



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 07:01 AM JST

PDB ID : 7DR1 / pdb_00007dr1
EMDB ID : EMD-30821
Title : Structure of Wild-type PSI monomer2 from *Cyanophora paradoxa*
Authors : Kato, K.; Nagao, R.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on : 2020-12-25
Resolution : 3.20 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

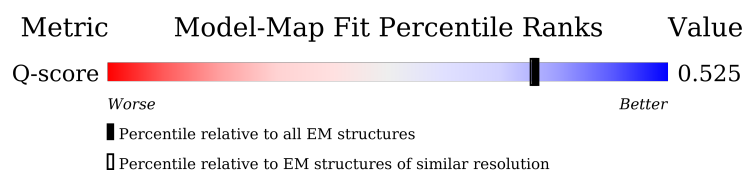
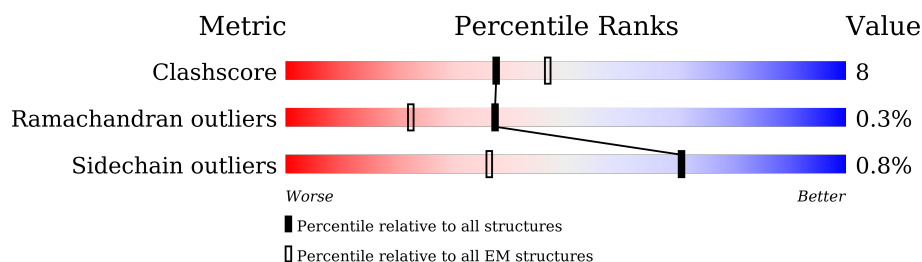
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



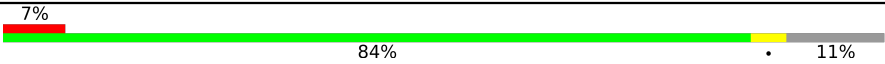
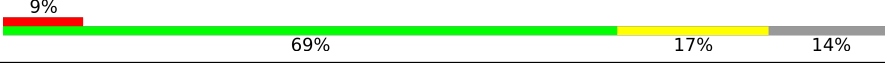
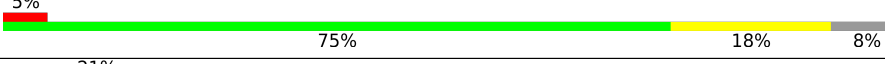
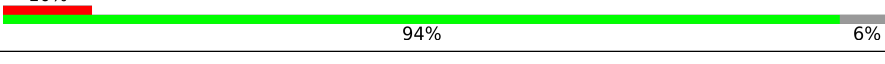
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	L	146	
10	M	31	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 22177 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	0	0
			292	199	43	50		

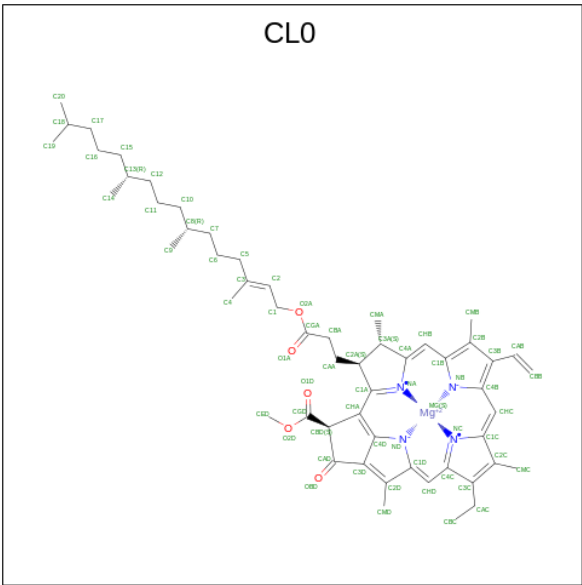
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

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

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

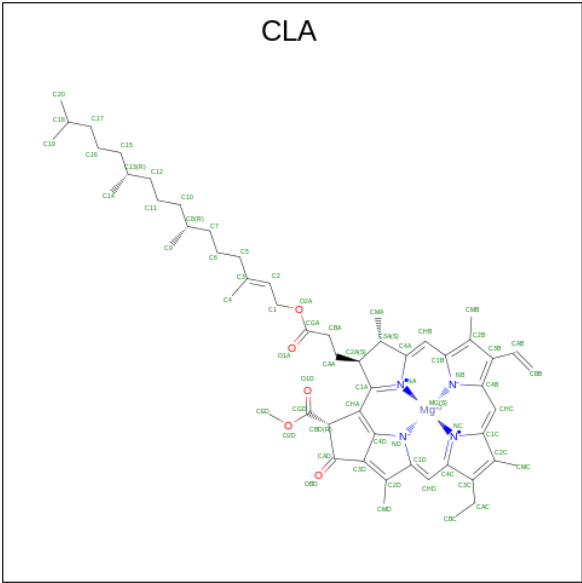
Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	29	Total	C	N	O	0	0
			215	145	34	36		

- Molecule 11 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

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



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 61	C 51	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
12	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
12	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
12	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
12	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	A	1	Total 52	C 42	Mg 1	N 4	O 5	0
12	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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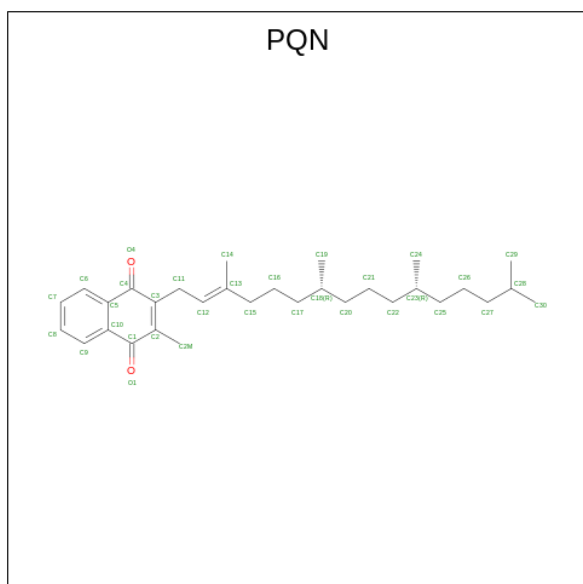
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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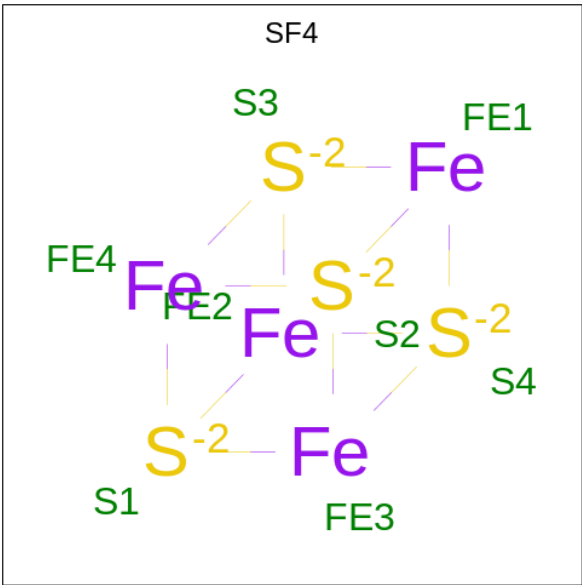
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



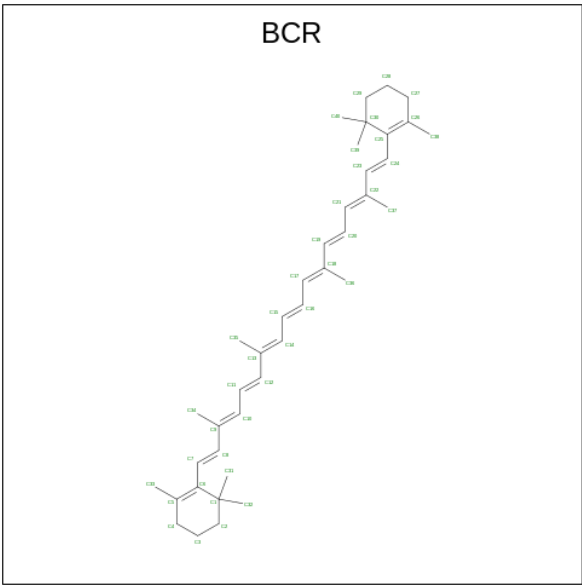
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			33	31	2	
13	B	1	Total	C	O	0
			33	31	2	

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



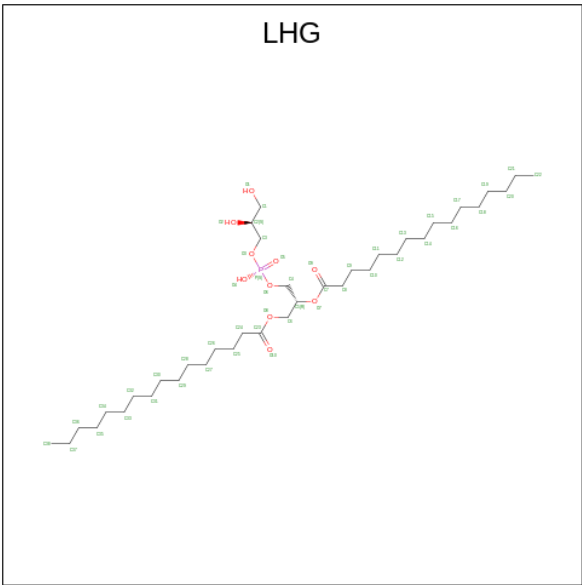
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	

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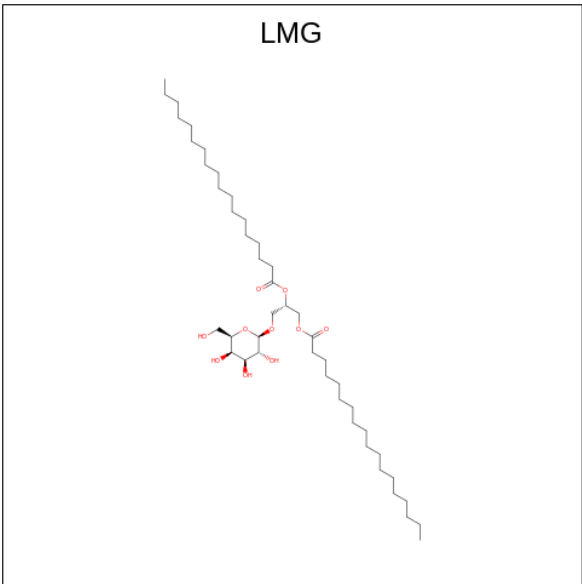
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C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

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

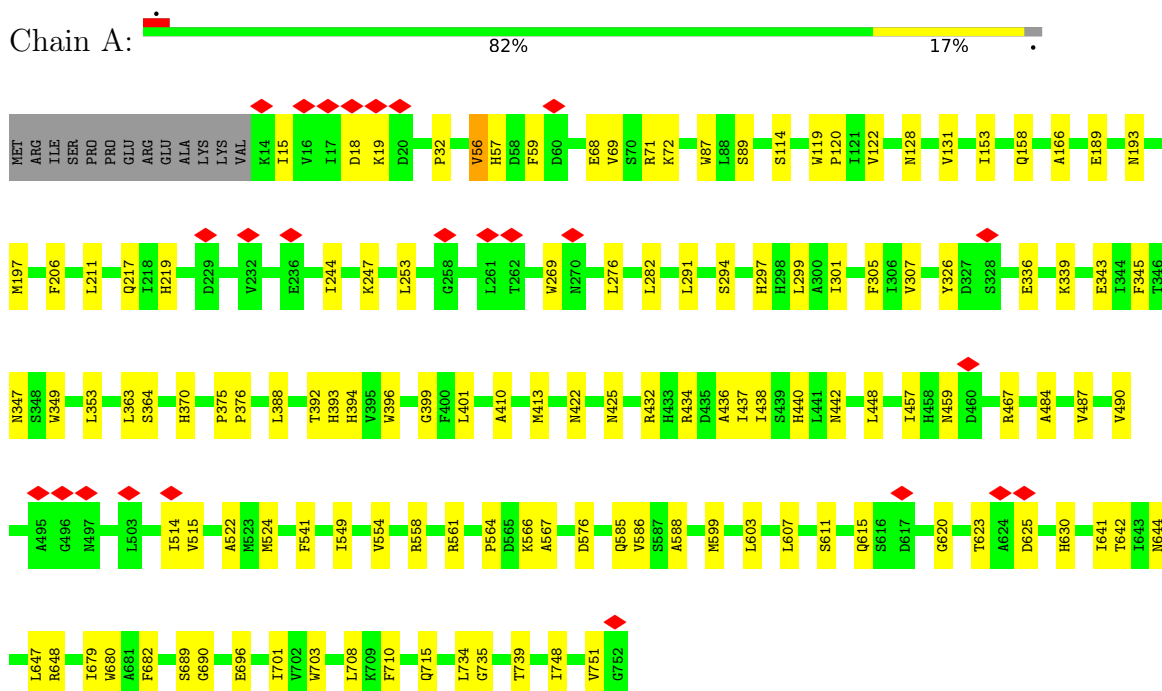


Mol	Chain	Residues	Atoms			AltConf
17	B	1	Total	C	O	0
			55	45	10	

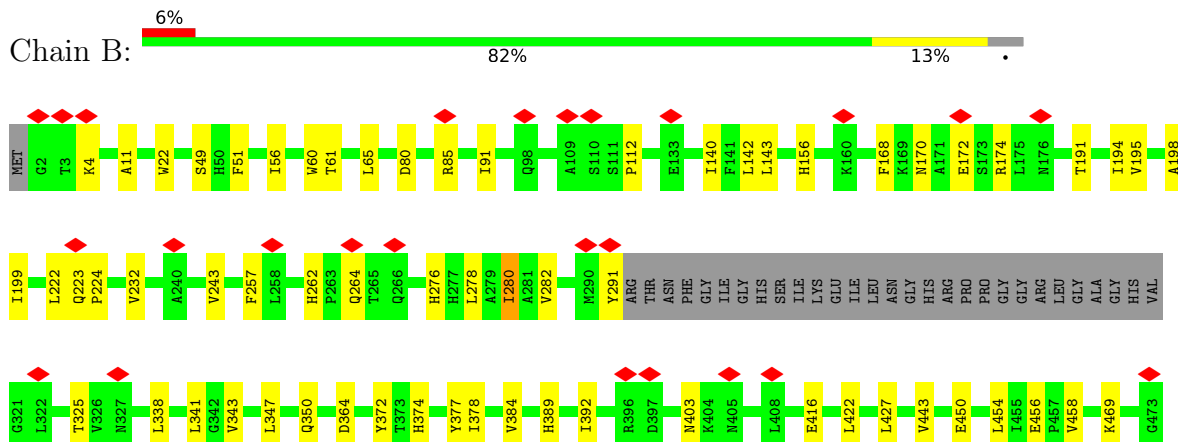
3 Residue-property plots

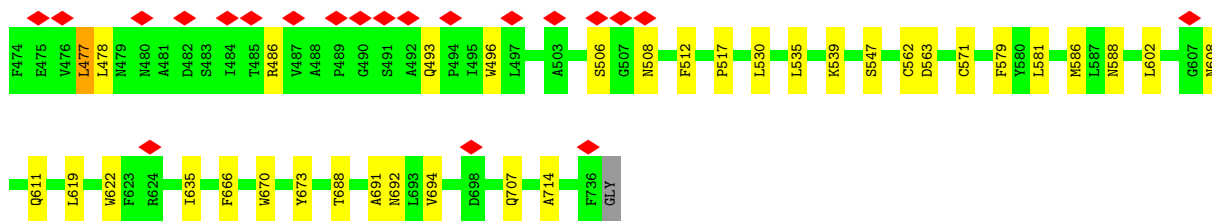
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

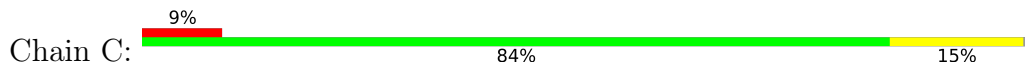


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

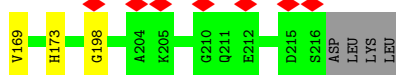




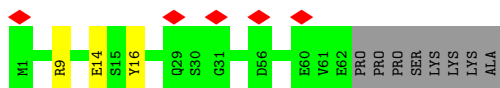
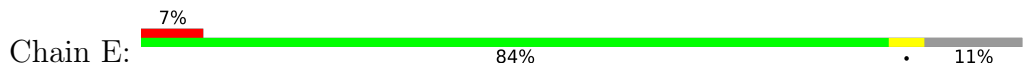
• Molecule 3: Photosystem I iron-sulfur center



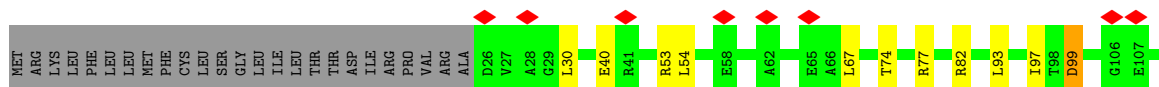
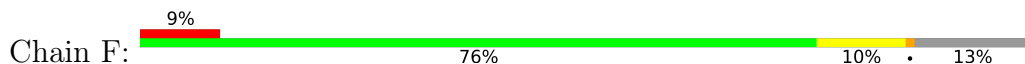
• Molecule 4: Photosystem I reaction center subunit II, cyanelle



• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III

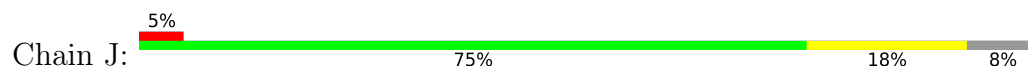


• Molecule 7: Photosystem I reaction center subunit VIII

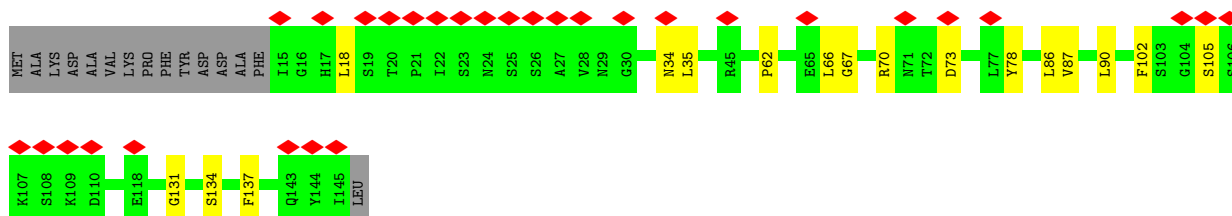
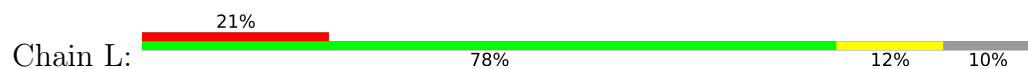




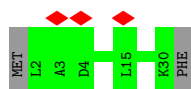
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110380	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	0.376	Depositor
Minimum map value	-0.292	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: PQN, LHG, BCR, CLA, CL0, LMG, SF4

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	0.22	0/6000	0.46	0/8177
2	B	0.31	0/5820	0.85	2/7955 (0.0%)
3	C	0.31	0/611	1.01	4/828 (0.5%)
4	D	0.24	0/1105	0.82	6/1489 (0.4%)
5	E	0.19	0/516	0.45	0/696
6	F	0.19	0/1281	0.55	2/1733 (0.1%)
7	I	0.27	0/232	0.59	0/319
8	J	0.19	0/300	0.54	0/410
9	L	0.22	0/988	0.60	2/1342 (0.1%)
10	M	0.18	0/217	0.41	0/295
All	All	0.26	0/17070	0.68	16/23244 (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
2	B	0	1
4	D	0	3
6	F	0	1
All	All	0	5

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	147	ASP	CA-C-N	7.04	124.67	120.24
6	F	147	ASP	C-N-CA	7.04	124.67	120.24
4	D	125	ALA	CA-C-N	6.95	134.47	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	125	ALA	C-N-CA	6.95	134.47	121.97
9	L	73	ASP	CA-C-N	6.26	132.97	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	493	GLN	Peptide
4	D	124	ALA	Peptide
4	D	125	ALA	Peptide
4	D	164	TYR	Peptide
6	F	99	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5803	0	5621	93	0
2	B	5622	0	5406	64	0
3	C	601	0	576	7	0
4	D	1082	0	1099	16	0
5	E	508	0	507	3	0
6	F	1255	0	1249	14	0
7	I	228	0	247	5	0
8	J	292	0	302	4	0
9	L	965	0	970	14	0
10	M	215	0	239	0	0
11	A	65	0	72	3	0
12	A	2407	0	2290	86	0
12	B	1900	0	1927	78	0
12	F	45	0	33	0	0
12	J	45	0	33	0	0
12	L	163	0	148	11	0
13	A	33	0	46	3	0
13	B	33	0	46	5	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	240	0	336	17	0
15	B	120	0	168	8	0
15	F	80	0	112	6	0
15	I	40	0	56	5	0
15	J	120	0	168	6	0
15	L	120	0	168	11	0
15	M	40	0	56	2	0
16	A	76	0	98	2	0
17	B	55	0	86	7	0
All	All	22177	0	22059	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 8.

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)
12:B:807:CLA:H162	12:B:822:CLA:HBB2	1.66	0.78
12:A:819:CLA:HAB	12:A:819:CLA:H8	1.72	0.71
12:B:802:CLA:H203	12:L:203:CLA:HBB1	1.73	0.71
1:A:307:VAL:HG12	15:A:846:BCR:H17C	1.75	0.68
12:B:829:CLA:H71	12:B:829:CLA:HBB1	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%)	701 (95%)	35 (5%)	1 (0%)	48 79
2	B	702/737 (95%)	669 (95%)	31 (4%)	2 (0%)	36 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	40
4	D	137/220 (62%)	114 (83%)	21 (15%)	2 (2%)	8	37
5	E	60/70 (86%)	53 (88%)	7 (12%)	0	100	100
6	F	159/186 (86%)	151 (95%)	8 (5%)	0	100	100
7	I	28/35 (80%)	27 (96%)	1 (4%)	0	100	100
8	J	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
9	L	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
10	M	27/31 (87%)	27 (100%)	0	0	100	100
All	All	2092/2298 (91%)	1966 (94%)	120 (6%)	6 (0%)	37	68

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	63	LEU
1	A	122	VAL
2	B	477	LEU
2	B	562	CYS
4	D	126	ILE

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%)	596 (100%)	2 (0%)	86	88
2	B	574/596 (96%)	564 (98%)	10 (2%)	53	75
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	114/171 (67%)	114 (100%)	0	100	100
5	E	58/65 (89%)	58 (100%)	0	100	100
6	F	133/156 (85%)	133 (100%)	0	100	100
7	I	27/31 (87%)	26 (96%)	1 (4%)	30	63
8	J	32/35 (91%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	L	99/111 (89%)	99 (100%)	0	100	100
10	M	21/23 (91%)	21 (100%)	0	100	100
All	All	1723/1866 (92%)	1710 (99%)	13 (1%)	70	82

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	539	LYS
2	B	571	CYS
7	I	31	THR
2	B	602	LEU
2	B	694	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	49	ASN
9	L	34	ASN
5	E	52	ASN
6	F	52	ASN
2	B	29	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](#)

108 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
12	CLA	A	807	1	55,59,73	2.31	21 (38%)	66,96,113	3.12	31 (46%)
12	CLA	A	821	-	69,73,73	2.03	20 (28%)	83,113,113	2.77	28 (33%)
12	CLA	A	830	1	69,73,73	2.01	17 (24%)	83,113,113	2.75	29 (34%)
15	BCR	L	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.35	10 (17%)
12	CLA	B	806	2	69,73,73	2.00	19 (27%)	83,113,113	2.87	32 (38%)
12	CLA	A	816	-	53,57,73	2.35	20 (37%)	62,93,113	3.12	26 (41%)
12	CLA	A	805	1	69,73,73	2.01	19 (27%)	83,113,113	2.84	34 (40%)
12	CLA	A	802	-	49,53,73	2.39	19 (38%)	59,89,113	3.28	28 (47%)
12	CLA	B	803	2	69,73,73	1.98	19 (27%)	83,113,113	2.87	34 (40%)
15	BCR	A	846	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	9 (16%)
17	LMG	B	837	-	55,55,55	0.78	1 (1%)	63,63,63	1.37	7 (11%)
12	CLA	A	804	1	49,53,73	2.41	19 (38%)	59,89,113	3.33	29 (49%)
12	CLA	B	825	2	69,73,73	2.01	19 (27%)	83,113,113	3.01	32 (38%)
15	BCR	A	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
12	CLA	A	820	1	65,69,73	2.12	19 (29%)	78,108,113	2.82	30 (38%)
12	CLA	A	835	1	58,62,73	2.20	19 (32%)	69,99,113	3.07	29 (42%)
15	BCR	A	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	7 (12%)
12	CLA	A	832	1	69,73,73	2.05	21 (30%)	83,113,113	2.85	31 (37%)
13	PQN	A	844	-	34,34,34	1.54	2 (5%)	42,45,45	1.04	2 (4%)
12	CLA	B	829	2	69,73,73	1.99	19 (27%)	83,113,113	2.84	30 (36%)
12	CLA	A	854	-	69,73,73	1.97	20 (28%)	83,113,113	2.89	32 (38%)
11	CL0	A	801	1	69,73,73	1.99	19 (27%)	83,113,113	2.85	36 (43%)
12	CLA	B	810	2	69,73,73	2.01	18 (26%)	83,113,113	2.58	30 (36%)
12	CLA	B	820	2	69,73,73	2.04	19 (27%)	83,113,113	2.89	30 (36%)
15	BCR	J	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.39	8 (14%)
15	BCR	L	205	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
12	CLA	B	824	2	53,57,73	2.36	20 (37%)	62,93,113	3.38	27 (43%)
12	CLA	A	828	1	69,73,73	2.03	21 (30%)	83,113,113	2.82	29 (34%)
15	BCR	B	834	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	LHG	A	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	7 (13%)
12	CLA	A	814	1	49,53,73	2.43	19 (38%)	59,89,113	3.27	28 (47%)
12	CLA	B	819	-	50,54,73	2.44	21 (42%)	60,90,113	3.38	29 (48%)
14	SF4	C	101	3	0,12,12	-	-	-	-	-
15	BCR	M	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	5 (8%)
12	CLA	B	808	2	69,73,73	2.01	18 (26%)	83,113,113	2.81	29 (34%)
12	CLA	J	101	8	49,53,73	2.42	20 (40%)	59,89,113	3.26	28 (47%)
12	CLA	A	817	1	69,73,73	2.04	20 (28%)	83,113,113	2.86	28 (33%)
12	CLA	A	825	-	69,73,73	1.97	21 (30%)	83,113,113	2.72	31 (37%)
13	PQN	B	833	-	34,34,34	1.50	2 (5%)	42,45,45	1.21	4 (9%)
12	CLA	A	806	1	69,73,73	1.99	20 (28%)	83,113,113	2.91	31 (37%)
12	CLA	A	809	1	49,53,73	2.39	20 (40%)	59,89,113	3.16	28 (47%)
12	CLA	A	842	1	69,73,73	2.03	21 (30%)	83,113,113	2.76	27 (32%)
12	CLA	A	841	-	55,59,73	2.31	20 (36%)	66,96,113	3.17	29 (43%)
12	CLA	A	831	1	54,58,73	2.29	20 (37%)	65,95,113	3.09	29 (44%)
12	CLA	B	807	2	69,73,73	2.02	19 (27%)	83,113,113	2.87	30 (36%)
12	CLA	A	833	1	69,73,73	2.02	20 (28%)	83,113,113	2.84	33 (39%)
12	CLA	A	840	1	69,73,73	2.06	22 (31%)	83,113,113	2.75	32 (38%)
12	CLA	L	204	-	56,60,73	2.26	20 (35%)	67,97,113	3.18	28 (41%)
12	CLA	A	812	1	58,62,73	2.25	20 (34%)	69,99,113	3.00	29 (42%)
12	CLA	B	827	2	49,53,73	2.43	20 (40%)	59,89,113	3.29	27 (45%)
12	CLA	B	831	-	69,73,73	2.05	20 (28%)	83,113,113	2.80	32 (38%)
15	BCR	B	835	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	B	826	2	62,66,73	2.14	19 (30%)	74,104,113	3.02	30 (40%)
12	CLA	B	817	2	63,67,73	2.15	20 (31%)	75,105,113	2.97	28 (37%)
15	BCR	B	836	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	B	832	2	69,73,73	2.04	19 (27%)	83,113,113	2.75	31 (37%)
12	CLA	A	815	1	49,53,73	2.44	20 (40%)	59,89,113	3.27	25 (42%)
12	CLA	B	812	2	49,53,73	2.45	20 (40%)	59,89,113	3.21	26 (44%)
12	CLA	L	202	9	50,54,73	2.43	20 (40%)	60,90,113	3.27	27 (45%)
12	CLA	A	822	1	50,54,73	2.38	19 (38%)	60,90,113	3.21	26 (43%)
12	CLA	A	818	1	58,62,73	2.24	21 (36%)	69,99,113	3.04	30 (43%)
15	BCR	I	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	8 (14%)
12	CLA	B	814	2	60,64,73	2.16	21 (35%)	72,102,113	2.95	30 (41%)
14	SF4	C	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	811	1	69,73,73	2.03	19 (27%)	83,113,113	2.84	29 (34%)
12	CLA	A	829	1	69,73,73	2.00	19 (27%)	83,113,113	2.74	31 (37%)
12	CLA	A	823	1	55,59,73	2.29	20 (36%)	66,96,113	3.15	31 (46%)
12	CLA	A	838	1	60,64,73	2.17	20 (33%)	72,102,113	3.01	30 (41%)
15	BCR	A	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.43	10 (17%)
15	BCR	F	202	-	41,41,41	1.02	2 (4%)	56,56,56	1.21	4 (7%)
15	BCR	F	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	5 (8%)
12	CLA	B	822	2	69,73,73	2.01	20 (28%)	83,113,113	2.73	30 (36%)
12	CLA	A	843	16	56,60,73	2.29	21 (37%)	67,97,113	3.12	25 (37%)
12	CLA	B	821	2	69,73,73	2.00	20 (28%)	83,113,113	2.89	30 (36%)
12	CLA	A	836	1	49,53,73	2.45	20 (40%)	59,89,113	3.30	29 (49%)
12	CLA	B	828	2	50,54,73	2.36	19 (38%)	60,90,113	3.29	28 (46%)
12	CLA	B	805	2	58,62,73	2.22	21 (36%)	69,99,113	3.10	28 (40%)
12	CLA	A	827	1	69,73,73	2.01	20 (28%)	83,113,113	2.87	31 (37%)
15	BCR	L	201	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	5 (8%)
12	CLA	A	834	1	69,73,73	2.03	19 (27%)	83,113,113	2.94	28 (33%)
12	CLA	A	808	1	69,73,73	2.05	21 (30%)	83,113,113	2.77	29 (34%)
14	SF4	A	845	2,1	0,12,12	-	-	-	-	-
12	CLA	A	839	1	54,58,73	2.26	21 (38%)	65,95,113	3.26	32 (49%)
12	CLA	A	813	1	49,53,73	2.42	21 (42%)	59,89,113	3.19	26 (44%)
15	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	5 (8%)
12	CLA	B	809	2	69,73,73	1.97	19 (27%)	83,113,113	2.89	31 (37%)
12	CLA	A	803	1	49,53,73	2.42	20 (40%)	59,89,113	3.24	28 (47%)
12	CLA	A	824	1	51,55,73	2.36	20 (39%)	61,91,113	3.22	29 (47%)
12	CLA	B	816	2	59,63,73	2.23	21 (35%)	71,101,113	3.09	29 (40%)
15	BCR	A	850	-	41,41,41	1.11	2 (4%)	56,56,56	1.33	7 (12%)
15	BCR	J	104	-	41,41,41	1.06	2 (4%)	56,56,56	1.29	6 (10%)
12	CLA	B	815	2	49,53,73	2.43	19 (38%)	59,89,113	3.28	27 (45%)
12	CLA	B	804	-	69,73,73	1.96	20 (28%)	83,113,113	2.77	28 (33%)
12	CLA	B	813	2	69,73,73	2.04	20 (28%)	83,113,113	2.85	31 (37%)
12	CLA	B	830	2	51,55,73	2.32	20 (39%)	61,91,113	3.25	26 (42%)
12	CLA	B	818	2	64,68,73	2.12	20 (31%)	77,107,113	2.87	31 (40%)
12	CLA	A	819	1	69,73,73	2.05	20 (28%)	83,113,113	2.73	30 (36%)
12	CLA	L	203	9	69,73,73	1.99	19 (27%)	83,113,113	2.84	28 (33%)
12	CLA	A	826	-	59,63,73	2.21	20 (33%)	71,101,113	3.09	33 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	F	203	6	49,53,73	2.45	20 (40%)	59,89,113	3.23	27 (45%)
15	BCR	A	847	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	7 (12%)
12	CLA	B	802	-	69,73,73	2.02	20 (28%)	83,113,113	2.70	29 (34%)
12	CLA	B	823	2	69,73,73	2.04	18 (26%)	83,113,113	2.77	30 (36%)
12	CLA	A	810	1	49,53,73	2.42	20 (40%)	59,89,113	3.24	26 (44%)
16	LHG	A	853	12	26,26,48	0.83	0	29,32,54	1.32	3 (10%)
12	CLA	B	801	-	69,73,73	1.98	19 (27%)	83,113,113	2.90	29 (34%)
12	CLA	A	837	1	55,59,73	2.27	20 (36%)	66,96,113	3.12	28 (42%)
12	CLA	B	811	2	69,73,73	2.03	20 (28%)	83,113,113	2.76	36 (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
12	CLA	A	807	1	-	10/23/99/115	-
12	CLA	A	821	-	-	15/39/115/115	-
12	CLA	A	830	1	-	10/39/115/115	-
15	BCR	L	206	-	-	15/29/63/63	0/2/2/2
12	CLA	B	806	2	-	17/39/115/115	-
12	CLA	A	816	-	-	2/20/96/115	-
12	CLA	A	805	1	-	18/39/115/115	-
12	CLA	A	802	-	-	3/15/91/115	-
12	CLA	B	803	2	-	13/39/115/115	-
15	BCR	A	846	-	-	9/29/63/63	0/2/2/2
17	LMG	B	837	-	-	24/50/70/70	0/1/1/1
12	CLA	A	804	1	-	4/15/91/115	-
12	CLA	B	825	2	-	13/39/115/115	-
15	BCR	A	851	-	-	18/29/63/63	0/2/2/2
12	CLA	A	820	1	-	10/35/111/115	-
12	CLA	A	835	1	-	8/26/102/115	-
15	BCR	A	849	-	-	7/29/63/63	0/2/2/2
12	CLA	A	832	1	-	9/39/115/115	-
13	PQN	A	844	-	-	2/23/43/43	0/2/2/2
12	CLA	B	829	2	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	854	-	-	7/39/115/115	-
11	CL0	A	801	1	-	4/39/115/115	-
12	CLA	B	810	2	-	14/39/115/115	-
12	CLA	B	820	2	-	8/39/115/115	-
15	BCR	J	103	-	-	16/29/63/63	0/2/2/2
15	BCR	L	205	-	-	10/29/63/63	0/2/2/2
12	CLA	B	824	2	-	9/20/96/115	-
12	CLA	A	828	1	-	12/39/115/115	-
15	BCR	B	834	-	-	10/29/63/63	0/2/2/2
16	LHG	A	852	-	-	22/53/53/53	-
12	CLA	A	814	1	-	3/15/91/115	-
12	CLA	B	819	-	-	6/17/93/115	-
14	SF4	C	101	3	-	-	0/6/5/5
15	BCR	M	101	-	-	13/29/63/63	0/2/2/2
12	CLA	B	808	2	-	3/39/115/115	-
12	CLA	J	101	8	-	8/15/91/115	-
12	CLA	A	817	1	-	10/39/115/115	-
12	CLA	A	825	-	-	12/39/115/115	-
13	PQN	B	833	-	-	5/23/43/43	0/2/2/2
12	CLA	A	806	1	-	14/39/115/115	-
12	CLA	A	809	1	-	4/15/91/115	-
12	CLA	A	842	1	-	7/39/115/115	-
12	CLA	A	841	-	-	7/23/99/115	-
12	CLA	A	831	1	-	7/21/97/115	-
12	CLA	B	807	2	-	14/39/115/115	-
12	CLA	A	833	1	-	9/39/115/115	-
12	CLA	A	840	1	-	16/39/115/115	-
12	CLA	L	204	-	-	9/24/100/115	-
12	CLA	A	812	1	-	10/26/102/115	-
12	CLA	B	827	2	-	8/15/91/115	-
12	CLA	B	831	-	-	11/39/115/115	-
15	BCR	B	835	-	-	12/29/63/63	0/2/2/2
12	CLA	B	826	2	-	13/31/107/115	-
12	CLA	B	817	2	-	11/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	B	836	-	-	10/29/63/63	0/2/2/2
12	CLA	B	832	2	-	17/39/115/115	-
12	CLA	A	815	1	-	5/15/91/115	-
12	CLA	B	812	2	-	3/15/91/115	-
12	CLA	L	202	9	-	6/17/93/115	-
12	CLA	A	822	1	-	5/17/93/115	-
12	CLA	A	818	1	-	9/26/102/115	-
15	BCR	I	101	-	-	9/29/63/63	0/2/2/2
12	CLA	B	814	2	-	10/29/105/115	-
14	SF4	C	102	3	-	-	0/6/5/5
12	CLA	A	811	1	-	12/39/115/115	-
12	CLA	A	829	1	-	12/39/115/115	-
12	CLA	A	823	1	-	10/23/99/115	-
12	CLA	A	838	1	-	12/29/105/115	-
15	BCR	A	848	-	-	11/29/63/63	0/2/2/2
15	BCR	F	202	-	-	11/29/63/63	0/2/2/2
15	BCR	F	201	-	-	12/29/63/63	0/2/2/2
12	CLA	B	822	2	-	12/39/115/115	-
12	CLA	A	843	16	-	14/24/100/115	-
12	CLA	B	821	2	-	19/39/115/115	-
12	CLA	A	836	1	-	5/15/91/115	-
12	CLA	B	828	2	-	6/17/93/115	-
12	CLA	B	805	2	-	4/26/102/115	-
12	CLA	A	827	1	-	13/39/115/115	-
15	BCR	L	201	-	-	11/29/63/63	0/2/2/2
12	CLA	A	834	1	-	16/39/115/115	-
12	CLA	A	808	1	-	17/39/115/115	-
14	SF4	A	845	2,1	-	-	0/6/5/5
12	CLA	A	839	1	-	5/21/97/115	-
12	CLA	A	813	1	-	10/15/91/115	-
15	BCR	J	102	-	-	14/29/63/63	0/2/2/2
12	CLA	B	809	2	-	9/39/115/115	-
12	CLA	A	803	1	-	6/15/91/115	-
12	CLA	A	824	1	-	4/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	816	2	-	5/27/103/115	-
15	BCR	A	850	-	-	10/29/63/63	0/2/2/2
15	BCR	J	104	-	-	13/29/63/63	0/2/2/2
12	CLA	B	815	2	-	6/15/91/115	-
12	CLA	B	804	-	-	7/39/115/115	-
12	CLA	B	813	2	-	20/39/115/115	-
12	CLA	B	830	2	-	5/18/94/115	-
12	CLA	B	818	2	-	5/33/109/115	-
12	CLA	A	819	1	-	14/39/115/115	-
12	CLA	L	203	9	-	13/39/115/115	-
12	CLA	A	826	-	-	10/27/103/115	-
12	CLA	F	203	6	-	5/15/91/115	-
15	BCR	A	847	-	-	8/29/63/63	0/2/2/2
12	CLA	B	802	-	-	14/39/115/115	-
12	CLA	B	823	2	-	15/39/115/115	-
12	CLA	A	810	1	-	4/15/91/115	-
16	LHG	A	853	12	-	10/31/31/53	-
12	CLA	B	801	-	-	5/39/115/115	-
12	CLA	A	837	1	-	8/23/99/115	-
12	CLA	B	811	2	-	11/39/115/115	-

The worst 5 of 1647 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	844	PQN	C3-C2	7.50	1.48	1.35
13	B	833	PQN	C3-C2	7.00	1.48	1.35
12	B	832	CLA	C3C-C2C	5.53	1.48	1.36
12	L	202	CLA	C3C-C2C	5.50	1.48	1.36
12	L	202	CLA	C1D-ND	5.50	1.44	1.37

The worst 5 of 2530 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	825	CLA	C1D-ND-C4D	-10.62	98.79	106.33
12	L	203	CLA	C1D-ND-C4D	-9.89	99.31	106.33
12	B	819	CLA	C2B-C1B-NB	9.75	116.77	110.23
12	A	822	CLA	C1D-ND-C4D	-9.67	99.47	106.33
12	A	817	CLA	C1D-ND-C4D	-9.61	99.51	106.33

There are no chirality outliers.

5 of 1054 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	803	CLA	CHA-CBD-CGD-O1D
12	A	803	CLA	CHA-CBD-CGD-O2D
12	A	804	CLA	C2B-C3B-CAB-CBB
12	A	804	CLA	C4B-C3B-CAB-CBB
12	A	804	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

95 monomers are involved in 205 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	807	CLA	2	0
12	A	821	CLA	3	0
12	A	830	CLA	4	0
15	L	206	BCR	3	0
12	B	806	CLA	4	0
12	A	805	CLA	8	0
12	A	802	CLA	2	0
12	B	803	CLA	2	0
15	A	846	BCR	2	0
17	B	837	LMG	7	0
12	A	804	CLA	2	0
12	B	825	CLA	2	0
15	A	851	BCR	1	0
12	A	820	CLA	2	0
12	A	835	CLA	1	0
15	A	849	BCR	1	0
12	A	832	CLA	5	0
13	A	844	PQN	3	0
12	B	829	CLA	4	0
12	A	854	CLA	5	0
11	A	801	CL0	3	0
12	B	810	CLA	2	0
12	B	820	CLA	3	0
15	J	103	BCR	1	0
15	L	205	BCR	3	0
12	B	824	CLA	3	0
12	A	828	CLA	7	0
15	B	834	BCR	2	0
16	A	852	LHG	2	0
12	B	819	CLA	1	0

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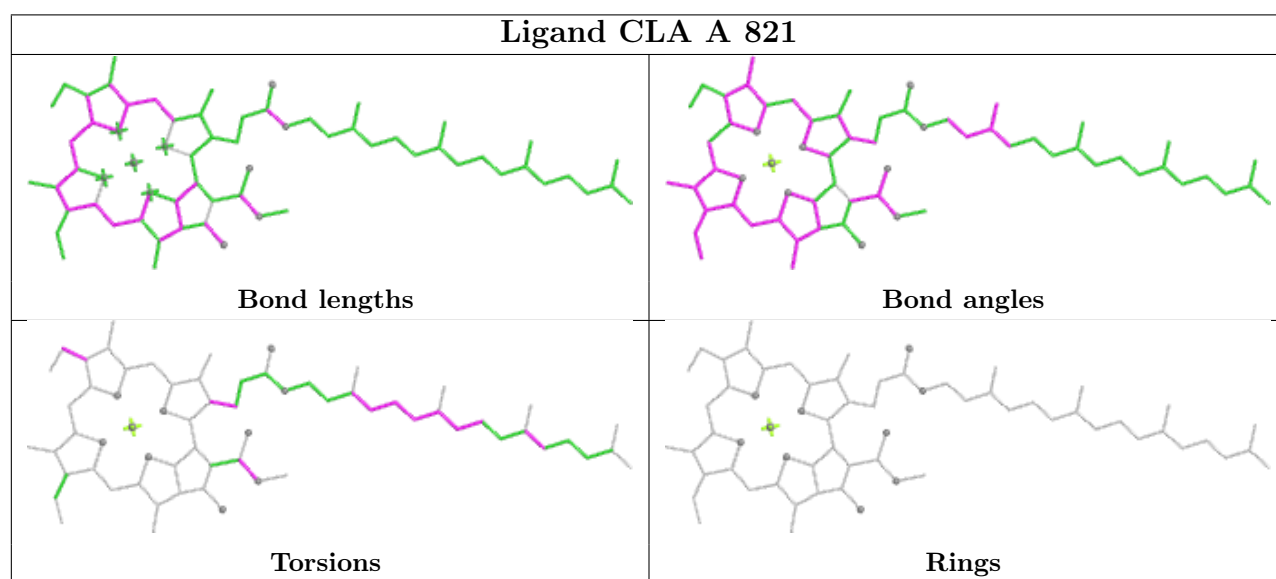
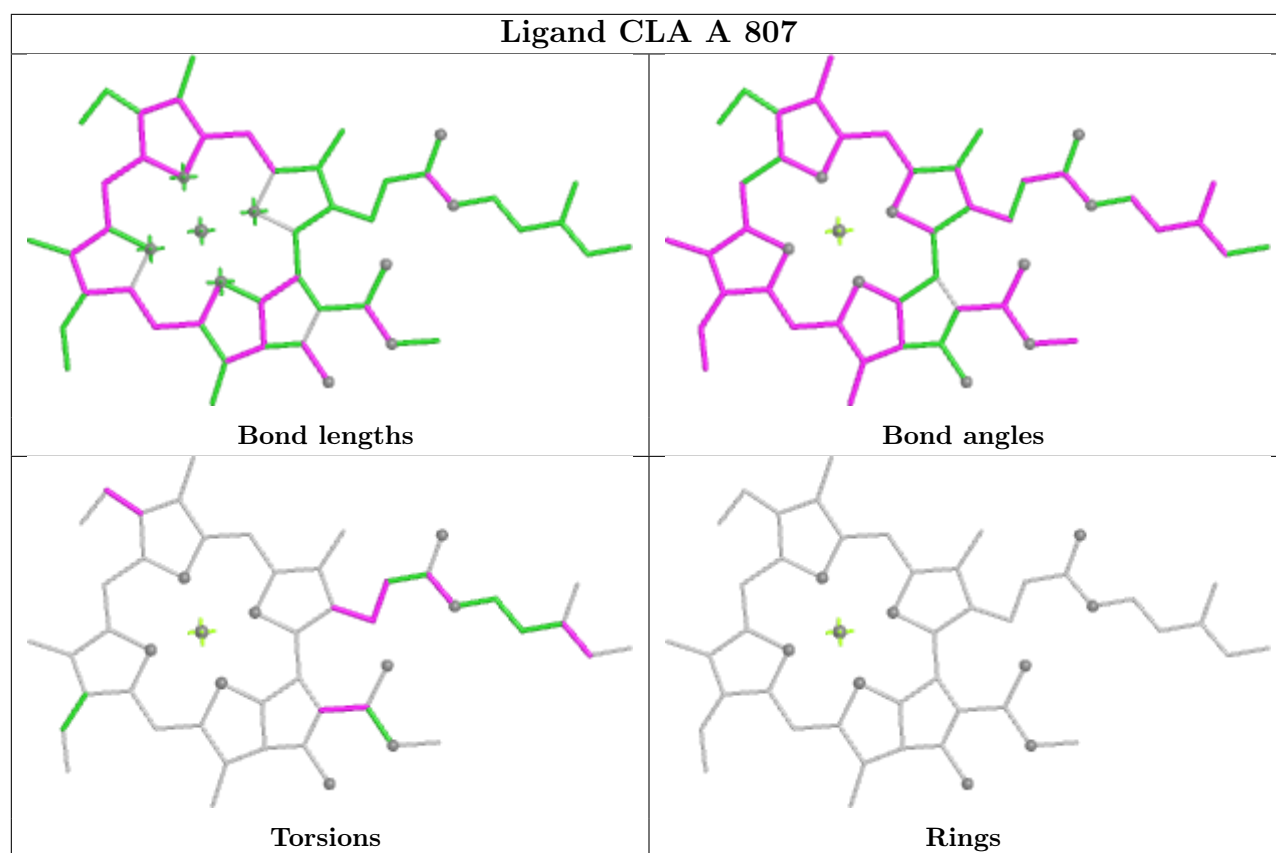
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	M	101	BCR	2	0
12	B	808	CLA	4	0
12	A	817	CLA	1	0
12	A	825	CLA	1	0
13	B	833	PQN	5	0
12	A	806	CLA	3	0
12	A	809	CLA	2	0
12	A	842	CLA	4	0
12	A	841	CLA	1	0
12	A	831	CLA	2	0
12	B	807	CLA	6	0
12	A	833	CLA	2	0
12	A	840	CLA	2	0
12	L	204	CLA	2	0
12	A	812	CLA	3	0
12	B	827	CLA	1	0
12	B	831	CLA	3	0
15	B	835	BCR	4	0
12	B	826	CLA	1	0
12	B	817	CLA	1	0
15	B	836	BCR	2	0
12	B	832	CLA	7	0
12	A	815	CLA	2	0
12	B	812	CLA	2	0
12	L	202	CLA	3	0
12	A	822	CLA	1	0
12	A	818	CLA	3	0
15	I	101	BCR	5	0
12	B	814	CLA	1	0
12	A	811	CLA	1	0
12	A	829	CLA	5	0
12	A	838	CLA	1	0
15	A	848	BCR	5	0
15	F	202	BCR	3	0
15	F	201	BCR	3	0
12	B	822	CLA	6	0
12	A	843	CLA	1	0
12	B	821	CLA	2	0
12	A	836	CLA	1	0
12	A	827	CLA	1	0
15	L	201	BCR	5	0
12	A	834	CLA	3	0

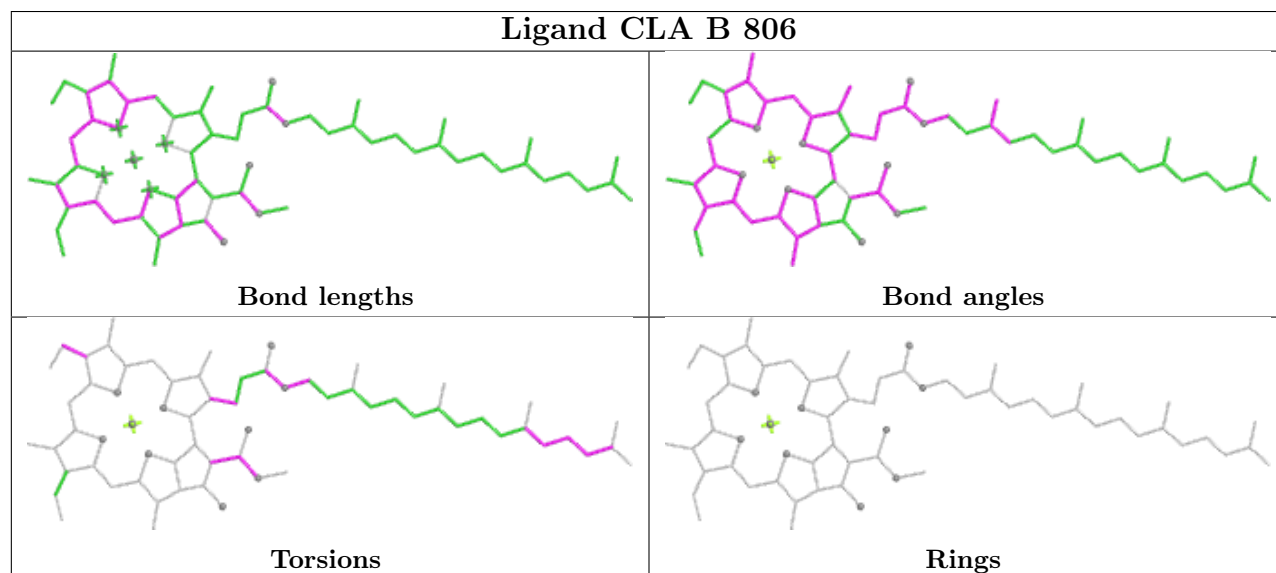
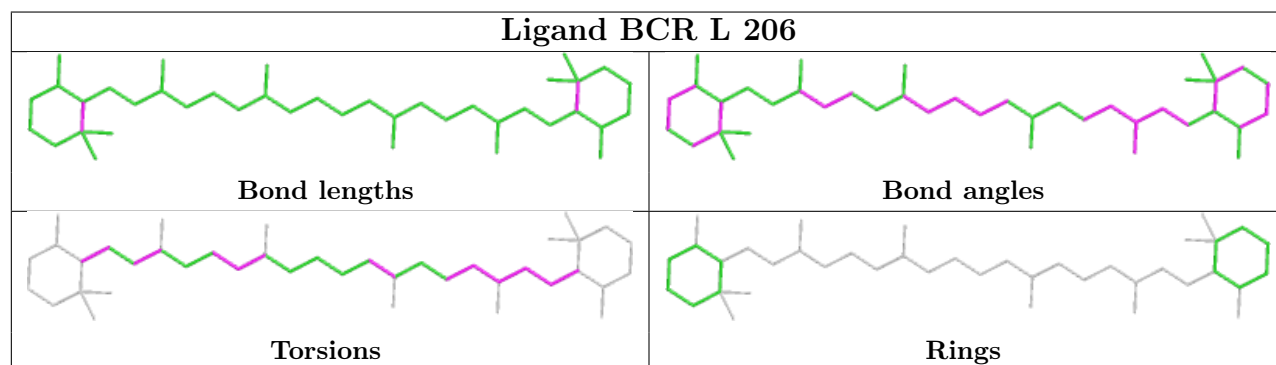
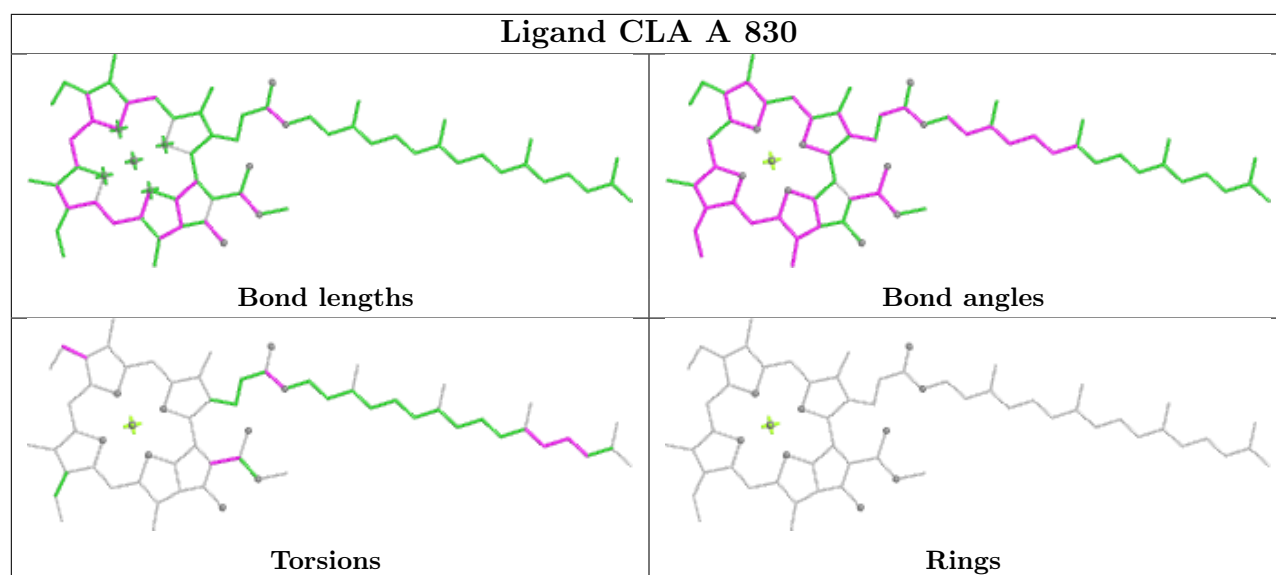
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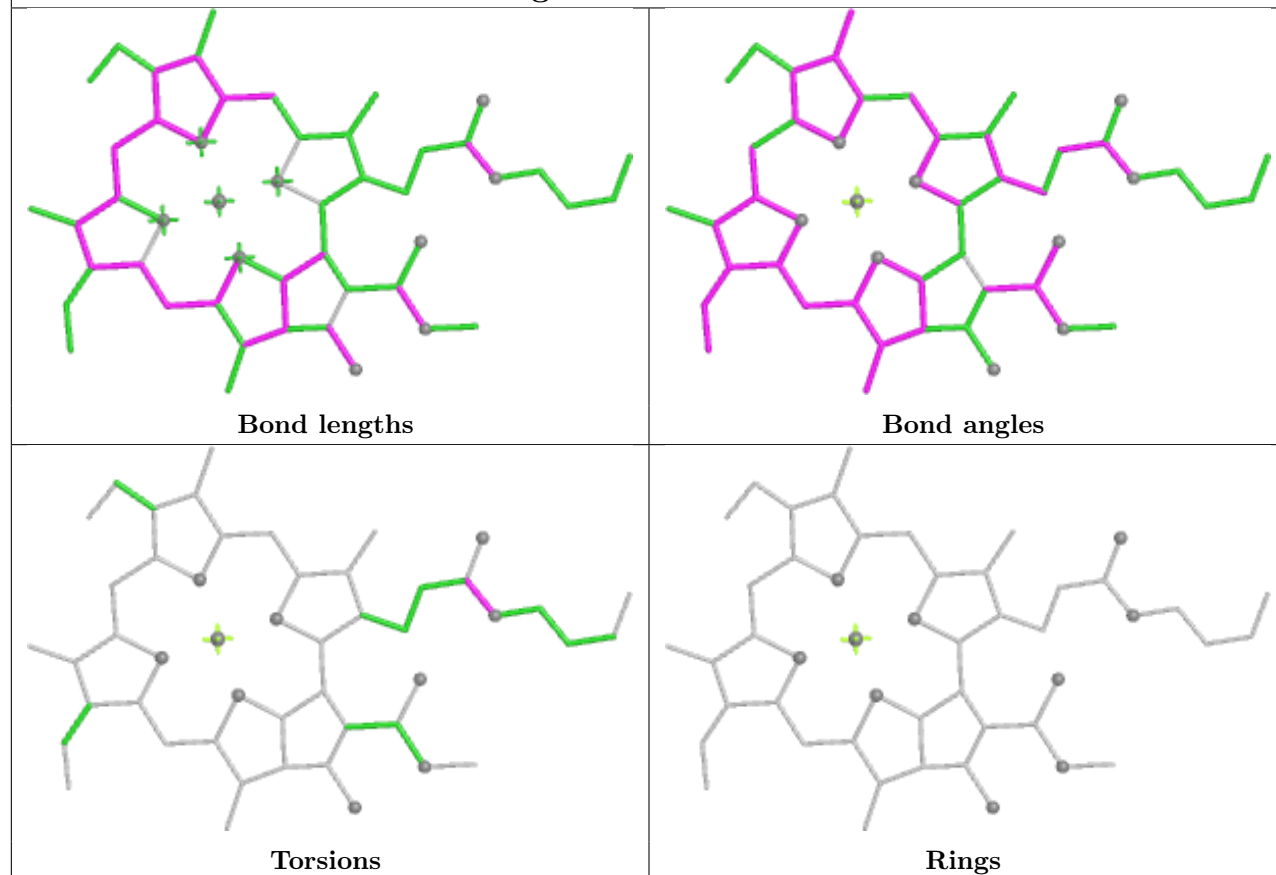
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	808	CLA	5	0
12	A	839	CLA	1	0
12	A	813	CLA	1	0
15	J	102	BCR	3	0
12	B	809	CLA	3	0
12	A	803	CLA	1	0
12	A	824	CLA	1	0
12	B	816	CLA	2	0
15	A	850	BCR	5	0
15	J	104	BCR	2	0
12	B	804	CLA	7	0
12	B	830	CLA	1	0
12	B	818	CLA	3	0
12	A	819	CLA	6	0
12	L	203	CLA	6	0
12	A	826	CLA	1	0
15	A	847	BCR	4	0
12	B	802	CLA	8	0
12	B	823	CLA	4	0
12	A	810	CLA	1	0
12	B	801	CLA	4	0
12	A	837	CLA	1	0
12	B	811	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.

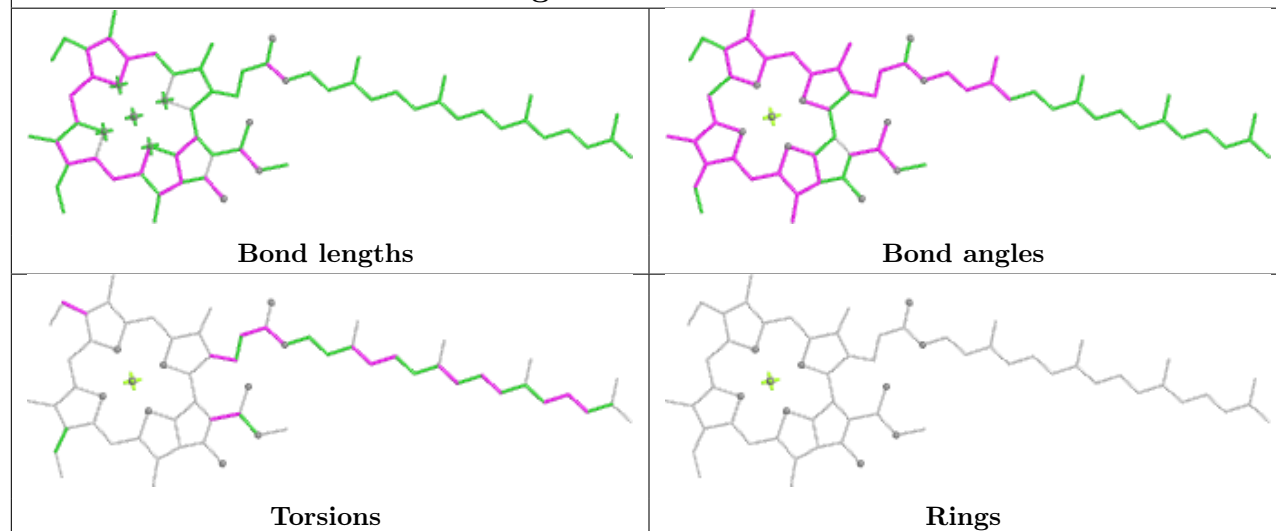


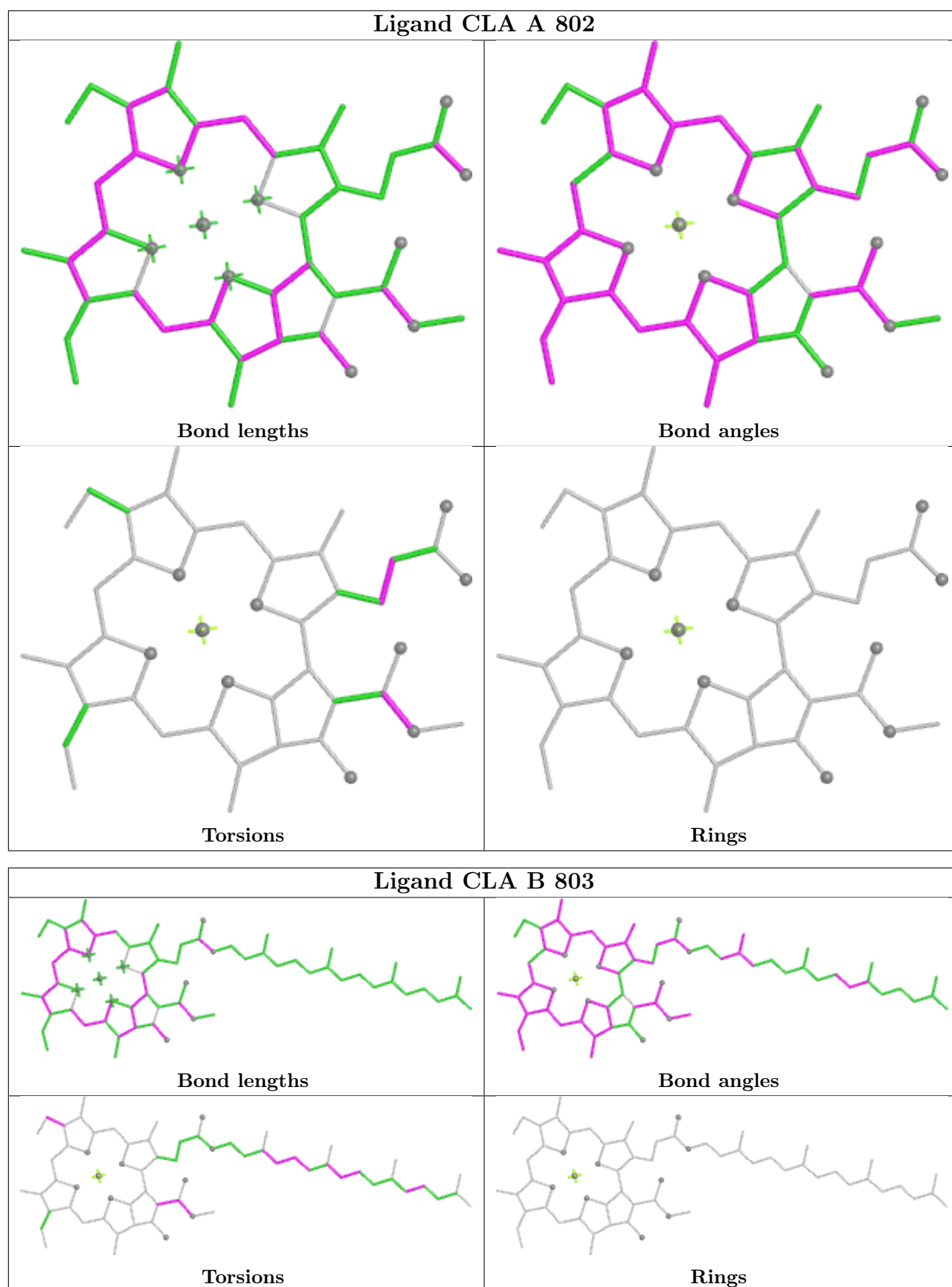


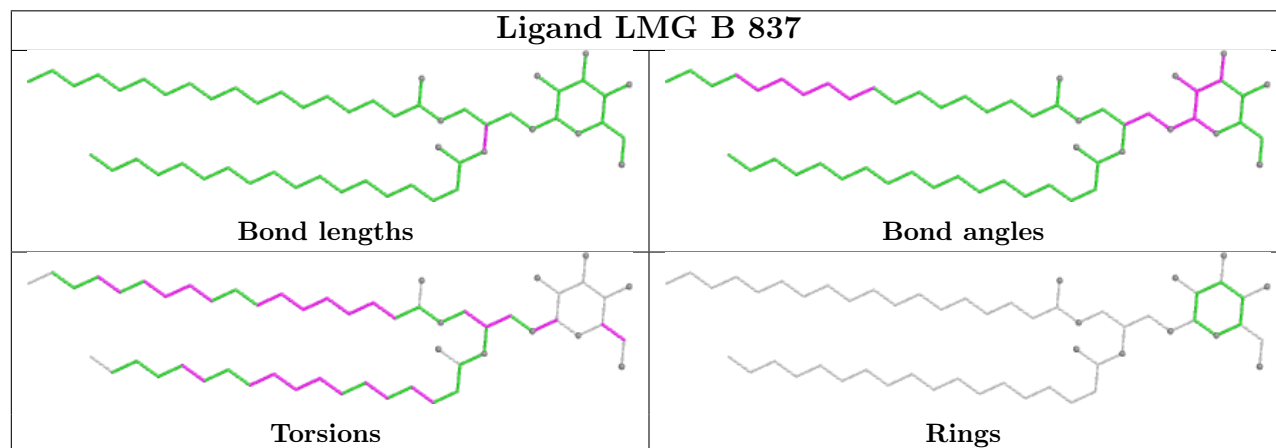
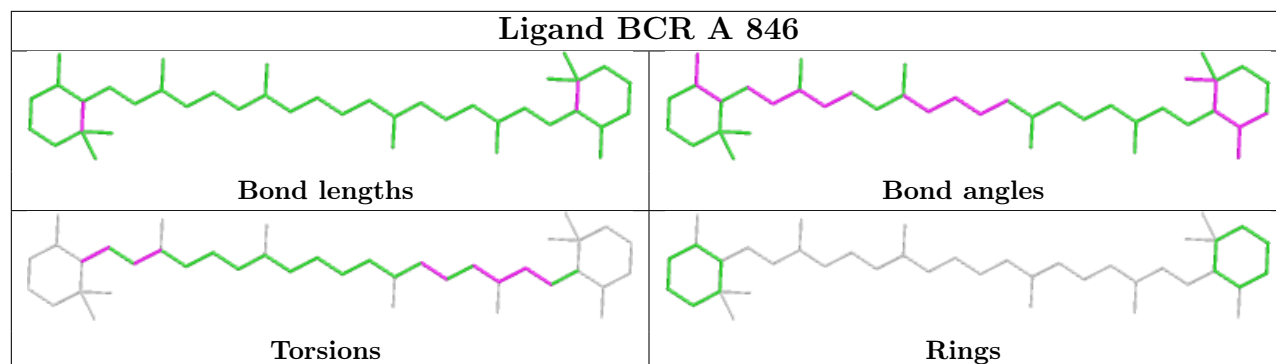
Ligand CLA A 816

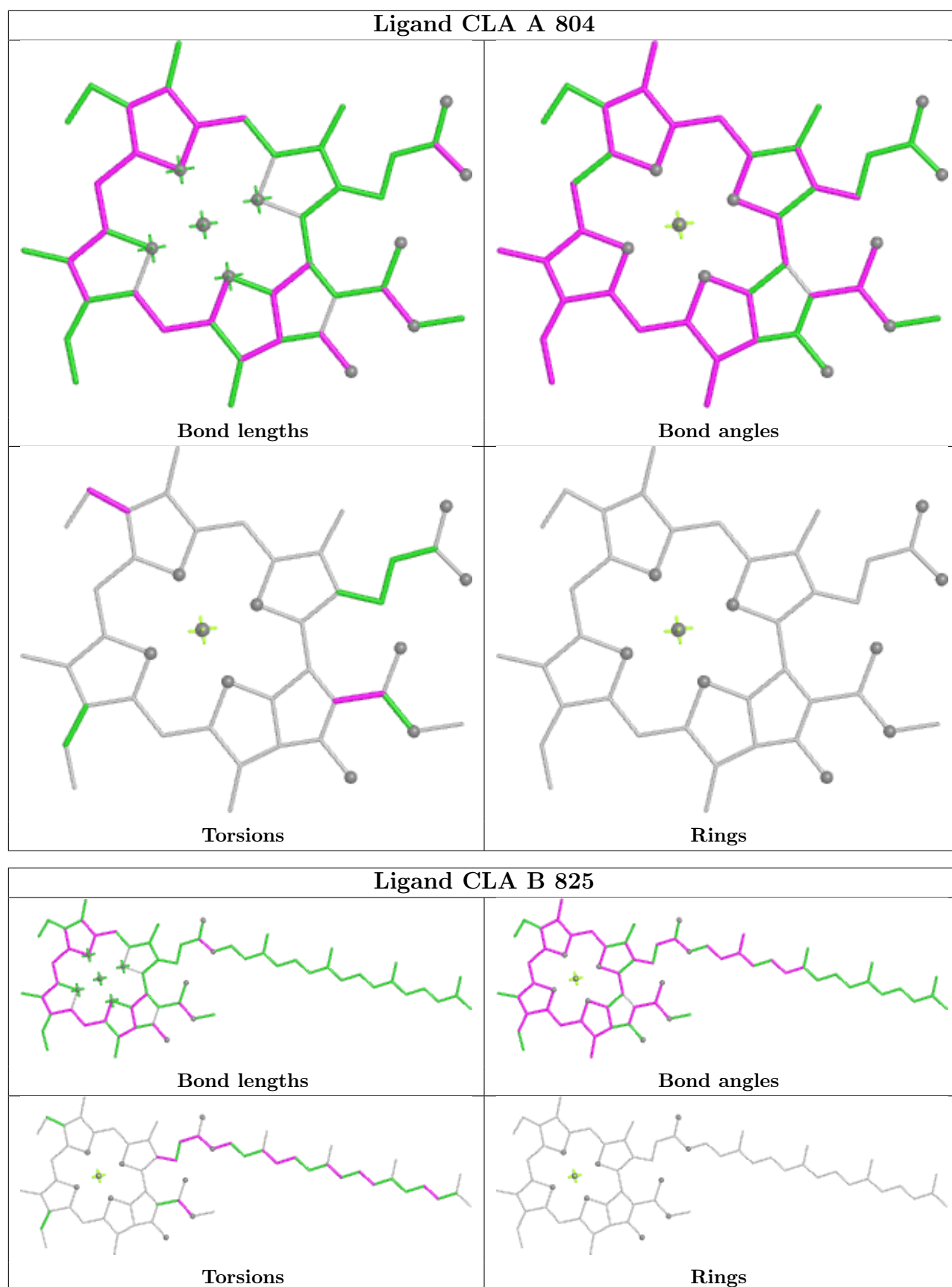


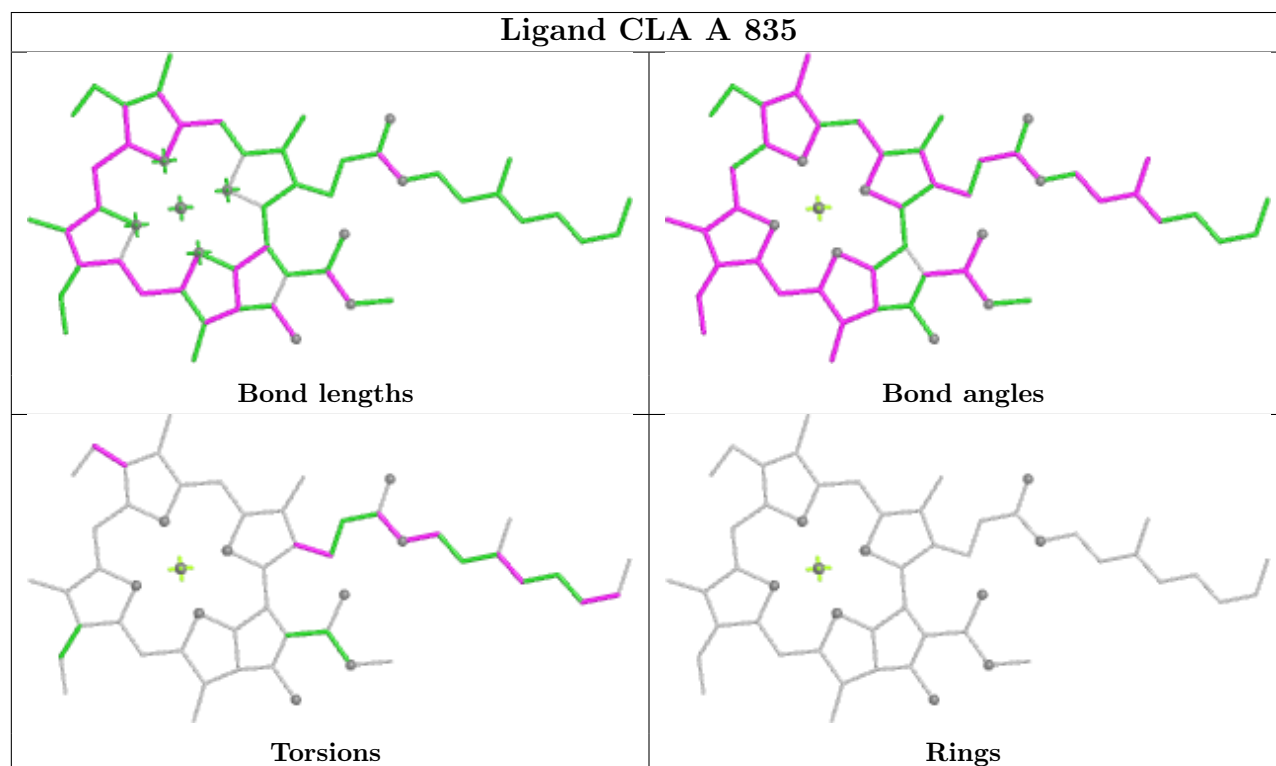
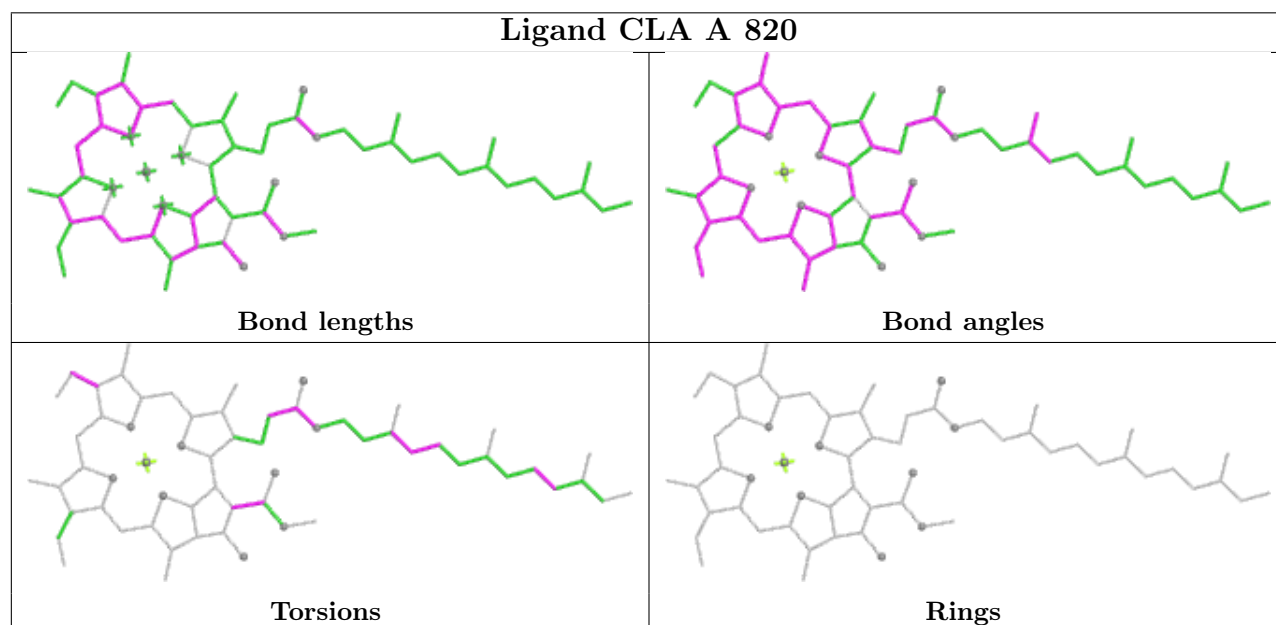
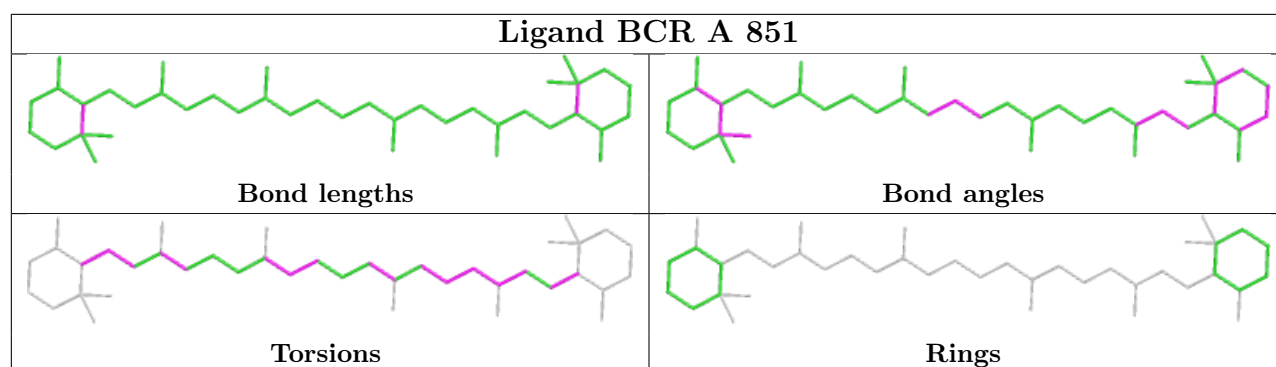
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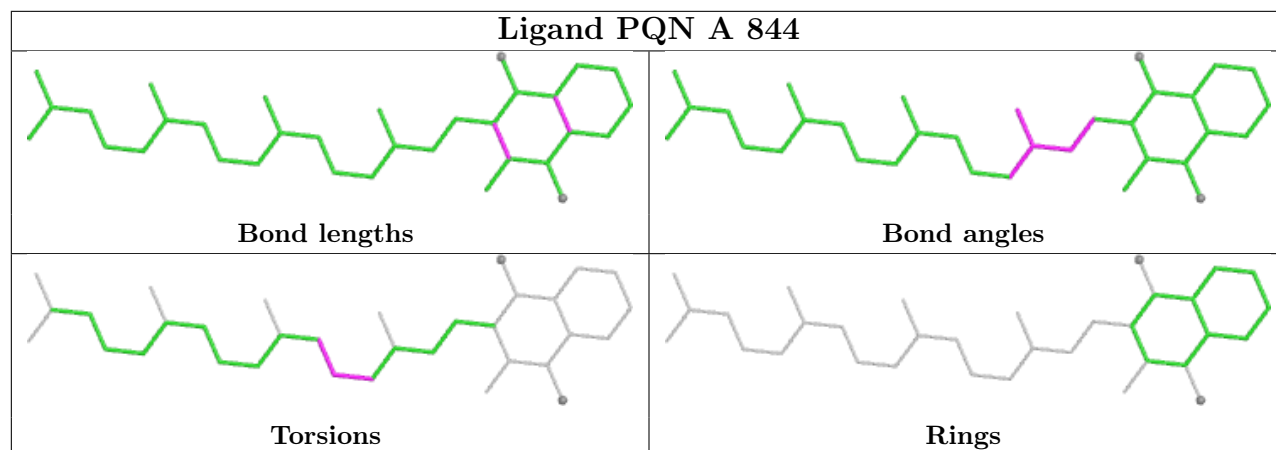
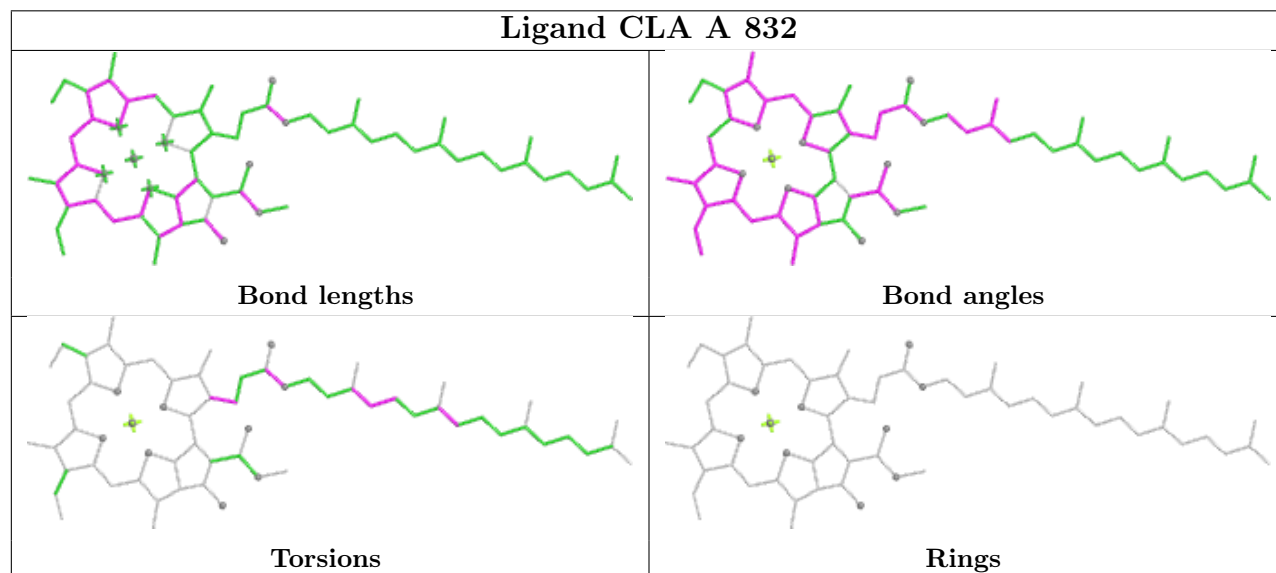
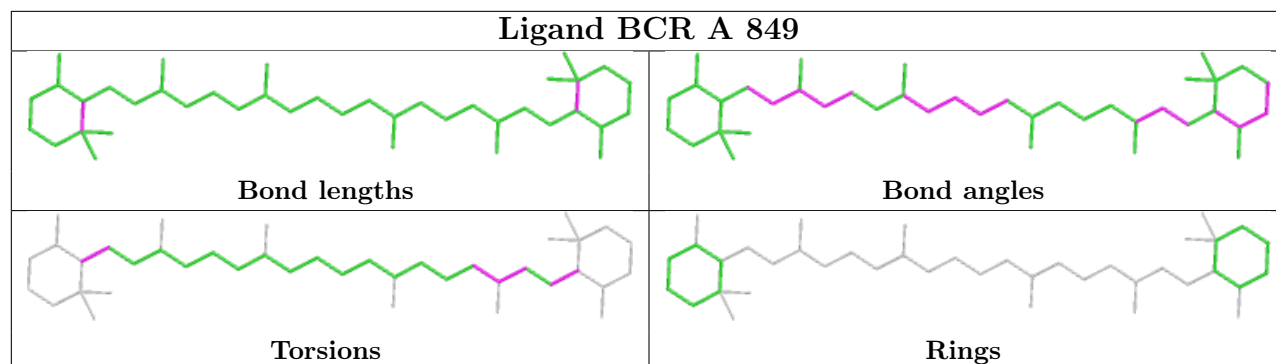


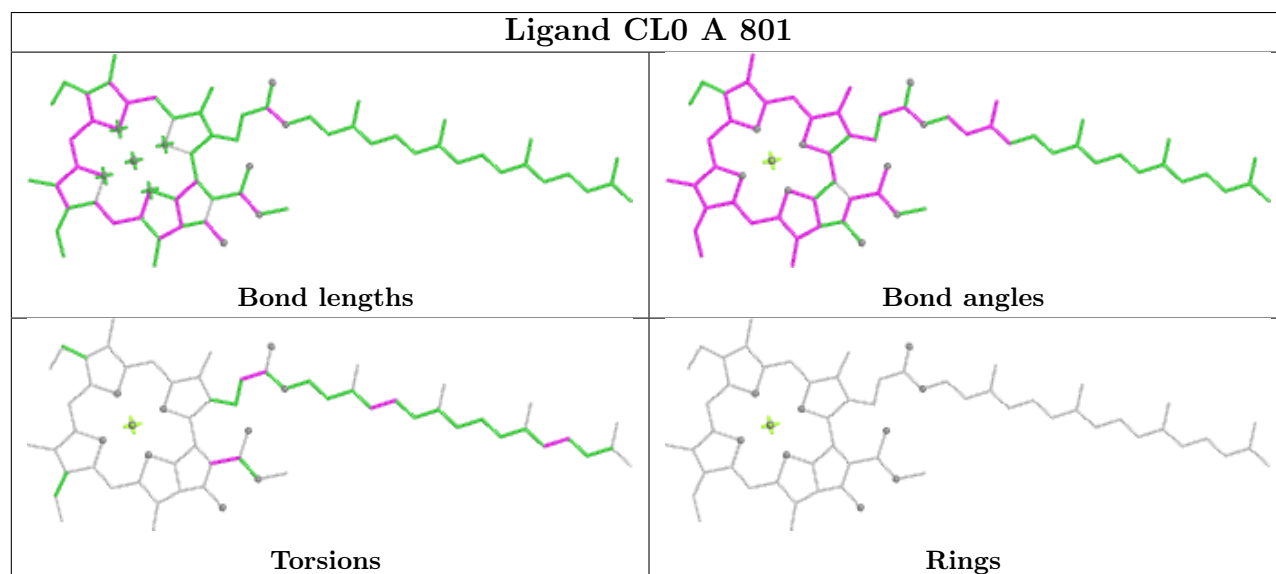
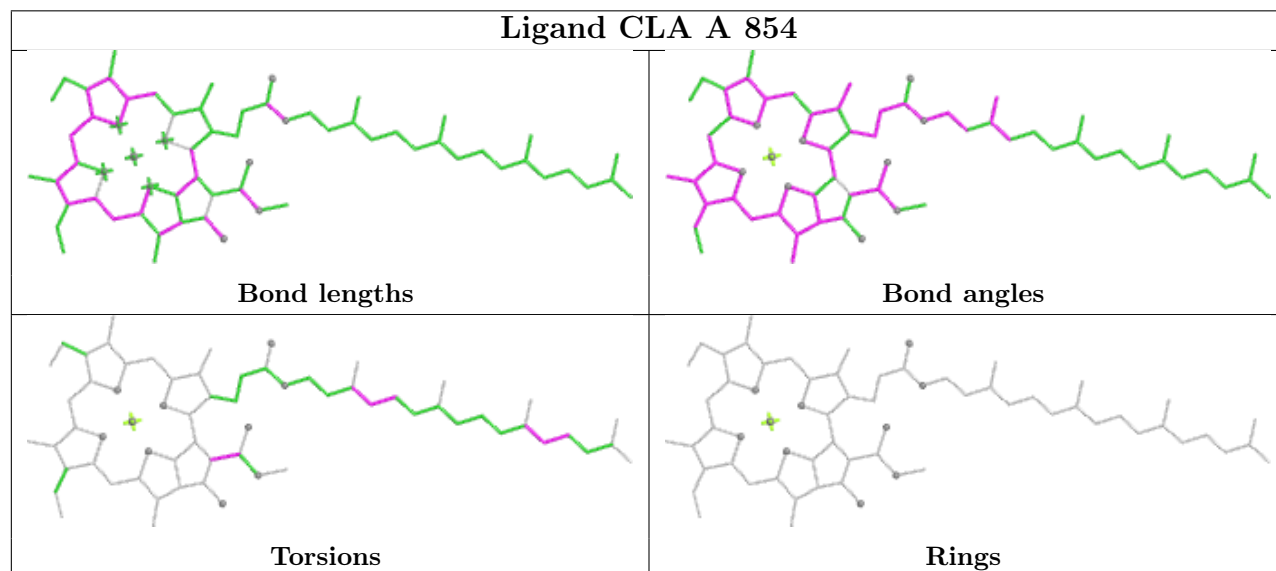
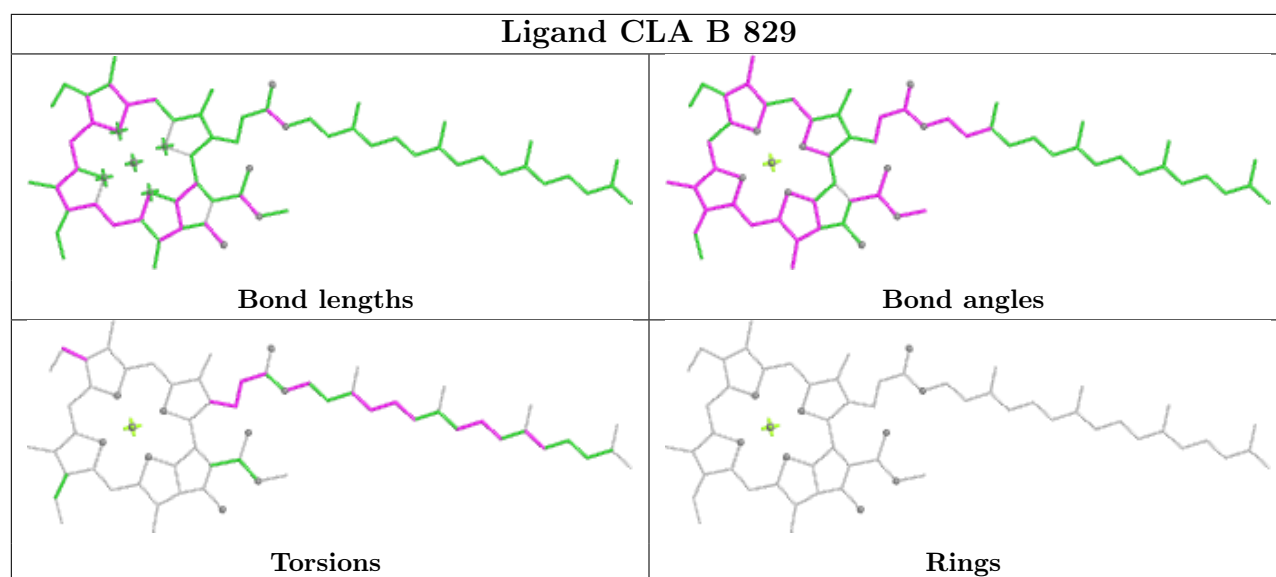


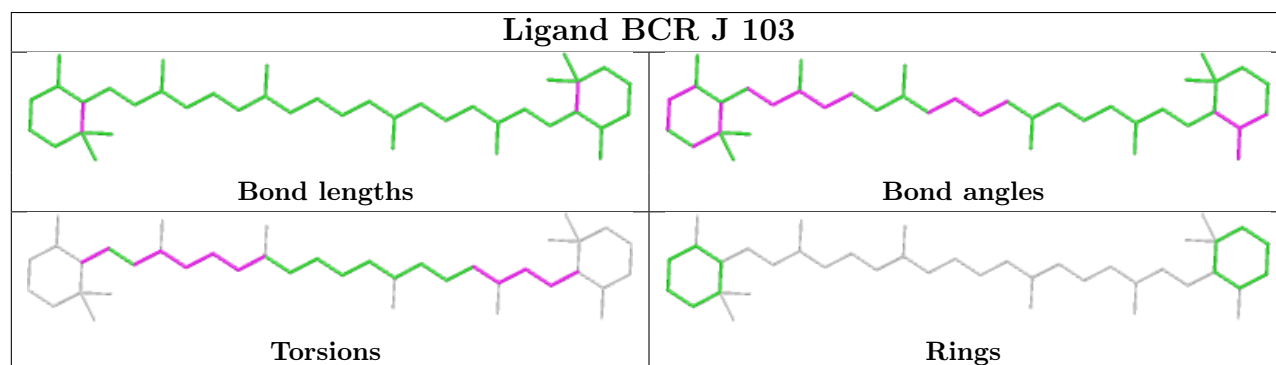
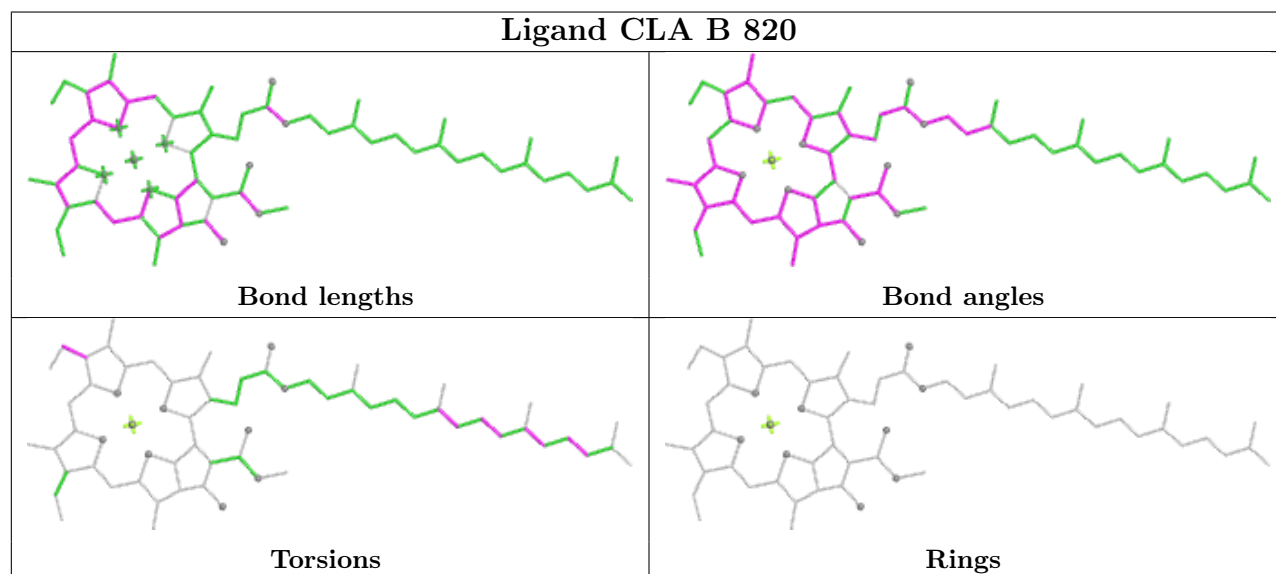
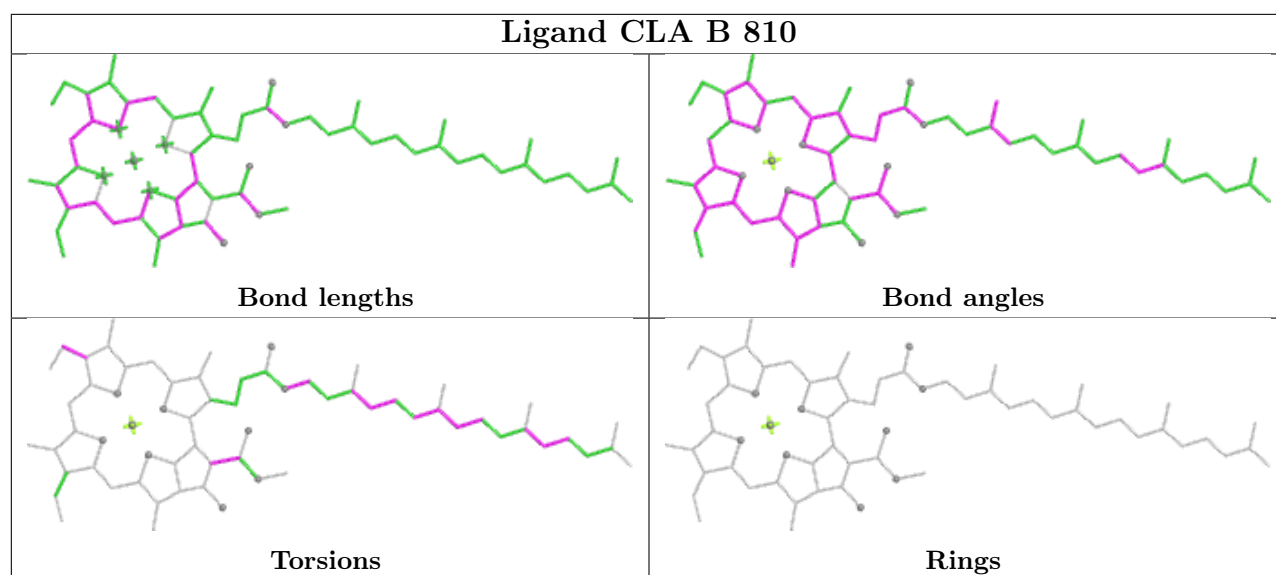


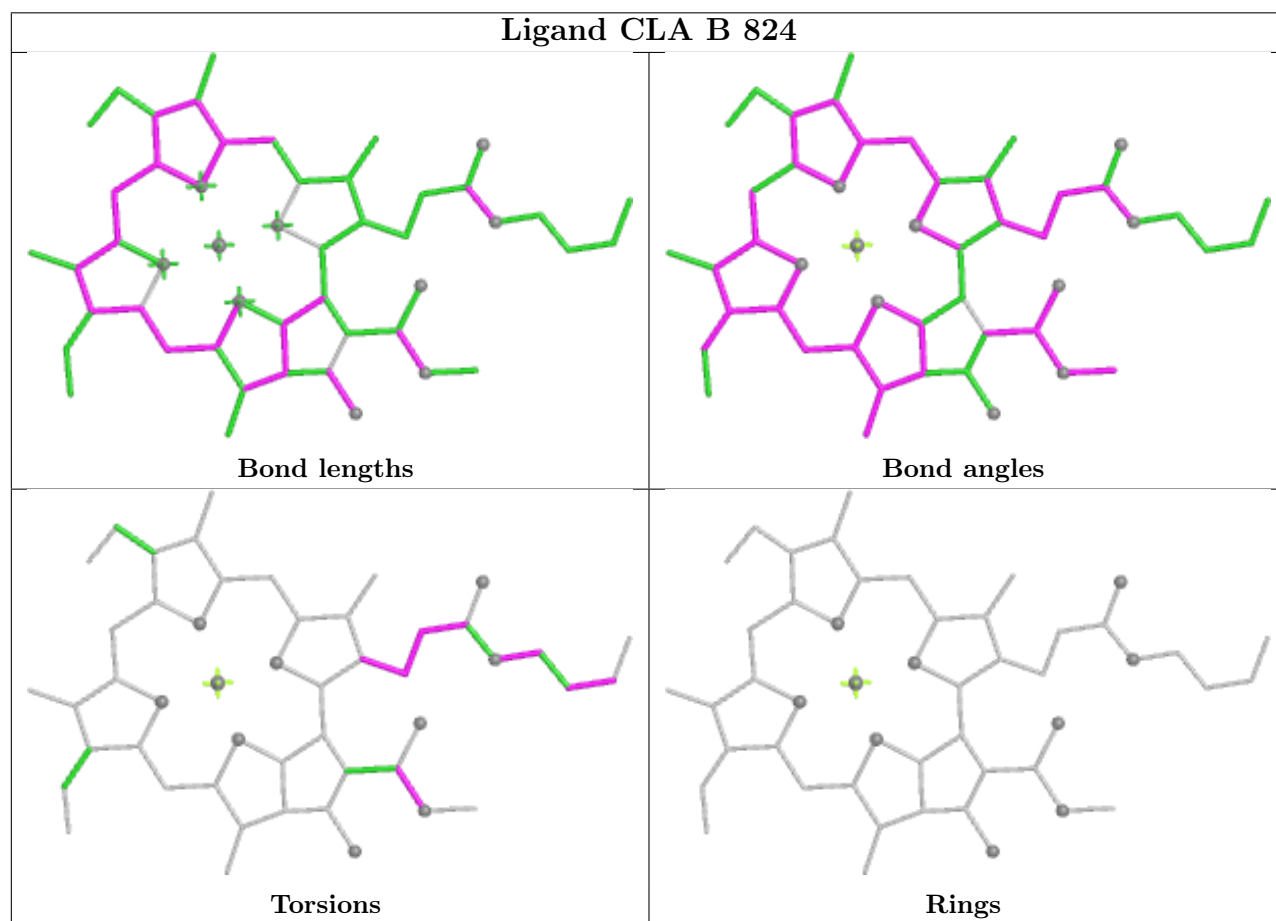
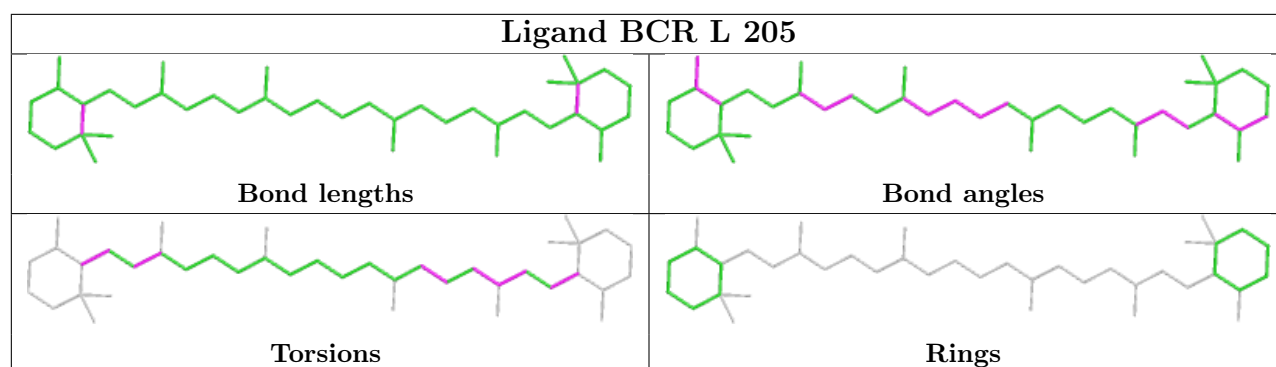


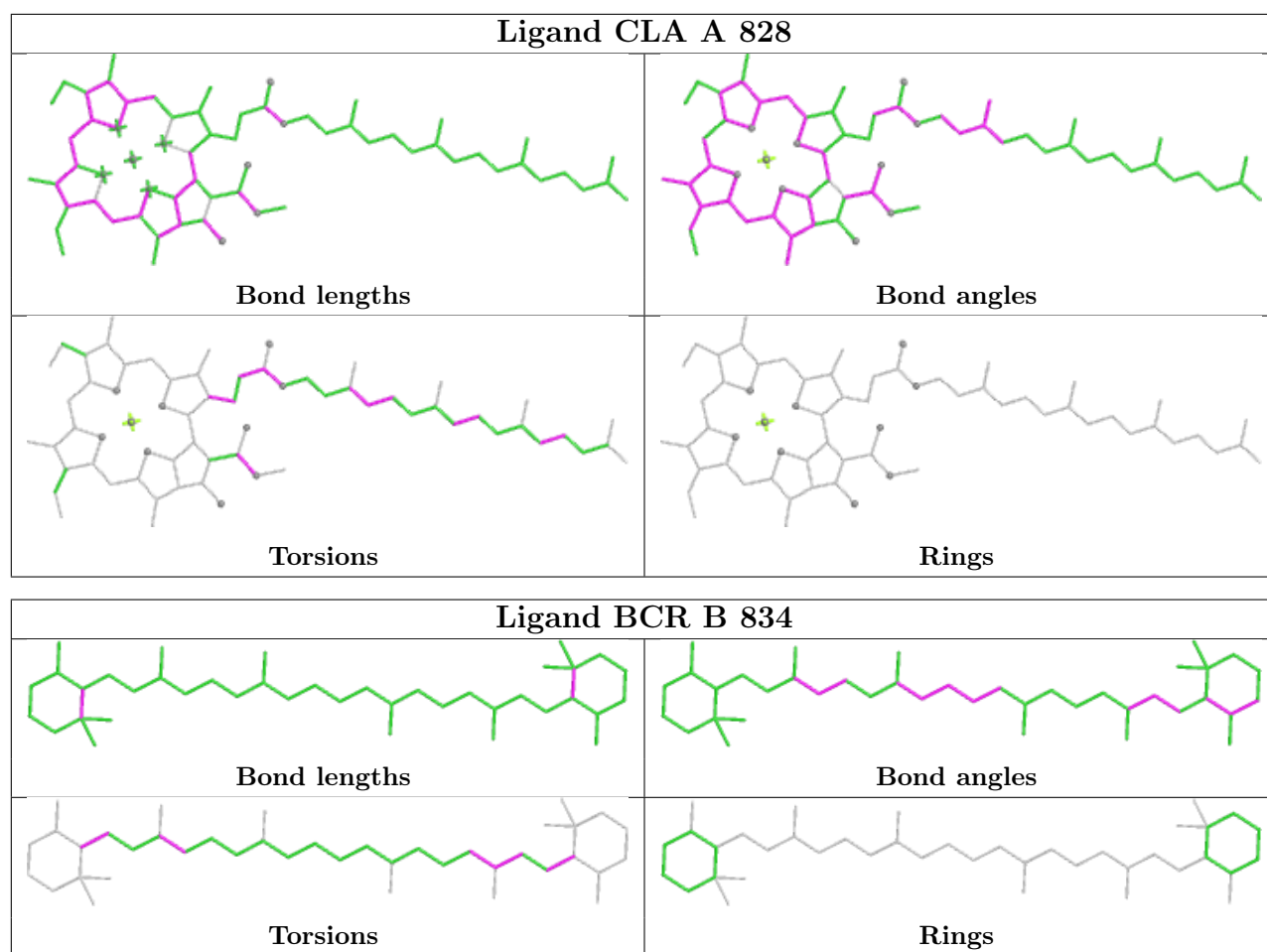


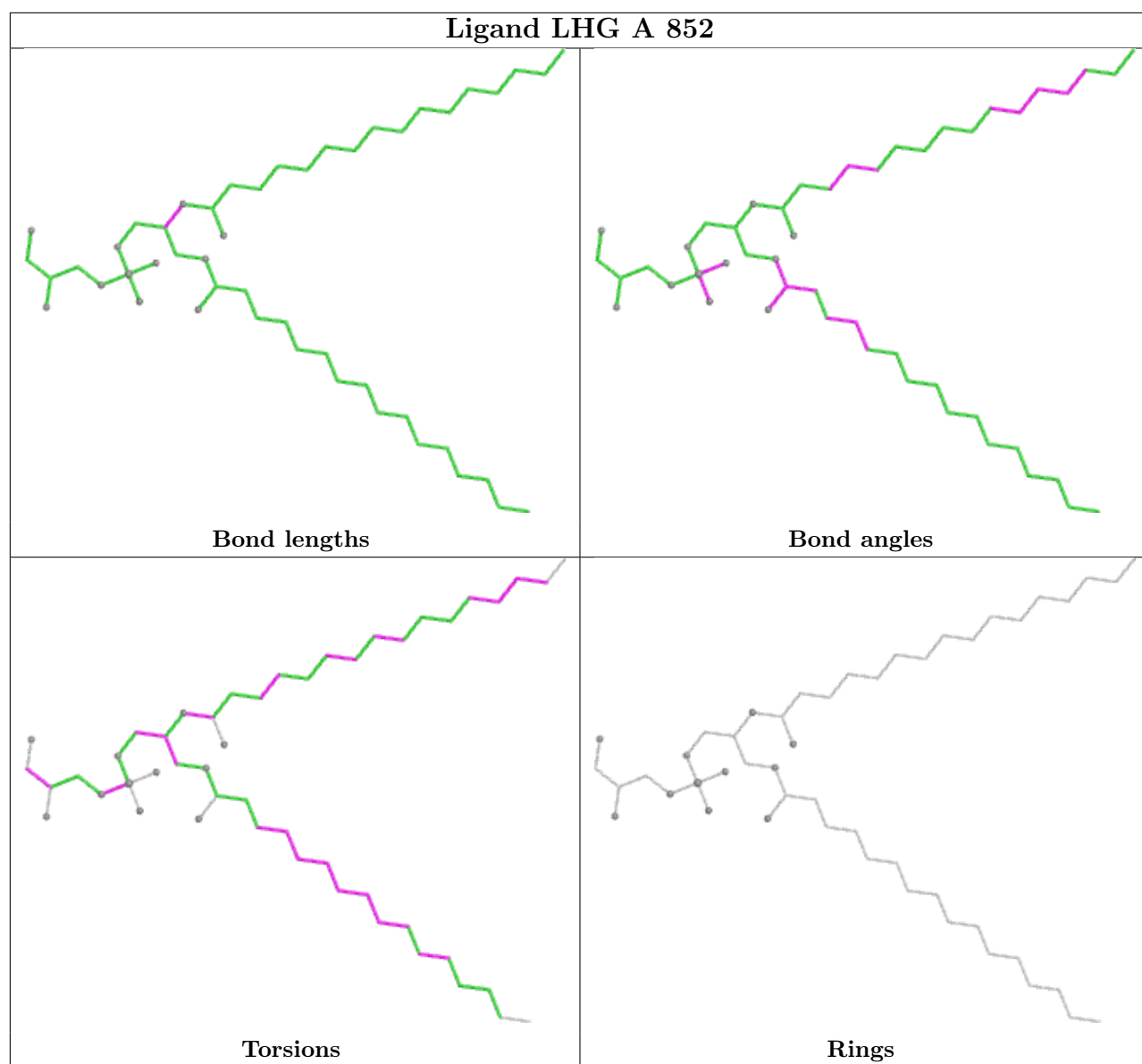


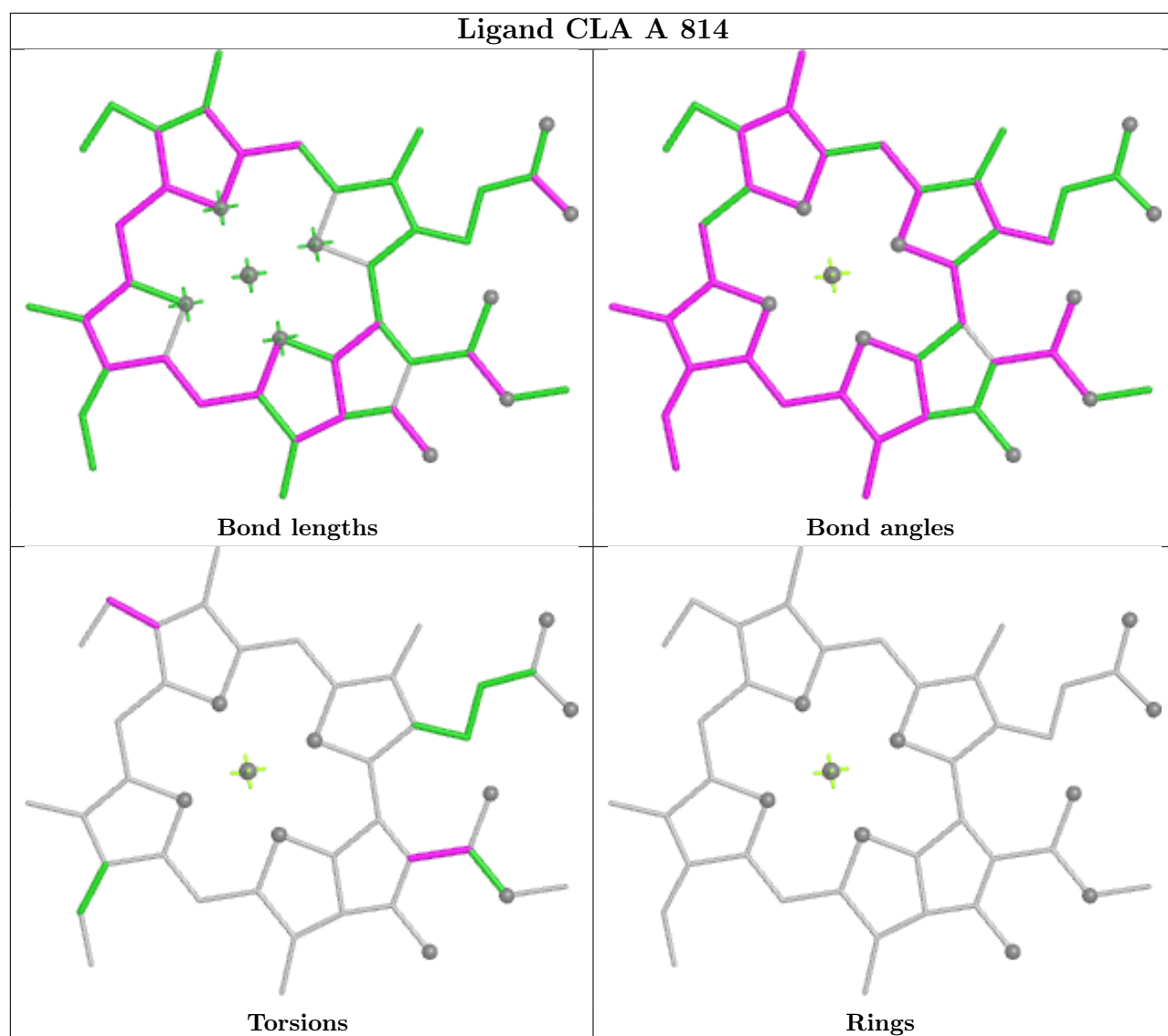


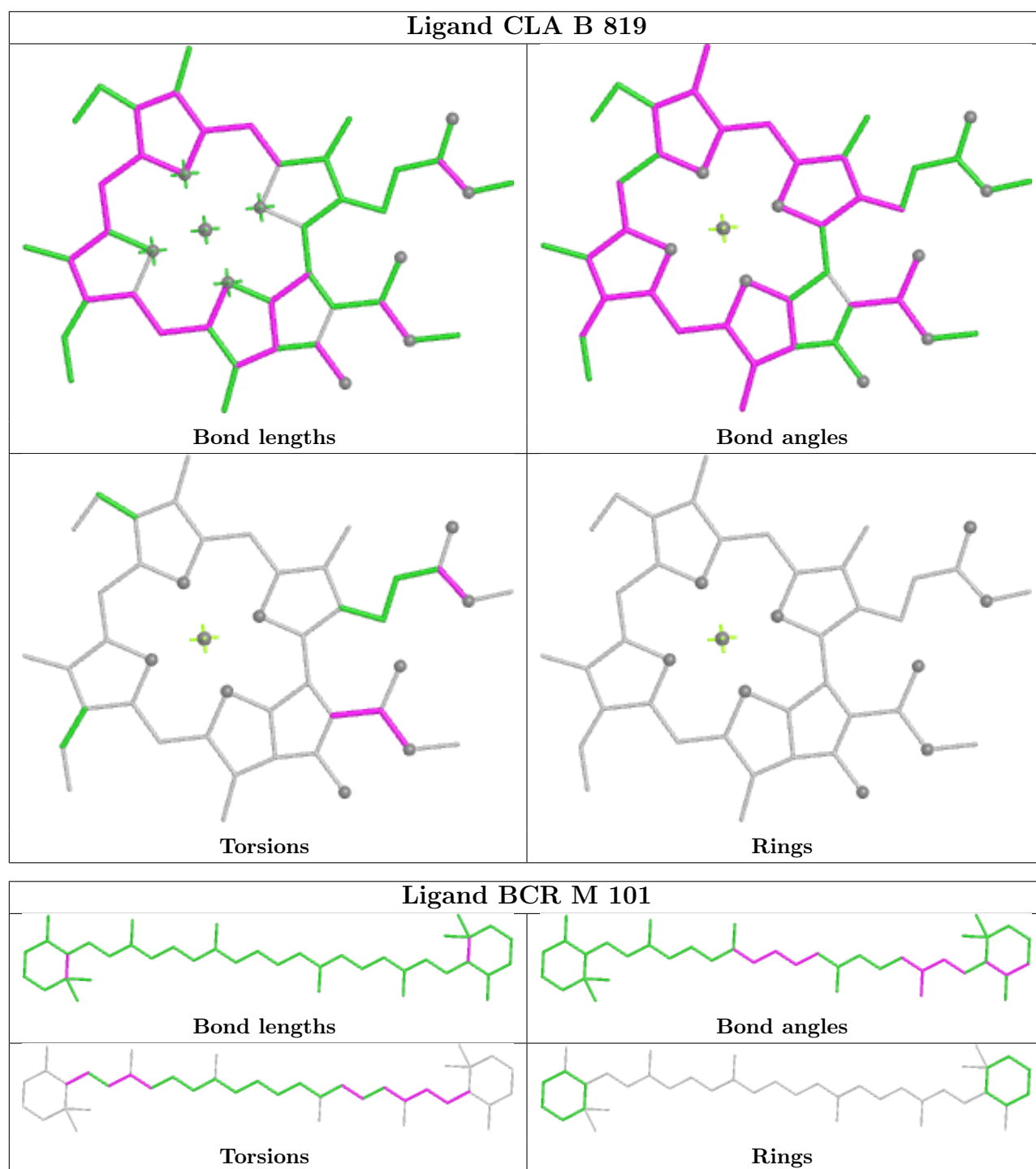


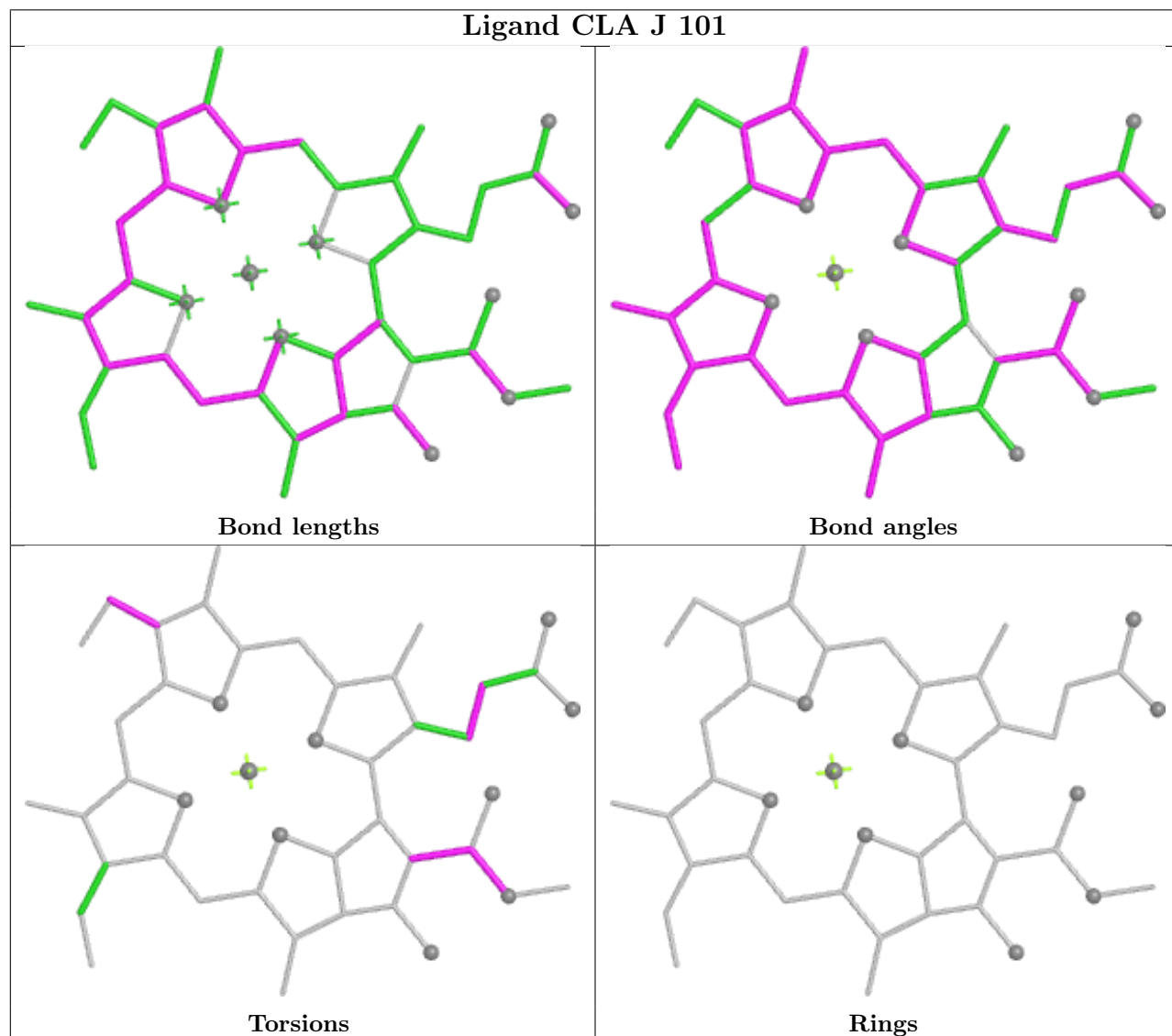
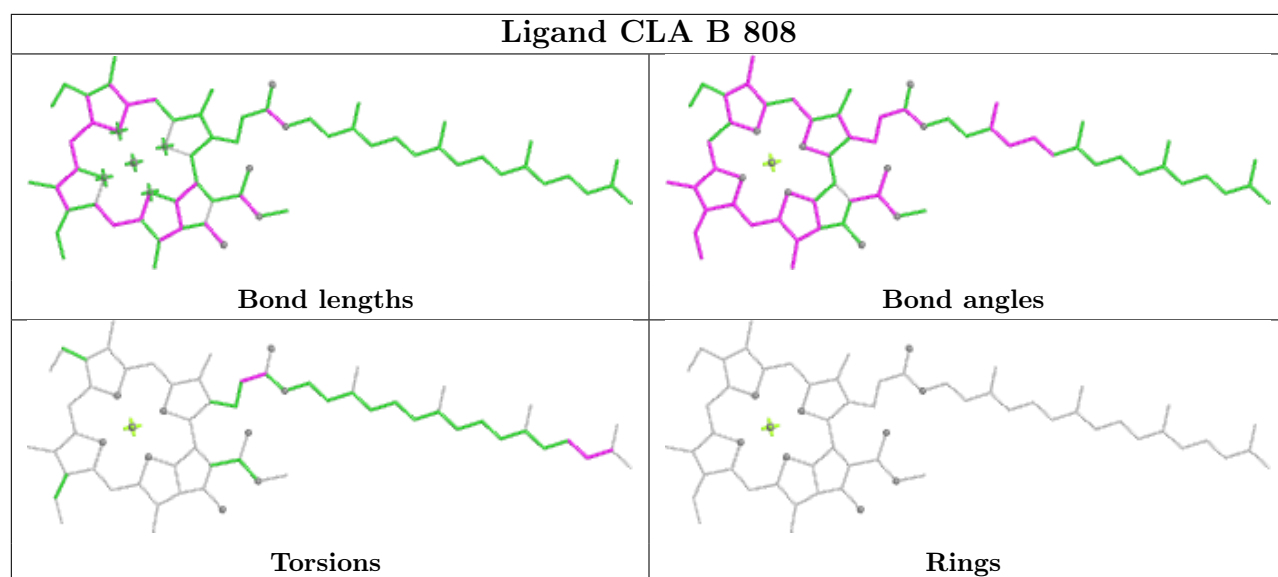


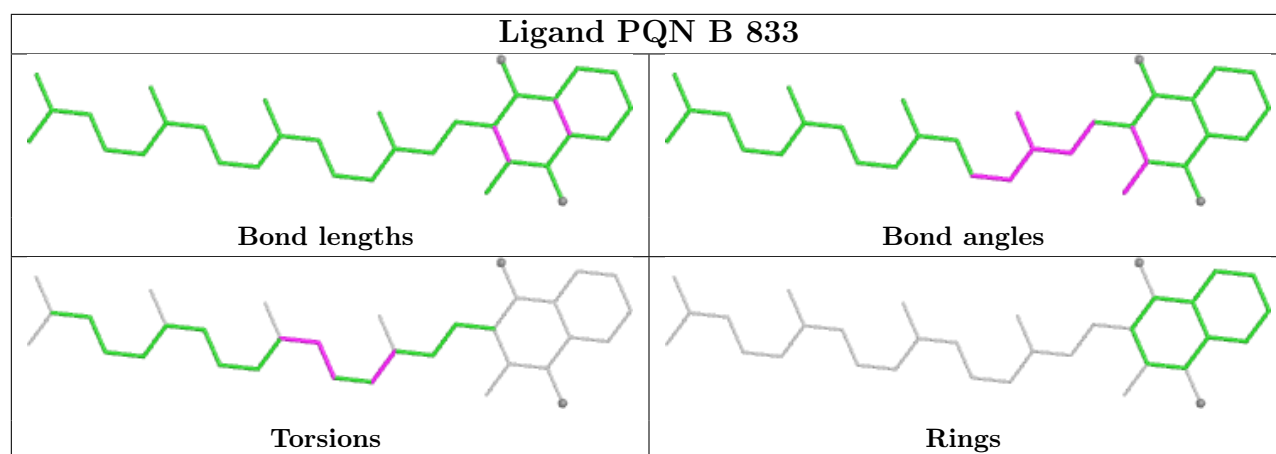
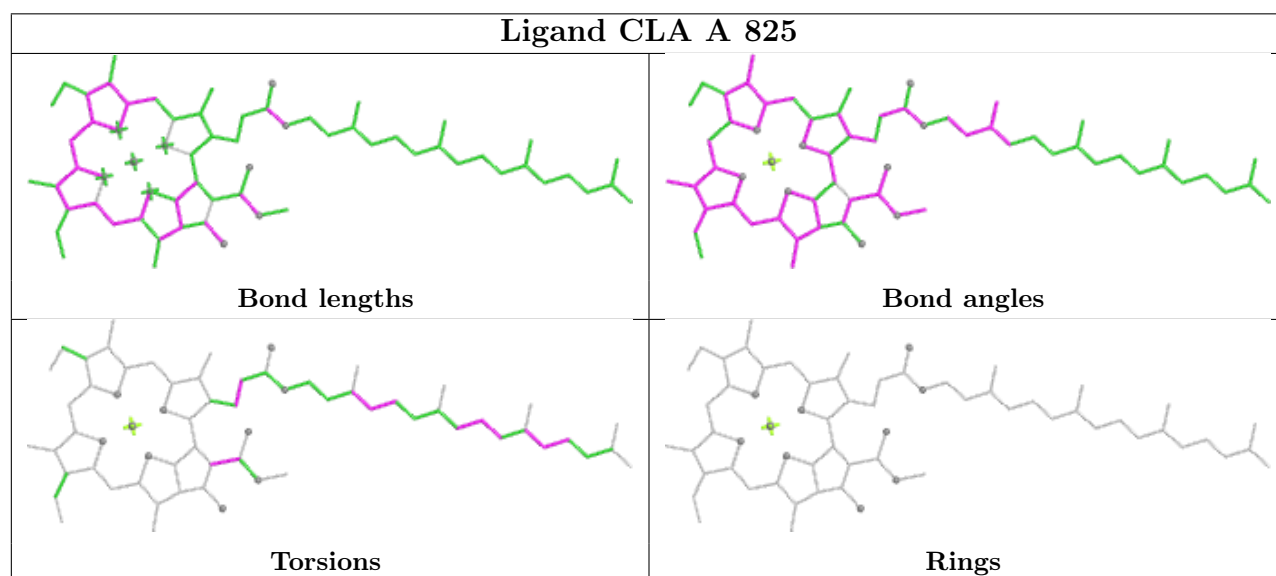
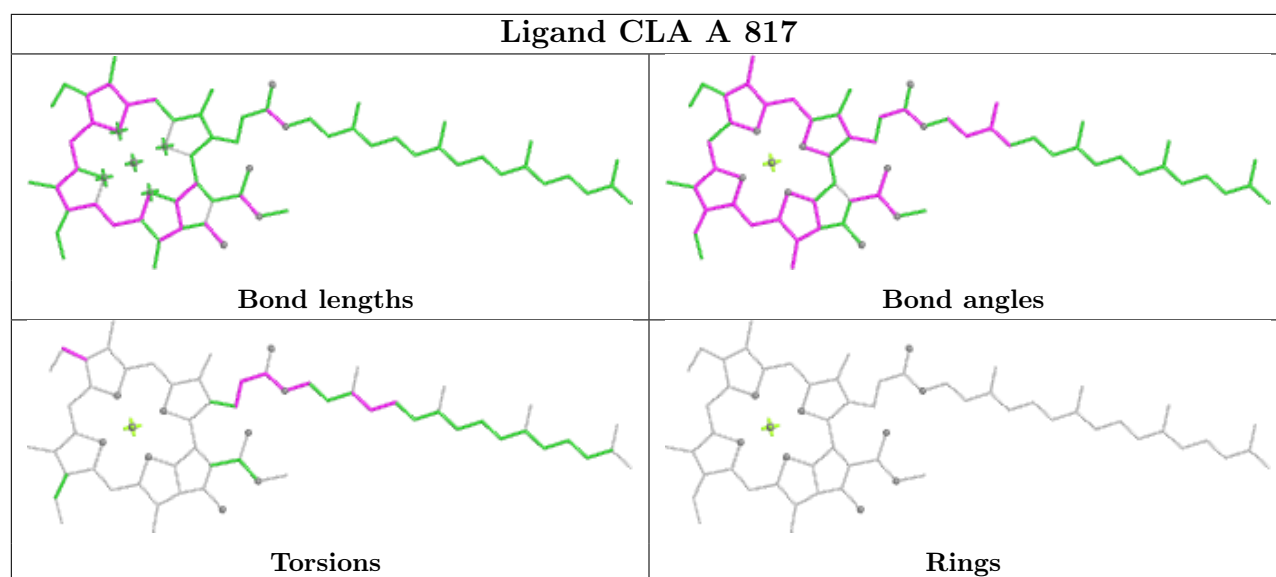


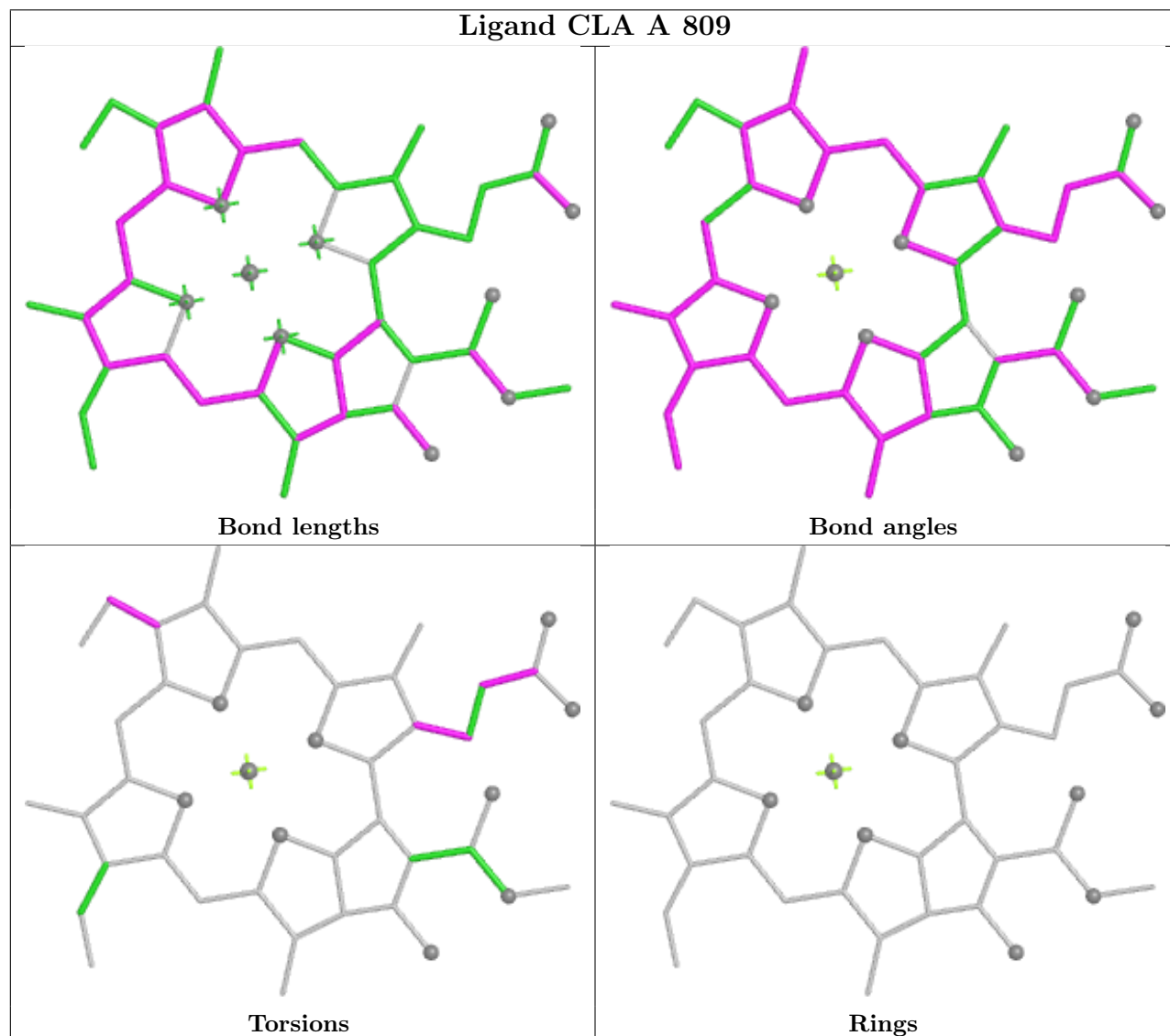
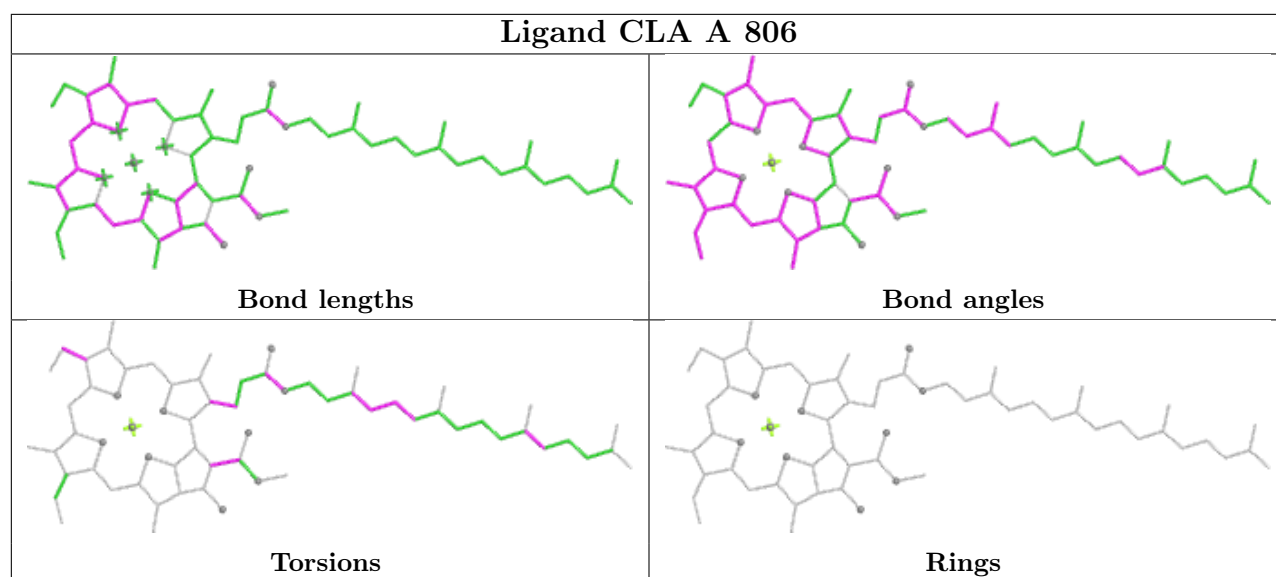


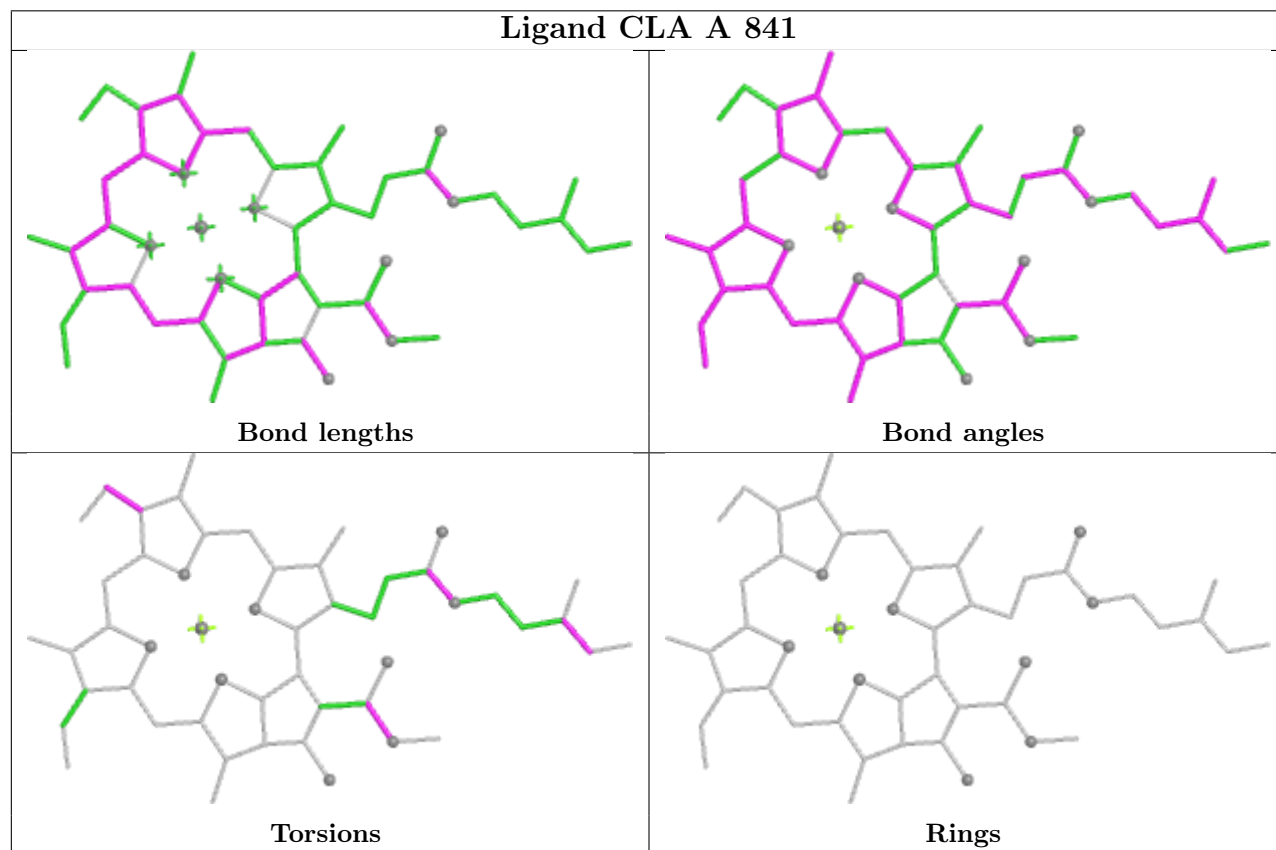
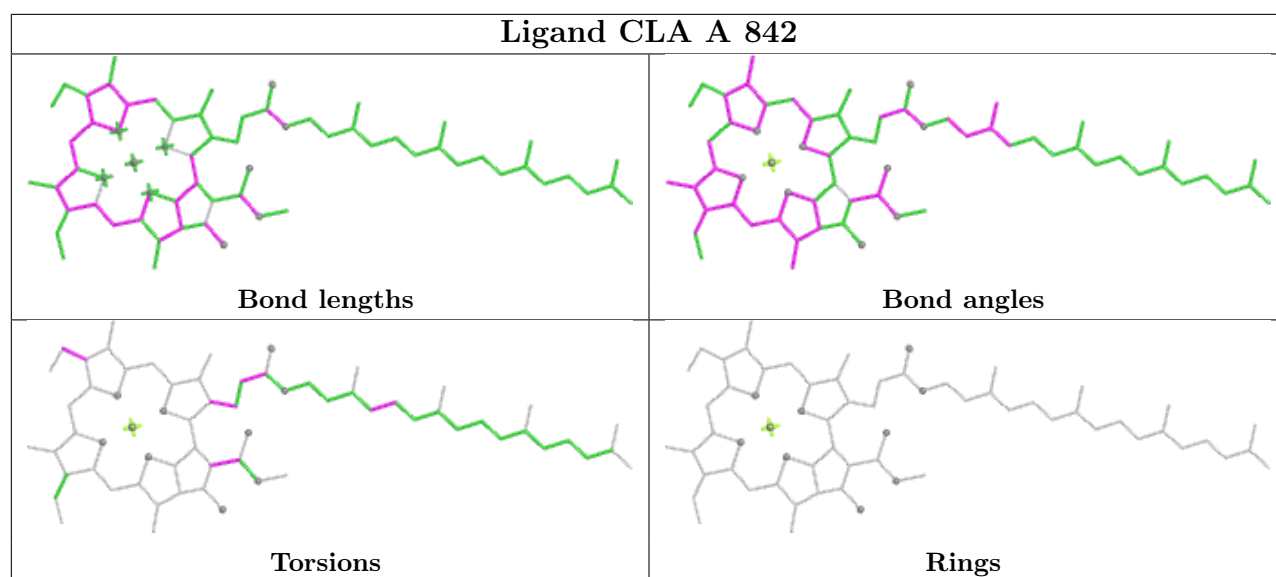




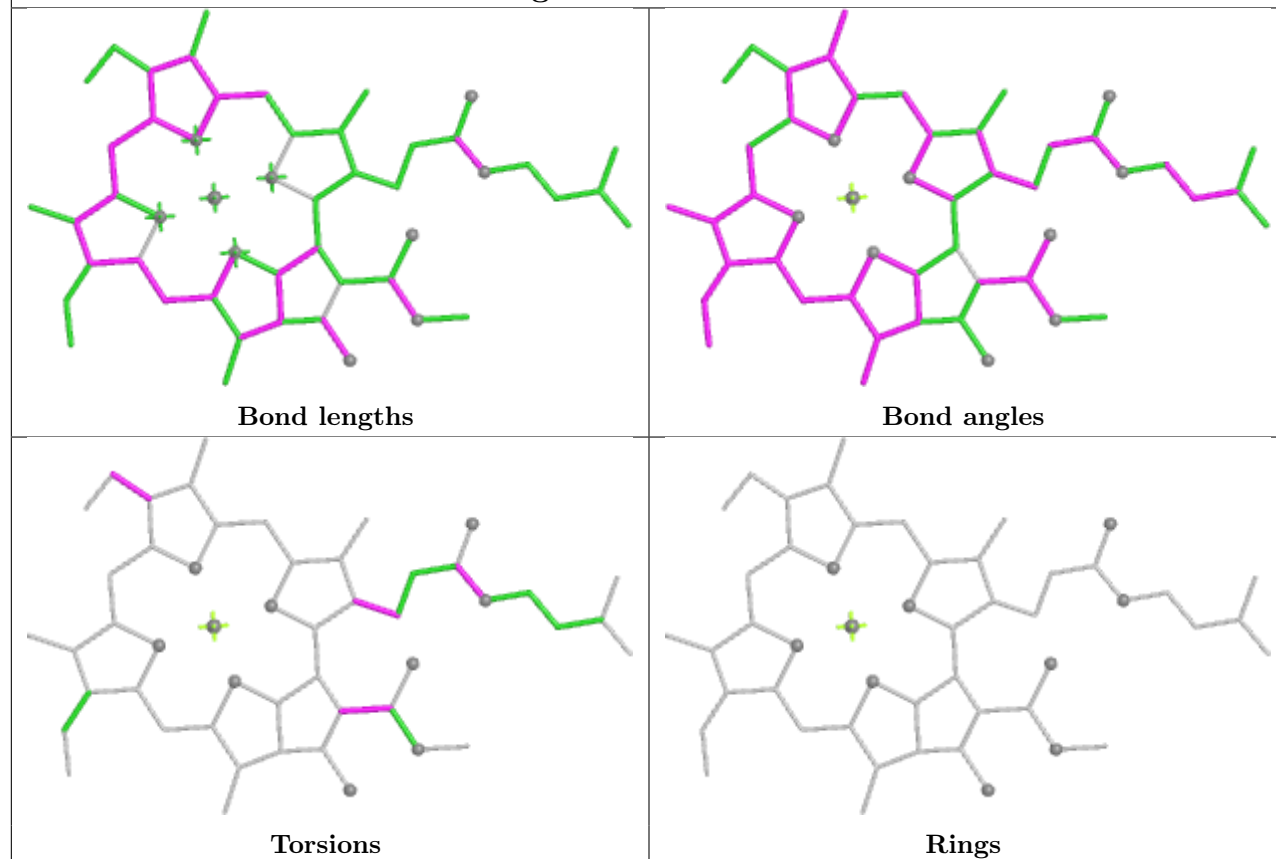




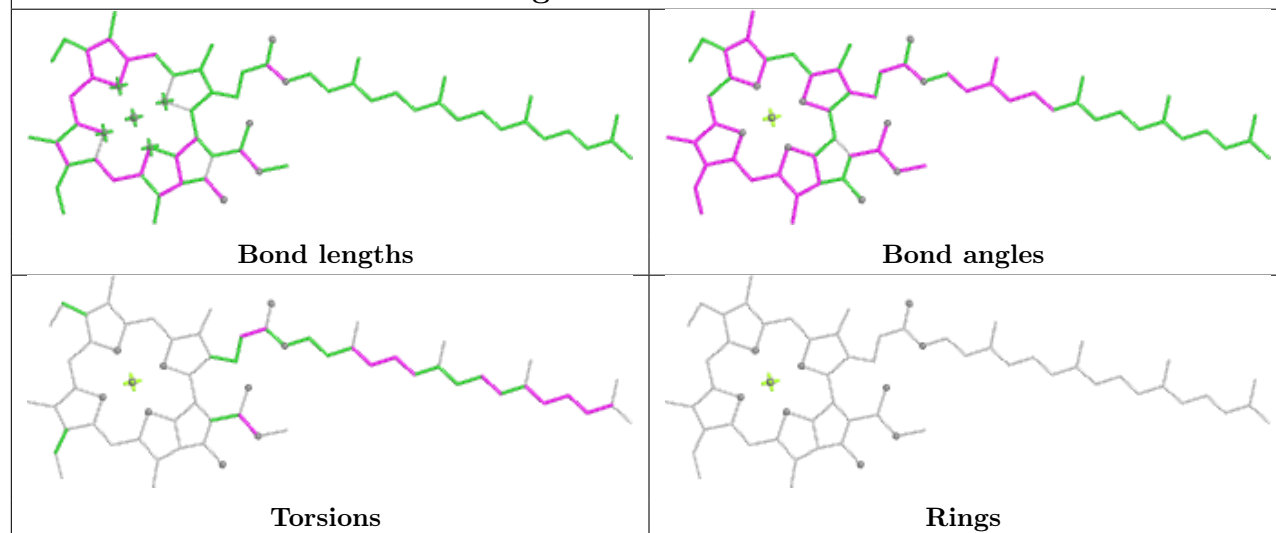


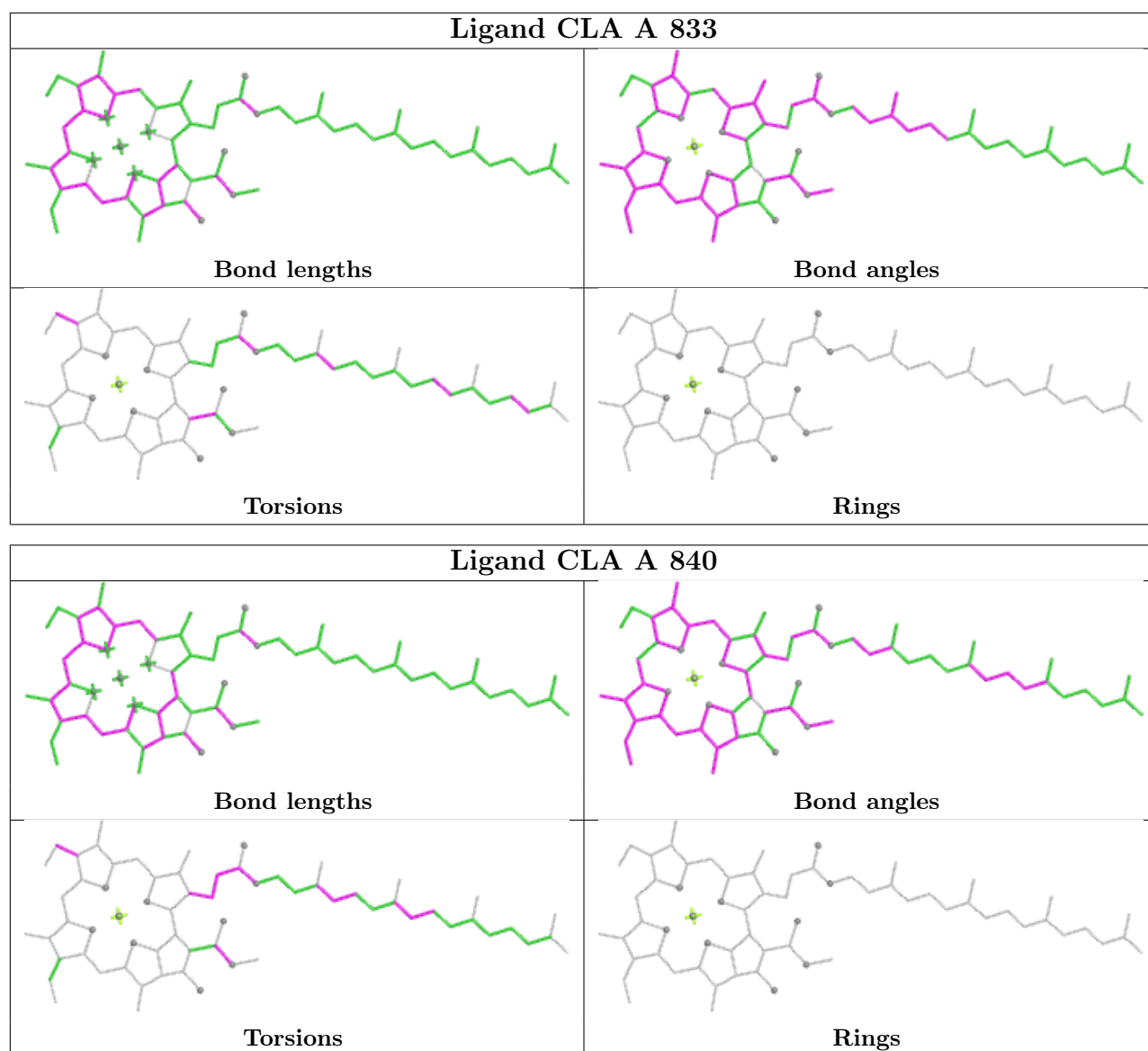


Ligand CLA A 831

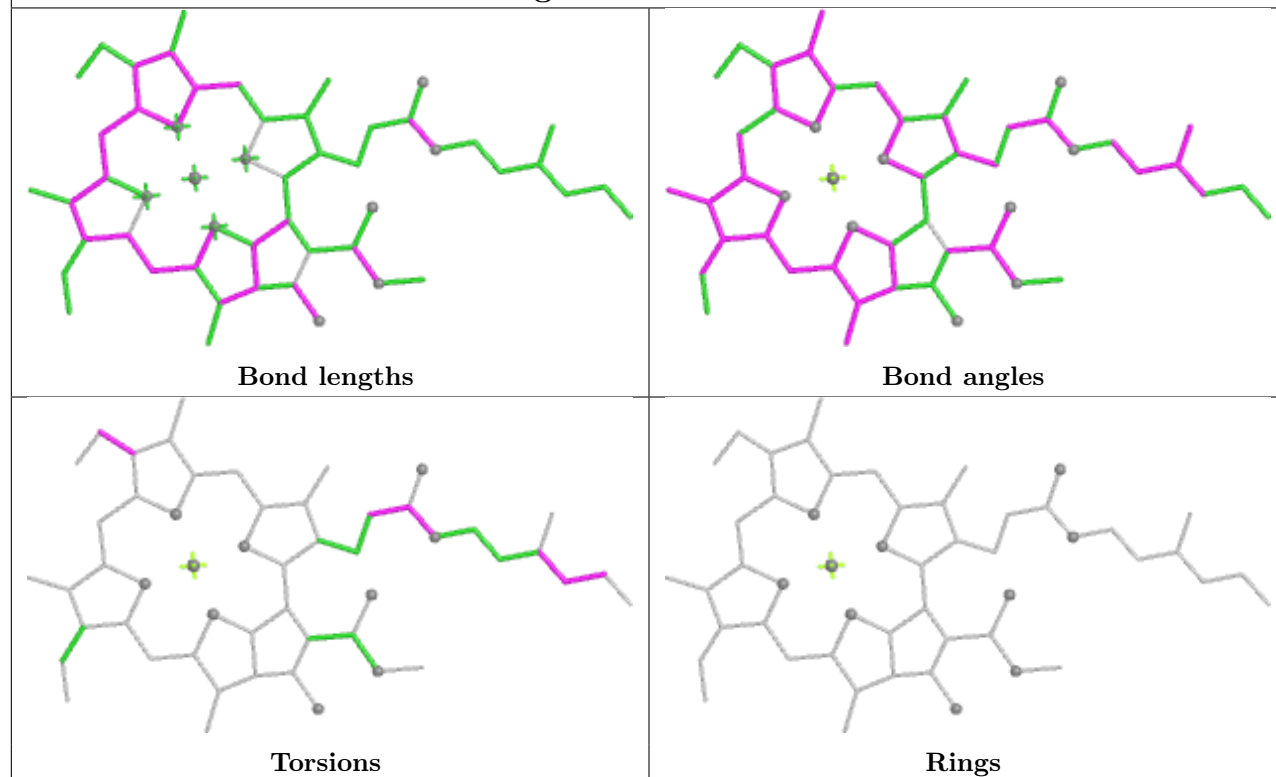


Ligand CLA B 807

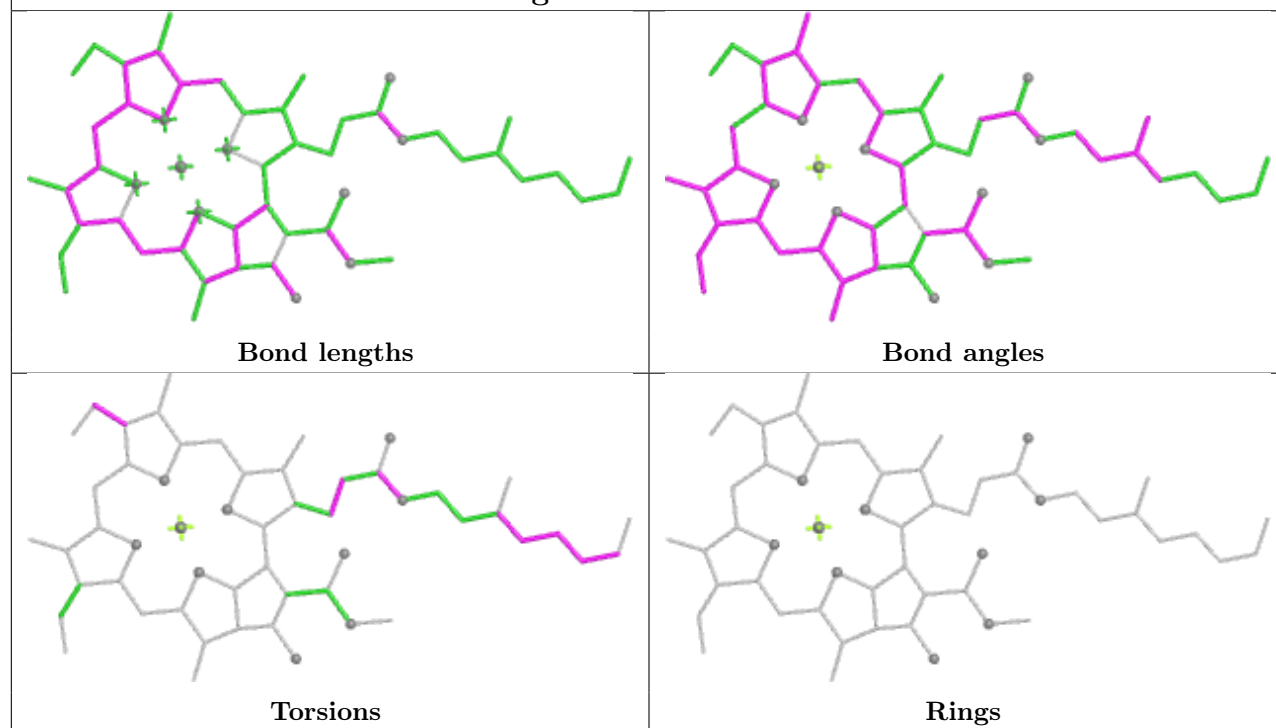




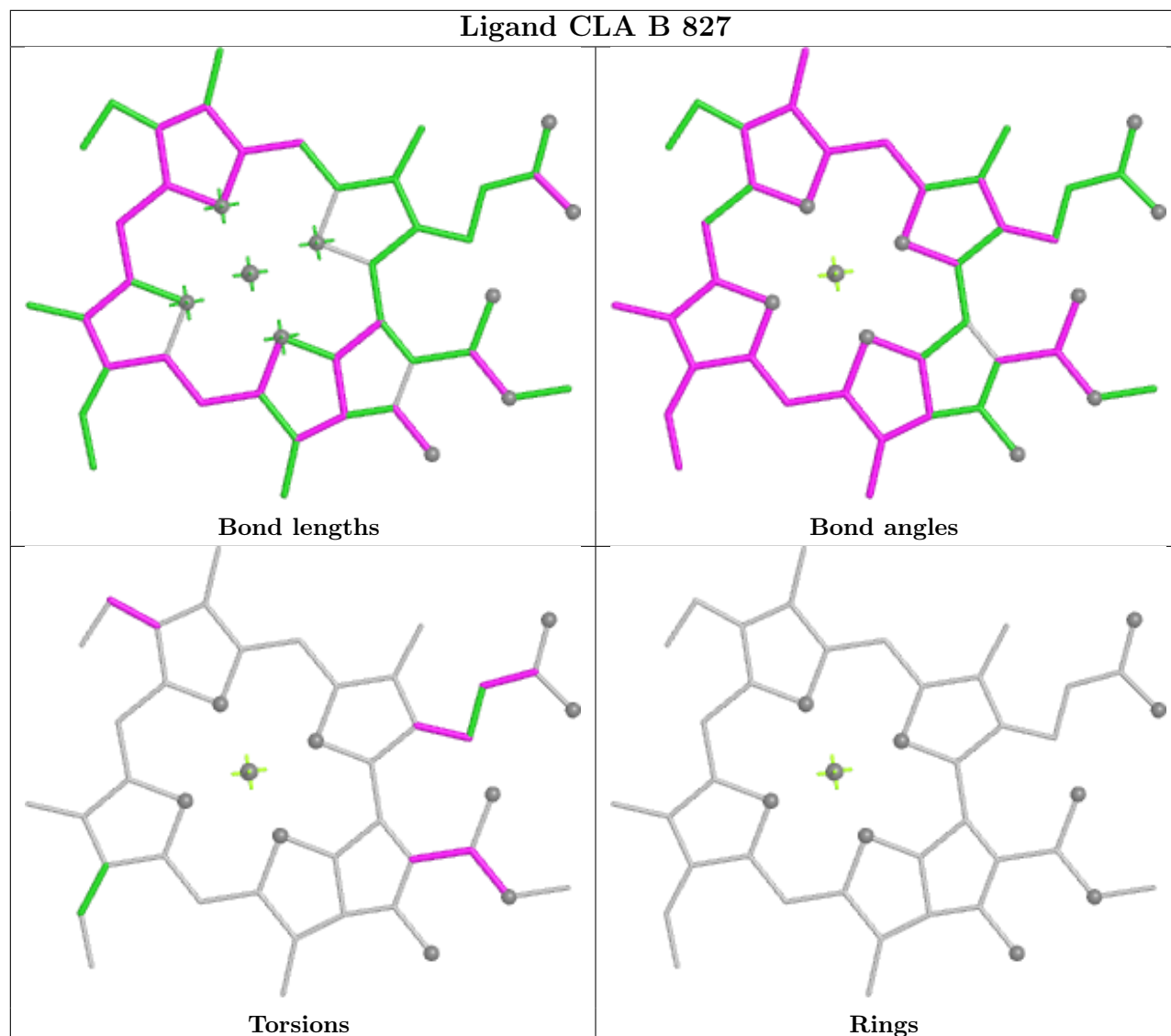
Ligand CLA L 204



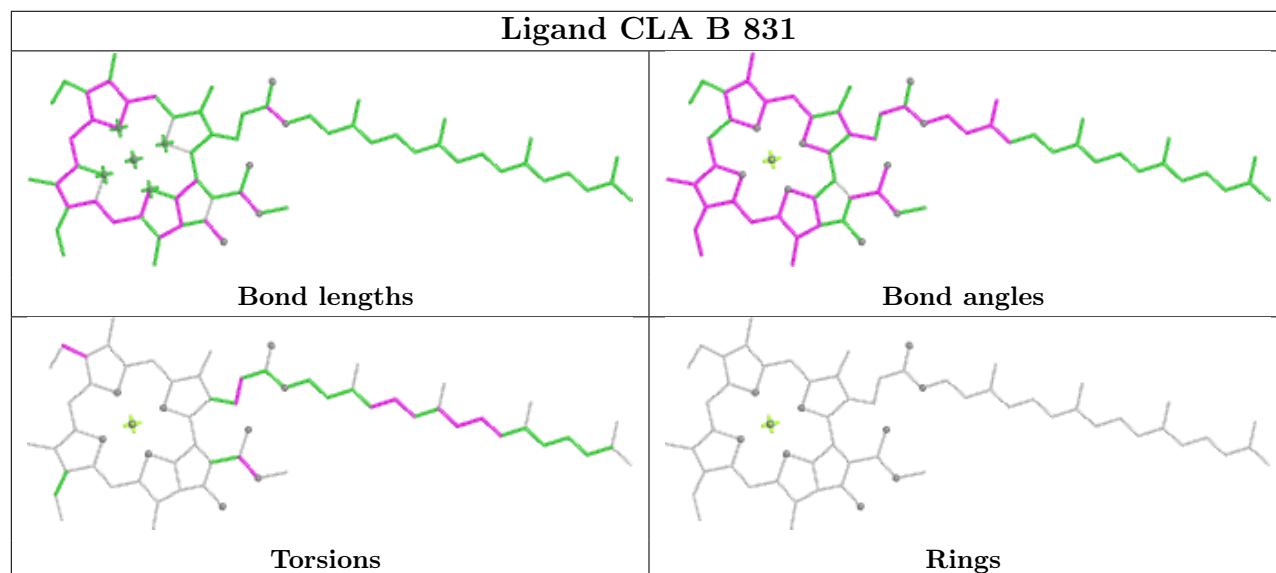
Ligand CLA A 812

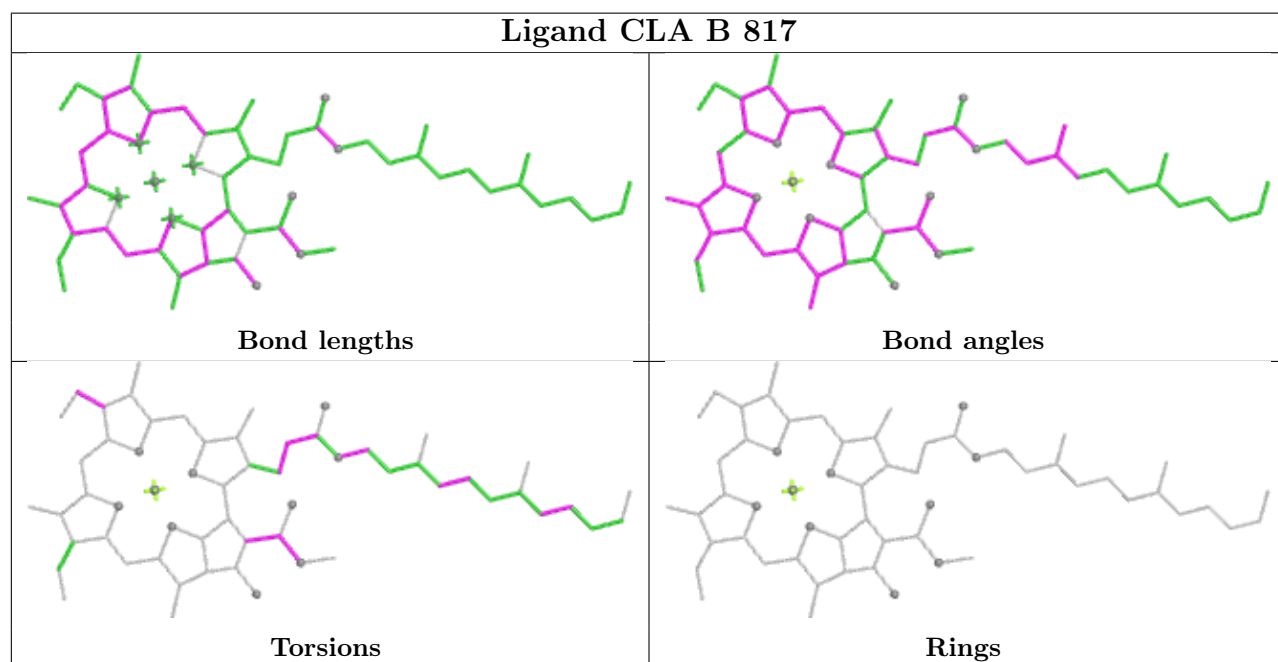
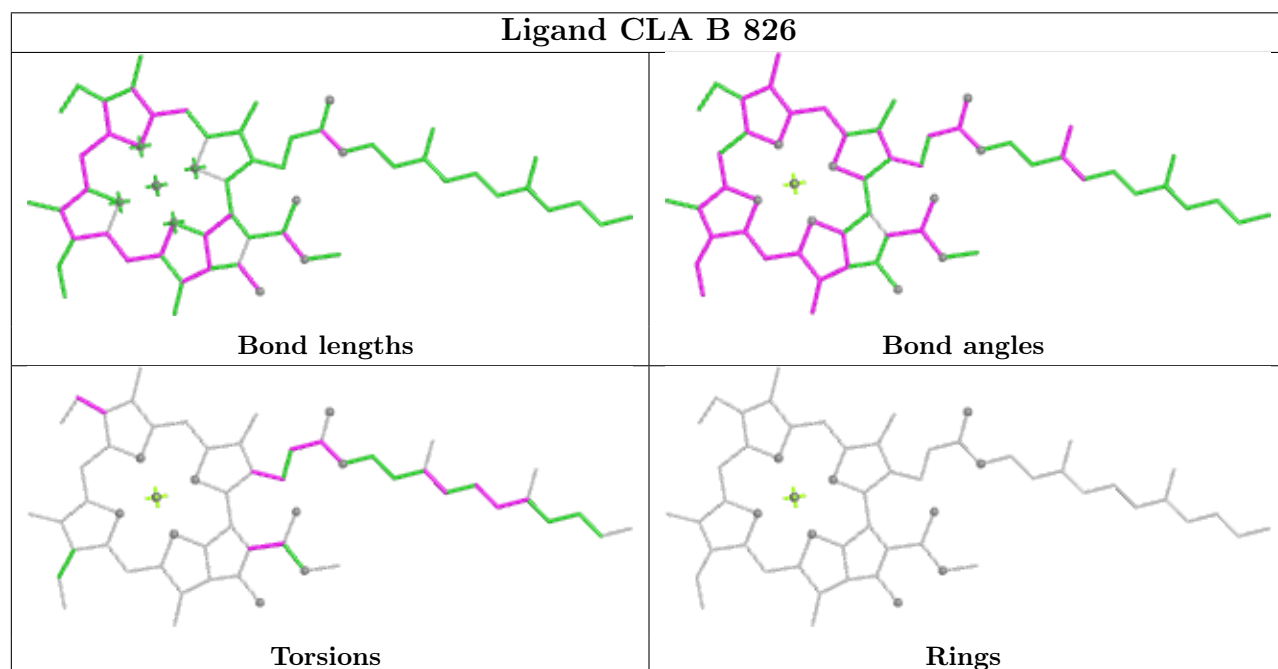
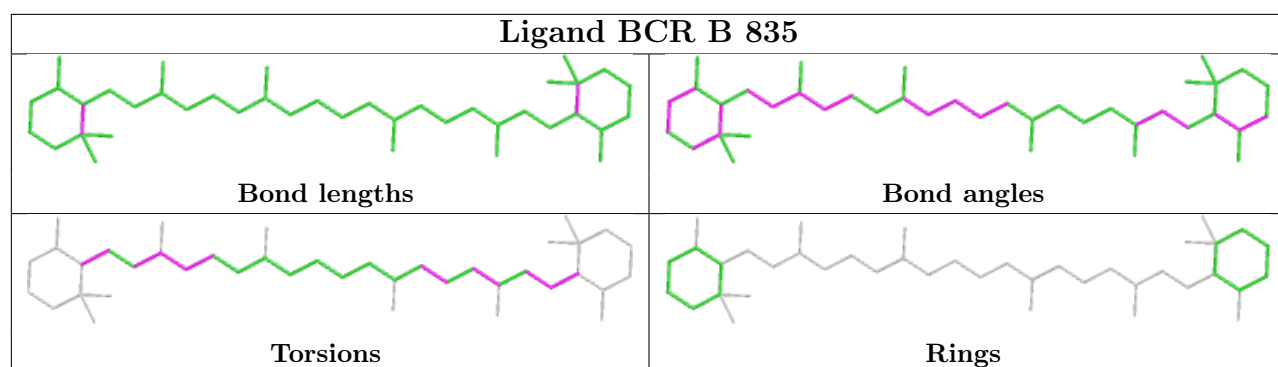


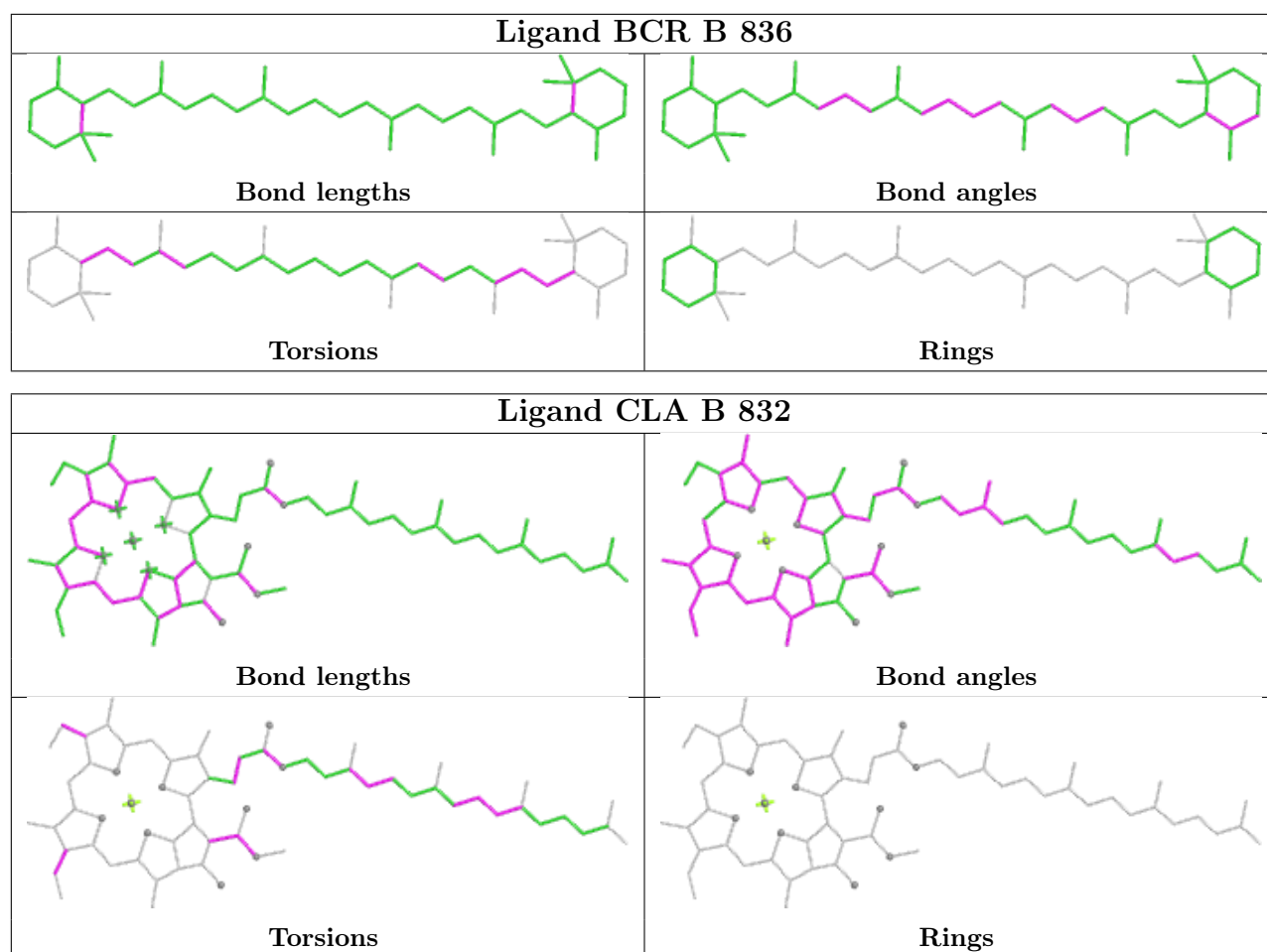
Ligand CLA B 827

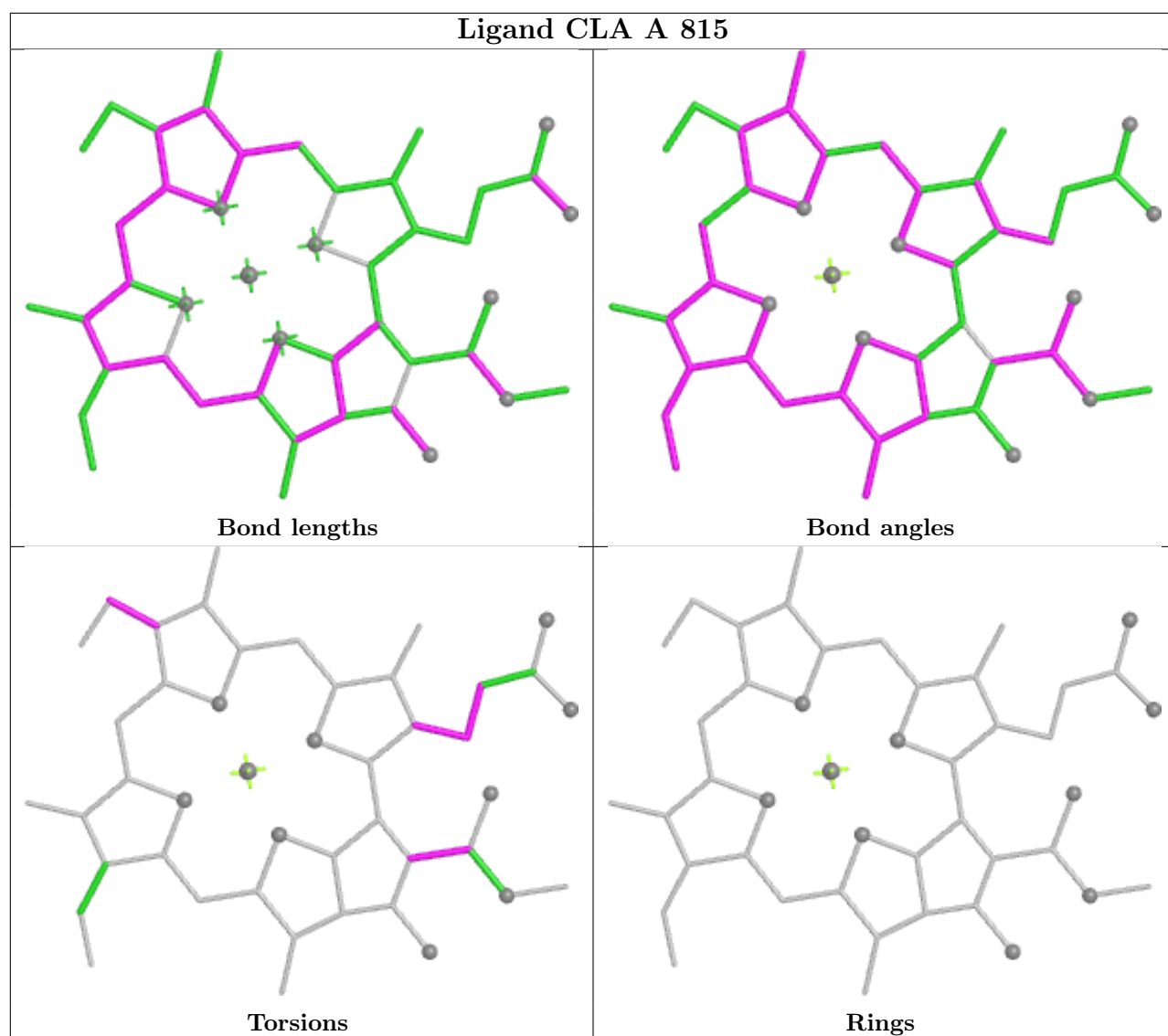


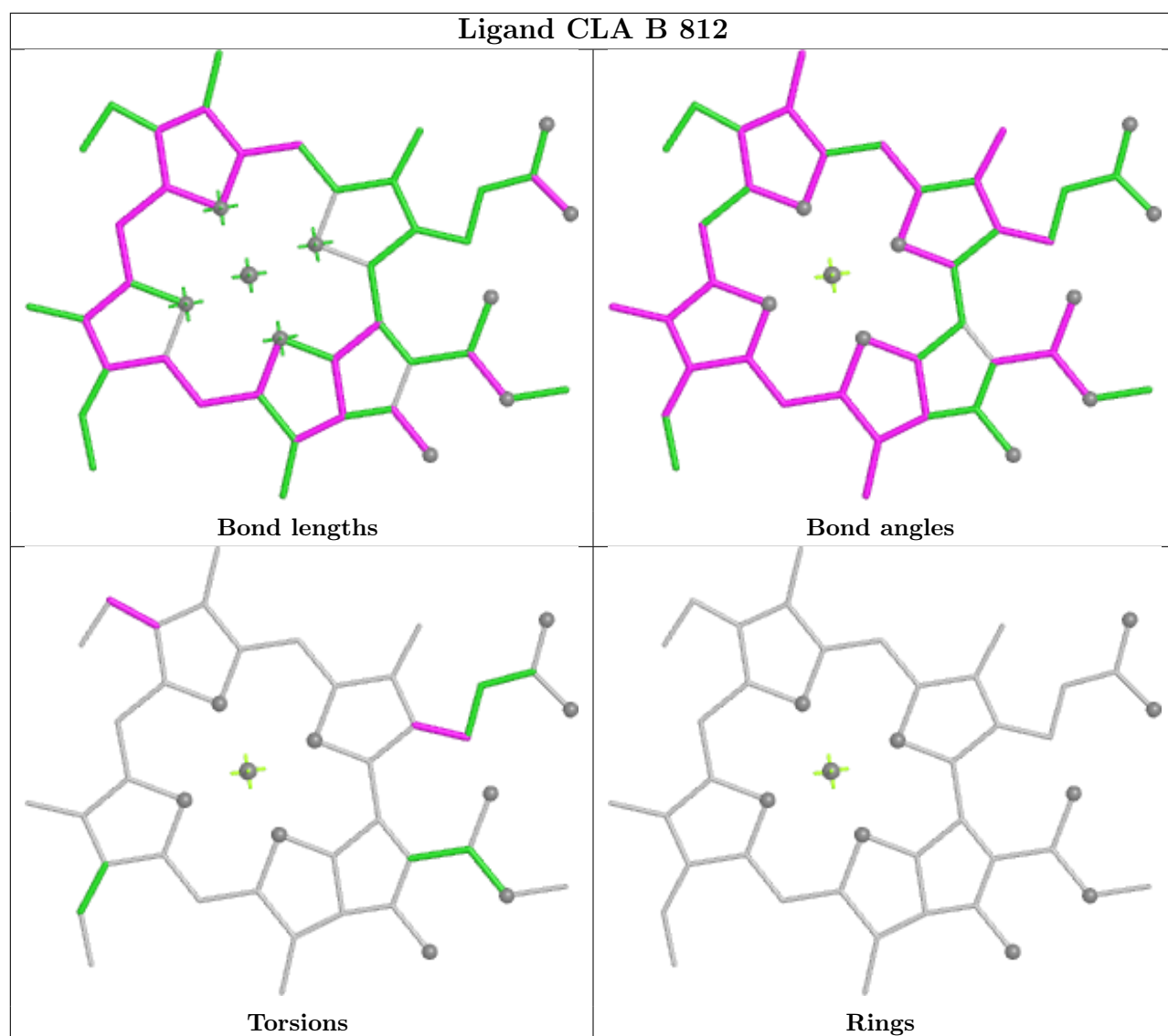
Ligand CLA B 831



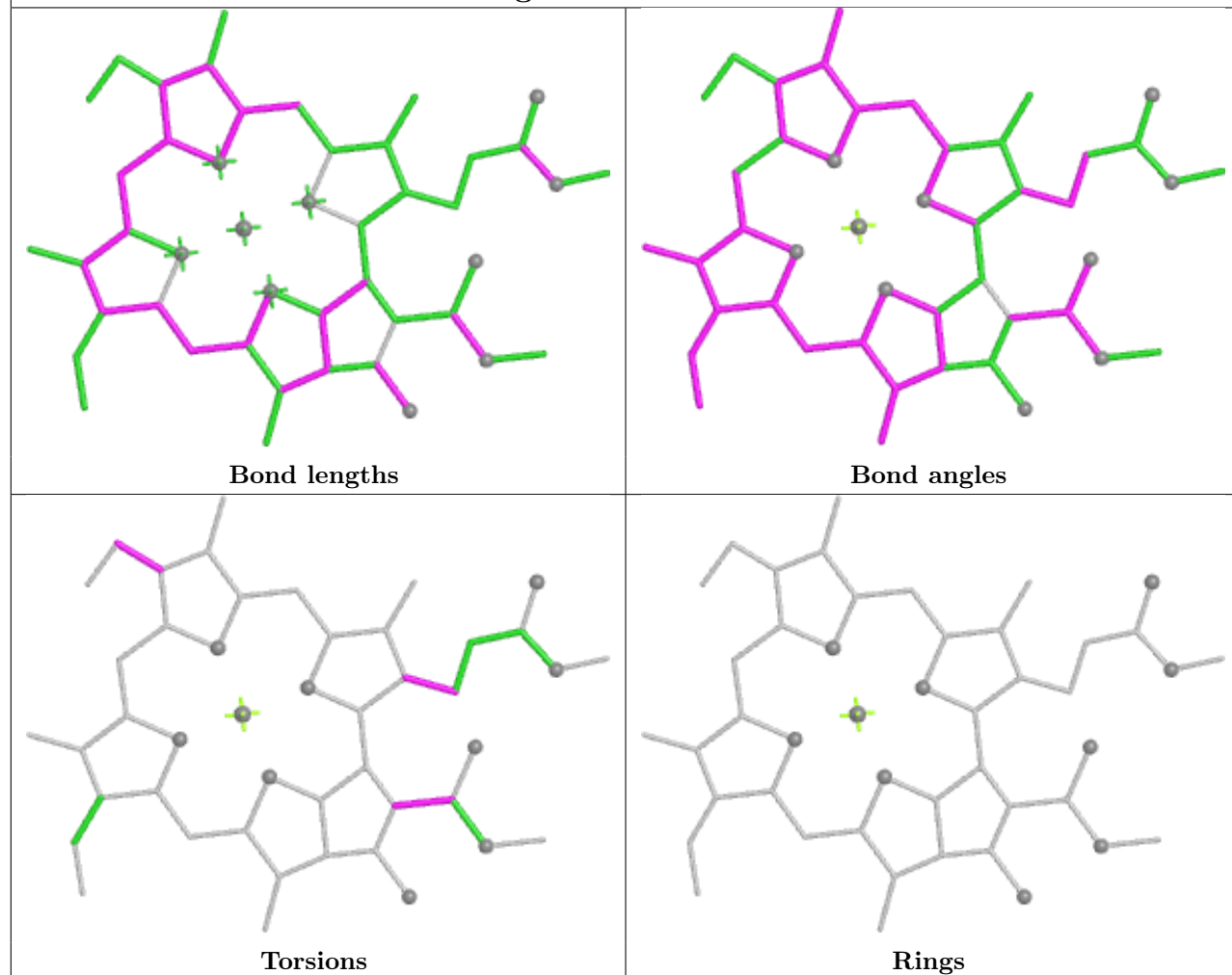


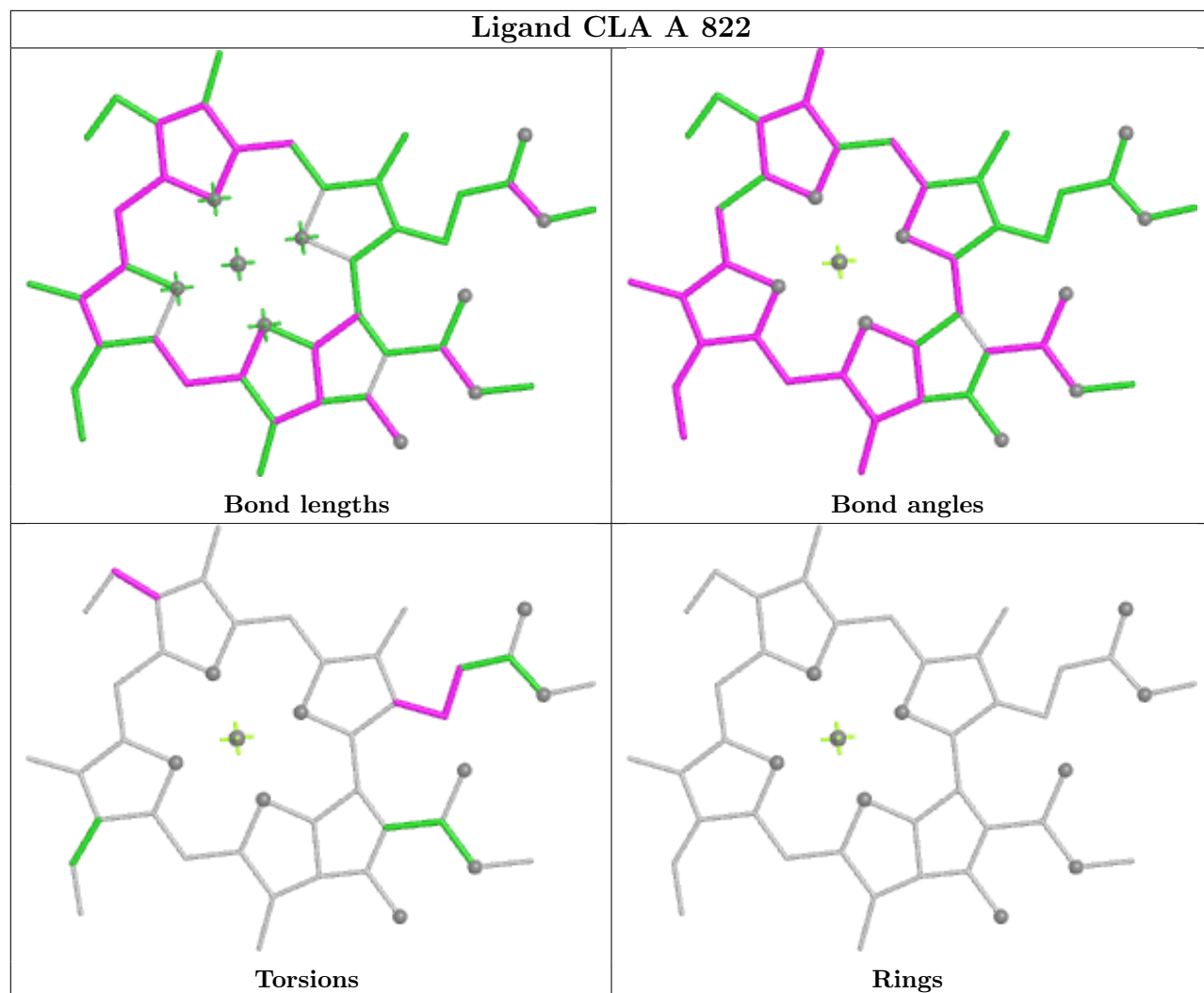


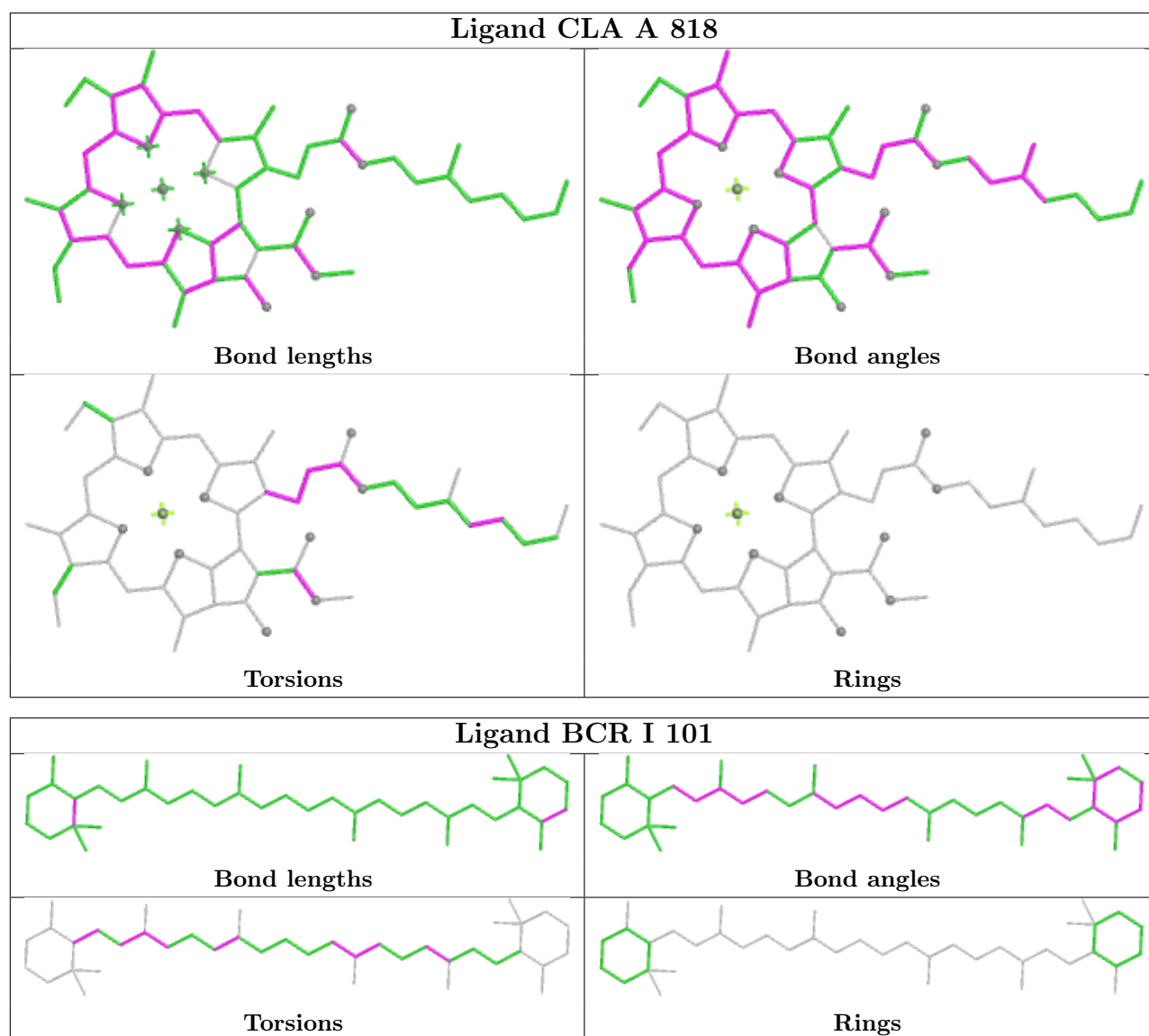


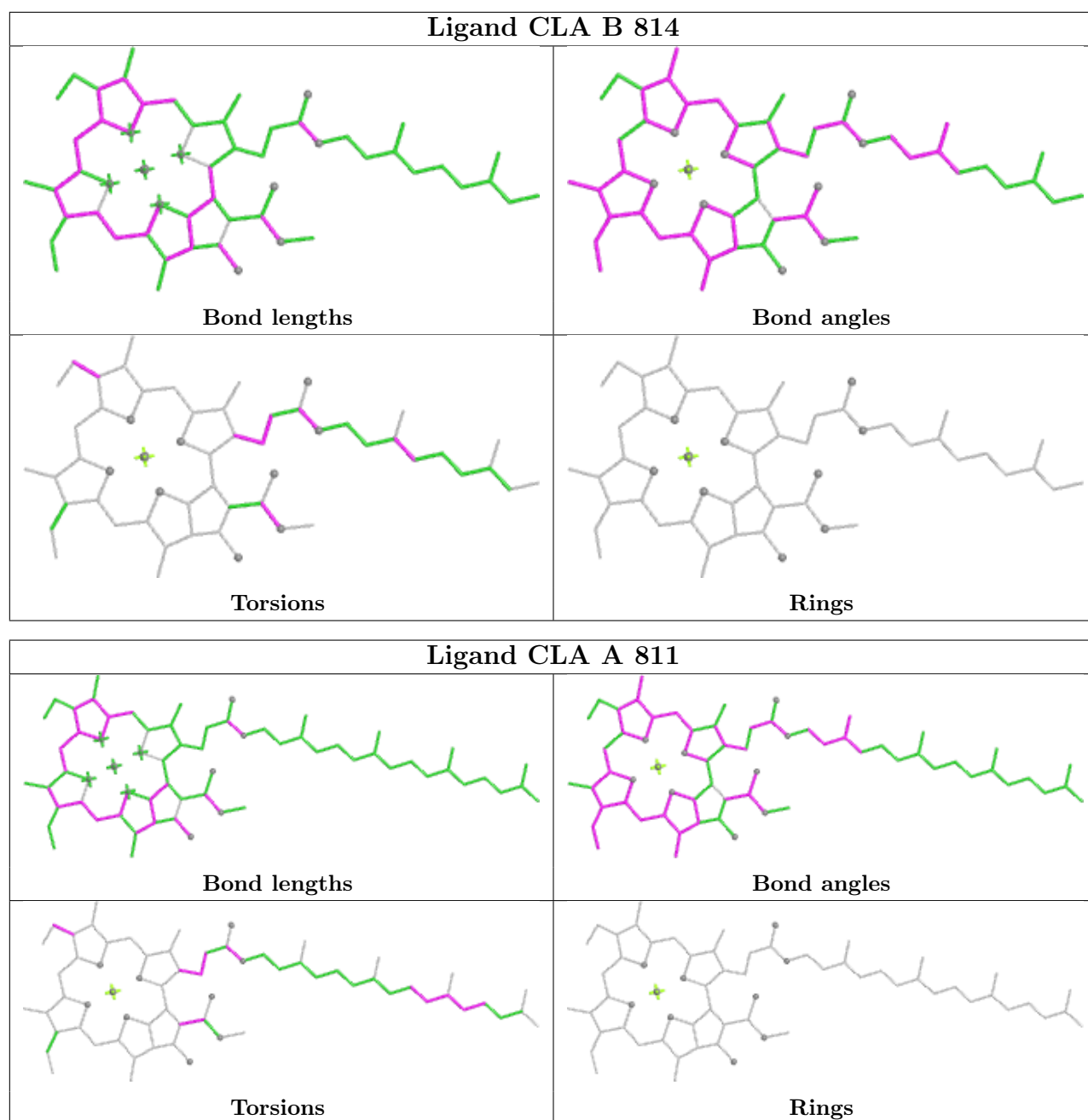


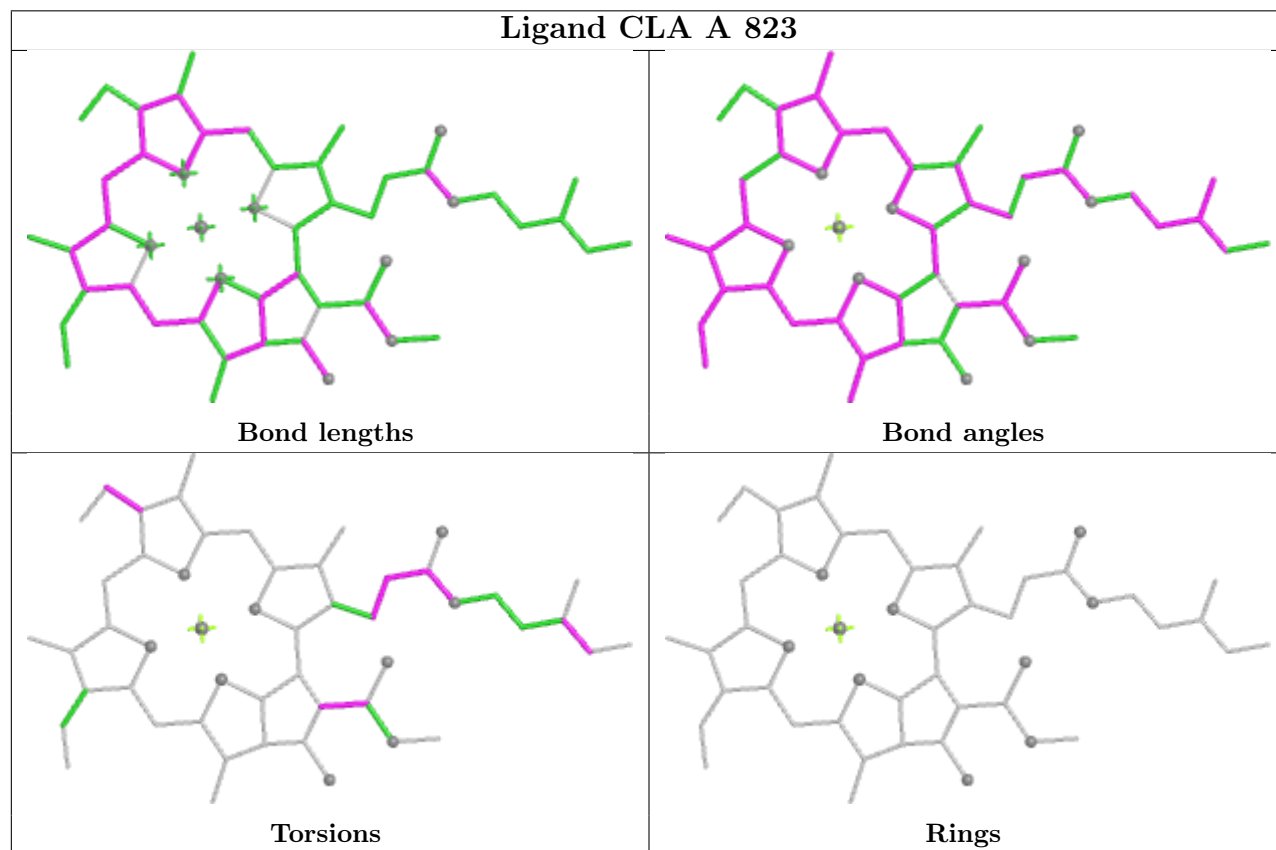
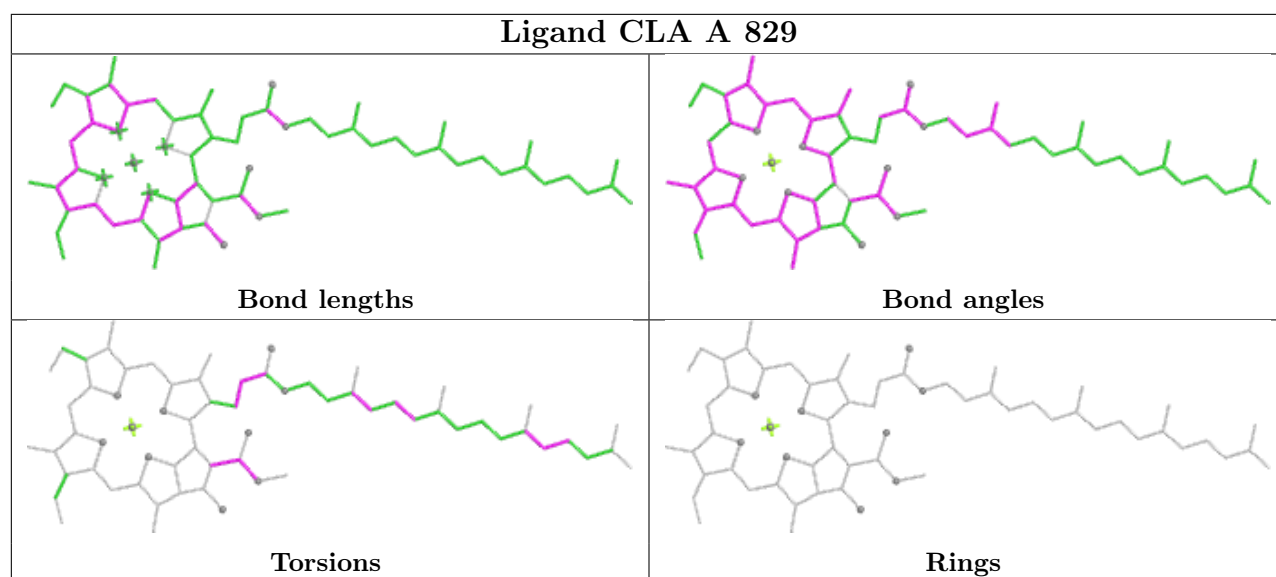
Ligand CLA L 202

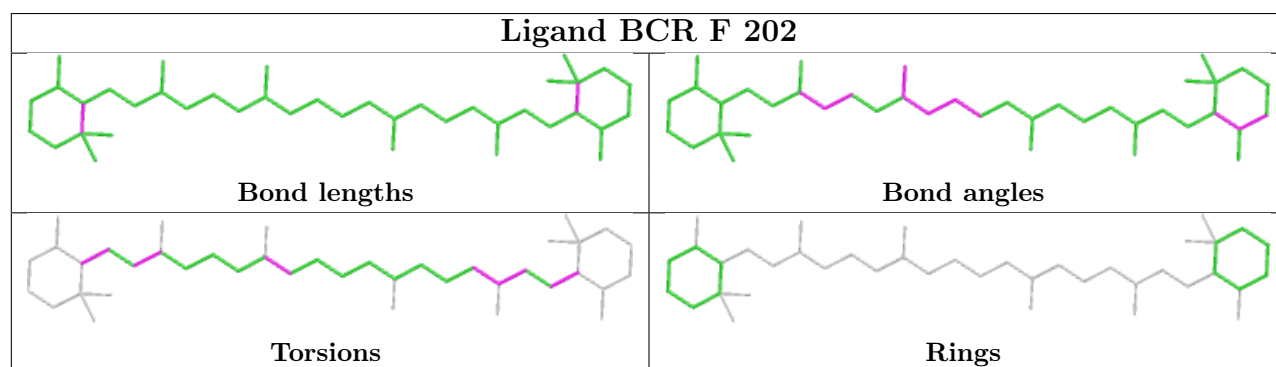
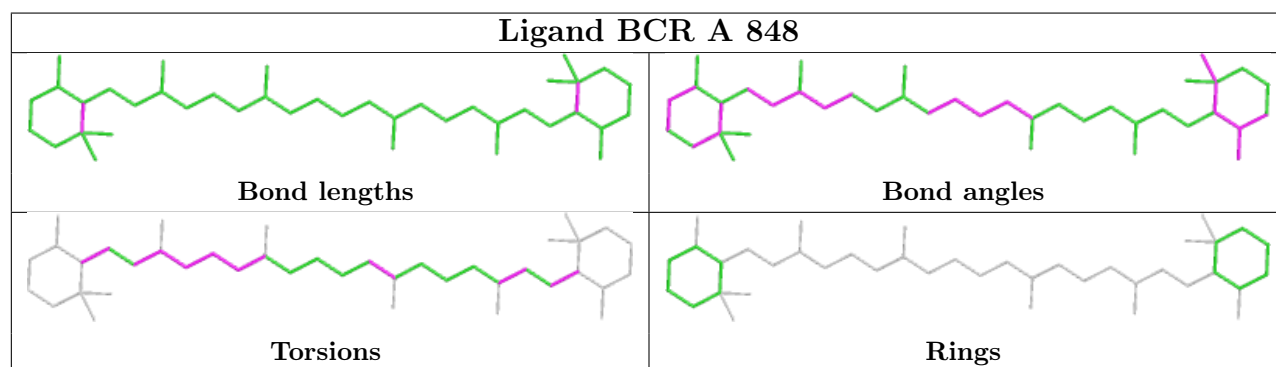
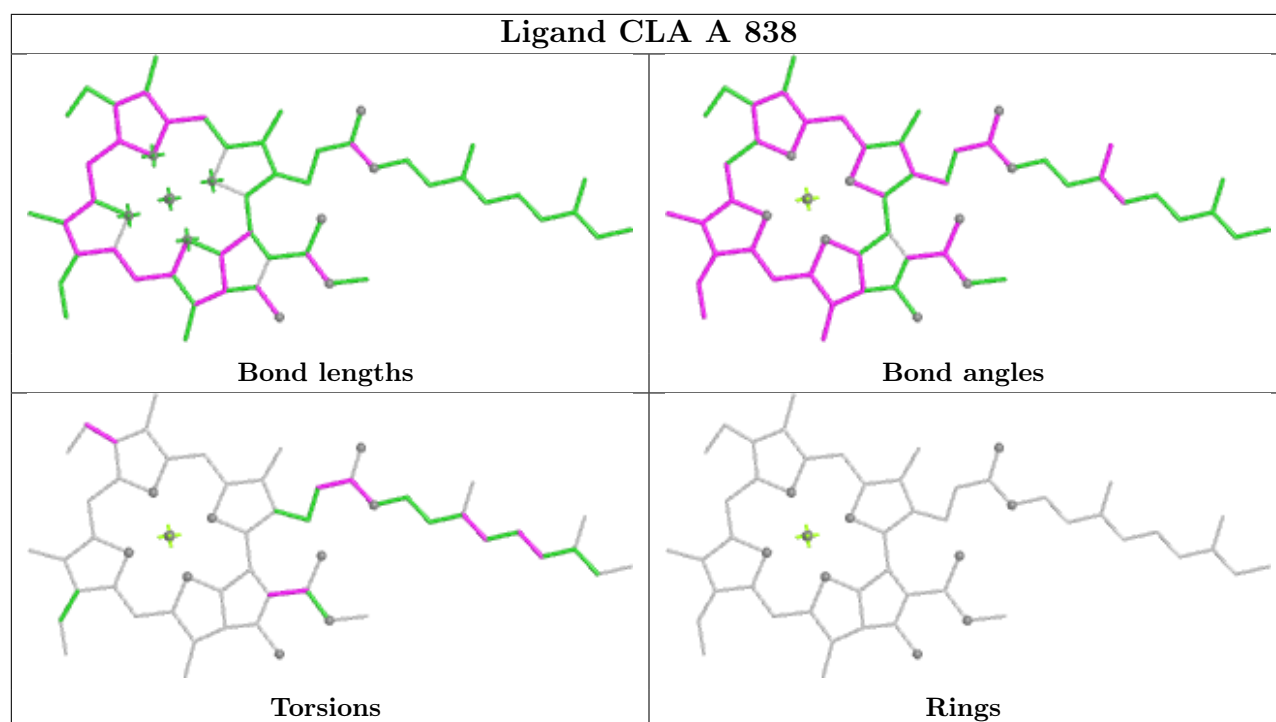


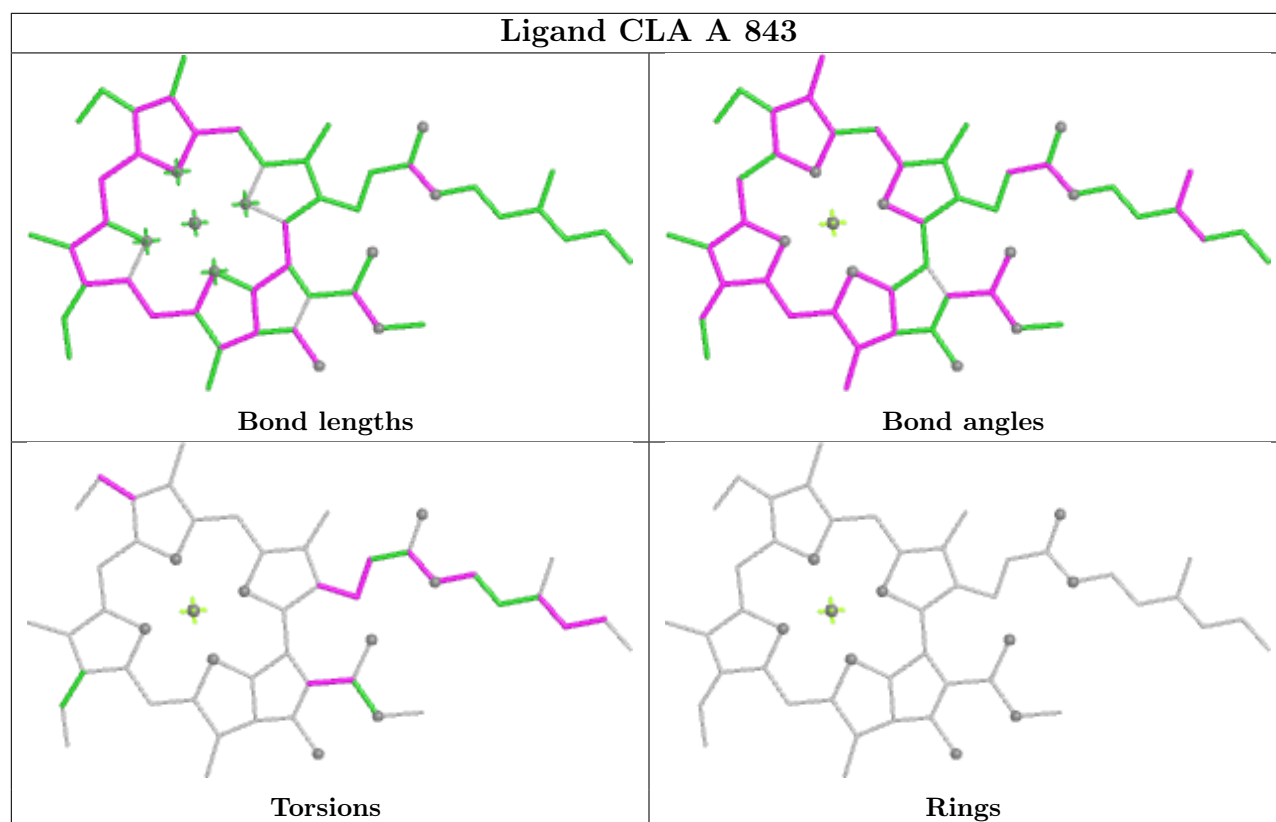
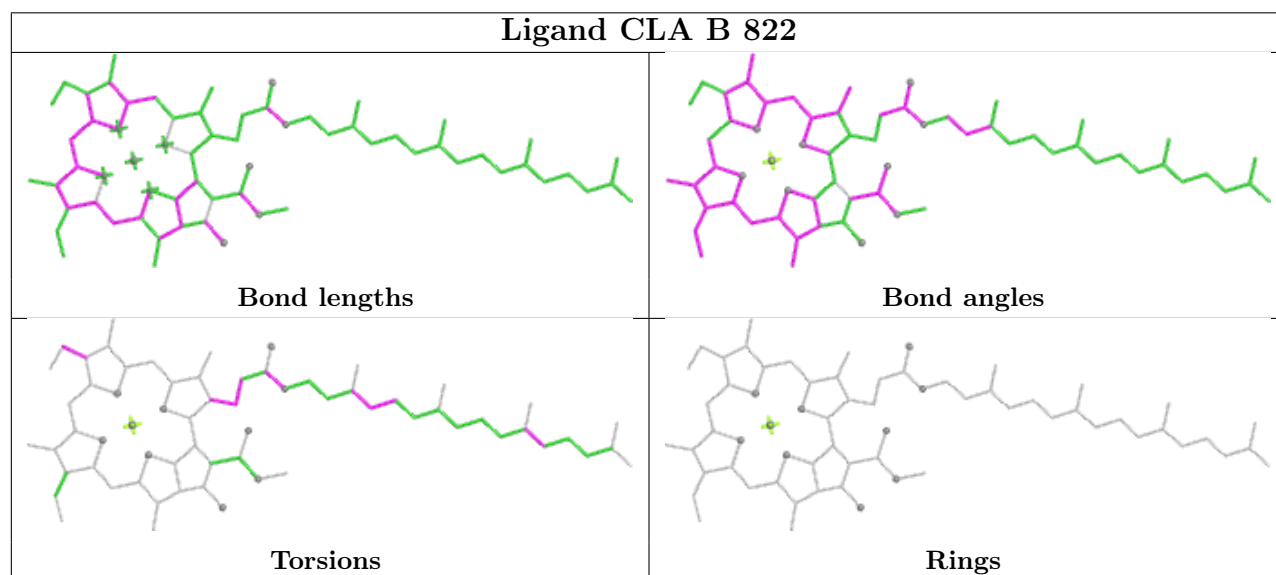
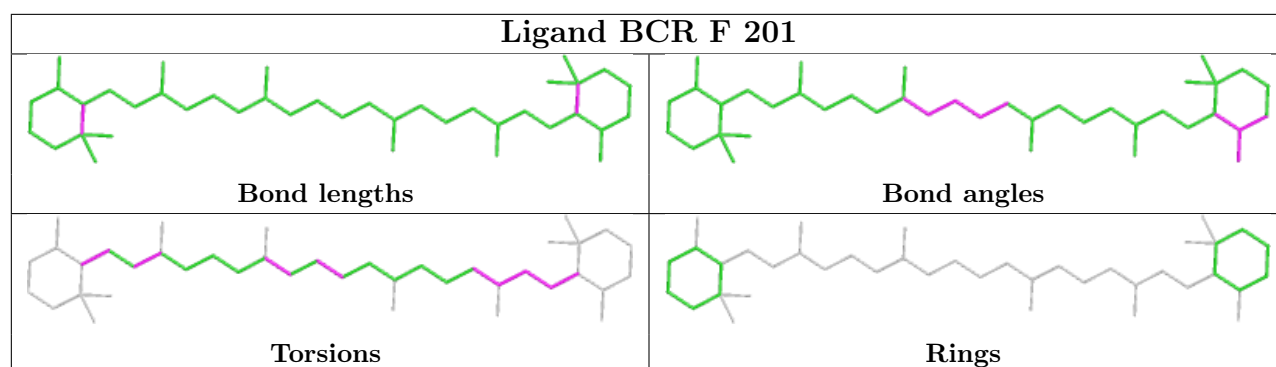


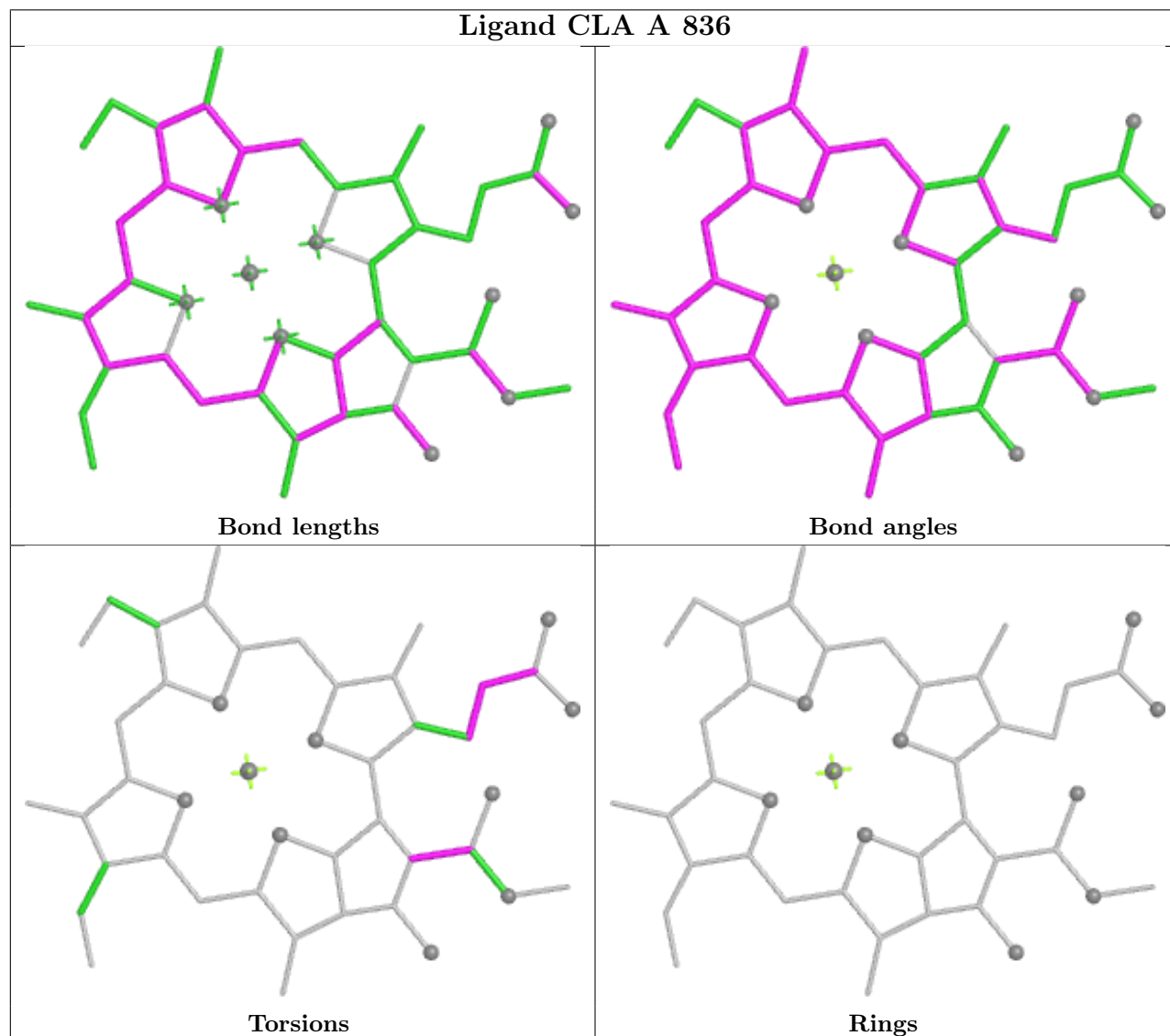
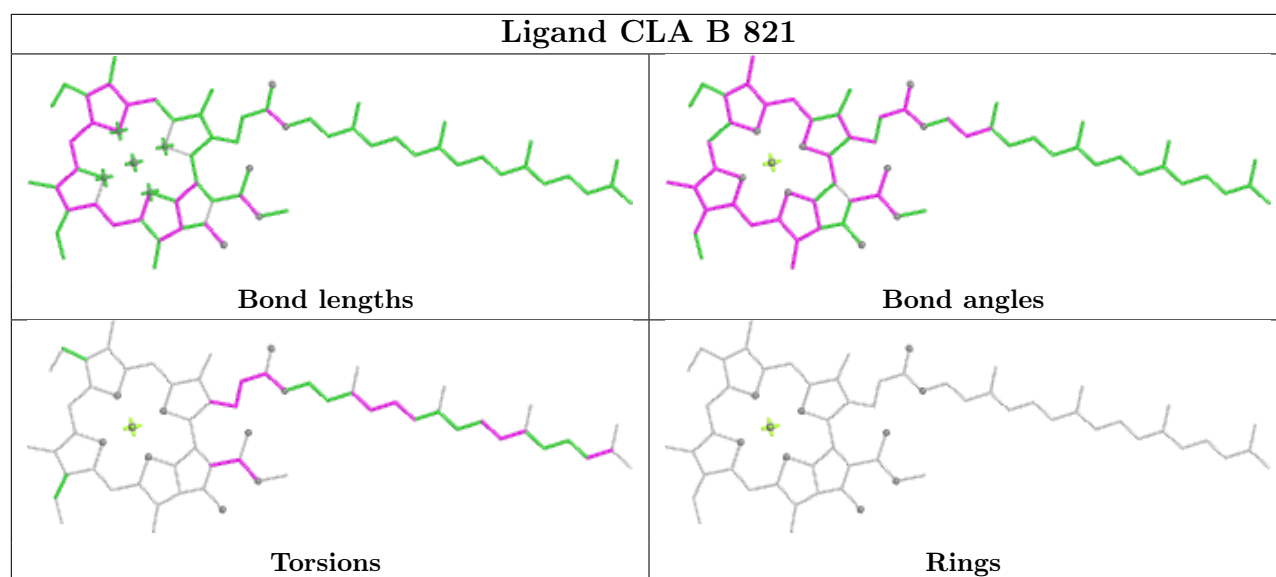


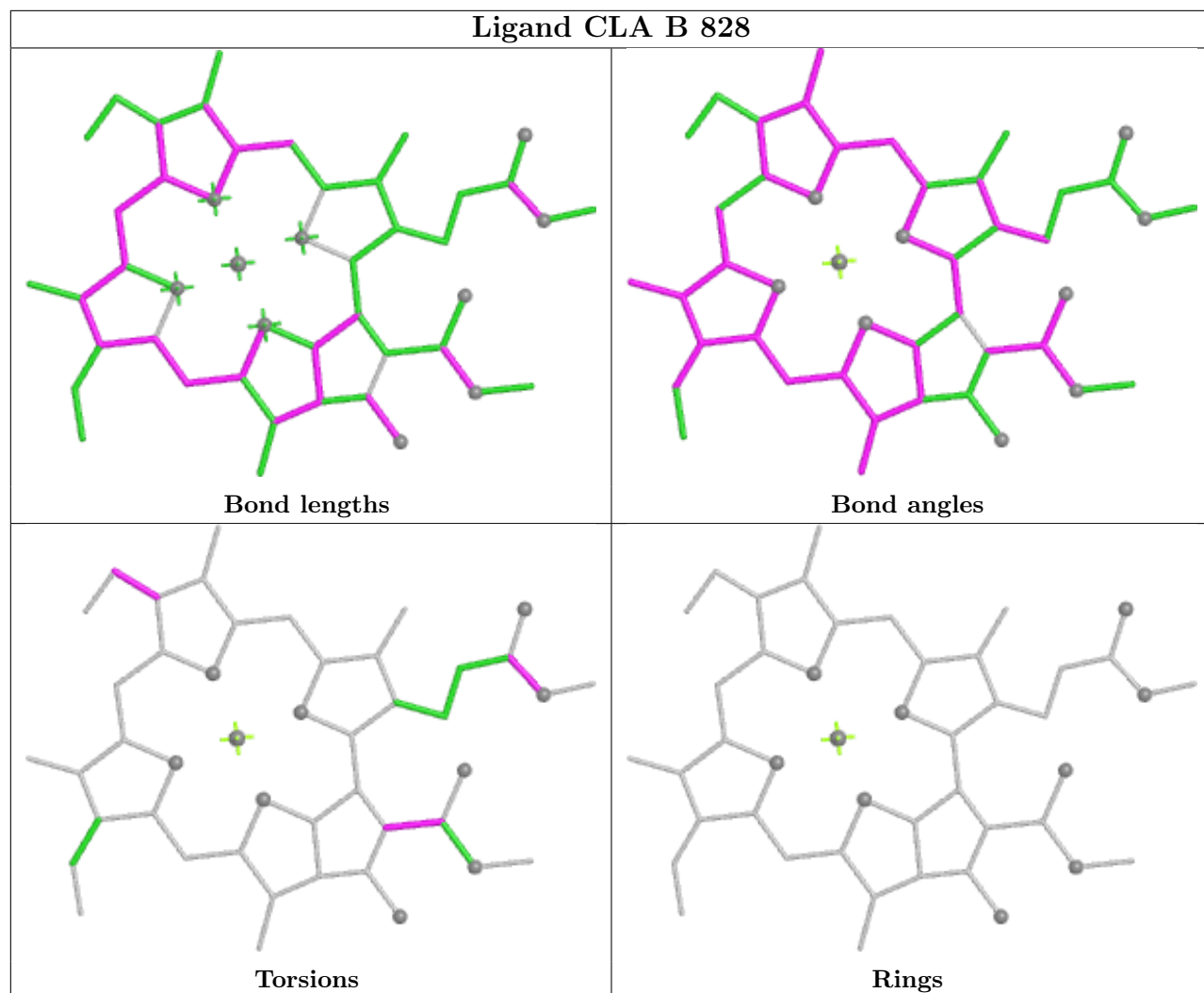


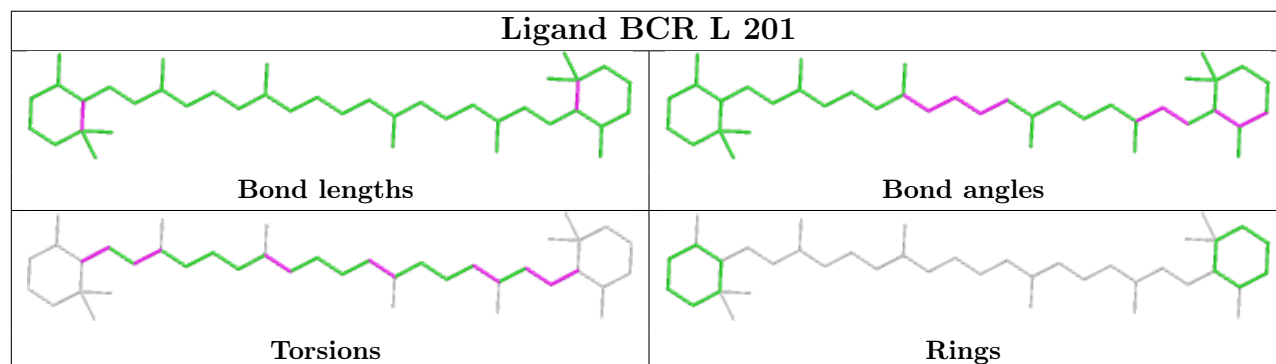
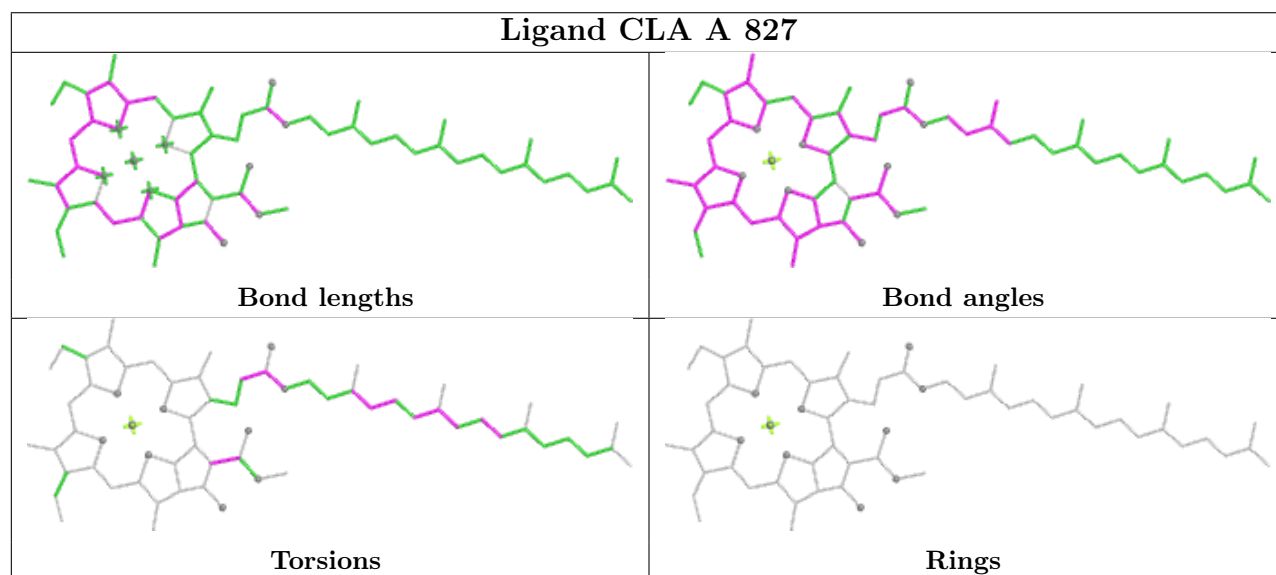
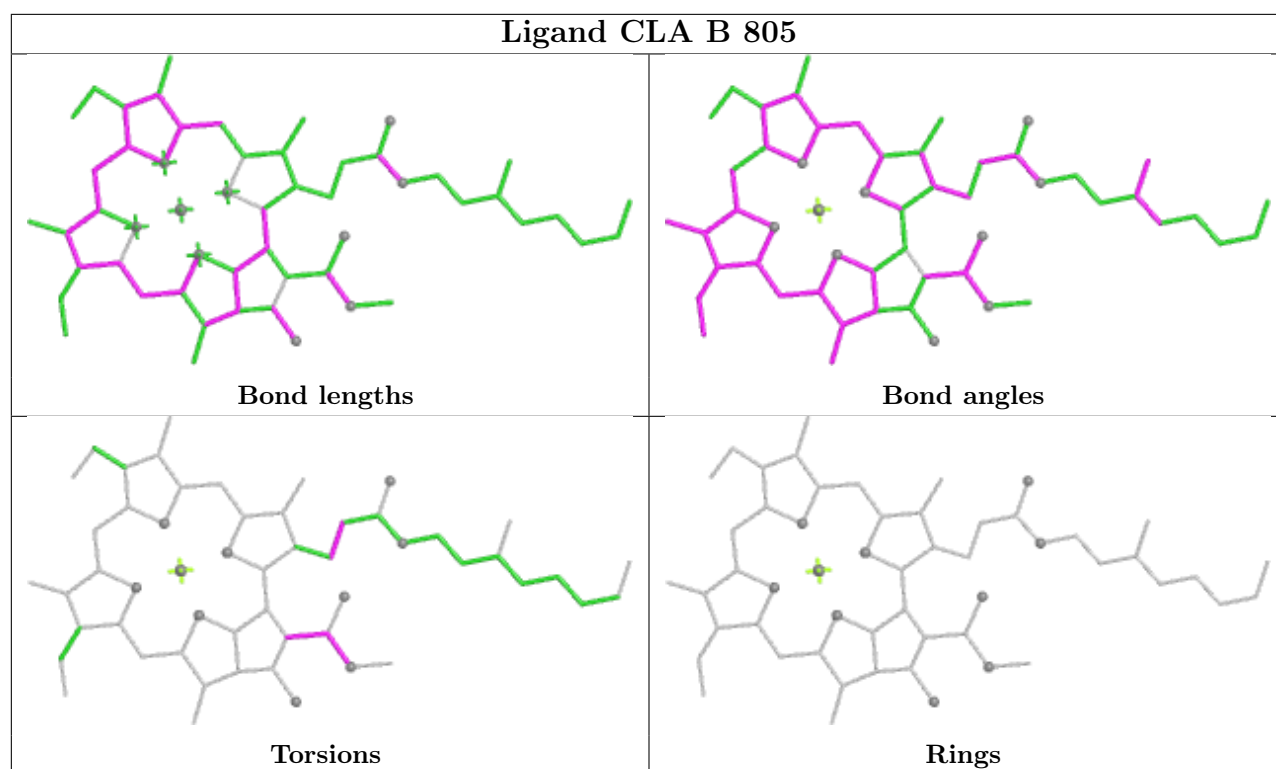


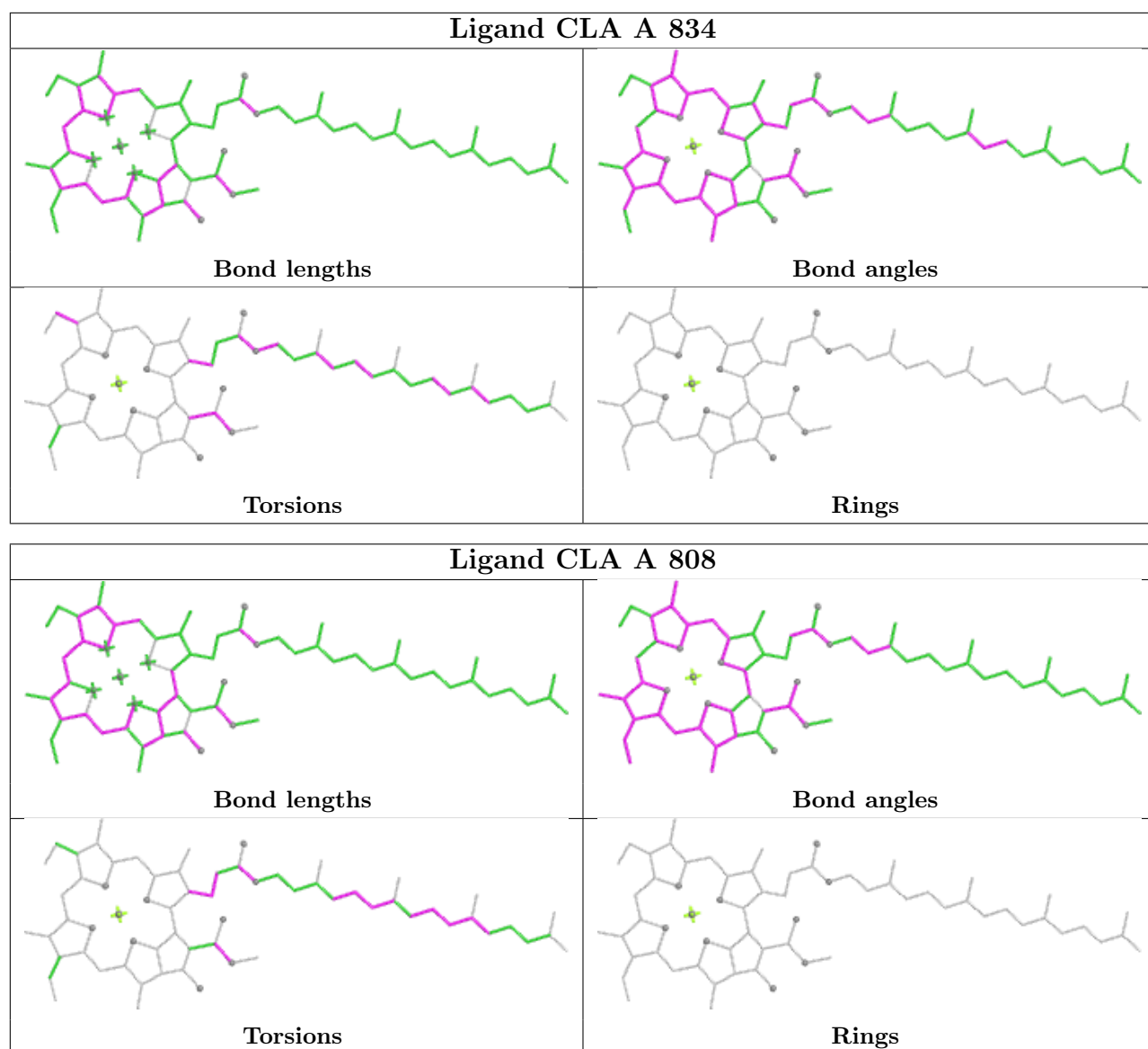


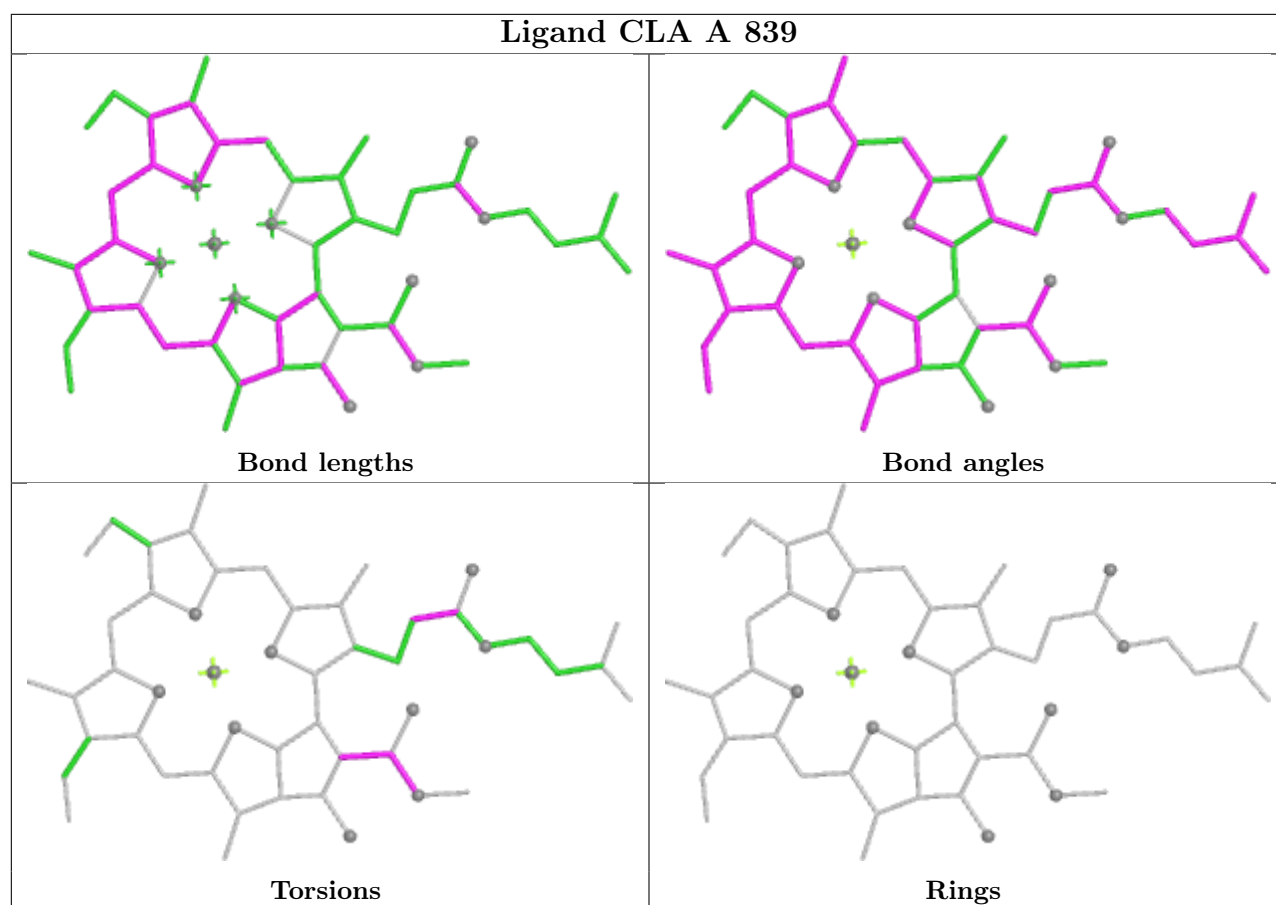


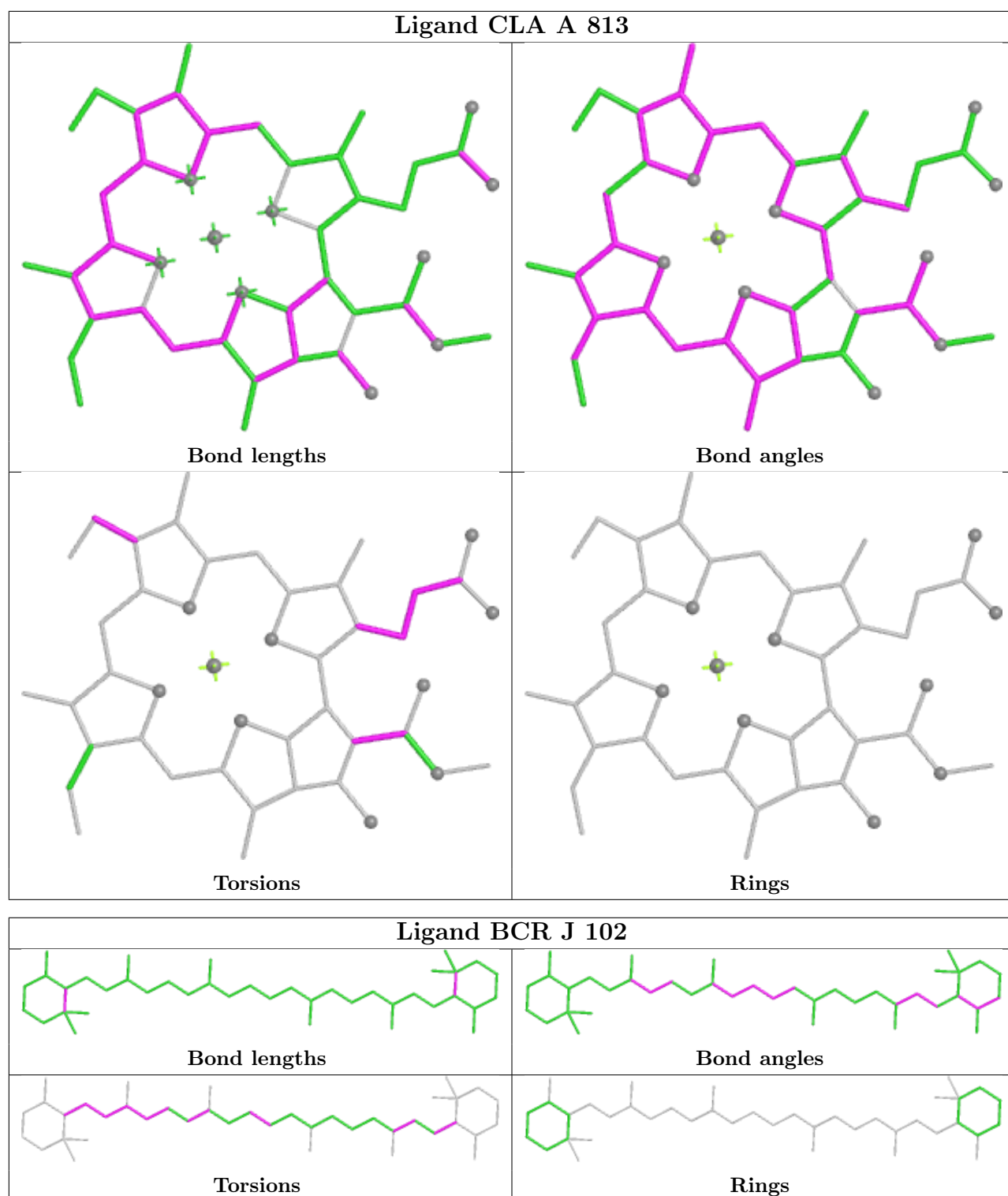


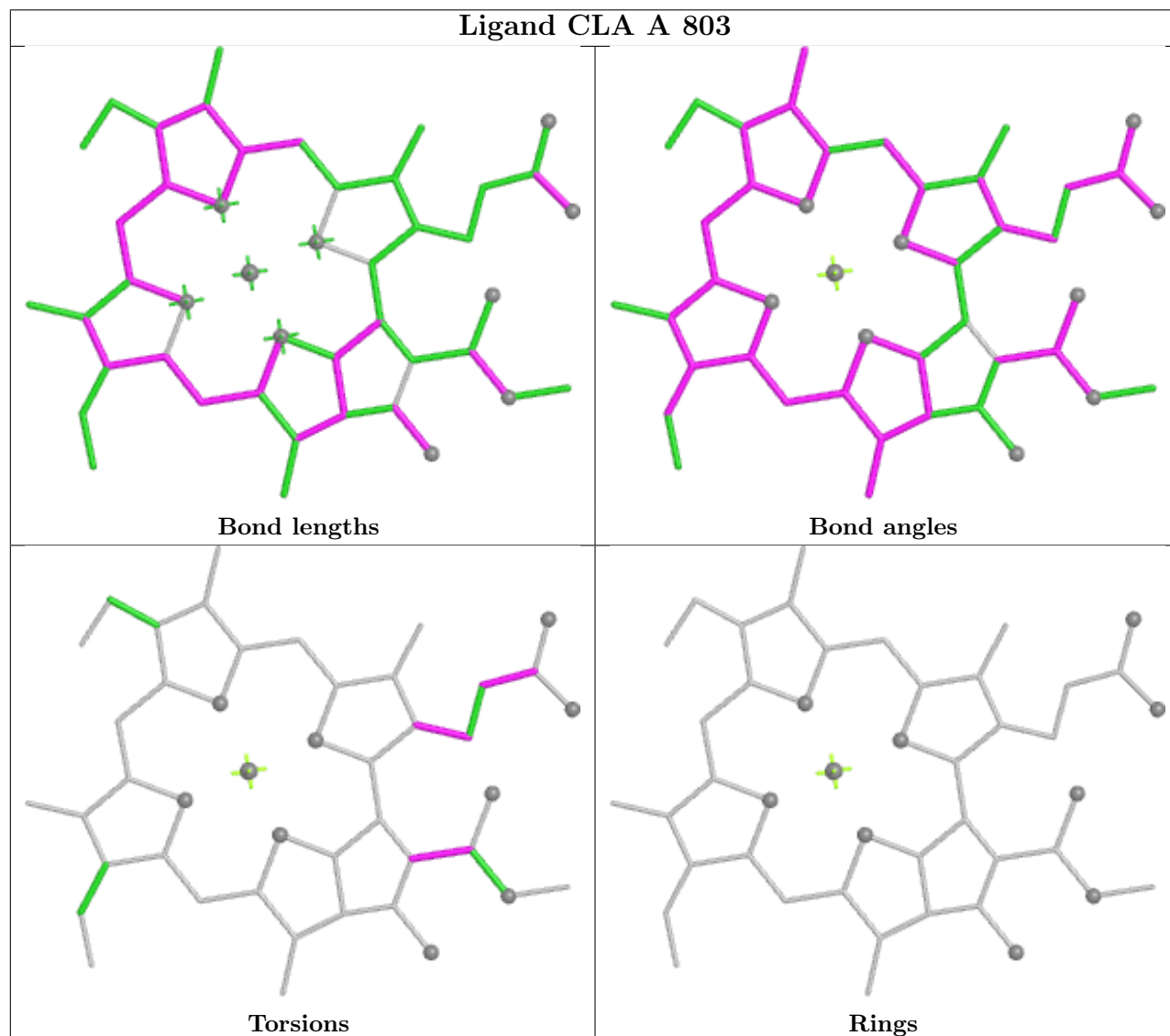
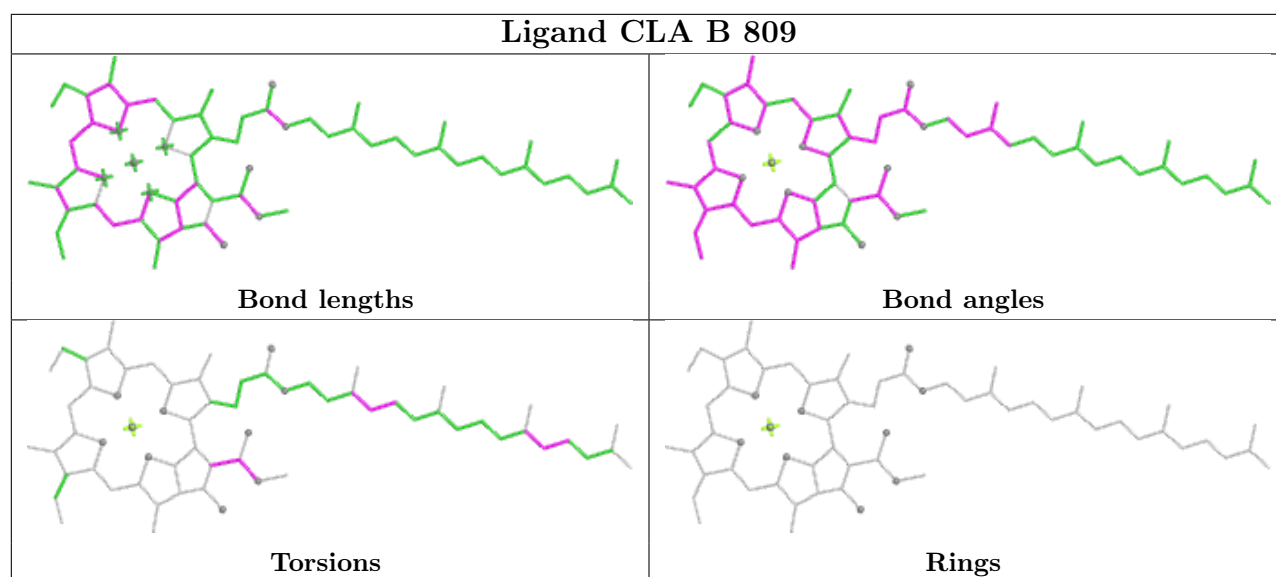




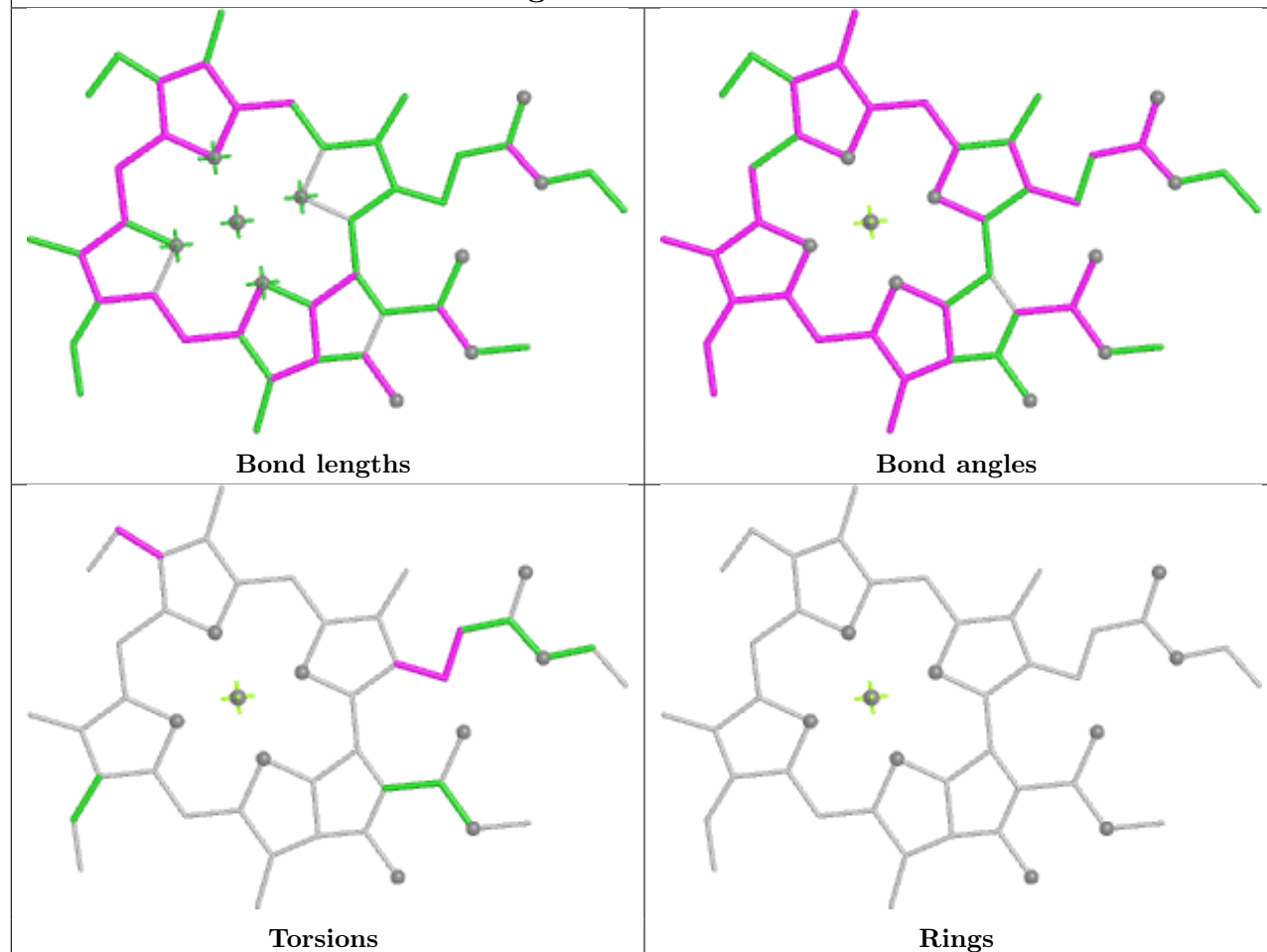




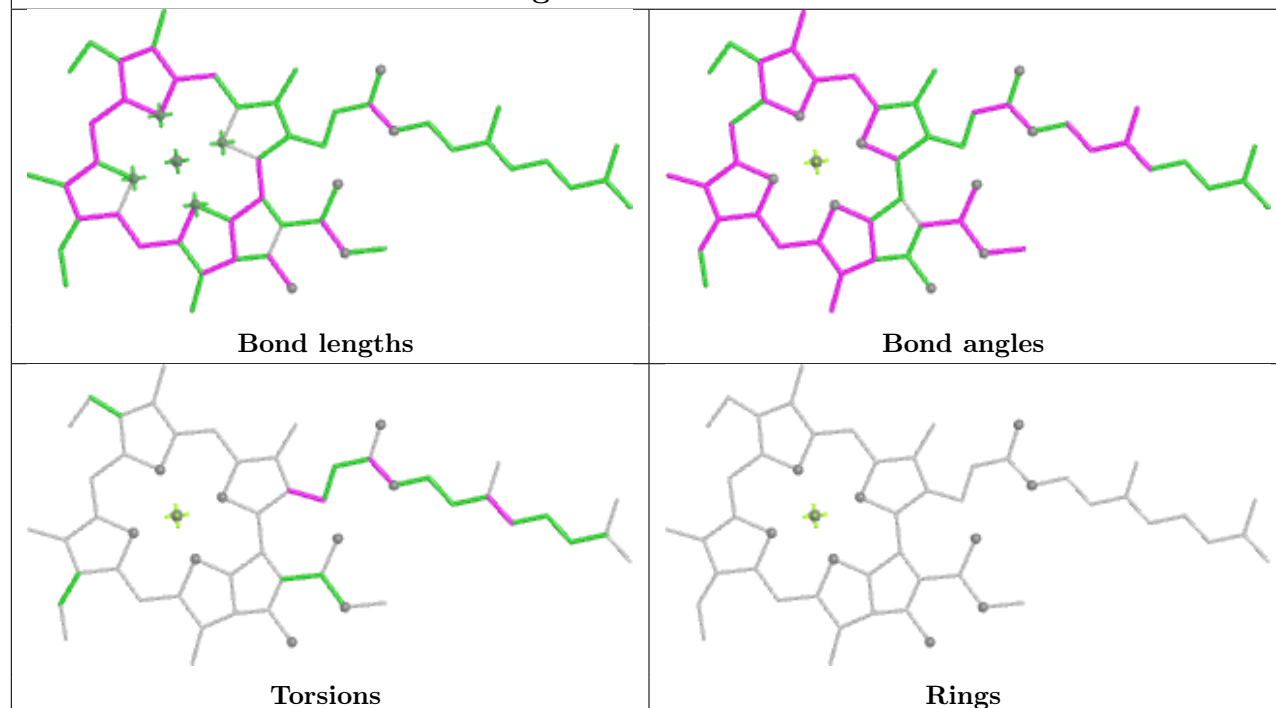


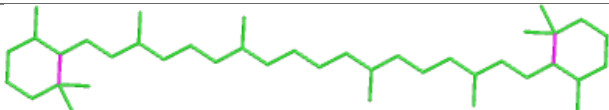
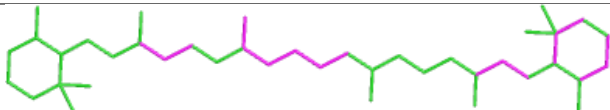
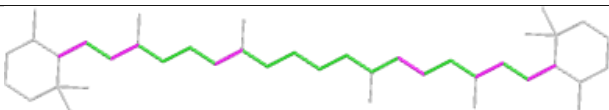
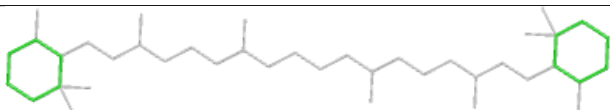


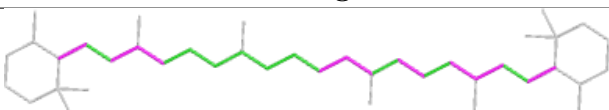
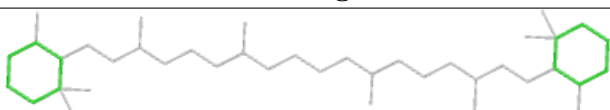
Ligand CLA A 824



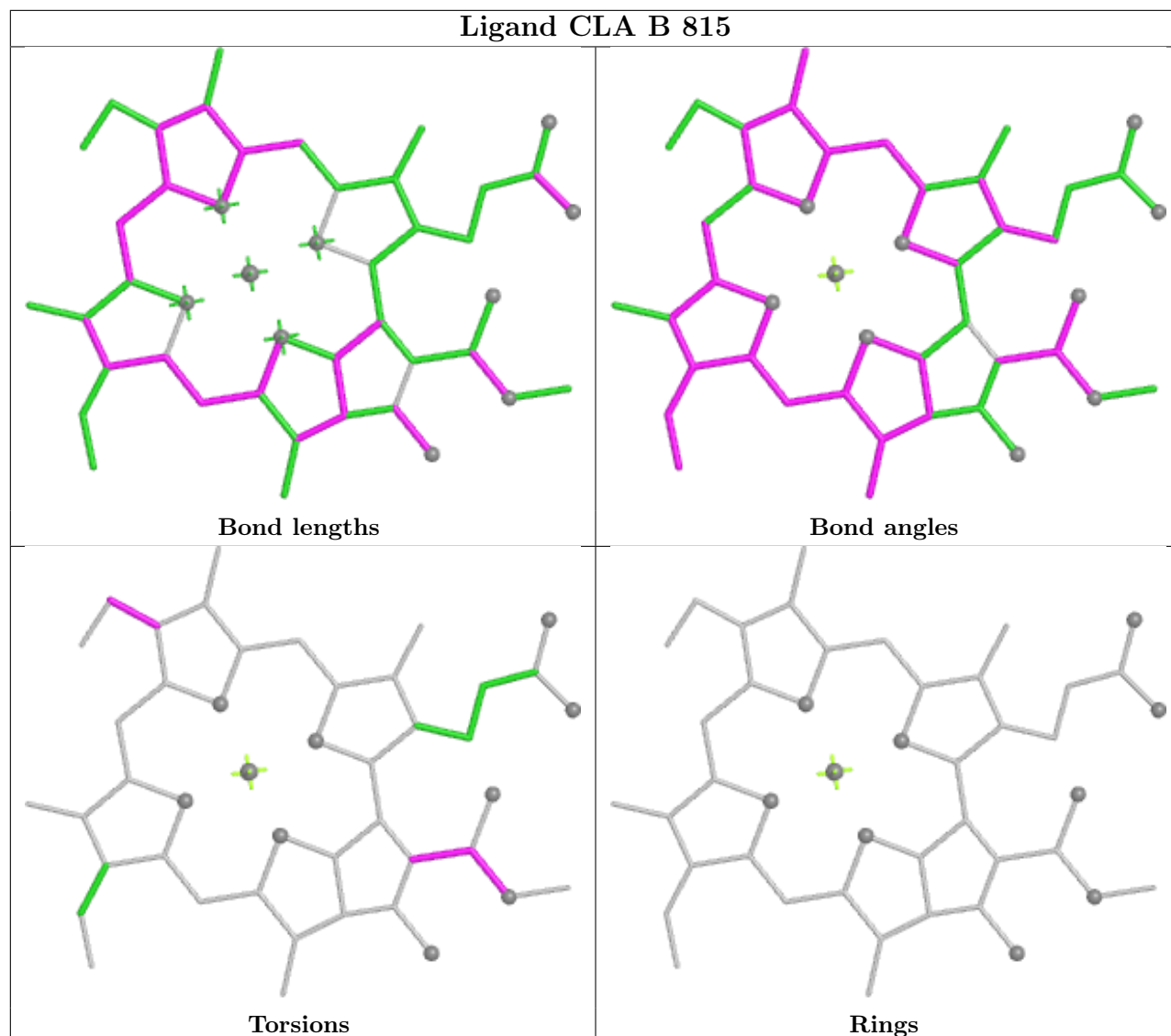
Ligand CLA B 816



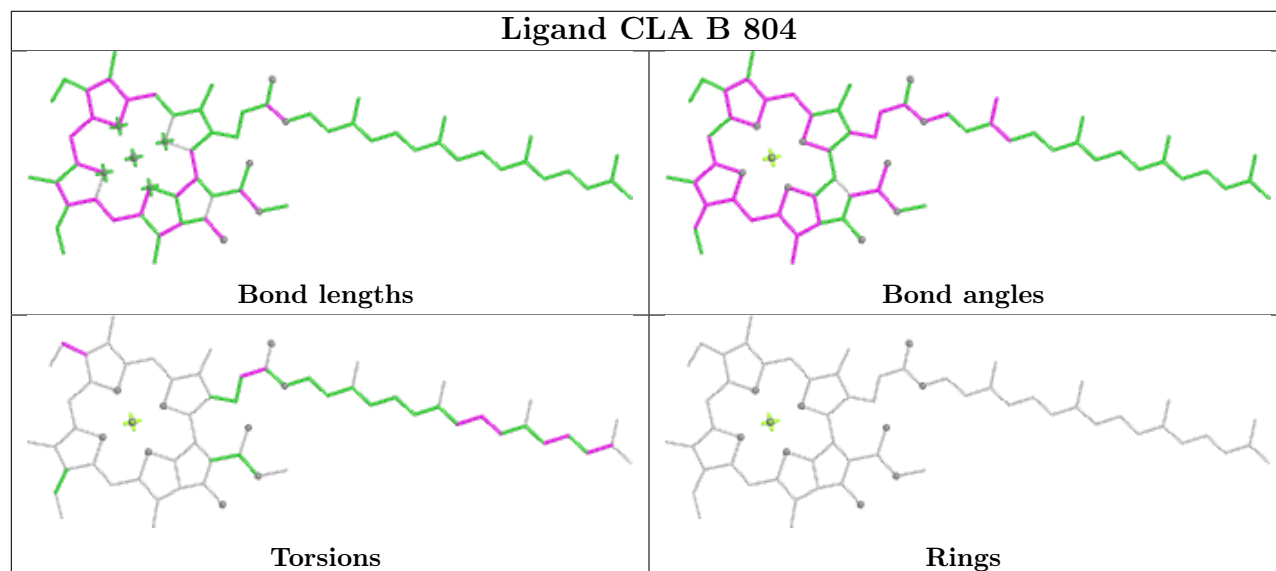
Ligand BCR A 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

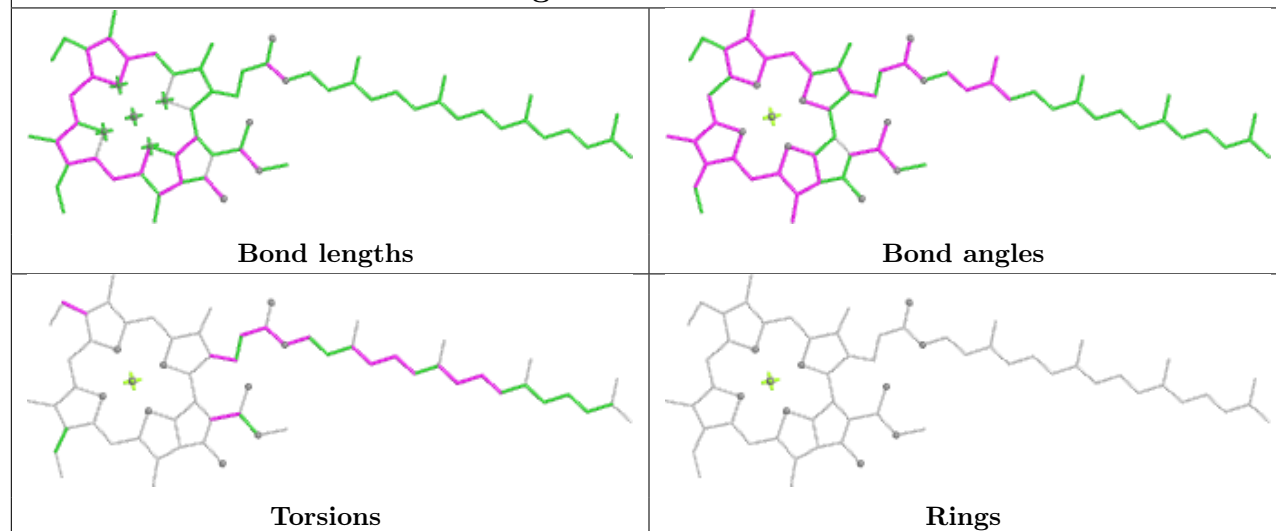
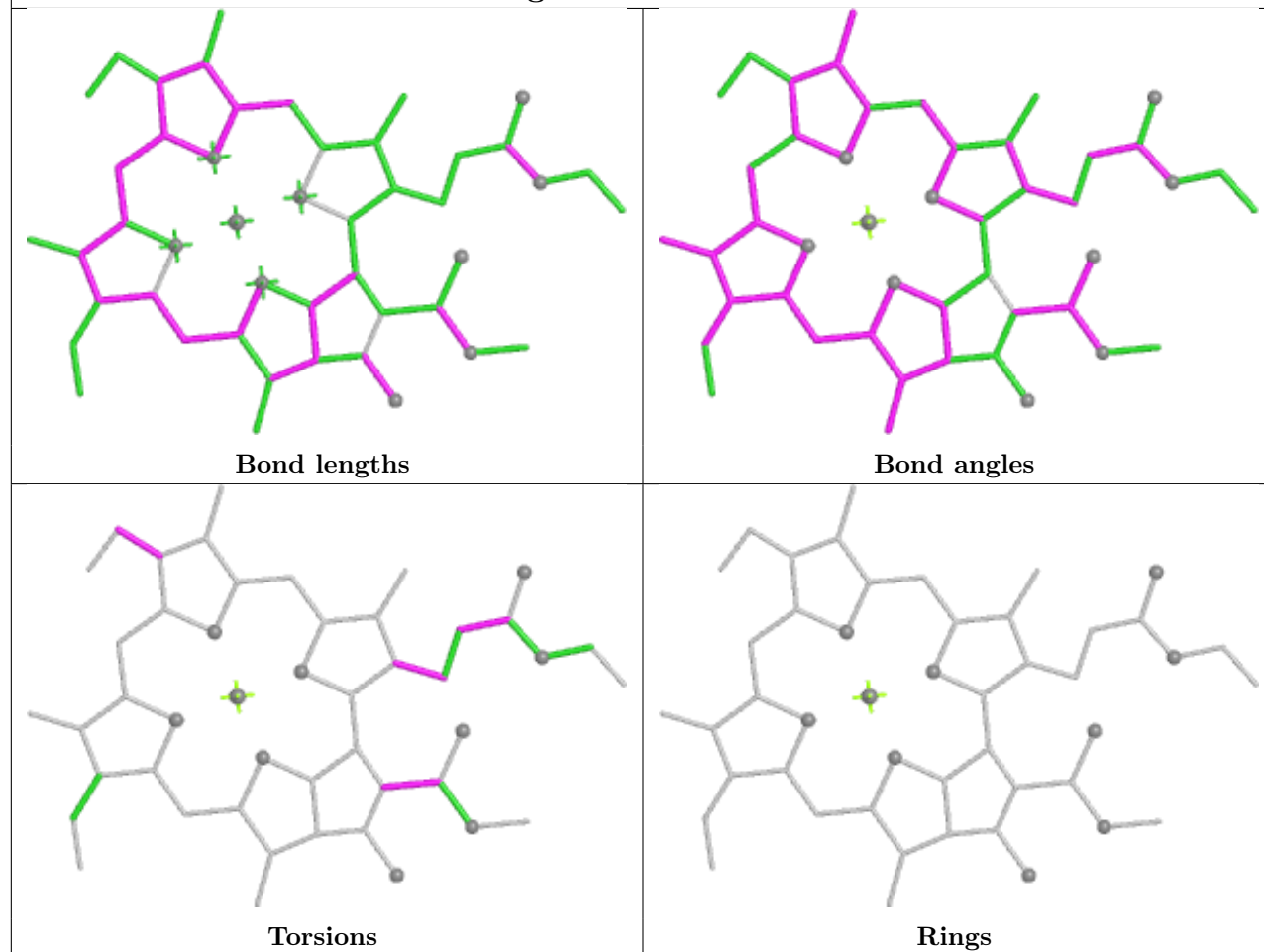
Ligand BCR J 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

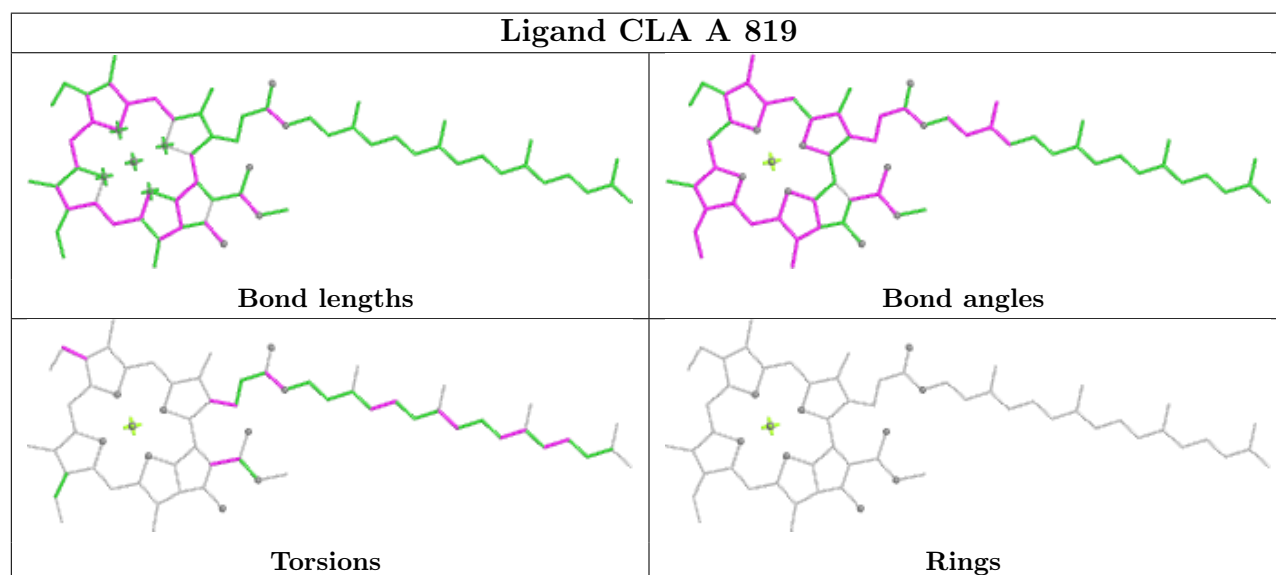
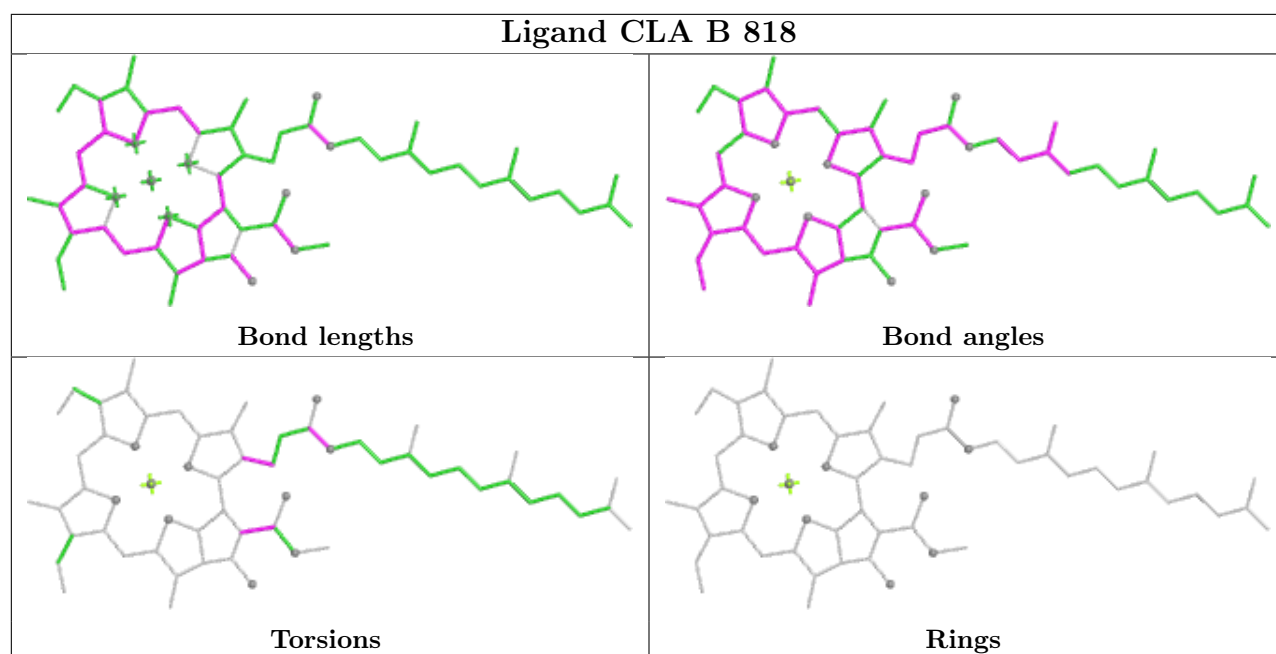
Ligand CLA B 815

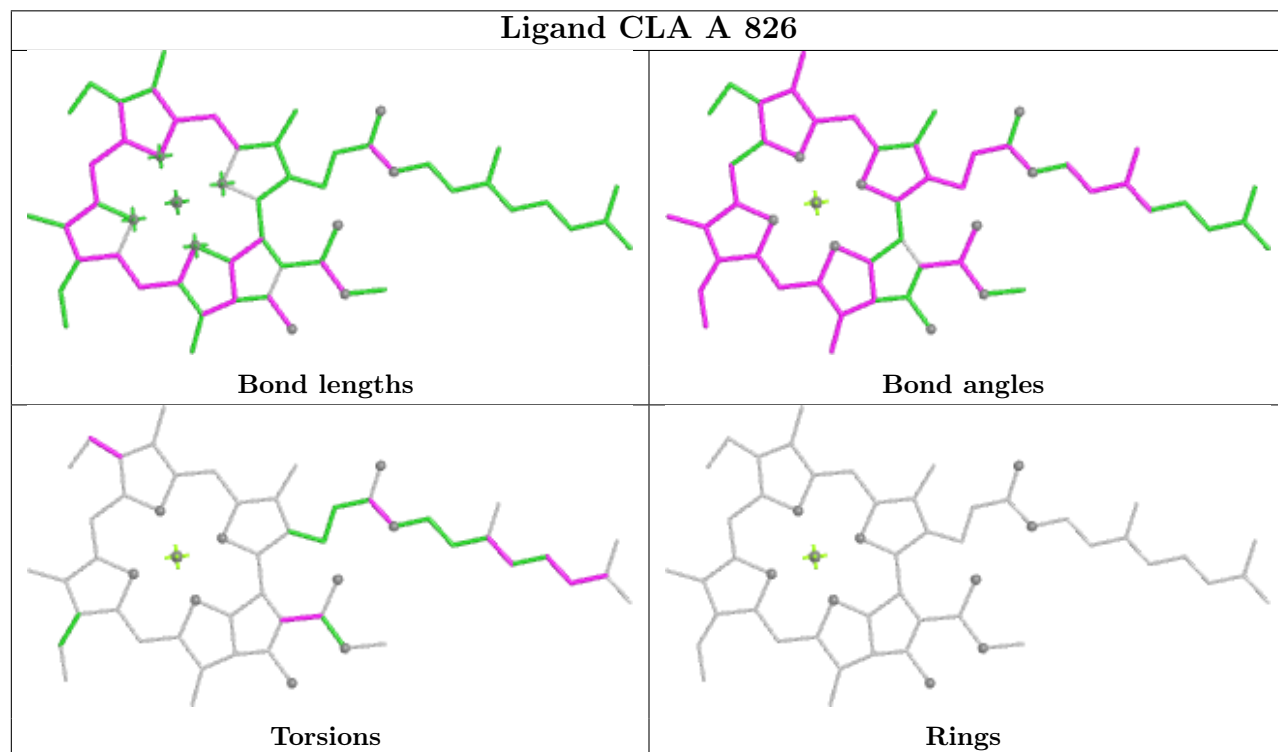
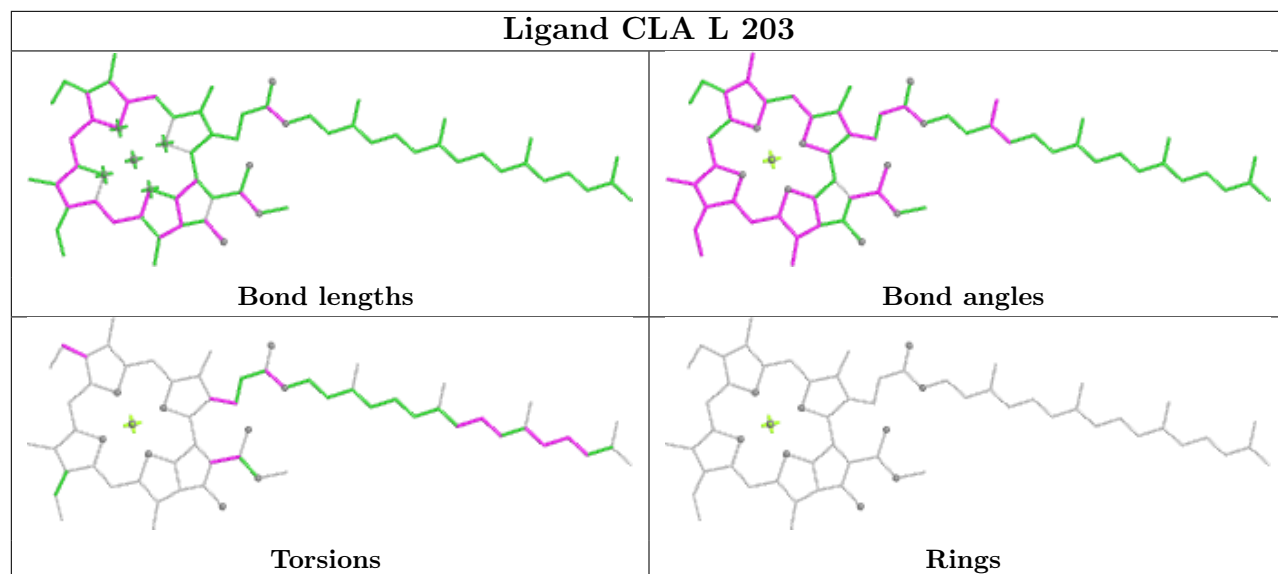


Ligand CLA B 804

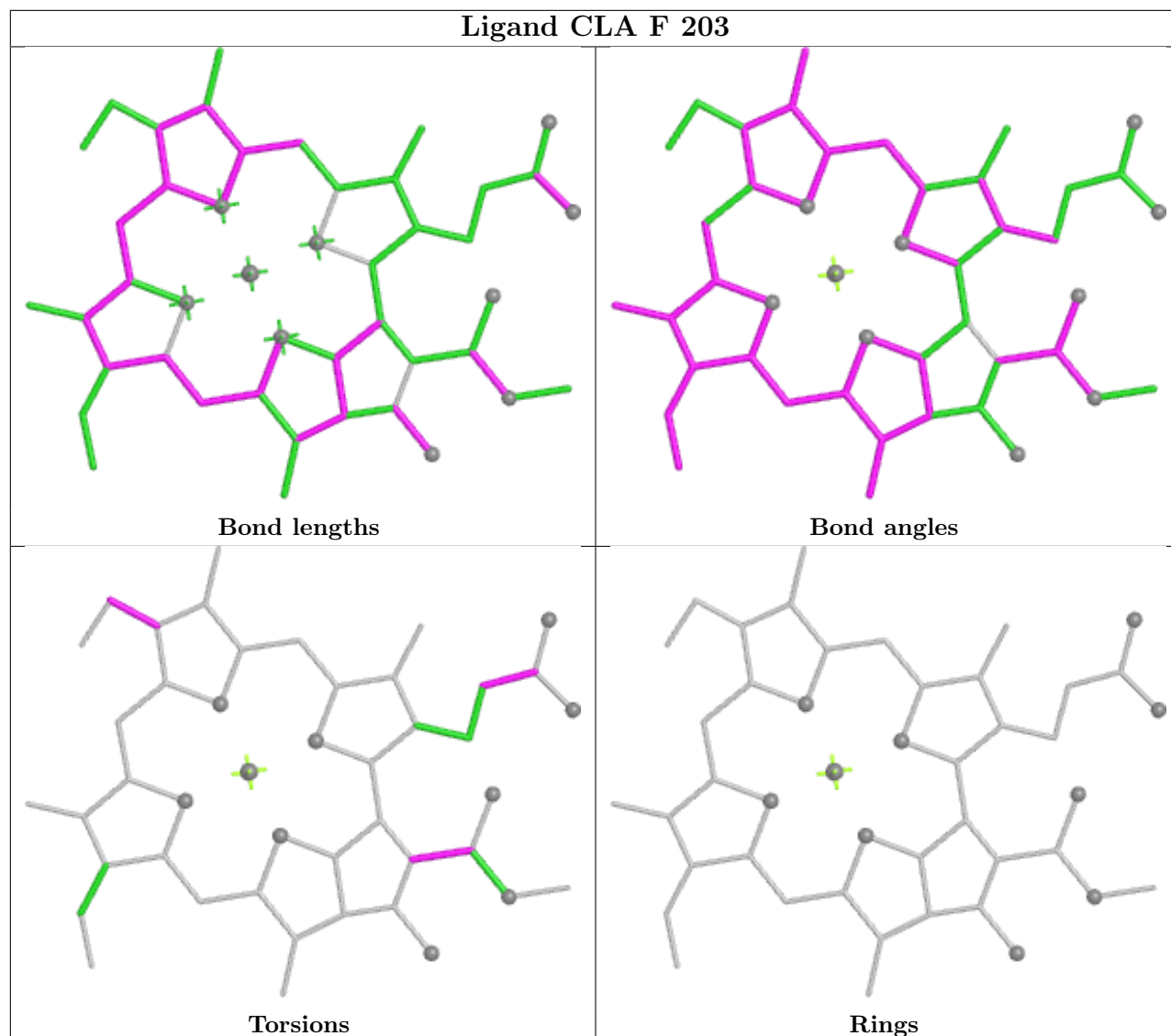


Ligand CLA B 813**Ligand CLA B 830**

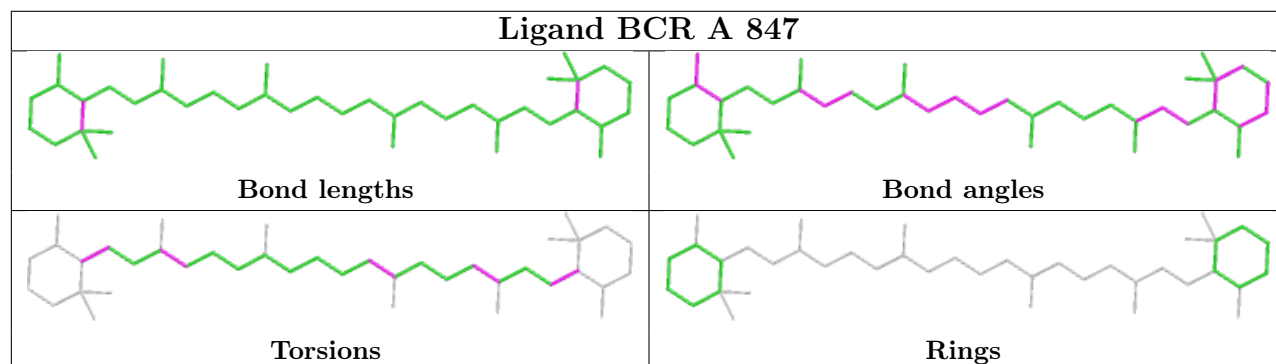


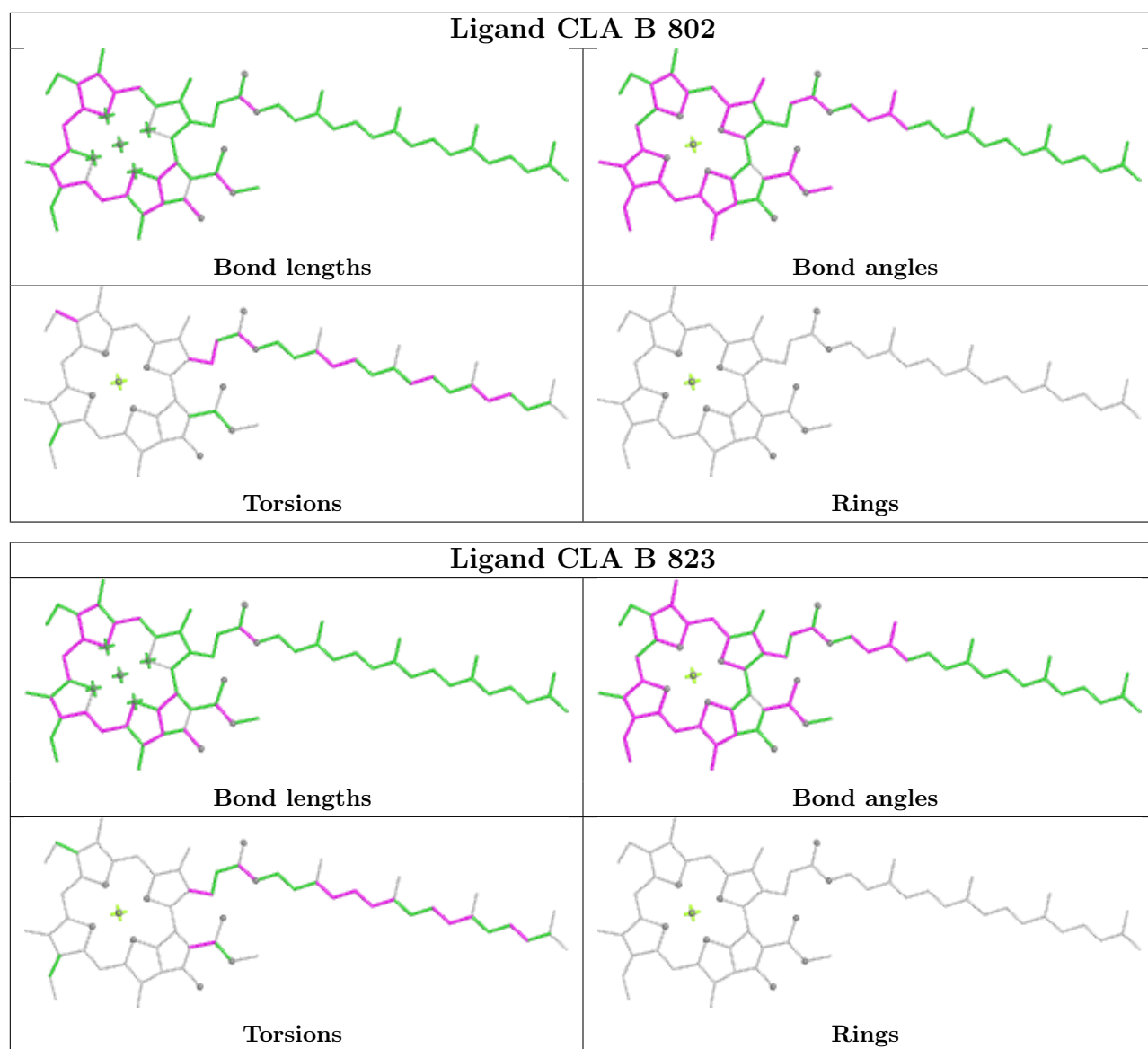


Ligand CLA F 203

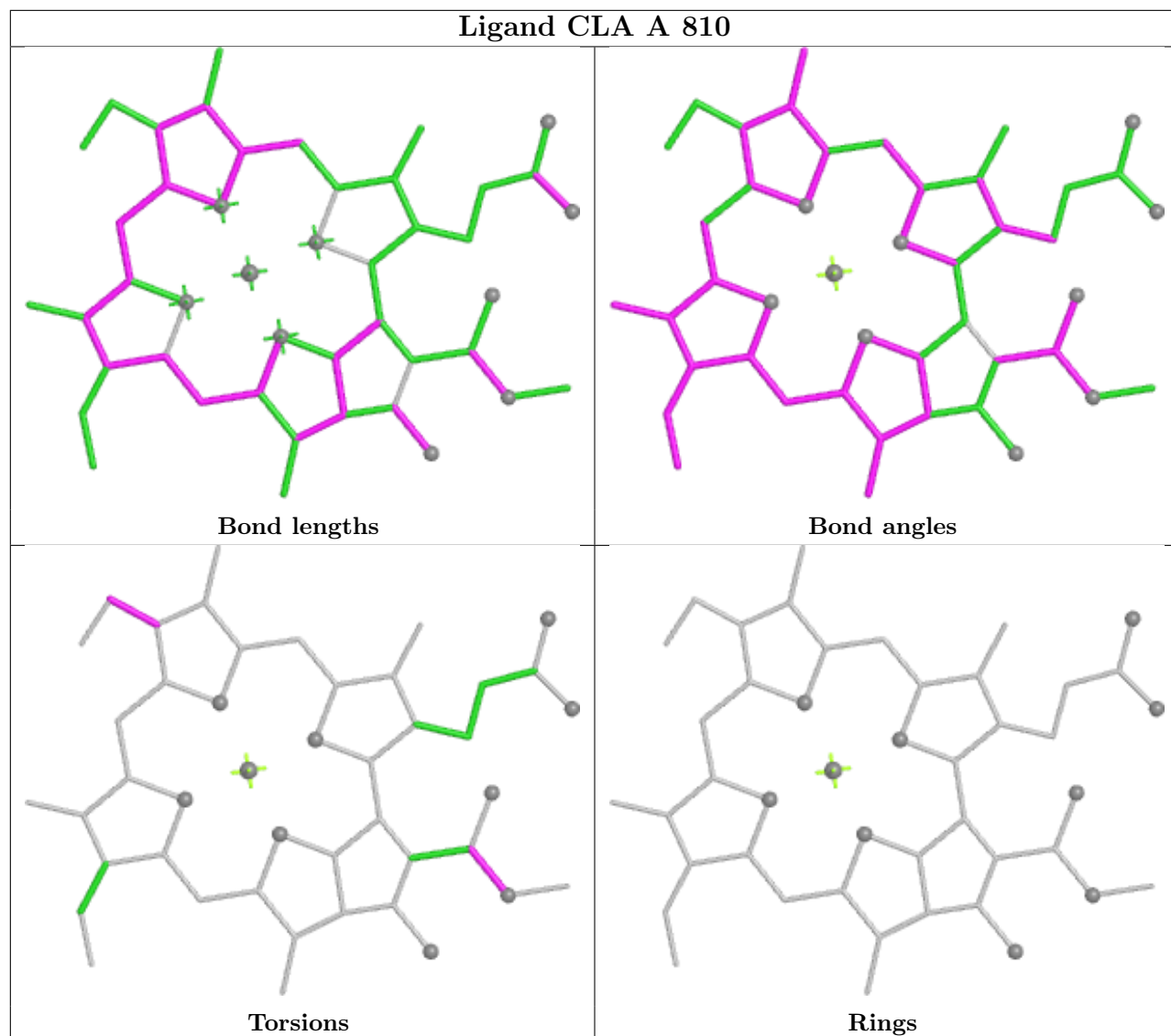


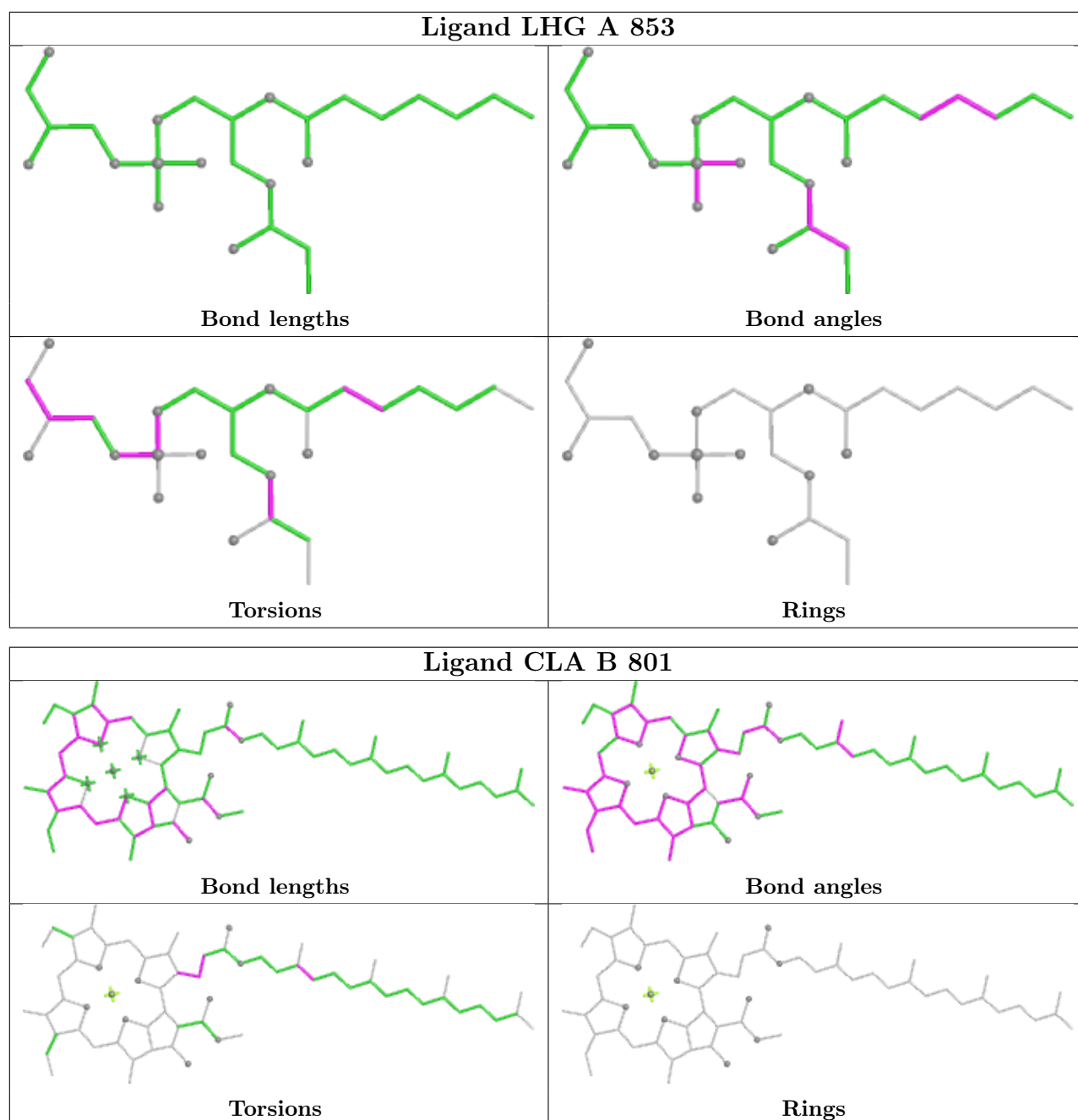
Ligand BCR A 847

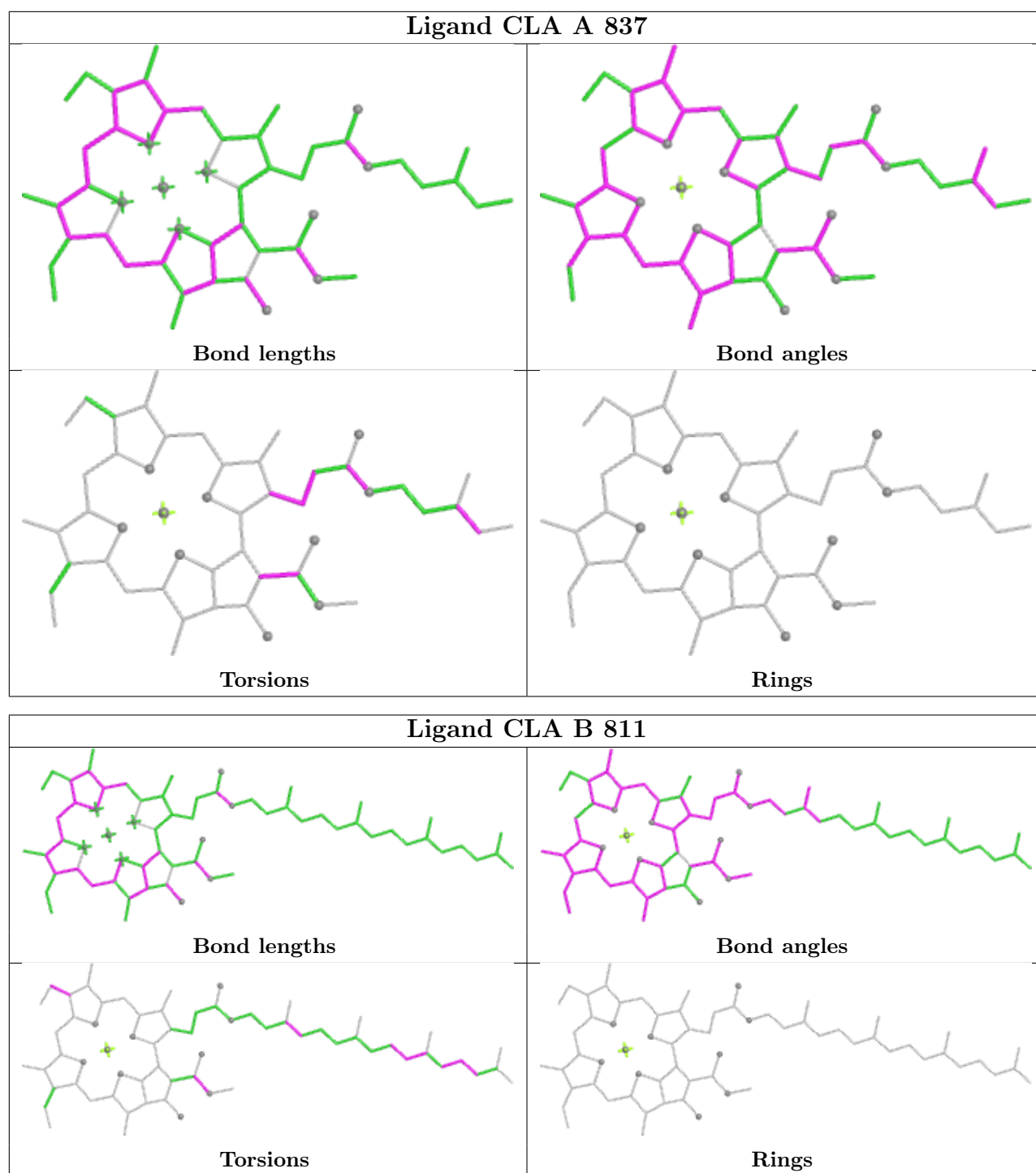




Ligand CLA A 810







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.

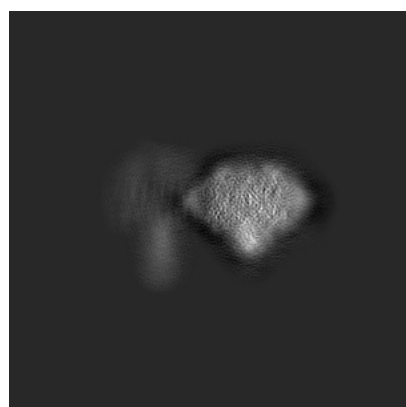
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30821. These allow visual inspection of the internal detail of the map and identification of artifacts.

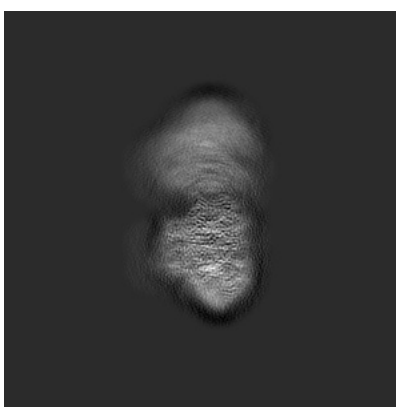
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

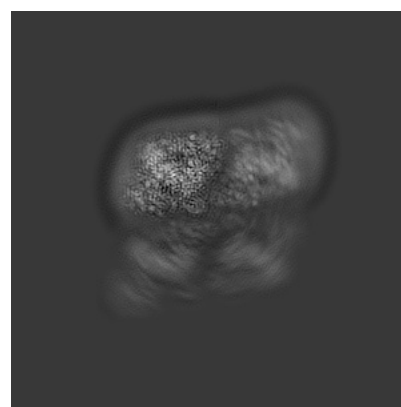
6.1.1 Primary map



X



Y

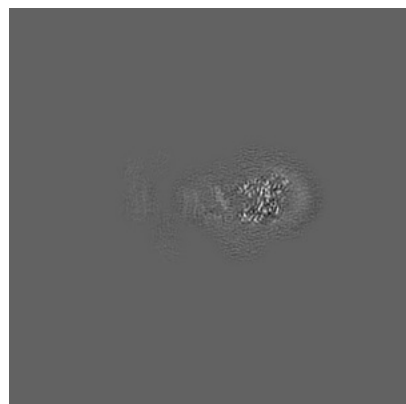


Z

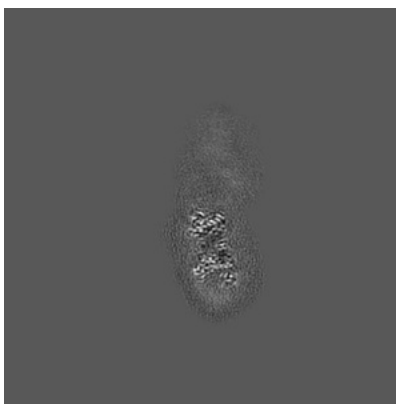
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

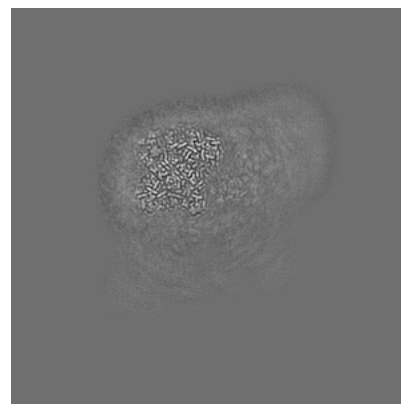
6.2.1 Primary map



X Index: 200



Y Index: 200

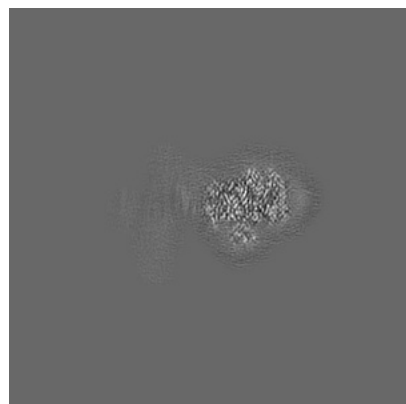


Z Index: 200

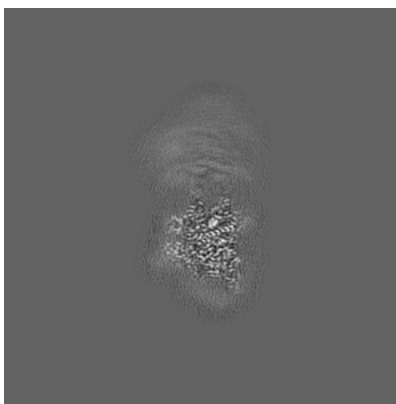
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

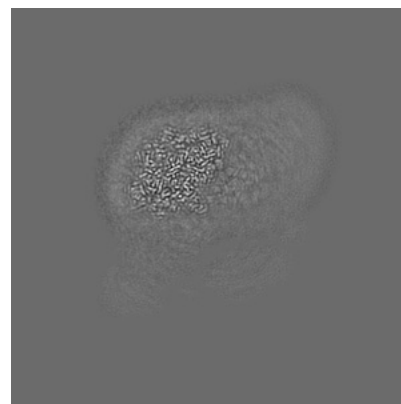
6.3.1 Primary map



X Index: 181



Y Index: 241

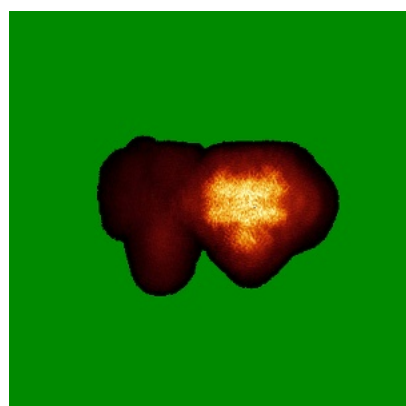


Z Index: 218

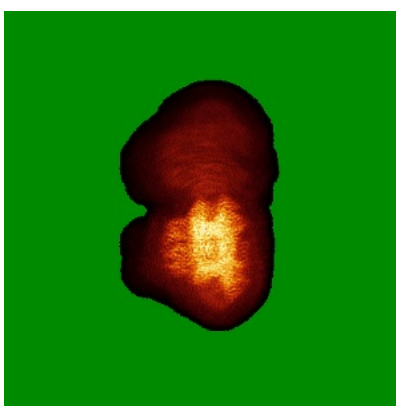
The images above show the largest variance slices of the map in three orthogonal directions.

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

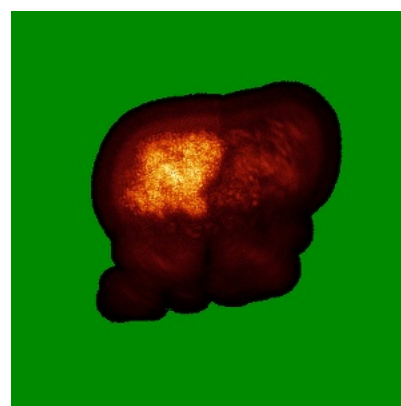
6.4.1 Primary map



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.

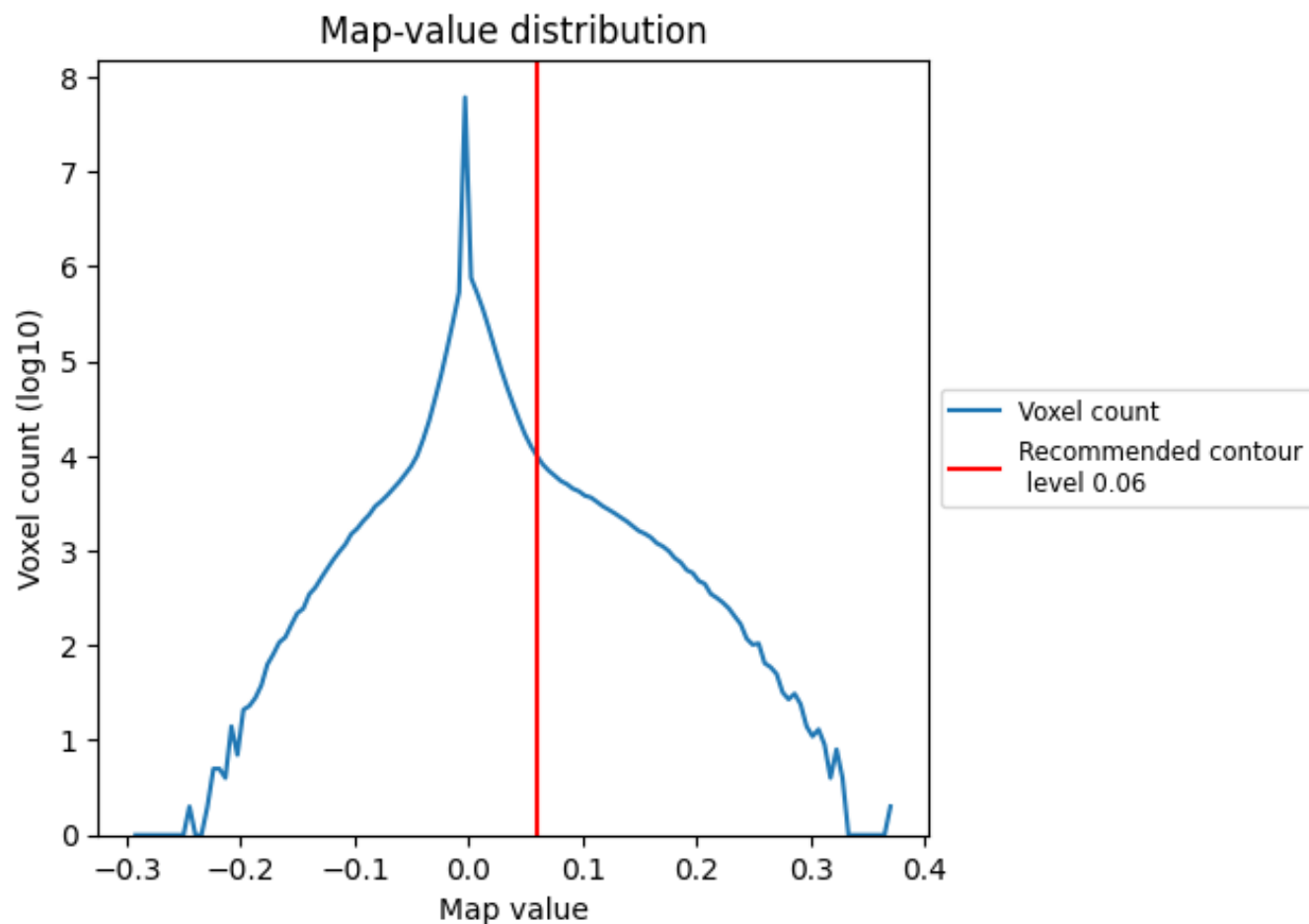
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

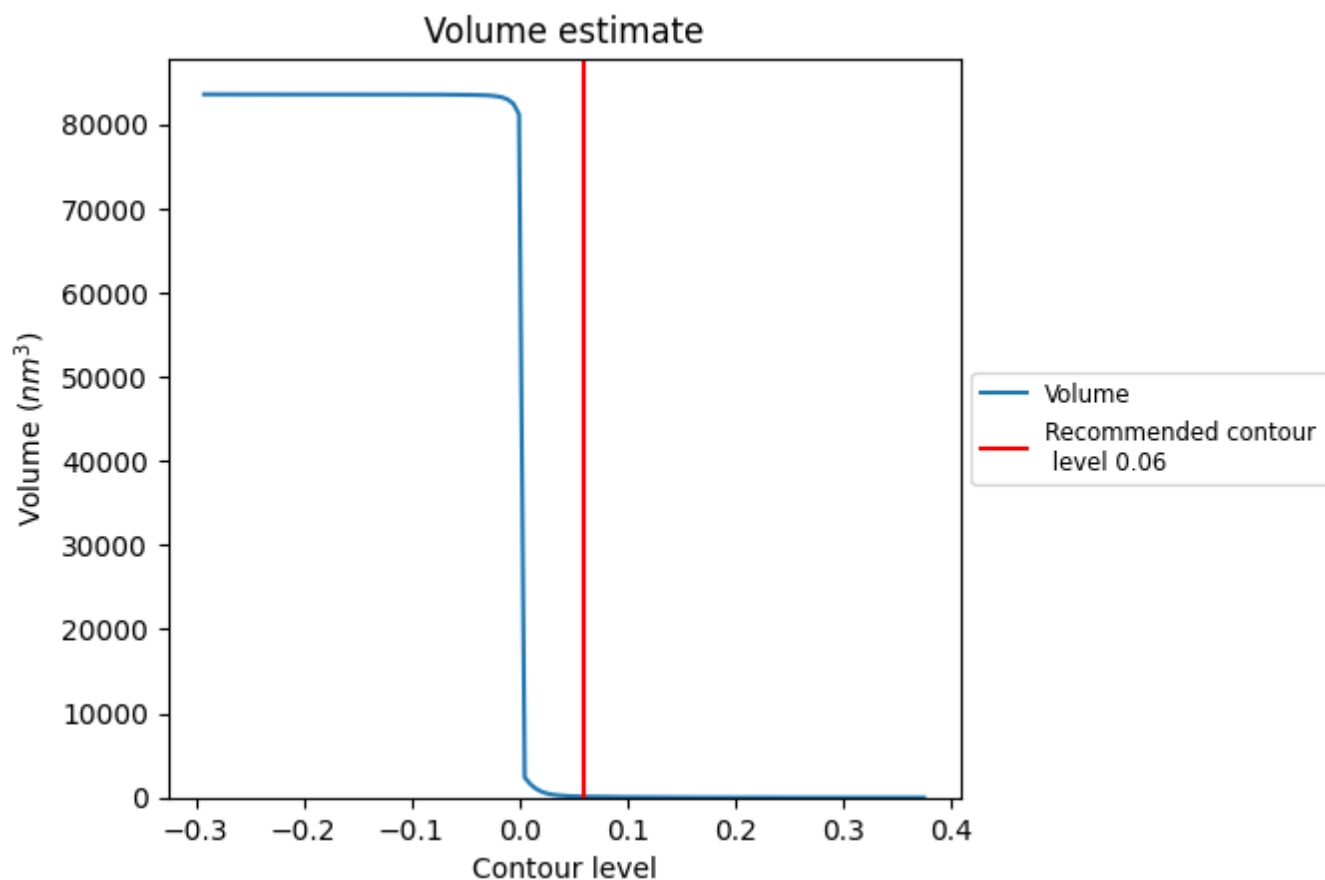
This section contains the results of statistical analysis of the map.

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.

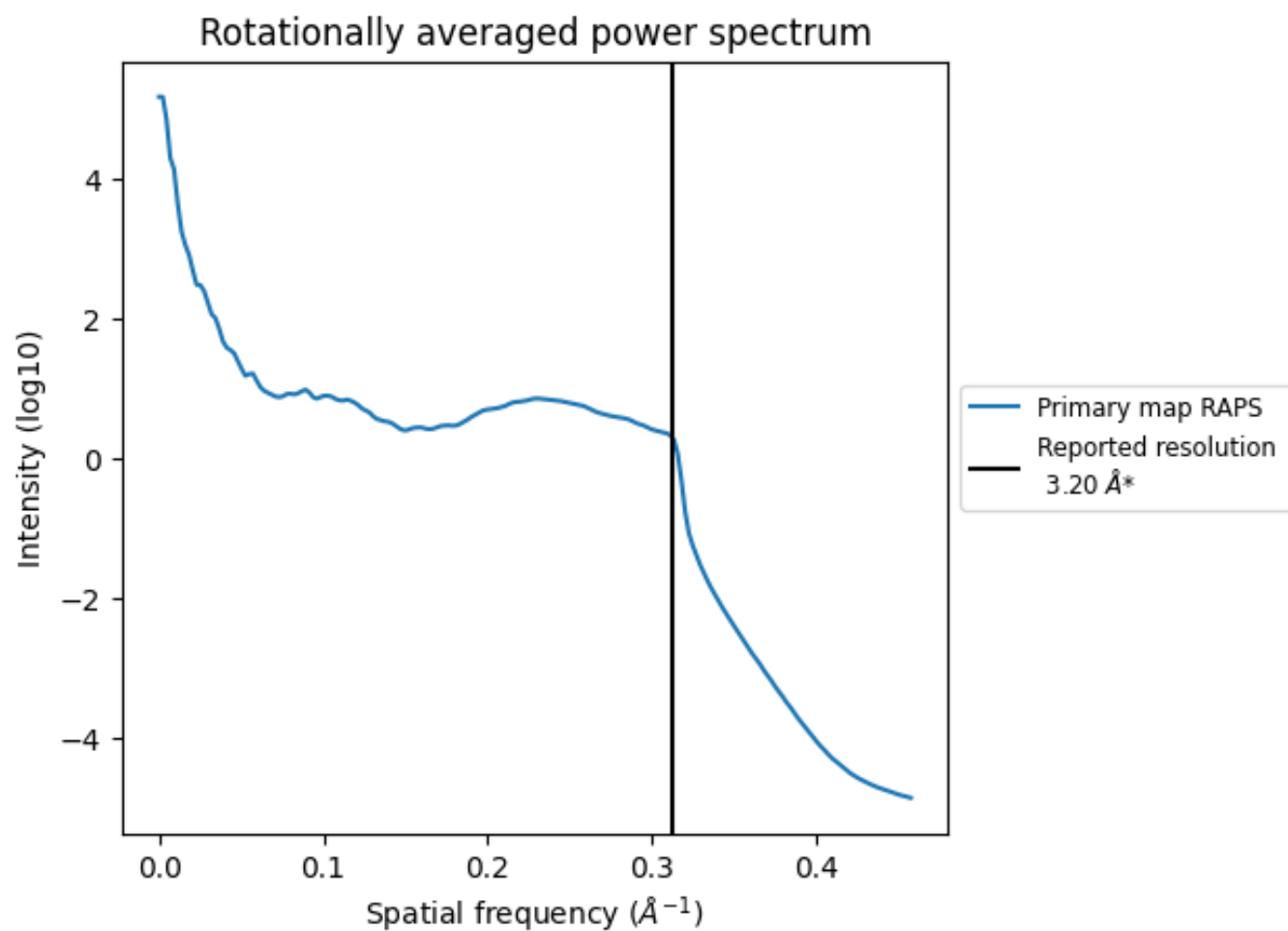
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm³; this corresponds to an approximate mass of 106 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 ⓘ

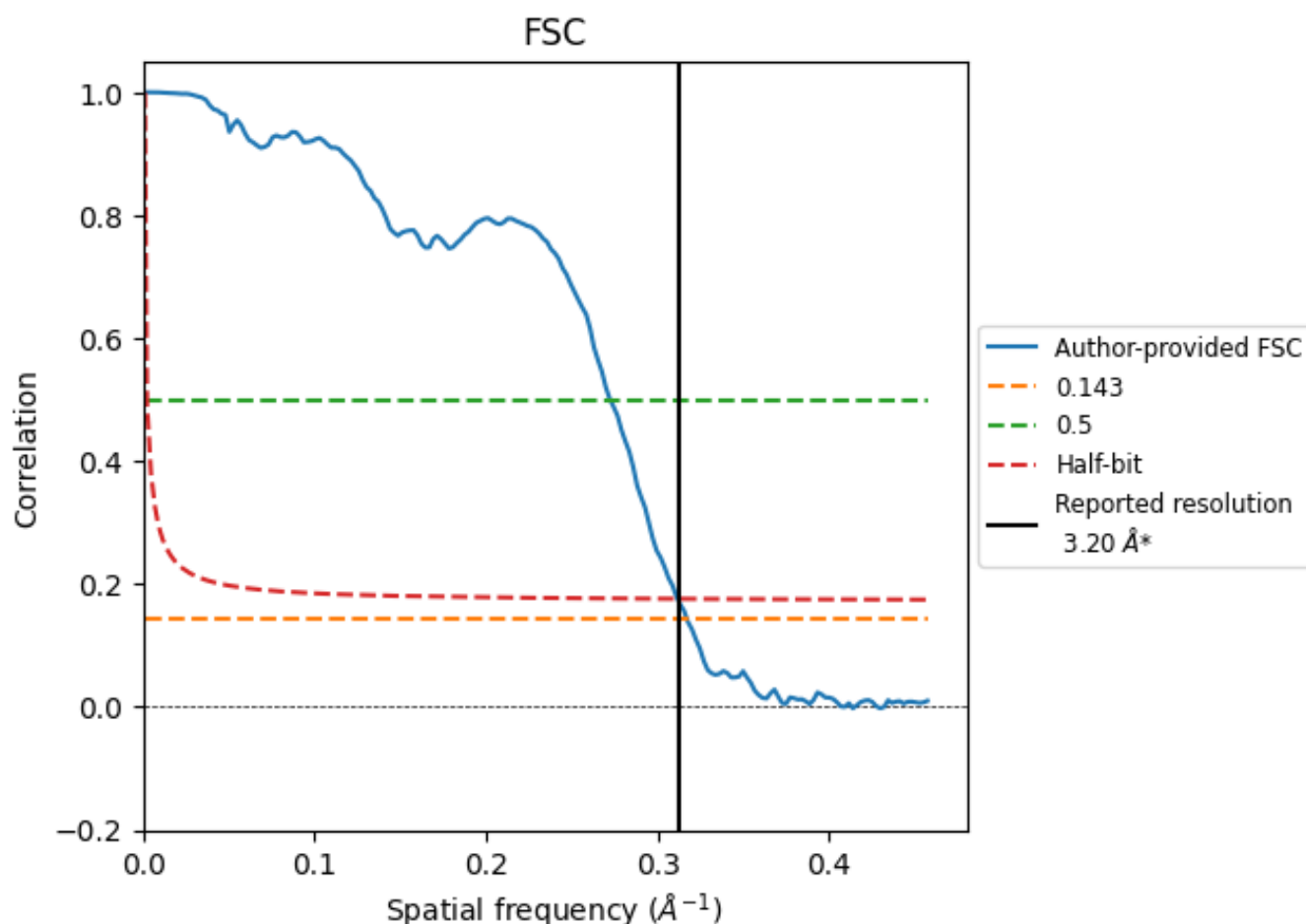


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

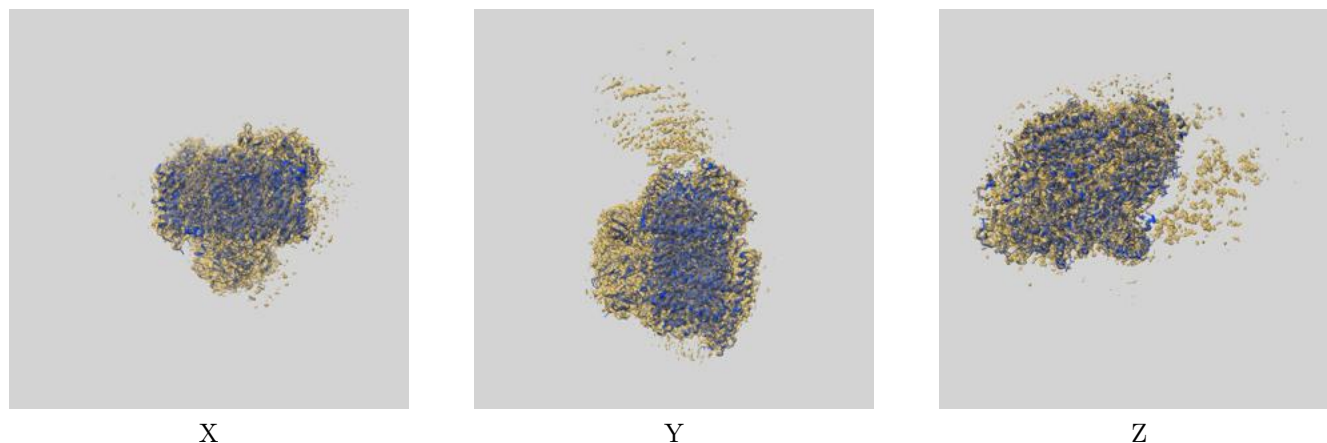
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.67	3.21
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

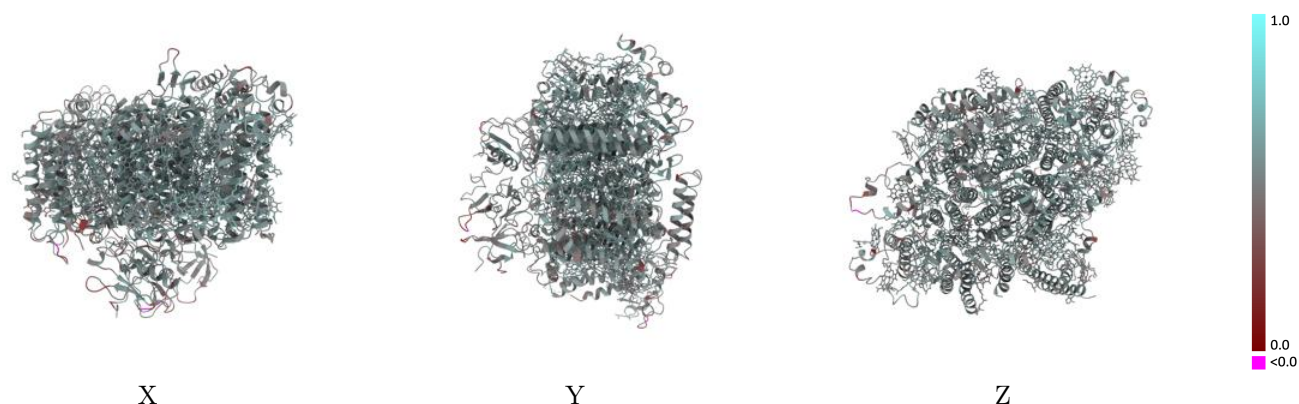
This section contains information regarding the fit between EMDB map EMD-30821 and PDB model 7DR1. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



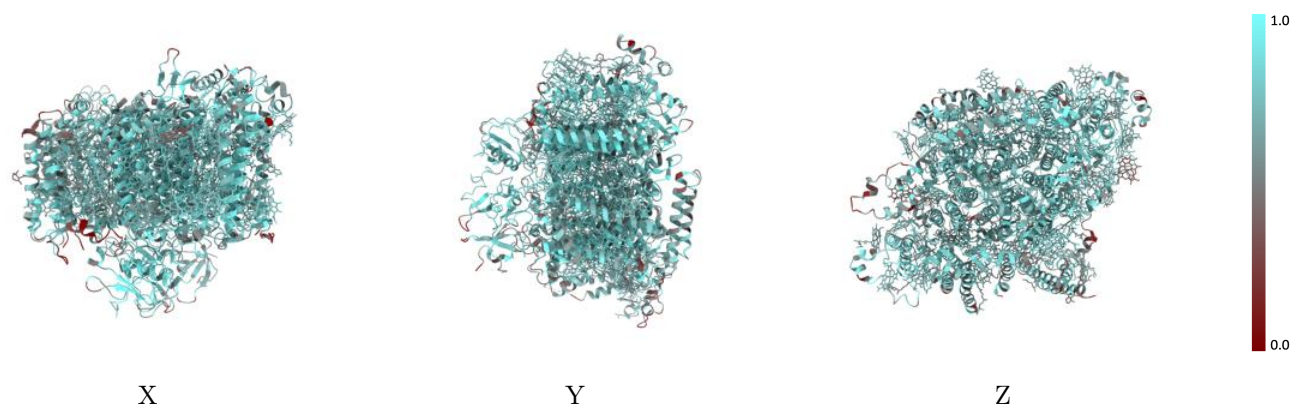
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



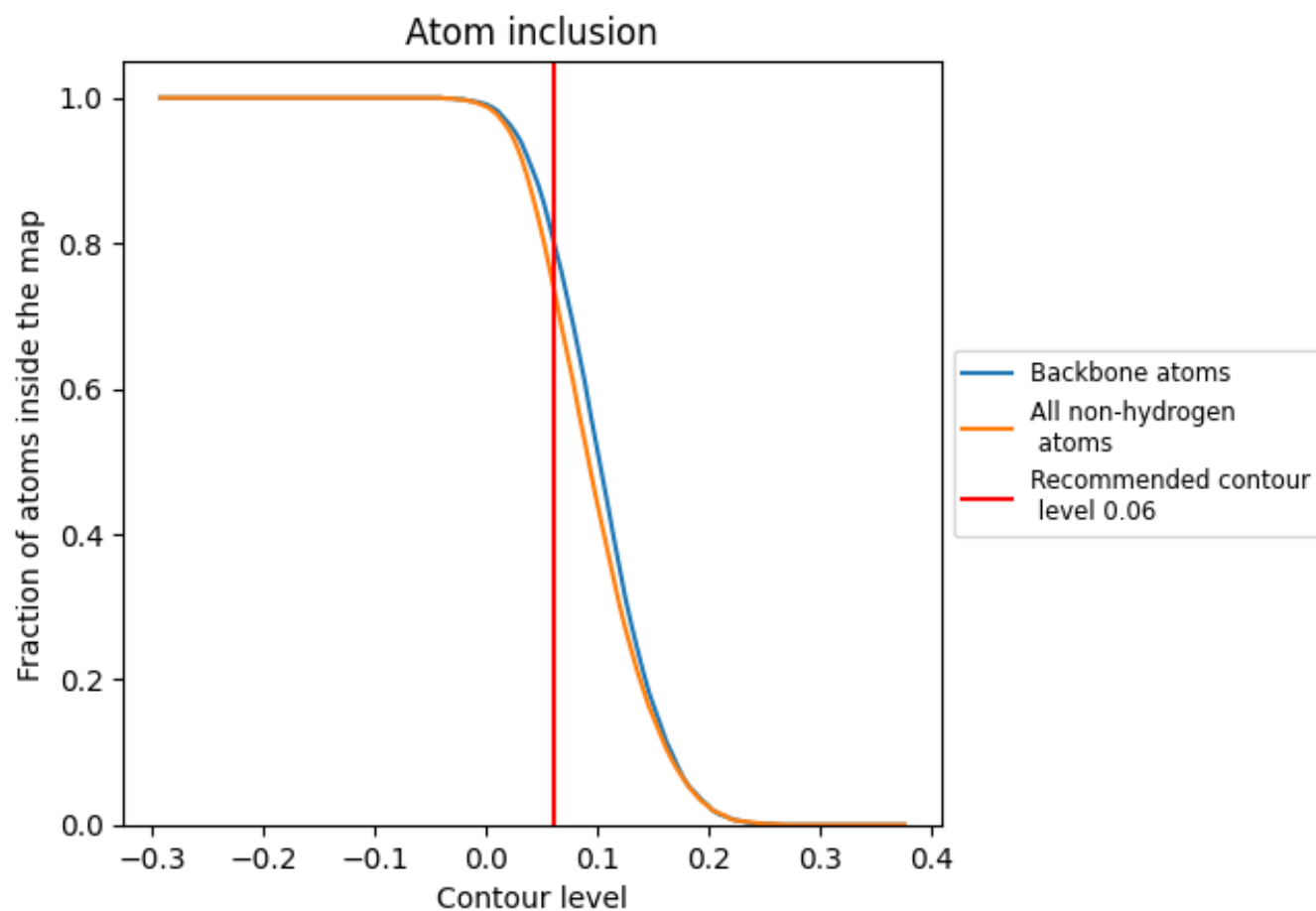
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 74% 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	0.7430	0.5250
A	0.7770	0.5470
B	0.7460	0.5200
C	0.7870	0.4730
D	0.7550	0.4870
E	0.7190	0.4730
F	0.6660	0.5050
I	0.6480	0.5250
J	0.6730	0.5290
L	0.6270	0.5050
M	0.6550	0.5200

1.0

0.0

<0.0