



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 05:15 AM JST

PDB ID : 7DR0 / pdb_00007dr0
EMDB ID : EMD-30820
Title : Structure of Wild-type PSI monomer1 from *Cyanophora paradoxa*
Authors : Kato, K.; Nagao, R.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on : 2020-12-25
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

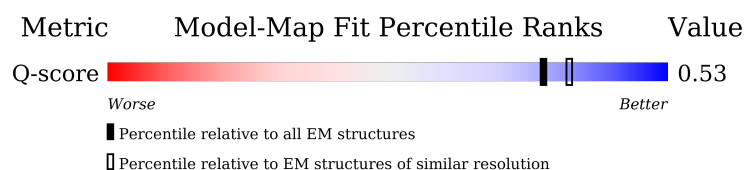
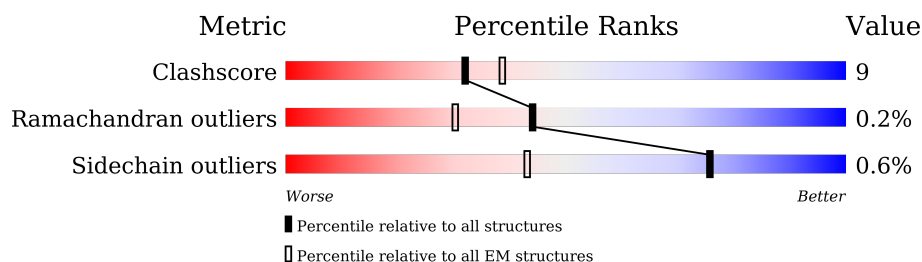
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



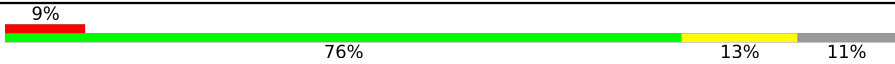
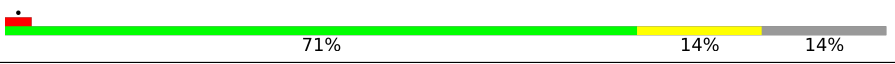
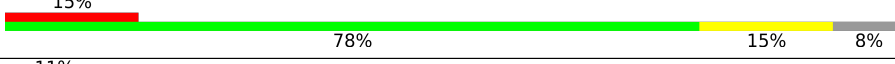
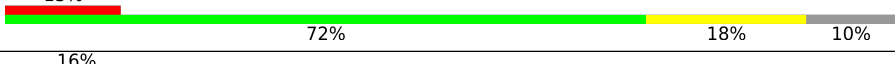
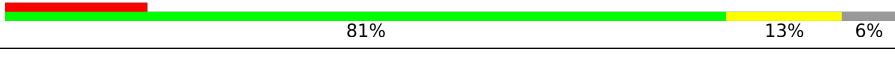
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	752	
2	B	737	
3	C	81	
4	D	220	

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Mol	Chain	Length	Quality of chain
5	E	70	
6	F	186	
7	I	35	
8	J	40	
9	K	157	
10	L	146	
11	M	31	

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
15	SF4	A	846	-	-	X	-
15	SF4	C	102	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 22745 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	739	Total	C	N	O	S	0	0
			5803	3794	987	999	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	706	Total	C	N	O	S	0	0
			5622	3688	950	972	12		

- 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	367	106	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1082	691	190	199	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	62	Total	C	N	O	S	0	0
			508	322	87	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	161	Total	C	N	O	S	0	0
			1255	795	220	238	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	30	Total	C	N	O	S	0	0
			228	155	31	40	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	37	Total	C	N	O	S	0	0
			292	199	43	50			

- Molecule 9 is a protein called Photosystem I reaction center subunit Psak 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	57	Total	C	N	O	S	0	0
			403	269	65	67	2		

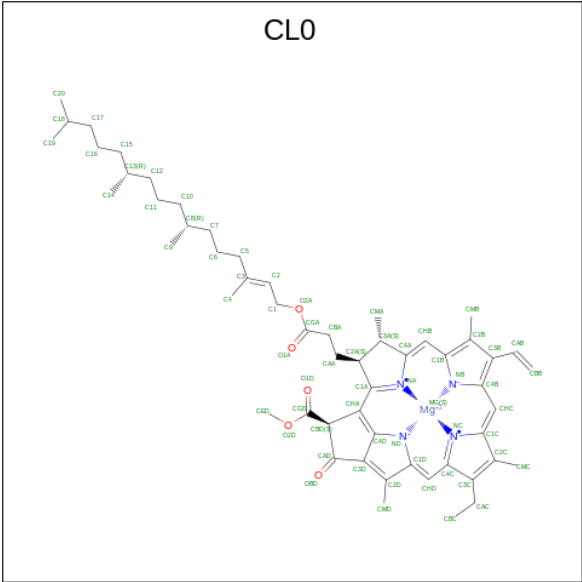
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	131	Total	C	N	O	S	0	0
			965	626	160	177	2		

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

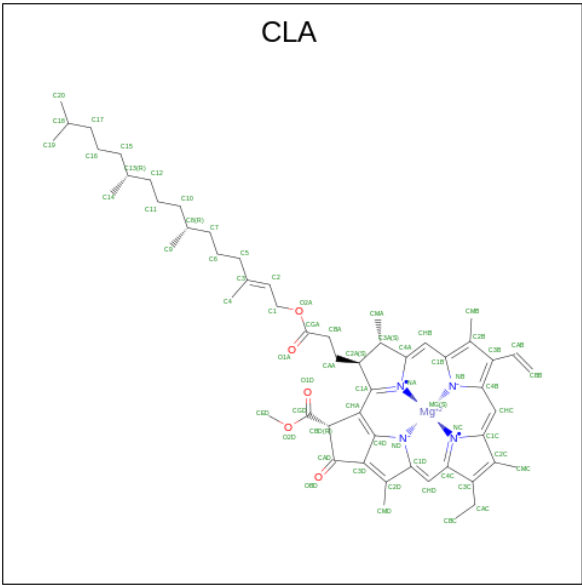
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	29	Total	C	N	O	S	0	0
			215	145	34	36			

- Molecule 12 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 45	C 35	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 51	C 41	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 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	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 54	C 44	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 49	C 39	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 54	C 44	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 61	C 51	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 51	C 41	Mg 1	N 4	O 5	0
13	A	1	Total 47	C 37	Mg 1	N 4	O 5	0

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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 55	C 45	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 50	C 40	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 54	C 44	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	A	1	Total 56	C 46	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 51	C 41	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 52	C 42	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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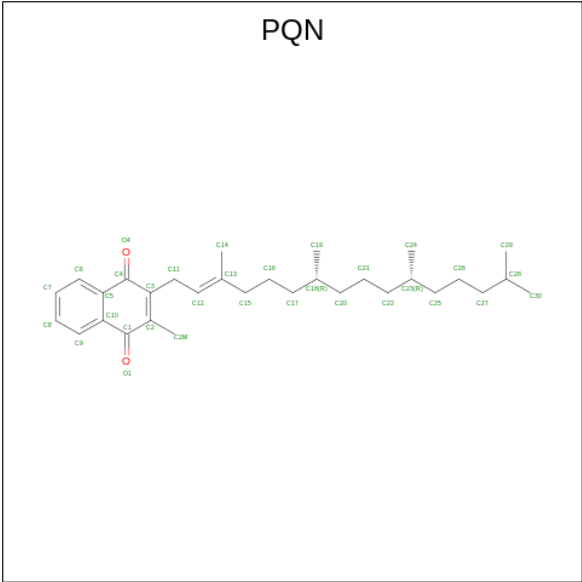
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13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 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
13	B	1	Total 45	C 35	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 56	C 46	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 46	C 36	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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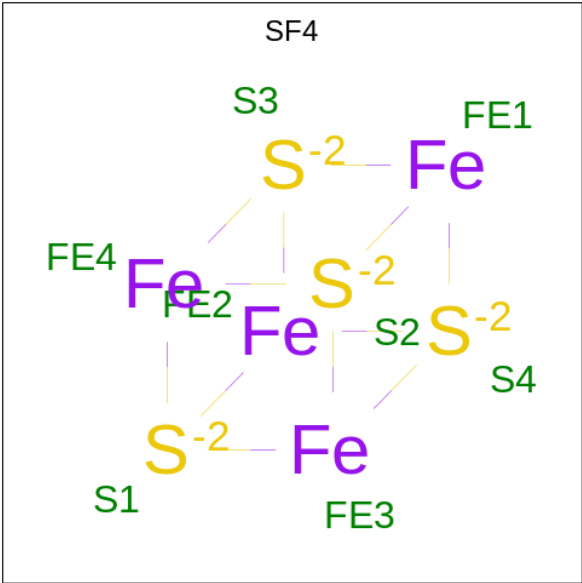
Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			47	37	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
			45	35	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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 IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



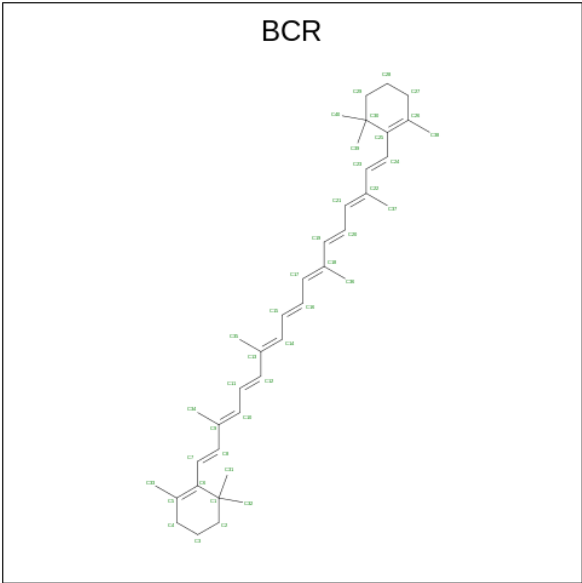
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



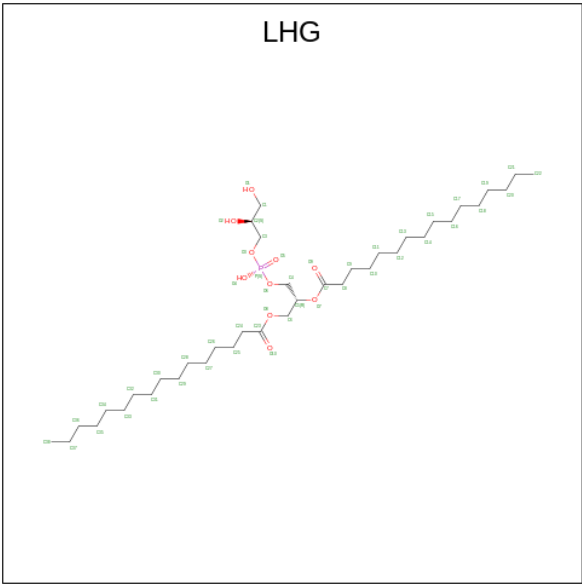
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	F	1	Total	C	0
			40	40	
16	F	1	Total	C	0
			40	40	

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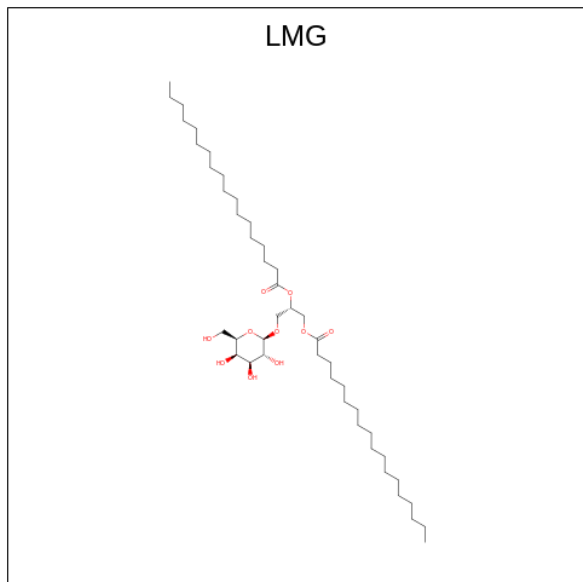
Mol	Chain	Residues	Atoms		AltConf
16	I	1	Total	C	0
			40	40	
16	J	1	Total	C	0
			40	40	
16	J	1	Total	C	0
			40	40	
16	J	1	Total	C	0
			40	40	
16	K	1	Total	C	0
			40	40	
16	L	1	Total	C	0
			40	40	
16	L	1	Total	C	0
			40	40	
16	L	1	Total	C	0
			40	40	
16	M	1	Total	C	0
			40	40	

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



Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

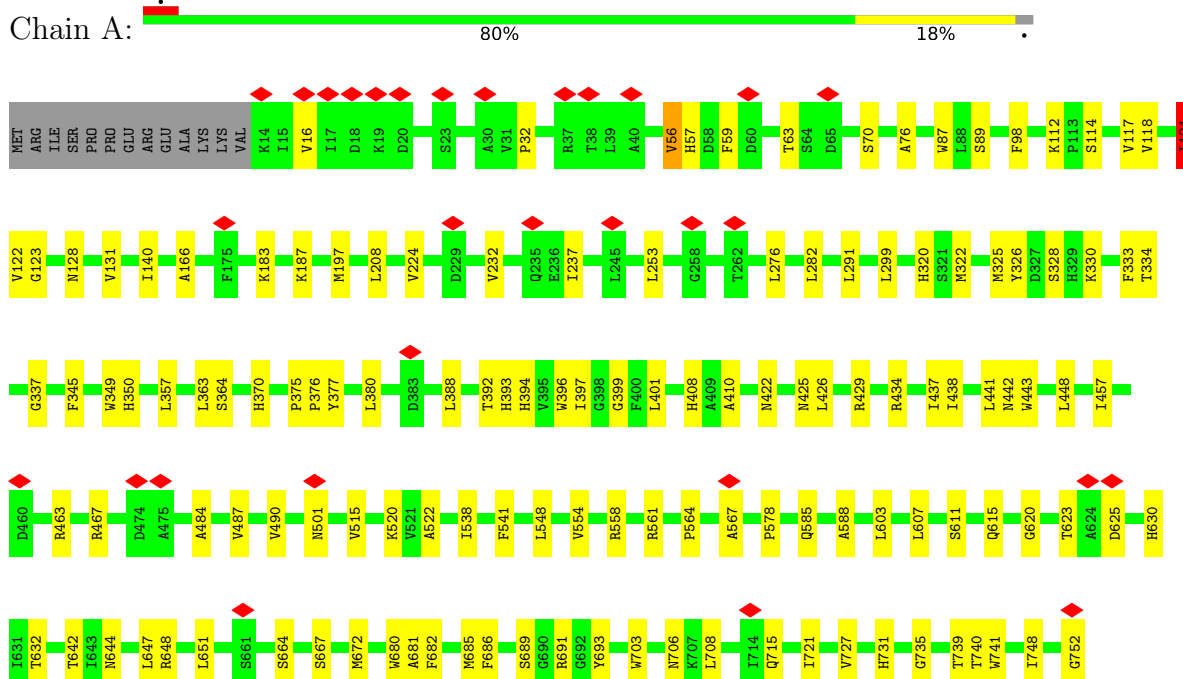


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	B	1	55	45	10	0

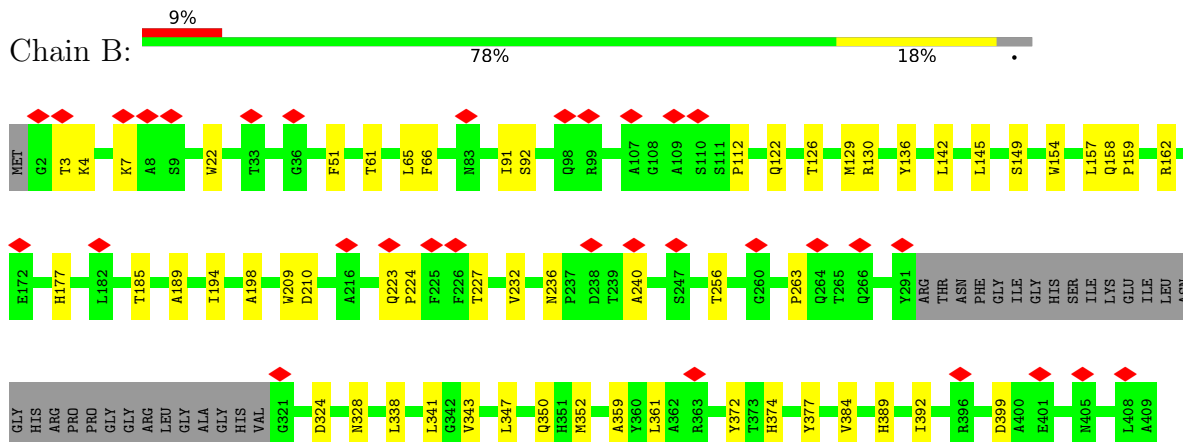
3 Residue-property plots

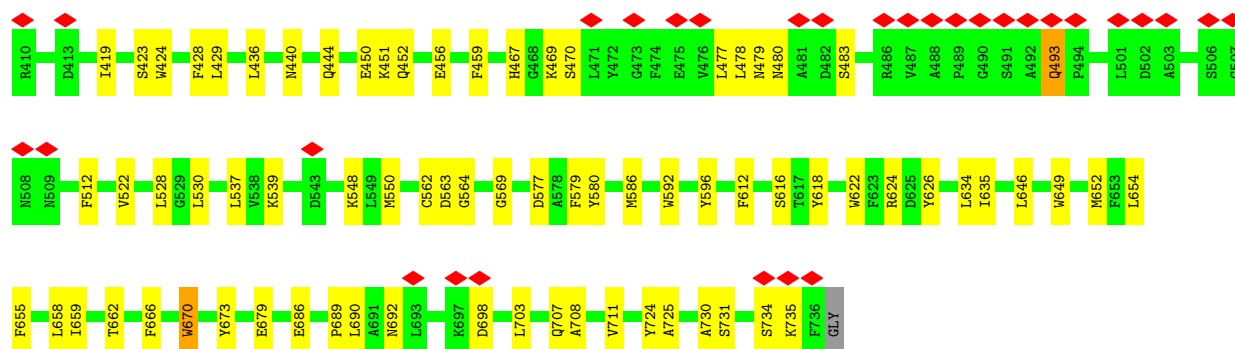
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

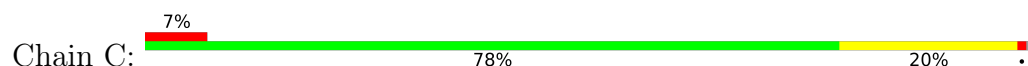


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

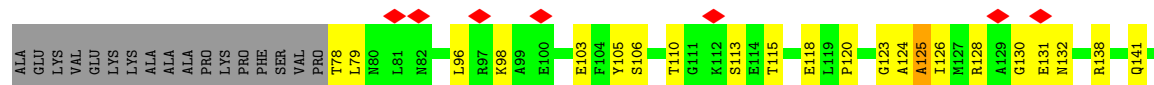
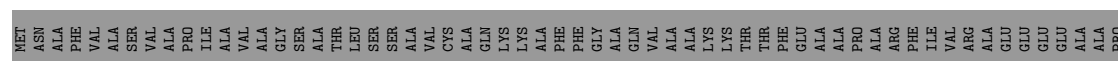




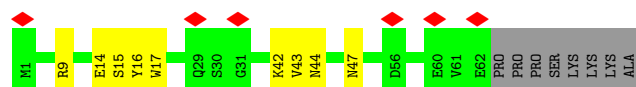
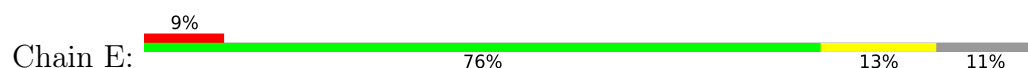
• Molecule 3: Photosystem I iron-sulfur center



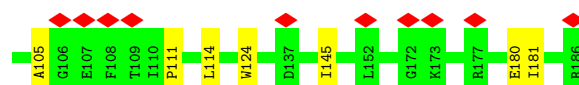
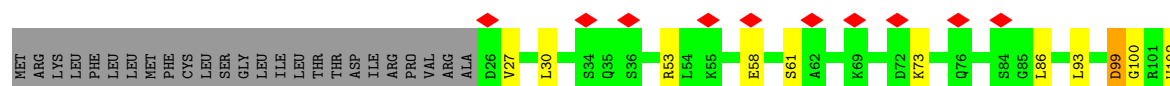
• Molecule 4: Photosystem I reaction center subunit II, cyanelle



• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III



Chain I:

Chain J:

[illegible]

Chain L:

13% 72% 18% 10%

MET ALA LYS ASP ASP VAL LYS PRO PHE TYR ASP ASP ALA PHE L115 L118 S119 N24 S25 S26 A27 V28 N29 G30 L31 L32 A33 N34 L35 T43 P44 P45 L46 R47 G61 P62 F65 L66 G67 R70 N71 T72 D73 V84 G85 L86 V87 V88 T91 L94

Chain M:

Amino Acid	Count	Percentage
MET	1	1%
L2	1	1%
A3	1	1%
D4	1	1%
I7	1	1%
F8	1	1%
T9	1	1%
A10	1	1%
A21	1	1%
L22	1	1%
L26	1	1%
E27	1	1%
K30	1	1%
PHE	1	1%
Green	81	81%
Red	16	16%
Yellow	13	13%
Grey	6	6%

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70920	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.396	Depositor
Minimum map value	-0.211	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	437.2, 437.2, 437.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.093, 1.093, 1.093	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.33	0/6000	0.49	2/8177 (0.0%)
2	B	0.29	0/5820	0.49	1/7955 (0.0%)
3	C	0.27	0/611	0.62	2/828 (0.2%)
4	D	0.28	0/1105	0.85	6/1489 (0.4%)
5	E	0.24	0/516	0.42	0/696
6	F	0.22	0/1281	0.51	0/1733
7	I	0.30	0/232	0.68	0/319
8	J	0.24	0/300	0.53	0/410
9	K	0.23	0/414	0.49	0/564
10	L	0.26	0/988	0.59	2/1342 (0.1%)
11	M	0.21	0/217	0.44	0/295
All	All	0.29	0/17484	0.53	13/23808 (0.1%)

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	3
4	D	0	3
6	F	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	125	ALA	CA-C-N	6.97	134.51	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	125	ALA	C-N-CA	6.97	134.51	121.97
4	D	130	GLY	CA-C-N	6.60	133.57	121.70
4	D	130	GLY	C-N-CA	6.60	133.57	121.70
10	L	73	ASP	CA-C-N	6.36	133.15	121.70

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	SER	Peptide
2	B	478	LEU	Peptide
2	B	493	GLN	Peptide
2	B	670	TRP	Peptide
4	D	124	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5803	0	5621	97	0
2	B	5622	0	5406	95	0
3	C	601	0	576	14	0
4	D	1082	0	1099	22	0
5	E	508	0	507	7	0
6	F	1255	0	1249	13	0
7	I	228	0	247	4	0
8	J	292	0	302	5	0
9	K	403	0	421	2	0
10	L	965	0	970	19	0
11	M	215	0	239	4	0
12	A	65	0	72	2	0
13	A	2441	0	2362	87	0
13	B	1945	0	1960	80	0
13	F	45	0	33	0	0
13	J	45	0	33	2	0
13	K	86	0	62	0	0
13	L	163	0	148	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	33	0	46	4	0
14	B	33	0	46	5	0
15	A	8	0	0	2	0
15	C	16	0	0	4	0
16	A	200	0	280	18	0
16	B	120	0	168	8	0
16	F	80	0	112	8	0
16	I	40	0	56	5	0
16	J	120	0	168	12	0
16	K	40	0	56	3	0
16	L	120	0	168	6	0
16	M	40	0	56	4	0
17	A	76	0	98	1	0
18	B	55	0	86	1	0
All	All	22745	0	22647	388	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 9.

The worst 5 of 388 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)
3:C:17:CYS:HB3	15:C:102:SF4:S4	2.29	0.72
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.72	0.70
13:B:830:CLA:H71	13:B:830:CLA:HBB1	1.73	0.69
15:A:846:SF4:S3	2:B:562:CYS:CB	2.78	0.69
2:B:338:LEU:HD21	13:B:823:CLA:HAB	1.75	0.68

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	737/752 (98%)	692 (94%)	44 (6%)	1 (0%)	48	75
2	B	702/737 (95%)	670 (95%)	32 (5%)	0	100	100
3	C	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	35
4	D	137/220 (62%)	110 (80%)	25 (18%)	2 (2%)	8	32
5	E	60/70 (86%)	53 (88%)	7 (12%)	0	100	100
6	F	159/186 (86%)	153 (96%)	5 (3%)	1 (1%)	21	52
7	I	28/35 (80%)	27 (96%)	1 (4%)	0	100	100
8	J	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
9	K	55/157 (35%)	53 (96%)	2 (4%)	0	100	100
10	L	129/146 (88%)	116 (90%)	13 (10%)	0	100	100
11	M	27/31 (87%)	27 (100%)	0	0	100	100
All	All	2147/2455 (88%)	2010 (94%)	132 (6%)	5 (0%)	44	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
3	C	63	LEU
4	D	126	ILE
4	D	165	PRO
6	F	100	GLY

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	598/610 (98%)	593 (99%)	5 (1%)	73	79
2	B	574/596 (96%)	572 (100%)	2 (0%)	86	86
3	C	67/68 (98%)	65 (97%)	2 (3%)	36	61
4	D	114/171 (67%)	114 (100%)	0	100	100
5	E	58/65 (89%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	133/156 (85%)	131 (98%)	2 (2%)	57	72
7	I	27/31 (87%)	27 (100%)	0	100	100
8	J	32/35 (91%)	32 (100%)	0	100	100
9	K	40/103 (39%)	40 (100%)	0	100	100
10	L	99/111 (89%)	99 (100%)	0	100	100
11	M	21/23 (91%)	21 (100%)	0	100	100
All	All	1763/1969 (90%)	1752 (99%)	11 (1%)	76	81

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	23	THR
3	C	63	LEU
6	F	145	ILE
6	F	27	VAL
1	A	740	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	262	HIS
6	F	131	GLN
2	B	440	ASN
9	K	120	GLN
4	D	173	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

111 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
13	CLA	A	806	1	69,73,73	1.93	19 (27%)	83,113,113	2.93	34 (40%)
16	BCR	A	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.35	8 (14%)
13	CLA	B	823	2	69,73,73	2.02	18 (26%)	83,113,113	2.78	29 (34%)
13	CLA	A	842	-	55,59,73	2.26	20 (36%)	66,96,113	3.23	32 (48%)
13	CLA	A	821	1	65,69,73	2.04	19 (29%)	78,108,113	2.90	30 (38%)
14	PQN	A	845	-	34,34,34	1.52	2 (5%)	42,45,45	1.09	3 (7%)
13	CLA	A	827	-	59,63,73	2.14	19 (32%)	71,101,113	3.13	32 (45%)
13	CLA	A	843	1	69,73,73	2.01	20 (28%)	83,113,113	2.79	29 (34%)
15	SF4	A	846	1,2	0,12,12	-	-	-	-	-
12	CL0	A	801	1	69,73,73	1.93	20 (28%)	83,113,113	2.86	35 (42%)
13	CLA	L	203	10	69,73,73	1.97	19 (27%)	83,113,113	2.91	28 (33%)
13	CLA	A	820	1	69,73,73	2.03	19 (27%)	83,113,113	2.76	32 (38%)
16	BCR	J	103	-	41,41,41	1.17	3 (7%)	56,56,56	1.38	9 (16%)
13	CLA	B	832	-	69,73,73	2.03	21 (30%)	83,113,113	2.82	30 (36%)
13	CLA	J	101	8	49,53,73	2.43	20 (40%)	59,89,113	3.24	28 (47%)
13	CLA	A	815	1	49,53,73	2.40	20 (40%)	59,89,113	3.26	29 (49%)
16	BCR	A	851	-	41,41,41	1.13	3 (7%)	56,56,56	1.27	6 (10%)
16	BCR	L	206	-	41,41,41	1.05	2 (4%)	56,56,56	1.37	8 (14%)
13	CLA	B	820	2	69,73,73	2.01	21 (30%)	83,113,113	2.82	30 (36%)
13	CLA	A	826	-	69,73,73	1.94	19 (27%)	83,113,113	2.67	28 (33%)
13	CLA	A	840	1	69,73,73	1.98	19 (27%)	83,113,113	2.88	33 (39%)
16	BCR	A	849	-	41,41,41	1.15	2 (4%)	56,56,56	1.33	8 (14%)
13	CLA	A	816	1	49,53,73	2.40	19 (38%)	59,89,113	3.29	25 (42%)
13	CLA	B	807	2	69,73,73	1.99	19 (27%)	83,113,113	2.82	30 (36%)
13	CLA	B	817	2	63,67,73	2.12	19 (30%)	75,105,113	2.95	29 (38%)
13	CLA	A	810	1	49,53,73	2.34	19 (38%)	59,89,113	3.16	30 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	825	2	69,73,73	1.95	18 (26%)	83,113,113	3.00	34 (40%)
16	BCR	B	836	-	41,41,41	1.13	2 (4%)	56,56,56	1.37	8 (14%)
13	CLA	B	813	2	69,73,73	2.02	21 (30%)	83,113,113	2.84	29 (34%)
13	CLA	B	818	2	64,68,73	2.07	18 (28%)	77,107,113	2.88	32 (41%)
13	CLA	A	834	1	69,73,73	1.99	20 (28%)	83,113,113	2.84	33 (39%)
13	CLA	A	838	1	55,59,73	2.21	20 (36%)	66,96,113	3.12	31 (46%)
16	BCR	B	837	-	41,41,41	1.21	4 (9%)	56,56,56	1.22	7 (12%)
13	CLA	A	809	1	69,73,73	2.00	21 (30%)	83,113,113	2.81	29 (34%)
14	PQN	B	834	-	34,34,34	1.44	2 (5%)	42,45,45	1.16	5 (11%)
13	CLA	B	809	2	69,73,73	1.97	18 (26%)	83,113,113	2.83	31 (37%)
13	CLA	B	805	2	58,62,73	2.17	18 (31%)	69,99,113	3.12	31 (44%)
13	CLA	A	819	1	58,62,73	2.19	20 (34%)	69,99,113	3.04	33 (47%)
13	CLA	A	824	1	55,59,73	2.24	22 (40%)	66,96,113	3.12	29 (43%)
13	CLA	B	830	2	69,73,73	1.98	18 (26%)	83,113,113	2.87	31 (37%)
13	CLA	B	814	2	60,64,73	2.14	20 (33%)	72,102,113	2.98	30 (41%)
13	CLA	A	805	1	49,53,73	2.40	19 (38%)	59,89,113	3.30	28 (47%)
13	CLA	A	832	1	54,58,73	2.26	17 (31%)	65,95,113	3.09	32 (49%)
13	CLA	A	804	1	49,53,73	2.37	18 (36%)	59,89,113	3.26	29 (49%)
16	BCR	J	104	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	7 (12%)
13	CLA	A	831	1	69,73,73	1.98	19 (27%)	83,113,113	2.83	28 (33%)
13	CLA	L	202	10	50,54,73	2.41	21 (42%)	60,90,113	3.34	25 (41%)
13	CLA	B	806	2	69,73,73	1.99	20 (28%)	83,113,113	2.79	28 (33%)
13	CLA	A	837	1	49,53,73	2.42	21 (42%)	59,89,113	3.35	27 (45%)
13	CLA	B	833	2	69,73,73	2.00	18 (26%)	83,113,113	2.74	31 (37%)
16	BCR	L	205	-	41,41,41	1.14	3 (7%)	56,56,56	1.30	6 (10%)
13	CLA	A	829	1	69,73,73	1.98	20 (28%)	83,113,113	2.90	31 (37%)
16	BCR	F	201	-	41,41,41	1.20	2 (4%)	56,56,56	1.34	6 (10%)
13	CLA	B	826	2	62,66,73	2.14	20 (32%)	74,104,113	3.06	32 (43%)
13	CLA	A	823	1	69,73,73	1.99	19 (27%)	83,113,113	2.82	28 (33%)
16	BCR	L	201	-	41,41,41	1.21	2 (4%)	56,56,56	1.28	5 (8%)
13	CLA	B	810	2	69,73,73	1.98	17 (24%)	83,113,113	2.70	30 (36%)
13	CLA	B	831	2	51,55,73	2.30	21 (41%)	61,91,113	3.26	28 (45%)
13	CLA	B	802	2	69,73,73	1.91	19 (27%)	83,113,113	2.99	35 (42%)
18	LMG	B	838	-	55,55,55	0.78	1 (1%)	63,63,63	1.42	7 (11%)
13	CLA	A	813	1	58,62,73	2.18	19 (32%)	69,99,113	3.00	28 (40%)

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	1.95	19 (27%)	83,113,113	2.85	34 (40%)
13	CLA	A	822	-	69,73,73	2.00	20 (28%)	83,113,113	2.75	28 (33%)
13	CLA	B	801	-	69,73,73	1.98	20 (28%)	83,113,113	2.70	32 (38%)
13	CLA	B	815	2	49,53,73	2.39	20 (40%)	59,89,113	3.29	26 (44%)
13	CLA	B	819	-	50,54,73	2.39	21 (42%)	60,90,113	3.26	28 (46%)
13	CLA	B	824	2	53,57,73	2.31	20 (37%)	62,93,113	3.36	28 (45%)
16	BCR	J	102	-	41,41,41	1.13	2 (4%)	56,56,56	1.30	7 (12%)
13	CLA	A	808	1	55,59,73	2.30	19 (34%)	66,96,113	3.05	30 (45%)
13	CLA	B	812	2	49,53,73	2.40	19 (38%)	59,89,113	3.24	28 (47%)
13	CLA	B	808	2	69,73,73	1.99	19 (27%)	83,113,113	2.86	31 (37%)
13	CLA	A	835	1	69,73,73	1.97	20 (28%)	83,113,113	2.97	31 (37%)
15	SF4	C	102	3	0,12,12	-	-	-	-	-
17	LHG	A	852	-	48,48,48	0.71	1 (2%)	51,54,54	1.30	7 (13%)
13	CLA	B	804	-	69,73,73	1.95	19 (27%)	83,113,113	2.83	30 (36%)
13	CLA	A	812	1	69,73,73	2.01	19 (27%)	83,113,113	2.83	30 (36%)
13	CLA	B	816	2	59,63,73	2.17	21 (35%)	71,101,113	3.06	29 (40%)
13	CLA	B	828	-	49,53,73	2.42	20 (40%)	59,89,113	3.37	28 (47%)
13	CLA	A	802	-	69,73,73	1.95	18 (26%)	83,113,113	2.94	31 (37%)
13	CLA	A	836	1	58,62,73	2.16	19 (32%)	69,99,113	3.00	29 (42%)
13	CLA	K	203	-	49,53,73	2.36	21 (42%)	59,89,113	3.20	29 (49%)
13	CLA	A	814	1	49,53,73	2.40	19 (38%)	59,89,113	3.16	27 (45%)
13	CLA	F	203	6	49,53,73	2.42	20 (40%)	59,89,113	3.21	26 (44%)
13	CLA	A	811	1	49,53,73	2.39	19 (38%)	59,89,113	3.20	27 (45%)
13	CLA	B	811	2	69,73,73	2.02	21 (30%)	83,113,113	2.79	31 (37%)
13	CLA	A	828	1	69,73,73	1.96	17 (24%)	83,113,113	2.83	30 (36%)
13	CLA	L	204	-	56,60,73	2.24	20 (35%)	67,97,113	3.15	29 (43%)
16	BCR	F	202	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	9 (16%)
16	BCR	K	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.35	9 (16%)
13	CLA	B	822	2	69,73,73	1.98	18 (26%)	83,113,113	2.74	30 (36%)
13	CLA	A	807	1	69,73,73	1.98	18 (26%)	83,113,113	2.91	32 (38%)
13	CLA	A	817	-	53,57,73	2.30	19 (35%)	62,93,113	3.09	27 (43%)
13	CLA	A	833	1	69,73,73	2.00	17 (24%)	83,113,113	2.81	30 (36%)
16	BCR	A	848	-	41,41,41	1.09	2 (4%)	56,56,56	1.49	12 (21%)
16	BCR	M	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	6 (10%)
16	BCR	A	850	-	41,41,41	1.20	2 (4%)	56,56,56	1.37	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	B	835	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	5 (8%)
13	CLA	A	841	1	69,73,73	2.04	22 (31%)	83,113,113	2.78	32 (38%)
15	SF4	C	101	3	0,12,12	-	-	-	-	-
13	CLA	A	818	1	69,73,73	1.98	19 (27%)	83,113,113	2.86	27 (32%)
17	LHG	A	853	13	26,26,48	0.84	0	29,32,54	1.32	3 (10%)
13	CLA	B	827	2	49,53,73	2.44	21 (42%)	59,89,113	3.23	28 (47%)
13	CLA	A	844	17	56,60,73	2.24	18 (32%)	67,97,113	3.20	28 (41%)
13	CLA	A	803	-	49,53,73	2.39	20 (40%)	59,89,113	3.23	27 (45%)
13	CLA	A	839	1	60,64,73	2.12	18 (30%)	72,102,113	3.01	30 (41%)
13	CLA	B	803	-	69,73,73	1.93	21 (30%)	83,113,113	2.97	31 (37%)
13	CLA	B	829	2	50,54,73	2.32	17 (34%)	60,90,113	3.25	29 (48%)
16	BCR	I	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.28	5 (8%)
13	CLA	A	830	1	69,73,73	1.96	20 (28%)	83,113,113	2.69	32 (38%)
13	CLA	A	825	1	51,55,73	2.36	19 (37%)	61,91,113	3.20	29 (47%)
13	CLA	K	201	9	46,49,73	2.34	17 (36%)	55,83,113	3.27	24 (43%)

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
13	CLA	A	806	1	-	14/39/115/115	-
16	BCR	A	847	-	-	11/29/63/63	0/2/2/2
13	CLA	B	823	2	-	16/39/115/115	-
13	CLA	A	842	-	-	8/23/99/115	-
13	CLA	A	821	1	-	9/35/111/115	-
14	PQN	A	845	-	-	2/23/43/43	0/2/2/2
13	CLA	A	827	-	-	9/27/103/115	-
13	CLA	A	843	1	-	12/39/115/115	-
15	SF4	A	846	1,2	-	-	0/6/5/5
12	CL0	A	801	1	-	5/39/115/115	-
13	CLA	L	203	10	-	15/39/115/115	-
13	CLA	A	820	1	-	14/39/115/115	-
16	BCR	J	103	-	-	17/29/63/63	0/2/2/2
13	CLA	B	832	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	J	101	8	-	8/15/91/115	-
13	CLA	A	815	1	-	7/15/91/115	-
16	BCR	A	851	-	-	21/29/63/63	0/2/2/2
16	BCR	L	206	-	-	18/29/63/63	0/2/2/2
13	CLA	B	820	2	-	10/39/115/115	-
13	CLA	A	826	-	-	17/39/115/115	-
13	CLA	A	840	1	-	16/39/115/115	-
16	BCR	A	849	-	-	11/29/63/63	0/2/2/2
13	CLA	A	816	1	-	9/15/91/115	-
13	CLA	B	807	2	-	14/39/115/115	-
13	CLA	B	817	2	-	16/32/108/115	-
13	CLA	A	810	1	-	5/15/91/115	-
13	CLA	B	825	2	-	12/39/115/115	-
16	BCR	B	836	-	-	10/29/63/63	0/2/2/2
13	CLA	B	813	2	-	20/39/115/115	-
13	CLA	B	818	2	-	5/33/109/115	-
13	CLA	A	834	1	-	16/39/115/115	-
13	CLA	A	838	1	-	7/23/99/115	-
16	BCR	B	837	-	-	9/29/63/63	0/2/2/2
13	CLA	A	809	1	-	19/39/115/115	-
14	PQN	B	834	-	-	9/23/43/43	0/2/2/2
13	CLA	B	809	2	-	9/39/115/115	-
13	CLA	B	805	2	-	11/26/102/115	-
13	CLA	A	819	1	-	10/26/102/115	-
13	CLA	A	824	1	-	12/23/99/115	-
13	CLA	B	830	2	-	9/39/115/115	-
13	CLA	B	814	2	-	8/29/105/115	-
13	CLA	A	805	1	-	4/15/91/115	-
13	CLA	A	832	1	-	8/21/97/115	-
13	CLA	A	804	1	-	6/15/91/115	-
16	BCR	J	104	-	-	9/29/63/63	0/2/2/2
13	CLA	A	831	1	-	11/39/115/115	-
13	CLA	L	202	10	-	7/17/93/115	-
13	CLA	B	806	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	837	1	-	9/15/91/115	-
13	CLA	B	833	2	-	18/39/115/115	-
16	BCR	L	205	-	-	11/29/63/63	0/2/2/2
13	CLA	A	829	1	-	16/39/115/115	-
16	BCR	F	201	-	-	12/29/63/63	0/2/2/2
13	CLA	B	826	2	-	15/31/107/115	-
13	CLA	A	823	1	-	17/39/115/115	-
16	BCR	L	201	-	-	9/29/63/63	0/2/2/2
13	CLA	B	810	2	-	13/39/115/115	-
13	CLA	B	831	2	-	4/18/94/115	-
13	CLA	B	802	2	-	19/39/115/115	-
18	LMG	B	838	-	-	27/50/70/70	0/1/1/1
13	CLA	A	813	1	-	7/26/102/115	-
13	CLA	B	821	2	-	19/39/115/115	-
13	CLA	A	822	-	-	14/39/115/115	-
13	CLA	B	801	-	-	12/39/115/115	-
13	CLA	B	815	2	-	8/15/91/115	-
13	CLA	B	819	-	-	6/17/93/115	-
13	CLA	B	824	2	-	11/20/96/115	-
16	BCR	J	102	-	-	13/29/63/63	0/2/2/2
13	CLA	A	808	1	-	9/23/99/115	-
13	CLA	B	812	2	-	2/15/91/115	-
13	CLA	B	808	2	-	11/39/115/115	-
13	CLA	A	835	1	-	16/39/115/115	-
17	LHG	A	852	-	-	18/53/53/53	-
15	SF4	C	102	3	-	-	0/6/5/5
13	CLA	B	804	-	-	15/39/115/115	-
13	CLA	A	812	1	-	12/39/115/115	-
13	CLA	B	816	2	-	7/27/103/115	-
13	CLA	B	828	-	-	4/15/91/115	-
13	CLA	A	802	-	-	6/39/115/115	-
13	CLA	A	836	1	-	11/26/102/115	-
13	CLA	K	203	-	-	5/15/91/115	-
13	CLA	A	814	1	-	12/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	F	203	6	-	4/15/91/115	-
13	CLA	A	811	1	-	8/15/91/115	-
13	CLA	B	811	2	-	12/39/115/115	-
13	CLA	A	828	1	-	14/39/115/115	-
13	CLA	L	204	-	-	9/24/100/115	-
16	BCR	F	202	-	-	13/29/63/63	0/2/2/2
16	BCR	K	202	-	-	8/29/63/63	0/2/2/2
13	CLA	B	822	2	-	16/39/115/115	-
13	CLA	A	807	1	-	13/39/115/115	-
13	CLA	A	817	-	-	3/20/96/115	-
13	CLA	A	833	1	-	10/39/115/115	-
16	BCR	A	848	-	-	10/29/63/63	0/2/2/2
16	BCR	M	101	-	-	14/29/63/63	0/2/2/2
16	BCR	A	850	-	-	15/29/63/63	0/2/2/2
16	BCR	B	835	-	-	11/29/63/63	0/2/2/2
13	CLA	A	841	1	-	12/39/115/115	-
15	SF4	C	101	3	-	-	0/6/5/5
13	CLA	A	818	1	-	12/39/115/115	-
17	LHG	A	853	13	-	12/31/31/53	-
13	CLA	B	827	2	-	1/15/91/115	-
13	CLA	A	844	17	-	13/24/100/115	-
13	CLA	A	803	-	-	3/15/91/115	-
13	CLA	A	839	1	-	9/29/105/115	-
13	CLA	B	803	-	-	14/39/115/115	-
13	CLA	B	829	2	-	9/17/93/115	-
16	BCR	I	101	-	-	7/29/63/63	0/2/2/2
13	CLA	A	830	1	-	15/39/115/115	-
13	CLA	A	825	1	-	5/18/94/115	-
13	CLA	K	201	9	-	3/9/81/115	-

The worst 5 of 1675 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	845	PQN	C3-C2	7.37	1.48	1.35
14	B	834	PQN	C3-C2	6.96	1.47	1.35
13	L	202	CLA	C3C-C2C	5.67	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	844	CLA	C3C-C2C	5.40	1.48	1.36
13	B	806	CLA	C3C-C2C	5.38	1.48	1.36

The worst 5 of 2657 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	825	CLA	C1D-ND-C4D	-10.56	98.84	106.33
13	A	803	CLA	C2B-C1B-NB	10.46	117.25	110.23
13	L	203	CLA	C1D-ND-C4D	-10.19	99.10	106.33
13	B	802	CLA	C1D-ND-C4D	-9.76	99.40	106.33
13	B	830	CLA	C1D-ND-C4D	-9.68	99.46	106.33

There are no chirality outliers.

5 of 1184 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	804	CLA	CHA-CBD-CGD-O1D
13	A	804	CLA	CHA-CBD-CGD-O2D
13	A	805	CLA	C2B-C3B-CAB-CBB
13	A	805	CLA	C4B-C3B-CAB-CBB
13	A	805	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

96 monomers are involved in 218 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	806	CLA	6	0
16	A	847	BCR	5	0
13	B	823	CLA	4	0
13	A	842	CLA	1	0
13	A	821	CLA	2	0
14	A	845	PQN	4	0
13	A	843	CLA	4	0
15	A	846	SF4	2	0
12	A	801	CL0	2	0
13	L	203	CLA	1	0
13	A	820	CLA	3	0
16	J	103	BCR	2	0
13	B	832	CLA	3	0
13	J	101	CLA	2	0
13	A	815	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	851	BCR	5	0
16	L	206	BCR	1	0
13	B	820	CLA	4	0
13	A	826	CLA	2	0
13	A	840	CLA	5	0
16	A	849	BCR	1	0
13	B	807	CLA	5	0
13	B	817	CLA	1	0
13	A	810	CLA	1	0
13	B	825	CLA	2	0
16	B	836	BCR	3	0
13	B	813	CLA	1	0
13	B	818	CLA	2	0
13	A	834	CLA	2	0
13	A	838	CLA	1	0
16	B	837	BCR	1	0
13	A	809	CLA	8	0
14	B	834	PQN	5	0
13	B	809	CLA	5	0
13	B	805	CLA	1	0
13	A	819	CLA	3	0
13	B	830	CLA	4	0
13	A	805	CLA	3	0
13	A	832	CLA	1	0
13	A	804	CLA	2	0
16	J	104	BCR	2	0
13	A	831	CLA	3	0
13	L	202	CLA	2	0
13	B	806	CLA	2	0
13	A	837	CLA	1	0
13	B	833	CLA	10	0
16	L	205	BCR	2	0
13	A	829	CLA	9	0
16	F	201	BCR	3	0
13	B	826	CLA	1	0
13	A	823	CLA	2	0
16	L	201	BCR	3	0
13	B	810	CLA	1	0
13	B	831	CLA	1	0
13	B	802	CLA	5	0
18	B	838	LMG	1	0
13	A	813	CLA	1	0

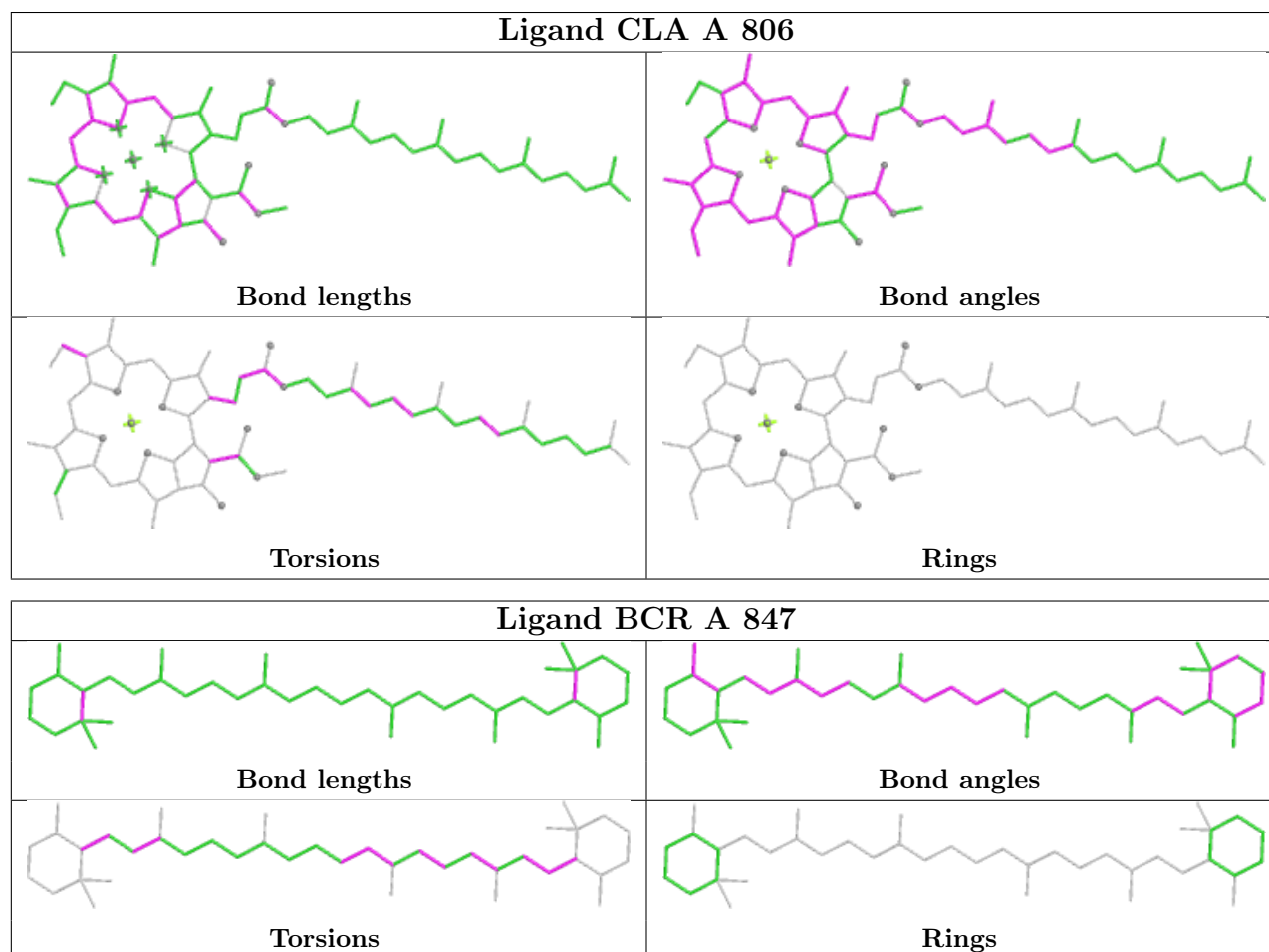
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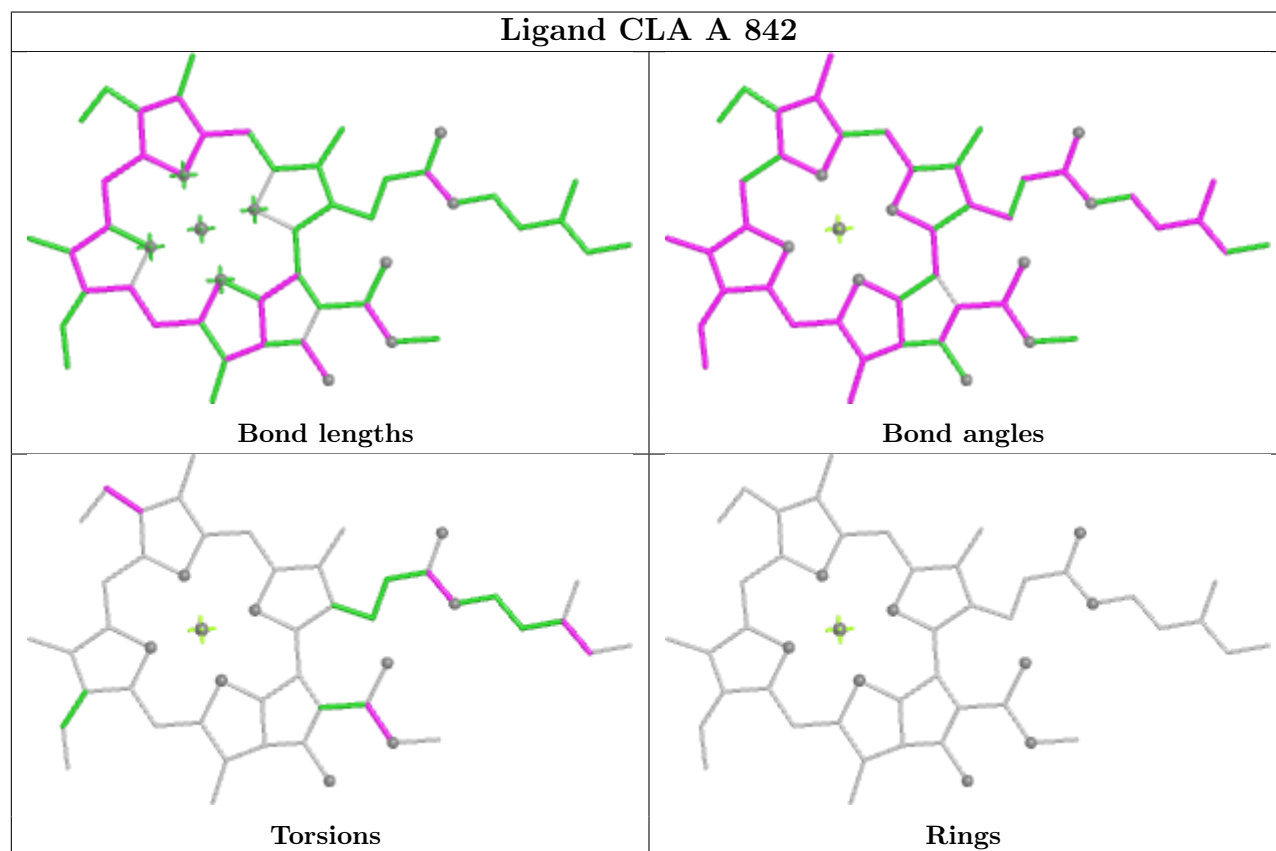
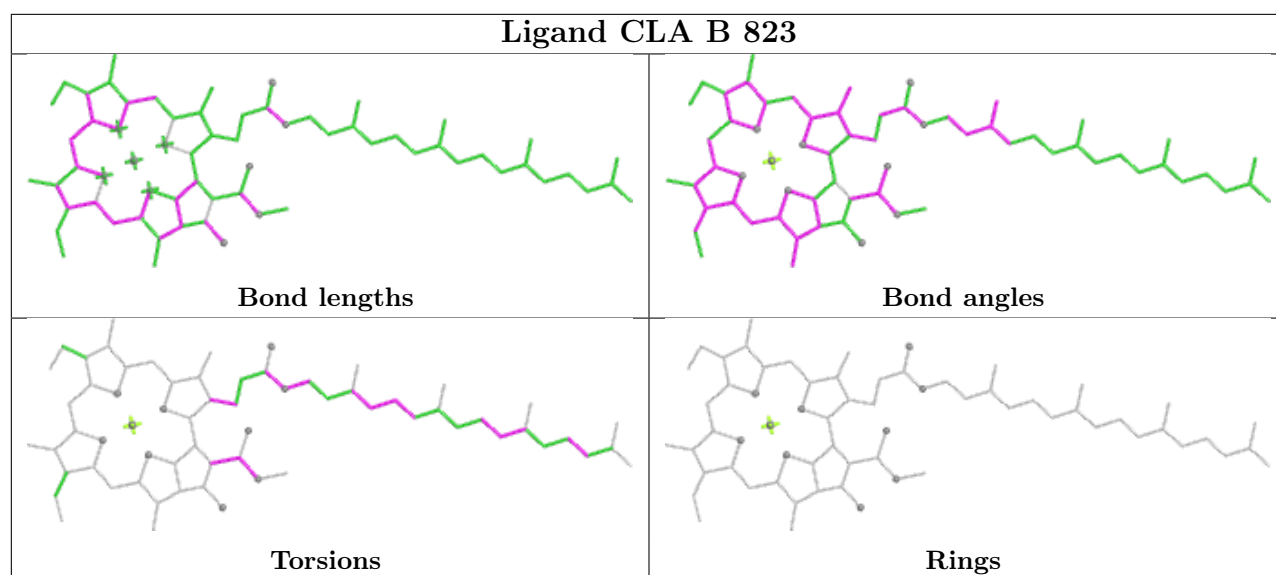
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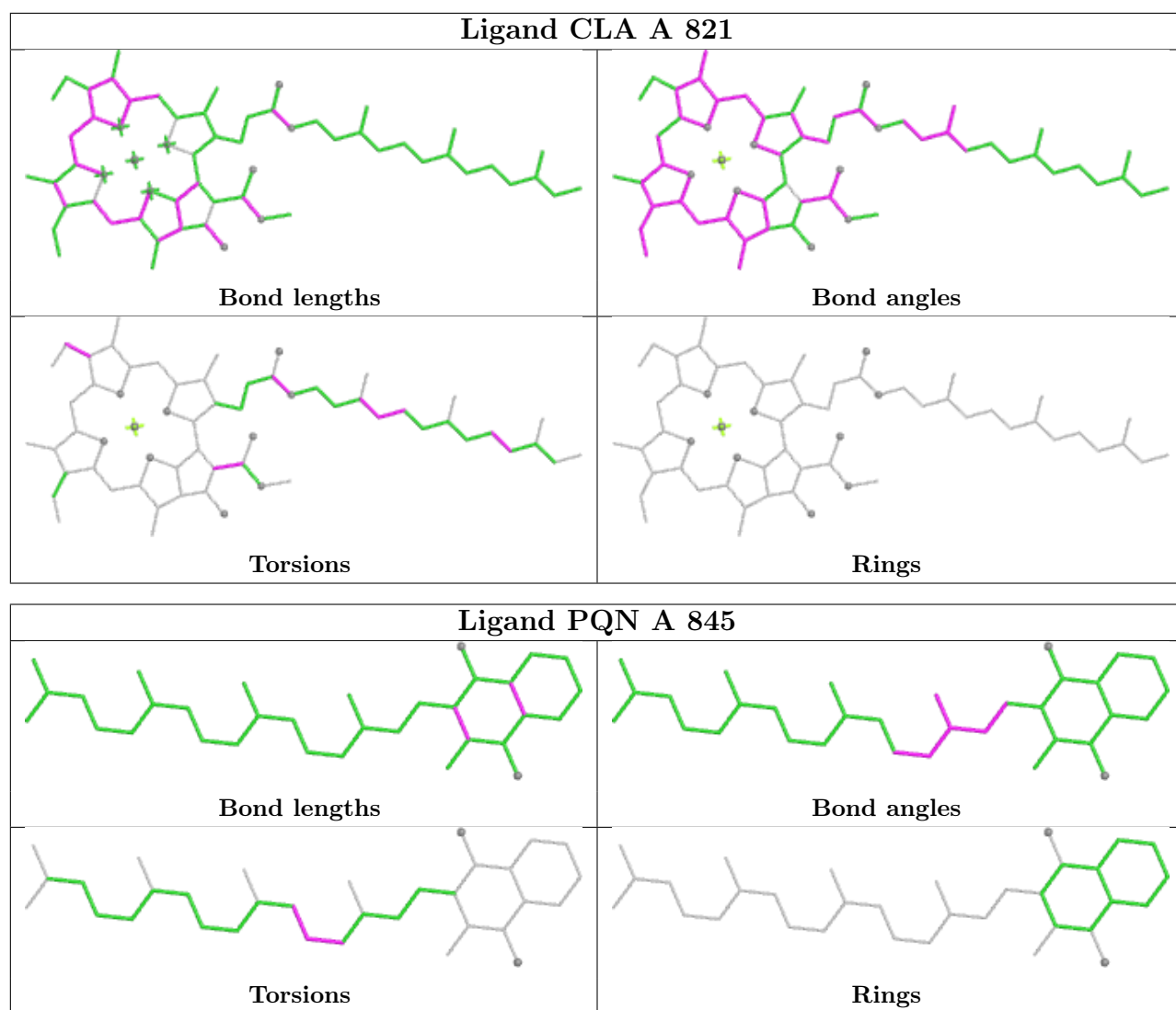
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	821	CLA	4	0
13	A	822	CLA	3	0
13	B	801	CLA	3	0
13	B	819	CLA	1	0
13	B	824	CLA	4	0
16	J	102	BCR	8	0
13	A	808	CLA	1	0
13	B	812	CLA	1	0
13	B	808	CLA	3	0
13	A	835	CLA	4	0
15	C	102	SF4	4	0
17	A	852	LHG	1	0
13	B	804	CLA	7	0
13	A	812	CLA	5	0
13	B	816	CLA	1	0
13	A	802	CLA	1	0
13	A	836	CLA	2	0
13	A	814	CLA	1	0
13	B	811	CLA	2	0
13	A	828	CLA	2	0
13	L	204	CLA	2	0
16	F	202	BCR	5	0
16	K	202	BCR	3	0
13	B	822	CLA	6	0
13	A	807	CLA	3	0
13	A	833	CLA	4	0
16	A	848	BCR	5	0
16	M	101	BCR	4	0
16	A	850	BCR	3	0
16	B	835	BCR	4	0
13	A	841	CLA	1	0
13	A	818	CLA	2	0
13	B	827	CLA	2	0
13	A	844	CLA	1	0
13	A	803	CLA	1	0
13	B	803	CLA	4	0
16	I	101	BCR	5	0
13	A	830	CLA	6	0
13	A	825	CLA	2	0

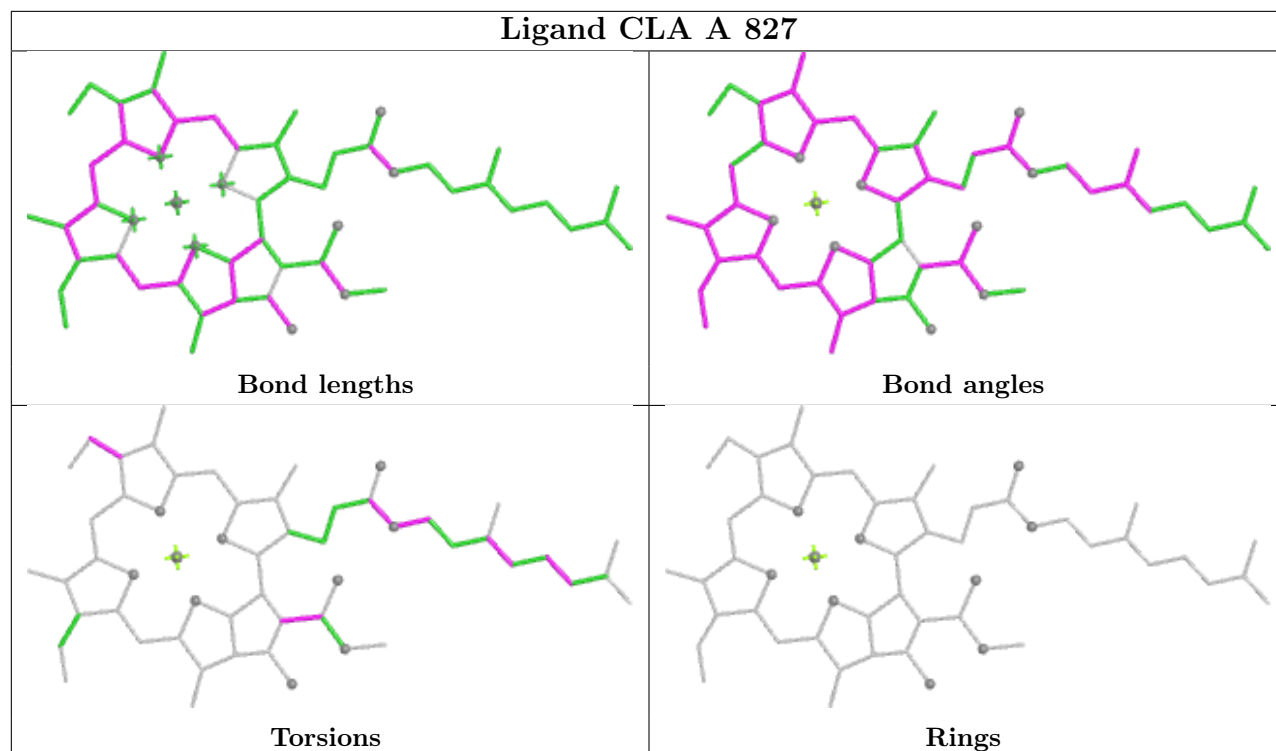
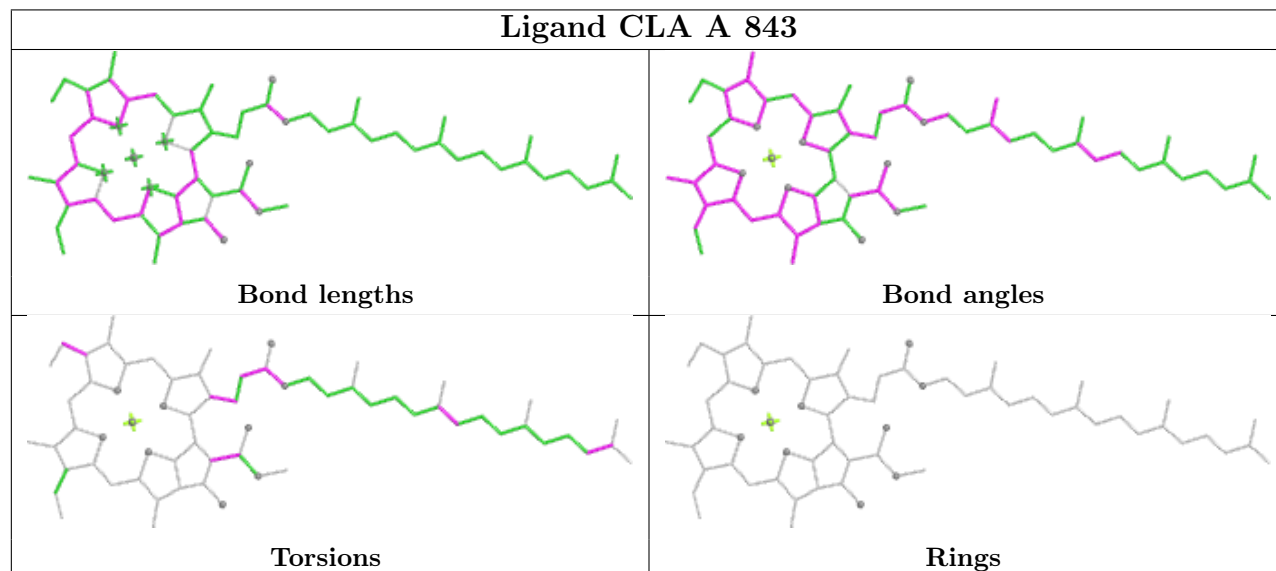
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

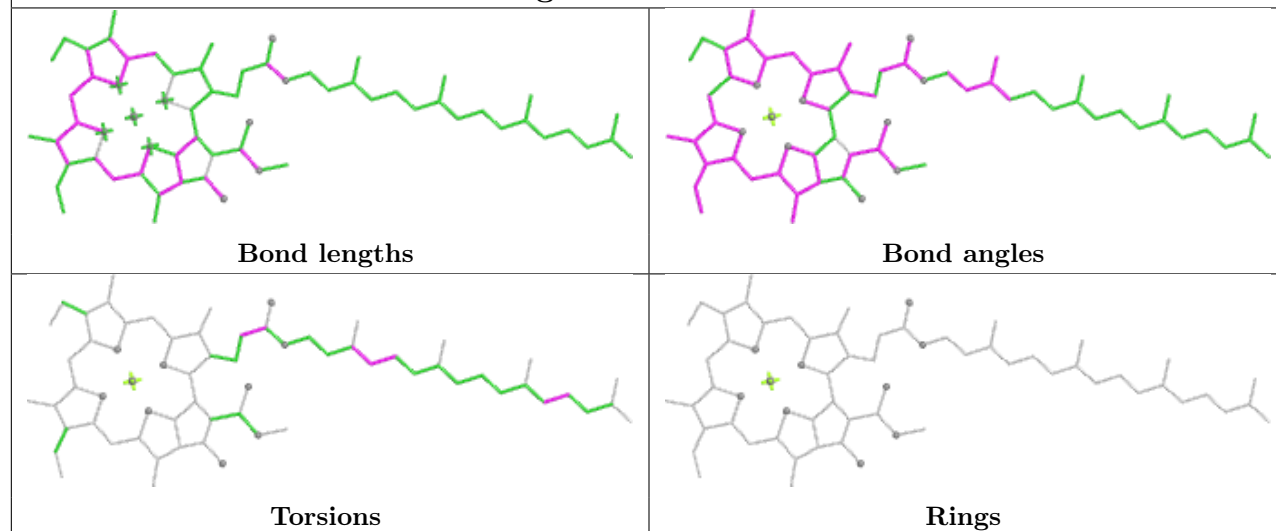
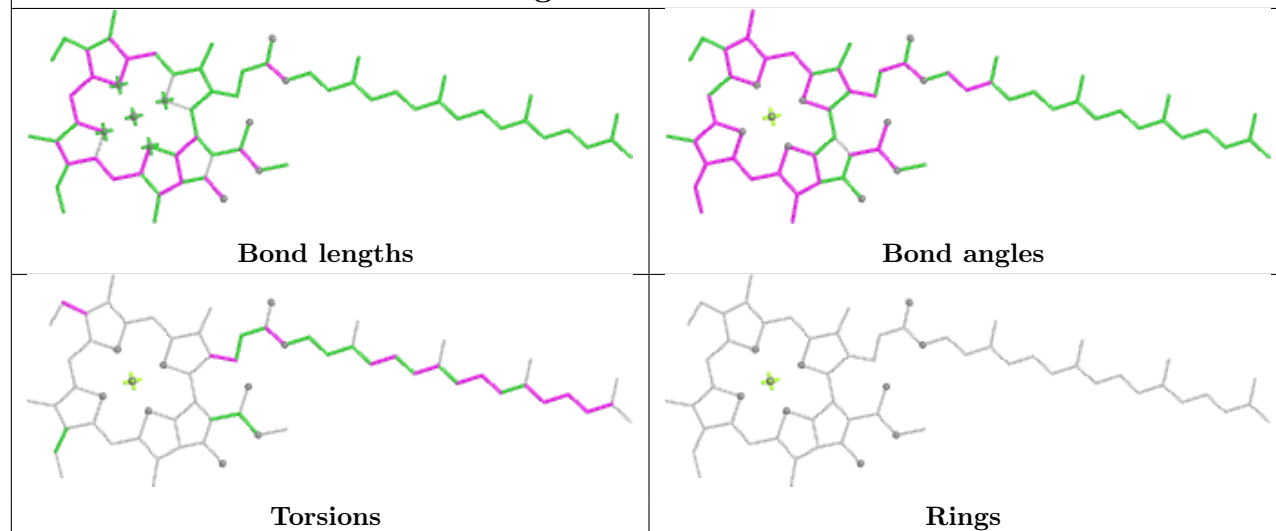
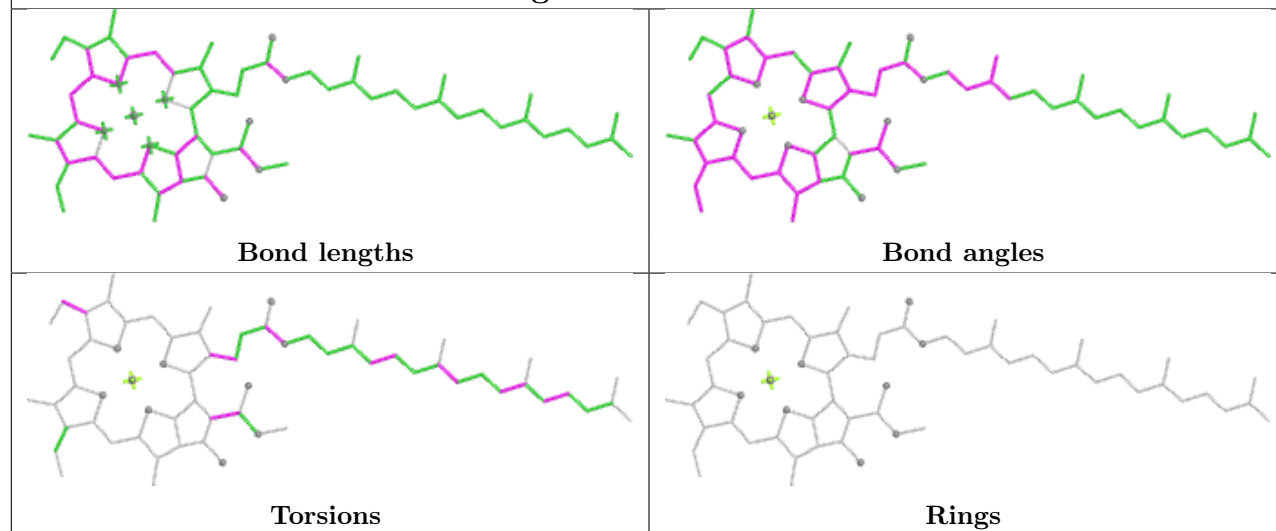
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted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

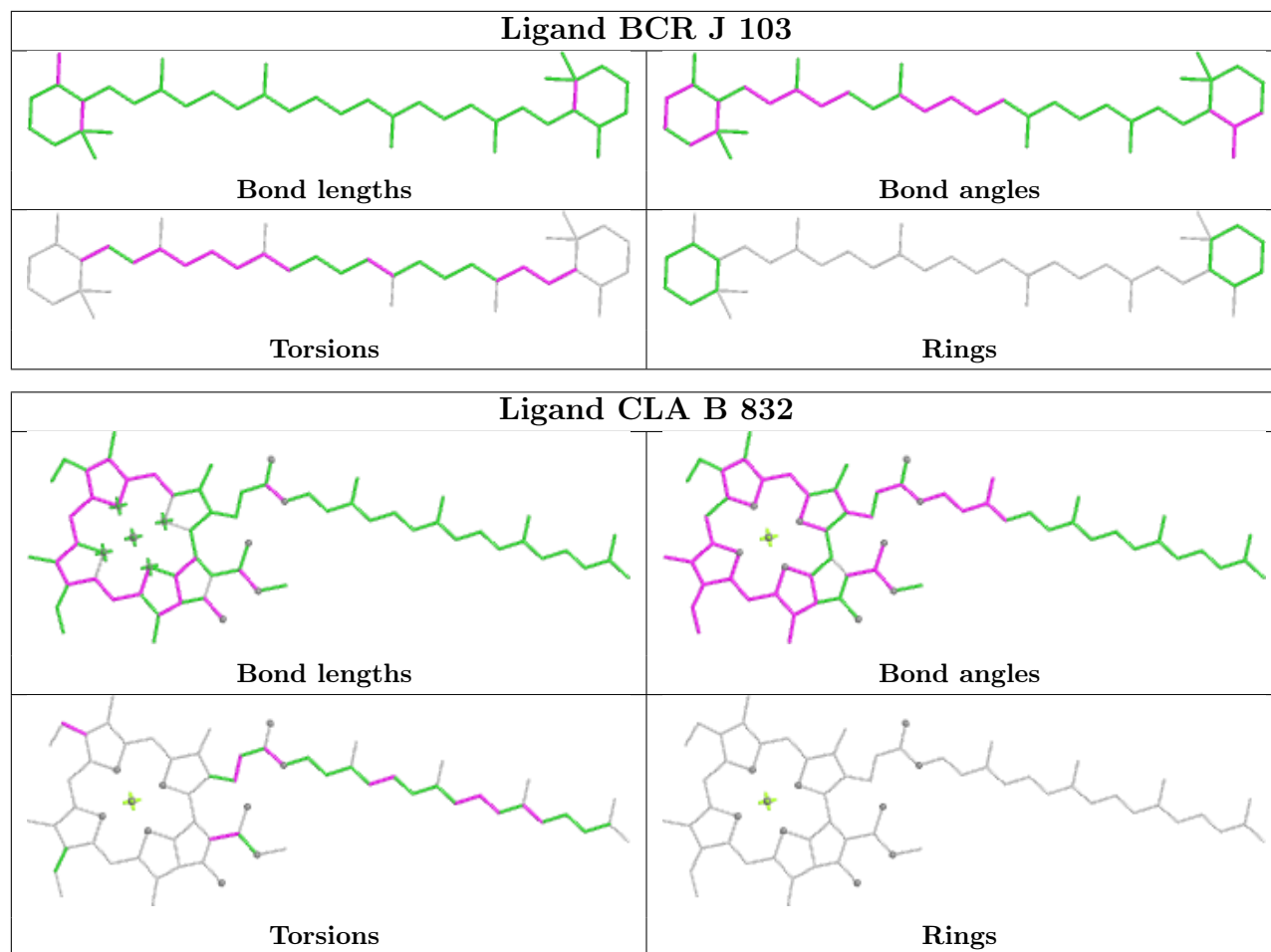




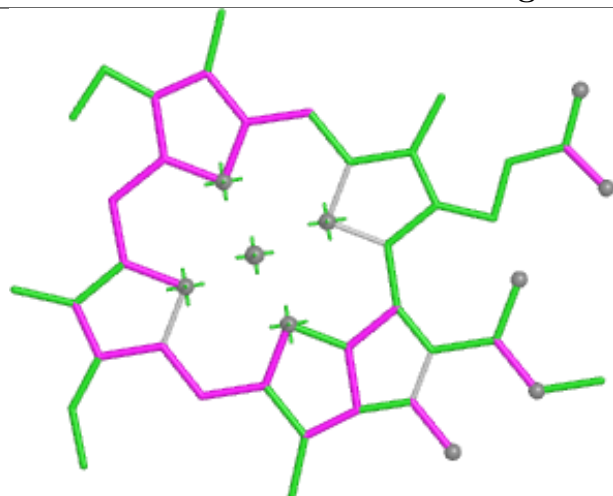


Ligand CLA A 827**Ligand CLA A 843**

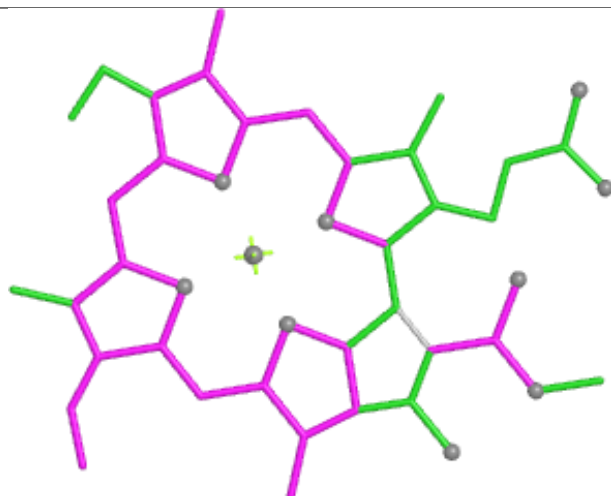
Ligand CL0 A 801**Ligand CLA L 203****Ligand CLA A 820**



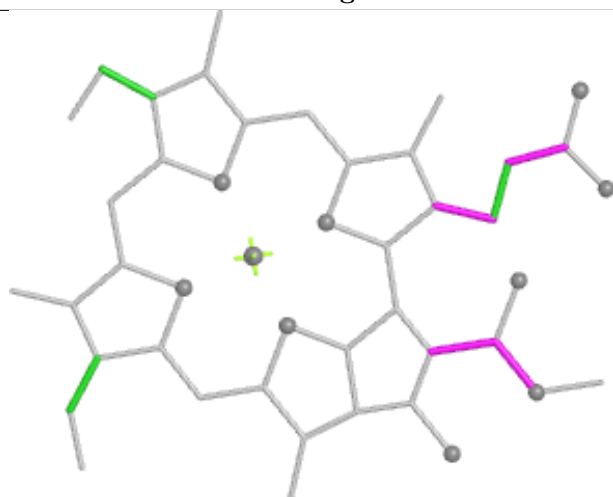
Ligand CLA J 101



Bond lengths



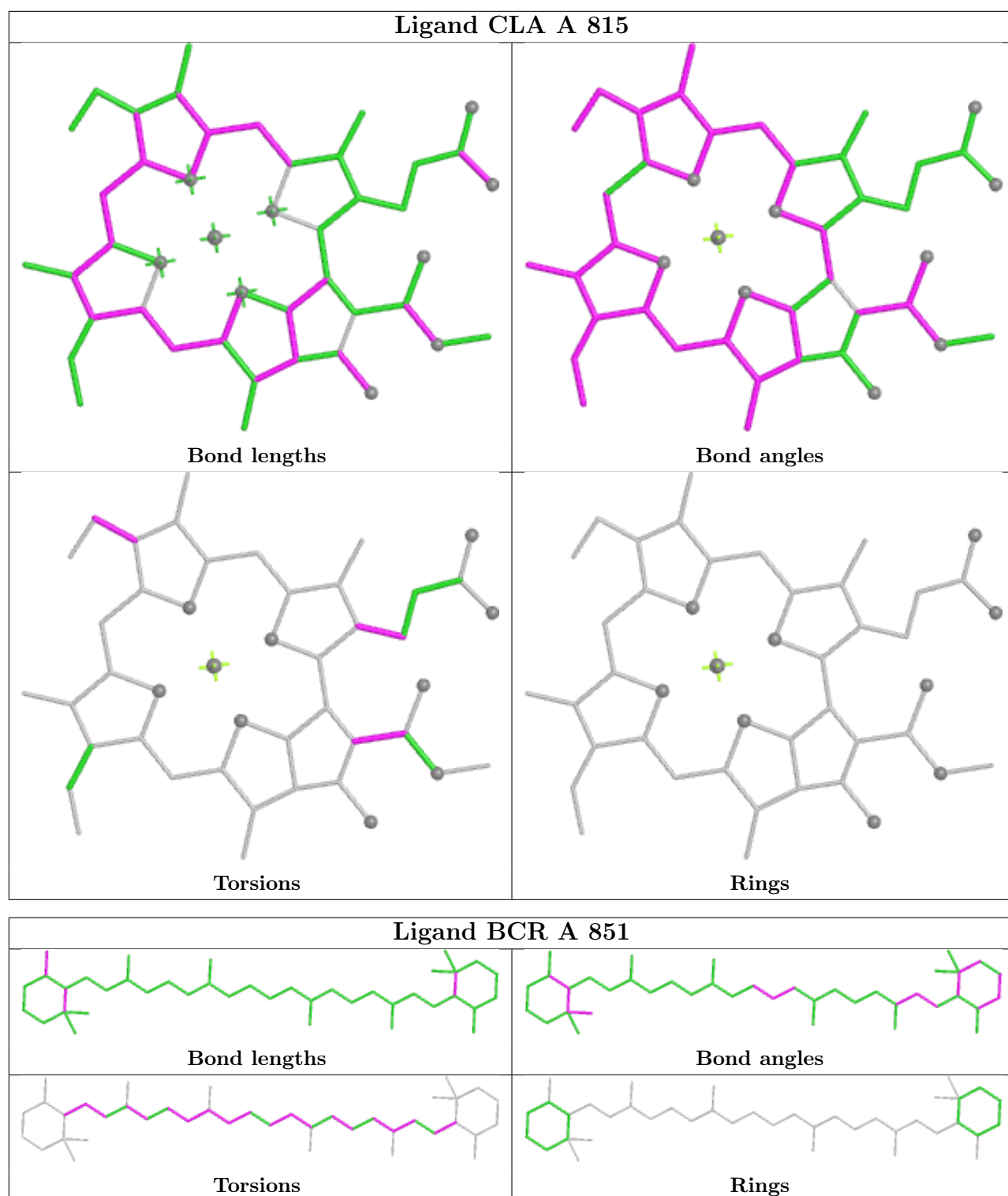
Bond angles

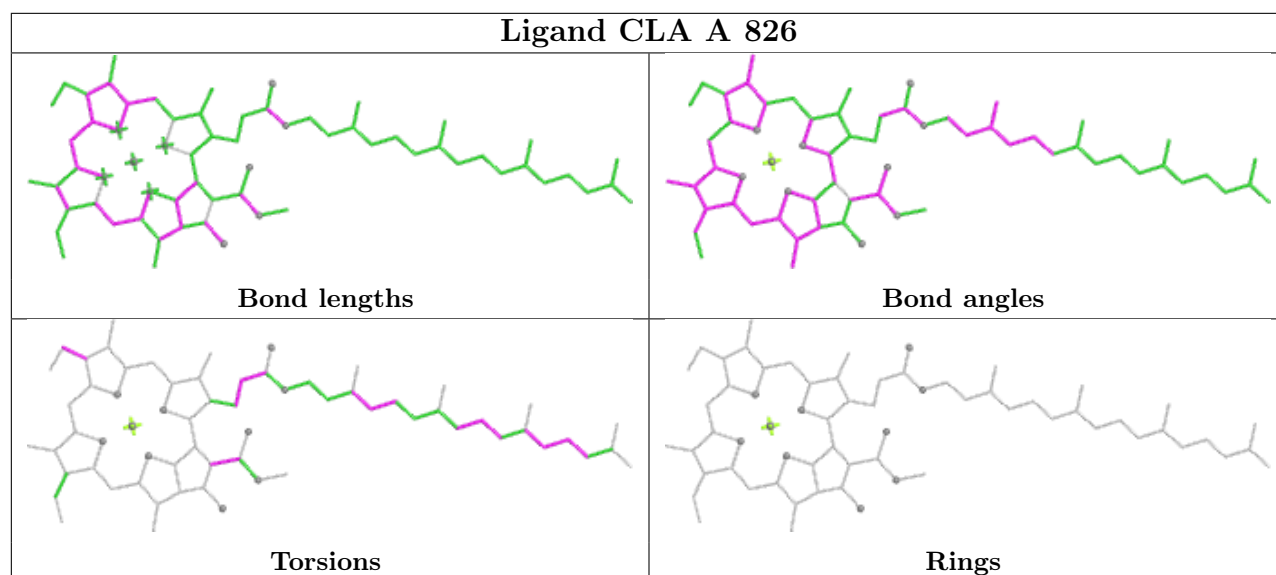
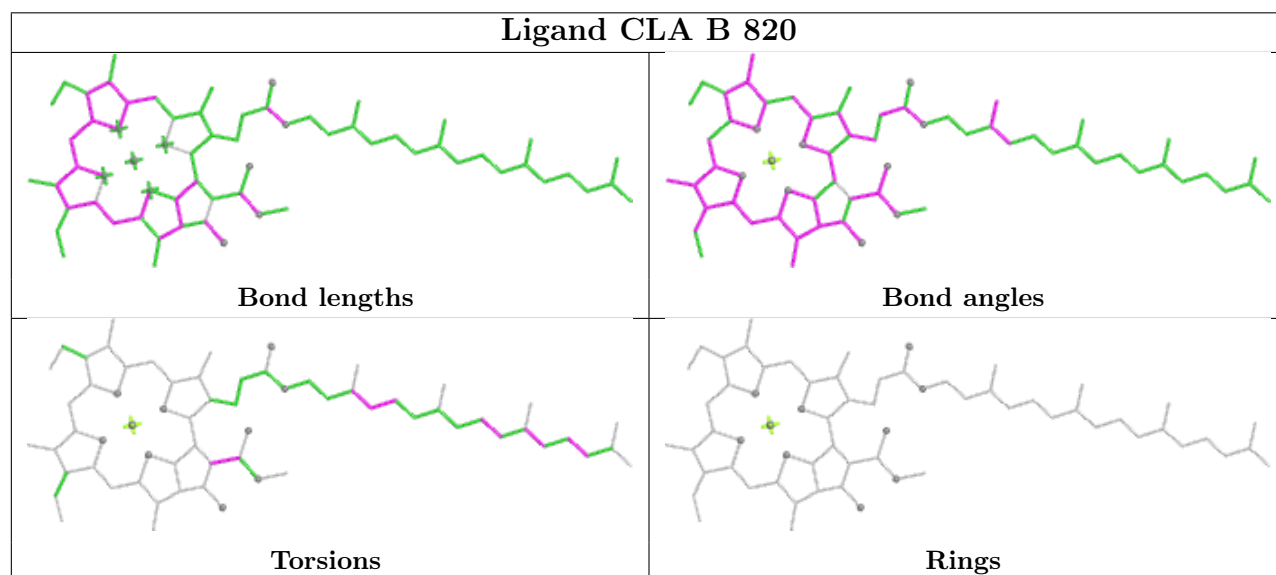
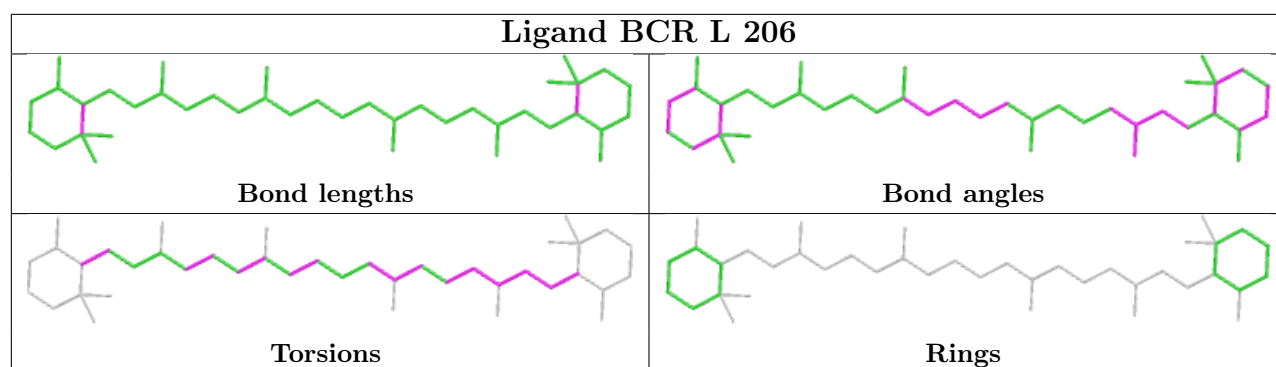


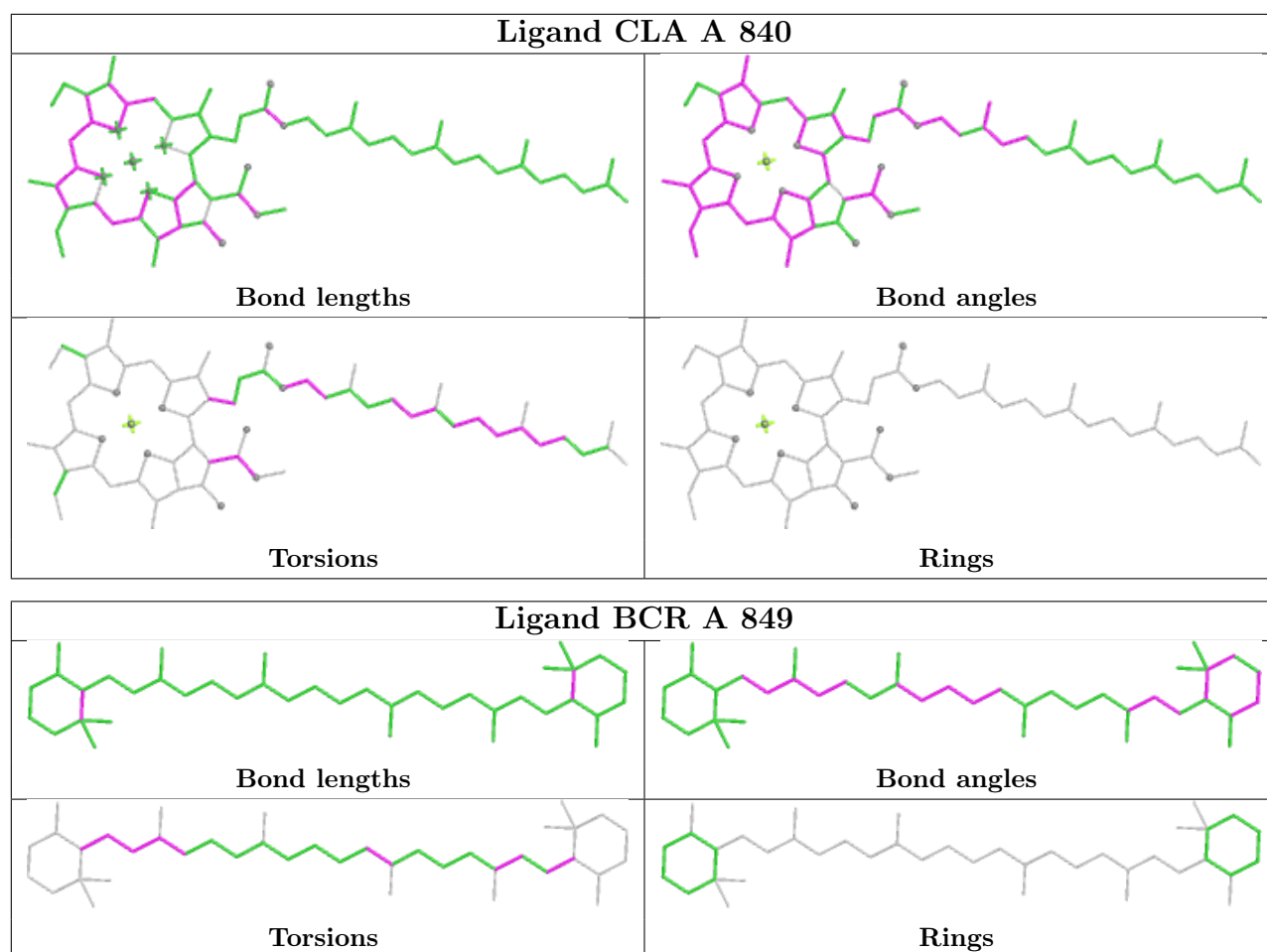
Torsions

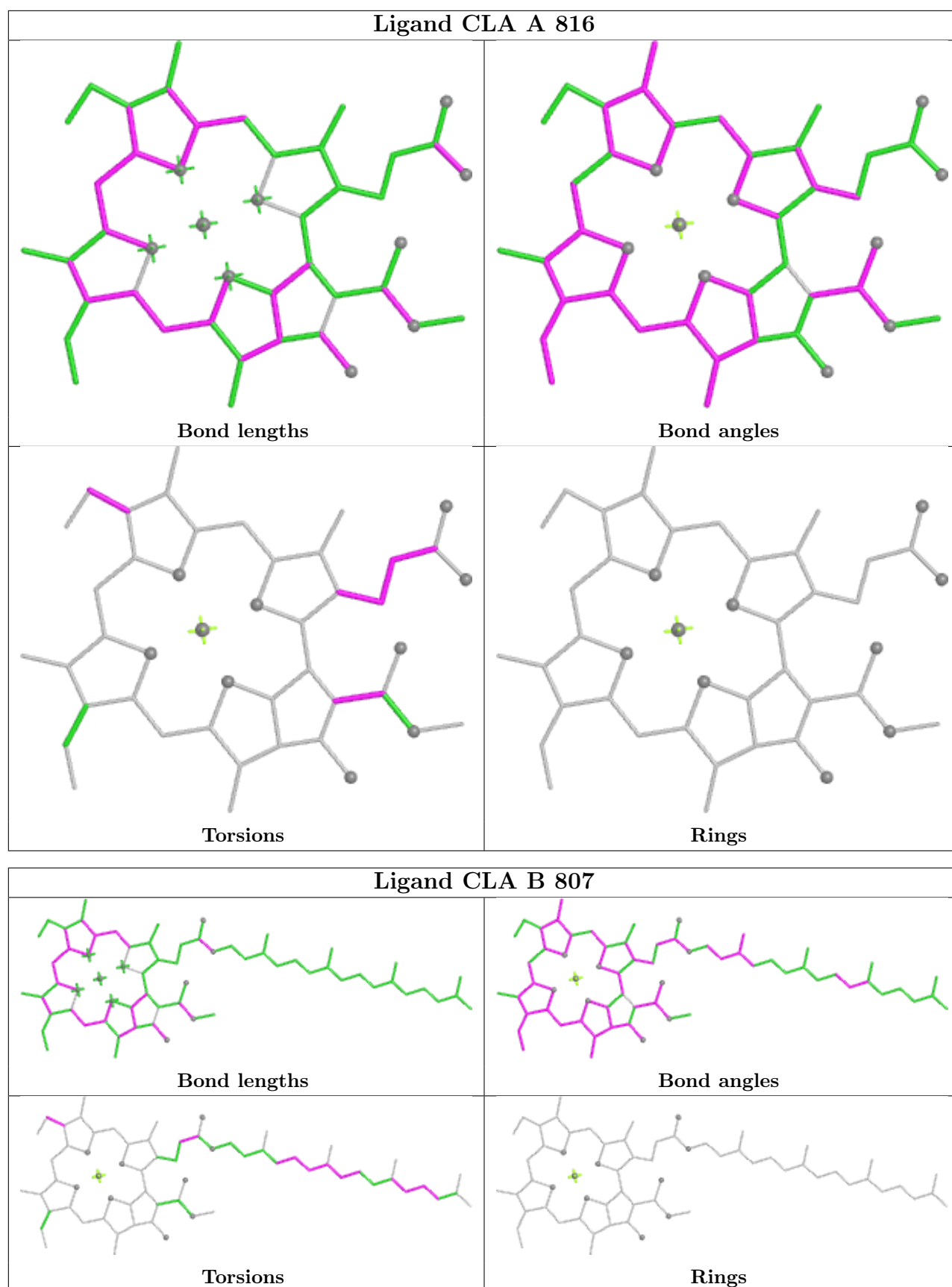


Rings

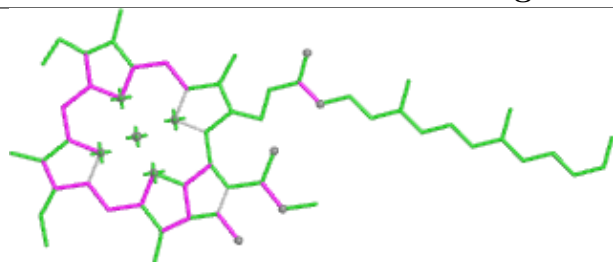




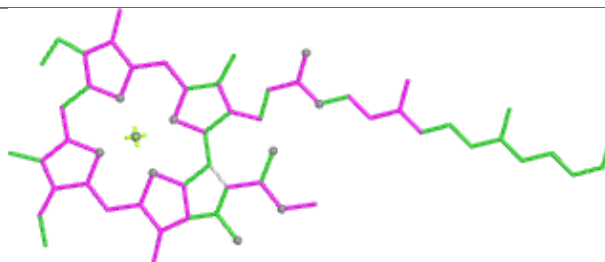




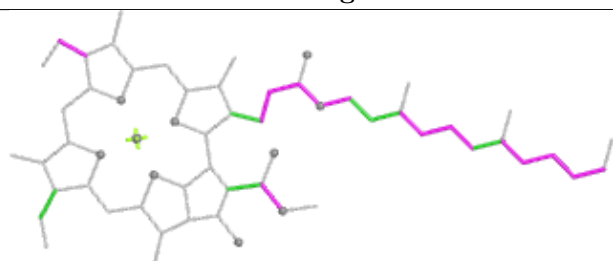
Ligand CLA B 817



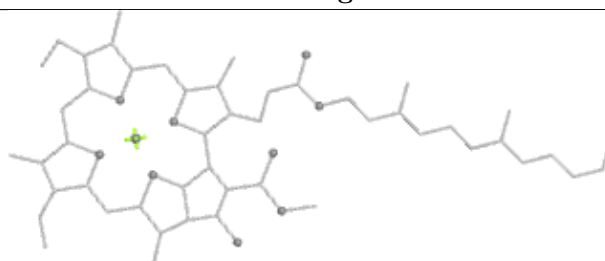
Bond lengths



Bond angles

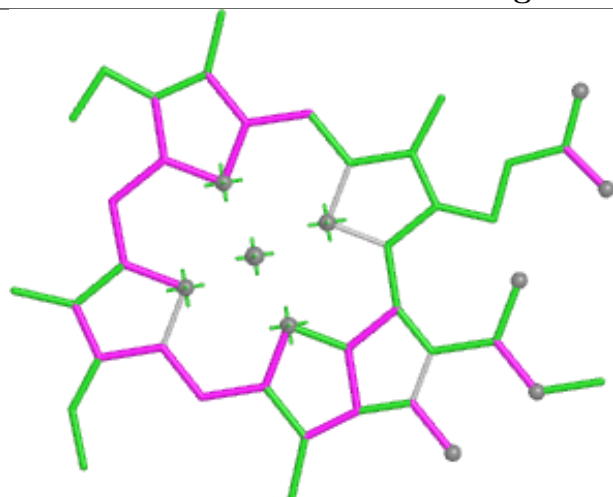


Torsions

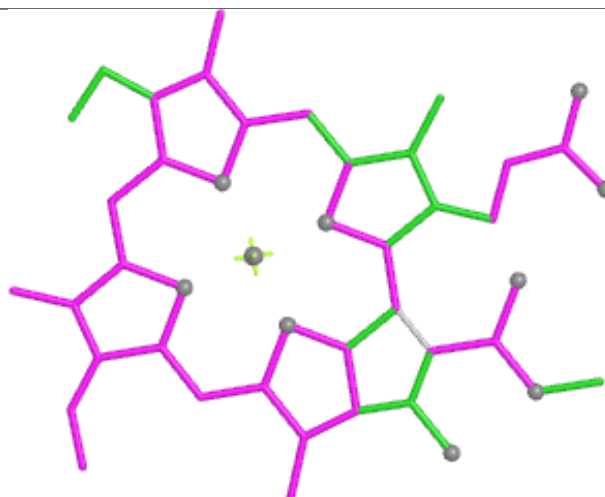


Rings

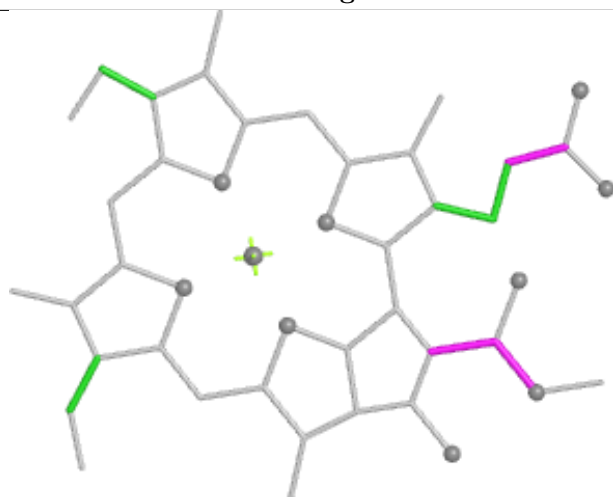
Ligand CLA A 810



Bond lengths



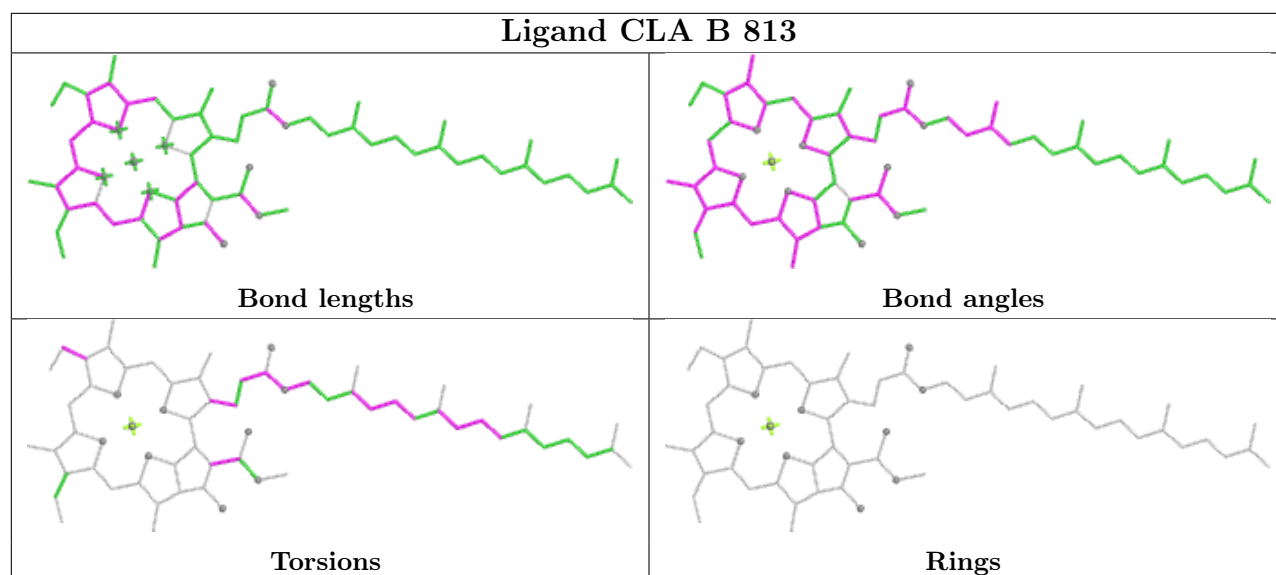
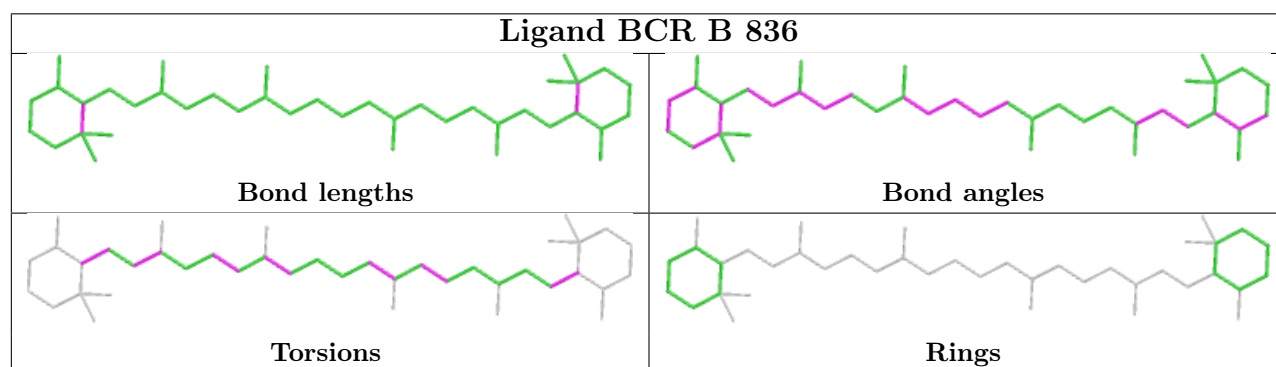
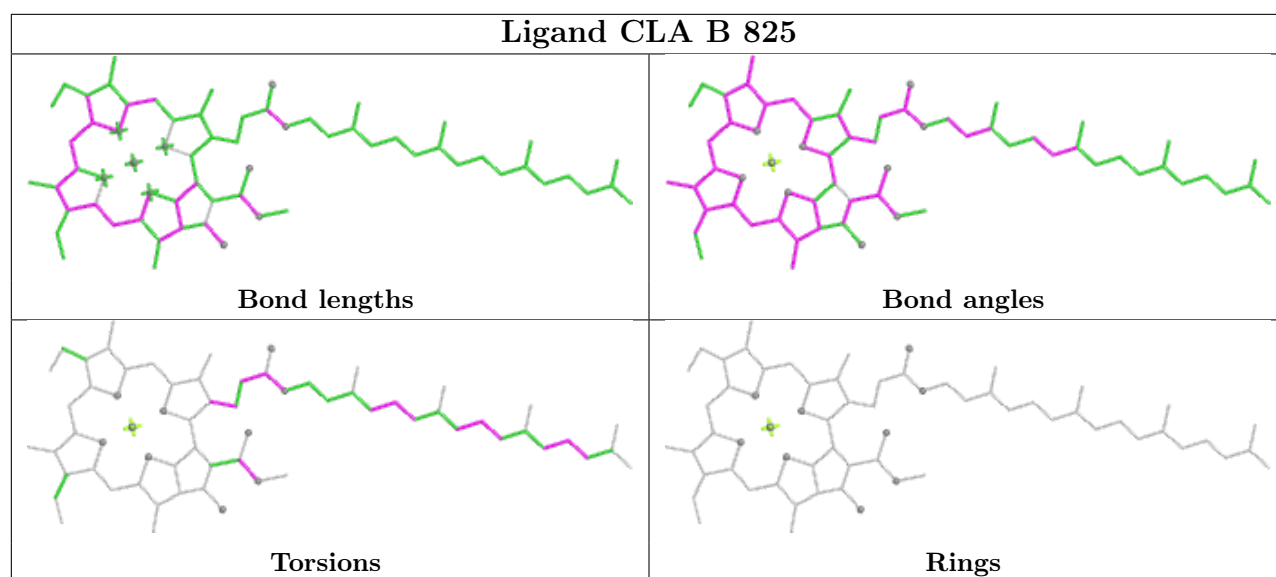
Bond angles

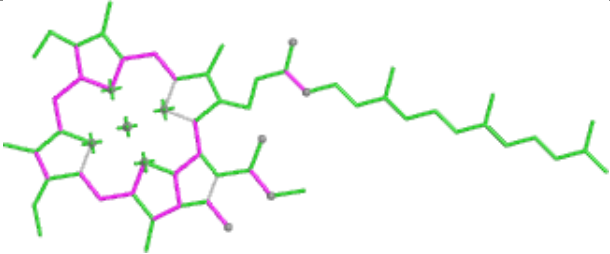
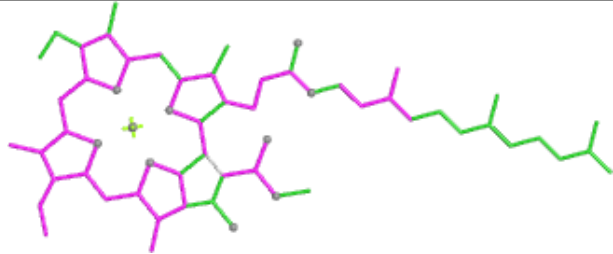
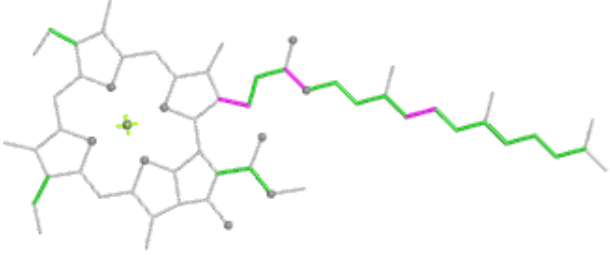
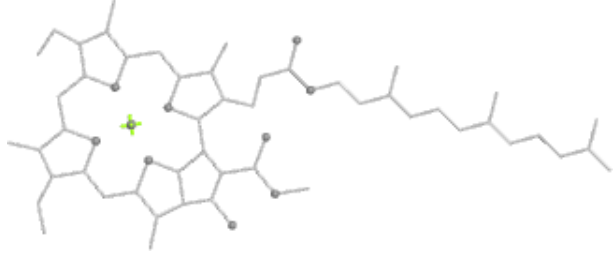
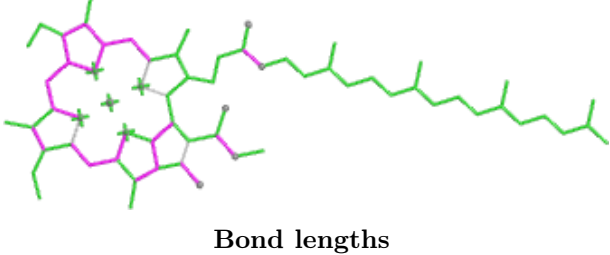
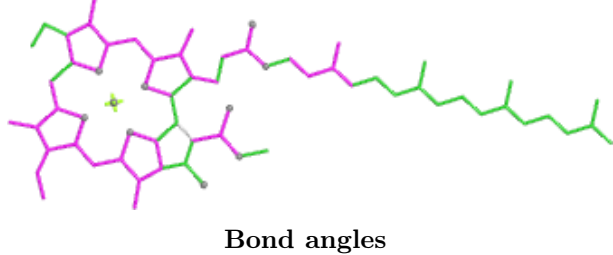
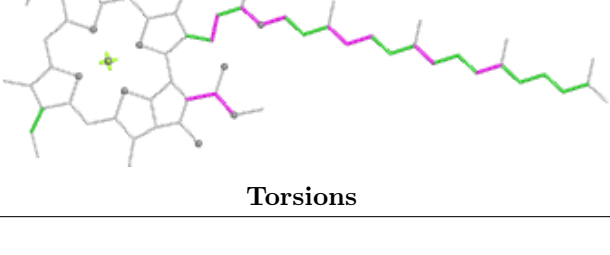
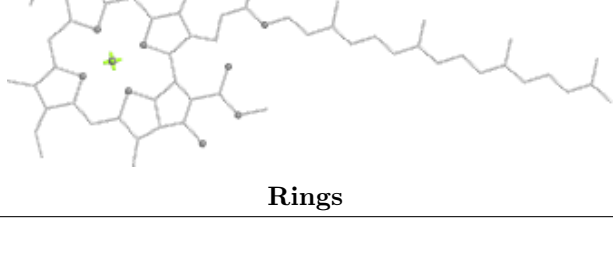


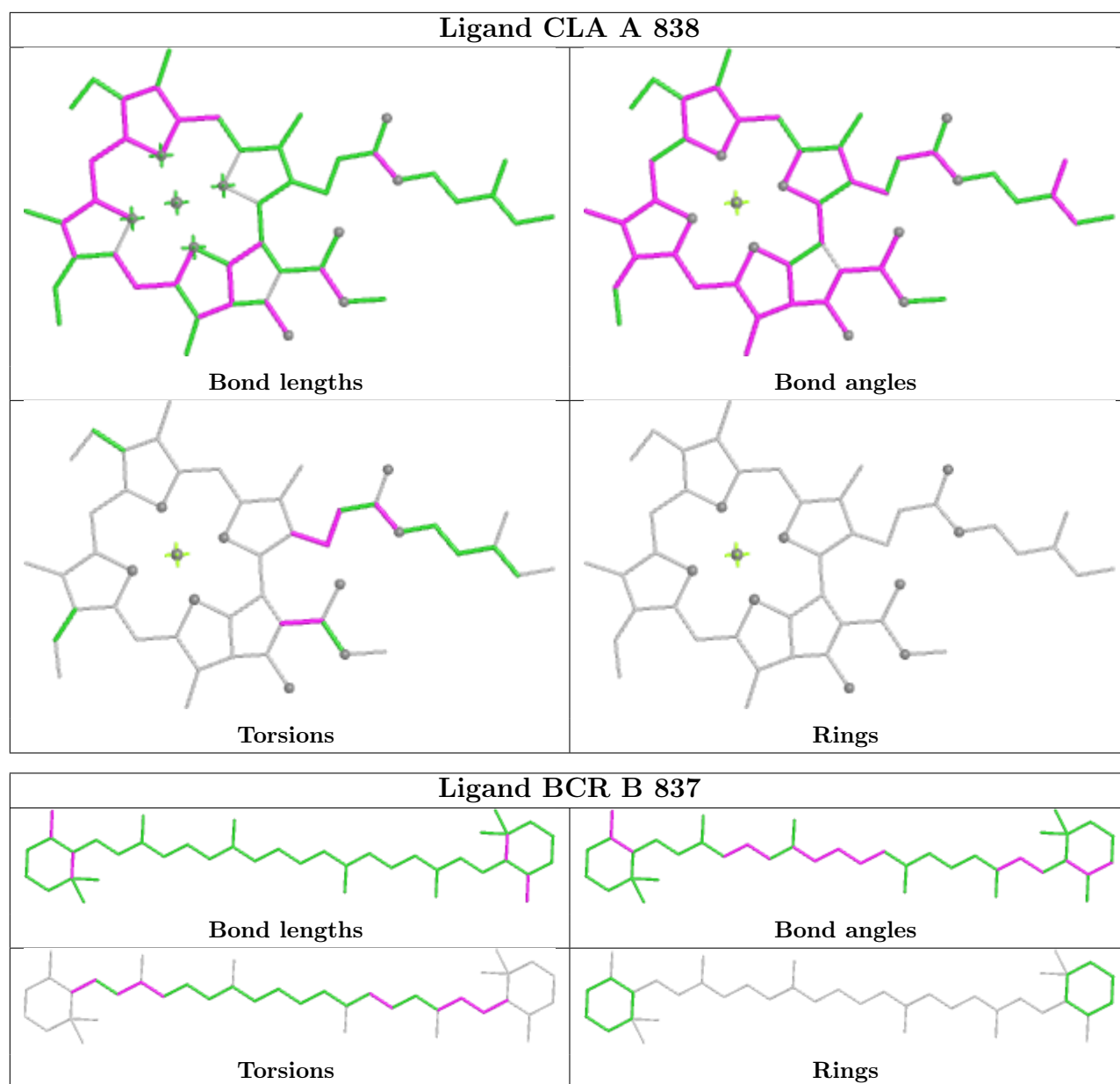
Torsions

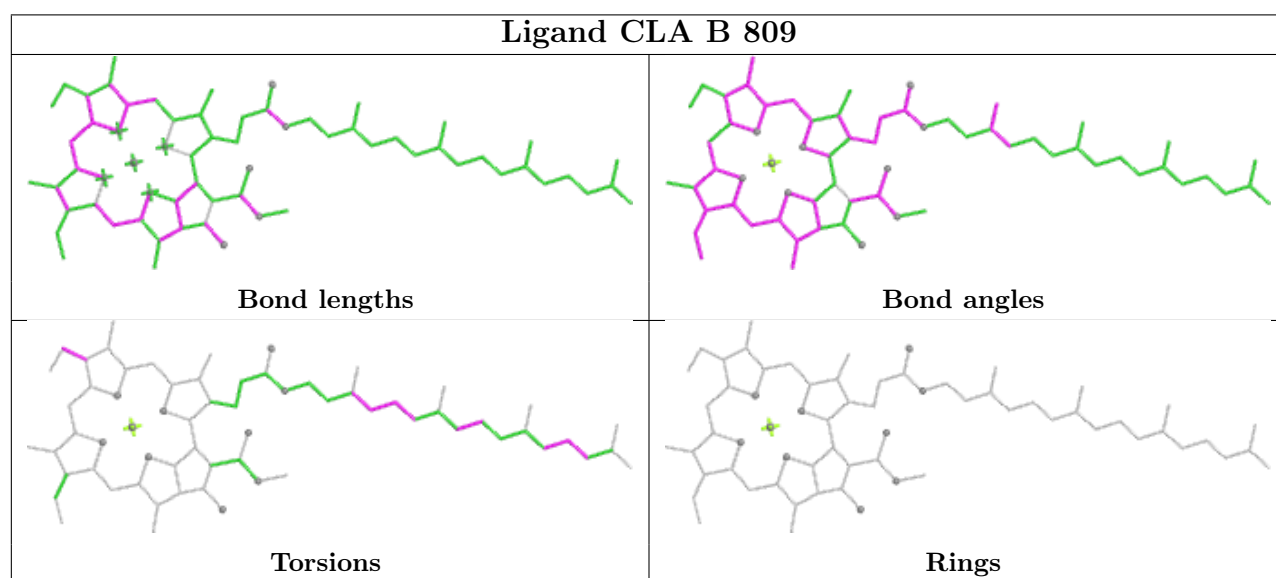
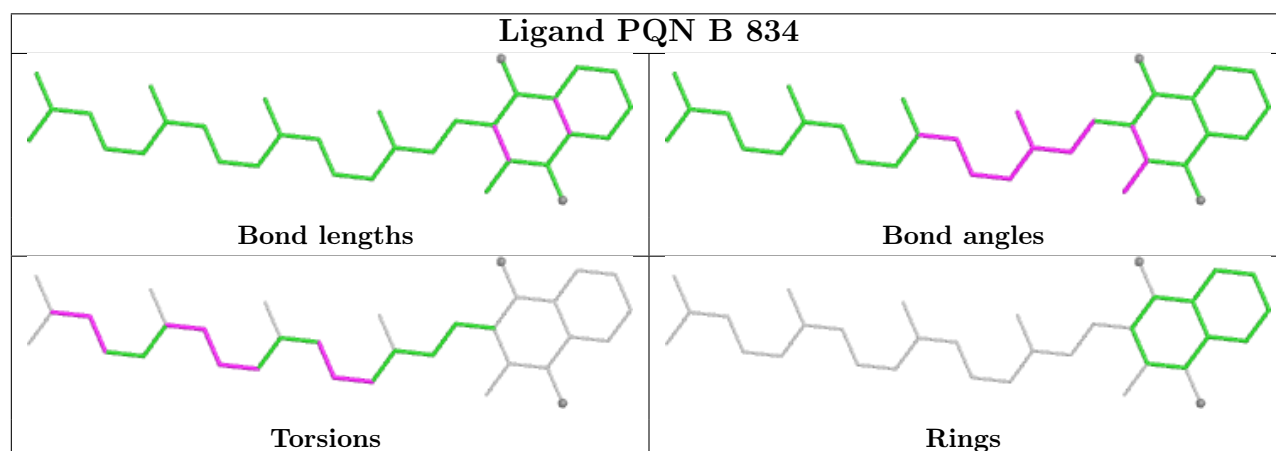
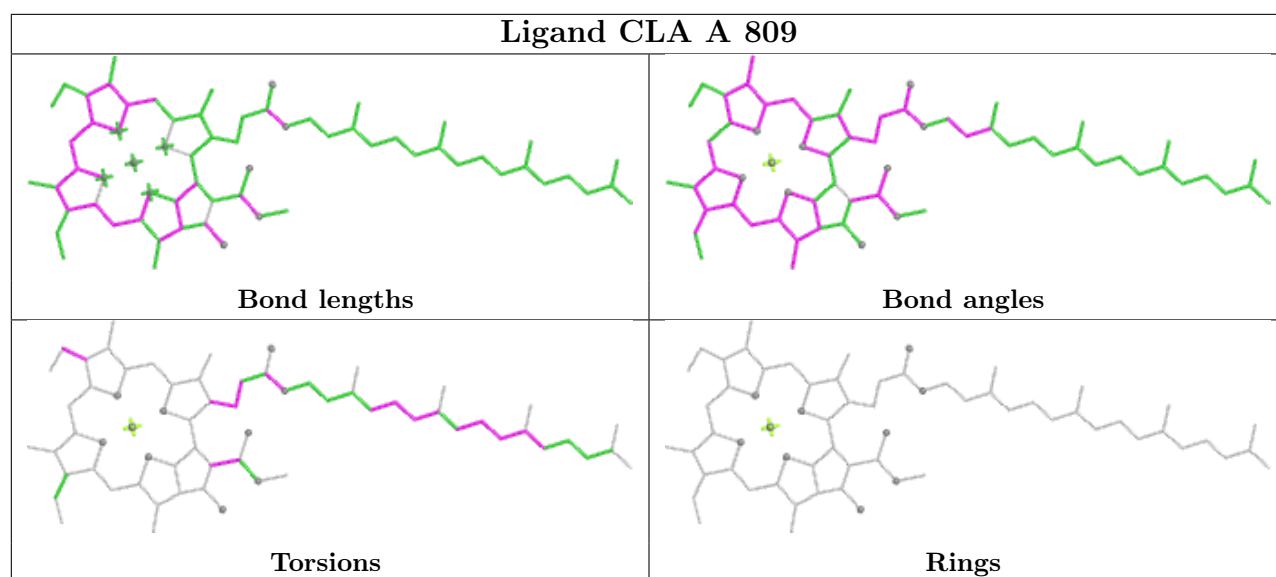


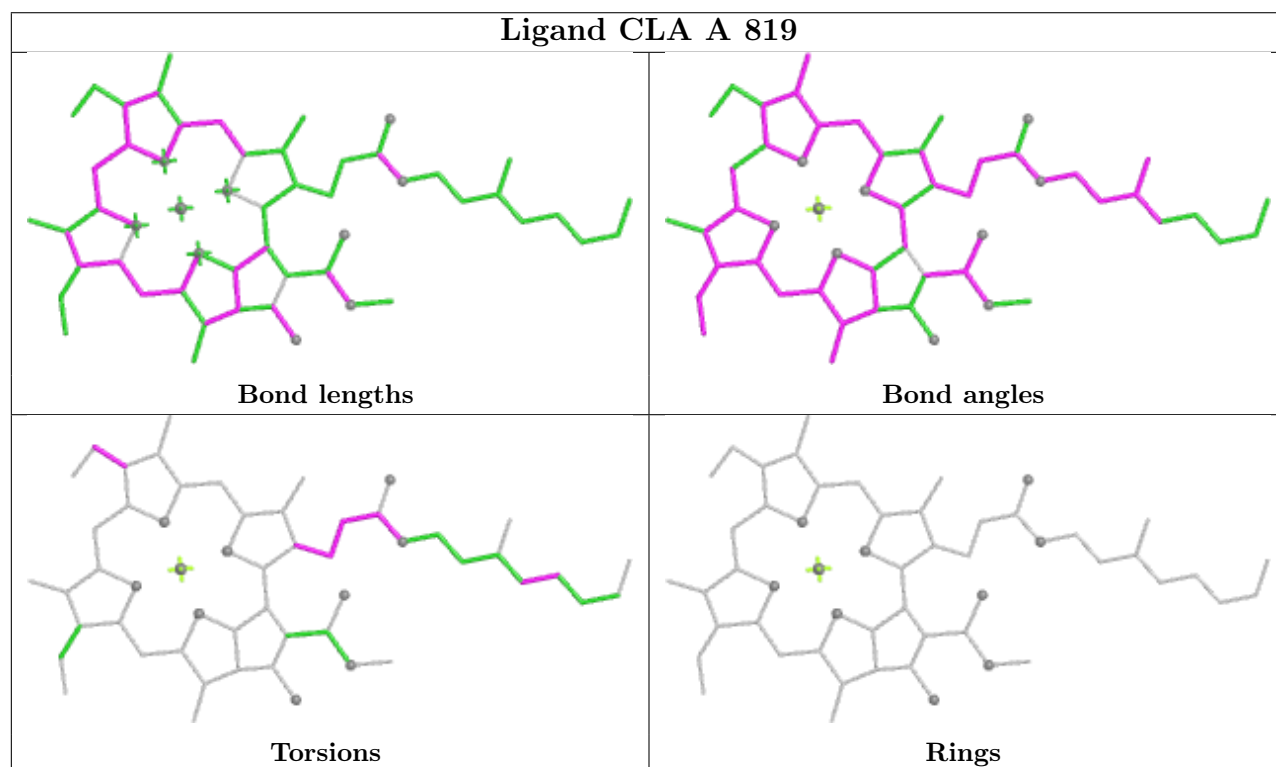
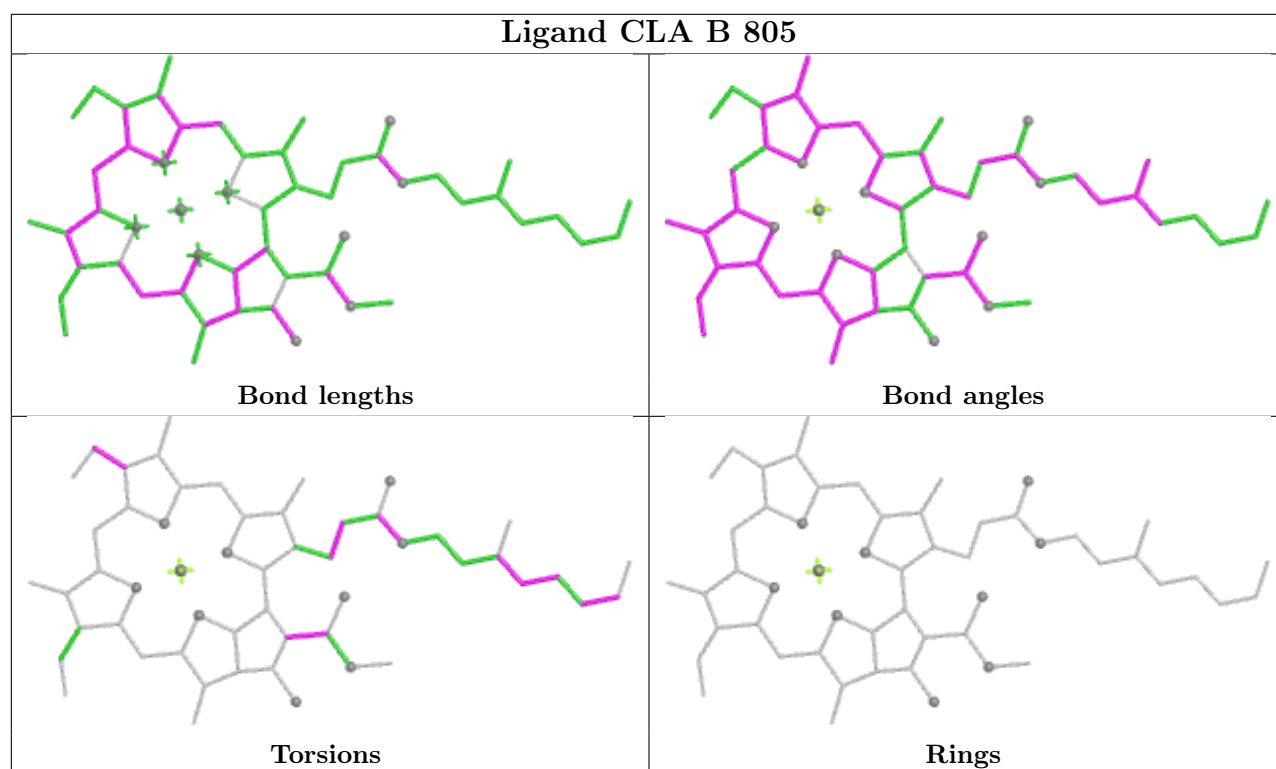
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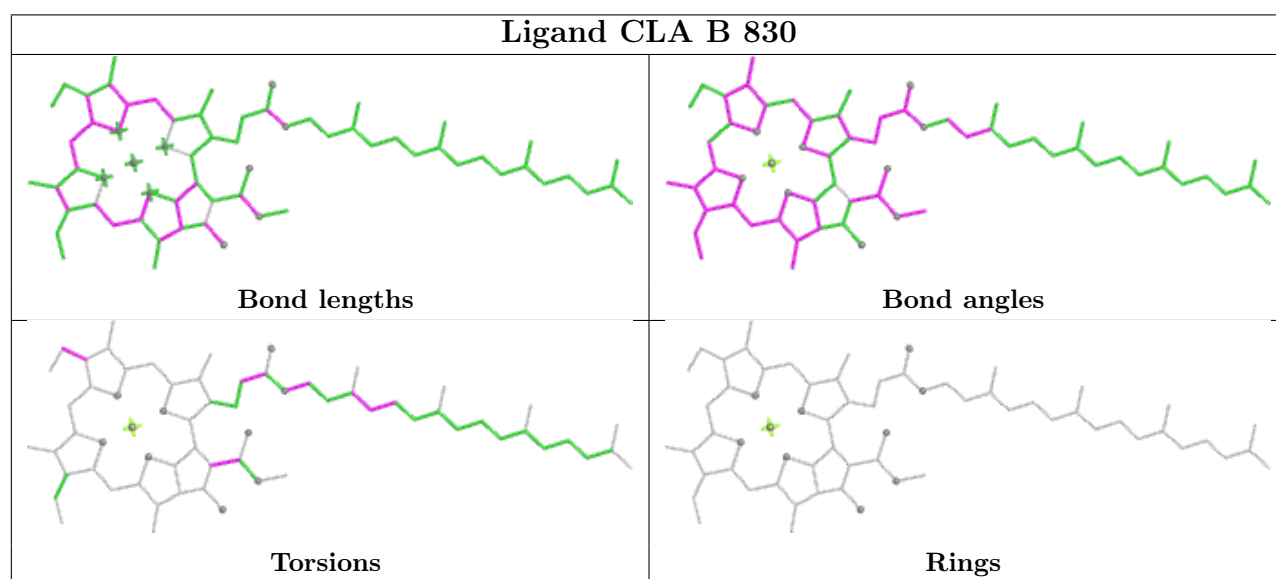
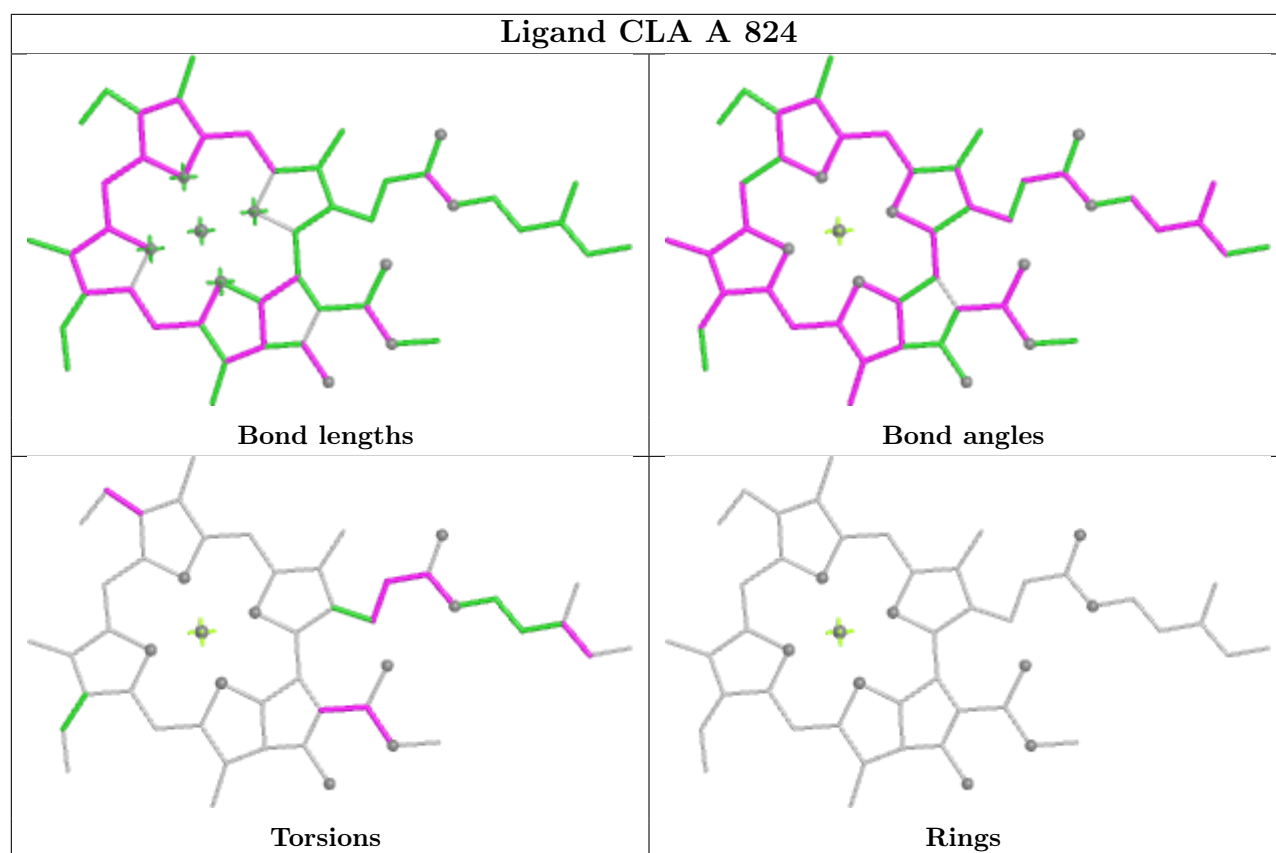


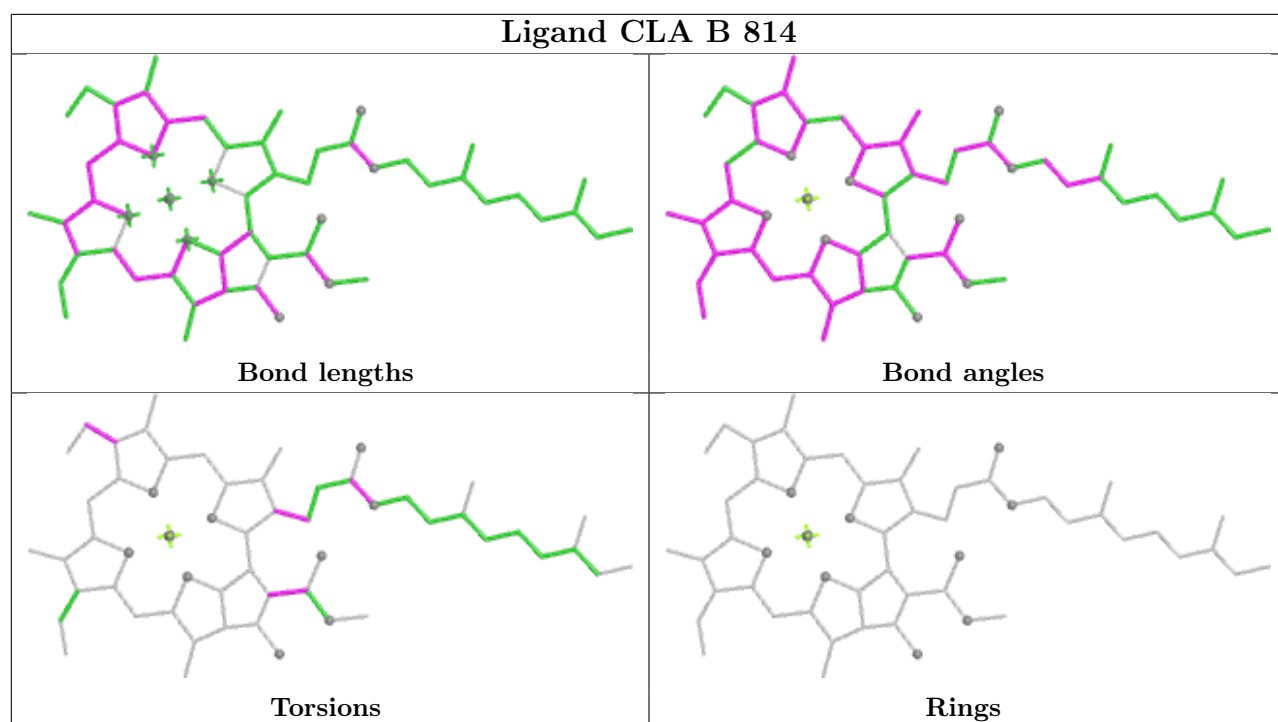
Ligand CLA B 818	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 834	
 Bond lengths	 Bond angles
 Torsions	 Rings

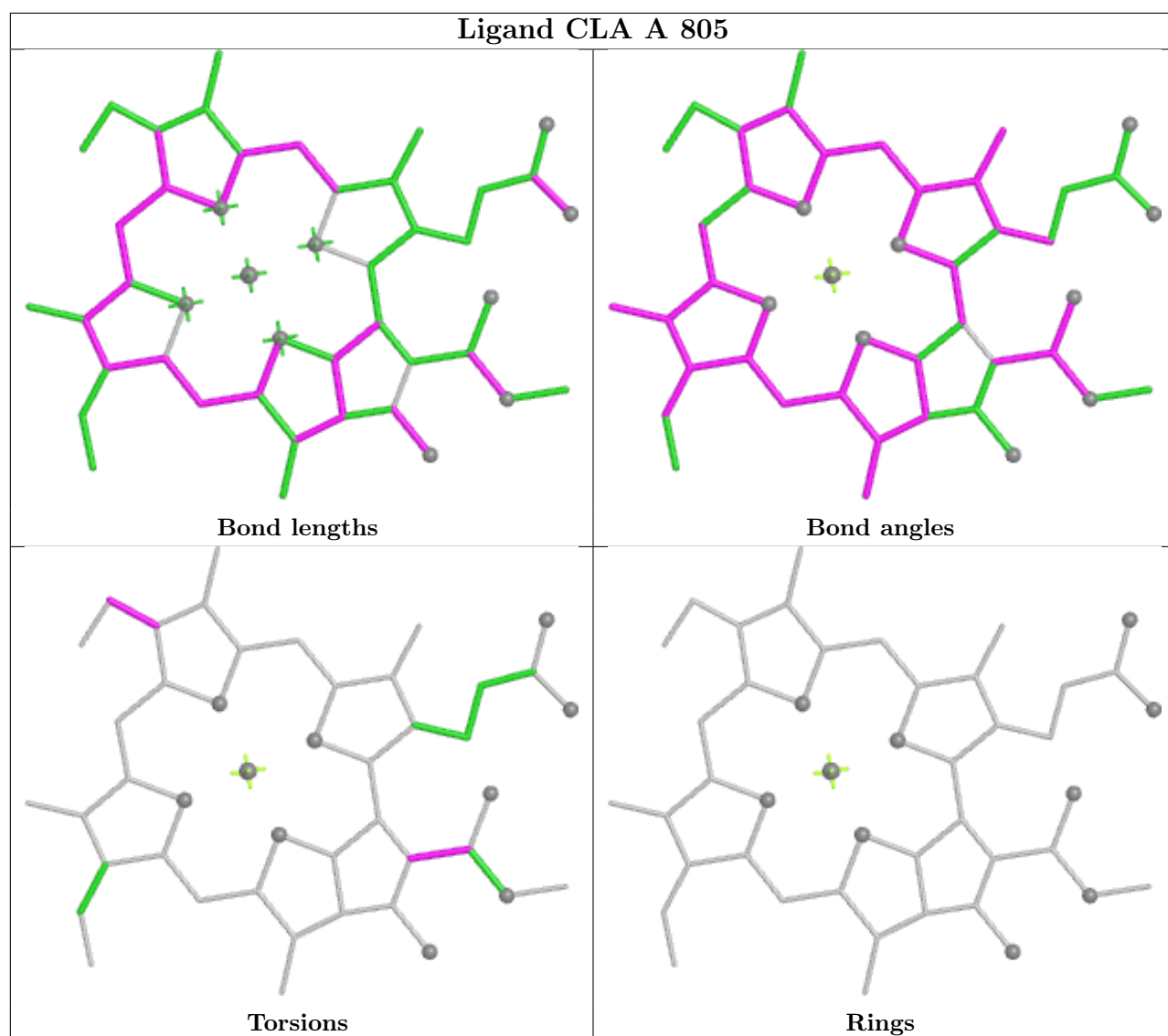


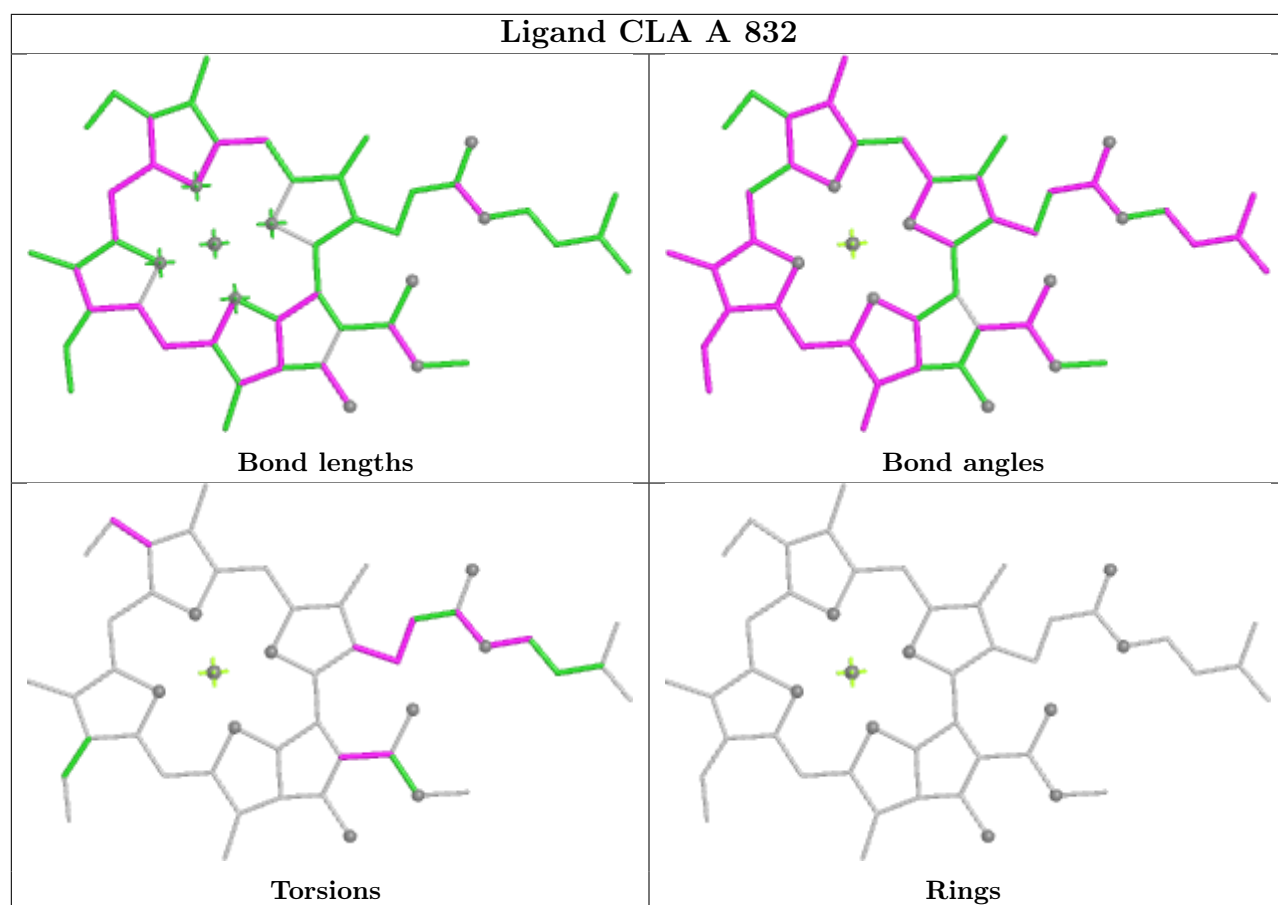


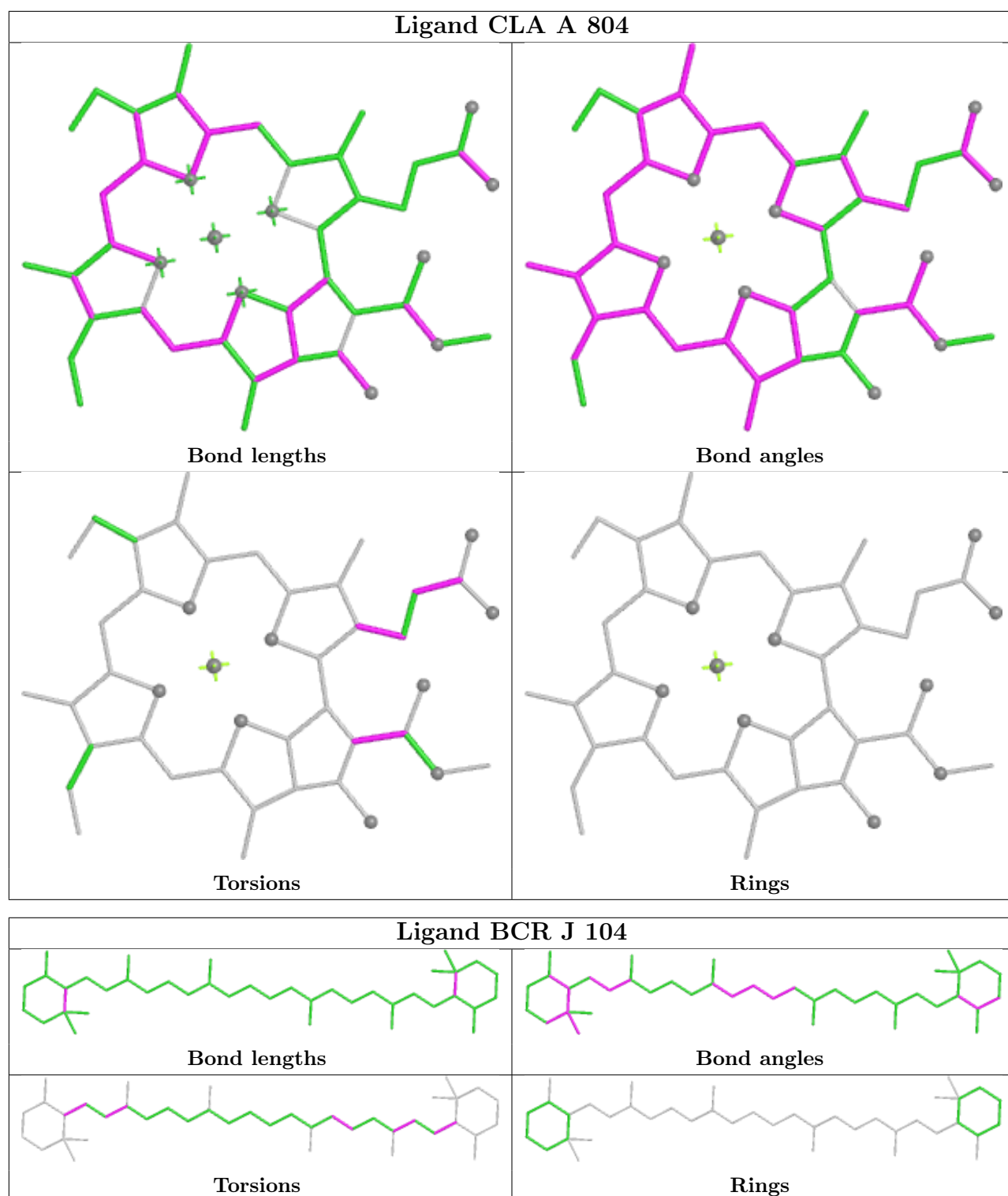




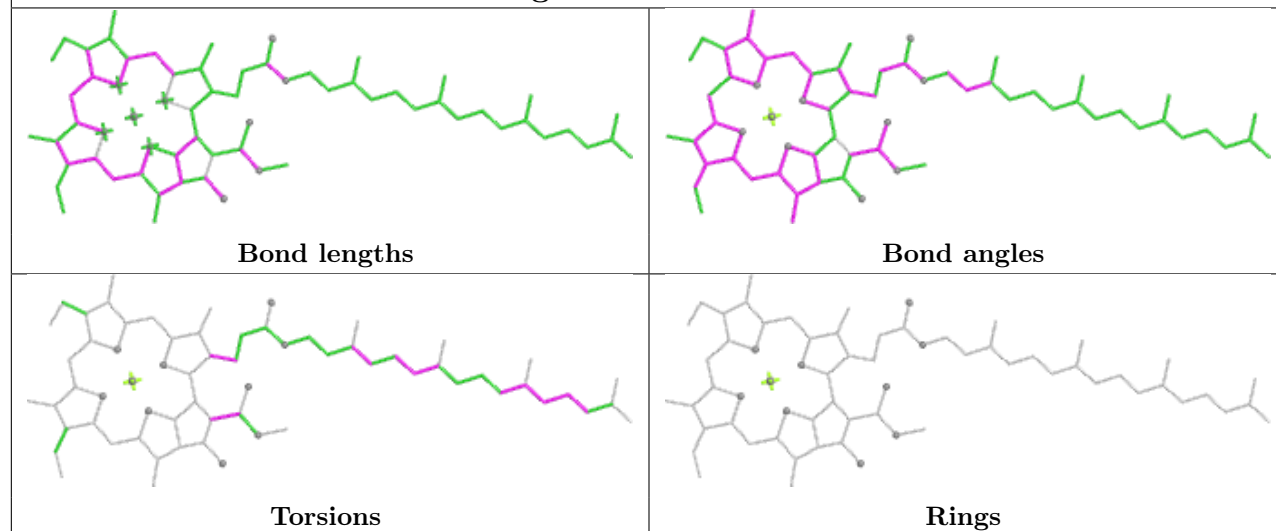




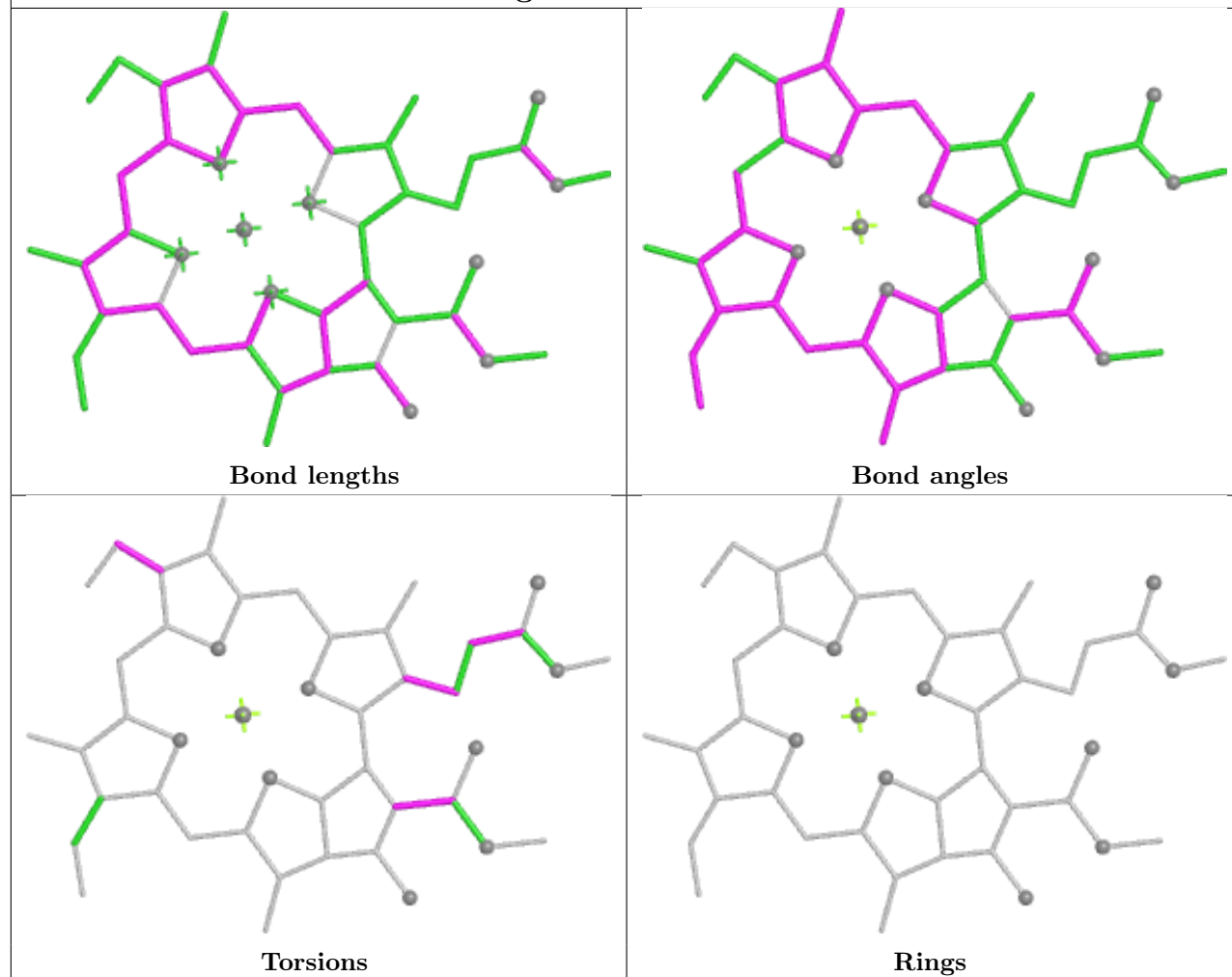


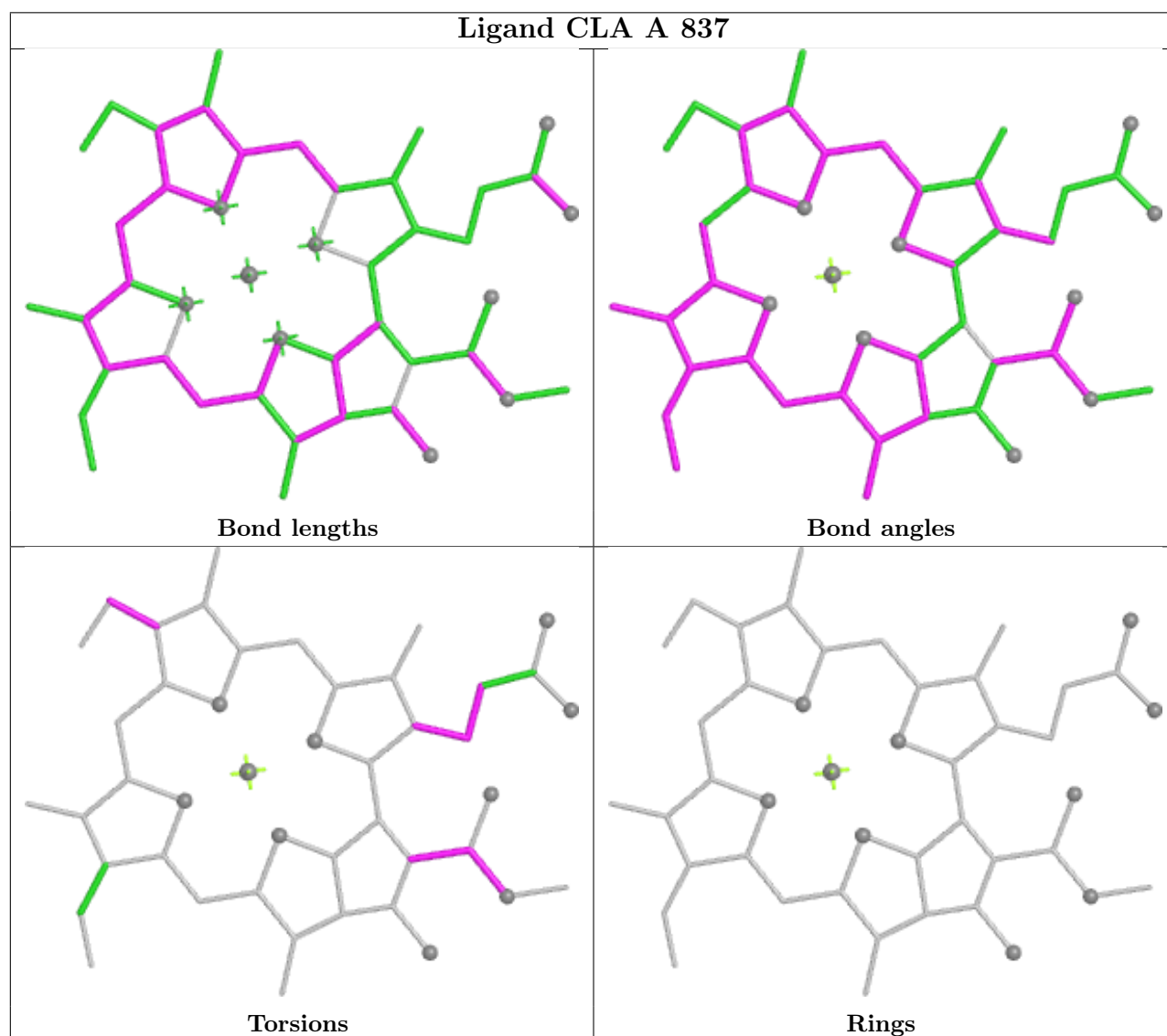
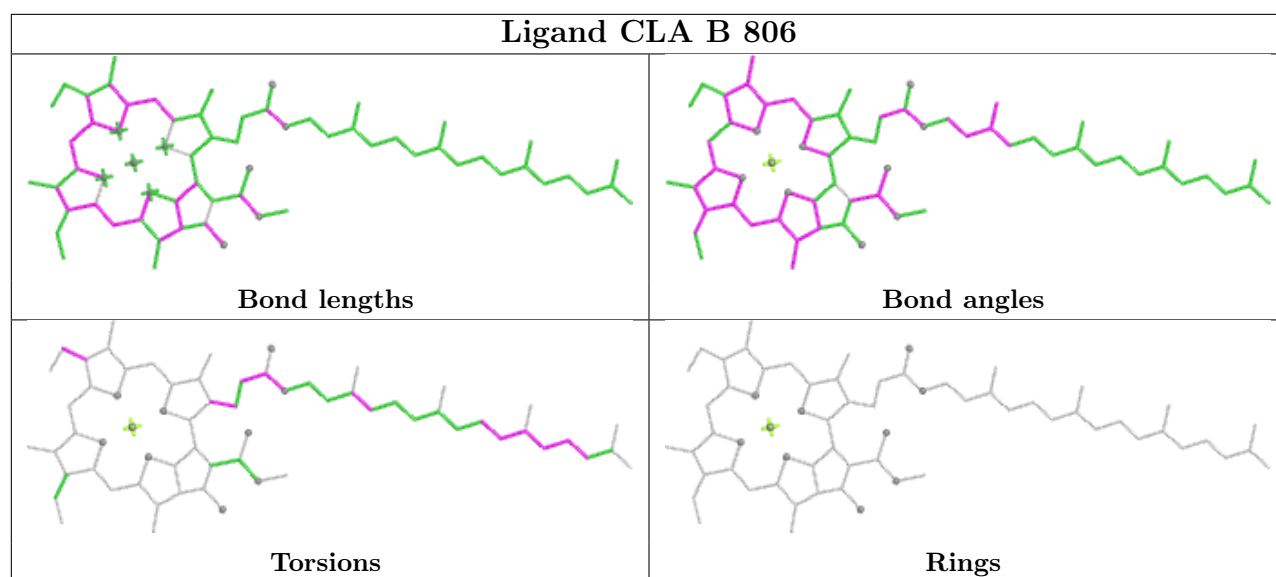


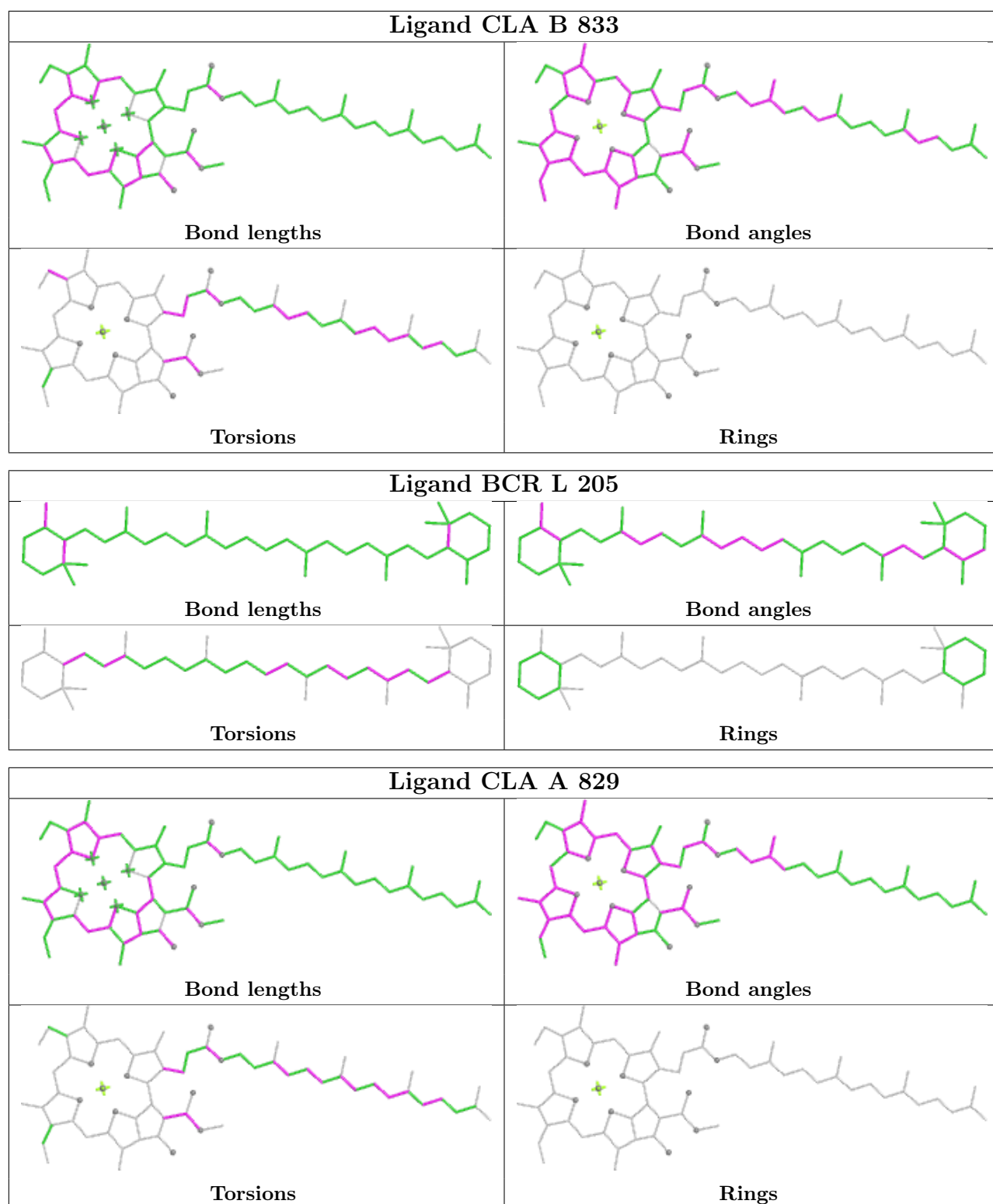
Ligand CLA A 831

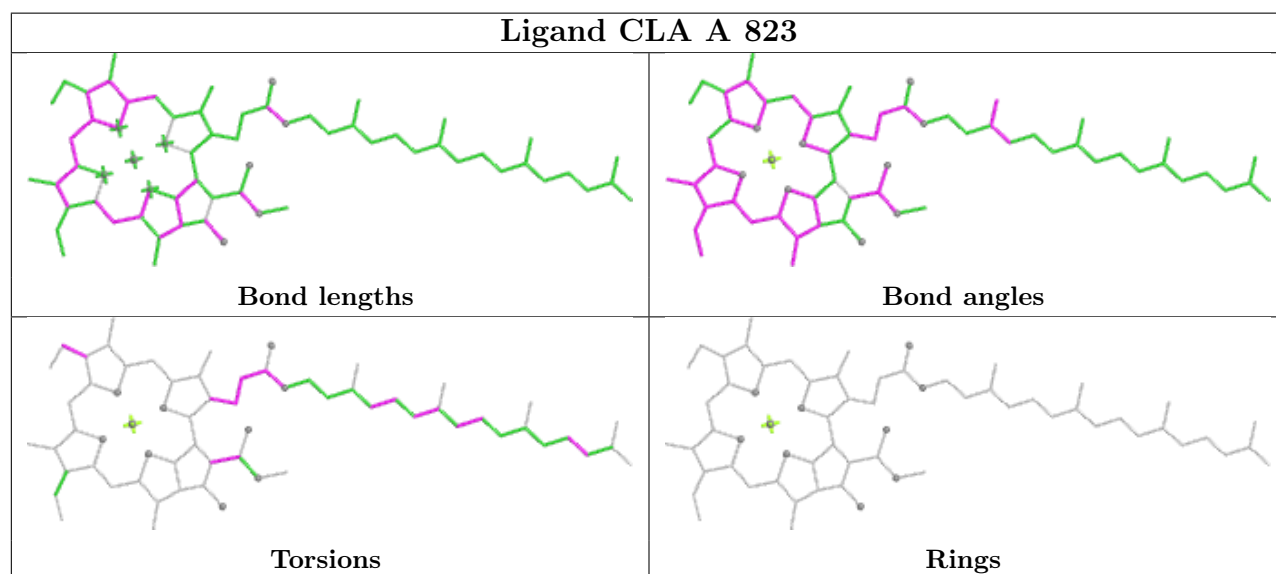
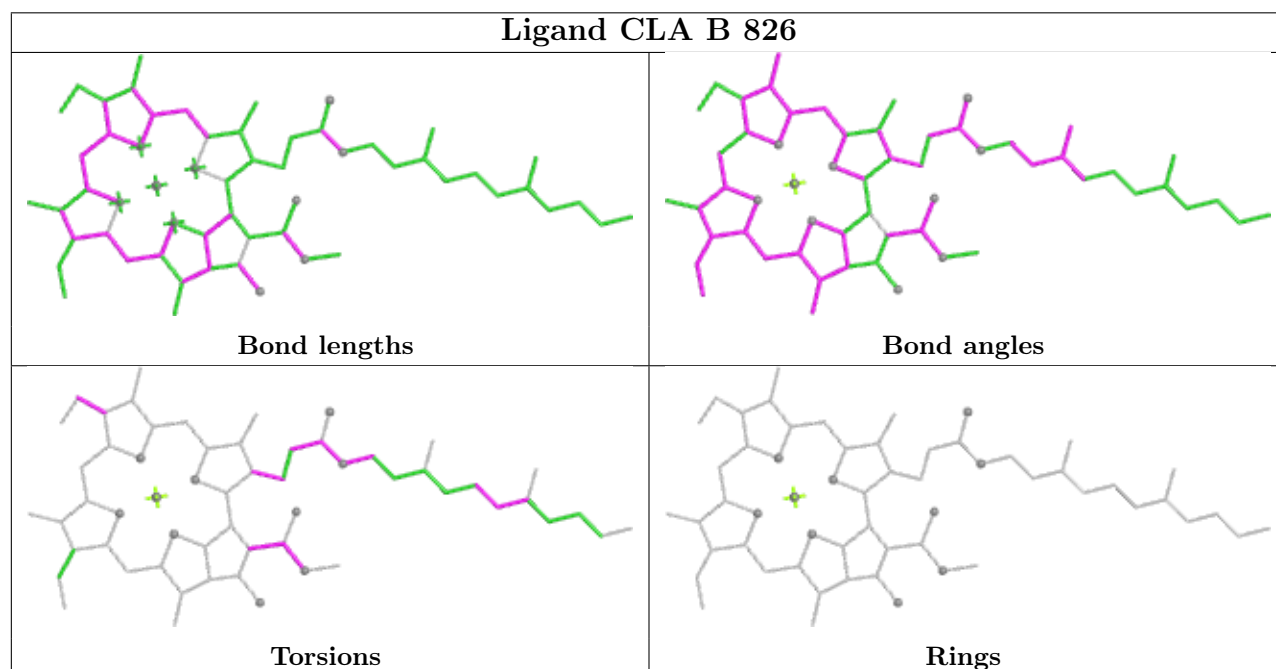
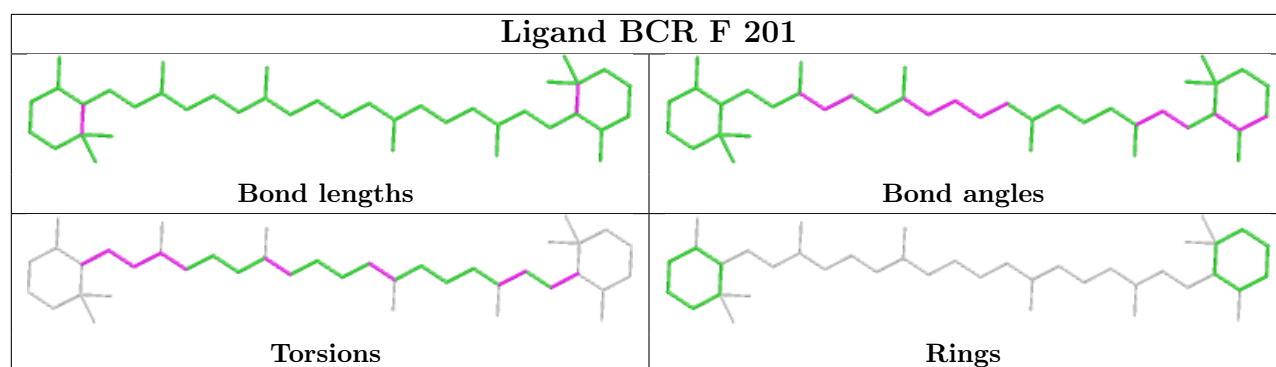


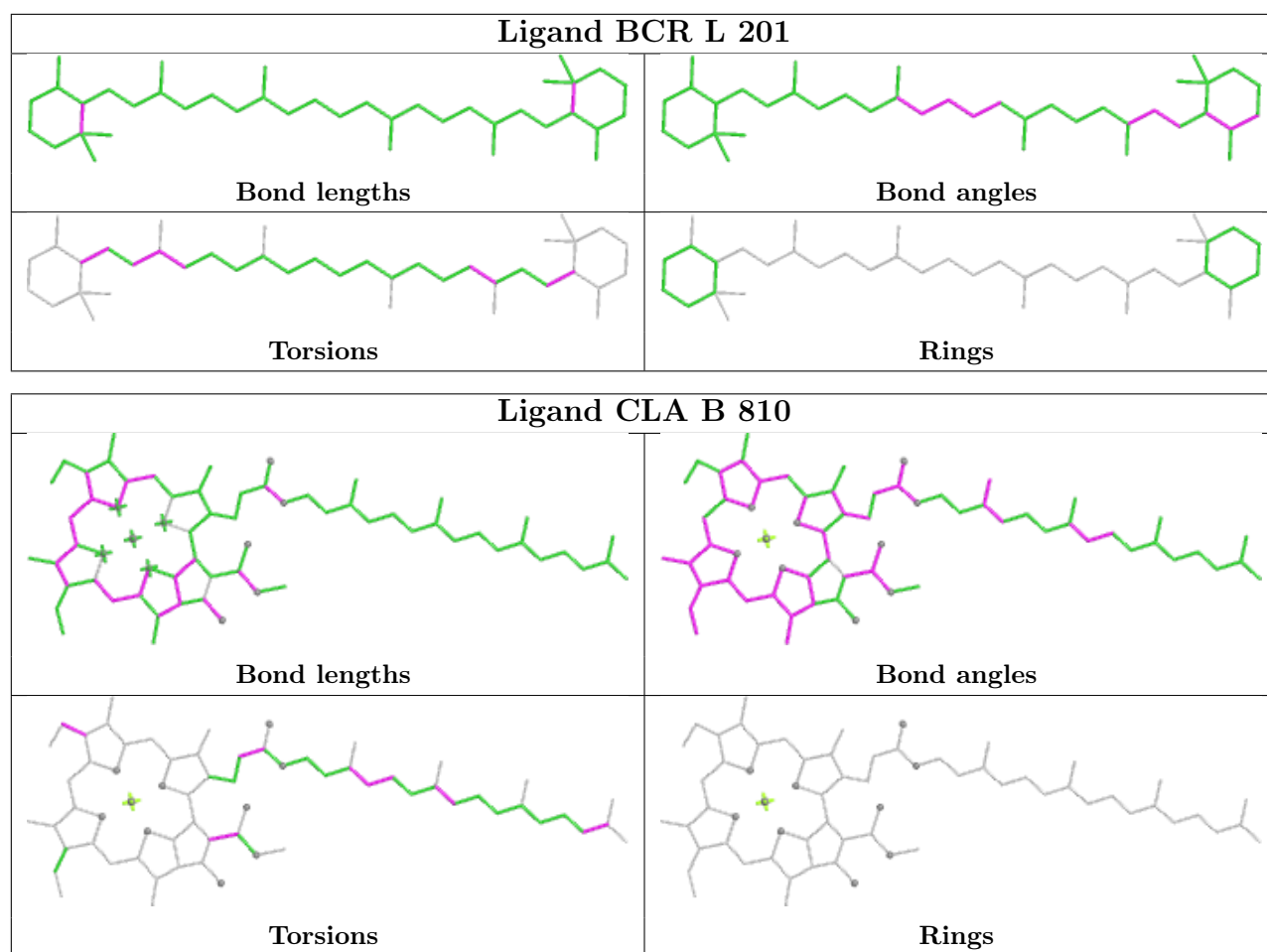
Ligand CLA L 202



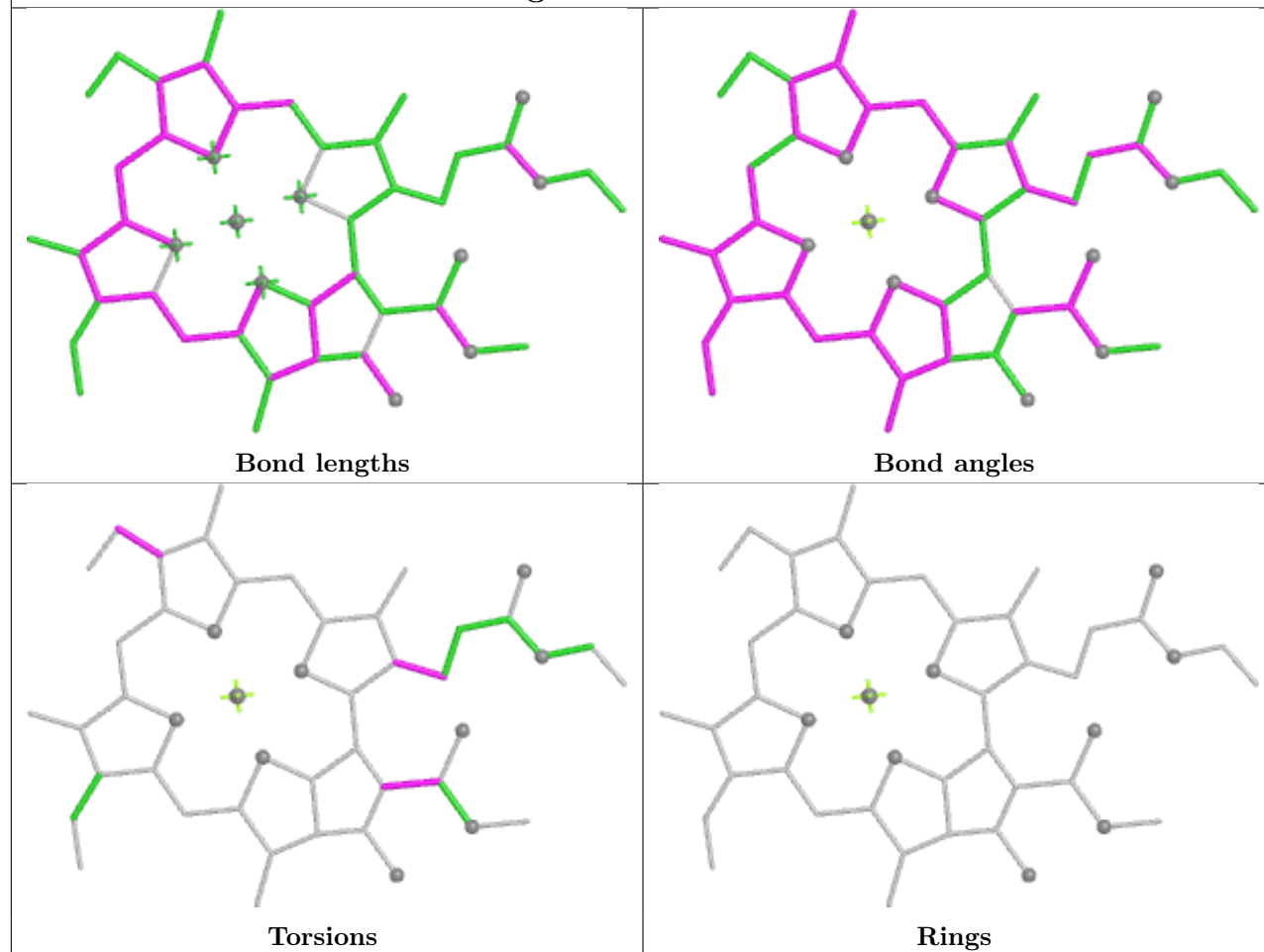




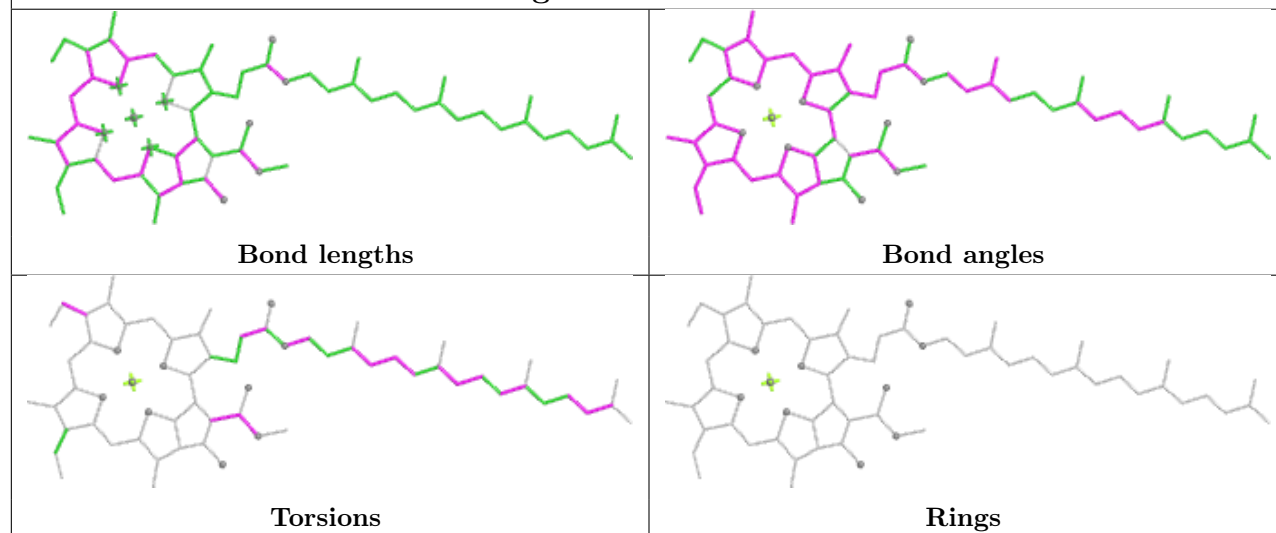


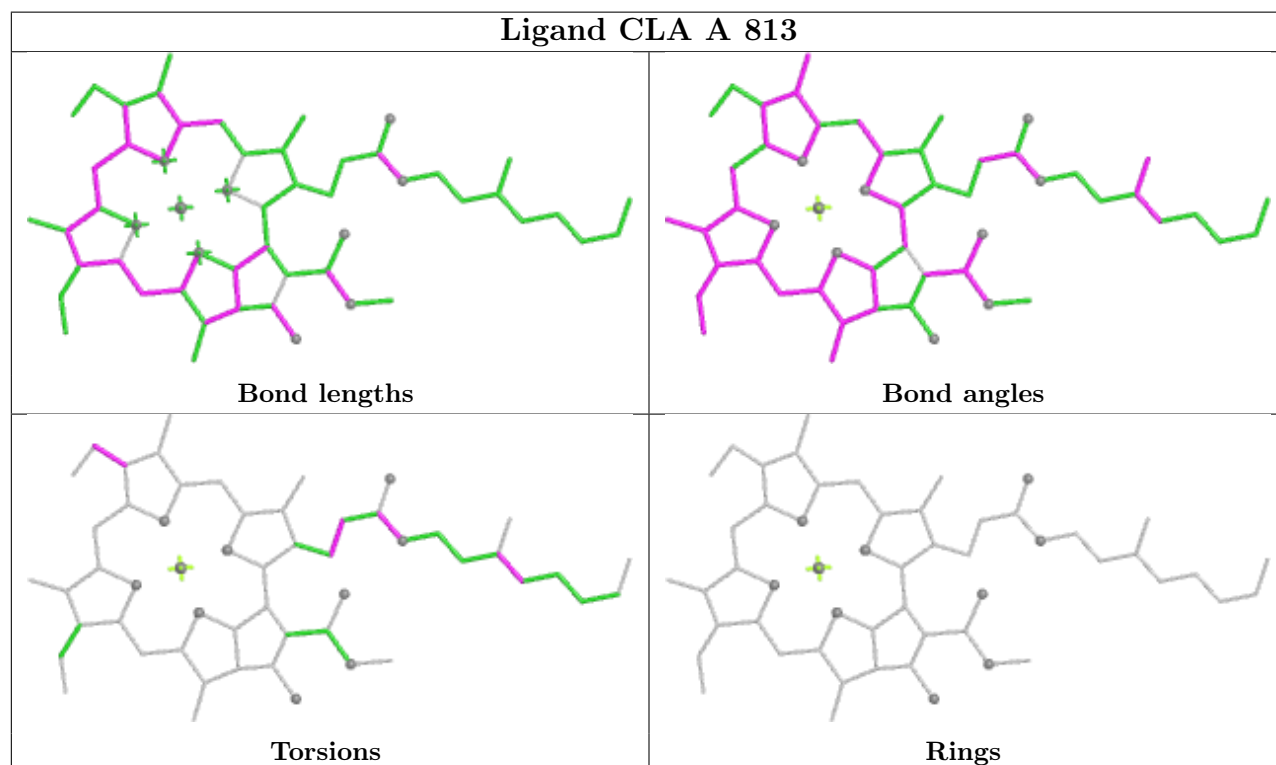
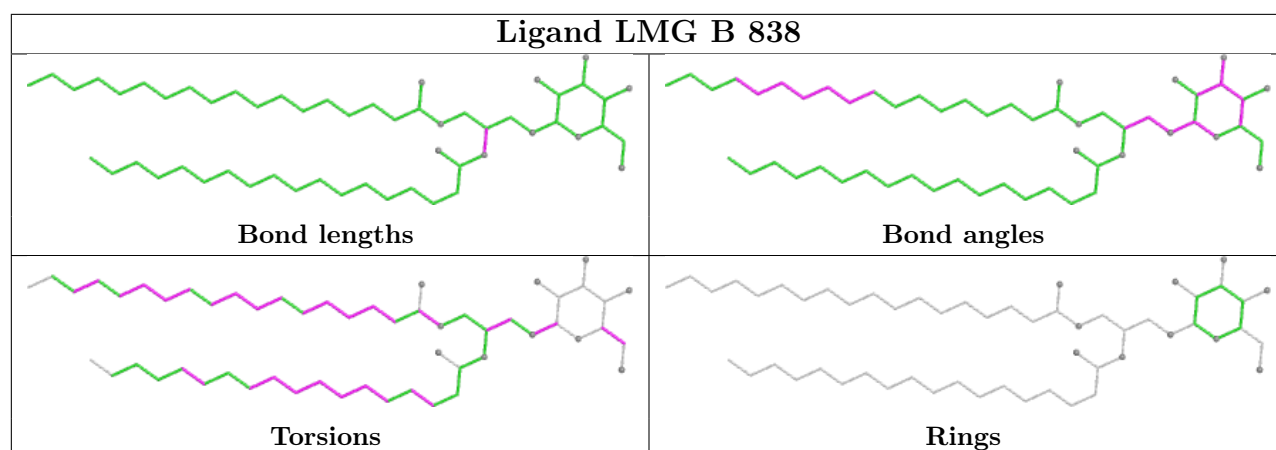


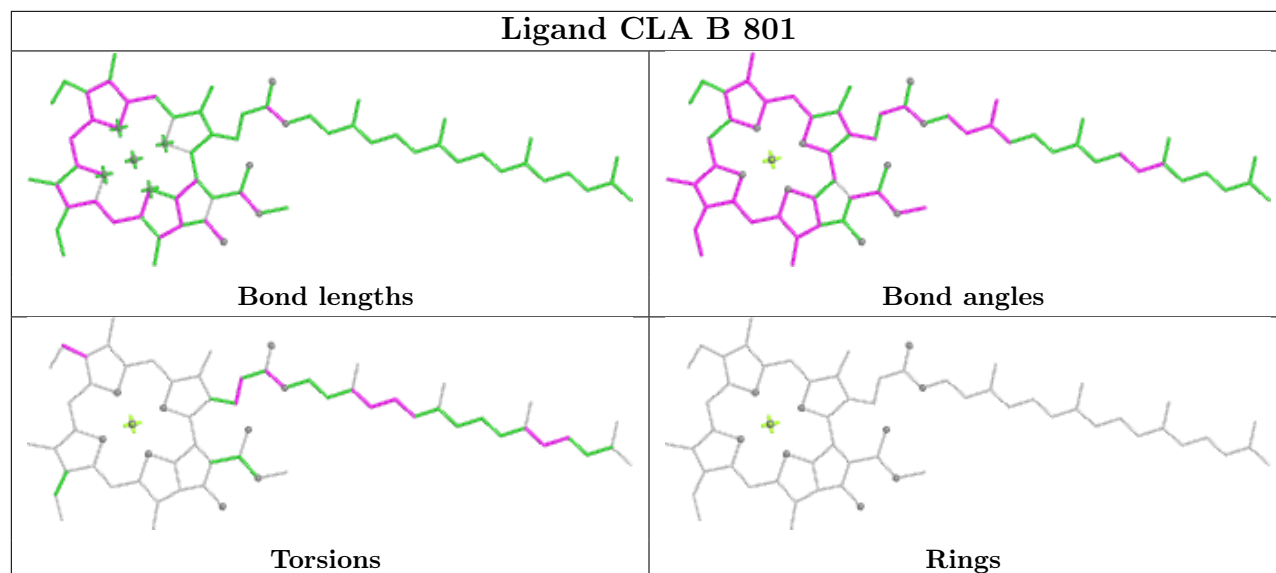
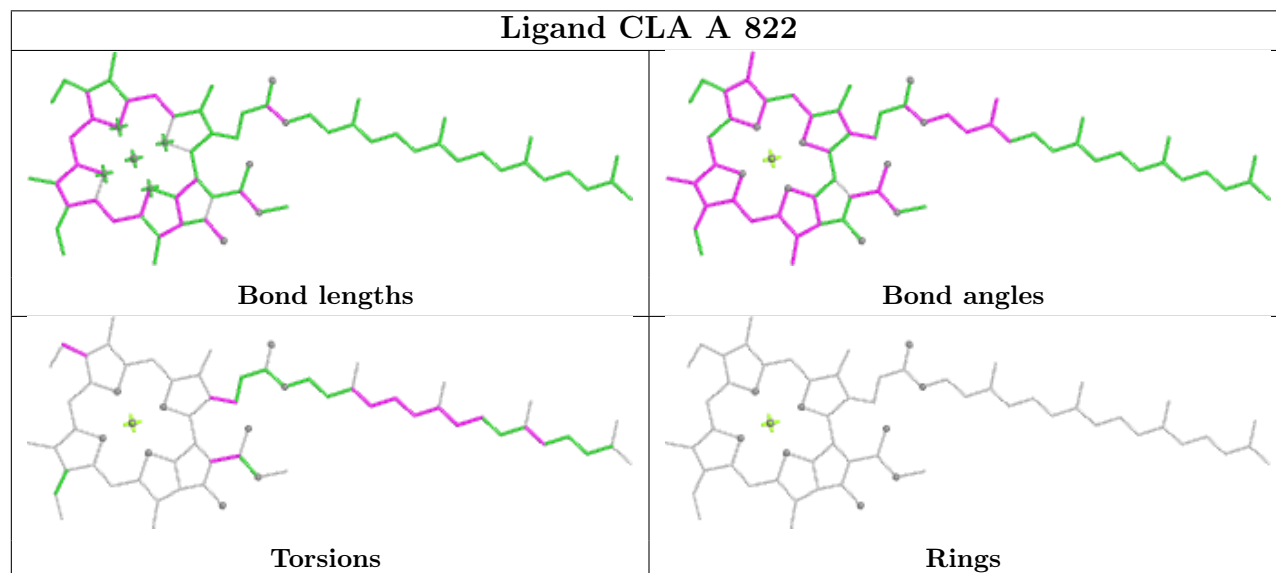
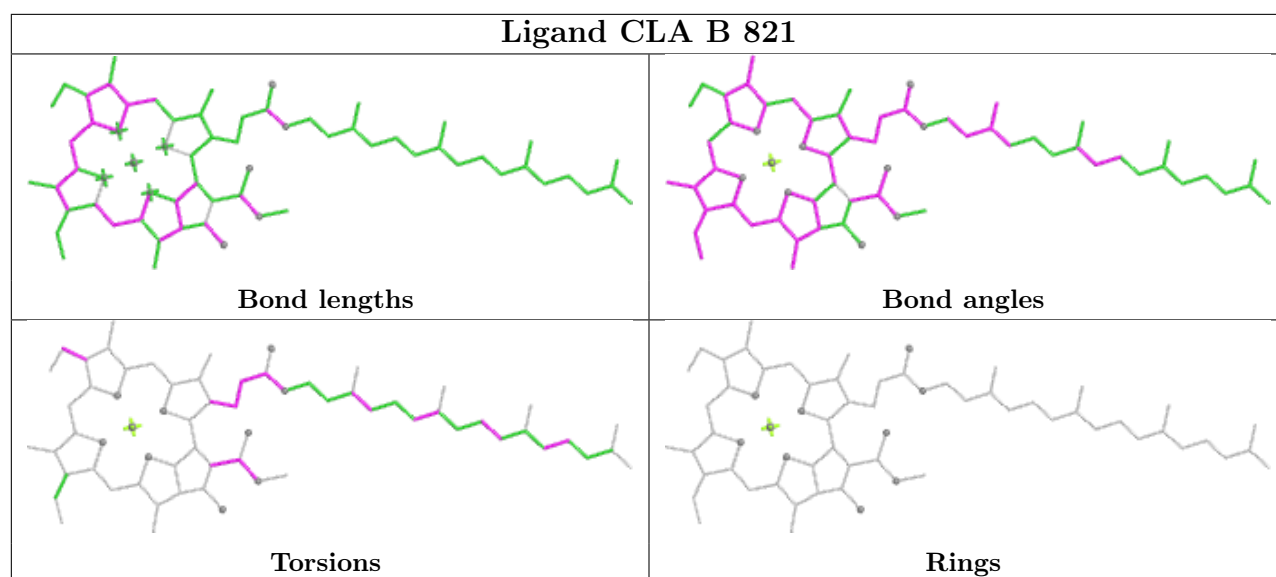
Ligand CLA B 831

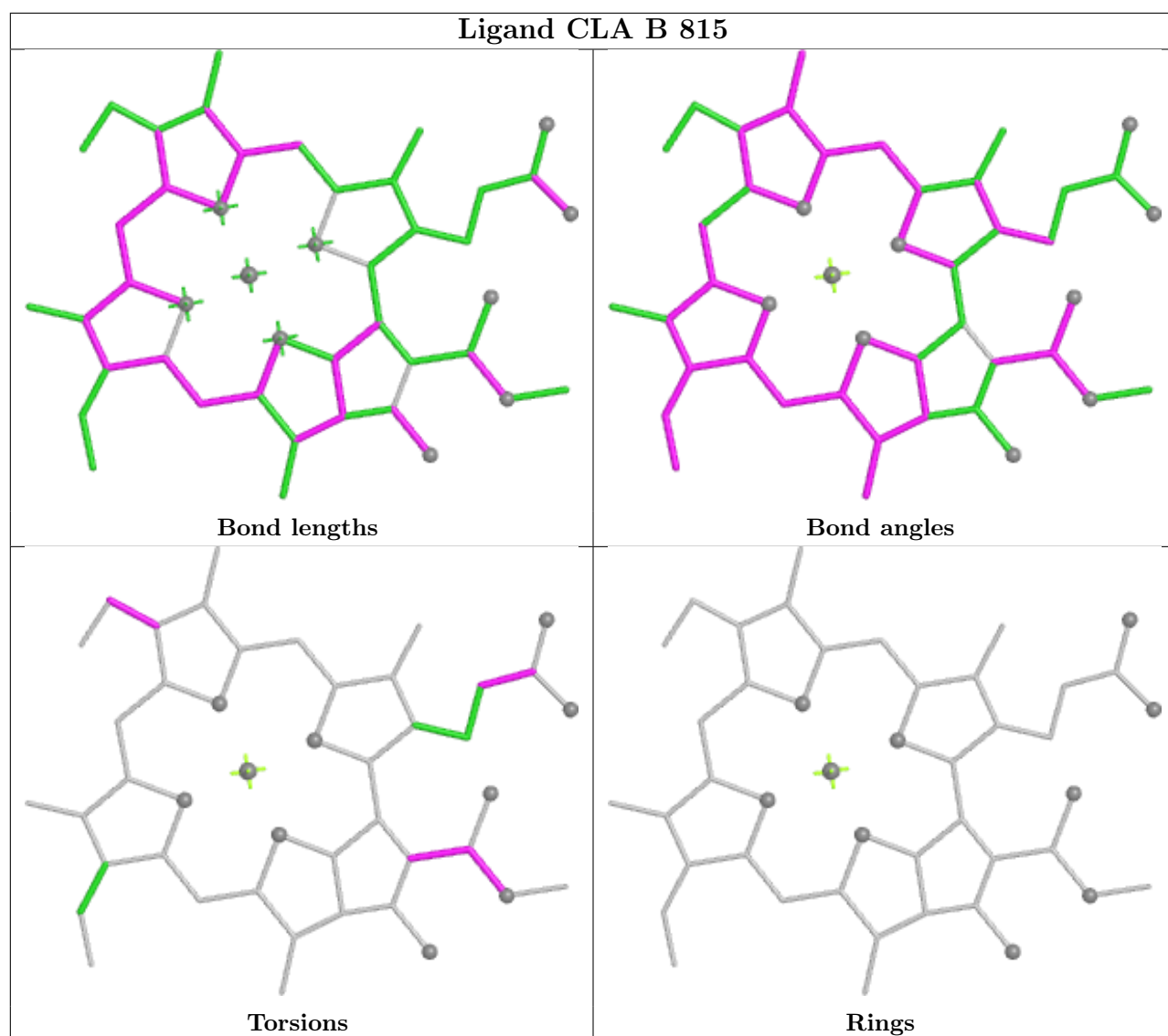


Ligand CLA B 802

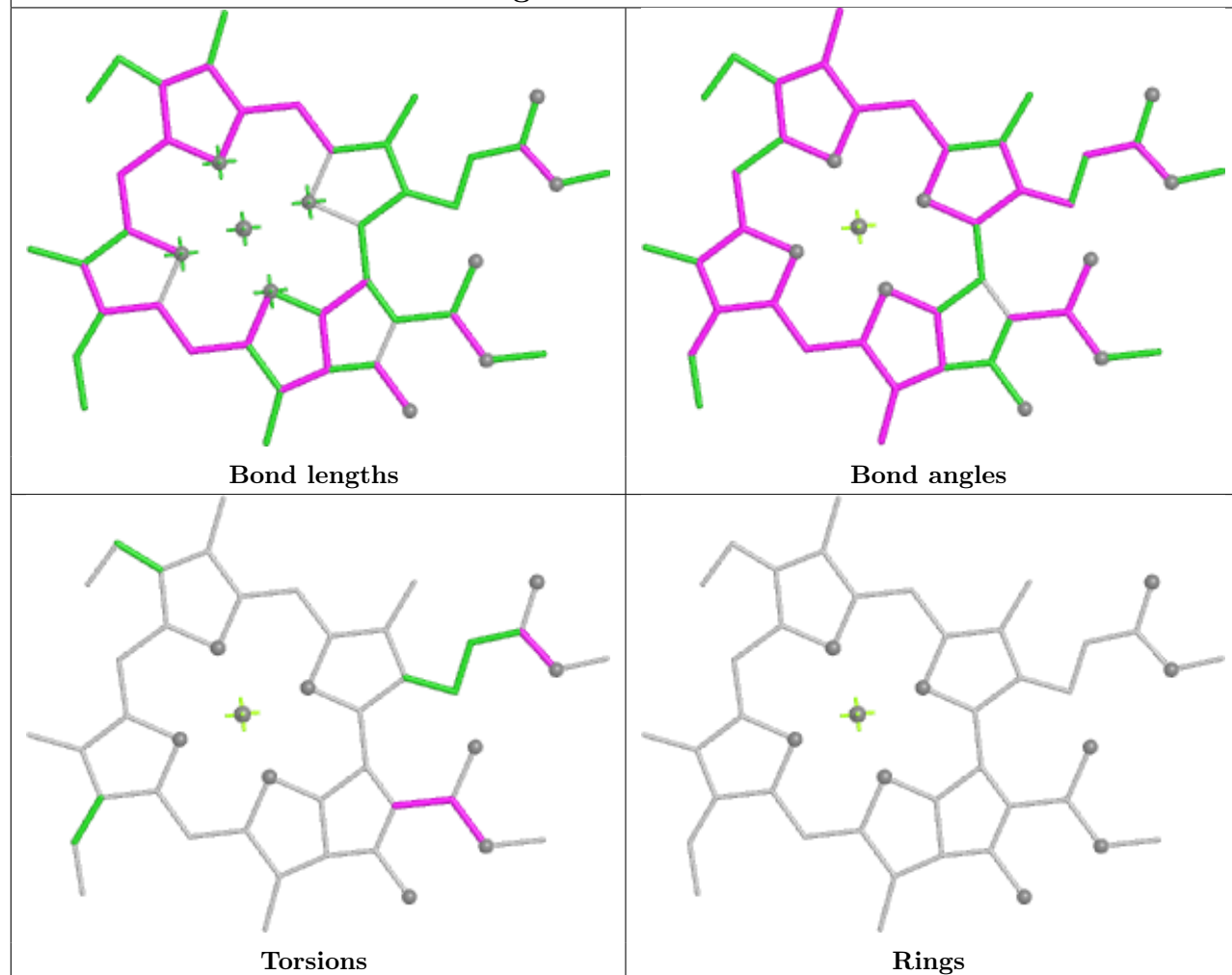


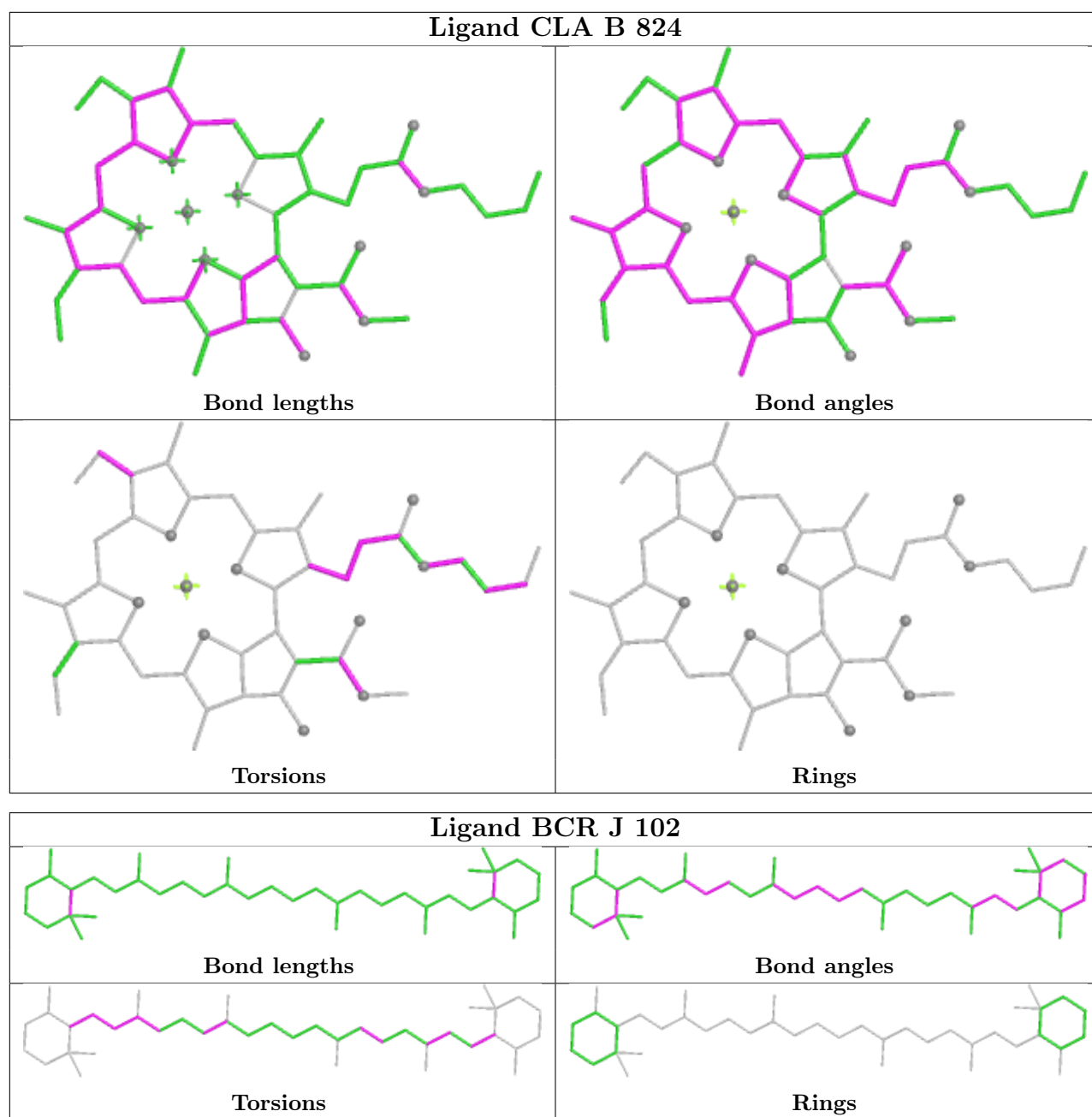


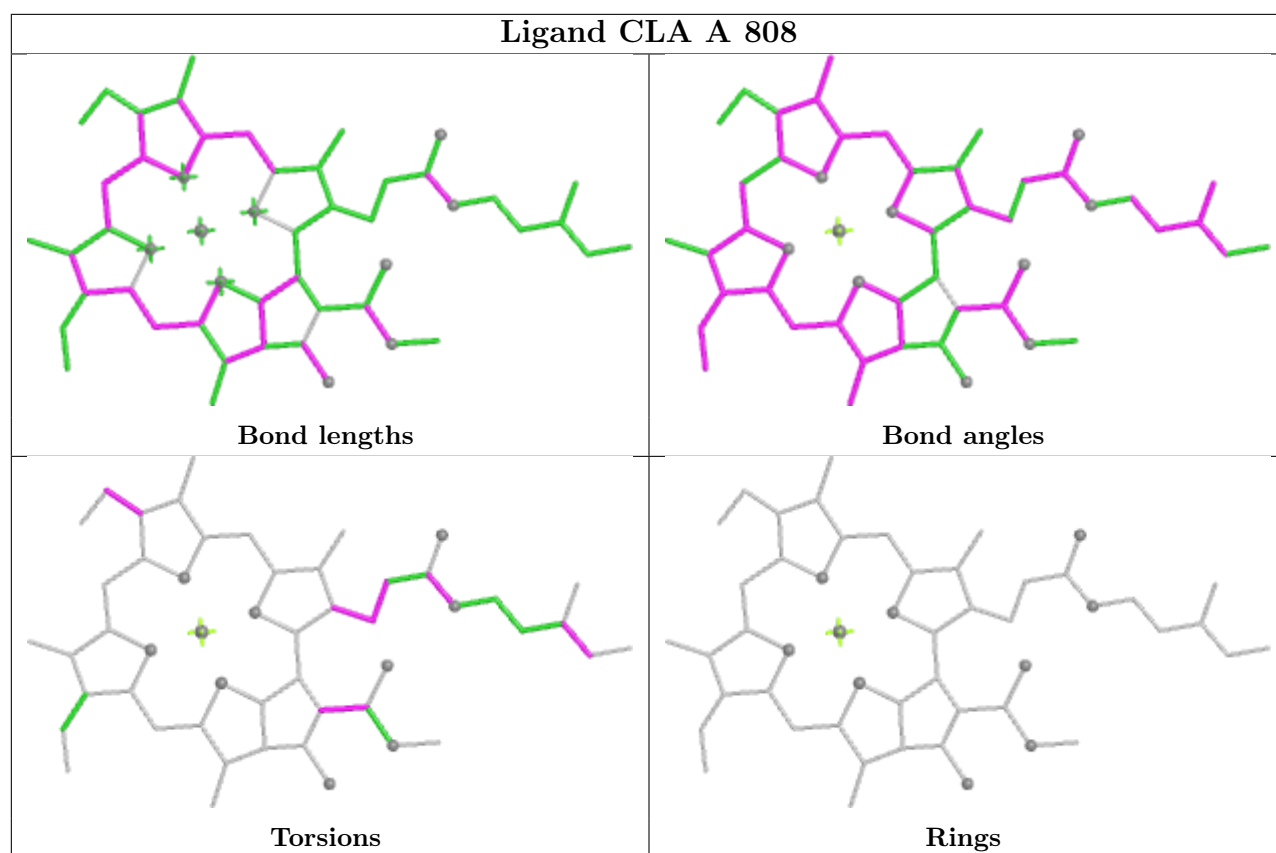


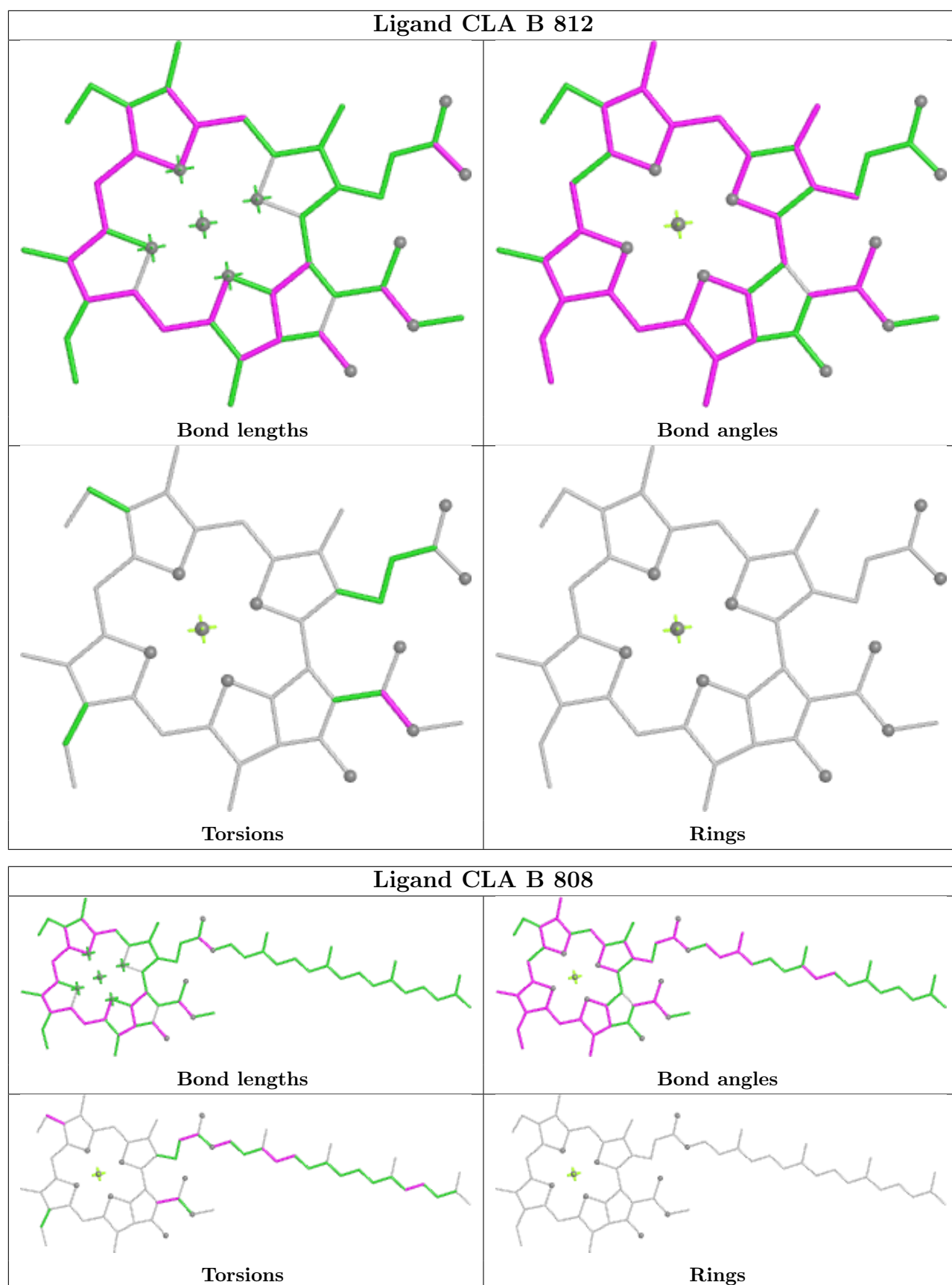


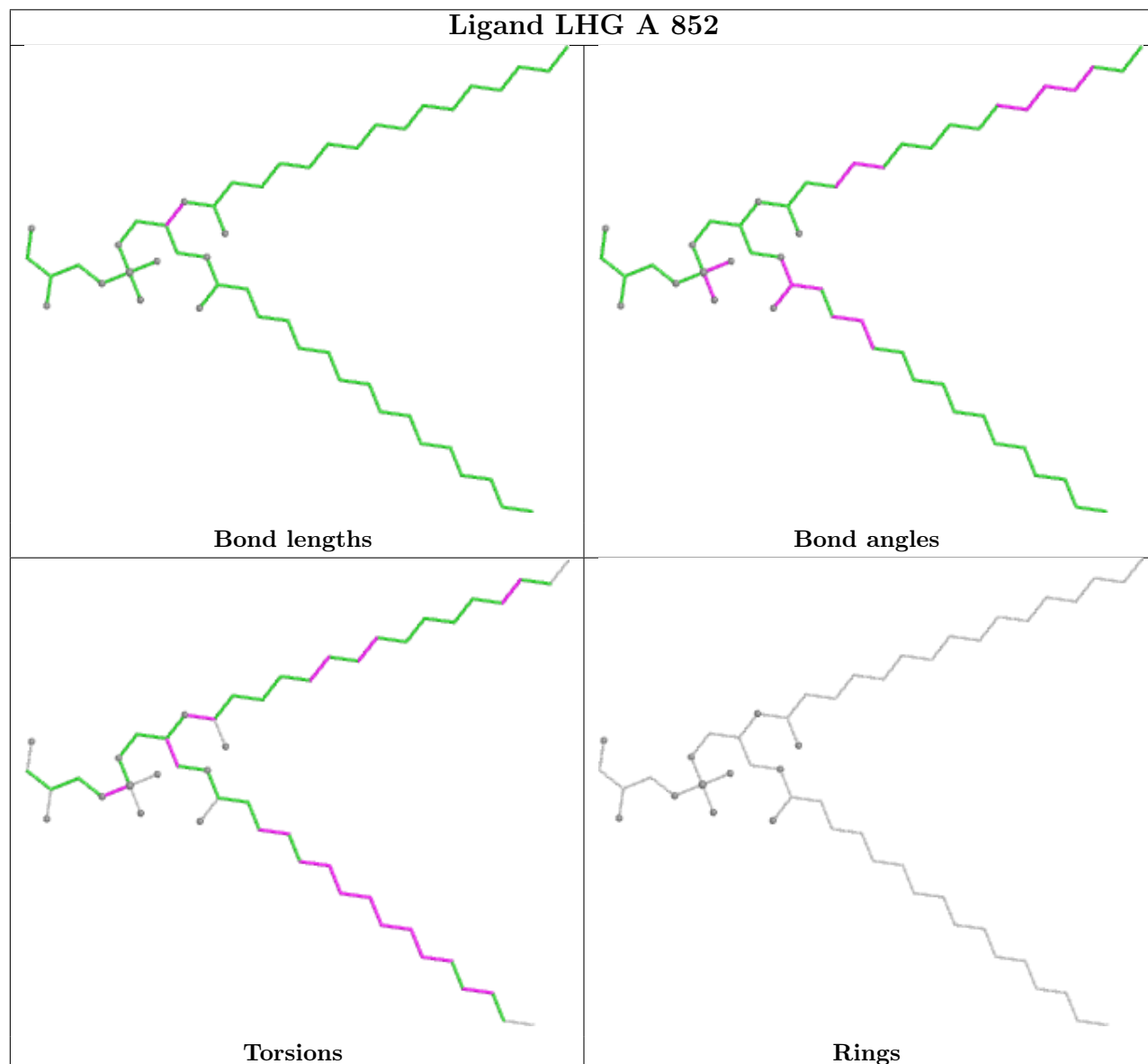
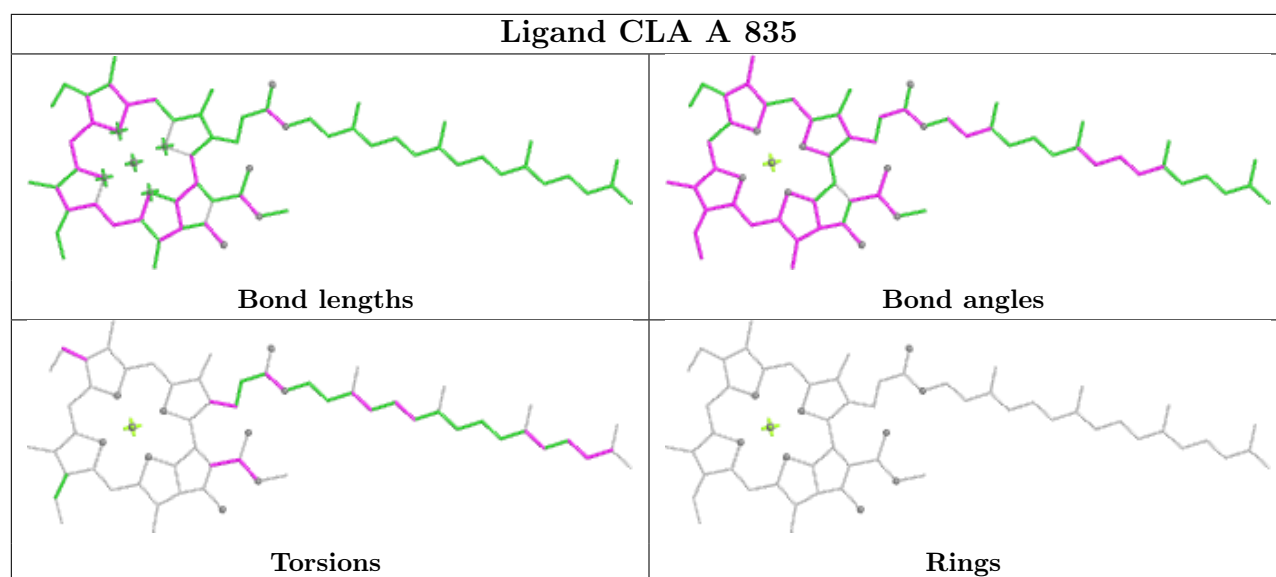
Ligand CLA B 819

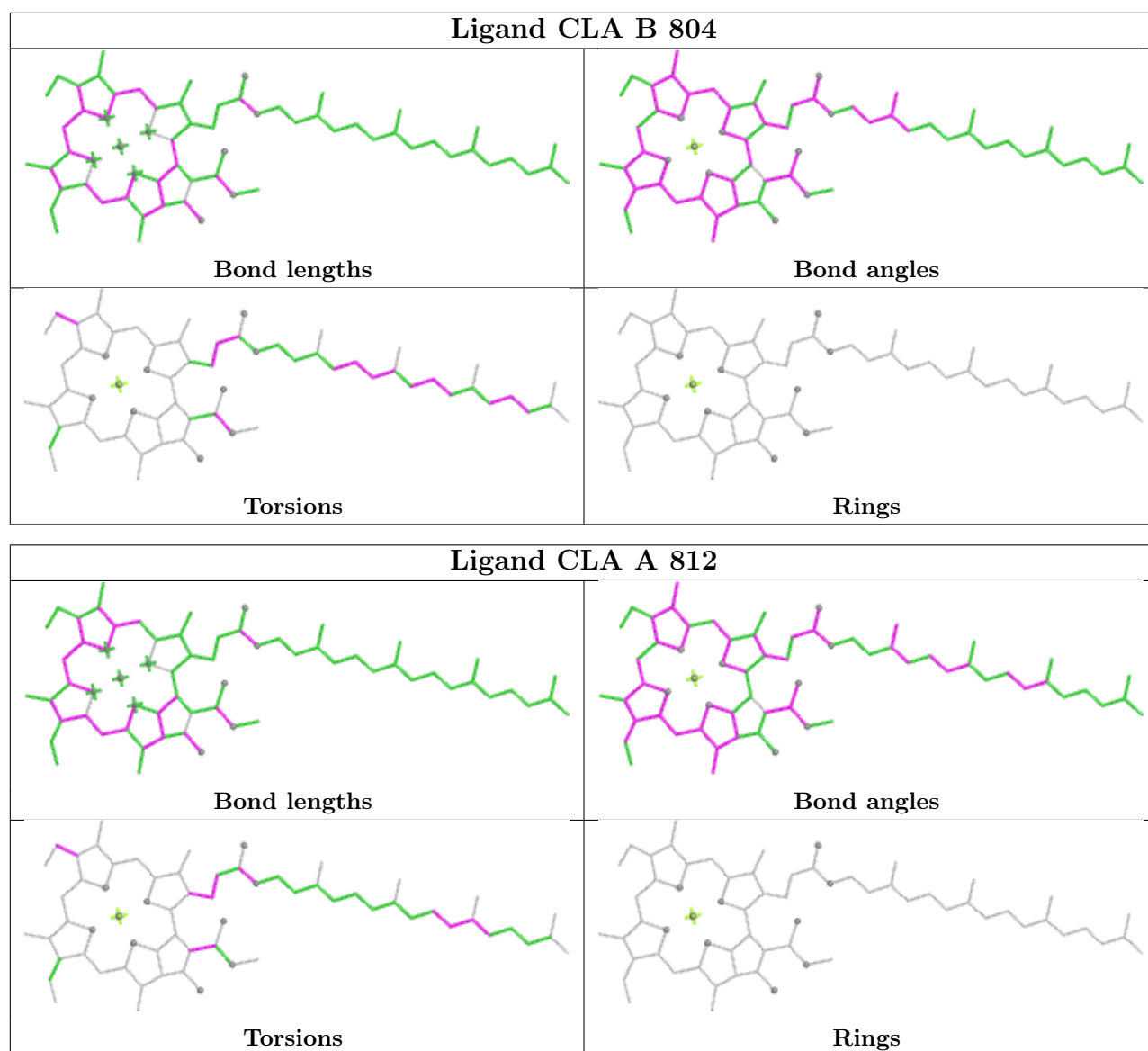


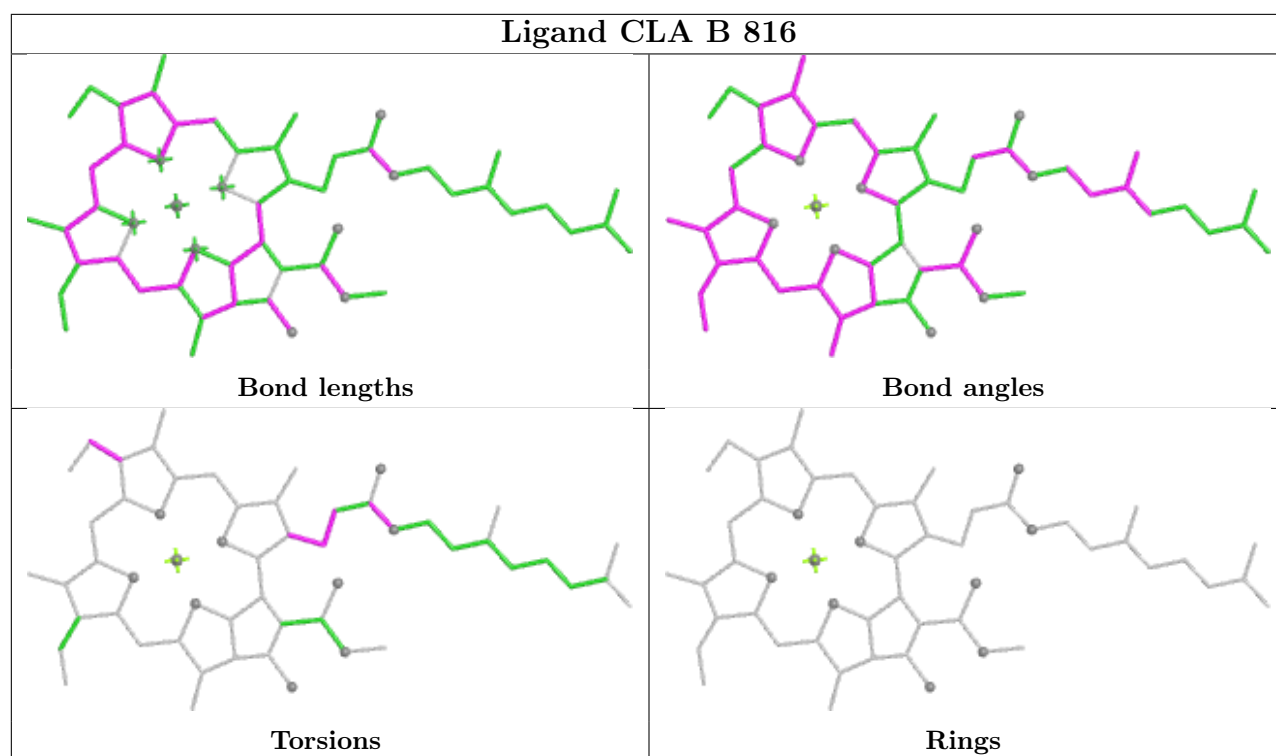


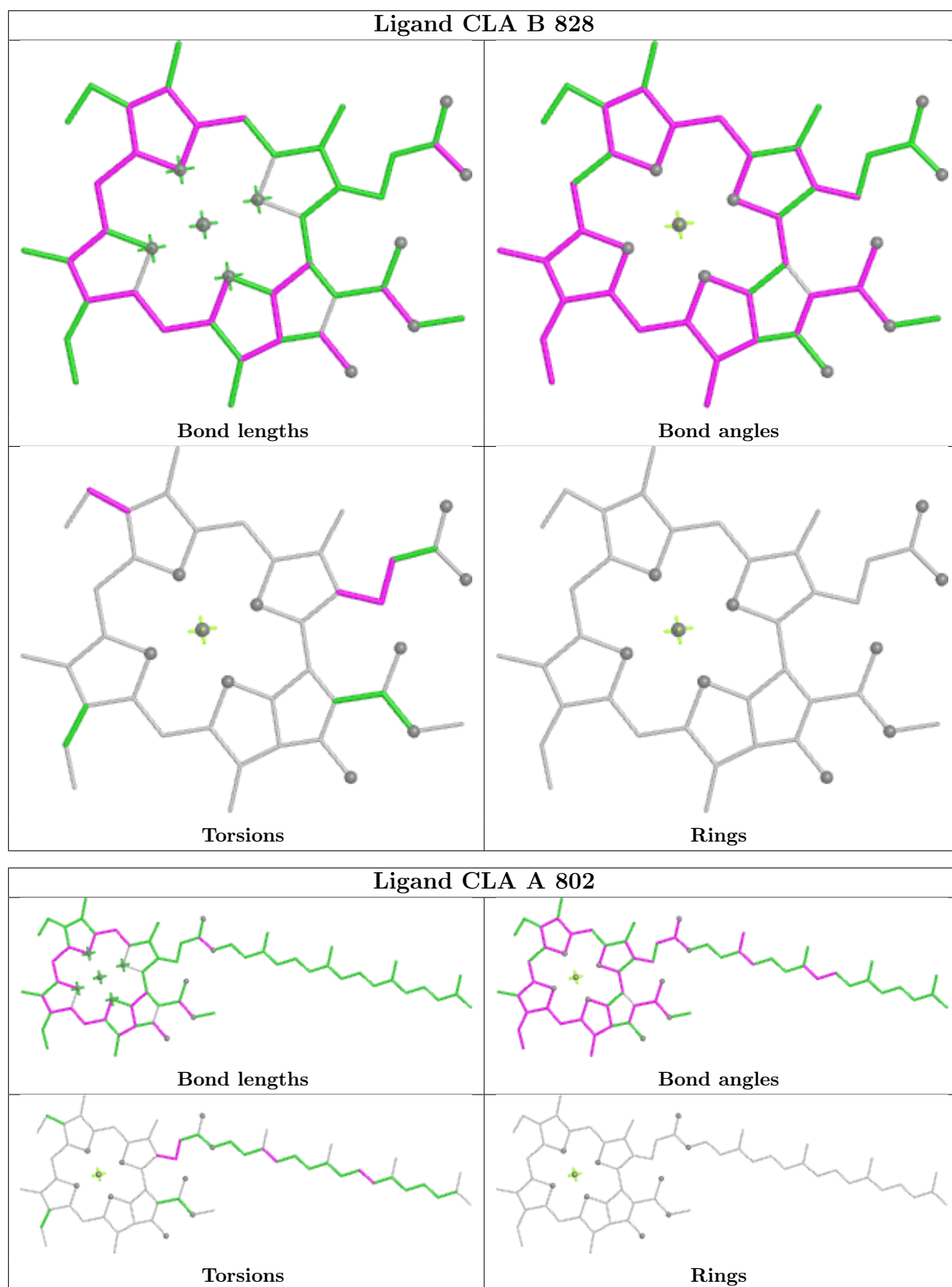


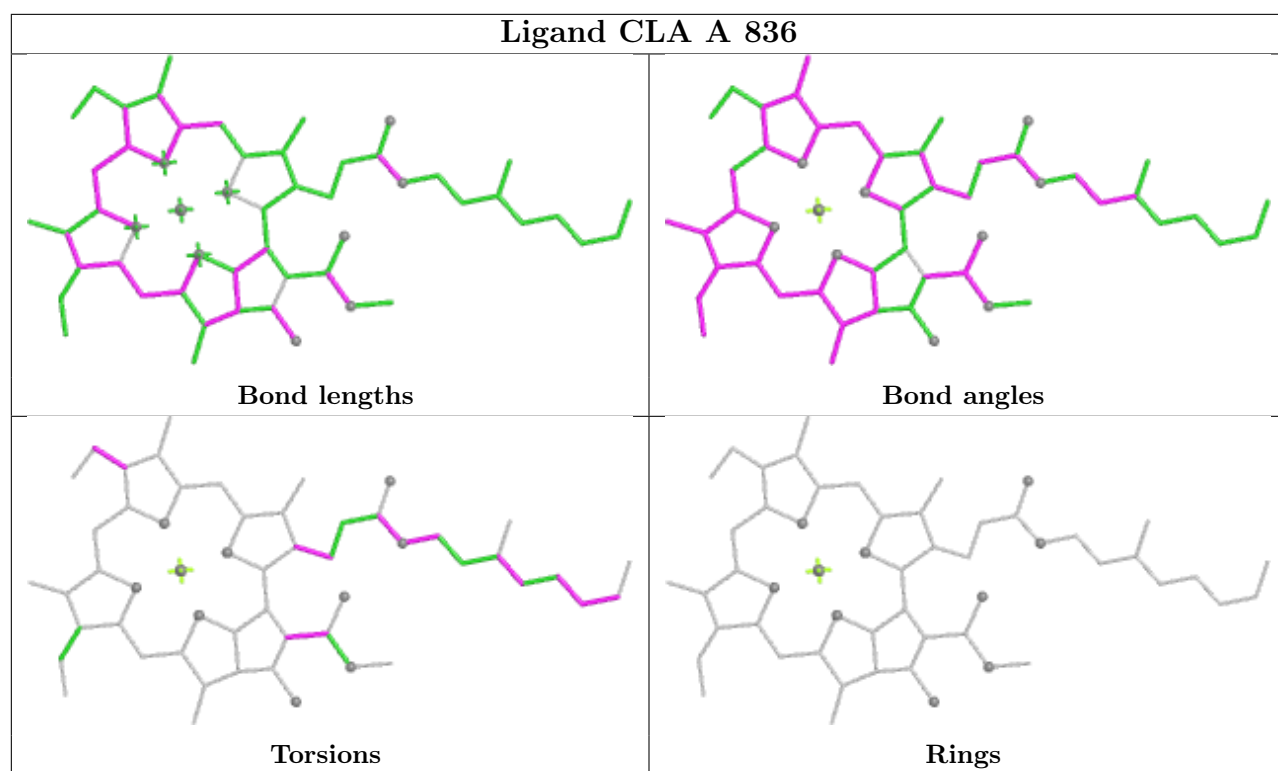




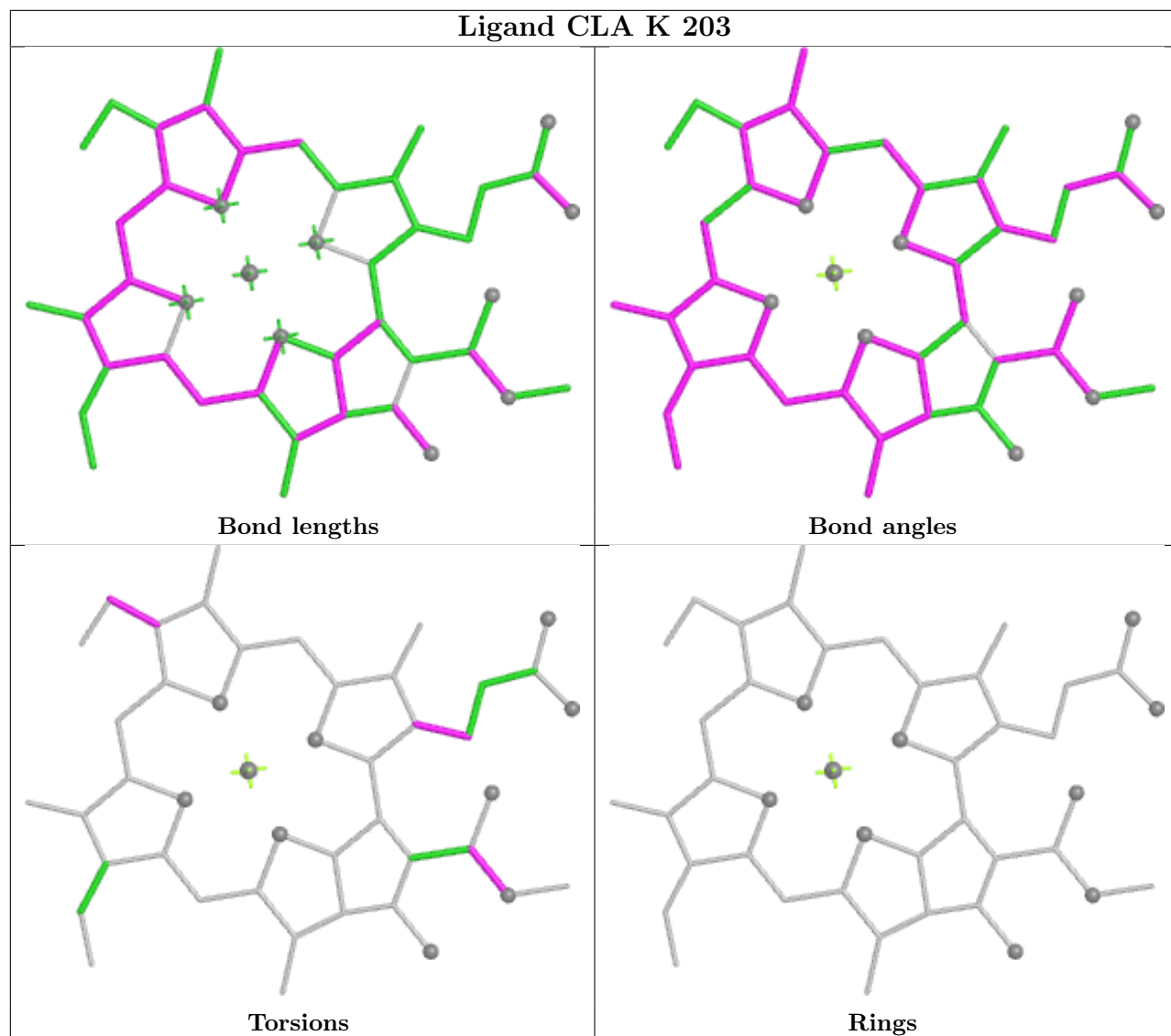


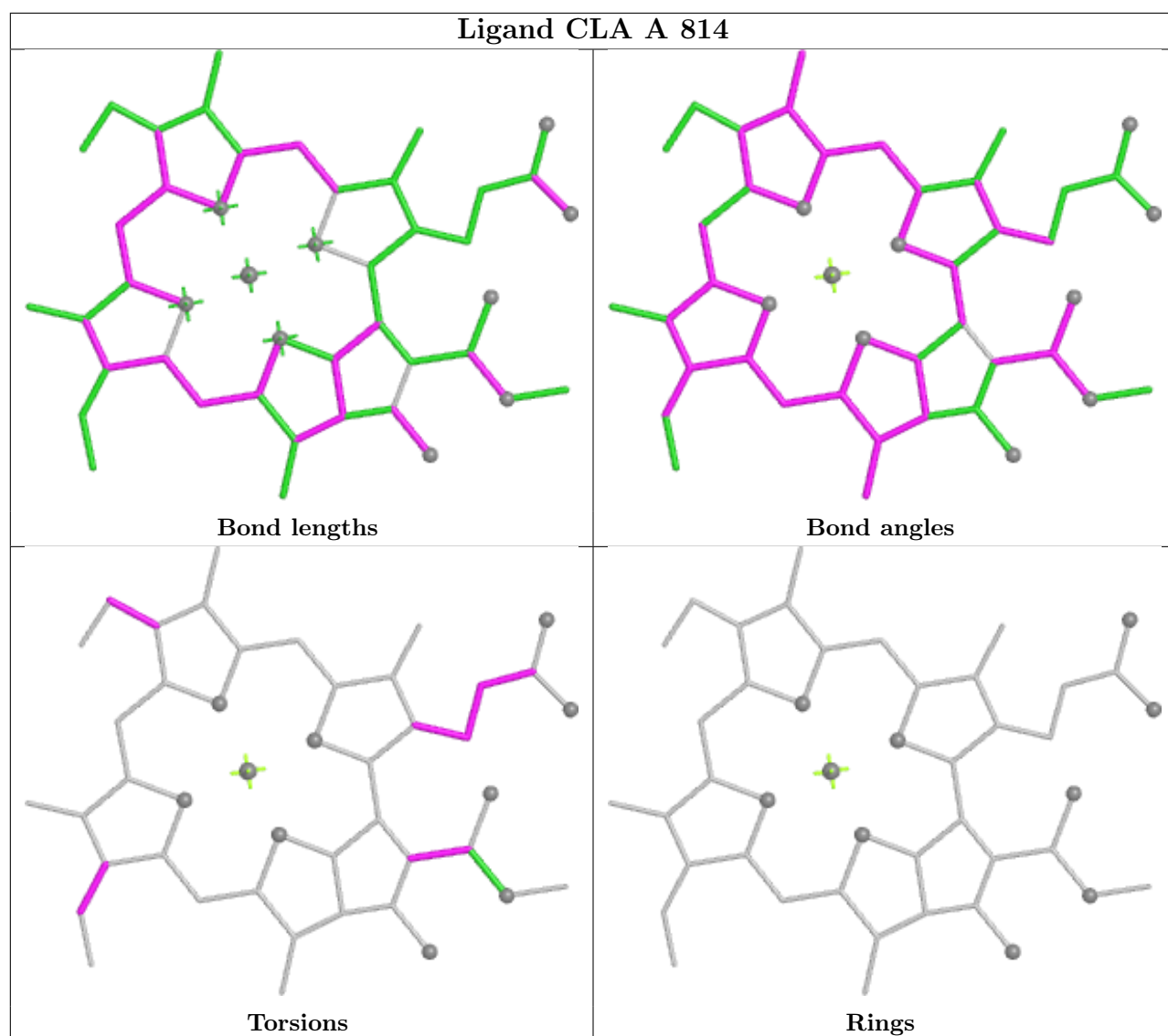




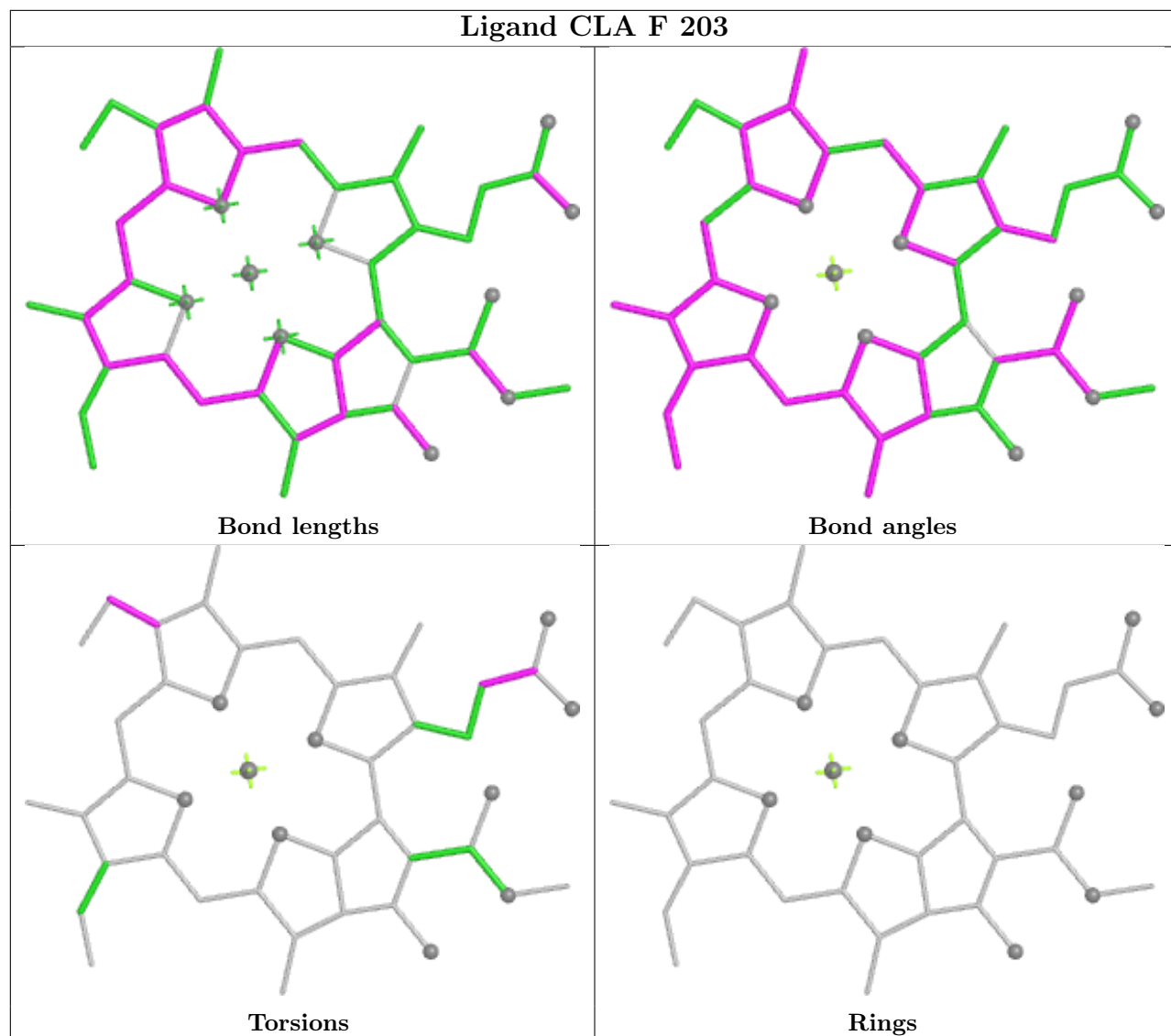


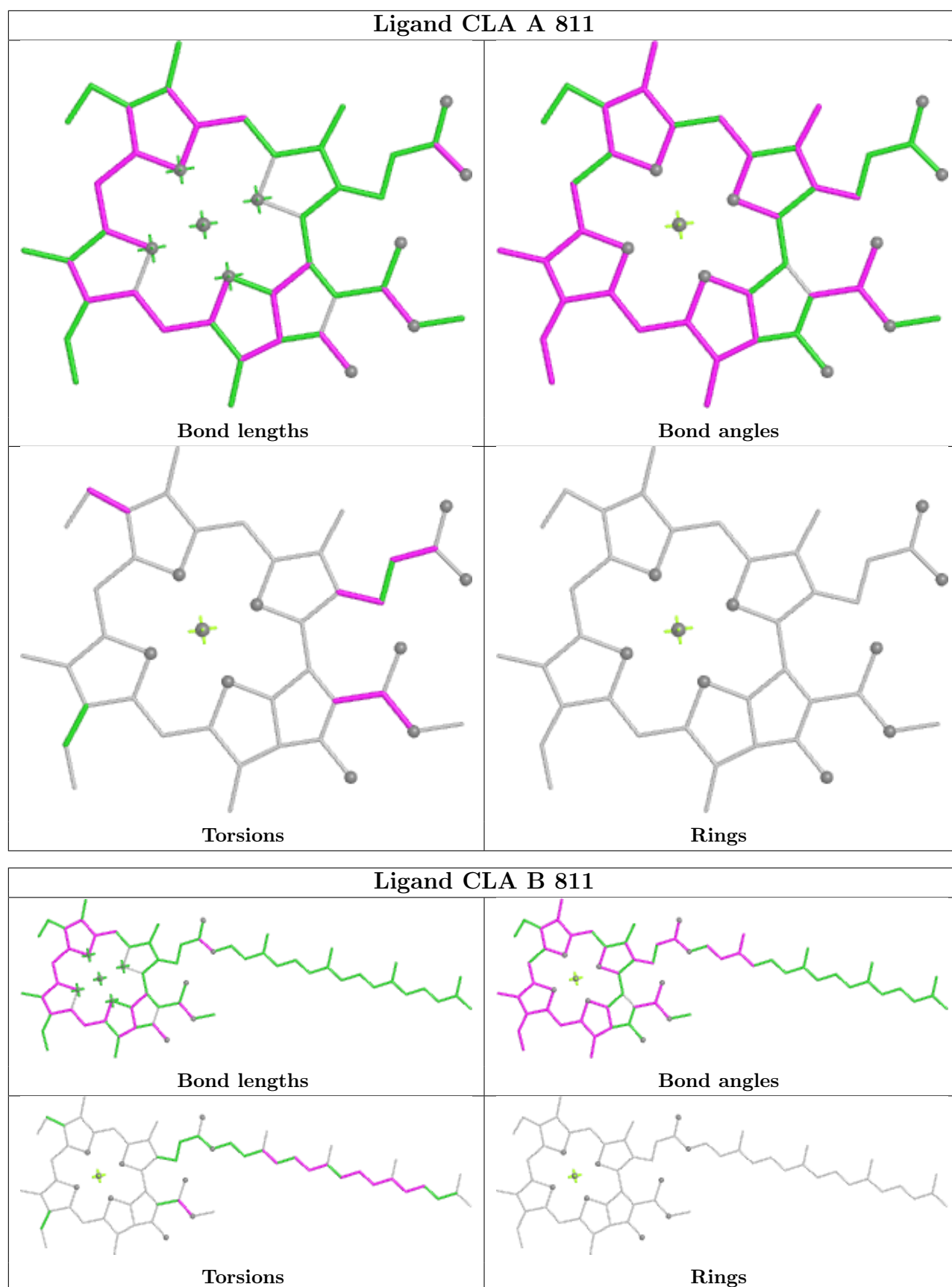
Ligand CLA K 203

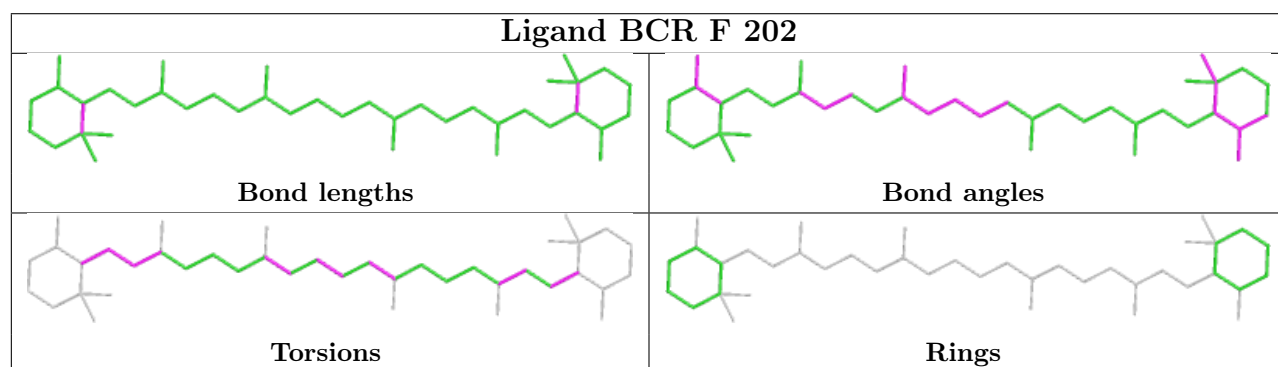
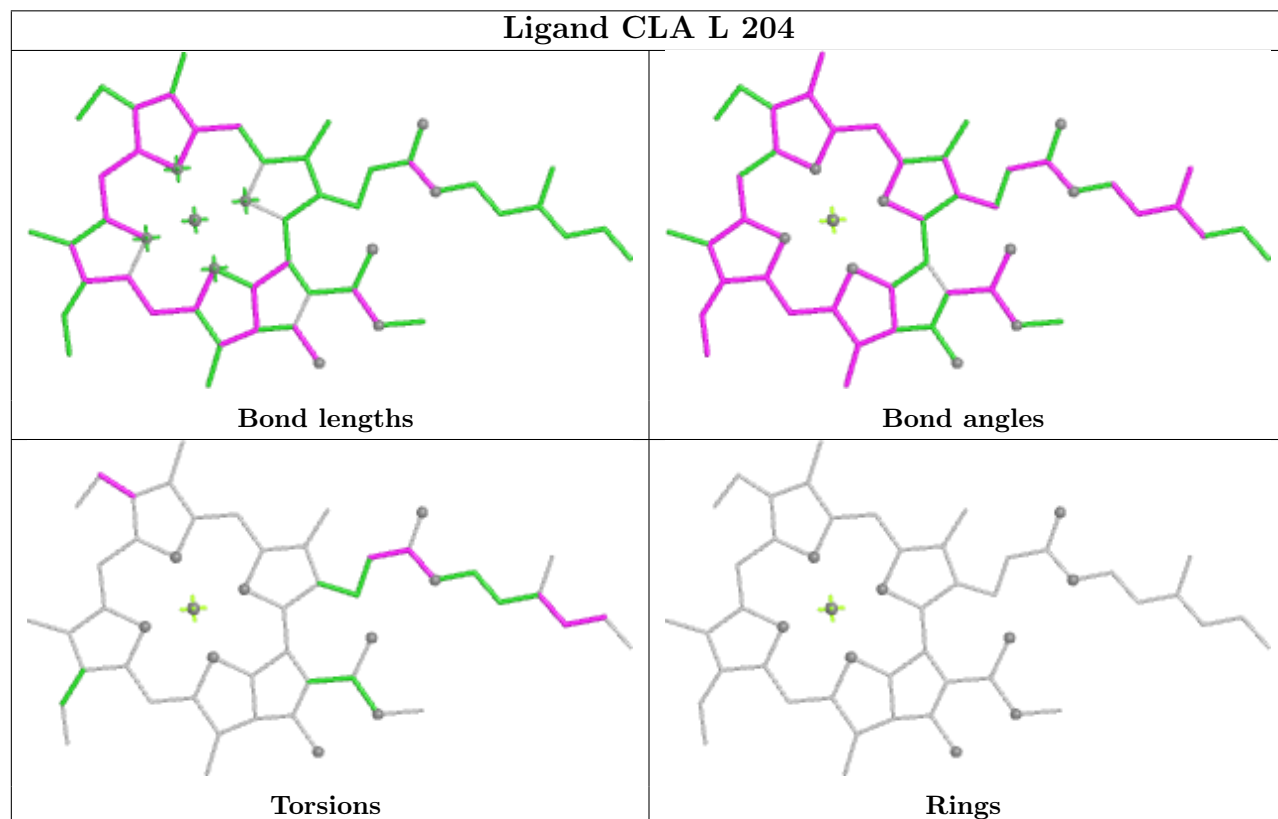
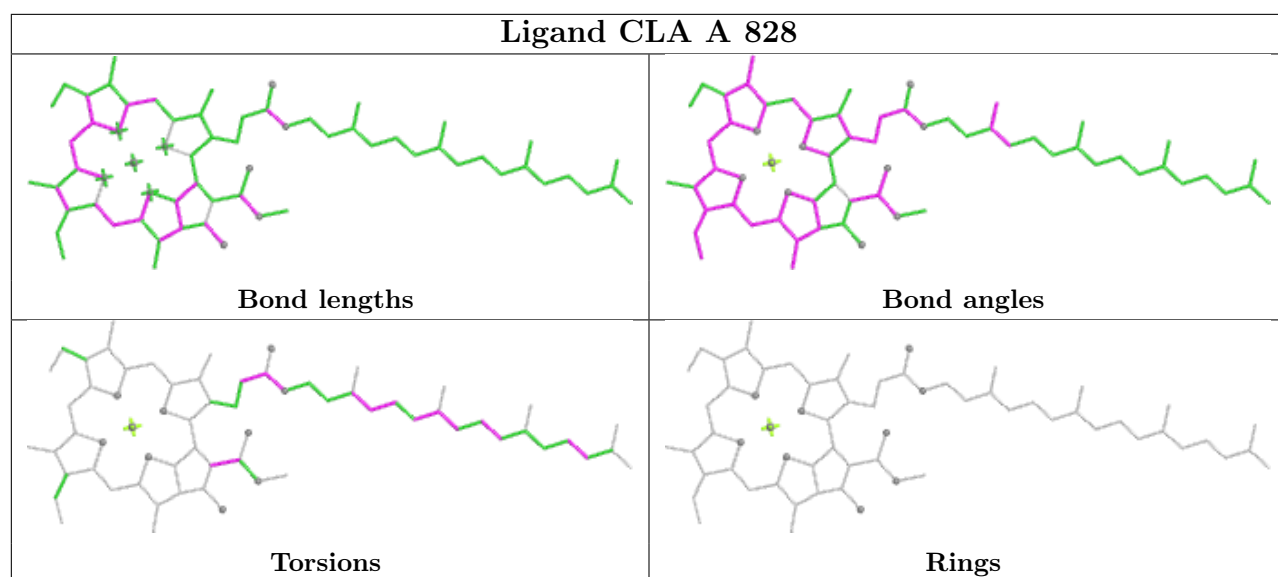


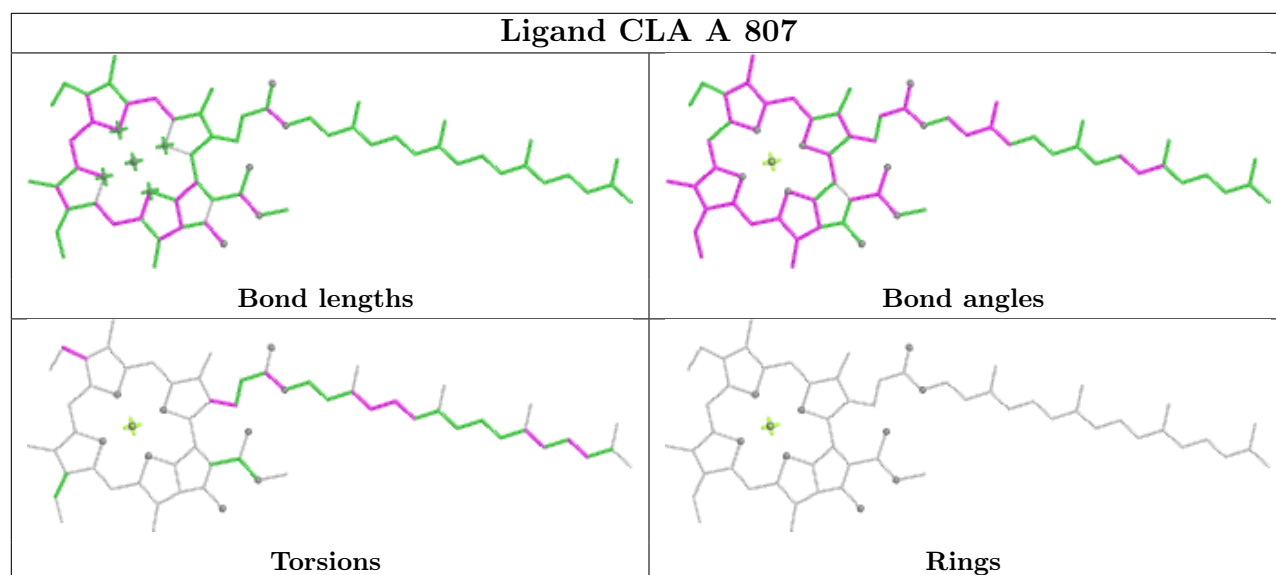
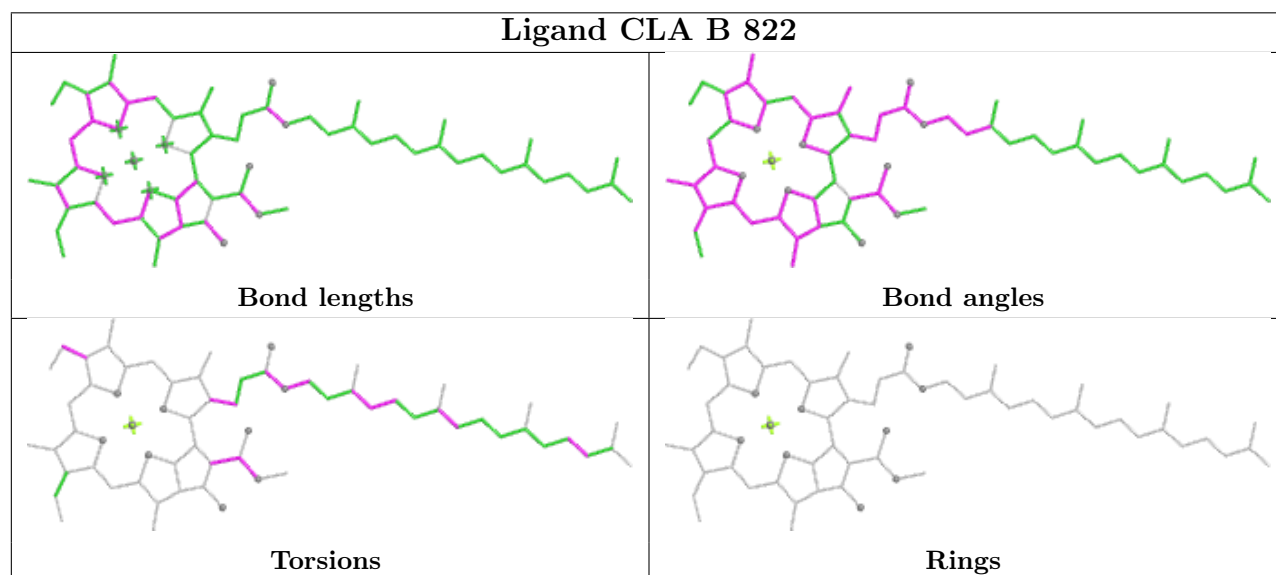
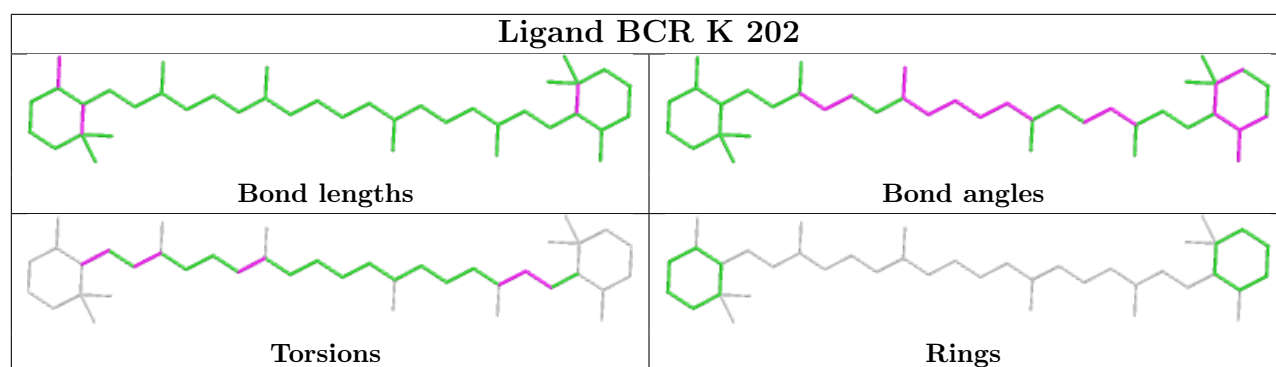


Ligand CLA F 203

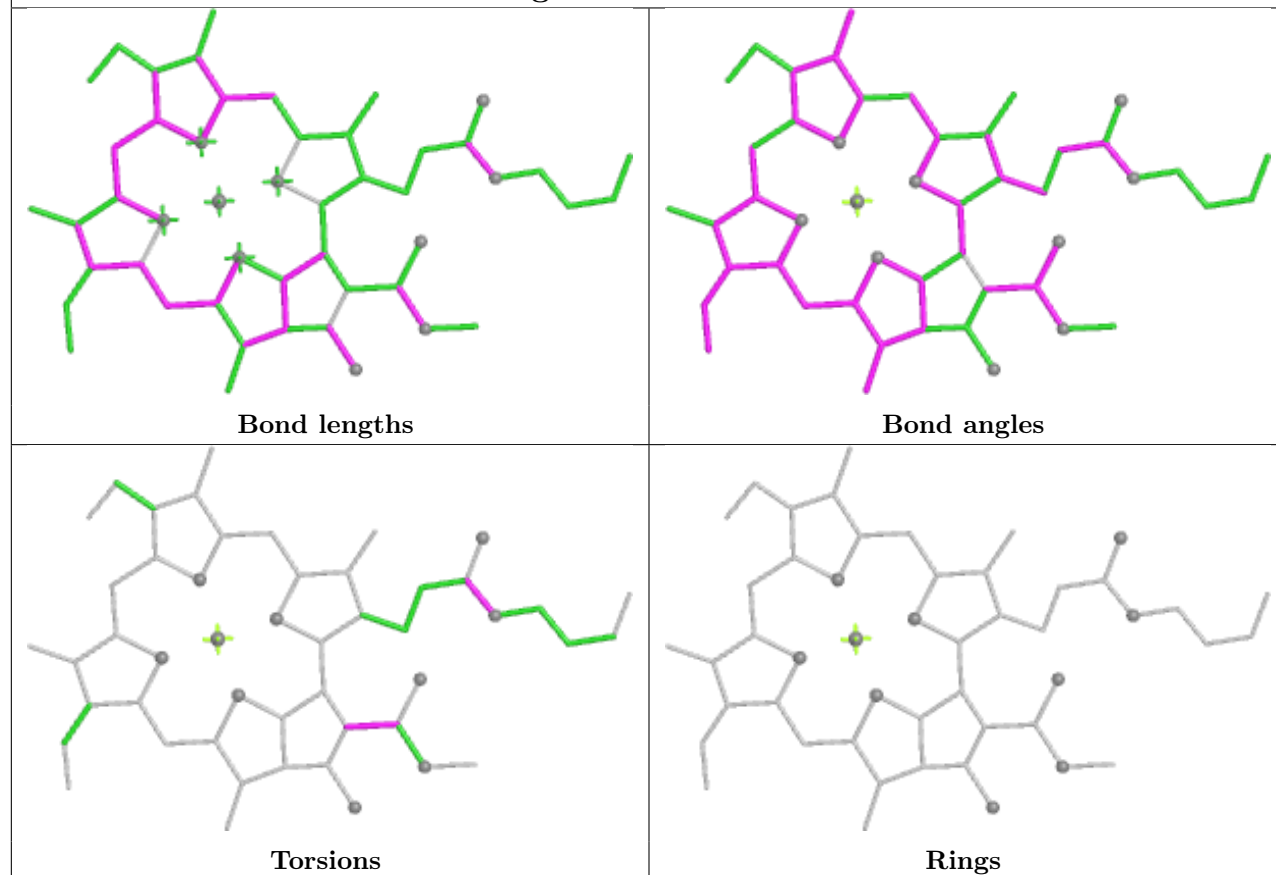




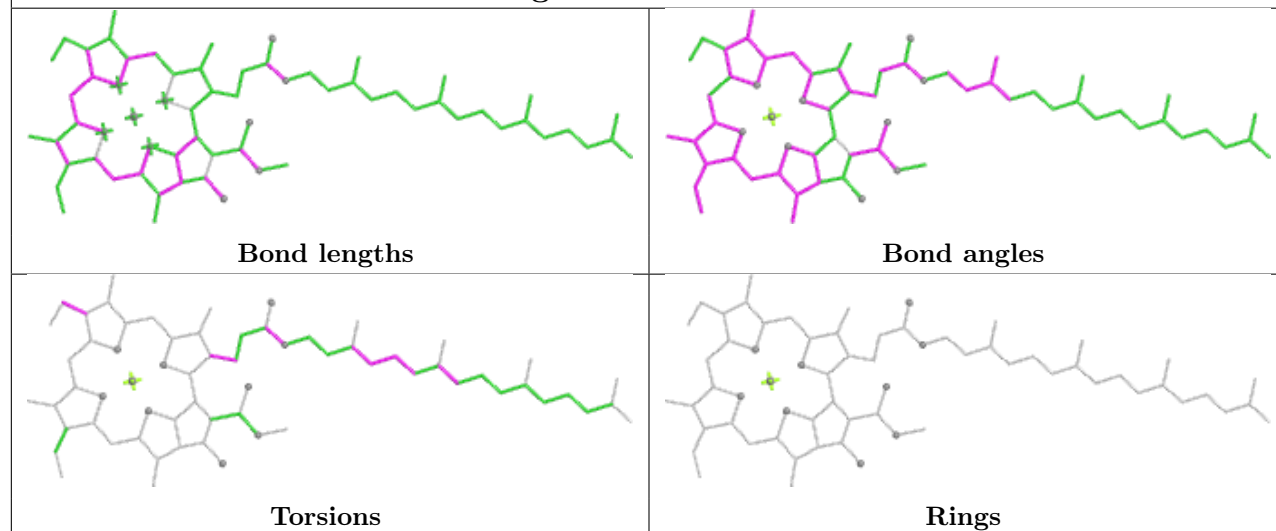


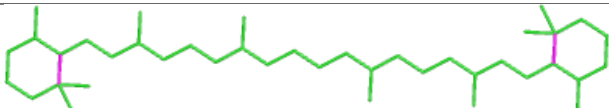
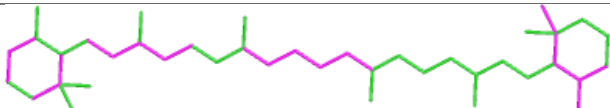
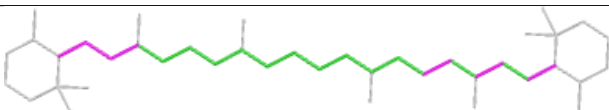
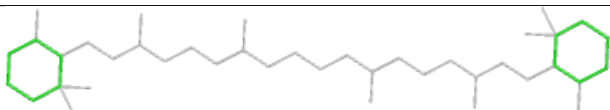


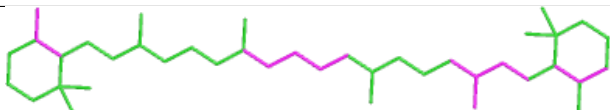
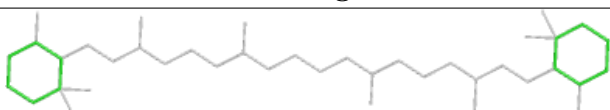
Ligand CLA A 817

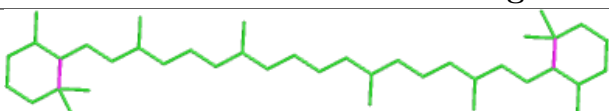
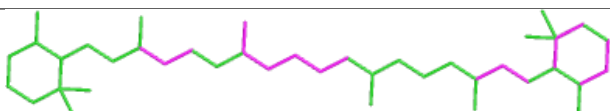
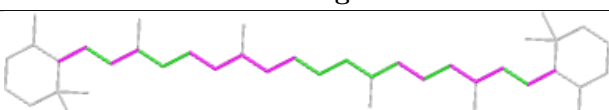
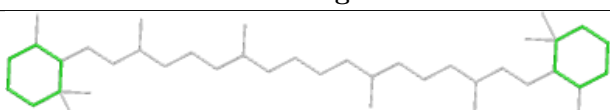


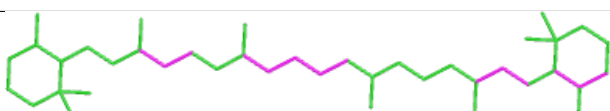
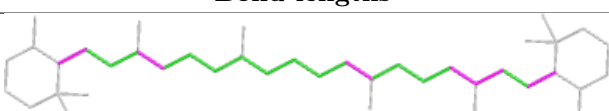
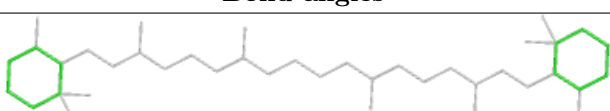
Ligand CLA A 833

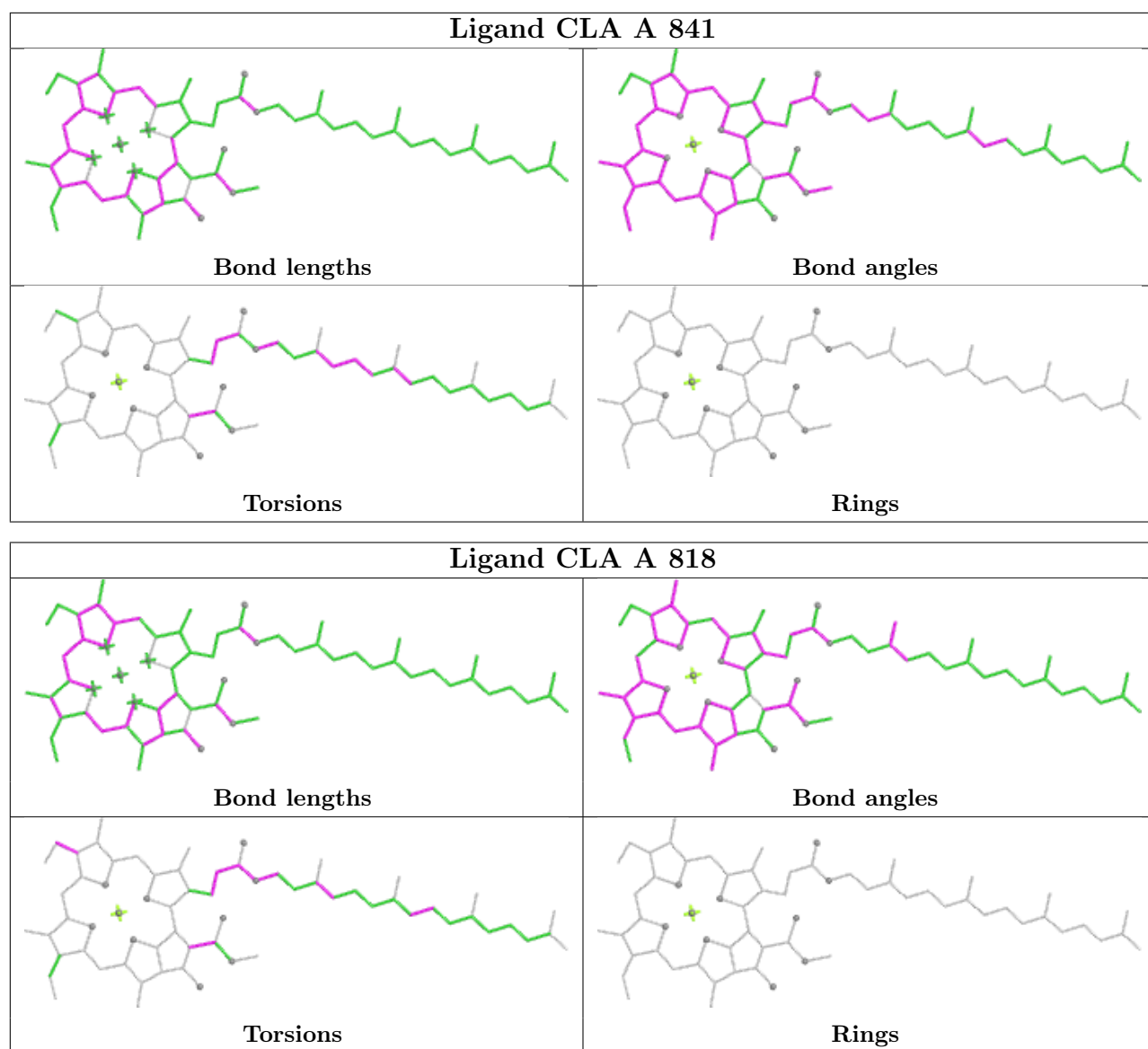


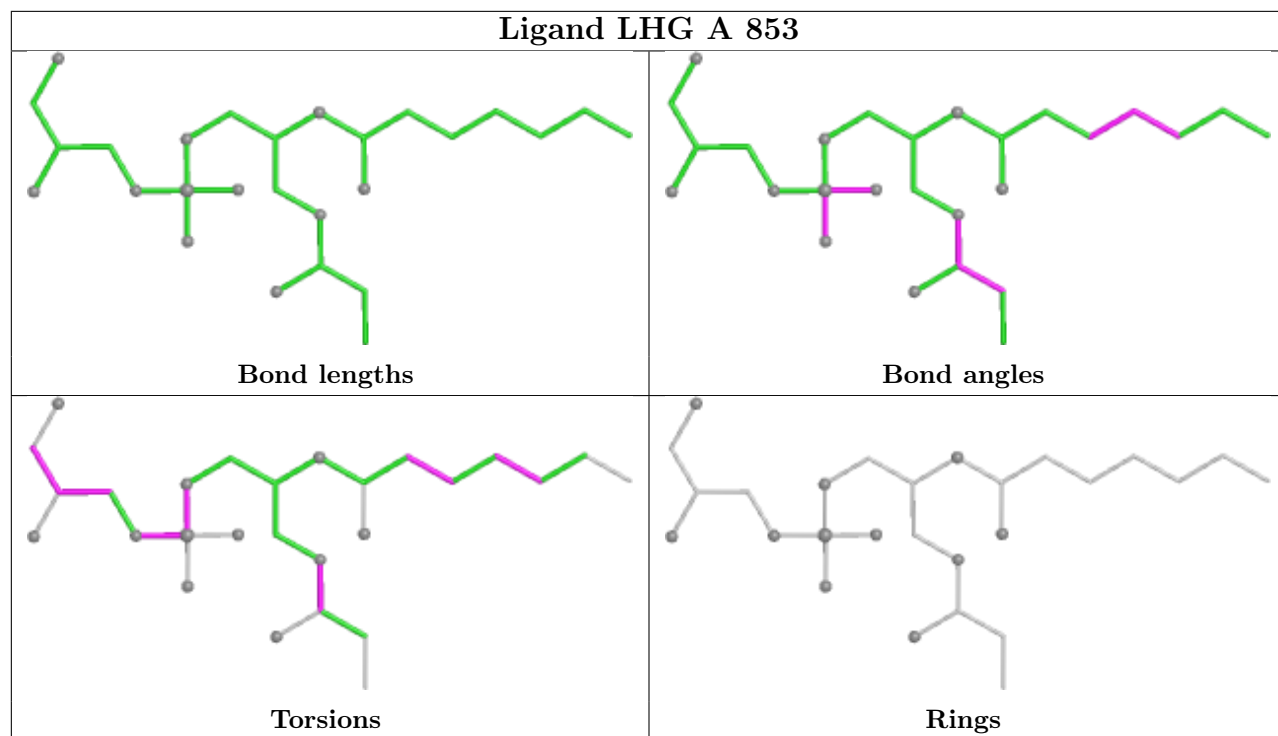
Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

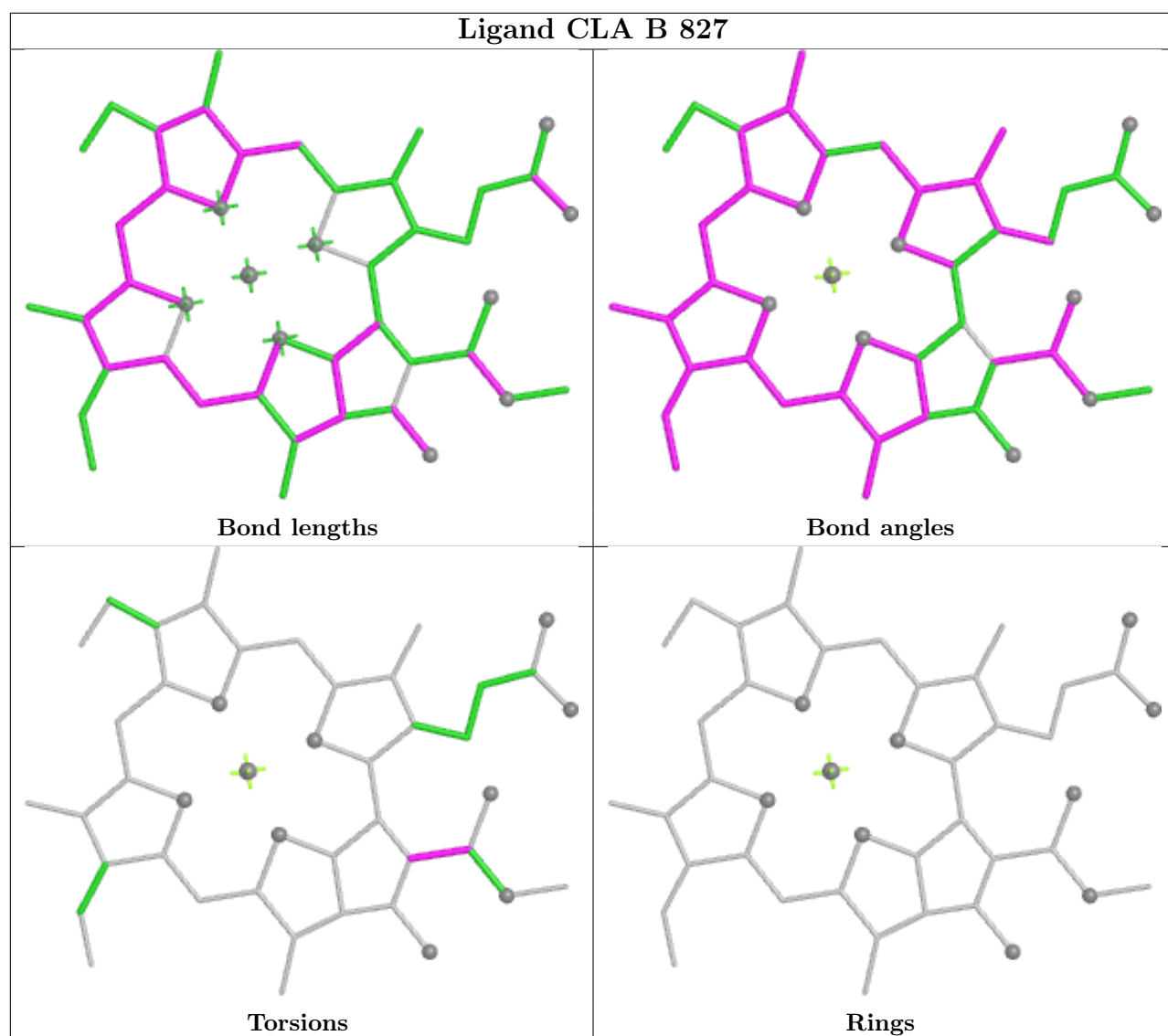
Ligand BCR M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

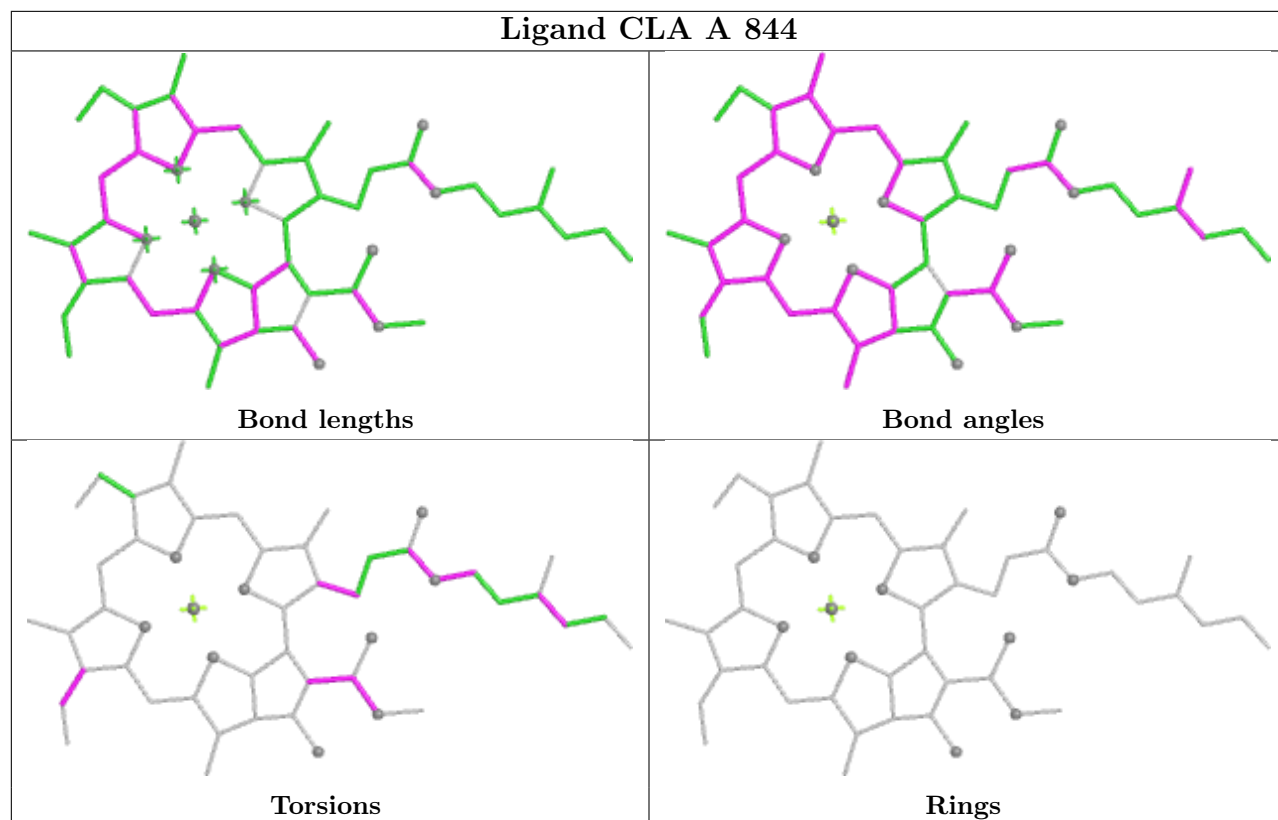
Ligand BCR A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

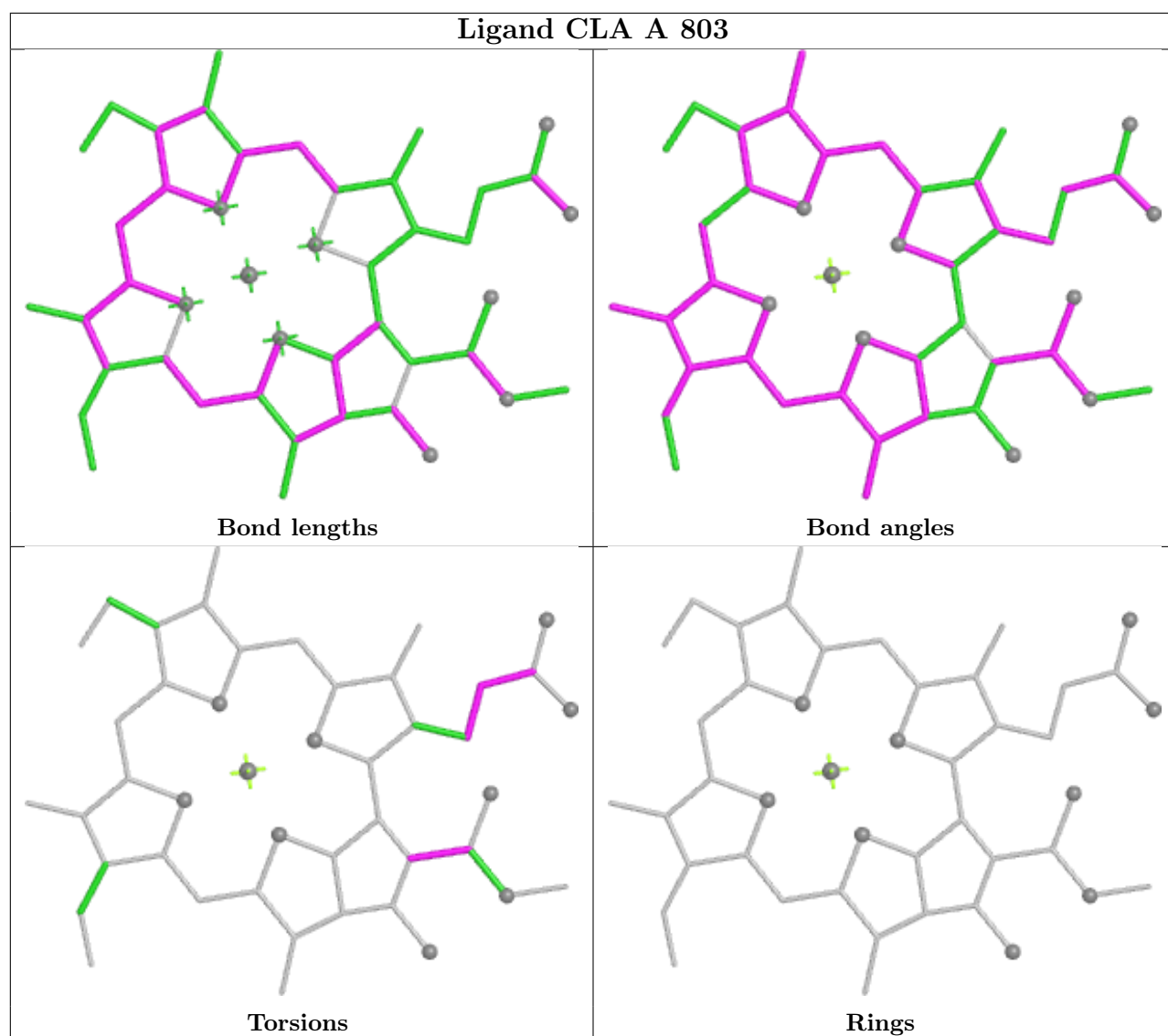
Ligand BCR B 835	
	
Bond lengths	Bond angles
	
Torsions	Rings

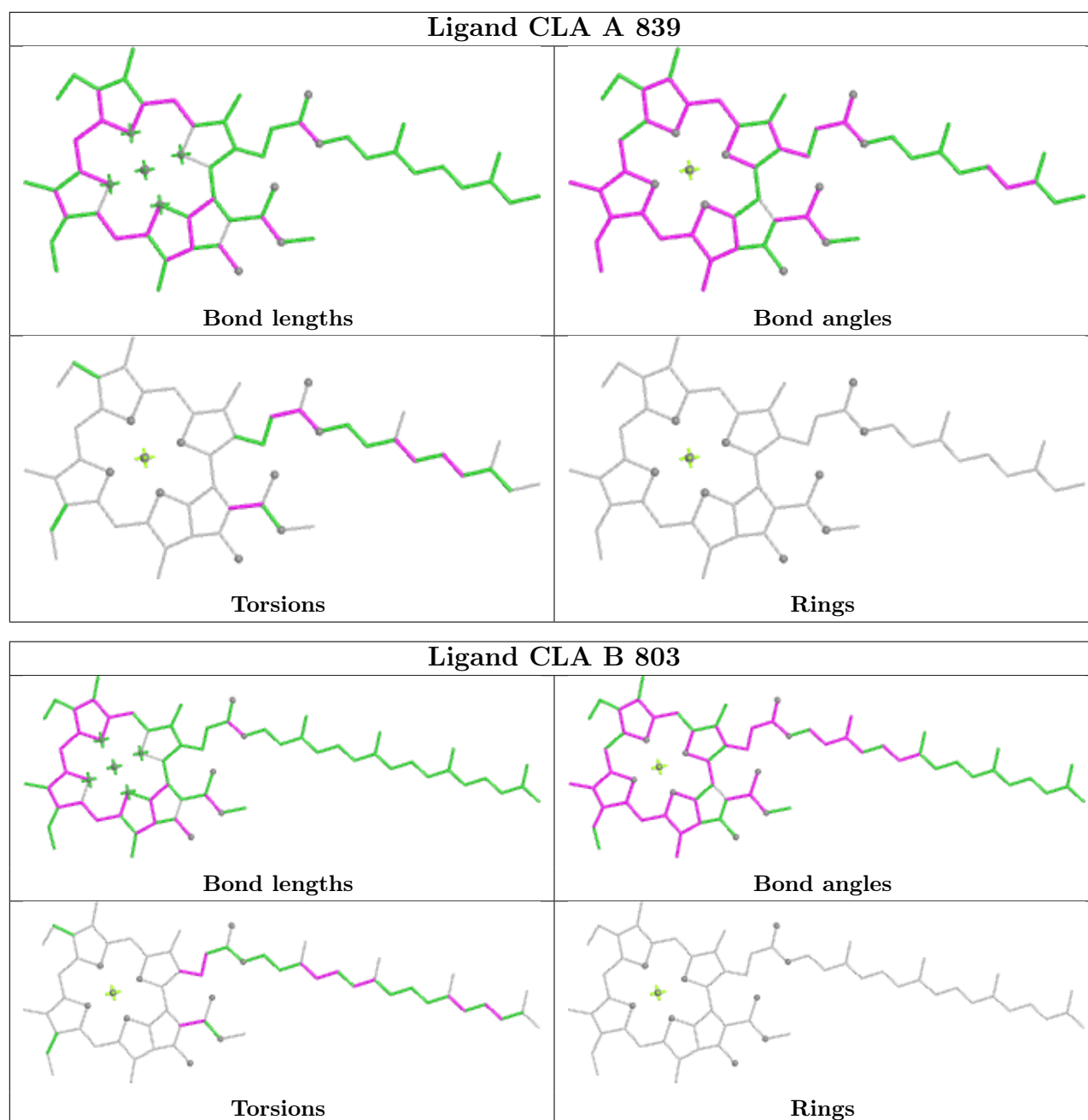


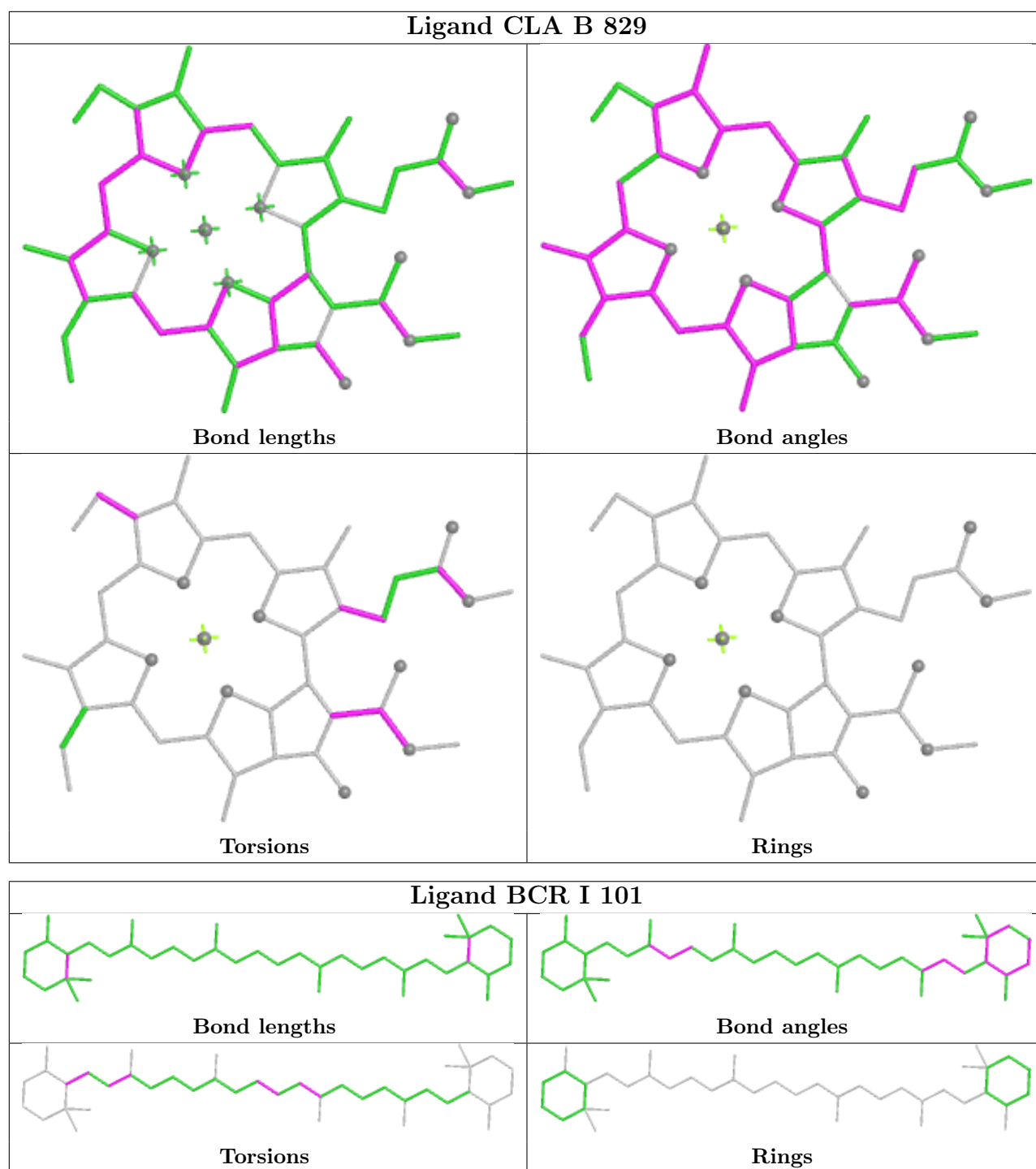


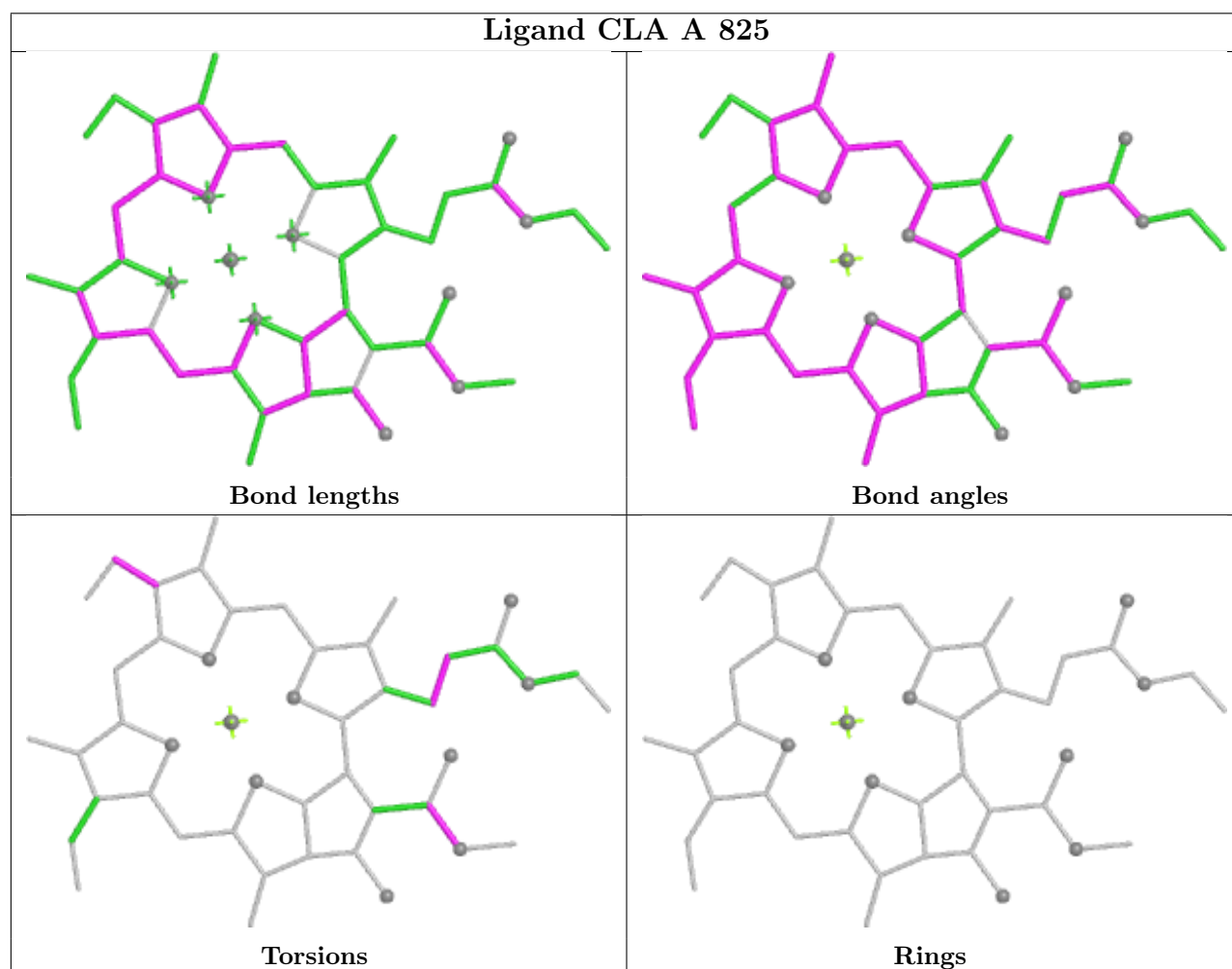
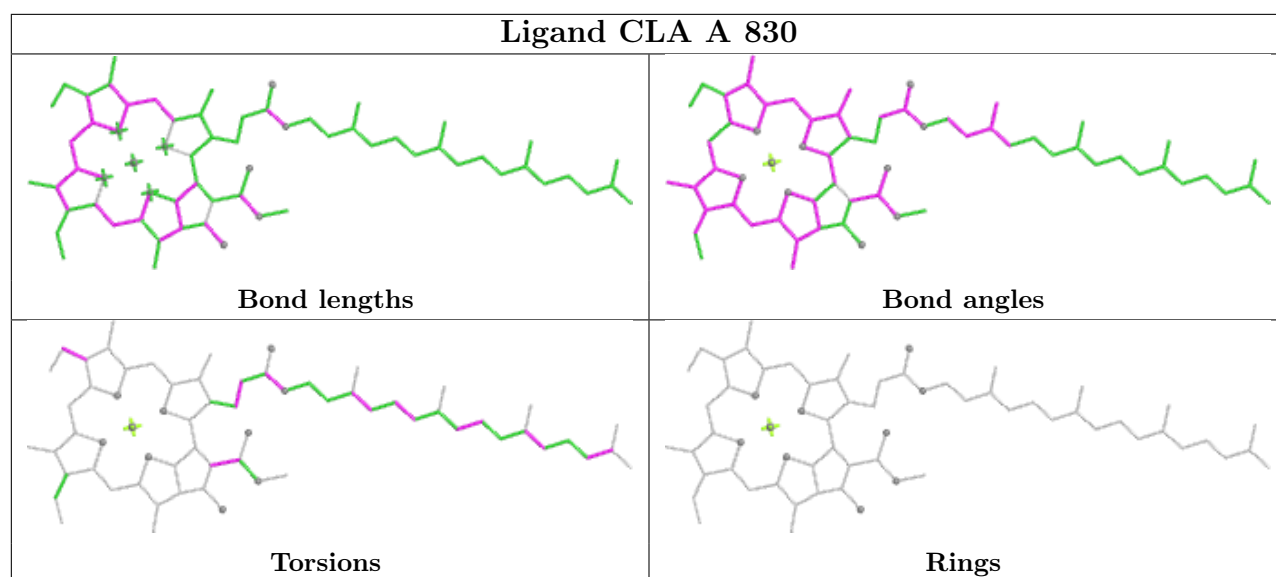


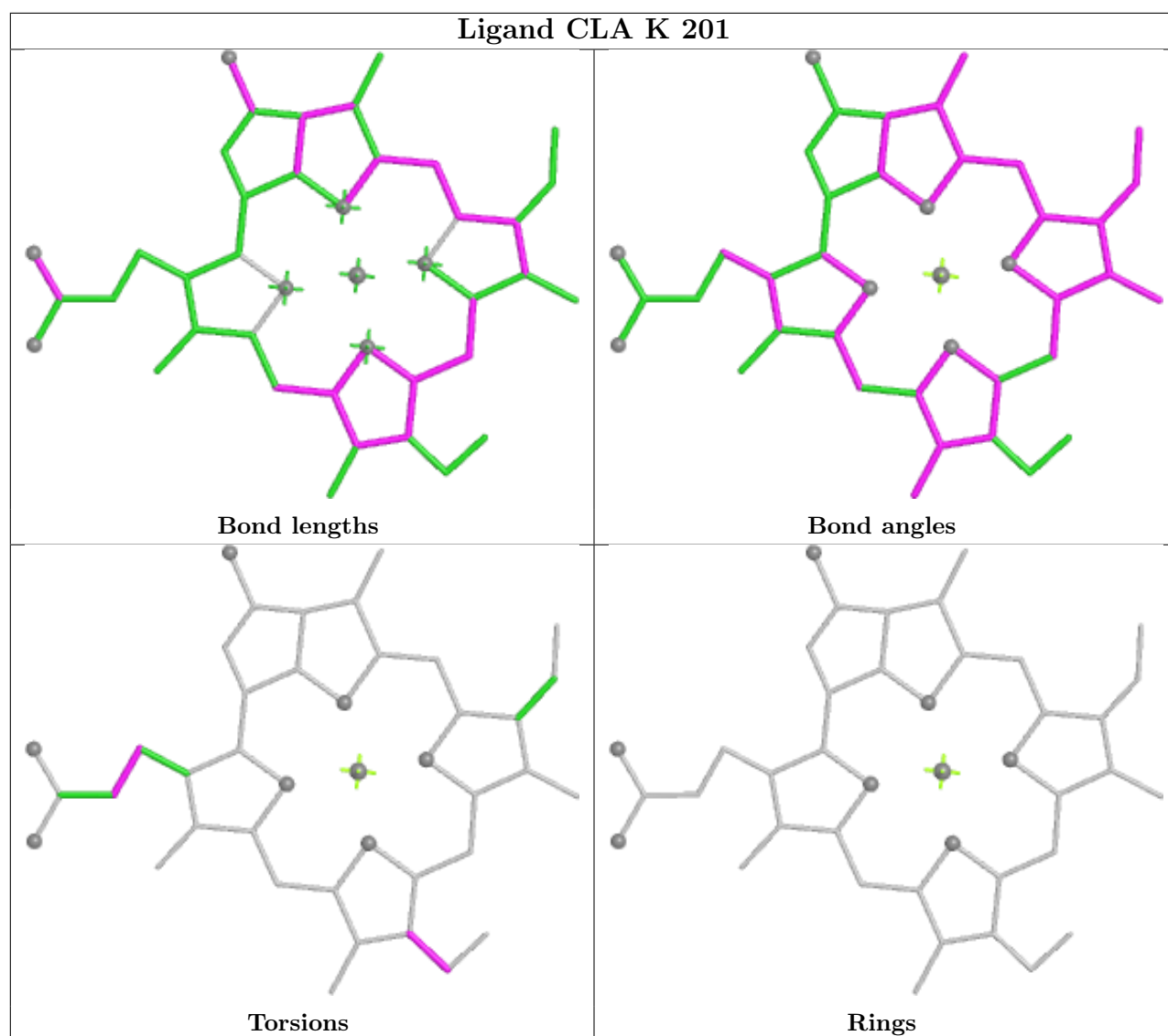












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

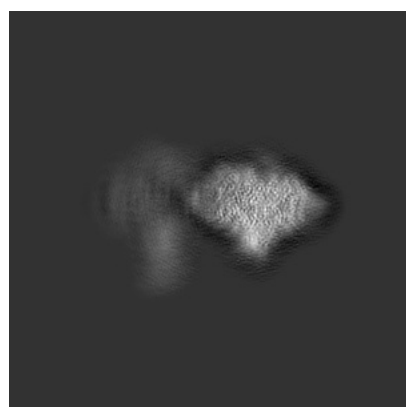
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30820. These allow visual inspection of the internal detail of the map and identification of artifacts.

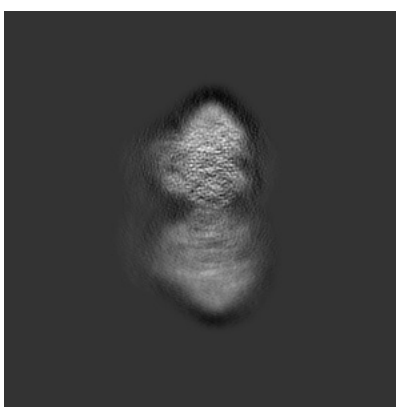
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

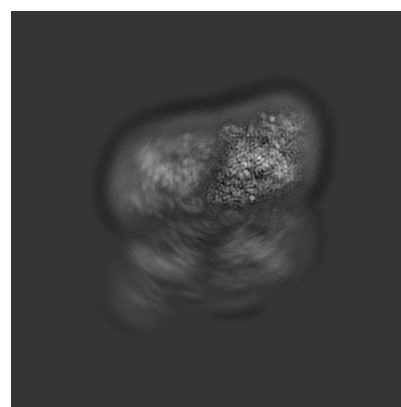
6.1.1 Primary map



X



Y

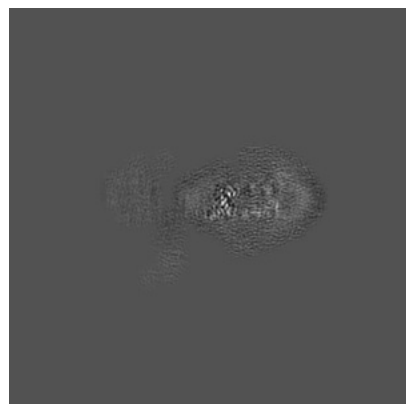


Z

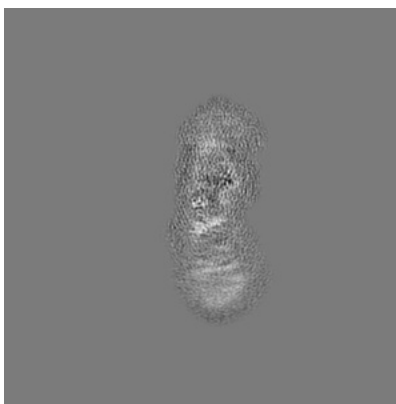
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

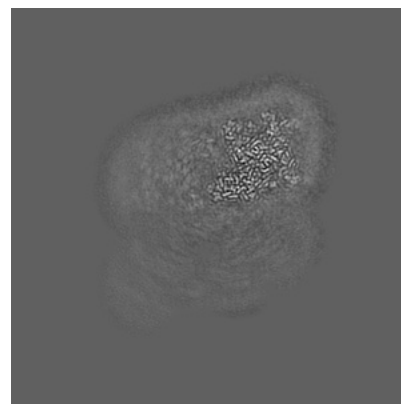
6.2.1 Primary map



X Index: 200



Y Index: 200

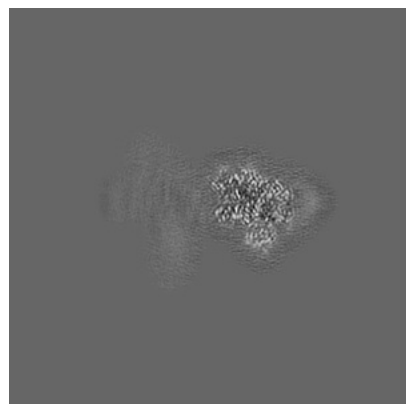


Z Index: 200

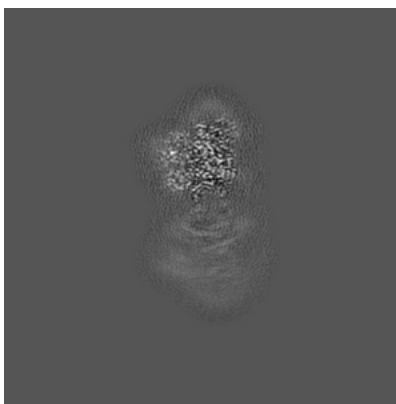
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

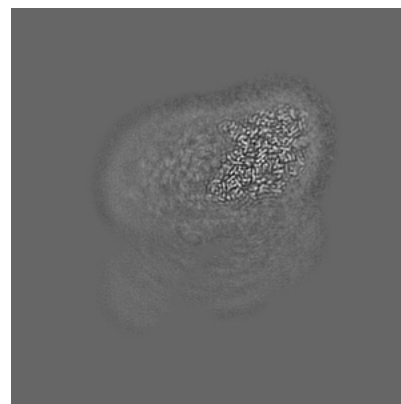
6.3.1 Primary map



X Index: 233



Y Index: 247

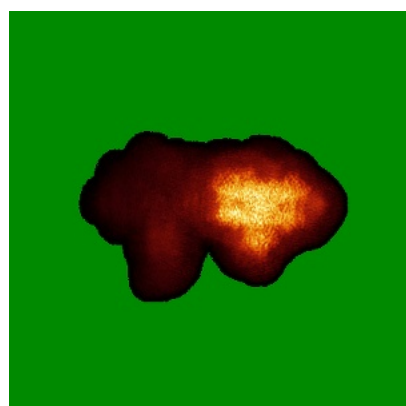


Z Index: 216

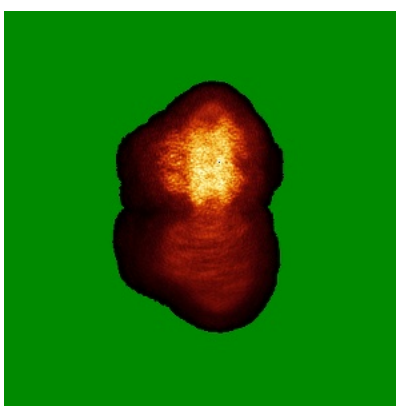
The images above show the largest variance slices of the map in three orthogonal directions.

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

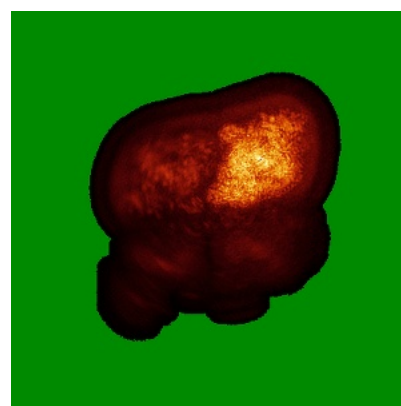
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

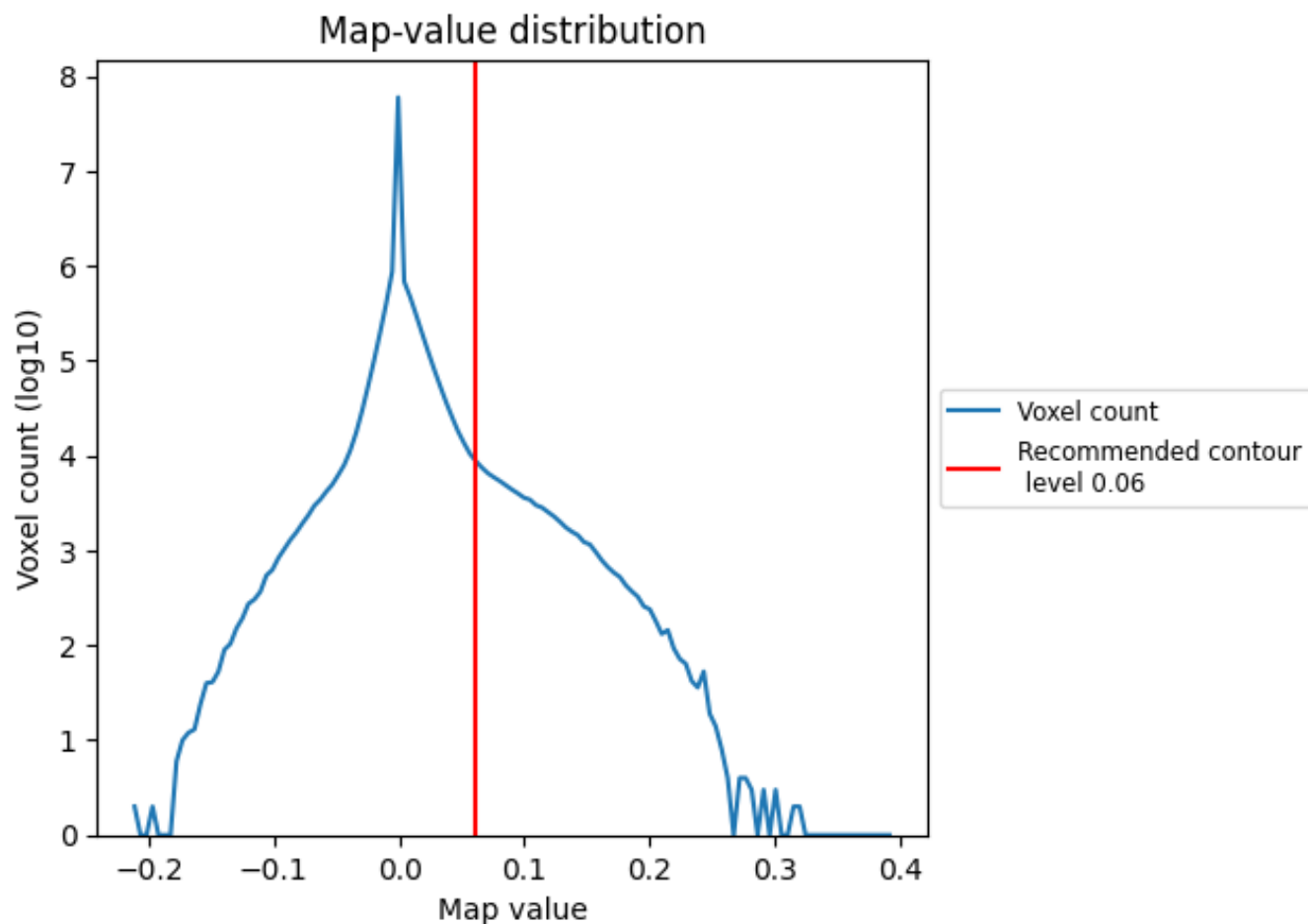
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

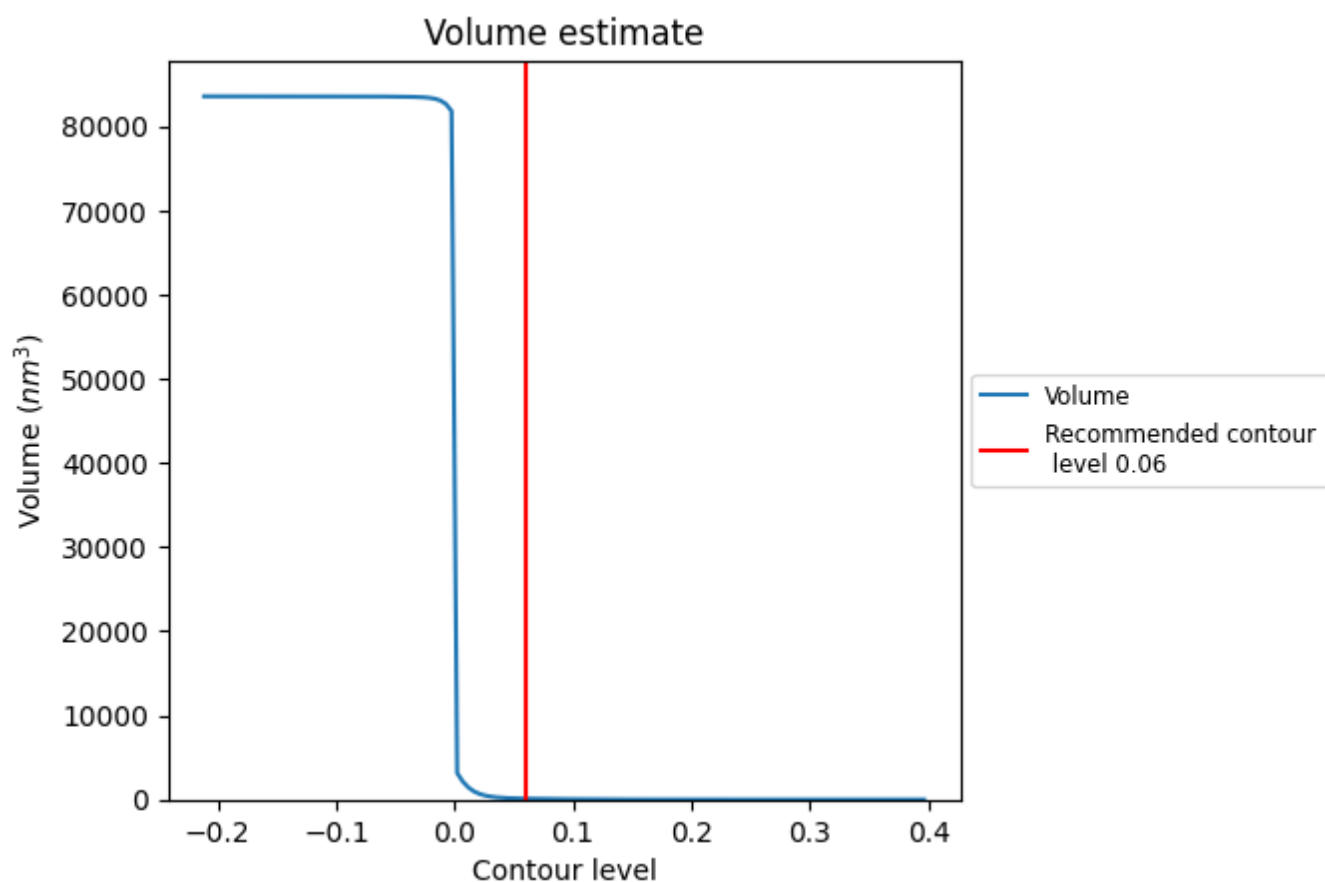
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

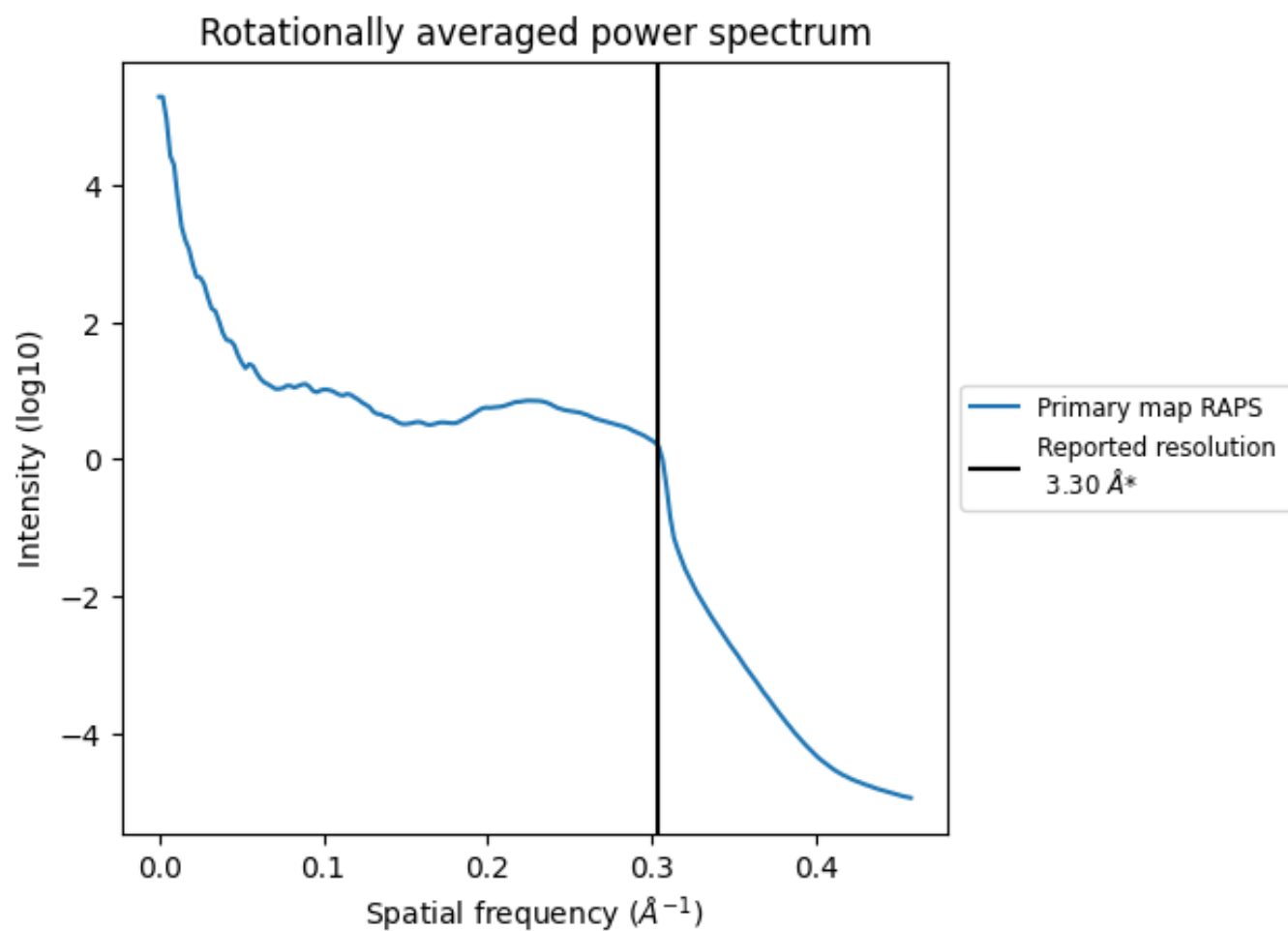
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm³; this corresponds to an approximate mass of 98 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 ⓘ

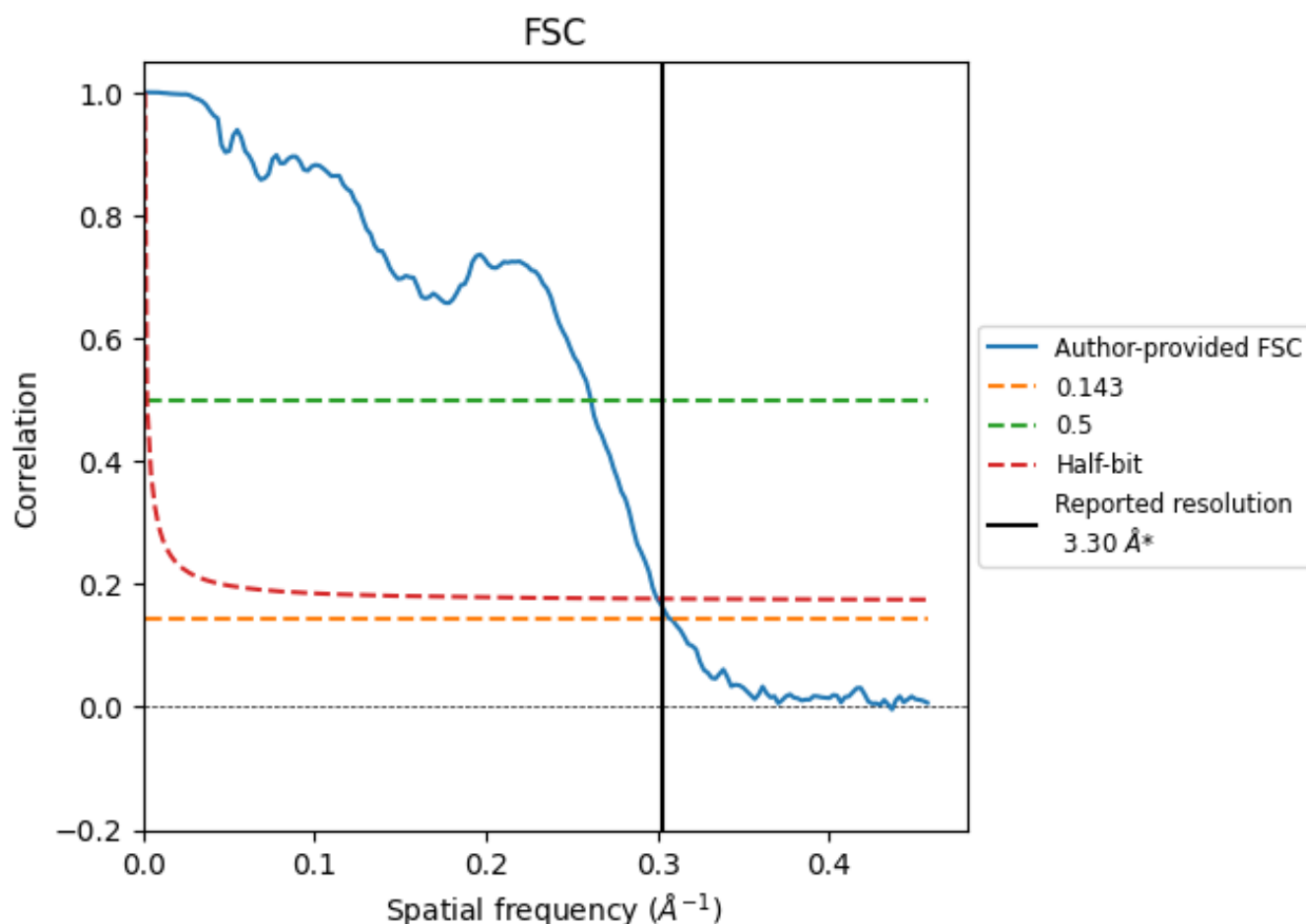


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

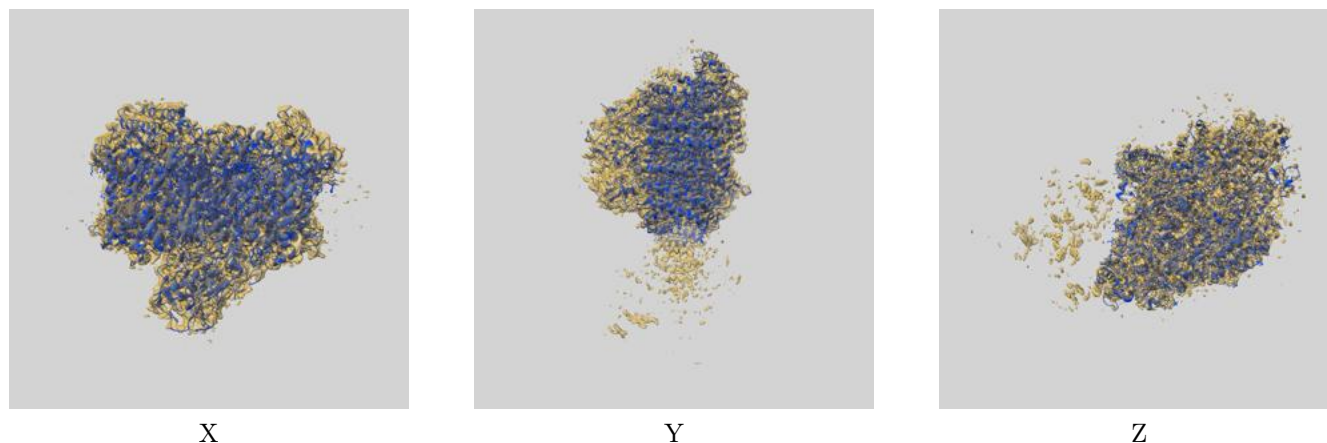
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.83	3.34
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

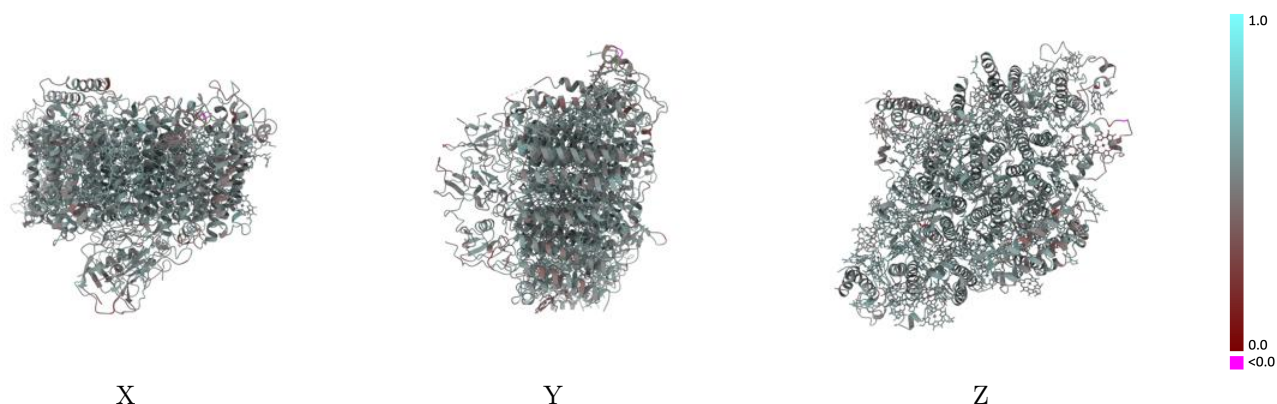
This section contains information regarding the fit between EMDB map EMD-30820 and PDB model 7DR0. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



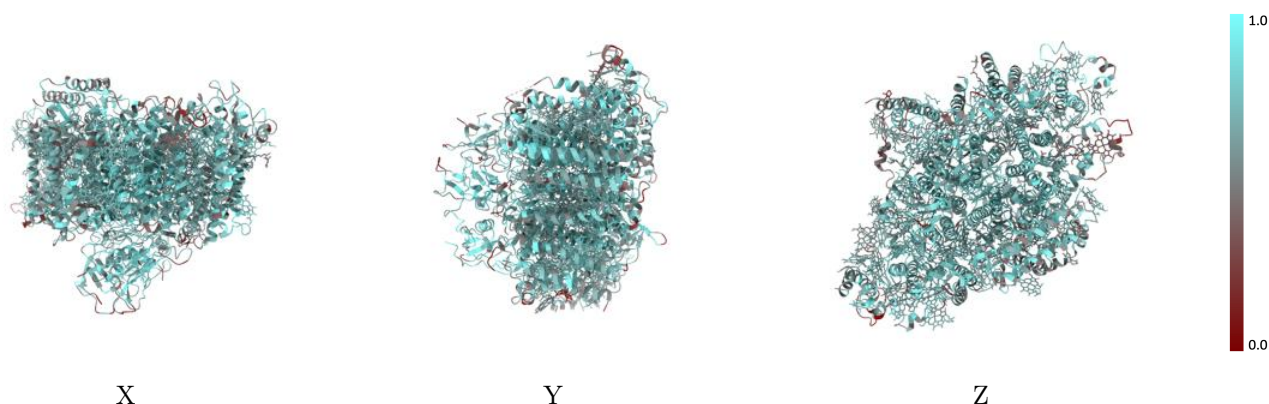
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



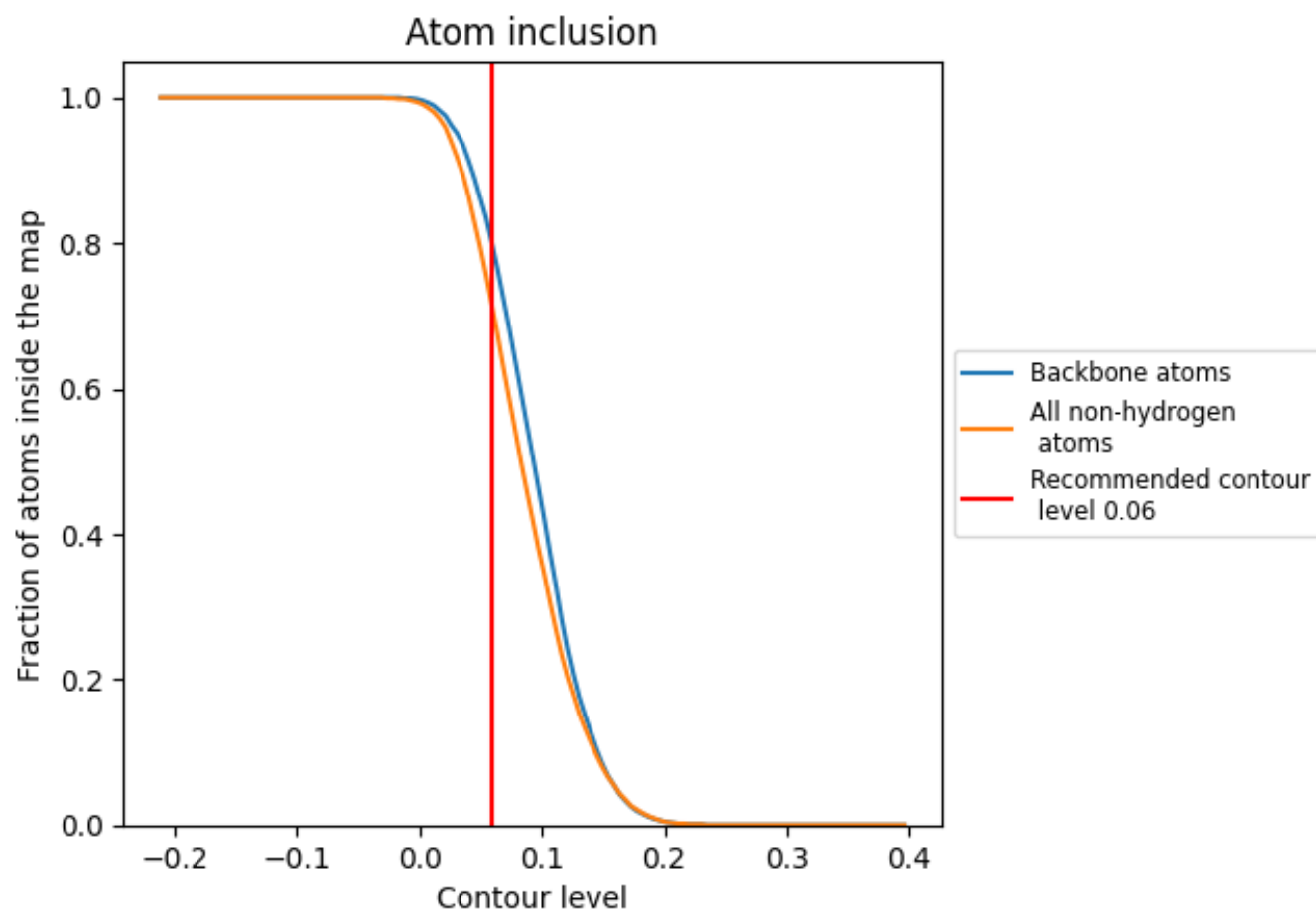
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 71% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.5300
A	0.7420	0.5480
B	0.7170	0.5290
C	0.7920	0.5060
D	0.7190	0.5020
E	0.6930	0.4980
F	0.6460	0.5030
I	0.6290	0.5120
J	0.5750	0.5230
K	0.5520	0.5180
L	0.6200	0.5010
M	0.5910	0.5210

