



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 02:29 PM UTC

PDB ID : 6LU1 / pdb_00006lu1
EMDB ID : EMD-0977
Title : Cyanobacterial PSI Monomer from *T. elongatus* by Single Particle CRYO-EM at 3.2 Å Resolution
Authors : Kurisu, G.; Coruh, O.; Tanaka, H.; Gerle, C.; Kawamoto, A.; Kato, T.; Namba, K.; Nowaczyk, M.M.; Rogner, M.; Misumi, Y.; Frank, A.; Eithar, E.M.
Deposited on : 2020-01-24
Resolution : 3.20 Å (reported)
Based on initial model : 1JB0

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 : **FAILED**
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

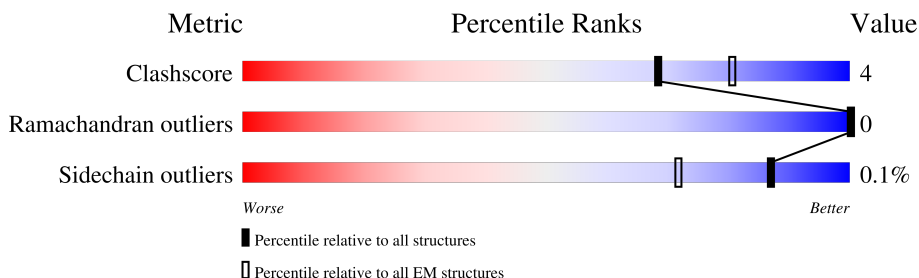
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	755	94% . .
2	B	741	91% 5% .
3	C	81	91% 7% .
4	D	139	94% 5% .
5	E	76	86% 5% 9%
6	F	164	17% . 82%
7	I	38	89% 11%

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Mol	Chain	Length	Quality of chain
8	J	41	
9	L	155	
10	M	31	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	801	X	-	-	-
11	CLA	A	802	X	-	-	-
11	CLA	A	803	X	-	-	-
11	CLA	A	804	X	-	-	-
11	CLA	A	805	X	-	-	-
11	CLA	A	806	X	-	-	-
11	CLA	A	807	X	-	-	-
11	CLA	A	808	X	-	-	-
11	CLA	A	809	X	-	-	-
11	CLA	A	810	X	-	-	-
11	CLA	A	811	X	-	-	-
11	CLA	A	812	X	-	-	-
11	CLA	A	813	X	-	-	-
11	CLA	A	814	X	-	-	-
11	CLA	A	815	X	-	-	-
11	CLA	A	816	X	-	-	-
11	CLA	A	817	X	-	-	-
11	CLA	A	818	X	-	-	-
11	CLA	A	819	X	-	-	-
11	CLA	A	820	X	-	-	-
11	CLA	A	821	X	-	-	-
11	CLA	A	822	X	-	-	-
11	CLA	A	823	X	-	-	-
11	CLA	A	824	X	-	-	-
11	CLA	A	825	X	-	-	-
11	CLA	A	826	X	-	-	-
11	CLA	A	827	X	-	-	-
11	CLA	A	828	X	-	-	-
11	CLA	A	829	X	-	-	-
11	CLA	A	830	X	-	-	-
11	CLA	A	831	X	-	-	-
11	CLA	A	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	833	X	-	-	-
11	CLA	A	834	X	-	-	-
11	CLA	A	835	X	-	-	-
11	CLA	A	836	X	-	-	-
11	CLA	A	837	X	-	-	-
11	CLA	A	838	X	-	-	-
11	CLA	A	839	X	-	-	-
11	CLA	A	840	X	-	-	-
11	CLA	A	841	X	-	-	-
11	CLA	A	842	X	-	-	-
11	CLA	A	859	X	-	-	-
11	CLA	A	860	X	-	-	-
11	CLA	B	801	X	-	-	-
11	CLA	B	802	X	-	-	-
11	CLA	B	803	X	-	-	-
11	CLA	B	805	X	-	-	-
11	CLA	B	806	X	-	-	-
11	CLA	B	807	X	-	-	-
11	CLA	B	808	X	-	-	-
11	CLA	B	809	X	-	-	-
11	CLA	B	810	X	-	-	-
11	CLA	B	811	X	-	-	-
11	CLA	B	812	X	-	-	-
11	CLA	B	813	X	-	-	-
11	CLA	B	814	X	-	-	-
11	CLA	B	815	X	-	-	-
11	CLA	B	816	X	-	-	-
11	CLA	B	817	X	-	-	-
11	CLA	B	818	X	-	-	-
11	CLA	B	819	X	-	-	-
11	CLA	B	820	X	-	-	-
11	CLA	B	821	X	-	-	-
11	CLA	B	822	X	-	-	-
11	CLA	B	823	X	-	-	-
11	CLA	B	824	X	-	-	-
11	CLA	B	825	X	-	-	-
11	CLA	B	826	X	-	-	-
11	CLA	B	827	X	-	-	-
11	CLA	B	828	X	-	-	-
11	CLA	B	829	X	-	-	-
11	CLA	B	830	X	-	-	-
11	CLA	B	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	832	X	-	-	-
11	CLA	B	833	X	-	-	-
11	CLA	B	834	X	-	-	-
11	CLA	B	835	X	-	-	-
11	CLA	B	836	X	-	-	-
11	CLA	L	1501	X	-	-	-
11	CLA	L	1502	X	-	-	-
11	CLA	L	1503	X	-	-	-
12	PQN	A	843	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 21198 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	745	Total	C	N	O	S	0	0
			5819	3818	994	981	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	713	Total	C	N	O	S	0	0
			5685	3747	952	967	19		

- 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
			598	367	103	117	11		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	69	Total	C	N	O	0	0
			539	342	93	104		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	F	29	Total	C	N	O	0	0
			231	160	37	34		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	J	8	Total	C	N	O	0	0
			67	44	12	11		

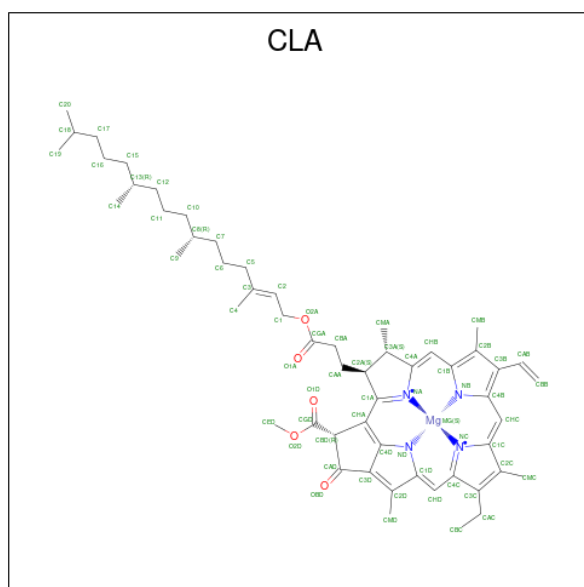
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	135	Total	C	N	O	S	0	0
			994	653	161	177	3		

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

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

- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			61	53	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			46	38	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			41	34	1	4	2	
11	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
11	A	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
11	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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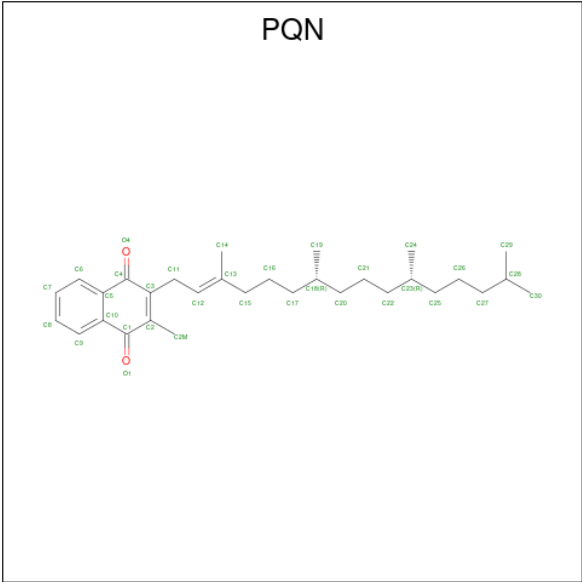
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
11	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
11	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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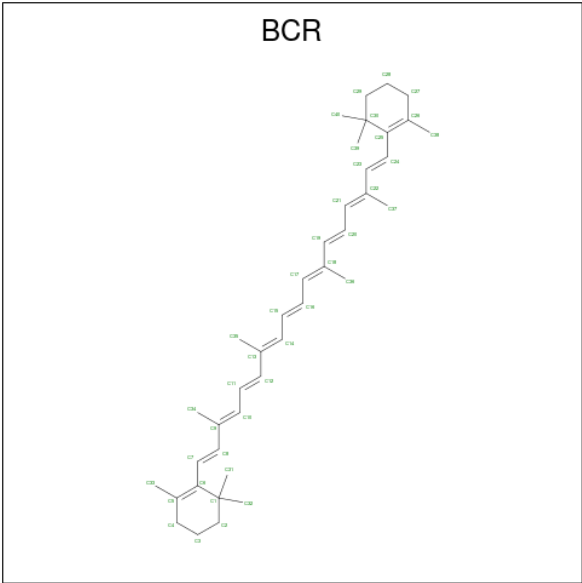
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
11	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
11	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
11	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
11	L	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
11	L	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
11	L	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

- Molecule 12 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 13 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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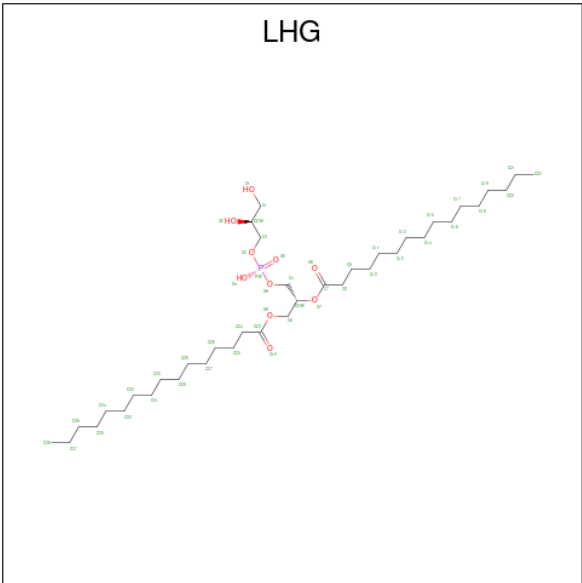
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 39 39	0
13	A	1	Total C 22 22	0
13	A	1	Total C 21 21	0
13	A	1	Total C 24 24	0
13	A	1	Total C 29 29	0
13	A	1	Total C 26 26	0
13	A	1	Total C 21 21	0
13	A	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 30 30	0
13	F	1	Total C 40 40	0
13	F	1	Total C 40 40	0
13	I	1	Total C 40 40	0

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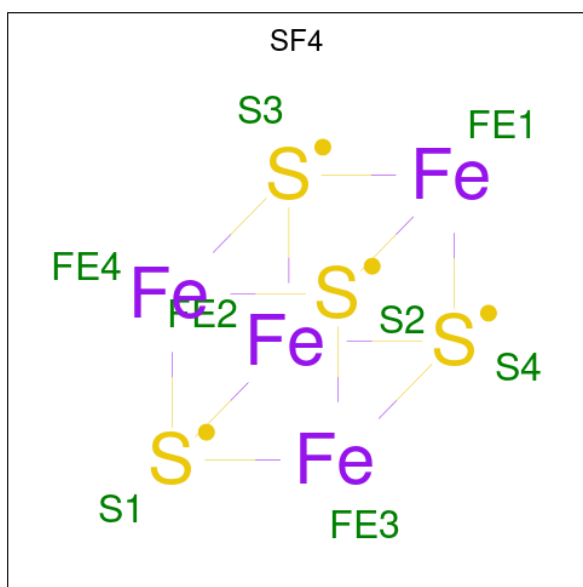
Mol	Chain	Residues	Atoms		AltConf
13	I	1	Total	C	0
			40	40	
13	L	1	Total	C	0
			40	40	
13	M	1	Total	C	0
			40	40	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



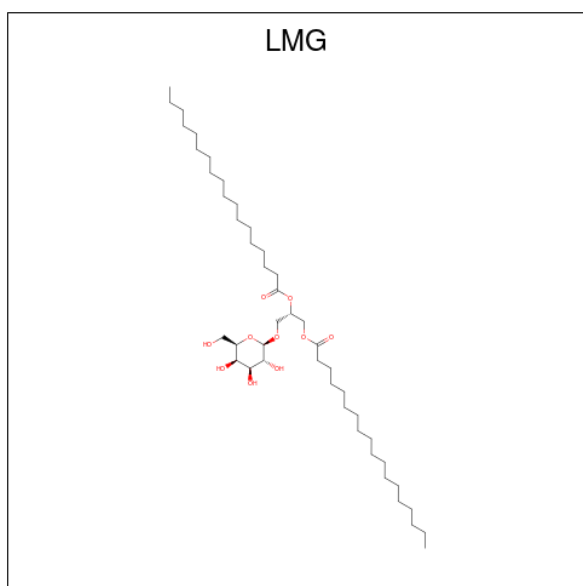
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			49	38	10	1	
14	A	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

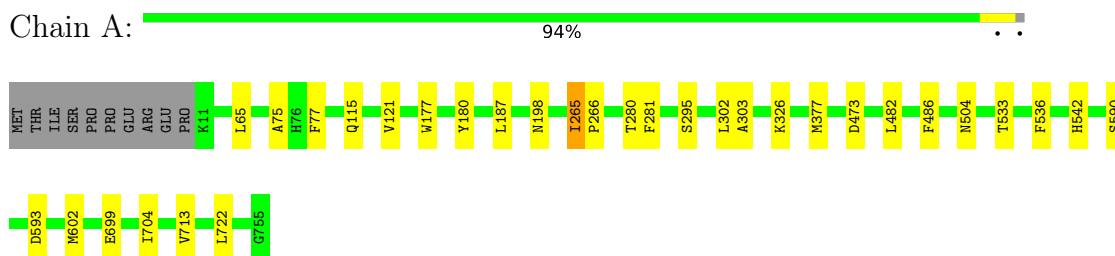
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	O	0
			1	1	
17	B	2	Total	O	0
			2	2	
17	C	1	Total	O	0
			1	1	
17	D	1	Total	O	0
			1	1	

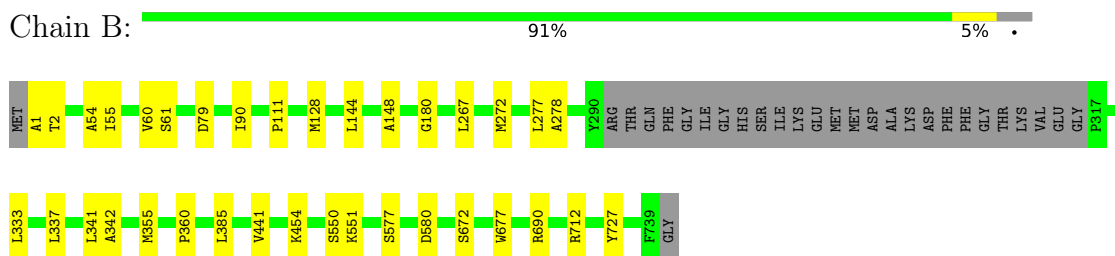
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

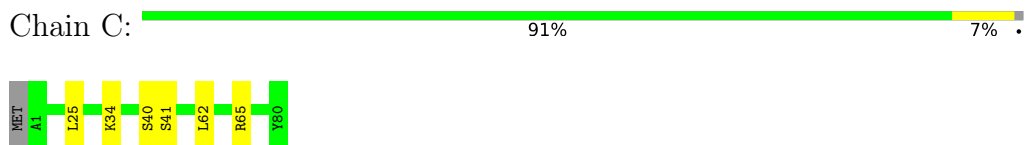
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



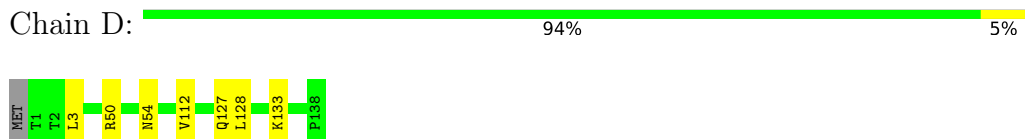
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



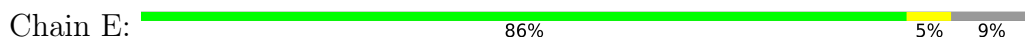
- Molecule 3: Photosystem I iron-sulfur center

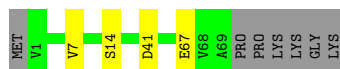


- Molecule 4: Photosystem I reaction center subunit II



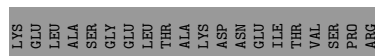
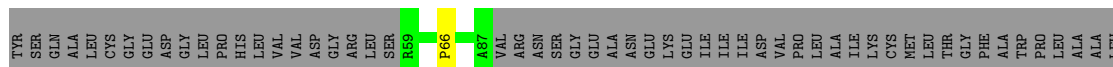
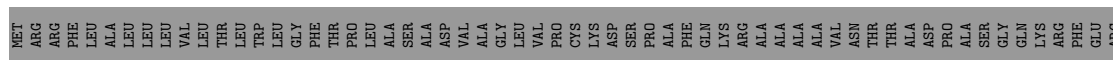
- Molecule 5: Photosystem I reaction center subunit IV





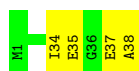
• Molecule 6: Photosystem I reaction center subunit III

Chain F: 17% 82%



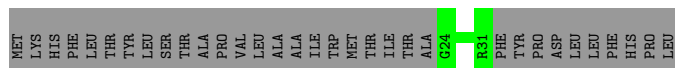
• Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 89% 11%



• Molecule 8: Photosystem I reaction center subunit IX

Chain J: 20% 80%



• Molecule 9: Photosystem I reaction center subunit XI

Chain L: 83% 13%



• Molecule 10: Photosystem I reaction center subunit XII

Chain M: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46105	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	56497	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.24	0/6019	0.42	0/8209
2	B	0.24	0/5898	0.43	1/8066 (0.0%)
3	C	0.24	0/608	0.49	0/824
4	D	0.21	0/1101	0.47	0/1492
5	E	0.16	0/551	0.37	0/750
6	F	0.23	0/239	0.58	0/326
7	I	0.24	0/312	0.53	0/425
8	J	0.15	0/67	0.40	0/88
9	L	0.17	0/1021	0.40	0/1387
10	M	0.19	0/244	0.47	0/332
All	All	0.23	0/16060	0.44	1/21899 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	55	ILE	N-CA-C	-5.60	107.36	112.96

There are no chirality outliers.

There are no planarity outliers.

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	5819	0	5686	29	0
2	B	5685	0	5453	28	0
3	C	598	0	588	4	0
4	D	1075	0	1077	5	0
5	E	539	0	528	3	0
6	F	231	0	235	1	0
7	I	301	0	306	3	0
8	J	67	0	69	0	0
9	L	994	0	1001	4	0
10	M	241	0	264	0	0
11	A	2422	0	2293	46	0
11	B	1932	0	1849	30	0
11	L	136	0	106	1	0
12	A	33	0	46	21	0
12	B	33	0	46	9	0
13	A	462	0	630	15	0
13	B	230	0	319	7	0
13	F	80	0	112	15	0
13	I	80	0	112	2	0
13	L	40	0	56	0	0
13	M	40	0	56	0	0
14	A	76	0	98	1	0
15	B	8	0	0	0	0
15	C	16	0	0	0	0
16	B	55	0	86	0	0
17	A	1	0	0	0	0
17	B	2	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
All	All	21198	0	21016	156	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 (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:843:PQN:H303	13:F:201:BCR:C19	1.72	1.20
12:A:843:PQN:H292	13:F:201:BCR:H17C	1.22	1.14
12:B:837:PQN:H242	12:B:837:PQN:H201	1.41	1.02
12:A:843:PQN:H303	13:F:201:BCR:C20	1.92	0.99
12:B:837:PQN:H272	12:B:837:PQN:H241	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:843:PQN:C29	13:F:201:BCR:H17C	2.02	0.90
12:A:843:PQN:H292	13:F:201:BCR:C17	2.09	0.80
12:B:837:PQN:H12	12:B:837:PQN:H2M1	1.62	0.79
12:A:843:PQN:C30	13:F:201:BCR:C19	2.58	0.79
12:B:837:PQN:H201	12:B:837:PQN:C24	2.13	0.78
12:A:843:PQN:H303	13:F:201:BCR:H20C	1.65	0.77
12:A:843:PQN:H303	13:F:201:BCR:H19C	1.66	0.76
12:B:837:PQN:H241	12:B:837:PQN:C27	2.10	0.75
12:A:843:PQN:C30	13:F:201:BCR:H20C	2.18	0.74
2:B:337:LEU:HD11	11:B:825:CLA:HBB1	1.73	0.71
12:A:843:PQN:C30	13:F:201:BCR:H19C	2.22	0.69
11:A:841:CLA:H41	12:A:843:PQN:H202	1.75	0.68
9:L:61:PRO:HG3	11:L:1503:CLA:HBB1	1.78	0.66
12:B:837:PQN:H2M1	12:B:837:PQN:C12	2.29	0.63
11:A:820:CLA:HBB1	13:A:844:BCR:H16C	1.80	0.63
1:A:486:PHE:HB3	11:A:837:CLA:H2	1.82	0.61
11:A:815:CLA:HBB1	13:A:844:BCR:H333	1.82	0.60
4:D:50:ARG:H	4:D:54:ASN:HD21	1.49	0.60
1:A:542:HIS:HB3	11:A:837:CLA:HBB1	1.85	0.59
11:B:808:CLA:H151	11:B:824:CLA:HBB2	1.85	0.58
11:A:860:CLA:H143	13:B:842:BCR:H362	1.87	0.57
11:A:831:CLA:HBA2	14:A:851:LHG:HC81	1.86	0.56
11:A:805:CLA:H42	11:A:806:CLA:HAB	1.87	0.56
3:C:40:SER:HB2	4:D:112:VAL:H	1.71	0.56
1:A:473:ASP:OD1	9:L:69:ARG:NH1	2.40	0.55
11:A:806:CLA:H3A	11:A:830:CLA:HAB	1.89	0.55
9:L:73:VAL:HG13	9:L:76:LEU:HB2	1.89	0.55
11:A:859:CLA:H43	2:B:441:VAL:HG22	1.89	0.54
11:B:802:CLA:H52	13:F:201:BCR:H362	1.89	0.54
11:A:821:CLA:H52	11:A:824:CLA:H51	1.88	0.54
1:A:536:PHE:HA	11:A:838:CLA:HED1	1.88	0.54
1:A:590:SER:OG	1:A:593:ASP:OD1	2.25	0.53
2:B:360:PRO:HG3	11:B:820:CLA:HBA2	1.90	0.53
12:A:843:PQN:H302	12:A:843:PQN:H252	1.90	0.53
11:A:859:CLA:HMB3	11:B:805:CLA:H18	1.91	0.53
1:A:115:GLN:NE2	11:A:809:CLA:OBD	2.42	0.52
11:B:808:CLA:H42	11:B:808:CLA:HMA2	1.90	0.52
6:F:66:PRO:HG3	13:F:202:BCR:H12C	1.90	0.52
2:B:1:ALA:HA	7:I:38:ALA:H	1.74	0.52
12:B:837:PQN:C24	12:B:837:PQN:C20	2.85	0.52
11:A:840:CLA:HAB	12:A:843:PQN:H193	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TRP:HB2	11:A:811:CLA:HMC3	1.92	0.52
1:A:482:LEU:HB2	1:A:533:THR:HG23	1.93	0.51
11:B:836:CLA:HBA1	12:B:837:PQN:H262	1.93	0.51
13:A:845:BCR:H362	13:A:846:BCR:H10C	1.92	0.50
2:B:577:SER:OG	2:B:580:ASP:OD1	2.30	0.49
4:D:128:LEU:HD22	4:D:133:LYS:HB2	1.94	0.49
13:F:201:BCR:H372	13:F:201:BCR:H361	1.95	0.49
11:A:828:CLA:H52	13:A:849:BCR:H343	1.92	0.49
1:A:75:ALA:HB1	11:A:805:CLA:HBB1	1.95	0.49
2:B:144:LEU:HD11	11:B:816:CLA:H152	1.93	0.49
2:B:454:LYS:HE2	11:B:829:CLA:HED3	1.94	0.49
3:C:62:LEU:HD12	3:C:65:ARG:HH11	1.78	0.48
12:A:843:PQN:C2M	12:A:843:PQN:H12	2.44	0.48
11:A:819:CLA:H92	11:A:829:CLA:H91	1.95	0.47
1:A:265:ILE:HG13	1:A:266:PRO:HD3	1.96	0.47
5:E:7:VAL:HG12	5:E:67:GLU:HA	1.97	0.47
2:B:672:SER:HB3	2:B:677:TRP:HE1	1.79	0.47
1:A:377:MET:HE2	11:A:827:CLA:HMC2	1.97	0.47
11:A:802:CLA:H143	11:B:812:CLA:HBC3	1.97	0.47
11:A:821:CLA:HAA2	11:A:825:CLA:HAB	1.95	0.47
11:A:826:CLA:H51	11:A:837:CLA:H43	1.97	0.47
13:A:858:BCR:H24C	13:A:858:BCR:H371	1.74	0.47
2:B:267:LEU:HB2	2:B:272:MET:HE2	1.96	0.47
2:B:90:ILE:HB	2:B:111:PRO:HB2	1.98	0.46
1:A:602:MET:HE3	1:A:602:MET:HB3	1.83	0.45
11:B:817:CLA:HBB1	13:B:838:BCR:H333	1.97	0.45
12:A:843:PQN:H272	11:B:802:CLA:H92	1.97	0.45
2:B:551:LYS:NZ	5:E:14:SER:O	2.47	0.45
1:A:722:LEU:HG	12:A:843:PQN:H143	1.99	0.45
11:B:807:CLA:H3A	11:B:807:CLA:HBA1	1.79	0.45
7:I:34:ILE:HG13	7:I:35:GLU:HG2	1.99	0.45
11:A:817:CLA:HAC1	13:A:855:BCR:H353	1.97	0.45
12:A:843:PQN:H12	12:A:843:PQN:H2M1	1.98	0.45
13:A:845:BCR:H24C	13:A:845:BCR:H371	1.85	0.45
11:B:813:CLA:HBB2	11:B:815:CLA:HMA3	1.98	0.45
2:B:277:LEU:HG	11:B:818:CLA:HAB	1.99	0.45
11:A:805:CLA:H71	11:A:813:CLA:H11	1.99	0.45
12:A:843:PQN:C2M	12:A:843:PQN:C12	2.95	0.45
1:A:504:ASN:HB2	11:A:836:CLA:HED2	1.98	0.44
1:A:704:ILE:HD13	11:B:802:CLA:HMD1	2.00	0.44
12:B:837:PQN:H193	12:B:837:PQN:H162	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:SER:O	2:B:61:SER:OG	2.31	0.44
11:B:828:CLA:H41	11:B:828:CLA:H62	1.80	0.44
2:B:128:MET:HE3	11:B:816:CLA:HMA2	1.98	0.44
11:A:821:CLA:H102	13:A:848:BCR:H10C	2.01	0.43
13:A:857:BCR:H24C	13:A:857:BCR:H371	1.80	0.43
2:B:278:ALA:HA	11:B:818:CLA:HMC3	2.01	0.43
1:A:180:TYR:OH	11:A:811:CLA:O1D	2.33	0.43
1:A:65:LEU:HD23	1:A:187:LEU:HD21	2.01	0.43
11:A:821:CLA:HMB2	11:A:825:CLA:HMA3	2.00	0.43
2:B:2:THR:H	7:I:37:GLU:HA	1.83	0.43
1:A:121:VAL:HG21	11:A:809:CLA:HAB	2.00	0.43
1:A:302:LEU:HG	11:A:817:CLA:HBB1	2.01	0.43
2:B:355:MET:HE2	2:B:355:MET:HB3	1.84	0.43
13:B:841:BCR:H24C	13:B:841:BCR:H371	1.90	0.42
1:A:326:LYS:HB3	1:A:326:LYS:HE3	1.83	0.42
13:A:849:BCR:H24C	13:A:849:BCR:H371	1.76	0.42
4:D:3:LEU:HD23	4:D:3:LEU:HA	1.85	0.42
9:L:38:ARG:HB3	9:L:41:LEU:HG	2.00	0.42
11:A:841:CLA:H41	12:A:843:PQN:C20	2.44	0.42
13:A:852:BCR:H24C	13:A:852:BCR:H371	1.84	0.42
13:B:840:BCR:H361	13:B:840:BCR:H21C	2.02	0.42
2:B:60:VAL:HG21	11:B:824:CLA:H42	2.02	0.42
2:B:180:GLY:HA3	11:B:815:CLA:HBB1	2.00	0.42
1:A:722:LEU:CD2	12:A:843:PQN:H143	2.50	0.42
11:A:808:CLA:H11	11:A:808:CLA:H51	1.76	0.41
11:A:817:CLA:HBA2	13:A:855:BCR:H362	2.01	0.41
1:A:281:PHE:HE2	11:A:818:CLA:HAB	1.86	0.41
1:A:303:ALA:HA	11:A:817:CLA:HMC3	2.02	0.41
11:A:811:CLA:H61	11:A:811:CLA:H41	1.75	0.41
2:B:333:LEU:HD21	11:B:807:CLA:H192	2.02	0.41
13:I:101:BCR:H24C	13:I:101:BCR:H371	1.93	0.41
1:A:280:THR:OG1	1:A:295:SER:OG	2.31	0.41
1:A:77:PHE:CZ	11:A:810:CLA:HBB1	2.56	0.41
1:A:713:VAL:HG21	11:B:802:CLA:HMB3	2.03	0.41
13:F:202:BCR:H20C	13:F:202:BCR:H361	1.91	0.41
3:C:25:LEU:HD23	3:C:41:SER:HB3	2.01	0.41
2:B:727:TYR:HB2	11:B:805:CLA:HED2	2.03	0.41
11:B:816:CLA:H13	11:B:824:CLA:H141	2.01	0.41
13:B:844:BCR:H20C	13:B:844:BCR:H361	1.82	0.41
1:A:77:PHE:CE1	11:A:810:CLA:HBB1	2.56	0.41
11:A:813:CLA:H62	11:A:813:CLA:H102	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:818:CLA:HBA2	11:A:818:CLA:H3A	1.84	0.41
13:A:857:BCR:H20C	13:A:857:BCR:H361	1.86	0.41
11:B:811:CLA:H61	11:B:811:CLA:H41	1.69	0.41
11:B:828:CLA:H162	11:B:828:CLA:H122	1.93	0.41
13:I:101:BCR:H20C	13:I:101:BCR:H361	1.91	0.41
11:A:824:CLA:H61	11:A:824:CLA:H41	1.90	0.41
2:B:341:LEU:HD22	2:B:385:LEU:HD22	2.03	0.41
13:A:858:BCR:H20C	13:A:858:BCR:H361	1.86	0.40
1:A:198:ASN:HB3	11:A:820:CLA:HMD1	2.03	0.40
11:A:808:CLA:HBA2	11:A:808:CLA:H3A	1.93	0.40
11:A:835:CLA:H61	11:A:835:CLA:H41	1.77	0.40
2:B:54:ALA:HB2	2:B:148:ALA:HB3	2.04	0.40
11:B:805:CLA:H111	11:B:805:CLA:H152	1.89	0.40
11:B:821:CLA:HBB1	11:B:834:CLA:HBB	2.03	0.40
11:A:818:CLA:H41	11:A:818:CLA:H62	1.73	0.40
2:B:580:ASP:OD2	2:B:712:ARG:NH1	2.54	0.40
2:B:690:ARG:HA	2:B:690:ARG:HD3	1.93	0.40
11:B:815:CLA:H52	11:B:815:CLA:H8	1.93	0.40
13:B:844:BCR:H24C	13:B:844:BCR:H371	1.76	0.40
4:D:127:GLN:HG3	4:D:128:LEU:HG	2.03	0.40
5:E:41:ASP:OD1	5:E:41:ASP:N	2.54	0.40
1:A:699:GLU:OE1	2:B:550:SER:OG	2.35	0.40
13:A:852:BCR:H20C	13:A:852:BCR:H361	1.89	0.40
2:B:342:ALA:HB2	13:B:841:BCR:H372	2.03	0.40
3:C:34:LYS:HB3	3:C:34:LYS:HE2	1.87	0.40
12:A:843:PQN:H192	12:A:843:PQN:H161	1.82	0.40
2:B:79:ASP:OD1	2:B:79:ASP:N	2.54	0.40
13:F:201:BCR:H392	13:F:201:BCR:H24C	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	743/755 (98%)	712 (96%)	31 (4%)	0	100	100
2	B	709/741 (96%)	671 (95%)	38 (5%)	0	100	100
3	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	D	136/139 (98%)	122 (90%)	14 (10%)	0	100	100
5	E	67/76 (88%)	62 (92%)	5 (8%)	0	100	100
6	F	27/164 (16%)	26 (96%)	1 (4%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	J	6/41 (15%)	6 (100%)	0	0	100	100
9	L	133/155 (86%)	128 (96%)	5 (4%)	0	100	100
10	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	1964/2221 (88%)	1859 (95%)	105 (5%)	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	593/603 (98%)	592 (100%)	1 (0%)	87	89
2	B	576/598 (96%)	576 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/116 (99%)	115 (100%)	0	100	100
5	E	59/65 (91%)	59 (100%)	0	100	100
6	F	21/128 (16%)	21 (100%)	0	100	100
7	I	32/32 (100%)	32 (100%)	0	100	100
8	J	7/36 (19%)	7 (100%)	0	100	100
9	L	103/120 (86%)	103 (100%)	0	100	100
10	M	26/26 (100%)	26 (100%)	0	100	100
All	All	1599/1792 (89%)	1598 (100%)	1 (0%)	87	91

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

Mol	Chain	Res	Type
1	A	265	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	50	ASN
1	A	181	HIS
1	A	224	ASN
1	A	286	ASN
1	A	299	HIS
1	A	323	HIS
1	A	341	HIS
1	A	359	ASN
1	A	426	GLN
1	A	461	HIS
1	A	542	HIS
2	B	13	GLN
2	B	28	HIS
2	B	49	HIS
2	B	247	GLN
2	B	322	HIS
2	B	378	HIS
2	B	604	HIS
2	B	678	GLN
2	B	688	HIS
2	B	695	ASN
2	B	710	GLN
4	D	54	ASN
4	D	71	GLN
4	D	121	GLN
5	E	18	ASN
5	E	56	ASN
5	E	63	HIS
9	L	9	ASN
9	L	16	HIS
9	L	75	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

116 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	$\# Z > 2$
11	CLA	A	813	-	69,73,73	1.60	9 (13%)	82,113,113	1.15	8 (9%)
11	CLA	B	809	-	69,73,73	1.59	9 (13%)	82,113,113	1.10	8 (9%)
11	CLA	B	811	-	69,73,73	1.61	8 (11%)	82,113,113	1.09	8 (9%)
11	CLA	B	814	-	49,53,73	1.97	9 (18%)	58,89,113	1.38	9 (15%)
15	SF4	C	102	-	0,12,12	-	-	-	-	-
11	CLA	A	824	-	68,72,73	1.61	9 (13%)	81,112,113	1.01	6 (7%)
13	BCR	B	840	-	41,41,41	0.25	0	56,56,56	0.73	2 (3%)
11	CLA	A	859	-	60,64,73	1.70	8 (13%)	71,102,113	1.16	7 (9%)
11	CLA	A	812	-	57,61,73	1.84	9 (15%)	67,98,113	1.17	8 (11%)
11	CLA	A	840	-	44,49,73	2.11	10 (22%)	50,83,113	1.35	7 (14%)
11	CLA	B	823	-	61,65,73	1.70	9 (14%)	72,103,113	1.19	10 (13%)
15	SF4	B	804	-	0,12,12	-	-	-	-	-
11	CLA	B	824	-	69,73,73	1.61	8 (11%)	82,113,113	1.25	9 (10%)
13	BCR	A	856	-	29,29,41	0.36	0	37,37,56	1.14	3 (8%)
13	BCR	A	848	-	41,41,41	0.30	0	56,56,56	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	827	-	69,73,73	1.61	9 (13%)	82,113,113	1.05	9 (10%)
13	BCR	A	849	-	41,41,41	0.43	1 (2%)	56,56,56	1.14	6 (10%)
13	BCR	L	1504	-	41,41,41	0.31	0	56,56,56	0.72	1 (1%)
11	CLA	A	801	-	65,69,73	1.66	10 (15%)	78,107,113	1.12	9 (11%)
11	CLA	A	834	-	69,73,73	1.58	8 (11%)	82,113,113	1.05	9 (10%)
16	LMG	B	843	-	55,55,55	0.79	2 (3%)	63,63,63	1.37	9 (14%)
11	CLA	B	818	-	59,63,73	1.82	10 (16%)	70,101,113	1.14	6 (8%)
11	CLA	A	821	-	69,73,73	1.61	9 (13%)	82,113,113	1.02	8 (9%)
11	CLA	A	819	-	69,73,73	1.61	8 (11%)	82,113,113	1.21	10 (12%)
11	CLA	A	839	-	53,57,73	1.81	10 (18%)	61,93,113	1.22	8 (13%)
11	CLA	L	1502	-	62,66,73	1.79	10 (16%)	73,104,113	1.38	9 (12%)
11	CLA	B	830	-	45,49,73	2.11	9 (20%)	54,84,113	1.38	8 (14%)
11	CLA	L	1503	-	46,50,73	2.02	8 (17%)	53,85,113	1.52	8 (15%)
11	CLA	B	820	-	64,68,73	1.67	9 (14%)	76,107,113	1.23	8 (10%)
11	CLA	B	812	-	47,51,73	2.01	9 (19%)	55,86,113	1.35	8 (14%)
13	BCR	B	839	-	41,41,41	0.29	0	56,56,56	0.51	0
13	BCR	F	201	-	41,41,41	0.51	1 (2%)	56,56,56	1.63	10 (17%)
13	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.34	0
11	CLA	A	838	-	59,63,73	1.75	9 (15%)	70,101,113	1.13	7 (10%)
11	CLA	B	807	-	69,73,73	1.59	9 (13%)	82,113,113	1.09	7 (8%)
11	CLA	A	825	-	69,73,73	1.62	8 (11%)	82,113,113	1.08	9 (10%)
11	CLA	A	842	-	44,48,73	2.07	9 (20%)	51,82,113	1.38	9 (17%)
11	CLA	B	803	-	69,73,73	1.66	10 (14%)	82,113,113	1.22	9 (10%)
11	CLA	B	822	-	47,52,73	1.97	8 (17%)	55,88,113	1.36	9 (16%)
11	CLA	A	802	-	69,73,73	1.58	8 (11%)	82,113,113	1.06	6 (7%)
15	SF4	C	101	-	0,12,12	-	-	-	-	-
11	CLA	B	831	-	49,53,73	1.88	8 (16%)	58,89,113	1.21	9 (15%)
11	CLA	B	816	-	69,73,73	1.61	9 (13%)	82,113,113	1.03	6 (7%)
11	CLA	B	825	-	69,73,73	1.65	9 (13%)	82,113,113	1.00	7 (8%)
11	CLA	A	815	-	49,53,73	1.91	9 (18%)	58,89,113	1.18	8 (13%)
11	CLA	B	819	-	63,67,73	1.74	9 (14%)	74,105,113	1.22	9 (12%)
11	CLA	A	832	-	55,59,73	1.83	9 (16%)	64,96,113	1.26	8 (12%)
11	CLA	B	810	-	69,73,73	1.60	9 (13%)	82,113,113	1.01	7 (8%)
13	BCR	M	101	-	41,41,41	0.33	0	56,56,56	0.42	0
13	BCR	A	857	-	25,26,41	0.36	0	32,34,56	0.45	0
11	CLA	A	804	-	63,67,73	1.69	9 (14%)	74,105,113	1.17	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	815	-	69,73,73	1.64	9 (13%)	82,113,113	1.14	9 (10%)
11	CLA	B	826	-	49,53,73	1.90	9 (18%)	58,89,113	1.24	8 (13%)
11	CLA	A	833	-	69,73,73	1.62	9 (13%)	82,113,113	1.06	9 (10%)
11	CLA	A	837	-	55,59,73	1.83	10 (18%)	64,96,113	1.25	9 (14%)
11	CLA	A	818	-	58,62,73	1.74	9 (15%)	68,99,113	1.21	10 (14%)
11	CLA	A	828	-	69,73,73	1.58	9 (13%)	82,113,113	1.13	7 (8%)
11	CLA	A	808	-	58,62,73	1.80	9 (15%)	68,99,113	1.25	9 (13%)
11	CLA	B	832	-	54,58,73	1.85	9 (16%)	64,95,113	1.24	9 (14%)
11	CLA	A	805	-	69,73,73	1.59	9 (13%)	82,113,113	1.20	7 (8%)
11	CLA	A	820	-	45,49,73	2.14	10 (22%)	54,84,113	1.40	9 (16%)
11	CLA	B	808	-	66,70,73	1.63	8 (12%)	78,109,113	1.04	8 (10%)
11	CLA	B	805	-	69,73,73	1.61	9 (13%)	82,113,113	1.05	9 (10%)
11	CLA	B	828	-	69,73,73	1.62	9 (13%)	82,113,113	1.10	8 (9%)
13	BCR	A	845	-	41,41,41	0.35	0	56,56,56	0.63	1 (1%)
11	CLA	B	835	-	69,73,73	1.62	9 (13%)	82,113,113	0.99	8 (9%)
13	BCR	A	854	-	21,21,41	0.39	0	28,28,56	0.51	0
13	BCR	B	842	-	41,41,41	0.21	0	56,56,56	0.39	0
13	BCR	A	852	-	39,40,41	0.32	0	51,53,56	0.92	3 (5%)
11	CLA	A	831	-	53,57,73	1.80	8 (15%)	61,93,113	1.23	8 (13%)
11	CLA	A	809	-	49,53,73	1.96	8 (16%)	58,89,113	1.23	7 (12%)
11	CLA	B	827	-	45,49,73	2.08	9 (20%)	54,84,113	1.40	9 (16%)
11	CLA	A	814	-	45,49,73	2.13	10 (22%)	54,84,113	1.34	7 (12%)
13	BCR	B	841	-	41,41,41	0.27	0	56,56,56	0.46	0
11	CLA	A	841	-	53,57,73	1.85	9 (16%)	61,93,113	1.14	7 (11%)
13	BCR	A	855	-	23,24,41	0.51	0	28,30,56	0.66	1 (3%)
13	BCR	A	858	-	21,21,41	0.30	0	28,28,56	0.64	1 (3%)
13	BCR	A	861	-	41,41,41	0.29	0	56,56,56	0.58	0
13	BCR	F	202	-	41,41,41	0.29	0	56,56,56	1.11	3 (5%)
13	BCR	I	101	-	41,41,41	0.34	0	56,56,56	0.50	0
11	CLA	B	821	-	50,54,73	1.92	10 (20%)	59,90,113	1.24	7 (11%)
13	BCR	A	847	-	41,41,41	0.29	0	56,56,56	0.33	0
11	CLA	B	833	-	69,73,73	1.64	9 (13%)	82,113,113	1.04	6 (7%)
11	CLA	A	836	-	49,53,73	1.92	9 (18%)	58,89,113	1.30	8 (13%)
11	CLA	B	813	-	47,51,73	1.96	9 (19%)	55,86,113	1.29	7 (12%)
12	PQN	B	837	-	34,34,34	0.38	0	43,45,45	0.52	1 (2%)
11	CLA	B	829	-	46,50,73	2.01	8 (17%)	53,85,113	1.26	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	835	-	58,62,73	1.76	9 (15%)	68,99,113	1.09	8 (11%)
13	BCR	B	838	-	41,41,41	0.33	0	56,56,56	0.55	1 (1%)
13	BCR	A	853	-	22,22,41	0.50	0	29,29,56	0.42	0
11	CLA	B	802	-	69,73,73	1.60	9 (13%)	82,113,113	1.03	8 (9%)
11	CLA	A	830	-	69,73,73	1.62	9 (13%)	82,113,113	1.01	8 (9%)
12	PQN	A	843	-	34,34,34	0.38	0	43,45,45	0.56	1 (2%)
11	CLA	B	836	-	47,51,73	1.99	9 (19%)	55,86,113	1.42	8 (14%)
13	BCR	A	846	-	41,41,41	0.31	0	56,56,56	0.40	0
14	LHG	A	850	-	48,48,48	0.70	1 (2%)	51,54,54	1.28	6 (11%)
11	CLA	A	822	-	53,57,73	1.90	8 (15%)	61,93,113	1.25	7 (11%)
11	CLA	A	803	-	46,50,73	1.99	9 (19%)	53,85,113	1.30	9 (16%)
11	CLA	A	826	-	64,68,73	1.69	10 (15%)	76,107,113	1.16	7 (9%)
11	CLA	L	1501	-	38,44,73	2.24	8 (21%)	48,77,113	1.82	11 (22%)
11	CLA	A	806	-	69,73,73	1.63	9 (13%)	82,113,113	1.08	8 (9%)
11	CLA	A	860	-	69,73,73	1.61	9 (13%)	82,113,113	0.95	7 (8%)
11	CLA	A	811	-	69,73,73	1.64	8 (11%)	82,113,113	1.22	10 (12%)
11	CLA	A	823	-	47,51,73	1.94	9 (19%)	55,86,113	1.38	7 (12%)
11	CLA	A	816	-	50,54,73	1.93	10 (20%)	60,89,113	1.38	11 (18%)
13	BCR	A	844	-	41,41,41	0.36	0	56,56,56	0.53	0
14	LHG	A	851	-	26,26,48	0.90	1 (3%)	29,32,54	1.34	3 (10%)
11	CLA	A	817	-	58,62,73	1.77	9 (15%)	68,99,113	1.16	7 (10%)
13	BCR	B	844	-	30,30,41	0.43	0	39,39,56	0.80	2 (5%)
11	CLA	A	810	-	49,53,73	1.88	7 (14%)	58,89,113	1.16	8 (13%)
11	CLA	A	807	-	55,59,73	1.78	8 (14%)	64,96,113	1.21	8 (12%)
11	CLA	A	829	-	69,73,73	1.55	9 (13%)	82,113,113	1.06	9 (10%)
11	CLA	B	801	-	69,73,73	1.59	9 (13%)	82,113,113	1.09	9 (10%)
11	CLA	B	806	-	50,54,73	1.92	9 (18%)	59,90,113	1.21	7 (11%)
11	CLA	B	834	-	51,55,73	1.86	8 (15%)	60,91,113	1.26	9 (15%)
11	CLA	B	817	-	46,51,73	1.99	8 (17%)	53,86,113	1.45	7 (13%)

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
11	CLA	A	813	-	1/1/15/20	12/39/115/115	-
11	CLA	B	809	-	1/1/15/20	5/39/115/115	-
11	CLA	B	811	-	1/1/15/20	11/39/115/115	-
11	CLA	B	814	-	1/1/11/20	5/15/91/115	-
15	SF4	C	102	-	-	-	0/6/5/5
11	CLA	A	824	-	1/1/15/20	7/37/113/115	-
13	BCR	B	840	-	-	4/29/63/63	0/2/2/2
11	CLA	A	859	-	1/1/13/20	8/29/105/115	-
11	CLA	A	812	-	1/1/12/20	3/24/100/115	-
11	CLA	A	840	-	1/1/9/20	2/7/85/115	-
11	CLA	B	823	-	1/1/13/20	8/30/106/115	-
15	SF4	B	804	-	-	-	0/6/5/5
11	CLA	B	824	-	1/1/15/20	4/39/115/115	-
13	BCR	A	856	-	-	9/23/40/63	0/1/1/2
13	BCR	A	848	-	-	2/29/63/63	0/2/2/2
11	CLA	A	827	-	1/1/15/20	12/39/115/115	-
13	BCR	A	849	-	-	10/29/63/63	0/2/2/2
13	BCR	L	1504	-	-	3/29/63/63	0/2/2/2
11	CLA	A	801	-	1/1/13/20	4/33/105/115	-
11	CLA	A	834	-	1/1/15/20	8/39/115/115	-
16	LMG	B	843	-	-	24/50/70/70	0/1/1/1
11	CLA	B	818	-	1/1/13/20	4/27/103/115	-
11	CLA	A	821	-	1/1/15/20	5/39/115/115	-
11	CLA	A	819	-	1/1/15/20	12/39/115/115	-
11	CLA	A	839	-	1/1/11/20	2/20/96/115	-
11	CLA	L	1502	-	1/1/13/20	2/31/107/115	-
11	CLA	B	830	-	1/1/10/20	4/10/86/115	-
11	CLA	L	1503	-	1/1/10/20	2/12/88/115	-
11	CLA	B	820	-	1/1/14/20	7/33/109/115	-
11	CLA	B	812	-	1/1/10/20	2/13/89/115	-
13	BCR	B	839	-	-	4/29/63/63	0/2/2/2
13	BCR	F	201	-	-	12/29/63/63	0/2/2/2
13	BCR	I	102	-	-	4/29/63/63	0/2/2/2
11	CLA	A	838	-	1/1/13/20	2/27/103/115	-
11	CLA	B	807	-	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	825	-	1/1/15/20	12/39/115/115	-
11	CLA	A	842	-	1/1/9/20	2/10/82/115	-
11	CLA	B	803	-	1/1/15/20	9/39/115/115	-
11	CLA	B	822	-	1/1/11/20	9/13/89/115	-
11	CLA	A	802	-	1/1/15/20	4/39/115/115	-
15	SF4	C	101	-	-	-	0/6/5/5
11	CLA	B	831	-	1/1/11/20	5/15/91/115	-
11	CLA	B	816	-	1/1/15/20	7/39/115/115	-
11	CLA	B	825	-	1/1/15/20	5/39/115/115	-
11	CLA	A	815	-	1/1/11/20	5/15/91/115	-
11	CLA	B	819	-	1/1/13/20	5/32/108/115	-
11	CLA	A	832	-	1/1/12/20	5/23/99/115	-
11	CLA	B	810	-	1/1/15/20	7/39/115/115	-
13	BCR	M	101	-	-	2/29/63/63	0/2/2/2
13	BCR	A	857	-	-	0/20/37/63	0/1/1/2
11	CLA	A	804	-	1/1/13/20	6/32/108/115	-
11	CLA	B	815	-	1/1/15/20	10/39/115/115	-
11	CLA	B	826	-	1/1/11/20	2/15/91/115	-
11	CLA	A	833	-	1/1/15/20	3/39/115/115	-
11	CLA	A	837	-	1/1/12/20	5/23/99/115	-
11	CLA	A	818	-	1/1/12/20	8/26/102/115	-
11	CLA	A	828	-	1/1/15/20	5/39/115/115	-
11	CLA	A	808	-	1/1/12/20	7/26/102/115	-
11	CLA	B	832	-	1/1/12/20	4/21/97/115	-
11	CLA	A	805	-	1/1/15/20	10/39/115/115	-
11	CLA	A	820	-	1/1/10/20	4/10/86/115	-
11	CLA	B	808	-	1/1/14/20	6/36/112/115	-
11	CLA	B	805	-	1/1/15/20	6/39/115/115	-
11	CLA	B	828	-	1/1/15/20	4/39/115/115	-
13	BCR	A	845	-	-	2/29/63/63	0/2/2/2
11	CLA	B	835	-	1/1/15/20	5/39/115/115	-
13	BCR	A	854	-	-	0/14/31/63	0/1/1/2
13	BCR	B	842	-	-	3/29/63/63	0/2/2/2
13	BCR	A	852	-	-	14/29/60/63	0/2/2/2
11	CLA	A	831	-	1/1/11/20	4/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	809	-	1/1/11/20	2/15/91/115	-
11	CLA	B	827	-	1/1/10/20	2/10/86/115	-
11	CLA	A	814	-	1/1/10/20	2/10/86/115	-
13	BCR	B	841	-	-	2/29/63/63	0/2/2/2
11	CLA	A	841	-	1/1/11/20	6/20/96/115	-
13	BCR	A	855	-	-	1/18/32/63	0/1/1/2
13	BCR	A	858	-	-	2/14/31/63	0/1/1/2
13	BCR	A	861	-	-	2/29/63/63	0/2/2/2
13	BCR	F	202	-	-	0/29/63/63	0/2/2/2
13	BCR	I	101	-	-	0/29/63/63	0/2/2/2
11	CLA	B	821	-	1/1/11/20	4/17/93/115	-
13	BCR	A	847	-	-	2/29/63/63	0/2/2/2
11	CLA	B	833	-	1/1/15/20	4/39/115/115	-
11	CLA	A	836	-	1/1/11/20	4/15/91/115	-
11	CLA	B	813	-	1/1/10/20	0/13/89/115	-
12	PQN	B	837	-	-	10/23/43/43	0/2/2/2
11	CLA	B	829	-	1/1/10/20	4/12/88/115	-
11	CLA	A	835	-	1/1/12/20	4/26/102/115	-
13	BCR	B	838	-	-	0/29/63/63	0/2/2/2
13	BCR	A	853	-	-	0/15/32/63	0/1/1/2
11	CLA	B	802	-	1/1/15/20	5/39/115/115	-
11	CLA	A	830	-	1/1/15/20	7/39/115/115	-
12	PQN	A	843	-	-	15/23/43/43	0/2/2/2
11	CLA	B	836	-	1/1/10/20	6/13/89/115	-
13	BCR	A	846	-	-	0/29/63/63	0/2/2/2
14	LHG	A	850	-	-	22/53/53/53	-
11	CLA	A	822	-	1/1/11/20	4/20/96/115	-
11	CLA	A	803	-	1/1/10/20	4/12/88/115	-
11	CLA	A	826	-	1/1/14/20	6/33/109/115	-
11	CLA	L	1501	-	1/1/8/20	2/2/74/115	-
11	CLA	A	806	-	1/1/15/20	10/39/115/115	-
11	CLA	A	860	-	1/1/15/20	4/39/115/115	-
11	CLA	A	811	-	1/1/15/20	10/39/115/115	-
11	CLA	A	823	-	1/1/10/20	2/13/89/115	-
11	CLA	A	816	-	1/1/10/20	4/15/87/115	-
13	BCR	A	844	-	-	0/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LHG	A	851	-	-	15/31/31/53	-
11	CLA	A	817	-	1/1/12/20	8/26/102/115	-
13	BCR	B	844	-	-	0/24/41/63	0/1/1/2
11	CLA	A	810	-	1/1/11/20	4/15/91/115	-
11	CLA	A	807	-	1/1/12/20	3/23/99/115	-
11	CLA	A	829	-	1/1/15/20	6/39/115/115	-
11	CLA	B	801	-	1/1/15/20	4/39/115/115	-
11	CLA	B	806	-	1/1/11/20	5/17/93/115	-
11	CLA	B	834	-	1/1/11/20	4/18/94/115	-
11	CLA	B	817	-	1/1/10/20	6/9/87/115	-

All (734) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	812	CLA	C4B-NB	8.11	1.48	1.37
11	A	816	CLA	C4B-NB	7.87	1.48	1.37
11	B	825	CLA	C4B-NB	7.82	1.48	1.37
11	B	832	CLA	C4B-NB	7.81	1.48	1.37
11	A	814	CLA	C4B-NB	7.80	1.48	1.37
11	B	828	CLA	C4B-NB	7.77	1.48	1.37
11	B	806	CLA	C4B-NB	7.75	1.48	1.37
11	L	1502	CLA	C4B-NB	7.71	1.48	1.37
11	A	809	CLA	C4B-NB	7.71	1.48	1.37
11	A	825	CLA	C4B-NB	7.69	1.48	1.37
11	B	819	CLA	C4B-NB	7.63	1.47	1.37
11	B	818	CLA	C4B-NB	7.62	1.47	1.37
11	A	832	CLA	C4B-NB	7.60	1.47	1.37
11	A	808	CLA	C4B-NB	7.59	1.47	1.37
11	A	840	CLA	C4B-NB	7.59	1.47	1.37
11	B	829	CLA	C4B-NB	7.58	1.47	1.37
11	A	830	CLA	C4B-NB	7.53	1.47	1.37
11	A	804	CLA	C4B-NB	7.53	1.47	1.37
11	A	822	CLA	C4B-NB	7.52	1.47	1.37
11	A	803	CLA	C4B-NB	7.52	1.47	1.37
11	A	838	CLA	C4B-NB	7.51	1.47	1.37
11	A	837	CLA	C4B-NB	7.49	1.47	1.37
11	L	1503	CLA	C4B-NB	7.48	1.47	1.37
11	B	827	CLA	C4B-NB	7.47	1.47	1.37
11	A	824	CLA	C4B-NB	7.47	1.47	1.37
11	B	831	CLA	C4B-NB	7.47	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	807	CLA	C4B-NB	7.46	1.47	1.37
11	B	833	CLA	C4B-NB	7.45	1.47	1.37
11	B	826	CLA	C4B-NB	7.44	1.47	1.37
11	L	1501	CLA	C4B-NB	7.43	1.47	1.37
11	B	811	CLA	C4B-NB	7.43	1.47	1.37
11	B	816	CLA	C4B-NB	7.43	1.47	1.37
11	B	812	CLA	C4B-NB	7.41	1.47	1.37
11	B	814	CLA	C4B-NB	7.40	1.47	1.37
11	A	820	CLA	C4B-NB	7.36	1.47	1.37
11	A	815	CLA	C4B-NB	7.36	1.47	1.37
11	B	830	CLA	C4B-NB	7.33	1.47	1.37
11	A	819	CLA	C4B-NB	7.32	1.47	1.37
11	A	836	CLA	C4B-NB	7.32	1.47	1.37
11	B	835	CLA	C4B-NB	7.32	1.47	1.37
11	A	860	CLA	C4B-NB	7.31	1.47	1.37
11	A	842	CLA	C4B-NB	7.31	1.47	1.37
11	A	817	CLA	C4B-NB	7.29	1.47	1.37
11	A	827	CLA	C4B-NB	7.29	1.47	1.37
11	A	818	CLA	C4B-NB	7.29	1.47	1.37
11	B	823	CLA	C4B-NB	7.27	1.47	1.37
11	B	813	CLA	C4B-NB	7.27	1.47	1.37
11	A	813	CLA	C4B-NB	7.25	1.47	1.37
11	A	811	CLA	C4B-NB	7.21	1.47	1.37
11	A	823	CLA	C4B-NB	7.20	1.47	1.37
11	B	815	CLA	C4B-NB	7.20	1.47	1.37
11	A	841	CLA	C4B-NB	7.18	1.47	1.37
11	B	834	CLA	C4B-NB	7.18	1.47	1.37
11	B	803	CLA	C4B-NB	7.17	1.47	1.37
11	A	821	CLA	C4B-NB	7.16	1.47	1.37
11	A	829	CLA	C4B-NB	7.15	1.47	1.37
11	A	806	CLA	C4B-NB	7.14	1.47	1.37
11	B	820	CLA	C4B-NB	7.14	1.47	1.37
11	A	859	CLA	C4B-NB	7.10	1.47	1.37
11	B	801	CLA	C4B-NB	7.08	1.47	1.37
11	A	810	CLA	C4B-NB	7.06	1.47	1.37
11	A	839	CLA	C4B-NB	7.05	1.47	1.37
11	A	833	CLA	C4B-NB	7.03	1.47	1.37
11	B	809	CLA	C4B-NB	7.03	1.47	1.37
11	A	802	CLA	C4B-NB	7.01	1.47	1.37
11	B	808	CLA	C4B-NB	7.00	1.47	1.37
11	B	807	CLA	C4B-NB	6.98	1.47	1.37
11	B	822	CLA	C4B-NB	6.96	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	805	CLA	C4B-NB	6.95	1.47	1.37
11	B	802	CLA	C4B-NB	6.95	1.47	1.37
11	B	817	CLA	C4B-NB	6.92	1.47	1.37
11	B	824	CLA	C4B-NB	6.88	1.46	1.37
11	A	826	CLA	C4B-NB	6.86	1.46	1.37
11	A	835	CLA	C4B-NB	6.85	1.46	1.37
11	A	831	CLA	C4B-NB	6.85	1.46	1.37
11	B	821	CLA	C4B-NB	6.82	1.46	1.37
11	B	810	CLA	C4B-NB	6.79	1.46	1.37
11	A	834	CLA	C4B-NB	6.75	1.46	1.37
11	B	805	CLA	C4B-NB	6.68	1.46	1.37
11	B	836	CLA	C4B-NB	6.67	1.46	1.37
11	A	801	CLA	C4B-NB	6.62	1.46	1.37
11	A	828	CLA	C4B-NB	6.55	1.46	1.37
11	B	805	CLA	MG-NB	-5.71	1.94	2.05
11	B	803	CLA	MG-NB	-5.66	1.94	2.05
11	A	802	CLA	MG-ND	-5.62	1.94	2.05
11	A	802	CLA	MG-NB	-5.60	1.94	2.05
11	B	836	CLA	MG-NB	-5.60	1.94	2.05
11	A	801	CLA	MG-NB	-5.59	1.94	2.05
11	B	805	CLA	MG-ND	-5.57	1.94	2.05
11	A	859	CLA	MG-NB	-5.55	1.94	2.05
11	A	859	CLA	MG-ND	-5.47	1.94	2.05
11	B	822	CLA	MG-NB	-5.47	1.94	2.05
11	B	810	CLA	MG-NB	-5.45	1.95	2.05
11	B	824	CLA	MG-NB	-5.45	1.95	2.05
11	B	811	CLA	MG-ND	-5.45	1.95	2.05
11	B	821	CLA	MG-NB	-5.44	1.95	2.05
11	B	818	CLA	MG-NB	-5.44	1.95	2.05
11	A	821	CLA	MG-NB	-5.43	1.95	2.05
11	L	1502	CLA	MG-NB	-5.43	1.95	2.05
11	A	828	CLA	MG-NB	-5.41	1.95	2.05
11	A	819	CLA	MG-NB	-5.39	1.95	2.05
11	B	815	CLA	MG-NB	-5.38	1.95	2.05
11	A	806	CLA	MG-ND	-5.37	1.95	2.05
11	B	822	CLA	MG-ND	-5.37	1.95	2.05
11	B	811	CLA	MG-NB	-5.36	1.95	2.05
11	A	805	CLA	MG-NB	-5.36	1.95	2.05
11	B	817	CLA	MG-NB	-5.34	1.95	2.05
11	B	820	CLA	MG-NB	-5.33	1.95	2.05
11	A	833	CLA	MG-NB	-5.30	1.95	2.05
11	B	823	CLA	MG-NB	-5.29	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	829	CLA	MG-NB	-5.28	1.95	2.05
11	B	830	CLA	MG-NB	-5.28	1.95	2.05
11	A	806	CLA	MG-NB	-5.26	1.95	2.05
11	A	811	CLA	MG-NB	-5.26	1.95	2.05
11	B	812	CLA	MG-NB	-5.26	1.95	2.05
11	B	808	CLA	MG-ND	-5.25	1.95	2.05
11	A	801	CLA	MG-ND	-5.25	1.95	2.05
11	B	821	CLA	MG-ND	-5.25	1.95	2.05
11	B	817	CLA	MG-ND	-5.23	1.95	2.05
11	A	823	CLA	MG-NB	-5.23	1.95	2.05
11	B	826	CLA	MG-NB	-5.23	1.95	2.05
11	B	818	CLA	MG-ND	-5.23	1.95	2.05
11	B	807	CLA	MG-NB	-5.22	1.95	2.05
11	A	808	CLA	MG-NB	-5.22	1.95	2.05
11	B	836	CLA	MG-ND	-5.21	1.95	2.05
11	A	822	CLA	MG-NB	-5.21	1.95	2.05
11	B	814	CLA	MG-NB	-5.21	1.95	2.05
11	A	835	CLA	MG-NB	-5.20	1.95	2.05
11	A	840	CLA	MG-NB	-5.19	1.95	2.05
11	L	1503	CLA	MG-NB	-5.19	1.95	2.05
11	A	831	CLA	MG-NB	-5.18	1.95	2.05
11	A	826	CLA	MG-NB	-5.18	1.95	2.05
11	B	824	CLA	MG-ND	-5.18	1.95	2.05
11	A	808	CLA	MG-ND	-5.18	1.95	2.05
11	B	827	CLA	MG-NB	-5.16	1.95	2.05
11	B	835	CLA	MG-NB	-5.16	1.95	2.05
11	A	814	CLA	MG-NB	-5.16	1.95	2.05
11	A	831	CLA	MG-ND	-5.16	1.95	2.05
11	A	820	CLA	MG-NB	-5.15	1.95	2.05
11	A	835	CLA	MG-ND	-5.14	1.95	2.05
11	L	1501	CLA	MG-NB	-5.13	1.95	2.05
11	A	830	CLA	MG-NB	-5.13	1.95	2.05
11	B	819	CLA	MG-NB	-5.13	1.95	2.05
11	A	860	CLA	MG-ND	-5.12	1.95	2.05
11	B	803	CLA	MG-ND	-5.12	1.95	2.05
11	A	838	CLA	MG-NB	-5.10	1.95	2.05
11	A	842	CLA	MG-NB	-5.10	1.95	2.05
11	B	808	CLA	MG-NB	-5.10	1.95	2.05
11	A	818	CLA	MG-NB	-5.09	1.95	2.05
11	A	811	CLA	MG-ND	-5.09	1.95	2.05
11	B	823	CLA	MG-ND	-5.08	1.95	2.05
11	A	803	CLA	MG-NB	-5.08	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	819	CLA	MG-ND	-5.08	1.95	2.05
11	A	837	CLA	MG-NB	-5.08	1.95	2.05
11	B	834	CLA	MG-NB	-5.07	1.95	2.05
11	A	825	CLA	MG-ND	-5.07	1.95	2.05
11	L	1501	CLA	MG-ND	-5.05	1.95	2.05
11	A	827	CLA	MG-ND	-5.05	1.95	2.05
11	B	810	CLA	MG-ND	-5.05	1.95	2.05
11	A	837	CLA	MG-ND	-5.05	1.95	2.05
11	L	1502	CLA	MG-ND	-5.05	1.95	2.05
11	B	809	CLA	MG-NB	-5.05	1.95	2.05
11	A	804	CLA	MG-NB	-5.05	1.95	2.05
11	B	802	CLA	MG-NB	-5.04	1.95	2.05
11	B	834	CLA	MG-ND	-5.04	1.95	2.05
11	A	828	CLA	MG-ND	-5.04	1.95	2.05
11	A	819	CLA	MG-ND	-5.04	1.95	2.05
11	A	832	CLA	MG-NB	-5.04	1.95	2.05
11	A	809	CLA	MG-ND	-5.04	1.95	2.05
11	A	817	CLA	MG-NB	-5.03	1.95	2.05
11	B	812	CLA	MG-ND	-5.03	1.95	2.05
11	B	813	CLA	MG-NB	-5.02	1.95	2.05
11	A	834	CLA	MG-NB	-5.02	1.95	2.05
11	A	836	CLA	MG-NB	-5.01	1.95	2.05
11	A	833	CLA	MG-ND	-5.01	1.95	2.05
11	A	834	CLA	MG-ND	-5.00	1.95	2.05
11	A	824	CLA	MG-NB	-5.00	1.95	2.05
11	B	816	CLA	MG-ND	-5.00	1.95	2.05
11	A	832	CLA	MG-ND	-5.00	1.95	2.05
11	A	839	CLA	MG-ND	-5.00	1.95	2.05
11	A	812	CLA	MG-ND	-4.99	1.95	2.05
11	A	817	CLA	MG-ND	-4.99	1.95	2.05
11	A	810	CLA	MG-NB	-4.99	1.95	2.05
11	A	826	CLA	MG-ND	-4.99	1.95	2.05
11	B	833	CLA	MG-NB	-4.99	1.95	2.05
11	A	813	CLA	MG-NB	-4.98	1.95	2.05
11	B	825	CLA	MG-NB	-4.97	1.95	2.05
11	A	841	CLA	MG-NB	-4.97	1.95	2.05
11	A	860	CLA	MG-NB	-4.97	1.95	2.05
11	A	842	CLA	MG-ND	-4.97	1.95	2.05
11	A	823	CLA	MG-ND	-4.97	1.95	2.05
11	B	826	CLA	MG-ND	-4.96	1.95	2.05
11	A	813	CLA	MG-ND	-4.96	1.95	2.05
11	B	832	CLA	MG-NB	-4.96	1.95	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	821	CLA	MG-ND	-4.96	1.96	2.05
11	B	820	CLA	MG-ND	-4.95	1.96	2.05
11	B	814	CLA	MG-ND	-4.95	1.96	2.05
11	A	822	CLA	MG-ND	-4.95	1.96	2.05
11	B	825	CLA	MG-ND	-4.93	1.96	2.05
11	A	809	CLA	MG-NB	-4.92	1.96	2.05
11	B	835	CLA	MG-ND	-4.92	1.96	2.05
11	B	809	CLA	MG-ND	-4.91	1.96	2.05
11	B	806	CLA	MG-NB	-4.91	1.96	2.05
11	A	820	CLA	MG-ND	-4.91	1.96	2.05
11	A	818	CLA	MG-ND	-4.90	1.96	2.05
11	A	814	CLA	C3A-C2A	-4.90	1.50	1.54
11	B	813	CLA	MG-ND	-4.90	1.96	2.05
11	A	814	CLA	MG-ND	-4.88	1.96	2.05
11	B	833	CLA	MG-ND	-4.88	1.96	2.05
11	B	832	CLA	MG-ND	-4.88	1.96	2.05
11	B	827	CLA	MG-ND	-4.88	1.96	2.05
11	A	830	CLA	MG-ND	-4.87	1.96	2.05
11	B	831	CLA	MG-ND	-4.87	1.96	2.05
11	A	836	CLA	MG-ND	-4.86	1.96	2.05
11	B	830	CLA	MG-ND	-4.86	1.96	2.05
11	A	839	CLA	MG-NB	-4.85	1.96	2.05
11	L	1503	CLA	MG-ND	-4.84	1.96	2.05
11	A	838	CLA	MG-ND	-4.84	1.96	2.05
11	A	805	CLA	MG-ND	-4.83	1.96	2.05
11	A	816	CLA	MG-ND	-4.83	1.96	2.05
11	A	841	CLA	MG-ND	-4.83	1.96	2.05
11	B	831	CLA	MG-NB	-4.83	1.96	2.05
11	A	815	CLA	MG-NB	-4.83	1.96	2.05
11	A	824	CLA	MG-ND	-4.82	1.96	2.05
11	B	801	CLA	MG-NB	-4.82	1.96	2.05
11	A	840	CLA	MG-ND	-4.81	1.96	2.05
11	B	828	CLA	MG-ND	-4.81	1.96	2.05
11	B	807	CLA	MG-ND	-4.80	1.96	2.05
11	B	815	CLA	MG-ND	-4.80	1.96	2.05
11	L	1502	CLA	MG-NA	-4.80	1.94	2.06
11	A	807	CLA	MG-NB	-4.79	1.96	2.05
11	A	803	CLA	MG-ND	-4.78	1.96	2.05
11	B	802	CLA	MG-ND	-4.78	1.96	2.05
11	B	829	CLA	MG-ND	-4.78	1.96	2.05
11	A	810	CLA	MG-ND	-4.77	1.96	2.05
11	B	816	CLA	MG-NB	-4.77	1.96	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	829	CLA	MG-ND	-4.77	1.96	2.05
11	B	801	CLA	MG-ND	-4.77	1.96	2.05
11	A	807	CLA	MG-ND	-4.76	1.96	2.05
11	A	812	CLA	MG-NB	-4.76	1.96	2.05
11	A	815	CLA	MG-ND	-4.76	1.96	2.05
11	B	828	CLA	MG-NB	-4.76	1.96	2.05
11	A	829	CLA	MG-NB	-4.75	1.96	2.05
11	A	827	CLA	MG-NB	-4.74	1.96	2.05
11	A	820	CLA	C3A-C2A	-4.70	1.50	1.54
11	A	804	CLA	MG-ND	-4.68	1.96	2.05
11	L	1501	CLA	MG-NA	-4.63	1.95	2.06
11	B	836	CLA	MG-NA	-4.62	1.95	2.06
11	B	827	CLA	C3A-C2A	-4.61	1.50	1.54
11	B	814	CLA	MG-NA	-4.57	1.95	2.06
11	A	825	CLA	MG-NB	-4.57	1.96	2.05
11	A	811	CLA	MG-NA	-4.57	1.95	2.06
11	B	806	CLA	MG-ND	-4.53	1.96	2.05
11	L	1503	CLA	MG-NA	-4.52	1.95	2.06
11	B	801	CLA	MG-NA	-4.47	1.95	2.06
11	A	826	CLA	MG-NA	-4.47	1.95	2.06
11	B	820	CLA	MG-NA	-4.46	1.95	2.06
11	B	830	CLA	MG-NA	-4.46	1.95	2.06
11	A	828	CLA	MG-NA	-4.46	1.95	2.06
11	A	816	CLA	MG-NB	-4.45	1.97	2.05
11	A	804	CLA	MG-NA	-4.43	1.95	2.06
11	B	813	CLA	MG-NA	-4.42	1.95	2.06
11	A	822	CLA	MG-NA	-4.41	1.95	2.06
11	B	806	CLA	MG-NA	-4.41	1.95	2.06
11	B	803	CLA	MG-NA	-4.39	1.95	2.06
11	B	817	CLA	MG-NA	-4.39	1.95	2.06
11	A	808	CLA	MG-NA	-4.37	1.95	2.06
11	B	810	CLA	MG-NA	-4.35	1.95	2.06
11	A	819	CLA	MG-NA	-4.34	1.96	2.06
11	A	840	CLA	MG-NA	-4.33	1.96	2.06
11	A	836	CLA	MG-NA	-4.32	1.96	2.06
11	B	802	CLA	MG-NA	-4.31	1.96	2.06
11	A	803	CLA	MG-NA	-4.29	1.96	2.06
11	B	833	CLA	MG-NA	-4.29	1.96	2.06
11	B	829	CLA	MG-NA	-4.28	1.96	2.06
11	B	824	CLA	MG-NA	-4.27	1.96	2.06
11	B	818	CLA	MG-NA	-4.27	1.96	2.06
11	B	822	CLA	MG-NA	-4.23	1.96	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	807	CLA	MG-NA	-4.22	1.96	2.06
11	B	819	CLA	MG-NA	-4.22	1.96	2.06
11	B	830	CLA	C3A-C2A	-4.22	1.50	1.54
11	A	810	CLA	MG-NA	-4.21	1.96	2.06
11	A	835	CLA	MG-NA	-4.21	1.96	2.06
11	A	823	CLA	MG-NA	-4.21	1.96	2.06
11	A	834	CLA	MG-NA	-4.20	1.96	2.06
11	A	821	CLA	MG-NA	-4.19	1.96	2.06
11	B	821	CLA	MG-NA	-4.19	1.96	2.06
11	A	820	CLA	MG-NA	-4.19	1.96	2.06
11	A	833	CLA	MG-NA	-4.17	1.96	2.06
11	A	805	CLA	MG-NA	-4.16	1.96	2.06
11	A	817	CLA	MG-NA	-4.16	1.96	2.06
11	A	841	CLA	MG-NA	-4.15	1.96	2.06
11	A	842	CLA	MG-NA	-4.14	1.96	2.06
11	A	806	CLA	MG-NA	-4.13	1.96	2.06
11	A	827	CLA	MG-NA	-4.13	1.96	2.06
11	A	838	CLA	MG-NA	-4.11	1.96	2.06
11	A	830	CLA	MG-NA	-4.09	1.96	2.06
11	B	809	CLA	MG-NA	-4.08	1.96	2.06
11	A	815	CLA	MG-NA	-4.06	1.96	2.06
11	A	814	CLA	MG-NA	-4.04	1.96	2.06
11	B	823	CLA	MG-NA	-4.04	1.96	2.06
11	B	812	CLA	MG-NA	-4.02	1.96	2.06
11	B	827	CLA	MG-NA	-4.02	1.96	2.06
11	B	815	CLA	MG-NA	-4.01	1.96	2.06
11	A	832	CLA	MG-NA	-4.01	1.96	2.06
11	A	842	CLA	C1D-ND	4.00	1.43	1.37
11	A	860	CLA	MG-NA	-4.00	1.96	2.06
11	B	830	CLA	MG-NC	-3.98	1.96	2.06
11	B	835	CLA	MG-NA	-3.94	1.96	2.06
11	B	808	CLA	MG-NA	-3.93	1.96	2.06
11	L	1501	CLA	MG-NC	-3.93	1.96	2.06
11	B	814	CLA	MG-NC	-3.93	1.96	2.06
11	B	817	CLA	MG-NC	-3.92	1.97	2.06
11	A	807	CLA	MG-NA	-3.91	1.97	2.06
11	B	834	CLA	MG-NA	-3.89	1.97	2.06
11	L	1502	CLA	MG-NC	-3.89	1.97	2.06
11	B	813	CLA	MG-NC	-3.88	1.97	2.06
11	A	801	CLA	MG-NA	-3.88	1.97	2.06
11	B	805	CLA	MG-NA	-3.88	1.97	2.06
11	B	825	CLA	MG-NA	-3.86	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	826	CLA	MG-NC	-3.85	1.97	2.06
11	A	839	CLA	MG-NA	-3.82	1.97	2.06
11	B	801	CLA	MG-NC	-3.80	1.97	2.06
11	A	822	CLA	MG-NC	-3.80	1.97	2.06
11	A	812	CLA	MG-NA	-3.79	1.97	2.06
11	A	809	CLA	MG-NA	-3.78	1.97	2.06
11	B	821	CLA	MG-NC	-3.78	1.97	2.06
11	L	1503	CLA	MG-NC	-3.77	1.97	2.06
11	B	836	CLA	MG-NC	-3.77	1.97	2.06
11	A	837	CLA	MG-NA	-3.76	1.97	2.06
11	B	829	CLA	MG-NC	-3.76	1.97	2.06
11	A	824	CLA	MG-NA	-3.75	1.97	2.06
11	B	828	CLA	MG-NA	-3.74	1.97	2.06
11	A	825	CLA	C1D-ND	3.73	1.42	1.37
11	B	833	CLA	MG-NC	-3.73	1.97	2.06
11	A	840	CLA	MG-NC	-3.73	1.97	2.06
11	B	832	CLA	MG-NA	-3.73	1.97	2.06
11	B	802	CLA	MG-NC	-3.73	1.97	2.06
11	A	811	CLA	MG-NC	-3.71	1.97	2.06
11	A	829	CLA	MG-NA	-3.70	1.97	2.06
11	B	816	CLA	C1D-ND	3.69	1.42	1.37
11	A	813	CLA	C1D-ND	3.69	1.42	1.37
11	B	826	CLA	MG-NA	-3.68	1.97	2.06
11	B	831	CLA	MG-NA	-3.68	1.97	2.06
11	A	835	CLA	MG-NC	-3.68	1.97	2.06
11	A	818	CLA	MG-NA	-3.67	1.97	2.06
11	B	803	CLA	MG-NC	-3.67	1.97	2.06
11	B	818	CLA	MG-NC	-3.67	1.97	2.06
11	A	817	CLA	MG-NC	-3.66	1.97	2.06
11	B	811	CLA	MG-NA	-3.65	1.97	2.06
11	A	825	CLA	MG-NA	-3.65	1.97	2.06
11	B	831	CLA	C1D-ND	3.65	1.42	1.37
11	A	815	CLA	MG-NC	-3.65	1.97	2.06
11	A	803	CLA	MG-NC	-3.64	1.97	2.06
11	A	831	CLA	MG-NA	-3.63	1.97	2.06
11	A	810	CLA	MG-NC	-3.63	1.97	2.06
11	B	812	CLA	MG-NC	-3.62	1.97	2.06
11	A	841	CLA	MG-NC	-3.60	1.97	2.06
11	L	1501	CLA	C1D-ND	3.60	1.42	1.37
11	A	816	CLA	MG-NA	-3.60	1.97	2.06
11	B	816	CLA	MG-NA	-3.59	1.97	2.06
11	B	834	CLA	MG-NC	-3.59	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	820	CLA	MG-NC	-3.59	1.97	2.06
11	A	820	CLA	MG-NC	-3.58	1.97	2.06
11	B	827	CLA	MG-NC	-3.56	1.97	2.06
11	B	828	CLA	C1D-ND	3.56	1.42	1.37
11	A	836	CLA	MG-NC	-3.56	1.97	2.06
11	A	812	CLA	MG-NC	-3.56	1.97	2.06
11	B	806	CLA	MG-NC	-3.55	1.97	2.06
11	B	809	CLA	MG-NC	-3.55	1.97	2.06
11	A	809	CLA	MG-NC	-3.55	1.97	2.06
11	A	823	CLA	MG-NC	-3.54	1.97	2.06
11	A	840	CLA	O1D-CGD	3.54	1.33	1.20
11	B	810	CLA	MG-NC	-3.54	1.97	2.06
11	A	808	CLA	MG-NC	-3.54	1.97	2.06
11	A	834	CLA	MG-NC	-3.54	1.97	2.06
11	B	835	CLA	C1D-ND	3.53	1.42	1.37
11	A	828	CLA	MG-NC	-3.53	1.97	2.06
11	A	805	CLA	MG-NC	-3.52	1.97	2.06
11	A	809	CLA	C1D-ND	3.52	1.42	1.37
11	B	807	CLA	MG-NC	-3.51	1.97	2.06
11	A	812	CLA	C1D-ND	3.51	1.42	1.37
11	A	838	CLA	MG-NC	-3.50	1.98	2.06
11	A	837	CLA	MG-NC	-3.50	1.98	2.06
11	A	804	CLA	MG-NC	-3.49	1.98	2.06
11	B	825	CLA	C1D-ND	3.49	1.42	1.37
11	B	829	CLA	C1D-ND	3.49	1.42	1.37
11	A	819	CLA	MG-NC	-3.48	1.98	2.06
11	A	841	CLA	C1D-ND	3.47	1.42	1.37
11	A	827	CLA	C1D-ND	3.47	1.42	1.37
11	A	859	CLA	MG-NA	-3.47	1.98	2.06
11	A	832	CLA	MG-NC	-3.44	1.98	2.06
11	A	802	CLA	MG-NA	-3.43	1.98	2.06
11	L	1503	CLA	C1D-ND	3.43	1.42	1.37
11	A	842	CLA	MG-NC	-3.42	1.98	2.06
11	B	835	CLA	MG-NC	-3.42	1.98	2.06
11	A	816	CLA	C1D-ND	3.42	1.42	1.37
11	B	819	CLA	MG-NC	-3.42	1.98	2.06
11	B	819	CLA	C1D-ND	3.40	1.42	1.37
11	B	824	CLA	MG-NC	-3.40	1.98	2.06
11	B	815	CLA	MG-NC	-3.40	1.98	2.06
11	B	815	CLA	C1D-ND	3.40	1.42	1.37
11	B	806	CLA	C1D-ND	3.39	1.42	1.37
11	A	816	CLA	MG-NC	-3.38	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	812	CLA	C1D-ND	3.37	1.42	1.37
11	A	820	CLA	C1D-ND	3.37	1.42	1.37
11	A	860	CLA	MG-NC	-3.37	1.98	2.06
11	B	814	CLA	C1D-ND	3.37	1.42	1.37
11	B	822	CLA	MG-NC	-3.36	1.98	2.06
11	A	830	CLA	MG-NC	-3.36	1.98	2.06
11	A	813	CLA	MG-NA	-3.36	1.98	2.06
11	A	825	CLA	MG-NC	-3.36	1.98	2.06
11	B	832	CLA	C1D-ND	3.35	1.42	1.37
11	A	821	CLA	MG-NC	-3.35	1.98	2.06
11	A	824	CLA	C1D-ND	3.35	1.42	1.37
11	B	828	CLA	MG-NC	-3.34	1.98	2.06
11	B	830	CLA	C1D-ND	3.34	1.42	1.37
11	A	827	CLA	MG-NC	-3.33	1.98	2.06
11	A	807	CLA	MG-NC	-3.33	1.98	2.06
11	B	825	CLA	MG-NC	-3.30	1.98	2.06
11	B	808	CLA	MG-NC	-3.30	1.98	2.06
11	A	813	CLA	MG-NC	-3.30	1.98	2.06
11	B	823	CLA	MG-NC	-3.29	1.98	2.06
11	A	807	CLA	C1D-ND	3.29	1.42	1.37
11	A	824	CLA	MG-NC	-3.28	1.98	2.06
11	A	833	CLA	MG-NC	-3.28	1.98	2.06
11	B	803	CLA	C1D-ND	3.28	1.42	1.37
11	A	831	CLA	C1D-ND	3.25	1.42	1.37
11	B	826	CLA	MG-NC	-3.25	1.98	2.06
11	A	831	CLA	MG-NC	-3.24	1.98	2.06
11	A	814	CLA	MG-NC	-3.24	1.98	2.06
11	A	801	CLA	MG-NC	-3.23	1.98	2.06
11	A	839	CLA	MG-NC	-3.22	1.98	2.06
11	A	832	CLA	C1D-ND	3.22	1.42	1.37
11	A	806	CLA	MG-NC	-3.22	1.98	2.06
11	A	822	CLA	C1D-ND	3.21	1.42	1.37
11	A	837	CLA	C1D-ND	3.20	1.42	1.37
11	A	818	CLA	MG-NC	-3.20	1.98	2.06
11	B	822	CLA	C1D-ND	3.19	1.42	1.37
11	A	834	CLA	C1D-ND	3.18	1.42	1.37
11	B	805	CLA	MG-NC	-3.17	1.98	2.06
11	B	833	CLA	C1D-ND	3.16	1.42	1.37
11	B	826	CLA	C1D-ND	3.16	1.42	1.37
11	B	832	CLA	MG-NC	-3.16	1.98	2.06
11	A	817	CLA	C1D-ND	3.15	1.42	1.37
11	B	824	CLA	C1D-ND	3.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	815	CLA	C1D-ND	3.13	1.42	1.37
11	A	802	CLA	MG-NC	-3.13	1.98	2.06
11	B	831	CLA	MG-NC	-3.12	1.98	2.06
11	B	802	CLA	C1D-ND	3.10	1.41	1.37
11	B	811	CLA	MG-NC	-3.09	1.98	2.06
11	A	818	CLA	C1D-ND	3.09	1.41	1.37
11	A	805	CLA	C1D-ND	3.08	1.41	1.37
11	A	842	CLA	C1B-NB	3.07	1.41	1.37
11	A	839	CLA	C1D-ND	3.07	1.41	1.37
11	A	803	CLA	C1D-ND	3.06	1.41	1.37
11	A	829	CLA	MG-NC	-3.06	1.99	2.06
11	B	836	CLA	C1D-ND	3.05	1.41	1.37
11	A	835	CLA	C1D-ND	3.05	1.41	1.37
11	A	833	CLA	C1D-ND	3.05	1.41	1.37
11	A	806	CLA	C1D-ND	3.04	1.41	1.37
11	A	814	CLA	C1D-ND	3.04	1.41	1.37
11	B	816	CLA	MG-NC	-3.03	1.99	2.06
11	A	830	CLA	C1D-ND	3.02	1.41	1.37
11	B	818	CLA	C1D-ND	3.01	1.41	1.37
11	A	829	CLA	C1D-ND	3.00	1.41	1.37
11	L	1501	CLA	C1B-NB	2.94	1.41	1.37
11	A	840	CLA	C1D-ND	2.94	1.41	1.37
11	A	823	CLA	C1D-ND	2.94	1.41	1.37
11	A	811	CLA	C1D-ND	2.94	1.41	1.37
11	B	813	CLA	C1D-ND	2.93	1.41	1.37
14	A	850	LHG	O7-C5	-2.88	1.39	1.46
11	A	810	CLA	C1D-ND	2.86	1.41	1.37
11	A	801	CLA	C4D-CHA	-2.86	1.34	1.43
11	B	834	CLA	C1D-ND	2.85	1.41	1.37
11	A	859	CLA	MG-NC	-2.83	1.99	2.06
11	A	820	CLA	C1B-NB	2.83	1.41	1.37
11	A	838	CLA	C1D-ND	2.82	1.41	1.37
11	B	809	CLA	C1D-ND	2.82	1.41	1.37
11	A	804	CLA	C1D-ND	2.81	1.41	1.37
11	B	814	CLA	C1B-NB	2.81	1.41	1.37
11	L	1502	CLA	C1D-ND	2.80	1.41	1.37
11	A	821	CLA	C1D-ND	2.79	1.41	1.37
11	B	827	CLA	C1D-ND	2.79	1.41	1.37
11	B	812	CLA	C1B-NB	2.77	1.41	1.37
11	L	1503	CLA	C1B-NB	2.76	1.41	1.37
11	B	807	CLA	C1D-ND	2.76	1.41	1.37
11	B	805	CLA	C1D-C2D	-2.76	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	826	CLA	C1D-ND	2.74	1.41	1.37
11	A	822	CLA	C1B-NB	2.74	1.41	1.37
11	B	808	CLA	C1D-ND	2.73	1.41	1.37
11	L	1502	CLA	C1B-NB	2.72	1.41	1.37
11	A	860	CLA	C1D-C2D	-2.72	1.40	1.45
11	B	815	CLA	C1B-NB	2.70	1.41	1.37
11	B	810	CLA	C1D-C2D	-2.69	1.40	1.45
11	B	829	CLA	C1B-NB	2.69	1.41	1.37
11	A	801	CLA	C1D-ND	2.69	1.41	1.37
11	A	813	CLA	C1B-NB	2.68	1.41	1.37
11	A	836	CLA	C1D-ND	2.68	1.41	1.37
11	B	821	CLA	C1D-ND	2.67	1.41	1.37
11	B	811	CLA	C1D-ND	2.66	1.41	1.37
11	A	816	CLA	C1D-C2D	-2.64	1.40	1.45
11	A	825	CLA	C1D-C2D	-2.63	1.40	1.45
11	B	833	CLA	C1B-NB	2.61	1.41	1.37
11	A	809	CLA	C1D-C2D	-2.61	1.40	1.45
11	A	841	CLA	C1B-NB	2.61	1.41	1.37
11	B	818	CLA	C1B-NB	2.59	1.41	1.37
11	B	817	CLA	C1D-ND	2.59	1.41	1.37
11	A	829	CLA	C1D-C2D	-2.59	1.40	1.45
11	A	827	CLA	C1D-C2D	-2.58	1.40	1.45
11	B	808	CLA	C1D-C2D	-2.58	1.40	1.45
11	A	828	CLA	C1D-ND	2.58	1.41	1.37
11	A	808	CLA	C1D-ND	2.58	1.41	1.37
11	A	806	CLA	C1D-C2D	-2.57	1.40	1.45
11	B	836	CLA	C1D-C2D	-2.57	1.40	1.45
11	B	832	CLA	C1D-C2D	-2.57	1.40	1.45
11	B	823	CLA	C1D-ND	2.57	1.41	1.37
11	A	810	CLA	C1D-C2D	-2.56	1.40	1.45
11	B	801	CLA	C1D-ND	2.56	1.41	1.37
11	A	812	CLA	C1D-C2D	-2.56	1.40	1.45
11	B	824	CLA	C1D-C2D	-2.55	1.40	1.45
11	A	859	CLA	C1D-ND	2.55	1.41	1.37
11	A	828	CLA	C1D-C2D	-2.55	1.40	1.45
11	A	837	CLA	C1D-C2D	-2.55	1.40	1.45
11	A	819	CLA	C1D-C2D	-2.55	1.40	1.45
11	A	830	CLA	C1D-C2D	-2.54	1.40	1.45
11	A	831	CLA	C1D-C2D	-2.54	1.40	1.45
11	A	839	CLA	C1D-C2D	-2.54	1.40	1.45
11	B	825	CLA	C1D-C2D	-2.53	1.40	1.45
11	A	860	CLA	C1D-ND	2.53	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	808	CLA	C1D-C2D	-2.53	1.40	1.45
11	A	838	CLA	C1D-C2D	-2.53	1.40	1.45
11	A	801	CLA	C1D-C2D	-2.53	1.40	1.45
11	B	835	CLA	C1D-C2D	-2.52	1.40	1.45
14	A	851	LHG	O7-C5	-2.52	1.40	1.46
11	A	835	CLA	C1D-C2D	-2.52	1.40	1.45
11	B	821	CLA	C1D-C2D	-2.52	1.40	1.45
11	B	801	CLA	C1D-C2D	-2.52	1.40	1.45
11	B	811	CLA	C1D-C2D	-2.51	1.40	1.45
11	A	833	CLA	C1D-C2D	-2.51	1.40	1.45
11	B	819	CLA	C1B-NB	2.51	1.41	1.37
11	A	815	CLA	C1D-C2D	-2.50	1.40	1.45
11	B	802	CLA	C1D-C2D	-2.50	1.40	1.45
11	A	807	CLA	C1D-C2D	-2.50	1.40	1.45
11	B	828	CLA	C1D-C2D	-2.50	1.40	1.45
11	B	826	CLA	C1B-NB	2.49	1.41	1.37
11	A	859	CLA	C1D-C2D	-2.49	1.40	1.45
11	A	812	CLA	C1B-NB	2.49	1.41	1.37
11	B	831	CLA	C1B-NB	2.49	1.41	1.37
11	A	822	CLA	C1D-C2D	-2.49	1.40	1.45
11	B	805	CLA	C3A-C2A	-2.49	1.47	1.54
11	A	824	CLA	C1D-C2D	-2.49	1.40	1.45
11	L	1502	CLA	C1D-C2D	-2.48	1.40	1.45
11	B	823	CLA	C1D-C2D	-2.48	1.40	1.45
11	A	836	CLA	C1D-C2D	-2.48	1.40	1.45
11	A	818	CLA	C1D-C2D	-2.48	1.40	1.45
11	B	803	CLA	C1D-C2D	-2.48	1.40	1.45
11	B	815	CLA	C1D-C2D	-2.48	1.40	1.45
11	B	816	CLA	C1D-C2D	-2.47	1.40	1.45
11	A	811	CLA	C1D-C2D	-2.47	1.40	1.45
11	A	813	CLA	C1D-C2D	-2.47	1.40	1.45
11	A	804	CLA	C1D-C2D	-2.46	1.40	1.45
11	B	812	CLA	C1D-C2D	-2.46	1.40	1.45
11	A	803	CLA	C1D-C2D	-2.46	1.40	1.45
11	B	806	CLA	C1B-NB	2.46	1.41	1.37
11	B	820	CLA	C1D-C2D	-2.46	1.40	1.45
11	B	834	CLA	C1D-C2D	-2.46	1.40	1.45
11	A	842	CLA	C1D-C2D	-2.45	1.40	1.45
11	A	826	CLA	C1D-C2D	-2.45	1.40	1.45
11	B	818	CLA	C1D-C2D	-2.45	1.40	1.45
11	B	822	CLA	C1D-C2D	-2.45	1.40	1.45
11	B	831	CLA	C1D-C2D	-2.45	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	807	CLA	C1D-C2D	-2.45	1.40	1.45
11	A	841	CLA	C1D-C2D	-2.45	1.40	1.45
11	A	815	CLA	C1B-NB	2.44	1.41	1.37
11	B	813	CLA	C1B-NB	2.43	1.41	1.37
11	A	805	CLA	C1D-C2D	-2.43	1.40	1.45
11	B	816	CLA	C1B-NB	2.43	1.41	1.37
11	B	809	CLA	C1D-C2D	-2.42	1.40	1.45
11	A	834	CLA	C1D-C2D	-2.42	1.40	1.45
11	A	802	CLA	C1D-C2D	-2.42	1.40	1.45
11	A	820	CLA	C1D-C2D	-2.42	1.40	1.45
16	B	843	LMG	O7-C8	-2.41	1.40	1.46
11	A	819	CLA	C1D-ND	2.40	1.41	1.37
11	A	836	CLA	C1B-NB	2.40	1.41	1.37
11	B	829	CLA	C1D-C2D	-2.38	1.40	1.45
11	B	817	CLA	C1D-C2D	-2.38	1.40	1.45
11	A	817	CLA	C1D-C2D	-2.38	1.40	1.45
11	A	821	CLA	C1D-C2D	-2.38	1.40	1.45
11	A	832	CLA	C1B-NB	2.38	1.41	1.37
11	A	803	CLA	C1B-NB	2.38	1.41	1.37
11	A	859	CLA	C3D-C4D	-2.37	1.38	1.44
11	B	830	CLA	C1D-C2D	-2.36	1.40	1.45
11	A	814	CLA	C1B-NB	2.36	1.41	1.37
11	B	827	CLA	C1D-C2D	-2.36	1.40	1.45
11	A	818	CLA	C1B-NB	2.36	1.41	1.37
11	A	840	CLA	C1D-C2D	-2.36	1.40	1.45
11	A	832	CLA	C1D-C2D	-2.36	1.40	1.45
11	B	806	CLA	C1D-C2D	-2.36	1.40	1.45
11	A	814	CLA	C1D-C2D	-2.36	1.40	1.45
11	A	835	CLA	C1B-NB	2.34	1.40	1.37
11	A	806	CLA	C3A-C2A	-2.33	1.48	1.54
11	A	833	CLA	C3A-C2A	-2.33	1.48	1.54
11	B	813	CLA	C1D-C2D	-2.33	1.40	1.45
11	B	826	CLA	C1D-C2D	-2.33	1.40	1.45
11	L	1503	CLA	C1D-C2D	-2.32	1.40	1.45
11	B	825	CLA	C1B-NB	2.32	1.40	1.37
11	B	833	CLA	C1D-C2D	-2.32	1.40	1.45
11	B	802	CLA	C1B-NB	2.31	1.40	1.37
11	B	820	CLA	C1D-ND	2.30	1.40	1.37
11	B	819	CLA	C1D-C2D	-2.29	1.40	1.45
11	B	810	CLA	C1D-ND	2.27	1.40	1.37
11	B	816	CLA	C1C-C2C	2.27	1.49	1.44
11	B	814	CLA	C1D-C2D	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	830	CLA	C1B-NB	2.26	1.40	1.37
11	A	823	CLA	C1D-C2D	-2.26	1.40	1.45
11	A	823	CLA	C1B-NB	2.25	1.40	1.37
11	A	802	CLA	C3D-C4D	-2.25	1.39	1.44
11	B	805	CLA	C1D-ND	2.25	1.40	1.37
11	B	809	CLA	C1B-NB	2.25	1.40	1.37
11	A	801	CLA	C3A-C2A	-2.24	1.48	1.54
11	L	1501	CLA	C1D-C2D	-2.24	1.40	1.45
11	B	834	CLA	C3D-C4D	-2.23	1.39	1.44
11	A	811	CLA	C3D-C4D	-2.22	1.39	1.44
11	A	804	CLA	C1B-NB	2.22	1.40	1.37
11	A	826	CLA	C3D-C4D	-2.22	1.39	1.44
11	A	809	CLA	C3A-C2A	-2.21	1.48	1.54
11	A	814	CLA	C3D-C4D	-2.21	1.39	1.44
11	B	823	CLA	C3D-C4D	-2.20	1.39	1.44
11	A	841	CLA	C3D-C4D	-2.20	1.39	1.44
11	A	805	CLA	C1B-NB	2.19	1.40	1.37
11	B	821	CLA	C3D-C4D	-2.19	1.39	1.44
11	A	817	CLA	C1B-NB	2.18	1.40	1.37
11	A	828	CLA	C3D-C4D	-2.18	1.39	1.44
11	B	836	CLA	C1B-NB	2.18	1.40	1.37
11	B	810	CLA	C1B-NB	2.18	1.40	1.37
11	A	837	CLA	C3A-C2A	-2.18	1.48	1.54
11	B	810	CLA	C3D-C4D	-2.18	1.39	1.44
11	A	839	CLA	C3A-C2A	-2.17	1.48	1.54
11	A	816	CLA	C1B-NB	2.17	1.40	1.37
11	A	838	CLA	C3D-C4D	-2.17	1.39	1.44
11	B	820	CLA	C1B-NB	2.17	1.40	1.37
11	B	830	CLA	C1B-NB	2.17	1.40	1.37
11	A	837	CLA	C1B-NB	2.17	1.40	1.37
11	B	817	CLA	C3D-C4D	-2.17	1.39	1.44
11	A	840	CLA	C1B-NB	2.16	1.40	1.37
11	A	826	CLA	C3A-C2A	-2.16	1.48	1.54
11	A	821	CLA	C1B-NB	2.16	1.40	1.37
11	A	827	CLA	C1B-NB	2.16	1.40	1.37
11	A	837	CLA	C3D-C4D	-2.16	1.39	1.44
11	B	807	CLA	C3D-C4D	-2.15	1.39	1.44
11	A	808	CLA	C3D-C4D	-2.15	1.39	1.44
11	A	824	CLA	C1B-NB	2.15	1.40	1.37
11	A	832	CLA	C3D-C4D	-2.15	1.39	1.44
11	B	833	CLA	C3D-C4D	-2.15	1.39	1.44
11	A	834	CLA	C3D-C4D	-2.15	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	820	CLA	C3D-C4D	-2.15	1.39	1.44
11	A	838	CLA	C1B-NB	2.15	1.40	1.37
11	B	835	CLA	C1B-NB	2.15	1.40	1.37
11	A	816	CLA	C3A-C2A	-2.14	1.48	1.54
11	A	821	CLA	C3D-C4D	-2.14	1.39	1.44
11	A	819	CLA	C3D-C4D	-2.14	1.39	1.44
11	A	840	CLA	C3D-C4D	-2.14	1.39	1.44
11	A	801	CLA	C3D-C4D	-2.13	1.39	1.44
11	B	807	CLA	C1B-NB	2.13	1.40	1.37
11	A	839	CLA	C3D-C4D	-2.13	1.39	1.44
11	B	815	CLA	C3D-C4D	-2.13	1.39	1.44
16	B	843	LMG	O1-C7	-2.13	1.40	1.43
11	B	809	CLA	C3D-C4D	-2.12	1.39	1.44
11	A	830	CLA	C3D-C4D	-2.12	1.39	1.44
11	B	801	CLA	C1B-NB	2.12	1.40	1.37
11	B	803	CLA	C3A-C2A	-2.12	1.48	1.54
11	A	804	CLA	C3D-C4D	-2.11	1.39	1.44
11	A	833	CLA	C3D-C4D	-2.10	1.39	1.44
11	A	836	CLA	C3D-C4D	-2.10	1.39	1.44
11	B	812	CLA	C3D-C4D	-2.10	1.39	1.44
11	A	842	CLA	C2A-C3A	-2.10	1.48	1.53
11	A	803	CLA	C3D-C4D	-2.10	1.39	1.44
13	A	849	BCR	C20-C21	2.10	1.49	1.43
11	A	802	CLA	C1D-ND	2.10	1.40	1.37
11	B	825	CLA	C3D-C4D	-2.10	1.39	1.44
11	B	803	CLA	C3D-C4D	-2.10	1.39	1.44
11	B	821	CLA	C1B-NB	2.10	1.40	1.37
11	B	811	CLA	C3D-C4D	-2.10	1.39	1.44
11	B	824	CLA	C3D-C4D	-2.10	1.39	1.44
11	A	839	CLA	CBD-CAD	-2.10	1.47	1.56
11	A	826	CLA	C1B-NB	2.09	1.40	1.37
11	B	828	CLA	C1B-NB	2.09	1.40	1.37
11	B	827	CLA	C3D-C4D	-2.09	1.39	1.44
11	B	819	CLA	C3D-C4D	-2.09	1.39	1.44
11	A	820	CLA	C3D-C4D	-2.08	1.39	1.44
11	A	829	CLA	C3D-C4D	-2.08	1.39	1.44
11	A	823	CLA	C3D-C4D	-2.08	1.39	1.44
11	A	807	CLA	C3D-C4D	-2.08	1.39	1.44
11	A	835	CLA	C3D-C4D	-2.08	1.39	1.44
11	B	836	CLA	C3D-C4D	-2.08	1.39	1.44
11	A	828	CLA	C1C-C2C	2.07	1.48	1.44
11	A	812	CLA	C3D-C4D	-2.07	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	201	BCR	C24-C25	2.07	1.52	1.45
11	B	821	CLA	C1C-C2C	2.07	1.48	1.44
11	A	860	CLA	C1B-NB	2.07	1.40	1.37
11	A	829	CLA	C1C-C2C	2.07	1.48	1.44
11	A	827	CLA	C3D-C4D	-2.06	1.39	1.44
11	B	801	CLA	C3D-C4D	-2.06	1.39	1.44
11	B	813	CLA	C3D-C4D	-2.06	1.39	1.44
11	A	860	CLA	C3D-C4D	-2.06	1.39	1.44
11	B	814	CLA	C3D-C4D	-2.06	1.39	1.44
11	B	832	CLA	C3D-C4D	-2.06	1.39	1.44
11	L	1502	CLA	C3D-C4D	-2.06	1.39	1.44
11	B	803	CLA	C1B-NB	2.06	1.40	1.37
11	B	805	CLA	CHD-C4C	-2.06	1.34	1.39
11	B	826	CLA	C3D-C4D	-2.05	1.39	1.44
11	B	835	CLA	C3D-C4D	-2.05	1.39	1.44
11	B	832	CLA	C3A-C2A	-2.05	1.48	1.54
11	B	806	CLA	C3D-C4D	-2.05	1.39	1.44
11	A	831	CLA	C3D-C4D	-2.05	1.39	1.44
11	A	813	CLA	C3D-C4D	-2.04	1.39	1.44
11	A	805	CLA	C3D-C4D	-2.04	1.39	1.44
11	A	818	CLA	C3D-C4D	-2.04	1.39	1.44
11	L	1502	CLA	C1C-C2C	2.04	1.48	1.44
11	A	817	CLA	C3D-C4D	-2.04	1.39	1.44
11	A	808	CLA	C1B-NB	2.04	1.40	1.37
11	B	822	CLA	C3D-C4D	-2.03	1.39	1.44
11	A	825	CLA	CHD-C4C	-2.03	1.34	1.39
11	A	806	CLA	C3D-C4D	-2.03	1.39	1.44
11	B	818	CLA	C3D-C4D	-2.03	1.39	1.44
11	B	808	CLA	C3D-C4D	-2.03	1.39	1.44
11	A	815	CLA	C3D-C4D	-2.02	1.39	1.44
11	B	823	CLA	C1B-NB	2.02	1.40	1.37
11	A	824	CLA	C3D-C4D	-2.02	1.39	1.44
11	B	818	CLA	C1C-C2C	2.02	1.48	1.44
11	A	816	CLA	CHD-C4C	-2.01	1.34	1.39
11	B	802	CLA	C3D-C4D	-2.01	1.39	1.44
11	B	828	CLA	C3D-C4D	-2.01	1.39	1.44

All (717) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	1502	CLA	C4A-NA-C1A	-7.26	103.37	106.68
13	F	201	BCR	C21-C20-C19	7.01	143.51	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	805	CLA	C4A-NA-C1A	-6.69	103.63	106.68
11	B	824	CLA	C4A-NA-C1A	-6.64	103.65	106.68
11	L	1503	CLA	C4A-NA-C1A	-6.59	103.67	106.68
11	B	803	CLA	C4A-NA-C1A	-6.59	103.67	106.68
11	B	836	CLA	C4A-NA-C1A	-6.50	103.71	106.68
11	L	1501	CLA	C3A-C2A-C1A	-6.50	99.65	106.30
11	L	1501	CLA	C4A-NA-C1A	-6.39	103.76	106.68
11	B	817	CLA	C4A-NA-C1A	-6.31	103.80	106.68
11	A	823	CLA	C4A-NA-C1A	-6.15	103.87	106.68
11	B	814	CLA	C4A-NA-C1A	-6.12	103.89	106.68
11	A	811	CLA	C4A-NA-C1A	-6.12	103.89	106.68
11	B	812	CLA	C4A-NA-C1A	-6.07	103.91	106.68
11	B	819	CLA	C4A-NA-C1A	-6.01	103.94	106.68
11	A	828	CLA	C4A-NA-C1A	-5.98	103.95	106.68
11	B	822	CLA	C4A-NA-C1A	-5.92	103.98	106.68
11	B	815	CLA	C4A-NA-C1A	-5.89	103.99	106.68
11	B	807	CLA	C4A-NA-C1A	-5.88	104.00	106.68
11	A	808	CLA	C4A-NA-C1A	-5.76	104.05	106.68
11	A	832	CLA	C4A-NA-C1A	-5.71	104.08	106.68
11	B	827	CLA	C4A-NA-C1A	-5.67	104.09	106.68
11	B	821	CLA	C4A-NA-C1A	-5.64	104.11	106.68
11	A	822	CLA	C4A-NA-C1A	-5.62	104.12	106.68
11	A	801	CLA	C4A-NA-C1A	-5.61	104.12	106.68
11	A	813	CLA	C4A-NA-C1A	-5.59	104.13	106.68
11	A	826	CLA	C4A-NA-C1A	-5.55	104.14	106.68
11	B	830	CLA	C4A-NA-C1A	-5.50	104.17	106.68
11	B	823	CLA	C4A-NA-C1A	-5.44	104.20	106.68
11	B	820	CLA	C4A-NA-C1A	-5.37	104.23	106.68
11	A	804	CLA	C4A-NA-C1A	-5.35	104.24	106.68
11	A	814	CLA	C4A-NA-C1A	-5.34	104.24	106.68
11	B	818	CLA	C4A-NA-C1A	-5.32	104.25	106.68
11	B	813	CLA	C4A-NA-C1A	-5.29	104.27	106.68
11	B	809	CLA	C4A-NA-C1A	-5.27	104.28	106.68
11	A	842	CLA	C4A-NA-C1A	-5.22	104.30	106.68
11	A	802	CLA	C4A-NA-C1A	-5.21	104.30	106.68
11	A	836	CLA	C4A-NA-C1A	-5.20	104.31	106.68
11	A	840	CLA	C4A-NA-C1A	-5.17	104.32	106.68
11	A	820	CLA	C4A-NA-C1A	-5.16	104.32	106.68
11	A	819	CLA	C4A-NA-C1A	-5.06	104.37	106.68
11	B	811	CLA	C4A-NA-C1A	-5.01	104.39	106.68
11	A	837	CLA	C4A-NA-C1A	-4.99	104.40	106.68
11	B	828	CLA	C4A-NA-C1A	-4.99	104.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	806	CLA	C4A-NA-C1A	-4.98	104.41	106.68
11	B	834	CLA	C4A-NA-C1A	-4.98	104.41	106.68
11	A	833	CLA	C4A-NA-C1A	-4.97	104.41	106.68
11	A	831	CLA	C4A-NA-C1A	-4.96	104.42	106.68
11	A	859	CLA	C4A-NA-C1A	-4.93	104.43	106.68
13	F	202	BCR	C23-C24-C25	4.91	140.11	127.00
11	A	818	CLA	C4A-NA-C1A	-4.87	104.45	106.68
11	A	806	CLA	C4A-NA-C1A	-4.86	104.46	106.68
11	A	803	CLA	C4A-NA-C1A	-4.85	104.47	106.68
11	A	829	CLA	C4A-NA-C1A	-4.80	104.49	106.68
11	A	817	CLA	C4A-NA-C1A	-4.78	104.50	106.68
11	B	816	CLA	C4A-NA-C1A	-4.73	104.52	106.68
11	B	801	CLA	C4A-NA-C1A	-4.71	104.53	106.68
13	F	202	BCR	C24-C23-C22	4.67	133.15	126.23
11	B	826	CLA	C4A-NA-C1A	-4.65	104.56	106.68
11	B	832	CLA	C4A-NA-C1A	-4.61	104.57	106.68
11	A	838	CLA	C4A-NA-C1A	-4.59	104.58	106.68
11	A	807	CLA	C4A-NA-C1A	-4.58	104.59	106.68
11	B	810	CLA	C4A-NA-C1A	-4.49	104.63	106.68
11	B	829	CLA	C4A-NA-C1A	-4.46	104.64	106.68
11	A	824	CLA	C4A-NA-C1A	-4.41	104.67	106.68
11	A	827	CLA	C4A-NA-C1A	-4.40	104.67	106.68
11	A	830	CLA	C4A-NA-C1A	-4.40	104.67	106.68
11	A	834	CLA	C4A-NA-C1A	-4.39	104.68	106.68
14	A	850	LHG	O4-P-O5	4.39	132.84	112.44
14	A	851	LHG	O4-P-O5	4.35	132.70	112.44
11	A	821	CLA	C4A-NA-C1A	-4.30	104.72	106.68
11	A	839	CLA	C4A-NA-C1A	-4.29	104.72	106.68
11	B	805	CLA	C4A-NA-C1A	-4.24	104.75	106.68
13	F	201	BCR	C15-C16-C17	4.20	132.11	123.52
11	A	825	CLA	C4A-NA-C1A	-4.14	104.79	106.68
11	A	812	CLA	C4A-NA-C1A	-4.13	104.80	106.68
11	A	815	CLA	C4A-NA-C1A	-4.10	104.81	106.68
11	B	831	CLA	C4A-NA-C1A	-4.10	104.81	106.68
11	B	825	CLA	C4A-NA-C1A	-4.06	104.83	106.68
11	B	802	CLA	C4A-NA-C1A	-4.04	104.84	106.68
11	A	809	CLA	C4A-NA-C1A	-4.00	104.85	106.68
11	B	808	CLA	C4A-NA-C1A	-3.95	104.88	106.68
11	A	841	CLA	C4A-NA-C1A	-3.86	104.92	106.68
11	B	835	CLA	C4A-NA-C1A	-3.84	104.92	106.68
11	A	816	CLA	C4A-NA-C1A	-3.79	104.95	106.68
11	B	833	CLA	C4A-NA-C1A	-3.76	104.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	820	CLA	CAA-C2A-C1A	-3.74	99.72	111.97
11	A	835	CLA	C4A-NA-C1A	-3.74	104.97	106.68
13	A	849	BCR	C21-C20-C19	3.68	133.86	123.20
13	A	856	BCR	C16-C15-C14	3.66	131.00	123.52
11	A	810	CLA	C4A-NA-C1A	-3.54	105.06	106.68
13	F	201	BCR	C16-C17-C18	3.54	132.24	127.28
13	L	1504	BCR	C23-C24-C25	3.48	136.29	127.00
13	A	852	BCR	C8-C7-C6	3.47	131.59	125.61
11	A	860	CLA	C4A-NA-C1A	-3.46	105.10	106.68
11	A	804	CLA	CAA-C2A-C1A	-3.36	100.97	111.97
11	A	808	CLA	CAA-C2A-C1A	-3.31	101.13	111.97
13	A	856	BCR	C15-C14-C13	3.29	131.89	127.28
11	A	816	CLA	CHA-C1A-NA	-3.28	118.97	126.39
13	A	849	BCR	C16-C15-C14	3.27	130.20	123.52
13	F	201	BCR	C15-C14-C13	3.22	131.80	127.28
11	B	833	CLA	C1D-ND-C4D	-3.20	104.07	106.31
11	A	820	CLA	C1D-ND-C4D	-3.19	104.08	106.31
11	A	816	CLA	C2A-C1A-CHA	3.12	129.29	123.87
11	B	815	CLA	C1D-ND-C4D	-3.09	104.15	106.31
13	B	840	BCR	C21-C20-C19	3.09	132.14	123.20
11	A	842	CLA	C3A-C2A-C1A	-3.08	103.15	106.30
11	B	820	CLA	C1-C2-C3	-3.08	121.15	126.20
13	A	849	BCR	C20-C21-C22	3.08	131.59	127.28
11	A	838	CLA	C1D-ND-C4D	-3.08	104.15	106.31
11	A	828	CLA	C3B-C4B-NB	-3.07	107.79	110.53
11	B	824	CLA	C1-C2-C3	-3.05	121.20	126.20
13	A	849	BCR	C15-C16-C17	3.00	129.65	123.52
11	A	832	CLA	C1D-ND-C4D	-3.00	104.21	106.31
11	A	819	CLA	CAA-C2A-C1A	-2.99	102.16	111.97
11	B	809	CLA	C1D-ND-C4D	-2.99	104.21	106.31
11	A	819	CLA	C1-C2-C3	-2.99	121.30	126.20
13	B	840	BCR	C20-C19-C18	2.96	134.49	126.36
11	A	822	CLA	C1D-ND-C4D	-2.96	104.24	106.31
11	A	859	CLA	C3B-C4B-NB	-2.93	107.91	110.53
14	A	851	LHG	O8-C23-C24	2.92	120.03	111.15
11	A	819	CLA	O2A-C1-C2	2.92	119.35	108.11
11	A	826	CLA	C1D-ND-C4D	-2.92	104.26	106.31
11	A	837	CLA	C1D-ND-C4D	-2.92	104.26	106.31
11	A	813	CLA	CHA-C1A-NA	-2.91	119.79	126.39
11	A	825	CLA	CHA-C1A-NA	-2.89	119.84	126.39
11	A	805	CLA	C1-C2-C3	-2.89	121.46	126.20
11	A	809	CLA	CHA-C1A-NA	-2.88	119.87	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	201	BCR	C20-C21-C22	2.88	131.31	127.28
11	B	812	CLA	C1D-ND-C4D	-2.87	104.30	106.31
11	A	815	CLA	C1D-ND-C4D	-2.87	104.30	106.31
13	F	202	BCR	C8-C7-C6	2.87	134.67	127.00
11	L	1503	CLA	CAA-C2A-C1A	-2.87	105.79	112.14
16	B	843	LMG	O6-C1-O1	-2.87	103.27	110.04
13	A	849	BCR	C10-C11-C12	2.87	131.51	123.20
11	A	836	CLA	C1D-ND-C4D	-2.86	104.30	106.31
11	L	1502	CLA	C1D-ND-C4D	-2.86	104.30	106.31
11	A	859	CLA	C1-C2-C3	-2.85	121.52	126.20
11	A	802	CLA	C3B-C4B-NB	-2.85	107.99	110.53
11	B	817	CLA	C1D-ND-C4D	-2.84	104.32	106.31
13	B	844	BCR	C23-C24-C25	2.84	134.57	127.00
11	A	816	CLA	C2C-C1C-NC	2.83	112.96	109.98
11	A	840	CLA	C1D-ND-C4D	-2.83	104.33	106.31
11	A	816	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
11	B	833	CLA	CHD-C1D-ND	-2.81	120.85	124.80
11	A	826	CLA	CAA-C2A-C1A	-2.80	102.80	111.97
11	B	828	CLA	CHC-C1C-C2C	-2.79	119.01	126.95
11	L	1502	CLA	CHD-C1D-ND	-2.79	120.87	124.80
14	A	850	LHG	O8-C23-C24	2.79	120.33	111.83
11	B	817	CLA	CHD-C1D-ND	-2.78	120.89	124.80
11	A	803	CLA	C1D-ND-C4D	-2.78	104.36	106.31
11	L	1503	CLA	C1D-ND-C4D	-2.78	104.36	106.31
11	B	828	CLA	C1D-ND-C4D	-2.77	104.37	106.31
11	L	1503	CLA	CHD-C1D-ND	-2.77	120.90	124.80
11	B	819	CLA	C1D-ND-C4D	-2.77	104.37	106.31
11	B	818	CLA	C1D-ND-C4D	-2.76	104.37	106.31
11	B	802	CLA	C1D-ND-C4D	-2.76	104.38	106.31
11	B	813	CLA	CHD-C1D-ND	-2.75	120.94	124.80
11	A	820	CLA	CAA-C2A-C1A	-2.74	105.05	111.81
11	A	814	CLA	C1D-ND-C4D	-2.72	104.40	106.31
11	B	834	CLA	C1D-ND-C4D	-2.72	104.40	106.31
11	B	801	CLA	CHD-C1D-ND	-2.72	120.97	124.80
11	A	831	CLA	C2C-C1C-NC	2.72	112.84	109.98
11	A	824	CLA	C1D-ND-C4D	-2.71	104.41	106.31
11	B	809	CLA	CHD-C1D-ND	-2.71	120.99	124.80
11	A	823	CLA	CHD-C1D-ND	-2.70	121.00	124.80
11	A	840	CLA	CHD-C1D-ND	-2.70	121.00	124.80
11	A	812	CLA	C1D-ND-C4D	-2.70	104.42	106.31
11	B	823	CLA	CAA-C2A-C1A	-2.69	103.17	111.97
11	B	814	CLA	CHD-C1D-ND	-2.68	121.03	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	810	CLA	CHC-C1C-C2C	-2.68	119.33	126.95
11	A	817	CLA	C1D-ND-C4D	-2.68	104.43	106.31
11	B	814	CLA	C1D-ND-C4D	-2.67	104.44	106.31
11	A	813	CLA	CHC-C1C-C2C	-2.67	119.36	126.95
11	L	1502	CLA	C3A-C2A-C1A	-2.67	97.34	101.34
11	A	818	CLA	CAA-C2A-C1A	-2.66	103.24	111.97
11	A	841	CLA	C1D-ND-C4D	-2.66	104.44	106.31
11	B	829	CLA	C1D-ND-C4D	-2.66	104.44	106.31
11	A	834	CLA	C1D-ND-C4D	-2.66	104.44	106.31
11	B	827	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
11	A	811	CLA	CHD-C1D-ND	-2.66	121.06	124.80
11	A	836	CLA	CHD-C1D-ND	-2.66	121.06	124.80
11	A	828	CLA	C1D-ND-C4D	-2.66	104.45	106.31
11	A	813	CLA	C2C-C1C-NC	2.66	112.77	109.98
11	B	801	CLA	C1D-ND-C4D	-2.66	104.45	106.31
11	B	820	CLA	C1D-ND-C4D	-2.66	104.45	106.31
11	B	828	CLA	C2C-C1C-NC	2.66	112.77	109.98
11	L	1501	CLA	CHD-C1D-ND	-2.65	121.07	124.80
11	B	834	CLA	CHC-C1C-C2C	-2.65	119.41	126.95
11	A	826	CLA	CHD-C1D-ND	-2.65	121.07	124.80
11	A	820	CLA	CHC-C1C-C2C	-2.65	119.42	126.95
11	B	820	CLA	CHD-C1D-ND	-2.65	121.08	124.80
11	A	839	CLA	CHC-C1C-C2C	-2.65	119.43	126.95
11	A	831	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
11	A	827	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
11	A	834	CLA	CHC-C1C-C2C	-2.64	119.44	126.95
11	A	822	CLA	CHD-C1D-ND	-2.64	121.09	124.80
11	A	804	CLA	C1D-ND-C4D	-2.64	104.46	106.31
11	B	808	CLA	C2C-C1C-NC	2.64	112.75	109.98
11	B	824	CLA	CHA-C1A-NA	-2.63	120.43	126.39
11	B	819	CLA	CHD-C1D-ND	-2.63	121.10	124.80
11	A	838	CLA	C1-C2-C3	-2.63	121.89	126.20
11	B	832	CLA	C1D-ND-C4D	-2.63	104.47	106.31
11	A	803	CLA	CHD-C1D-ND	-2.62	121.11	124.80
11	B	827	CLA	CHD-C1D-ND	-2.62	121.11	124.80
11	B	832	CLA	CHC-C1C-C2C	-2.62	119.50	126.95
11	B	807	CLA	CHD-C1D-ND	-2.62	121.12	124.80
11	A	820	CLA	C2C-C1C-NC	2.61	112.73	109.98
11	A	831	CLA	CHA-C1A-NA	-2.61	120.48	126.39
11	B	801	CLA	CAA-C2A-C1A	-2.61	103.42	111.97
11	B	815	CLA	C2C-C1C-NC	2.61	112.72	109.98
11	A	807	CLA	C1D-ND-C4D	-2.61	104.48	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	829	CLA	C1D-ND-C4D	-2.61	104.48	106.31
11	A	818	CLA	C2C-C1C-NC	2.61	112.72	109.98
11	A	812	CLA	CHA-C1A-NA	-2.61	120.49	126.39
11	B	832	CLA	C2C-C1C-NC	2.60	112.72	109.98
11	B	831	CLA	CHC-C1C-C2C	-2.60	119.55	126.95
11	B	816	CLA	C1D-ND-C4D	-2.60	104.49	106.31
12	A	843	PQN	C11-C3-C2	-2.60	120.43	124.89
13	F	201	BCR	C16-C15-C14	2.60	128.84	123.52
11	A	820	CLA	CHD-C1D-ND	-2.60	121.14	124.80
11	B	830	CLA	CHD-C1D-ND	-2.60	121.15	124.80
11	B	806	CLA	CHD-C1D-ND	-2.60	121.15	124.80
11	B	828	CLA	CHA-C1A-NA	-2.60	120.51	126.39
11	A	818	CLA	C1D-ND-C4D	-2.60	104.49	106.31
13	F	201	BCR	C24-C25-C26	2.59	127.53	121.56
11	A	832	CLA	CHD-C1D-ND	-2.59	121.15	124.80
13	A	852	BCR	C10-C11-C12	2.59	130.72	123.20
11	A	828	CLA	CHD-C1D-ND	-2.59	121.15	124.80
11	A	804	CLA	CHD-C1D-ND	-2.59	121.16	124.80
11	A	812	CLA	CHC-C1C-C2C	-2.59	119.59	126.95
11	B	806	CLA	C1D-ND-C4D	-2.59	104.50	106.31
11	L	1501	CLA	CHC-C1C-NC	2.59	128.21	124.31
11	A	838	CLA	CHD-C1D-ND	-2.59	121.16	124.80
11	A	806	CLA	CHA-C1A-NA	-2.58	120.54	126.39
11	A	829	CLA	C1-C2-C3	-2.58	121.97	126.20
11	A	814	CLA	CHD-C1D-ND	-2.58	121.17	124.80
11	B	835	CLA	C1D-ND-C4D	-2.58	104.50	106.31
11	A	807	CLA	CHC-C1C-C2C	-2.58	119.62	126.95
11	B	835	CLA	CHC-C1C-C2C	-2.58	119.63	126.95
11	B	802	CLA	CHD-C1D-ND	-2.58	121.18	124.80
11	A	806	CLA	C2C-C1C-NC	2.58	112.69	109.98
11	A	809	CLA	CHC-C1C-NC	2.57	128.19	124.31
11	A	806	CLA	CHC-C1C-C2C	-2.57	119.64	126.95
11	B	826	CLA	C1D-ND-C4D	-2.57	104.51	106.31
11	A	807	CLA	CHC-C1C-NC	2.57	128.18	124.31
11	B	805	CLA	C3B-C4B-NB	-2.57	108.24	110.53
11	A	802	CLA	CHD-C1D-ND	-2.56	121.20	124.80
11	A	839	CLA	CHA-C1A-NA	-2.56	120.59	126.39
11	B	808	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
11	B	833	CLA	CHC-C1C-C2C	-2.56	119.67	126.95
11	A	835	CLA	C1D-ND-C4D	-2.56	104.52	106.31
11	A	825	CLA	CHC-C1C-C2C	-2.56	119.68	126.95
11	A	805	CLA	CHD-C1D-ND	-2.56	121.20	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	828	CLA	CHC-C1C-NC	2.56	128.16	124.31
11	B	802	CLA	C1-C2-C3	-2.56	122.01	126.20
11	A	803	CLA	CHC-C1C-C2C	-2.56	119.69	126.95
11	A	837	CLA	CHC-C1C-C2C	-2.55	119.69	126.95
11	B	827	CLA	CHC-C1C-NC	2.55	128.16	124.31
16	B	843	LMG	O1-C7-C8	-2.55	104.61	110.82
11	B	814	CLA	CHC-C1C-C2C	-2.55	119.70	126.95
11	B	826	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
11	A	809	CLA	CHC-C1C-C2C	-2.55	119.71	126.95
11	B	805	CLA	CHA-C1A-NA	-2.55	120.63	126.39
11	B	809	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
11	A	835	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
11	A	815	CLA	CHC-C1C-C2C	-2.54	119.72	126.95
11	A	816	CLA	C1D-ND-C4D	-2.54	104.53	106.31
11	B	822	CLA	C3B-C4B-NB	-2.54	108.26	110.53
11	B	816	CLA	CHA-C1A-NA	-2.54	120.64	126.39
11	B	825	CLA	C1D-ND-C4D	-2.54	104.53	106.31
11	B	819	CLA	CAA-C2A-C1A	-2.54	103.66	111.97
11	A	810	CLA	CHD-C1D-ND	-2.54	121.23	124.80
11	A	819	CLA	CHD-C1D-ND	-2.53	121.24	124.80
11	A	817	CLA	CHC-C1C-NC	2.53	128.12	124.31
11	A	818	CLA	CHC-C1C-C2C	-2.53	119.76	126.95
11	L	1501	CLA	CHC-C1C-C2C	-2.53	119.77	126.95
11	B	830	CLA	C1D-ND-C4D	-2.52	104.54	106.31
11	B	811	CLA	CHC-C1C-C2C	-2.52	119.78	126.95
11	B	824	CLA	CHD-C1D-ND	-2.52	121.25	124.80
11	A	827	CLA	C1D-ND-C4D	-2.52	104.54	106.31
11	A	831	CLA	C1D-ND-C4D	-2.52	104.54	106.31
11	A	805	CLA	CHA-C1A-NA	-2.52	120.69	126.39
13	A	852	BCR	C23-C24-C25	2.52	133.73	127.00
11	B	823	CLA	CHD-C1D-ND	-2.52	121.26	124.80
11	A	860	CLA	CHD-C1D-ND	-2.52	121.26	124.80
11	A	817	CLA	CHD-C1D-ND	-2.51	121.27	124.80
11	B	815	CLA	CHC-C1C-C2C	-2.51	119.81	126.95
11	B	832	CLA	CHA-C1A-NA	-2.51	120.70	126.39
11	A	816	CLA	CHB-C1B-NB	-2.51	120.28	124.05
11	A	834	CLA	CHC-C1C-NC	2.51	128.09	124.31
11	A	812	CLA	CHC-C1C-NC	2.51	128.09	124.31
11	B	820	CLA	CHC-C1C-C2C	-2.51	119.82	126.95
11	L	1501	CLA	C1D-ND-C4D	-2.51	104.55	106.31
11	A	840	CLA	CHC-C1C-NC	2.51	128.09	124.31
11	B	807	CLA	C1D-ND-C4D	-2.51	104.55	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	842	CLA	CHC-C1C-C2C	-2.51	119.83	126.95
11	B	827	CLA	C1D-ND-C4D	-2.50	104.56	106.31
11	A	841	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
11	A	837	CLA	CHD-C1D-ND	-2.50	121.28	124.80
11	B	801	CLA	CHC-C1C-C2C	-2.50	119.84	126.95
11	A	816	CLA	CHC-C1C-NC	2.50	128.08	124.31
11	B	822	CLA	CHA-C1A-NA	-2.50	120.73	126.39
11	B	812	CLA	CHD-C1D-ND	-2.50	121.29	124.80
11	B	818	CLA	CHD-C1D-ND	-2.50	121.29	124.80
11	B	801	CLA	CHC-C1C-NC	2.50	128.07	124.31
11	A	823	CLA	C1D-ND-C4D	-2.50	104.56	106.31
11	B	803	CLA	CHA-C1A-NA	-2.50	120.74	126.39
11	B	822	CLA	CHD-C1D-ND	-2.50	121.29	124.80
11	A	824	CLA	CHD-C1D-ND	-2.49	121.29	124.80
11	B	836	CLA	CHC-C1C-C2C	-2.49	119.86	126.95
11	B	811	CLA	C1-C2-C3	-2.49	122.11	126.20
11	A	819	CLA	CHC-C1C-C2C	-2.49	119.87	126.95
11	A	833	CLA	C1D-ND-C4D	-2.49	104.56	106.31
11	B	802	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
11	A	834	CLA	CHD-C1D-ND	-2.49	121.30	124.80
11	A	808	CLA	CHD-C1D-ND	-2.49	121.30	124.80
11	B	817	CLA	CHC-C1C-C2C	-2.49	119.88	126.95
11	B	808	CLA	CHD-C1D-ND	-2.48	121.31	124.80
11	A	832	CLA	CHC-C1C-C2C	-2.48	119.89	126.95
11	L	1501	CLA	C2A-C3A-C4A	-2.48	99.36	103.57
11	A	818	CLA	C1-C2-C3	-2.48	122.13	126.20
11	B	829	CLA	CHD-C1D-ND	-2.48	121.31	124.80
11	B	826	CLA	C2C-C1C-NC	2.48	112.59	109.98
11	B	833	CLA	CHC-C1C-NC	2.48	128.05	124.31
11	A	829	CLA	CHD-C1D-ND	-2.48	121.31	124.80
11	B	803	CLA	CHD-C1D-ND	-2.48	121.31	124.80
11	A	802	CLA	CHA-C1A-NA	-2.48	120.78	126.39
11	A	841	CLA	CHC-C1C-NC	2.48	128.04	124.31
11	B	834	CLA	CHC-C1C-NC	2.48	128.04	124.31
11	B	803	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
11	B	834	CLA	CHD-C1D-ND	-2.47	121.33	124.80
11	B	813	CLA	CHC-C1C-C2C	-2.47	119.93	126.95
11	A	835	CLA	CHD-C1D-ND	-2.47	121.33	124.80
11	B	812	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
11	A	817	CLA	CHC-C1C-C2C	-2.47	119.94	126.95
11	A	819	CLA	CHC-C1C-NC	2.47	128.02	124.31
11	A	821	CLA	CHC-C1C-C2C	-2.46	119.94	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	825	CLA	C1D-ND-C4D	-2.46	104.58	106.31
11	B	813	CLA	CHC-C1C-NC	2.46	128.02	124.31
11	A	815	CLA	CHD-C1D-ND	-2.46	121.34	124.80
11	A	833	CLA	CHC-C1C-C2C	-2.46	119.97	126.95
11	A	818	CLA	CHD-C1D-ND	-2.46	121.35	124.80
11	A	803	CLA	CHC-C1C-NC	2.45	128.01	124.31
11	A	833	CLA	CHD-C1D-ND	-2.45	121.35	124.80
11	B	826	CLA	CHD-C1D-ND	-2.45	121.35	124.80
11	B	825	CLA	CHC-C1C-C2C	-2.45	119.98	126.95
11	B	811	CLA	C3B-C4B-NB	-2.45	108.34	110.53
11	A	823	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
11	A	811	CLA	C1D-ND-C4D	-2.45	104.59	106.31
11	A	827	CLA	C2C-C1C-NC	2.45	112.55	109.98
11	B	835	CLA	CHA-C1A-NA	-2.45	120.85	126.39
11	A	836	CLA	CHC-C1C-C2C	-2.45	119.99	126.95
11	B	811	CLA	CHA-C1A-NA	-2.45	120.85	126.39
11	B	806	CLA	CHC-C1C-NC	2.45	127.99	124.31
11	L	1503	CLA	CHC-C1C-C2C	-2.45	120.00	126.95
11	B	830	CLA	CHC-C1C-C2C	-2.44	120.01	126.95
11	A	834	CLA	C1-C2-C3	-2.44	122.20	126.20
11	A	839	CLA	CHC-C1C-NC	2.44	127.99	124.31
11	A	811	CLA	C3B-C4B-NB	-2.44	108.35	110.53
11	A	822	CLA	CHC-C1C-C2C	-2.44	120.02	126.95
14	A	850	LHG	C20-C19-C18	-2.44	102.05	114.37
11	B	835	CLA	CHC-C1C-NC	2.43	127.98	124.31
11	L	1503	CLA	CHC-C1C-NC	2.43	127.98	124.31
11	A	810	CLA	C1D-ND-C4D	-2.43	104.61	106.31
11	A	837	CLA	CHA-C1A-NA	-2.43	120.88	126.39
11	B	836	CLA	C2C-C1C-NC	2.43	112.54	109.98
11	B	826	CLA	CHA-C1A-NA	-2.43	120.89	126.39
11	B	811	CLA	CHD-C1D-ND	-2.43	121.38	124.80
11	B	815	CLA	CHD-C1D-ND	-2.43	121.38	124.80
11	B	831	CLA	CHA-C1A-NA	-2.43	120.89	126.39
11	A	831	CLA	CHD-C1D-ND	-2.43	121.39	124.80
14	A	851	LHG	C11-C10-C9	-2.43	102.10	114.37
11	A	832	CLA	CHA-C1A-NA	-2.43	120.90	126.39
11	A	809	CLA	C1D-ND-C4D	-2.42	104.61	106.31
11	B	808	CLA	CHB-C1B-NB	-2.42	120.41	124.05
11	A	826	CLA	CHC-C1C-NC	2.42	127.96	124.31
11	B	836	CLA	CHD-C1D-ND	-2.42	121.39	124.80
11	B	819	CLA	CHC-C1C-C2C	-2.42	120.07	126.95
11	A	840	CLA	CHC-C1C-C2C	-2.42	120.07	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	816	CLA	CHD-C1D-ND	-2.42	121.40	124.80
11	A	822	CLA	CHC-C1C-NC	2.42	127.95	124.31
11	A	808	CLA	C1D-ND-C4D	-2.42	104.62	106.31
11	B	821	CLA	CHD-C1D-ND	-2.42	121.40	124.80
11	A	837	CLA	C2C-C1C-NC	2.42	112.52	109.98
11	B	822	CLA	CHC-C1C-C2C	-2.41	120.09	126.95
11	B	829	CLA	CHA-C1A-NA	-2.41	120.93	126.39
11	B	808	CLA	CHA-C1A-NA	-2.41	120.93	126.39
11	B	834	CLA	C2C-C1C-NC	2.41	112.52	109.98
11	B	814	CLA	CHC-C1C-NC	2.41	127.94	124.31
11	B	831	CLA	CHC-C1C-NC	2.41	127.94	124.31
11	B	831	CLA	C1D-ND-C4D	-2.41	104.62	106.31
11	A	812	CLA	CHD-C1D-ND	-2.41	121.42	124.80
11	B	828	CLA	CHD-C1D-ND	-2.41	121.42	124.80
11	A	859	CLA	CHA-C1A-NA	-2.41	120.94	126.39
11	B	831	CLA	CHD-C1D-ND	-2.40	121.42	124.80
11	B	806	CLA	CHC-C1C-C2C	-2.40	120.12	126.95
11	A	816	CLA	C1-C2-C3	-2.40	122.88	126.76
12	B	837	PQN	C11-C3-C2	-2.40	120.77	124.89
11	B	823	CLA	CHC-C1C-C2C	-2.40	120.13	126.95
11	A	815	CLA	CHC-C1C-NC	2.40	127.92	124.31
11	A	836	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
16	B	843	LMG	C38-C37-C36	-2.40	102.26	114.37
11	A	859	CLA	CHD-C1D-ND	-2.39	121.43	124.80
11	A	801	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
11	B	818	CLA	CHA-C1A-NA	-2.39	120.97	126.39
11	L	1502	CLA	CHA-C1A-NA	-2.39	120.97	126.39
11	B	805	CLA	CHC-C1C-C2C	-2.39	120.15	126.95
11	A	825	CLA	CHC-C1C-NC	2.39	127.91	124.31
11	A	829	CLA	CHA-C1A-NA	-2.39	120.98	126.39
11	A	806	CLA	C1-C2-C3	-2.39	122.28	126.20
11	B	830	CLA	CHA-C1A-NA	-2.39	120.98	126.39
11	A	807	CLA	CHD-C1D-ND	-2.39	121.44	124.80
13	A	858	BCR	C23-C24-C25	2.39	133.38	127.00
11	A	810	CLA	CHC-C1C-NC	2.39	127.91	124.31
11	B	810	CLA	CBA-CAA-C2A	2.39	120.89	113.79
11	B	829	CLA	CHC-C1C-NC	2.38	127.90	124.31
11	B	836	CLA	CHA-C1A-NA	-2.38	121.00	126.39
11	A	821	CLA	CHD-C1D-ND	-2.38	121.45	124.80
11	A	827	CLA	CHC-C1C-NC	2.38	127.89	124.31
11	A	839	CLA	CHB-C1B-NB	-2.38	120.48	124.05
11	B	820	CLA	CHC-C1C-NC	2.38	127.89	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	813	CLA	C1D-ND-C4D	-2.37	104.65	106.31
11	A	805	CLA	C1D-ND-C4D	-2.37	104.65	106.31
11	B	817	CLA	CHC-C1C-NC	2.37	127.88	124.31
11	B	802	CLA	CHC-C1C-NC	2.37	127.88	124.31
11	A	826	CLA	CHC-C1C-C2C	-2.37	120.21	126.95
11	B	829	CLA	CHC-C1C-C2C	-2.37	120.22	126.95
11	A	814	CLA	CHC-C1C-C2C	-2.37	120.22	126.95
11	B	835	CLA	CHD-C1D-ND	-2.37	121.47	124.80
11	B	810	CLA	CHC-C1C-C2C	-2.36	120.23	126.95
11	B	831	CLA	C2C-C1C-NC	2.36	112.47	109.98
11	A	804	CLA	CHC-C1C-C2C	-2.36	120.23	126.95
11	A	839	CLA	C2C-C1C-NC	2.36	112.46	109.98
11	A	811	CLA	CHC-C1C-NC	2.36	127.87	124.31
11	A	813	CLA	CHC-C1C-NC	2.36	127.87	124.31
11	A	841	CLA	CHD-C1D-ND	-2.36	121.48	124.80
11	A	817	CLA	CHA-C1A-NA	-2.36	121.05	126.39
11	A	827	CLA	CHD-C1D-ND	-2.36	121.48	124.80
11	A	811	CLA	CHC-C1C-C2C	-2.36	120.24	126.95
11	B	825	CLA	CHD-C1D-ND	-2.36	121.48	124.80
11	B	815	CLA	C1-C2-C3	-2.36	122.33	126.20
11	A	809	CLA	CHB-C1B-NB	-2.36	120.51	124.05
11	B	809	CLA	C2C-C1C-NC	2.36	112.46	109.98
11	B	827	CLA	C2C-C1C-NC	2.36	112.46	109.98
11	A	830	CLA	CHC-C1C-C2C	-2.36	120.25	126.95
11	B	830	CLA	CHC-C1C-NC	2.36	127.86	124.31
11	B	811	CLA	C2C-C1C-NC	2.35	112.45	109.98
11	B	834	CLA	CHA-C1A-NA	-2.35	121.06	126.39
11	A	806	CLA	CHD-C1D-ND	-2.35	121.50	124.80
11	A	806	CLA	CHB-C1B-NB	-2.34	120.53	124.05
11	A	839	CLA	C1D-ND-C4D	-2.34	104.67	106.31
11	A	803	CLA	CAA-C2A-C1A	-2.34	106.96	112.14
11	B	808	CLA	C1D-ND-C4D	-2.34	104.67	106.31
11	A	842	CLA	CHD-C1D-ND	-2.34	121.51	124.80
11	A	827	CLA	C1-C2-C3	-2.34	122.37	126.20
11	B	803	CLA	C1-C2-C3	-2.34	122.37	126.20
11	B	803	CLA	CHC-C1C-NC	2.34	127.83	124.31
11	B	807	CLA	CHC-C1C-C2C	-2.33	120.32	126.95
11	B	822	CLA	C1D-ND-C4D	-2.33	104.67	106.31
11	A	807	CLA	CHA-C1A-NA	-2.33	121.11	126.39
11	B	809	CLA	CHC-C1C-NC	2.33	127.82	124.31
13	B	838	BCR	C23-C24-C25	2.33	133.22	127.00
11	A	824	CLA	CHA-C1A-NA	-2.33	121.12	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	825	CLA	CHA-C1A-NA	-2.33	121.12	126.39
16	B	843	LMG	O2-C2-C1	-2.33	104.53	110.08
11	A	804	CLA	CHC-C1C-NC	2.33	127.81	124.31
11	B	814	CLA	CHA-C1A-NA	-2.32	121.13	126.39
11	A	814	CLA	CHC-C1C-NC	2.32	127.81	124.31
11	A	830	CLA	CHD-C1D-ND	-2.32	121.53	124.80
11	L	1502	CLA	C2A-C1A-CHA	2.32	127.90	123.87
11	A	824	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
11	A	839	CLA	CHD-C1D-ND	-2.32	121.54	124.80
11	B	825	CLA	CHC-C1C-NC	2.32	127.80	124.31
11	A	801	CLA	CHA-C1A-NA	-2.32	121.14	126.39
11	A	808	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
11	A	805	CLA	CHC-C1C-C2C	-2.32	120.36	126.95
11	B	821	CLA	C1D-ND-C4D	-2.31	104.69	106.31
11	A	820	CLA	CHC-C1C-NC	2.31	127.80	124.31
11	A	821	CLA	CHC-C1C-NC	2.31	127.80	124.31
11	A	809	CLA	CHD-C1D-ND	-2.31	121.55	124.80
11	L	1501	CLA	C2A-C1A-CHA	2.31	126.30	122.71
11	A	860	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
11	B	824	CLA	CHC-C1C-C2C	-2.31	120.38	126.95
11	B	823	CLA	CHC-C1C-NC	2.31	127.79	124.31
11	A	801	CLA	CHD-C1D-ND	-2.31	121.55	124.80
14	A	850	LHG	C11-C10-C9	-2.31	102.70	114.37
11	L	1502	CLA	C1-C2-C3	-2.31	122.42	126.20
11	B	832	CLA	CHD-C1D-ND	-2.31	121.56	124.80
11	A	842	CLA	CHC-C1C-NC	2.31	127.78	124.31
11	B	832	CLA	CHC-C1C-NC	2.30	127.78	124.31
11	A	823	CLA	CHC-C1C-NC	2.30	127.78	124.31
11	A	830	CLA	CHA-C1A-NA	-2.30	121.18	126.39
11	B	818	CLA	CHC-C1C-C2C	-2.30	120.41	126.95
11	B	827	CLA	CAA-C2A-C1A	-2.30	106.13	111.81
11	A	819	CLA	C1D-ND-C4D	-2.30	104.70	106.31
16	B	843	LMG	C40-C39-C38	-2.30	102.76	114.37
11	A	860	CLA	CHC-C1C-NC	2.30	127.77	124.31
11	A	825	CLA	C2C-C1C-NC	2.29	112.39	109.98
11	A	817	CLA	C3B-C4B-NB	-2.29	108.48	110.53
11	B	812	CLA	CHA-C1A-NA	-2.29	121.20	126.39
11	B	821	CLA	CHA-C1A-NA	-2.29	121.20	126.39
11	A	814	CLA	CHA-C1A-NA	-2.29	121.21	126.39
11	B	813	CLA	CAA-C2A-C1A	-2.29	104.47	111.97
11	A	837	CLA	CHC-C1C-NC	2.29	127.76	124.31
11	A	829	CLA	C3B-C4B-NB	-2.29	108.49	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	812	CLA	CHB-C1B-NB	-2.29	120.62	124.05
11	A	822	CLA	CHA-C1A-NA	-2.29	121.21	126.39
11	A	808	CLA	CHC-C1C-NC	2.28	127.75	124.31
11	B	831	CLA	C3B-C4B-NB	-2.28	108.49	110.53
11	A	813	CLA	CHD-C1D-ND	-2.28	121.59	124.80
11	A	833	CLA	CHA-C1A-NA	-2.28	121.23	126.39
11	B	811	CLA	CHC-C1C-NC	2.28	127.74	124.31
11	B	824	CLA	C3B-C4B-NB	-2.28	108.50	110.53
11	A	825	CLA	C1-C2-C3	-2.28	122.47	126.20
11	A	838	CLA	CHC-C1C-C2C	-2.27	120.48	126.95
13	A	849	BCR	C23-C24-C25	2.27	133.07	127.00
13	A	855	BCR	C8-C7-C6	2.27	129.53	125.61
11	A	808	CLA	C1-C2-C3	-2.27	122.48	126.20
11	A	835	CLA	CHC-C1C-NC	2.27	127.73	124.31
11	B	805	CLA	CHD-C1D-ND	-2.27	121.61	124.80
11	B	807	CLA	CHA-C1A-NA	-2.27	121.26	126.39
11	A	833	CLA	CHC-C1C-NC	2.27	127.72	124.31
11	B	821	CLA	CHC-C1C-C2C	-2.26	120.51	126.95
11	B	832	CLA	C1-C2-C3	-2.26	123.10	126.76
11	A	831	CLA	CHC-C1C-NC	2.26	127.72	124.31
11	A	842	CLA	C2C-C1C-NC	2.26	112.36	109.98
11	A	825	CLA	CHB-C1B-NB	-2.26	120.66	124.05
11	A	832	CLA	C2C-C1C-NC	2.26	112.36	109.98
11	A	823	CLA	CHA-C1A-NA	-2.26	121.28	126.39
11	A	811	CLA	CHA-C1A-NA	-2.26	121.28	126.39
11	B	803	CLA	C3B-C4B-NB	-2.26	108.52	110.53
11	B	816	CLA	CHD-C1D-ND	-2.26	121.63	124.80
11	B	816	CLA	CHC-C1C-C2C	-2.26	120.53	126.95
11	B	805	CLA	C1-C2-C3	-2.26	122.50	126.20
11	A	835	CLA	CHA-C1A-NA	-2.26	121.28	126.39
11	B	823	CLA	CHA-C1A-NA	-2.25	121.29	126.39
11	B	823	CLA	C1D-ND-C4D	-2.25	104.73	106.31
11	A	810	CLA	CHB-C1B-NB	-2.25	120.67	124.05
11	B	819	CLA	C1-C2-C3	-2.25	122.51	126.20
11	A	860	CLA	C1D-ND-C4D	-2.25	104.73	106.31
11	A	802	CLA	CHC-C1C-C2C	-2.25	120.57	126.95
11	A	826	CLA	C1-C2-C3	-2.24	122.52	126.20
11	B	812	CLA	CHC-C1C-NC	2.24	127.69	124.31
11	B	818	CLA	CHC-C1C-NC	2.24	127.69	124.31
11	A	835	CLA	C2C-C1C-NC	2.24	112.33	109.98
11	L	1503	CLA	CHA-C1A-NA	-2.24	121.32	126.39
11	A	833	CLA	CHB-C1B-NB	-2.24	120.69	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	836	CLA	C2C-C1C-NC	2.24	112.33	109.98
11	A	832	CLA	CHC-C1C-NC	2.24	127.68	124.31
11	A	807	CLA	CHB-C1B-NB	-2.23	120.70	124.05
11	A	806	CLA	CHC-C1C-NC	2.23	127.68	124.31
11	A	829	CLA	CHC-C1C-C2C	-2.23	120.60	126.95
11	B	819	CLA	CHC-C1C-NC	2.23	127.67	124.31
11	A	827	CLA	CHB-C1B-NB	-2.23	120.70	124.05
11	B	824	CLA	CHC-C1C-NC	2.23	127.67	124.31
11	A	811	CLA	C1-C2-C3	-2.23	122.55	126.20
14	A	850	LHG	C18-C17-C16	-2.23	103.11	114.37
11	B	801	CLA	C1-C2-C3	-2.23	122.55	126.20
13	B	844	BCR	C24-C25-C26	2.23	126.68	121.56
11	A	821	CLA	C1D-ND-C4D	-2.22	104.75	106.31
11	A	834	CLA	CHA-C1A-NA	-2.22	121.36	126.39
11	B	810	CLA	C1-C2-C3	-2.22	122.56	126.20
11	A	860	CLA	CHA-C1A-NA	-2.22	121.36	126.39
11	A	816	CLA	CAA-C2A-C3A	-2.22	107.01	113.00
11	B	807	CLA	CHC-C1C-NC	2.22	127.65	124.31
11	A	830	CLA	C1D-ND-C4D	-2.21	104.76	106.31
11	A	841	CLA	CHA-C1A-NA	-2.21	121.38	126.39
11	B	824	CLA	C1D-ND-C4D	-2.21	104.76	106.31
11	A	837	CLA	CHB-C1B-NB	-2.21	120.73	124.05
11	B	823	CLA	CHB-C1B-NB	-2.21	120.73	124.05
11	B	828	CLA	CHB-C1B-NB	-2.21	120.73	124.05
11	A	836	CLA	CHC-C1C-NC	2.21	127.64	124.31
11	B	817	CLA	CHA-C1A-NA	-2.21	121.39	126.39
13	F	201	BCR	C20-C19-C18	2.21	132.42	126.36
11	A	824	CLA	CHC-C1C-NC	2.21	127.64	124.31
11	A	810	CLA	CHA-C1A-NA	-2.21	121.39	126.39
11	A	828	CLA	CHA-C1A-NA	-2.21	121.39	126.39
11	A	830	CLA	CHC-C1C-NC	2.21	127.63	124.31
11	L	1502	CLA	CHC-C1C-NC	2.20	127.63	124.31
11	A	818	CLA	CHA-C1A-NA	-2.20	121.40	126.39
11	A	837	CLA	C1-C2-C3	-2.20	122.59	126.20
11	A	841	CLA	CHB-C1B-NB	-2.20	120.74	124.05
11	A	842	CLA	CHA-C1A-NA	-2.20	121.32	126.33
11	L	1501	CLA	CHB-C1B-NB	-2.20	120.75	124.05
11	A	810	CLA	C2C-C1C-NC	2.20	112.29	109.98
11	A	834	CLA	C2C-C1C-NC	2.20	112.29	109.98
11	A	827	CLA	CHA-C1A-NA	-2.19	121.42	126.39
11	L	1502	CLA	CHC-C1C-C2C	-2.19	120.72	126.95
11	B	817	CLA	CAA-C2A-C1A	-2.19	104.79	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	805	CLA	CHB-C1B-NB	-2.19	120.77	124.05
11	A	829	CLA	CHC-C1C-NC	2.19	127.61	124.31
11	A	803	CLA	C2C-C1C-NC	2.19	112.28	109.98
13	F	201	BCR	C30-C25-C24	-2.18	109.73	115.65
11	A	805	CLA	CHC-C1C-NC	2.18	127.60	124.31
11	L	1501	CLA	CHA-C1A-NA	-2.18	121.36	126.33
11	L	1501	CLA	CBD-CHA-C1A	2.18	130.34	128.03
11	A	819	CLA	CHA-C1A-NA	-2.17	121.47	126.39
11	A	859	CLA	CHC-C1C-C2C	-2.17	120.78	126.95
11	B	823	CLA	C3B-C4B-NB	-2.17	108.59	110.53
11	A	821	CLA	CHA-C1A-NA	-2.17	121.48	126.39
11	B	822	CLA	CHC-C1C-NC	2.16	127.57	124.31
11	B	806	CLA	CHA-C1A-NA	-2.16	121.49	126.39
11	A	801	CLA	C3B-C4B-NB	-2.16	108.60	110.53
11	A	820	CLA	CHA-C1A-NA	-2.16	121.49	126.39
11	B	801	CLA	CHB-C1B-NB	-2.16	120.81	124.05
11	B	808	CLA	CHC-C1C-NC	2.16	127.56	124.31
11	A	832	CLA	CHB-C1B-NB	-2.16	120.81	124.05
11	B	812	CLA	C2C-C1C-NC	2.16	112.25	109.98
13	A	856	BCR	C2-C1-C6	2.16	113.57	110.44
11	B	813	CLA	CHB-C1B-NB	-2.15	120.82	124.05
11	A	811	CLA	C2A-C1A-CHA	2.15	127.60	123.87
11	B	833	CLA	CHB-C1B-NB	-2.15	120.82	124.05
11	B	834	CLA	CHB-C1B-NB	-2.15	120.82	124.05
11	B	810	CLA	CHC-C1C-NC	2.15	127.55	124.31
11	A	842	CLA	C1D-ND-C4D	-2.15	104.81	106.31
11	B	836	CLA	C1D-ND-C4D	-2.15	104.81	106.31
11	A	819	CLA	C3B-C4B-NB	-2.14	108.62	110.53
11	A	815	CLA	CHA-C1A-NA	-2.14	121.54	126.39
11	B	826	CLA	CHC-C1C-NC	2.14	127.53	124.31
11	A	834	CLA	CHB-C1B-NB	-2.14	120.84	124.05
11	A	821	CLA	C3B-C4B-NB	-2.14	108.62	110.53
11	A	825	CLA	CHD-C1D-ND	-2.13	121.80	124.80
11	B	827	CLA	CHA-C1A-NA	-2.13	121.56	126.39
11	B	821	CLA	CHC-C1C-NC	2.13	127.52	124.31
11	A	821	CLA	C2C-C1C-NC	2.13	112.22	109.98
11	A	818	CLA	CHC-C1C-NC	2.13	127.52	124.31
11	B	809	CLA	CHB-C1B-NB	-2.13	120.86	124.05
11	A	830	CLA	C1-C2-C3	-2.13	122.71	126.20
11	A	815	CLA	CHB-C1B-NB	-2.13	120.86	124.05
16	B	843	LMG	O1-C1-C2	-2.13	105.04	108.27
11	A	838	CLA	CHC-C1C-NC	2.13	127.51	124.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	836	CLA	CHC-C1C-NC	2.12	127.51	124.31
11	B	815	CLA	CHA-C1A-NA	-2.12	121.58	126.39
11	B	814	CLA	C2C-C1C-NC	2.12	112.21	109.98
11	A	801	CLA	C1D-ND-C4D	-2.12	104.82	106.31
11	B	834	CLA	C3B-C4B-NB	-2.12	108.64	110.53
16	B	843	LMG	O3-C3-C2	-2.12	105.38	110.38
11	A	815	CLA	C2C-C1C-NC	2.12	112.20	109.98
11	A	813	CLA	C1D-ND-C4D	-2.12	104.83	106.31
11	A	831	CLA	CHB-C1B-NB	-2.11	120.88	124.05
11	B	820	CLA	C2C-C1C-NC	2.11	112.20	109.98
11	A	860	CLA	CHB-C1B-NB	-2.11	120.89	124.05
11	A	801	CLA	CHC-C1C-NC	2.11	127.48	124.31
11	B	809	CLA	CHA-C1A-NA	-2.10	121.63	126.39
11	B	819	CLA	C2C-C1C-NC	2.10	112.19	109.98
11	A	820	CLA	CHB-C1B-NB	-2.10	120.89	124.05
11	B	810	CLA	CHD-C1D-ND	-2.10	121.84	124.80
13	A	845	BCR	C23-C24-C25	2.10	132.61	127.00
11	A	801	CLA	CHB-C1B-NB	-2.10	120.90	124.05
11	A	811	CLA	CHB-C1B-NB	-2.10	120.90	124.05
11	B	803	CLA	C1D-ND-C4D	-2.10	104.84	106.31
11	B	815	CLA	CHC-C1C-NC	2.10	127.47	124.31
11	B	805	CLA	CHC-C1C-NC	2.10	127.47	124.31
11	A	807	CLA	C1-C2-C3	-2.09	122.77	126.20
16	B	843	LMG	C42-C41-C40	-2.09	103.81	114.37
11	A	813	CLA	CHB-C1B-NB	-2.09	120.92	124.05
11	B	806	CLA	CHB-C1B-NB	-2.09	120.92	124.05
11	B	814	CLA	CHB-C1B-NB	-2.08	120.92	124.05
11	B	832	CLA	CHB-C1B-NB	-2.08	120.92	124.05
11	B	816	CLA	CHC-C1C-NC	2.08	127.44	124.31
13	F	201	BCR	C19-C18-C17	-2.08	115.74	119.01
11	B	814	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
11	A	801	CLA	C2C-C1C-NC	2.08	112.17	109.98
11	B	826	CLA	CHB-C1B-NB	-2.08	120.93	124.05
11	B	823	CLA	C1-C2-C3	-2.08	122.80	126.20
11	B	827	CLA	CHB-C1B-NB	-2.07	120.94	124.05
11	A	829	CLA	CHB-C1B-NB	-2.07	120.94	124.05
11	L	1503	CLA	CHB-C1B-NB	-2.07	120.94	124.05
11	B	815	CLA	CHB-C1B-NB	-2.07	120.95	124.05
11	B	822	CLA	C2C-C1C-NC	2.06	112.15	109.98
11	B	836	CLA	C3B-C4B-NB	-2.06	108.69	110.53
11	B	812	CLA	CHB-C1B-NB	-2.06	120.95	124.05
11	A	804	CLA	C1-C2-C3	-2.06	122.82	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	823	CLA	C2C-C1C-NC	2.06	112.15	109.98
11	A	803	CLA	CHB-C1B-NB	-2.06	120.96	124.05
11	A	818	CLA	CHB-C1B-NB	-2.06	120.96	124.05
11	A	812	CLA	C2C-C1C-NC	2.06	112.14	109.98
11	A	808	CLA	CHA-C1A-NA	-2.06	121.73	126.39
11	B	831	CLA	CHB-C1B-NB	-2.06	120.96	124.05
11	B	807	CLA	CHB-C1B-NB	-2.06	120.96	124.05
11	A	822	CLA	CHB-C1B-NB	-2.06	120.97	124.05
11	A	828	CLA	CHC-C1C-C2C	-2.06	121.11	126.95
11	A	838	CLA	CHA-C1A-NA	-2.05	121.74	126.39
11	B	802	CLA	C2C-C1C-NC	2.05	112.14	109.98
16	B	843	LMG	O7-C10-O9	-2.05	118.91	123.70
11	B	803	CLA	C2C-C1C-NC	2.05	112.14	109.98
11	B	830	CLA	CHB-C1B-NB	-2.05	120.98	124.05
11	B	802	CLA	CHB-C1B-NB	-2.04	120.98	124.05
11	A	833	CLA	C3B-C4B-NB	-2.04	108.71	110.53
11	A	814	CLA	CHB-C1B-NB	-2.04	120.99	124.05
11	B	829	CLA	CBA-CAA-C2A	2.04	117.74	113.41
11	B	825	CLA	CHB-C1B-NB	-2.04	120.99	124.05
11	A	840	CLA	CHB-C1B-NB	-2.04	121.00	124.05
11	B	805	CLA	C2C-C1C-NC	2.03	112.12	109.98
11	A	808	CLA	CHB-C1B-NB	-2.03	121.00	124.05
11	A	859	CLA	C1D-ND-C4D	-2.03	104.89	106.31
14	A	850	LHG	C27-C26-C25	-2.03	104.10	114.37
11	B	819	CLA	CHA-C1A-NA	-2.03	121.79	126.39
11	A	833	CLA	C2C-C1C-NC	2.03	112.11	109.98
11	A	804	CLA	CHB-C1B-NB	-2.03	121.00	124.05
11	A	802	CLA	C2C-C1C-NC	2.03	112.11	109.98
11	A	830	CLA	CHB-C1B-NB	-2.03	121.01	124.05
11	B	830	CLA	CAA-C2A-C1A	-2.03	106.81	111.81
11	A	803	CLA	CHA-C1A-NA	-2.03	121.81	126.39
11	B	824	CLA	C2A-C1A-CHA	2.02	127.38	123.87
11	A	836	CLA	CHB-C1B-NB	-2.02	121.01	124.05
11	B	822	CLA	CHB-C1B-NB	-2.02	121.01	124.05
11	B	835	CLA	C2C-C1C-NC	2.02	112.10	109.98
11	B	835	CLA	CHB-C1B-NB	-2.01	121.03	124.05
11	A	828	CLA	CHC-C1C-NC	2.01	127.34	124.31
11	A	842	CLA	C2A-C1A-CHA	2.01	125.83	122.71
11	B	801	CLA	CHA-C1A-NA	-2.01	121.84	126.39
11	A	840	CLA	CHA-C1A-NA	-2.01	121.85	126.39
11	A	835	CLA	CHB-C1B-NB	-2.01	121.04	124.05
11	B	821	CLA	CHB-C1B-NB	-2.00	121.04	124.05

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	B	810	CLA	C1D-ND-C4D	-2.00	104.91	106.31

All (82) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	801	CLA	ND
11	A	802	CLA	ND
11	A	803	CLA	ND
11	A	804	CLA	ND
11	A	805	CLA	ND
11	A	806	CLA	ND
11	A	807	CLA	ND
11	A	808	CLA	ND
11	A	809	CLA	ND
11	A	810	CLA	ND
11	A	811	CLA	ND
11	A	812	CLA	ND
11	A	813	CLA	ND
11	A	814	CLA	ND
11	A	815	CLA	ND
11	A	816	CLA	ND
11	A	817	CLA	ND
11	A	818	CLA	ND
11	A	819	CLA	ND
11	A	820	CLA	ND
11	A	821	CLA	ND
11	A	822	CLA	ND
11	A	823	CLA	ND
11	A	824	CLA	ND
11	A	825	CLA	ND
11	A	826	CLA	ND
11	A	827	CLA	ND
11	A	828	CLA	ND
11	A	829	CLA	ND
11	A	830	CLA	ND
11	A	831	CLA	ND
11	A	832	CLA	ND
11	A	833	CLA	ND
11	A	834	CLA	ND
11	A	835	CLA	ND
11	A	836	CLA	ND
11	A	837	CLA	ND

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Mol	Chain	Res	Type	Atom
11	A	838	CLA	ND
11	A	839	CLA	ND
11	A	840	CLA	ND
11	A	841	CLA	ND
11	A	842	CLA	ND
11	A	859	CLA	ND
11	A	860	CLA	ND
11	B	801	CLA	ND
11	B	802	CLA	ND
11	B	803	CLA	ND
11	B	805	CLA	ND
11	B	806	CLA	ND
11	B	807	CLA	ND
11	B	808	CLA	ND
11	B	809	CLA	ND
11	B	810	CLA	ND
11	B	811	CLA	ND
11	B	812	CLA	ND
11	B	813	CLA	ND
11	B	814	CLA	ND
11	B	815	CLA	ND
11	B	816	CLA	ND
11	B	817	CLA	ND
11	B	818	CLA	ND
11	B	819	CLA	ND
11	B	820	CLA	ND
11	B	821	CLA	ND
11	B	822	CLA	ND
11	B	823	CLA	ND
11	B	824	CLA	ND
11	B	825	CLA	ND
11	B	826	CLA	ND
11	B	827	CLA	ND
11	B	828	CLA	ND
11	B	829	CLA	ND
11	B	830	CLA	ND
11	B	831	CLA	ND
11	B	832	CLA	ND
11	B	833	CLA	ND
11	B	834	CLA	ND
11	B	835	CLA	ND
11	B	836	CLA	ND

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Mol	Chain	Res	Type	Atom
11	L	1501	CLA	ND
11	L	1502	CLA	ND
11	L	1503	CLA	ND

All (605) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	803	CLA	CAD-CBD-CGD-O1D
11	A	803	CLA	CAD-CBD-CGD-O2D
11	A	806	CLA	C1A-C2A-CAA-CBA
11	A	808	CLA	CHA-CBD-CGD-O1D
11	A	808	CLA	CHA-CBD-CGD-O2D
11	A	810	CLA	C1A-C2A-CAA-CBA
11	A	811	CLA	C4B-C3B-CAB-CBB
11	A	812	CLA	C4B-C3B-CAB-CBB
11	A	815	CLA	C2B-C3B-CAB-CBB
11	A	815	CLA	C4B-C3B-CAB-CBB
11	A	816	CLA	C1A-C2A-CAA-CBA
11	A	818	CLA	C2-C3-C5-C6
11	A	819	CLA	C3A-C2A-CAA-CBA
11	A	824	CLA	C1A-C2A-CAA-CBA
11	A	827	CLA	CHA-CBD-CGD-O1D
11	A	827	CLA	CHA-CBD-CGD-O2D
11	A	830	CLA	CHA-CBD-CGD-O1D
11	A	830	CLA	CHA-CBD-CGD-O2D
11	A	831	CLA	C2B-C3B-CAB-CBB
11	A	831	CLA	C4B-C3B-CAB-CBB
11	A	834	CLA	C4B-C3B-CAB-CBB
11	A	835	CLA	C4B-C3B-CAB-CBB
11	A	840	CLA	C2B-C3B-CAB-CBB
11	A	840	CLA	C4B-C3B-CAB-CBB
11	A	841	CLA	C2B-C3B-CAB-CBB
11	A	841	CLA	C4B-C3B-CAB-CBB
11	A	841	CLA	C1-C2-C3-C4
11	A	842	CLA	C4B-C3B-CAB-CBB
11	B	802	CLA	C2B-C3B-CAB-CBB
11	B	802	CLA	C4B-C3B-CAB-CBB
11	B	803	CLA	C1A-C2A-CAA-CBA
11	B	805	CLA	C2B-C3B-CAB-CBB
11	B	805	CLA	C4B-C3B-CAB-CBB
11	B	807	CLA	CAD-CBD-CGD-O1D
11	B	807	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	B	810	CLA	CHA-CBD-CGD-O1D
11	B	810	CLA	CHA-CBD-CGD-O2D
11	B	815	CLA	C2B-C3B-CAB-CBB
11	B	815	CLA	C4B-C3B-CAB-CBB
11	B	816	CLA	CHA-CBD-CGD-O1D
11	B	816	CLA	CHA-CBD-CGD-O2D
11	B	817	CLA	C1A-C2A-CAA-CBA
11	B	818	CLA	C4B-C3B-CAB-CBB
11	B	821	CLA	C2B-C3B-CAB-CBB
11	B	821	CLA	C4B-C3B-CAB-CBB
11	B	821	CLA	CHA-CBD-CGD-O1D
11	B	821	CLA	CHA-CBD-CGD-O2D
11	B	822	CLA	C1A-C2A-CAA-CBA
11	B	822	CLA	C2B-C3B-CAB-CBB
11	B	822	CLA	C4B-C3B-CAB-CBB
11	B	822	CLA	CHA-CBD-CGD-O2D
11	B	825	CLA	C4B-C3B-CAB-CBB
11	B	825	CLA	CHA-CBD-CGD-O1D
11	B	825	CLA	CHA-CBD-CGD-O2D
11	B	826	CLA	C2B-C3B-CAB-CBB
11	B	826	CLA	C4B-C3B-CAB-CBB
11	B	827	CLA	C4B-C3B-CAB-CBB
11	B	830	CLA	CAD-CBD-CGD-O2D
11	B	832	CLA	CHA-CBD-CGD-O1D
11	B	832	CLA	CHA-CBD-CGD-O2D
11	B	835	CLA	C4B-C3B-CAB-CBB
11	B	836	CLA	C1A-C2A-CAA-CBA
11	B	836	CLA	CAD-CBD-CGD-O1D
11	B	836	CLA	CAD-CBD-CGD-O2D
11	L	1501	CLA	C4B-C3B-CAB-CBB
11	L	1503	CLA	C4B-C3B-CAB-CBB
13	A	845	BCR	C23-C24-C25-C26
13	A	845	BCR	C23-C24-C25-C30
13	A	849	BCR	C7-C8-C9-C10
13	A	849	BCR	C10-C11-C12-C13
13	A	849	BCR	C11-C12-C13-C35
13	A	852	BCR	C1-C6-C7-C8
13	A	852	BCR	C10-C11-C12-C13
13	A	852	BCR	C11-C12-C13-C14
13	A	852	BCR	C11-C12-C13-C35
13	A	856	BCR	C13-C14-C15-C16
13	A	858	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
13	F	201	BCR	C5-C6-C7-C8
13	F	201	BCR	C13-C14-C15-C16
13	F	201	BCR	C15-C16-C17-C18
13	F	201	BCR	C17-C18-C19-C20
13	F	201	BCR	C36-C18-C19-C20
13	F	201	BCR	C18-C19-C20-C21
13	F	201	BCR	C21-C22-C23-C24
13	F	201	BCR	C37-C22-C23-C24
13	L	1504	BCR	C23-C24-C25-C30
13	M	101	BCR	C1-C6-C7-C8
13	M	101	BCR	C5-C6-C7-C8
14	A	850	LHG	C3-O3-P-O4
14	A	850	LHG	C3-O3-P-O6
14	A	851	LHG	C3-O3-P-O6
14	A	851	LHG	C4-O6-P-O5
12	A	843	PQN	C25-C26-C27-C28
11	B	835	CLA	C3-C5-C6-C7
12	B	837	PQN	C13-C15-C16-C17
11	A	818	CLA	C4-C3-C5-C6
11	B	811	CLA	C4-C3-C5-C6
12	A	843	PQN	C14-C13-C15-C16
12	A	843	PQN	C12-C13-C15-C16
13	A	849	BCR	C19-C20-C21-C22
13	F	201	BCR	C19-C20-C21-C22
14	A	851	LHG	O2-C2-C3-O3
11	B	810	CLA	C3-C5-C6-C7
11	A	825	CLA	C13-C15-C16-C17
11	B	824	CLA	C2A-CAA-CBA-CGA
14	A	851	LHG	C1-C2-C3-O3
11	A	835	CLA	C2-C3-C5-C6
11	B	811	CLA	C2-C3-C5-C6
11	A	825	CLA	C11-C12-C13-C14
12	A	843	PQN	C16-C17-C18-C19
12	A	843	PQN	C19-C18-C20-C21
12	B	837	PQN	C16-C17-C18-C19
12	B	837	PQN	C24-C23-C25-C26
13	A	856	BCR	C11-C12-C13-C35
13	A	856	BCR	C11-C12-C13-C14
11	B	803	CLA	C2A-CAA-CBA-CGA
11	A	806	CLA	C13-C15-C16-C17
11	A	859	CLA	C3-C5-C6-C7
12	A	843	PQN	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	B	818	CLA	C5-C6-C7-C8
11	A	824	CLA	C13-C15-C16-C17
11	A	818	CLA	C2A-CAA-CBA-CGA
11	A	829	CLA	C2A-CAA-CBA-CGA
11	B	806	CLA	C2A-CAA-CBA-CGA
11	B	835	CLA	C2A-CAA-CBA-CGA
11	A	813	CLA	C10-C11-C12-C13
16	B	843	LMG	O6-C1-O1-C7
11	A	833	CLA	C5-C6-C7-C8
14	A	850	LHG	C23-C24-C25-C26
16	B	843	LMG	C28-C29-C30-C31
11	A	835	CLA	C4-C3-C5-C6
11	B	825	CLA	C8-C10-C11-C12
16	B	843	LMG	O6-C5-C6-O5
14	A	850	LHG	O9-C7-O7-C5
11	B	831	CLA	C2A-CAA-CBA-CGA
11	B	805	CLA	C13-C15-C16-C17
11	A	811	CLA	C15-C16-C17-C18
11	A	827	CLA	C13-C15-C16-C17
11	B	820	CLA	C4-C3-C5-C6
11	B	820	CLA	C2-C3-C5-C6
11	B	807	CLA	C13-C15-C16-C17
16	B	843	LMG	C2-C1-O1-C7
13	F	201	BCR	C35-C13-C14-C15
11	A	817	CLA	C2A-CAA-CBA-CGA
11	A	828	CLA	C2A-CAA-CBA-CGA
11	B	823	CLA	C2A-CAA-CBA-CGA
11	B	835	CLA	C13-C15-C16-C17
14	A	850	LHG	O1-C1-C2-C3
14	A	851	LHG	O1-C1-C2-C3
11	A	819	CLA	C16-C17-C18-C20
11	A	828	CLA	C16-C17-C18-C20
11	B	803	CLA	C3-C5-C6-C7
13	A	849	BCR	C11-C10-C9-C8
13	A	849	BCR	C12-C13-C14-C15
13	A	849	BCR	C16-C17-C18-C19
13	A	852	BCR	C11-C10-C9-C8
13	A	852	BCR	C12-C13-C14-C15
13	A	852	BCR	C16-C17-C18-C19
13	A	856	BCR	C12-C13-C14-C15
13	F	201	BCR	C12-C13-C14-C15
13	A	856	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
14	A	850	LHG	C31-C32-C33-C34
14	A	850	LHG	C27-C28-C29-C30
16	B	843	LMG	C16-C17-C18-C19
16	B	843	LMG	C29-C30-C31-C32
16	B	843	LMG	C40-C41-C42-C43
16	B	843	LMG	C41-C42-C43-C44
11	A	801	CLA	C4B-C3B-CAB-CBB
11	A	803	CLA	C4B-C3B-CAB-CBB
11	A	804	CLA	C4B-C3B-CAB-CBB
11	A	806	CLA	C4B-C3B-CAB-CBB
11	A	807	CLA	C4B-C3B-CAB-CBB
11	A	808	CLA	C4B-C3B-CAB-CBB
11	A	809	CLA	C4B-C3B-CAB-CBB
11	A	813	CLA	C4B-C3B-CAB-CBB
11	A	814	CLA	C4B-C3B-CAB-CBB
11	A	816	CLA	C4B-C3B-CAB-CBB
11	A	818	CLA	C4B-C3B-CAB-CBB
11	A	819	CLA	C4B-C3B-CAB-CBB
11	A	820	CLA	C4B-C3B-CAB-CBB
11	A	822	CLA	C4B-C3B-CAB-CBB
11	A	823	CLA	C4B-C3B-CAB-CBB
11	A	824	CLA	C4B-C3B-CAB-CBB
11	A	827	CLA	C4B-C3B-CAB-CBB
11	A	830	CLA	C4B-C3B-CAB-CBB
11	A	832	CLA	C4B-C3B-CAB-CBB
11	A	833	CLA	C4B-C3B-CAB-CBB
11	A	836	CLA	C4B-C3B-CAB-CBB
11	A	838	CLA	C4B-C3B-CAB-CBB
11	B	806	CLA	C4B-C3B-CAB-CBB
11	B	807	CLA	C4B-C3B-CAB-CBB
11	B	808	CLA	C4B-C3B-CAB-CBB
11	B	809	CLA	C4B-C3B-CAB-CBB
11	B	810	CLA	C4B-C3B-CAB-CBB
11	B	811	CLA	C4B-C3B-CAB-CBB
11	B	814	CLA	C4B-C3B-CAB-CBB
11	B	817	CLA	C4B-C3B-CAB-CBB
11	B	819	CLA	C4B-C3B-CAB-CBB
11	B	820	CLA	C4B-C3B-CAB-CBB
11	B	823	CLA	C4B-C3B-CAB-CBB
11	B	829	CLA	C4B-C3B-CAB-CBB
11	B	830	CLA	C4B-C3B-CAB-CBB
11	B	831	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	B	833	CLA	C4B-C3B-CAB-CBB
11	L	1502	CLA	C4B-C3B-CAB-CBB
11	A	828	CLA	C16-C17-C18-C19
16	B	843	LMG	C37-C38-C39-C40
12	B	837	PQN	C17-C18-C20-C21
14	A	850	LHG	C24-C25-C26-C27
11	A	805	CLA	C3A-C2A-CAA-CBA
11	A	810	CLA	C3A-C2A-CAA-CBA
11	A	816	CLA	C3A-C2A-CAA-CBA
11	A	837	CLA	C3A-C2A-CAA-CBA
11	A	859	CLA	C3A-C2A-CAA-CBA
11	B	808	CLA	C3A-C2A-CAA-CBA
11	B	815	CLA	C3A-C2A-CAA-CBA
14	A	851	LHG	C4-C5-C6-O8
16	B	843	LMG	C32-C33-C34-C35
11	A	803	CLA	C2B-C3B-CAB-CBB
11	A	806	CLA	C2B-C3B-CAB-CBB
11	A	811	CLA	C2B-C3B-CAB-CBB
11	A	812	CLA	C2B-C3B-CAB-CBB
11	A	816	CLA	C2B-C3B-CAB-CBB
11	A	818	CLA	C2B-C3B-CAB-CBB
11	A	819	CLA	C2B-C3B-CAB-CBB
11	A	820	CLA	C2B-C3B-CAB-CBB
11	A	823	CLA	C2B-C3B-CAB-CBB
11	A	827	CLA	C2B-C3B-CAB-CBB
11	A	833	CLA	C2B-C3B-CAB-CBB
11	A	834	CLA	C2B-C3B-CAB-CBB
11	A	835	CLA	C2B-C3B-CAB-CBB
11	A	836	CLA	C2B-C3B-CAB-CBB
11	A	838	CLA	C2B-C3B-CAB-CBB
11	A	842	CLA	C2B-C3B-CAB-CBB
11	B	808	CLA	C2B-C3B-CAB-CBB
11	B	809	CLA	C2B-C3B-CAB-CBB
11	B	810	CLA	C2B-C3B-CAB-CBB
11	B	814	CLA	C2B-C3B-CAB-CBB
11	B	818	CLA	C2B-C3B-CAB-CBB
11	B	819	CLA	C2B-C3B-CAB-CBB
11	B	825	CLA	C2B-C3B-CAB-CBB
11	B	827	CLA	C2B-C3B-CAB-CBB
11	B	830	CLA	C2B-C3B-CAB-CBB
11	B	835	CLA	C2B-C3B-CAB-CBB
11	B	836	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	L	1501	CLA	C2B-C3B-CAB-CBB
11	L	1503	CLA	C2B-C3B-CAB-CBB
13	A	856	BCR	C1-C6-C7-C8
13	A	856	BCR	C5-C6-C7-C8
13	A	858	BCR	C23-C24-C25-C30
13	B	839	BCR	C1-C6-C7-C8
13	B	839	BCR	C5-C6-C7-C8
13	F	201	BCR	C1-C6-C7-C8
13	L	1504	BCR	C23-C24-C25-C26
11	A	859	CLA	C2A-CAA-CBA-CGA
11	A	860	CLA	C2A-CAA-CBA-CGA
16	B	843	LMG	C34-C35-C36-C37
13	A	856	BCR	C10-C11-C12-C13
13	A	849	BCR	C14-C15-C16-C17
12	B	837	PQN	C15-C16-C17-C18
11	A	819	CLA	C16-C17-C18-C19
14	A	850	LHG	C8-C7-O7-C5
14	A	851	LHG	C7-C8-C9-C10
11	B	833	CLA	C4-C3-C5-C6
11	A	817	CLA	C3-C5-C6-C7
12	A	843	PQN	C20-C21-C22-C23
11	A	811	CLA	C4-C3-C5-C6
11	A	811	CLA	C2-C3-C5-C6
11	B	833	CLA	C2-C3-C5-C6
11	A	841	CLA	C2A-CAA-CBA-CGA
11	B	820	CLA	C2A-CAA-CBA-CGA
12	B	837	PQN	C11-C12-C13-C14
14	A	851	LHG	O1-C1-C2-O2
11	A	805	CLA	C1A-C2A-CAA-CBA
11	A	817	CLA	C1A-C2A-CAA-CBA
11	A	819	CLA	C1A-C2A-CAA-CBA
11	A	828	CLA	C1A-C2A-CAA-CBA
11	A	830	CLA	C1A-C2A-CAA-CBA
11	A	832	CLA	C1A-C2A-CAA-CBA
11	A	837	CLA	C1A-C2A-CAA-CBA
11	A	859	CLA	C1A-C2A-CAA-CBA
11	B	808	CLA	C1A-C2A-CAA-CBA
11	B	815	CLA	C1A-C2A-CAA-CBA
11	B	818	CLA	C1A-C2A-CAA-CBA
11	B	834	CLA	C1A-C2A-CAA-CBA
16	B	843	LMG	C33-C34-C35-C36
11	A	805	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
11	A	813	CLA	C12-C13-C15-C16
11	A	829	CLA	C12-C13-C15-C16
12	A	843	PQN	C22-C23-C25-C26
12	B	837	PQN	C16-C17-C18-C20
11	A	825	CLA	C4-C3-C5-C6
11	A	825	CLA	C2-C3-C5-C6
11	B	816	CLA	C2-C3-C5-C6
11	A	802	CLA	C2A-CAA-CBA-CGA
11	A	805	CLA	C11-C12-C13-C14
11	A	811	CLA	C11-C12-C13-C14
11	A	824	CLA	C11-C10-C8-C9
11	A	829	CLA	C14-C13-C15-C16
11	A	834	CLA	C14-C13-C15-C16
12	A	843	PQN	C24-C23-C25-C26
16	B	843	LMG	C23-C24-C25-C26
13	A	856	BCR	C35-C13-C14-C15
11	A	827	CLA	C2-C3-C5-C6
11	B	815	CLA	C2-C3-C5-C6
11	A	815	CLA	C2A-CAA-CBA-CGA
11	B	828	CLA	O2A-C1-C2-C3
16	B	843	LMG	C31-C32-C33-C34
14	A	850	LHG	O6-C4-C5-O7
11	B	815	CLA	C4-C3-C5-C6
11	B	819	CLA	C4-C3-C5-C6
14	A	850	LHG	O7-C5-C6-O8
14	A	850	LHG	C29-C30-C31-C32
11	A	827	CLA	C4-C3-C5-C6
11	B	810	CLA	C4-C3-C5-C6
11	A	813	CLA	C14-C13-C15-C16
11	A	825	CLA	C14-C13-C15-C16
11	A	827	CLA	C14-C13-C15-C16
11	B	815	CLA	C6-C7-C8-C9
12	B	837	PQN	C19-C18-C20-C21
11	A	805	CLA	C4B-C3B-CAB-CBB
11	A	810	CLA	C4B-C3B-CAB-CBB
11	A	817	CLA	C4B-C3B-CAB-CBB
11	A	821	CLA	C4B-C3B-CAB-CBB
11	A	826	CLA	C4B-C3B-CAB-CBB
11	A	829	CLA	C4B-C3B-CAB-CBB
11	A	837	CLA	C4B-C3B-CAB-CBB
11	A	839	CLA	C4B-C3B-CAB-CBB
11	A	859	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
11	B	803	CLA	C4B-C3B-CAB-CBB
11	B	812	CLA	C4B-C3B-CAB-CBB
11	B	816	CLA	C4B-C3B-CAB-CBB
11	B	824	CLA	C4B-C3B-CAB-CBB
11	B	832	CLA	C4B-C3B-CAB-CBB
11	B	836	CLA	C4B-C3B-CAB-CBB
11	A	811	CLA	C11-C12-C13-C15
11	A	813	CLA	C11-C12-C13-C15
11	A	824	CLA	C11-C10-C8-C7
11	A	825	CLA	C12-C13-C15-C16
11	A	827	CLA	C12-C13-C15-C16
11	A	834	CLA	C12-C13-C15-C16
12	A	843	PQN	C16-C17-C18-C20
13	A	852	BCR	C5-C6-C7-C8
11	A	806	CLA	C3A-C2A-CAA-CBA
11	A	813	CLA	C3A-C2A-CAA-CBA
11	A	824	CLA	C3A-C2A-CAA-CBA
11	A	808	CLA	C2A-CAA-CBA-CGA
16	B	843	LMG	C19-C20-C21-C22
11	A	808	CLA	C4-C3-C5-C6
11	B	816	CLA	C4-C3-C5-C6
11	B	810	CLA	C2-C3-C5-C6
11	B	828	CLA	C10-C11-C12-C13
11	B	803	CLA	C2B-C3B-CAB-CBB
13	A	861	BCR	C23-C24-C25-C26
13	A	861	BCR	C23-C24-C25-C30
13	B	842	BCR	C1-C6-C7-C8
13	I	102	BCR	C23-C24-C25-C30
16	B	843	LMG	C15-C16-C17-C18
11	A	834	CLA	C4-C3-C5-C6
11	A	813	CLA	C11-C12-C13-C14
11	A	825	CLA	C16-C17-C18-C20
11	A	821	CLA	C4-C3-C5-C6
11	B	811	CLA	C16-C17-C18-C19
14	A	850	LHG	C32-C33-C34-C35
13	A	852	BCR	C35-C13-C14-C15
11	A	819	CLA	C6-C7-C8-C10
11	A	827	CLA	C11-C10-C8-C7
11	B	815	CLA	C6-C7-C8-C10
12	A	843	PQN	C12-C11-C3-C2
11	A	859	CLA	C4-C3-C5-C6
11	A	813	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
11	A	822	CLA	O2A-C1-C2-C3
11	A	805	CLA	C2A-CAA-CBA-CGA
11	A	859	CLA	C2-C3-C5-C6
12	A	843	PQN	C12-C11-C3-C4
11	A	801	CLA	C3-C5-C6-C7
11	A	827	CLA	C11-C10-C8-C9
14	A	850	LHG	C11-C10-C9-C8
11	B	802	CLA	C3-C5-C6-C7
16	B	843	LMG	C4-C5-C6-O5
11	A	813	CLA	C1A-C2A-CAA-CBA
11	A	818	CLA	C1A-C2A-CAA-CBA
11	B	834	CLA	C4B-C3B-CAB-CBB
11	A	819	CLA	CBA-CGA-O2A-C1
11	B	803	CLA	C4-C3-C5-C6
13	A	849	BCR	C11-C12-C13-C14
11	A	832	CLA	C2-C3-C5-C6
11	A	806	CLA	C11-C12-C13-C15
11	A	826	CLA	C11-C10-C8-C7
11	B	805	CLA	C12-C13-C15-C16
12	A	843	PQN	C17-C18-C20-C21
12	B	837	PQN	C22-C23-C25-C26
16	B	843	LMG	C18-C19-C20-C21
11	B	811	CLA	C16-C17-C18-C20
11	A	834	CLA	C2-C3-C5-C6
13	A	852	BCR	C14-C15-C16-C17
11	A	819	CLA	C6-C7-C8-C9
11	A	822	CLA	C1-C2-C3-C4
11	A	831	CLA	C1-C2-C3-C4
14	A	851	LHG	O7-C5-C6-O8
11	A	821	CLA	C2-C3-C5-C6
11	A	805	CLA	CAD-CBD-CGD-O2D
11	A	815	CLA	CAD-CBD-CGD-O2D
11	A	820	CLA	CAD-CBD-CGD-O2D
11	A	805	CLA	CAD-CBD-CGD-O1D
11	A	815	CLA	CAD-CBD-CGD-O1D
11	A	820	CLA	CAD-CBD-CGD-O1D
11	B	806	CLA	CHA-CBD-CGD-O1D
11	B	806	CLA	CHA-CBD-CGD-O2D
11	B	820	CLA	CHA-CBD-CGD-O1D
11	B	829	CLA	CHA-CBD-CGD-O1D
11	B	829	CLA	CHA-CBD-CGD-O2D
11	B	830	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	A	855	BCR	C1-C6-C7-C8
14	A	851	LHG	C3-O3-P-O5
14	A	851	LHG	C4-O6-P-O3
14	A	851	LHG	C4-O6-P-O4
11	B	823	CLA	C4-C3-C5-C6
11	A	801	CLA	C2B-C3B-CAB-CBB
11	A	804	CLA	C2B-C3B-CAB-CBB
11	A	807	CLA	C2B-C3B-CAB-CBB
11	A	808	CLA	C2B-C3B-CAB-CBB
11	A	809	CLA	C2B-C3B-CAB-CBB
11	A	810	CLA	C2B-C3B-CAB-CBB
11	A	813	CLA	C2B-C3B-CAB-CBB
11	A	814	CLA	C2B-C3B-CAB-CBB
11	A	822	CLA	C2B-C3B-CAB-CBB
11	A	824	CLA	C2B-C3B-CAB-CBB
11	A	830	CLA	C2B-C3B-CAB-CBB
11	A	832	CLA	C2B-C3B-CAB-CBB
11	A	839	CLA	C2B-C3B-CAB-CBB
11	A	859	CLA	C2B-C3B-CAB-CBB
11	B	806	CLA	C2B-C3B-CAB-CBB
11	B	807	CLA	C2B-C3B-CAB-CBB
11	B	811	CLA	C2B-C3B-CAB-CBB
11	B	812	CLA	C2B-C3B-CAB-CBB
11	B	816	CLA	C2B-C3B-CAB-CBB
11	B	817	CLA	C2B-C3B-CAB-CBB
11	B	820	CLA	C2B-C3B-CAB-CBB
11	B	823	CLA	C2B-C3B-CAB-CBB
11	B	824	CLA	C2B-C3B-CAB-CBB
11	B	829	CLA	C2B-C3B-CAB-CBB
11	B	831	CLA	C2B-C3B-CAB-CBB
11	B	832	CLA	C2B-C3B-CAB-CBB
11	B	833	CLA	C2B-C3B-CAB-CBB
11	B	834	CLA	C2B-C3B-CAB-CBB
11	L	1502	CLA	C2B-C3B-CAB-CBB
13	A	848	BCR	C1-C6-C7-C8
13	B	840	BCR	C18-C19-C20-C21
11	B	803	CLA	C2-C3-C5-C6
14	A	850	LHG	O6-C4-C5-C6
11	A	830	CLA	C6-C7-C8-C9
11	A	808	CLA	C2-C3-C5-C6
16	B	843	LMG	C42-C43-C44-C45
11	A	827	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
11	A	819	CLA	C2A-CAA-CBA-CGA
11	B	819	CLA	C2-C3-C5-C6
14	A	850	LHG	C4-C5-C6-O8
14	A	850	LHG	C35-C36-C37-C38
12	A	843	PQN	C26-C27-C28-C29
11	B	823	CLA	C2-C3-C5-C6
11	A	841	CLA	O2A-C1-C2-C3
11	A	819	CLA	O1A-CGA-O2A-C1
11	B	809	CLA	C4-C3-C5-C6
11	B	822	CLA	C3A-C2A-CAA-CBA
11	B	836	CLA	C3A-C2A-CAA-CBA
16	B	843	LMG	C11-C12-C13-C14
13	B	839	BCR	C11-C10-C9-C34
13	B	840	BCR	C11-C10-C9-C34
13	I	102	BCR	C20-C21-C22-C37
11	A	825	CLA	C8-C10-C11-C12
11	A	832	CLA	C4-C3-C5-C6
13	L	1504	BCR	C21-C22-C23-C24
11	A	804	CLA	C6-C7-C8-C9
11	A	828	CLA	C11-C12-C13-C14
11	B	807	CLA	C11-C10-C8-C9
11	B	807	CLA	C14-C13-C15-C16
11	B	811	CLA	C11-C10-C8-C9
11	A	825	CLA	C16-C17-C18-C19
14	A	850	LHG	O1-C1-C2-O2
11	A	812	CLA	C1A-C2A-CAA-CBA
11	B	823	CLA	C1A-C2A-CAA-CBA
13	A	852	BCR	C20-C21-C22-C23
13	B	839	BCR	C11-C10-C9-C8
13	B	840	BCR	C11-C10-C9-C8
13	I	102	BCR	C20-C21-C22-C23
11	A	805	CLA	C2B-C3B-CAB-CBB
11	A	817	CLA	C2B-C3B-CAB-CBB
11	A	821	CLA	C2B-C3B-CAB-CBB
11	A	825	CLA	C2B-C3B-CAB-CBB
11	A	837	CLA	C2B-C3B-CAB-CBB
13	B	841	BCR	C23-C24-C25-C30
13	B	842	BCR	C5-C6-C7-C8
13	I	102	BCR	C23-C24-C25-C26
16	B	843	LMG	C30-C31-C32-C33
11	A	802	CLA	C4-C3-C5-C6
11	A	817	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
11	B	802	CLA	C4-C3-C5-C6
11	A	831	CLA	O2A-C1-C2-C3
11	B	802	CLA	C2A-CAA-CBA-CGA
11	A	834	CLA	C5-C6-C7-C8
11	A	836	CLA	CAA-CBA-CGA-O2A
11	A	829	CLA	C4-C3-C5-C6
11	A	819	CLA	C2-C1-O2A-CGA
11	A	836	CLA	CAA-CBA-CGA-O1A
11	A	804	CLA	C4-C3-C5-C6
11	A	806	CLA	C2-C3-C5-C6
14	A	850	LHG	C10-C11-C12-C13
11	B	809	CLA	C2A-CAA-CBA-CGA
11	B	815	CLA	C2A-CAA-CBA-CGA
11	A	802	CLA	C4B-C3B-CAB-CBB
11	A	825	CLA	C4B-C3B-CAB-CBB
11	B	805	CLA	CAA-CBA-CGA-O2A
13	A	849	BCR	C11-C10-C9-C34
11	B	815	CLA	C5-C6-C7-C8
11	A	801	CLA	CAA-CBA-CGA-O2A
11	B	807	CLA	C11-C10-C8-C7
11	A	818	CLA	CAA-CBA-CGA-O2A
11	A	826	CLA	C11-C10-C8-C9
11	B	828	CLA	C11-C12-C13-C14
11	A	806	CLA	C2-C1-O2A-CGA
11	A	807	CLA	C2-C1-O2A-CGA
11	A	860	CLA	C2-C1-O2A-CGA
11	B	823	CLA	C2-C1-O2A-CGA
11	A	818	CLA	C3A-C2A-CAA-CBA
11	B	828	CLA	C3-C5-C6-C7
11	B	819	CLA	CAA-CBA-CGA-O2A
11	B	809	CLA	C2-C3-C5-C6
11	A	826	CLA	C2A-CAA-CBA-CGA
11	A	811	CLA	CAA-CBA-CGA-O2A
11	B	808	CLA	CAA-CBA-CGA-O2A
14	A	850	LHG	C33-C34-C35-C36
11	B	831	CLA	CAA-CBA-CGA-O1A
11	A	804	CLA	CAA-CBA-CGA-O2A
11	B	811	CLA	CAA-CBA-CGA-O2A
11	B	814	CLA	CAA-CBA-CGA-O1A
12	A	843	PQN	C26-C27-C28-C30
11	B	814	CLA	CAA-CBA-CGA-O2A
11	B	831	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
11	A	825	CLA	C11-C12-C13-C15
11	B	801	CLA	C11-C10-C8-C7
11	B	807	CLA	C12-C13-C15-C16
11	B	811	CLA	C11-C12-C13-C15
11	B	816	CLA	C12-C13-C15-C16
11	A	802	CLA	C2B-C3B-CAB-CBB
11	A	826	CLA	C2B-C3B-CAB-CBB
11	A	829	CLA	C2B-C3B-CAB-CBB
13	A	847	BCR	C1-C6-C7-C8
13	A	847	BCR	C5-C6-C7-C8
13	A	848	BCR	C5-C6-C7-C8
13	B	840	BCR	C23-C24-C25-C30
13	B	841	BCR	C23-C24-C25-C26
13	B	842	BCR	C23-C24-C25-C30
11	A	817	CLA	C2-C1-O2A-CGA
11	A	837	CLA	C2-C1-O2A-CGA
11	B	801	CLA	C2-C1-O2A-CGA
11	B	817	CLA	CAA-CBA-CGA-O1A
11	B	822	CLA	CAA-CBA-CGA-O2A
11	A	860	CLA	CAA-CBA-CGA-O2A
13	A	852	BCR	C16-C17-C18-C36
11	B	822	CLA	C2A-CAA-CBA-CGA
11	A	806	CLA	C11-C12-C13-C14
11	B	811	CLA	C5-C6-C7-C8
11	B	807	CLA	C1A-C2A-CAA-CBA
11	B	801	CLA	CAA-CBA-CGA-O2A
13	A	852	BCR	C21-C22-C23-C24
11	B	803	CLA	CAA-CBA-CGA-O2A
14	A	850	LHG	O8-C23-C24-C25
16	B	843	LMG	C36-C37-C38-C39
11	A	813	CLA	C2-C1-O2A-CGA
11	A	821	CLA	C2-C1-O2A-CGA
12	B	837	PQN	C26-C27-C28-C30
14	A	851	LHG	O7-C7-C8-C9
11	A	804	CLA	CAA-CBA-CGA-O1A
11	B	822	CLA	CAA-CBA-CGA-O1A
11	B	814	CLA	C3A-C2A-CAA-CBA
11	B	817	CLA	C3A-C2A-CAA-CBA
11	B	822	CLA	CHA-CBD-CGD-O1D
14	A	850	LHG	O10-C23-C24-C25
11	B	824	CLA	C13-C15-C16-C17
11	A	813	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
11	B	805	CLA	C14-C13-C15-C16
16	B	843	LMG	O7-C10-C11-C12
11	B	817	CLA	CAA-CBA-CGA-O2A
11	A	826	CLA	C4-C3-C5-C6
11	B	808	CLA	CAA-CBA-CGA-O1A
11	B	823	CLA	CAA-CBA-CGA-O2A
13	A	852	BCR	C17-C18-C19-C20
11	B	811	CLA	CAA-CBA-CGA-O1A
14	A	851	LHG	O9-C7-C8-C9
11	A	860	CLA	CAA-CBA-CGA-O1A
11	A	811	CLA	CAA-CBA-CGA-O1A
11	A	806	CLA	C4-C3-C5-C6
11	A	830	CLA	C8-C10-C11-C12
11	A	817	CLA	C2-C3-C5-C6
11	B	803	CLA	CAA-CBA-CGA-O1A
11	B	834	CLA	CAD-CBD-CGD-O2D
11	A	805	CLA	CAA-CBA-CGA-O2A
16	B	843	LMG	C14-C15-C16-C17
11	A	811	CLA	C2-C1-O2A-CGA
11	A	834	CLA	C2-C1-O2A-CGA
11	A	841	CLA	C2-C1-O2A-CGA
11	B	820	CLA	CAA-CBA-CGA-O2A
14	A	851	LHG	C8-C7-O7-C5
11	B	801	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

70 monomers are involved in 120 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	813	CLA	2	0
11	B	811	CLA	1	0
11	A	824	CLA	2	0
13	B	840	BCR	1	0
11	A	859	CLA	2	0
11	A	840	CLA	1	0
11	B	824	CLA	3	0
13	A	848	BCR	1	0
11	A	827	CLA	1	0
13	A	849	BCR	2	0
11	B	818	CLA	2	0
11	A	821	CLA	4	0
11	A	819	CLA	1	0

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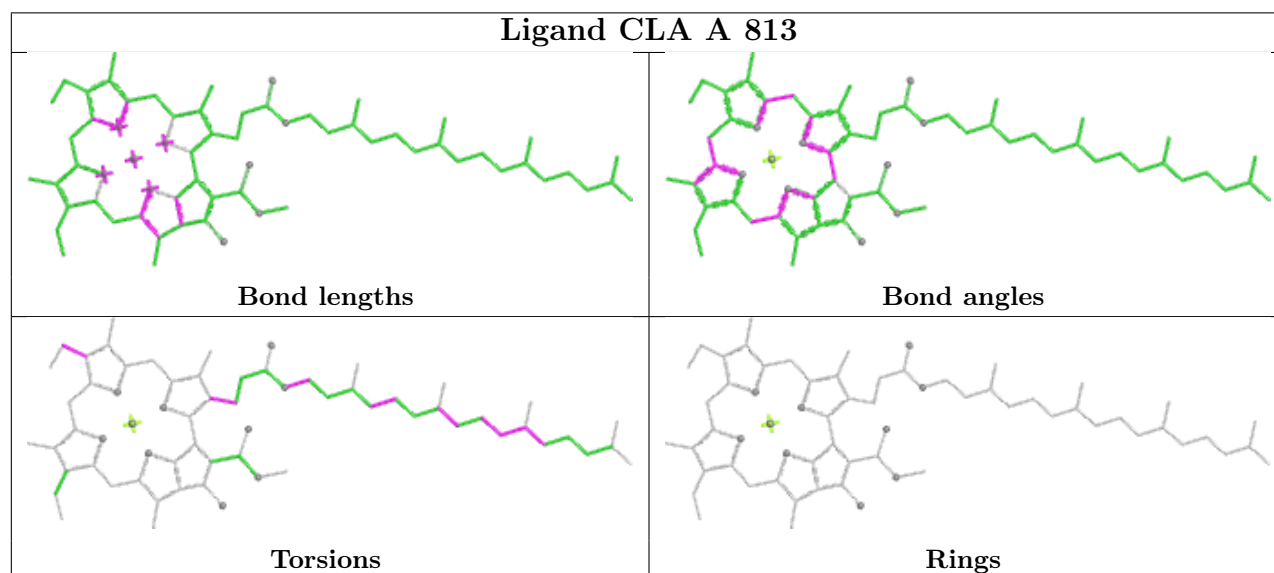
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	L	1503	CLA	1	0
11	B	820	CLA	1	0
11	B	812	CLA	1	0
13	F	201	BCR	13	0
11	A	838	CLA	1	0
11	B	807	CLA	2	0
11	A	825	CLA	2	0
11	A	802	CLA	1	0
11	B	816	CLA	3	0
11	B	825	CLA	1	0
11	A	815	CLA	1	0
13	A	857	BCR	2	0
11	B	815	CLA	3	0
11	A	837	CLA	3	0
11	A	818	CLA	3	0
11	A	828	CLA	1	0
11	A	808	CLA	2	0
11	A	805	CLA	3	0
11	A	820	CLA	2	0
11	B	808	CLA	2	0
11	B	805	CLA	3	0
11	B	828	CLA	2	0
13	A	845	BCR	2	0
13	B	842	BCR	1	0
13	A	852	BCR	2	0
11	A	831	CLA	1	0
11	A	809	CLA	2	0
13	B	841	BCR	2	0
11	A	841	CLA	2	0
13	A	855	BCR	2	0
13	A	858	BCR	2	0
13	F	202	BCR	2	0
13	I	101	BCR	2	0
11	B	821	CLA	1	0
11	A	836	CLA	1	0
11	B	813	CLA	1	0
12	B	837	PQN	9	0
11	B	829	CLA	1	0
11	A	835	CLA	1	0
13	B	838	BCR	1	0
11	B	802	CLA	4	0
11	A	830	CLA	1	0

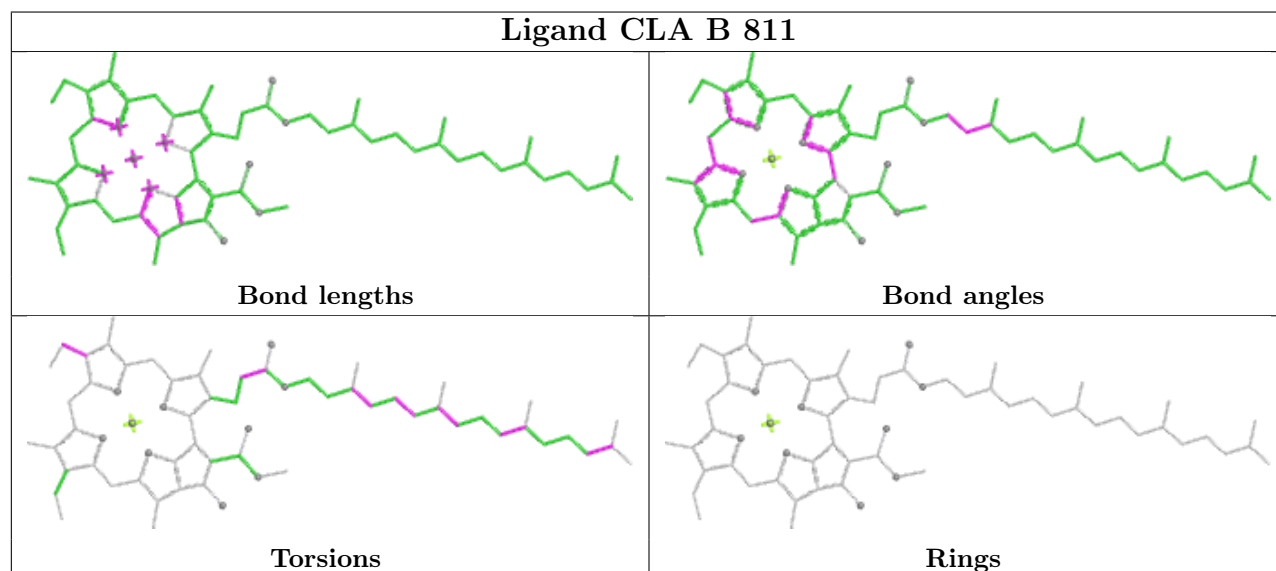
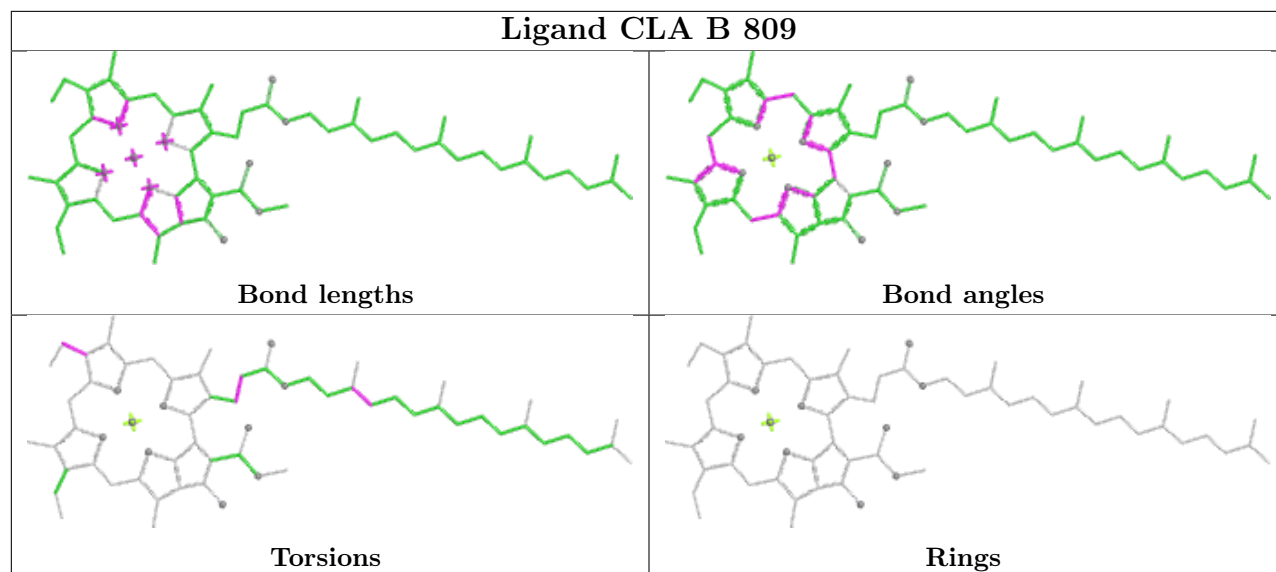
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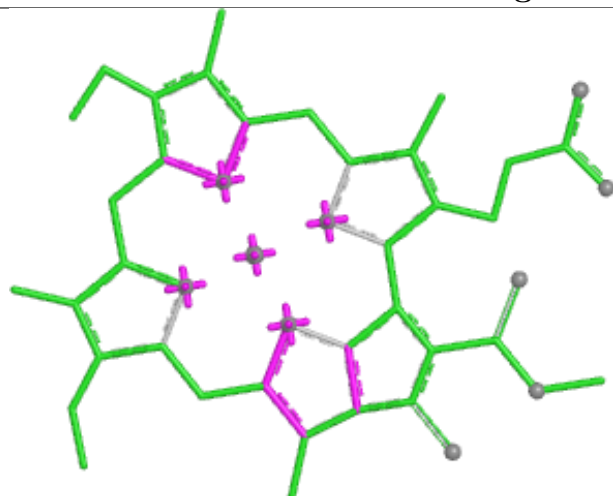
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	843	PQN	21	0
11	B	836	CLA	1	0
13	A	846	BCR	1	0
11	A	826	CLA	1	0
11	A	806	CLA	2	0
11	A	860	CLA	1	0
11	A	811	CLA	3	0
13	A	844	BCR	2	0
14	A	851	LHG	1	0
11	A	817	CLA	4	0
13	B	844	BCR	2	0
11	A	810	CLA	2	0
11	A	829	CLA	1	0
11	B	834	CLA	1	0
11	B	817	CLA	1	0

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

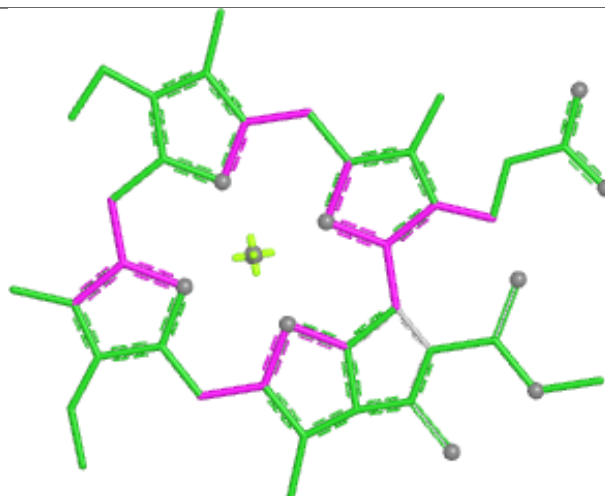




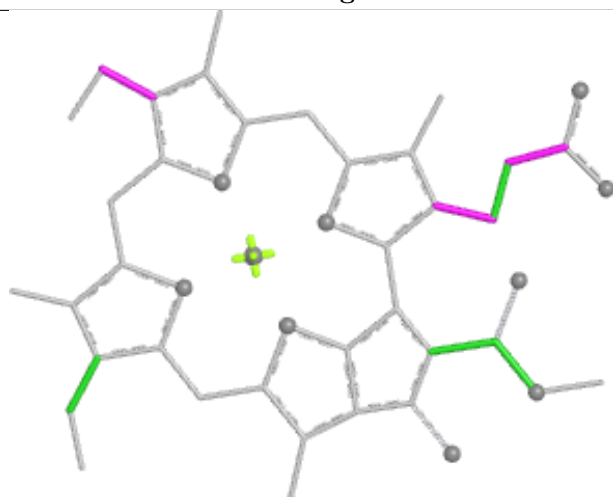
Ligand CLA B 814



Bond lengths



Bond angles

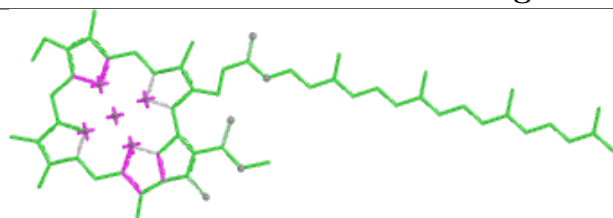


Torsions

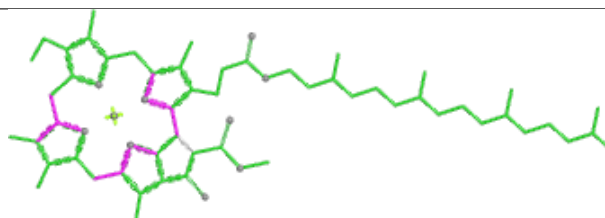


Rings

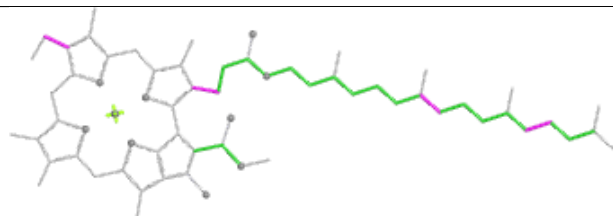
Ligand CLA A 824



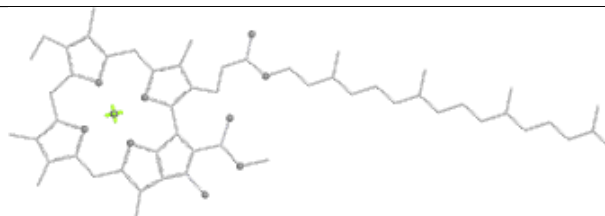
Bond lengths



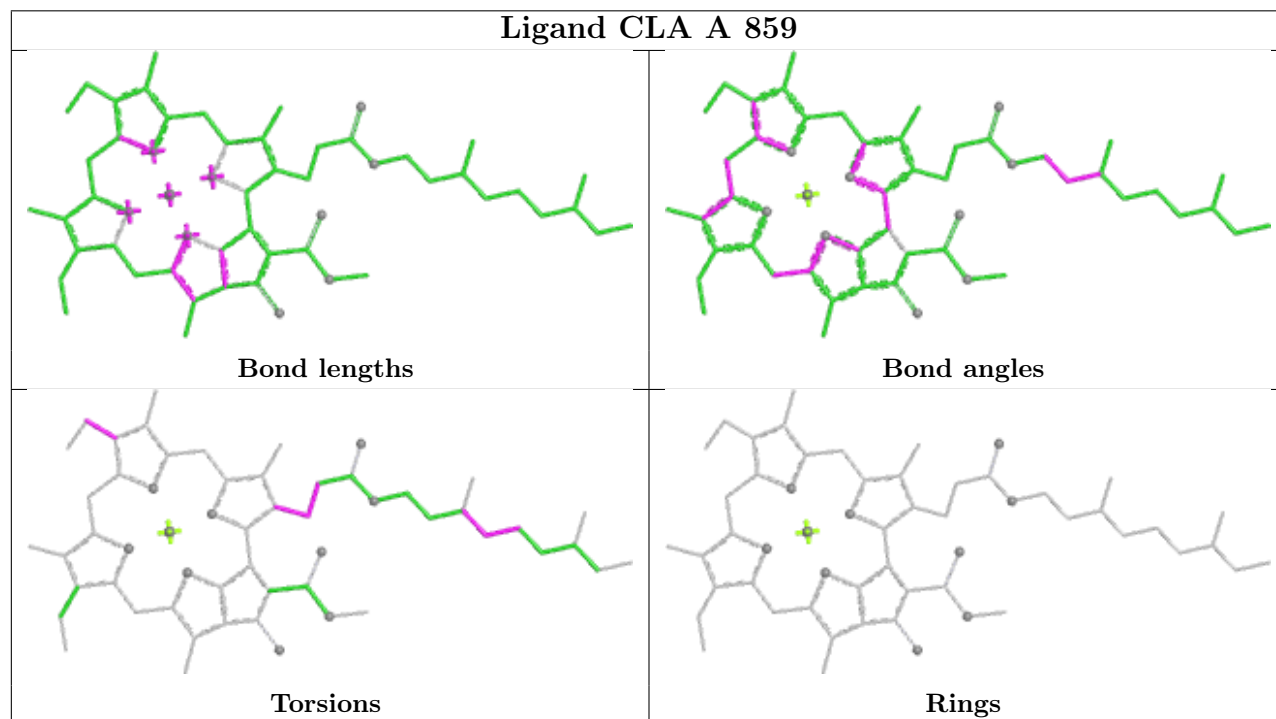
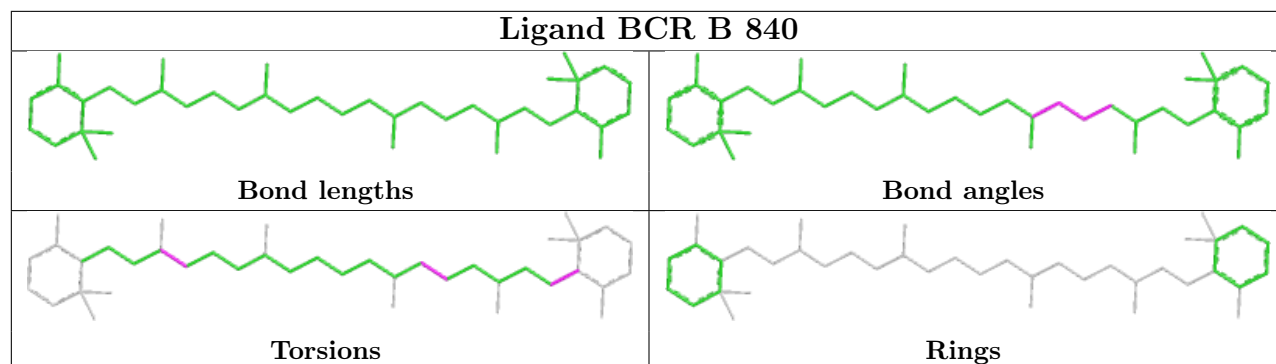
Bond angles

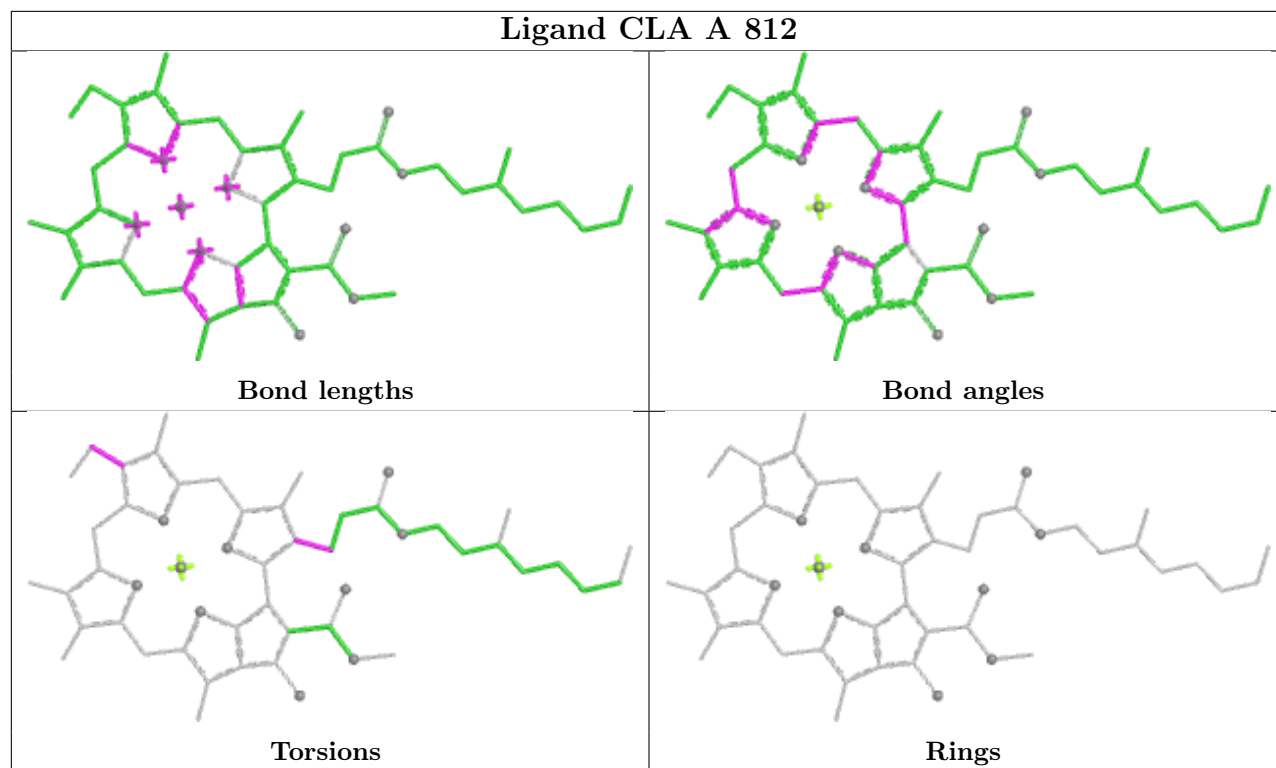


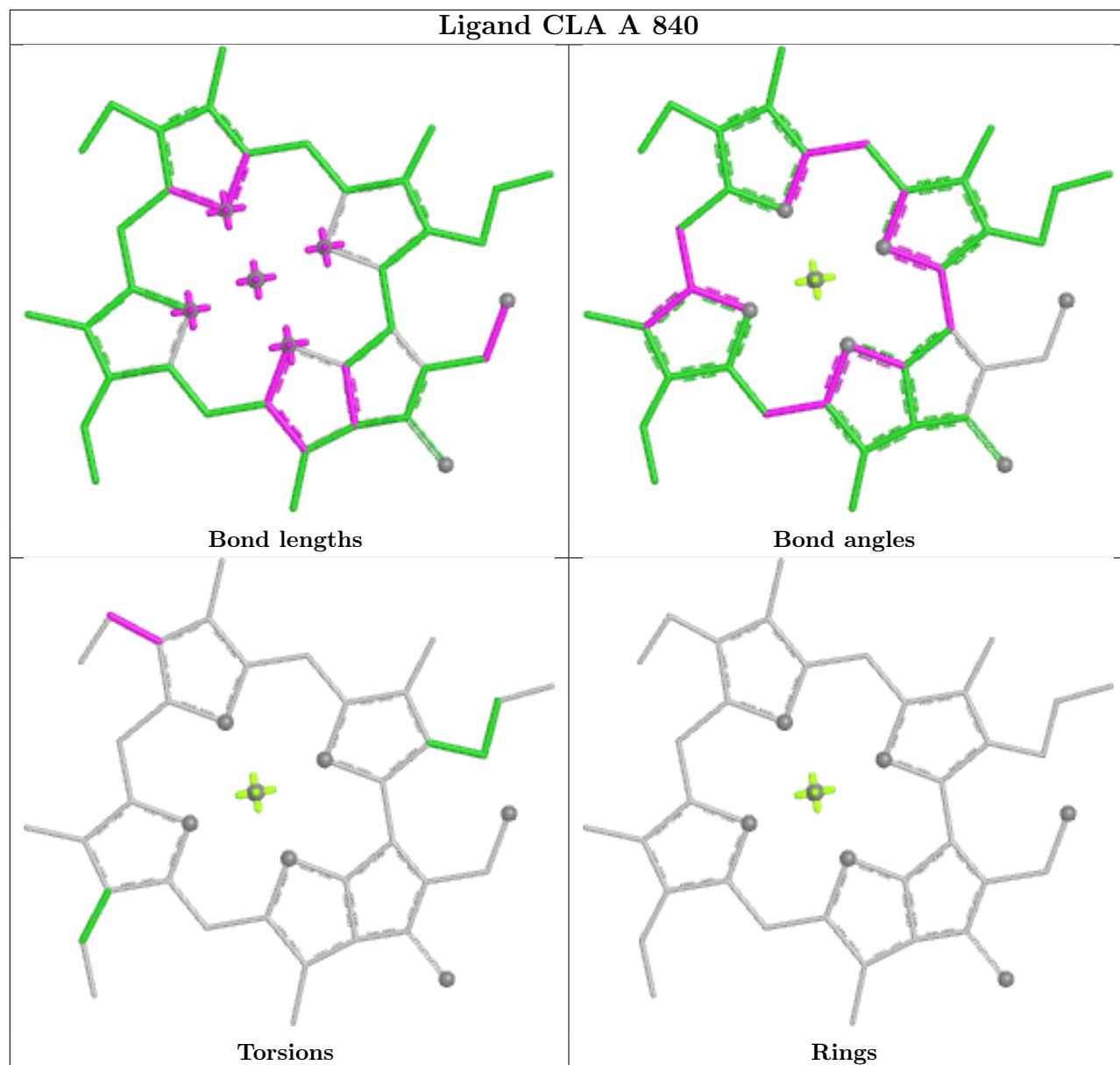
Torsions

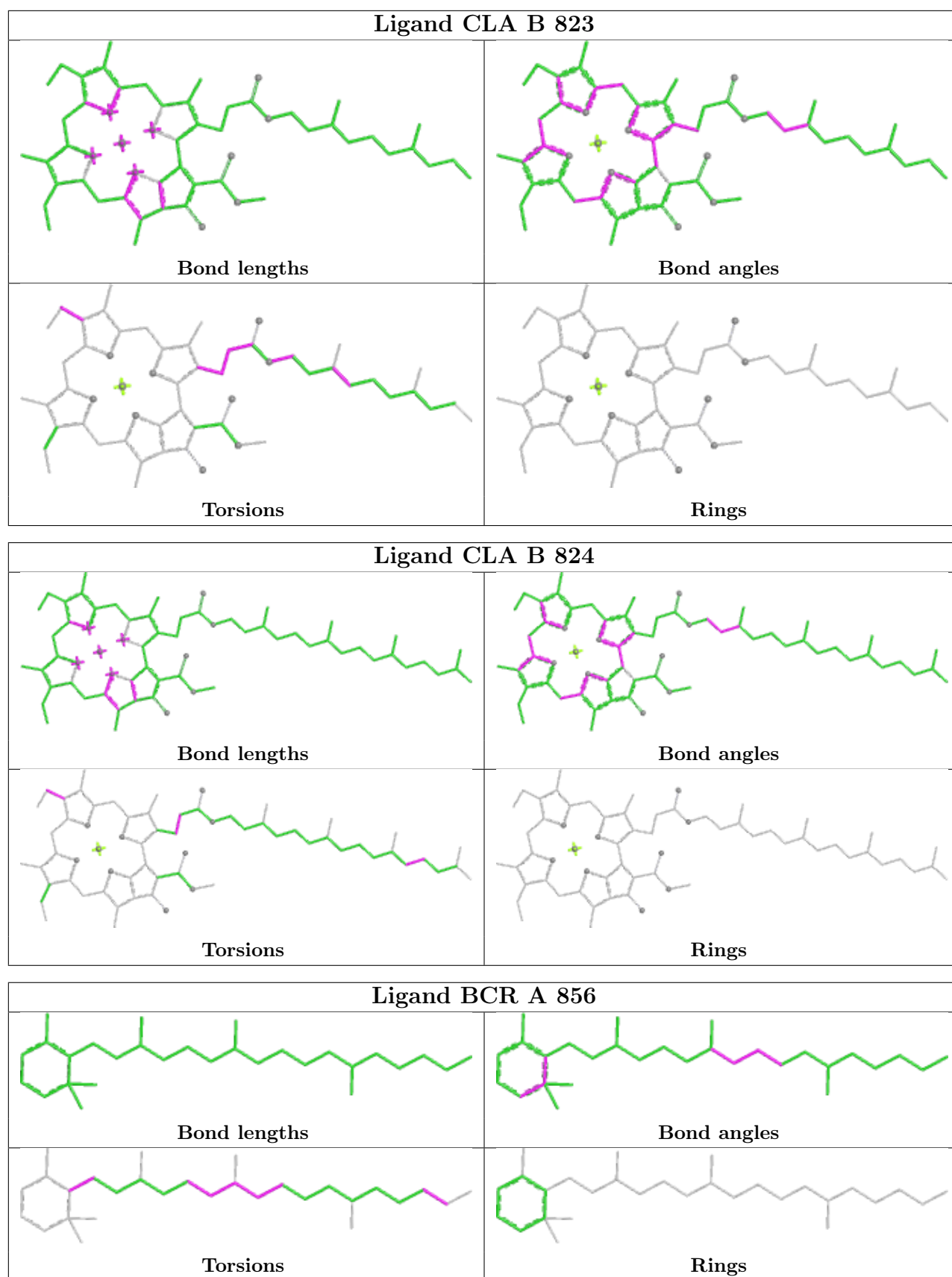


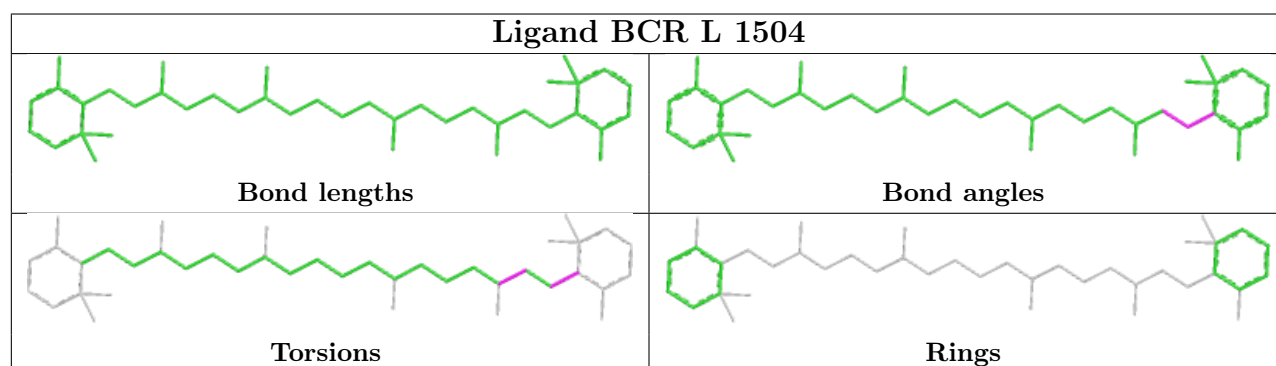
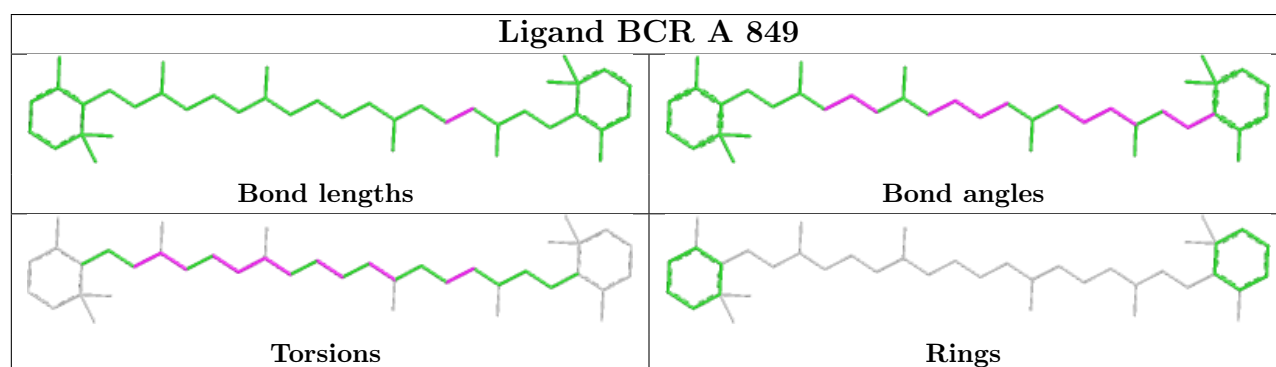
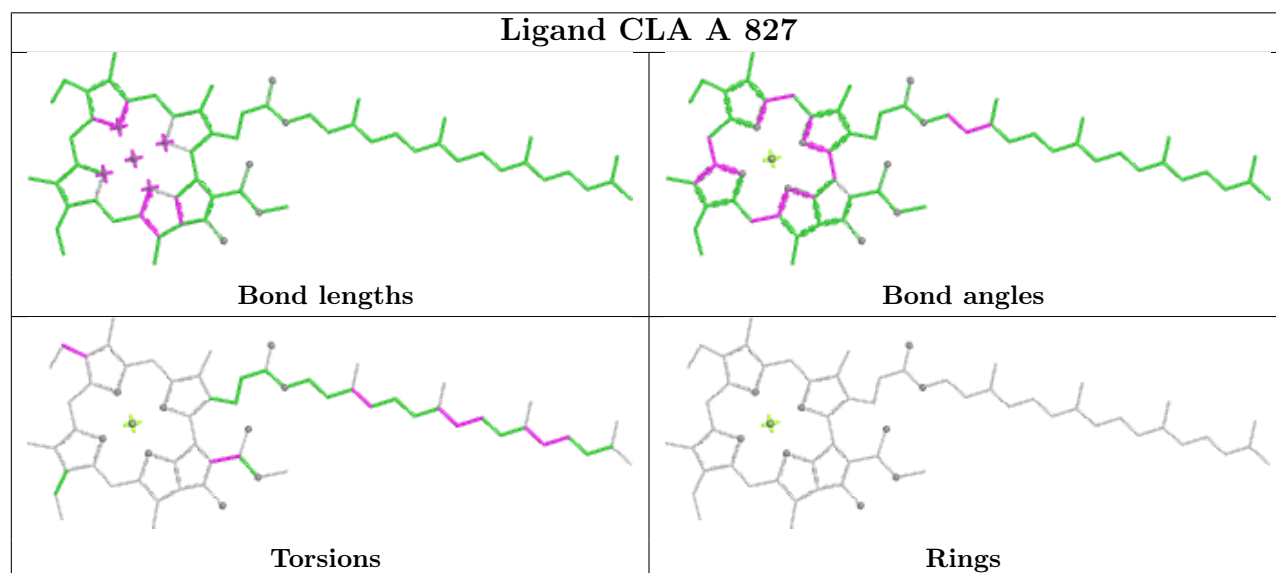
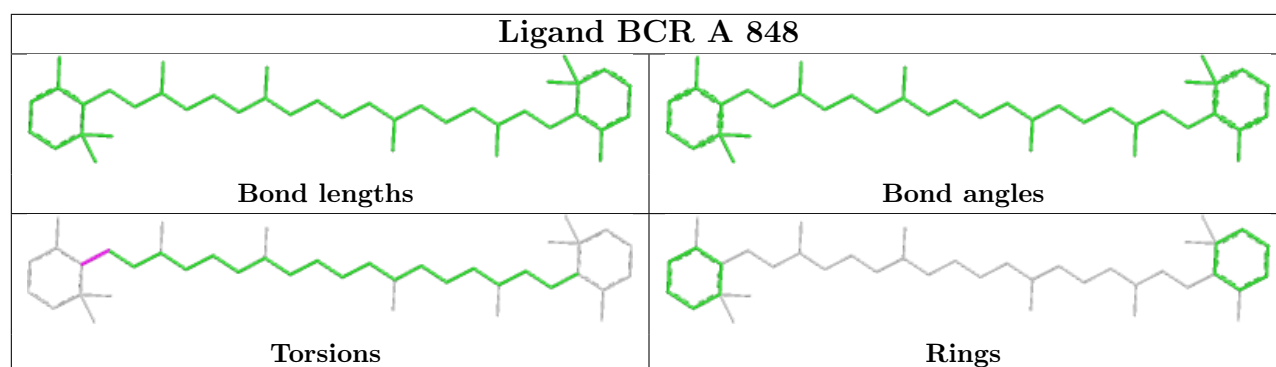
Rings

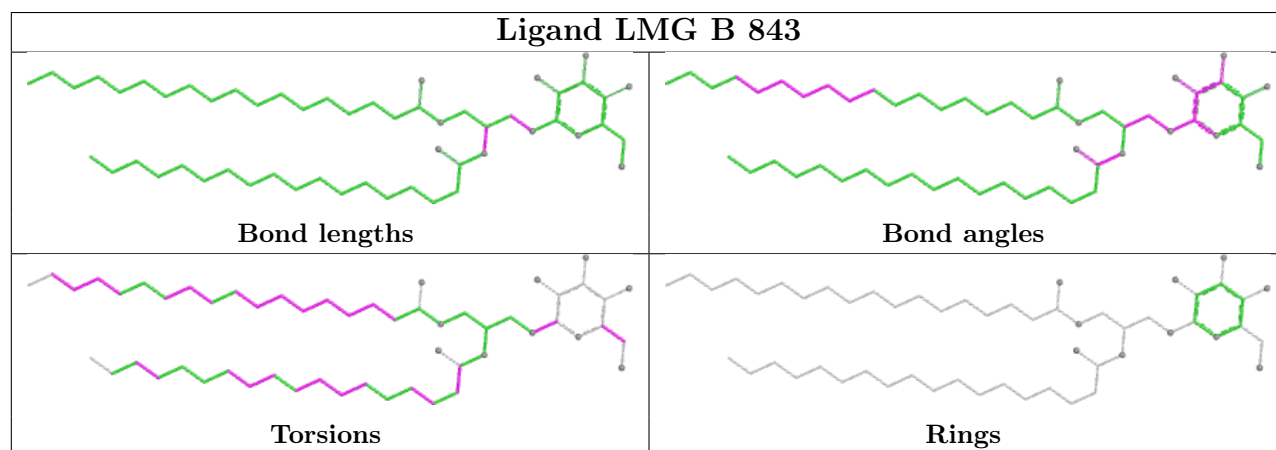
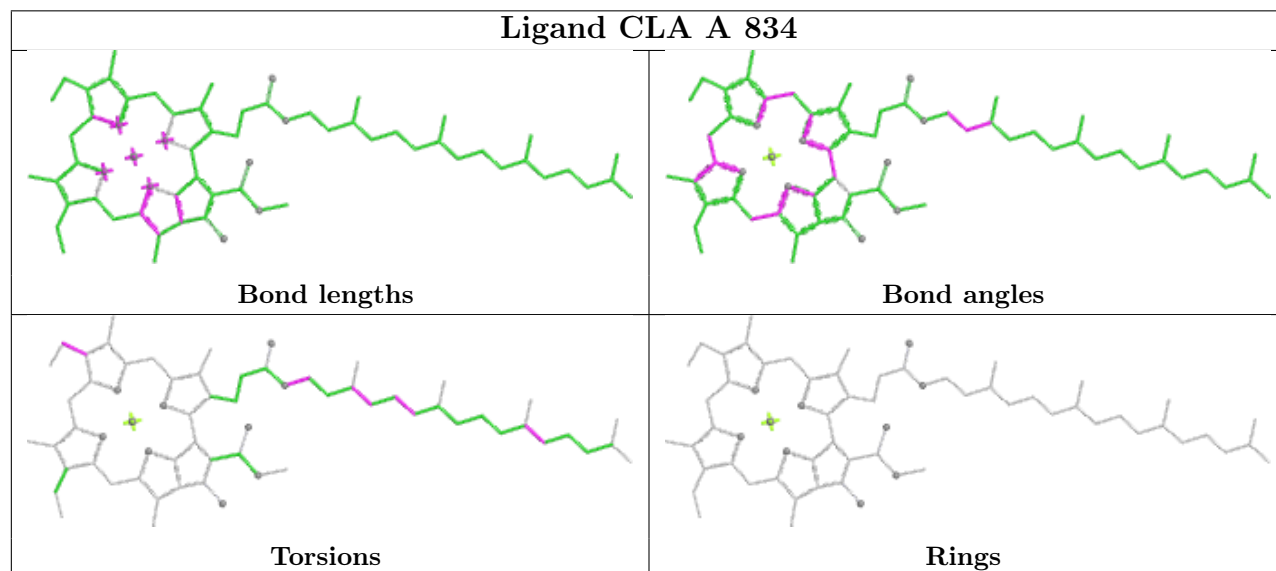
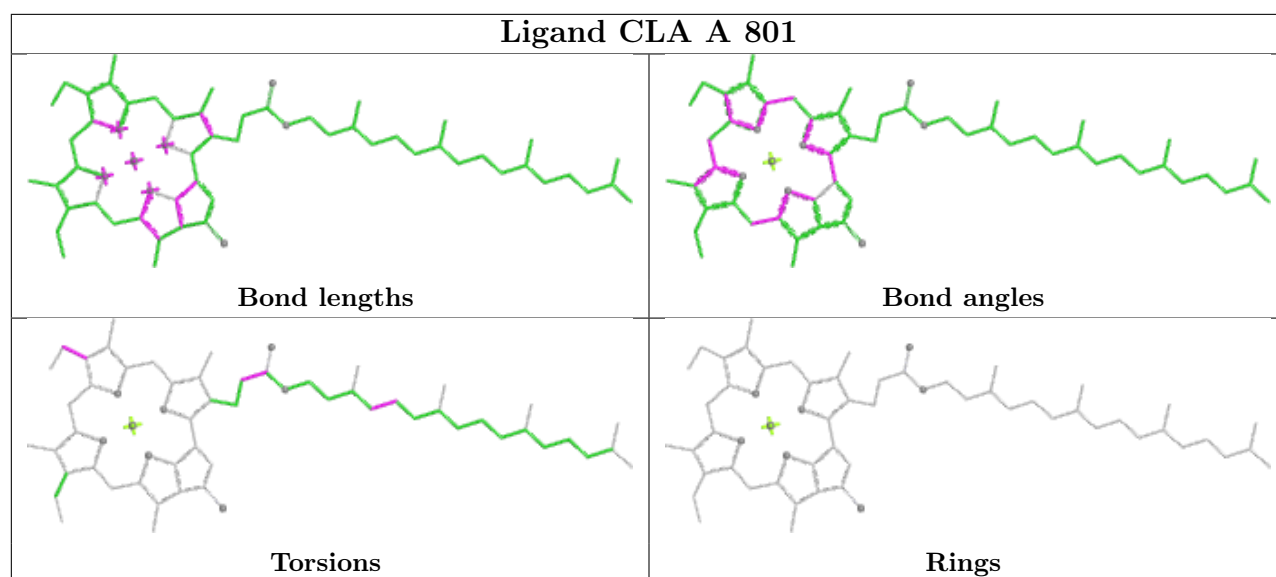




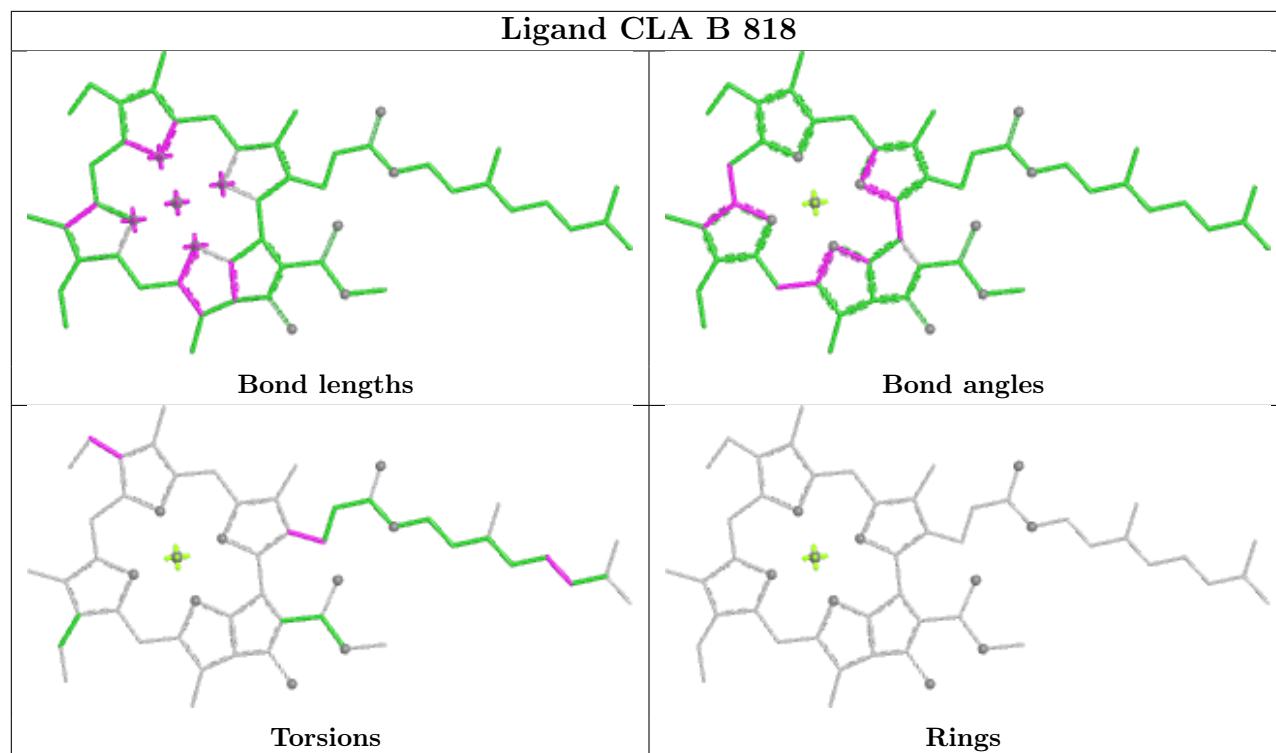




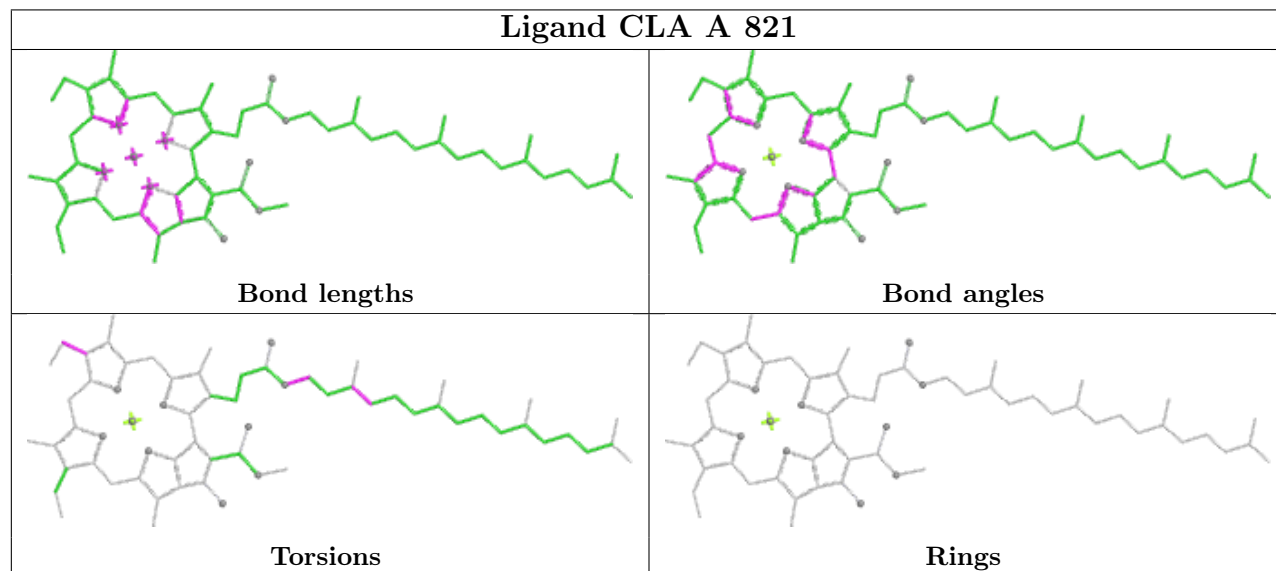


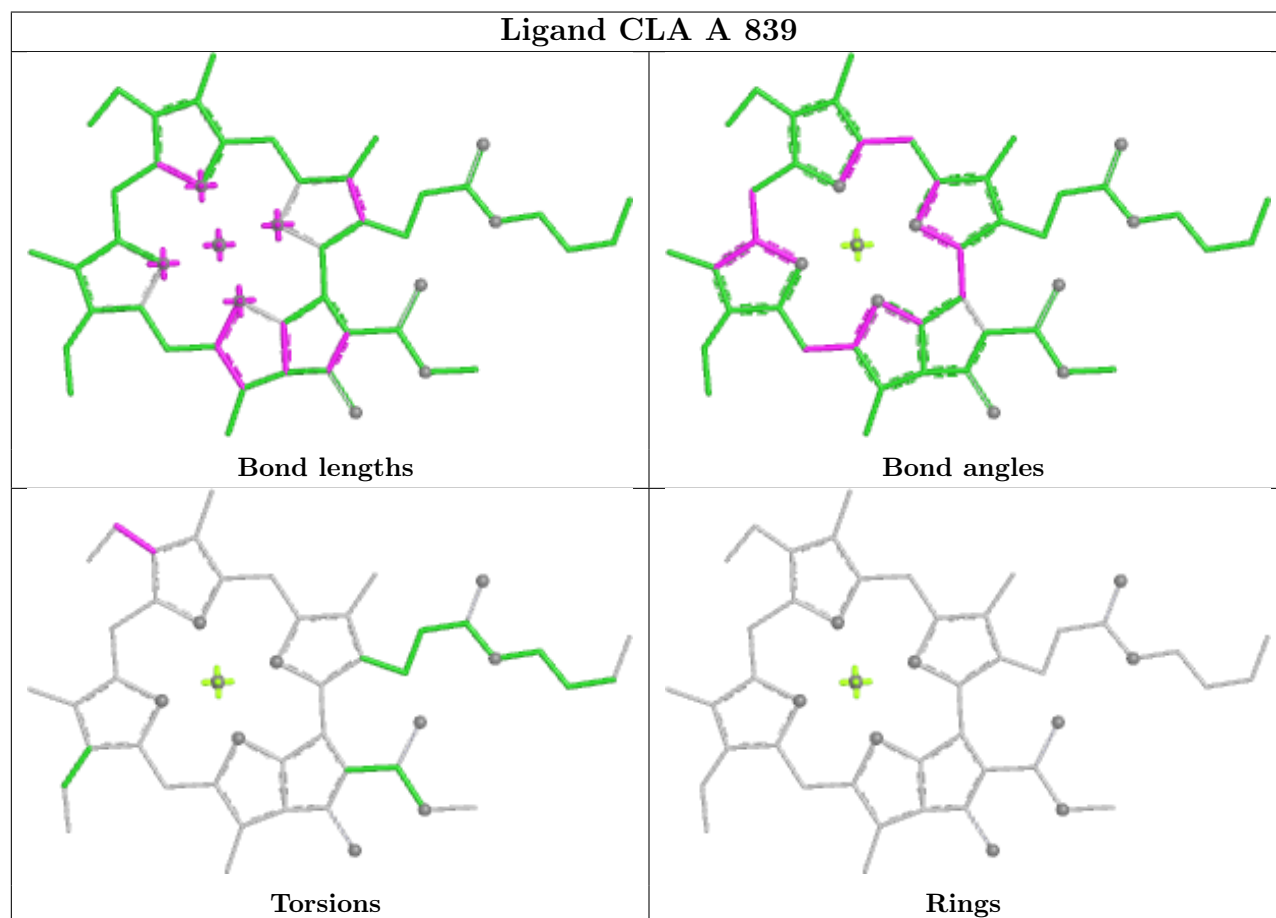
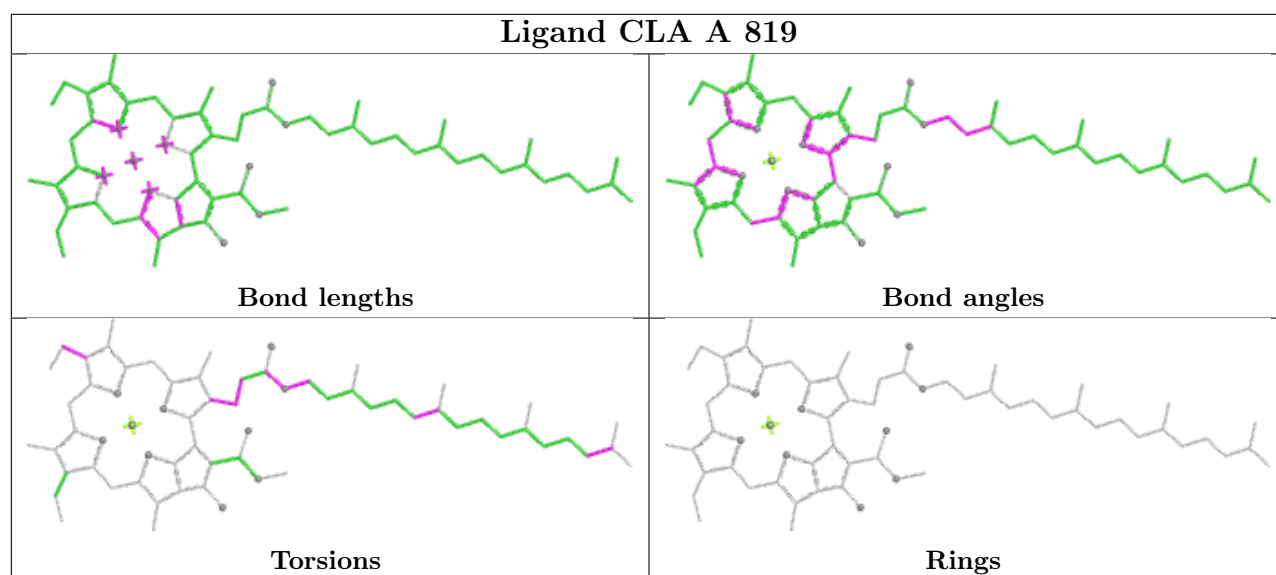


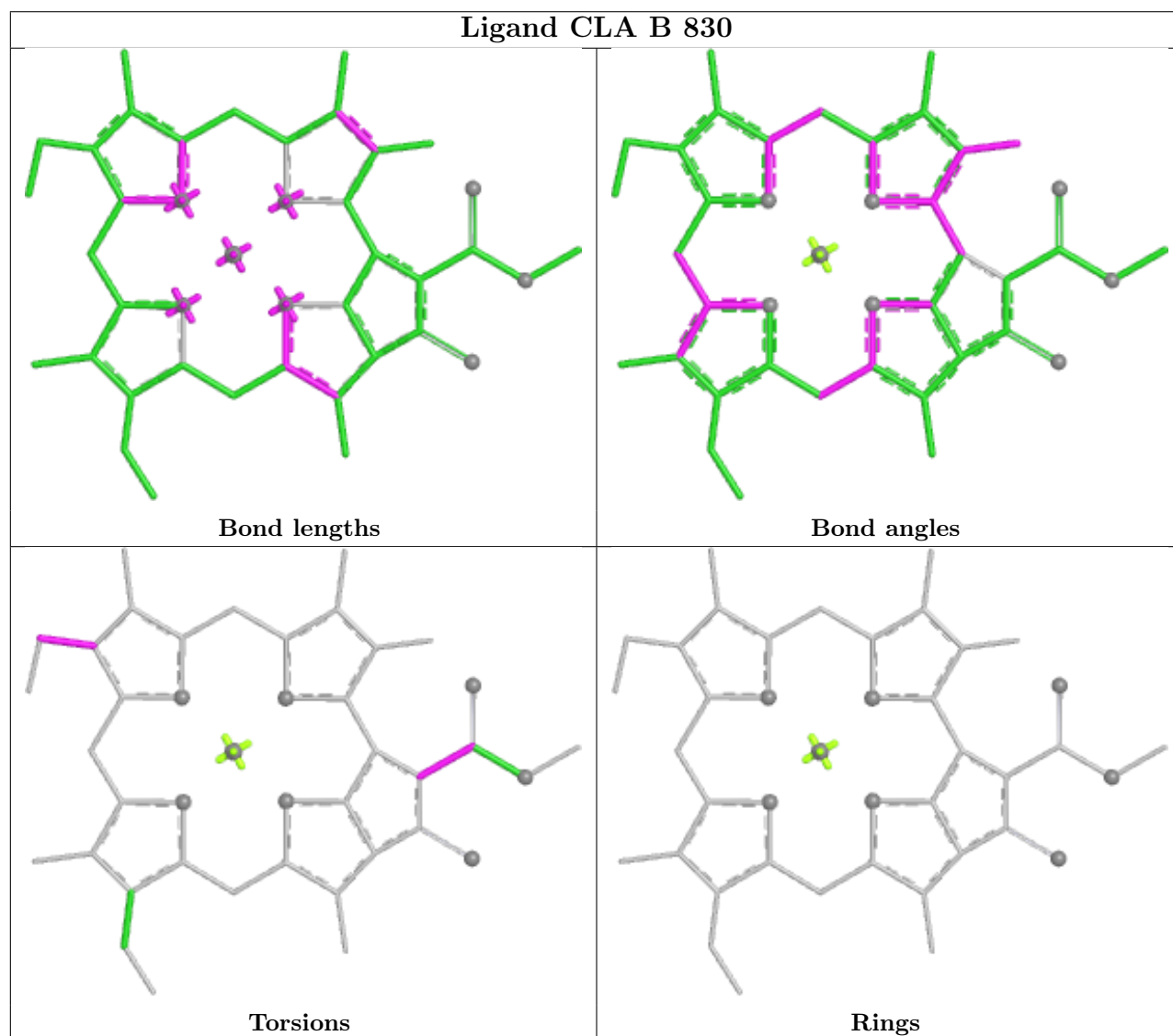
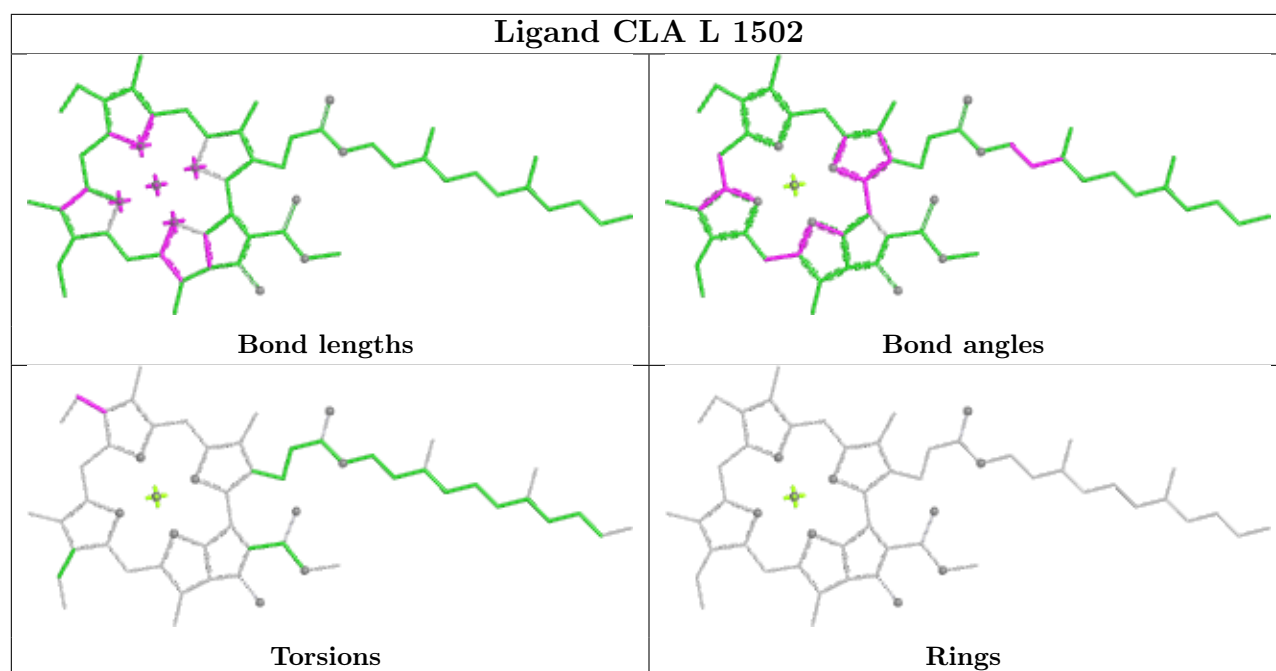
Ligand CLA B 818



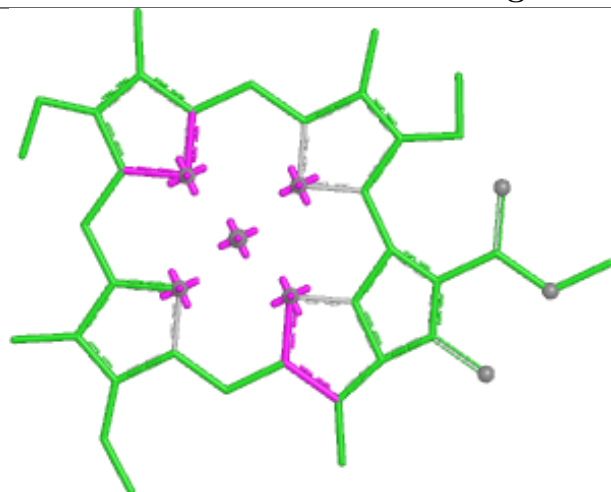
Ligand CLA A 821



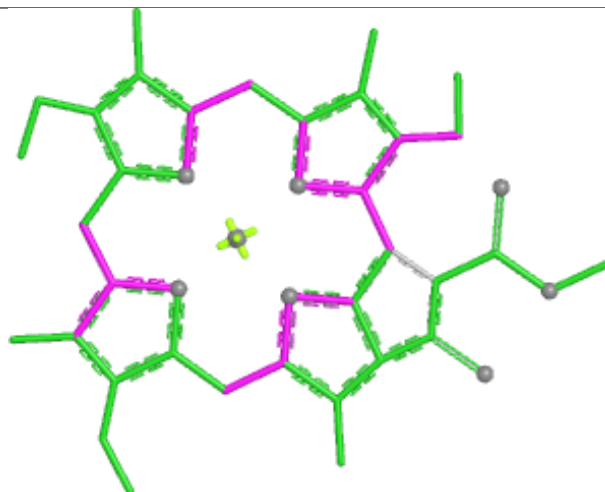




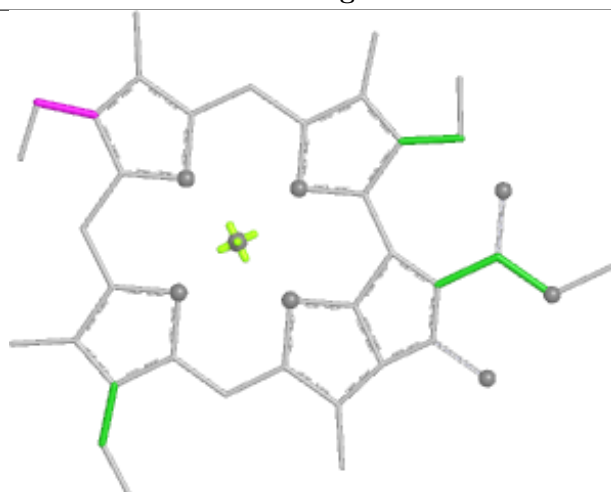
Ligand CLA L 1503



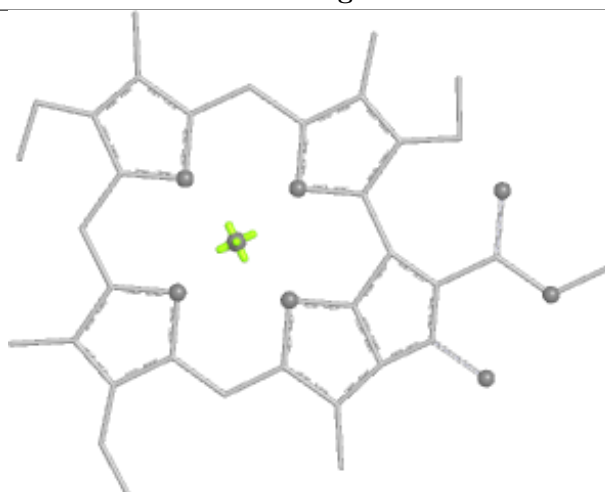
Bond lengths



Bond angles

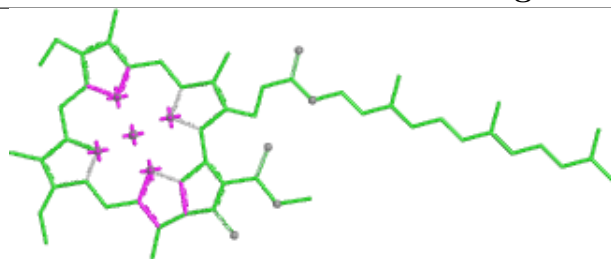


Torsions

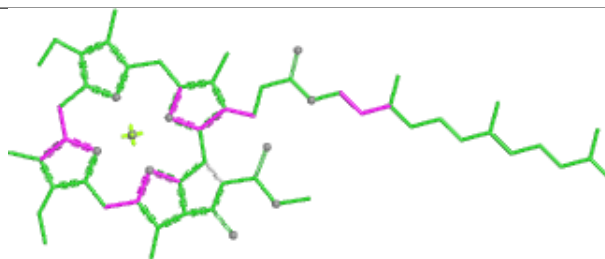


Rings

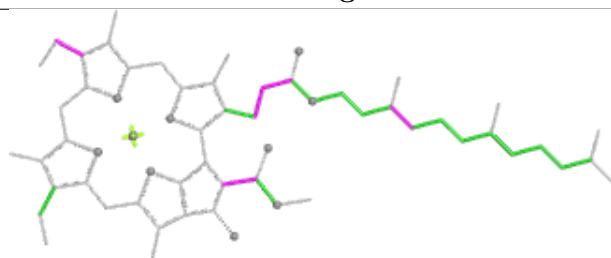
Ligand CLA B 820



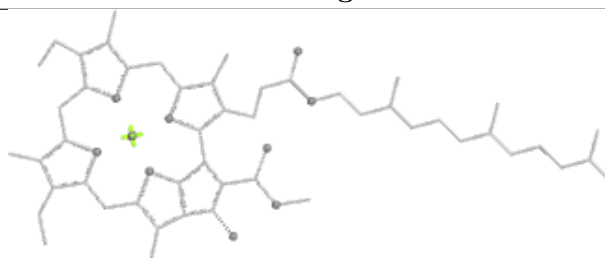
Bond lengths



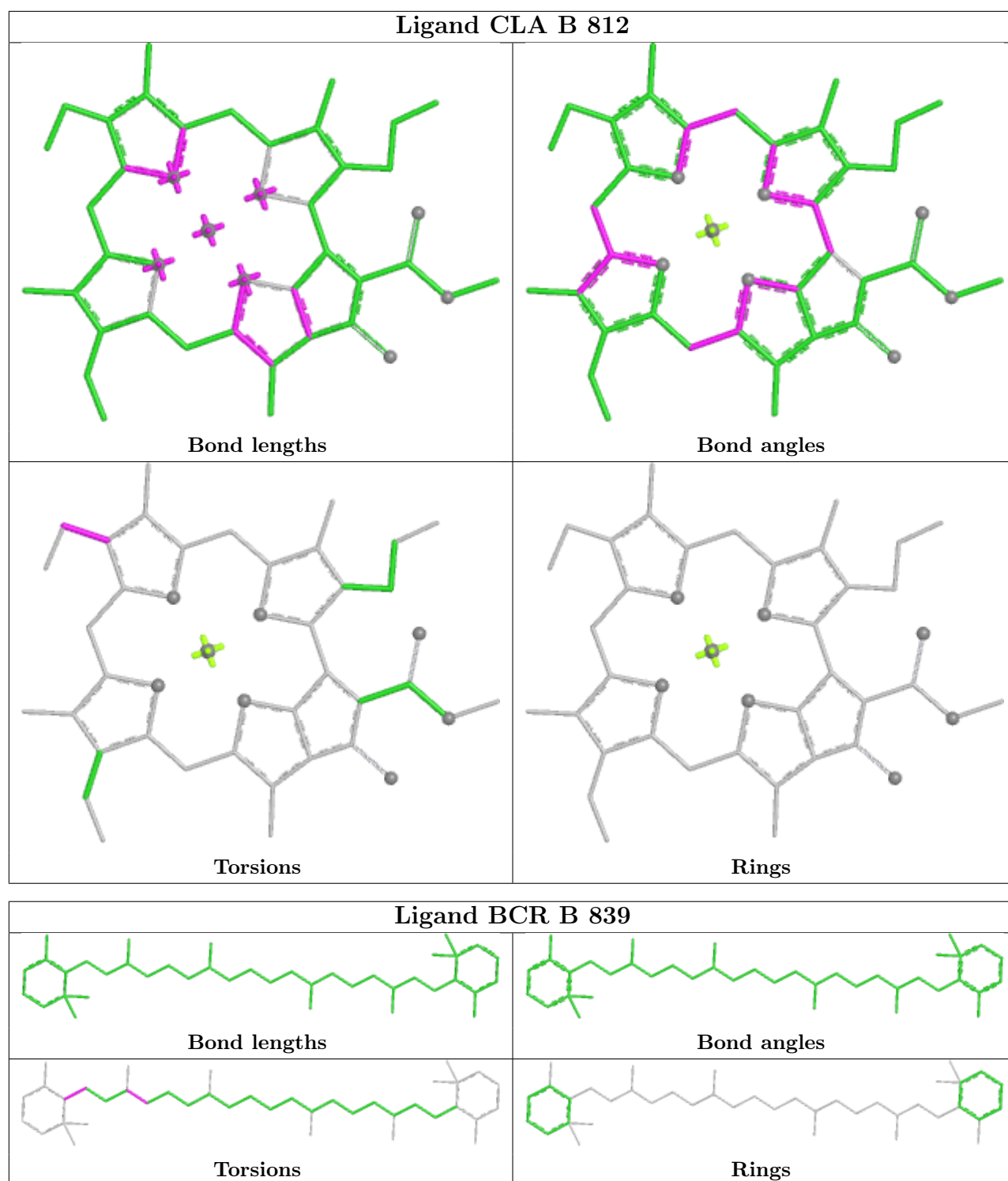
Bond angles

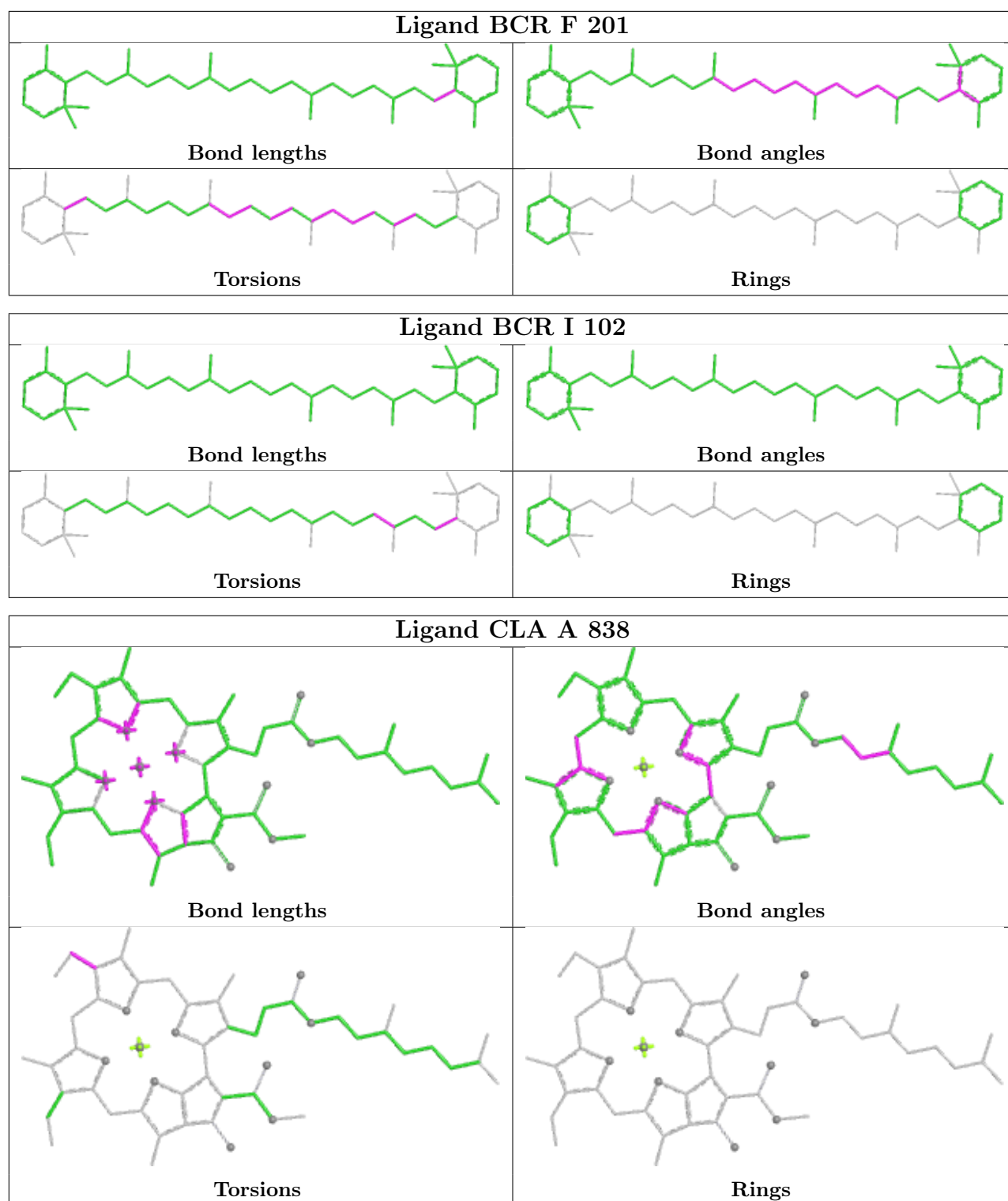


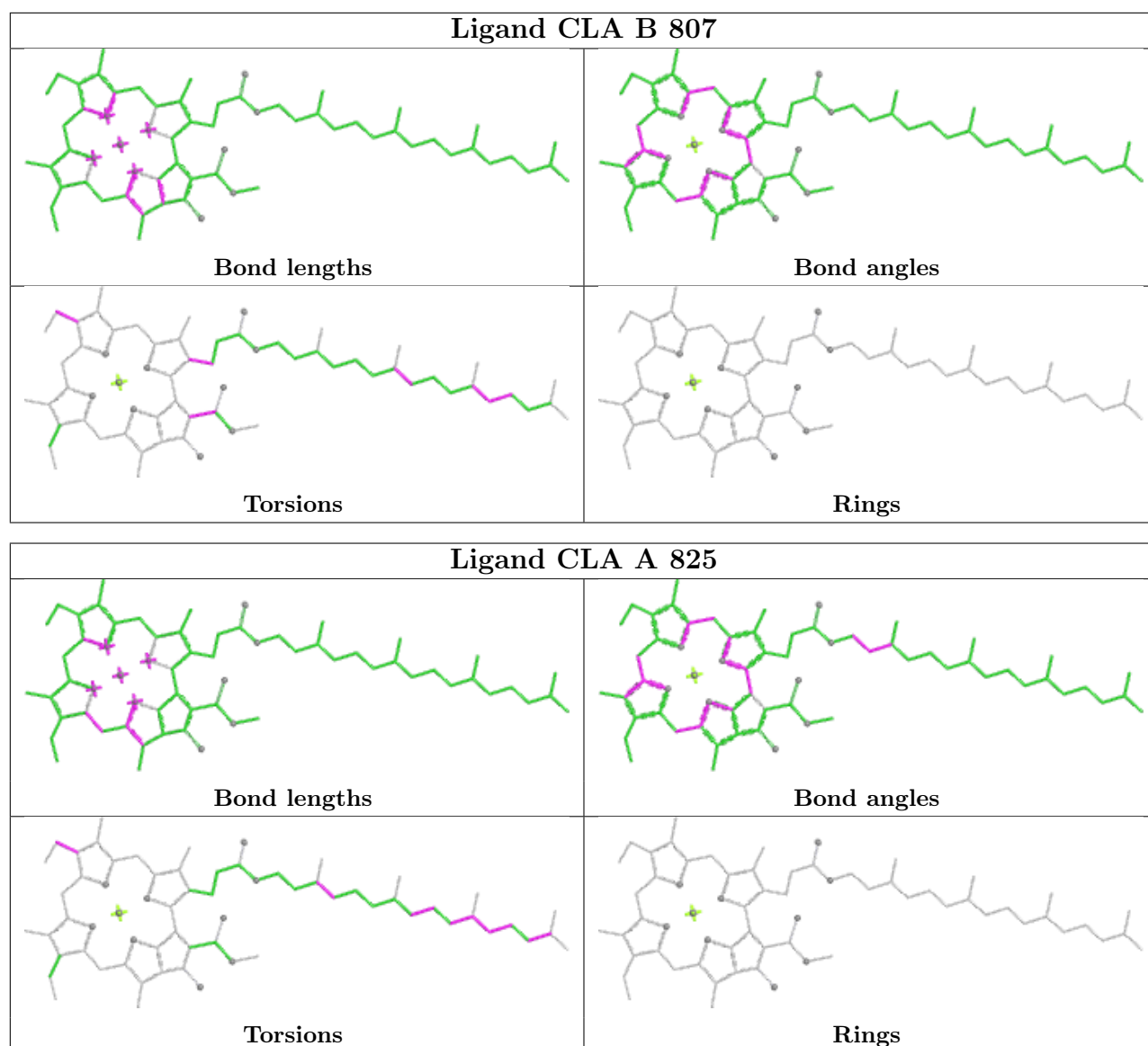
Torsions



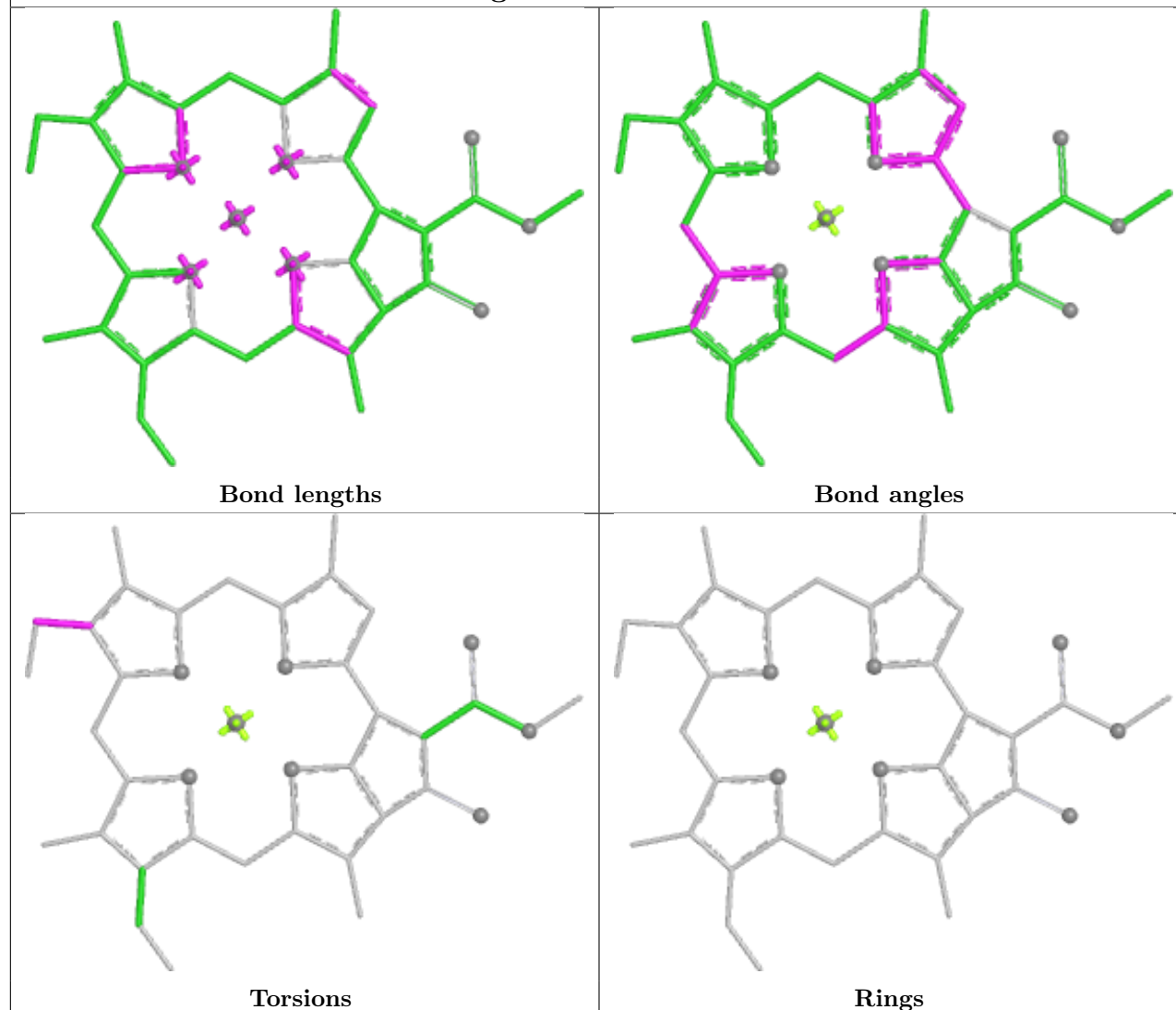
Rings



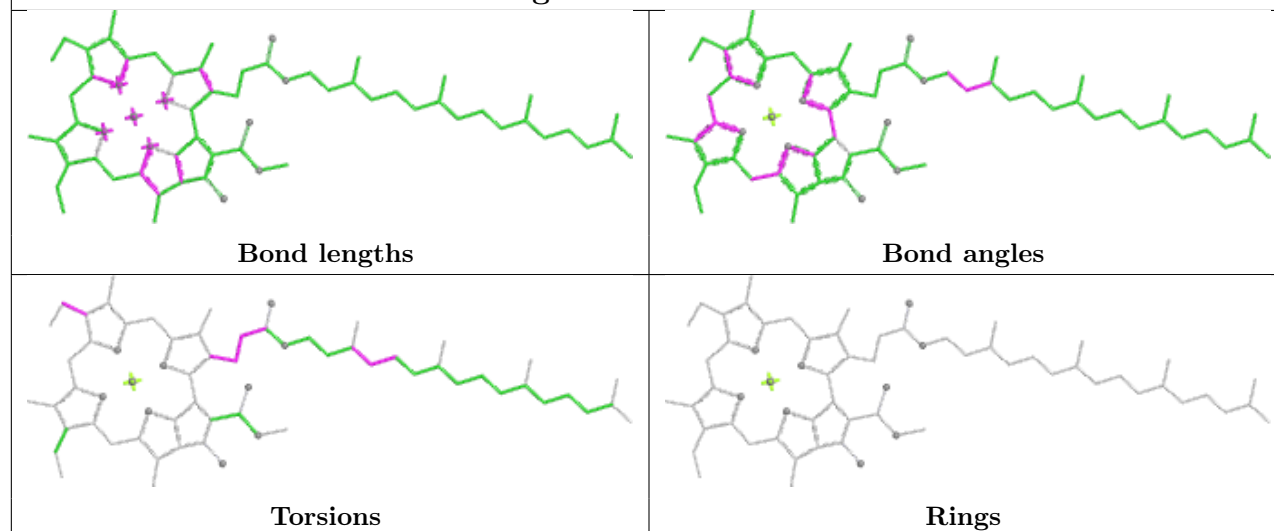




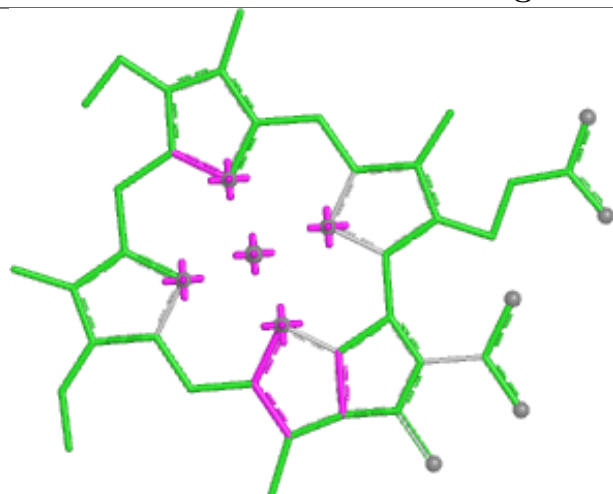
Ligand CLA A 842



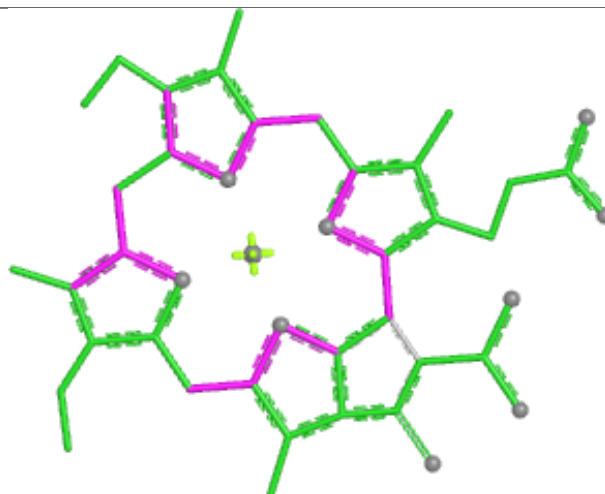
Ligand CLA B 803



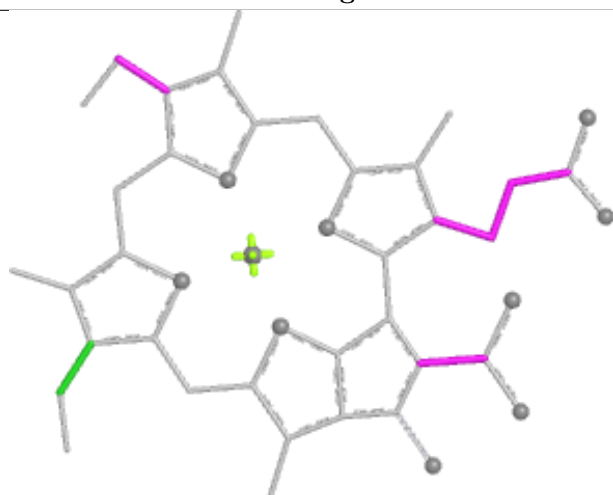
Ligand CLA B 822



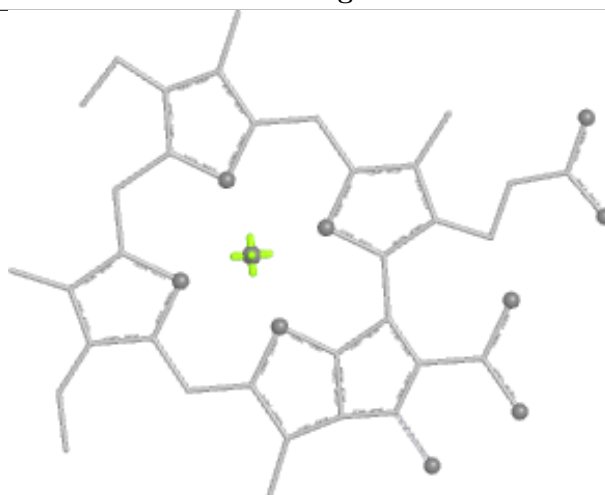
Bond lengths



Bond angles

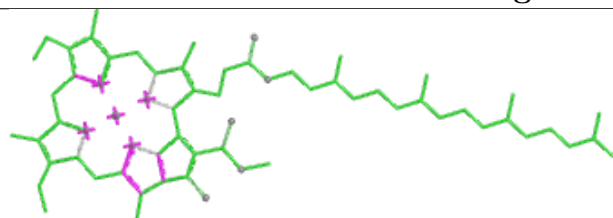


Torsions

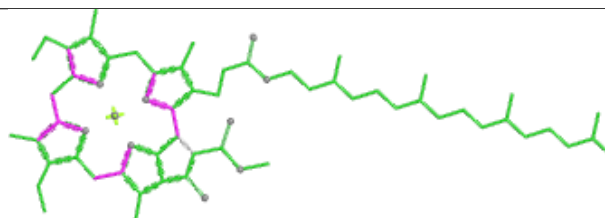


Rings

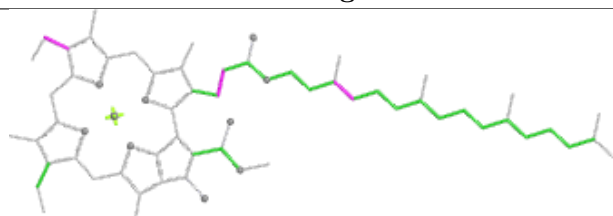
Ligand CLA A 802



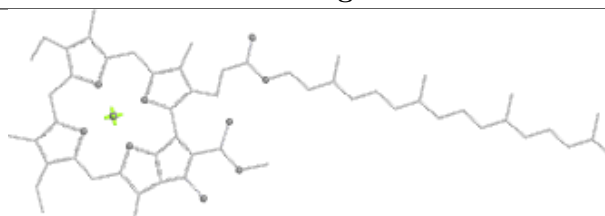
Bond lengths



Bond angles

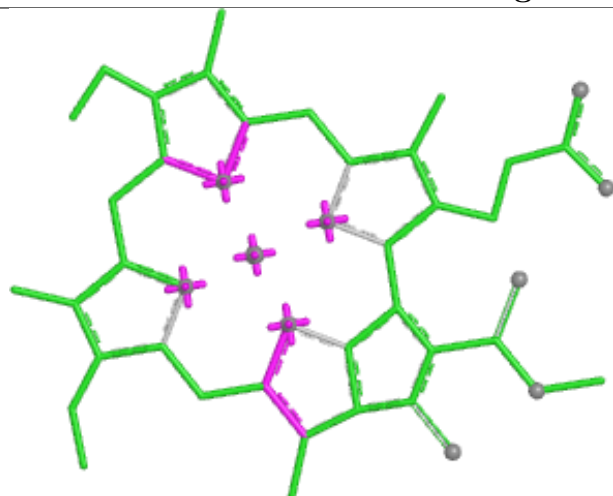


Torsions

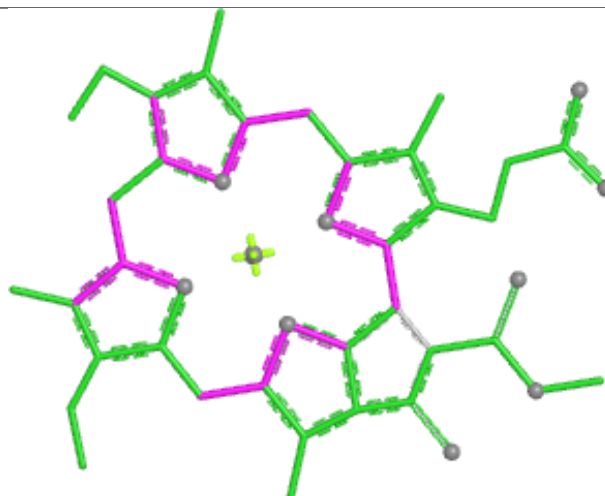


Rings

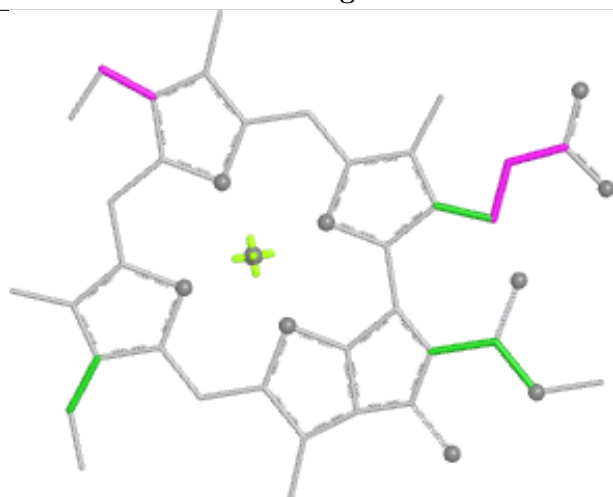
Ligand CLA B 831



Bond lengths



Bond angles

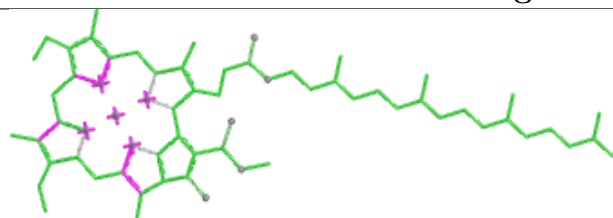


Torsions

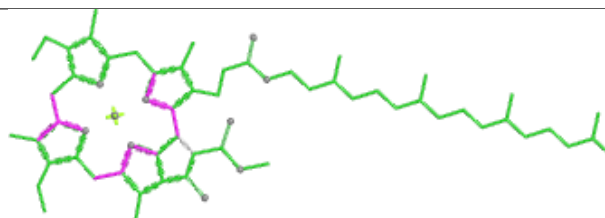


Rings

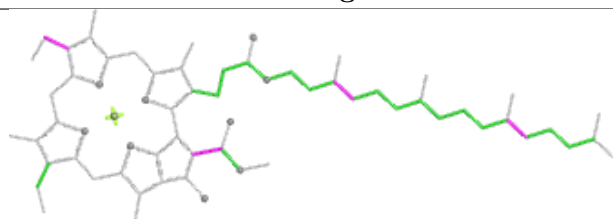
Ligand CLA B 816



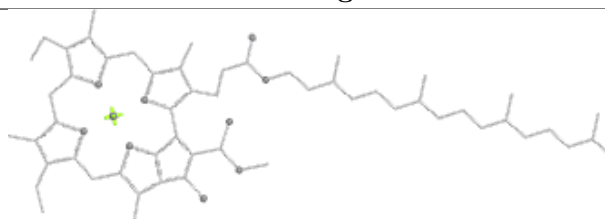
Bond lengths



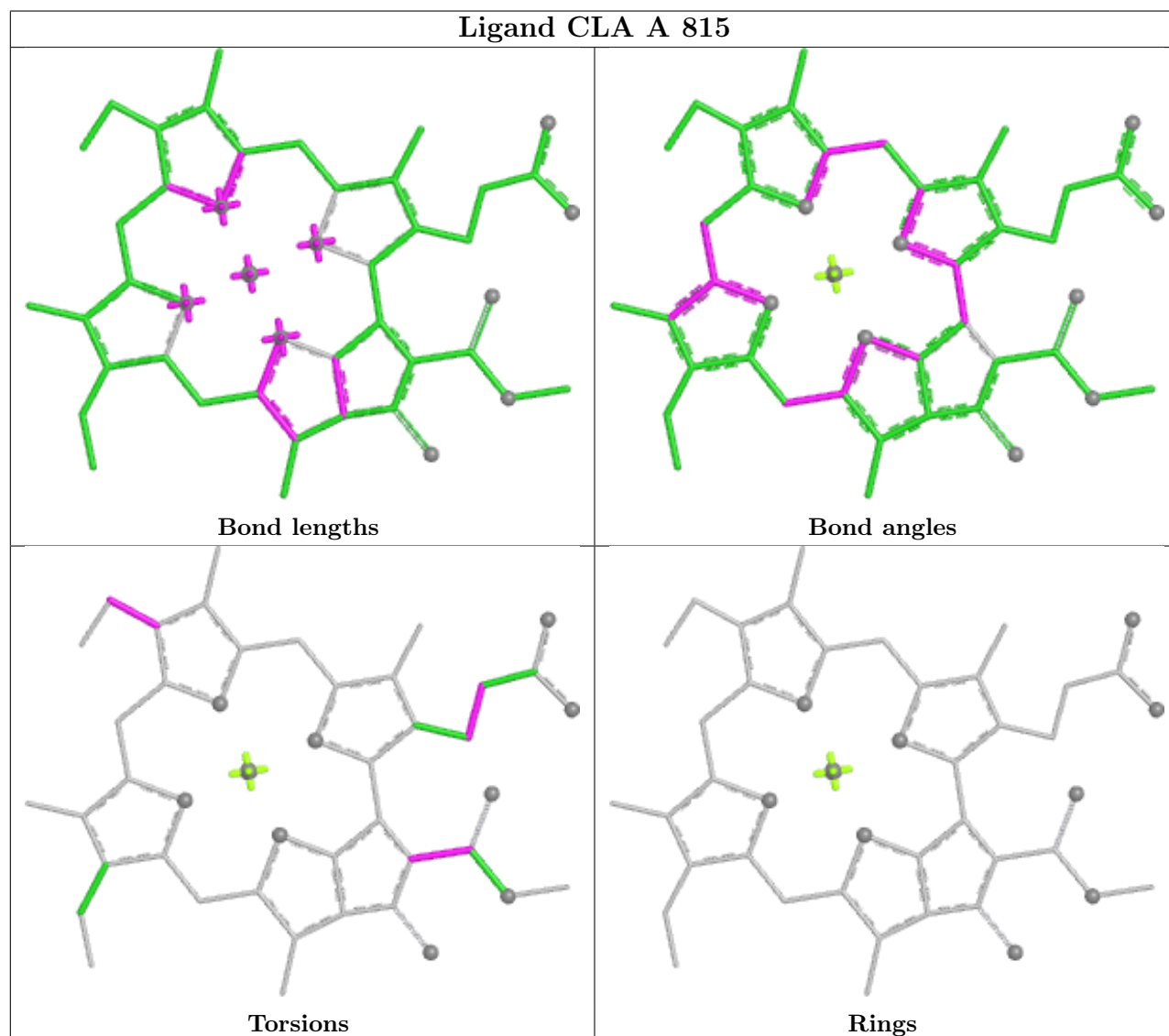
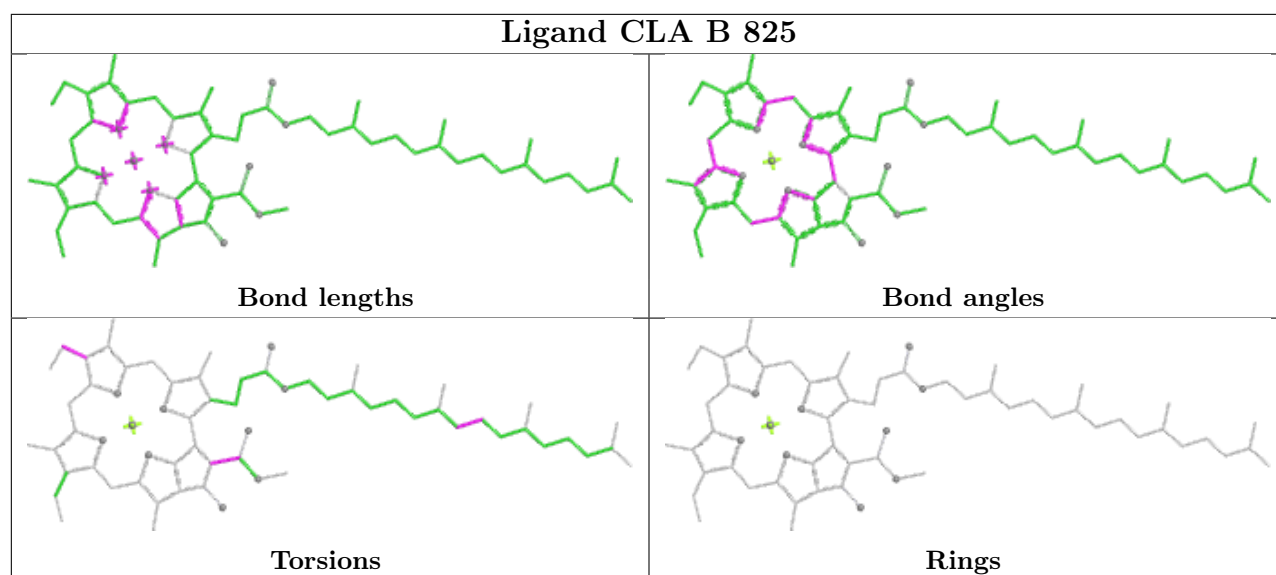
Bond angles



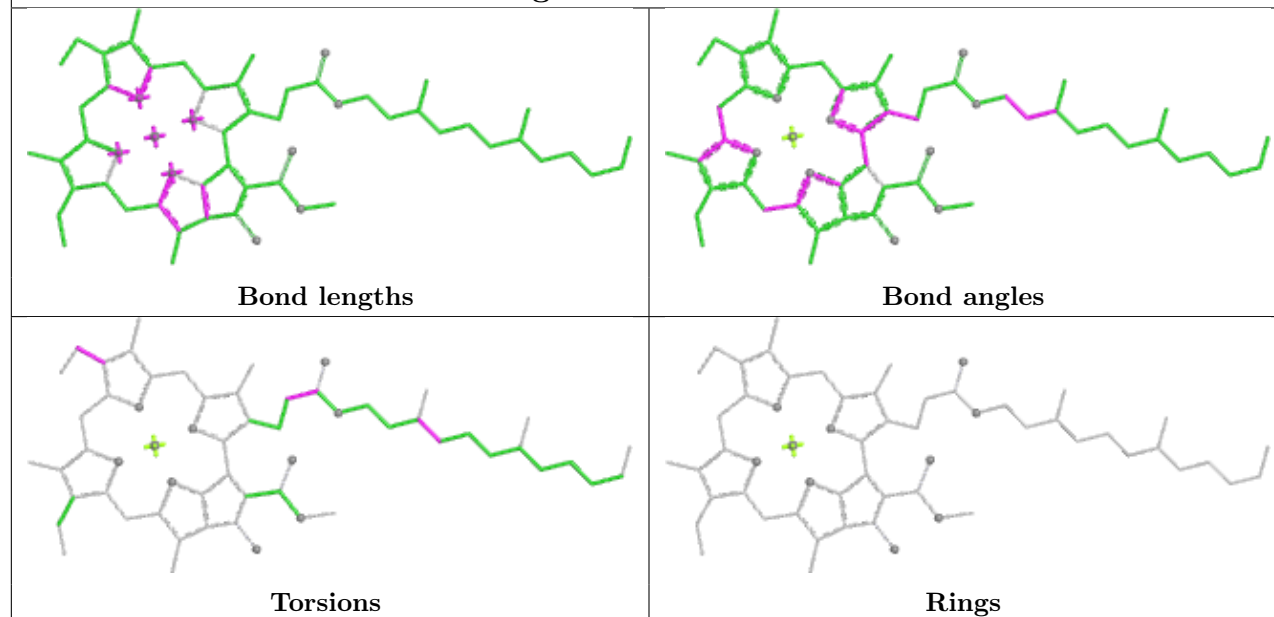
Torsions



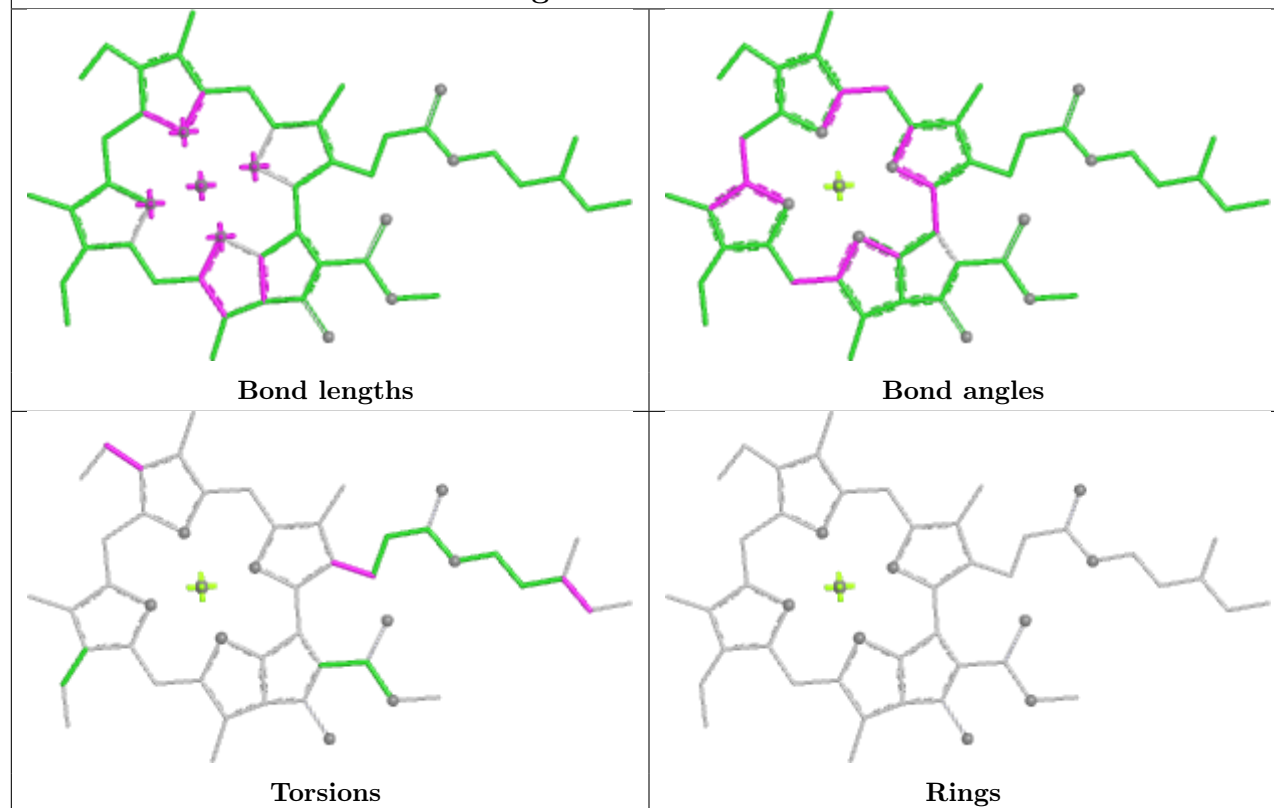
Rings

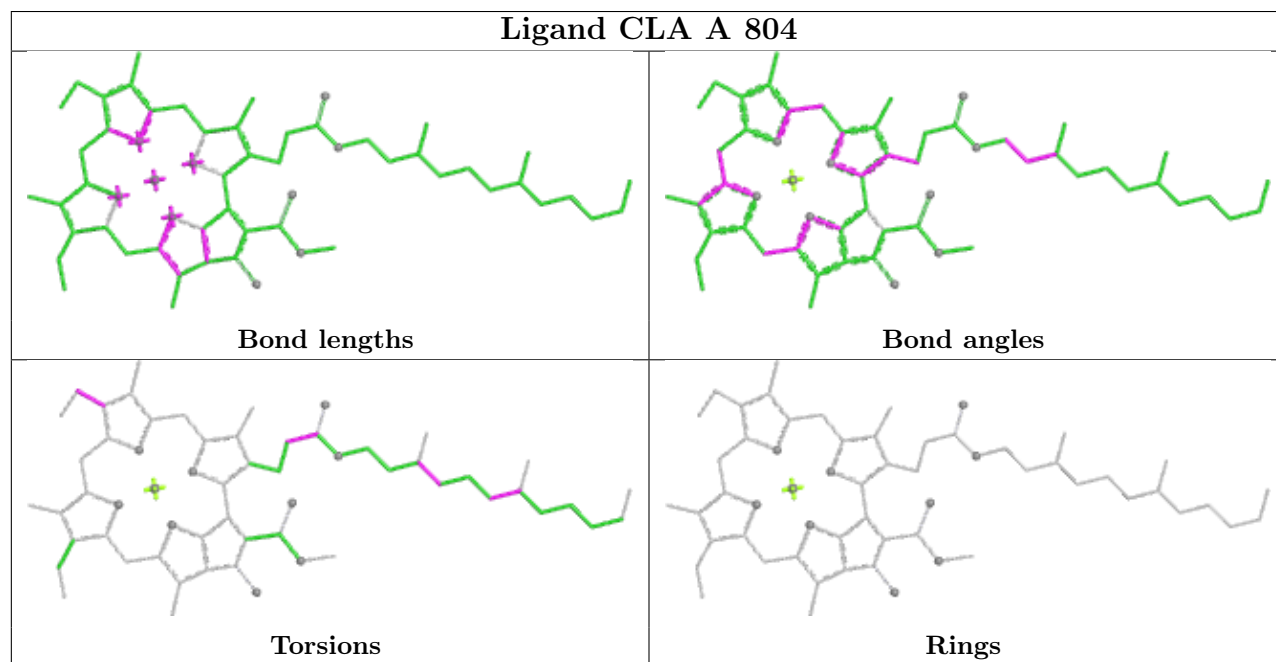
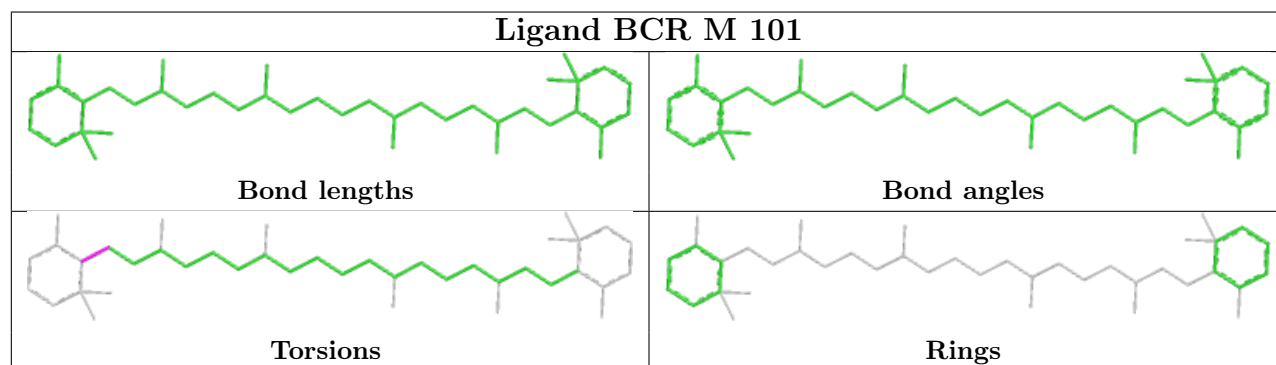
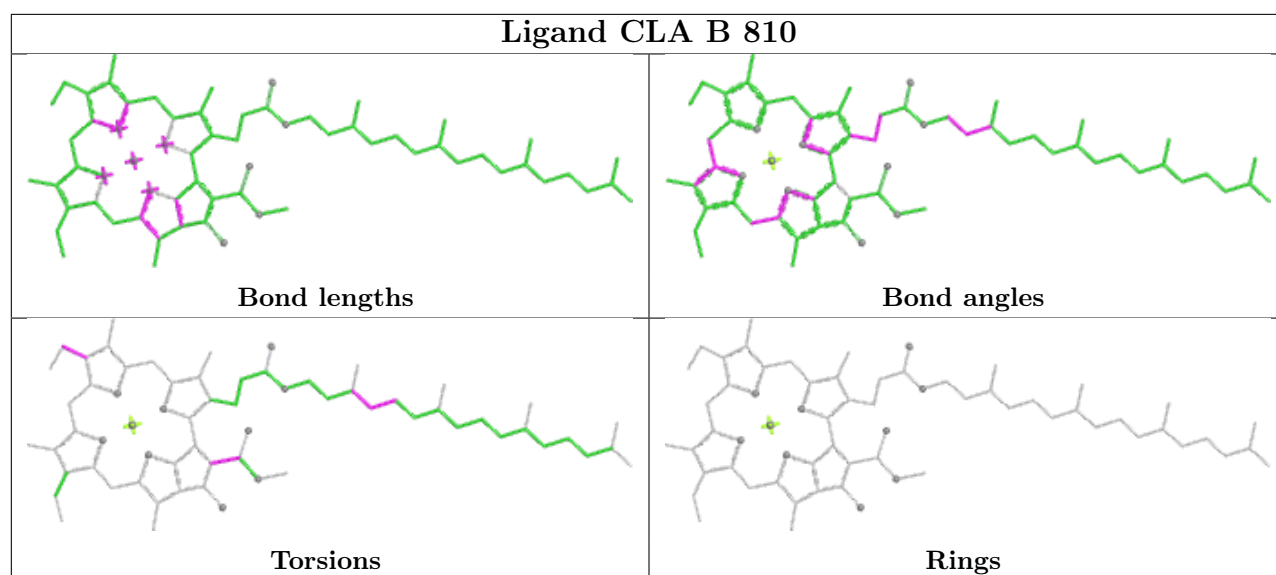


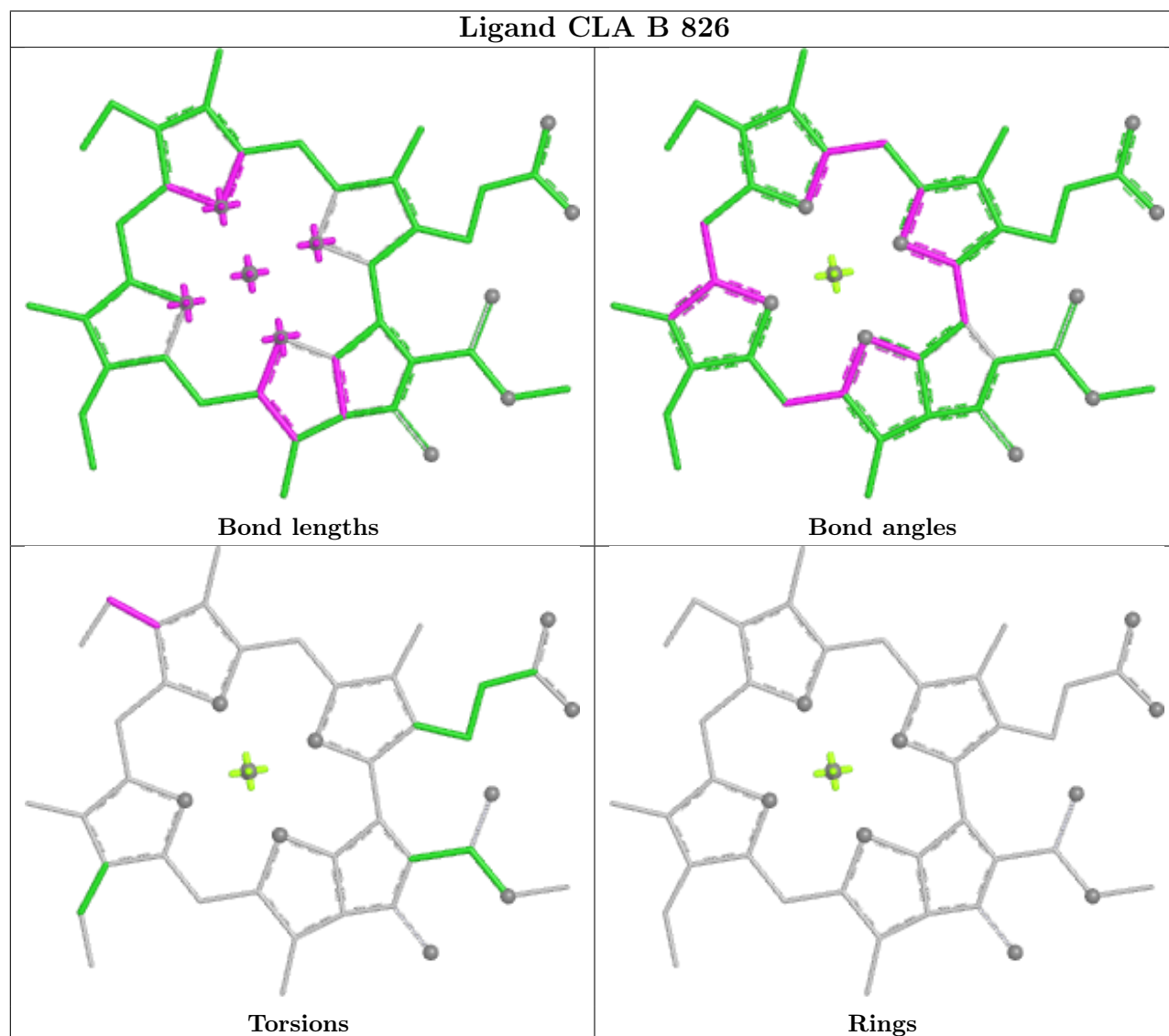
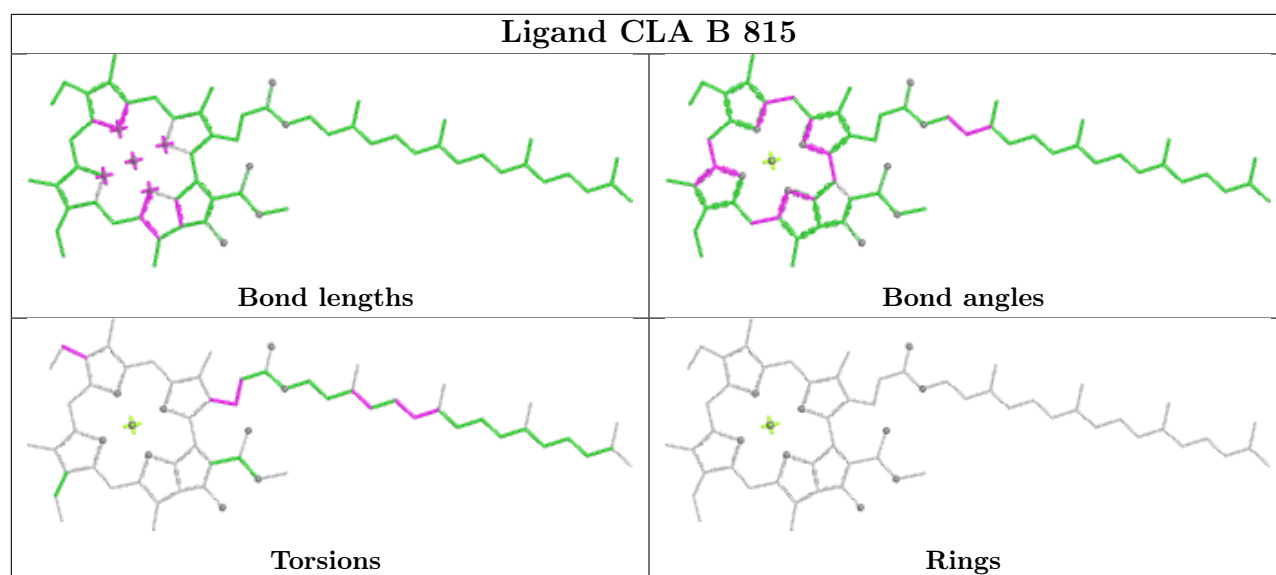
Ligand CLA B 819

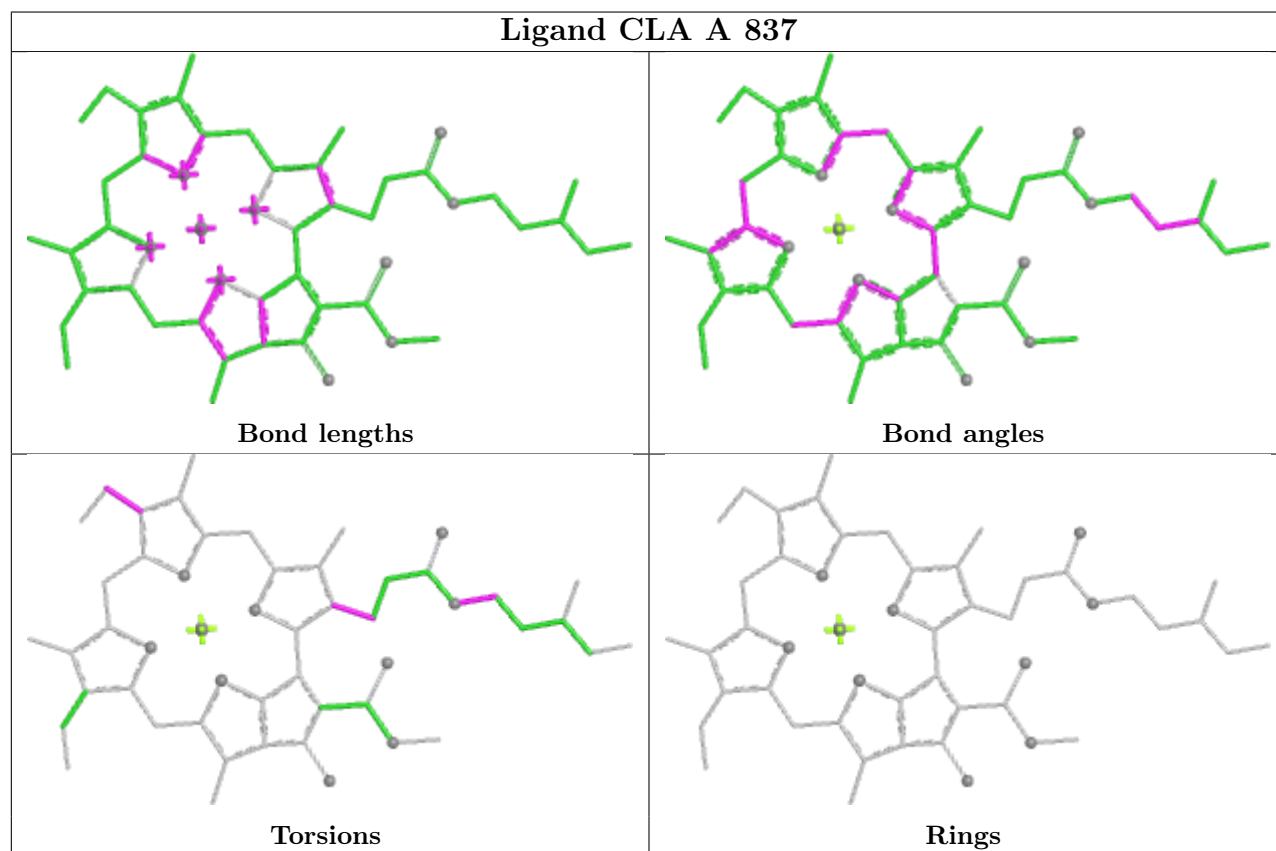
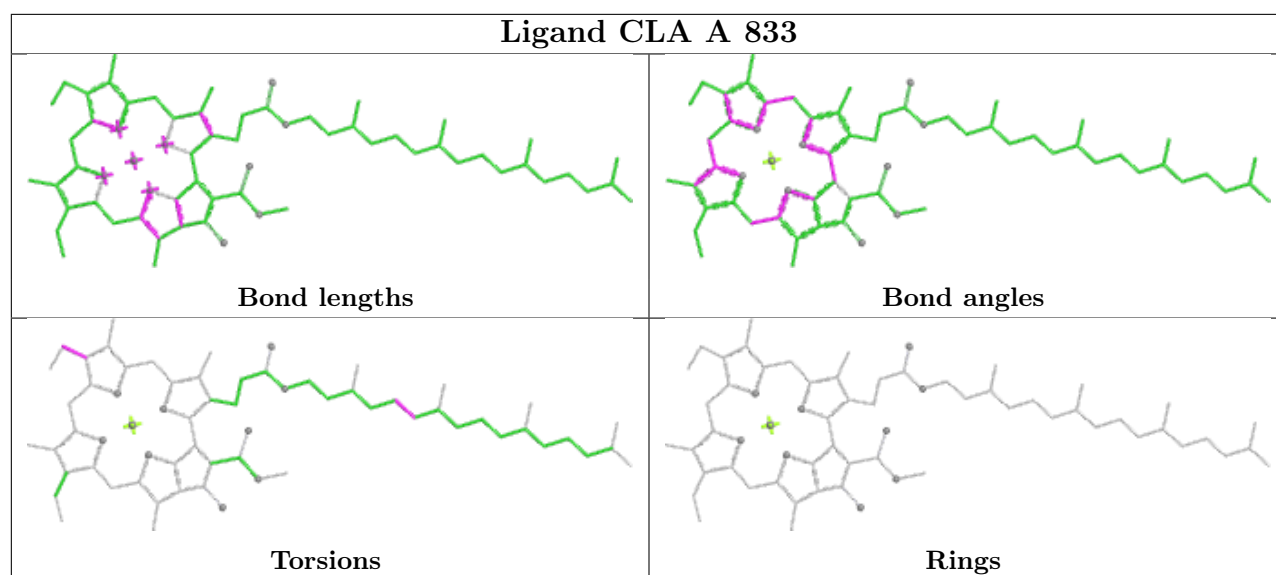


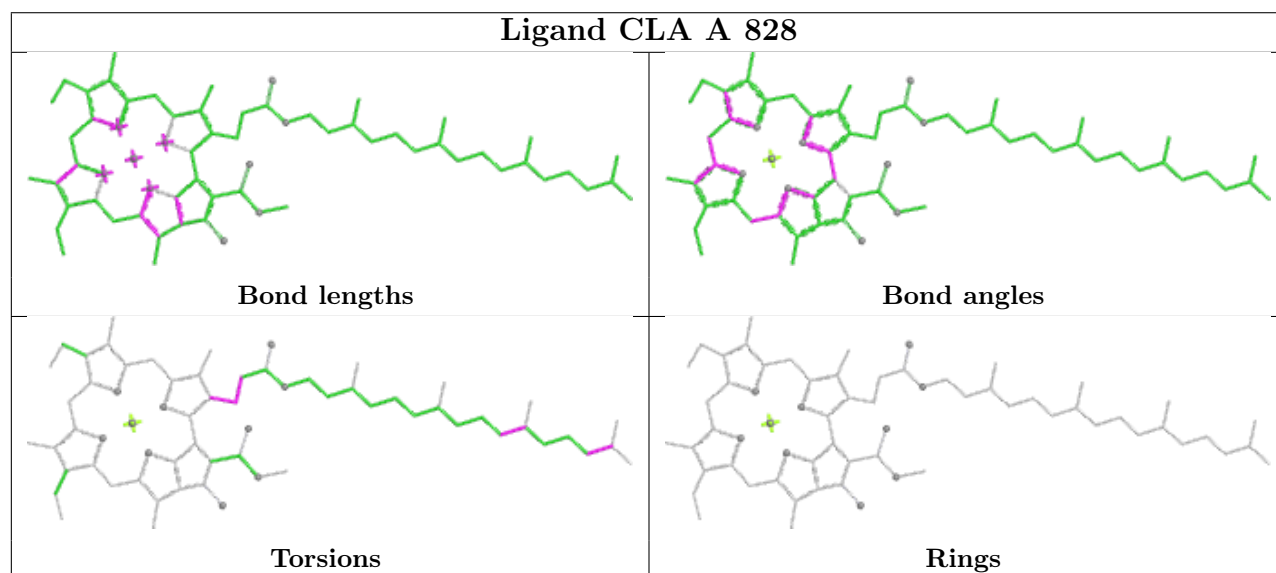
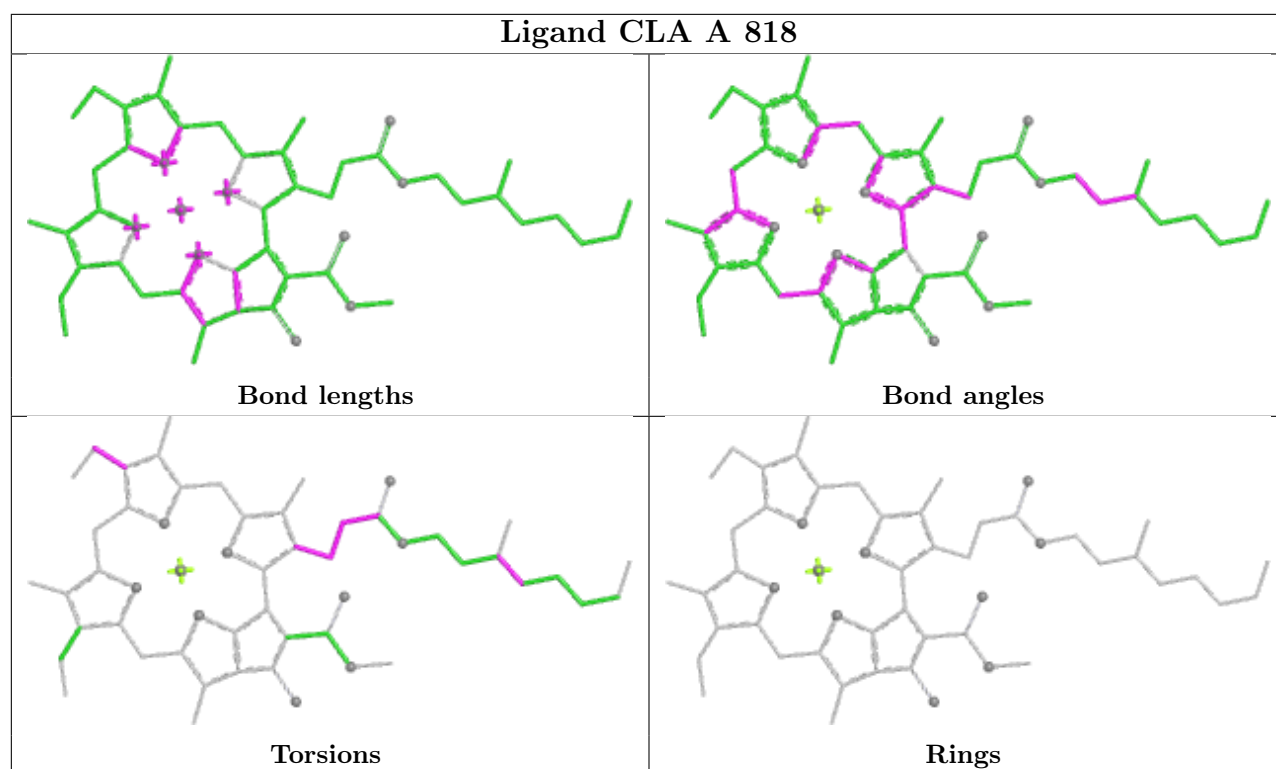
Ligand CLA A 832



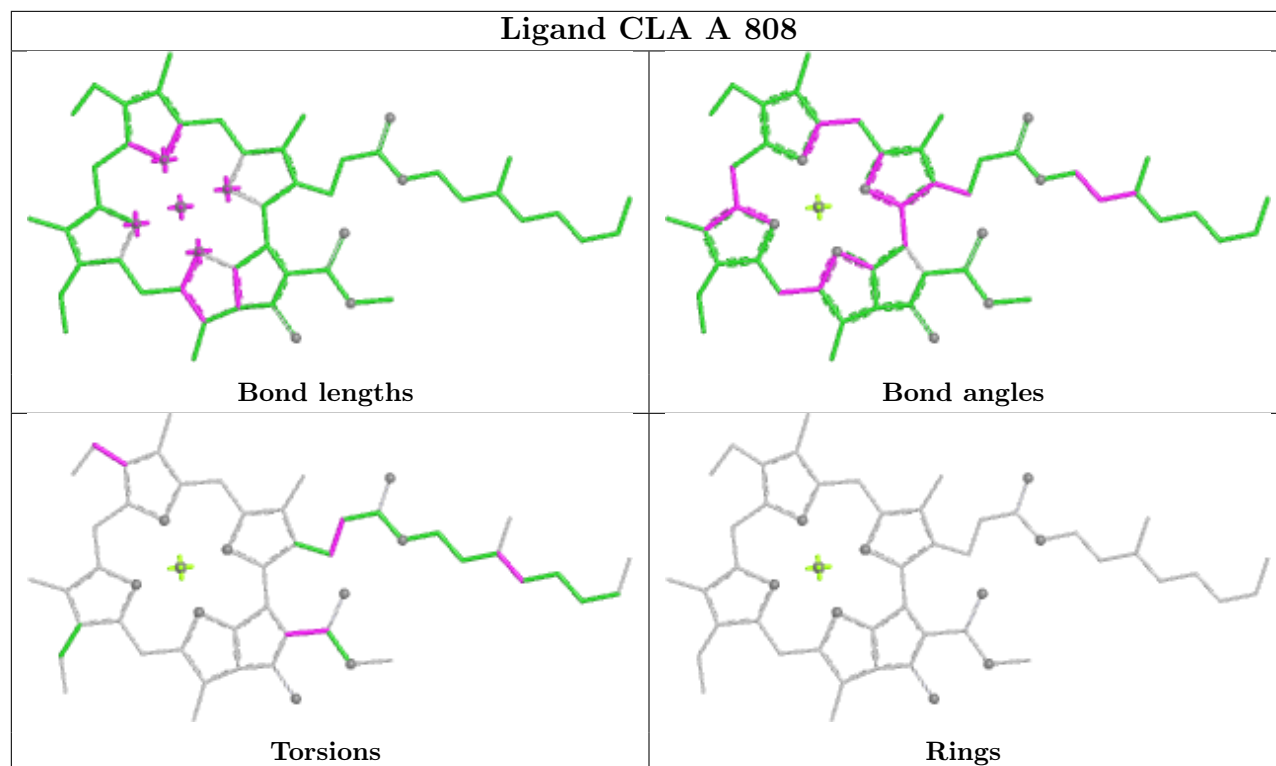




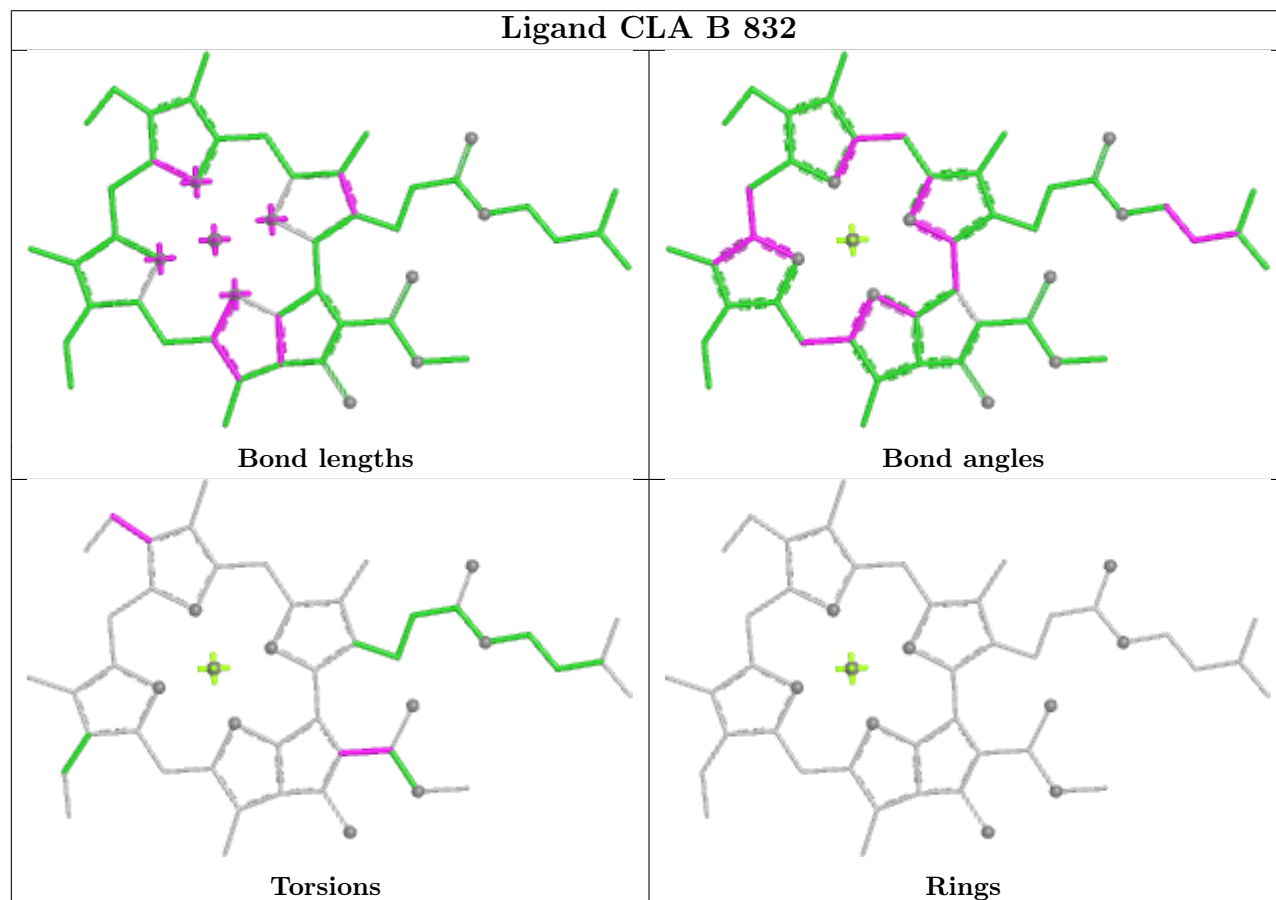


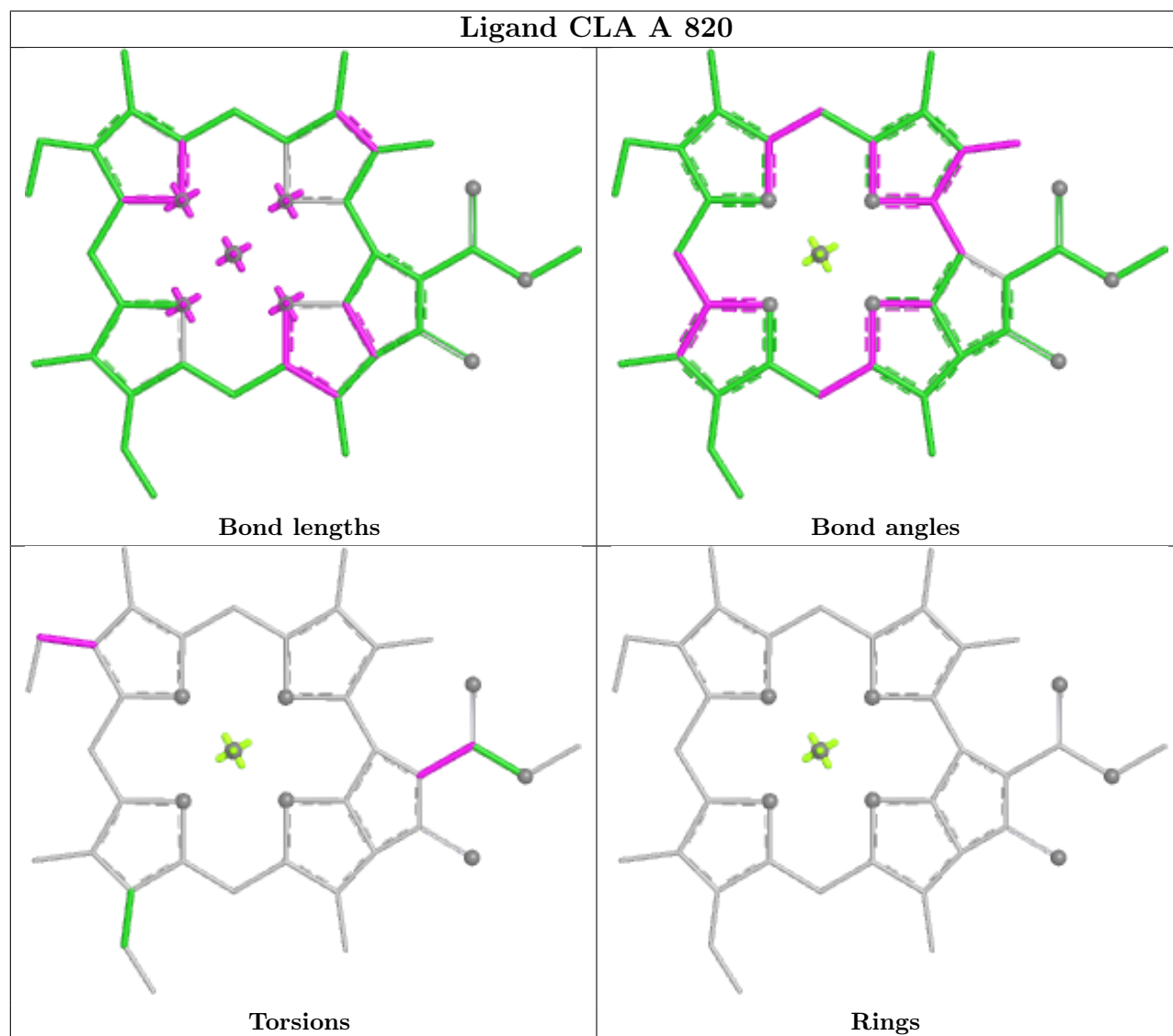
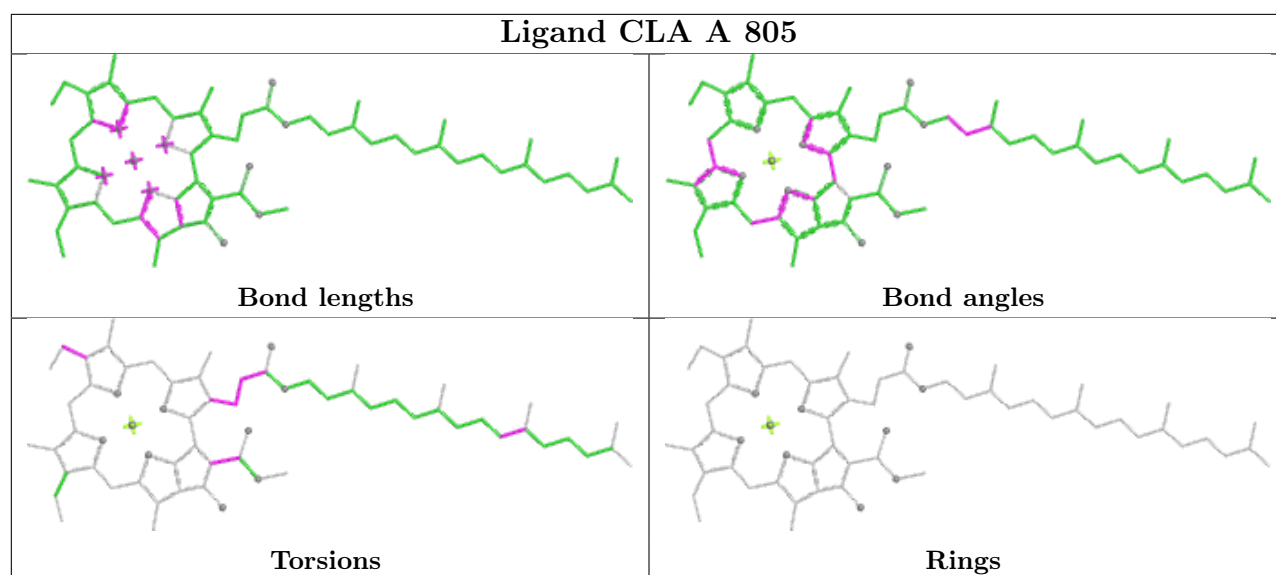


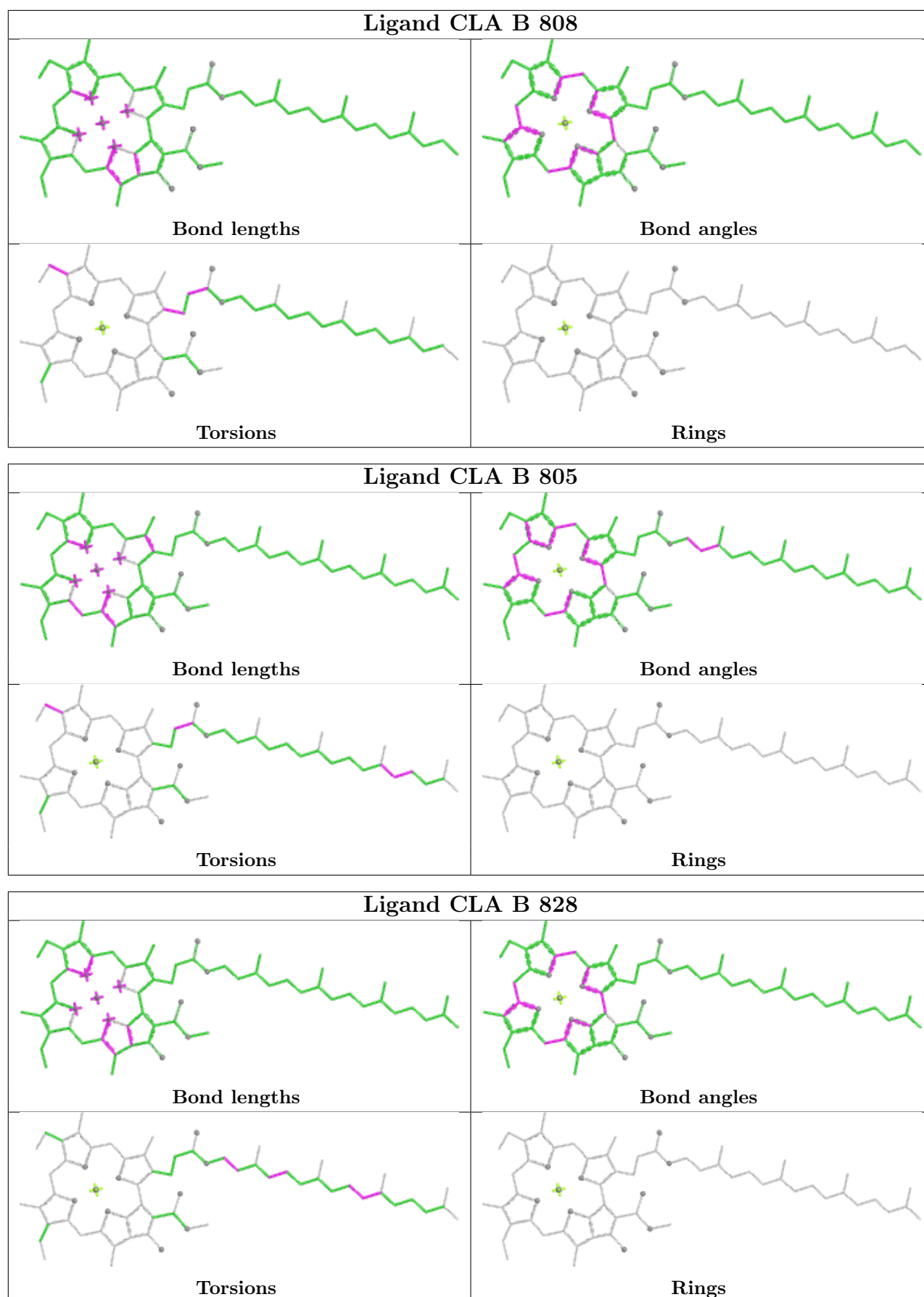
Ligand CLA A 808

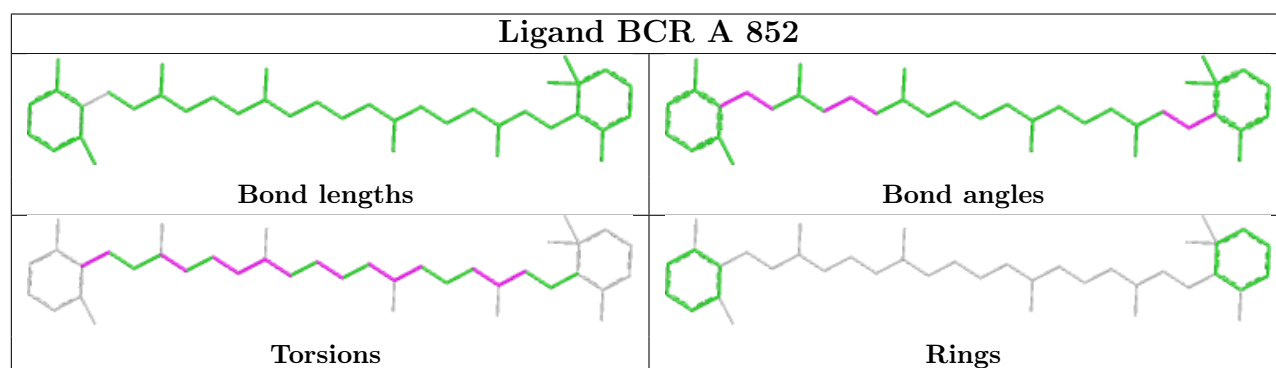
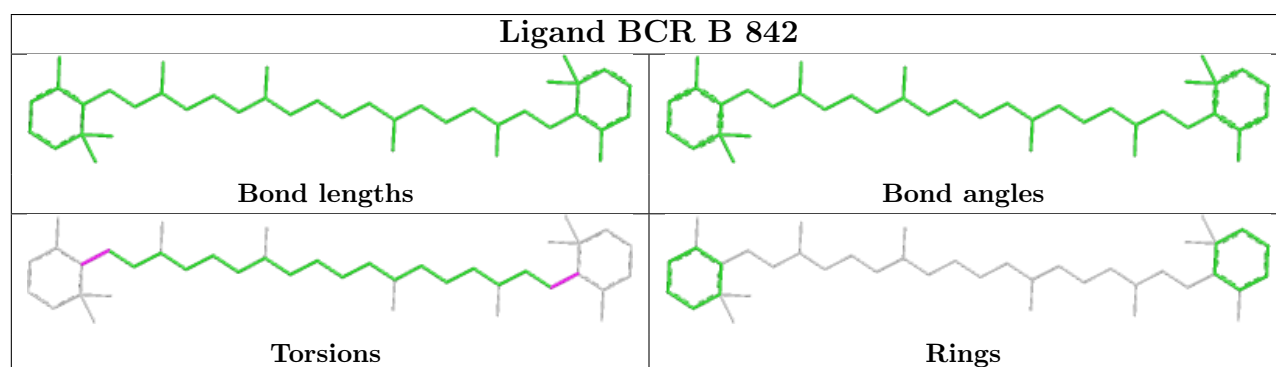
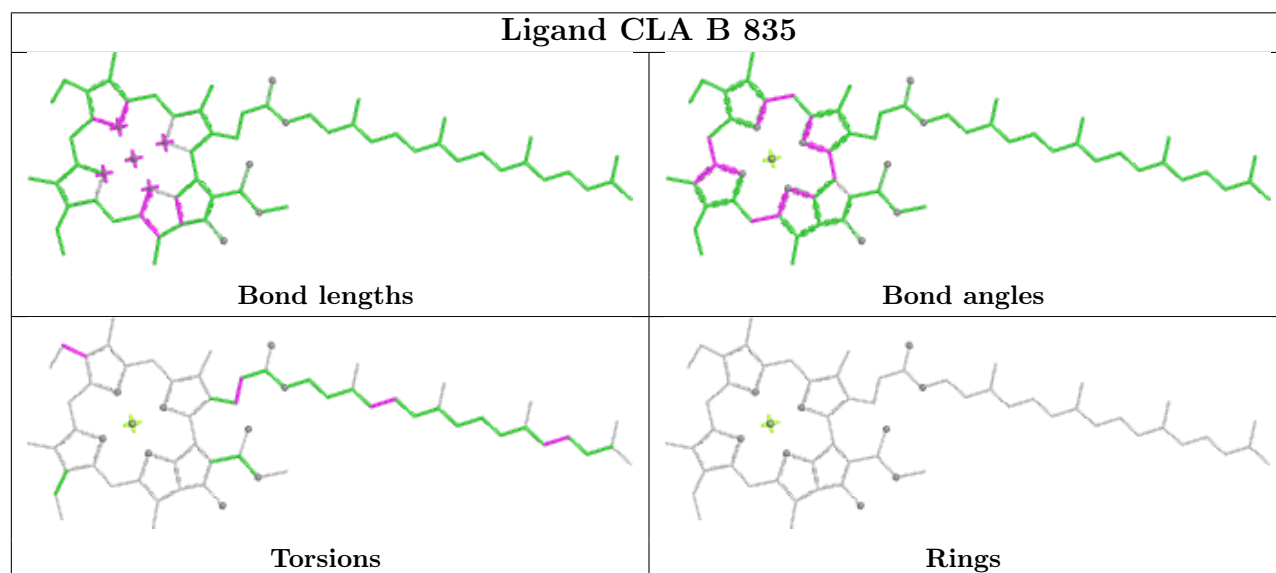
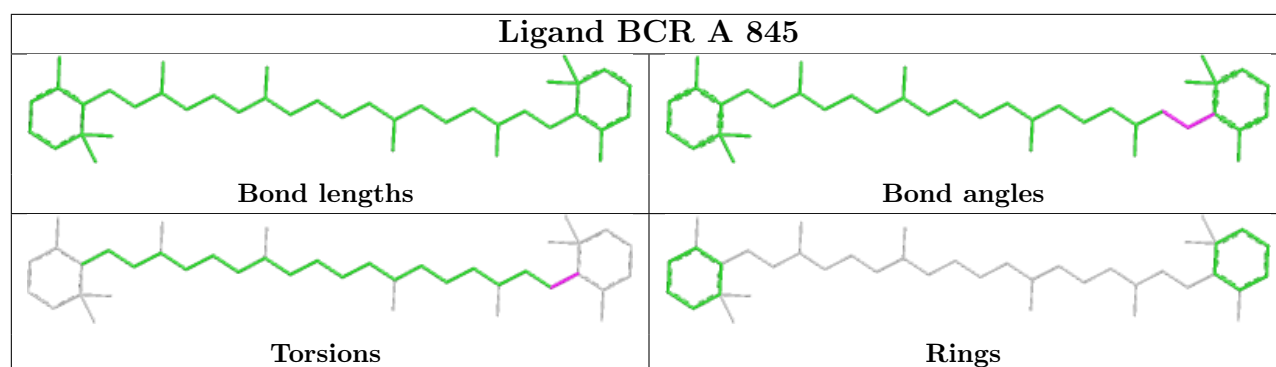


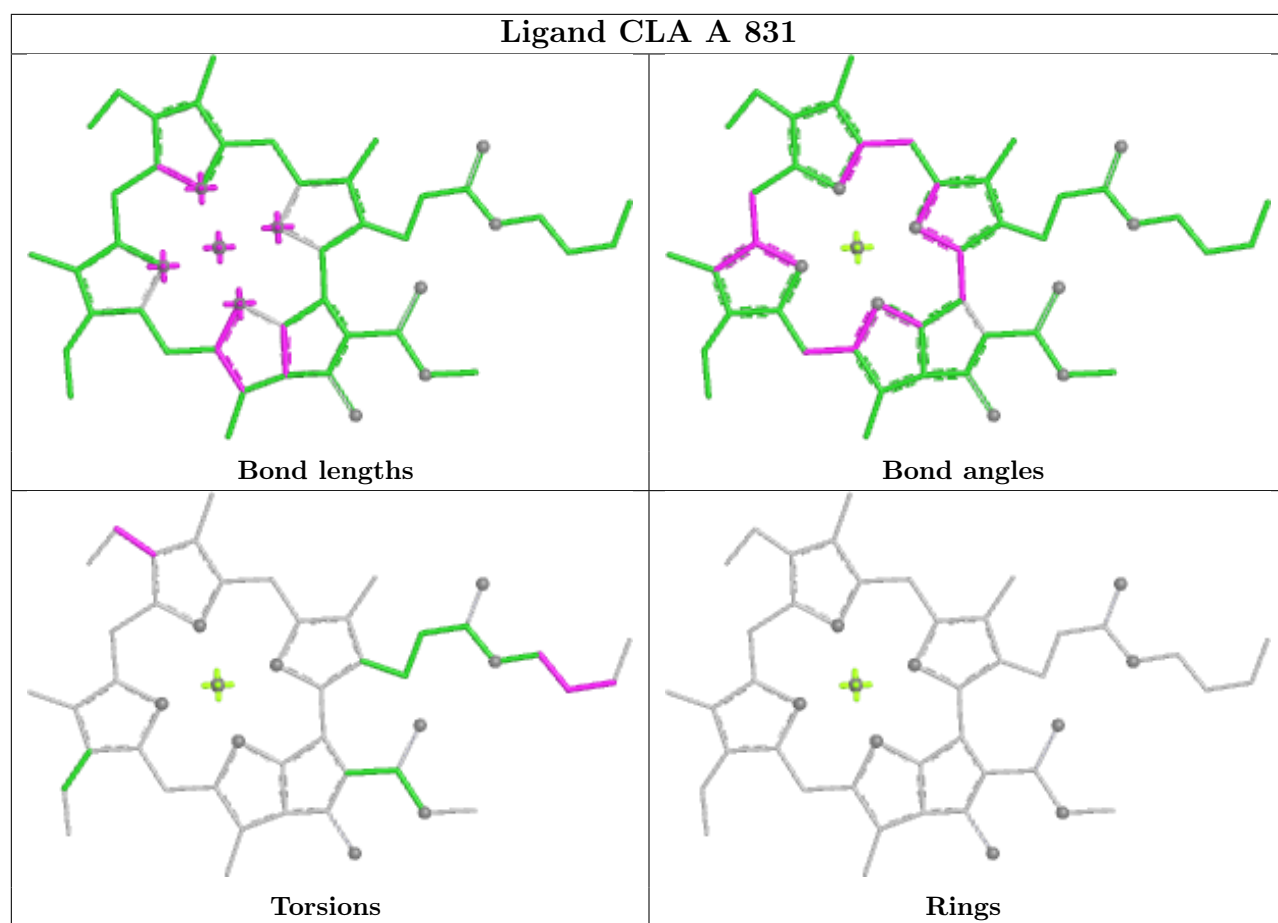
Ligand CLA B 832

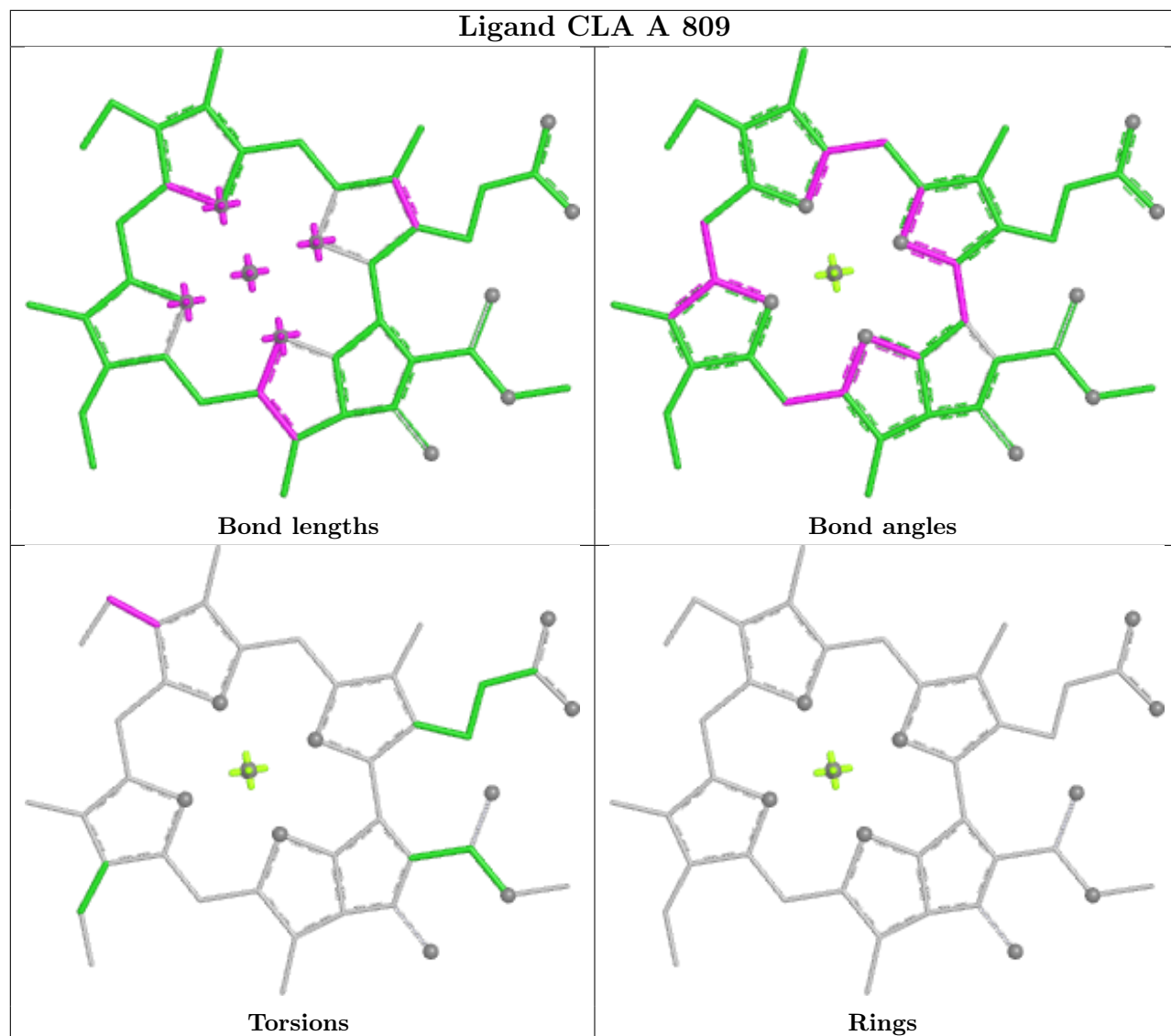




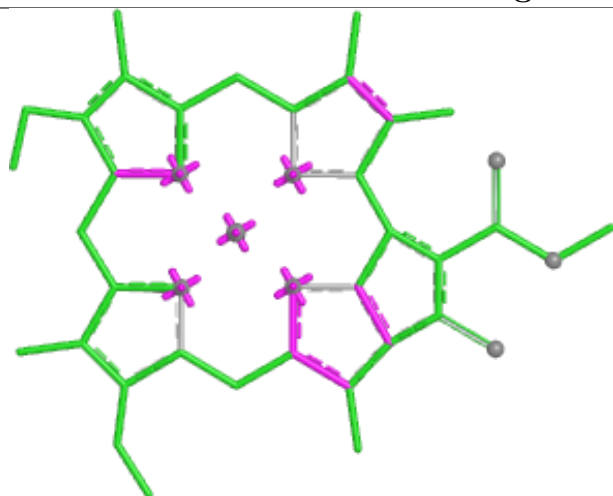




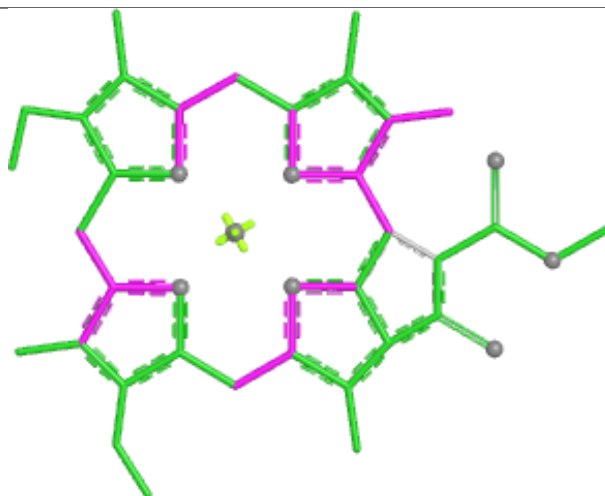




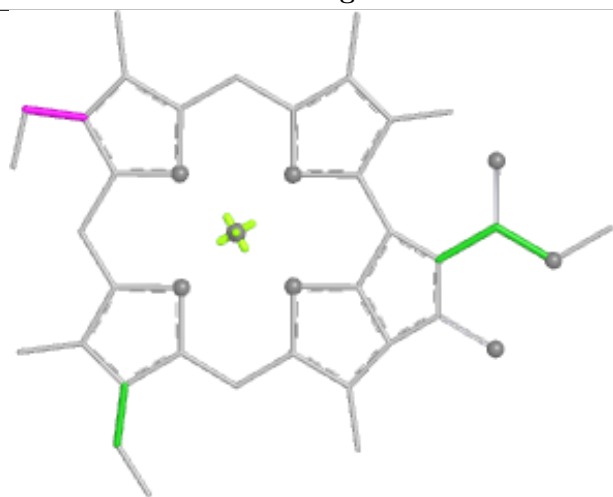
Ligand CLA B 827



Bond lengths



Bond angles

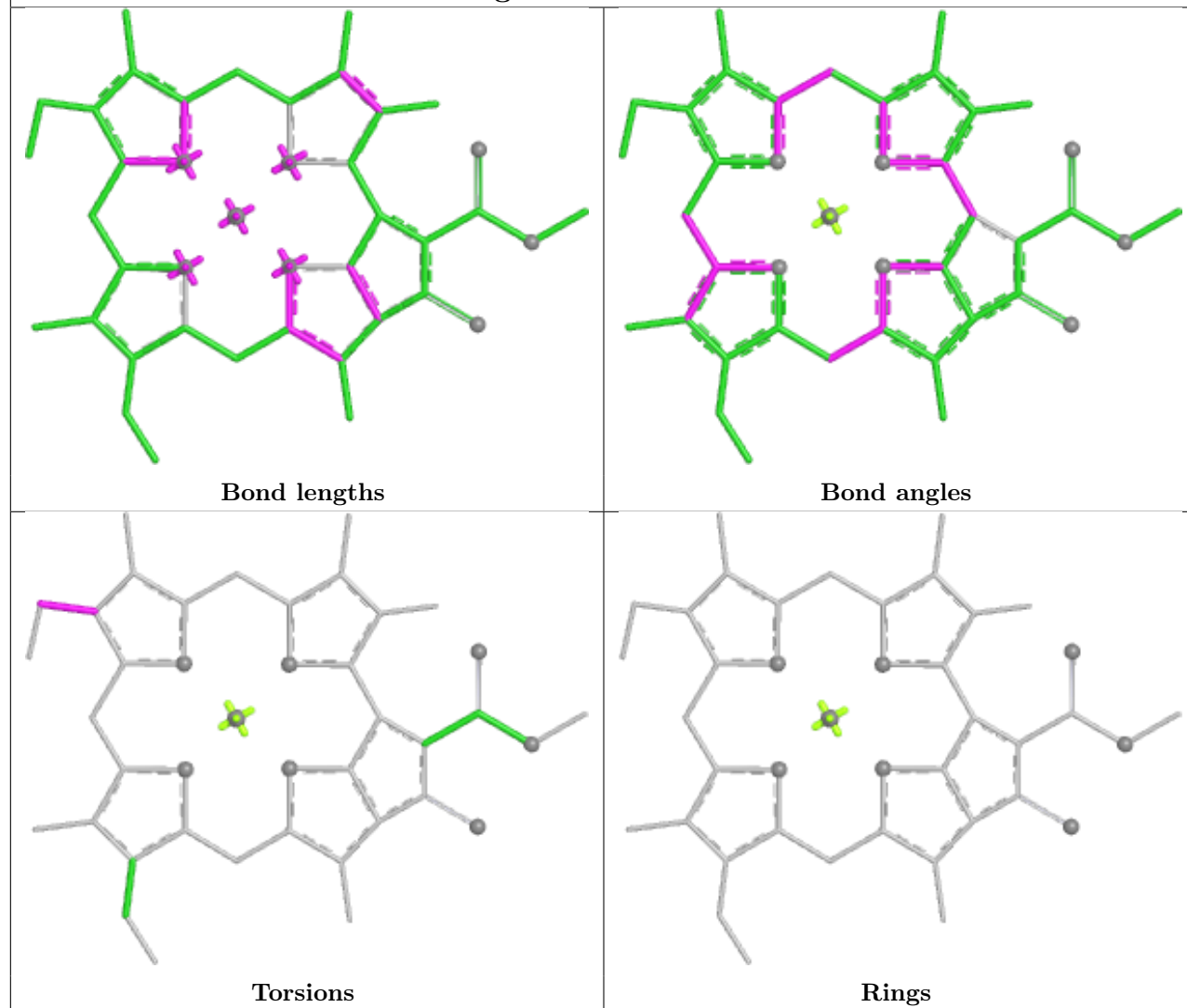


Torsions

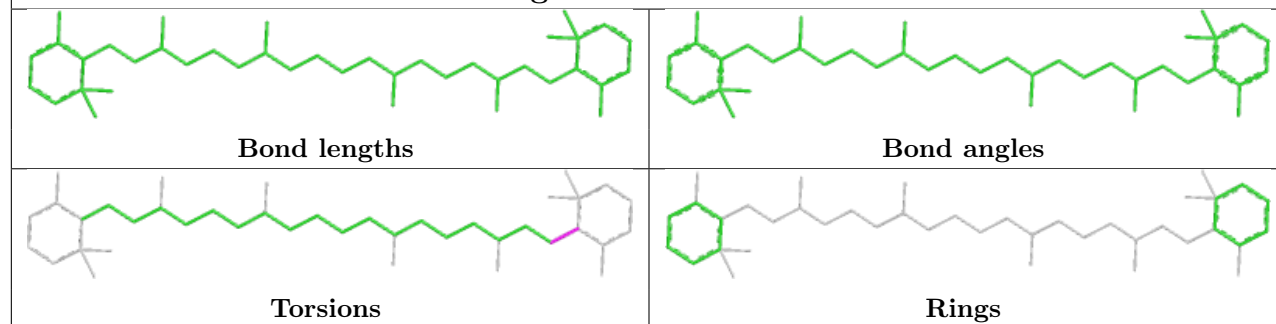


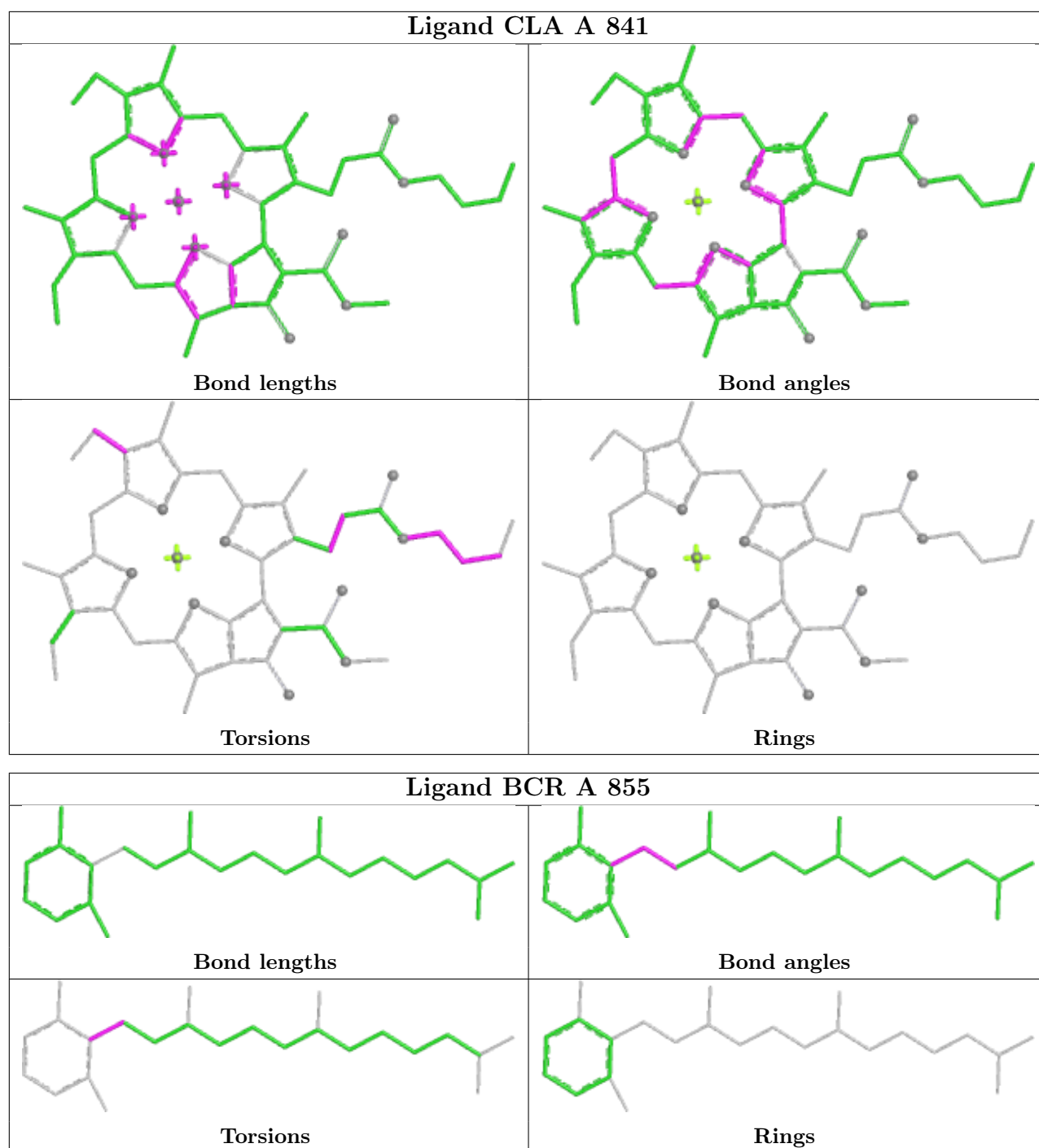
Rings

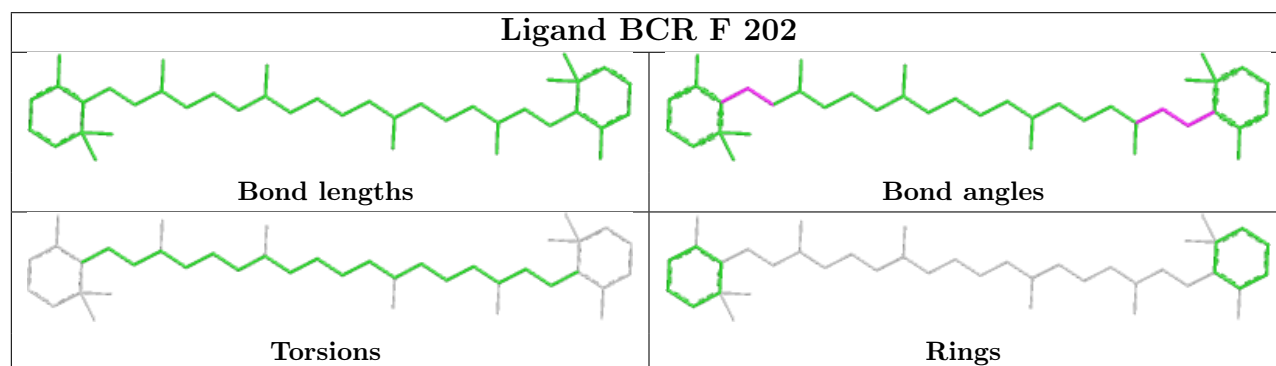
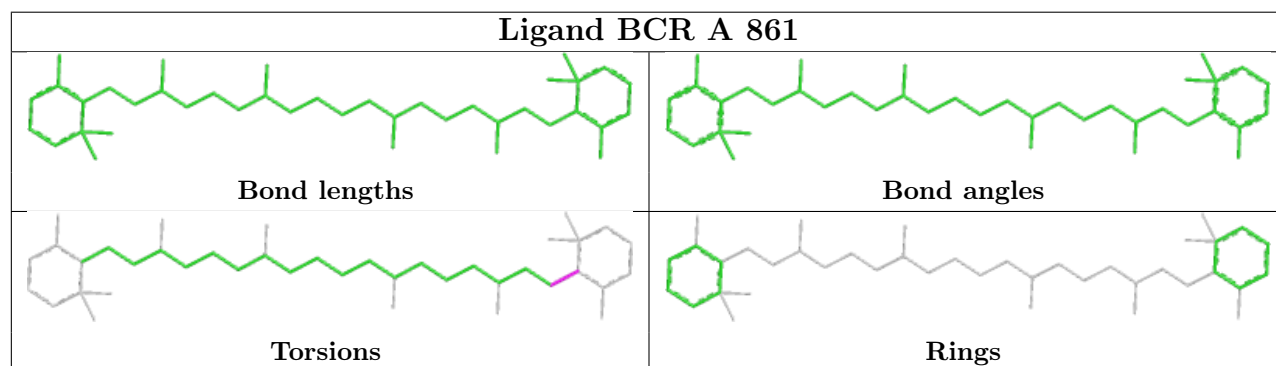
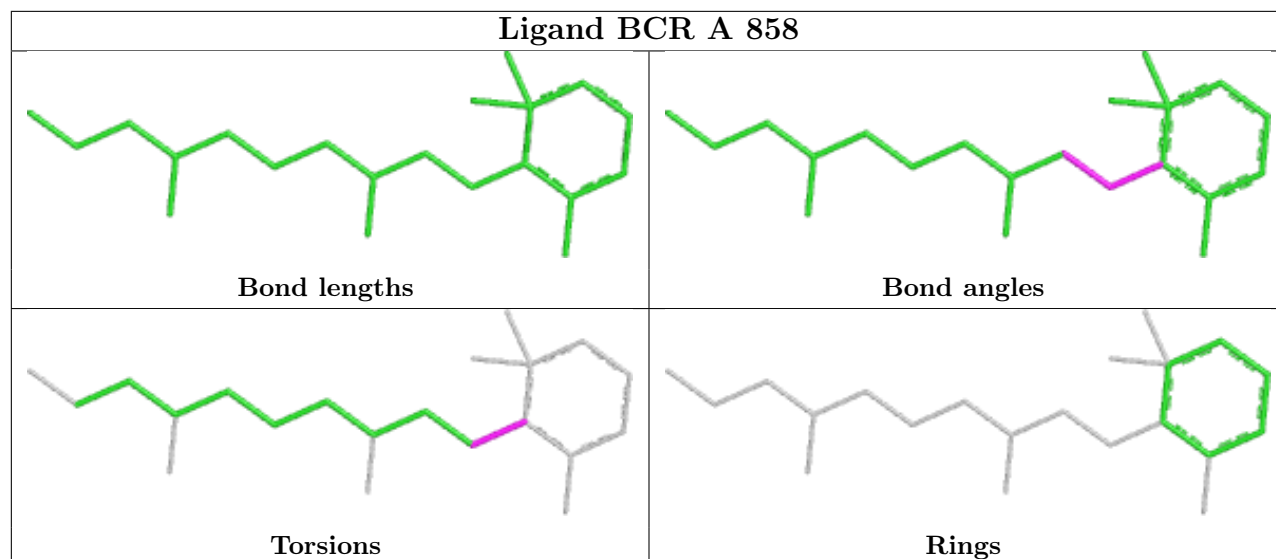
Ligand CLA A 814

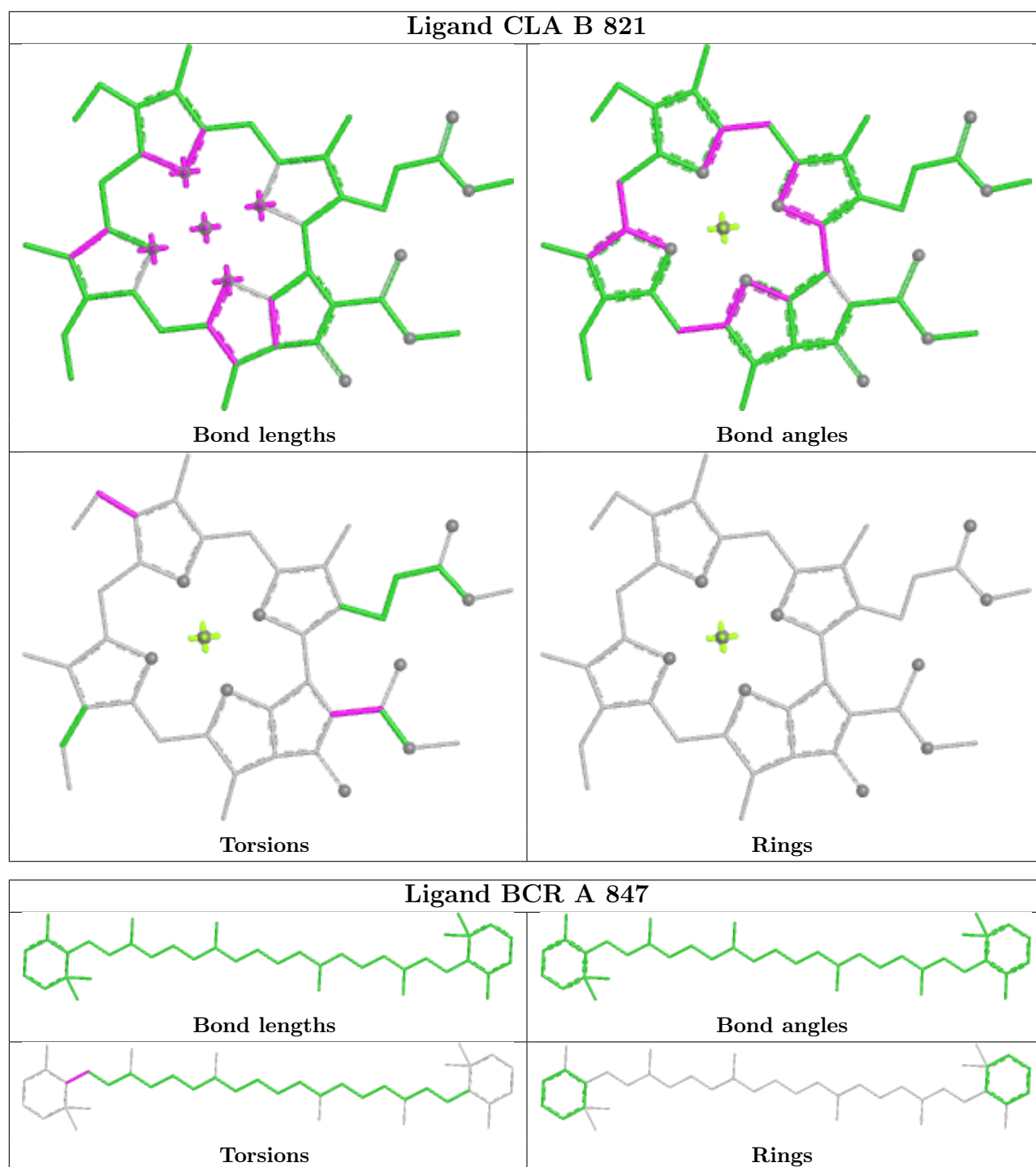


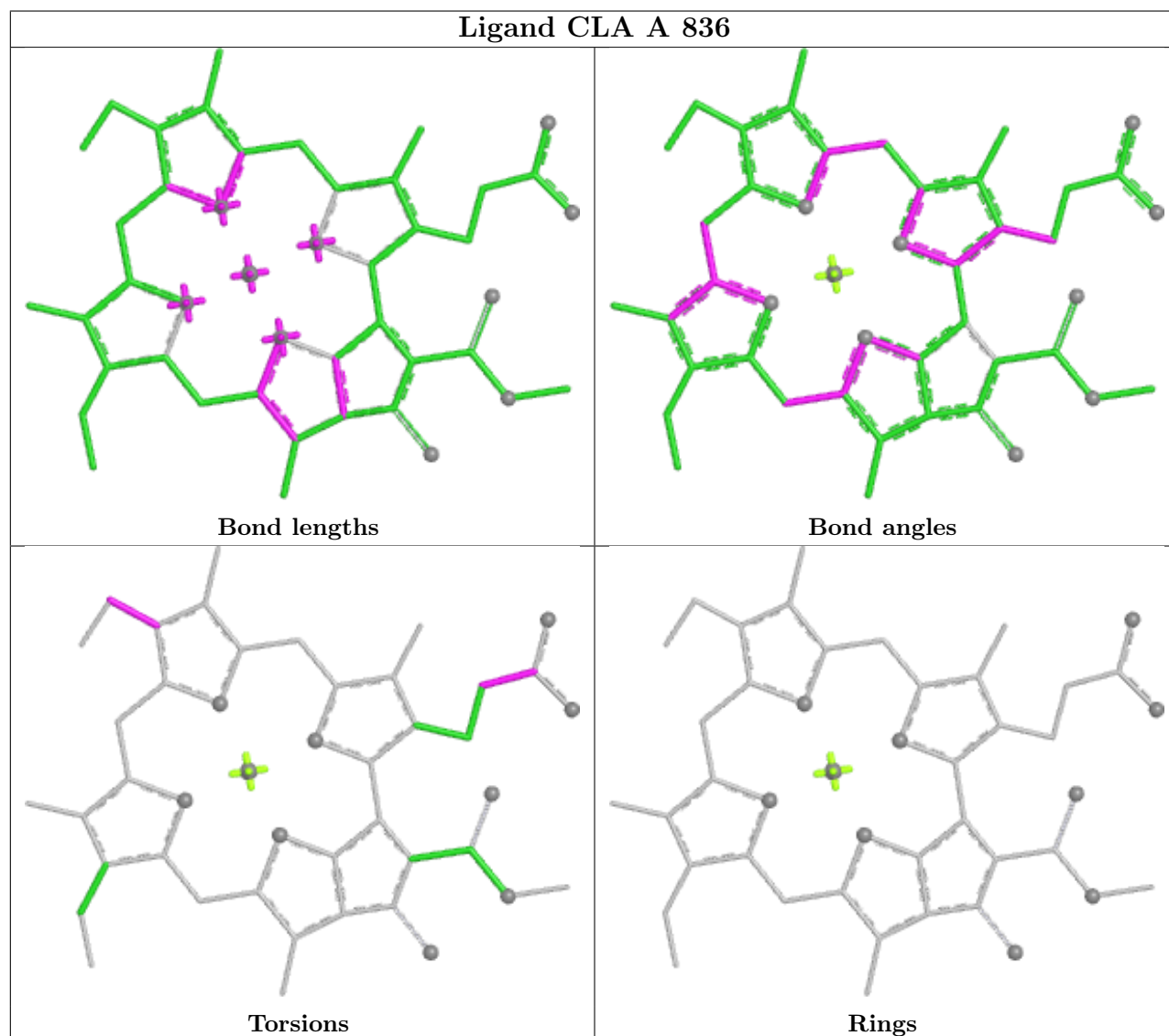
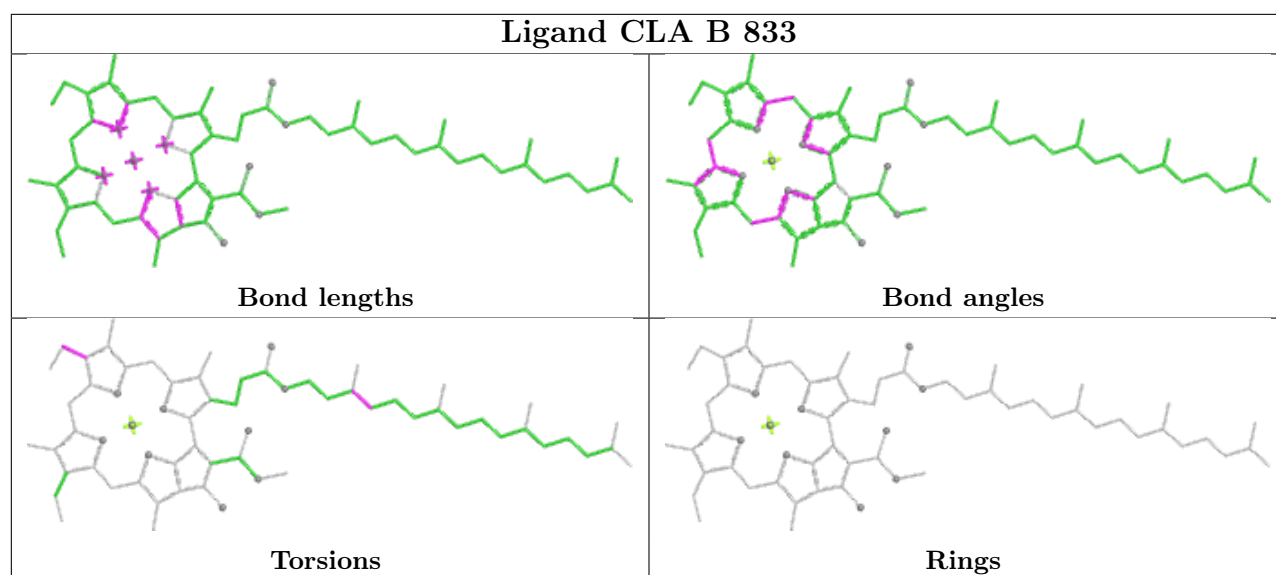
Ligand BCR B 841



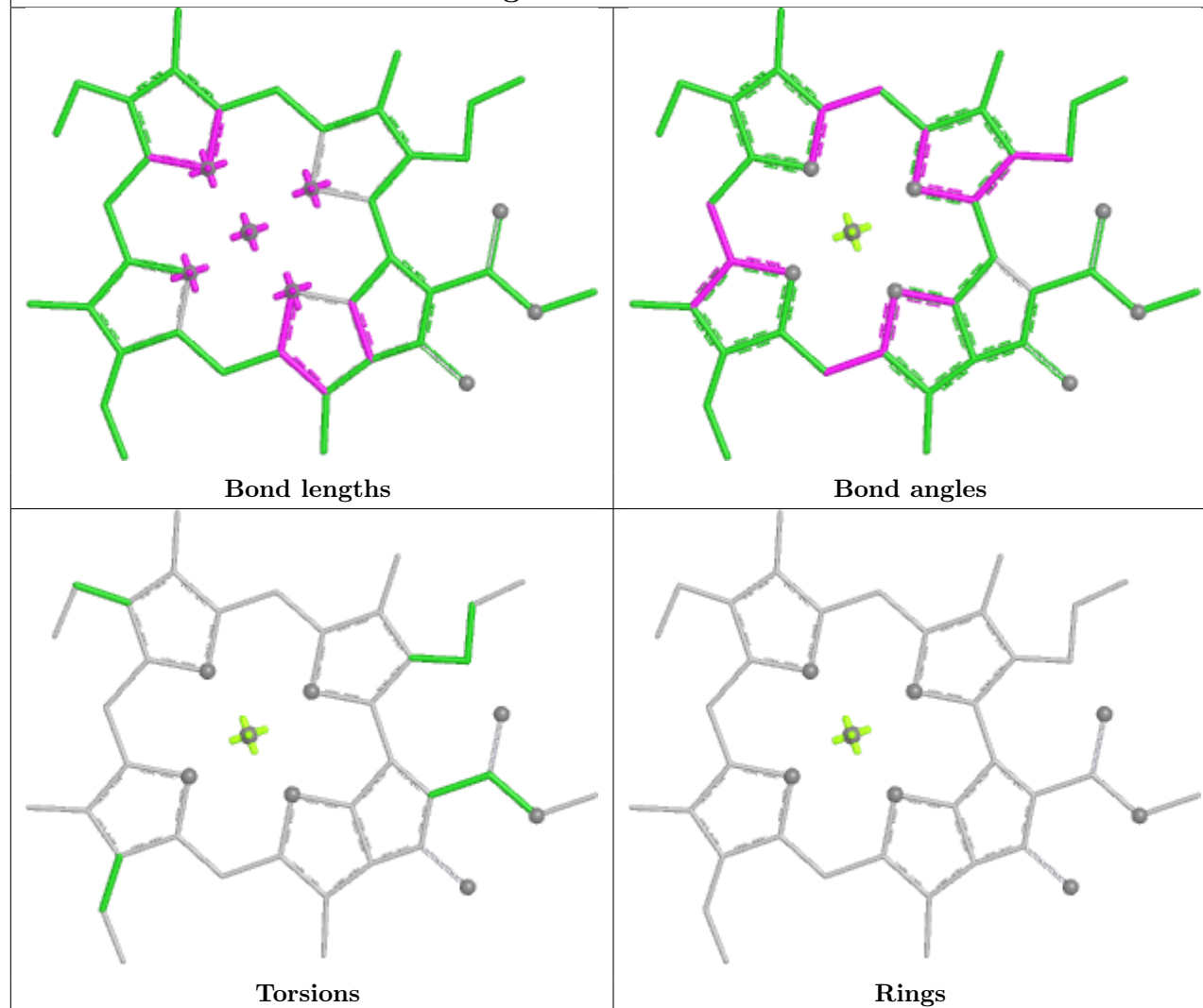




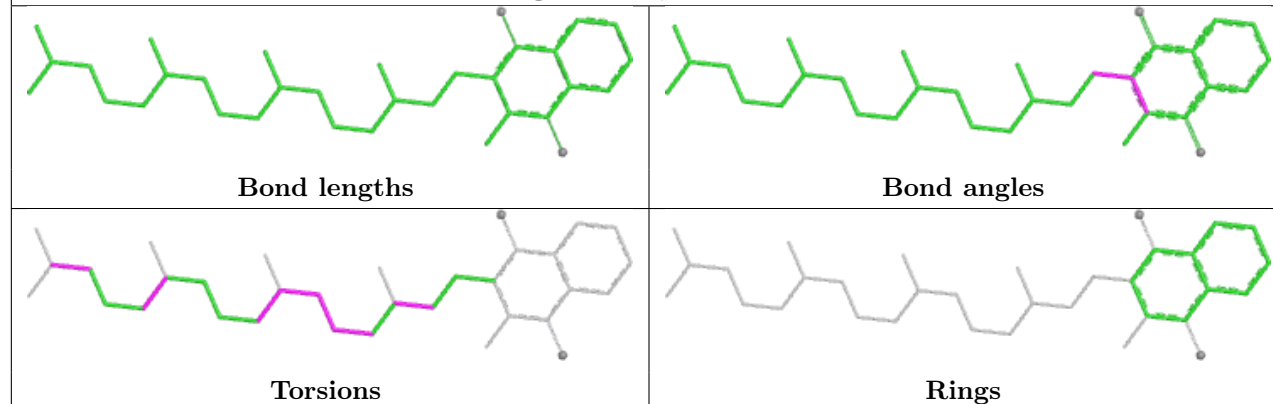




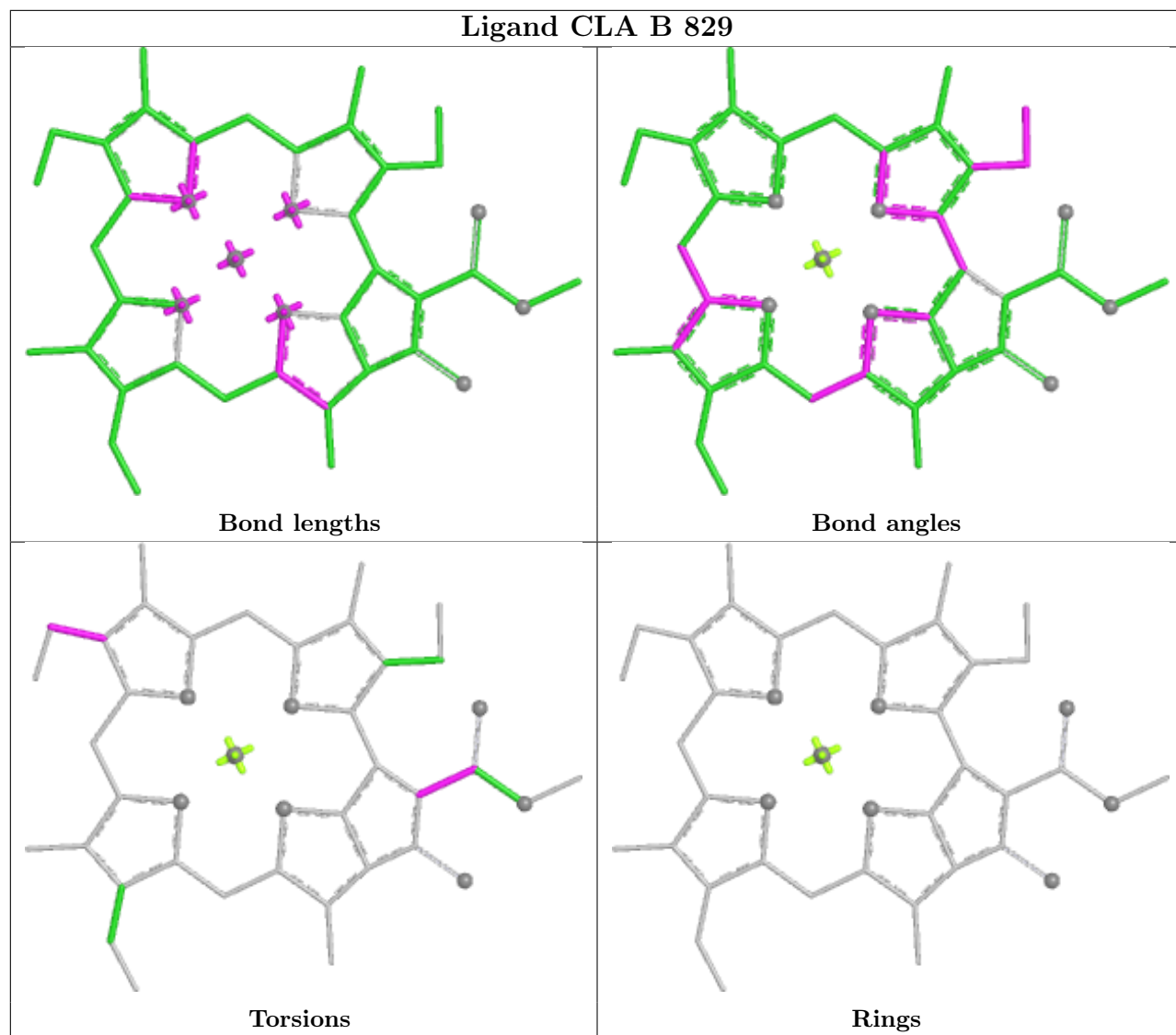
Ligand CLA B 813

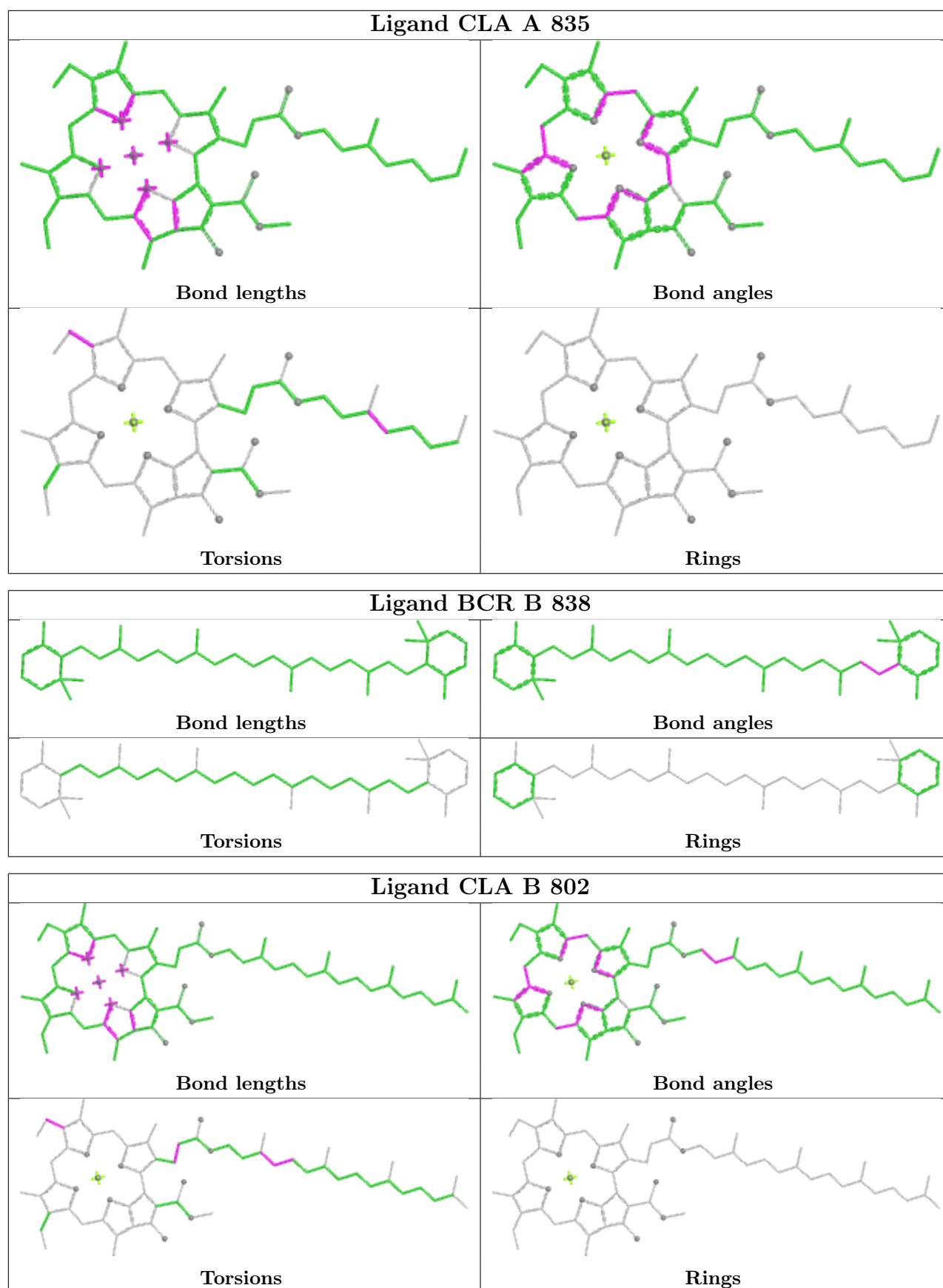


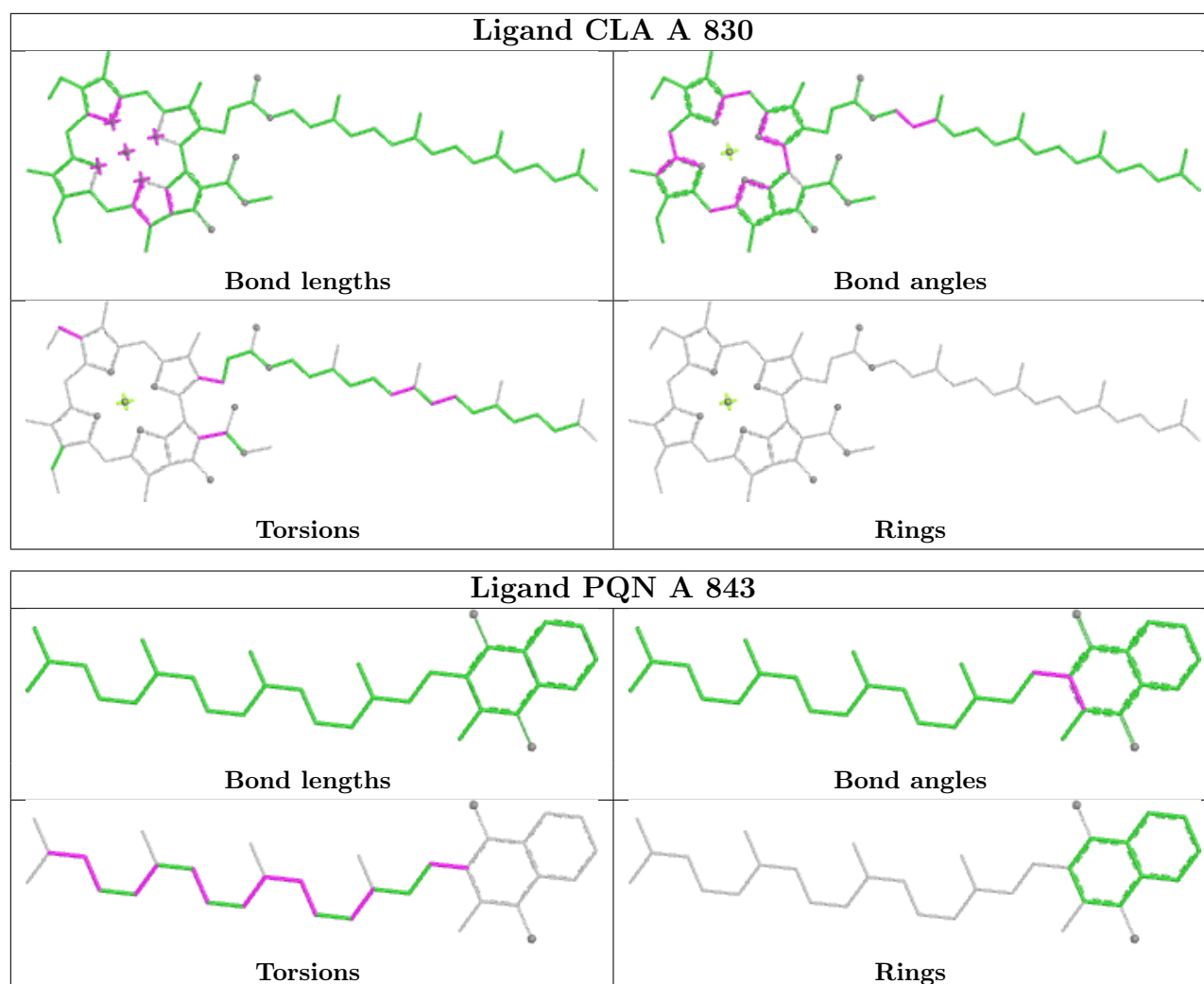
Ligand PQN B 837

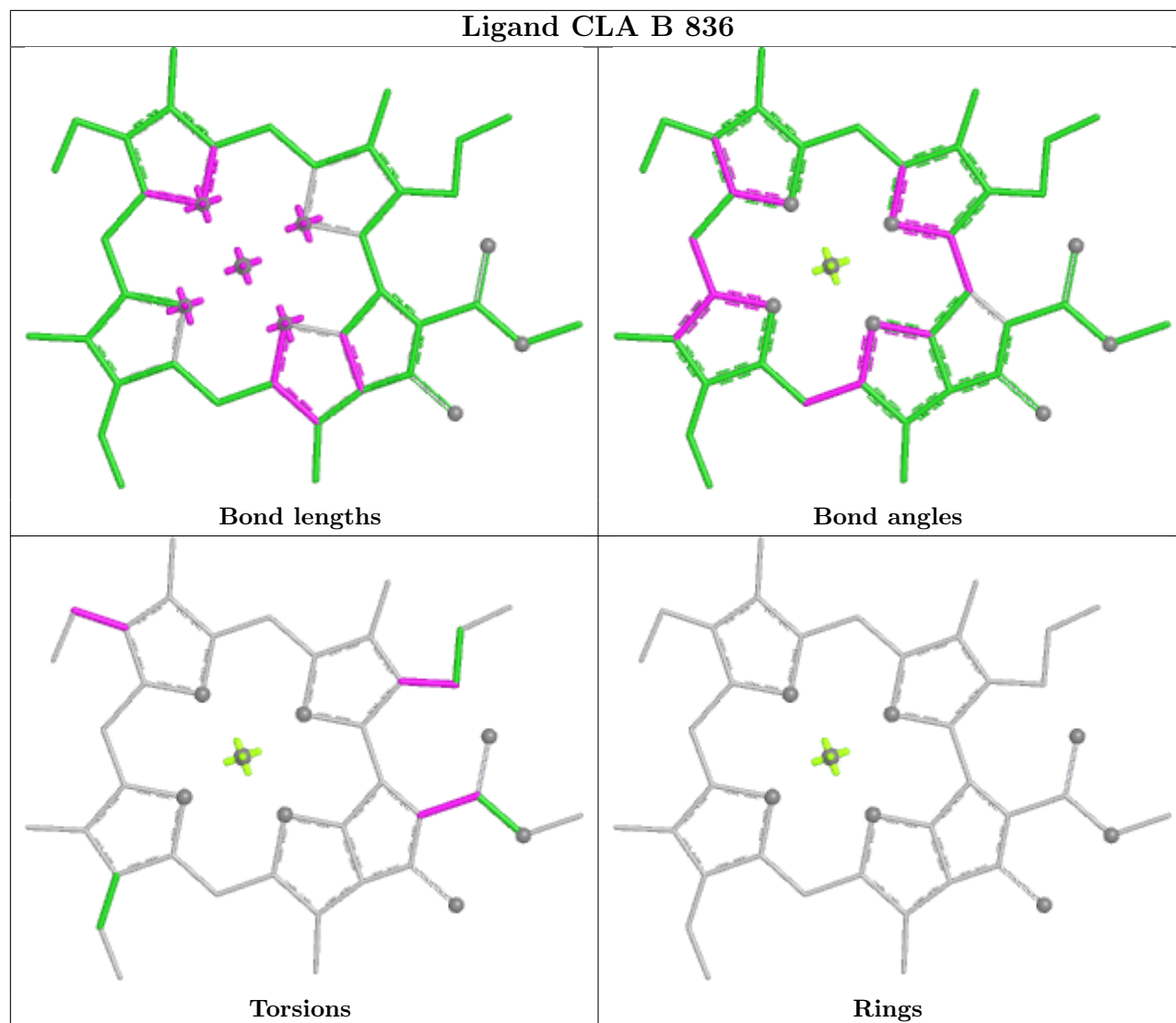


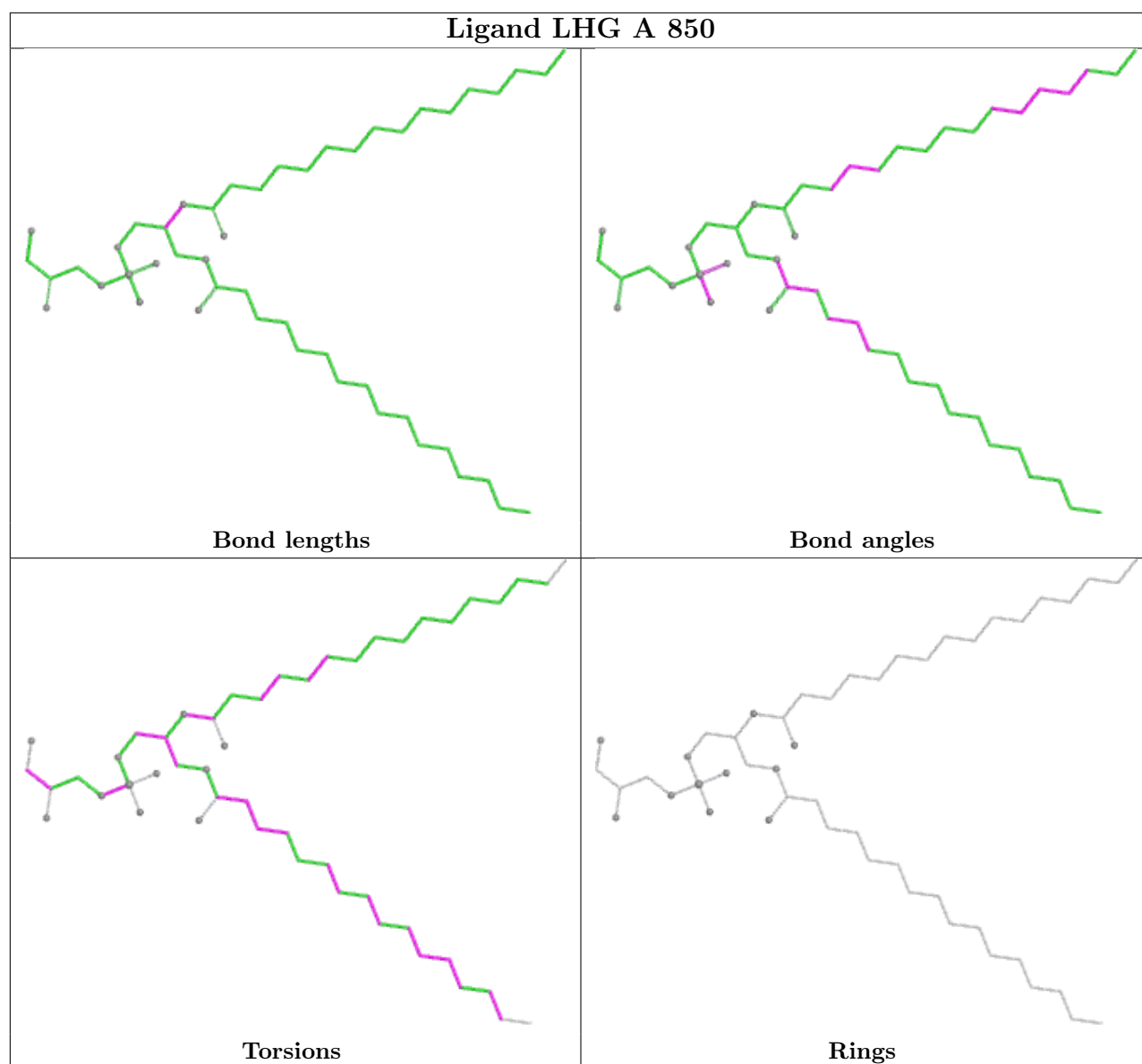
Ligand CLA B 829

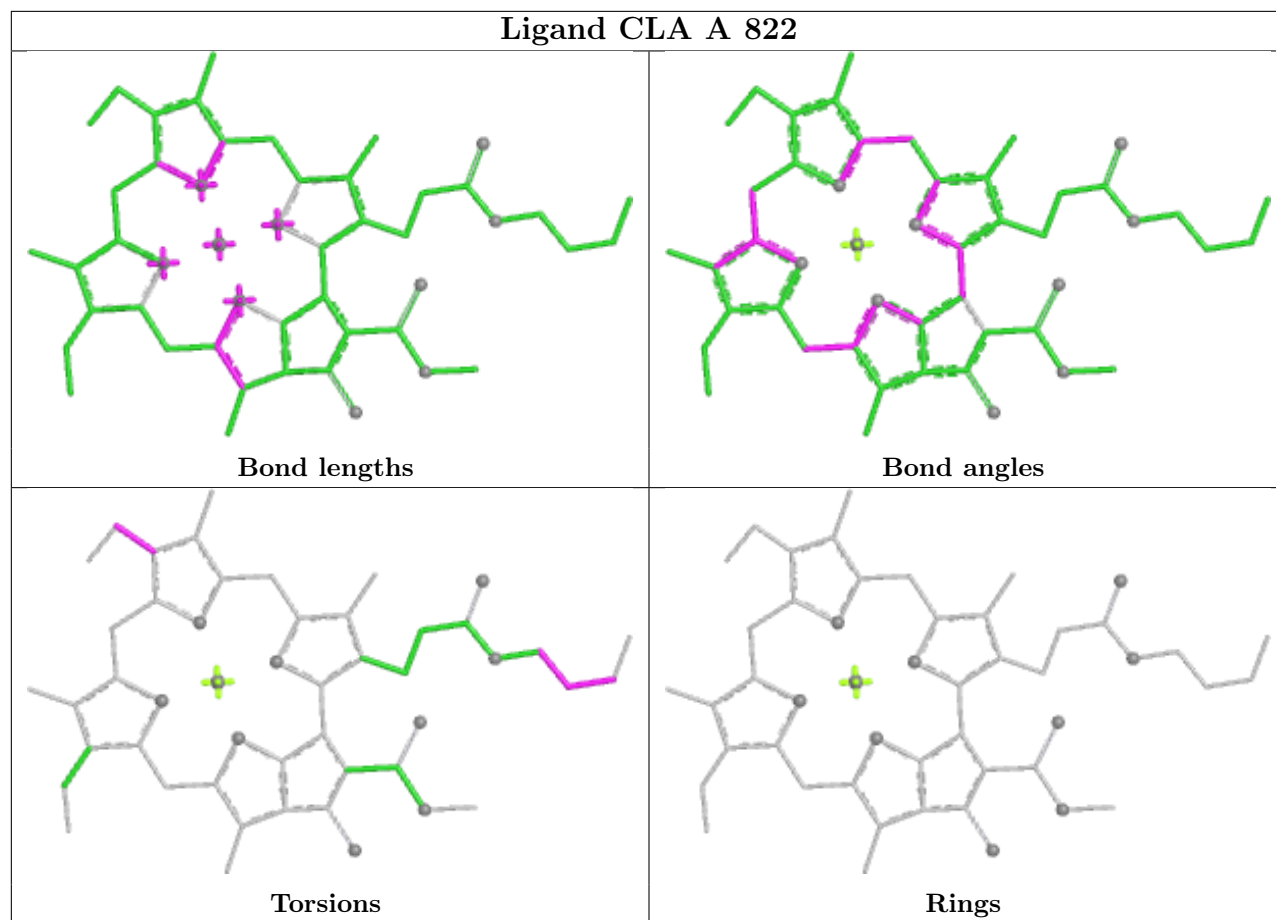




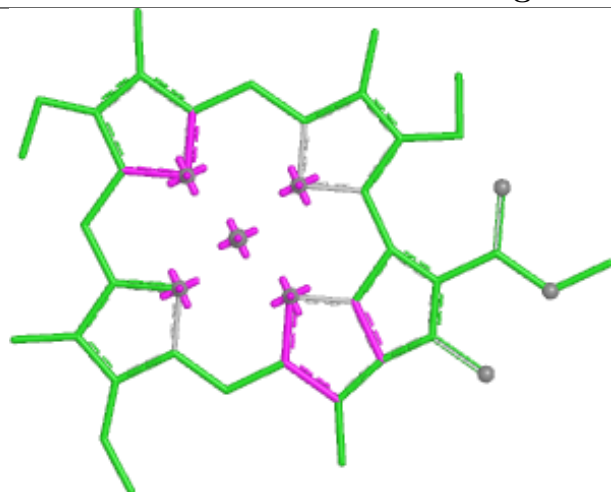




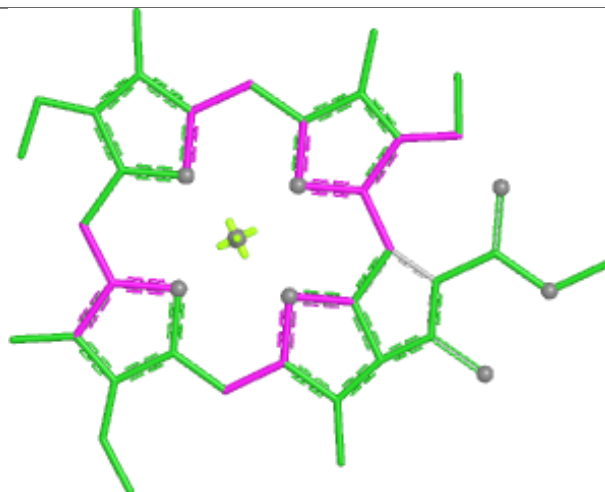




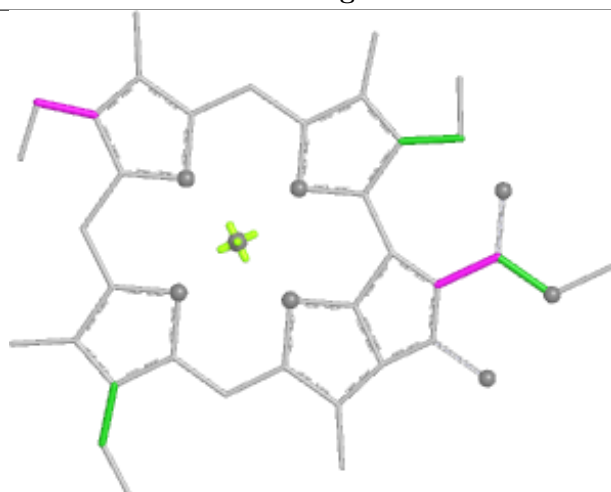
Ligand CLA A 803



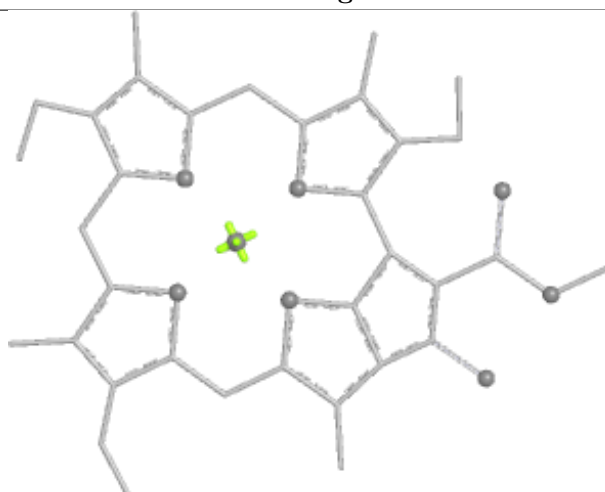
Bond lengths



Bond angles

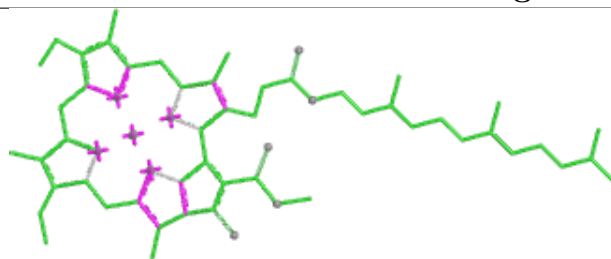


Torsions

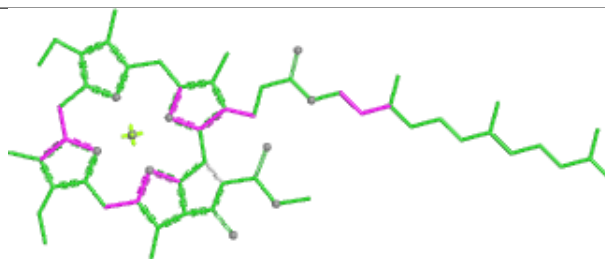


Rings

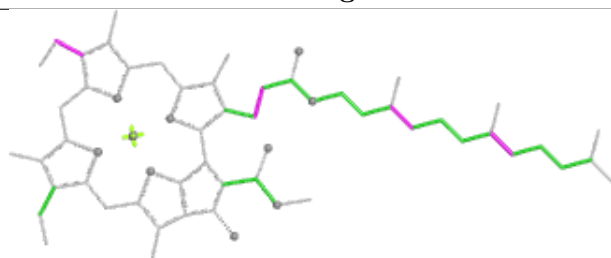
Ligand CLA A 826



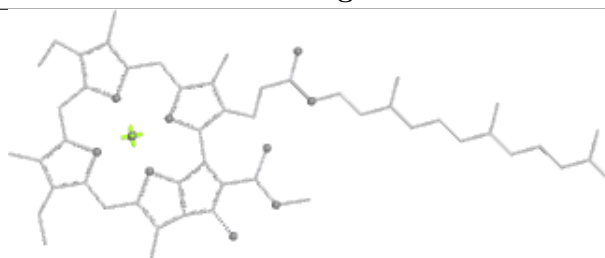
Bond lengths



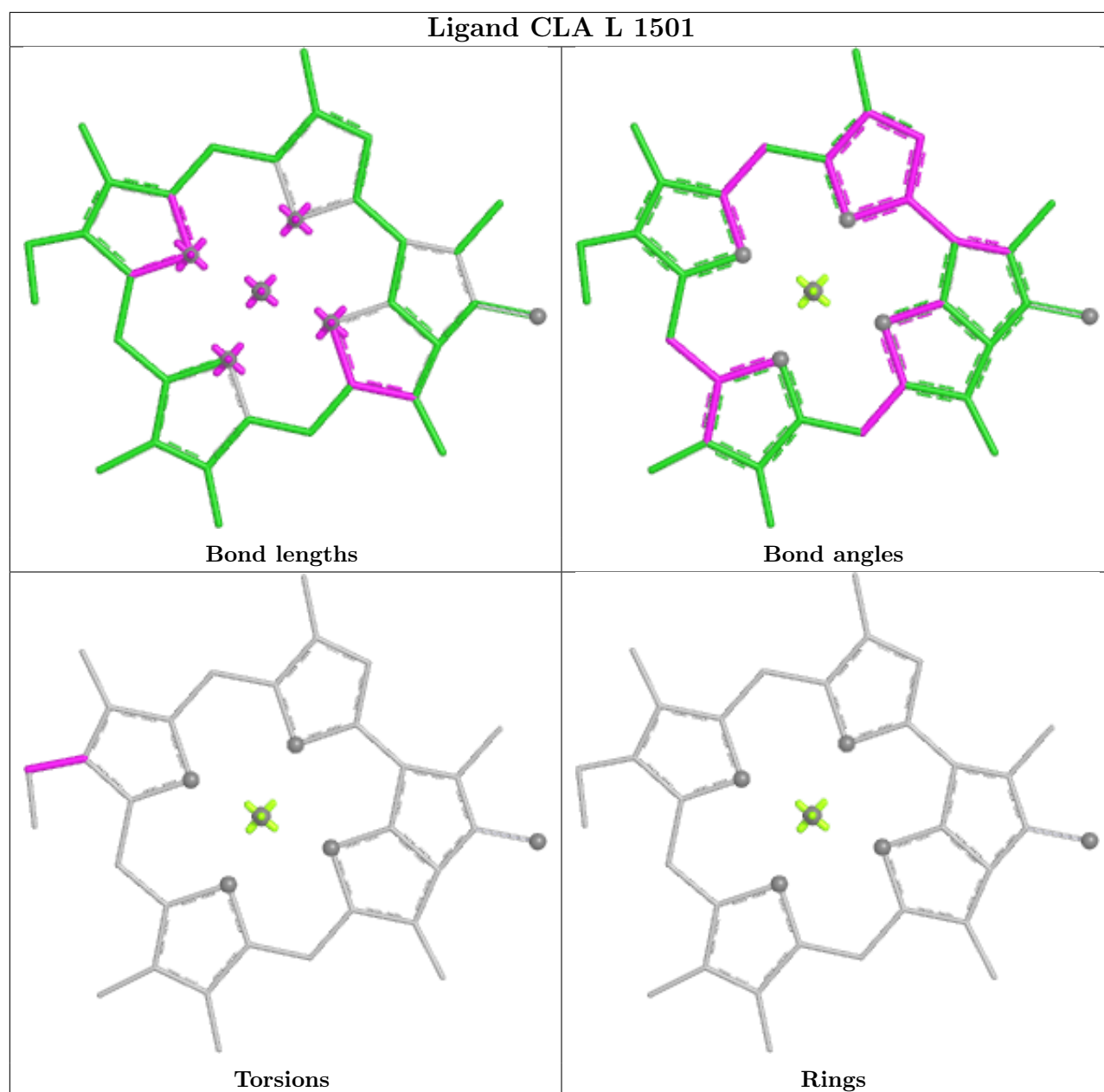
Bond angles

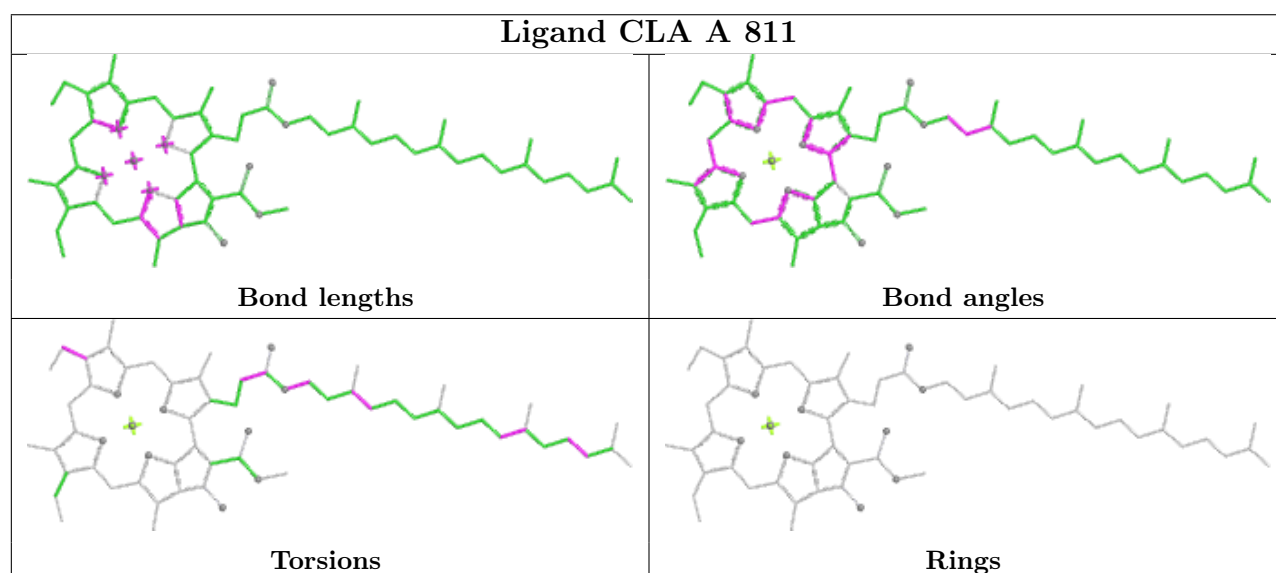
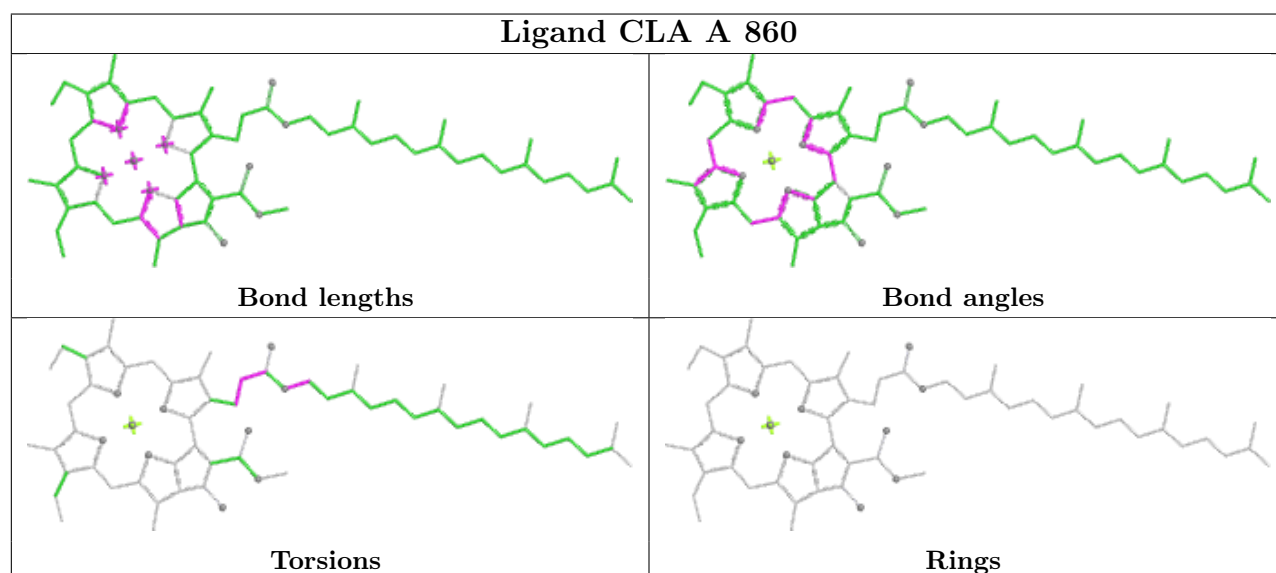
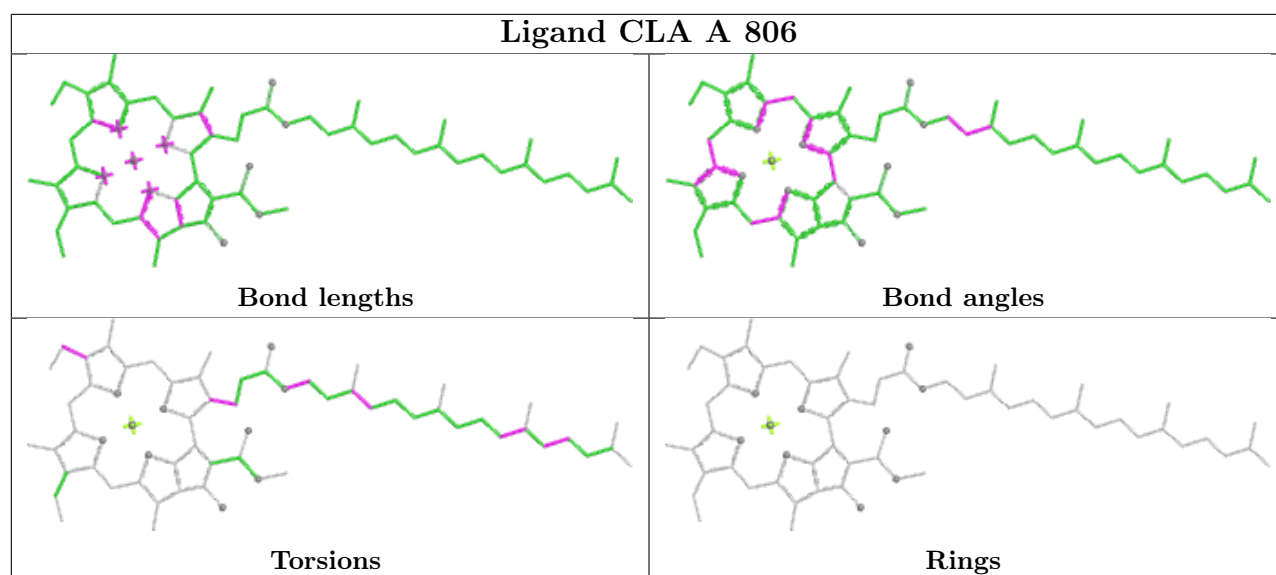


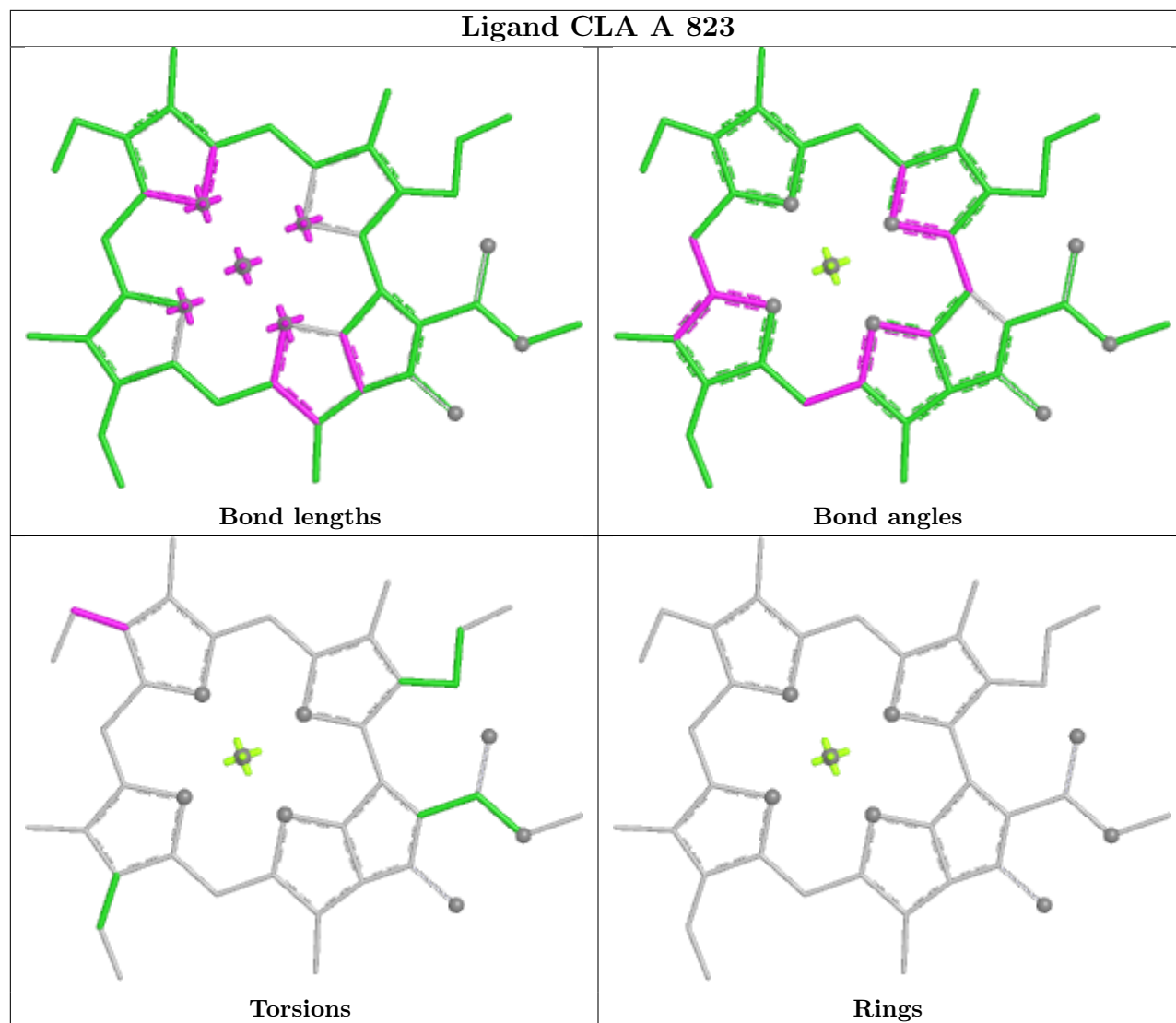
Torsions

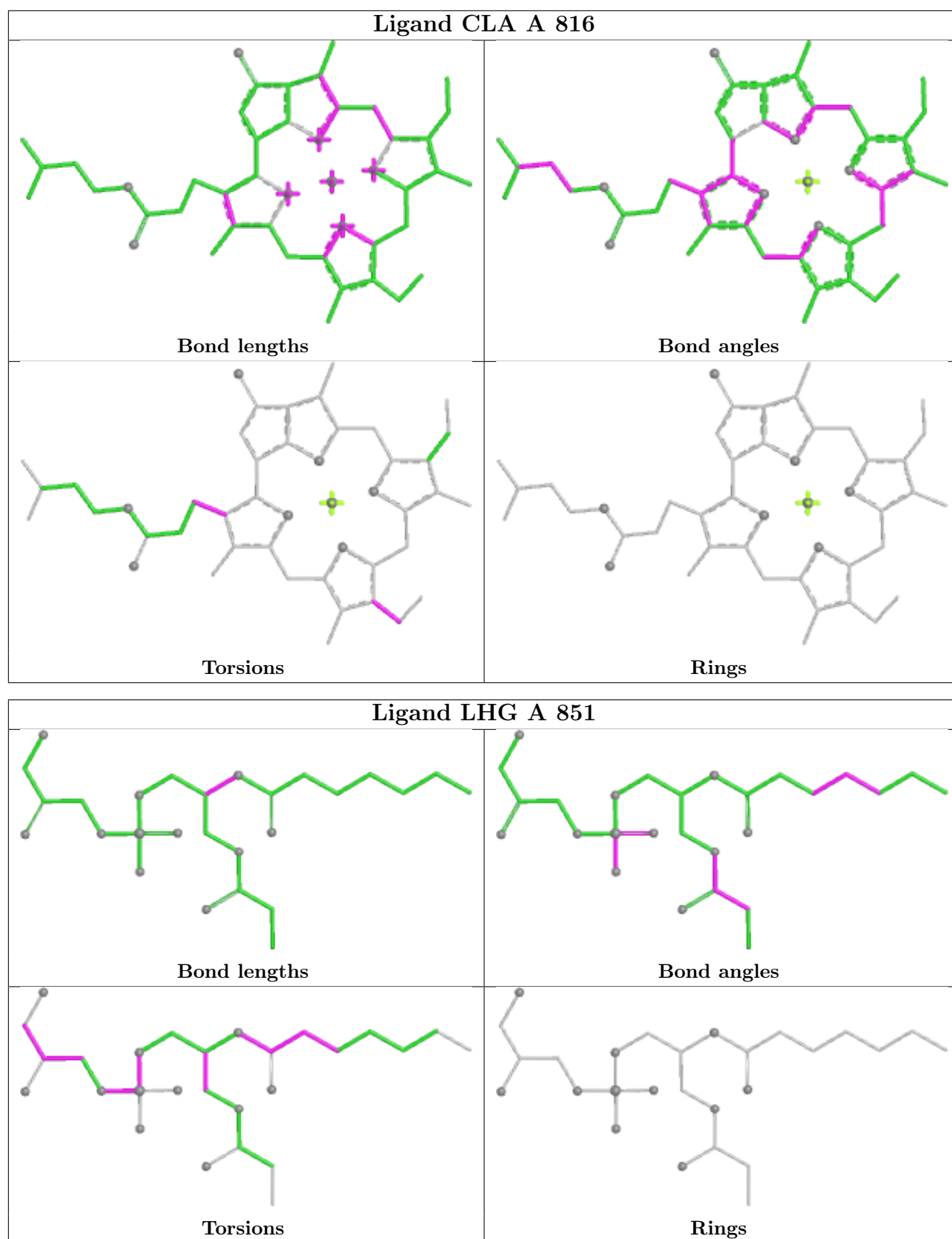


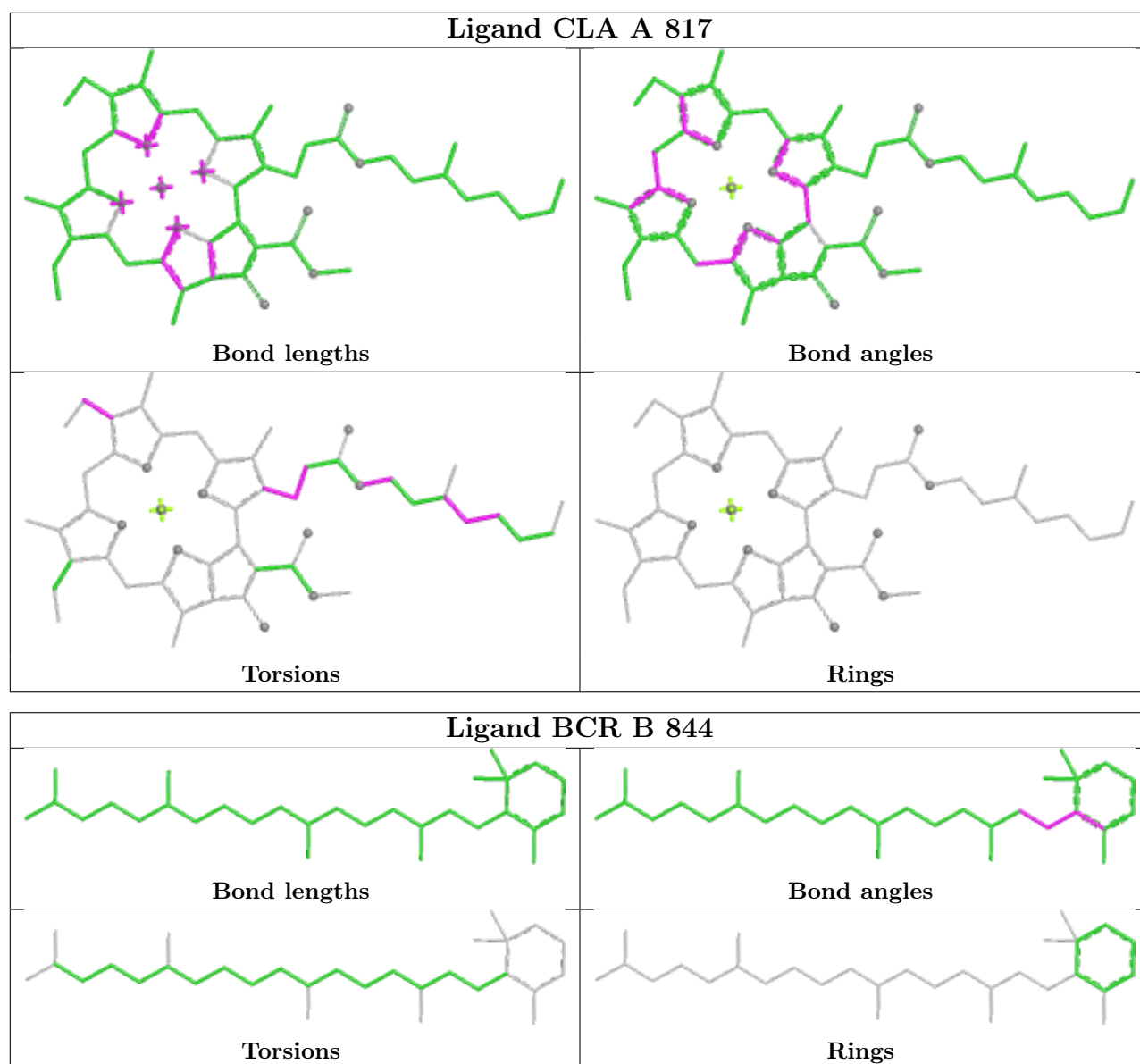
Rings

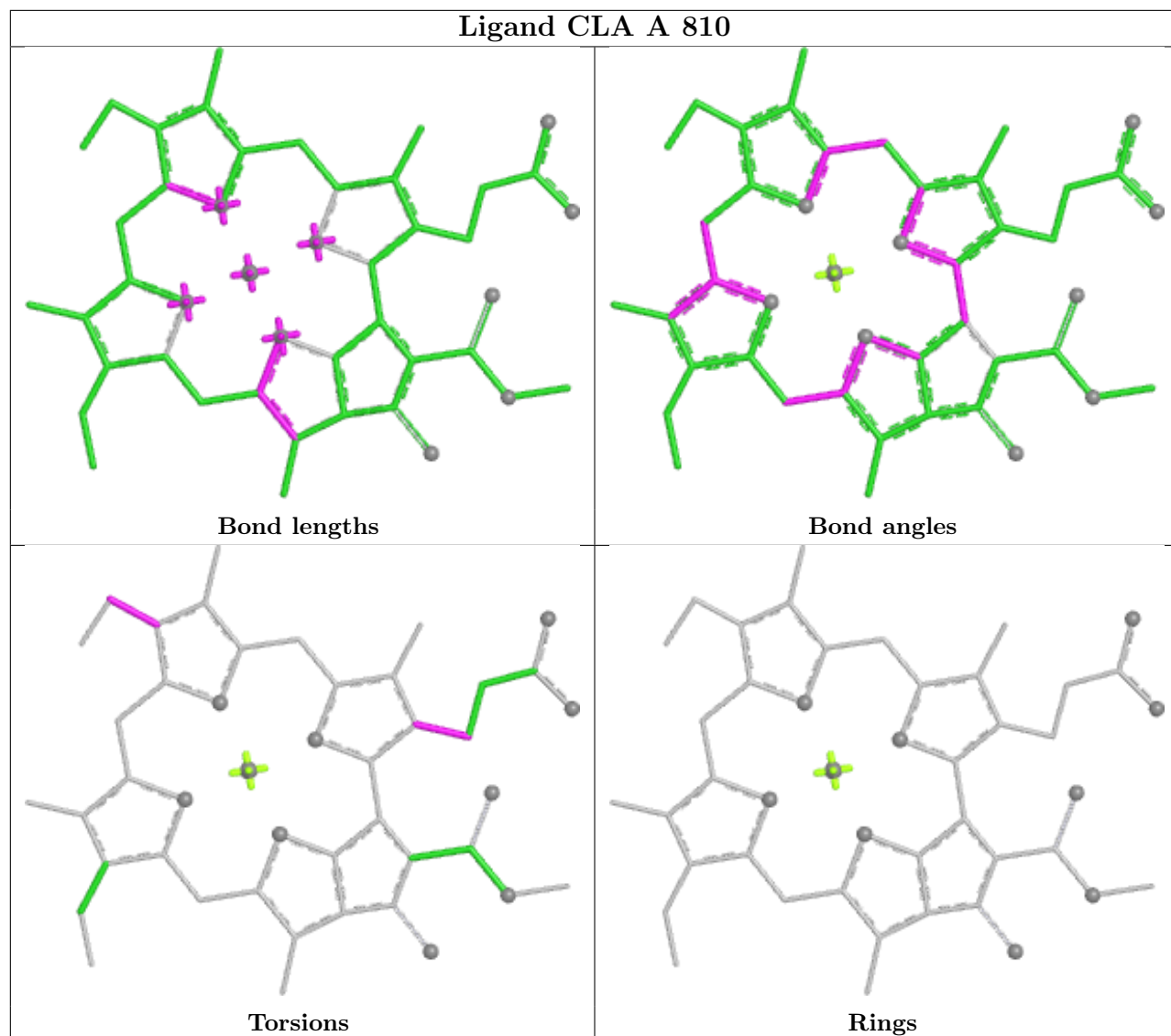


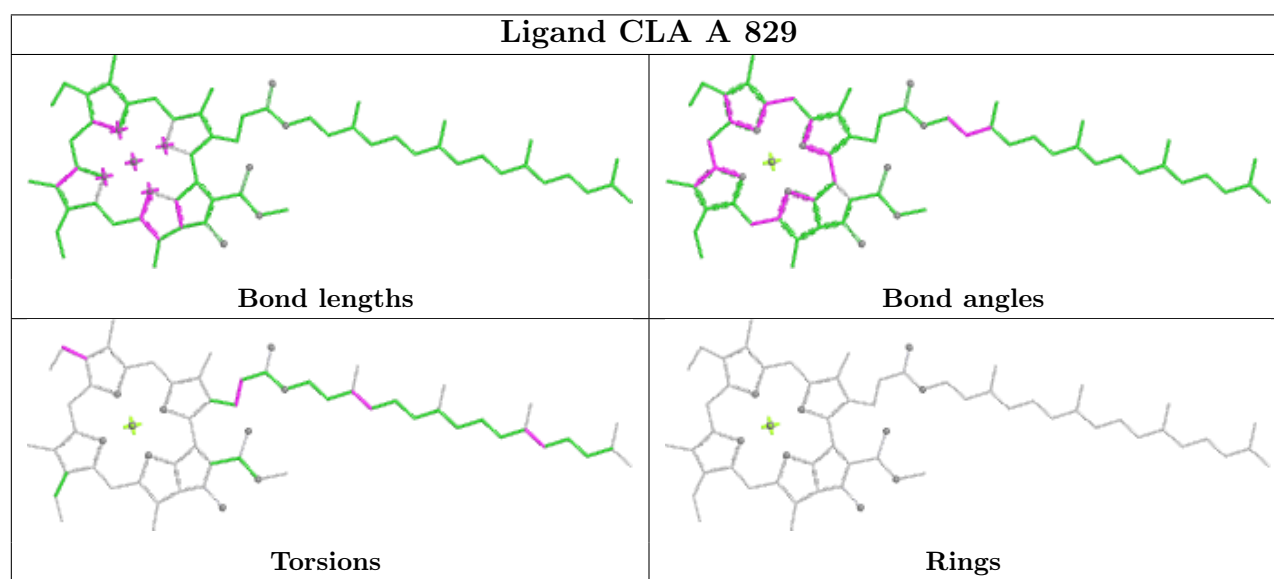
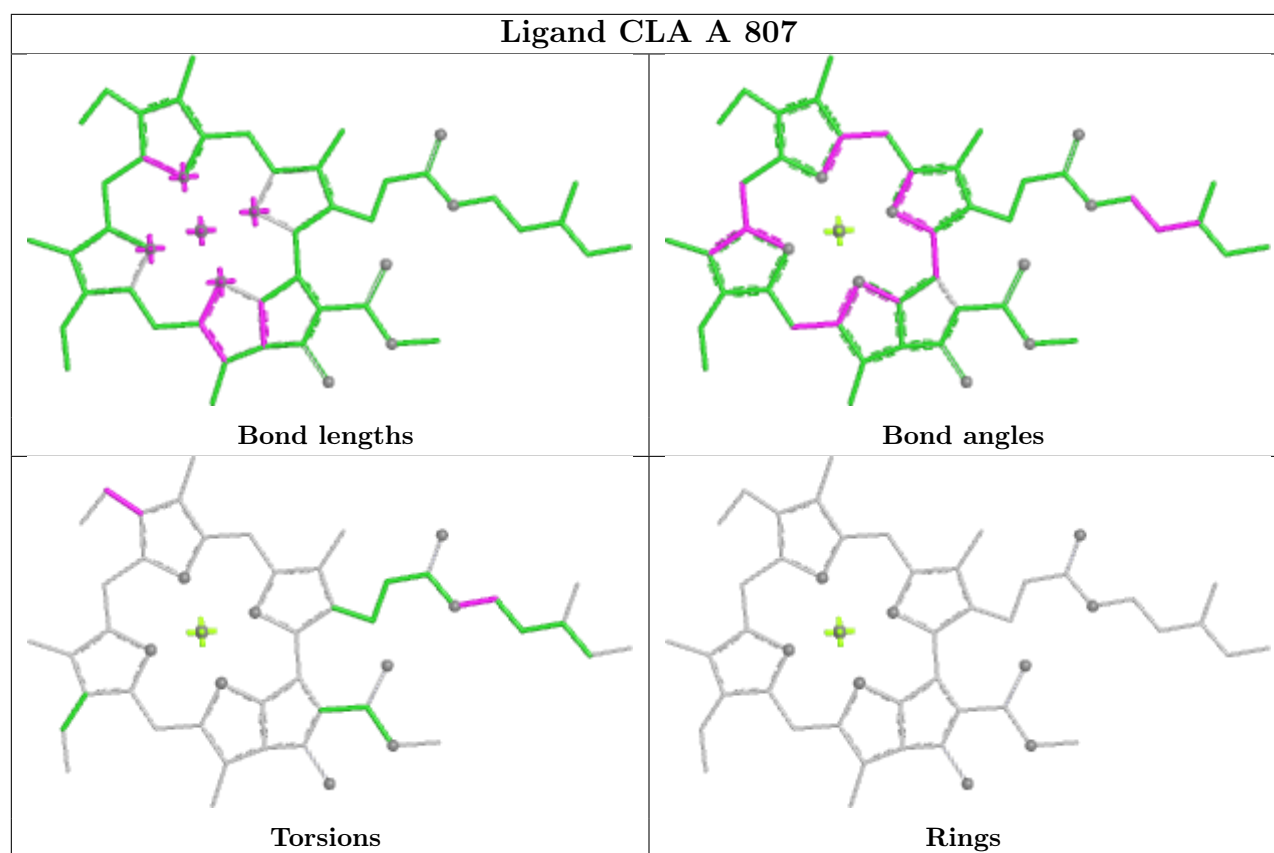




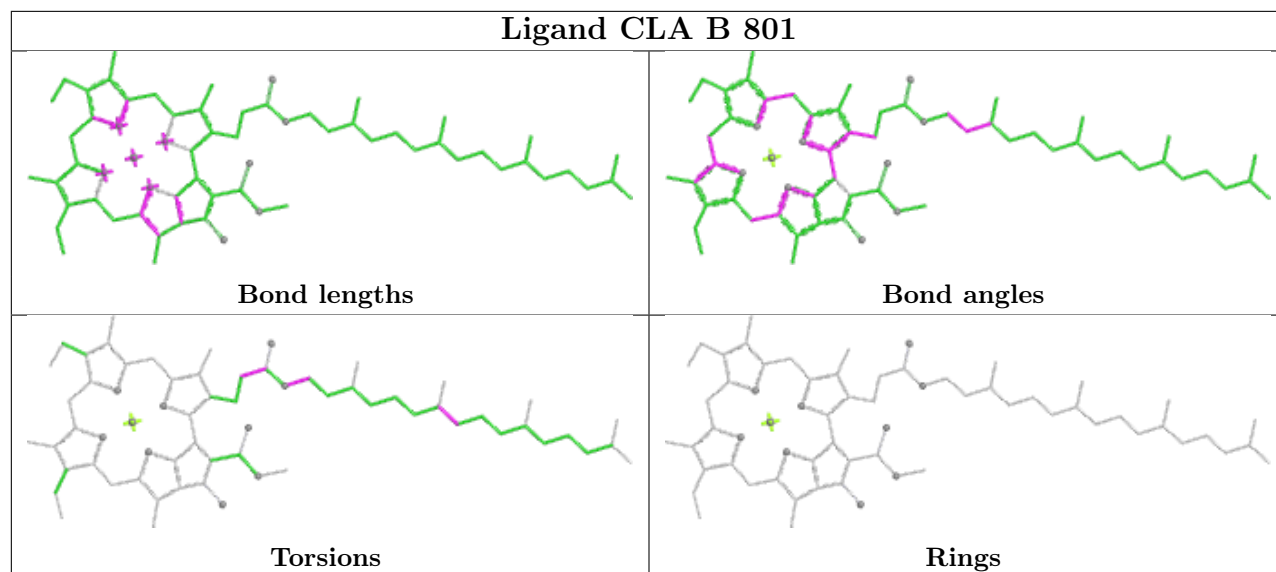




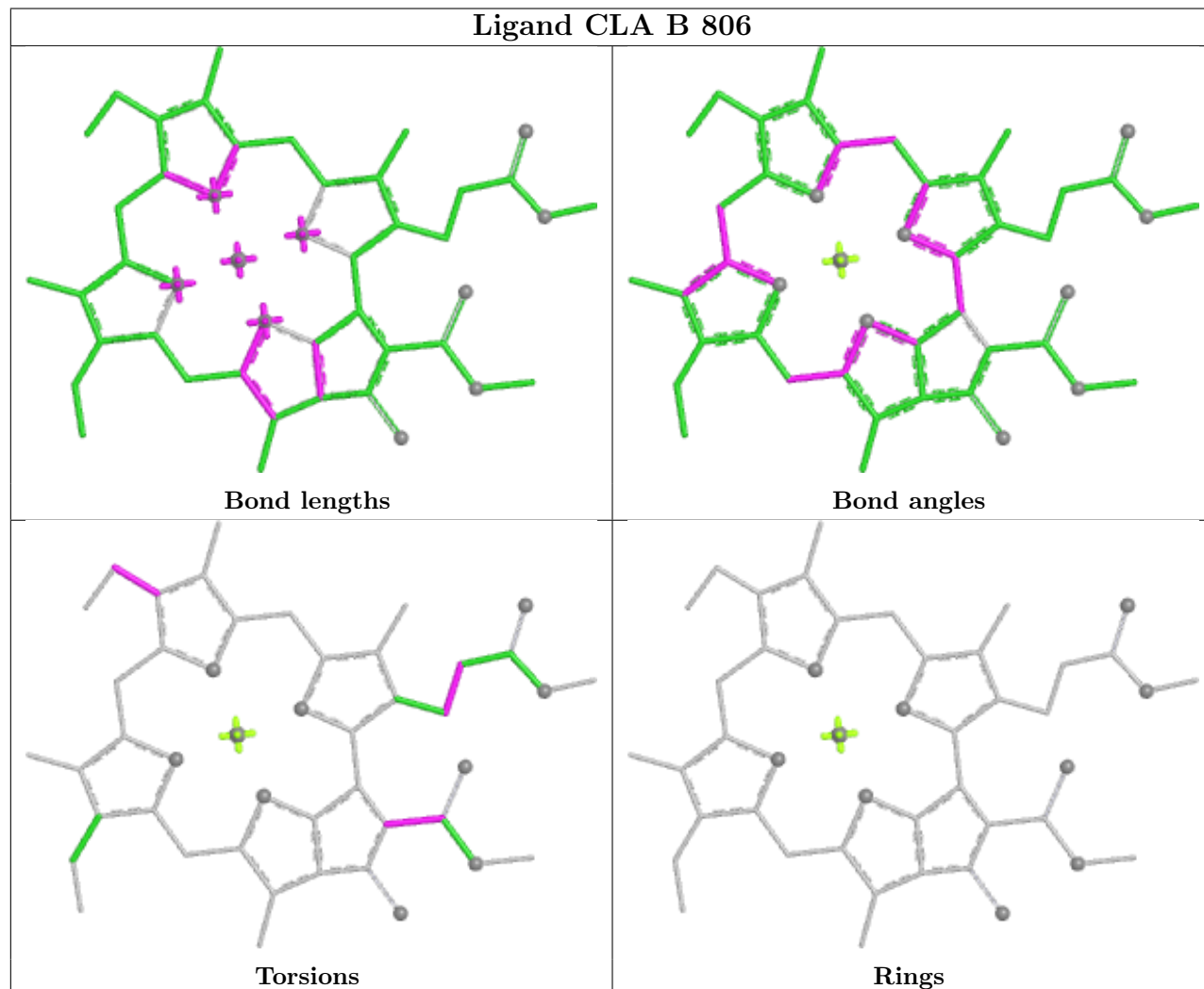




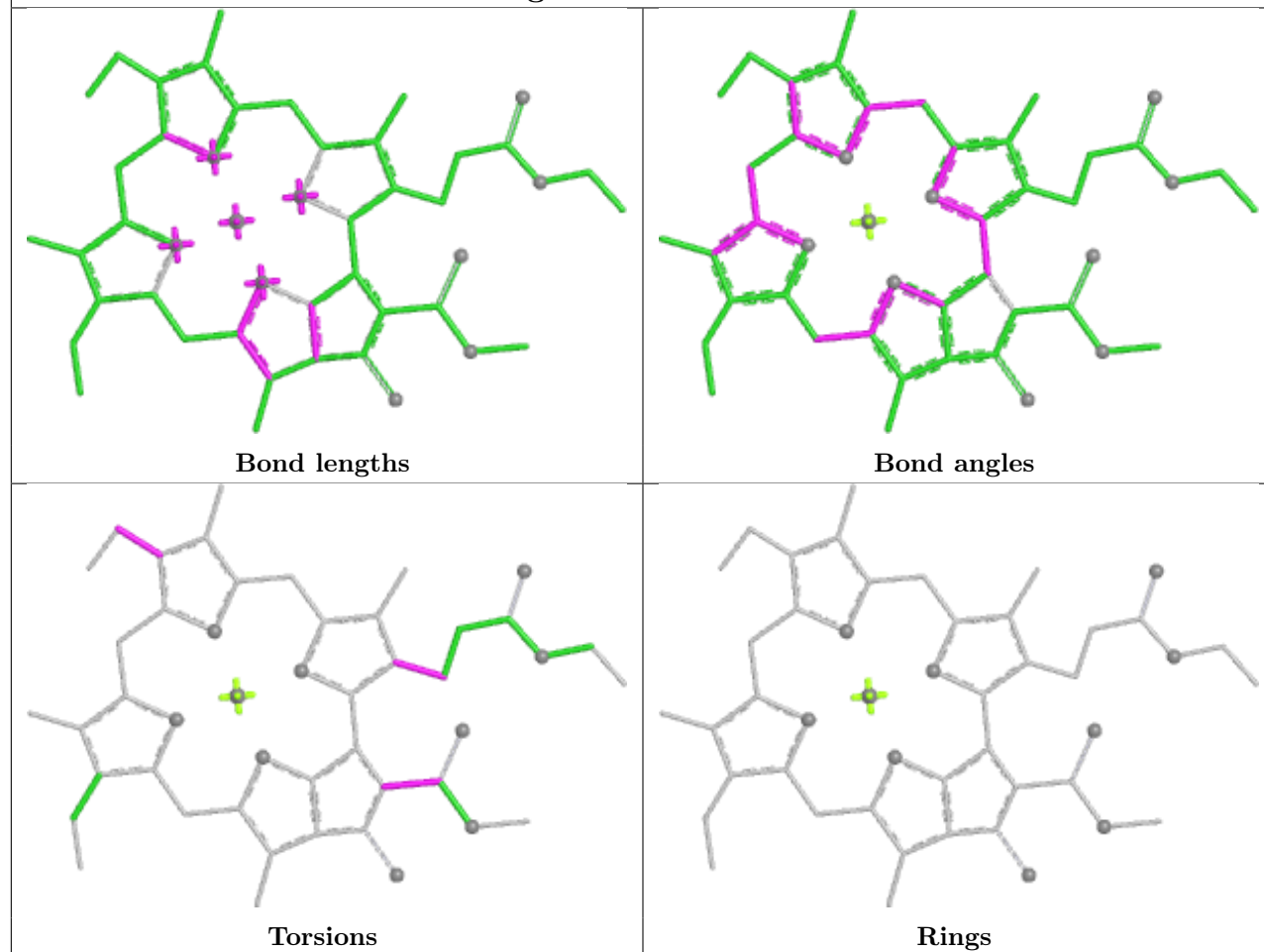
Ligand CLA B 801

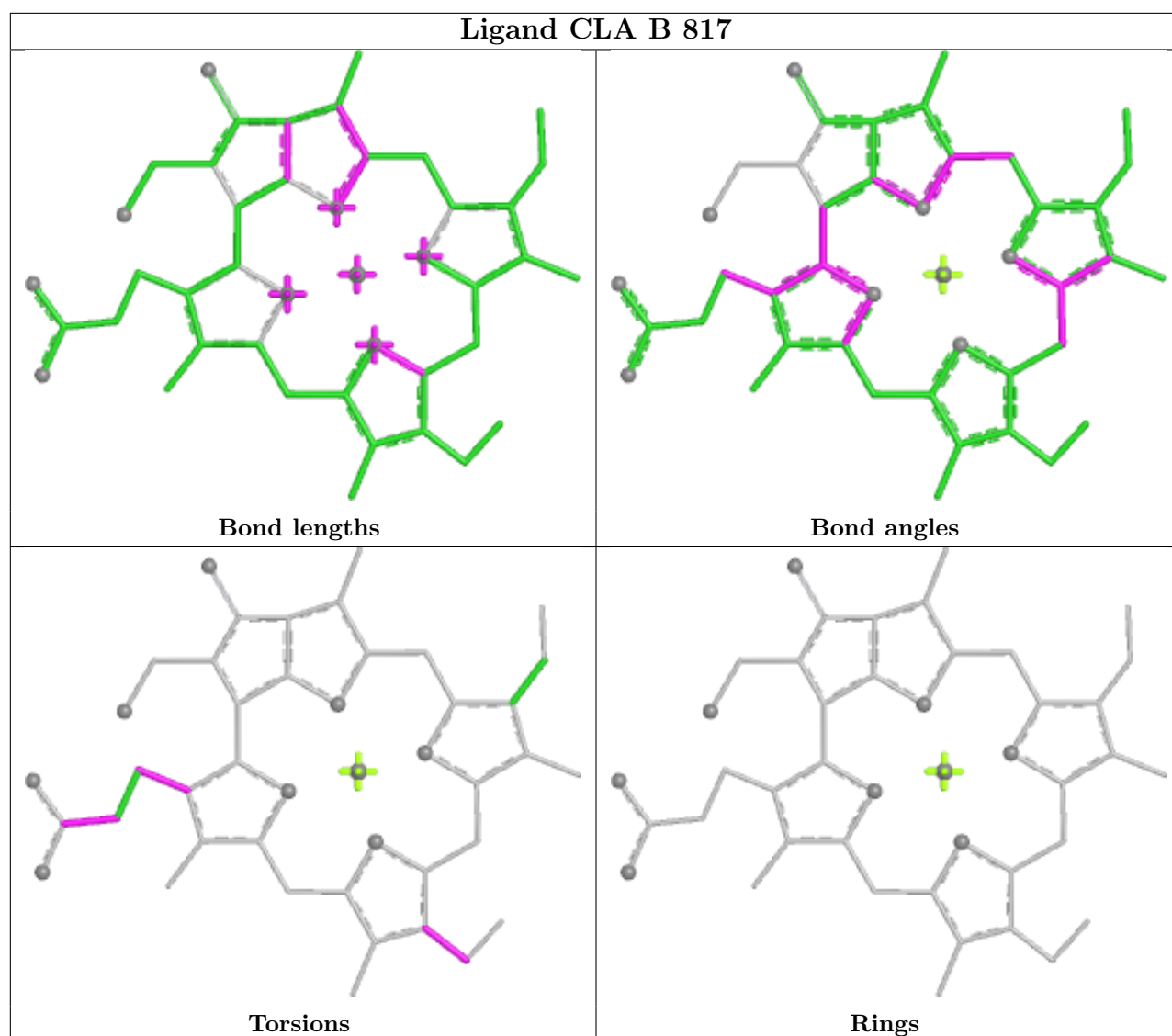


Ligand CLA B 806



Ligand CLA B 834





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.