



wwPDB EM Validation Summary Report ⓘ

Aug 24, 2026 – 12:03 am BST

PDB ID : 9SE7 / pdb_00009se7
EMDB ID : EMD-54804
Title : Structure of Cytochrome C6 bound Photosystem I from Chlamydomonas reinhardtii at 2.07 Å resolution
Authors : Mahapatra, G.P.; Schuller, J.M.
Deposited on : 2025-08-15
Resolution : 2.06 Å (reported)
Based on initial models : 7ZQC, 1CYI

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:

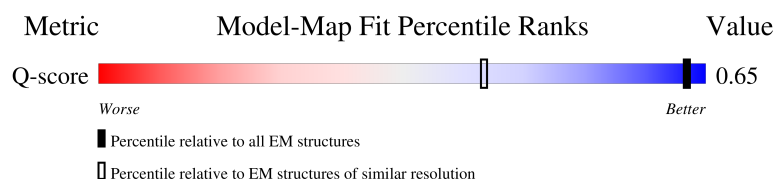
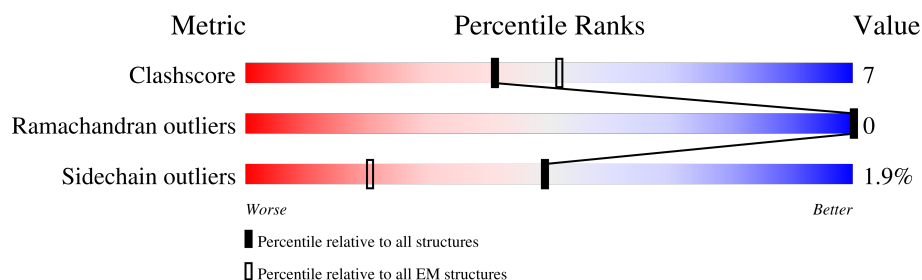
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

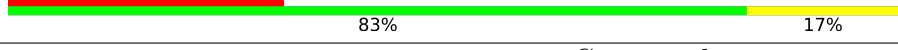
The reported resolution of this entry is 2.06 Å.

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	1895 (1.56 - 2.56)

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	742	
2	B	733	
3	C	80	
4	D	144	

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Mol	Chain	Length	Quality of chain
5	E	64	
6	I	37	
7	J	41	
8	T	89	
9	F	165	
10	L	138	

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
11	CLA	A	801	X	-	-	-
20	HEC	T	200	X	-	-	-

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 24300 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	742	Total	C	N	O	S	0	0
			5825	3808	994	1001	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5824	3824	977	1005	18		

- 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
			601	369	103	117	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	144	Total	C	N	O	S	0	0
			1133	725	200	201	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	64	Total	C	N	O	0	0
			506	322	89	95		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	41	Total	C	N	O	S	0	0
			329	224	46	58	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ACE	-	acetylation	UNP P59777

- Molecule 8 is a protein called Cytochrome c6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	89	Total	C	N	O	S	0	0
			674	424	114	131	5		

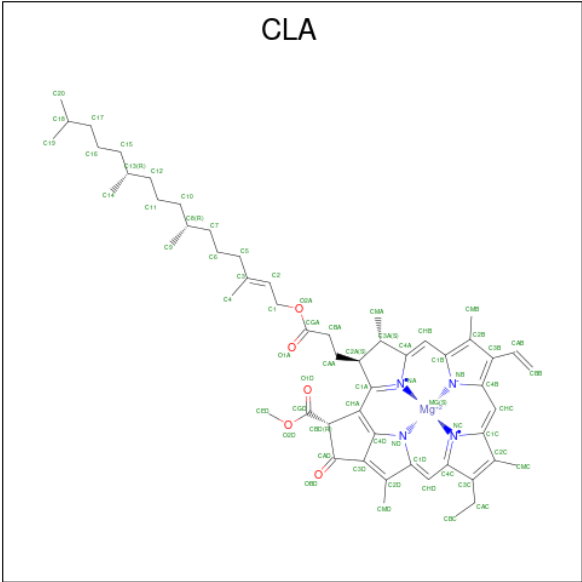
- Molecule 9 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	124	Total	C	N	O	S	0	0
			899	586	146	164	3		

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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

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

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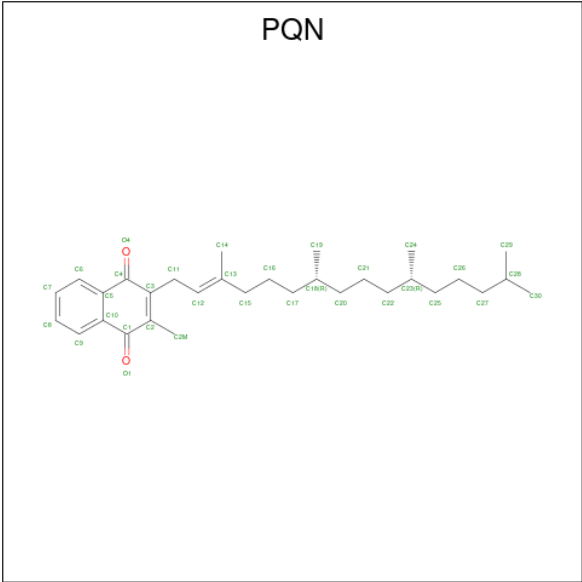
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
11	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
11	B	1	Total 42	C 34	Mg 1	N 4	O 3	0
11	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
11	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
11	B	1	Total 58	C 48	Mg 1	N 4	O 5	0

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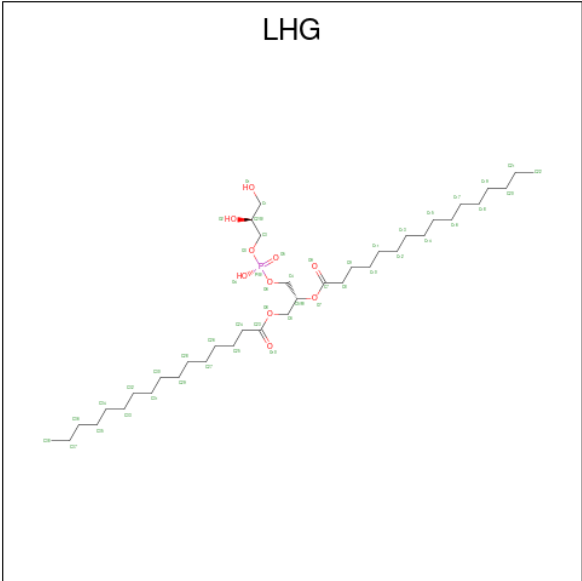
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	J	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 12 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 13 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



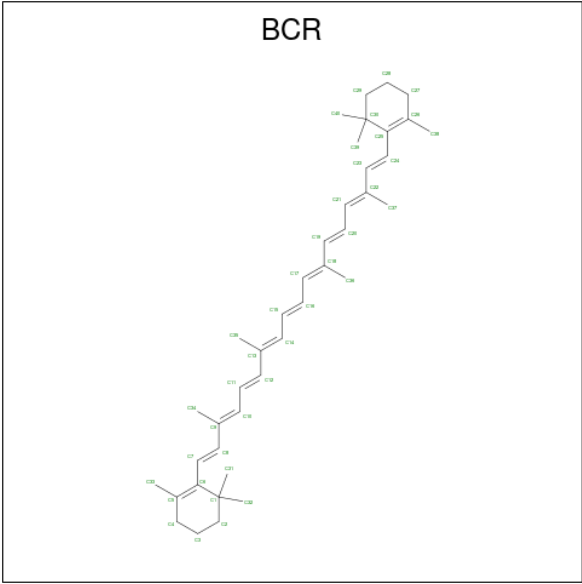
Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	O	P	0
			38	27	10	1	
13	B	1	Total	C	O	P	0
			45	34	10	1	

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



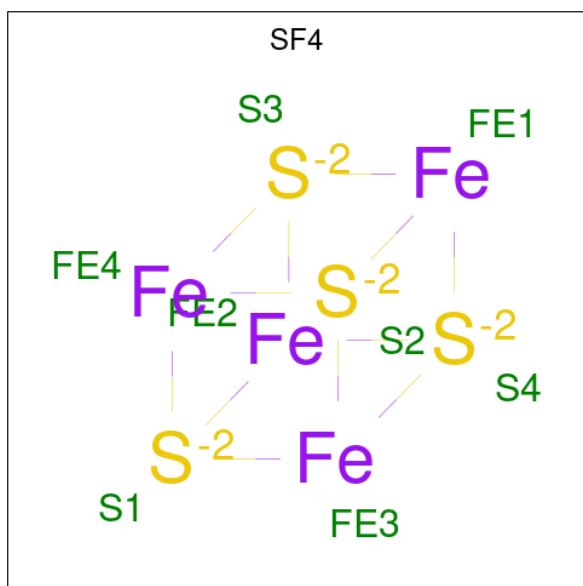
Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	A	1	Total	C	0
			40	40	
14	B	1	Total	C	0
			40	40	
14	B	1	Total	C	0
			40	40	
14	B	1	Total	C	0
			40	40	
14	B	1	Total	C	0
			40	40	

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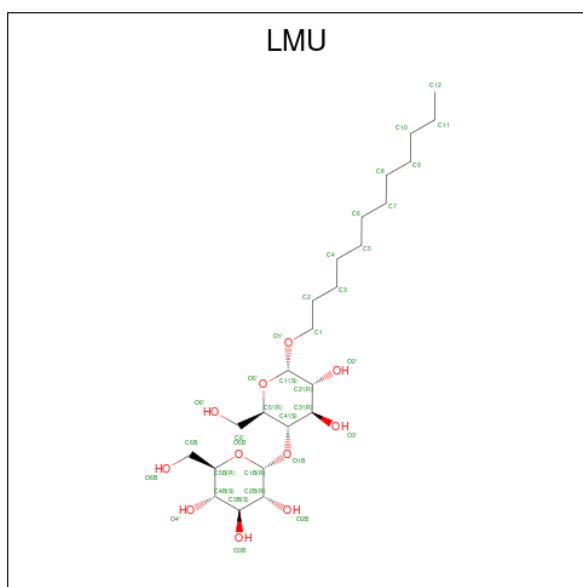
Mol	Chain	Residues	Atoms	AltConf
14	B	1	Total C 40 40	0
14	I	1	Total C 40 40	0
14	J	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	L	1	Total C 40 40	0
14	L	1	Total C 40 40	0

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



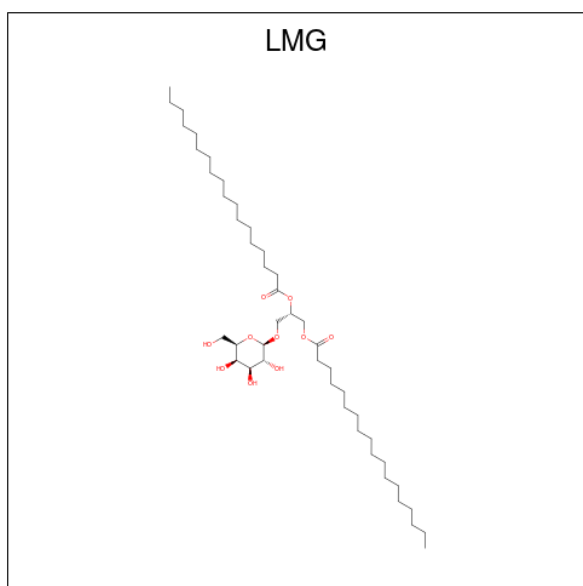
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total Fe S 8 4 4	0
15	C	1	Total Fe S 8 4 4	0
15	C	1	Total Fe S 8 4 4	0

- Molecule 16 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$).



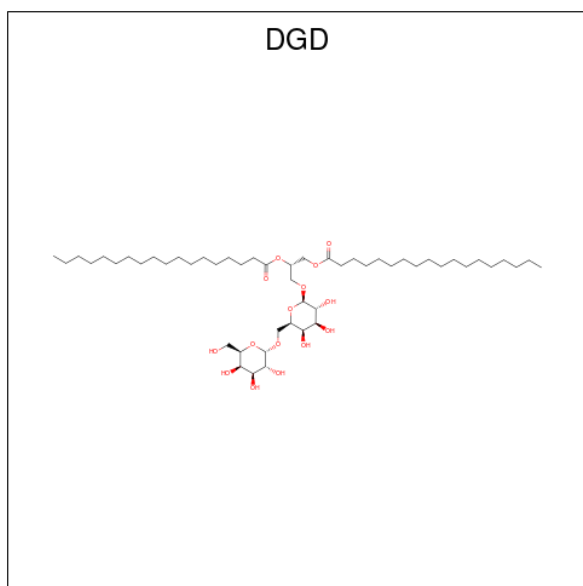
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			34	23	11	
16	A	1	Total	C	O	0
			35	24	11	
16	A	1	Total	C	O	0
			24	18	6	

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



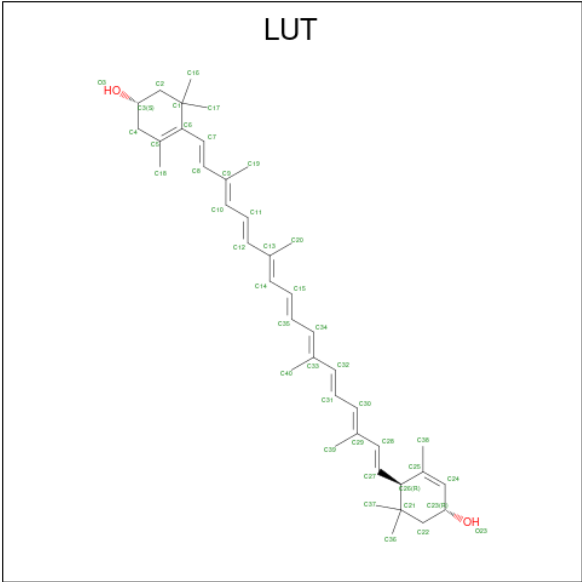
Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	C	O	0
			40	30	10	
17	B	1	Total	C	O	0
			43	33	10	
17	J	1	Total	C	O	0
			32	22	10	
17	J	1	Total	C	O	0
			42	32	10	
17	F	1	Total	C	O	0
			35	25	10	

- Molecule 18 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



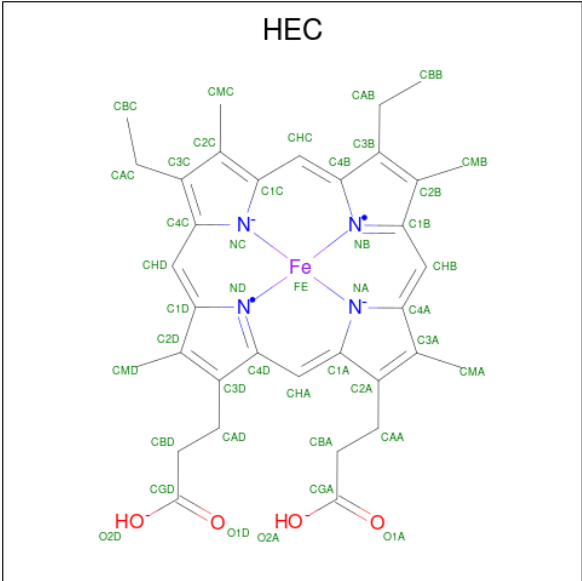
Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	C	O	0
			59	44	15	

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
19	J	1	Total	C	O	0
			42	40	2	
19	F	1	Total	C	O	0
			42	40	2	

- Molecule 20 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₆FeN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	T	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

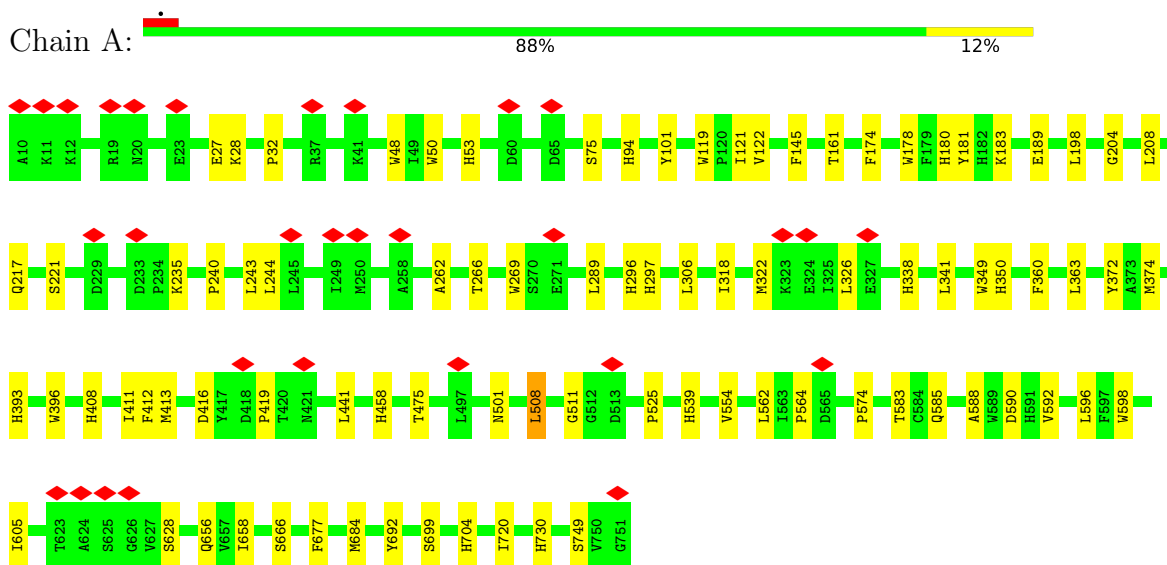
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	103	Total 103	O 103	0
21	B	107	Total 107	O 107	0
21	C	2	Total 2	O 2	0
21	D	3	Total 3	O 3	0
21	E	3	Total 3	O 3	0
21	J	6	Total 6	O 6	0
21	T	4	Total 4	O 4	0
21	F	24	Total 24	O 24	0

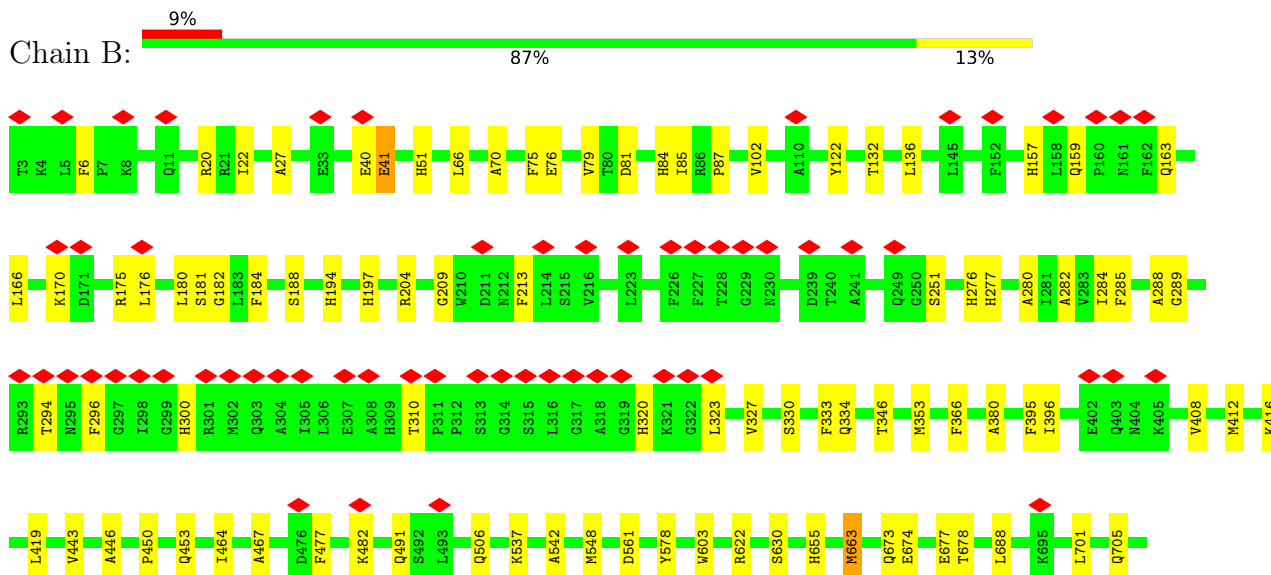
3 Residue-property plots

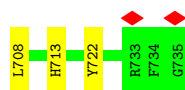
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

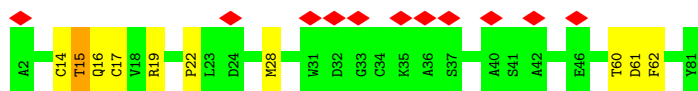
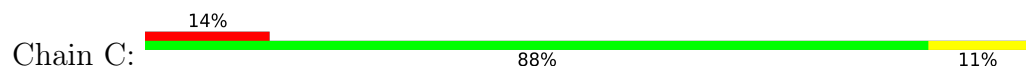


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

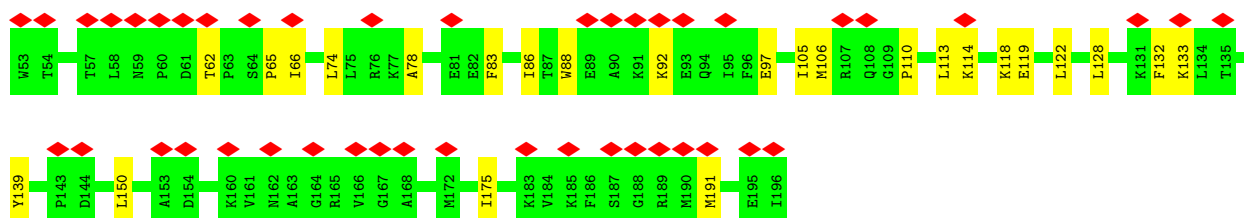
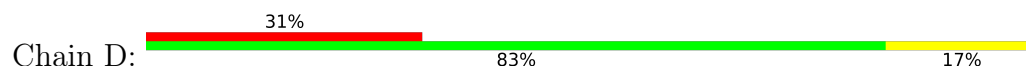




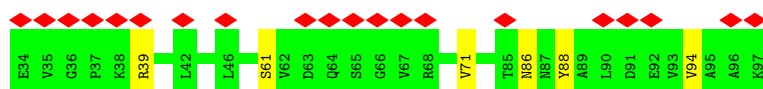
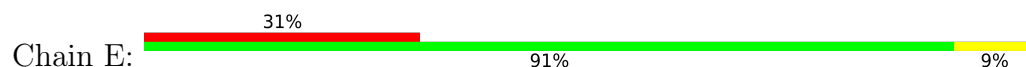
- Molecule 3: Photosystem I iron-sulfur center



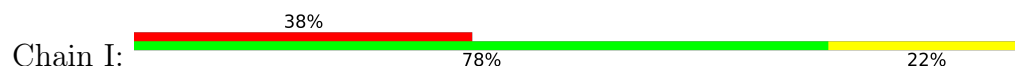
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic



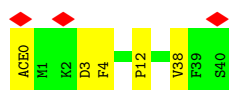
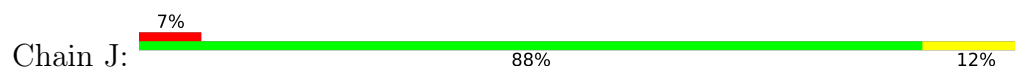
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



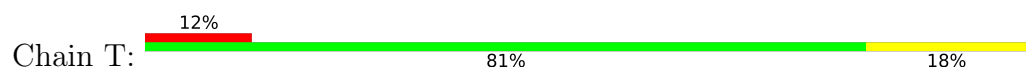
- Molecule 6: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit IX

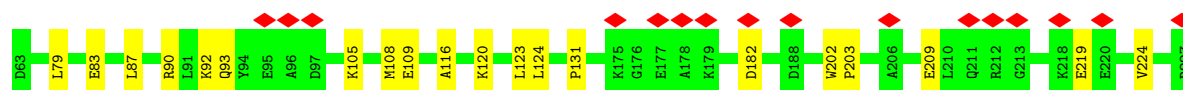
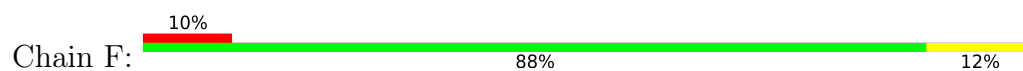


- Molecule 8: Cytochrome c6, chloroplastic

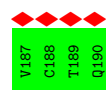
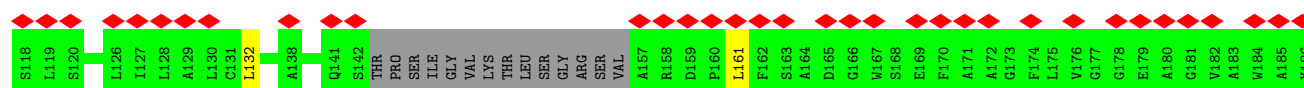
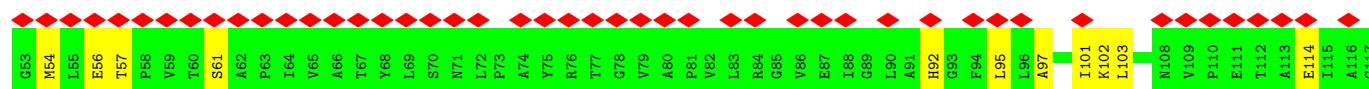
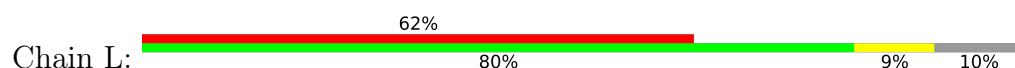




- Molecule 9: Photosystem I reaction center subunit III, chloroplastic



- Molecule 10: Photosystem I reaction center subunit XI, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	53904	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.266	Depositor
Minimum map value	-0.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.73, 0.73, 0.73	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.15	0/6021	0.31	0/8208
2	B	0.15	0/6036	0.32	1/8240 (0.0%)
3	C	0.13	0/611	0.35	0/826
4	D	0.11	0/1161	0.31	0/1567
5	E	0.11	0/516	0.28	0/700
6	I	0.15	0/293	0.32	0/406
7	J	0.18	0/338	0.36	0/464
8	T	0.11	0/686	0.30	0/925
9	F	0.14	0/1292	0.30	0/1747
10	L	0.11	0/920	0.27	0/1257
All	All	0.14	0/17874	0.31	1/24340 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	663	MET	CA-CB-CG	5.65	125.41	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	0	5675	68	0
2	B	5824	0	5577	76	0
3	C	601	0	581	7	0
4	D	1133	0	1150	13	0
5	E	506	0	504	2	0
6	I	281	0	292	8	0
7	J	329	0	328	4	0
8	T	674	0	650	8	0
9	F	1266	0	1300	9	0
10	L	899	0	905	10	0
11	A	2554	0	2596	84	0
11	B	2588	0	2666	98	0
11	F	110	0	105	2	0
11	J	55	0	49	1	0
11	L	110	0	105	5	0
12	A	33	0	46	2	0
12	B	33	0	46	3	0
13	A	87	0	123	2	0
13	B	45	0	63	2	0
14	A	200	0	280	13	0
14	B	200	0	280	10	0
14	F	40	0	56	1	0
14	I	40	0	56	3	0
14	J	40	0	56	2	0
14	L	80	0	112	5	0
15	A	8	0	0	0	0
15	C	16	0	0	1	0
16	A	93	0	122	3	0
17	A	40	0	50	1	0
17	B	43	0	56	2	0
17	F	35	0	40	0	0
17	J	74	0	91	1	0
18	B	59	0	79	5	0
19	F	42	0	56	1	0
19	J	42	0	56	2	0
20	T	43	0	31	2	0
21	A	103	0	0	0	0
21	B	107	0	0	0	0
21	C	2	0	0	0	0
21	D	3	0	0	0	0
21	E	3	0	0	0	0
21	F	24	0	0	0	0
21	J	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	T	4	0	0	0	0
All	All	24300	0	24182	333	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 333 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:198:LEU:HD12	1:A:322:MET:HE1	1.58	0.85
1:A:684:MET:HB2	11:A:802:CLA:C1C	2.09	0.82
2:B:663:MET:HB3	11:B:804:CLA:C1C	2.12	0.79
2:B:300:HIS:NE2	11:B:822:CLA:ND	2.31	0.78
11:A:840:CLA:H112	11:A:840:CLA:HAB	1.71	0.72

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	740/742 (100%)	726 (98%)	14 (2%)	0	100	100
2	B	731/733 (100%)	712 (97%)	19 (3%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
5	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
6	I	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
7	J	39/41 (95%)	39 (100%)	0	0	100	100
8	T	87/89 (98%)	86 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	F	163/165 (99%)	160 (98%)	3 (2%)	0	100	100
10	L	120/138 (87%)	117 (98%)	3 (2%)	0	100	100
All	All	2197/2233 (98%)	2147 (98%)	50 (2%)	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	601/601 (100%)	593 (99%)	8 (1%)	61	62
2	B	596/596 (100%)	590 (99%)	6 (1%)	68	71
3	C	69/69 (100%)	67 (97%)	2 (3%)	37	33
4	D	121/121 (100%)	117 (97%)	4 (3%)	33	28
5	E	55/55 (100%)	53 (96%)	2 (4%)	31	25
6	I	31/31 (100%)	31 (100%)	0	100	100
7	J	36/36 (100%)	36 (100%)	0	100	100
8	T	66/66 (100%)	61 (92%)	5 (8%)	12	6
9	F	127/127 (100%)	122 (96%)	5 (4%)	28	23
10	L	90/102 (88%)	88 (98%)	2 (2%)	45	43
All	All	1792/1804 (99%)	1758 (98%)	34 (2%)	49	49

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	F	182	ASP
9	F	209	GLU
10	L	54	MET
2	B	506	GLN
2	B	491	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	453	GLN
2	B	506	GLN
10	L	139	GLN
8	T	13	ASN
9	F	117	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](#)

126 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	CLA	A	817	1	69,73,73	1.25	7 (10%)	83,113,113	1.30	7 (8%)
11	CLA	B	835	2	64,68,73	1.29	6 (9%)	77,107,113	1.33	6 (7%)
11	CLA	B	837	2	64,68,73	1.30	8 (12%)	77,107,113	1.31	8 (10%)
11	CLA	B	813	2	45,49,73	1.52	6 (13%)	54,84,113	1.51	5 (9%)
11	CLA	B	824	2	69,73,73	1.25	7 (10%)	83,113,113	1.26	5 (6%)
11	CLA	B	806	2	69,73,73	1.24	8 (11%)	83,113,113	1.28	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	803	1	69,73,73	1.24	8 (11%)	83,113,113	1.34	9 (10%)
14	BCR	B	846	-	41,41,41	0.30	0	56,56,56	0.68	0
11	CLA	B	829	2	69,73,73	1.24	9 (13%)	83,113,113	1.23	7 (8%)
11	CLA	A	808	1	69,73,73	1.23	8 (11%)	83,113,113	1.33	6 (7%)
11	CLA	B	834	2	62,66,73	1.30	8 (12%)	74,104,113	1.39	10 (13%)
11	CLA	B	823	2	49,53,73	1.50	7 (14%)	59,89,113	1.42	4 (6%)
11	CLA	B	815	2	64,68,73	1.30	8 (12%)	77,107,113	1.28	5 (6%)
11	CLA	B	828	2	69,73,73	1.25	7 (10%)	83,113,113	1.27	7 (8%)
11	CLA	A	805	1	69,73,73	1.24	7 (10%)	83,113,113	1.27	6 (7%)
11	CLA	B	836	21	49,53,73	1.48	6 (12%)	59,89,113	1.44	5 (8%)
14	BCR	A	850	-	41,41,41	0.30	0	56,56,56	0.66	1 (1%)
11	CLA	B	818	2	69,73,73	1.26	9 (13%)	83,113,113	1.26	6 (7%)
11	CLA	J	103	7	59,63,73	1.34	8 (13%)	71,101,113	1.40	7 (9%)
16	LMU	A	853	-	35,35,36	0.47	0	46,46,47	0.77	1 (2%)
11	CLA	A	822	1	49,53,73	1.49	8 (16%)	59,89,113	1.44	6 (10%)
11	CLA	A	821	21	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
11	CLA	L	203	-	49,53,73	1.50	7 (14%)	59,89,113	1.39	6 (10%)
17	LMG	A	855	-	40,40,55	0.52	0	48,48,63	0.65	0
11	CLA	B	801	21	69,73,73	1.25	6 (8%)	83,113,113	1.23	5 (6%)
11	CLA	B	820	-	64,68,73	1.30	8 (12%)	77,107,113	1.34	8 (10%)
11	CLA	B	811	2	69,73,73	1.25	8 (11%)	83,113,113	1.31	5 (6%)
11	CLA	A	804	1,11	59,63,73	1.35	7 (11%)	71,101,113	1.35	8 (11%)
11	CLA	A	813	1	69,73,73	1.25	9 (13%)	83,113,113	1.30	5 (6%)
11	CLA	A	830	1	69,73,73	1.24	9 (13%)	83,113,113	1.28	6 (7%)
11	CLA	A	812	1	59,63,73	1.34	7 (11%)	71,101,113	1.38	6 (8%)
11	CLA	B	809	2	69,73,73	1.24	8 (11%)	83,113,113	1.31	8 (9%)
11	CLA	B	802	21	69,73,73	1.25	7 (10%)	83,113,113	1.22	4 (4%)
11	CLA	B	831	2	49,53,73	1.48	8 (16%)	59,89,113	1.44	6 (10%)
14	BCR	A	851	-	41,41,41	0.33	0	56,56,56	0.53	0
15	SF4	C	101	3	0,12,12	-	-	-	-	-
11	CLA	A	825	21	69,73,73	1.26	8 (11%)	83,113,113	1.29	5 (6%)
11	CLA	A	840	1	69,73,73	1.23	8 (11%)	83,113,113	1.27	5 (6%)
13	LHG	A	845	-	48,48,48	0.52	0	51,54,54	0.55	0
14	BCR	L	204	-	41,41,41	0.34	0	56,56,56	0.57	0
11	CLA	A	809	1	69,73,73	1.23	8 (11%)	83,113,113	1.35	10 (12%)
11	CLA	A	826	21	69,73,73	1.24	8 (11%)	83,113,113	1.35	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	BCR	F	801	-	41,41,41	0.34	0	56,56,56	1.08	3 (5%)
11	CLA	A	816	21	59,63,73	1.36	7 (11%)	71,101,113	1.41	5 (7%)
13	LHG	A	846	11	37,37,48	0.58	0	40,43,54	0.55	0
17	LMG	F	802	-	35,35,55	0.57	0	43,43,63	0.76	0
13	LHG	B	850	11	44,44,48	0.53	0	47,50,54	0.56	0
11	CLA	B	825	21	69,73,73	1.26	7 (10%)	83,113,113	1.26	5 (6%)
11	CLA	A	810	1	66,70,73	1.27	7 (10%)	77,108,113	1.31	8 (10%)
11	CLA	B	807	2	69,73,73	1.26	8 (11%)	83,113,113	1.28	6 (7%)
11	CLA	B	819	2	69,73,73	1.25	10 (14%)	83,113,113	1.30	8 (9%)
11	CLA	A	802	-	69,73,73	1.22	6 (8%)	83,113,113	1.23	9 (10%)
11	CLA	A	835	1	69,73,73	1.25	8 (11%)	83,113,113	1.28	6 (7%)
11	CLA	A	842	21	69,73,73	1.25	9 (13%)	83,113,113	1.28	5 (6%)
11	CLA	A	827	1	69,73,73	1.25	9 (13%)	83,113,113	1.28	5 (6%)
11	CLA	B	817	2	60,64,73	1.34	8 (13%)	72,102,113	1.35	6 (8%)
11	CLA	L	202	10	69,73,73	1.25	6 (8%)	83,113,113	1.29	7 (8%)
11	CLA	A	829	1	69,73,73	1.25	8 (11%)	83,113,113	1.26	7 (8%)
11	CLA	B	810	2	69,73,73	1.26	8 (11%)	83,113,113	1.29	6 (7%)
12	PQN	A	843	-	34,34,34	0.35	0	42,45,45	0.54	0
11	CLA	A	834	1	69,73,73	1.25	8 (11%)	83,113,113	1.32	8 (9%)
11	CLA	B	805	2	49,53,73	1.48	8 (16%)	59,89,113	1.43	6 (10%)
17	LMG	B	851	-	43,43,55	0.53	0	51,51,63	0.68	0
11	CLA	A	844	13	49,53,73	1.49	8 (16%)	59,89,113	1.45	4 (6%)
14	BCR	B	845	-	41,41,41	0.35	0	56,56,56	0.54	0
11	CLA	A	841	1	69,73,73	1.25	9 (13%)	83,113,113	1.25	7 (8%)
11	CLA	A	801	1	69,73,73	0.85	5 (7%)	83,113,113	1.10	7 (8%)
11	CLA	B	804	-	69,73,73	1.24	7 (10%)	83,113,113	1.27	9 (10%)
11	CLA	B	821	2	60,64,73	1.36	7 (11%)	72,102,113	1.34	6 (8%)
11	CLA	B	838	2	69,73,73	1.24	8 (11%)	83,113,113	1.27	7 (8%)
11	CLA	B	827	2	69,73,73	1.26	10 (14%)	83,113,113	1.27	6 (7%)
11	CLA	B	830	2	69,73,73	1.25	8 (11%)	83,113,113	1.23	7 (8%)
15	SF4	C	102	3	0,12,12	-	-	-	-	-
11	CLA	A	818	1	64,68,73	1.32	9 (14%)	77,107,113	1.30	7 (9%)
14	BCR	A	847	-	41,41,41	0.32	0	56,56,56	0.47	0
11	CLA	B	826	21	69,73,73	1.23	7 (10%)	83,113,113	1.32	7 (8%)
11	CLA	F	803	21	69,73,73	1.25	8 (11%)	83,113,113	1.30	7 (8%)
11	CLA	B	840	-	69,73,73	1.25	8 (11%)	83,113,113	1.29	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LMG	J	105	-	42,42,55	0.53	0	50,50,63	0.68	0
11	CLA	B	816	2	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
11	CLA	A	832	1	49,53,73	1.49	9 (18%)	59,89,113	1.49	8 (13%)
11	CLA	A	815	1	46,50,73	1.50	8 (17%)	55,85,113	1.52	6 (10%)
16	LMU	A	856	-	24,24,36	0.36	0	29,29,47	0.79	1 (3%)
11	CLA	B	812	2	69,73,73	1.25	6 (8%)	83,113,113	1.24	6 (7%)
11	CLA	A	819	1	69,73,73	1.25	9 (13%)	83,113,113	1.31	10 (12%)
17	LMG	J	102	-	32,32,55	0.59	0	40,40,63	0.67	0
11	CLA	A	839	1	69,73,73	1.26	9 (13%)	83,113,113	1.30	6 (7%)
14	BCR	I	201	-	41,41,41	0.32	0	56,56,56	0.83	1 (1%)
14	BCR	B	844	-	41,41,41	0.36	0	56,56,56	0.68	0
15	SF4	A	852	2,1	0,12,12	-	-	-	-	-
11	CLA	A	837	1	55,59,73	1.40	8 (14%)	66,96,113	1.43	8 (12%)
11	CLA	A	824	1	59,63,73	1.36	7 (11%)	71,101,113	1.36	8 (11%)
12	PQN	B	843	-	34,34,34	0.35	0	42,45,45	0.59	1 (2%)
11	CLA	B	839	2	54,58,73	1.41	8 (14%)	65,95,113	1.41	6 (9%)
11	CLA	A	831	1	59,63,73	1.35	8 (13%)	71,101,113	1.34	6 (8%)
11	CLA	A	820	1	46,50,73	1.50	7 (15%)	55,85,113	1.48	6 (10%)
11	CLA	A	838	1	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
14	BCR	J	104	-	41,41,41	0.31	0	56,56,56	0.72	1 (1%)
11	CLA	A	814	1	59,63,73	1.35	8 (13%)	71,101,113	1.33	6 (8%)
11	CLA	A	833	1	69,73,73	1.25	9 (13%)	83,113,113	1.29	6 (7%)
19	LUT	F	805	-	42,43,43	0.30	0	51,60,60	0.75	2 (3%)
20	HEC	T	200	8	50,50,50	1.68	5 (10%)	68,82,82	1.48	8 (11%)
11	CLA	A	836	1	49,53,73	1.49	9 (18%)	59,89,113	1.45	7 (11%)
16	LMU	A	854	-	36,36,36	0.44	0	47,47,47	1.18	4 (8%)
19	LUT	J	101	-	42,43,43	0.31	0	51,60,60	0.66	1 (1%)
11	CLA	B	822	2	46,50,73	1.51	8 (17%)	55,85,113	1.46	5 (9%)
11	CLA	A	828	1	69,73,73	1.23	6 (8%)	83,113,113	1.27	6 (7%)
14	BCR	B	847	-	41,41,41	0.31	0	56,56,56	0.87	0
14	BCR	L	201	-	41,41,41	0.33	0	56,56,56	0.54	0
11	CLA	B	808	2	59,63,73	1.34	9 (15%)	71,101,113	1.34	7 (9%)
11	CLA	A	811	1,11	69,73,73	1.23	7 (10%)	83,113,113	1.26	7 (8%)
11	CLA	F	804	21	49,53,73	1.49	8 (16%)	59,89,113	1.45	5 (8%)
14	BCR	A	848	-	41,41,41	0.34	0	56,56,56	0.44	0
11	CLA	A	807	1	54,58,73	1.40	7 (12%)	65,95,113	1.43	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	852	9	69,73,73	1.26	7 (10%)	83,113,113	1.21	4 (4%)
11	CLA	B	842	13	69,73,73	1.26	8 (11%)	83,113,113	1.31	8 (9%)
18	DGD	B	849	-	60,60,67	0.55	0	74,74,81	0.79	1 (1%)
11	CLA	B	832	2	59,63,73	1.35	8 (13%)	71,101,113	1.34	6 (8%)
14	BCR	B	848	-	41,41,41	0.31	0	56,56,56	0.72	0
11	CLA	B	833	2	69,73,73	1.25	8 (11%)	83,113,113	1.29	6 (7%)
11	CLA	A	806	1	69,73,73	1.26	7 (10%)	83,113,113	1.29	6 (7%)
11	CLA	A	823	1	49,53,73	1.48	7 (14%)	59,89,113	1.40	5 (8%)
11	CLA	B	841	2	69,73,73	1.25	8 (11%)	83,113,113	1.31	6 (7%)
14	BCR	A	849	-	41,41,41	0.31	0	56,56,56	0.60	0
11	CLA	B	814	2	69,73,73	1.27	8 (11%)	83,113,113	1.28	6 (7%)
11	CLA	B	803	2	69,73,73	1.22	7 (10%)	83,113,113	1.31	6 (7%)

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
11	CLA	A	817	1	-	9/39/115/115	-
11	CLA	B	835	2	-	8/33/109/115	-
11	CLA	B	837	2	-	10/33/109/115	-
11	CLA	B	813	2	-	0/10/86/115	-
11	CLA	B	824	2	-	15/39/115/115	-
11	CLA	B	806	2	-	11/39/115/115	-
11	CLA	A	803	1	-	2/39/115/115	-
14	BCR	B	846	-	-	3/29/63/63	0/2/2/2
11	CLA	B	829	2	-	10/39/115/115	-
11	CLA	A	808	1	-	11/39/115/115	-
11	CLA	B	834	2	-	9/31/107/115	-
11	CLA	B	823	2	-	3/15/91/115	-
11	CLA	B	815	2	-	8/33/109/115	-
11	CLA	B	828	2	-	12/39/115/115	-
11	CLA	A	805	1	-	17/39/115/115	-
11	CLA	B	836	21	-	5/15/91/115	-
14	BCR	A	850	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	818	2	-	13/39/115/115	-
11	CLA	J	103	7	-	11/27/103/115	-
16	LMU	A	853	-	-	1/20/60/61	0/2/2/2
11	CLA	A	822	1	-	10/15/91/115	-
11	CLA	A	821	21	-	6/39/115/115	-
11	CLA	L	203	-	-	6/15/91/115	-
17	LMG	A	855	-	-	11/35/55/70	0/1/1/1
11	CLA	B	801	21	-	7/39/115/115	-
11	CLA	B	820	-	-	12/33/109/115	-
11	CLA	B	811	2	-	10/39/115/115	-
11	CLA	A	804	1,11	-	6/27/103/115	-
11	CLA	A	813	1	-	11/39/115/115	-
11	CLA	A	830	1	-	9/39/115/115	-
11	CLA	A	812	1	-	3/27/103/115	-
11	CLA	B	809	2	-	12/39/115/115	-
11	CLA	B	802	21	-	15/39/115/115	-
11	CLA	B	831	2	-	1/15/91/115	-
14	BCR	A	851	-	-	8/29/63/63	0/2/2/2
15	SF4	C	101	3	-	-	0/6/5/5
11	CLA	A	825	21	-	10/39/115/115	-
11	CLA	A	840	1	-	11/39/115/115	-
13	LHG	A	845	-	-	10/53/53/53	-
14	BCR	L	204	-	-	6/29/63/63	0/2/2/2
11	CLA	A	809	1	-	12/39/115/115	-
11	CLA	A	826	21	-	10/39/115/115	-
14	BCR	F	801	-	-	4/29/63/63	0/2/2/2
11	CLA	A	816	21	-	7/27/103/115	-
13	LHG	A	846	11	-	12/42/42/53	-
17	LMG	F	802	-	-	12/30/50/70	0/1/1/1
13	LHG	B	850	11	-	16/49/49/53	-
11	CLA	B	825	21	-	6/39/115/115	-
11	CLA	A	810	1	-	9/33/109/115	-
11	CLA	B	807	2	-	8/39/115/115	-
11	CLA	B	819	2	-	9/39/115/115	-
11	CLA	A	802	-	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	835	1	-	8/39/115/115	-
11	CLA	A	842	21	-	17/39/115/115	-
11	CLA	A	827	1	-	7/39/115/115	-
11	CLA	B	817	2	-	5/29/105/115	-
11	CLA	L	202	10	-	18/39/115/115	-
11	CLA	A	829	1	-	4/39/115/115	-
11	CLA	B	810	2	-	10/39/115/115	-
12	PQN	A	843	-	-	2/23/43/43	0/2/2/2
11	CLA	A	834	1	-	9/39/115/115	-
11	CLA	B	805	2	-	4/15/91/115	-
17	LMG	B	851	-	-	10/38/58/70	0/1/1/1
11	CLA	A	844	13	-	8/15/91/115	-
14	BCR	B	845	-	-	5/29/63/63	0/2/2/2
11	CLA	A	841	1	-	7/39/115/115	-
11	CLA	A	801	1	1/1/15/20	2/39/115/115	-
11	CLA	B	804	-	-	8/39/115/115	-
11	CLA	B	821	2	-	14/29/105/115	-
11	CLA	B	838	2	-	9/39/115/115	-
11	CLA	B	827	2	-	6/39/115/115	-
11	CLA	B	830	2	-	8/39/115/115	-
15	SF4	C	102	3	-	-	0/6/5/5
11	CLA	A	818	1	-	13/33/109/115	-
14	BCR	A	847	-	-	5/29/63/63	0/2/2/2
11	CLA	B	826	21	-	12/39/115/115	-
11	CLA	F	803	21	-	7/39/115/115	-
11	CLA	B	840	-	-	12/39/115/115	-
17	LMG	J	105	-	-	7/37/57/70	0/1/1/1
11	CLA	B	816	2	-	17/39/115/115	-
11	CLA	A	832	1	-	3/15/91/115	-
11	CLA	A	815	1	-	4/12/88/115	-
16	LMU	A	856	-	-	5/15/35/61	0/1/1/2
11	CLA	B	812	2	-	13/39/115/115	-
11	CLA	A	819	1	-	4/39/115/115	-
17	LMG	J	102	-	-	11/27/47/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	839	1	-	11/39/115/115	-
14	BCR	I	201	-	-	5/29/63/63	0/2/2/2
14	BCR	B	844	-	-	8/29/63/63	0/2/2/2
15	SF4	A	852	2,1	-	-	0/6/5/5
11	CLA	A	837	1	-	5/23/99/115	-
11	CLA	A	824	1	-	11/27/103/115	-
12	PQN	B	843	-	-	0/23/43/43	0/2/2/2
11	CLA	B	839	2	-	4/21/97/115	-
11	CLA	A	831	1	-	8/27/103/115	-
11	CLA	A	820	1	-	3/12/88/115	-
11	CLA	A	838	1	-	9/39/115/115	-
14	BCR	J	104	-	-	7/29/63/63	0/2/2/2
11	CLA	A	814	1	-	8/27/103/115	-
11	CLA	A	833	1	-	5/39/115/115	-
19	LUT	F	805	-	-	7/29/67/67	0/2/2/2
20	HEC	T	200	8	1/1/3/7	4/14/54/54	-
11	CLA	A	836	1	-	5/15/91/115	-
16	LMU	A	854	-	-	11/21/61/61	0/2/2/2
19	LUT	J	101	-	-	6/29/67/67	0/2/2/2
11	CLA	B	822	2	-	5/12/88/115	-
11	CLA	A	828	1	-	11/39/115/115	-
14	BCR	B	847	-	-	2/29/63/63	0/2/2/2
14	BCR	L	201	-	-	4/29/63/63	0/2/2/2
11	CLA	B	808	2	-	6/27/103/115	-
11	CLA	A	811	1,11	-	9/39/115/115	-
11	CLA	F	804	21	-	2/15/91/115	-
14	BCR	A	848	-	-	0/29/63/63	0/2/2/2
11	CLA	A	807	1	-	3/21/97/115	-
11	CLA	B	852	9	-	25/39/115/115	-
11	CLA	B	842	13	-	15/39/115/115	-
18	DGD	B	849	-	-	16/48/88/95	0/2/2/2
11	CLA	B	832	2	-	4/27/103/115	-
14	BCR	B	848	-	-	3/29/63/63	0/2/2/2
11	CLA	B	833	2	-	9/39/115/115	-
11	CLA	A	806	1	-	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	823	1	-	5/15/91/115	-
11	CLA	B	841	2	-	12/39/115/115	-
14	BCR	A	849	-	-	3/29/63/63	0/2/2/2
11	CLA	B	814	2	-	13/39/115/115	-
11	CLA	B	803	2	-	7/39/115/115	-

The worst 5 of 709 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	T	200	HEC	C3D-C2D	7.95	1.53	1.36
11	A	820	CLA	C1D-ND	3.96	1.42	1.37
11	A	834	CLA	C1D-ND	3.94	1.42	1.37
11	A	832	CLA	C1D-ND	3.93	1.42	1.37
11	B	811	CLA	C1D-ND	3.92	1.42	1.37

The worst 5 of 619 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	803	CLA	C4A-NA-C1A	8.01	110.31	106.71
11	A	808	CLA	C4A-NA-C1A	7.52	110.08	106.71
11	B	841	CLA	C4A-NA-C1A	7.30	109.99	106.71
11	A	816	CLA	C4A-NA-C1A	7.16	109.92	106.71
11	A	828	CLA	C4A-NA-C1A	7.10	109.90	106.71

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	801	CLA	CBD
20	T	200	HEC	NA

5 of 994 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	805	CLA	C3A-C2A-CAA-CBA
11	A	815	CLA	CHA-CBD-CGD-O2D
11	A	818	CLA	C1A-C2A-CAA-CBA
11	A	818	CLA	C3A-C2A-CAA-CBA
11	A	822	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

107 monomers are involved in 222 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	817	CLA	4	0
11	B	835	CLA	1	0
11	B	837	CLA	3	0
11	B	824	CLA	3	0
11	B	806	CLA	2	0
11	A	803	CLA	2	0
14	B	846	BCR	1	0
11	B	829	CLA	2	0
11	A	808	CLA	3	0
11	B	834	CLA	4	0
11	B	815	CLA	2	0
11	B	828	CLA	2	0
11	A	805	CLA	6	0
11	B	836	CLA	2	0
14	A	850	BCR	3	0
11	B	818	CLA	8	0
11	J	103	CLA	1	0
11	A	821	CLA	2	0
17	A	855	LMG	1	0
11	B	801	CLA	1	0
11	B	820	CLA	4	0
11	B	811	CLA	4	0
11	A	813	CLA	1	0
11	A	830	CLA	3	0
11	A	812	CLA	1	0
11	B	809	CLA	4	0
11	B	802	CLA	3	0
11	B	831	CLA	3	0
14	A	851	BCR	4	0
11	A	825	CLA	2	0
11	A	840	CLA	6	0
14	L	204	BCR	4	0
11	A	809	CLA	6	0
11	A	826	CLA	3	0
14	F	801	BCR	1	0
11	A	816	CLA	1	0
13	A	846	LHG	2	0
13	B	850	LHG	2	0
11	A	810	CLA	2	0
11	B	807	CLA	3	0
11	B	819	CLA	2	0
11	A	802	CLA	3	0

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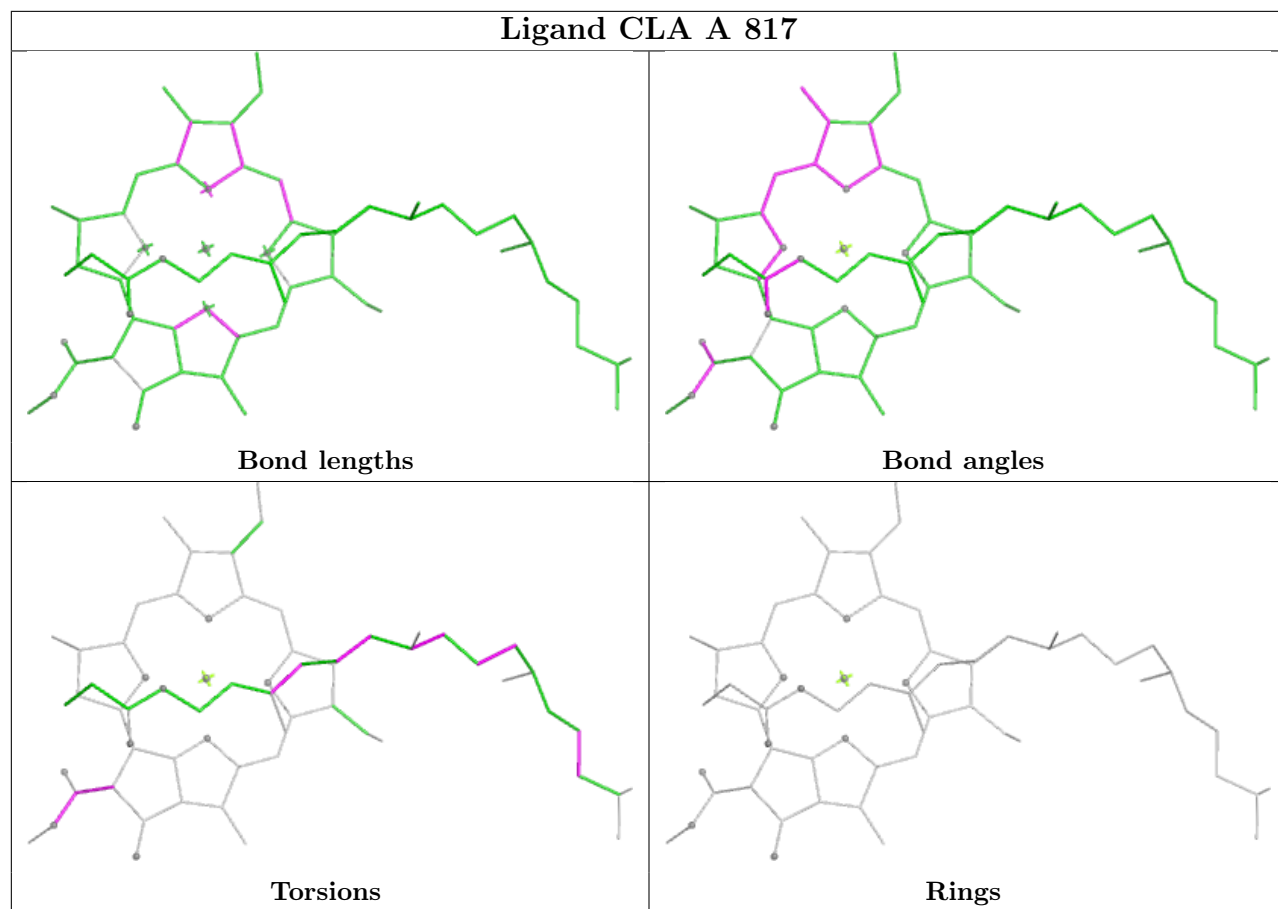
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	835	CLA	1	0
11	A	842	CLA	3	0
11	A	827	CLA	2	0
11	B	817	CLA	3	0
11	L	202	CLA	5	0
11	A	829	CLA	2	0
11	B	810	CLA	1	0
12	A	843	PQN	2	0
11	A	834	CLA	3	0
11	B	805	CLA	1	0
17	B	851	LMG	2	0
14	B	845	BCR	3	0
11	A	841	CLA	1	0
11	B	804	CLA	5	0
11	B	821	CLA	1	0
11	B	838	CLA	1	0
11	B	827	CLA	1	0
11	B	830	CLA	1	0
15	C	102	SF4	1	0
11	A	818	CLA	2	0
14	A	847	BCR	2	0
11	B	826	CLA	4	0
11	F	803	CLA	2	0
11	B	840	CLA	6	0
11	B	816	CLA	2	0
11	A	832	CLA	1	0
16	A	856	LMU	2	0
11	B	812	CLA	4	0
11	A	819	CLA	4	0
17	J	102	LMG	1	0
11	A	839	CLA	6	0
14	I	201	BCR	3	0
14	B	844	BCR	4	0
11	A	837	CLA	2	0
11	A	824	CLA	2	0
12	B	843	PQN	3	0
11	B	839	CLA	2	0
11	A	831	CLA	3	0
11	A	820	CLA	3	0
11	A	838	CLA	2	0
14	J	104	BCR	2	0
11	A	833	CLA	3	0

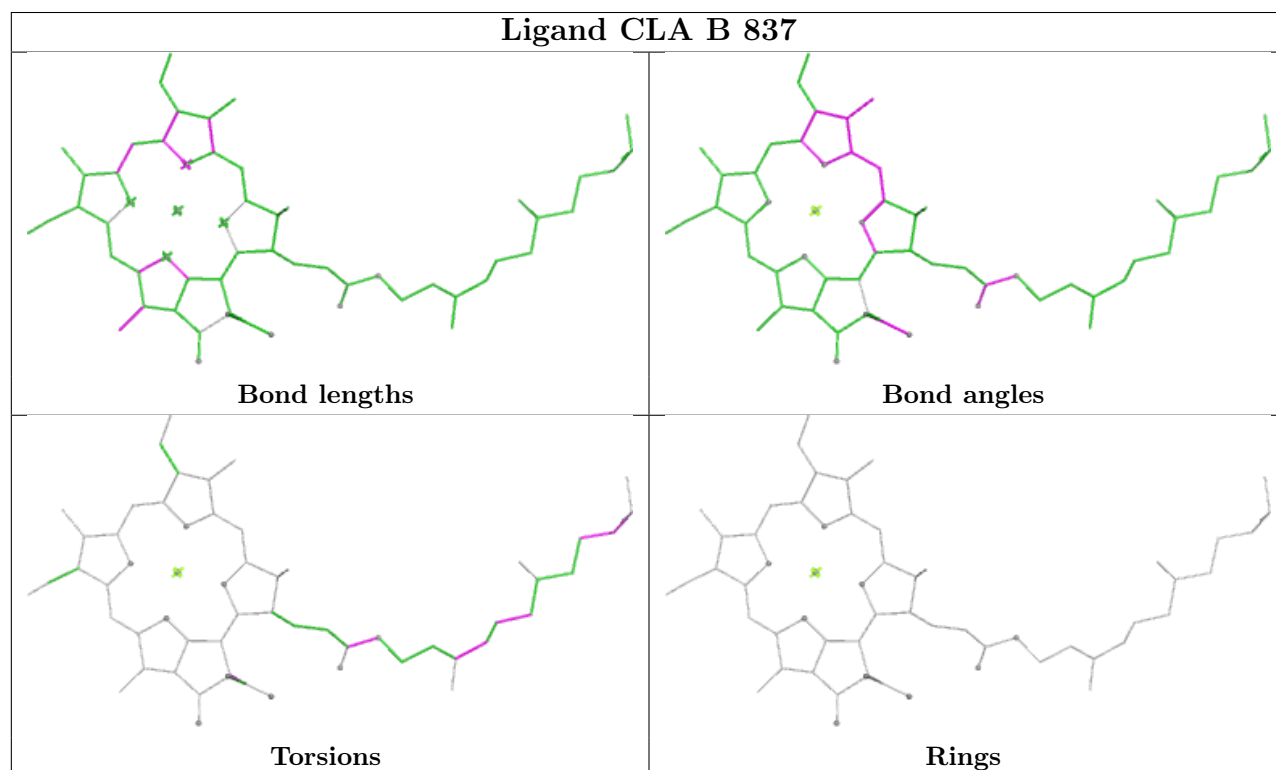
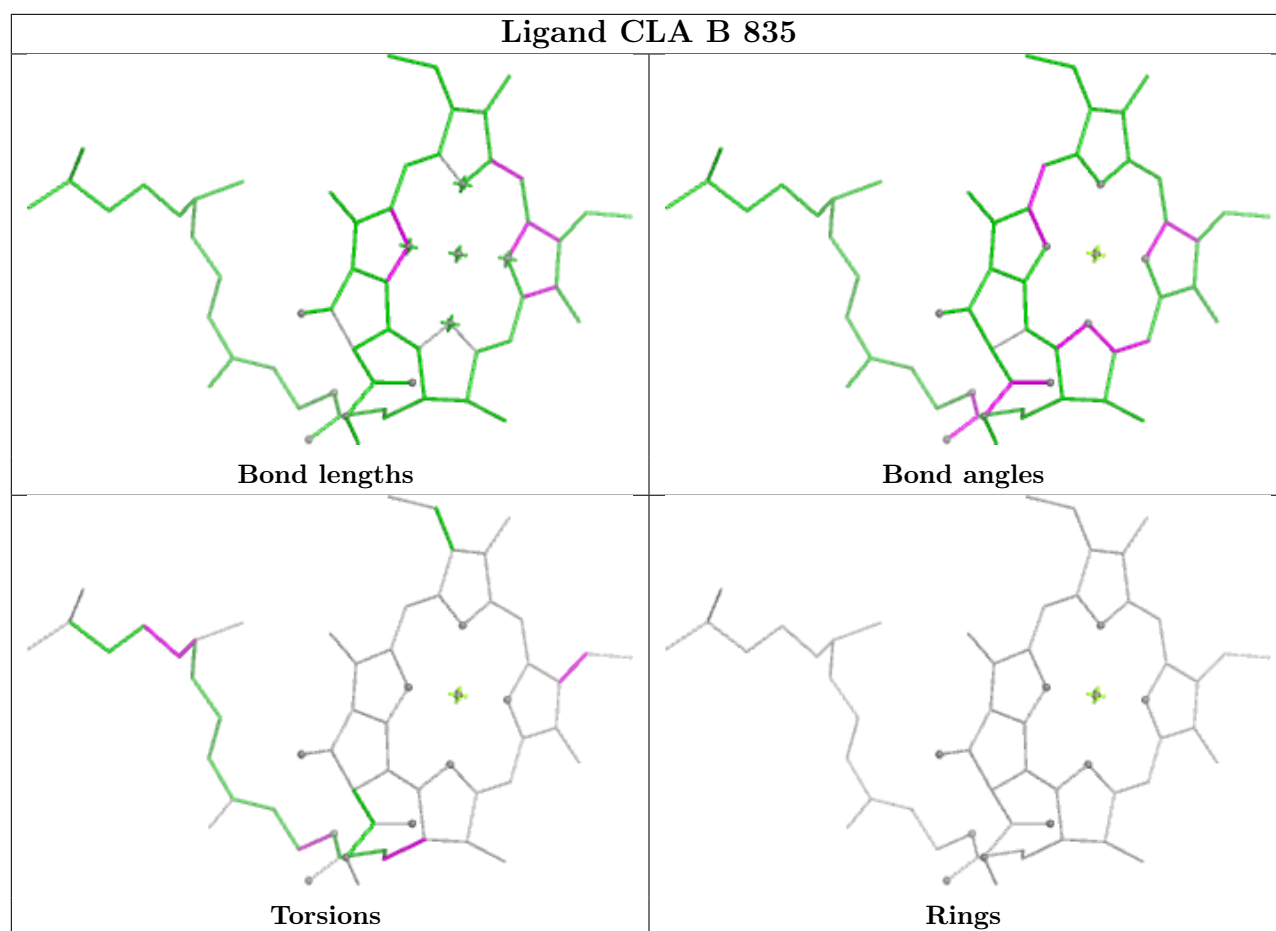
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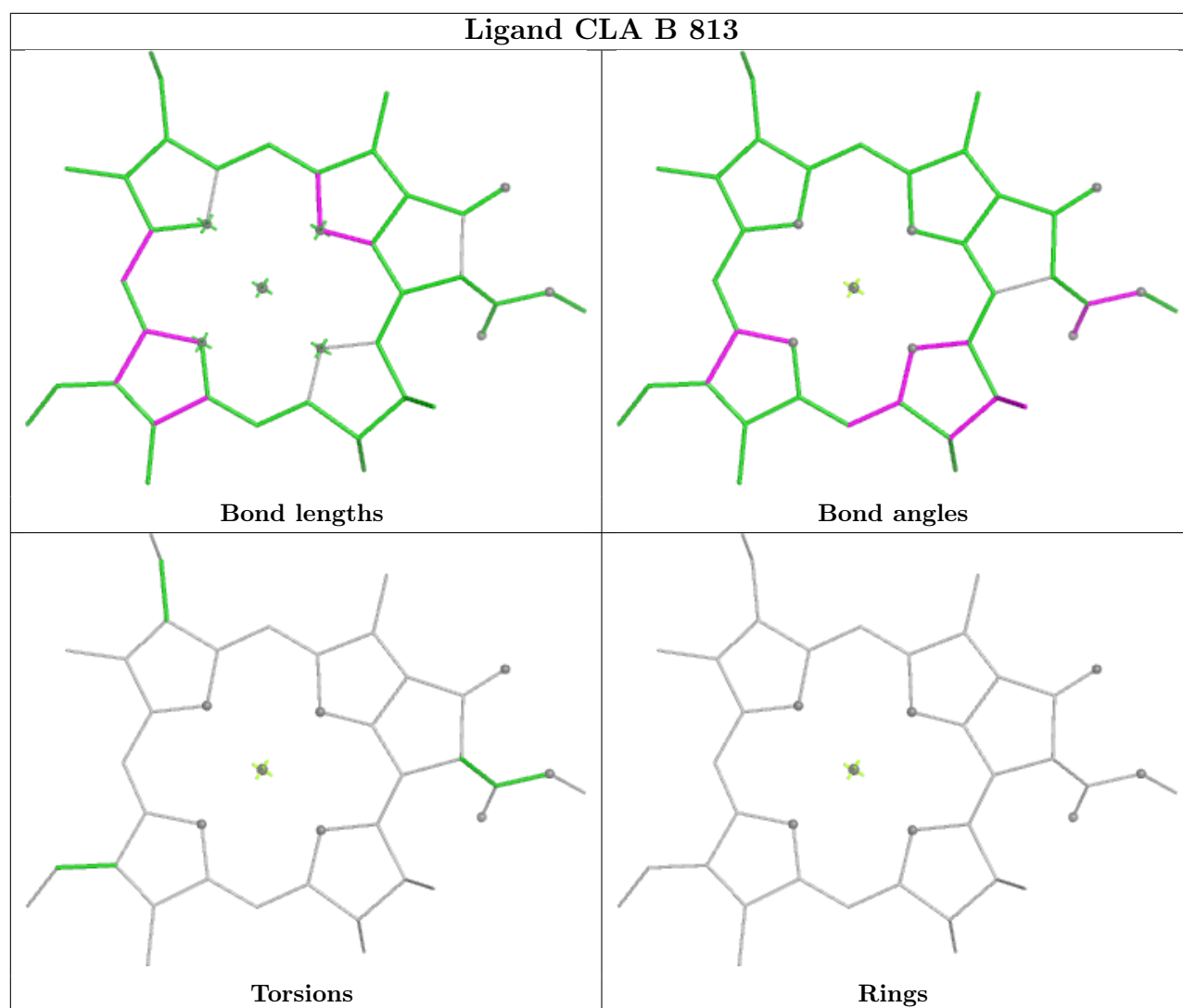
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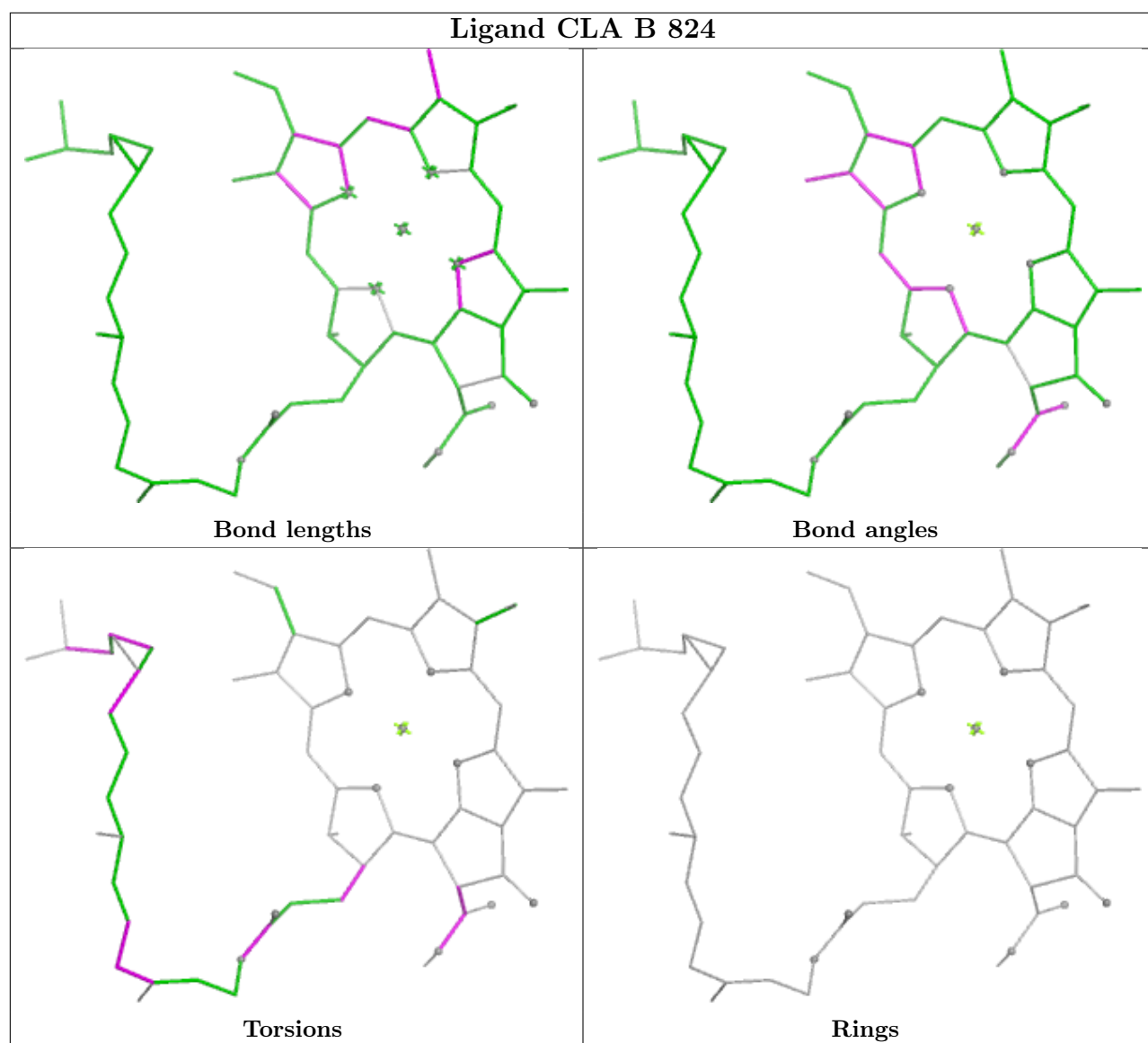
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	F	805	LUT	1	0
20	T	200	HEC	2	0
11	A	836	CLA	1	0
16	A	854	LMU	1	0
19	J	101	LUT	2	0
11	B	822	CLA	3	0
11	A	828	CLA	3	0
14	B	847	BCR	1	0
14	L	201	BCR	1	0
11	A	811	CLA	2	0
14	A	848	BCR	2	0
11	A	807	CLA	1	0
11	B	852	CLA	2	0
11	B	842	CLA	2	0
18	B	849	DGD	5	0
11	B	832	CLA	3	0
14	B	848	BCR	1	0
11	B	833	CLA	1	0
11	A	806	CLA	2	0
11	B	841	CLA	7	0
14	A	849	BCR	2	0
11	B	814	CLA	6	0
11	B	803	CLA	4	0

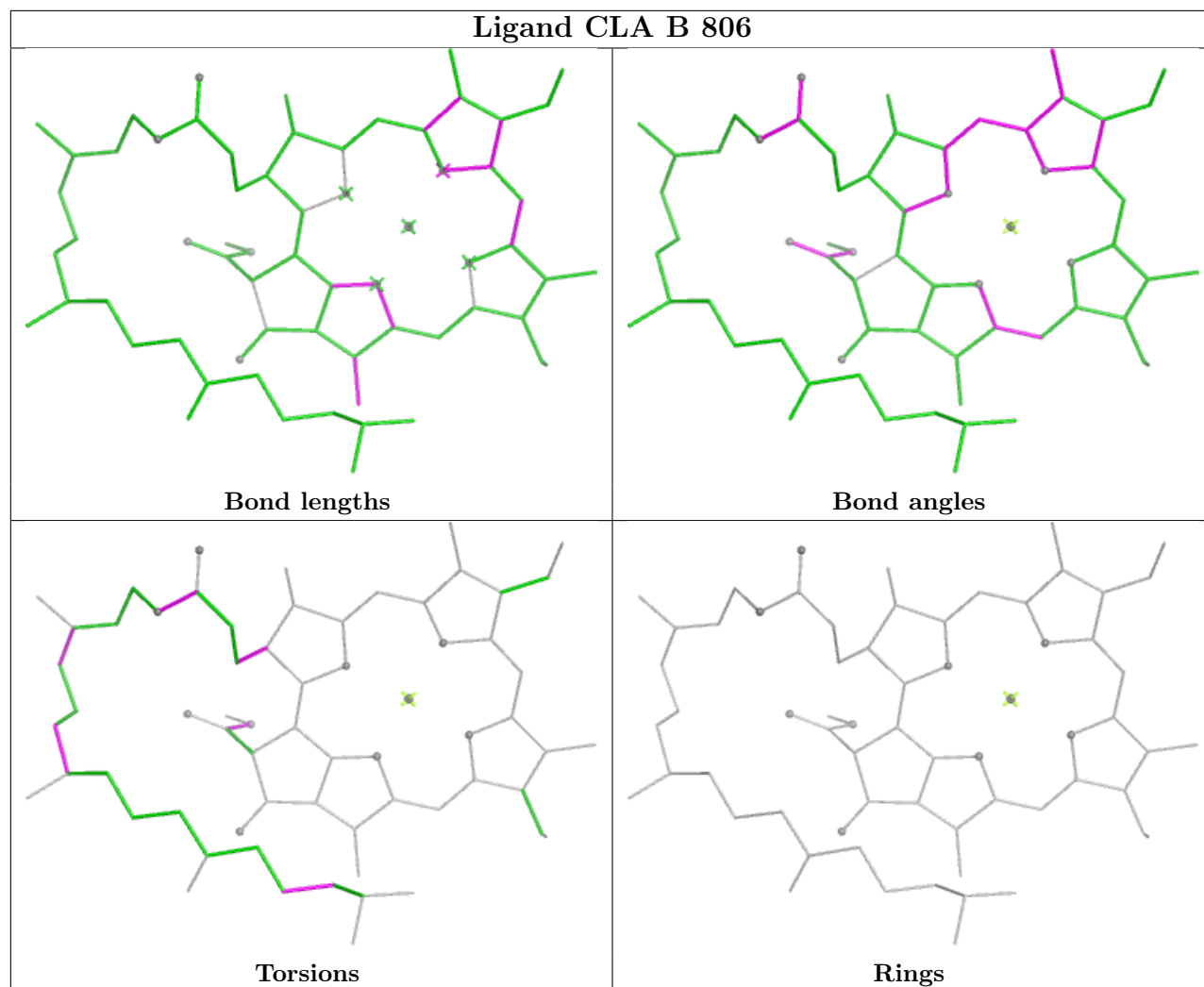
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

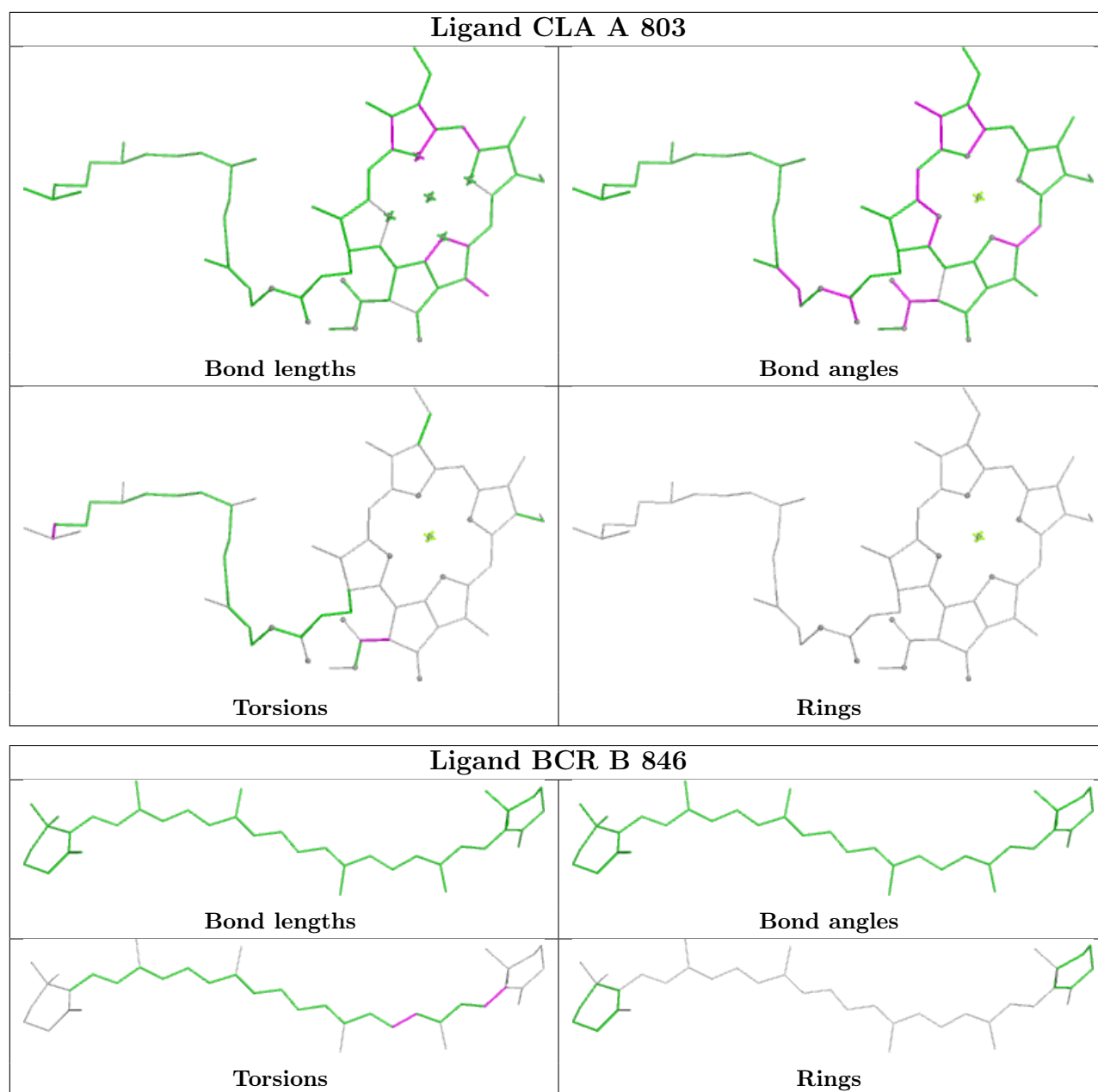


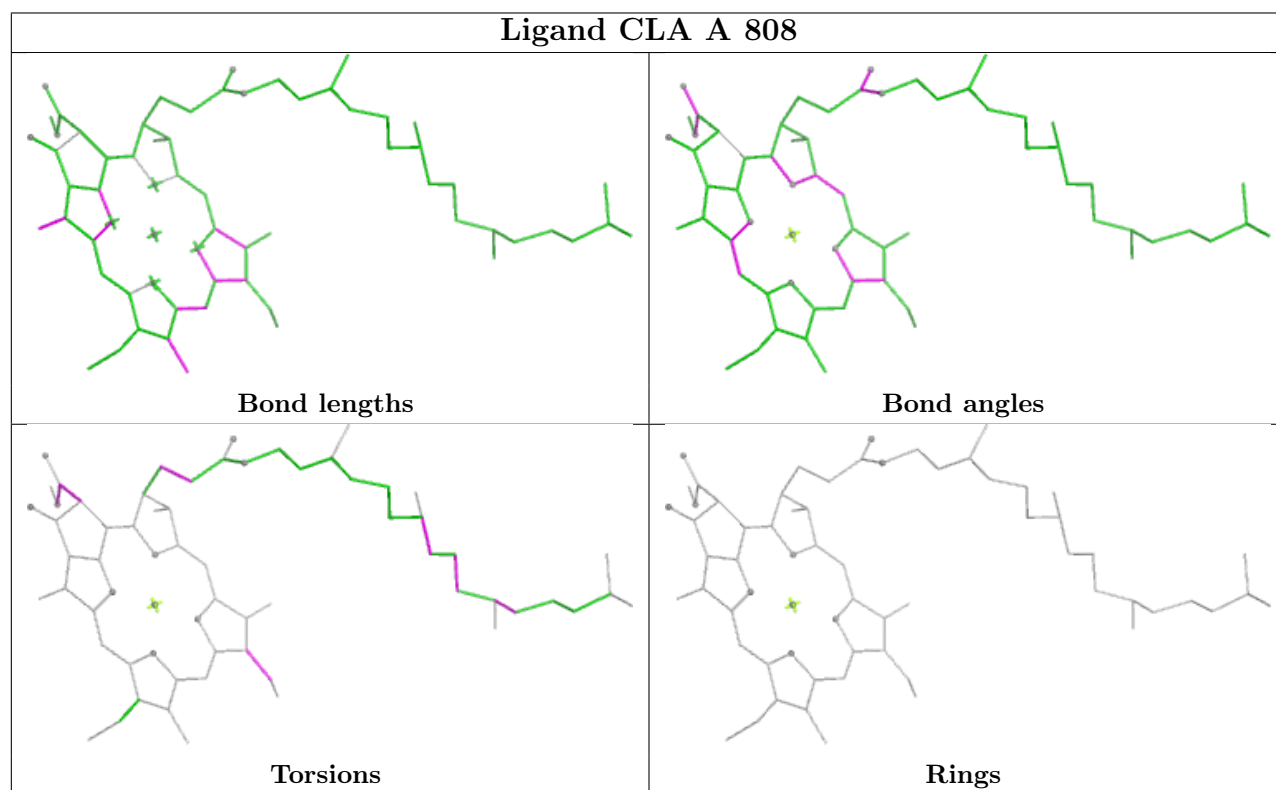
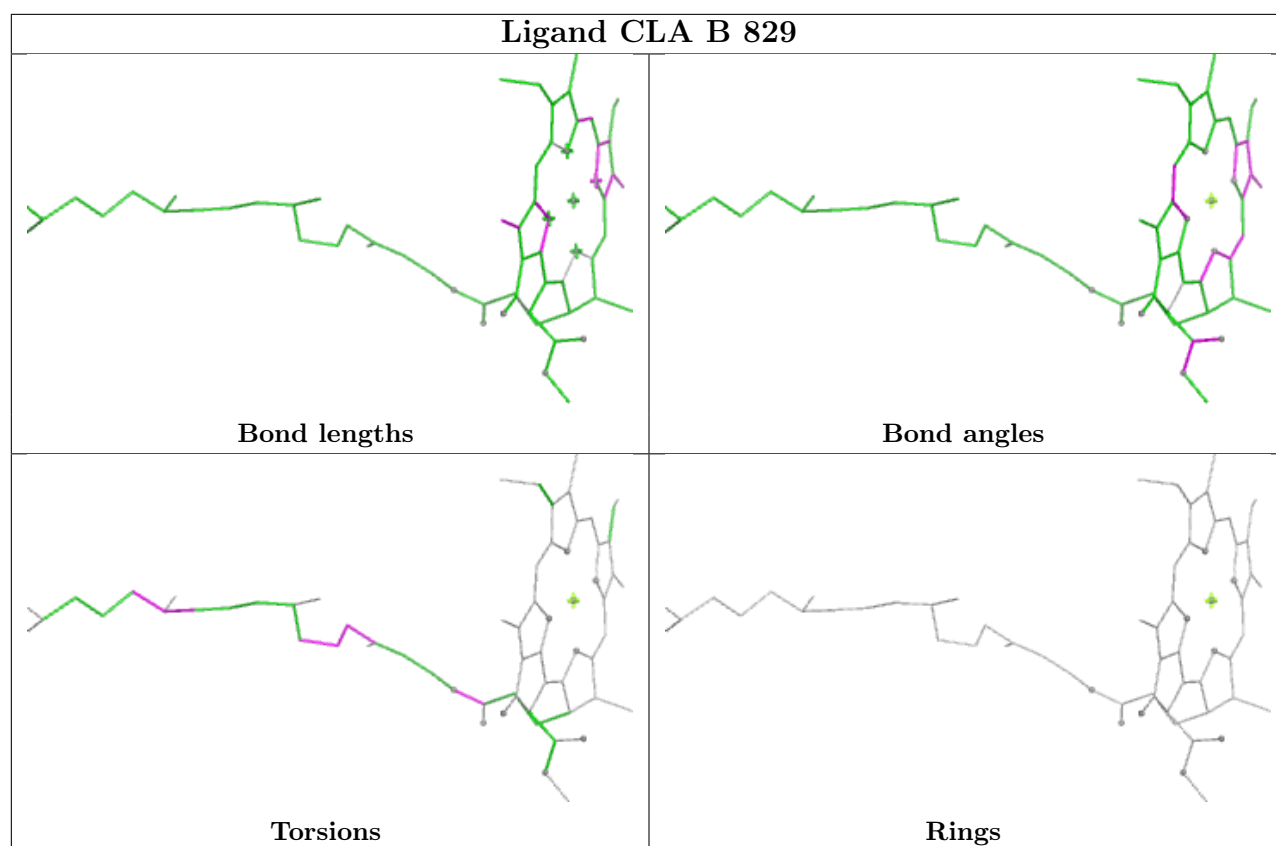


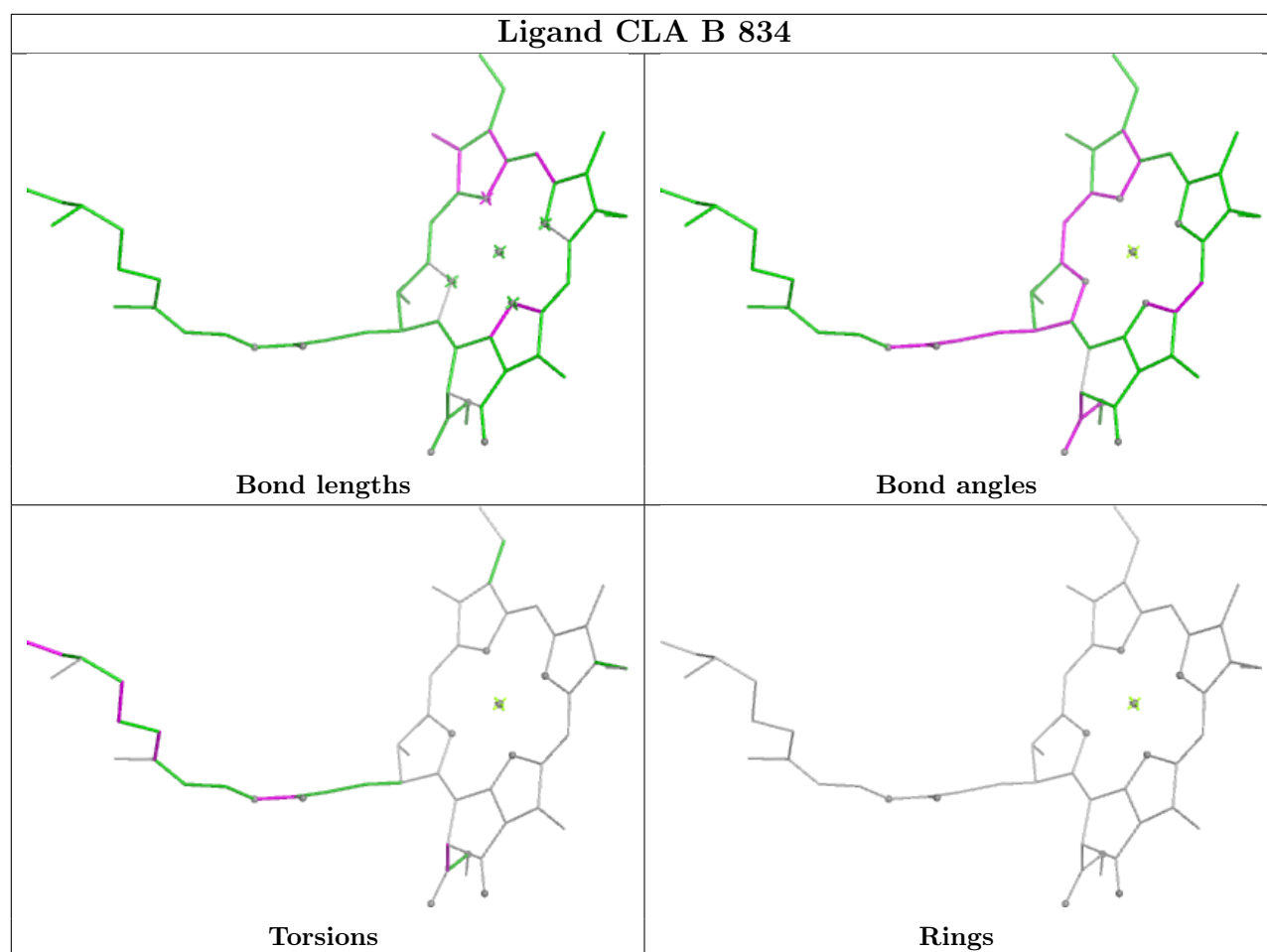


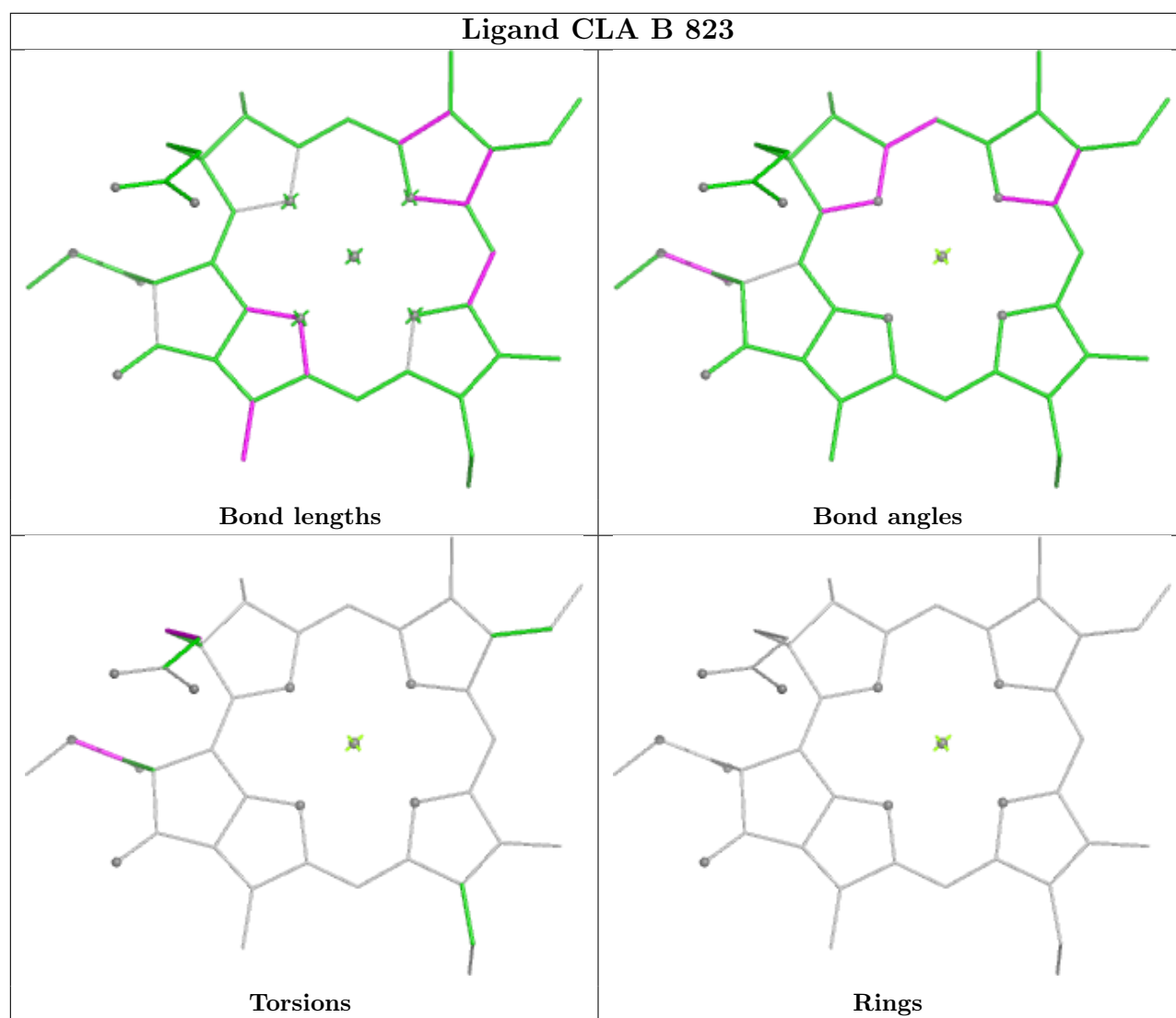




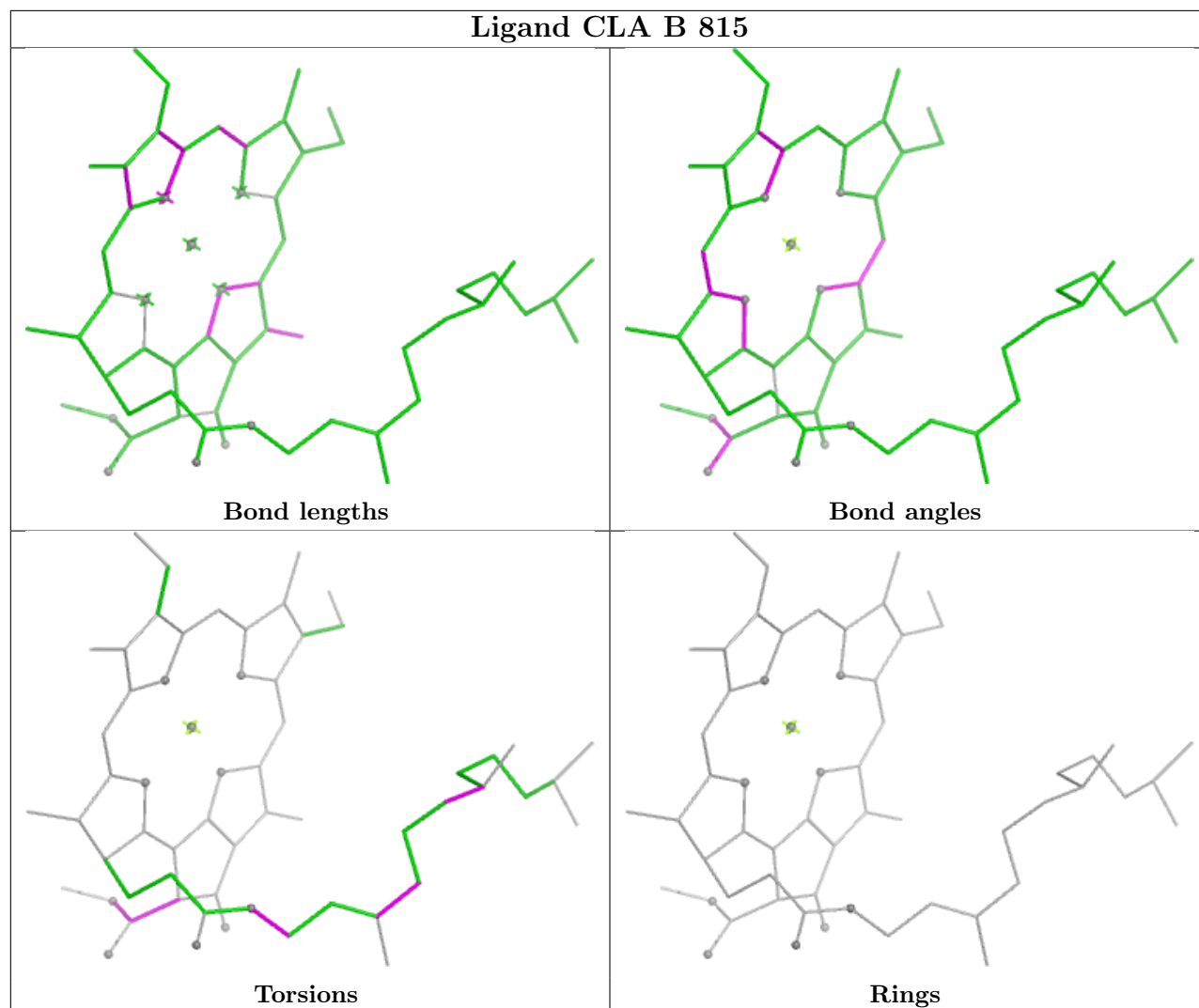




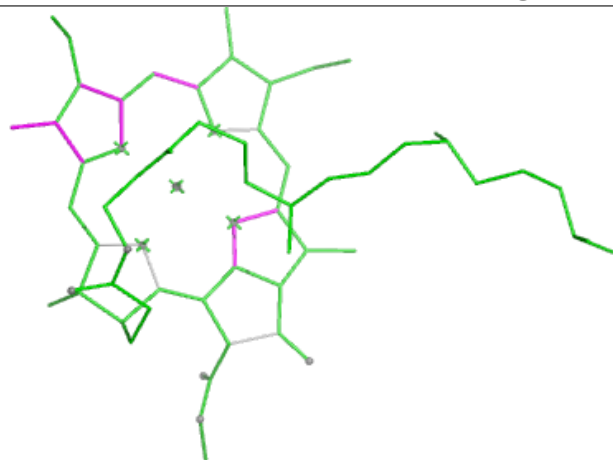




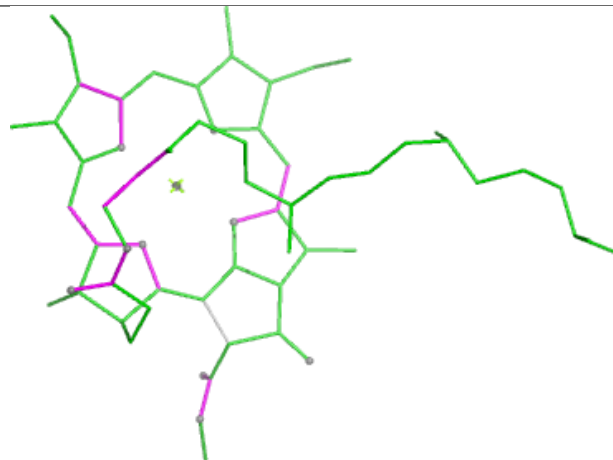
Ligand CLA B 815



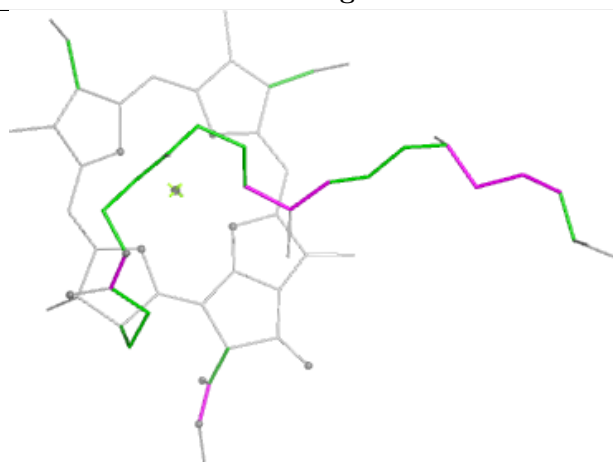
Ligand CLA B 828



Bond lengths



Bond angles

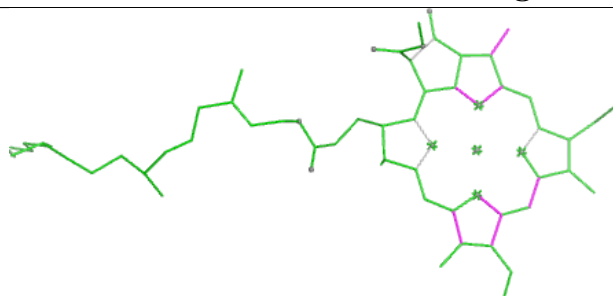


Torsions

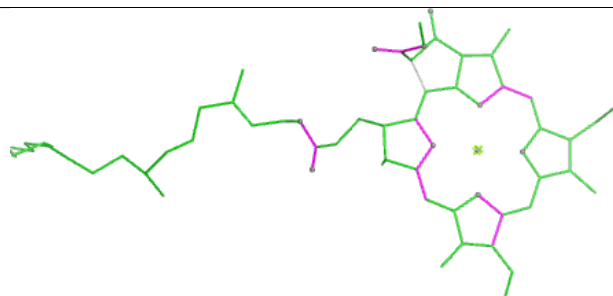


Rings

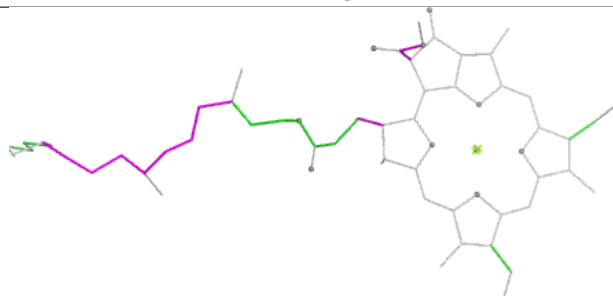
Ligand CLA A 805



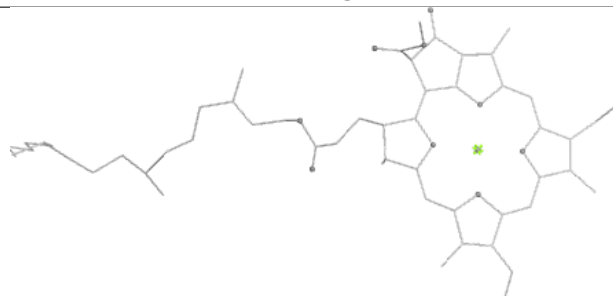
Bond lengths



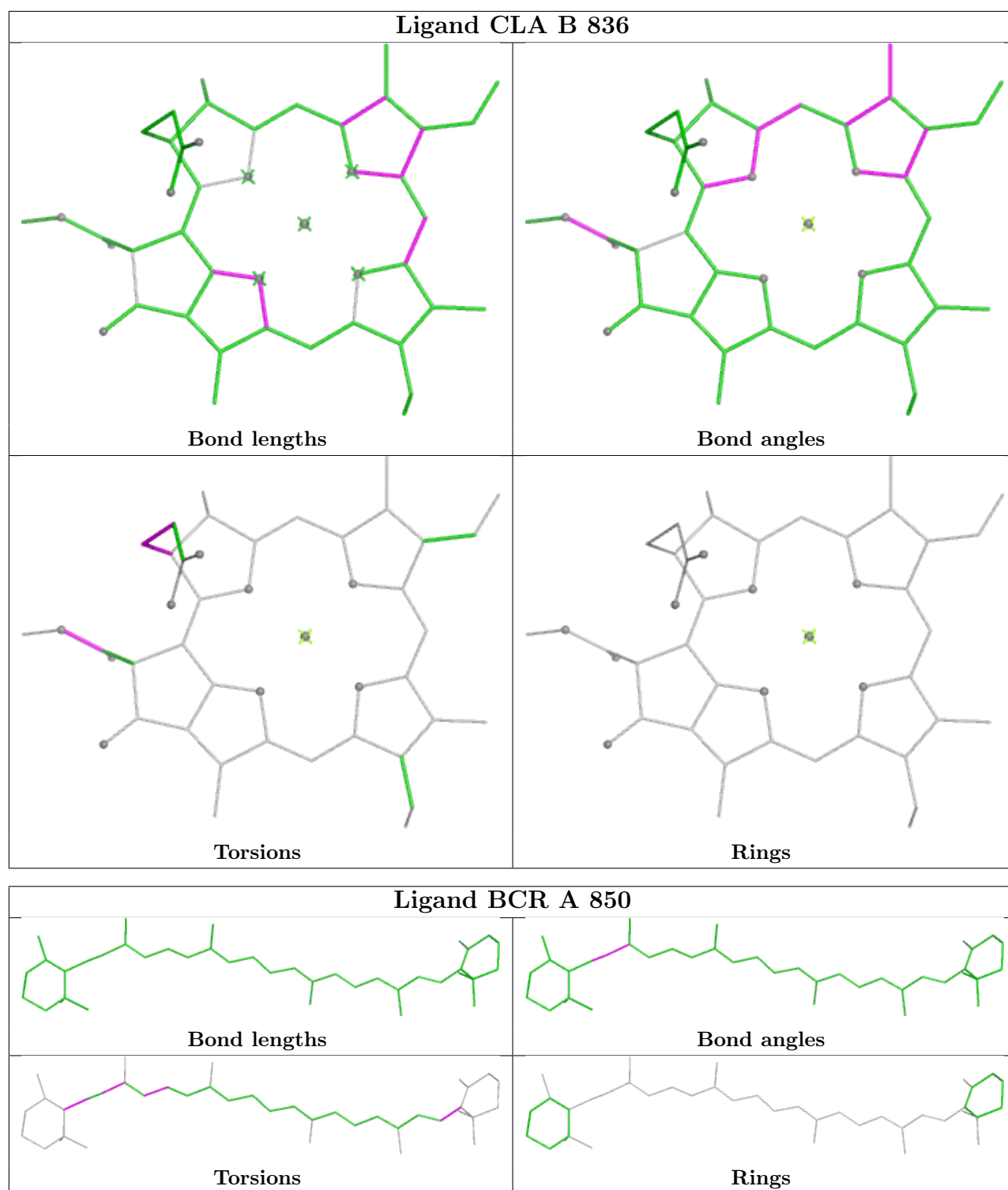
Bond angles

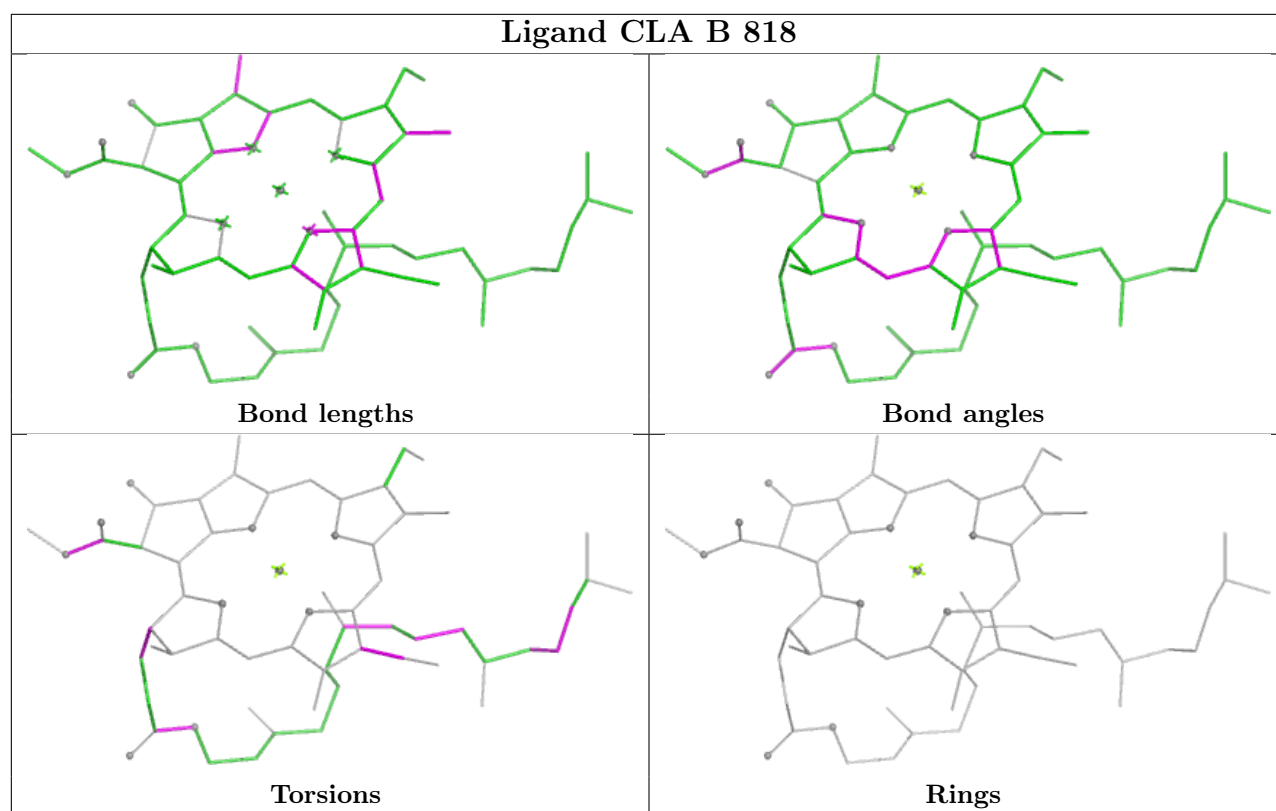


Torsions

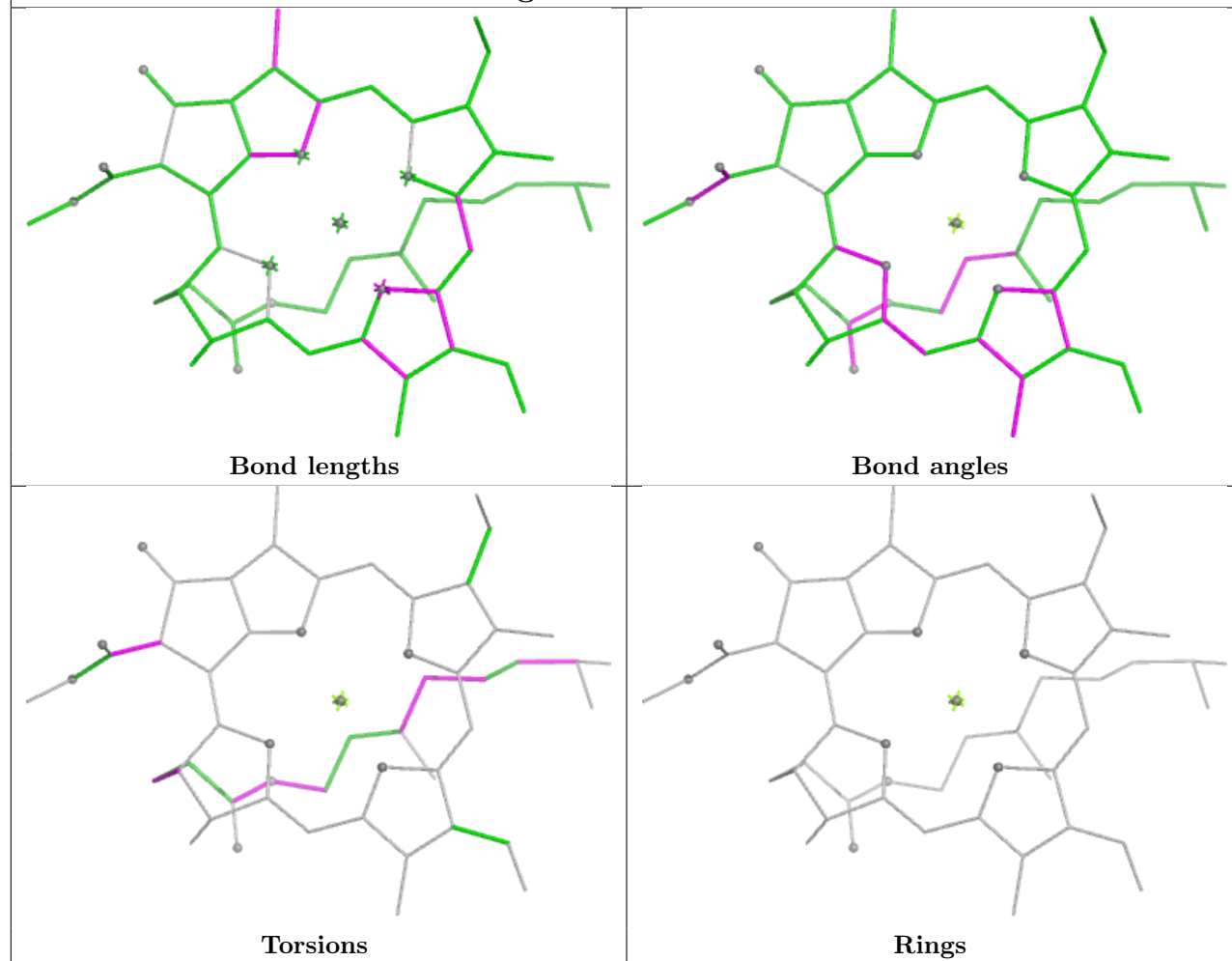


Rings

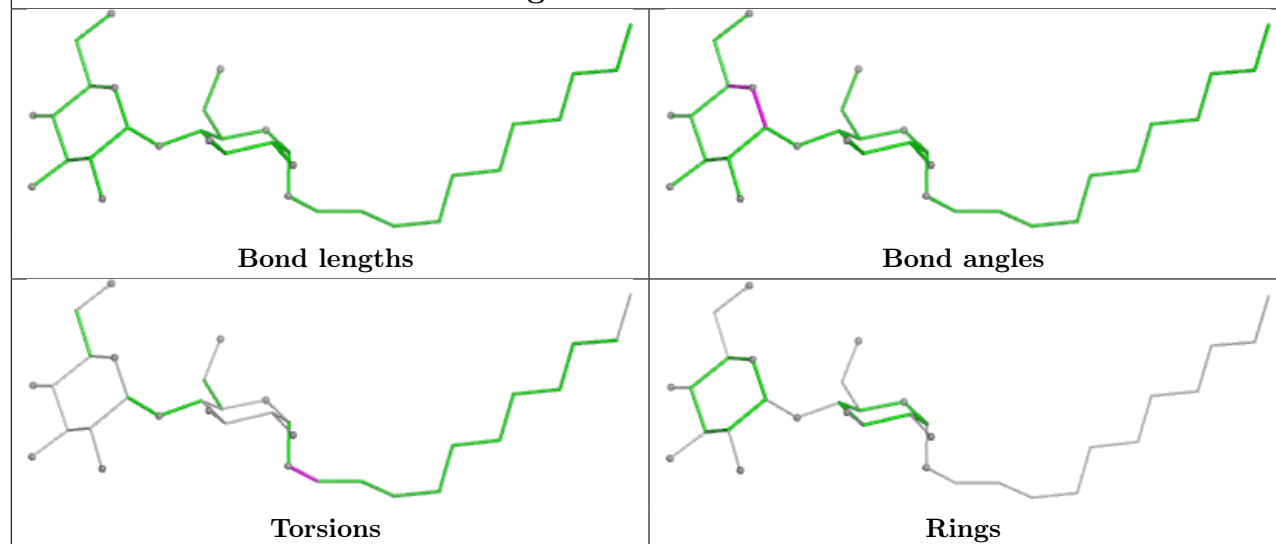


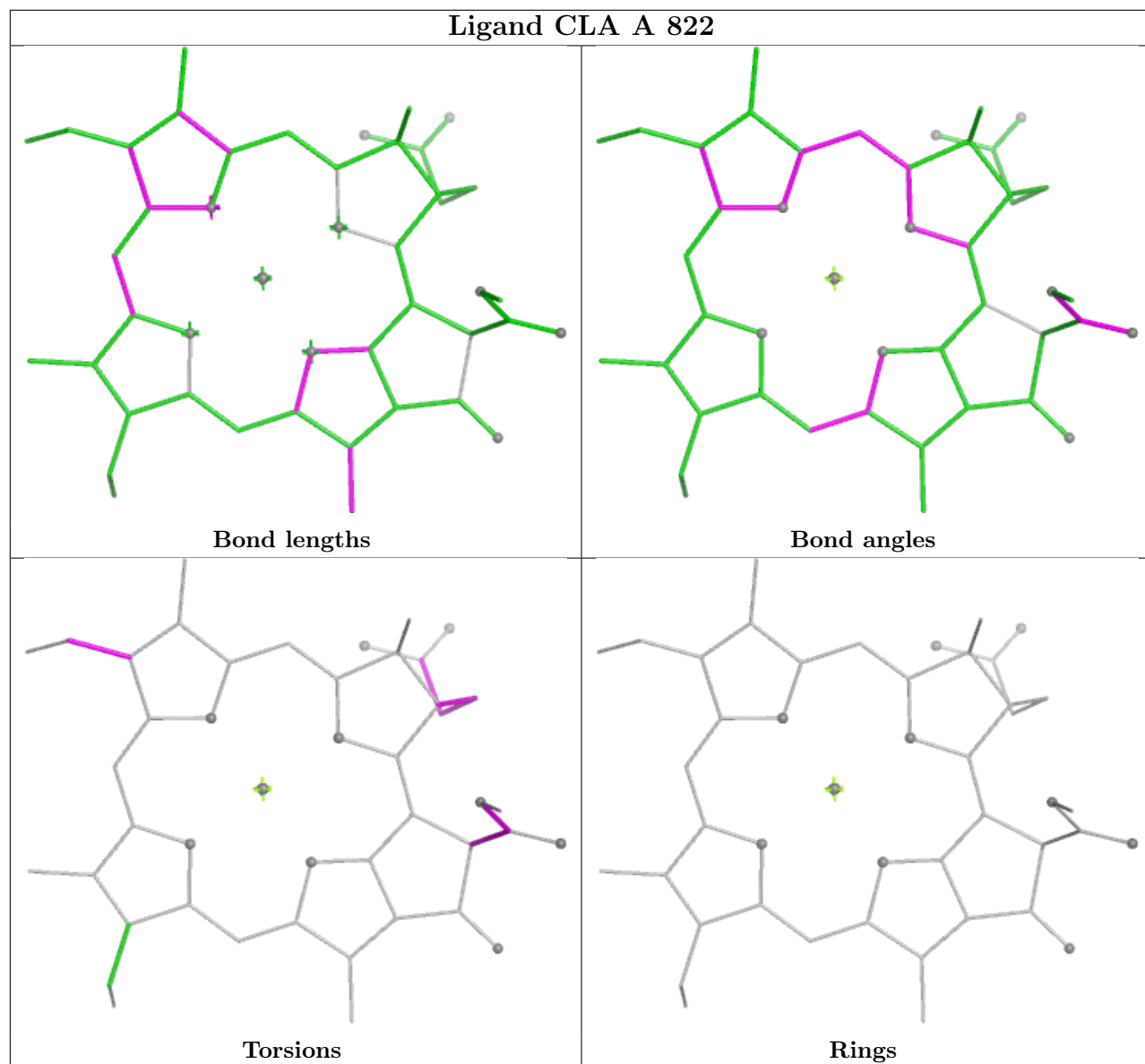


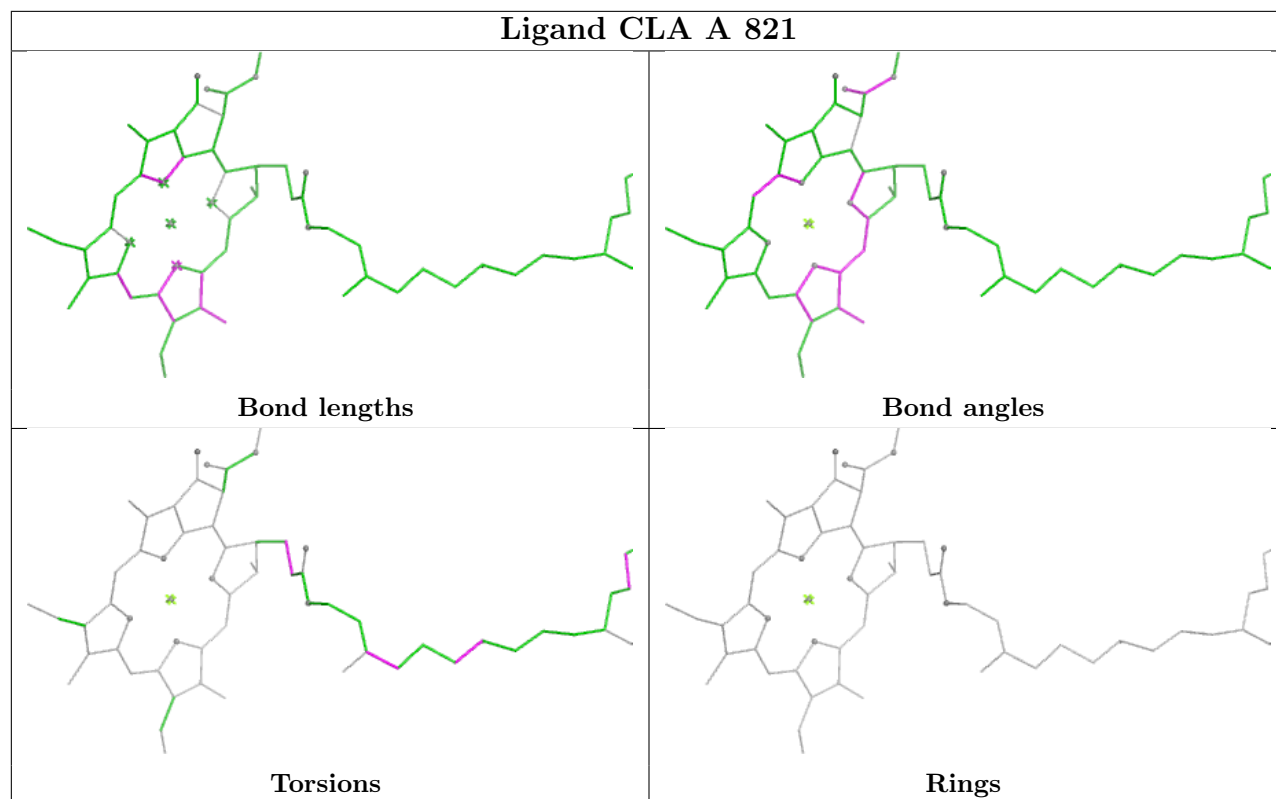
Ligand CLA J 103

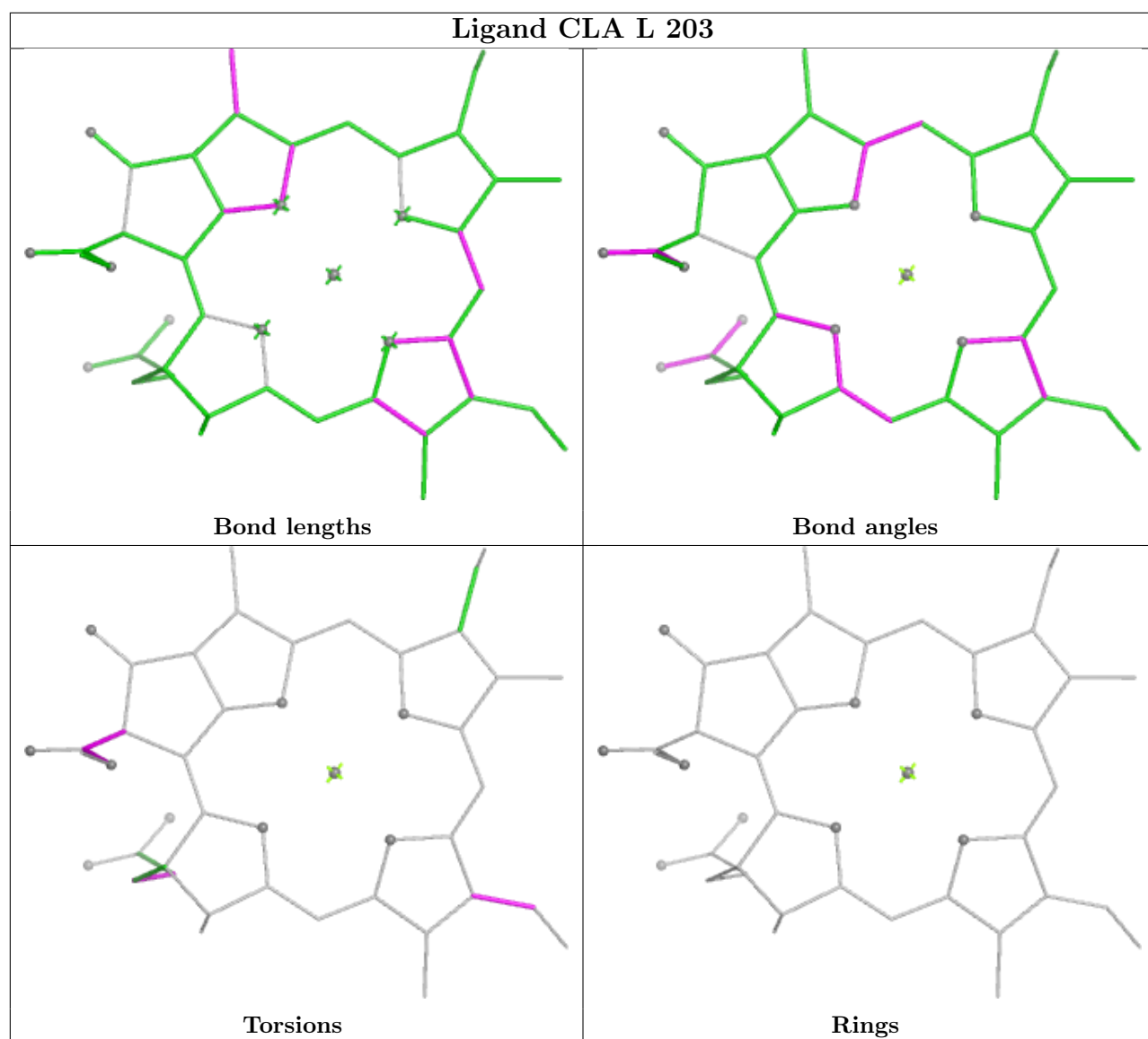


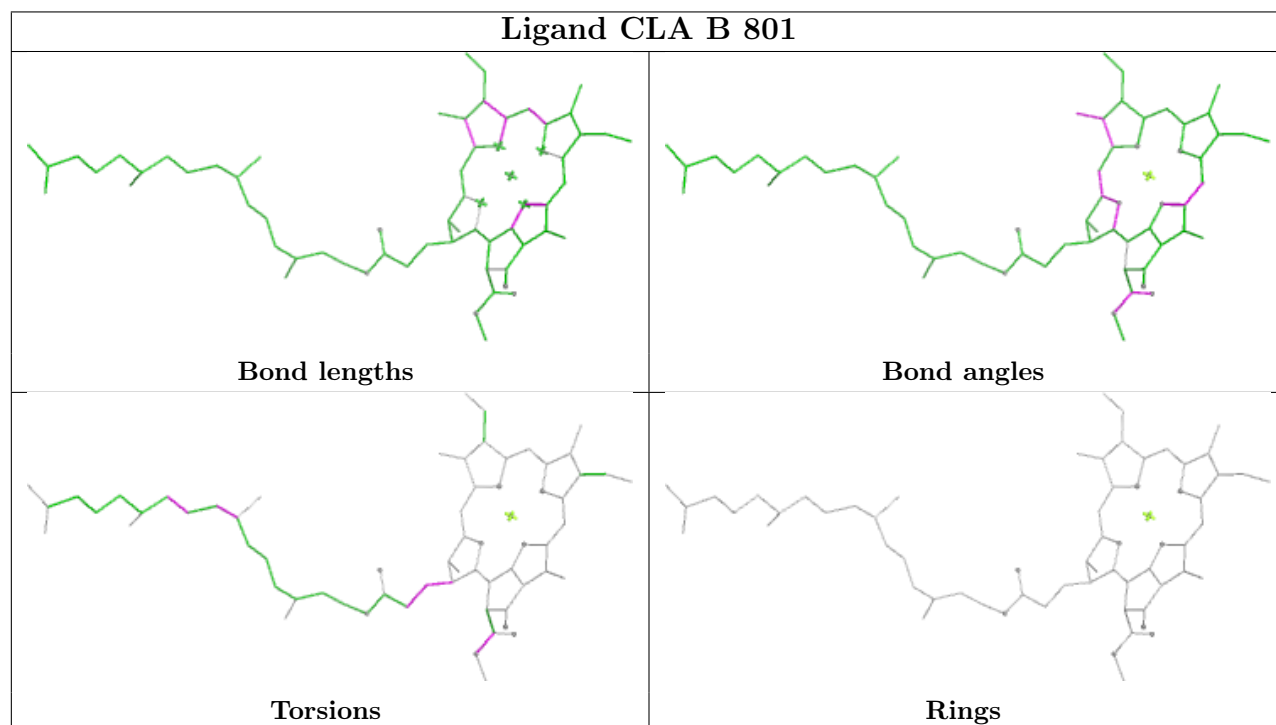
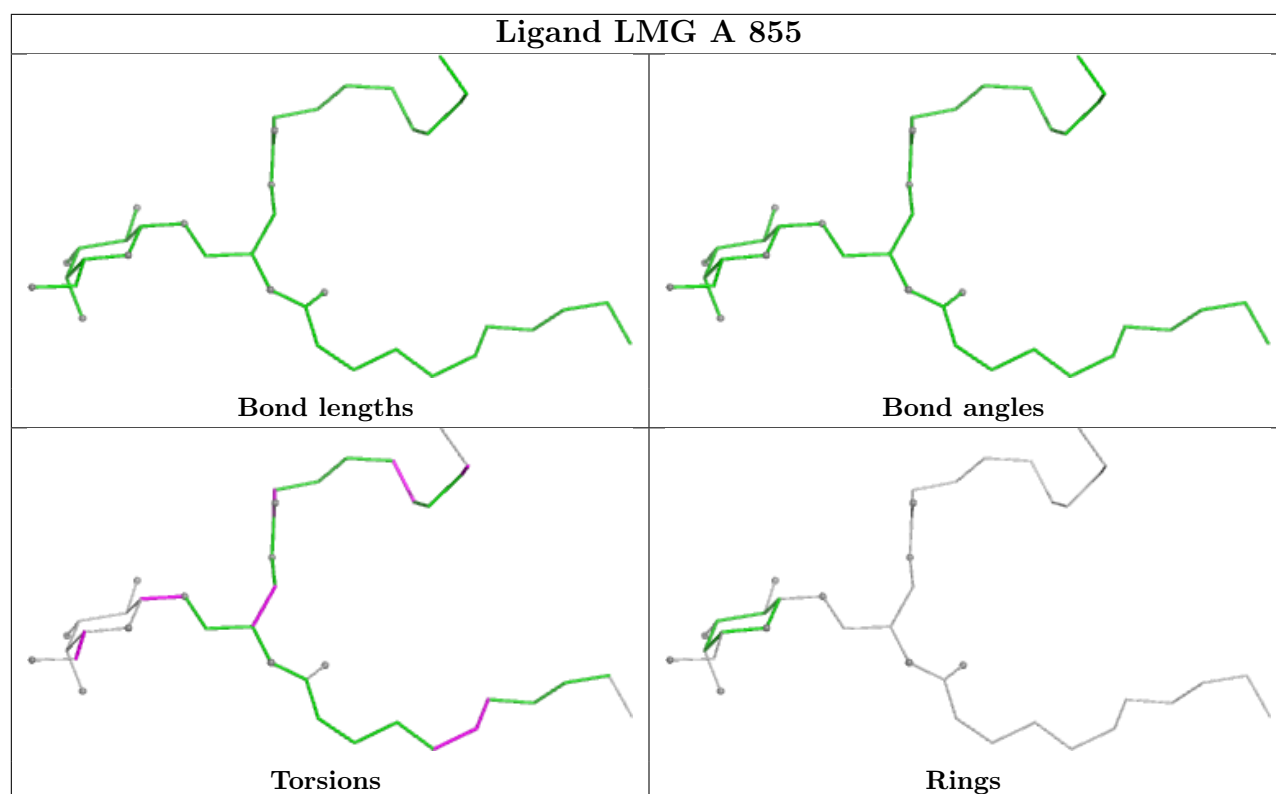
Ligand LMU A 853

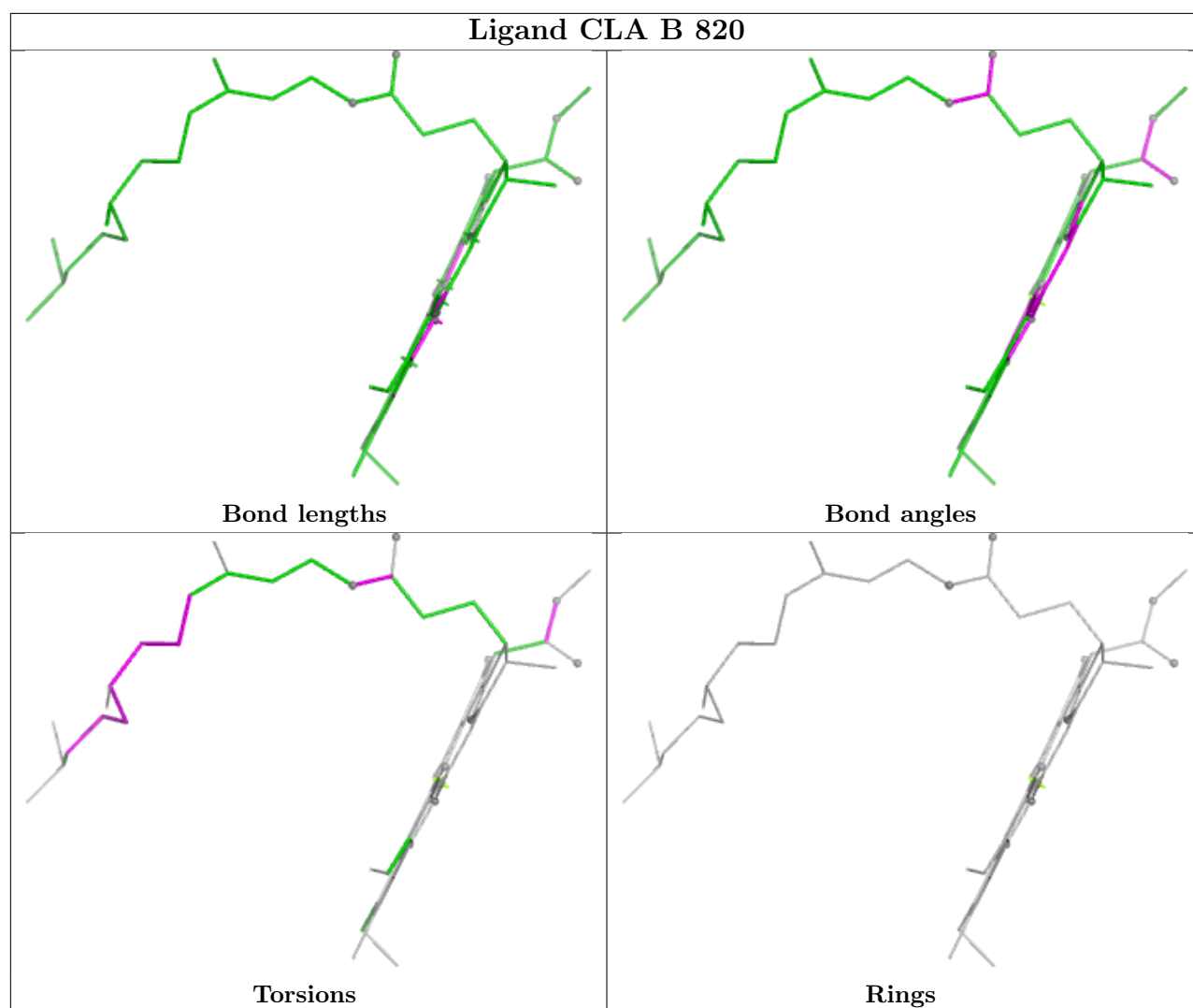


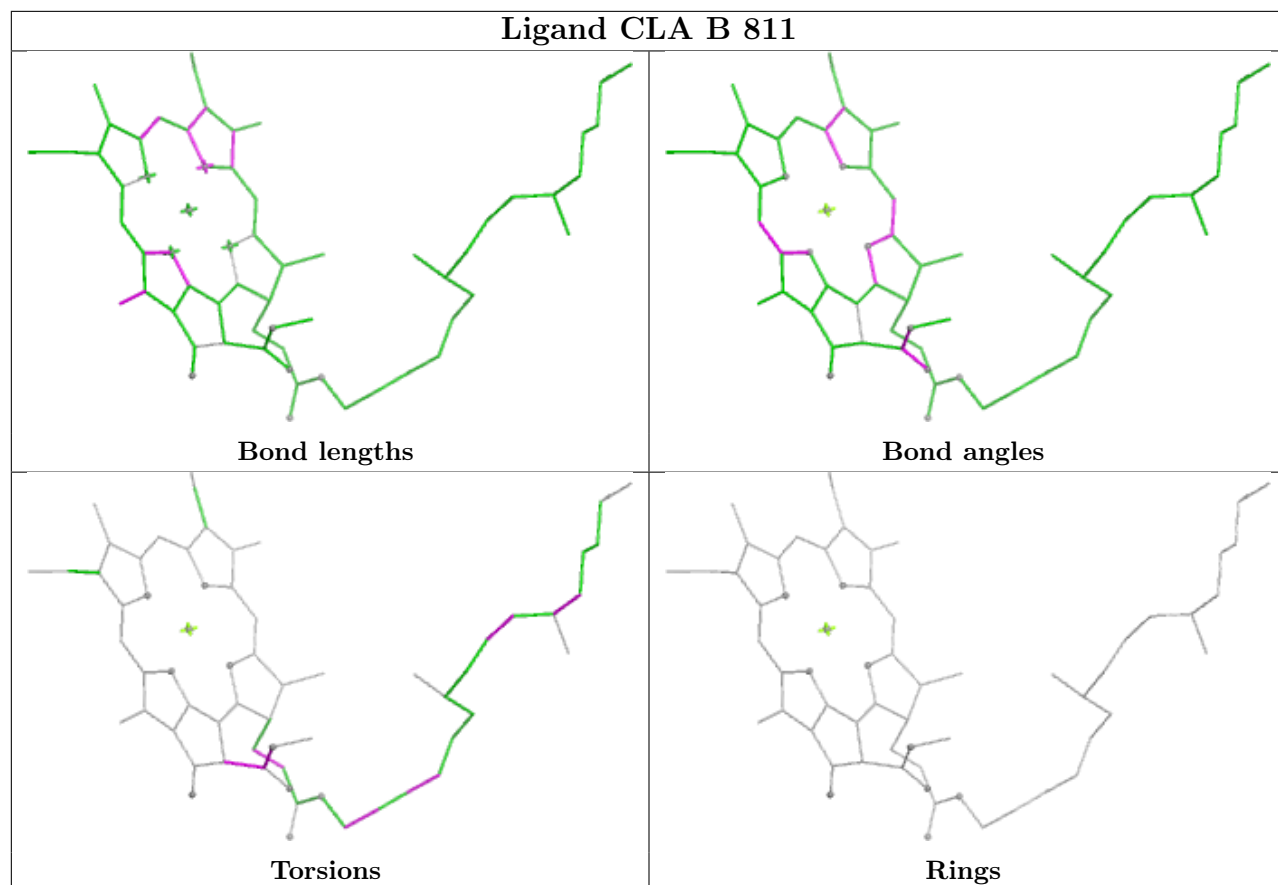


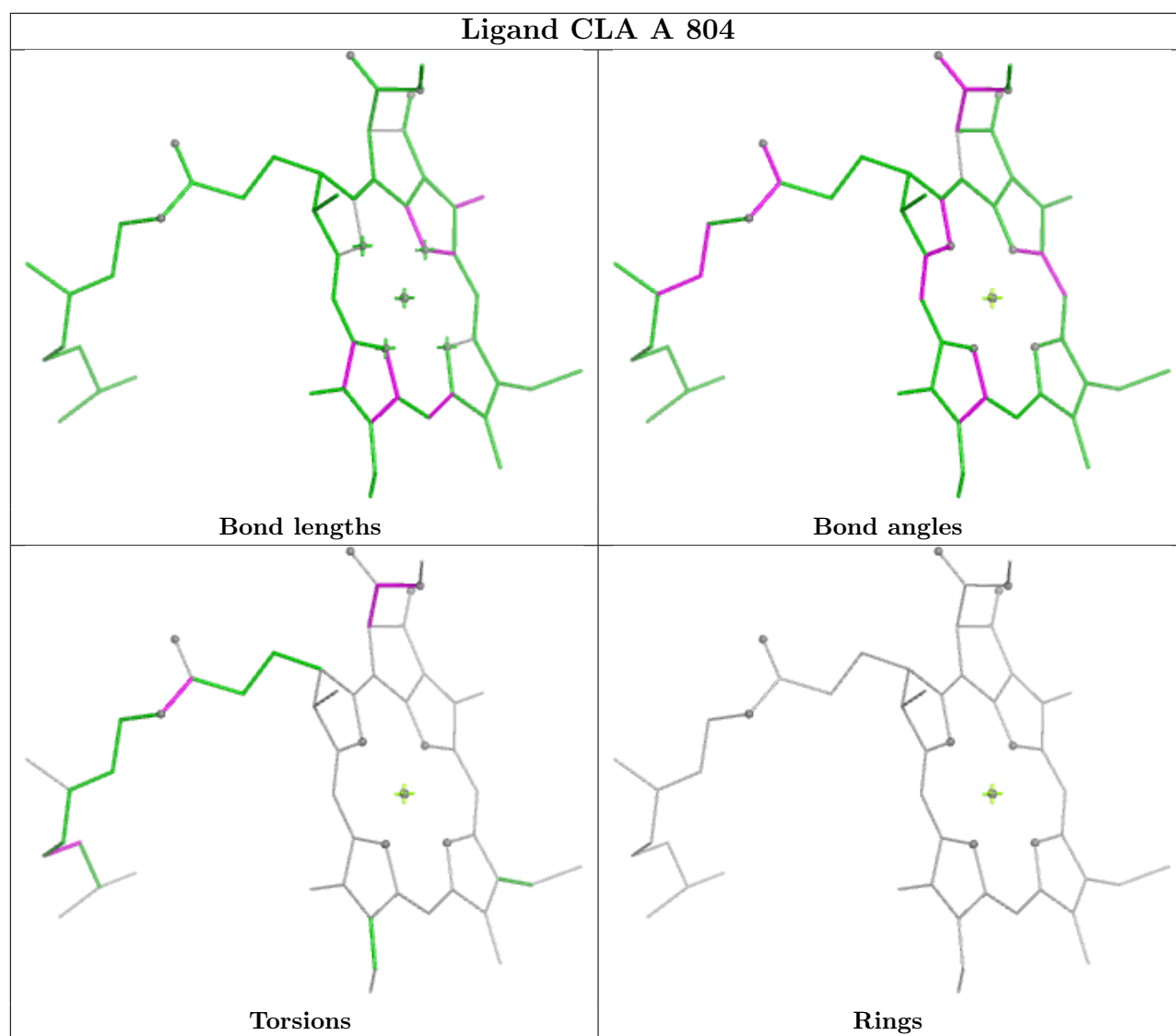


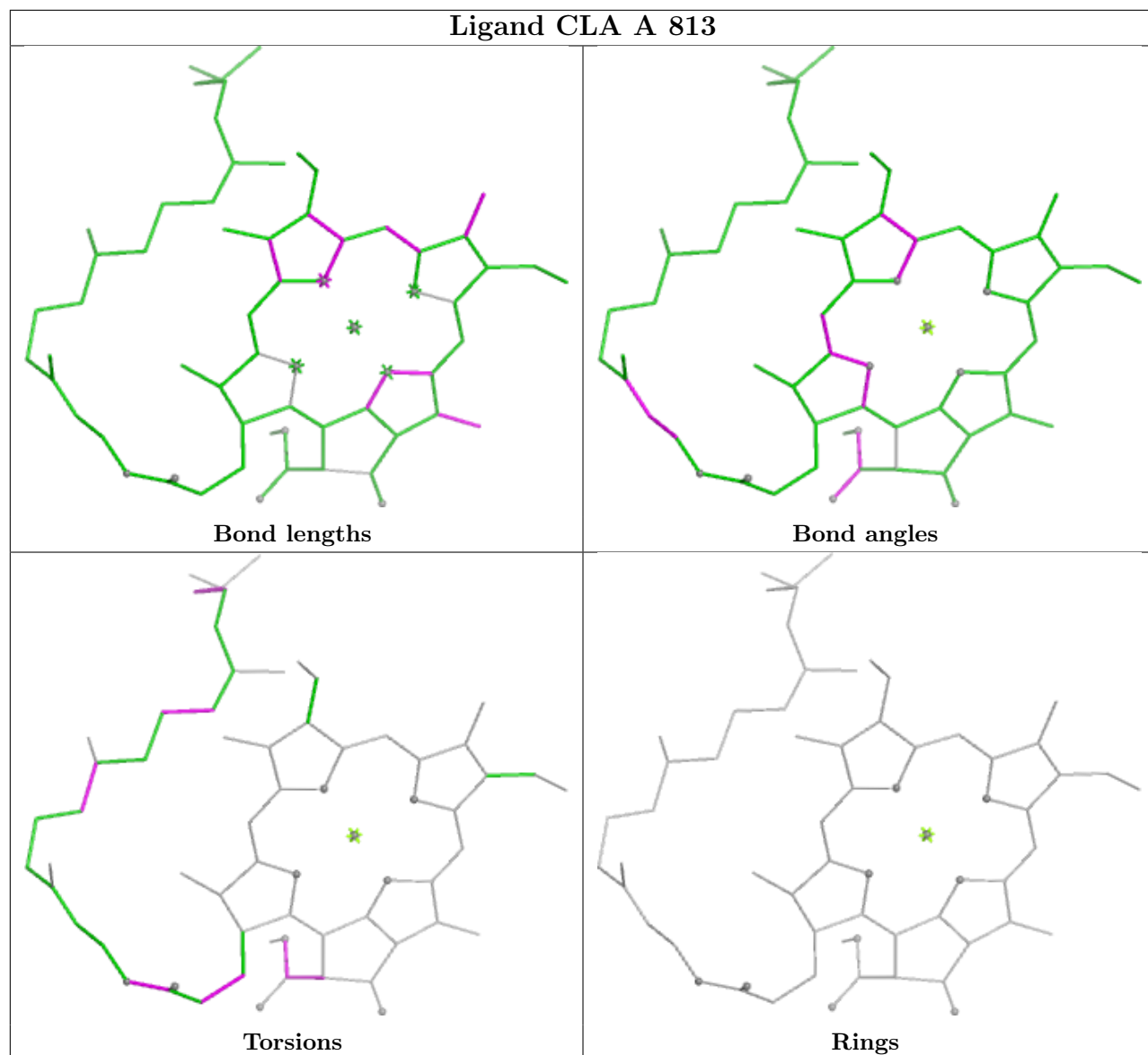


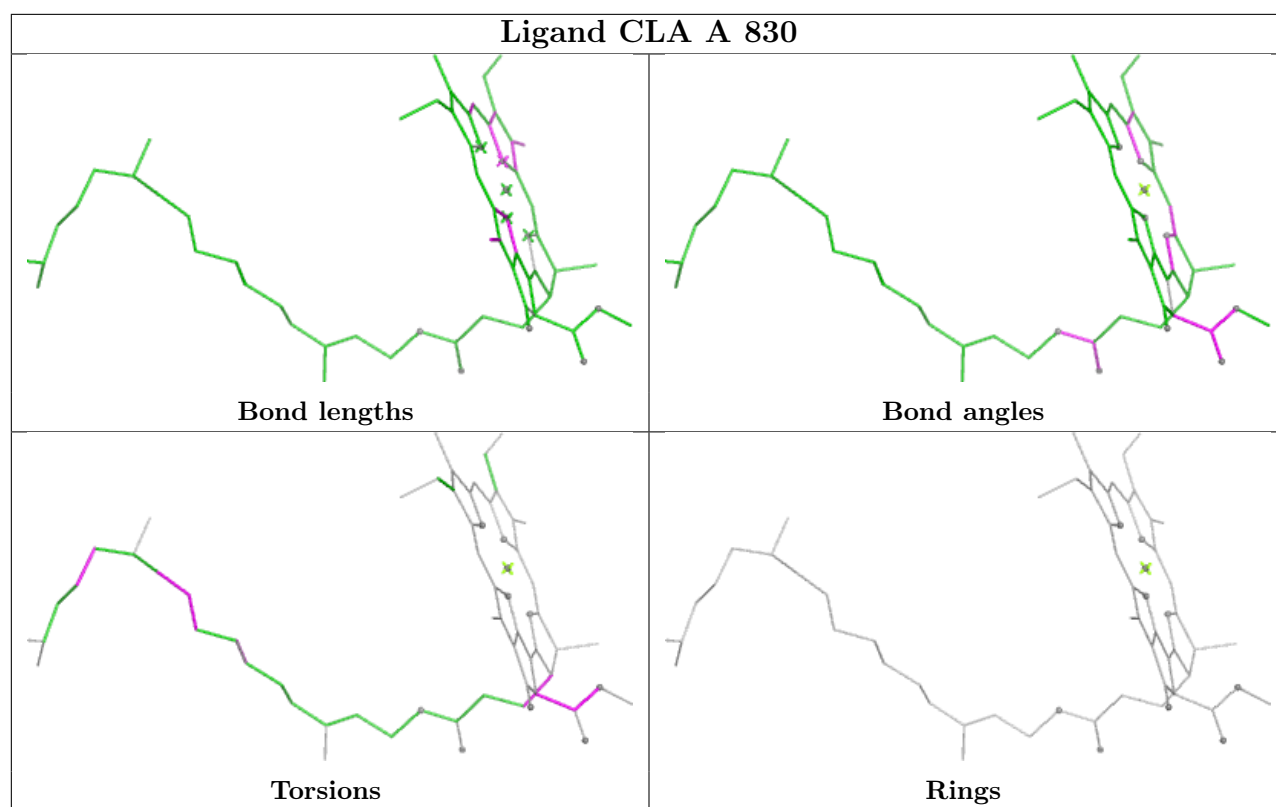




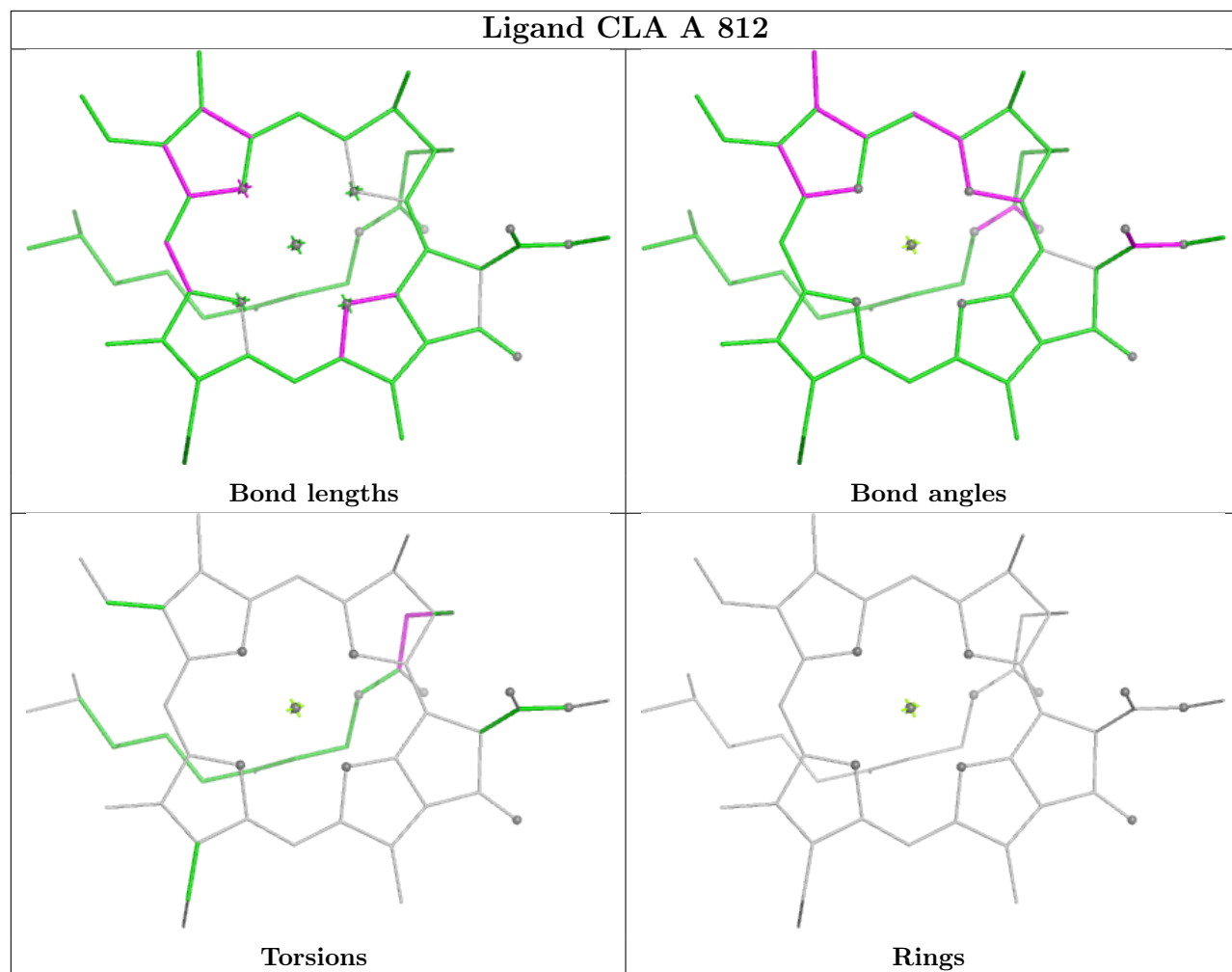


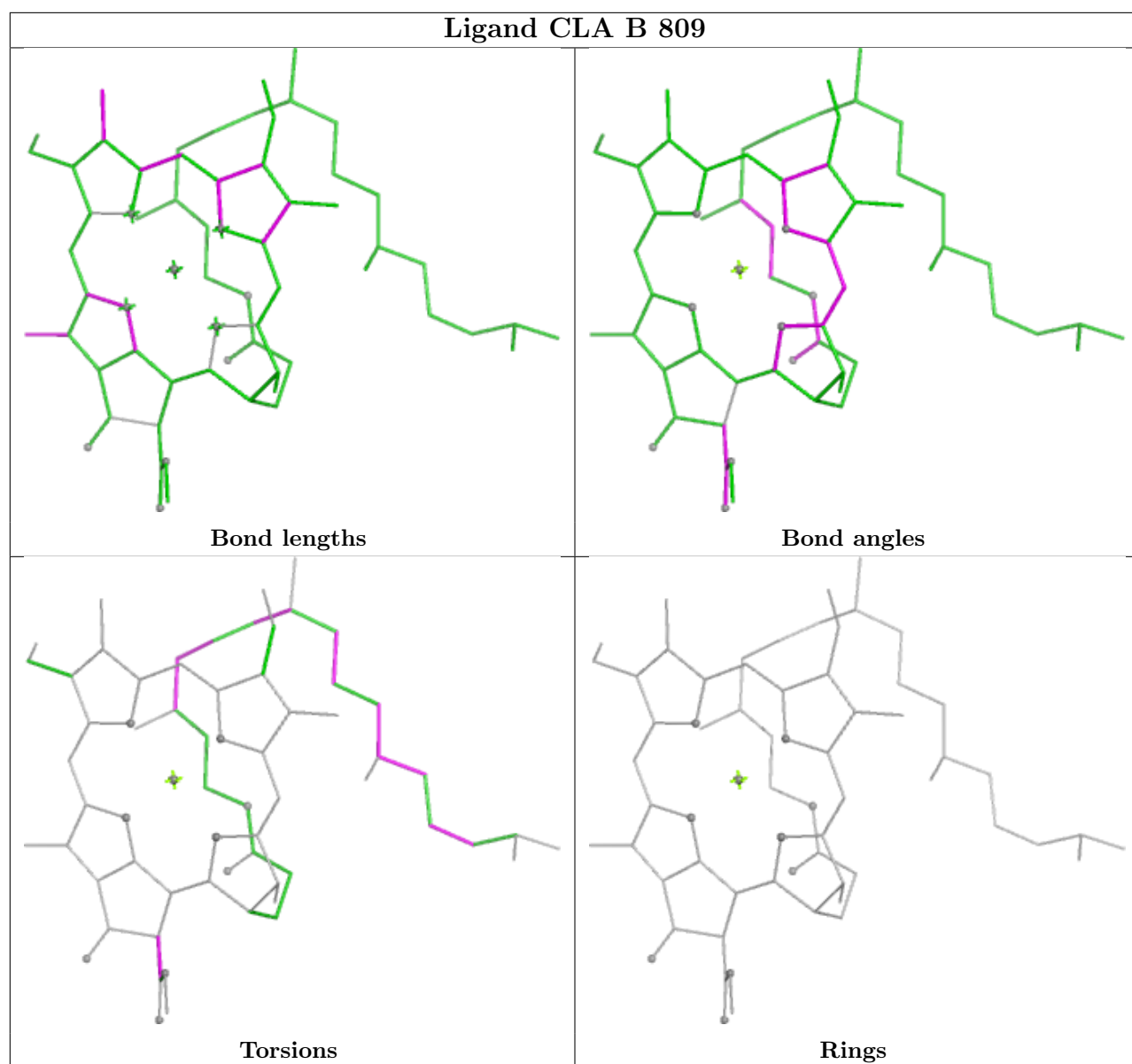


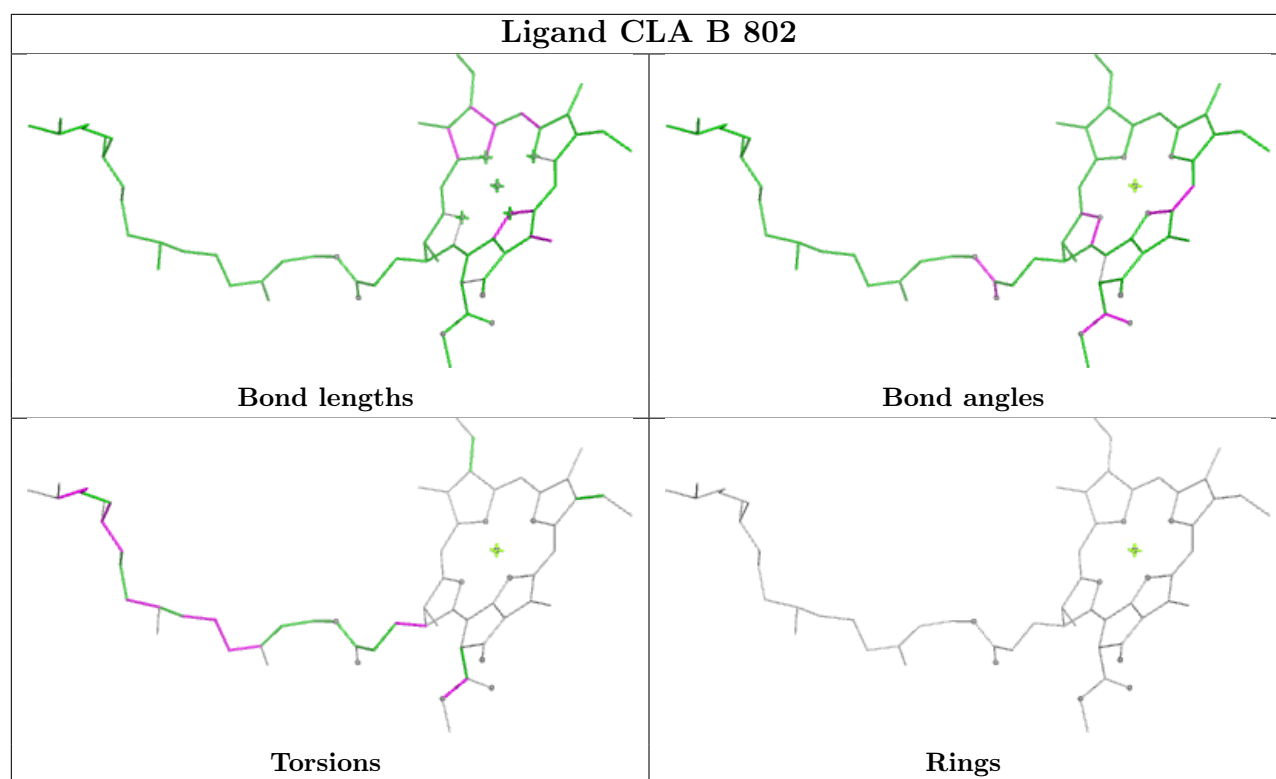




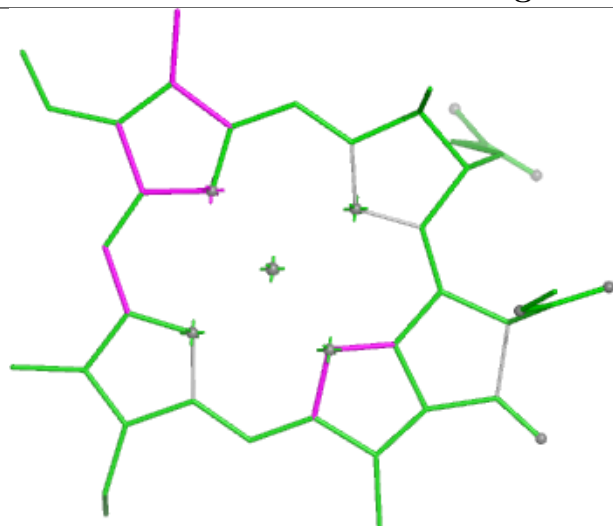
Ligand CLA A 812



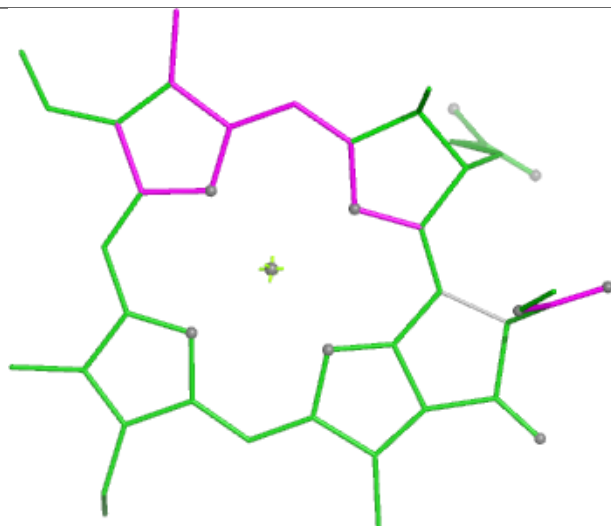




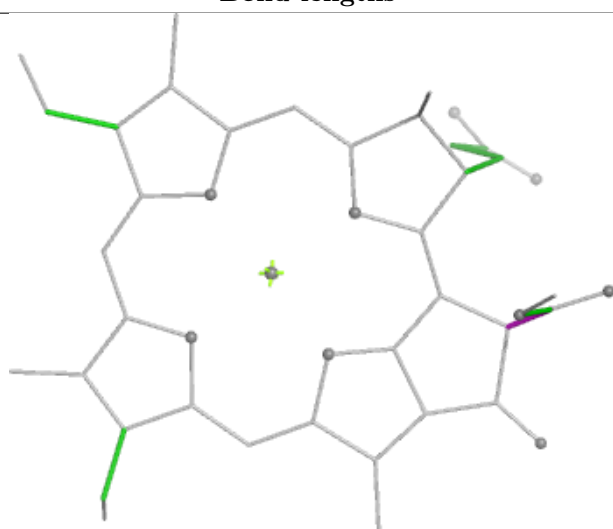
Ligand CLA B 831



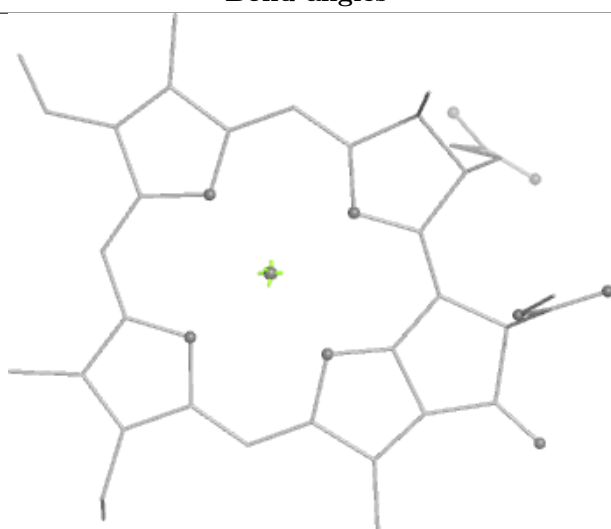
Bond lengths



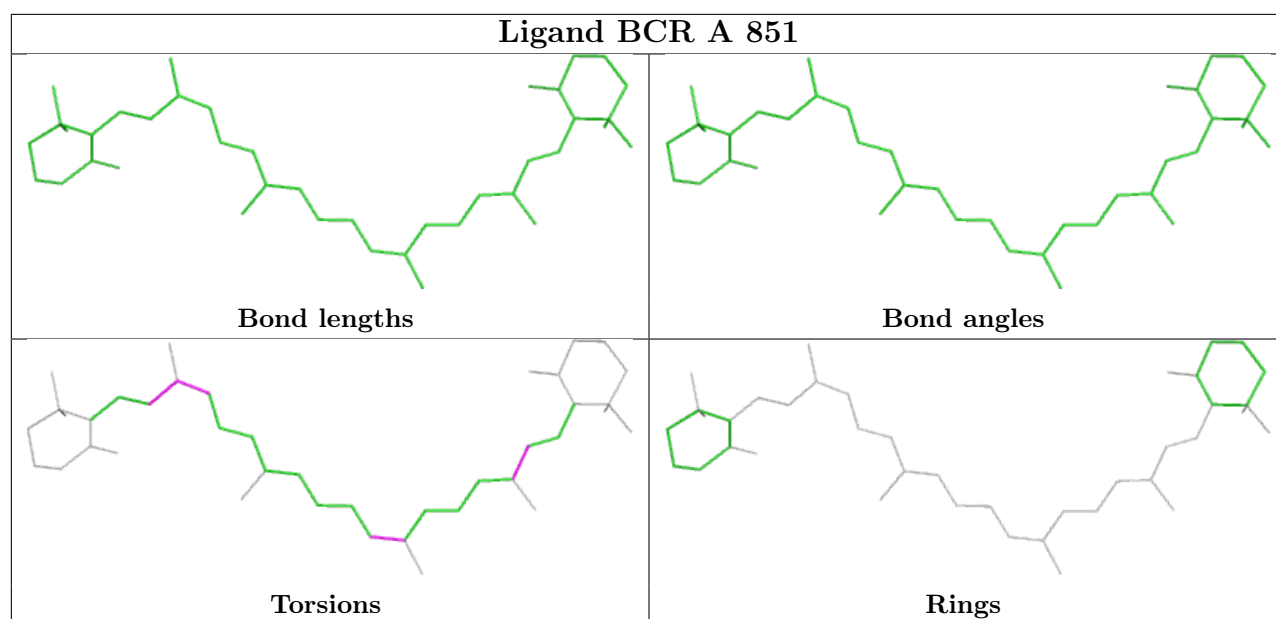
Bond angles

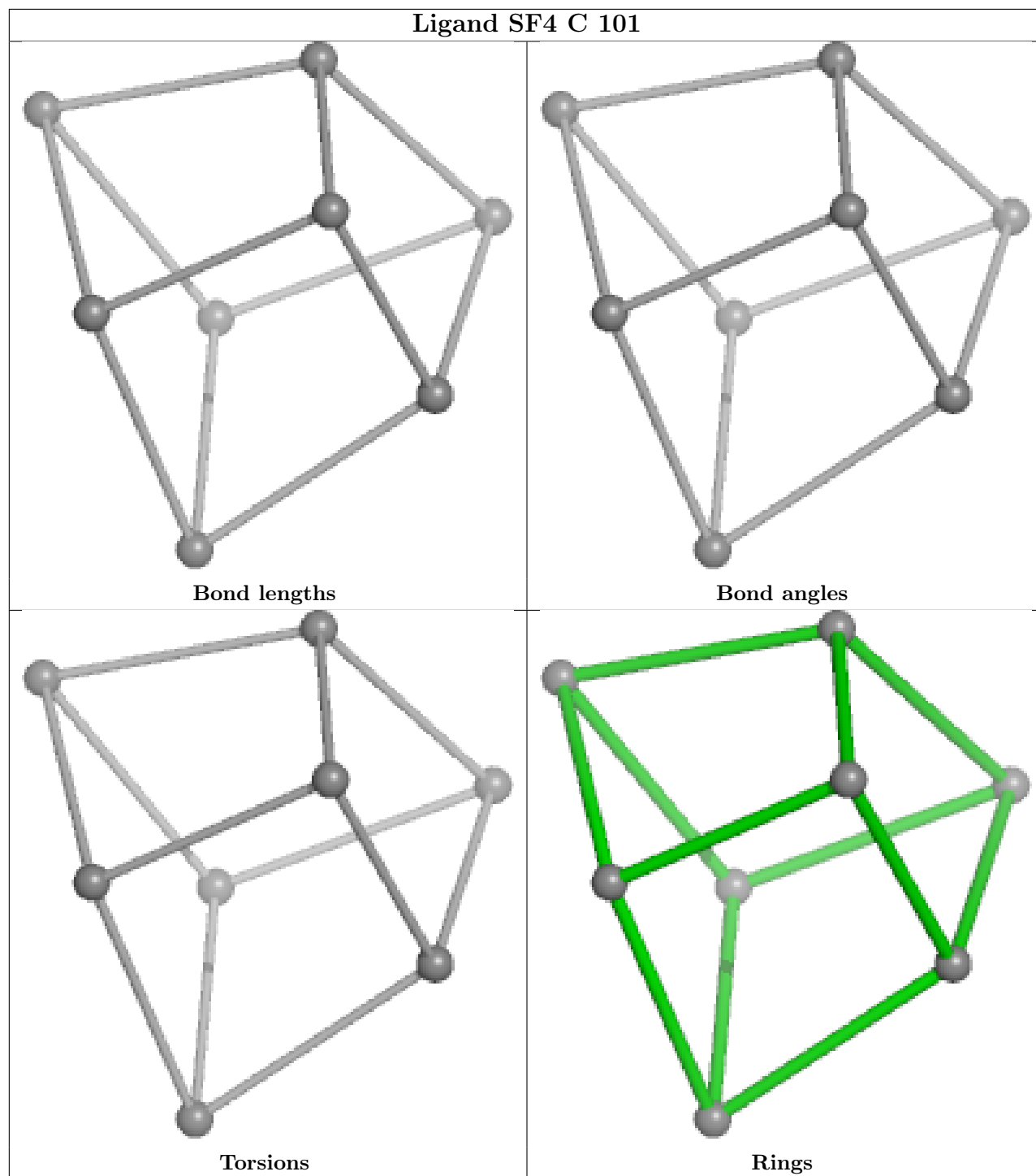


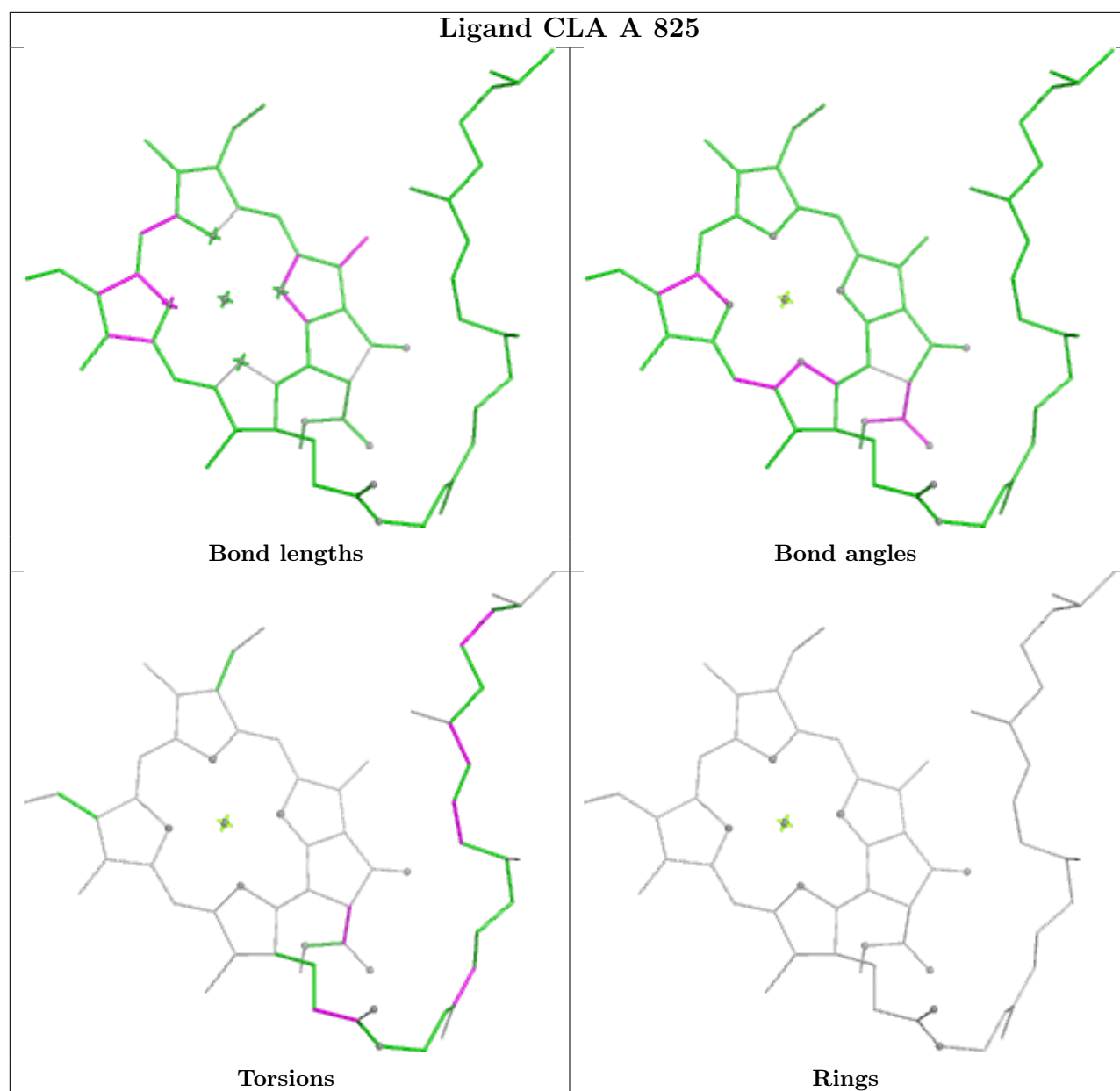
Torsions

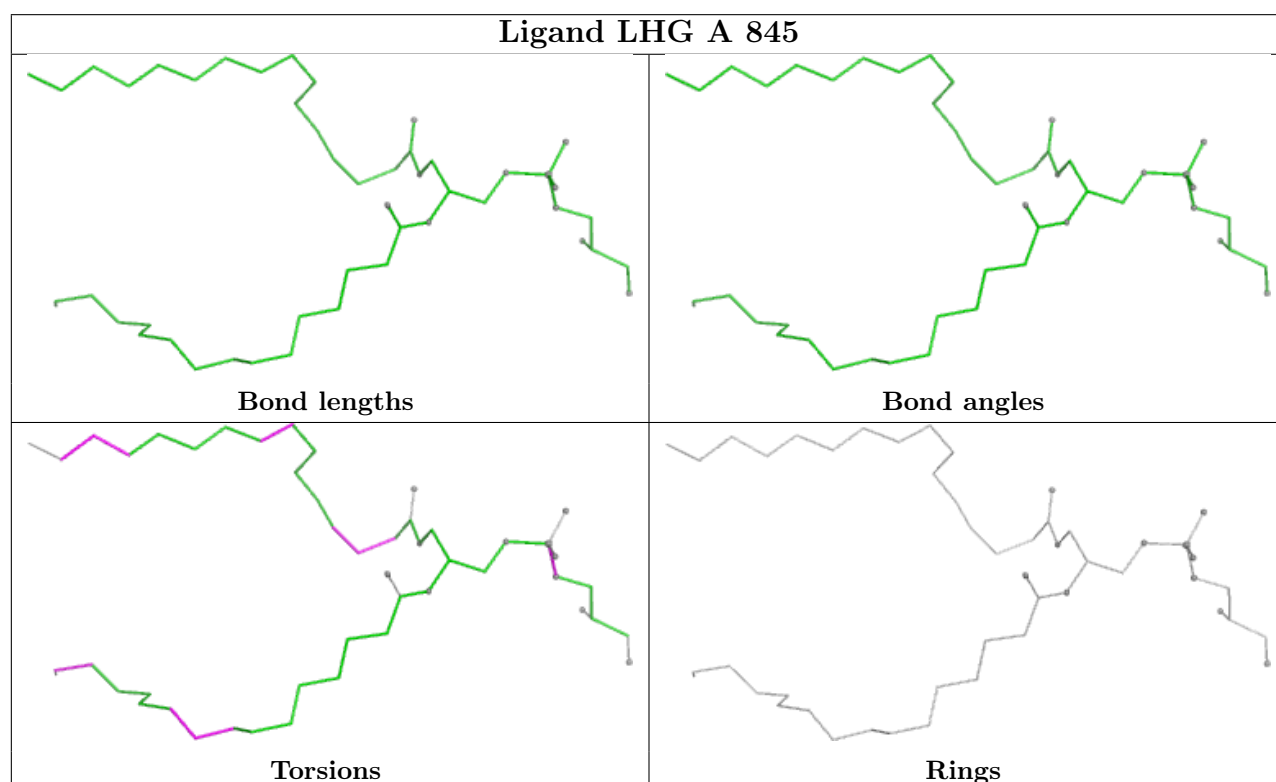
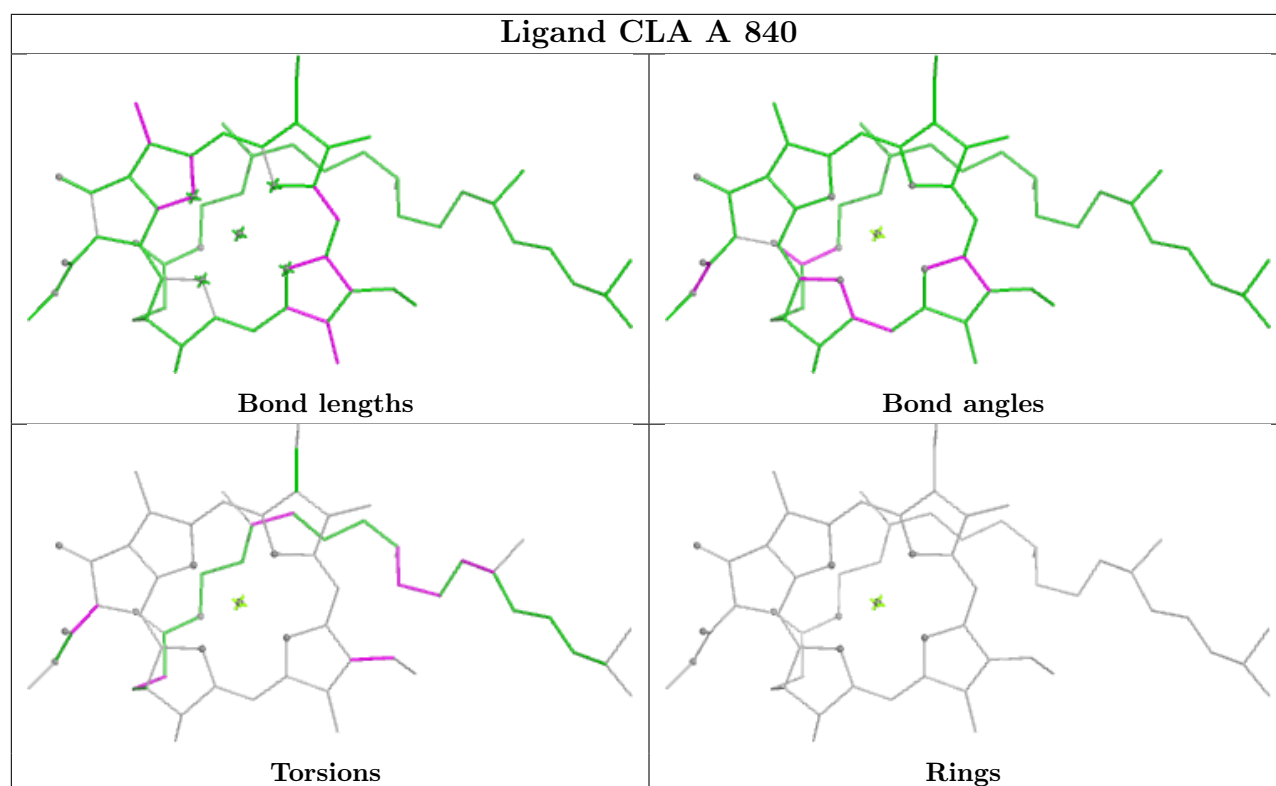


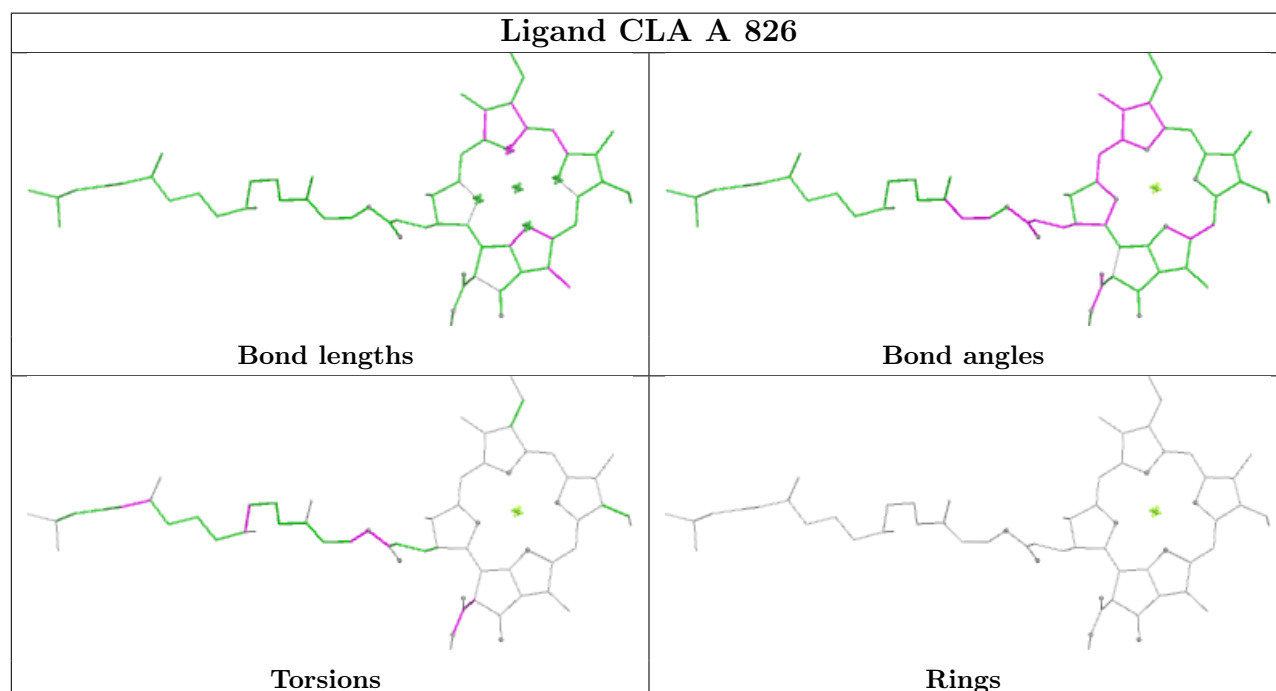
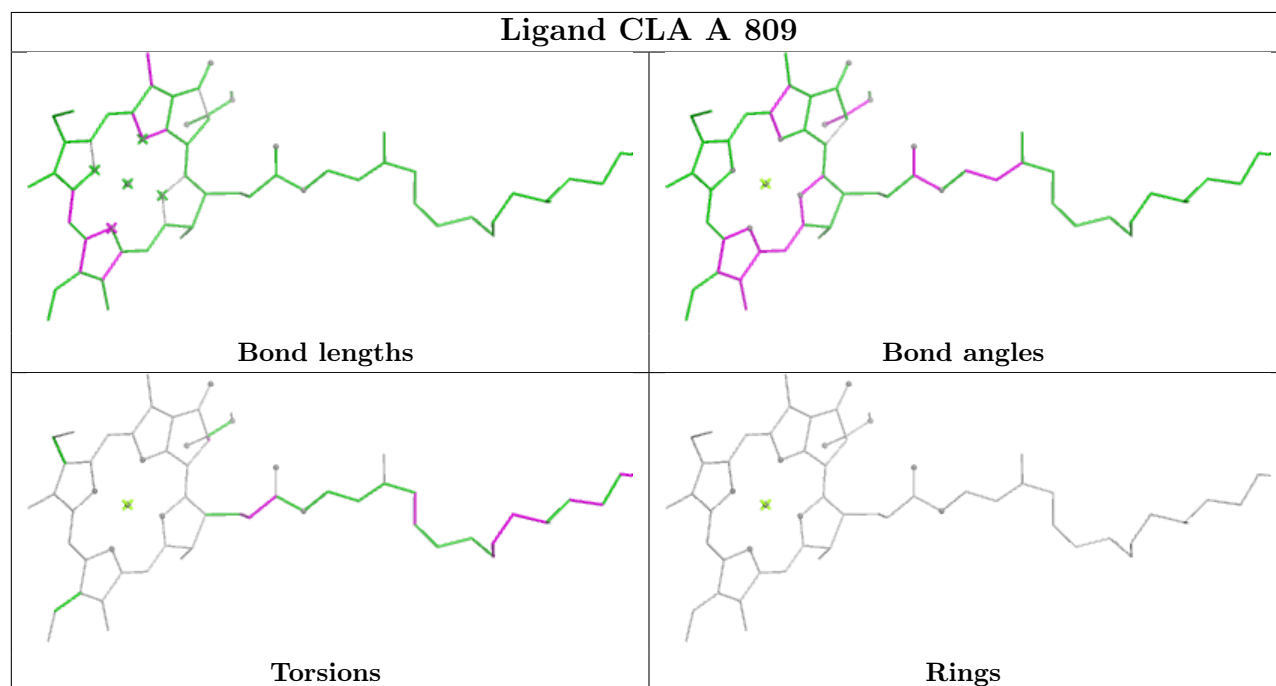
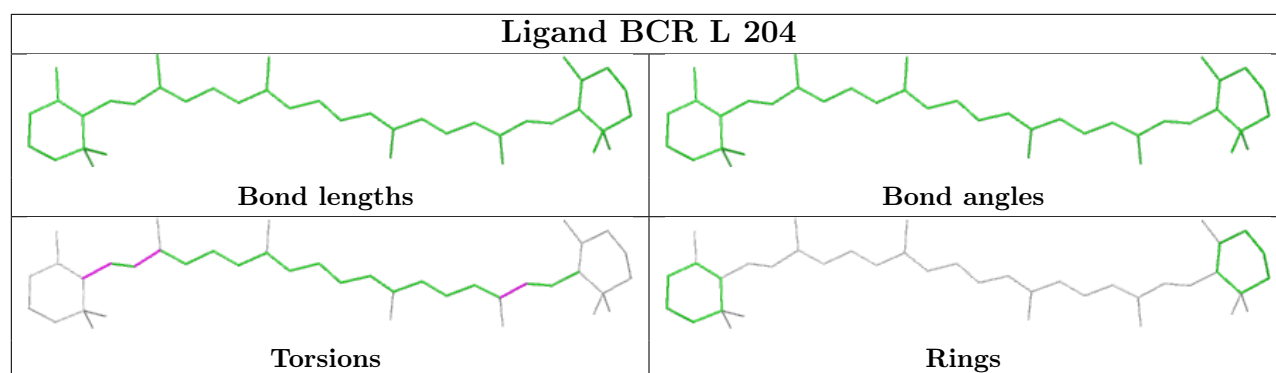
Rings

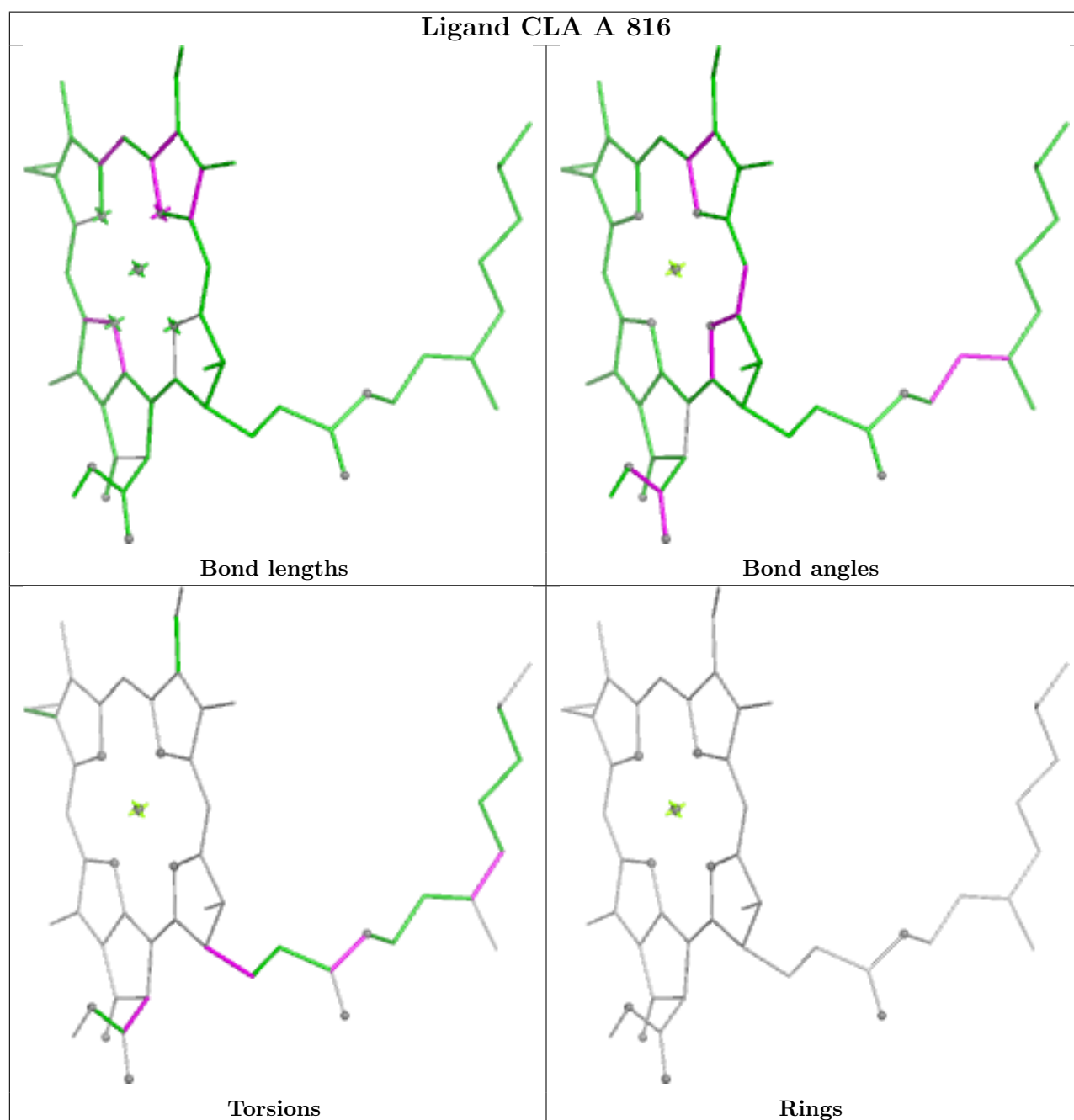
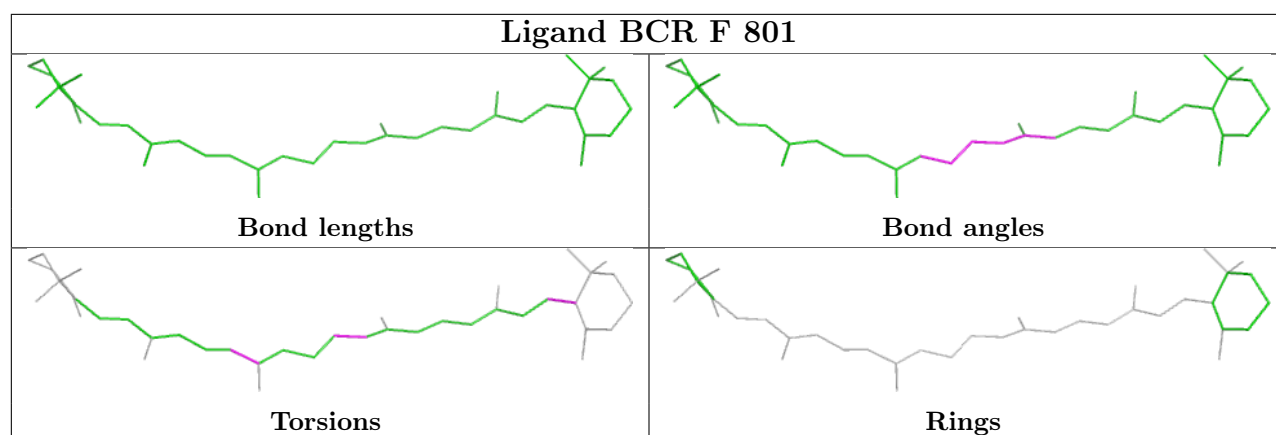


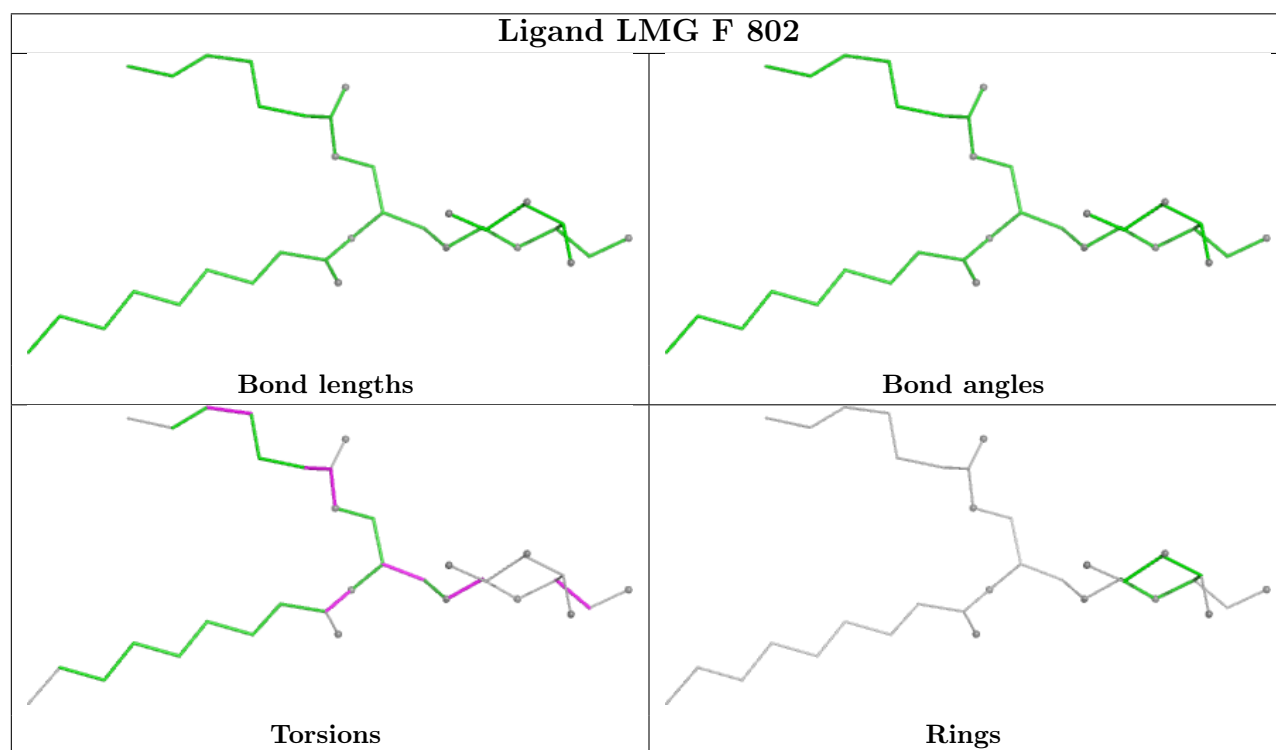
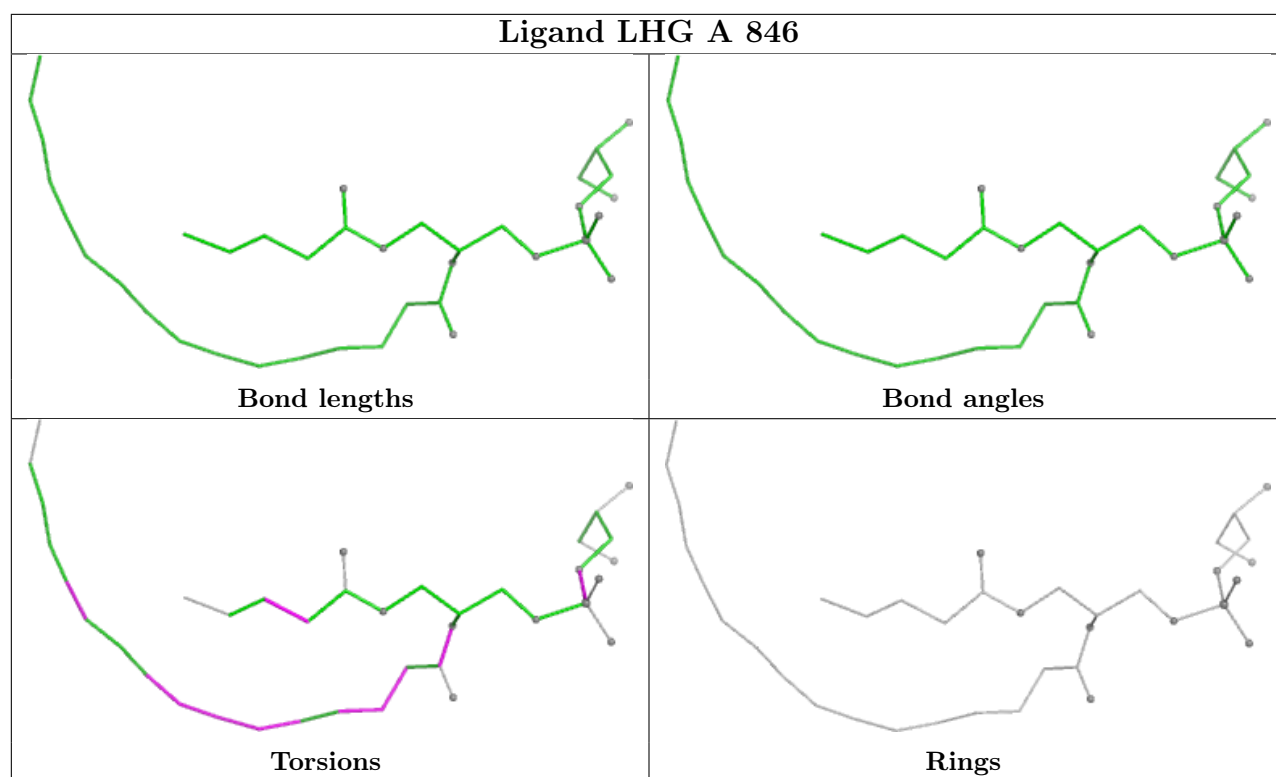


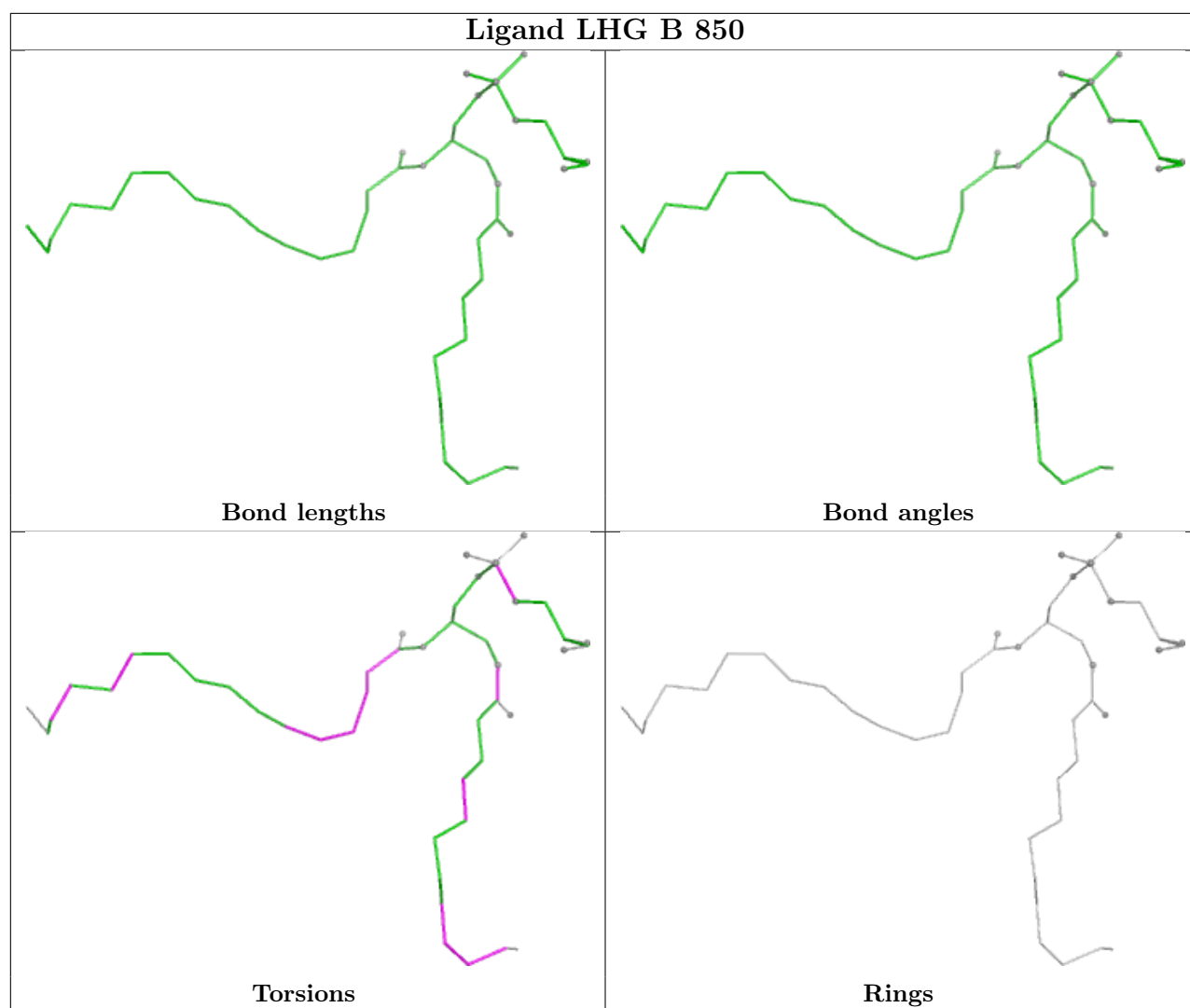


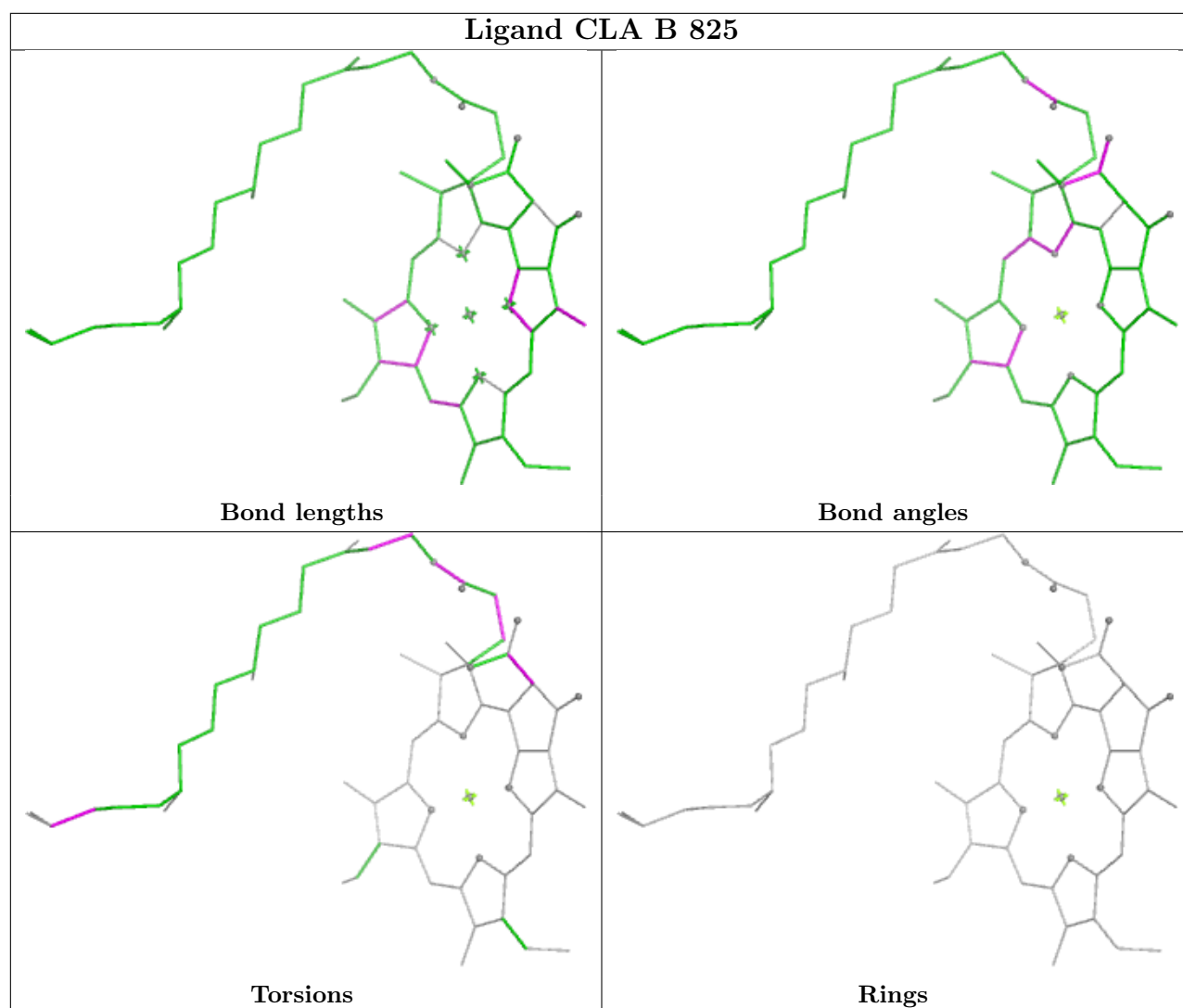


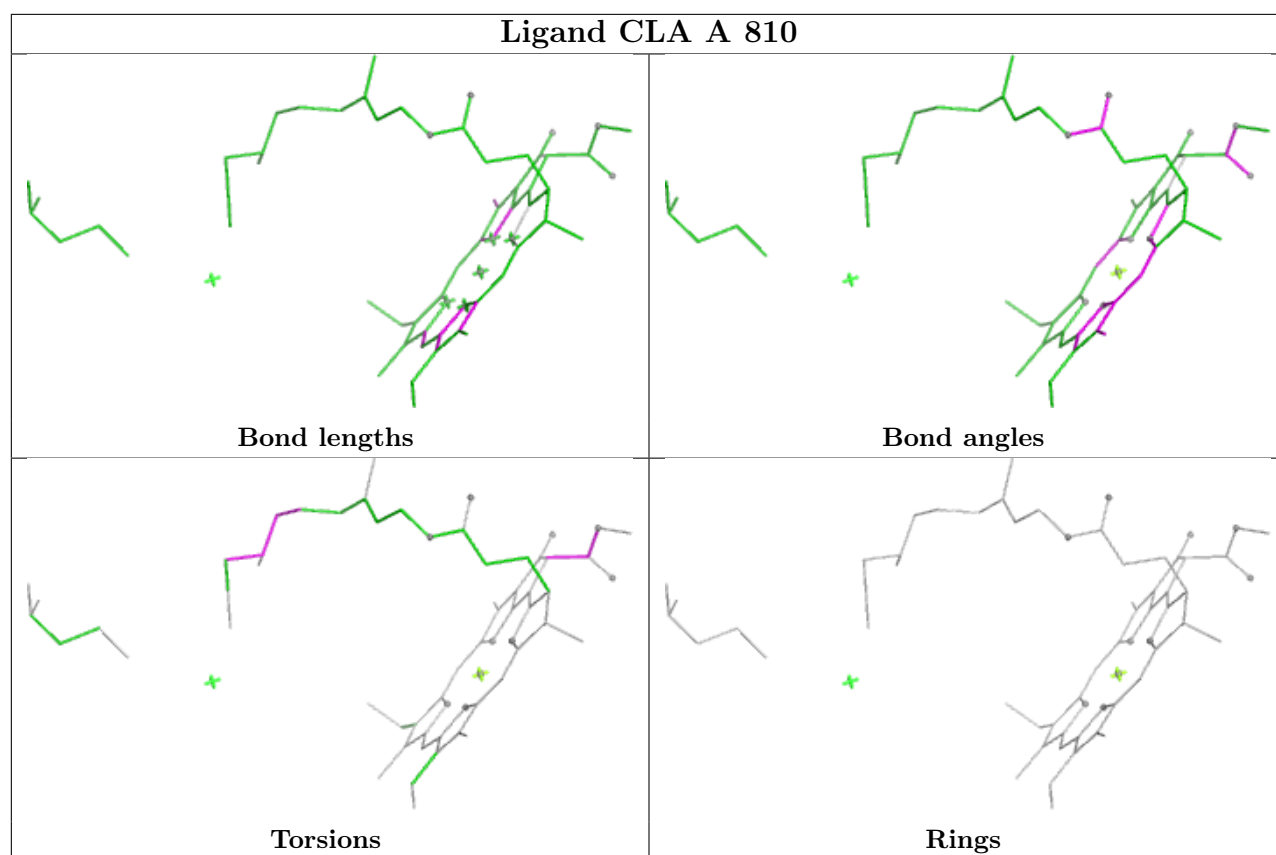




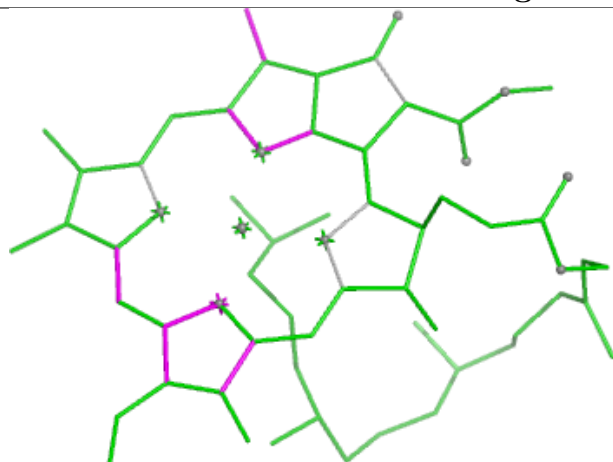




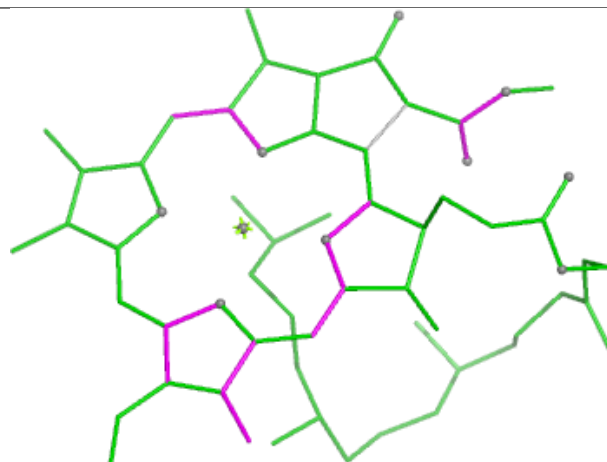




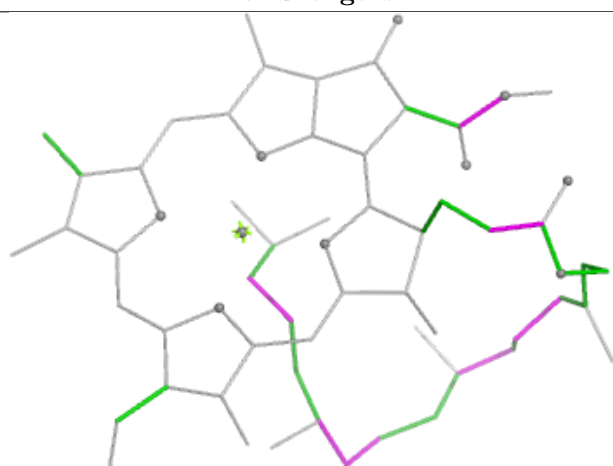
Ligand CLA B 807



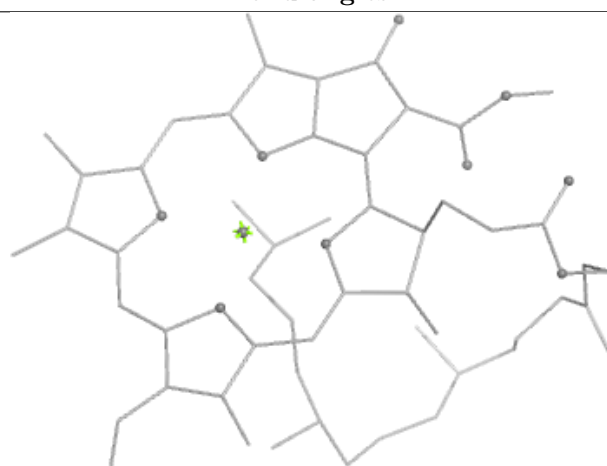
Bond lengths



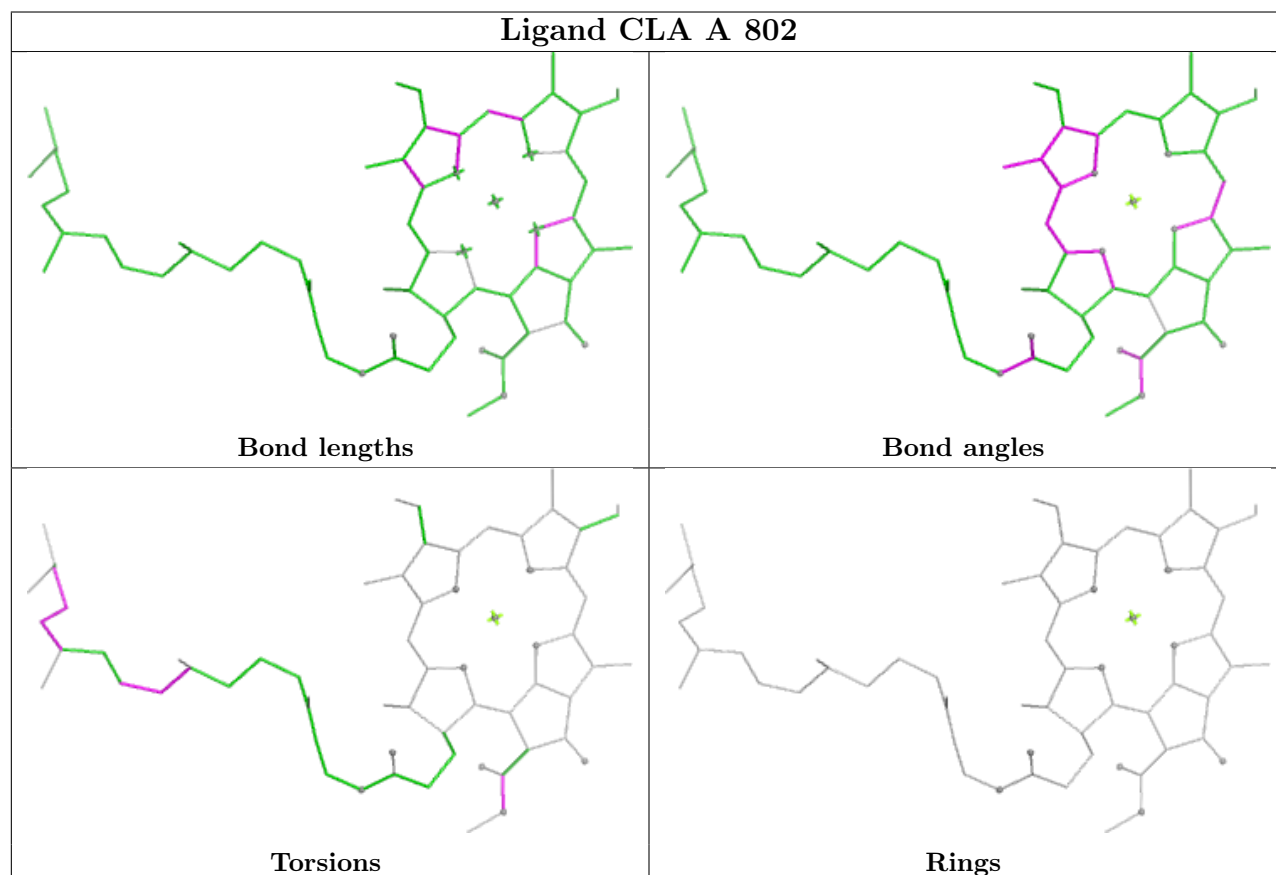
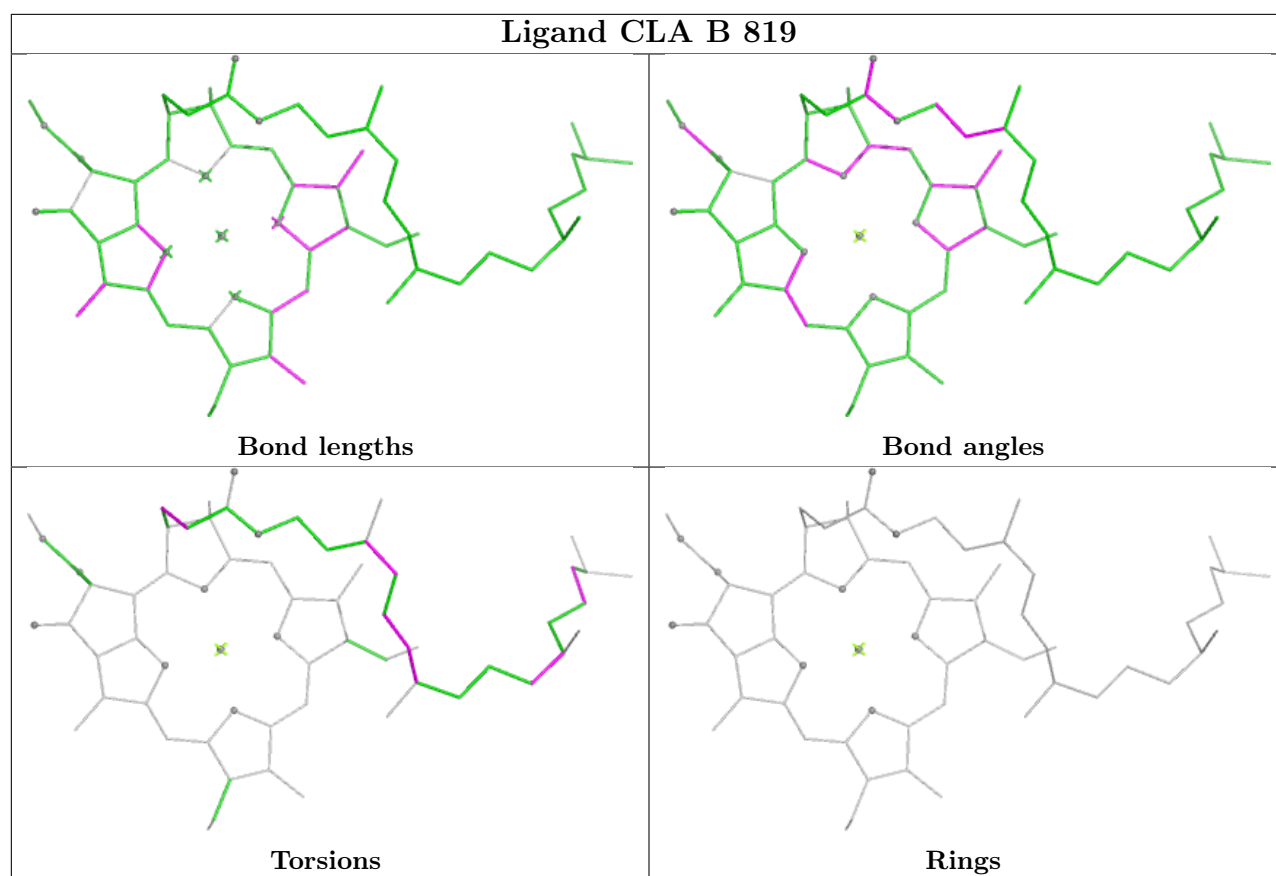
Bond angles

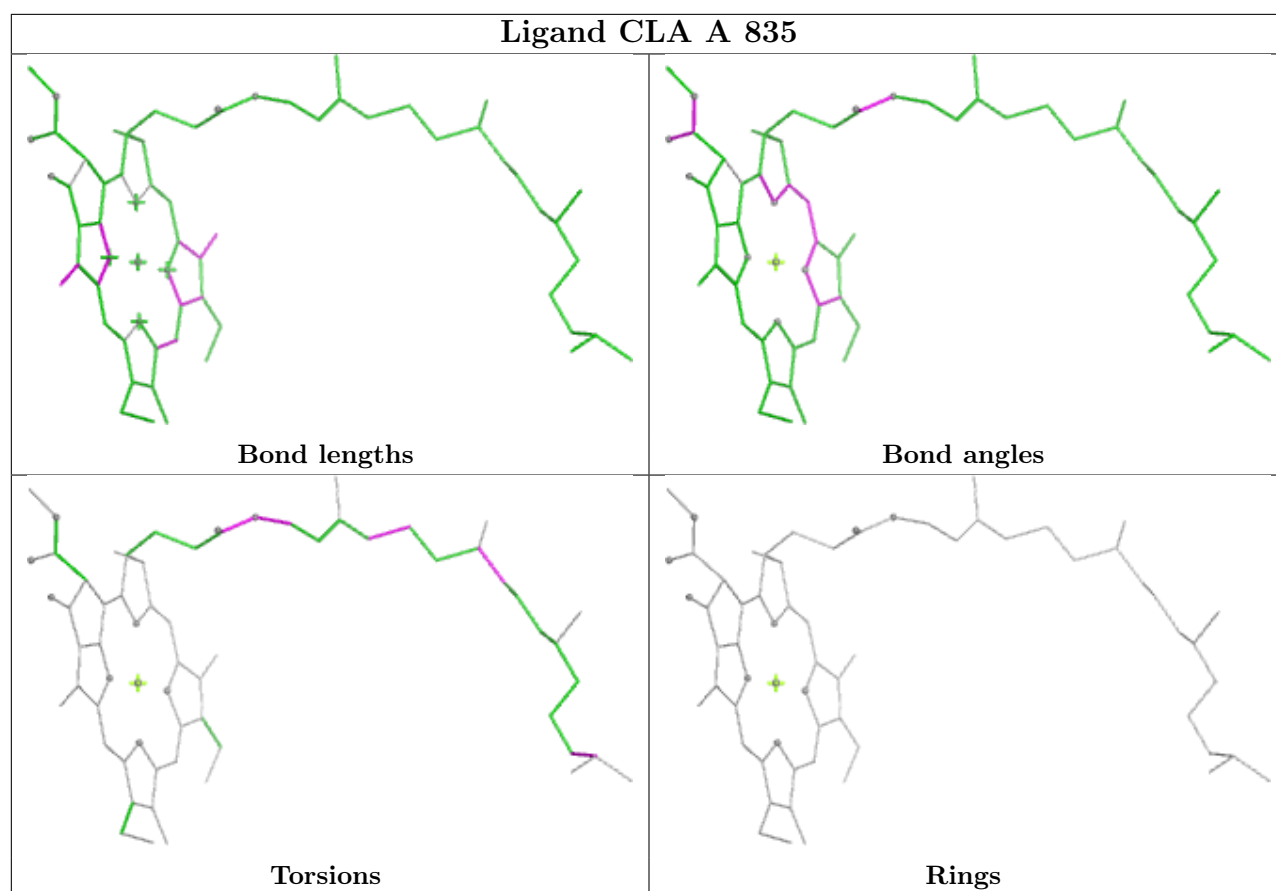


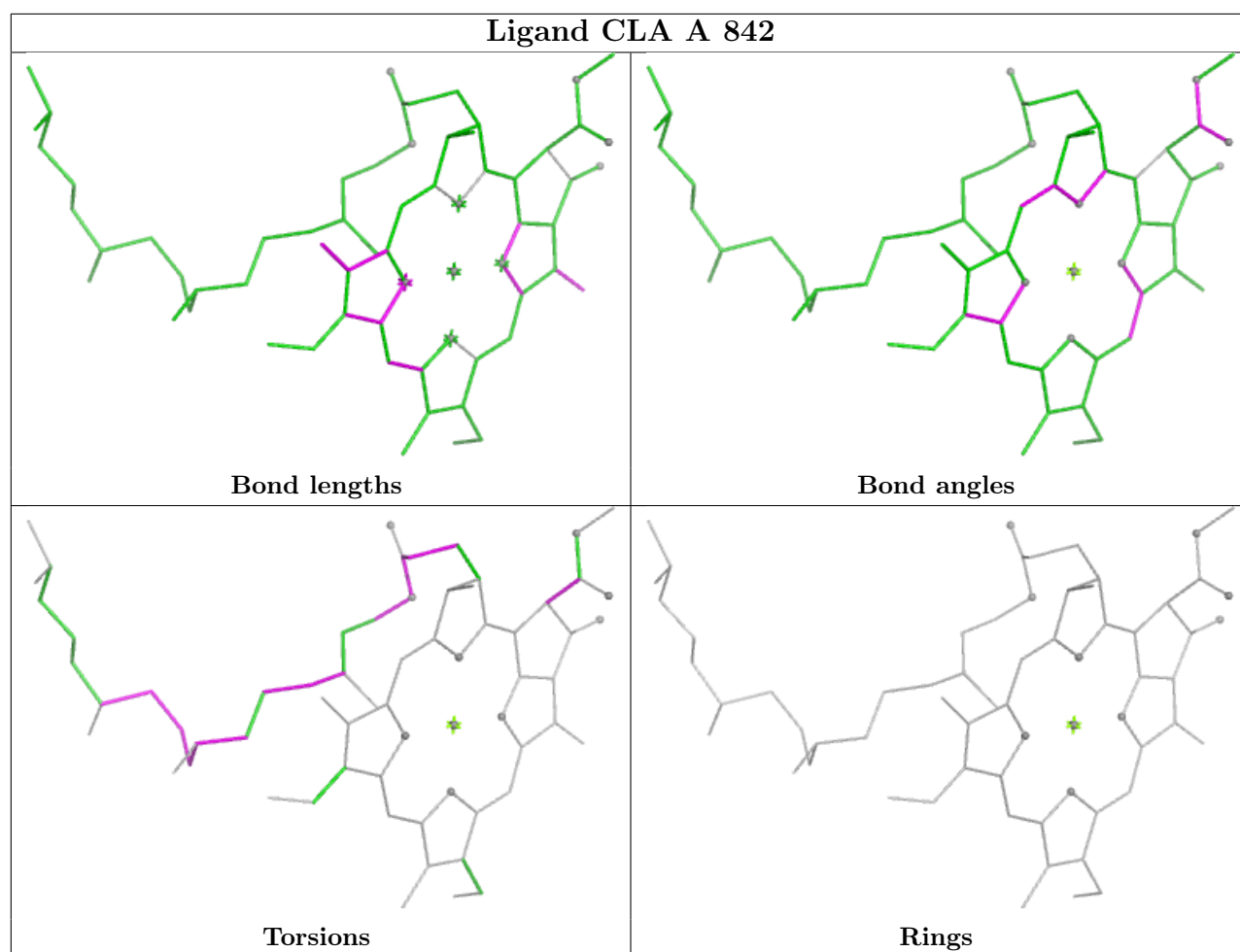
Torsions

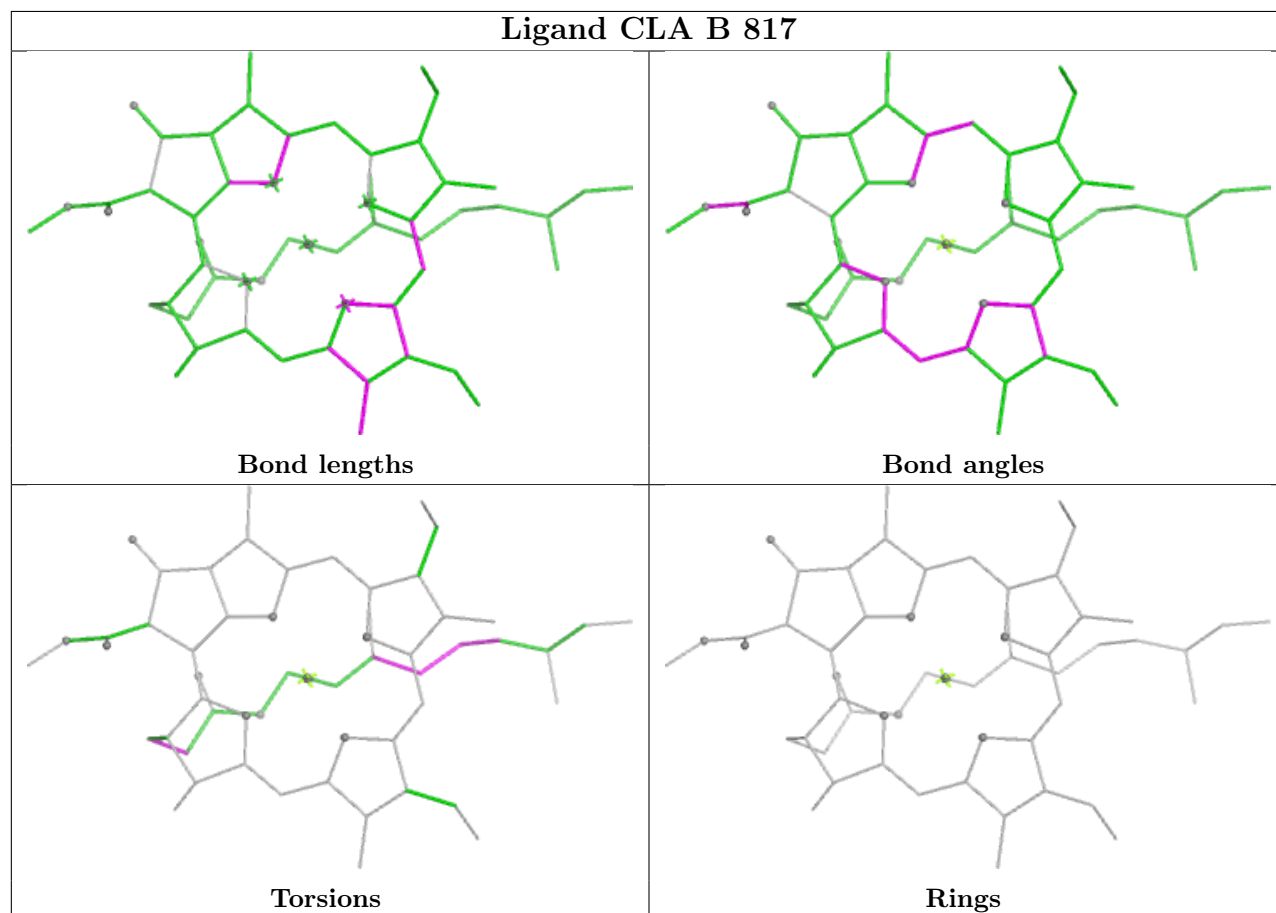
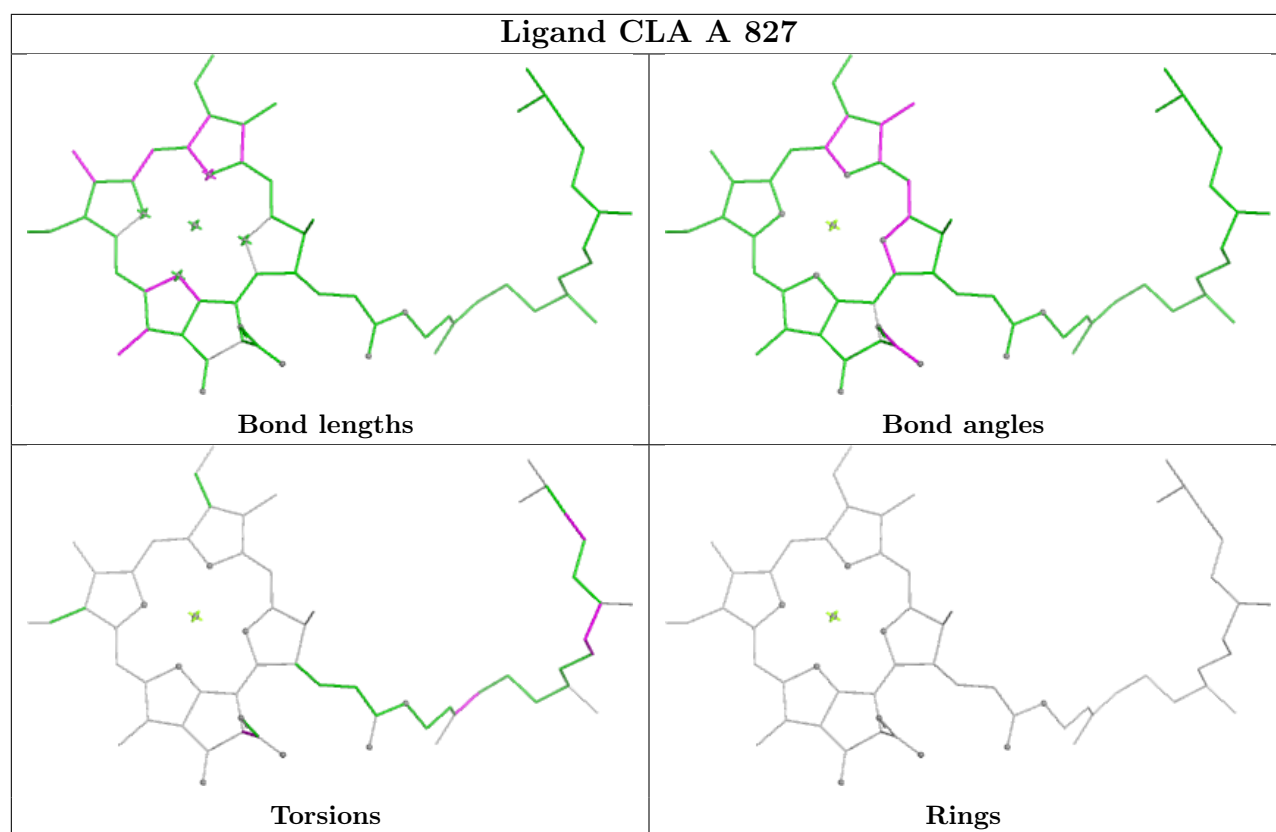


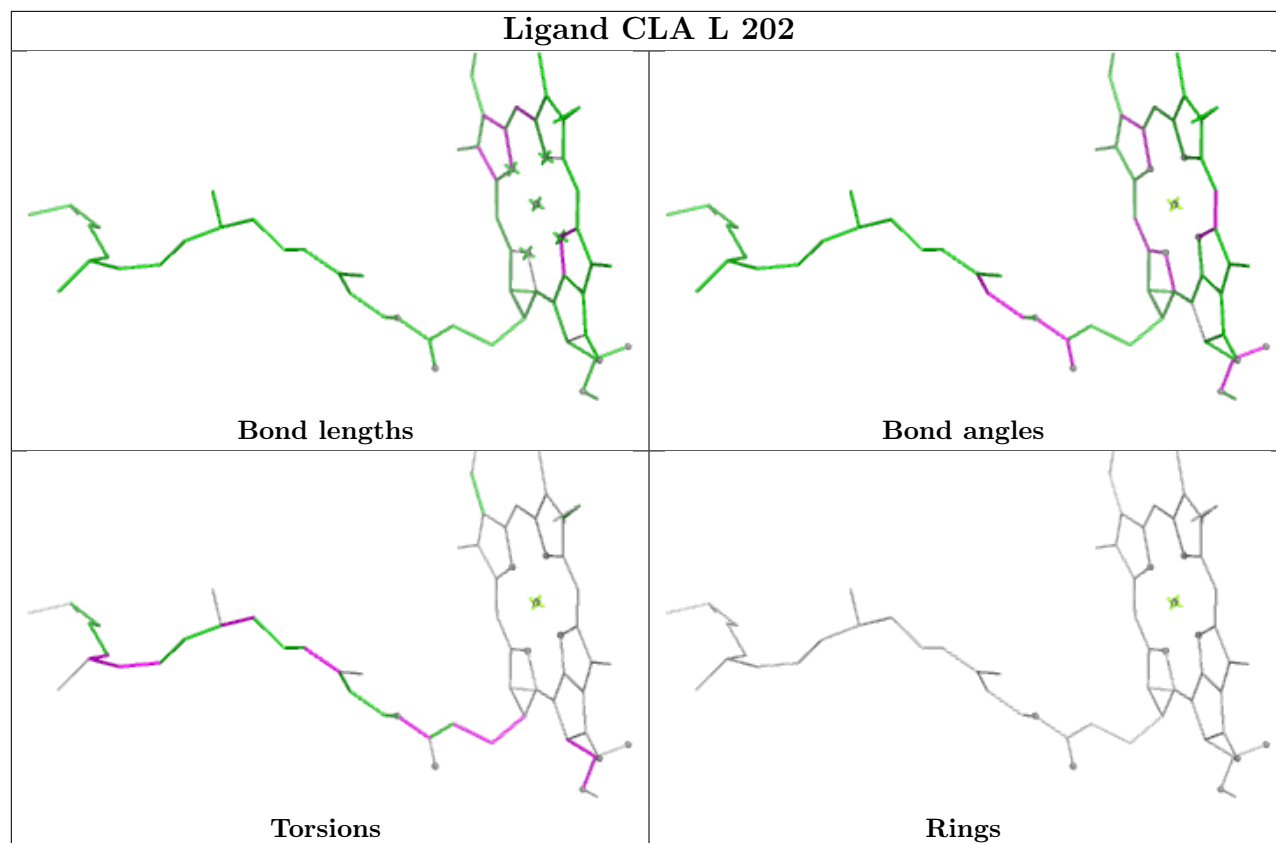
Rings



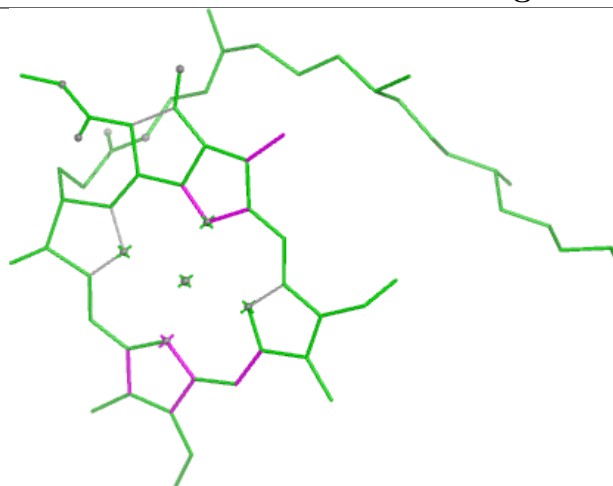




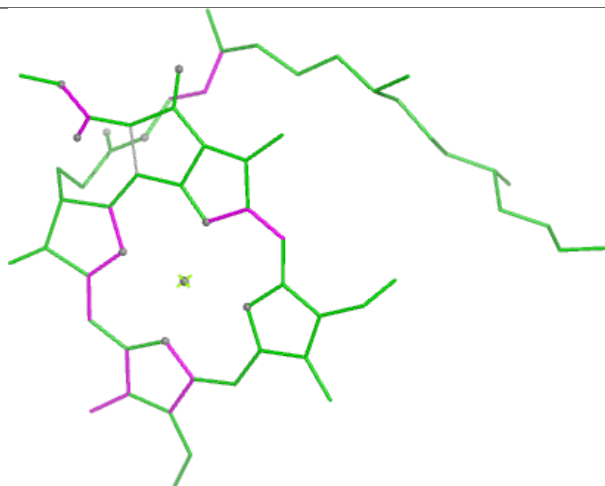




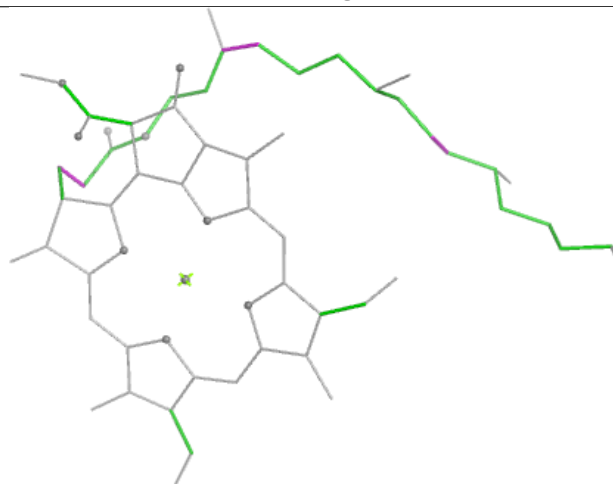
Ligand CLA A 829



Bond lengths



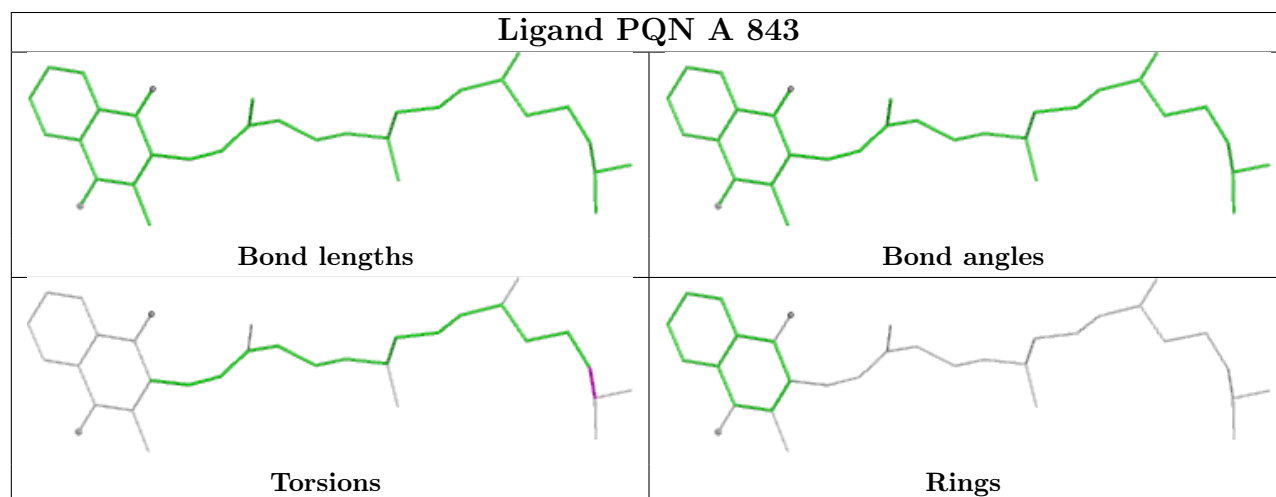
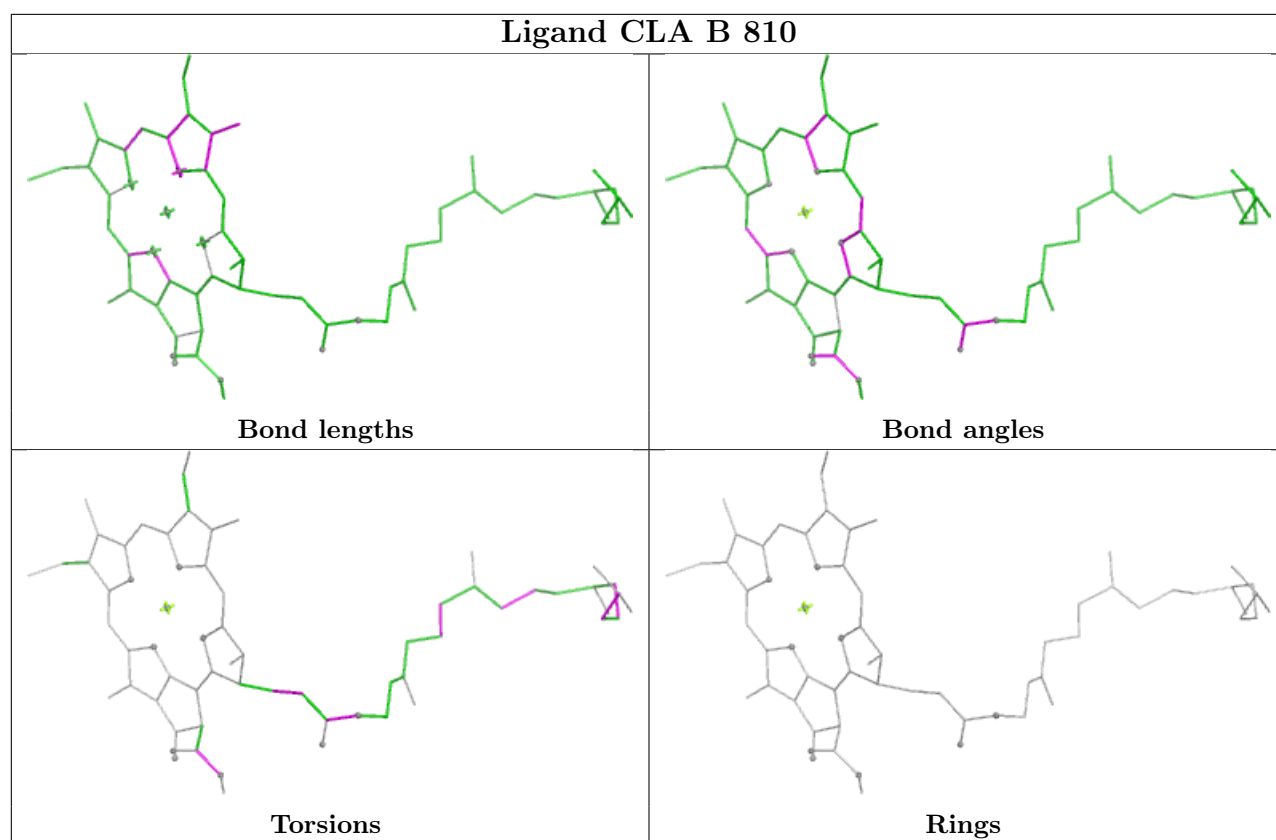
Bond angles

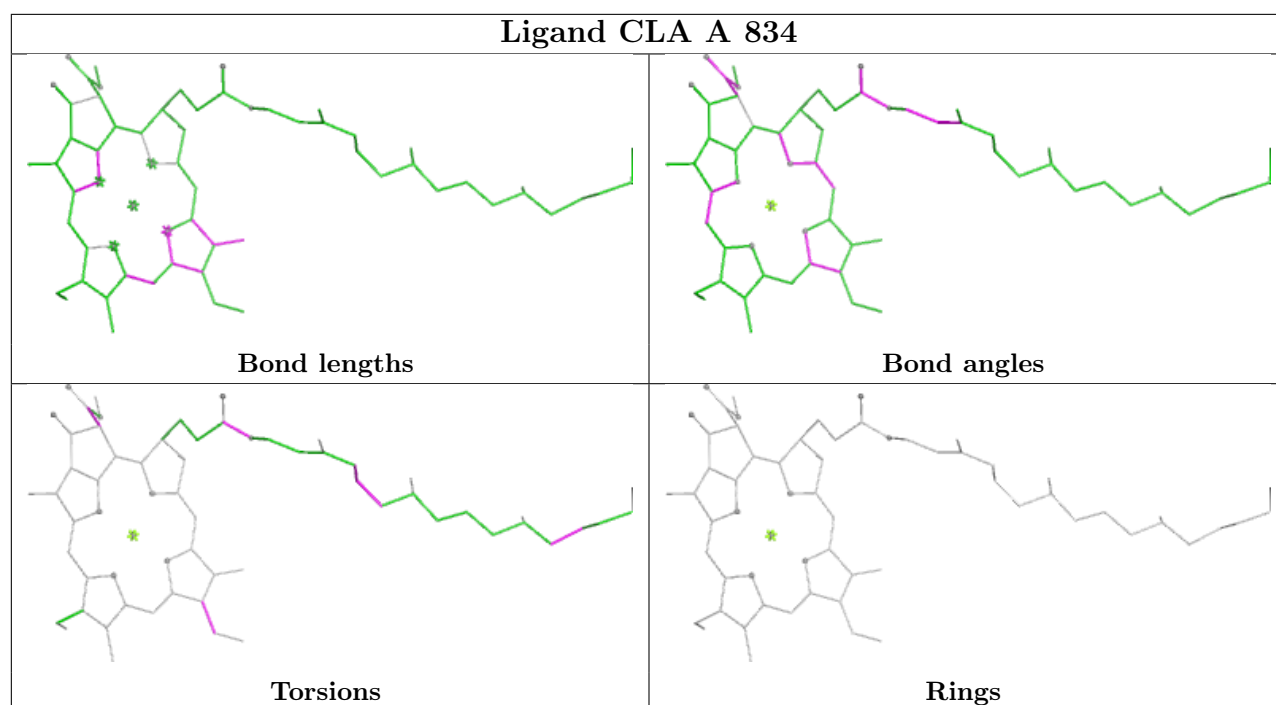


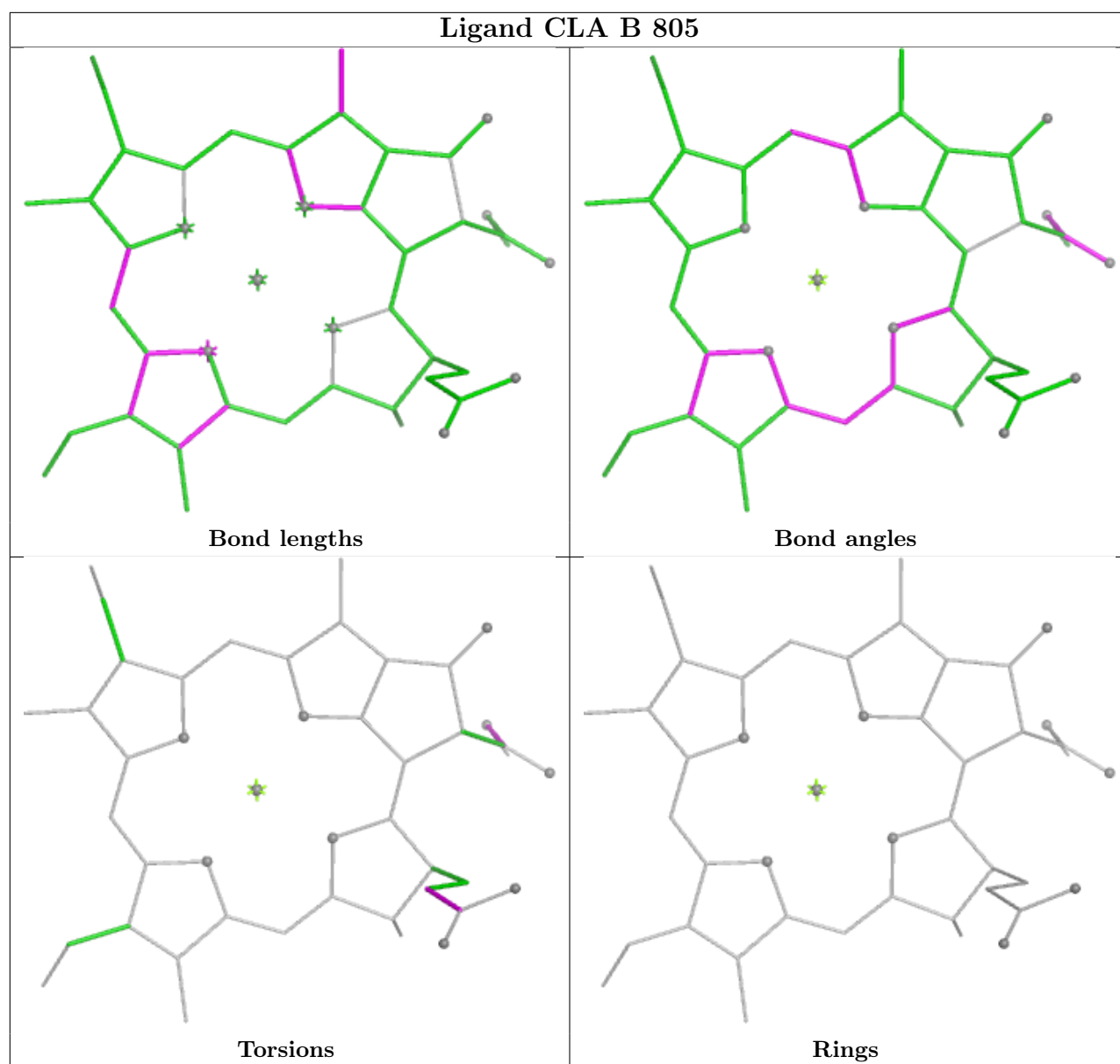
Torsions

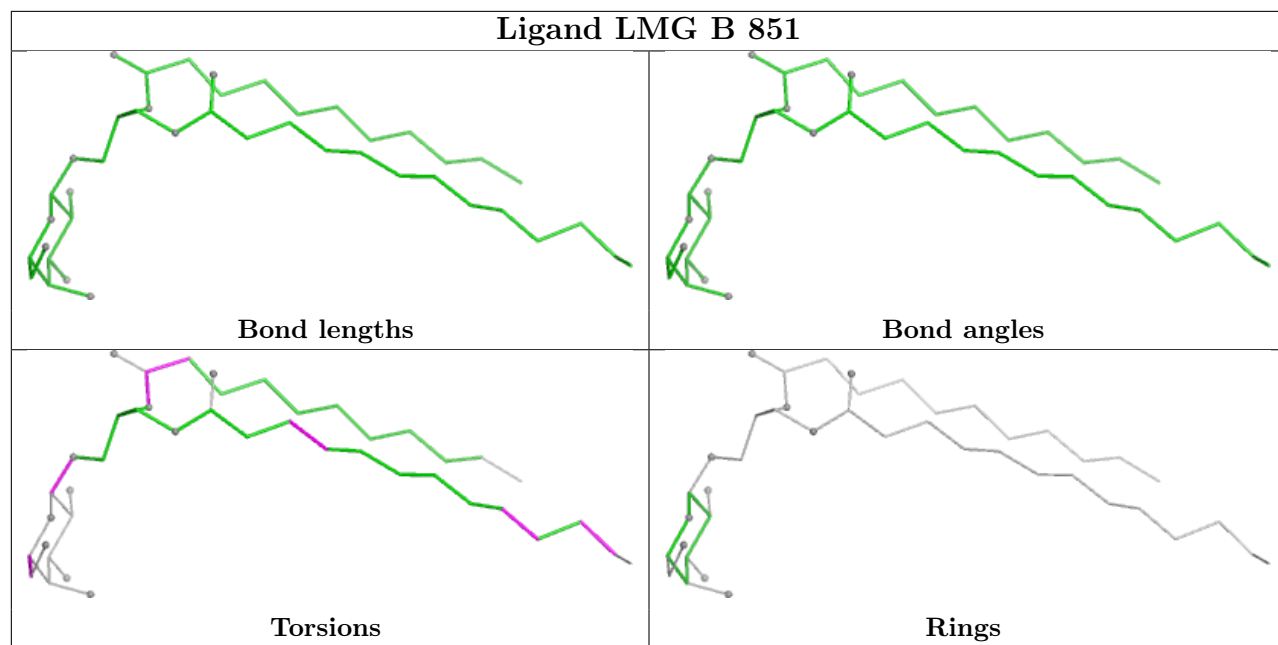


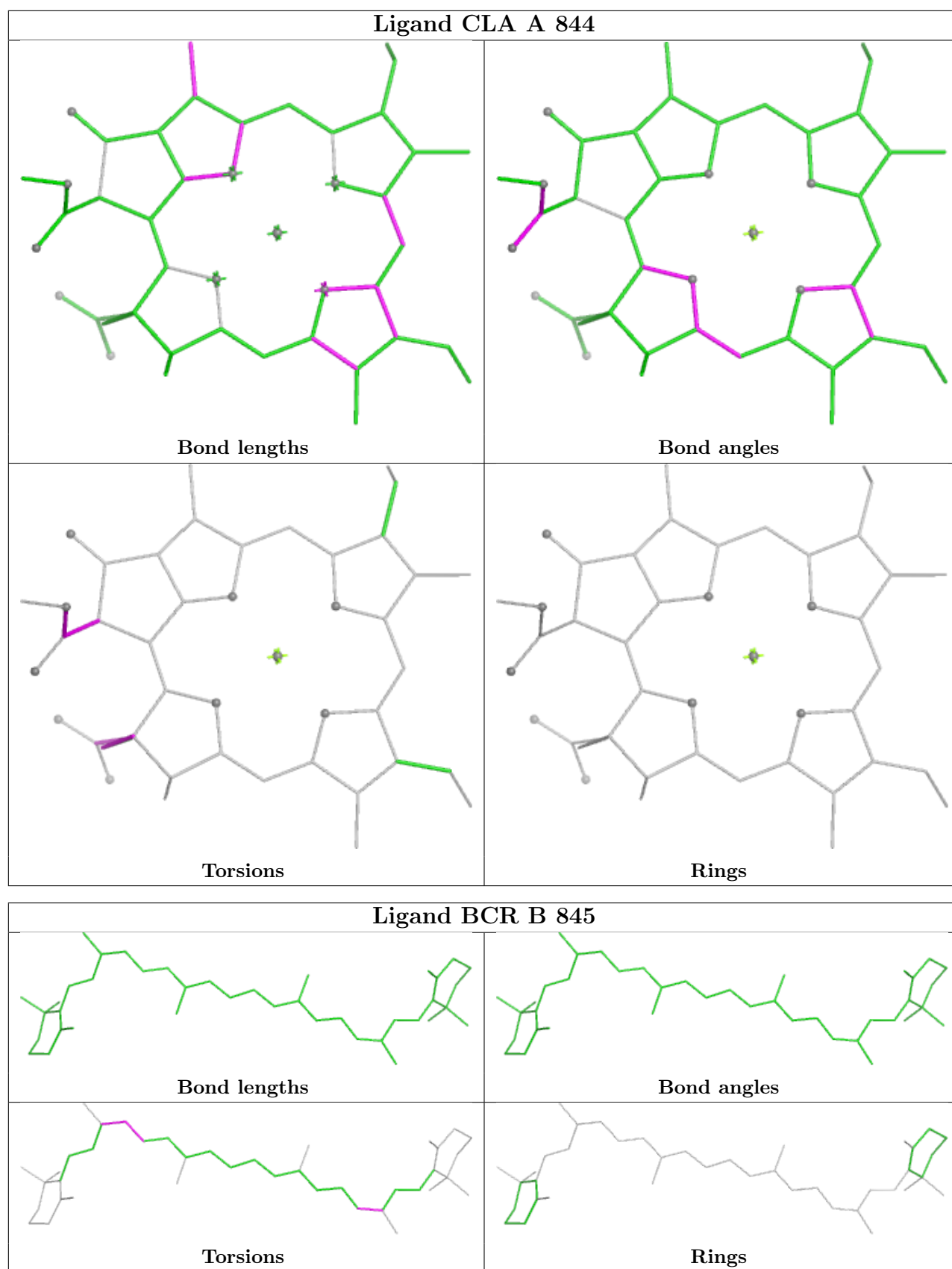
Rings

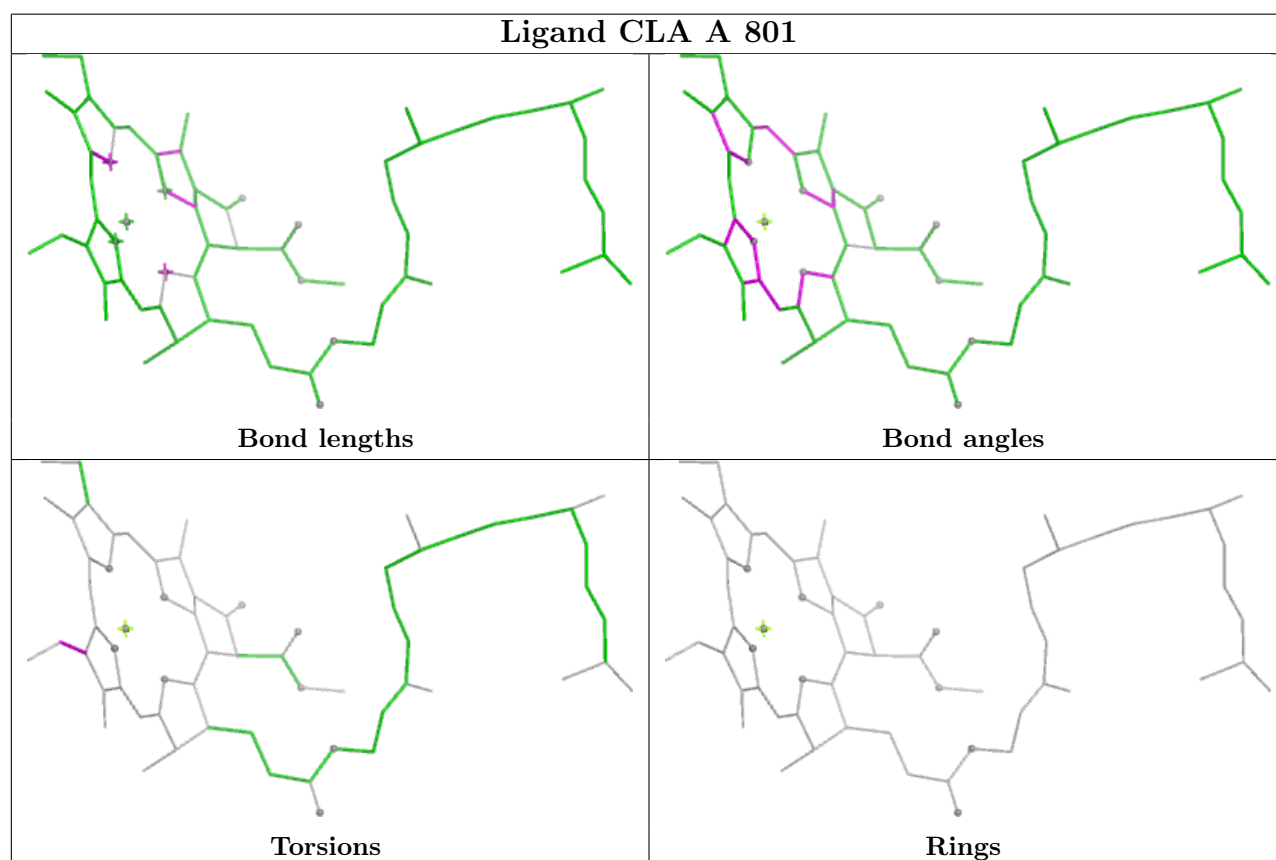
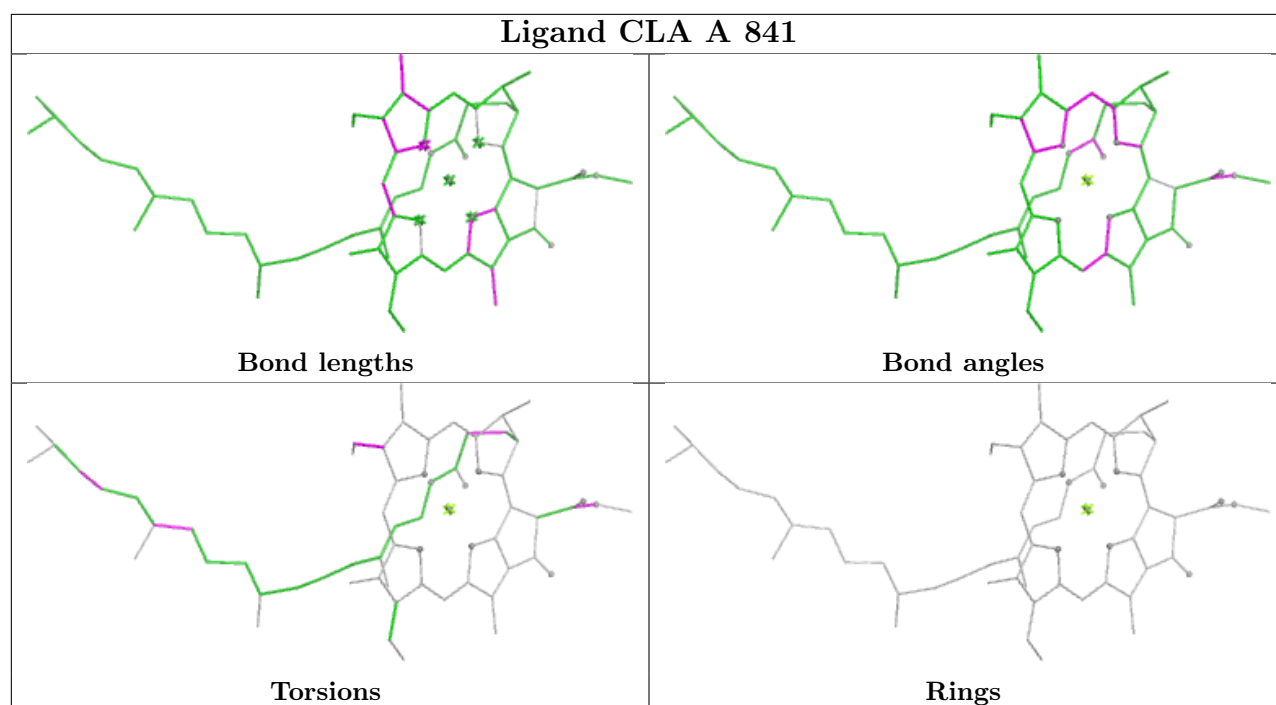


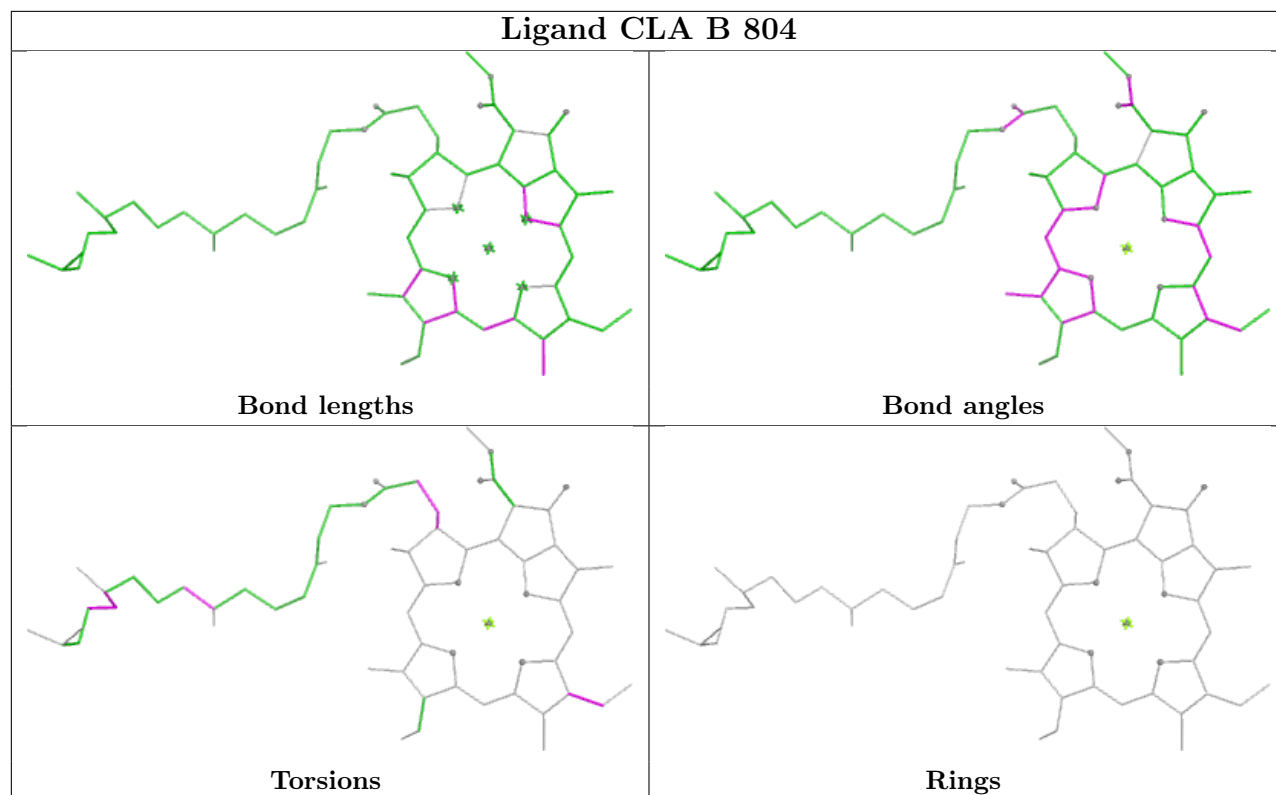




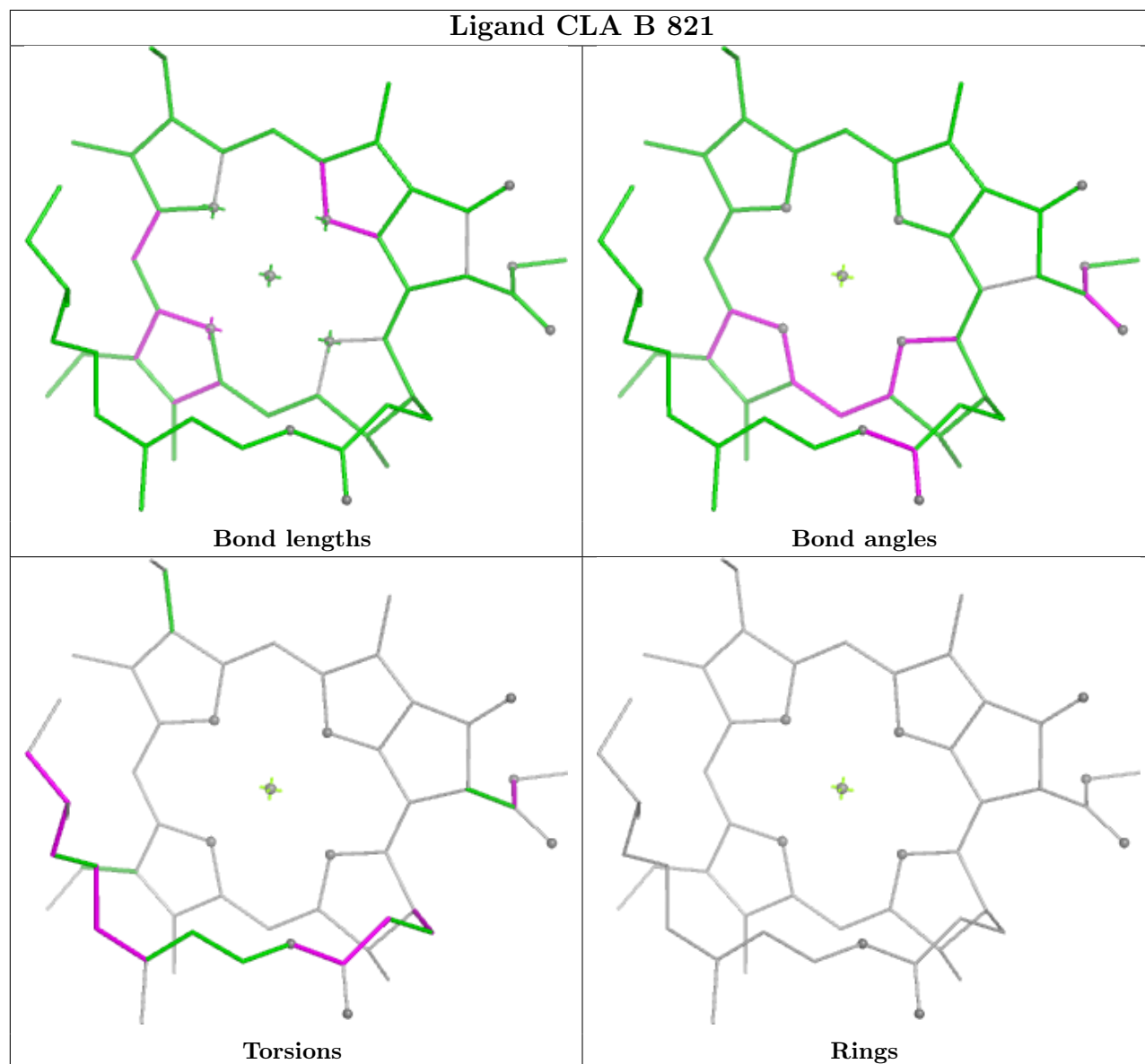


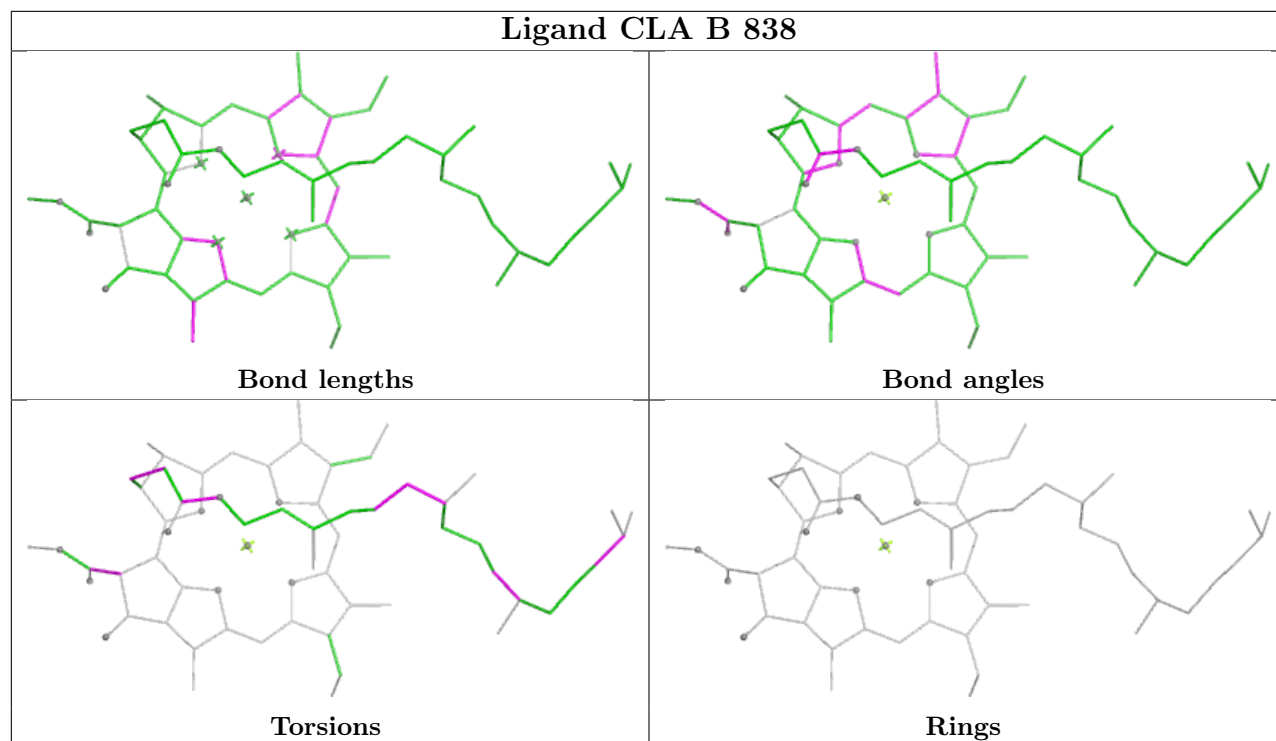
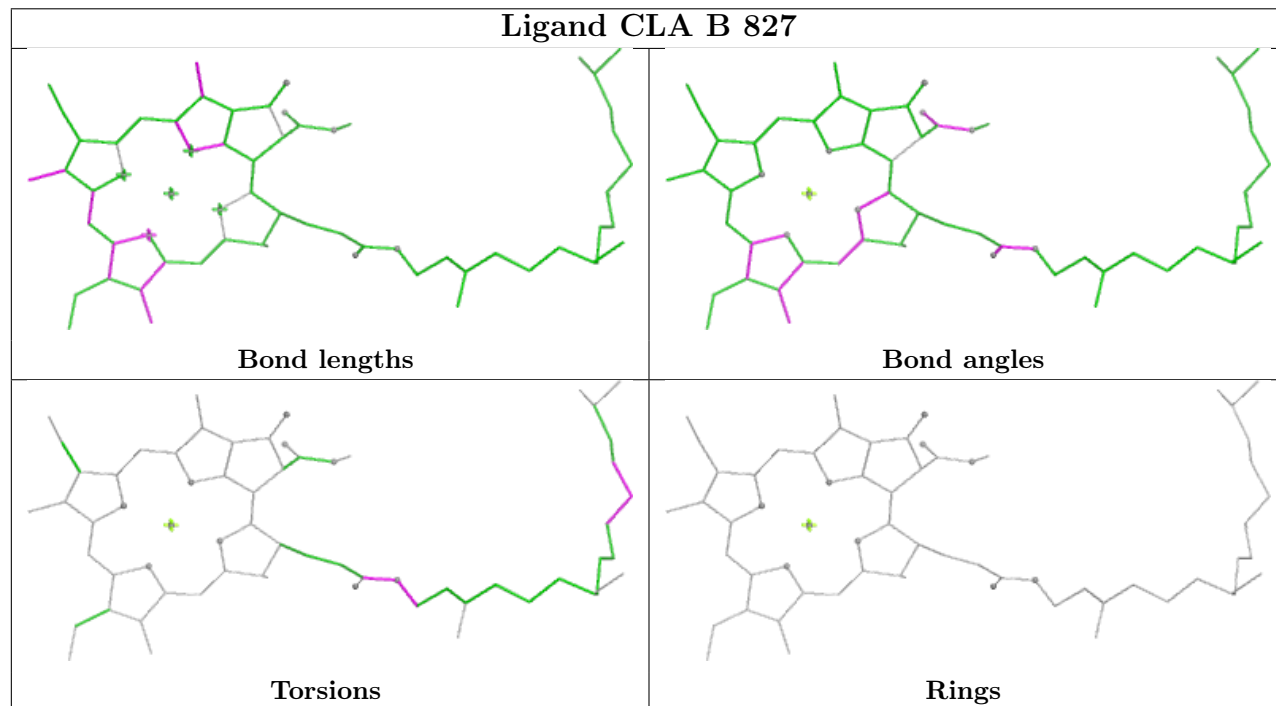


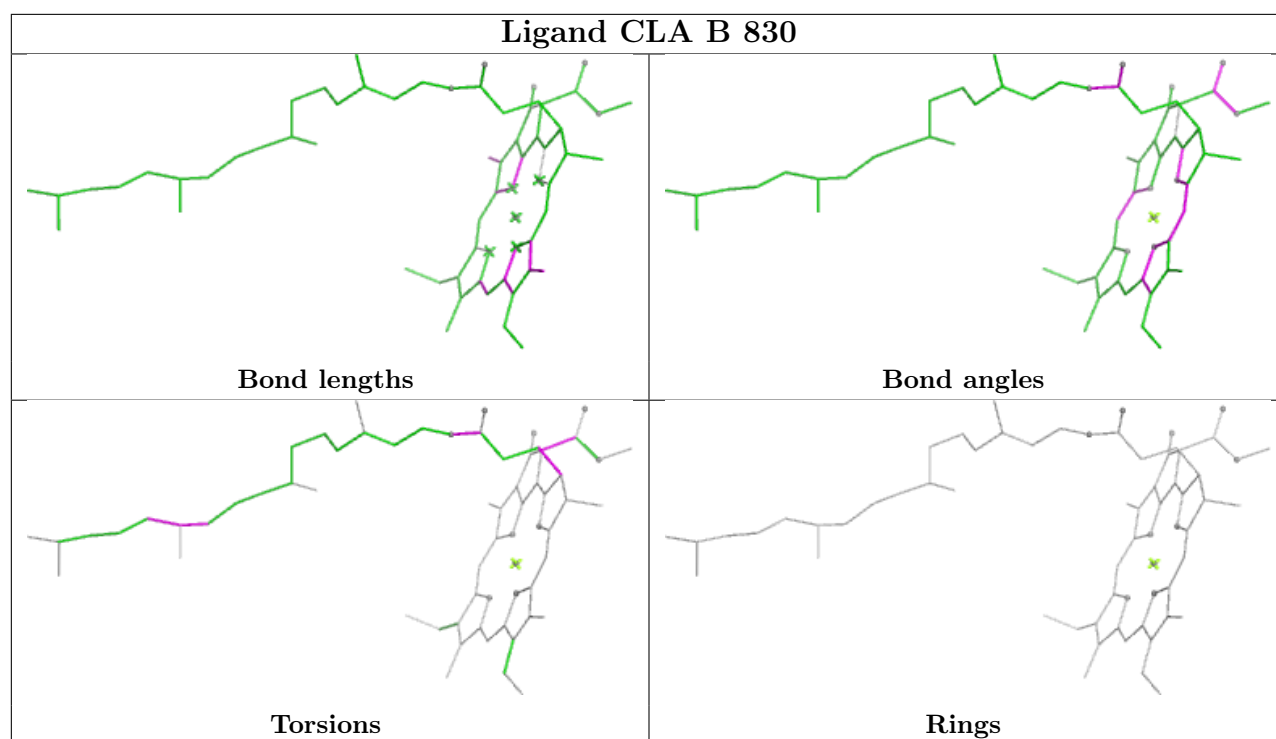


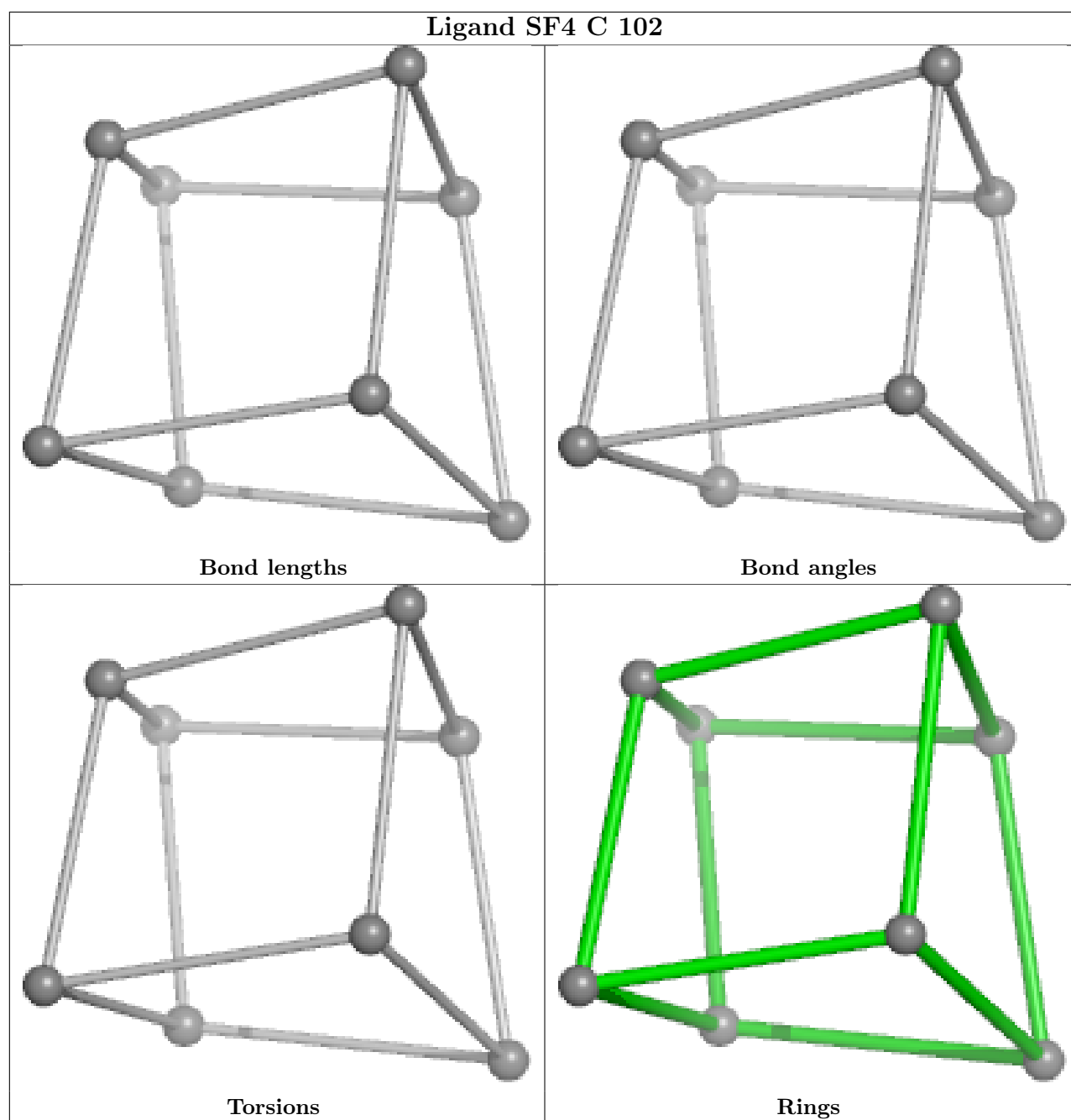


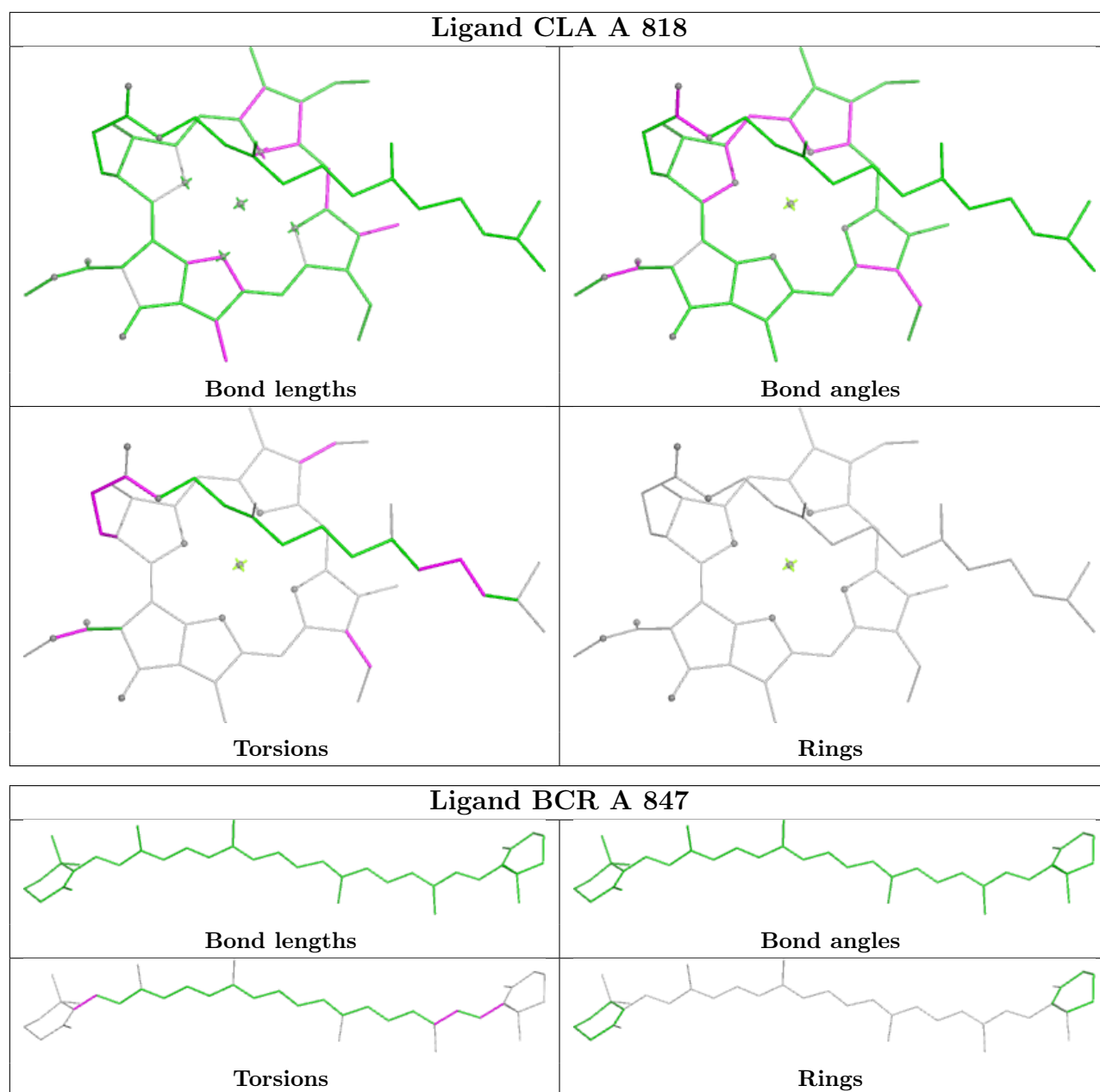
Ligand CLA B 821

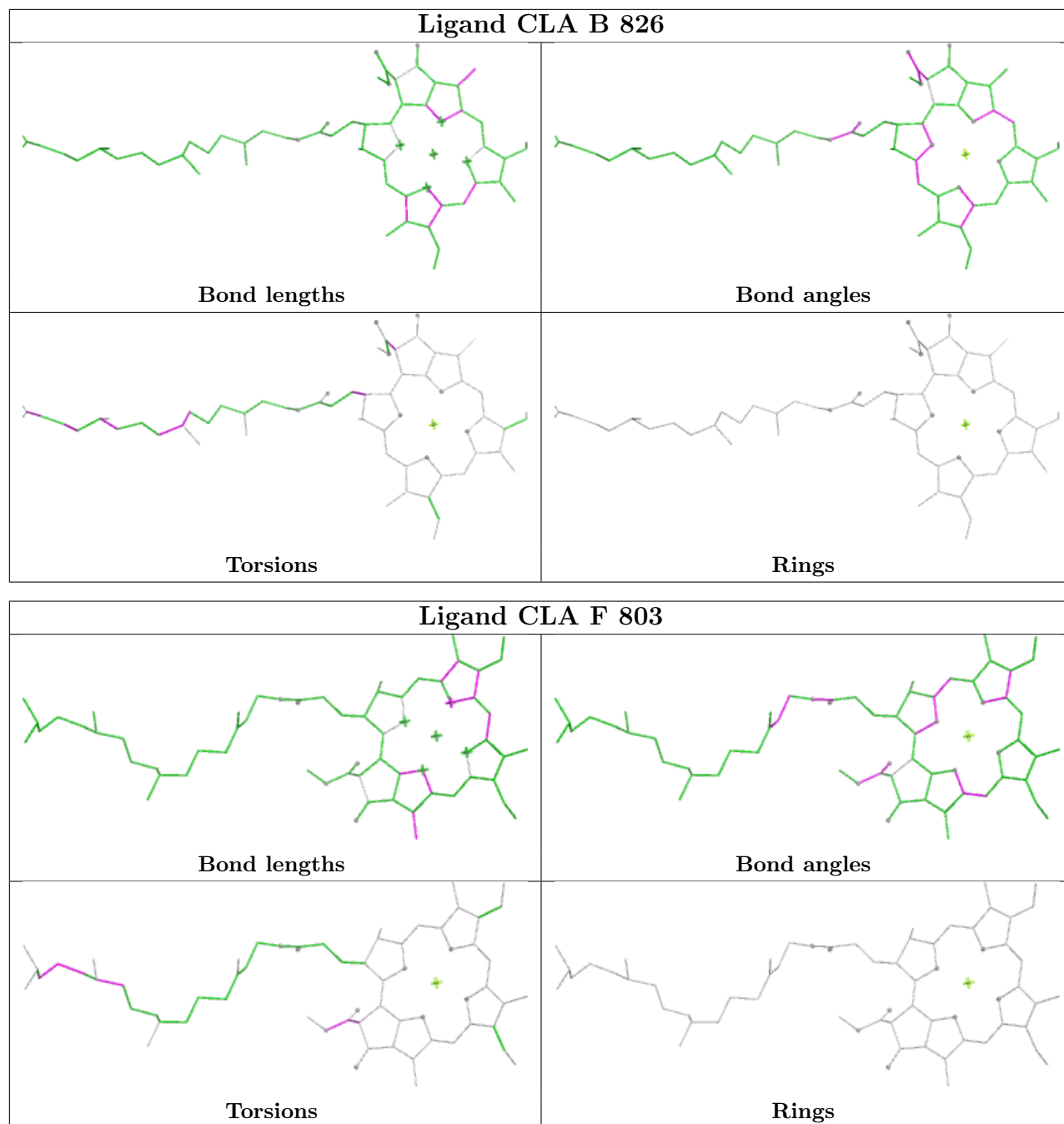


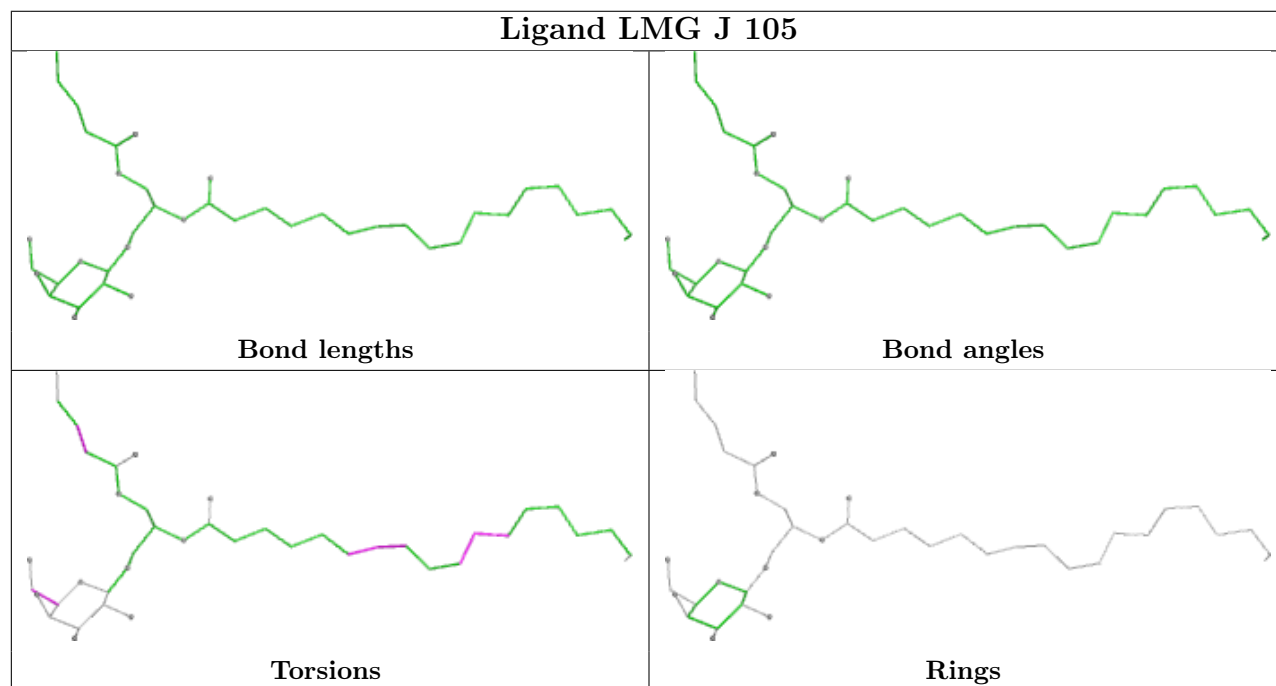
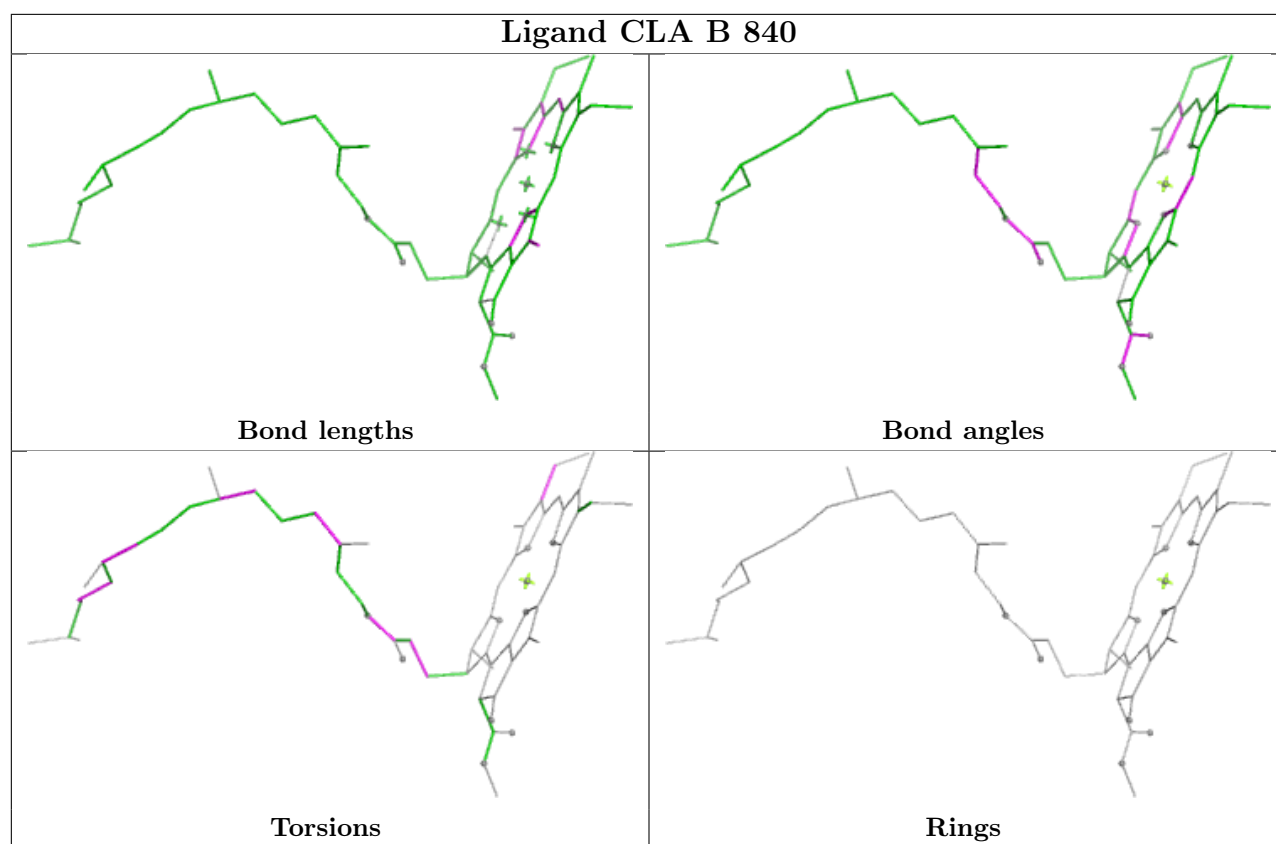
Ligand CLA B 838**Ligand CLA B 827**



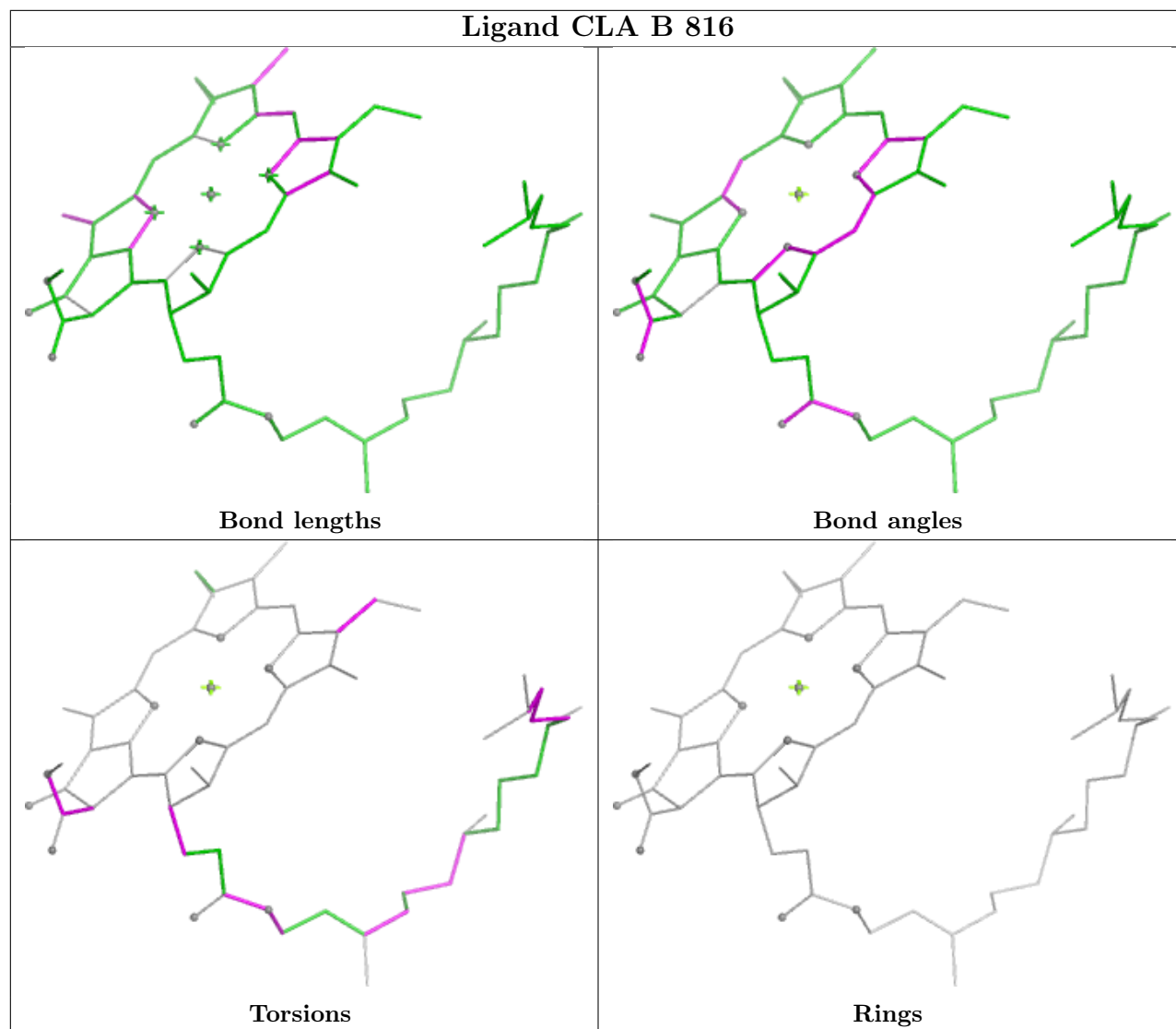




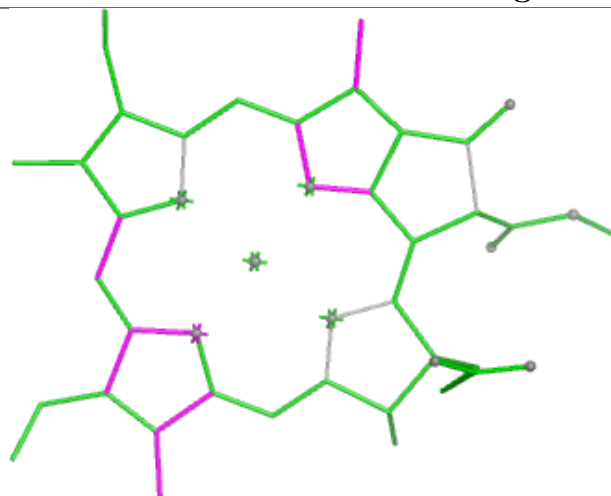




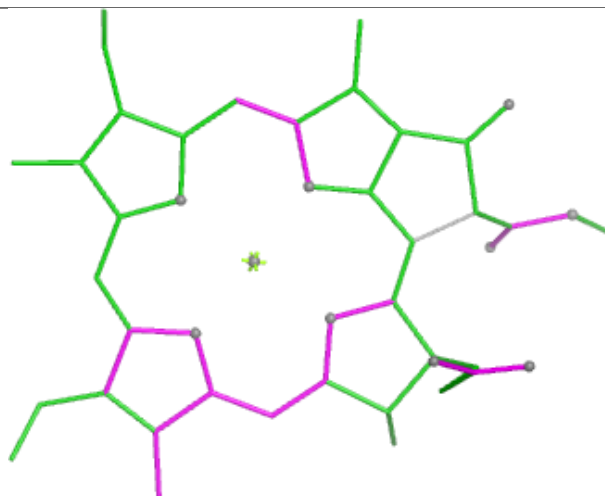
Ligand CLA B 816



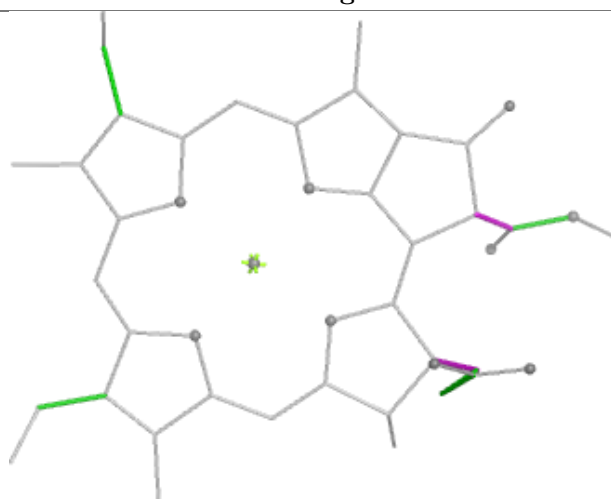
Ligand CLA A 832



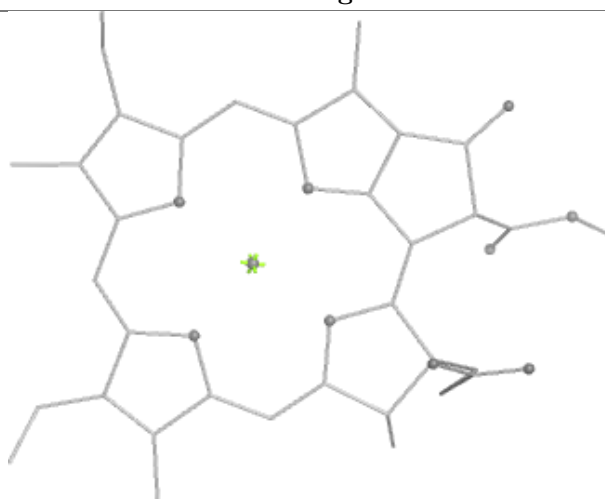
Bond lengths



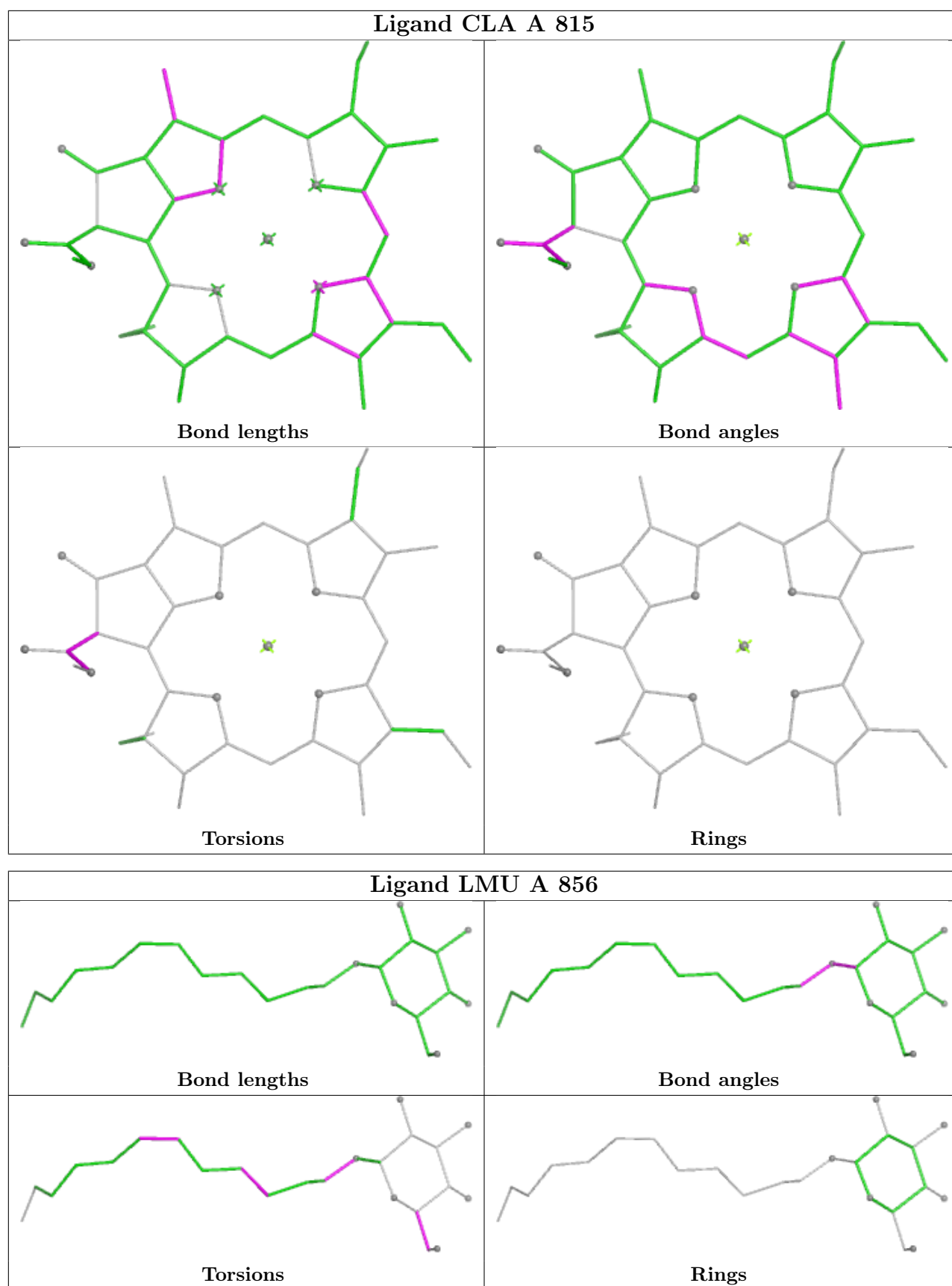
Bond angles

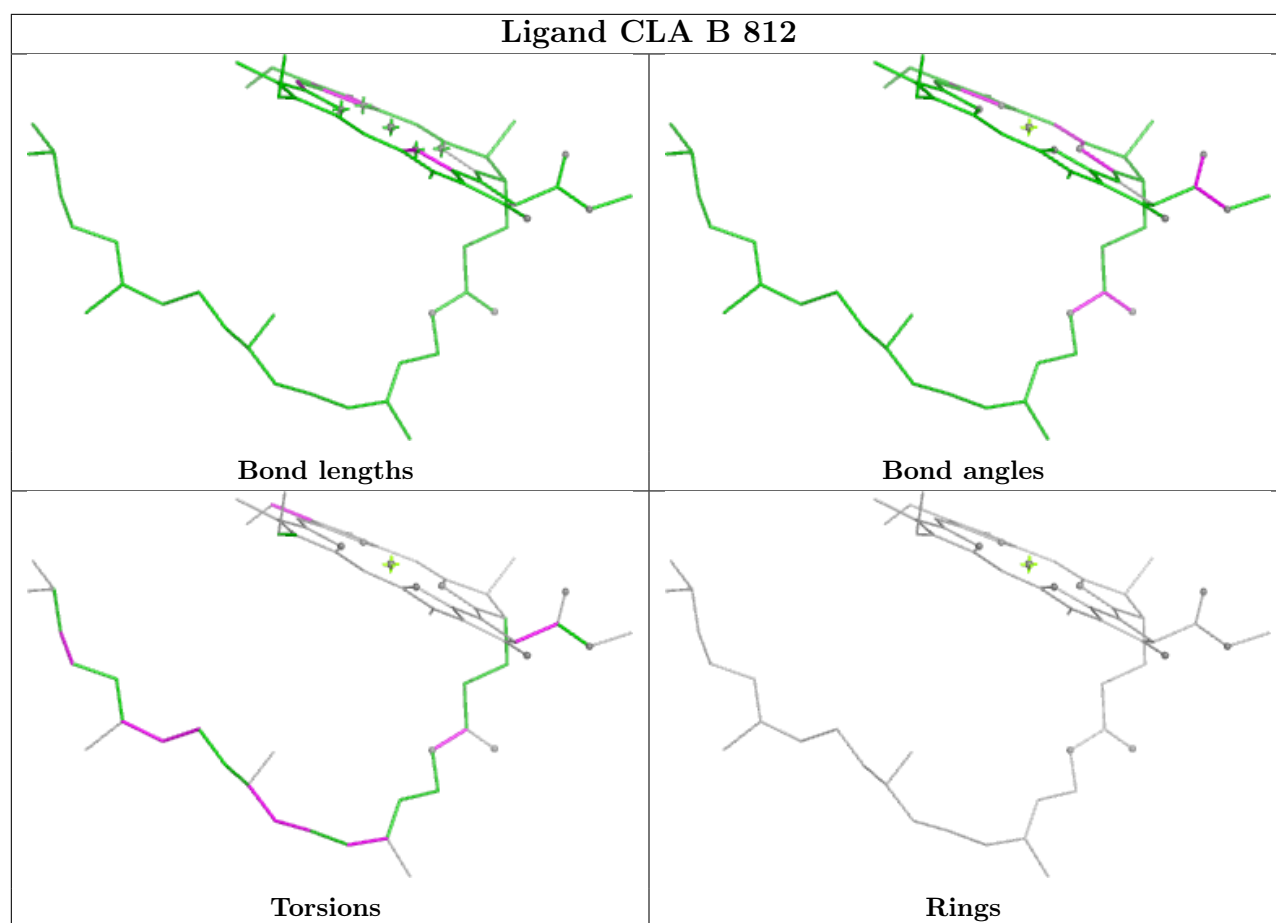


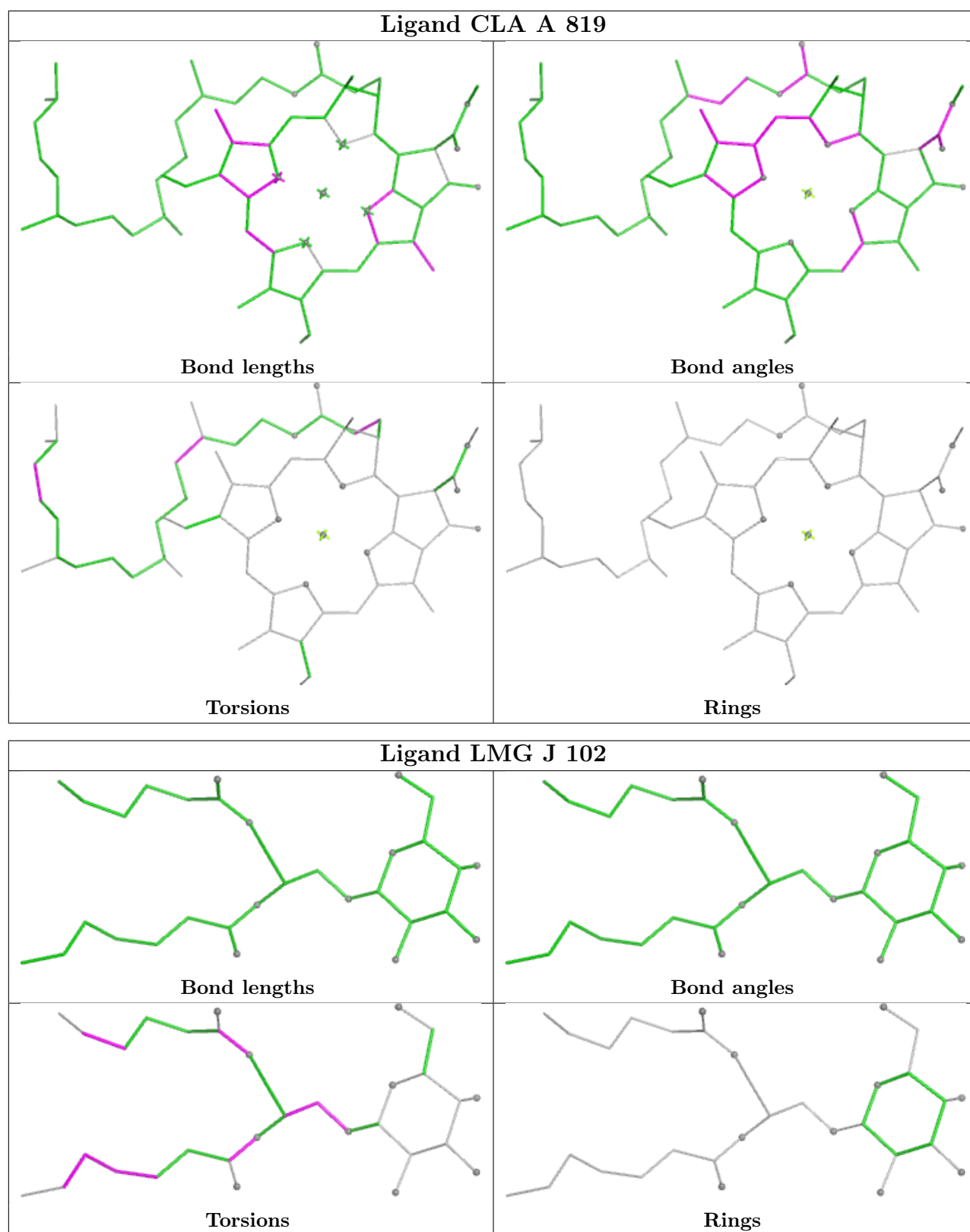
Torsions

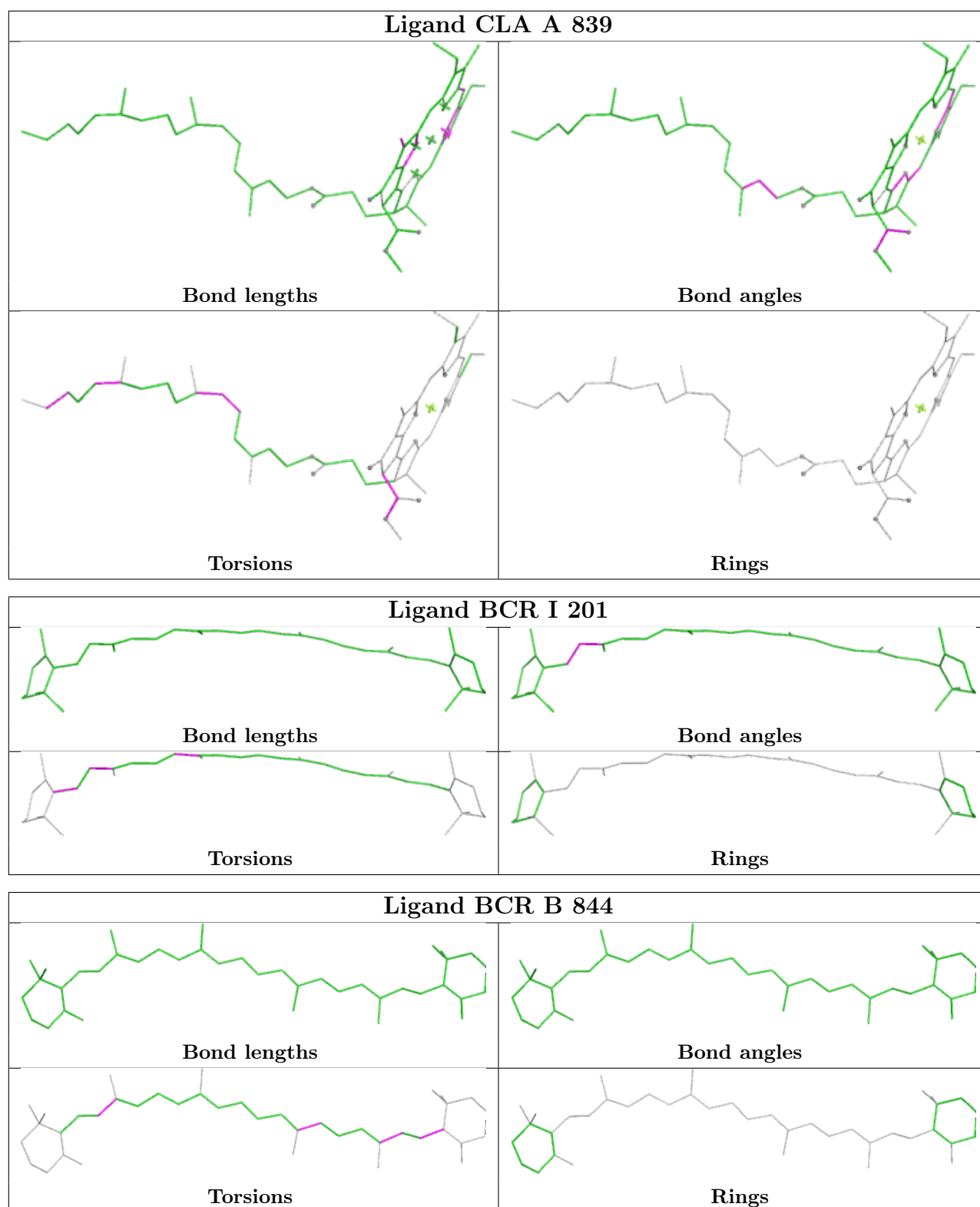


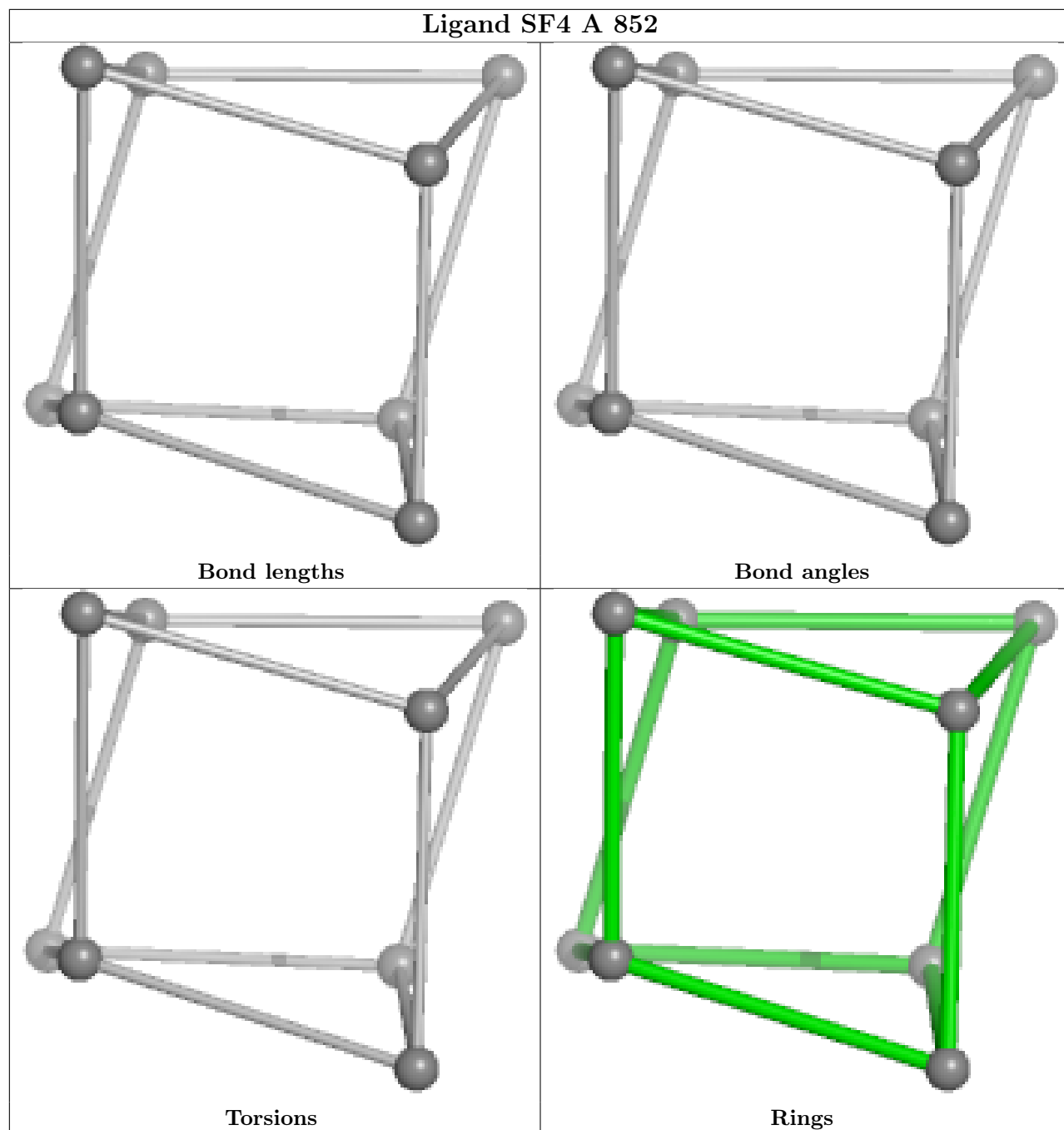
Rings

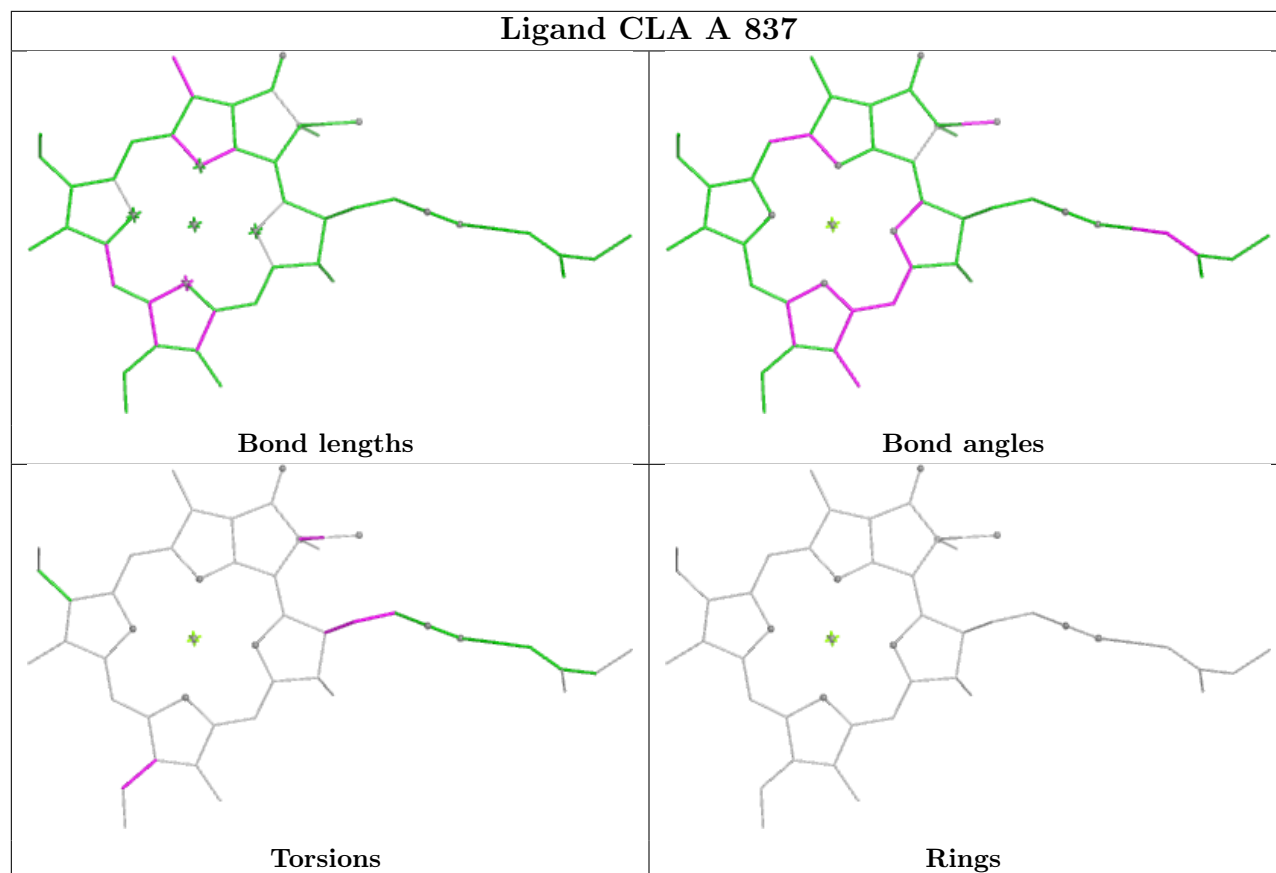


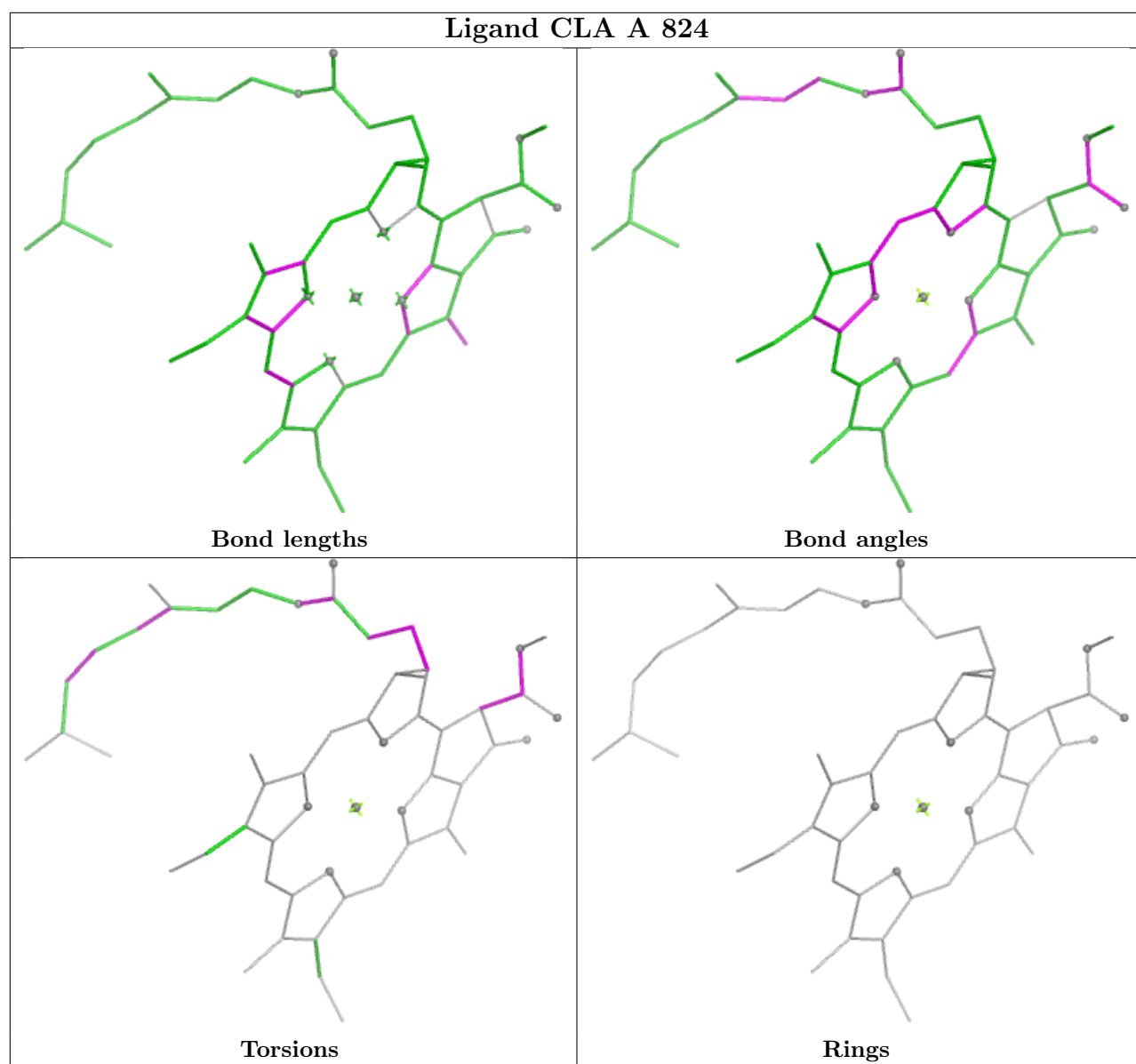


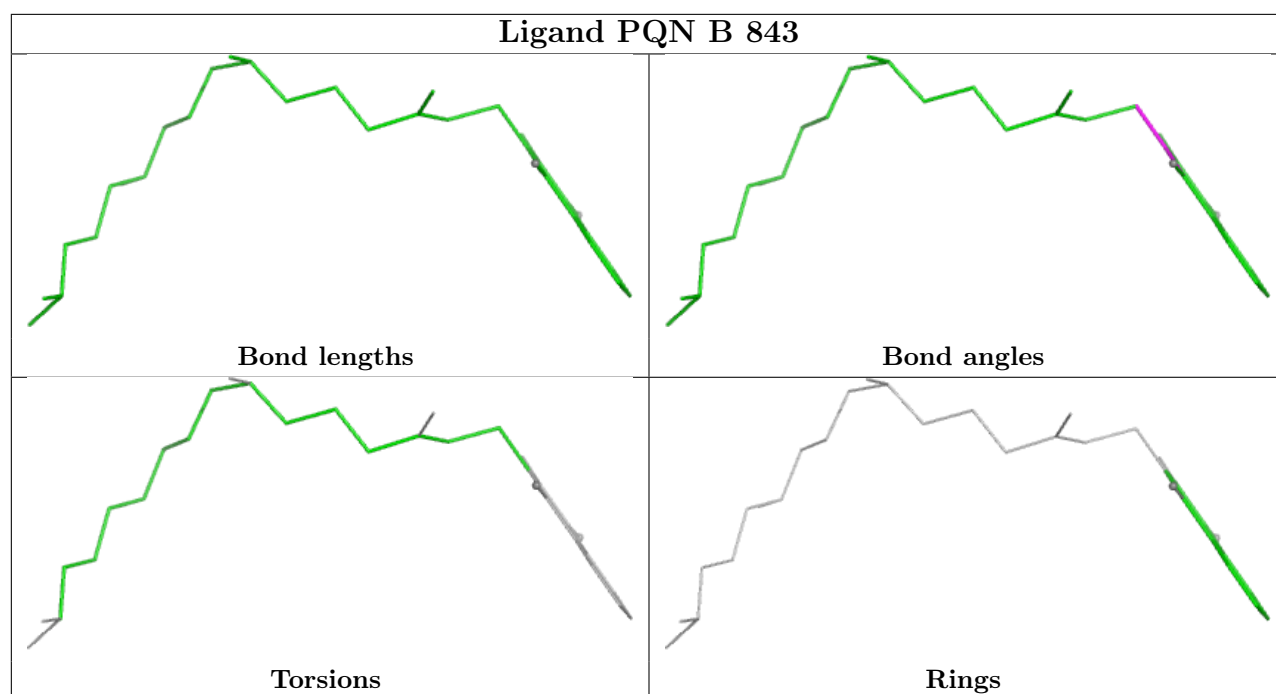




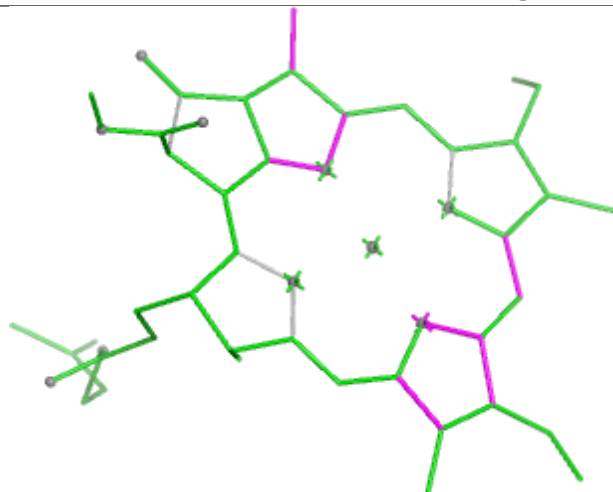




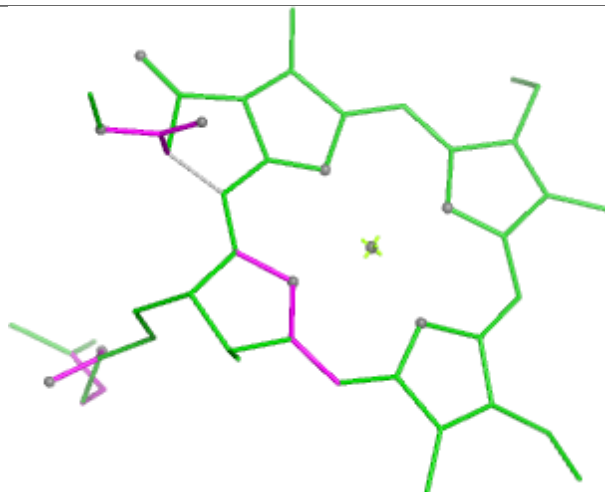




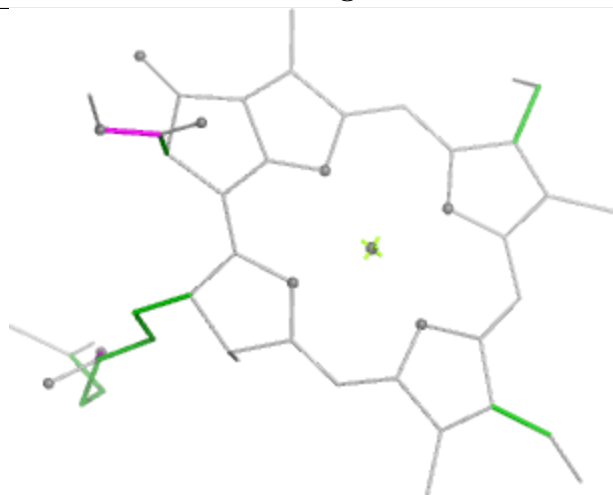
Ligand CLA B 839



Bond lengths



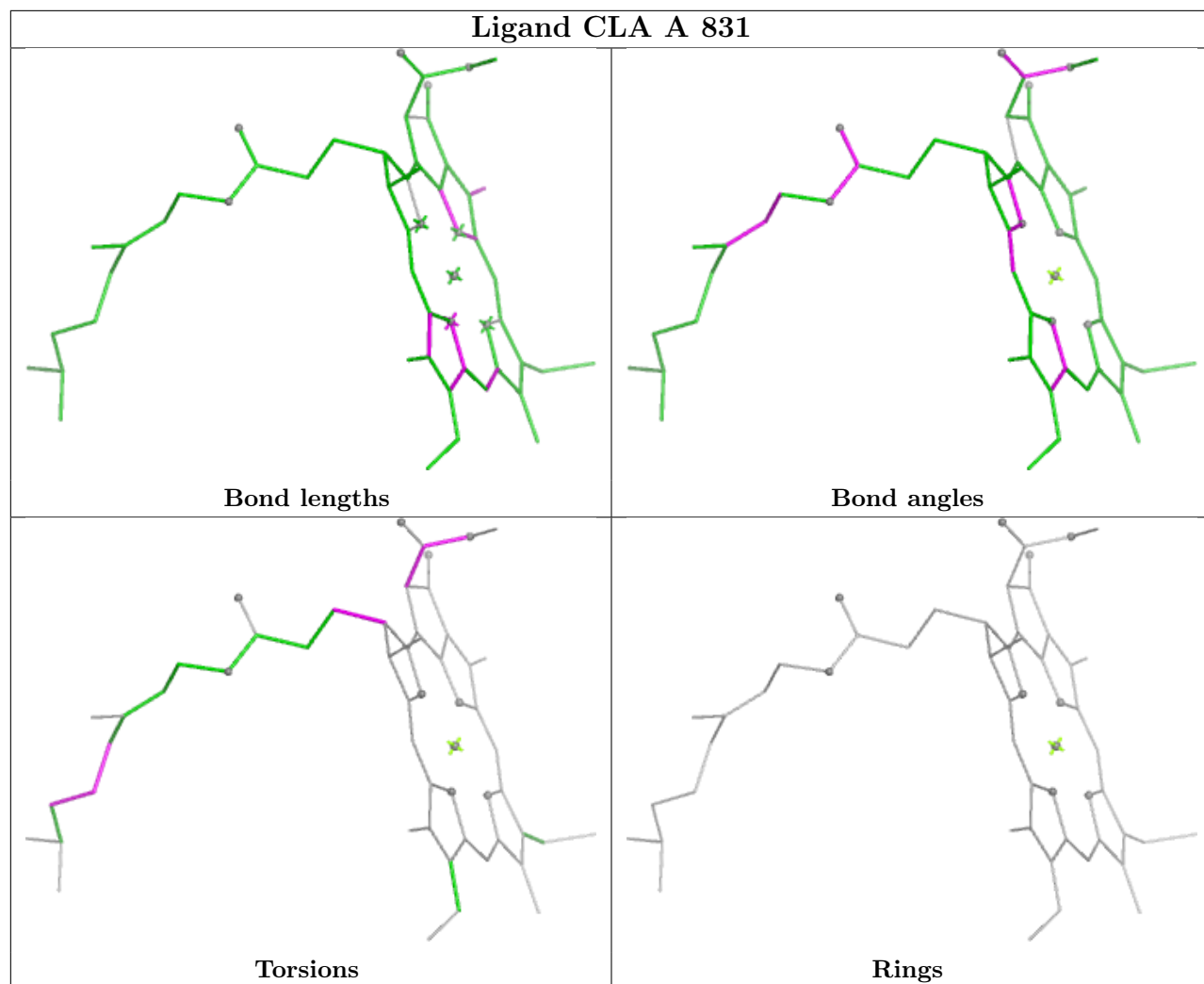
Bond angles

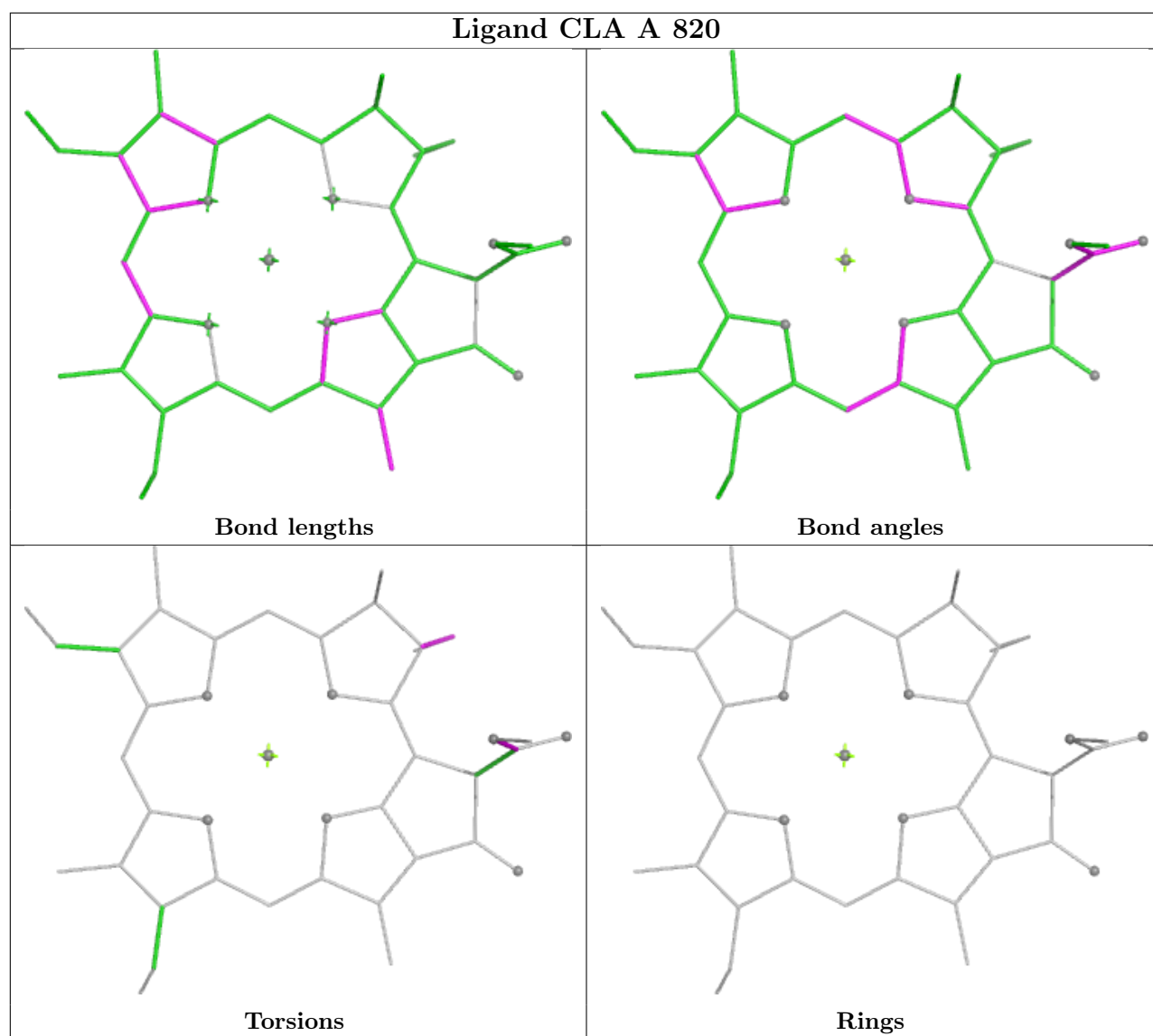


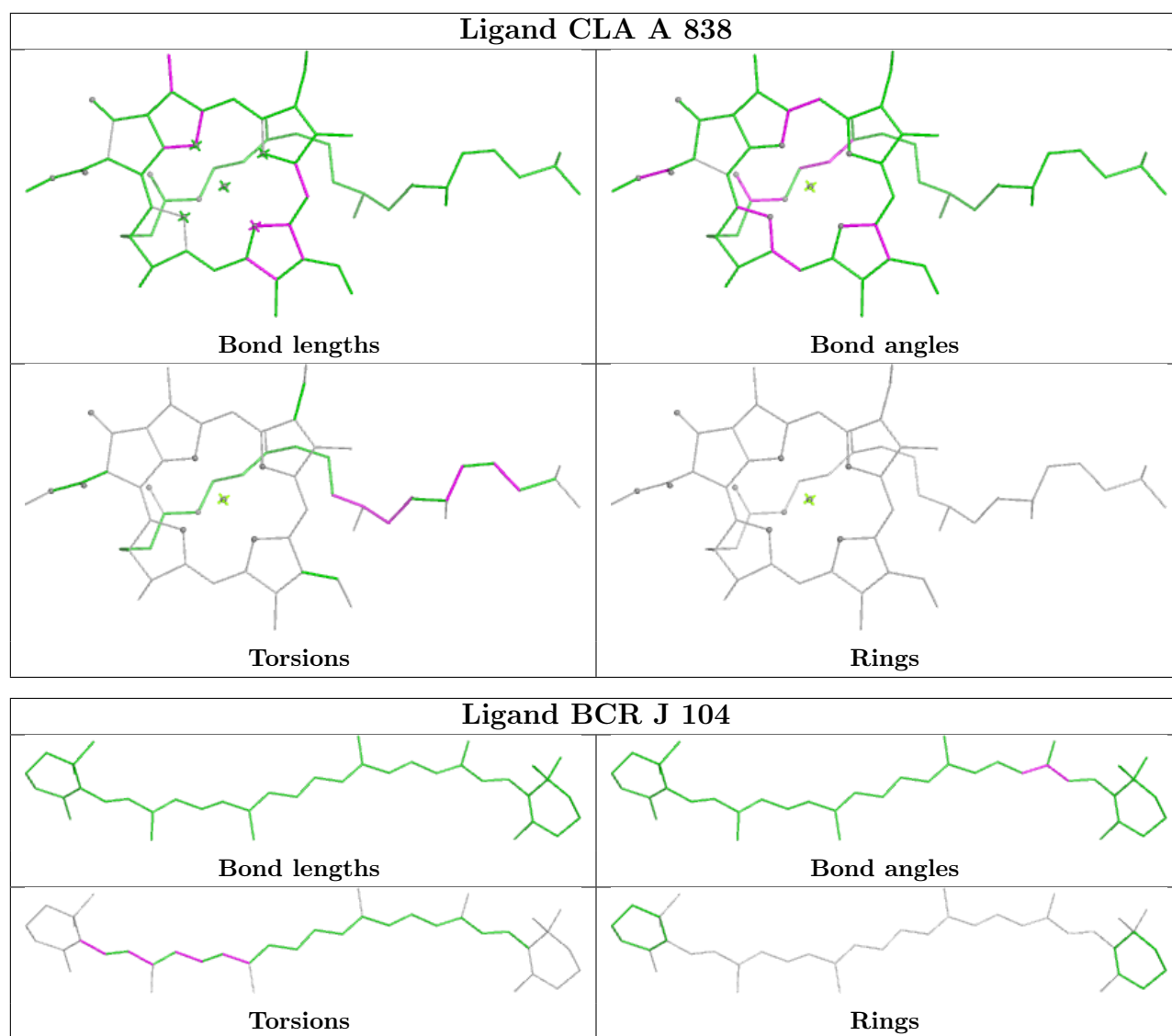
Torsions

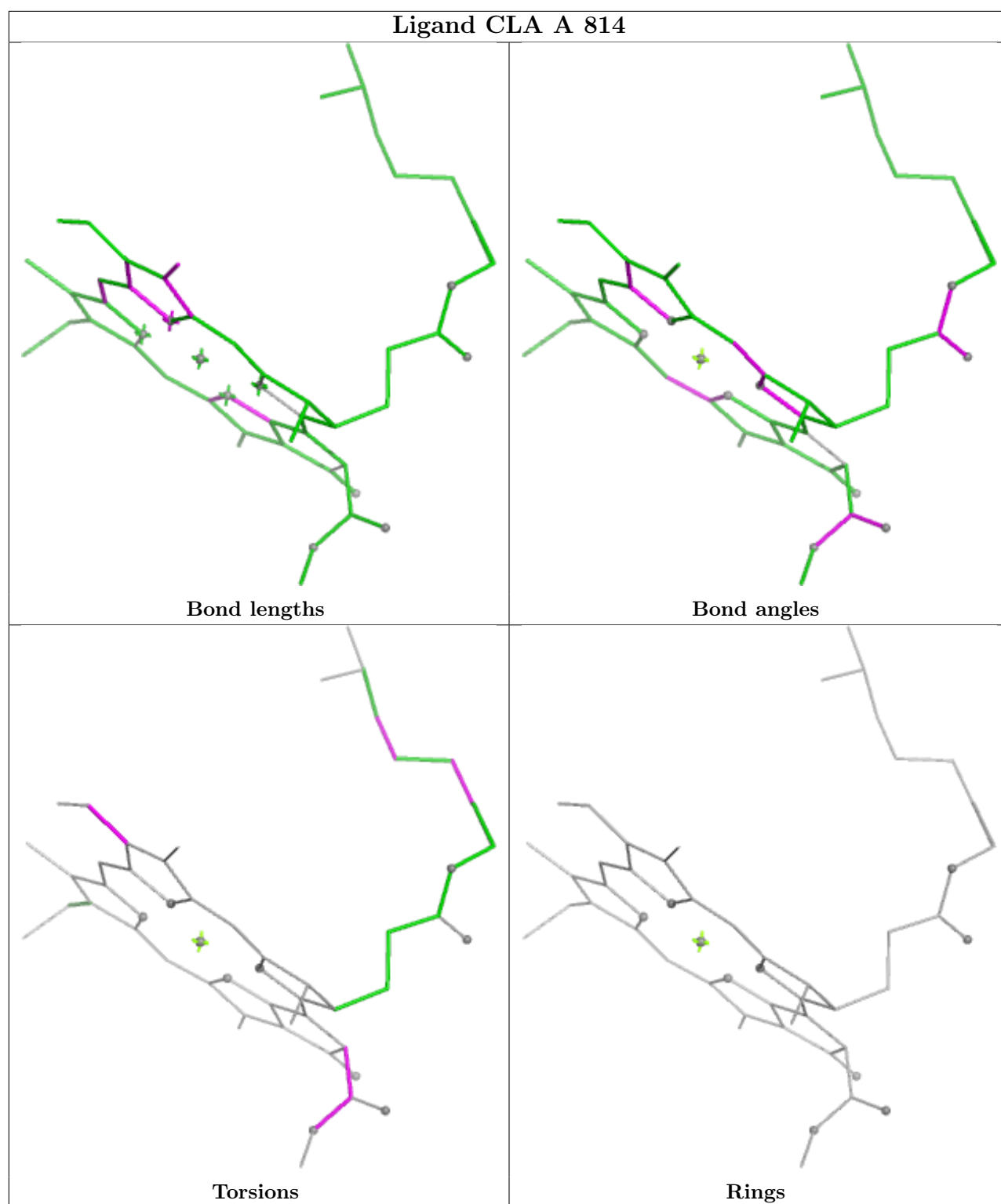


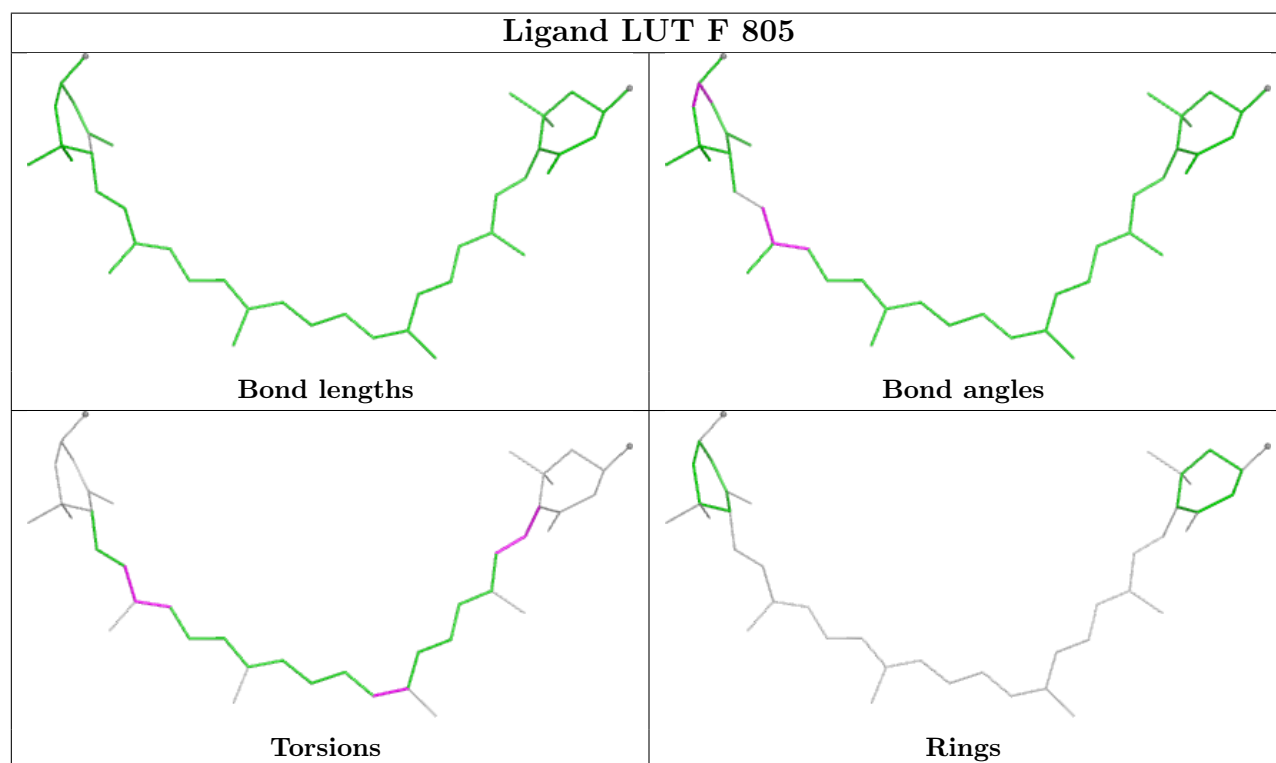
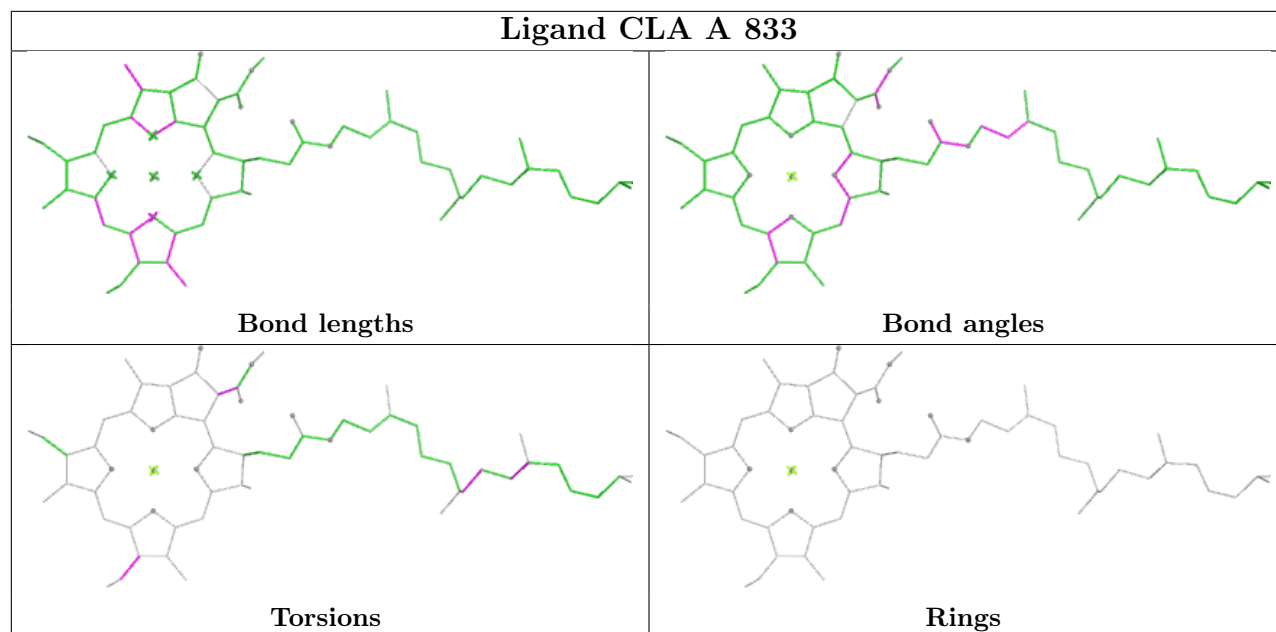
Rings

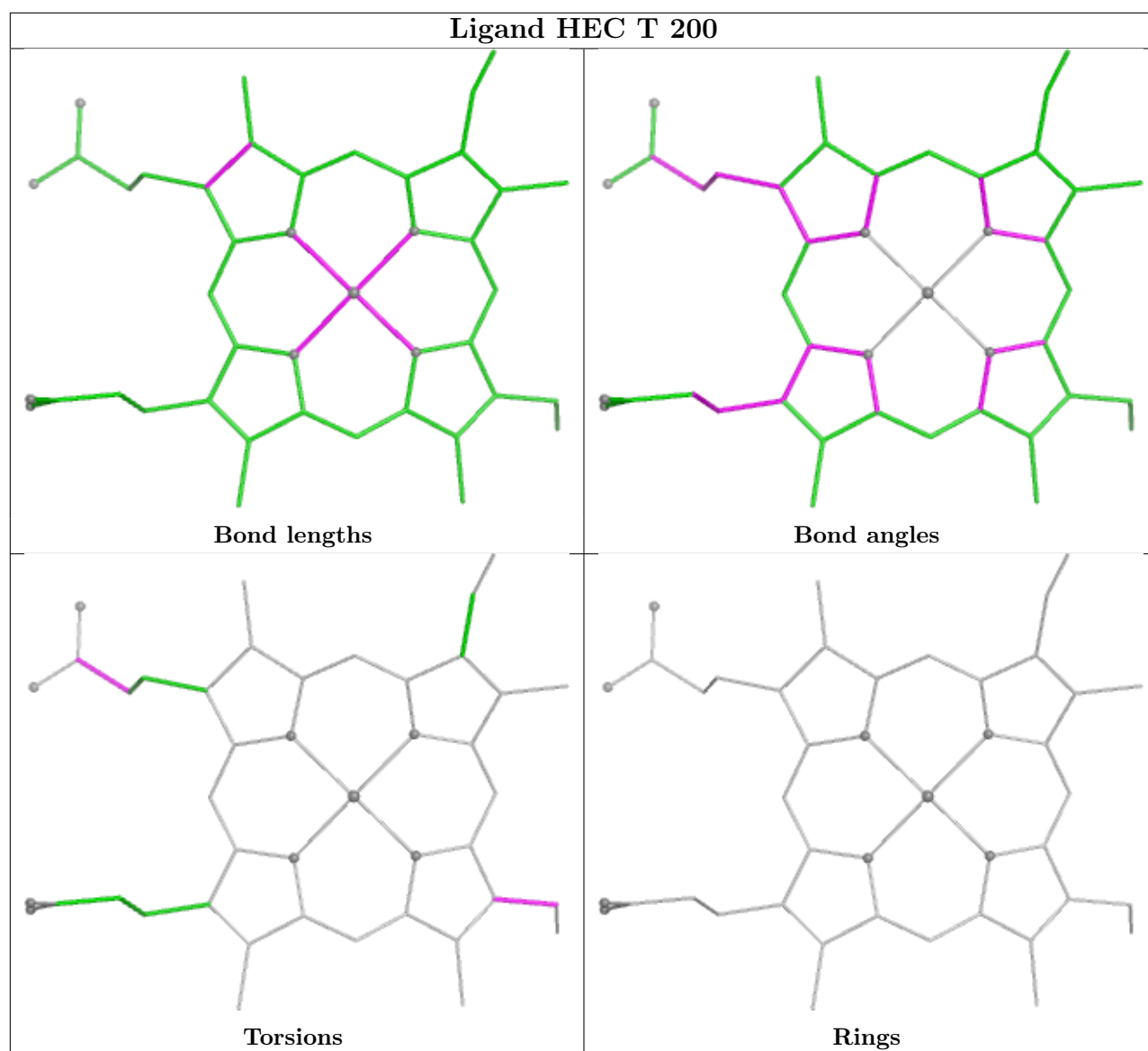




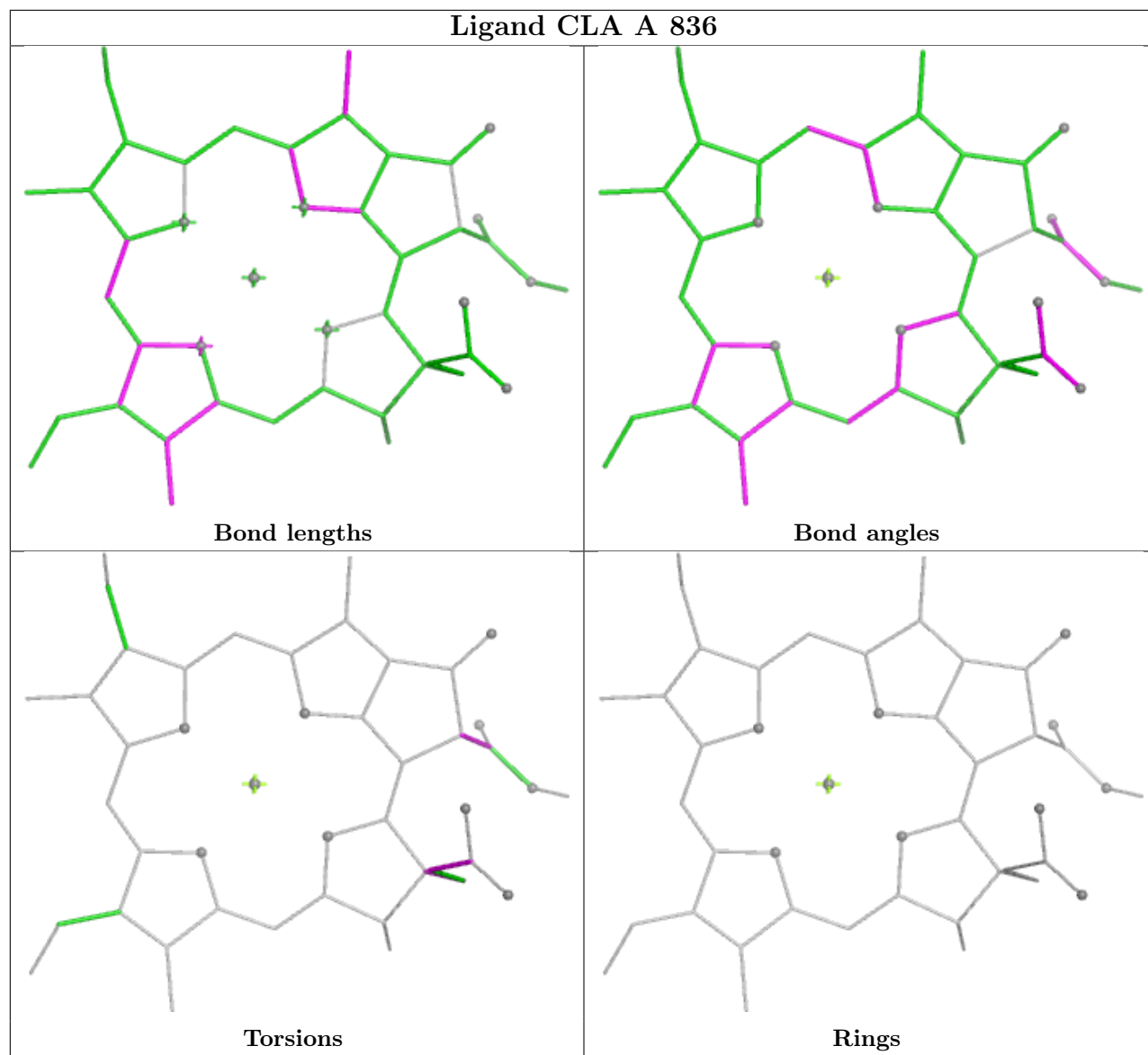




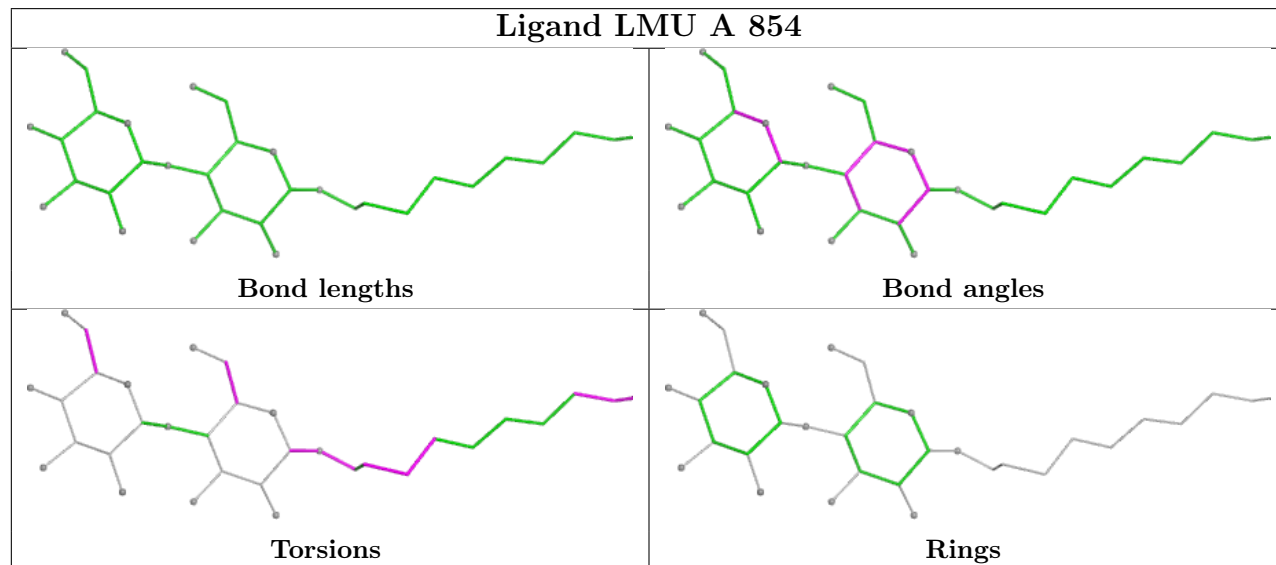


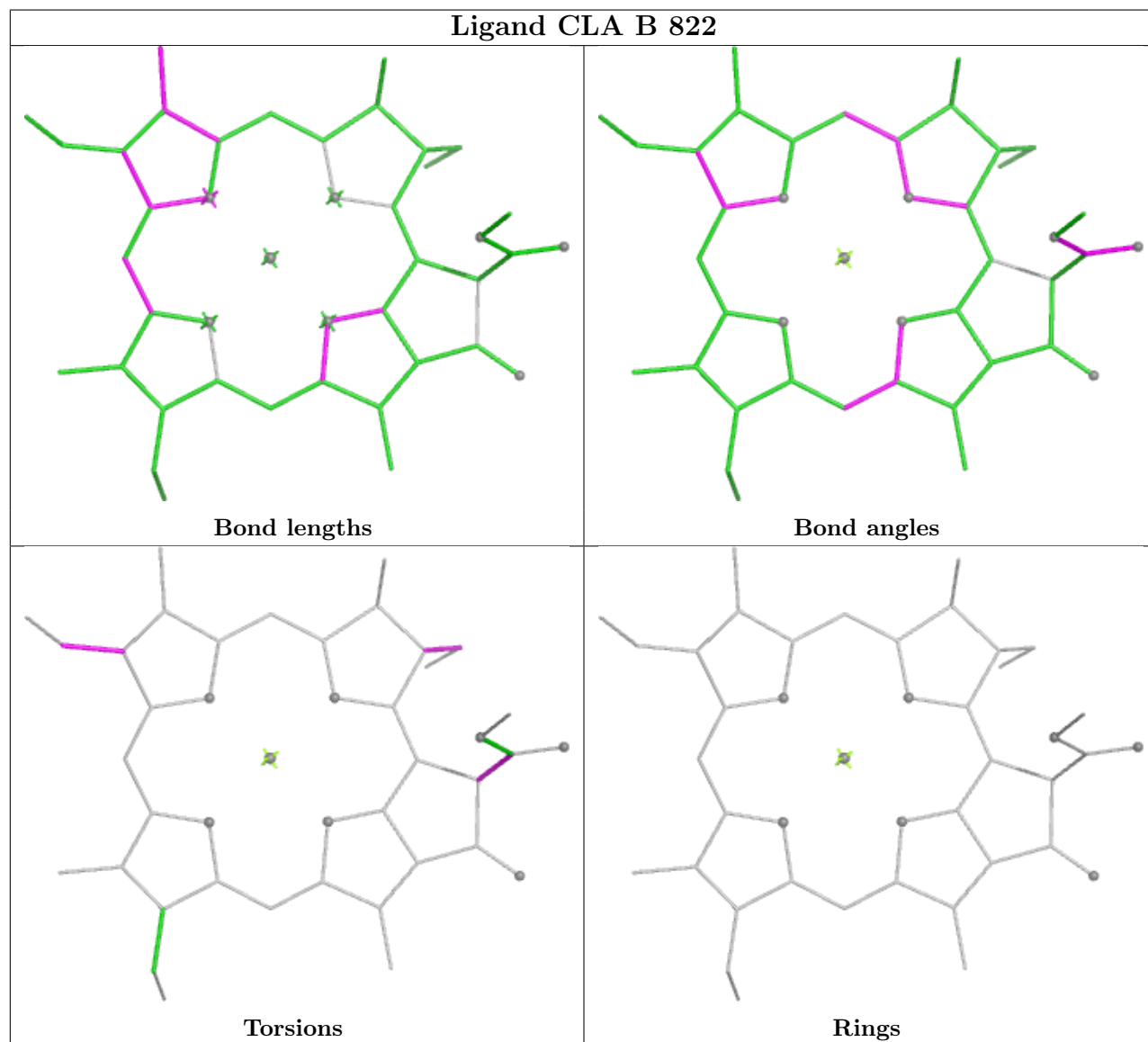
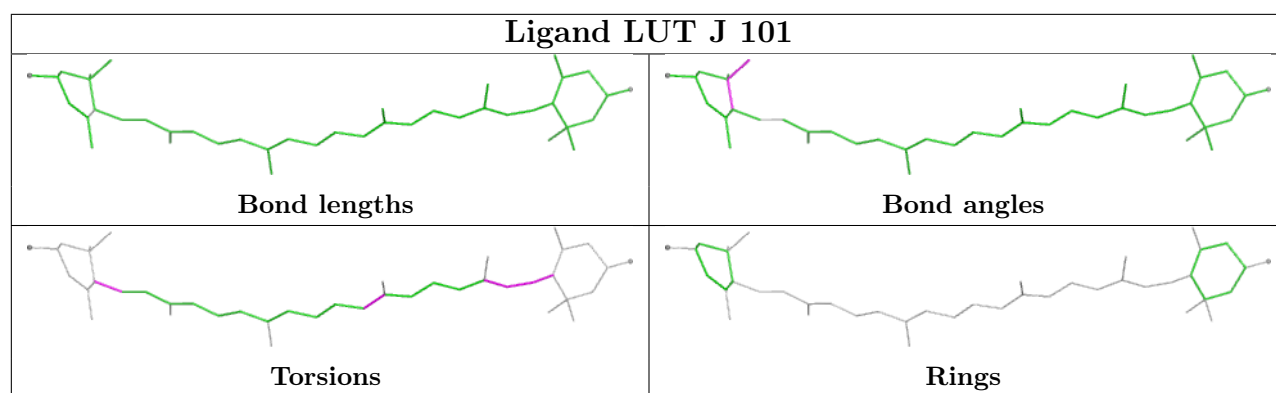


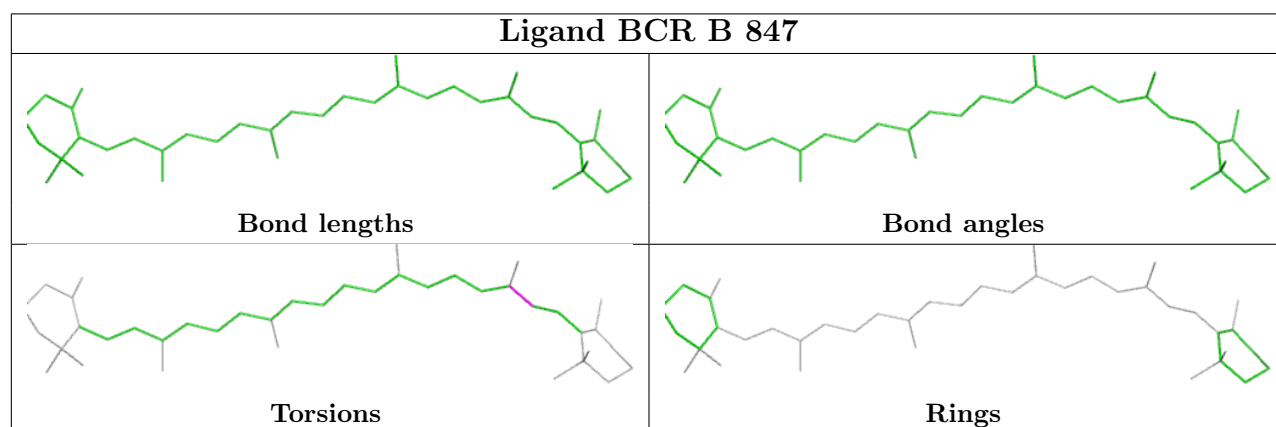
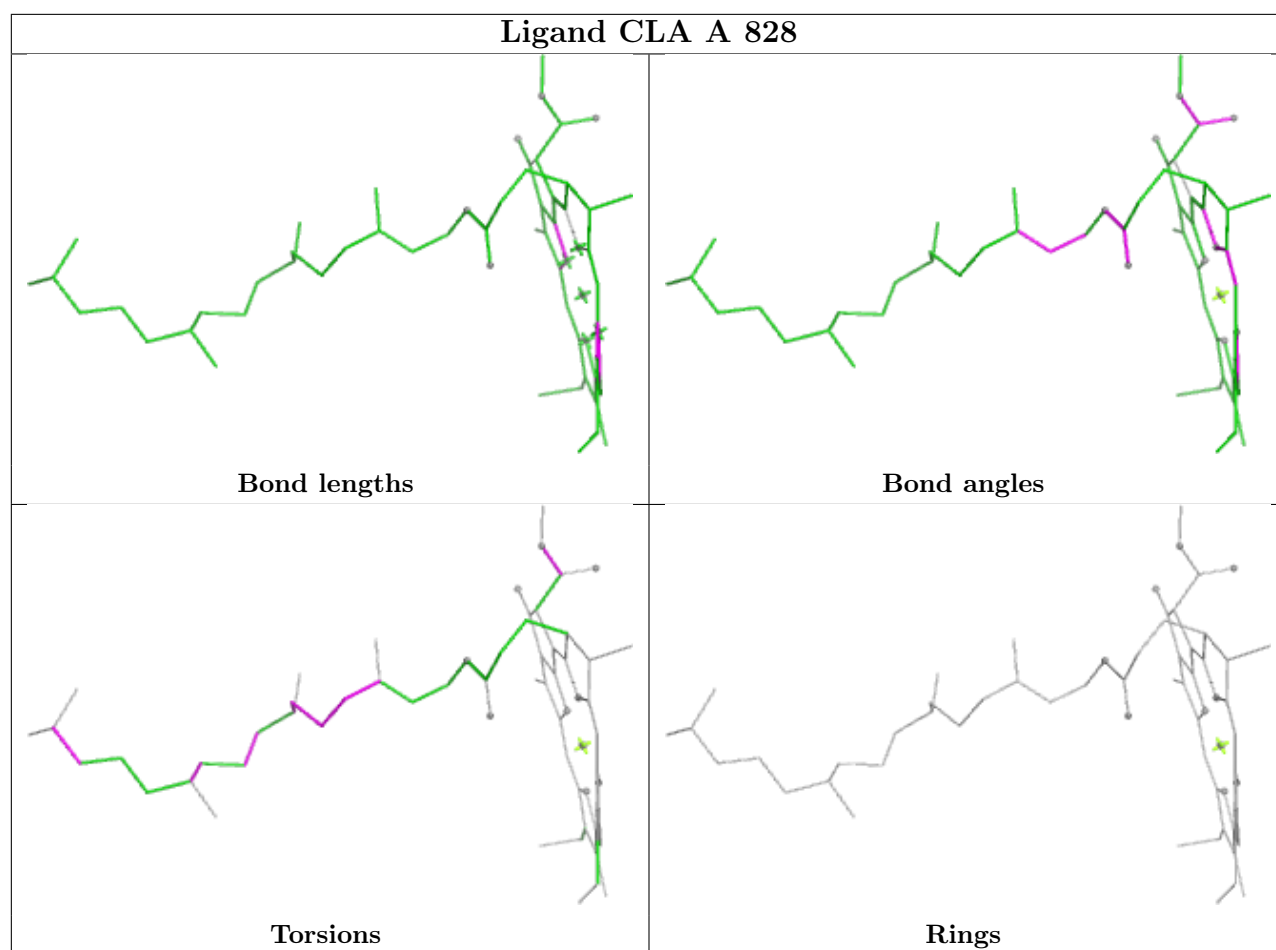
Ligand CLA A 836

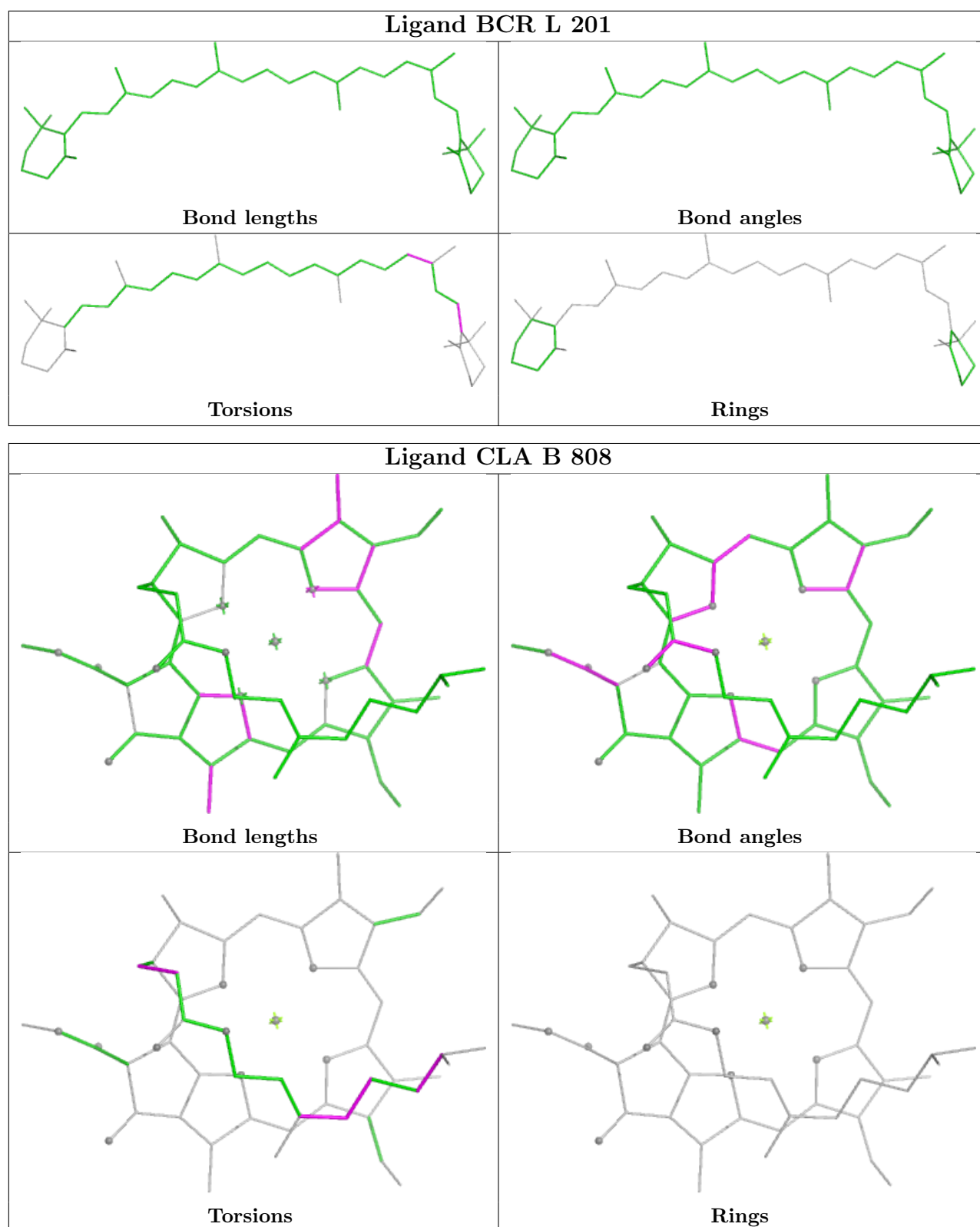


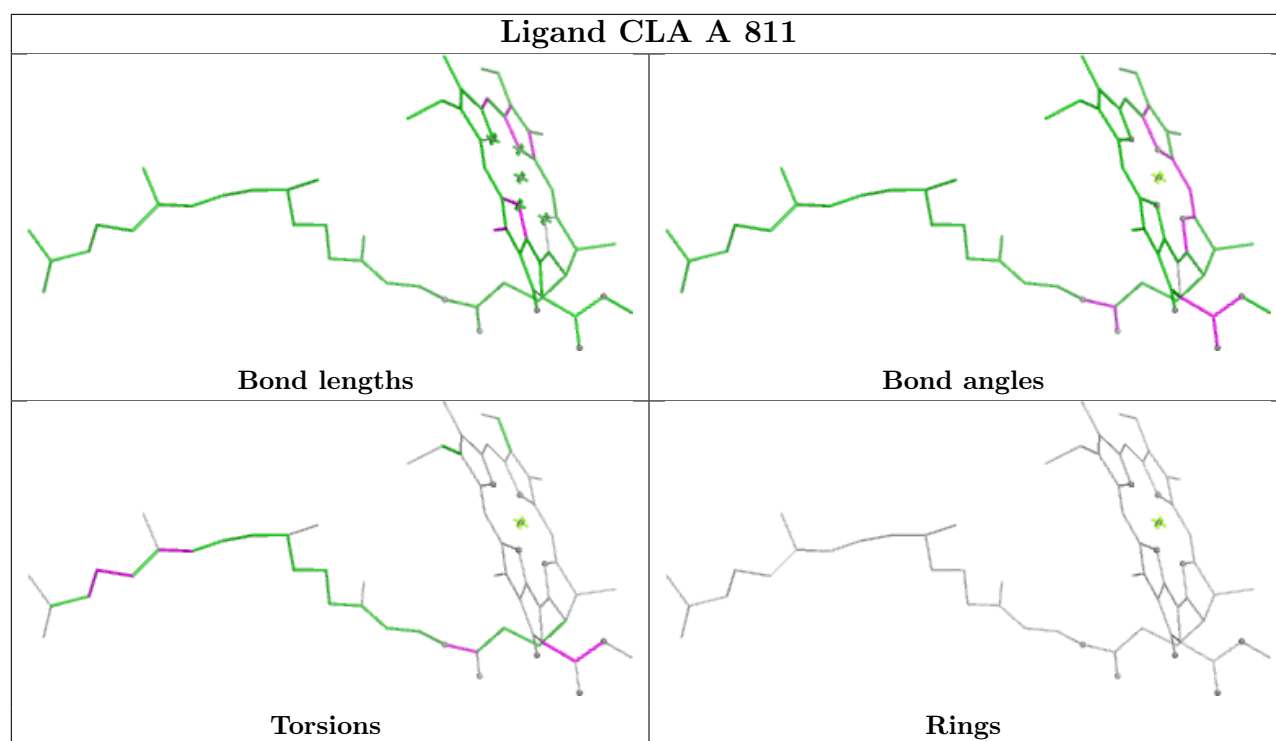
Ligand LMU A 854



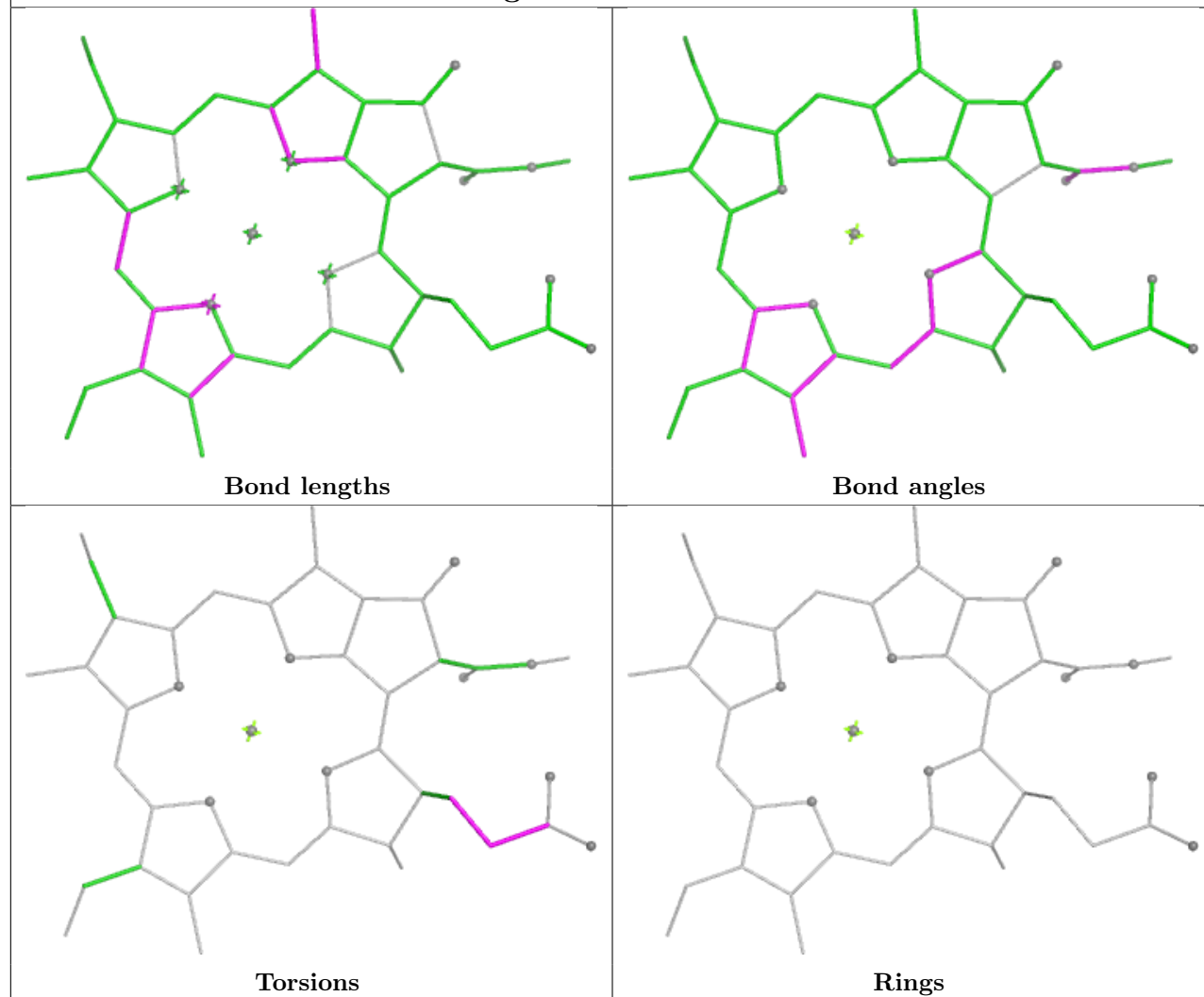




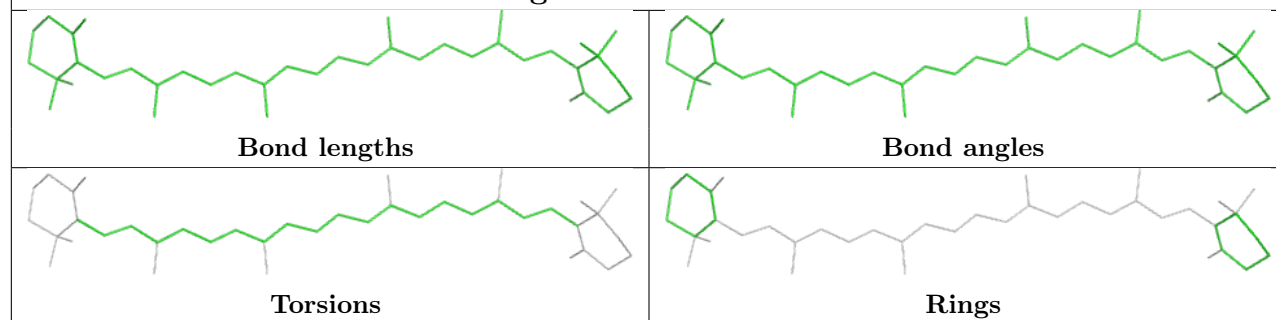




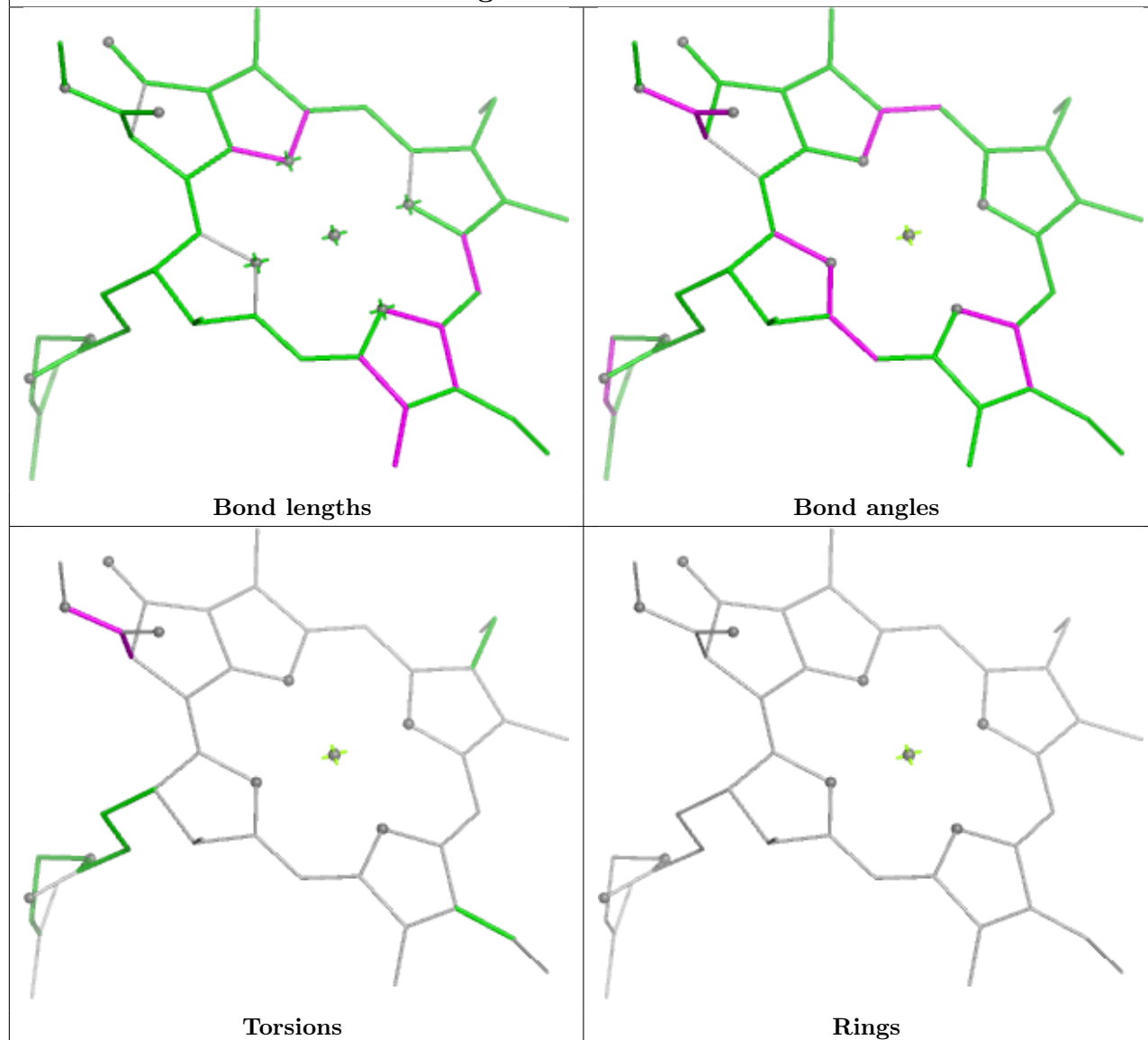
Ligand CLA F 804

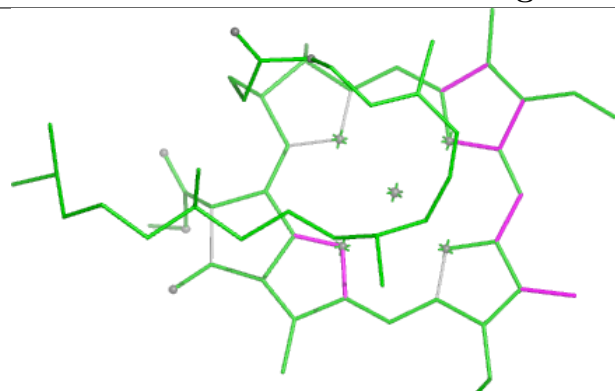
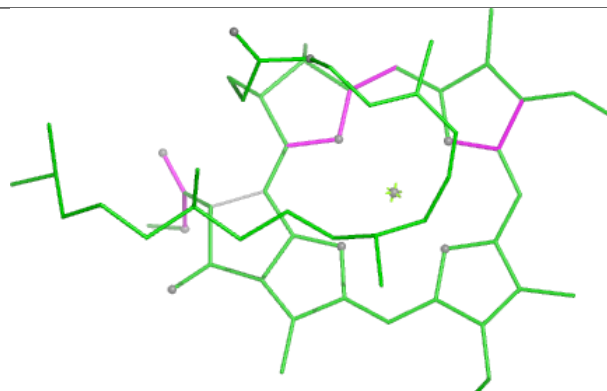
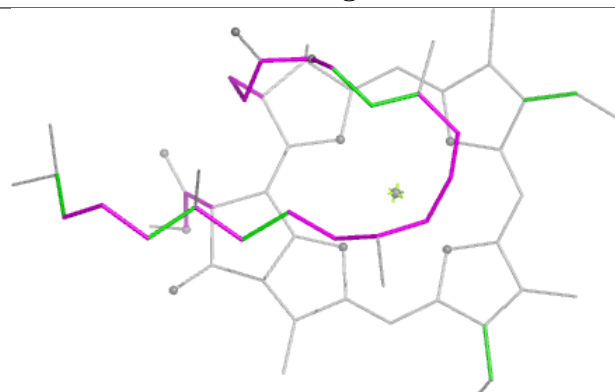
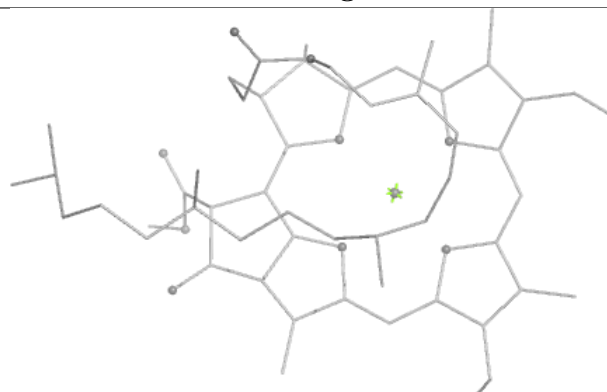
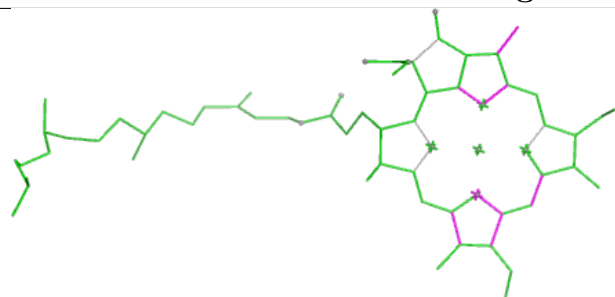
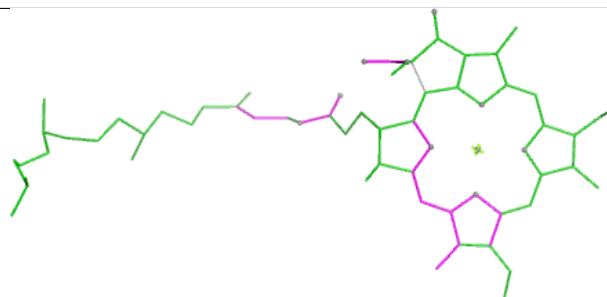
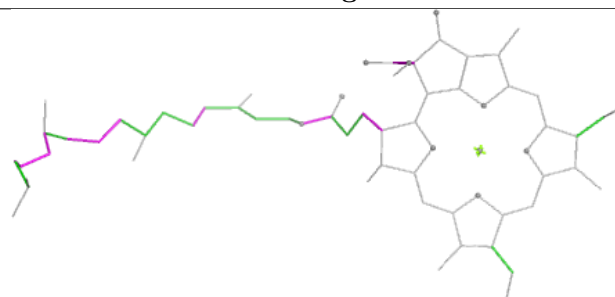
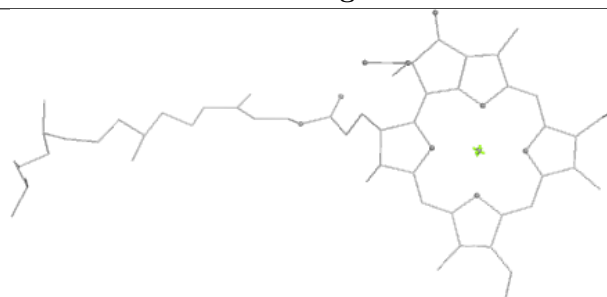


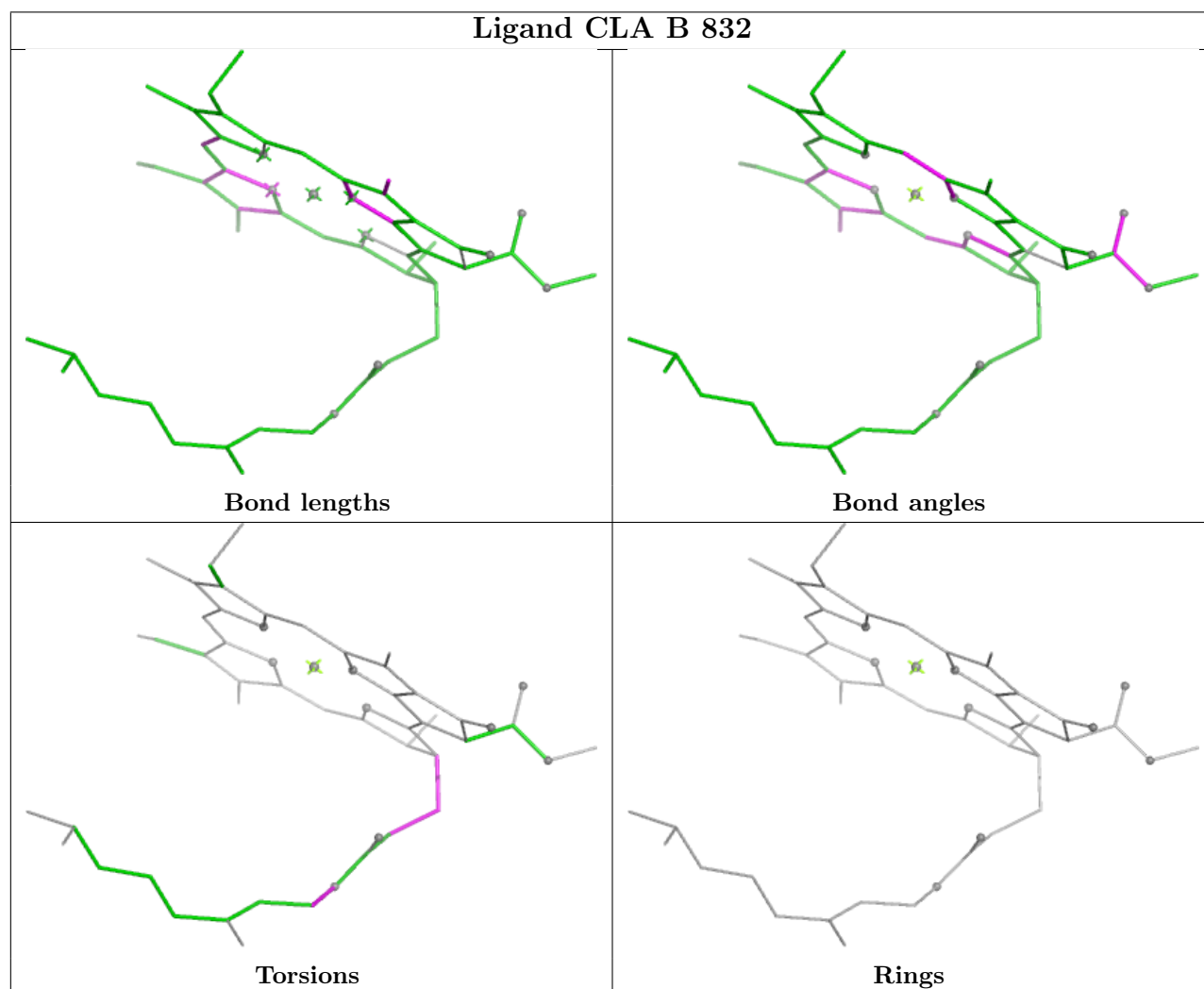
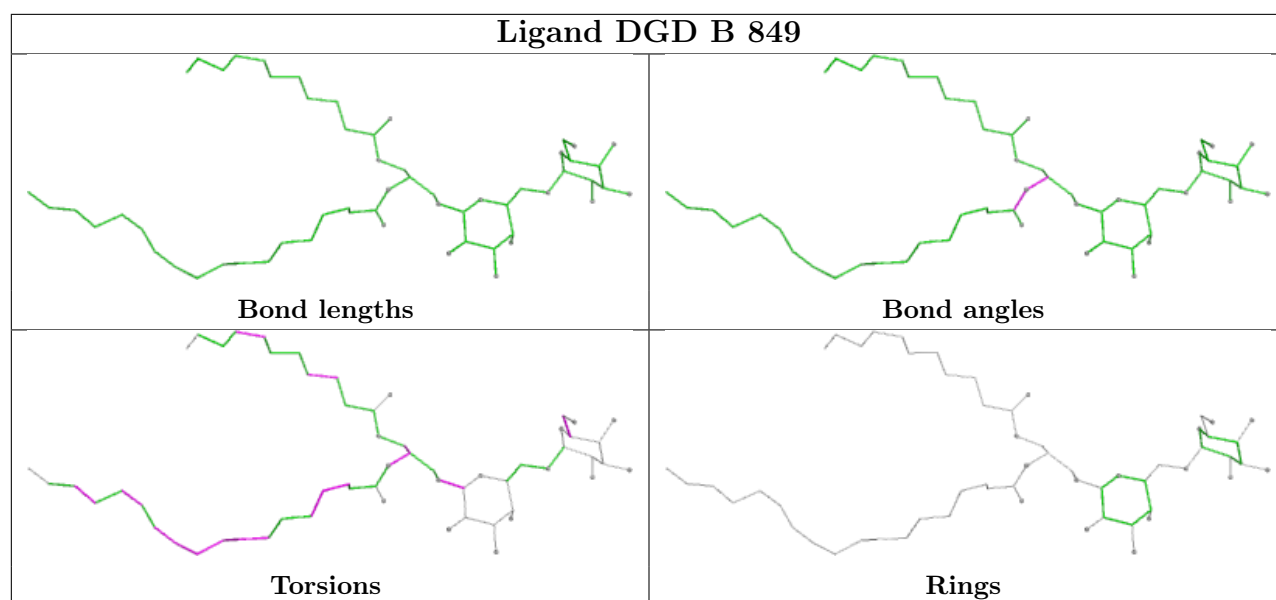
Ligand BCR A 848

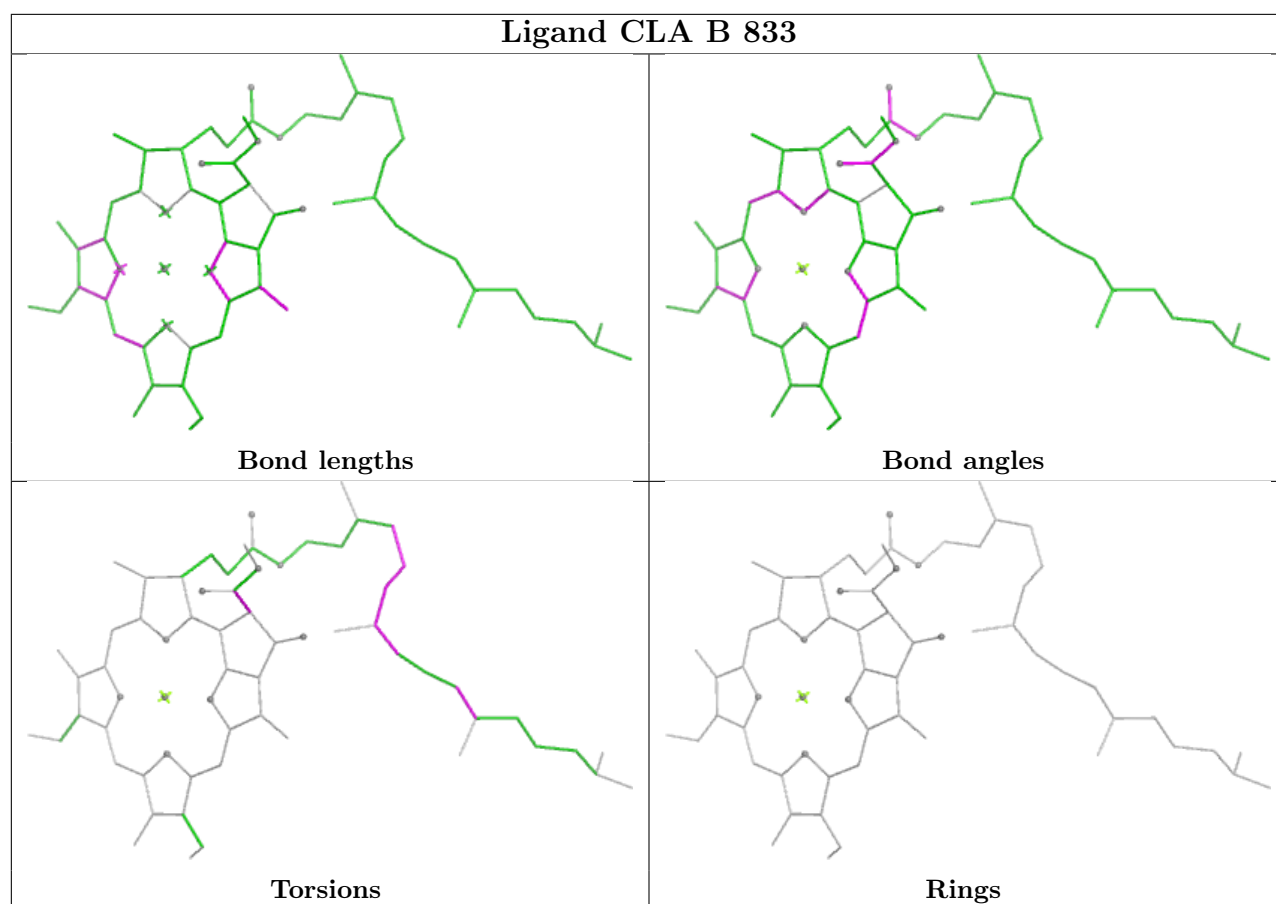
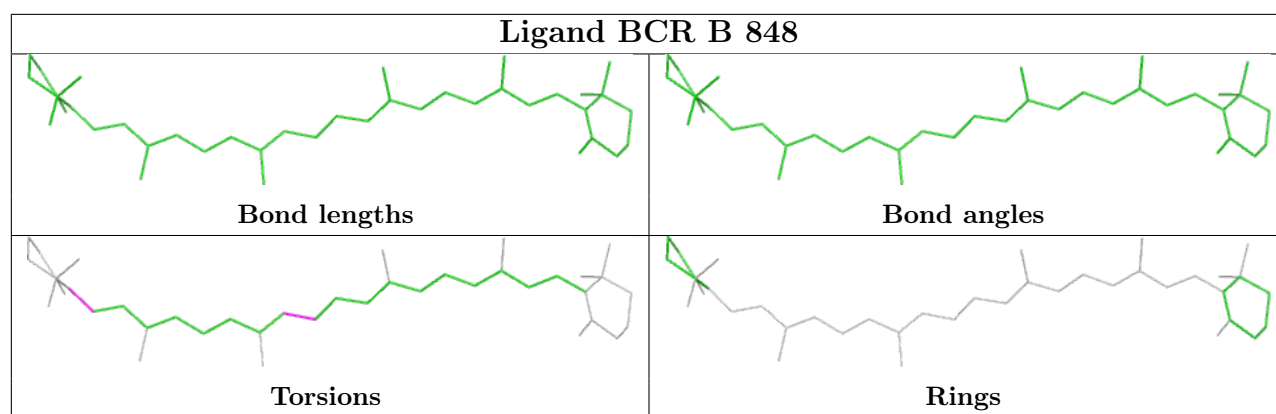


Ligand CLA A 807

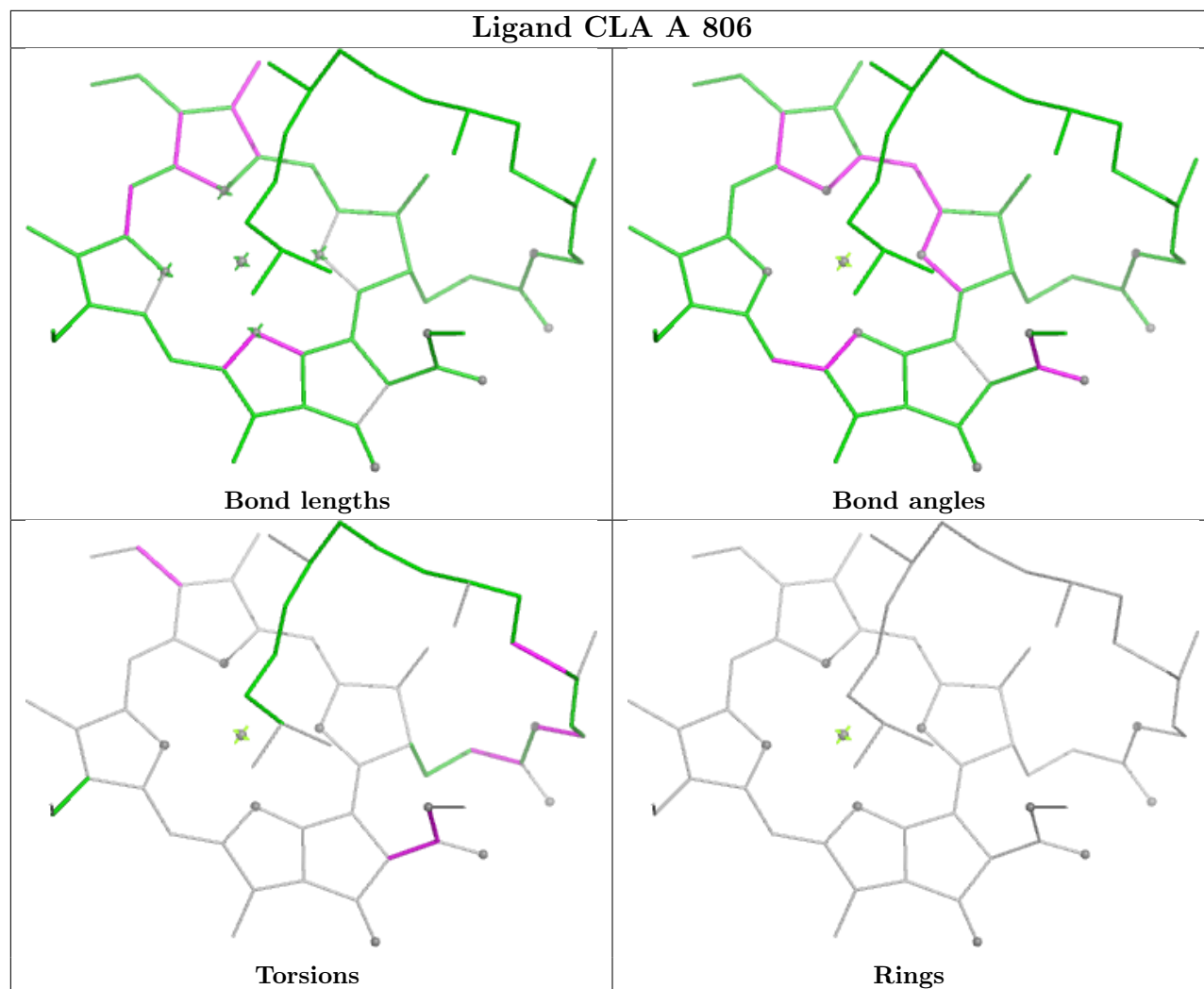


Ligand CLA B 852**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 842****Bond lengths****Bond angles****Torsions****Rings**

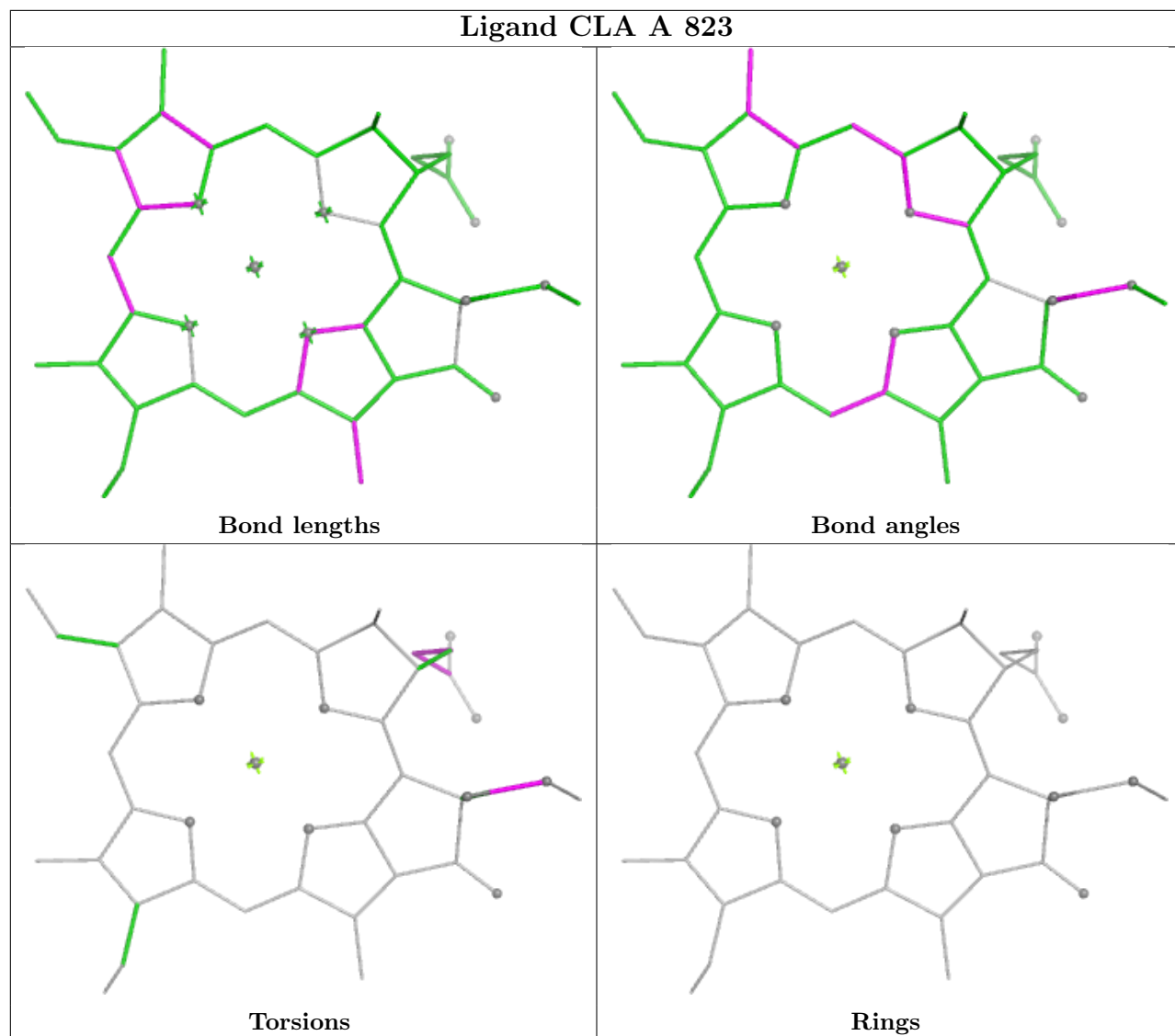


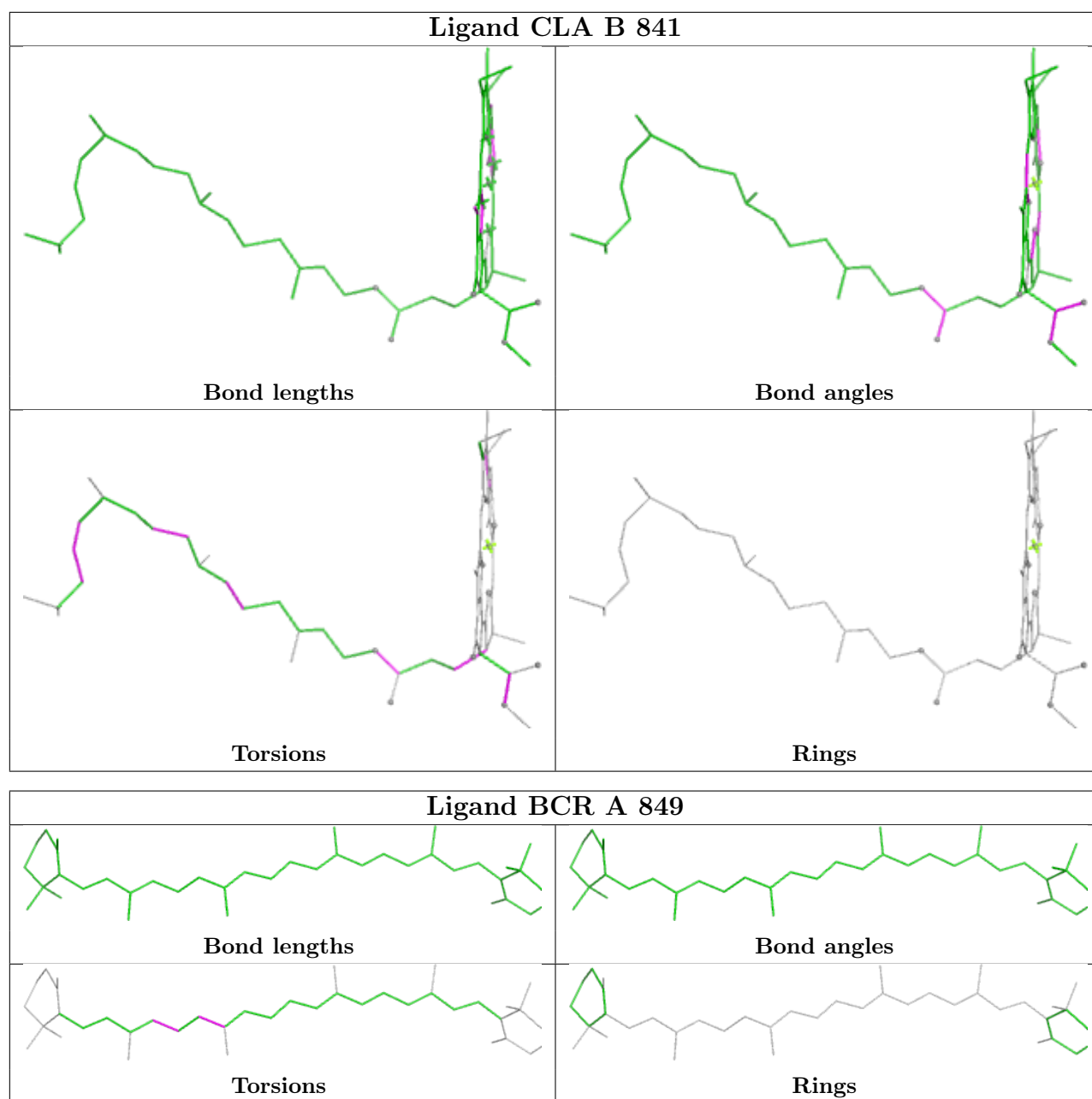


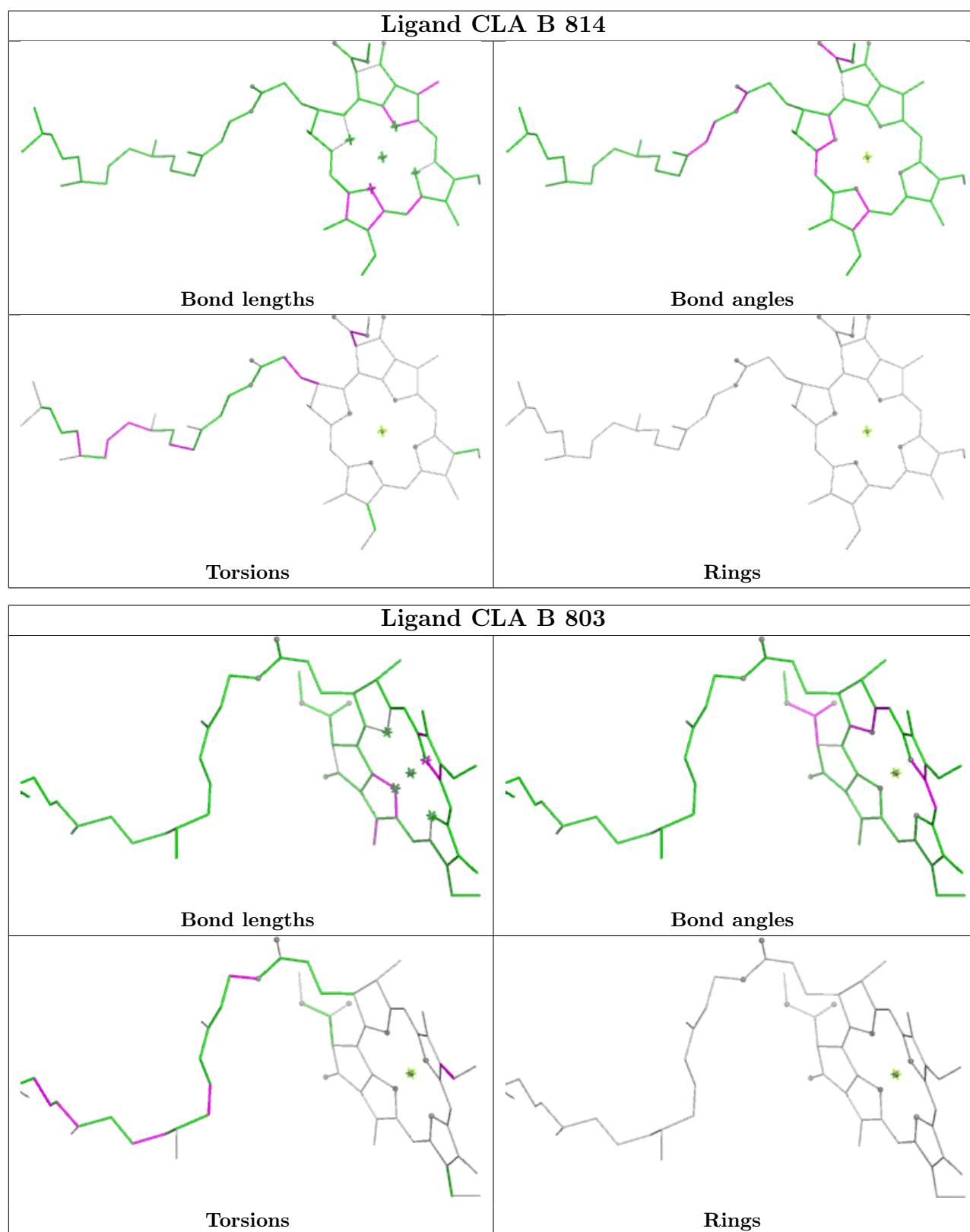
Ligand CLA A 806



Ligand CLA A 823







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

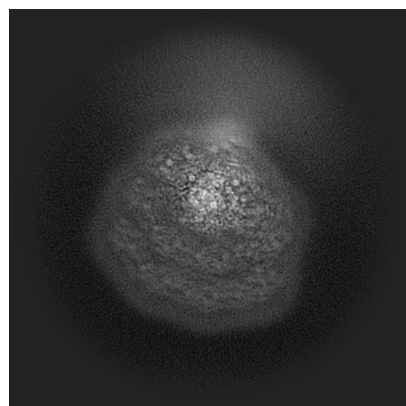
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54804. These allow visual inspection of the internal detail of the map and identification of artifacts.

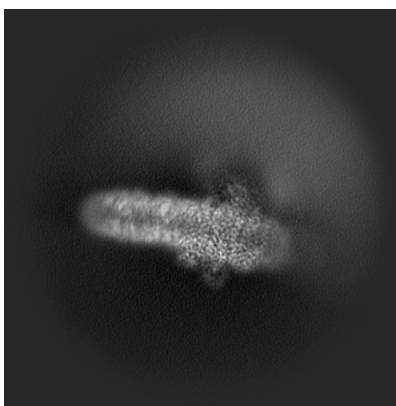
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

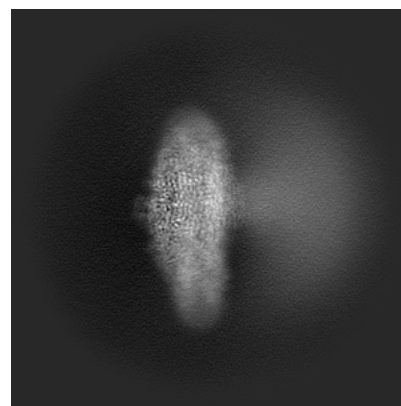
6.1.1 Primary map



X

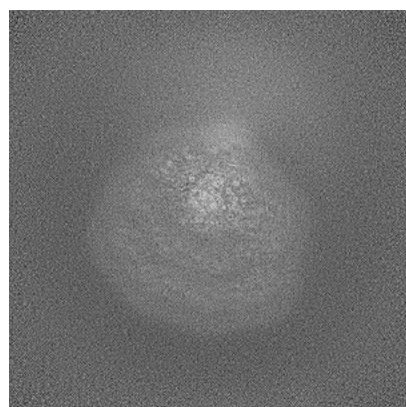


Y

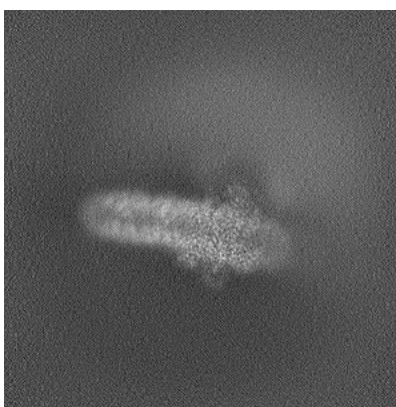


Z

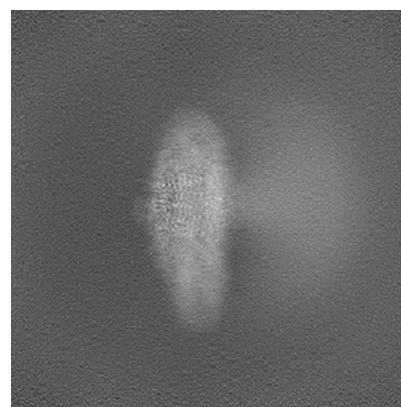
6.1.2 Raw map



X



Y

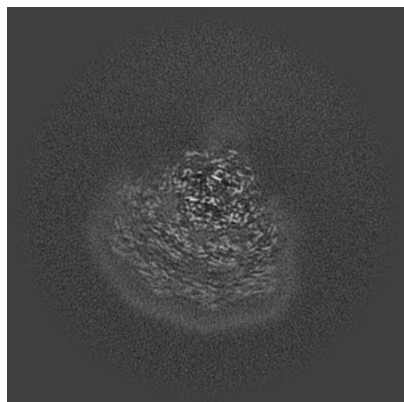


Z

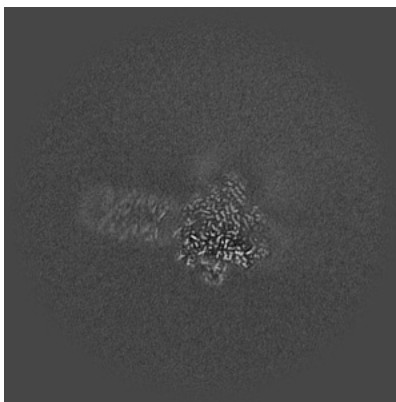
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

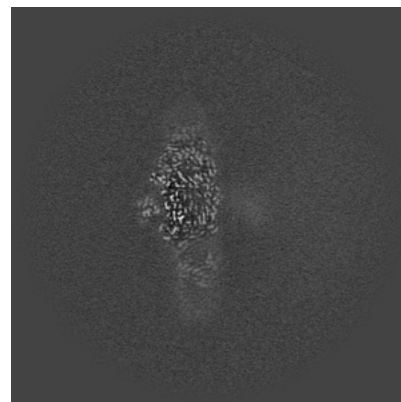
6.2.1 Primary map



X Index: 256

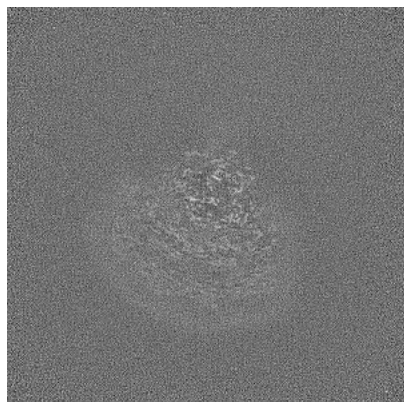


Y Index: 256

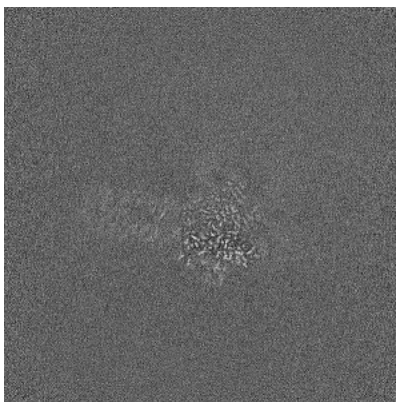


Z Index: 256

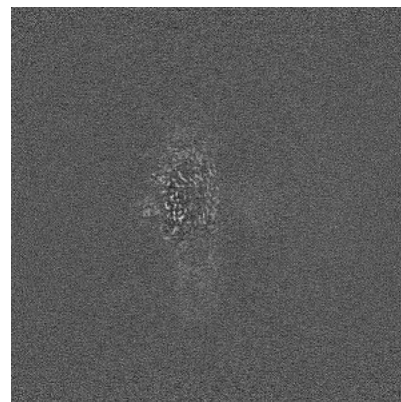
6.2.2 Raw map



X Index: 256



Y Index: 256

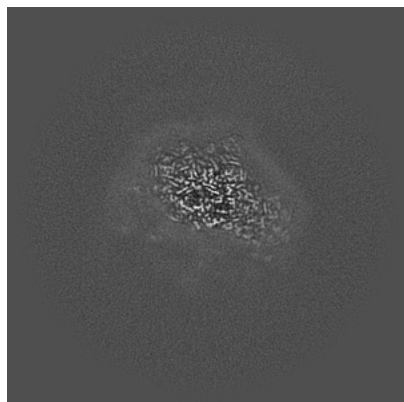


Z Index: 256

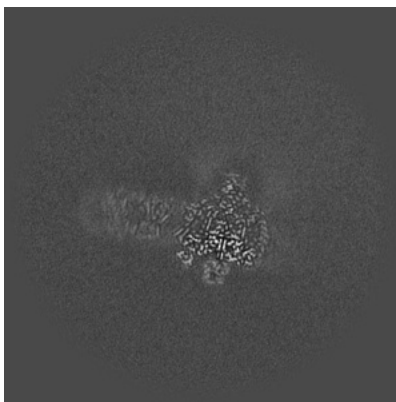
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

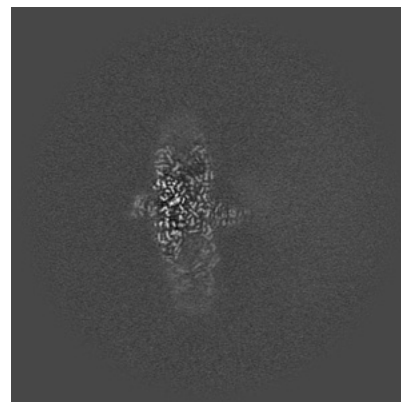
6.3.1 Primary map



X Index: 209

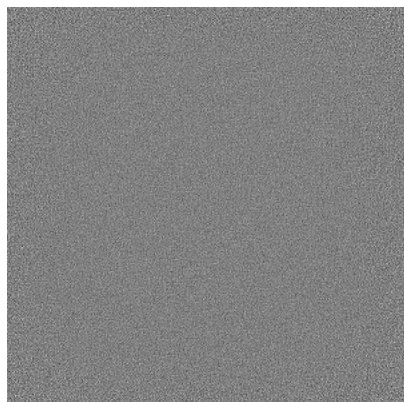


Y Index: 261

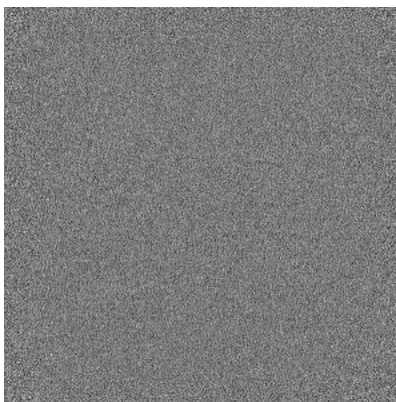


Z Index: 276

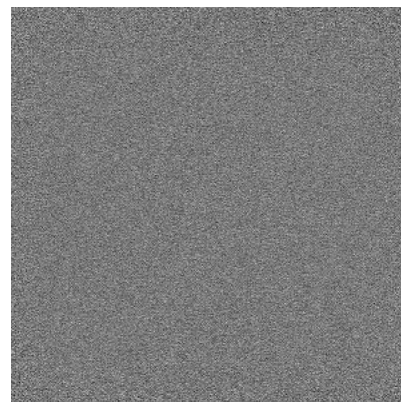
6.3.2 Raw map



X Index: 0



Y Index: 0

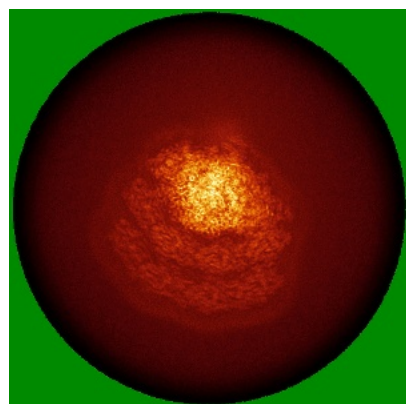


Z Index: 0

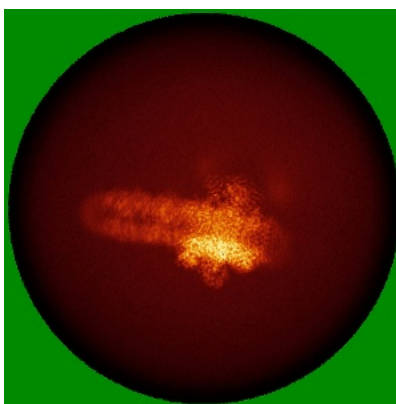
The images above show the largest variance slices of the map in three orthogonal directions.

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

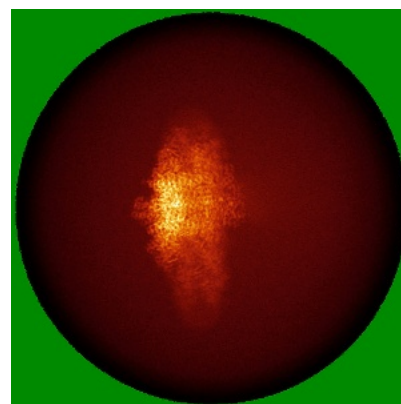
6.4.1 Primary map



X

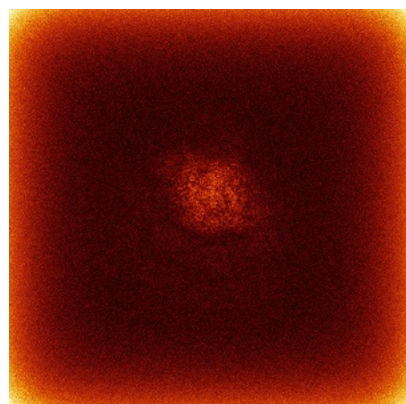


Y

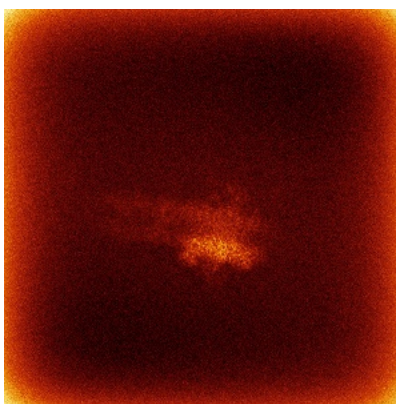


Z

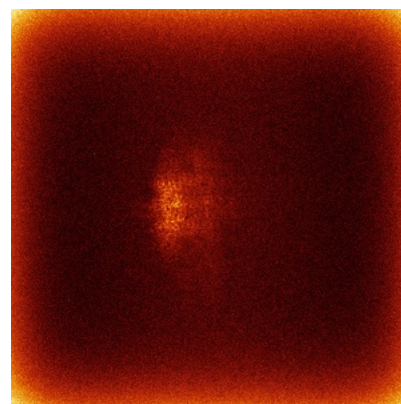
6.4.2 Raw map



X



Y

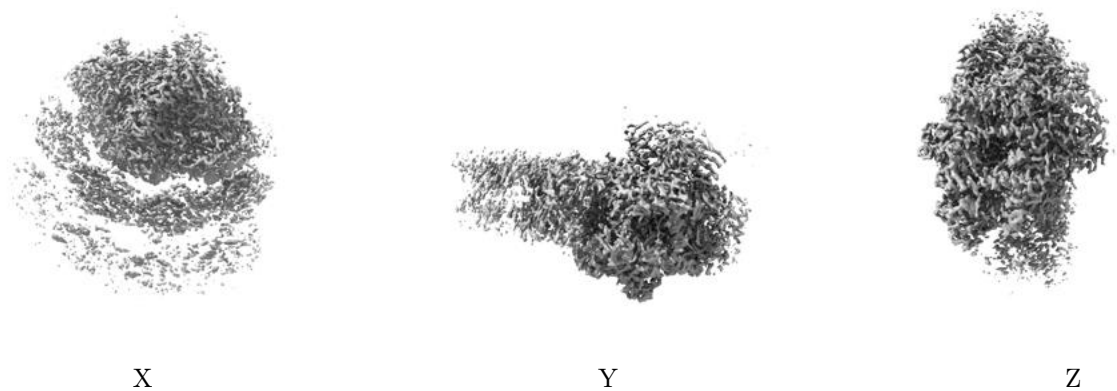


Z

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.

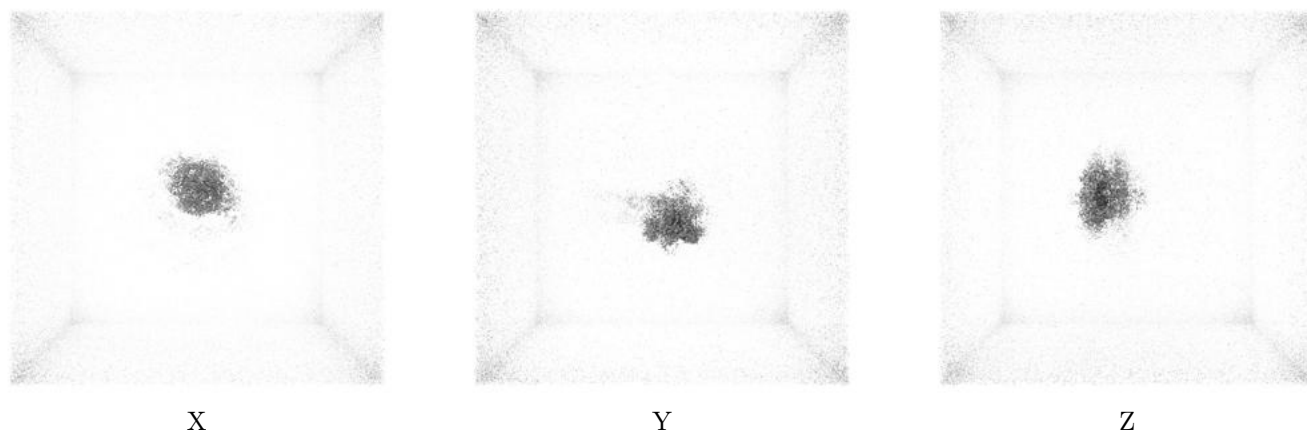
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

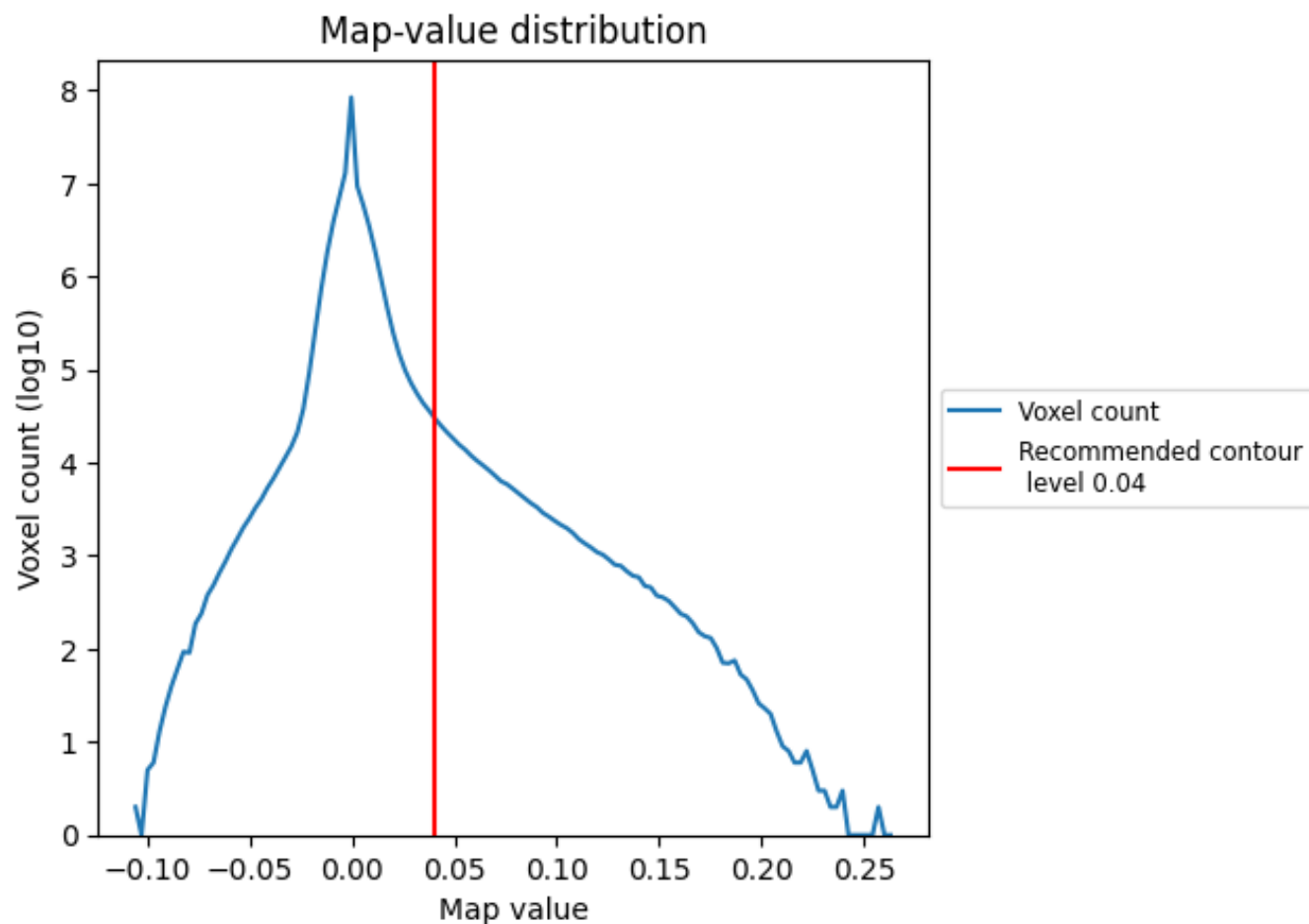
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

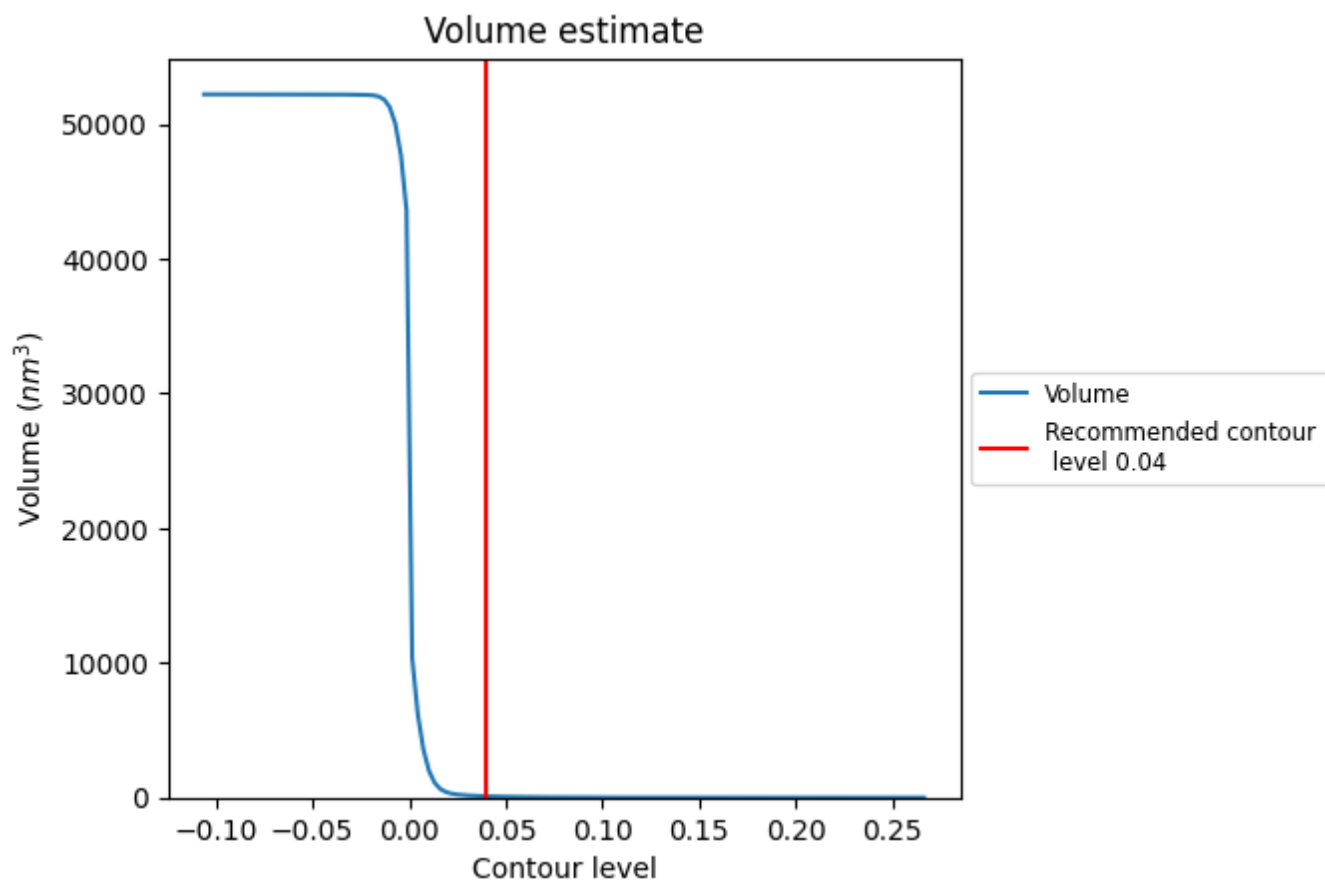
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

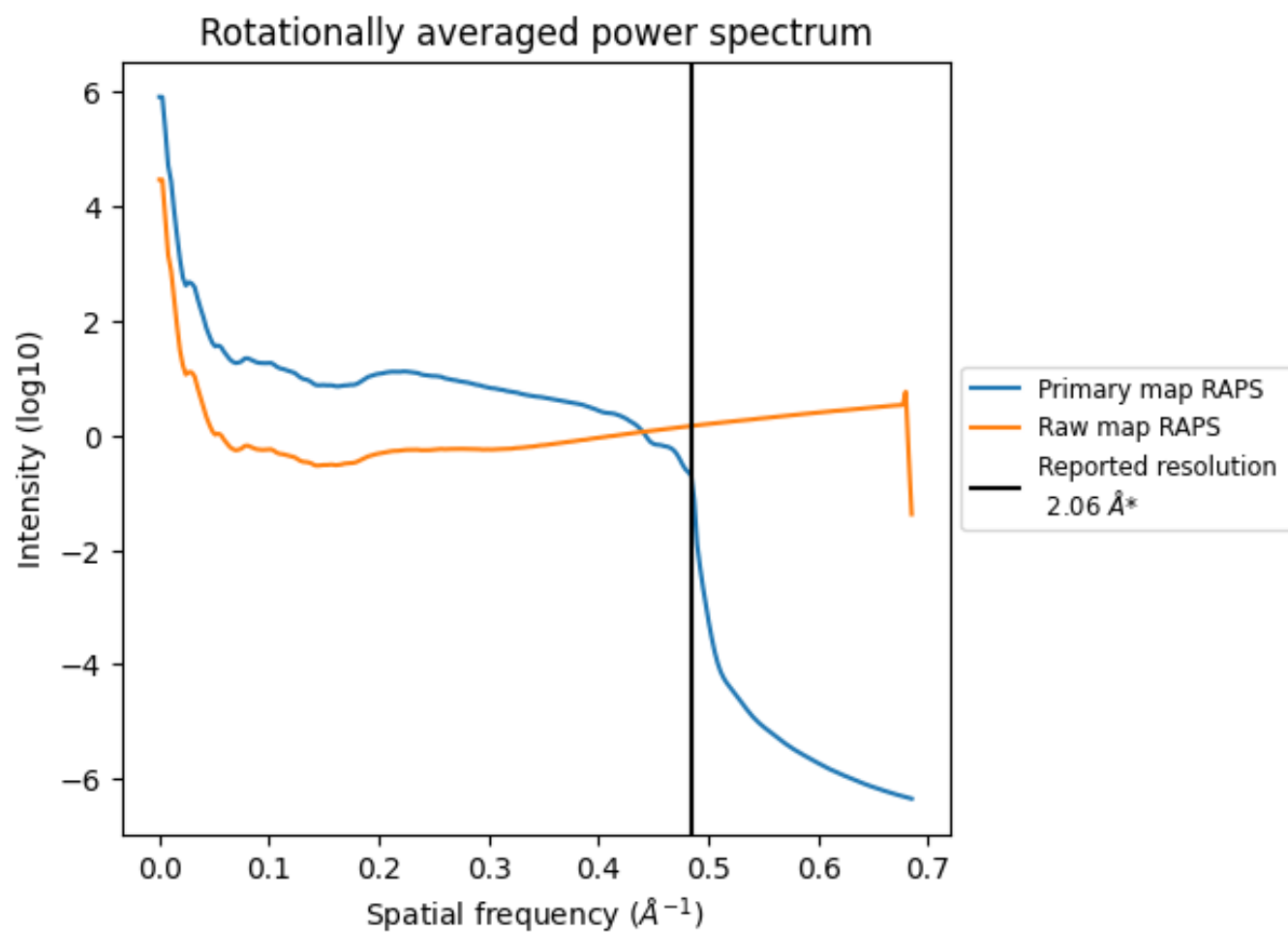
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 93 nm^3 ; this corresponds to an approximate mass of 84 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 ⓘ

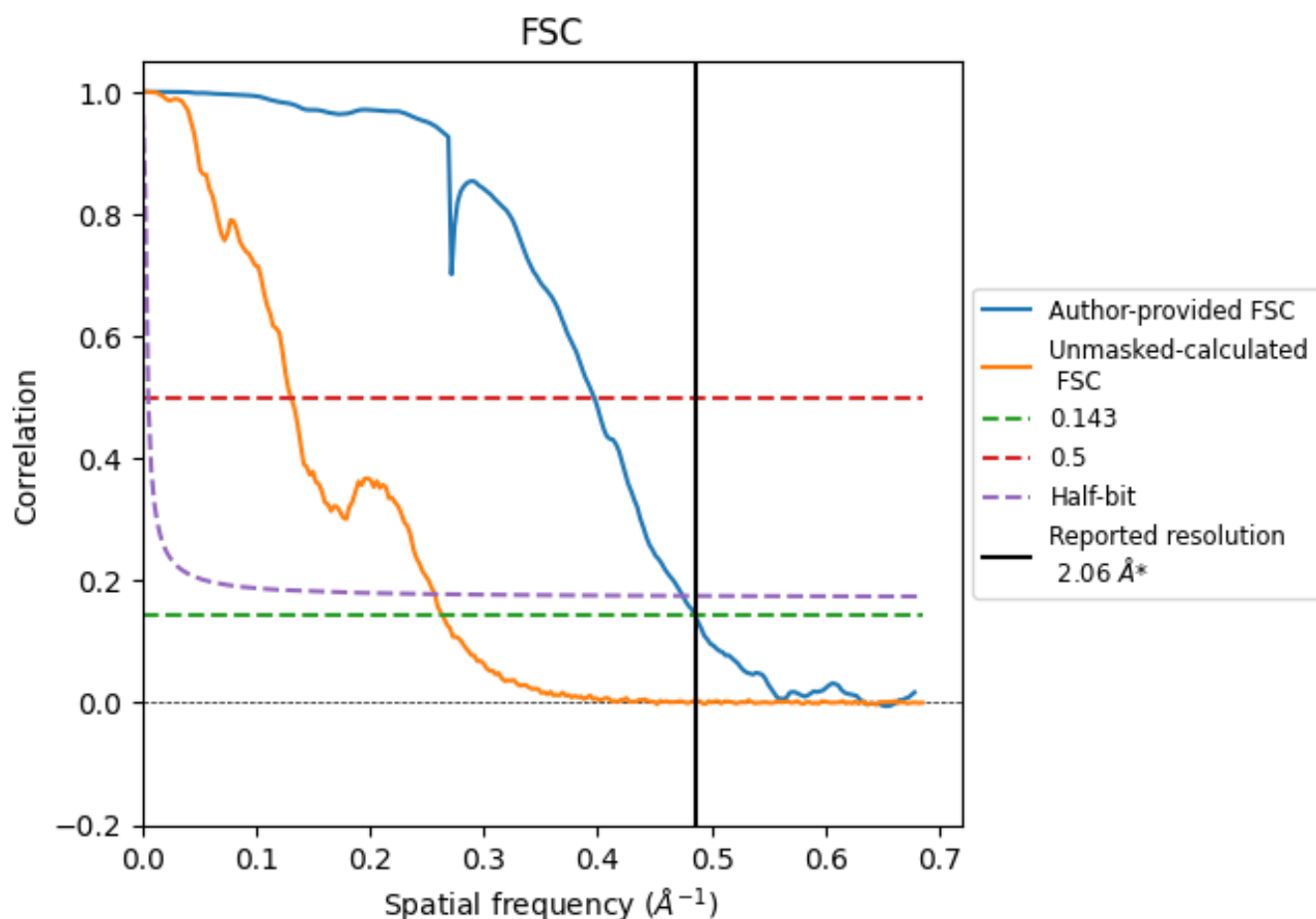


*Reported resolution corresponds to spatial frequency of $0.485 \text{ \AA}^{-1}$

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 0.485 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

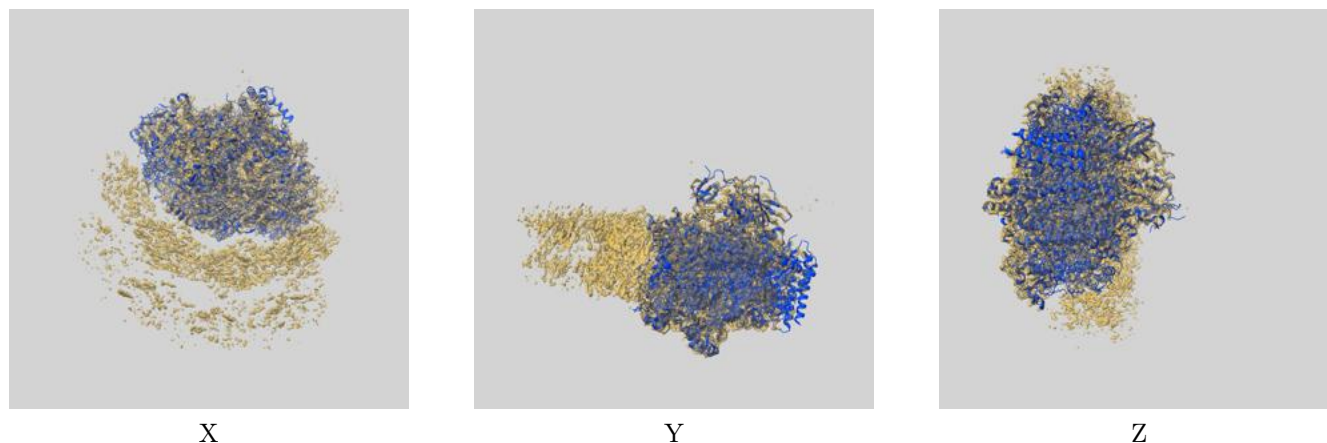
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.06	-	-
Author-provided FSC curve	2.06	2.52	2.11
Unmasked-calculated*	3.79	7.66	3.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.79 differs from the reported value 2.06 by more than 10 %

9 Map-model fit [i](#)

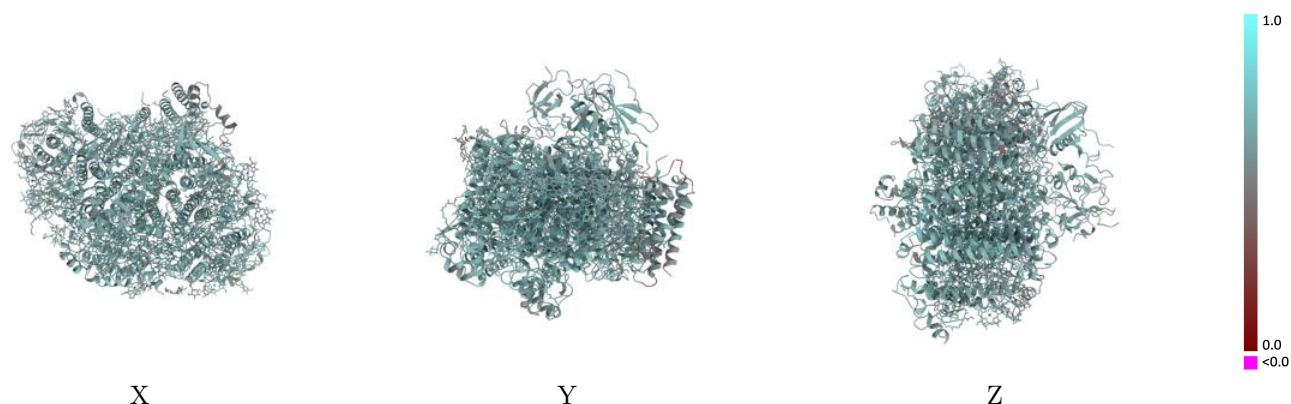
This section contains information regarding the fit between EMDB map EMD-54804 and PDB model 9SE7. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



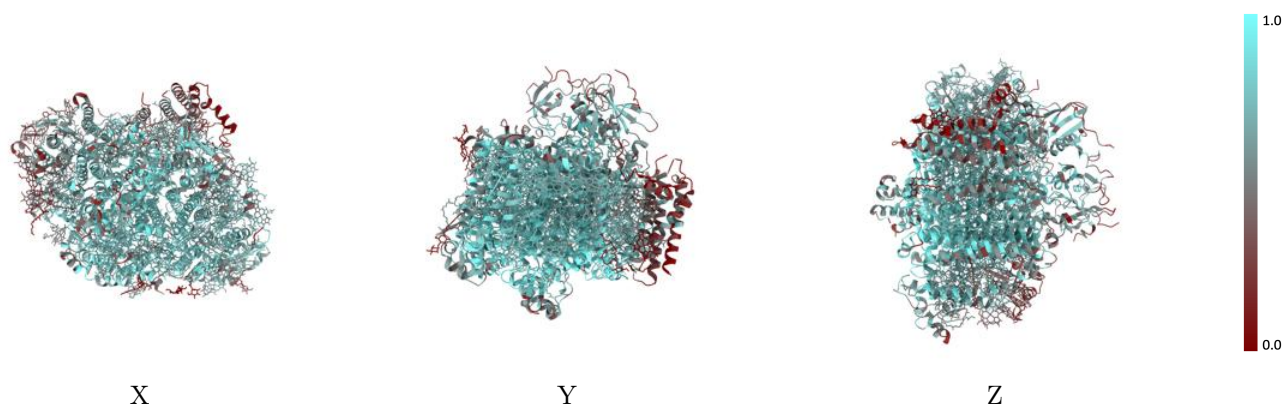
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



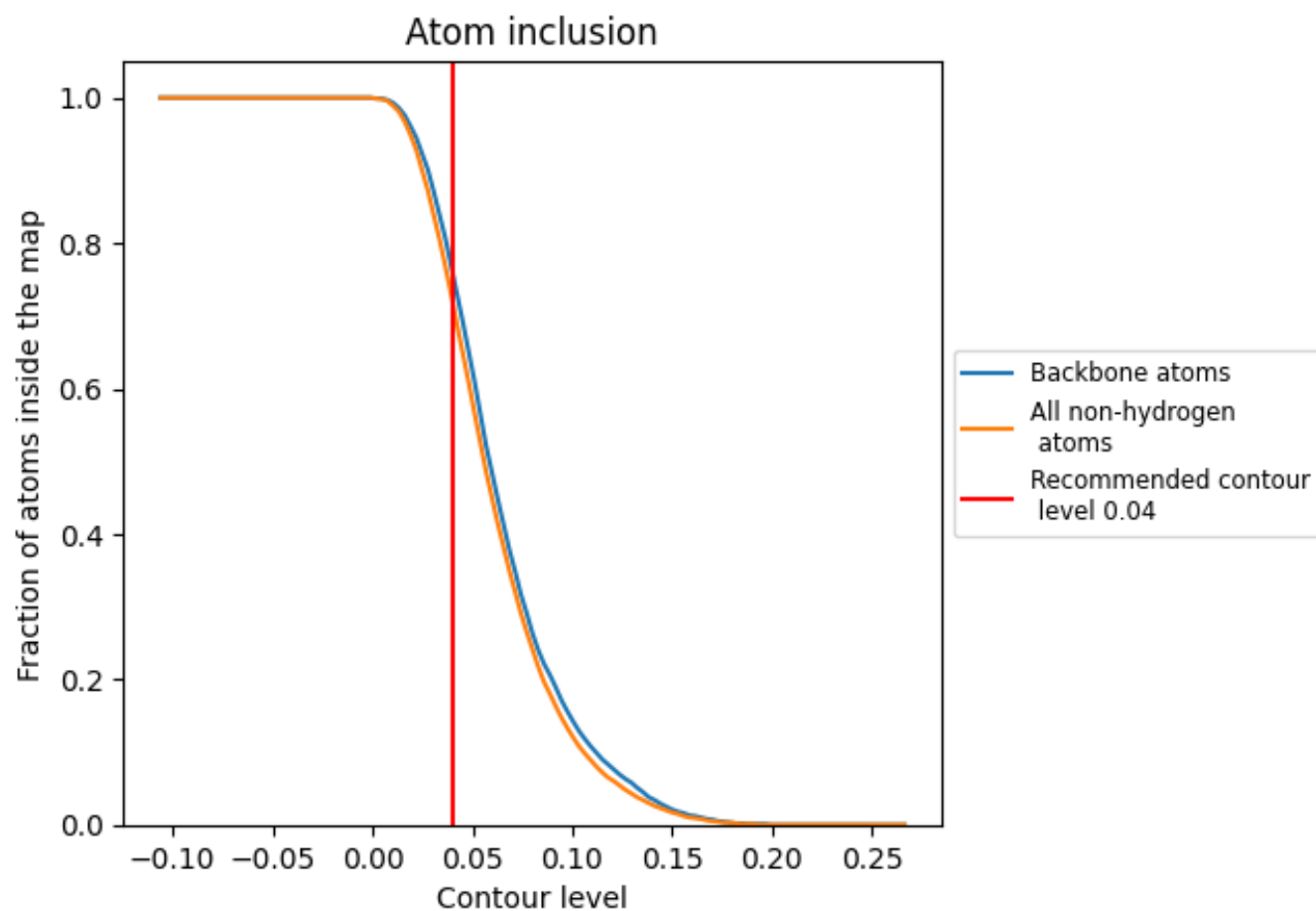
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7210	0.6500
A	0.8010	0.6660
B	0.7490	0.6590
C	0.6900	0.6350
D	0.5190	0.6200
E	0.5210	0.6040
F	0.7400	0.6460
I	0.4670	0.6210
J	0.6830	0.6380
L	0.2720	0.5550
T	0.6650	0.6120

1.0

0.0

<0.0