



wwPDB EM Validation Summary Report ⓘ

Sep 20, 2026 – 11:16 pm BST

PDB ID : 9QFP / pdb_00009qfp
EMDB ID : EMD-53120
Title : Monomeric Photosystem I Cryo-EM structure at 1.8 Å resolution
Authors : Gaullier, G.; Boyka, J.; Zouni, A.; Blikstad, C.
Deposited on : 2025-03-12
Resolution : 1.74 Å (reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

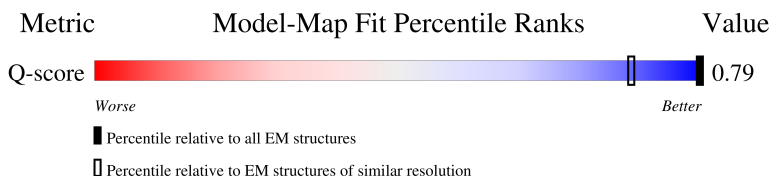
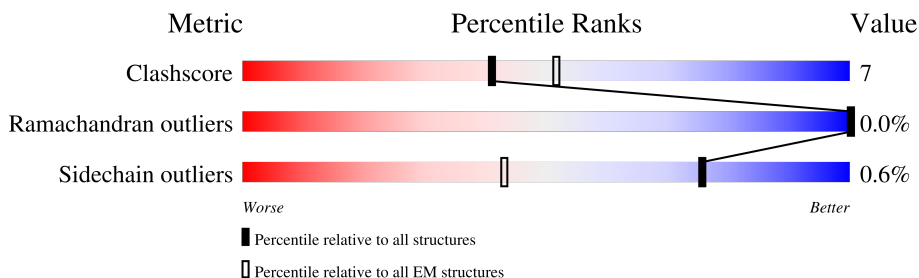
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 1.74 Å.

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



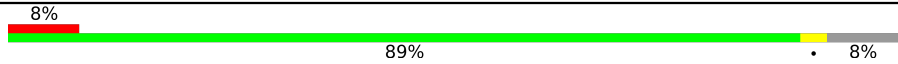
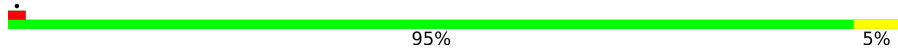
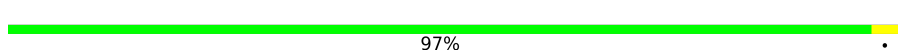
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	645 (1.25 - 2.24)

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	
2	B	741	
3	C	81	
4	D	139	

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Mol	Chain	Length	Quality of chain
5	E	76	
6	F	164	
7	I	38	
8	J	41	
9	K	83	
10	M	31	
11	X	39	

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	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	809	X	-	-	-
13	CLA	A	810	X	-	-	-
13	CLA	A	811	X	-	-	-
13	CLA	A	812	X	-	-	-
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	-
13	CLA	A	816	X	-	-	-
13	CLA	A	817	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	-
13	CLA	A	823	X	-	-	-
13	CLA	A	824	X	-	-	-
13	CLA	A	825	X	-	-	-
13	CLA	A	827	X	-	-	-
13	CLA	A	830	X	-	-	-
13	CLA	A	831	X	-	-	-
13	CLA	A	832	X	-	-	-
13	CLA	A	844	X	-	-	-
13	CLA	A	848	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	849	X	-	-	-
13	CLA	A	851	X	-	-	-
13	CLA	A	854	X	-	-	-
13	CLA	A	856	X	-	-	-
13	CLA	A	858	X	-	-	-
13	CLA	A	859	X	-	-	-
13	CLA	A	860	X	-	-	-
13	CLA	A	861	X	-	-	-
13	CLA	B	813	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	821	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	839	X	-	-	-
13	CLA	B	841	X	-	-	-
13	CLA	B	842	X	-	-	-
13	CLA	B	843	X	-	-	-
13	CLA	F	201	X	-	-	-
13	CLA	F	204	X	-	-	-
13	CLA	J	102	X	-	-	-
13	CLA	K	101	X	-	-	-
13	CLA	K	104	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 25572 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	747	Total	C	N	O	S	0	0
			5835	3828	996	985	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	S	0	0
			547	347	94	105	1		

- 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	37	Total	C	N	O	S	0	0
			293	203	39	47	4		

- 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
			338	231	51	54	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		

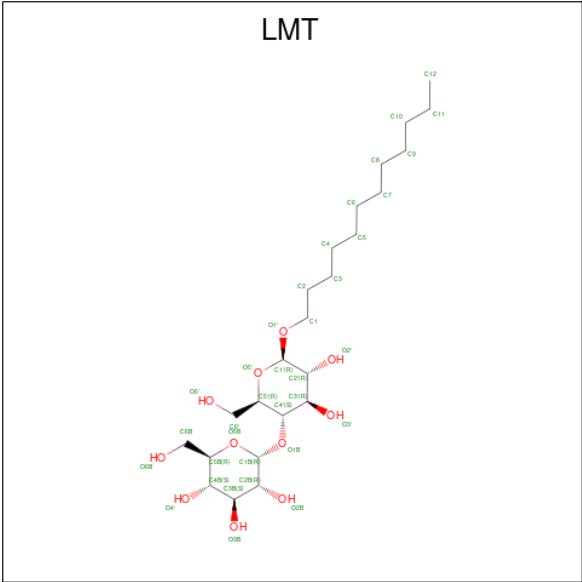
- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 11 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	X	30	Total	C	N	O	0	0
			252	178	37	37		

- Molecule 12 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



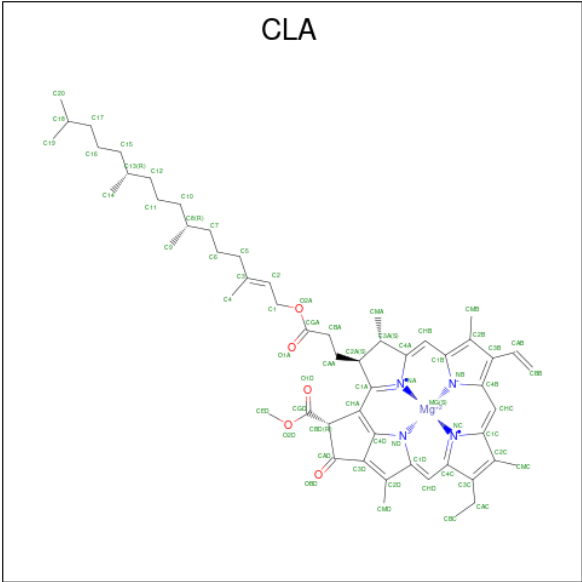
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			35	24	11	
12	A	1	Total	C	O	0
			35	24	11	
12	A	1	Total	C	O	0
			35	24	11	
12	A	1	Total	C	O	0
			35	24	11	
12	A	1	Total	C	O	0
			35	24	11	
12	A	1	Total	C	O	0
			35	24	11	
12	A	1	Total	C	O	0
			35	24	11	
12	B	1	Total	C	O	0
			35	24	11	
12	B	1	Total	C	O	0
			35	24	11	
12	B	1	Total	C	O	0
			35	24	11	
12	B	1	Total	C	O	0
			35	24	11	
12	F	1	Total	C	O	0
			35	24	11	
12	K	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
12	K	1	Total	C	O	0
			35	24	11	
12	X	1	Total	C	O	0
			35	24	11	

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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

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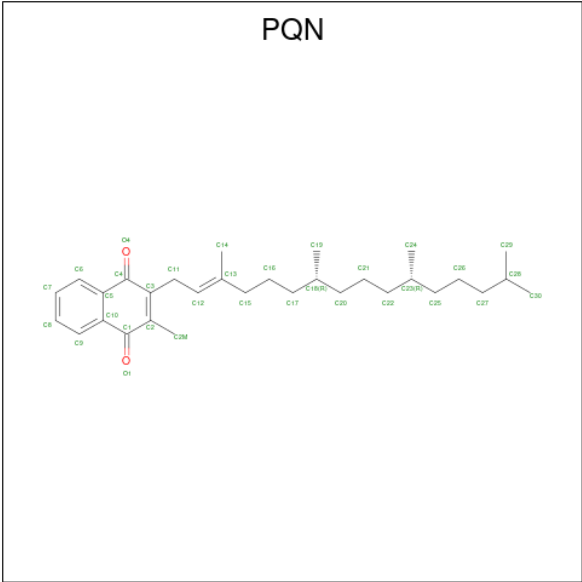
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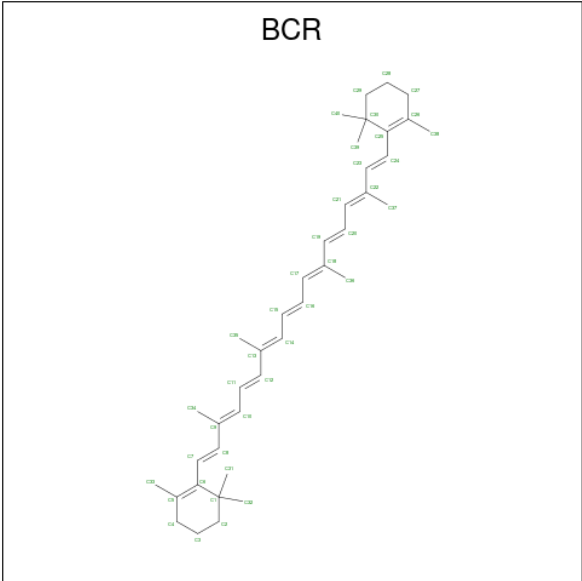
Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	X	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



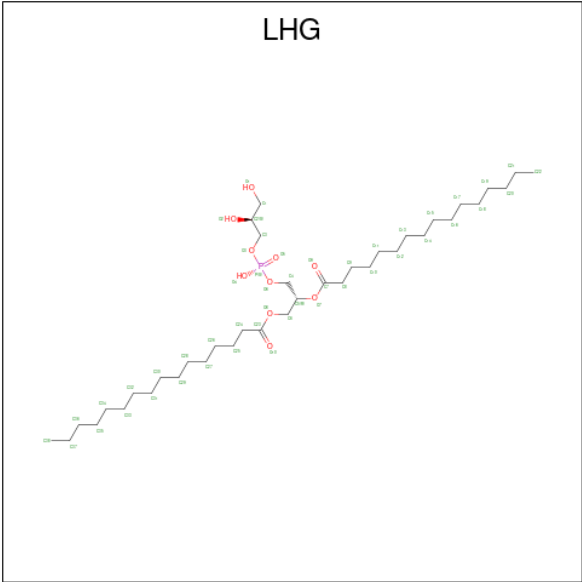
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	

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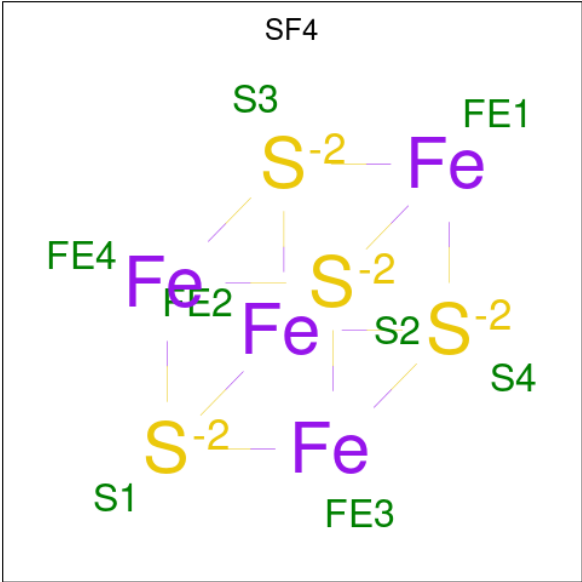
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	K	1	Total C 40 40	0
15	M	1	Total C 40 40	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



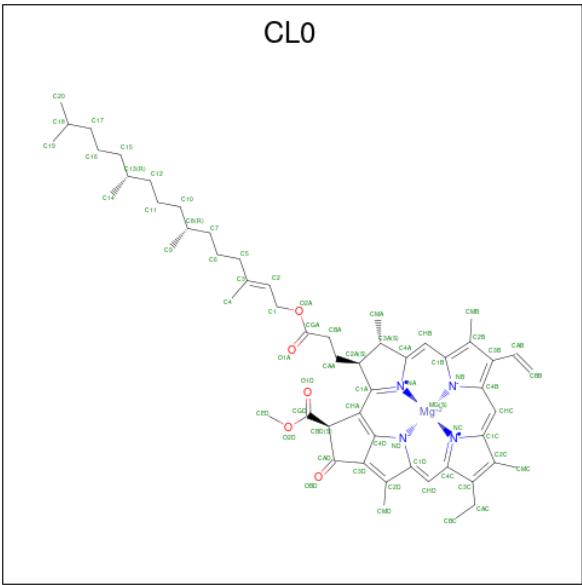
Mol	Chain	Residues	Atoms				AltConf
16	A	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			49	38	10	1	
16	I	1	Total	C	O	P	0
			49	38	10	1	
16	X	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



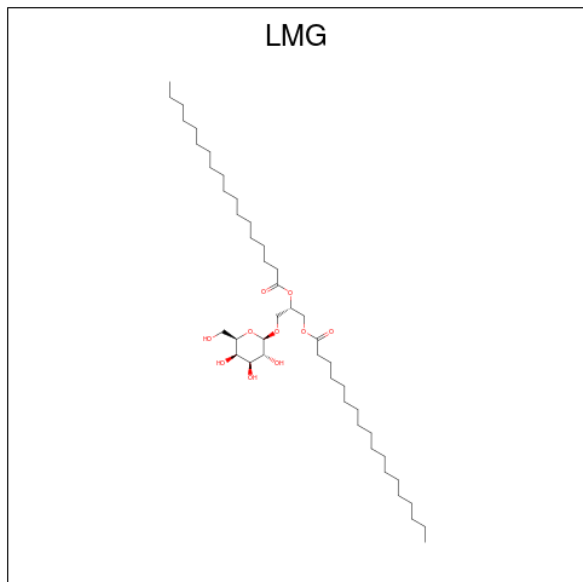
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).

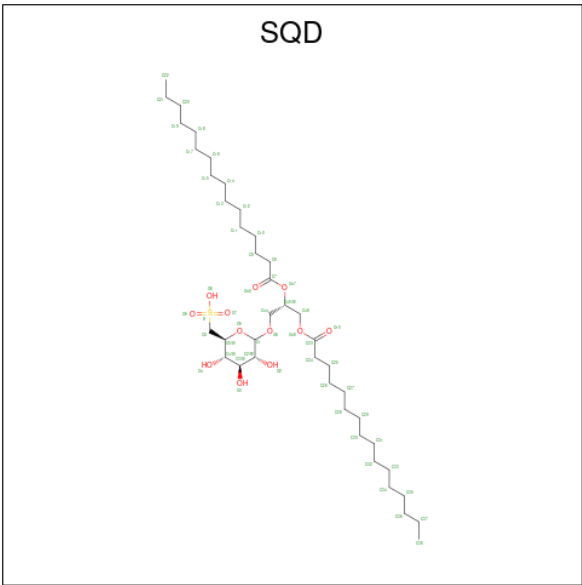


Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			55	45	10	

- Molecule 20 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
20	B	1	Total	Mg	0
			1	1	

- Molecule 21 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
21	X	1	Total	C	O	S	0
			54	41	12	1	

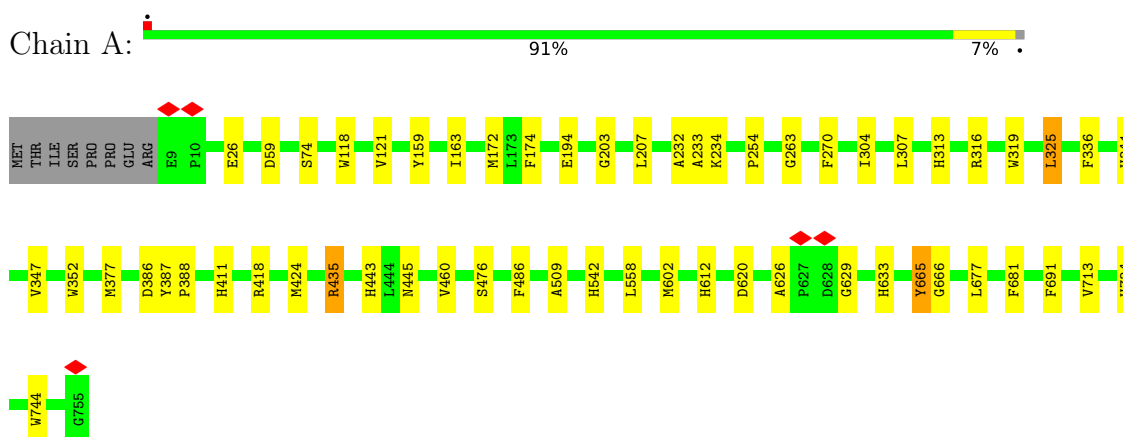
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	A	348	Total	O	0
			348	348	
22	B	442	Total	O	0
			442	442	
22	C	96	Total	O	0
			96	96	
22	D	107	Total	O	0
			107	107	
22	E	68	Total	O	0
			68	68	
22	F	74	Total	O	0
			74	74	
22	I	5	Total	O	0
			5	5	
22	J	12	Total	O	0
			12	12	
22	K	12	Total	O	0
			12	12	
22	M	13	Total	O	0
			13	13	
22	X	6	Total	O	0
			6	6	

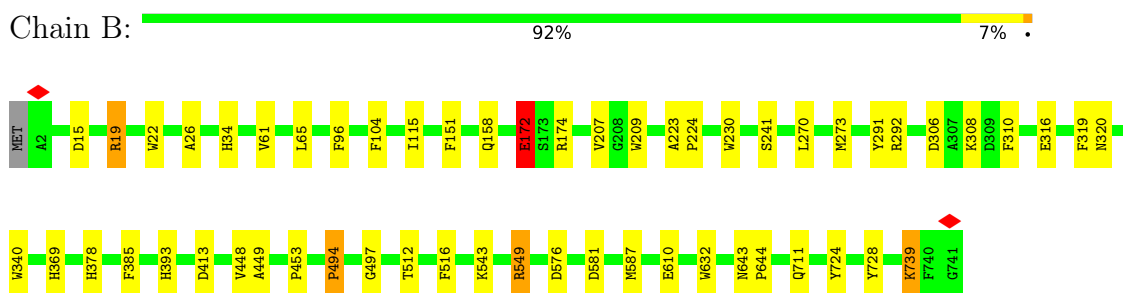
3 Residue-property plots

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.

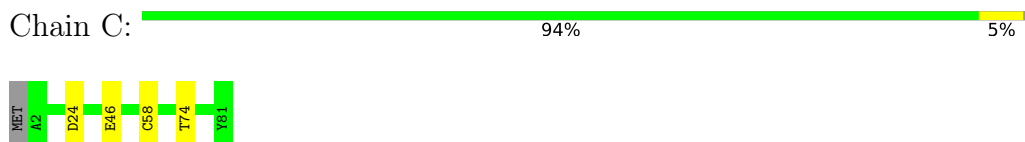
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

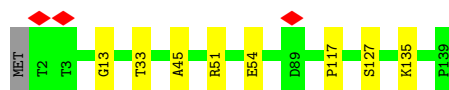


- Molecule 3: Photosystem I iron-sulfur center

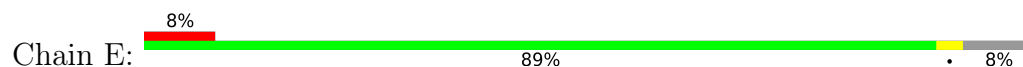


- Molecule 4: Photosystem I reaction center subunit II

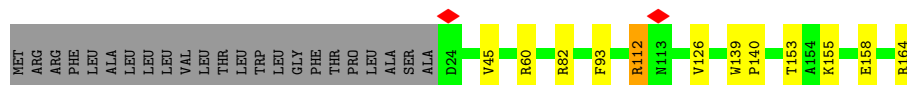
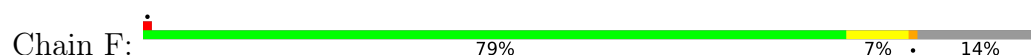




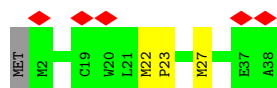
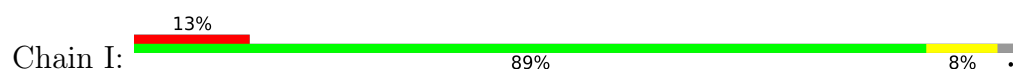
- Molecule 5: Photosystem I reaction center subunit IV



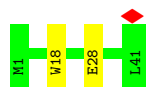
- Molecule 6: Photosystem I reaction center subunit III



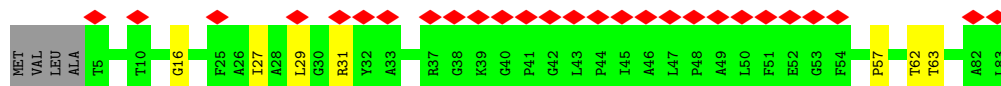
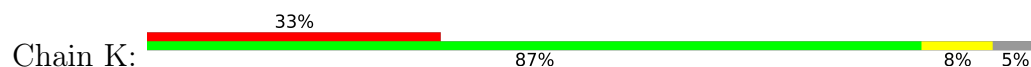
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



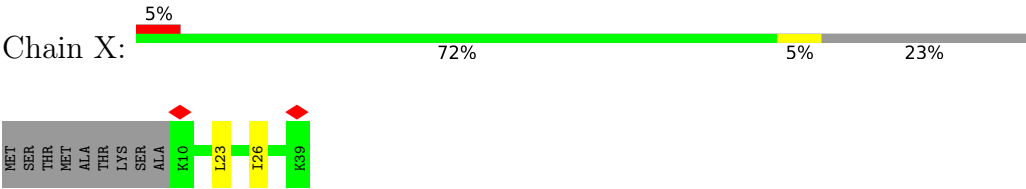
- Molecule 9: Photosystem I reaction center subunit PsaK



- Molecule 10: Photosystem I reaction center subunit XII



- Molecule 11: 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	712866	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Patch CTF estimation job in CryoSPARC, run with default settings.	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.468	Depositor
Minimum map value	-0.511	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.08	Depositor
Map size ($\text{\AA}$)	331.776, 331.776, 331.776	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.648, 0.648, 0.648	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SQD, LMG, SF4, BCR, LHG, CL0, CLA, MG, PQN, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.92	5/6036 (0.1%)	1.13	12/8233 (0.1%)
2	B	0.89	1/6112 (0.0%)	1.12	15/8350 (0.2%)
3	C	0.81	0/608	1.12	1/824 (0.1%)
4	D	0.69	1/1101 (0.1%)	1.11	2/1492 (0.1%)
5	E	0.63	0/559	1.10	1/760 (0.1%)
6	F	0.66	0/1087	1.08	5/1476 (0.3%)
7	I	0.58	0/304	0.85	0/415
8	J	0.58	0/350	1.02	0/477
9	K	0.53	0/585	0.97	0/800
10	M	0.70	0/244	1.05	1/332 (0.3%)
11	X	0.63	0/261	1.00	0/354
All	All	0.84	7/17247 (0.0%)	1.11	37/23513 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	2
4	D	0	1
6	F	0	1
All	All	0	5

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	341	HIS	CE1-NE2	-6.71	1.25	1.32
4	D	117	PRO	CA-CB	6.65	1.58	1.53
1	A	666	GLY	N-CA	5.58	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	ILE	CB-CG1	-5.22	1.43	1.53
2	B	378	HIS	CE1-NE2	5.18	1.37	1.32

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	665	TYR	O-C-N	-10.84	110.82	122.09
4	D	135	LYS	CB-CA-C	10.19	124.22	108.84
1	A	665	TYR	CA-C-N	-9.29	103.21	121.41
1	A	665	TYR	C-N-CA	-9.29	103.21	121.41
1	A	435	ARG	NE-CZ-NH1	-7.83	113.67	121.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	316	ARG	Sidechain
2	B	19	ARG	Sidechain
2	B	292	ARG	Sidechain
4	D	51	ARG	Sidechain
6	F	164	ARG	Sidechain

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	5835	0	5697	52	0
2	B	5894	0	5649	48	0
3	C	598	0	577	3	0
4	D	1075	0	1074	2	0
5	E	547	0	537	0	0
6	F	1065	0	1074	5	0
7	I	293	0	294	4	0
8	J	338	0	347	2	0
9	K	571	0	593	5	0
10	M	241	0	264	0	0
11	X	252	0	260	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	280	0	368	7	0
12	B	140	0	184	2	0
12	F	35	0	46	0	0
12	K	70	0	92	0	0
12	X	35	0	46	0	0
13	A	2860	0	3129	130	0
13	B	2535	0	2775	82	0
13	F	130	0	142	6	0
13	J	130	0	143	4	0
13	K	130	0	144	11	0
13	X	65	0	72	1	0
14	A	33	0	46	0	0
14	B	33	0	46	0	0
15	A	240	0	336	30	0
15	B	240	0	334	22	0
15	F	120	0	168	10	0
15	J	80	0	112	8	0
15	K	40	0	56	7	0
15	M	40	0	56	1	0
16	A	147	0	222	1	0
16	I	49	0	74	0	0
16	X	49	0	74	2	0
17	A	8	0	0	0	0
17	C	16	0	0	1	0
18	A	65	0	72	0	0
19	B	55	0	86	0	0
20	B	1	0	0	0	0
21	X	54	0	78	0	0
22	A	348	0	0	2	0
22	B	442	0	0	16	0
22	C	96	0	0	1	0
22	D	107	0	0	0	0
22	E	68	0	0	0	0
22	F	74	0	0	1	0
22	I	5	0	0	0	0
22	J	12	0	0	0	0
22	K	12	0	0	0	0
22	M	13	0	0	0	0
22	X	6	0	0	0	0
All	All	25572	0	25267	340	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 7.

The worst 5 of 340 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)
13:A:826:CLA:C1	13:A:826:CLA:O2A	1.72	1.36
13:A:826:CLA:C1	13:A:826:CLA:O1A	1.85	1.24
13:A:826:CLA:C1	13:A:826:CLA:CGA	2.25	1.14
1:A:633:HIS:ND1	22:A:901:HOH:O	1.86	1.04
2:B:448:VAL:HG13	22:B:1286:HOH:O	1.58	1.04

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	745/755 (99%)	727 (98%)	18 (2%)	0	100	100
2	B	738/741 (100%)	725 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	78 (100%)	0	0	100	100
4	D	136/139 (98%)	131 (96%)	4 (3%)	1 (1%)	18	6
5	E	68/76 (90%)	65 (96%)	3 (4%)	0	100	100
6	F	139/164 (85%)	137 (99%)	2 (1%)	0	100	100
7	I	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
8	J	39/41 (95%)	38 (97%)	1 (3%)	0	100	100
9	K	77/83 (93%)	76 (99%)	1 (1%)	0	100	100
10	M	29/31 (94%)	29 (100%)	0	0	100	100
11	X	28/39 (72%)	28 (100%)	0	0	100	100
All	All	2112/2188 (96%)	2068 (98%)	43 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	45	ALA

5.3.2 Protein sidechains [i](#)

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	595/603 (99%)	592 (100%)	3 (0%)	81	75
2	B	597/598 (100%)	594 (100%)	3 (0%)	81	75
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/116 (99%)	114 (99%)	1 (1%)	70	59
5	E	60/65 (92%)	59 (98%)	1 (2%)	53	32
6	F	109/128 (85%)	108 (99%)	1 (1%)	70	59
7	I	31/32 (97%)	31 (100%)	0	100	100
8	J	36/36 (100%)	36 (100%)	0	100	100
9	K	58/61 (95%)	57 (98%)	1 (2%)	53	32
10	M	26/26 (100%)	26 (100%)	0	100	100
11	X	24/31 (77%)	24 (100%)	0	100	100
All	All	1718/1764 (97%)	1708 (99%)	10 (1%)	76	71

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	30	THR
6	F	82	ARG
9	K	31	ARG
2	B	172	GLU
2	B	319	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	79	ASN

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Mol	Chain	Res	Type
6	F	118	ASN
9	K	23	ASN
5	E	60	ASN
2	B	320	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 139 ligands modelled in this entry, 1 is monoatomic - leaving 138 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	$\# Z > 2$
15	BCR	B	825	-	41,41,41	1.61	7 (17%)	56,56,56	1.56	12 (21%)
13	CLA	A	860	1	69,73,73	1.66	15 (21%)	83,113,113	3.13	35 (42%)
16	LHG	A	852	-	48,48,48	0.75	1 (2%)	51,54,54	0.60	1 (1%)
13	CLA	B	829	2	69,73,73	1.94	15 (21%)	83,113,113	3.02	33 (39%)
13	CLA	A	810	1	69,73,73	1.79	17 (24%)	83,113,113	2.68	27 (32%)
16	LHG	A	843	13	48,48,48	0.51	0	51,54,54	1.03	4 (7%)
17	SF4	C	1001	3	0,12,12	-	-	-		
15	BCR	A	842	-	41,41,41	1.76	8 (19%)	56,56,56	1.45	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	F	202	-	41,41,41	1.44	5 (12%)	56,56,56	1.57	8 (14%)
13	CLA	B	808	2	69,73,73	1.56	15 (21%)	83,113,113	2.06	27 (32%)
13	CLA	A	805	1	69,73,73	1.73	18 (26%)	83,113,113	2.68	23 (27%)
13	CLA	B	806	2	69,73,73	1.67	12 (17%)	83,113,113	2.00	24 (28%)
12	LMT	B	827	-	36,36,36	0.36	0	47,47,47	0.57	0
13	CLA	A	816	1	69,73,73	1.84	15 (21%)	83,113,113	2.75	30 (36%)
18	CL0	A	847	1	69,73,73	1.53	11 (15%)	83,113,113	2.33	28 (33%)
12	LMT	B	852	-	36,36,36	0.34	0	47,47,47	0.75	2 (4%)
13	CLA	A	826	1	69,73,73	2.21	20 (28%)	83,113,113	3.18	32 (38%)
12	LMT	F	205	-	36,36,36	0.28	0	47,47,47	0.54	0
13	CLA	A	807	1	69,73,73	1.77	13 (18%)	83,113,113	2.85	30 (36%)
13	CLA	A	848	1	69,73,73	1.78	18 (26%)	83,113,113	3.51	38 (45%)
13	CLA	F	204	22	69,73,73	1.73	15 (21%)	83,113,113	3.30	28 (33%)
13	CLA	A	854	1,13	69,73,73	1.66	16 (23%)	83,113,113	2.61	21 (25%)
13	CLA	B	837	2	69,73,73	1.72	18 (26%)	83,113,113	2.73	23 (27%)
13	CLA	K	104	22	69,73,73	1.98	17 (24%)	83,113,113	3.00	24 (28%)
12	LMT	B	851	-	36,36,36	0.27	0	47,47,47	0.68	1 (2%)
15	BCR	M	101	-	41,41,41	1.66	8 (19%)	56,56,56	1.44	9 (16%)
12	LMT	A	802	-	36,36,36	0.20	0	47,47,47	0.41	0
13	CLA	A	811	1	69,73,73	1.79	14 (20%)	83,113,113	2.88	34 (40%)
13	CLA	A	832	1	69,73,73	1.61	14 (20%)	83,113,113	2.65	28 (33%)
13	CLA	A	859	1	69,73,73	1.94	16 (23%)	83,113,113	2.98	27 (32%)
13	CLA	A	820	1	69,73,73	1.76	18 (26%)	83,113,113	2.41	27 (32%)
13	CLA	B	805	2	69,73,73	1.46	13 (18%)	83,113,113	2.61	28 (33%)
21	SQD	X	101	-	53,54,54	0.54	1 (1%)	62,65,65	1.52	7 (11%)
13	CLA	B	814	2	69,73,73	1.67	13 (18%)	83,113,113	2.41	24 (28%)
12	LMT	K	102	-	36,36,36	0.28	0	47,47,47	0.51	1 (2%)
13	CLA	A	861	1	69,73,73	1.61	12 (17%)	83,113,113	2.70	29 (34%)
15	BCR	A	862	-	41,41,41	1.66	12 (29%)	56,56,56	1.55	8 (14%)
13	CLA	B	848	22	69,73,73	1.51	11 (15%)	83,113,113	2.04	21 (25%)
15	BCR	B	802	-	41,41,41	2.25	11 (26%)	56,56,56	2.84	15 (26%)
14	PQN	B	823	-	34,34,34	0.69	1 (2%)	42,45,45	0.60	0
13	CLA	A	856	1	69,73,73	1.64	10 (14%)	83,113,113	2.78	29 (34%)
15	BCR	A	838	-	41,41,41	1.57	7 (17%)	56,56,56	1.53	14 (25%)
13	CLA	A	822	22	69,73,73	1.91	14 (20%)	83,113,113	2.57	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	820	2	69,73,73	1.50	15 (21%)	83,113,113	2.83	30 (36%)
15	BCR	B	803	-	41,41,41	1.63	7 (17%)	56,56,56	1.45	9 (16%)
13	CLA	A	812	1	69,73,73	1.84	15 (21%)	83,113,113	2.63	29 (34%)
13	CLA	A	850	-	69,73,73	1.61	14 (20%)	83,113,113	2.62	31 (37%)
13	CLA	B	836	2	69,73,73	1.61	13 (18%)	83,113,113	2.62	24 (28%)
15	BCR	A	840	-	41,41,41	1.71	8 (19%)	56,56,56	1.36	9 (16%)
15	BCR	B	822	-	41,41,41	1.57	7 (17%)	56,56,56	1.24	5 (8%)
13	CLA	B	834	2	69,73,73	1.45	15 (21%)	83,113,113	2.32	24 (28%)
13	CLA	J	102	8	69,73,73	1.94	16 (23%)	83,113,113	2.99	30 (36%)
12	LMT	B	801	-	36,36,36	0.35	0	47,47,47	0.76	2 (4%)
13	CLA	B	840	2	69,73,73	1.55	13 (18%)	83,113,113	2.88	33 (39%)
15	BCR	A	839	-	41,41,41	1.53	6 (14%)	56,56,56	1.44	8 (14%)
13	CLA	B	819	22	69,73,73	2.00	15 (21%)	83,113,113	3.07	29 (34%)
13	CLA	A	824	22	69,73,73	1.73	16 (23%)	83,113,113	2.64	27 (32%)
13	CLA	B	828	2	69,73,73	1.69	13 (18%)	83,113,113	2.72	30 (36%)
13	CLA	F	201	22	69,73,73	1.76	15 (21%)	83,113,113	2.85	27 (32%)
12	LMT	A	845	-	36,36,36	0.47	0	47,47,47	0.71	0
13	CLA	B	845	22	69,73,73	2.00	16 (23%)	83,113,113	2.59	27 (32%)
12	LMT	K	105	-	36,36,36	0.30	0	47,47,47	0.72	1 (2%)
13	CLA	X	102	11	69,73,73	1.62	15 (21%)	83,113,113	2.12	22 (26%)
19	LMG	B	804	-	55,55,55	0.80	2 (3%)	63,63,63	0.59	0
13	CLA	A	808	1	69,73,73	1.94	20 (28%)	83,113,113	2.85	35 (42%)
13	CLA	B	807	2	69,73,73	1.69	17 (24%)	83,113,113	2.22	24 (28%)
13	CLA	B	850	2	69,73,73	1.68	16 (23%)	83,113,113	2.08	24 (28%)
13	CLA	B	849	2	69,73,73	1.44	12 (17%)	83,113,113	2.09	19 (22%)
15	BCR	J	104	-	41,41,41	1.50	7 (17%)	56,56,56	2.21	11 (19%)
13	CLA	A	809	1	69,73,73	1.76	16 (23%)	83,113,113	2.57	30 (36%)
13	CLA	B	842	2	69,73,73	1.75	18 (26%)	83,113,113	2.93	33 (39%)
13	CLA	B	815	2	69,73,73	1.62	14 (20%)	83,113,113	2.46	25 (30%)
15	BCR	B	826	-	41,41,41	1.57	7 (17%)	56,56,56	1.47	11 (19%)
13	CLA	A	815	1	69,73,73	1.57	13 (18%)	83,113,113	2.20	22 (26%)
15	BCR	A	841	-	41,41,41	1.79	11 (26%)	56,56,56	1.62	13 (23%)
15	BCR	F	206	-	41,41,41	1.65	10 (24%)	56,56,56	1.48	8 (14%)
13	CLA	A	863	-	69,73,73	1.47	14 (20%)	83,113,113	2.69	27 (32%)
13	CLA	B	816	2	69,73,73	1.60	12 (17%)	83,113,113	2.86	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	851	22	69,73,73	1.76	14 (20%)	83,113,113	2.86	26 (31%)
12	LMT	A	804	-	36,36,36	0.26	0	47,47,47	0.56	0
16	LHG	I	101	-	48,48,48	0.27	0	51,54,54	0.34	0
13	CLA	A	817	1	69,73,73	1.69	14 (20%)	83,113,113	2.94	36 (43%)
13	CLA	A	827	1	69,73,73	1.84	15 (21%)	83,113,113	2.97	29 (34%)
13	CLA	A	857	1,13	69,73,73	1.71	15 (21%)	83,113,113	2.39	20 (24%)
13	CLA	B	818	2	69,73,73	1.78	13 (18%)	83,113,113	2.69	30 (36%)
15	BCR	F	203	-	41,41,41	1.62	8 (19%)	56,56,56	1.61	10 (17%)
17	SF4	A	846	1,2	0,12,12	-	-	-	-	-
16	LHG	X	104	-	48,48,48	0.35	0	51,54,54	0.43	0
13	CLA	A	828	1	69,73,73	1.73	15 (21%)	83,113,113	2.37	31 (37%)
12	LMT	A	836	-	36,36,36	0.19	0	47,47,47	0.50	0
13	CLA	B	839	22	69,73,73	1.76	16 (23%)	83,113,113	2.59	25 (30%)
13	CLA	A	829	1	69,73,73	1.56	14 (20%)	83,113,113	2.57	24 (28%)
13	CLA	A	855	1	69,73,73	1.68	15 (21%)	83,113,113	2.84	29 (34%)
13	CLA	A	853	1	69,73,73	1.59	14 (20%)	83,113,113	2.74	30 (36%)
13	CLA	B	811	2	69,73,73	1.86	17 (24%)	83,113,113	2.40	25 (30%)
13	CLA	K	101	-	69,73,73	2.02	19 (27%)	83,113,113	3.16	27 (32%)
13	CLA	A	821	22	69,73,73	1.89	15 (21%)	83,113,113	2.91	24 (28%)
13	CLA	B	847	2	69,73,73	1.97	13 (18%)	83,113,113	2.28	22 (26%)
12	LMT	X	103	-	36,36,36	0.39	0	47,47,47	0.47	0
12	LMT	A	835	-	36,36,36	0.43	0	47,47,47	0.81	1 (2%)
13	CLA	A	831	1	69,73,73	1.78	17 (24%)	83,113,113	2.80	25 (30%)
16	LHG	A	864	-	48,48,48	0.29	0	51,54,54	0.35	0
13	CLA	A	833	1	69,73,73	1.65	15 (21%)	83,113,113	2.81	29 (34%)
13	CLA	B	833	2	69,73,73	1.53	12 (17%)	83,113,113	2.69	28 (33%)
13	CLA	B	810	2	69,73,73	1.68	15 (21%)	83,113,113	1.87	23 (27%)
13	CLA	A	844	1	69,73,73	1.88	15 (21%)	83,113,113	2.72	32 (38%)
13	CLA	A	830	16	69,73,73	1.85	16 (23%)	83,113,113	2.92	29 (34%)
13	CLA	B	835	2	69,73,73	1.76	13 (18%)	83,113,113	3.04	37 (44%)
15	BCR	K	103	-	41,41,41	2.00	7 (17%)	56,56,56	2.01	13 (23%)
15	BCR	B	824	-	41,41,41	1.50	5 (12%)	56,56,56	1.28	8 (14%)
14	PQN	A	837	-	34,34,34	0.65	0	42,45,45	0.64	0
13	CLA	A	813	1	69,73,73	1.95	15 (21%)	83,113,113	2.93	29 (34%)
13	CLA	A	825	1	69,73,73	1.71	14 (20%)	83,113,113	2.85	23 (27%)
12	LMT	A	834	-	36,36,36	0.38	0	47,47,47	0.92	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	821	2	69,73,73	1.57	17 (24%)	83,113,113	2.61	28 (33%)
13	CLA	B	841	2	69,73,73	1.58	11 (15%)	83,113,113	3.11	30 (36%)
13	CLA	B	838	2	69,73,73	1.80	15 (21%)	83,113,113	2.05	19 (22%)
13	CLA	A	806	22	69,73,73	1.61	10 (14%)	83,113,113	2.86	33 (39%)
13	CLA	B	843	2	69,73,73	1.70	15 (21%)	83,113,113	2.90	28 (33%)
13	CLA	A	814	1	69,73,73	1.86	16 (23%)	83,113,113	2.92	32 (38%)
13	CLA	B	831	2	69,73,73	1.81	15 (21%)	83,113,113	2.81	31 (37%)
13	CLA	A	823	1	69,73,73	1.54	16 (23%)	83,113,113	2.42	27 (32%)
17	SF4	C	1002	3	0,12,12	-	-	-	-	-
13	CLA	A	849	22	69,73,73	1.64	15 (21%)	83,113,113	2.71	30 (36%)
13	CLA	A	858	1	69,73,73	1.49	14 (20%)	83,113,113	2.76	32 (38%)
12	LMT	A	801	-	36,36,36	0.68	0	47,47,47	1.50	5 (10%)
13	CLA	B	844	2	69,73,73	1.64	11 (15%)	83,113,113	1.99	20 (24%)
13	CLA	A	819	1	69,73,73	1.94	21 (30%)	83,113,113	2.93	25 (30%)
13	CLA	B	830	2	69,73,73	1.42	11 (15%)	83,113,113	1.83	18 (21%)
13	CLA	B	832	2	69,73,73	1.80	15 (21%)	83,113,113	3.07	34 (40%)
13	CLA	J	101	8	69,73,73	1.98	16 (23%)	83,113,113	3.11	32 (38%)
15	BCR	J	103	-	41,41,41	1.62	10 (24%)	56,56,56	1.45	11 (19%)
13	CLA	B	813	22	69,73,73	1.55	14 (20%)	83,113,113	2.95	28 (33%)
13	CLA	A	818	1	69,73,73	1.82	19 (27%)	83,113,113	2.61	32 (38%)
13	CLA	B	817	2	69,73,73	1.73	15 (21%)	83,113,113	2.85	27 (32%)
13	CLA	B	809	22	69,73,73	1.67	13 (18%)	83,113,113	2.27	21 (25%)
13	CLA	B	846	22	69,73,73	1.74	15 (21%)	83,113,113	2.17	25 (30%)
12	LMT	A	803	-	36,36,36	0.23	0	47,47,47	0.61	1 (2%)

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
15	BCR	B	825	-	-	2/29/63/63	0/2/2/2
13	CLA	A	860	1	1/1/15/20	9/39/115/115	-
16	LHG	A	852	-	-	8/53/53/53	-
13	CLA	B	829	2	1/1/15/20	7/39/115/115	-
13	CLA	A	810	1	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LHG	A	843	13	-	13/53/53/53	-
17	SF4	C	1001	3	-	-	0/6/5/5
15	BCR	A	842	-	-	0/29/63/63	0/2/2/2
15	BCR	F	202	-	-	0/29/63/63	0/2/2/2
13	CLA	B	808	2	-	7/39/115/115	-
13	CLA	A	805	1	1/1/15/20	11/39/115/115	-
13	CLA	B	806	2	-	9/39/115/115	-
13	CLA	A	816	1	1/1/15/20	15/39/115/115	-
12	LMT	B	827	-	-	8/21/61/61	0/2/2/2
18	CL0	A	847	1	-	2/39/115/115	-
12	LMT	B	852	-	-	2/21/61/61	0/2/2/2
13	CLA	A	826	1	-	10/39/115/115	-
12	LMT	F	205	-	-	2/21/61/61	0/2/2/2
13	CLA	A	807	1	1/1/15/20	8/39/115/115	-
13	CLA	A	848	1	1/1/15/20	5/39/115/115	-
13	CLA	F	204	22	1/1/15/20	13/39/115/115	-
13	CLA	A	854	1,13	1/1/15/20	11/39/115/115	-
13	CLA	B	837	2	1/1/15/20	8/39/115/115	-
13	CLA	K	104	22	1/1/15/20	7/39/115/115	-
12	LMT	B	851	-	-	2/21/61/61	0/2/2/2
15	BCR	M	101	-	-	0/29/63/63	0/2/2/2
13	CLA	A	811	1	1/1/15/20	12/39/115/115	-
13	CLA	A	859	1	1/1/15/20	8/39/115/115	-
13	CLA	A	832	1	1/1/15/20	8/39/115/115	-
12	LMT	A	802	-	-	4/21/61/61	0/2/2/2
13	CLA	A	820	1	-	15/39/115/115	-
13	CLA	B	805	2	-	10/39/115/115	-
21	SQD	X	101	-	-	13/49/69/69	0/1/1/1
13	CLA	B	814	2	-	7/39/115/115	-
12	LMT	K	102	-	-	1/21/61/61	0/2/2/2
13	CLA	A	861	1	1/1/15/20	9/39/115/115	-
15	BCR	A	862	-	-	2/29/63/63	0/2/2/2
13	CLA	B	848	22	-	7/39/115/115	-
15	BCR	B	802	-	-	5/29/63/63	0/2/2/2
14	PQN	B	823	-	-	3/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	856	1	1/1/15/20	9/39/115/115	-
15	BCR	A	838	-	-	2/29/63/63	0/2/2/2
13	CLA	A	822	22	1/1/15/20	10/39/115/115	-
13	CLA	B	820	2	1/1/15/20	11/39/115/115	-
15	BCR	B	803	-	-	1/29/63/63	0/2/2/2
13	CLA	A	812	1	1/1/15/20	15/39/115/115	-
13	CLA	A	850	-	-	4/39/115/115	-
13	CLA	B	836	2	-	8/39/115/115	-
15	BCR	A	840	-	-	4/29/63/63	0/2/2/2
15	BCR	B	822	-	-	2/29/63/63	0/2/2/2
13	CLA	B	834	2	-	3/39/115/115	-
13	CLA	J	102	8	1/1/15/20	14/39/115/115	-
12	LMT	B	801	-	-	8/21/61/61	0/2/2/2
13	CLA	B	840	2	-	10/39/115/115	-
15	BCR	A	839	-	-	0/29/63/63	0/2/2/2
13	CLA	B	819	22	1/1/15/20	12/39/115/115	-
13	CLA	A	824	22	1/1/15/20	4/39/115/115	-
13	CLA	B	828	2	1/1/15/20	13/39/115/115	-
13	CLA	F	201	22	1/1/15/20	6/39/115/115	-
12	LMT	A	845	-	-	2/21/61/61	0/2/2/2
13	CLA	B	845	22	-	14/39/115/115	-
12	LMT	K	105	-	-	6/21/61/61	0/2/2/2
13	CLA	X	102	11	-	6/39/115/115	-
19	LMG	B	804	-	-	16/50/70/70	0/1/1/1
13	CLA	A	808	1	1/1/15/20	16/39/115/115	-
13	CLA	B	807	2	-	11/39/115/115	-
13	CLA	B	850	2	-	10/39/115/115	-
13	CLA	B	849	2	-	7/39/115/115	-
15	BCR	J	104	-	-	6/29/63/63	0/2/2/2
13	CLA	A	809	1	1/1/15/20	12/39/115/115	-
13	CLA	B	842	2	1/1/15/20	11/39/115/115	-
13	CLA	B	815	2	1/1/15/20	9/39/115/115	-
15	BCR	B	826	-	-	2/29/63/63	0/2/2/2
13	CLA	A	815	1	1/1/15/20	9/39/115/115	-
15	BCR	A	841	-	-	1/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	F	206	-	-	1/29/63/63	0/2/2/2
13	CLA	A	863	-	-	5/39/115/115	-
13	CLA	B	816	2	1/1/15/20	11/39/115/115	-
13	CLA	A	851	22	1/1/15/20	14/39/115/115	-
12	LMT	A	804	-	-	6/21/61/61	0/2/2/2
16	LHG	I	101	-	-	18/53/53/53	-
13	CLA	A	817	1	1/1/15/20	12/39/115/115	-
13	CLA	A	827	1	1/1/15/20	7/39/115/115	-
13	CLA	B	818	2	1/1/15/20	5/39/115/115	-
13	CLA	A	857	1,13	-	5/39/115/115	-
15	BCR	F	203	-	-	2/29/63/63	0/2/2/2
17	SF4	A	846	1,2	-	-	0/6/5/5
16	LHG	X	104	-	-	20/53/53/53	-
13	CLA	A	828	1	-	6/39/115/115	-
13	CLA	B	839	22	1/1/15/20	9/39/115/115	-
12	LMT	A	836	-	-	3/21/61/61	0/2/2/2
13	CLA	A	829	1	-	7/39/115/115	-
13	CLA	A	855	1	-	5/39/115/115	-
13	CLA	A	853	1	-	8/39/115/115	-
13	CLA	B	811	2	-	10/39/115/115	-
13	CLA	K	101	-	1/1/15/20	9/39/115/115	-
13	CLA	A	821	22	1/1/15/20	10/39/115/115	-
13	CLA	B	847	2	-	7/39/115/115	-
12	LMT	X	103	-	-	9/21/61/61	0/2/2/2
12	LMT	A	835	-	-	5/21/61/61	0/2/2/2
13	CLA	A	831	1	1/1/15/20	9/39/115/115	-
16	LHG	A	864	-	-	14/53/53/53	-
13	CLA	A	833	1	-	13/39/115/115	-
13	CLA	B	833	2	1/1/15/20	9/39/115/115	-
13	CLA	B	810	2	-	5/39/115/115	-
13	CLA	A	844	1	1/1/15/20	8/39/115/115	-
13	CLA	A	830	16	1/1/15/20	8/39/115/115	-
13	CLA	B	835	2	1/1/15/20	13/39/115/115	-
15	BCR	K	103	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	B	824	-	-	5/29/63/63	0/2/2/2
14	PQN	A	837	-	-	6/23/43/43	0/2/2/2
13	CLA	A	813	1	1/1/15/20	5/39/115/115	-
13	CLA	A	825	1	1/1/15/20	7/39/115/115	-
12	LMT	A	834	-	-	8/21/61/61	0/2/2/2
13	CLA	B	821	2	1/1/15/20	4/39/115/115	-
13	CLA	B	841	2	1/1/15/20	13/39/115/115	-
13	CLA	B	838	2	-	6/39/115/115	-
13	CLA	A	806	22	1/1/15/20	10/39/115/115	-
13	CLA	B	843	2	1/1/15/20	10/39/115/115	-
13	CLA	A	814	1	1/1/15/20	10/39/115/115	-
13	CLA	B	831	2	1/1/15/20	12/39/115/115	-
13	CLA	A	823	1	1/1/15/20	9/39/115/115	-
17	SF4	C	1002	3	-	-	0/6/5/5
13	CLA	A	849	22	1/1/15/20	4/39/115/115	-
13	CLA	A	858	1	1/1/15/20	7/39/115/115	-
12	LMT	A	801	-	-	9/21/61/61	0/2/2/2
13	CLA	B	844	2	-	4/39/115/115	-
13	CLA	A	819	1	-	13/39/115/115	-
13	CLA	B	830	2	-	1/39/115/115	-
13	CLA	B	832	2	1/1/15/20	9/39/115/115	-
13	CLA	J	101	8	-	14/39/115/115	-
15	BCR	J	103	-	-	2/29/63/63	0/2/2/2
13	CLA	B	813	22	1/1/15/20	11/39/115/115	-
13	CLA	A	818	1	1/1/15/20	10/39/115/115	-
13	CLA	B	817	2	1/1/15/20	10/39/115/115	-
13	CLA	B	809	22	-	2/39/115/115	-
13	CLA	B	846	22	-	4/39/115/115	-
12	LMT	A	803	-	-	1/21/61/61	0/2/2/2

The worst 5 of 1504 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	826	CLA	O2A-C1	9.51	1.72	1.46
13	B	847	CLA	O2A-C1	-8.62	1.21	1.46
13	J	101	CLA	C1D-ND	8.11	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	819	CLA	C1D-ND	7.93	1.47	1.37
13	B	845	CLA	C1D-ND	7.82	1.47	1.37

The worst 5 of 2734 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	826	CLA	O2A-C1-C2	16.73	152.61	108.64
13	A	819	CLA	C4A-NA-C1A	14.15	113.07	106.71
13	A	848	CLA	O2D-CGD-CBD	13.97	136.08	111.27
13	A	814	CLA	C4A-NA-C1A	13.83	112.92	106.71
13	K	101	CLA	C1D-ND-C4D	-13.63	96.66	106.33

5 of 57 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	805	CLA	C8
13	A	806	CLA	C8
13	A	807	CLA	C8
13	A	808	CLA	C8
13	A	809	CLA	C8

5 of 1026 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	804	LMT	C2'-C1'-O1'-C1
12	A	804	LMT	O5'-C1'-O1'-C1
12	A	834	LMT	C2-C1-O1'-C1'
12	B	827	LMT	O5'-C1'-O1'-C1
12	X	103	LMT	C2-C1-O1'-C1'

There are no ring outliers.

108 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	825	BCR	2	0
13	A	860	CLA	5	0
13	B	829	CLA	1	0
13	A	810	CLA	2	0
16	A	843	LHG	1	0
17	C	1001	SF4	1	0
15	A	842	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	F	202	BCR	4	0
13	B	808	CLA	2	0
13	A	805	CLA	1	0
13	B	806	CLA	3	0
12	B	827	LMT	1	0
13	A	816	CLA	1	0
13	A	826	CLA	6	0
13	A	848	CLA	4	0
13	F	204	CLA	5	0
13	K	104	CLA	5	0
12	B	851	LMT	1	0
15	M	101	BCR	1	0
12	A	802	LMT	1	0
13	A	811	CLA	5	0
13	A	832	CLA	10	0
13	A	859	CLA	3	0
13	A	820	CLA	10	0
13	B	805	CLA	3	0
13	B	814	CLA	4	0
13	A	861	CLA	4	0
15	A	862	BCR	5	0
15	B	802	BCR	3	0
13	A	856	CLA	7	0
15	A	838	BCR	5	0
13	A	822	CLA	5	0
13	B	820	CLA	3	0
15	B	803	BCR	6	0
13	A	812	CLA	4	0
13	A	850	CLA	3	0
15	A	840	BCR	8	0
15	B	822	BCR	5	0
13	B	834	CLA	2	0
13	J	102	CLA	3	0
13	B	840	CLA	2	0
15	A	839	BCR	4	0
13	B	819	CLA	2	0
13	A	824	CLA	5	0
13	F	201	CLA	1	0
12	A	845	LMT	1	0
13	B	845	CLA	9	0
13	X	102	CLA	1	0
13	A	808	CLA	4	0

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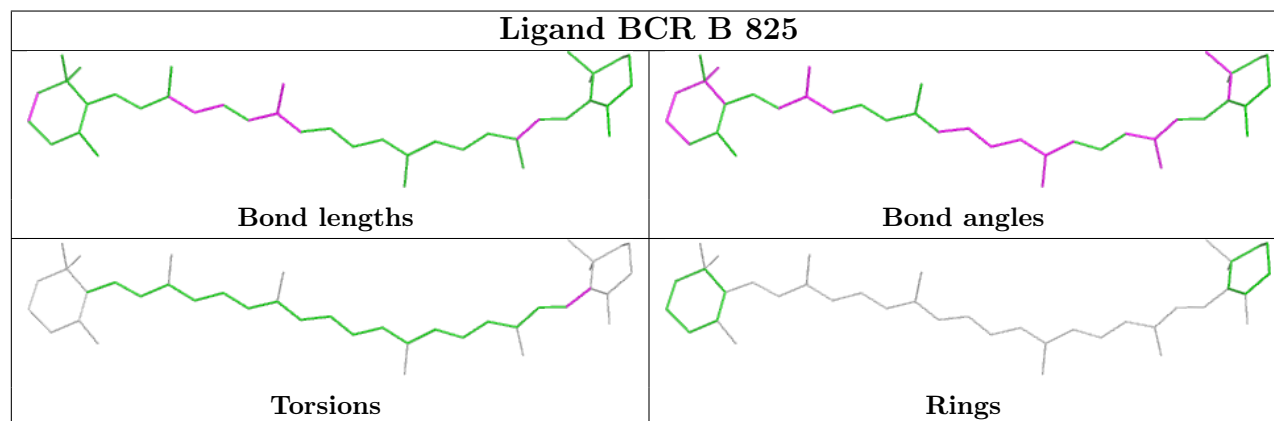
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	807	CLA	3	0
13	B	850	CLA	1	0
13	B	849	CLA	2	0
15	J	104	BCR	4	0
13	A	809	CLA	2	0
13	B	842	CLA	4	0
13	B	815	CLA	5	0
15	B	826	BCR	2	0
13	A	815	CLA	1	0
15	A	841	BCR	5	0
15	F	206	BCR	4	0
13	A	863	CLA	2	0
13	B	816	CLA	5	0
13	A	851	CLA	5	0
13	A	817	CLA	3	0
13	A	827	CLA	2	0
13	A	857	CLA	2	0
13	B	818	CLA	2	0
15	F	203	BCR	2	0
16	X	104	LHG	2	0
13	A	828	CLA	3	0
13	A	829	CLA	4	0
13	A	855	CLA	2	0
13	A	853	CLA	3	0
13	B	811	CLA	1	0
13	K	101	CLA	6	0
13	A	821	CLA	1	0
13	B	847	CLA	4	0
12	A	835	LMT	2	0
13	A	831	CLA	3	0
13	A	833	CLA	1	0
13	B	833	CLA	4	0
13	B	810	CLA	2	0
13	A	844	CLA	1	0
13	A	830	CLA	1	0
13	B	835	CLA	1	0
15	K	103	BCR	7	0
15	B	824	BCR	4	0
13	A	813	CLA	2	0
13	A	825	CLA	11	0
12	A	834	LMT	3	0
13	B	841	CLA	4	0

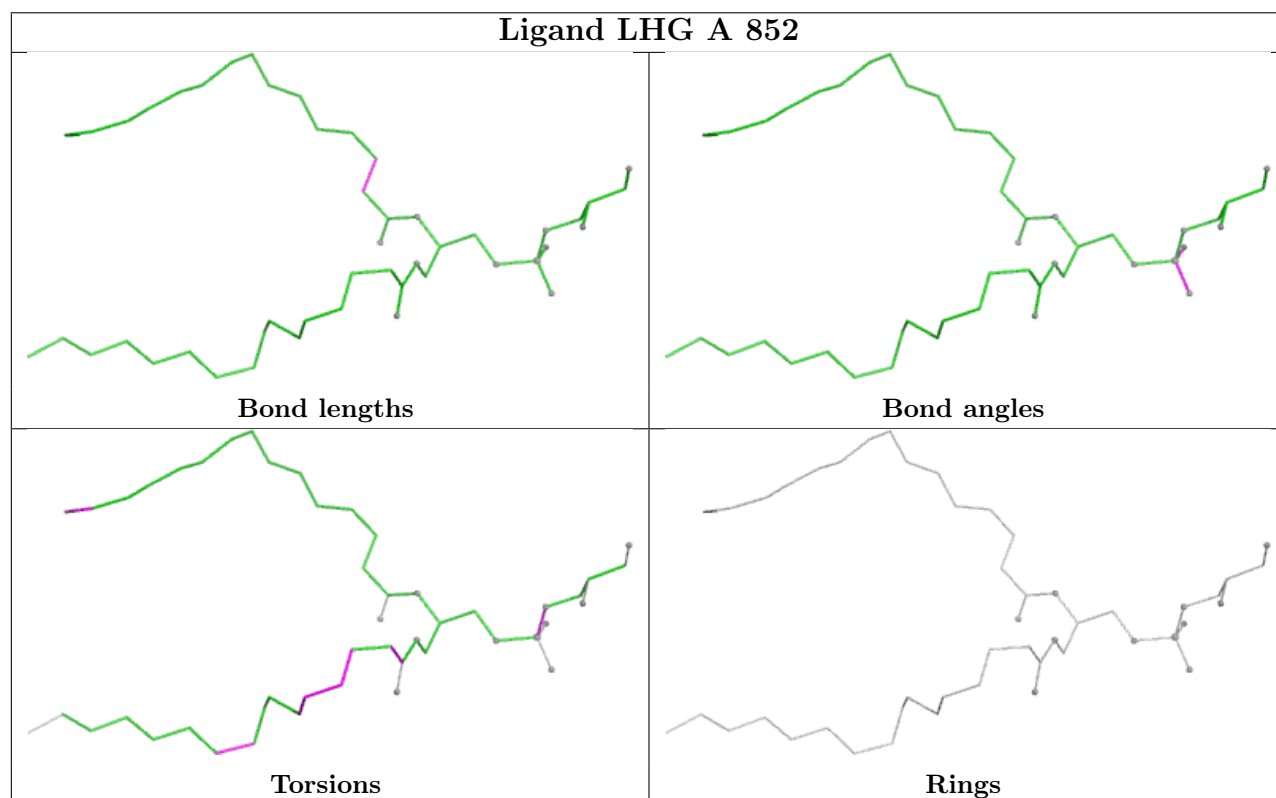
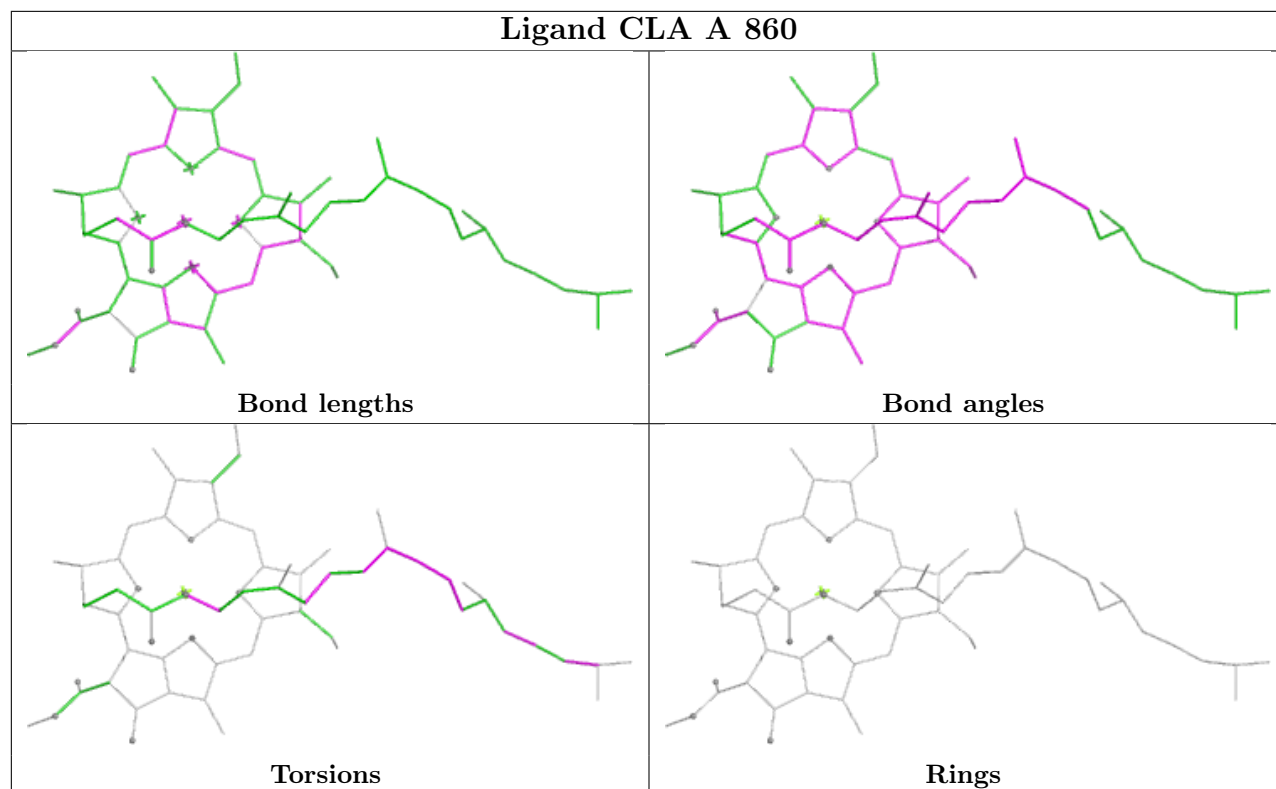
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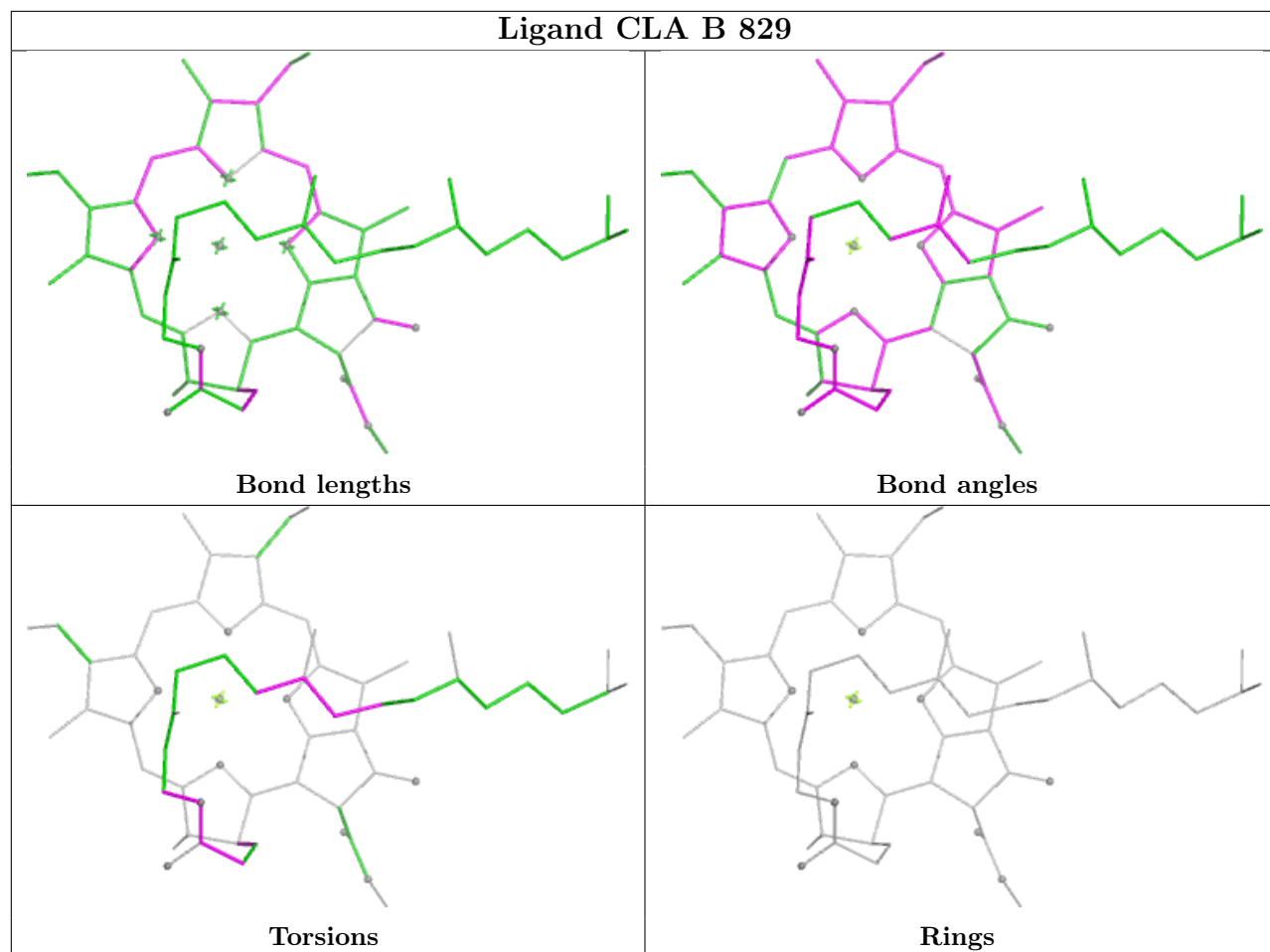
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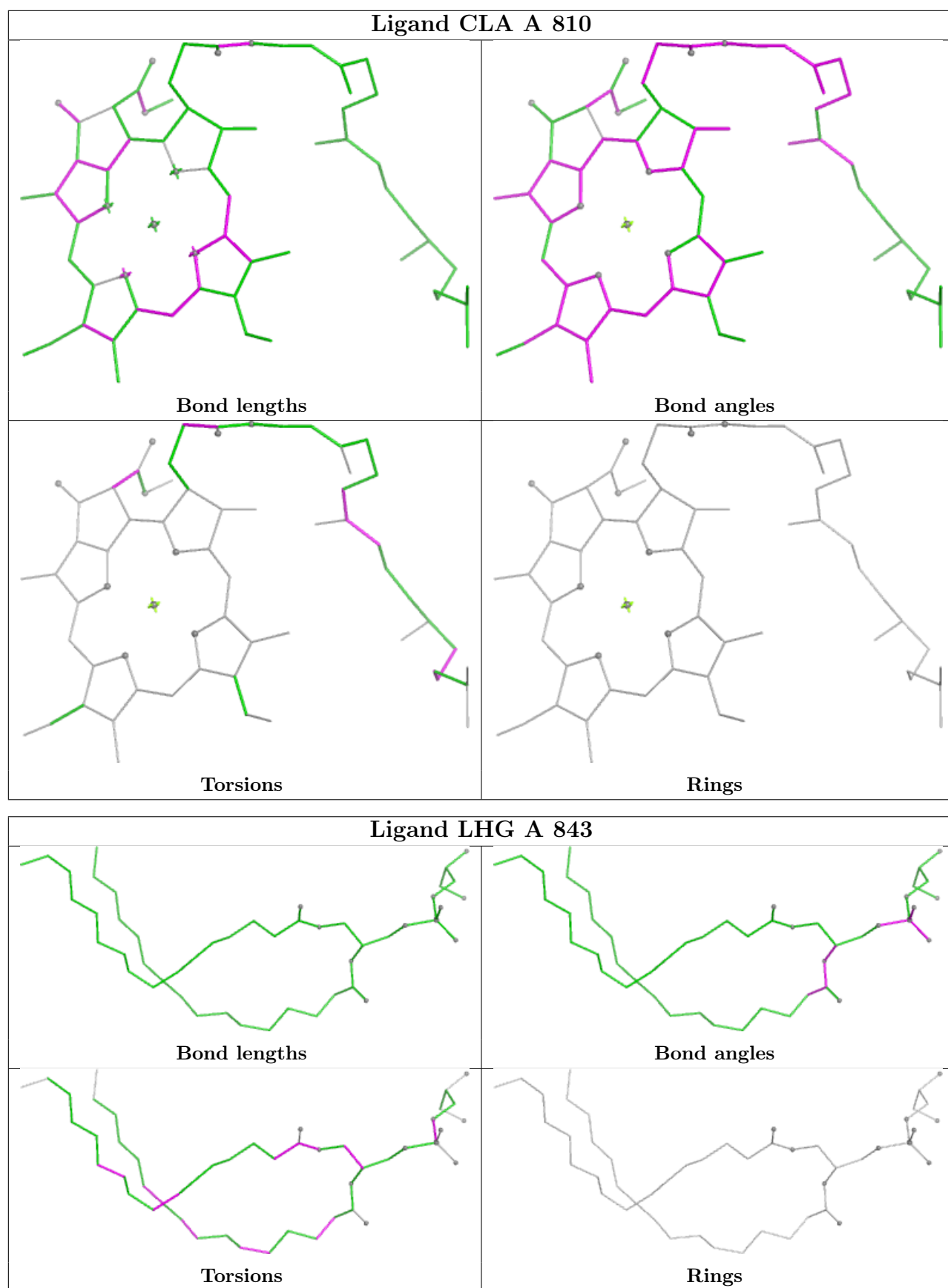
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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13	A	806	CLA	1	0
13	B	843	CLA	7	0
13	A	814	CLA	1	0
13	B	831	CLA	3	0
13	A	823	CLA	8	0
13	A	849	CLA	2	0
13	A	858	CLA	2	0
13	B	844	CLA	3	0
13	A	819	CLA	2	0
13	B	832	CLA	1	0
13	J	101	CLA	1	0
15	J	103	BCR	4	0
13	B	813	CLA	4	0
13	A	818	CLA	1	0
13	B	809	CLA	2	0
13	B	846	CLA	3	0

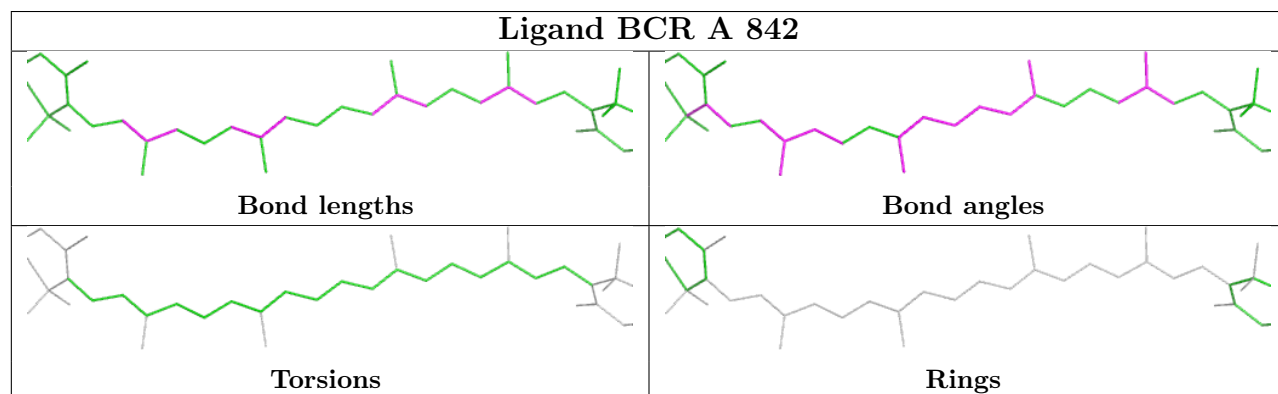
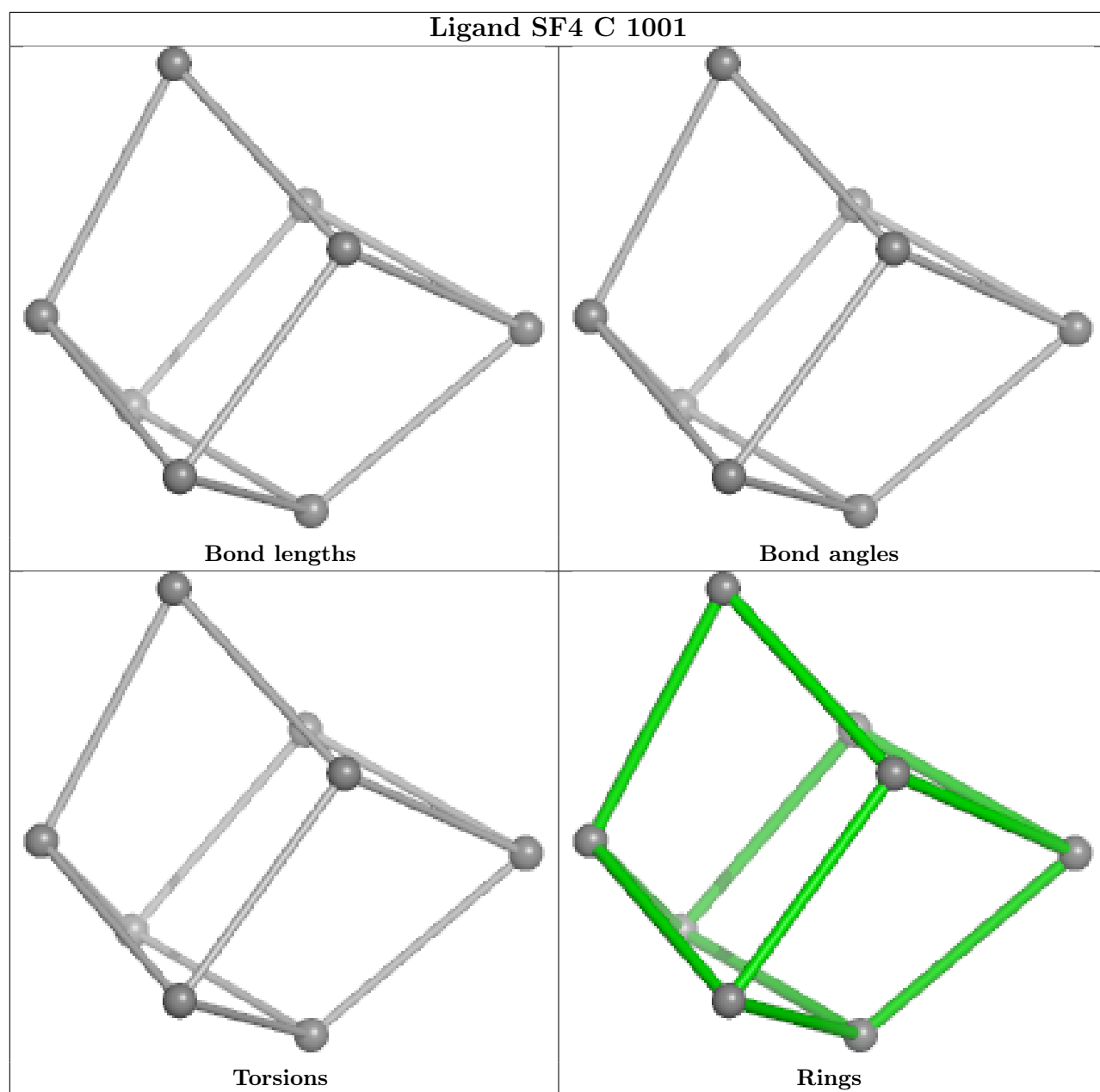
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

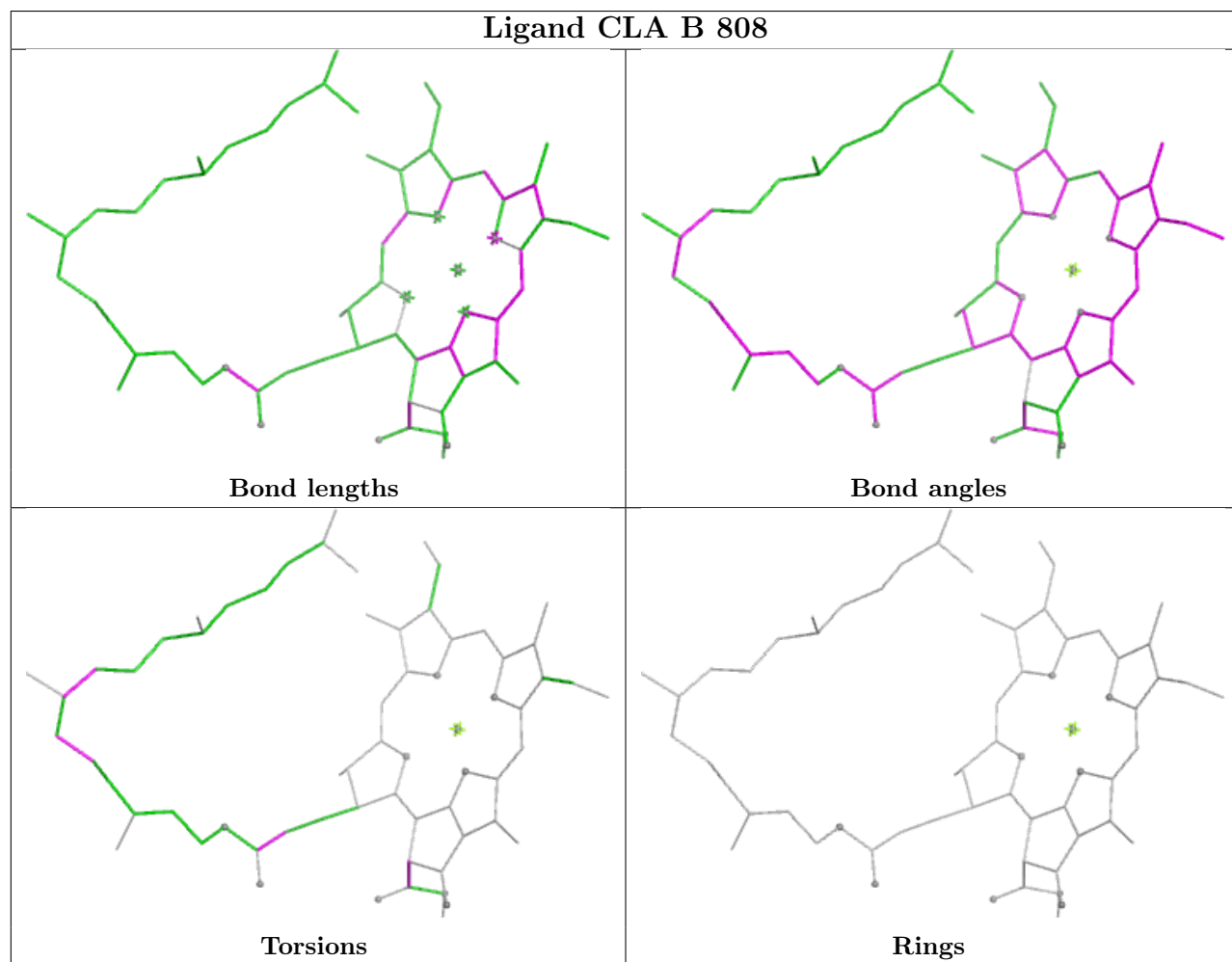
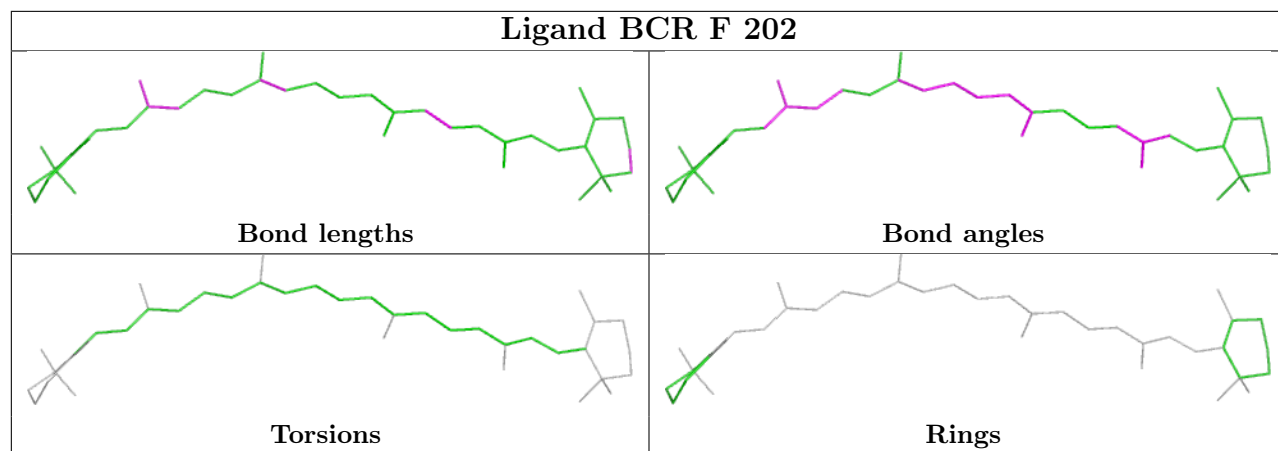


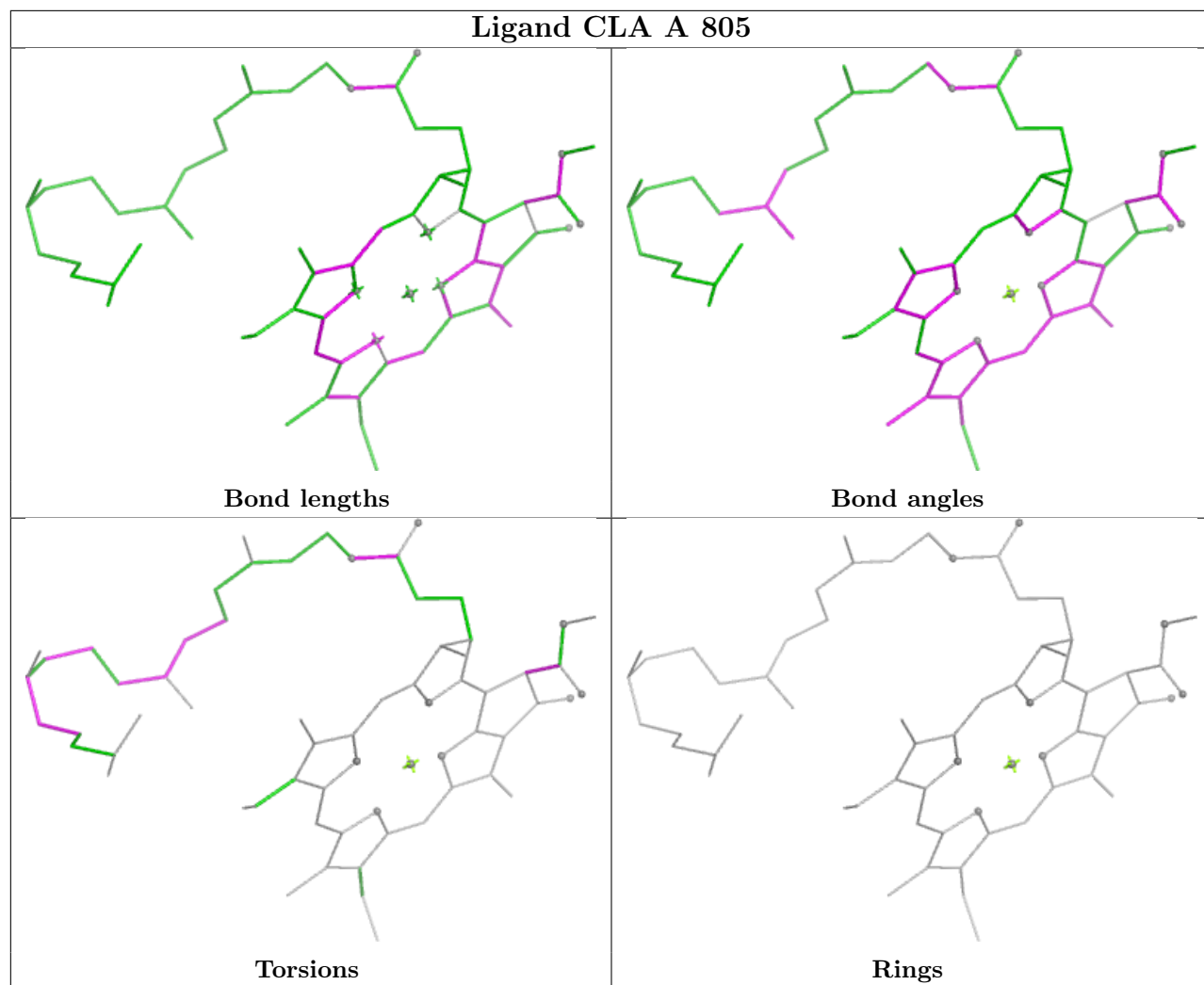


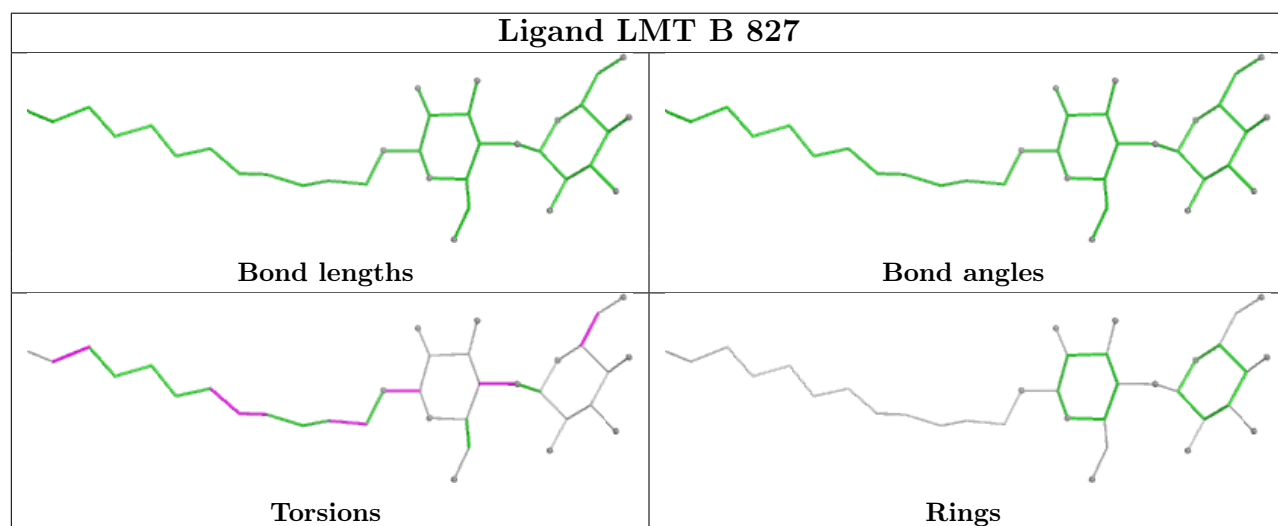
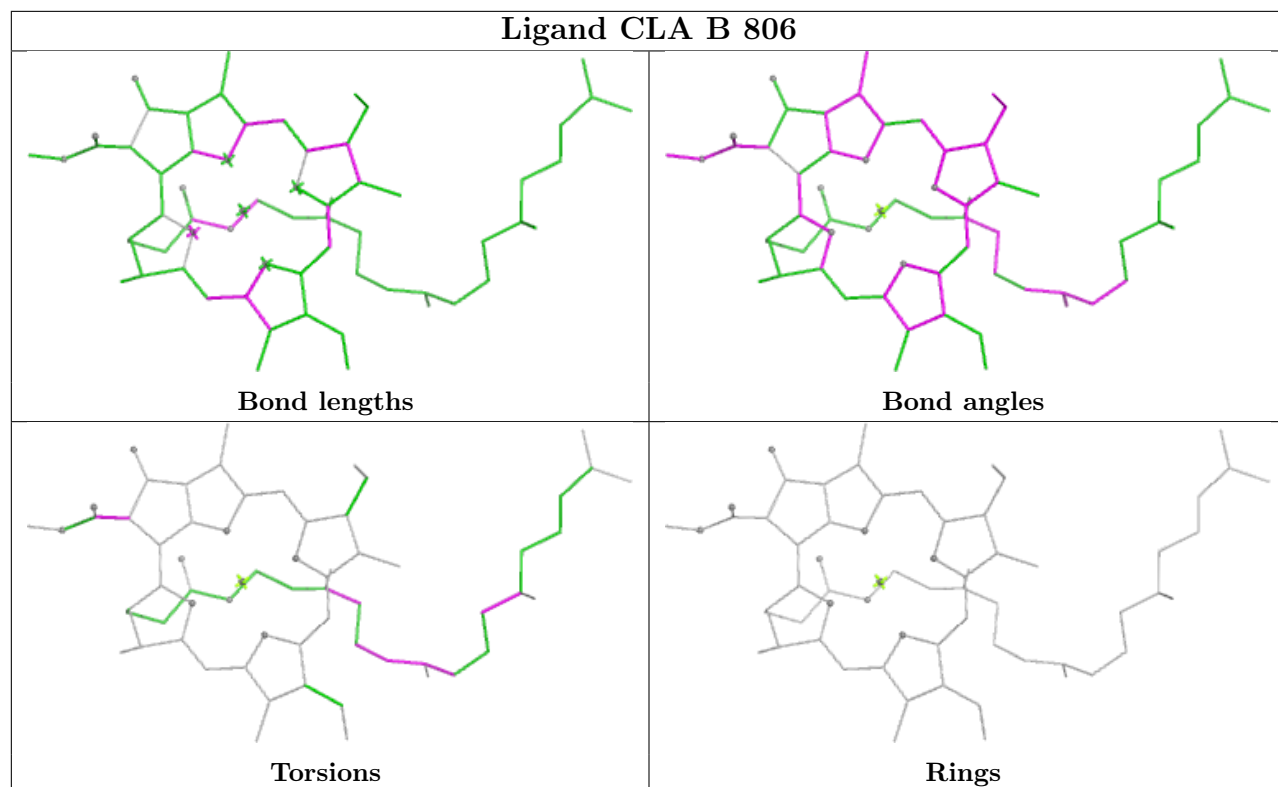


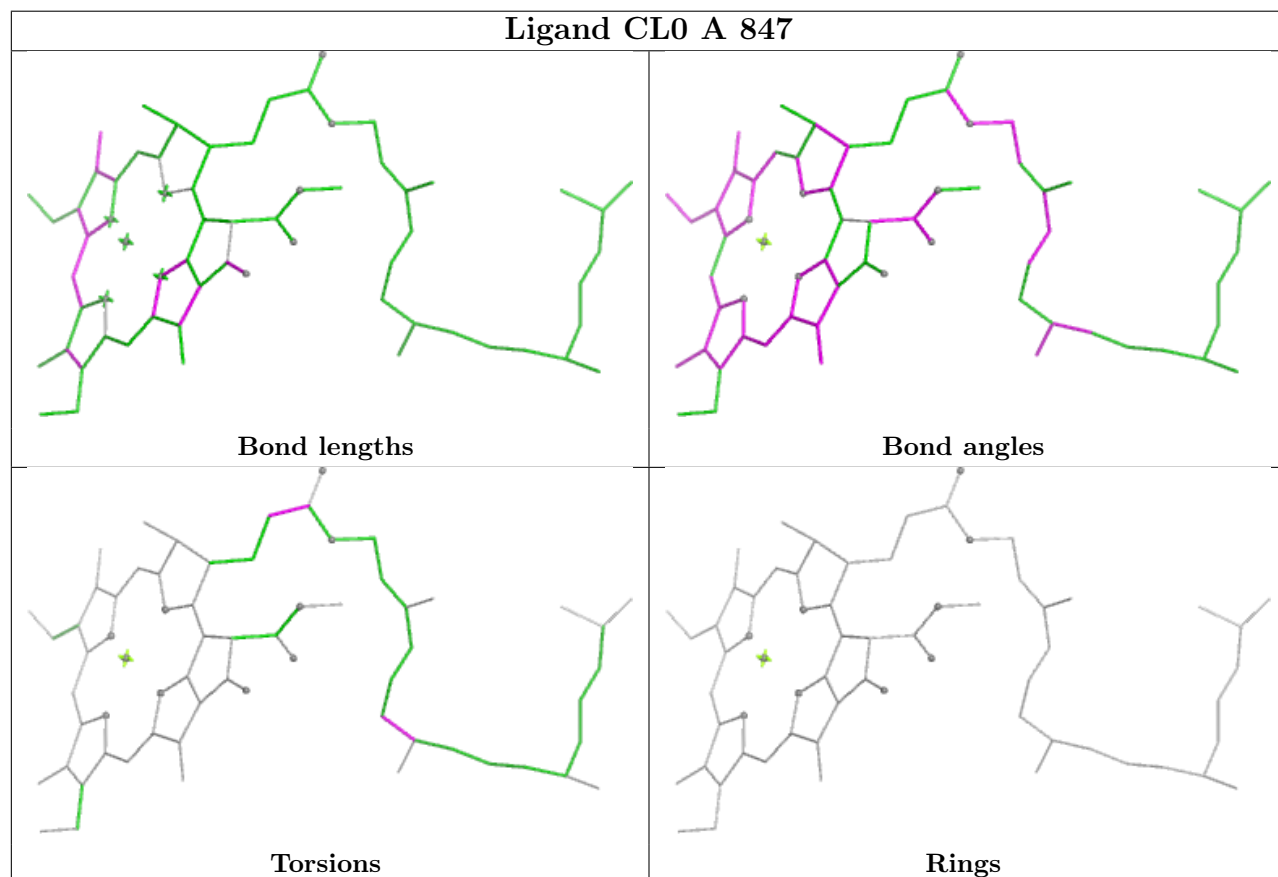
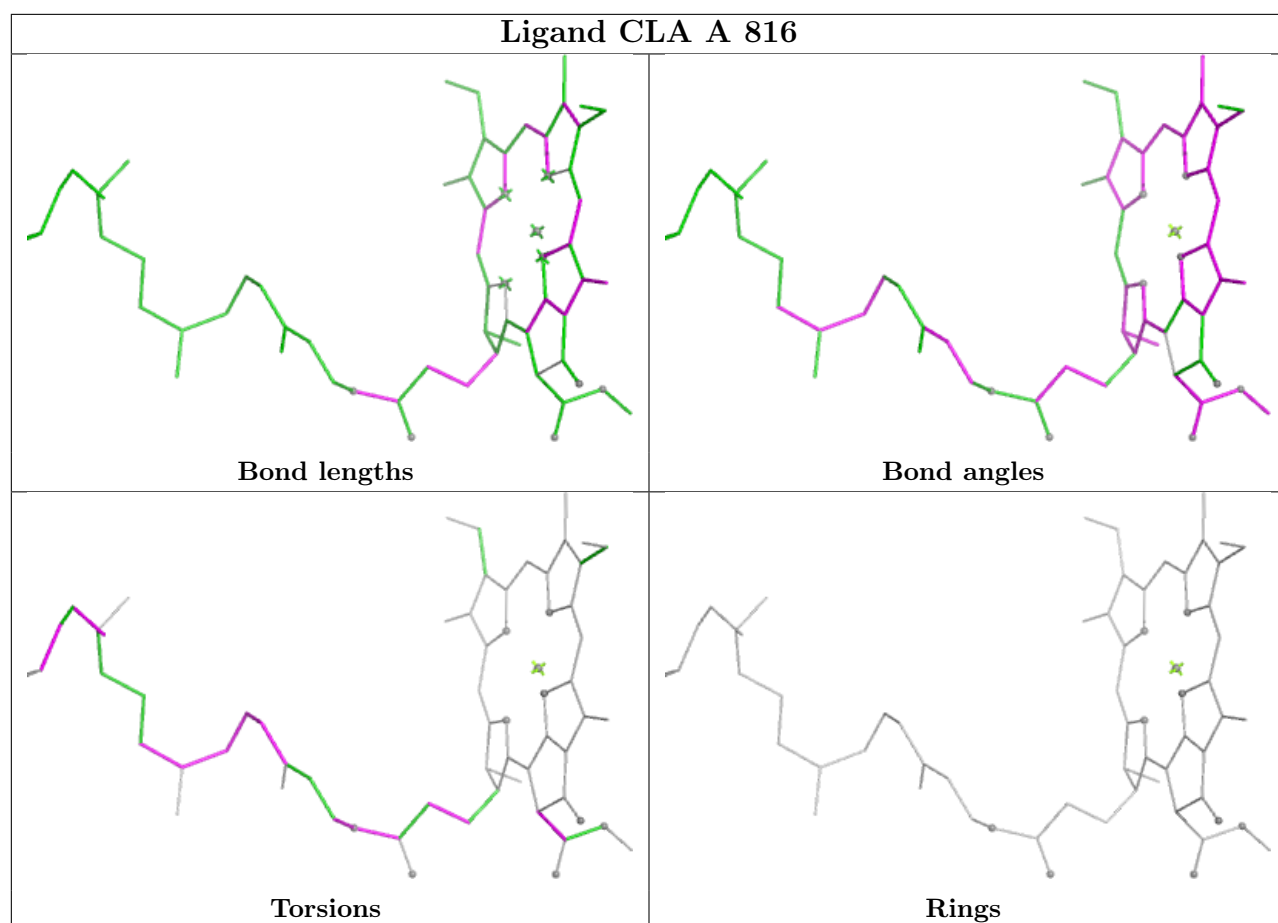


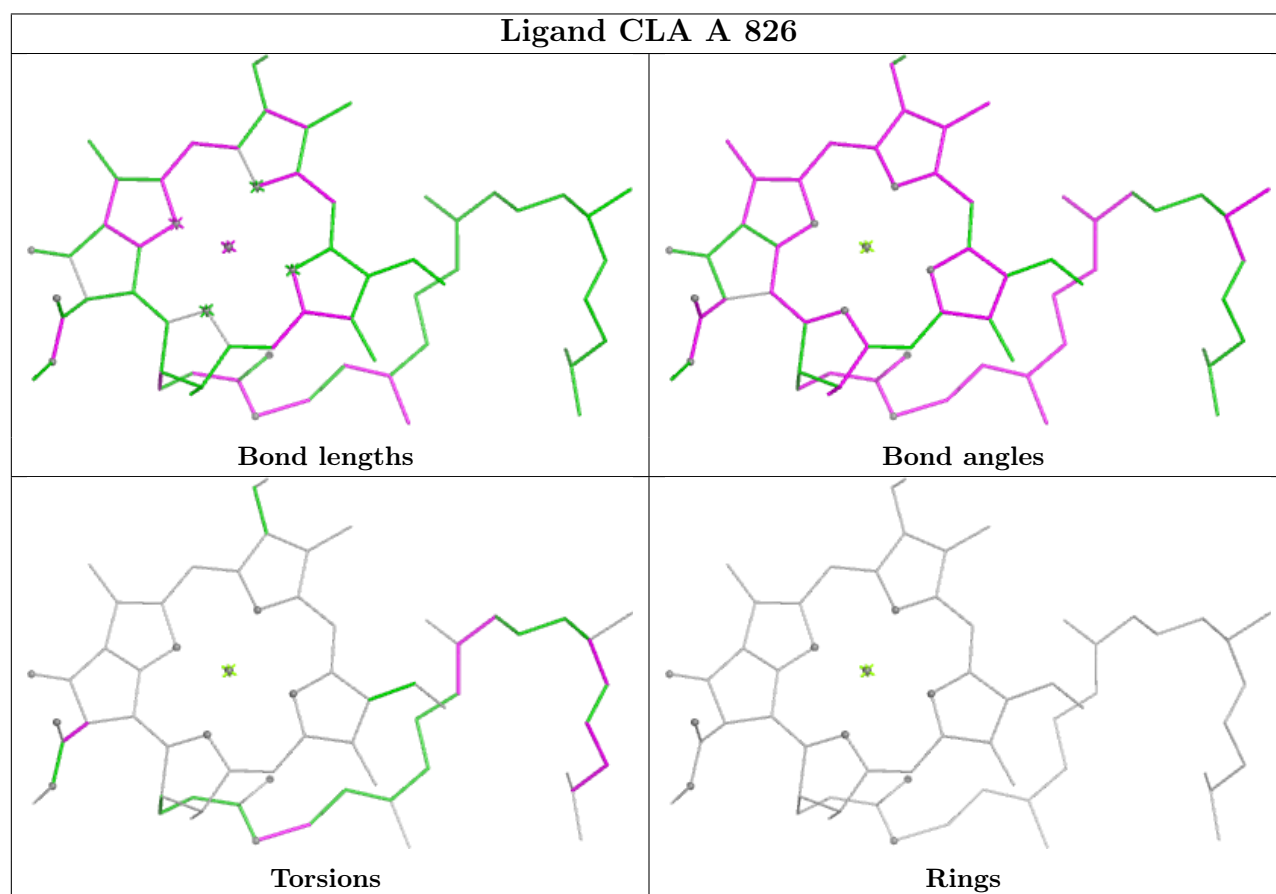
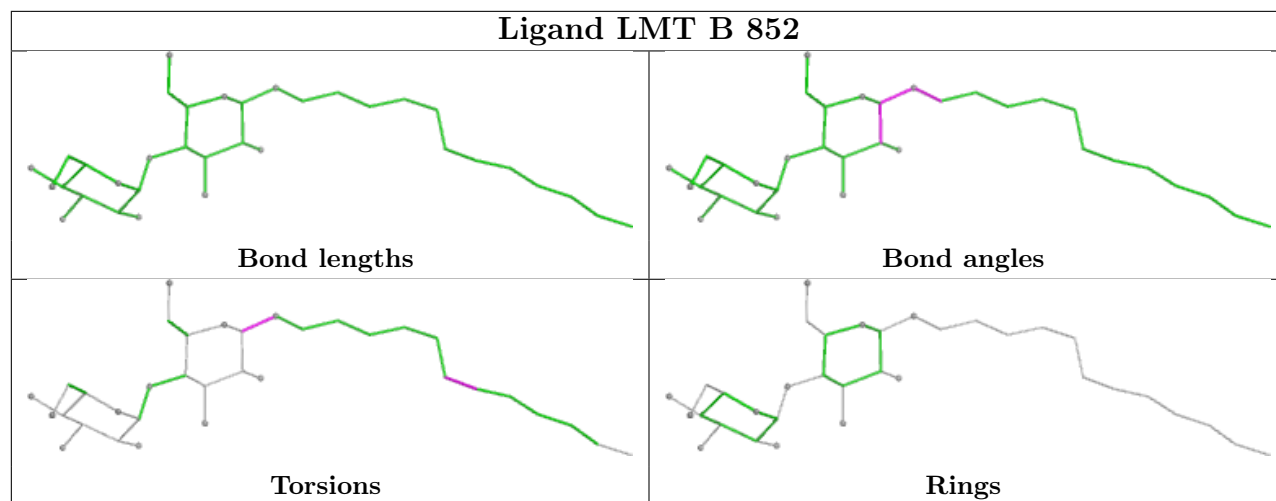


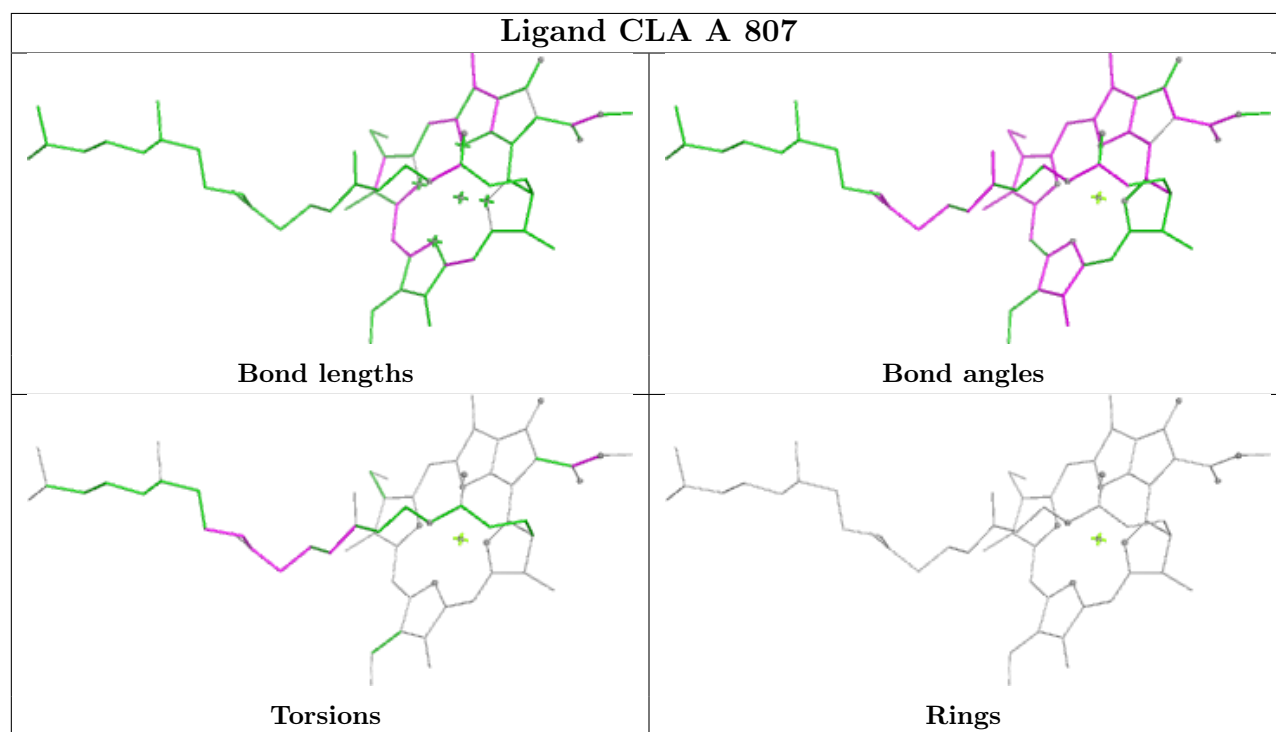
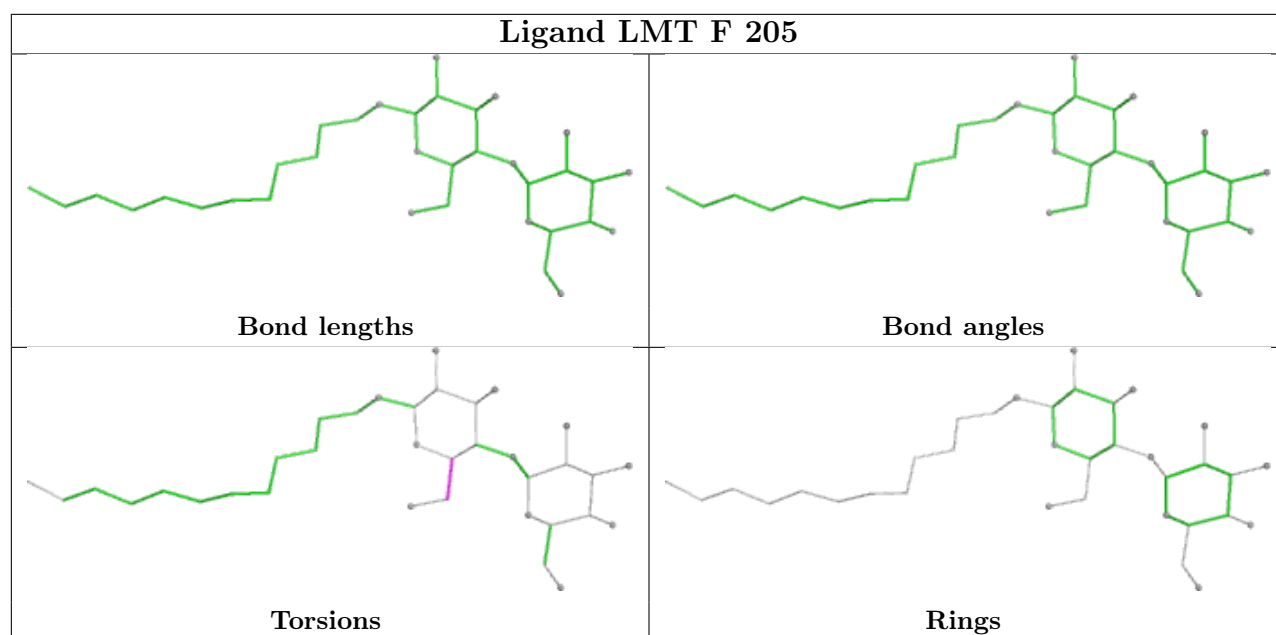


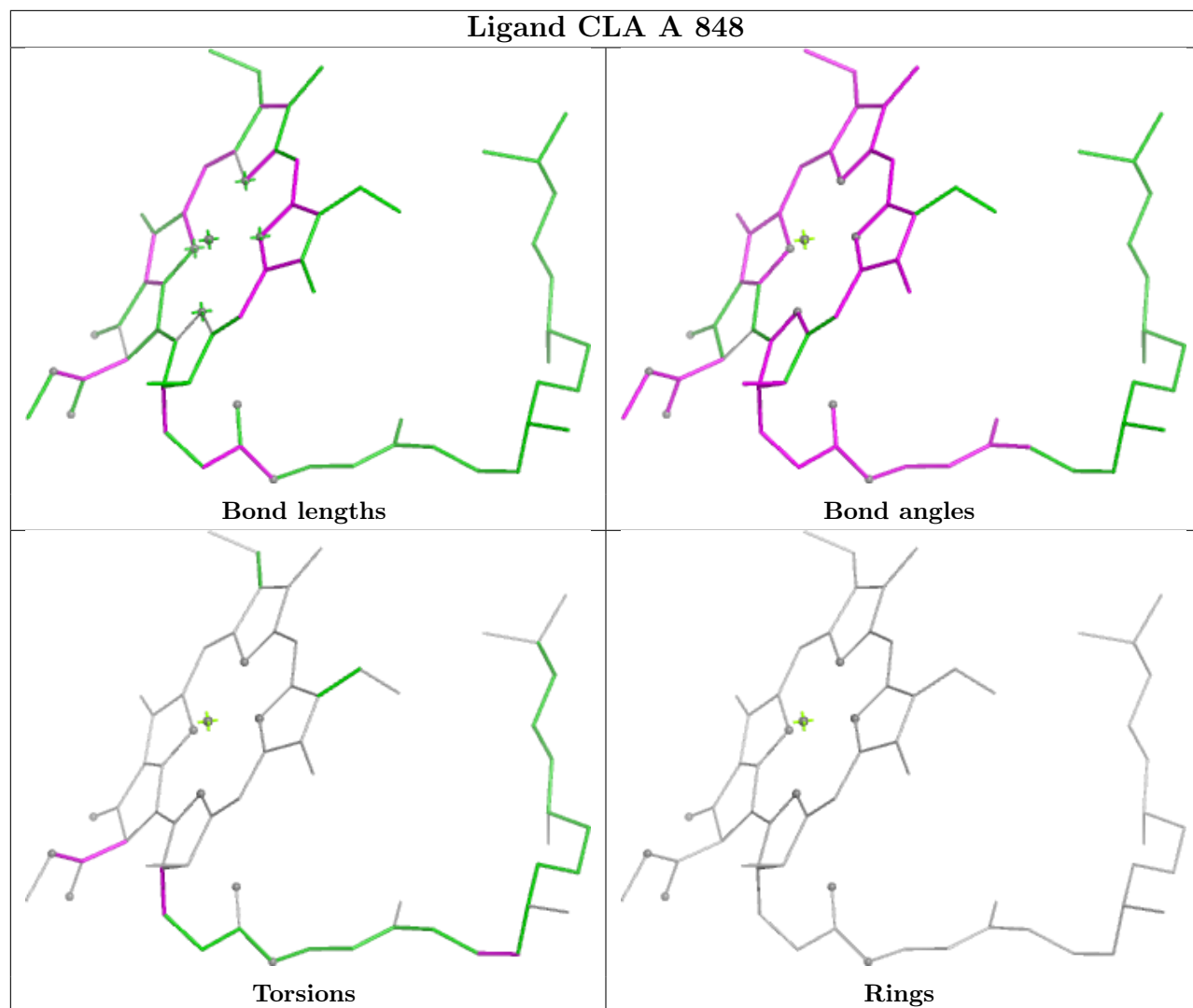


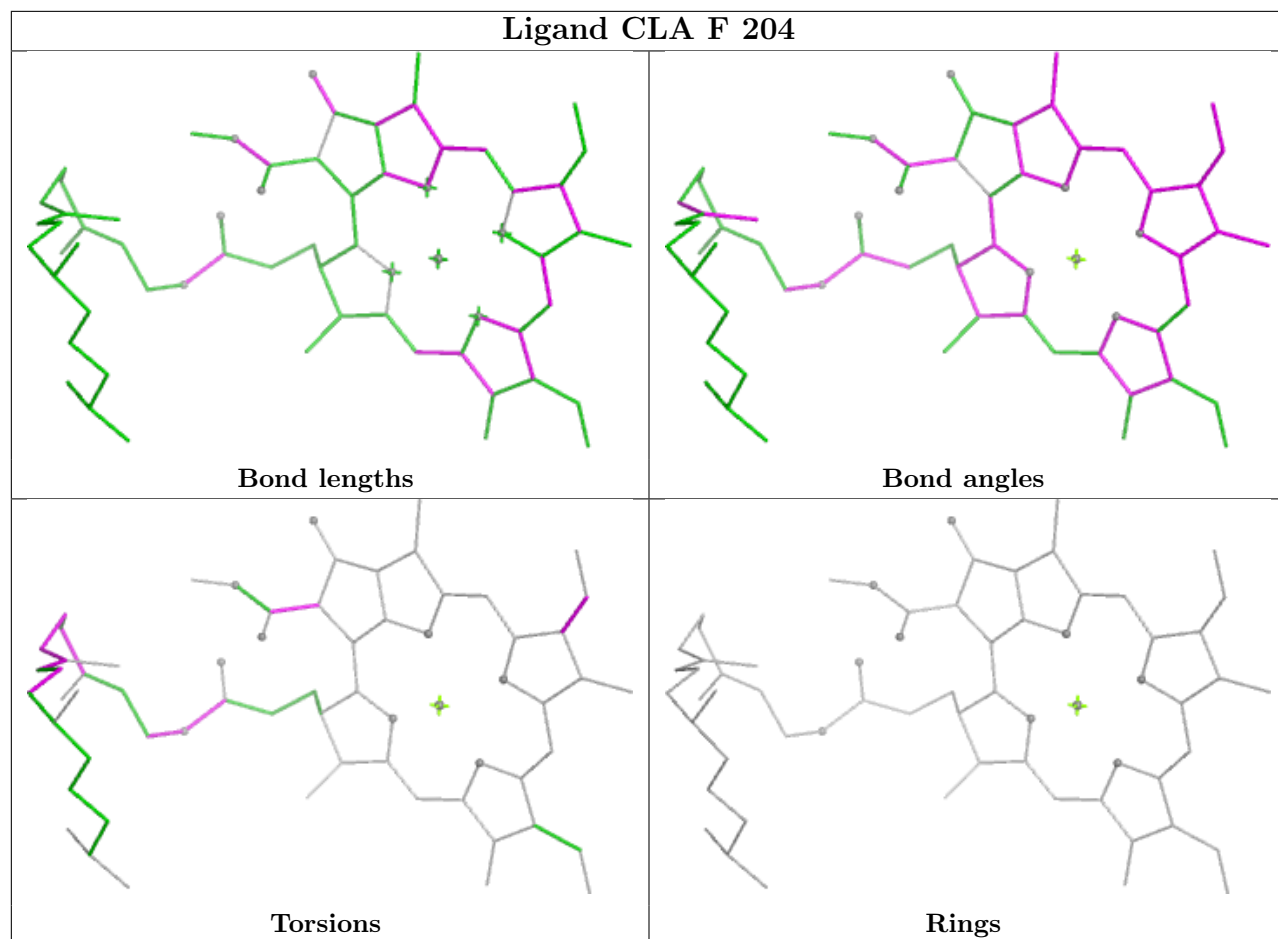


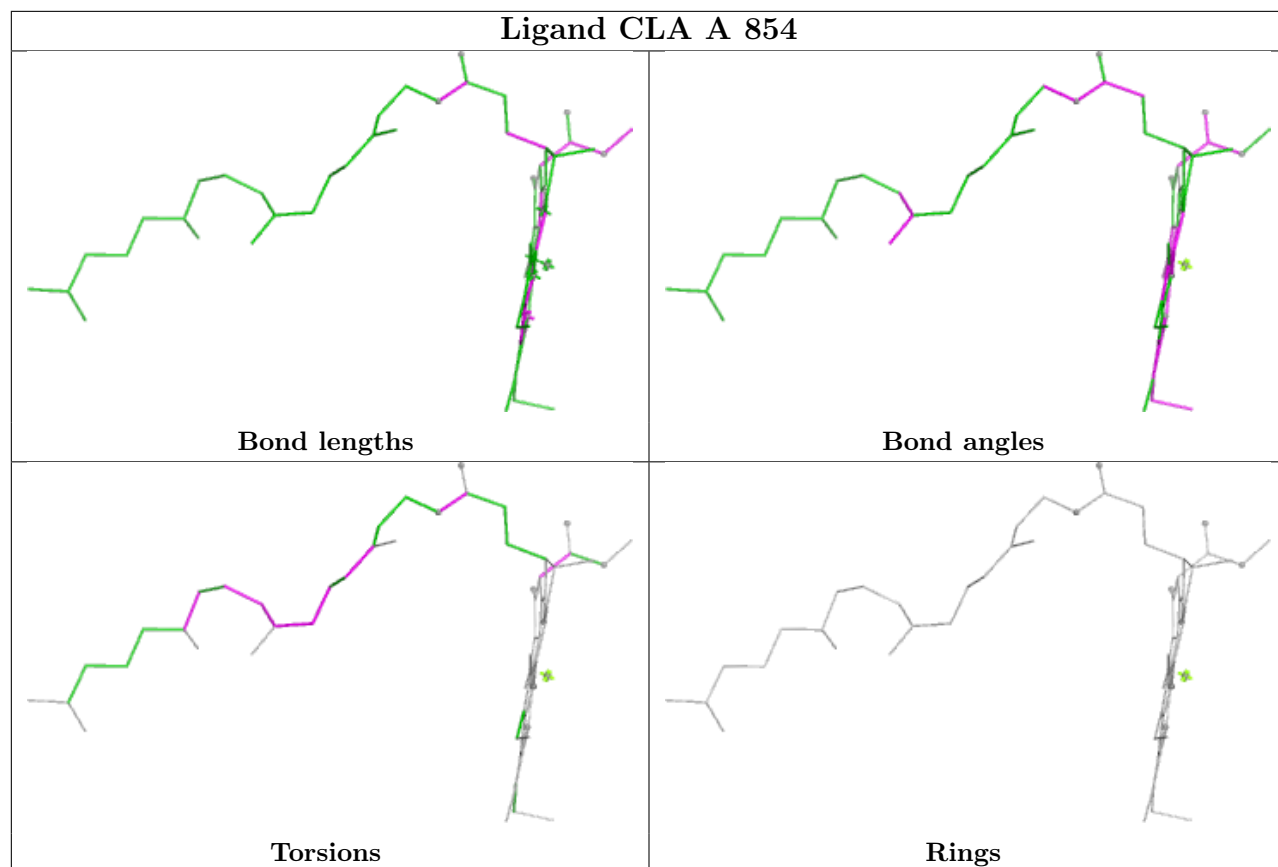


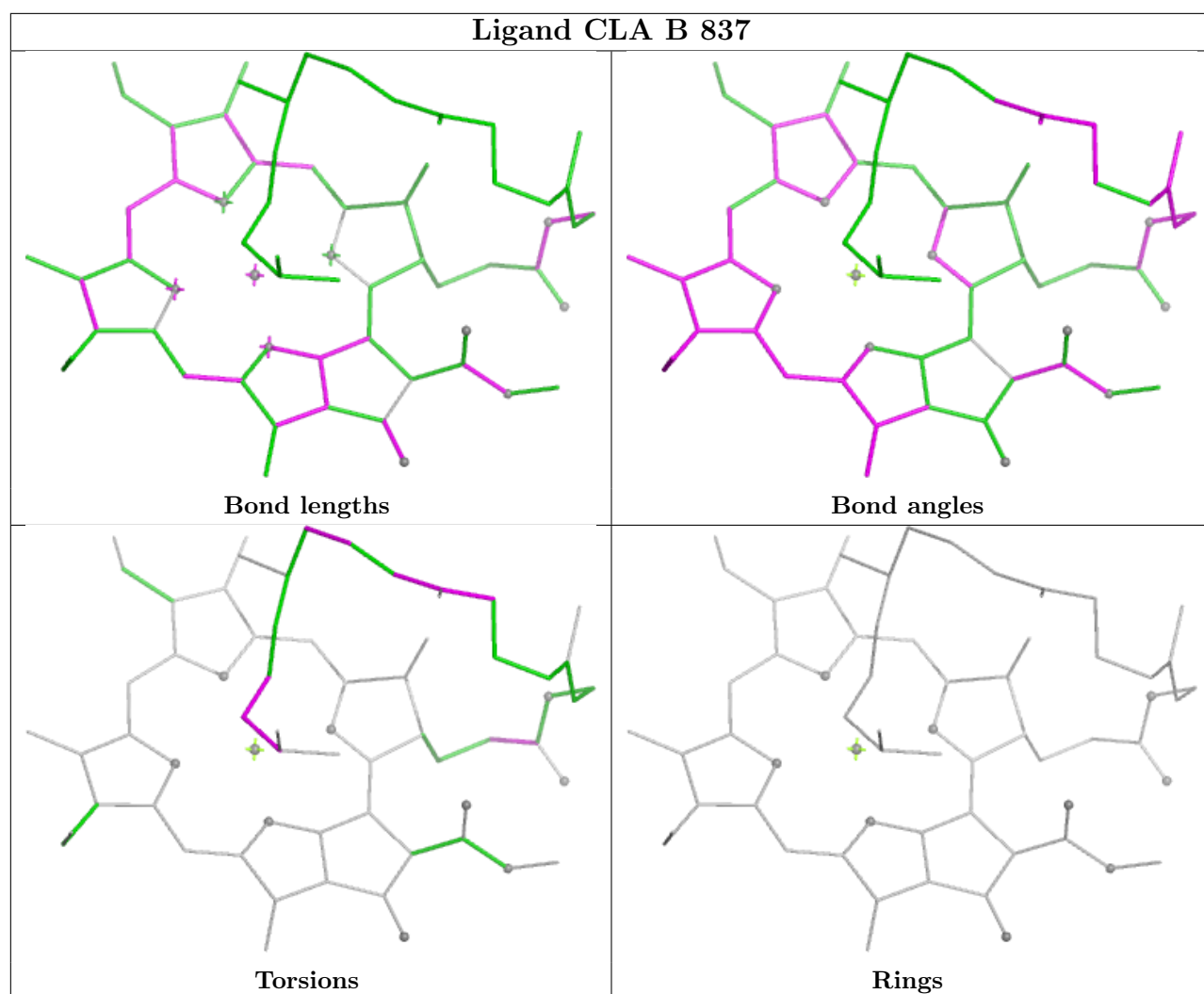


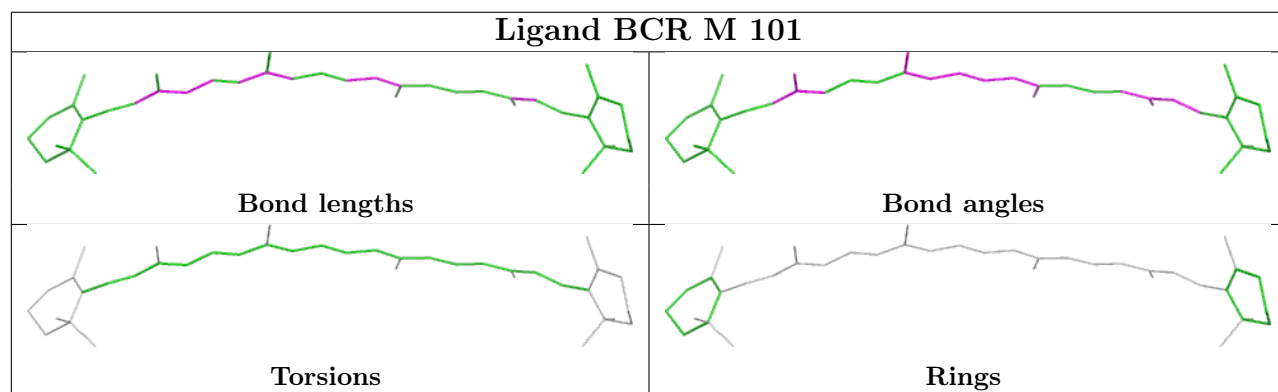
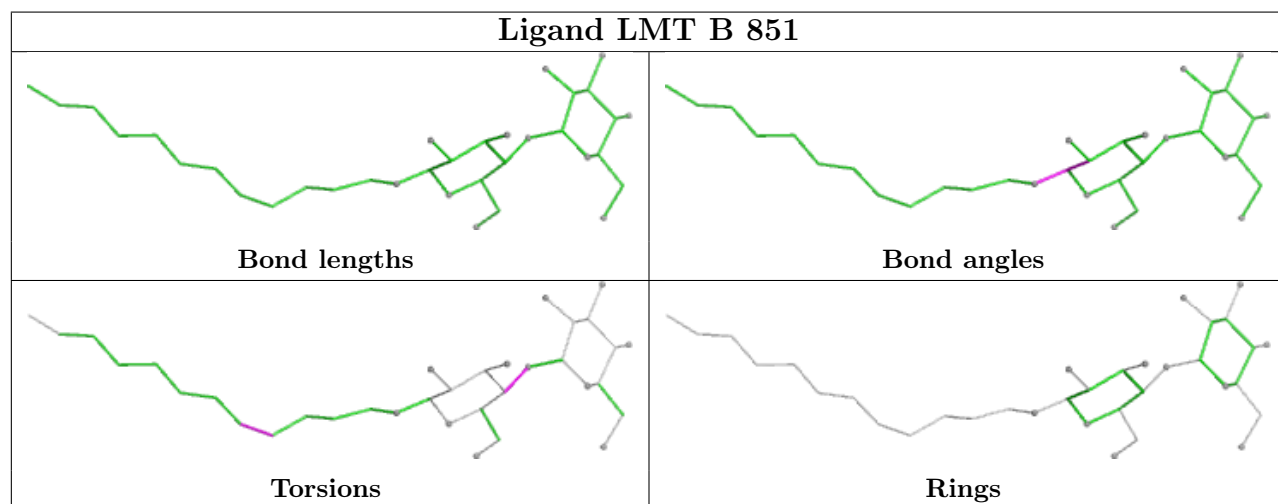
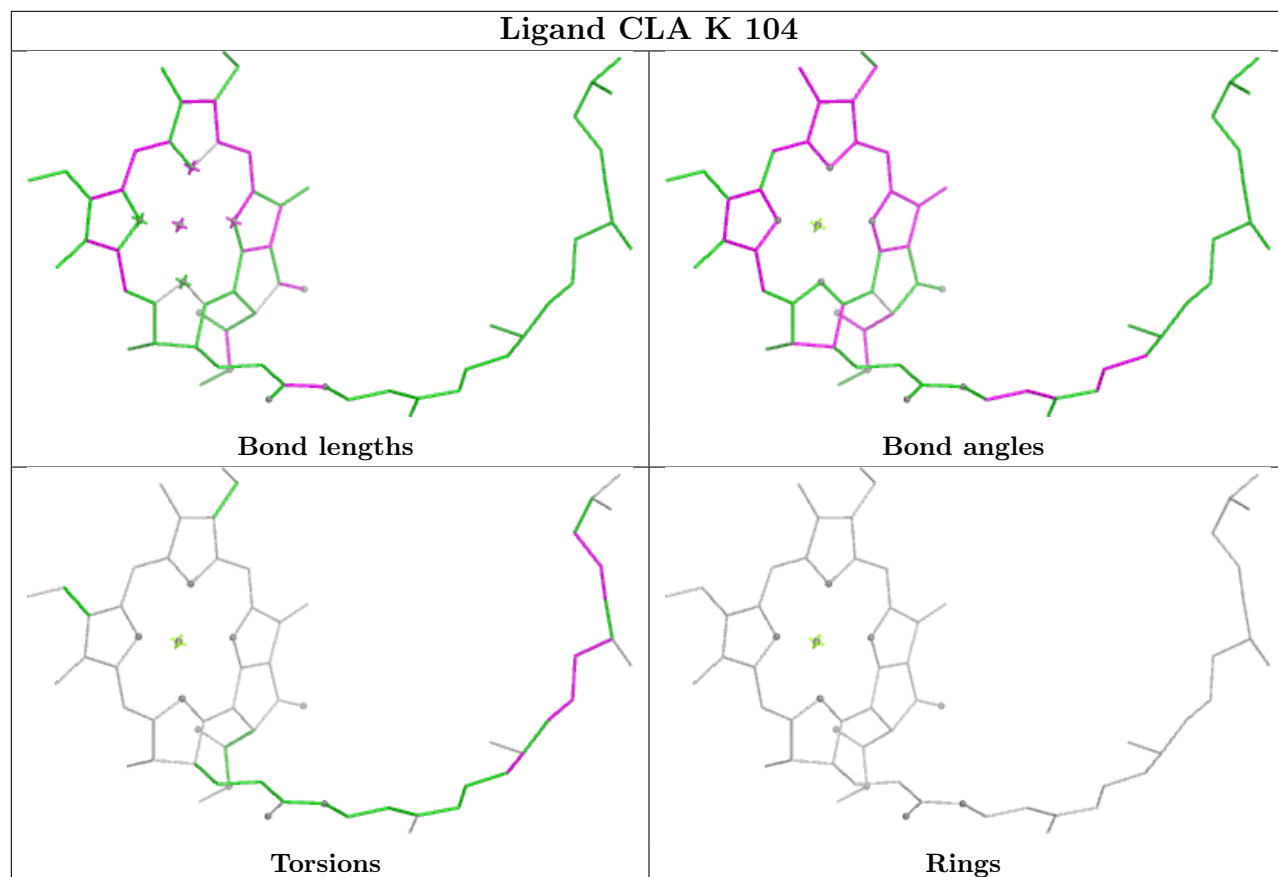


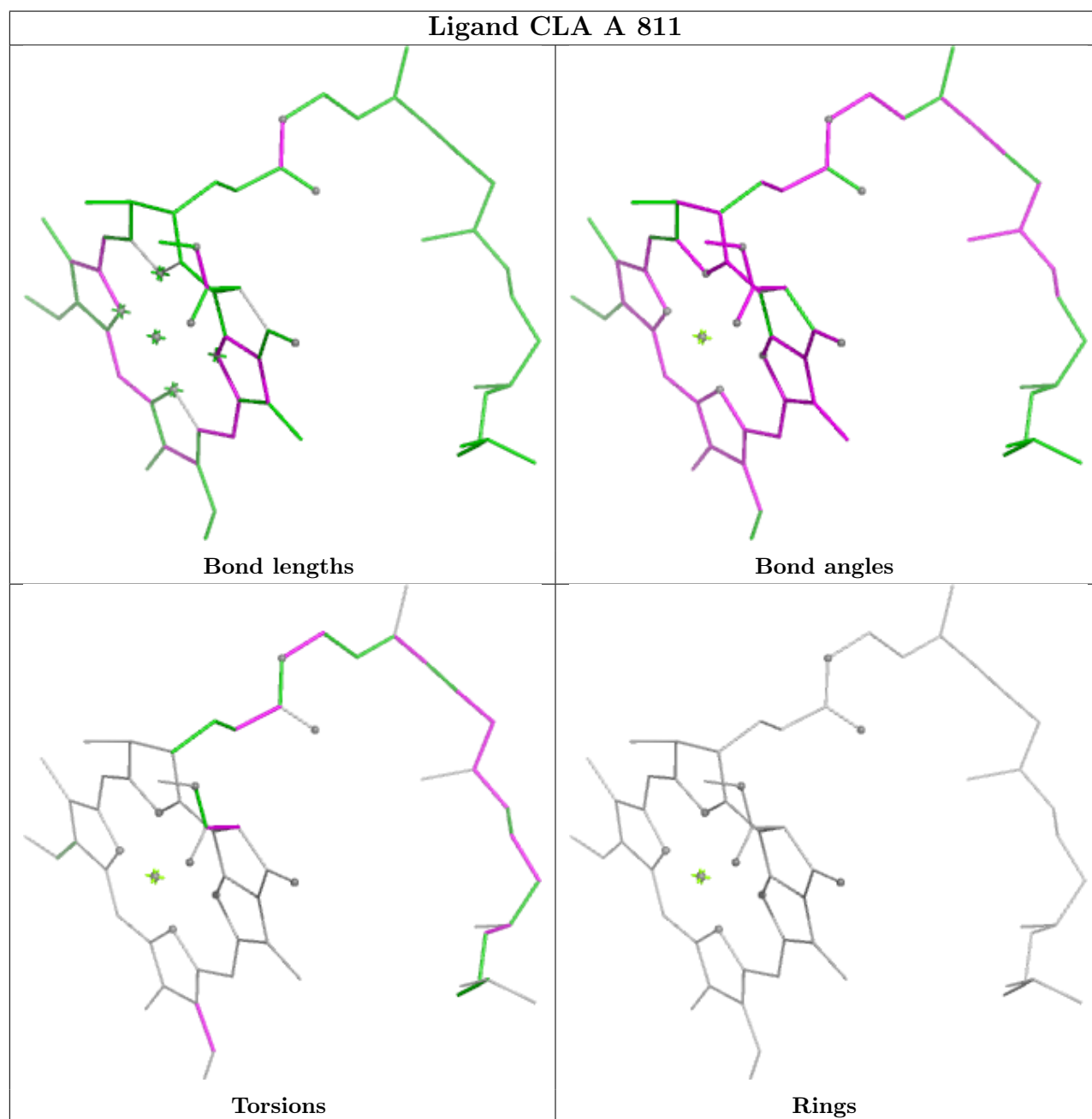
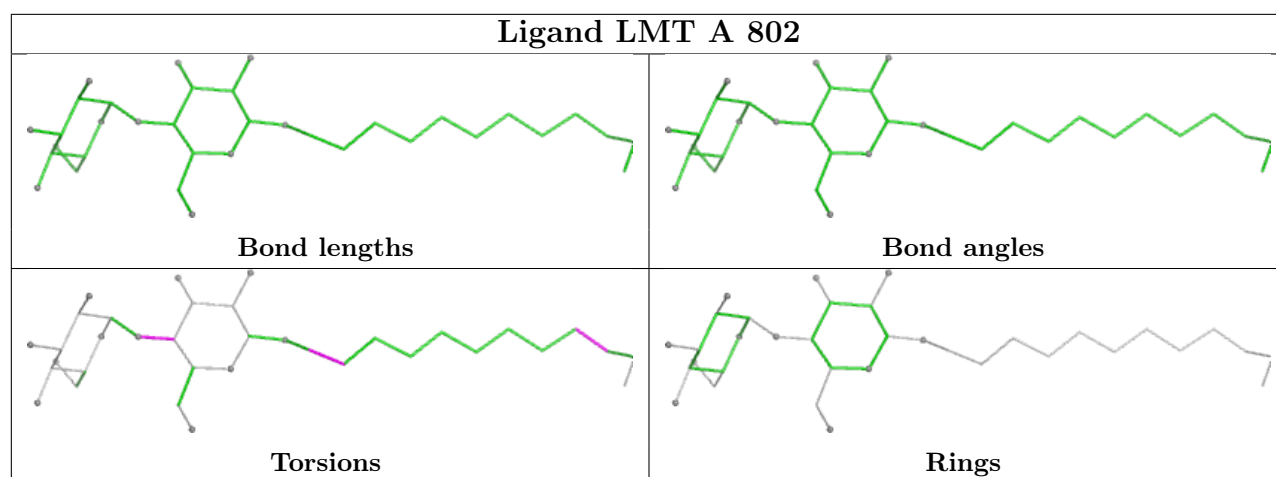


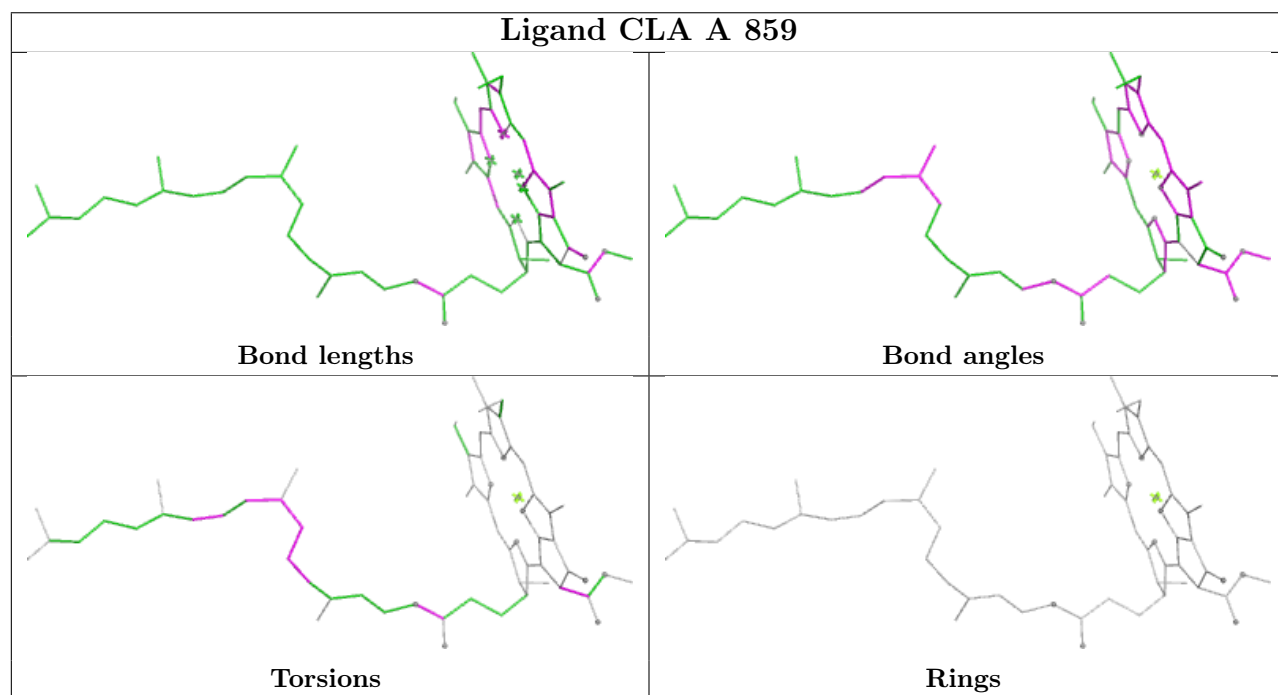
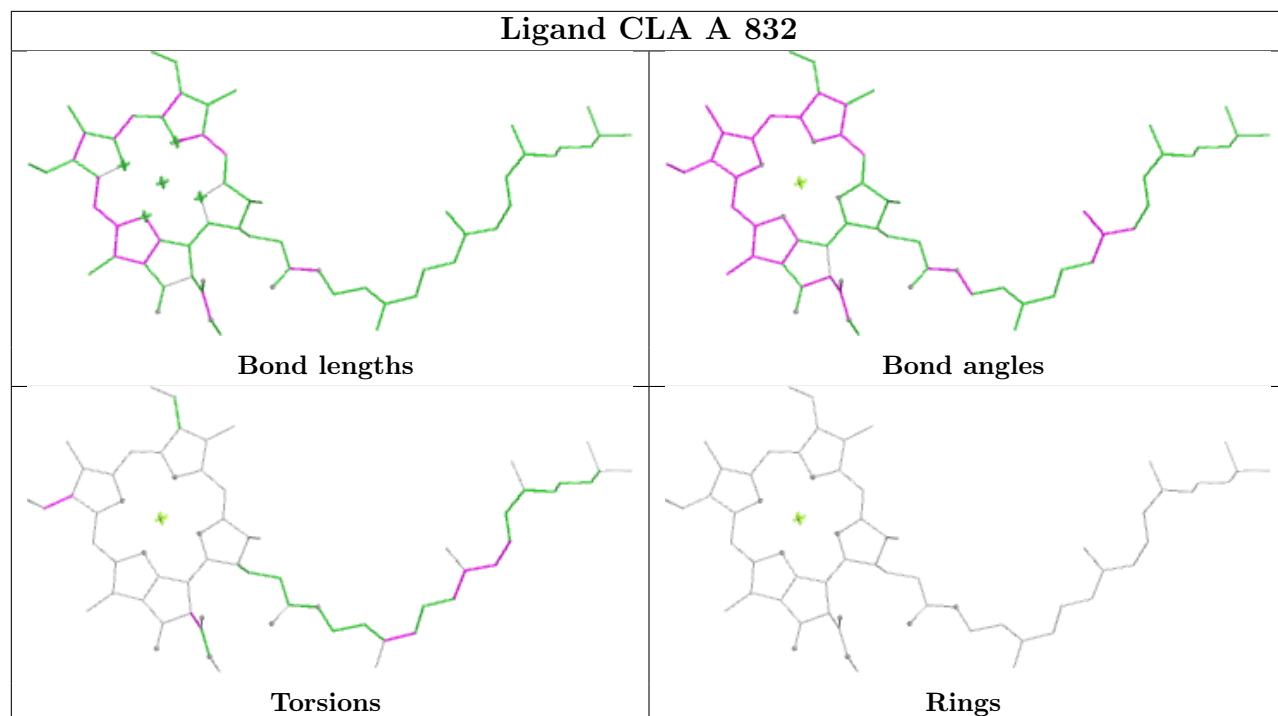


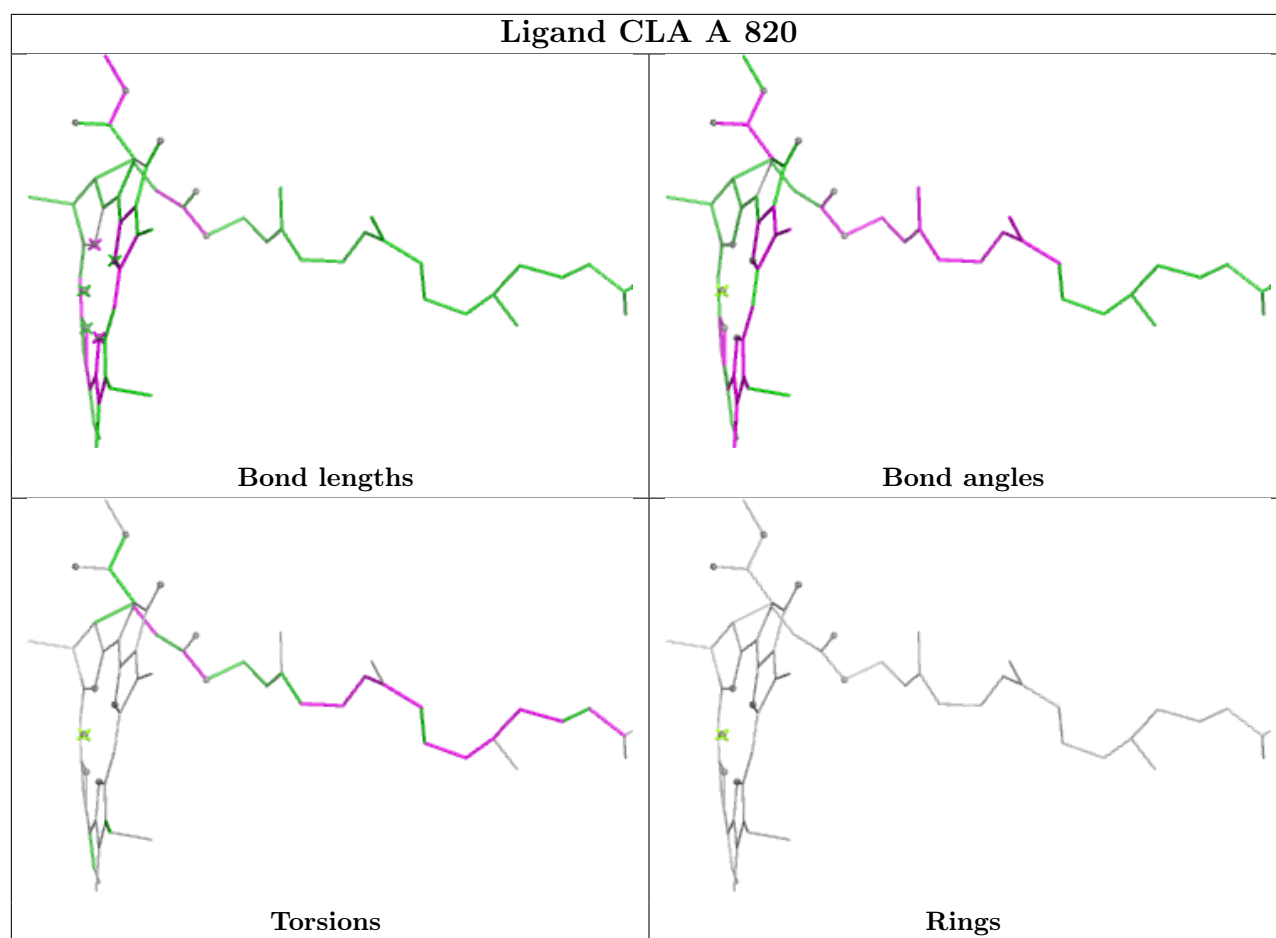


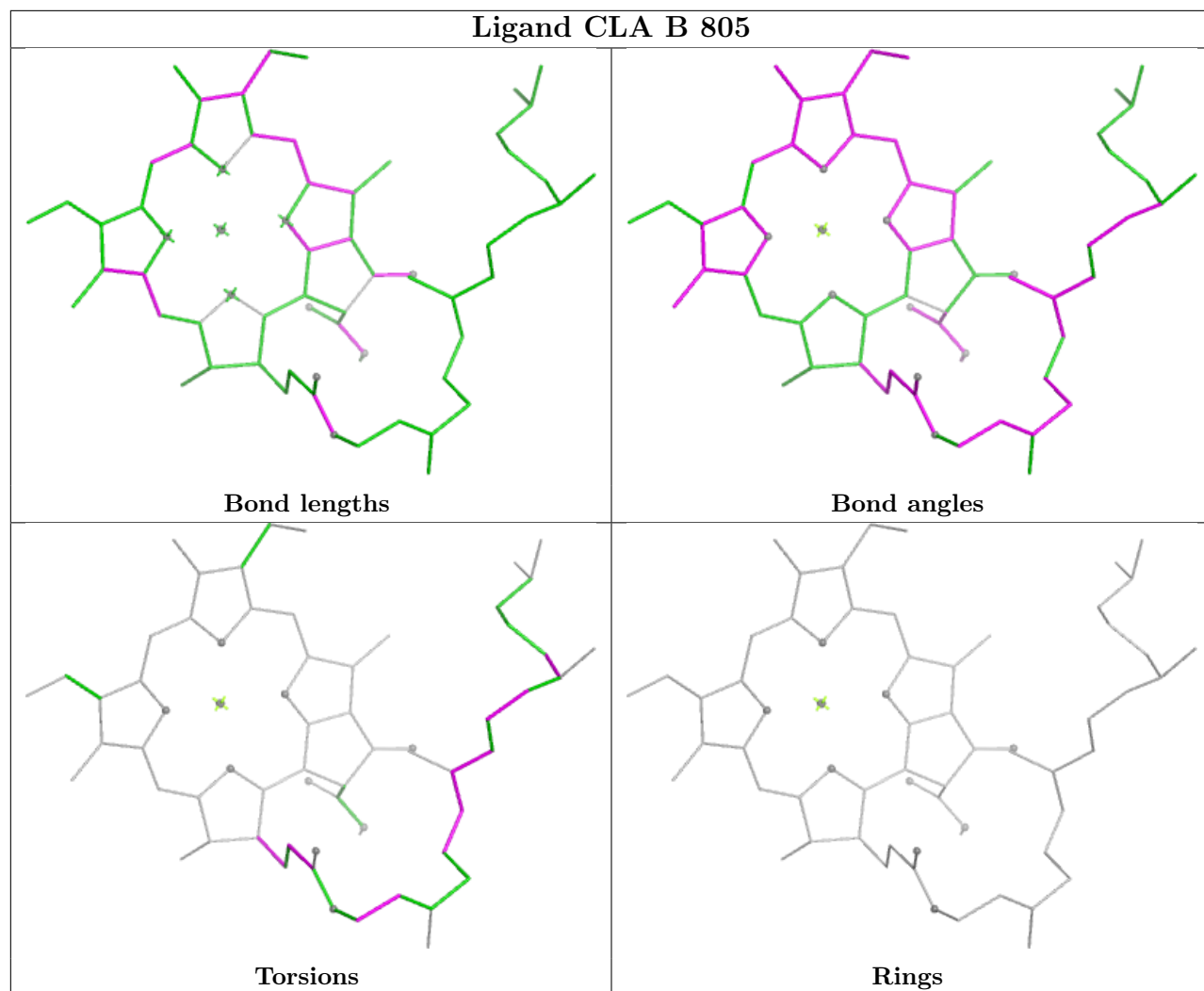


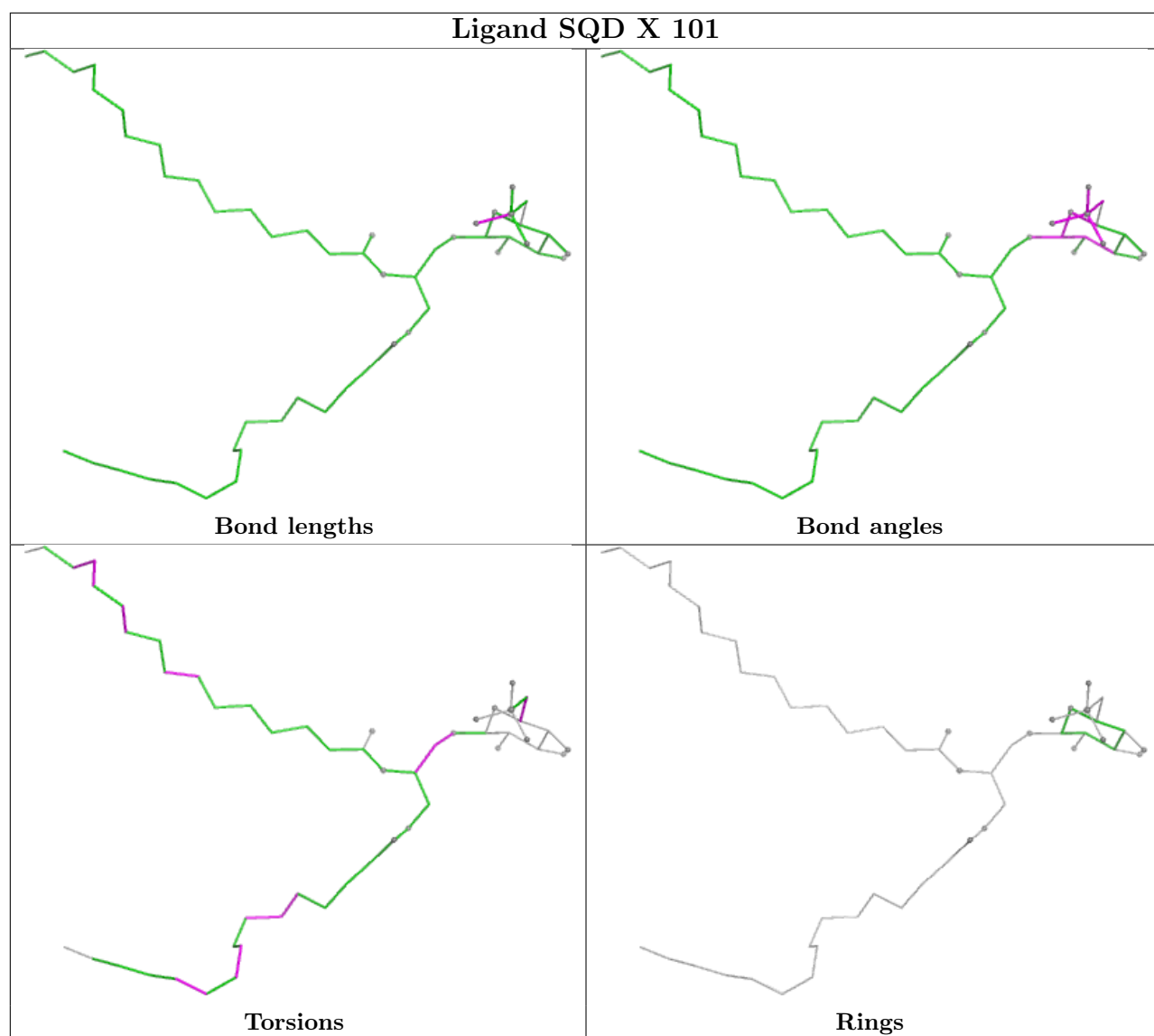


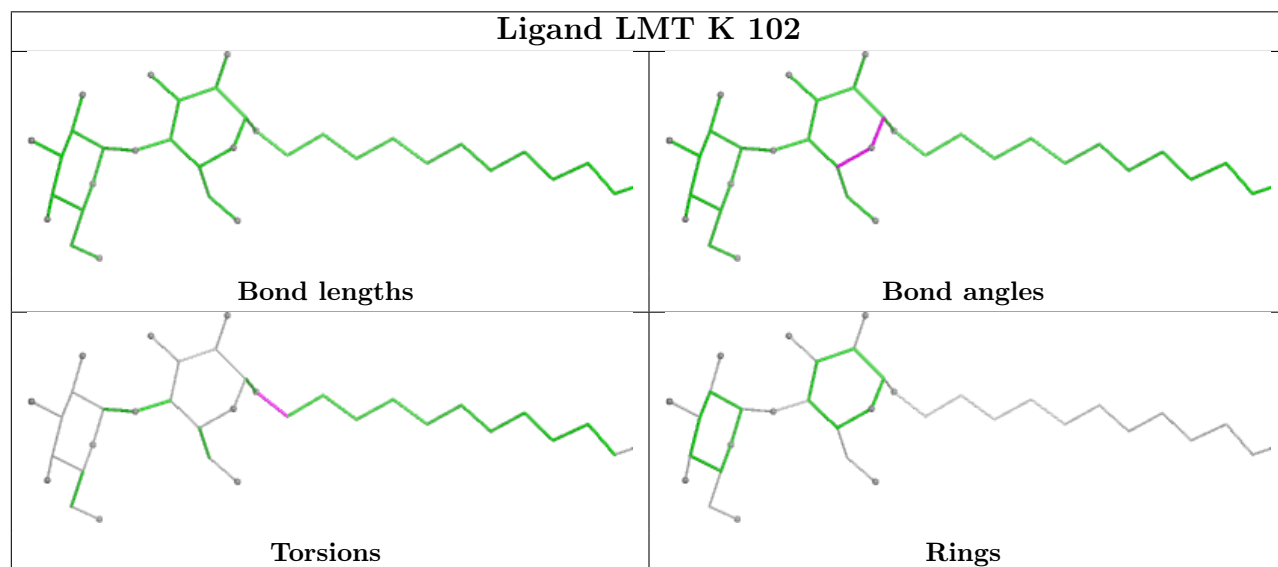
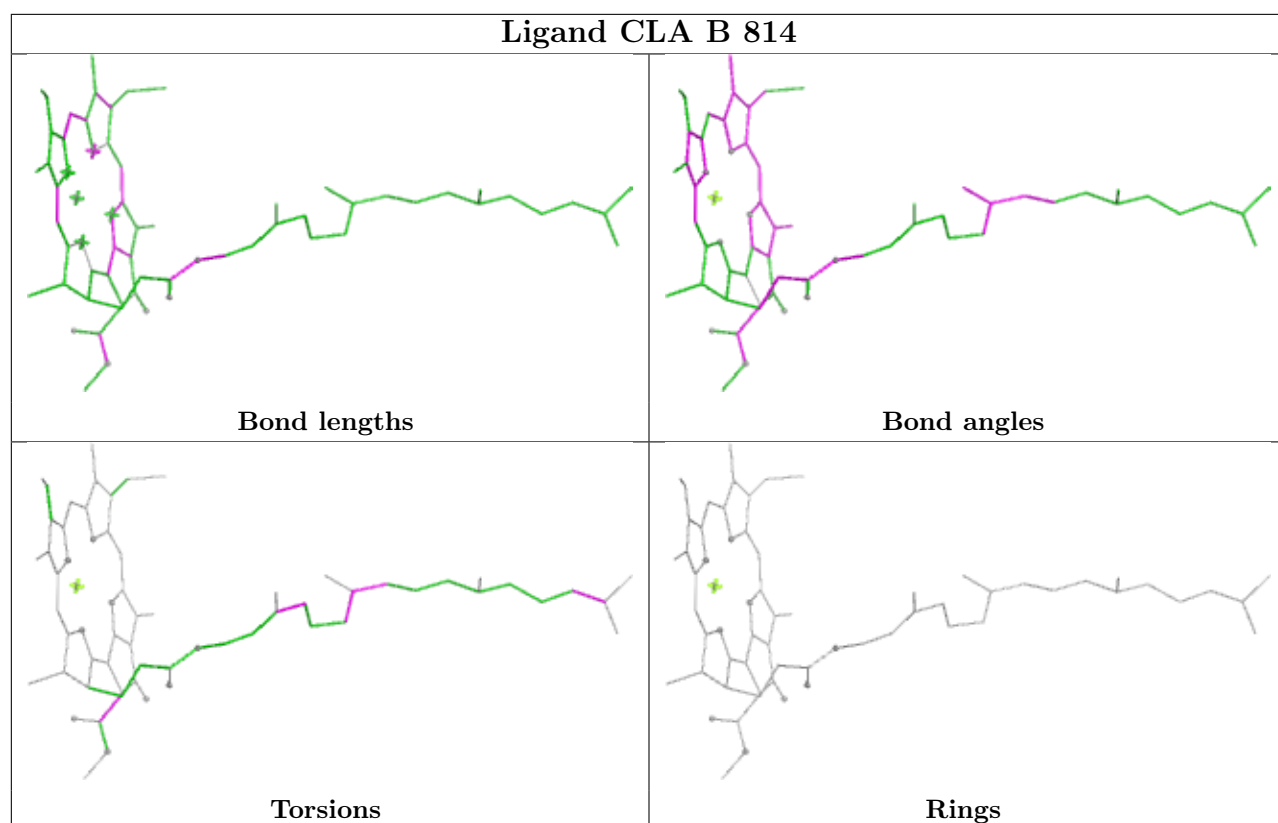


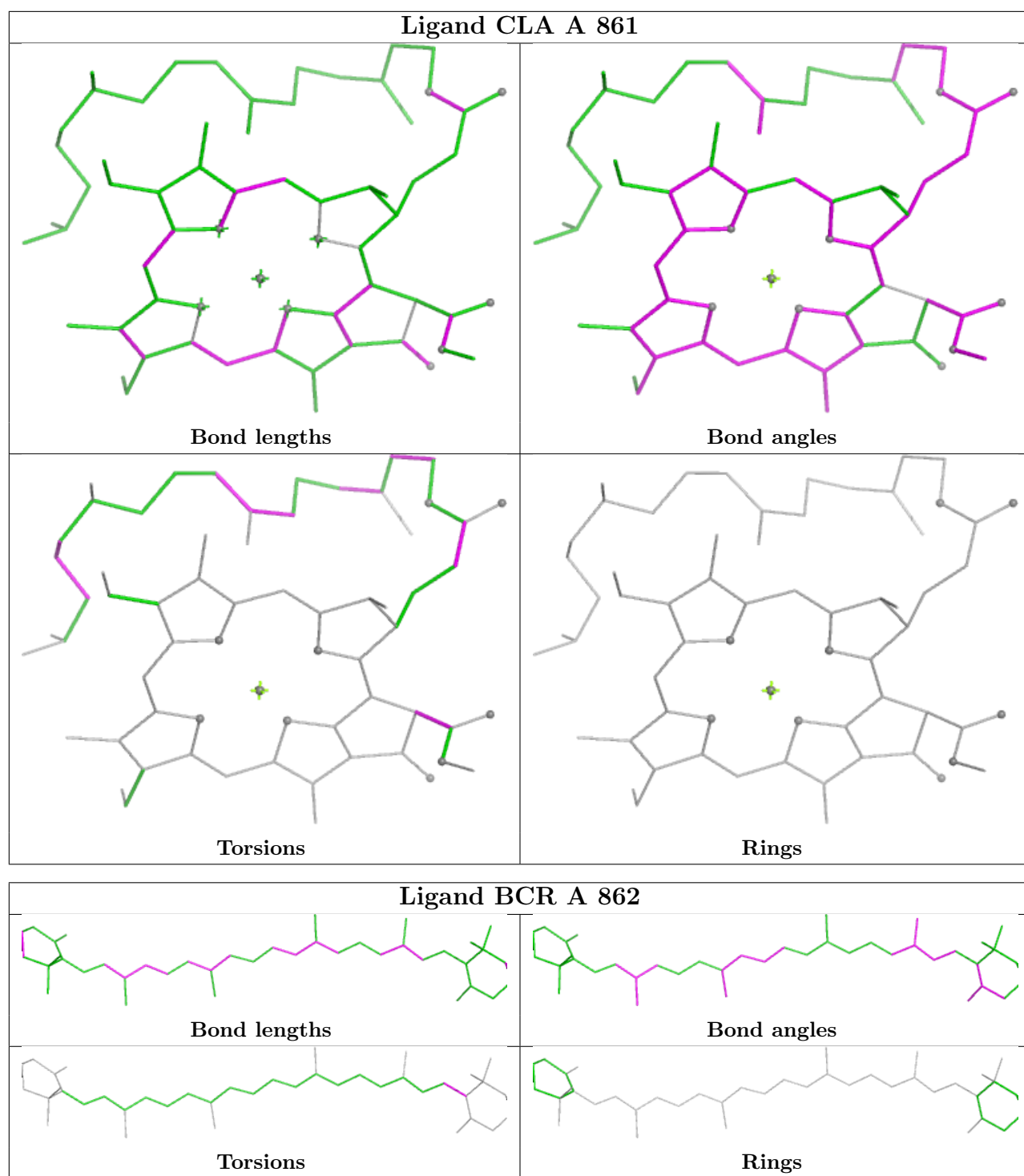


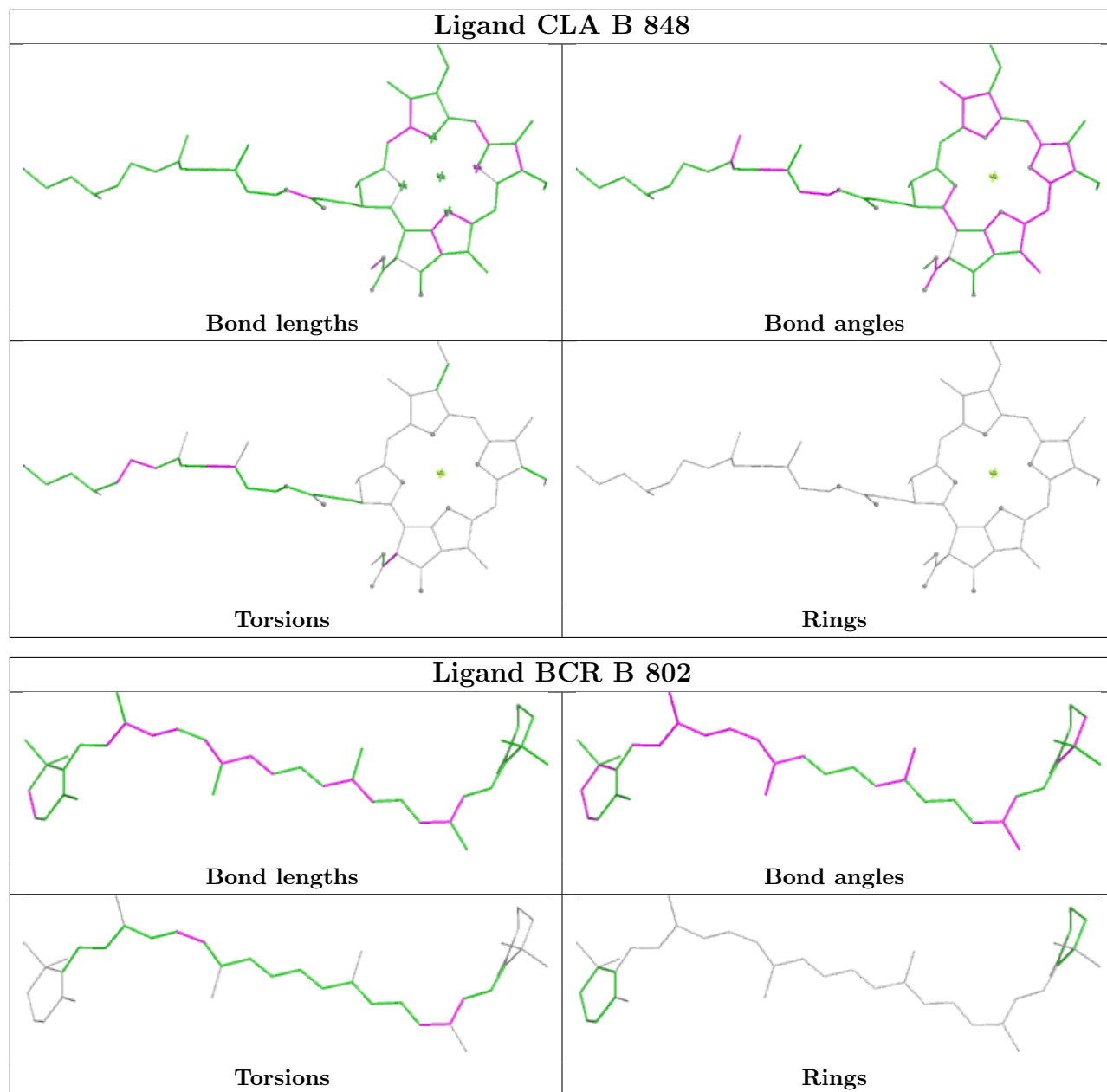


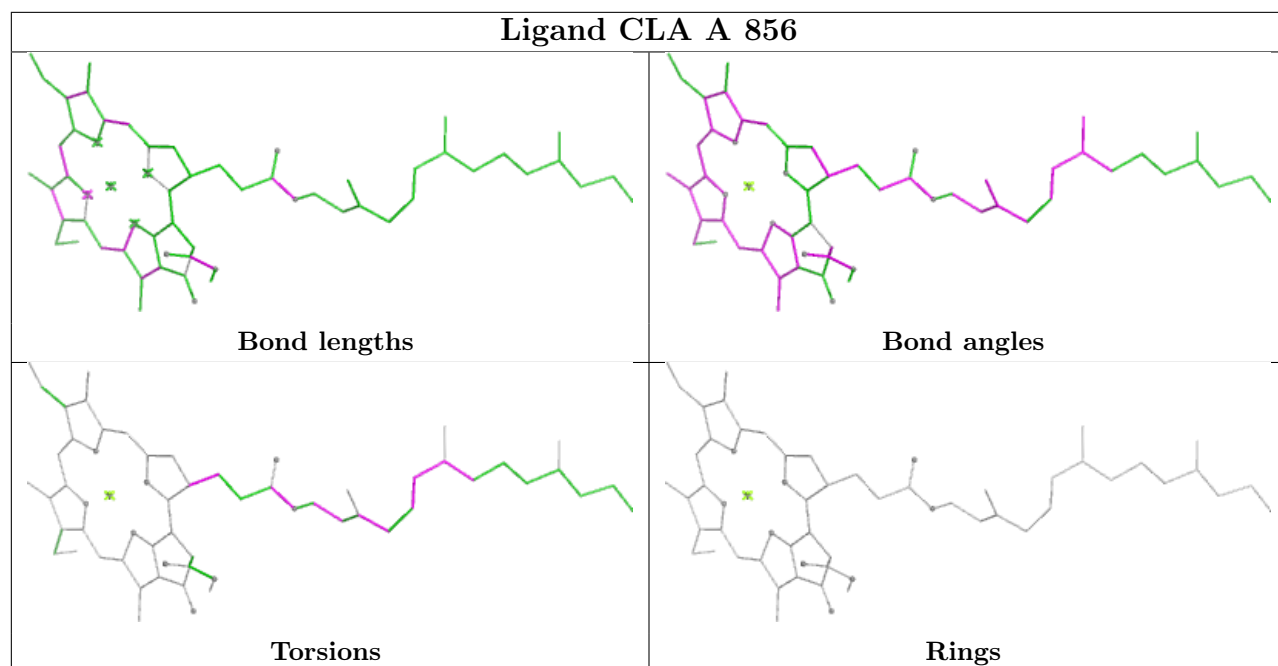
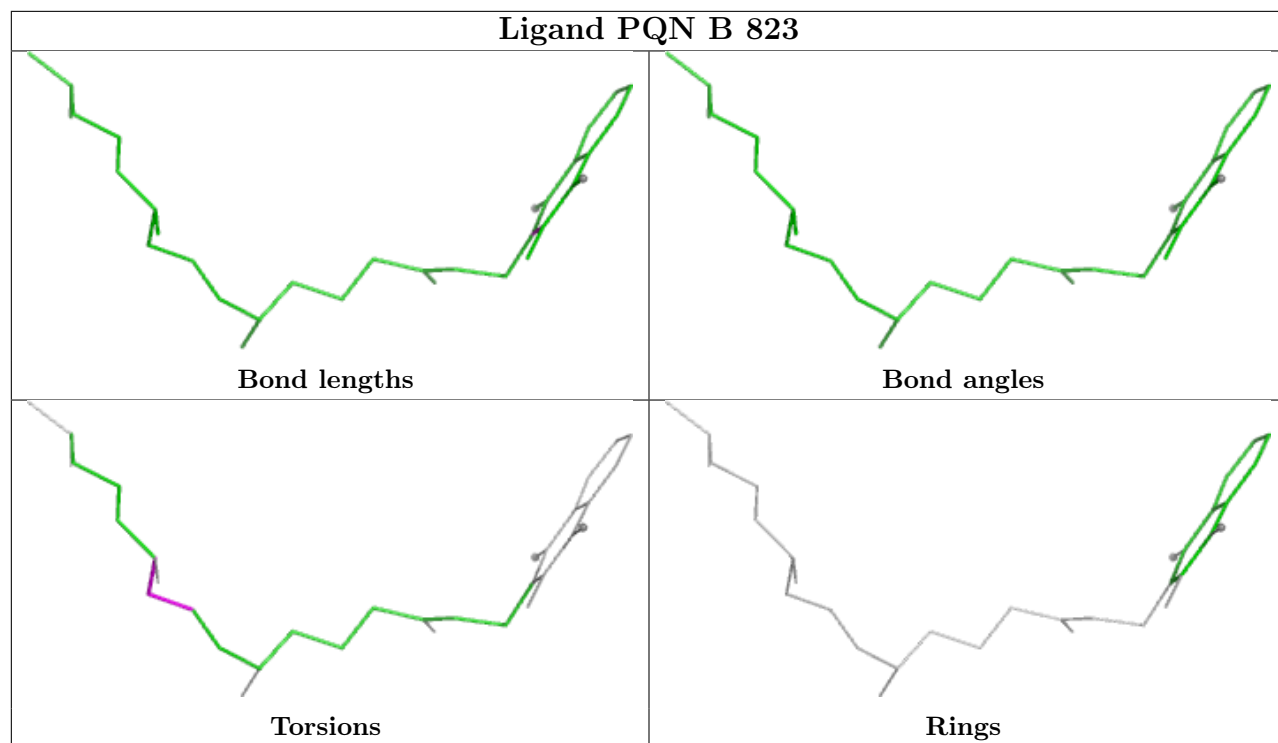


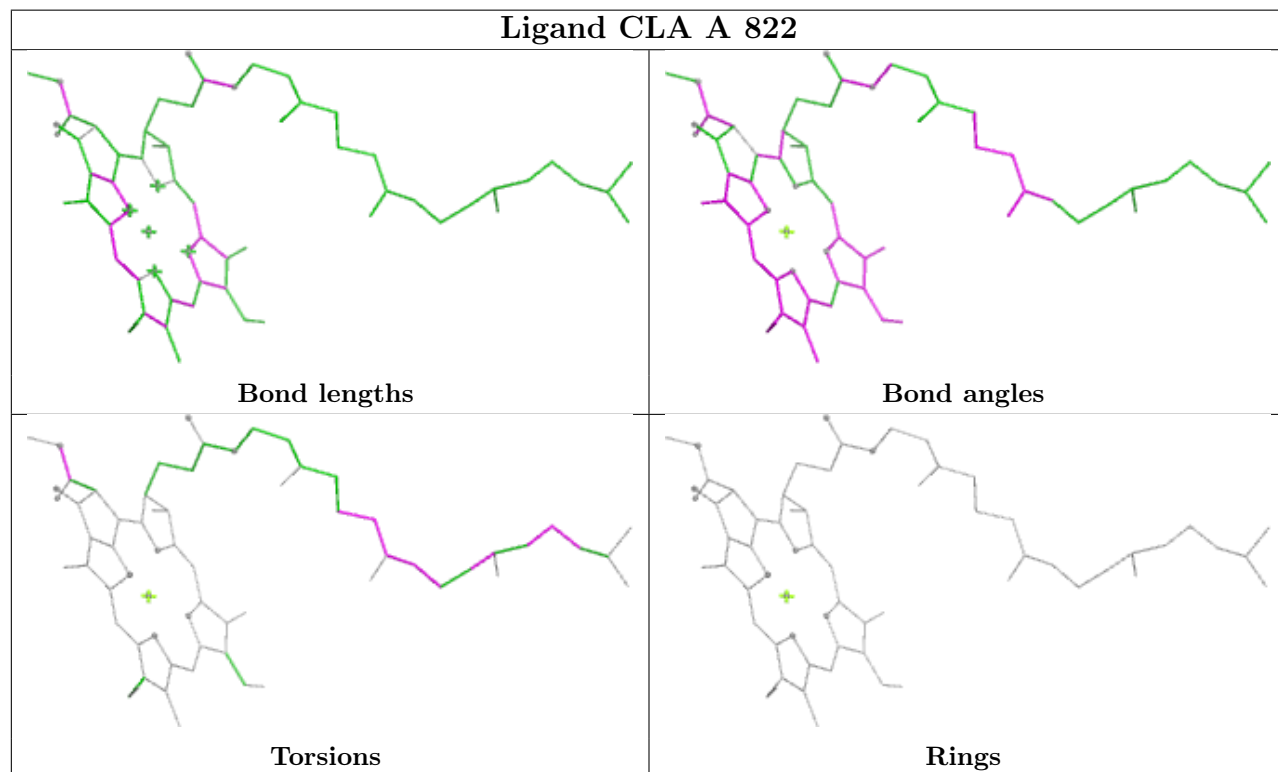
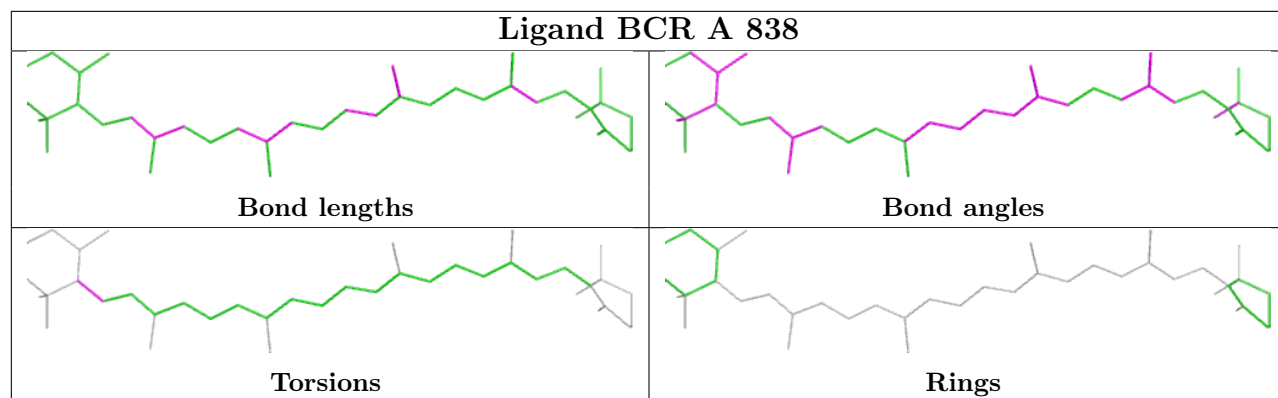


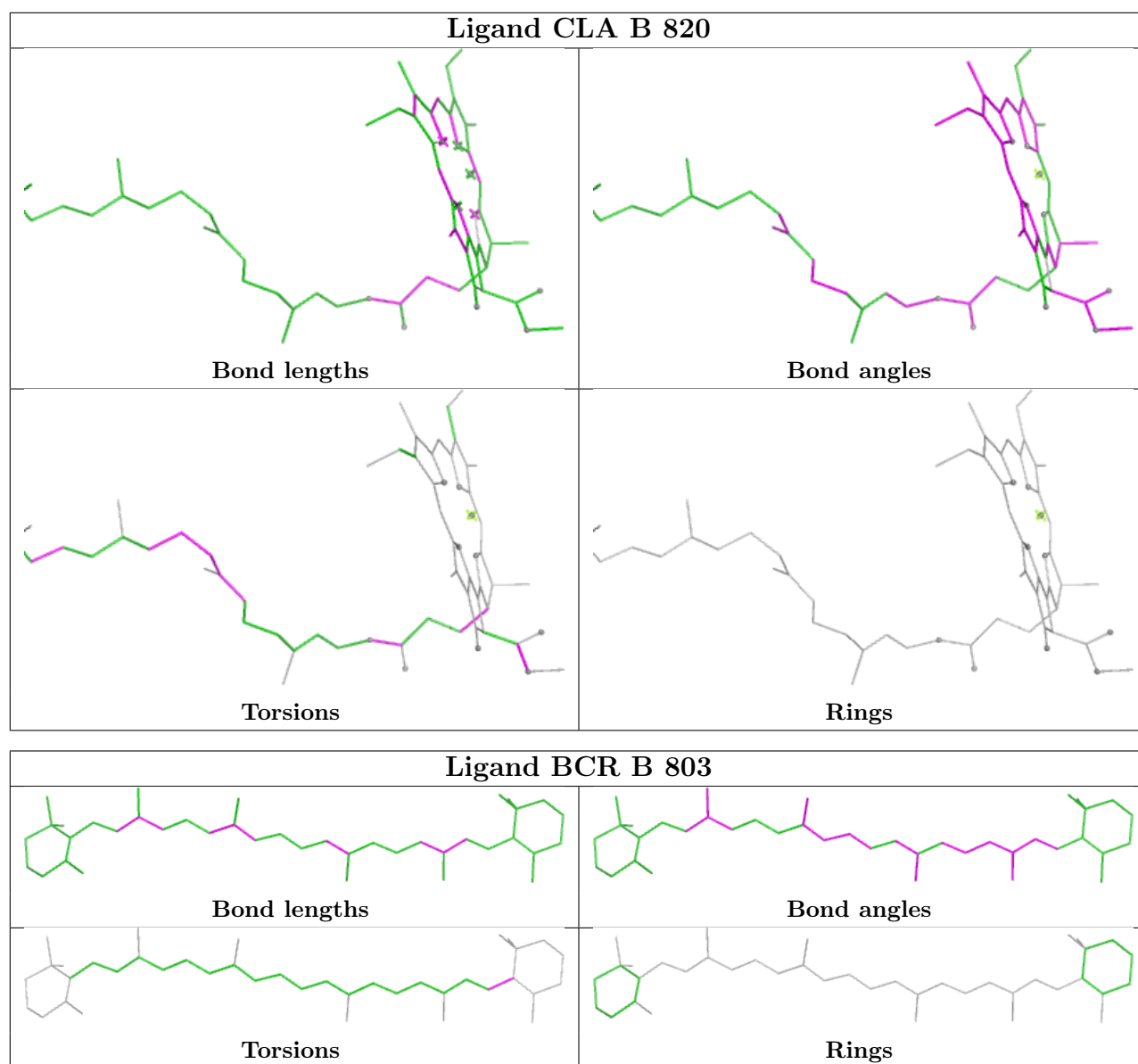


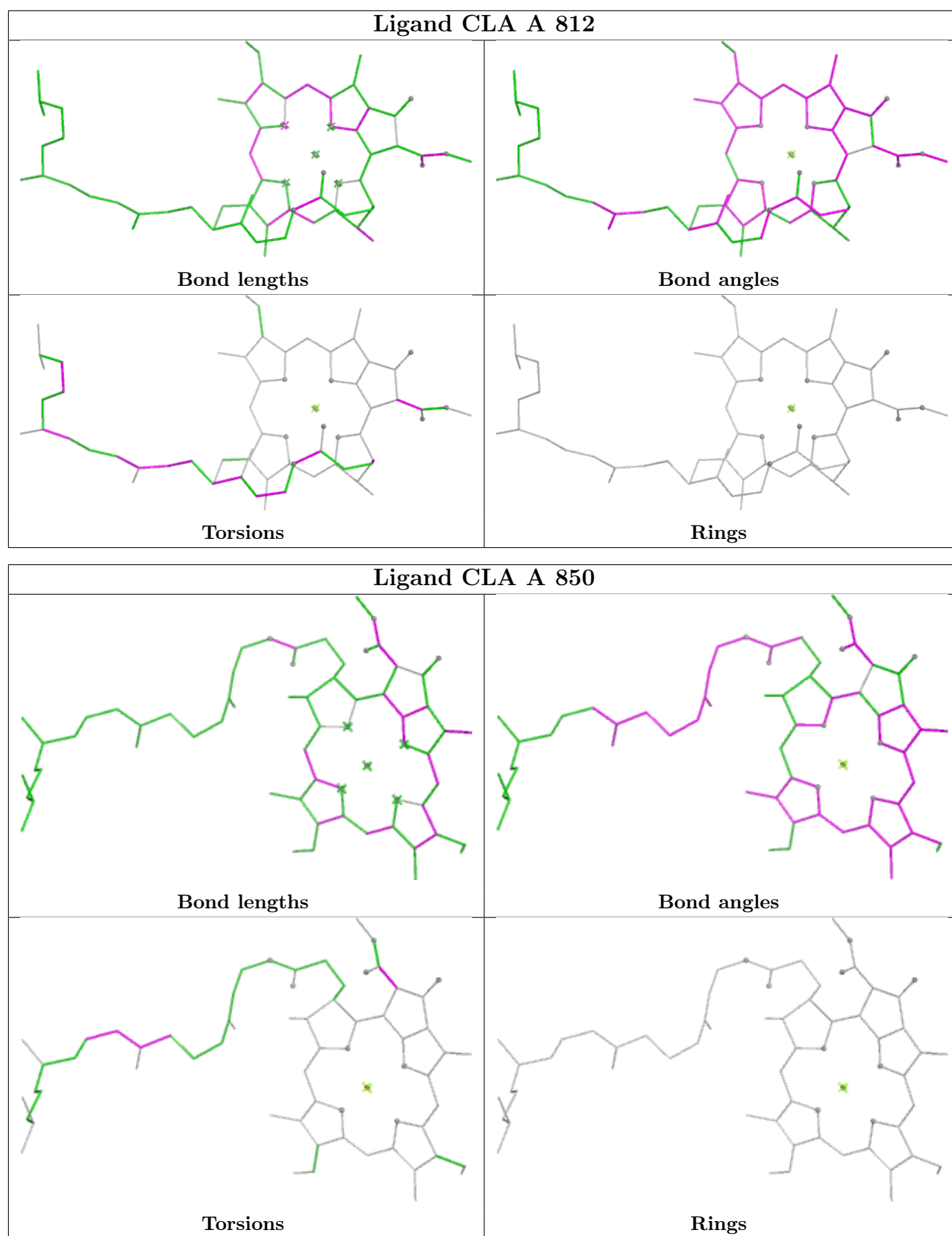


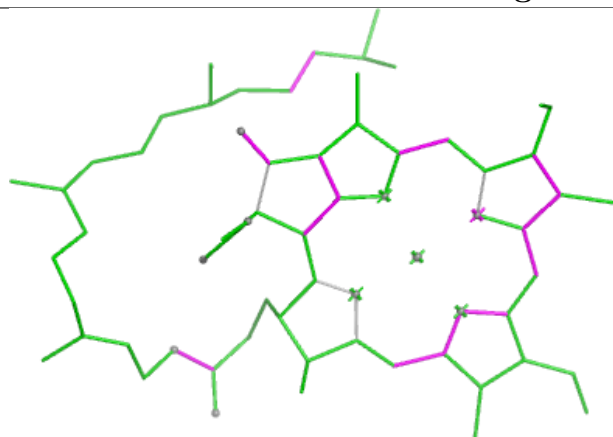
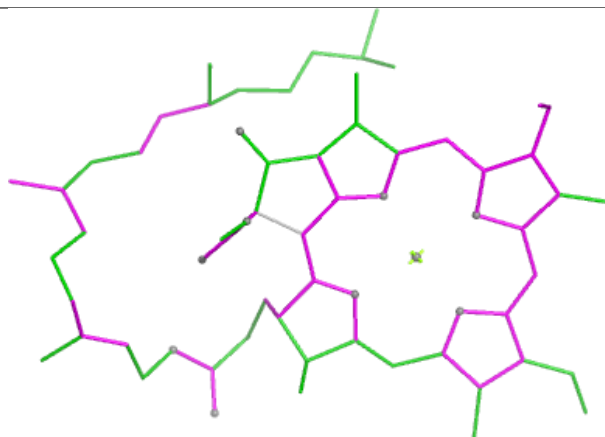
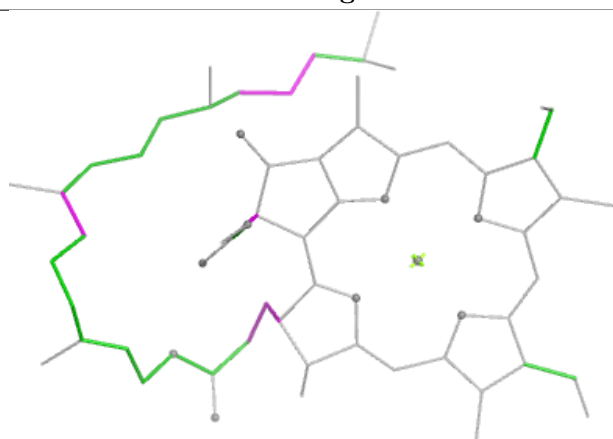
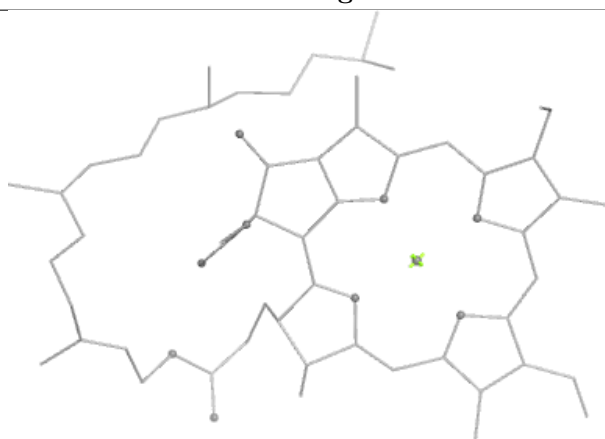
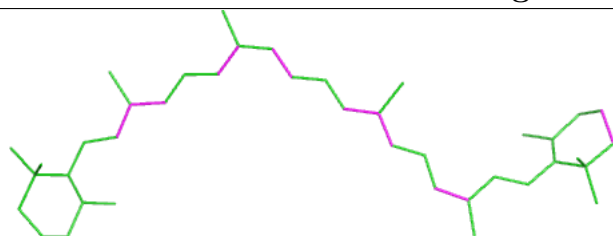
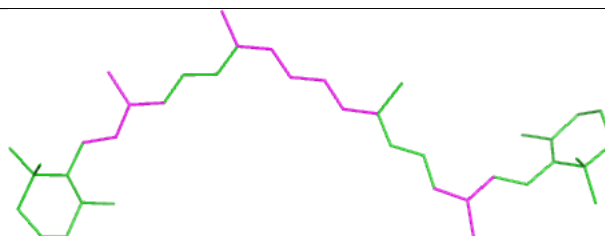
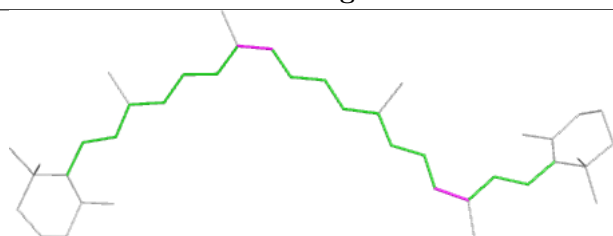
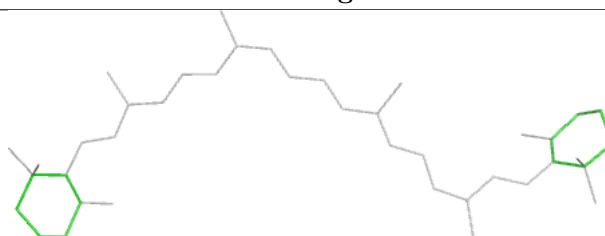


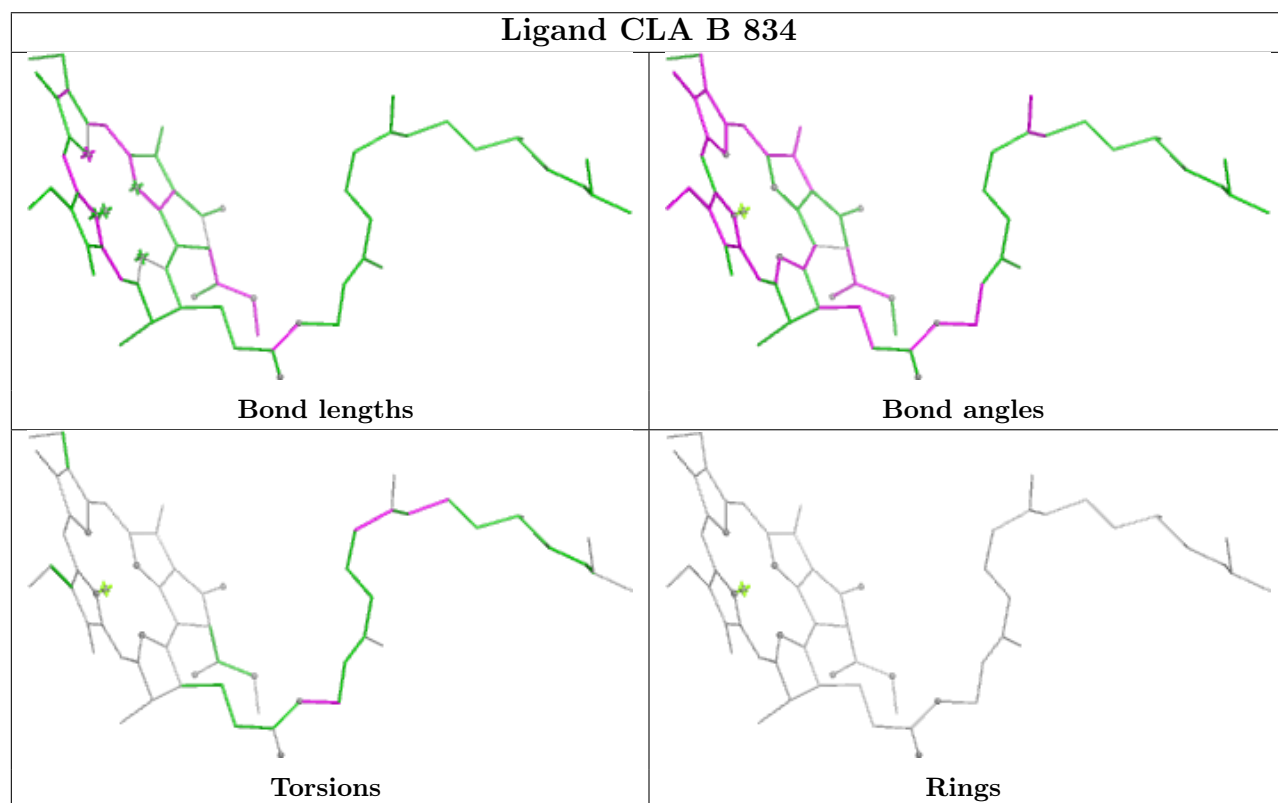
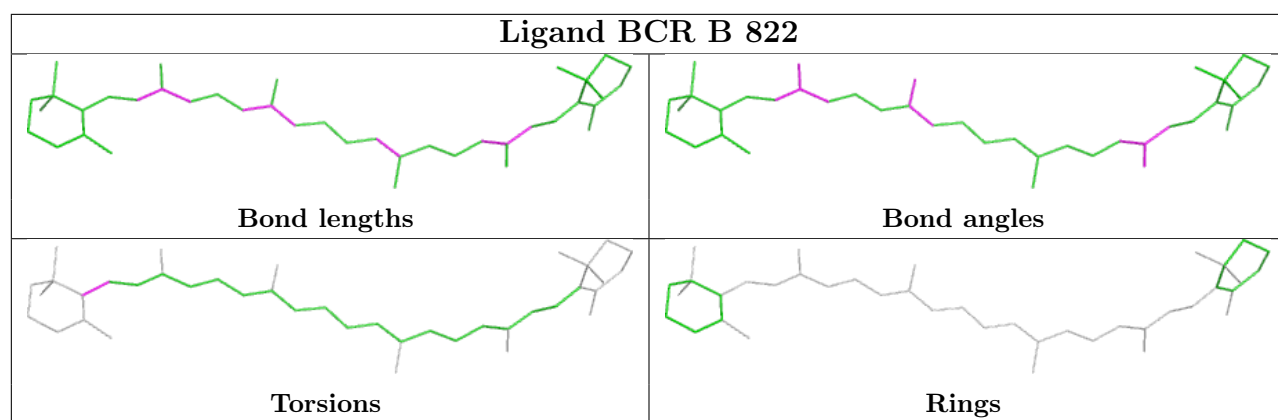


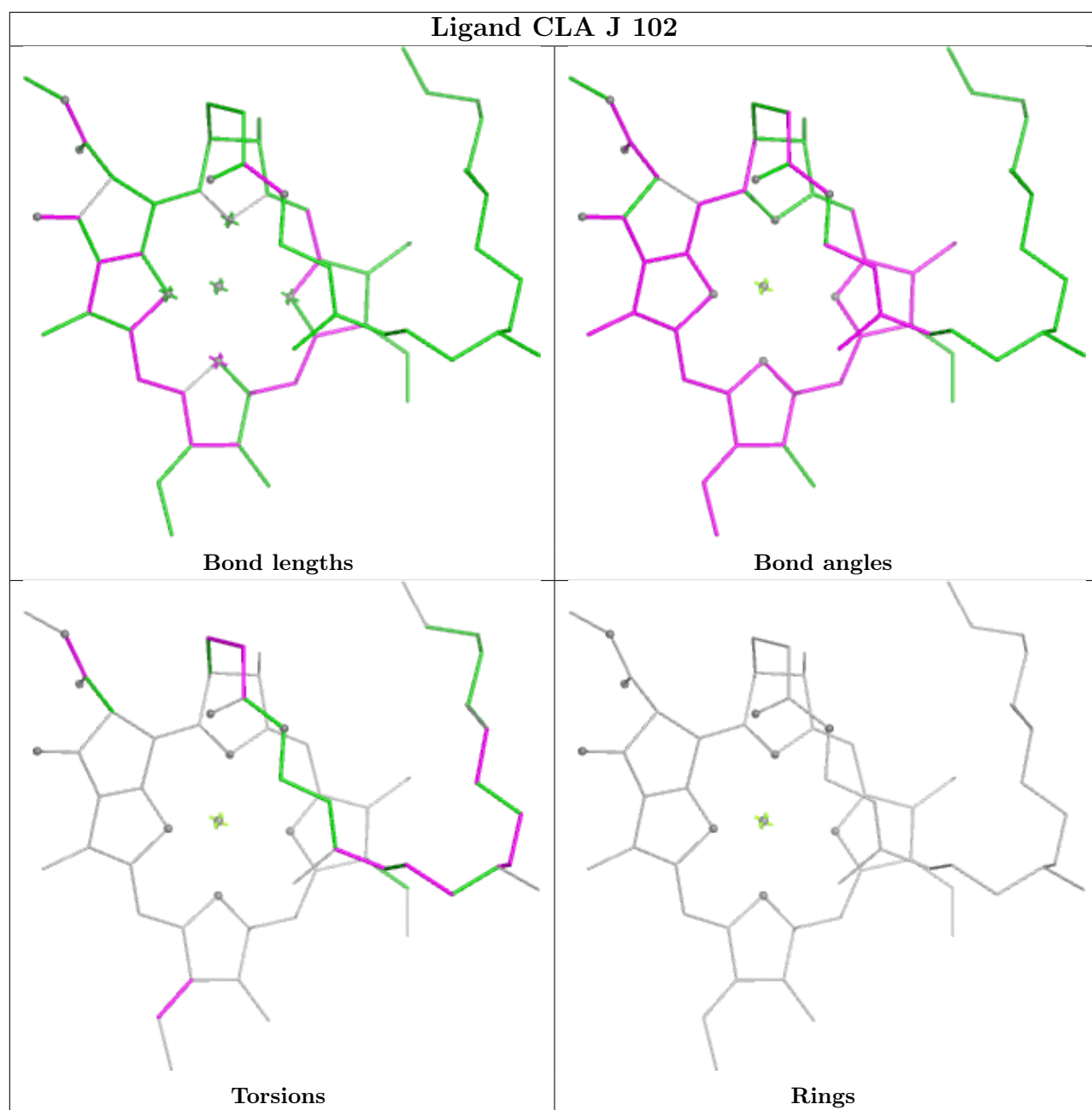


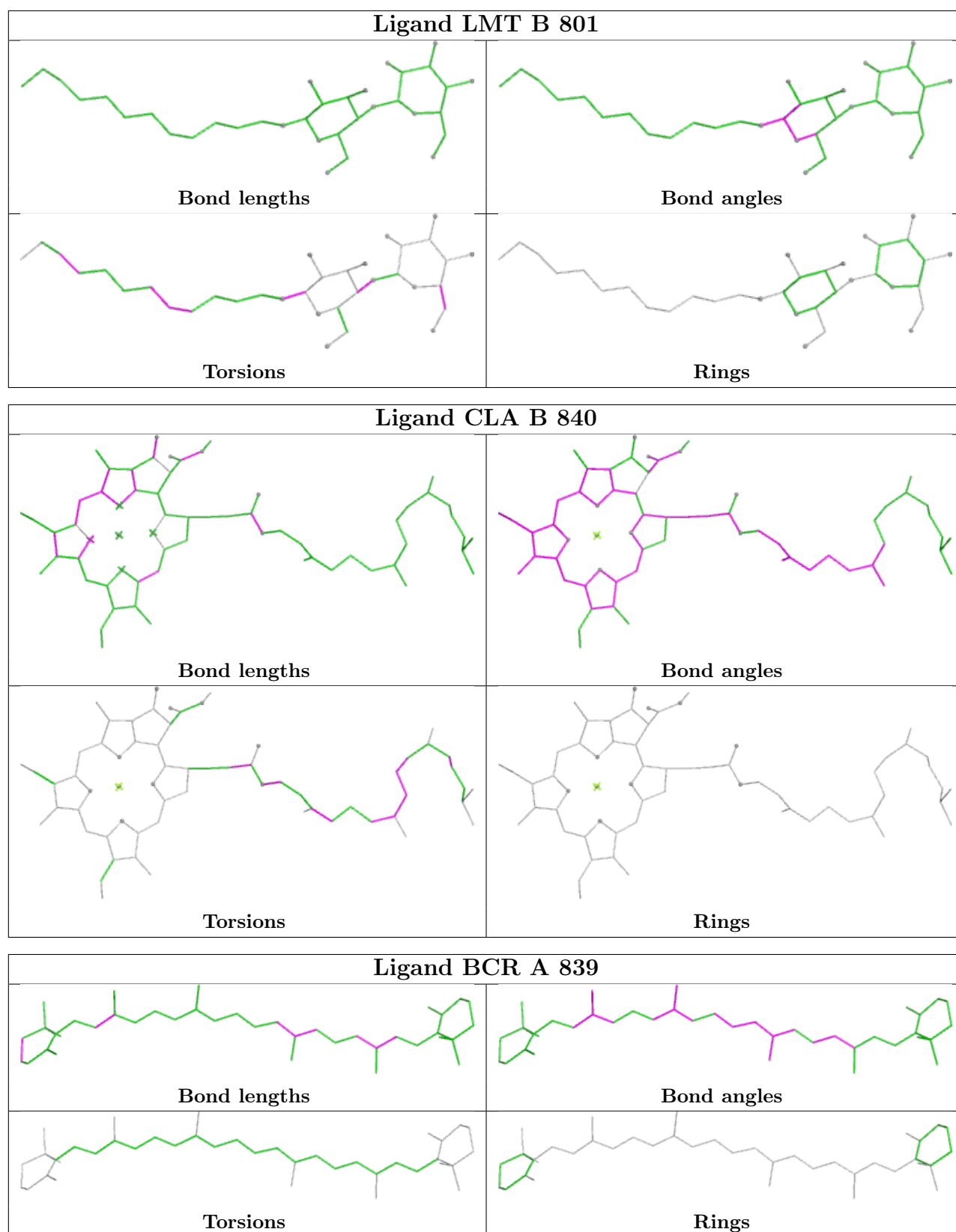


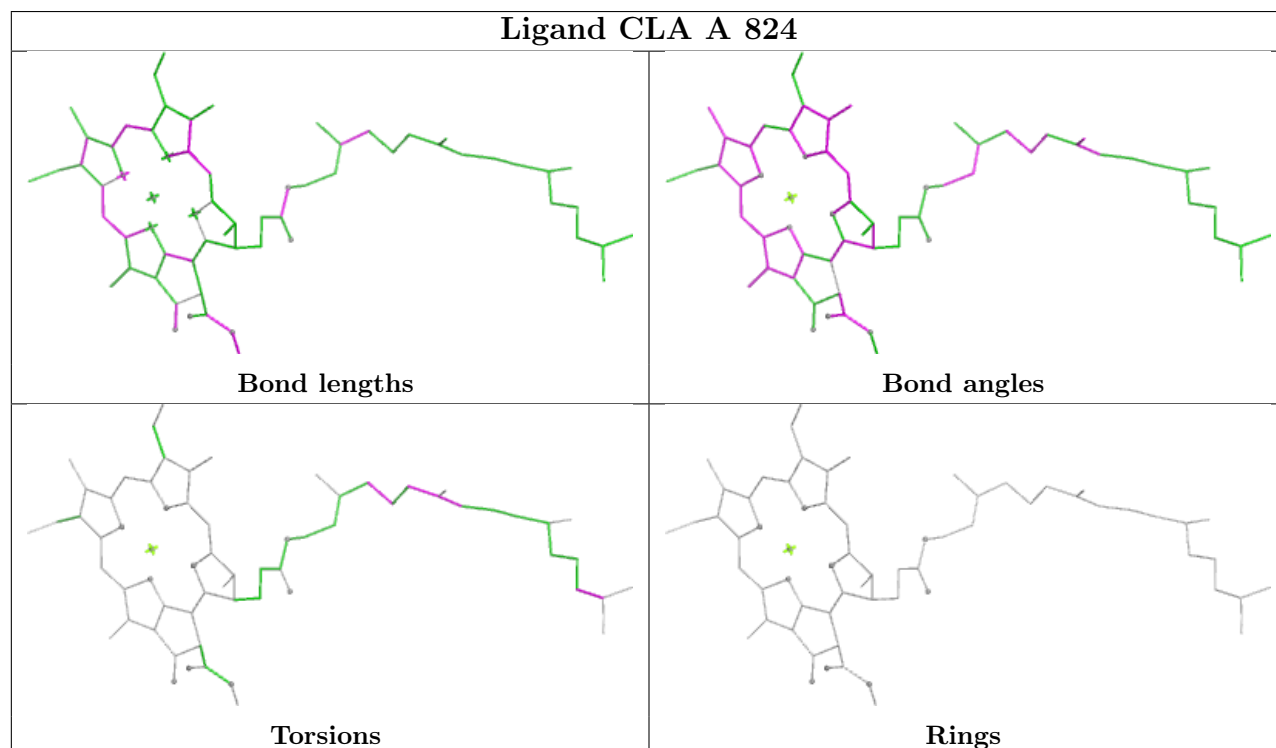
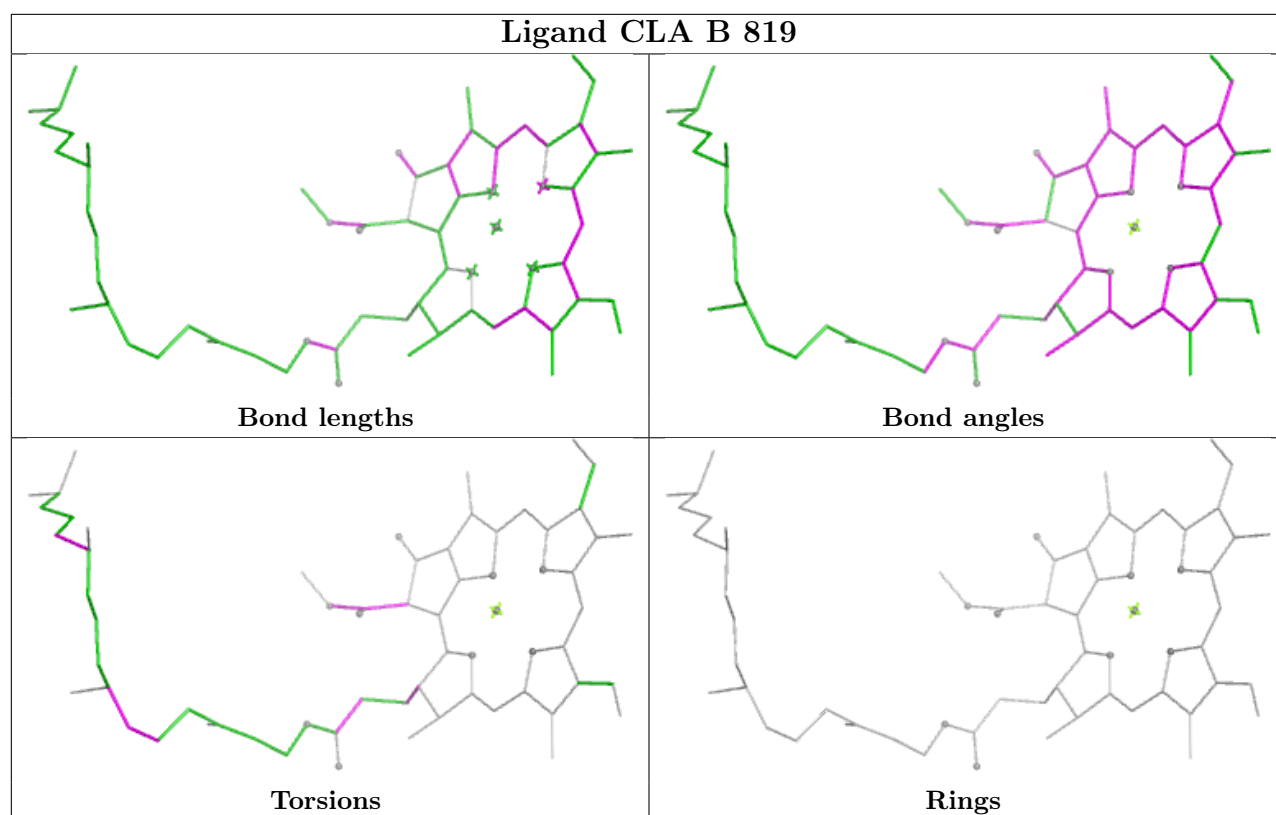


Ligand CLA B 836**Bond lengths****Bond angles****Torsions****Rings****Ligand BCR A 840****Bond lengths****Bond angles****Torsions****Rings**

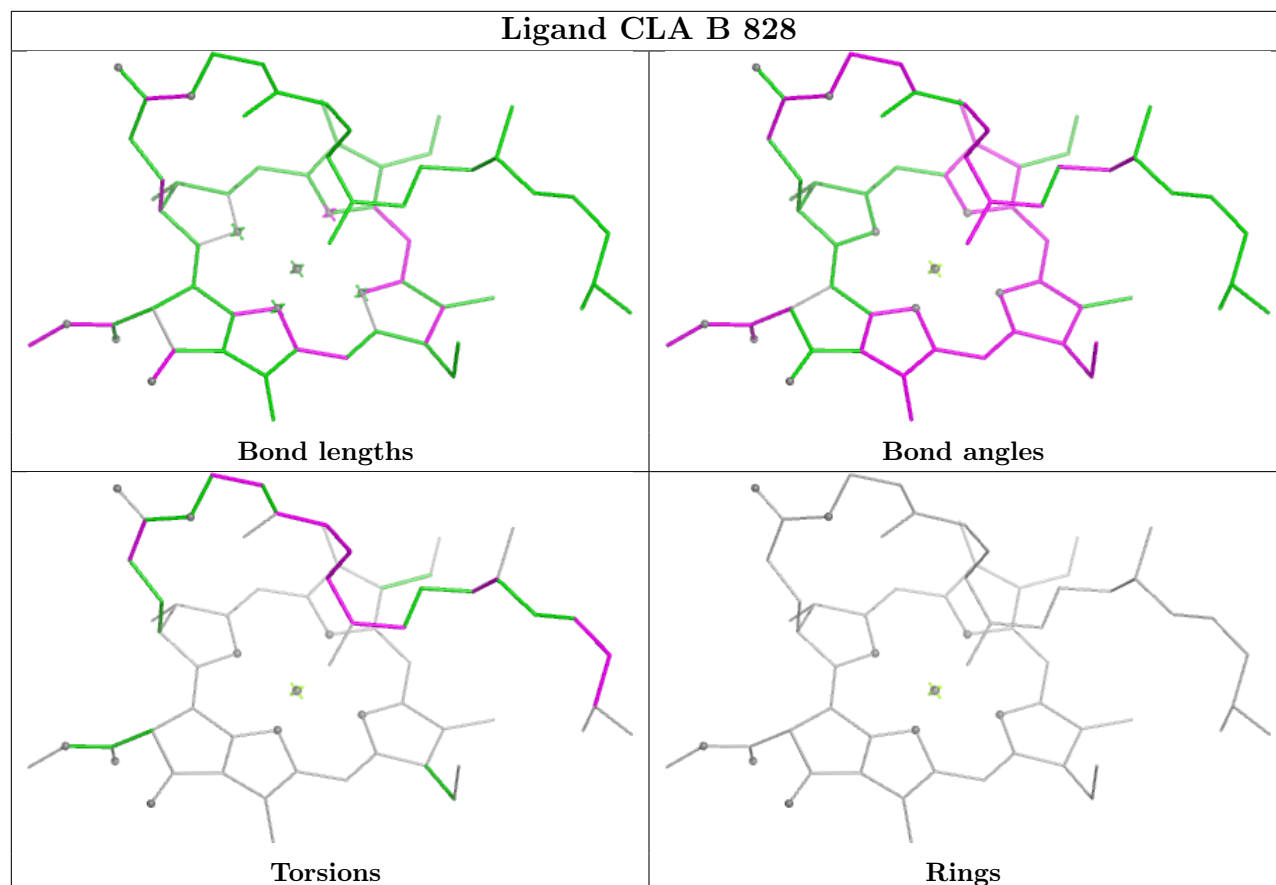




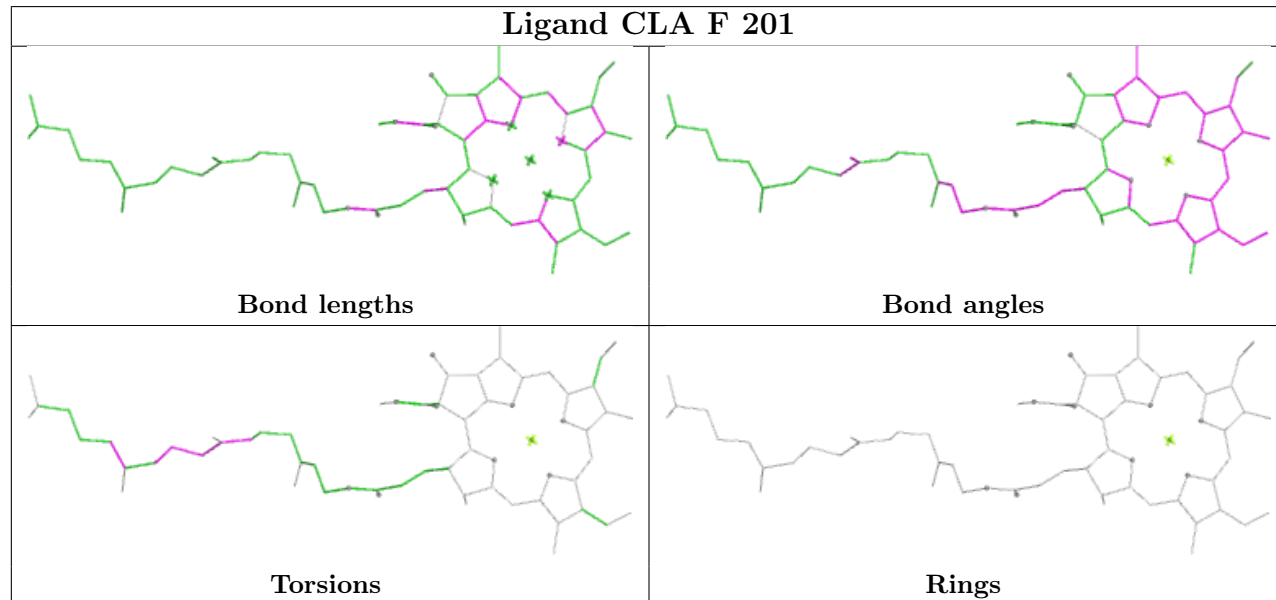


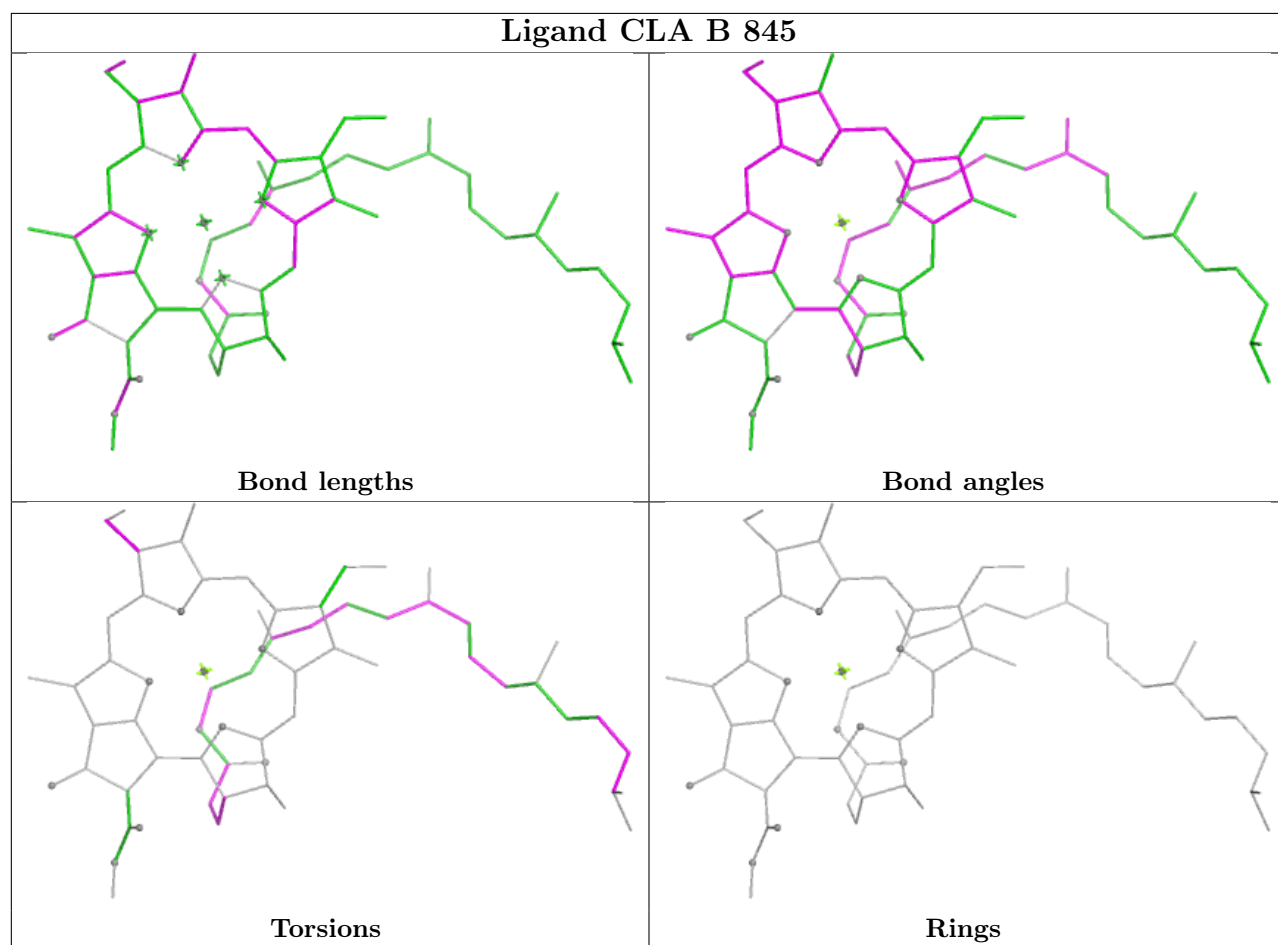
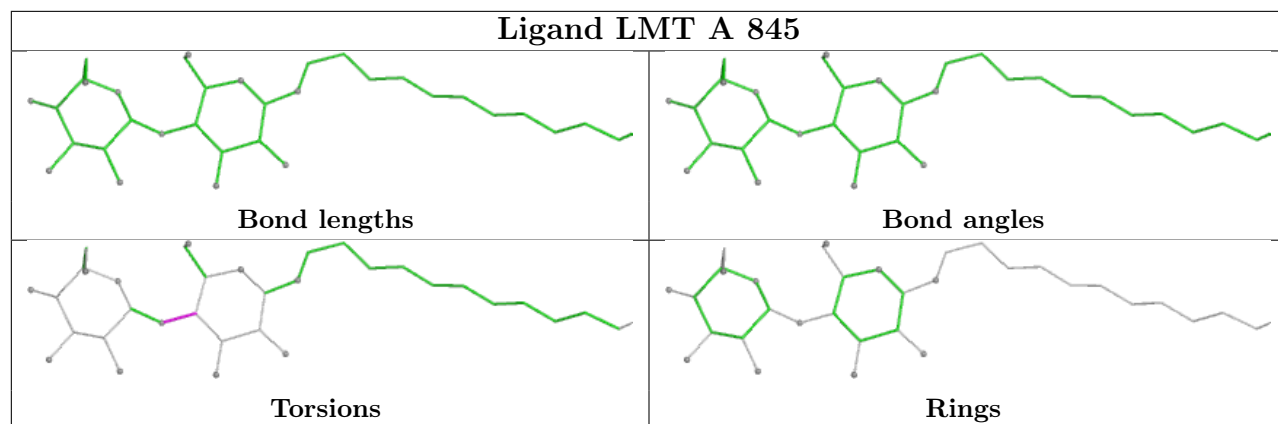


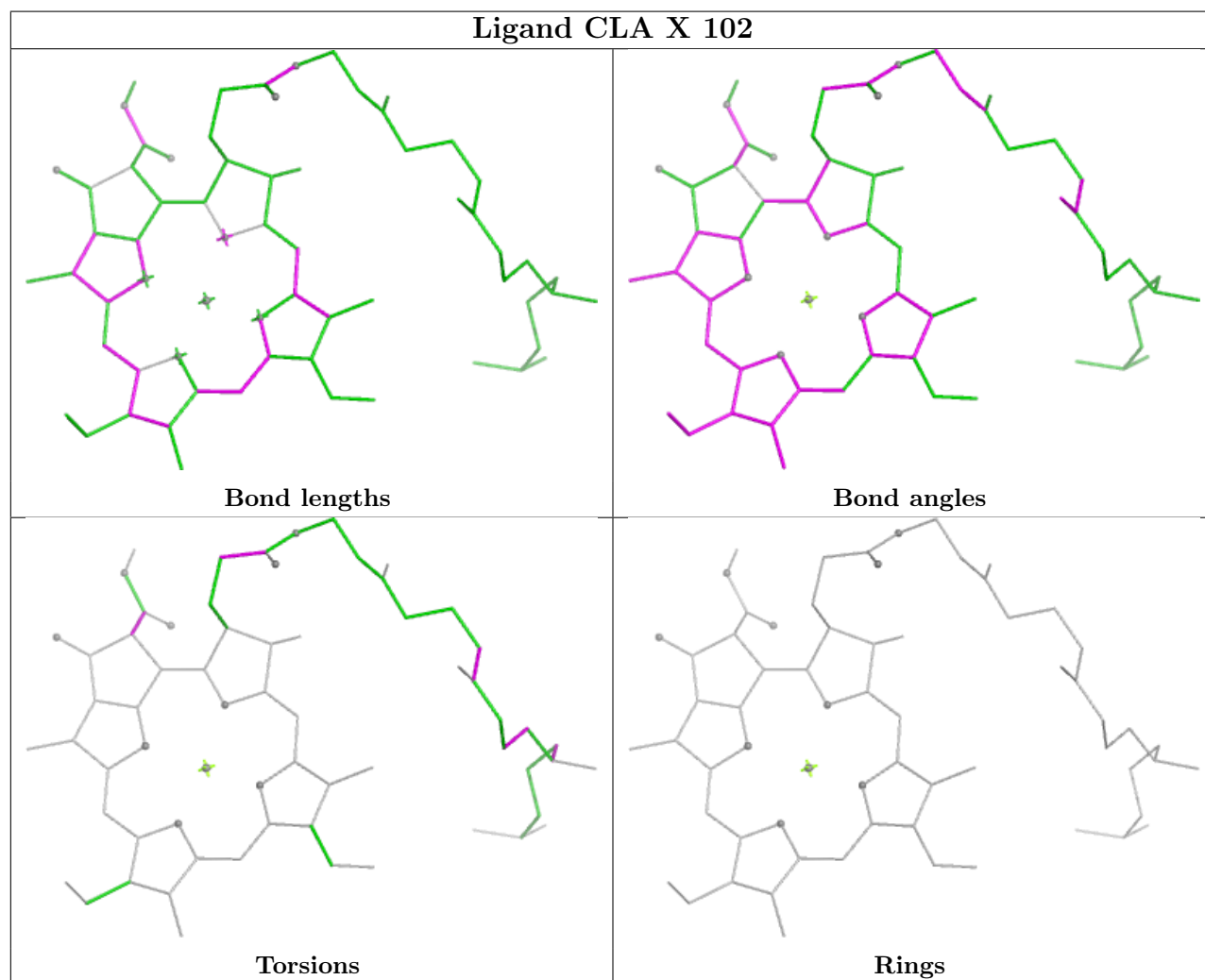
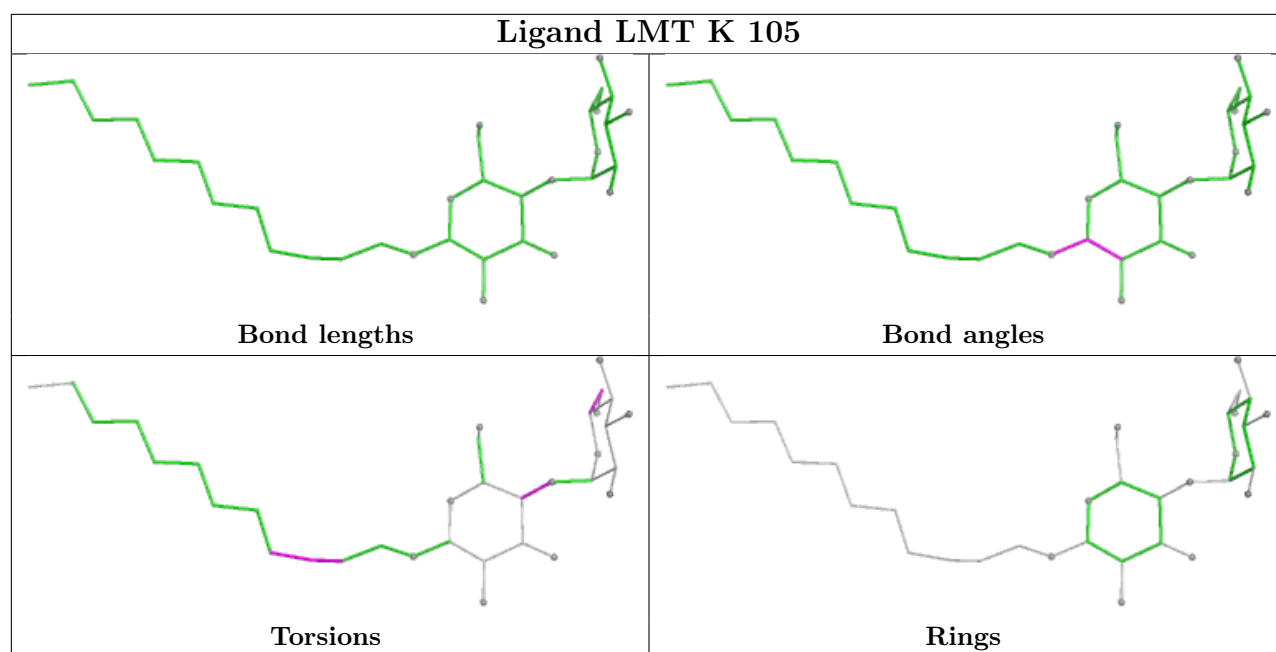
Ligand CLA B 828

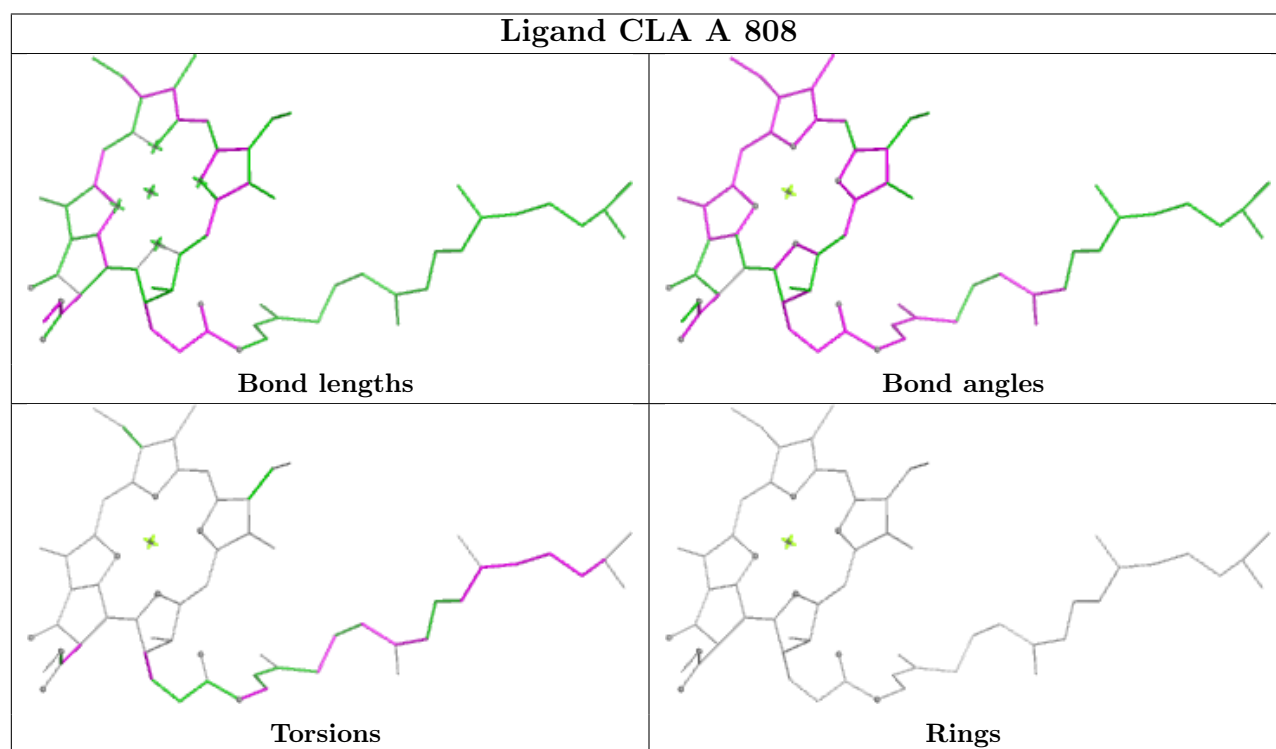
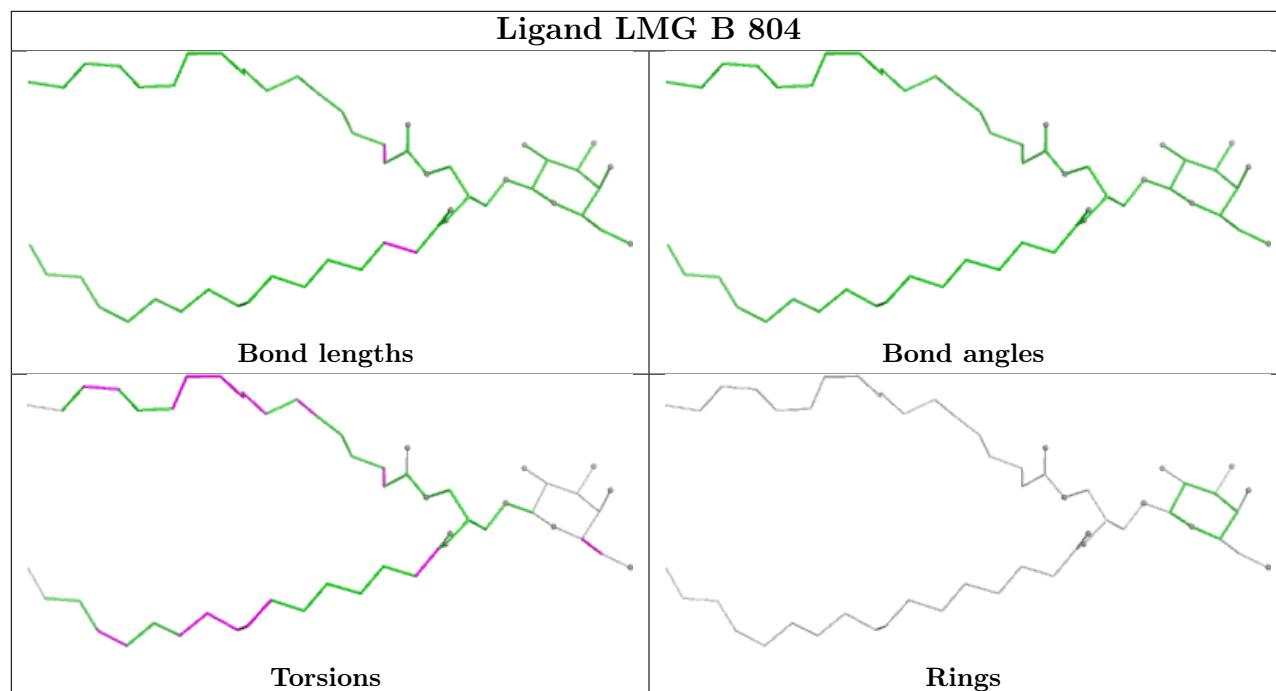


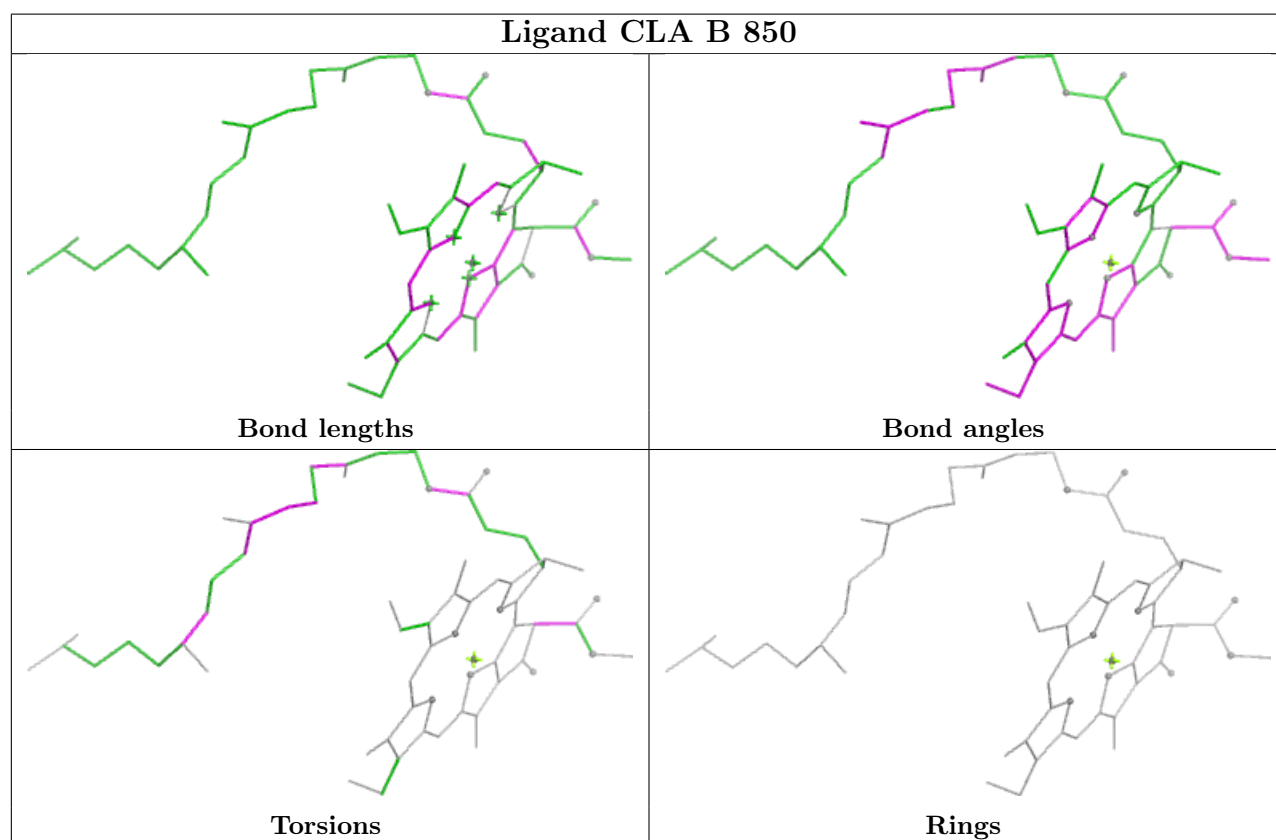
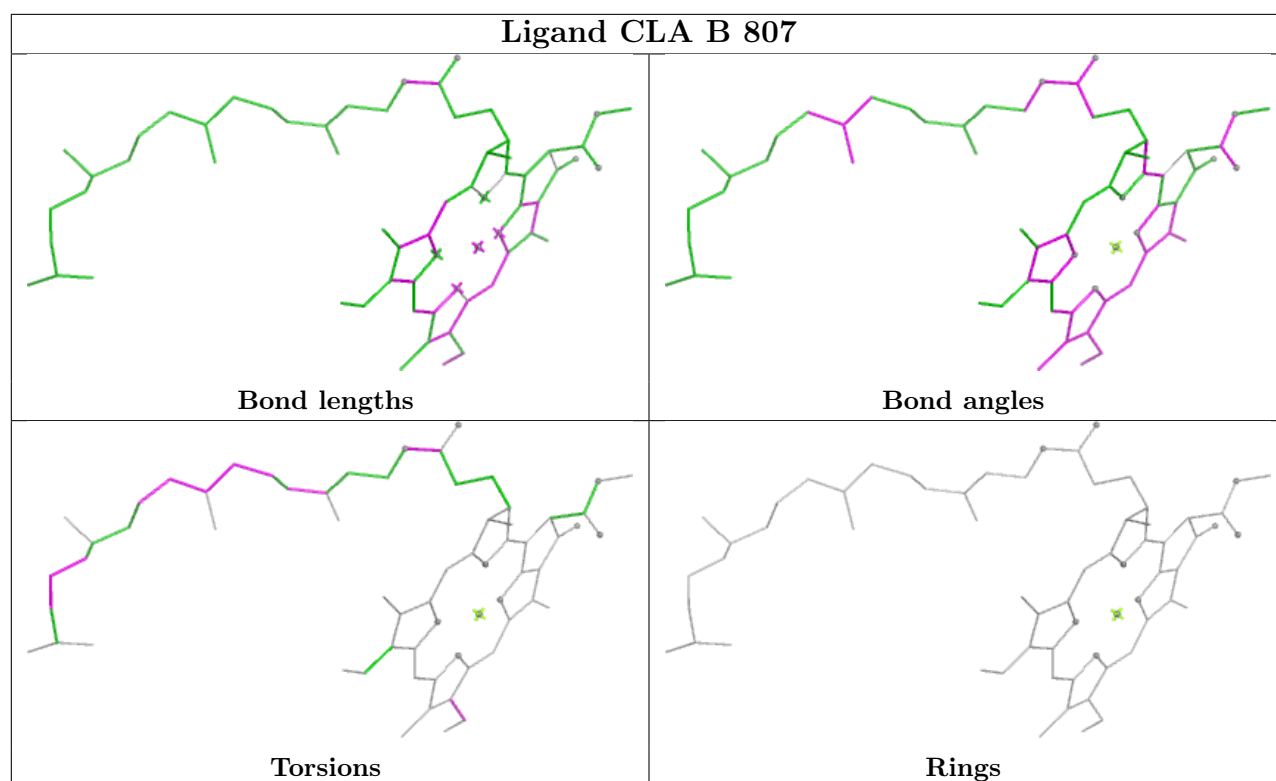
Ligand CLA F 201

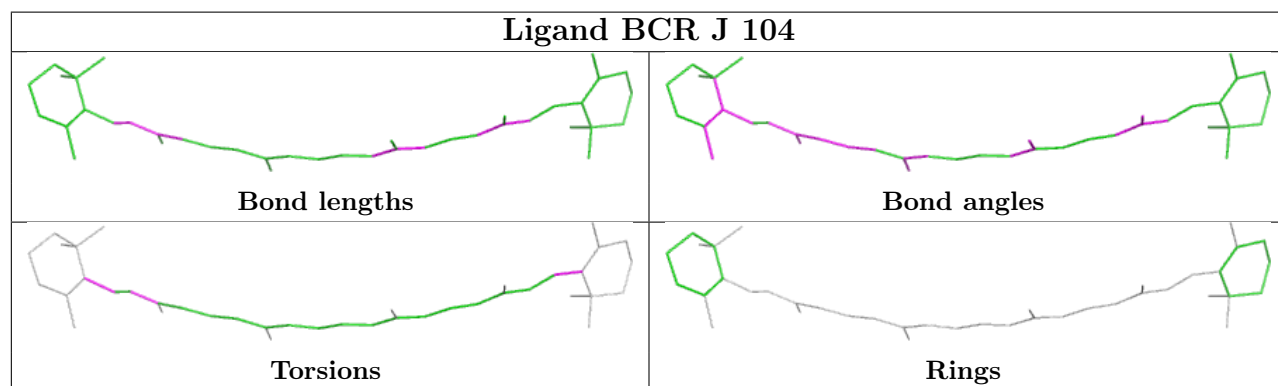
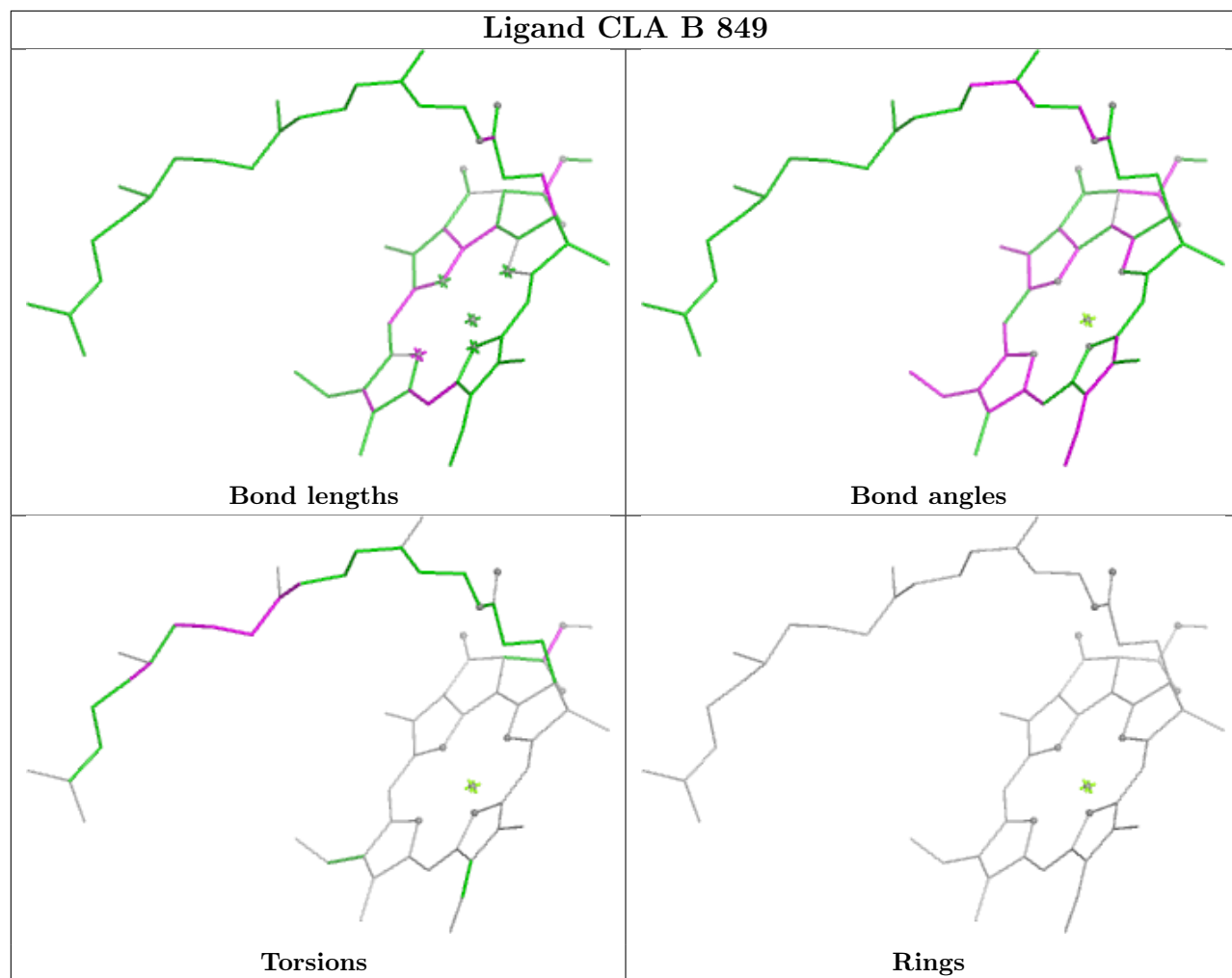


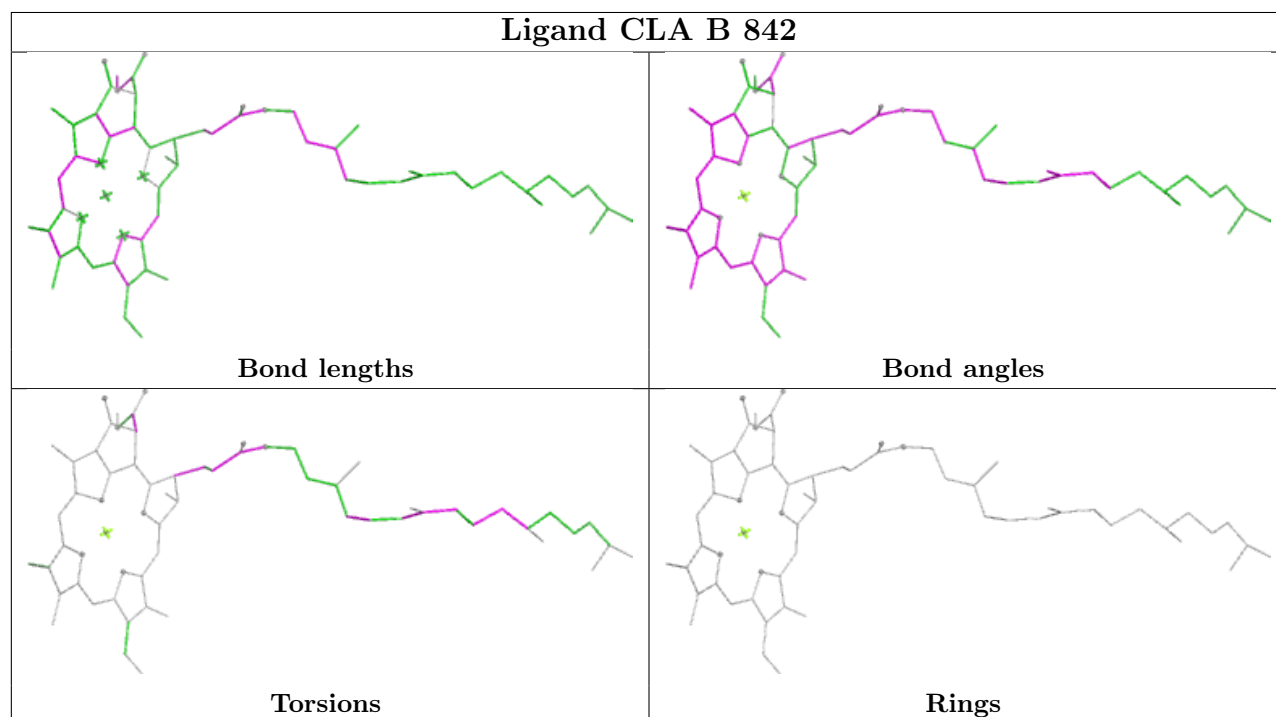
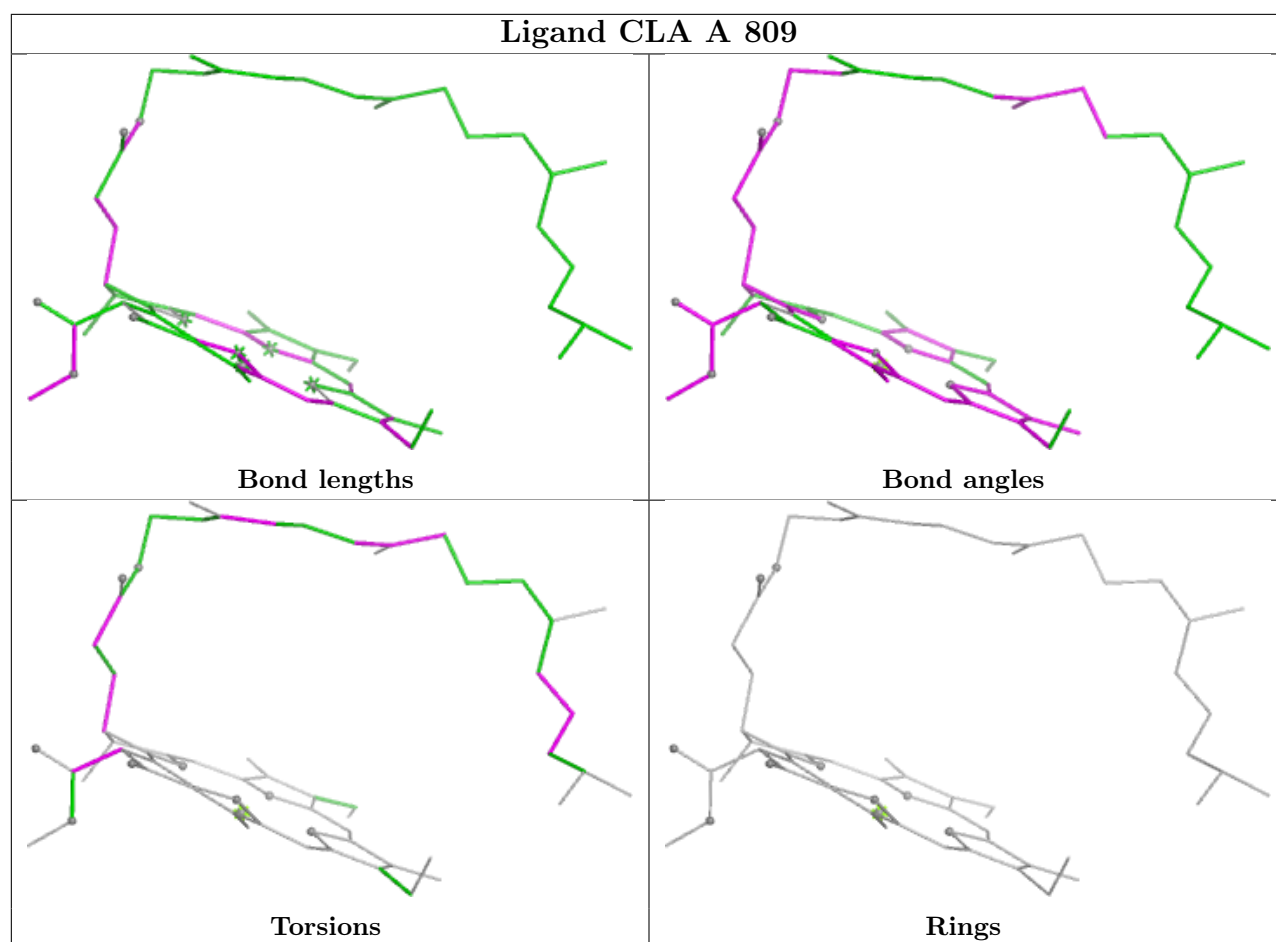


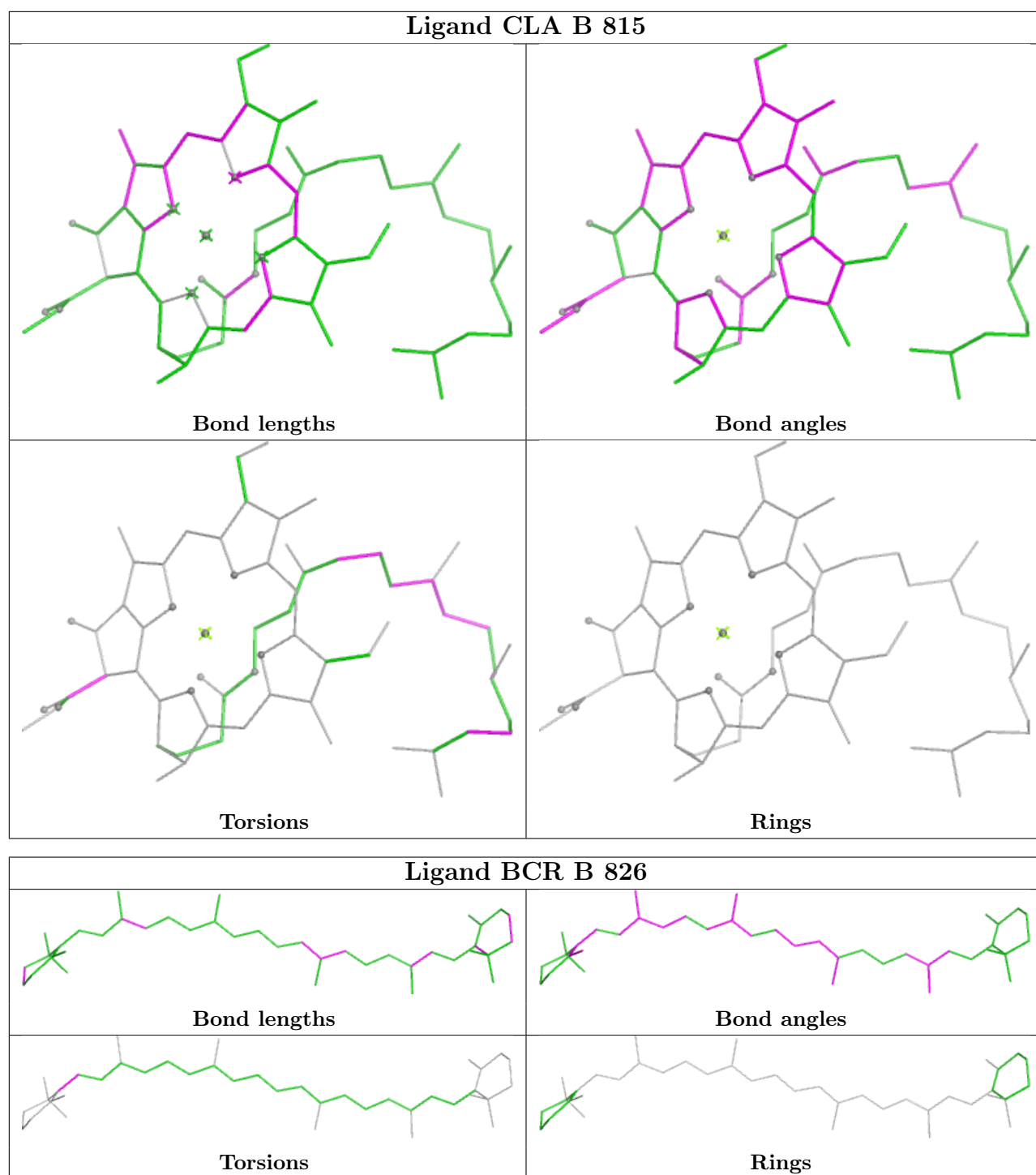


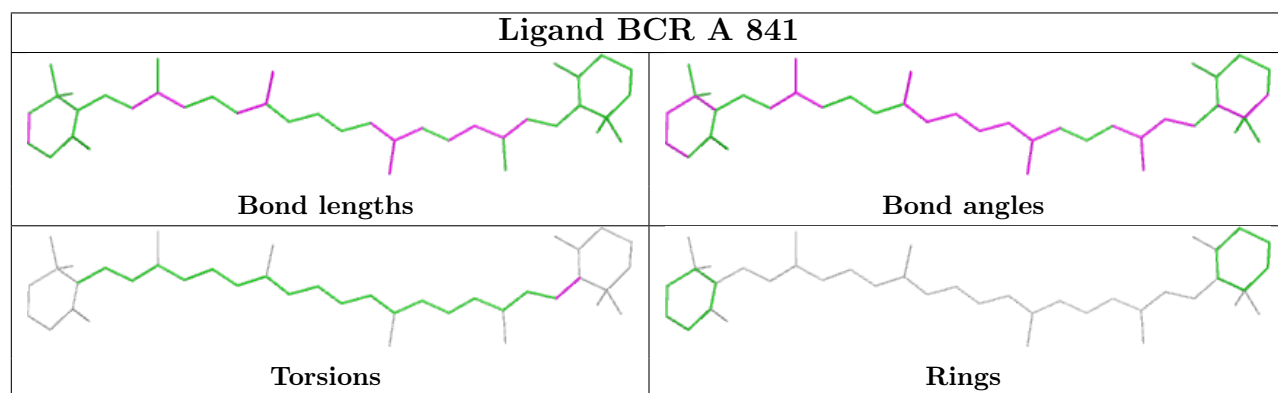
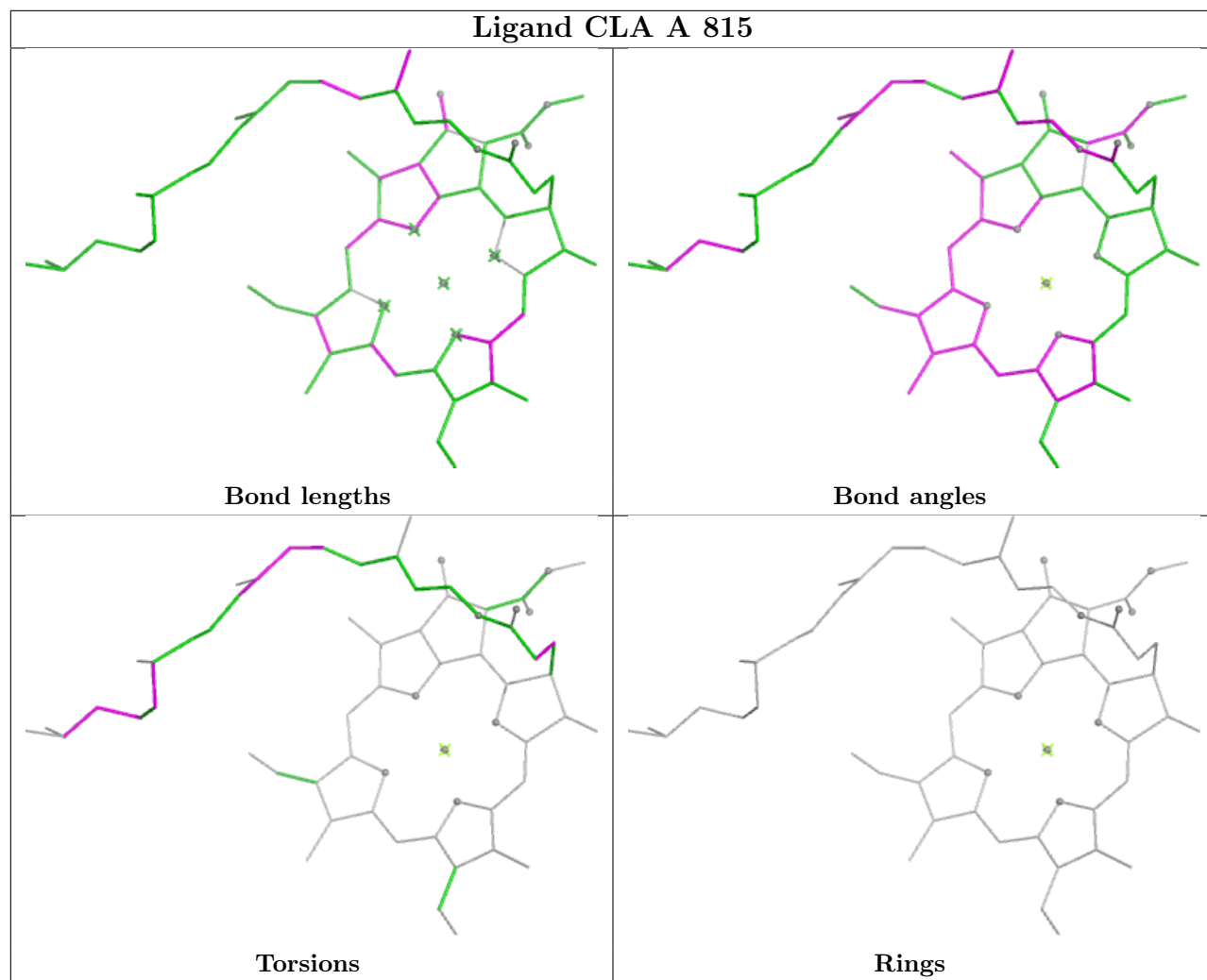


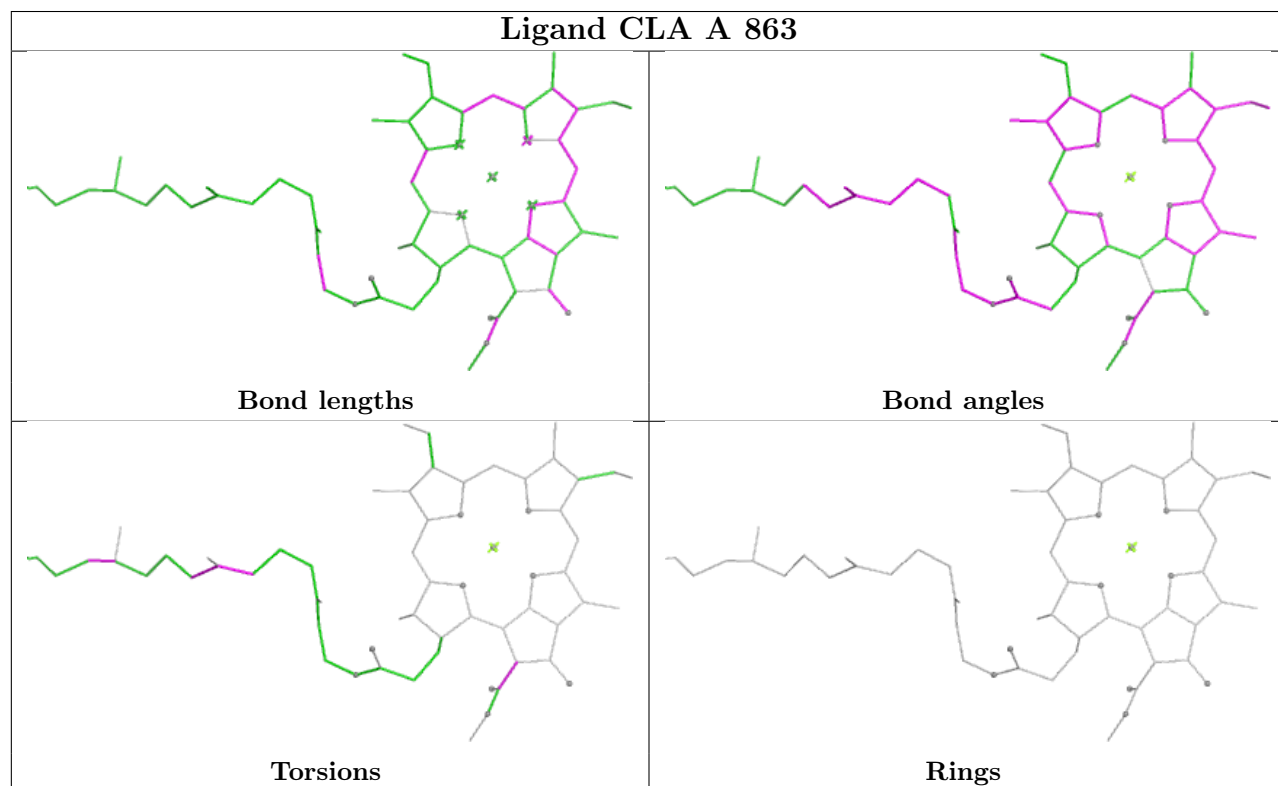
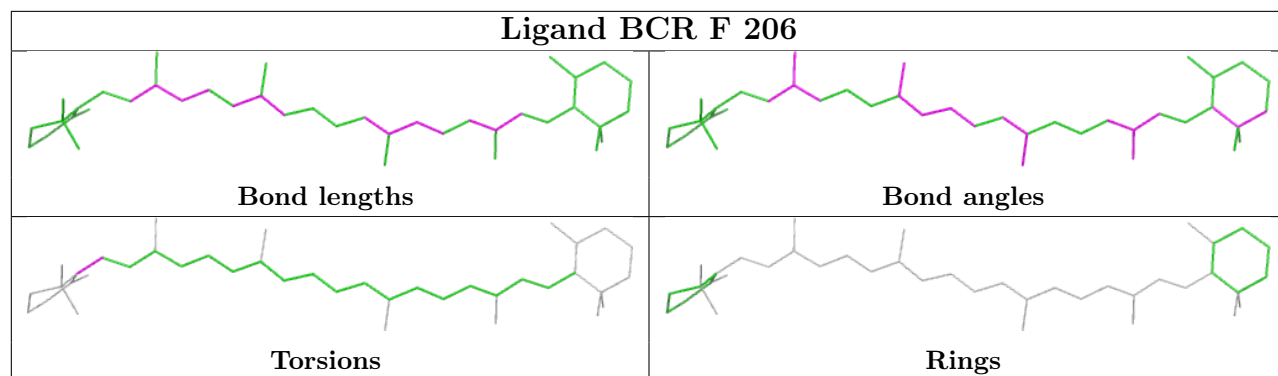


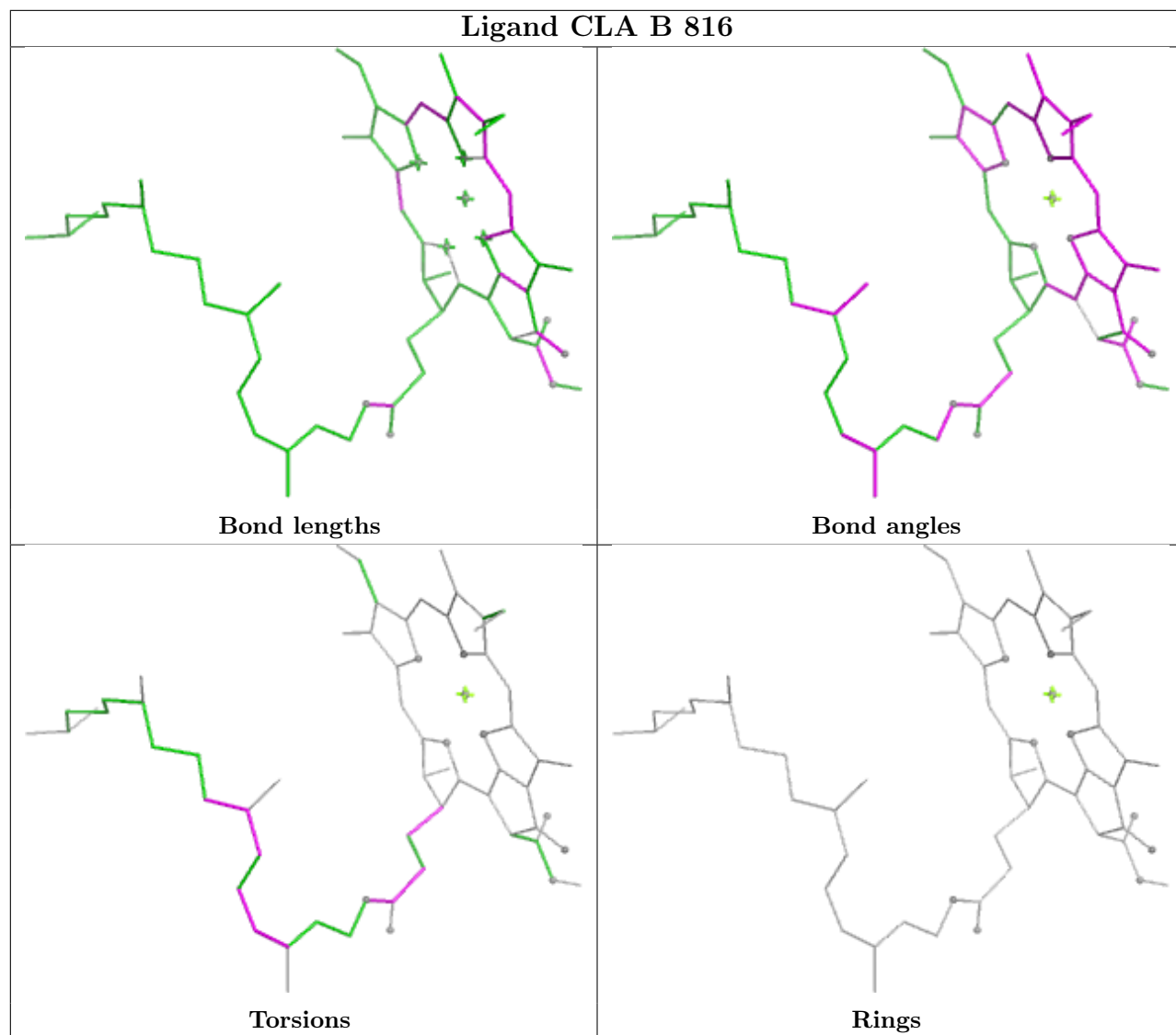


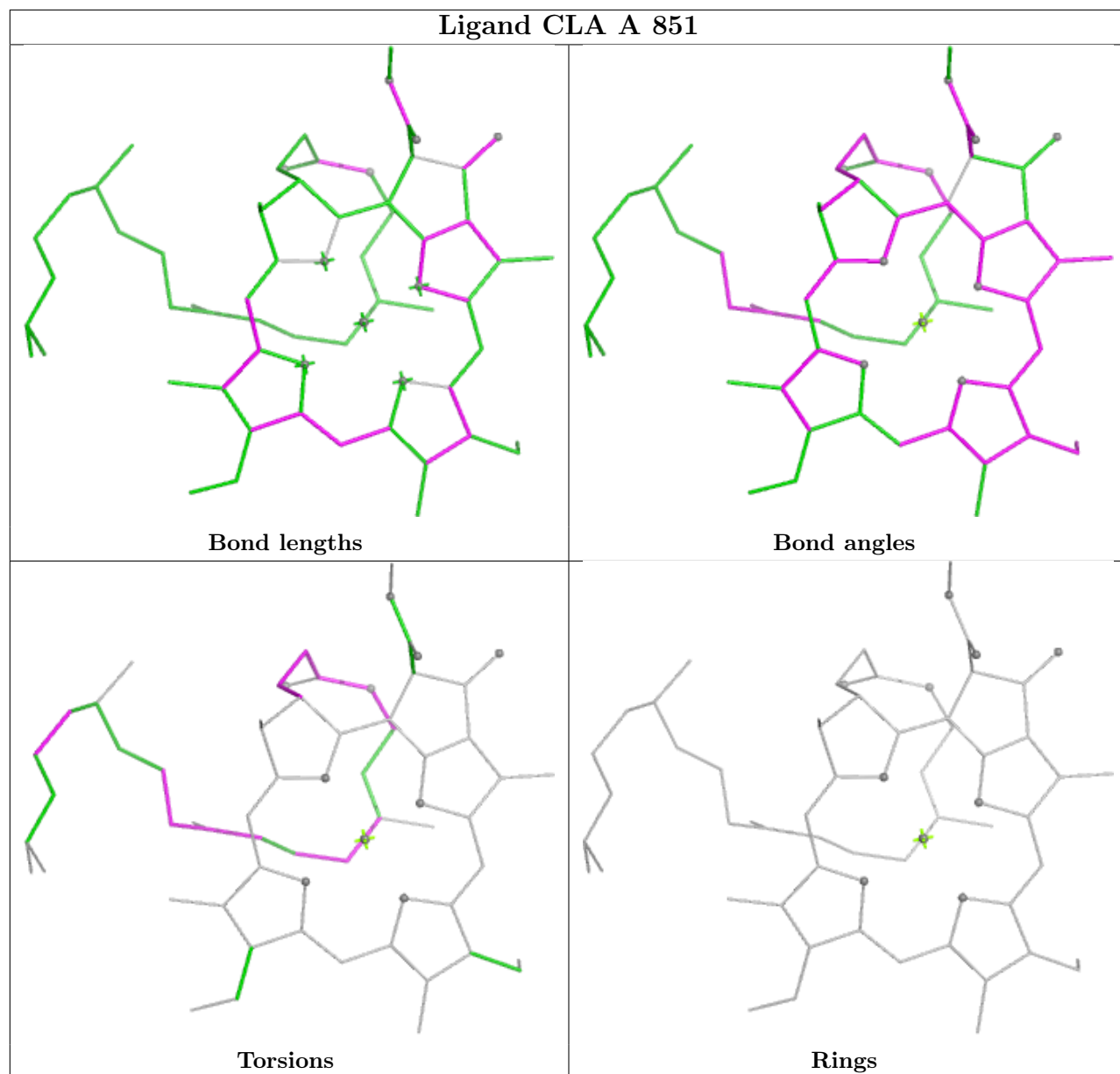


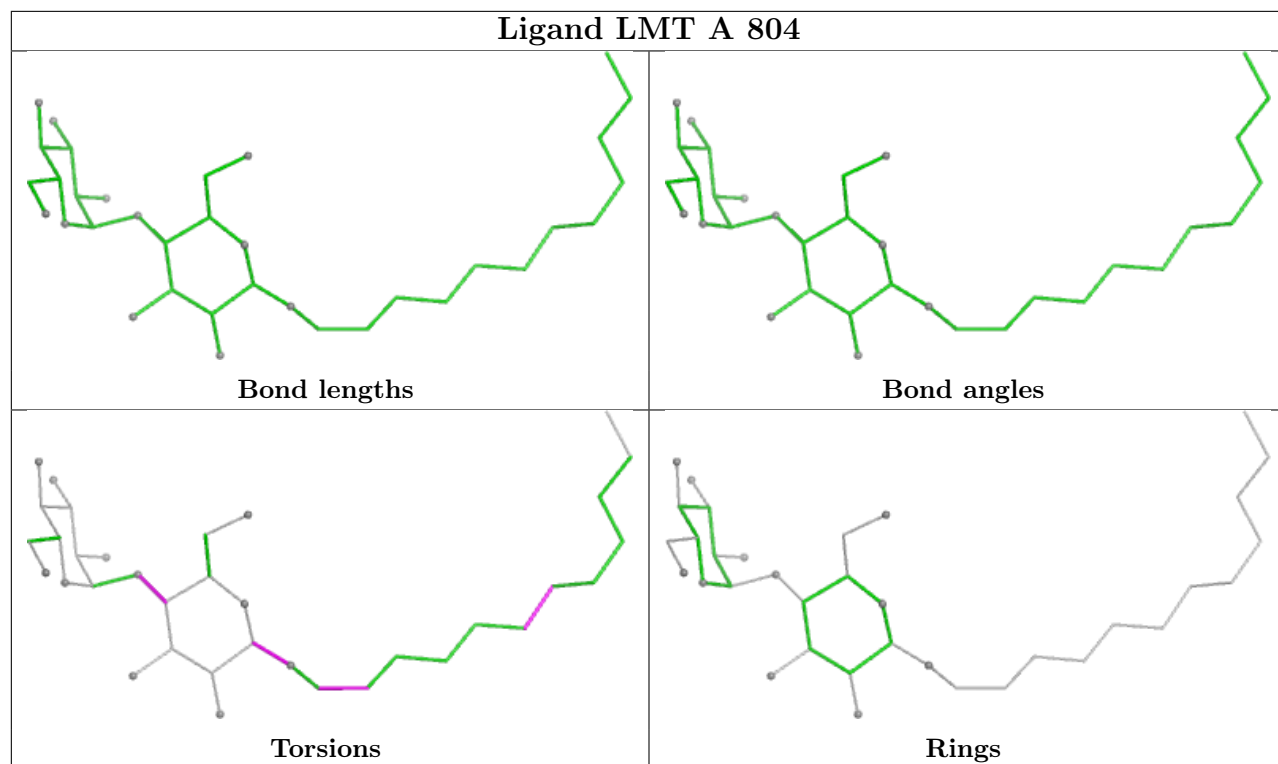


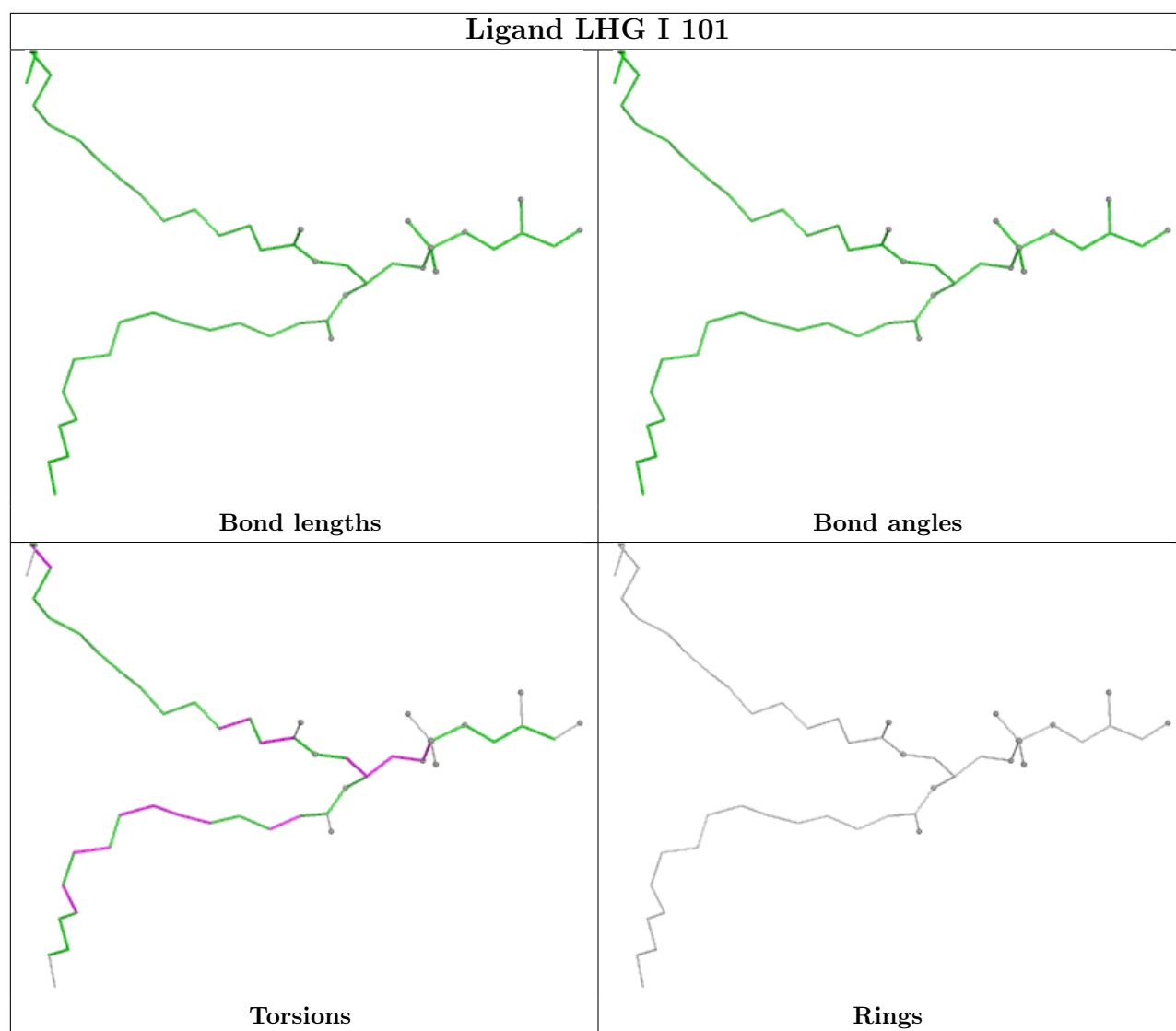


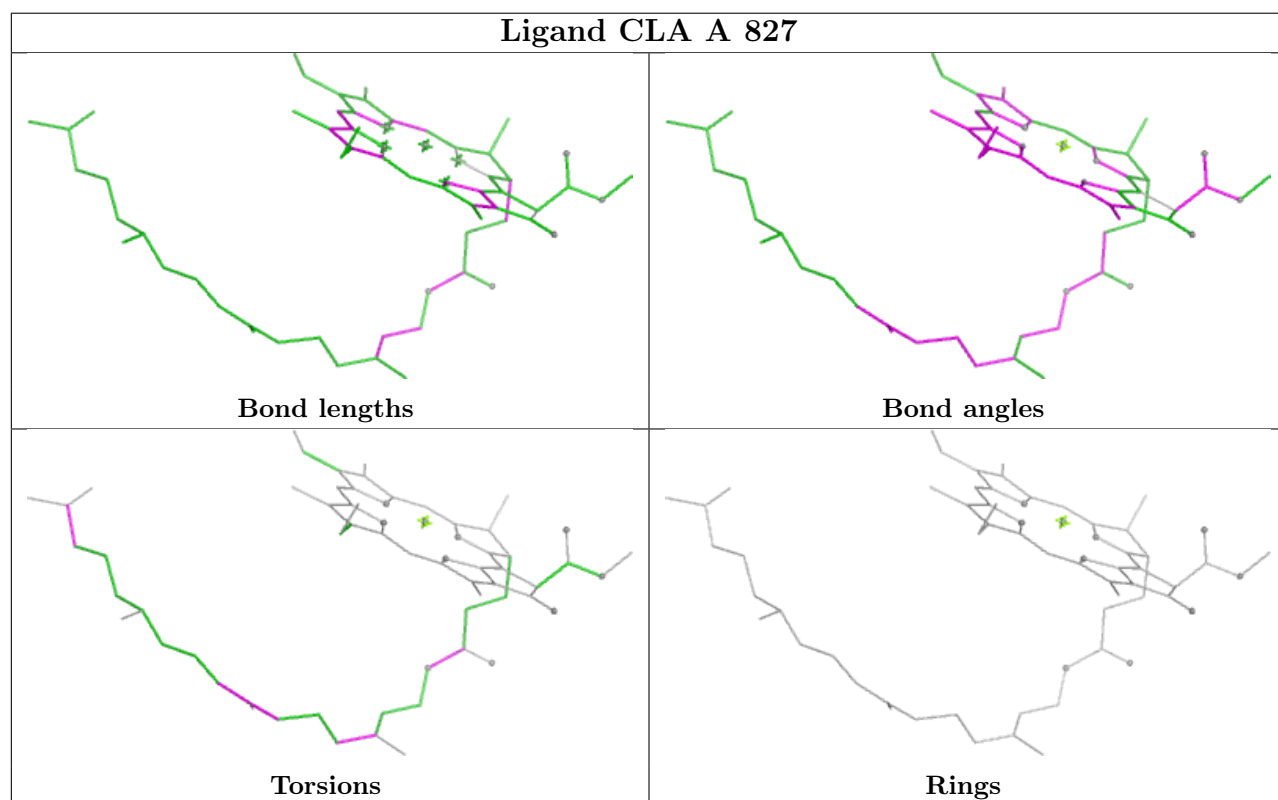
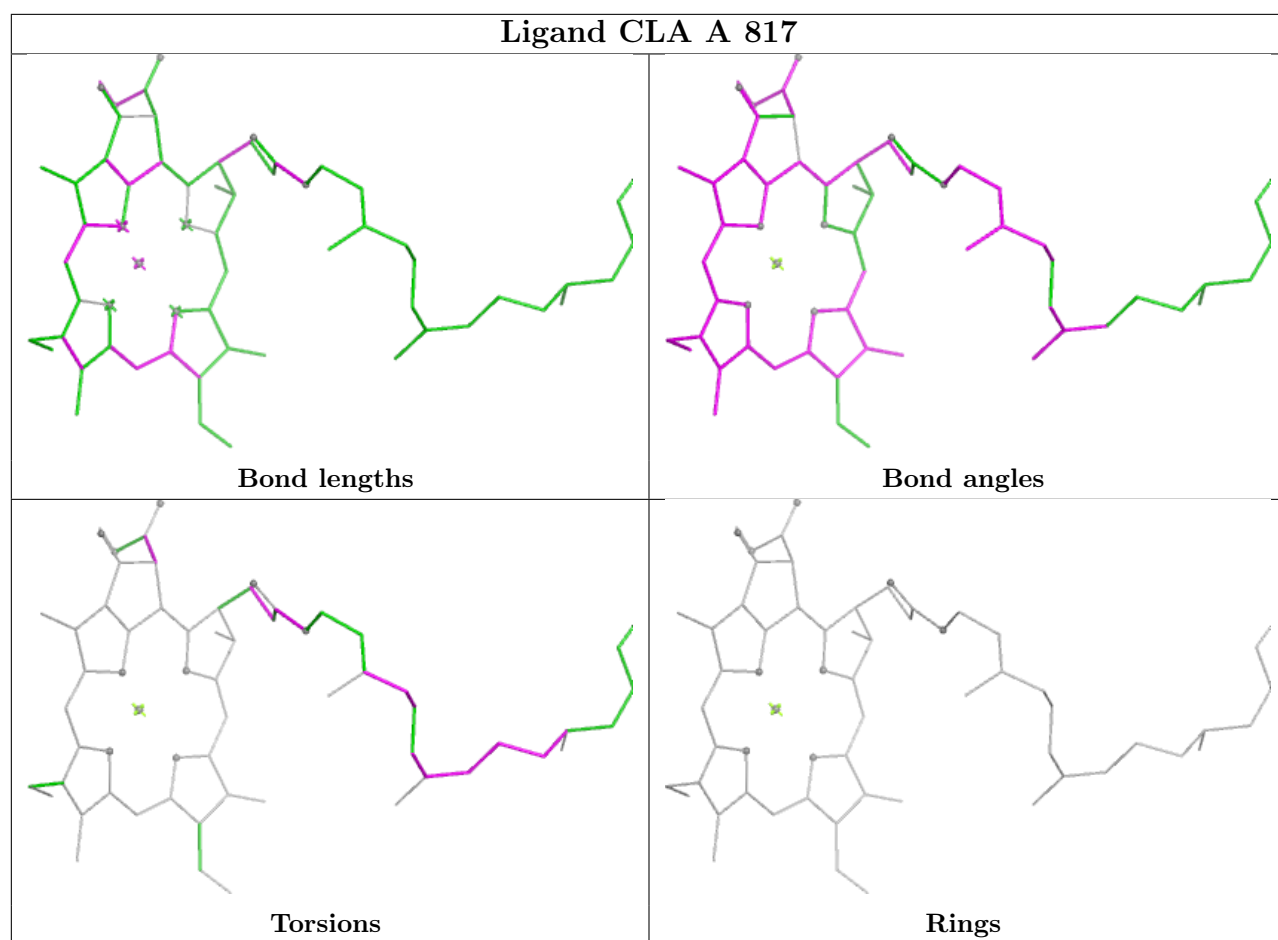


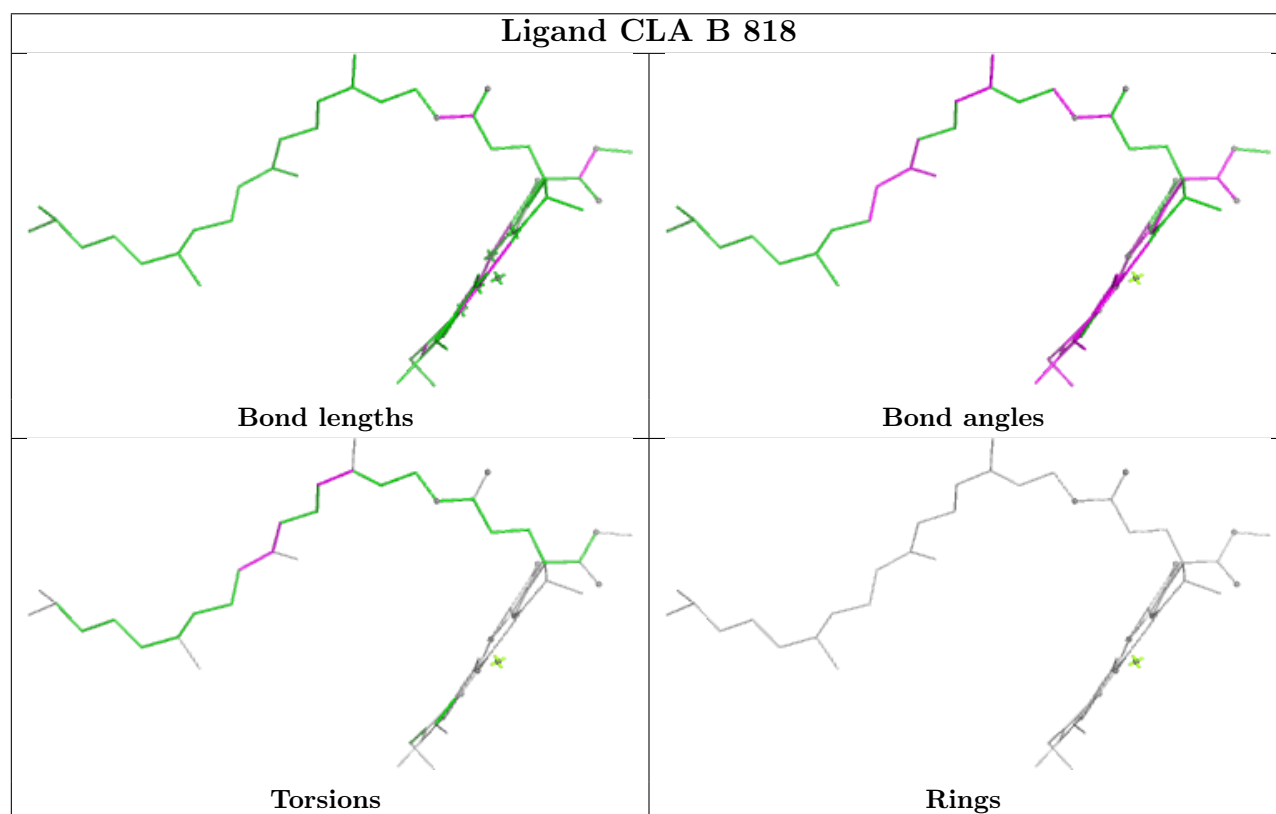
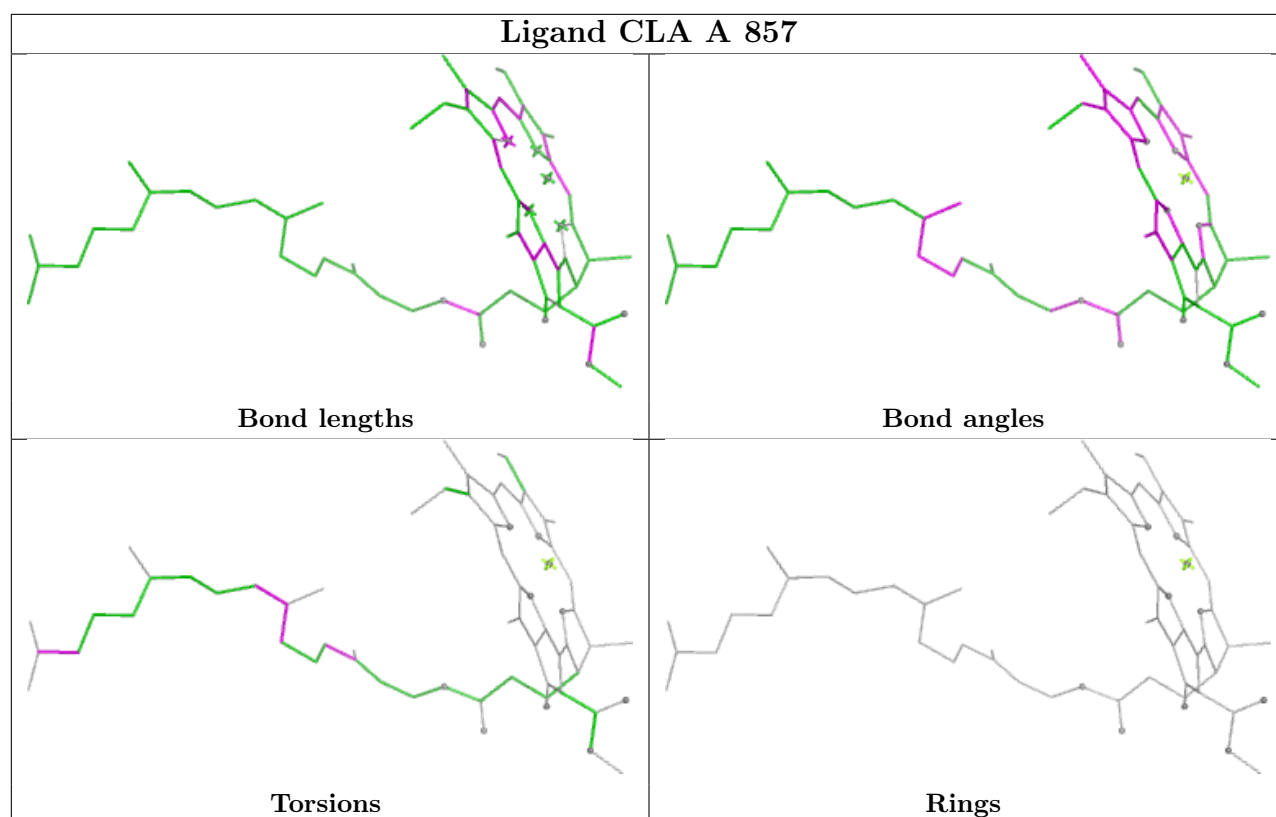


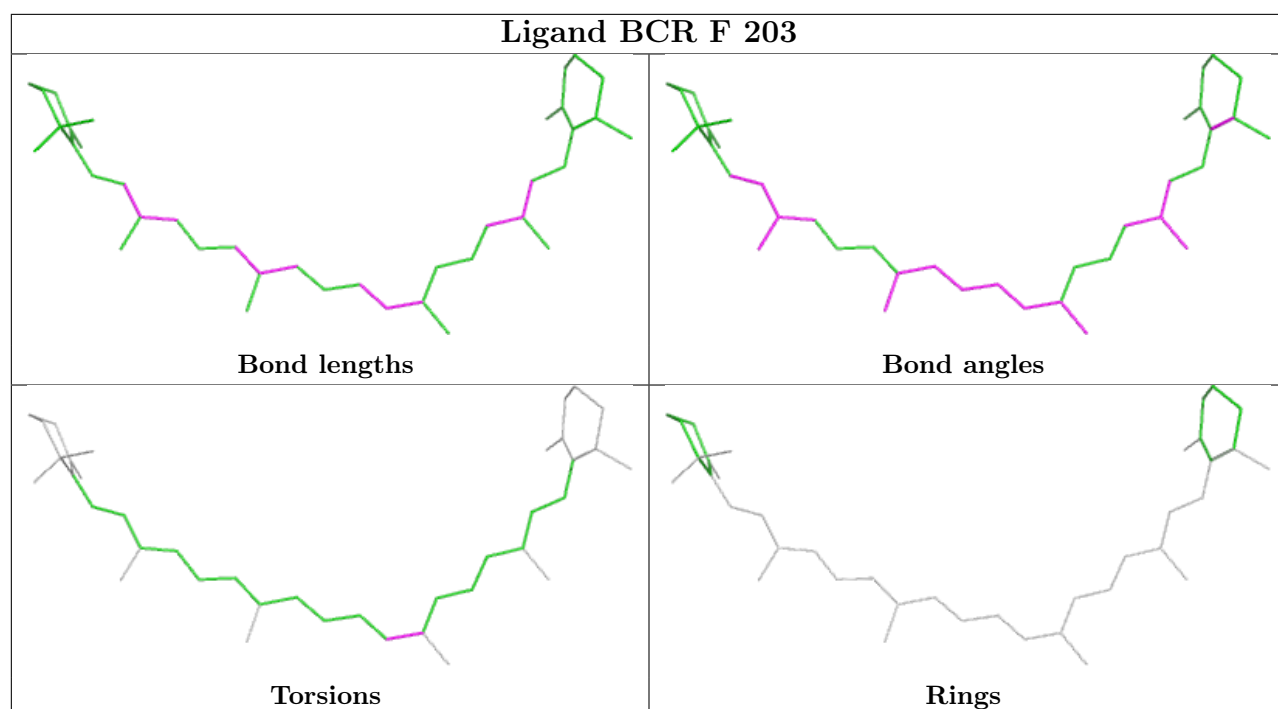




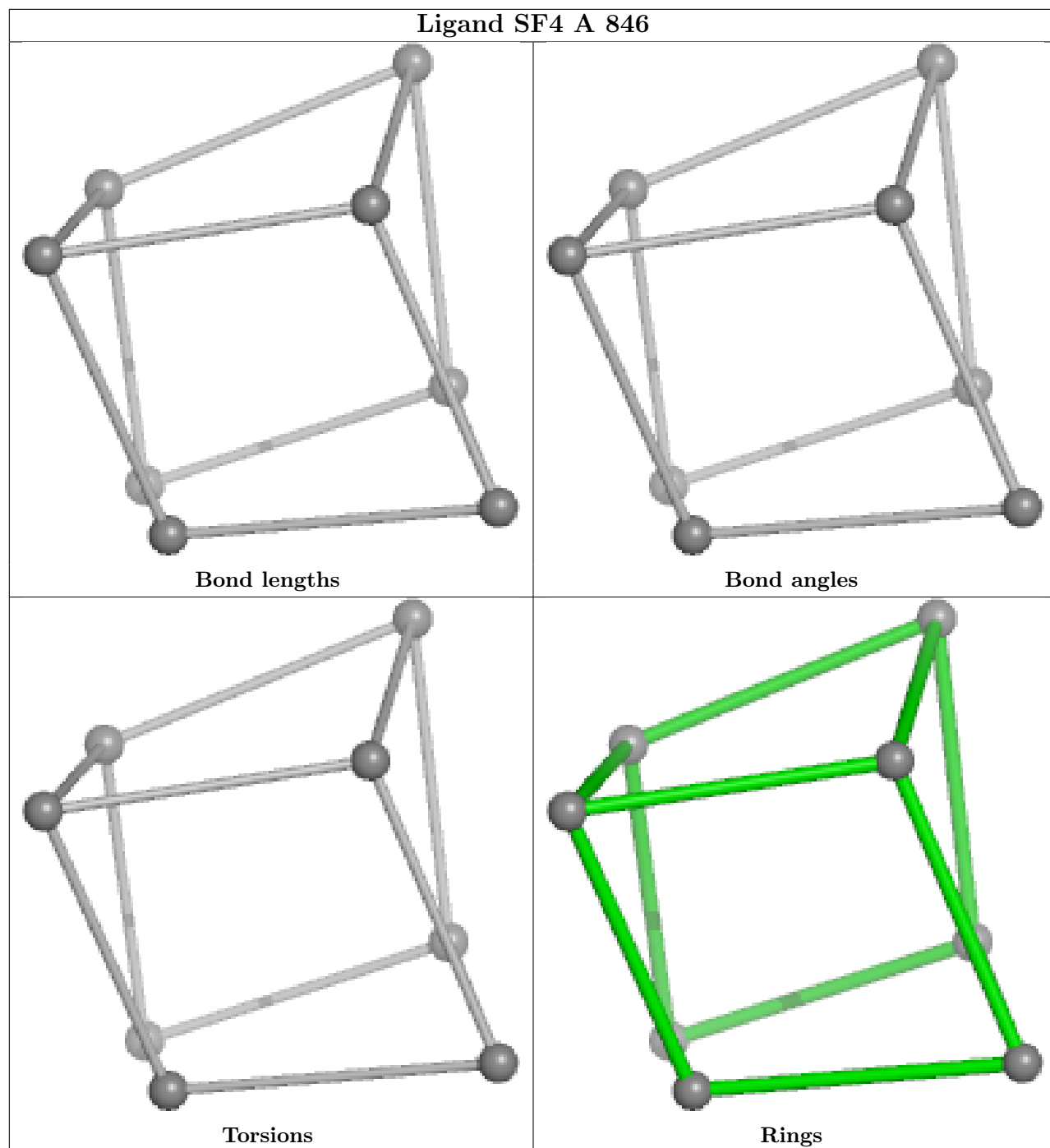


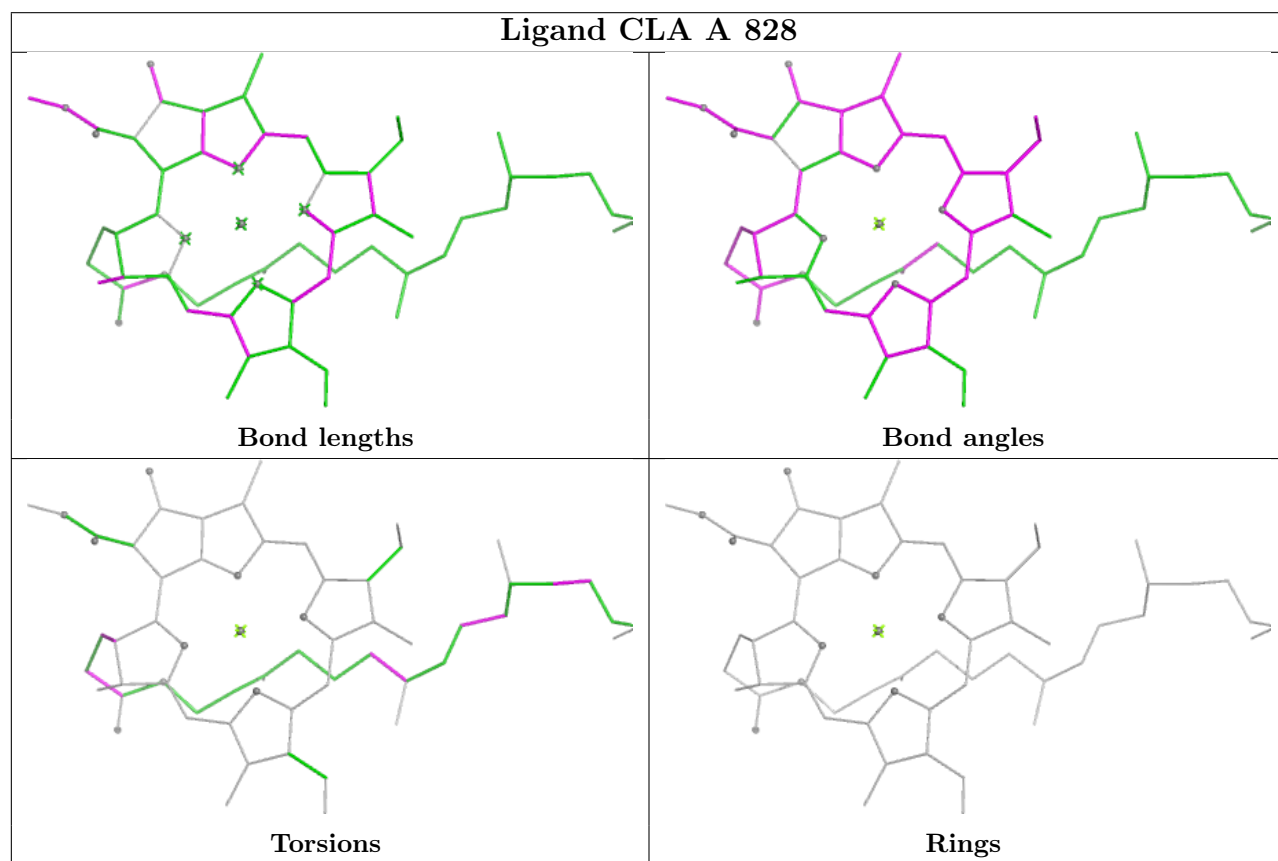
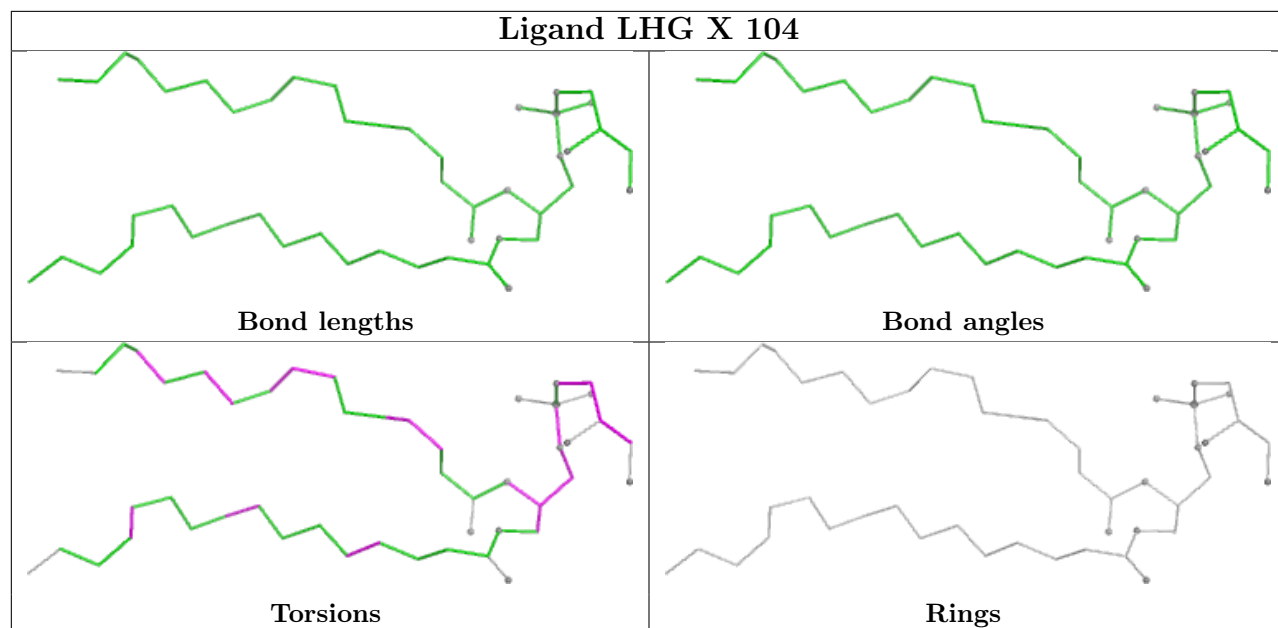


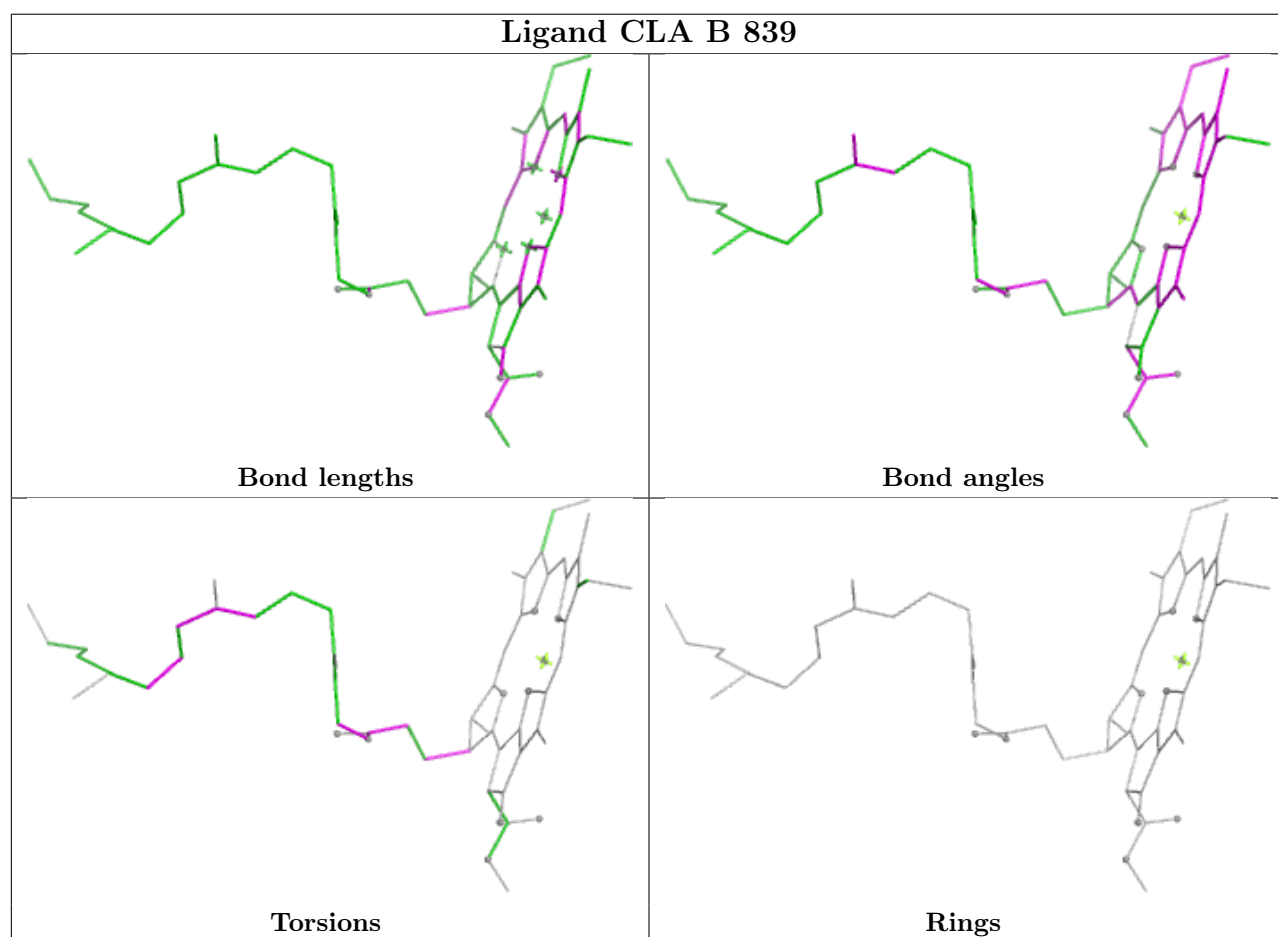
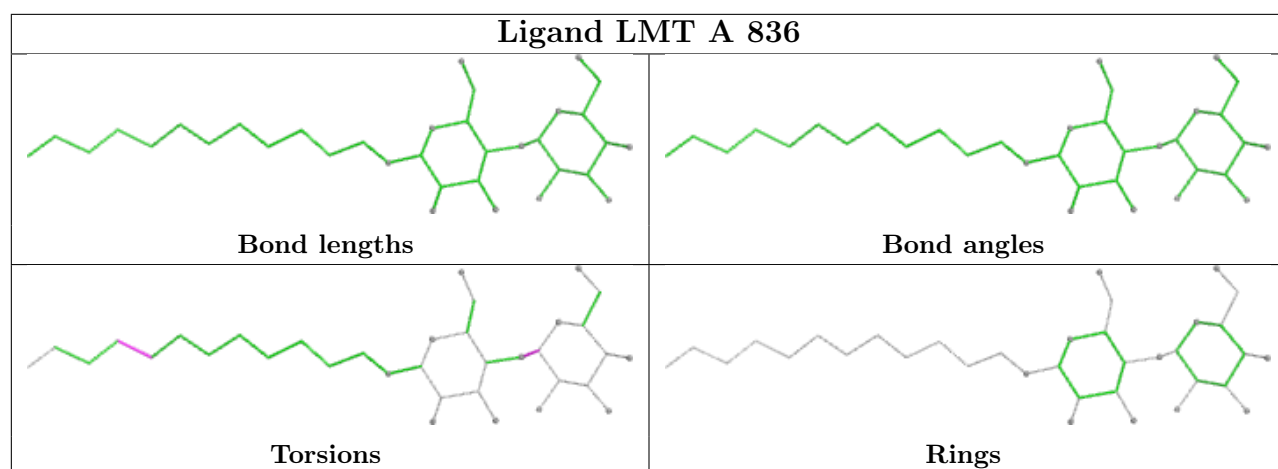


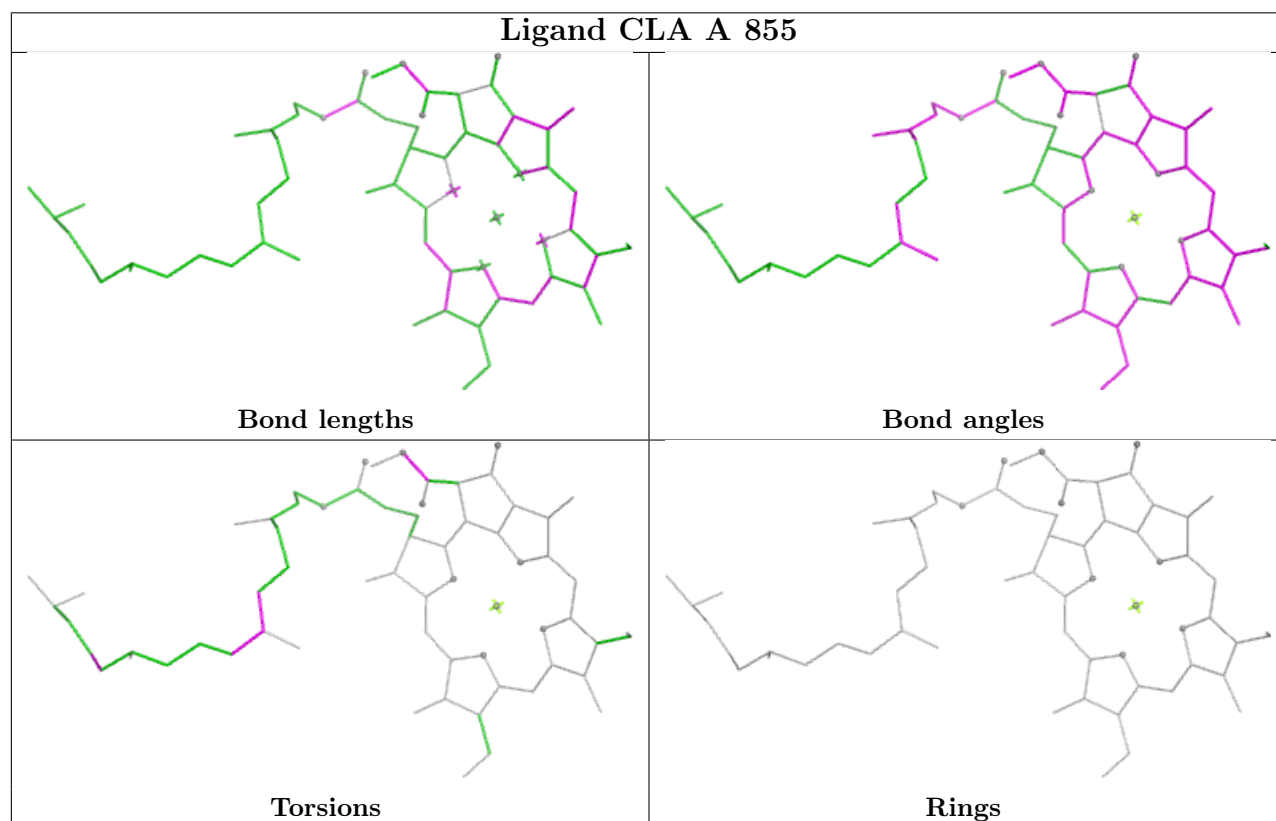
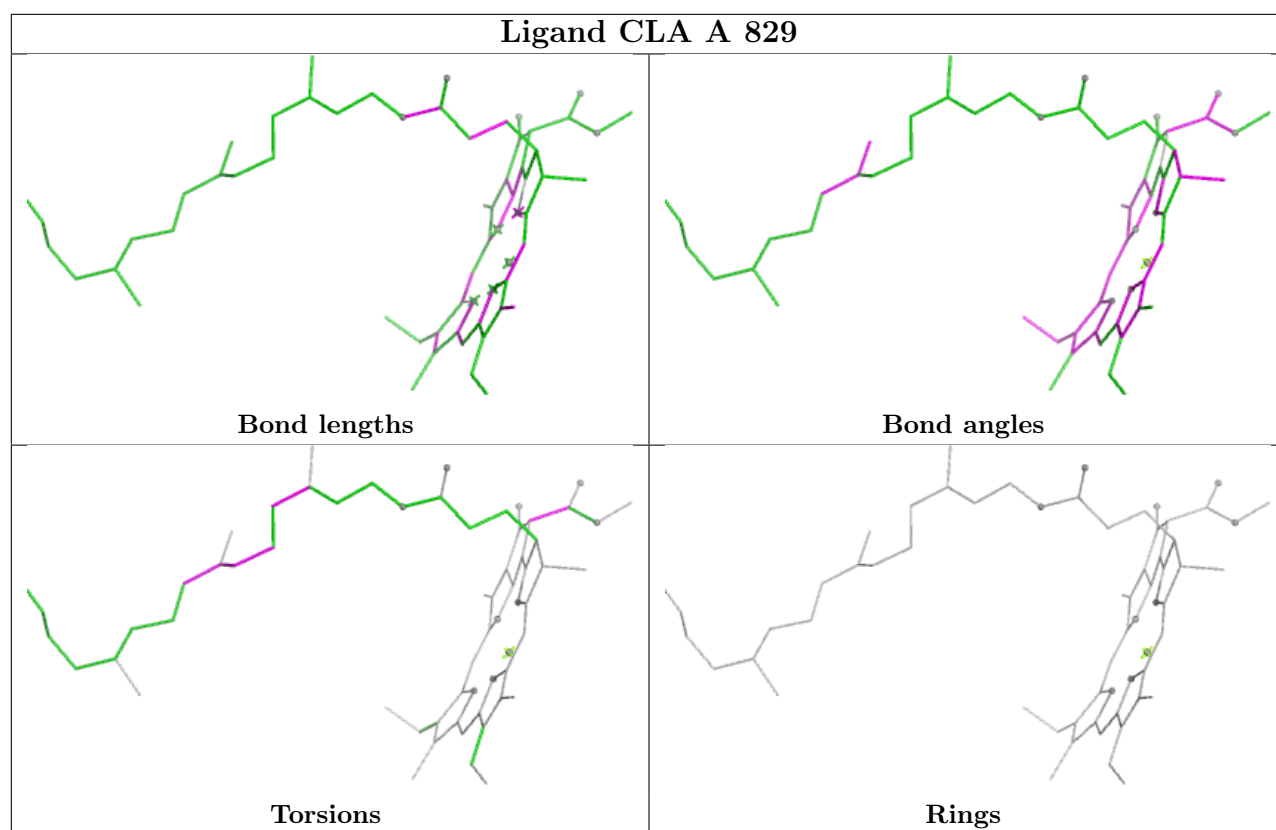


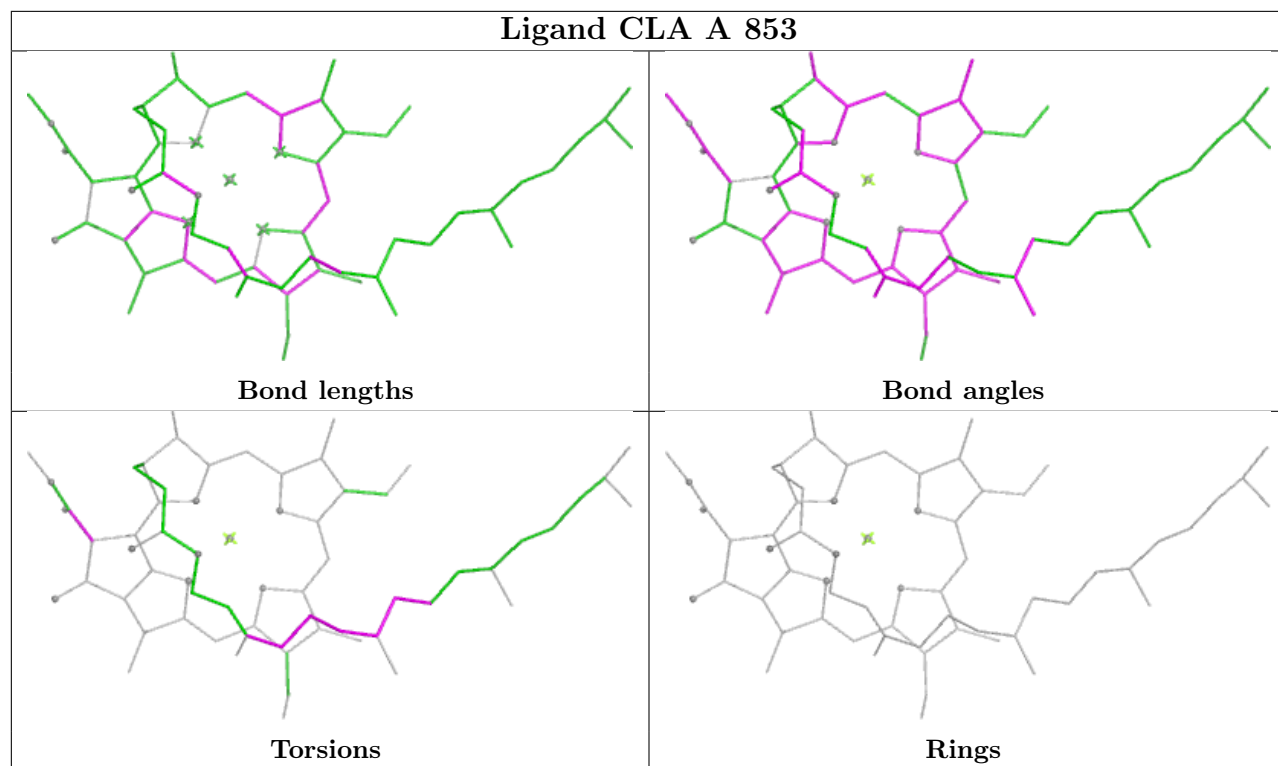
Ligand SF4 A 846



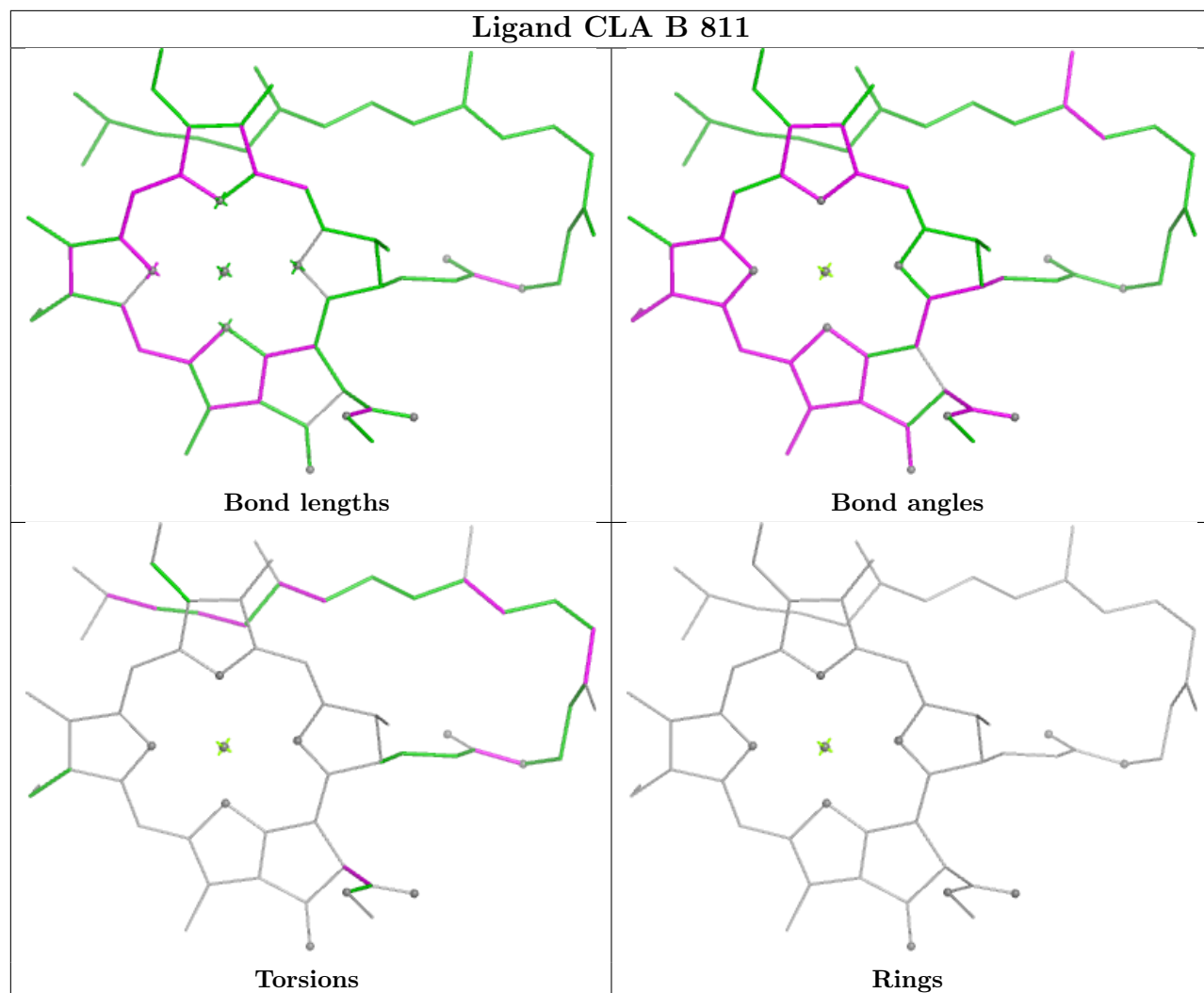


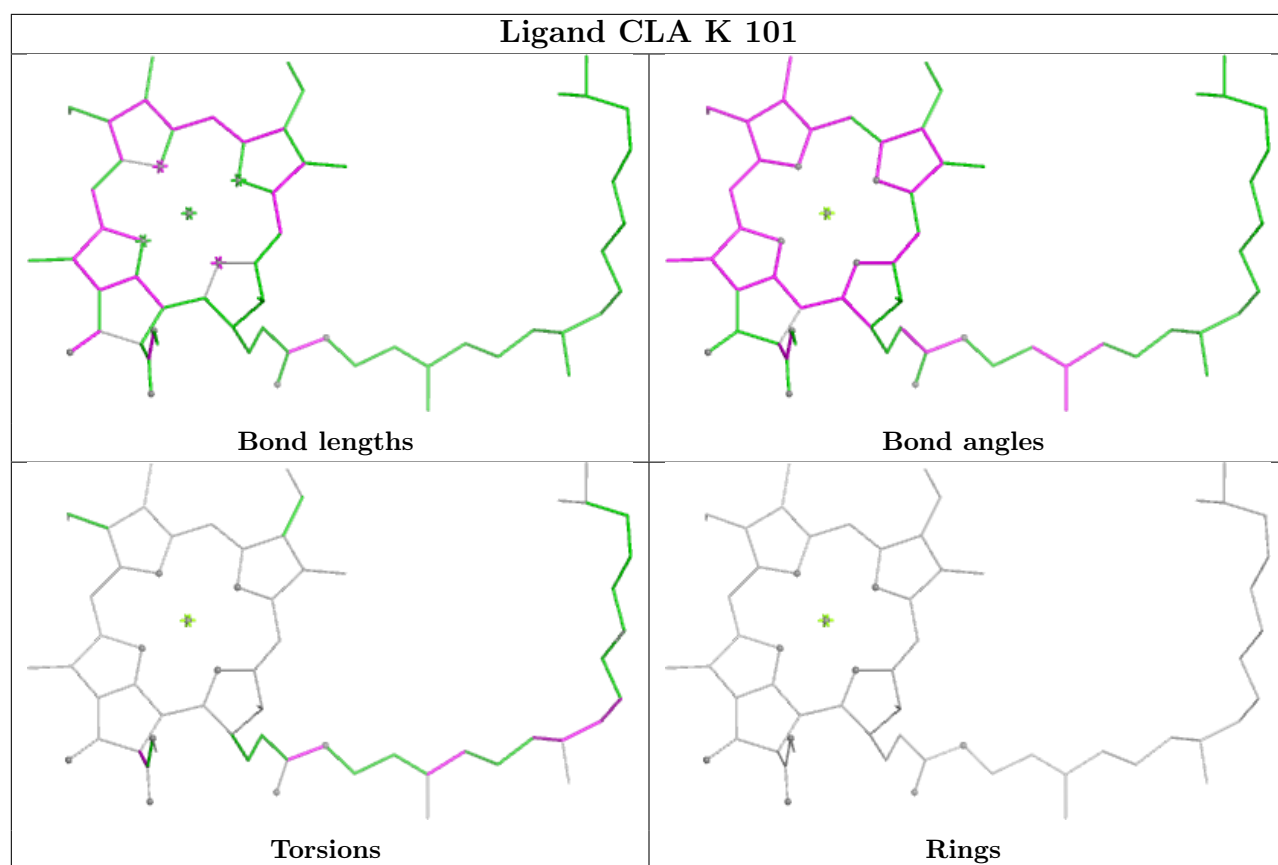


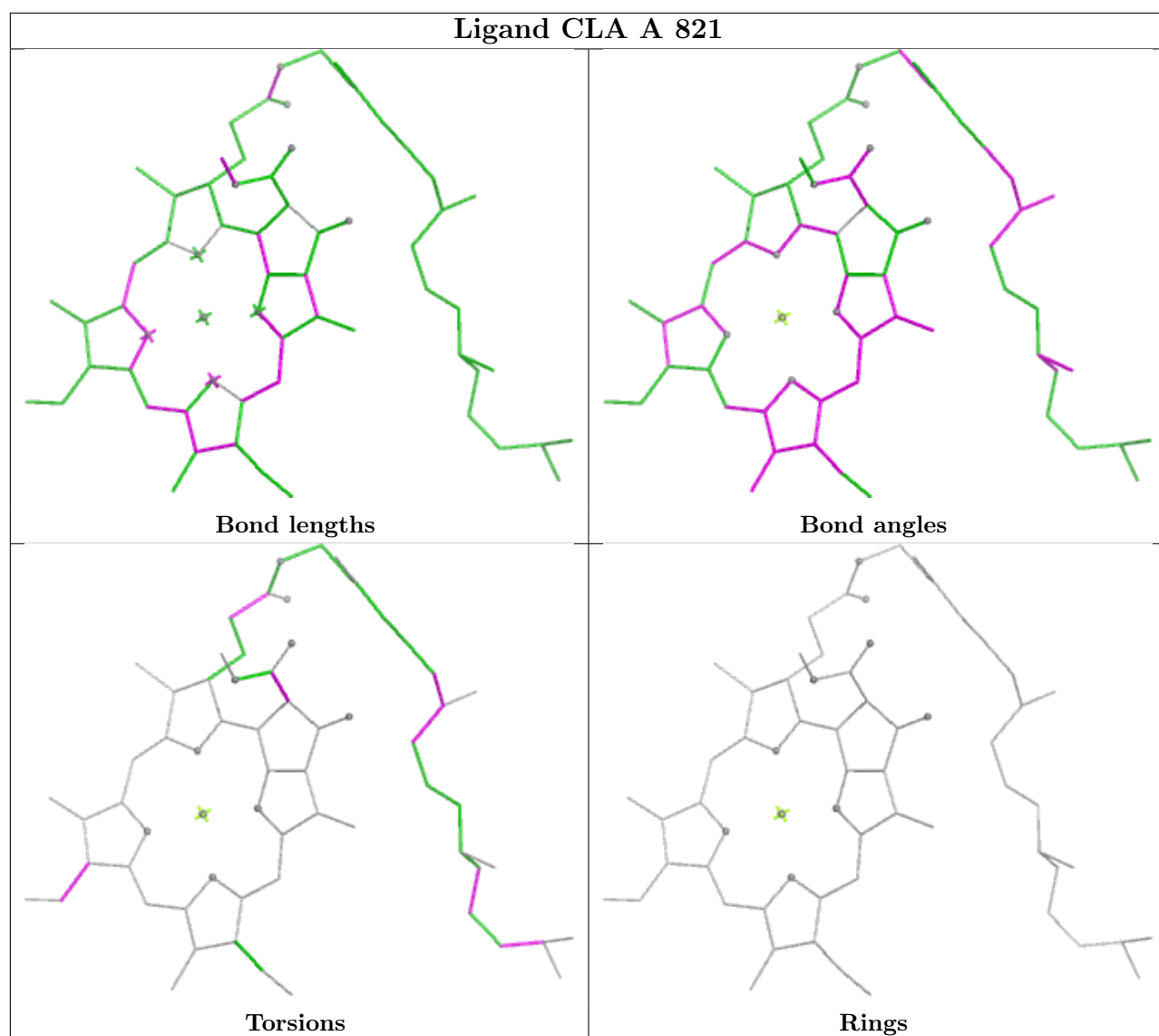


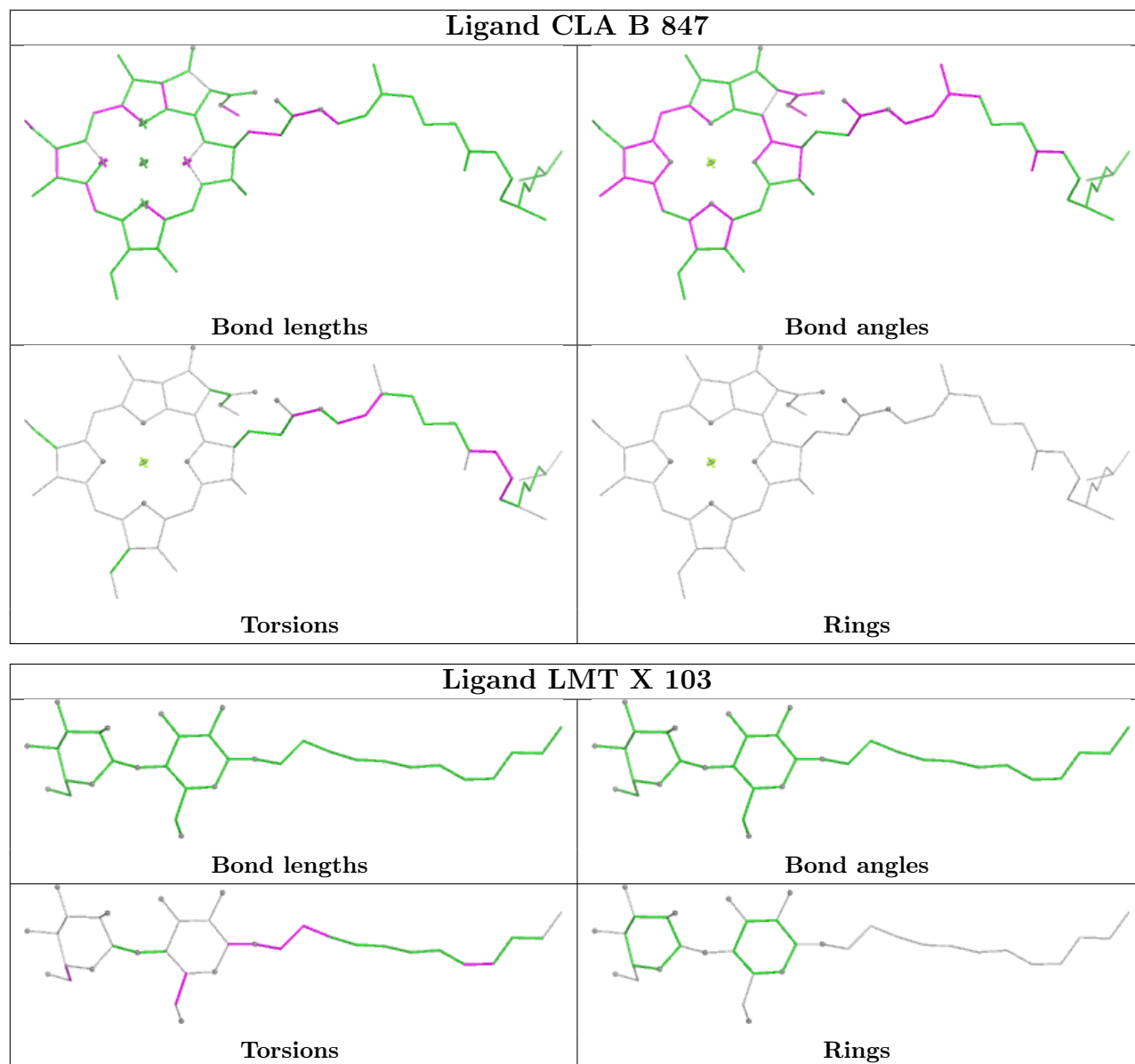


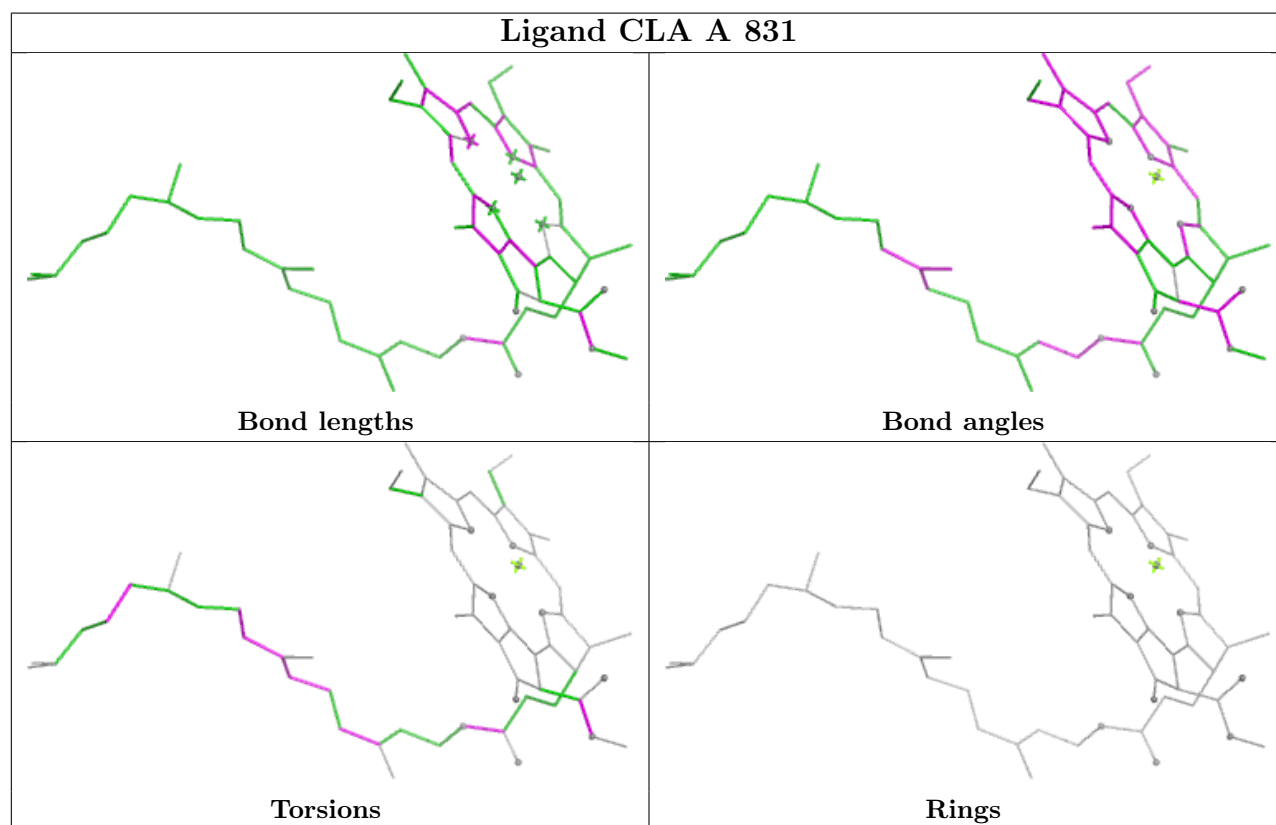
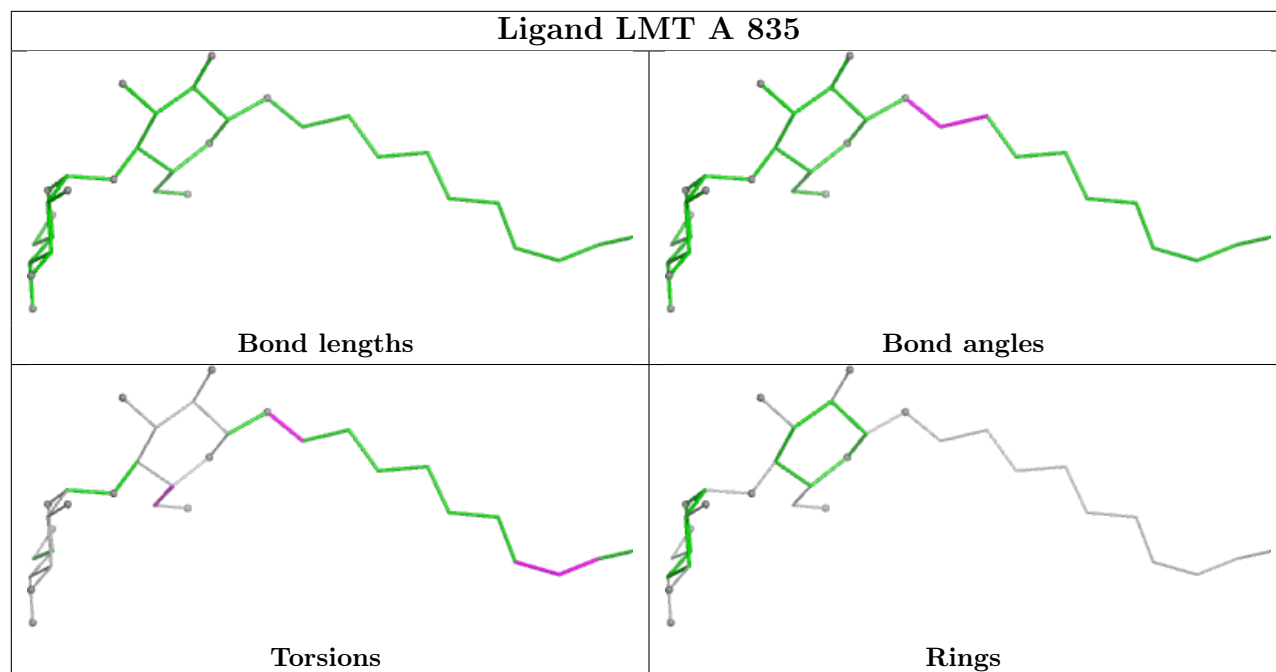
Ligand CLA B 811

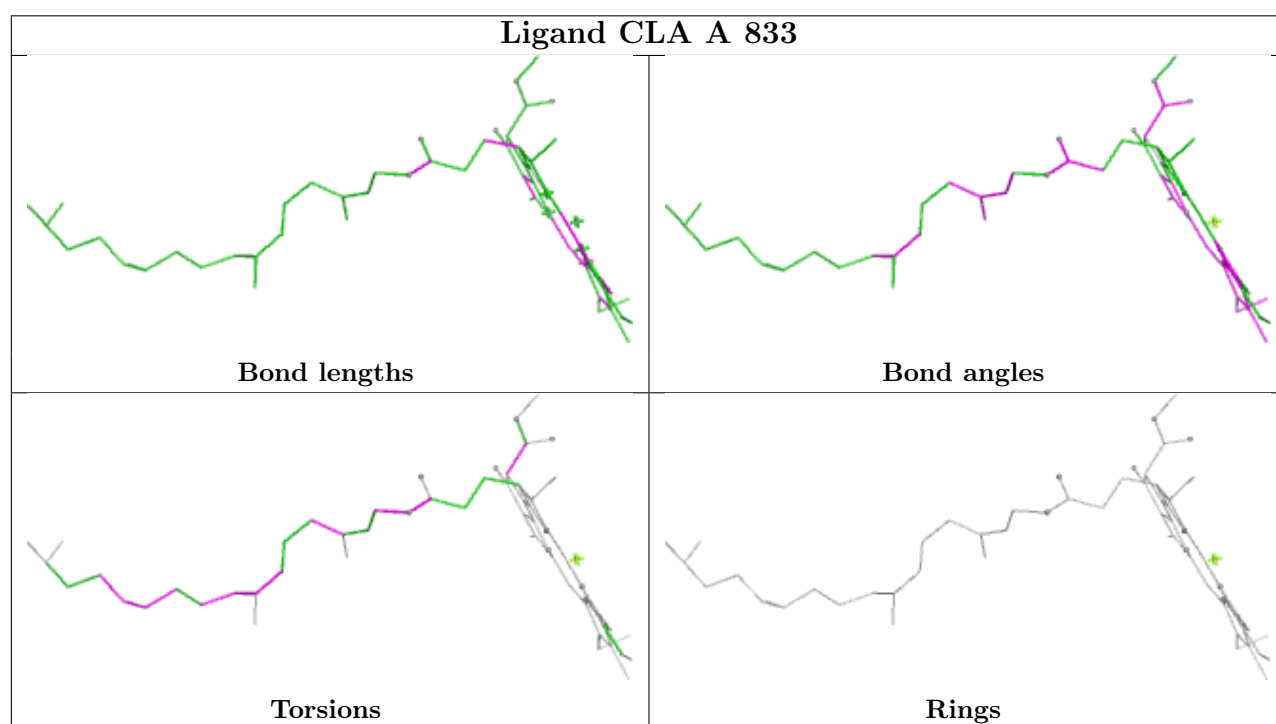
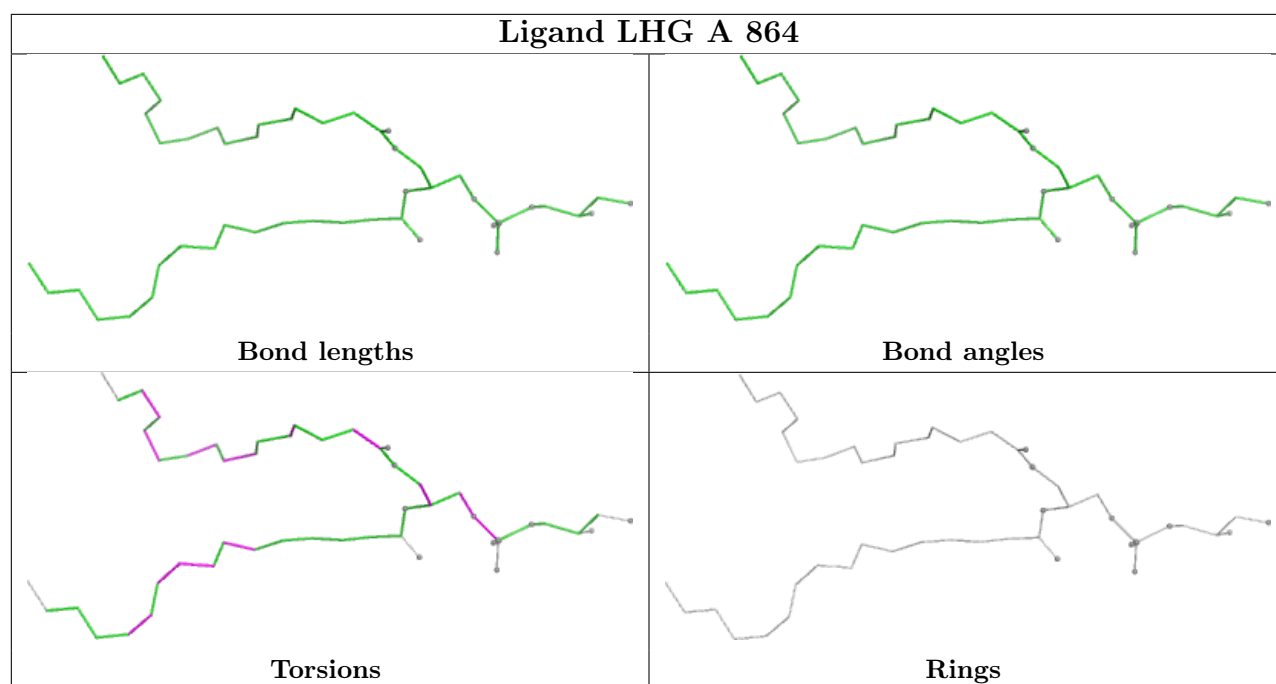


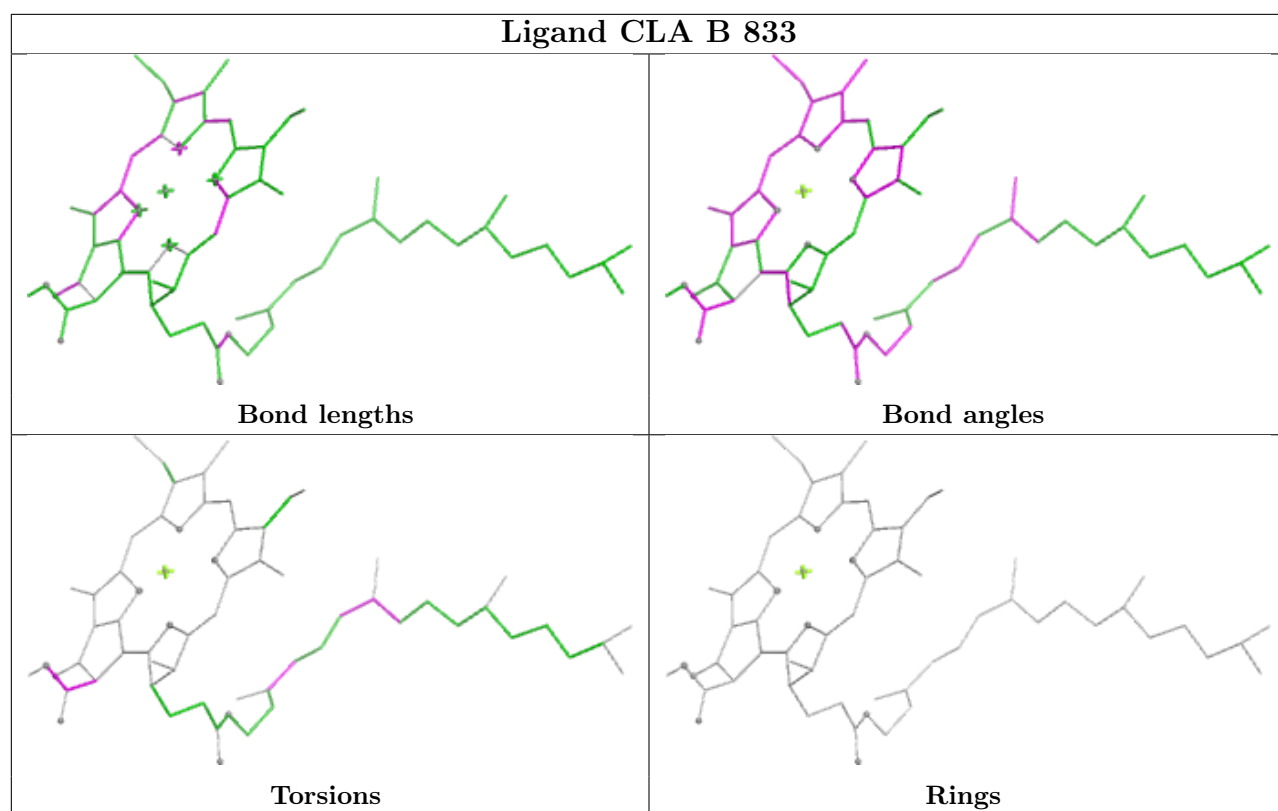


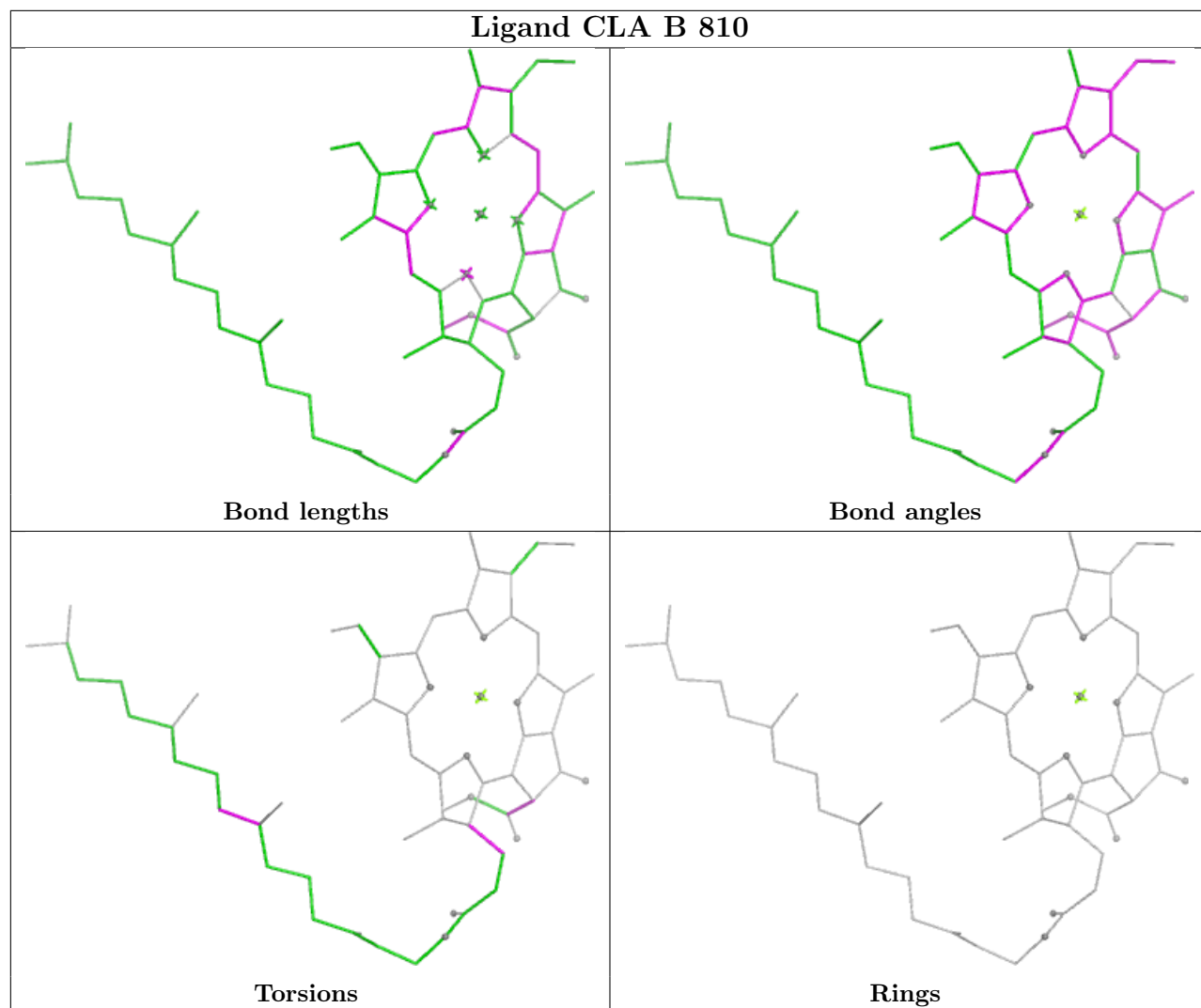


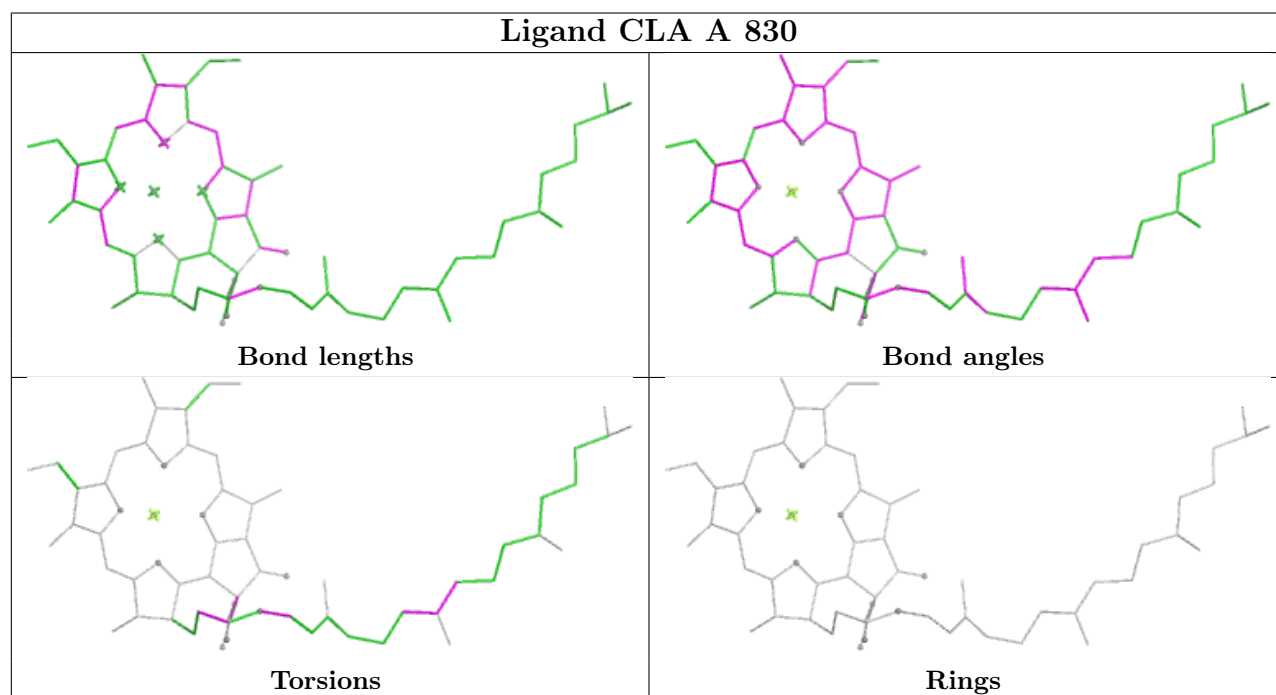
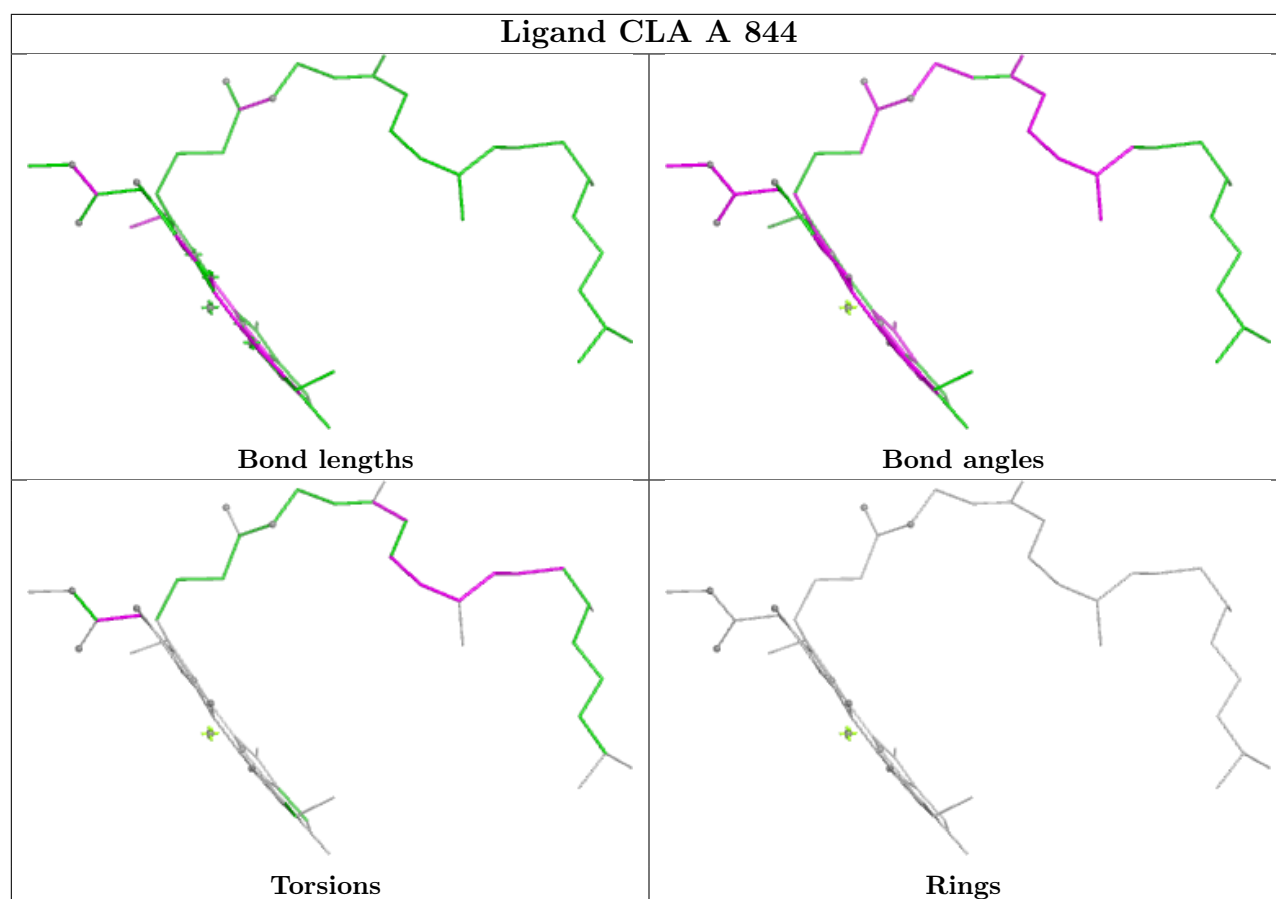


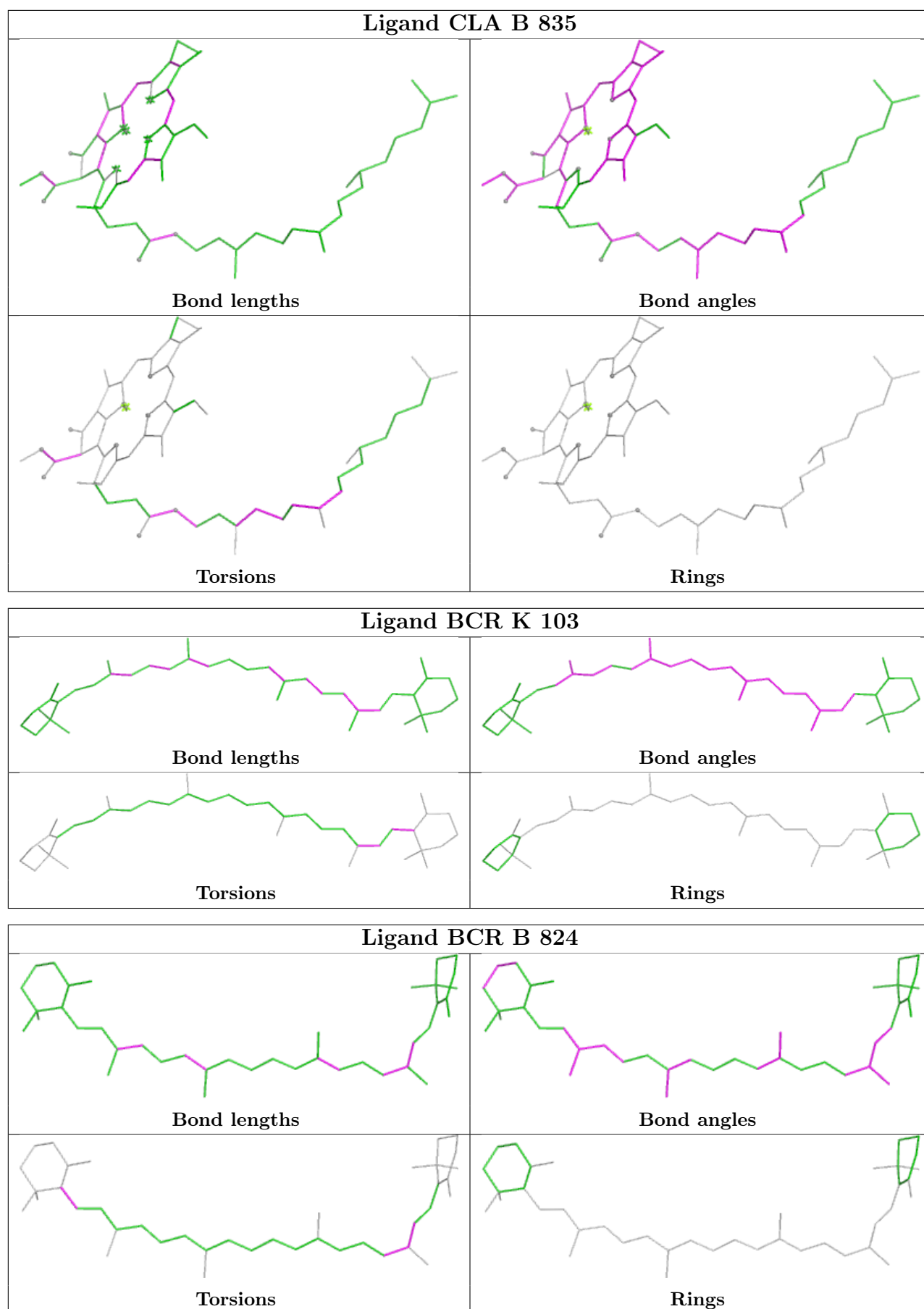


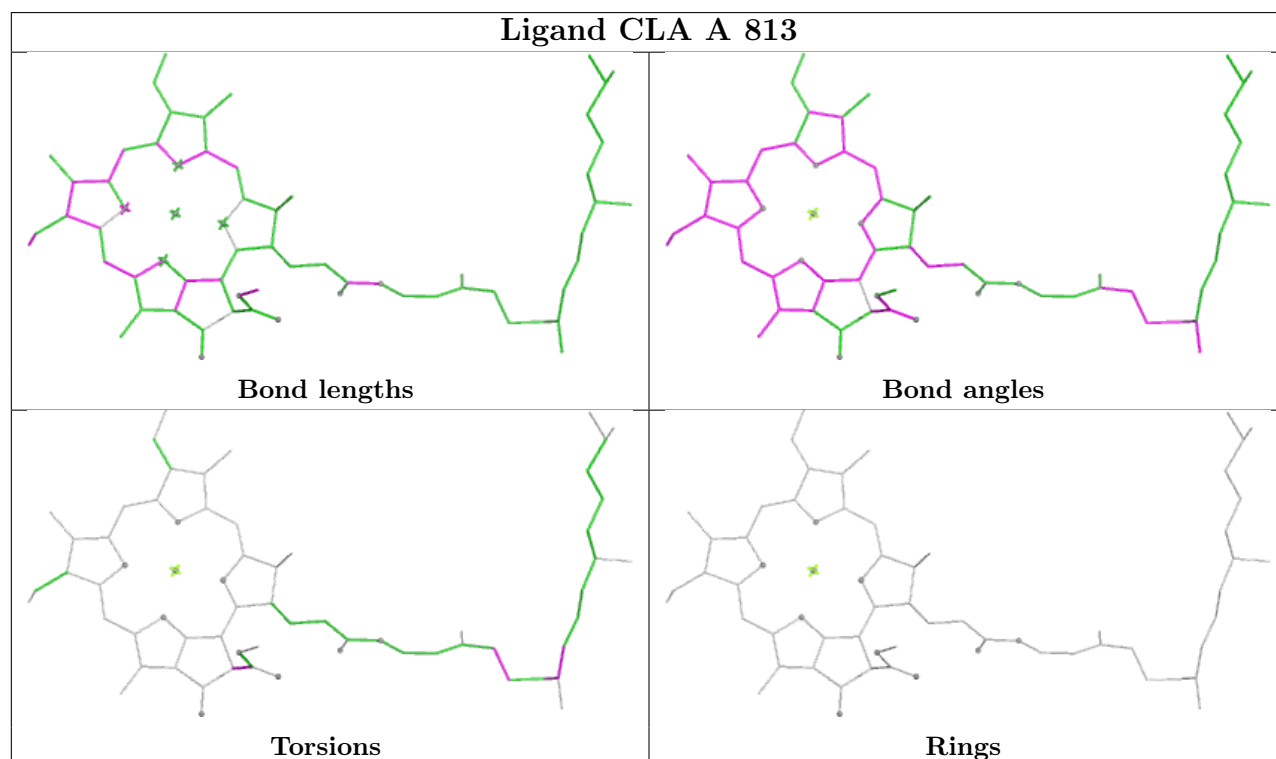
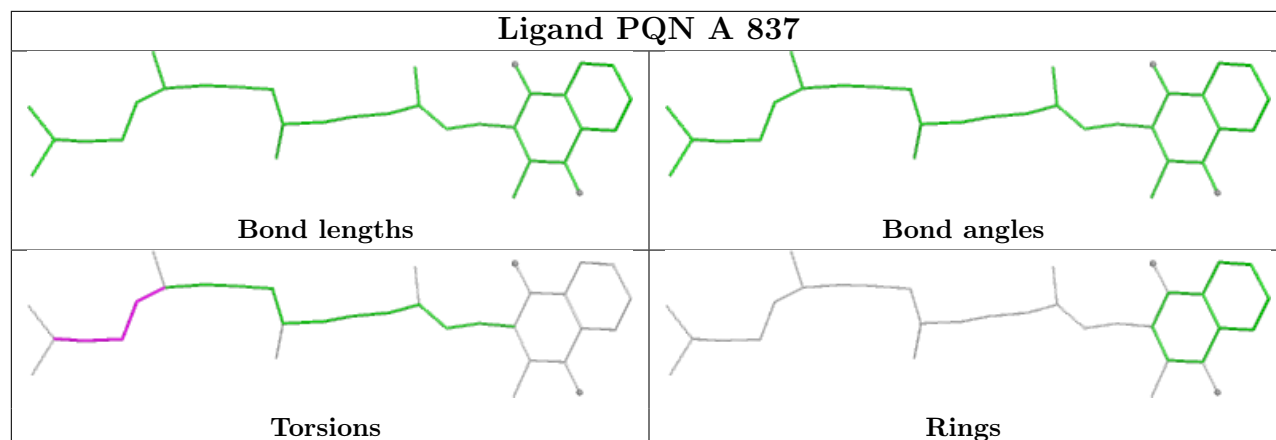


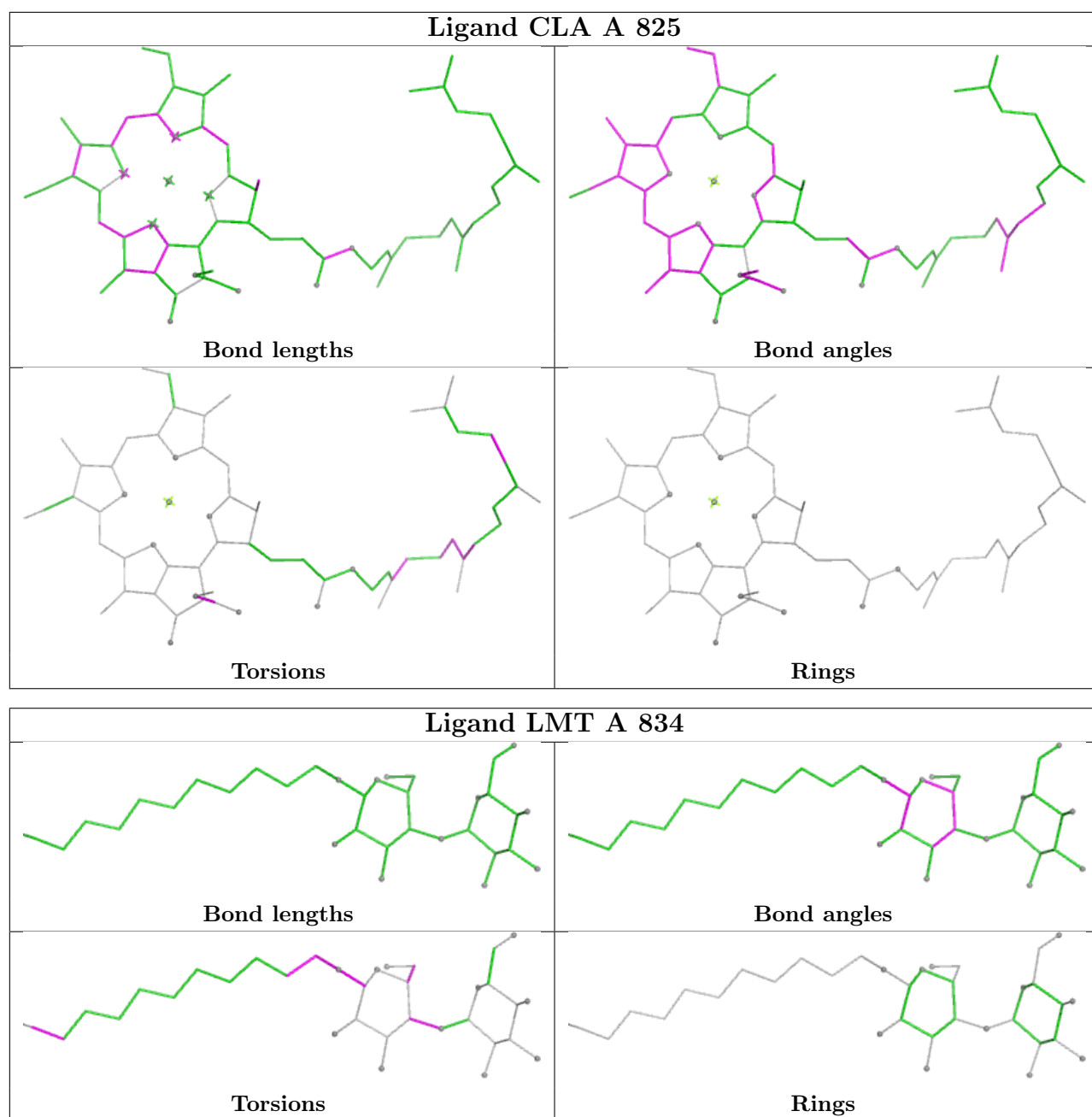


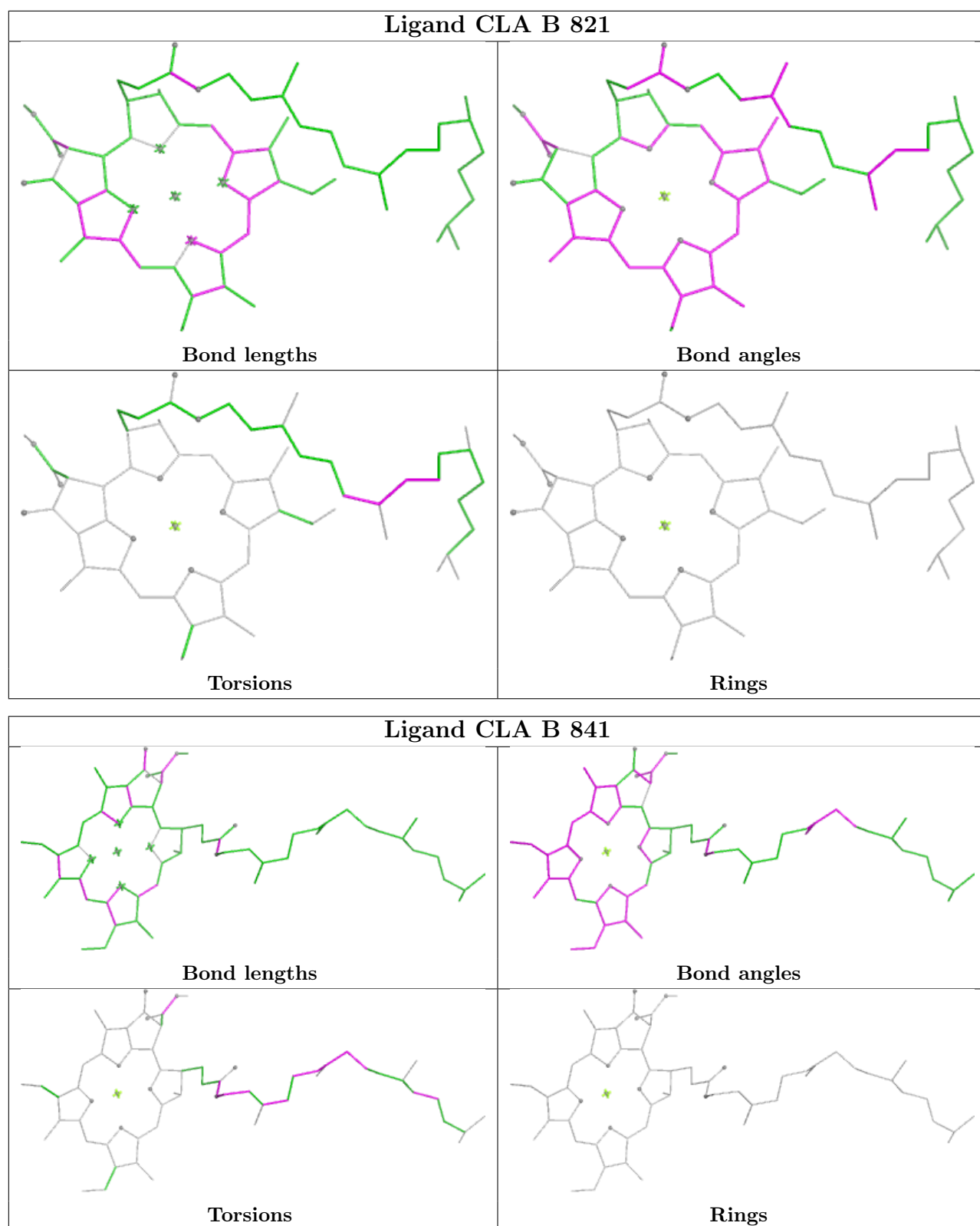


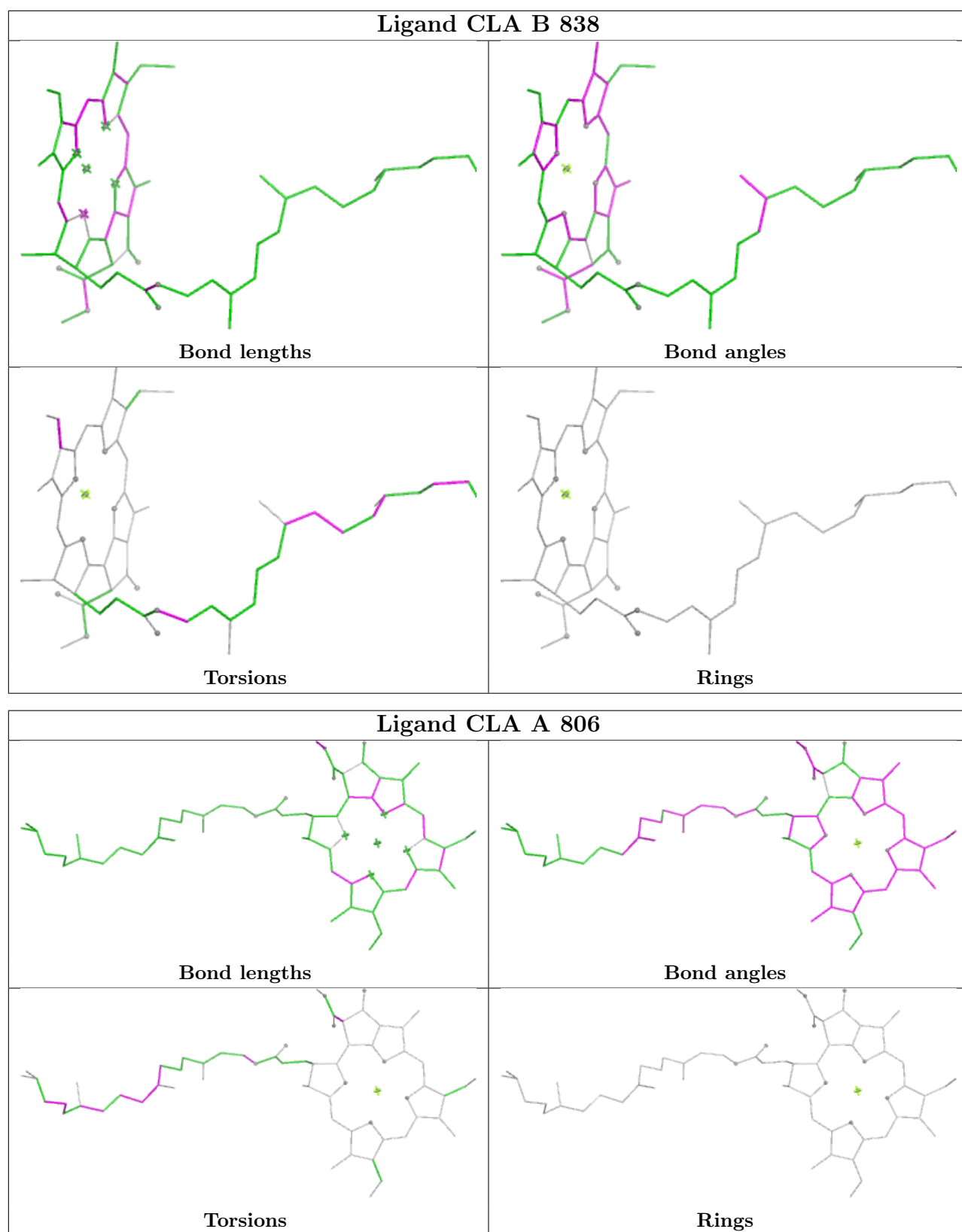


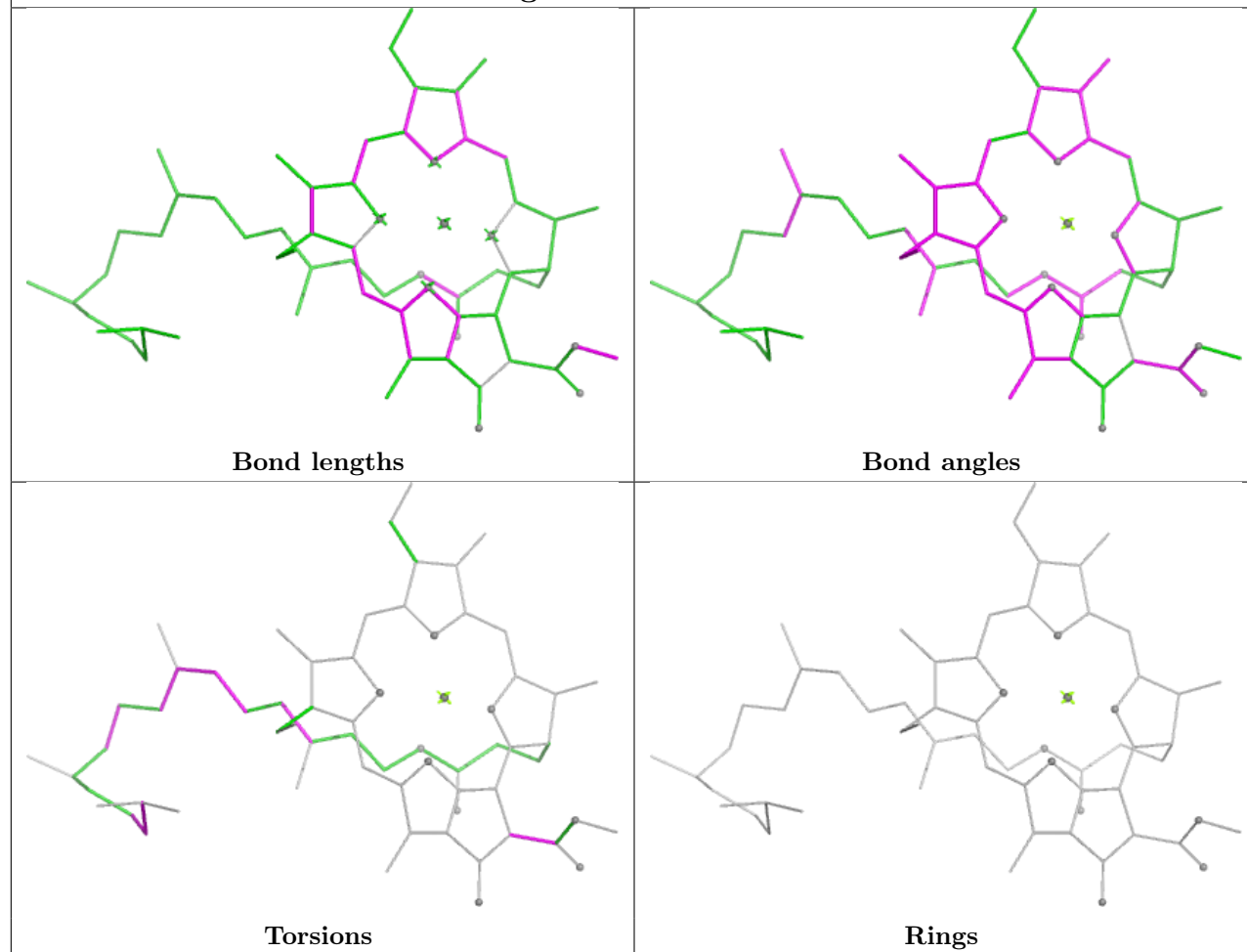
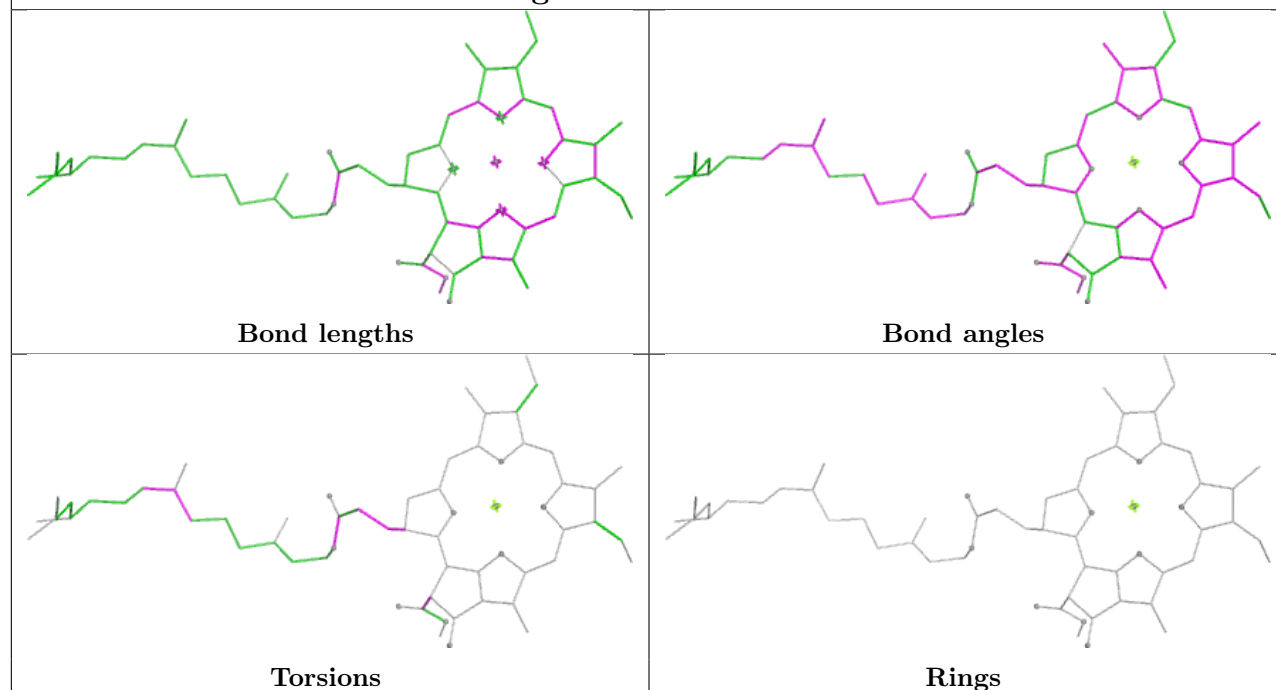


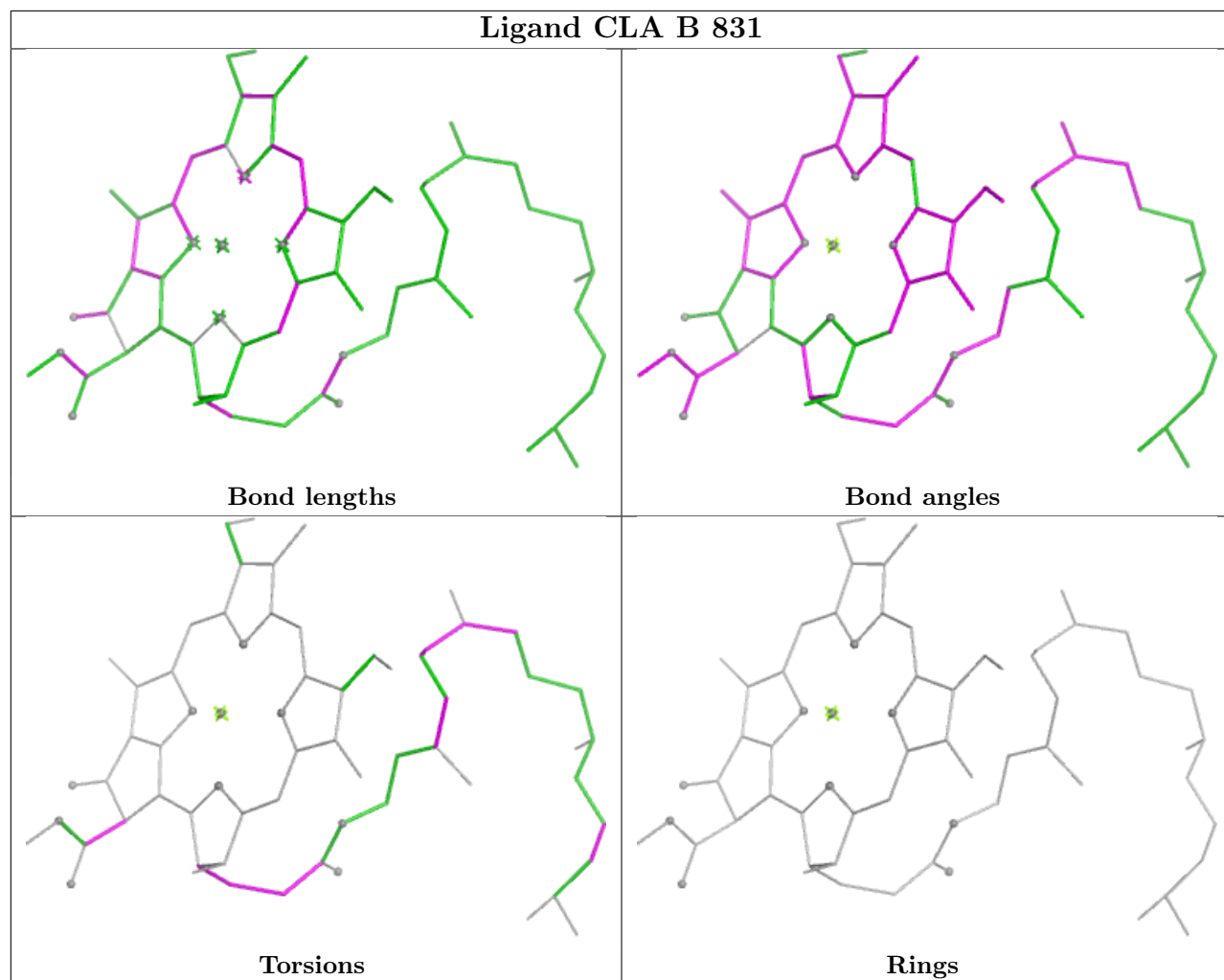


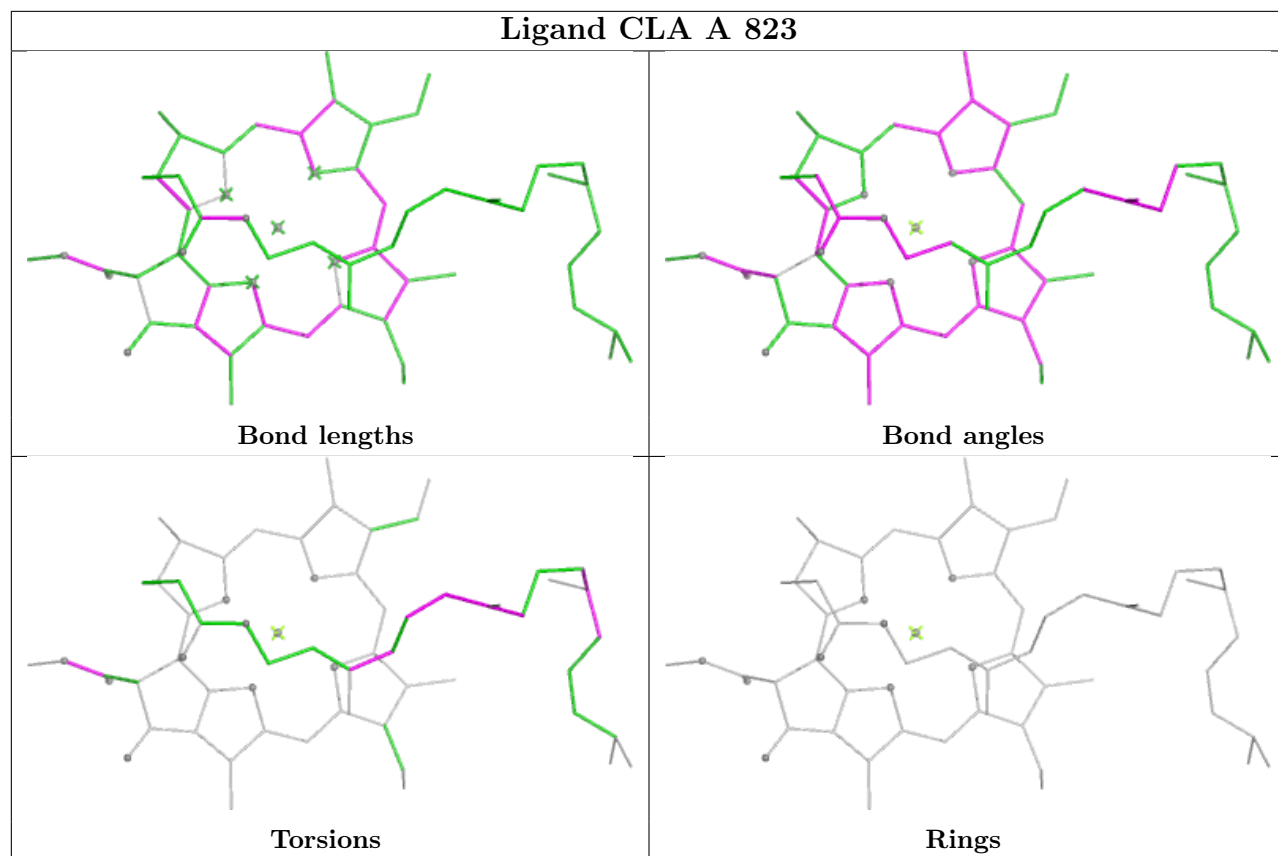


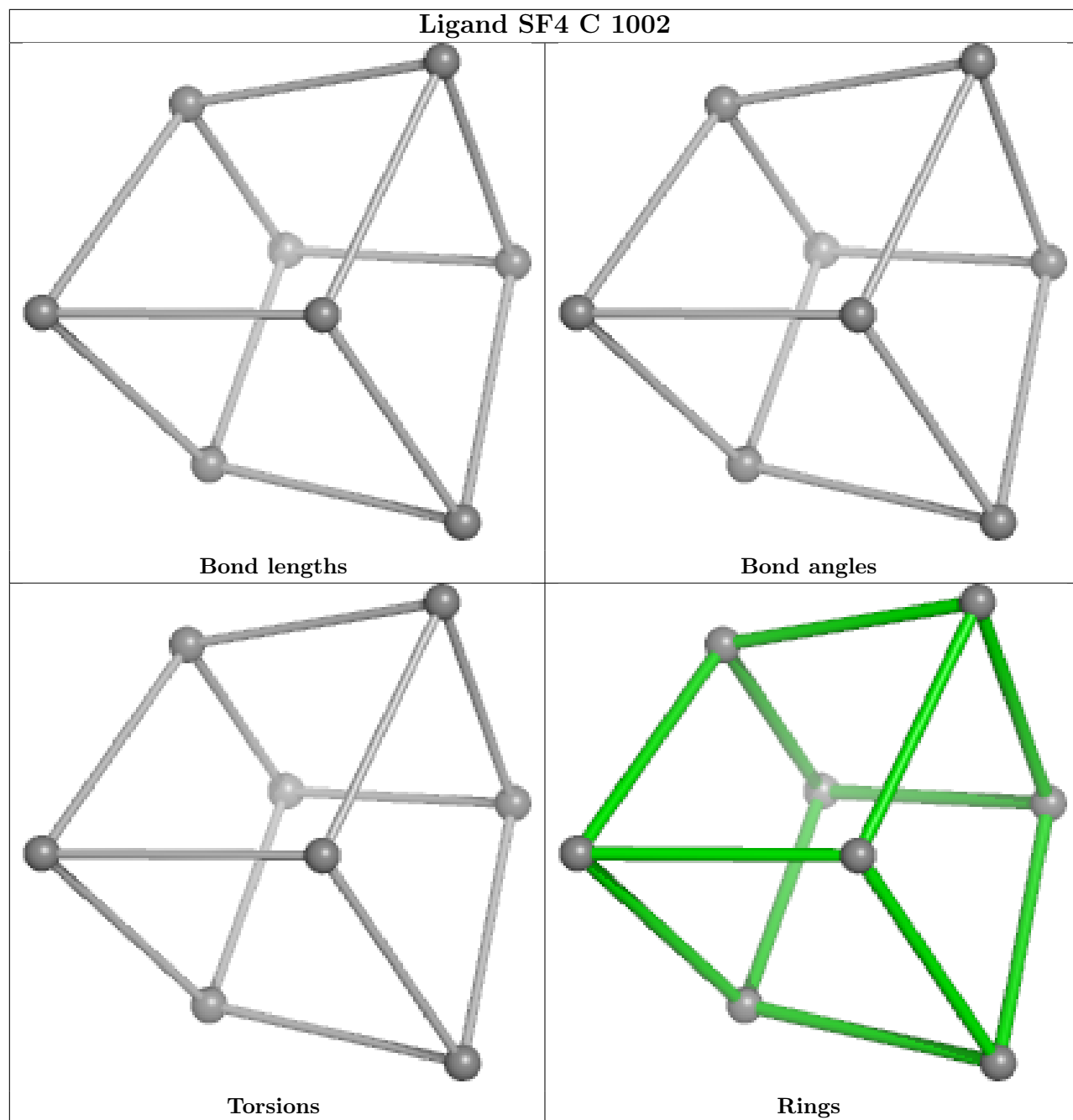


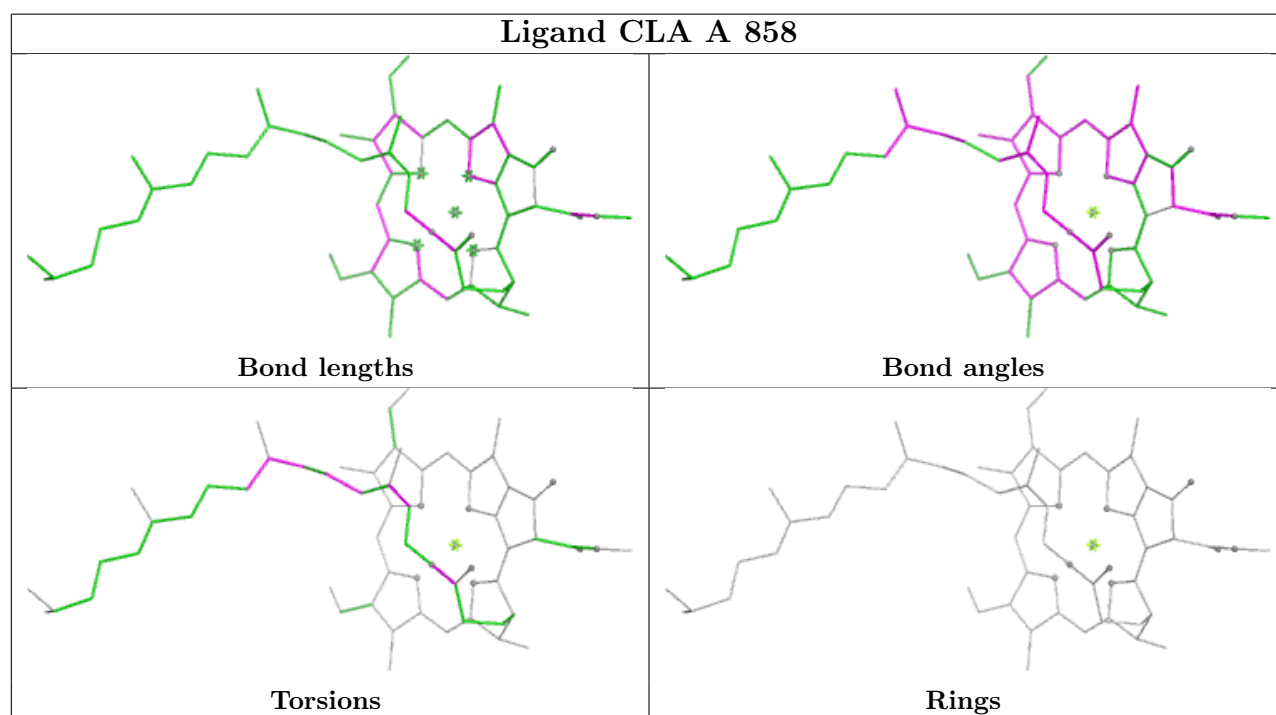
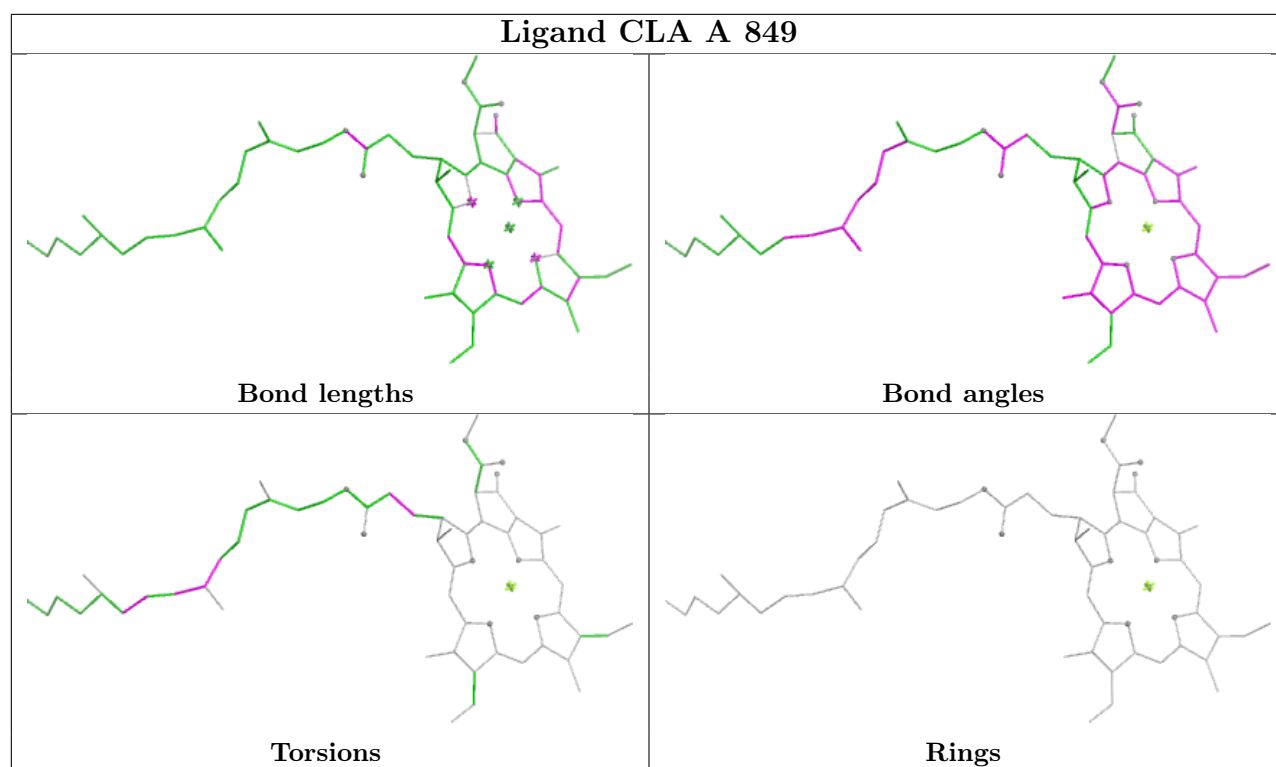


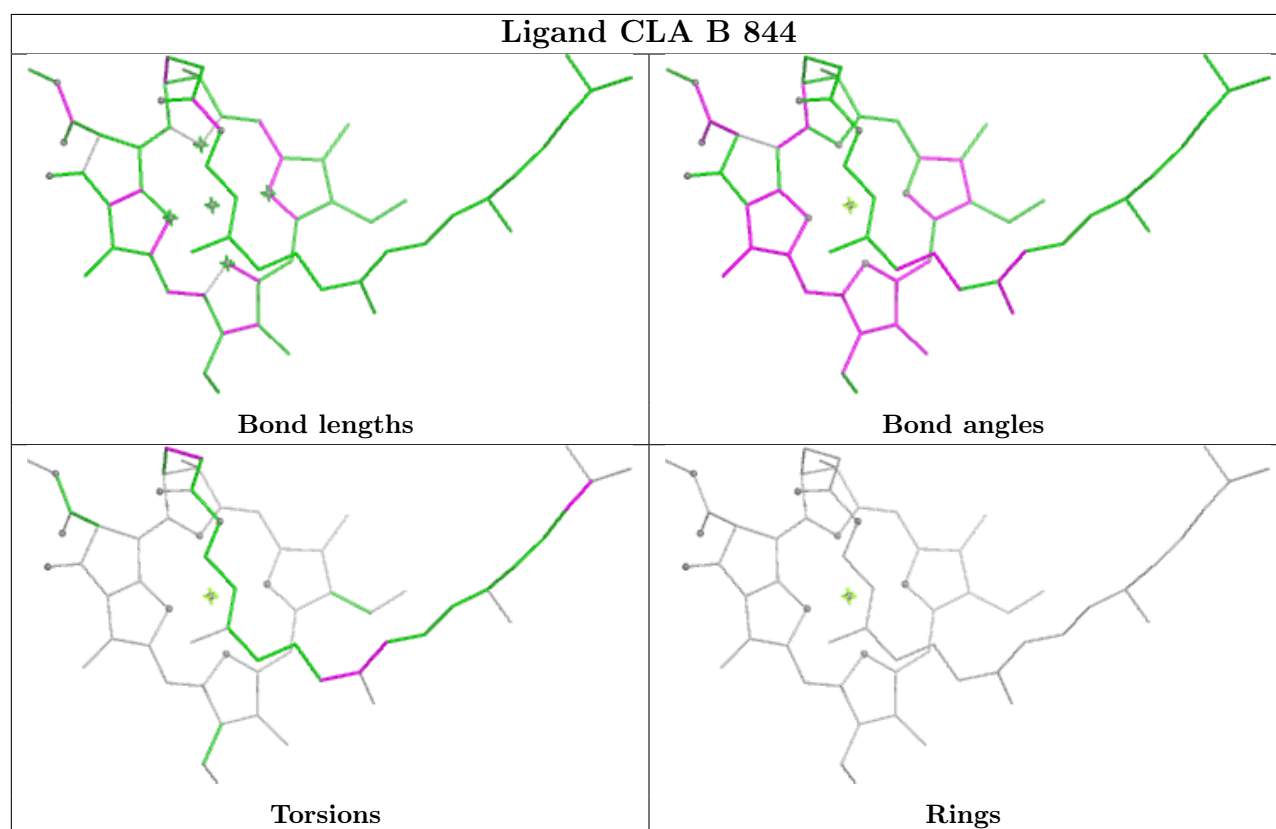
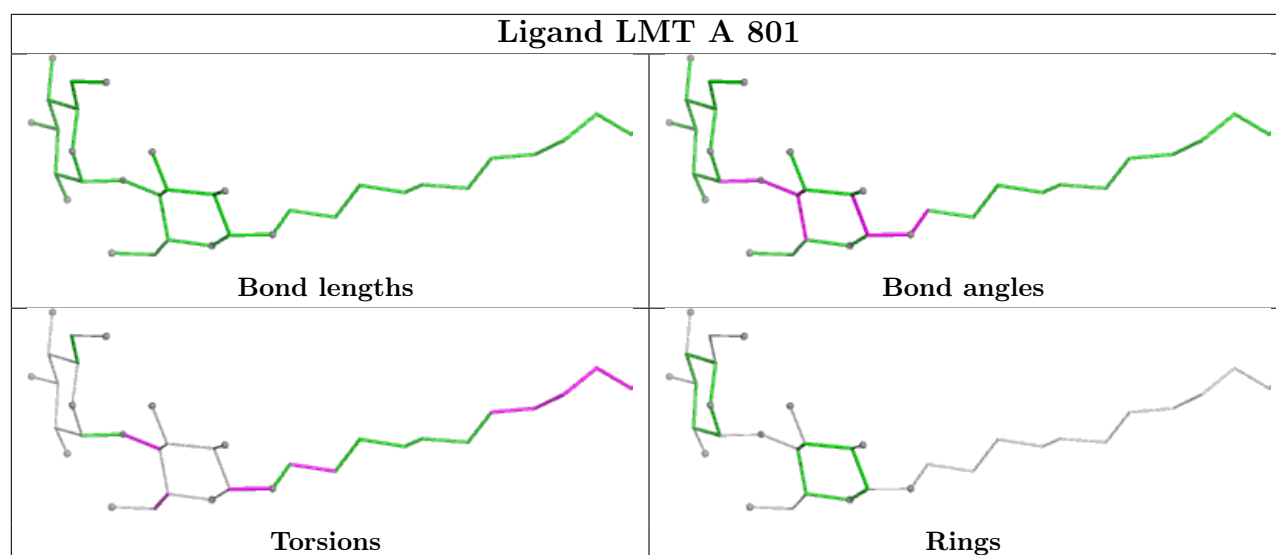
Ligand CLA B 843**Ligand CLA A 814**

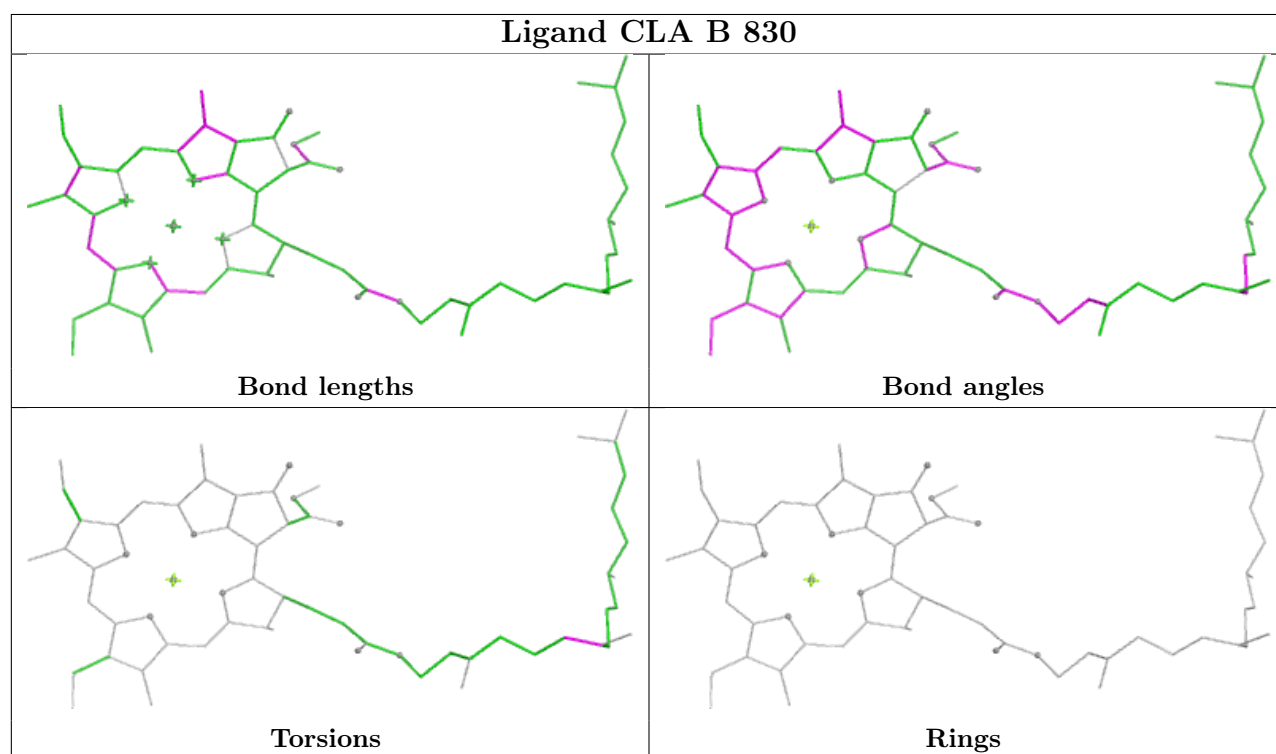
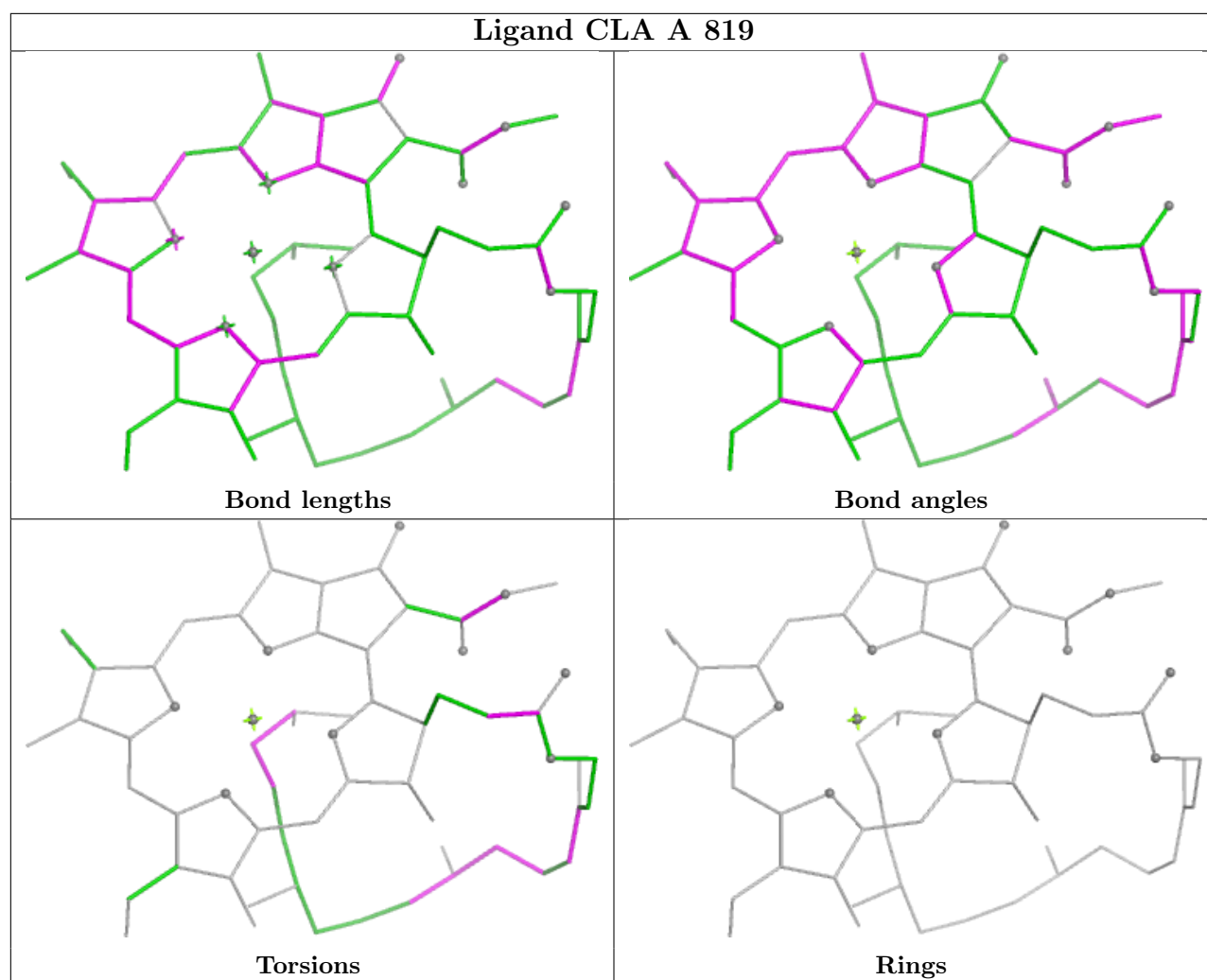


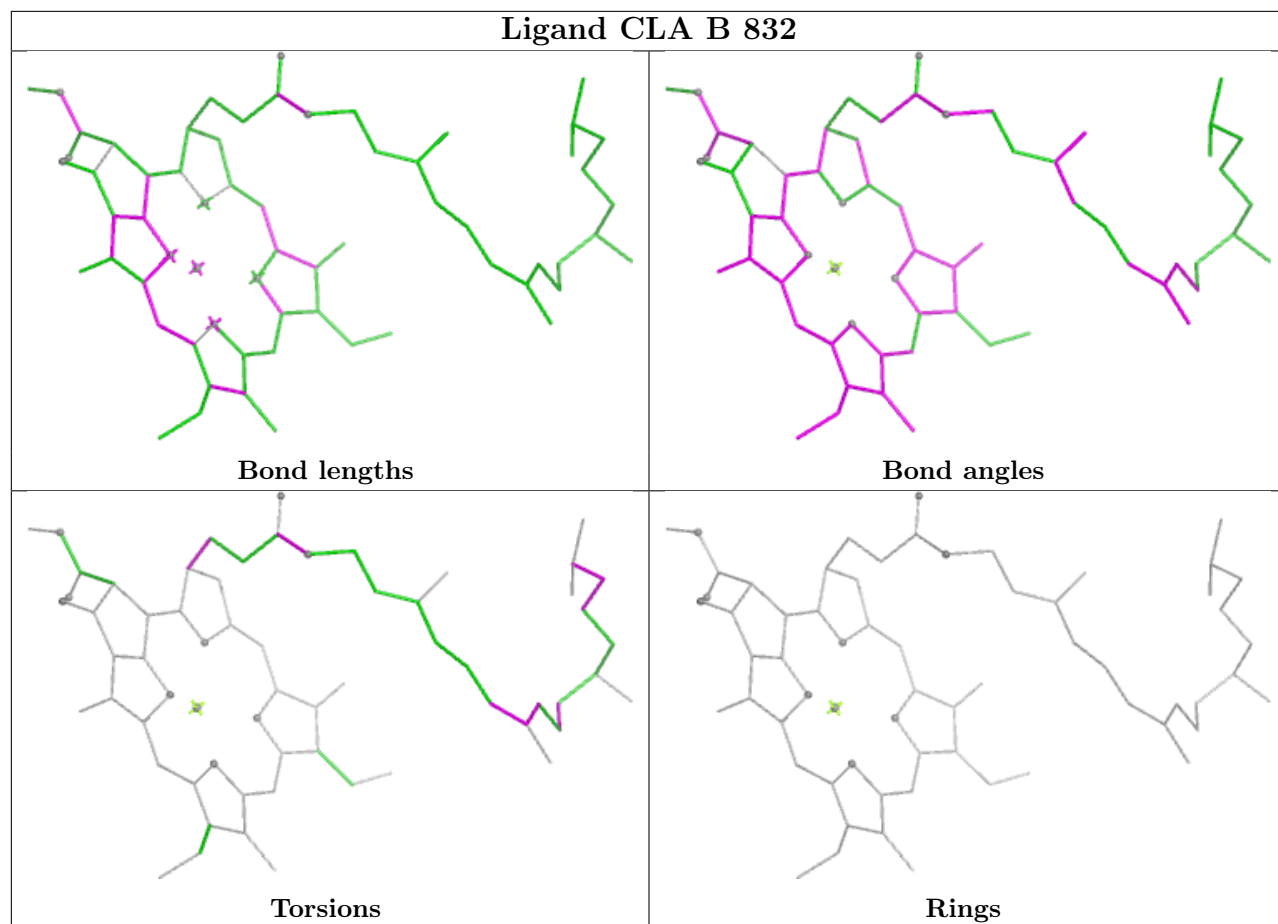




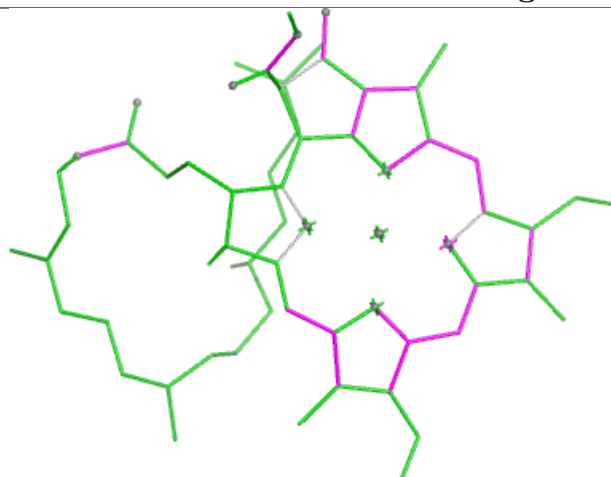




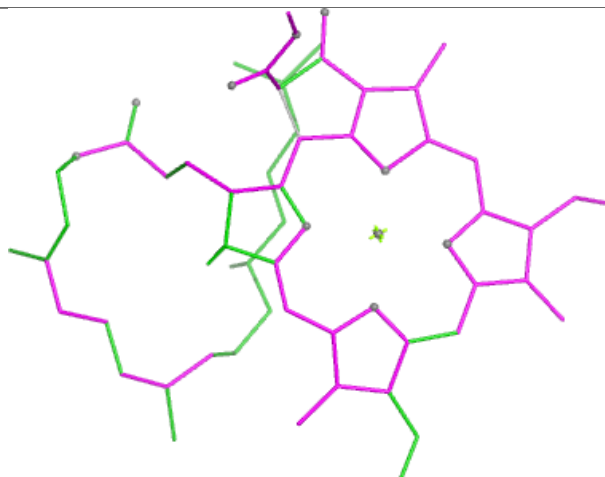




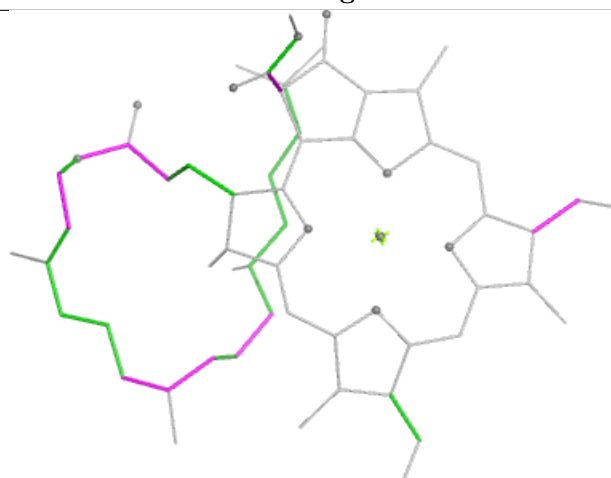
Ligand CLA J 101



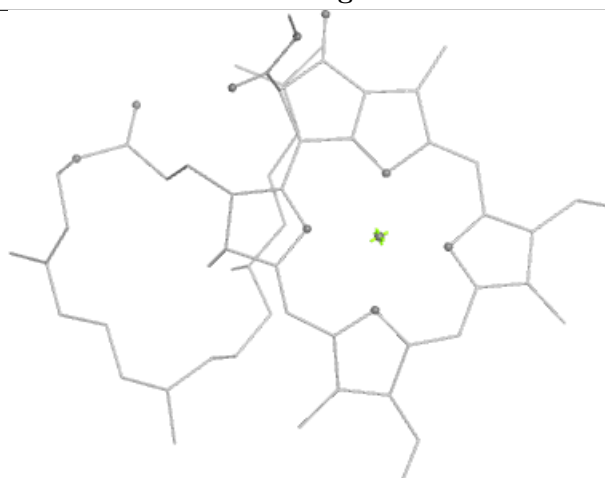
Bond lengths



Bond angles

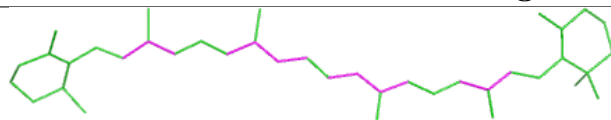


Torsions

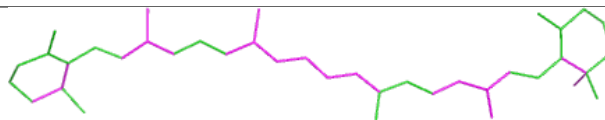


Rings

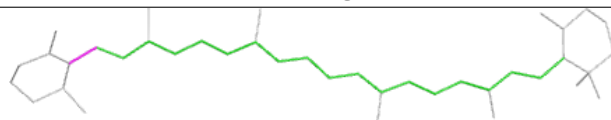
Ligand BCR J 103



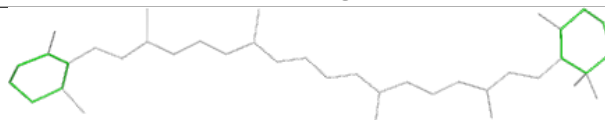
Bond lengths



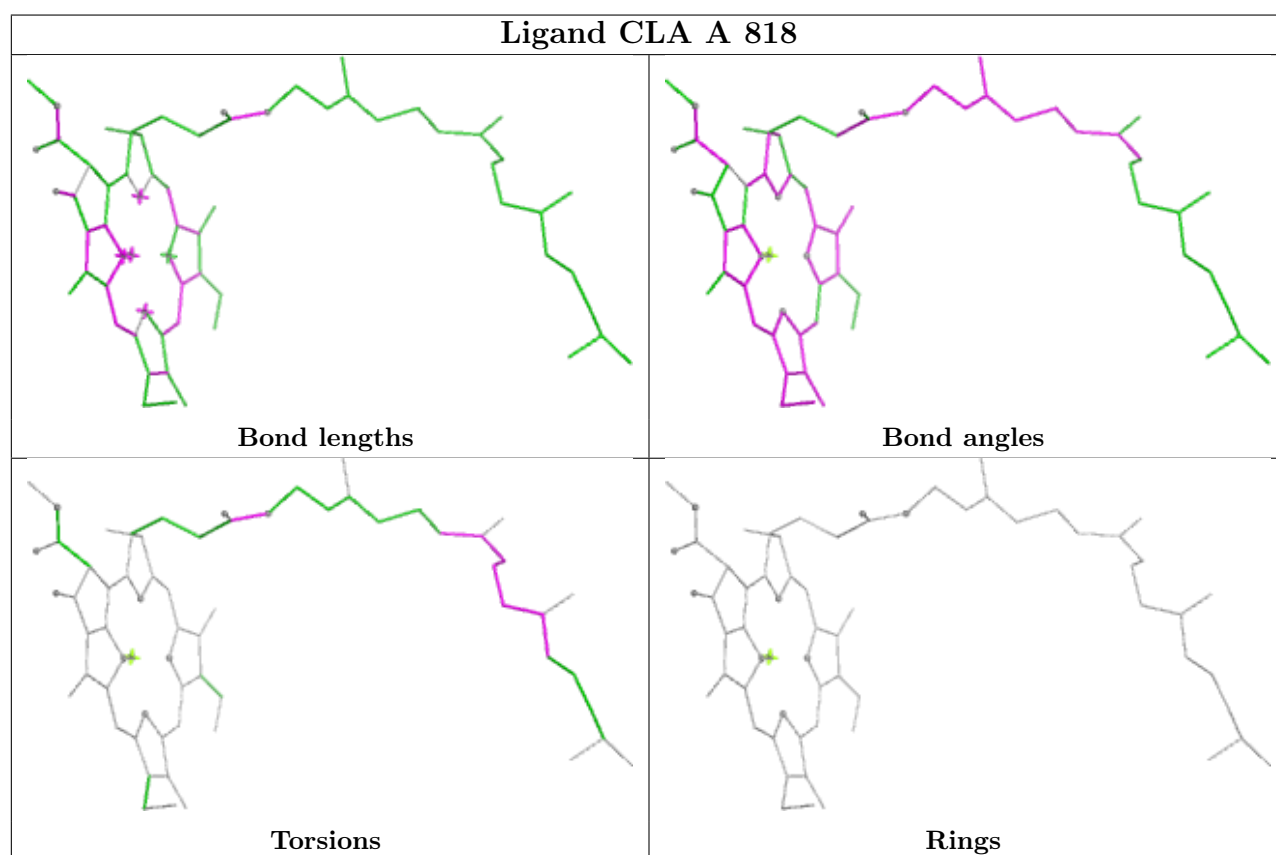
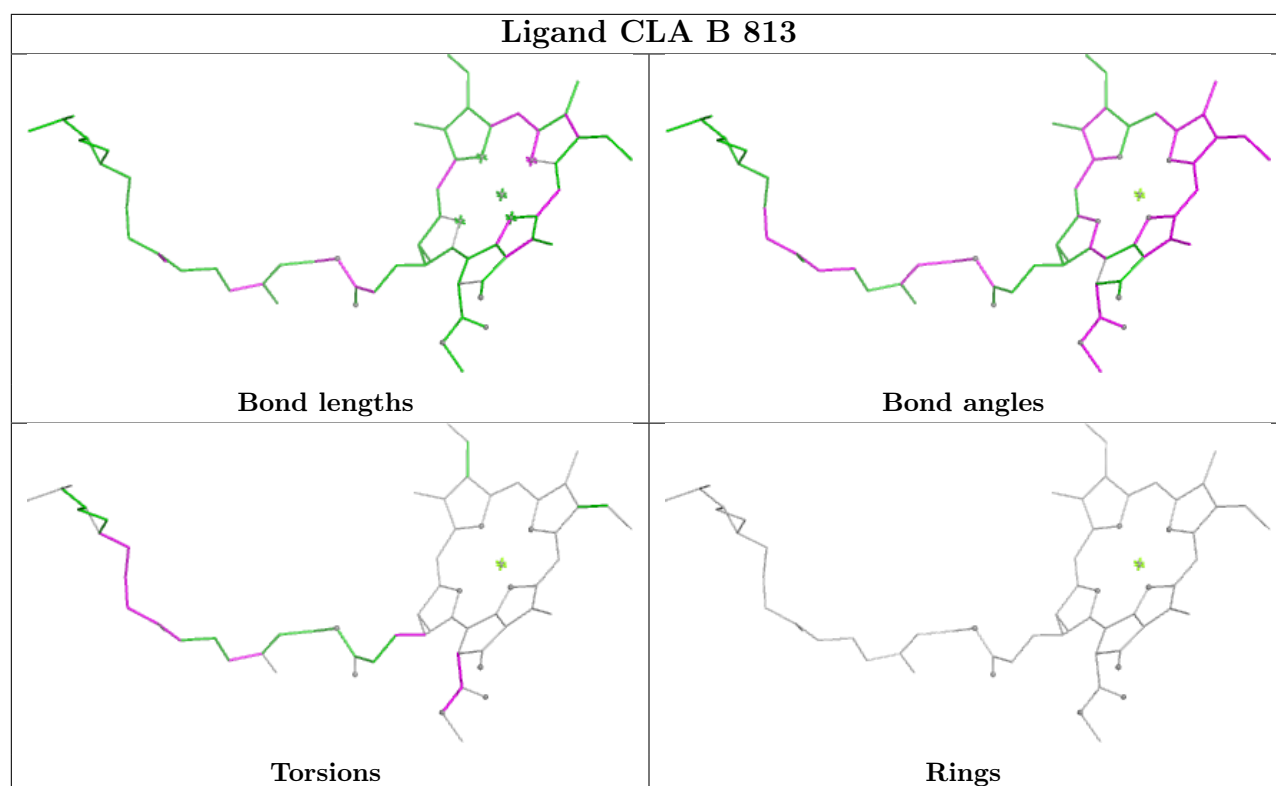
Bond angles

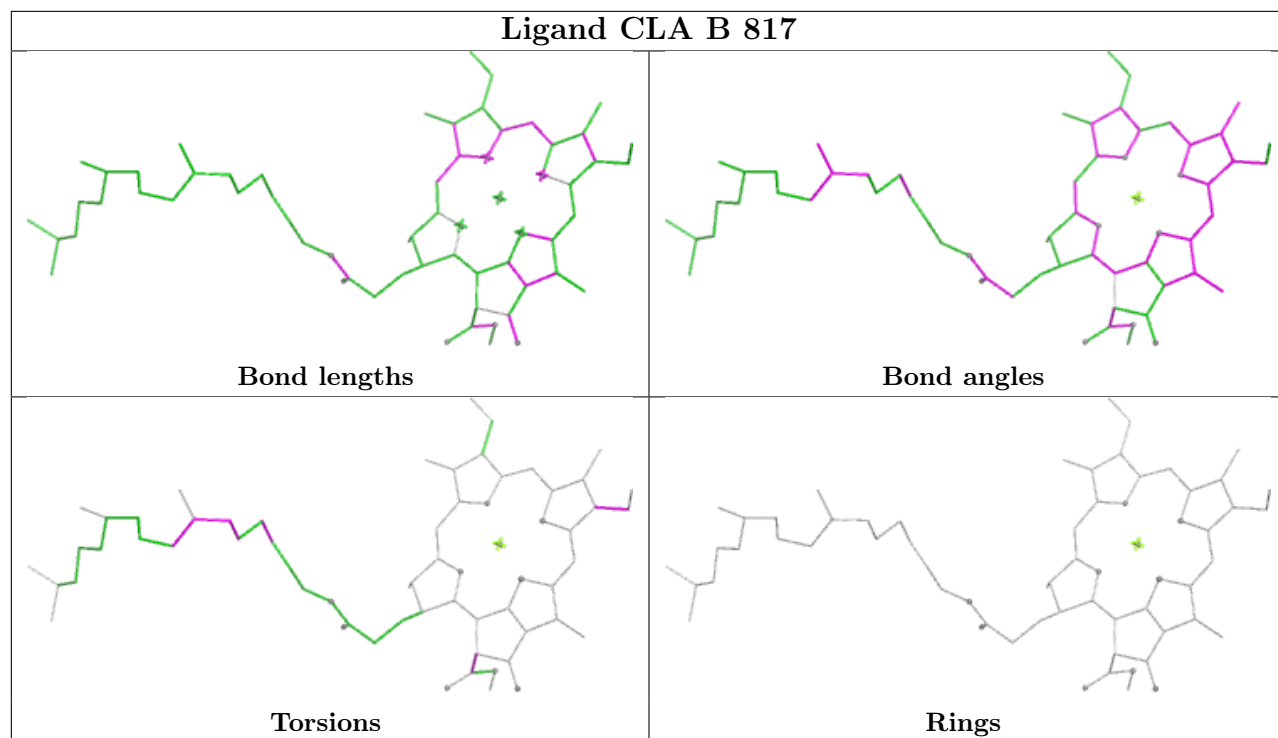


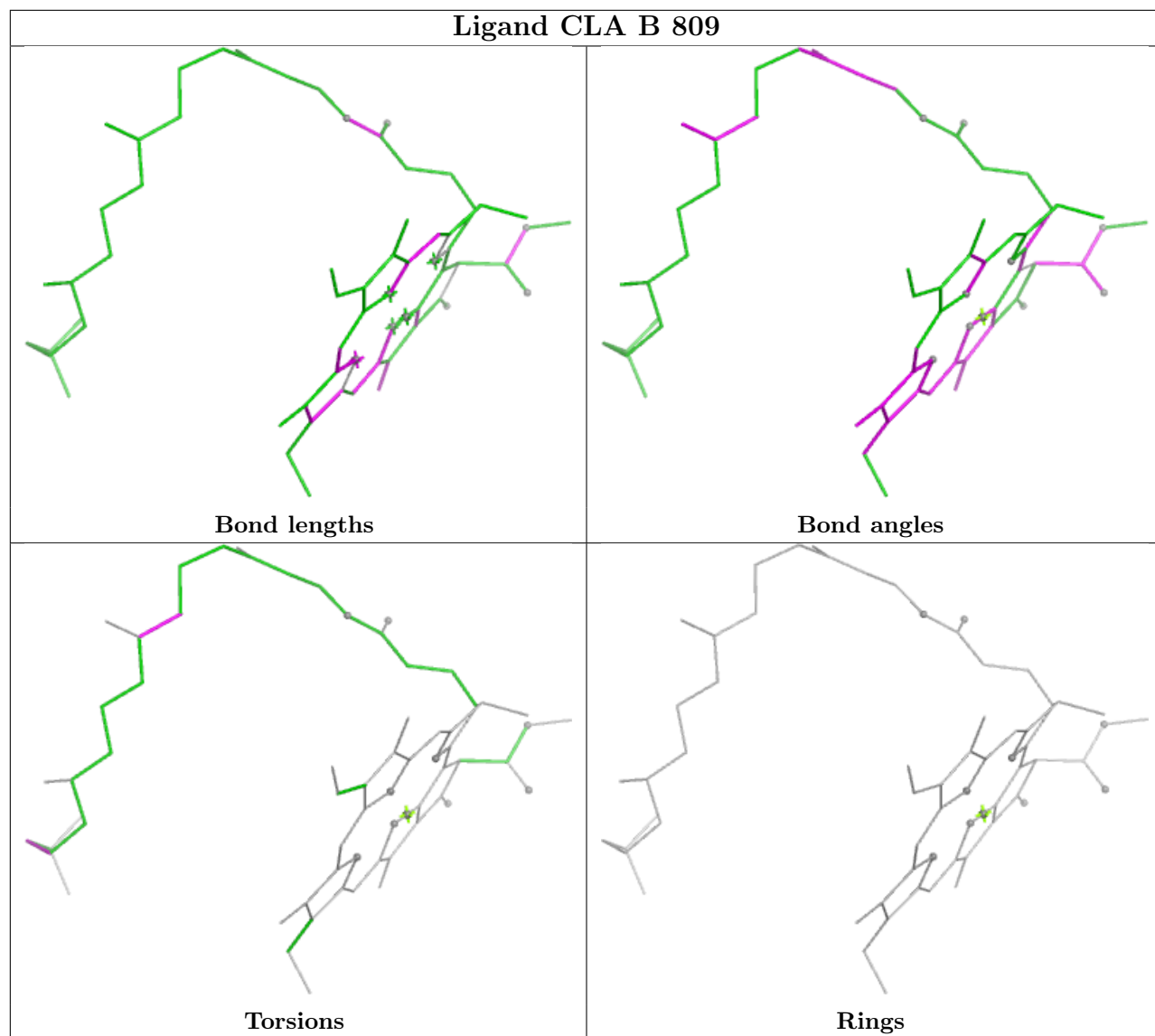
Torsions

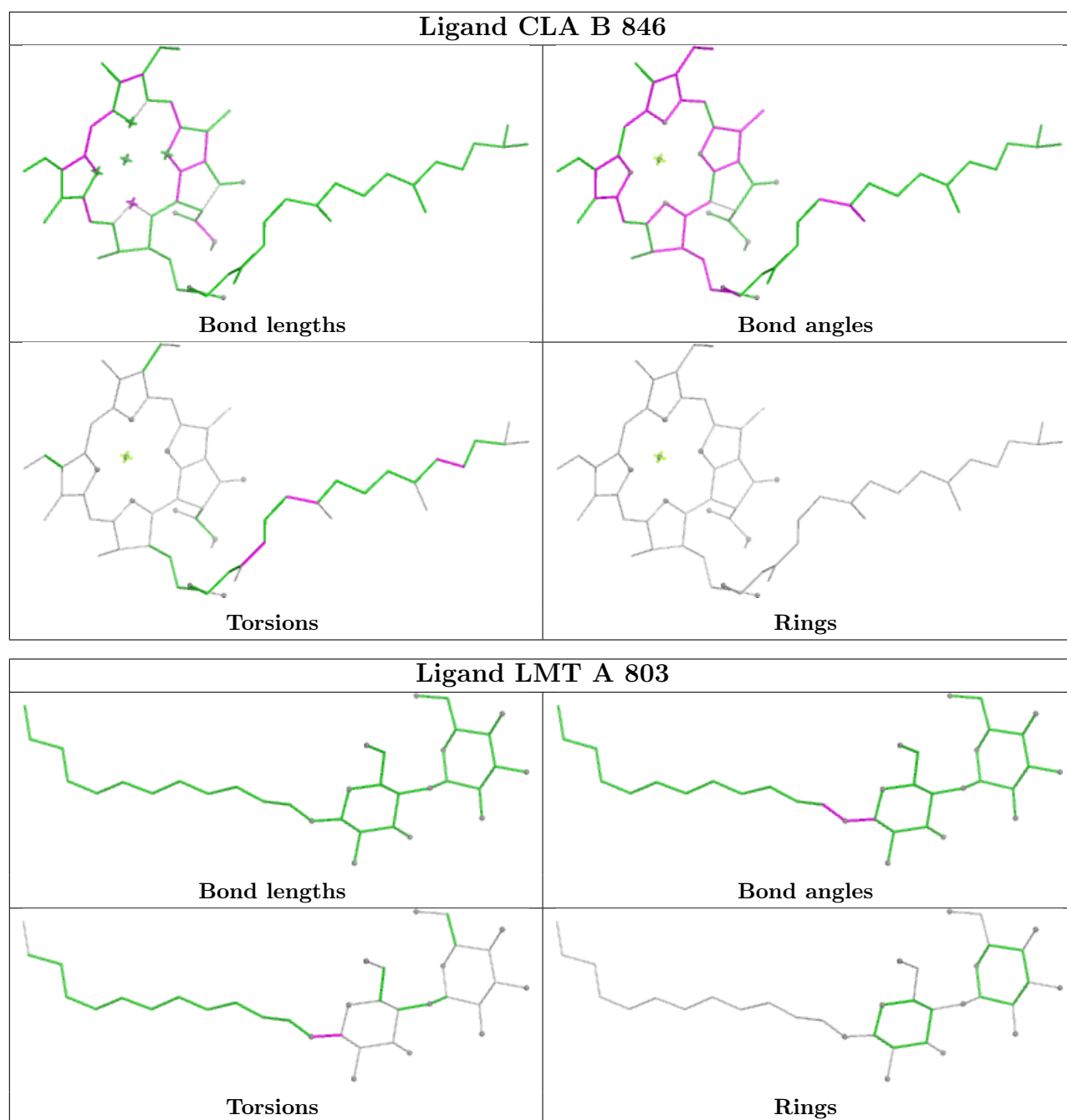


Rings









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.

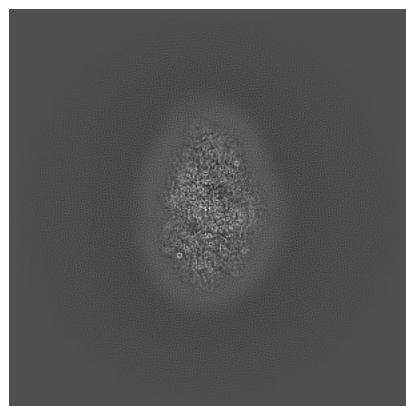
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53120. These allow visual inspection of the internal detail of the map and identification of artifacts.

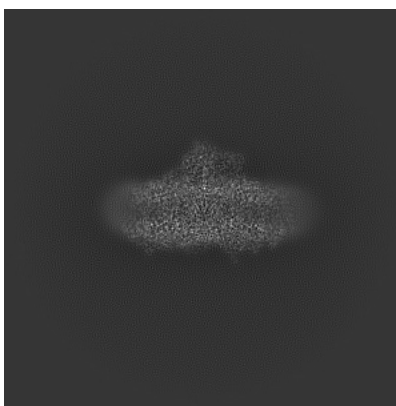
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

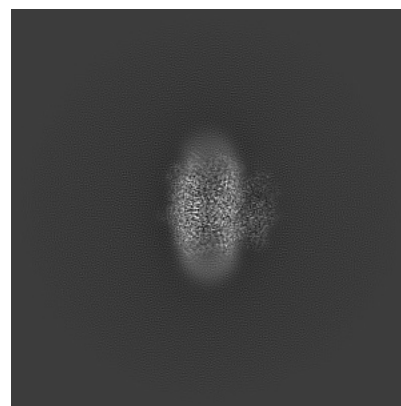
6.1.1 Primary map



X

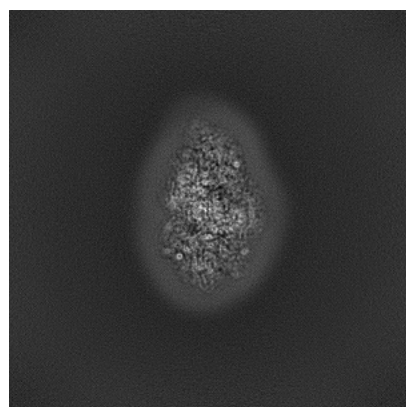


Y

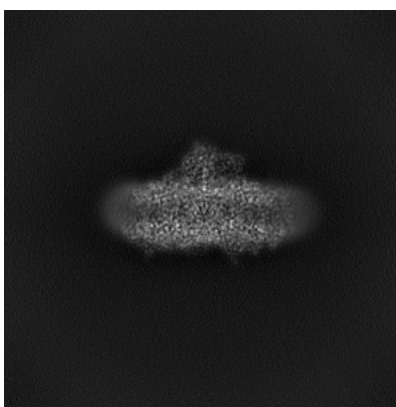


Z

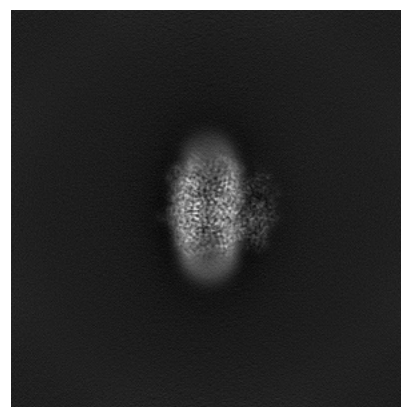
6.1.2 Raw map



X



Y

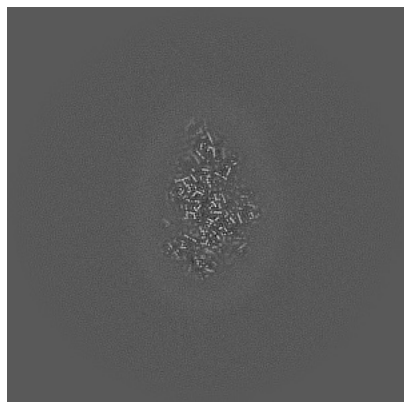


Z

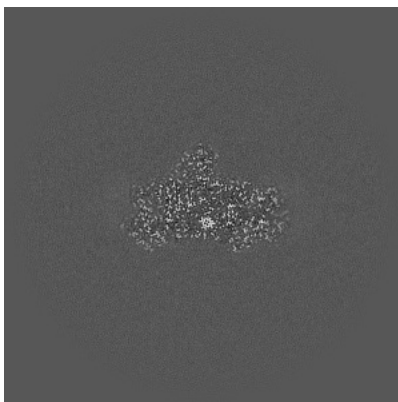
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

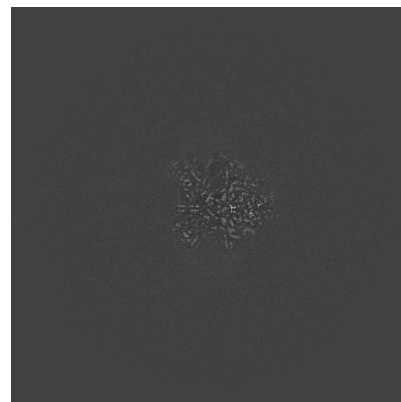
6.2.1 Primary map



X Index: 256

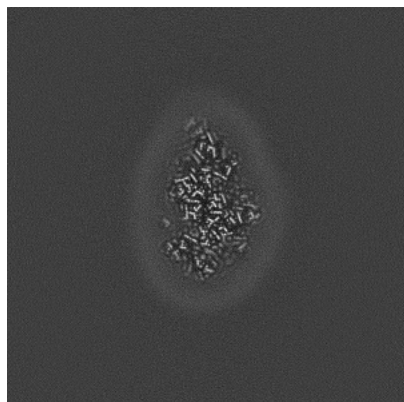


Y Index: 256

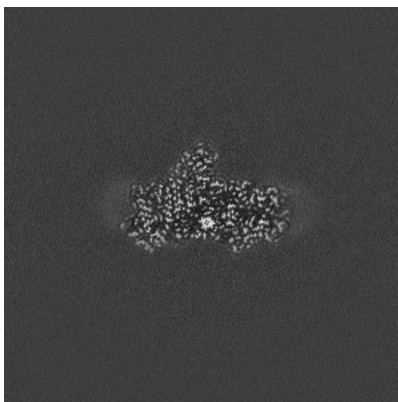


Z Index: 256

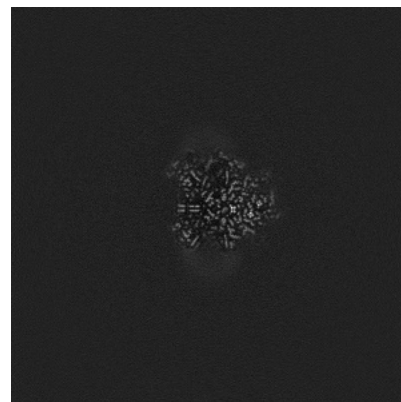
6.2.2 Raw map



X Index: 256



Y Index: 256

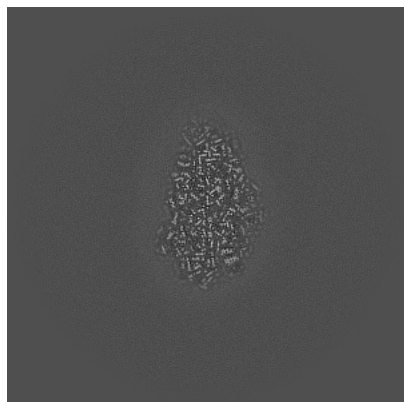


Z Index: 256

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

6.3 Largest variance slices [i](#)

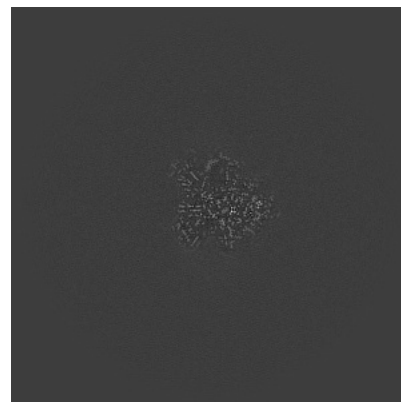
6.3.1 Primary map



X Index: 235

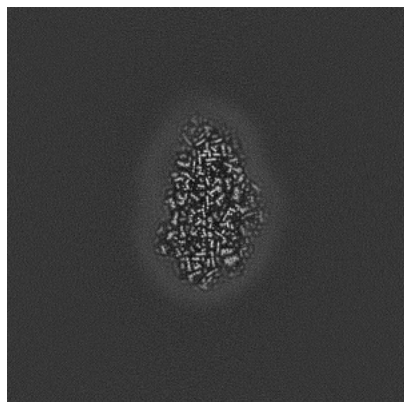


Y Index: 252

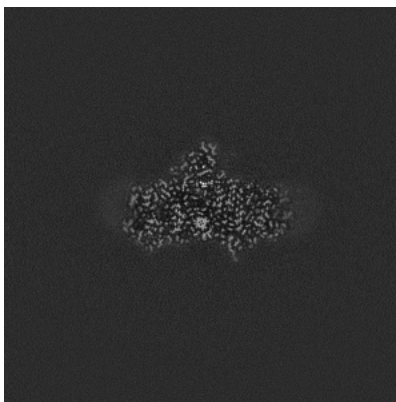


Z Index: 257

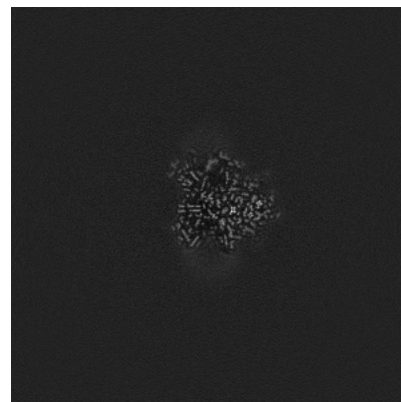
6.3.2 Raw map



X Index: 235



Y Index: 251

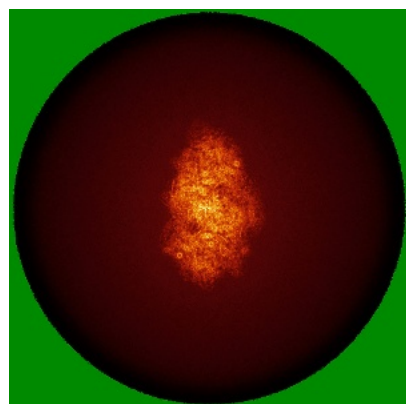


Z Index: 257

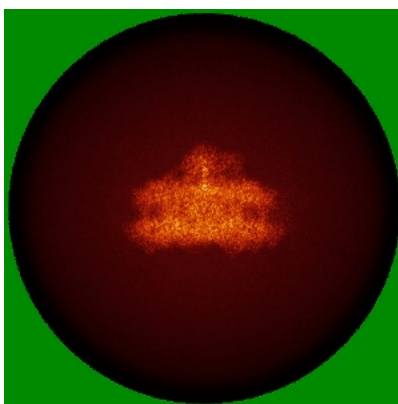
The images above show the largest variance slices of the map in three orthogonal directions.

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

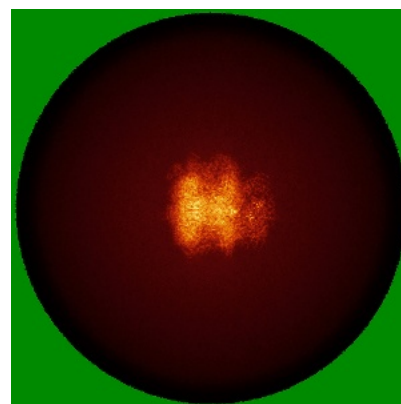
6.4.1 Primary map



X

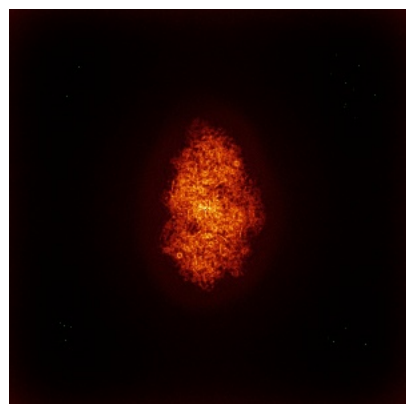


Y

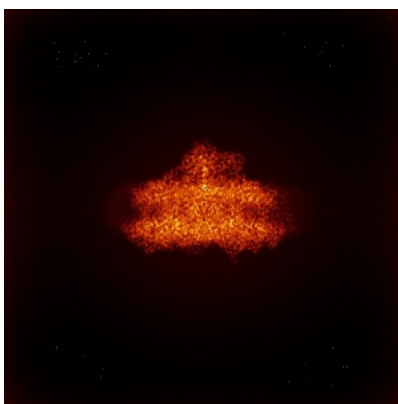


Z

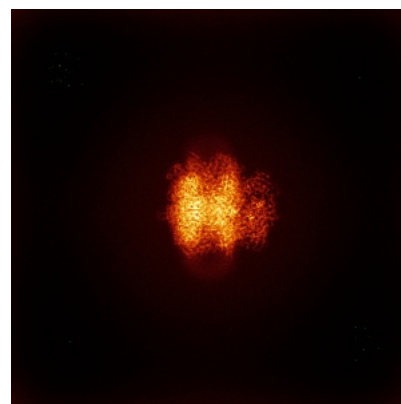
6.4.2 Raw map



X



Y

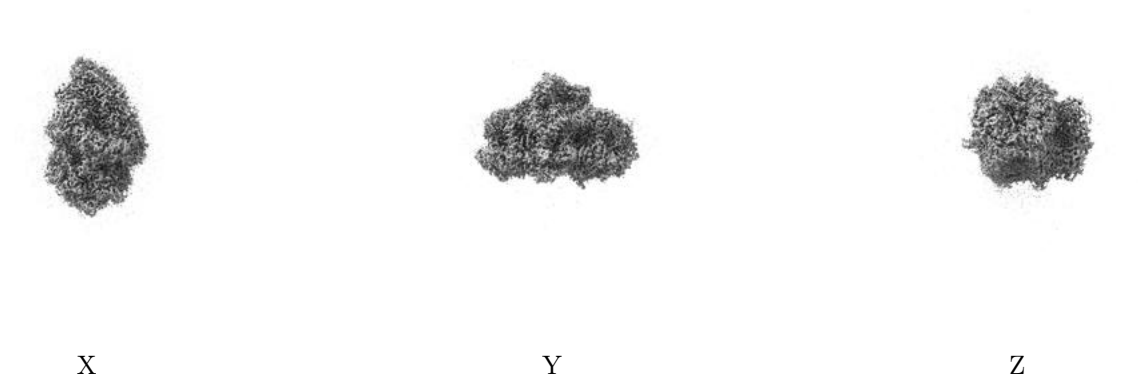


Z

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

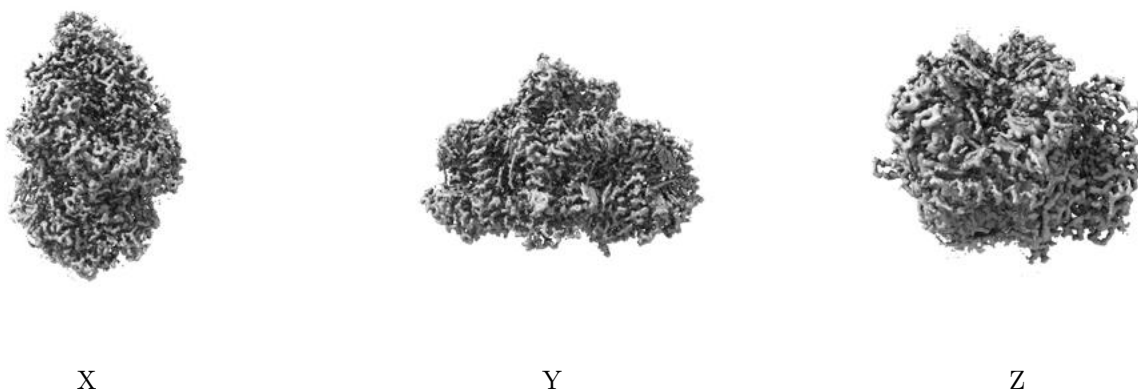
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

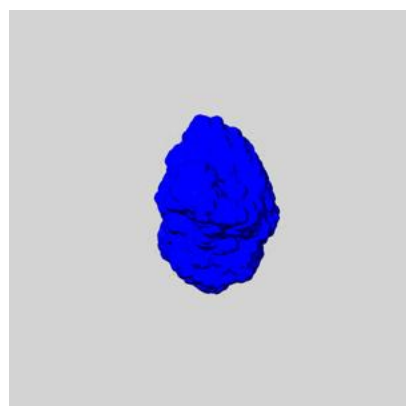
6.6 Mask visualisation [i](#)

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

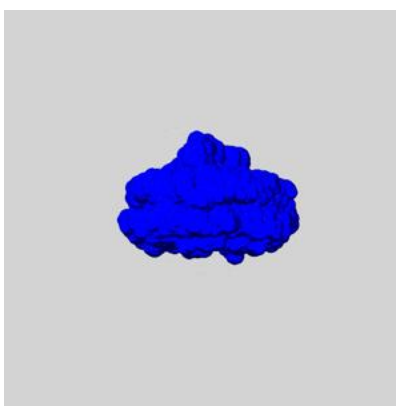
A mask typically either:

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

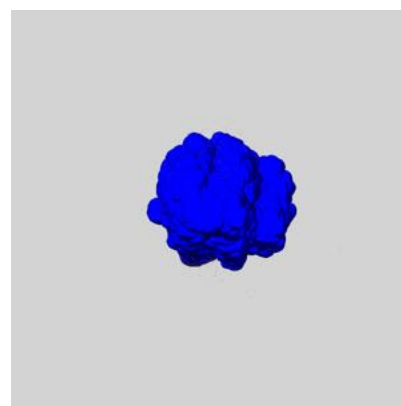
6.6.1 emd_53120_msk_1.map [i](#)



X

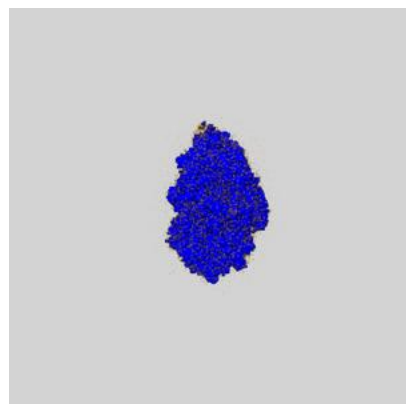


Y

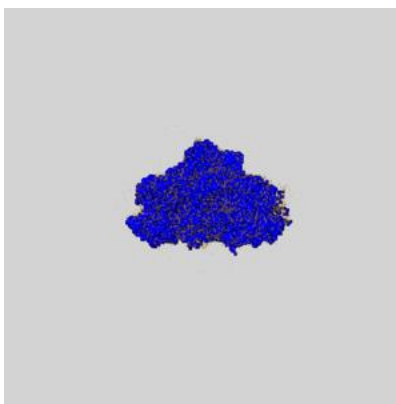


Z

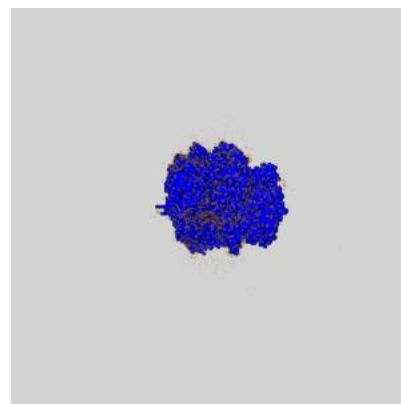
6.6.2 emd_53120_msk_2.map [i](#)



X



Y

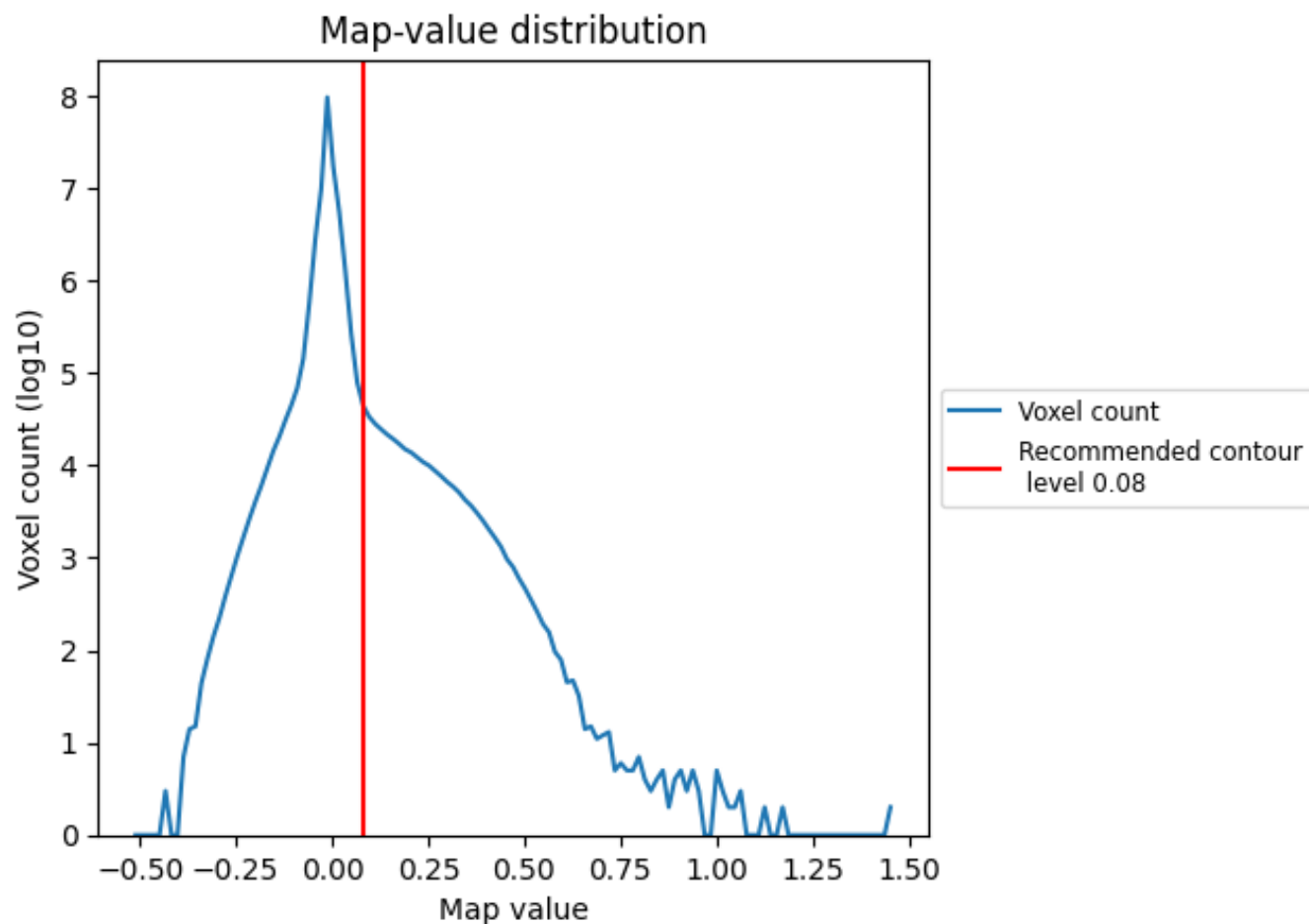


Z

7 Map analysis [i](#)

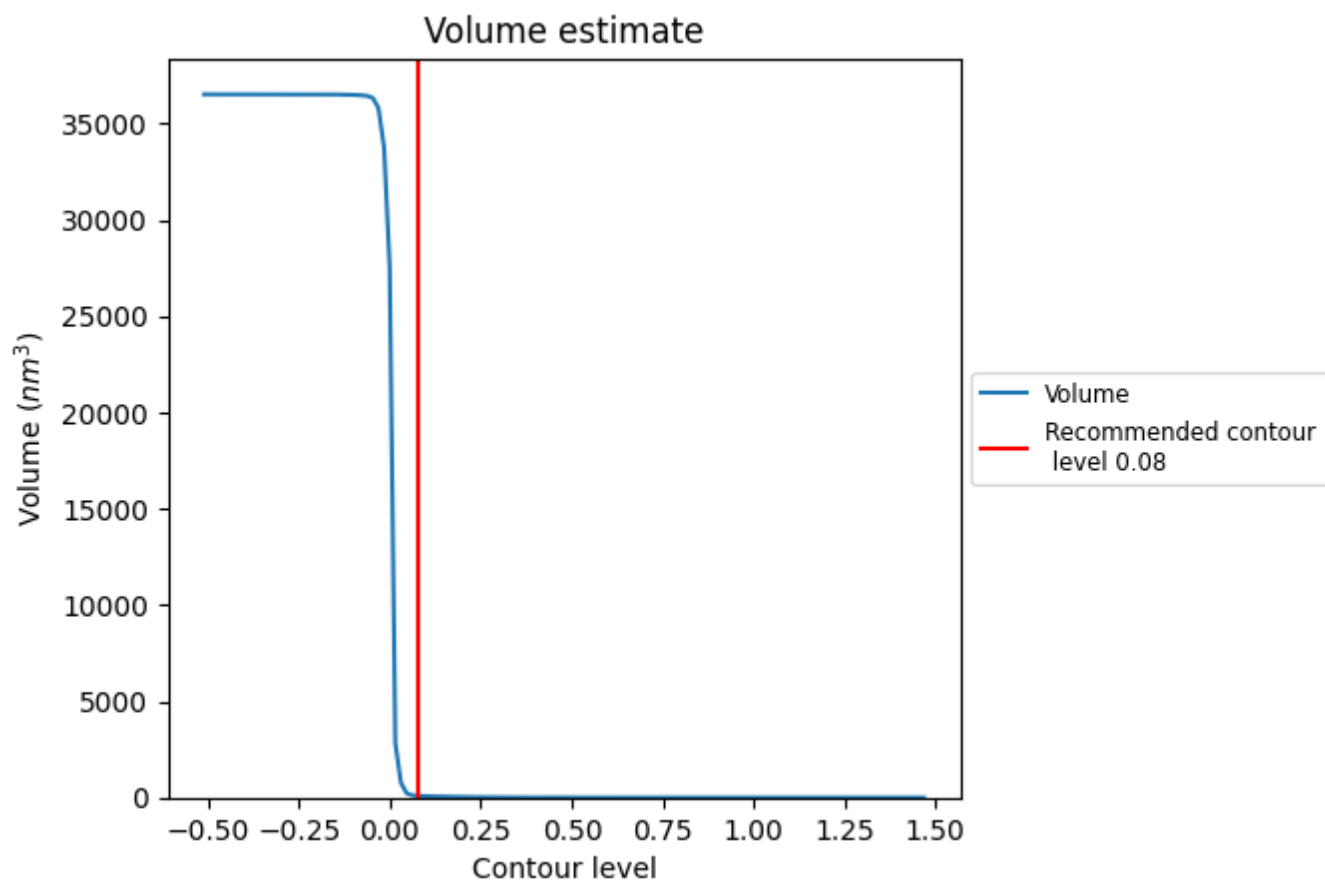
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

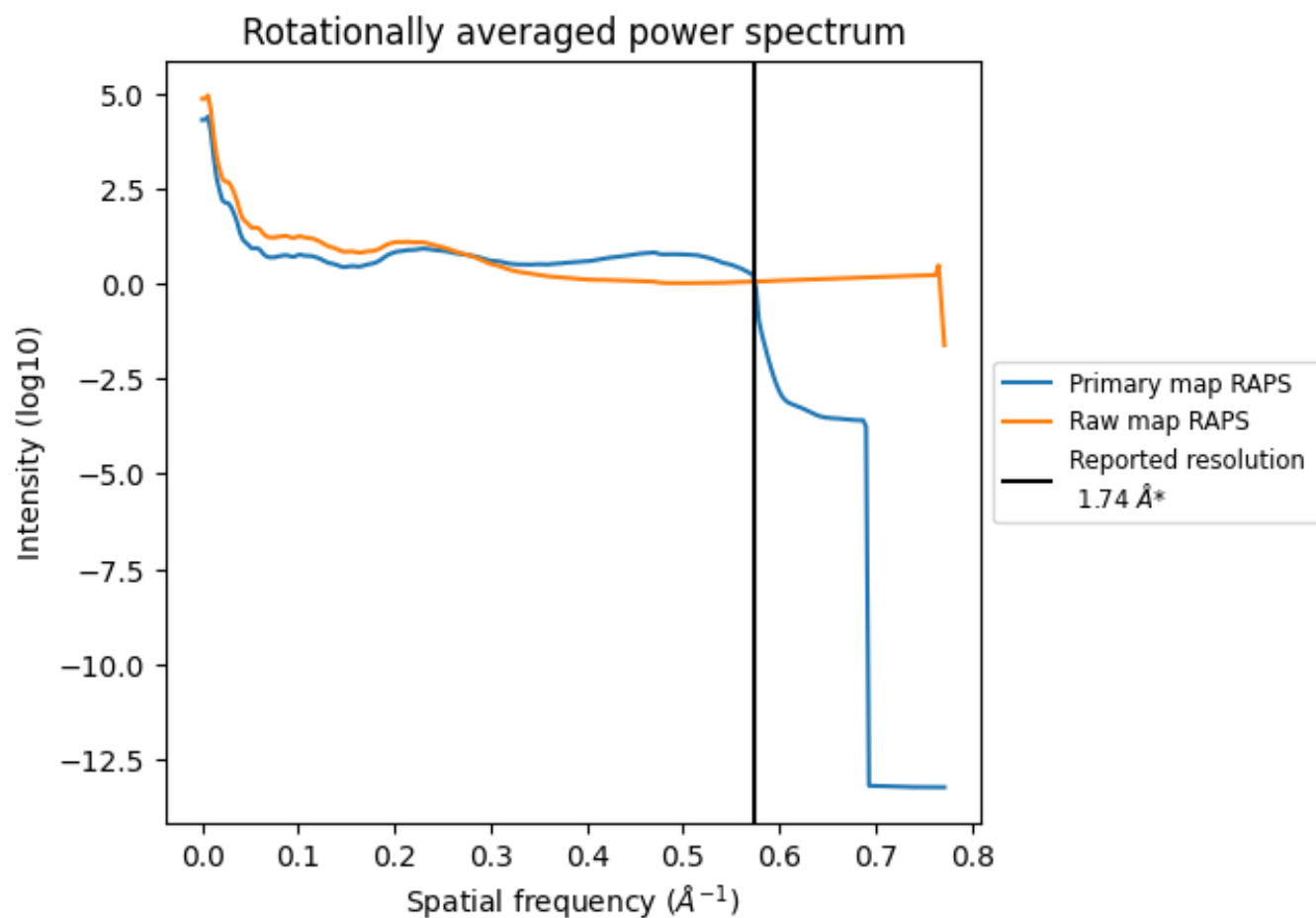
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm^3 ; this corresponds to an approximate mass of 77 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

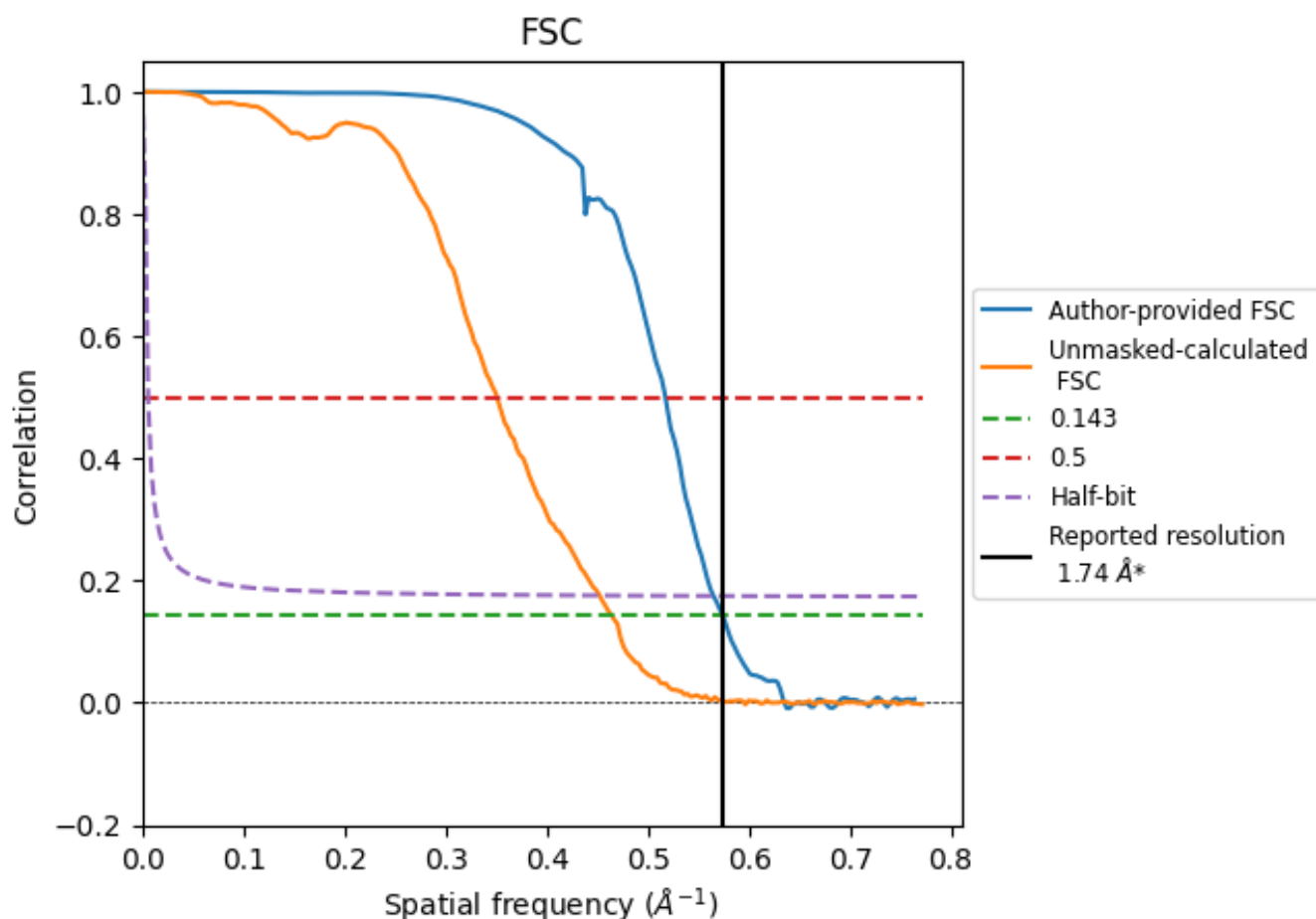


*Reported resolution corresponds to spatial frequency of 0.575 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.575 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

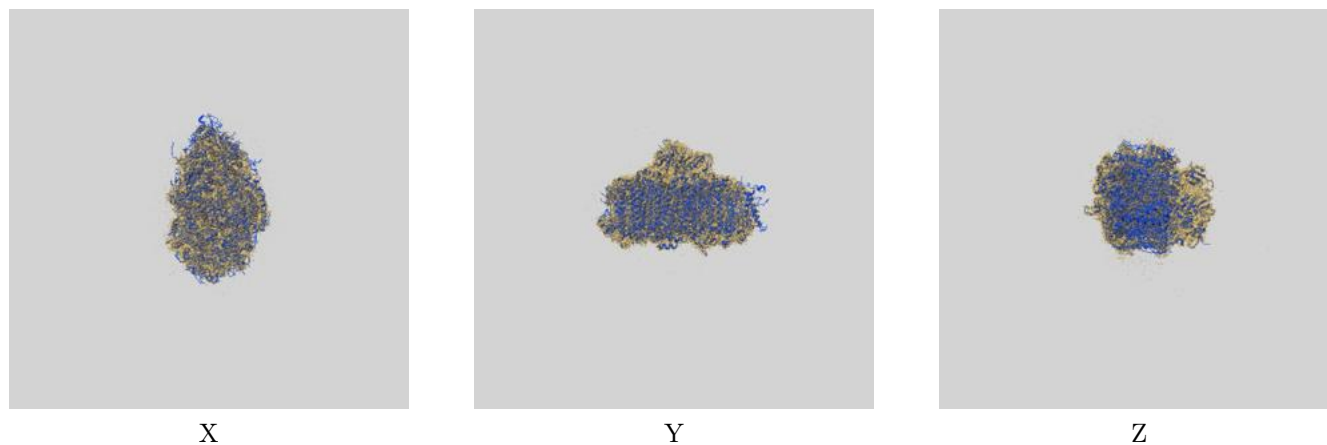
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.74	-	-
Author-provided FSC curve	1.74	1.93	1.77
Unmasked-calculated*	2.15	2.85	2.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.15 differs from the reported value 1.74 by more than 10 %

9 Map-model fit [i](#)

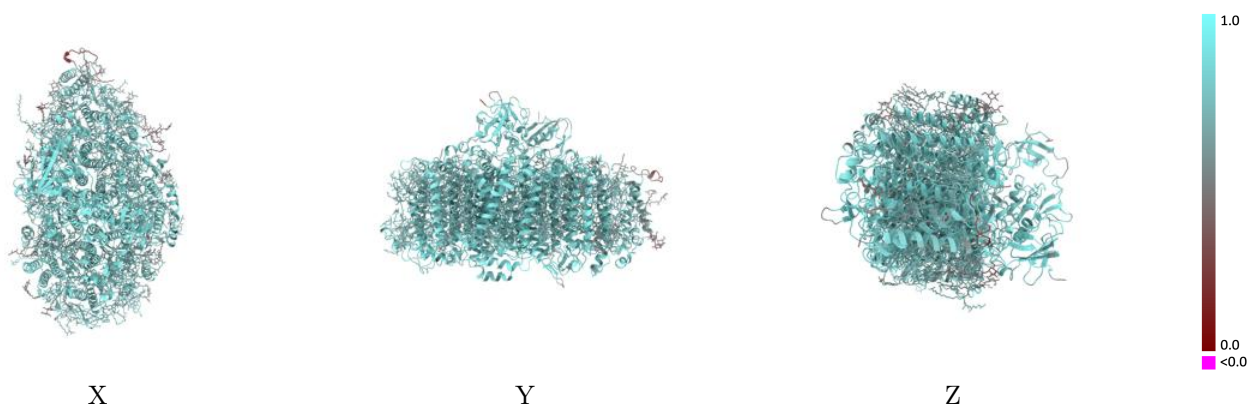
This section contains information regarding the fit between EMDB map EMD-53120 and PDB model 9QFP. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



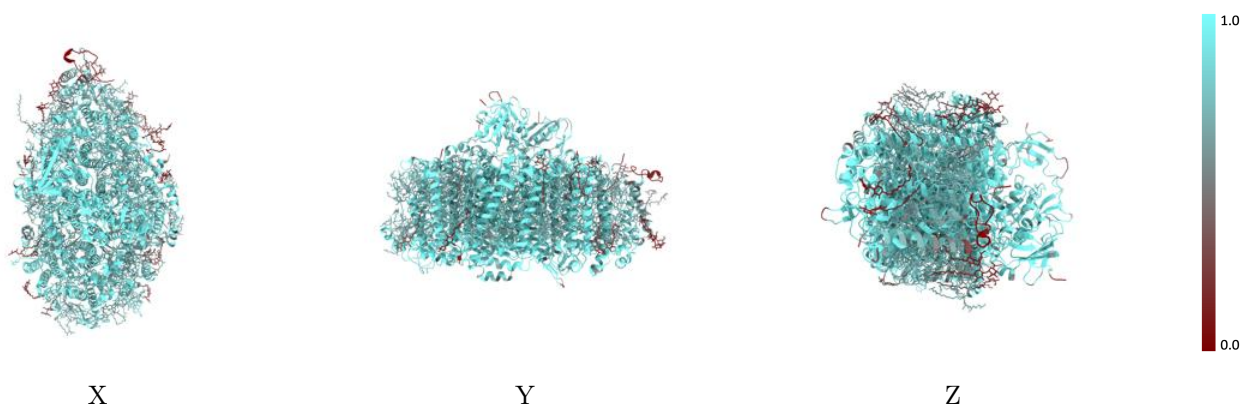
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



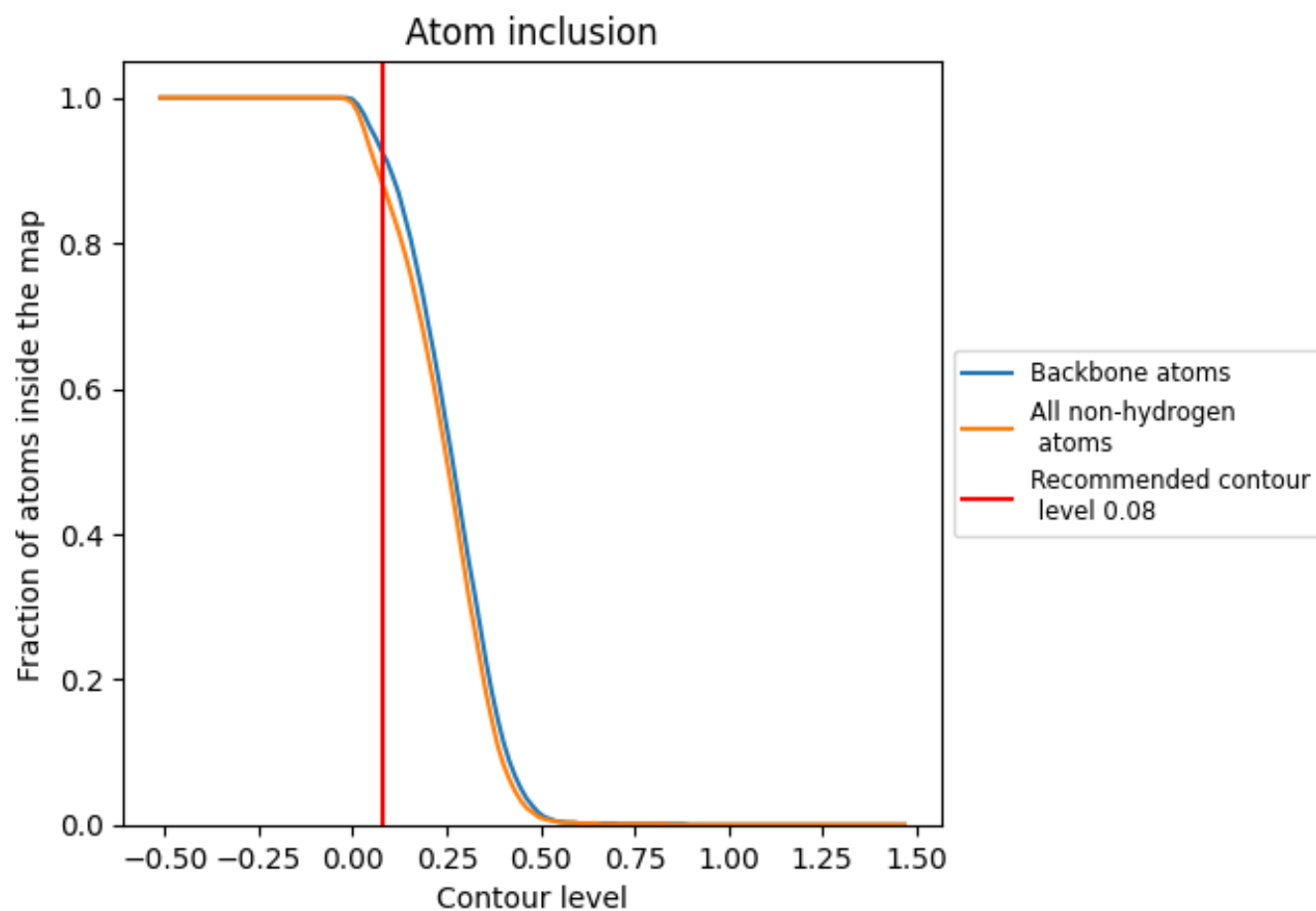
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.08).

9.4 Atom inclusion ⓘ



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8810	0.7900
A	0.8940	0.7960
B	0.9120	0.8060
C	0.9880	0.8460
D	0.9120	0.7930
E	0.8670	0.7770
F	0.8650	0.7820
I	0.6330	0.6640
J	0.8510	0.7650
K	0.5070	0.6220
M	0.9390	0.8070
X	0.6810	0.6970

1.0

0.0

<0.0