



wwPDB EM Validation Summary Report ⓘ

Nov 21, 2022 – 11:32 PM JST

PDB ID : 7DR1
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)

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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:

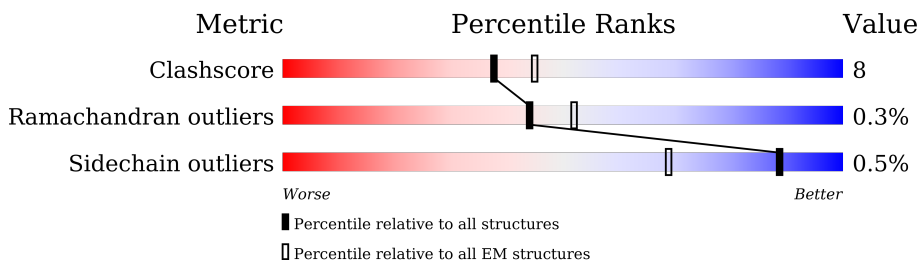
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	
5	E	70	
6	F	186	
7	I	35	
8	J	40	

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Mol	Chain	Length	Quality of chain			
9	L	146				
10	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
11	CL0	A	801	X	-	-	-
12	CLA	A	802	X	-	-	-
12	CLA	A	803	X	-	-	-
12	CLA	A	804	X	-	-	-
12	CLA	A	805	X	-	-	-
12	CLA	A	806	X	-	-	-
12	CLA	A	807	X	-	-	-
12	CLA	A	808	X	-	-	-
12	CLA	A	809	X	-	-	-
12	CLA	A	810	X	-	-	-
12	CLA	A	811	X	-	-	-
12	CLA	A	813	X	-	-	-
12	CLA	A	814	X	-	-	-
12	CLA	A	816	X	-	-	-
12	CLA	A	818	X	-	-	-
12	CLA	A	819	X	-	-	-
12	CLA	A	820	X	-	-	-
12	CLA	A	821	X	-	-	-
12	CLA	A	824	X	-	-	-
12	CLA	A	825	X	-	-	-
12	CLA	A	826	X	-	-	-
12	CLA	A	827	X	-	-	-
12	CLA	A	828	X	-	-	-
12	CLA	A	829	X	-	-	-
12	CLA	A	830	X	-	-	-
12	CLA	A	831	X	-	-	-
12	CLA	A	832	X	-	-	-
12	CLA	A	833	X	-	-	-
12	CLA	A	835	X	-	-	-
12	CLA	A	836	X	-	-	-
12	CLA	A	837	X	-	-	-
12	CLA	A	838	X	-	-	-
12	CLA	A	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	841	X	-	-	-
12	CLA	A	842	X	-	-	-
12	CLA	A	854	X	-	-	-
12	CLA	B	801	X	-	-	-
12	CLA	B	802	X	-	-	-
12	CLA	B	803	X	-	-	-
12	CLA	B	804	X	-	-	-
12	CLA	B	805	X	-	-	-
12	CLA	B	806	X	-	-	-
12	CLA	B	807	X	-	-	-
12	CLA	B	808	X	-	-	-
12	CLA	B	809	X	-	-	-
12	CLA	B	810	X	-	-	-
12	CLA	B	811	X	-	-	-
12	CLA	B	812	X	-	-	-
12	CLA	B	813	X	-	-	-
12	CLA	B	814	X	-	-	-
12	CLA	B	815	X	-	-	-
12	CLA	B	817	X	-	-	-
12	CLA	B	818	X	-	-	-
12	CLA	B	819	X	-	-	-
12	CLA	B	820	X	-	-	-
12	CLA	B	821	X	-	-	-
12	CLA	B	822	X	-	-	-
12	CLA	B	823	X	-	-	-
12	CLA	B	825	X	-	-	-
12	CLA	B	826	X	-	-	-
12	CLA	B	828	X	-	-	-
12	CLA	B	829	X	-	-	-
12	CLA	B	830	X	-	-	-
12	CLA	B	832	X	-	-	-
12	CLA	F	203	X	-	-	-
12	CLA	J	101	X	-	-	-

2 Entry composition [i](#)

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
			Total	C	N	O	S		
1	A	739	5803	3794	987	999	23	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	601	367	106	117	11	0	0

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

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

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

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

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

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

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

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

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

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

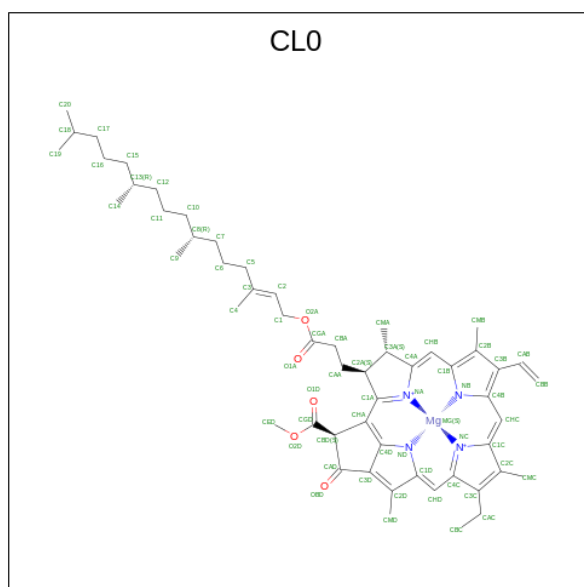
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

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

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

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

- Molecule 11 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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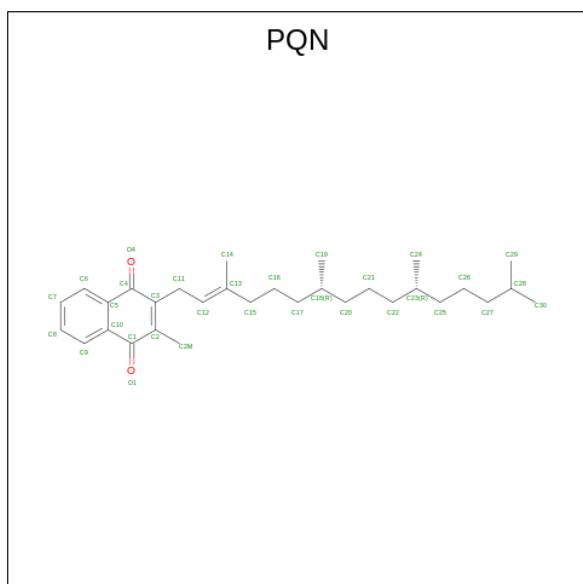
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	A	1	2407	1977	43	172	215	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0
12	B	1	1900	1580	32	128	160	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
12	B	1	Total 1900	C 1580	Mg 32	N 128	O 160	0
12	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	L	1	Total 163	C 133	Mg 3	N 12	O 15	0
12	L	1	Total 163	C 133	Mg 3	N 12	O 15	0
12	L	1	Total 163	C 133	Mg 3	N 12	O 15	0

- Molecule 13 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



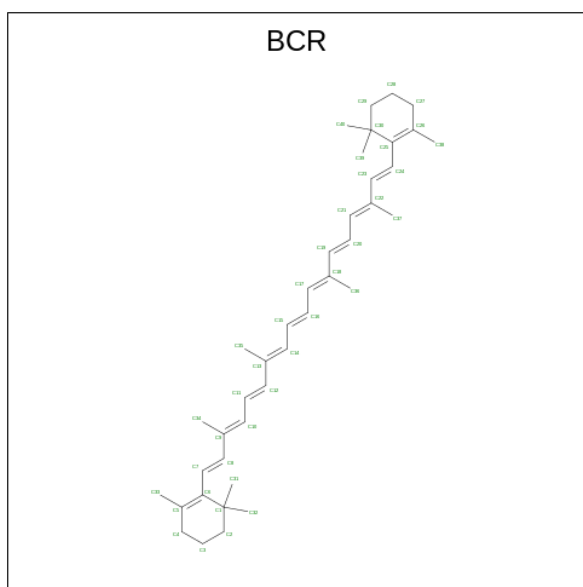
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
13	A	1	Total 33	C 31	O 2	0
13	B	1	Total 33	C 31	O 2	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms	AltConf
14	A	1	Total Fe S 8 4 4	0
14	C	1	Total Fe S 16 8 8	0
14	C	1	Total Fe S 16 8 8	0

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



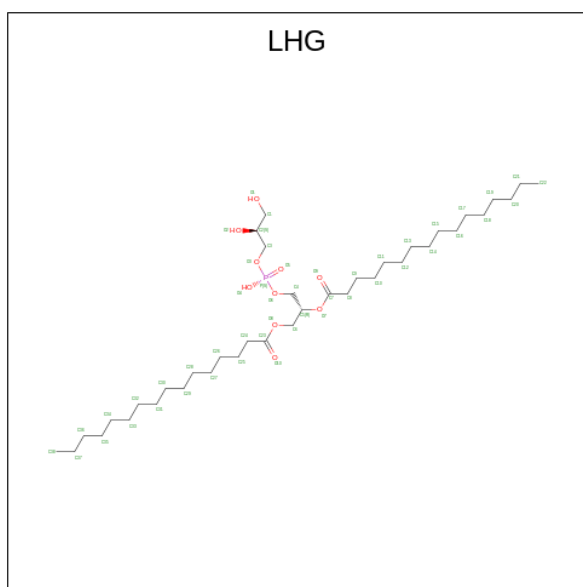
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 240 240	0

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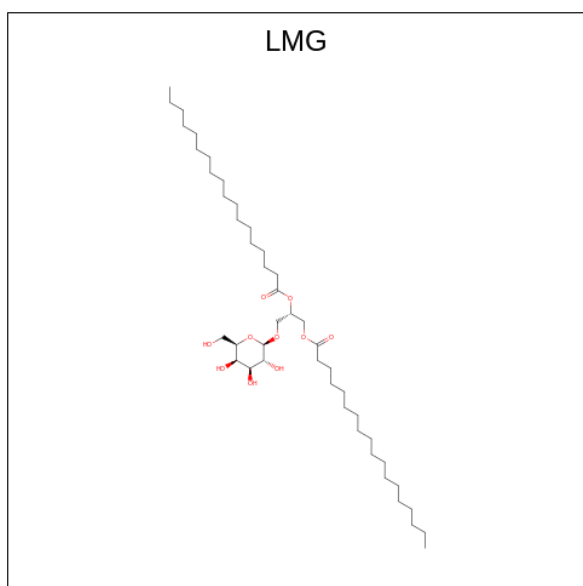
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total 240	C 240	0
15	A	1	Total 240	C 240	0
15	A	1	Total 240	C 240	0
15	A	1	Total 240	C 240	0
15	A	1	Total 240	C 240	0
15	B	1	Total 120	C 120	0
15	B	1	Total 120	C 120	0
15	B	1	Total 120	C 120	0
15	F	1	Total 80	C 80	0
15	F	1	Total 80	C 80	0
15	I	1	Total 40	C 40	0
15	J	1	Total 120	C 120	0
15	J	1	Total 120	C 120	0
15	J	1	Total 120	C 120	0
15	L	1	Total 120	C 120	0
15	L	1	Total 120	C 120	0
15	L	1	Total 120	C 120	0
15	M	1	Total 40	C 40	0

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).

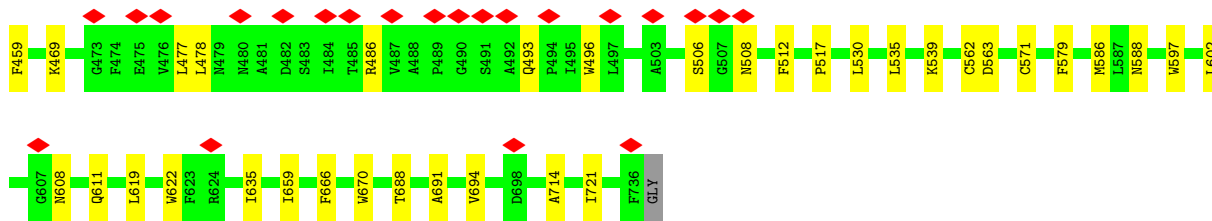


Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
16	A	1	76	54	20	2	0
16	A	1	76	54	20	2	0

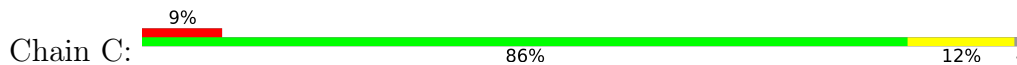
- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



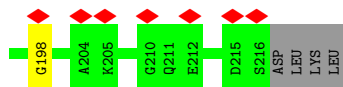
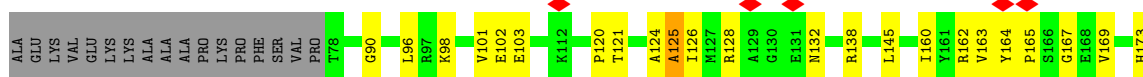
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	B	1	55	45	10	0



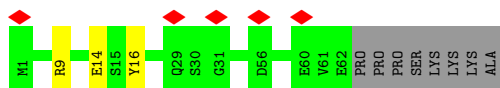
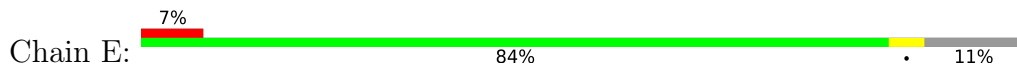
• Molecule 3: Photosystem I iron-sulfur center



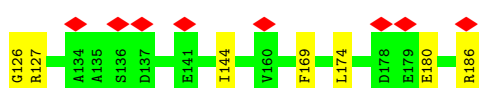
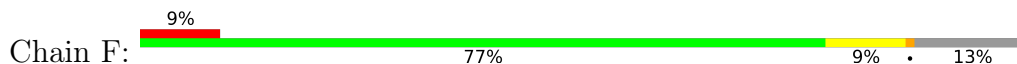
• Molecule 4: Photosystem I reaction center subunit II, cyanelle



• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III



• Molecule 7: Photosystem I reaction center subunit VIII

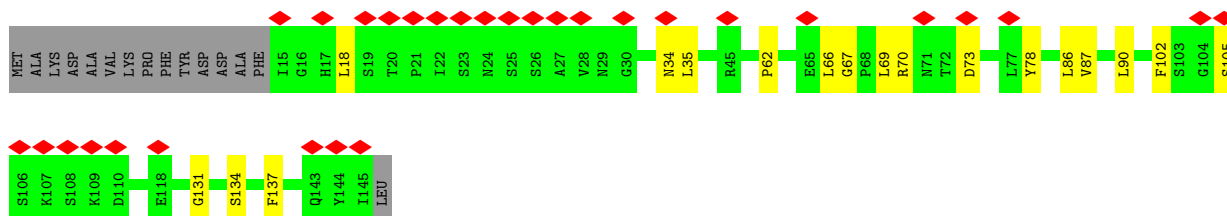
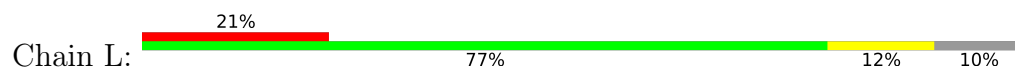




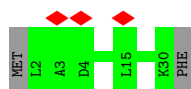
- Molecule 8: Photosystem I reaction center subunit IX



- 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/6000	0.47	0/8177
2	B	0.33	0/5820	0.62	1/7955 (0.0%)
3	C	0.35	0/611	0.74	0/828
4	D	0.31	0/1105	0.67	1/1489 (0.1%)
5	E	0.29	0/516	0.49	0/696
6	F	0.26	0/1281	0.49	0/1733
7	I	0.31	0/232	0.60	0/319
8	J	0.28	0/300	0.55	0/410
9	L	0.28	0/988	0.56	2/1342 (0.1%)
10	M	0.26	0/217	0.49	0/295
All	All	0.31	0/17070	0.56	4/23244 (0.0%)

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.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	69	LEU	CA-CB-CG	6.07	129.25	115.30
2	B	93	ASP	CB-CG-OD1	5.33	123.09	118.30
4	D	125	ALA	C-N-CA	5.11	134.47	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	L	73	ASP	C-N-CA	5.08	132.97	122.30

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	96	0
2	B	5622	0	5406	71	0
3	C	601	0	576	7	0
4	D	1082	0	1099	15	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	6	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	103	0
12	B	1900	0	1927	89	0
12	F	45	0	33	1	0
12	J	45	0	33	1	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
15	A	240	0	336	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	B	120	0	168	8	0
15	F	80	0	112	7	0
15	I	40	0	56	5	0
15	J	120	0	168	8	0
15	L	120	0	168	11	0
15	M	40	0	56	2	0
16	A	76	0	98	3	0
17	B	55	0	86	7	0
All	All	22177	0	22059	358	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 358 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%)	51 83
2	B	702/737 (95%)	669 (95%)	31 (4%)	2 (0%)	41 74
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	12 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	137/220 (62%)	114 (83%)	21 (15%)	2 (2%)	10	44
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%)	44	74

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	598/610 (98%)	596 (100%)	2 (0%)	92	96
2	B	574/596 (96%)	568 (99%)	6 (1%)	76	90
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%)	27 (100%)	0	100	100
8	J	32/35 (91%)	32 (100%)	0	100	100
9	L	99/111 (89%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	M	21/23 (91%)	21 (100%)	0	100	100
All	All	1723/1866 (92%)	1715 (100%)	8 (0%)	89	95

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	694	VAL
2	B	602	LEU
2	B	571	CYS
2	B	539	LYS
2	B	579	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	611	GLN
4	D	148	GLN
2	B	675	GLN
5	E	52	ASN
1	A	350	HIS

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 monosaccharides 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	B	808	-	65,73,73	2.00	16 (24%)	76,113,113	2.77	26 (34%)
12	CLA	A	812	-	54,62,73	2.27	17 (31%)	62,99,113	2.91	27 (43%)
12	CLA	A	836	1	45,53,73	2.49	17 (37%)	52,89,113	3.24	25 (48%)
12	CLA	A	830	-	65,73,73	2.02	16 (24%)	76,113,113	2.72	28 (36%)
12	CLA	L	203	-	65,73,73	1.99	16 (24%)	76,113,113	2.76	26 (34%)
12	CLA	A	805	-	65,73,73	2.03	15 (23%)	76,113,113	2.72	31 (40%)
15	BCR	M	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	5 (8%)
12	CLA	A	825	-	65,73,73	1.98	18 (27%)	76,113,113	2.62	28 (36%)
12	CLA	A	802	-	45,53,73	2.44	15 (33%)	52,89,113	3.20	26 (50%)
12	CLA	A	823	-	51,59,73	2.33	17 (33%)	59,96,113	3.02	28 (47%)
12	CLA	A	854	-	65,73,73	1.98	17 (26%)	76,113,113	2.85	30 (39%)
12	CLA	J	101	8	45,53,73	2.47	17 (37%)	52,89,113	3.17	25 (48%)
15	BCR	A	850	-	41,41,41	1.11	2 (4%)	56,56,56	1.33	7 (12%)
15	BCR	F	202	-	41,41,41	1.02	2 (4%)	56,56,56	1.21	4 (7%)
12	CLA	A	840	-	65,73,73	2.06	17 (26%)	76,113,113	2.64	29 (38%)
12	CLA	A	817	-	65,73,73	2.04	15 (23%)	76,113,113	2.75	25 (32%)
12	CLA	B	810	2	65,73,73	2.01	16 (24%)	76,113,113	2.57	29 (38%)
17	LMG	B	837	-	55,55,55	0.78	1 (1%)	63,63,63	1.37	7 (11%)
12	CLA	A	815	-	45,53,73	2.48	16 (35%)	52,89,113	3.18	23 (44%)
12	CLA	B	828	-	46,54,73	2.38	17 (36%)	53,90,113	3.22	25 (47%)
12	CLA	A	827	-	65,73,73	1.99	17 (26%)	76,113,113	2.77	28 (36%)
13	PQN	A	844	-	34,34,34	1.54	2 (5%)	42,45,45	1.04	2 (4%)
12	CLA	B	815	-	45,53,73	2.46	15 (33%)	52,89,113	3.18	24 (46%)
12	CLA	A	811	-	65,73,73	2.04	16 (24%)	76,113,113	2.74	26 (34%)
12	CLA	B	801	-	65,73,73	1.99	16 (24%)	76,113,113	2.82	28 (36%)
15	BCR	B	835	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	A	841	-	51,59,73	2.34	16 (31%)	59,96,113	3.09	27 (45%)
12	CLA	A	831	-	50,58,73	2.32	17 (34%)	58,95,113	3.04	27 (46%)
15	BCR	B	834	-	41,41,41	1.08	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	B	813	-	65,73,73	2.04	16 (24%)	76,113,113	2.72	28 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	830	-	47,55,73	2.35	17 (36%)	54,91,113	3.16	24 (44%)
12	CLA	B	825	-	65,73,73	1.99	17 (26%)	76,113,113	2.92	28 (36%)
12	CLA	B	805	2	54,62,73	2.26	17 (31%)	62,99,113	2.99	26 (41%)
12	CLA	B	802	-	65,73,73	2.03	17 (26%)	76,113,113	2.62	28 (36%)
12	CLA	A	806	-	65,73,73	1.99	17 (26%)	76,113,113	2.83	28 (36%)
16	LHG	A	853	12	26,26,48	0.83	0	29,32,54	1.32	3 (10%)
12	CLA	A	833	-	65,73,73	2.02	16 (24%)	76,113,113	2.74	31 (40%)
12	CLA	A	834	-	65,73,73	2.02	15 (23%)	76,113,113	2.80	25 (32%)
12	CLA	A	819	-	65,73,73	2.05	16 (24%)	76,113,113	2.64	27 (35%)
12	CLA	A	832	-	65,73,73	2.05	18 (27%)	76,113,113	2.77	28 (36%)
16	LHG	A	852	-	48,48,48	0.66	1 (2%)	51,54,54	1.28	7 (13%)
12	CLA	B	807	-	65,73,73	2.02	16 (24%)	76,113,113	2.78	28 (36%)
12	CLA	A	803	-	45,53,73	2.45	17 (37%)	52,89,113	3.15	25 (48%)
12	CLA	A	826	-	55,63,73	2.22	16 (29%)	64,101,113	2.98	30 (46%)
15	BCR	A	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.23	6 (10%)
12	CLA	A	816	-	49,57,73	2.38	17 (34%)	55,93,113	3.07	24 (43%)
15	BCR	A	847	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	7 (12%)
15	BCR	A	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.33	7 (12%)
12	CLA	B	811	-	65,73,73	2.04	17 (26%)	76,113,113	2.67	33 (43%)
14	SF4	C	102	3	0,12,12	-	-	-	-	-
12	CLA	B	829	-	65,73,73	1.99	16 (24%)	76,113,113	2.76	28 (36%)
13	PQN	B	833	-	34,34,34	1.50	2 (5%)	42,45,45	1.21	4 (9%)
12	CLA	A	821	-	65,73,73	2.01	15 (23%)	76,113,113	2.66	26 (34%)
12	CLA	B	803	-	65,73,73	1.97	16 (24%)	76,113,113	2.78	31 (40%)
12	CLA	L	204	-	52,60,73	2.28	16 (30%)	60,97,113	3.09	26 (43%)
12	CLA	B	819	-	46,54,73	2.48	16 (34%)	53,90,113	3.27	26 (49%)
15	BCR	B	836	-	41,41,41	1.15	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	A	822	-	46,54,73	2.42	16 (34%)	53,90,113	3.18	24 (45%)
12	CLA	B	812	-	45,53,73	2.48	16 (35%)	52,89,113	3.16	24 (46%)
12	CLA	B	818	-	60,68,73	2.12	17 (28%)	70,107,113	2.84	29 (41%)
12	CLA	A	828	-	65,73,73	2.05	17 (26%)	76,113,113	2.68	27 (35%)
12	CLA	B	832	-	65,73,73	2.04	16 (24%)	76,113,113	2.70	28 (36%)
15	BCR	J	104	-	41,41,41	1.06	2 (4%)	56,56,56	1.29	6 (10%)
12	CLA	B	806	-	65,73,73	2.02	14 (21%)	76,113,113	2.75	28 (36%)
12	CLA	A	818	-	54,62,73	2.24	16 (29%)	62,99,113	2.92	26 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	5 (8%)
12	CLA	A	820	-	61,69,73	2.14	16 (26%)	71,108,113	2.73	27 (38%)
14	SF4	A	845	2,1	0,12,12	-	-	-	-	-
12	CLA	A	808	1	65,73,73	2.05	17 (26%)	76,113,113	2.65	26 (34%)
12	CLA	B	826	-	58,66,73	2.14	16 (27%)	67,104,113	2.88	26 (38%)
15	BCR	A	846	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	9 (16%)
12	CLA	B	823	-	65,73,73	2.06	16 (24%)	76,113,113	2.76	27 (35%)
12	CLA	B	820	-	65,73,73	2.04	16 (24%)	76,113,113	2.82	28 (36%)
12	CLA	A	804	-	45,53,73	2.44	15 (33%)	52,89,113	3.24	26 (50%)
11	CLO	A	801	-	65,73,73	1.97	16 (24%)	76,113,113	2.74	31 (40%)
12	CLA	L	202	9	46,54,73	2.47	16 (34%)	53,90,113	3.19	24 (45%)
15	BCR	F	201	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	5 (8%)
15	BCR	J	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.39	8 (14%)
15	BCR	L	201	-	41,41,41	1.10	2 (4%)	56,56,56	1.22	5 (8%)
12	CLA	B	821	-	65,73,73	2.02	16 (24%)	76,113,113	2.77	27 (35%)
12	CLA	A	838	-	56,64,73	2.19	16 (28%)	65,102,113	2.94	28 (43%)
12	CLA	A	837	-	51,59,73	2.32	17 (33%)	59,96,113	3.03	25 (42%)
12	CLA	B	824	-	49,57,73	2.40	17 (34%)	55,93,113	3.30	25 (45%)
12	CLA	B	804	-	65,73,73	1.97	16 (24%)	76,113,113	2.61	25 (32%)
12	CLA	A	813	-	45,53,73	2.45	18 (40%)	52,89,113	3.09	23 (44%)
12	CLA	B	816	-	55,63,73	2.29	18 (32%)	64,101,113	2.99	26 (40%)
12	CLA	A	810	-	45,53,73	2.46	16 (35%)	52,89,113	3.17	23 (44%)
12	CLA	B	814	-	56,64,73	2.18	17 (30%)	65,102,113	2.85	27 (41%)
15	BCR	I	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	8 (14%)
12	CLA	F	203	6	45,53,73	2.50	16 (35%)	52,89,113	3.13	24 (46%)
15	BCR	L	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.35	10 (17%)
12	CLA	A	814	-	45,53,73	2.45	17 (37%)	52,89,113	3.15	26 (50%)
12	CLA	A	809	1	45,53,73	2.42	17 (37%)	52,89,113	3.09	25 (48%)
12	CLA	A	829	-	65,73,73	1.98	16 (24%)	76,113,113	2.62	28 (36%)
12	CLA	A	843	16	52,60,73	2.31	18 (34%)	60,97,113	3.02	23 (38%)
12	CLA	B	822	-	65,73,73	2.00	17 (26%)	76,113,113	2.60	27 (35%)
15	BCR	L	205	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	6 (10%)
12	CLA	B	831	-	65,73,73	2.06	16 (24%)	76,113,113	2.70	29 (38%)
12	CLA	A	835	1	54,62,73	2.21	16 (29%)	62,99,113	2.99	27 (43%)
12	CLA	A	824	-	47,55,73	2.39	16 (34%)	54,91,113	3.11	26 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	817	-	59,67,73	2.15	16 (27%)	68,105,113	2.87	26 (38%)
12	CLA	A	839	-	50,58,73	2.28	18 (36%)	58,95,113	3.17	29 (50%)
12	CLA	B	827	-	45,53,73	2.46	16 (35%)	52,89,113	3.21	24 (46%)
12	CLA	B	809	-	65,73,73	1.98	15 (23%)	76,113,113	2.84	29 (38%)
14	SF4	C	101	3	0,12,12	-	-	-	-	-
12	CLA	A	842	-	65,73,73	2.04	18 (27%)	76,113,113	2.66	25 (32%)
15	BCR	A	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.43	10 (17%)
12	CLA	A	807	-	51,59,73	2.33	16 (31%)	59,96,113	3.03	28 (47%)

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	B	808	-	1/1/15/20	3/37/115/115	-
12	CLA	A	812	-	-	8/24/102/115	-
12	CLA	A	836	1	1/1/11/20	5/13/91/115	-
12	CLA	A	830	-	1/1/15/20	8/37/115/115	-
12	CLA	L	203	-	-	11/37/115/115	-
12	CLA	A	805	-	1/1/15/20	16/37/115/115	-
15	BCR	M	101	-	-	13/29/63/63	0/2/2/2
12	CLA	A	825	-	1/1/15/20	12/37/115/115	-
12	CLA	A	802	-	1/1/11/20	3/13/91/115	-
12	CLA	J	101	8	1/1/11/20	6/13/91/115	-
12	CLA	A	854	-	1/1/15/20	7/37/115/115	-
12	CLA	A	823	-	-	8/21/99/115	-
15	BCR	A	850	-	-	10/29/63/63	0/2/2/2
15	BCR	F	202	-	-	11/29/63/63	0/2/2/2
12	CLA	A	840	-	1/1/15/20	14/37/115/115	-
12	CLA	A	817	-	-	8/37/115/115	-
12	CLA	B	810	2	1/1/15/20	12/37/115/115	-
17	LMG	B	837	-	-	24/50/70/70	0/1/1/1
12	CLA	B	828	-	1/1/11/20	4/15/93/115	-
12	CLA	A	815	-	-	3/13/91/115	-
12	CLA	A	827	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	PQN	A	844	-	-	2/23/43/43	0/2/2/2
12	CLA	B	815	-	1/1/11/20	4/13/91/115	-
12	CLA	A	811	-	1/1/15/20	10/37/115/115	-
12	CLA	B	801	-	1/1/15/20	5/37/115/115	-
15	BCR	B	835	-	-	12/29/63/63	0/2/2/2
12	CLA	A	841	-	1/1/12/20	5/21/99/115	-
12	CLA	A	831	-	1/1/12/20	5/19/97/115	-
15	BCR	B	834	-	-	10/29/63/63	0/2/2/2
12	CLA	B	813	-	1/1/15/20	18/37/115/115	-
12	CLA	B	830	-	1/1/11/20	3/16/94/115	-
12	CLA	B	825	-	1/1/15/20	13/37/115/115	-
12	CLA	B	805	2	1/1/12/20	4/24/102/115	-
12	CLA	B	802	-	1/1/15/20	12/37/115/115	-
12	CLA	A	806	-	1/1/15/20	12/37/115/115	-
16	LHG	A	853	12	-	10/31/31/53	-
12	CLA	A	833	-	1/1/15/20	7/37/115/115	-
12	CLA	A	834	-	-	14/37/115/115	-
12	CLA	A	819	-	1/1/15/20	12/37/115/115	-
12	CLA	A	832	-	1/1/15/20	9/37/115/115	-
16	LHG	A	852	-	-	22/53/53/53	-
12	CLA	B	807	-	1/1/15/20	14/37/115/115	-
12	CLA	A	803	-	1/1/11/20	6/13/91/115	-
12	CLA	A	826	-	1/1/13/20	8/25/103/115	-
15	BCR	A	851	-	-	18/29/63/63	0/2/2/2
12	CLA	A	816	-	1/1/11/20	2/18/96/115	-
15	BCR	A	847	-	-	8/29/63/63	0/2/2/2
15	BCR	A	849	-	-	7/29/63/63	0/2/2/2
12	CLA	B	811	-	1/1/15/20	9/37/115/115	-
14	SF4	C	102	3	-	-	0/6/5/5
12	CLA	B	829	-	1/1/15/20	14/37/115/115	-
13	PQN	B	833	-	-	5/23/43/43	0/2/2/2
12	CLA	A	821	-	1/1/15/20	13/37/115/115	-
12	CLA	B	803	-	1/1/15/20	11/37/115/115	-
12	CLA	L	204	-	-	7/22/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	819	-	1/1/11/20	6/15/93/115	-
15	BCR	B	836	-	-	10/29/63/63	0/2/2/2
12	CLA	A	822	-	-	3/15/93/115	-
12	CLA	B	812	-	1/1/11/20	1/13/91/115	-
12	CLA	B	818	-	1/1/14/20	5/31/109/115	-
12	CLA	A	828	-	1/1/15/20	12/37/115/115	-
12	CLA	B	832	-	1/1/15/20	16/37/115/115	-
15	BCR	J	104	-	-	13/29/63/63	0/2/2/2
12	CLA	B	806	-	1/1/15/20	15/37/115/115	-
12	CLA	A	818	-	1/1/12/20	9/24/102/115	-
15	BCR	J	102	-	-	14/29/63/63	0/2/2/2
12	CLA	A	820	-	1/1/14/20	8/33/111/115	-
14	SF4	A	845	2,1	-	-	0/6/5/5
12	CLA	A	808	1	1/1/15/20	17/37/115/115	-
12	CLA	B	826	-	1/1/13/20	11/29/107/115	-
15	BCR	A	846	-	-	9/29/63/63	0/2/2/2
12	CLA	B	823	-	1/1/15/20	15/37/115/115	-
12	CLA	B	820	-	1/1/15/20	6/37/115/115	-
12	CLA	A	804	-	1/1/11/20	2/13/91/115	-
11	CL0	A	801	-	3/3/20/25	4/37/135/135	-
12	CLA	L	202	9	-	4/15/93/115	-
15	BCR	F	201	-	-	12/29/63/63	0/2/2/2
15	BCR	J	103	-	-	16/29/63/63	0/2/2/2
15	BCR	L	201	-	-	11/29/63/63	0/2/2/2
12	CLA	B	821	-	1/1/15/20	19/37/115/115	-
12	CLA	A	838	-	1/1/13/20	10/27/105/115	-
12	CLA	A	837	-	1/1/12/20	8/21/99/115	-
12	CLA	B	824	-	-	9/18/96/115	-
12	CLA	B	804	-	1/1/15/20	5/37/115/115	-
12	CLA	A	813	-	1/1/11/20	8/13/91/115	-
12	CLA	B	816	-	-	5/25/103/115	-
12	CLA	A	810	-	1/1/11/20	2/13/91/115	-
12	CLA	B	814	-	1/1/13/20	8/27/105/115	-
15	BCR	I	101	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	F	203	6	1/1/11/20	3/13/91/115	-
15	BCR	L	206	-	-	15/29/63/63	0/2/2/2
12	CLA	A	814	-	1/1/11/20	1/13/91/115	-
12	CLA	A	809	1	1/1/11/20	3/13/91/115	-
12	CLA	A	829	-	1/1/15/20	12/37/115/115	-
12	CLA	A	843	16	-	12/22/100/115	-
12	CLA	B	822	-	1/1/15/20	10/37/115/115	-
15	BCR	L	205	-	-	10/29/63/63	0/2/2/2
12	CLA	B	831	-	-	9/37/115/115	-
12	CLA	A	835	1	1/1/12/20	6/24/102/115	-
12	CLA	A	824	-	1/1/11/20	2/16/94/115	-
12	CLA	B	817	-	1/1/13/20	9/30/108/115	-
12	CLA	A	839	-	-	5/19/97/115	-
12	CLA	B	827	-	-	6/13/91/115	-
12	CLA	B	809	-	1/1/15/20	9/37/115/115	-
14	SF4	C	101	3	-	-	0/6/5/5
12	CLA	A	842	-	1/1/15/20	5/37/115/115	-
15	BCR	A	848	-	-	11/29/63/63	0/2/2/2
12	CLA	A	807	-	1/1/12/20	8/21/99/115	-

The worst 5 of 1370 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	816	CLA	C3B-C2B	6.54	1.49	1.40
12	A	837	CLA	C3B-C2B	6.27	1.49	1.40
12	B	805	CLA	C3B-C2B	6.19	1.49	1.40

The worst 5 of 2316 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	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
12	B	825	CLA	C2D-C1D-ND	9.58	117.16	110.10

5 of 68 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	801	CL0	NC
11	A	801	CL0	ND
11	A	801	CL0	NA
12	A	802	CLA	ND
12	A	803	CLA	ND

5 of 948 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	CHA-CBD-CGD-O1D
12	A	804	CLA	CHA-CBD-CGD-O2D
12	A	805	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

100 monomers are involved in 234 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	808	CLA	3	0
12	A	812	CLA	3	0
12	A	836	CLA	2	0
12	A	830	CLA	5	0
12	L	203	CLA	6	0
12	A	805	CLA	9	0
15	M	101	BCR	2	0
12	A	825	CLA	2	0
12	A	802	CLA	2	0
12	A	854	CLA	4	0
12	J	101	CLA	1	0
15	A	850	BCR	6	0
15	F	202	BCR	3	0
12	A	840	CLA	1	0
12	A	817	CLA	1	0
12	B	810	CLA	2	0
17	B	837	LMG	7	0
12	A	815	CLA	2	0
12	B	828	CLA	1	0
12	A	827	CLA	2	0
13	A	844	PQN	3	0
12	A	811	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	801	CLA	4	0
15	B	835	BCR	4	0
12	A	841	CLA	2	0
12	A	831	CLA	2	0
15	B	834	BCR	2	0
12	B	813	CLA	2	0
12	B	830	CLA	1	0
12	B	825	CLA	2	0
12	B	805	CLA	1	0
12	B	802	CLA	9	0
12	A	806	CLA	3	0
12	A	833	CLA	3	0
12	A	834	CLA	4	0
12	A	819	CLA	6	0
12	A	832	CLA	6	0
16	A	852	LHG	3	0
12	B	807	CLA	8	0
12	A	803	CLA	3	0
12	A	826	CLA	1	0
15	A	851	BCR	1	0
15	A	847	BCR	4	0
15	A	849	BCR	1	0
12	B	811	CLA	2	0
12	B	829	CLA	5	0
13	B	833	PQN	5	0
12	A	821	CLA	4	0
12	B	803	CLA	2	0
12	L	204	CLA	2	0
12	B	819	CLA	1	0
15	B	836	BCR	2	0
12	A	822	CLA	1	0
12	B	812	CLA	2	0
12	B	818	CLA	4	0
12	A	828	CLA	8	0
12	B	832	CLA	8	0
15	J	104	BCR	2	0
12	B	806	CLA	5	0
12	A	818	CLA	3	0
15	J	102	BCR	4	0
12	A	820	CLA	2	0
12	A	808	CLA	6	0
12	B	826	CLA	1	0

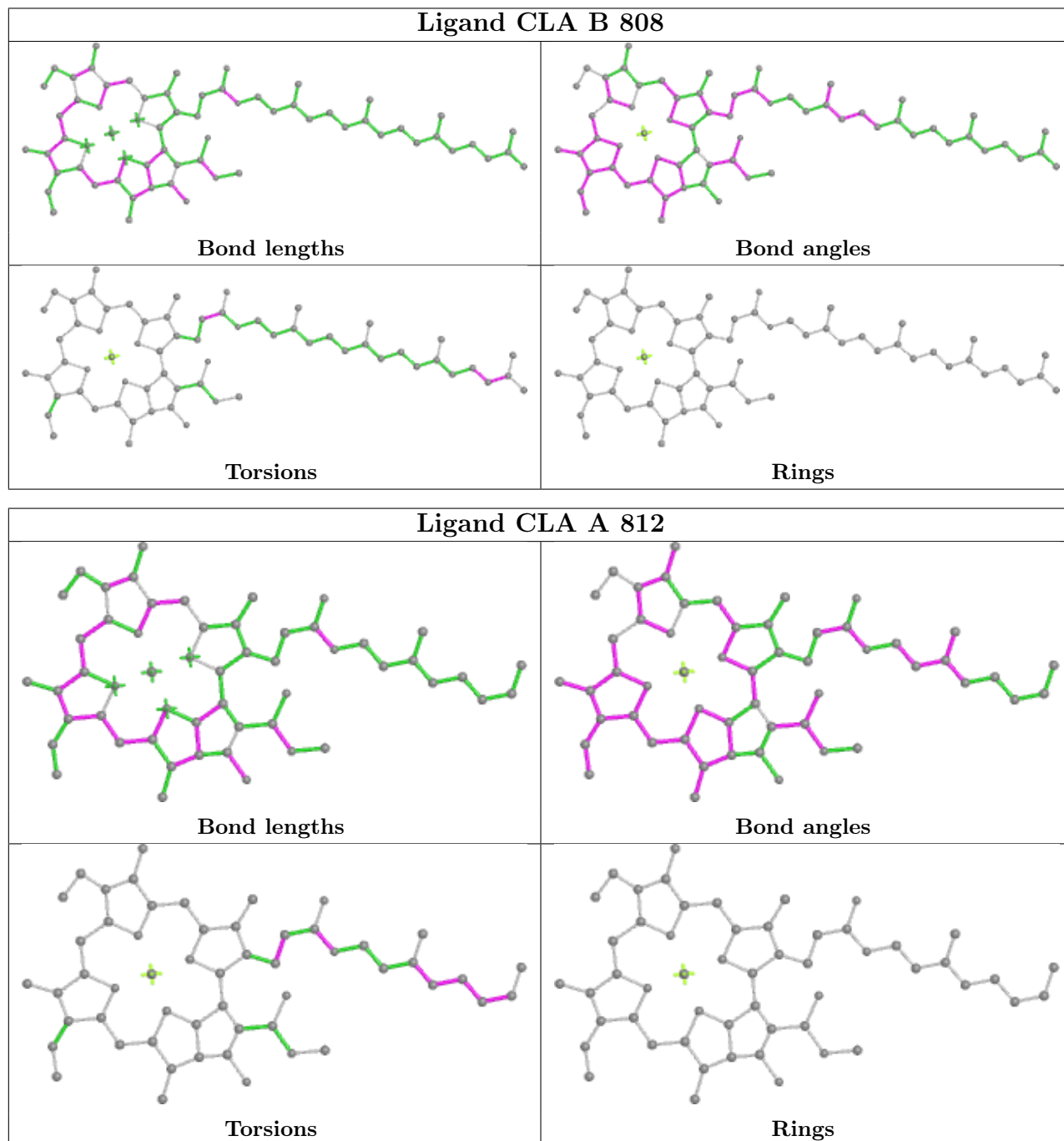
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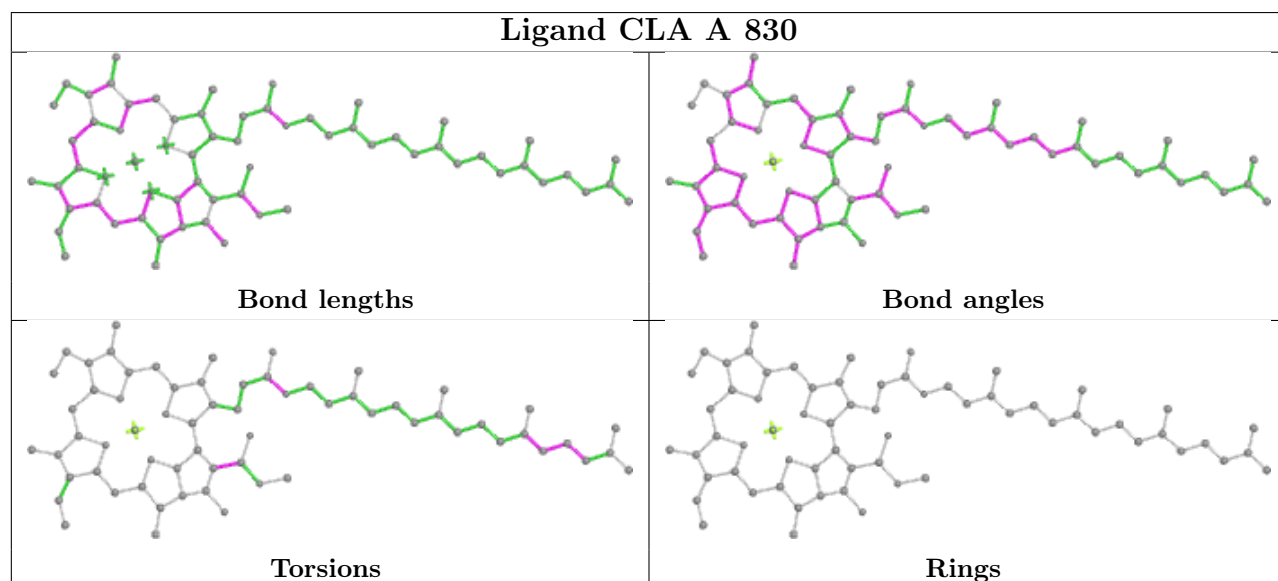
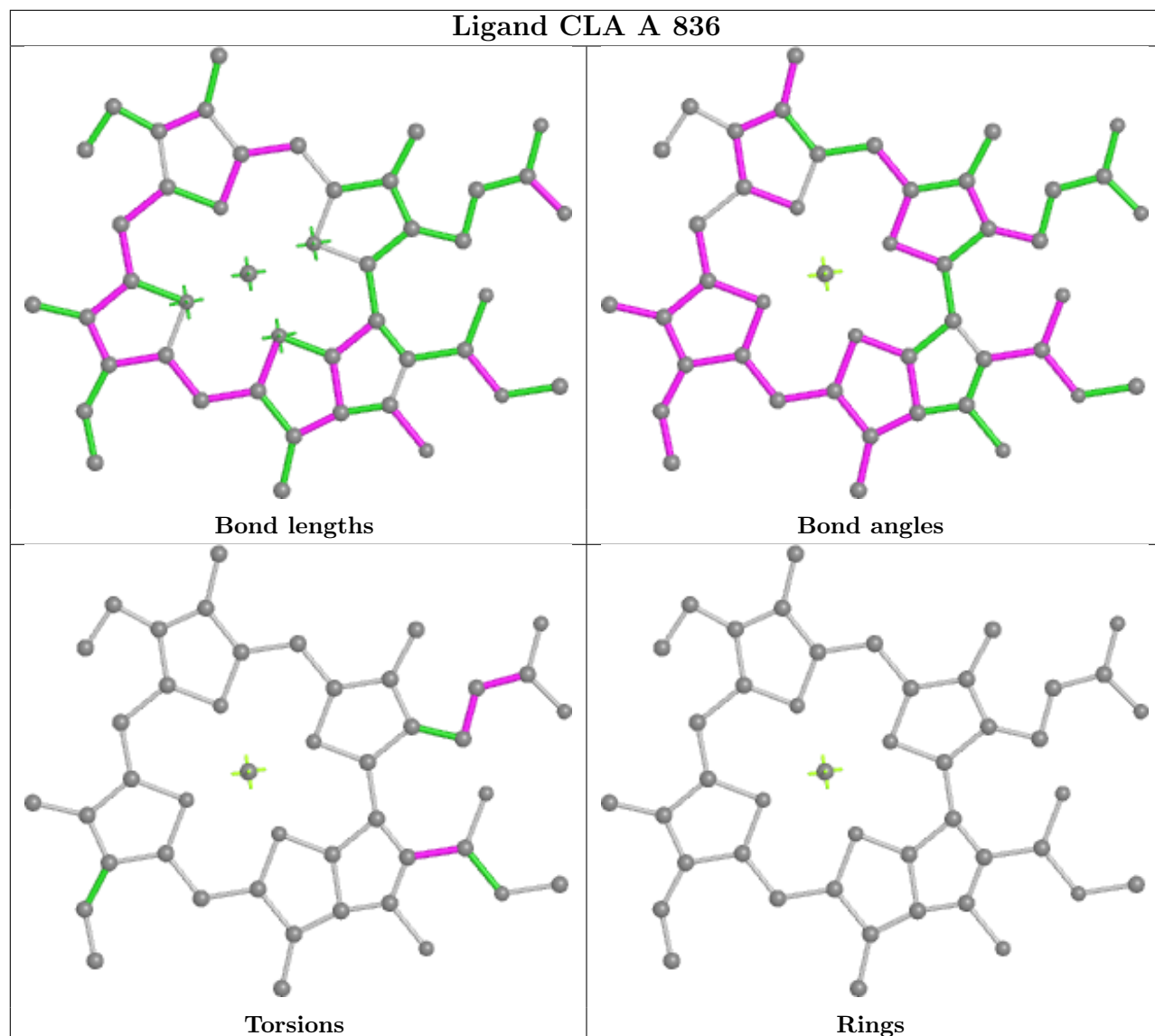
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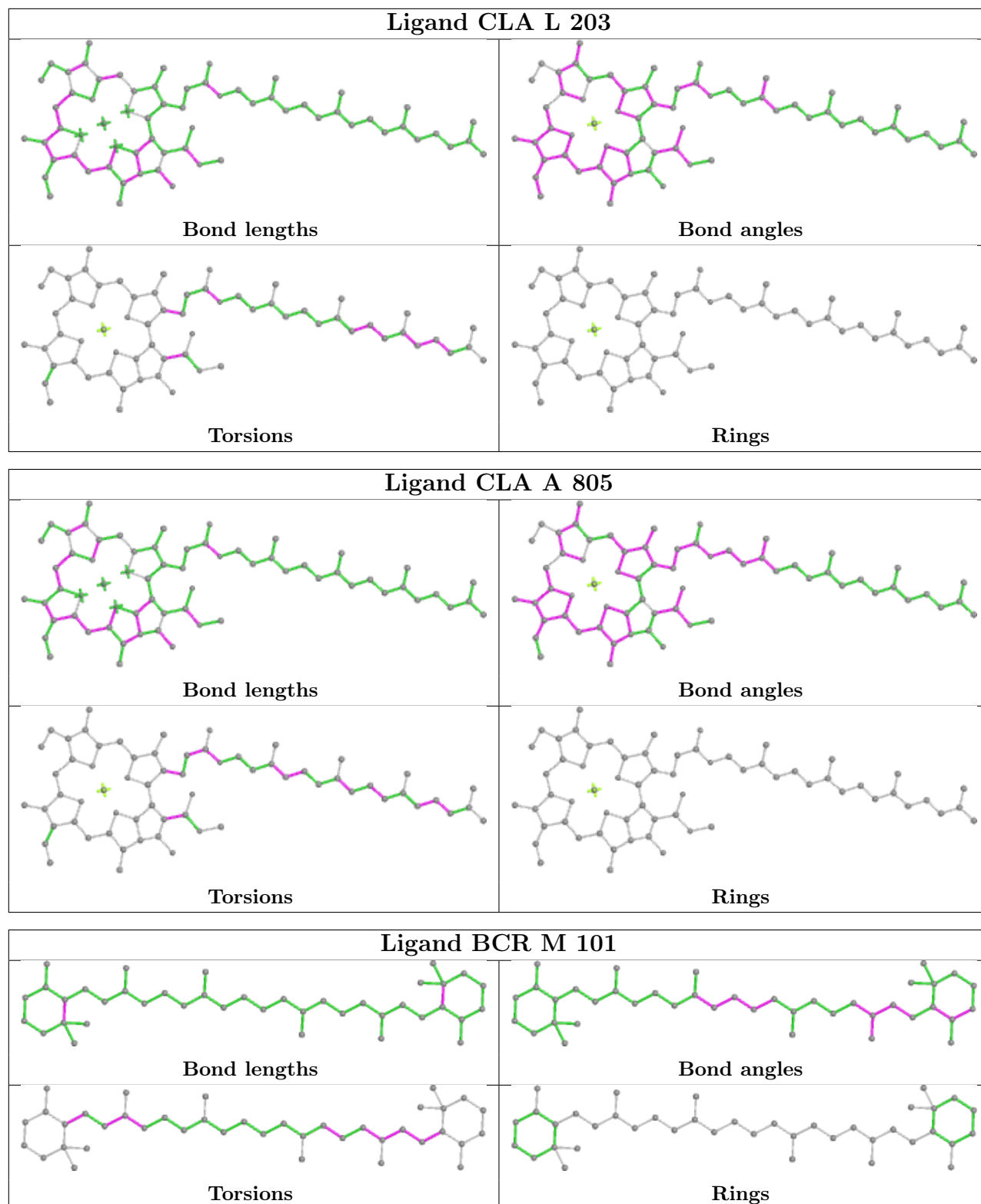
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	846	BCR	2	0
12	B	823	CLA	4	0
12	B	820	CLA	3	0
12	A	804	CLA	1	0
11	A	801	CL0	3	0
12	L	202	CLA	3	0
15	F	201	BCR	4	0
15	J	103	BCR	2	0
15	L	201	BCR	5	0
12	B	821	CLA	5	0
12	A	838	CLA	4	0
12	A	837	CLA	1	0
12	B	824	CLA	3	0
12	B	804	CLA	5	0
12	A	813	CLA	2	0
12	B	816	CLA	2	0
12	A	810	CLA	1	0
12	B	814	CLA	1	0
15	I	101	BCR	5	0
12	F	203	CLA	1	0
15	L	206	BCR	3	0
12	A	809	CLA	3	0
12	A	829	CLA	5	0
12	A	843	CLA	1	0
12	B	822	CLA	9	0
15	L	205	BCR	3	0
12	B	831	CLA	3	0
12	A	835	CLA	2	0
12	A	824	CLA	2	0
12	B	817	CLA	1	0
12	A	839	CLA	1	0
12	B	827	CLA	1	0
12	B	809	CLA	1	0
12	A	842	CLA	6	0
15	A	848	BCR	5	0
12	A	807	CLA	3	0

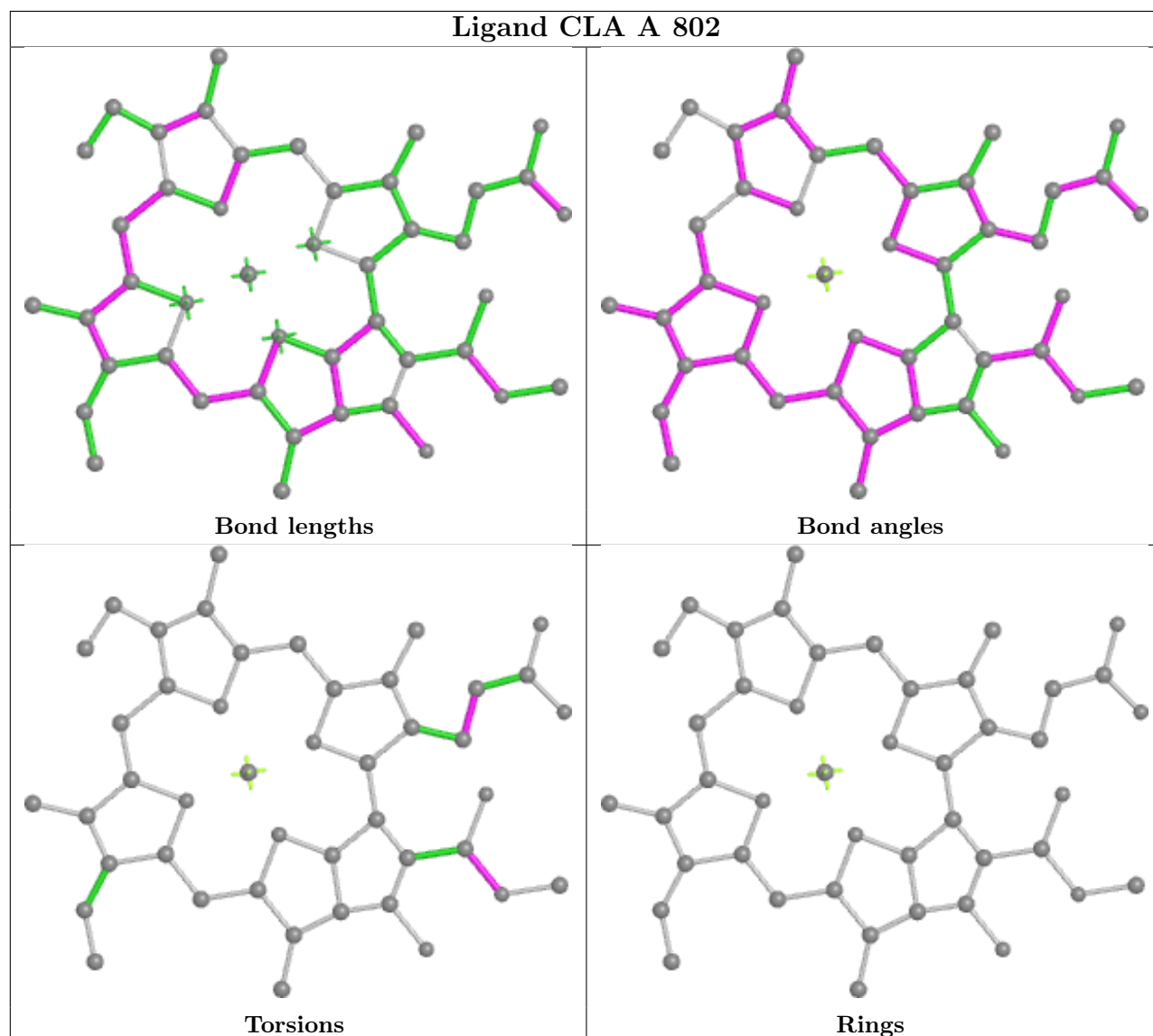
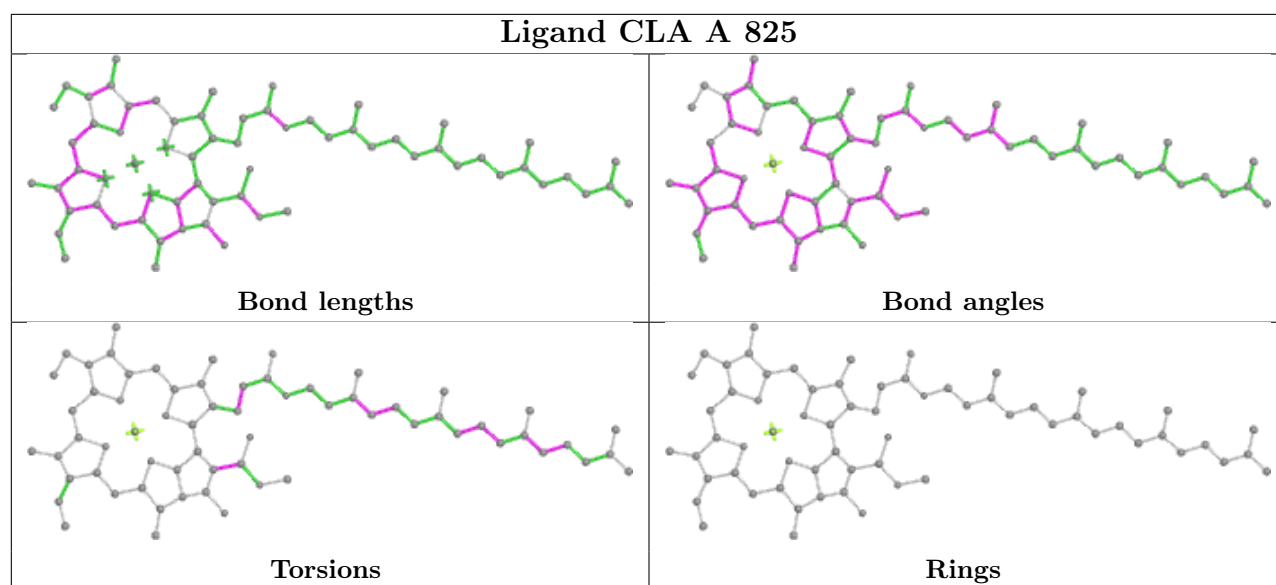
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

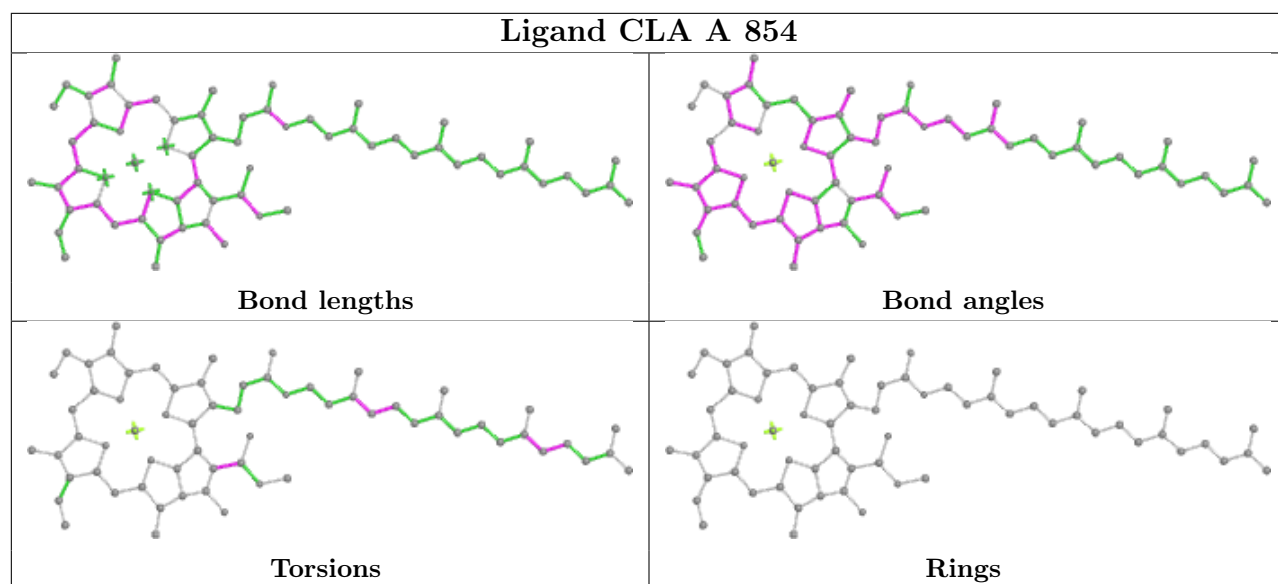
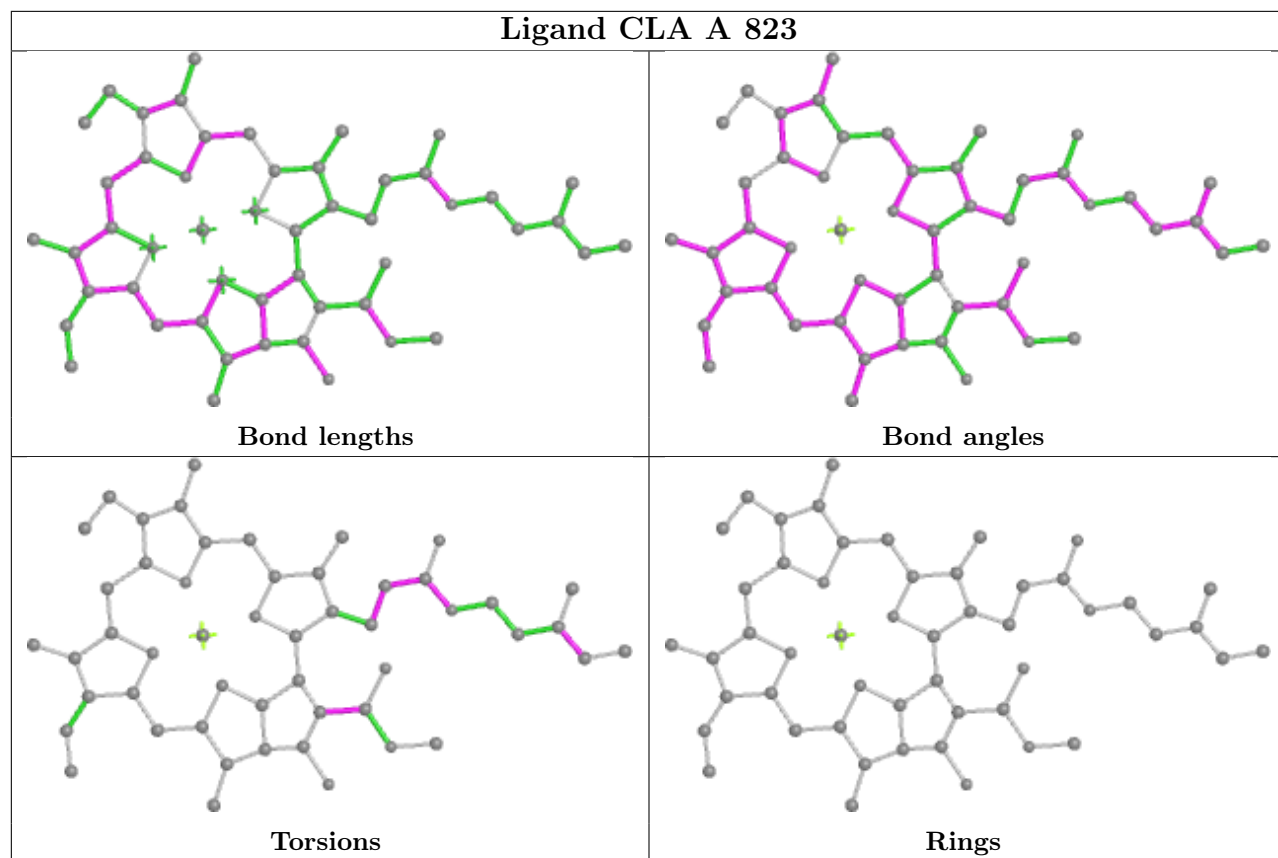
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

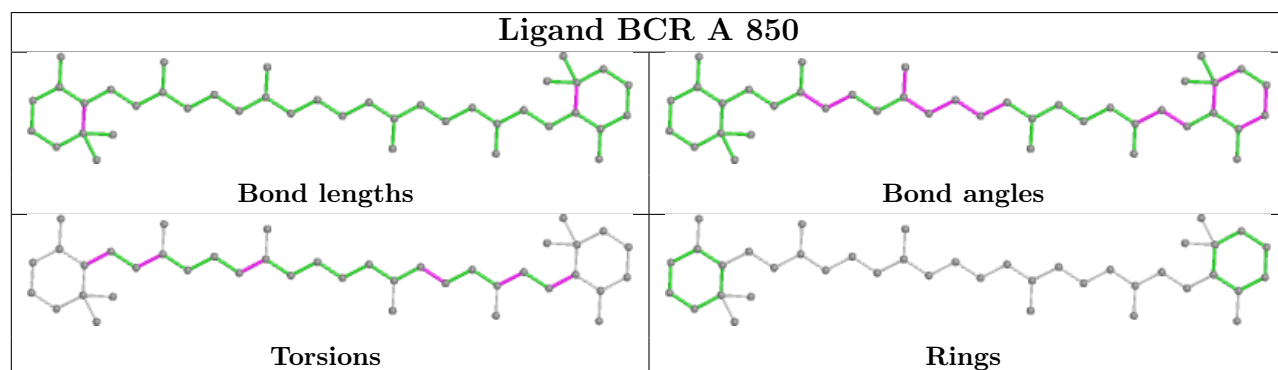
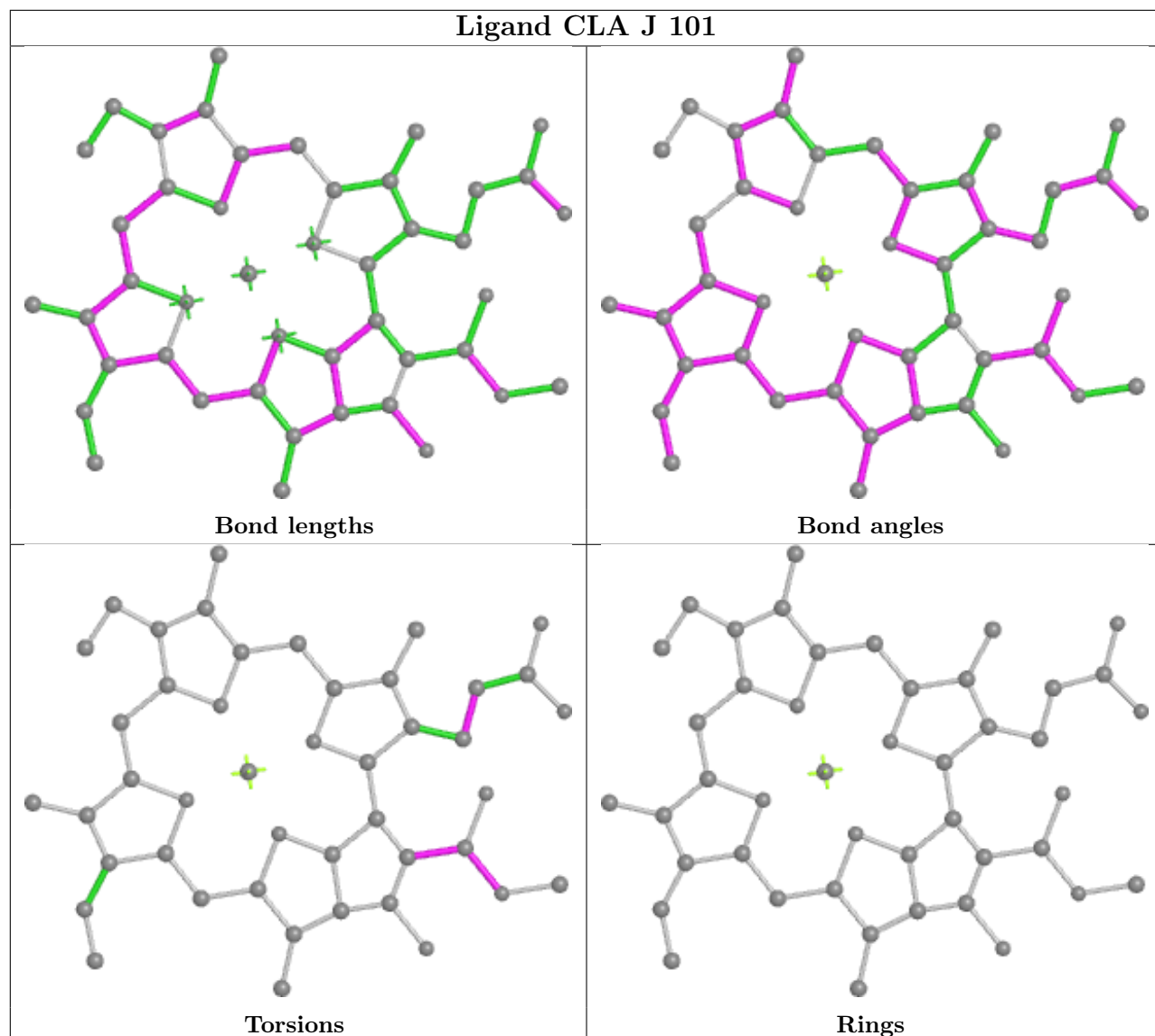


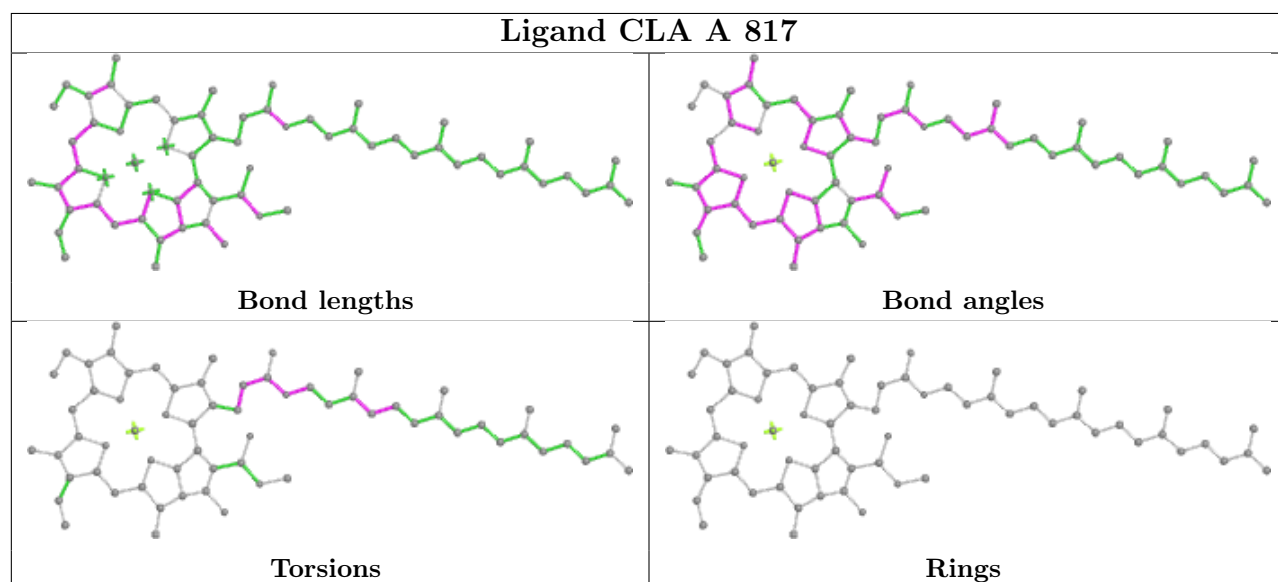
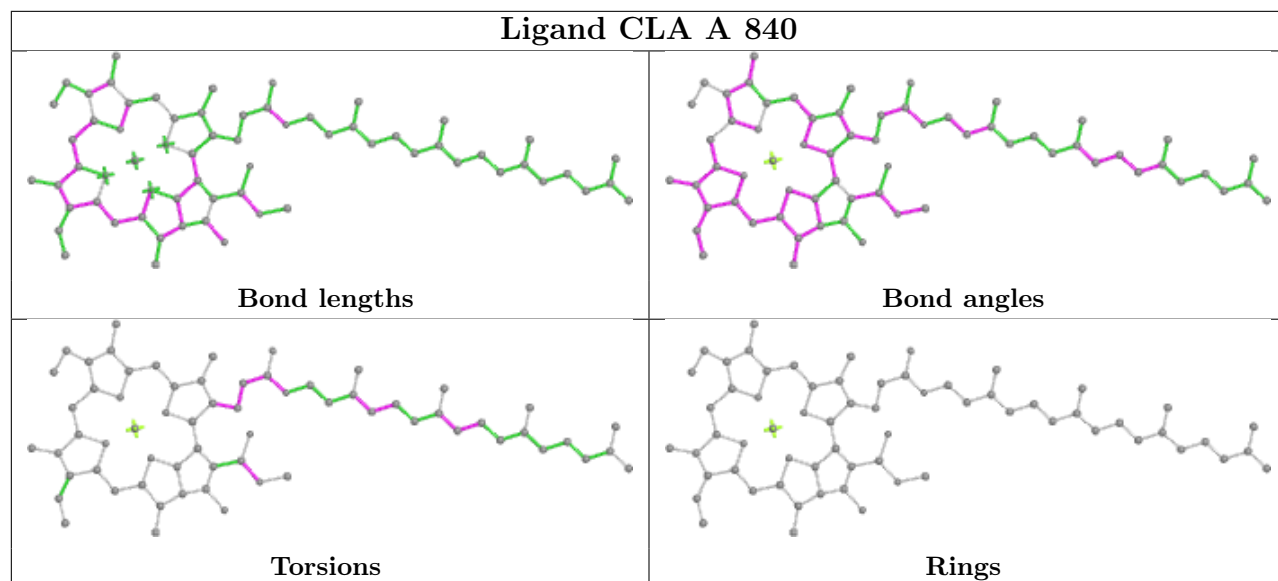
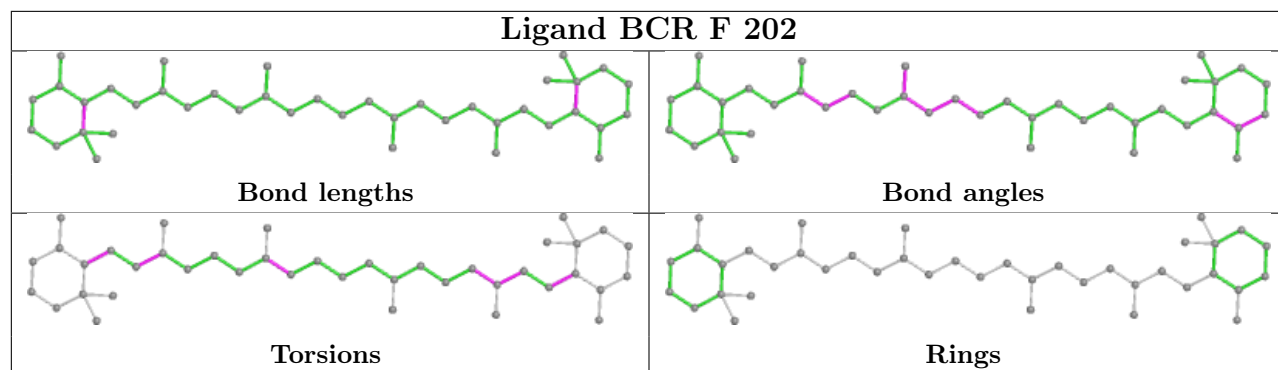


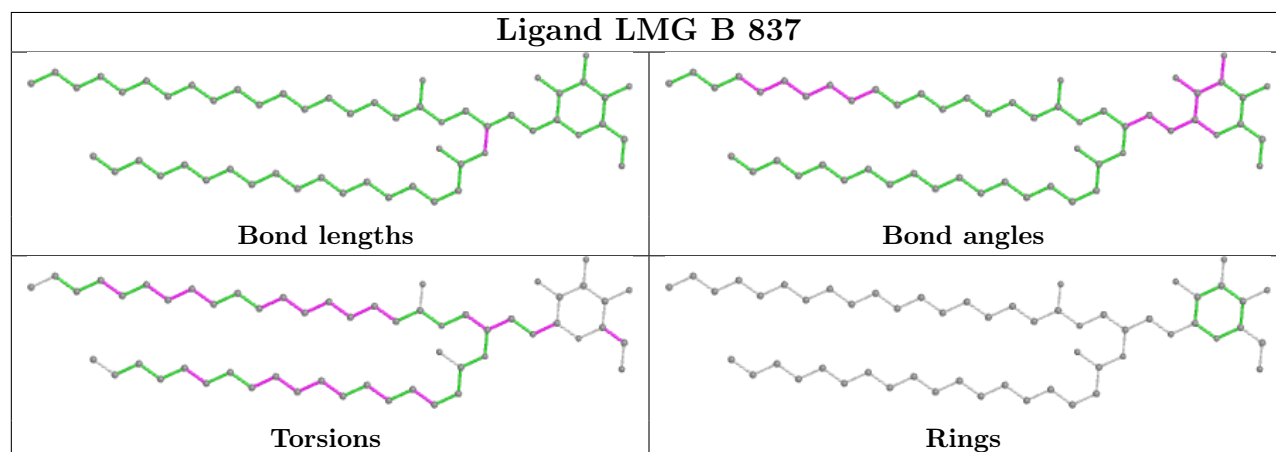
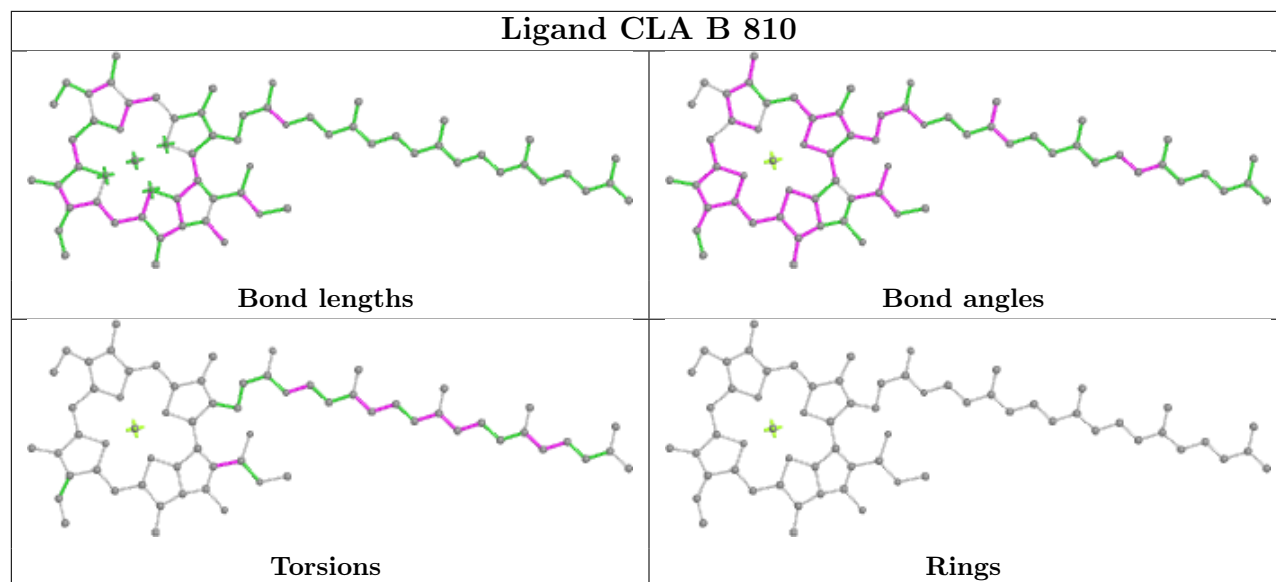


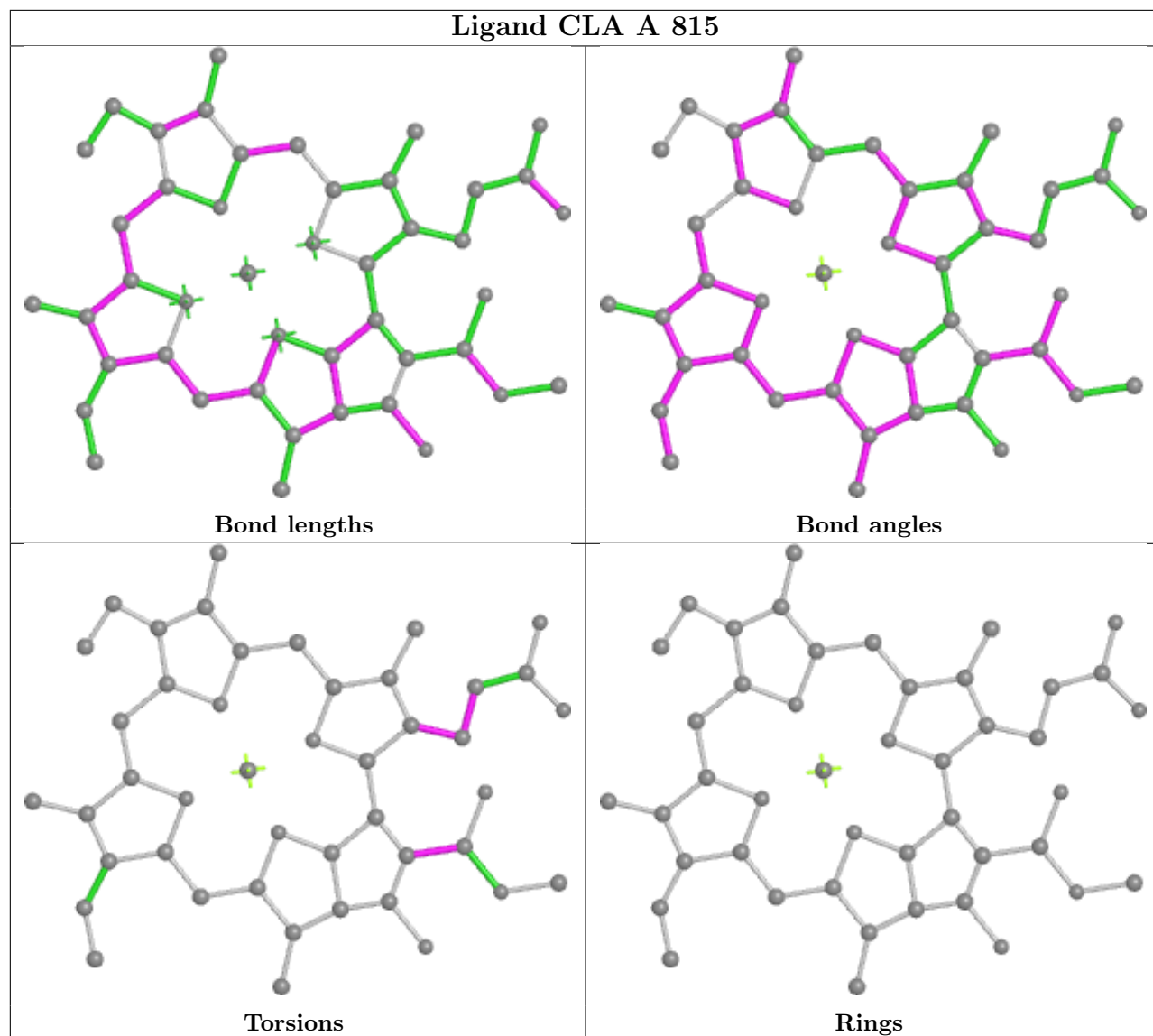


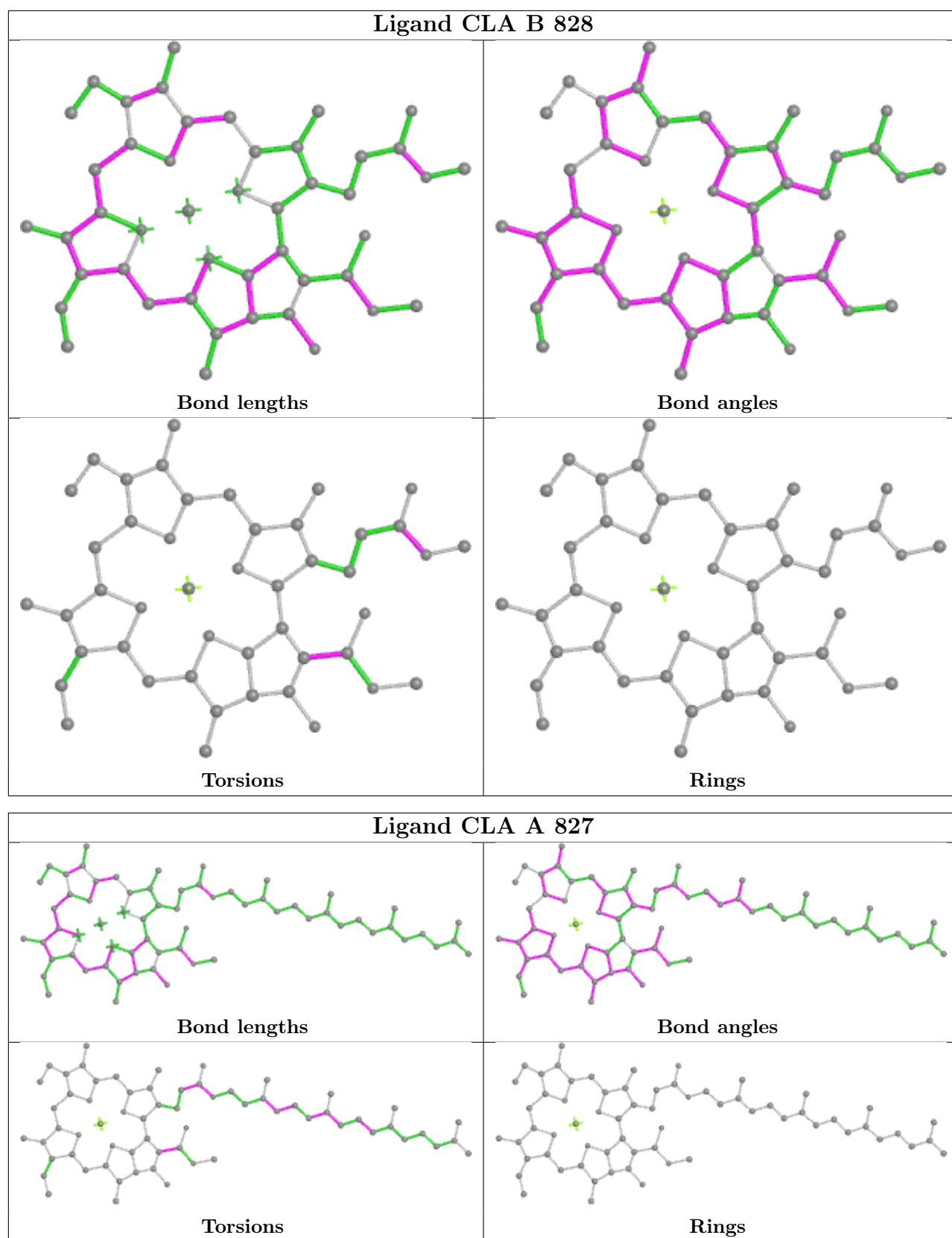


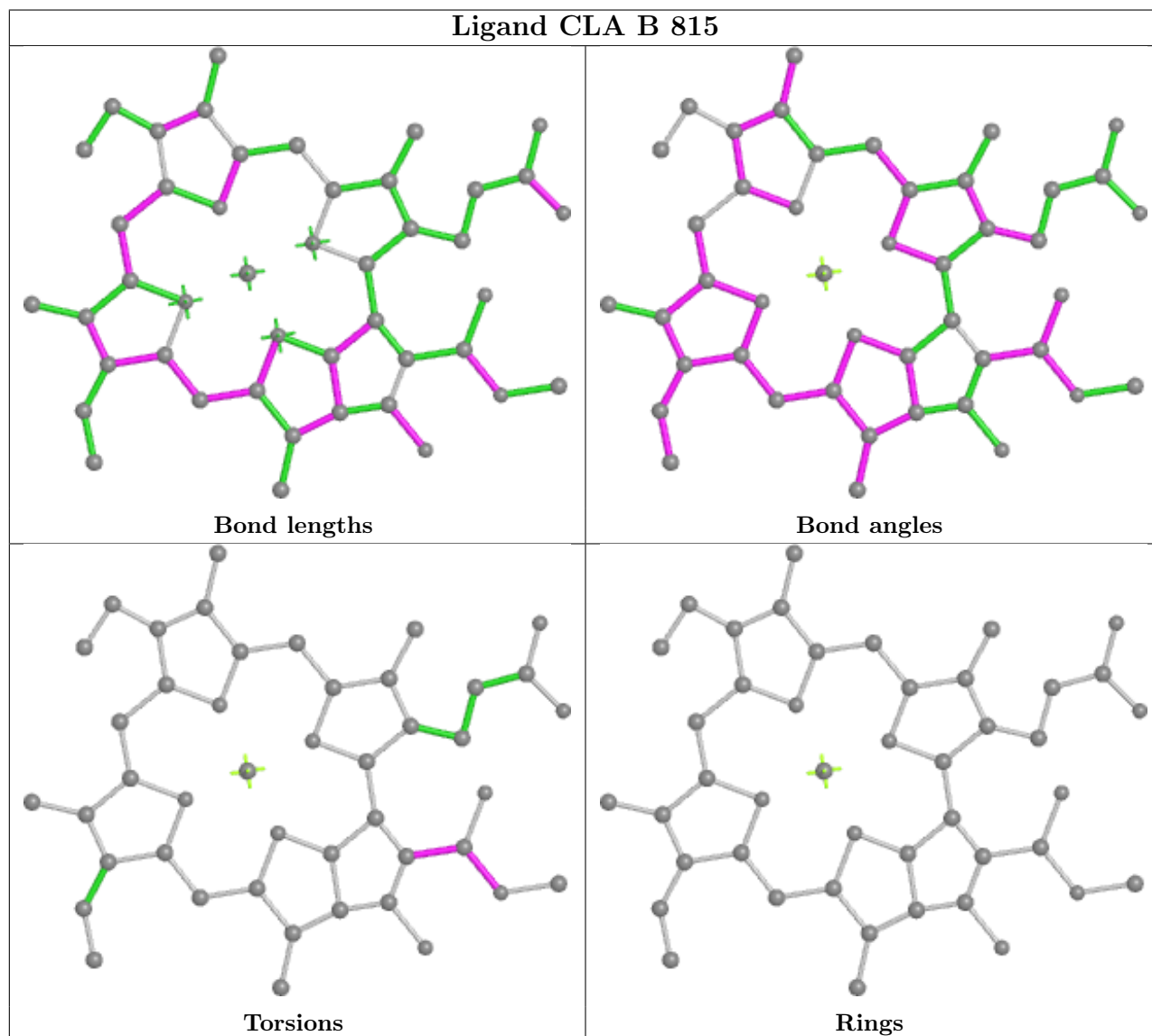
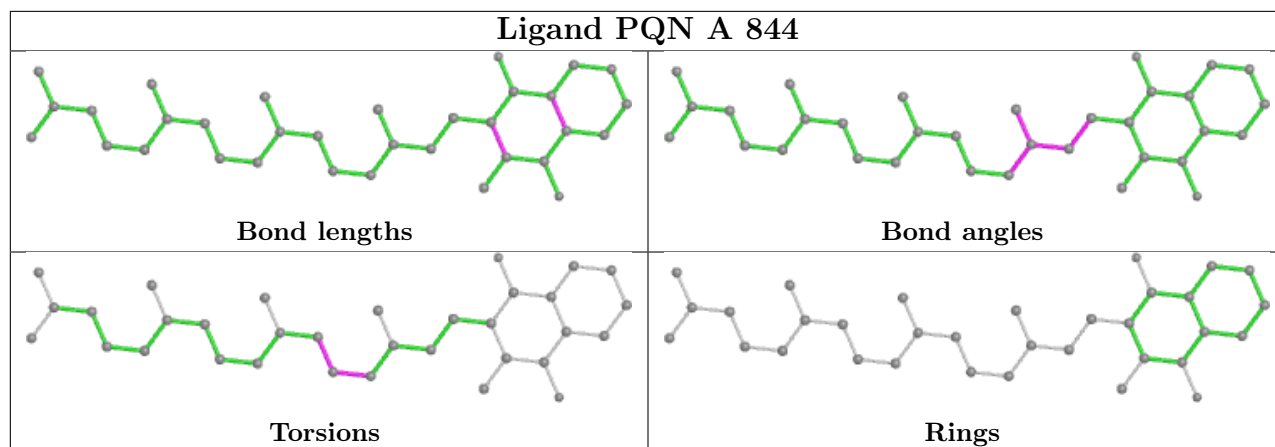


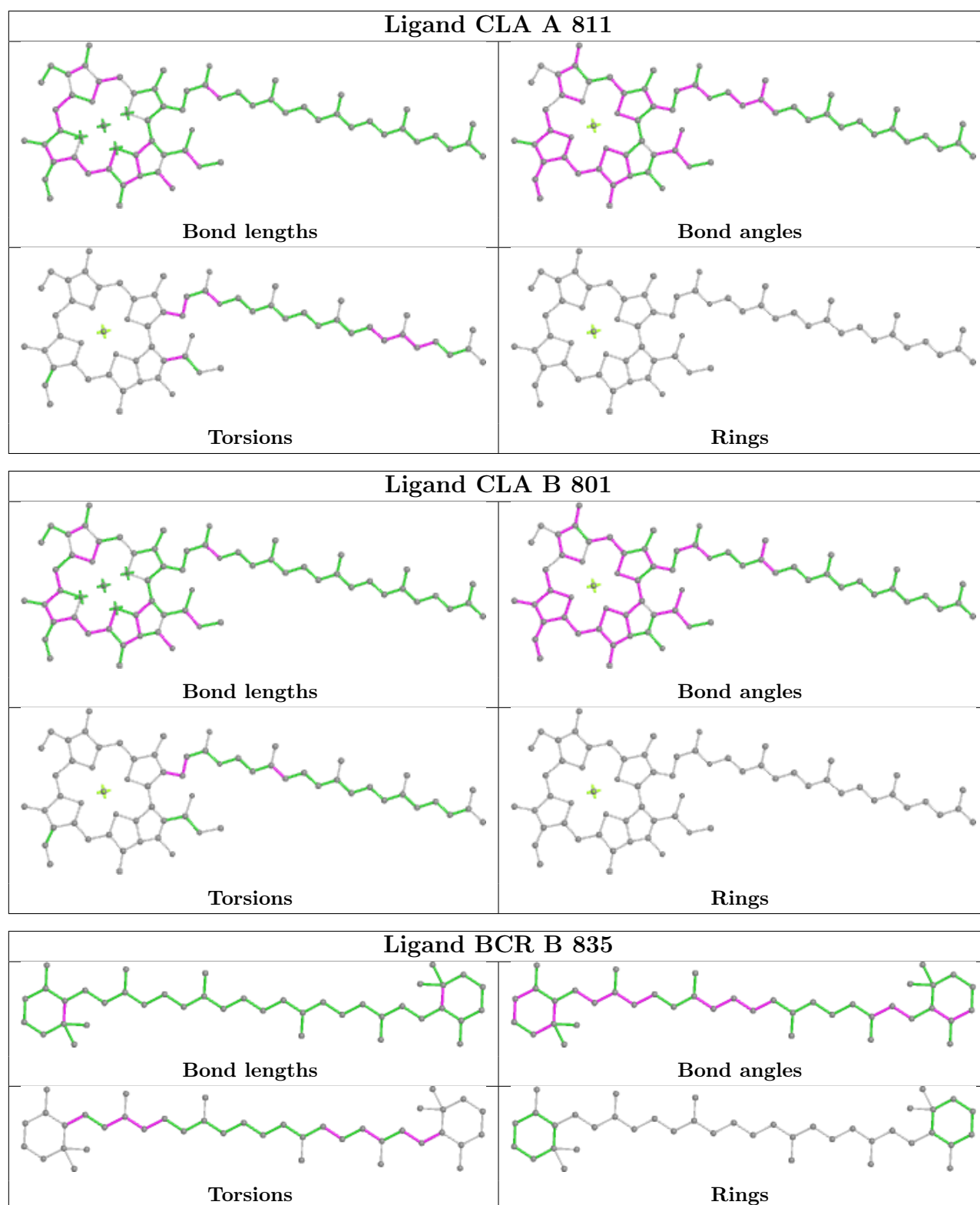


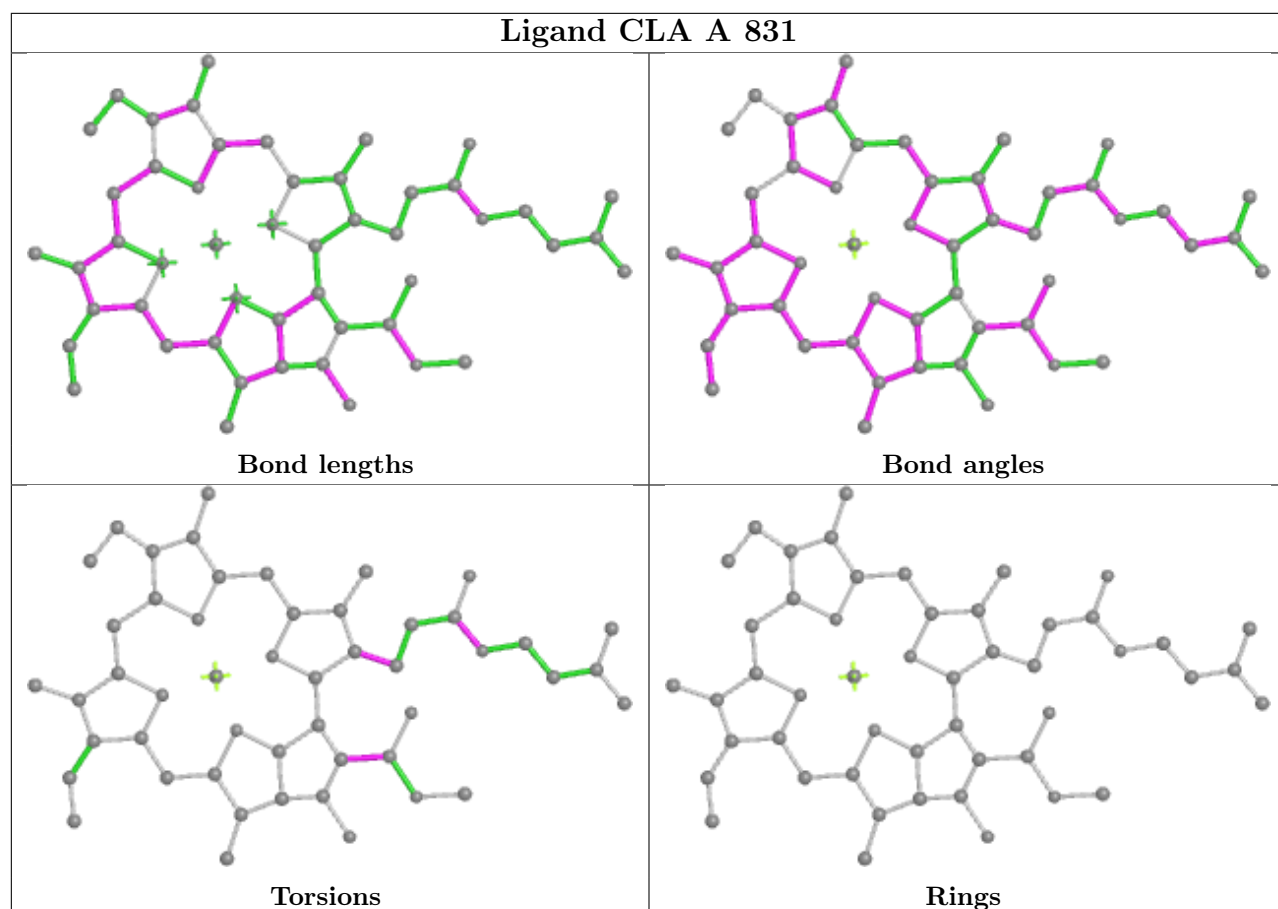
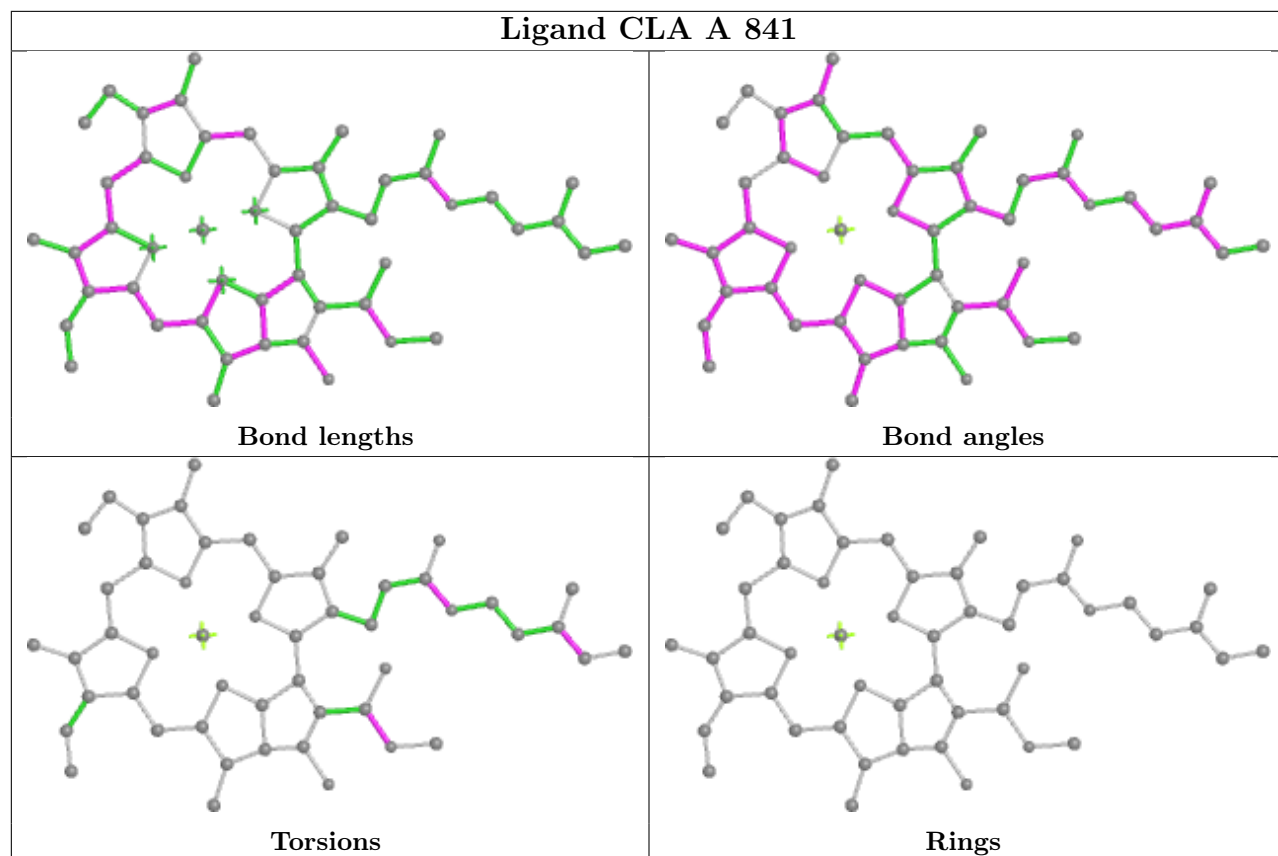


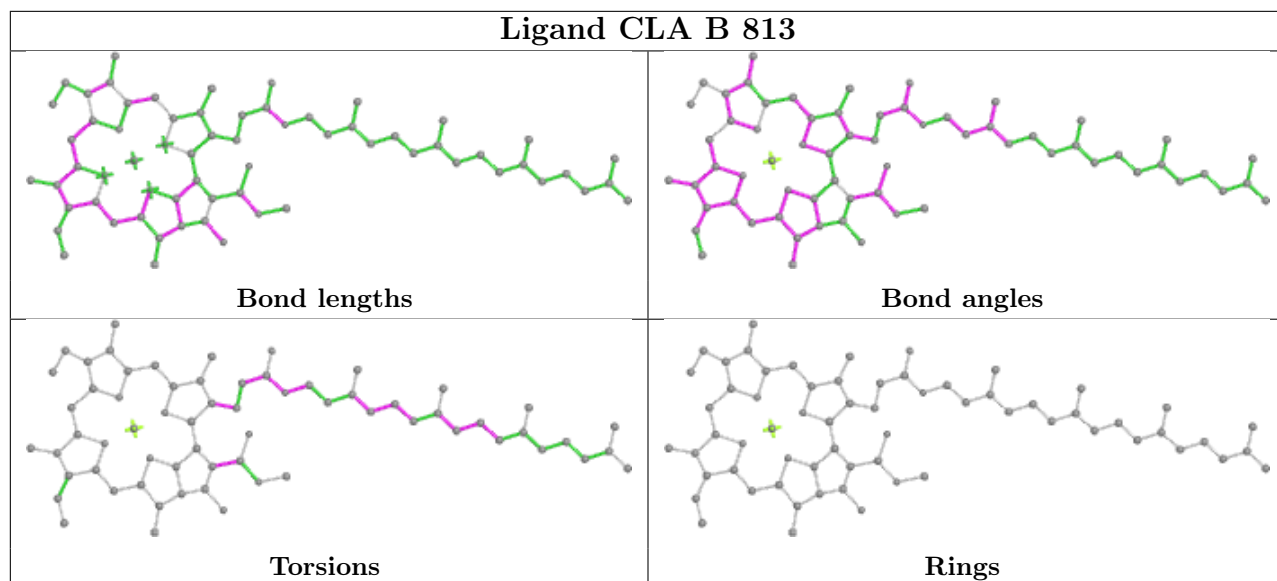
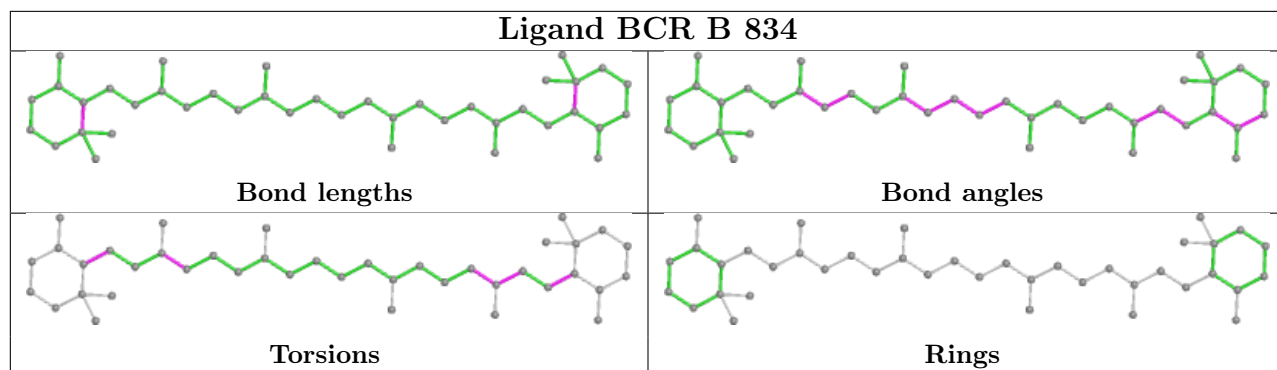


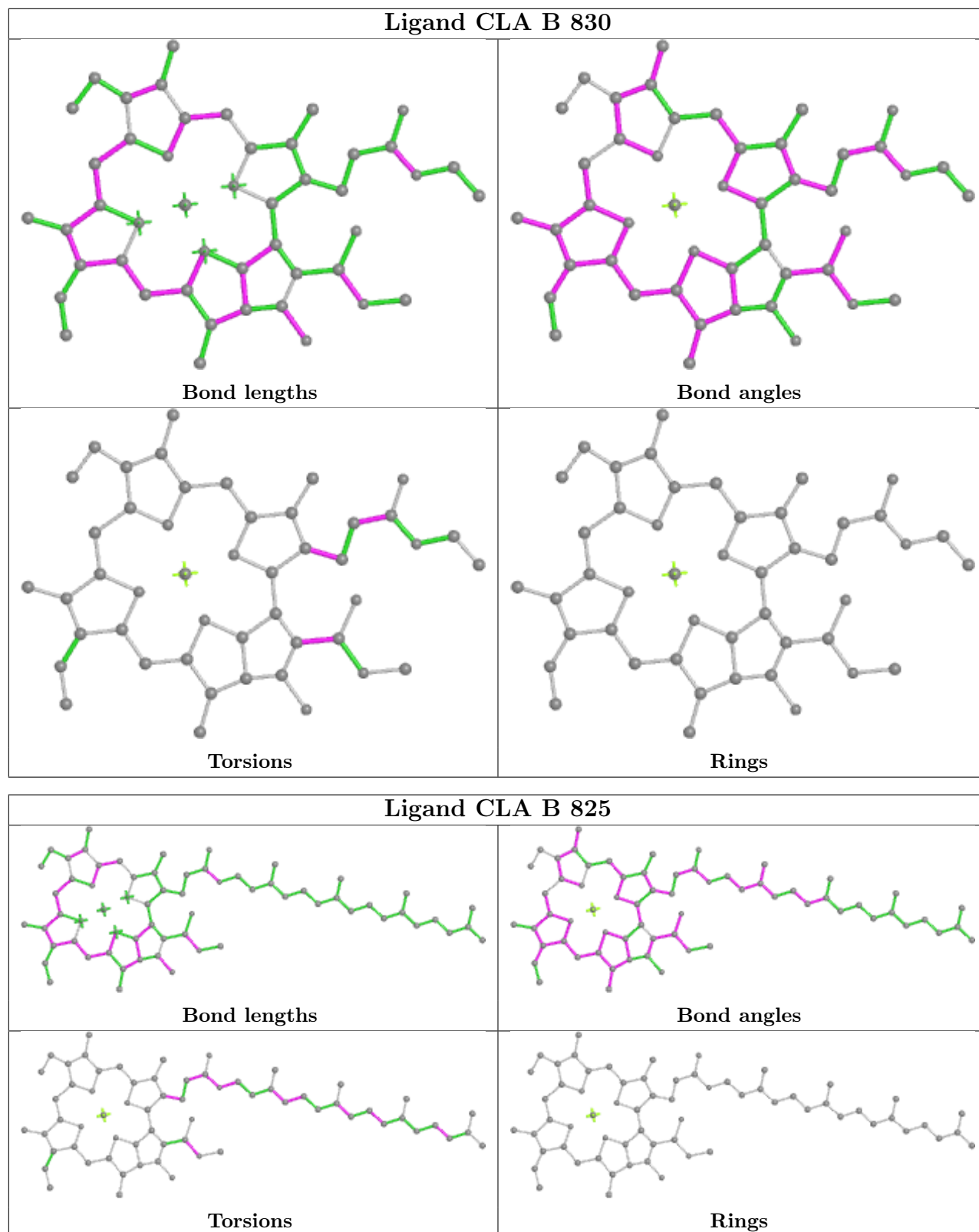


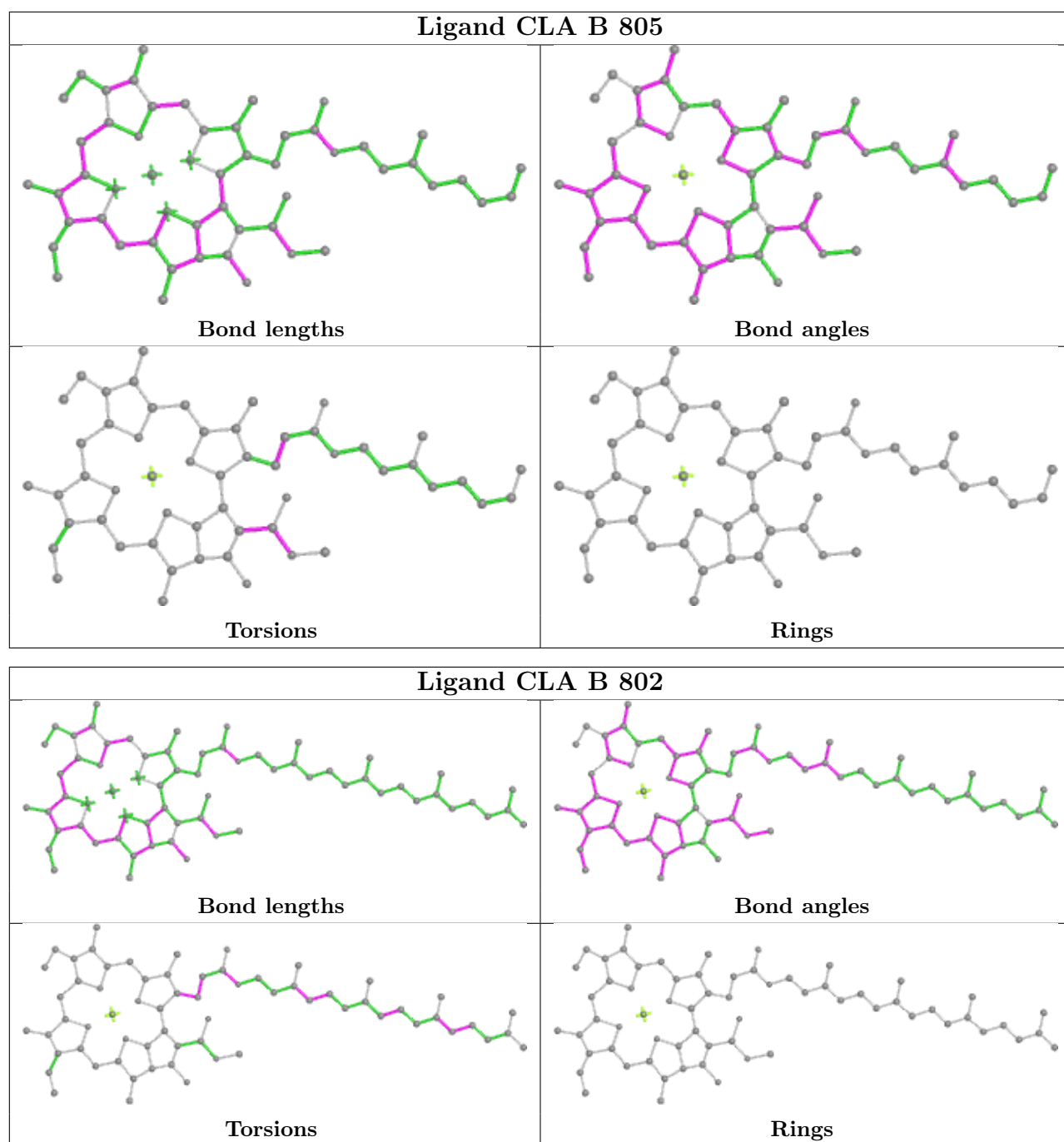


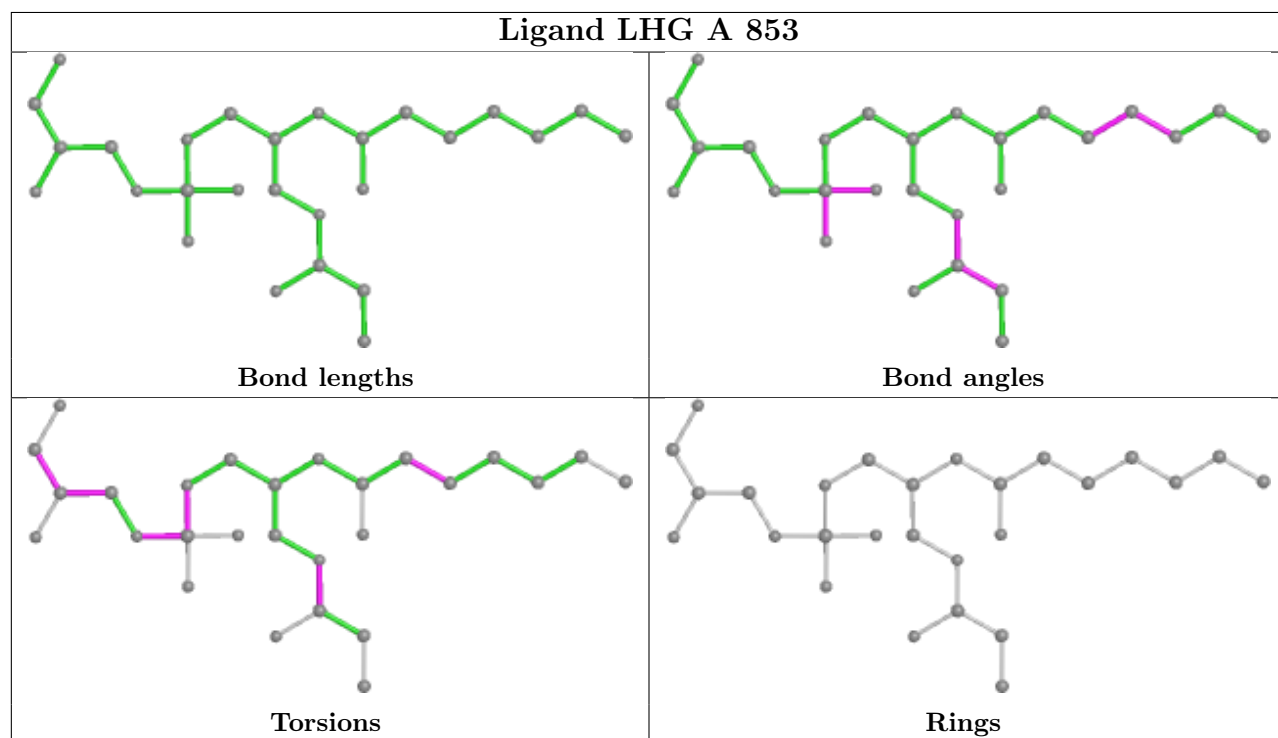
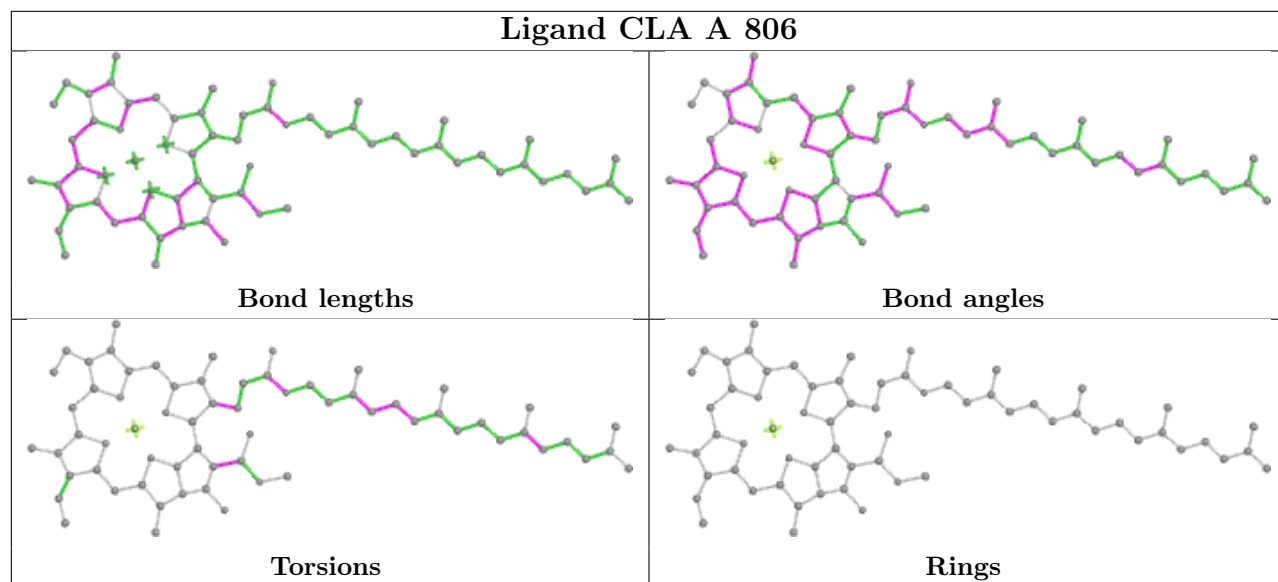


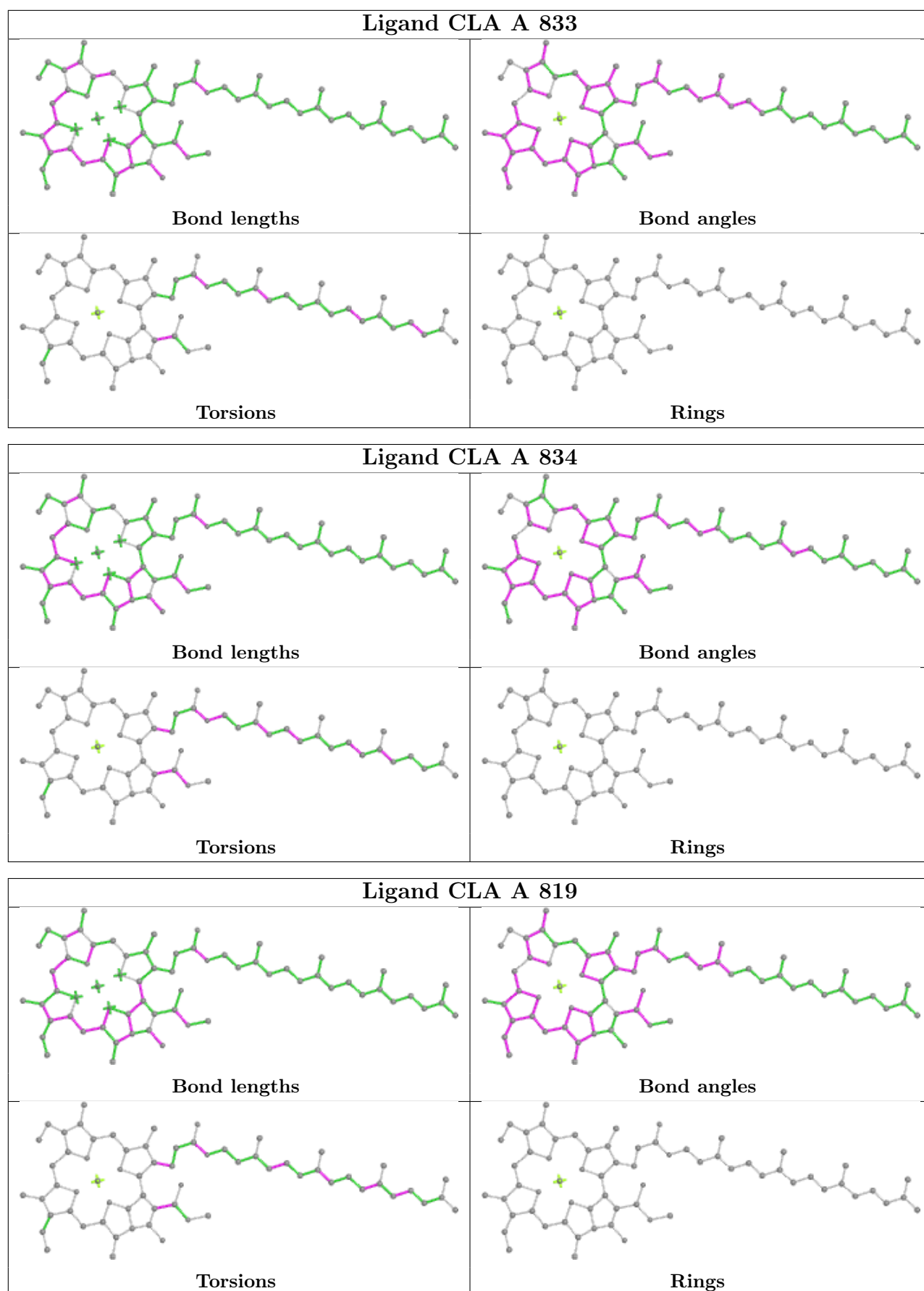


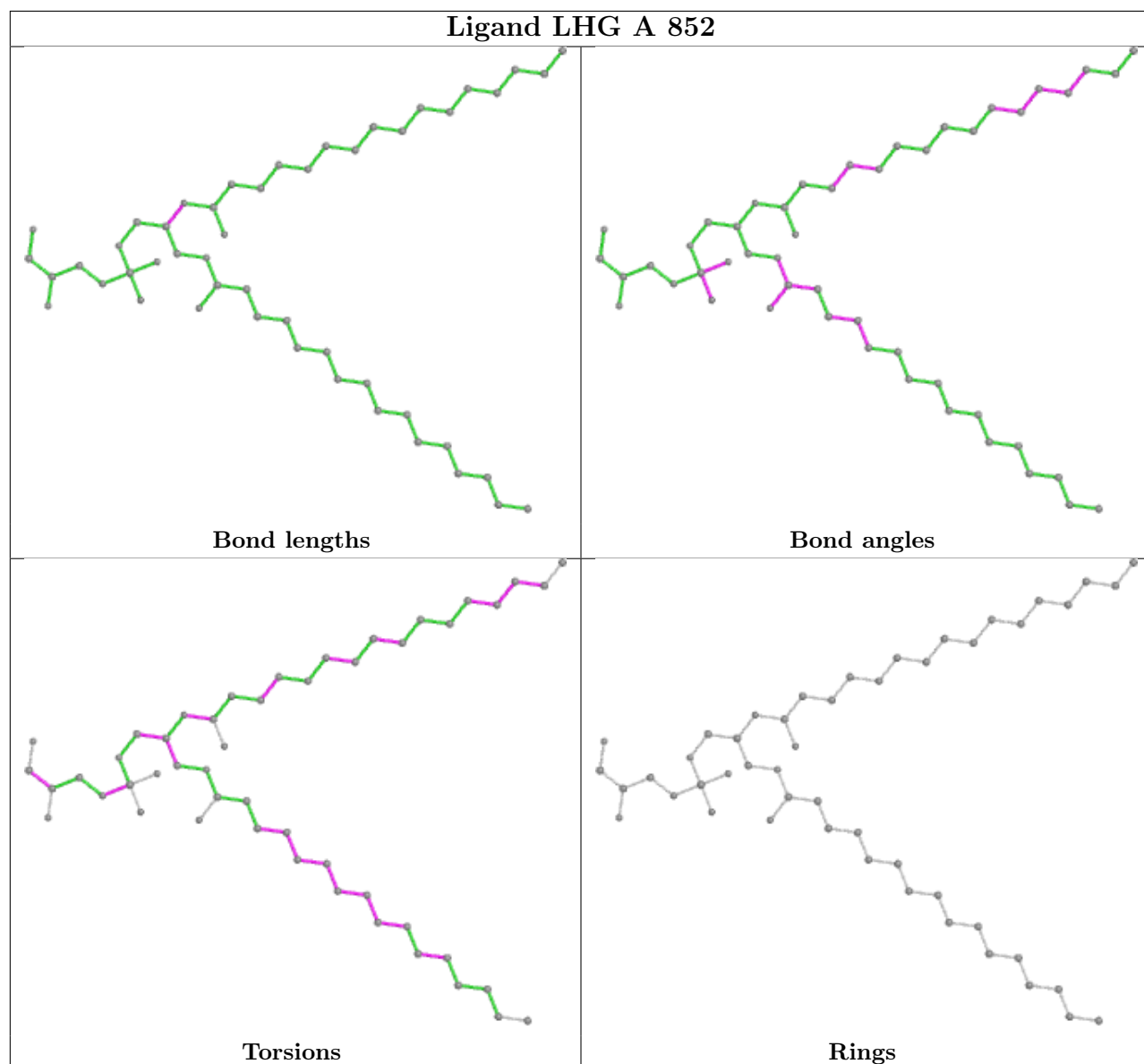
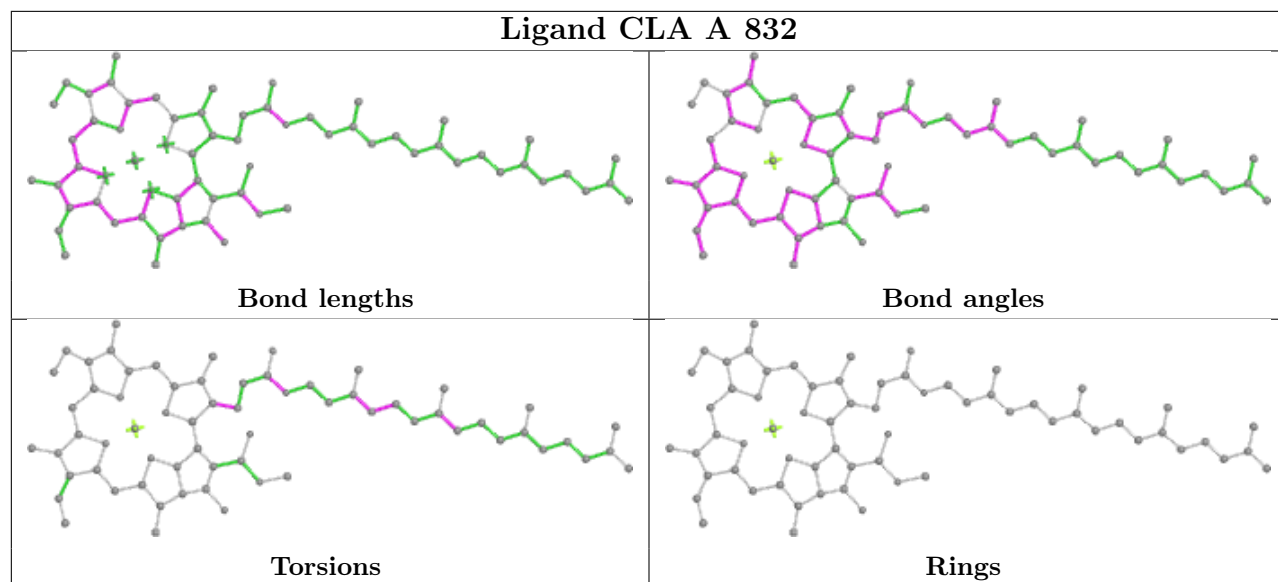


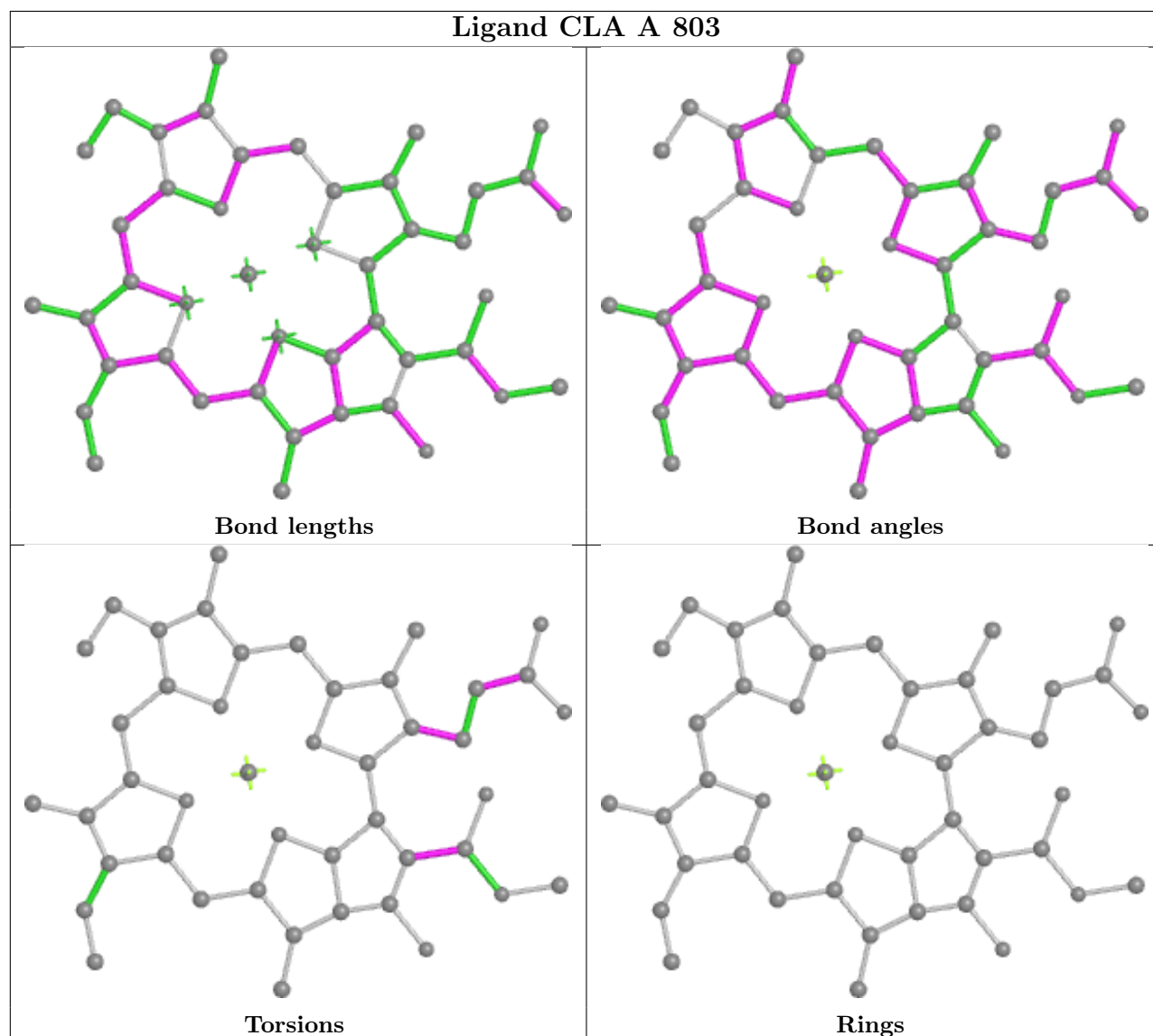
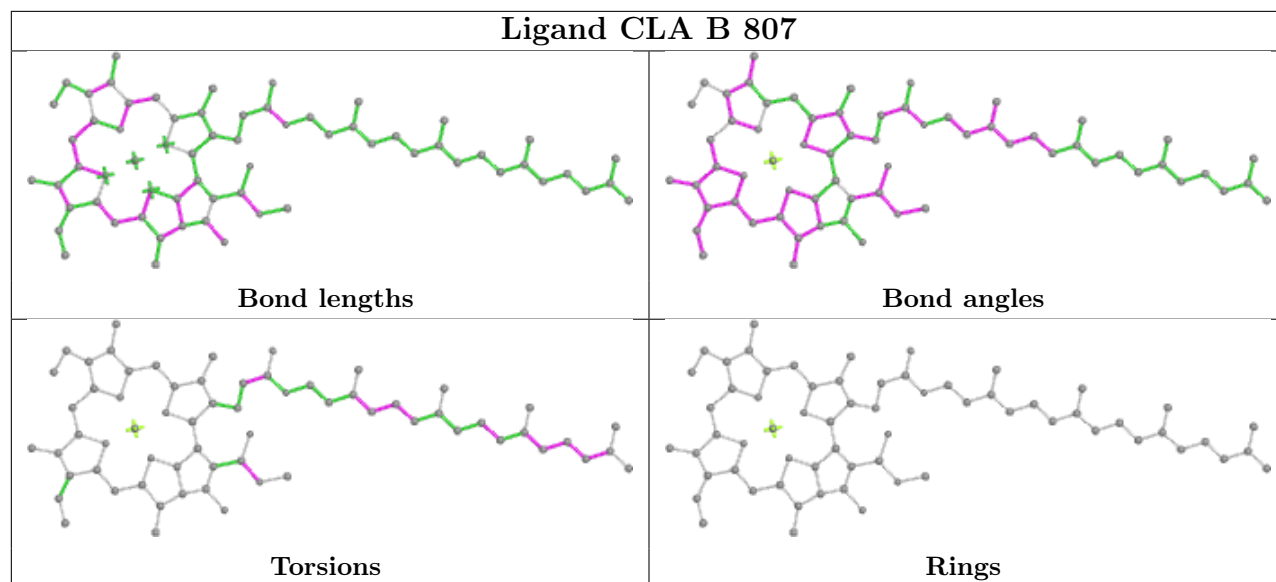


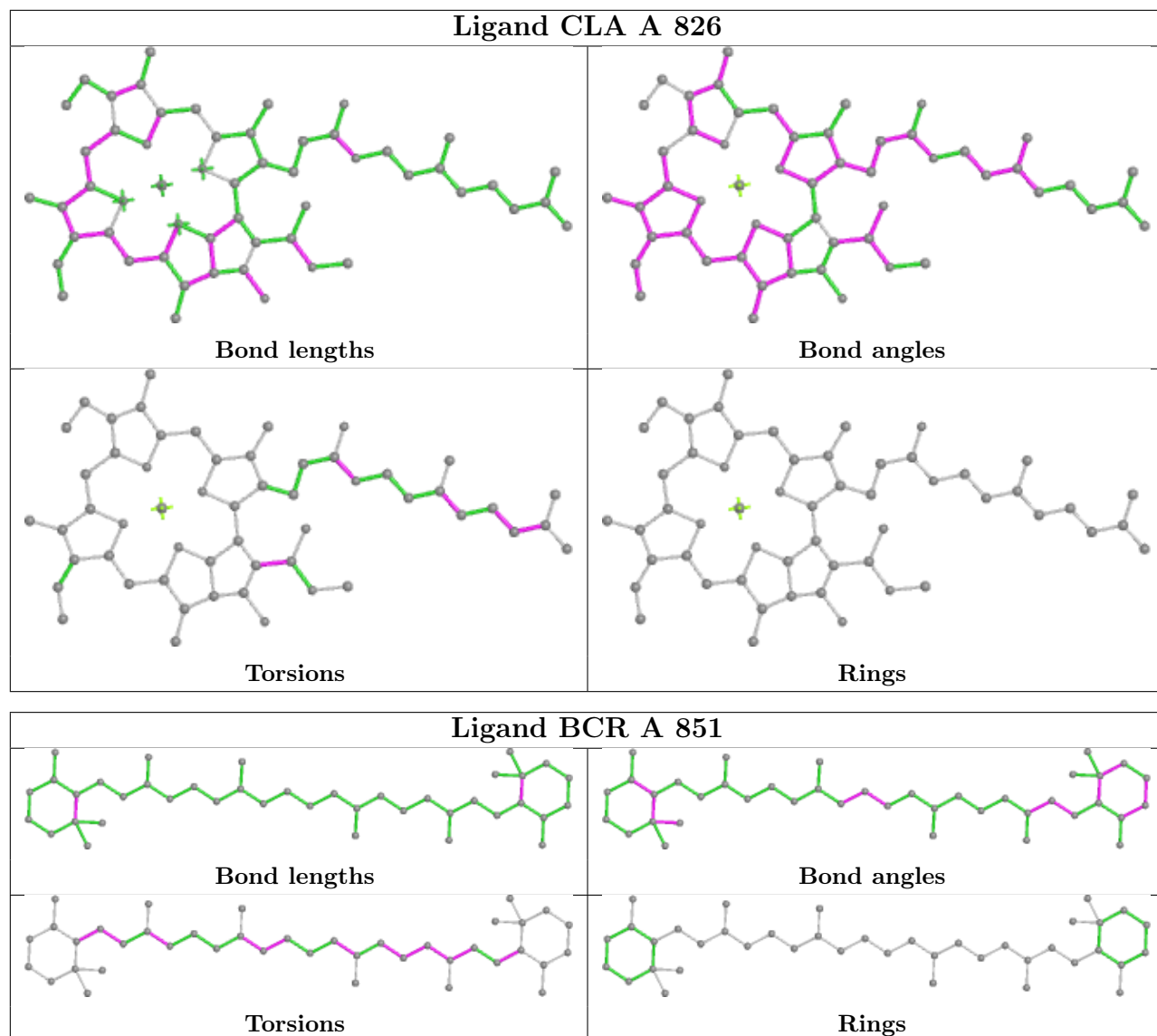


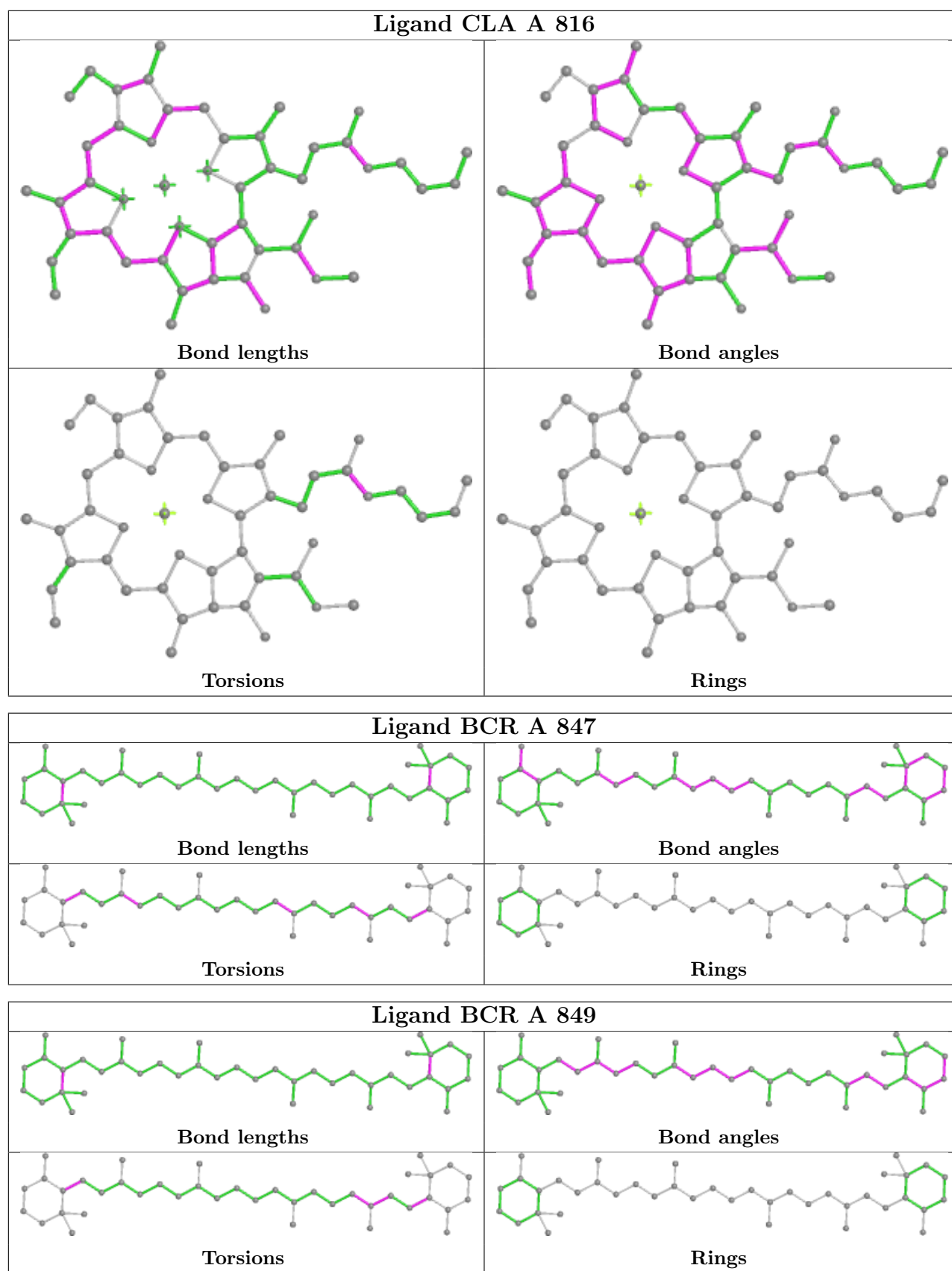


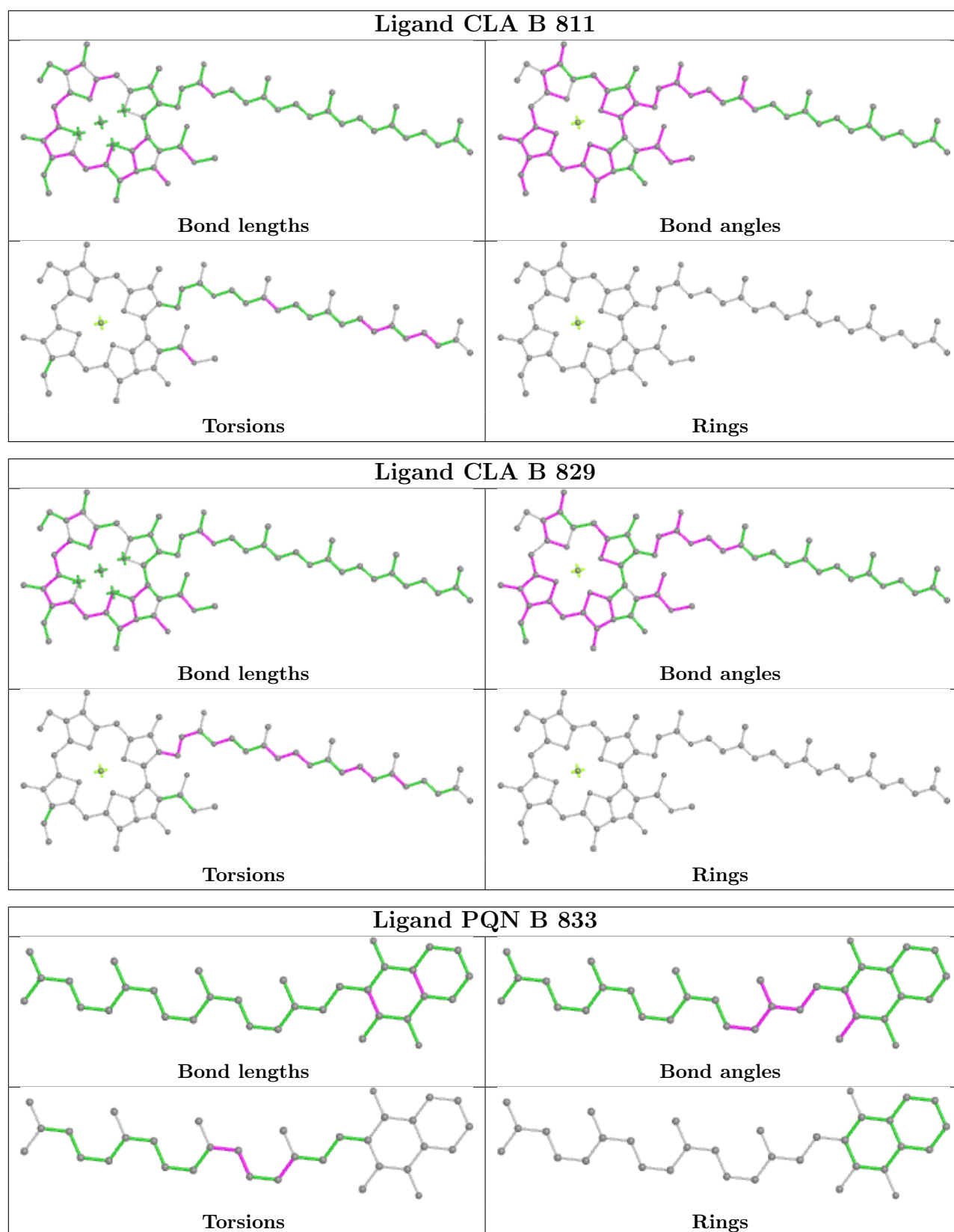


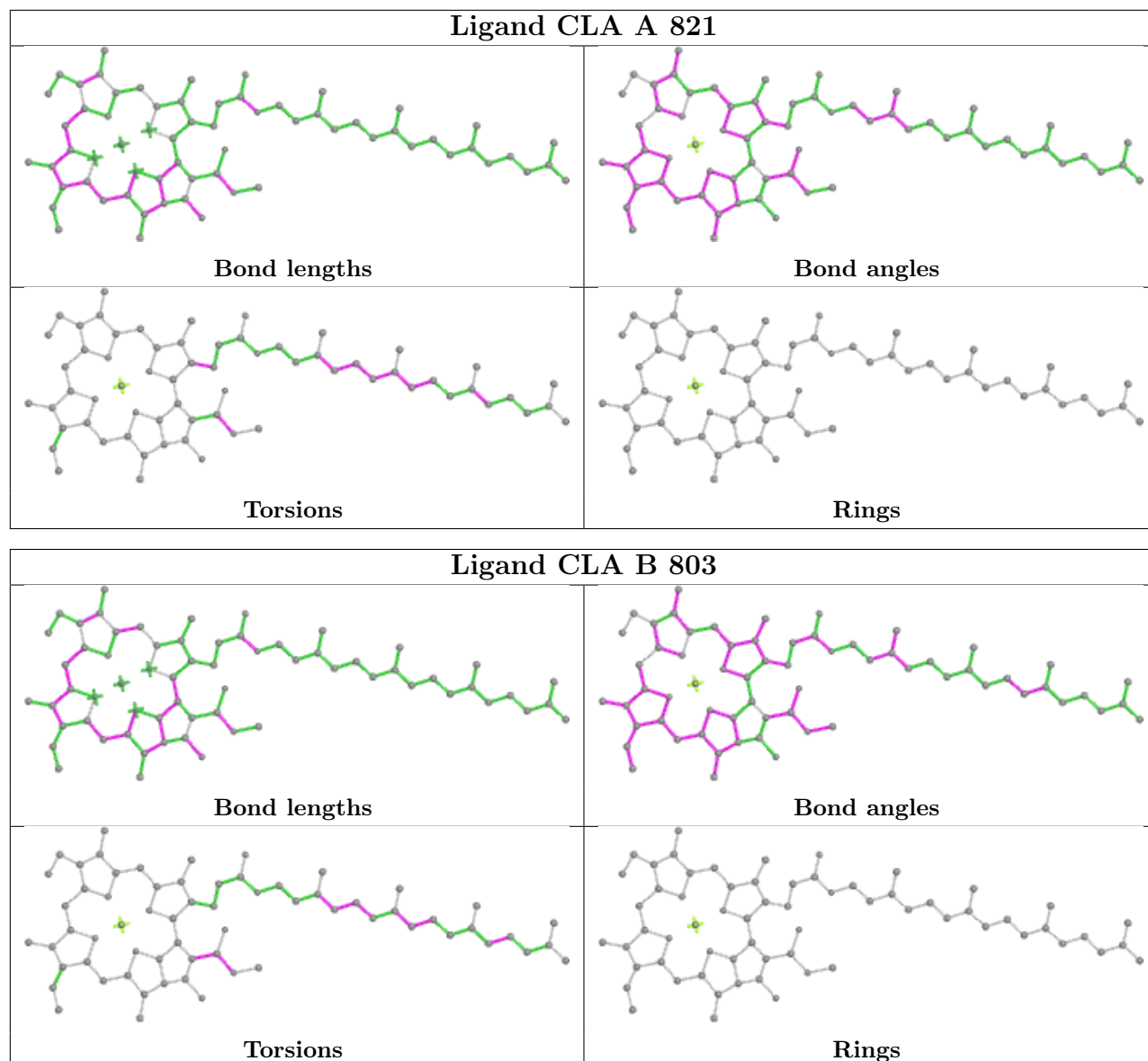


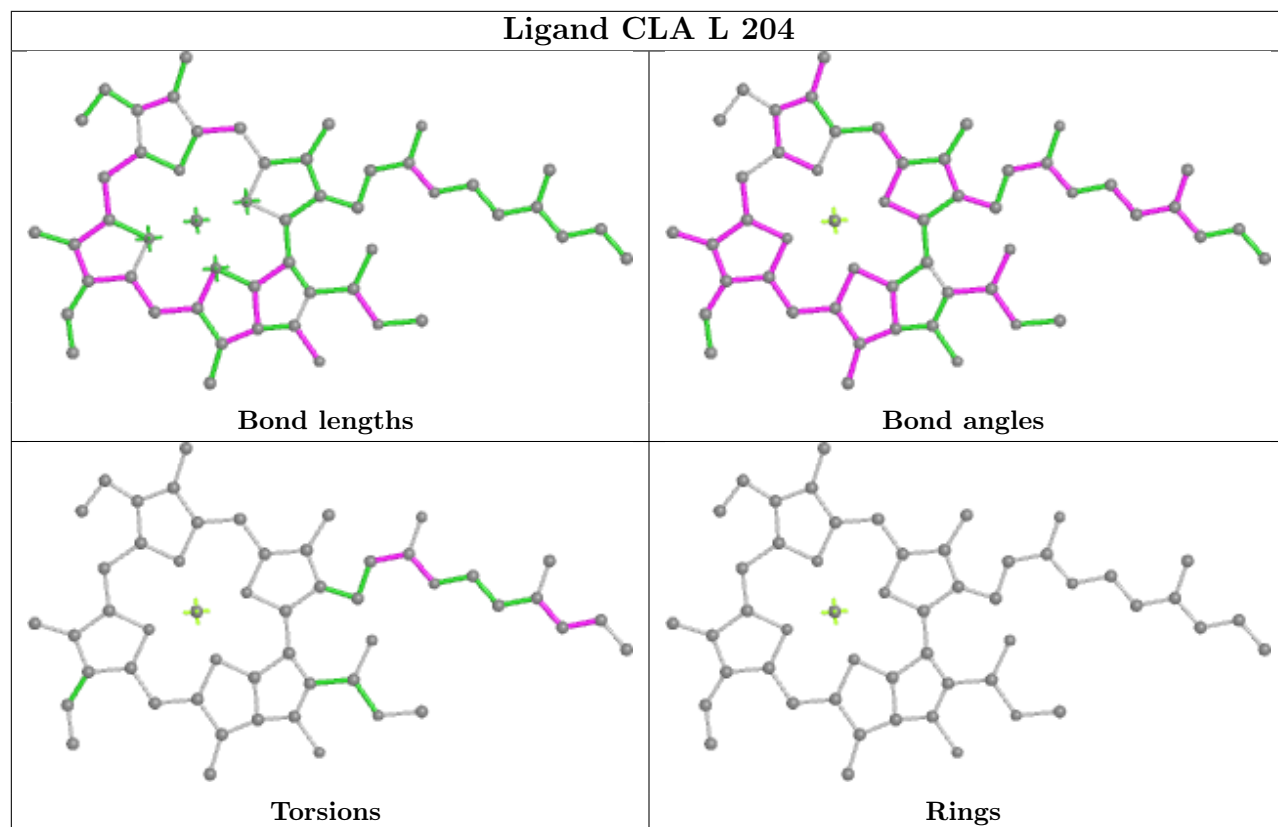


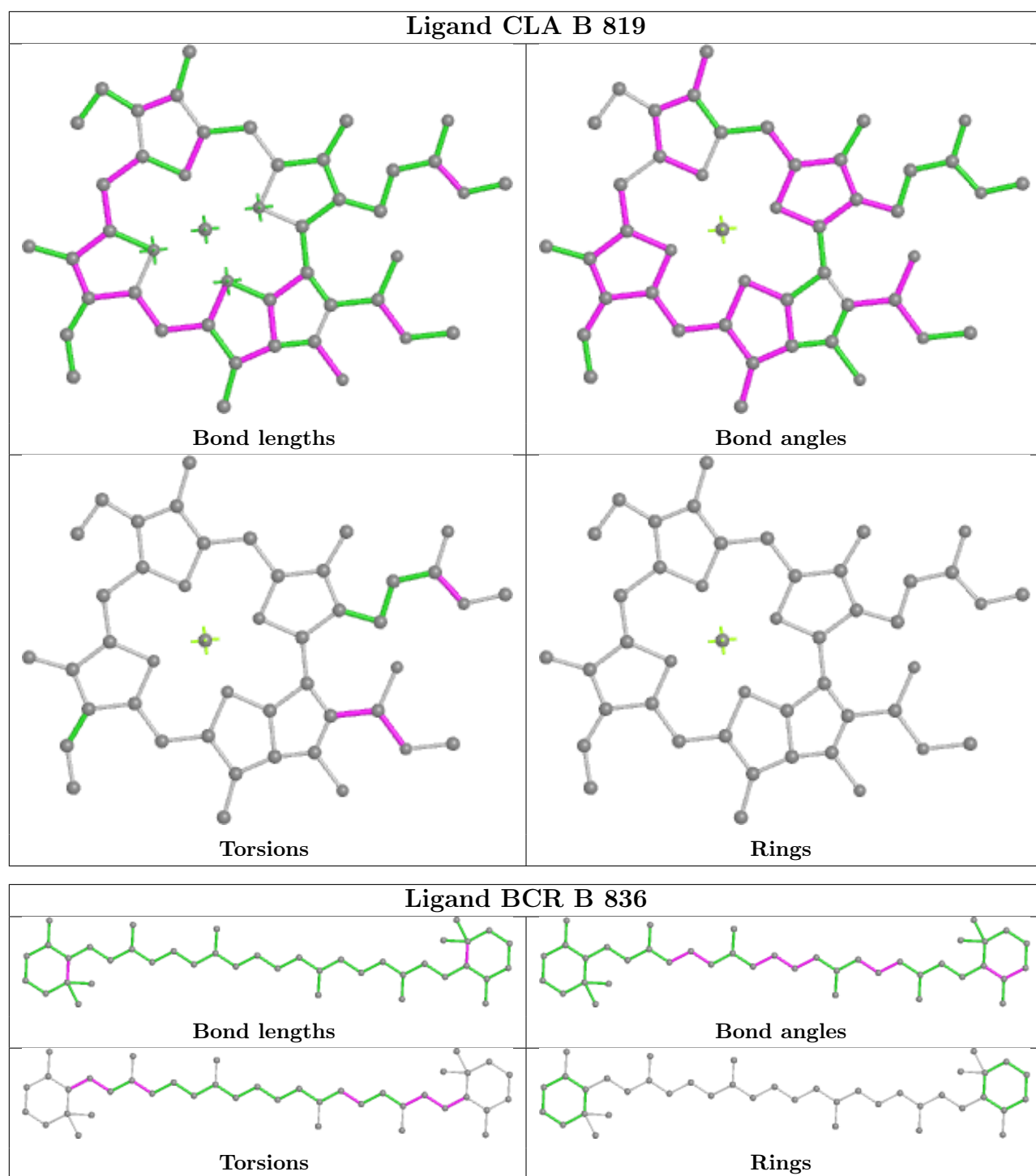


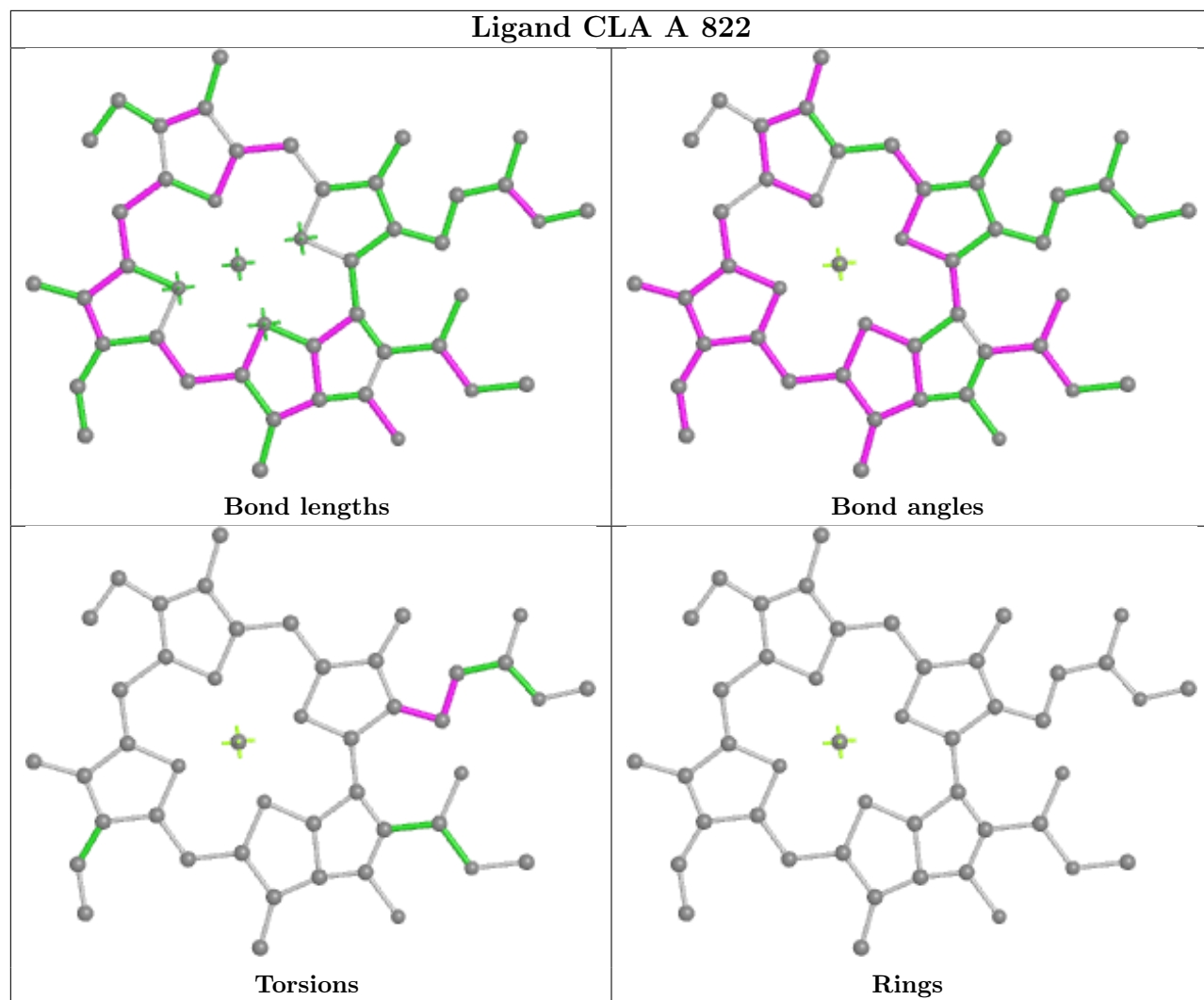


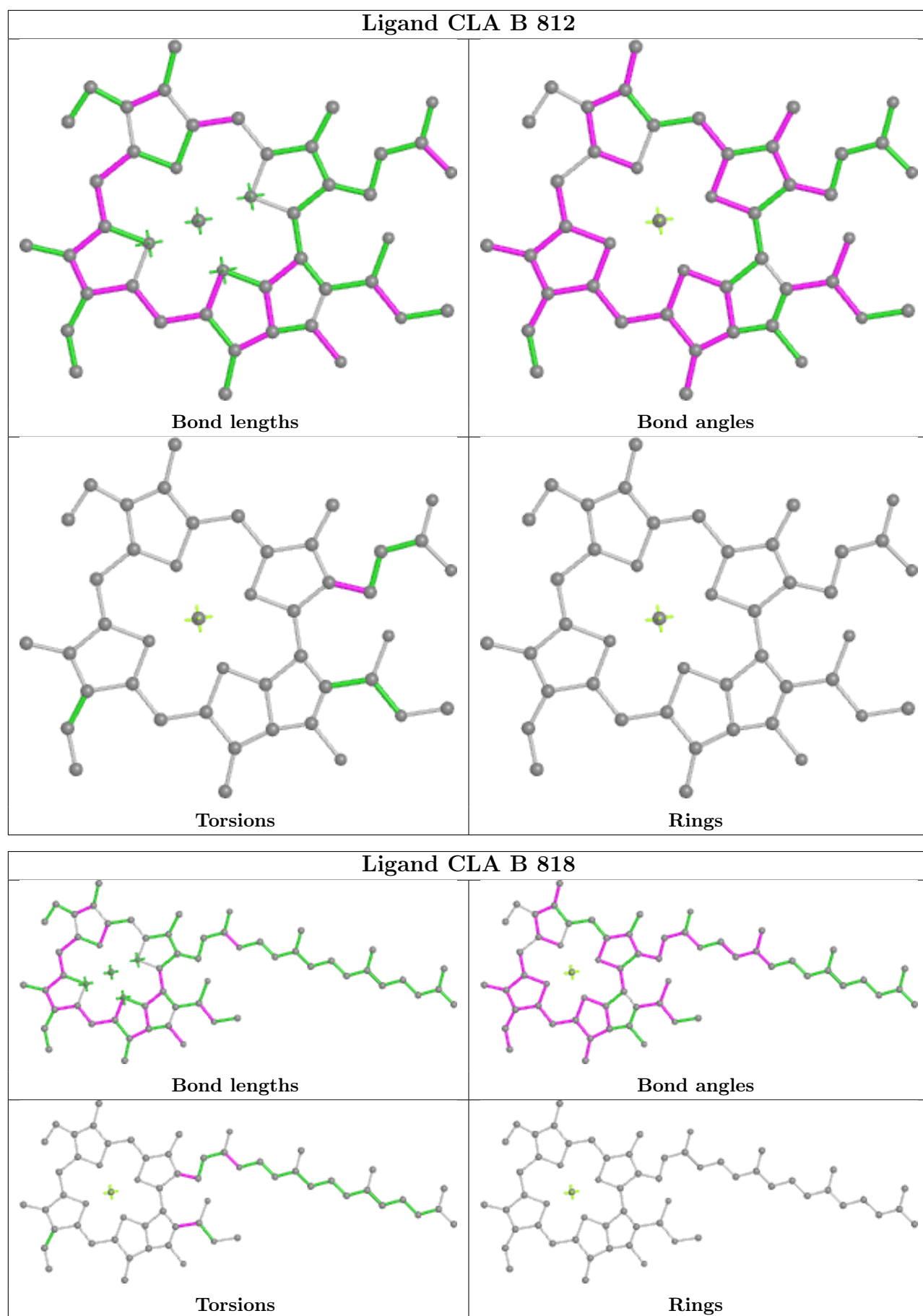


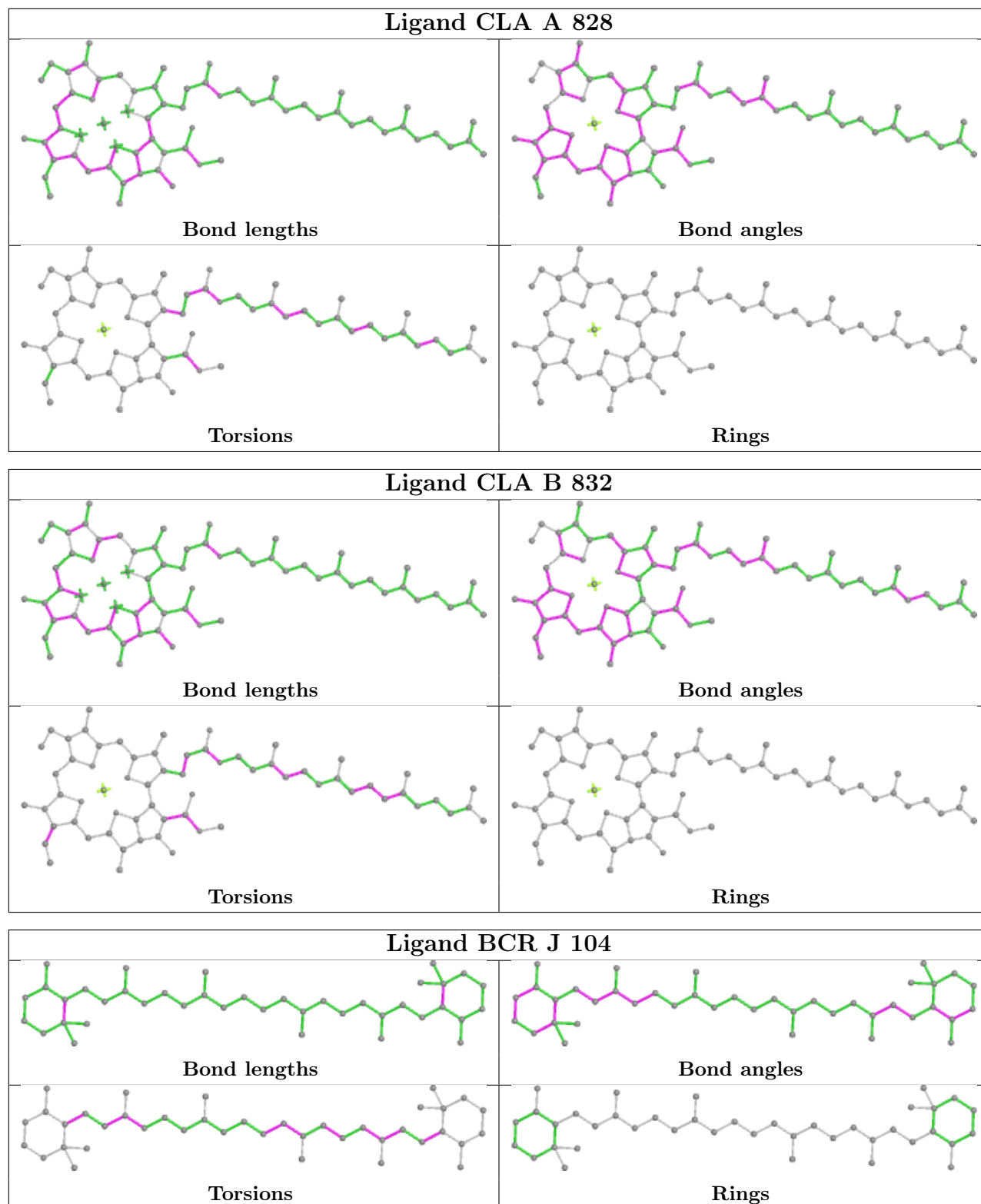


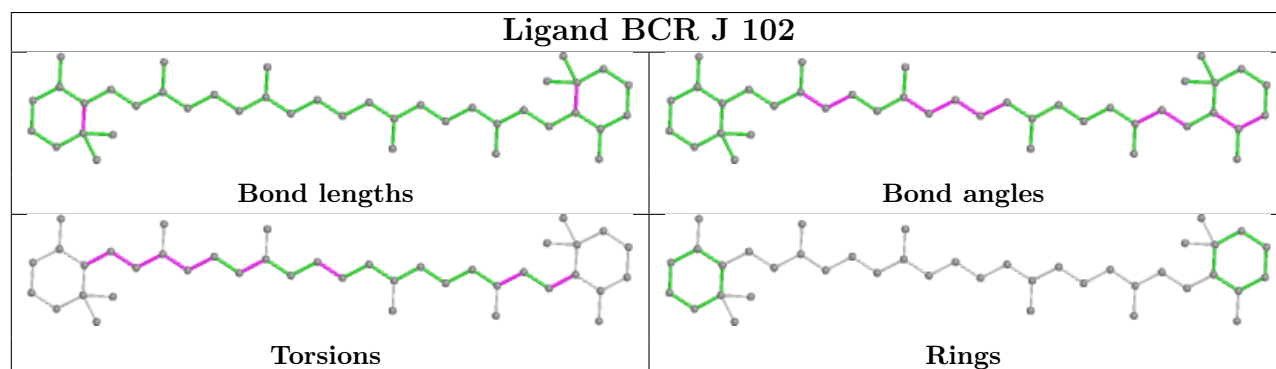
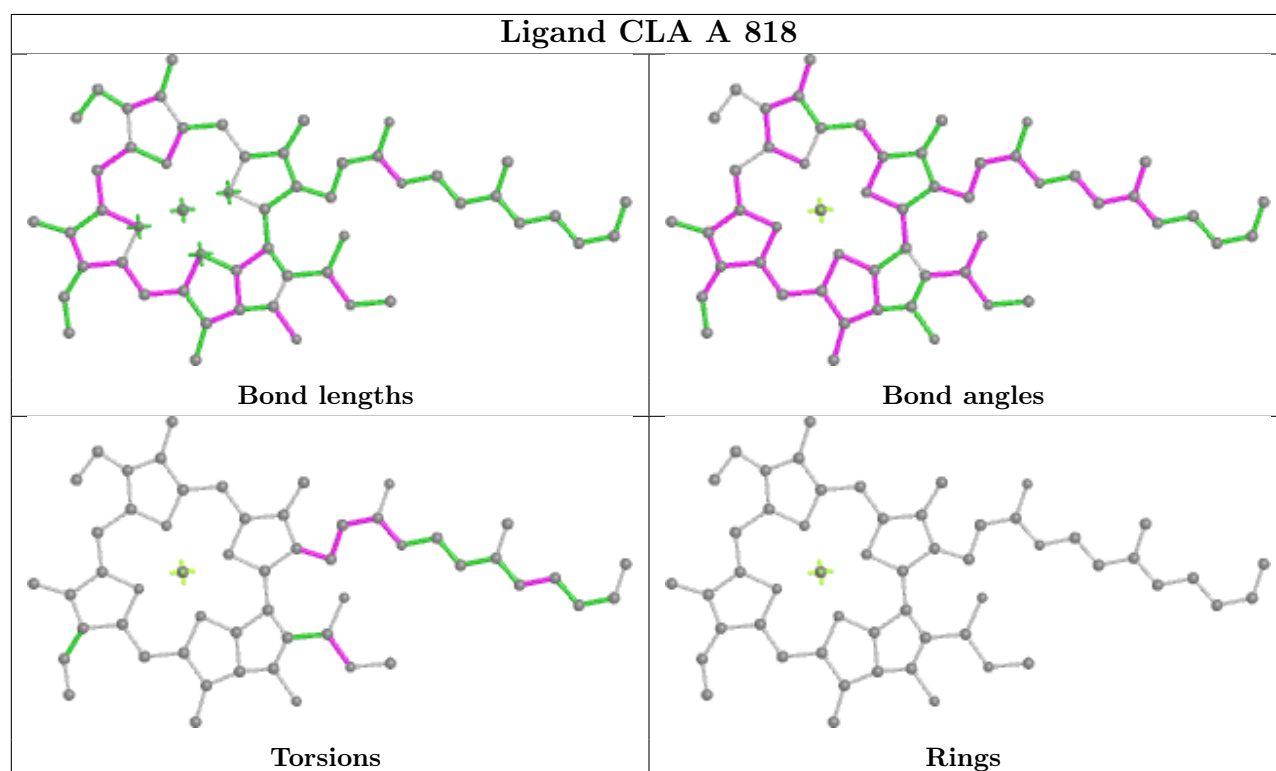
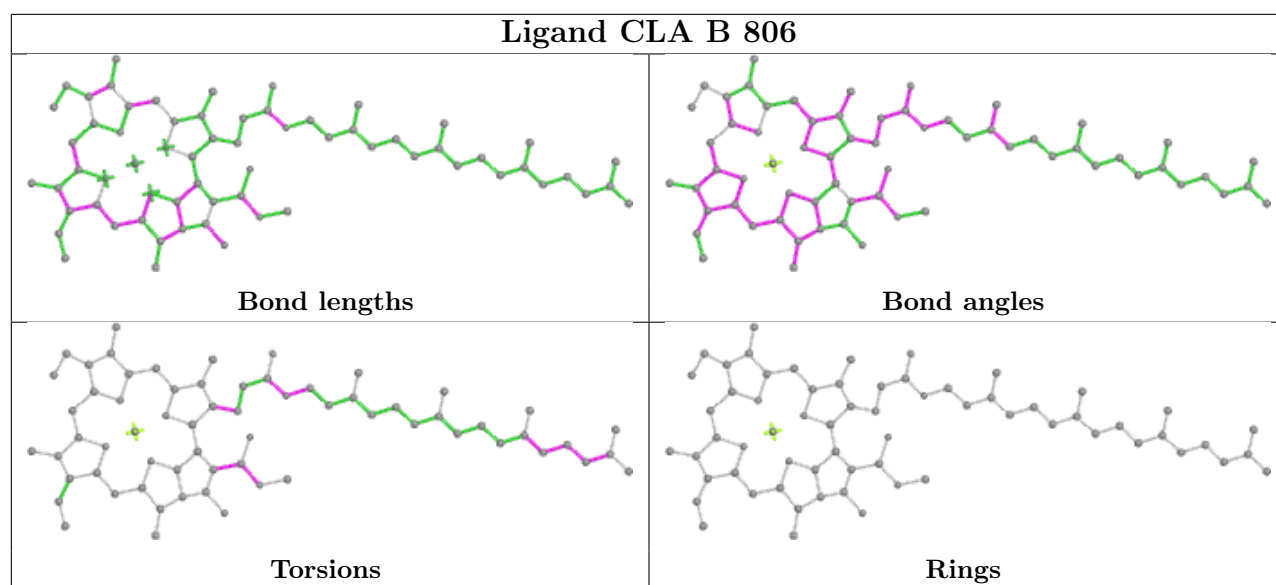


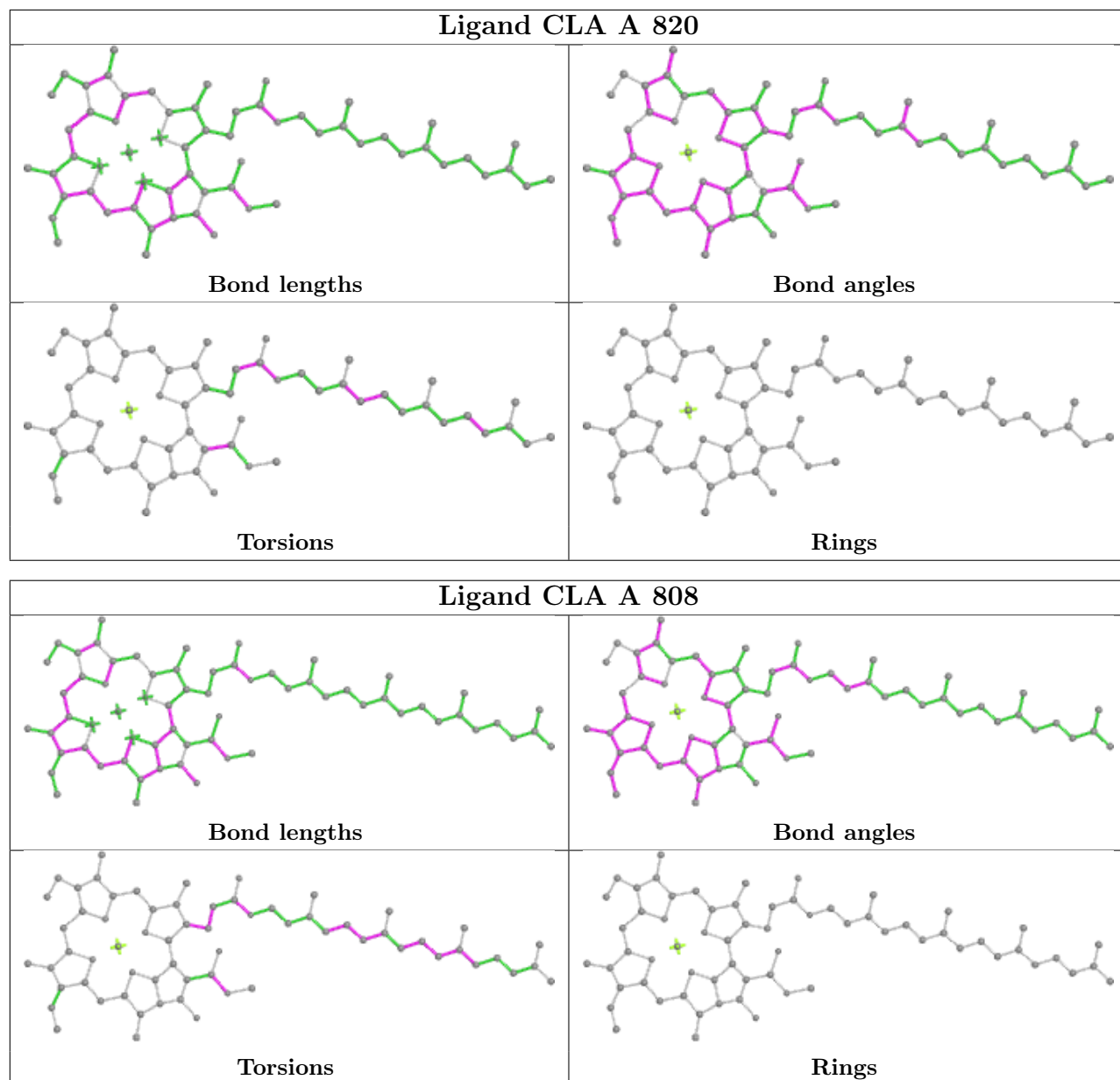


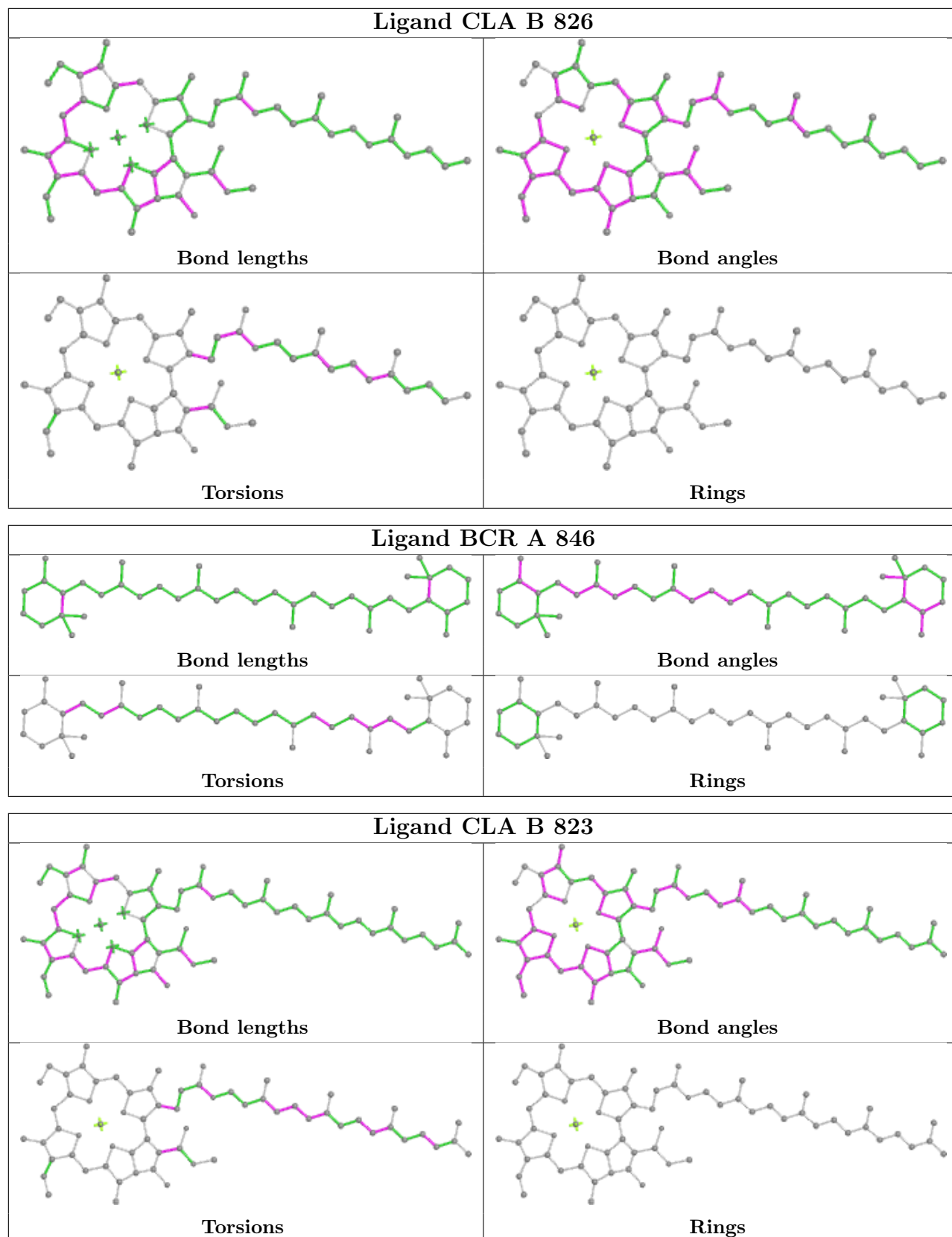


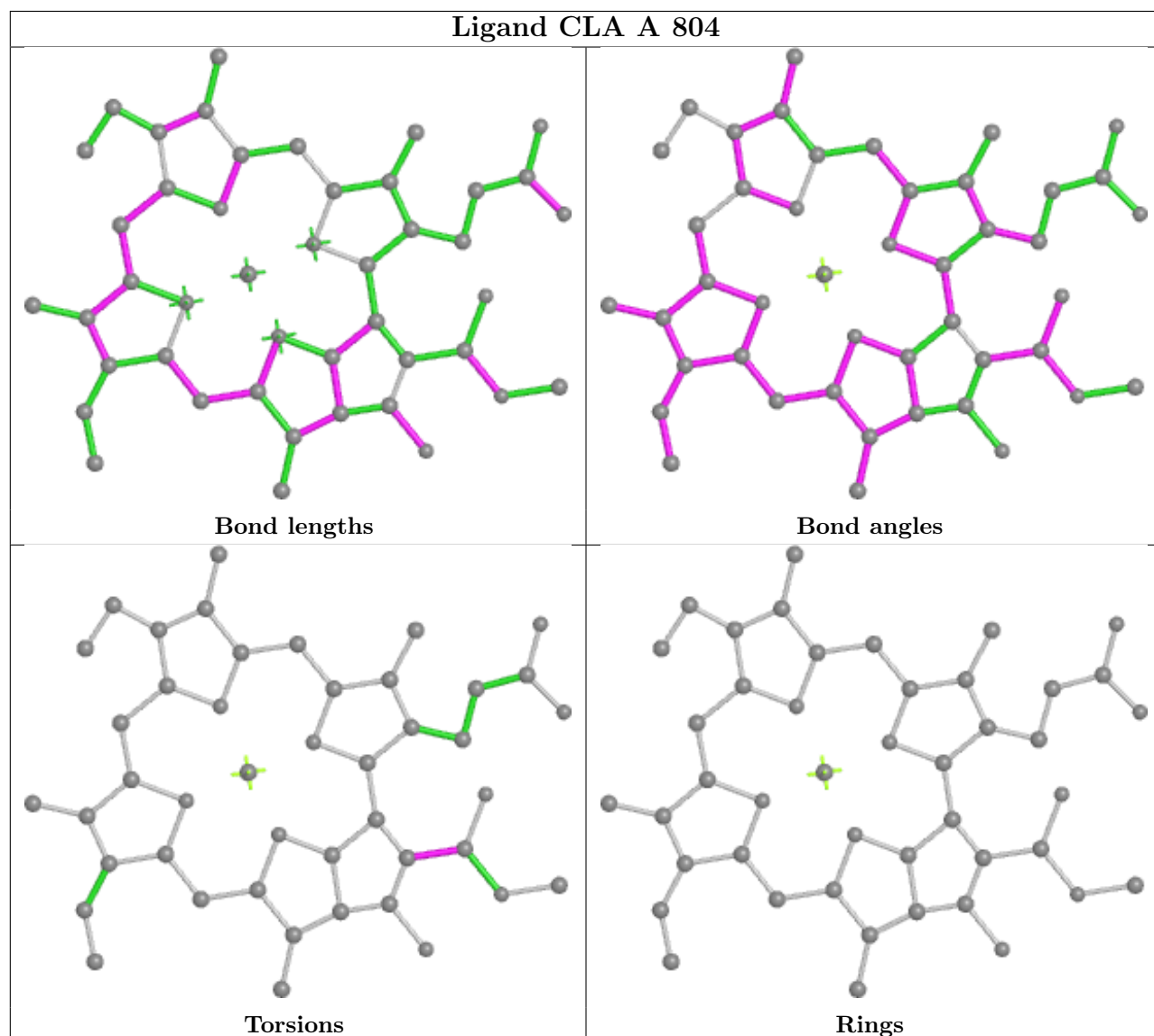
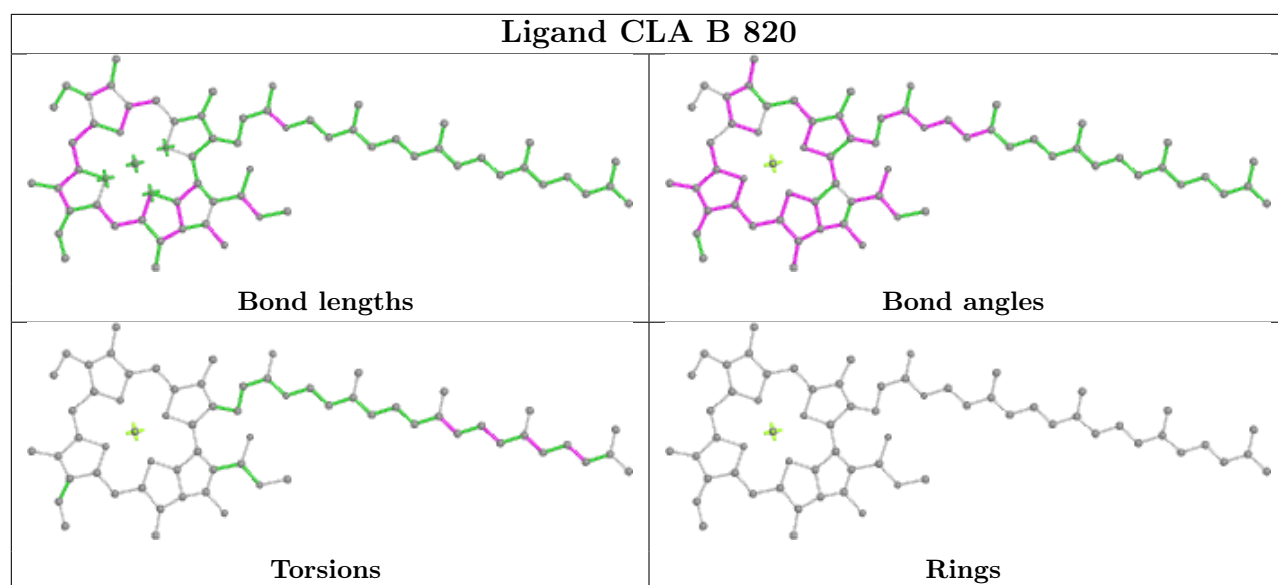


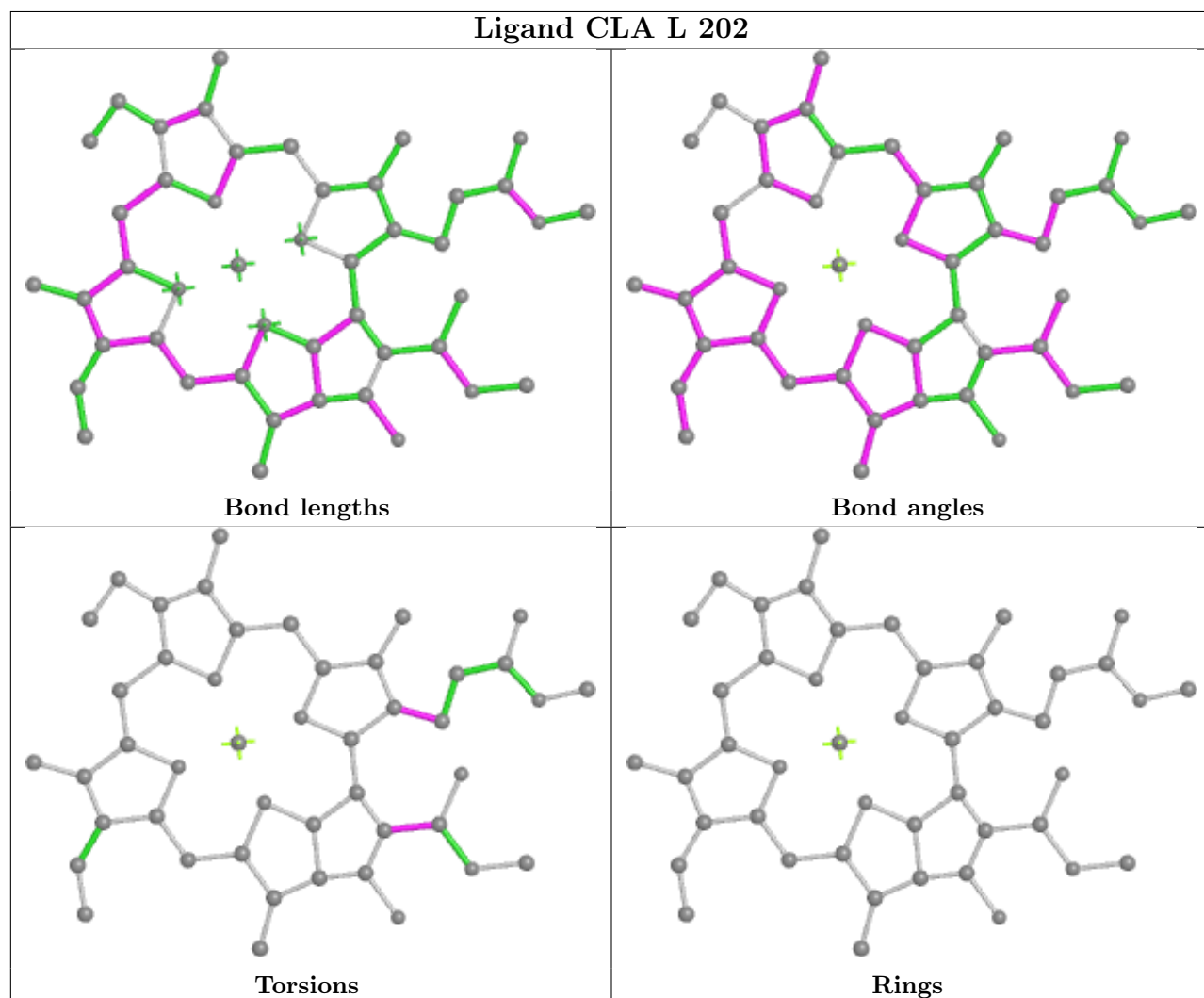
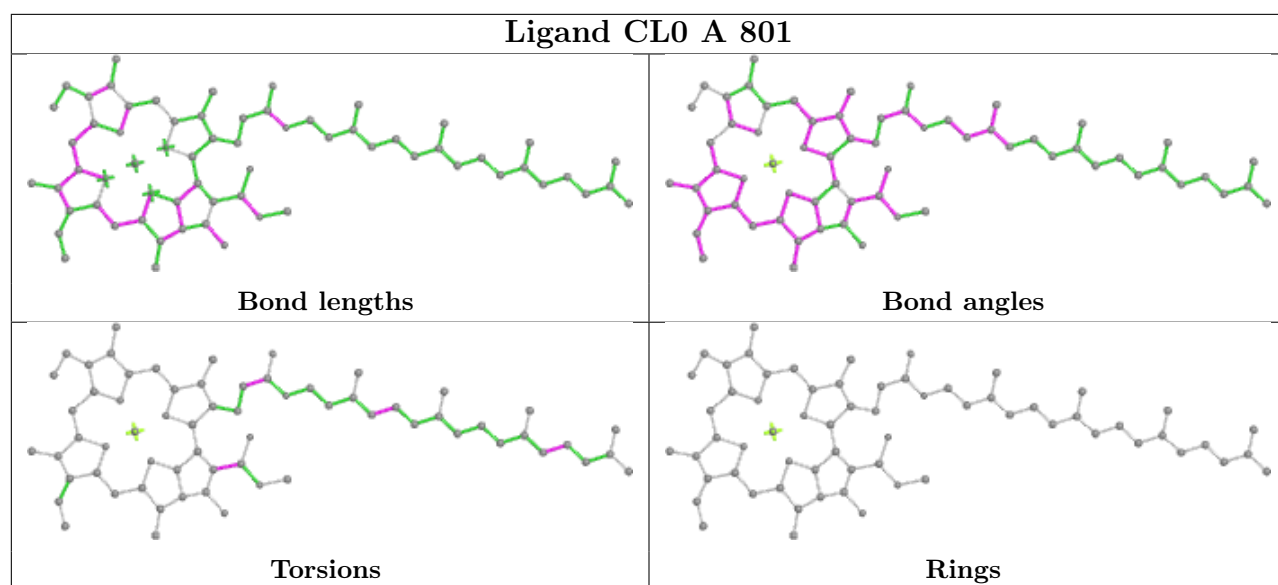


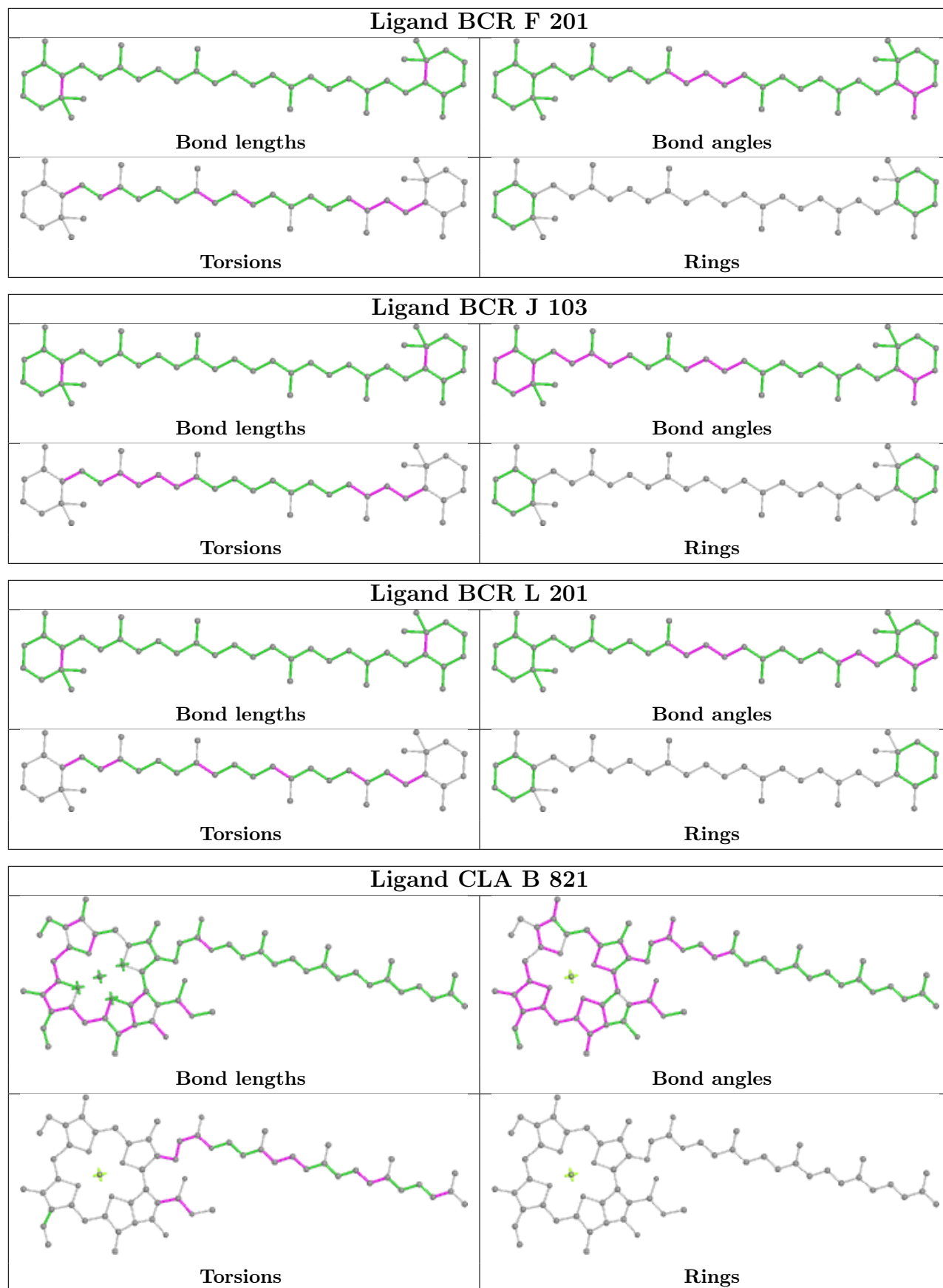


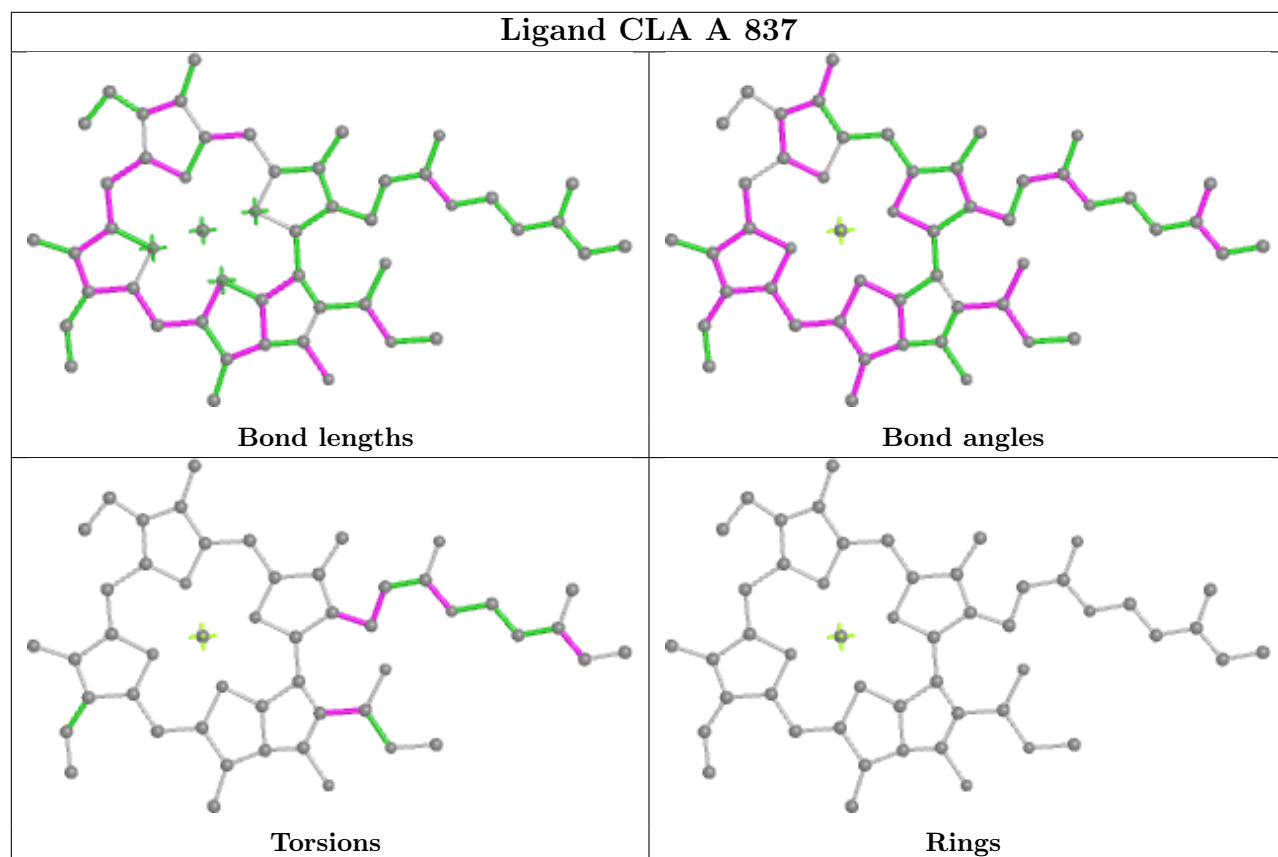
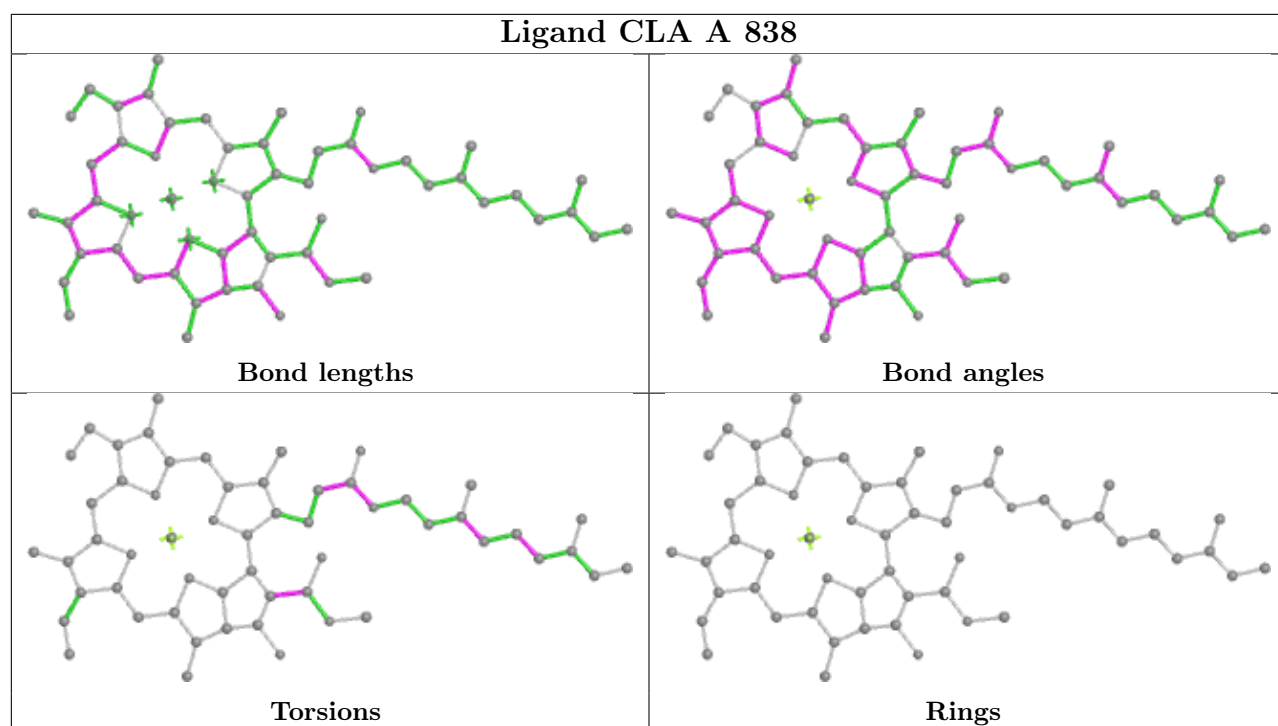


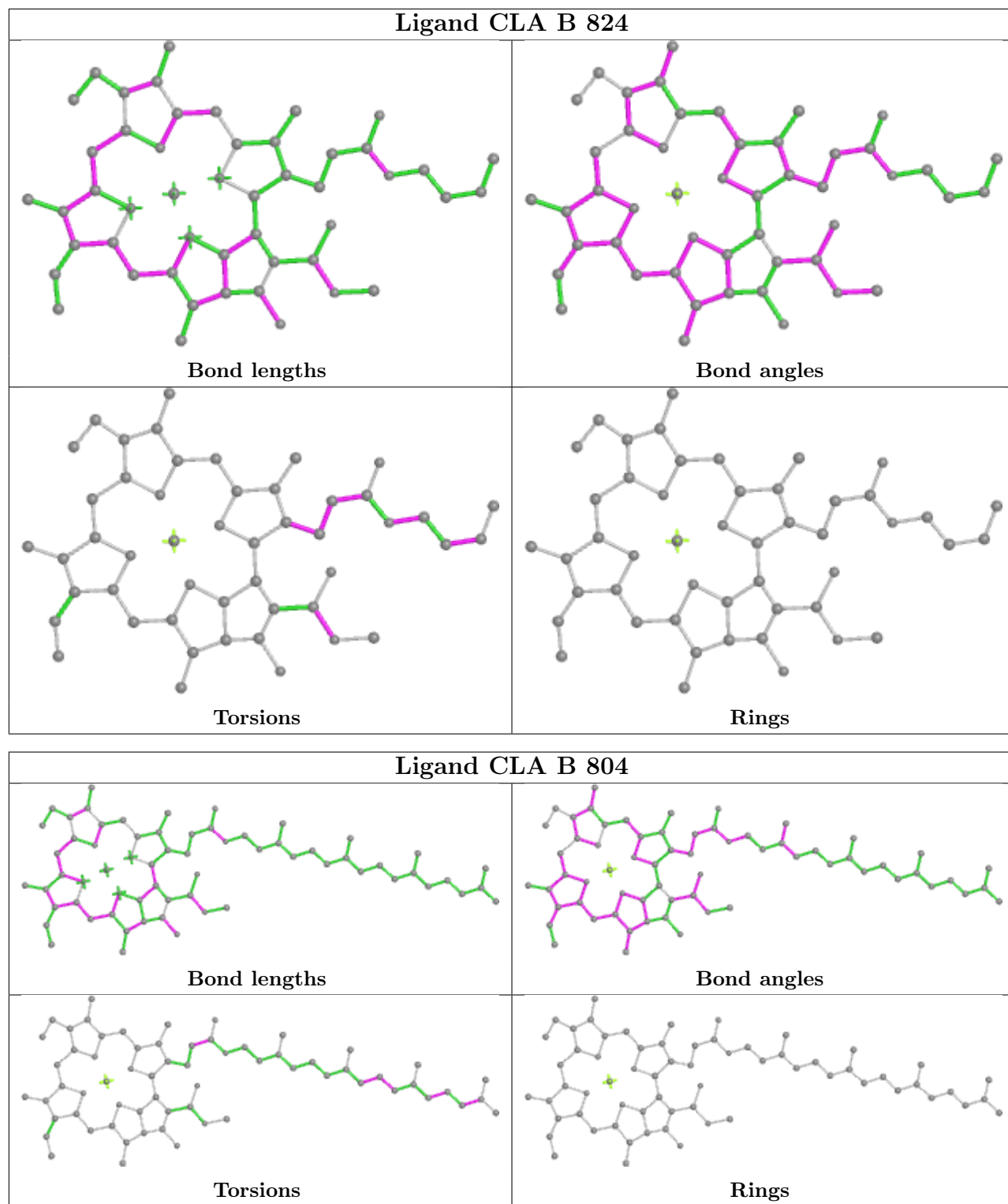


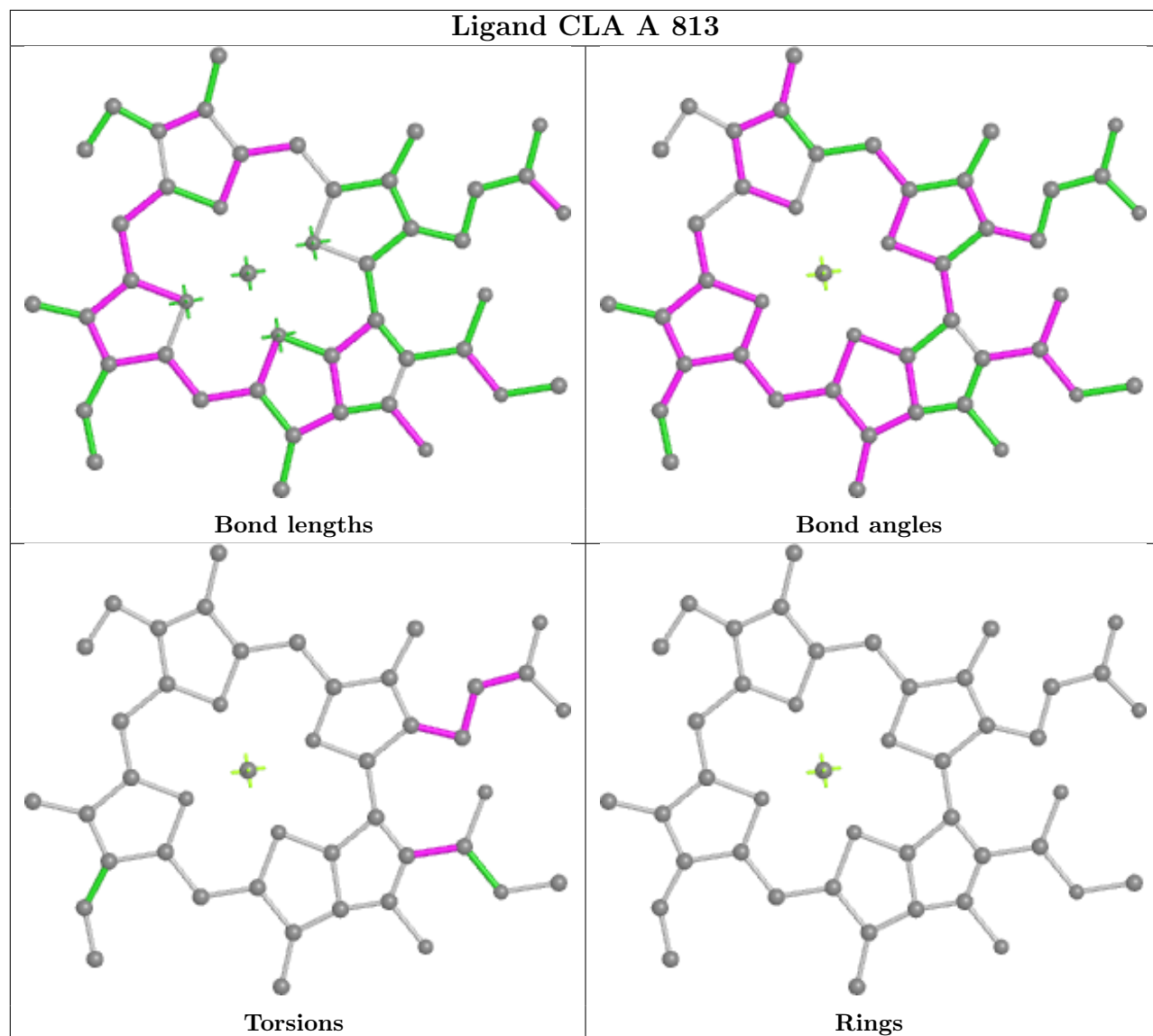


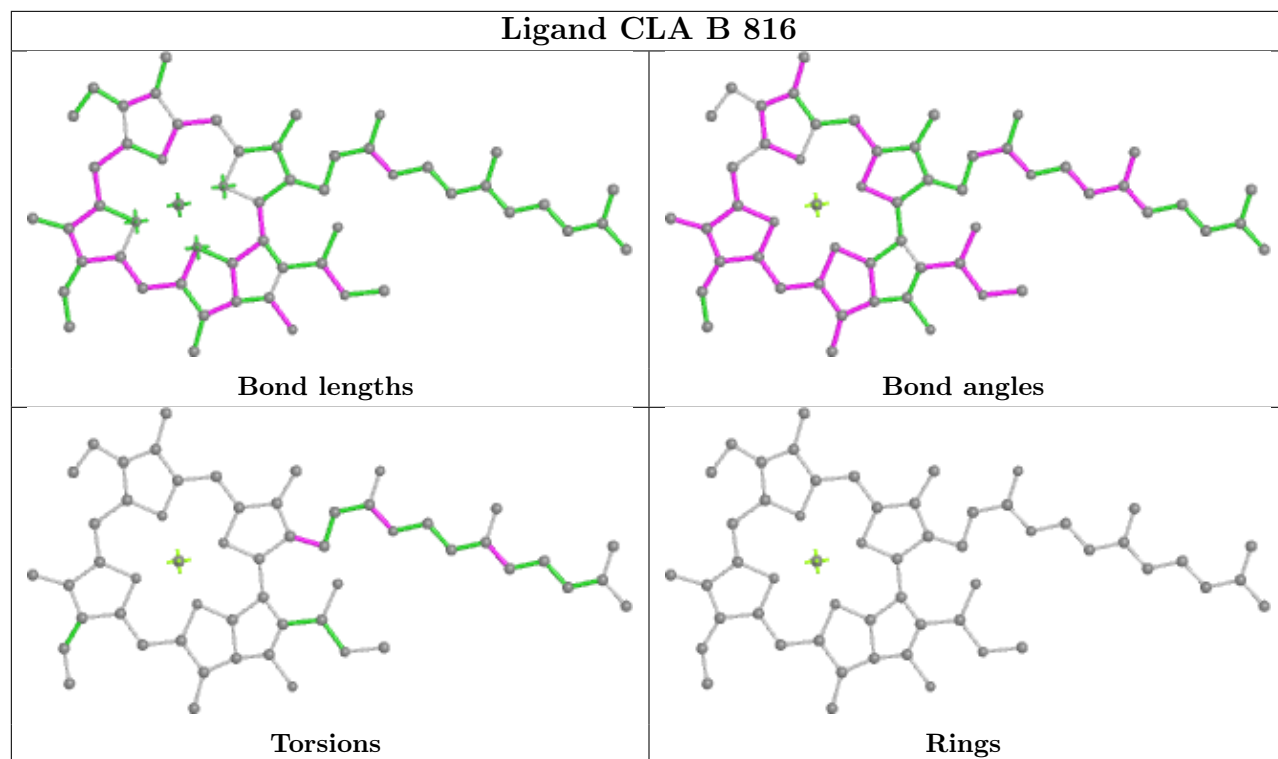


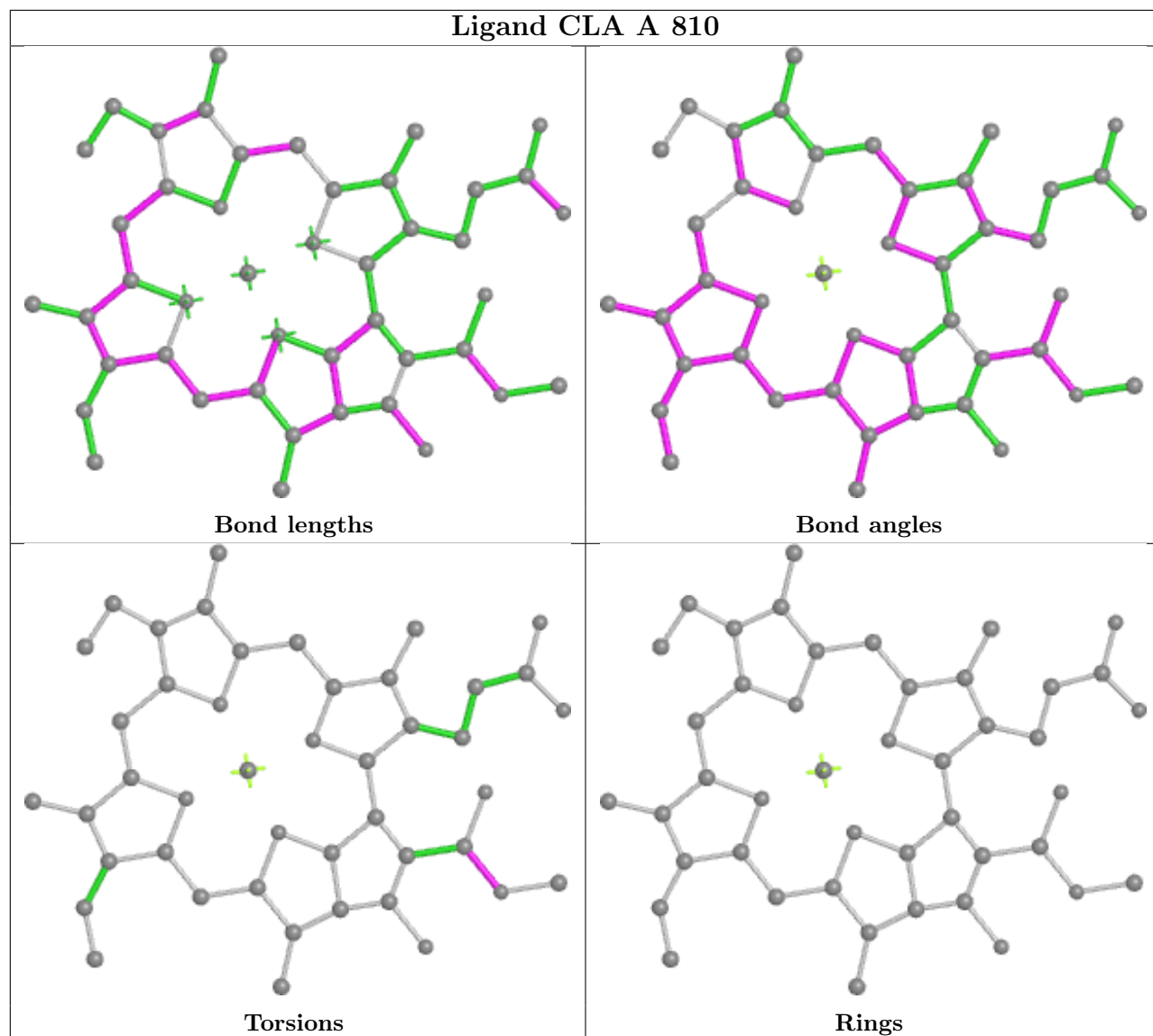


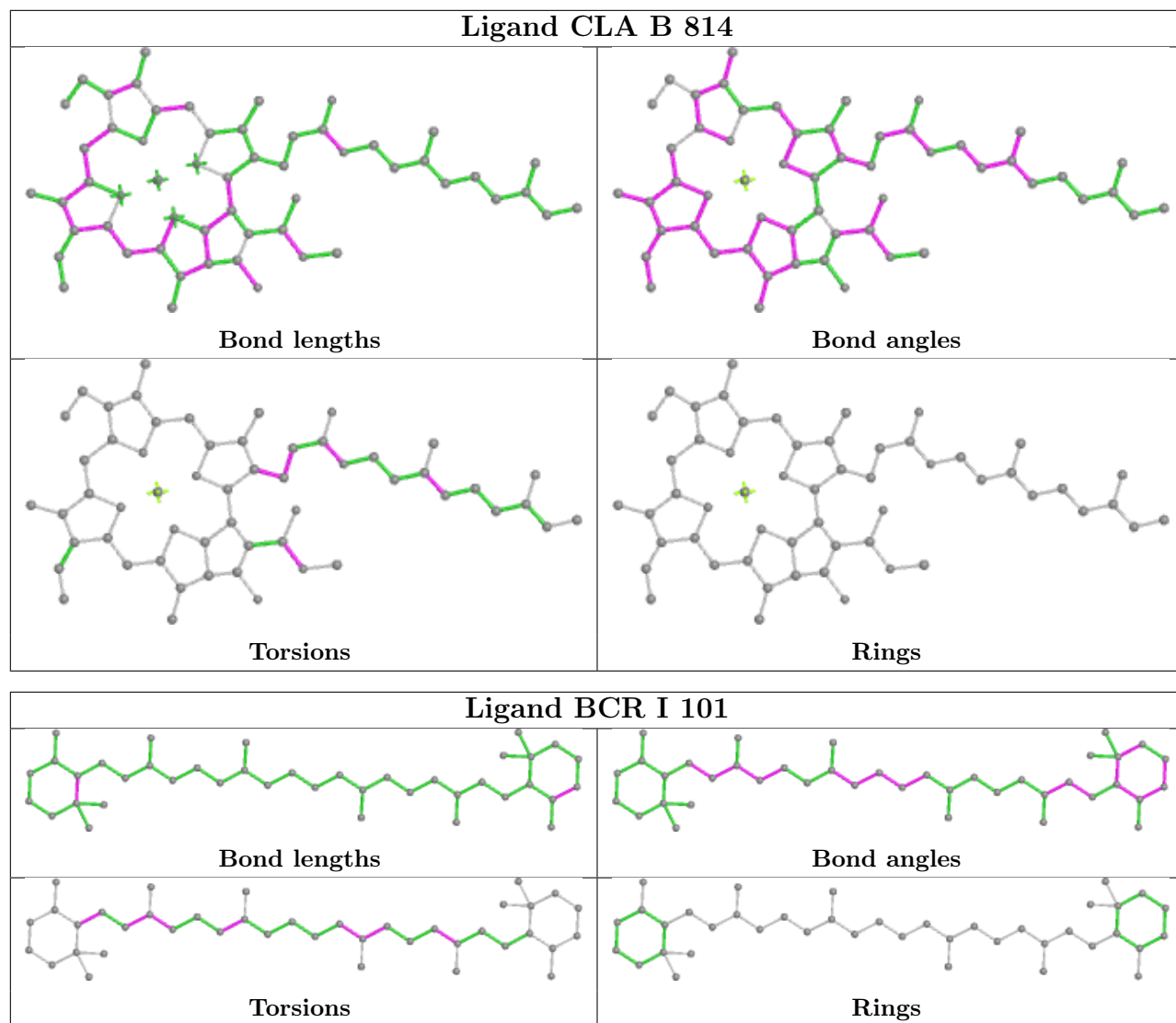


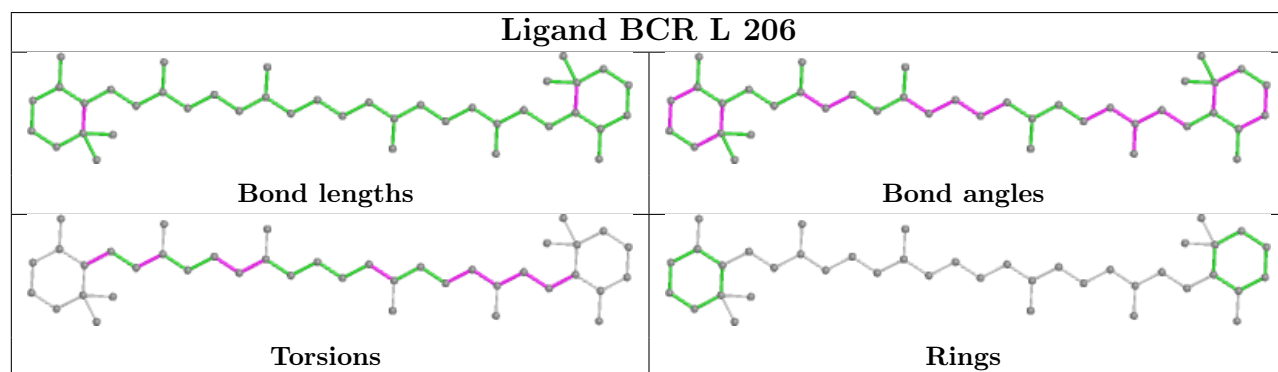
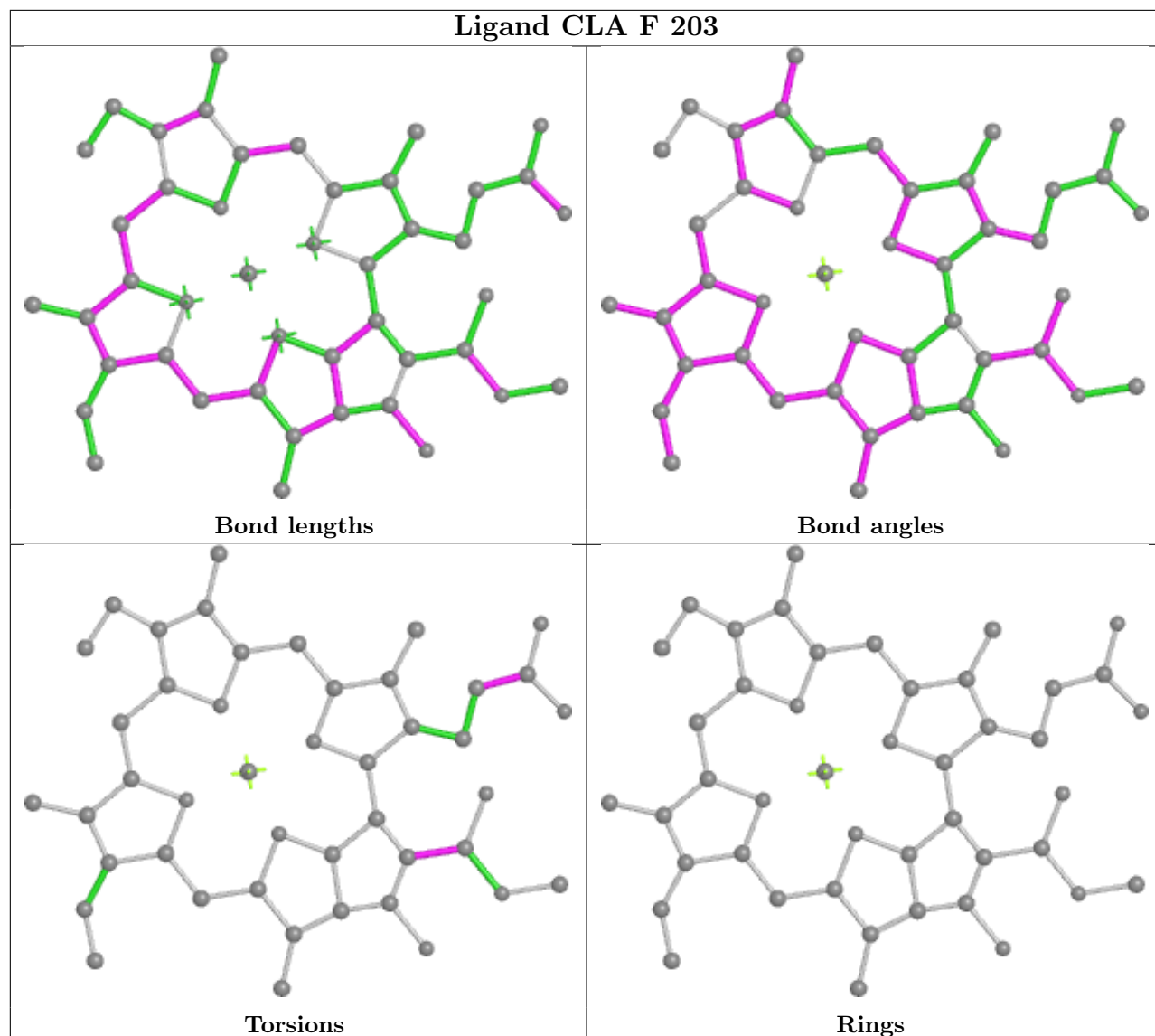


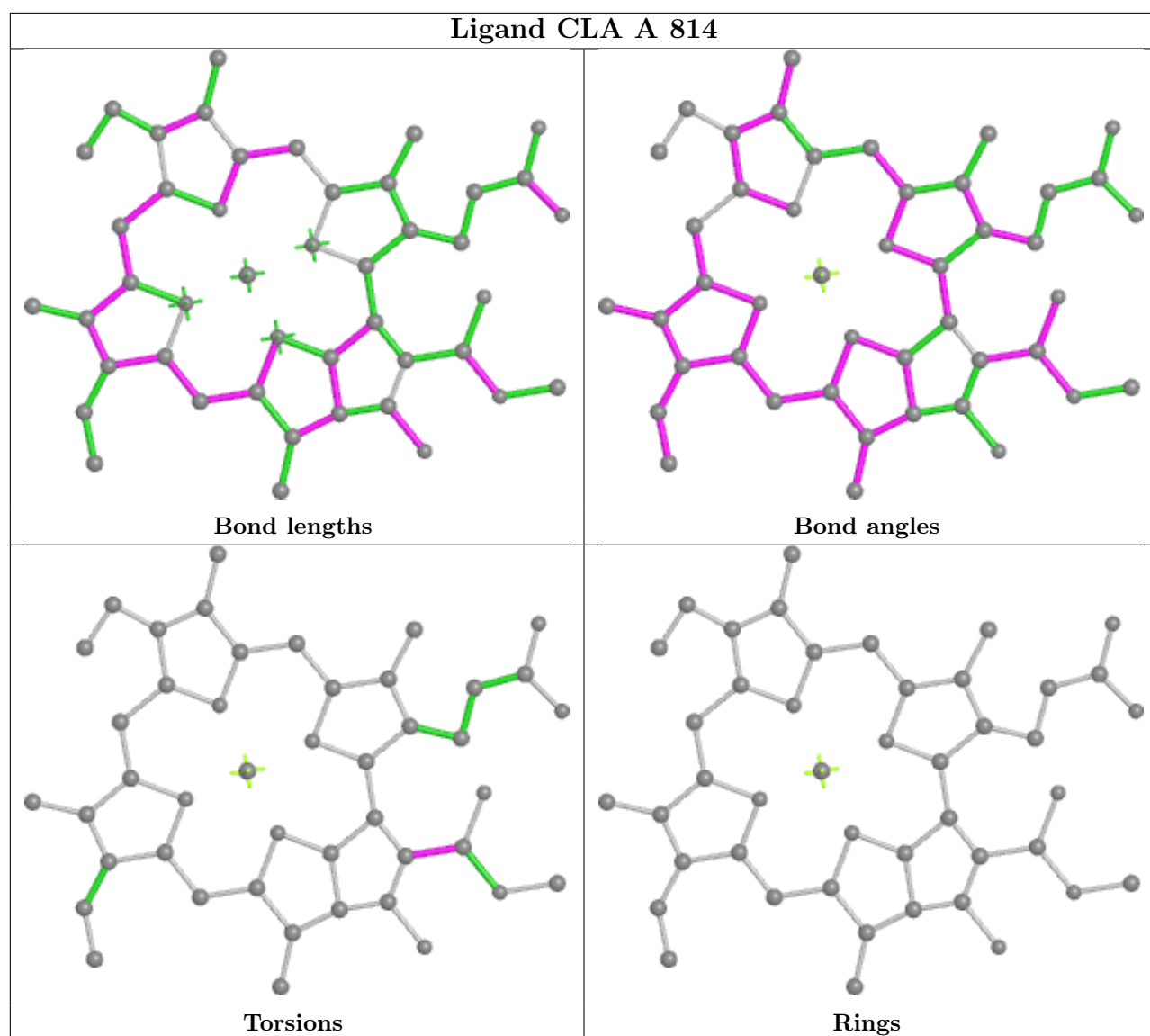


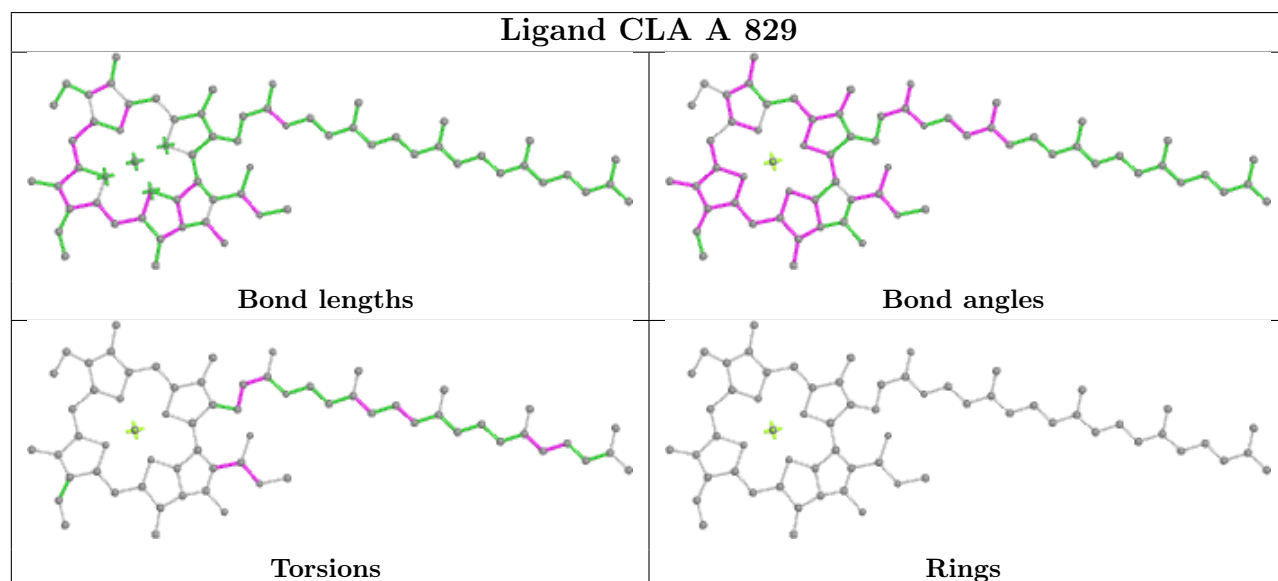
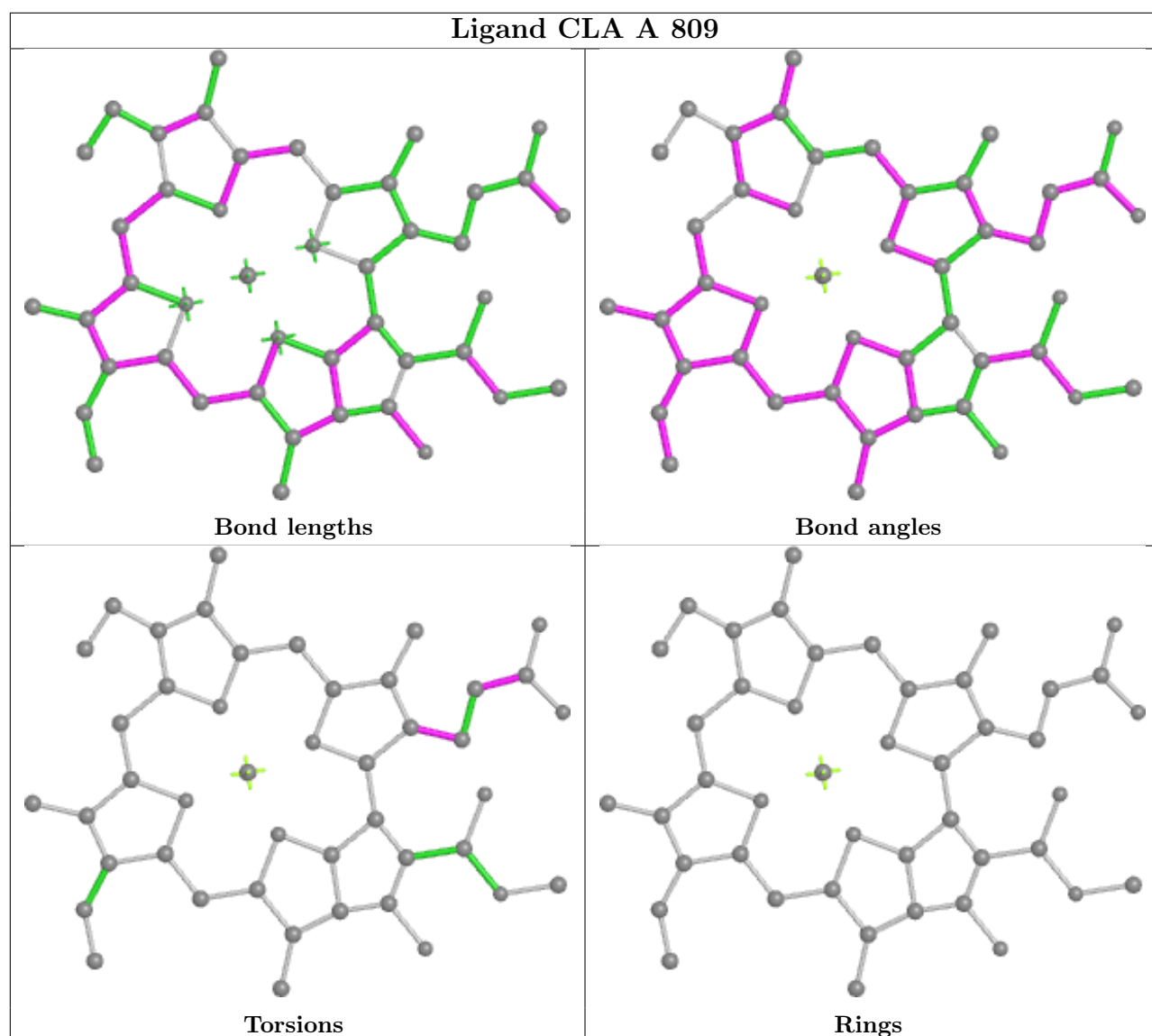


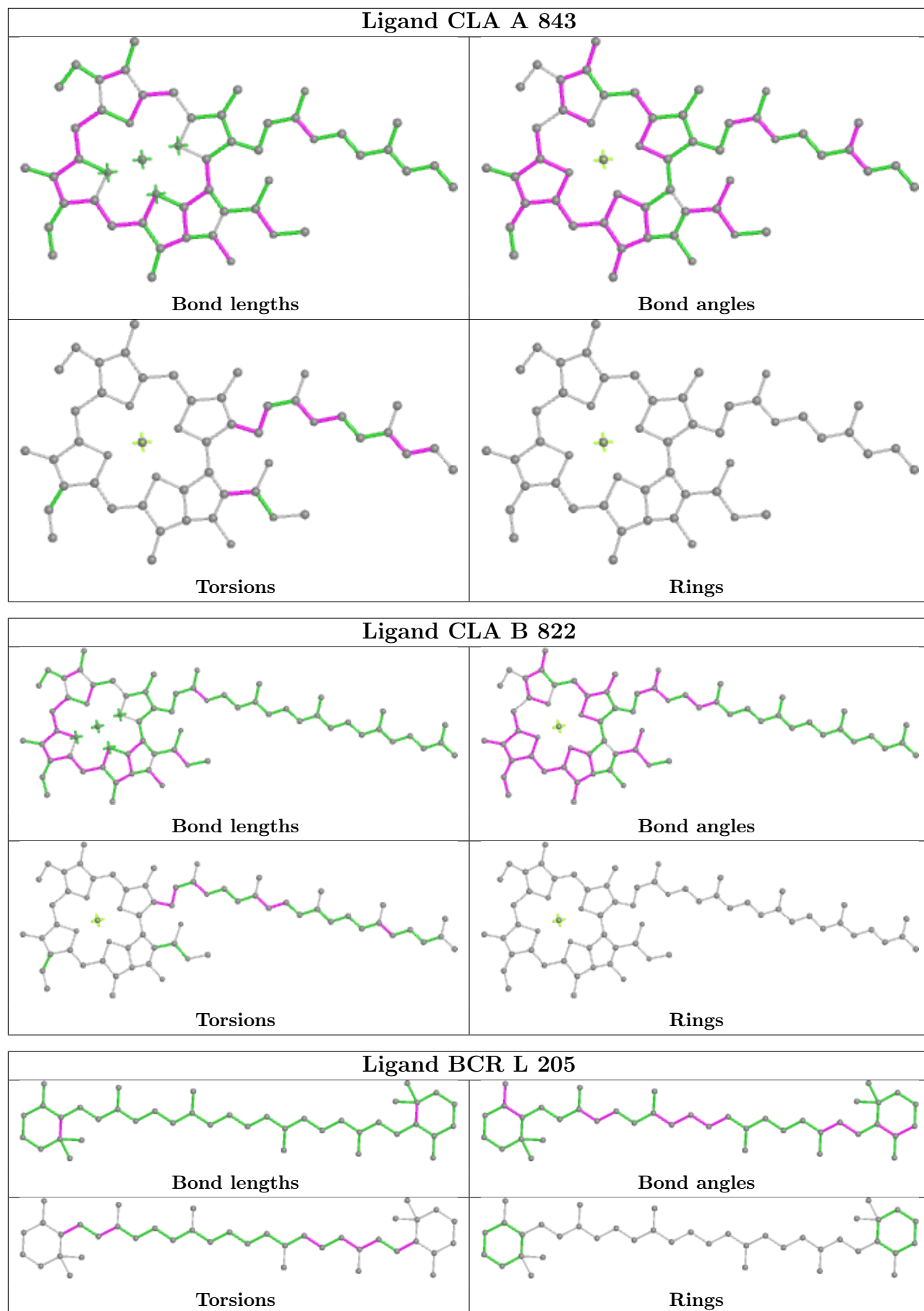


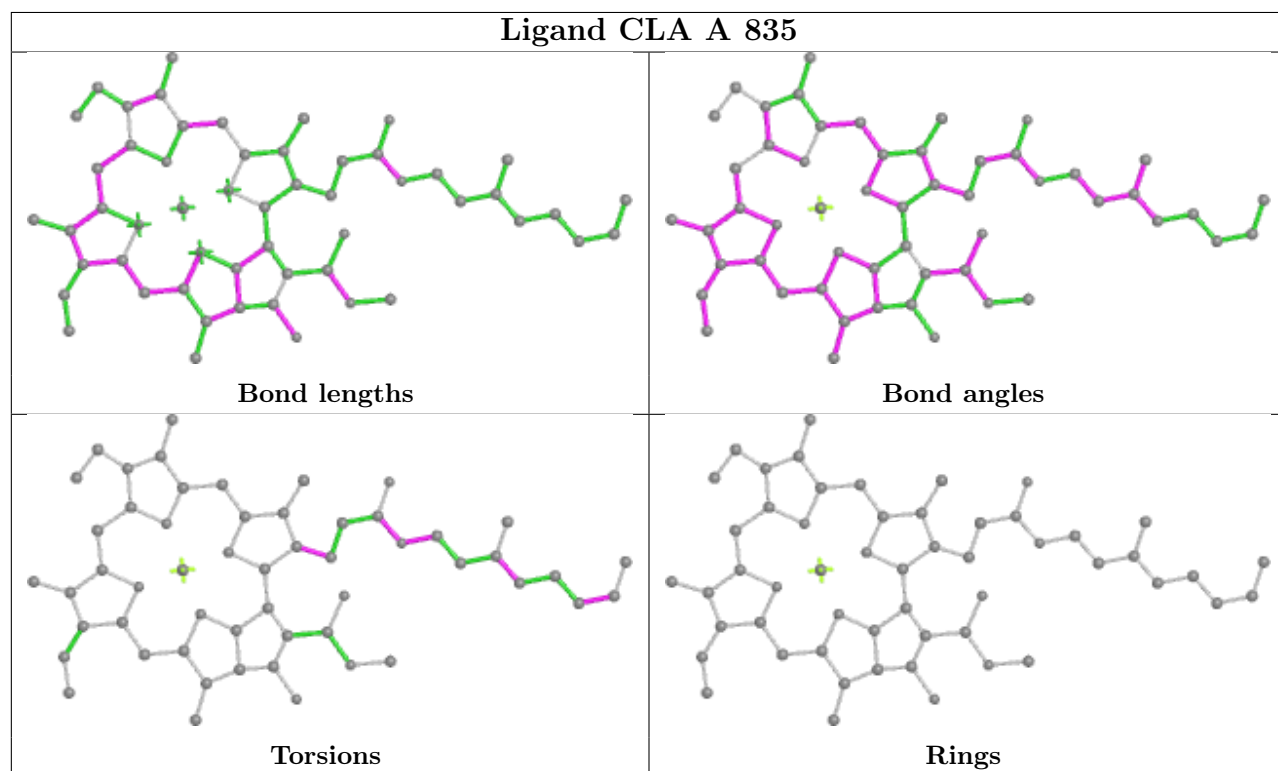
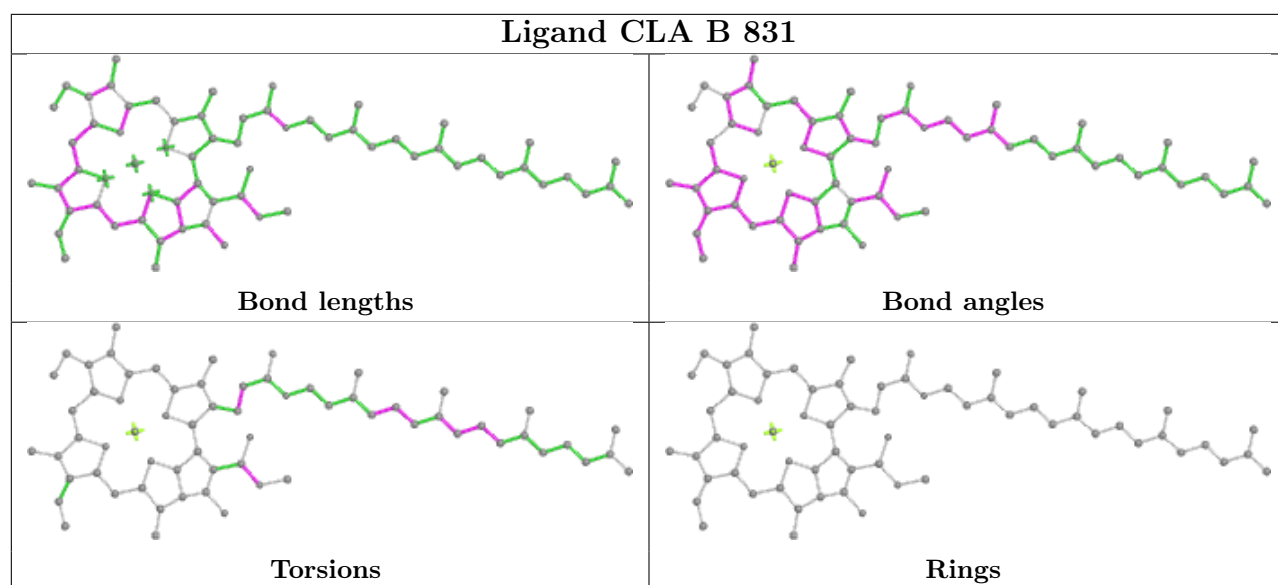


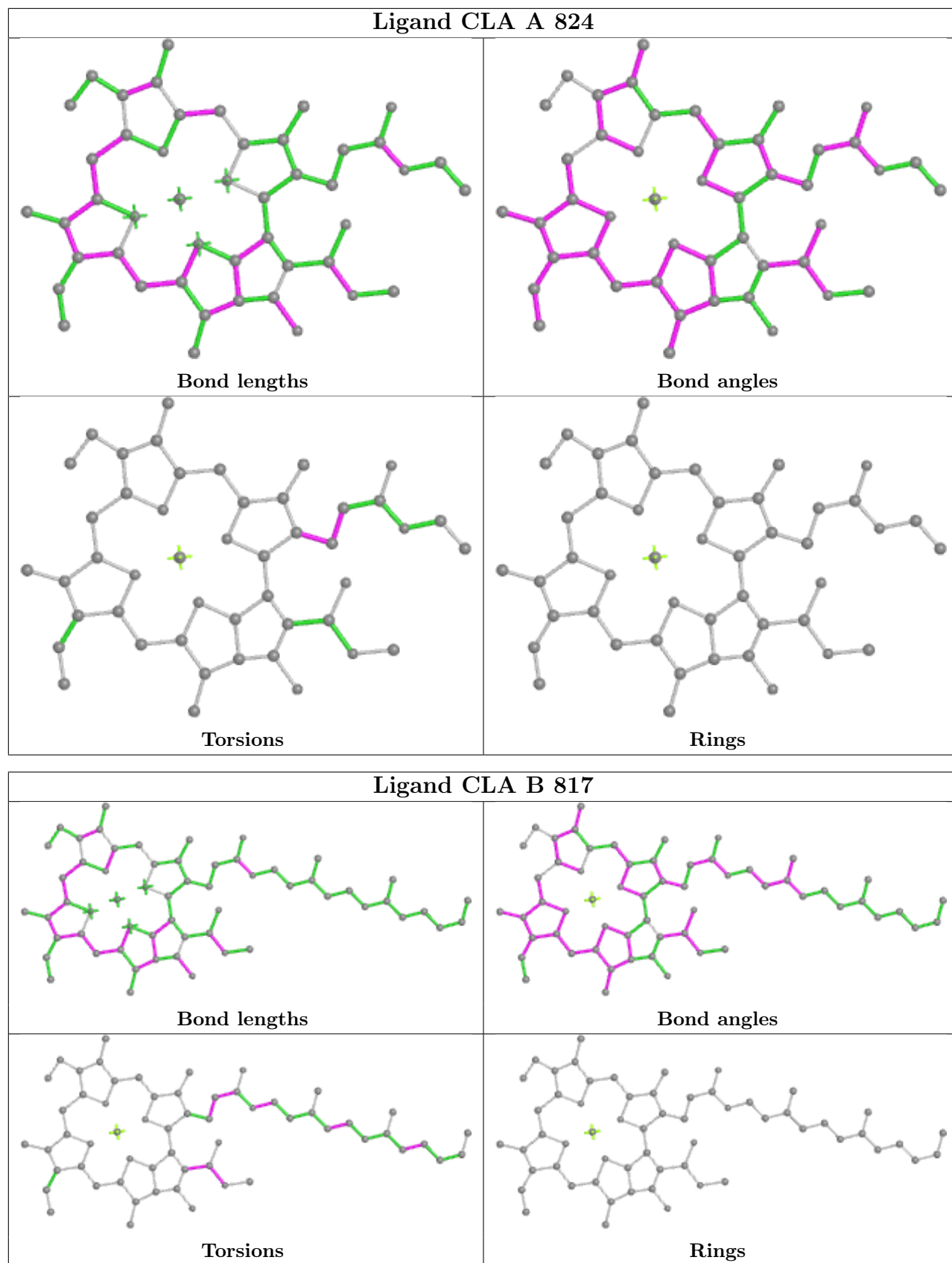


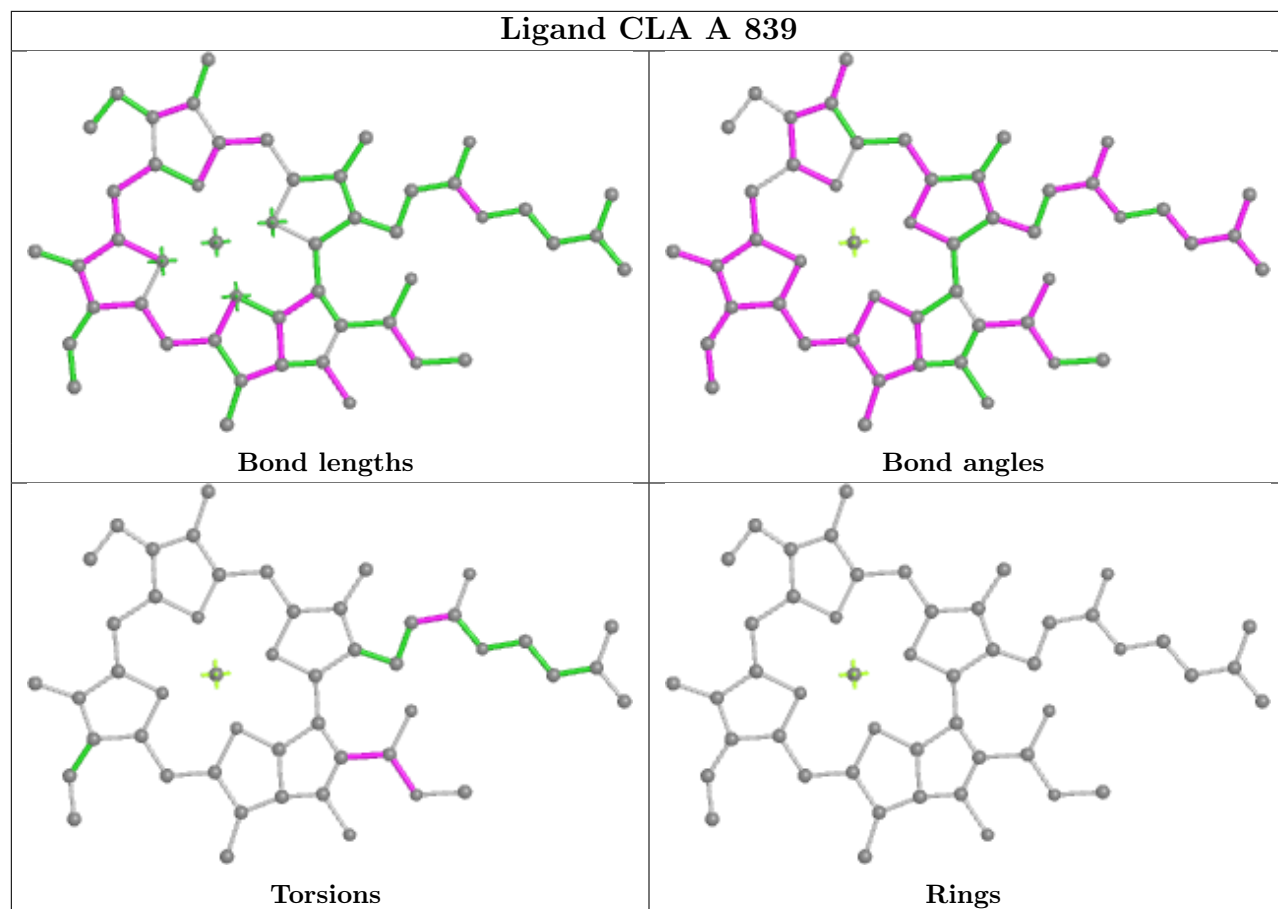


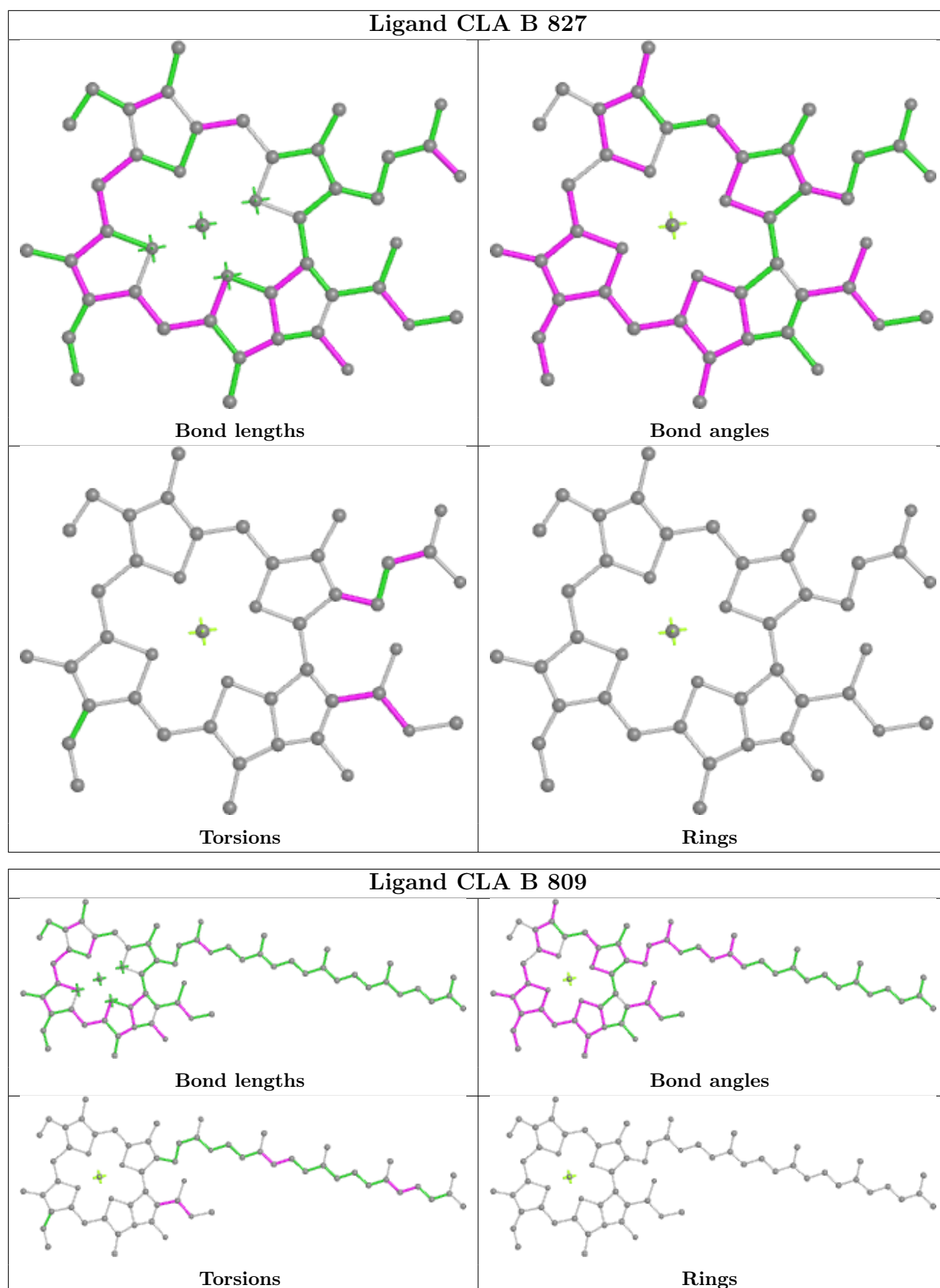


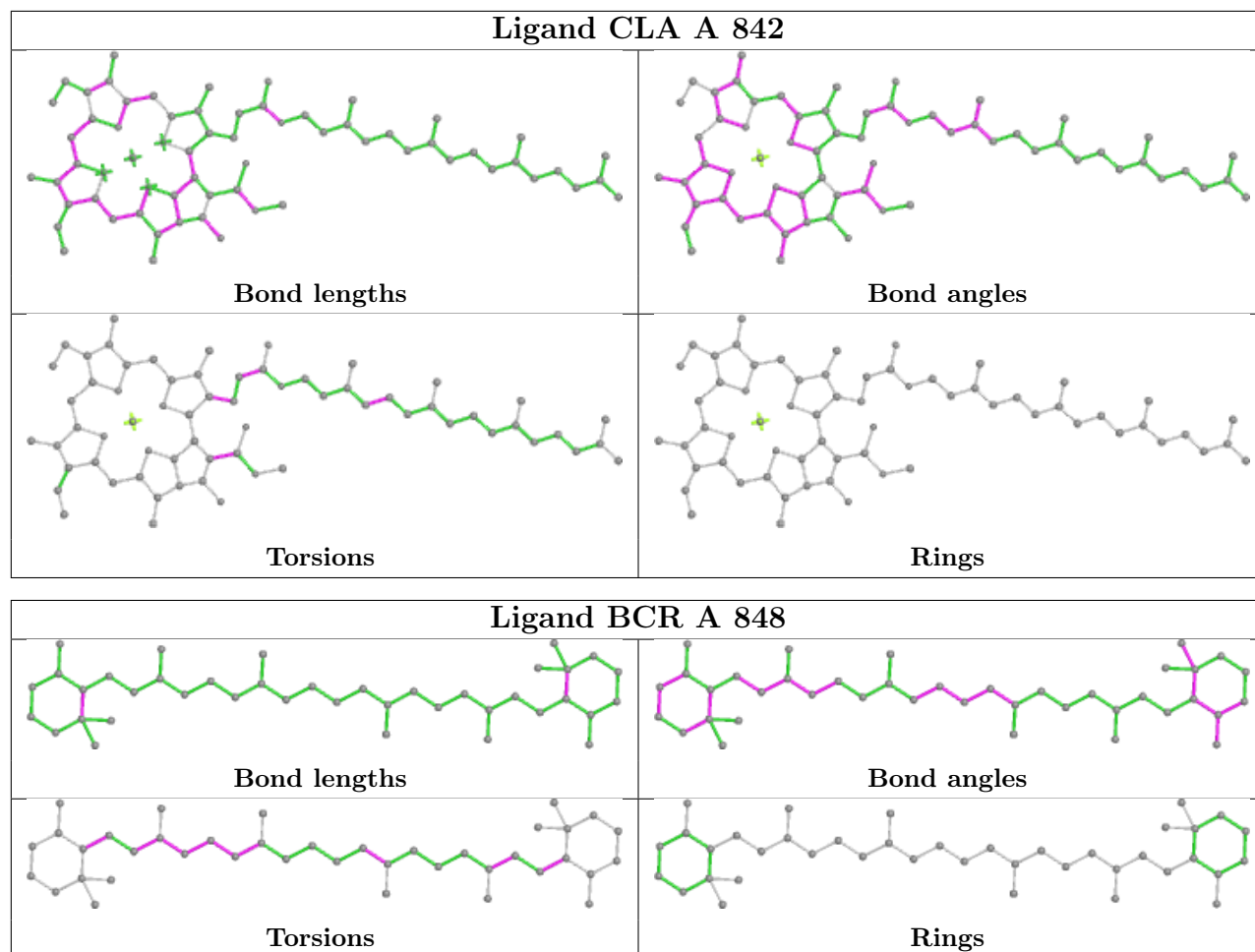


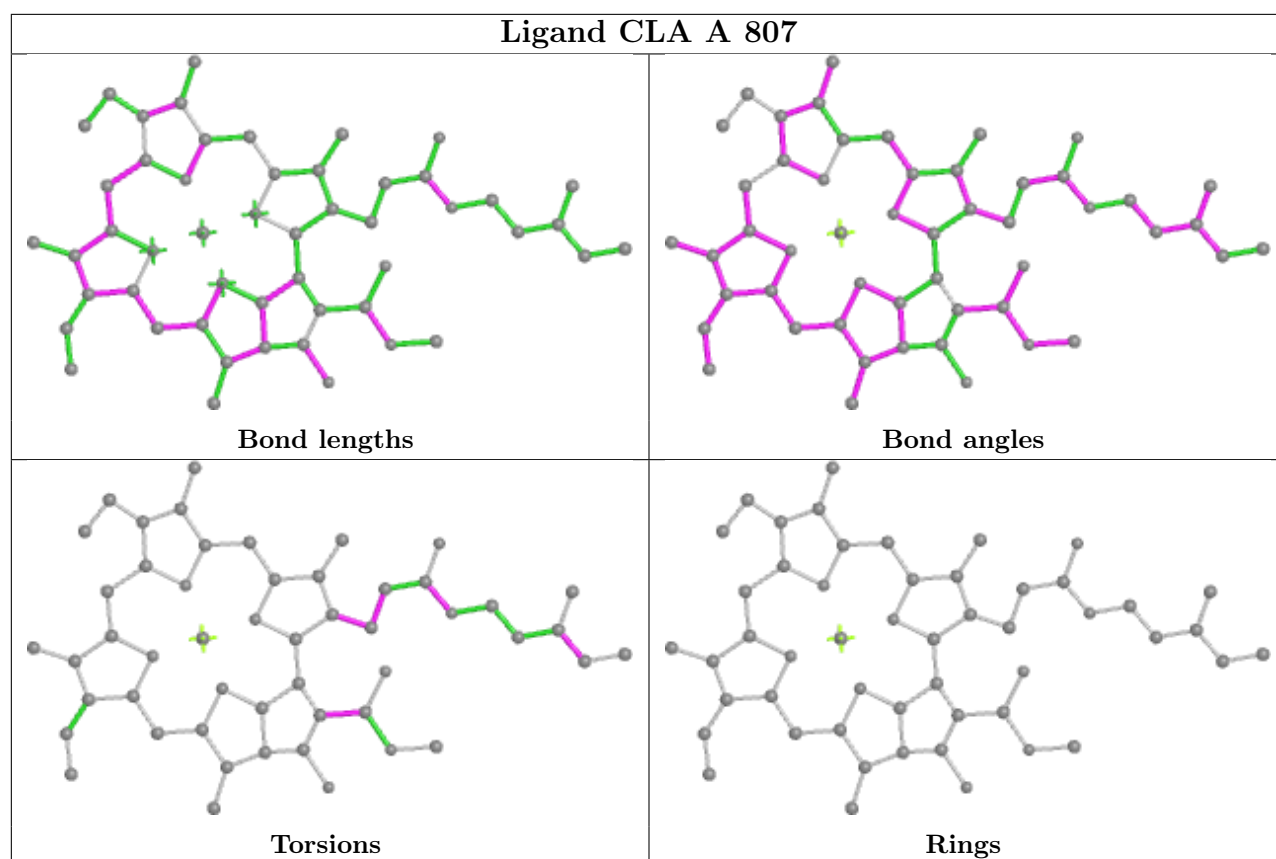












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

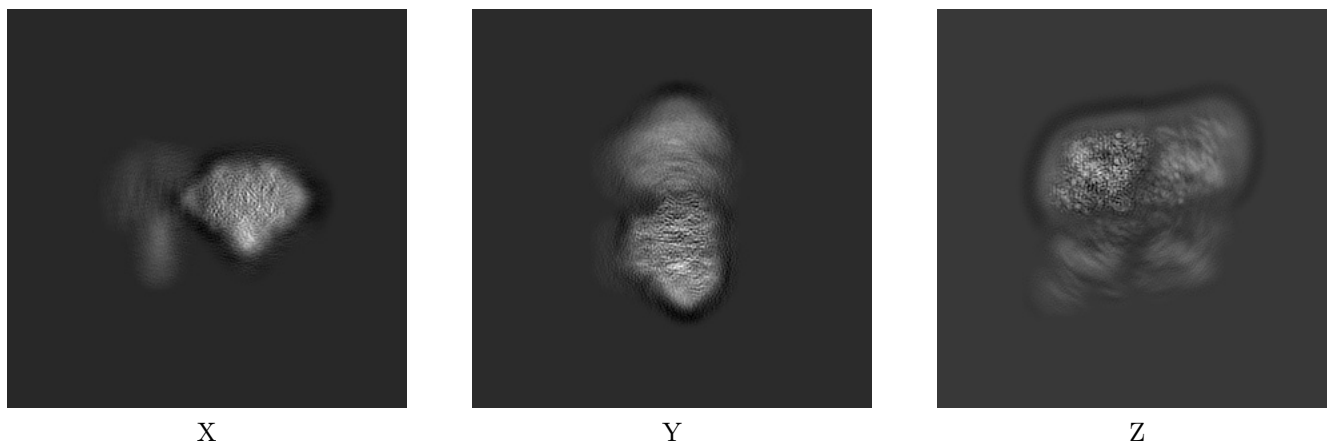
6 Map visualisation [i](#)

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](#)

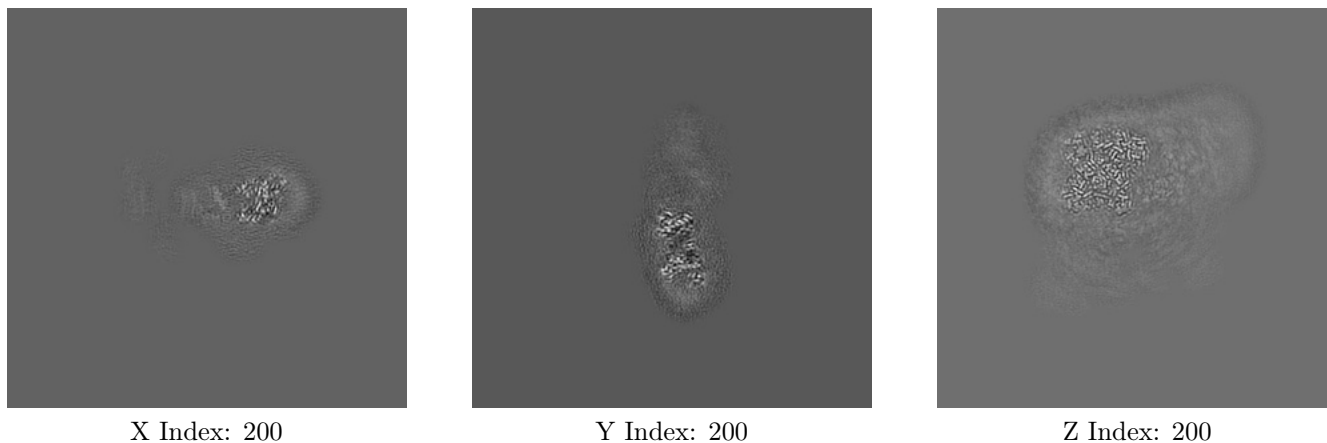
6.1.1 Primary map



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

6.2 Central slices [i](#)

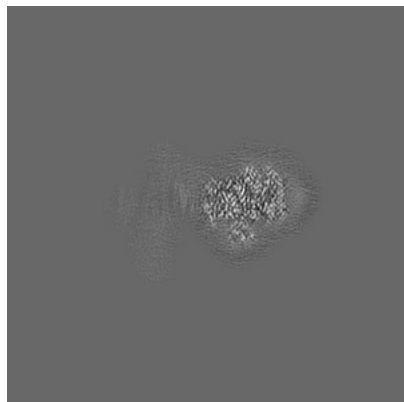
6.2.1 Primary map



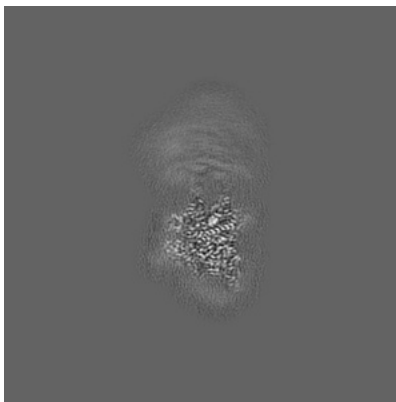
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

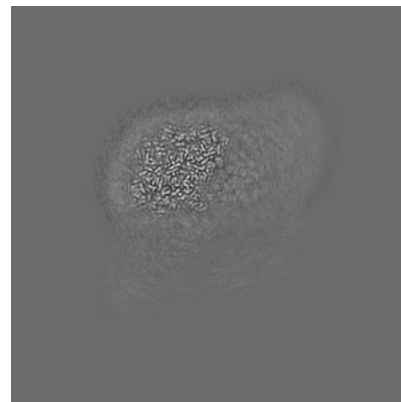
6.3.1 Primary map



X Index: 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 surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

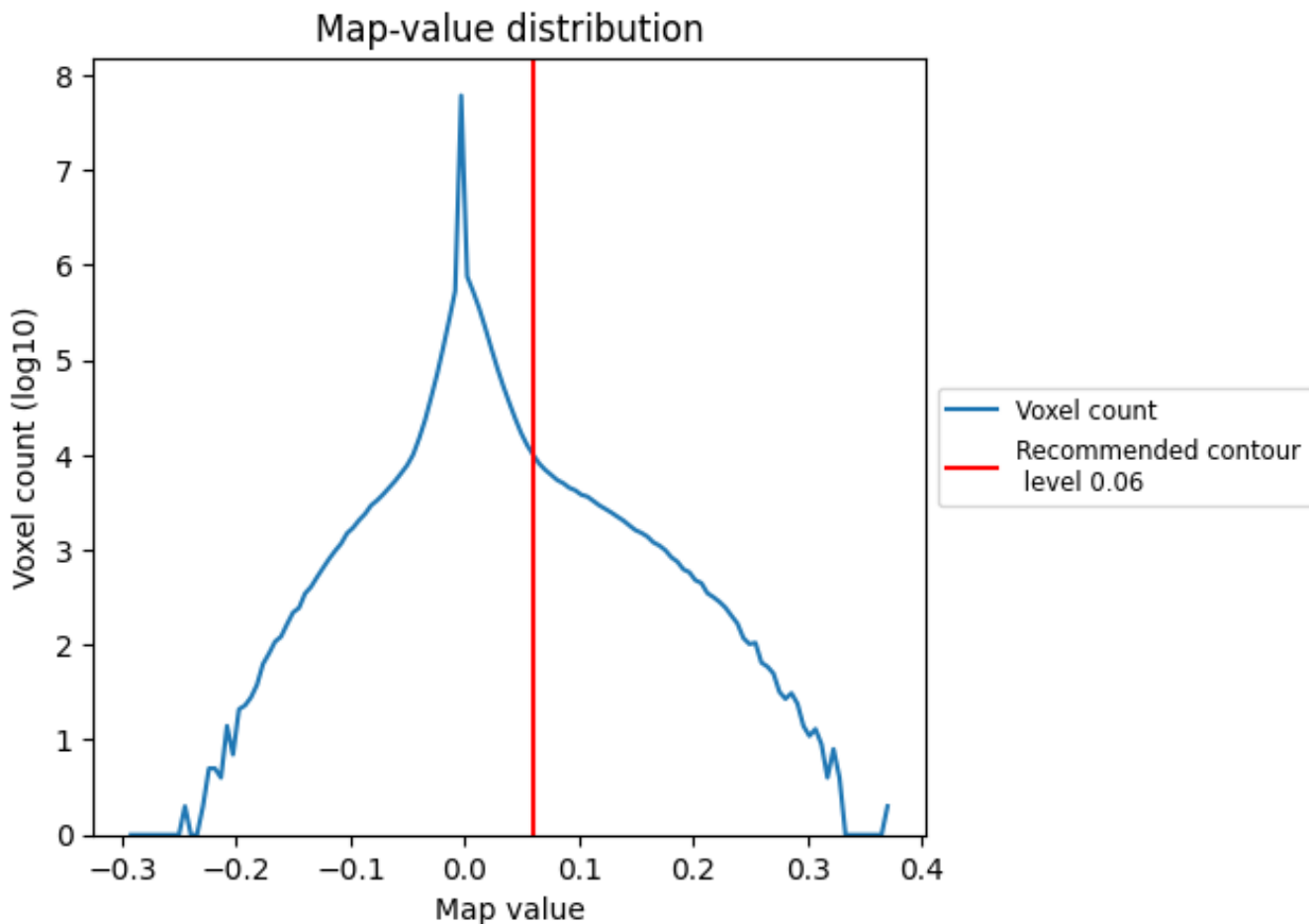
6.5 Mask visualisation

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

7 Map analysis [i](#)

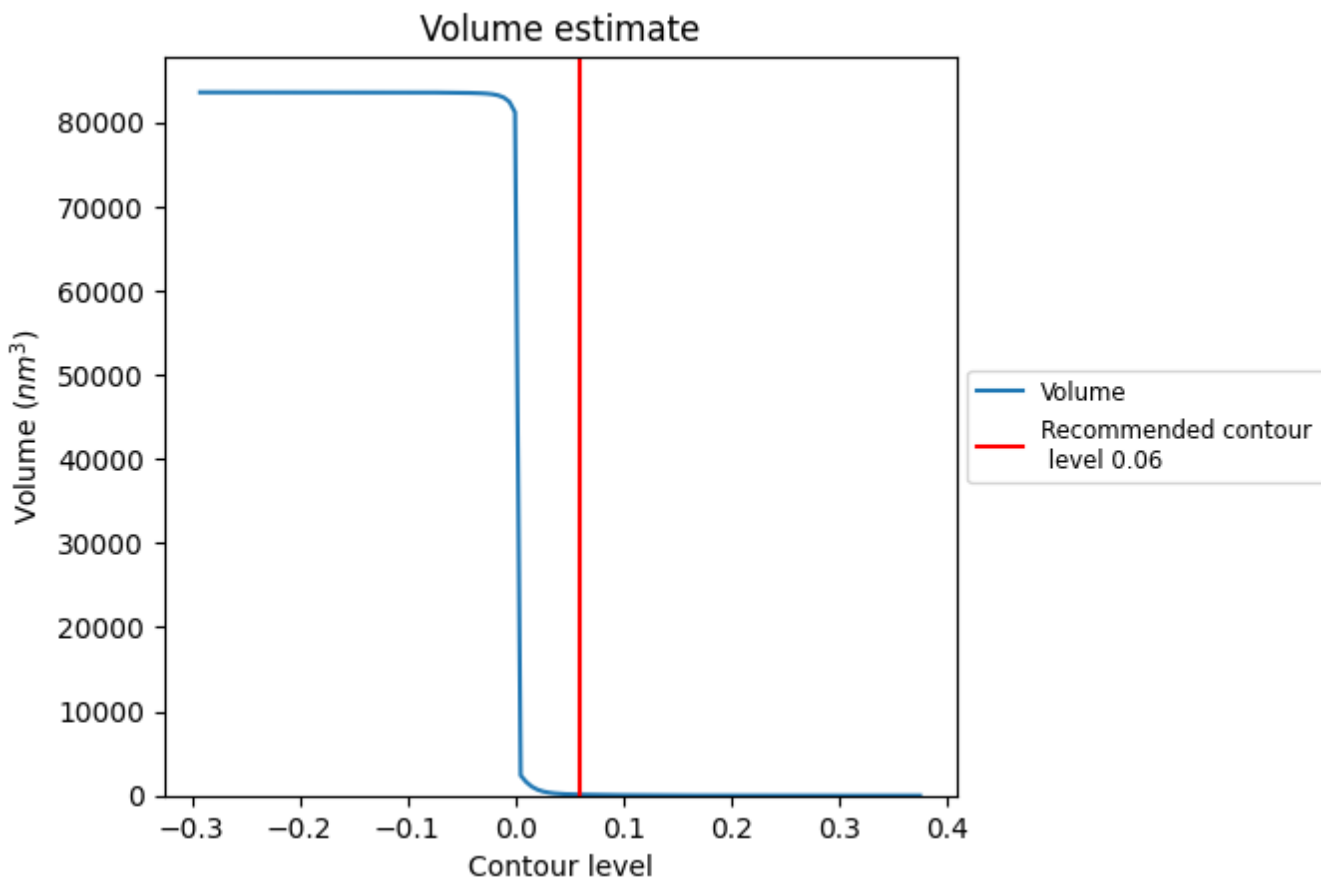
This section contains the results of statistical analysis of the map.

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.

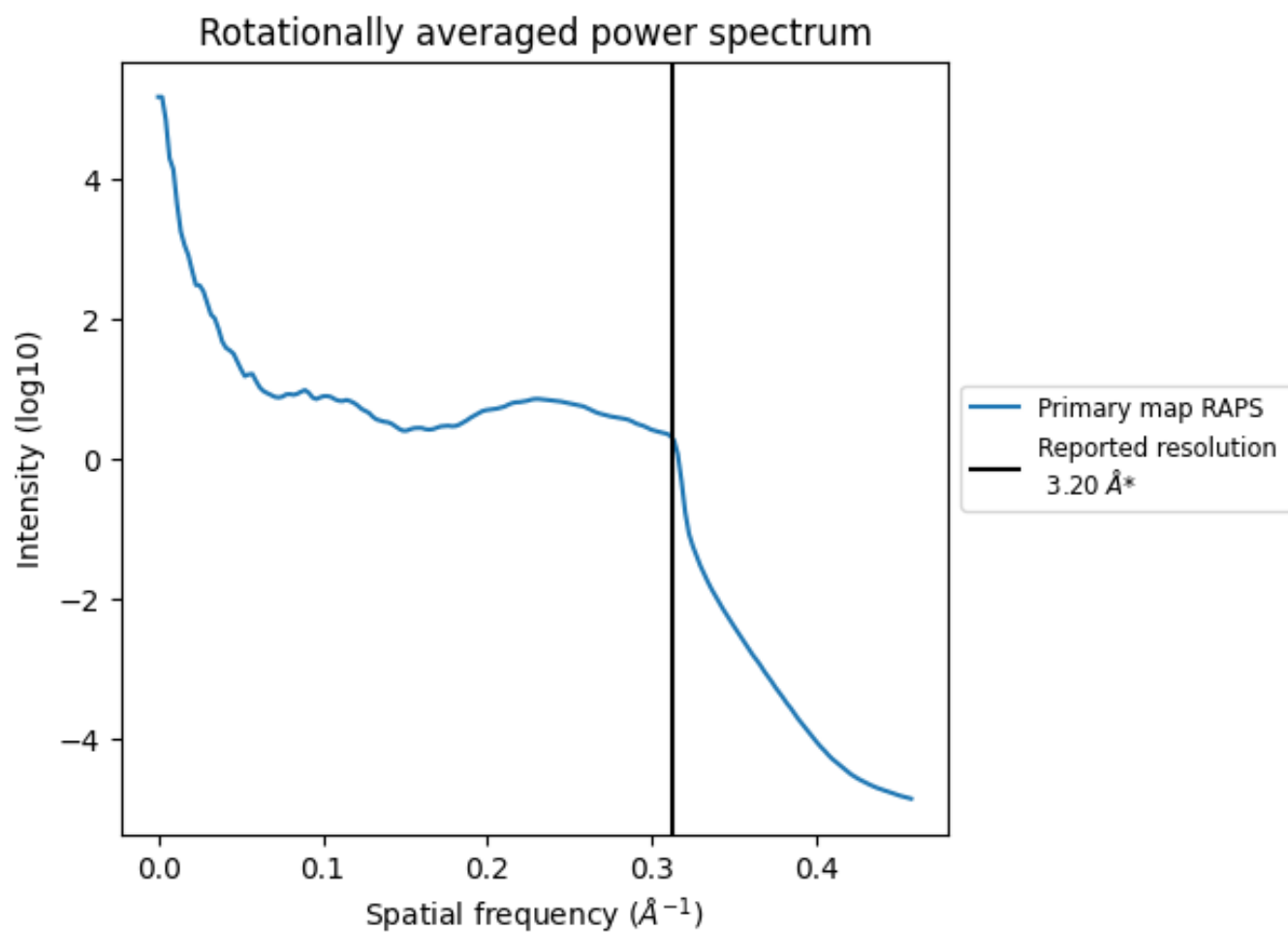
7.2 Volume estimate [i](#)



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 [i](#)

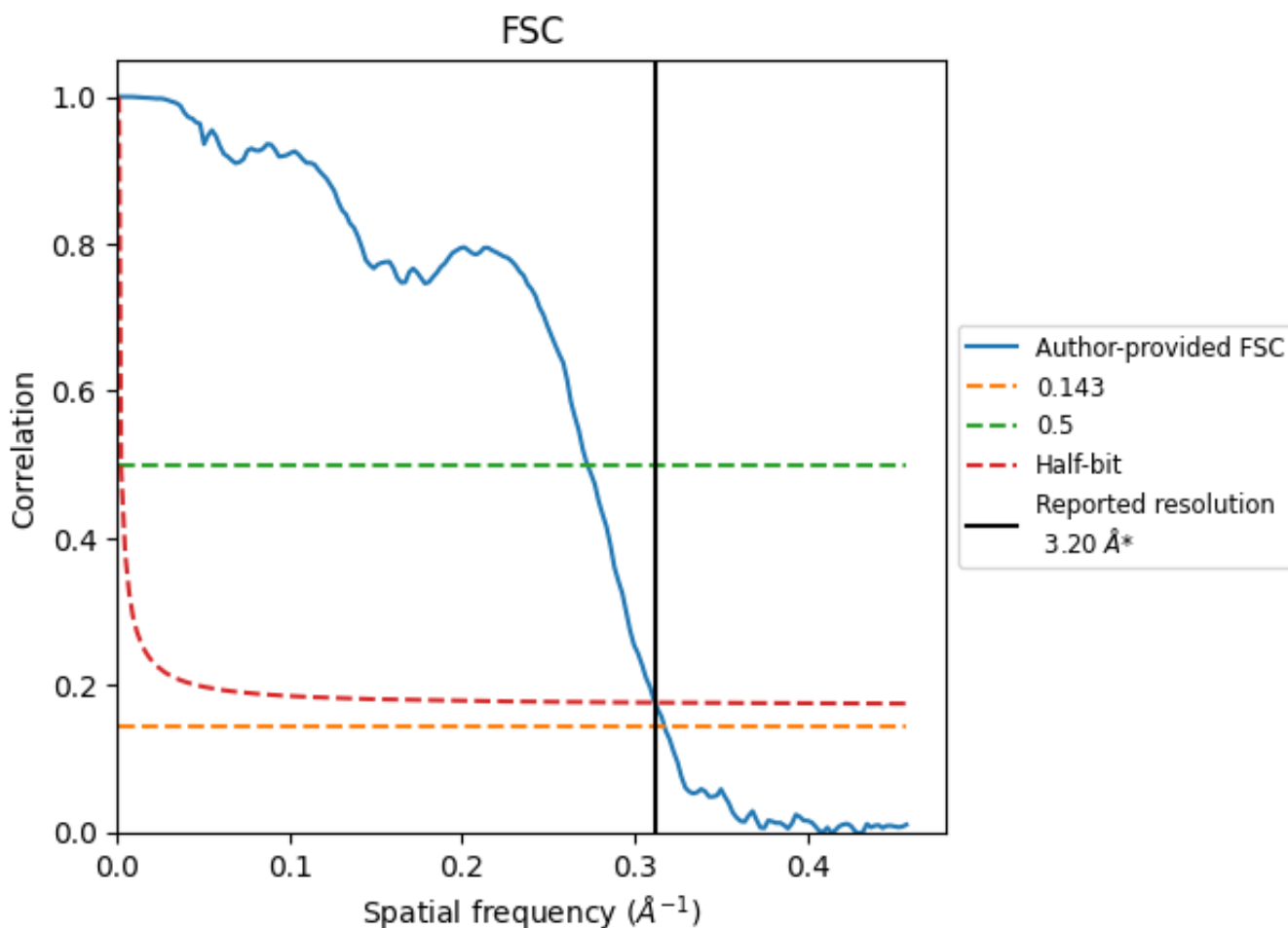


*Reported resolution corresponds to spatial frequency of 0.312\AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

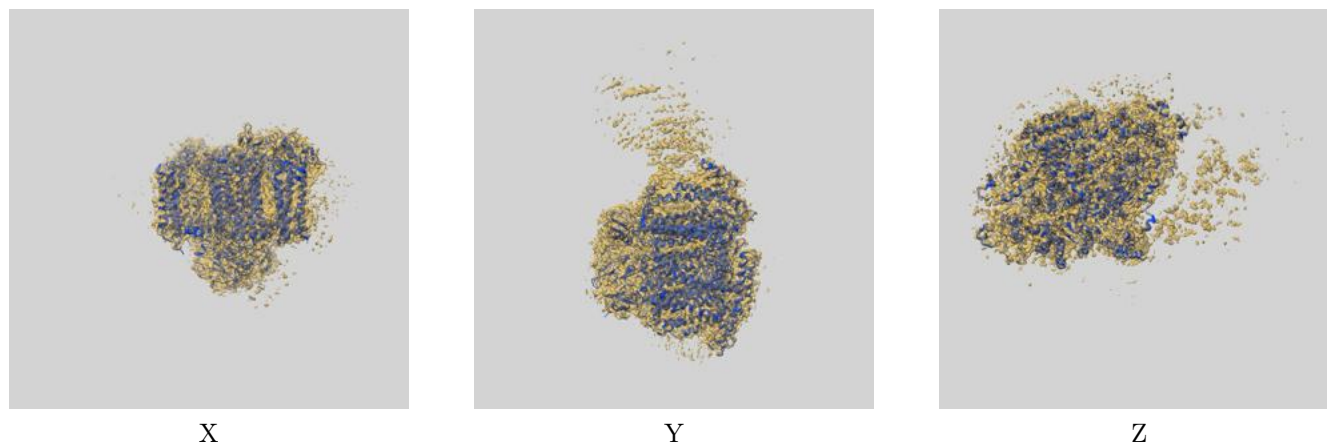
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.67	3.21
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

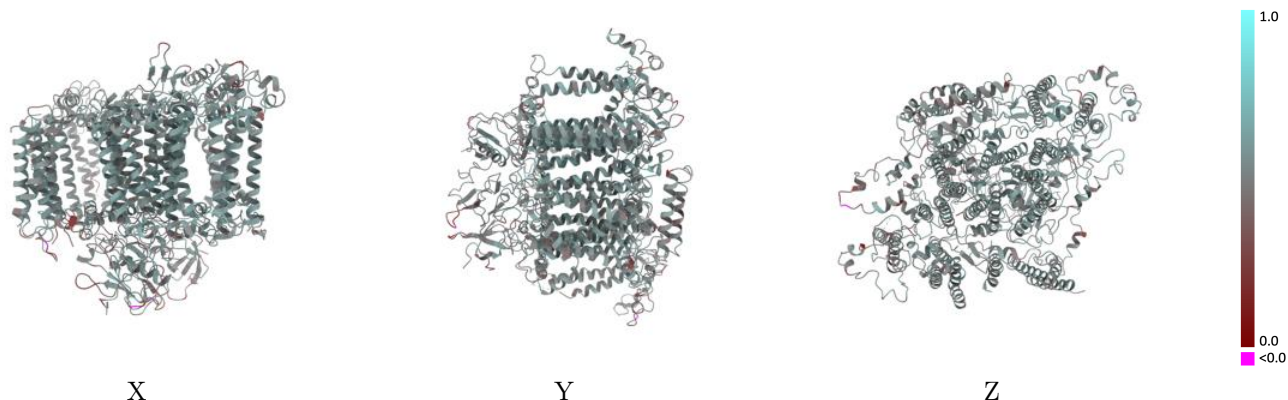
This section contains information regarding the fit between EMDB map EMD-30821 and PDB model 7DR1. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



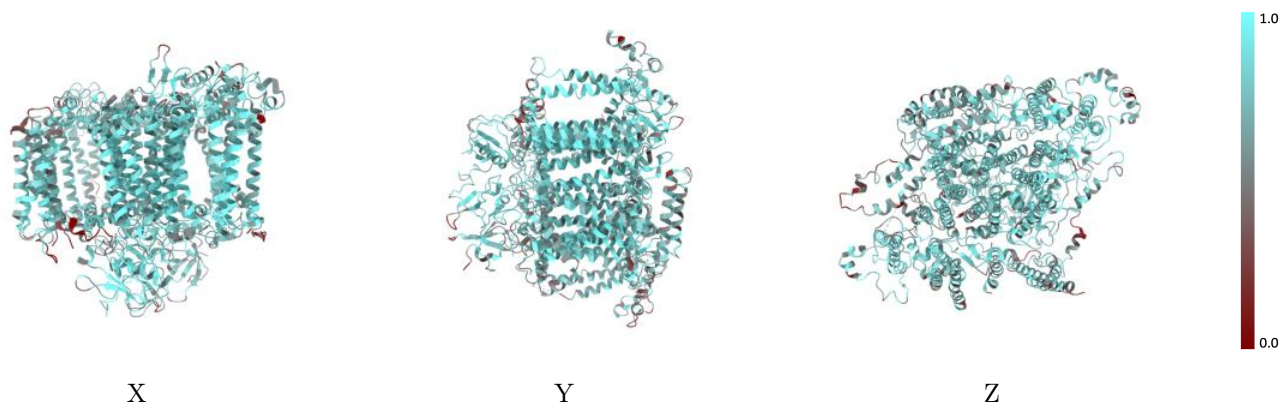
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



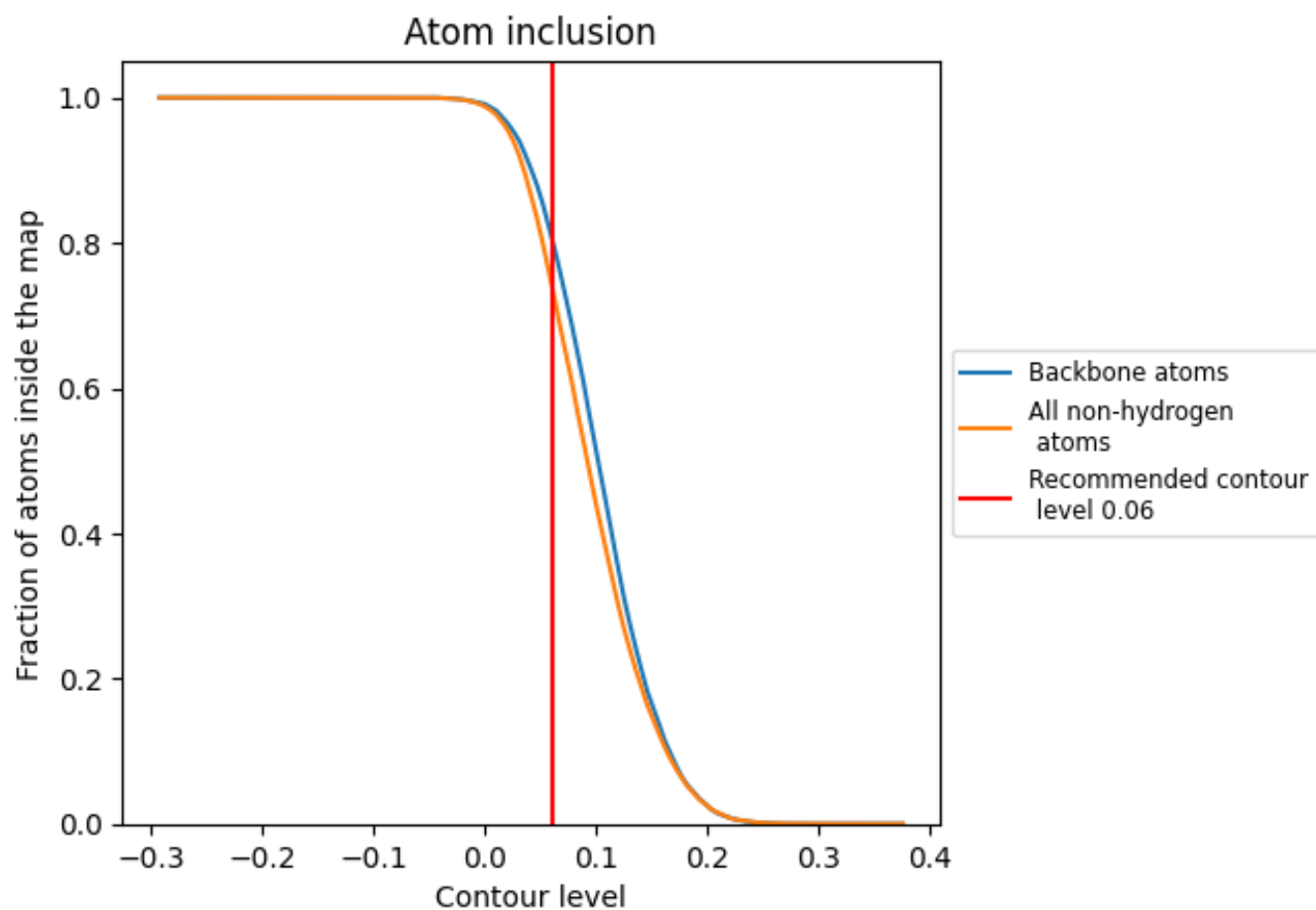
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 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	 0.7434	 0.5250
A	 0.7773	 0.5470
B	 0.7456	 0.5200
C	 0.7870	 0.4730
D	 0.7549	 0.4870
E	 0.7192	 0.4730
F	 0.6664	 0.5050
I	 0.6479	 0.5250
J	 0.6726	 0.5290
L	 0.6267	 0.5050
M	 0.6548	 0.5200

