



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:33 PM UTC

PDB ID : 6TRA / pdb_00006tra
EMDB ID : EMD-10557
Title : Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6
Authors : Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Miehke, T.; Lisdat, F.; Zouni, A.; Wendler, P.
Deposited on : 2019-12-18
Resolution : 2.85 Å (reported)
Based on initial model : 1JB0

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:

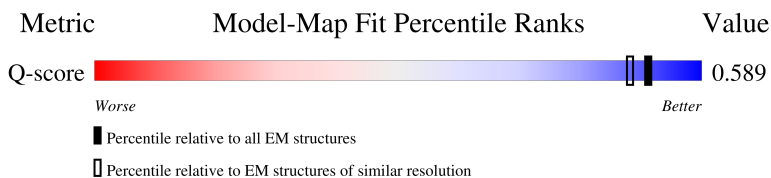
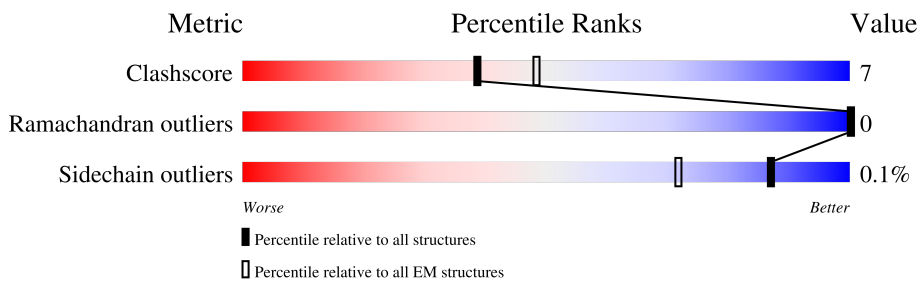
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.85 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	11965 (2.35 - 3.35)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	755	<div style="display: flex; justify-content: space-between;"> 9% 83% 16% </div>
2	B	741	<div style="display: flex; justify-content: space-between;"> 11% 85% 15% </div>
3	C	81	<div style="display: flex; justify-content: space-between;"> 11% 79% 20% </div>

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Mol	Chain	Length	Quality of chain
4	D	139	
5	E	76	
6	F	141	
7	I	38	
8	J	41	
9	K	83	
10	L	155	
11	M	31	
12	X	36	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	854	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	B	842	X	-	-	-
14	CLA	F	201	X	-	-	-
14	CLA	F	203	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	M	102	X	-	-	-
14	CLA	X	1701	X	-	-	-

2 Entry composition i

There are 21 unique types of molecules in this entry. The entry contains 25197 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	746	5826	3823	995	982	26	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	740	5894	3878	988	1007	21	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	598	367	103	117	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	138	1075	682	186	204	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	70	546	347	94	105	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	141	1065	680	184	197	4	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	38	303	209	40	49	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	J	41	340	232	51	55	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K	79	571	377	92	101	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	L	152	1124	738	180	202	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4

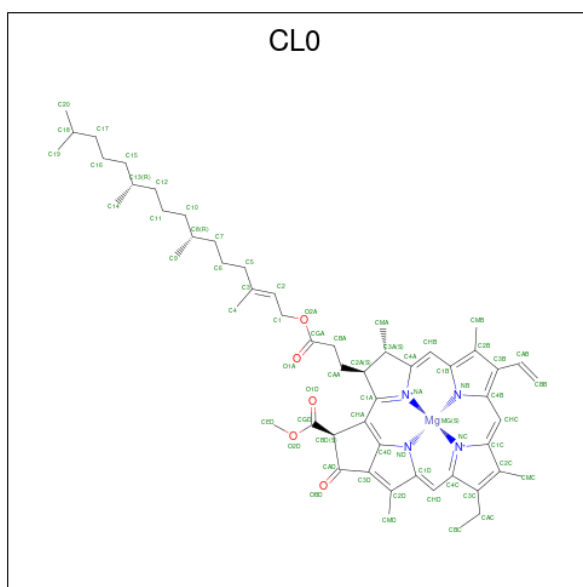
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

- Molecule 12 is a protein called Photosystem I 4.8K protein.

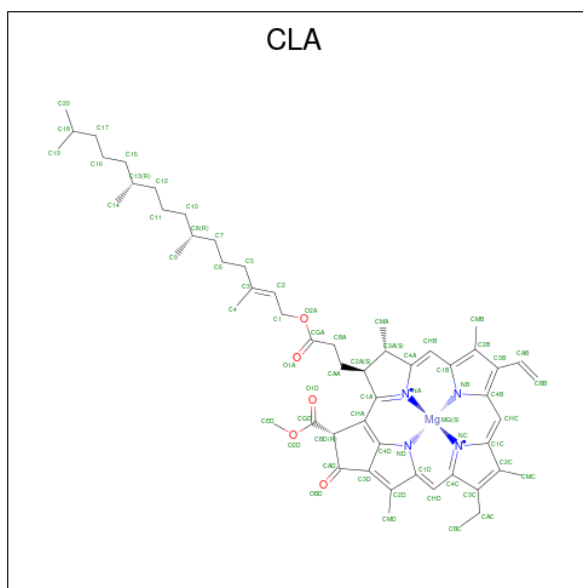
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	X	27	228	163	33	32	0	0

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	60	50	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	45	35	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	65	55	1	4	5	0
14	A	1	45	35	1	4	5	0
14	A	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	45	35	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	45	35	1	4	5	0
14	B	1	55	45	1	4	5	0
14	B	1	45	35	1	4	5	0
14	B	1	65	55	1	4	5	0

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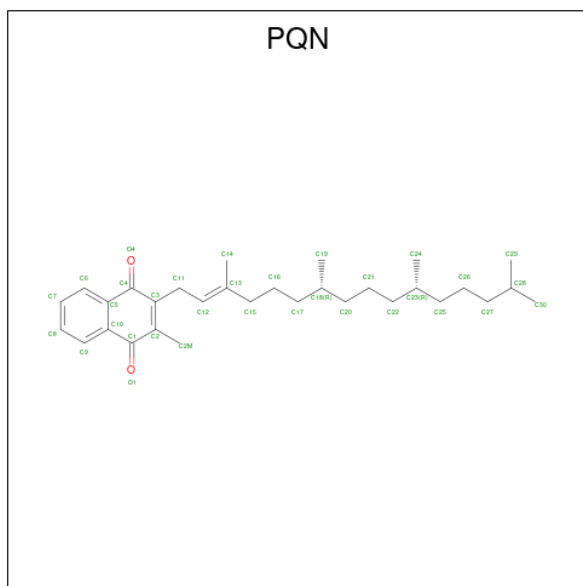
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	55	45	1	4	5	0
14	B	1	49	39	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	50	40	1	4	5	0
14	B	1	45	35	1	4	5	0
14	B	1	60	50	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	47	37	1	4	5	0
14	B	1	65	55	1	4	5	0
14	B	1	65	55	1	4	5	0
14	F	1	58	48	1	4	5	0
14	F	1	45	35	1	4	5	0
14	F	1	50	40	1	4	5	0
14	J	1	45	35	1	4	5	0

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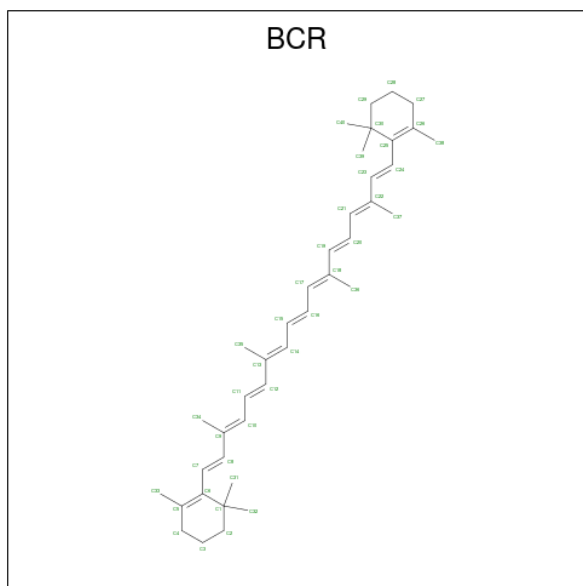
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	J	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	K	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	M	1	Total 36	C 30	Mg 1	N 4	O 1	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



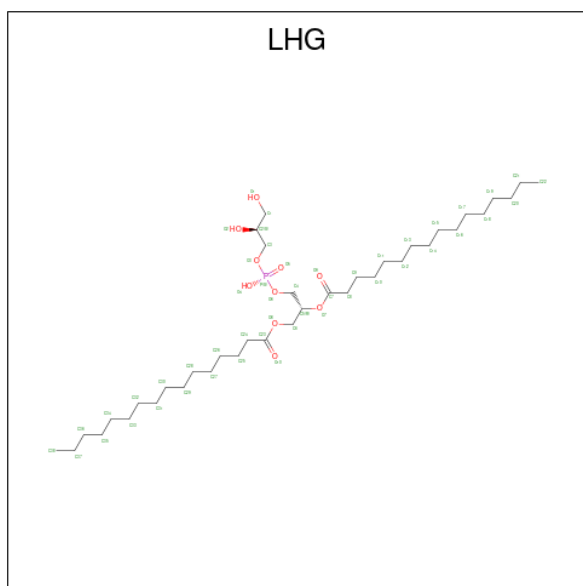
Mol	Chain	Residues	Atoms	AltConf
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 40 40	0
16	A	1	Total C 25 25	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0

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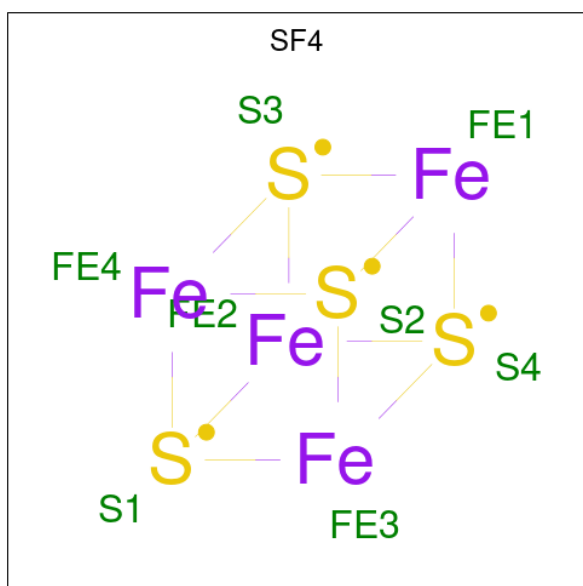
Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 25 25	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms			AltConf	
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	B	1	Total	C	O	P	0
			49	38	10	1	
17	I	1	Total	C	O	P	0
			39	28	10	1	
17	M	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

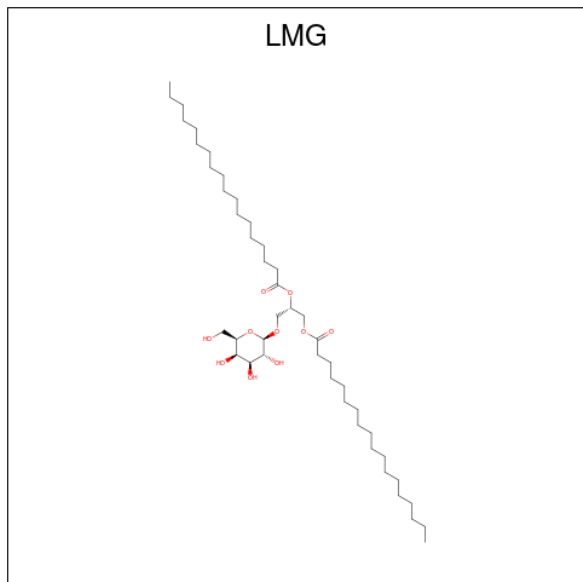


Mol	Chain	Residues	Atoms		AltConf
18	B	1	Total	Fe S	0
			8	4 4	
18	C	1	Total	Fe S	0
			8	4 4	
18	C	1	Total	Fe S	0
			8	4 4	

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
19	B	1	Total Ca	0
			1 1	
19	L	1	Total Ca	0
			1 1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
21	A	65	65	65	0
21	B	77	77	77	0
21	C	25	25	25	0
21	D	23	23	23	0
21	E	9	9	9	0
21	F	4	4	4	0
21	I	1	1	1	0
21	J	1	1	1	0
21	K	1	1	1	0

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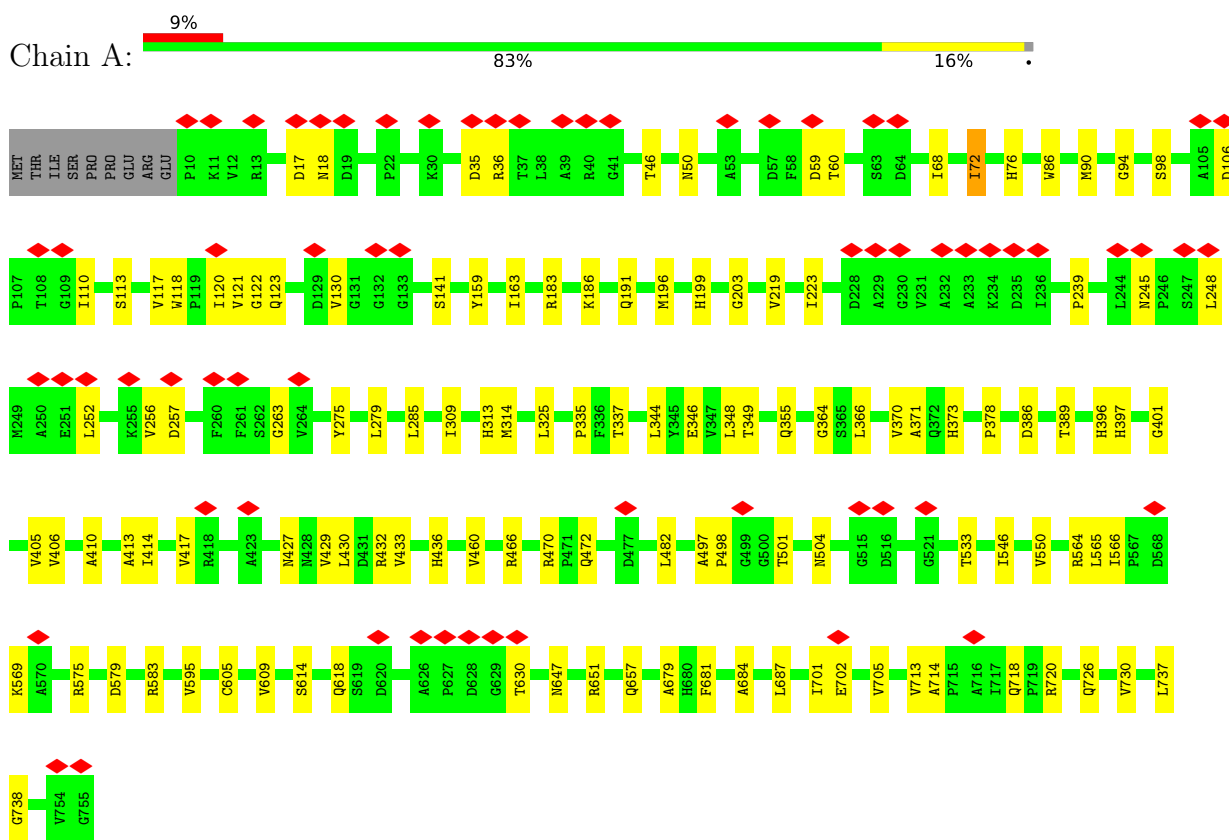
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Mol	Chain	Residues	Atoms		AltConf
21	L	10	Total 10	O 10	0
21	M	1	Total 1	O 1	0

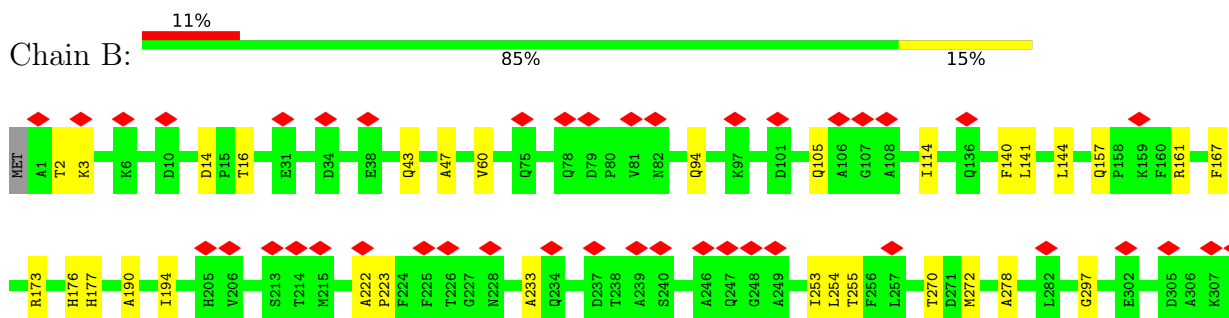
3 Residue-property plots [i](#)

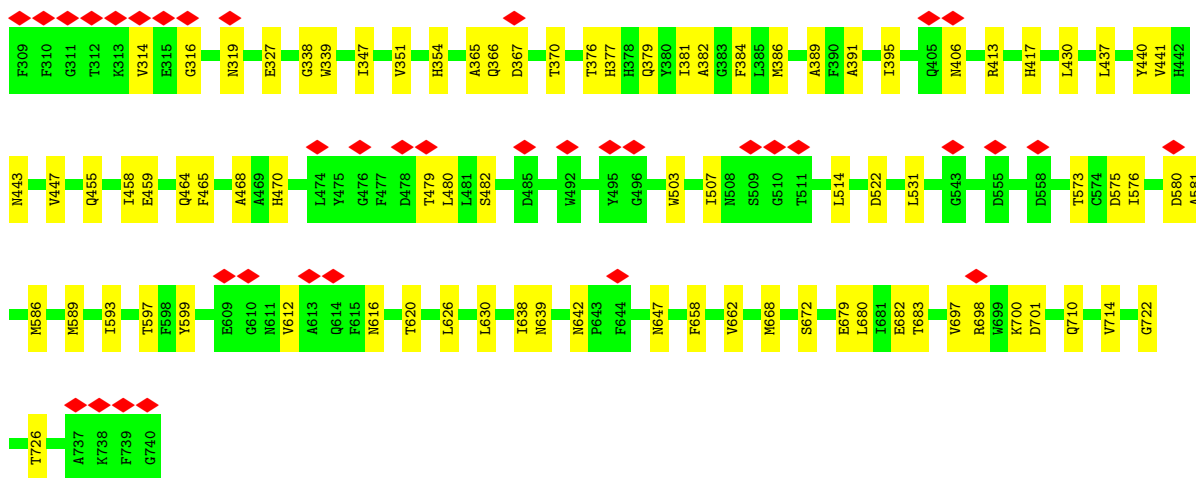
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

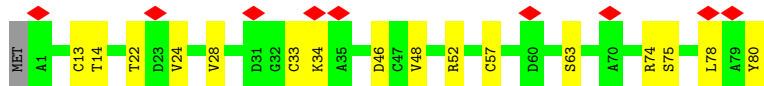
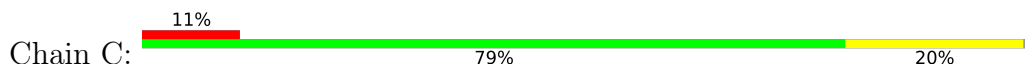


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

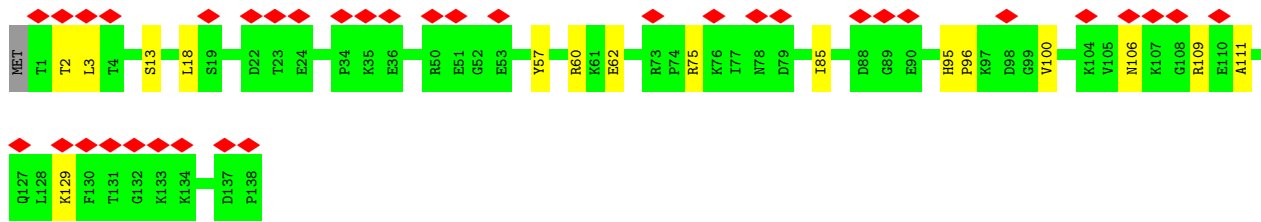
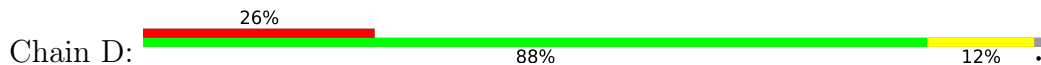




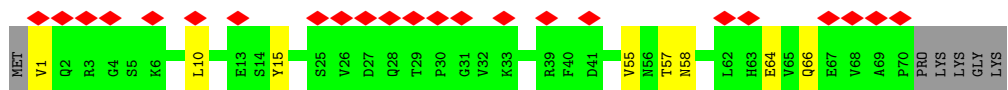
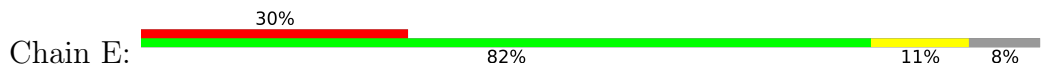
• Molecule 3: Photosystem I iron-sulfur center



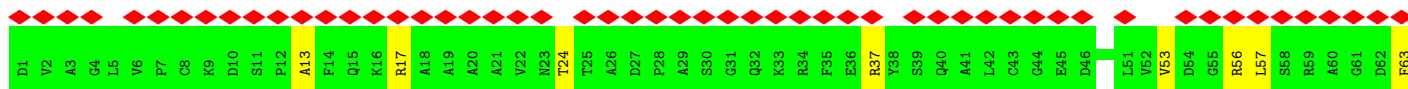
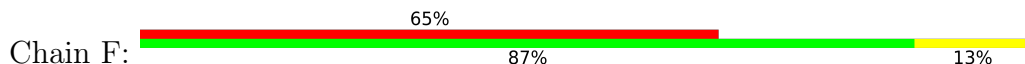
• Molecule 4: Photosystem I reaction center subunit II

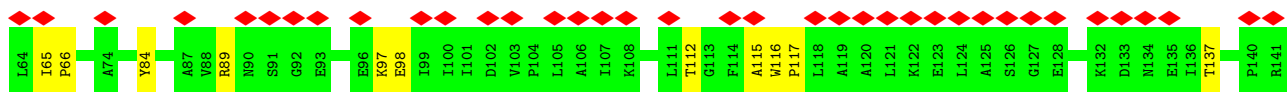


• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III

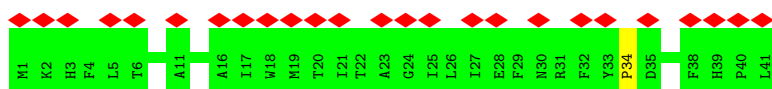




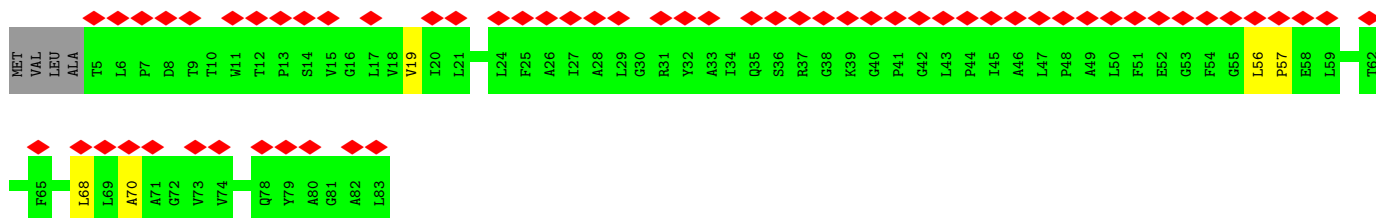
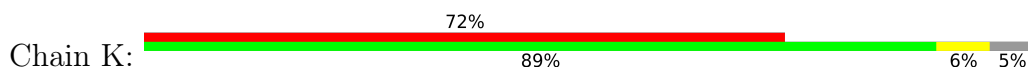
- Molecule 7: Photosystem I reaction center subunit VIII



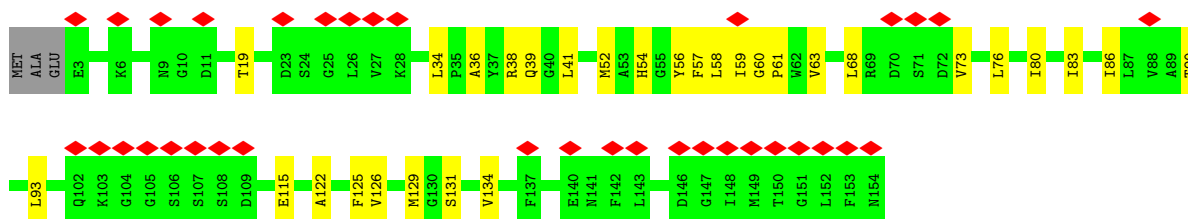
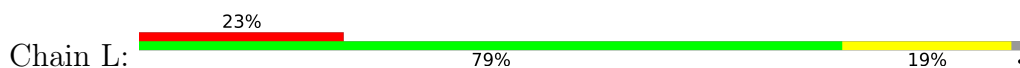
- Molecule 8: Photosystem I reaction center subunit IX



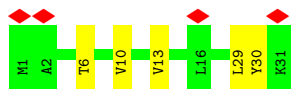
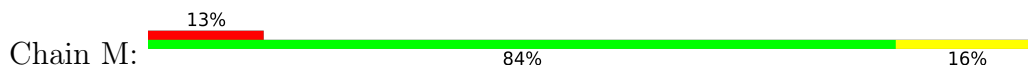
- Molecule 9: Photosystem I reaction center subunit PsaK



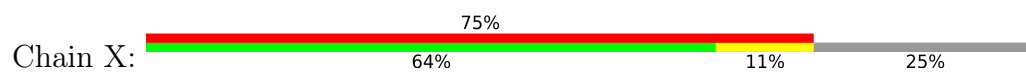
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I 4.8K protein



MET	ALA	THR	LYS	SER	ALA	LYS	PRO	THR	Y9	A10	F11	R12	T13	F14	M15	A16	V17	L18	L19	L20	A21	I22	N23	F24	L25	V26	A27	A28	Y29	Y30	F31	G32	I33	L34	K35
-----	-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.049	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.017	Depositor
Map size (\AA)	351.68002, 351.68002, 351.68002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.628, 0.628, 0.628	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: CA, LMG, LHG, BCR, CL0, PQN, SF4, FME, CLA

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	0.21	0/6027	0.35	0/8220
2	B	0.21	0/6112	0.37	0/8350
3	C	0.24	0/608	0.39	0/824
4	D	0.20	0/1101	0.38	0/1492
5	E	0.19	0/559	0.35	0/762
6	F	0.17	0/1087	0.35	0/1476
7	I	0.22	0/304	0.51	0/415
8	J	0.14	0/342	0.29	0/467
9	K	0.17	0/585	0.35	0/800
10	L	0.19	0/1153	0.35	0/1565
11	M	0.23	0/244	0.36	0/332
12	X	0.13	0/236	0.28	0/321
All	All	0.21	0/18358	0.36	0/25024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5826	0	5692	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5894	0	5653	95	0
3	C	598	0	580	13	0
4	D	1075	0	1077	19	0
5	E	546	0	535	7	0
6	F	1065	0	1077	14	0
7	I	303	0	305	8	0
8	J	340	0	346	1	0
9	K	571	0	593	3	0
10	L	1124	0	1127	23	0
11	M	241	0	264	4	0
12	X	228	0	234	4	0
13	A	65	0	72	1	0
14	A	2674	0	2849	56	0
14	B	2446	0	2562	40	0
14	F	153	0	127	1	0
14	J	82	0	58	0	0
14	K	104	0	88	2	0
14	L	260	0	288	6	0
14	M	36	0	24	0	0
14	X	45	0	33	1	0
15	A	33	0	46	2	0
15	B	33	0	46	0	0
16	A	265	0	369	18	0
16	B	320	0	448	13	0
16	F	80	0	112	1	0
16	I	80	0	112	3	0
16	J	80	0	112	5	0
16	K	25	0	33	4	0
16	L	80	0	112	1	0
17	A	90	0	129	4	0
17	B	49	0	74	1	0
17	I	39	0	51	2	0
17	M	49	0	74	1	0
18	B	8	0	0	0	0
18	C	16	0	0	0	0
19	B	1	0	0	0	0
19	L	1	0	0	0	0
20	B	55	0	86	3	0
21	A	65	0	0	21	0
21	B	77	0	0	11	0
21	C	25	0	0	5	0
21	D	23	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	E	9	0	0	5	0
21	F	4	0	0	1	0
21	I	1	0	0	1	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	10	0	0	6	0
21	M	1	0	0	0	0
All	All	25197	0	25388	369	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 369 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:OD1	1:A:183:ARG:NH1	2.08	0.87
4:D:95:HIS:O	21:D:201:HOH:O	1.96	0.84
7:I:33:TYR:OH	11:M:30:TYR:OH	1.92	0.84
4:D:60:ARG:NH2	4:D:62:GLU:OE1	2.11	0.82
1:A:569:LYS:NZ	2:B:679:GLU:OE2	2.13	0.82

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	744/755 (98%)	712 (96%)	32 (4%)	0	100	100
2	B	738/741 (100%)	706 (96%)	32 (4%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	D	136/139 (98%)	124 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	68/76 (90%)	68 (100%)	0	0	100	100
6	F	139/141 (99%)	129 (93%)	10 (7%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	J	39/41 (95%)	39 (100%)	0	0	100	100
9	K	77/83 (93%)	72 (94%)	5 (6%)	0	100	100
10	L	150/155 (97%)	145 (97%)	5 (3%)	0	100	100
11	M	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	X	25/36 (69%)	25 (100%)	0	0	100	100
All	All	2259/2317 (98%)	2154 (95%)	105 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	594/603 (98%)	593 (100%)	1 (0%)	87	95
2	B	597/598 (100%)	597 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/116 (99%)	115 (100%)	0	100	100
5	E	60/65 (92%)	60 (100%)	0	100	100
6	F	109/109 (100%)	109 (100%)	0	100	100
7	I	31/31 (100%)	31 (100%)	0	100	100
8	J	35/35 (100%)	35 (100%)	0	100	100
9	K	58/61 (95%)	58 (100%)	0	100	100
10	L	117/120 (98%)	117 (100%)	0	100	100
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	21/28 (75%)	21 (100%)	0	100	100
All	All	1830/1860 (98%)	1829 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	611	ASN
11	M	7	GLN
4	D	106	ASN
10	L	39	GLN
3	C	15	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
8	FME	J	1	8	8,9,10	0.97	0	8,9,11	0.92	0
7	FME	I	1	7	8,9,10	1.01	0	8,9,11	0.82	0

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
8	FME	J	1	8	-	1/7/9/11	-
7	FME	I	1	7	-	0/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 134 ligands modelled in this entry, 2 are monoatomic - leaving 132 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
17	LHG	B	851	-	48,48,48	0.68	2 (4%)	51,54,54	1.22	5 (9%)
14	CLA	B	819	-	69,73,73	1.15	9 (13%)	82,113,113	1.26	6 (7%)
14	CLA	K	102	21	62,66,73	1.23	8 (12%)	73,104,113	1.28	6 (8%)
14	CLA	B	821	-	69,73,73	1.18	9 (13%)	82,113,113	1.19	5 (6%)
14	CLA	B	842	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
14	CLA	A	831	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	7 (8%)
14	CLA	B	830	-	69,73,73	1.16	7 (10%)	82,113,113	1.30	6 (7%)
14	CLA	B	832	-	53,57,73	1.31	8 (15%)	61,93,113	1.34	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	816	-	69,73,73	1.14	9 (13%)	82,113,113	1.24	5 (6%)
14	CLA	A	837	1	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
14	CLA	B	827	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
14	CLA	A	841	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
14	CLA	B	836	21	54,58,73	1.33	8 (14%)	64,95,113	1.40	7 (10%)
14	CLA	A	821	-	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
14	CLA	L	201	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	B	811	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
16	BCR	B	847	-	41,41,41	1.20	2 (4%)	56,56,56	1.24	8 (14%)
14	CLA	L	205	-	69,73,73	1.14	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	B	838	-	64,68,73	1.22	9 (14%)	76,107,113	1.27	5 (6%)
14	CLA	A	817	21	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
14	CLA	B	841	21	69,73,73	1.17	9 (13%)	82,113,113	1.22	5 (6%)
14	CLA	B	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	A	826	21	69,73,73	1.16	8 (11%)	82,113,113	1.23	4 (4%)
14	CLA	A	836	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
14	CLA	B	801	21	69,73,73	1.17	9 (13%)	82,113,113	1.24	4 (4%)
14	CLA	M	102	-	39,44,73	1.51	9 (23%)	47,76,113	1.45	4 (8%)
14	CLA	A	833	-	69,73,73	1.15	8 (11%)	82,113,113	1.21	5 (6%)
14	CLA	B	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	8 (9%)
14	CLA	A	816	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	4 (4%)
14	CLA	A	829	-	69,73,73	1.14	9 (13%)	82,113,113	1.21	7 (8%)
14	CLA	B	820	21	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
14	CLA	A	812	14	69,73,73	1.15	8 (11%)	82,113,113	1.22	4 (4%)
14	CLA	B	837	21	49,53,73	1.40	7 (14%)	58,89,113	1.40	4 (6%)
17	LHG	I	102	-	38,38,48	0.71	0	41,44,54	1.29	4 (9%)
14	CLA	A	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
16	BCR	I	103	-	41,41,41	1.13	3 (7%)	56,56,56	1.32	8 (14%)
14	CLA	A	835	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	5 (6%)
14	CLA	B	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	A	814	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	4 (4%)
14	CLA	A	822	21	69,73,73	1.15	9 (13%)	82,113,113	1.22	4 (4%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	B	817	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
14	CLA	A	808	-	55,59,73	1.29	8 (14%)	64,96,113	1.32	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	A	848	-	41,41,41	1.14	3 (7%)	56,56,56	1.18	5 (8%)
14	CLA	A	819	-	69,73,73	1.17	9 (13%)	82,113,113	1.20	5 (6%)
14	CLA	B	823	21	59,63,73	1.26	8 (13%)	70,101,113	1.28	5 (7%)
14	CLA	B	810	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
16	BCR	J	103	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	6 (10%)
14	CLA	A	807	-	69,73,73	1.17	9 (13%)	82,113,113	1.19	5 (6%)
14	CLA	B	805	-	69,73,73	1.14	8 (11%)	82,113,113	1.31	5 (6%)
14	CLA	A	834	-	69,73,73	1.15	8 (11%)	82,113,113	1.29	8 (9%)
16	BCR	A	849	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	5 (8%)
16	BCR	K	103	-	25,25,41	1.17	1 (4%)	33,33,56	1.35	5 (15%)
16	BCR	A	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	8 (14%)
16	BCR	L	207	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	7 (12%)
14	CLA	B	809	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
14	CLA	A	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	5 (6%)
13	CL0	A	801	-	58,73,73	2.20	10 (17%)	60,113,113	1.64	14 (23%)
14	CLA	A	805	14	63,67,73	1.21	8 (12%)	74,105,113	1.30	7 (9%)
14	CLA	A	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.20	5 (6%)
16	BCR	A	851	-	25,25,41	1.19	2 (8%)	33,33,56	1.46	6 (18%)
14	CLA	X	1701	12	49,53,73	1.39	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	B	808	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	4 (4%)
14	CLA	L	206	21	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
14	CLA	A	818	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	6 (7%)
14	CLA	B	812	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
15	PQN	A	844	-	34,34,34	0.42	0	43,45,45	0.52	1 (2%)
14	CLA	A	827	21	69,73,73	1.15	9 (13%)	82,113,113	1.30	8 (9%)
14	CLA	K	101	-	50,54,73	1.36	9 (18%)	59,90,113	1.39	4 (6%)
16	BCR	B	852	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	B	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
16	BCR	B	849	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	7 (12%)
16	BCR	L	202	-	41,41,41	1.22	3 (7%)	56,56,56	1.31	8 (14%)
16	BCR	B	844	-	41,41,41	1.19	2 (4%)	56,56,56	1.24	7 (12%)
14	CLA	F	204	-	54,58,73	1.31	8 (14%)	64,95,113	1.37	6 (9%)
16	BCR	B	853	-	41,41,41	1.17	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	B	829	-	69,73,73	1.17	9 (13%)	82,113,113	1.24	6 (7%)
16	BCR	B	845	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	833	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	5 (6%)
14	CLA	A	815	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	4 (4%)
14	CLA	A	854	21	69,73,73	1.15	9 (13%)	82,113,113	1.30	6 (7%)
20	LMG	B	850	-	55,55,55	0.71	1 (1%)	63,63,63	1.34	8 (12%)
14	CLA	A	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	6 (7%)
17	LHG	M	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	B	831	-	59,63,73	1.25	9 (15%)	70,101,113	1.30	4 (5%)
14	CLA	A	811	-	53,57,73	1.32	8 (15%)	61,93,113	1.31	5 (8%)
15	PQN	B	843	-	34,34,34	0.43	0	43,45,45	0.53	1 (2%)
14	CLA	A	804	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	B	818	-	69,73,73	1.15	9 (13%)	82,113,113	1.33	8 (9%)
14	CLA	F	203	21	49,53,73	1.38	8 (16%)	58,89,113	1.43	4 (6%)
16	BCR	A	850	-	41,41,41	1.21	2 (4%)	56,56,56	1.47	11 (19%)
17	LHG	A	853	14	40,40,48	0.73	1 (2%)	43,46,54	1.22	4 (9%)
14	CLA	B	824	-	49,53,73	1.39	5 (10%)	58,89,113	1.38	4 (6%)
16	BCR	F	202	-	41,41,41	1.22	3 (7%)	56,56,56	1.28	9 (16%)
14	CLA	A	820	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
16	BCR	J	104	-	41,41,41	1.23	3 (7%)	56,56,56	1.40	10 (17%)
14	CLA	B	834	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	4 (4%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	A	832	-	64,68,73	1.21	9 (14%)	76,107,113	1.27	5 (6%)
14	CLA	B	822	-	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
14	CLA	B	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.15	5 (6%)
14	CLA	A	810	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
14	CLA	B	825	2	69,73,73	1.17	8 (11%)	82,113,113	1.17	5 (6%)
17	LHG	A	852	-	48,48,48	0.67	1 (2%)	51,54,54	1.23	5 (9%)
14	CLA	A	806	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	5 (6%)
14	CLA	A	809	1	69,73,73	1.15	9 (13%)	82,113,113	1.26	4 (4%)
14	CLA	B	826	21	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
16	BCR	A	845	-	41,41,41	1.15	3 (7%)	56,56,56	1.31	7 (12%)
16	BCR	F	205	-	41,41,41	1.15	3 (7%)	56,56,56	1.30	8 (14%)
14	CLA	A	823	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	5 (8%)
14	CLA	A	840	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	4 (4%)
14	CLA	J	101	8	49,53,73	1.38	9 (18%)	58,89,113	1.38	5 (8%)
14	CLA	A	802	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	J	102	-	41,45,73	1.48	7 (17%)	50,78,113	1.37	3 (6%)
14	CLA	A	803	21	69,73,73	1.18	9 (13%)	82,113,113	1.14	5 (6%)
14	CLA	A	843	17	49,53,73	1.38	9 (18%)	58,89,113	1.40	4 (6%)
16	BCR	B	848	-	41,41,41	1.21	3 (7%)	56,56,56	1.29	6 (10%)
14	CLA	B	839	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
14	CLA	A	824	-	69,73,73	1.18	7 (10%)	82,113,113	1.16	4 (4%)
16	BCR	B	846	-	41,41,41	1.19	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	L	204	10	69,73,73	1.18	8 (11%)	82,113,113	1.41	9 (10%)
14	CLA	B	813	-	49,53,73	1.37	9 (18%)	58,89,113	1.41	4 (6%)
14	CLA	B	835	-	69,73,73	1.16	9 (13%)	82,113,113	1.26	4 (4%)
14	CLA	B	840	-	51,55,73	1.34	9 (17%)	60,91,113	1.38	6 (10%)
18	SF4	B	802	1,2	0,12,12	-	-	-	-	-
14	CLA	B	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	4 (4%)
16	BCR	I	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.26	7 (12%)
16	BCR	A	847	-	41,41,41	1.19	4 (9%)	56,56,56	1.36	8 (14%)
14	CLA	A	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	6 (7%)
14	CLA	A	838	-	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
14	CLA	F	201	21	62,66,73	1.24	8 (12%)	73,104,113	1.25	5 (6%)
14	CLA	A	813	-	49,53,73	1.40	9 (18%)	58,89,113	1.36	5 (8%)

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
17	LHG	B	851	-	-	27/53/53/53	-
14	CLA	B	819	-	1/1/15/20	14/39/115/115	-
14	CLA	K	102	21	1/1/13/20	13/31/107/115	-
14	CLA	B	821	-	1/1/15/20	12/39/115/115	-
14	CLA	B	842	-	1/1/15/20	8/39/115/115	-
14	CLA	A	831	-	1/1/15/20	7/39/115/115	-
14	CLA	B	830	-	1/1/15/20	7/39/115/115	-
14	CLA	B	832	-	1/1/11/20	5/20/96/115	-
14	CLA	B	816	-	1/1/15/20	12/39/115/115	-
14	CLA	A	837	1	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	827	-	1/1/15/20	7/39/115/115	-
14	CLA	A	841	-	1/1/15/20	13/39/115/115	-
14	CLA	B	836	21	1/1/12/20	5/21/97/115	-
14	CLA	A	821	-	1/1/15/20	12/39/115/115	-
14	CLA	L	201	2	1/1/15/20	11/39/115/115	-
14	CLA	B	811	2	1/1/15/20	9/39/115/115	-
16	BCR	B	847	-	-	10/29/63/63	0/2/2/2
14	CLA	L	205	-	1/1/15/20	10/39/115/115	-
14	CLA	B	838	-	1/1/14/20	8/33/109/115	-
14	CLA	A	817	21	1/1/15/20	9/39/115/115	-
14	CLA	B	841	21	1/1/15/20	11/39/115/115	-
14	CLA	B	815	-	1/1/15/20	20/39/115/115	-
14	CLA	A	826	21	1/1/15/20	14/39/115/115	-
14	CLA	A	836	-	1/1/15/20	13/39/115/115	-
14	CLA	B	801	21	1/1/15/20	15/39/115/115	-
14	CLA	M	102	-	1/1/7/20	2/4/72/115	-
14	CLA	A	833	-	1/1/15/20	12/39/115/115	-
14	CLA	B	814	-	1/1/15/20	18/39/115/115	-
14	CLA	A	816	-	1/1/15/20	16/39/115/115	-
14	CLA	A	829	-	1/1/15/20	13/39/115/115	-
14	CLA	B	820	21	1/1/15/20	17/39/115/115	-
14	CLA	A	812	14	1/1/15/20	11/39/115/115	-
14	CLA	B	837	21	1/1/11/20	6/15/91/115	-
17	LHG	I	102	-	-	23/43/43/53	-
14	CLA	A	825	-	1/1/15/20	13/39/115/115	-
16	BCR	I	103	-	-	9/29/63/63	0/2/2/2
14	CLA	A	835	-	1/1/15/20	7/39/115/115	-
14	CLA	B	806	-	1/1/15/20	10/39/115/115	-
14	CLA	A	814	-	1/1/15/20	13/39/115/115	-
14	CLA	A	822	21	1/1/15/20	5/39/115/115	-
18	SF4	C	102	3	-	-	0/6/5/5
14	CLA	B	817	-	1/1/15/20	17/39/115/115	-
14	CLA	A	808	-	1/1/12/20	3/23/99/115	-
16	BCR	A	848	-	-	7/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	819	-	1/1/15/20	12/39/115/115	-
14	CLA	B	823	21	1/1/13/20	4/27/103/115	-
14	CLA	B	810	-	1/1/15/20	5/39/115/115	-
16	BCR	J	103	-	-	13/29/63/63	0/2/2/2
14	CLA	A	807	-	1/1/15/20	14/39/115/115	-
14	CLA	B	805	-	1/1/15/20	12/39/115/115	-
14	CLA	A	834	-	1/1/15/20	12/39/115/115	-
16	BCR	A	849	-	-	5/29/63/63	0/2/2/2
16	BCR	K	103	-	-	4/18/35/63	0/1/1/2
16	BCR	A	846	-	-	11/29/63/63	0/2/2/2
16	BCR	L	207	-	-	17/29/63/63	0/2/2/2
14	CLA	B	809	-	1/1/15/20	9/39/115/115	-
14	CLA	A	842	-	1/1/15/20	4/39/115/115	-
13	CL0	A	801	-	3/3/20/25	7/37/135/135	-
14	CLA	A	805	14	1/1/13/20	9/32/108/115	-
14	CLA	A	830	-	1/1/15/20	9/39/115/115	-
16	BCR	A	851	-	-	13/18/35/63	0/1/1/2
14	CLA	X	1701	12	1/1/11/20	4/15/91/115	-
14	CLA	B	808	-	1/1/15/20	8/39/115/115	-
14	CLA	L	206	21	1/1/15/20	5/39/115/115	-
14	CLA	A	818	-	1/1/15/20	11/39/115/115	-
14	CLA	B	812	-	1/1/15/20	7/39/115/115	-
15	PQN	A	844	-	-	1/23/43/43	0/2/2/2
14	CLA	A	827	21	1/1/15/20	10/39/115/115	-
14	CLA	K	101	-	1/1/11/20	8/17/93/115	-
16	BCR	B	852	-	-	12/29/63/63	0/2/2/2
14	CLA	B	807	-	1/1/15/20	16/39/115/115	-
16	BCR	B	849	-	-	4/29/63/63	0/2/2/2
16	BCR	L	202	-	-	12/29/63/63	0/2/2/2
16	BCR	B	844	-	-	11/29/63/63	0/2/2/2
14	CLA	F	204	-	1/1/12/20	8/21/97/115	-
16	BCR	B	853	-	-	13/29/63/63	0/2/2/2
14	CLA	B	829	-	1/1/15/20	14/39/115/115	-
16	BCR	B	845	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	833	-	1/1/15/20	12/39/115/115	-
14	CLA	A	815	-	1/1/15/20	12/39/115/115	-
14	CLA	A	854	21	1/1/15/20	15/39/115/115	-
20	LMG	B	850	-	-	23/50/70/70	0/1/1/1
14	CLA	A	828	-	1/1/15/20	6/39/115/115	-
17	LHG	M	101	-	-	20/53/53/53	-
14	CLA	B	831	-	1/1/13/20	7/27/103/115	-
14	CLA	A	811	-	1/1/11/20	5/20/96/115	-
15	PQN	B	843	-	-	2/23/43/43	0/2/2/2
14	CLA	A	804	-	1/1/15/20	10/39/115/115	-
14	CLA	B	818	-	1/1/15/20	12/39/115/115	-
14	CLA	F	203	21	1/1/11/20	4/15/91/115	-
16	BCR	A	850	-	-	18/29/63/63	0/2/2/2
17	LHG	A	853	14	-	13/45/45/53	-
14	CLA	B	824	-	1/1/11/20	6/15/91/115	-
16	BCR	F	202	-	-	8/29/63/63	0/2/2/2
14	CLA	A	820	-	1/1/15/20	6/39/115/115	-
16	BCR	J	104	-	-	10/29/63/63	0/2/2/2
14	CLA	B	834	-	1/1/15/20	9/39/115/115	-
18	SF4	C	101	3	-	-	0/6/5/5
14	CLA	A	832	-	1/1/14/20	8/33/109/115	-
14	CLA	B	822	-	1/1/11/20	7/15/91/115	-
14	CLA	B	828	-	1/1/15/20	17/39/115/115	-
14	CLA	A	810	1	1/1/15/20	13/39/115/115	-
14	CLA	B	825	2	1/1/15/20	12/39/115/115	-
17	LHG	A	852	-	-	22/53/53/53	-
14	CLA	A	806	-	1/1/15/20	24/39/115/115	-
14	CLA	A	809	1	1/1/15/20	9/39/115/115	-
14	CLA	B	826	21	1/1/15/20	15/39/115/115	-
16	BCR	A	845	-	-	4/29/63/63	0/2/2/2
16	BCR	F	205	-	-	10/29/63/63	0/2/2/2
14	CLA	A	823	-	1/1/11/20	6/15/91/115	-
14	CLA	A	840	-	1/1/15/20	6/39/115/115	-
14	CLA	J	101	8	1/1/11/20	2/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	802	-	1/1/15/20	11/39/115/115	-
14	CLA	J	102	-	1/1/8/20	0/4/76/115	-
14	CLA	A	803	21	1/1/15/20	11/39/115/115	-
14	CLA	A	843	17	1/1/11/20	3/15/91/115	-
16	BCR	B	848	-	-	6/29/63/63	0/2/2/2
14	CLA	B	839	-	1/1/15/20	10/39/115/115	-
14	CLA	A	824	-	1/1/15/20	7/39/115/115	-
16	BCR	B	846	-	-	8/29/63/63	0/2/2/2
14	CLA	L	204	10	1/1/15/20	15/39/115/115	-
14	CLA	B	813	-	1/1/11/20	5/15/91/115	-
14	CLA	B	835	-	1/1/15/20	10/39/115/115	-
14	CLA	B	840	-	1/1/11/20	4/18/94/115	-
18	SF4	B	802	1,2	-	-	0/6/5/5
14	CLA	B	804	-	1/1/15/20	11/39/115/115	-
16	BCR	I	101	-	-	11/29/63/63	0/2/2/2
16	BCR	A	847	-	-	12/29/63/63	0/2/2/2
14	CLA	A	839	-	1/1/15/20	14/39/115/115	-
14	CLA	A	838	-	1/1/15/20	13/39/115/115	-
14	CLA	F	201	21	1/1/13/20	8/31/107/115	-
14	CLA	A	813	-	1/1/11/20	2/15/91/115	-

The worst 5 of 895 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	C1B-C2B	9.07	1.49	1.39
13	A	801	CL0	C3B-C4B	7.40	1.48	1.41
13	A	801	CL0	C1D-C2D	7.18	1.47	1.39
16	B	847	BCR	C30-C25	-4.33	1.48	1.53
13	A	801	CL0	C3D-C4D	4.32	1.48	1.41

The worst 5 of 724 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	835	CLA	C4A-NA-C1A	7.41	110.06	106.68
14	L	201	CLA	C4A-NA-C1A	7.29	110.01	106.68
14	B	805	CLA	C4A-NA-C1A	7.02	109.88	106.68
14	A	837	CLA	C4A-NA-C1A	6.94	109.85	106.68
14	B	839	CLA	C4A-NA-C1A	6.93	109.84	106.68

5 of 99 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NC
13	A	801	CL0	ND
13	A	801	CL0	NA
14	A	802	CLA	ND
14	A	803	CLA	ND

5 of 1311 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

89 monomers are involved in 145 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	B	851	LHG	1	0
14	B	819	CLA	1	0
14	B	842	CLA	1	0
14	B	830	CLA	2	0
14	A	837	CLA	2	0
14	B	827	CLA	2	0
14	A	841	CLA	1	0
14	B	836	CLA	2	0
14	A	821	CLA	3	0
14	L	201	CLA	3	0
16	B	847	BCR	3	0
14	L	205	CLA	1	0
14	B	838	CLA	1	0
14	B	815	CLA	1	0
14	A	826	CLA	2	0
14	A	836	CLA	4	0
14	B	801	CLA	2	0
14	A	833	CLA	3	0
14	B	814	CLA	2	0
14	A	816	CLA	2	0
14	A	829	CLA	4	0
14	A	812	CLA	1	0

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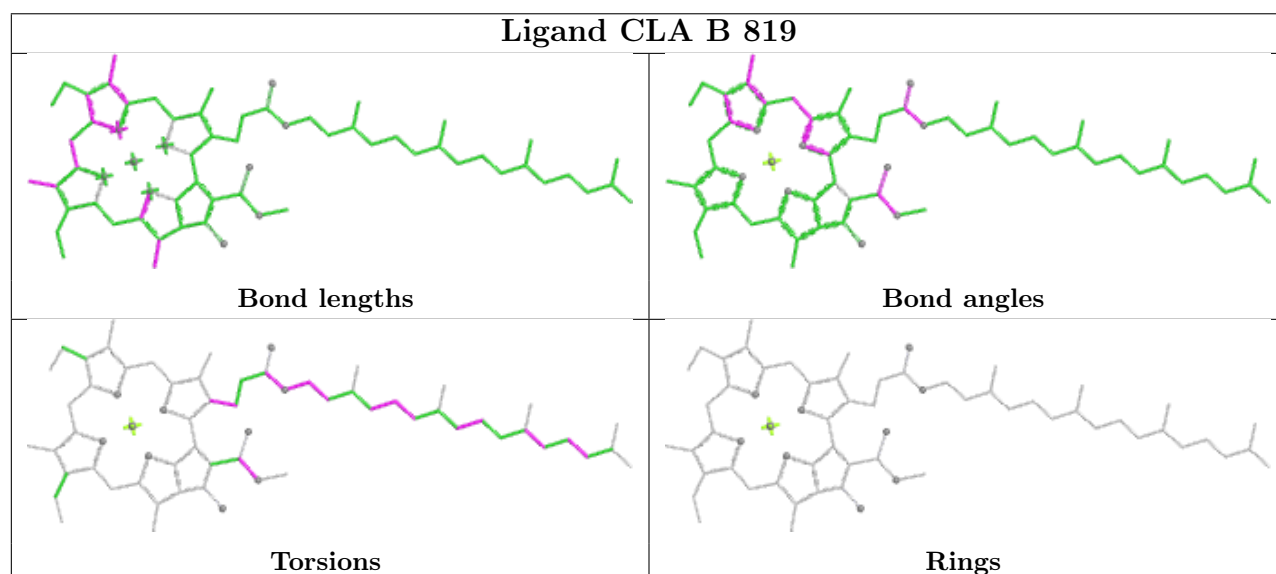
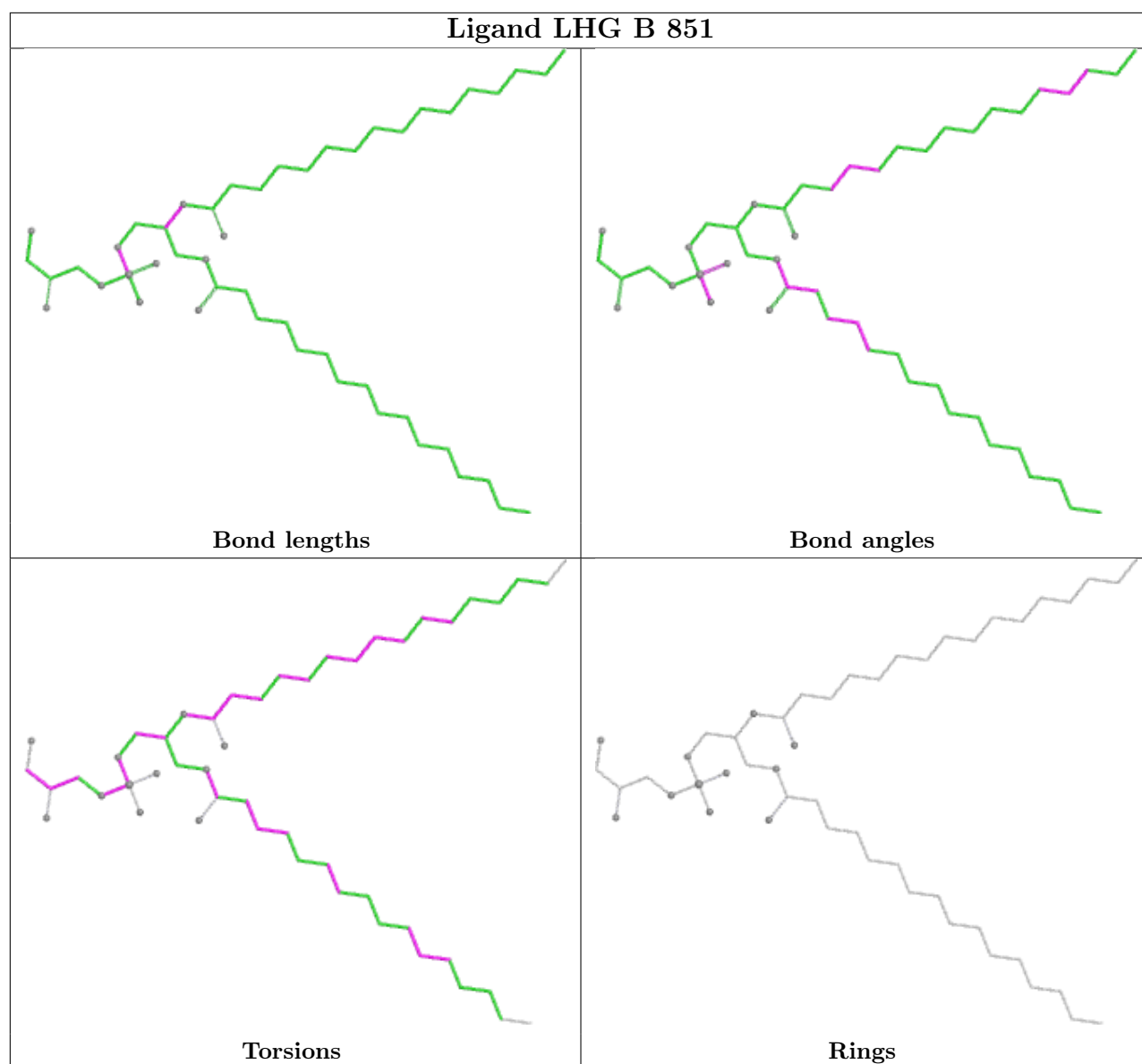
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	I	102	LHG	2	0
14	A	825	CLA	7	0
16	I	103	BCR	1	0
14	A	835	CLA	3	0
14	A	822	CLA	2	0
14	B	817	CLA	1	0
16	A	848	BCR	2	0
14	A	819	CLA	3	0
14	B	810	CLA	2	0
16	J	103	BCR	3	0
14	A	807	CLA	1	0
14	B	805	CLA	1	0
16	A	849	BCR	2	0
16	K	103	BCR	4	0
16	A	846	BCR	5	0
14	A	842	CLA	2	0
13	A	801	CL0	1	0
14	A	805	CLA	1	0
14	A	830	CLA	1	0
16	A	851	BCR	2	0
14	X	1701	CLA	1	0
14	B	808	CLA	1	0
15	A	844	PQN	2	0
14	K	101	CLA	2	0
16	B	852	BCR	2	0
16	B	849	BCR	1	0
16	L	202	BCR	1	0
16	B	844	BCR	1	0
14	F	204	CLA	1	0
16	B	853	BCR	3	0
14	B	829	CLA	2	0
14	B	833	CLA	1	0
14	A	854	CLA	4	0
20	B	850	LMG	3	0
14	A	828	CLA	1	0
17	M	101	LHG	1	0
14	B	831	CLA	1	0
14	A	811	CLA	1	0
14	A	804	CLA	1	0
14	B	818	CLA	1	0
16	A	850	BCR	6	0
17	A	853	LHG	2	0

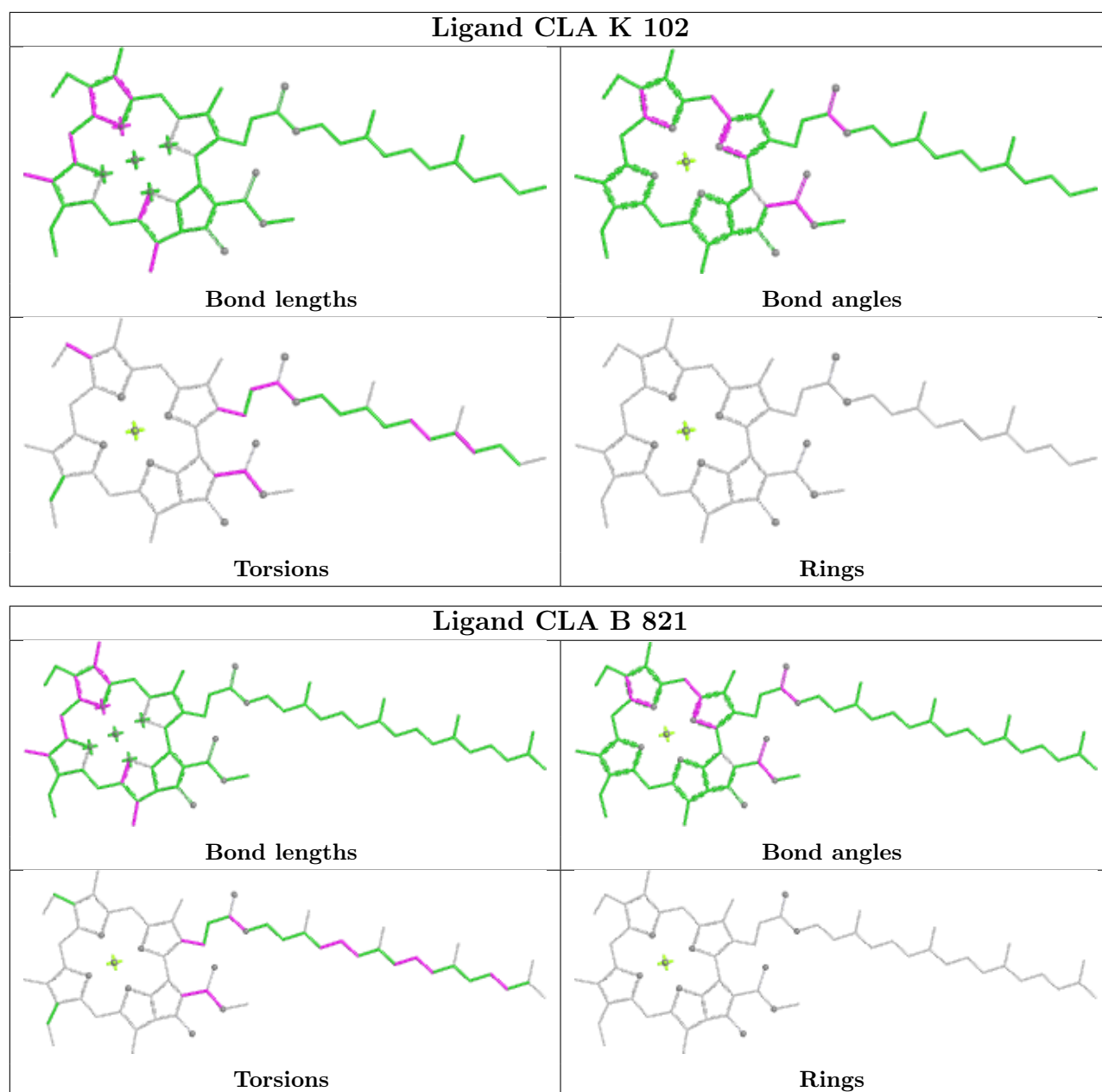
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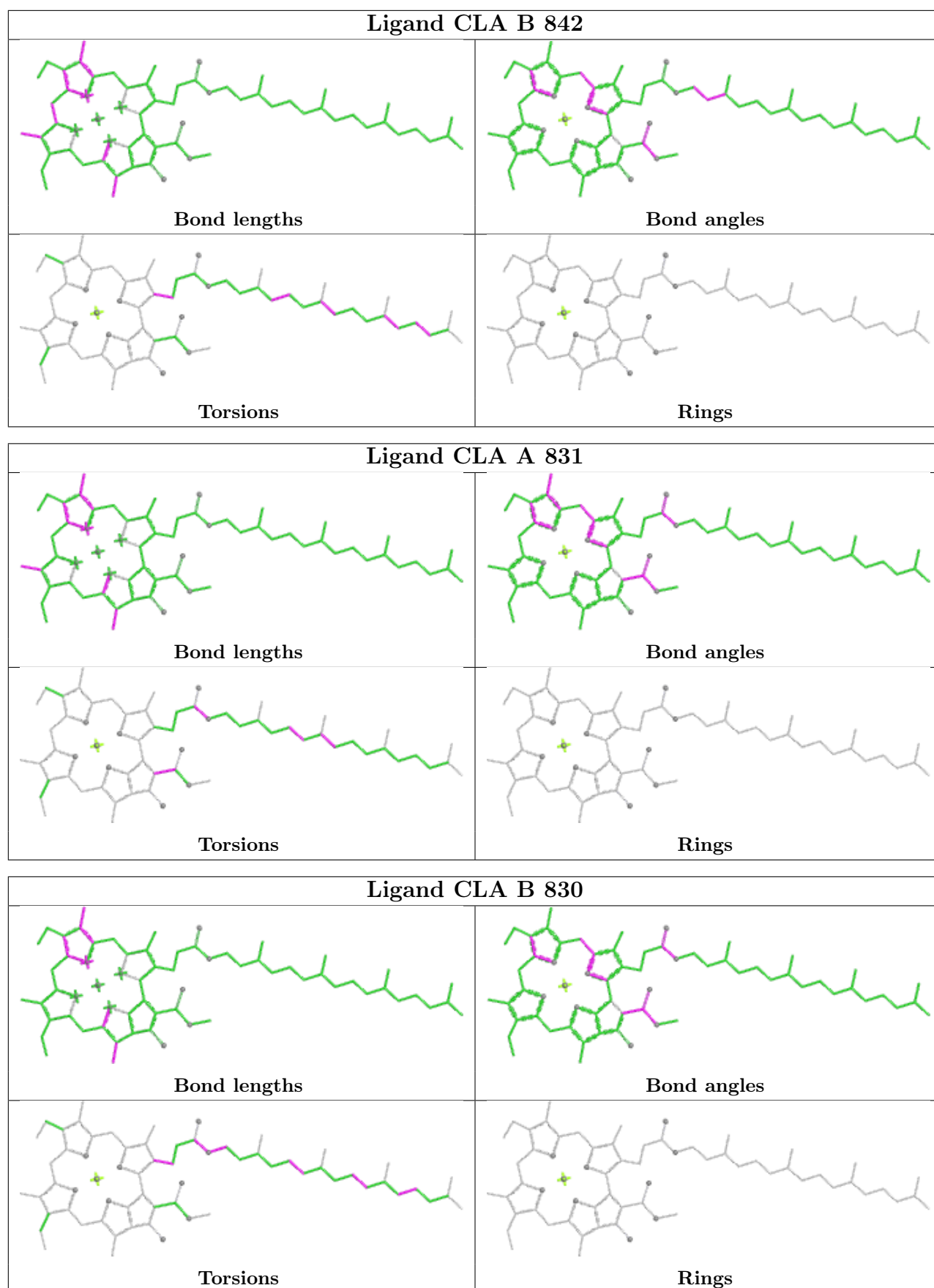
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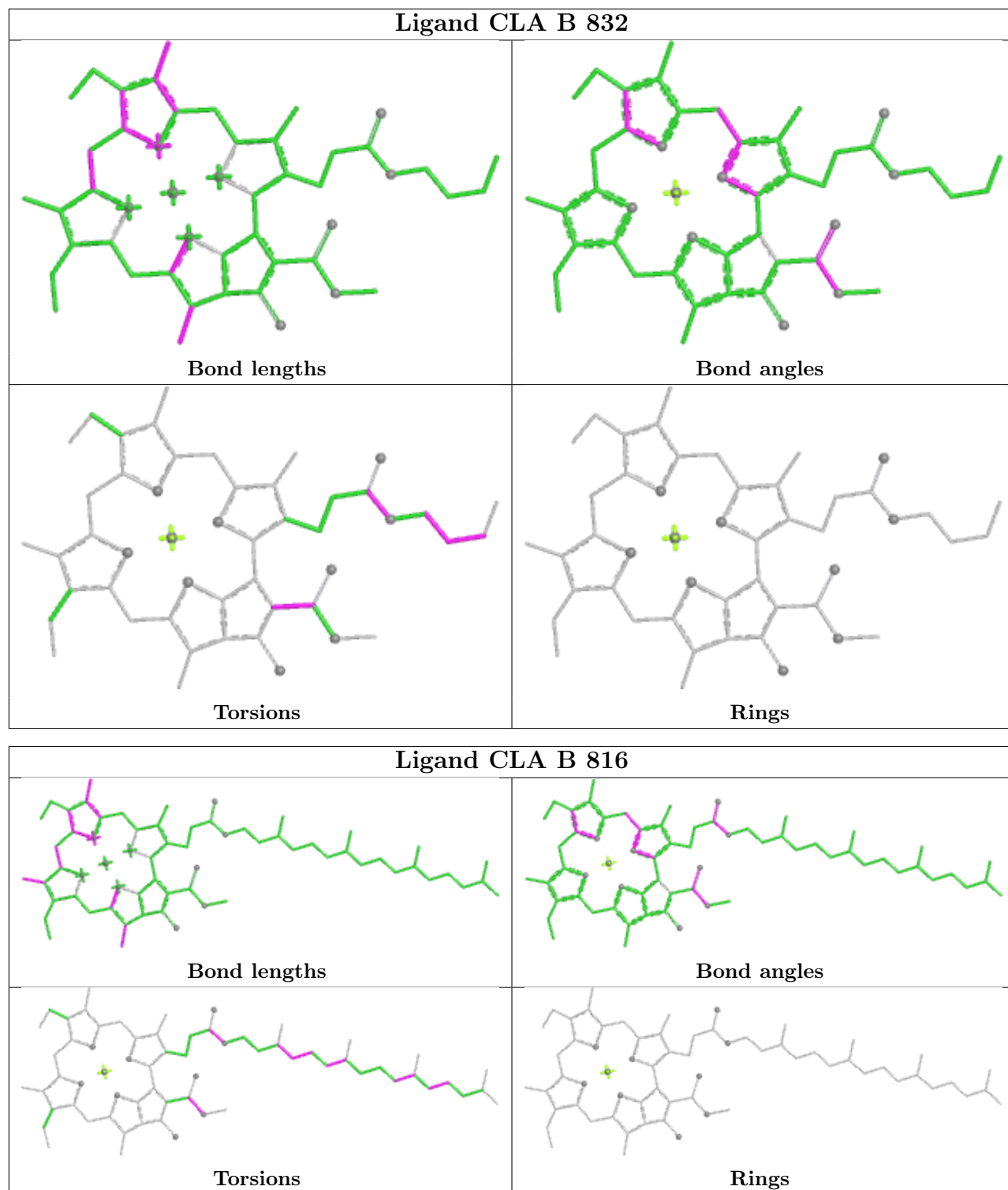
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	820	CLA	1	0
16	J	104	BCR	2	0
14	B	834	CLA	1	0
14	A	832	CLA	1	0
14	B	822	CLA	1	0
14	B	828	CLA	5	0
14	B	825	CLA	3	0
17	A	852	LHG	2	0
14	A	809	CLA	1	0
14	B	826	CLA	3	0
16	A	845	BCR	1	0
16	F	205	BCR	1	0
14	A	840	CLA	1	0
14	A	802	CLA	6	0
14	A	803	CLA	1	0
16	B	848	BCR	2	0
14	B	839	CLA	1	0
16	B	846	BCR	1	0
14	L	204	CLA	2	0
14	B	835	CLA	2	0
14	B	804	CLA	3	0
16	I	101	BCR	2	0
16	A	847	BCR	3	0
14	A	838	CLA	1	0
14	A	813	CLA	1	0

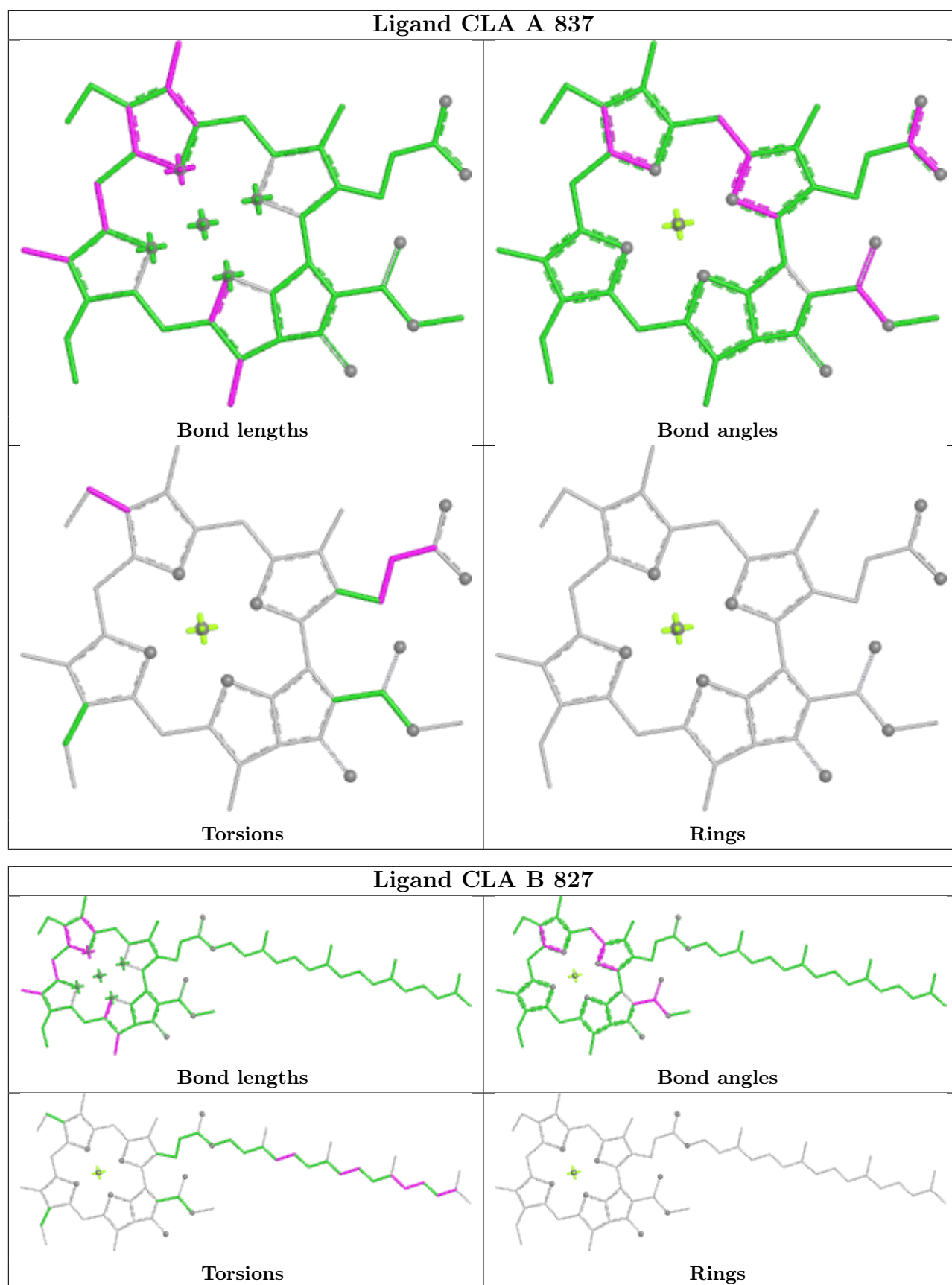
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

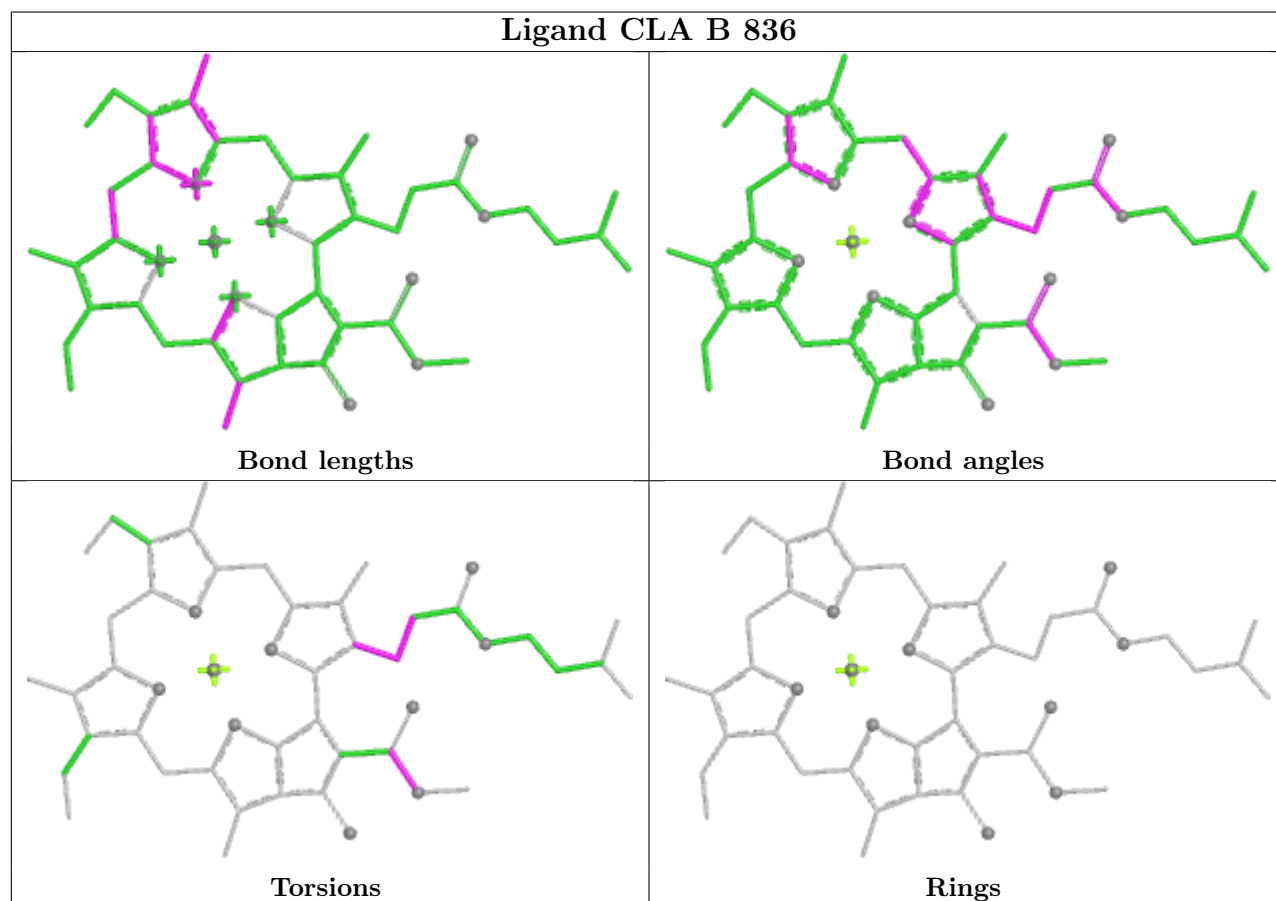
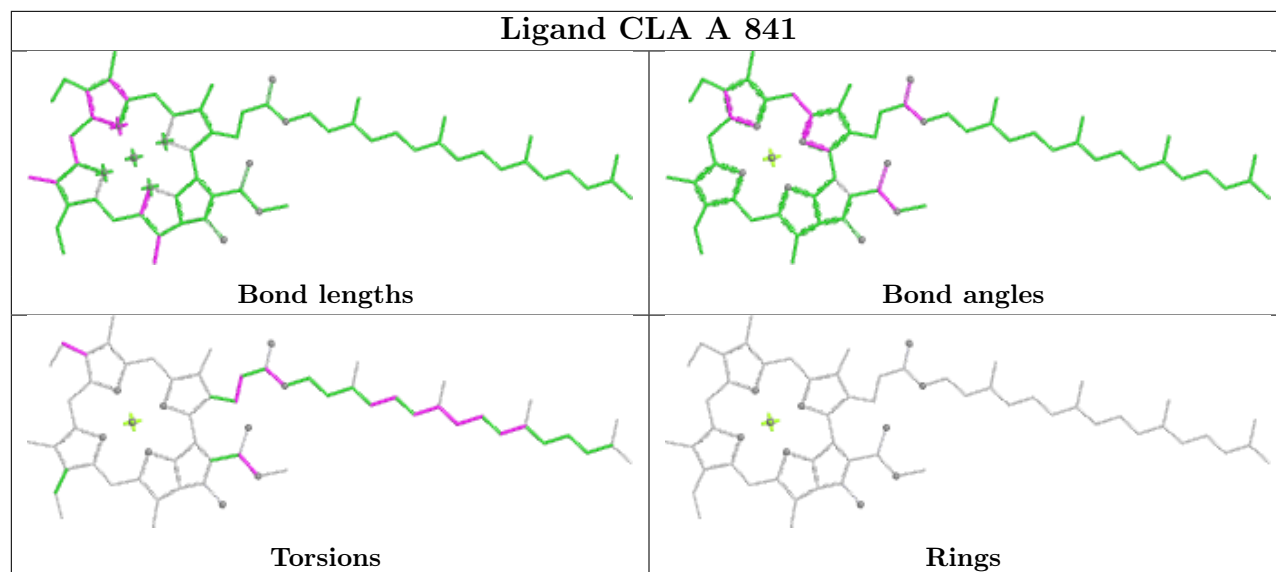


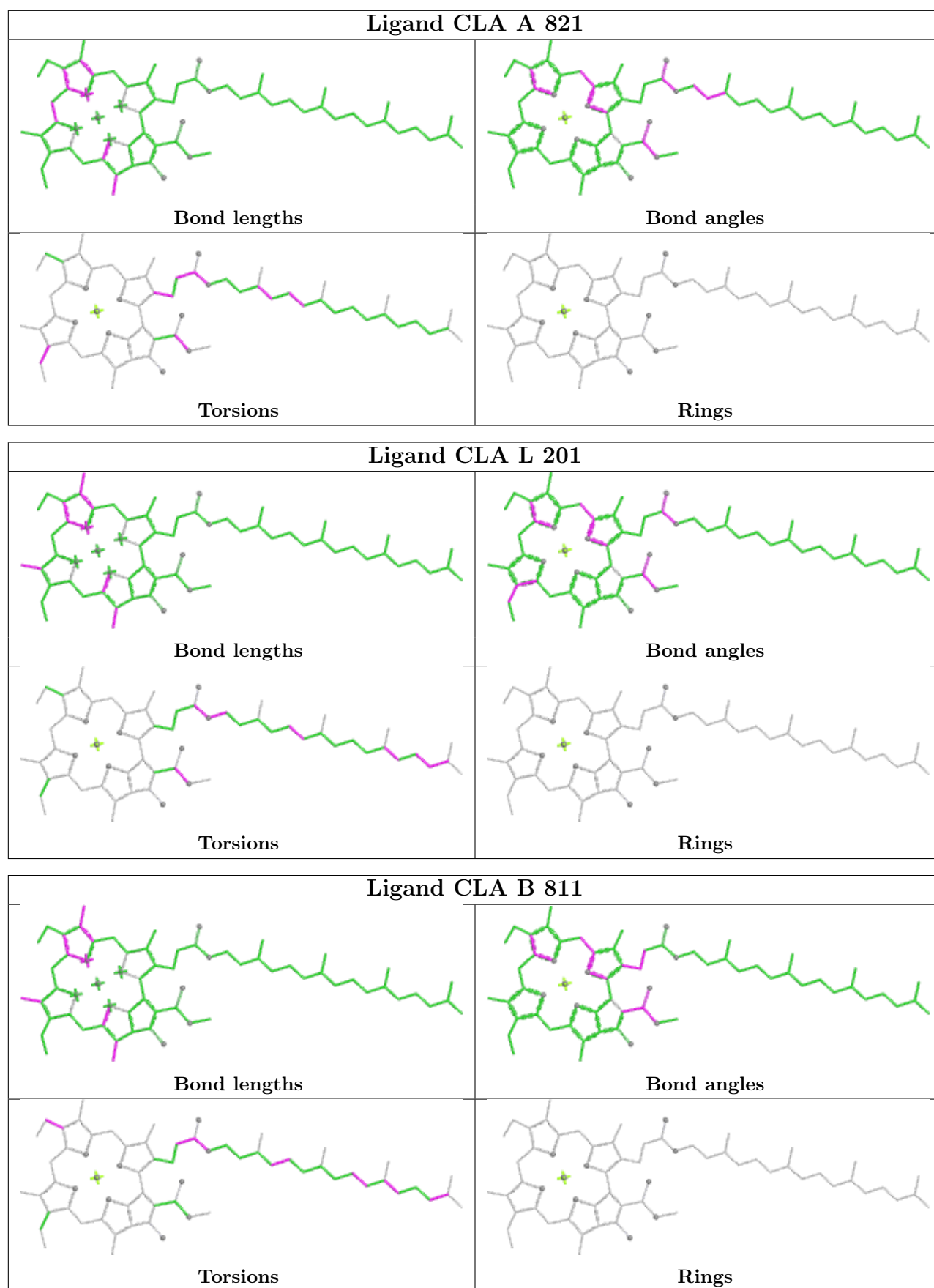


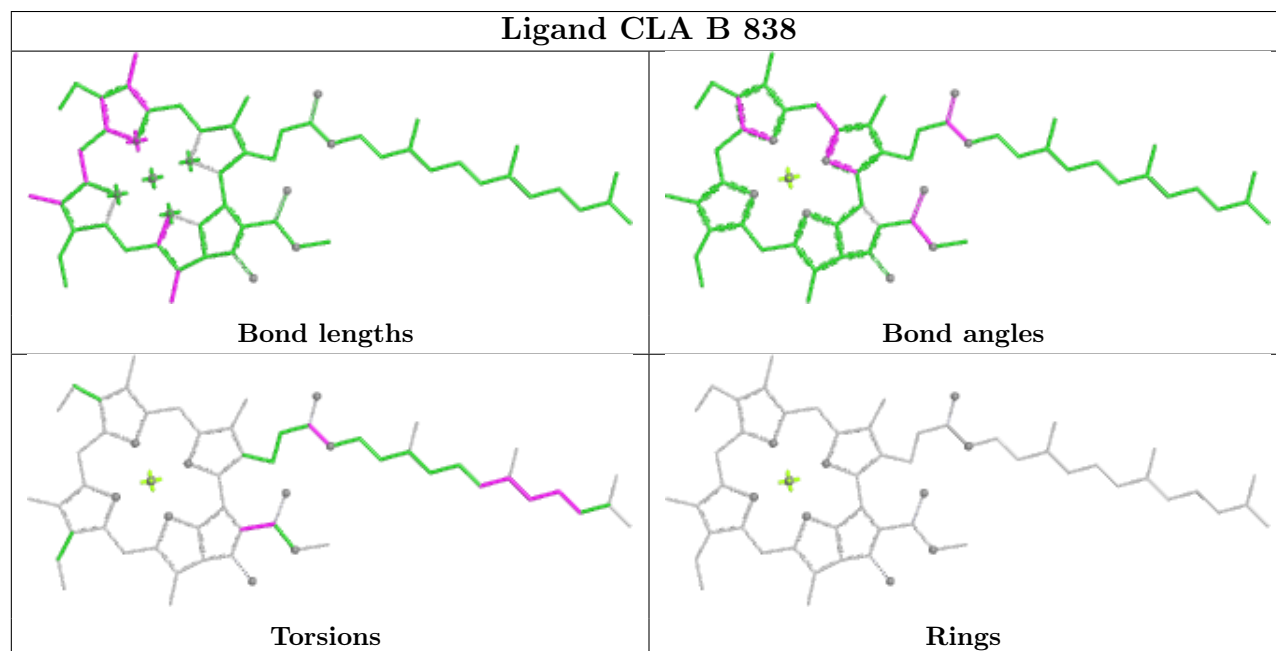
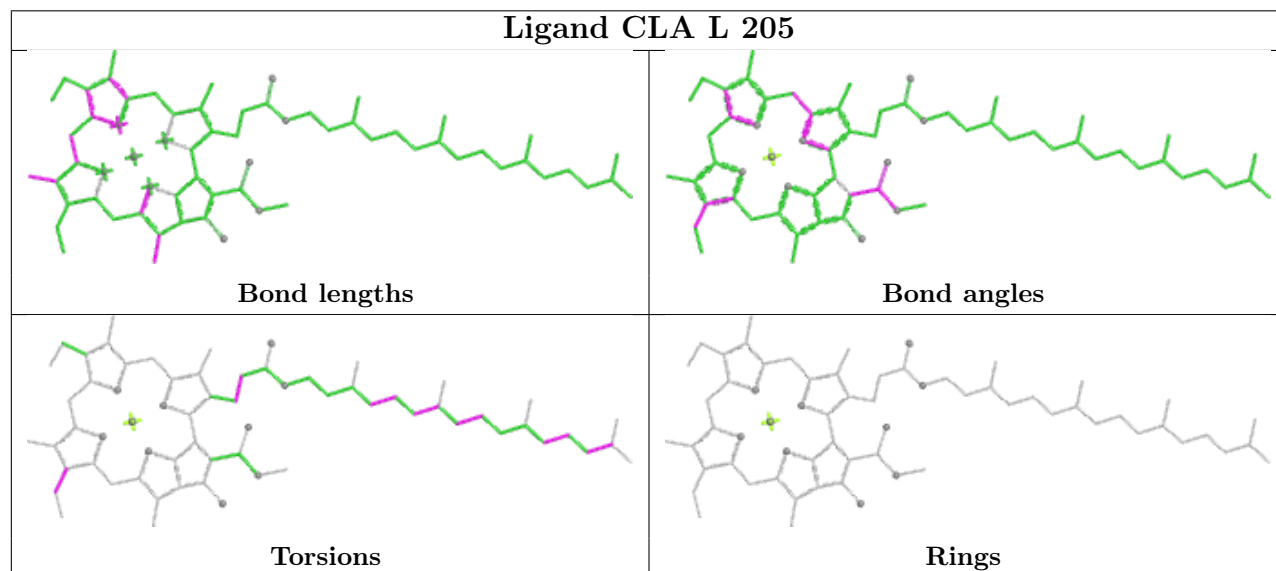
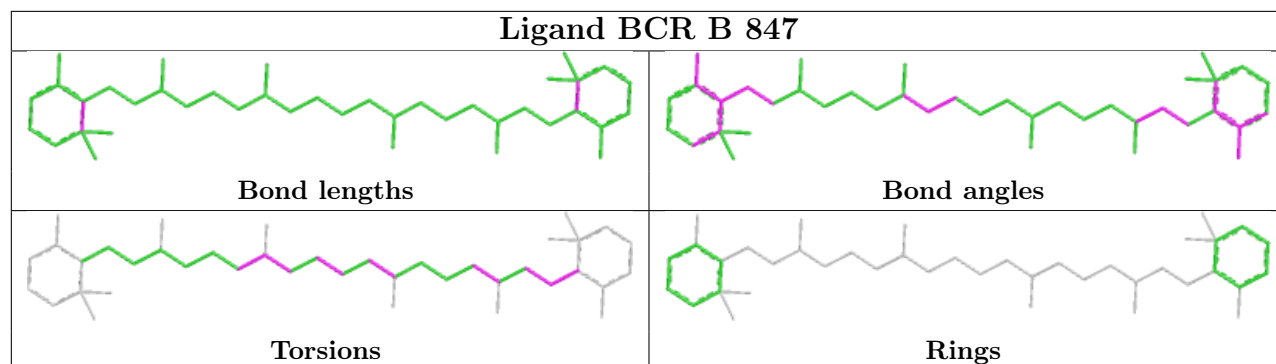


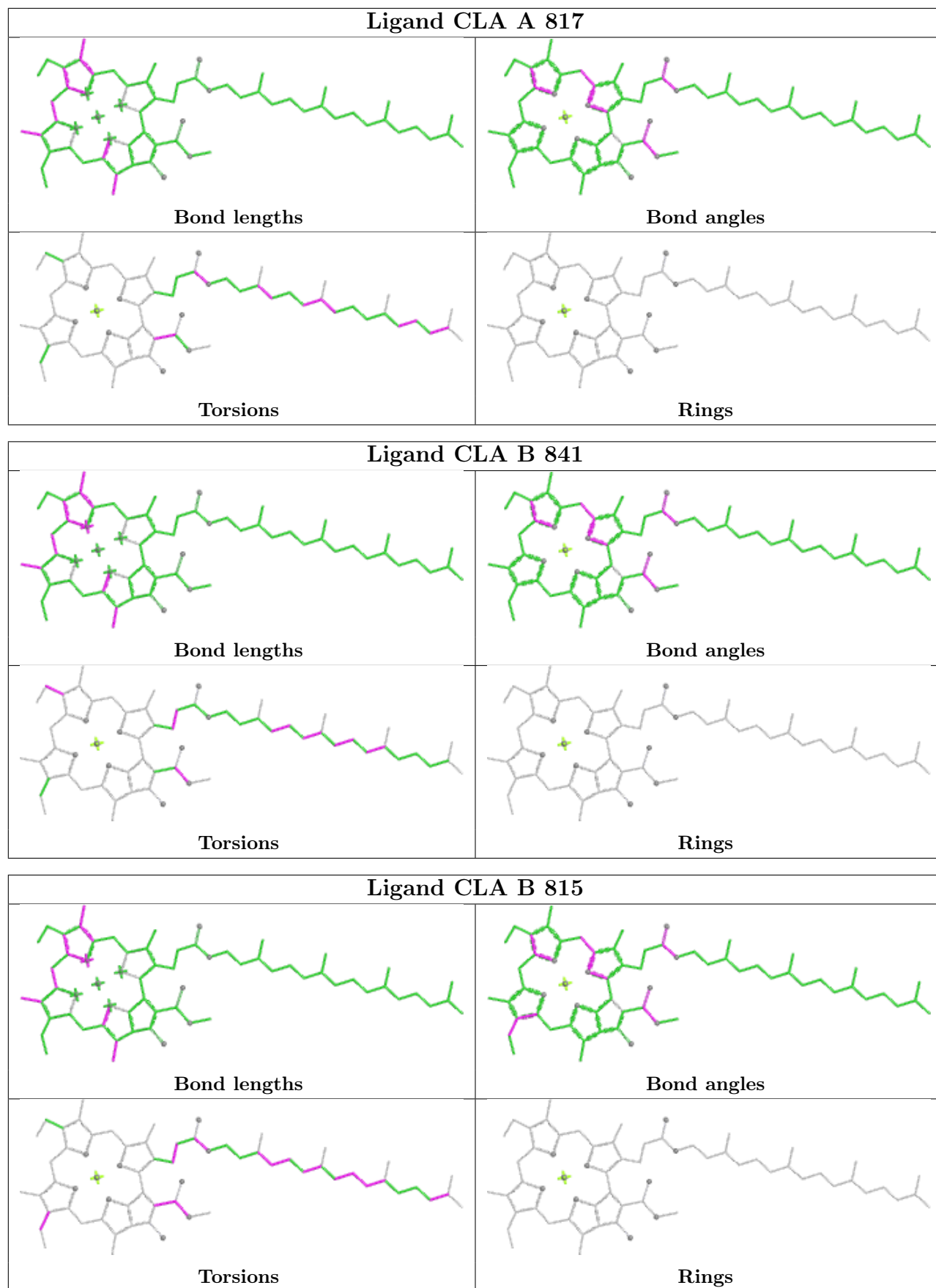


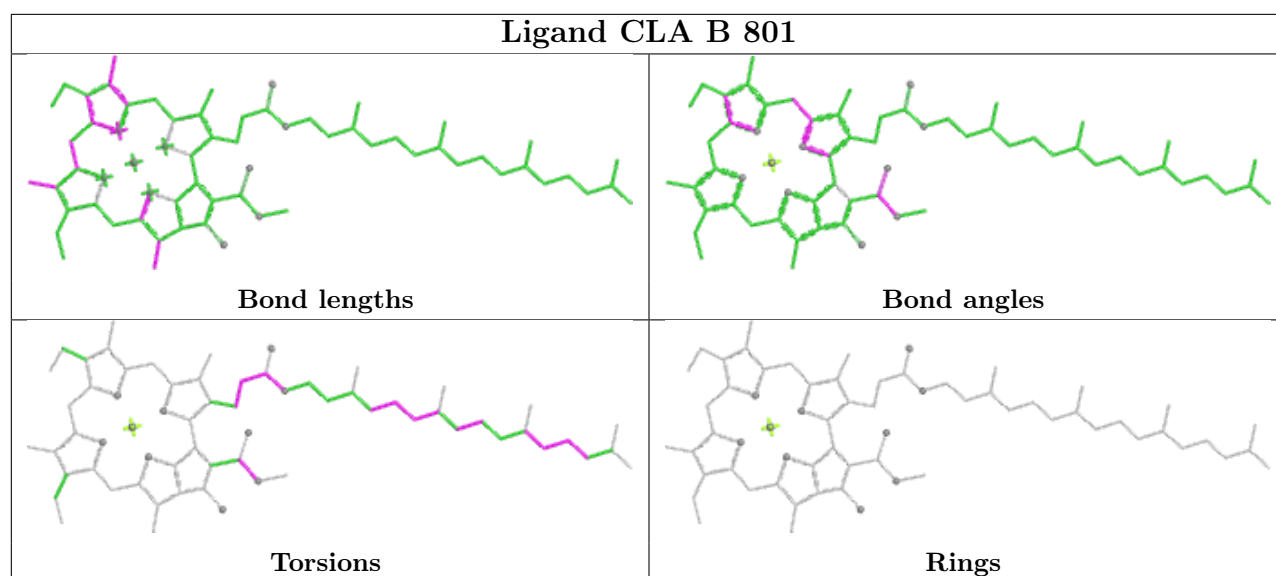
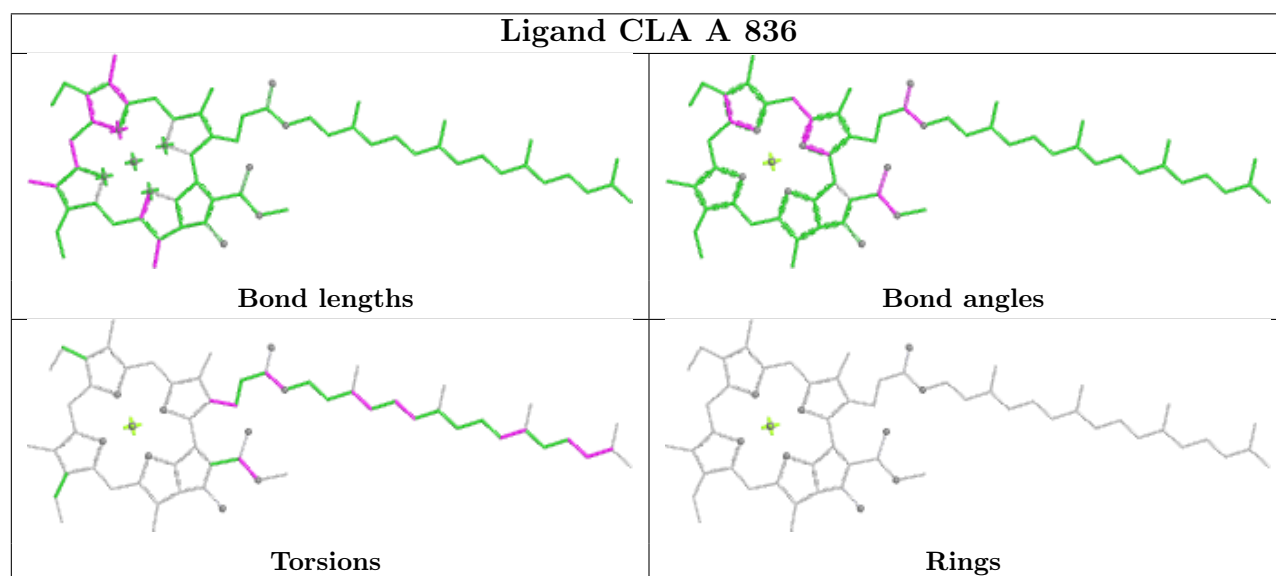
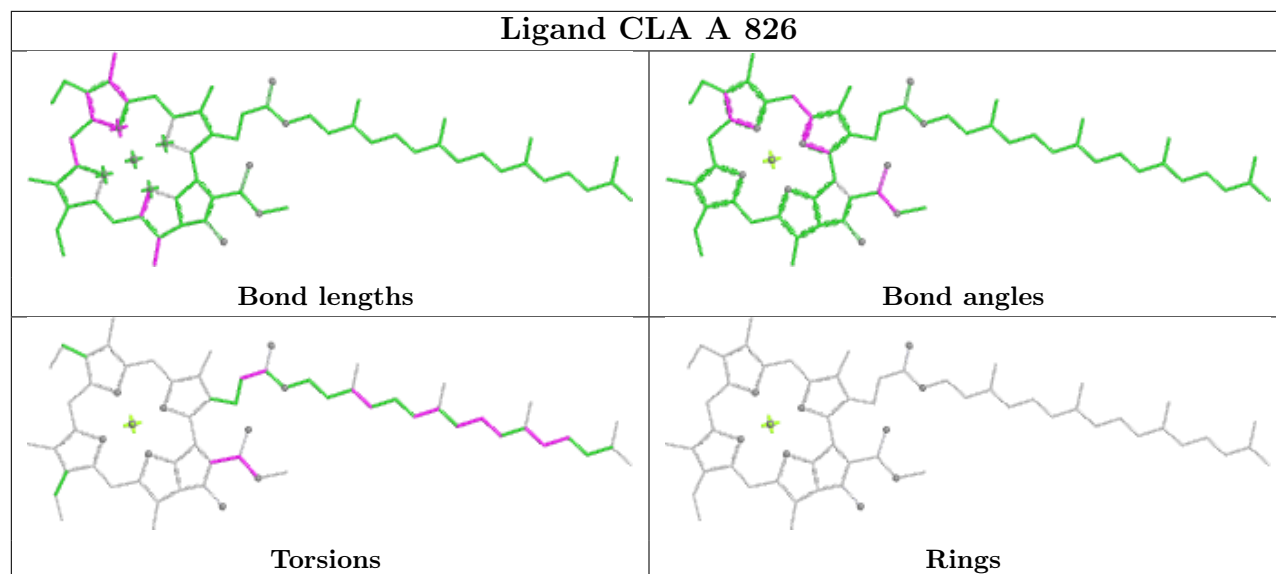


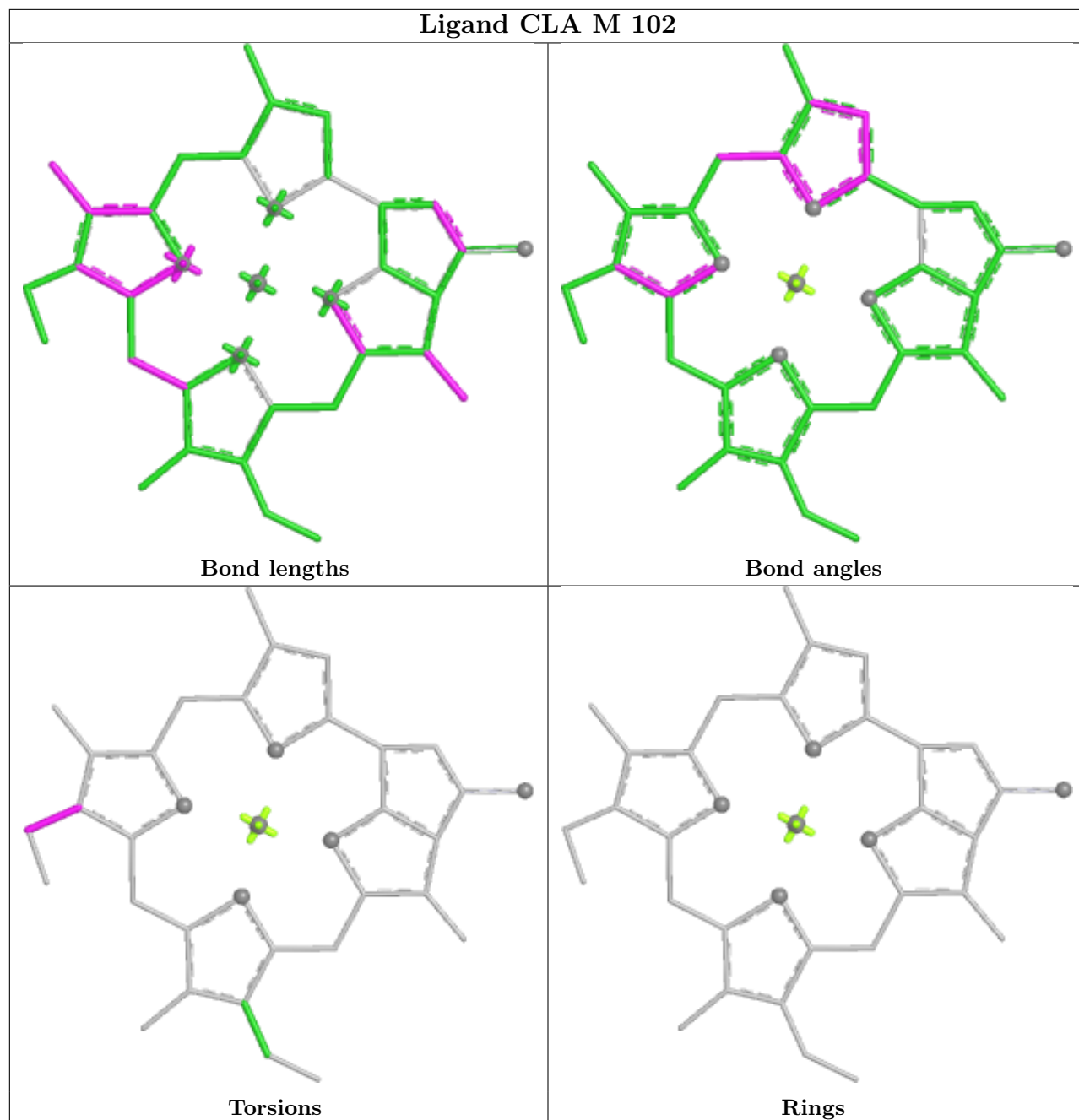


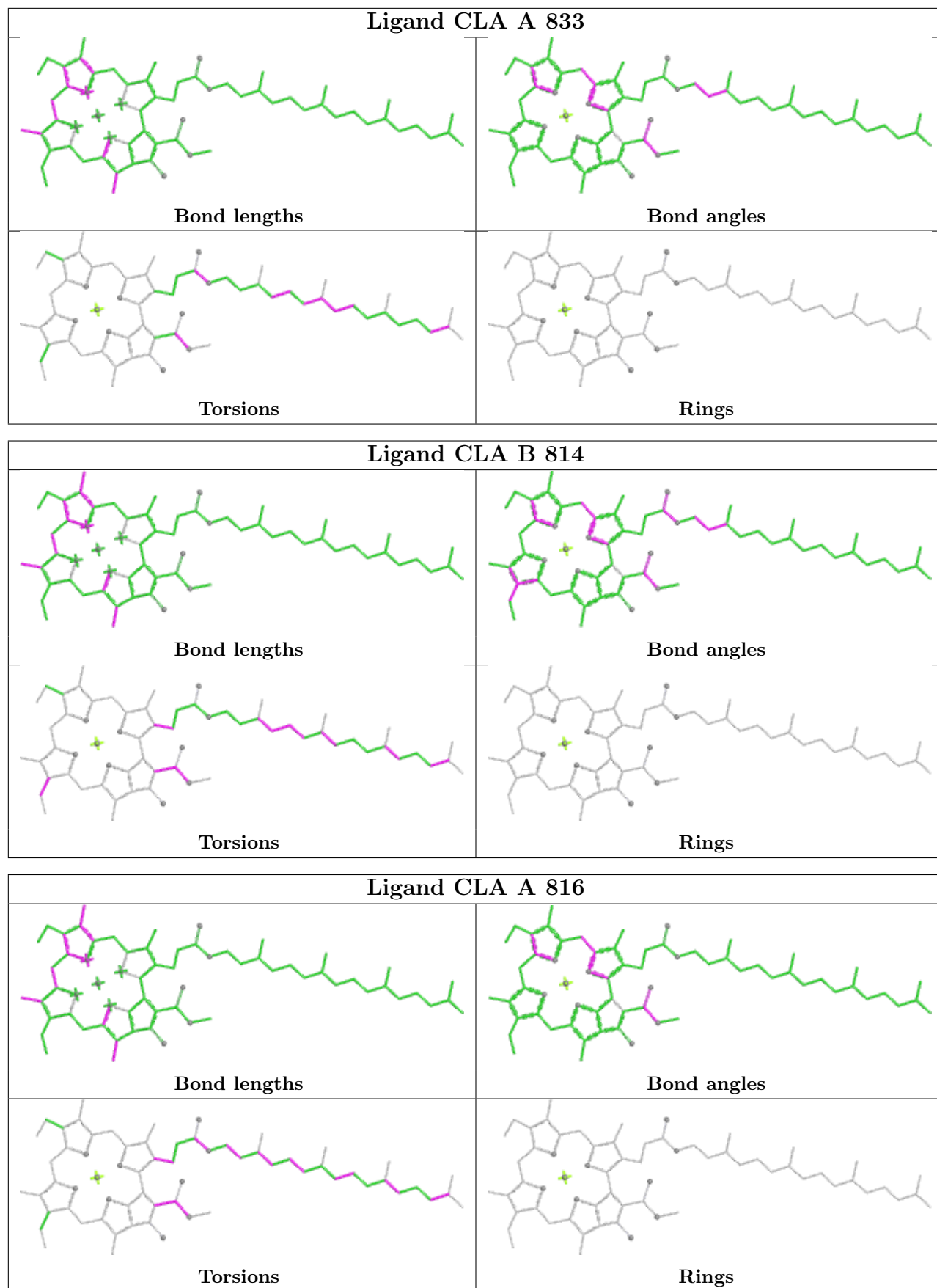


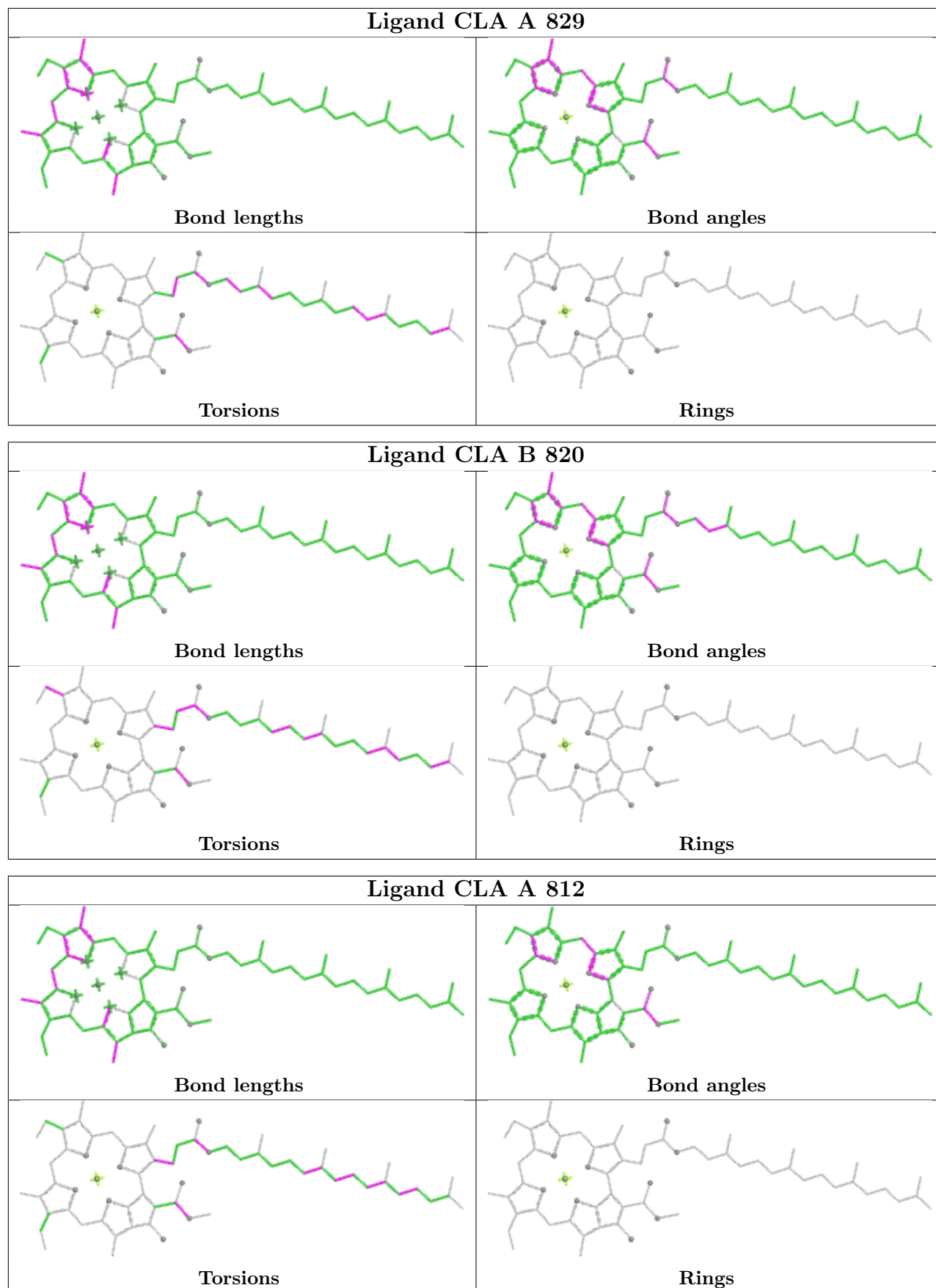


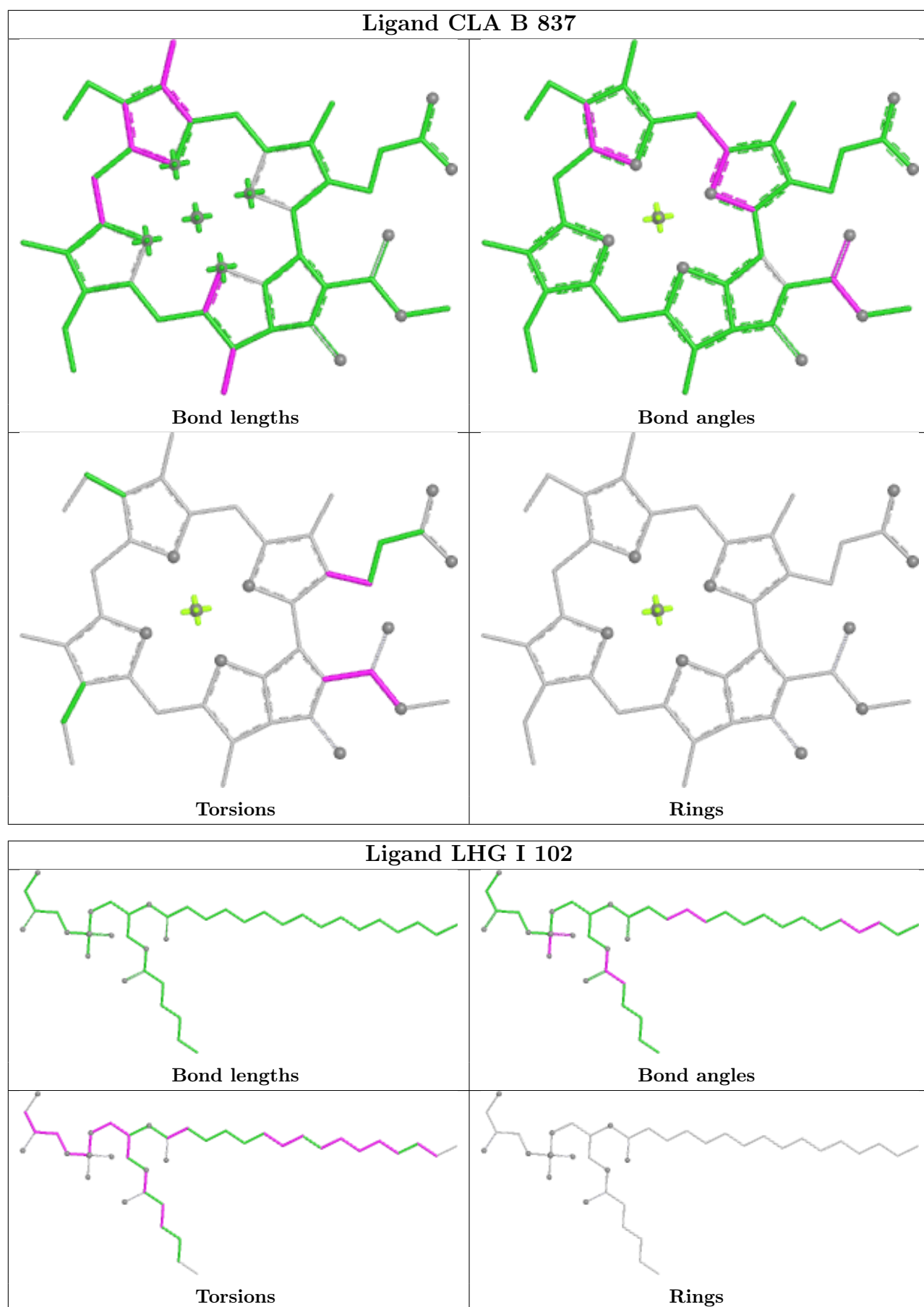


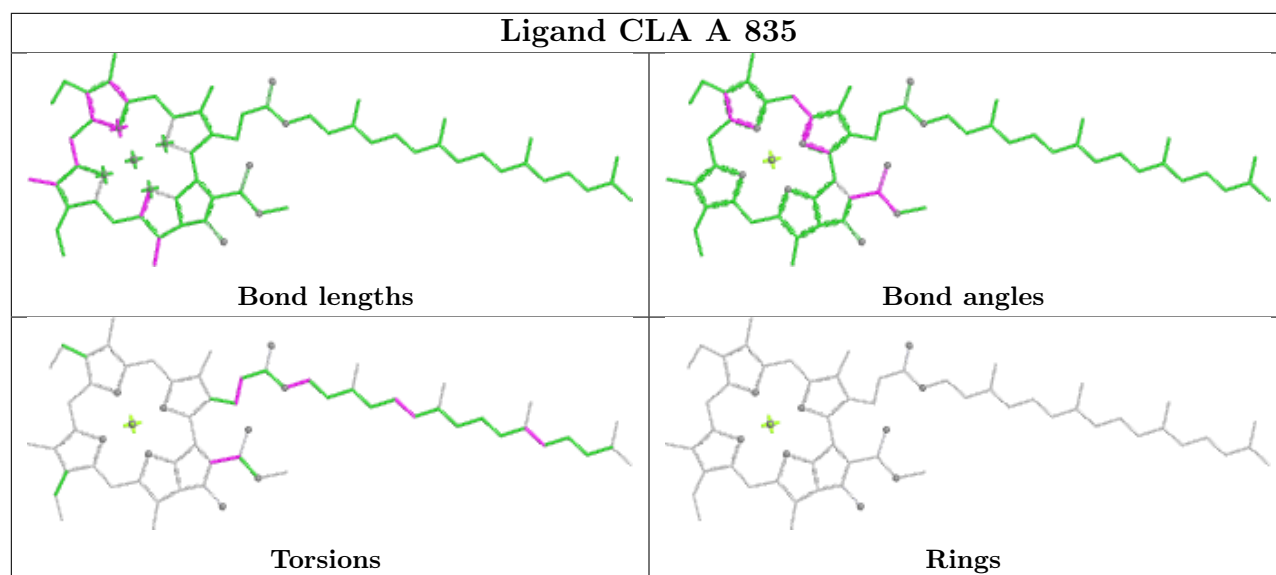
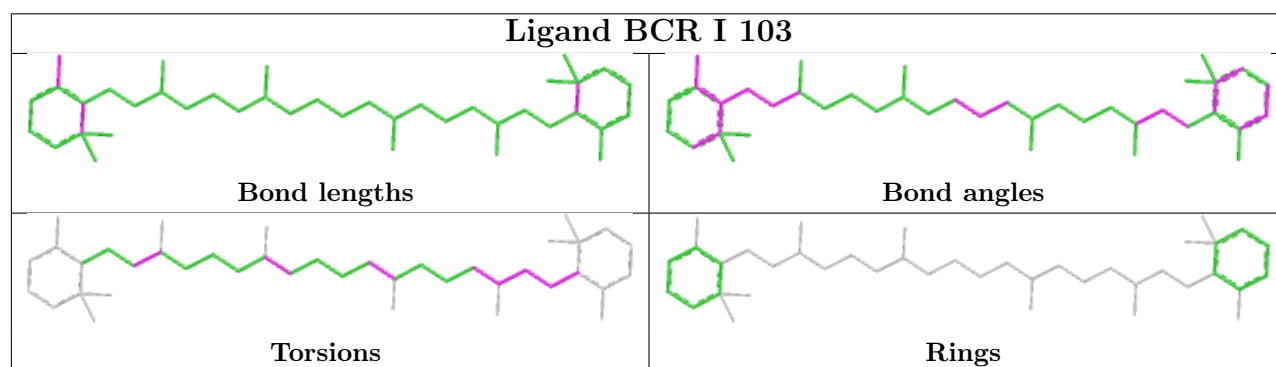
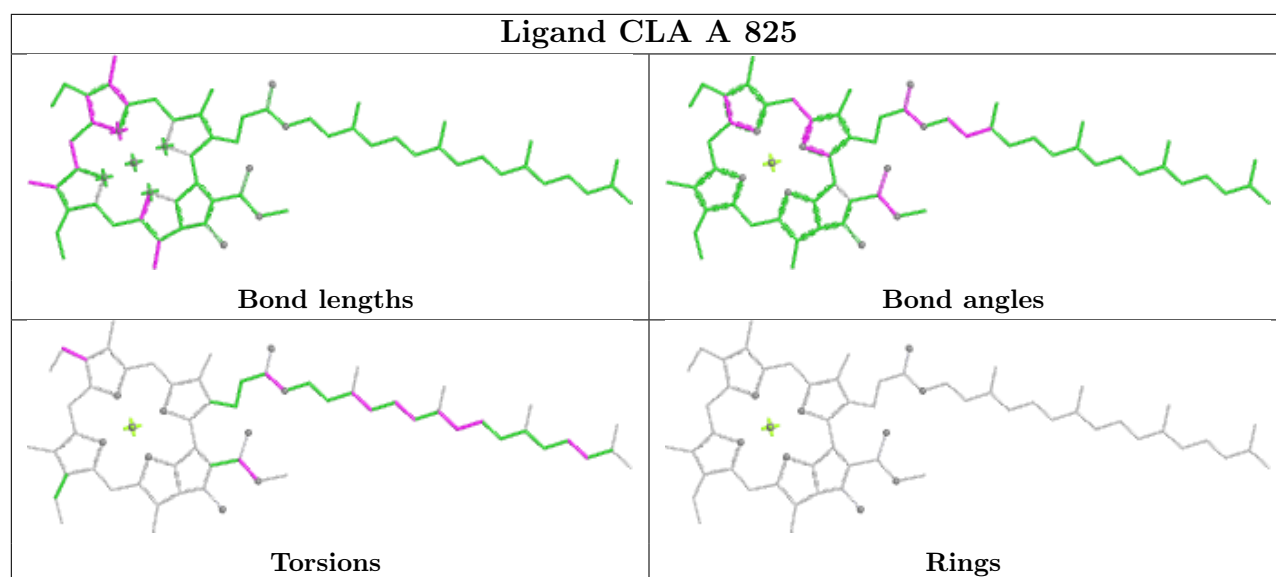


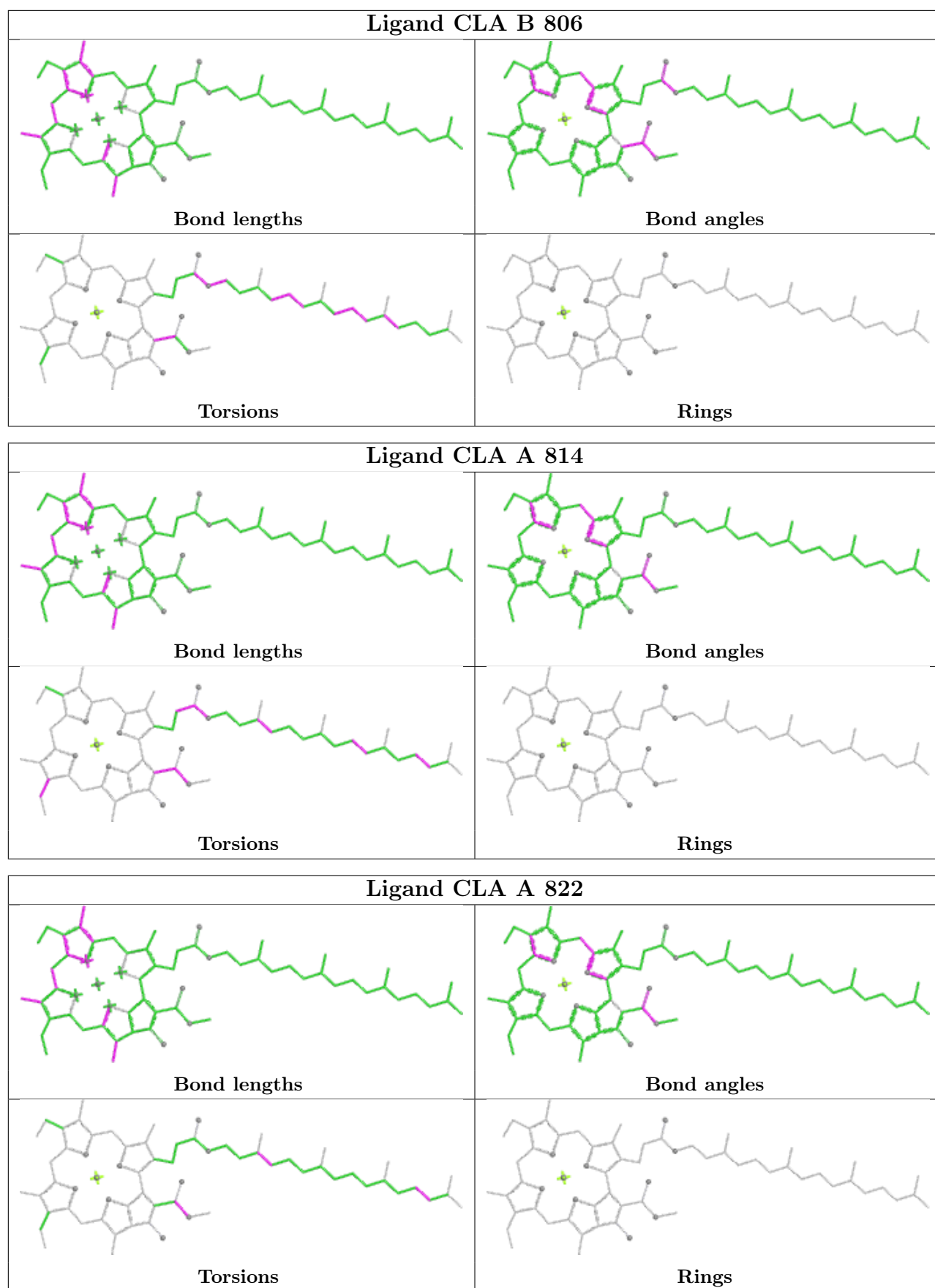


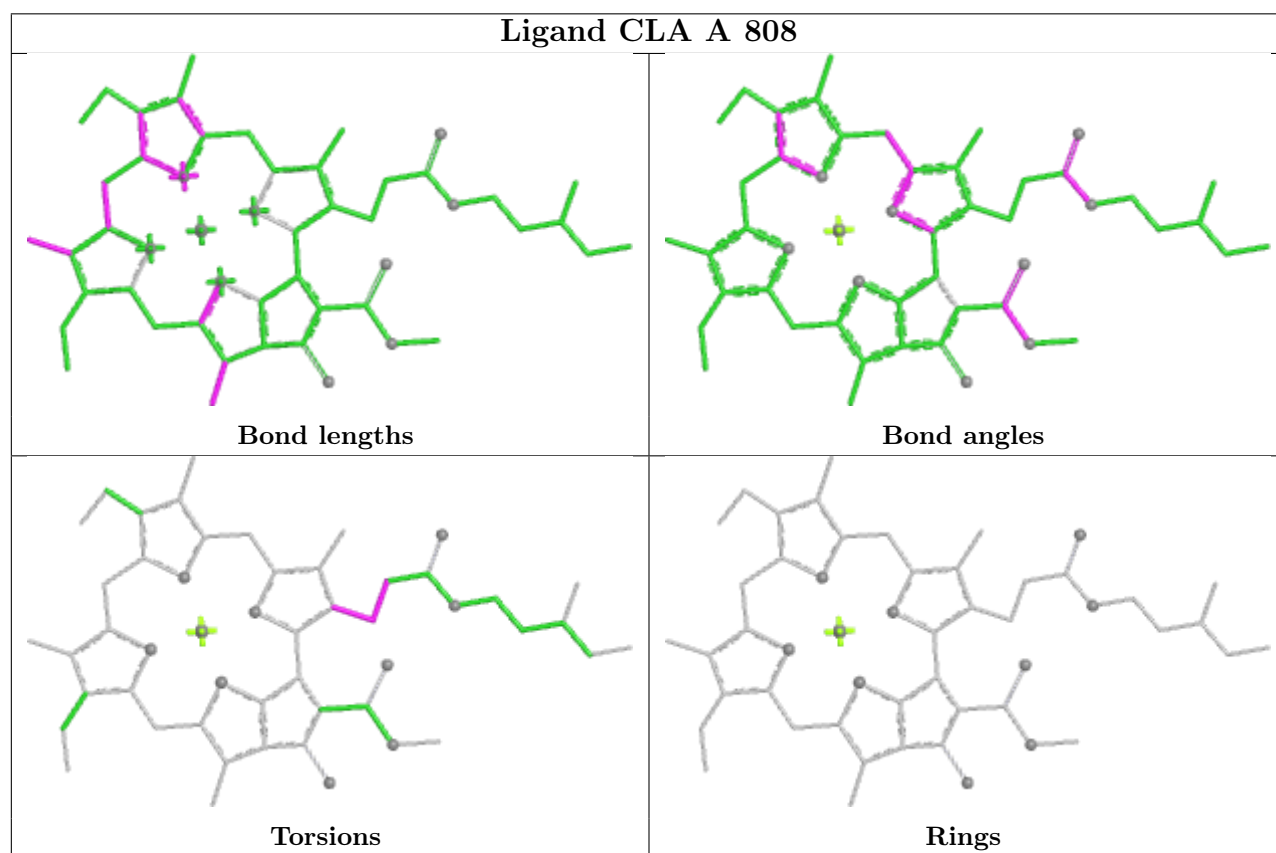
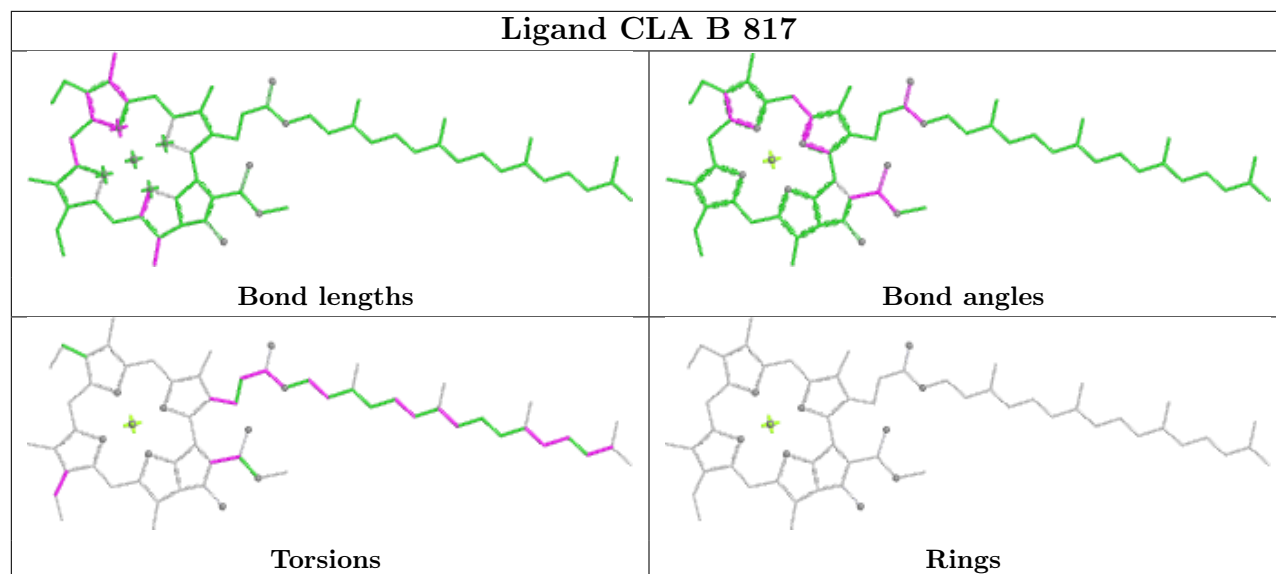


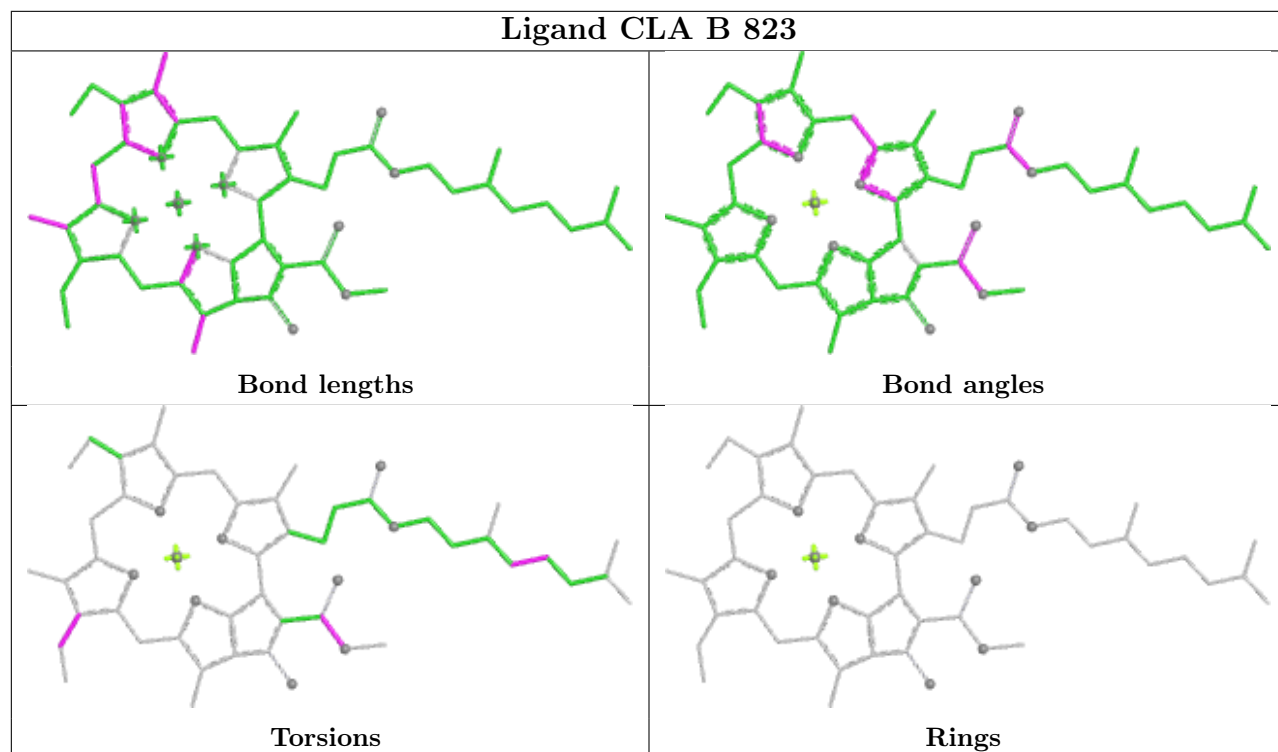
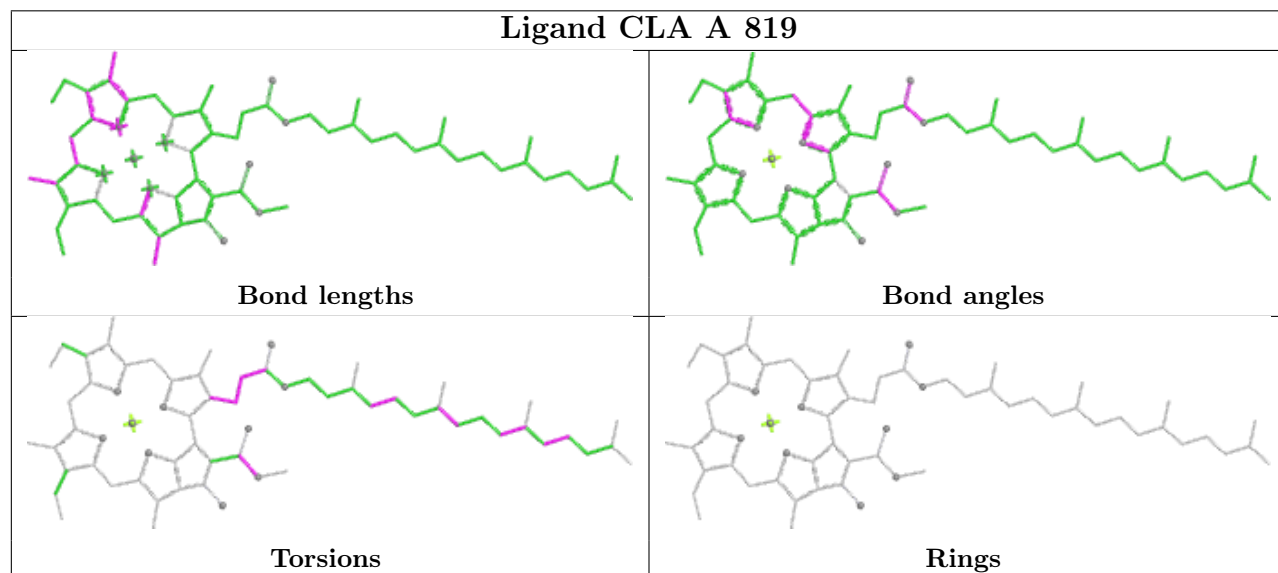
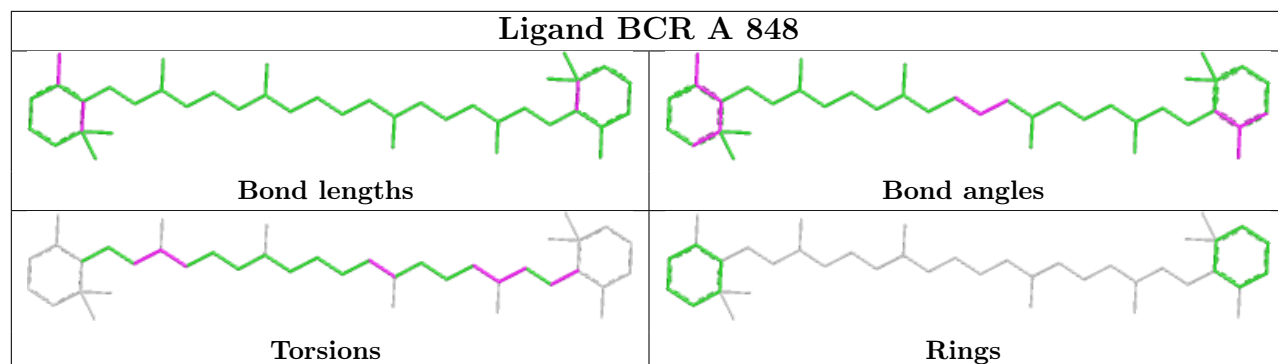


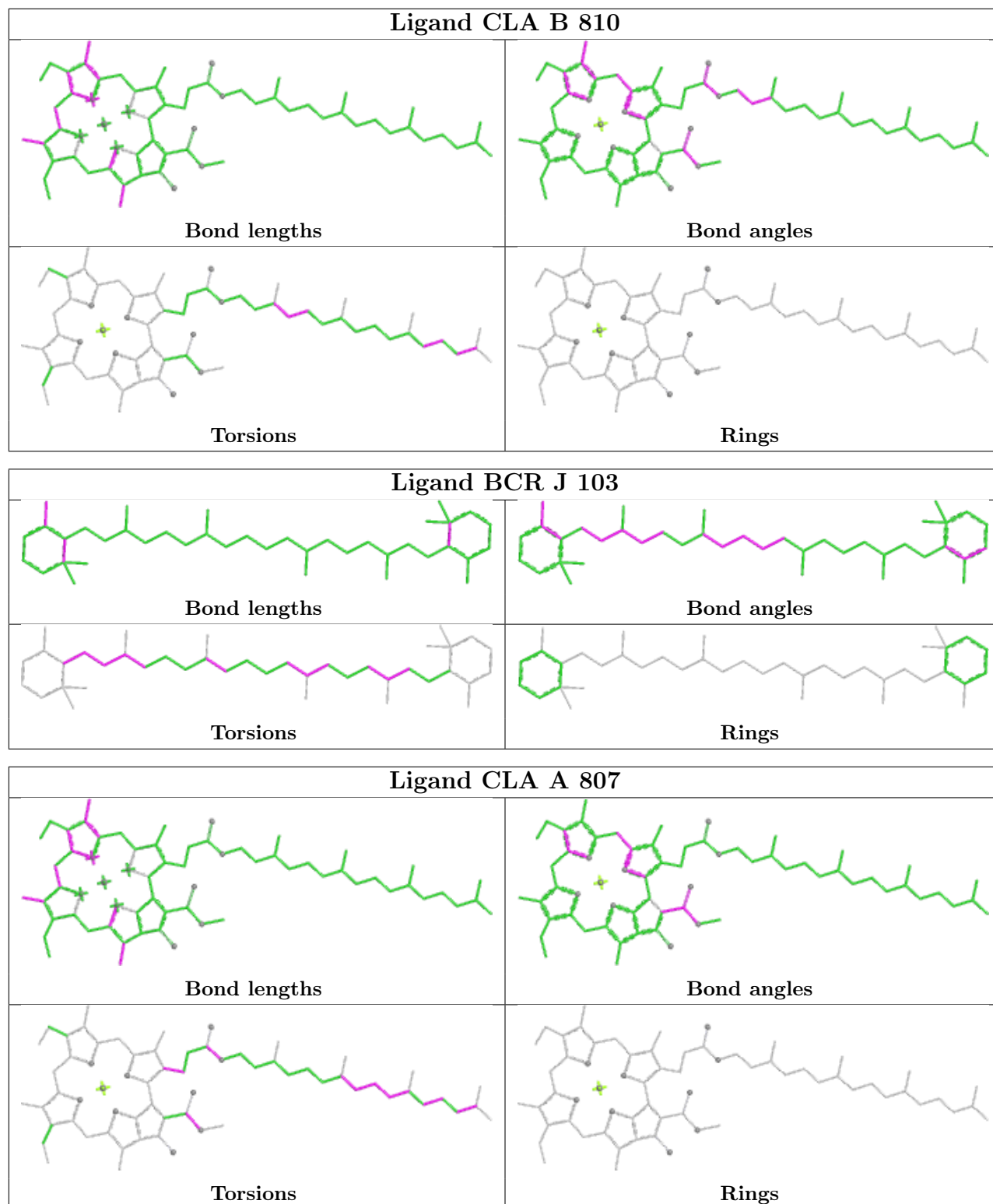


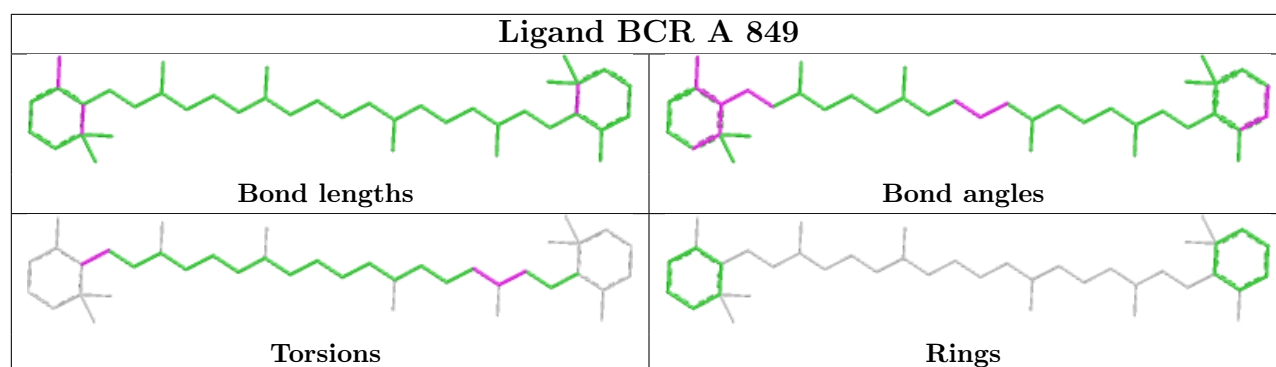
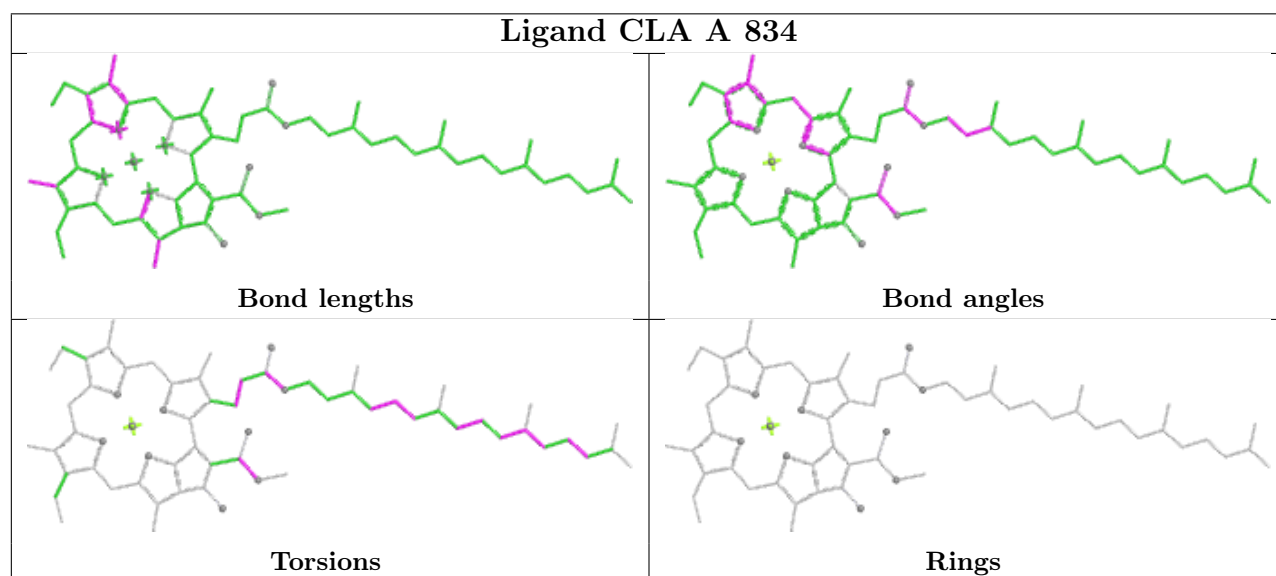
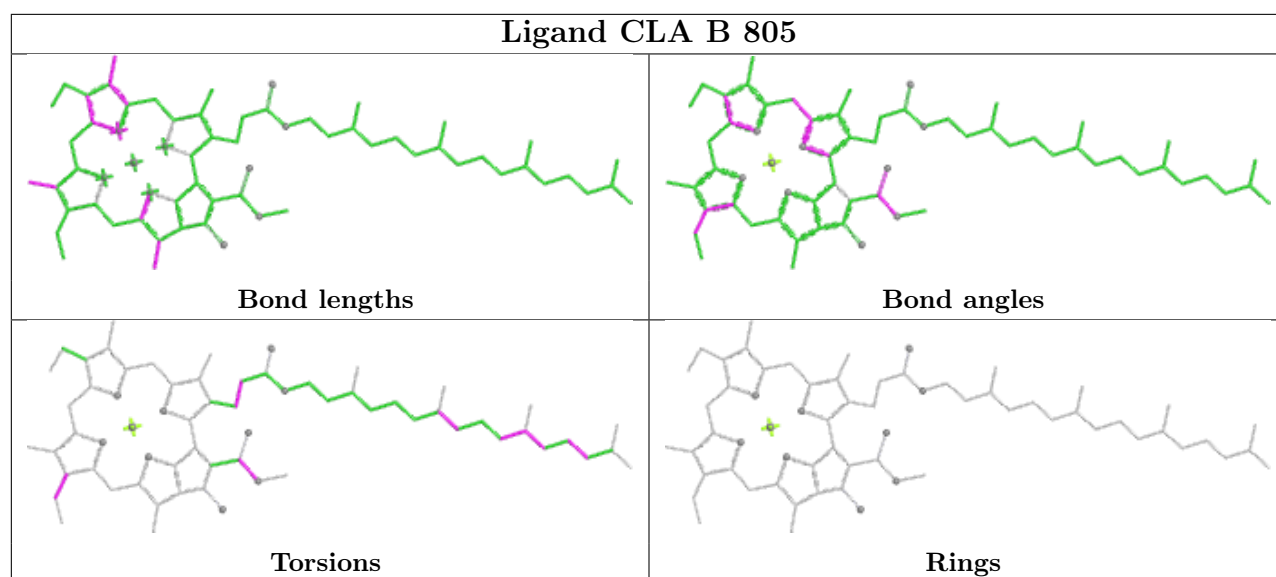


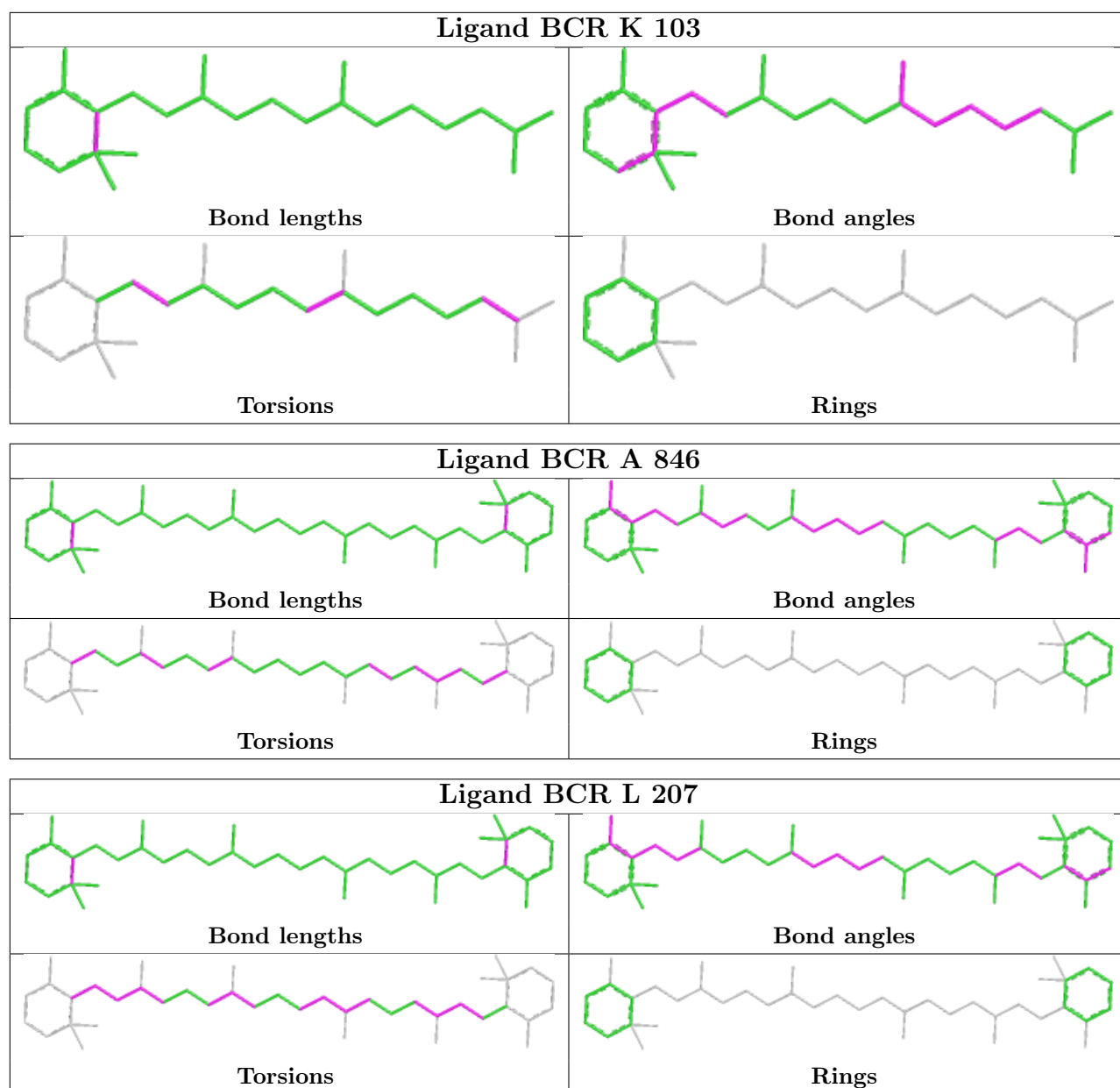


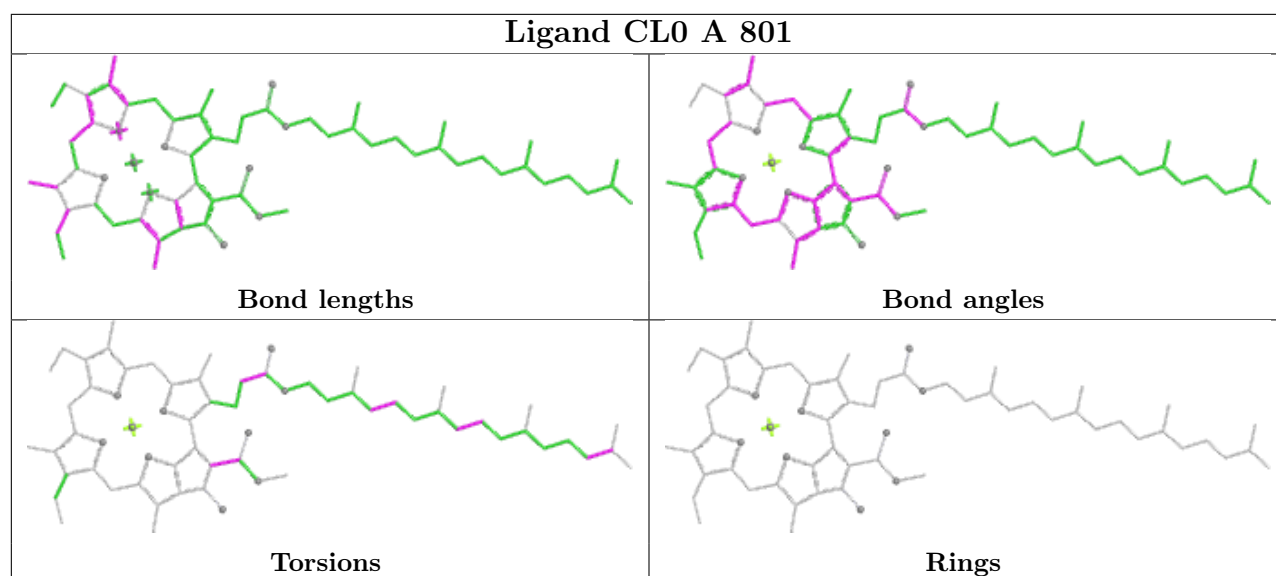
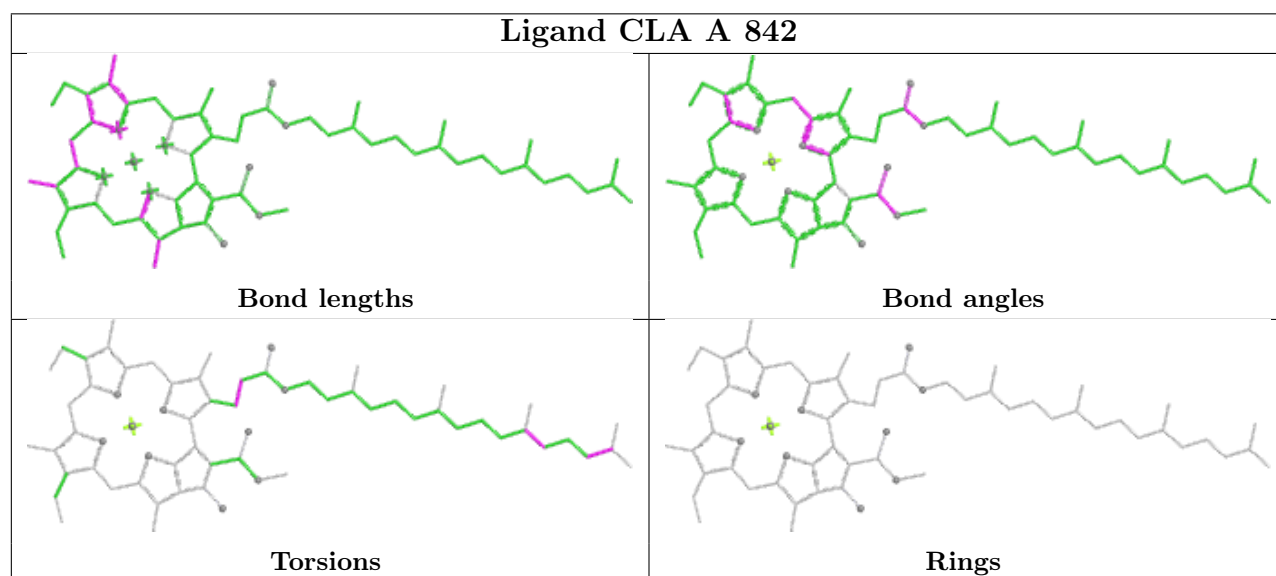
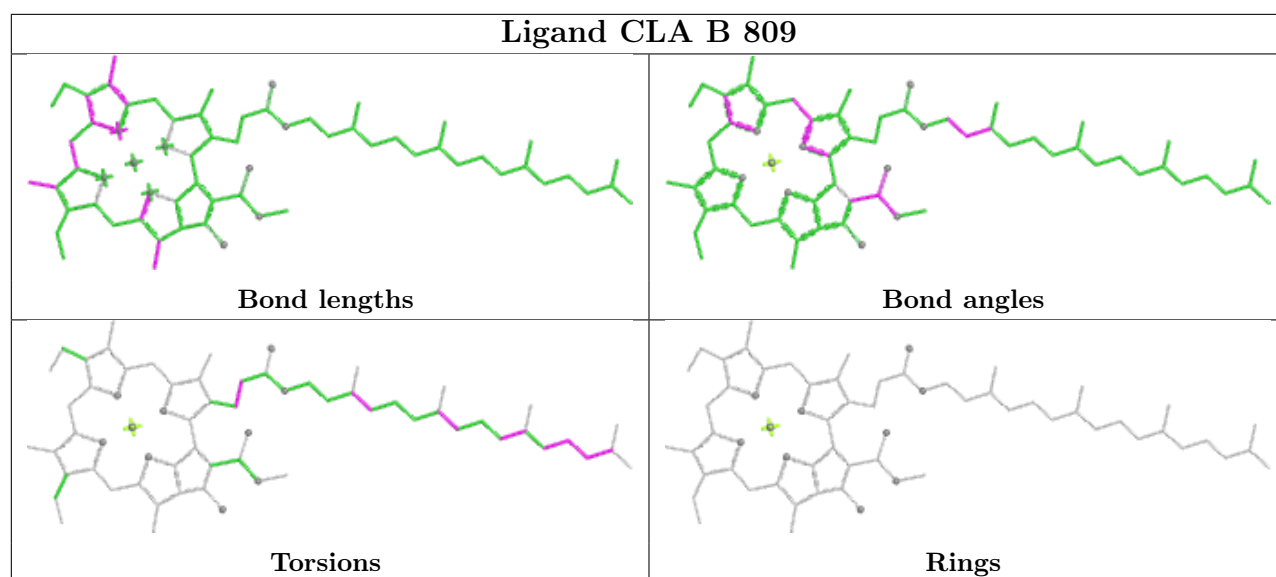


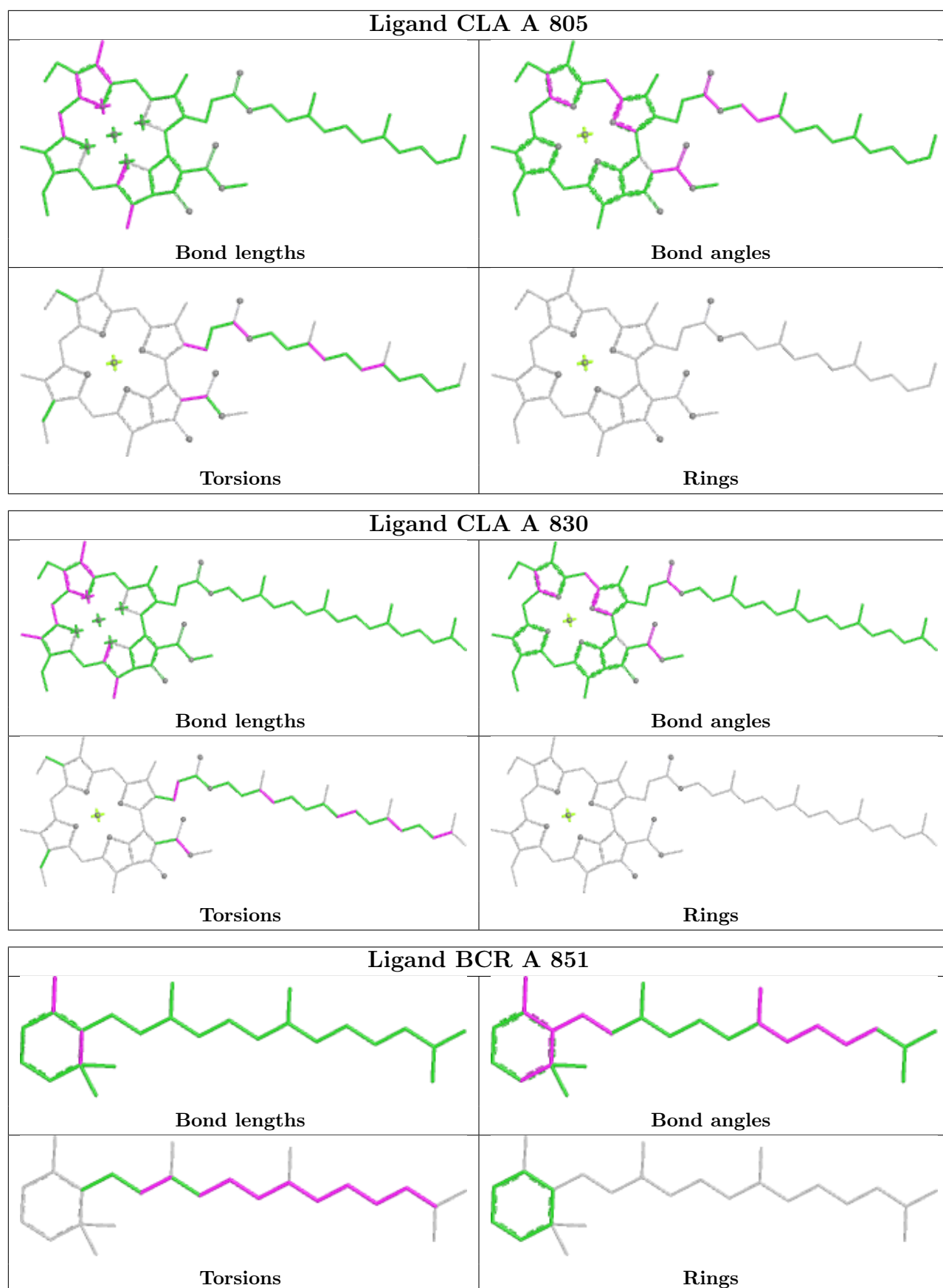


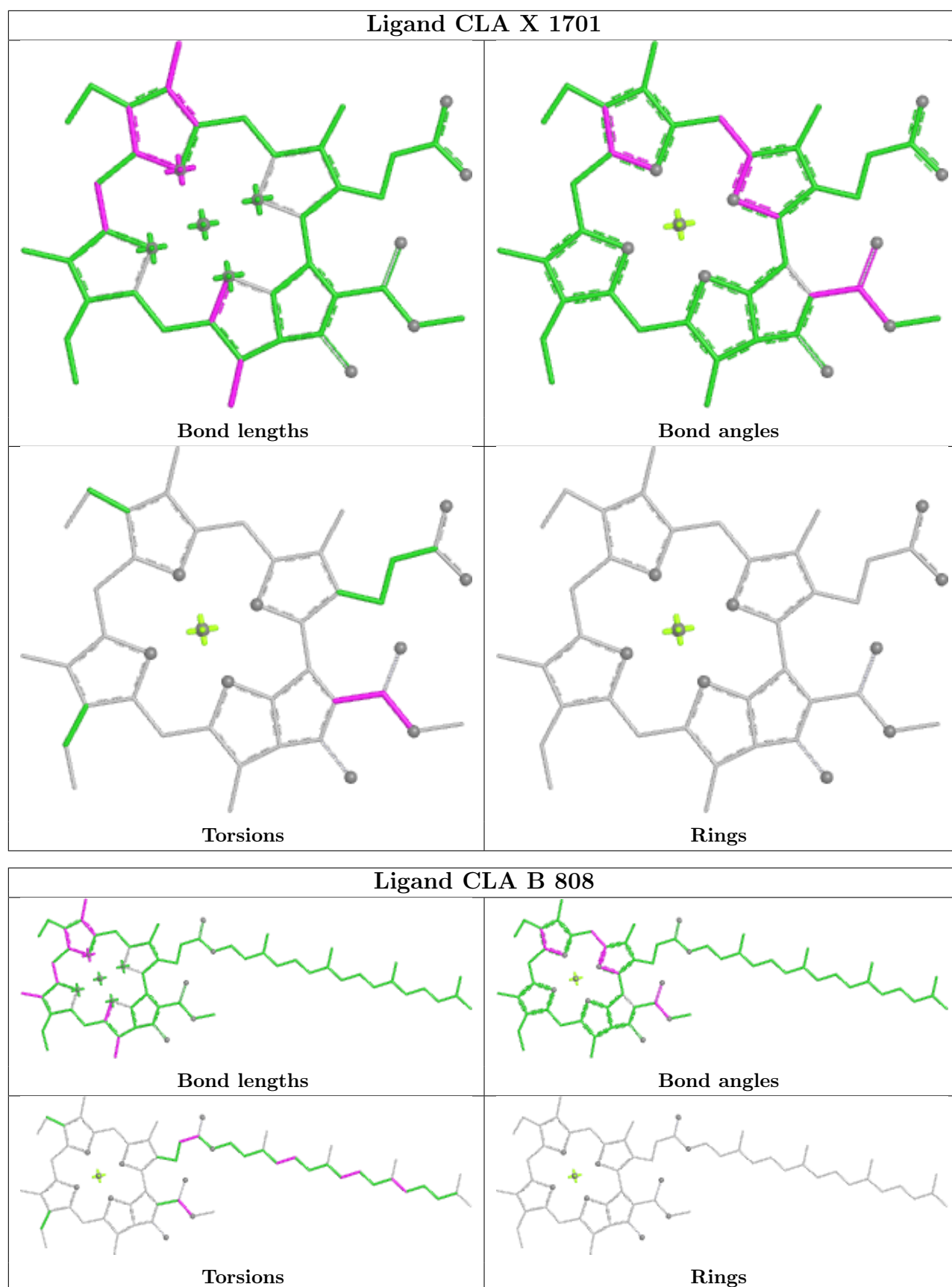


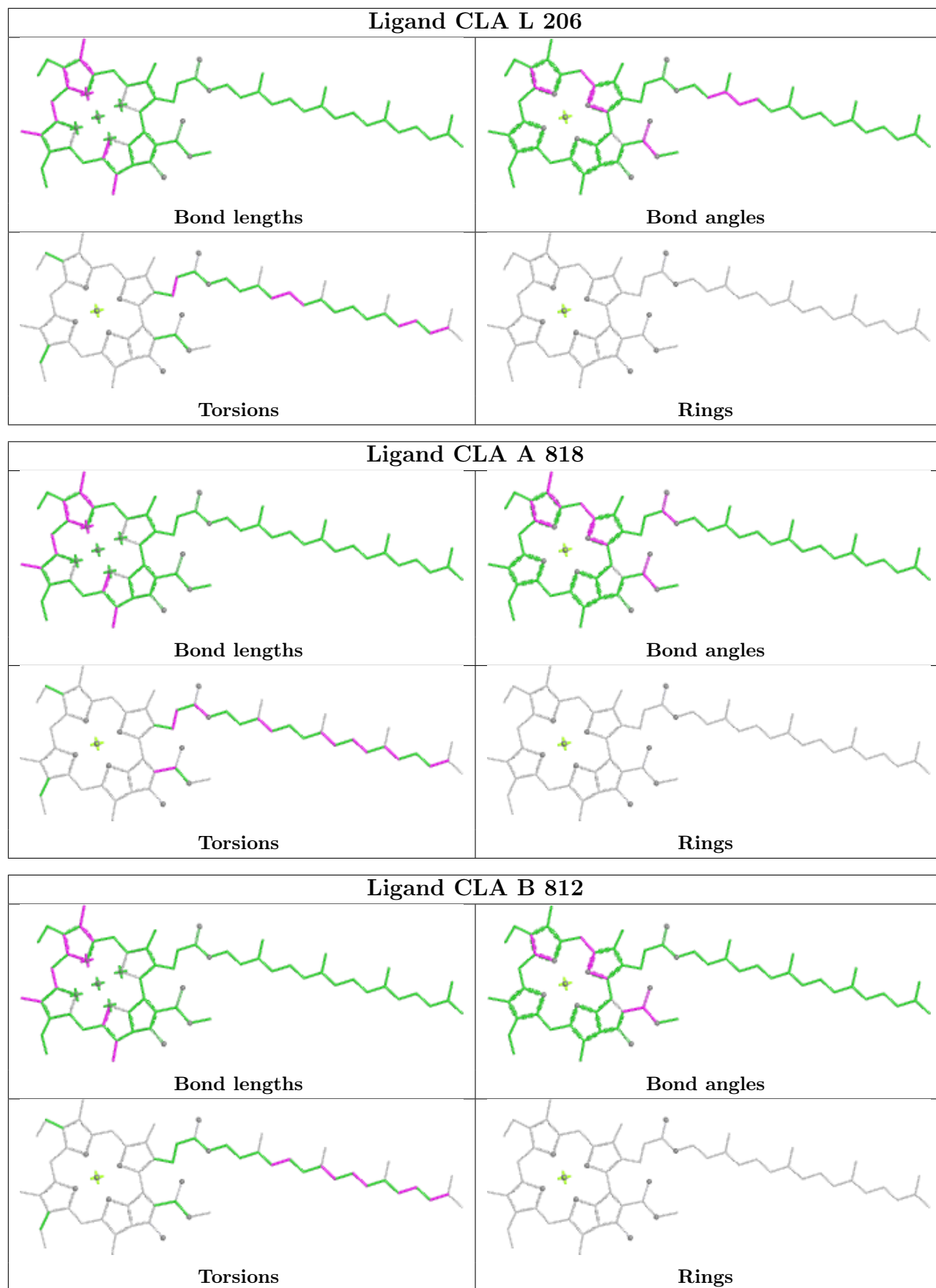


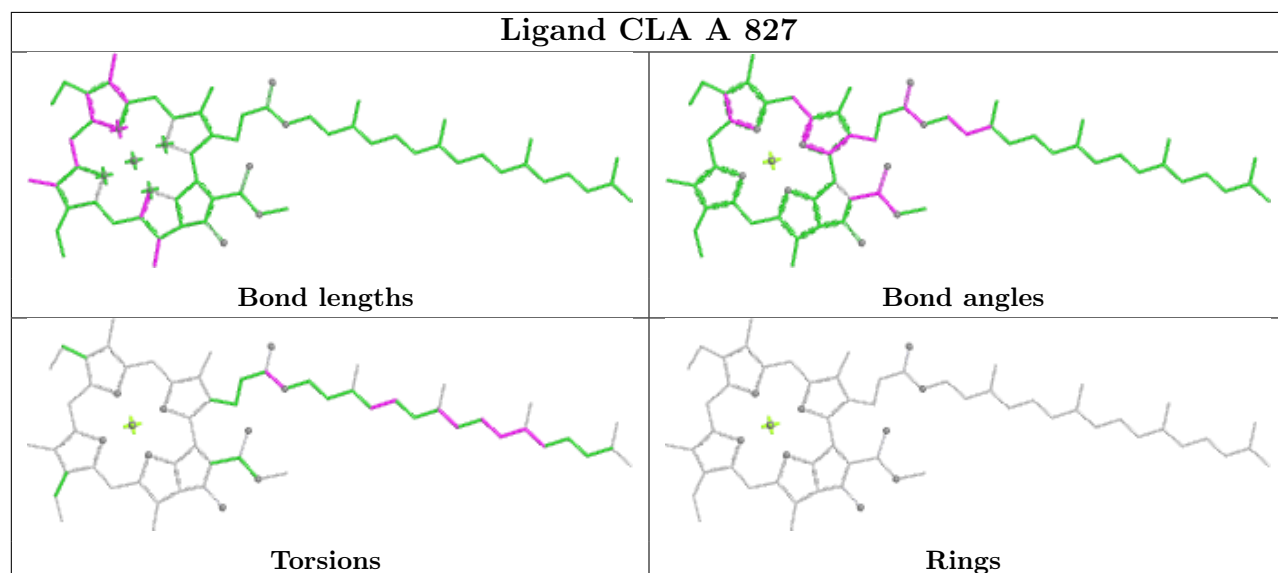
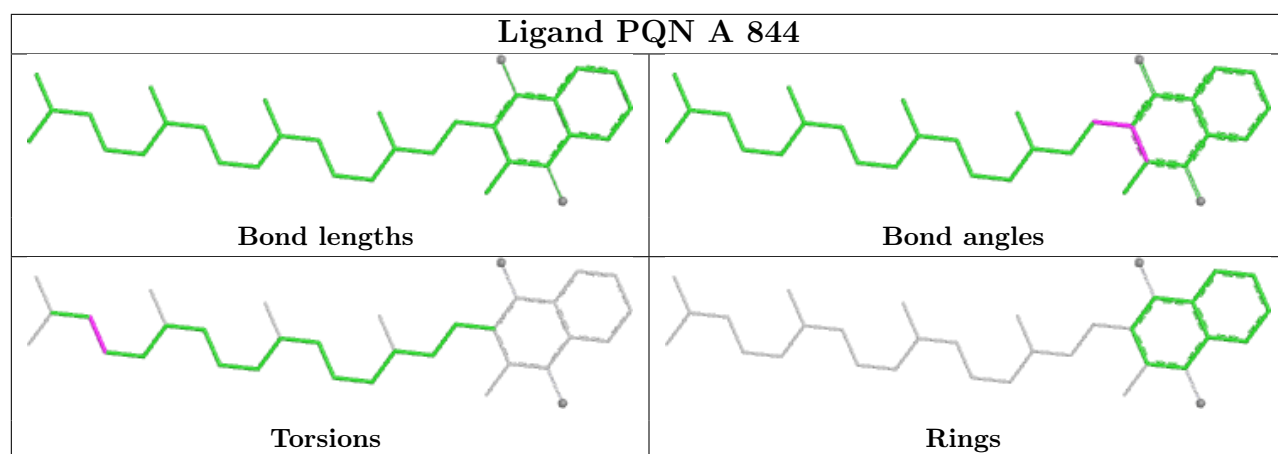


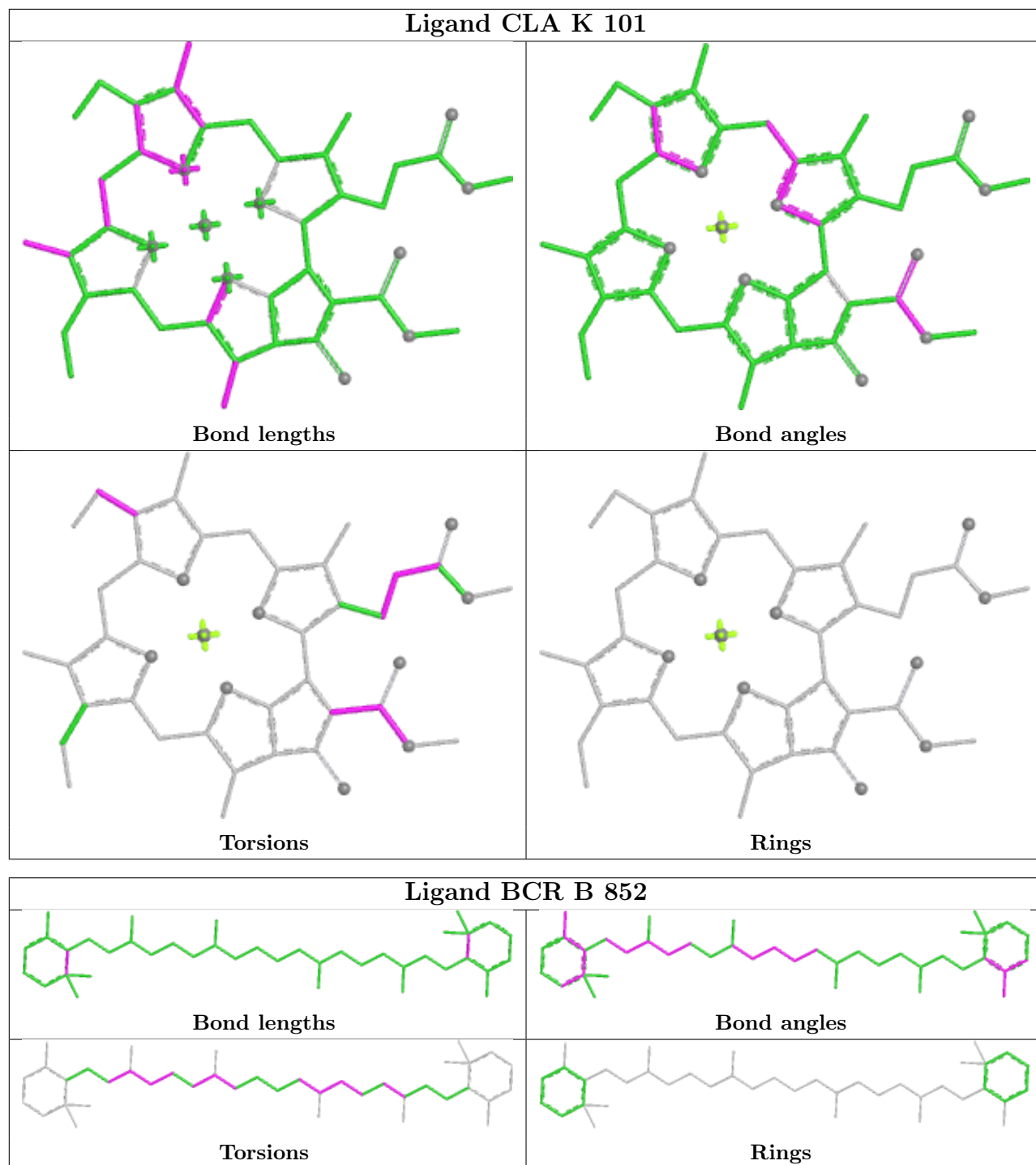


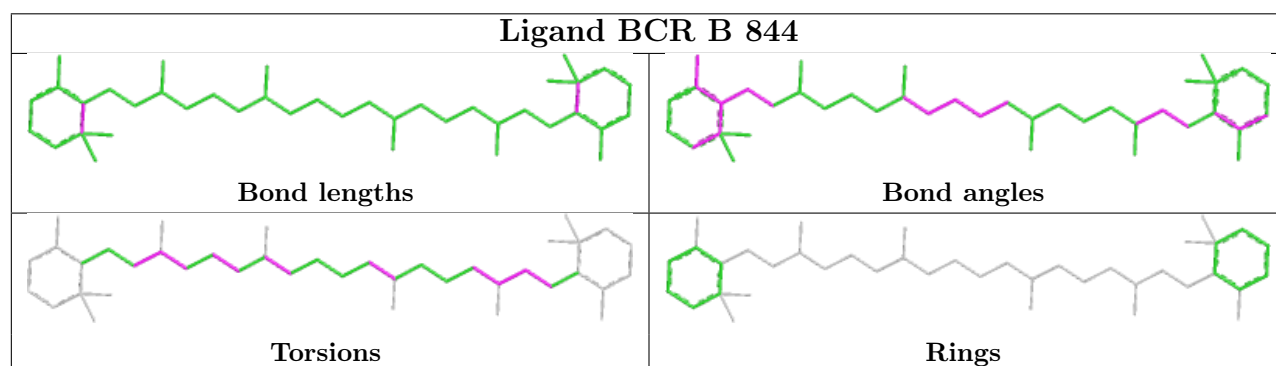
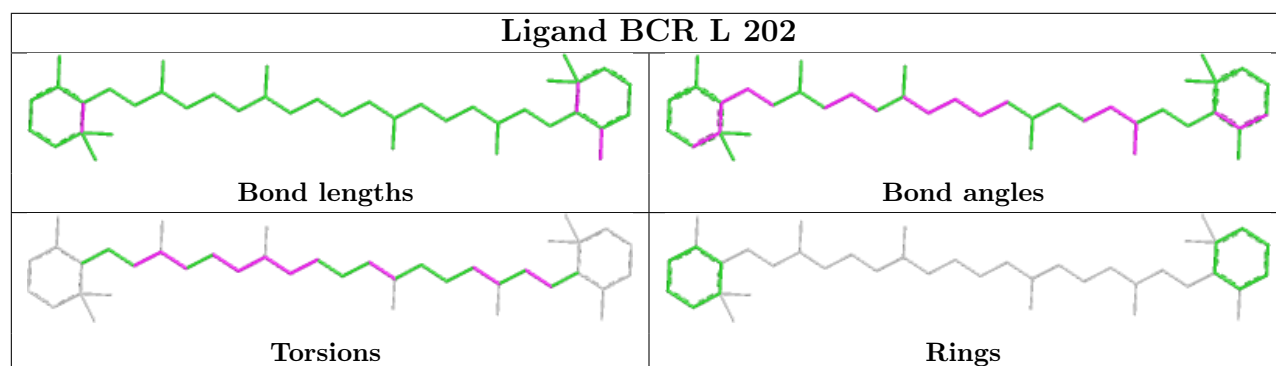
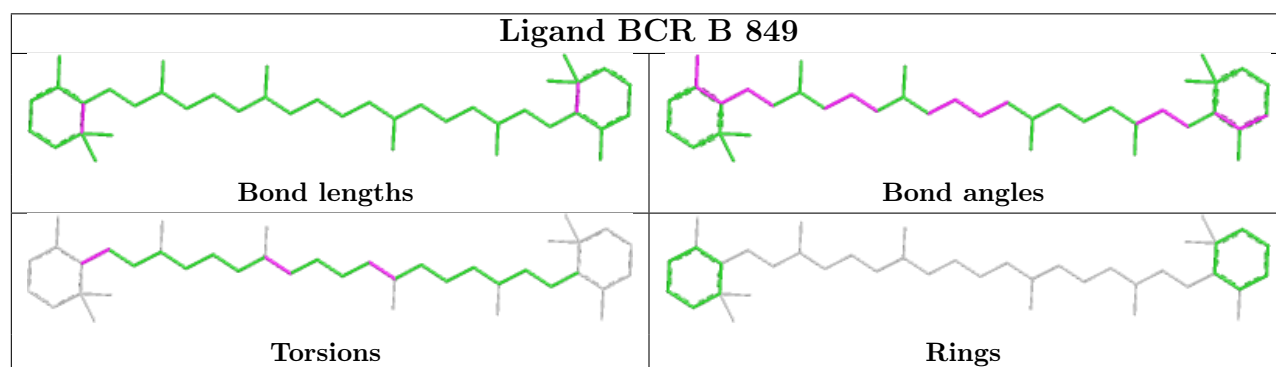
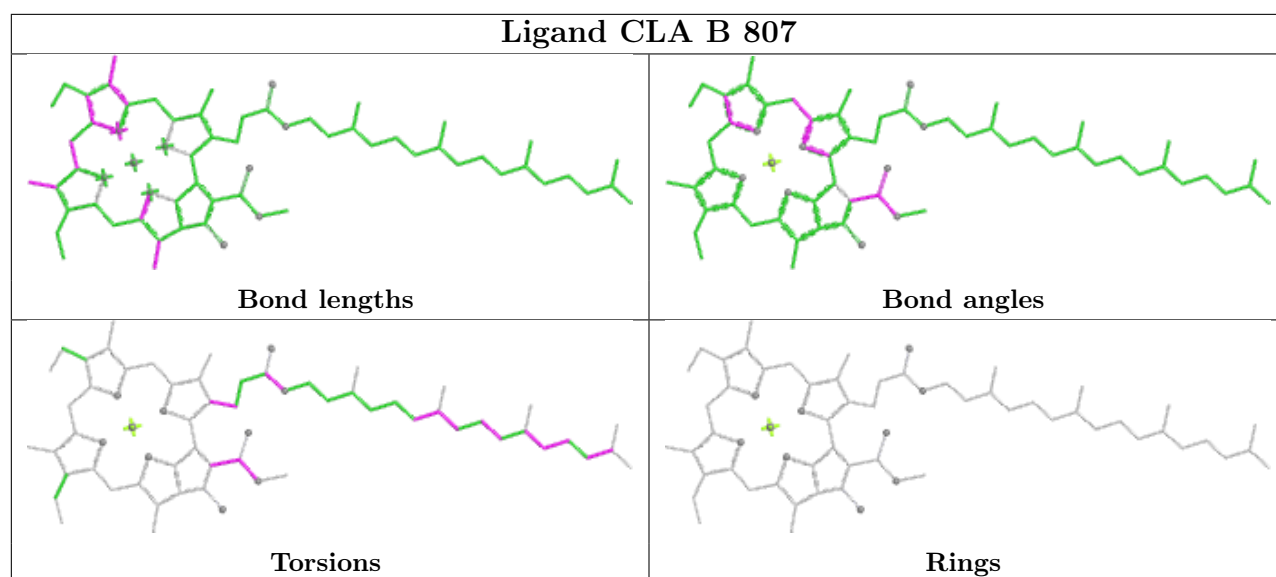


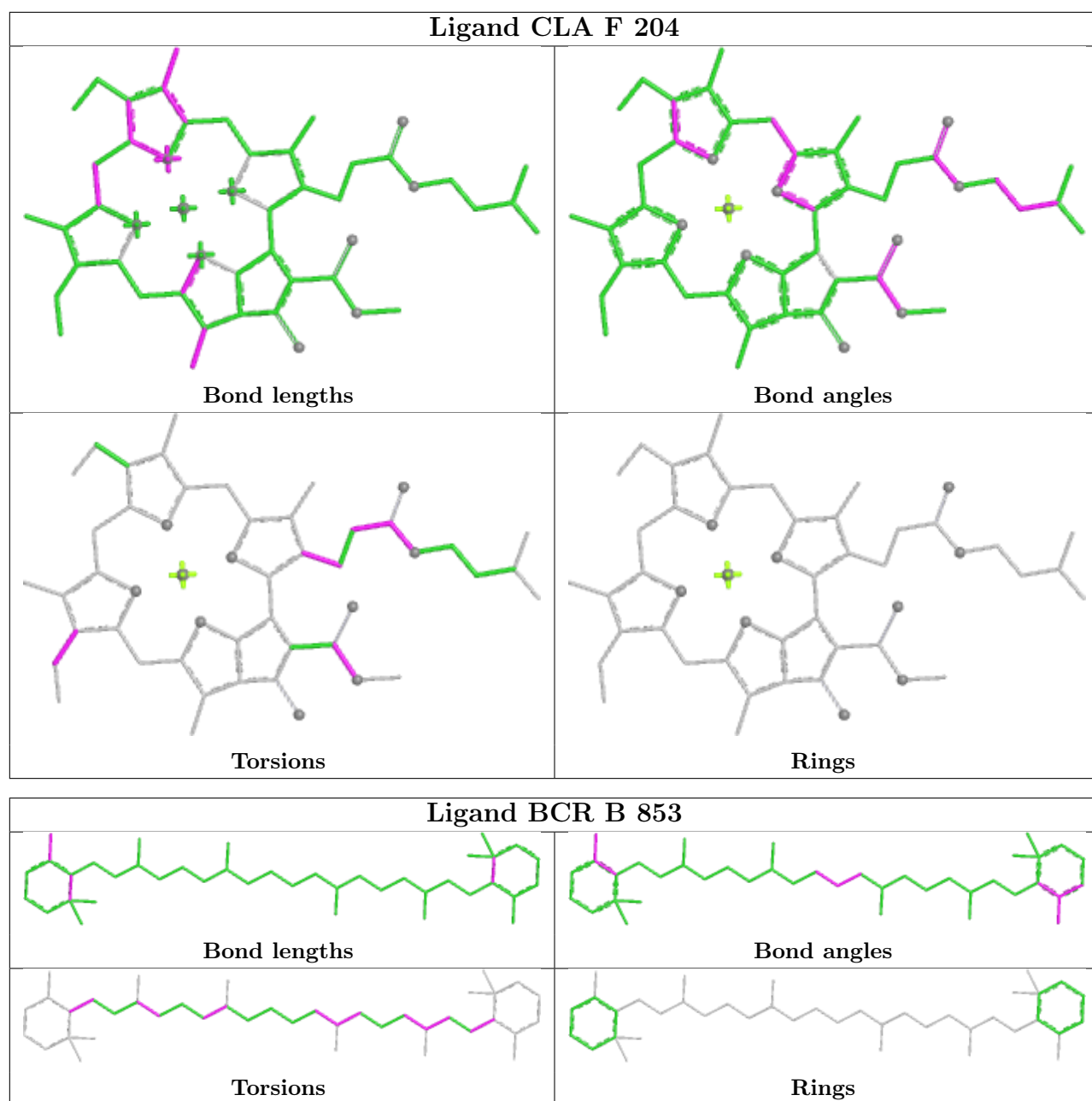


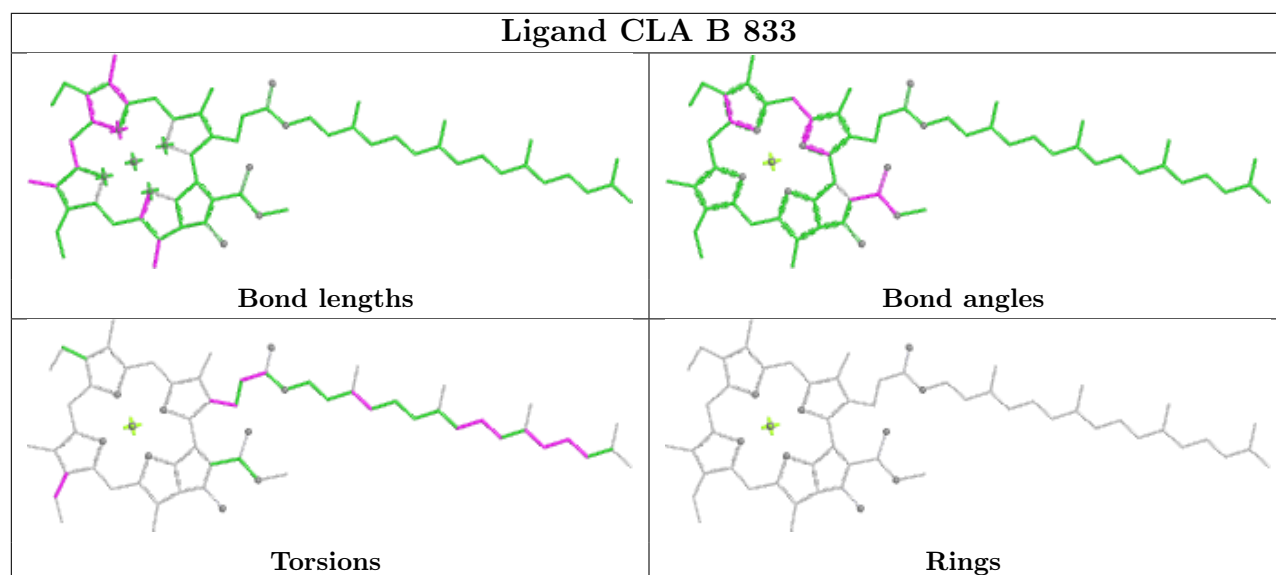
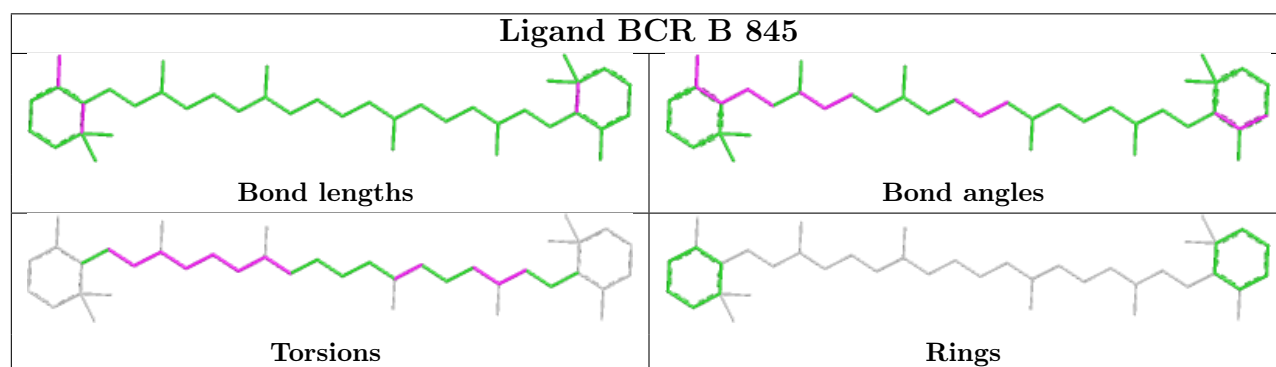
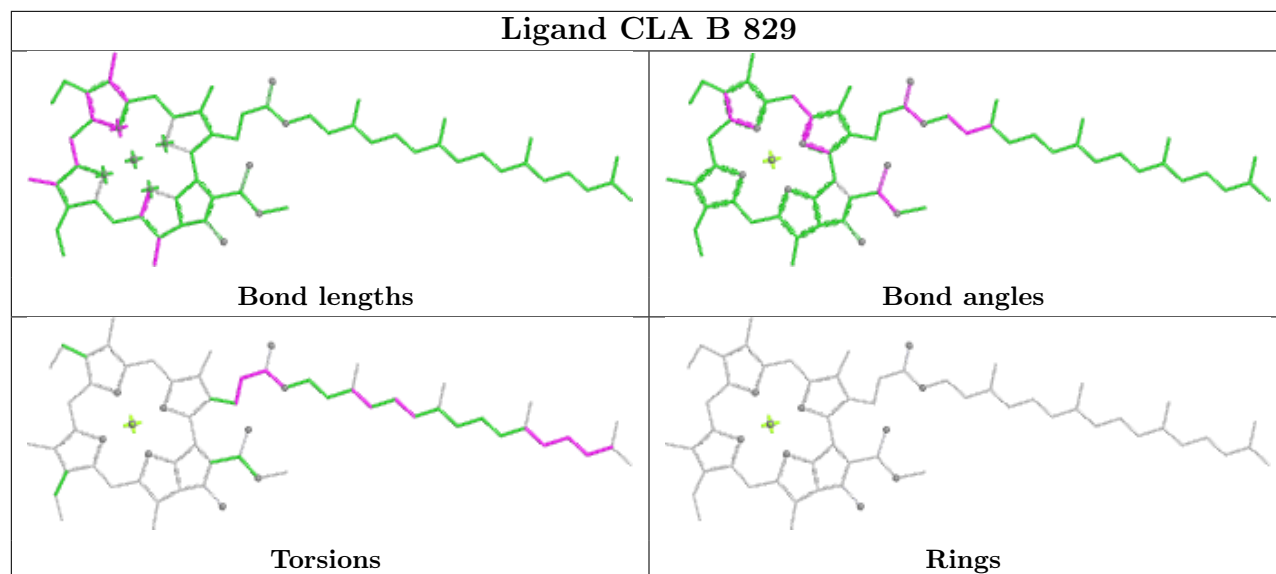


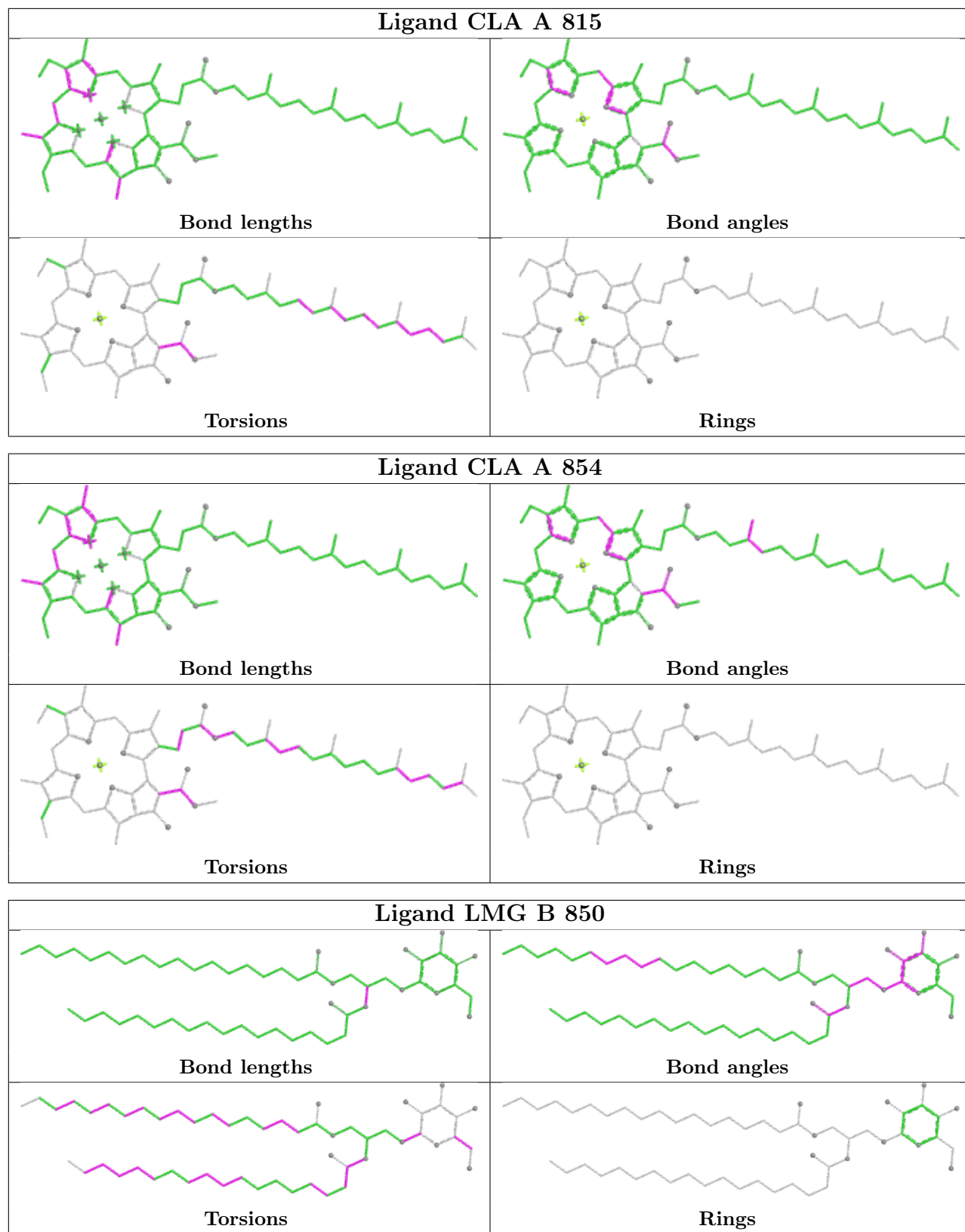


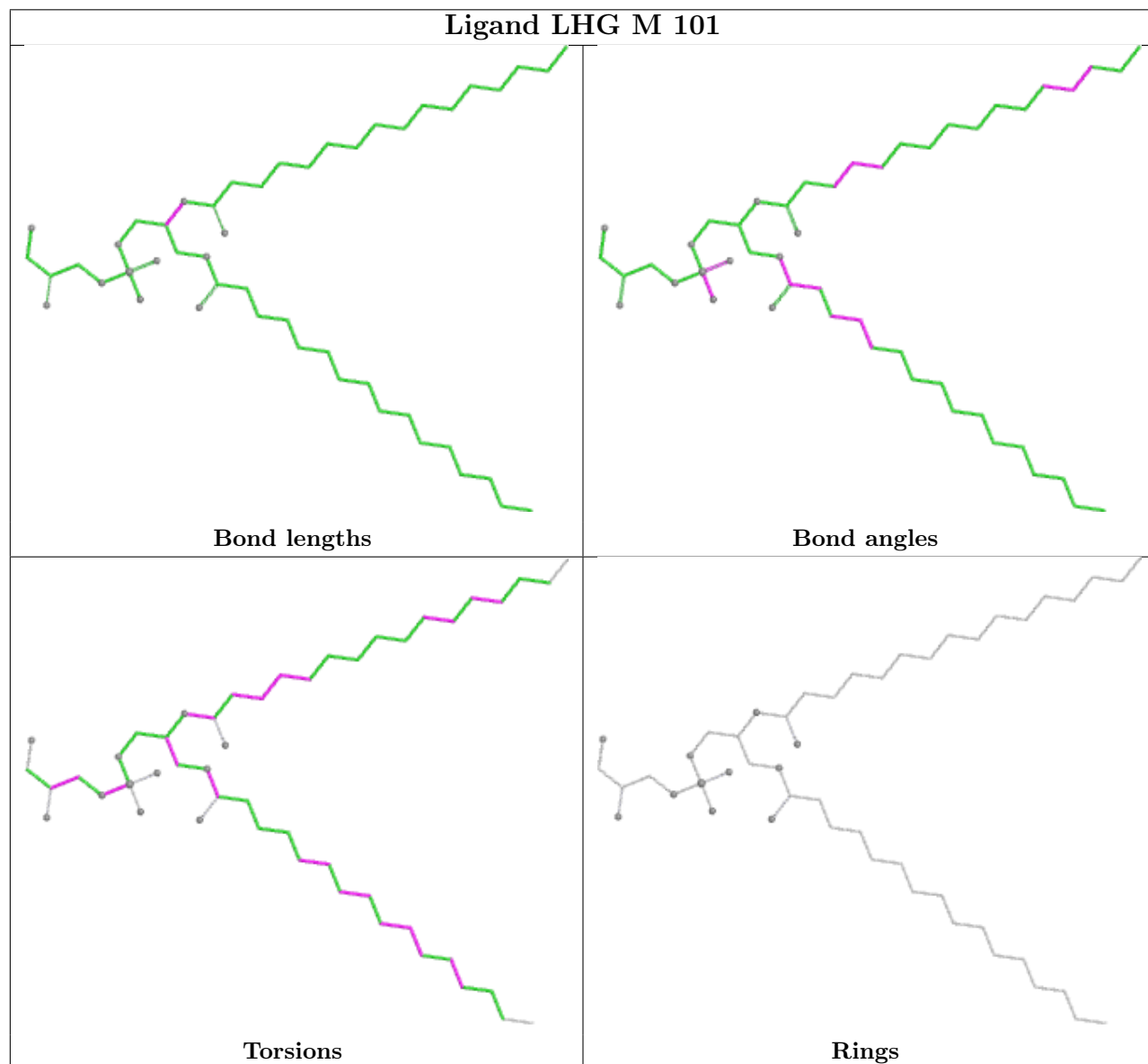
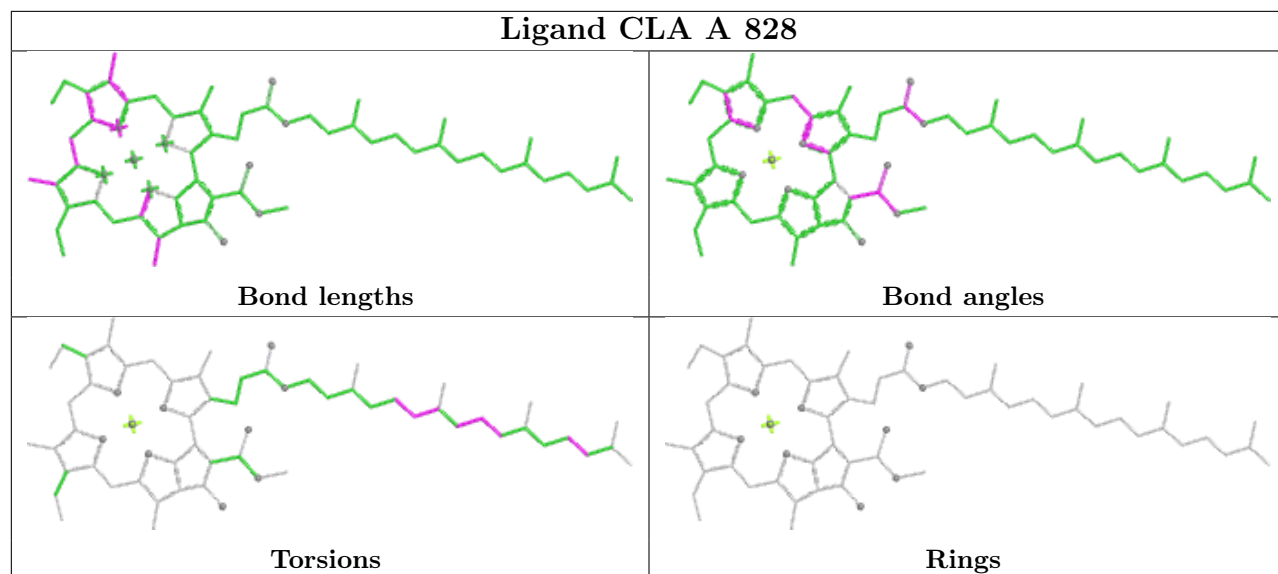


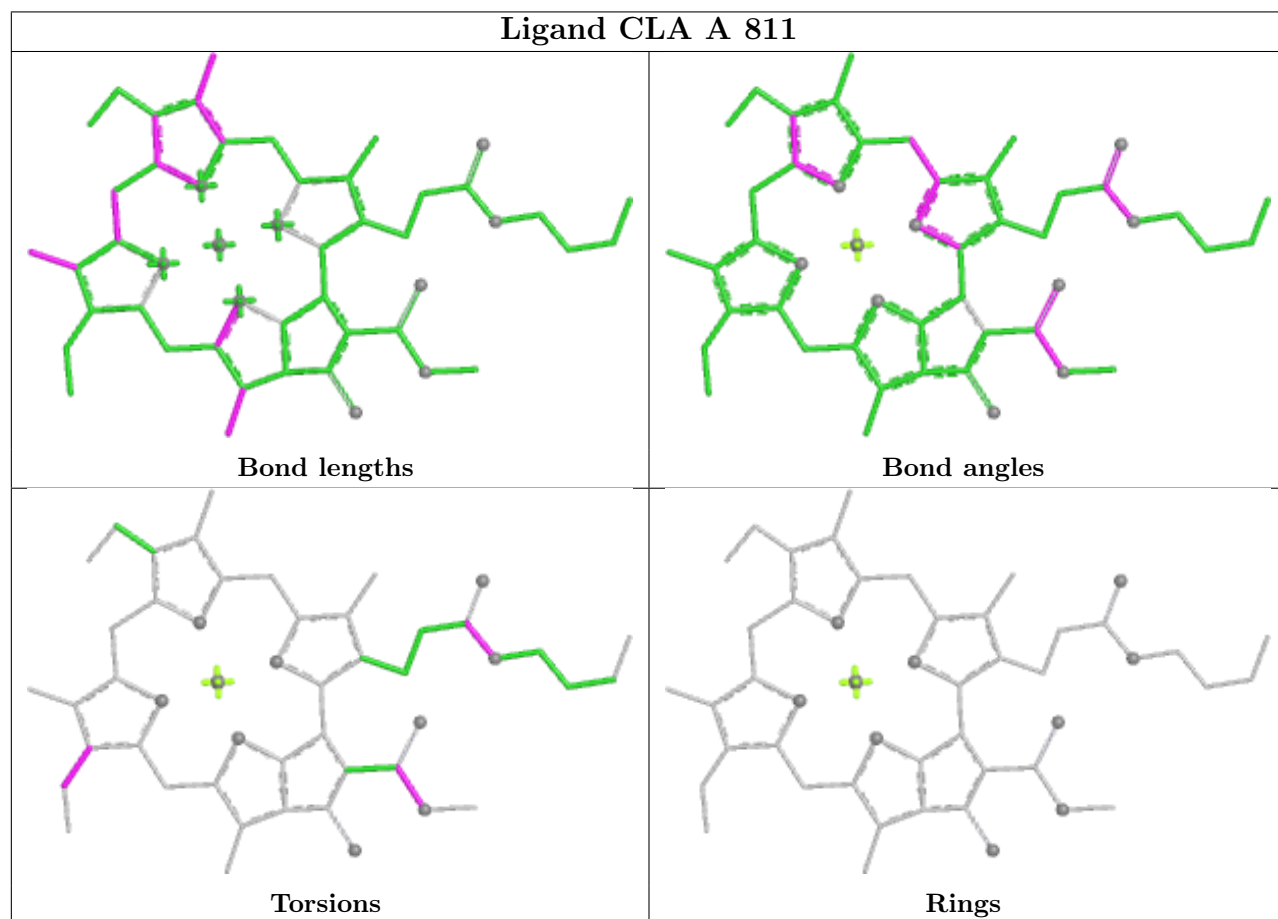
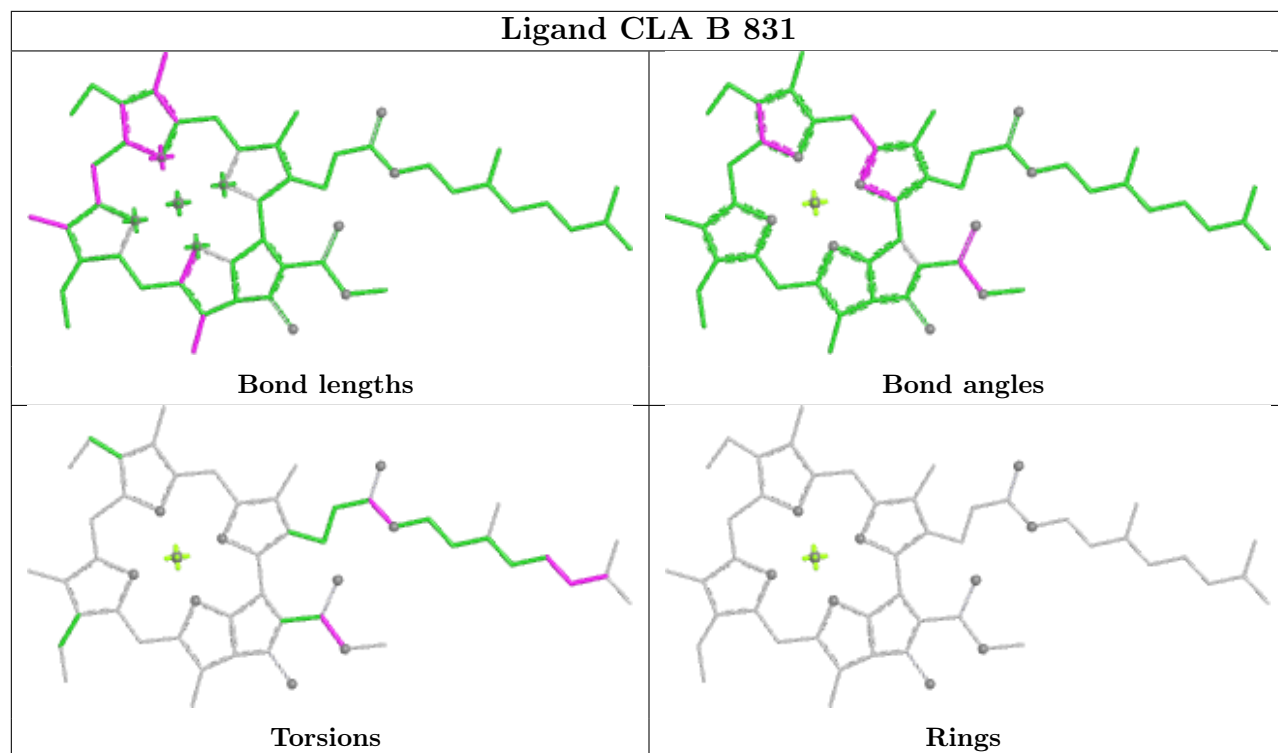


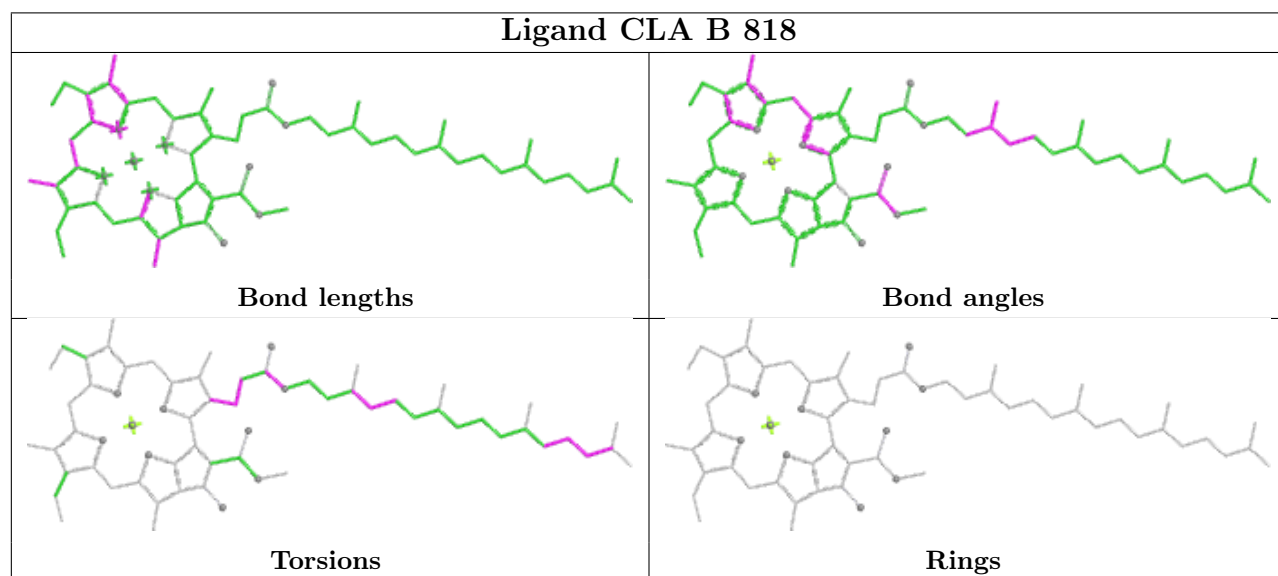
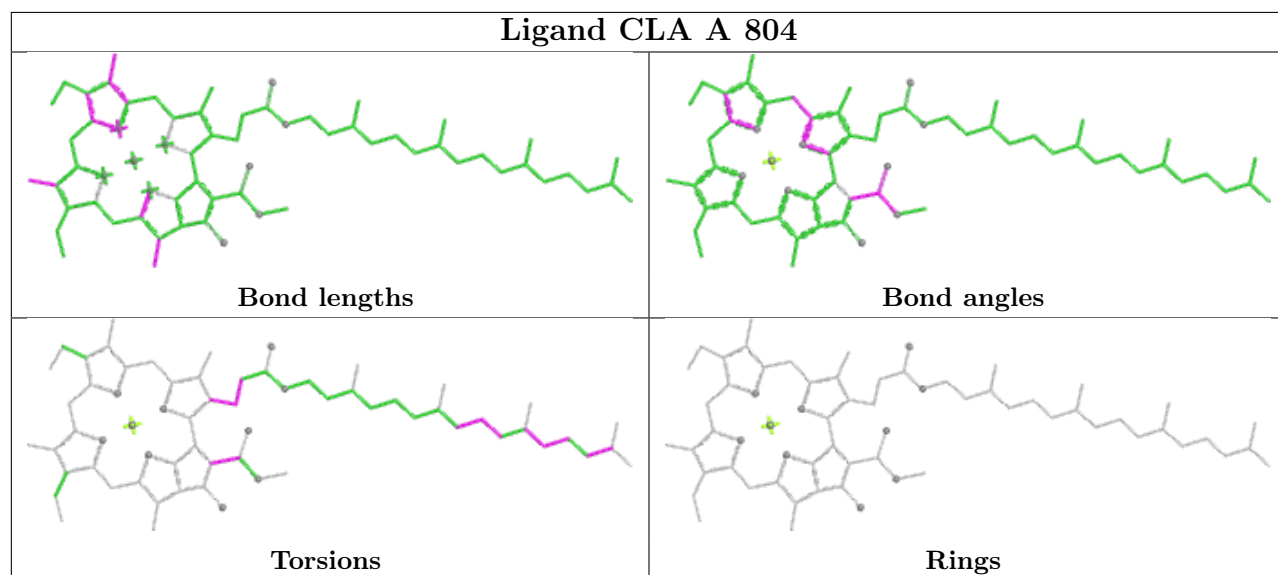
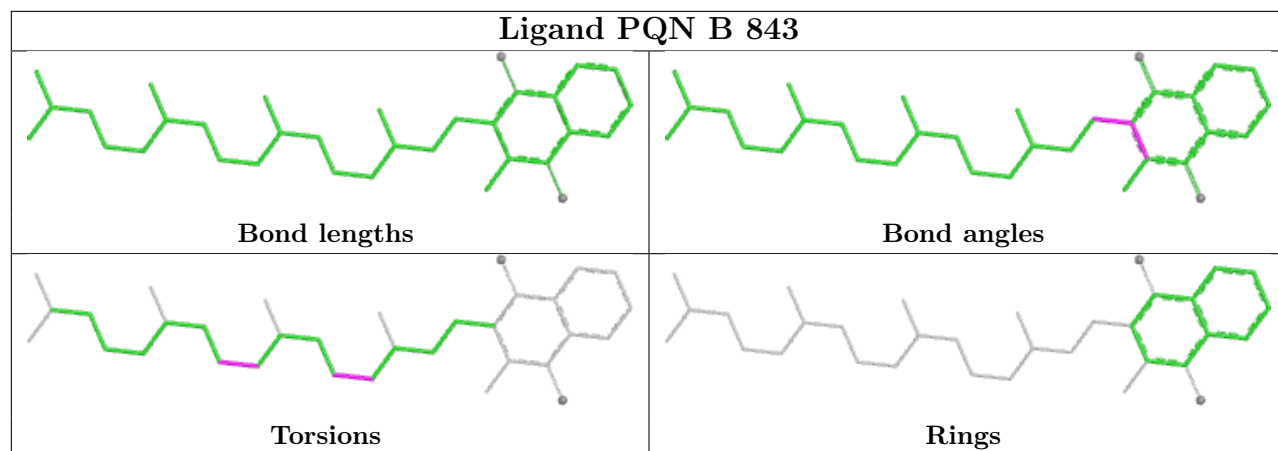


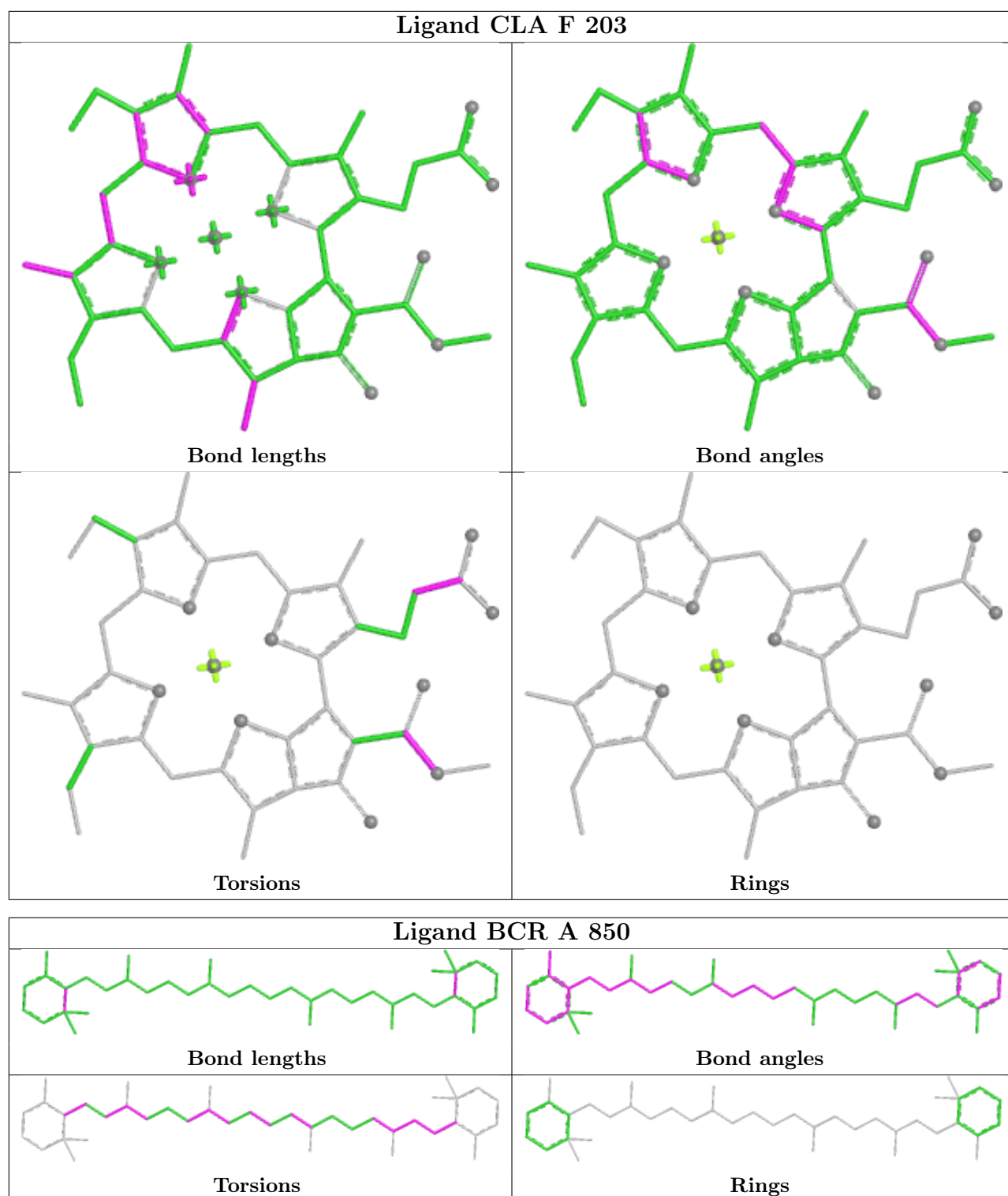


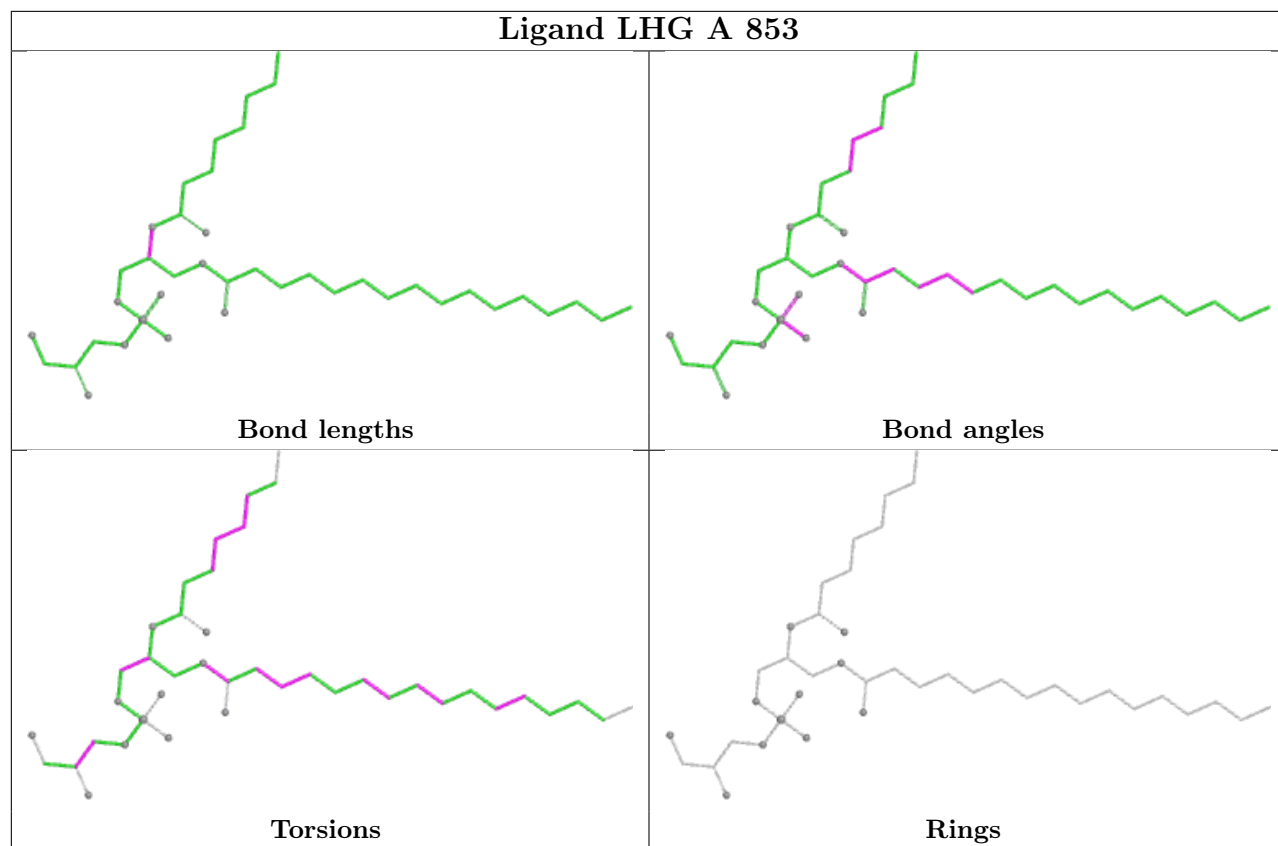


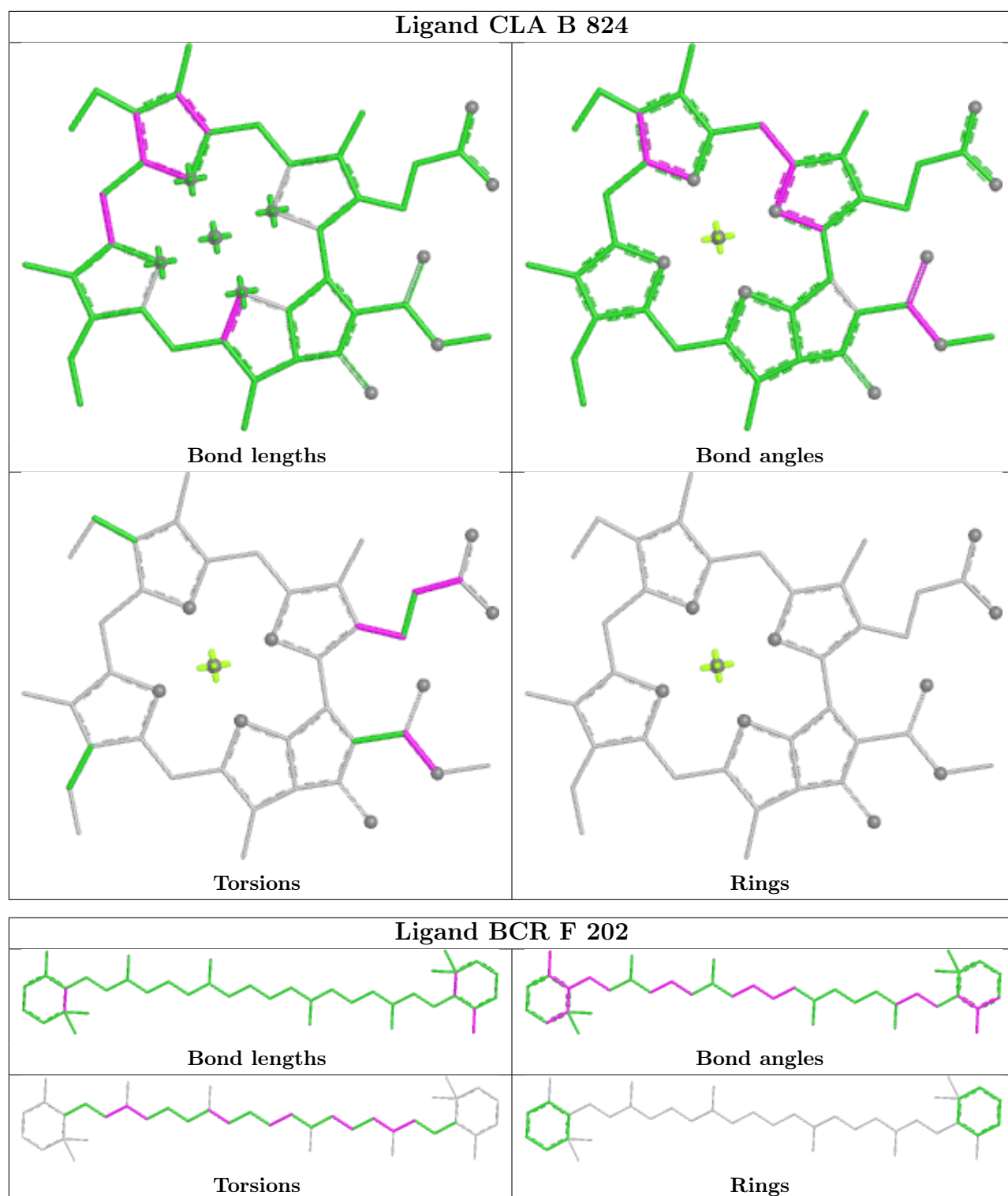


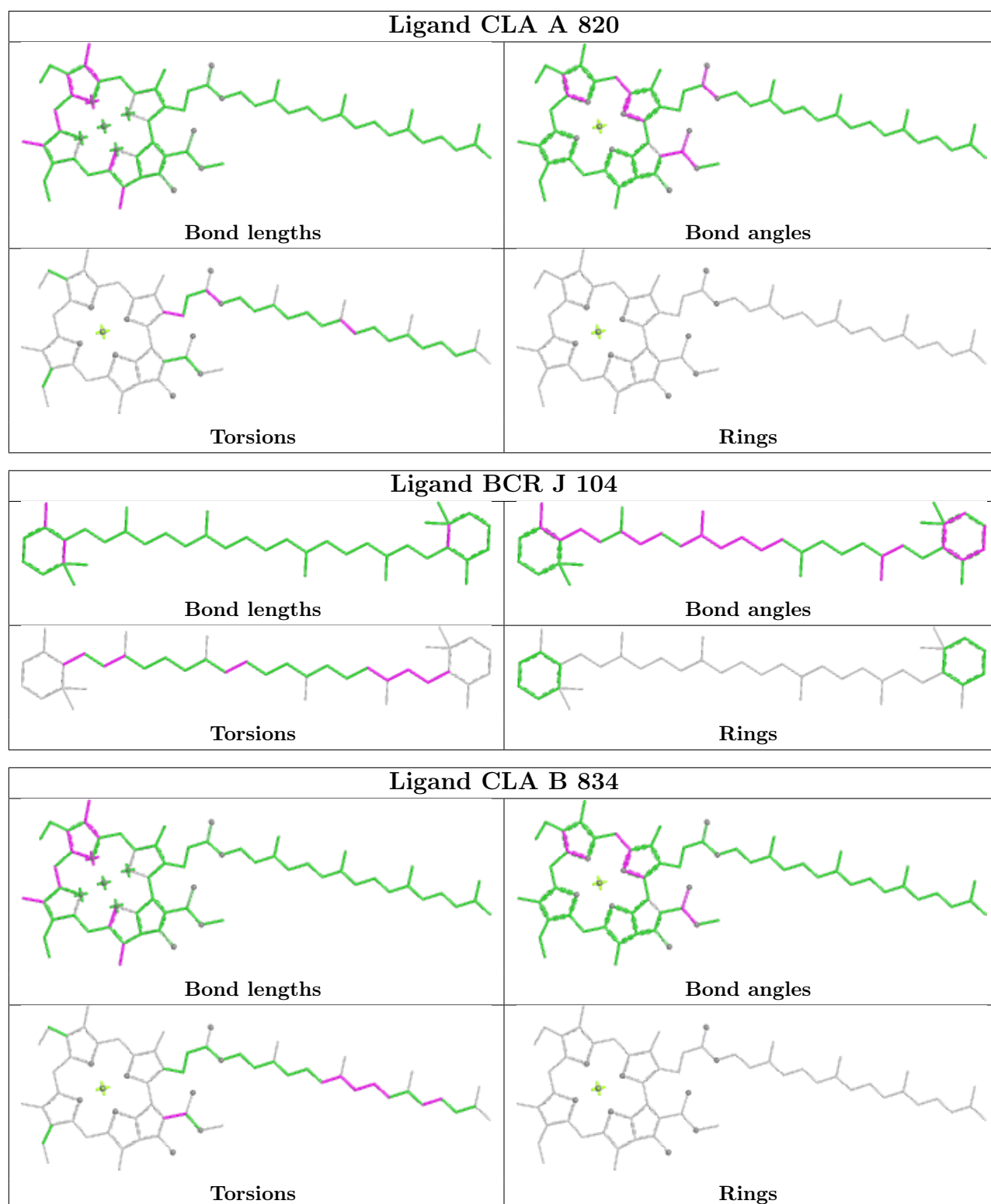


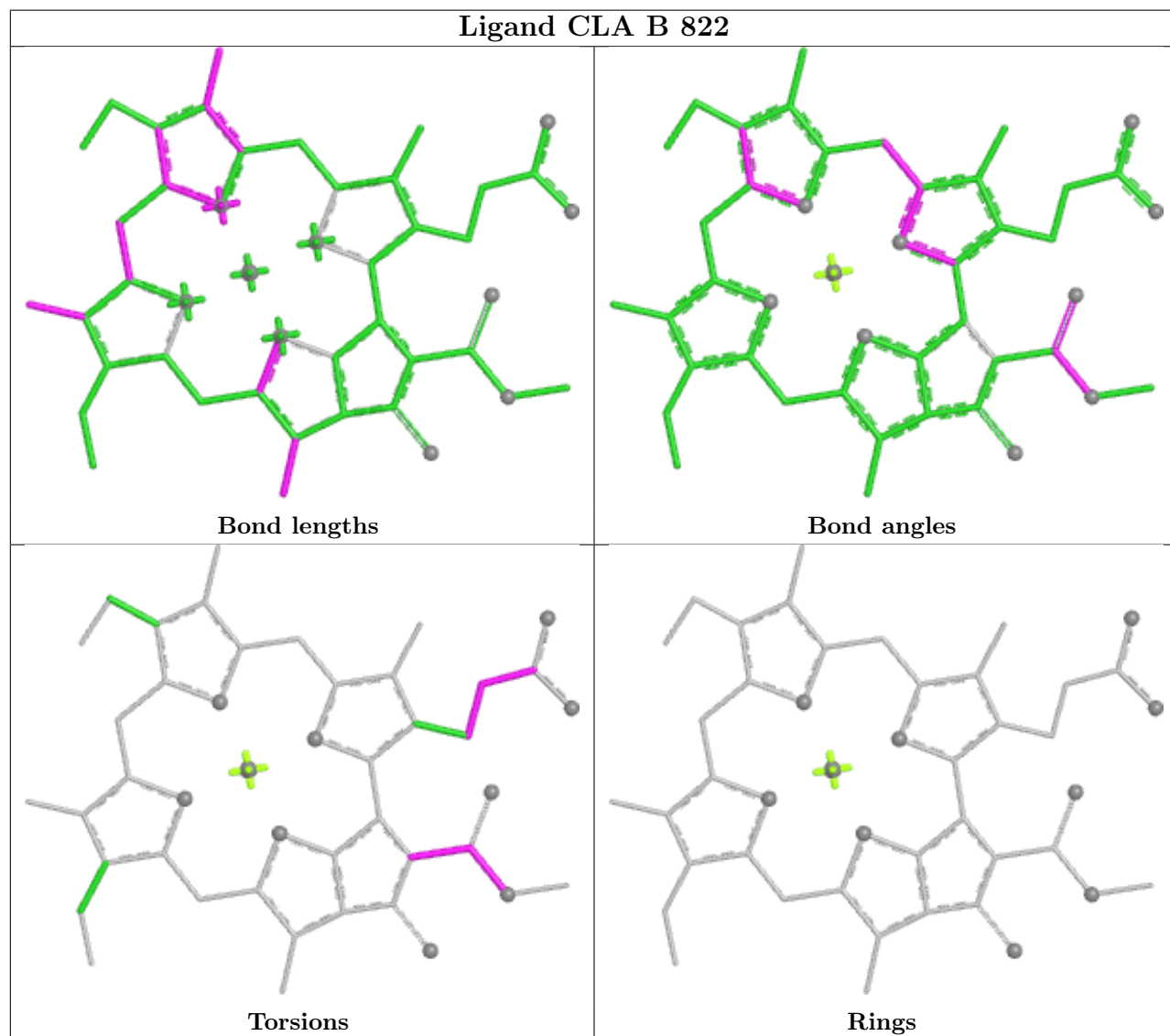
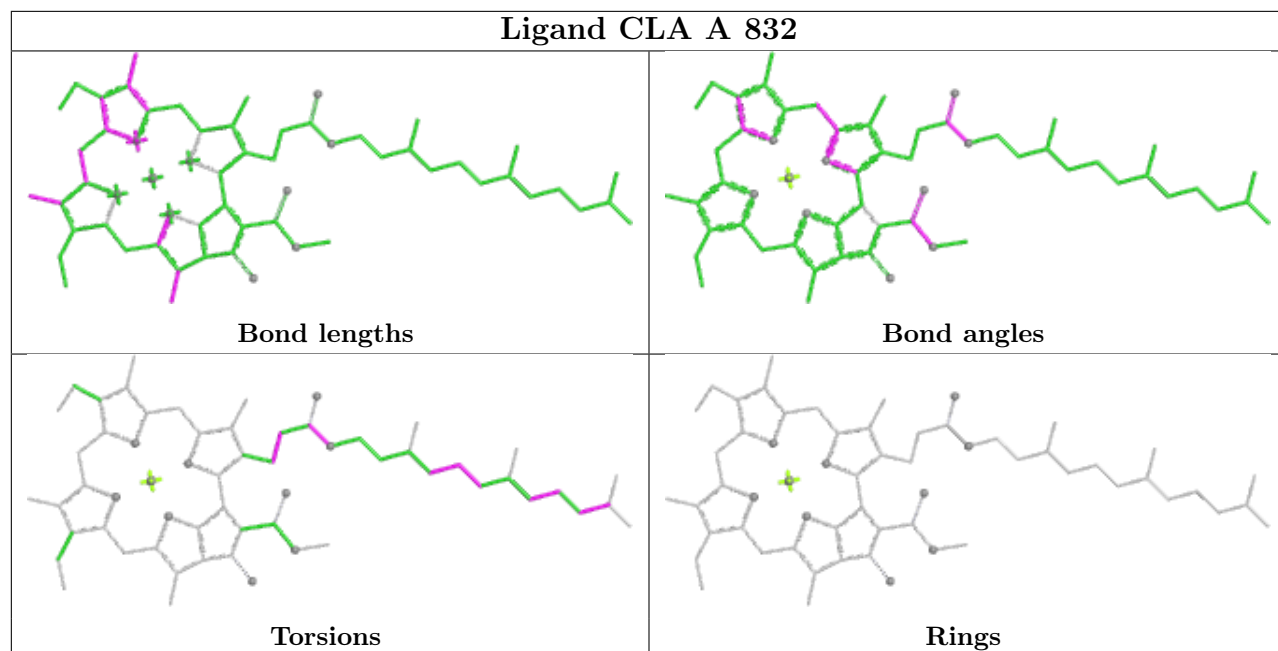


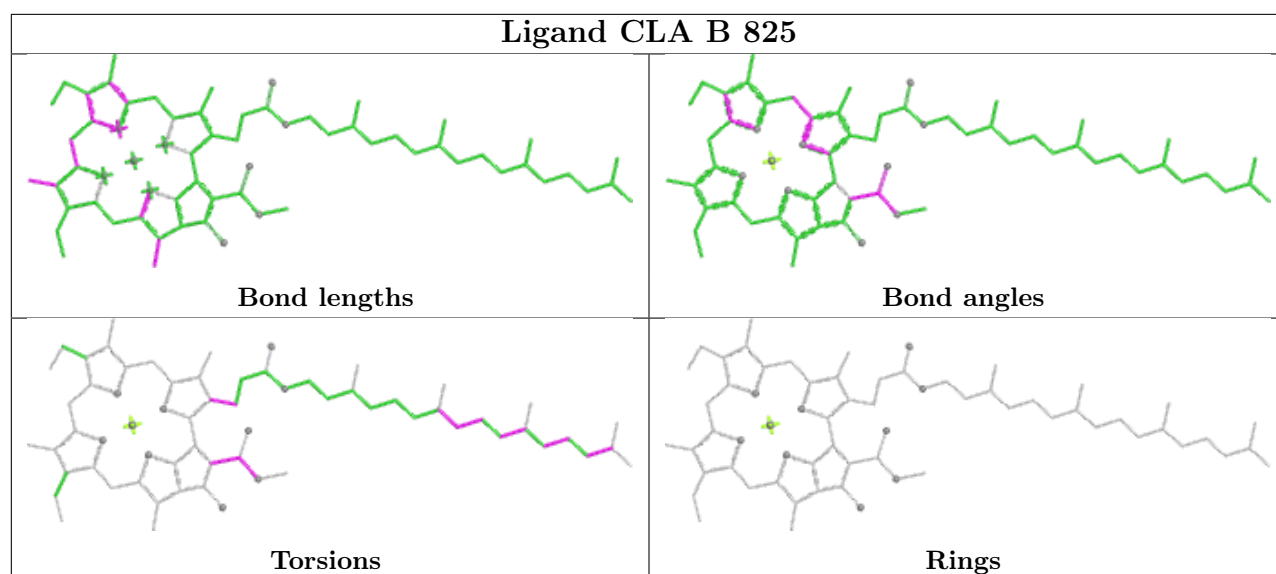
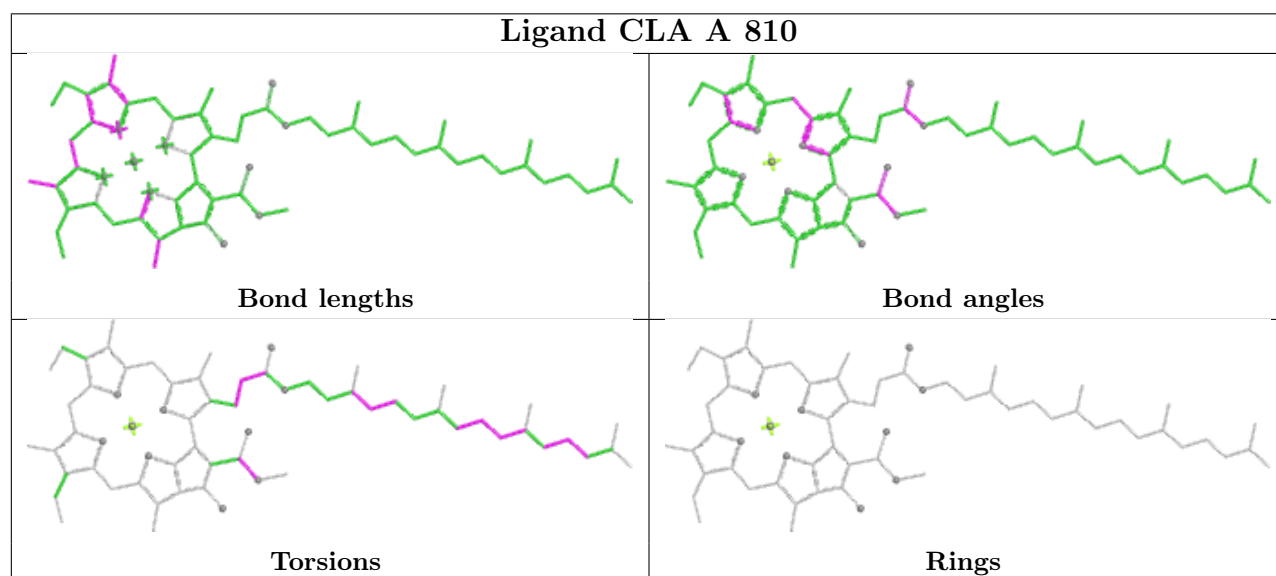
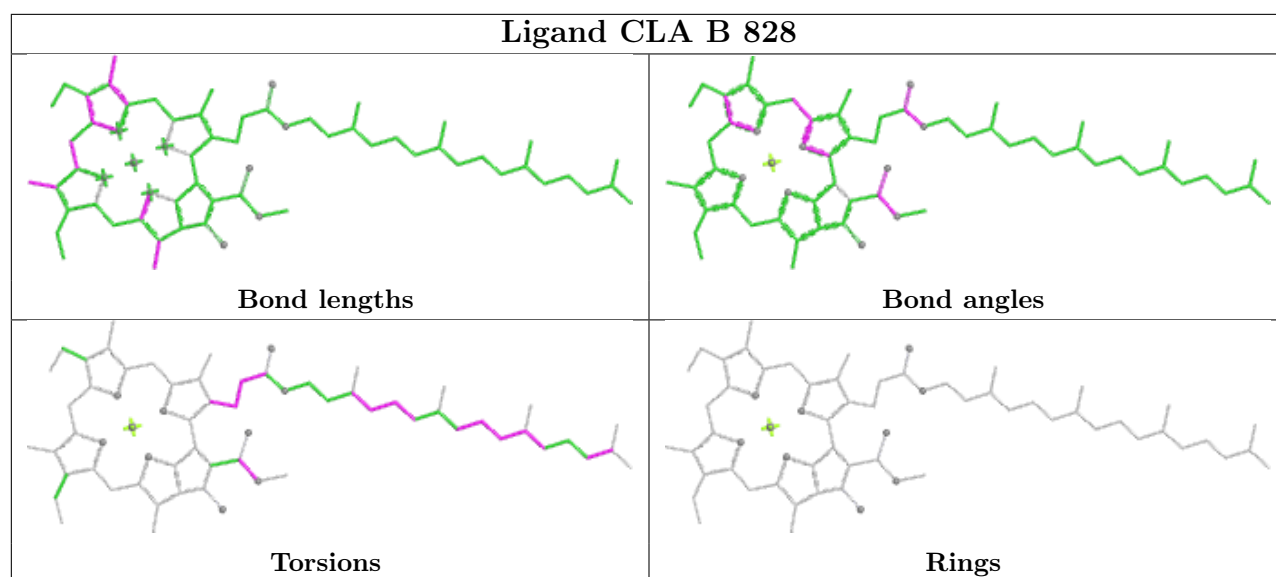


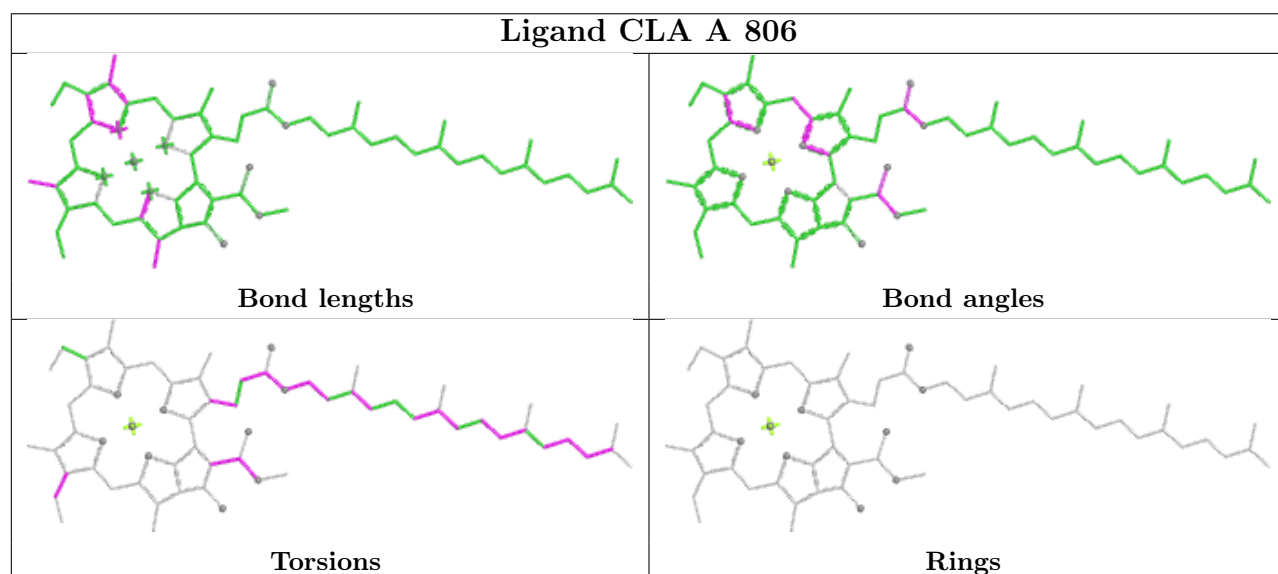
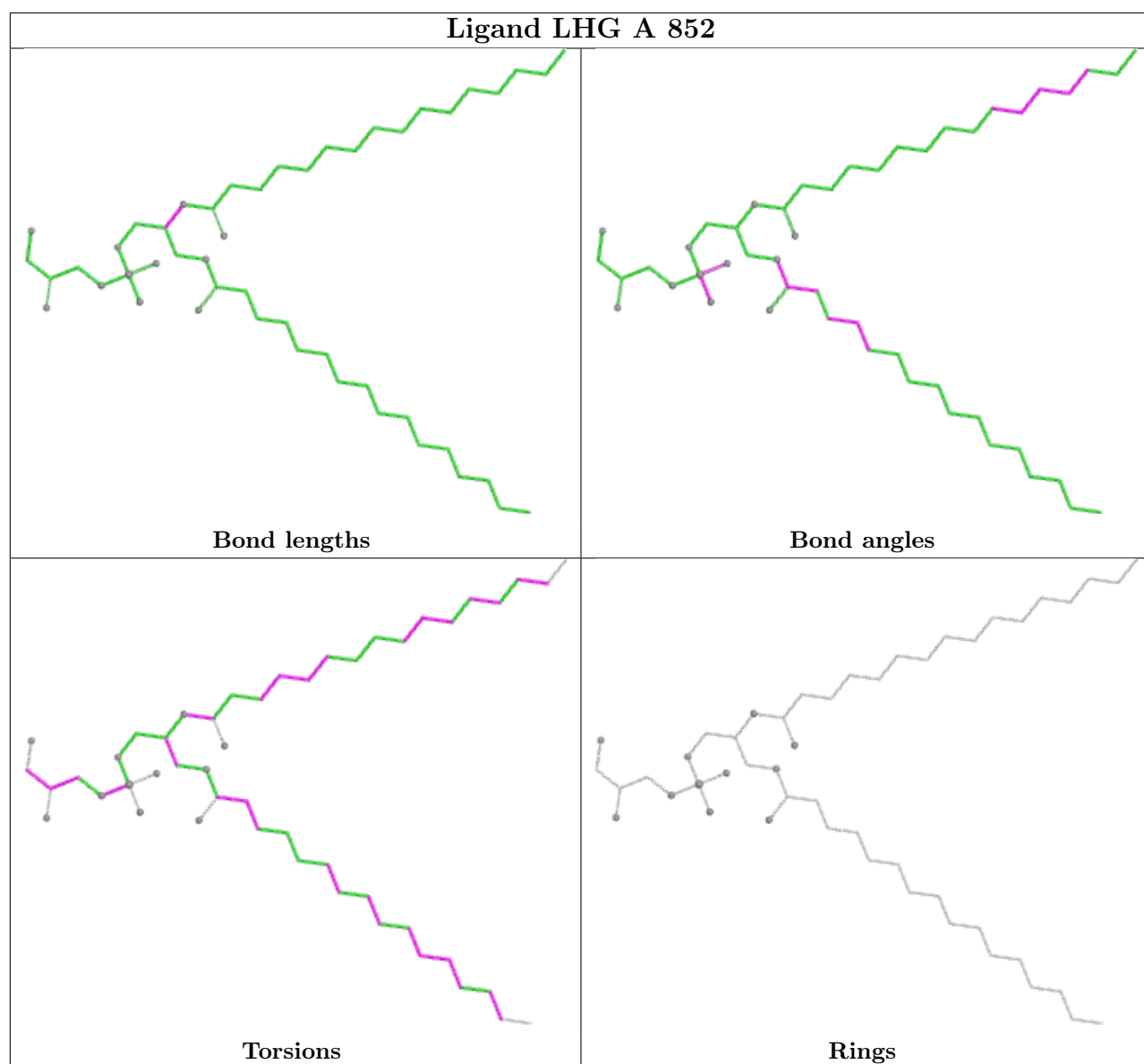


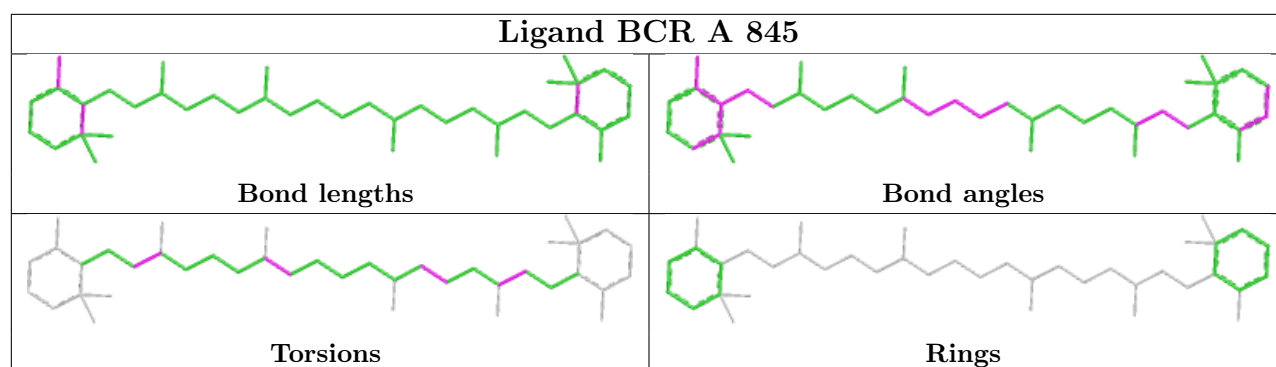
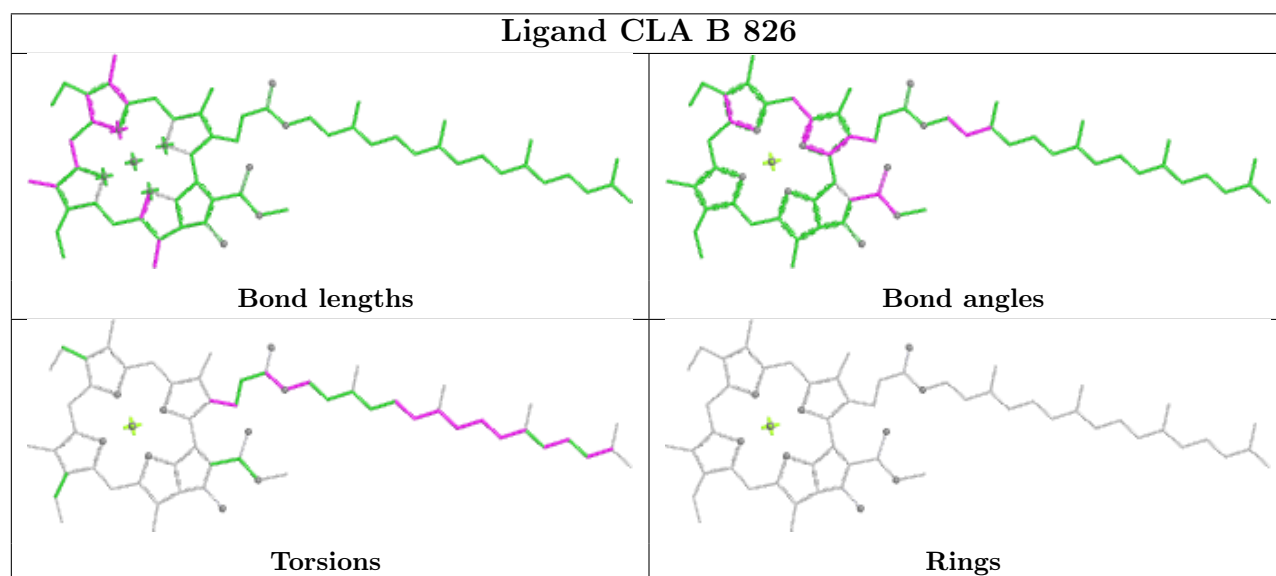
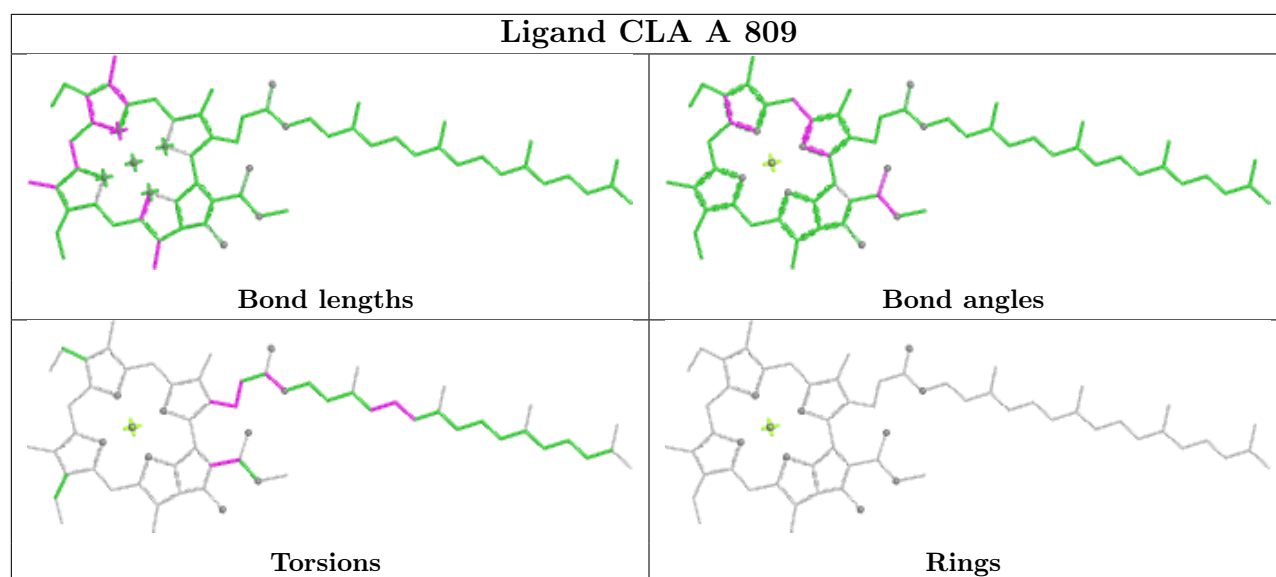


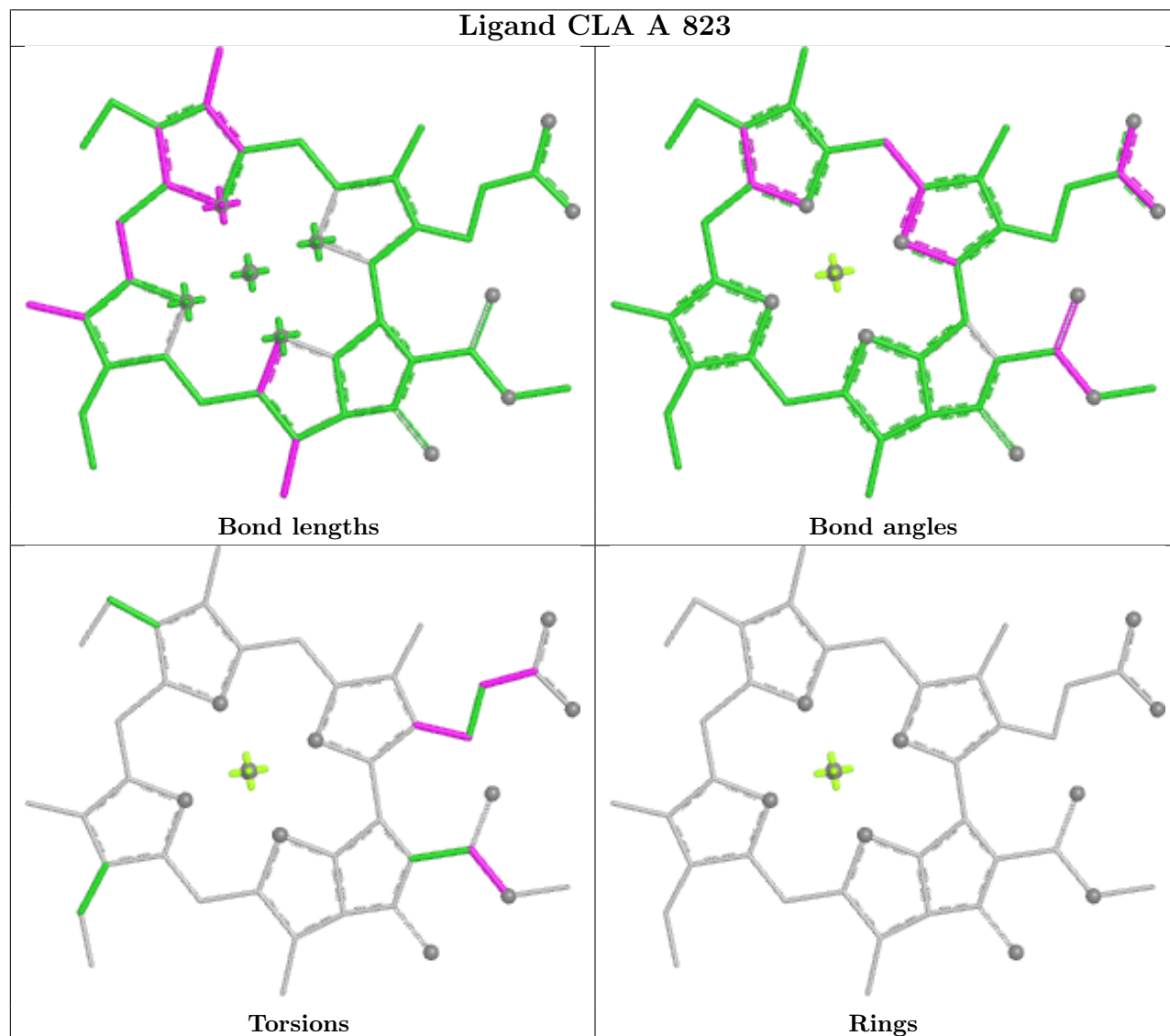
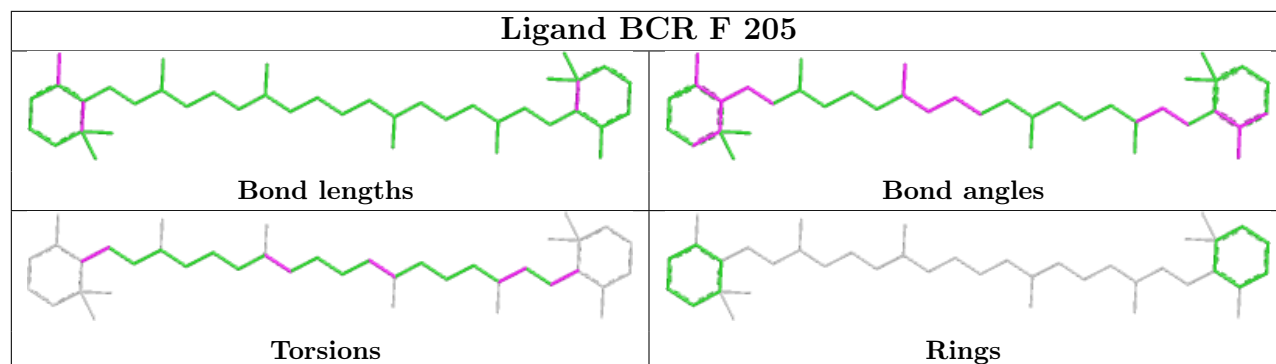


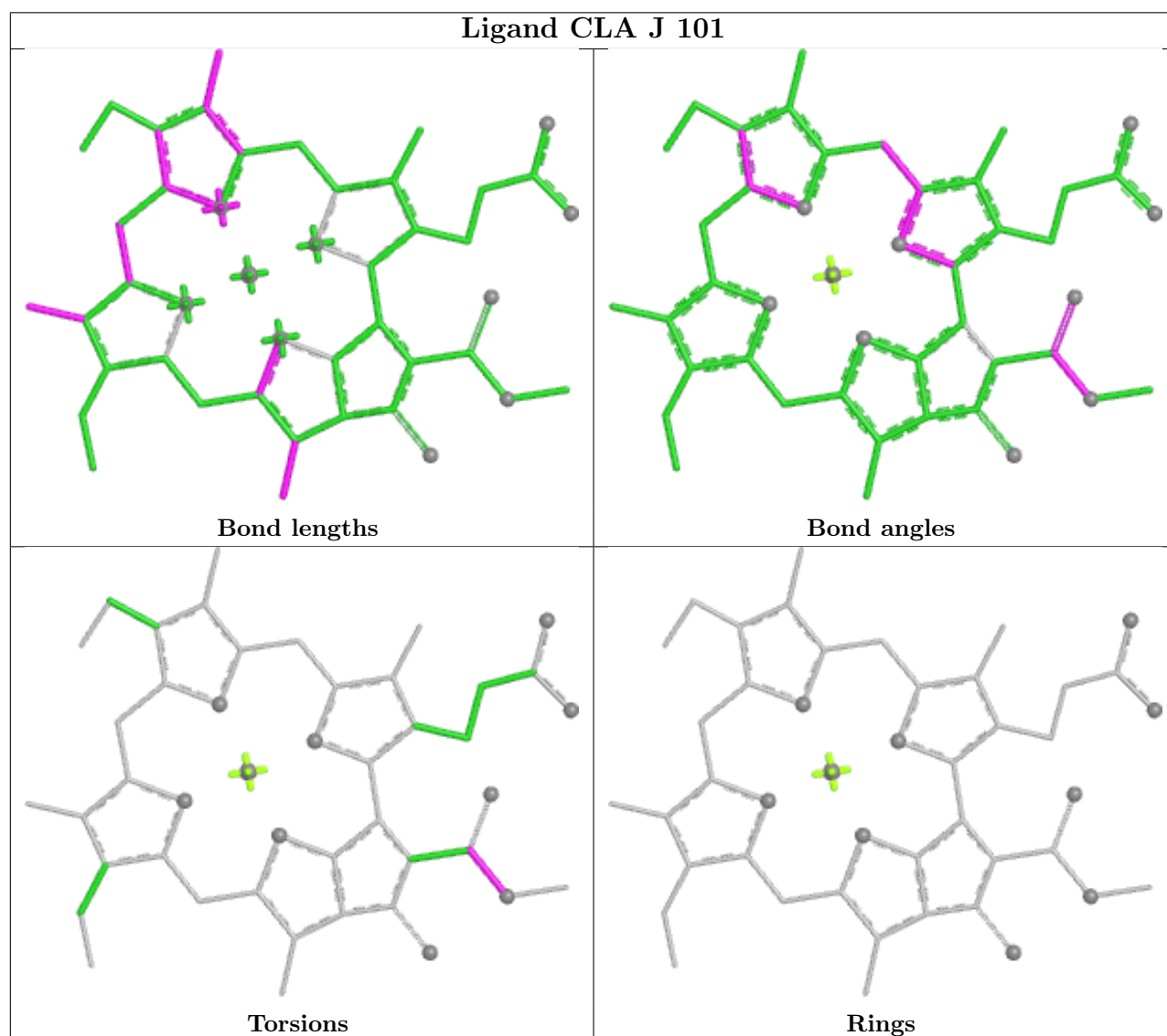
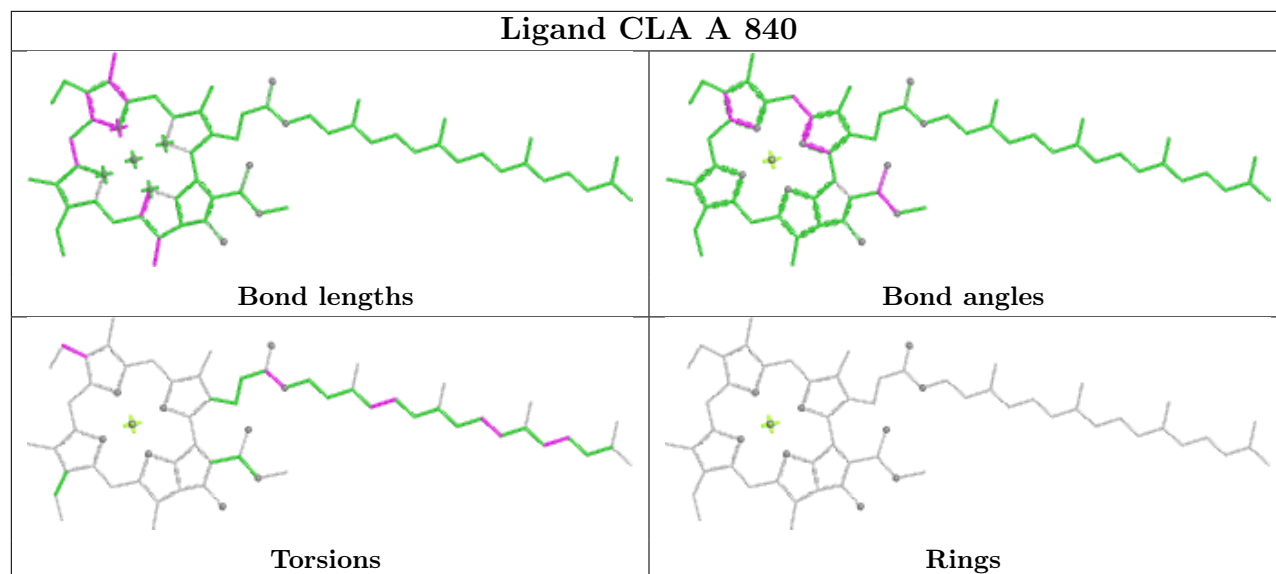


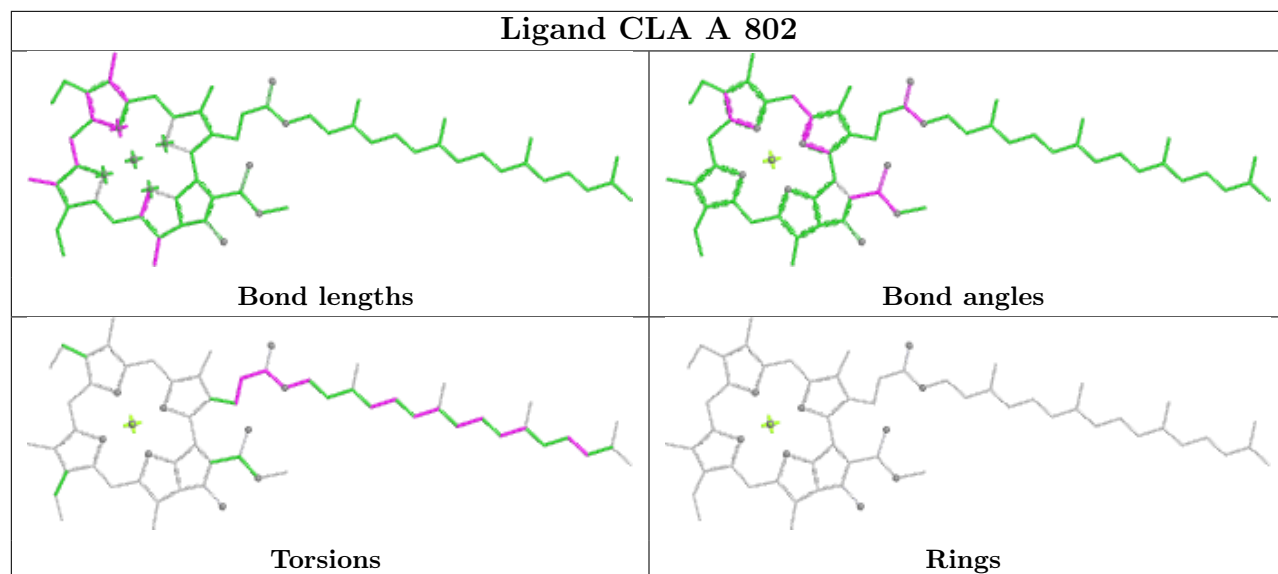


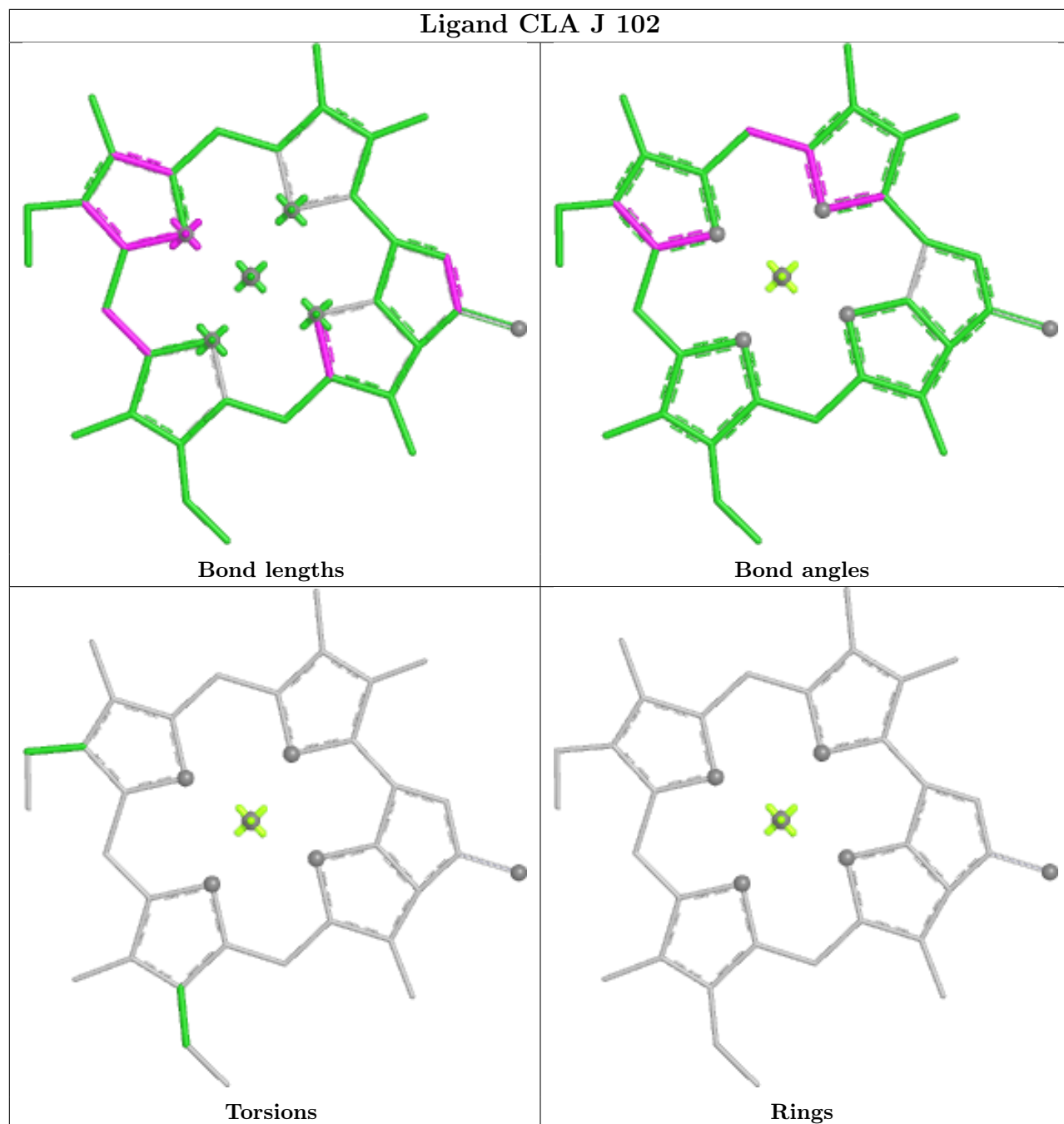


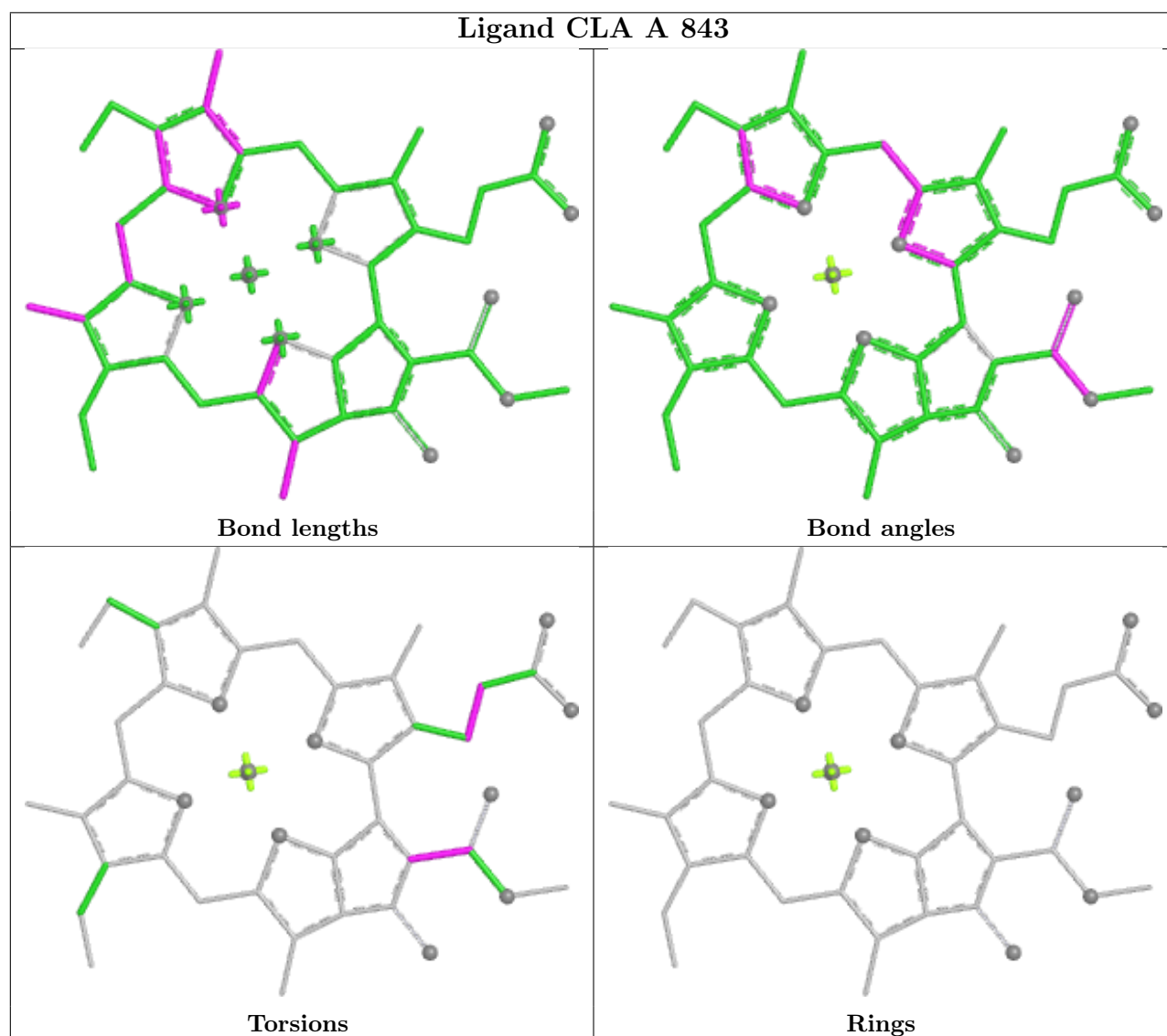
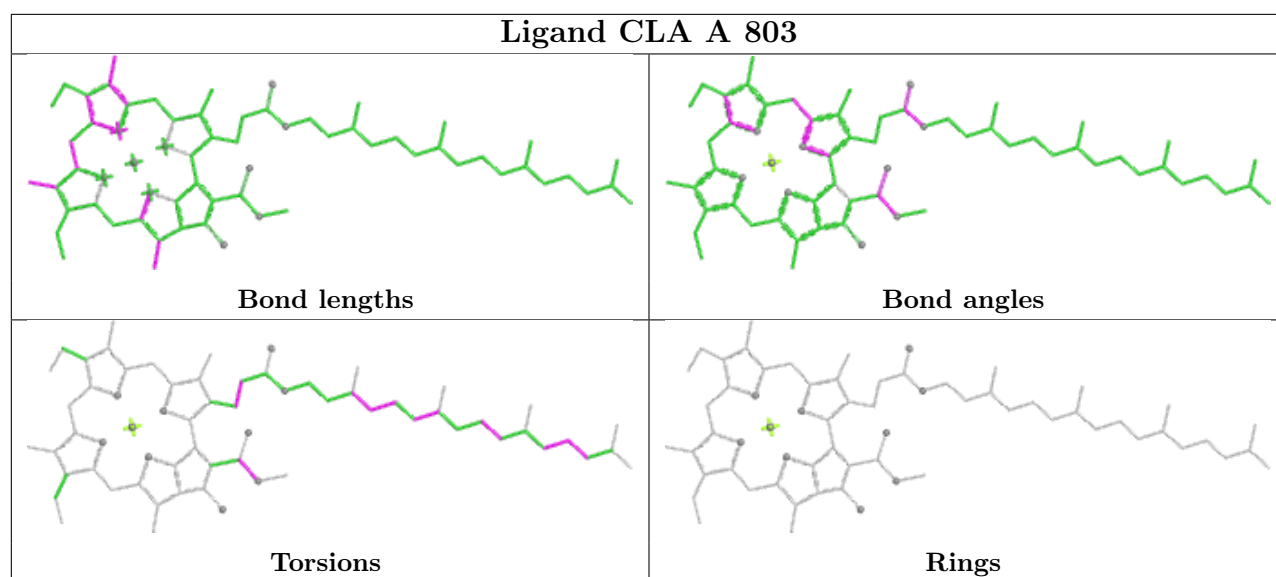


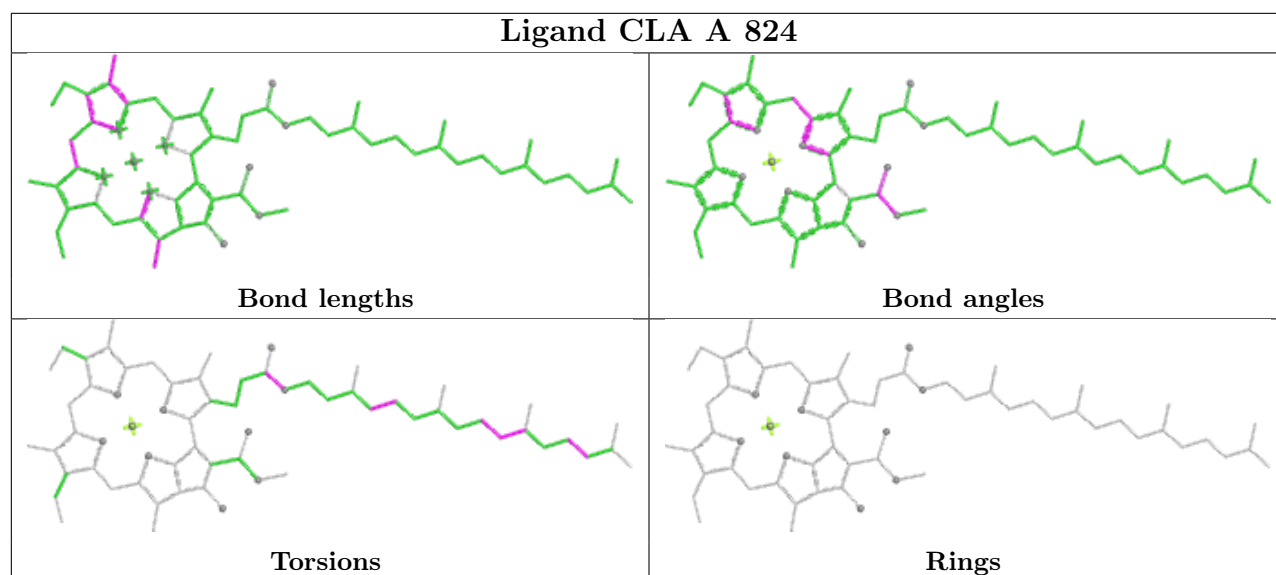
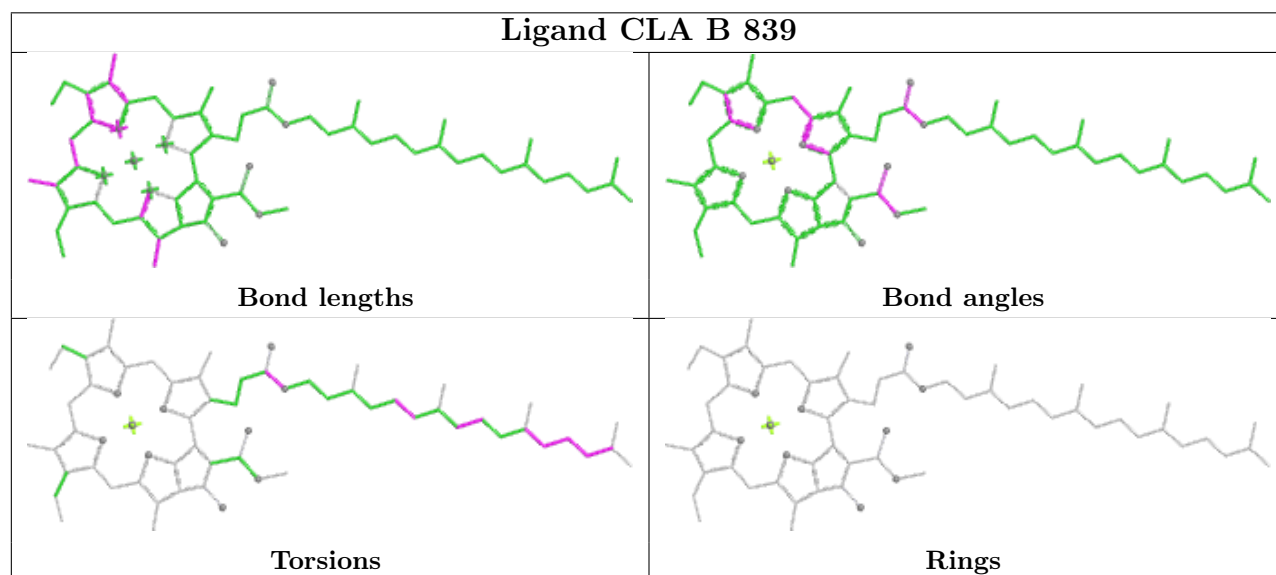
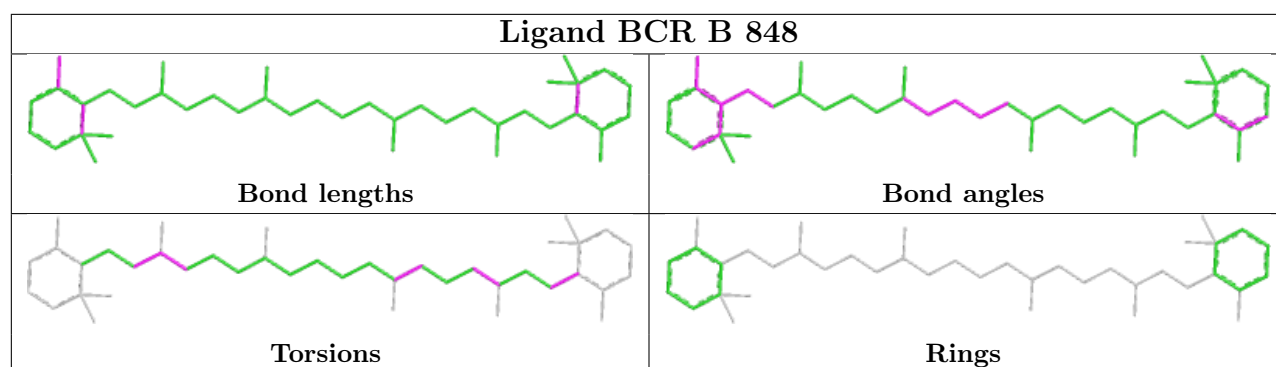


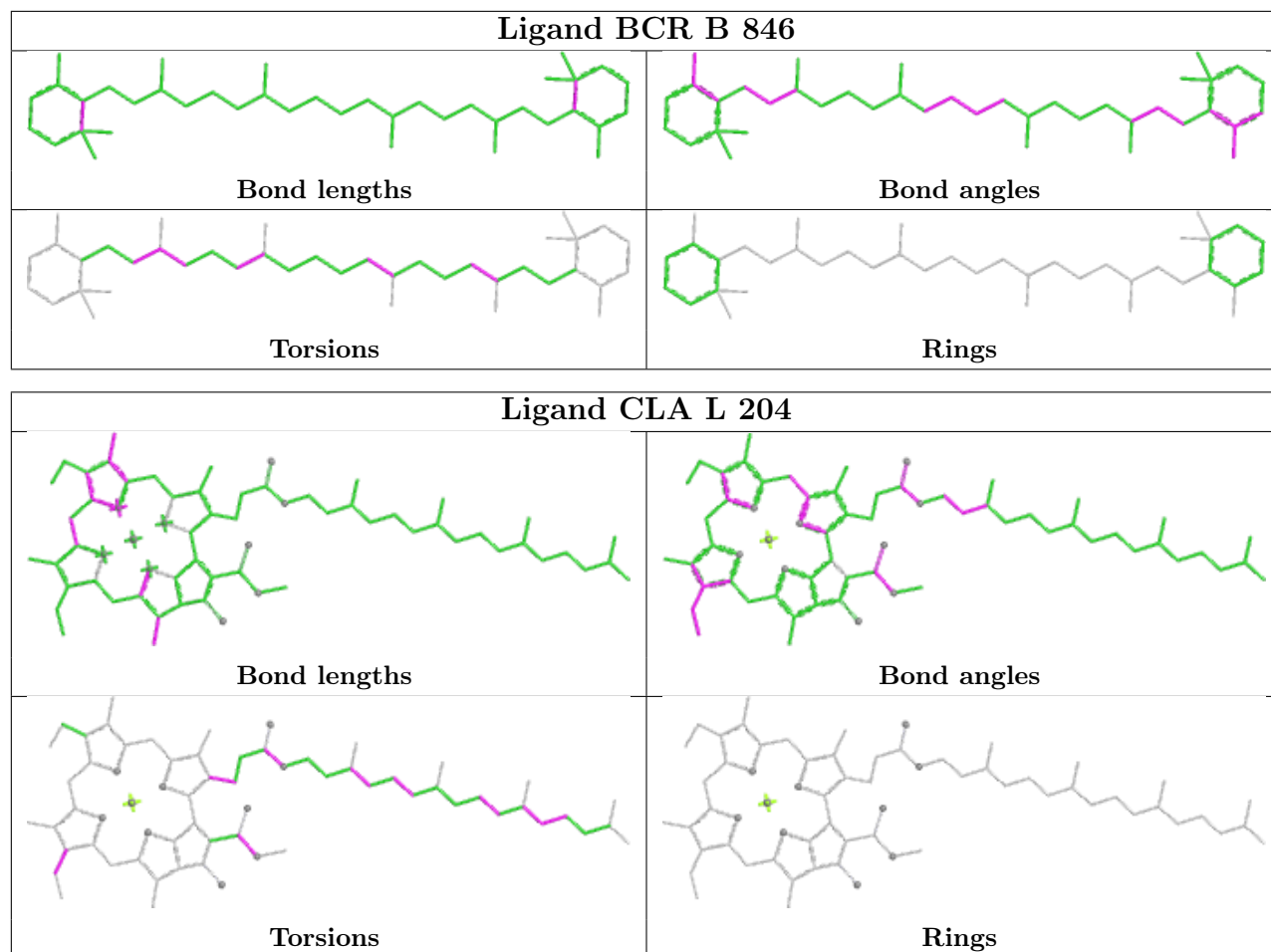


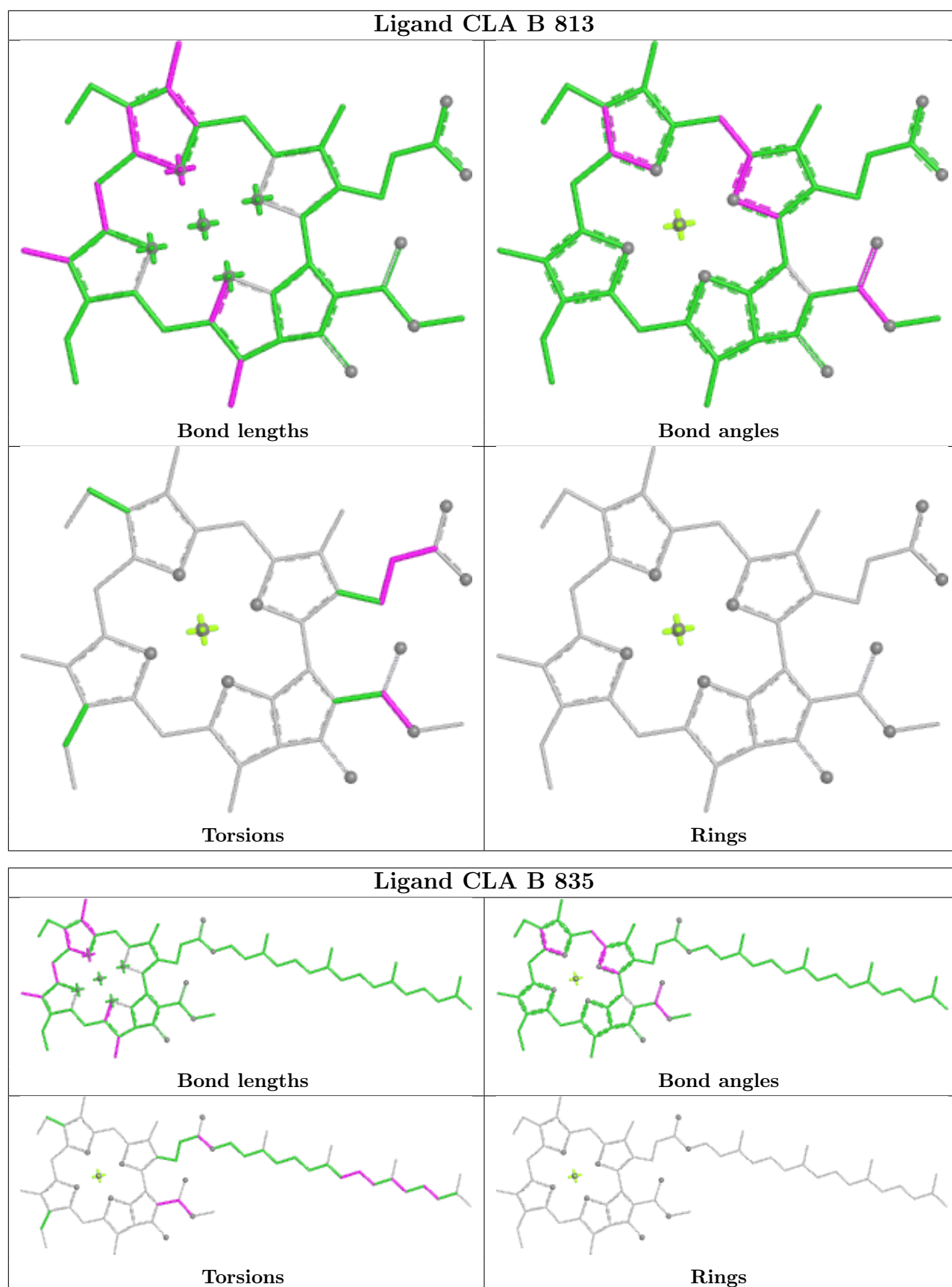


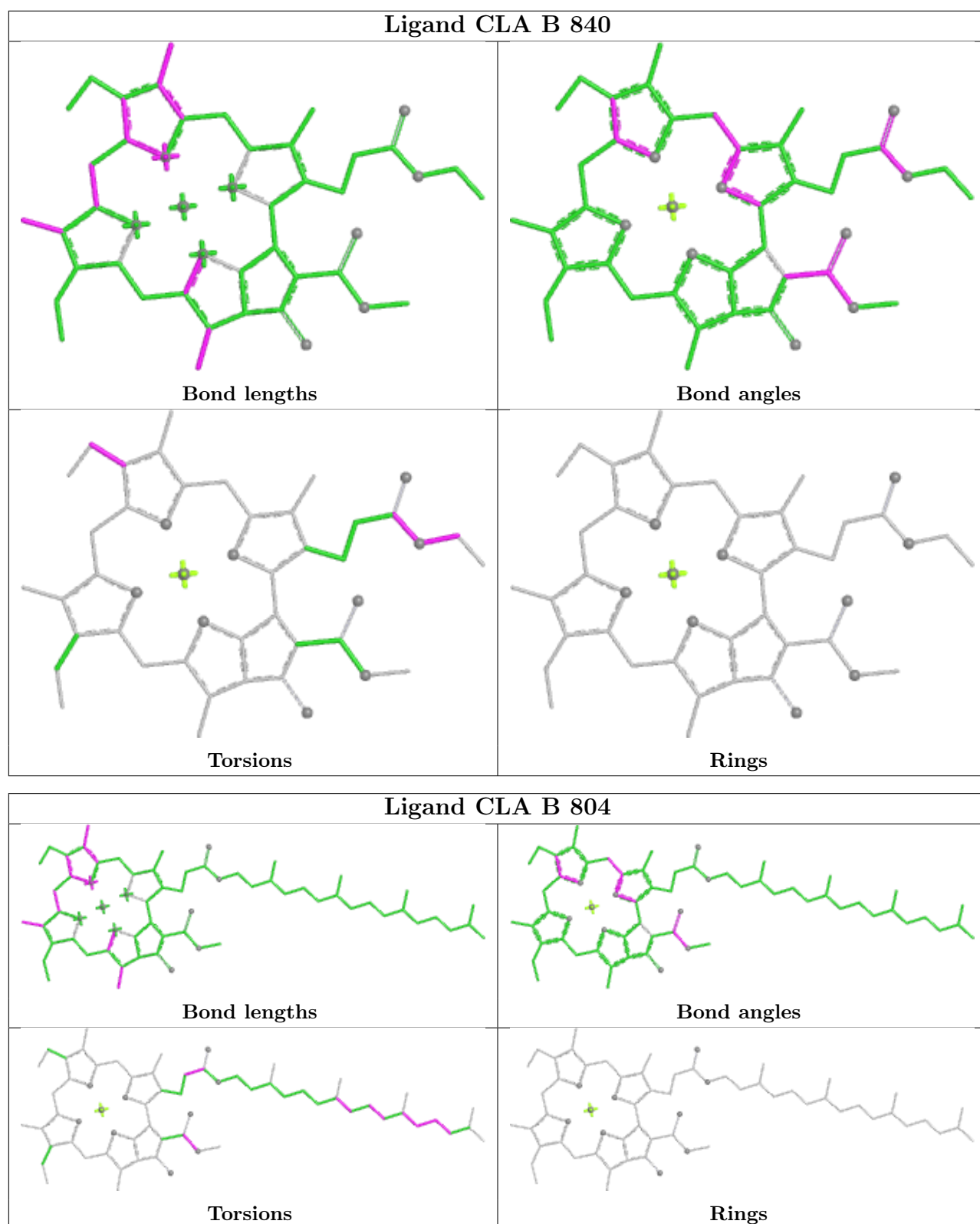


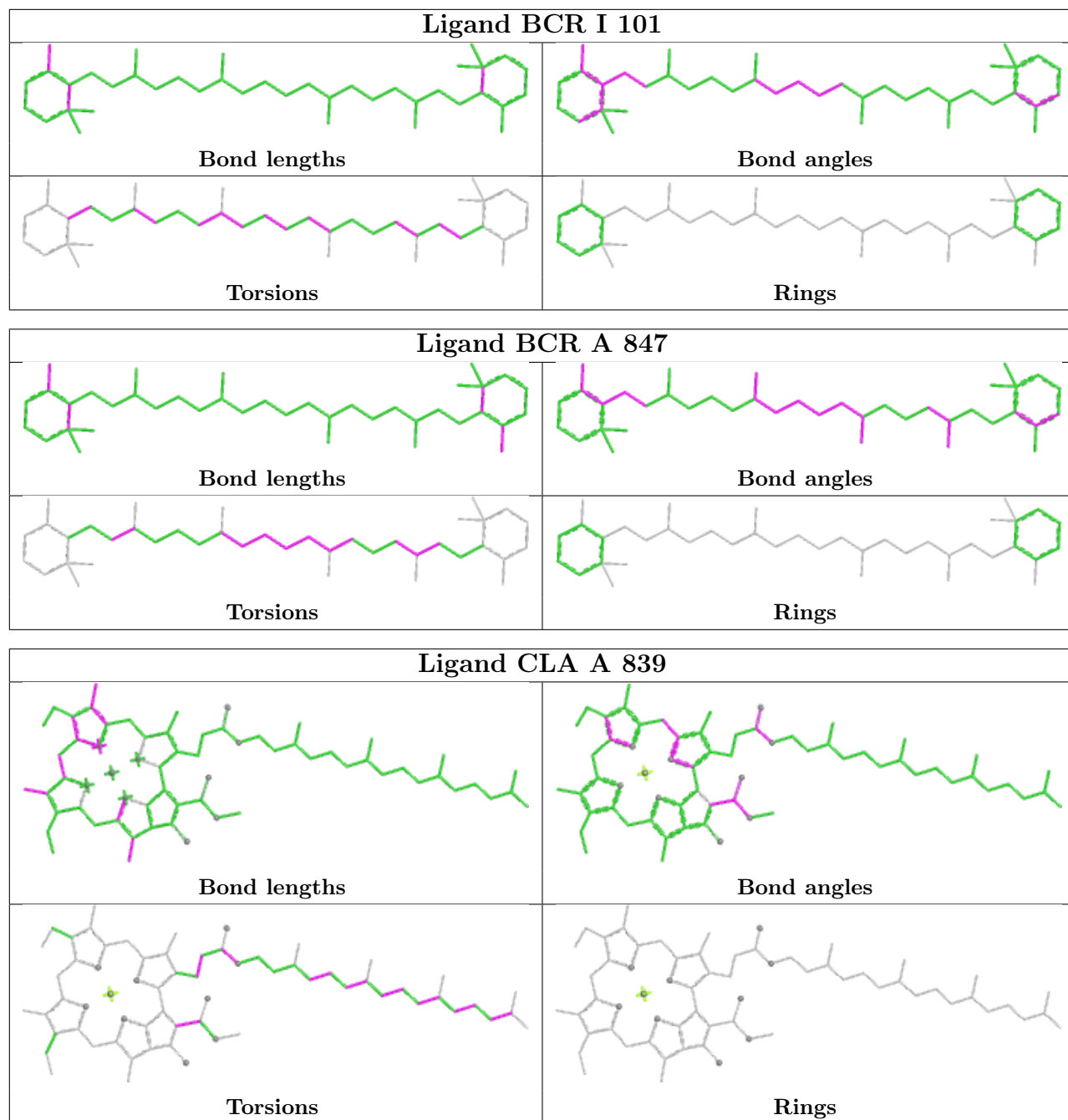


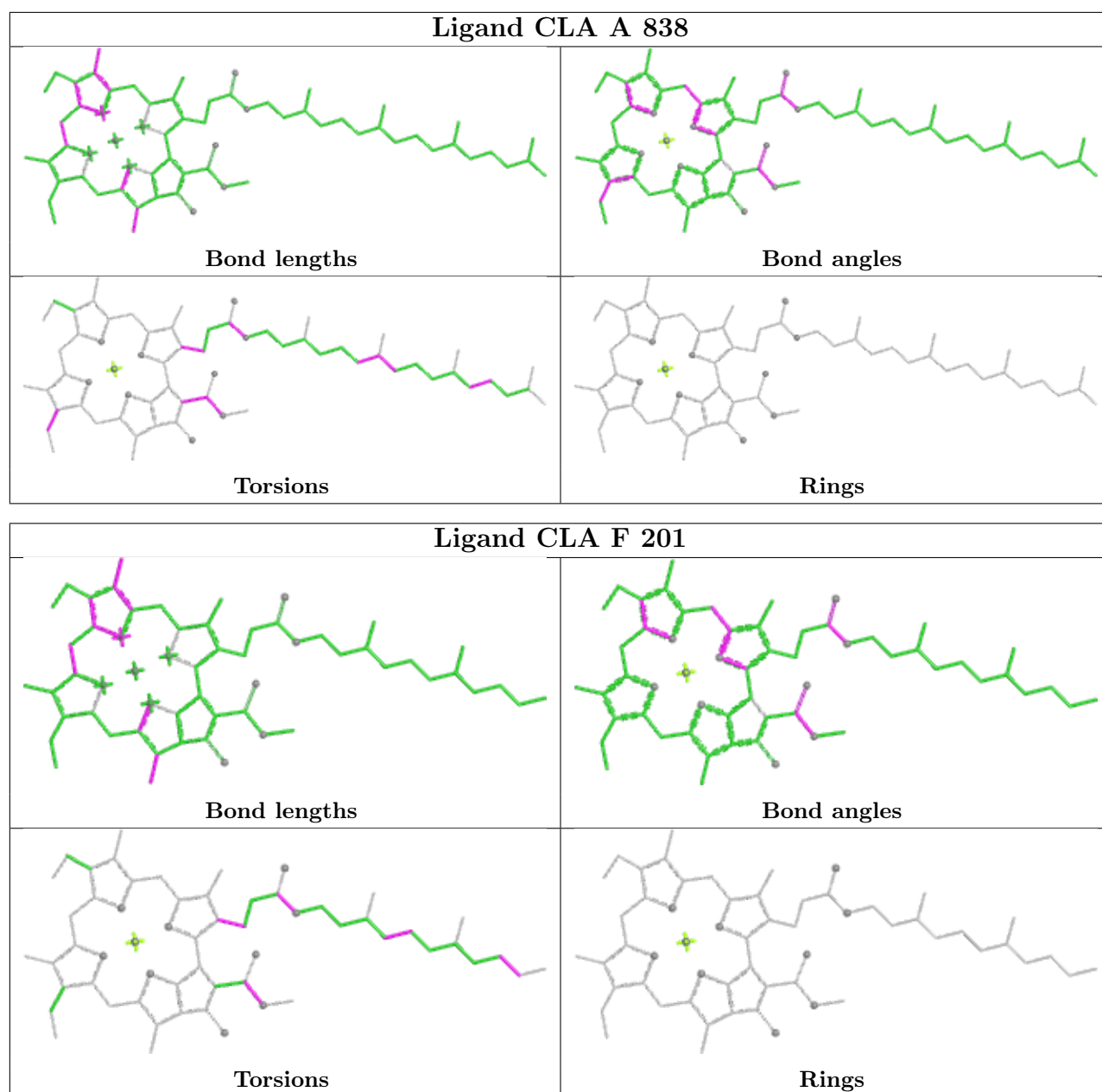


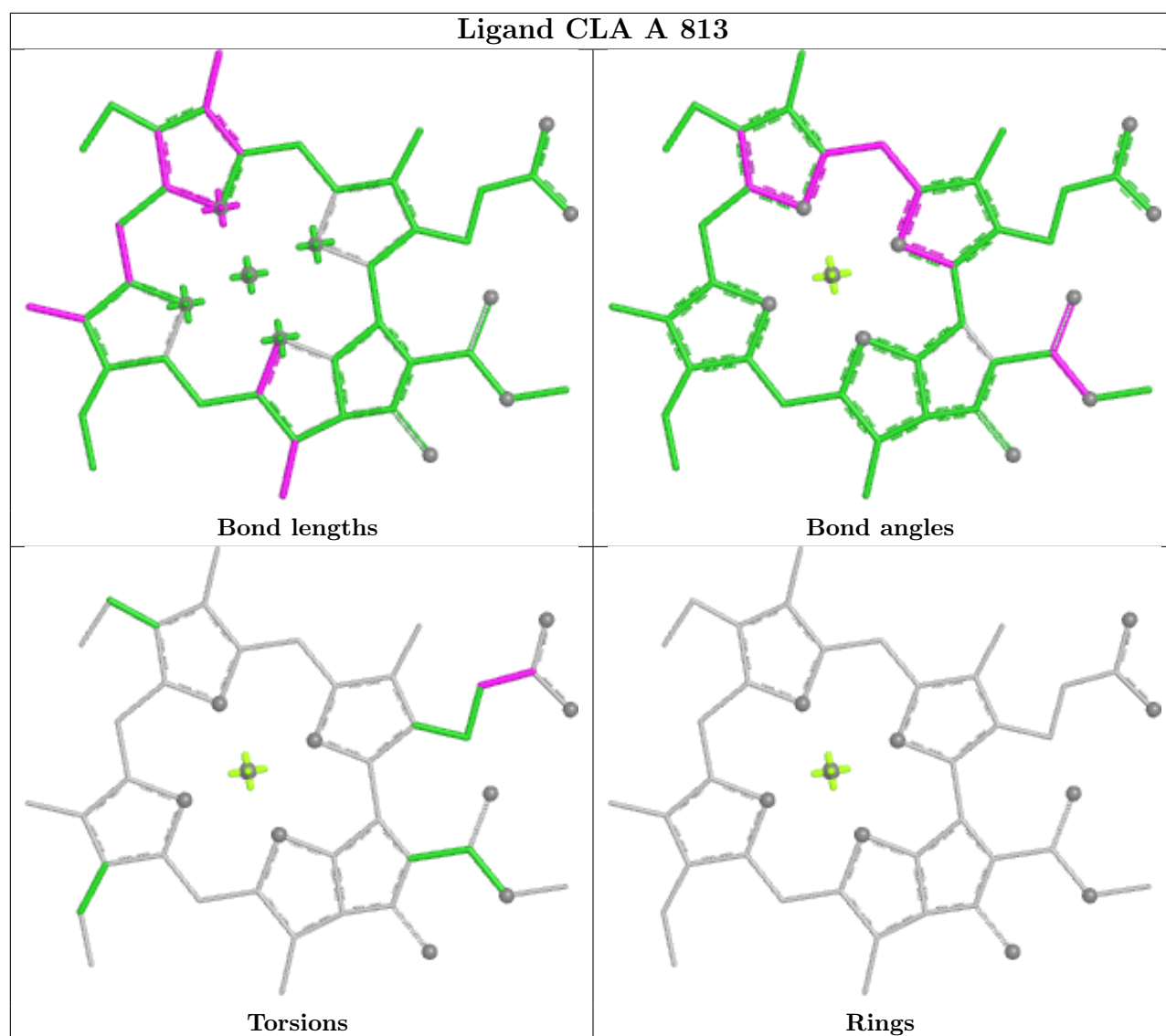












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

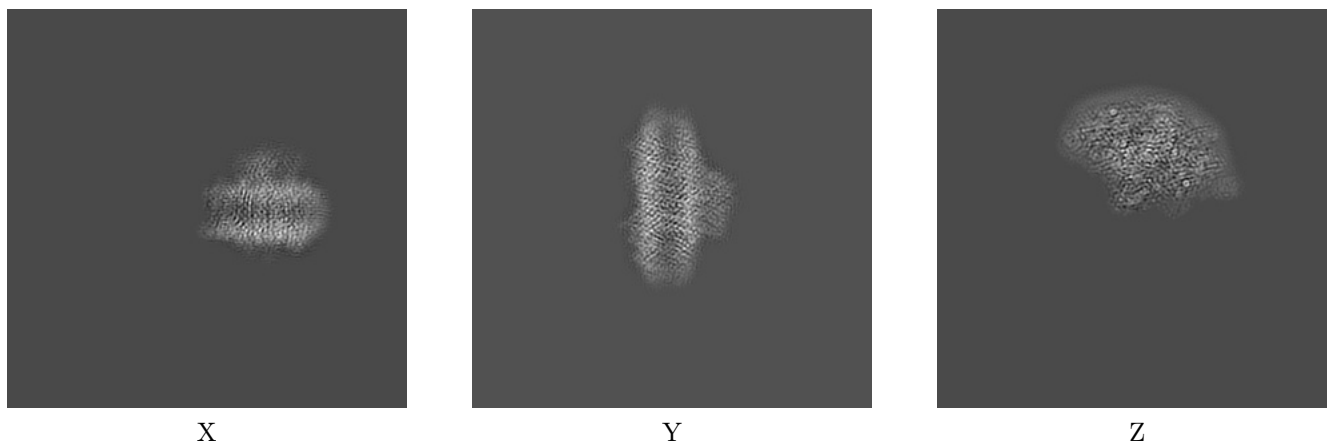
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10557. 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](#)

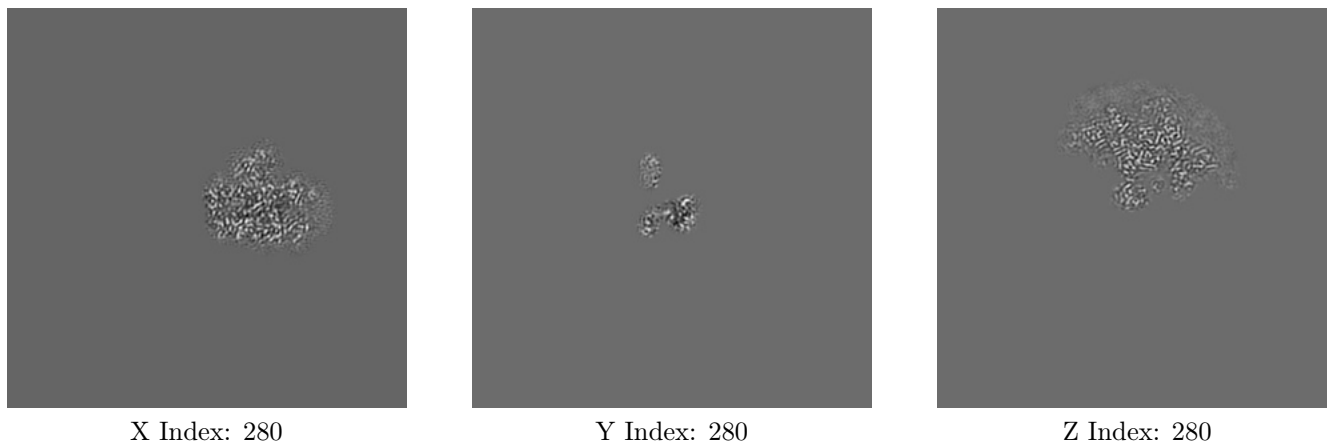
6.1.1 Primary map



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

6.2 Central slices [i](#)

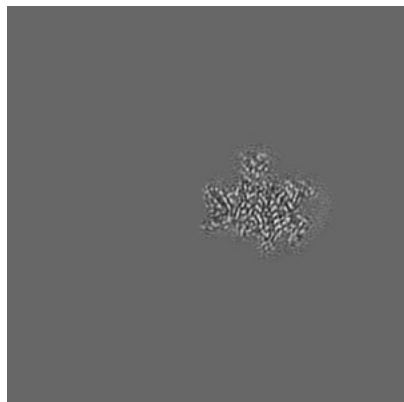
6.2.1 Primary map



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

6.3 Largest variance slices [i](#)

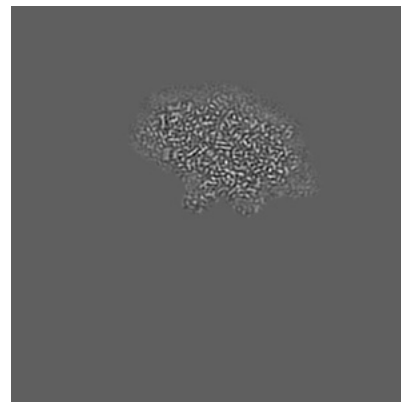
6.3.1 Primary map



X Index: 265



Y Index: 354

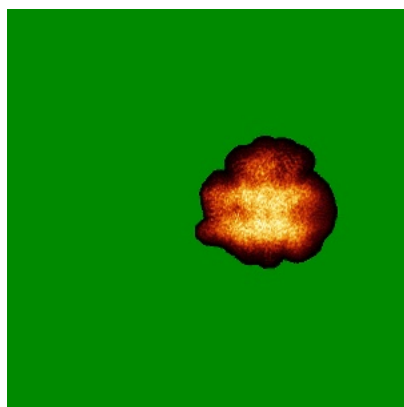


Z Index: 251

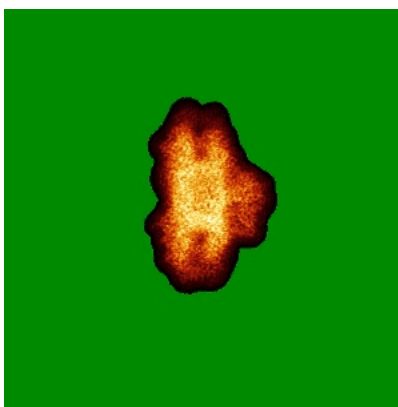
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



Y

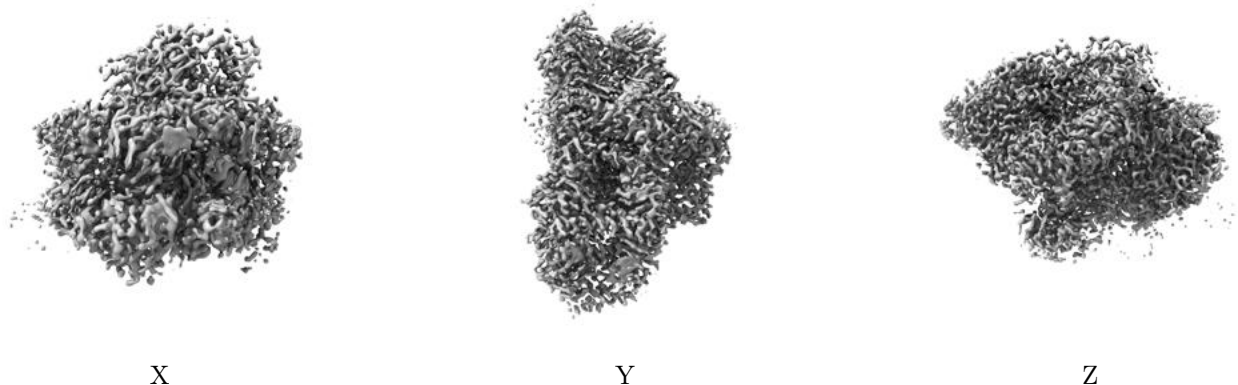


Z

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 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

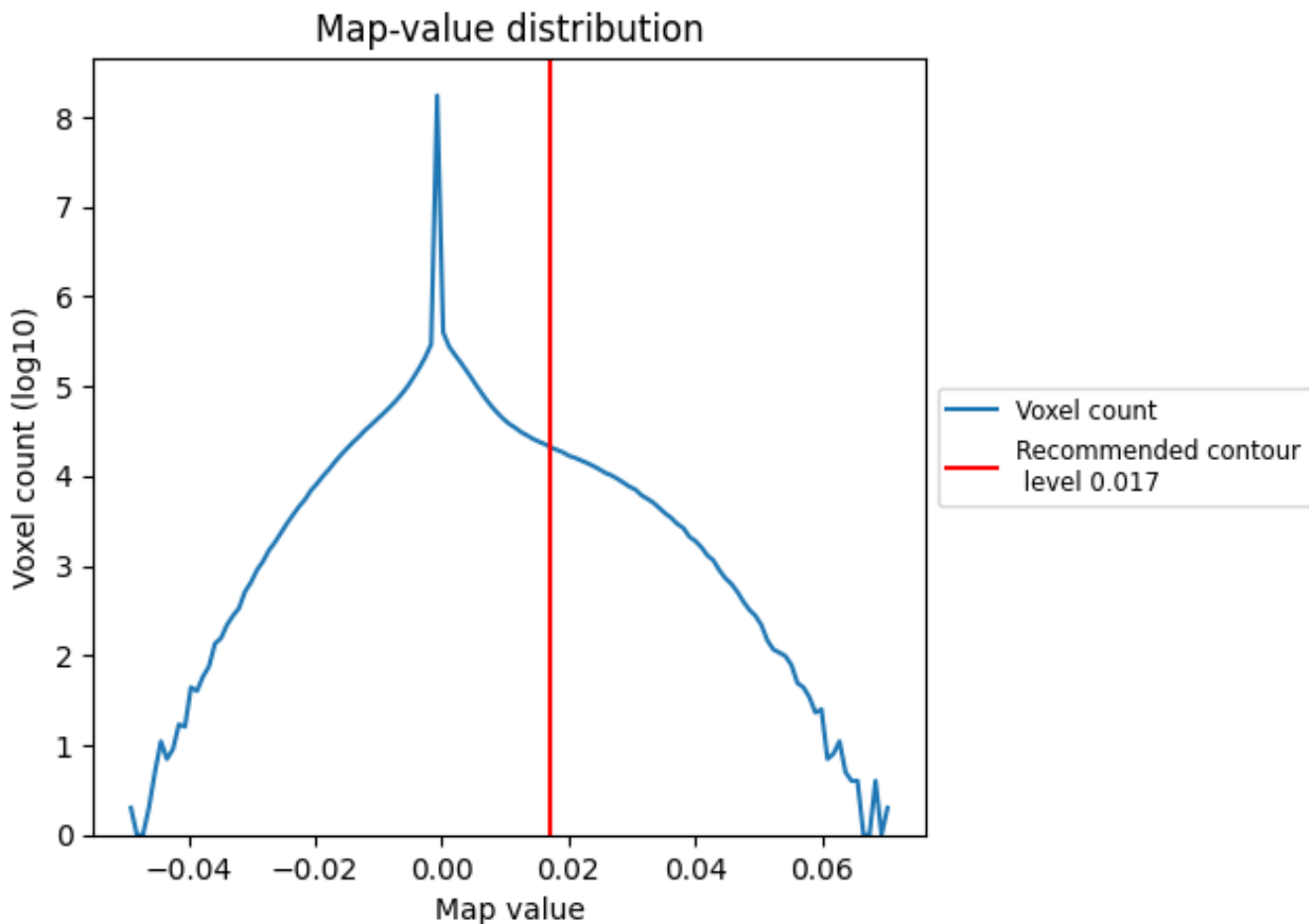
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

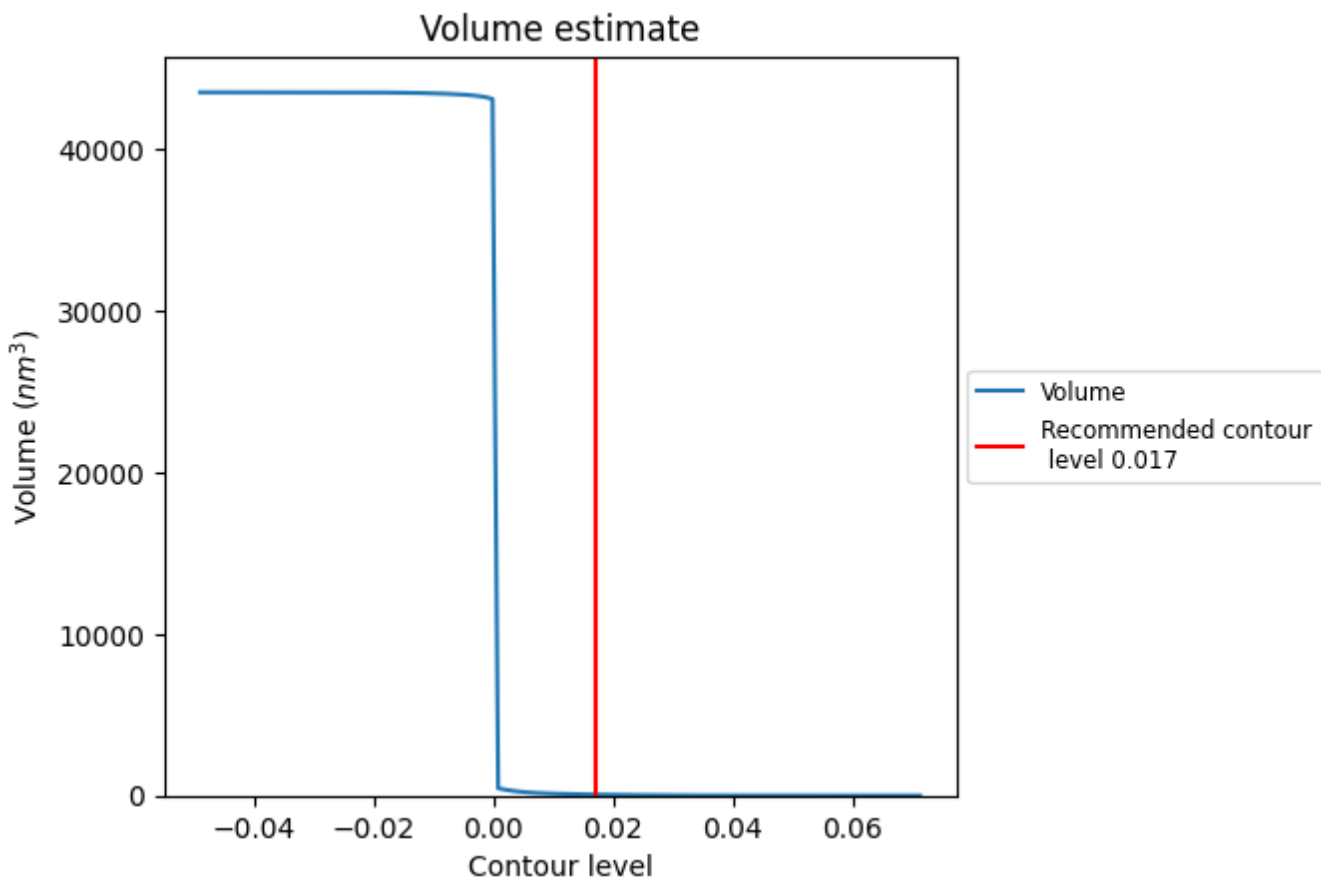
This section contains the results of statistical analysis of the map.

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.

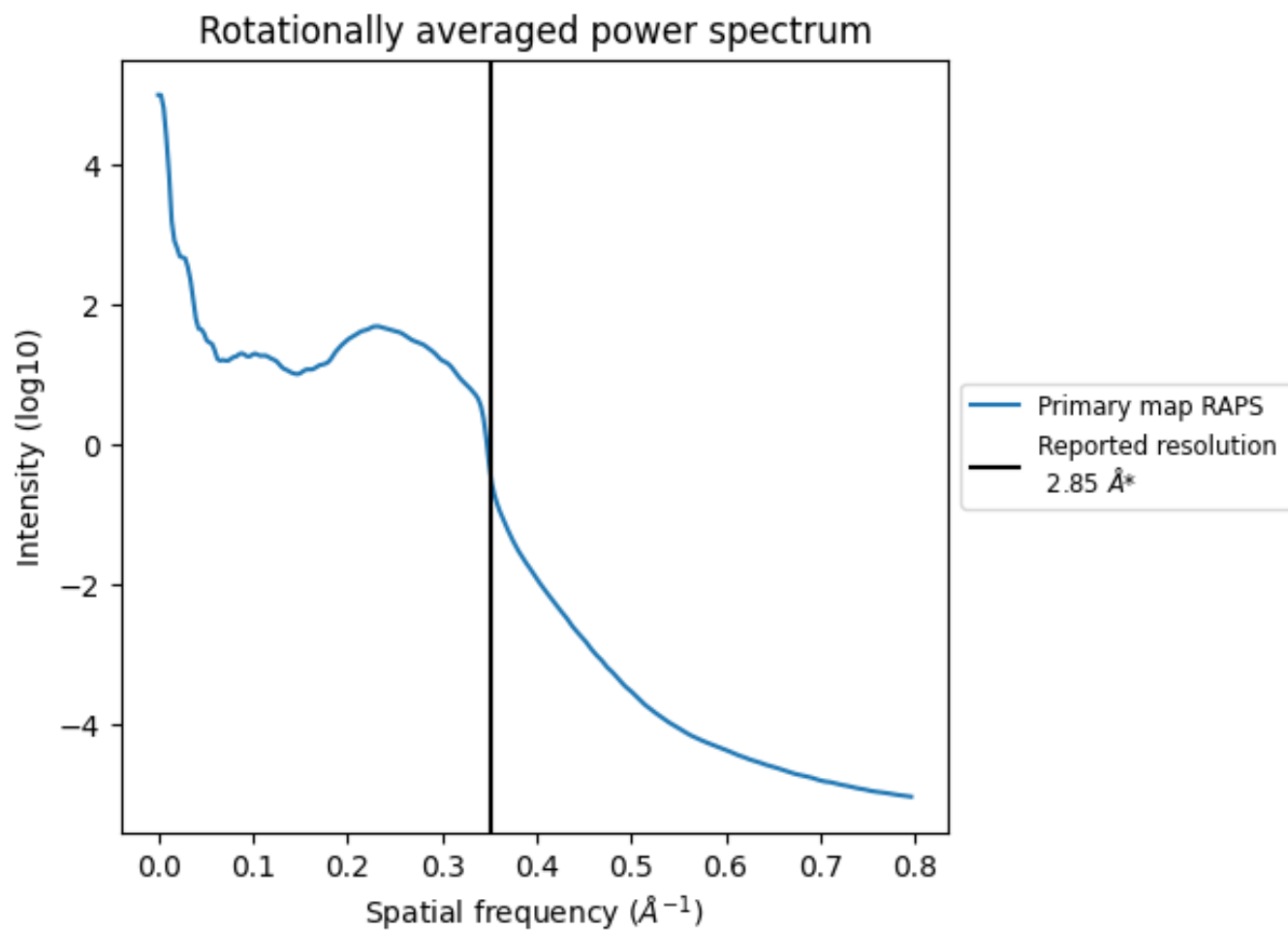
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 62 nm³; this corresponds to an approximate mass of 56 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](#)

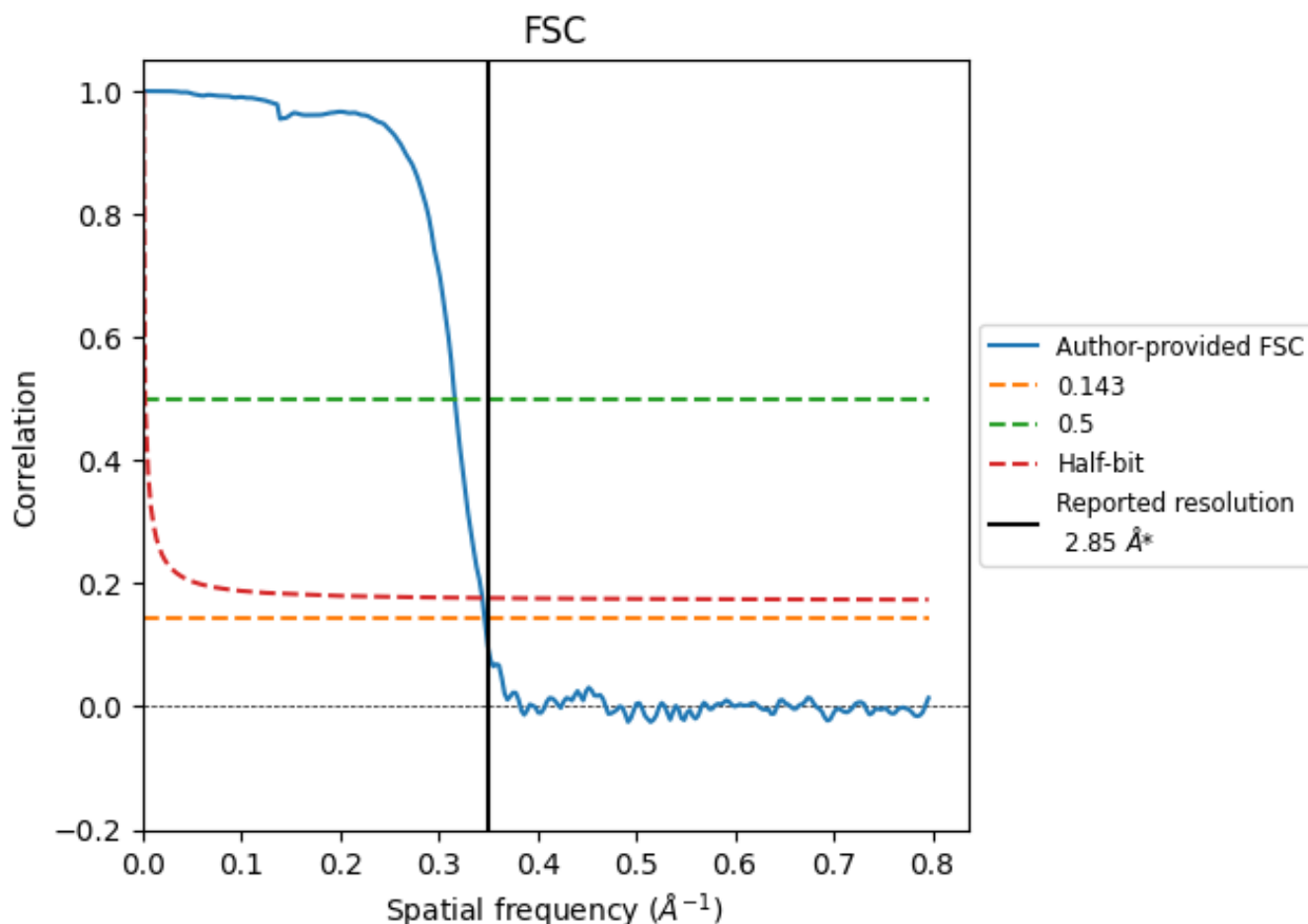


*Reported resolution corresponds to spatial frequency of 0.351 Å⁻¹

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 0.351 Å⁻¹

8.2 Resolution estimates [i](#)

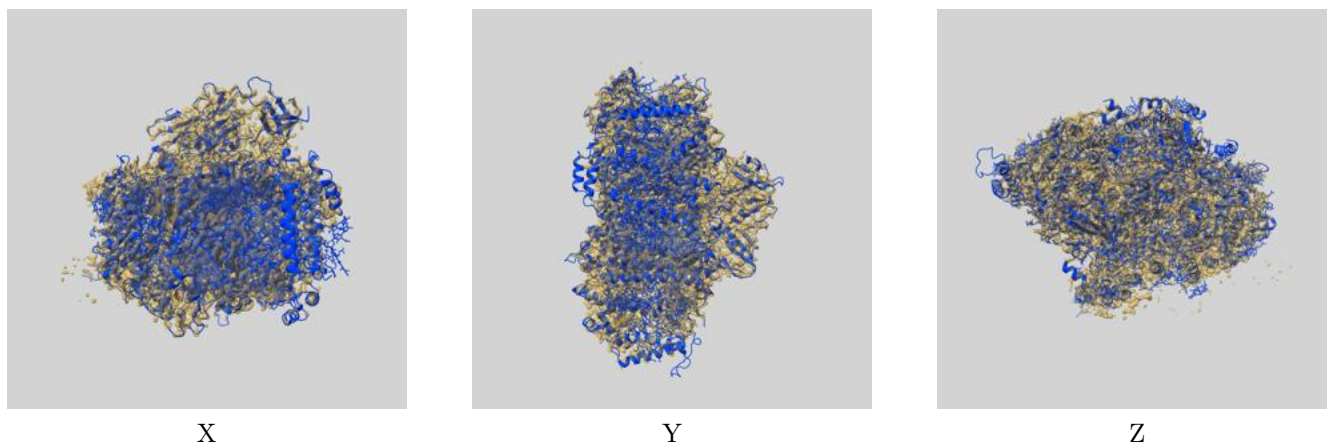
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.89	3.16	2.91
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

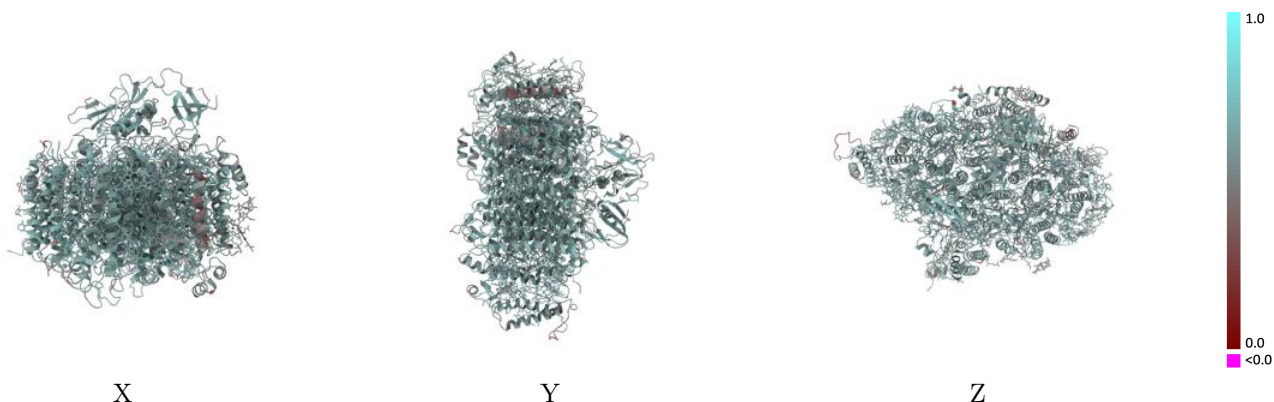
This section contains information regarding the fit between EMDB map EMD-10557 and PDB model 6TRA. Per-residue inclusion information can be found in section 3 on page 19.

9.1 Map-model overlay [i](#)



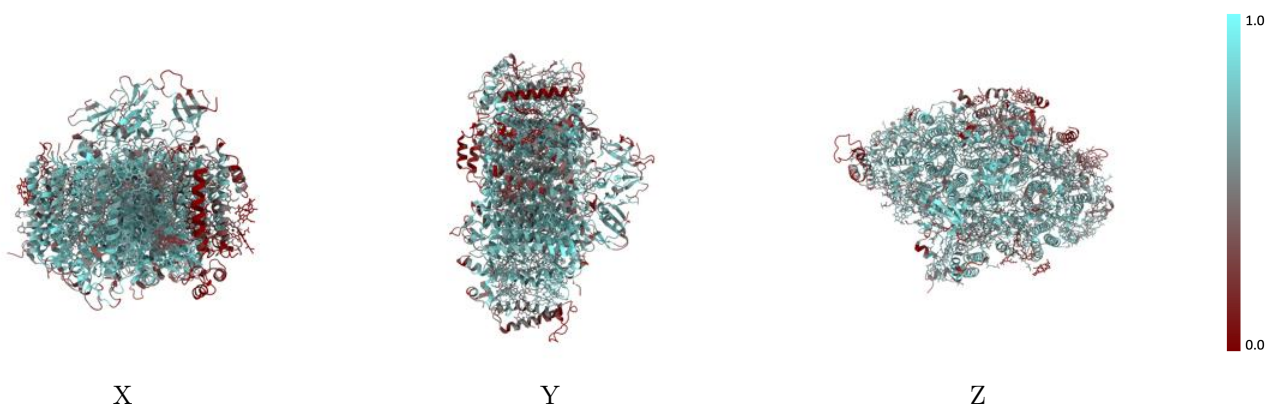
The images above show the 3D surface view of the map at the recommended contour level 0.017 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



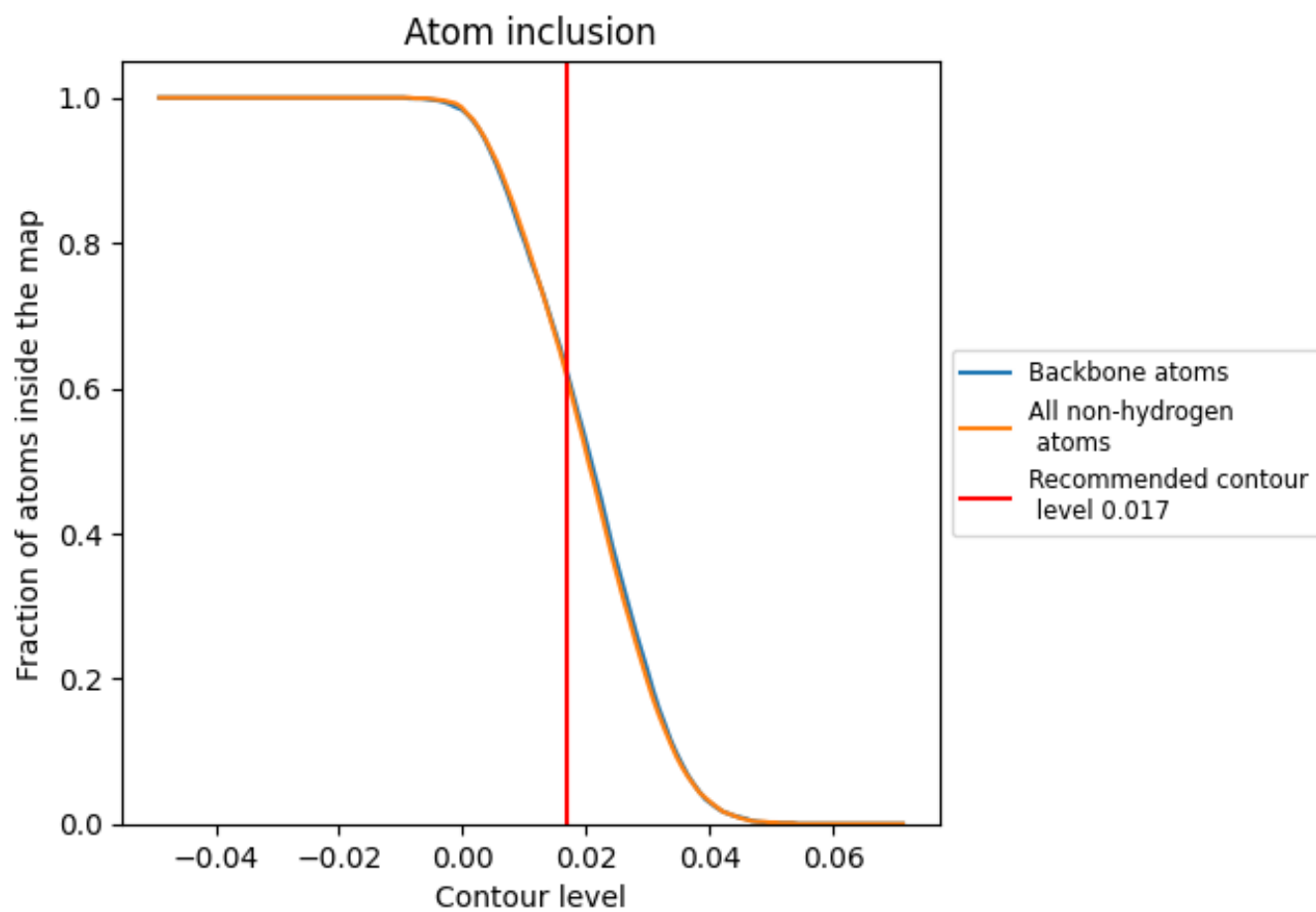
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.017).



























9.4 Atom inclusion [i](#)



At the recommended contour level, 62% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6120	 0.5890
A	 0.6900	 0.6030
B	 0.6630	 0.5960
C	 0.6800	 0.5910
D	 0.5620	 0.5780
E	 0.5090	 0.5760
F	 0.3120	 0.5470
I	 0.5890	 0.5890
J	 0.2920	 0.5530
K	 0.2630	 0.5270
L	 0.5880	 0.5790
M	 0.4870	 0.5700
X	 0.0150	 0.4450

