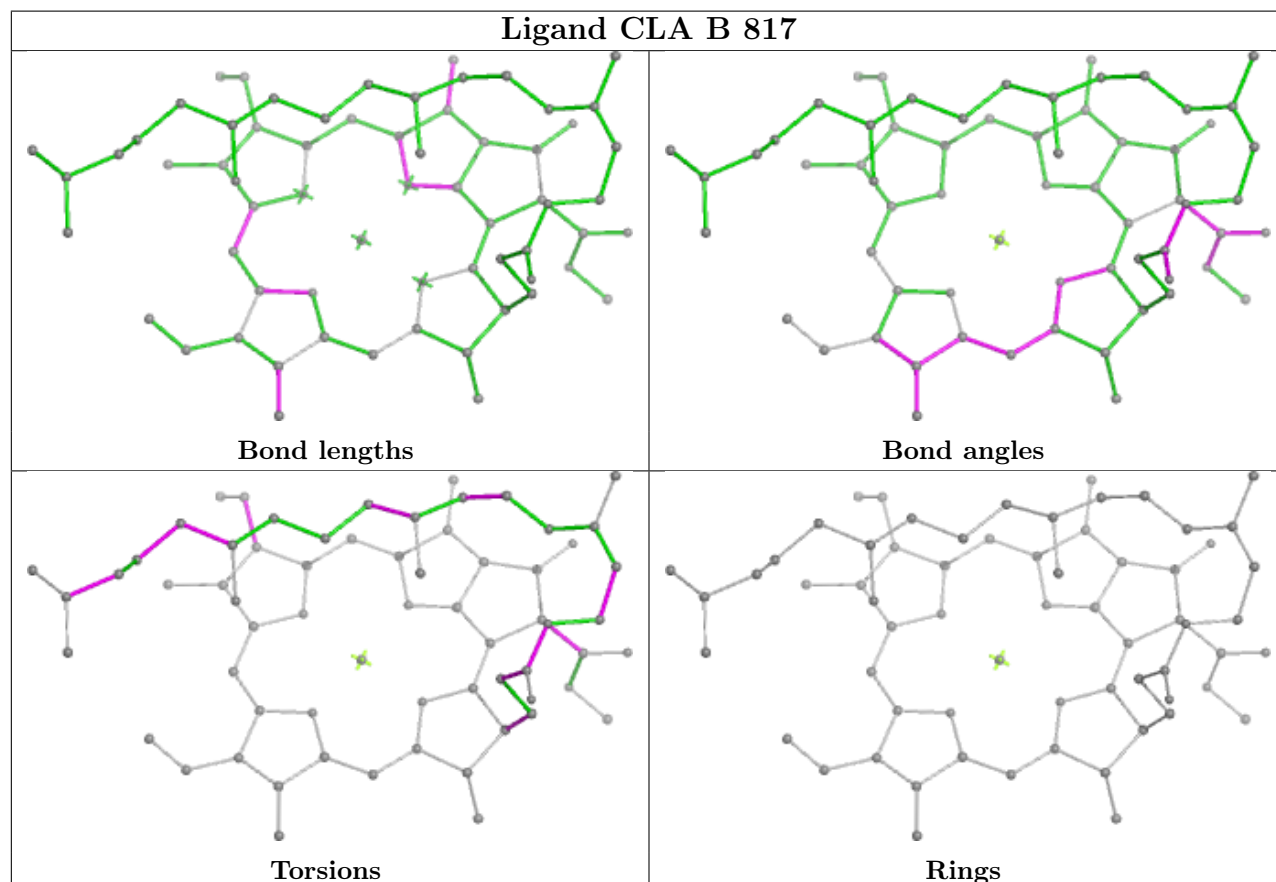




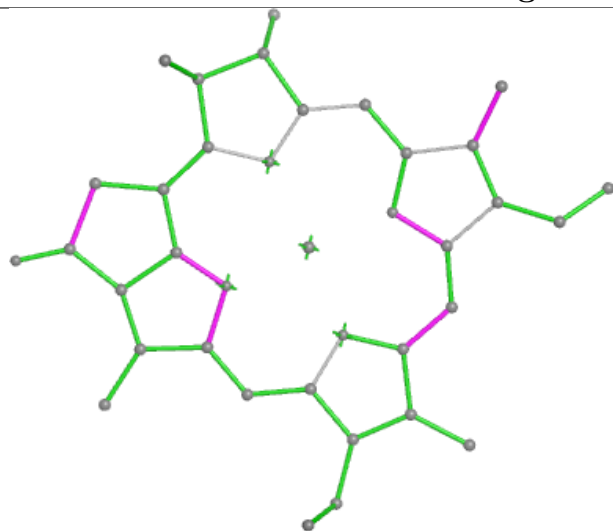
Ligand CLA A 831



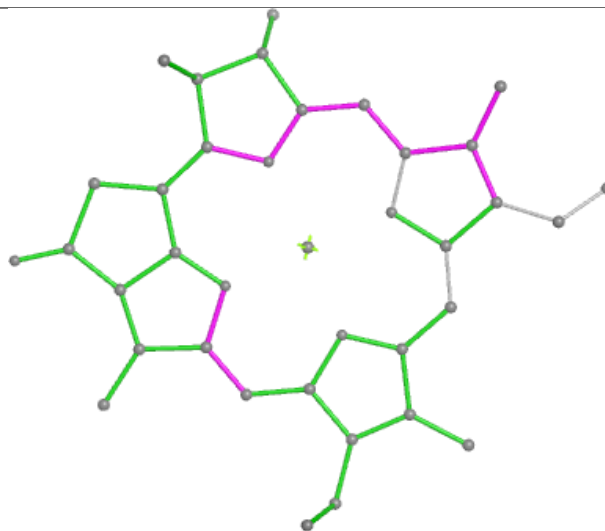
Ligand CLA B 817



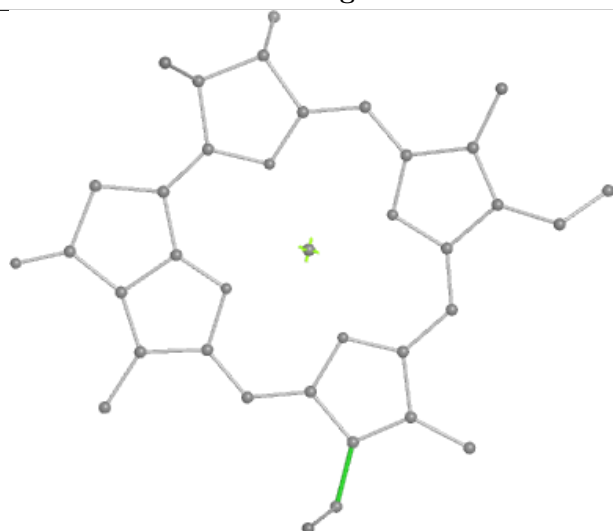
Ligand CLA J 102



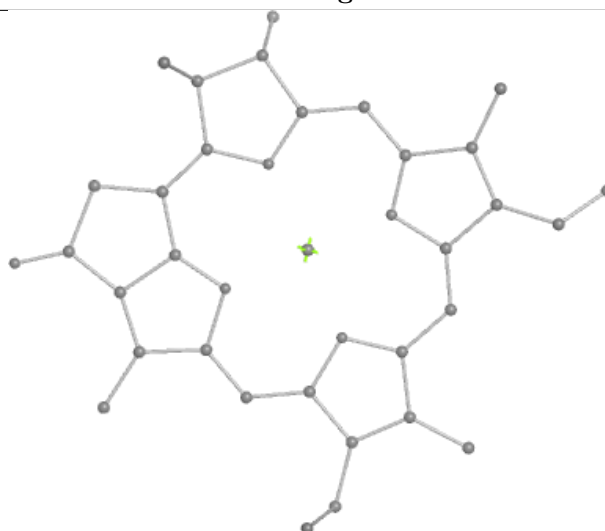
Bond lengths



Bond angles

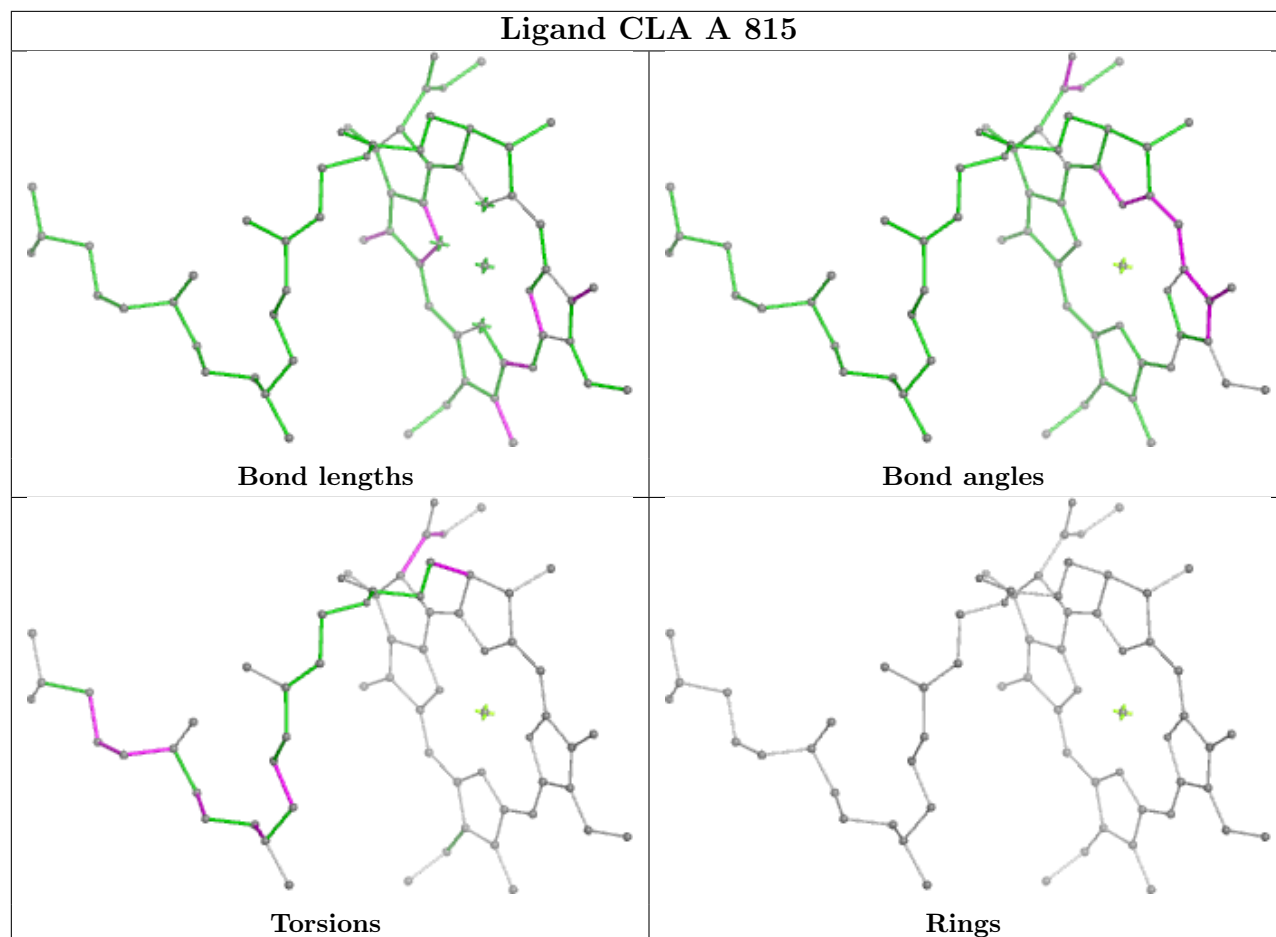


Torsions

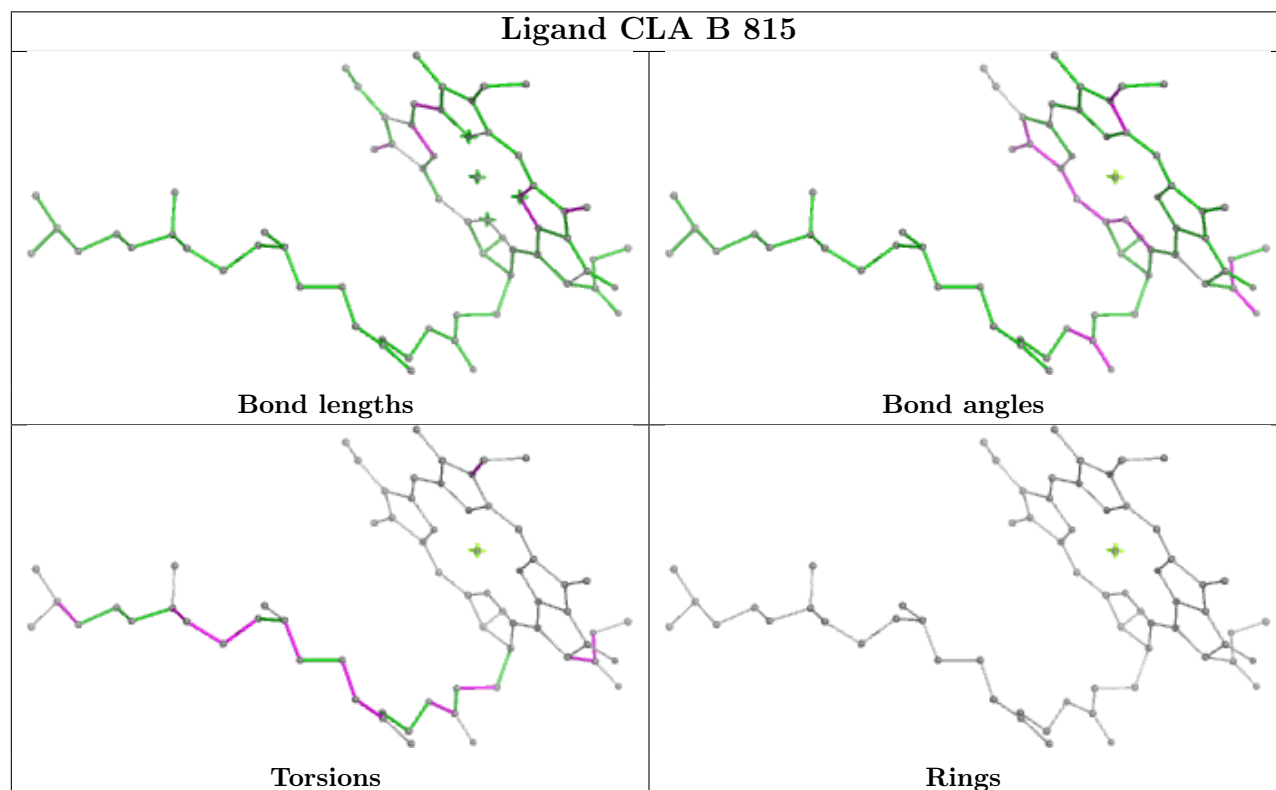


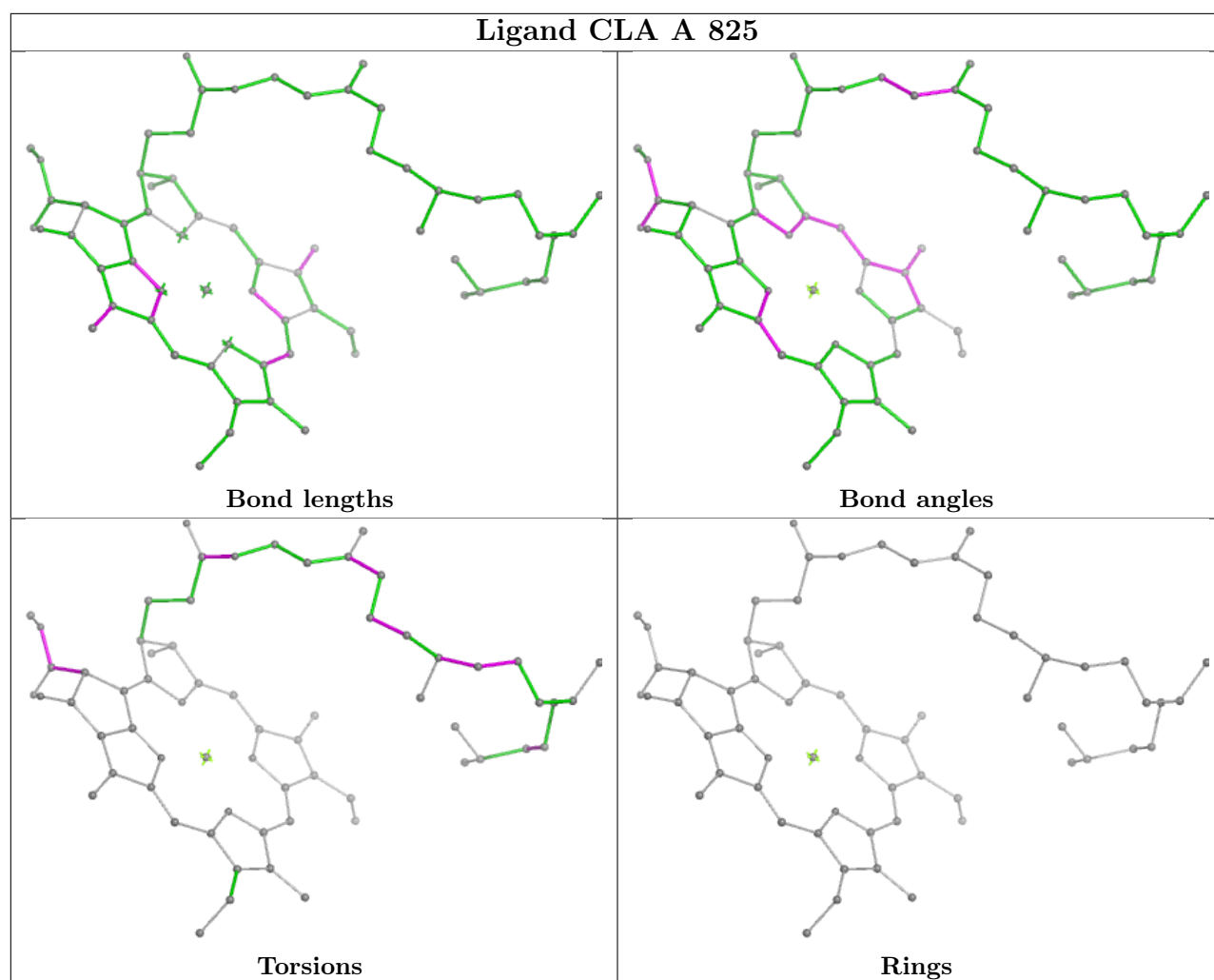
Rings

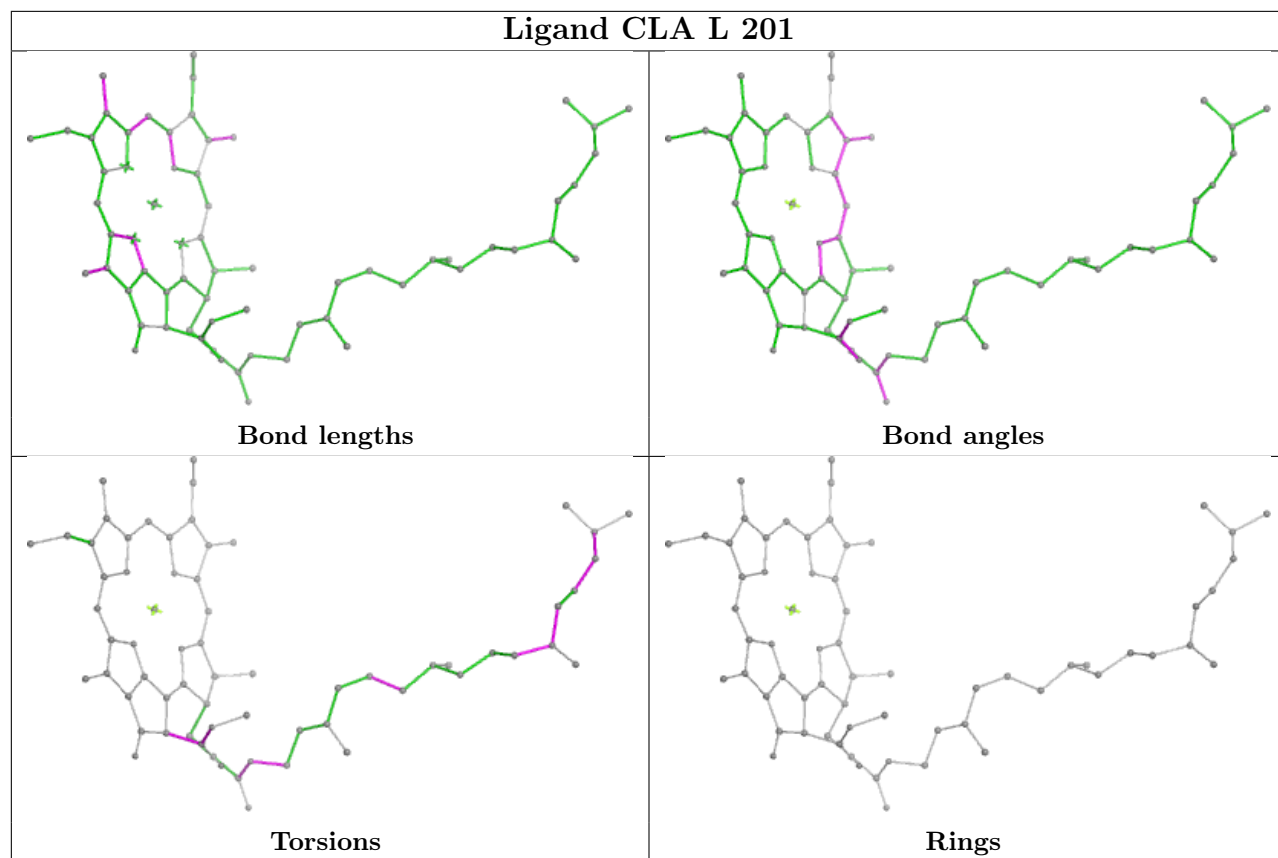
Ligand CLA A 815



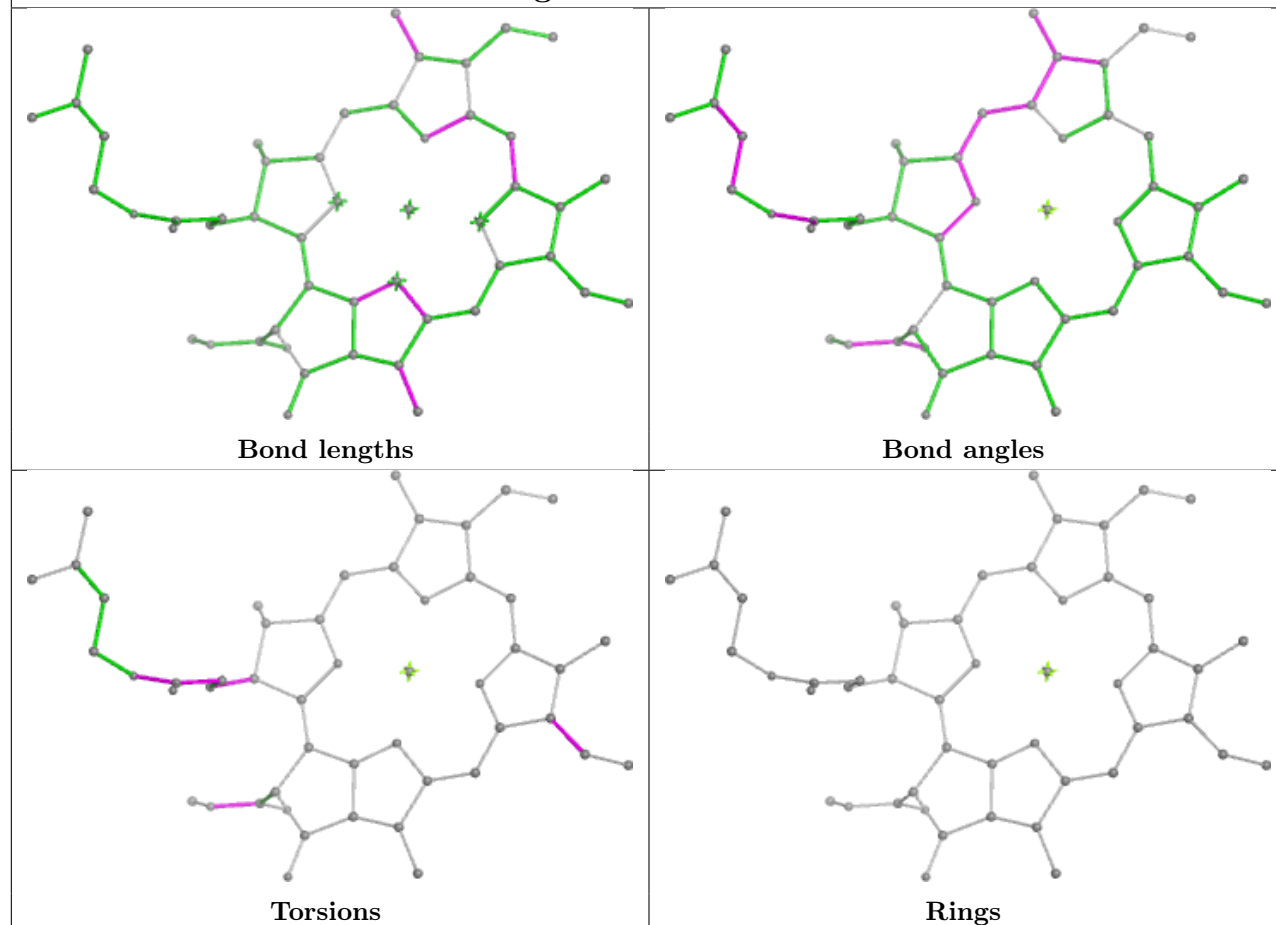
Ligand CLA B 815



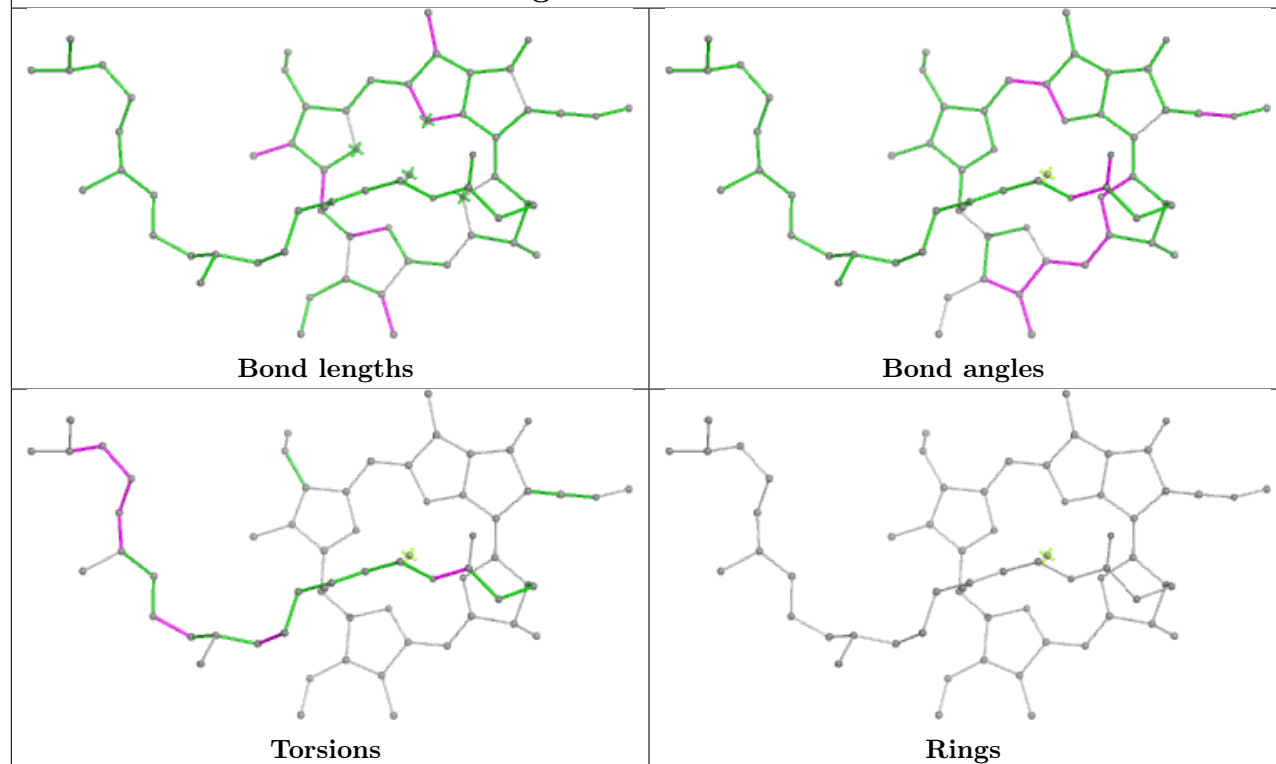




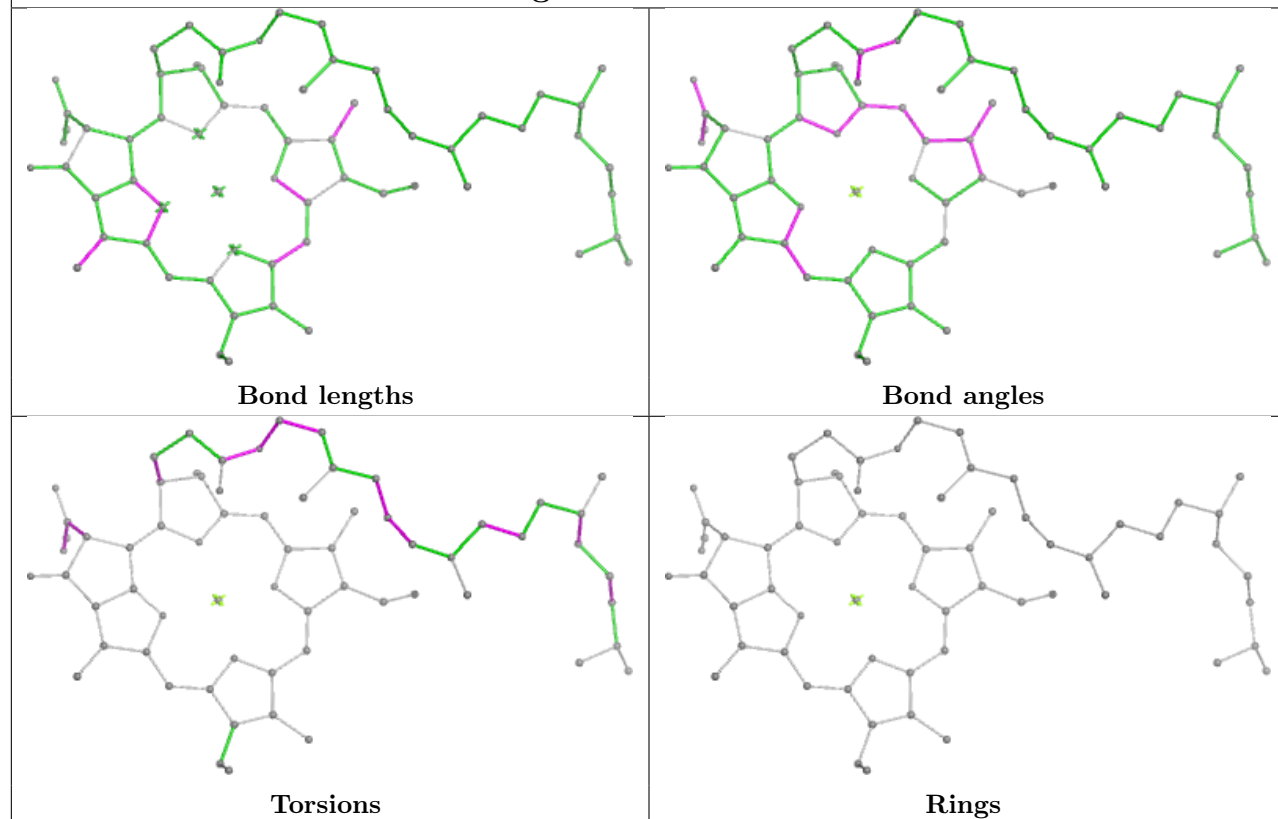
Ligand CLA F 204



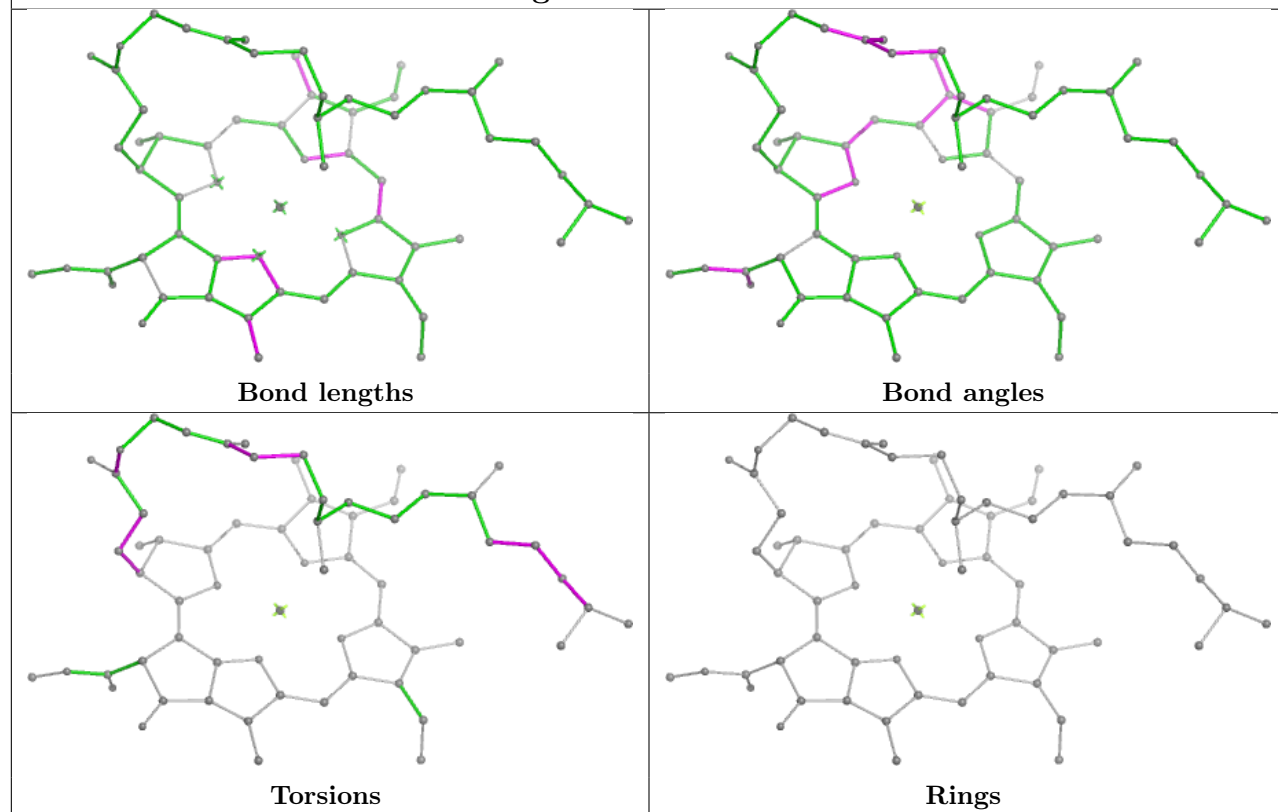
Ligand CLA B 839



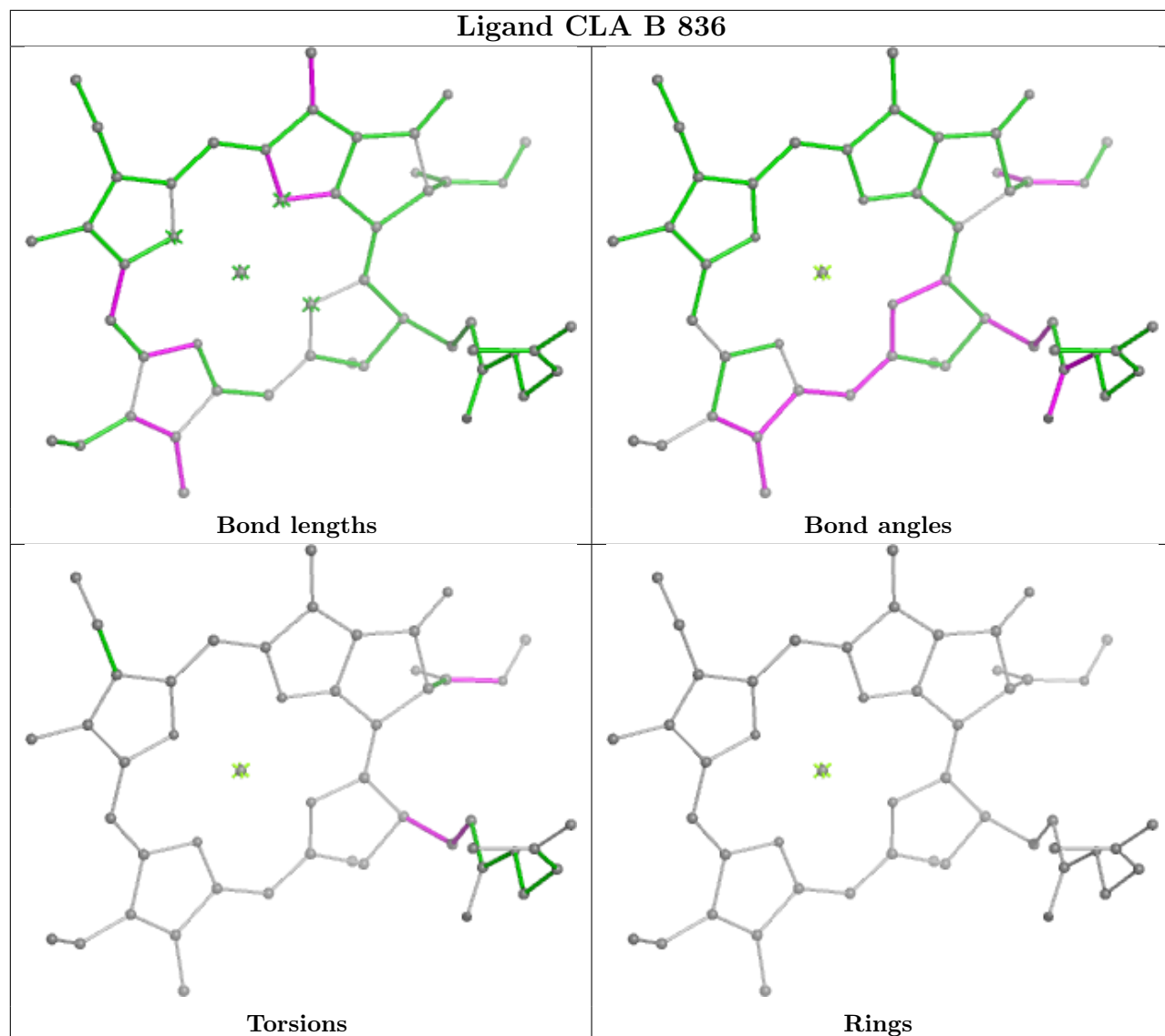
Ligand CLA B 819

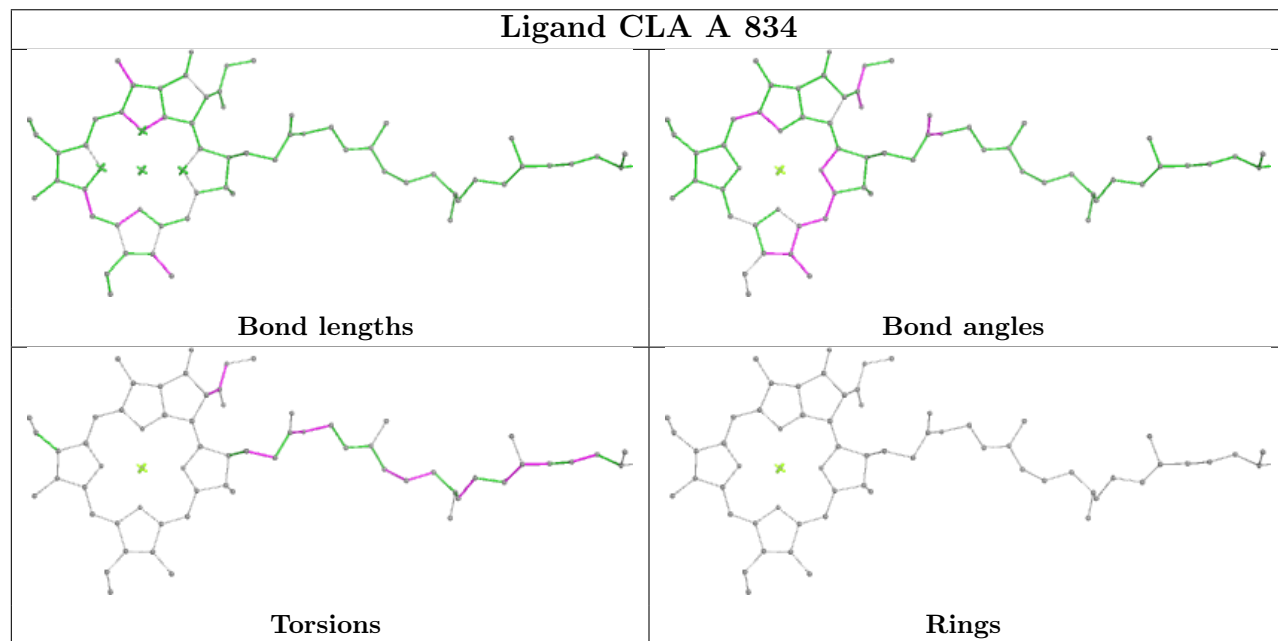
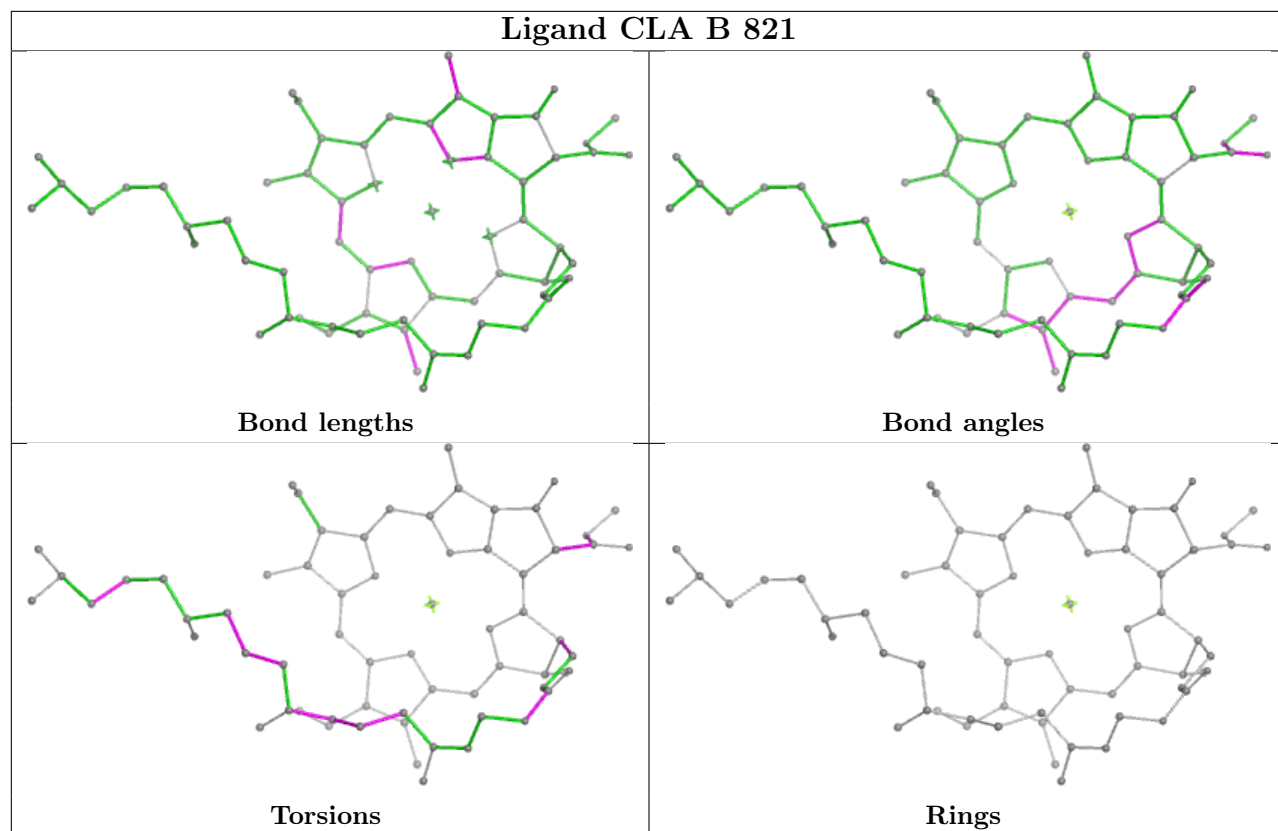


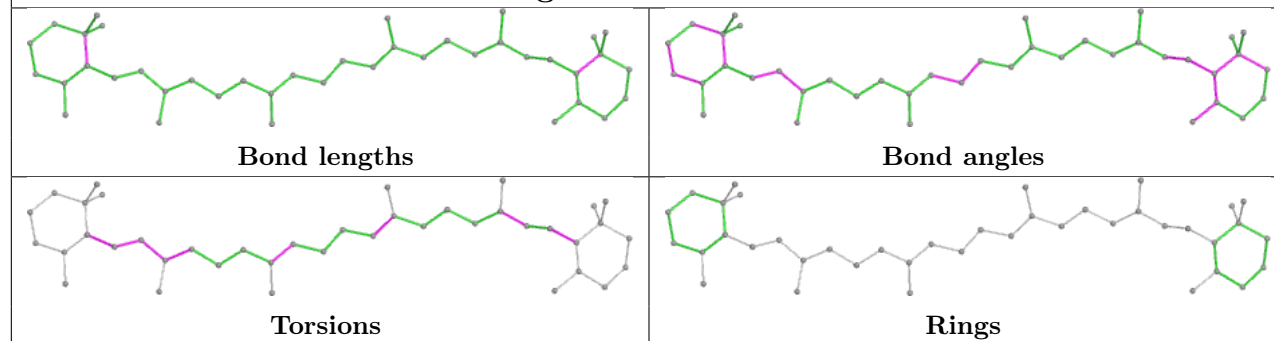
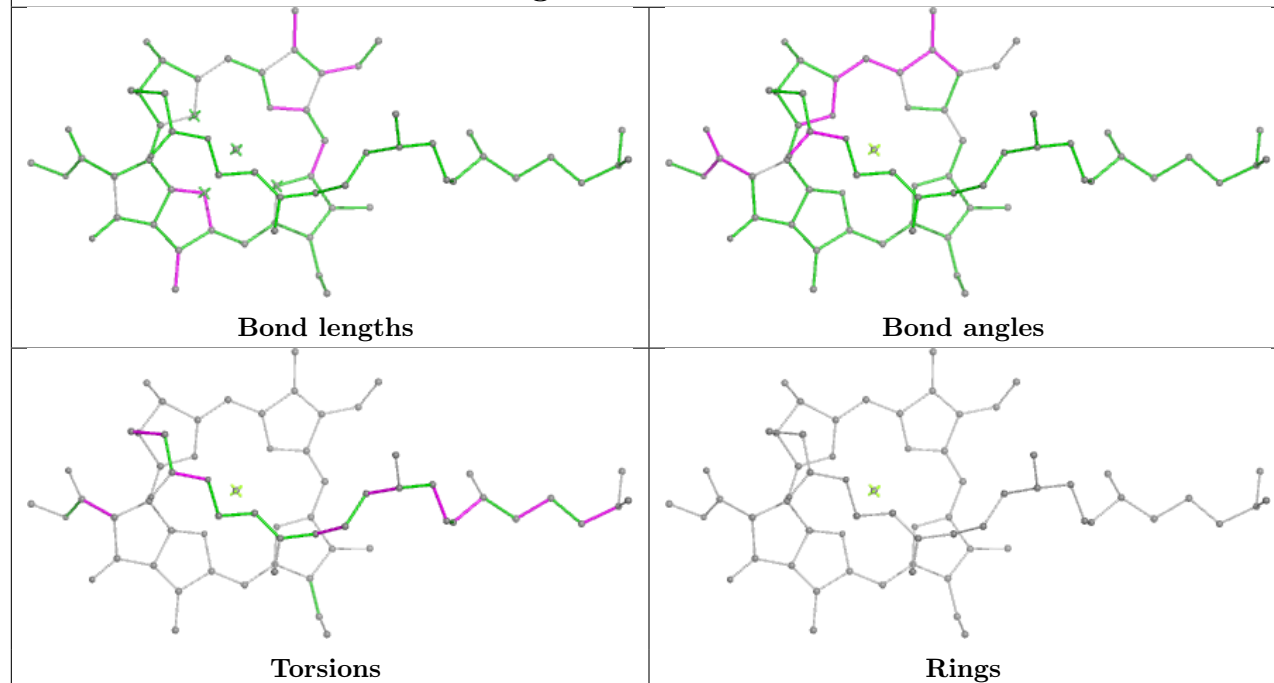
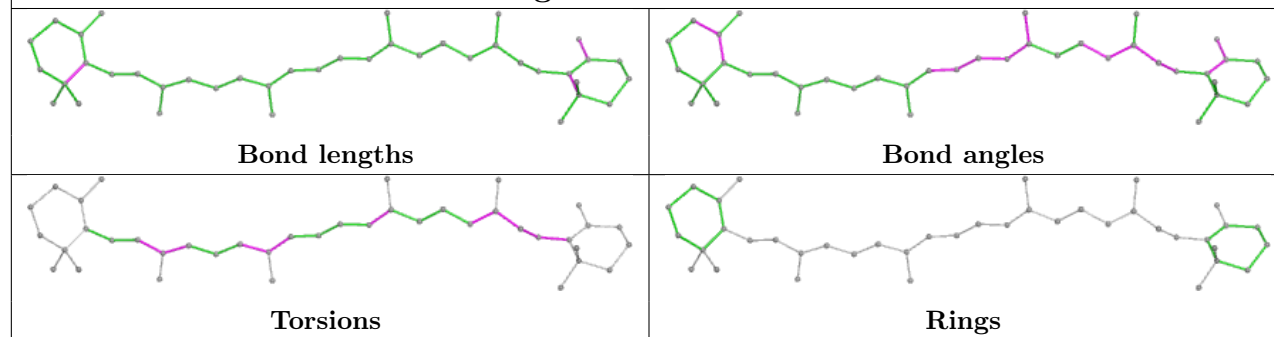
Ligand CLA B 818



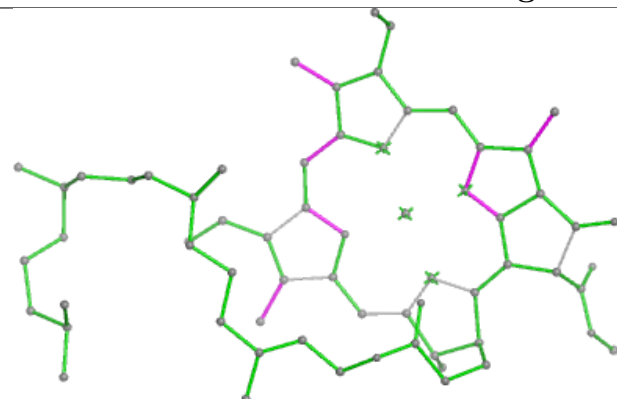
Ligand CLA B 836



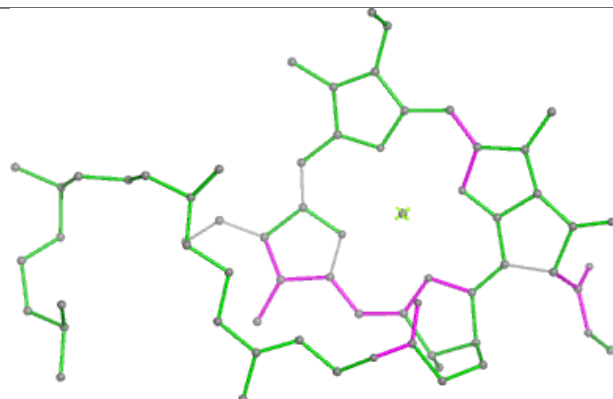


Ligand BCR I 103**Ligand CLA A 839****Ligand BCR J 103**

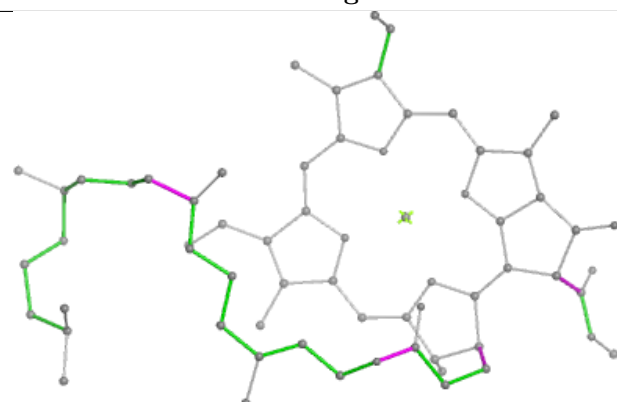
Ligand CLA A 820



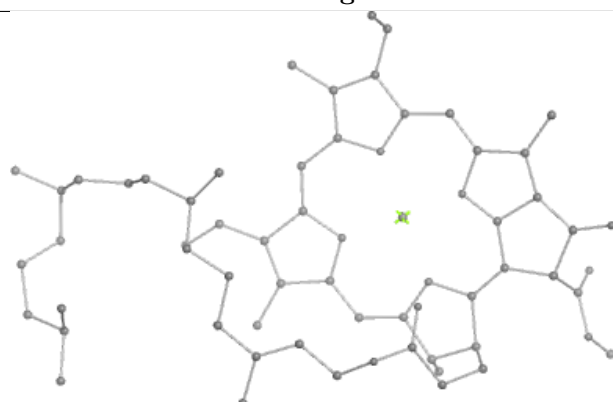
Bond lengths



Bond angles

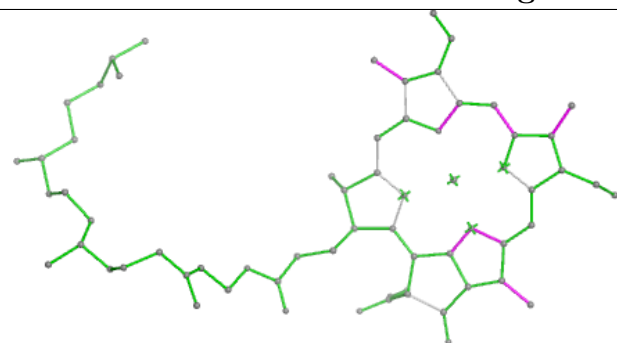


Torsions

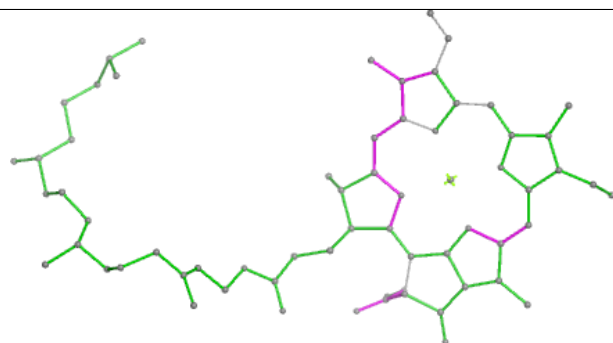


Rings

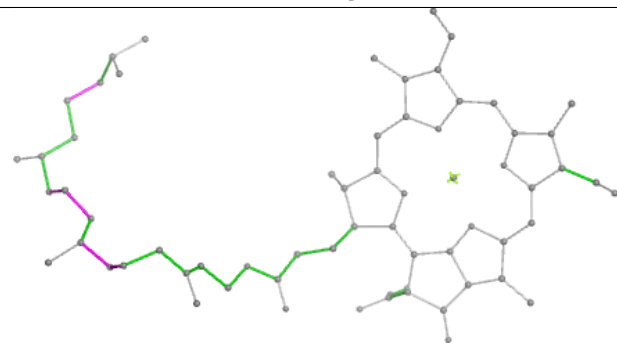
Ligand CLA A 828



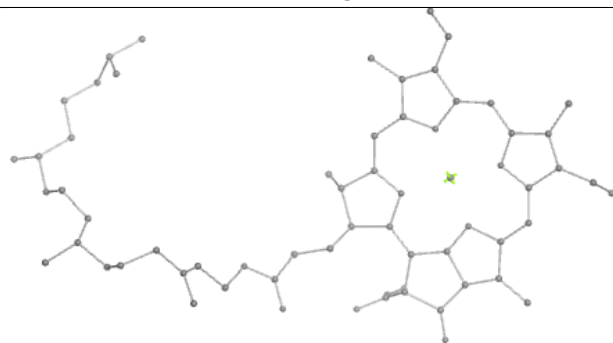
Bond lengths



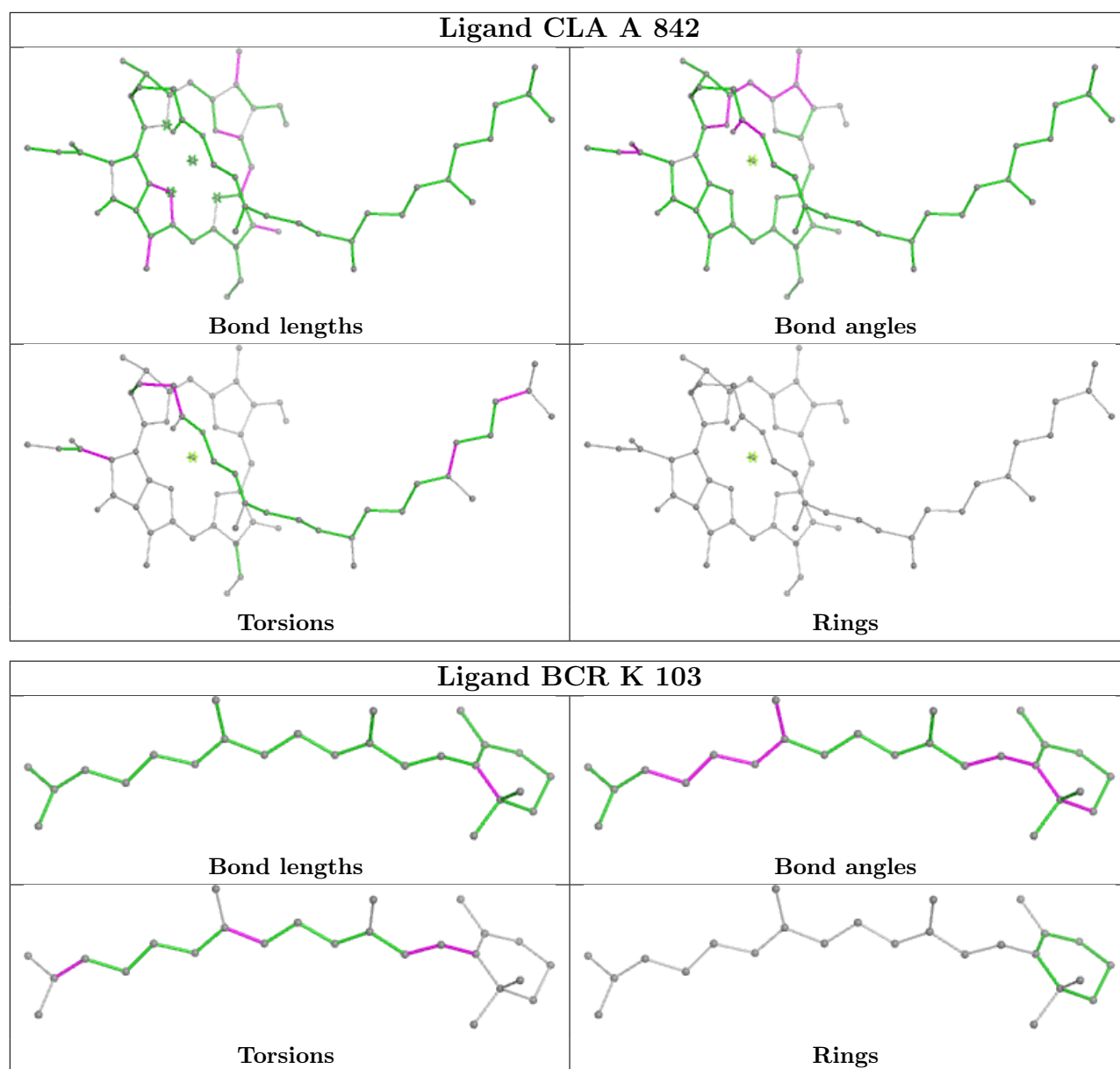
Bond angles



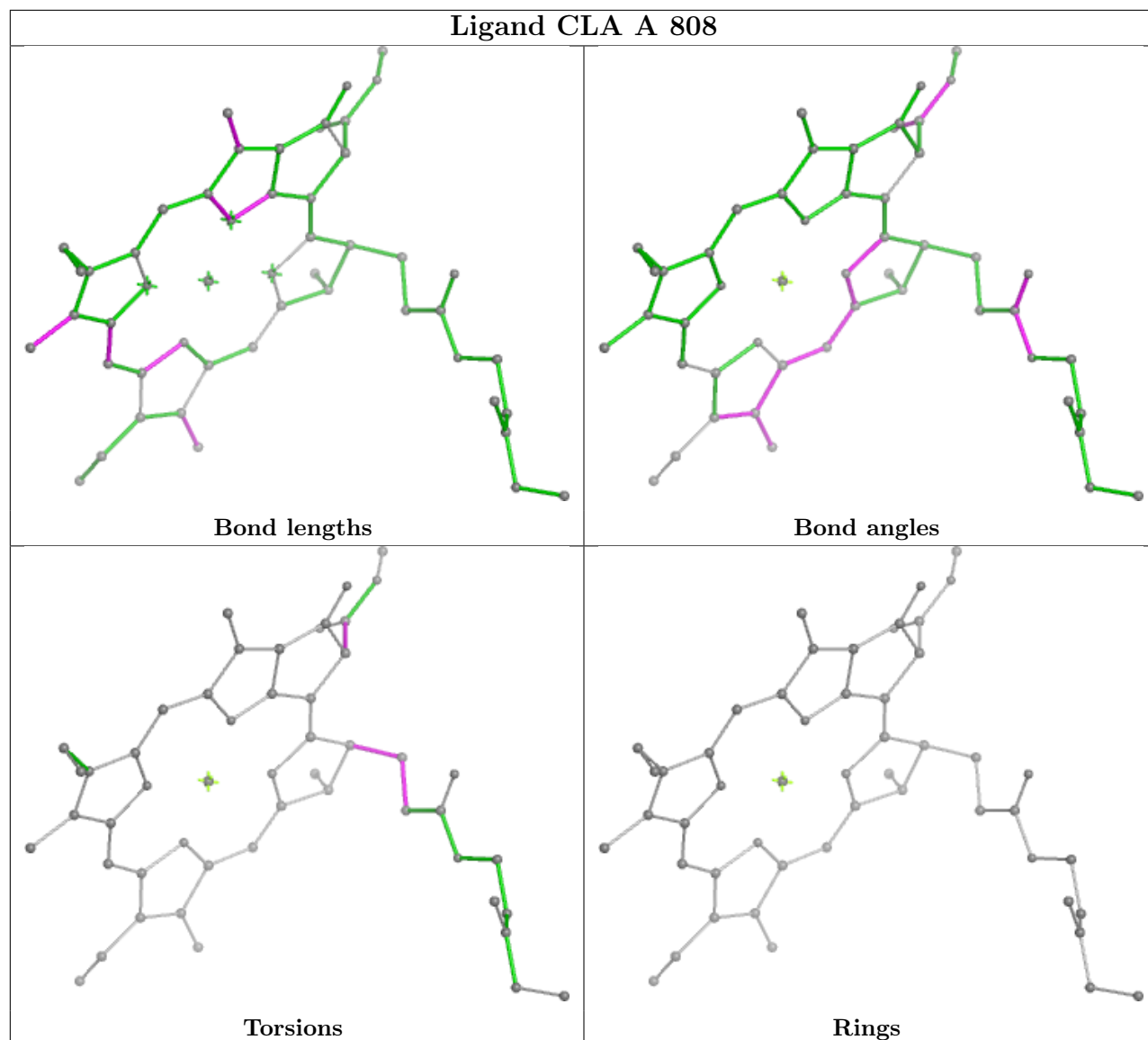
Torsions



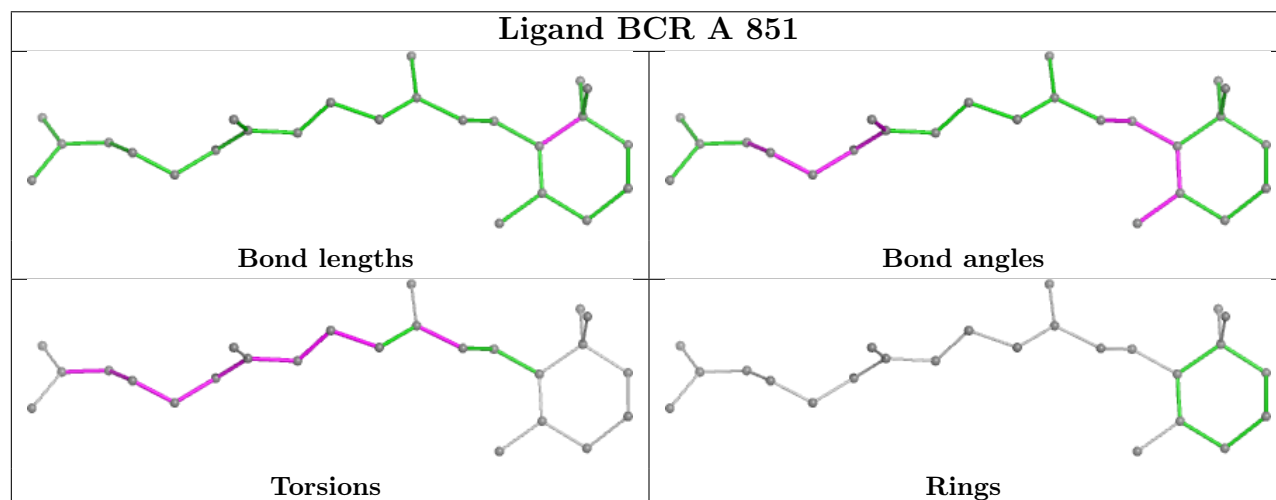
Rings

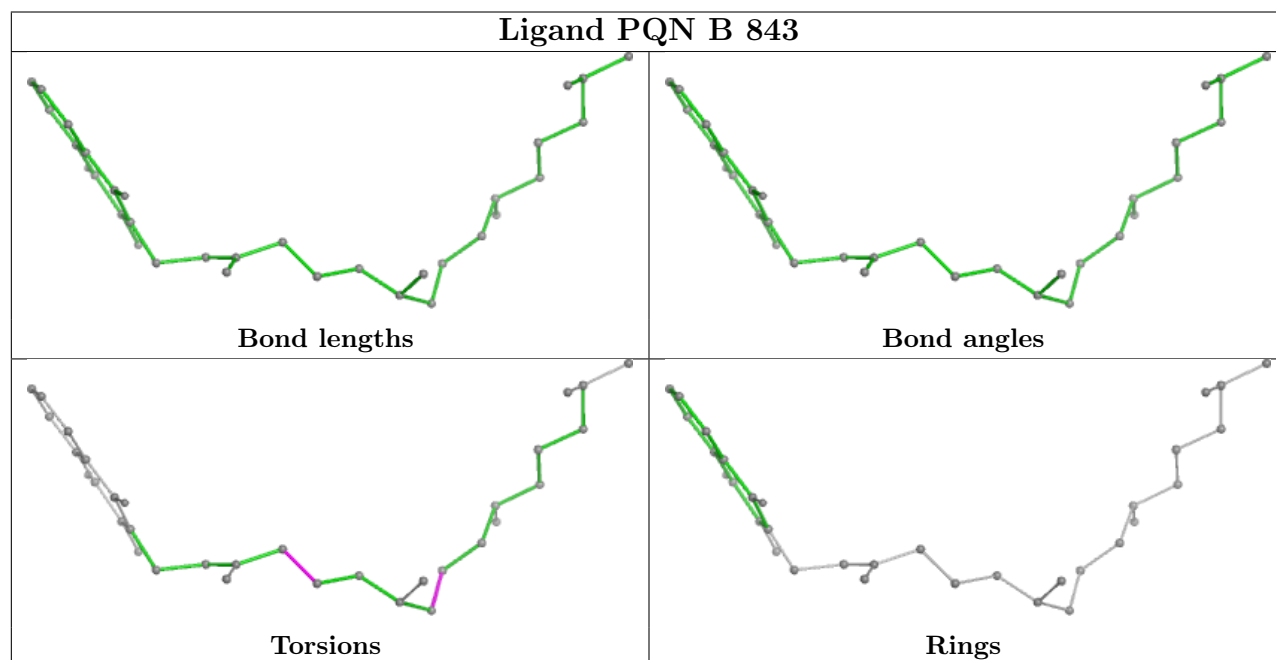
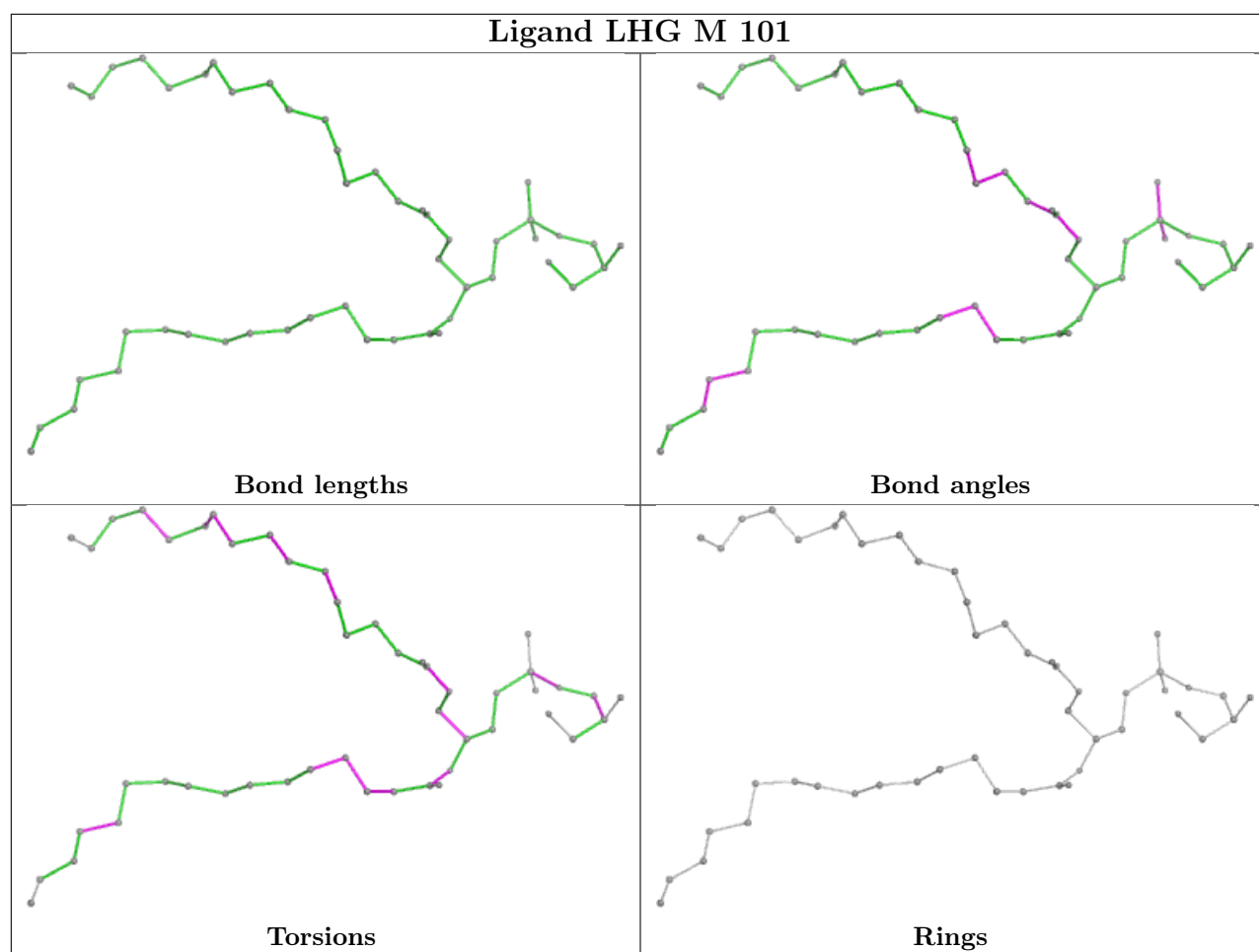


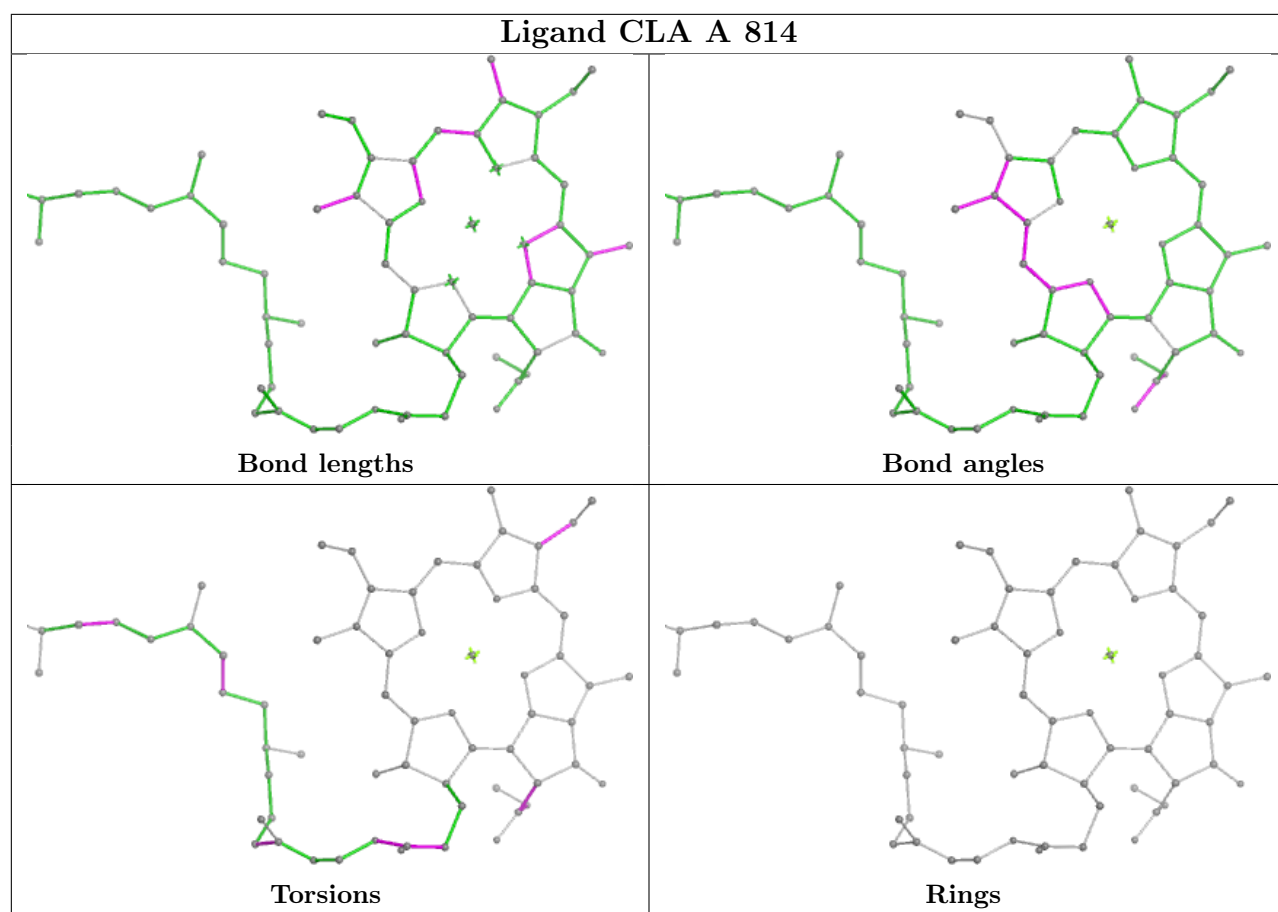
Ligand CLA A 808

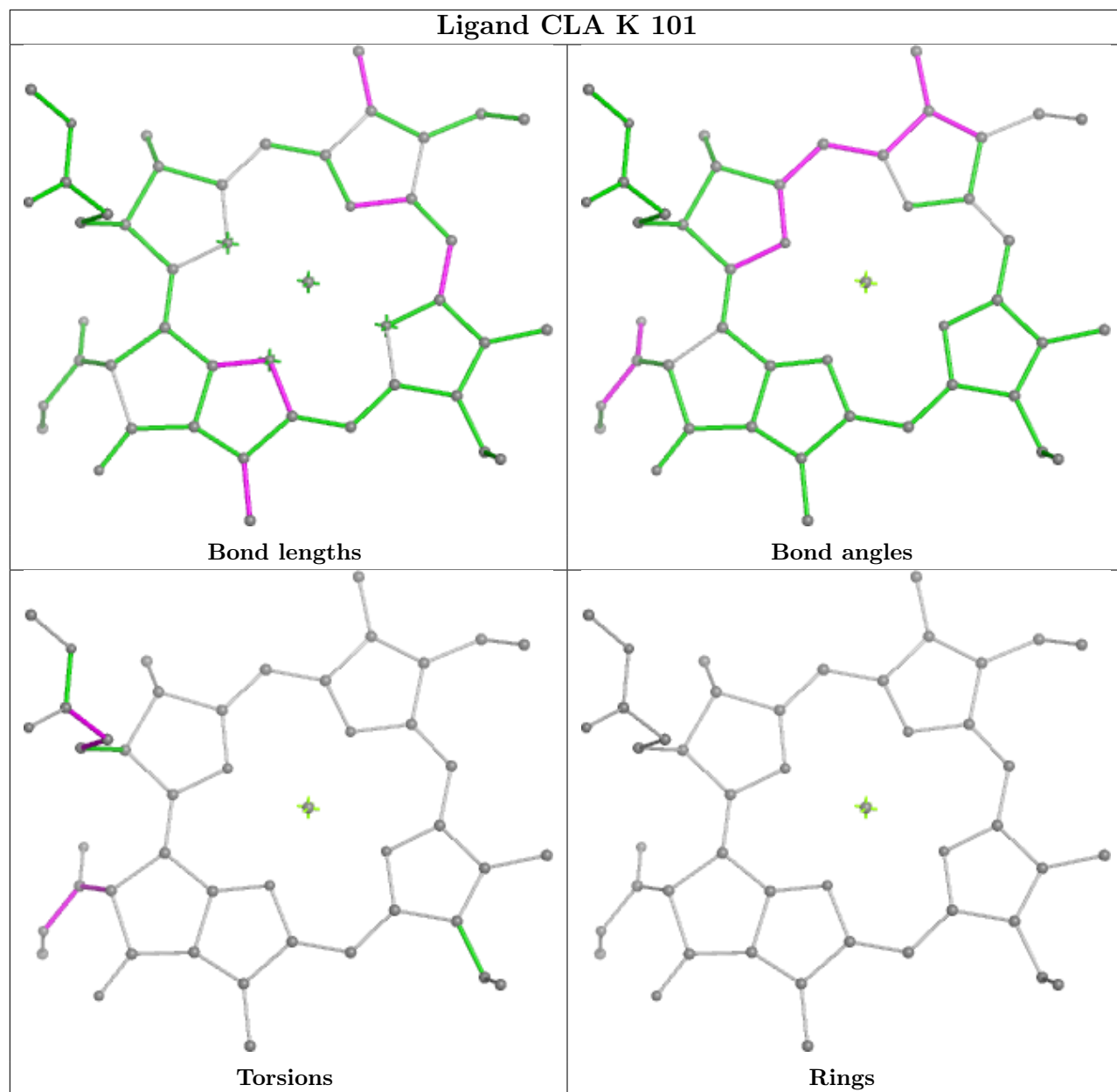


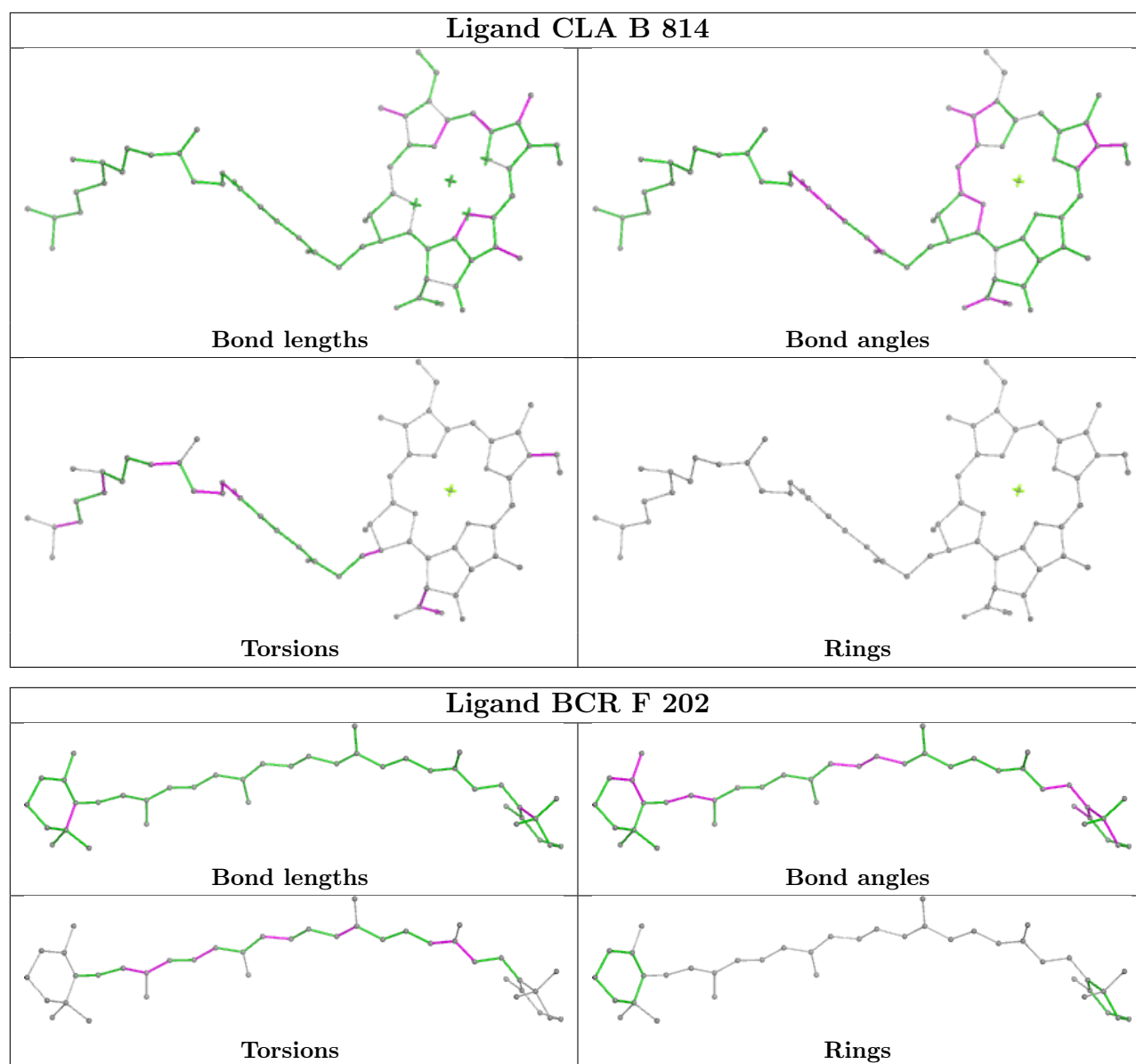
Ligand BCR A 851



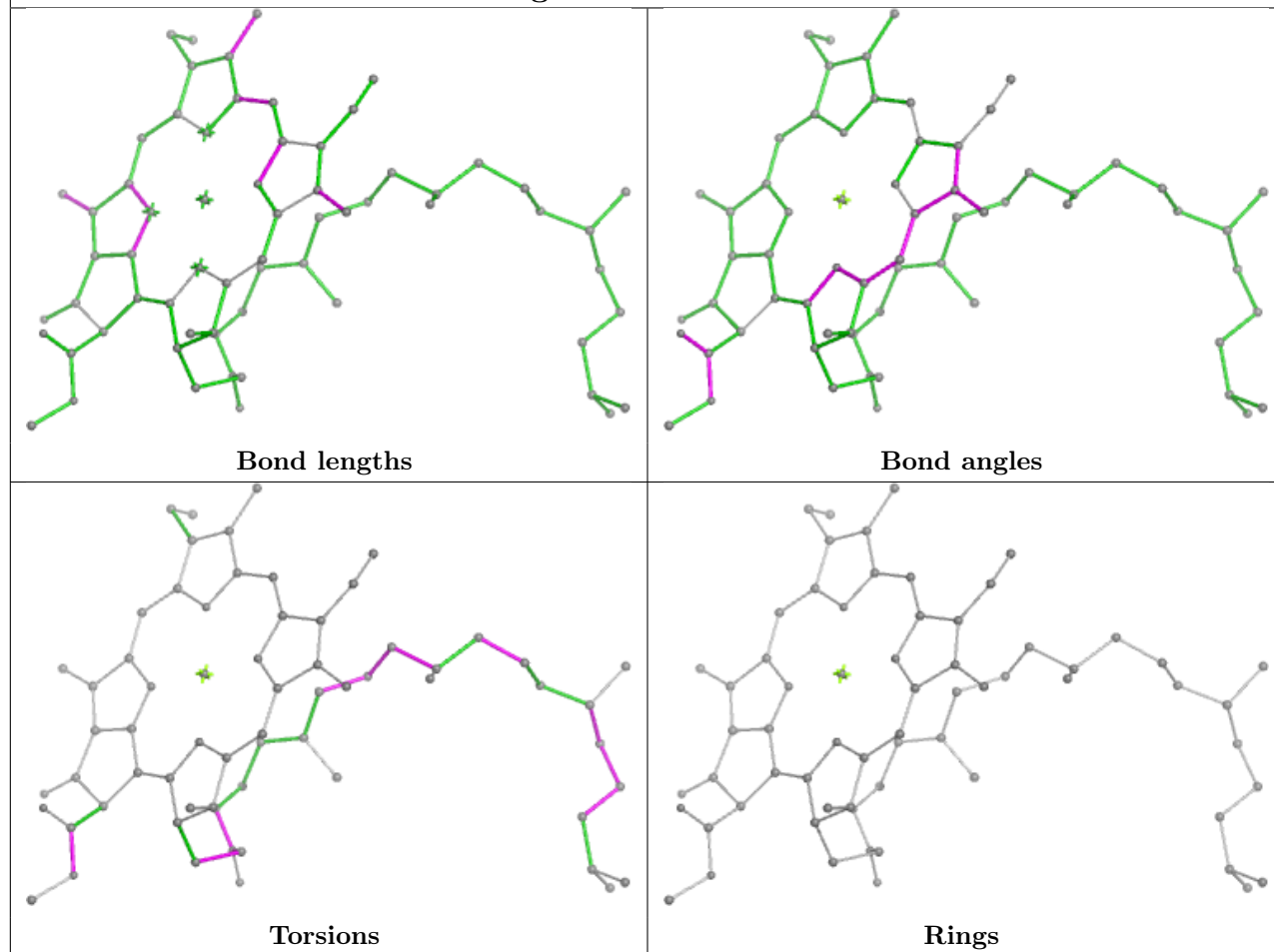




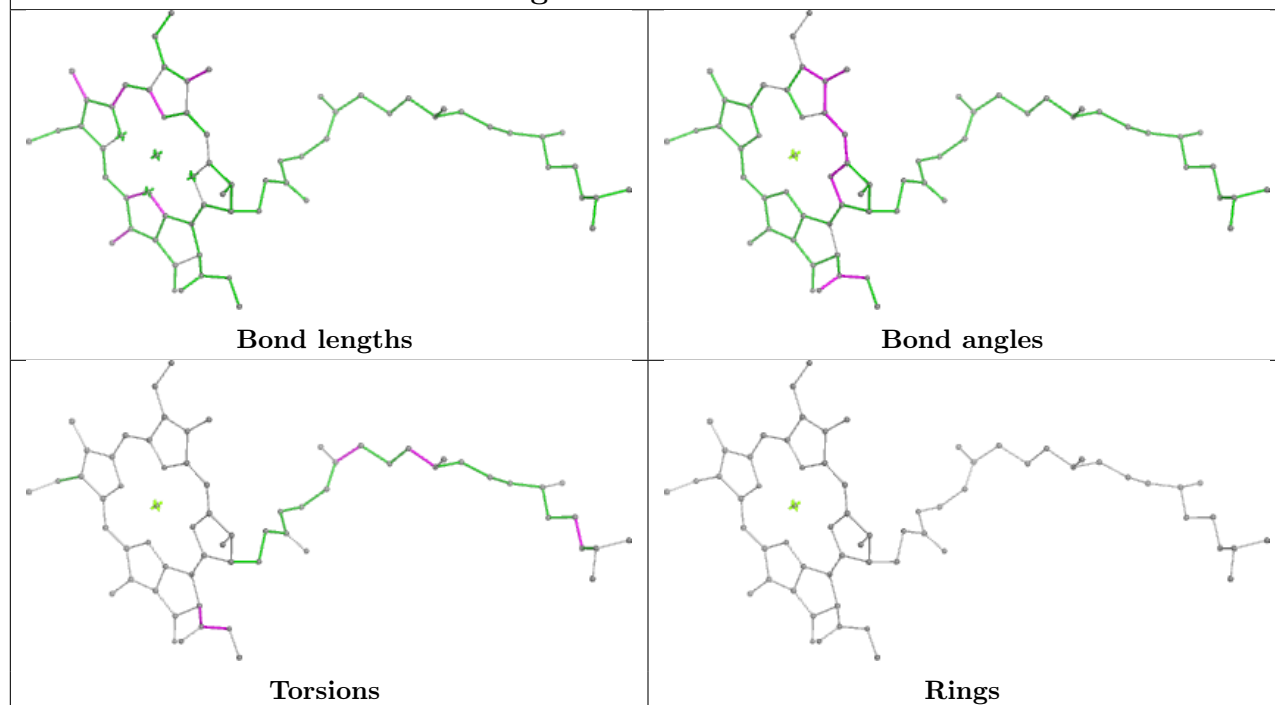


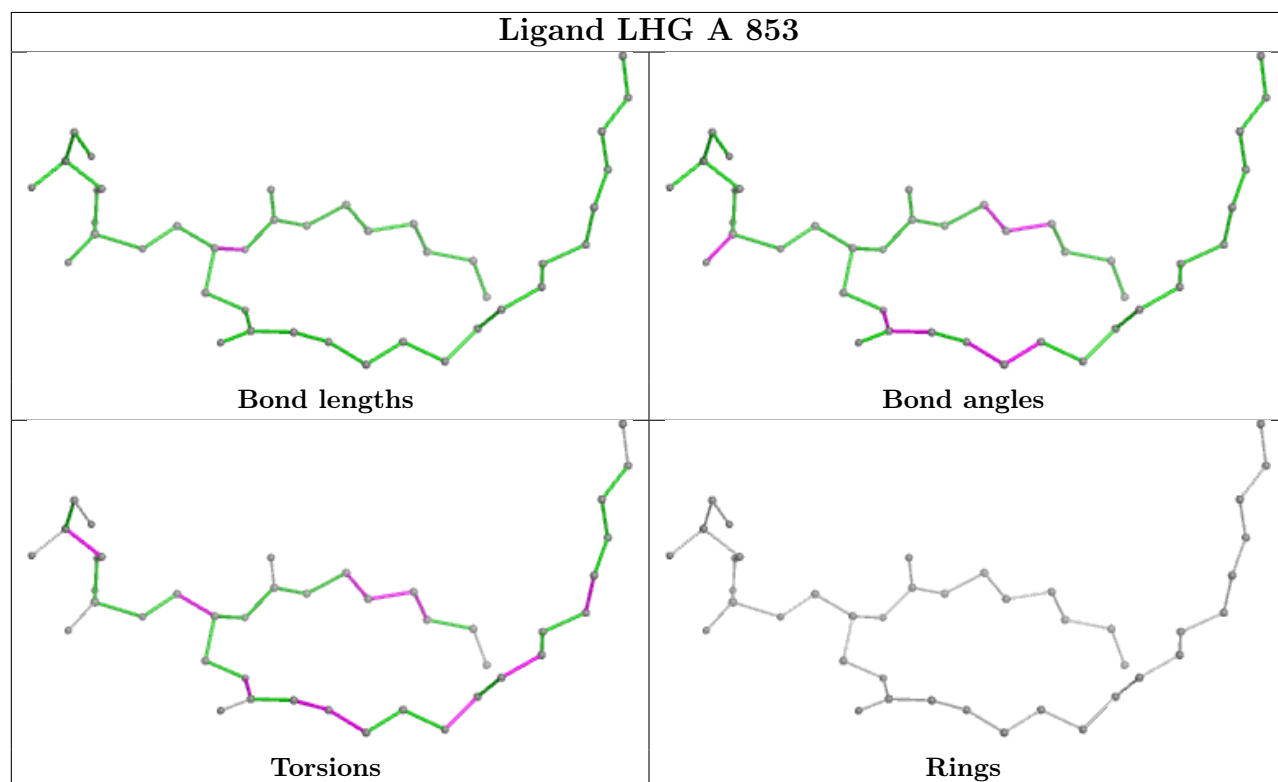
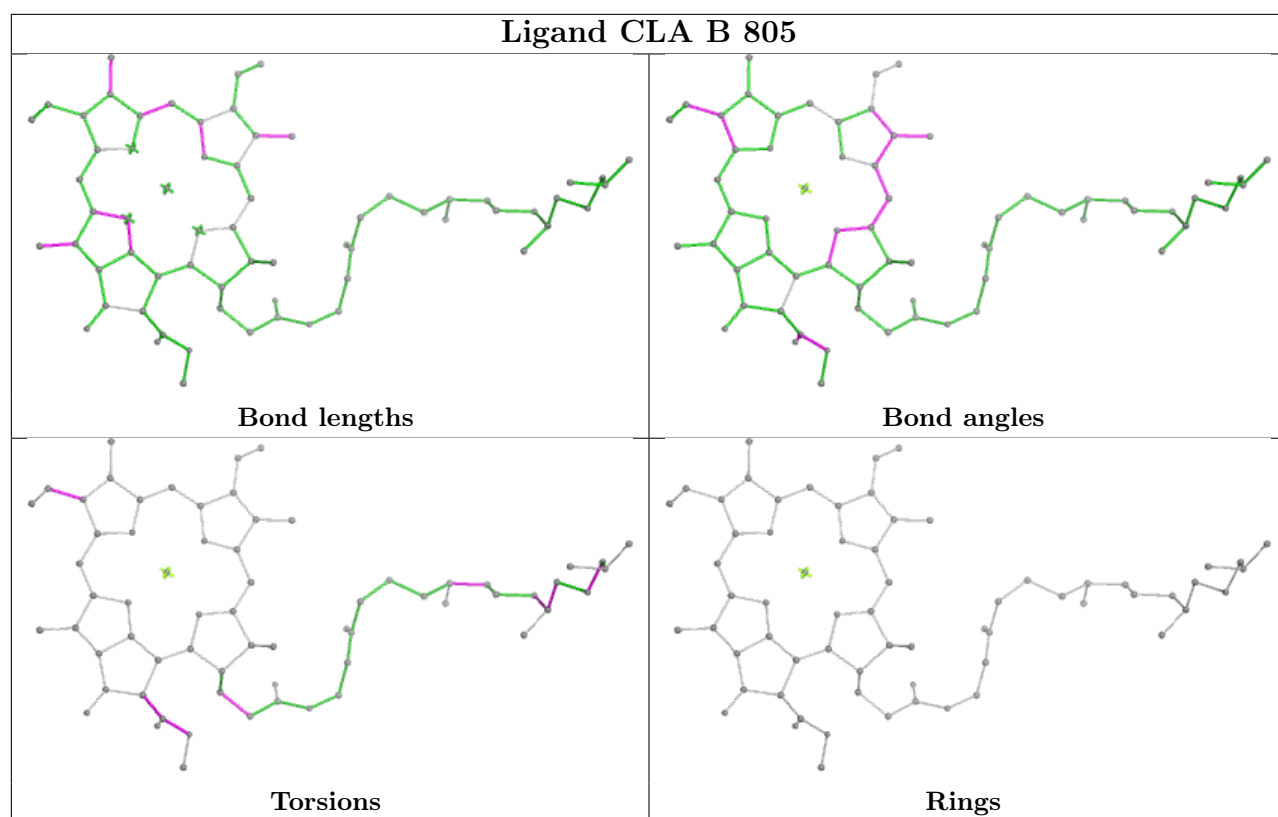


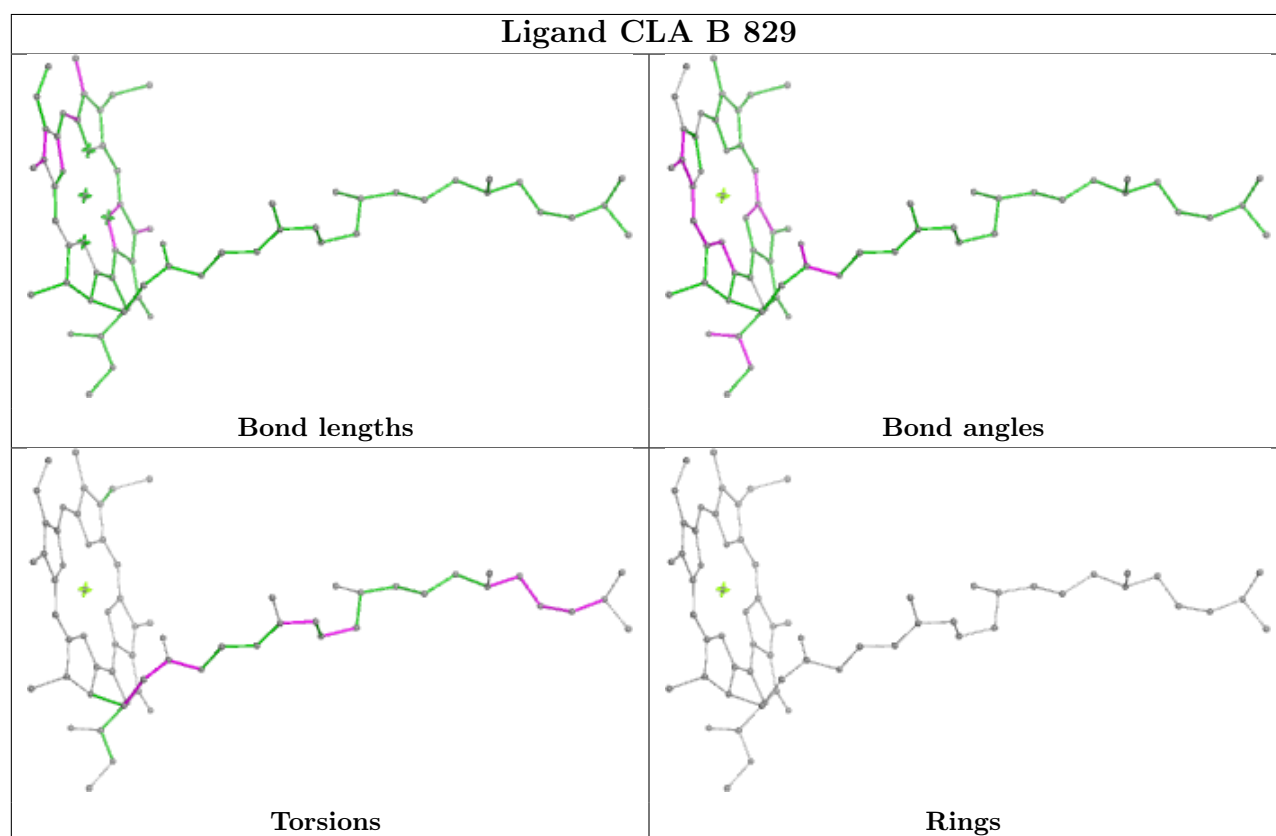
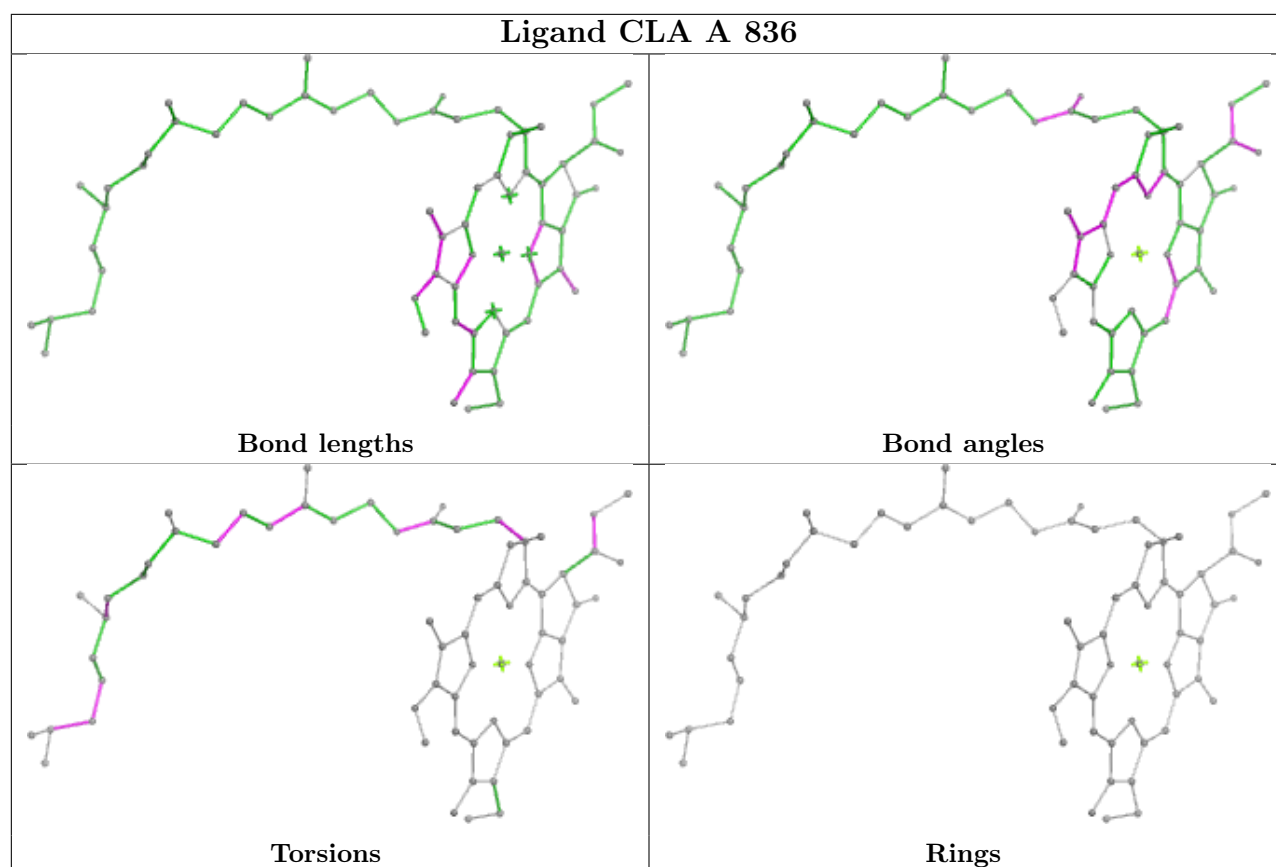
Ligand CLA B 801



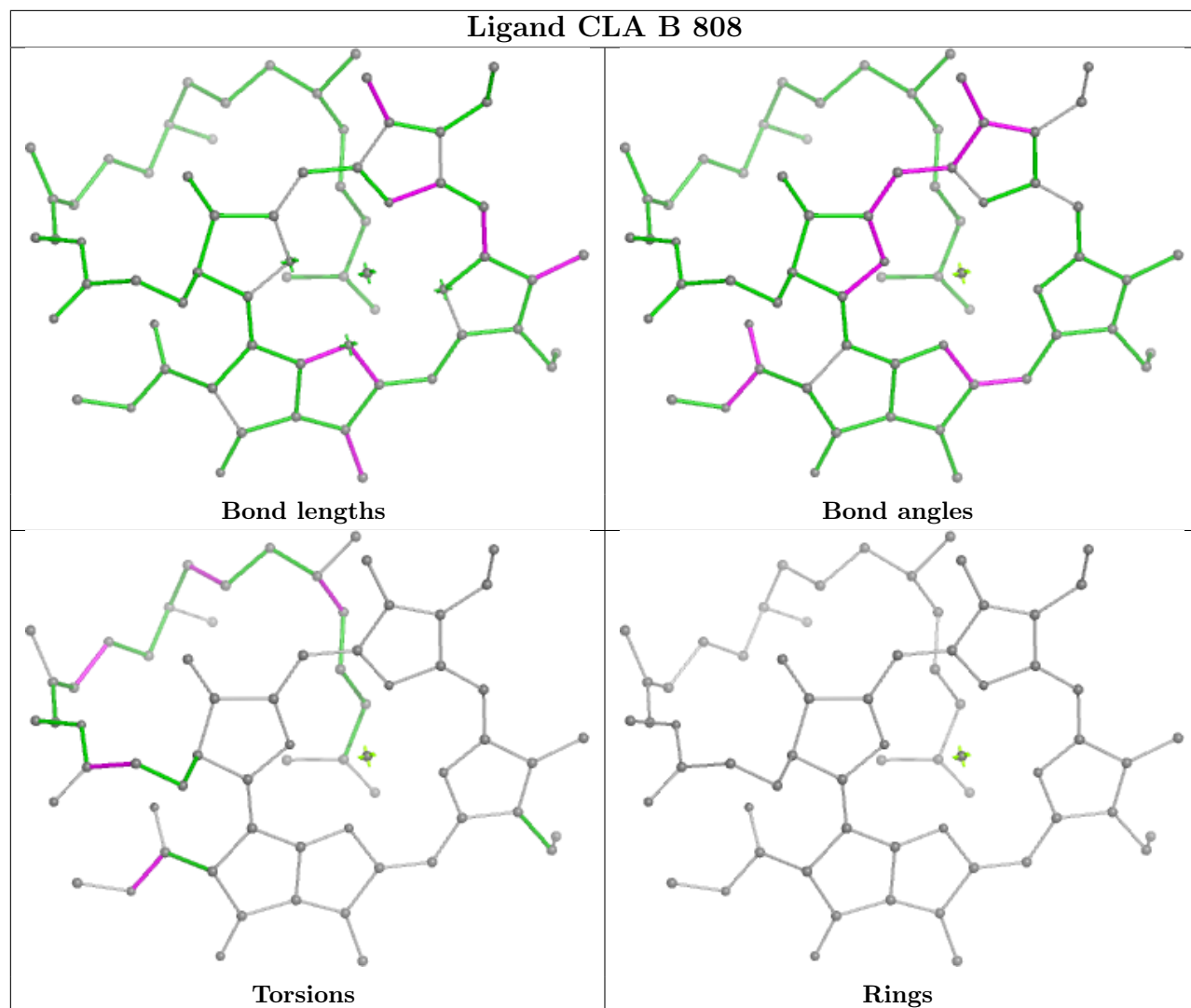
Ligand CLA A 822

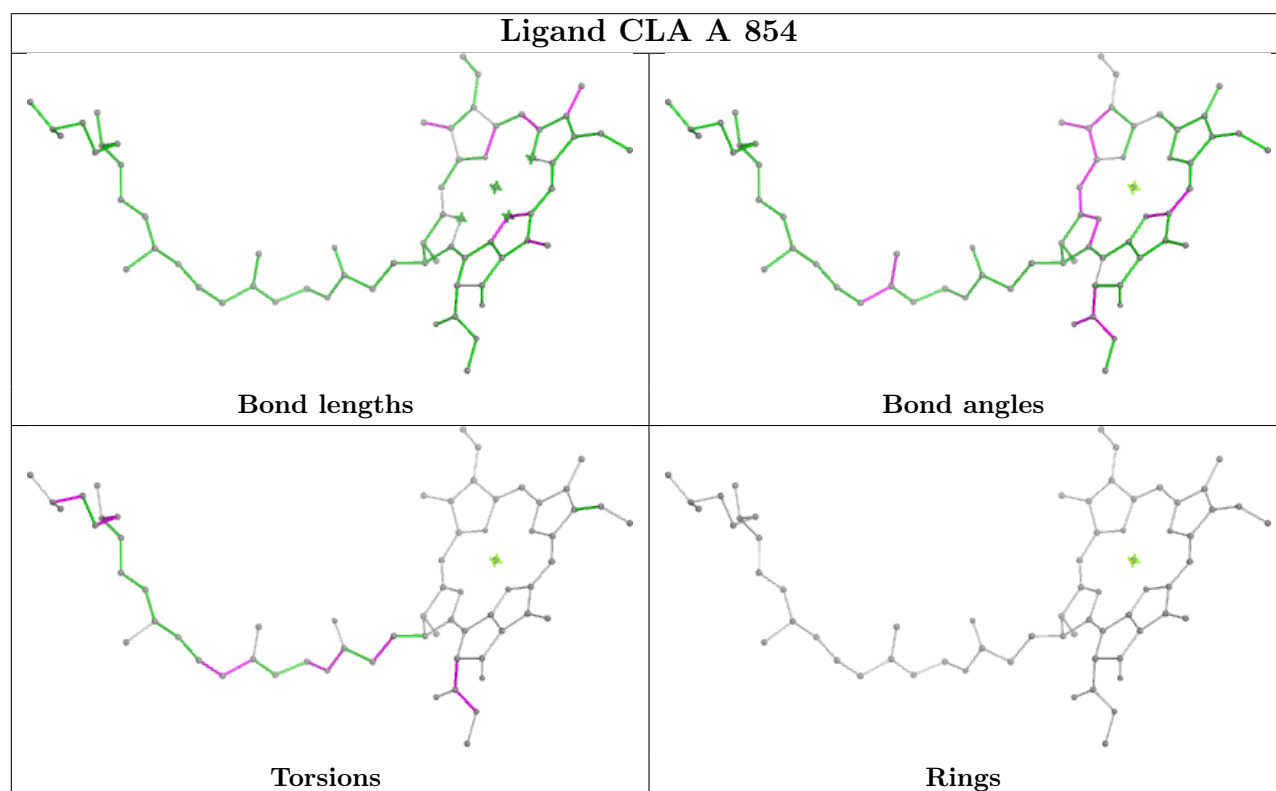
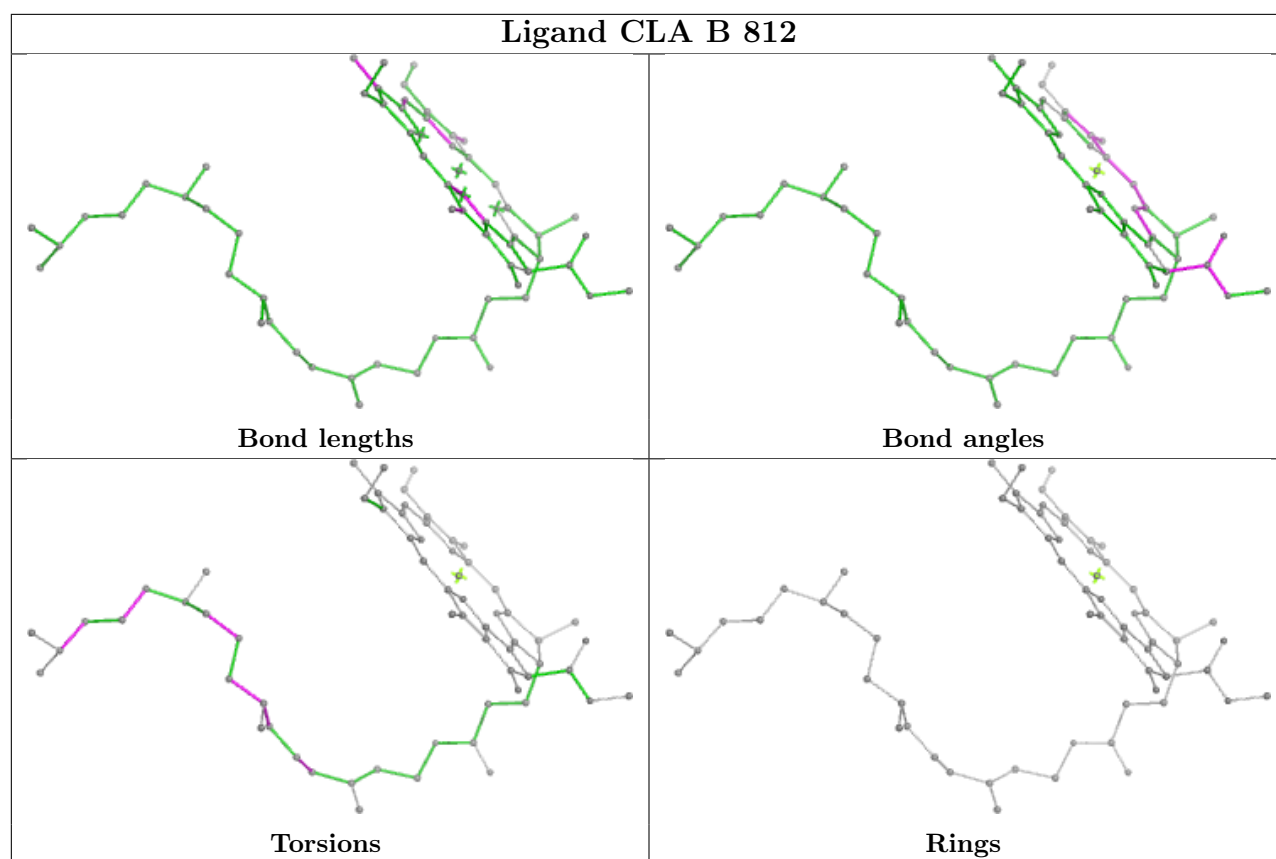


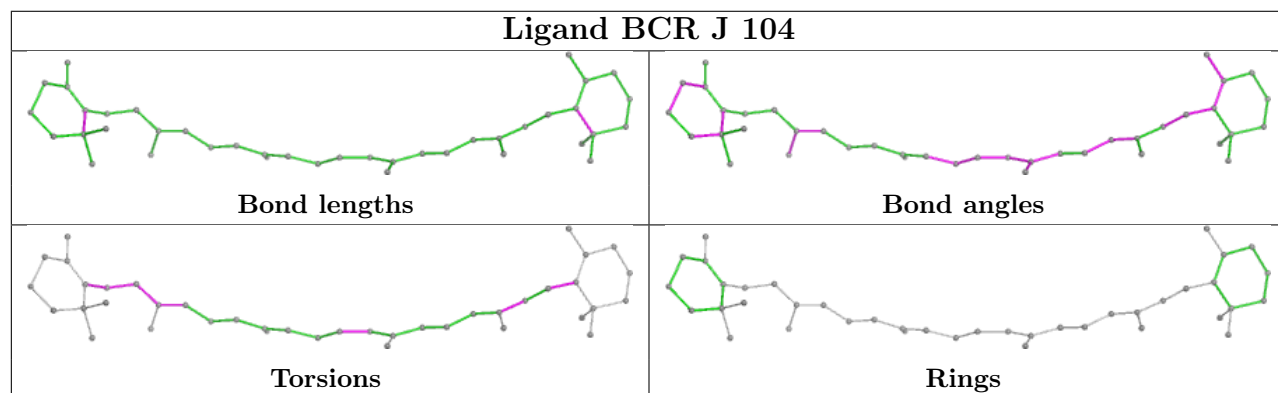
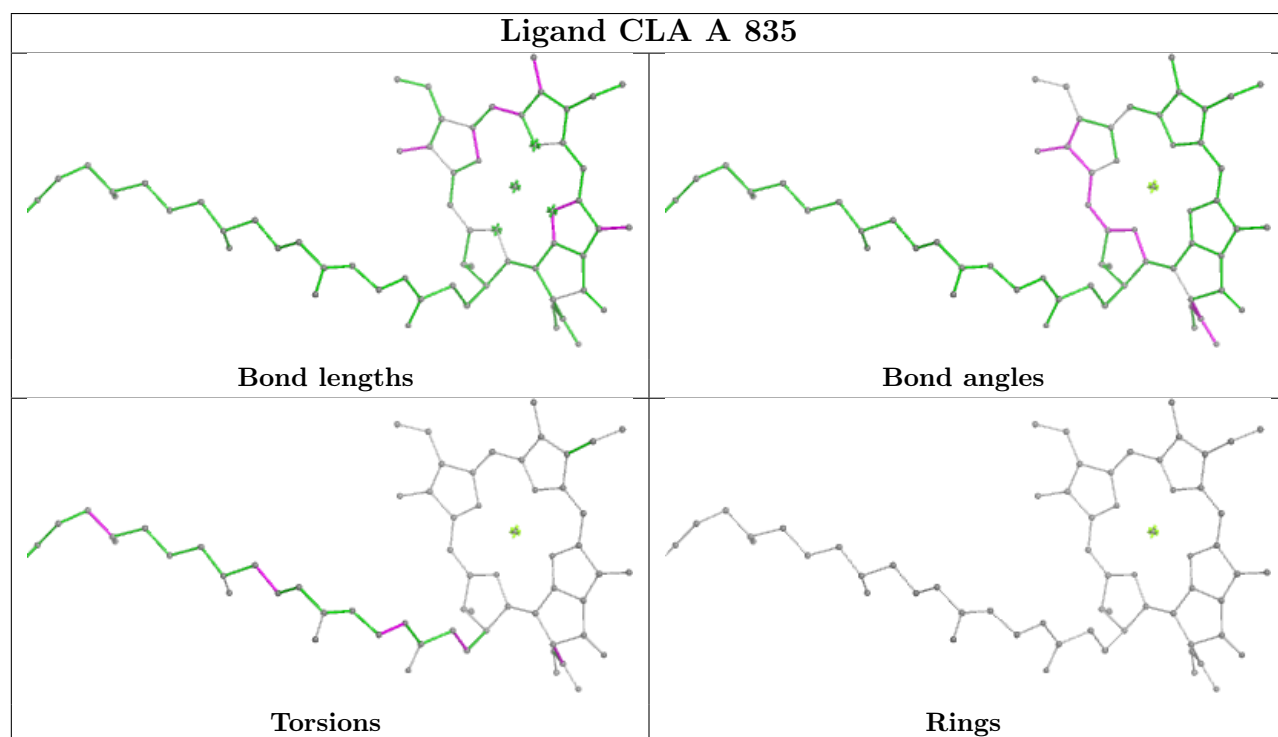
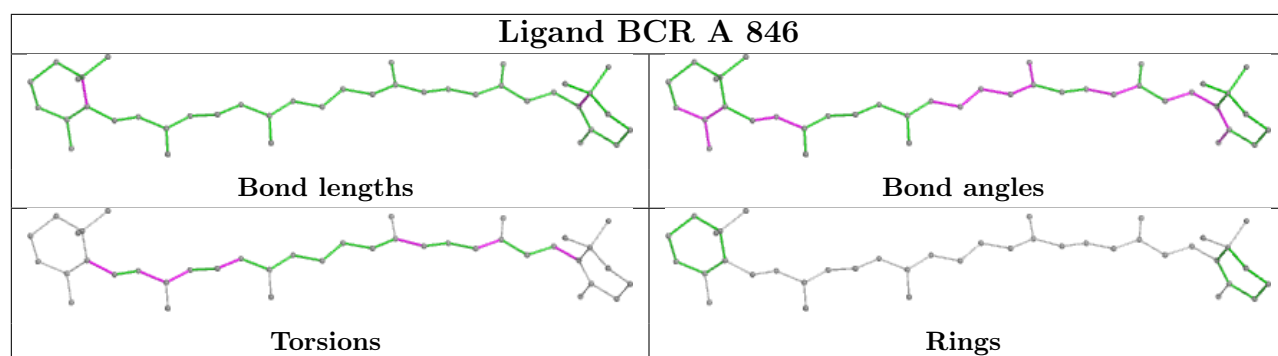




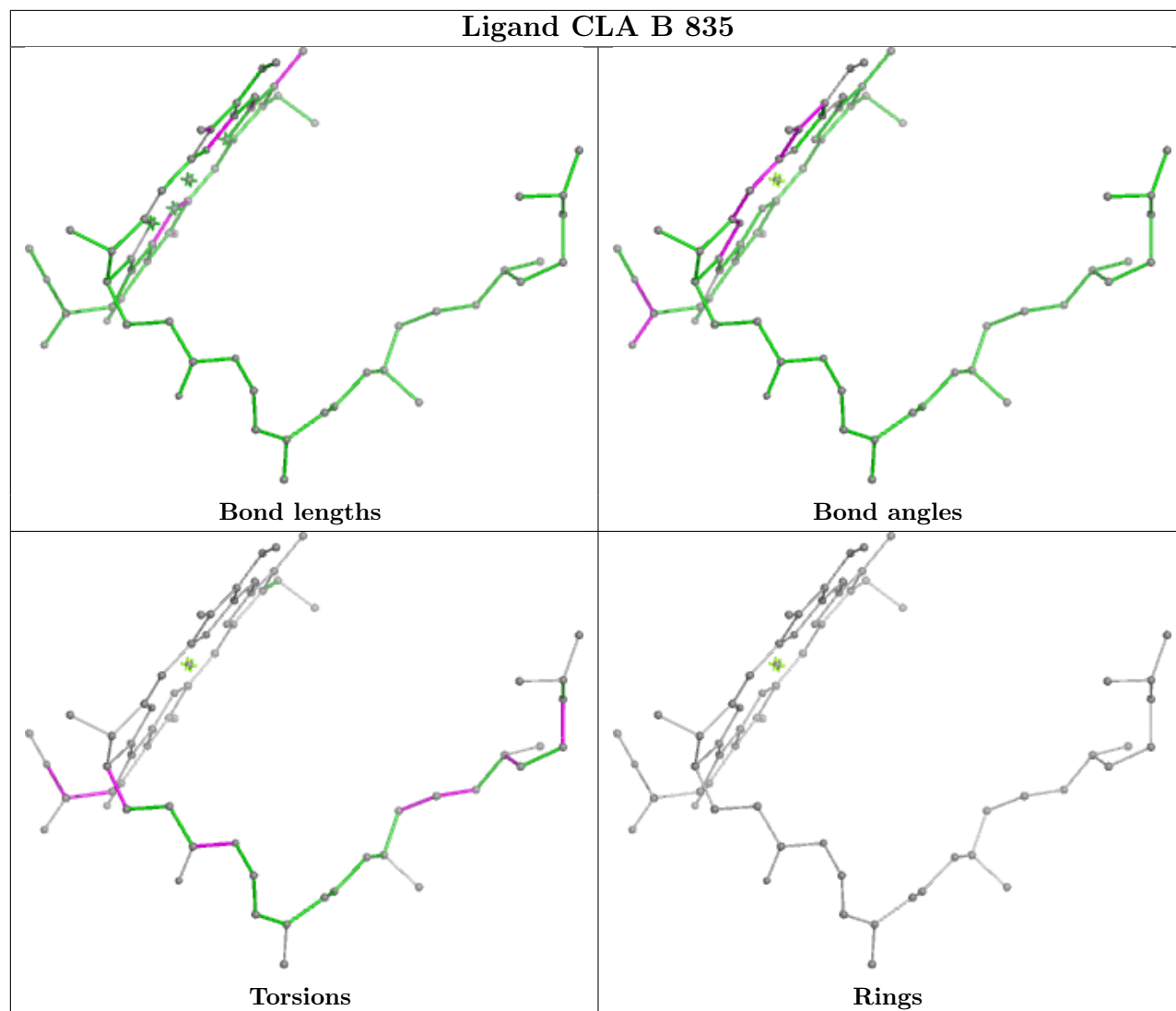
Ligand CLA B 808



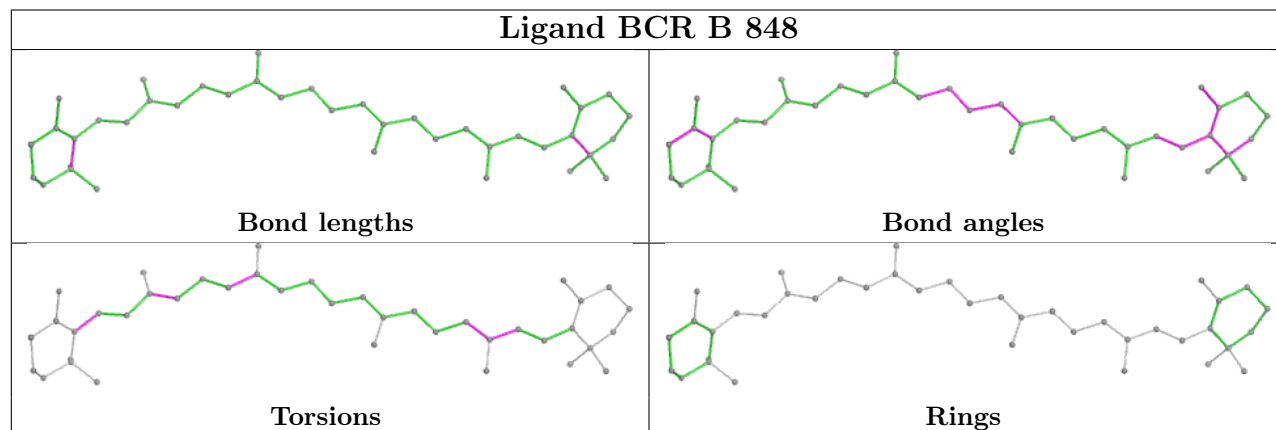


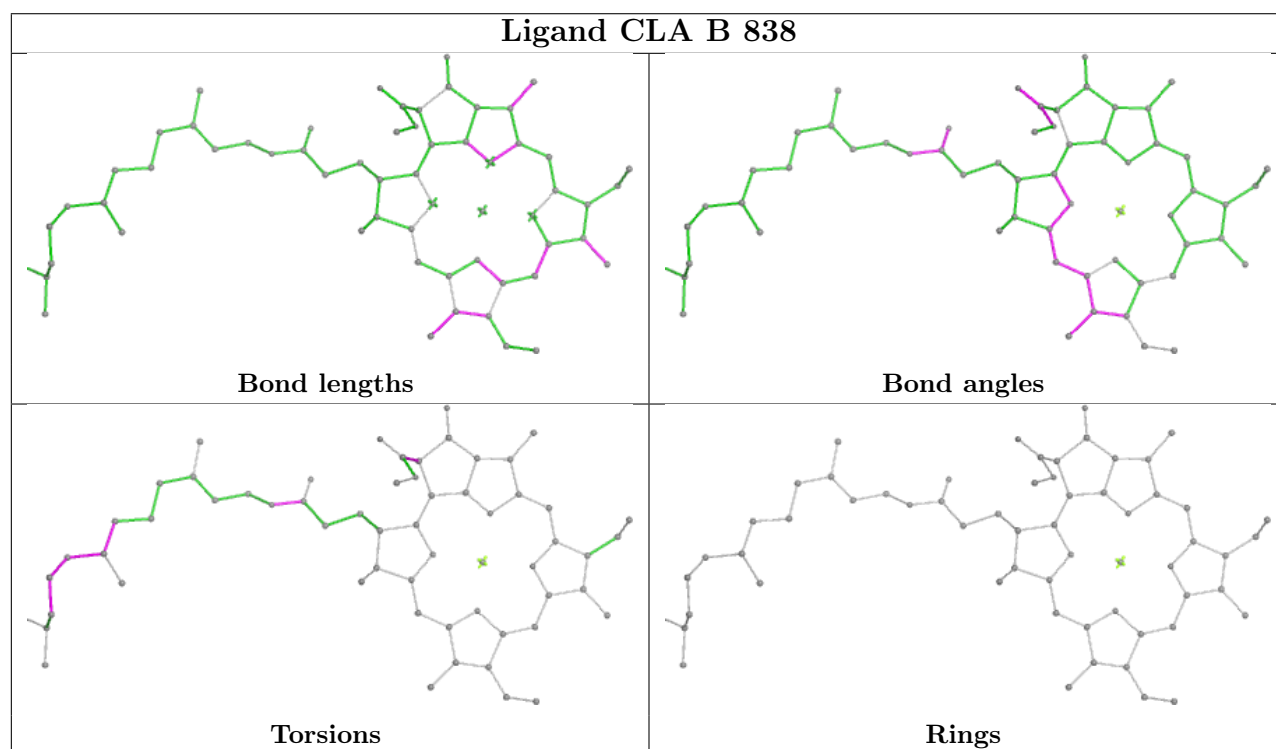
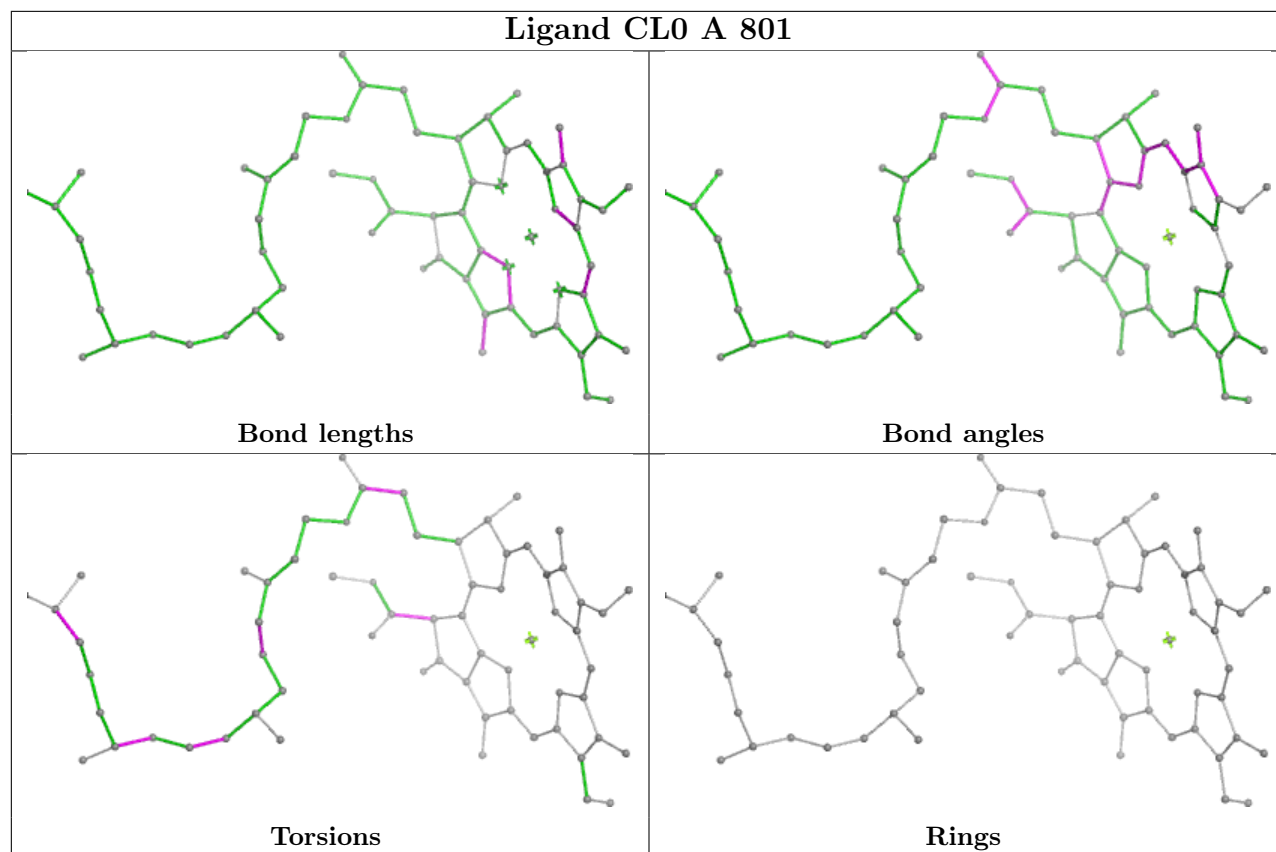


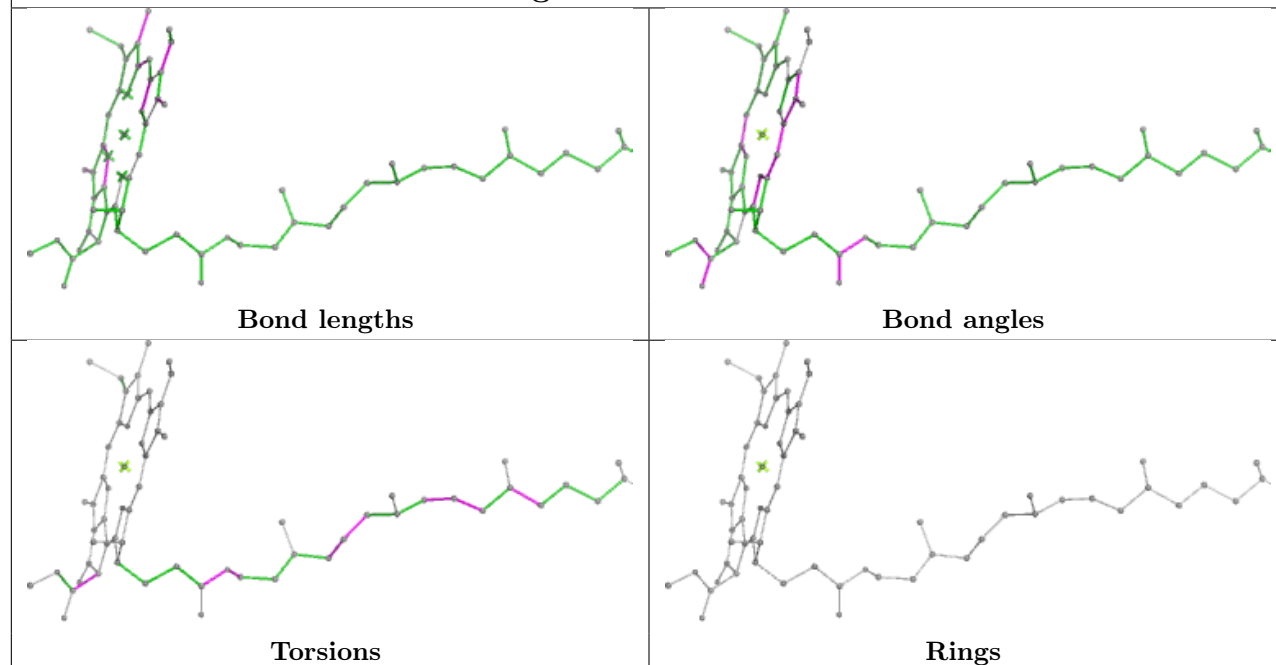
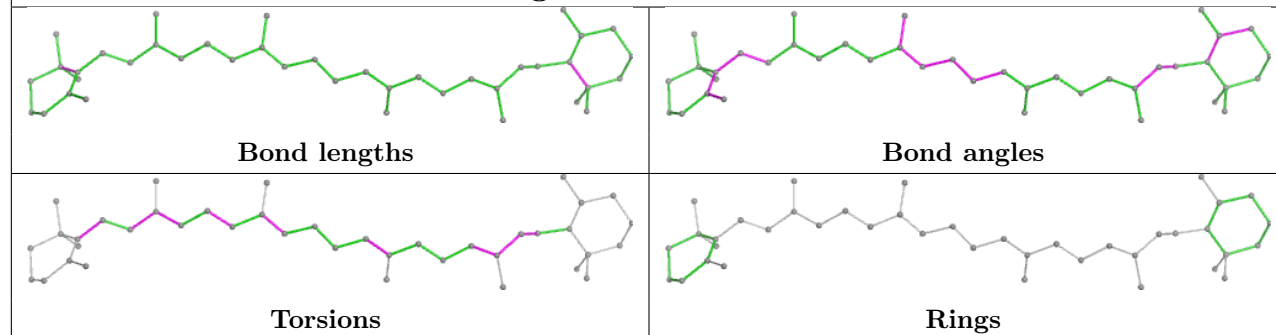
Ligand CLA B 835



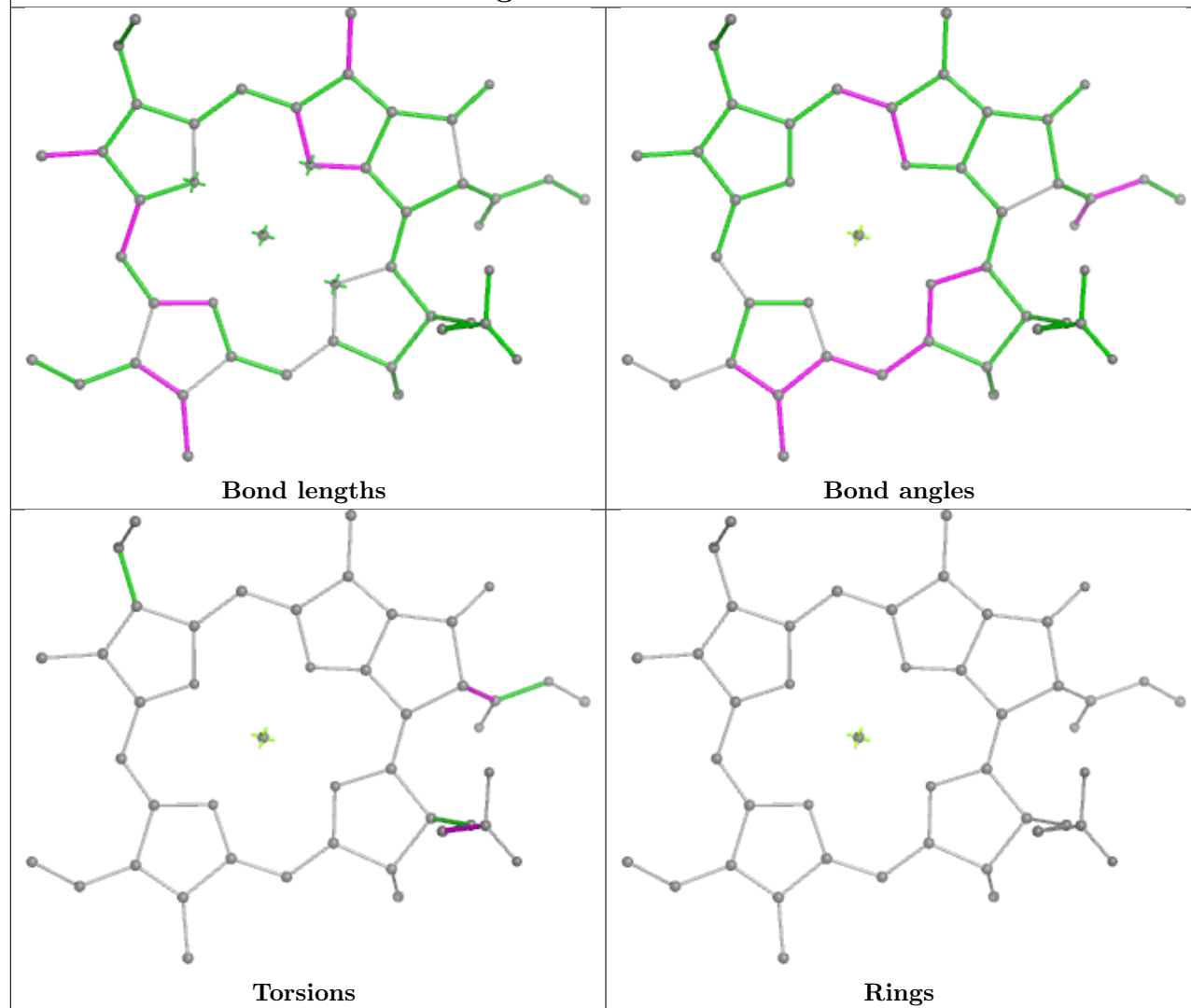
Ligand BCR B 848



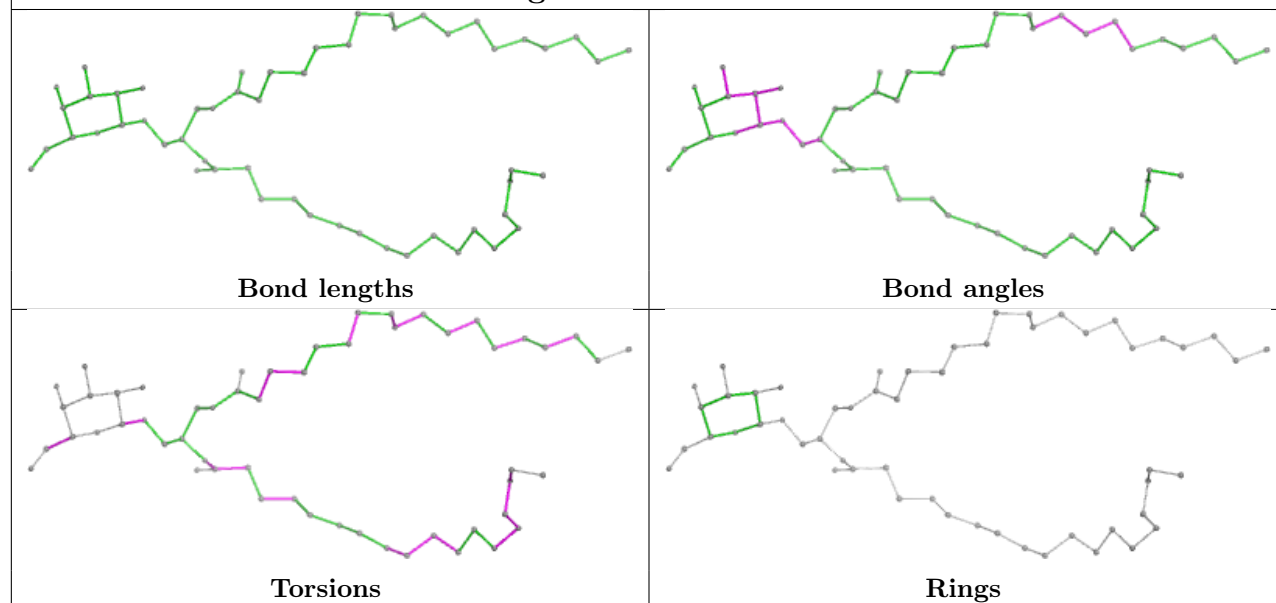


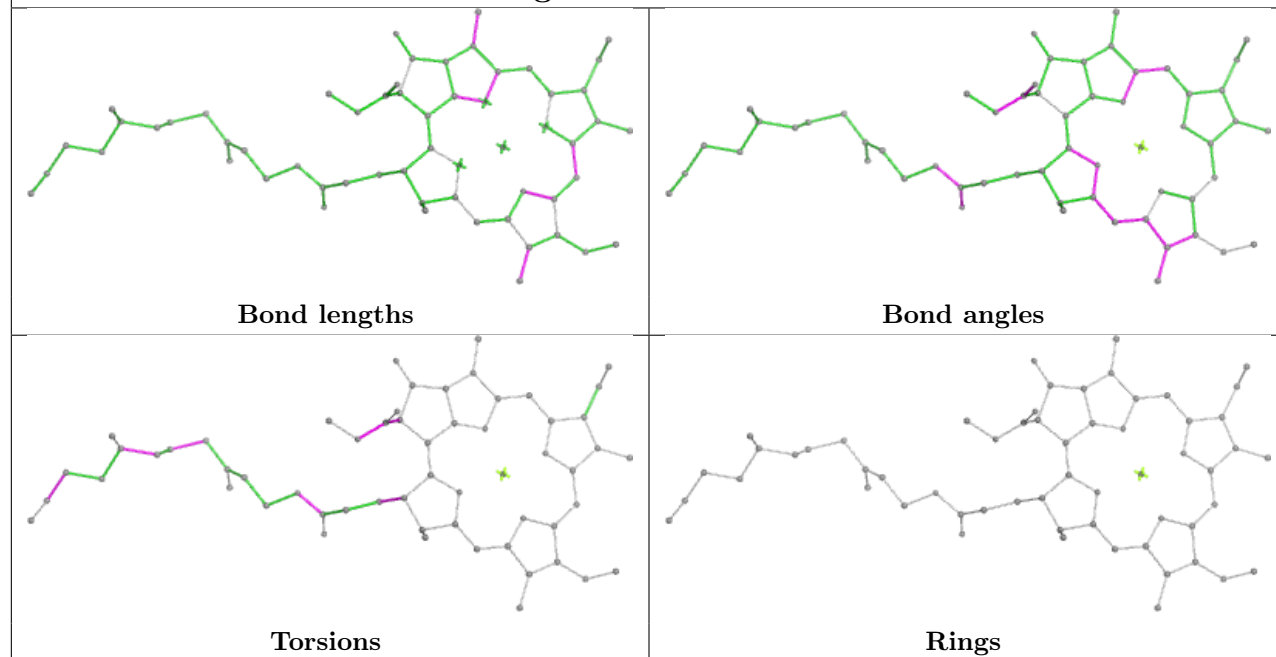
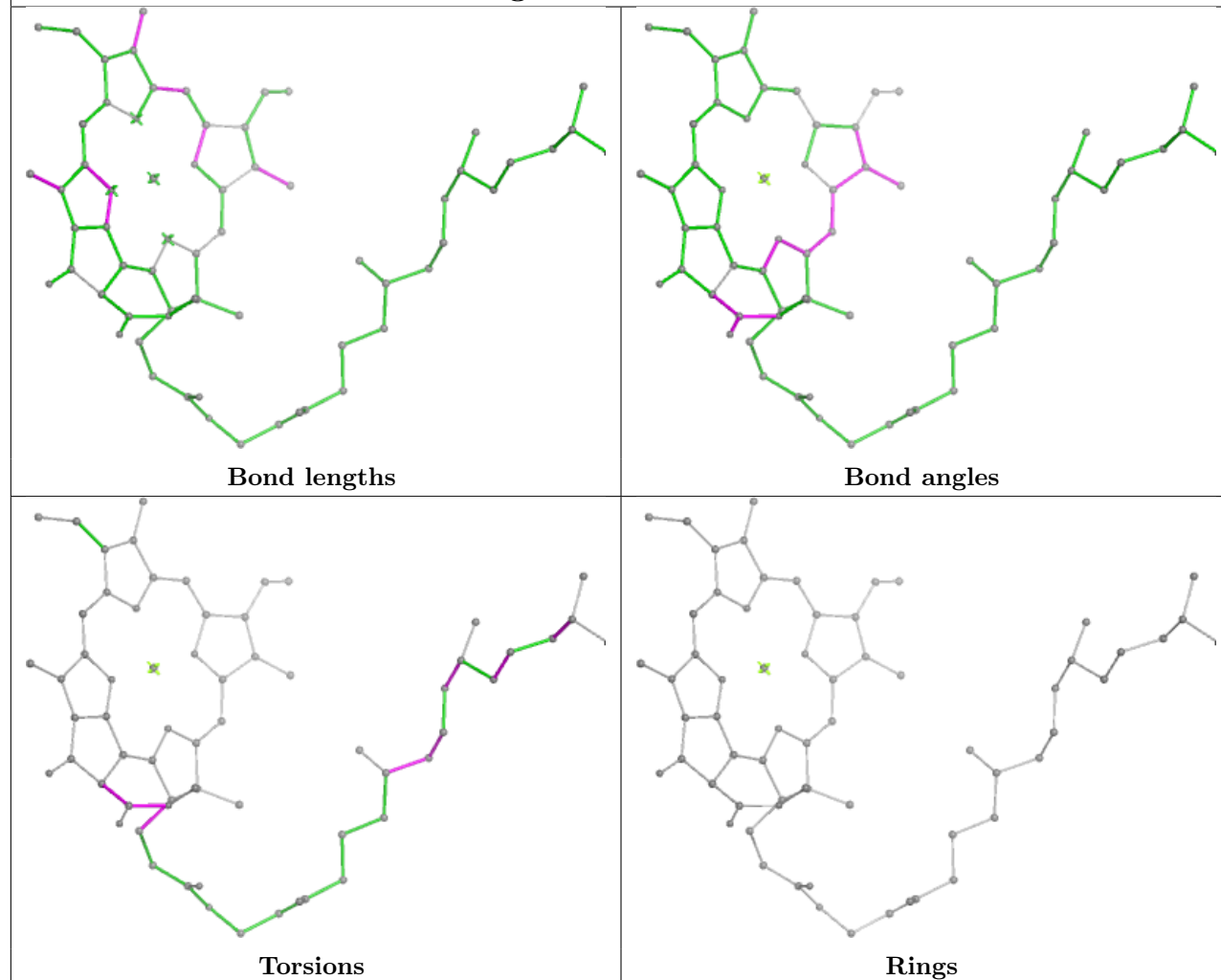
Ligand CLA B 806**Ligand BCR B 844**

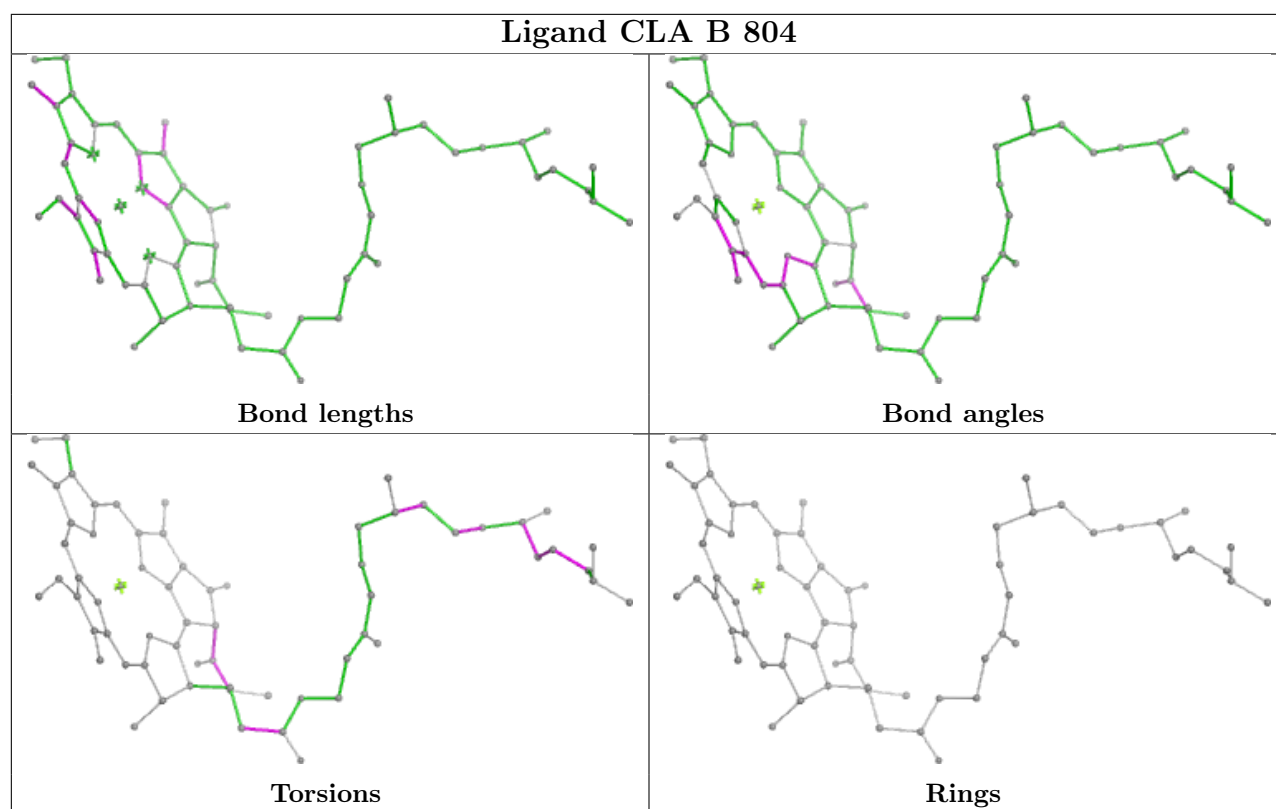
Ligand CLA A 813



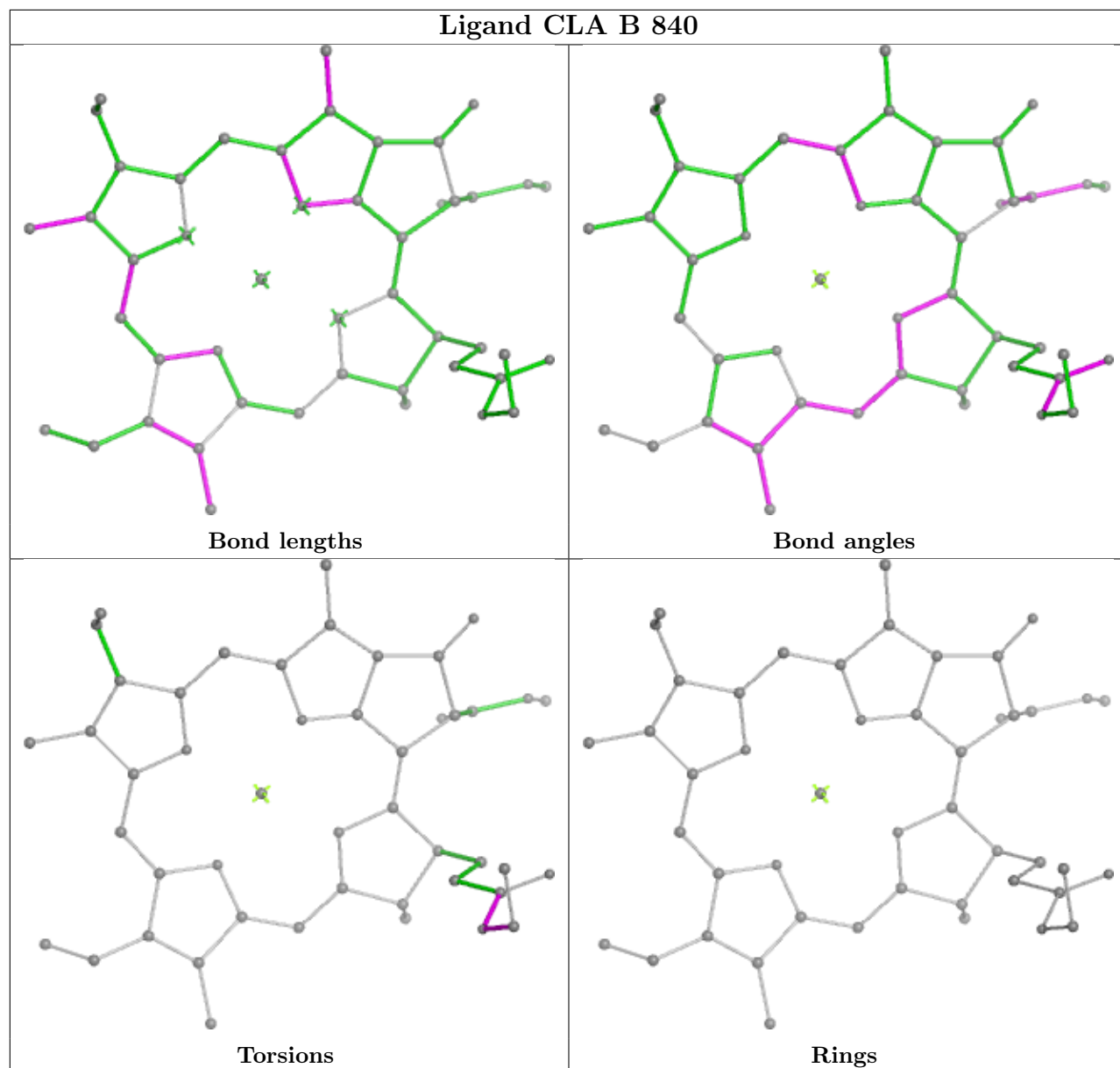
Ligand LMG B 850

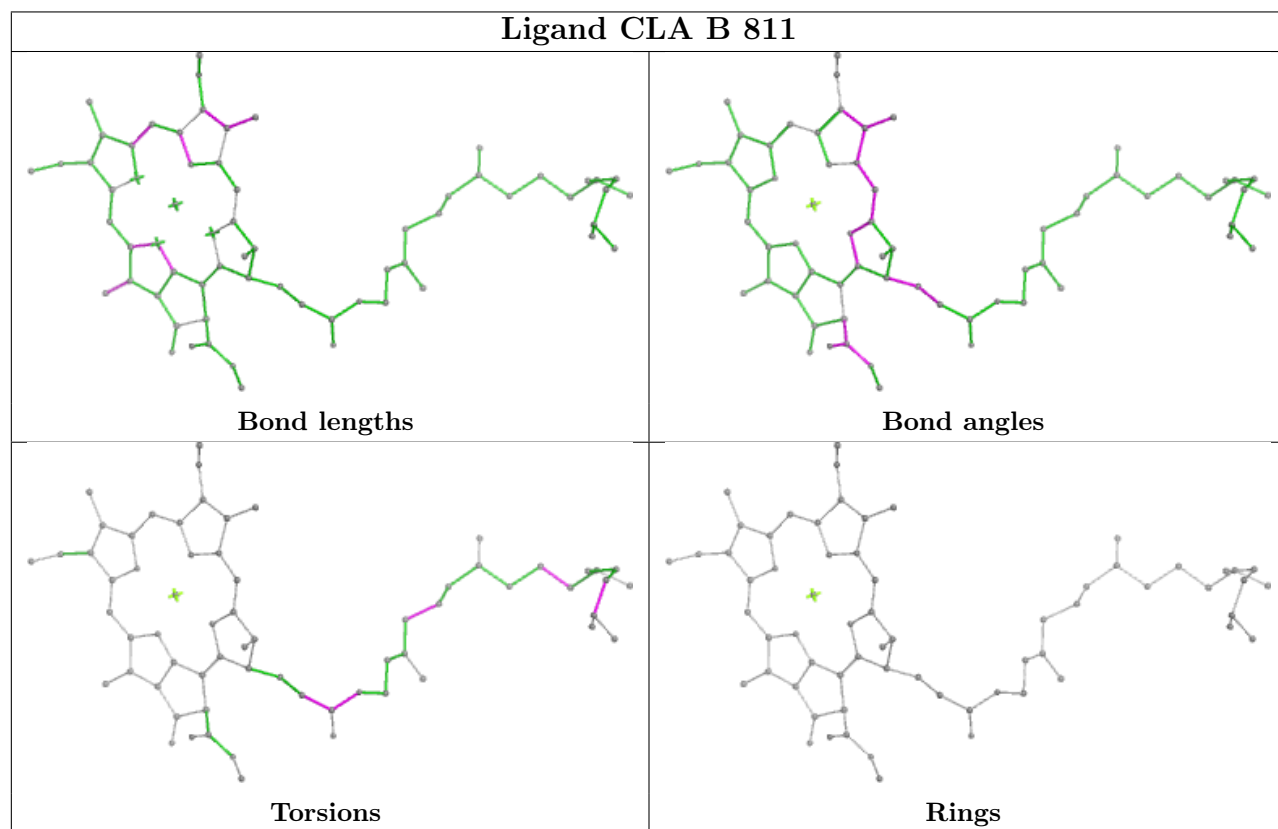
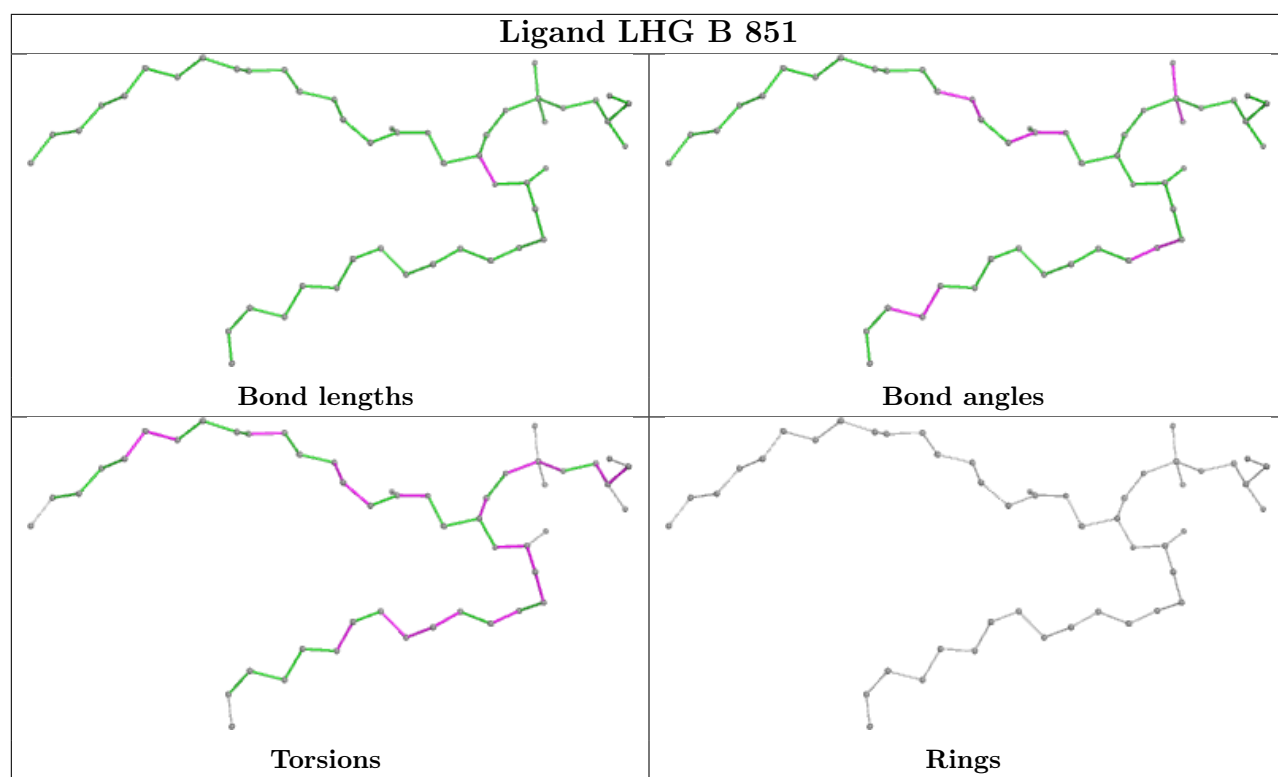


Ligand CLA F 201**Ligand CLA B 825**

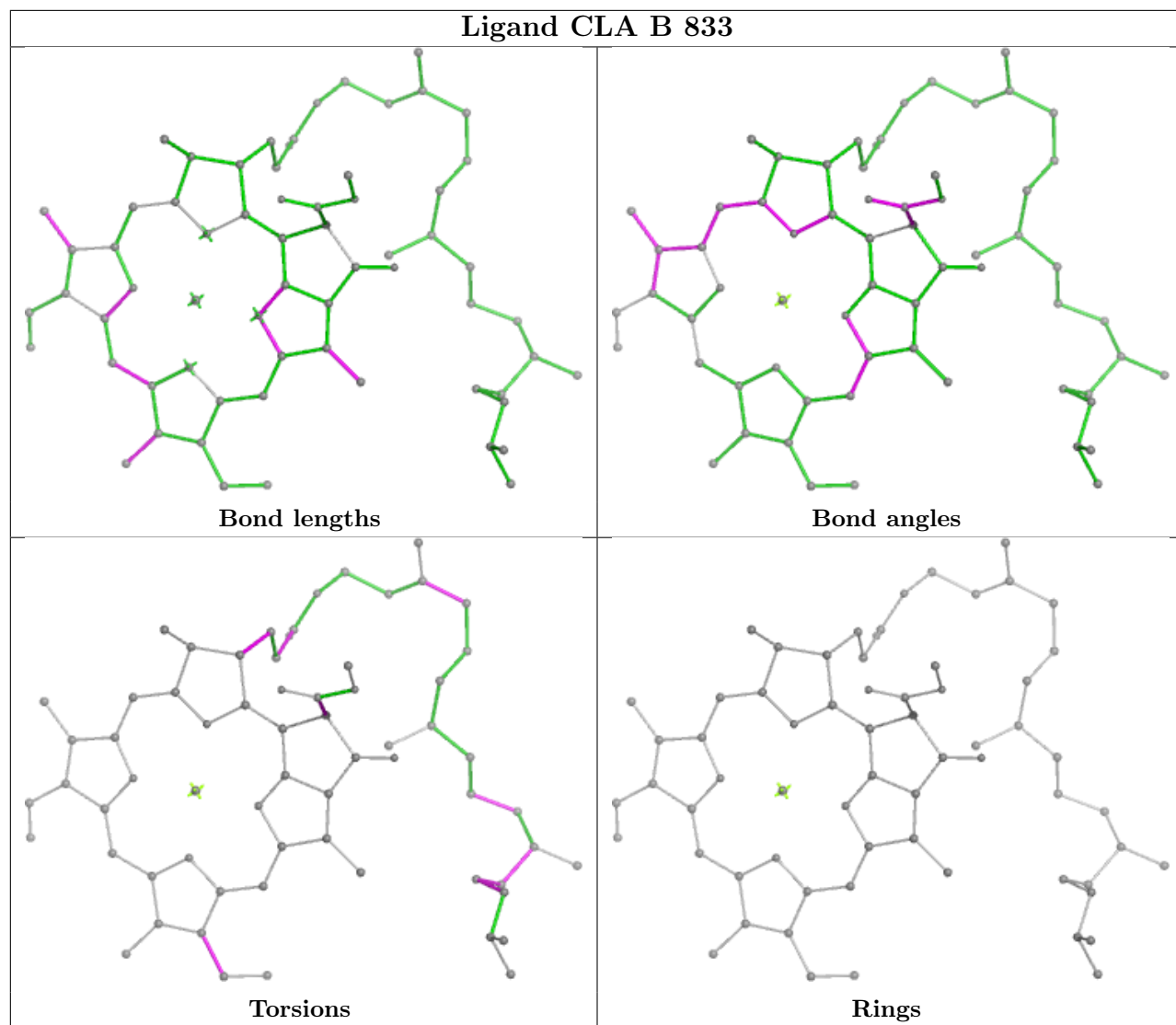


Ligand CLA B 840

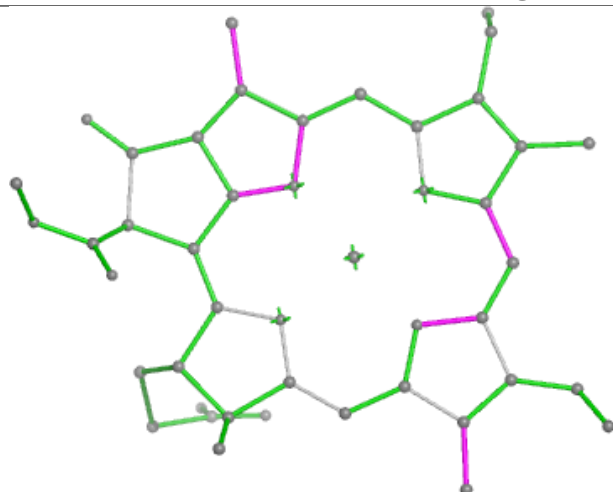




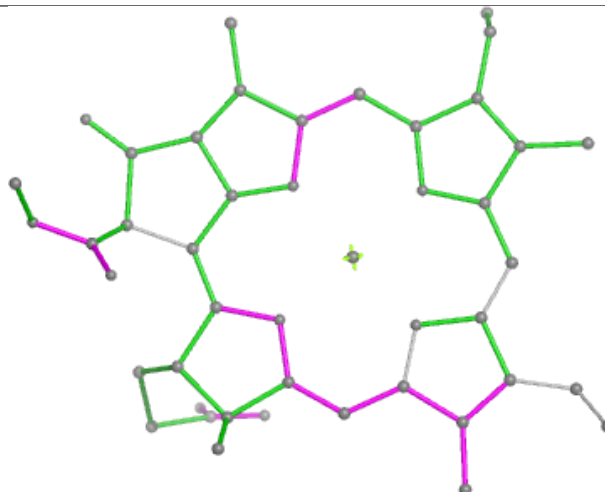
Ligand CLA B 833



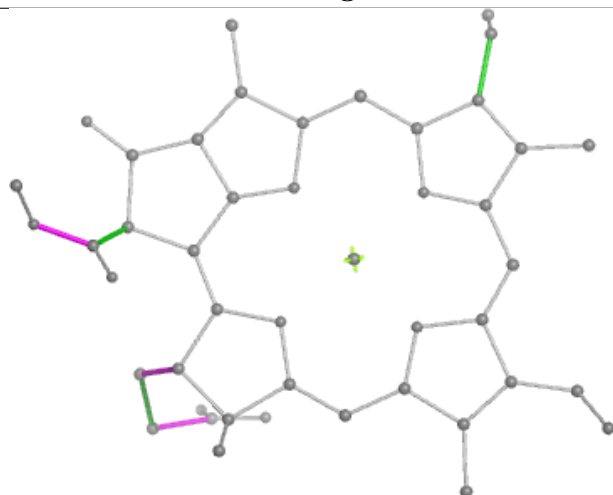
Ligand CLA A 823



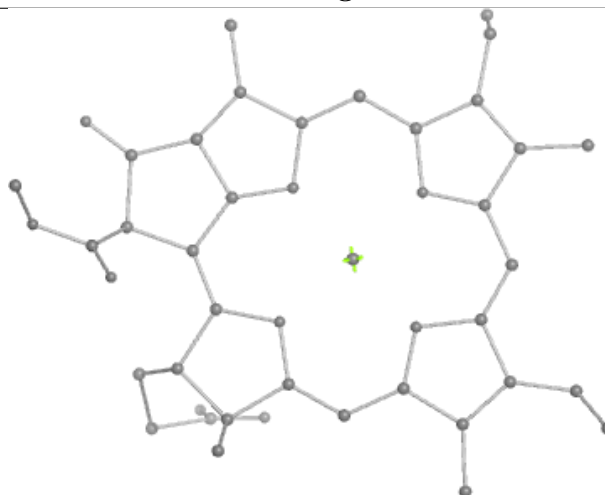
Bond lengths



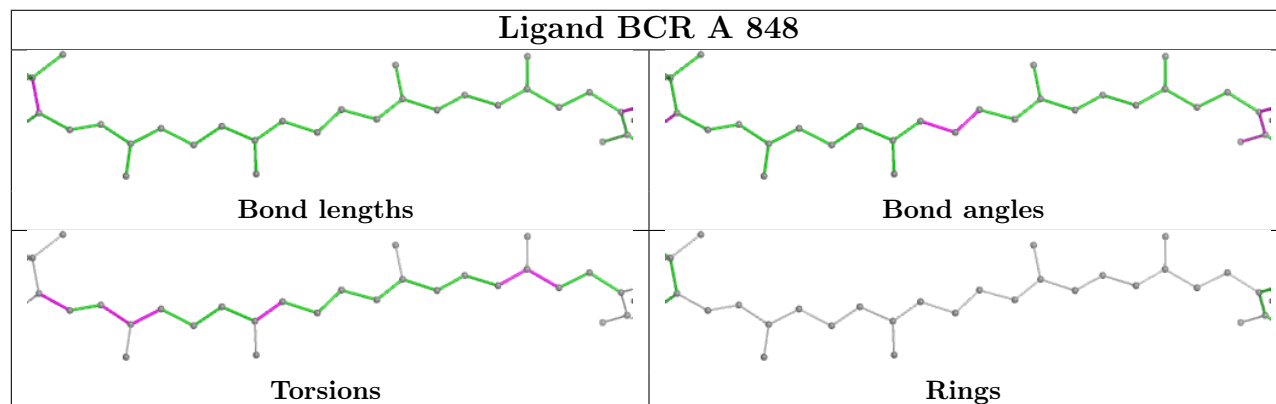
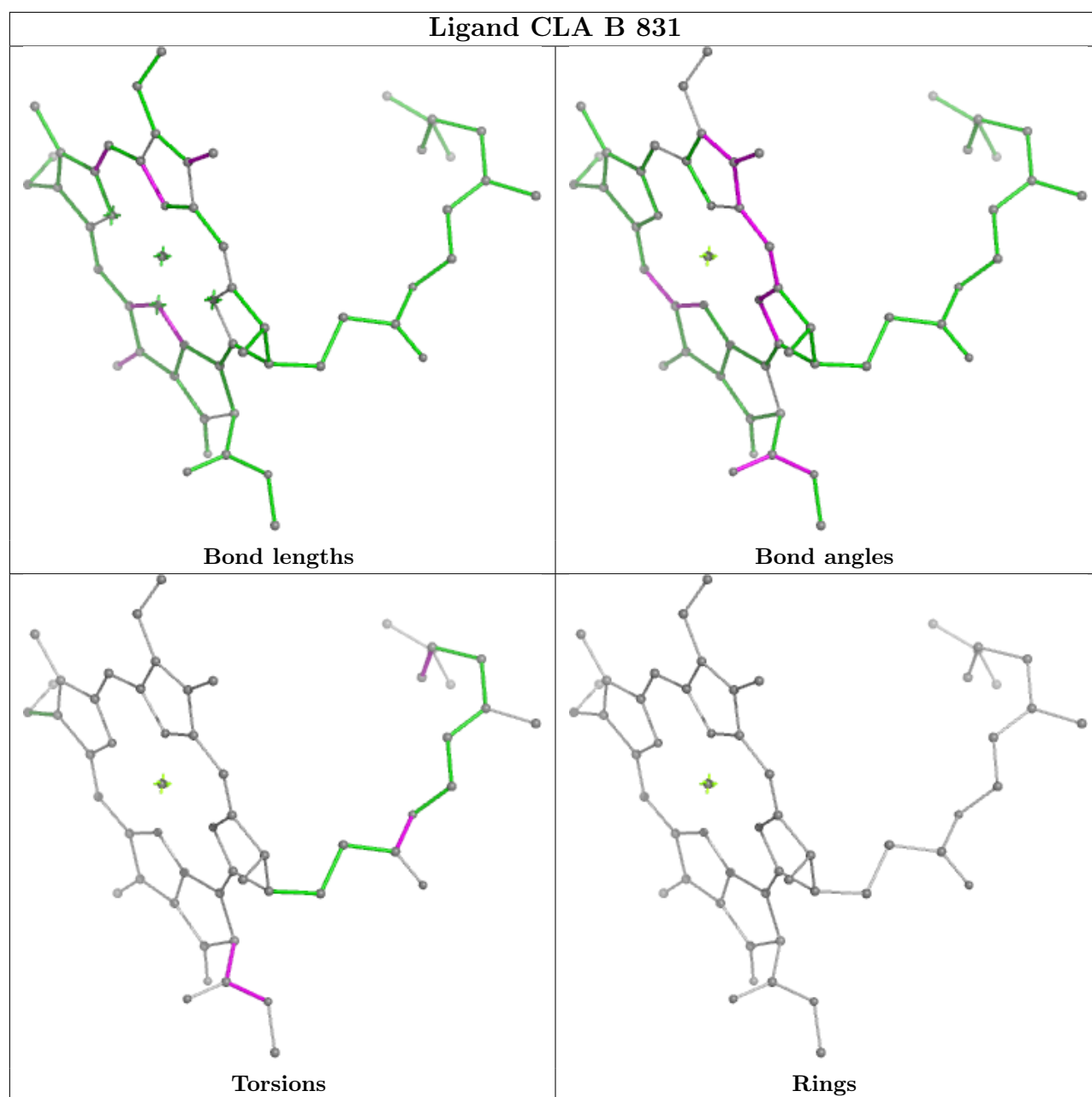
Bond angles



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.

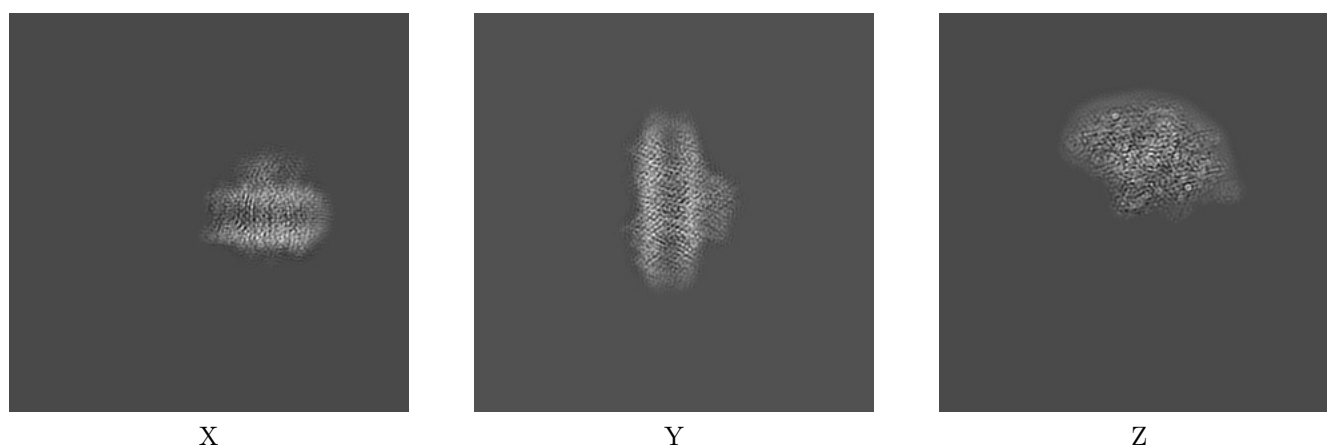
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10557. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

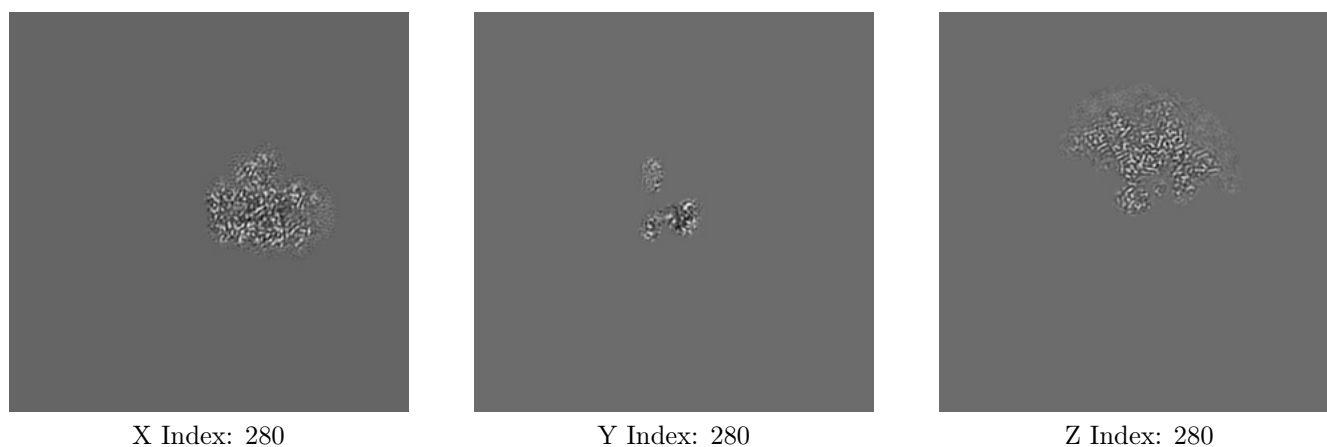
6.1.1 Primary map



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

6.2 Central slices [i](#)

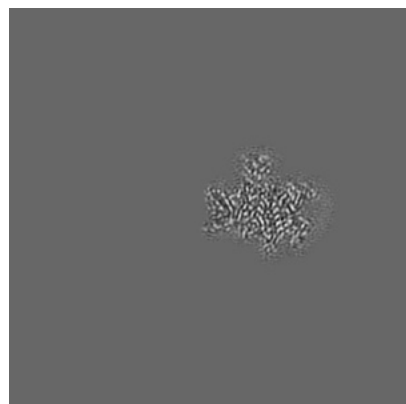
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

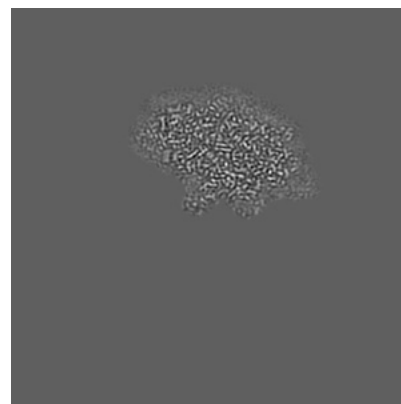
6.3.1 Primary map



X Index: 265



Y Index: 354

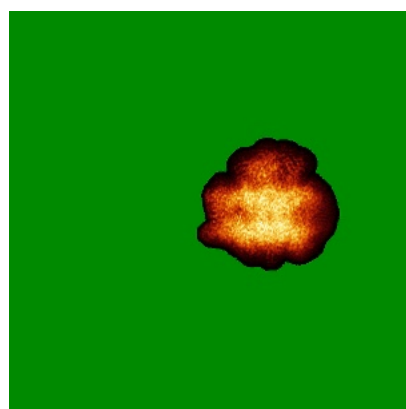


Z Index: 251

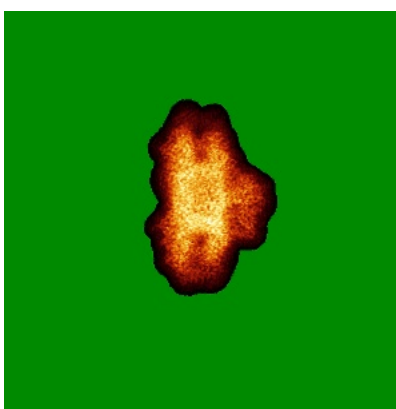
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

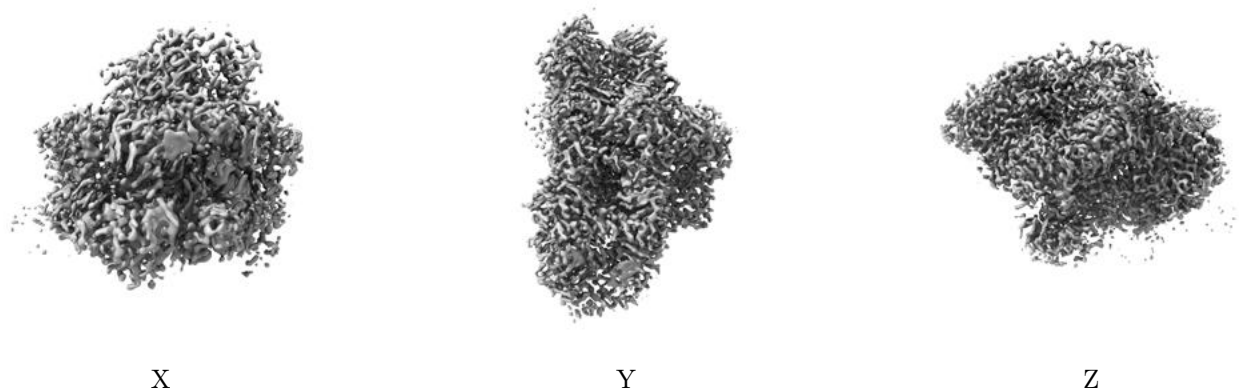


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

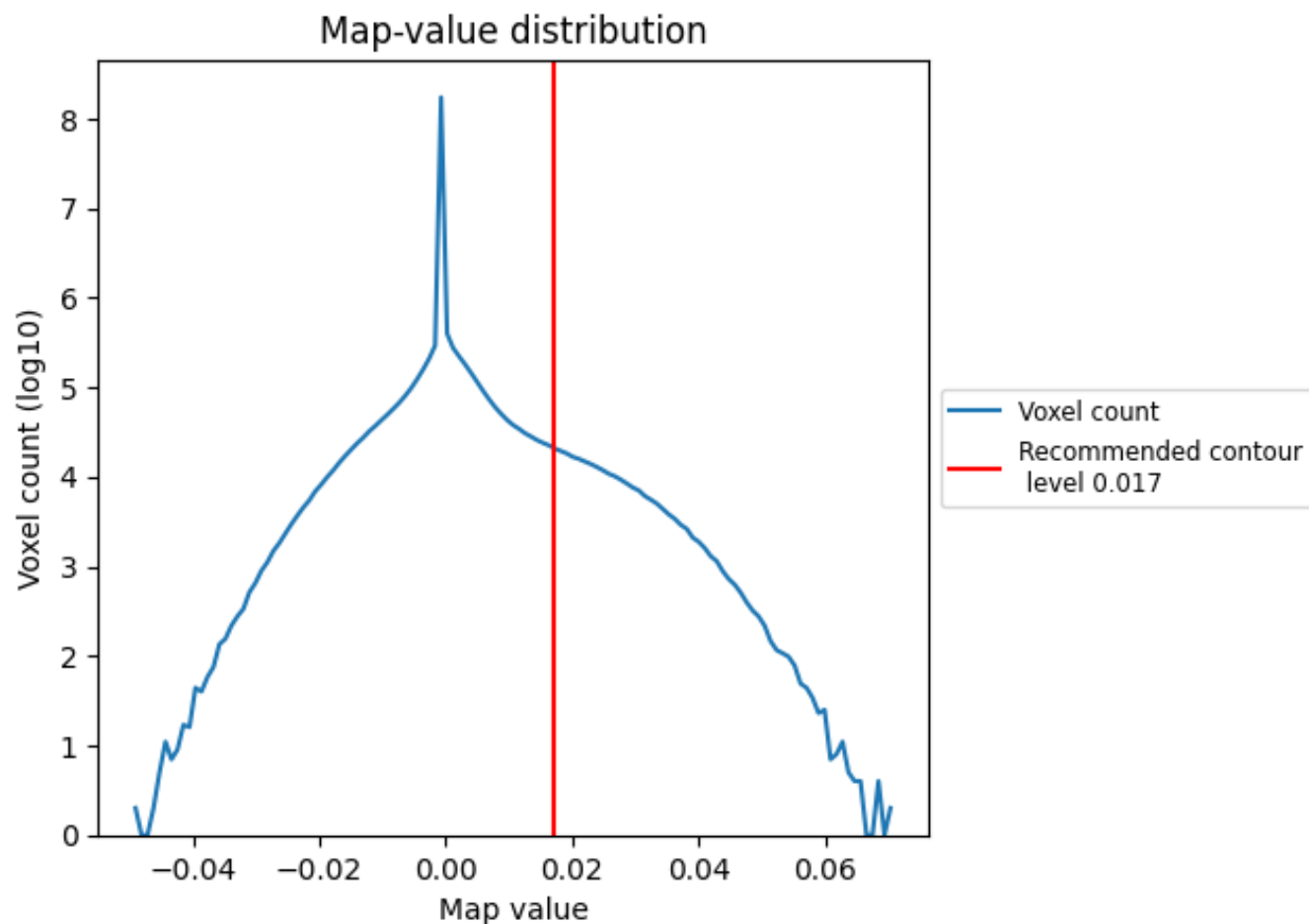
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

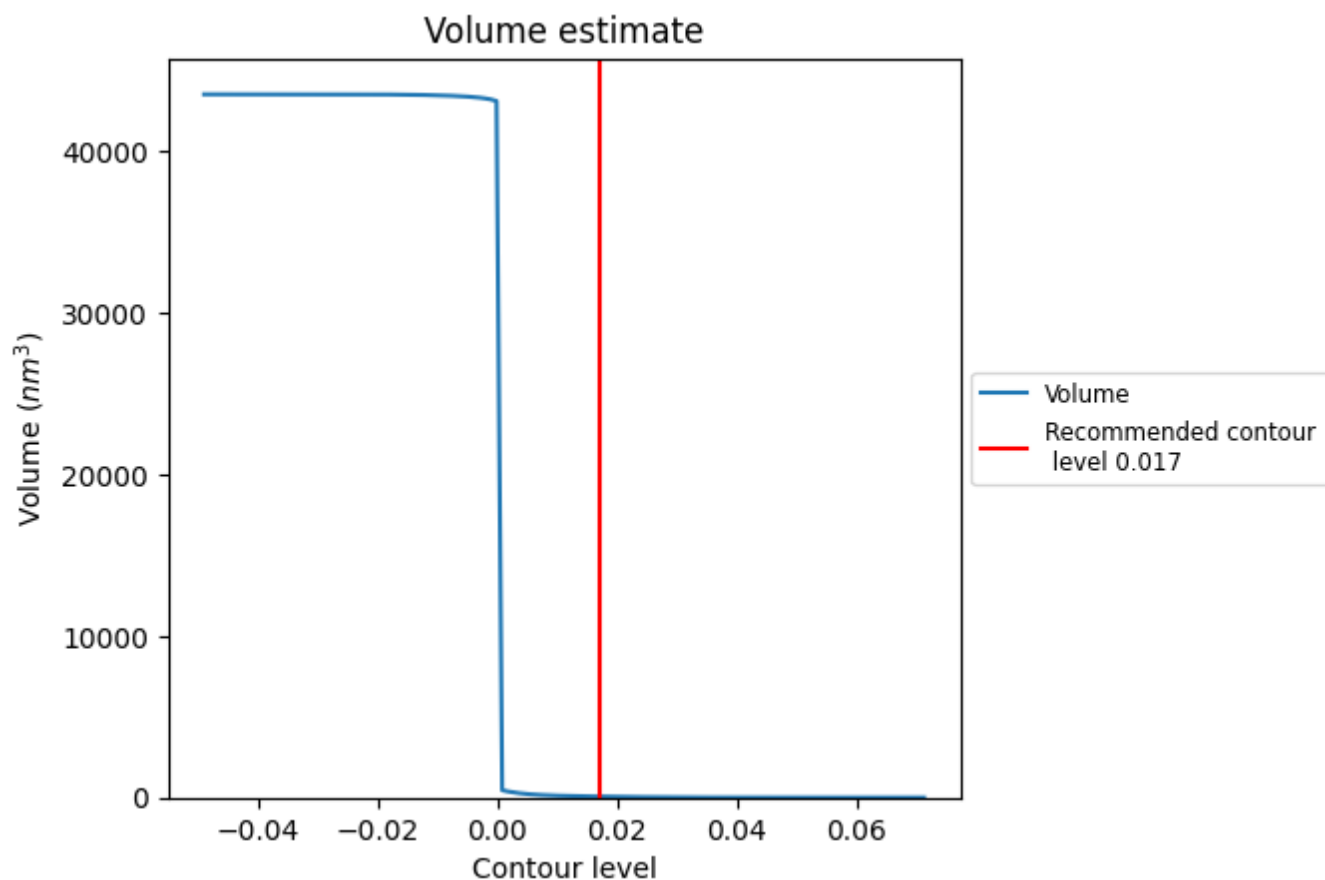
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

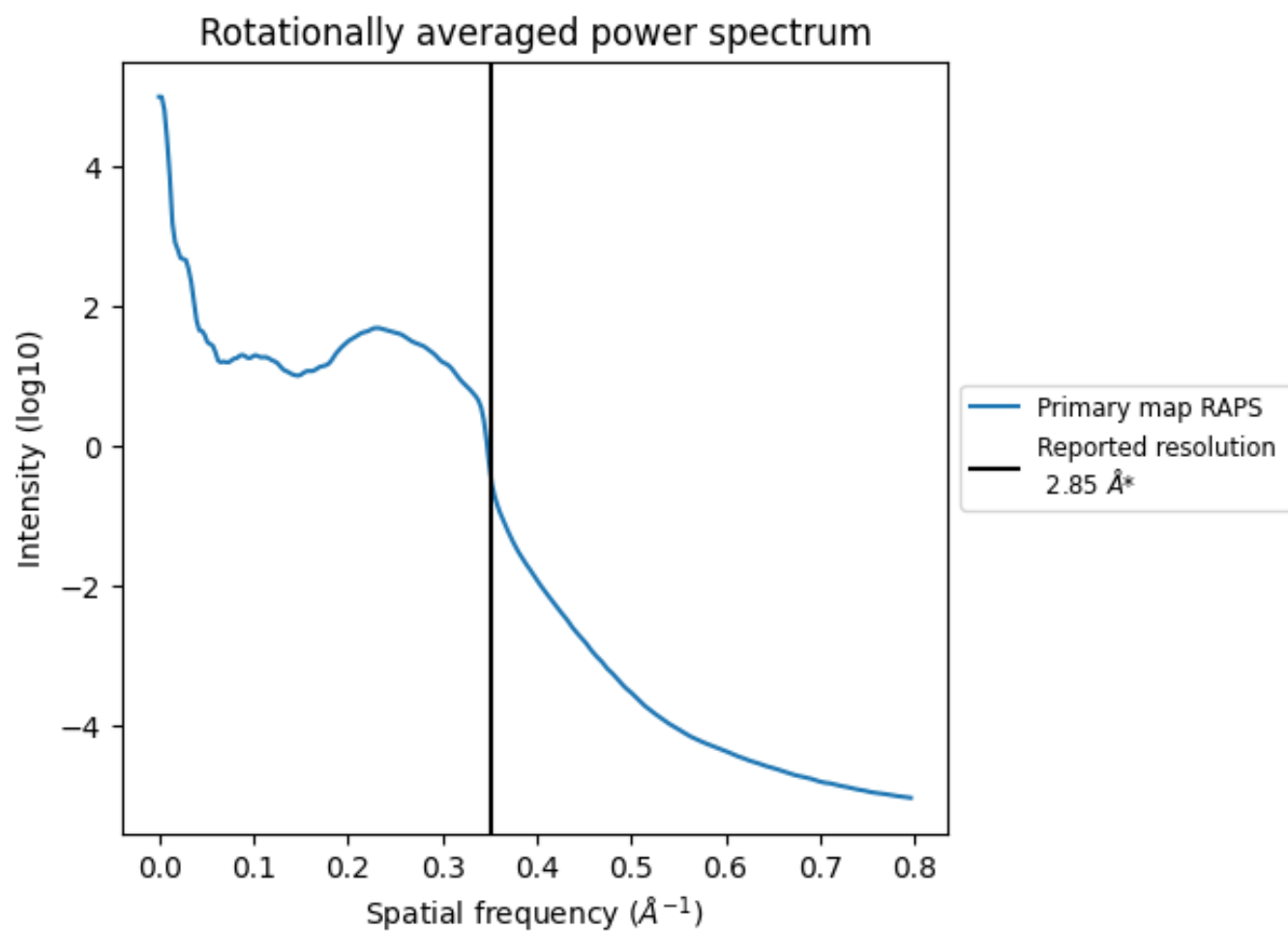
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm³; this corresponds to an approximate mass of 56 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 [i](#)

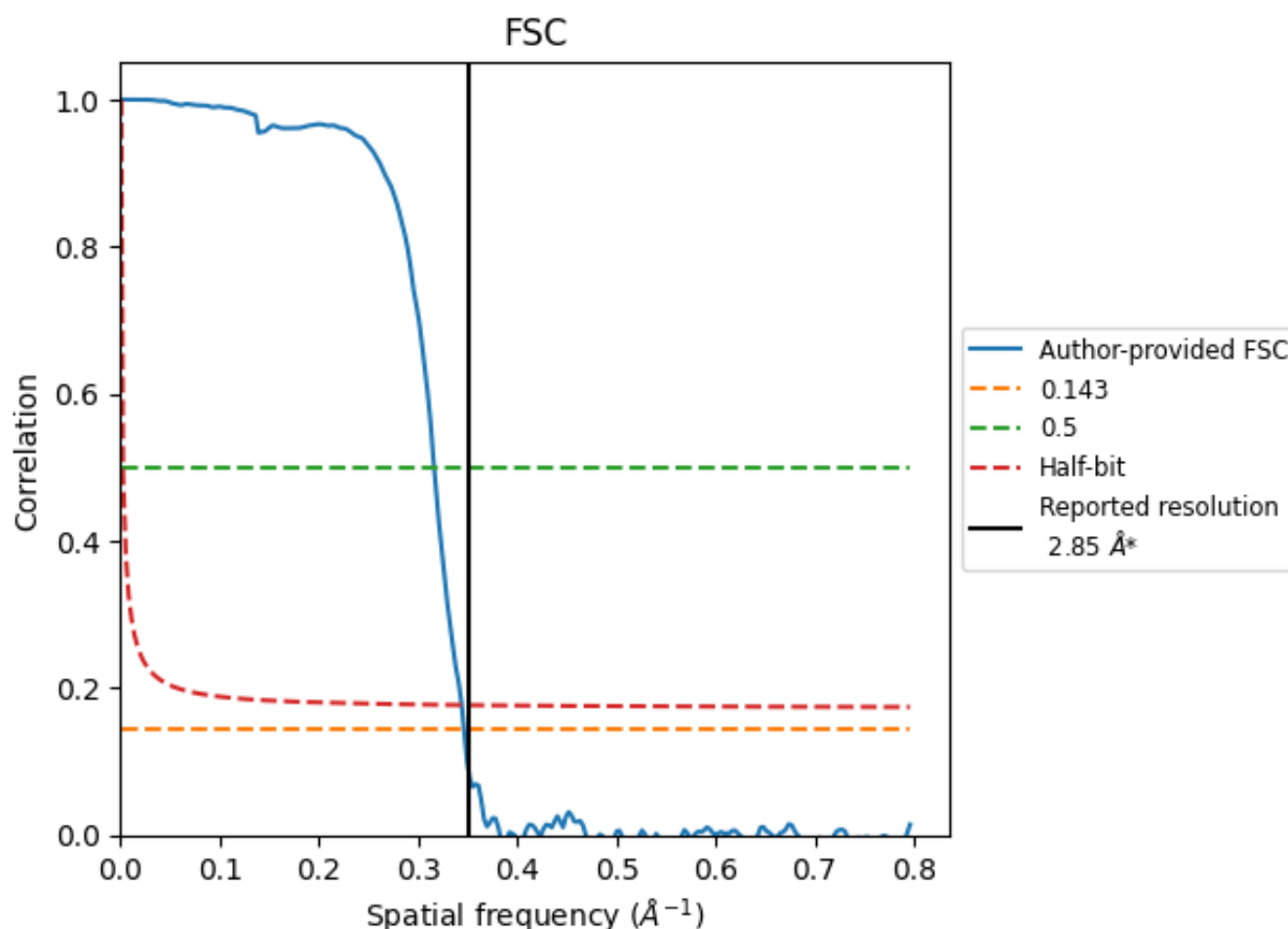


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 Å⁻¹

8.2 Resolution estimates [i](#)

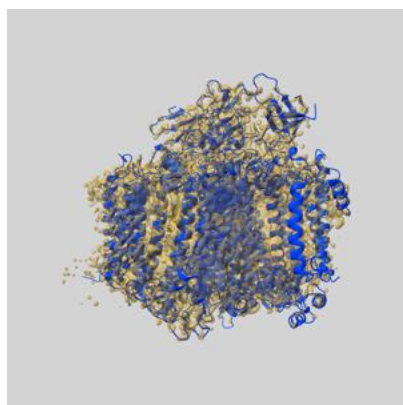
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.89	3.16	2.91
Unmasked-calculated*	-	-	-

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

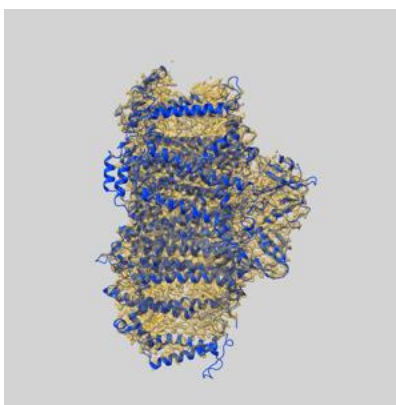
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10557 and PDB model 6TRA. Per-residue inclusion information can be found in section [3](#) on page [19](#).

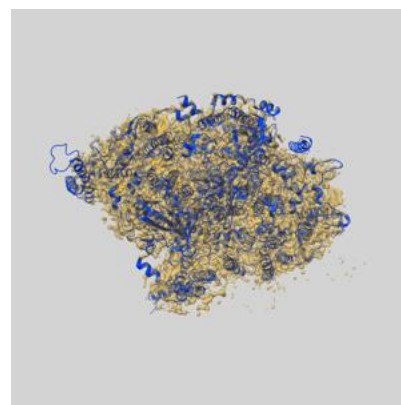
9.1 Map-model overlay [i](#)



X



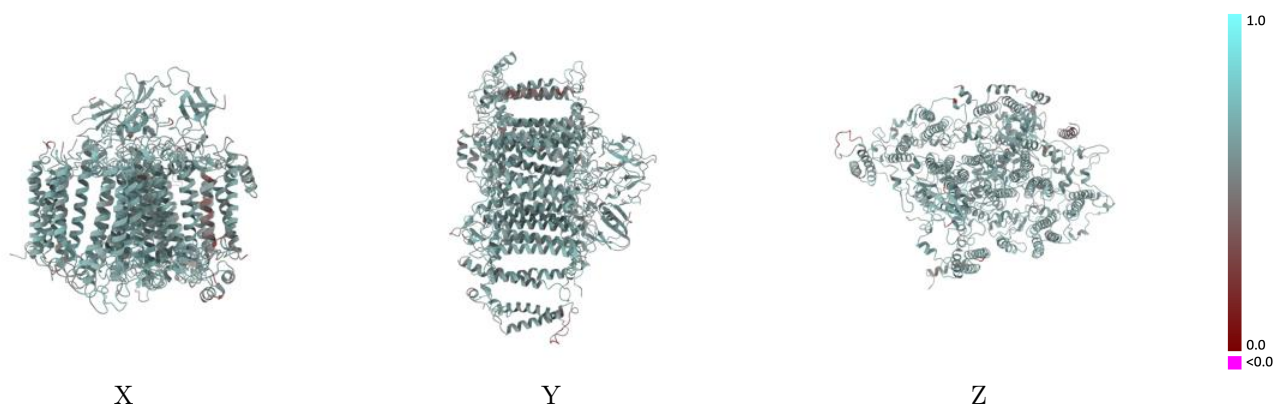
Y



Z

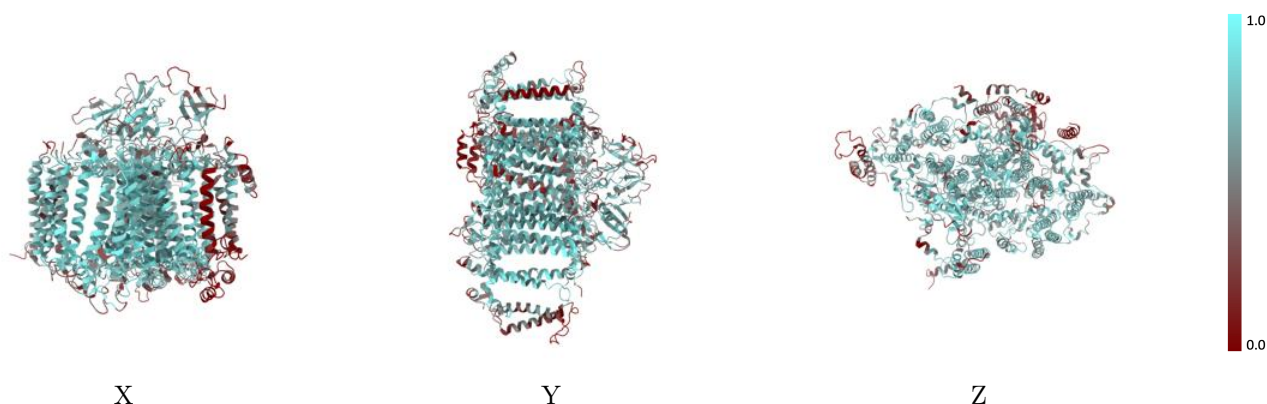
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



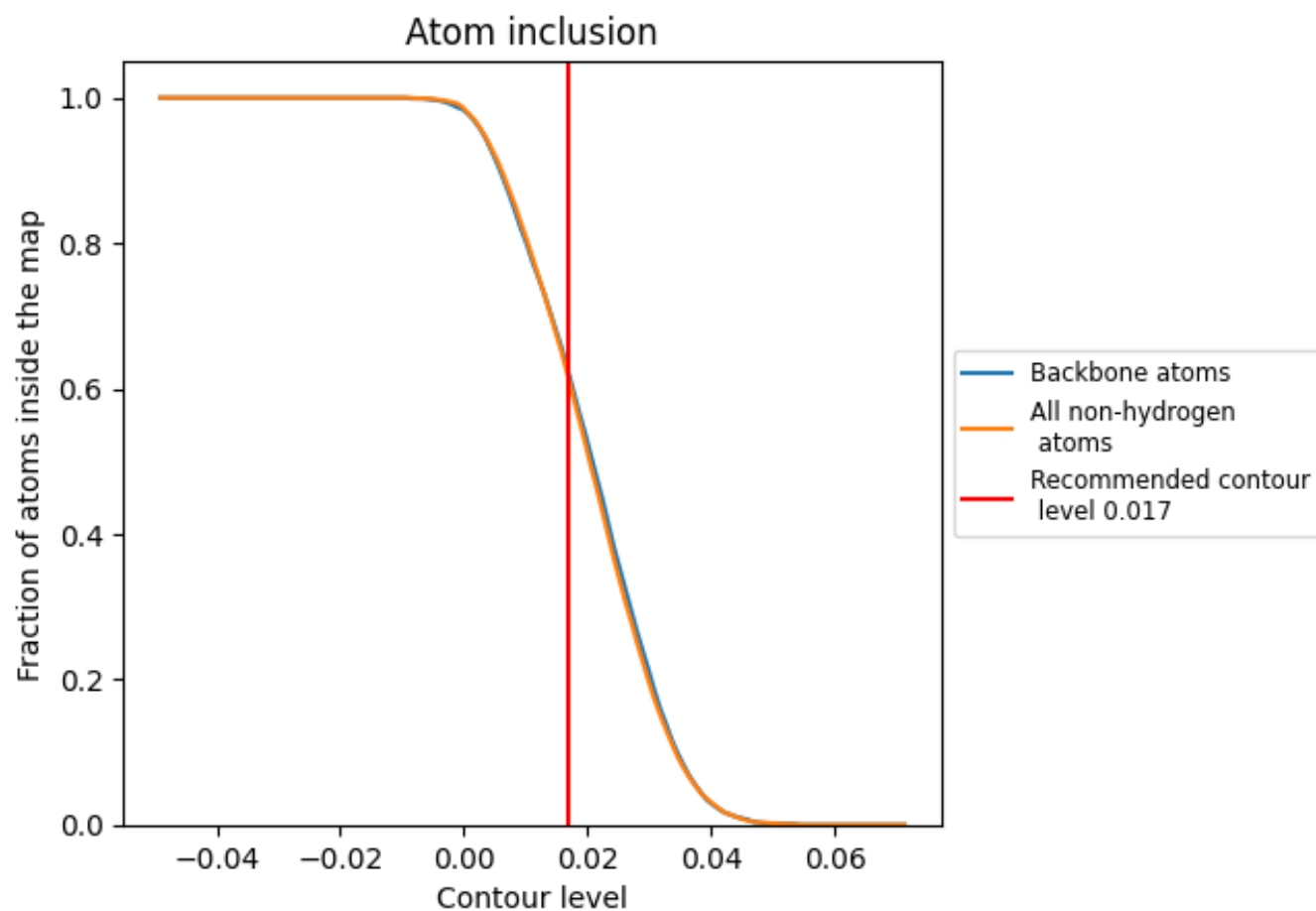
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).

9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 61% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6120	<div></div> 0.5890
A	<div></div> 0.6900	<div></div> 0.6030
B	<div></div> 0.6630	<div></div> 0.5960
C	<div></div> 0.6800	<div></div> 0.5910
D	<div></div> 0.5620	<div></div> 0.5780
E	<div></div> 0.5090	<div></div> 0.5760
F	<div></div> 0.3120	<div></div> 0.5470
I	<div></div> 0.5890	<div></div> 0.5890
J	<div></div> 0.2920	<div></div> 0.5530
K	<div></div> 0.2630	<div></div> 0.5270
L	<div></div> 0.5880	<div></div> 0.5790
M	<div></div> 0.4870	<div></div> 0.5700
X	<div></div> 0.0150	<div></div> 0.4450

