



Full wwPDB EM Validation Report ⓘ

Jun 28, 2025 – 09:58 pm BST

PDB ID : 8BCW / pdb_00008bcw
EMDB ID : EMD-15970
Title : Photosystem I assembly intermediate of Avena sativa
Authors : Naschberger, A.; Amunts, A.; Nelson, N.
Deposited on : 2022-10-17
Resolution : 2.11 Å(reported)

This is a Full wwPDB EM Validation 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

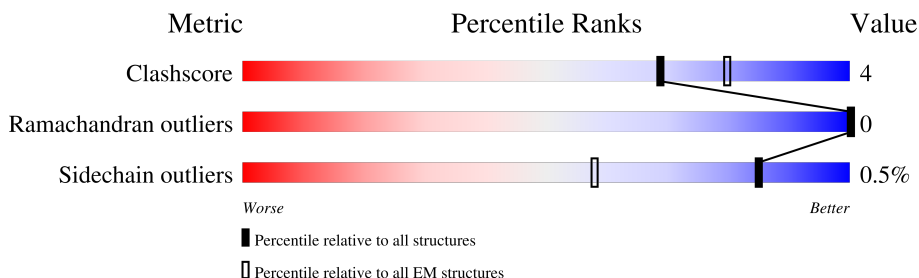
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.11 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	750	<div> <div>10%</div> <div>91%</div> <div>5%</div> <div>•</div> </div>
2	B	734	<div> <div>13%</div> <div>92%</div> <div>8%</div> </div>
3	C	81	<div> <div>94%</div> <div>5%</div> <div>•</div> </div>
4	D	206	<div> <div>6%</div> <div>65%</div> <div>5%</div> <div>31%</div> </div>
5	E	143	<div> <div>13%</div> <div>45%</div> <div>•</div> <div>53%</div> </div>
6	H	94	<div> <div>39%</div> <div>93%</div> <div>7%</div> </div>
7	I	33	<div> <div>12%</div> <div>91%</div> <div>9%</div> </div>
8	L	213	<div> <div>14%</div> <div>68%</div> <div>7%</div> <div>25%</div> </div>

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
10	CLA	A	802	X	-	-	-
10	CLA	A	803	X	-	-	-
10	CLA	A	804	X	-	-	-
10	CLA	A	805	X	-	-	-
10	CLA	A	806	X	-	-	-
10	CLA	A	807	X	-	-	-
10	CLA	A	808	X	-	-	-
10	CLA	A	809	X	-	-	-
10	CLA	A	810	X	-	-	-
10	CLA	A	811	X	-	-	-
10	CLA	A	812	X	-	-	-
10	CLA	A	813	X	-	-	-
10	CLA	A	814	X	-	-	-
10	CLA	A	815	X	-	-	-
10	CLA	A	816	X	-	-	-
10	CLA	A	817	X	-	-	-
10	CLA	A	818	X	-	-	-
10	CLA	A	819	X	-	-	-
10	CLA	A	820	X	-	-	-
10	CLA	A	821	X	-	-	-
10	CLA	A	822	X	-	-	-
10	CLA	A	823	X	-	-	-
10	CLA	A	824	X	-	-	-
10	CLA	A	825	X	-	-	-
10	CLA	A	826	X	-	-	-
10	CLA	A	827	X	-	-	-
10	CLA	A	828	X	-	-	-
10	CLA	A	829	X	-	-	-
10	CLA	A	830	X	-	-	-
10	CLA	A	831	X	-	-	-
10	CLA	A	832	X	-	-	-
10	CLA	A	833	X	-	-	-
10	CLA	A	834	X	-	-	-
10	CLA	A	835	X	-	-	-
10	CLA	A	836	X	-	-	-
10	CLA	A	837	X	-	-	-
10	CLA	A	838	X	-	-	-
10	CLA	A	839	X	-	-	-
10	CLA	A	840	X	-	-	-
10	CLA	A	841	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	A	842	X	-	-	-
10	CLA	A	843	X	-	-	-
10	CLA	A	845	X	-	-	-
10	CLA	A	854	X	-	-	-
10	CLA	A	856	X	-	-	-
10	CLA	B	801	X	-	-	-
10	CLA	B	802	X	-	-	-
10	CLA	B	803	X	-	-	-
10	CLA	B	804	X	-	-	-
10	CLA	B	805	X	-	-	-
10	CLA	B	806	X	-	-	-
10	CLA	B	807	X	-	-	-
10	CLA	B	808	X	-	-	-
10	CLA	B	809	X	-	-	-
10	CLA	B	810	X	-	-	-
10	CLA	B	811	X	-	-	-
10	CLA	B	812	X	-	-	-
10	CLA	B	813	X	-	-	-
10	CLA	B	814	X	-	-	-
10	CLA	B	815	X	-	-	-
10	CLA	B	816	X	-	-	-
10	CLA	B	817	X	-	-	-
10	CLA	B	818	X	-	-	-
10	CLA	B	819	X	-	-	-
10	CLA	B	820	X	-	-	-
10	CLA	B	821	X	-	-	-
10	CLA	B	822	X	-	-	-
10	CLA	B	823	X	-	-	-
10	CLA	B	824	X	-	-	-
10	CLA	B	825	X	-	-	-
10	CLA	B	826	X	-	-	-
10	CLA	B	827	X	-	-	-
10	CLA	B	828	X	-	-	-
10	CLA	B	829	X	-	-	-
10	CLA	B	830	X	-	-	-
10	CLA	B	831	X	-	-	-
10	CLA	B	832	X	-	-	-
10	CLA	B	833	X	-	-	-
10	CLA	B	834	X	-	-	-
10	CLA	B	835	X	-	-	-
10	CLA	B	836	X	-	-	-
10	CLA	B	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	B	838	X	-	-	-
10	CLA	L	302	X	-	-	-
10	CLA	L	303	X	-	-	-
10	CLA	L	304	X	-	-	-
9	CL0	A	801	X	-	-	-
9	CL0	H	201	X	-	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 22313 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	720	Total	C	N	O	S	0	0
			5660	3711	961	969	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5864	3848	996	1007	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			605	372	104	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	143	Total	C	N	O	S	0	0
			1124	722	196	203	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	67	Total	C	N	O	0	0
			533	340	94	99		

- Molecule 6 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	H	94	Total	C	N	O	0	0
			715	469	114	132		

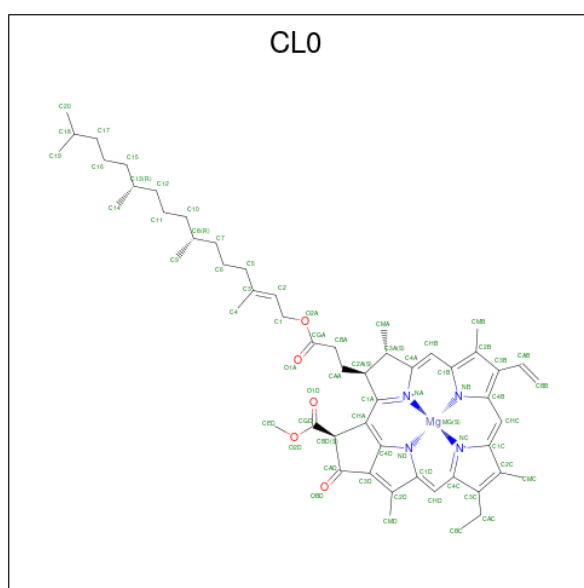
- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	33	Total	C	N	O	S	0	0
			258	178	38	41	1		

- Molecule 8 is a protein called PSI subunit V.

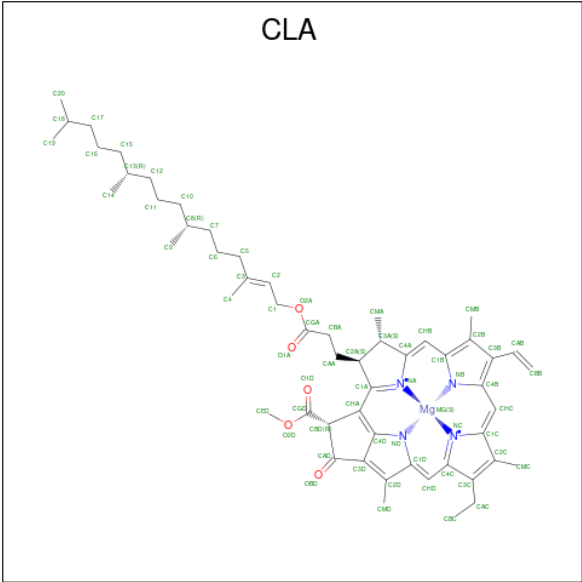
Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	159	Total	C	N	O	S	0	0
			1192	788	189	214	1		

- Molecule 9 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
9	H	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 10 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
10	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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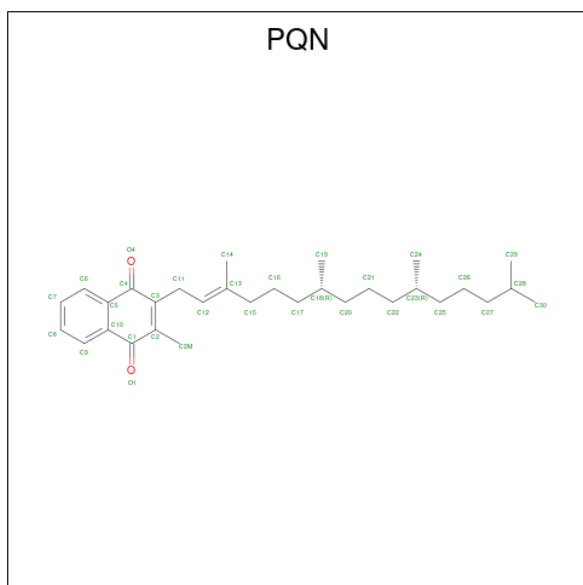
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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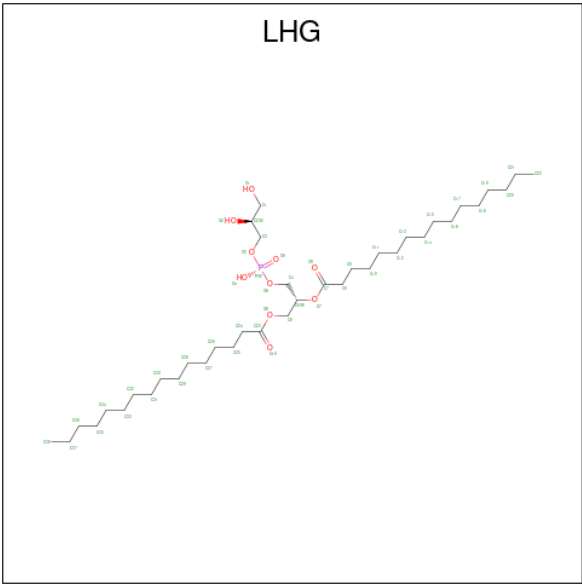
Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
10	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 11 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



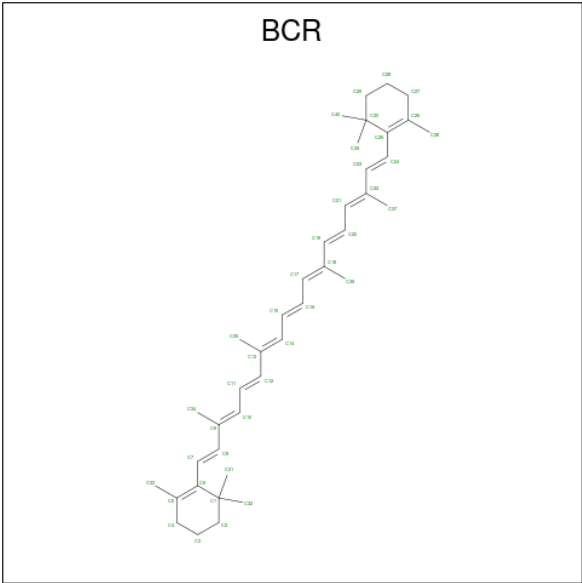
Mol	Chain	Residues	Atoms			AltConf
11	A	1	Total	C	O	0
			33	31	2	
11	B	1	Total	C	O	0
			33	31	2	

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



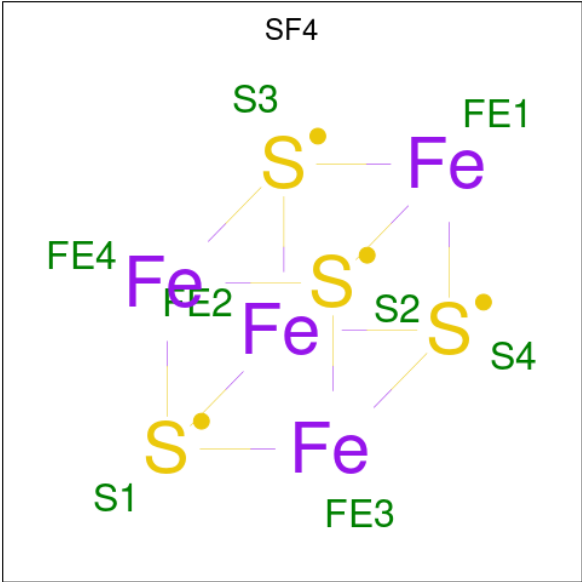
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	A	1	41	30	10	1	0
12	A	1	31	20	10	1	0
12	B	1	49	38	10	1	0

- Molecule 13 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



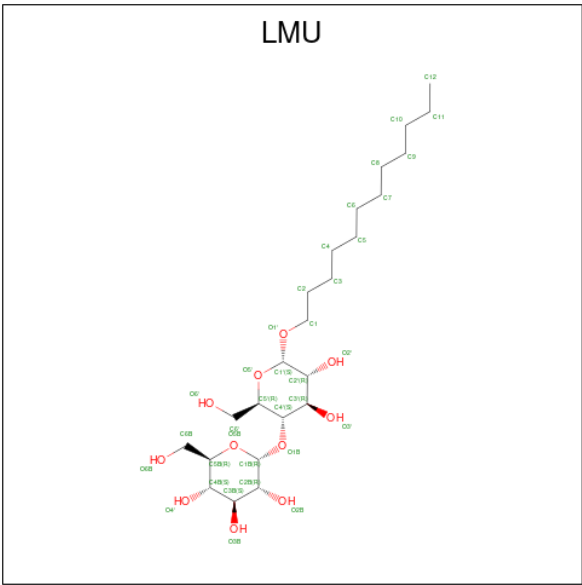
Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total 40	C 40	0
13	A	1	Total 40	C 40	0
13	A	1	Total 40	C 40	0
13	A	1	Total 40	C 40	0
13	A	1	Total 40	C 40	0
13	B	1	Total 40	C 40	0
13	B	1	Total 40	C 40	0
13	B	1	Total 40	C 40	0
13	B	1	Total 40	C 40	0
13	I	1	Total 40	C 40	0
13	L	1	Total 40	C 40	0
13	L	1	Total 40	C 40	0
13	L	1	Total 40	C 40	0

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 15 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁).



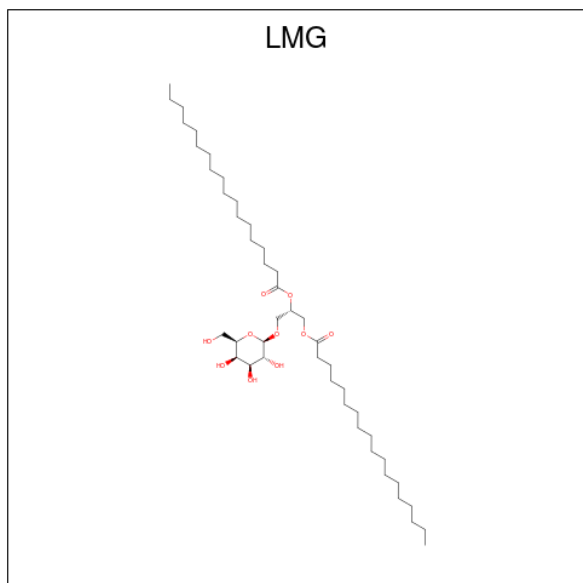
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			35	24	11	

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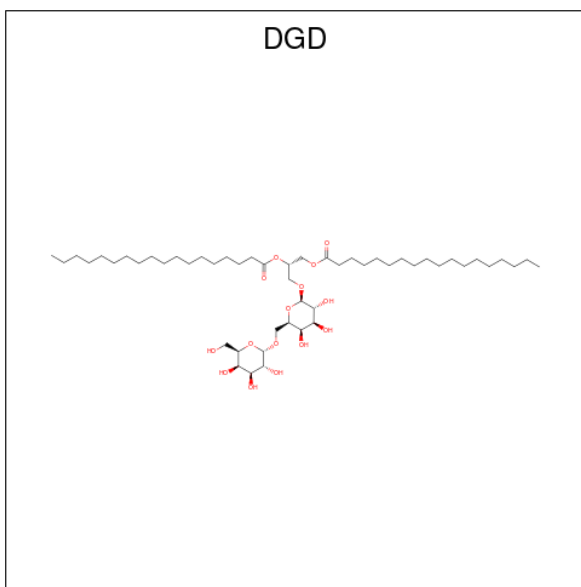
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			24	18	6	
15	A	1	Total	C	O	0
			21	15	6	

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			43	33	10	

- Molecule 17 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	B	1	Total	C	O	0
			61	46	15	

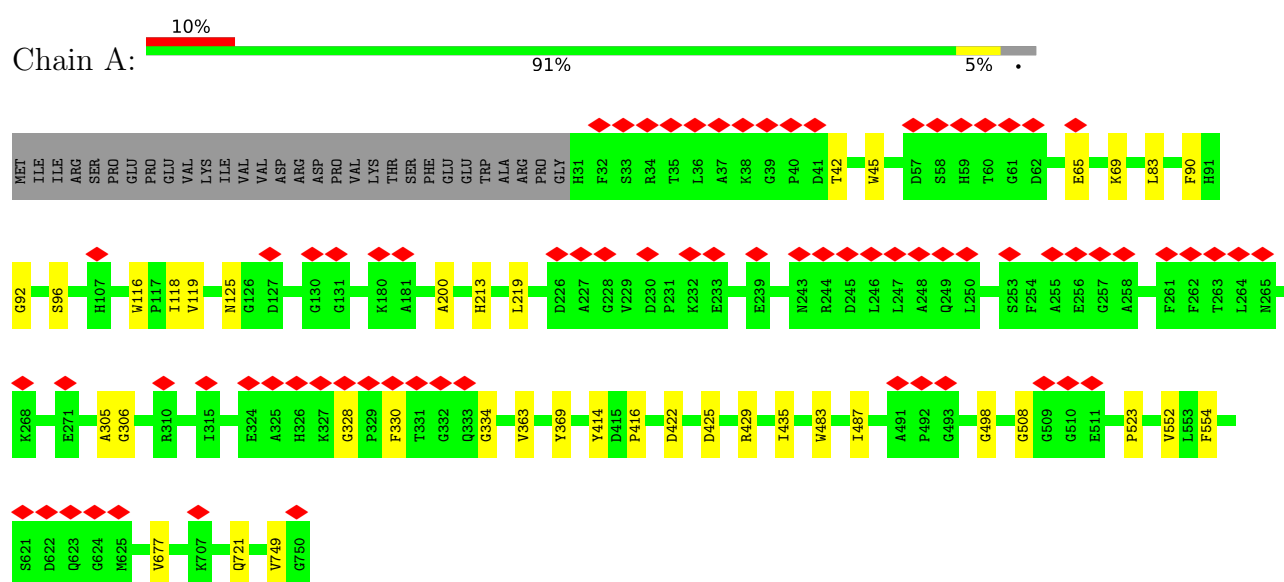
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
18	A	155	Total	O	0
			155	155	
18	B	203	Total	O	0
			203	203	
18	C	62	Total	O	0
			62	62	
18	D	47	Total	O	0
			47	47	
18	E	13	Total	O	0
			13	13	
18	H	9	Total	O	0
			9	9	
18	I	4	Total	O	0
			4	4	
18	L	24	Total	O	0
			24	24	

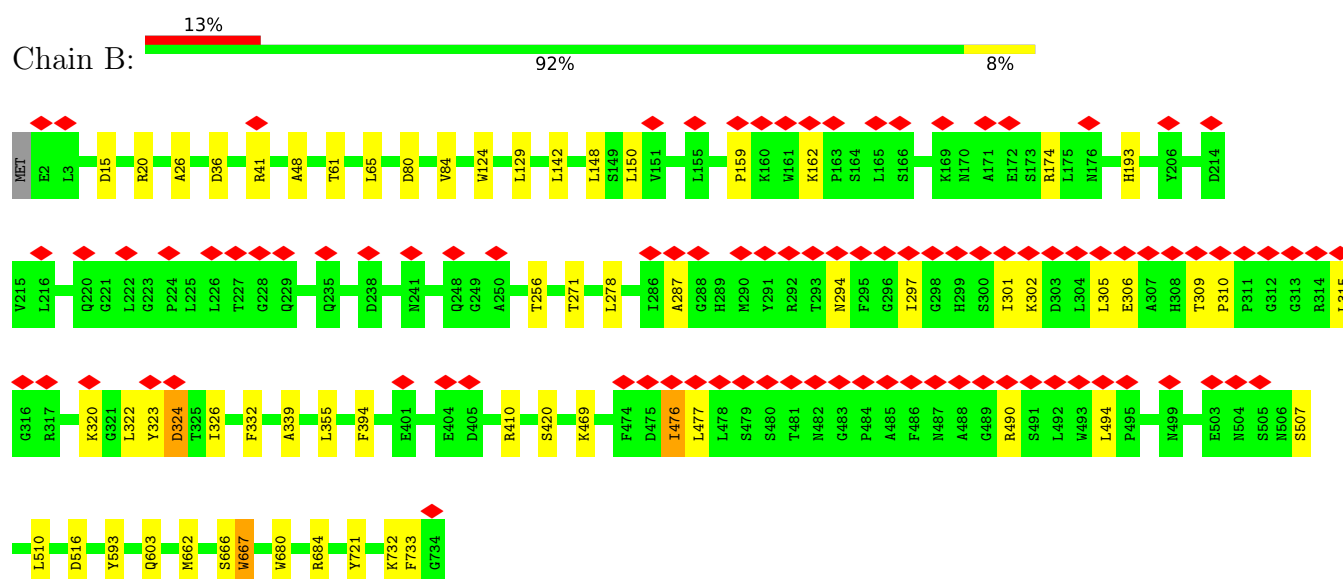
3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



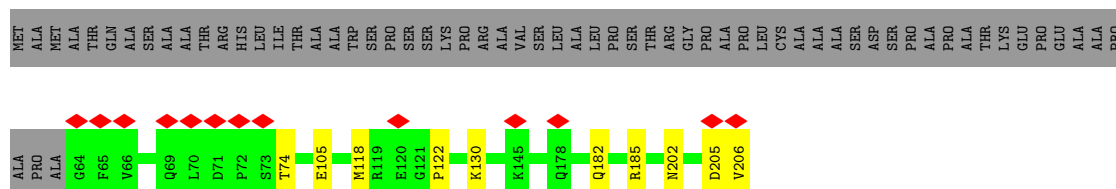
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  94% 5%



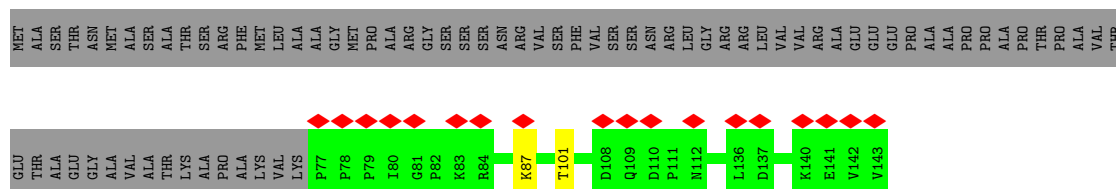
- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

Chain D:  6% 65% 5% 31%

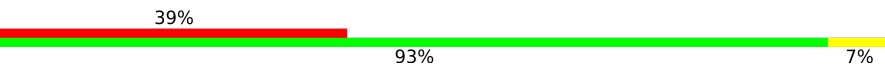


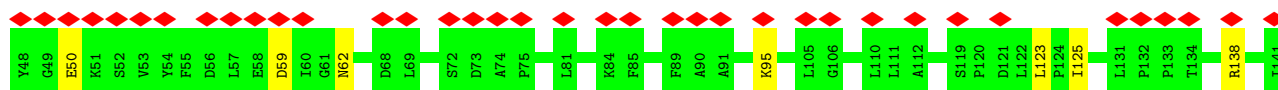
- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

Chain E:  13% 45% 53%

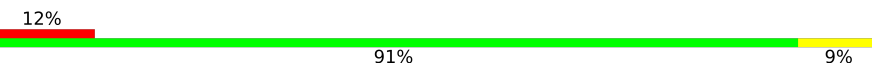


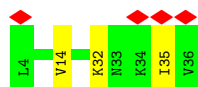
- Molecule 6: Photosystem I reaction center subunit VI, chloroplastic

Chain H:  39% 93% 7%



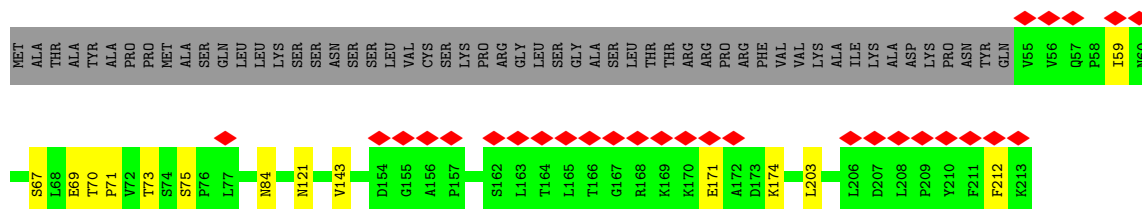
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  12% 91% 9%



- Molecule 8: PSI subunit V

Chain L:  14% 68% 7% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169213	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51.346	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.470	Depositor
Minimum map value	-0.159	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.053	Depositor
Map size (\AA)	336.0, 336.0, 336.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84, 0.84, 0.84	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: PQN, LHG, LMU, DGD, CLA, SF4, BCR, LMG, CL0

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/5853	0.30	0/7985
2	B	0.15	0/6075	0.31	0/8297
3	C	0.13	0/616	0.33	0/834
4	D	0.11	0/1153	0.34	0/1557
5	E	0.09	0/546	0.24	0/743
6	H	0.11	0/737	0.27	0/1002
7	I	0.13	0/264	0.28	0/359
8	L	0.12	0/1228	0.27	0/1681
All	All	0.14	0/16472	0.30	0/22458

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	667	TRP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5660	0	5513	27	0
2	B	5864	0	5642	44	0
3	C	605	0	587	3	0
4	D	1124	0	1128	6	0
5	E	533	0	538	1	0
6	H	715	0	715	4	0
7	I	258	0	285	2	0
8	L	1192	0	1197	9	0
9	A	65	0	72	0	0
9	H	55	0	49	1	0
10	A	2520	0	2393	35	0
10	B	2140	0	2054	36	0
10	L	150	0	125	3	0
11	A	33	0	46	1	0
11	B	33	0	46	1	0
12	A	72	0	87	3	0
12	B	49	0	74	6	0
13	A	200	0	280	15	0
13	B	160	0	224	8	0
13	I	40	0	56	2	0
13	L	120	0	168	3	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
15	A	80	0	107	3	0
16	A	43	0	56	1	0
17	B	61	0	83	1	0
18	A	155	0	0	1	0
18	B	203	0	0	1	0
18	C	62	0	0	0	0
18	D	47	0	0	0	0
18	E	13	0	0	0	0
18	H	9	0	0	0	0
18	I	4	0	0	0	0
18	L	24	0	0	1	0
All	All	22313	0	21525	153	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 4.

All (153) 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:125:ASN:ND2	15:A:855:LMU:O6'	2.24	0.70
2:B:490:ARG:HA	2:B:494:LEU:HD12	1.76	0.68
10:B:802:CLA:H143	13:B:843:BCR:H362	1.76	0.66
2:B:150:LEU:HD11	12:B:845:LHG:H382	1.80	0.63
8:L:59:ILE:HA	8:L:69:GLU:HG3	1.79	0.63
1:A:552:VAL:HG21	13:A:851:BCR:H282	1.81	0.62
10:A:805:CLA:HBA2	10:A:812:CLA:H51	1.83	0.60
10:B:816:CLA:HBA2	10:B:825:CLA:HBB2	1.83	0.60
1:A:118:ILE:HD11	15:A:855:LMU:H71	1.83	0.60
2:B:36:ASP:O	2:B:41:ARG:NH1	2.35	0.60
2:B:278:LEU:HD11	10:B:814:CLA:H92	1.84	0.59
1:A:677:VAL:HG22	10:A:842:CLA:HBB1	1.83	0.59
10:B:826:CLA:HBC2	10:B:826:CLA:H142	1.86	0.57
8:L:171:GLU:OE2	8:L:174:LYS:NZ	2.38	0.57
2:B:469:LYS:NZ	18:B:904:HOH:O	2.33	0.56
2:B:410:ARG:NH1	10:B:829:CLA:OBD	2.34	0.56
1:A:200:ALA:HB2	1:A:306:GLY:HA3	1.88	0.56
10:B:824:CLA:H43	10:B:833:CLA:HBB2	1.88	0.56
10:A:803:CLA:HBB1	10:A:803:CLA:HMB1	1.87	0.56
6:H:59:ASP:OD2	6:H:62:ASN:ND2	2.37	0.56
13:A:851:BCR:HC8	13:A:851:BCR:H321	1.89	0.55
2:B:15:ASP:HB3	2:B:20:ARG:HB2	1.88	0.55
2:B:48:ALA:HB1	12:B:845:LHG:H272	1.88	0.55
4:D:202:ASN:ND2	4:D:205:ASP:OD2	2.39	0.55
6:H:123:LEU:HG	6:H:125:ILE:HG22	1.88	0.55
2:B:129:LEU:HD23	10:B:813:CLA:HED2	1.88	0.53
13:A:852:BCR:H362	10:A:854:CLA:H2	1.91	0.53
10:B:807:CLA:H72	10:B:807:CLA:HBB1	1.90	0.53
1:A:330:PHE:HE2	12:A:847:LHG:HC5	1.74	0.52
2:B:309:THR:HG21	2:B:320:LYS:HE3	1.91	0.52
13:A:852:BCR:H392	13:A:852:BCR:H23C	1.92	0.52
1:A:92:GLY:O	1:A:96:SER:OG	2.19	0.51
2:B:322:LEU:O	2:B:326:ILE:HG12	2.09	0.51
2:B:721:TYR:HB2	10:B:801:CLA:HED2	1.93	0.51
10:A:843:CLA:H52	10:B:837:CLA:H43	1.94	0.50
1:A:83:LEU:HD23	10:A:809:CLA:H91	1.93	0.50
2:B:174:ARG:HB2	10:B:812:CLA:HBC2	1.92	0.50
12:A:847:LHG:H281	13:A:850:BCR:H20C	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:B:825:CLA:H161	13:B:842:BCR:H15C	1.92	0.50
4:D:105:GLU:HA	4:D:118:MET:O	2.12	0.49
2:B:302:LYS:O	2:B:306:GLU:HG2	2.13	0.49
2:B:310:PRO:HG2	2:B:315:LEU:HD12	1.94	0.49
2:B:680:TRP:CE2	2:B:684:ARG:HG3	2.47	0.49
12:B:845:LHG:H202	12:B:845:LHG:H342	1.95	0.48
2:B:193:HIS:HB2	10:B:813:CLA:CHC	2.43	0.48
1:A:213:HIS:HB2	10:A:815:CLA:CHC	2.44	0.48
10:B:833:CLA:HBB1	13:B:842:BCR:H333	1.94	0.48
10:A:804:CLA:H3A	11:A:844:PQN:H292	1.95	0.48
13:A:852:BCR:H272	10:B:831:CLA:HMA1	1.94	0.48
2:B:324:ASP:N	2:B:324:ASP:OD1	2.46	0.48
2:B:355:LEU:HD11	10:B:825:CLA:HAB	1.96	0.48
10:B:827:CLA:H12	13:B:840:BCR:H393	1.95	0.47
10:B:816:CLA:H61	10:B:816:CLA:H111	1.95	0.47
10:A:809:CLA:H3A	10:A:809:CLA:HBA2	1.69	0.47
10:A:819:CLA:H72	10:A:836:CLA:H12	1.95	0.47
2:B:150:LEU:HD21	12:B:845:LHG:H361	1.97	0.47
2:B:301:ILE:HG21	10:B:823:CLA:HAC1	1.95	0.47
8:L:121:ASN:ND2	18:L:402:HOH:O	2.44	0.47
1:A:425:ASP:O	1:A:429:ARG:HG3	2.15	0.47
13:A:852:BCR:H393	15:A:859:LMU:H81	1.97	0.47
10:B:827:CLA:H3A	10:B:827:CLA:HBA2	1.69	0.47
9:H:201:CL0:H16	13:L:306:BCR:H311	1.95	0.47
8:L:203:LEU:HG	10:L:304:CLA:HED3	1.97	0.47
3:C:15:THR:HG22	3:C:28:MET:HG3	1.98	0.46
2:B:80:ASP:HB3	2:B:84:VAL:HG23	1.97	0.46
2:B:287:ALA:HB2	10:B:818:CLA:HBC2	1.98	0.46
1:A:721:GLN:OE1	18:A:901:HOH:O	2.21	0.46
1:A:42:THR:O	1:A:45:TRP:HD1	1.98	0.46
2:B:662:MET:HB2	10:B:802:CLA:C1C	2.46	0.46
10:A:822:CLA:HAA2	10:A:826:CLA:HAB	1.98	0.45
3:C:29:ILE:HD11	4:D:182:GLN:HE22	1.81	0.45
10:A:812:CLA:H62	10:A:812:CLA:H41	1.54	0.45
13:L:305:BCR:H23C	13:L:305:BCR:H392	1.98	0.45
1:A:116:TRP:CD2	10:A:810:CLA:HED3	2.51	0.45
2:B:507:SER:HA	2:B:510:LEU:HD21	1.97	0.45
10:B:818:CLA:H41	10:B:818:CLA:H61	1.71	0.45
10:B:821:CLA:HBC2	10:B:822:CLA:HBA2	1.99	0.45
1:A:213:HIS:HB2	10:A:815:CLA:C1C	2.47	0.45
10:A:843:CLA:H62	10:A:843:CLA:H41	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:59:ILE:HG21	8:L:67:SER:HB3	1.98	0.44
10:A:843:CLA:H61	10:A:843:CLA:H112	1.99	0.44
4:D:74:THR:HG23	4:D:122:PRO:HB2	2.00	0.44
10:A:841:CLA:HED2	2:B:420:SER:HB3	1.99	0.44
1:A:328:GLY:HA3	12:A:847:LHG:HC2	1.98	0.44
10:A:826:CLA:HAA2	10:A:826:CLA:HBD	2.00	0.44
2:B:332:PHE:CE1	13:B:842:BCR:H401	2.53	0.44
1:A:435:ILE:HG13	1:A:554:PHE:HE1	1.83	0.44
13:A:848:BCR:H362	13:A:849:BCR:H10C	1.99	0.44
2:B:256:THR:HG23	2:B:271:THR:HG21	1.99	0.44
1:A:118:ILE:HG22	1:A:119:VAL:HG13	2.00	0.44
2:B:305:LEU:HD12	2:B:323:TYR:HB2	2.00	0.44
2:B:733:PHE:HA	6:H:138:ARG:HD3	2.00	0.44
13:A:852:BCR:H24C	13:A:852:BCR:H371	1.73	0.44
8:L:212:PHE:CE2	10:L:304:CLA:HBA1	2.52	0.44
10:A:822:CLA:HBC1	16:A:858:LMG:H201	1.99	0.43
1:A:414:TYR:CE2	1:A:416:PRO:HD3	2.53	0.43
2:B:124:TRP:HB3	2:B:129:LEU:HD12	2.00	0.43
2:B:301:ILE:HG23	10:B:818:CLA:HED3	2.00	0.43
10:A:814:CLA:HAA2	10:A:826:CLA:H52	2.01	0.43
7:I:32:LYS:HE2	7:I:35:ILE:HD11	2.01	0.43
10:B:824:CLA:C4	10:B:833:CLA:HBB2	2.49	0.43
1:A:508:GLY:HA2	1:A:523:PRO:HB3	2.01	0.43
2:B:476:ILE:HG22	2:B:477:LEU:H	1.84	0.42
10:B:803:CLA:O1A	12:B:845:LHG:H141	2.19	0.42
8:L:70:THR:H	8:L:73:THR:HG1	1.67	0.42
1:A:65:GLU:HG3	1:A:69:LYS:HE2	2.02	0.42
13:I:101:BCR:H24C	13:I:101:BCR:H371	1.90	0.42
8:L:71:PRO:O	8:L:75:SER:OG	2.36	0.42
4:D:185:ARG:HH12	4:D:206:VAL:HB	1.84	0.42
10:A:828:CLA:HED1	10:A:836:CLA:HAB	2.01	0.42
2:B:516:ASP:OD2	2:B:593:TYR:OH	2.32	0.42
1:A:498:GLY:HA3	10:A:837:CLA:HED2	2.02	0.42
10:B:806:CLA:H13	12:B:845:LHG:H381	2.02	0.42
10:B:806:CLA:H61	13:I:101:BCR:H281	2.01	0.42
10:A:825:CLA:HBA2	13:A:850:BCR:H351	2.02	0.42
2:B:666:SER:C	2:B:667:TRP:HD1	2.28	0.42
6:H:95:LYS:HE2	6:H:95:LYS:HB2	1.89	0.41
1:A:90:PHE:CG	10:A:808:CLA:HBC3	2.56	0.41
10:A:815:CLA:CHD	10:A:817:CLA:HBB1	2.50	0.41
13:L:301:BCR:H24C	13:L:301:BCR:H371	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:802:CLA:H112	13:A:852:BCR:H403	2.01	0.41
10:A:830:CLA:H62	13:A:849:BCR:H373	2.03	0.41
2:B:26:ALA:HA	10:B:828:CLA:H42	2.03	0.41
1:A:334:GLY:HA2	1:A:422:ASP:HB3	2.03	0.41
10:A:802:CLA:H41	10:A:802:CLA:H62	1.90	0.41
10:A:822:CLA:H171	10:A:832:CLA:HBC1	2.01	0.41
10:B:813:CLA:HMA1	13:B:841:BCR:H392	2.02	0.41
8:L:84:ASN:HB3	10:L:302:CLA:HAC1	2.03	0.41
10:A:828:CLA:H2	10:A:828:CLA:H61	1.88	0.41
2:B:294:ASN:OD1	2:B:294:ASN:N	2.53	0.41
10:B:806:CLA:H12	7:I:14:VAL:HG21	2.02	0.41
11:B:839:PQN:H302	17:B:844:DGD:HA92	2.01	0.41
13:A:848:BCR:H20C	13:A:848:BCR:H361	1.88	0.41
13:A:850:BCR:H24C	13:A:850:BCR:H371	1.84	0.41
2:B:61:THR:HG23	2:B:142:LEU:HD13	2.03	0.41
2:B:159:PRO:HA	2:B:162:LYS:HE2	2.03	0.41
10:B:807:CLA:CGA	10:B:807:CLA:C1A	2.99	0.41
1:A:305:ALA:HB2	10:A:822:CLA:HBC2	2.03	0.41
1:A:363:VAL:HG11	10:A:820:CLA:H201	2.02	0.41
1:A:425:ASP:OD2	1:A:429:ARG:NH1	2.50	0.41
10:A:814:CLA:H61	10:A:814:CLA:H102	1.97	0.41
2:B:65:LEU:HD12	2:B:142:LEU:HD12	2.02	0.41
2:B:603:GLN:HE21	2:B:732:LYS:HD3	1.86	0.41
3:C:47:ASP:OD2	4:D:130:LYS:NZ	2.51	0.41
5:E:87:LYS:HG3	5:E:101:THR:HG23	2.03	0.41
13:A:852:BCR:H362	10:A:854:CLA:C2	2.51	0.41
10:B:808:CLA:H61	10:B:808:CLA:H41	1.86	0.41
13:B:842:BCR:H20C	13:B:842:BCR:H361	1.97	0.41
10:A:819:CLA:HMC1	10:A:819:CLA:H93	2.03	0.40
2:B:148:LEU:HD23	10:B:813:CLA:H202	2.03	0.40
2:B:339:ALA:HB2	13:B:842:BCR:H372	2.03	0.40
2:B:410:ARG:HD3	10:B:829:CLA:OBD	2.21	0.40
1:A:483:TRP:CE2	1:A:487:ILE:HD11	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	718/750 (96%)	703 (98%)	15 (2%)	0	100	100
2	B	731/734 (100%)	716 (98%)	15 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/206 (68%)	138 (98%)	3 (2%)	0	100	100
5	E	65/143 (46%)	65 (100%)	0	0	100	100
6	H	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
7	I	31/33 (94%)	31 (100%)	0	0	100	100
8	L	157/213 (74%)	154 (98%)	3 (2%)	0	100	100
All	All	2013/2254 (89%)	1974 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	580/608 (95%)	577 (100%)	3 (0%)	86	91
2	B	598/599 (100%)	594 (99%)	4 (1%)	81	86
3	C	70/71 (99%)	70 (100%)	0	100	100
4	D	120/163 (74%)	120 (100%)	0	100	100
5	E	59/115 (51%)	59 (100%)	0	100	100
6	H	76/76 (100%)	75 (99%)	1 (1%)	65	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	30/30 (100%)	30 (100%)	0	100	100
8	L	123/168 (73%)	122 (99%)	1 (1%)	79	84
All	All	1656/1830 (90%)	1647 (100%)	9 (0%)	85	91

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	219	LEU
1	A	369	TYR
1	A	749	VAL
2	B	297	ILE
2	B	324	ASP
2	B	394	PHE
2	B	476	ILE
6	H	50	GLU
8	L	143	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	384	GLN
1	A	439	ASN
1	A	486	ASN
2	B	231	ASN
2	B	333	GLN
2	B	627	ASN
3	C	38	GLN
6	H	66	GLN
6	H	79	ASN
6	H	130	GLN
8	L	121	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

114 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	LHG	B	845	-	48,48,48	0.23	0	51,54,54	0.24	0
10	CLA	A	818	-	45,53,73	1.25	3 (6%)	52,89,113	1.02	2 (3%)
10	CLA	B	819	-	45,53,73	1.26	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	A	833	-	55,63,73	1.08	3 (5%)	64,101,113	0.92	2 (3%)
10	CLA	A	831	-	65,73,73	1.01	3 (4%)	76,113,113	0.81	2 (2%)
10	CLA	B	833	-	45,53,73	1.22	3 (6%)	52,89,113	1.05	2 (3%)
10	CLA	A	815	-	54,62,73	1.15	3 (5%)	62,99,113	0.93	2 (3%)
13	BCR	B	841	-	41,41,41	0.14	0	56,56,56	0.30	0
10	CLA	A	830	-	65,73,73	1.03	3 (4%)	76,113,113	0.82	2 (2%)
10	CLA	A	841	-	55,63,73	1.10	3 (5%)	64,101,113	0.91	2 (3%)
10	CLA	A	832	-	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
13	BCR	A	851	-	41,41,41	0.18	0	56,56,56	0.34	0
9	CL0	H	201	6	55,63,73	2.23	7 (12%)	64,101,113	1.27	6 (9%)
10	CLA	A	820	-	65,73,73	1.02	3 (4%)	76,113,113	0.89	2 (2%)
10	CLA	B	818	18	55,63,73	1.14	3 (5%)	64,101,113	0.95	2 (3%)
10	CLA	A	819	-	56,64,73	1.12	3 (5%)	65,102,113	0.91	2 (3%)
10	CLA	A	813	-	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
13	BCR	L	306	-	41,41,41	0.12	0	56,56,56	0.24	0
10	CLA	A	804	-	45,53,73	1.25	3 (6%)	52,89,113	1.05	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	A	845	12	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	A	803	18	65,73,73	1.06	3 (4%)	76,113,113	0.88	3 (3%)
14	SF4	A	853	1,2	0,12,12	-	-	-		
10	CLA	A	829	-	60,68,73	1.07	3 (5%)	70,107,113	0.87	2 (2%)
10	CLA	B	824	18	50,58,73	1.13	3 (6%)	58,95,113	0.95	2 (3%)
10	CLA	A	825	-	60,68,73	1.07	3 (5%)	70,107,113	0.88	2 (2%)
10	CLA	B	830	-	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
10	CLA	A	843	18	65,73,73	1.01	3 (4%)	76,113,113	0.88	2 (2%)
10	CLA	A	826	18	65,73,73	1.06	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	B	817	-	65,73,73	1.02	3 (4%)	76,113,113	0.88	2 (2%)
10	CLA	B	826	-	65,73,73	1.01	3 (4%)	76,113,113	0.89	3 (3%)
10	CLA	B	834	-	51,59,73	1.18	3 (5%)	59,96,113	0.97	2 (3%)
10	CLA	A	835	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
10	CLA	B	804	-	65,73,73	1.01	3 (4%)	76,113,113	0.87	2 (2%)
10	CLA	L	304	18	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
10	CLA	A	839	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
15	LMU	A	859	-	21,21,36	0.13	0	26,26,47	0.28	0
10	CLA	A	837	1	45,53,73	1.24	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	A	817	18	45,53,73	1.28	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	A	854	18	55,63,73	1.07	3 (5%)	64,101,113	1.00	3 (4%)
10	CLA	A	856	18	50,58,73	1.17	3 (6%)	58,95,113	0.97	2 (3%)
10	CLA	B	828	-	65,73,73	0.95	4 (6%)	76,113,113	0.85	2 (2%)
12	LHG	A	846	-	40,40,48	0.26	0	43,46,54	0.28	0
10	CLA	A	805	10	50,58,73	1.17	3 (6%)	58,95,113	0.93	2 (3%)
13	BCR	I	101	-	41,41,41	0.16	0	56,56,56	0.44	0
10	CLA	A	834	-	65,73,73	1.00	3 (4%)	76,113,113	0.88	2 (2%)
13	BCR	A	849	-	41,41,41	0.13	0	56,56,56	0.28	0
13	BCR	A	852	-	41,41,41	0.27	0	56,56,56	0.83	1 (1%)
15	LMU	A	857	-	24,24,36	0.13	0	29,29,47	0.29	0
10	CLA	B	832	-	45,53,73	1.21	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	B	820	-	45,53,73	1.25	3 (6%)	52,89,113	1.05	2 (3%)
10	CLA	A	838	-	51,59,73	1.18	3 (5%)	59,96,113	0.97	2 (3%)
9	CL0	A	801	-	65,73,73	2.00	8 (12%)	76,113,113	1.12	6 (7%)
13	BCR	A	848	-	41,41,41	0.12	0	56,56,56	0.26	0
10	CLA	B	803	-	45,53,73	1.24	3 (6%)	52,89,113	1.01	2 (3%)
10	CLA	B	808	2	65,73,73	1.01	3 (4%)	76,113,113	0.83	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	L	301	-	41,41,41	0.14	0	56,56,56	0.32	0
10	CLA	B	816	-	60,68,73	1.08	3 (5%)	70,107,113	0.88	2 (2%)
10	CLA	A	842	-	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
10	CLA	B	825	-	65,73,73	1.02	3 (4%)	76,113,113	0.83	2 (2%)
13	BCR	B	843	-	41,41,41	0.14	0	56,56,56	0.42	0
10	CLA	B	809	-	65,73,73	1.04	3 (4%)	76,113,113	0.83	2 (2%)
10	CLA	A	807	1	65,73,73	1.02	3 (4%)	76,113,113	0.85	2 (2%)
11	PQN	A	844	-	34,34,34	0.32	0	42,45,45	0.35	0
14	SF4	C	101	3	0,12,12	-	-	-	-	-
10	CLA	A	828	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
10	CLA	A	810	1	50,58,73	1.17	3 (6%)	58,95,113	0.97	2 (3%)
10	CLA	B	810	-	56,64,73	1.12	3 (5%)	65,102,113	0.90	2 (3%)
10	CLA	L	302	8	45,53,73	1.24	3 (6%)	52,89,113	1.02	2 (3%)
13	BCR	A	850	-	41,41,41	0.15	0	56,56,56	0.34	0
11	PQN	B	839	-	34,34,34	0.32	0	42,45,45	0.32	0
10	CLA	A	811	-	45,53,73	1.23	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	A	822	18	65,73,73	1.02	3 (4%)	76,113,113	0.88	2 (2%)
10	CLA	B	837	18	65,73,73	0.99	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	B	805	2	65,73,73	1.03	3 (4%)	76,113,113	0.81	2 (2%)
10	CLA	B	814	-	55,63,73	1.10	3 (5%)	64,101,113	0.91	2 (3%)
10	CLA	A	836	-	65,73,73	1.01	3 (4%)	76,113,113	0.84	2 (2%)
10	CLA	B	831	-	45,53,73	1.22	3 (6%)	52,89,113	1.08	3 (5%)
10	CLA	A	808	-	47,55,73	1.20	3 (6%)	54,91,113	1.00	2 (3%)
10	CLA	B	815	-	57,65,73	1.10	3 (5%)	66,103,113	0.91	2 (3%)
10	CLA	A	816	-	60,68,73	1.04	3 (5%)	70,107,113	0.89	2 (2%)
13	BCR	B	842	-	41,41,41	0.13	0	56,56,56	0.41	0
10	CLA	B	836	-	50,58,73	1.17	3 (6%)	58,95,113	0.94	2 (3%)
17	DGD	B	844	-	62,62,67	0.18	0	76,76,81	0.30	0
10	CLA	B	838	-	65,73,73	1.03	3 (4%)	76,113,113	0.86	2 (2%)
10	CLA	B	806	-	60,68,73	1.04	3 (5%)	70,107,113	0.88	2 (2%)
10	CLA	A	823	-	52,60,73	1.16	3 (5%)	60,97,113	0.97	2 (3%)
10	CLA	B	823	18	56,64,73	1.14	3 (5%)	65,102,113	0.90	2 (3%)
10	CLA	A	809	1	55,63,73	1.09	3 (5%)	64,101,113	0.91	2 (3%)
12	LHG	A	847	10	30,30,48	0.29	0	33,36,54	0.31	0
10	CLA	B	801	-	65,73,73	1.00	3 (4%)	76,113,113	0.80	2 (2%)
10	CLA	B	813	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	A	802	-	65,73,73	0.97	3 (4%)	76,113,113	0.86	2 (2%)
13	BCR	L	305	-	41,41,41	0.27	0	56,56,56	0.46	1 (1%)
10	CLA	A	827	18	55,63,73	1.09	3 (5%)	64,101,113	0.90	2 (3%)
15	LMU	A	855	-	36,36,36	0.12	0	47,47,47	0.25	0
10	CLA	B	827	-	65,73,73	1.01	3 (4%)	76,113,113	0.89	3 (3%)
10	CLA	L	303	-	60,68,73	1.04	3 (5%)	70,107,113	0.90	2 (2%)
10	CLA	B	807	-	65,73,73	1.03	3 (4%)	76,113,113	0.84	2 (2%)
10	CLA	B	822	-	45,53,73	1.24	3 (6%)	52,89,113	1.03	2 (3%)
10	CLA	A	812	10	65,73,73	1.01	3 (4%)	76,113,113	0.84	2 (2%)
10	CLA	A	840	-	55,63,73	1.07	3 (5%)	64,101,113	0.93	2 (3%)
16	LMG	A	858	-	43,43,55	0.18	0	51,51,63	0.17	0
10	CLA	B	812	-	65,73,73	1.05	3 (4%)	76,113,113	0.85	2 (2%)
14	SF4	C	102	3	0,12,12	-	-	-	-	-
10	CLA	B	835	-	55,63,73	1.09	3 (5%)	64,101,113	0.94	2 (3%)
10	CLA	A	821	-	45,53,73	1.24	3 (6%)	52,89,113	1.01	2 (3%)
10	CLA	B	802	-	65,73,73	0.98	3 (4%)	76,113,113	0.82	3 (3%)
10	CLA	A	814	-	65,73,73	1.04	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	B	821	-	45,53,73	1.25	3 (6%)	52,89,113	1.03	2 (3%)
13	BCR	B	840	-	41,41,41	0.19	0	56,56,56	0.44	0
10	CLA	A	824	-	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)
10	CLA	B	829	-	45,53,73	1.25	3 (6%)	52,89,113	1.05	2 (3%)
10	CLA	A	806	-	65,73,73	1.03	3 (4%)	76,113,113	0.85	2 (2%)
10	CLA	B	811	-	45,53,73	1.25	3 (6%)	52,89,113	1.04	2 (3%)

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	LHG	B	845	-	-	18/53/53/53	-
10	CLA	A	818	-	1/1/11/20	4/13/91/115	-
10	CLA	B	819	-	1/1/11/20	2/13/91/115	-
10	CLA	A	833	-	1/1/13/20	0/25/103/115	-
10	CLA	A	831	-	1/1/15/20	2/37/115/115	-
10	CLA	B	833	-	1/1/11/20	2/13/91/115	-
10	CLA	A	815	-	1/1/12/20	3/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	B	841	-	-	6/29/63/63	0/2/2/2
10	CLA	A	830	-	1/1/15/20	2/37/115/115	-
10	CLA	A	841	-	1/1/13/20	2/25/103/115	-
10	CLA	A	832	-	1/1/11/20	3/13/91/115	-
13	BCR	A	851	-	-	2/29/63/63	0/2/2/2
9	CL0	H	201	6	3/3/18/25	4/25/123/135	-
10	CLA	A	820	-	1/1/15/20	6/37/115/115	-
10	CLA	B	818	18	1/1/13/20	2/25/103/115	-
10	CLA	A	819	-	1/1/13/20	5/27/105/115	-
10	CLA	A	813	-	1/1/11/20	3/13/91/115	-
13	BCR	L	306	-	-	1/29/63/63	0/2/2/2
10	CLA	A	804	-	1/1/11/20	4/13/91/115	-
10	CLA	A	845	12	1/1/11/20	5/13/91/115	-
10	CLA	A	803	18	1/1/15/20	1/37/115/115	-
14	SF4	A	853	1,2	-	-	0/6/5/5
10	CLA	A	829	-	1/1/14/20	2/31/109/115	-
10	CLA	B	824	18	1/1/12/20	2/19/97/115	-
10	CLA	A	825	-	1/1/14/20	2/31/109/115	-
10	CLA	B	830	-	1/1/11/20	2/13/91/115	-
10	CLA	A	843	18	1/1/15/20	5/37/115/115	-
10	CLA	A	826	18	1/1/15/20	7/37/115/115	-
10	CLA	B	817	-	1/1/15/20	4/37/115/115	-
10	CLA	B	826	-	1/1/15/20	6/37/115/115	-
10	CLA	B	834	-	1/1/12/20	4/21/99/115	-
10	CLA	A	835	-	1/1/15/20	2/37/115/115	-
10	CLA	B	804	-	1/1/15/20	5/37/115/115	-
10	CLA	L	304	18	1/1/11/20	0/13/91/115	-
10	CLA	A	839	-	1/1/15/20	4/37/115/115	-
15	LMU	A	859	-	-	4/12/32/61	0/1/1/2
10	CLA	A	837	1	1/1/11/20	1/13/91/115	-
10	CLA	A	817	18	1/1/11/20	1/13/91/115	-
10	CLA	A	854	18	1/1/13/20	3/25/103/115	-
10	CLA	A	856	18	1/1/12/20	0/19/97/115	-
10	CLA	B	828	-	1/1/15/20	8/37/115/115	-
12	LHG	A	846	-	-	7/45/45/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	805	10	1/1/12/20	3/19/97/115	-
13	BCR	I	101	-	-	0/29/63/63	0/2/2/2
10	CLA	A	834	-	1/1/15/20	3/37/115/115	-
13	BCR	A	849	-	-	2/29/63/63	0/2/2/2
13	BCR	A	852	-	-	4/29/63/63	0/2/2/2
15	LMU	A	857	-	-	3/15/35/61	0/1/1/2
10	CLA	B	832	-	1/1/11/20	3/13/91/115	-
10	CLA	B	820	-	1/1/11/20	4/13/91/115	-
10	CLA	A	838	-	1/1/12/20	1/21/99/115	-
9	CL0	A	801	-	3/3/20/25	2/37/135/135	-
13	BCR	A	848	-	-	4/29/63/63	0/2/2/2
10	CLA	B	803	-	1/1/11/20	4/13/91/115	-
10	CLA	B	808	2	1/1/15/20	6/37/115/115	-
13	BCR	L	301	-	-	4/29/63/63	0/2/2/2
10	CLA	B	816	-	1/1/14/20	4/31/109/115	-
10	CLA	A	842	-	1/1/11/20	2/13/91/115	-
10	CLA	B	825	-	1/1/15/20	3/37/115/115	-
13	BCR	B	843	-	-	1/29/63/63	0/2/2/2
10	CLA	B	809	-	1/1/15/20	2/37/115/115	-
10	CLA	A	807	1	1/1/15/20	6/37/115/115	-
11	PQN	A	844	-	-	0/23/43/43	0/2/2/2
14	SF4	C	101	3	-	-	0/6/5/5
10	CLA	A	828	-	1/1/15/20	2/37/115/115	-
10	CLA	A	810	1	1/1/12/20	2/19/97/115	-
10	CLA	B	810	-	1/1/13/20	4/27/105/115	-
10	CLA	L	302	8	1/1/11/20	2/13/91/115	-
13	BCR	A	850	-	-	2/29/63/63	0/2/2/2
11	PQN	B	839	-	-	3/23/43/43	0/2/2/2
10	CLA	A	811	-	1/1/11/20	1/13/91/115	-
10	CLA	A	822	18	1/1/15/20	0/37/115/115	-
10	CLA	B	837	18	1/1/15/20	3/37/115/115	-
10	CLA	B	805	2	1/1/15/20	2/37/115/115	-
10	CLA	B	814	-	1/1/13/20	5/25/103/115	-
10	CLA	A	836	-	1/1/15/20	5/37/115/115	-
10	CLA	B	831	-	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	808	-	1/1/11/20	2/16/94/115	-
10	CLA	B	815	-	1/1/13/20	4/28/106/115	-
10	CLA	A	816	-	1/1/14/20	4/31/109/115	-
13	BCR	B	842	-	-	2/29/63/63	0/2/2/2
10	CLA	B	836	-	1/1/12/20	0/19/97/115	-
17	DGD	B	844	-	-	11/50/90/95	0/2/2/2
10	CLA	B	838	-	1/1/15/20	2/37/115/115	-
10	CLA	B	806	-	1/1/14/20	4/31/109/115	-
10	CLA	A	823	-	1/1/12/20	5/22/100/115	-
10	CLA	B	823	18	1/1/13/20	5/27/105/115	-
10	CLA	A	809	1	1/1/13/20	7/25/103/115	-
12	LHG	A	847	10	-	10/35/35/53	-
10	CLA	B	801	-	1/1/15/20	4/37/115/115	-
10	CLA	B	813	-	1/1/15/20	4/37/115/115	-
10	CLA	A	802	-	1/1/15/20	0/37/115/115	-
13	BCR	L	305	-	-	2/29/63/63	0/2/2/2
10	CLA	A	827	18	1/1/13/20	1/25/103/115	-
15	LMU	A	855	-	-	4/21/61/61	0/2/2/2
10	CLA	B	827	-	1/1/15/20	8/37/115/115	-
10	CLA	L	303	-	1/1/14/20	3/31/109/115	-
10	CLA	B	807	-	1/1/15/20	5/37/115/115	-
10	CLA	B	822	-	1/1/11/20	3/13/91/115	-
10	CLA	A	812	10	1/1/15/20	7/37/115/115	-
10	CLA	A	840	-	1/1/13/20	2/25/103/115	-
16	LMG	A	858	-	-	2/38/58/70	0/1/1/1
10	CLA	B	812	-	1/1/15/20	7/37/115/115	-
14	SF4	C	102	3	-	-	0/6/5/5
10	CLA	B	835	-	1/1/13/20	2/25/103/115	-
10	CLA	A	821	-	1/1/11/20	3/13/91/115	-
10	CLA	B	802	-	1/1/15/20	1/37/115/115	-
10	CLA	A	814	-	1/1/15/20	6/37/115/115	-
10	CLA	B	821	-	1/1/11/20	5/13/91/115	-
13	BCR	B	840	-	-	1/29/63/63	0/2/2/2
10	CLA	A	824	-	1/1/11/20	3/13/91/115	-
10	CLA	B	829	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	806	-	1/1/15/20	3/37/115/115	-
10	CLA	B	811	-	1/1/11/20	3/13/91/115	-

All (274) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	801	CL0	C4B-NB	10.89	1.44	1.35
9	H	201	CL0	C4B-NB	10.55	1.44	1.35
9	H	201	CL0	C1B-NB	7.30	1.41	1.35
9	A	801	CL0	C1B-NB	6.71	1.41	1.35
10	B	823	CLA	C1D-ND	5.91	1.45	1.37
10	A	803	CLA	C1D-ND	5.88	1.45	1.37
10	A	838	CLA	C1D-ND	5.88	1.45	1.37
10	A	826	CLA	C1D-ND	5.85	1.45	1.37
10	A	817	CLA	C1D-ND	5.84	1.45	1.37
10	B	834	CLA	C1D-ND	5.82	1.44	1.37
10	A	828	CLA	C1D-ND	5.80	1.44	1.37
10	B	838	CLA	C1D-ND	5.74	1.44	1.37
10	B	812	CLA	C1D-ND	5.71	1.44	1.37
10	B	819	CLA	C1D-ND	5.69	1.44	1.37
10	B	803	CLA	C1D-ND	5.69	1.44	1.37
10	B	807	CLA	C1D-ND	5.69	1.44	1.37
10	A	829	CLA	C1D-ND	5.68	1.44	1.37
10	B	810	CLA	C1D-ND	5.68	1.44	1.37
10	A	815	CLA	C1D-ND	5.67	1.44	1.37
10	A	842	CLA	C1D-ND	5.66	1.44	1.37
10	A	839	CLA	C1D-ND	5.65	1.44	1.37
10	A	814	CLA	C1D-ND	5.64	1.44	1.37
10	A	819	CLA	C1D-ND	5.64	1.44	1.37
10	L	304	CLA	C1D-ND	5.62	1.44	1.37
10	B	801	CLA	C1D-ND	5.61	1.44	1.37
10	B	818	CLA	C1D-ND	5.61	1.44	1.37
10	A	823	CLA	C1D-ND	5.60	1.44	1.37
10	A	804	CLA	C1D-ND	5.58	1.44	1.37
10	A	845	CLA	C1D-ND	5.57	1.44	1.37
10	A	820	CLA	C1D-ND	5.55	1.44	1.37
10	B	827	CLA	C1D-ND	5.55	1.44	1.37
10	B	829	CLA	C1D-ND	5.53	1.44	1.37
10	B	808	CLA	C1D-ND	5.53	1.44	1.37
10	A	856	CLA	C1D-ND	5.53	1.44	1.37
10	B	809	CLA	C1D-ND	5.52	1.44	1.37
10	A	808	CLA	C1D-ND	5.52	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	805	CLA	C1D-ND	5.51	1.44	1.37
10	B	821	CLA	C1D-ND	5.51	1.44	1.37
10	A	806	CLA	C1D-ND	5.50	1.44	1.37
10	A	831	CLA	C1D-ND	5.50	1.44	1.37
10	B	820	CLA	C1D-ND	5.50	1.44	1.37
10	A	818	CLA	C1D-ND	5.49	1.44	1.37
10	B	816	CLA	C1D-ND	5.49	1.44	1.37
10	B	811	CLA	C1D-ND	5.49	1.44	1.37
10	A	813	CLA	C1D-ND	5.49	1.44	1.37
10	A	822	CLA	C1D-ND	5.49	1.44	1.37
10	B	836	CLA	C1D-ND	5.48	1.44	1.37
10	A	830	CLA	C1D-ND	5.48	1.44	1.37
10	A	832	CLA	C1D-ND	5.48	1.44	1.37
10	A	821	CLA	C1D-ND	5.47	1.44	1.37
10	B	817	CLA	C1D-ND	5.47	1.44	1.37
10	B	813	CLA	C1D-ND	5.47	1.44	1.37
10	B	826	CLA	C1D-ND	5.46	1.44	1.37
10	A	824	CLA	C1D-ND	5.45	1.44	1.37
10	A	837	CLA	C1D-ND	5.44	1.44	1.37
10	A	825	CLA	C1D-ND	5.43	1.44	1.37
10	A	807	CLA	C1D-ND	5.43	1.44	1.37
10	B	815	CLA	C1D-ND	5.42	1.44	1.37
10	B	822	CLA	C1D-ND	5.39	1.44	1.37
10	B	805	CLA	C1D-ND	5.38	1.44	1.37
10	A	811	CLA	C1D-ND	5.36	1.44	1.37
10	B	833	CLA	C1D-ND	5.34	1.44	1.37
10	A	834	CLA	C1D-ND	5.33	1.44	1.37
10	L	302	CLA	C1D-ND	5.33	1.44	1.37
10	A	841	CLA	C1D-ND	5.33	1.44	1.37
10	A	835	CLA	C1D-ND	5.31	1.44	1.37
10	A	843	CLA	C1D-ND	5.31	1.44	1.37
10	B	832	CLA	C1D-ND	5.31	1.44	1.37
10	B	830	CLA	C1D-ND	5.31	1.44	1.37
10	A	810	CLA	C1D-ND	5.29	1.44	1.37
10	B	804	CLA	C1D-ND	5.28	1.44	1.37
10	A	840	CLA	C1D-ND	5.28	1.44	1.37
10	B	825	CLA	C1D-ND	5.27	1.44	1.37
10	A	816	CLA	C1D-ND	5.26	1.44	1.37
10	A	809	CLA	C1D-ND	5.26	1.44	1.37
10	B	835	CLA	C1D-ND	5.26	1.44	1.37
10	B	837	CLA	C1D-ND	5.22	1.44	1.37
10	B	814	CLA	C1D-ND	5.22	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	303	CLA	C1D-ND	5.21	1.44	1.37
10	A	836	CLA	C1D-ND	5.21	1.44	1.37
10	A	812	CLA	C1D-ND	5.19	1.44	1.37
9	A	801	CL0	C1D-ND	5.19	1.44	1.37
10	B	824	CLA	C1D-ND	5.18	1.44	1.37
10	B	831	CLA	C1D-ND	5.17	1.44	1.37
10	B	806	CLA	C1D-ND	5.16	1.44	1.37
10	A	854	CLA	C1D-ND	5.14	1.44	1.37
10	A	827	CLA	C1D-ND	5.12	1.44	1.37
10	A	833	CLA	C1D-ND	5.09	1.44	1.37
9	H	201	CL0	C1D-ND	5.07	1.44	1.37
10	B	802	CLA	C1D-ND	4.94	1.43	1.37
10	A	802	CLA	C1D-ND	4.73	1.43	1.37
9	H	201	CL0	MG-NA	-4.61	1.95	2.06
10	B	828	CLA	C1D-ND	4.46	1.43	1.37
9	H	201	CL0	MG-ND	-4.44	1.97	2.05
10	A	835	CLA	MG-ND	-4.30	1.97	2.05
9	A	801	CL0	MG-ND	-4.29	1.97	2.05
10	A	824	CLA	MG-ND	-4.22	1.97	2.05
10	A	818	CLA	MG-ND	-4.20	1.97	2.05
10	B	830	CLA	MG-ND	-4.18	1.97	2.05
10	L	302	CLA	MG-ND	-4.18	1.97	2.05
10	A	810	CLA	MG-ND	-4.18	1.97	2.05
10	B	825	CLA	MG-ND	-4.18	1.97	2.05
10	A	817	CLA	MG-ND	-4.17	1.97	2.05
10	A	813	CLA	MG-ND	-4.16	1.97	2.05
10	B	811	CLA	MG-ND	-4.14	1.97	2.05
10	B	816	CLA	MG-ND	-4.14	1.97	2.05
10	A	815	CLA	MG-ND	-4.14	1.97	2.05
10	A	812	CLA	MG-ND	-4.12	1.97	2.05
10	A	832	CLA	MG-ND	-4.10	1.97	2.05
10	B	820	CLA	MG-ND	-4.10	1.97	2.05
10	A	821	CLA	MG-ND	-4.09	1.97	2.05
10	B	815	CLA	MG-ND	-4.09	1.97	2.05
10	B	805	CLA	MG-ND	-4.08	1.97	2.05
10	B	821	CLA	MG-ND	-4.08	1.97	2.05
9	A	801	CL0	MG-NA	-4.08	1.96	2.06
10	B	818	CLA	MG-ND	-4.07	1.97	2.05
10	B	814	CLA	MG-ND	-4.06	1.97	2.05
10	A	845	CLA	MG-ND	-4.06	1.97	2.05
10	A	819	CLA	MG-ND	-4.04	1.97	2.05
10	A	837	CLA	MG-ND	-4.03	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	836	CLA	MG-ND	-4.03	1.97	2.05
10	A	836	CLA	MG-ND	-4.03	1.97	2.05
10	A	826	CLA	MG-ND	-4.02	1.97	2.05
10	B	819	CLA	MG-ND	-4.02	1.97	2.05
10	A	803	CLA	MG-ND	-4.02	1.97	2.05
10	L	304	CLA	MG-ND	-4.01	1.97	2.05
10	A	825	CLA	MG-ND	-4.01	1.97	2.05
10	A	827	CLA	MG-ND	-4.01	1.97	2.05
10	B	829	CLA	MG-ND	-4.00	1.97	2.05
10	A	843	CLA	MG-ND	-4.00	1.97	2.05
10	B	810	CLA	MG-ND	-4.00	1.97	2.05
10	A	802	CLA	MG-ND	-4.00	1.97	2.05
10	B	813	CLA	MG-ND	-3.99	1.97	2.05
10	B	823	CLA	MG-ND	-3.99	1.97	2.05
10	A	811	CLA	MG-ND	-3.98	1.97	2.05
10	A	833	CLA	MG-ND	-3.97	1.97	2.05
10	B	802	CLA	MG-ND	-3.97	1.97	2.05
10	B	817	CLA	MG-ND	-3.97	1.97	2.05
10	B	812	CLA	MG-ND	-3.97	1.97	2.05
10	A	804	CLA	MG-ND	-3.96	1.97	2.05
10	B	822	CLA	MG-ND	-3.96	1.97	2.05
10	A	823	CLA	MG-ND	-3.96	1.97	2.05
10	B	831	CLA	MG-ND	-3.96	1.97	2.05
10	A	841	CLA	MG-ND	-3.95	1.97	2.05
10	A	816	CLA	MG-ND	-3.95	1.98	2.05
10	A	842	CLA	MG-ND	-3.94	1.98	2.05
10	B	809	CLA	MG-ND	-3.93	1.98	2.05
10	A	807	CLA	MG-ND	-3.93	1.98	2.05
10	A	856	CLA	MG-ND	-3.93	1.98	2.05
9	H	201	CL0	MG-NC	-3.92	1.97	2.06
10	L	303	CLA	MG-ND	-3.91	1.98	2.05
10	A	806	CLA	MG-ND	-3.91	1.98	2.05
10	A	830	CLA	MG-ND	-3.89	1.98	2.05
10	A	805	CLA	MG-ND	-3.89	1.98	2.05
10	A	808	CLA	MG-ND	-3.88	1.98	2.05
10	B	806	CLA	MG-ND	-3.88	1.98	2.05
10	B	833	CLA	MG-ND	-3.88	1.98	2.05
10	A	829	CLA	MG-ND	-3.87	1.98	2.05
10	B	804	CLA	MG-ND	-3.87	1.98	2.05
10	B	832	CLA	MG-ND	-3.86	1.98	2.05
10	A	809	CLA	MG-ND	-3.84	1.98	2.05
10	A	814	CLA	MG-ND	-3.84	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	822	CLA	MG-ND	-3.83	1.98	2.05
10	A	854	CLA	MG-ND	-3.83	1.98	2.05
10	B	837	CLA	MG-ND	-3.82	1.98	2.05
10	A	820	CLA	MG-ND	-3.79	1.98	2.05
10	B	828	CLA	MG-ND	-3.79	1.98	2.05
10	A	834	CLA	MG-ND	-3.77	1.98	2.05
10	B	835	CLA	MG-ND	-3.77	1.98	2.05
10	A	839	CLA	MG-ND	-3.77	1.98	2.05
10	B	824	CLA	MG-ND	-3.76	1.98	2.05
10	B	826	CLA	MG-ND	-3.76	1.98	2.05
10	B	808	CLA	MG-ND	-3.75	1.98	2.05
10	B	834	CLA	MG-ND	-3.70	1.98	2.05
10	B	803	CLA	MG-ND	-3.69	1.98	2.05
10	A	838	CLA	MG-ND	-3.69	1.98	2.05
10	A	828	CLA	MG-ND	-3.61	1.98	2.05
10	A	840	CLA	MG-ND	-3.60	1.98	2.05
10	B	838	CLA	MG-ND	-3.58	1.98	2.05
10	B	807	CLA	MG-ND	-3.53	1.98	2.05
10	B	827	CLA	MG-ND	-3.52	1.98	2.05
10	A	831	CLA	MG-ND	-3.50	1.98	2.05
10	B	801	CLA	MG-ND	-3.25	1.99	2.05
9	A	801	CL0	MG-NC	-3.16	1.98	2.06
10	B	807	CLA	C1D-C2D	-2.49	1.40	1.45
10	A	831	CLA	C1D-C2D	-2.45	1.40	1.45
10	B	801	CLA	C1D-C2D	-2.45	1.40	1.45
10	A	826	CLA	C1D-C2D	-2.45	1.40	1.45
10	A	805	CLA	C1D-C2D	-2.44	1.40	1.45
10	A	832	CLA	C1D-C2D	-2.43	1.40	1.45
10	B	836	CLA	C1D-C2D	-2.43	1.40	1.45
10	A	843	CLA	C1D-C2D	-2.42	1.40	1.45
10	B	809	CLA	C1D-C2D	-2.41	1.40	1.45
10	B	814	CLA	C1D-C2D	-2.41	1.40	1.45
10	B	802	CLA	C1D-C2D	-2.41	1.40	1.45
10	A	842	CLA	C1D-C2D	-2.40	1.40	1.45
10	B	816	CLA	C1D-C2D	-2.40	1.40	1.45
10	A	815	CLA	C1D-C2D	-2.40	1.40	1.45
10	A	830	CLA	C1D-C2D	-2.40	1.40	1.45
10	A	818	CLA	C1D-C2D	-2.40	1.40	1.45
10	A	829	CLA	C1D-C2D	-2.40	1.40	1.45
10	B	813	CLA	C1D-C2D	-2.39	1.40	1.45
10	B	823	CLA	C1D-C2D	-2.39	1.40	1.45
10	A	817	CLA	C1D-C2D	-2.39	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	856	CLA	C1D-C2D	-2.39	1.40	1.45
10	A	834	CLA	C1D-C2D	-2.39	1.40	1.45
10	B	805	CLA	C1D-C2D	-2.39	1.40	1.45
10	B	826	CLA	C1D-C2D	-2.39	1.40	1.45
10	B	825	CLA	C1D-C2D	-2.38	1.40	1.45
10	B	837	CLA	C1D-C2D	-2.38	1.40	1.45
10	B	834	CLA	C1D-C2D	-2.37	1.40	1.45
10	B	812	CLA	C1D-C2D	-2.37	1.40	1.45
10	A	808	CLA	C1D-C2D	-2.37	1.40	1.45
10	A	839	CLA	C1D-C2D	-2.37	1.40	1.45
10	A	838	CLA	C1D-C2D	-2.37	1.40	1.45
10	A	841	CLA	C1D-C2D	-2.37	1.40	1.45
10	B	835	CLA	C1D-C2D	-2.37	1.40	1.45
10	A	807	CLA	C1D-C2D	-2.36	1.40	1.45
10	L	304	CLA	C1D-C2D	-2.36	1.40	1.45
10	A	813	CLA	C1D-C2D	-2.36	1.40	1.45
10	A	824	CLA	C1D-C2D	-2.36	1.40	1.45
10	A	812	CLA	C1D-C2D	-2.36	1.40	1.45
10	B	815	CLA	C1D-C2D	-2.36	1.40	1.45
10	B	803	CLA	C1D-C2D	-2.36	1.40	1.45
10	B	824	CLA	C1D-C2D	-2.35	1.40	1.45
10	B	827	CLA	C1D-C2D	-2.35	1.40	1.45
10	A	810	CLA	C1D-C2D	-2.35	1.40	1.45
10	A	809	CLA	C1D-C2D	-2.35	1.40	1.45
10	A	854	CLA	C1D-C2D	-2.35	1.40	1.45
10	B	828	CLA	C1D-C2D	-2.35	1.40	1.45
10	A	802	CLA	C1D-C2D	-2.35	1.40	1.45
10	B	829	CLA	C1D-C2D	-2.35	1.40	1.45
10	B	811	CLA	C1D-C2D	-2.35	1.40	1.45
10	B	808	CLA	C1D-C2D	-2.35	1.40	1.45
10	B	819	CLA	C1D-C2D	-2.34	1.40	1.45
10	A	821	CLA	C1D-C2D	-2.34	1.40	1.45
10	A	819	CLA	C1D-C2D	-2.34	1.40	1.45
10	B	817	CLA	C1D-C2D	-2.34	1.40	1.45
10	A	835	CLA	C1D-C2D	-2.34	1.40	1.45
10	A	825	CLA	C1D-C2D	-2.34	1.40	1.45
9	H	201	CL0	C1D-C2D	-2.33	1.40	1.45
10	A	814	CLA	C1D-C2D	-2.33	1.40	1.45
10	B	810	CLA	C1D-C2D	-2.32	1.40	1.45
10	A	828	CLA	C1D-C2D	-2.31	1.40	1.45
10	A	811	CLA	C1D-C2D	-2.31	1.40	1.45
10	B	838	CLA	C1D-C2D	-2.31	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	822	CLA	C1D-C2D	-2.31	1.40	1.45
10	A	804	CLA	C1D-C2D	-2.30	1.40	1.45
10	A	816	CLA	C1D-C2D	-2.30	1.40	1.45
10	A	820	CLA	C1D-C2D	-2.30	1.40	1.45
10	A	803	CLA	C1D-C2D	-2.30	1.40	1.45
10	A	806	CLA	C1D-C2D	-2.30	1.40	1.45
10	B	818	CLA	C1D-C2D	-2.30	1.40	1.45
10	A	827	CLA	C1D-C2D	-2.30	1.40	1.45
10	A	833	CLA	C1D-C2D	-2.30	1.40	1.45
10	L	303	CLA	C1D-C2D	-2.29	1.40	1.45
10	A	822	CLA	C1D-C2D	-2.29	1.40	1.45
10	B	820	CLA	C1D-C2D	-2.29	1.40	1.45
10	L	302	CLA	C1D-C2D	-2.29	1.40	1.45
10	A	823	CLA	C1D-C2D	-2.29	1.40	1.45
10	B	804	CLA	C1D-C2D	-2.29	1.40	1.45
10	A	837	CLA	C1D-C2D	-2.28	1.40	1.45
10	A	840	CLA	C1D-C2D	-2.28	1.40	1.45
10	B	821	CLA	C1D-C2D	-2.28	1.40	1.45
10	A	845	CLA	C1D-C2D	-2.28	1.40	1.45
10	B	832	CLA	C1D-C2D	-2.28	1.40	1.45
10	B	806	CLA	C1D-C2D	-2.27	1.40	1.45
10	A	836	CLA	C1D-C2D	-2.27	1.40	1.45
10	B	833	CLA	C1D-C2D	-2.27	1.40	1.45
10	B	831	CLA	C1D-C2D	-2.26	1.40	1.45
10	B	830	CLA	C1D-C2D	-2.26	1.40	1.45
9	A	801	CL0	C1D-C2D	-2.23	1.40	1.45
9	A	801	CL0	C1C-C2C	2.07	1.48	1.44
10	B	828	CLA	C3D-C4D	-2.02	1.39	1.44

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	831	CLA	C1D-ND-C4D	-4.27	103.30	106.33
10	A	820	CLA	C1D-ND-C4D	-4.25	103.31	106.33
10	A	828	CLA	C1D-ND-C4D	-4.21	103.34	106.33
10	A	804	CLA	C1D-ND-C4D	-4.21	103.34	106.33
10	B	807	CLA	C1D-ND-C4D	-4.20	103.35	106.33
10	B	833	CLA	C1D-ND-C4D	-4.19	103.36	106.33
10	B	818	CLA	C1D-ND-C4D	-4.19	103.36	106.33
10	A	811	CLA	C1D-ND-C4D	-4.17	103.37	106.33
10	B	817	CLA	C1D-ND-C4D	-4.17	103.38	106.33
10	A	822	CLA	C1D-ND-C4D	-4.16	103.38	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	835	CLA	C1D-ND-C4D	-4.16	103.38	106.33
10	A	816	CLA	C1D-ND-C4D	-4.16	103.38	106.33
10	A	839	CLA	C1D-ND-C4D	-4.16	103.38	106.33
10	A	845	CLA	C1D-ND-C4D	-4.15	103.39	106.33
10	B	804	CLA	C1D-ND-C4D	-4.14	103.40	106.33
10	A	823	CLA	C1D-ND-C4D	-4.13	103.40	106.33
10	B	838	CLA	C1D-ND-C4D	-4.12	103.41	106.33
10	B	834	CLA	C1D-ND-C4D	-4.12	103.41	106.33
10	A	837	CLA	C1D-ND-C4D	-4.12	103.41	106.33
9	H	201	CL0	CHC-C1C-NC	4.11	130.44	124.20
10	A	808	CLA	C1D-ND-C4D	-4.10	103.42	106.33
10	B	819	CLA	C1D-ND-C4D	-4.08	103.43	106.33
10	B	820	CLA	C1D-ND-C4D	-4.08	103.44	106.33
10	A	814	CLA	C1D-ND-C4D	-4.06	103.45	106.33
10	B	829	CLA	C1D-ND-C4D	-4.06	103.45	106.33
10	B	812	CLA	C1D-ND-C4D	-4.06	103.45	106.33
10	B	815	CLA	C1D-ND-C4D	-4.06	103.45	106.33
10	B	830	CLA	C1D-ND-C4D	-4.06	103.45	106.33
10	A	856	CLA	C1D-ND-C4D	-4.05	103.46	106.33
10	B	832	CLA	C1D-ND-C4D	-4.04	103.47	106.33
10	A	806	CLA	C1D-ND-C4D	-4.04	103.47	106.33
10	A	813	CLA	C1D-ND-C4D	-4.04	103.47	106.33
10	A	817	CLA	C1D-ND-C4D	-4.03	103.47	106.33
10	B	827	CLA	C1D-ND-C4D	-4.02	103.48	106.33
10	B	837	CLA	C1D-ND-C4D	-4.01	103.48	106.33
10	B	822	CLA	C1D-ND-C4D	-4.01	103.48	106.33
10	B	811	CLA	C1D-ND-C4D	-4.00	103.49	106.33
10	A	824	CLA	C1D-ND-C4D	-4.00	103.49	106.33
10	L	303	CLA	C1D-ND-C4D	-4.00	103.49	106.33
10	A	812	CLA	C1D-ND-C4D	-3.98	103.51	106.33
10	A	825	CLA	C1D-ND-C4D	-3.98	103.51	106.33
10	A	840	CLA	C1D-ND-C4D	-3.97	103.52	106.33
10	B	810	CLA	C1D-ND-C4D	-3.97	103.52	106.33
10	A	818	CLA	C1D-ND-C4D	-3.96	103.52	106.33
10	A	809	CLA	C1D-ND-C4D	-3.96	103.52	106.33
10	A	854	CLA	C1D-ND-C4D	-3.96	103.52	106.33
10	B	803	CLA	C1D-ND-C4D	-3.96	103.52	106.33
10	A	832	CLA	C1D-ND-C4D	-3.96	103.53	106.33
10	A	836	CLA	C1D-ND-C4D	-3.94	103.53	106.33
9	A	801	CL0	C1D-ND-C4D	-3.94	103.53	106.33
10	B	809	CLA	C1D-ND-C4D	-3.94	103.54	106.33
10	A	841	CLA	C1D-ND-C4D	-3.94	103.54	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	827	CLA	C1D-ND-C4D	-3.94	103.54	106.33
10	A	831	CLA	C1D-ND-C4D	-3.93	103.54	106.33
10	L	302	CLA	C1D-ND-C4D	-3.93	103.54	106.33
9	H	201	CL0	C1D-ND-C4D	-3.93	103.55	106.33
10	A	810	CLA	C1D-ND-C4D	-3.93	103.55	106.33
10	B	824	CLA	C1D-ND-C4D	-3.93	103.55	106.33
10	A	838	CLA	C1D-ND-C4D	-3.91	103.56	106.33
10	A	833	CLA	C1D-ND-C4D	-3.91	103.56	106.33
10	A	821	CLA	C1D-ND-C4D	-3.90	103.56	106.33
10	B	814	CLA	C1D-ND-C4D	-3.90	103.56	106.33
10	B	821	CLA	C1D-ND-C4D	-3.90	103.57	106.33
9	H	201	CL0	CHD-C1D-ND	-3.88	120.89	124.45
10	A	815	CLA	C1D-ND-C4D	-3.87	103.59	106.33
10	B	806	CLA	C1D-ND-C4D	-3.86	103.59	106.33
10	A	807	CLA	C1D-ND-C4D	-3.86	103.59	106.33
10	A	803	CLA	C1D-ND-C4D	-3.85	103.60	106.33
10	A	819	CLA	C1D-ND-C4D	-3.85	103.60	106.33
10	A	842	CLA	C1D-ND-C4D	-3.84	103.60	106.33
10	A	843	CLA	C1D-ND-C4D	-3.84	103.60	106.33
10	L	304	CLA	C1D-ND-C4D	-3.84	103.60	106.33
10	B	813	CLA	C1D-ND-C4D	-3.84	103.61	106.33
10	A	805	CLA	C1D-ND-C4D	-3.83	103.61	106.33
10	A	829	CLA	C1D-ND-C4D	-3.82	103.62	106.33
10	A	834	CLA	C1D-ND-C4D	-3.82	103.62	106.33
10	B	816	CLA	C1D-ND-C4D	-3.82	103.62	106.33
10	B	808	CLA	C1D-ND-C4D	-3.82	103.62	106.33
10	B	823	CLA	C1D-ND-C4D	-3.82	103.62	106.33
10	A	835	CLA	C1D-ND-C4D	-3.82	103.62	106.33
9	A	801	CL0	CHD-C1D-ND	-3.80	120.96	124.45
10	A	826	CLA	C1D-ND-C4D	-3.79	103.64	106.33
10	B	828	CLA	C1D-ND-C4D	-3.78	103.65	106.33
10	B	836	CLA	C1D-ND-C4D	-3.78	103.65	106.33
10	B	801	CLA	C1D-ND-C4D	-3.77	103.66	106.33
10	A	802	CLA	C1D-ND-C4D	-3.76	103.66	106.33
10	B	826	CLA	C1D-ND-C4D	-3.71	103.70	106.33
10	A	830	CLA	C1D-ND-C4D	-3.66	103.73	106.33
10	B	825	CLA	C1D-ND-C4D	-3.65	103.74	106.33
9	A	801	CL0	CHC-C1C-NC	3.64	129.73	124.20
10	A	802	CLA	CHD-C1D-ND	-3.63	121.11	124.45
10	B	805	CLA	C1D-ND-C4D	-3.61	103.77	106.33
10	B	831	CLA	CHD-C1D-ND	-3.55	121.19	124.45
10	B	833	CLA	CHD-C1D-ND	-3.51	121.23	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	832	CLA	CHD-C1D-ND	-3.47	121.27	124.45
10	L	303	CLA	CHD-C1D-ND	-3.47	121.27	124.45
10	A	820	CLA	CHD-C1D-ND	-3.45	121.28	124.45
10	B	828	CLA	CHD-C1D-ND	-3.45	121.28	124.45
10	A	822	CLA	CHD-C1D-ND	-3.45	121.28	124.45
10	A	854	CLA	CHD-C1D-ND	-3.45	121.28	124.45
10	A	813	CLA	CHD-C1D-ND	-3.44	121.29	124.45
10	A	811	CLA	CHD-C1D-ND	-3.44	121.30	124.45
9	H	201	CL0	CHC-C1C-C2C	-3.43	117.24	126.72
10	B	804	CLA	CHD-C1D-ND	-3.41	121.32	124.45
10	B	829	CLA	CHD-C1D-ND	-3.40	121.33	124.45
10	B	817	CLA	CHD-C1D-ND	-3.40	121.33	124.45
10	A	837	CLA	CHD-C1D-ND	-3.38	121.35	124.45
10	B	820	CLA	CHD-C1D-ND	-3.38	121.35	124.45
10	B	818	CLA	CHD-C1D-ND	-3.37	121.36	124.45
10	A	833	CLA	CHD-C1D-ND	-3.36	121.36	124.45
10	A	812	CLA	CHD-C1D-ND	-3.36	121.36	124.45
10	B	806	CLA	CHD-C1D-ND	-3.36	121.37	124.45
10	B	802	CLA	C1D-ND-C4D	-3.36	103.95	106.33
10	A	824	CLA	CHD-C1D-ND	-3.35	121.37	124.45
10	B	822	CLA	CHD-C1D-ND	-3.34	121.38	124.45
10	A	845	CLA	CHD-C1D-ND	-3.34	121.38	124.45
10	B	825	CLA	CHD-C1D-ND	-3.34	121.38	124.45
10	A	825	CLA	CHD-C1D-ND	-3.34	121.39	124.45
10	A	836	CLA	CHD-C1D-ND	-3.34	121.39	124.45
10	A	828	CLA	CHD-C1D-ND	-3.33	121.39	124.45
10	A	840	CLA	CHD-C1D-ND	-3.33	121.39	124.45
10	B	809	CLA	CHD-C1D-ND	-3.33	121.40	124.45
10	B	835	CLA	CHD-C1D-ND	-3.33	121.40	124.45
10	A	806	CLA	CHD-C1D-ND	-3.33	121.40	124.45
10	A	835	CLA	CHD-C1D-ND	-3.32	121.40	124.45
10	B	830	CLA	CHD-C1D-ND	-3.32	121.41	124.45
10	B	802	CLA	CHD-C1D-ND	-3.31	121.41	124.45
10	L	302	CLA	CHD-C1D-ND	-3.31	121.41	124.45
10	A	803	CLA	CHD-C1D-ND	-3.31	121.41	124.45
10	A	814	CLA	CHD-C1D-ND	-3.31	121.42	124.45
10	B	811	CLA	CHD-C1D-ND	-3.30	121.42	124.45
10	B	824	CLA	CHD-C1D-ND	-3.30	121.42	124.45
10	A	804	CLA	CHD-C1D-ND	-3.30	121.42	124.45
10	B	837	CLA	CHD-C1D-ND	-3.30	121.42	124.45
10	B	819	CLA	CHD-C1D-ND	-3.29	121.43	124.45
10	A	809	CLA	CHD-C1D-ND	-3.26	121.46	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	816	CLA	CHD-C1D-ND	-3.26	121.46	124.45
10	B	821	CLA	CHD-C1D-ND	-3.26	121.46	124.45
10	A	823	CLA	CHD-C1D-ND	-3.24	121.47	124.45
10	A	821	CLA	CHD-C1D-ND	-3.24	121.48	124.45
10	B	838	CLA	CHD-C1D-ND	-3.24	121.48	124.45
10	A	827	CLA	CHD-C1D-ND	-3.23	121.48	124.45
10	A	807	CLA	CHD-C1D-ND	-3.23	121.49	124.45
10	A	810	CLA	CHD-C1D-ND	-3.22	121.50	124.45
10	B	814	CLA	CHD-C1D-ND	-3.22	121.50	124.45
10	A	841	CLA	CHD-C1D-ND	-3.21	121.50	124.45
10	L	304	CLA	CHD-C1D-ND	-3.20	121.51	124.45
10	A	808	CLA	CHD-C1D-ND	-3.20	121.52	124.45
10	B	808	CLA	CHD-C1D-ND	-3.19	121.52	124.45
10	B	827	CLA	CHD-C1D-ND	-3.19	121.52	124.45
10	B	815	CLA	CHD-C1D-ND	-3.19	121.53	124.45
10	A	856	CLA	CHD-C1D-ND	-3.18	121.53	124.45
10	B	834	CLA	CHD-C1D-ND	-3.18	121.53	124.45
10	B	803	CLA	CHD-C1D-ND	-3.18	121.53	124.45
9	A	801	CL0	CHC-C1C-C2C	-3.18	117.93	126.72
10	B	807	CLA	CHD-C1D-ND	-3.17	121.54	124.45
10	A	834	CLA	CHD-C1D-ND	-3.17	121.54	124.45
10	B	810	CLA	CHD-C1D-ND	-3.16	121.55	124.45
10	B	816	CLA	CHD-C1D-ND	-3.15	121.56	124.45
10	A	838	CLA	CHD-C1D-ND	-3.13	121.58	124.45
10	A	839	CLA	CHD-C1D-ND	-3.13	121.58	124.45
10	B	812	CLA	CHD-C1D-ND	-3.12	121.58	124.45
10	A	817	CLA	CHD-C1D-ND	-3.12	121.59	124.45
10	A	832	CLA	CHD-C1D-ND	-3.12	121.59	124.45
10	A	829	CLA	CHD-C1D-ND	-3.11	121.59	124.45
10	A	819	CLA	CHD-C1D-ND	-3.10	121.60	124.45
10	A	818	CLA	CHD-C1D-ND	-3.08	121.62	124.45
10	B	813	CLA	CHD-C1D-ND	-3.08	121.63	124.45
10	A	831	CLA	CHD-C1D-ND	-3.06	121.64	124.45
10	A	830	CLA	CHD-C1D-ND	-3.04	121.66	124.45
10	B	836	CLA	CHD-C1D-ND	-3.04	121.66	124.45
10	A	826	CLA	CHD-C1D-ND	-3.04	121.66	124.45
10	A	805	CLA	CHD-C1D-ND	-3.03	121.67	124.45
10	B	823	CLA	CHD-C1D-ND	-3.03	121.67	124.45
10	A	815	CLA	CHD-C1D-ND	-3.03	121.67	124.45
10	A	843	CLA	CHD-C1D-ND	-3.03	121.67	124.45
10	B	805	CLA	CHD-C1D-ND	-3.03	121.67	124.45
10	B	801	CLA	CHD-C1D-ND	-2.99	121.70	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	826	CLA	CHD-C1D-ND	-2.97	121.72	124.45
13	A	852	BCR	C23-C24-C25	2.97	135.54	127.20
10	A	842	CLA	CHD-C1D-ND	-2.91	121.78	124.45
9	A	801	CL0	C2C-C1C-NC	2.49	112.31	109.97
9	H	201	CL0	C2C-C1C-NC	2.40	112.22	109.97
10	B	827	CLA	O2A-C1-C2	2.34	114.79	108.64
10	B	826	CLA	O2A-C1-C2	-2.17	102.92	108.64
10	A	854	CLA	C1-C2-C3	2.16	129.78	126.04
9	A	801	CL0	CHA-C1A-NA	-2.12	121.54	126.40
10	B	831	CLA	C3D-C4D-ND	2.10	113.64	110.24
13	L	305	BCR	C23-C24-C25	2.07	133.03	127.20
10	A	803	CLA	C4A-NA-C1A	2.06	107.63	106.71
9	H	201	CL0	CHA-C1A-NA	-2.03	121.76	126.40
10	B	802	CLA	C4A-NA-C1A	2.02	107.61	106.71

All (92) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	801	CL0	ND
9	A	801	CL0	NA
9	A	801	CL0	NC
9	H	201	CL0	ND
9	H	201	CL0	NA
9	H	201	CL0	NC
10	A	802	CLA	ND
10	A	803	CLA	ND
10	A	804	CLA	ND
10	A	805	CLA	ND
10	A	806	CLA	ND
10	A	807	CLA	ND
10	A	808	CLA	ND
10	A	809	CLA	ND
10	A	810	CLA	ND
10	A	811	CLA	ND
10	A	812	CLA	ND
10	A	813	CLA	ND
10	A	814	CLA	ND
10	A	815	CLA	ND
10	A	816	CLA	ND
10	A	817	CLA	ND
10	A	818	CLA	ND
10	A	819	CLA	ND

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Mol	Chain	Res	Type	Atom
10	A	820	CLA	ND
10	A	821	CLA	ND
10	A	822	CLA	ND
10	A	823	CLA	ND
10	A	824	CLA	ND
10	A	825	CLA	ND
10	A	826	CLA	ND
10	A	827	CLA	ND
10	A	828	CLA	ND
10	A	829	CLA	ND
10	A	830	CLA	ND
10	A	831	CLA	ND
10	A	832	CLA	ND
10	A	833	CLA	ND
10	A	834	CLA	ND
10	A	835	CLA	ND
10	A	836	CLA	ND
10	A	837	CLA	ND
10	A	838	CLA	ND
10	A	839	CLA	ND
10	A	840	CLA	ND
10	A	841	CLA	ND
10	A	842	CLA	ND
10	A	843	CLA	ND
10	A	845	CLA	ND
10	A	854	CLA	ND
10	A	856	CLA	ND
10	B	801	CLA	ND
10	B	802	CLA	ND
10	B	803	CLA	ND
10	B	804	CLA	ND
10	B	805	CLA	ND
10	B	806	CLA	ND
10	B	807	CLA	ND
10	B	808	CLA	ND
10	B	809	CLA	ND
10	B	810	CLA	ND
10	B	811	CLA	ND
10	B	812	CLA	ND
10	B	813	CLA	ND
10	B	814	CLA	ND
10	B	815	CLA	ND

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Mol	Chain	Res	Type	Atom
10	B	816	CLA	ND
10	B	817	CLA	ND
10	B	818	CLA	ND
10	B	819	CLA	ND
10	B	820	CLA	ND
10	B	821	CLA	ND
10	B	822	CLA	ND
10	B	823	CLA	ND
10	B	824	CLA	ND
10	B	825	CLA	ND
10	B	826	CLA	ND
10	B	827	CLA	ND
10	B	828	CLA	ND
10	B	829	CLA	ND
10	B	830	CLA	ND
10	B	831	CLA	ND
10	B	832	CLA	ND
10	B	833	CLA	ND
10	B	834	CLA	ND
10	B	835	CLA	ND
10	B	836	CLA	ND
10	B	837	CLA	ND
10	B	838	CLA	ND
10	L	302	CLA	ND
10	L	303	CLA	ND
10	L	304	CLA	ND

All (379) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	812	CLA	CHA-CBD-CGD-O2D
10	A	818	CLA	CHA-CBD-CGD-O2D
10	A	819	CLA	C1A-C2A-CAA-CBA
10	A	819	CLA	C3A-C2A-CAA-CBA
10	A	823	CLA	C2-C3-C5-C6
10	A	823	CLA	C4-C3-C5-C6
10	A	825	CLA	CHA-CBD-CGD-O1D
10	A	825	CLA	CHA-CBD-CGD-O2D
10	A	830	CLA	C2A-CAA-CBA-CGA
10	A	835	CLA	CHA-CBD-CGD-O1D
10	A	835	CLA	CHA-CBD-CGD-O2D
10	A	843	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	A	843	CLA	C4-C3-C5-C6
10	A	845	CLA	CHA-CBD-CGD-O1D
10	A	845	CLA	CHA-CBD-CGD-O2D
10	A	845	CLA	CAD-CBD-CGD-O1D
10	B	803	CLA	C1A-C2A-CAA-CBA
10	B	804	CLA	C1A-C2A-CAA-CBA
10	B	808	CLA	C2-C3-C5-C6
10	B	808	CLA	C4-C3-C5-C6
10	B	821	CLA	CAD-CBD-CGD-O1D
10	B	821	CLA	CAD-CBD-CGD-O2D
10	B	822	CLA	CHA-CBD-CGD-O1D
10	B	822	CLA	CHA-CBD-CGD-O2D
10	B	823	CLA	C1A-C2A-CAA-CBA
10	B	824	CLA	CHA-CBD-CGD-O2D
10	B	825	CLA	C11-C10-C8-C9
10	B	827	CLA	C1A-C2A-CAA-CBA
10	B	827	CLA	C3A-C2A-CAA-CBA
10	B	829	CLA	C1A-C2A-CAA-CBA
10	B	834	CLA	C2-C3-C5-C6
10	B	834	CLA	C4-C3-C5-C6
12	A	846	LHG	C1-C2-C3-O3
12	A	846	LHG	C3-O3-P-O4
12	A	847	LHG	C3-O3-P-O4
12	A	847	LHG	C3-O3-P-O5
12	B	845	LHG	C4-O6-P-O4
12	B	845	LHG	C4-O6-P-O5
13	A	848	BCR	C1-C6-C7-C8
13	B	841	BCR	C1-C6-C7-C8
13	B	841	BCR	C5-C6-C7-C8
13	L	301	BCR	C23-C24-C25-C30
15	A	855	LMU	O5'-C1'-O1'-C1
15	A	857	LMU	C2'-C1'-O1'-C1
15	A	857	LMU	O5'-C1'-O1'-C1
15	A	859	LMU	C2'-C1'-O1'-C1
15	A	859	LMU	O5'-C1'-O1'-C1
15	A	859	LMU	C2-C1-O1'-C1'
10	A	836	CLA	C4-C3-C5-C6
10	B	837	CLA	C2A-CAA-CBA-CGA
12	A	846	LHG	O2-C2-C3-O3
12	B	845	LHG	O2-C2-C3-O3
10	A	836	CLA	C3-C5-C6-C7
10	A	812	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	A	812	CLA	C2-C3-C5-C6
10	B	813	CLA	C2A-CAA-CBA-CGA
12	B	845	LHG	C1-C2-C3-O3
12	A	847	LHG	O7-C5-C6-O8
10	A	836	CLA	C2-C3-C5-C6
10	B	826	CLA	C11-C12-C13-C14
11	B	839	PQN	C24-C23-C25-C26
10	B	808	CLA	C13-C15-C16-C17
15	A	855	LMU	C5'-C4'-O1B-C1B
10	B	812	CLA	C8-C10-C11-C12
12	A	846	LHG	C3-O3-P-O6
12	A	847	LHG	C3-O3-P-O6
12	A	847	LHG	C4-O6-P-O3
12	B	845	LHG	C4-O6-P-O3
10	B	818	CLA	C4-C3-C5-C6
17	B	844	DGD	C2B-C3B-C4B-C5B
10	B	835	CLA	C6-C7-C8-C9
17	B	844	DGD	C2D-C1D-O3G-C3G
10	A	839	CLA	C14-C13-C15-C16
10	B	814	CLA	C2A-CAA-CBA-CGA
10	B	807	CLA	C3-C5-C6-C7
10	B	835	CLA	C6-C7-C8-C10
10	B	823	CLA	C3A-C2A-CAA-CBA
10	A	843	CLA	O2A-C1-C2-C3
10	A	820	CLA	C4-C3-C5-C6
10	A	826	CLA	C4-C3-C5-C6
10	A	828	CLA	C4-C3-C5-C6
10	B	837	CLA	C4-C3-C5-C6
10	A	820	CLA	C2-C3-C5-C6
10	A	828	CLA	C2-C3-C5-C6
10	B	837	CLA	C2-C3-C5-C6
13	A	848	BCR	C5-C6-C7-C8
13	A	848	BCR	C23-C24-C25-C30
13	A	850	BCR	C1-C6-C7-C8
13	A	850	BCR	C5-C6-C7-C8
13	A	851	BCR	C1-C6-C7-C8
13	A	851	BCR	C5-C6-C7-C8
13	B	842	BCR	C23-C24-C25-C26
13	B	842	BCR	C23-C24-C25-C30
13	L	301	BCR	C23-C24-C25-C26
12	B	845	LHG	C12-C13-C14-C15
10	A	815	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
10	A	815	CLA	C2-C3-C5-C6
10	A	826	CLA	C2-C3-C5-C6
10	A	839	CLA	C11-C12-C13-C15
10	B	809	CLA	C2-C3-C5-C6
10	B	810	CLA	C2-C3-C5-C6
10	B	826	CLA	C11-C12-C13-C15
10	B	827	CLA	C2-C3-C5-C6
10	B	828	CLA	C11-C10-C8-C7
15	A	855	LMU	C3'-C4'-O1B-C1B
10	B	816	CLA	C2A-CAA-CBA-CGA
17	B	844	DGD	O6D-C1D-O3G-C3G
15	A	855	LMU	C2'-C1'-O1'-C1
16	A	858	LMG	C2-C1-O1-C7
15	A	859	LMU	O5'-C5'-C6'-O6'
12	B	845	LHG	C13-C14-C15-C16
10	B	809	CLA	C4-C3-C5-C6
10	B	827	CLA	C4-C3-C5-C6
10	B	818	CLA	C2-C3-C5-C6
10	A	839	CLA	C11-C12-C13-C14
10	B	828	CLA	C14-C13-C15-C16
10	A	803	CLA	C2A-CAA-CBA-CGA
10	A	821	CLA	C1A-C2A-CAA-CBA
10	B	821	CLA	C1A-C2A-CAA-CBA
10	B	822	CLA	C1A-C2A-CAA-CBA
10	A	807	CLA	C5-C6-C7-C8
12	B	845	LHG	C5-C4-O6-P
10	B	806	CLA	C4-C3-C5-C6
10	B	810	CLA	C4-C3-C5-C6
17	B	844	DGD	O1G-C1G-C2G-C3G
10	A	834	CLA	C4-C3-C5-C6
10	A	819	CLA	CAA-CBA-CGA-O2A
10	A	826	CLA	C11-C10-C8-C7
10	A	820	CLA	C14-C13-C15-C16
10	A	826	CLA	C11-C10-C8-C9
10	B	812	CLA	C6-C7-C8-C9
12	A	846	LHG	C24-C25-C26-C27
10	A	807	CLA	C15-C16-C17-C18
10	L	303	CLA	C10-C11-C12-C13
10	A	834	CLA	C2-C3-C5-C6
10	A	809	CLA	C3A-C2A-CAA-CBA
10	B	803	CLA	C3A-C2A-CAA-CBA
10	B	804	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
10	B	813	CLA	C15-C16-C17-C18
15	A	857	LMU	C2-C1-O1'-C1'
12	A	847	LHG	C4-C5-C6-O8
10	B	814	CLA	O2A-C1-C2-C3
10	A	841	CLA	C4-C3-C5-C6
17	B	844	DGD	O1G-C1G-C2G-O2G
10	A	805	CLA	C2-C1-O2A-CGA
10	A	809	CLA	C2-C1-O2A-CGA
10	A	823	CLA	C2-C1-O2A-CGA
10	A	854	CLA	C2-C1-O2A-CGA
10	B	806	CLA	C11-C10-C8-C9
10	A	816	CLA	C8-C10-C11-C12
12	A	847	LHG	C5-C4-O6-P
10	A	810	CLA	C2A-CAA-CBA-CGA
13	A	848	BCR	C23-C24-C25-C26
13	A	849	BCR	C1-C6-C7-C8
13	A	849	BCR	C5-C6-C7-C8
10	A	820	CLA	C12-C13-C15-C16
10	B	806	CLA	C2-C3-C5-C6
10	B	812	CLA	C6-C7-C8-C10
10	A	805	CLA	CAD-CBD-CGD-O2D
10	A	832	CLA	CAD-CBD-CGD-O2D
10	A	838	CLA	CAD-CBD-CGD-O2D
10	B	811	CLA	CAD-CBD-CGD-O2D
10	B	815	CLA	CAD-CBD-CGD-O2D
10	B	819	CLA	CAD-CBD-CGD-O2D
10	B	834	CLA	CAD-CBD-CGD-O2D
10	A	816	CLA	C2-C3-C5-C6
10	A	841	CLA	C2-C3-C5-C6
10	A	829	CLA	C11-C12-C13-C15
10	A	806	CLA	CHA-CBD-CGD-O1D
10	A	806	CLA	CHA-CBD-CGD-O2D
10	A	812	CLA	CHA-CBD-CGD-O1D
10	A	818	CLA	CHA-CBD-CGD-O1D
10	A	831	CLA	CHA-CBD-CGD-O1D
10	A	840	CLA	CHA-CBD-CGD-O1D
10	A	840	CLA	CHA-CBD-CGD-O2D
10	B	807	CLA	CHA-CBD-CGD-O1D
10	B	807	CLA	CHA-CBD-CGD-O2D
10	B	810	CLA	CHA-CBD-CGD-O1D
10	B	810	CLA	CHA-CBD-CGD-O2D
10	B	820	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
10	B	824	CLA	CHA-CBD-CGD-O1D
10	B	834	CLA	CHA-CBD-CGD-O1D
10	A	816	CLA	C4-C3-C5-C6
10	B	817	CLA	C14-C13-C15-C16
10	L	303	CLA	C11-C10-C8-C9
10	A	809	CLA	C1A-C2A-CAA-CBA
10	A	854	CLA	C1A-C2A-CAA-CBA
10	B	819	CLA	C1A-C2A-CAA-CBA
10	A	820	CLA	C15-C16-C17-C18
12	B	845	LHG	C3-O3-P-O6
12	B	845	LHG	O6-C4-C5-C6
10	A	814	CLA	C8-C10-C11-C12
10	A	804	CLA	CAD-CBD-CGD-O1D
10	A	806	CLA	CAD-CBD-CGD-O1D
12	B	845	LHG	C25-C26-C27-C28
10	A	814	CLA	C11-C10-C8-C7
10	A	854	CLA	C3A-C2A-CAA-CBA
10	B	817	CLA	C6-C7-C8-C10
12	B	845	LHG	O6-C4-C5-O7
16	A	858	LMG	O8-C28-C29-C30
10	A	829	CLA	C11-C10-C8-C9
9	H	201	CL0	C2-C1-O2A-CGA
10	B	814	CLA	C2-C1-O2A-CGA
10	B	827	CLA	C2-C1-O2A-CGA
10	A	807	CLA	C3-C5-C6-C7
13	B	843	BCR	C1-C6-C7-C8
10	B	826	CLA	C3-C5-C6-C7
10	B	827	CLA	C2A-CAA-CBA-CGA
10	B	826	CLA	C4-C3-C5-C6
10	B	828	CLA	C11-C10-C8-C9
10	B	830	CLA	CAA-CBA-CGA-O1A
10	A	820	CLA	C16-C17-C18-C20
10	B	815	CLA	C4-C3-C5-C6
10	A	821	CLA	CAA-CBA-CGA-O2A
10	A	809	CLA	C2-C3-C5-C6
10	B	815	CLA	C2-C3-C5-C6
17	B	844	DGD	C9A-CAA-CBA-CCA
10	A	818	CLA	CAA-CBA-CGA-O2A
10	B	801	CLA	C2-C1-O2A-CGA
10	B	838	CLA	C16-C17-C18-C20
17	B	844	DGD	C3B-C4B-C5B-C6B
17	B	844	DGD	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
10	A	809	CLA	C4-C3-C5-C6
12	B	845	LHG	C30-C31-C32-C33
10	B	826	CLA	C2-C3-C5-C6
10	A	810	CLA	CAA-CBA-CGA-O2A
10	A	812	CLA	C6-C7-C8-C9
10	B	816	CLA	C11-C10-C8-C9
10	A	845	CLA	CAA-CBA-CGA-O1A
13	A	852	BCR	C11-C10-C9-C34
13	A	852	BCR	C16-C17-C18-C36
13	B	841	BCR	C11-C10-C9-C34
13	B	841	BCR	C20-C21-C22-C37
13	L	301	BCR	C20-C21-C22-C37
10	A	819	CLA	C2A-CAA-CBA-CGA
9	H	201	CL0	C6-C7-C8-C10
10	B	820	CLA	CAA-CBA-CGA-O1A
10	B	830	CLA	CAA-CBA-CGA-O2A
10	B	816	CLA	C1A-C2A-CAA-CBA
10	B	826	CLA	C1A-C2A-CAA-CBA
11	B	839	PQN	C17-C18-C20-C21
10	A	818	CLA	CAA-CBA-CGA-O1A
10	A	842	CLA	CAA-CBA-CGA-O2A
10	B	831	CLA	CAA-CBA-CGA-O2A
10	B	831	CLA	CAA-CBA-CGA-O1A
12	B	845	LHG	C11-C12-C13-C14
10	B	820	CLA	CAA-CBA-CGA-O2A
10	B	804	CLA	C4-C3-C5-C6
10	B	807	CLA	C4-C3-C5-C6
12	A	847	LHG	O2-C2-C3-O3
10	A	842	CLA	CAA-CBA-CGA-O1A
10	A	845	CLA	CAA-CBA-CGA-O2A
10	B	832	CLA	CAA-CBA-CGA-O2A
10	A	812	CLA	C3-C5-C6-C7
13	A	852	BCR	C11-C10-C9-C8
13	A	852	BCR	C16-C17-C18-C19
13	B	841	BCR	C11-C10-C9-C8
13	B	841	BCR	C20-C21-C22-C23
13	L	301	BCR	C20-C21-C22-C23
10	A	821	CLA	CAA-CBA-CGA-O1A
10	L	302	CLA	CAA-CBA-CGA-O2A
10	B	808	CLA	C2-C1-O2A-CGA
10	B	833	CLA	CAA-CBA-CGA-O2A
13	B	840	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	L	305	BCR	C23-C24-C25-C30
13	L	306	BCR	C23-C24-C25-C30
10	B	832	CLA	CAA-CBA-CGA-O1A
10	B	833	CLA	CAA-CBA-CGA-O1A
10	B	817	CLA	C4-C3-C5-C6
10	A	804	CLA	CAA-CBA-CGA-O2A
10	A	832	CLA	CAA-CBA-CGA-O2A
10	L	302	CLA	CAA-CBA-CGA-O1A
10	B	838	CLA	C15-C16-C17-C18
10	B	811	CLA	CAA-CBA-CGA-O2A
9	H	201	CL0	C6-C7-C8-C9
10	L	303	CLA	C11-C12-C13-C14
10	B	811	CLA	CAA-CBA-CGA-O1A
12	B	845	LHG	C32-C33-C34-C35
10	A	819	CLA	CAA-CBA-CGA-O1A
10	A	839	CLA	C12-C13-C15-C16
10	B	829	CLA	CAA-CBA-CGA-O2A
10	B	803	CLA	CAA-CBA-CGA-O2A
10	A	813	CLA	CAA-CBA-CGA-O1A
10	B	804	CLA	C2-C3-C5-C6
10	A	814	CLA	C11-C10-C8-C9
10	B	817	CLA	C6-C7-C8-C9
10	A	807	CLA	CAA-CBA-CGA-O2A
10	A	807	CLA	CAD-CBD-CGD-O2D
10	A	813	CLA	CAD-CBD-CGD-O2D
10	A	814	CLA	CAD-CBD-CGD-O2D
10	A	815	CLA	CAD-CBD-CGD-O2D
10	A	816	CLA	CAD-CBD-CGD-O2D
10	A	817	CLA	CAD-CBD-CGD-O2D
10	A	823	CLA	CAD-CBD-CGD-O2D
10	A	827	CLA	CAD-CBD-CGD-O2D
10	A	834	CLA	CAD-CBD-CGD-O2D
10	B	820	CLA	CAD-CBD-CGD-O2D
10	B	828	CLA	CAD-CBD-CGD-O2D
10	A	814	CLA	CAA-CBA-CGA-O2A
10	B	828	CLA	C4-C3-C5-C6
10	A	832	CLA	CAA-CBA-CGA-O1A
10	B	807	CLA	C2-C3-C5-C6
10	A	826	CLA	CAA-CBA-CGA-O2A
12	A	846	LHG	O8-C23-C24-C25
10	A	804	CLA	CAA-CBA-CGA-O1A
10	A	826	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
10	B	829	CLA	CAA-CBA-CGA-O1A
10	A	804	CLA	CHA-CBD-CGD-O1D
10	A	809	CLA	CHA-CBD-CGD-O1D
10	A	809	CLA	CHA-CBD-CGD-O2D
10	A	824	CLA	CHA-CBD-CGD-O1D
10	A	824	CLA	CHA-CBD-CGD-O2D
10	A	831	CLA	CHA-CBD-CGD-O2D
10	B	801	CLA	CHA-CBD-CGD-O1D
10	B	801	CLA	CHA-CBD-CGD-O2D
10	B	812	CLA	CHA-CBD-CGD-O2D
10	B	813	CLA	CHA-CBD-CGD-O1D
10	B	813	CLA	CHA-CBD-CGD-O2D
10	B	814	CLA	CHA-CBD-CGD-O1D
10	B	814	CLA	CHA-CBD-CGD-O2D
10	B	821	CLA	CHA-CBD-CGD-O1D
10	B	821	CLA	CHA-CBD-CGD-O2D
10	B	823	CLA	CHA-CBD-CGD-O1D
10	B	823	CLA	CHA-CBD-CGD-O2D
10	B	825	CLA	CHA-CBD-CGD-O2D
10	B	832	CLA	CHA-CBD-CGD-O1D
10	B	823	CLA	C2-C3-C5-C6
10	B	803	CLA	CAA-CBA-CGA-O1A
10	B	805	CLA	CAA-CBA-CGA-O2A
10	A	836	CLA	CAA-CBA-CGA-O2A
10	B	808	CLA	CAA-CBA-CGA-O2A
17	B	844	DGD	O2G-C1B-C2B-C3B
10	A	808	CLA	CAA-CBA-CGA-O2A
10	B	812	CLA	C4-C3-C5-C6
10	A	812	CLA	C6-C7-C8-C10
10	B	827	CLA	CAA-CBA-CGA-O2A
17	B	844	DGD	C6B-C7B-C8B-C9B
10	A	843	CLA	CAA-CBA-CGA-O2A
10	A	823	CLA	C2A-CAA-CBA-CGA
10	B	802	CLA	C2A-CAA-CBA-CGA
10	B	815	CLA	C2A-CAA-CBA-CGA
10	A	813	CLA	CAA-CBA-CGA-O2A
10	A	826	CLA	CAA-CBA-CGA-O1A
10	A	807	CLA	CAA-CBA-CGA-O1A
10	A	805	CLA	C1A-C2A-CAA-CBA
10	B	806	CLA	C1A-C2A-CAA-CBA
10	B	812	CLA	C1A-C2A-CAA-CBA
9	A	801	CL0	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
12	A	846	LHG	O10-C23-C24-C25
10	A	824	CLA	CAA-CBA-CGA-O2A
10	B	805	CLA	CAA-CBA-CGA-O1A
10	B	828	CLA	C2-C3-C5-C6
12	A	847	LHG	C4-O6-P-O4
12	A	847	LHG	C4-O6-P-O5
10	B	827	CLA	CAA-CBA-CGA-O1A
13	L	305	BCR	C23-C24-C25-C26
10	B	812	CLA	C16-C17-C18-C20
10	A	814	CLA	CAA-CBA-CGA-O1A
9	H	201	CL0	CAD-CBD-CGD-O1D
10	A	830	CLA	C11-C10-C8-C9
10	A	843	CLA	CAA-CBA-CGA-O1A
10	B	804	CLA	CAA-CBA-CGA-O2A
9	A	801	CL0	CAA-CBA-CGA-O2A
10	A	808	CLA	CAA-CBA-CGA-O1A
10	B	816	CLA	C11-C10-C8-C7
10	B	825	CLA	C11-C10-C8-C7
10	B	828	CLA	C3A-C2A-CAA-CBA
10	B	829	CLA	C3A-C2A-CAA-CBA
11	B	839	PQN	C22-C23-C25-C26
10	A	836	CLA	CAA-CBA-CGA-O1A
10	B	808	CLA	CAA-CBA-CGA-O1A
10	A	811	CLA	CAA-CBA-CGA-O2A
10	B	801	CLA	CAA-CBA-CGA-O2A
12	B	845	LHG	O9-C7-C8-C9
17	B	844	DGD	O1B-C1B-C2B-C3B
12	B	845	LHG	O7-C7-C8-C9
12	B	845	LHG	C33-C34-C35-C36
10	B	828	CLA	CAA-CBA-CGA-O2A
10	A	837	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

72 monomers are involved in 98 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	845	LHG	6	0
10	B	833	CLA	3	0
10	A	815	CLA	3	0
13	B	841	BCR	1	0
10	A	830	CLA	1	0
10	A	841	CLA	1	0

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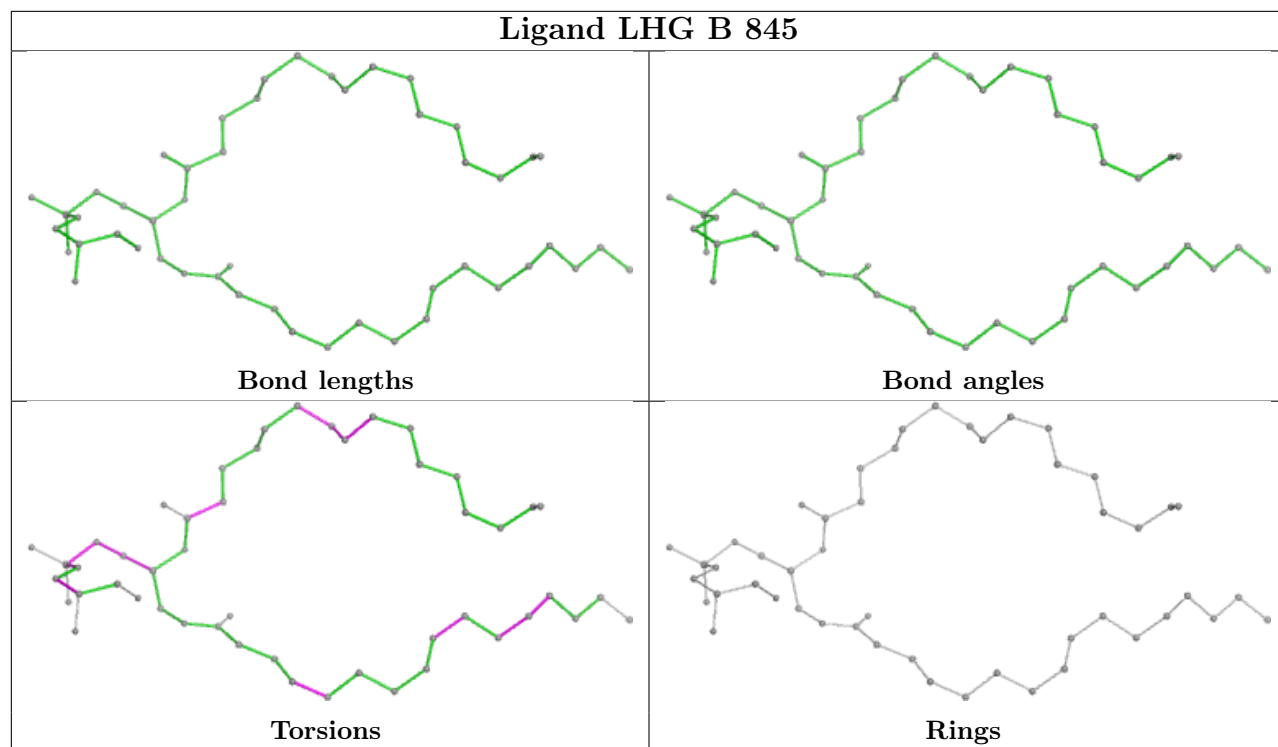
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	832	CLA	1	0
13	A	851	BCR	2	0
9	H	201	CL0	1	0
10	A	820	CLA	1	0
10	B	818	CLA	3	0
10	A	819	CLA	2	0
13	L	306	BCR	1	0
10	A	804	CLA	1	0
10	A	803	CLA	1	0
10	B	824	CLA	2	0
10	A	825	CLA	1	0
10	A	843	CLA	3	0
10	A	826	CLA	3	0
10	B	826	CLA	1	0
10	L	304	CLA	2	0
15	A	859	LMU	1	0
10	A	837	CLA	1	0
10	A	817	CLA	1	0
10	A	854	CLA	2	0
10	B	828	CLA	1	0
10	A	805	CLA	1	0
13	I	101	BCR	2	0
13	A	849	BCR	2	0
13	A	852	BCR	7	0
13	A	848	BCR	2	0
10	B	803	CLA	1	0
10	B	808	CLA	1	0
13	L	301	BCR	1	0
10	B	816	CLA	2	0
10	A	842	CLA	1	0
10	B	825	CLA	3	0
13	B	843	BCR	1	0
11	A	844	PQN	1	0
10	A	828	CLA	2	0
10	A	810	CLA	1	0
10	L	302	CLA	1	0
13	A	850	BCR	3	0
11	B	839	PQN	1	0
10	A	822	CLA	4	0
10	B	837	CLA	1	0
10	B	814	CLA	1	0
10	A	836	CLA	2	0

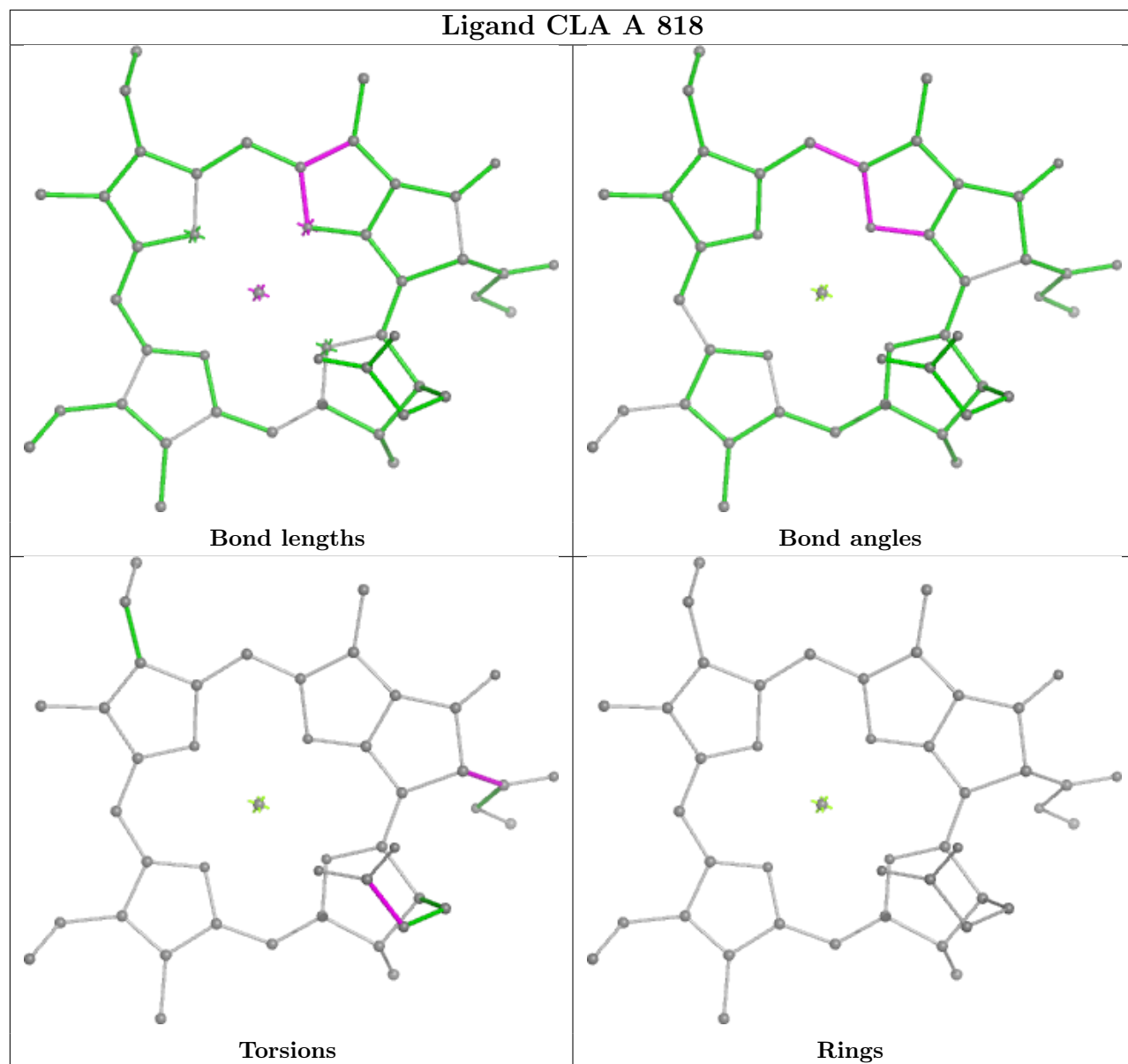
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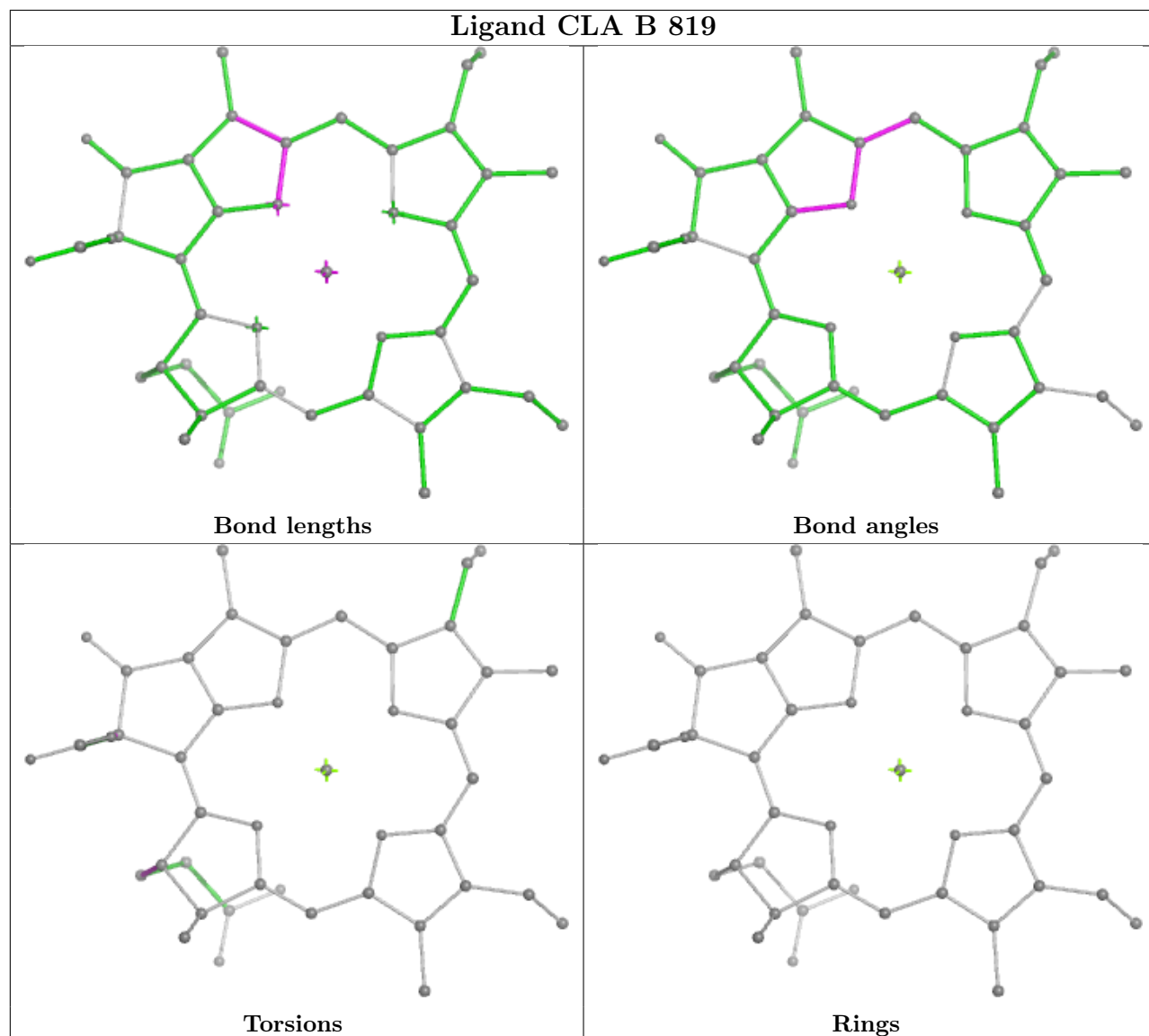
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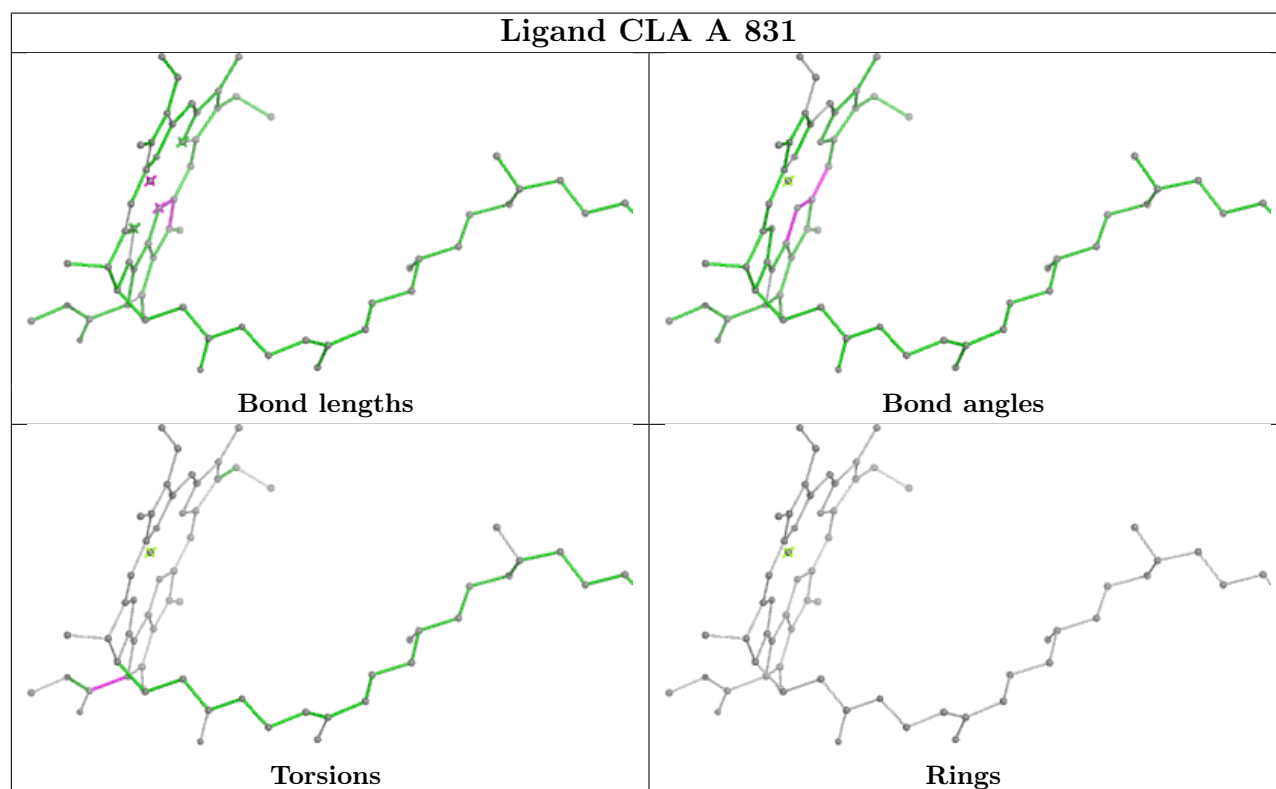
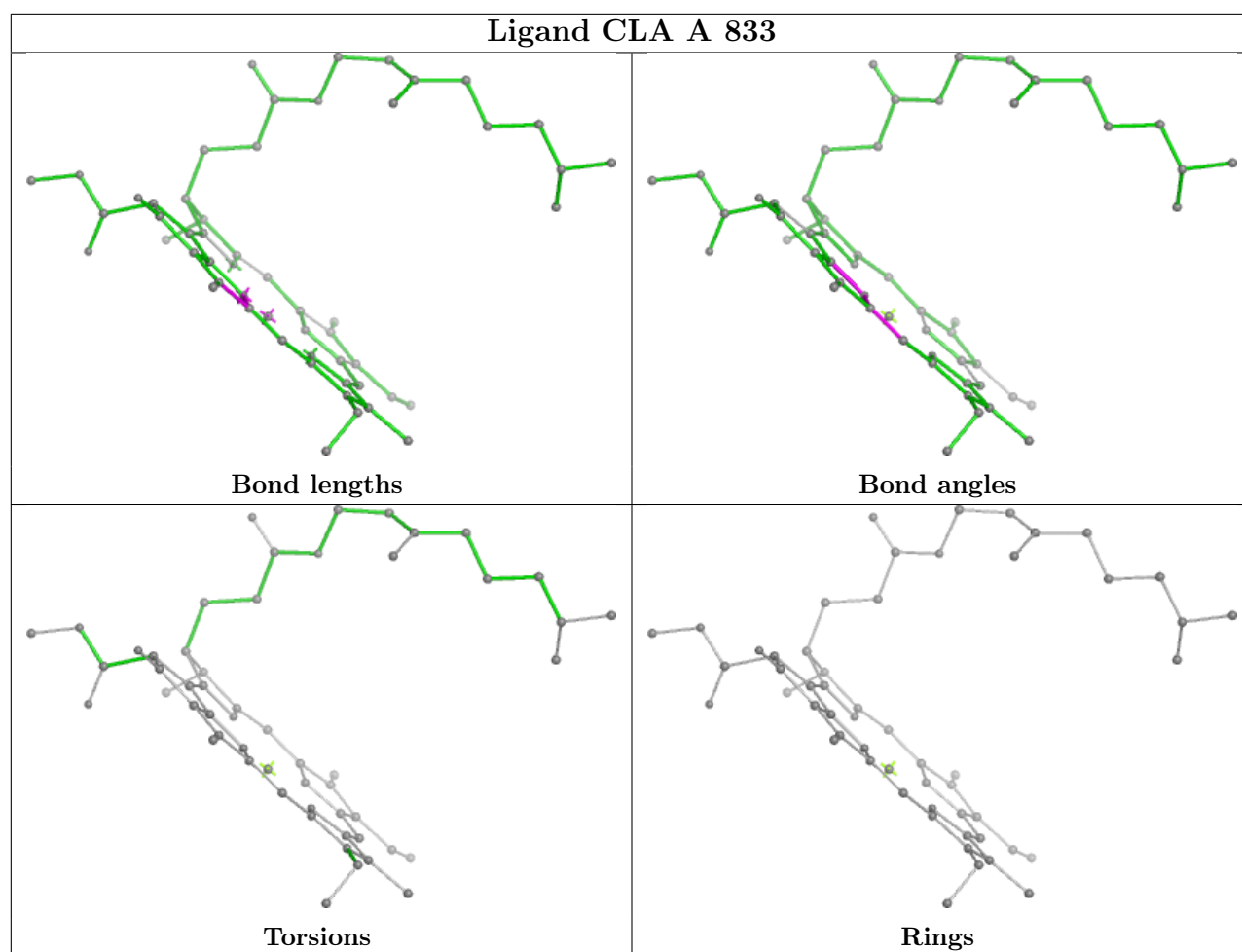
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	831	CLA	1	0
10	A	808	CLA	1	0
13	B	842	BCR	5	0
17	B	844	DGD	1	0
10	B	806	CLA	3	0
10	B	823	CLA	1	0
10	A	809	CLA	2	0
12	A	847	LHG	3	0
10	B	801	CLA	1	0
10	B	813	CLA	4	0
10	A	802	CLA	2	0
13	L	305	BCR	1	0
15	A	855	LMU	2	0
10	B	827	CLA	2	0
10	B	807	CLA	2	0
10	B	822	CLA	1	0
10	A	812	CLA	2	0
16	A	858	LMG	1	0
10	B	812	CLA	1	0
10	B	802	CLA	2	0
10	A	814	CLA	2	0
10	B	821	CLA	1	0
13	B	840	BCR	1	0
10	B	829	CLA	2	0

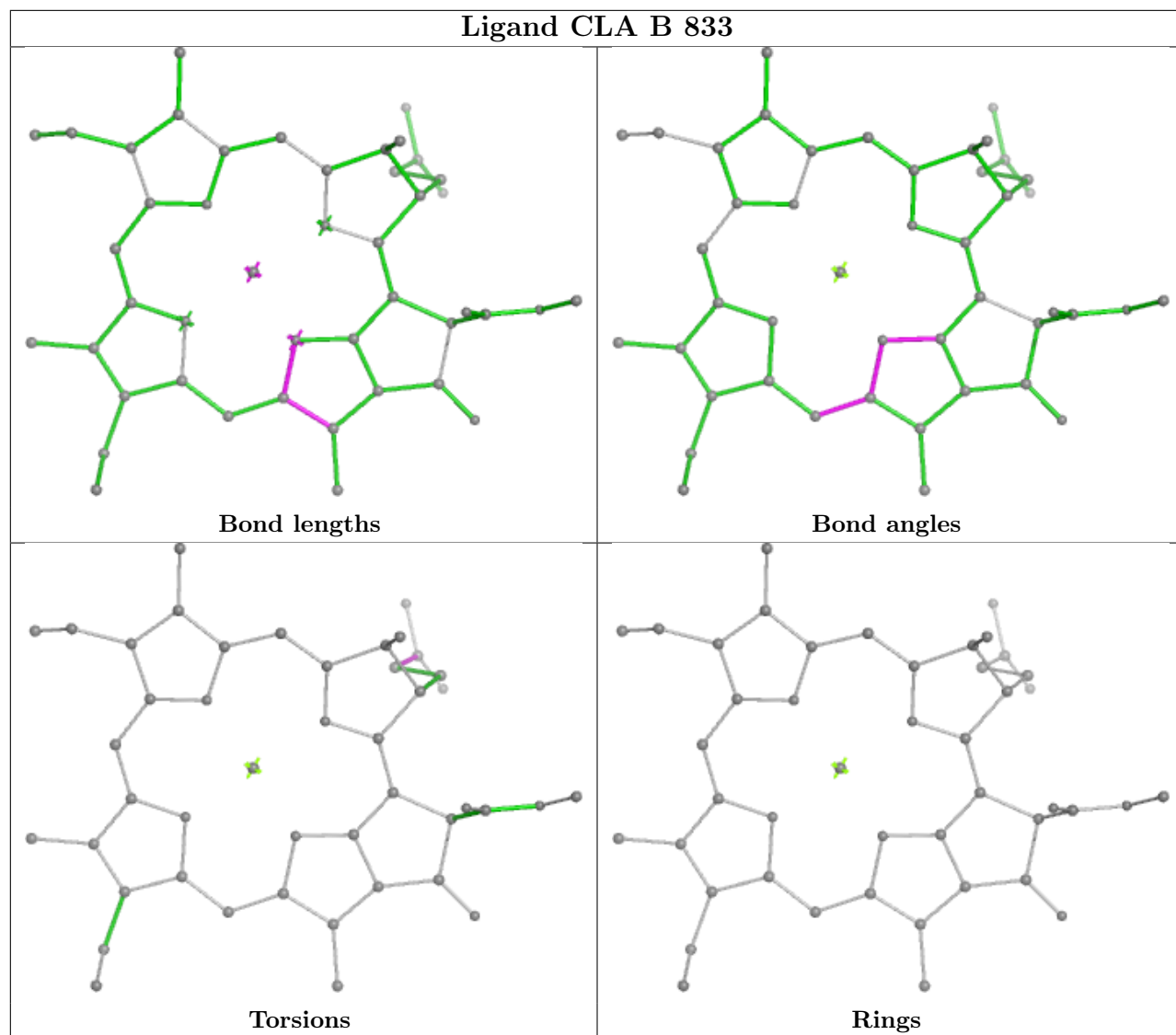
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

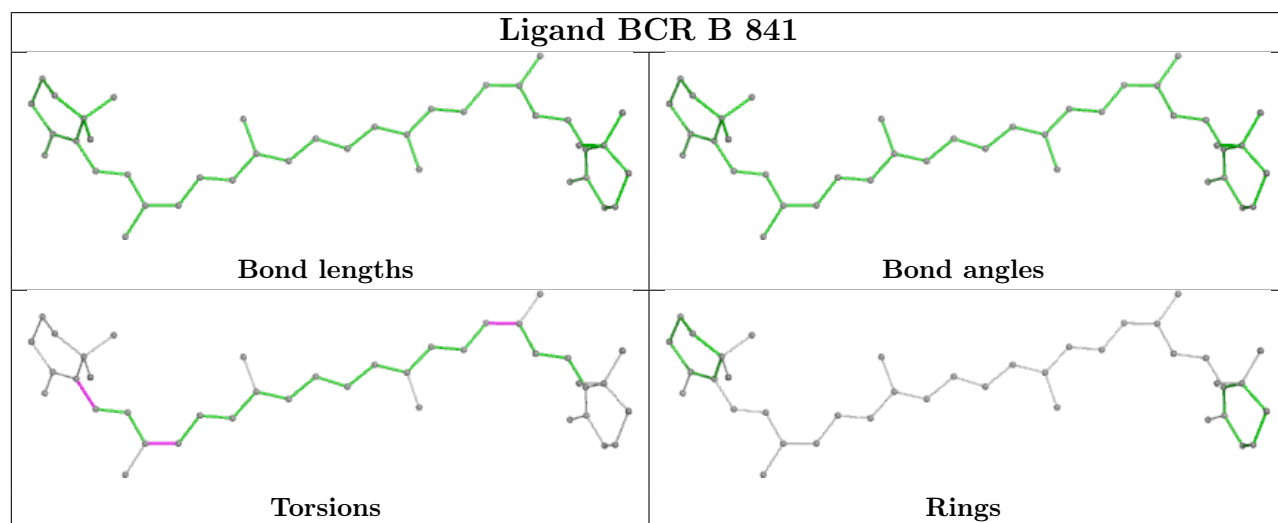
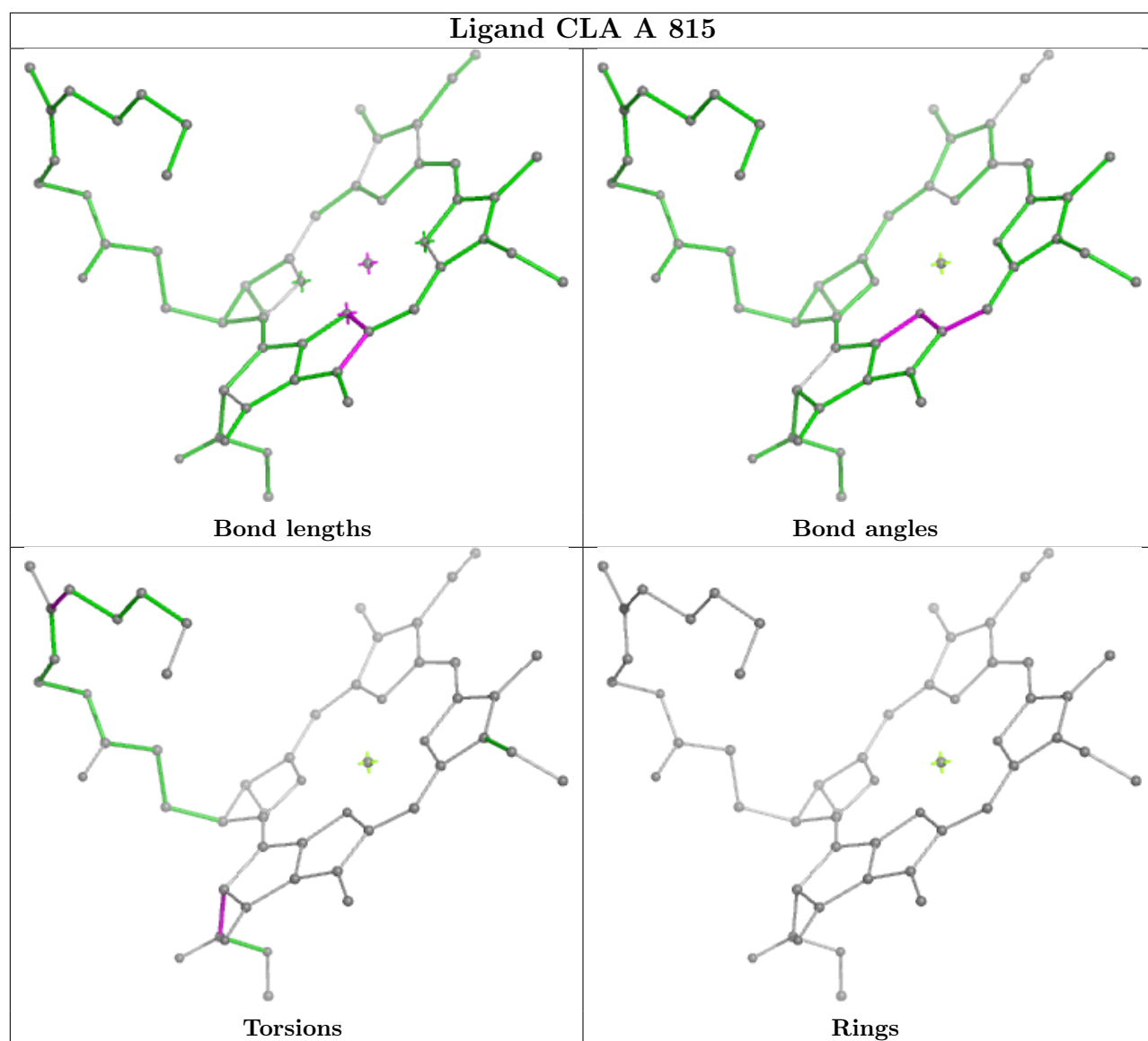




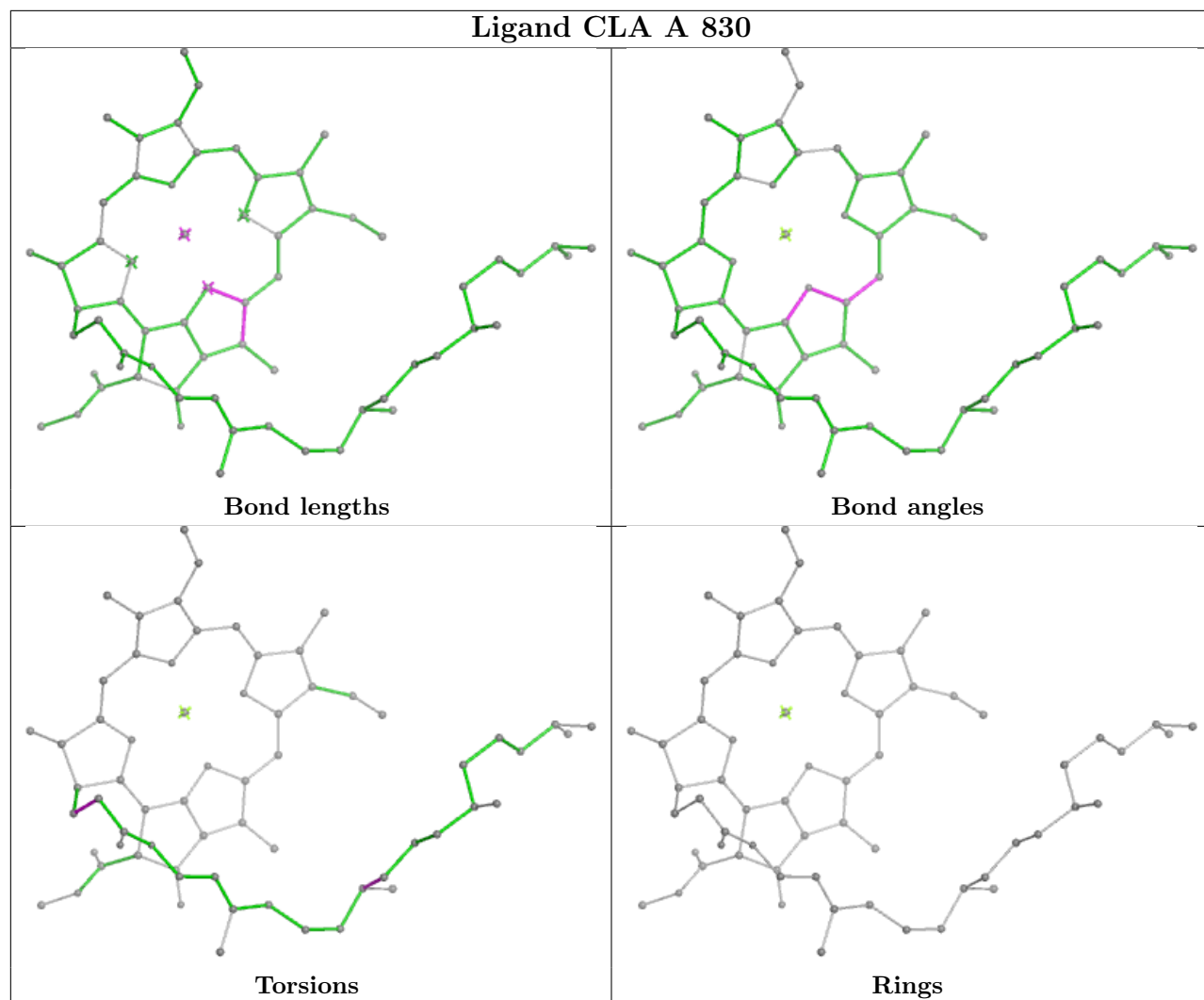


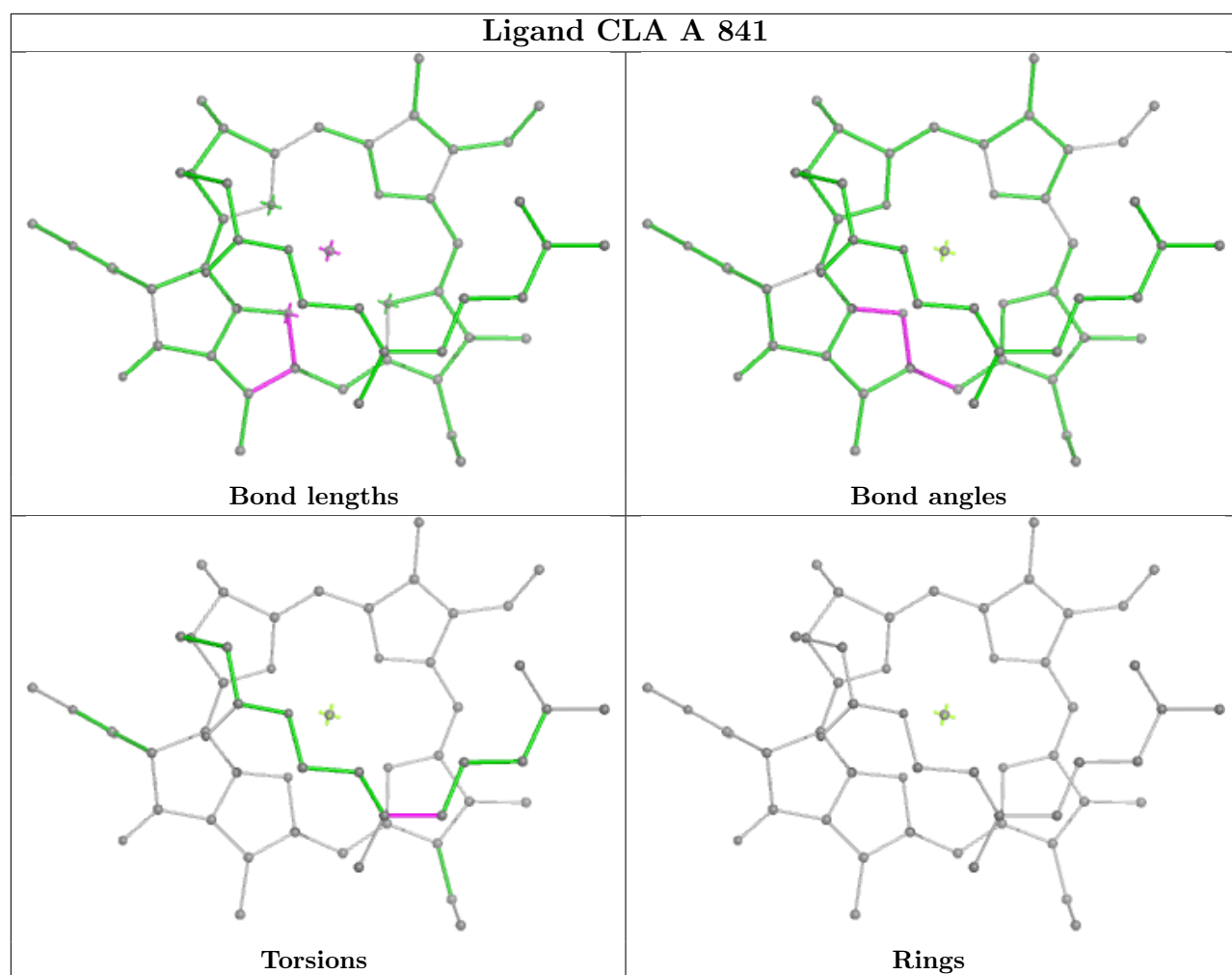


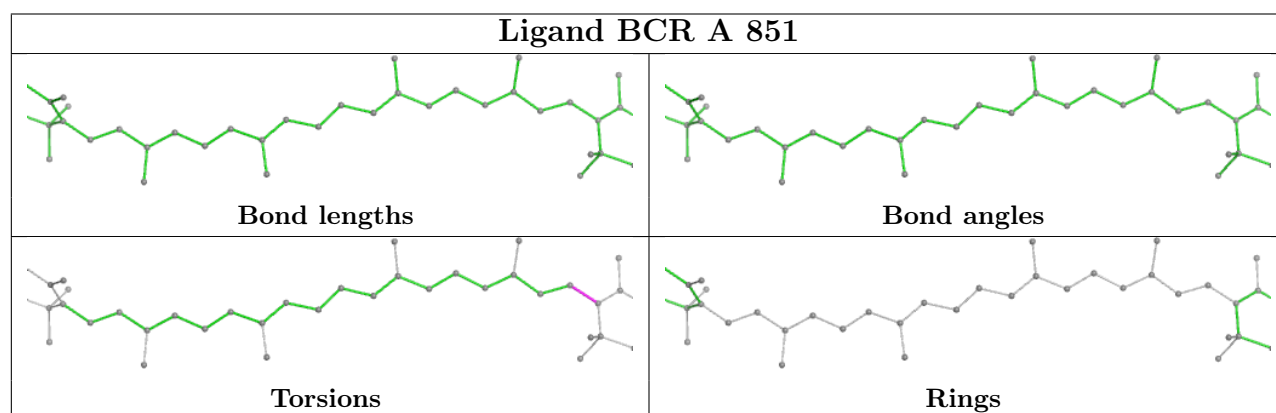
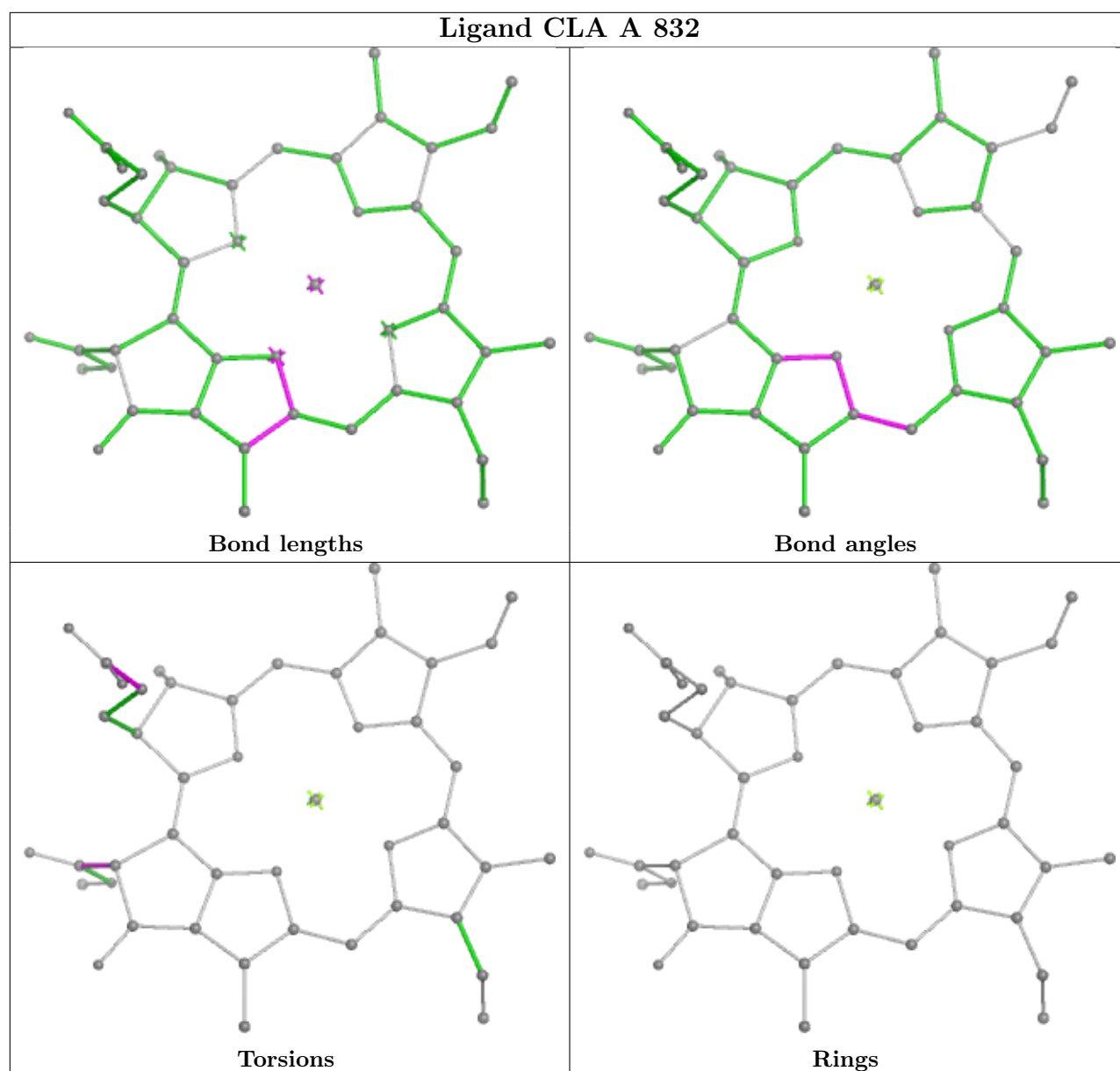


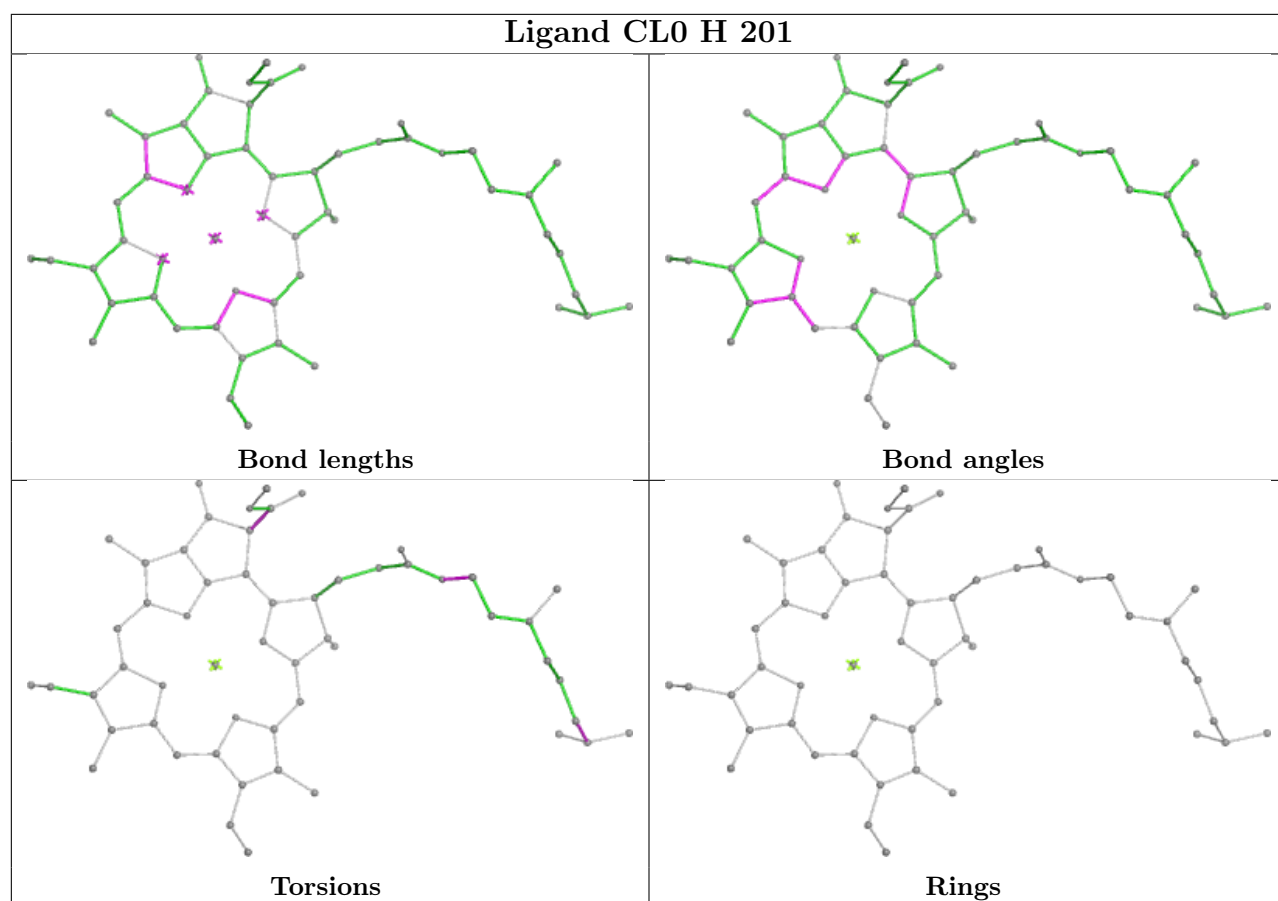


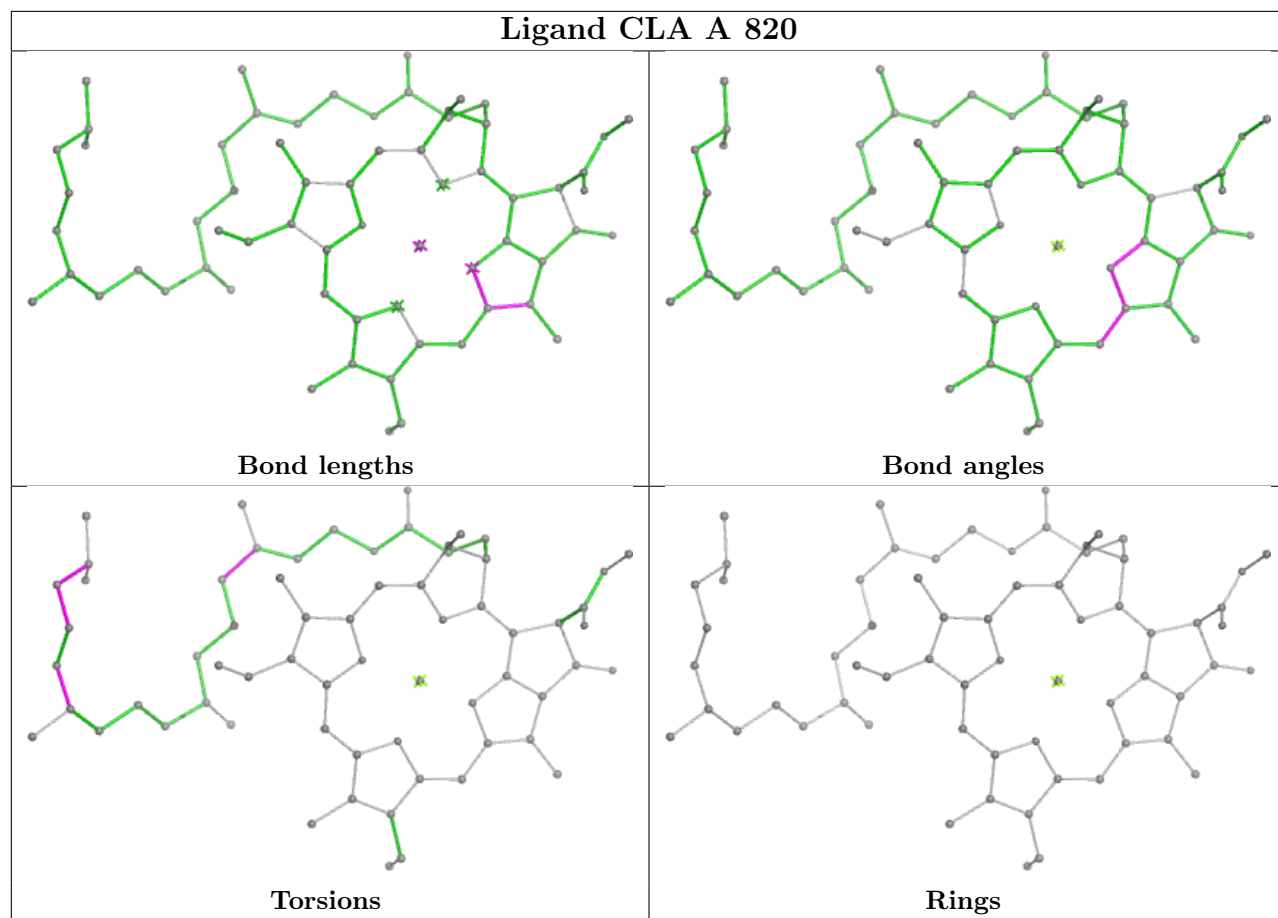
Ligand CLA A 830

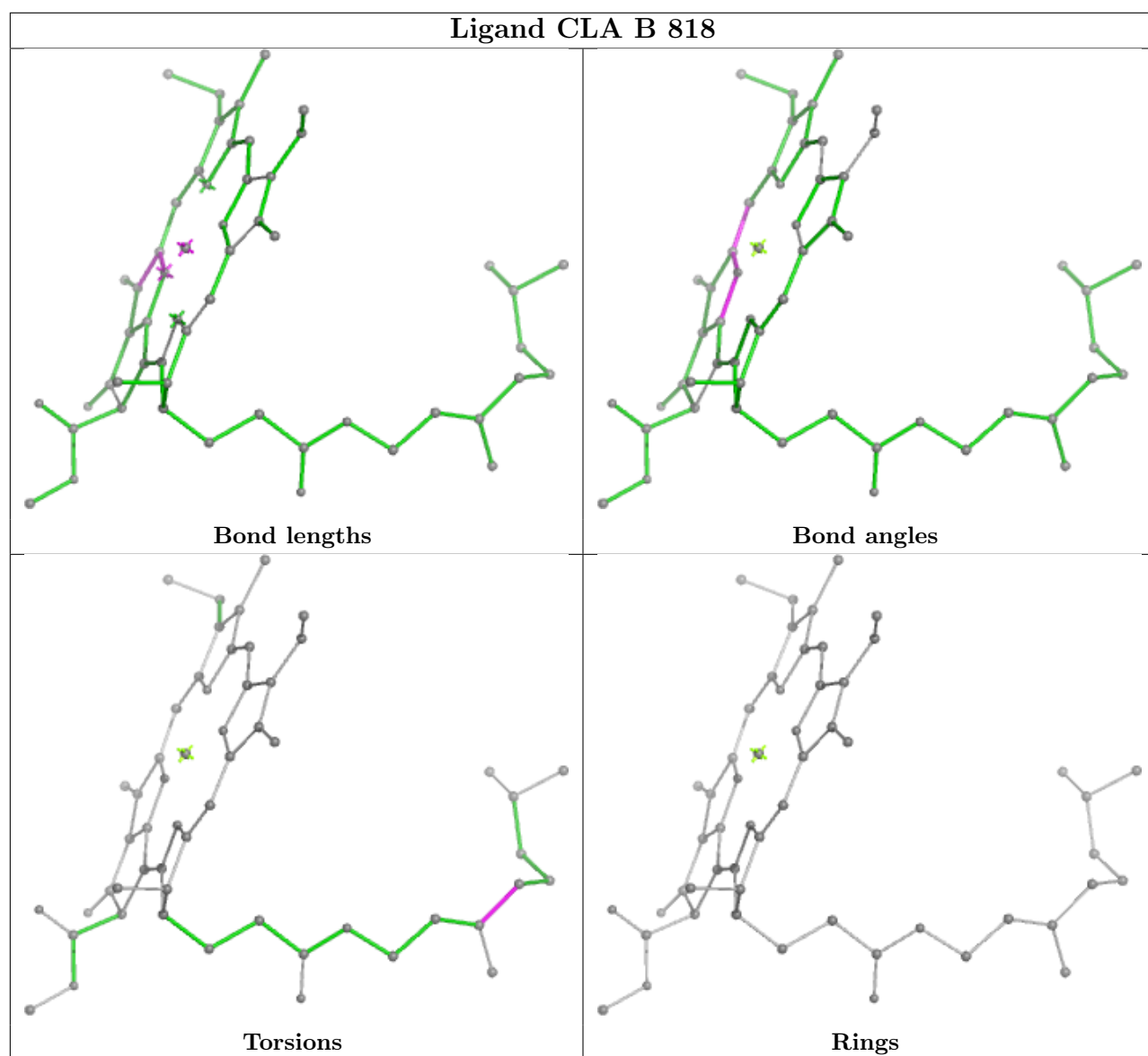




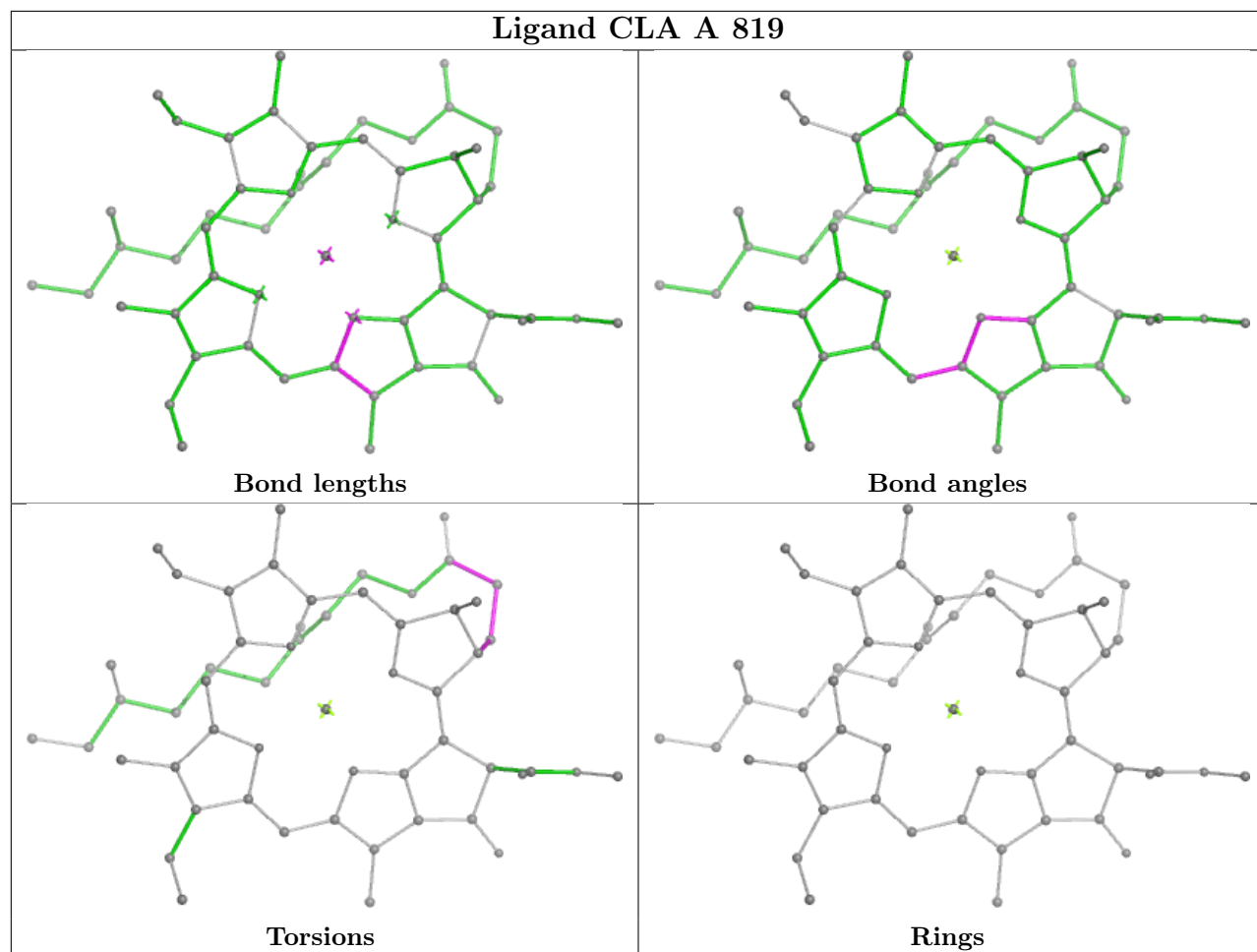




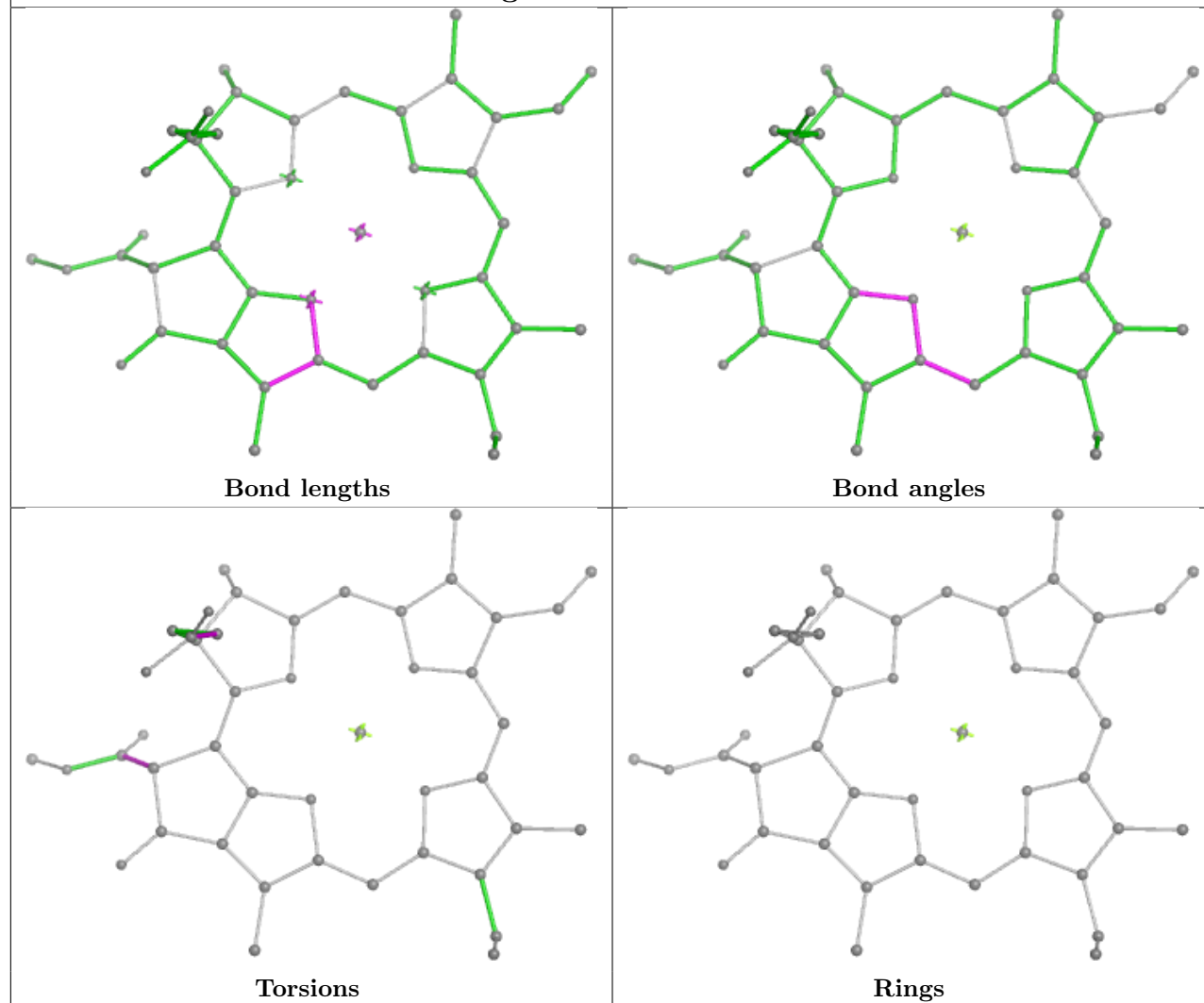




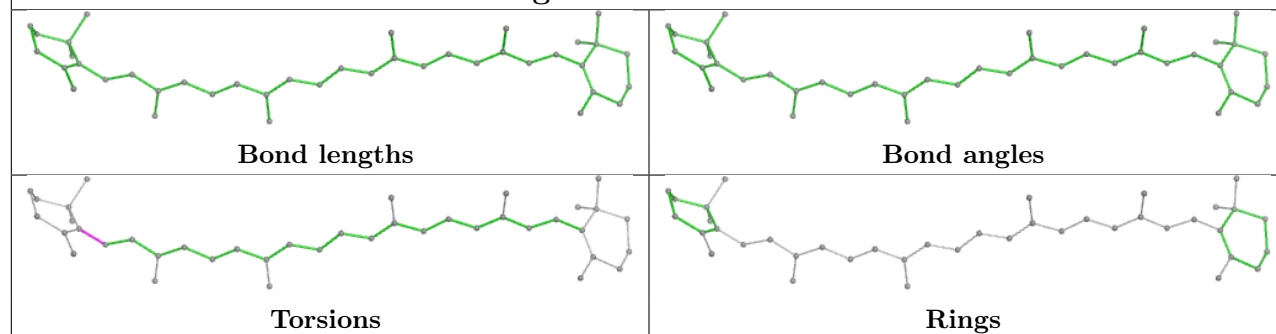
Ligand CLA A 819

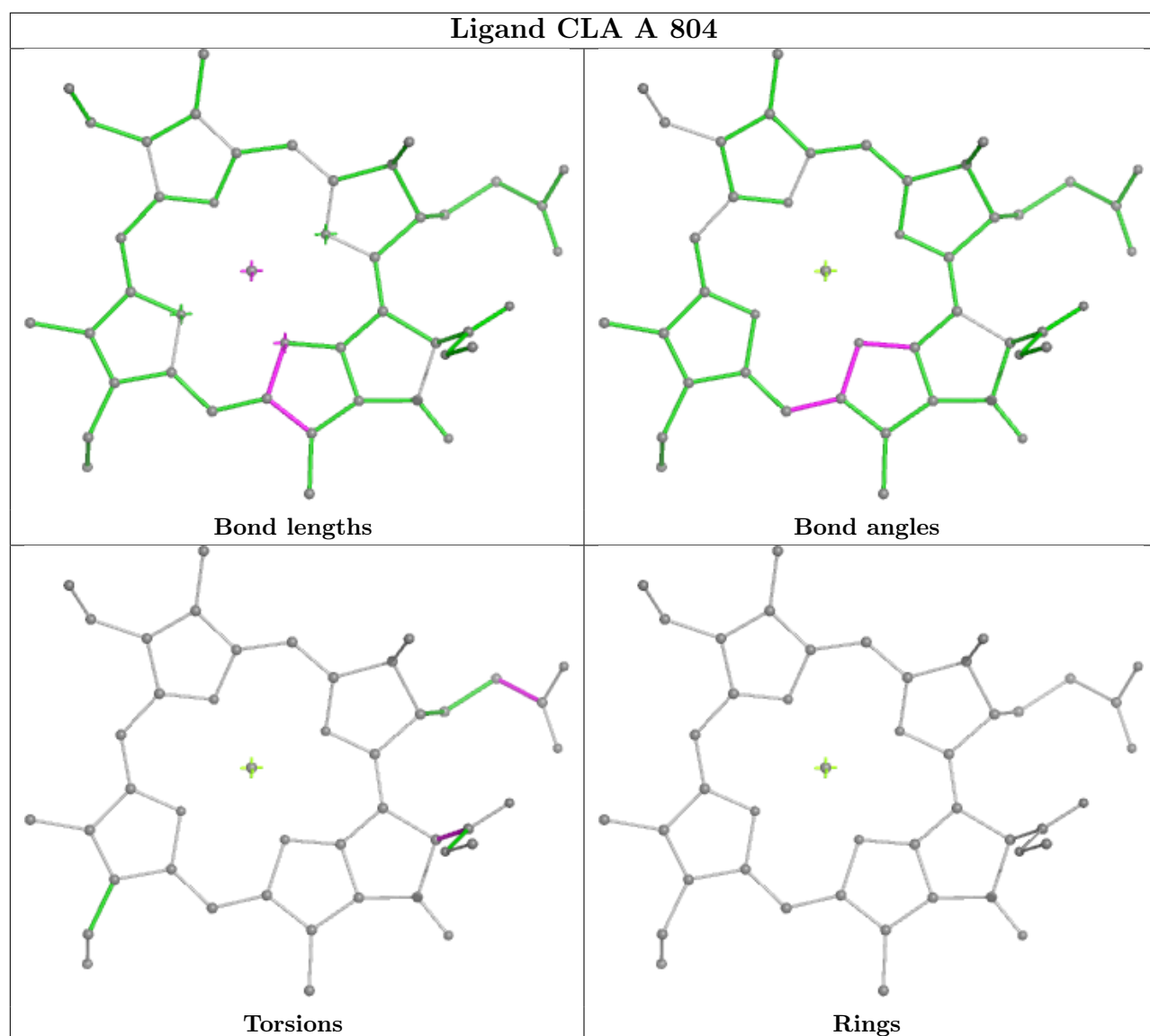


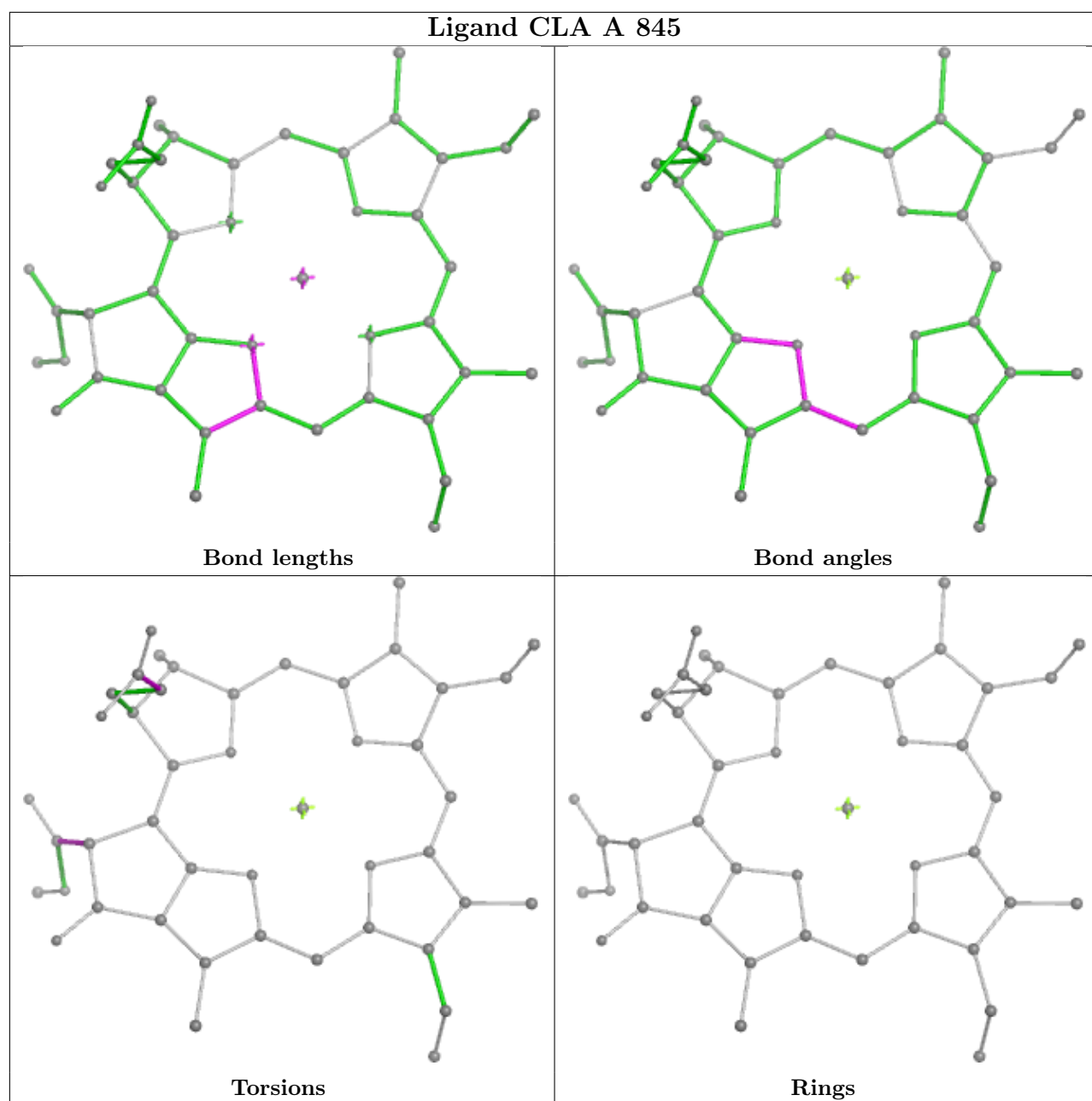
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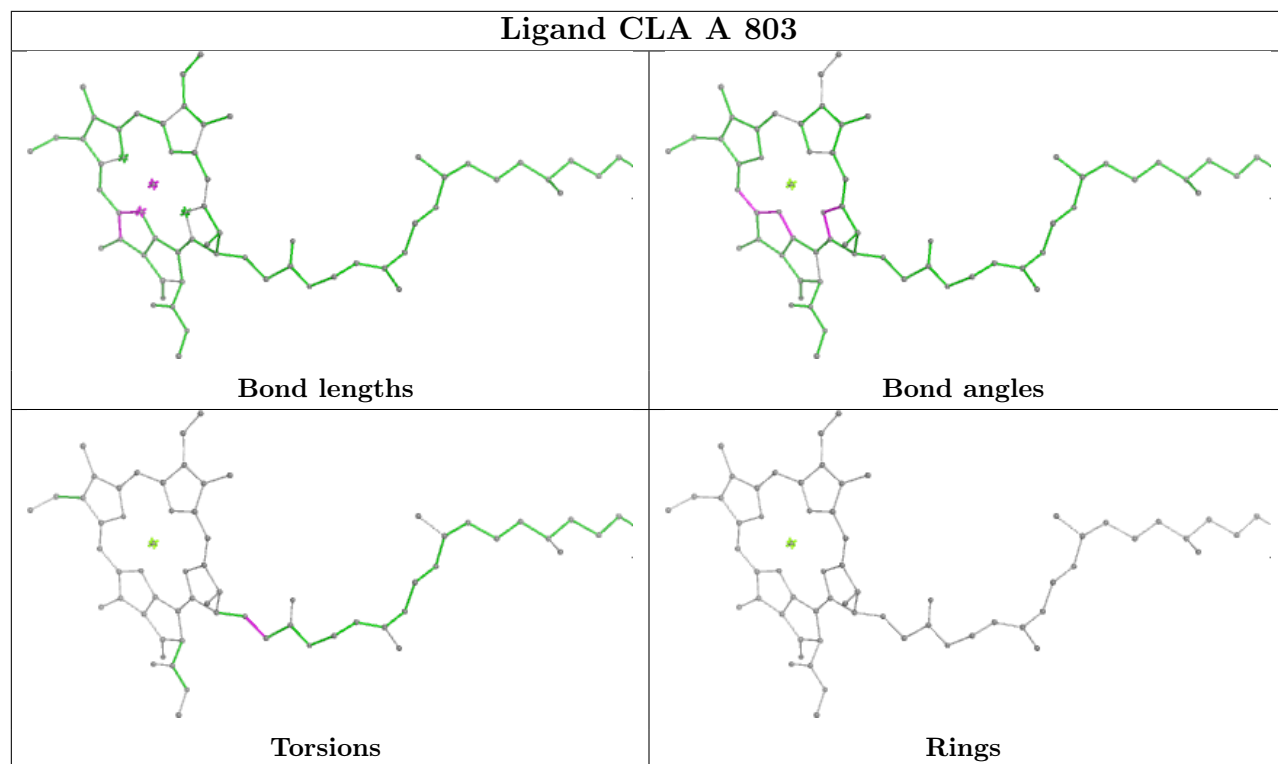


Ligand BCR L 306

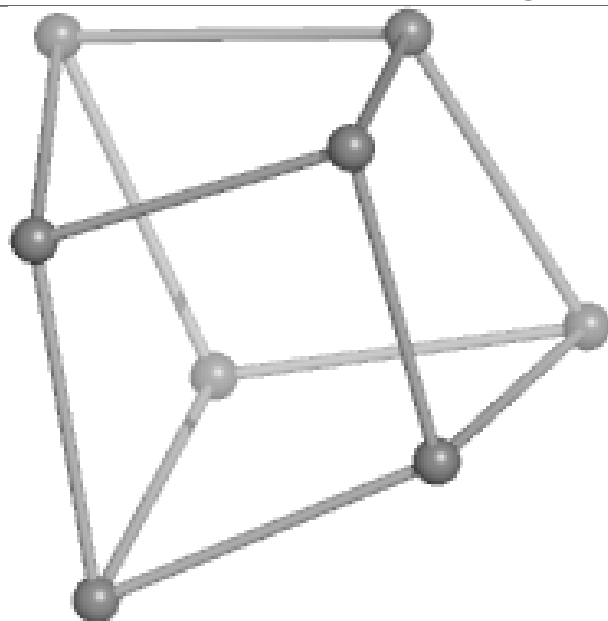




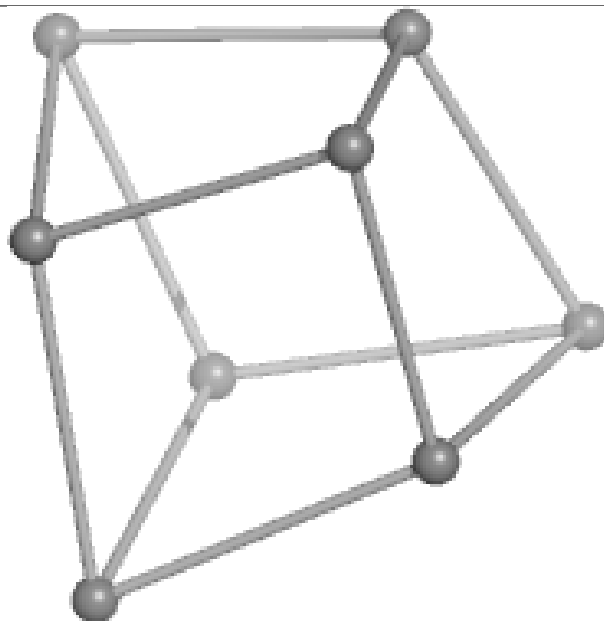




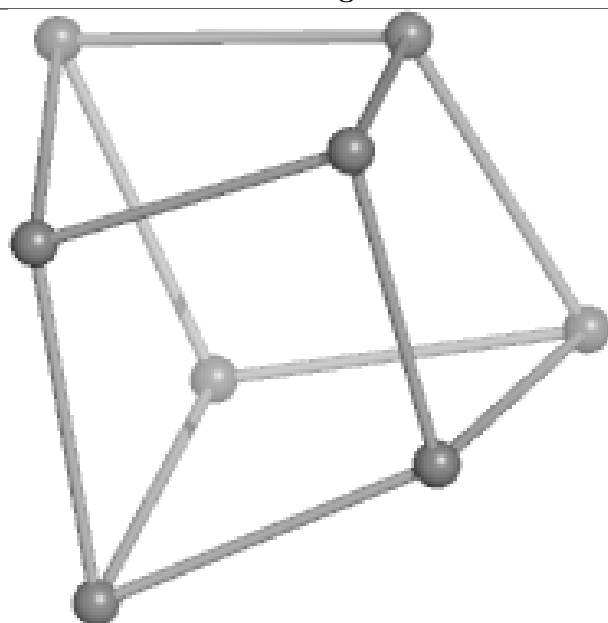
Ligand SF4 A 853



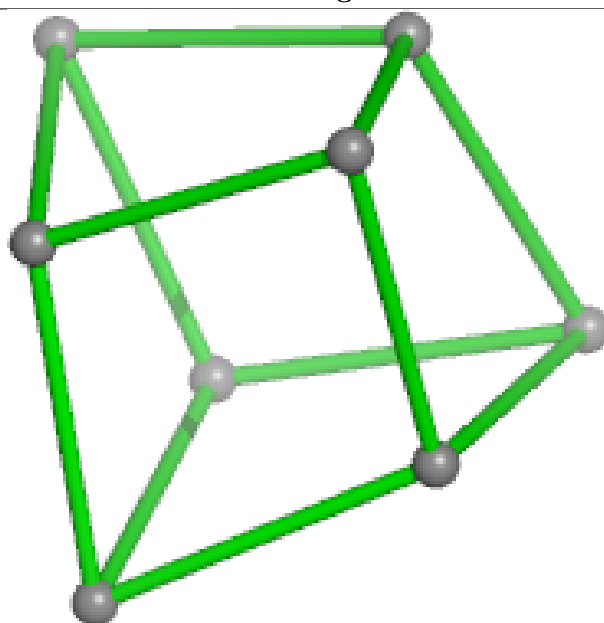
Bond lengths



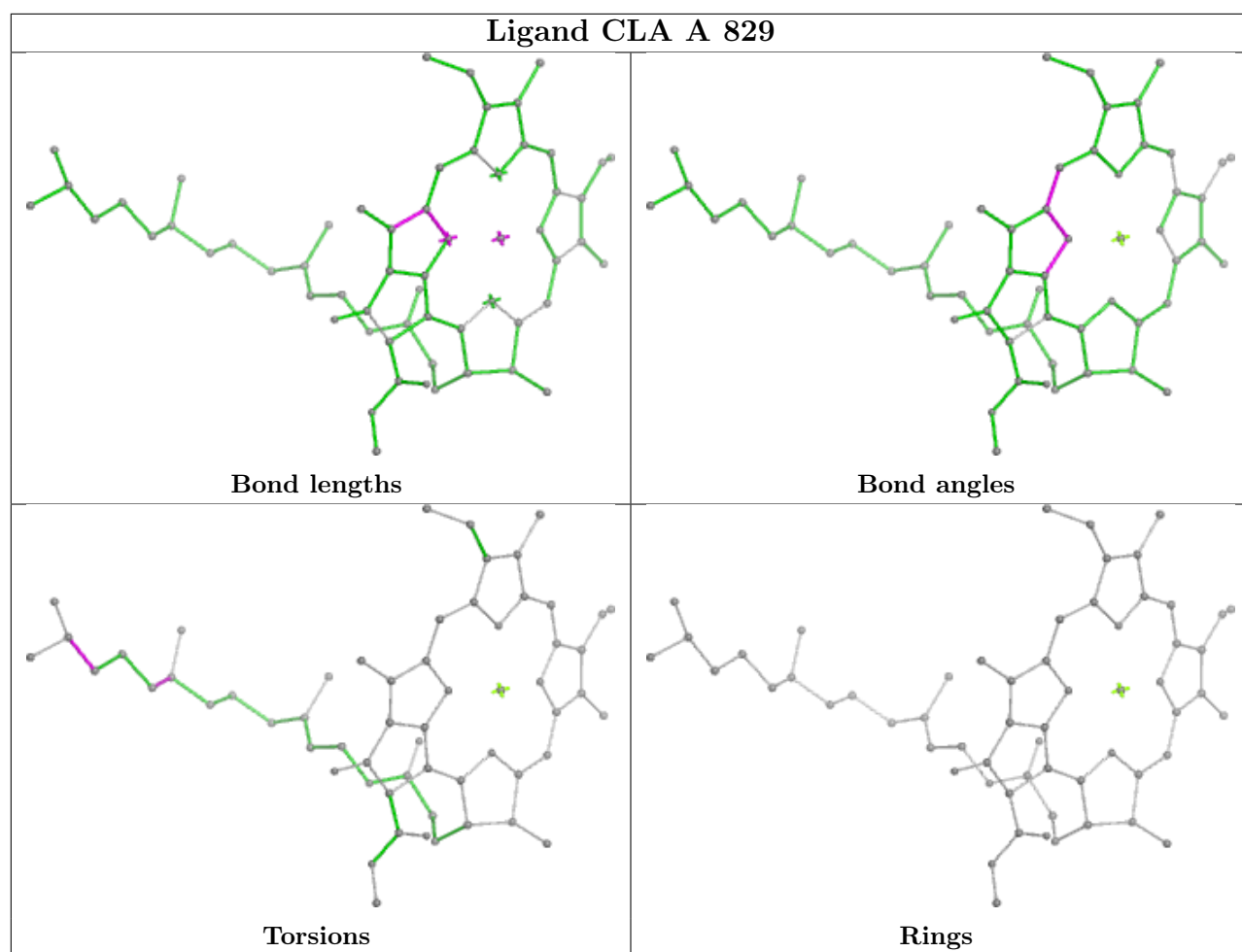
Bond angles

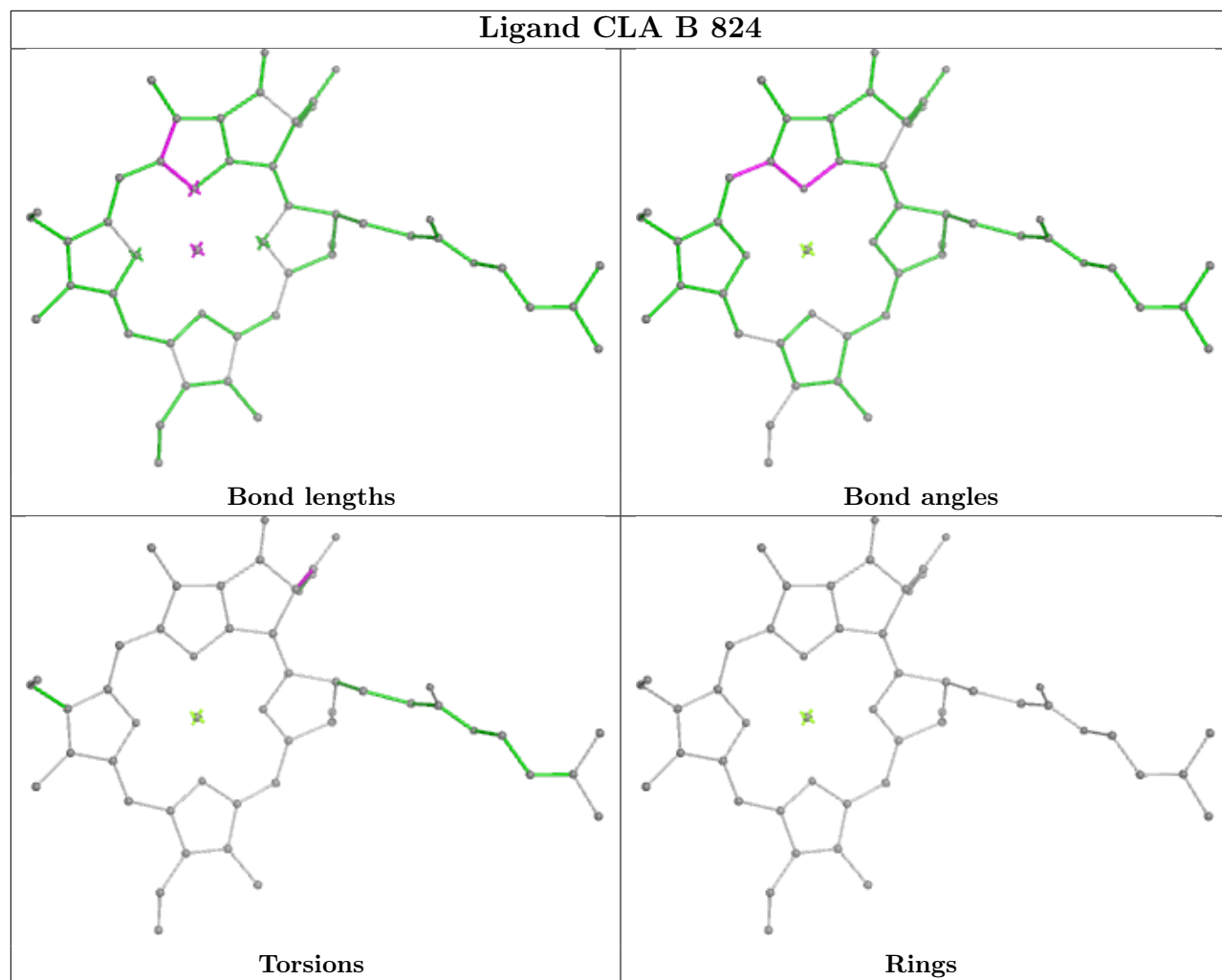


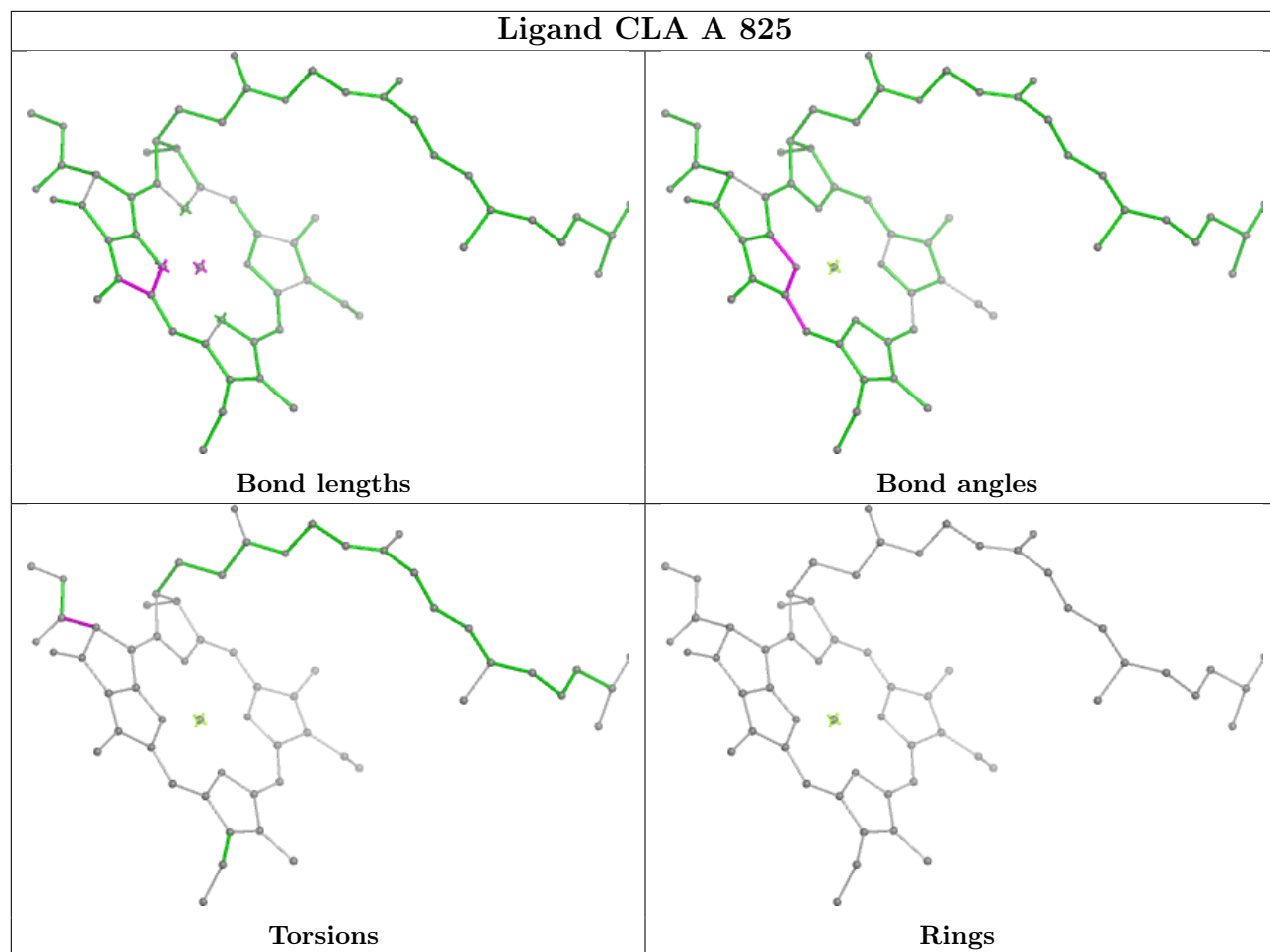
Torsions



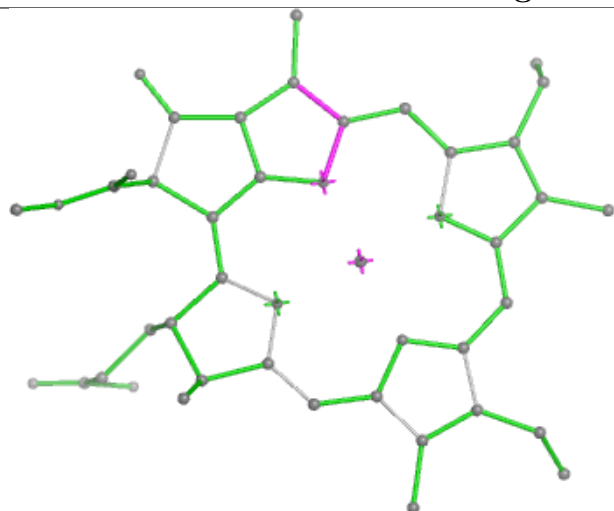
Rings



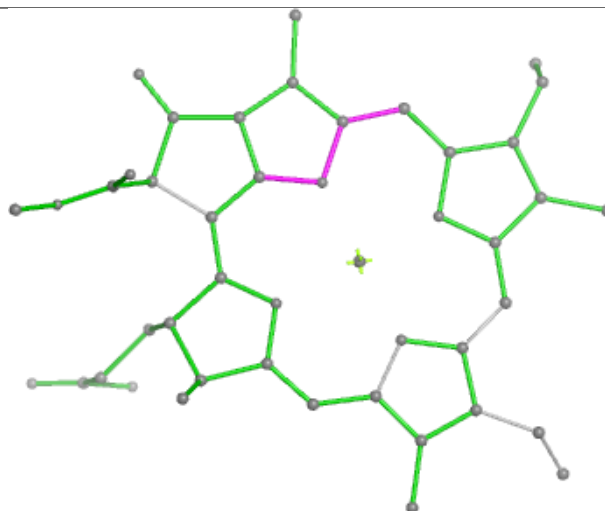




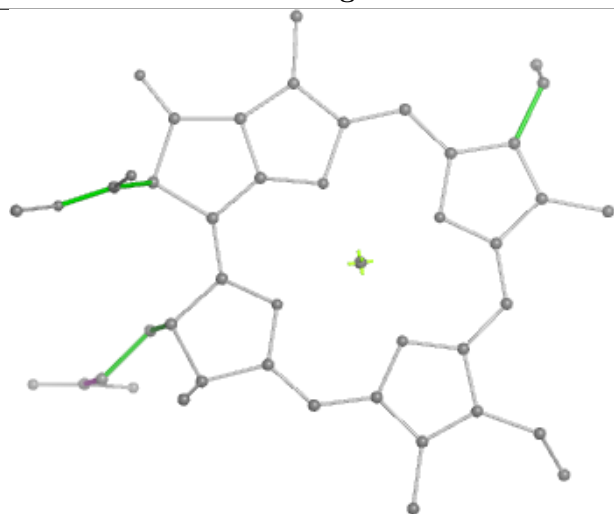
Ligand CLA B 830



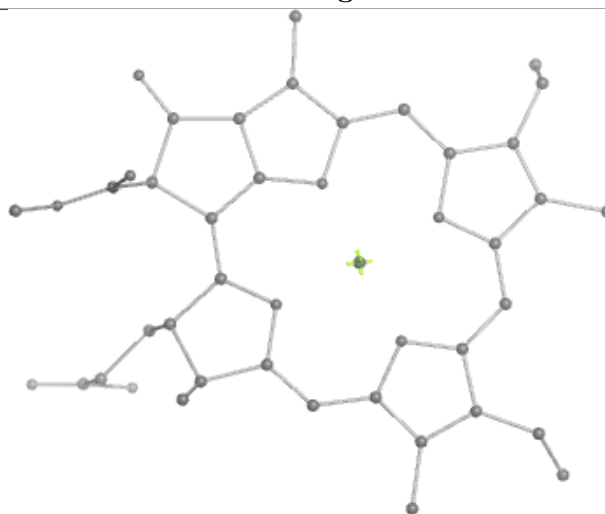
Bond lengths



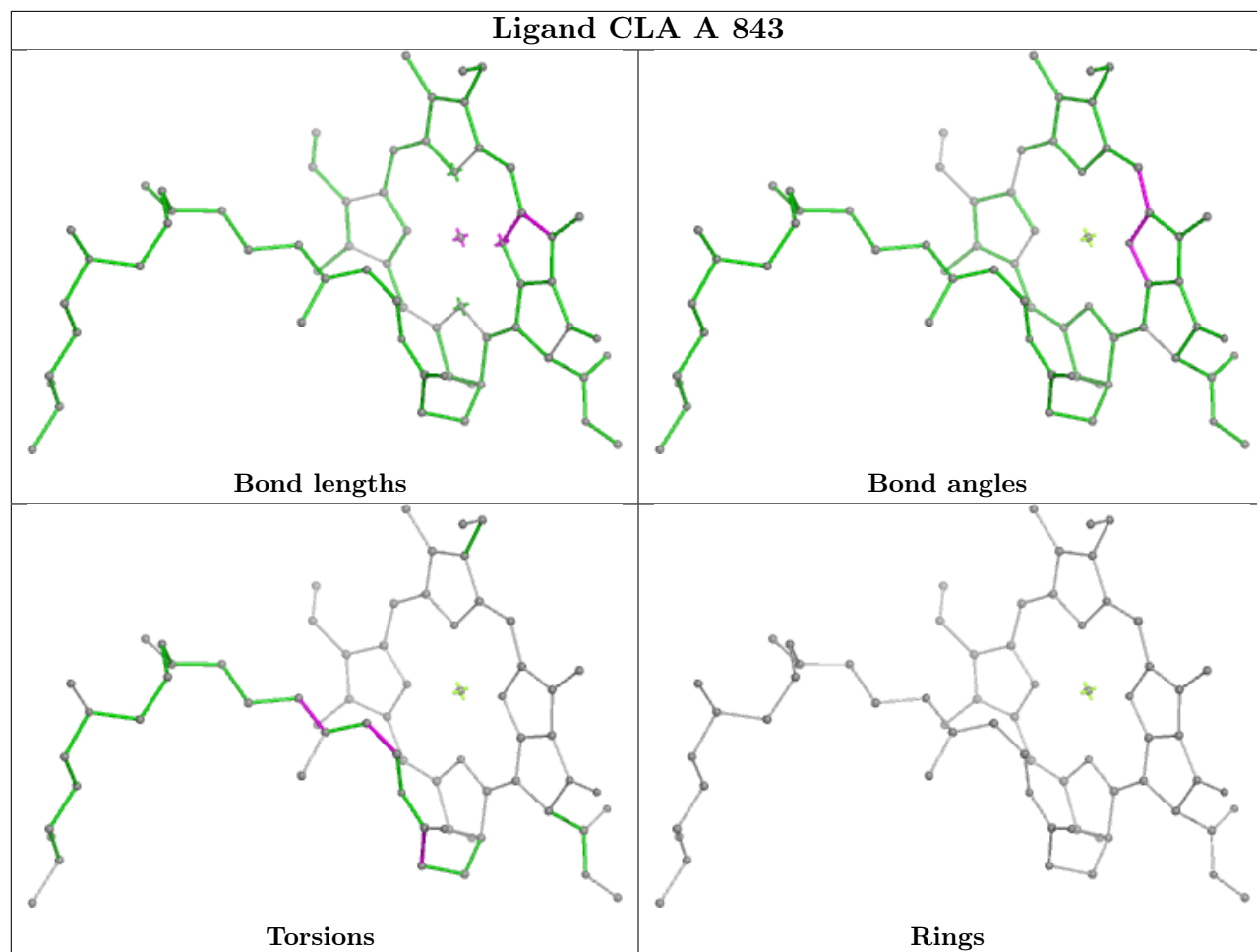
Bond angles

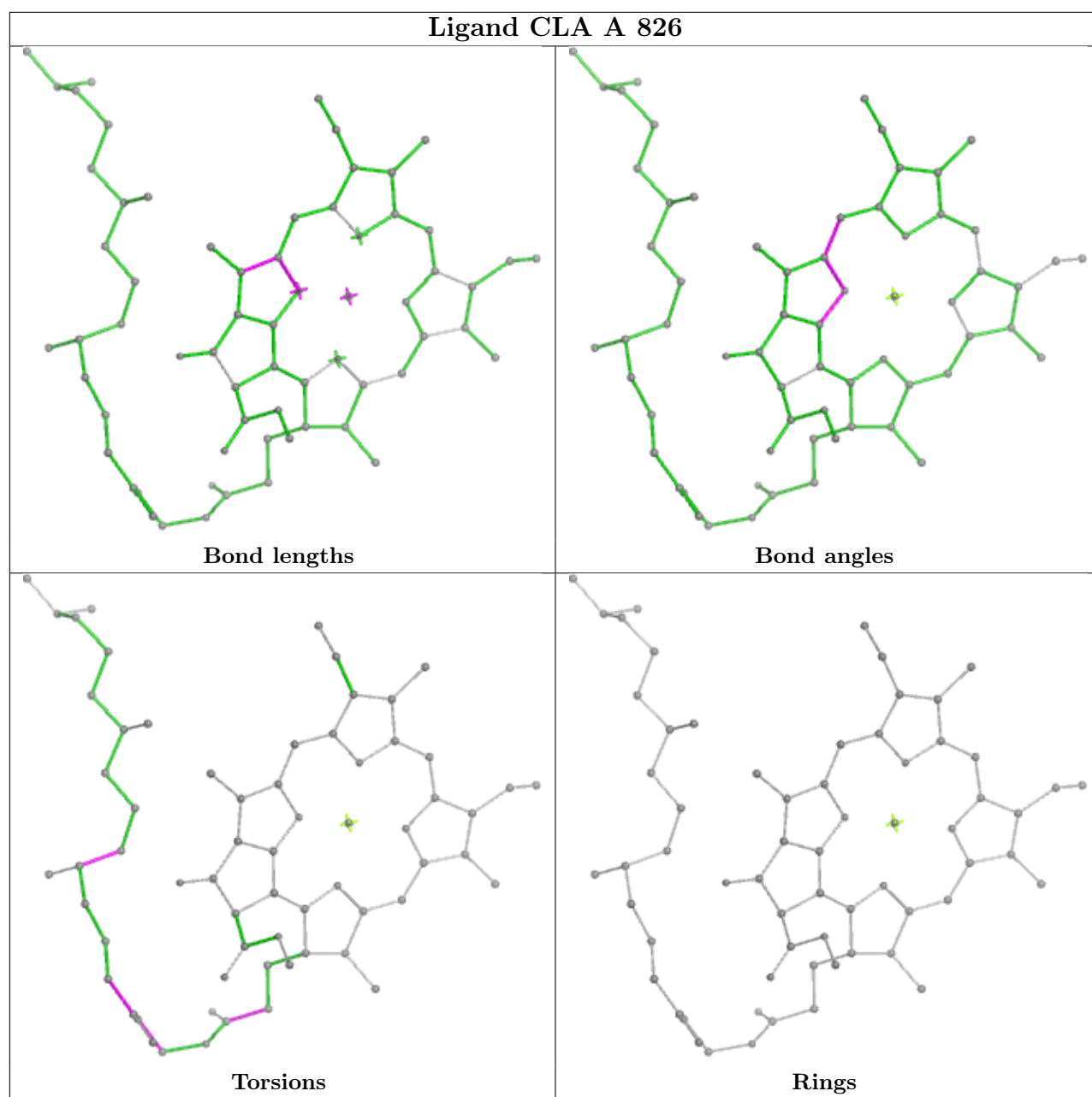


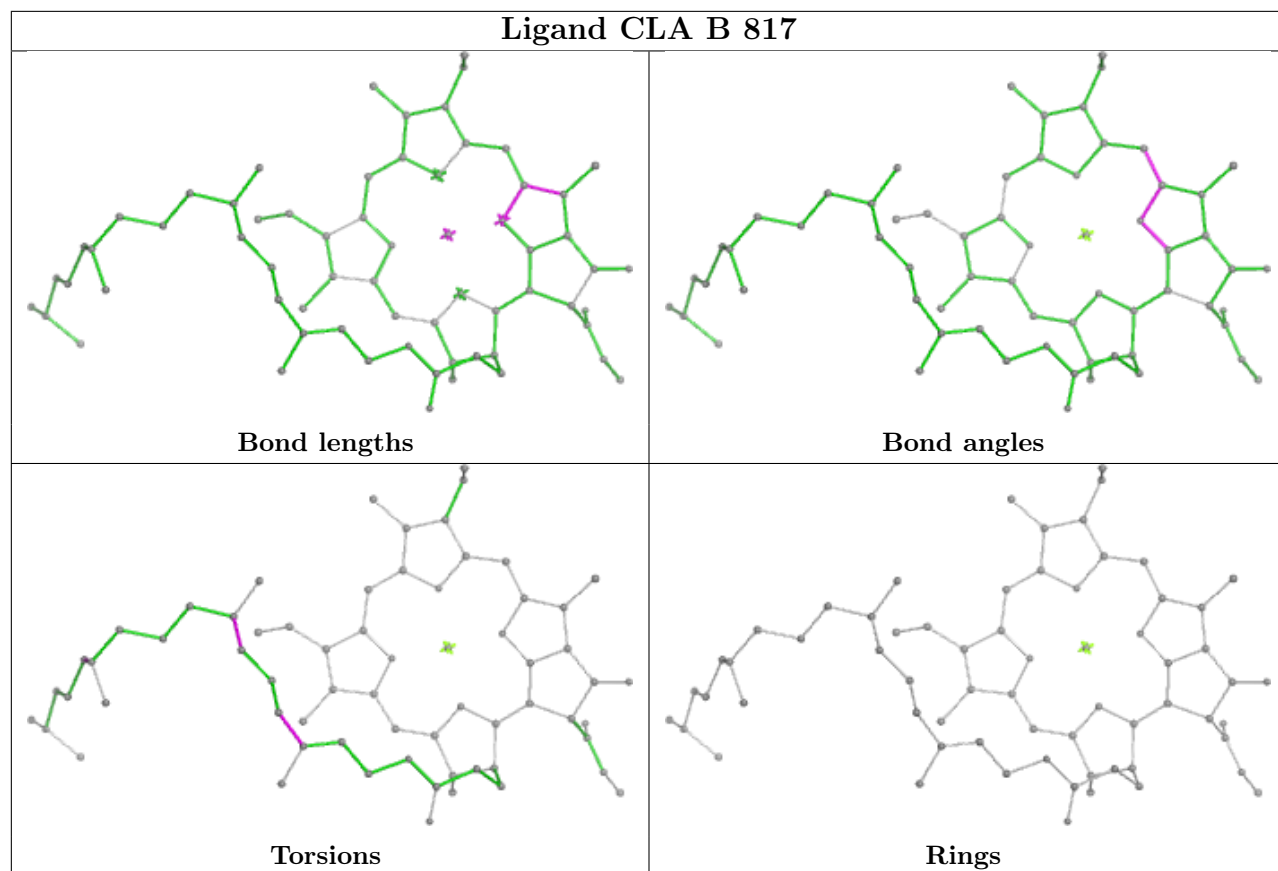
Torsions



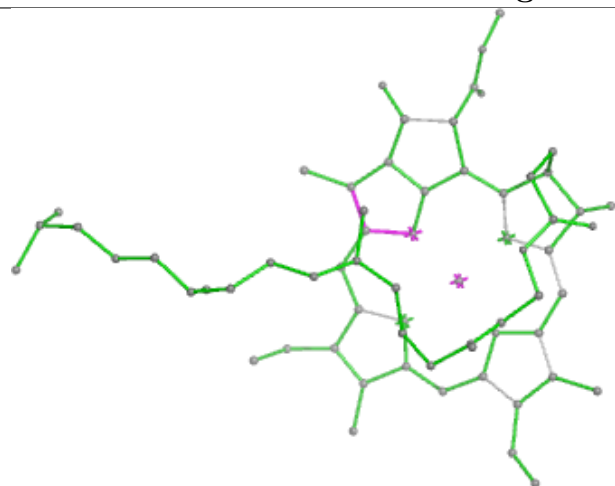
Rings



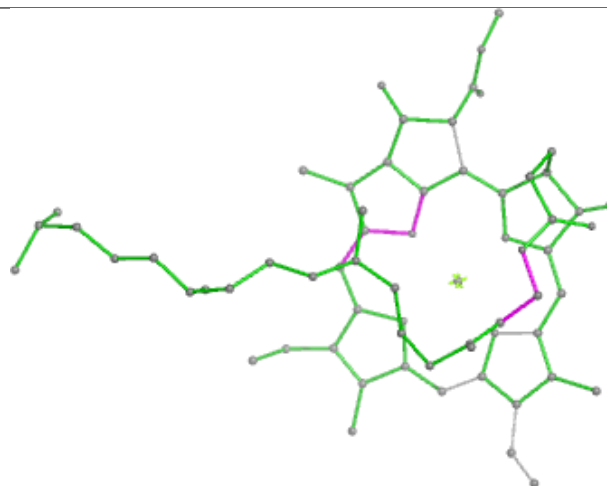




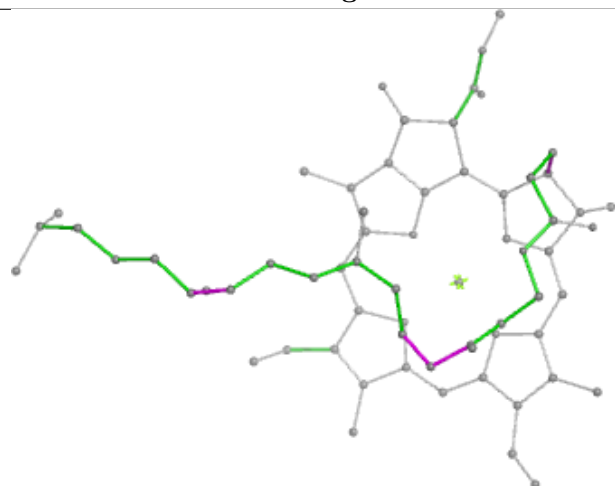
Ligand CLA B 826



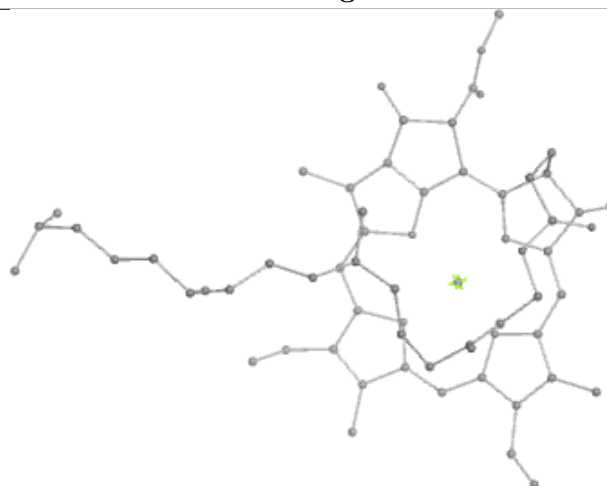
Bond lengths



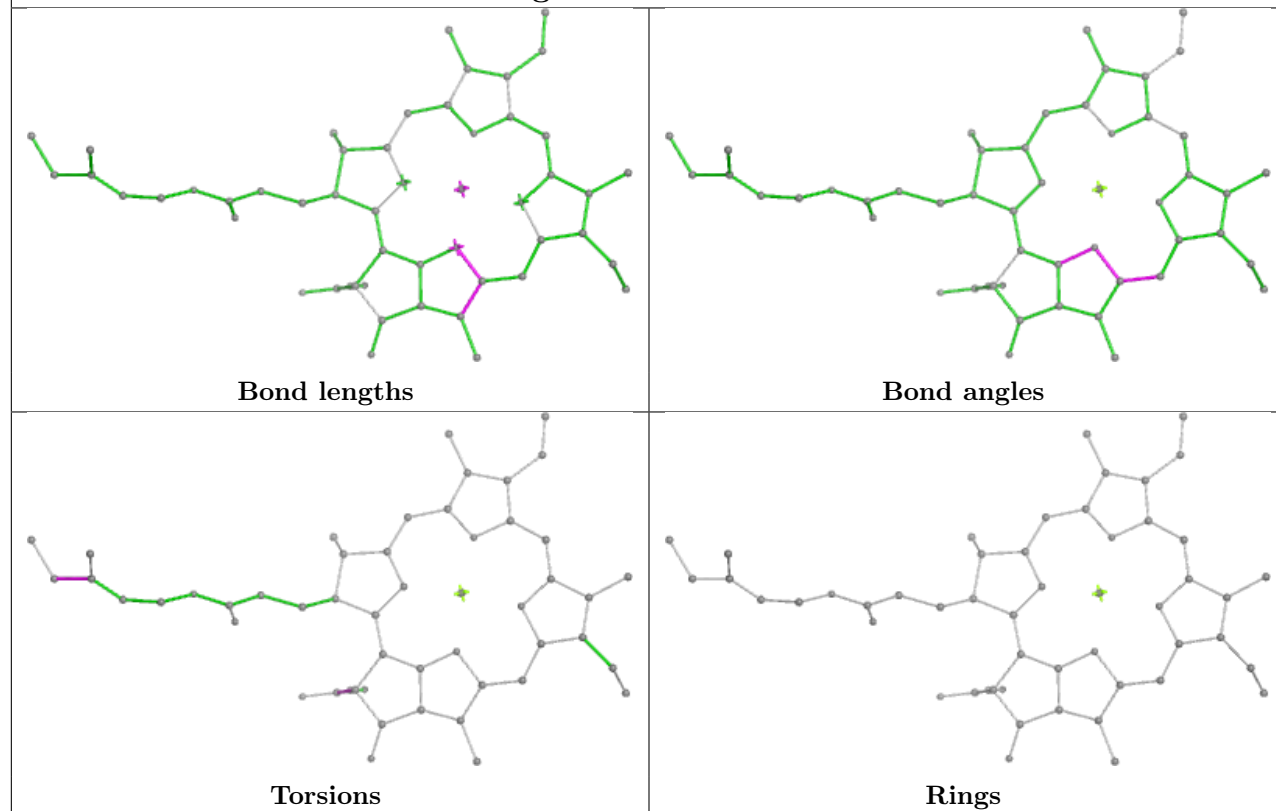
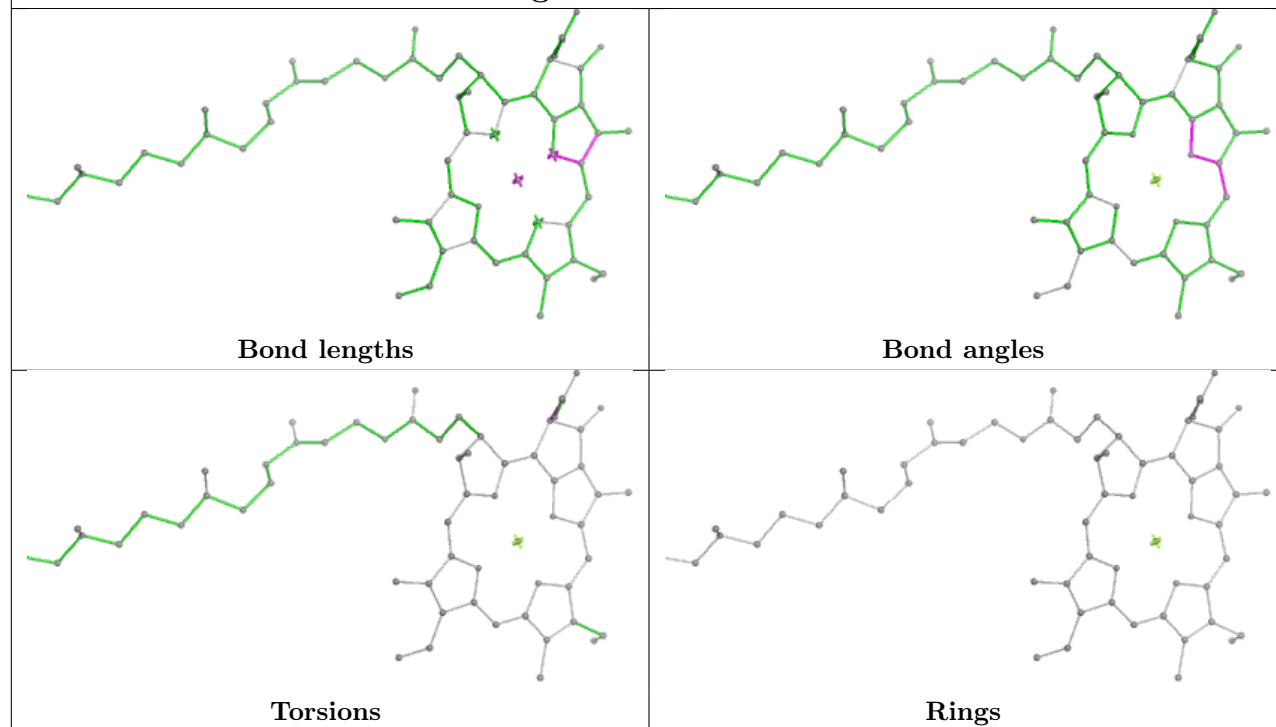
Bond angles

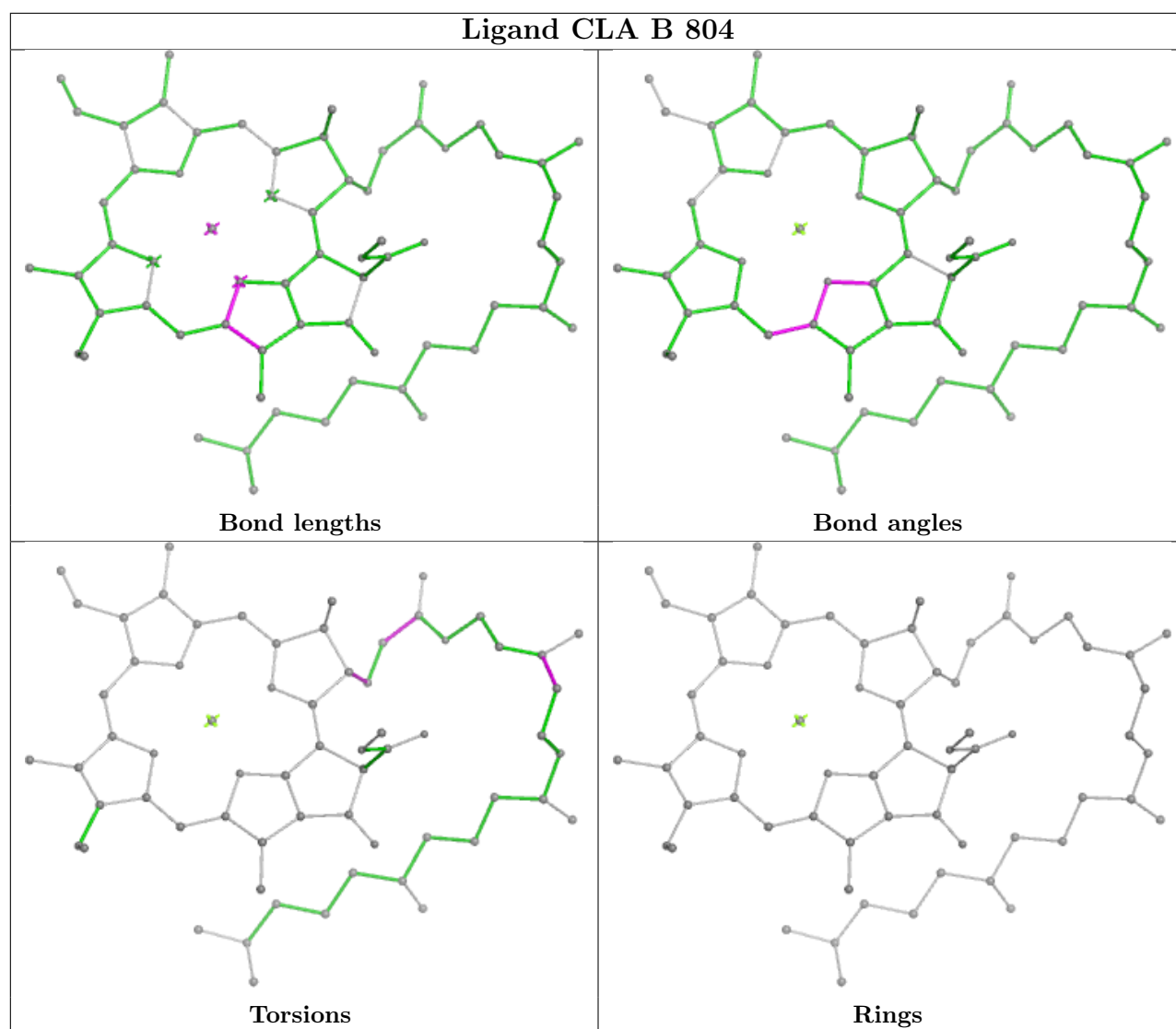


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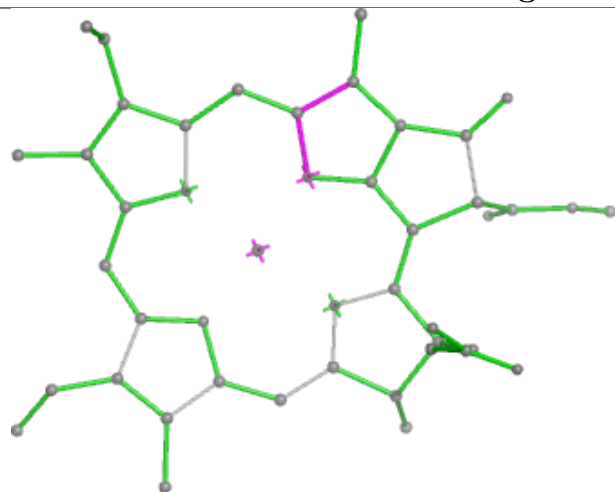


Rings

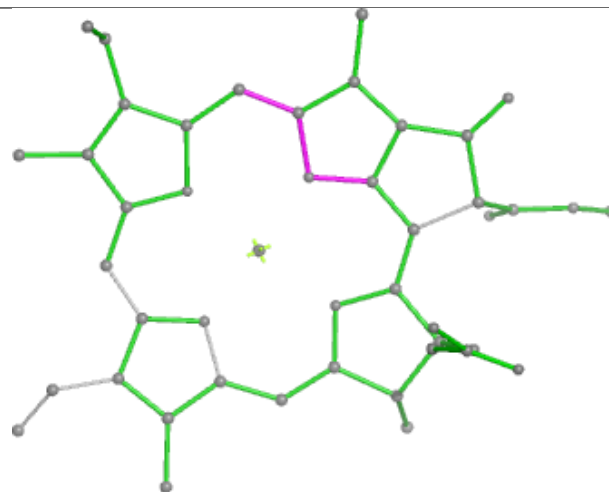
Ligand CLA B 834**Ligand CLA A 835**



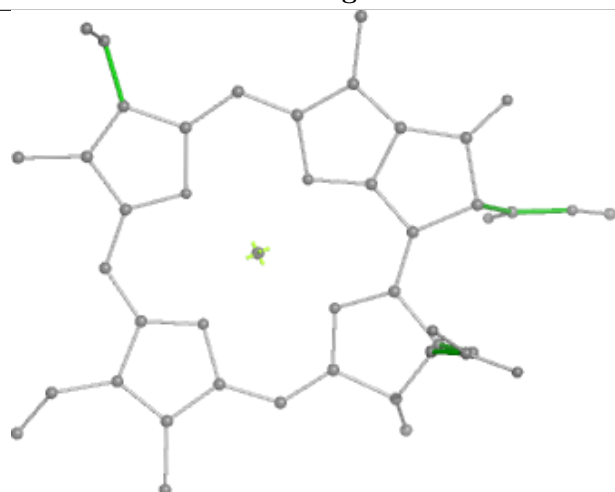
Ligand CLA L 304



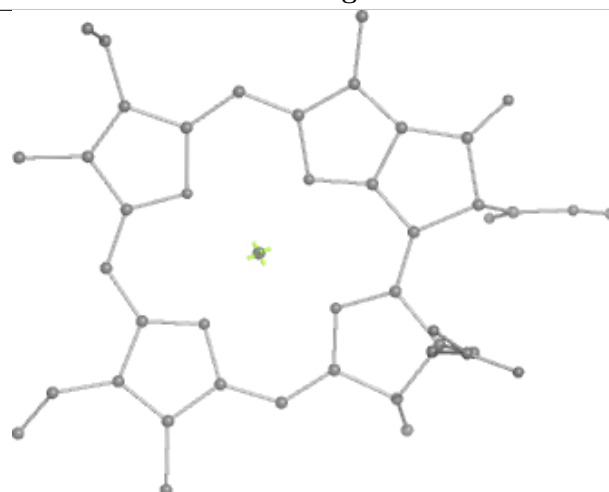
Bond lengths



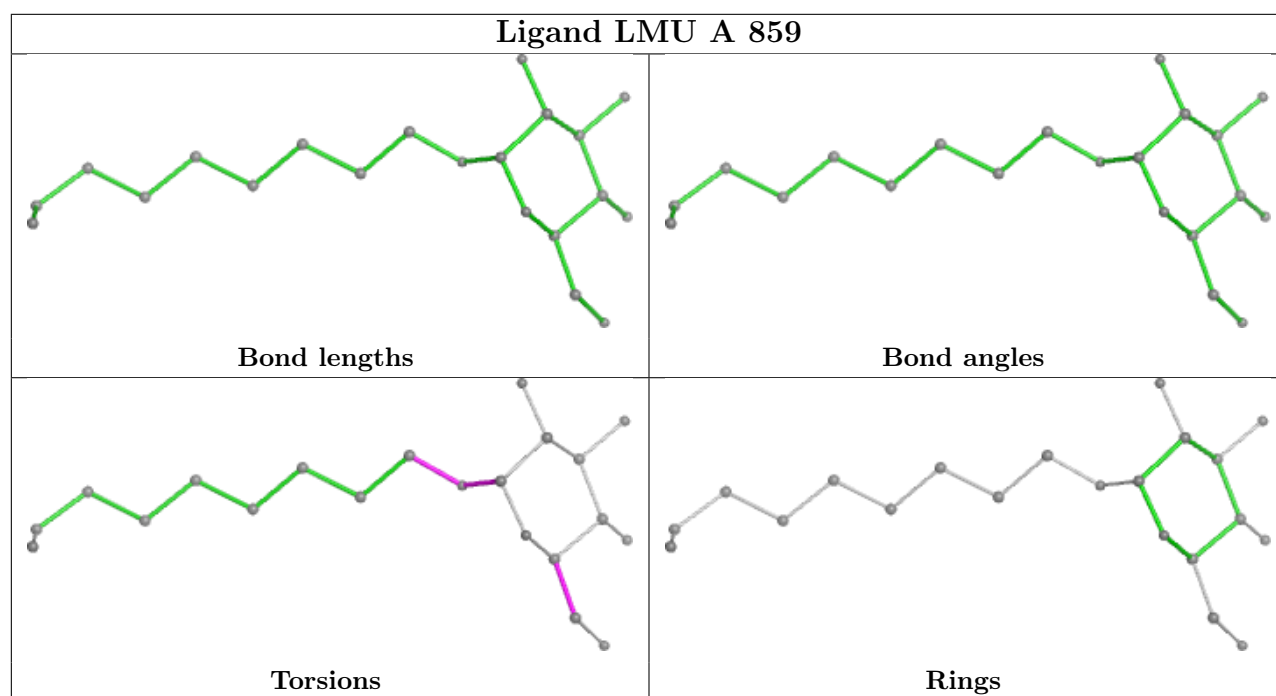
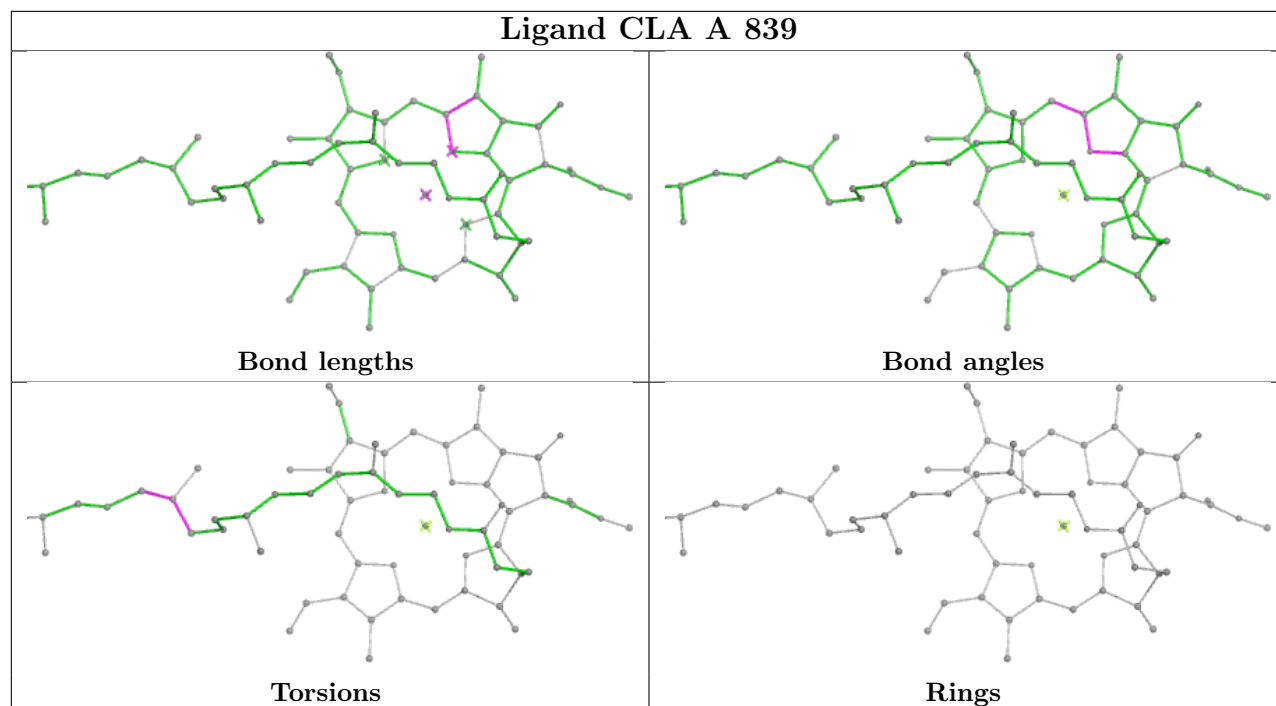
Bond angles

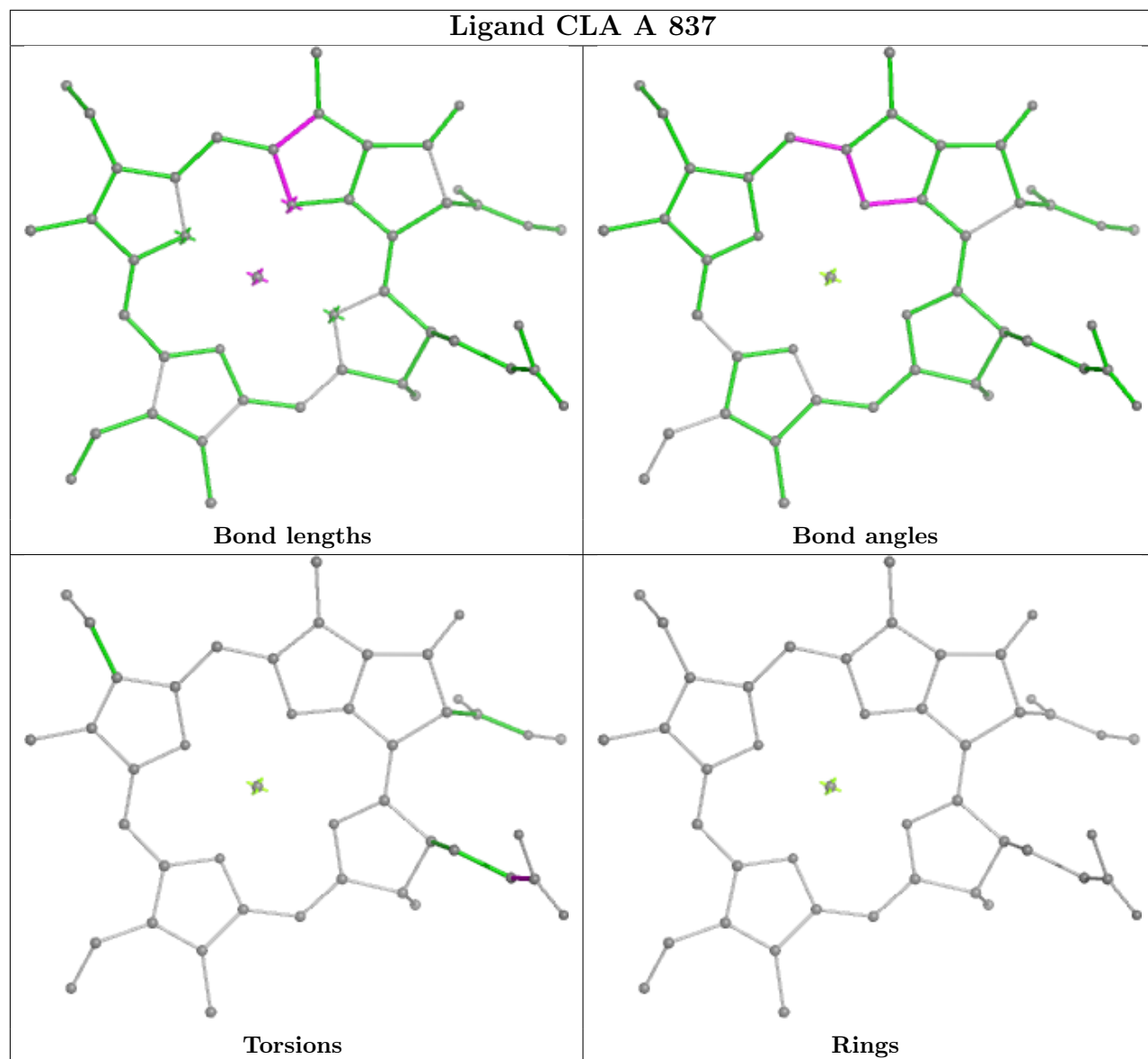


Torsions

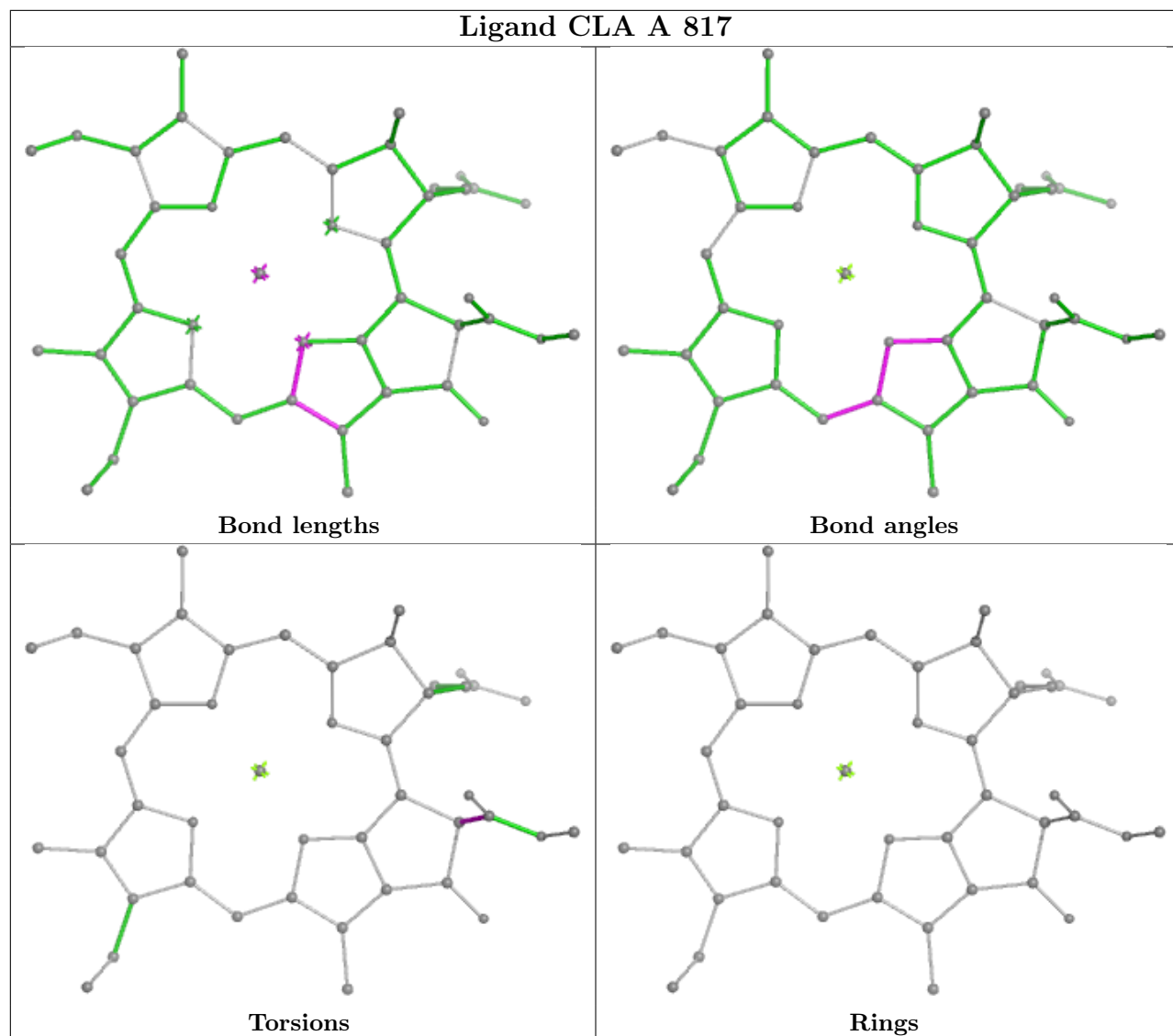


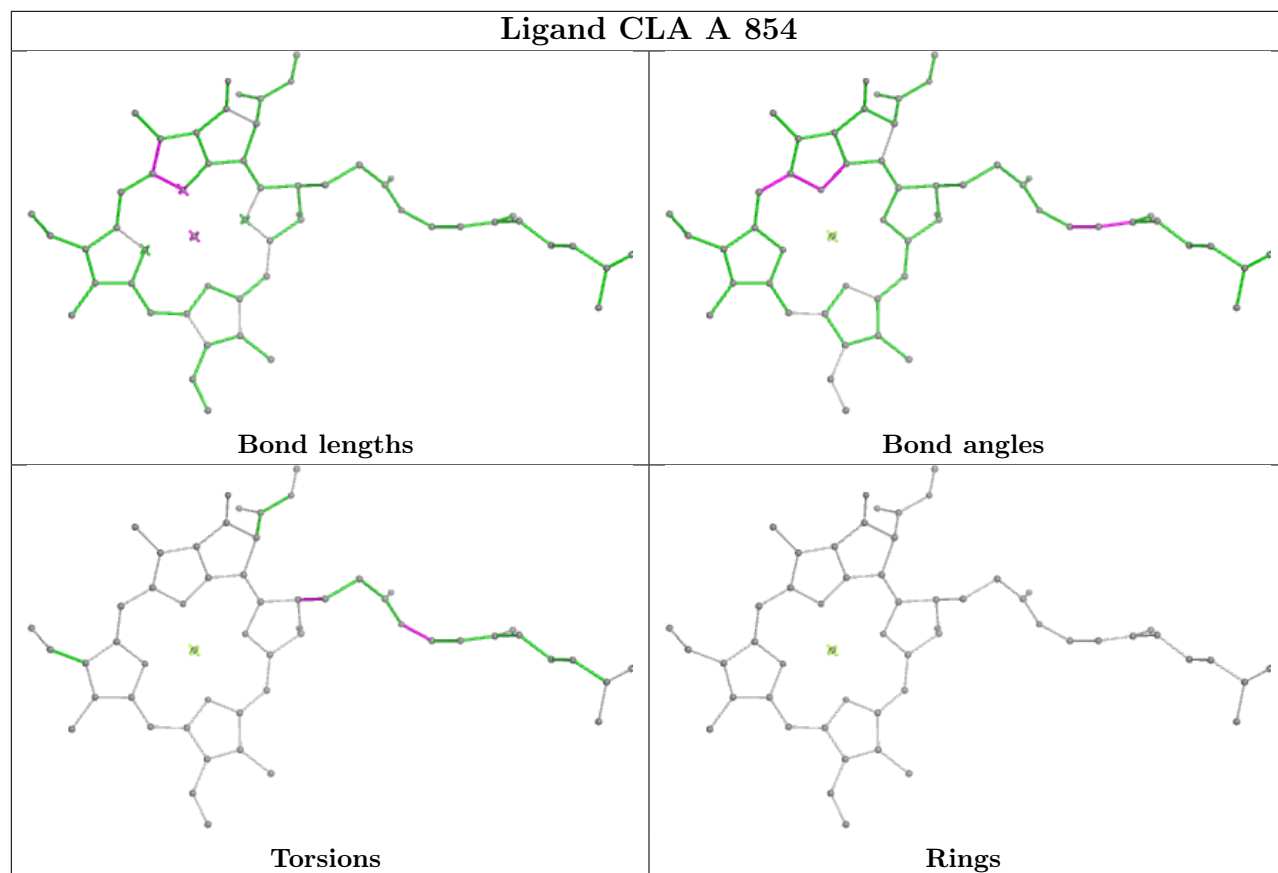
Rings



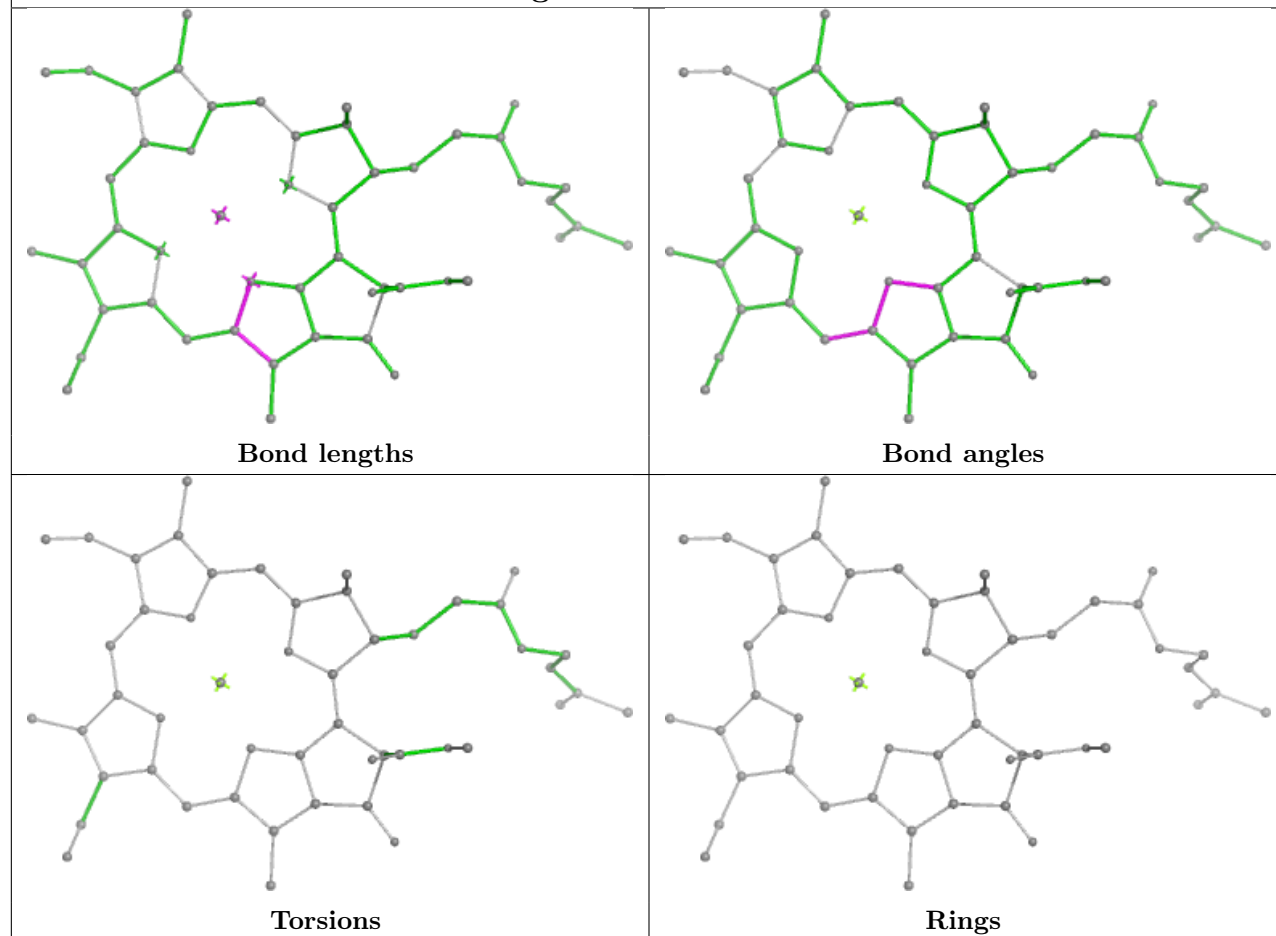


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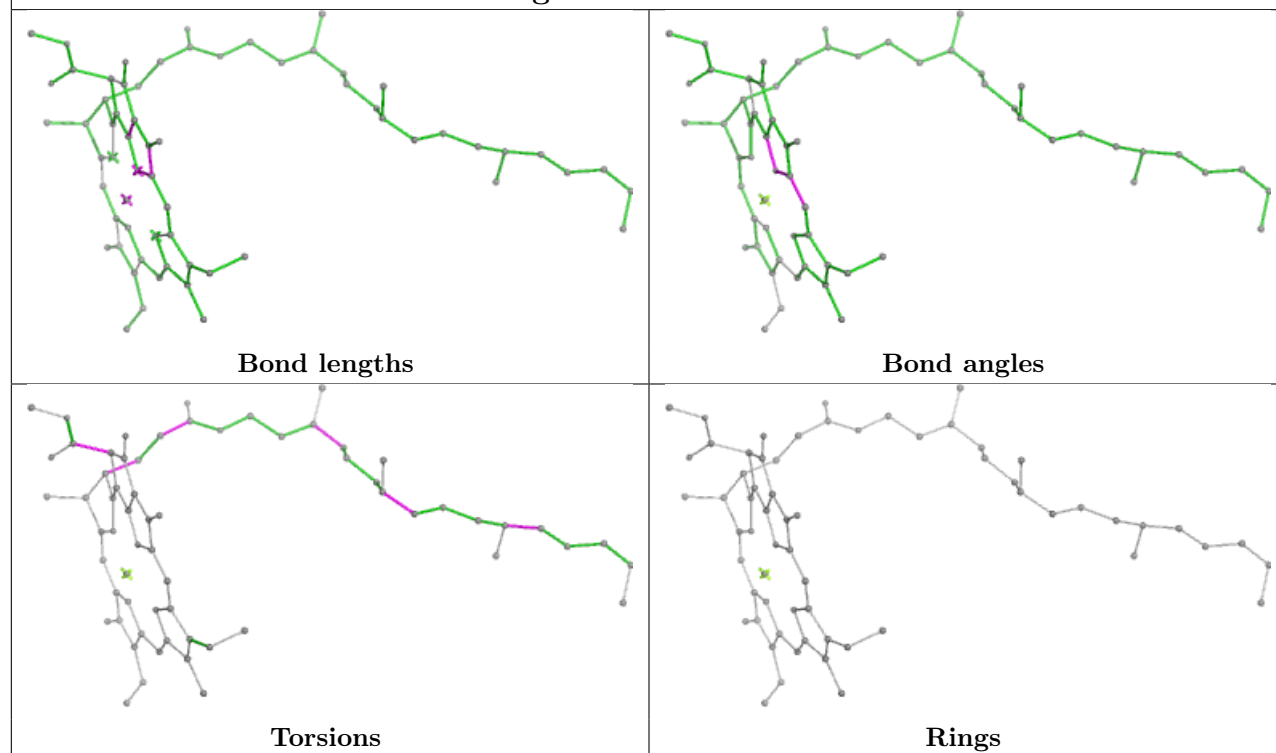


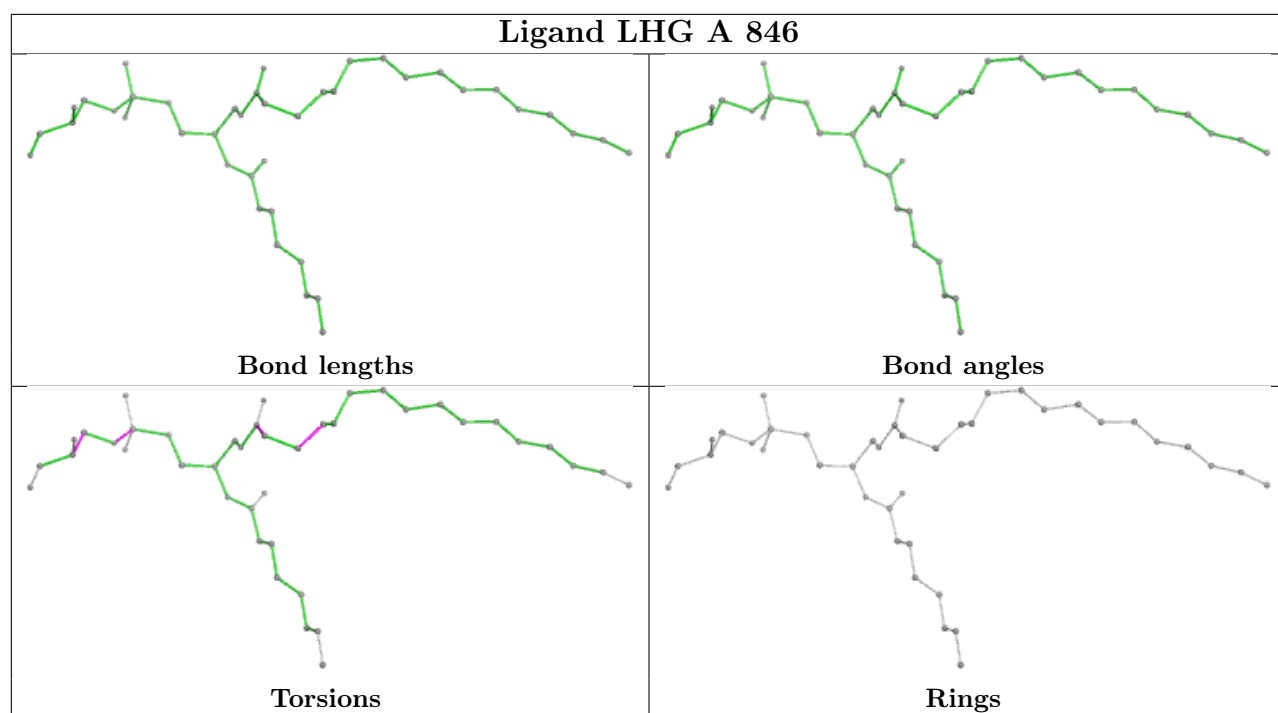


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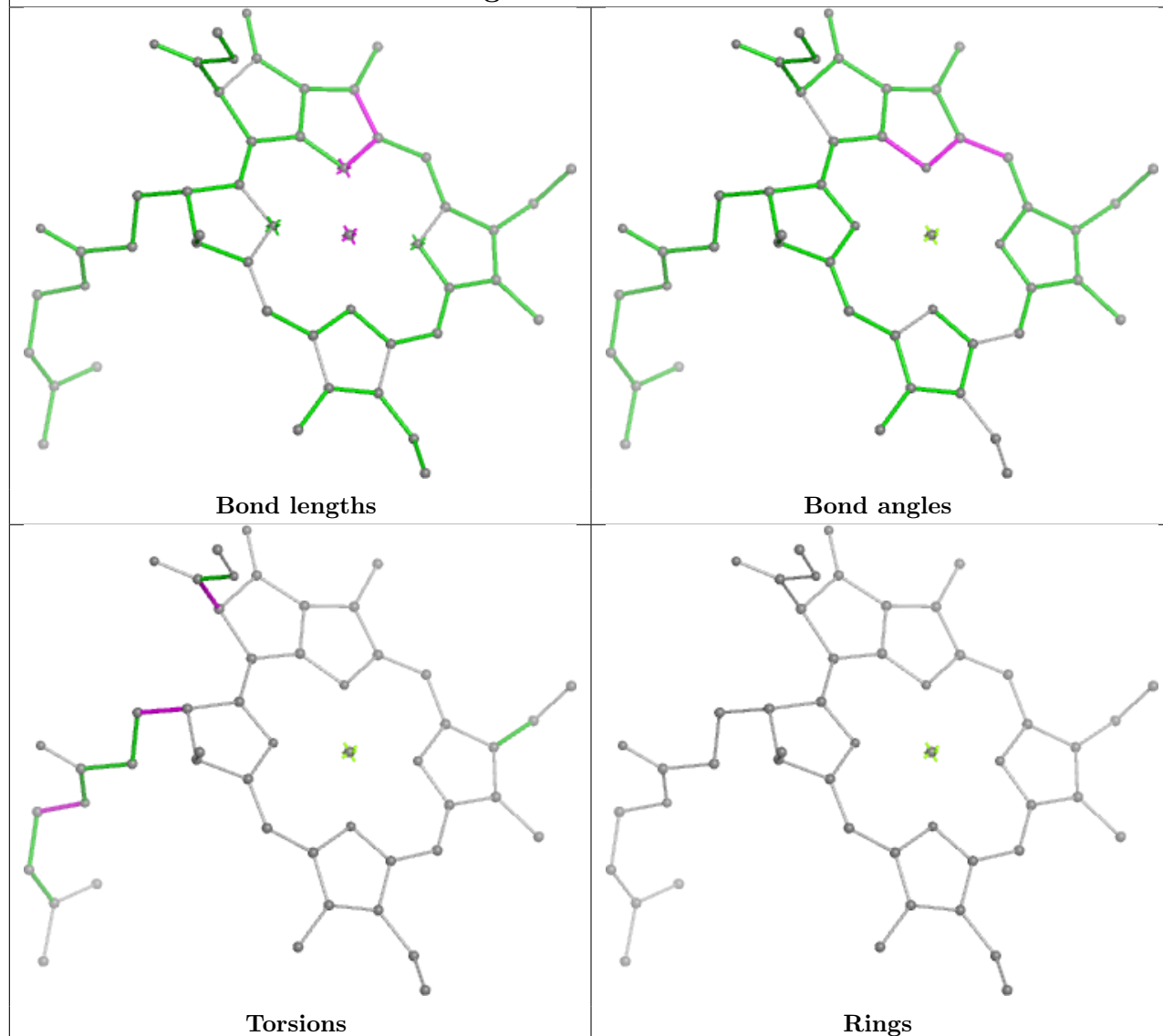


Ligand CLA B 828

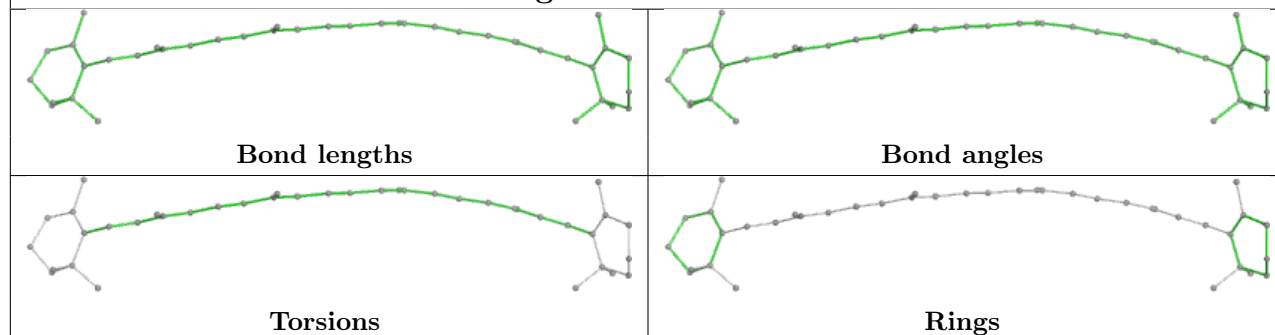


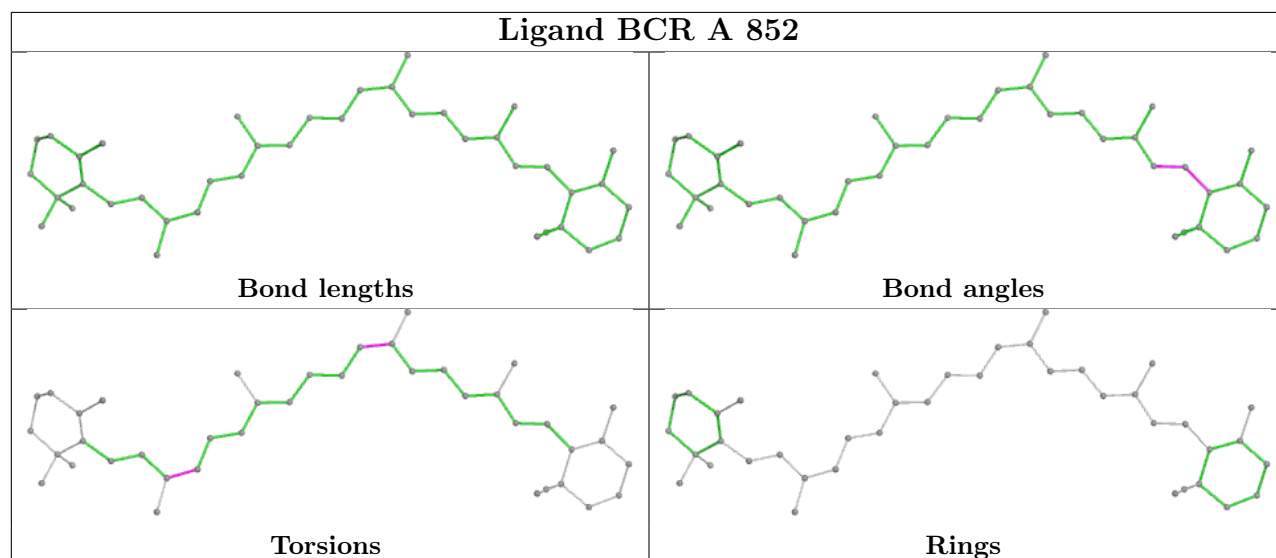
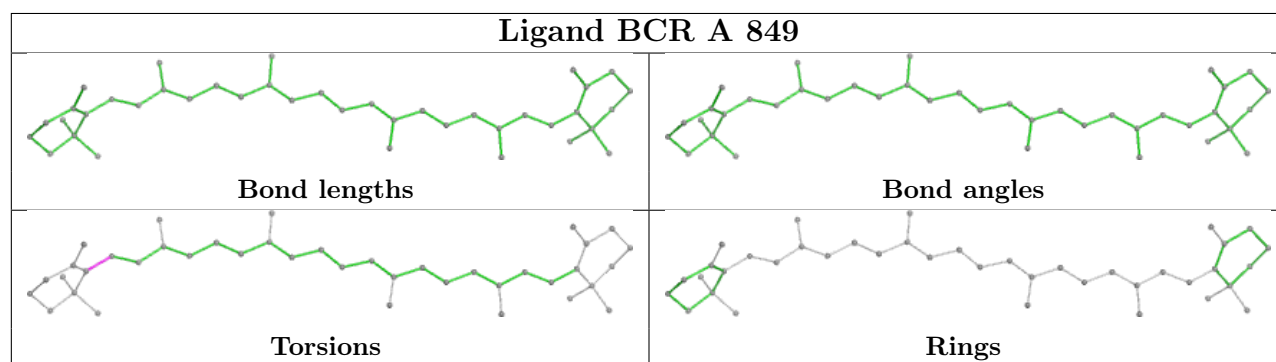
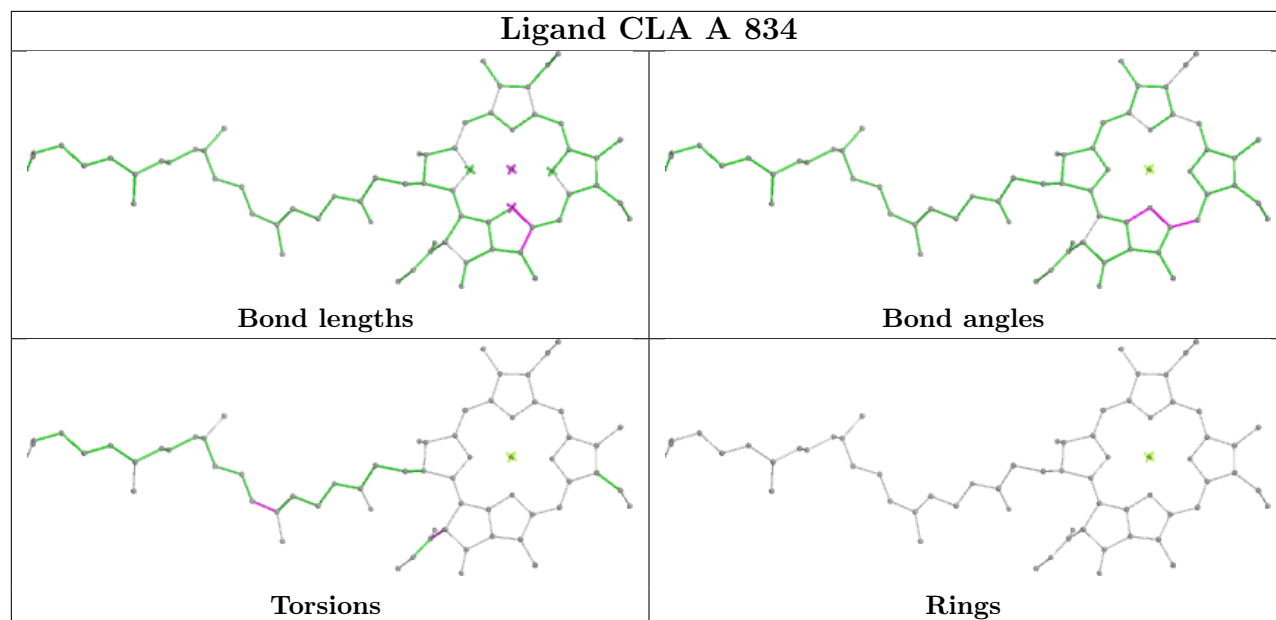


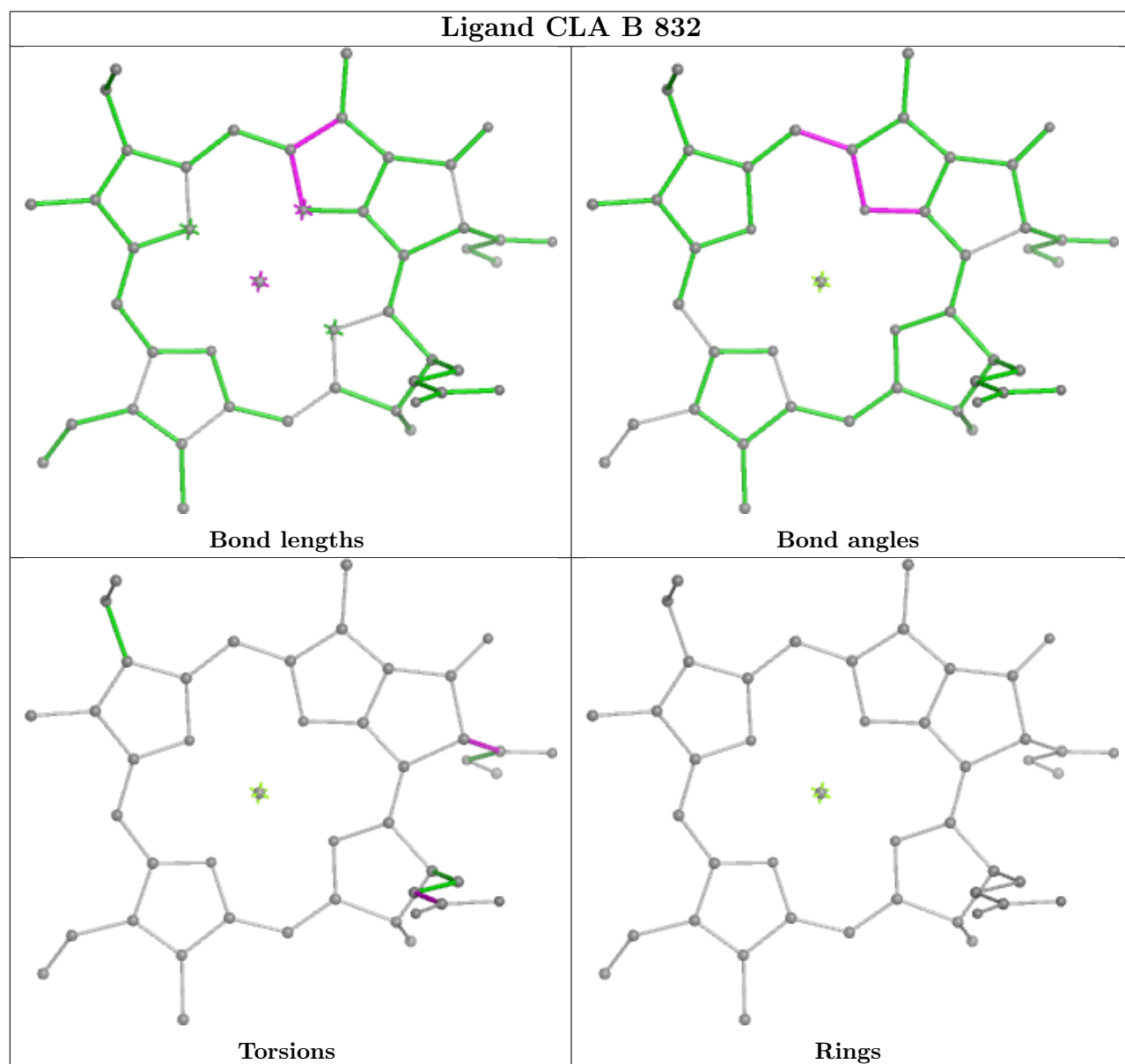
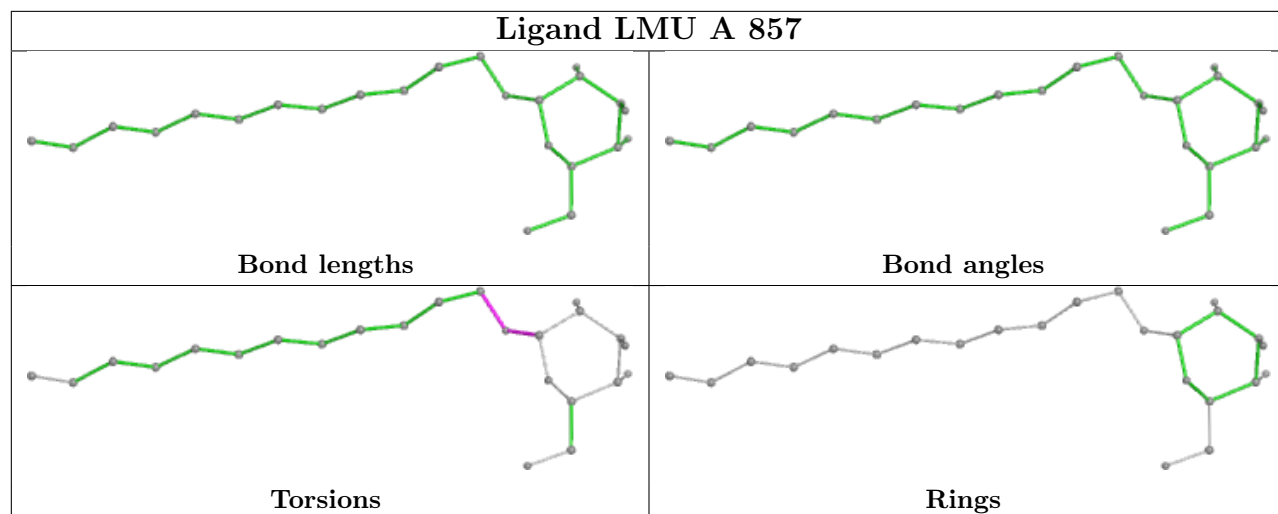
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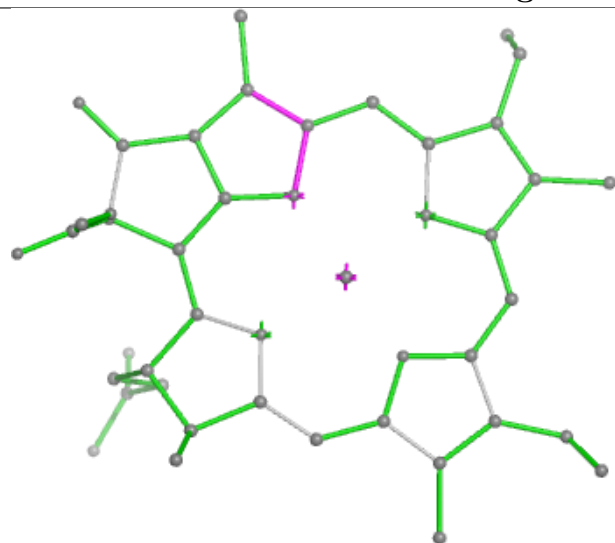
Ligand BCR I 101



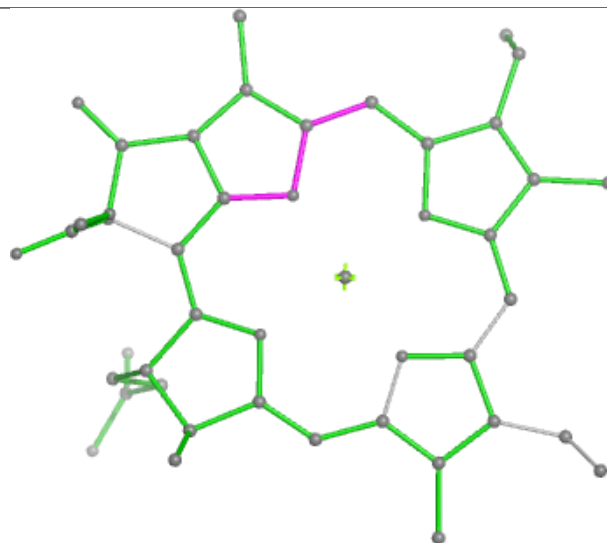




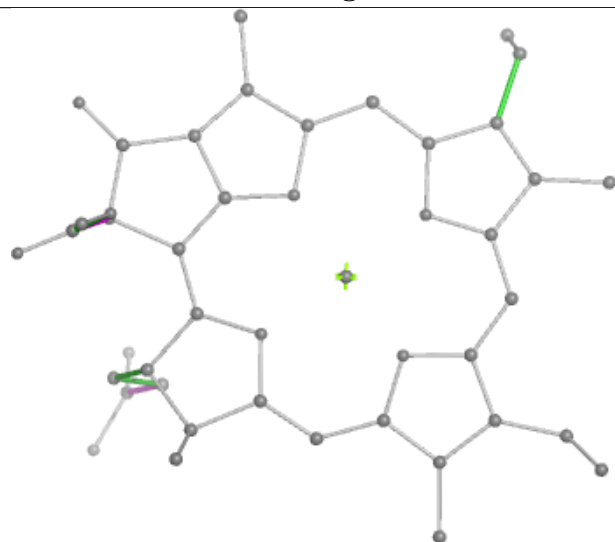
Ligand CLA B 820



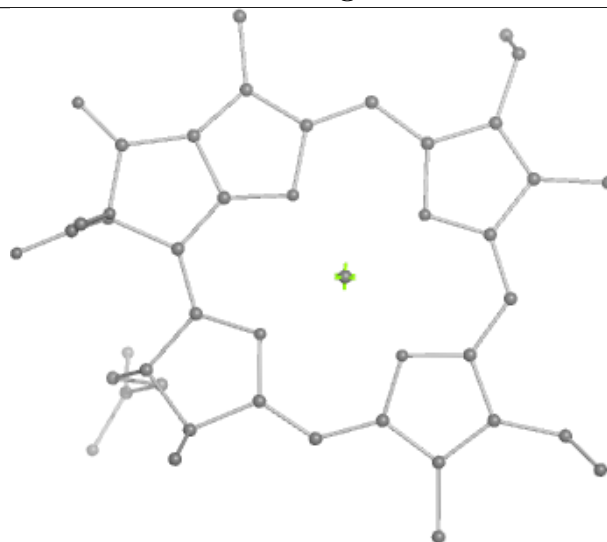
Bond lengths



Bond angles

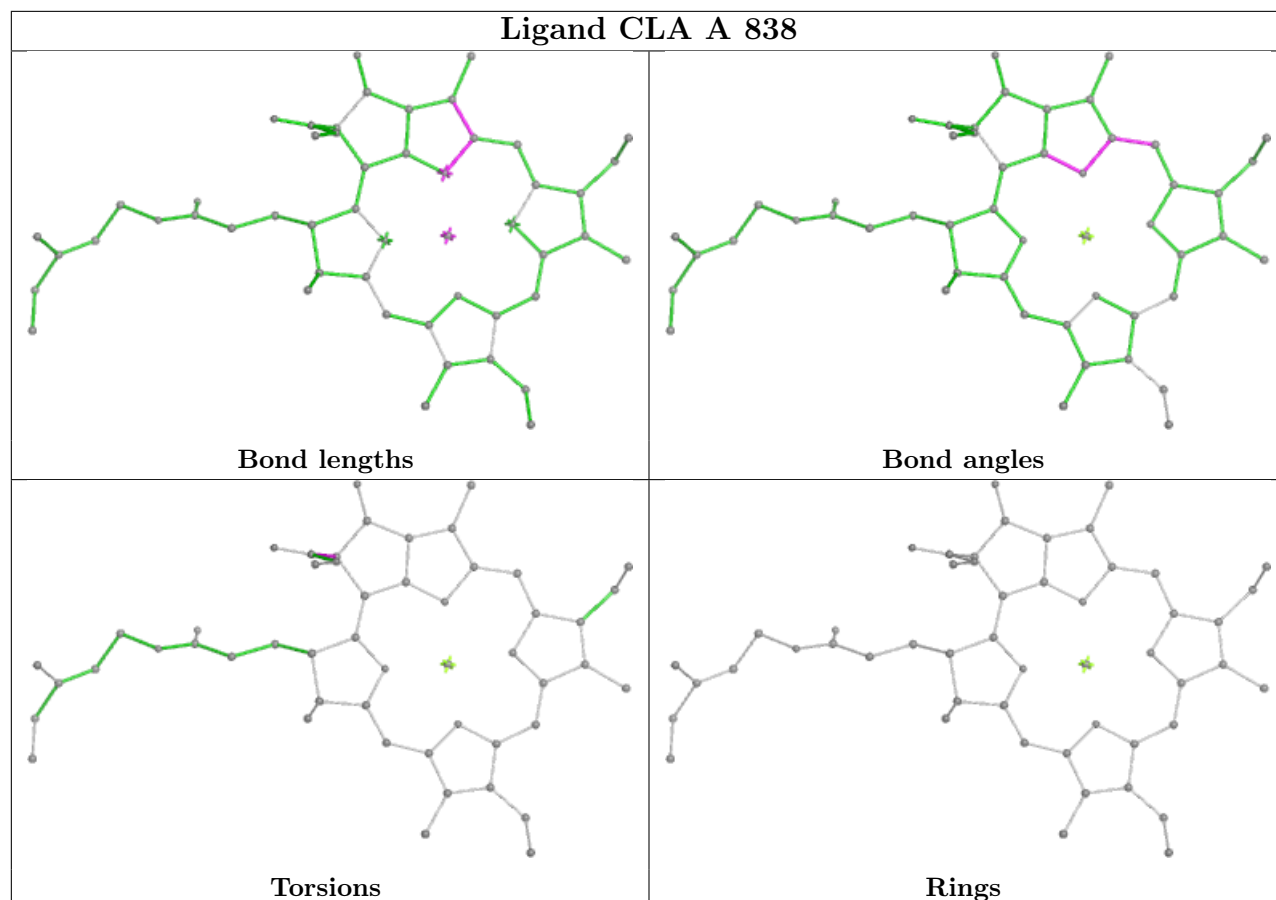


Torsions

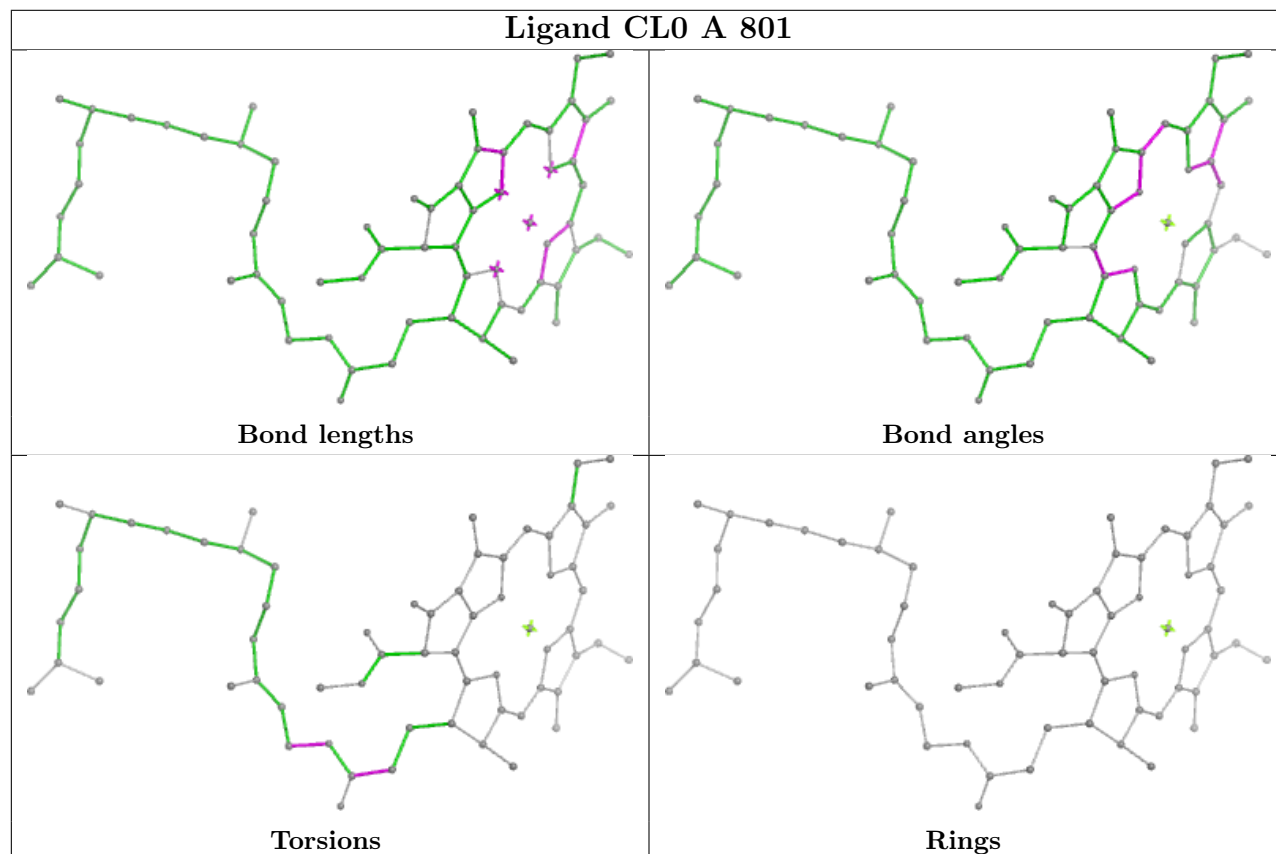


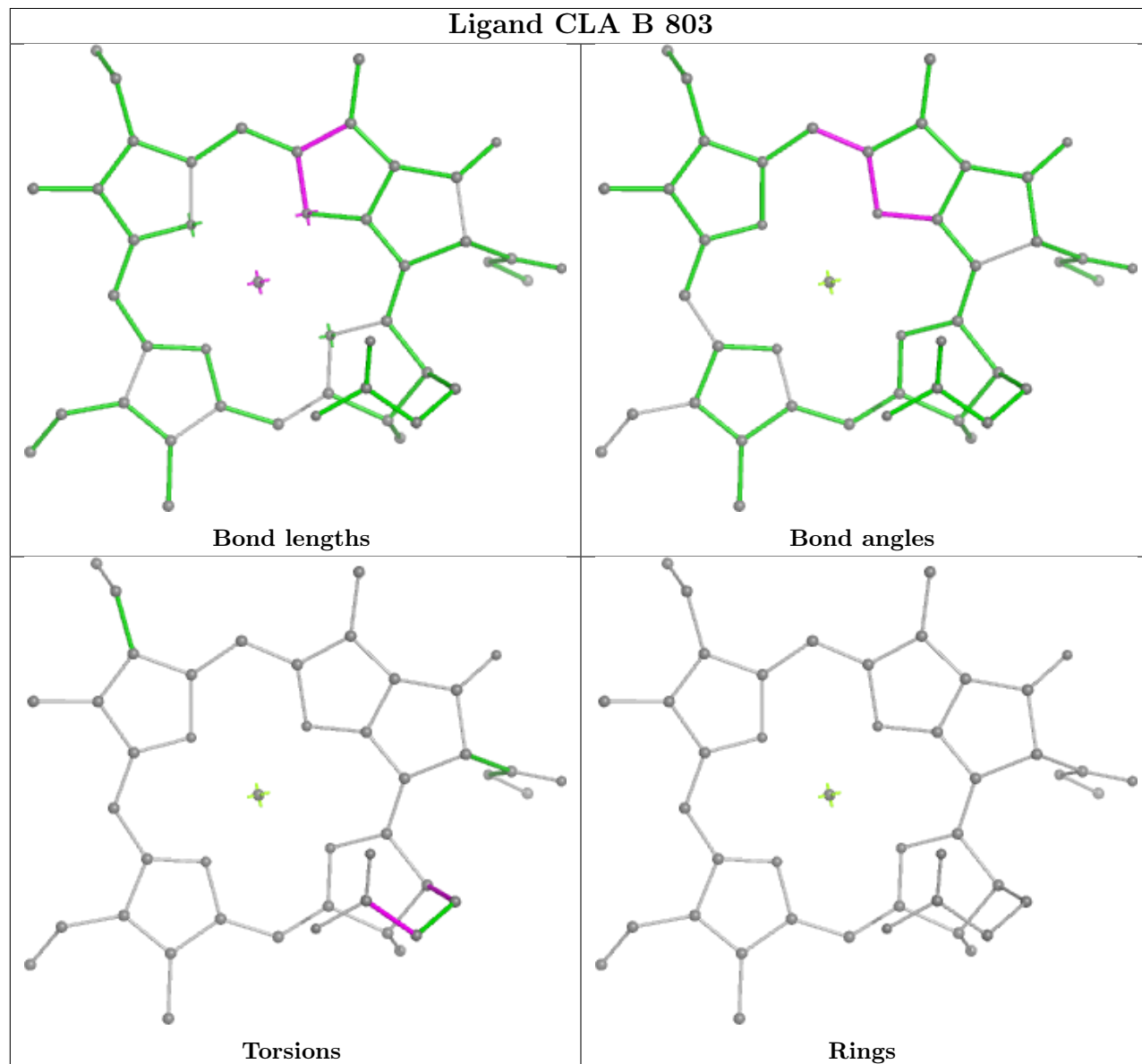
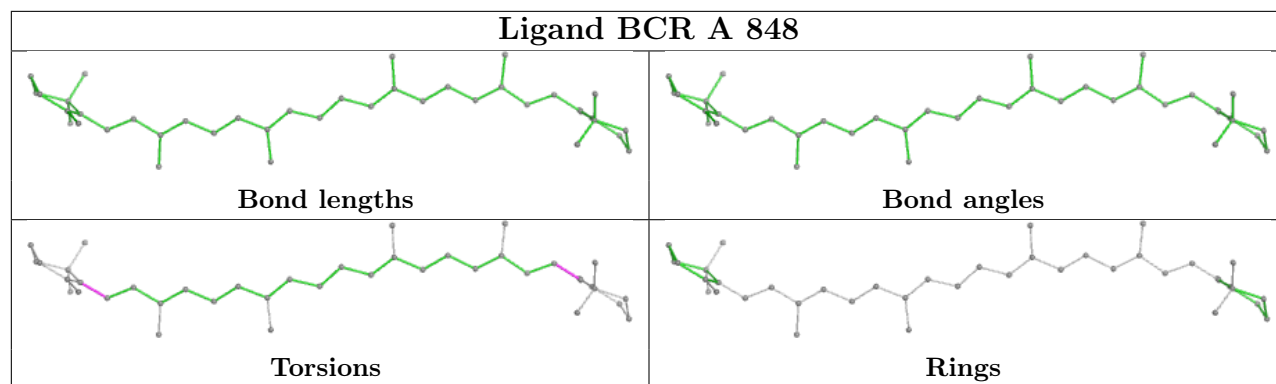
Rings

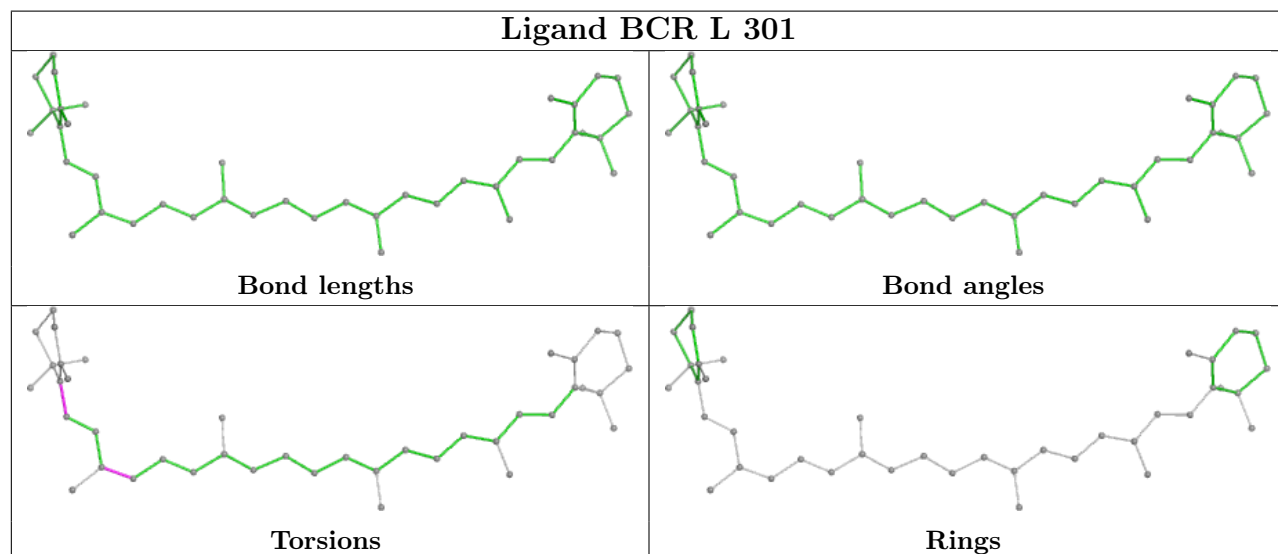
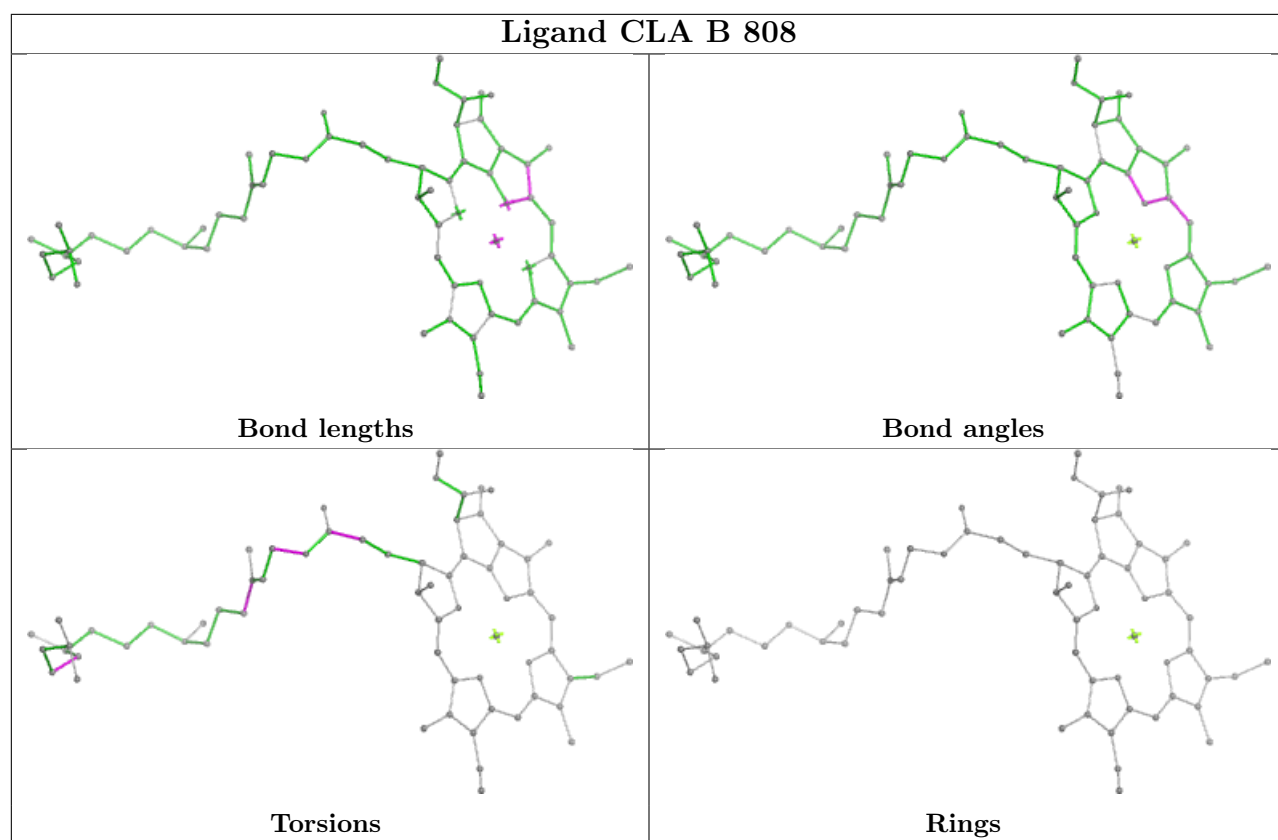
Ligand CLA A 838



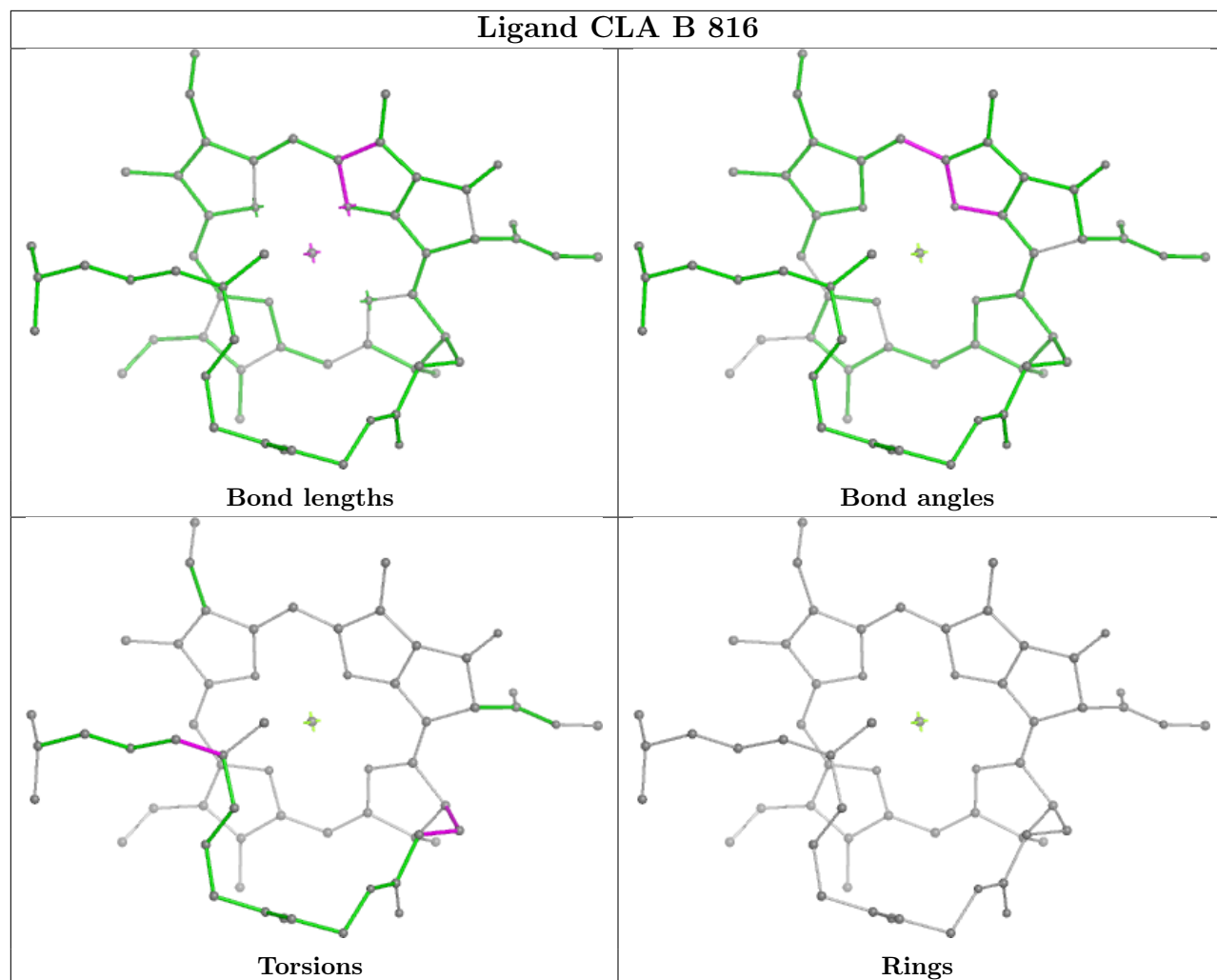
Ligand CL0 A 801

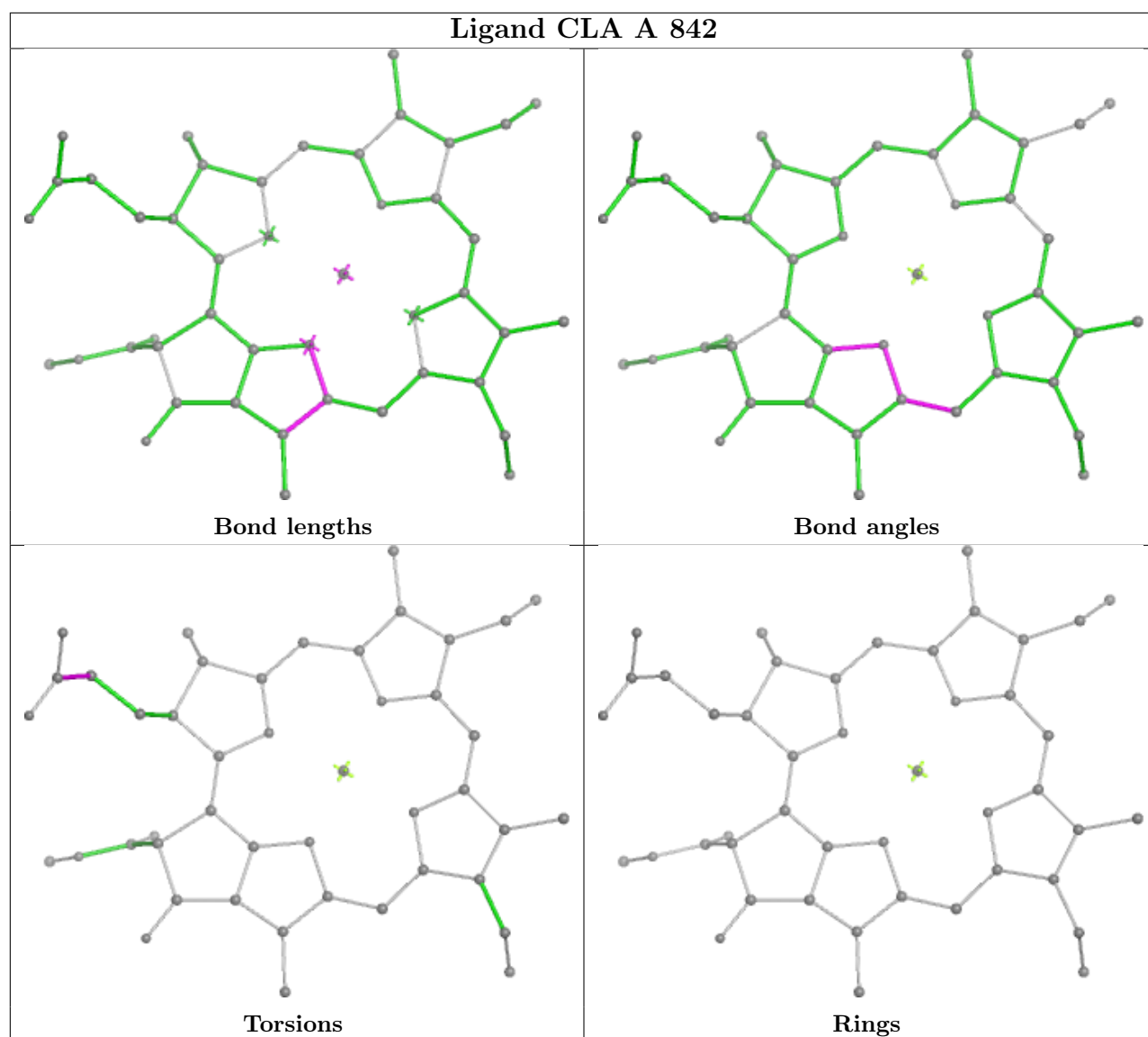


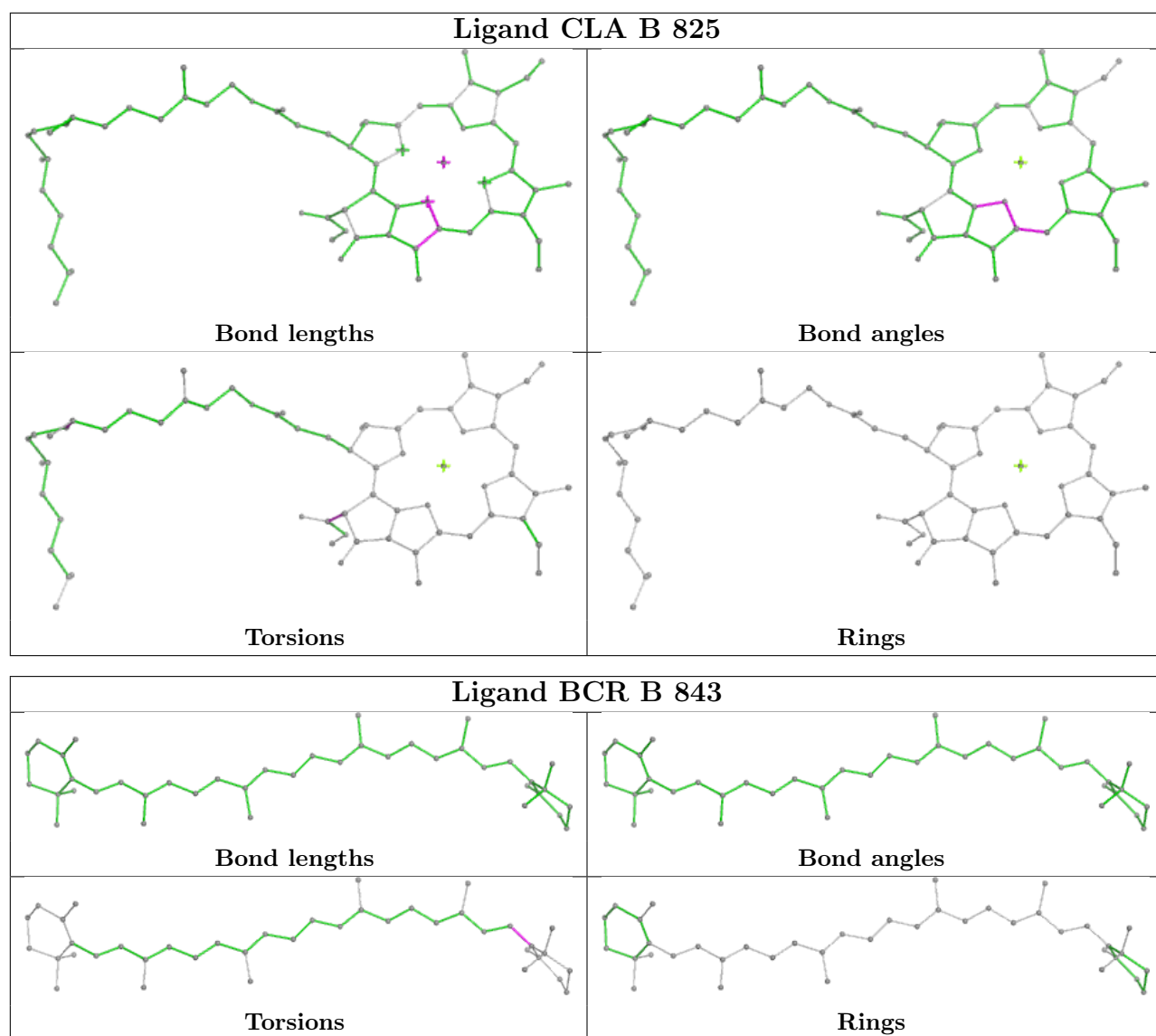


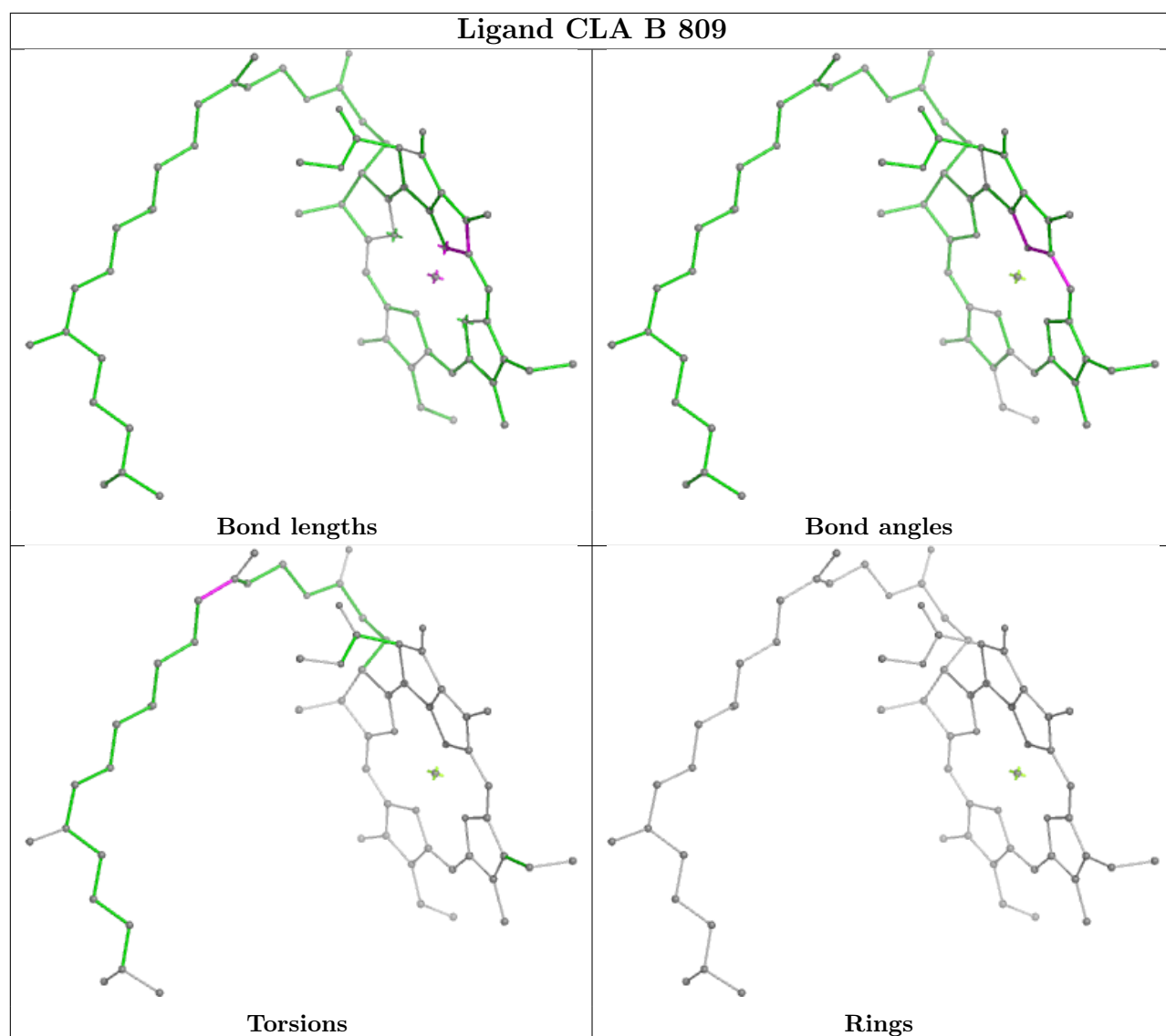


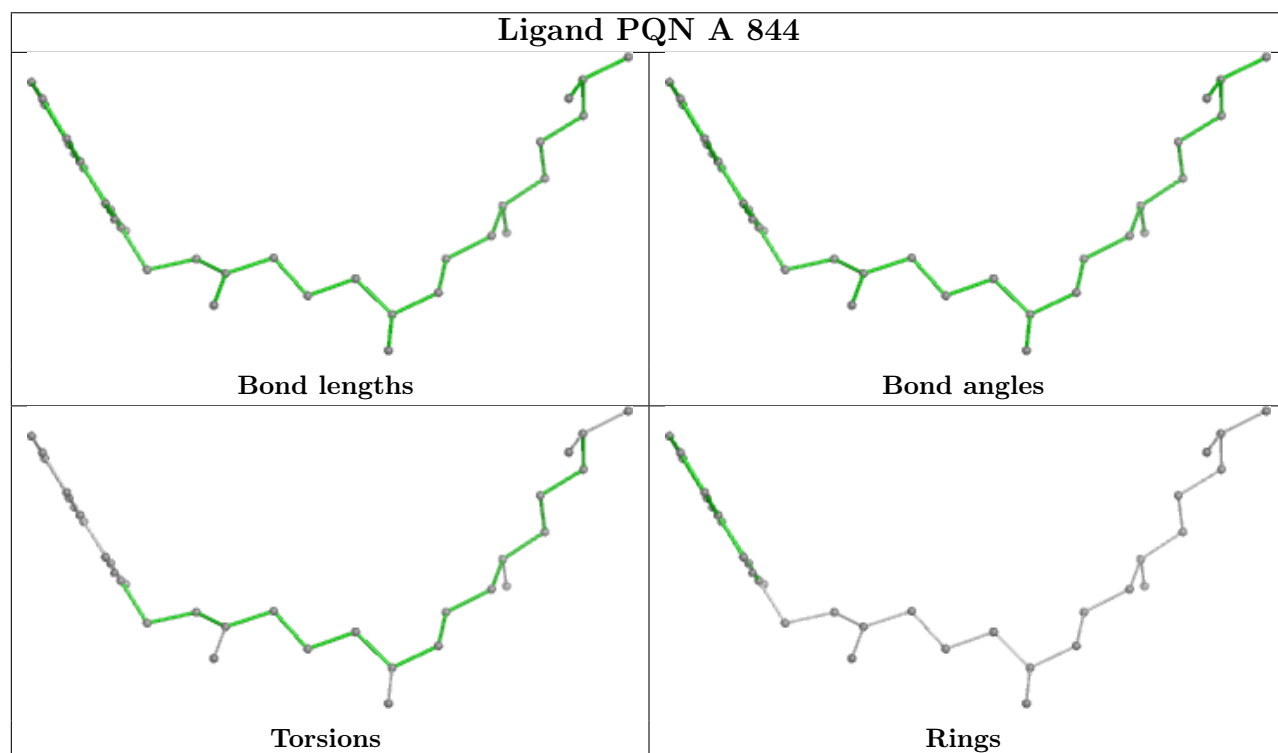
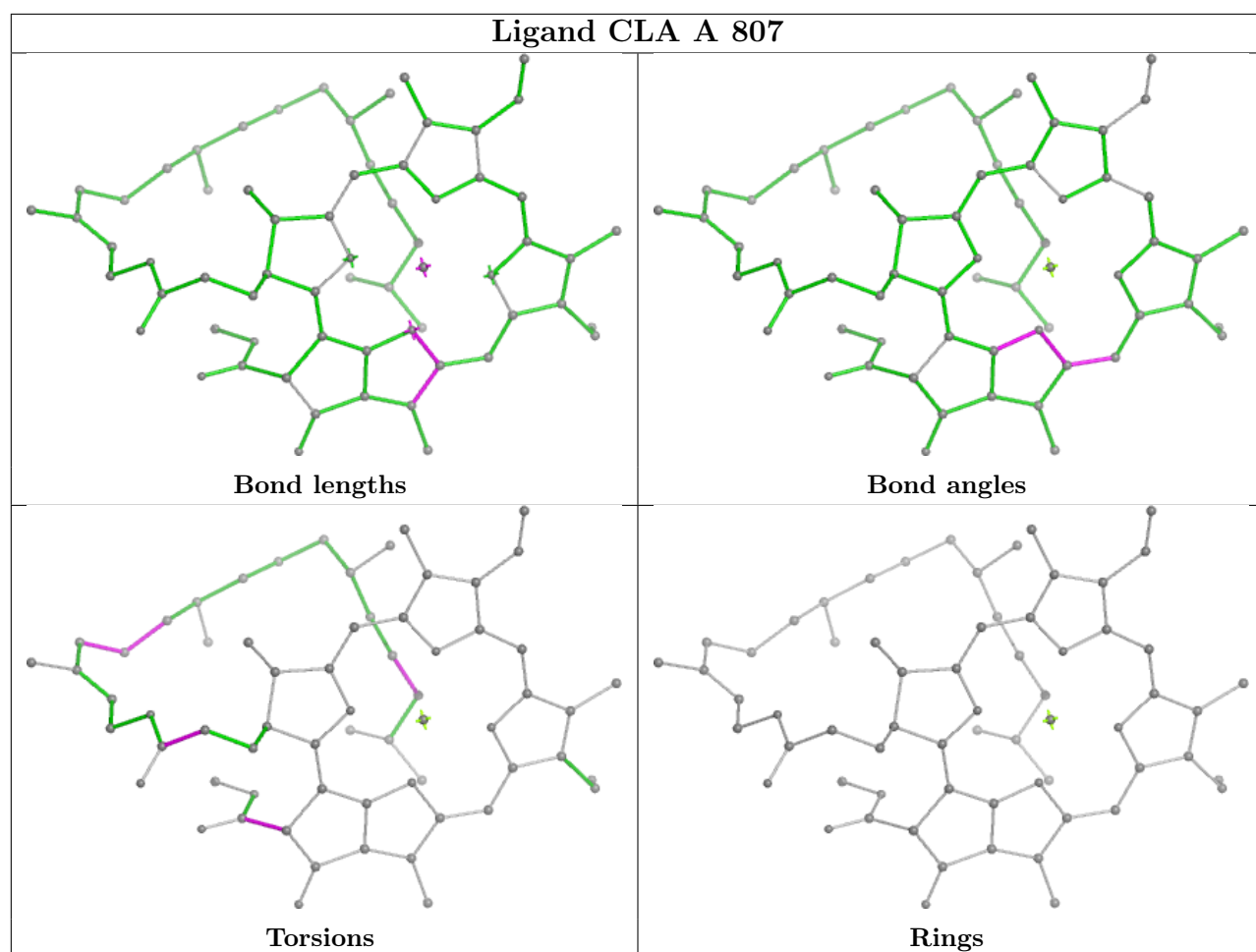
Ligand CLA B 816



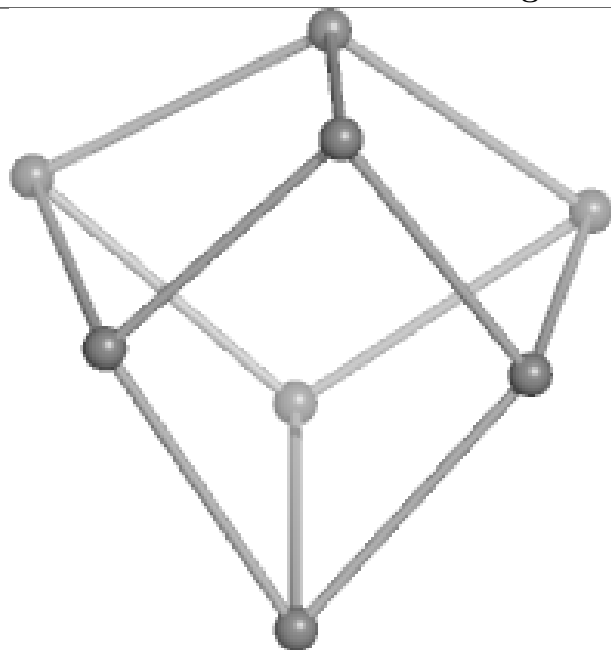




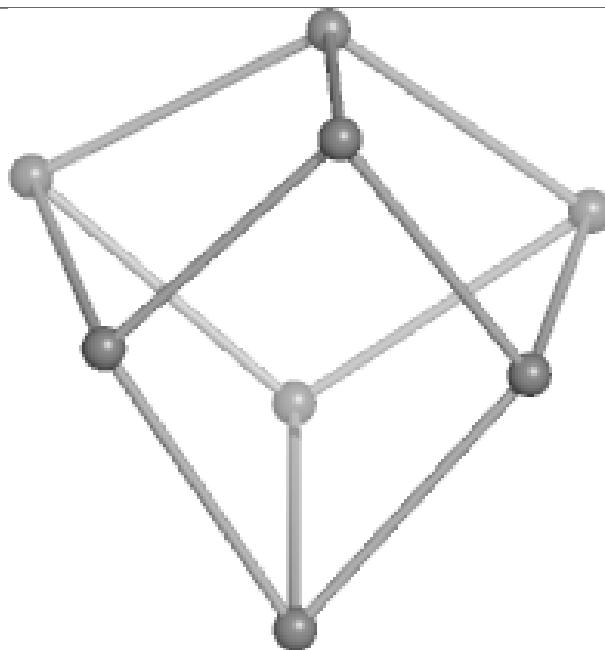




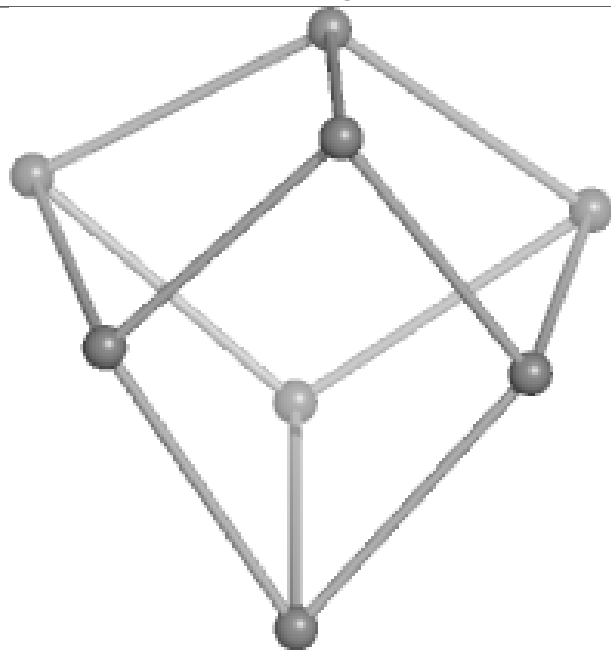
Ligand SF4 C 101



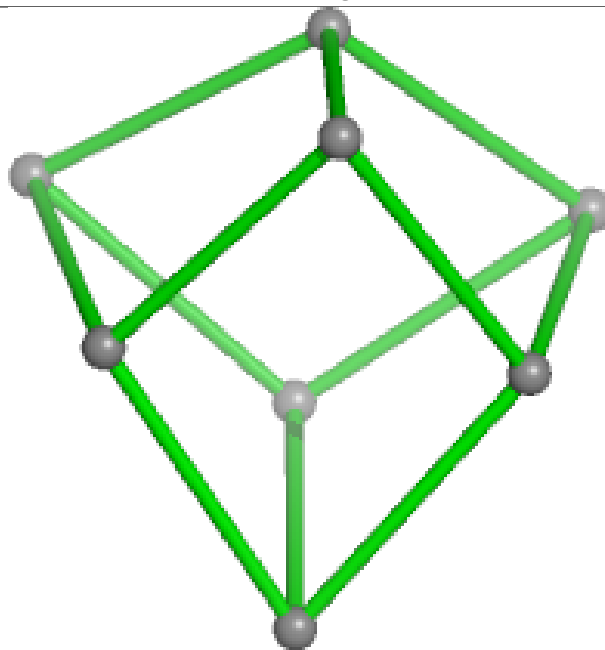
Bond lengths



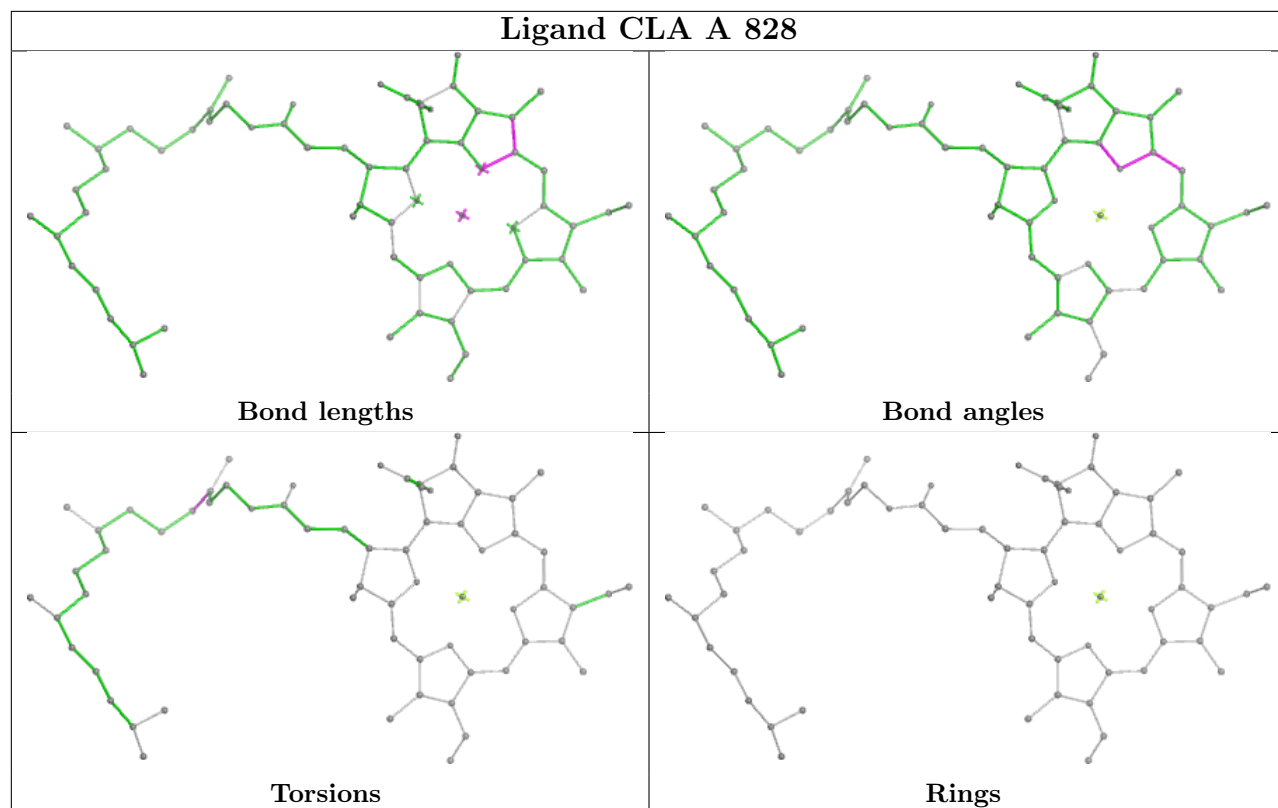
Bond angles



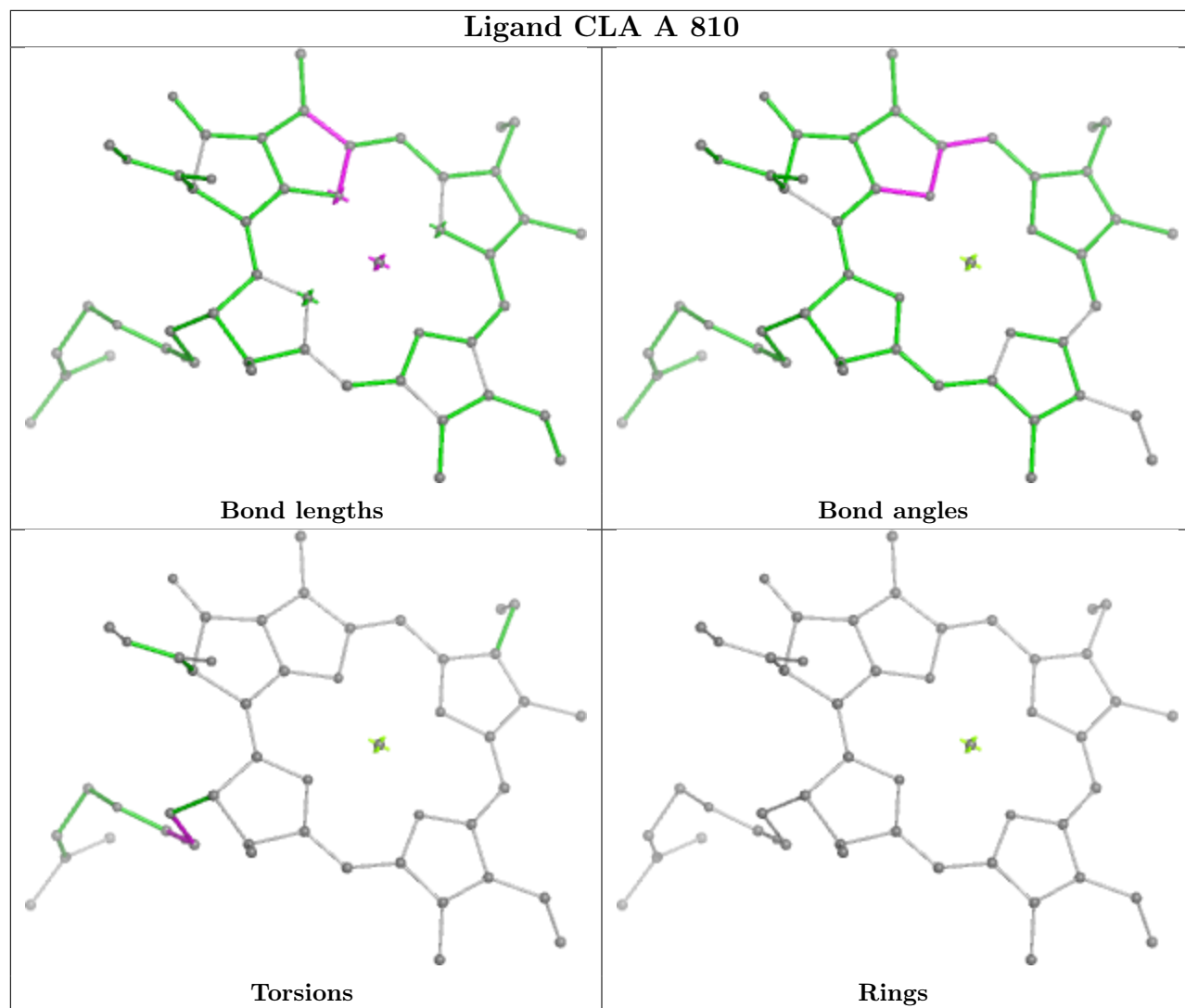
Torsions

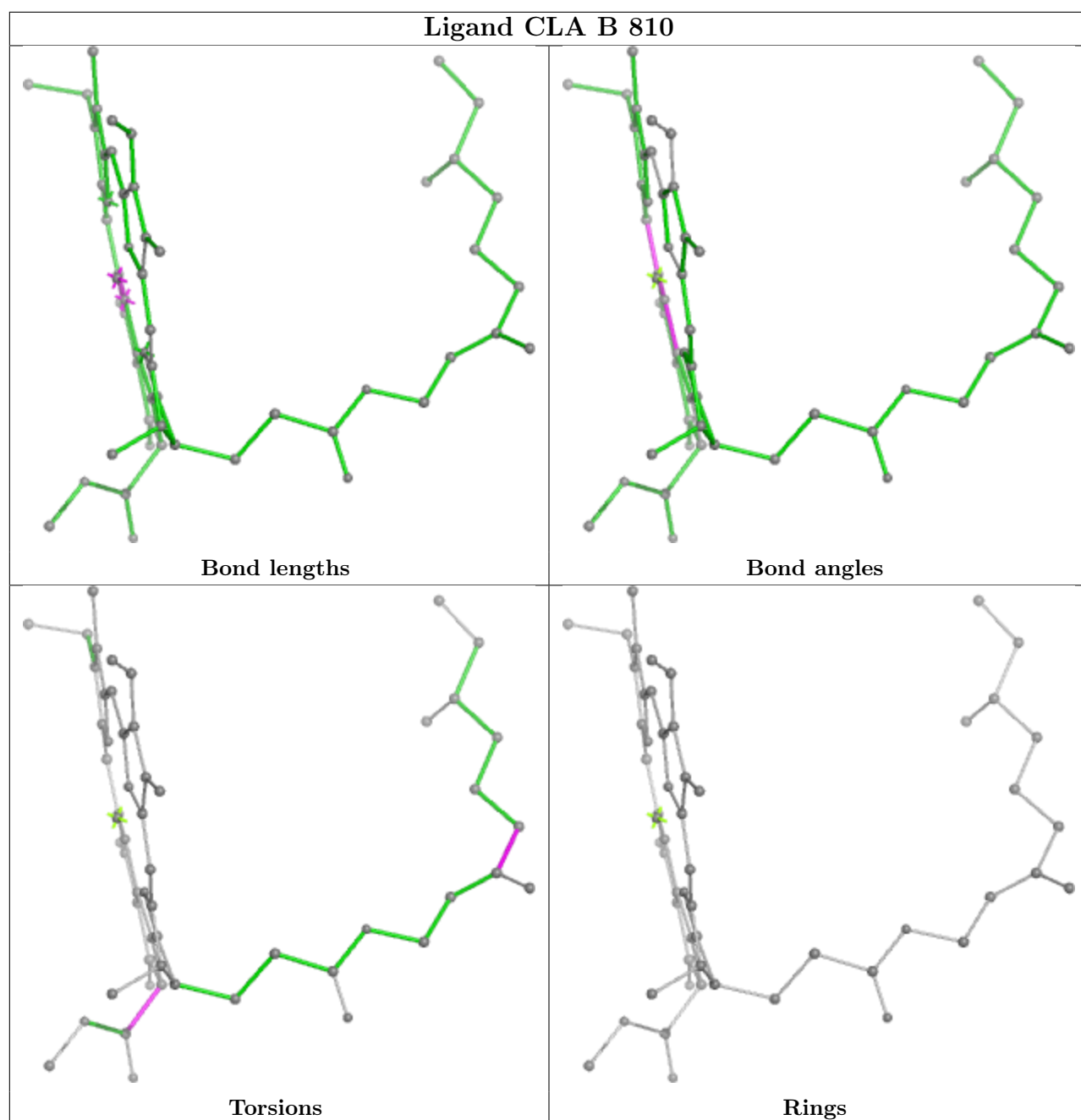


Rings

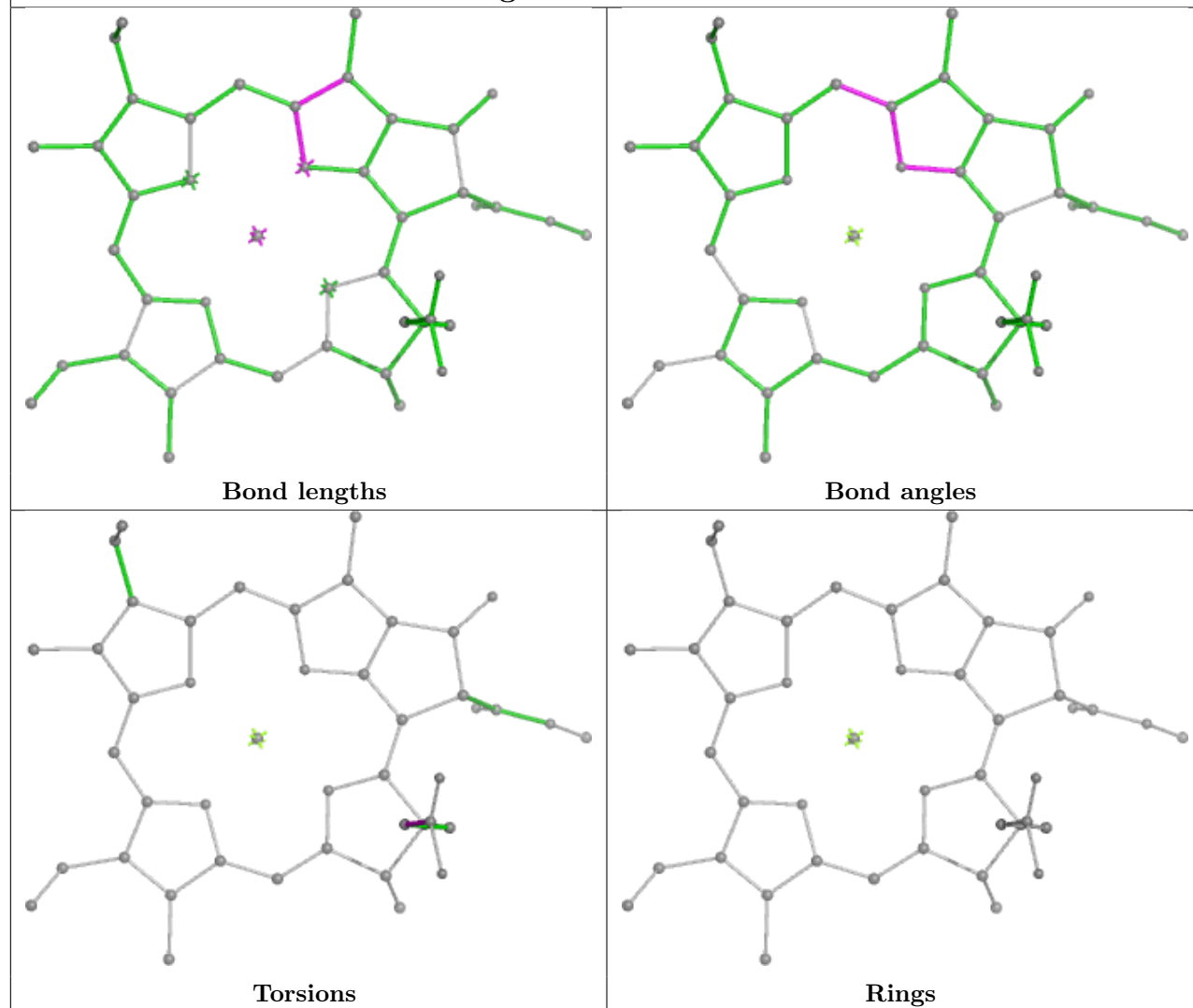


Ligand CLA A 810

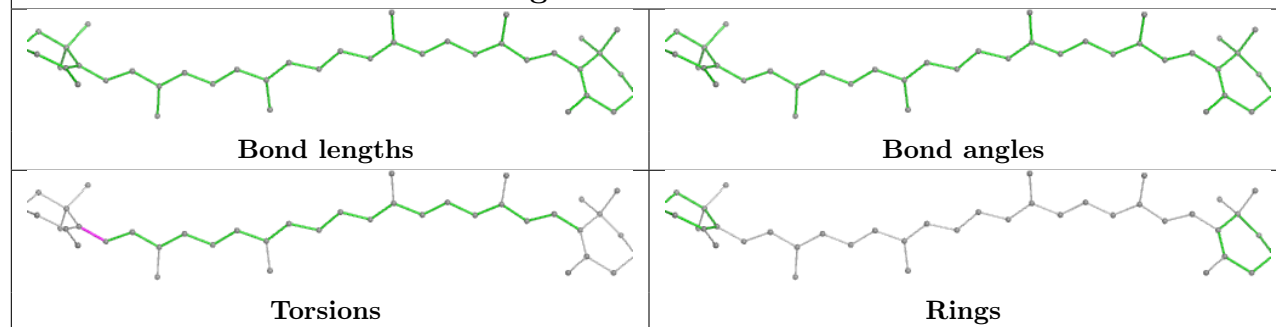


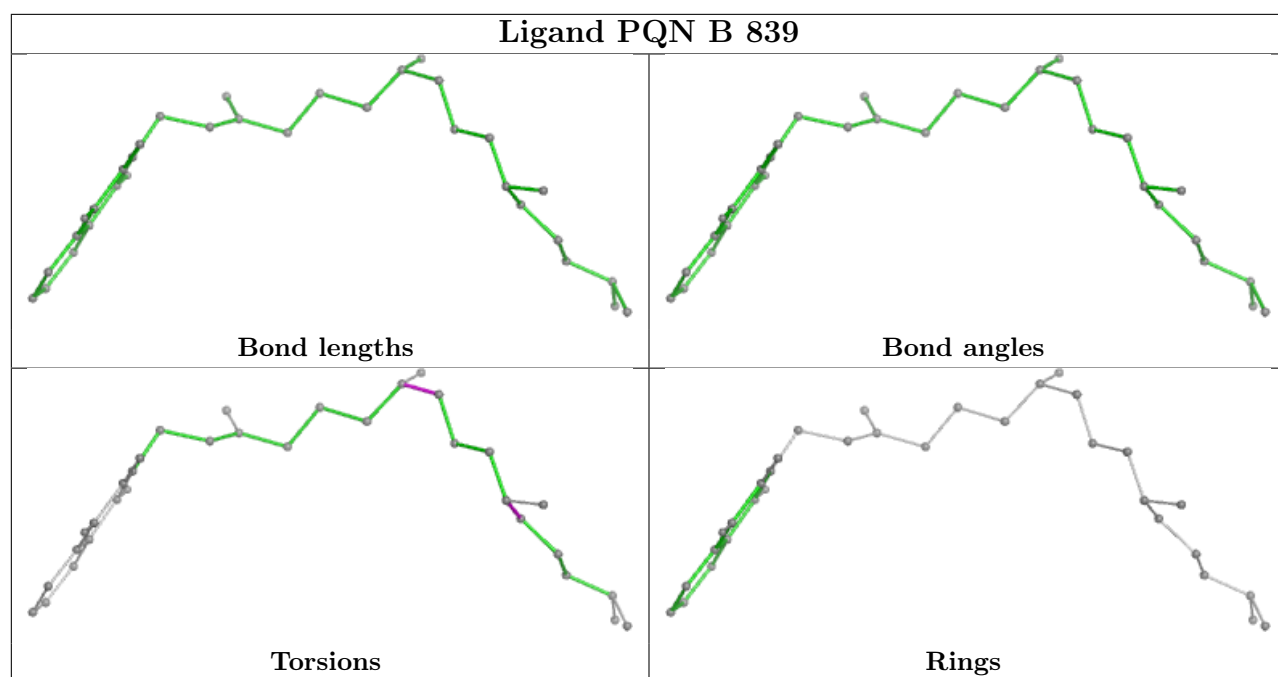


Ligand CLA L 302

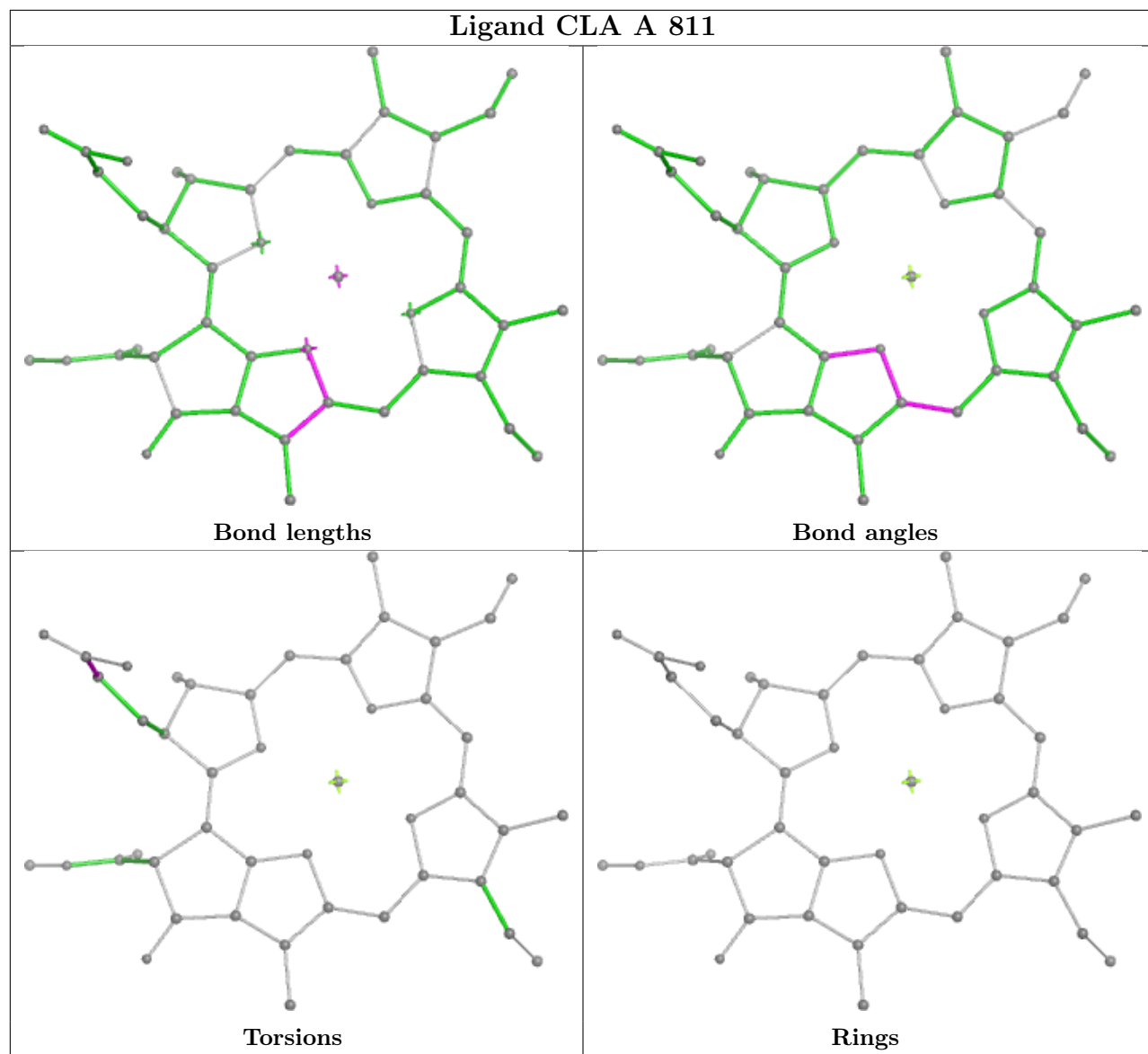


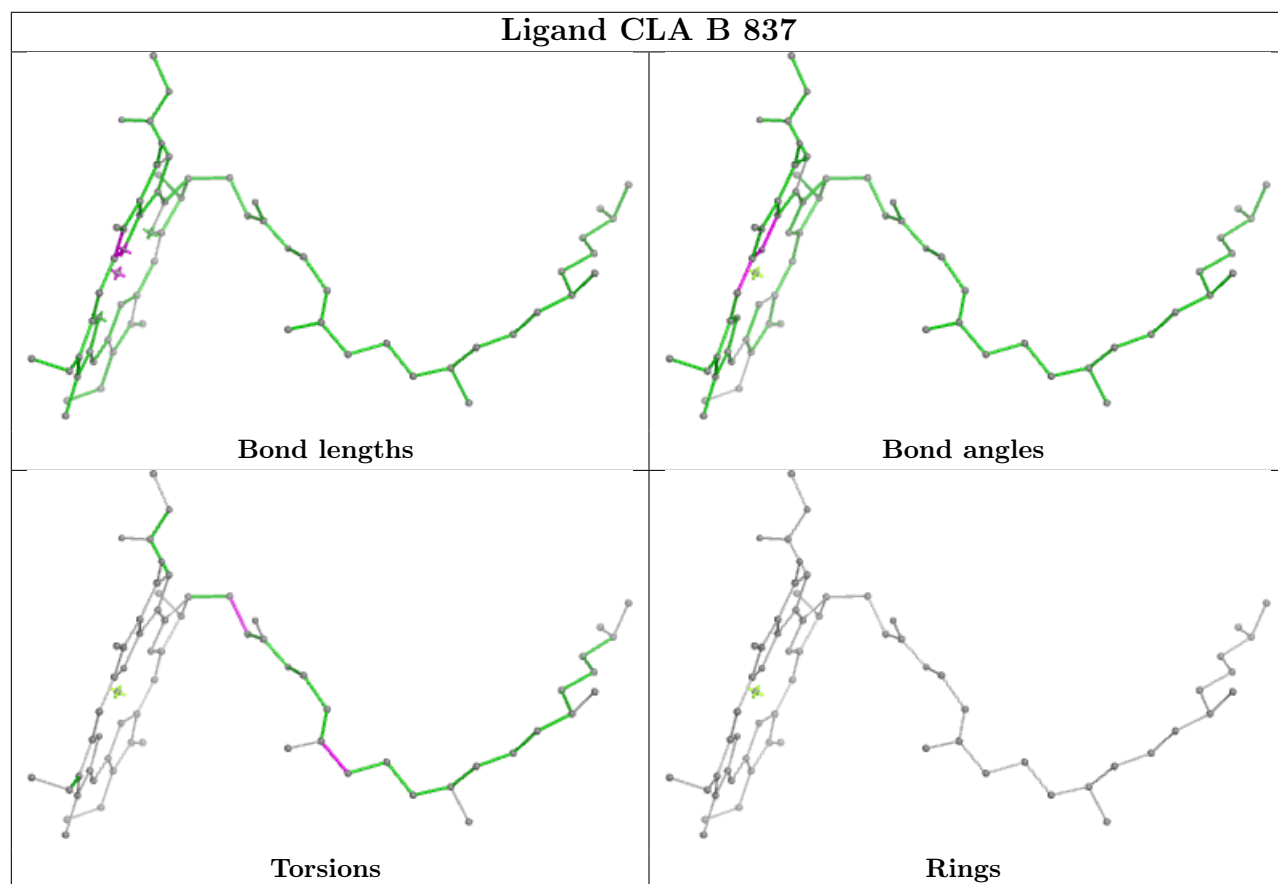
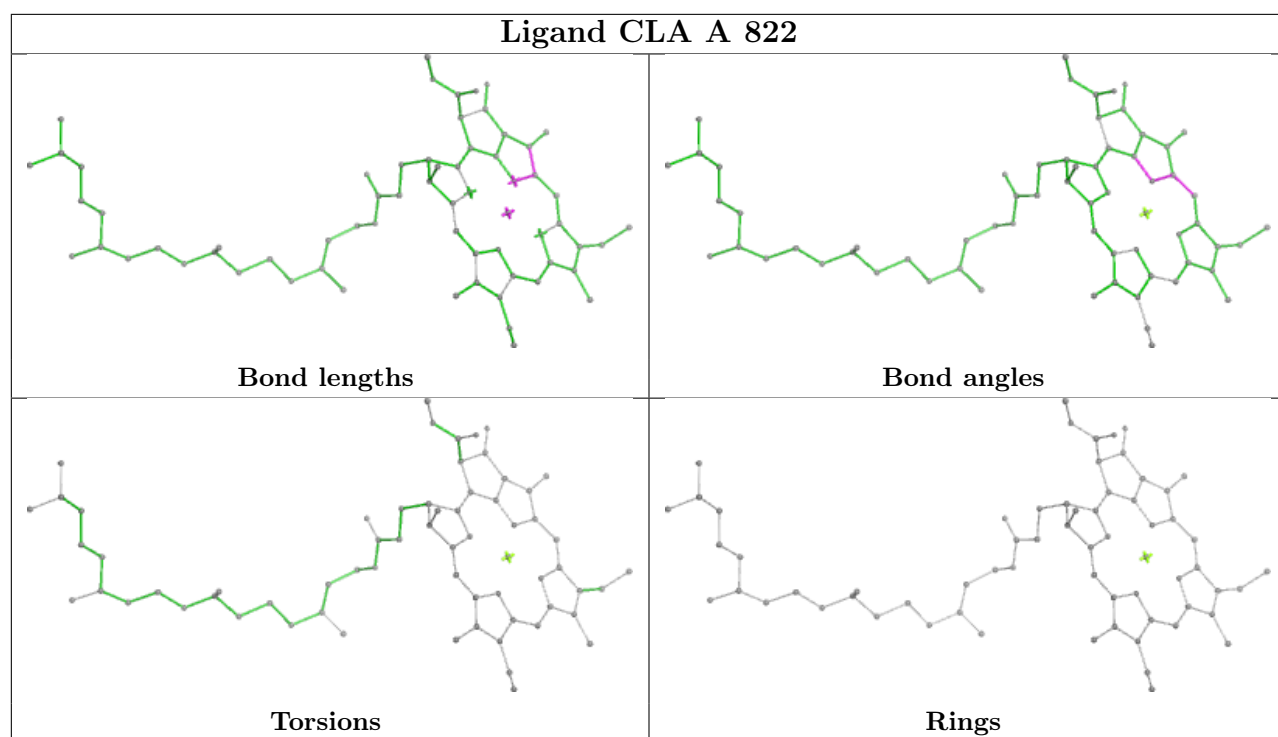
Ligand BCR A 850



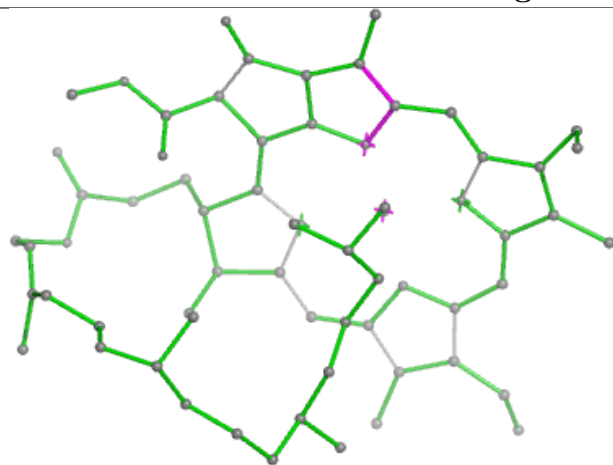


Ligand CLA A 811

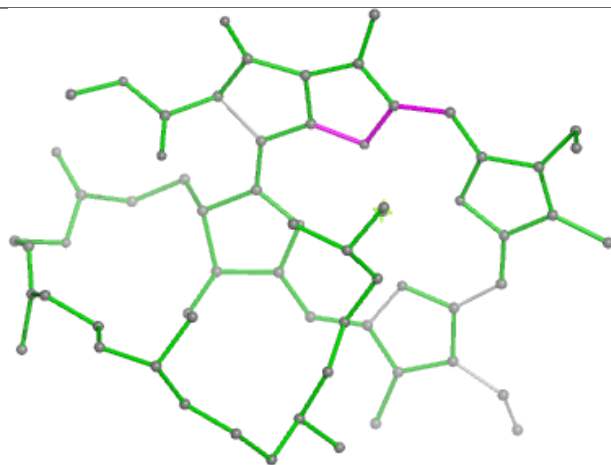




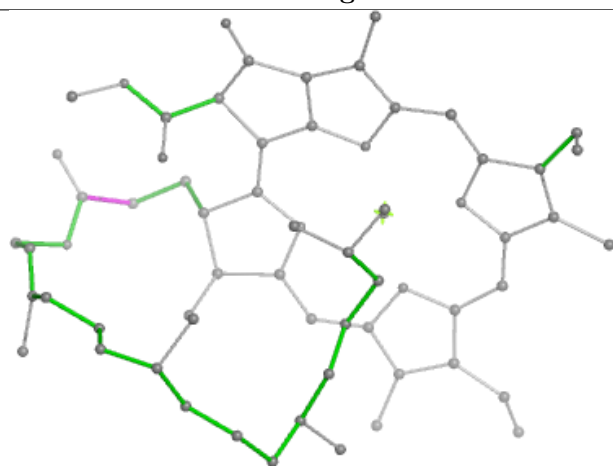
Ligand CLA B 805



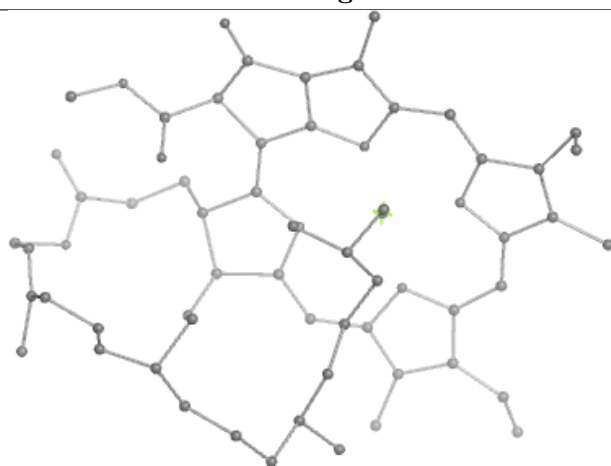
Bond lengths



Bond angles

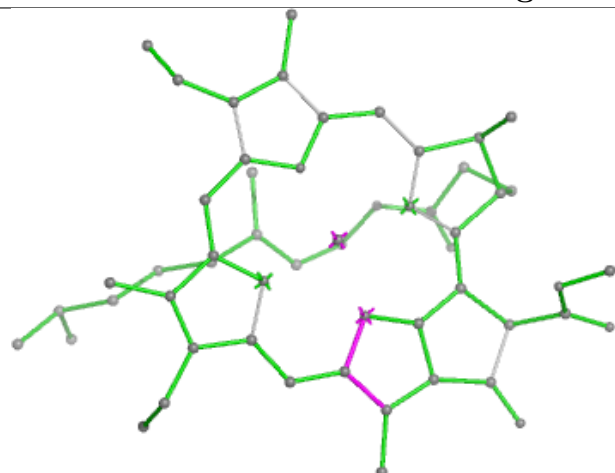


Torsions

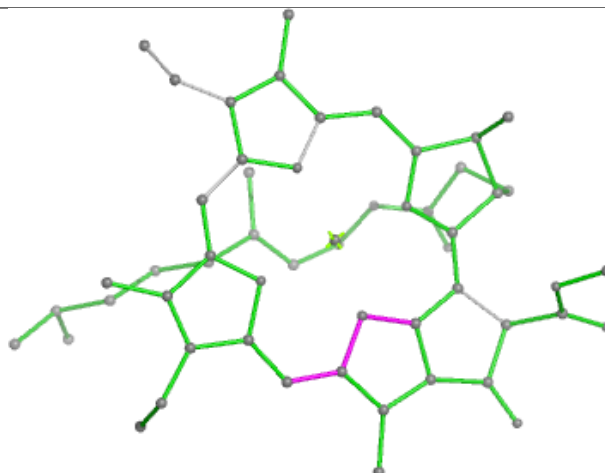


Rings

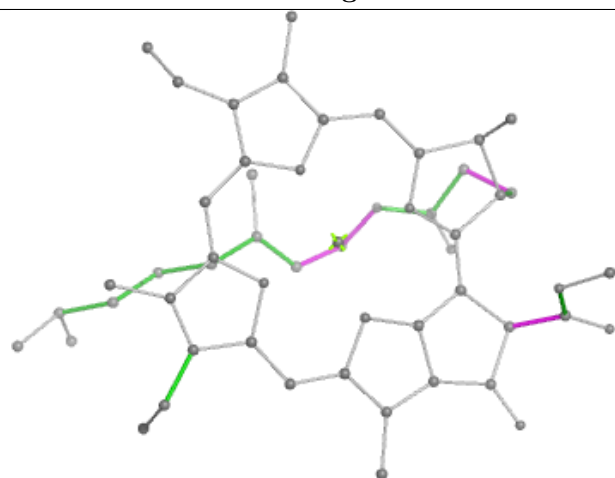
Ligand CLA B 814



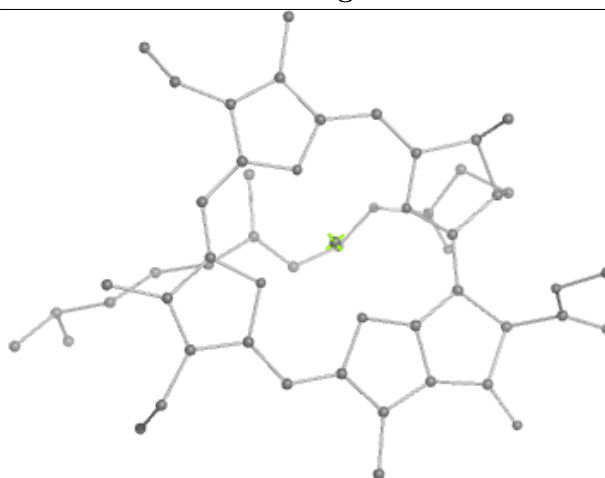
Bond lengths



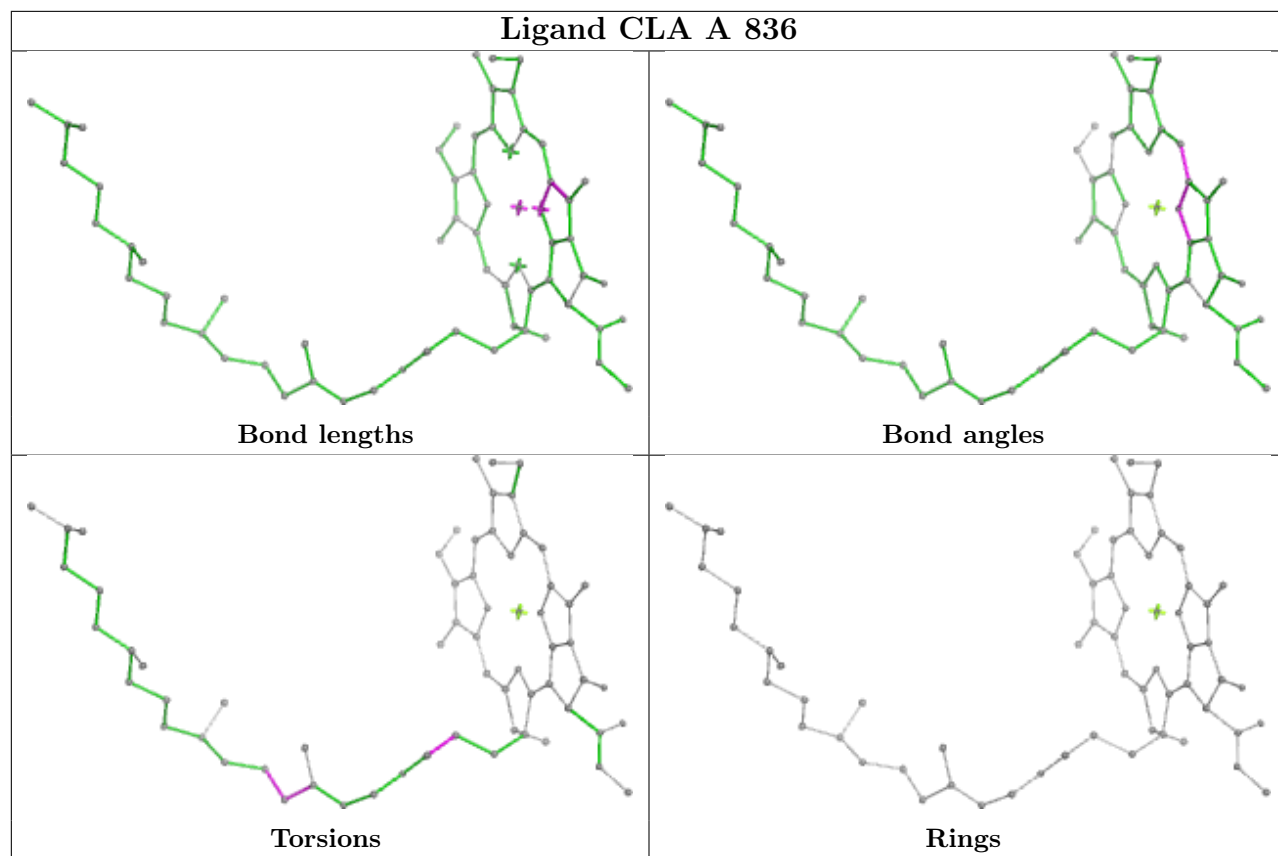
Bond angles



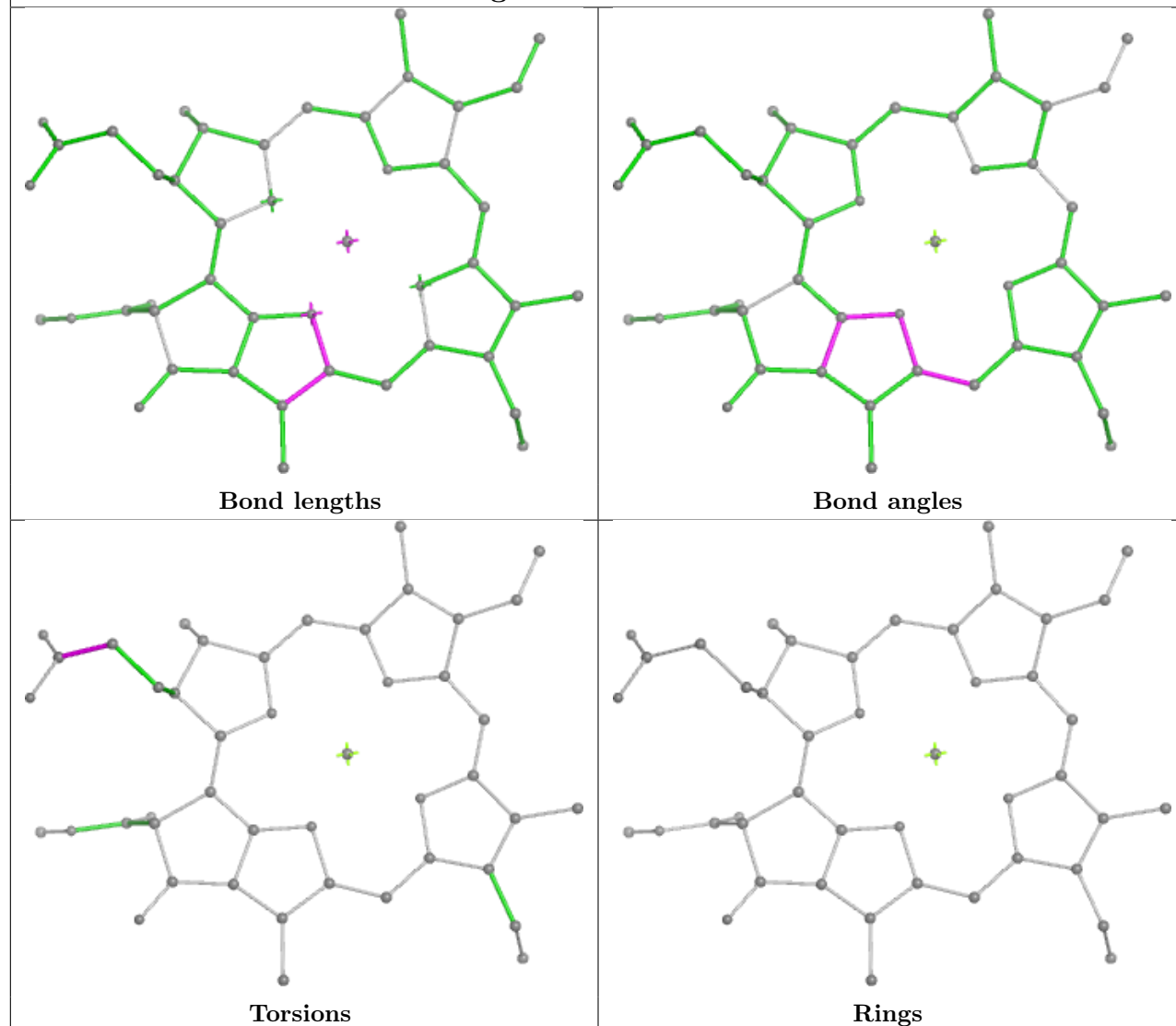
Torsions



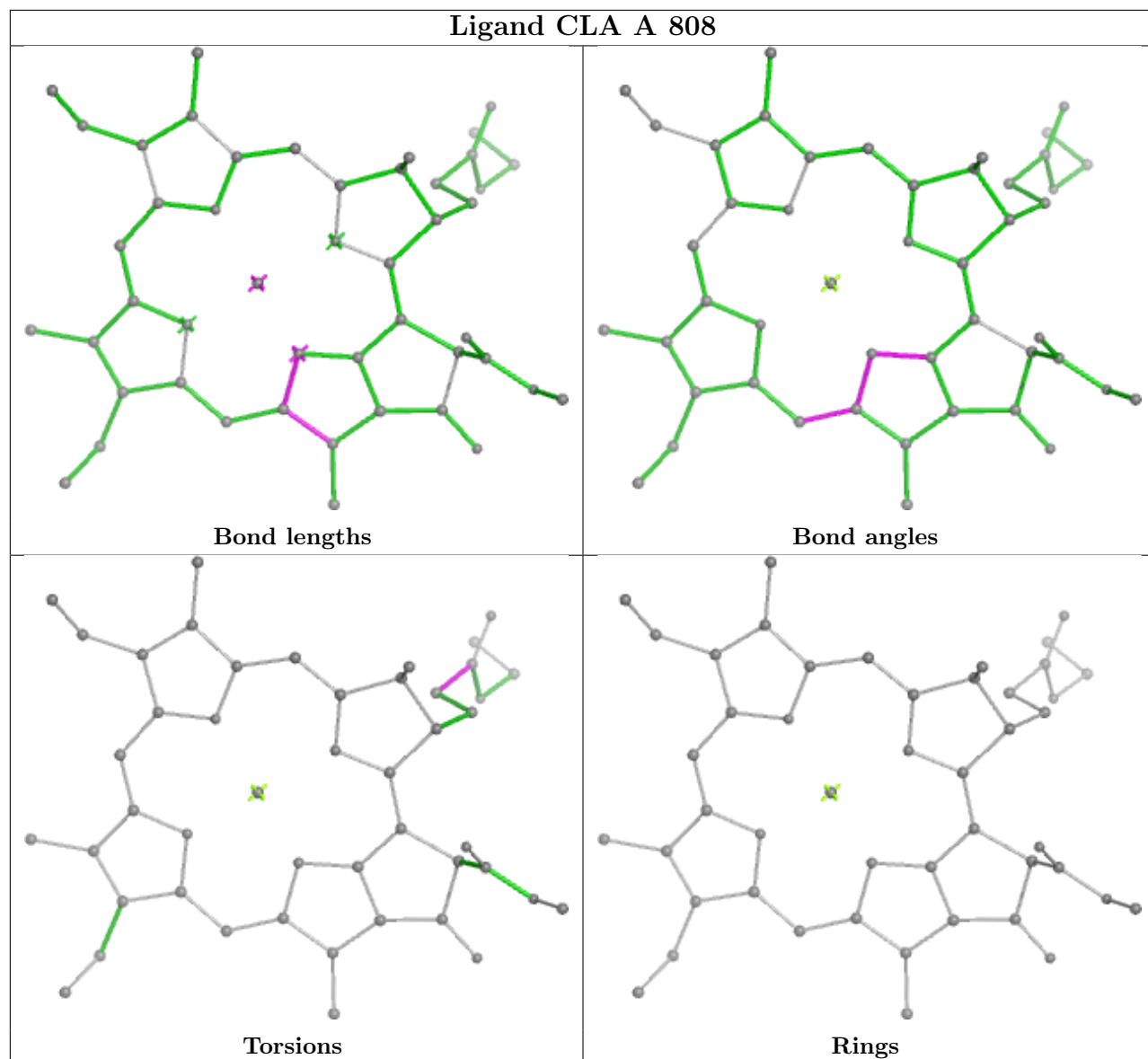
Rings



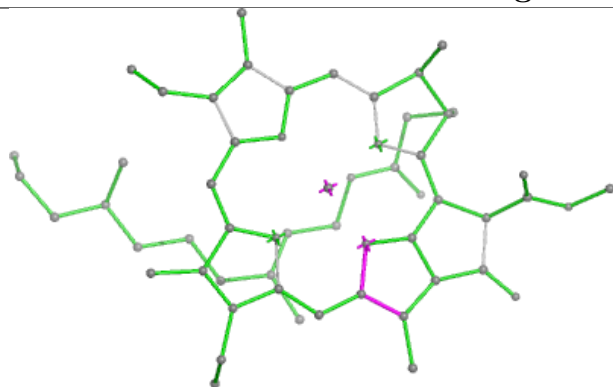
Ligand CLA B 831



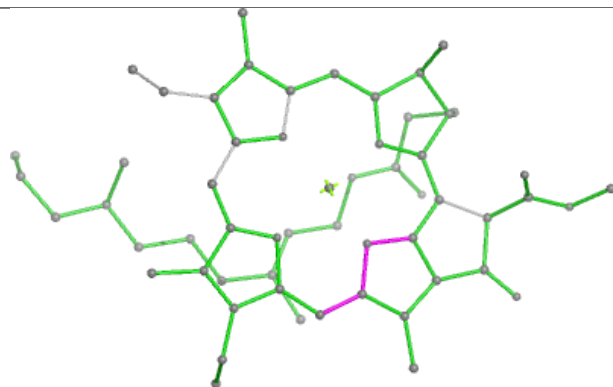
Ligand CLA A 808



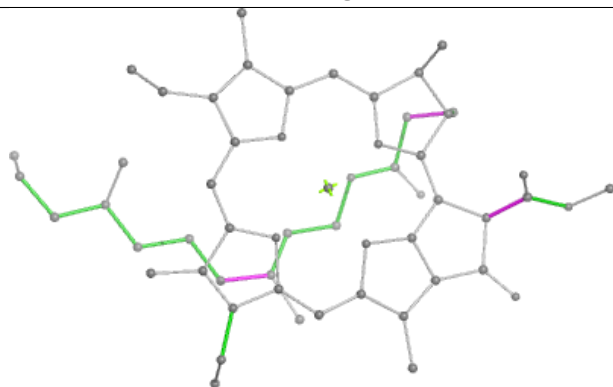
Ligand CLA B 815



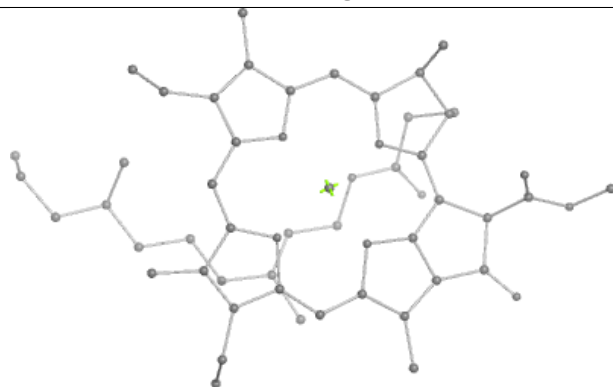
Bond lengths



Bond angles

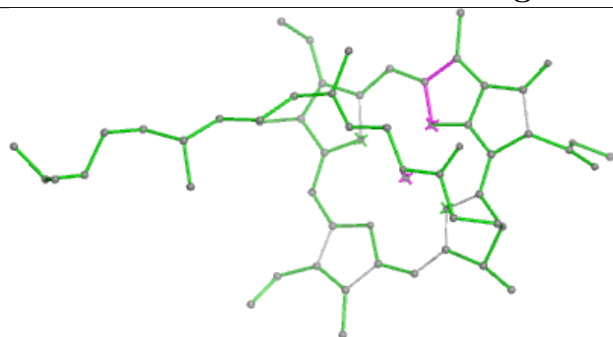


Torsions

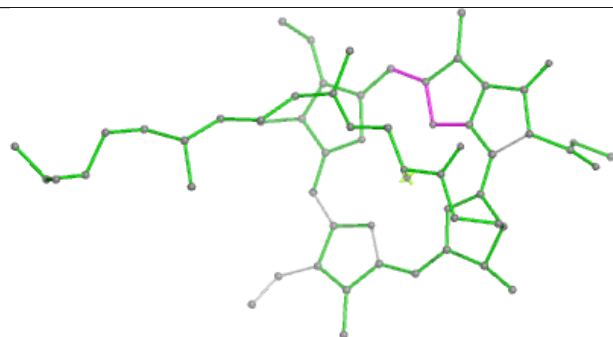


Rings

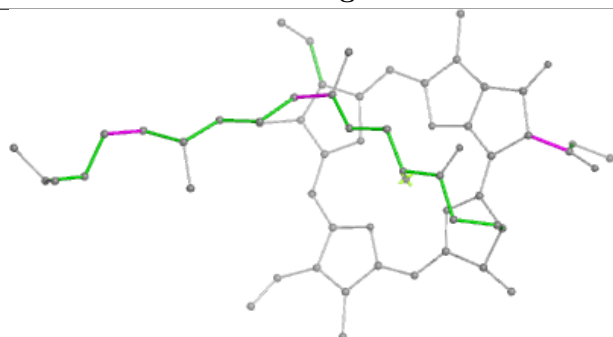
Ligand CLA A 816



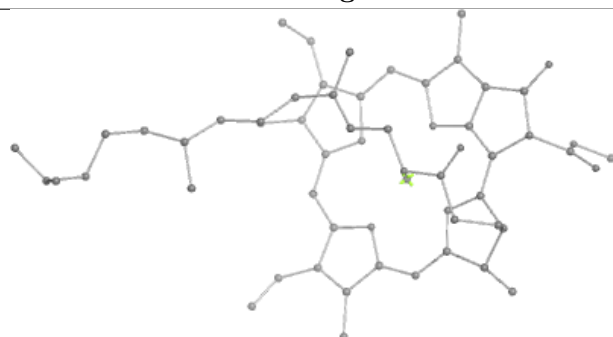
Bond lengths



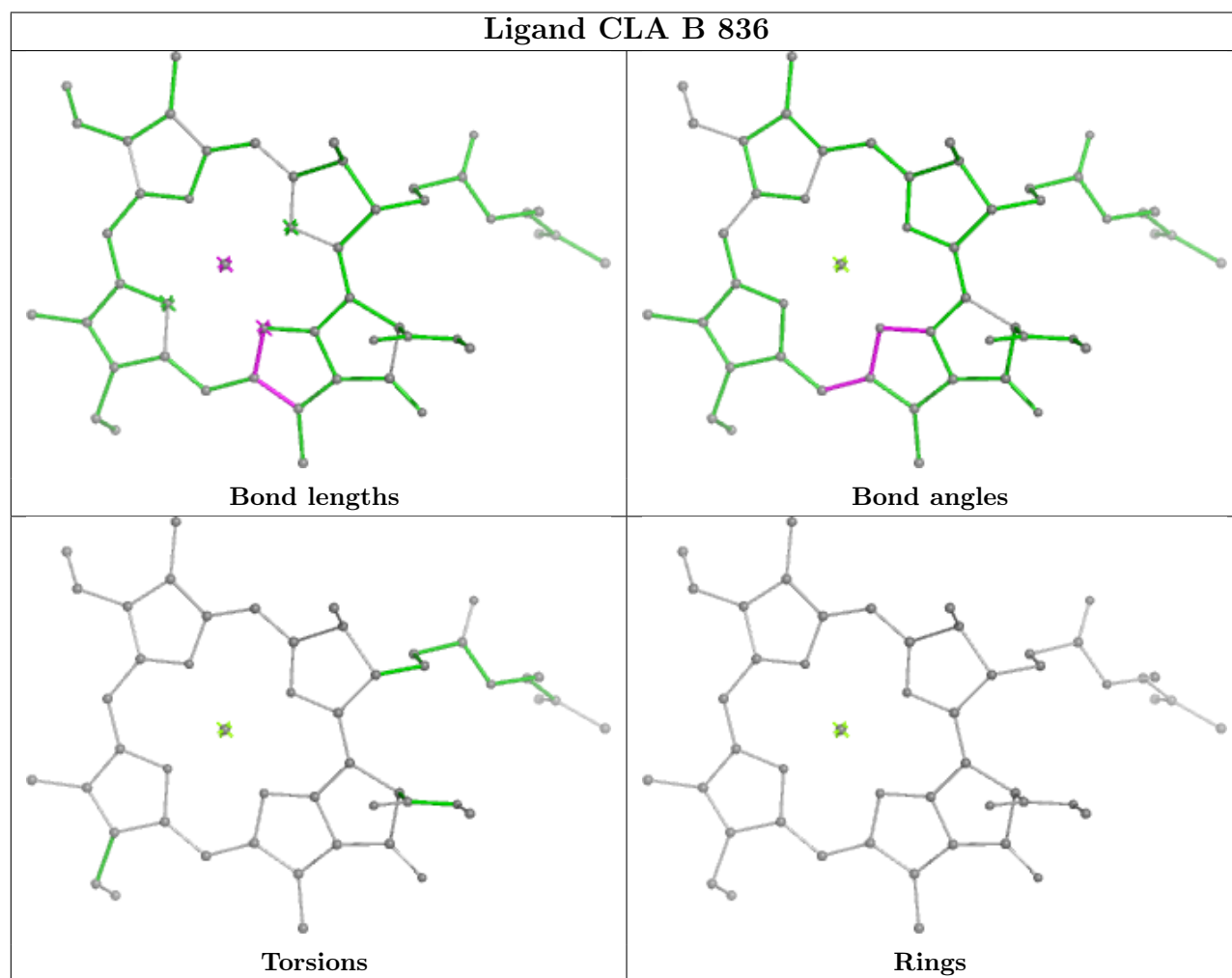
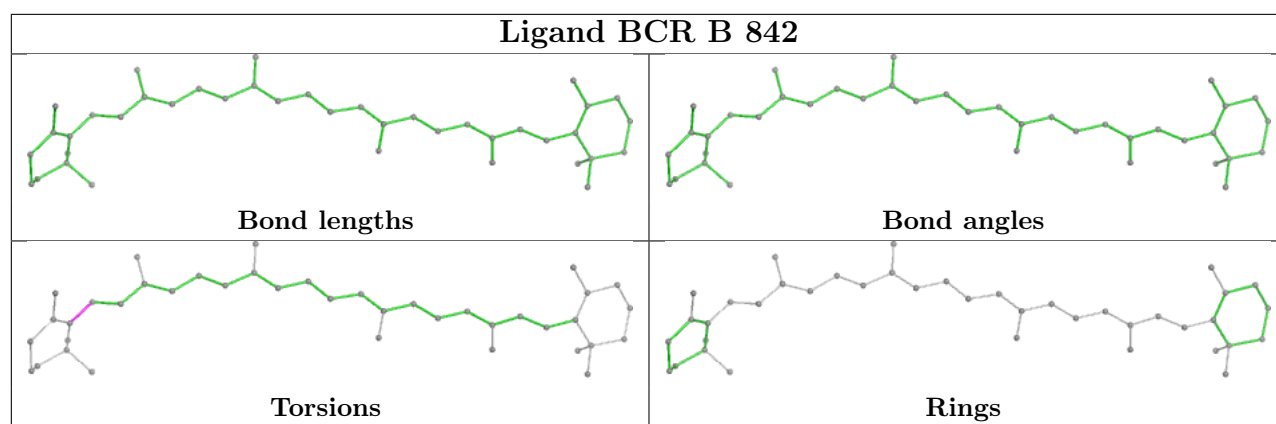
Bond angles

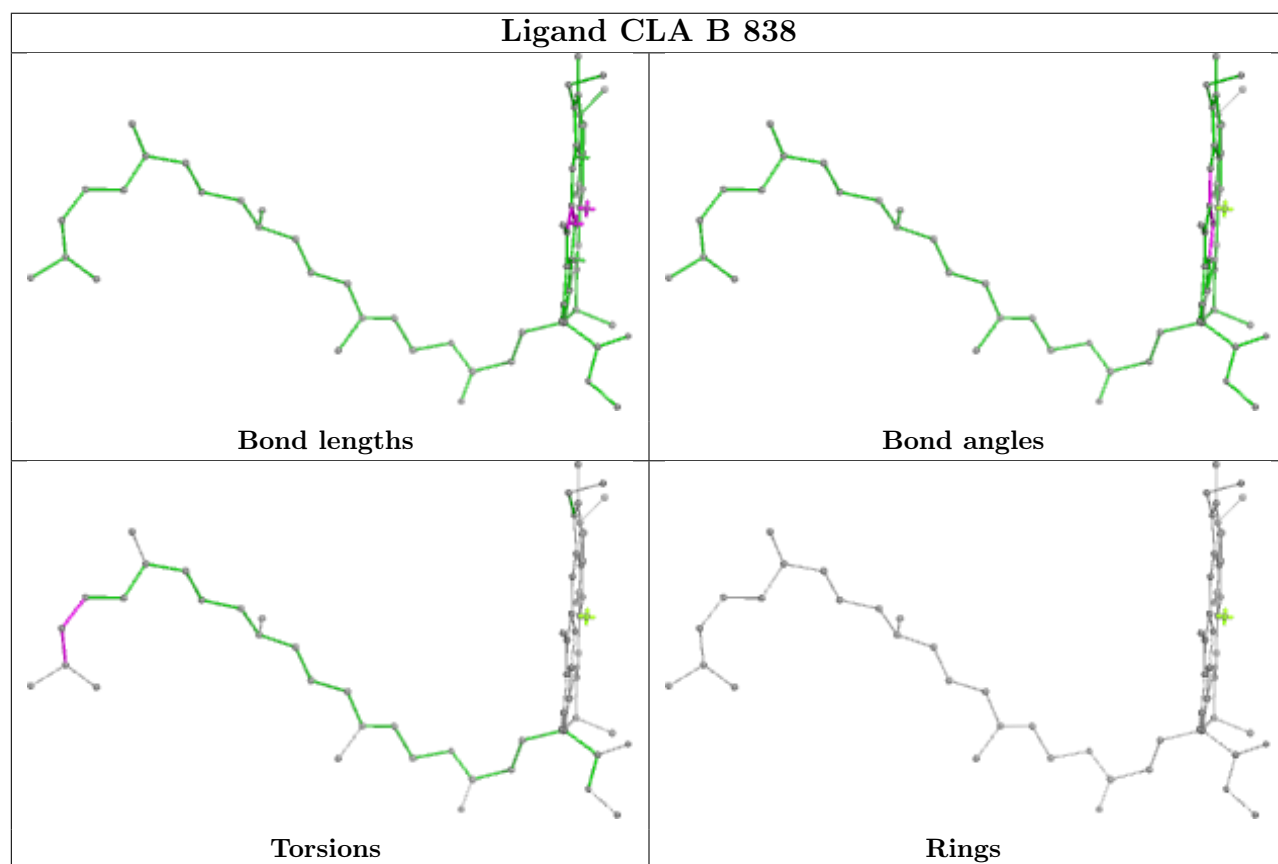
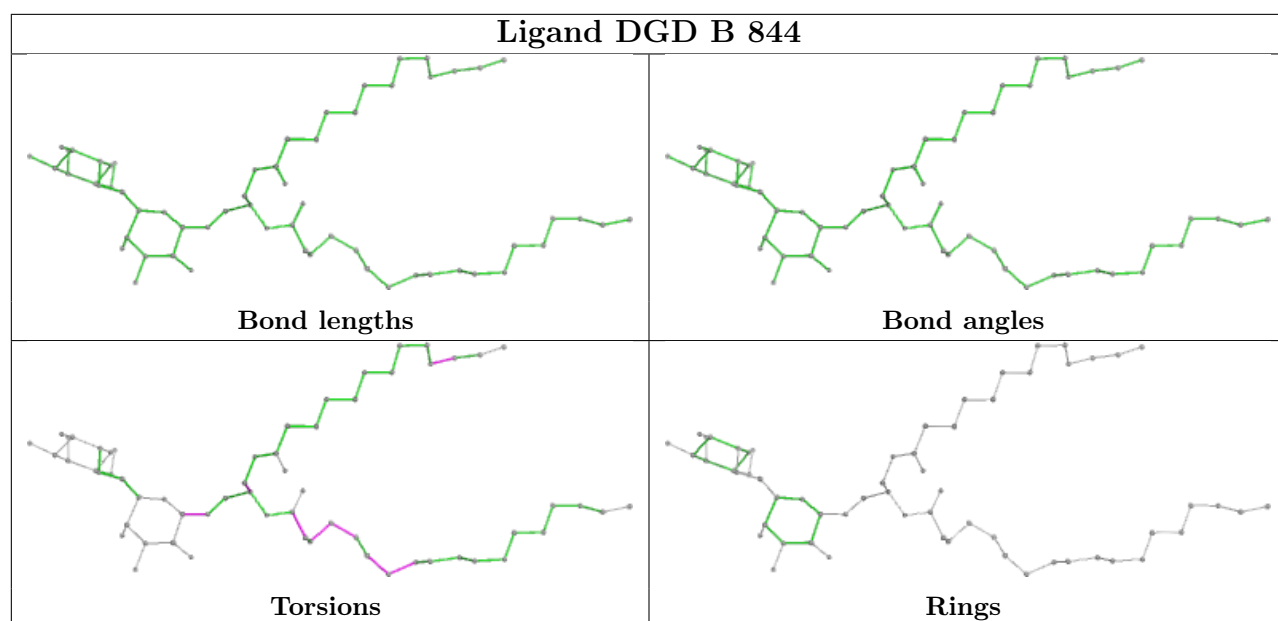


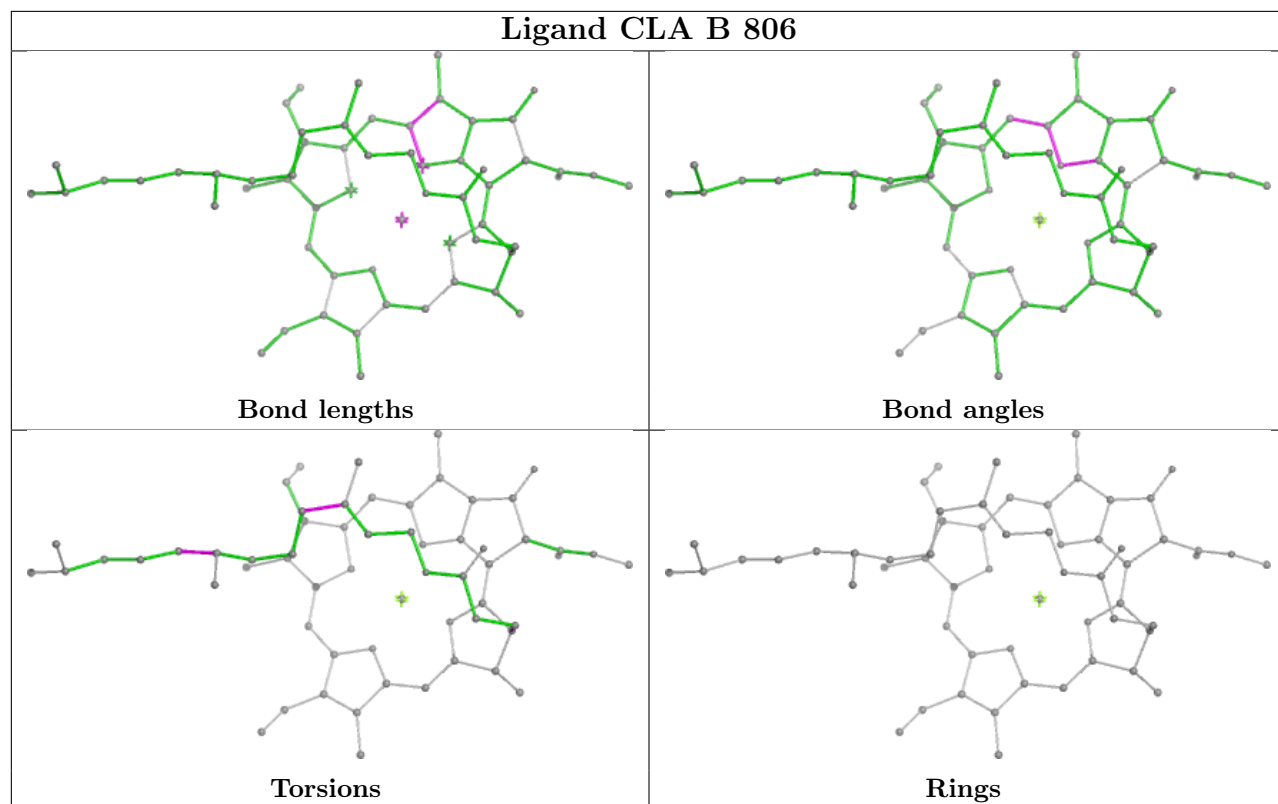
Torsions

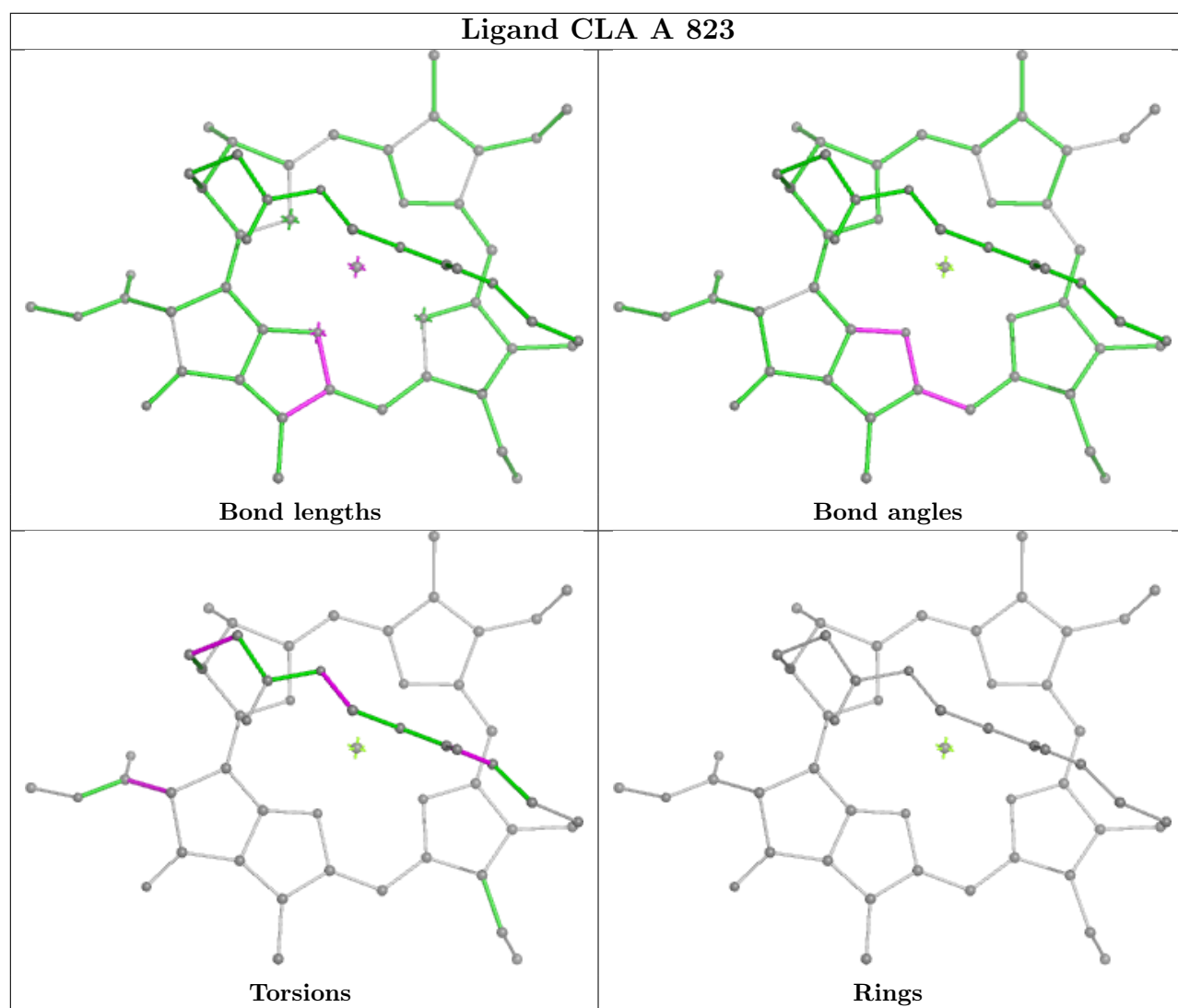


Rings

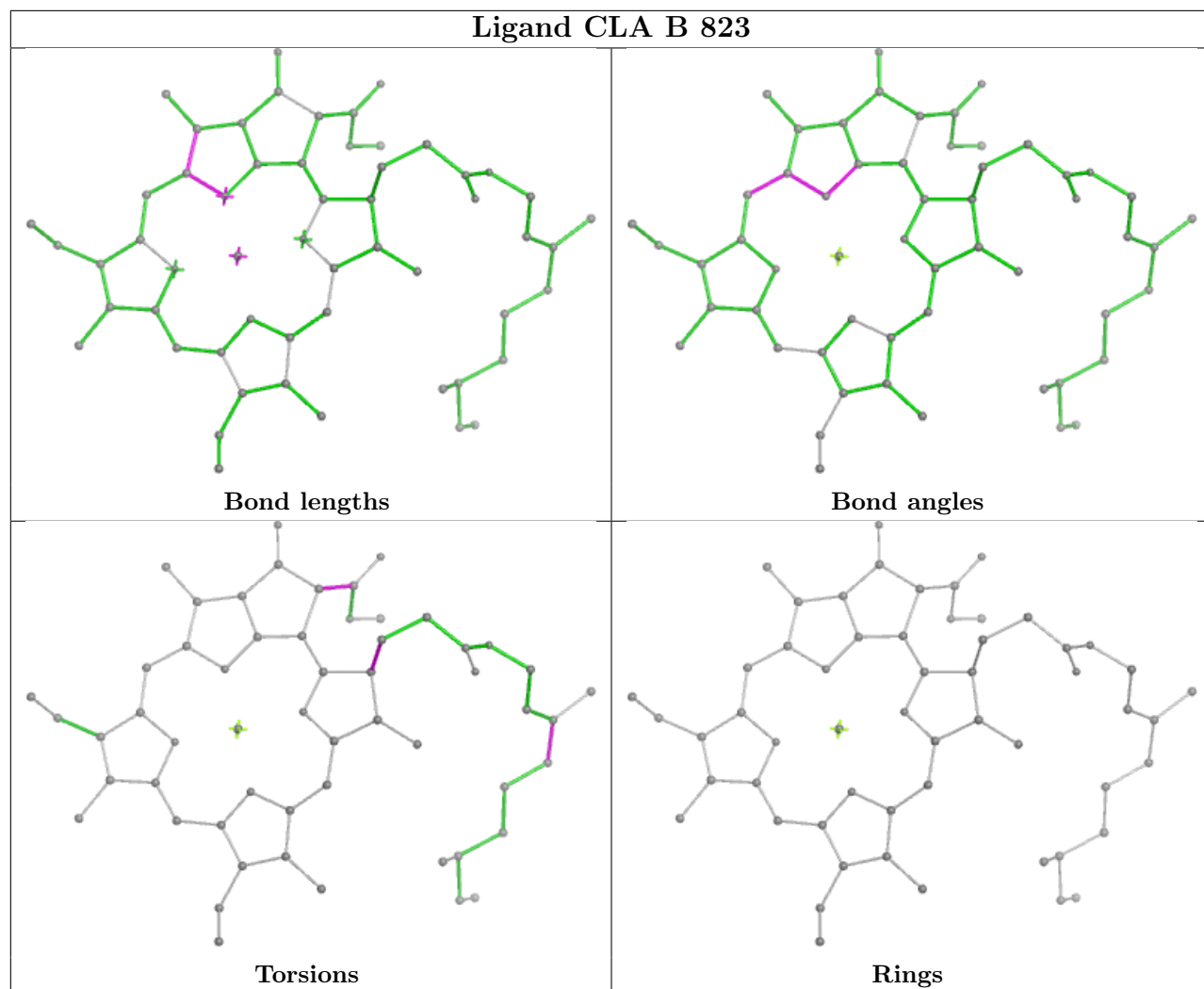




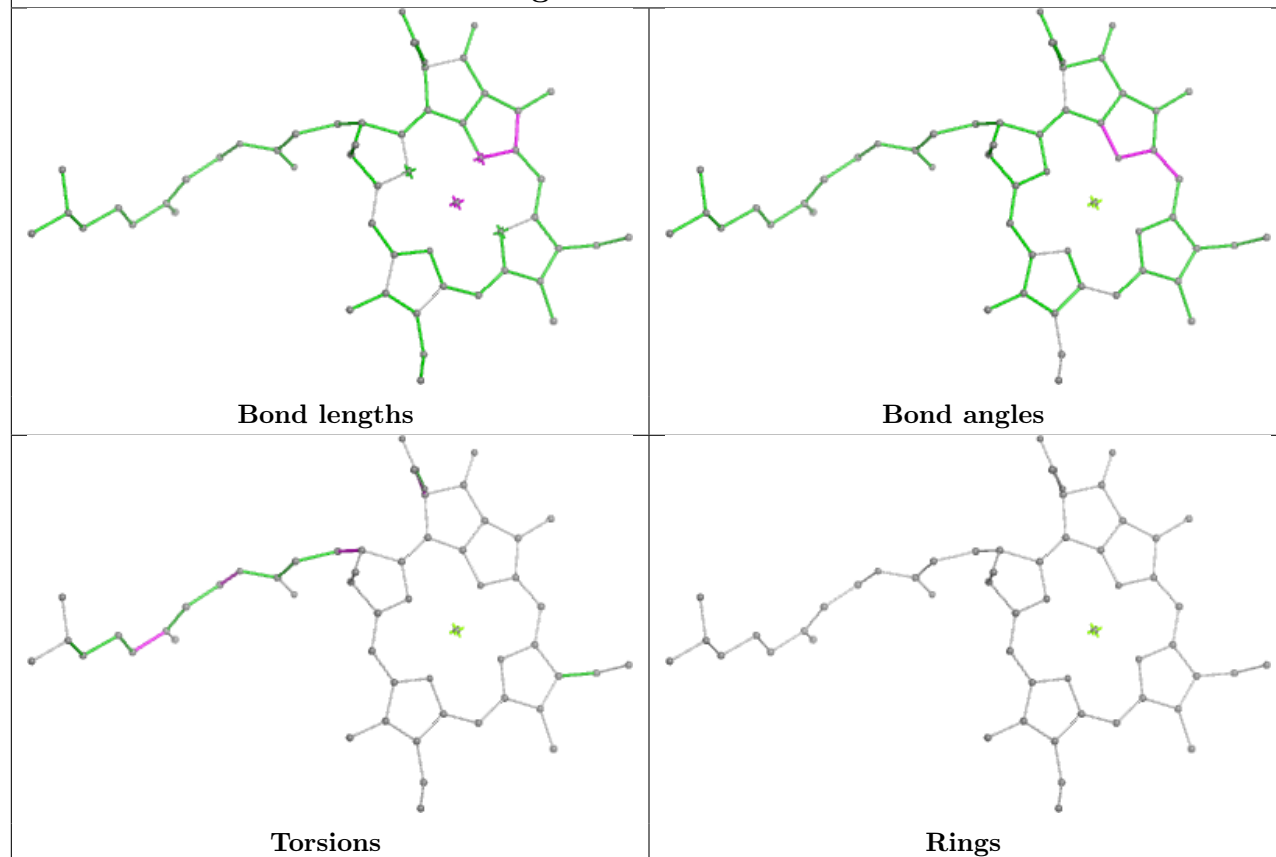




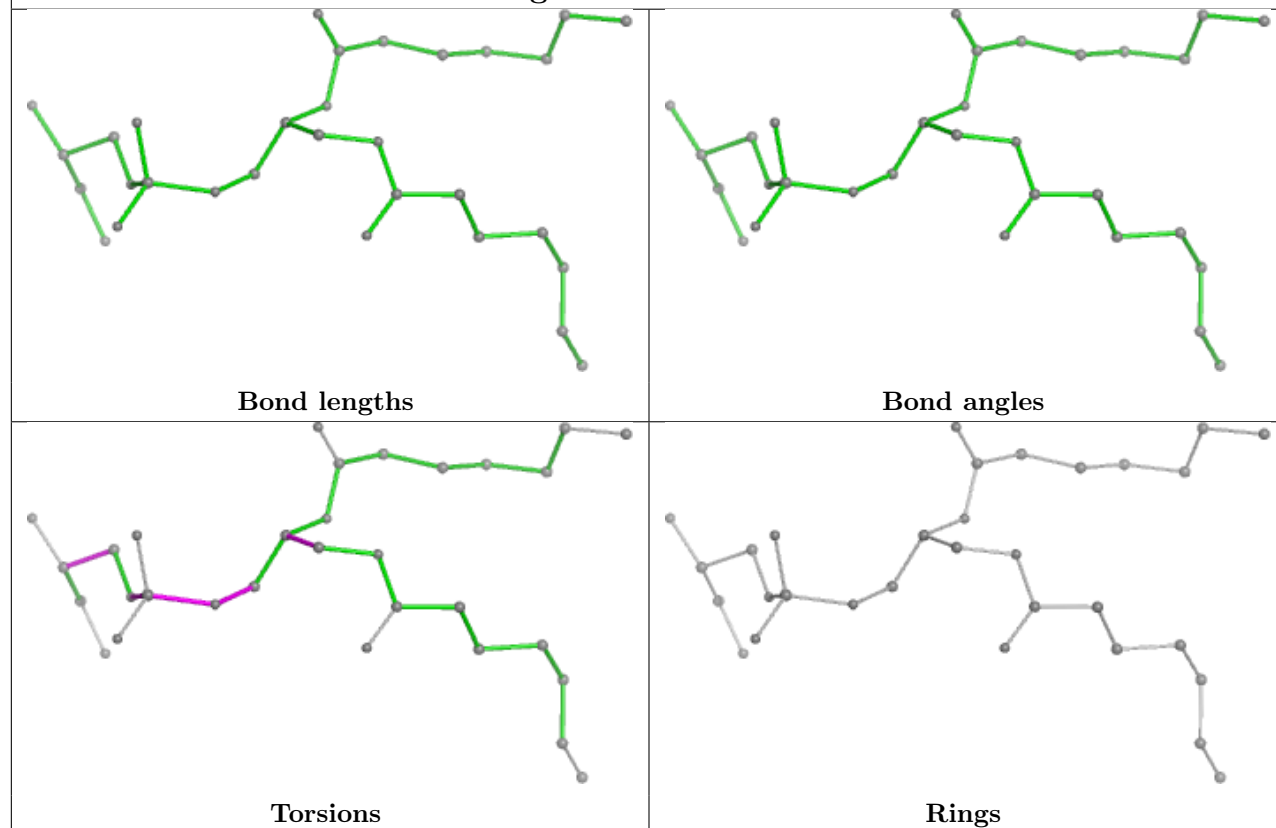
Ligand CLA B 823

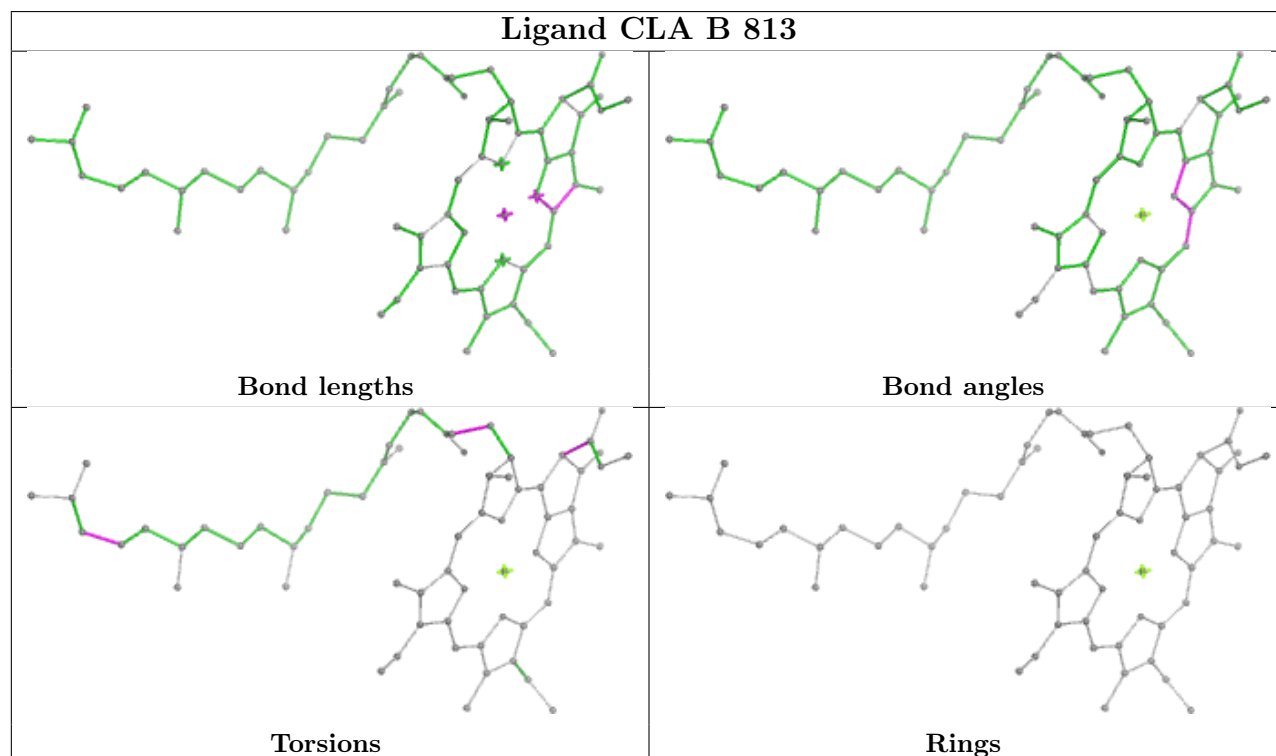
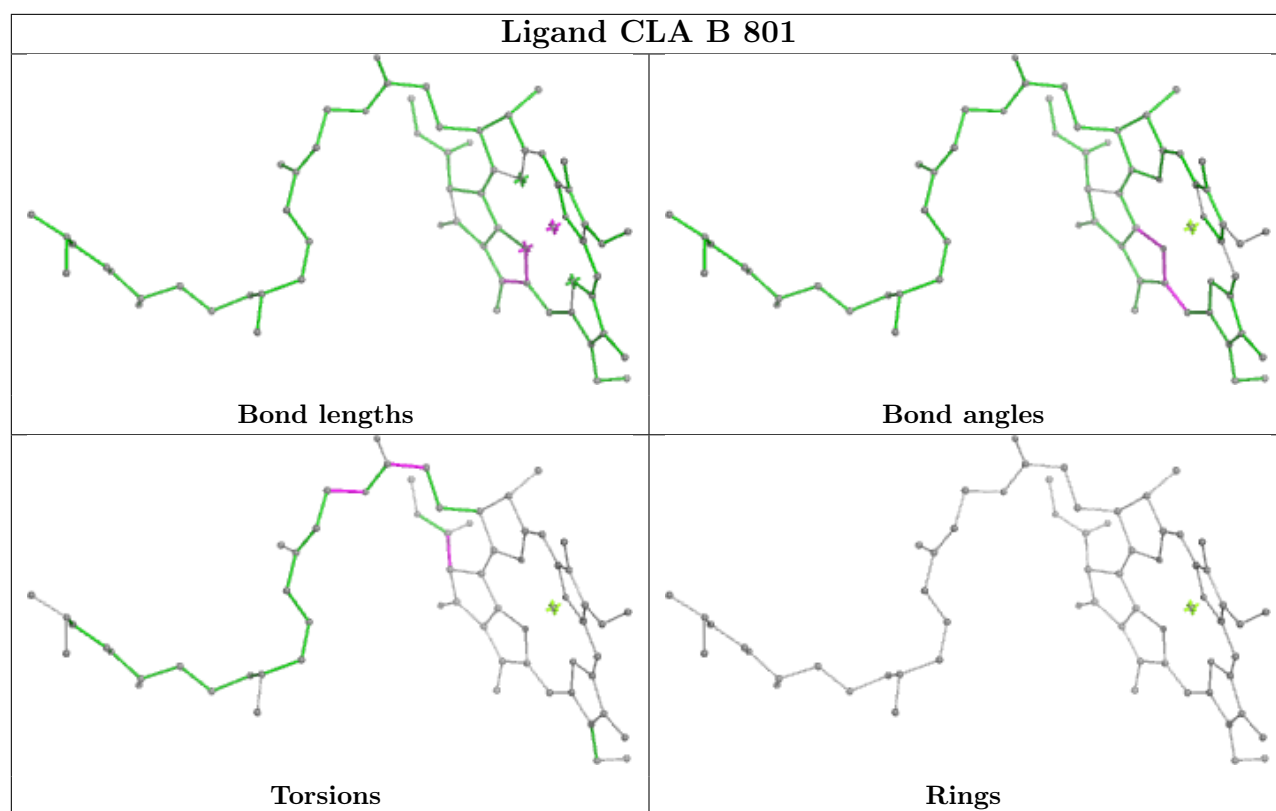


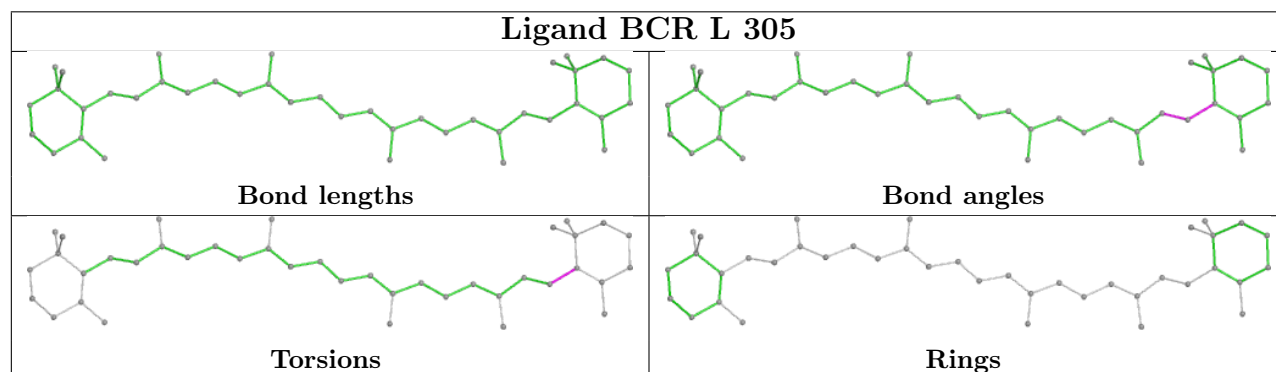
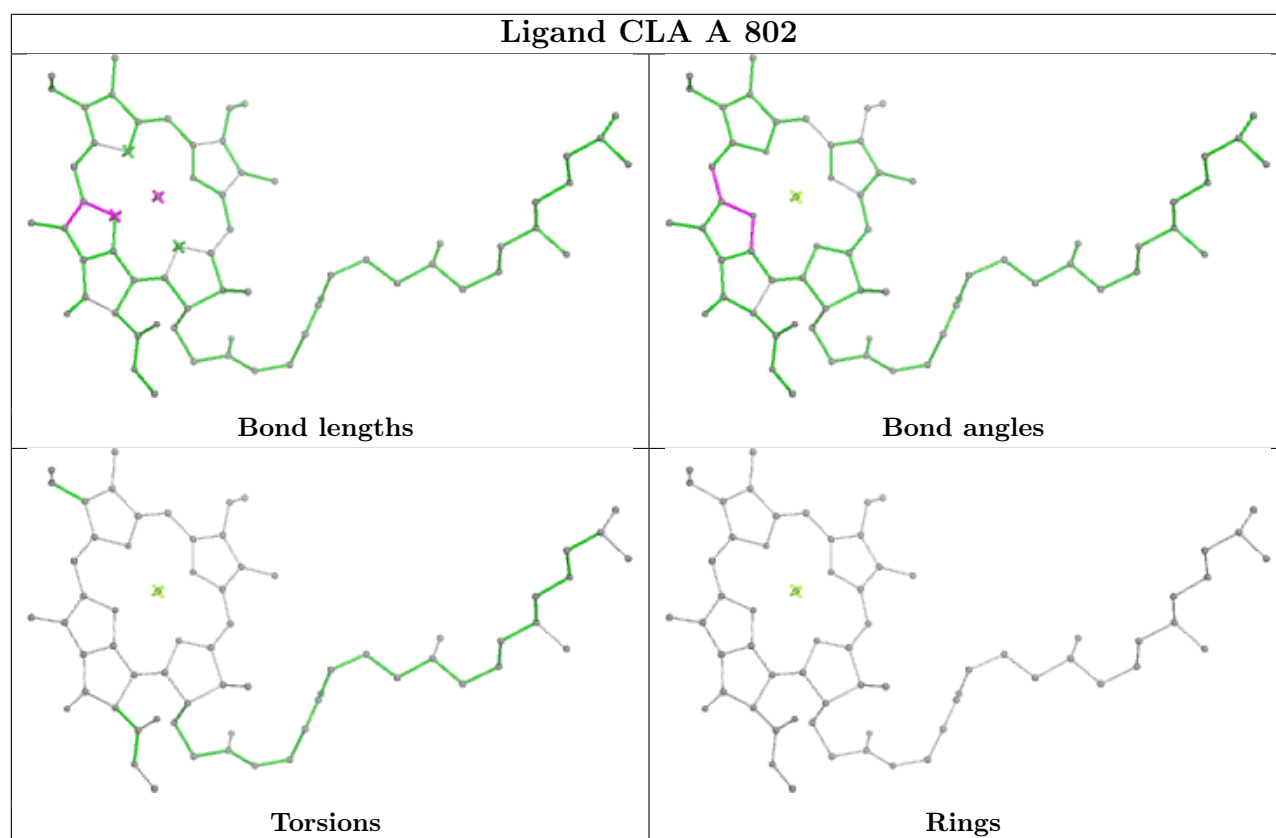
Ligand CLA A 809

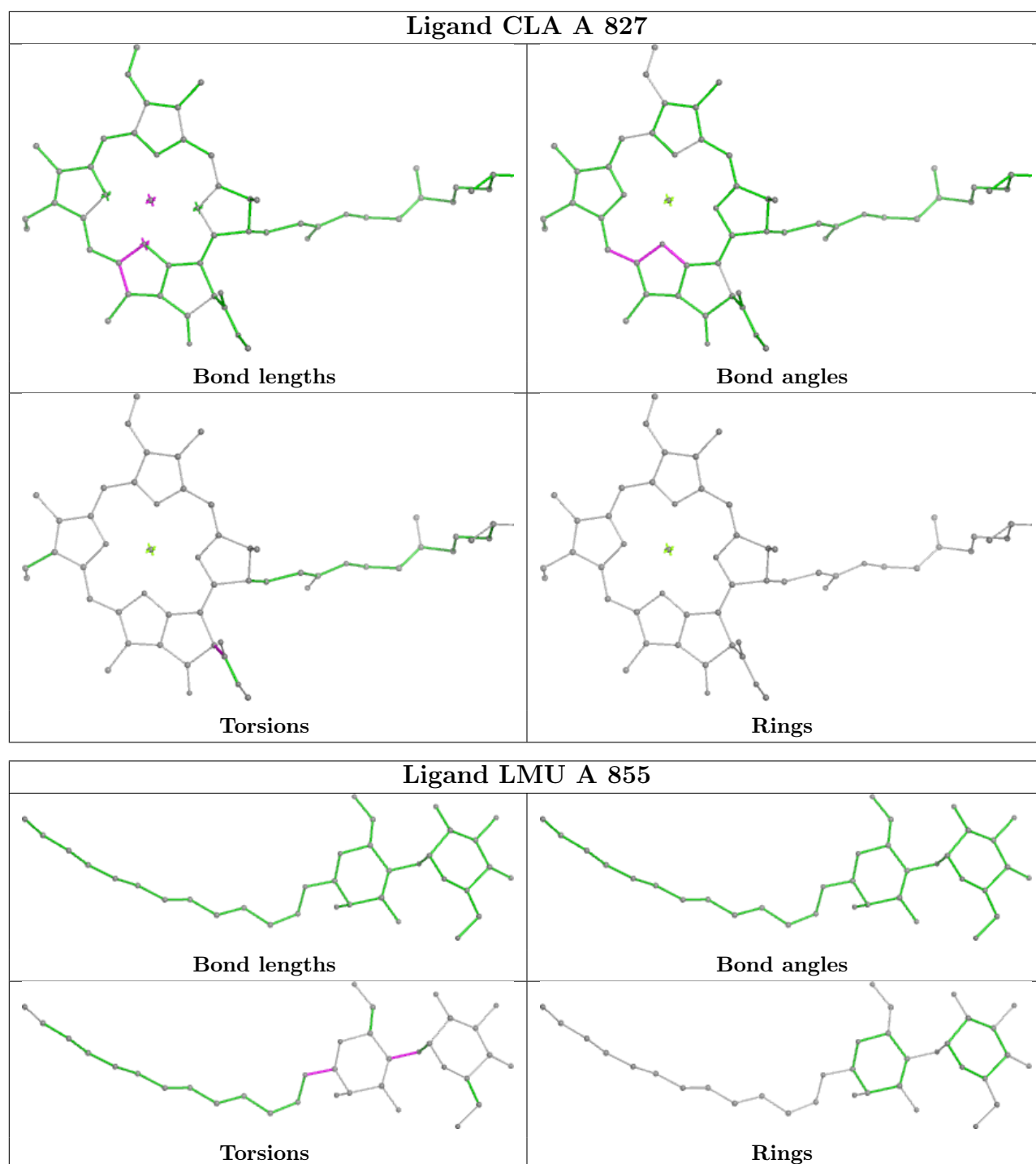


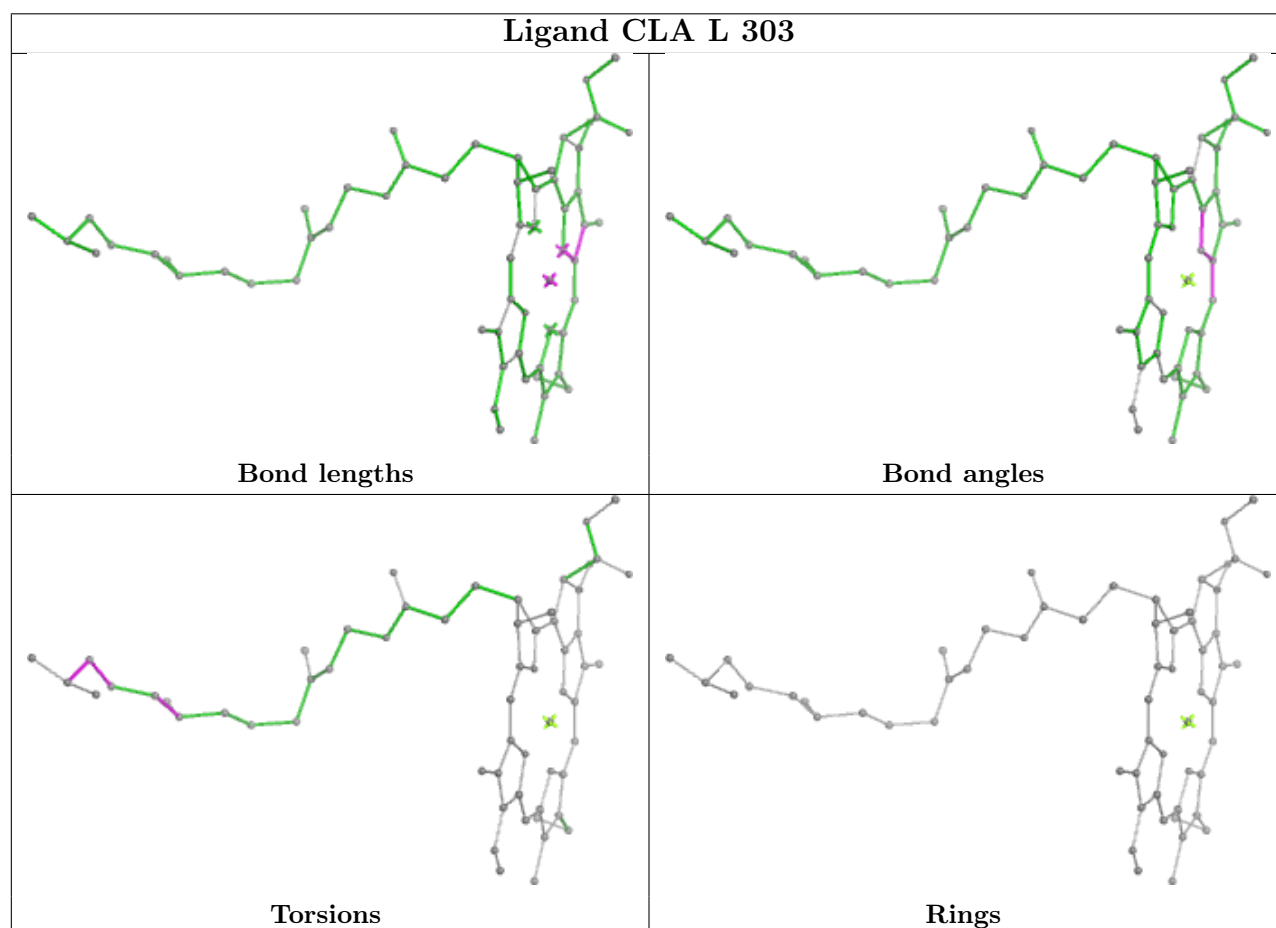
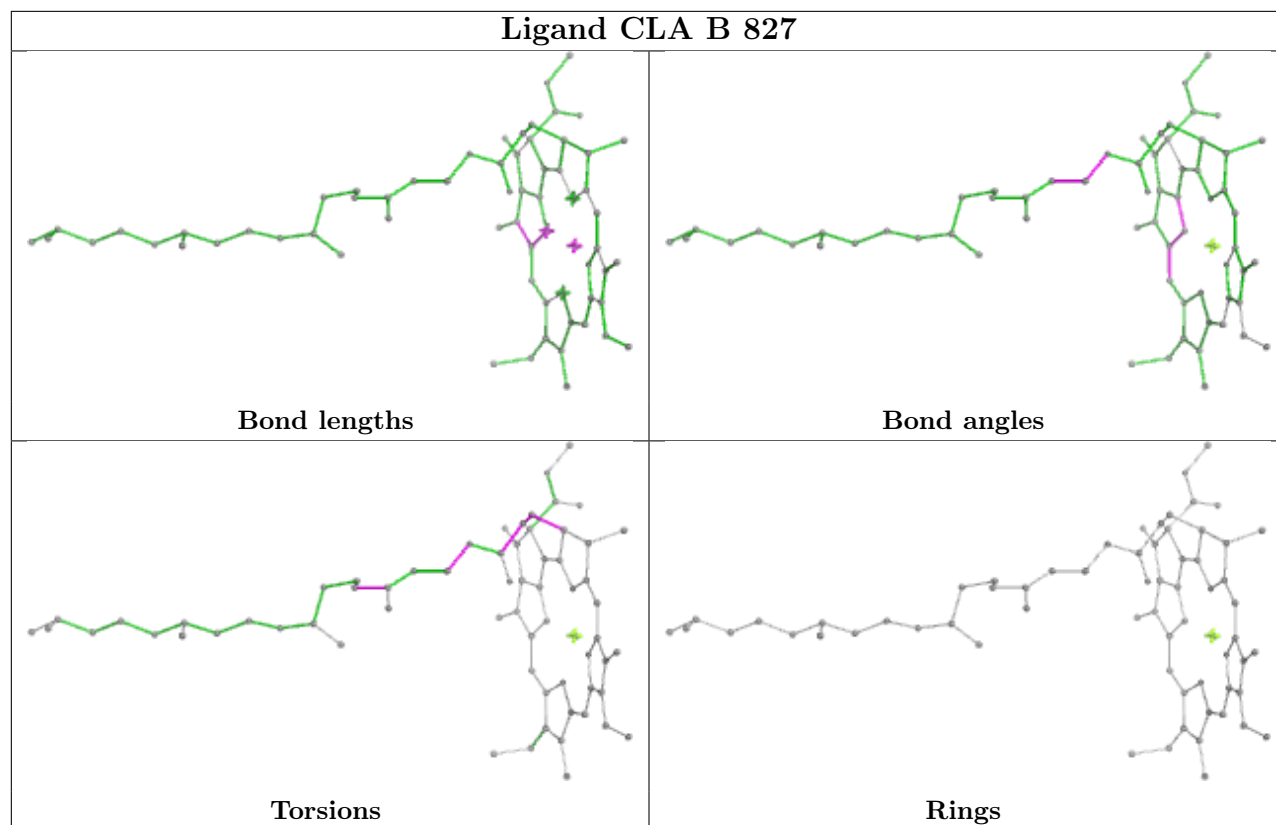
Ligand LHG A 847

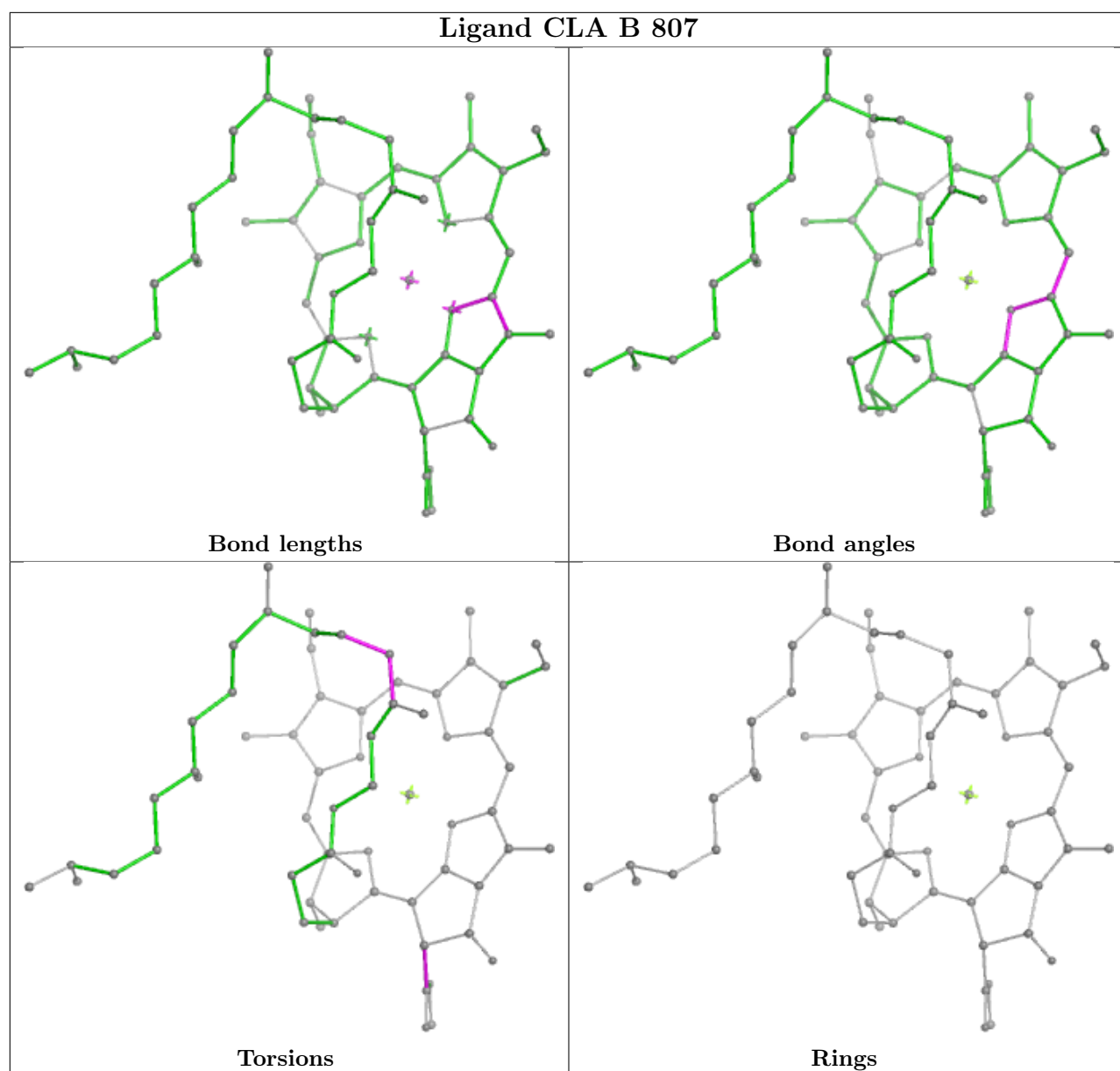




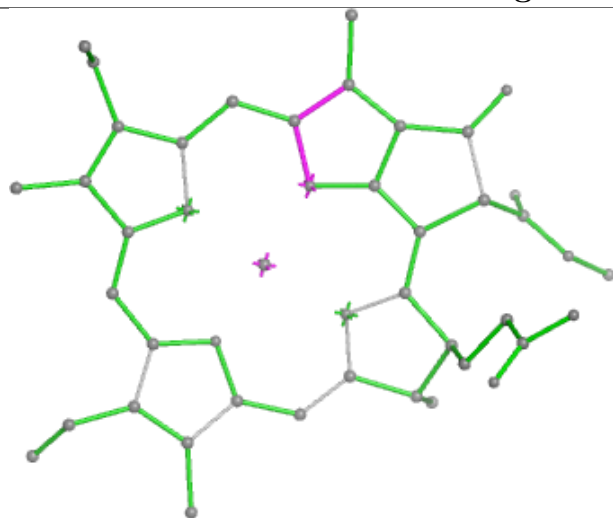




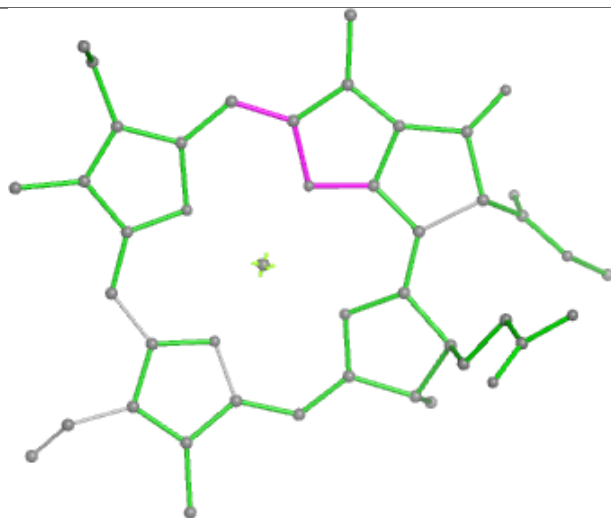




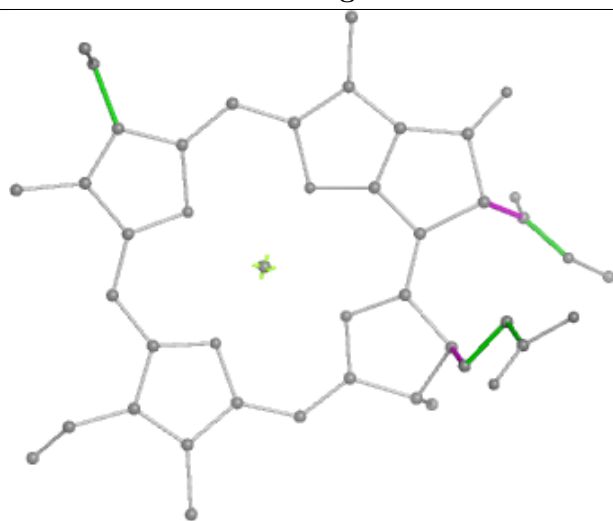
Ligand CLA B 822



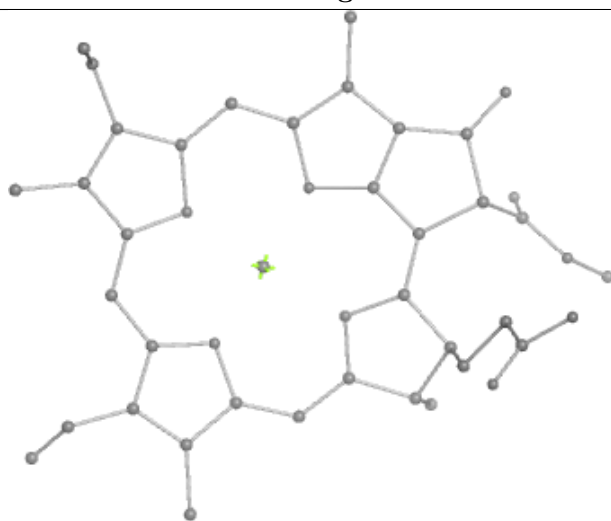
Bond lengths



Bond angles

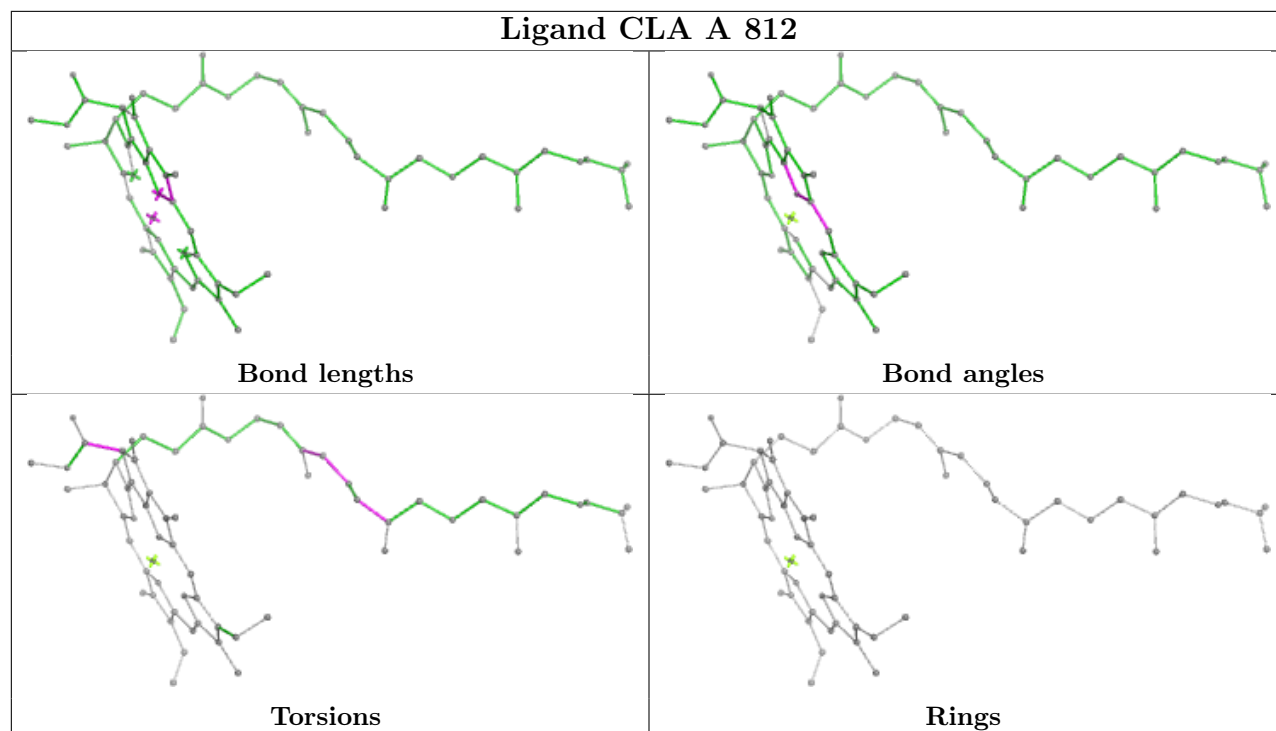


Torsions

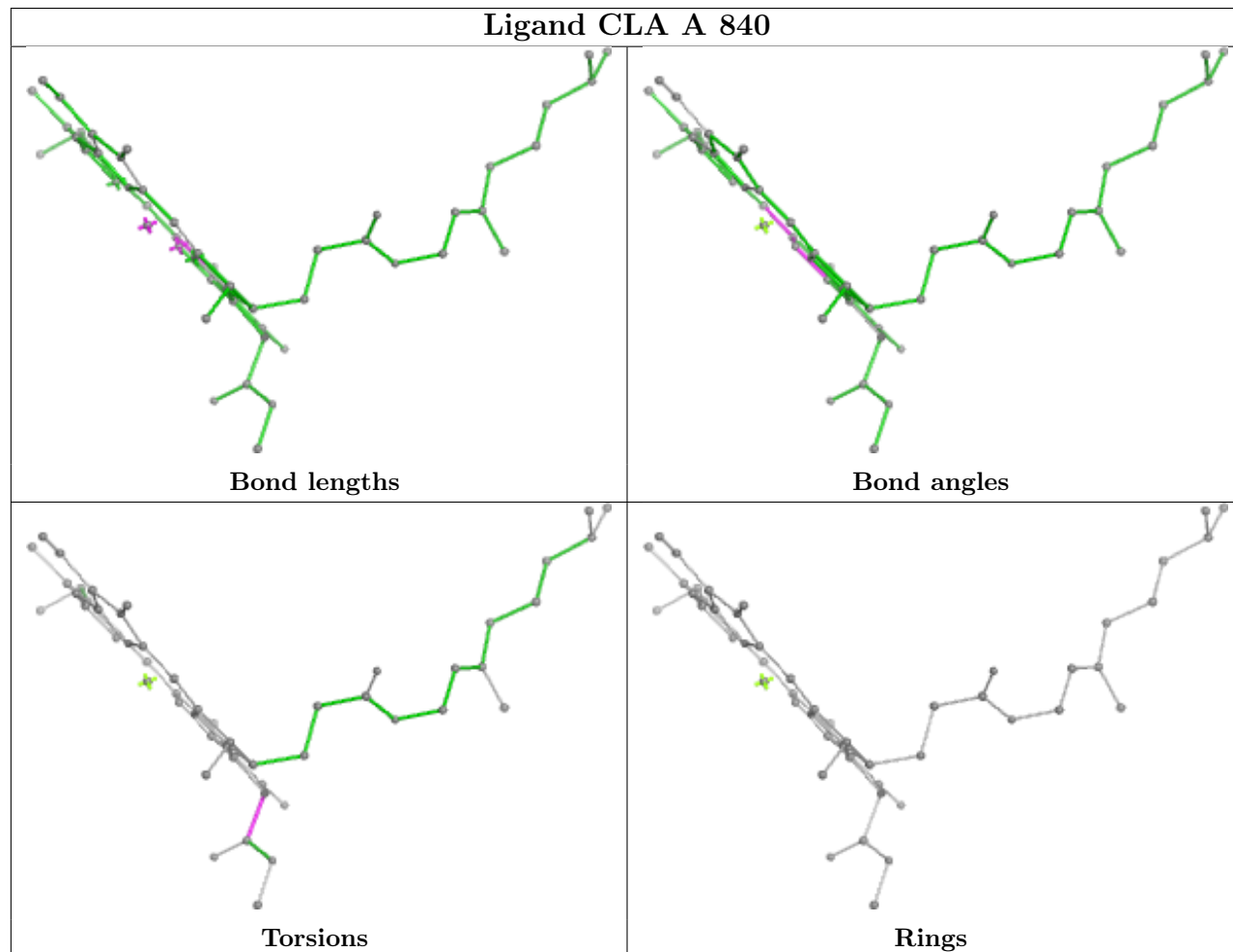


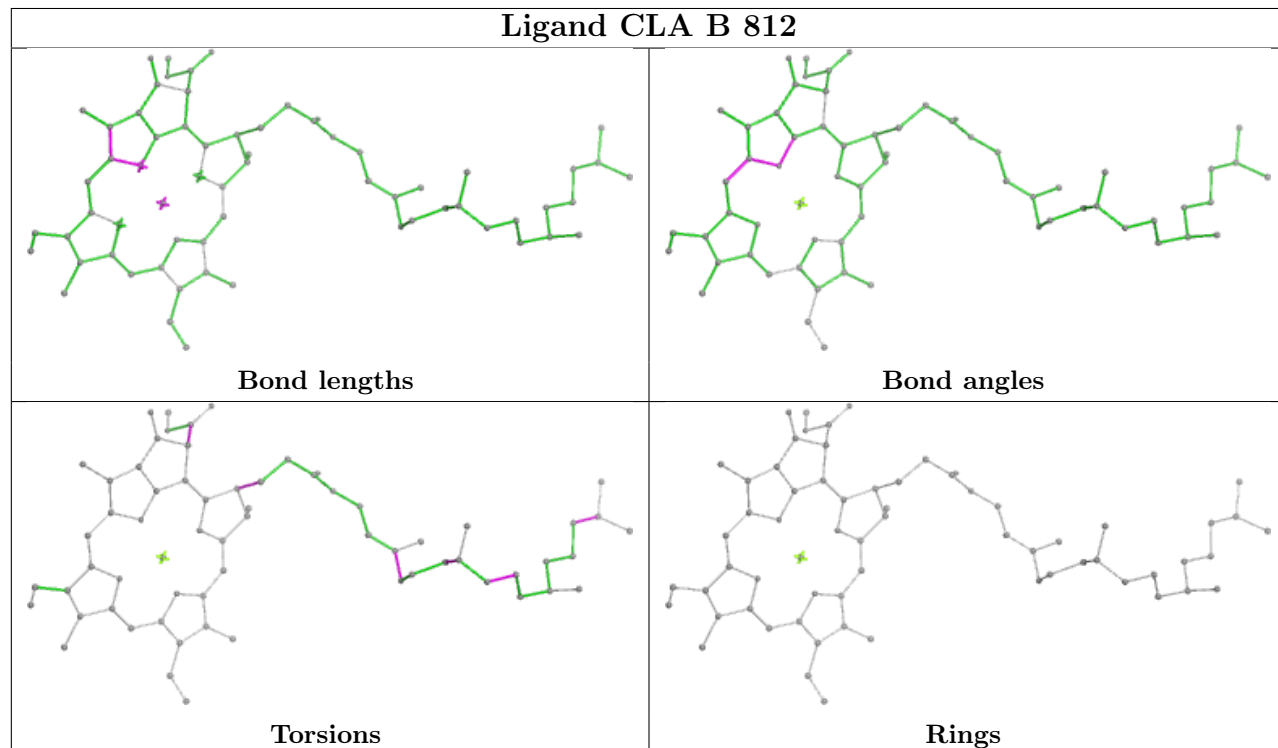
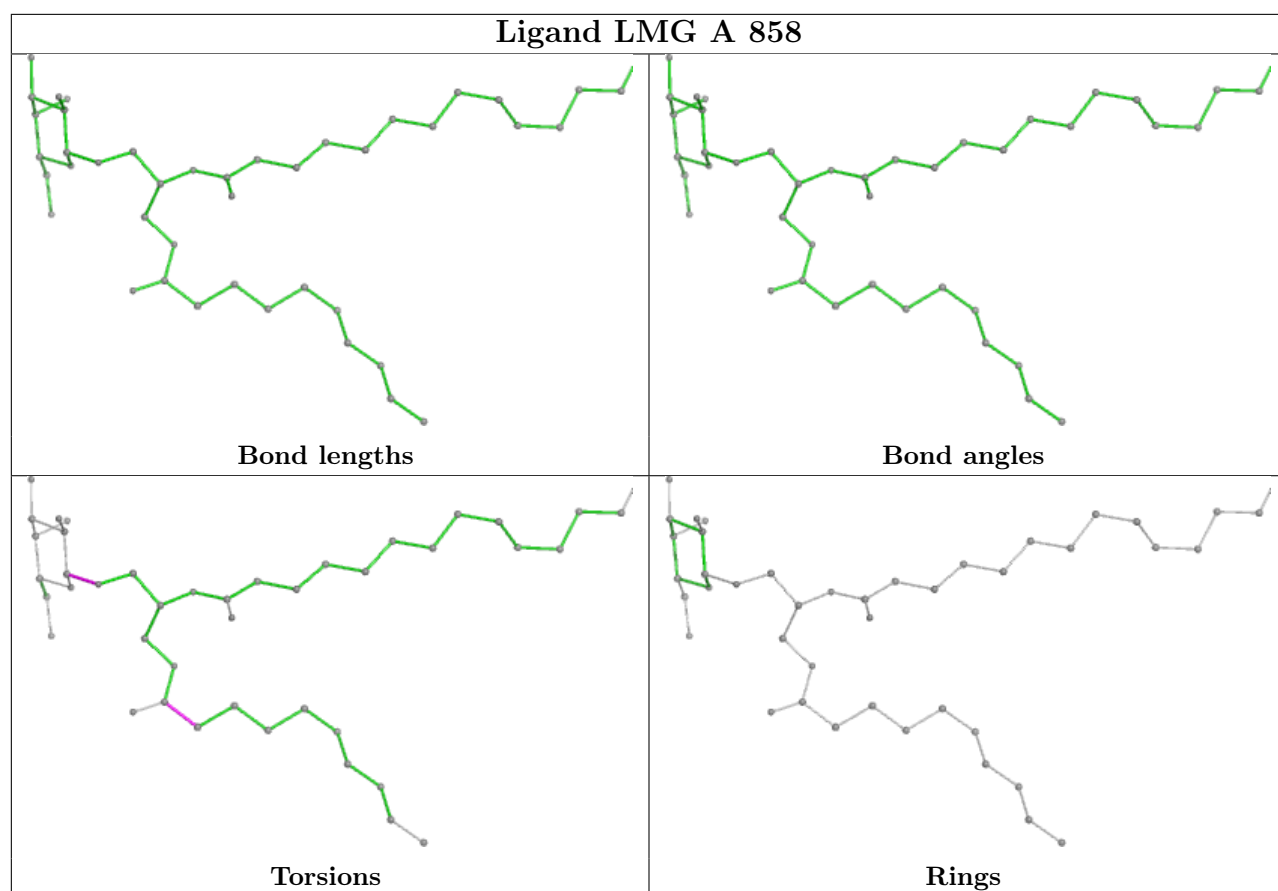
Rings

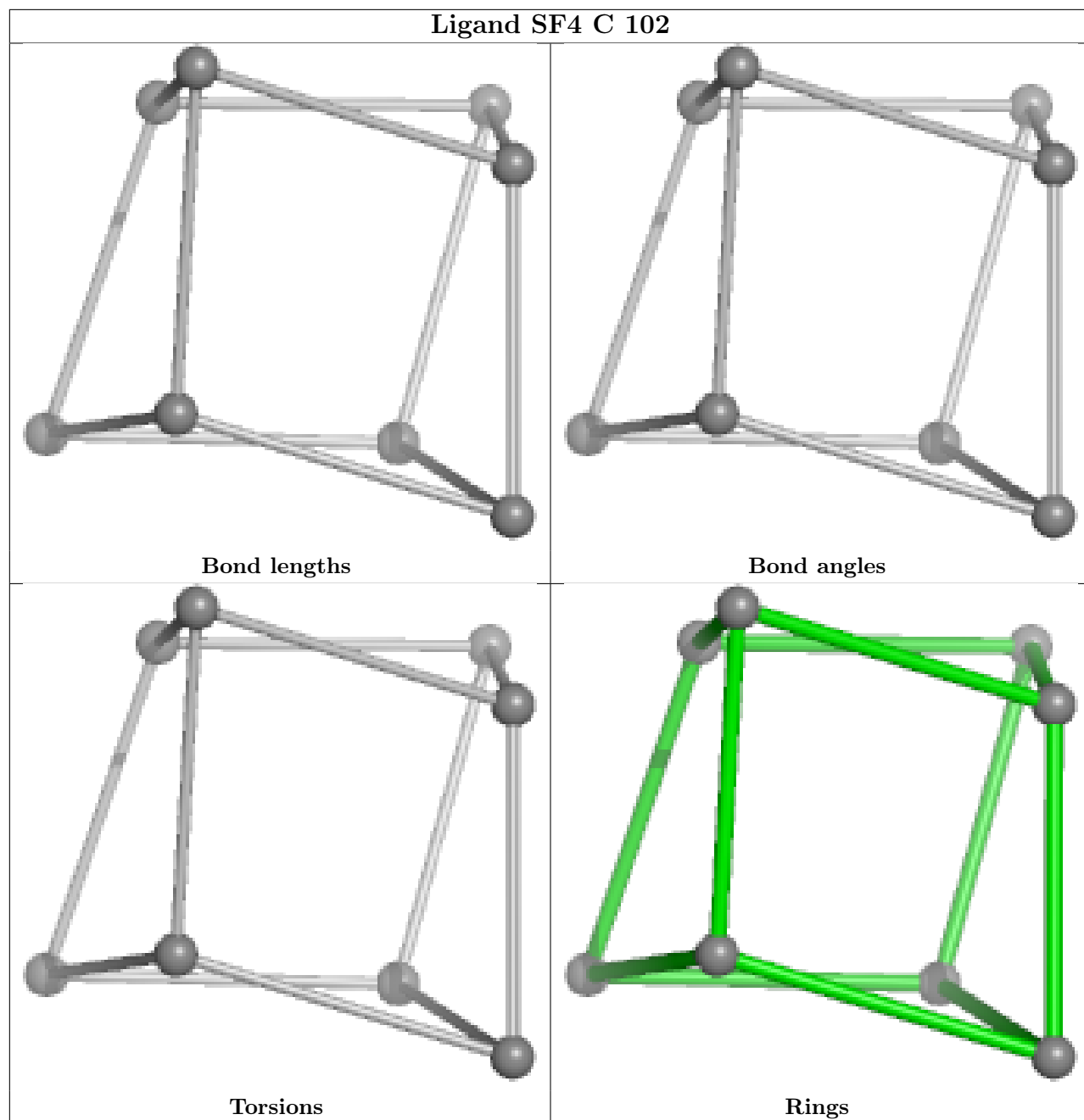
Ligand CLA A 812



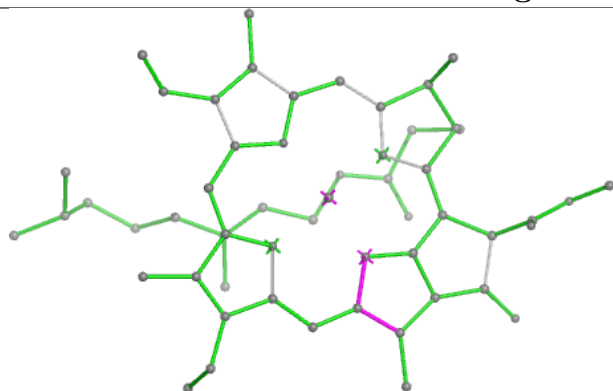
Ligand CLA A 840



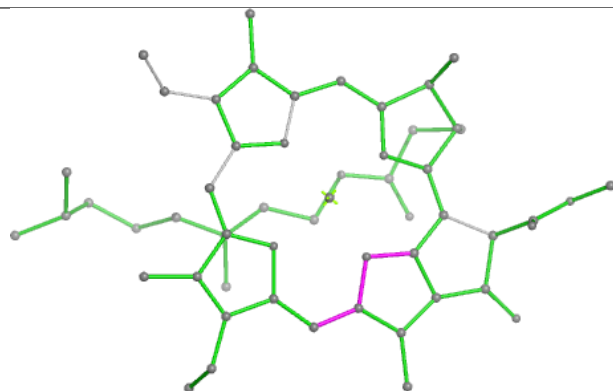




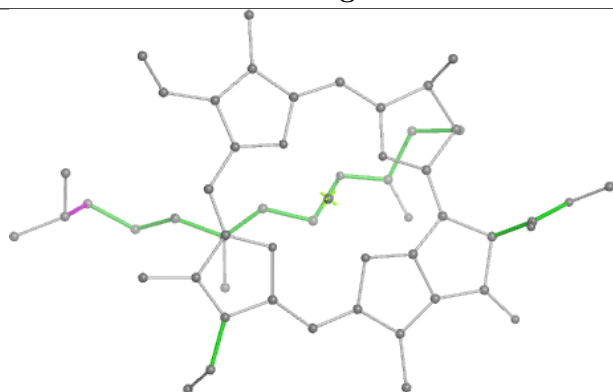
Ligand CLA B 835



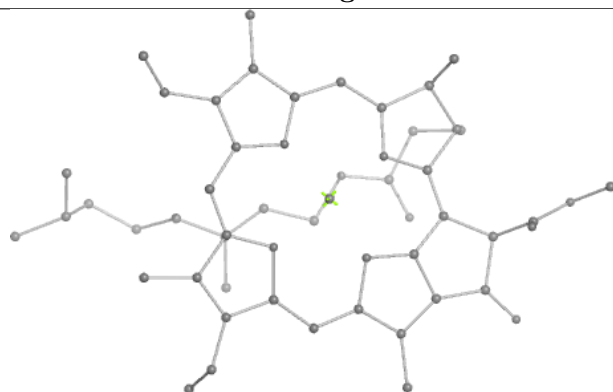
Bond lengths



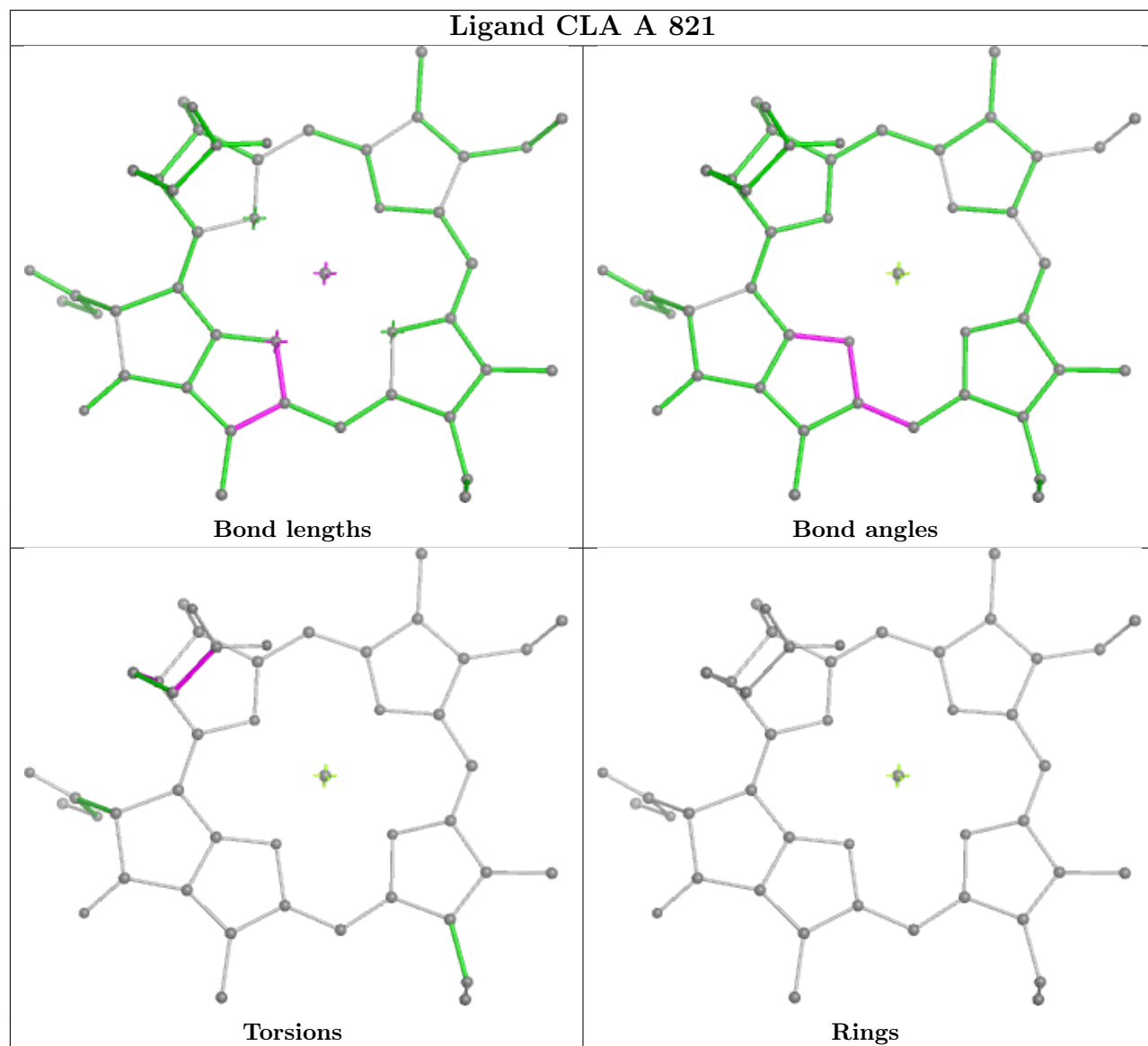
Bond angles



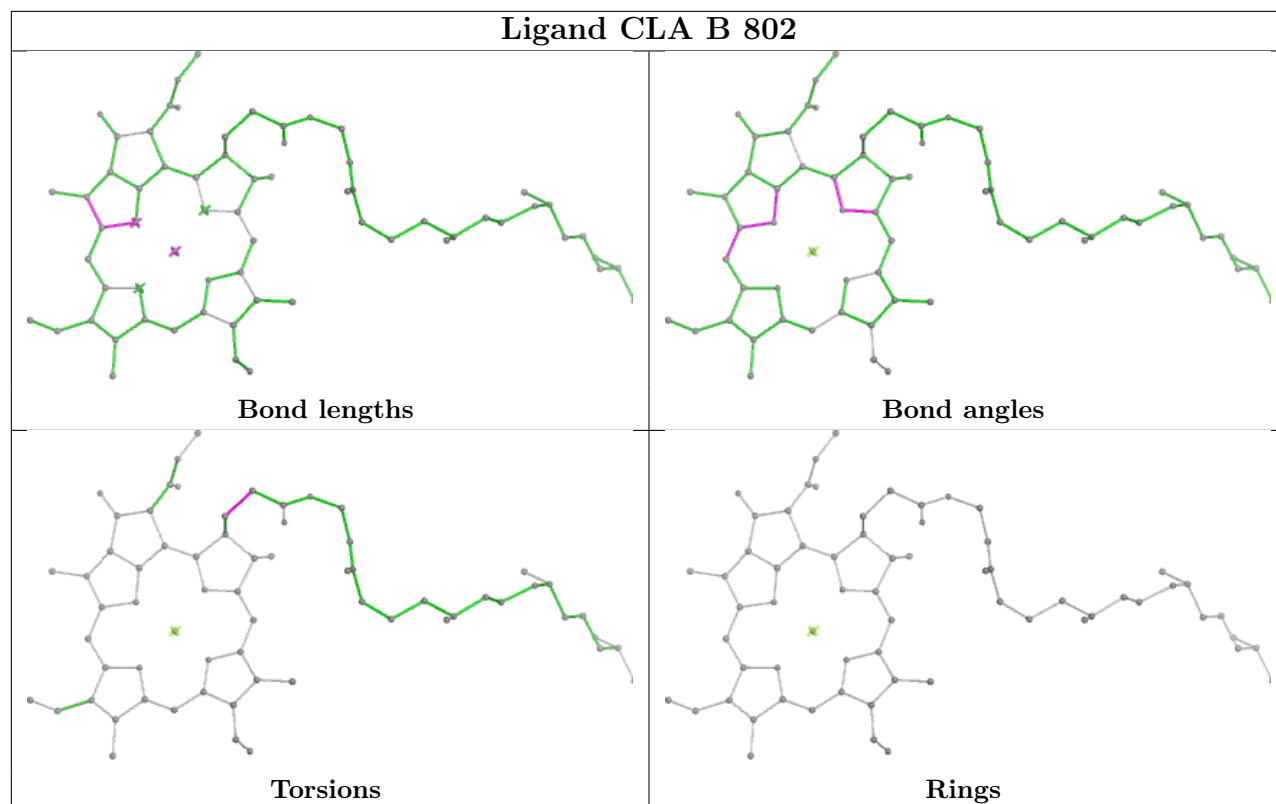
Torsions



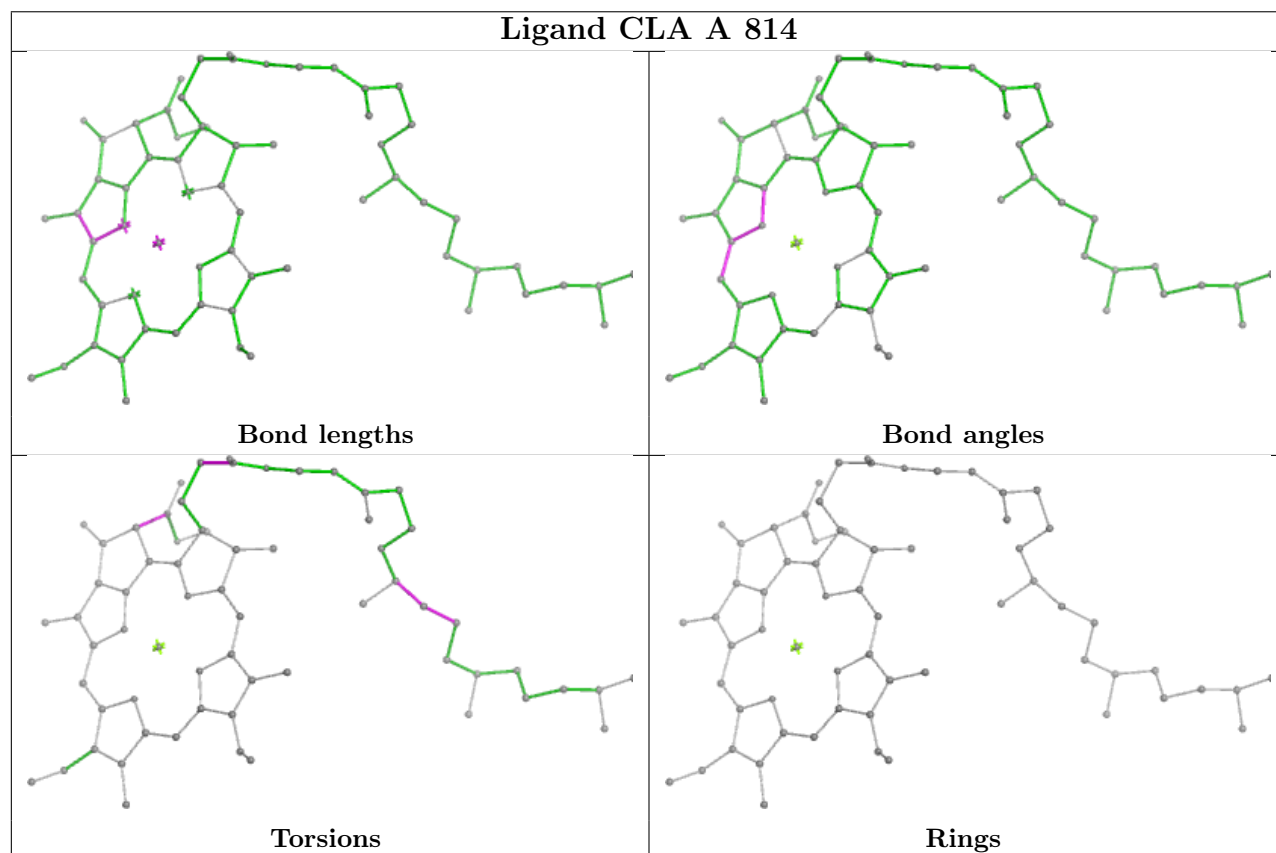
Rings



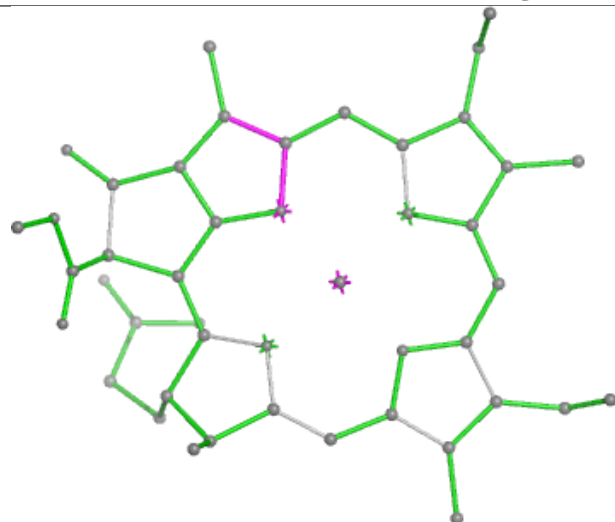
Ligand CLA B 802



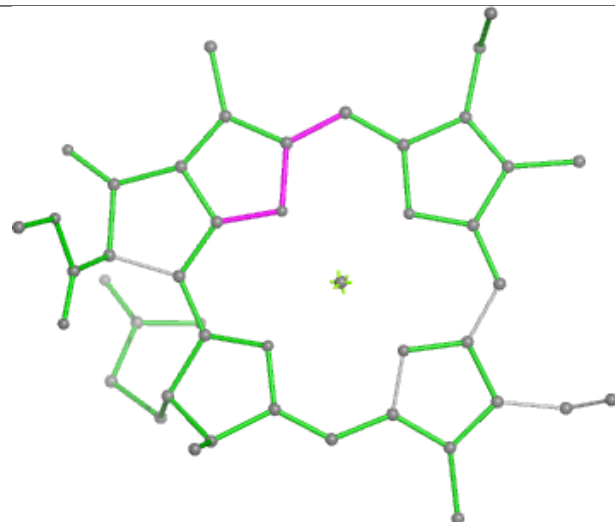
Ligand CLA A 814



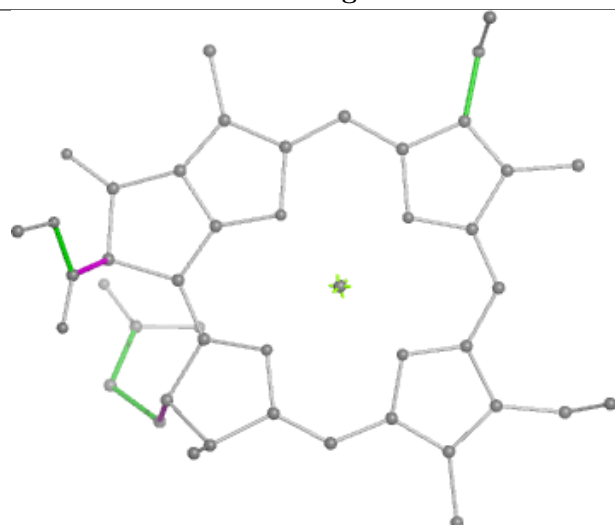
Ligand CLA B 821



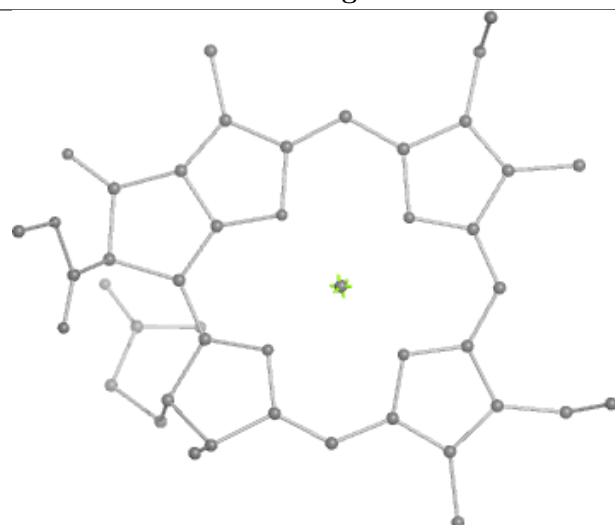
Bond lengths



Bond angles

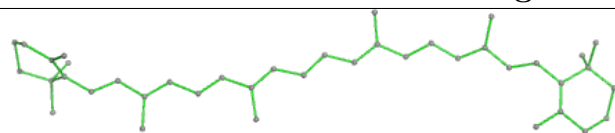


Torsions

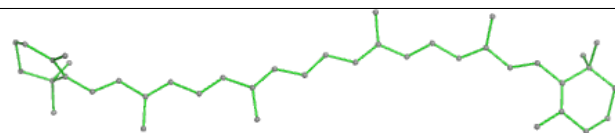


Rings

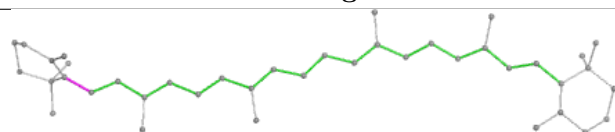
Ligand BCR B 840



Bond lengths



Bond angles

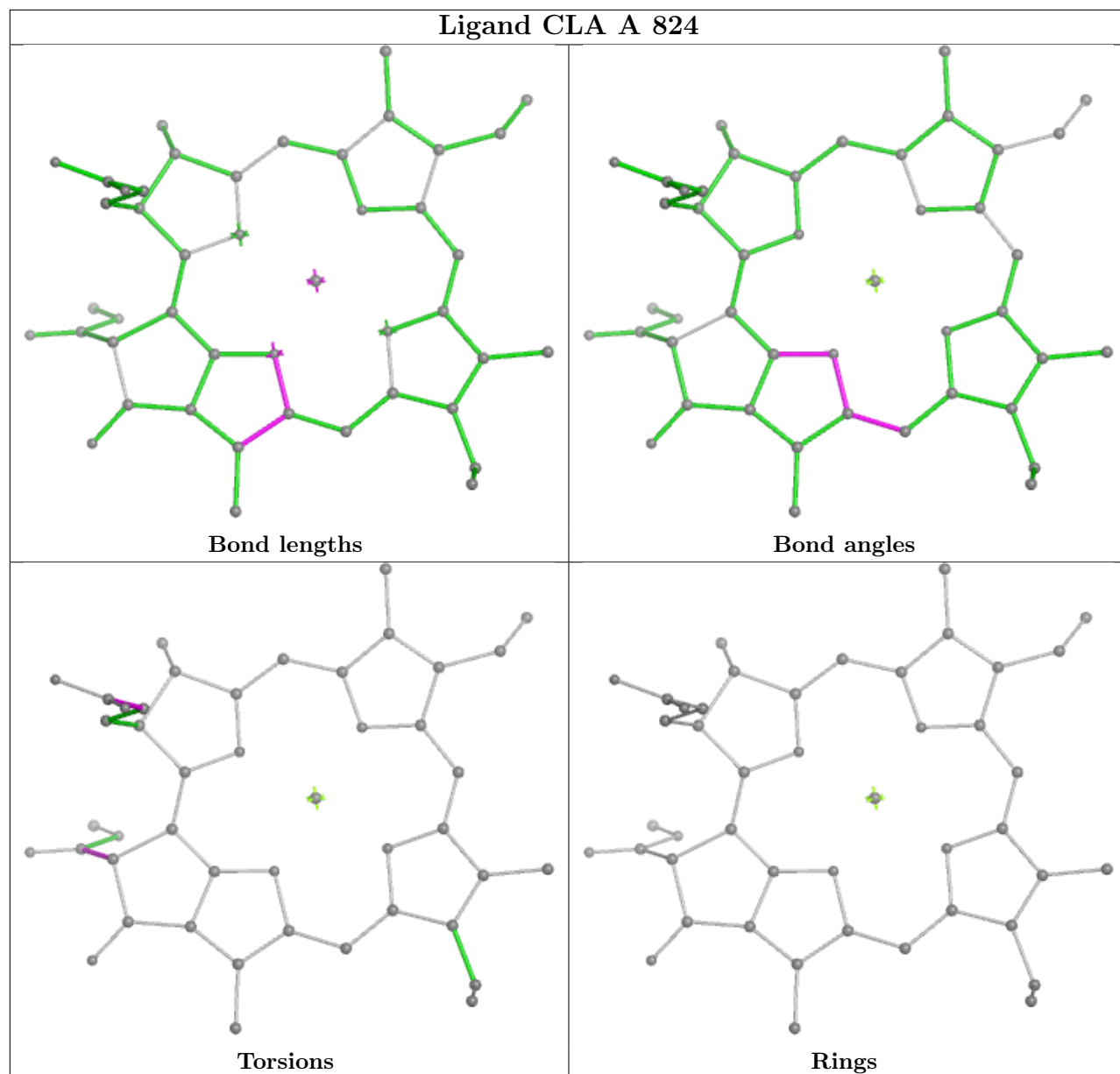


Torsions

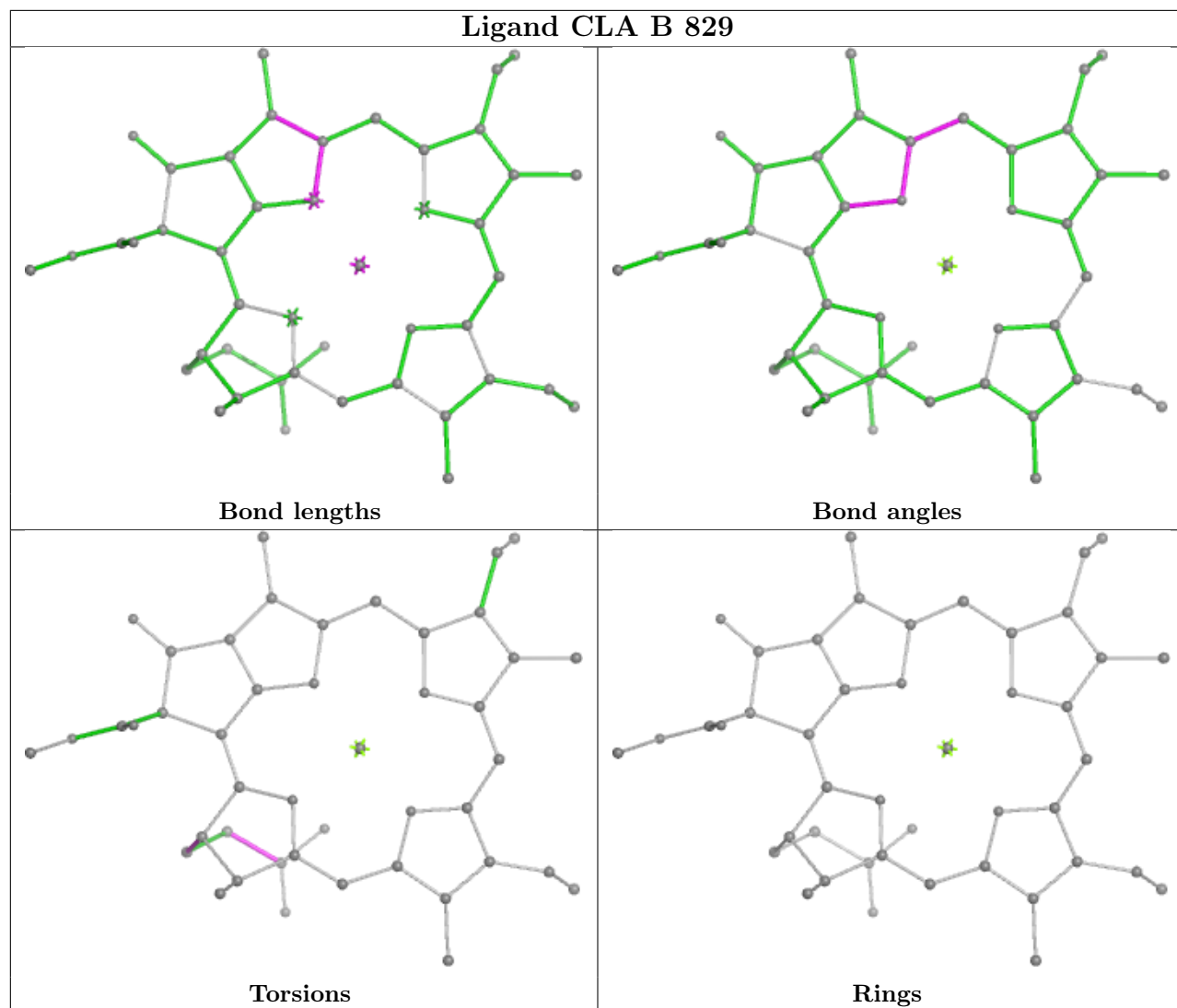


Rings

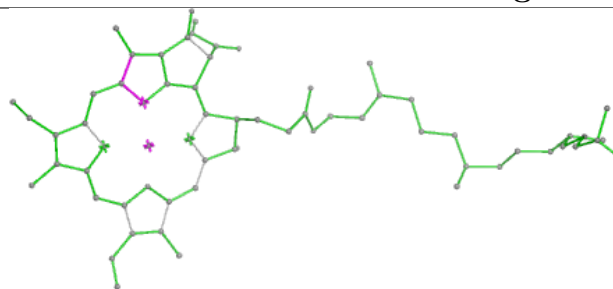
Ligand CLA A 824



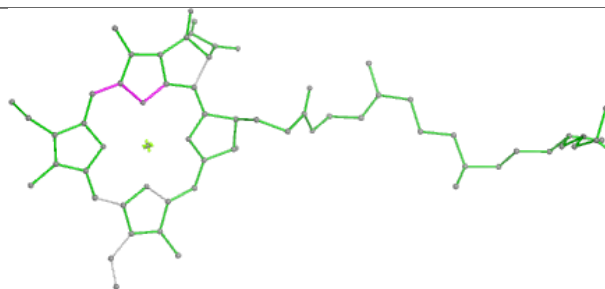
Ligand CLA B 829



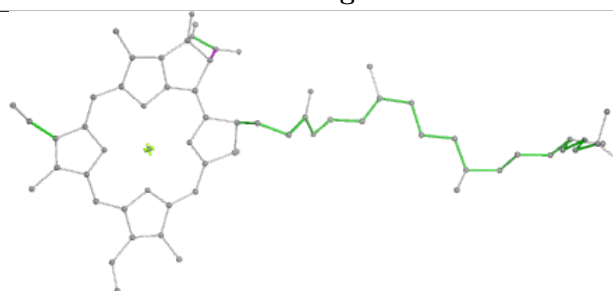
Ligand CLA A 806



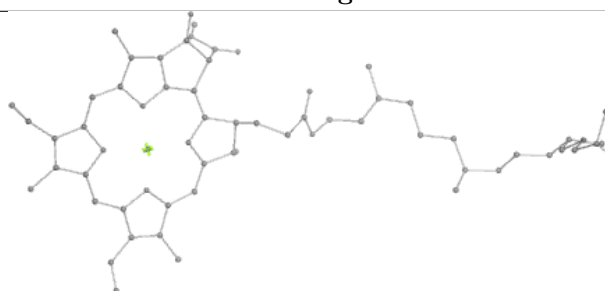
Bond lengths



Bond angles

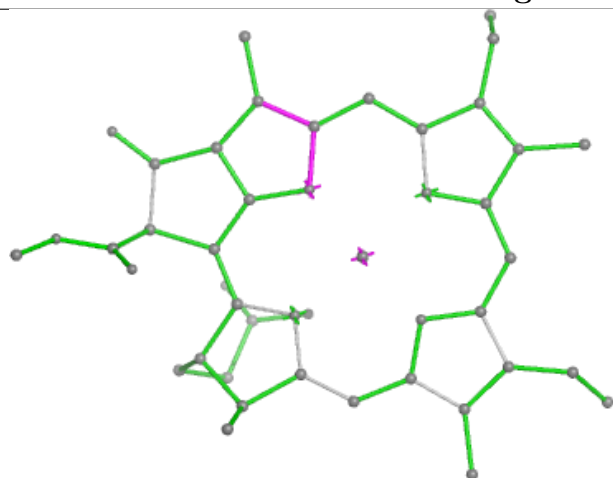


Torsions

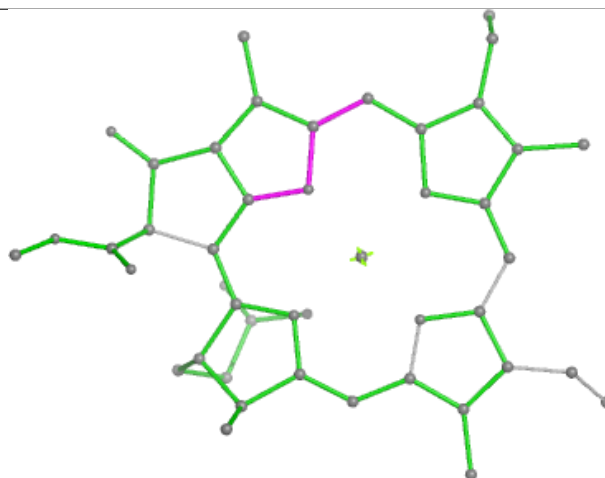


Rings

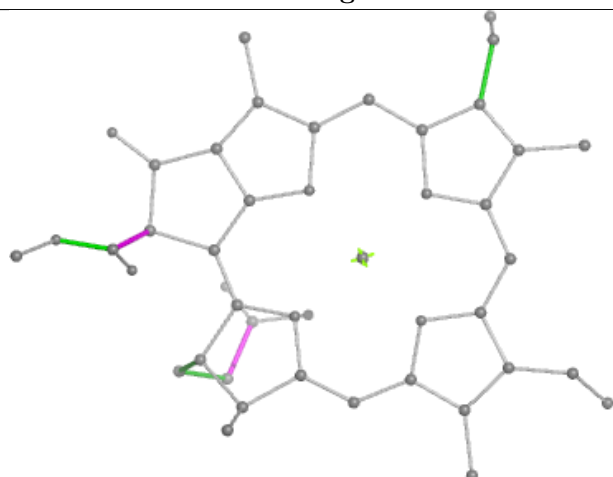
Ligand CLA B 811



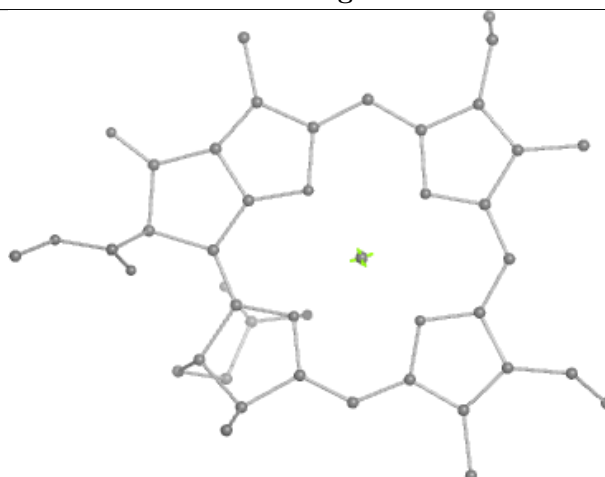
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

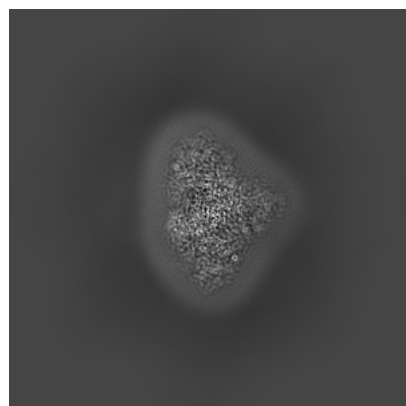
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15970. These allow visual inspection of the internal detail of the map and identification of artifacts.

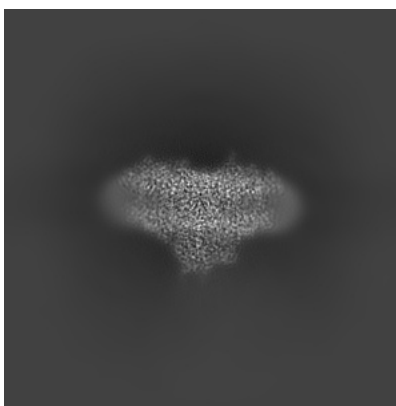
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

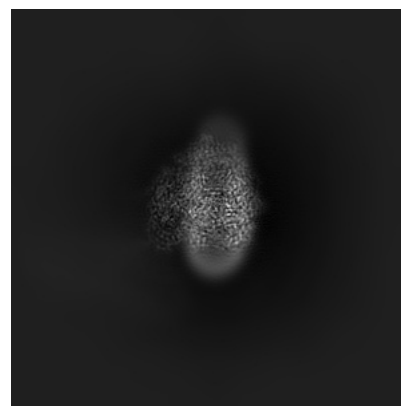
6.1.1 Primary map



X

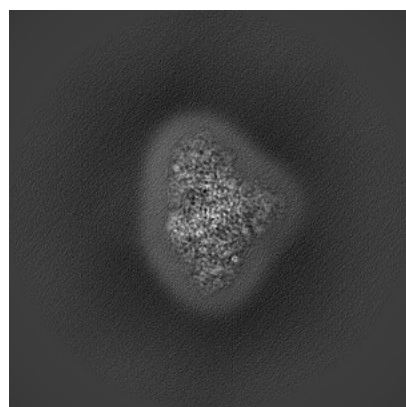


Y

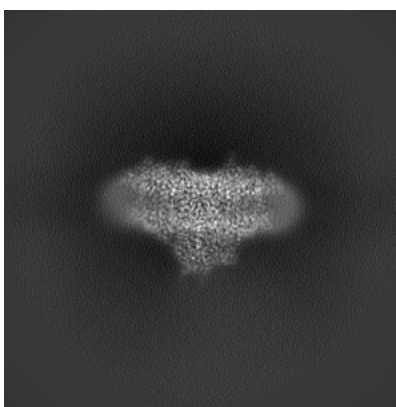


Z

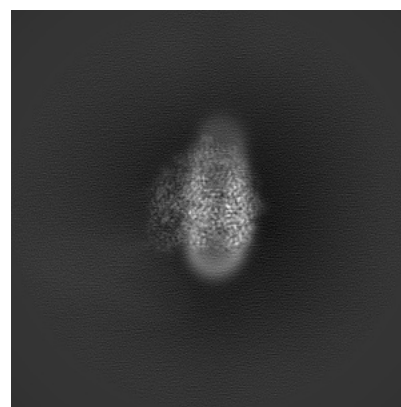
6.1.2 Raw map



X



Y

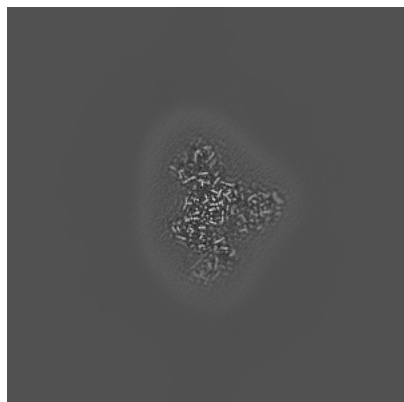


Z

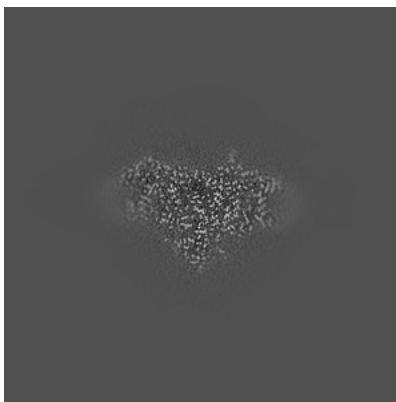
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

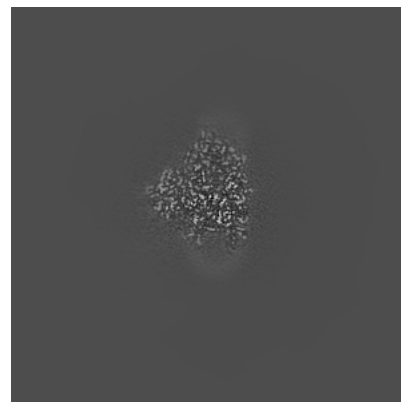
6.2.1 Primary map



X Index: 200

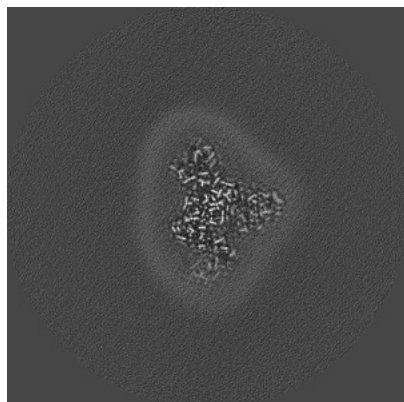


Y Index: 200

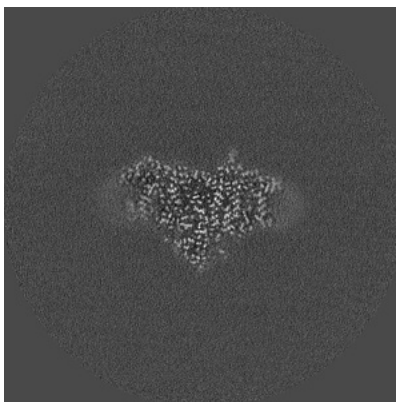


Z Index: 200

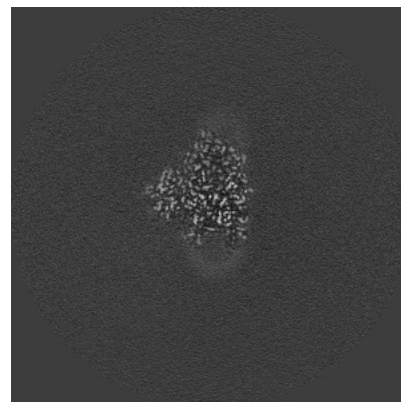
6.2.2 Raw map



X Index: 200



Y Index: 200

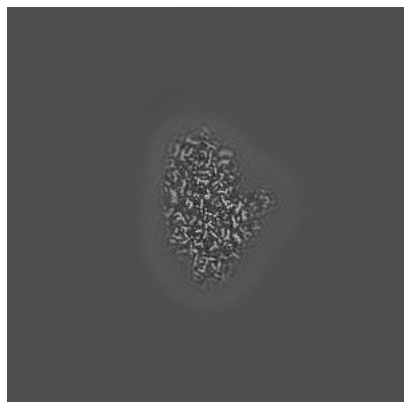


Z Index: 200

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

6.3 Largest variance slices [i](#)

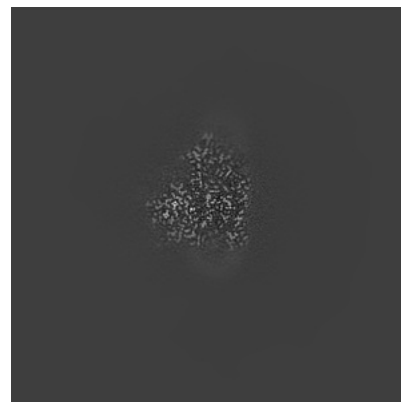
6.3.1 Primary map



X Index: 219

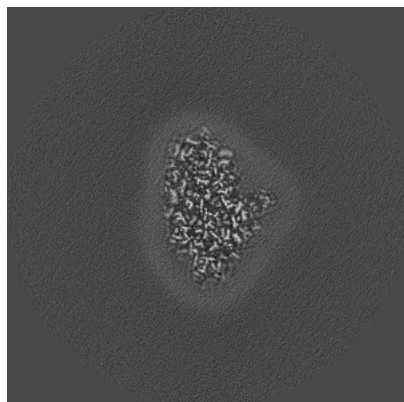


Y Index: 198

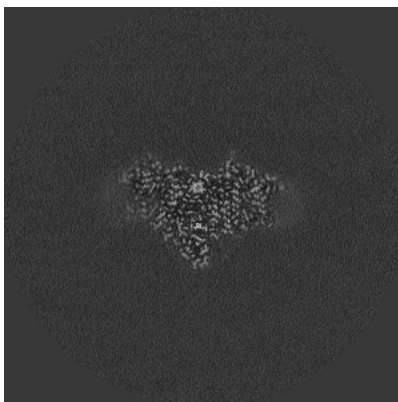


Z Index: 193

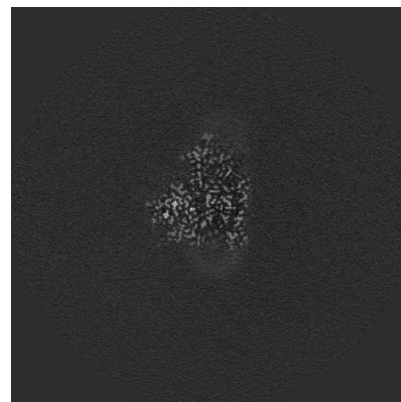
6.3.2 Raw map



X Index: 219



Y Index: 198

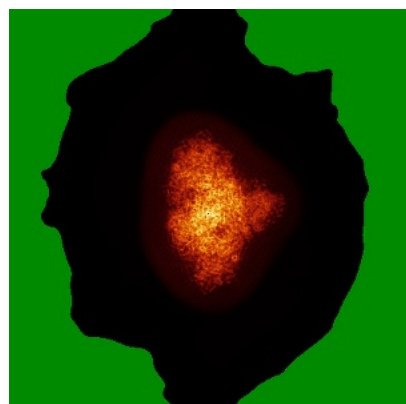


Z Index: 193

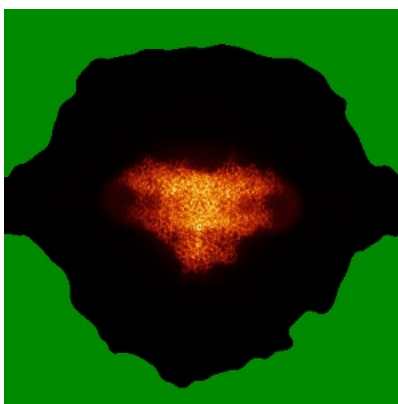
The images above show the largest variance slices of the map in three orthogonal directions.

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

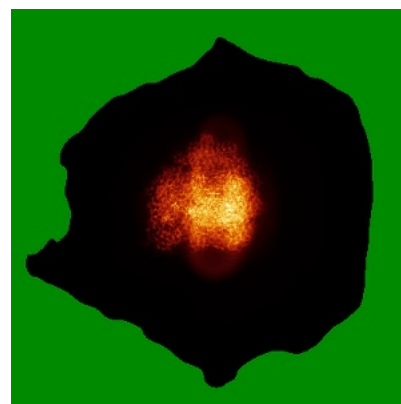
6.4.1 Primary map



X

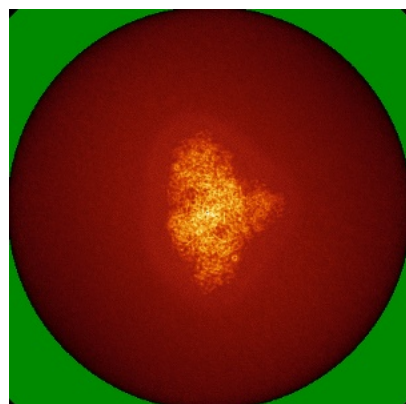


Y

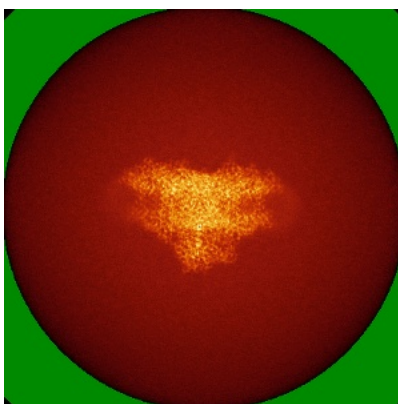


Z

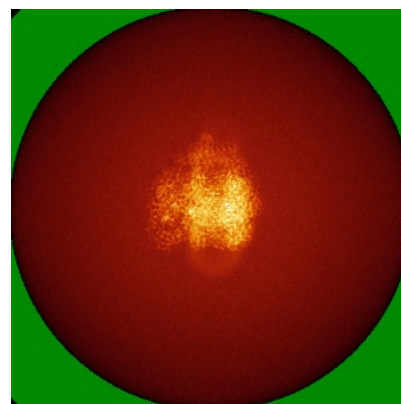
6.4.2 Raw map



X



Y

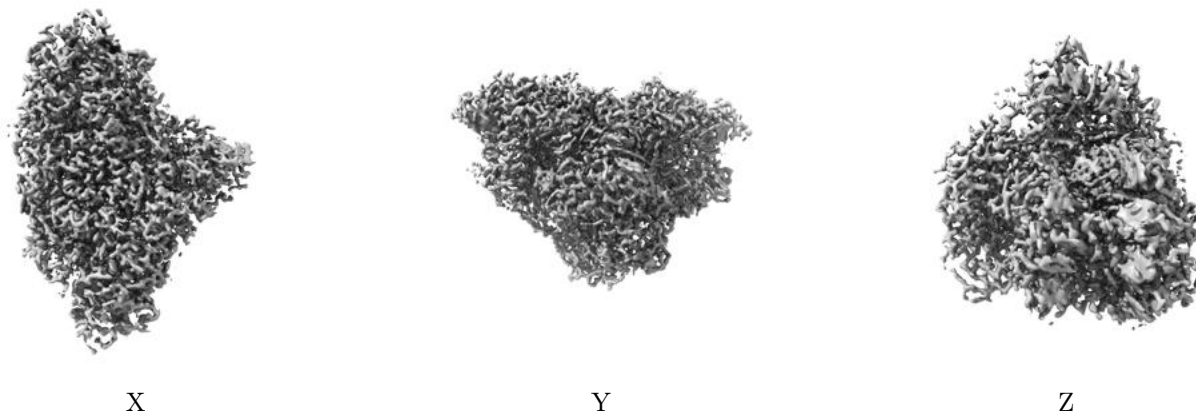


Z

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

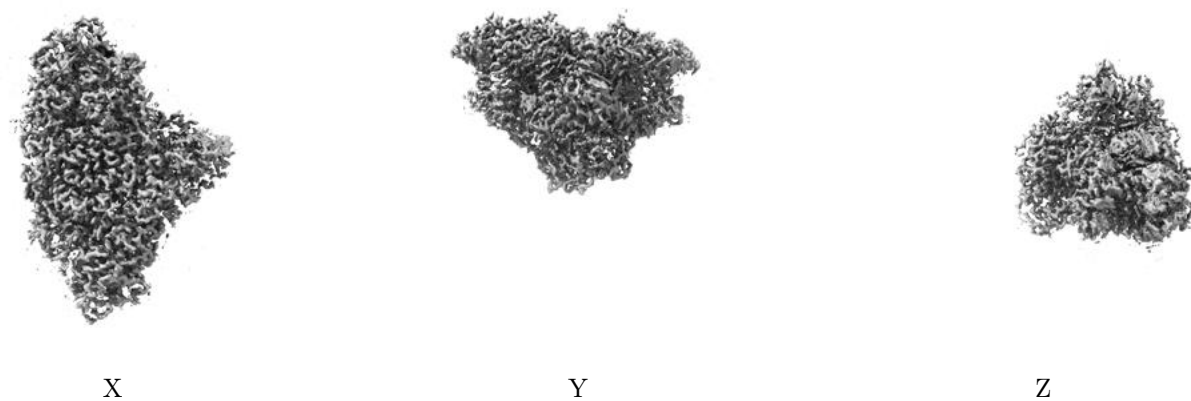
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.053. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

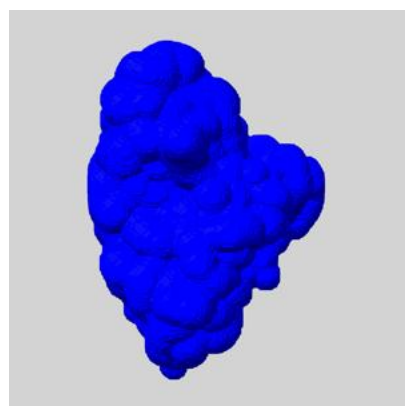
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

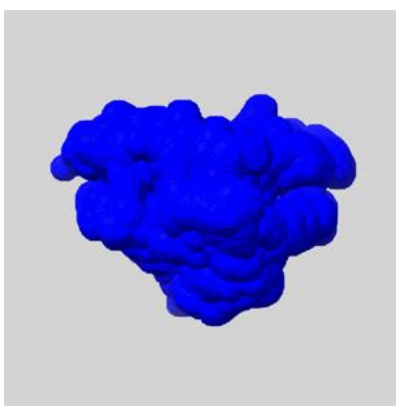
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

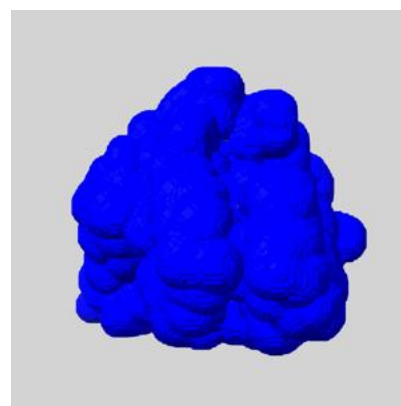
6.6.1 emd_15970_msk_1.map [i](#)



X



Y

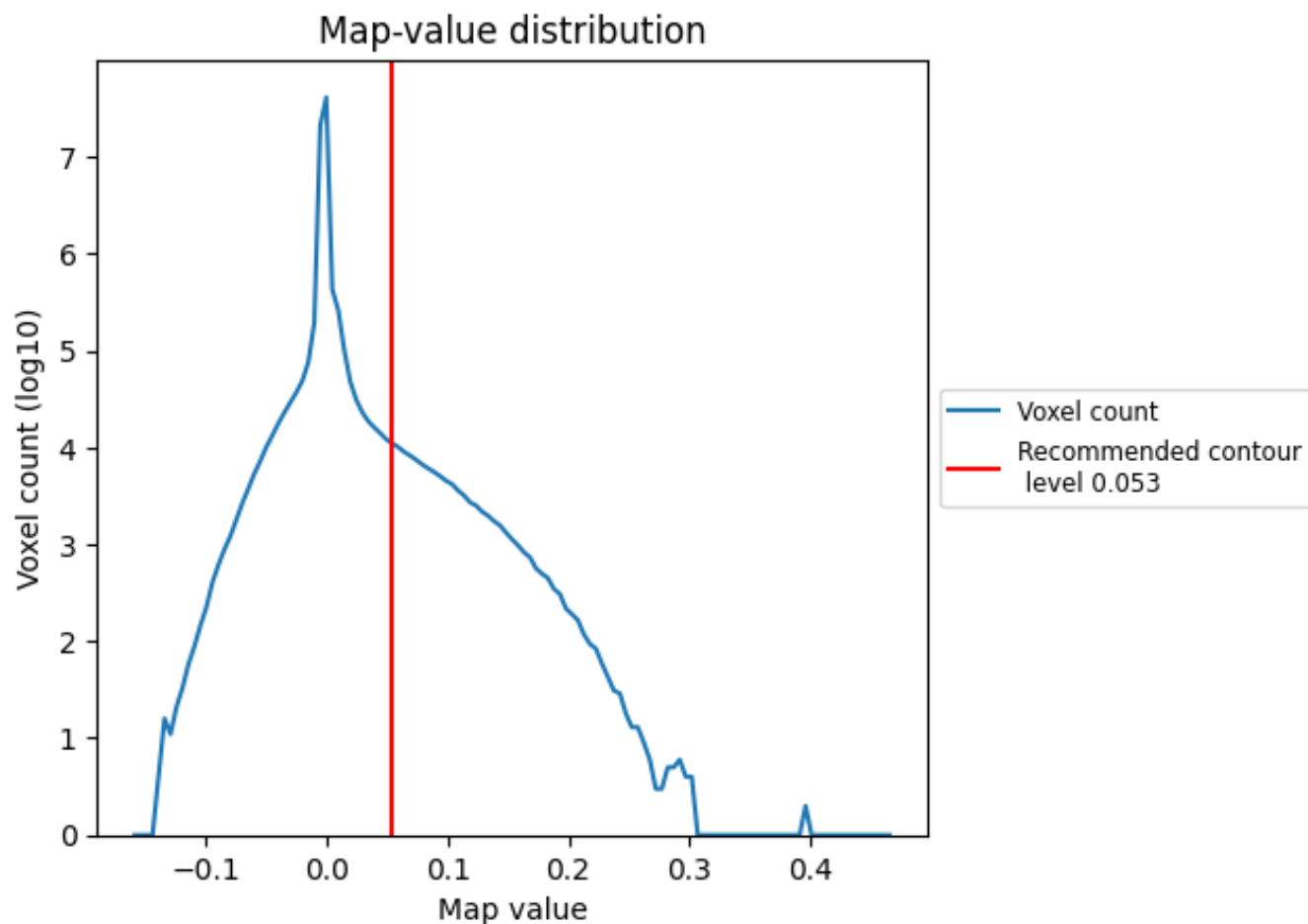


Z

7 Map analysis [i](#)

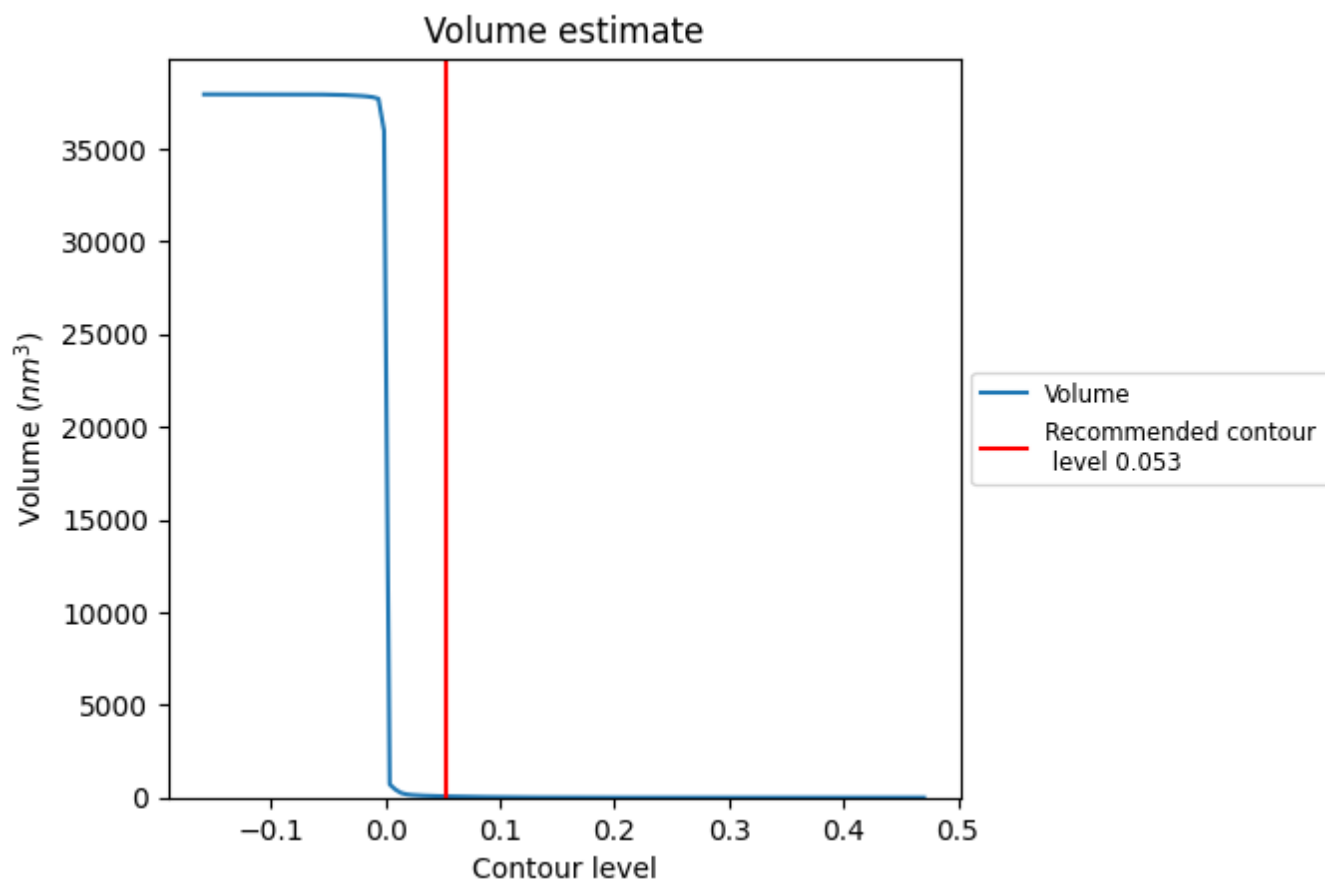
This section contains the results of statistical analysis of the map.

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.

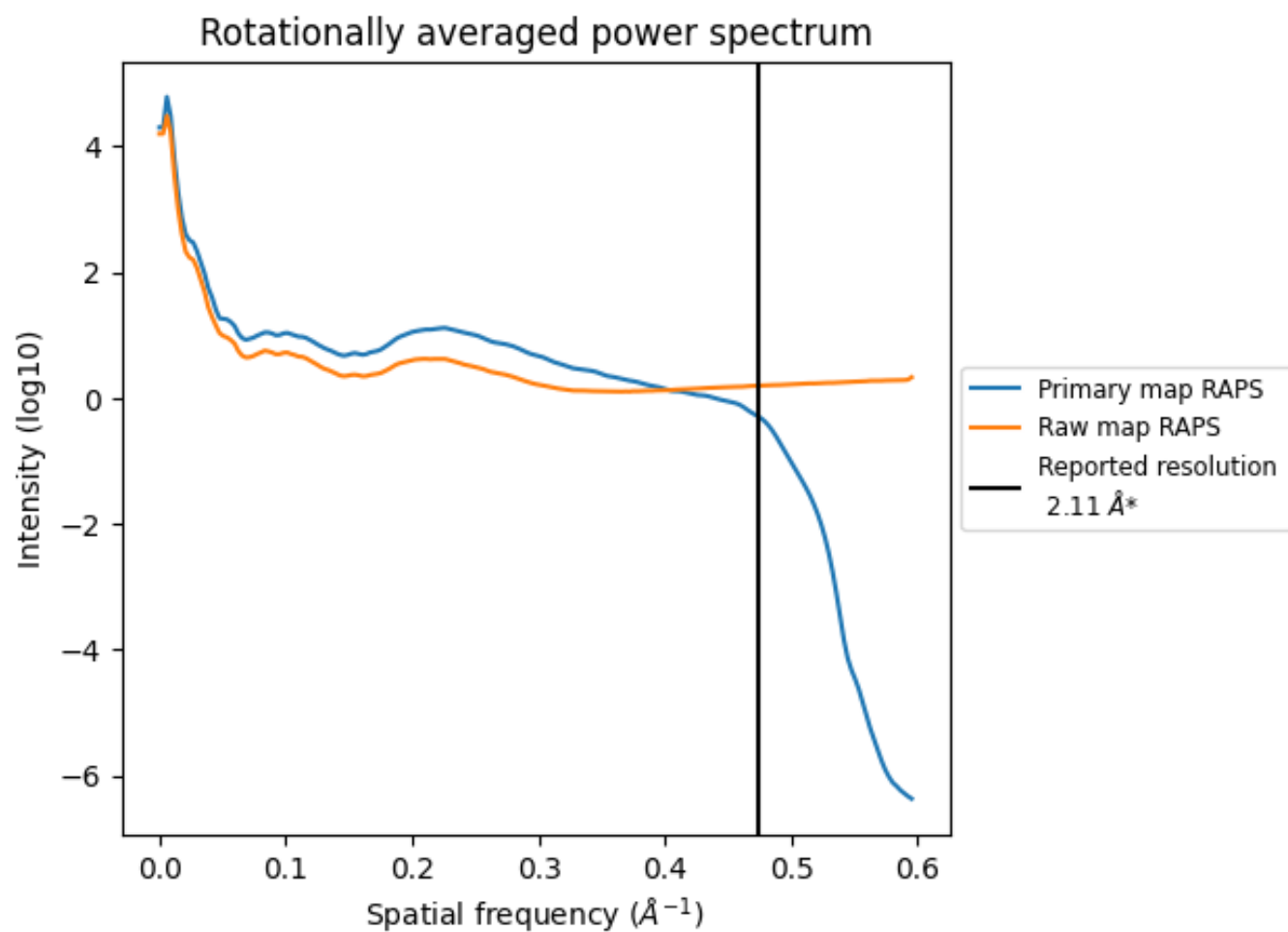
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm^3 ; this corresponds to an approximate mass of 58 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

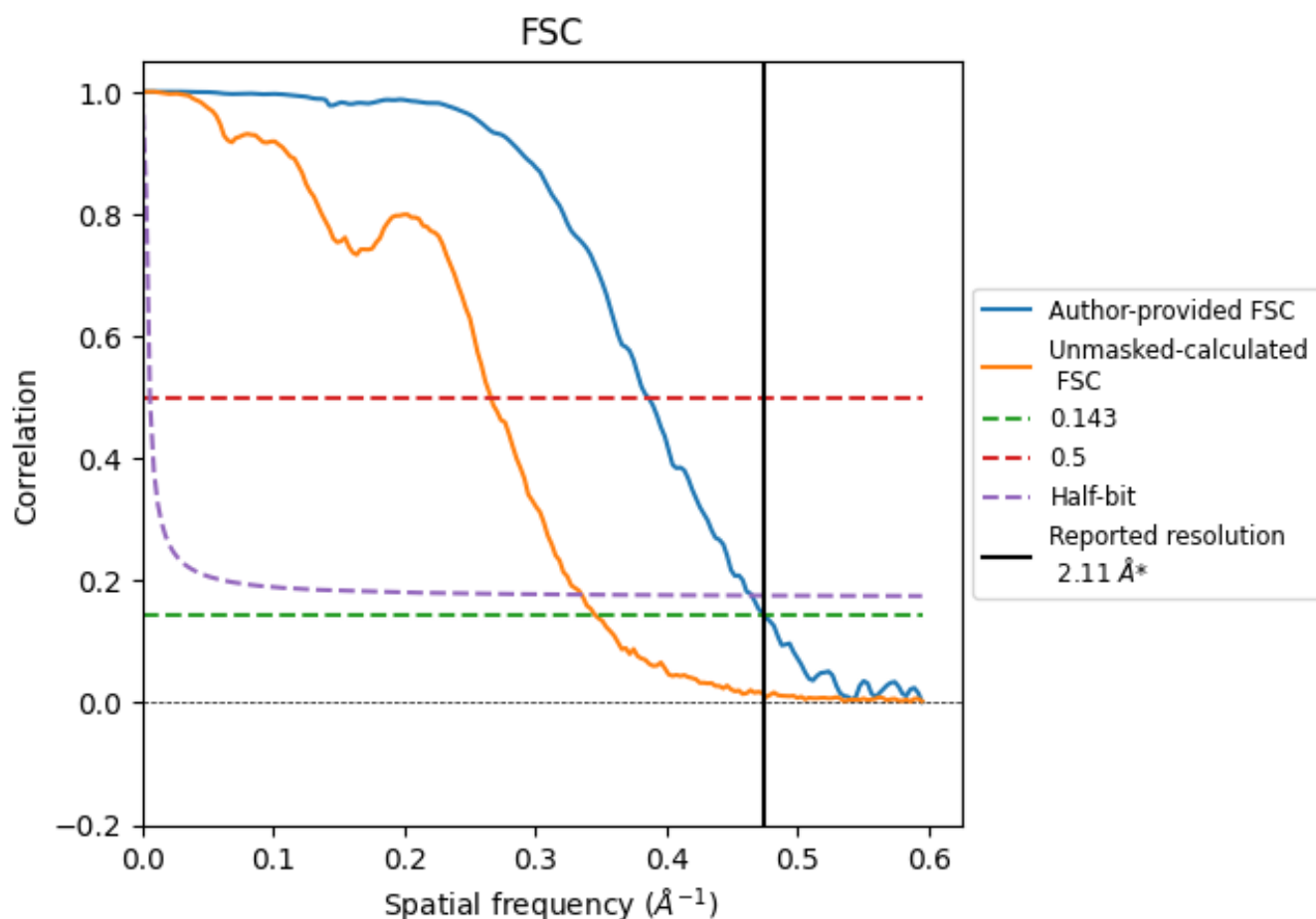


*Reported resolution corresponds to spatial frequency of 0.474 \AA^{-1}

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 0.474 \AA^{-1}

8.2 Resolution estimates [i](#)

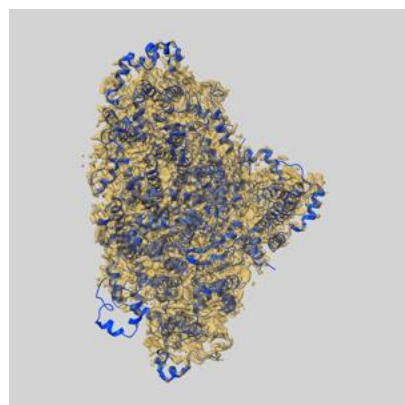
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.11	-	-
Author-provided FSC curve	2.11	2.59	2.15
Unmasked-calculated*	2.89	3.76	2.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.89 differs from the reported value 2.11 by more than 10 %

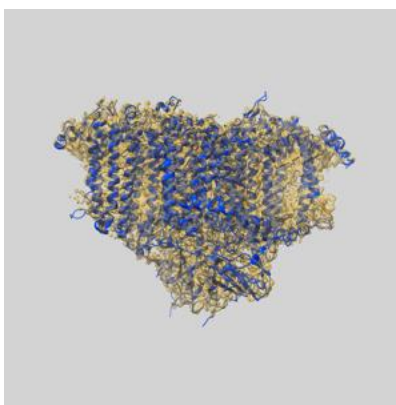
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15970 and PDB model 8BCW. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

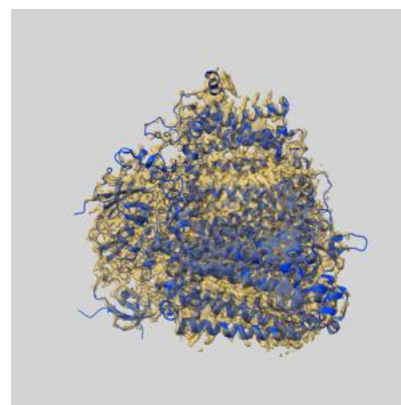
9.1 Map-model overlay [i](#)



X



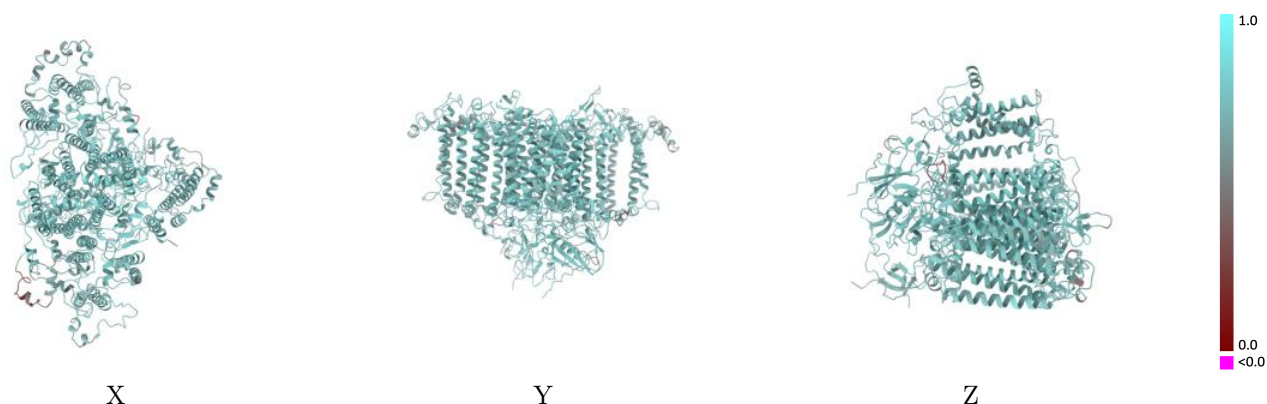
Y



Z

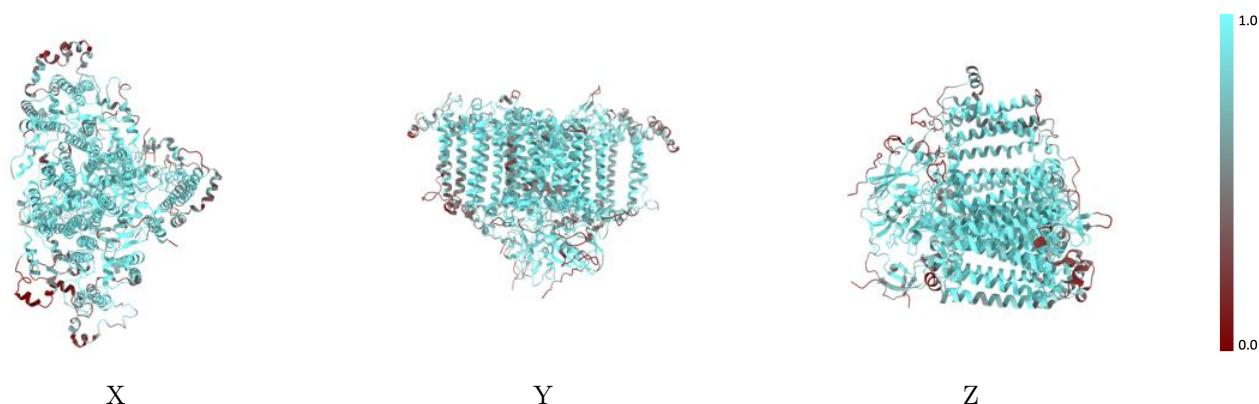
The images above show the 3D surface view of the map at the recommended contour level 0.053 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



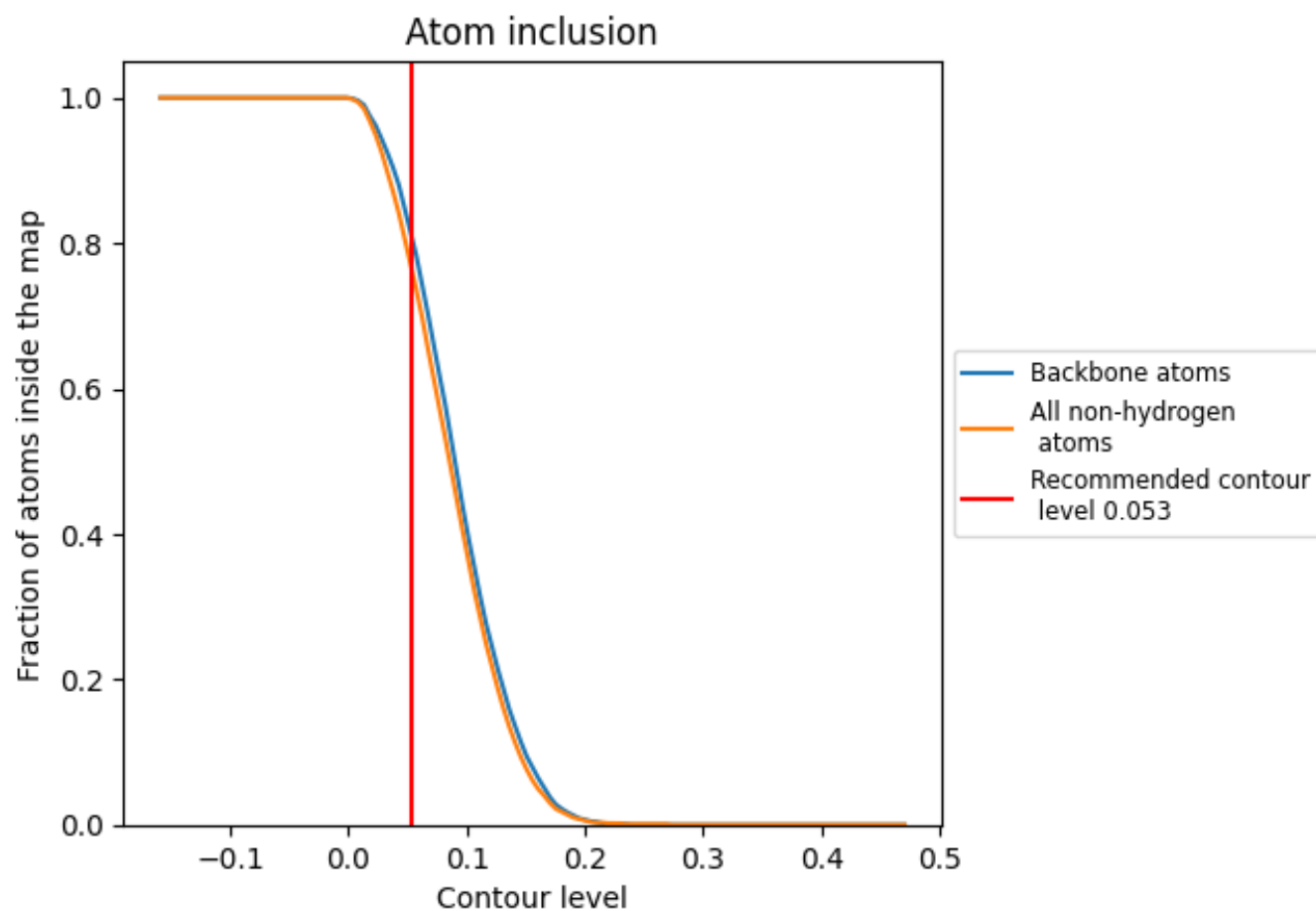
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.053).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 77% 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 (0.053) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7680	<div></div> 0.7070
A	<div></div> 0.8030	<div></div> 0.7130
B	<div></div> 0.7530	<div></div> 0.7060
C	<div></div> 0.9490	<div></div> 0.7580
D	<div></div> 0.8140	<div></div> 0.7130
E	<div></div> 0.6400	<div></div> 0.6690
H	<div></div> 0.4850	<div></div> 0.6610
I	<div></div> 0.7610	<div></div> 0.7030
L	<div></div> 0.7210	<div></div> 0.6940

