



Full wwPDB EM Validation Report ⓘ

Dec 13, 2022 – 05:04 PM JST

PDB ID : 6LU1
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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

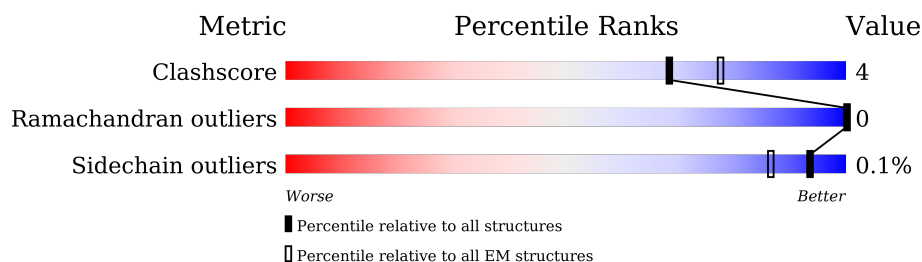
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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




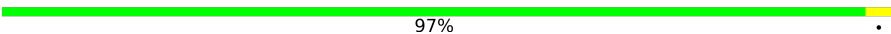
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	755	95% . .
2	B	741	92% . .
3	C	81	91% 7% .
4	D	139	94% 5% .
5	E	76	86% 5% 9%
6	F	164	16% . 82%
7	I	38	89% 11%
8	J	41	20% 80%

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Mol	Chain	Length	Quality of chain
9	L	155	 83% 13%
10	M	31	 97%

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	-	-	-
11	CLA	A	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
11	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-

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		

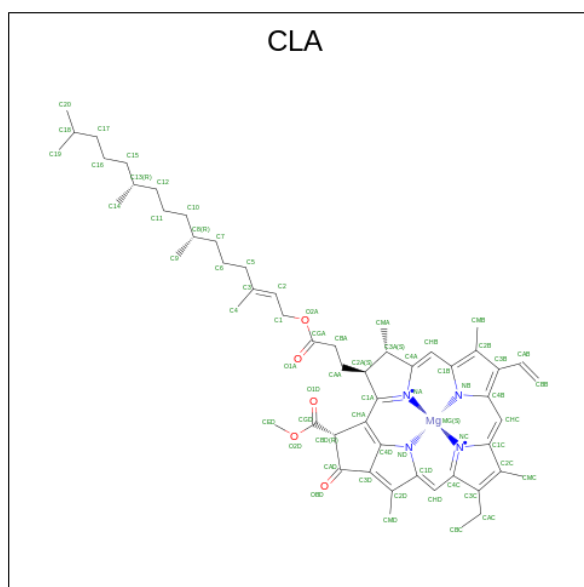
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

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 (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0
11	A	1	Total	C	Mg	N	O	0
11	A	1	2422	1999	44	176	203	0

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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0

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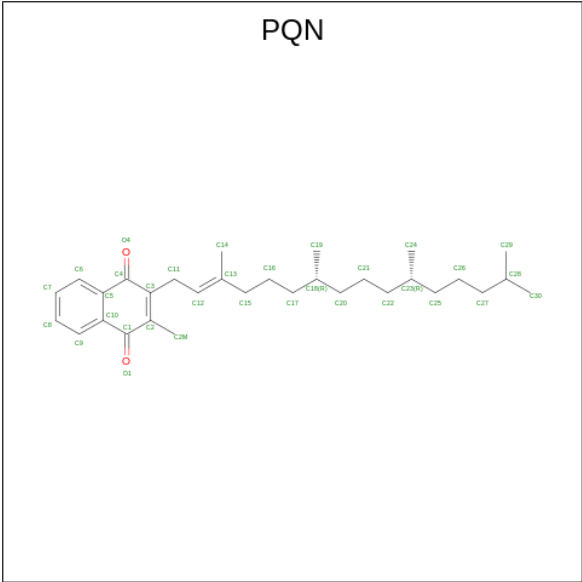
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0

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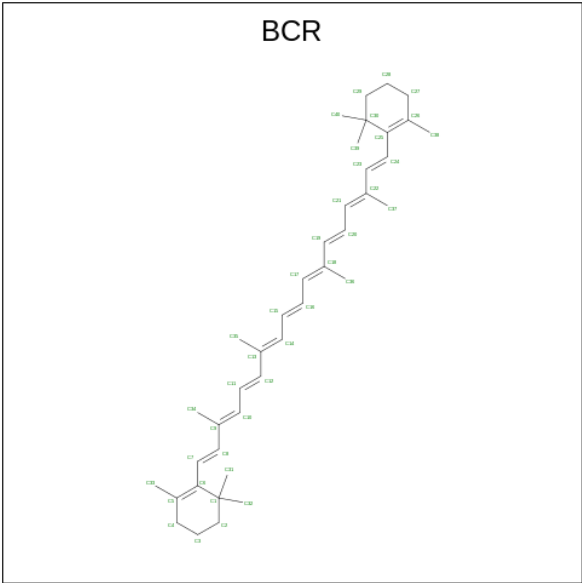
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	B	1	Total	C	Mg	N	O	0
			1932	1595	35	140	162	
11	L	1	Total	C	Mg	N	O	0
			136	112	3	12	9	
11	L	1	Total	C	Mg	N	O	0
			136	112	3	12	9	
11	L	1	Total	C	Mg	N	O	0
			136	112	3	12	9	

- Molecule 12 is PHYLLOQUINONE (three-letter code: 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 (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	C	0
			462	462	
13	A	1	Total	C	0
			462	462	

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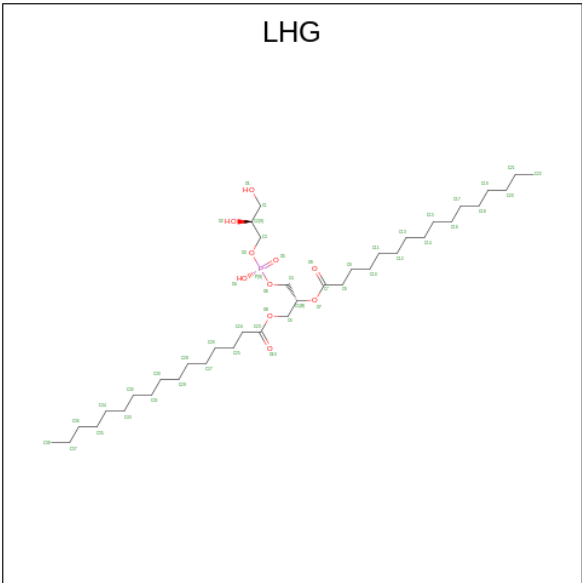
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	A	1	Total C 462 462	0
13	B	1	Total C 230 230	0
13	B	1	Total C 230 230	0
13	B	1	Total C 230 230	0
13	B	1	Total C 230 230	0
13	B	1	Total C 230 230	0
13	B	1	Total C 230 230	0
13	F	1	Total C 80 80	0
13	F	1	Total C 80 80	0
13	I	1	Total C 80 80	0

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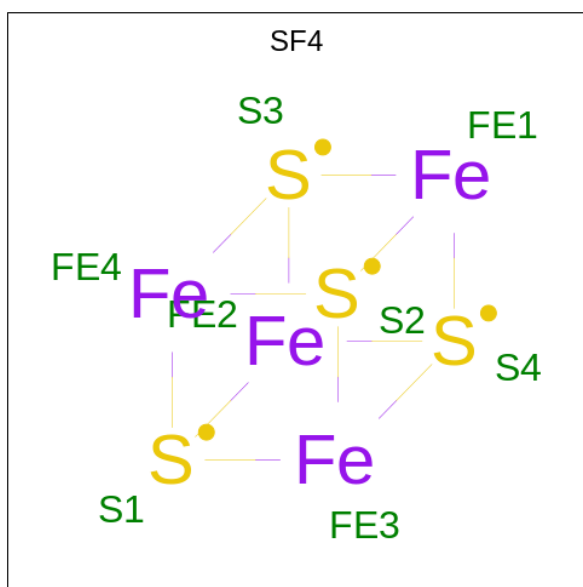
Mol	Chain	Residues	Atoms		AltConf
13	I	1	Total	C	0
			80	80	
13	L	1	Total	C	0
			40	40	
13	M	1	Total	C	0
			40	40	

- Molecule 14 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



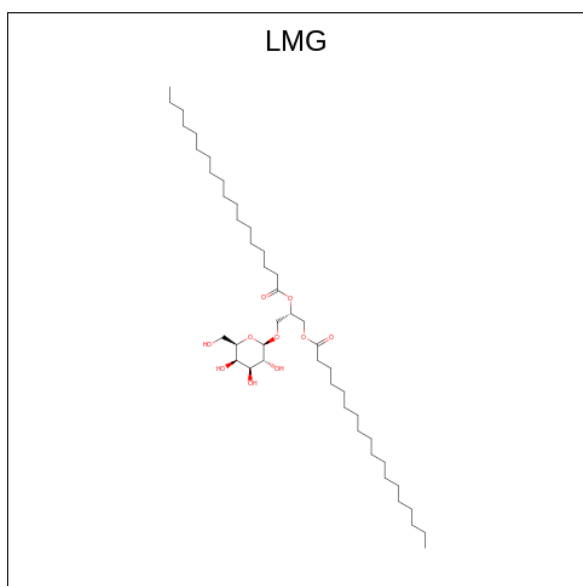
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			76	54	20	2	
14	A	1	Total	C	O	P	0
			76	54	20	2	

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: 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
			16	8	8	
15	C	1	Total	Fe	S	0
			16	8	8	

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



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

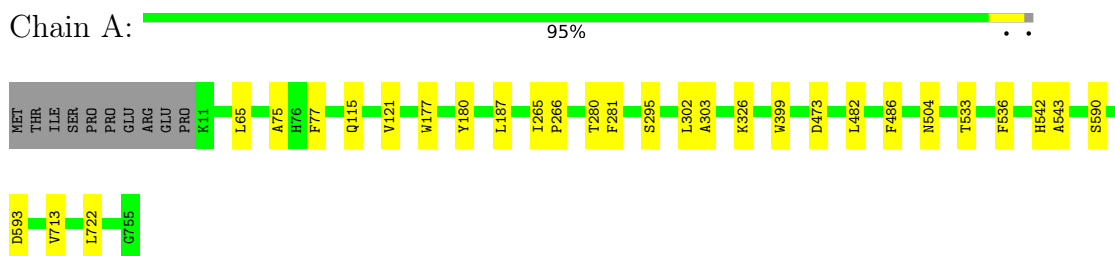
- Molecule 17 is water.

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	

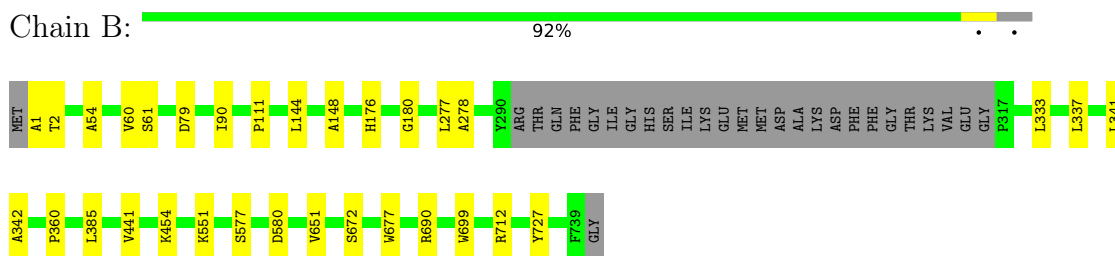
3 Residue-property plots [i](#)

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.

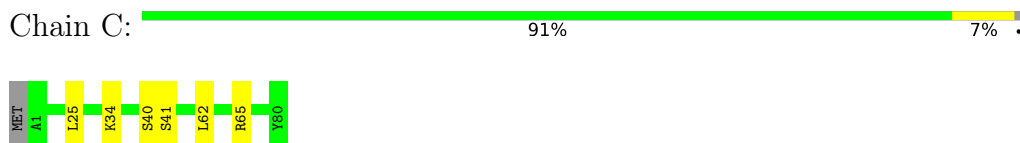
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



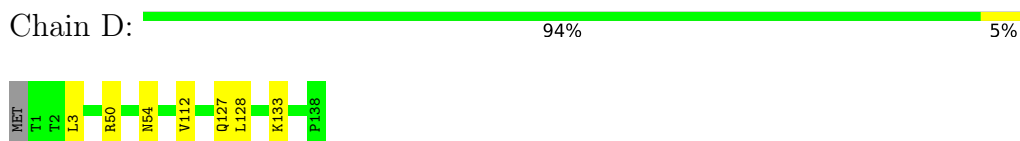
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



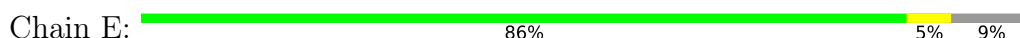
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II



- Molecule 5: Photosystem I reaction center subunit IV





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: SF4, CLA, LMG, BCR, LHG, PQN

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	0.31	0/6019	0.49	0/8209
2	B	0.31	0/5898	0.50	0/8066
3	C	0.34	0/608	0.55	0/824
4	D	0.30	0/1101	0.53	0/1492
5	E	0.29	0/551	0.48	0/750
6	F	0.29	0/239	0.63	0/326
7	I	0.31	0/312	0.60	0/425
8	J	0.28	0/67	0.49	0/88
9	L	0.28	0/1021	0.48	0/1387
10	M	0.25	0/244	0.51	0/332
All	All	0.31	0/16060	0.50	0/21899

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	26	0
2	B	5685	0	5453	27	0
3	C	598	0	588	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	50	0
11	B	1932	0	1849	34	0
11	L	136	0	106	1	0
12	A	33	0	46	20	0
12	B	33	0	46	9	0
13	A	462	0	630	16	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	2	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	159	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 (159) 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
12:A:843:PQN:C29	13:F:201:BCR:H17C	2.02	0.90
12:A:843:PQN:H2M1	12:A:843:PQN:H12	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
12:A:843:PQN:H2M1	12:A:843:PQN:C12	2.23	0.62
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:B:802:CLA:HMC2	11:B:802:CLA:H122	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:808:CLA:HMC3	11:A:809:CLA:HMD2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
11:A:835:CLA:HMD2	11:A:836:CLA:HBB1	1.96	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
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:90:ILE:HB	2:B:111:PRO:HB2	1.98	0.46
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
11:B:809:CLA:HMC2	11:B:809:CLA:H92	1.99	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
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
1:A:504:ASN:HB2	11:A:836:CLA:HED2	1.98	0.44
12:B:837:PQN:H193	12:B:837:PQN:H162	1.77	0.44
11:A:842:CLA:HMC3	14:A:851:LHG:HC62	2.00	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:699:TRP:HE3	11:B:835:CLA:HMD3	1.83	0.44
2:B:651:VAL:HG11	11:B:811:CLA:HMD2	1.98	0.43
11:A:812:CLA:HMD2	13:A:854:BCR:H313	2.00	0.43
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
1:A:399:TRP:HB3	11:A:828:CLA:HMC3	2.00	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
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
11:B:803:CLA:HMC2	11:B:835:CLA:H11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:813:CLA:H62	11:A:813:CLA:H102	1.82	0.41
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
1:A:543:ALA:HB1	11:A:838:CLA:HMB3	2.03	0.40
13:A:858:BCR:H20C	13:A:858:BCR:H361	1.86	0.40
2:B:176:HIS:CG	11:B:815:CLA:HMC2	2.55	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
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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	593 (100%)	0	100	100
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%)	20 (95%)	1 (5%)	25	61
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%)	25 (96%)	1 (4%)	33	67
All	All	1599/1792 (89%)	1597 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	82	ARG
10	M	30	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	61	HIS
1	A	282	ASN
1	A	286	ASN
1	A	341	HIS
1	A	359	ASN
1	A	373	HIS
1	A	461	HIS
1	A	542	HIS
1	A	718	GLN
2	B	13	GLN
2	B	49	HIS
2	B	322	HIS
4	D	54	ASN
4	D	71	GLN
5	E	18	ASN
9	L	16	HIS

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 monosaccharides 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	B	805	-	65,73,73	2.09	9 (13%)	76,113,113	1.08	8 (10%)
14	LHG	A	851	-	26,26,48	0.88	1 (3%)	29,32,54	1.34	3 (10%)
11	CLA	A	830	-	65,73,73	2.25	8 (12%)	76,113,113	1.07	8 (10%)
11	CLA	B	829	-	42,50,73	2.85	7 (16%)	48,85,113	1.37	8 (16%)
13	BCR	A	848	-	41,41,41	0.30	0	56,56,56	0.44	0
11	CLA	B	819	-	59,67,73	2.41	8 (13%)	68,105,113	1.32	10 (14%)
11	CLA	A	824	-	64,72,73	2.25	9 (14%)	75,112,113	1.09	8 (10%)
11	CLA	B	825	-	65,73,73	2.30	8 (12%)	76,113,113	1.06	8 (10%)
11	CLA	A	801	-	62,69,73	2.18	10 (16%)	72,107,113	1.18	8 (11%)
13	BCR	A	857	-	26,26,41	0.35	0	34,34,56	0.42	0
11	CLA	B	812	-	43,51,73	2.81	8 (18%)	49,86,113	1.47	7 (14%)
13	BCR	M	101	-	41,41,41	0.32	0	56,56,56	0.39	0
11	CLA	A	828	-	65,73,73	2.09	9 (13%)	76,113,113	1.20	8 (10%)
11	CLA	A	808	-	54,62,73	2.48	8 (14%)	62,99,113	1.34	9 (14%)
11	CLA	A	840	-	41,49,73	2.90	9 (21%)	44,83,113	1.48	6 (13%)
11	CLA	A	821	-	65,73,73	2.18	8 (12%)	76,113,113	1.10	9 (11%)
11	CLA	A	804	-	59,67,73	2.36	8 (13%)	68,105,113	1.26	8 (11%)
11	CLA	B	836	-	43,51,73	2.67	8 (18%)	49,86,113	1.56	8 (16%)
15	SF4	C	102	-	0,12,12	-	-	-	-	-
11	CLA	B	815	-	65,73,73	2.25	8 (12%)	76,113,113	1.23	8 (10%)
13	BCR	A	844	-	41,41,41	0.35	0	56,56,56	0.51	0
11	CLA	A	814	-	41,49,73	2.95	9 (21%)	47,84,113	1.47	8 (17%)
11	CLA	B	827	-	41,49,73	2.85	9 (21%)	47,84,113	1.53	8 (17%)
11	CLA	L	1501	-	34,44,73	3.20	7 (20%)	40,77,113	1.78	10 (25%)
12	PQN	B	837	-	34,34,34	0.37	0	42,45,45	0.38	0
13	BCR	A	853	-	22,22,41	0.53	0	29,29,56	0.42	0
11	CLA	B	820	-	60,68,73	2.28	8 (13%)	70,107,113	1.32	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	818	-	55,63,73	2.51	9 (16%)	64,101,113	1.24	7 (10%)
11	CLA	B	811	-	65,73,73	2.19	9 (13%)	76,113,113	1.14	9 (11%)
11	CLA	B	830	-	41,49,73	2.89	9 (21%)	47,84,113	1.51	9 (19%)
11	CLA	A	832	-	51,59,73	2.56	8 (15%)	59,96,113	1.36	8 (13%)
11	CLA	A	827	-	65,73,73	2.23	8 (12%)	76,113,113	1.12	9 (11%)
13	BCR	A	861	-	41,41,41	0.28	0	56,56,56	0.56	0
11	CLA	A	860	-	65,73,73	2.20	8 (12%)	76,113,113	1.03	7 (9%)
11	CLA	A	834	-	65,73,73	2.14	8 (12%)	76,113,113	1.12	8 (10%)
11	CLA	A	822	-	49,57,73	2.65	7 (14%)	55,93,113	1.37	8 (14%)
11	CLA	A	815	-	45,53,73	2.70	9 (20%)	52,89,113	1.29	7 (13%)
12	PQN	A	843	-	34,34,34	0.36	0	42,45,45	0.40	0
11	CLA	A	816	-	47,54,73	2.74	10 (21%)	54,89,113	1.46	11 (20%)
11	CLA	A	813	-	65,73,73	2.23	8 (12%)	76,113,113	1.24	8 (10%)
11	CLA	A	837	-	51,59,73	2.54	9 (17%)	59,96,113	1.34	8 (13%)
13	BCR	A	845	-	41,41,41	0.34	0	56,56,56	0.60	0
11	CLA	B	807	-	65,73,73	2.17	8 (12%)	76,113,113	1.18	9 (11%)
11	CLA	B	808	-	62,70,73	2.21	8 (12%)	72,109,113	1.10	7 (9%)
11	CLA	A	836	-	45,53,73	2.68	8 (17%)	52,89,113	1.42	9 (17%)
11	CLA	A	833	-	65,73,73	2.17	9 (13%)	76,113,113	1.12	8 (10%)
11	CLA	A	842	-	39,48,73	2.98	8 (20%)	45,82,113	1.51	11 (24%)
11	CLA	B	828	-	65,73,73	2.27	7 (10%)	76,113,113	1.17	7 (9%)
13	BCR	B	841	-	41,41,41	0.26	0	56,56,56	0.45	0
11	CLA	B	801	-	65,73,73	2.18	8 (12%)	76,113,113	1.18	10 (13%)
11	CLA	A	805	-	65,73,73	2.16	8 (12%)	76,113,113	1.29	10 (13%)
11	CLA	B	835	-	65,73,73	2.22	8 (12%)	76,113,113	1.05	8 (10%)
11	CLA	B	821	-	46,54,73	2.59	9 (19%)	53,90,113	1.35	8 (15%)
11	CLA	B	810	-	65,73,73	2.15	8 (12%)	76,113,113	1.08	9 (11%)
13	BCR	A	847	-	41,41,41	0.28	0	56,56,56	0.32	0
11	CLA	B	802	-	65,73,73	2.19	8 (12%)	76,113,113	1.10	8 (10%)
16	LMG	B	843	-	55,55,55	0.78	2 (3%)	63,63,63	1.36	8 (12%)
11	CLA	A	803	-	42,50,73	2.82	8 (19%)	48,85,113	1.42	8 (16%)
13	BCR	I	101	-	41,41,41	0.34	0	56,56,56	0.49	0
11	CLA	B	816	-	65,73,73	2.25	8 (12%)	76,113,113	1.11	9 (11%)
13	BCR	A	852	-	39,40,41	0.32	0	52,53,56	0.98	4 (7%)
11	CLA	B	806	-	46,54,73	2.73	8 (17%)	53,90,113	1.33	7 (13%)
11	CLA	A	807	-	51,59,73	2.49	8 (15%)	59,96,113	1.27	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	841	-	49,57,73	2.58	8 (16%)	55,93,113	1.23	7 (12%)
11	CLA	B	831	-	45,53,73	2.69	7 (15%)	52,89,113	1.31	9 (17%)
11	CLA	B	826	-	45,53,73	2.69	8 (17%)	52,89,113	1.34	7 (13%)
11	CLA	B	814	-	45,53,73	2.76	8 (17%)	52,89,113	1.52	10 (19%)
11	CLA	A	859	-	56,64,73	2.28	9 (16%)	65,102,113	1.22	9 (13%)
11	CLA	B	822	-	43,52,73	2.68	8 (18%)	49,88,113	1.47	8 (16%)
11	CLA	B	833	-	65,73,73	2.27	8 (12%)	76,113,113	1.13	7 (9%)
11	CLA	L	1503	-	42,50,73	2.85	7 (16%)	48,85,113	1.64	9 (18%)
11	CLA	A	838	-	55,63,73	2.44	8 (14%)	64,101,113	1.22	9 (14%)
11	CLA	A	835	-	54,62,73	2.39	8 (14%)	62,99,113	1.19	8 (12%)
11	CLA	B	817	-	43,51,73	2.68	9 (20%)	47,86,113	1.60	10 (21%)
13	BCR	B	839	-	41,41,41	0.28	0	56,56,56	0.50	0
11	CLA	A	823	-	43,51,73	2.71	8 (18%)	49,86,113	1.51	8 (16%)
13	BCR	B	844	-	30,30,41	0.41	0	39,39,56	0.78	2 (5%)
11	CLA	A	817	-	54,62,73	2.45	8 (14%)	62,99,113	1.22	7 (11%)
11	CLA	A	802	-	65,73,73	2.10	8 (12%)	76,113,113	1.12	8 (10%)
13	BCR	A	846	-	41,41,41	0.31	0	56,56,56	0.39	0
11	CLA	B	809	-	65,73,73	2.18	8 (12%)	76,113,113	1.18	7 (9%)
11	CLA	A	809	-	45,53,73	2.74	8 (17%)	52,89,113	1.31	8 (15%)
11	CLA	A	825	-	65,73,73	2.26	8 (12%)	76,113,113	1.14	9 (11%)
13	BCR	A	856	-	29,29,41	0.40	0	37,37,56	1.14	3 (8%)
13	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.33	0
11	CLA	A	818	-	54,62,73	2.42	8 (14%)	62,99,113	1.29	10 (16%)
11	CLA	A	811	-	65,73,73	2.21	8 (12%)	76,113,113	1.28	9 (11%)
11	CLA	A	819	-	65,73,73	2.20	8 (12%)	76,113,113	1.33	12 (15%)
11	CLA	B	834	-	47,55,73	2.55	8 (17%)	54,91,113	1.35	7 (12%)
15	SF4	C	101	-	0,12,12	-	-	-	-	-
11	CLA	B	813	-	43,51,73	2.75	8 (18%)	49,86,113	1.42	7 (14%)
11	CLA	L	1502	-	58,66,73	2.47	9 (15%)	67,104,113	1.48	11 (16%)
13	BCR	B	842	-	41,41,41	0.21	0	56,56,56	0.39	0
11	CLA	A	831	-	49,57,73	2.46	9 (18%)	55,93,113	1.33	7 (12%)
11	CLA	B	823	-	57,65,73	2.33	8 (14%)	66,103,113	1.26	9 (13%)
11	CLA	A	839	-	49,57,73	2.49	9 (18%)	55,93,113	1.32	8 (14%)
15	SF4	B	804	-	0,12,12	-	-	-	-	-
13	BCR	B	840	-	41,41,41	0.25	0	56,56,56	0.70	2 (3%)
11	CLA	B	803	-	65,73,73	2.22	9 (13%)	76,113,113	1.29	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	812	-	53,61,73	2.61	8 (15%)	61,98,113	1.26	8 (13%)
11	CLA	A	806	-	65,73,73	2.20	9 (13%)	76,113,113	1.13	7 (9%)
13	BCR	B	838	-	41,41,41	0.32	0	56,56,56	0.53	1 (1%)
11	CLA	B	824	-	65,73,73	2.14	8 (12%)	76,113,113	1.32	11 (14%)
11	CLA	A	810	-	45,53,73	2.59	7 (15%)	52,89,113	1.26	7 (13%)
13	BCR	F	201	-	41,41,41	0.52	0	56,56,56	1.58	10 (17%)
11	CLA	A	829	-	65,73,73	2.15	9 (13%)	76,113,113	1.12	8 (10%)
11	CLA	A	820	-	41,49,73	2.94	9 (21%)	47,84,113	1.53	8 (17%)
13	BCR	A	858	-	21,21,41	0.31	0	28,28,56	0.62	1 (3%)
13	BCR	A	854	-	21,21,41	0.40	0	28,28,56	0.49	0
14	LHG	A	850	-	48,48,48	0.68	1 (2%)	51,54,54	1.26	6 (11%)
13	BCR	A	855	-	23,24,41	0.49	0	29,30,56	0.94	2 (6%)
11	CLA	A	826	-	60,68,73	2.27	9 (15%)	70,107,113	1.25	8 (11%)
13	BCR	A	849	-	41,41,41	0.44	1 (2%)	56,56,56	1.12	6 (10%)
13	BCR	L	1504	-	41,41,41	0.30	0	56,56,56	0.68	1 (1%)
11	CLA	B	832	-	50,58,73	2.59	8 (16%)	58,95,113	1.33	9 (15%)
13	BCR	F	202	-	41,41,41	0.28	0	56,56,56	1.07	3 (5%)

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	B	805	-	1/1/15/20	4/37/115/115	-
14	LHG	A	851	-	-	14/31/31/53	-
11	CLA	A	830	-	1/1/15/20	5/37/115/115	-
11	CLA	B	829	-	1/1/10/20	1/10/88/115	-
13	BCR	A	848	-	-	2/29/63/63	0/2/2/2
11	CLA	B	819	-	1/1/13/20	3/30/108/115	-
11	CLA	A	824	-	1/1/15/20	7/35/113/115	-
11	CLA	B	825	-	1/1/15/20	3/37/115/115	-
11	CLA	A	801	-	1/1/13/20	2/31/105/115	-
13	BCR	A	857	-	-	0/20/37/63	0/1/1/2
11	CLA	B	812	-	1/1/10/20	1/11/89/115	-
13	BCR	M	101	-	-	2/29/63/63	0/2/2/2
11	CLA	A	828	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	808	-	1/1/12/20	6/24/102/115	-
11	CLA	A	840	-	1/1/9/20	0/5/85/115	-
11	CLA	A	821	-	1/1/15/20	3/37/115/115	-
11	CLA	A	804	-	1/1/13/20	6/30/108/115	-
11	CLA	B	836	-	1/1/10/20	6/11/89/115	-
15	SF4	C	102	-	-	-	0/6/5/5
11	CLA	B	815	-	1/1/15/20	9/37/115/115	-
13	BCR	A	844	-	-	0/29/63/63	0/2/2/2
11	CLA	A	814	-	1/1/10/20	1/8/86/115	-
11	CLA	B	827	-	1/1/10/20	0/8/86/115	-
11	CLA	L	1501	-	1/1/8/20	0/0/74/115	-
12	PQN	B	837	-	-	10/23/43/43	0/2/2/2
13	BCR	A	853	-	-	0/15/32/63	0/1/1/2
11	CLA	B	820	-	1/1/14/20	4/31/109/115	-
11	CLA	B	818	-	1/1/13/20	2/25/103/115	-
11	CLA	B	811	-	1/1/15/20	9/37/115/115	-
11	CLA	B	830	-	1/1/10/20	3/8/86/115	-
11	CLA	A	832	-	1/1/12/20	3/21/99/115	-
11	CLA	A	827	-	1/1/15/20	10/37/115/115	-
13	BCR	A	861	-	-	3/29/63/63	0/2/2/2
11	CLA	A	860	-	1/1/15/20	6/37/115/115	-
11	CLA	A	834	-	1/1/15/20	8/37/115/115	-
11	CLA	A	822	-	1/1/11/20	3/18/96/115	-
11	CLA	A	815	-	1/1/11/20	4/13/91/115	-
12	PQN	A	843	-	-	15/23/43/43	0/2/2/2
11	CLA	A	816	-	1/1/10/20	2/13/87/115	-
11	CLA	A	813	-	1/1/15/20	11/37/115/115	-
11	CLA	A	837	-	1/1/12/20	4/21/99/115	-
13	BCR	A	845	-	-	2/29/63/63	0/2/2/2
11	CLA	B	807	-	1/1/15/20	10/37/115/115	-
11	CLA	B	808	-	1/1/14/20	4/34/112/115	-
11	CLA	A	836	-	1/1/11/20	4/13/91/115	-
11	CLA	A	833	-	1/1/15/20	4/37/115/115	-
11	CLA	A	842	-	1/1/9/20	2/8/82/115	-
11	CLA	B	828	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	B	841	-	-	2/29/63/63	0/2/2/2
11	CLA	B	801	-	1/1/15/20	4/37/115/115	-
11	CLA	A	805	-	1/1/15/20	12/37/115/115	-
11	CLA	B	835	-	1/1/15/20	3/37/115/115	-
11	CLA	B	821	-	1/1/11/20	2/15/93/115	-
11	CLA	B	810	-	1/1/15/20	5/37/115/115	-
13	BCR	A	847	-	-	4/29/63/63	0/2/2/2
11	CLA	B	802	-	1/1/15/20	6/37/115/115	-
16	LMG	B	843	-	-	24/50/70/70	0/1/1/1
11	CLA	A	803	-	1/1/10/20	4/10/88/115	-
13	BCR	I	101	-	-	0/29/63/63	0/2/2/2
11	CLA	B	816	-	1/1/15/20	6/37/115/115	-
13	BCR	A	852	-	-	14/29/60/63	0/2/2/2
11	CLA	B	806	-	1/1/11/20	2/15/93/115	-
11	CLA	A	807	-	1/1/12/20	2/21/99/115	-
11	CLA	A	841	-	1/1/11/20	5/18/96/115	-
11	CLA	B	831	-	1/1/11/20	3/13/91/115	-
11	CLA	B	826	-	1/1/11/20	1/13/91/115	-
11	CLA	B	814	-	1/1/11/20	5/13/91/115	-
11	CLA	A	859	-	1/1/13/20	6/27/105/115	-
11	CLA	B	822	-	1/1/11/20	7/11/89/115	-
11	CLA	B	833	-	1/1/15/20	2/37/115/115	-
11	CLA	L	1503	-	1/1/10/20	0/10/88/115	-
11	CLA	A	838	-	1/1/13/20	2/25/103/115	-
11	CLA	A	835	-	1/1/12/20	2/24/102/115	-
11	CLA	B	817	-	1/1/10/20	4/7/87/115	-
13	BCR	B	839	-	-	4/29/63/63	0/2/2/2
11	CLA	A	823	-	1/1/10/20	2/11/89/115	-
13	BCR	B	844	-	-	0/24/41/63	0/1/1/2
11	CLA	A	817	-	1/1/12/20	6/24/102/115	-
11	CLA	A	802	-	1/1/15/20	2/37/115/115	-
13	BCR	A	846	-	-	0/29/63/63	0/2/2/2
11	CLA	B	809	-	1/1/15/20	3/37/115/115	-
11	CLA	A	809	-	1/1/11/20	0/13/91/115	-
11	CLA	A	825	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	A	856	-	-	9/23/40/63	0/1/1/2
13	BCR	I	102	-	-	4/29/63/63	0/2/2/2
11	CLA	A	818	-	1/1/12/20	6/24/102/115	-
11	CLA	A	811	-	1/1/15/20	11/37/115/115	-
11	CLA	A	819	-	1/1/15/20	12/37/115/115	-
11	CLA	B	834	-	1/1/11/20	2/16/94/115	-
15	SF4	C	101	-	-	-	0/6/5/5
11	CLA	B	813	-	1/1/10/20	0/11/89/115	-
11	CLA	L	1502	-	1/1/13/20	2/29/107/115	-
13	BCR	B	842	-	-	4/29/63/63	0/2/2/2
11	CLA	A	831	-	1/1/11/20	4/18/96/115	-
11	CLA	B	823	-	1/1/13/20	7/28/106/115	-
11	CLA	A	839	-	1/1/11/20	2/18/96/115	-
15	SF4	B	804	-	-	-	0/6/5/5
13	BCR	B	840	-	-	6/29/63/63	0/2/2/2
11	CLA	B	803	-	1/1/15/20	7/37/115/115	-
11	CLA	A	812	-	1/1/12/20	2/22/100/115	-
11	CLA	A	806	-	1/1/15/20	7/37/115/115	-
13	BCR	B	838	-	-	0/29/63/63	0/2/2/2
11	CLA	B	824	-	1/1/15/20	4/37/115/115	-
11	CLA	A	810	-	1/1/11/20	4/13/91/115	-
13	BCR	F	201	-	-	12/29/63/63	0/2/2/2
11	CLA	A	829	-	1/1/15/20	5/37/115/115	-
11	CLA	A	820	-	1/1/10/20	2/8/86/115	-
13	BCR	A	858	-	-	2/14/31/63	0/1/1/2
13	BCR	A	854	-	-	0/14/31/63	0/1/1/2
14	LHG	A	850	-	-	22/53/53/53	-
13	BCR	A	855	-	-	1/18/32/63	0/1/1/2
11	CLA	A	826	-	1/1/14/20	4/31/109/115	-
13	BCR	A	849	-	-	12/29/63/63	0/2/2/2
13	BCR	L	1504	-	-	3/29/63/63	0/2/2/2
11	CLA	B	832	-	1/1/12/20	2/19/97/115	-
13	BCR	F	202	-	-	0/29/63/63	0/2/2/2

All (681) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	812	CLA	C4B-NB	14.92	1.48	1.35
11	A	816	CLA	C4B-NB	14.56	1.48	1.35
11	B	825	CLA	C4B-NB	14.49	1.48	1.35
11	B	832	CLA	C4B-NB	14.47	1.48	1.35
11	A	814	CLA	C4B-NB	14.46	1.48	1.35
11	B	828	CLA	C4B-NB	14.41	1.48	1.35
11	B	806	CLA	C4B-NB	14.39	1.48	1.35
11	L	1502	CLA	C4B-NB	14.32	1.48	1.35
11	A	809	CLA	C4B-NB	14.32	1.48	1.35
11	A	825	CLA	C4B-NB	14.29	1.48	1.35
11	B	819	CLA	C4B-NB	14.21	1.47	1.35
11	B	818	CLA	C4B-NB	14.19	1.47	1.35
11	A	832	CLA	C4B-NB	14.16	1.47	1.35
11	A	808	CLA	C4B-NB	14.16	1.47	1.35
11	A	840	CLA	C4B-NB	14.15	1.47	1.35
11	B	829	CLA	C4B-NB	14.13	1.47	1.35
11	A	830	CLA	C4B-NB	14.07	1.47	1.35
11	A	804	CLA	C4B-NB	14.06	1.47	1.35
11	A	822	CLA	C4B-NB	14.05	1.47	1.35
11	A	803	CLA	C4B-NB	14.04	1.47	1.35
11	A	838	CLA	C4B-NB	14.04	1.47	1.35
11	A	837	CLA	C4B-NB	14.01	1.47	1.35
11	L	1503	CLA	C4B-NB	13.99	1.47	1.35
11	B	827	CLA	C4B-NB	13.98	1.47	1.35
11	A	824	CLA	C4B-NB	13.98	1.47	1.35
11	B	831	CLA	C4B-NB	13.97	1.47	1.35
11	A	807	CLA	C4B-NB	13.96	1.47	1.35
11	B	833	CLA	C4B-NB	13.94	1.47	1.35
11	B	826	CLA	C4B-NB	13.93	1.47	1.35
11	L	1501	CLA	C4B-NB	13.92	1.47	1.35
11	B	811	CLA	C4B-NB	13.92	1.47	1.35
11	B	816	CLA	C4B-NB	13.91	1.47	1.35
11	B	812	CLA	C4B-NB	13.88	1.47	1.35
11	B	814	CLA	C4B-NB	13.87	1.47	1.35
11	A	820	CLA	C4B-NB	13.82	1.47	1.35
11	A	815	CLA	C4B-NB	13.81	1.47	1.35
11	B	830	CLA	C4B-NB	13.77	1.47	1.35
11	A	819	CLA	C4B-NB	13.76	1.47	1.35
11	A	836	CLA	C4B-NB	13.75	1.47	1.35
11	B	835	CLA	C4B-NB	13.75	1.47	1.35
11	A	860	CLA	C4B-NB	13.74	1.47	1.35
11	A	842	CLA	C4B-NB	13.74	1.47	1.35
11	A	817	CLA	C4B-NB	13.71	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	827	CLA	C4B-NB	13.71	1.47	1.35
11	A	818	CLA	C4B-NB	13.71	1.47	1.35
11	B	823	CLA	C4B-NB	13.69	1.47	1.35
11	B	813	CLA	C4B-NB	13.68	1.47	1.35
11	A	813	CLA	C4B-NB	13.65	1.47	1.35
11	A	811	CLA	C4B-NB	13.60	1.47	1.35
11	A	823	CLA	C4B-NB	13.57	1.47	1.35
11	B	815	CLA	C4B-NB	13.57	1.47	1.35
11	A	841	CLA	C4B-NB	13.55	1.47	1.35
11	B	834	CLA	C4B-NB	13.54	1.47	1.35
11	B	803	CLA	C4B-NB	13.54	1.47	1.35
11	A	821	CLA	C4B-NB	13.51	1.47	1.35
11	A	829	CLA	C4B-NB	13.51	1.47	1.35
11	A	806	CLA	C4B-NB	13.49	1.47	1.35
11	B	820	CLA	C4B-NB	13.48	1.47	1.35
11	A	859	CLA	C4B-NB	13.43	1.47	1.35
11	B	801	CLA	C4B-NB	13.40	1.47	1.35
11	A	810	CLA	C4B-NB	13.38	1.47	1.35
11	A	839	CLA	C4B-NB	13.35	1.47	1.35
11	A	833	CLA	C4B-NB	13.33	1.47	1.35
11	B	809	CLA	C4B-NB	13.33	1.47	1.35
11	A	802	CLA	C4B-NB	13.30	1.47	1.35
11	B	808	CLA	C4B-NB	13.28	1.47	1.35
11	B	807	CLA	C4B-NB	13.25	1.47	1.35
11	B	822	CLA	C4B-NB	13.22	1.47	1.35
11	A	805	CLA	C4B-NB	13.21	1.47	1.35
11	B	802	CLA	C4B-NB	13.21	1.47	1.35
11	B	817	CLA	C4B-NB	13.17	1.47	1.35
11	B	824	CLA	C4B-NB	13.11	1.46	1.35
11	A	826	CLA	C4B-NB	13.08	1.46	1.35
11	A	835	CLA	C4B-NB	13.07	1.46	1.35
11	A	831	CLA	C4B-NB	13.06	1.46	1.35
11	B	821	CLA	C4B-NB	13.01	1.46	1.35
11	B	810	CLA	C4B-NB	12.97	1.46	1.35
11	A	834	CLA	C4B-NB	12.92	1.46	1.35
11	B	805	CLA	C4B-NB	12.81	1.46	1.35
11	B	836	CLA	C4B-NB	12.80	1.46	1.35
11	A	801	CLA	C4B-NB	12.72	1.46	1.35
11	A	828	CLA	C4B-NB	12.62	1.46	1.35
11	A	842	CLA	C1B-NB	7.49	1.41	1.35
11	L	1501	CLA	C1B-NB	7.31	1.41	1.35
11	A	820	CLA	C1B-NB	7.13	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	814	CLA	C1B-NB	7.11	1.41	1.35
11	B	812	CLA	C1B-NB	7.05	1.41	1.35
11	L	1503	CLA	C1B-NB	7.04	1.41	1.35
11	A	822	CLA	C1B-NB	7.00	1.41	1.35
11	L	1502	CLA	C1B-NB	6.98	1.41	1.35
11	B	815	CLA	C1B-NB	6.96	1.41	1.35
11	B	829	CLA	C1B-NB	6.94	1.41	1.35
11	A	813	CLA	C1B-NB	6.92	1.41	1.35
11	B	833	CLA	C1B-NB	6.81	1.41	1.35
11	A	841	CLA	C1B-NB	6.81	1.41	1.35
11	B	818	CLA	C1B-NB	6.79	1.41	1.35
11	B	819	CLA	C1B-NB	6.66	1.41	1.35
11	B	826	CLA	C1B-NB	6.65	1.41	1.35
11	A	812	CLA	C1B-NB	6.64	1.41	1.35
11	B	831	CLA	C1B-NB	6.64	1.41	1.35
11	B	806	CLA	C1B-NB	6.60	1.41	1.35
11	A	815	CLA	C1B-NB	6.57	1.41	1.35
11	B	813	CLA	C1B-NB	6.55	1.41	1.35
11	B	816	CLA	C1B-NB	6.55	1.41	1.35
11	A	836	CLA	C1B-NB	6.51	1.41	1.35
11	A	832	CLA	C1B-NB	6.48	1.41	1.35
11	A	803	CLA	C1B-NB	6.48	1.41	1.35
11	A	814	CLA	C1B-NB	6.45	1.41	1.35
11	A	818	CLA	C1B-NB	6.45	1.41	1.35
11	A	835	CLA	C1B-NB	6.42	1.40	1.35
11	B	825	CLA	C1B-NB	6.39	1.40	1.35
11	B	802	CLA	C1B-NB	6.38	1.40	1.35
11	A	830	CLA	C1B-NB	6.30	1.40	1.35
11	A	823	CLA	C1B-NB	6.29	1.40	1.35
11	B	809	CLA	C1B-NB	6.28	1.40	1.35
11	A	804	CLA	C1B-NB	6.24	1.40	1.35
11	A	805	CLA	C1B-NB	6.20	1.40	1.35
11	A	817	CLA	C1B-NB	6.19	1.40	1.35
11	B	836	CLA	C1B-NB	6.19	1.40	1.35
11	B	810	CLA	C1B-NB	6.19	1.40	1.35
11	A	816	CLA	C1B-NB	6.18	1.40	1.35
11	B	820	CLA	C1B-NB	6.17	1.40	1.35
11	B	830	CLA	C1B-NB	6.17	1.40	1.35
11	A	837	CLA	C1B-NB	6.17	1.40	1.35
11	A	840	CLA	C1B-NB	6.16	1.40	1.35
11	A	821	CLA	C1B-NB	6.15	1.40	1.35
11	A	827	CLA	C1B-NB	6.15	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	824	CLA	C1B-NB	6.14	1.40	1.35
11	A	838	CLA	C1B-NB	6.13	1.40	1.35
11	B	835	CLA	C1B-NB	6.13	1.40	1.35
11	B	807	CLA	C1B-NB	6.11	1.40	1.35
11	B	801	CLA	C1B-NB	6.09	1.40	1.35
11	B	821	CLA	C1B-NB	6.06	1.40	1.35
11	A	826	CLA	C1B-NB	6.06	1.40	1.35
11	B	828	CLA	C1B-NB	6.05	1.40	1.35
11	A	860	CLA	C1B-NB	6.02	1.40	1.35
11	B	803	CLA	C1B-NB	6.00	1.40	1.35
11	A	808	CLA	C1B-NB	5.97	1.40	1.35
11	B	823	CLA	C1B-NB	5.95	1.40	1.35
11	A	819	CLA	C1B-NB	5.90	1.40	1.35
11	A	811	CLA	C1B-NB	5.89	1.40	1.35
11	B	822	CLA	C1B-NB	5.88	1.40	1.35
11	B	808	CLA	C1B-NB	5.85	1.40	1.35
11	B	827	CLA	C1B-NB	5.84	1.40	1.35
11	A	834	CLA	C1B-NB	5.80	1.40	1.35
11	B	832	CLA	C1B-NB	5.79	1.40	1.35
11	A	806	CLA	C1B-NB	5.78	1.40	1.35
11	A	809	CLA	C1B-NB	5.75	1.40	1.35
11	A	831	CLA	C1B-NB	5.69	1.40	1.35
11	A	807	CLA	C1B-NB	5.68	1.40	1.35
11	A	833	CLA	C1B-NB	5.65	1.40	1.35
11	B	817	CLA	C1B-NB	5.65	1.40	1.35
11	A	825	CLA	C1B-NB	5.64	1.40	1.35
11	A	802	CLA	MG-ND	-5.62	1.94	2.05
11	A	839	CLA	C1B-NB	5.60	1.40	1.35
11	A	810	CLA	C1B-NB	5.57	1.40	1.35
11	B	805	CLA	MG-ND	-5.57	1.94	2.05
11	B	824	CLA	C1B-NB	5.55	1.40	1.35
11	B	834	CLA	C1B-NB	5.52	1.40	1.35
11	A	829	CLA	C1B-NB	5.50	1.40	1.35
11	A	801	CLA	C1B-NB	5.47	1.40	1.35
11	A	859	CLA	MG-ND	-5.47	1.94	2.05
11	B	811	CLA	MG-ND	-5.45	1.95	2.05
11	A	828	CLA	C1B-NB	5.40	1.40	1.35
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	817	CLA	MG-ND	-5.23	1.95	2.05
11	B	818	CLA	MG-ND	-5.23	1.95	2.05
11	B	836	CLA	MG-ND	-5.21	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	A	831	CLA	MG-ND	-5.16	1.95	2.05
11	A	835	CLA	MG-ND	-5.14	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	811	CLA	MG-ND	-5.09	1.95	2.05
11	B	823	CLA	MG-ND	-5.08	1.95	2.05
11	B	819	CLA	MG-ND	-5.08	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	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	809	CLA	MG-ND	-5.04	1.95	2.05
11	B	812	CLA	MG-ND	-5.03	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	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	826	CLA	MG-ND	-4.99	1.95	2.05
11	B	811	CLA	C1B-NB	4.98	1.39	1.35
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	A	821	CLA	MG-ND	-4.96	1.96	2.05
11	A	859	CLA	C1B-NB	4.95	1.39	1.35
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	A	820	CLA	MG-ND	-4.91	1.96	2.05
11	A	818	CLA	MG-ND	-4.90	1.96	2.05
11	B	813	CLA	MG-ND	-4.90	1.96	2.05
11	B	805	CLA	C1B-NB	4.89	1.39	1.35
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	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	802	CLA	C1B-NB	4.84	1.39	1.35
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	A	824	CLA	MG-ND	-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	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	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	815	CLA	MG-ND	-4.76	1.96	2.05
11	A	804	CLA	MG-ND	-4.68	1.96	2.05
11	A	814	CLA	C3A-C2A	-4.66	1.50	1.54
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	814	CLA	MG-NA	-4.57	1.95	2.06
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	A	820	CLA	C3A-C2A	-4.47	1.50	1.54
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	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	B	827	CLA	C3A-C2A	-4.38	1.50	1.54
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	842	CLA	C1D-ND	4.33	1.43	1.37
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
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	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	825	CLA	C1D-ND	4.05	1.42	1.37
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	816	CLA	C1D-ND	4.01	1.42	1.37
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	B	830	CLA	C3A-C2A	-4.00	1.50	1.54
11	A	813	CLA	C1D-ND	4.00	1.42	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	831	CLA	C1D-ND	3.96	1.42	1.37
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	L	1501	CLA	C1D-ND	3.91	1.42	1.37
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	828	CLA	C1D-ND	3.87	1.42	1.37
11	B	825	CLA	MG-NA	-3.86	1.97	2.06
11	A	826	CLA	MG-NC	-3.85	1.97	2.06
11	B	835	CLA	C1D-ND	3.84	1.42	1.37
11	A	809	CLA	C1D-ND	3.83	1.42	1.37
11	A	839	CLA	MG-NA	-3.82	1.97	2.06
11	A	812	CLA	C1D-ND	3.81	1.42	1.37
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	B	825	CLA	C1D-ND	3.79	1.42	1.37
11	B	829	CLA	C1D-ND	3.79	1.42	1.37
11	A	809	CLA	MG-NA	-3.78	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	A	841	CLA	C1D-ND	3.77	1.42	1.37
11	B	836	CLA	MG-NC	-3.77	1.97	2.06
11	A	827	CLA	C1D-ND	3.77	1.42	1.37
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	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	L	1503	CLA	C1D-ND	3.72	1.42	1.37
11	A	816	CLA	C1D-ND	3.72	1.42	1.37
11	A	811	CLA	MG-NC	-3.71	1.97	2.06
11	B	819	CLA	C1D-ND	3.70	1.42	1.37
11	A	829	CLA	MG-NA	-3.70	1.97	2.06
11	B	815	CLA	C1D-ND	3.69	1.42	1.37
11	B	826	CLA	MG-NA	-3.68	1.97	2.06
11	B	806	CLA	C1D-ND	3.68	1.42	1.37
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	B	812	CLA	C1D-ND	3.67	1.42	1.37
11	A	820	CLA	C1D-ND	3.66	1.42	1.37
11	B	814	CLA	C1D-ND	3.66	1.42	1.37
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	832	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	824	CLA	C1D-ND	3.64	1.42	1.37
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	830	CLA	C1D-ND	3.63	1.42	1.37
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	A	816	CLA	MG-NA	-3.60	1.97	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	816	CLA	MG-NA	-3.59	1.97	2.06
11	B	834	CLA	MG-NC	-3.59	1.97	2.06
11	B	820	CLA	MG-NC	-3.59	1.97	2.06
11	A	807	CLA	C1D-ND	3.58	1.42	1.37
11	A	820	CLA	MG-NC	-3.58	1.97	2.06
11	B	803	CLA	C1D-ND	3.56	1.42	1.37
11	B	827	CLA	MG-NC	-3.56	1.97	2.06
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	831	CLA	C1D-ND	3.54	1.42	1.37
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	A	828	CLA	MG-NC	-3.53	1.97	2.06
11	A	805	CLA	MG-NC	-3.52	1.97	2.06
11	B	807	CLA	MG-NC	-3.51	1.97	2.06
11	A	832	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	A	822	CLA	C1D-ND	3.49	1.42	1.37
11	A	837	CLA	C1D-ND	3.48	1.42	1.37
11	A	819	CLA	MG-NC	-3.48	1.98	2.06
11	B	822	CLA	C1D-ND	3.47	1.42	1.37
11	A	859	CLA	MG-NA	-3.47	1.98	2.06
11	A	834	CLA	C1D-ND	3.46	1.42	1.37
11	B	833	CLA	C1D-ND	3.44	1.42	1.37
11	B	826	CLA	C1D-ND	3.44	1.42	1.37
11	A	832	CLA	MG-NC	-3.44	1.98	2.06
11	A	817	CLA	C1D-ND	3.43	1.42	1.37
11	A	802	CLA	MG-NA	-3.43	1.98	2.06
11	B	824	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	B	819	CLA	MG-NC	-3.42	1.98	2.06
11	A	815	CLA	C1D-ND	3.41	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	840	CLA	O1D-CGD	3.39	1.33	1.19
11	A	816	CLA	MG-NC	-3.38	1.98	2.06
11	B	802	CLA	C1D-ND	3.38	1.41	1.37
11	A	860	CLA	MG-NC	-3.37	1.98	2.06
11	A	818	CLA	C1D-ND	3.36	1.41	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	A	805	CLA	C1D-ND	3.35	1.41	1.37
11	A	821	CLA	MG-NC	-3.35	1.98	2.06
11	B	828	CLA	MG-NC	-3.34	1.98	2.06
11	A	839	CLA	C1D-ND	3.34	1.41	1.37
11	A	803	CLA	C1D-ND	3.34	1.41	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	836	CLA	C1D-ND	3.32	1.41	1.37
11	A	835	CLA	C1D-ND	3.32	1.41	1.37
11	A	833	CLA	C1D-ND	3.32	1.41	1.37
11	A	806	CLA	C1D-ND	3.31	1.41	1.37
11	A	814	CLA	C1D-ND	3.31	1.41	1.37
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	830	CLA	C1D-ND	3.28	1.41	1.37
11	B	818	CLA	C1D-ND	3.28	1.41	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	A	829	CLA	C1D-ND	3.27	1.41	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	806	CLA	MG-NC	-3.22	1.98	2.06
11	A	840	CLA	C1D-ND	3.21	1.41	1.37
11	A	823	CLA	C1D-ND	3.20	1.41	1.37
11	A	818	CLA	MG-NC	-3.20	1.98	2.06
11	A	811	CLA	C1D-ND	3.20	1.41	1.37
11	B	813	CLA	C1D-ND	3.19	1.41	1.37
11	B	805	CLA	MG-NC	-3.17	1.98	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	832	CLA	MG-NC	-3.16	1.98	2.06
11	A	802	CLA	MG-NC	-3.13	1.98	2.06
11	A	810	CLA	C1D-ND	3.12	1.41	1.37
11	B	831	CLA	MG-NC	-3.12	1.98	2.06
11	B	834	CLA	C1D-ND	3.11	1.41	1.37
11	B	811	CLA	MG-NC	-3.09	1.98	2.06
11	A	838	CLA	C1D-ND	3.08	1.41	1.37
11	B	809	CLA	C1D-ND	3.08	1.41	1.37
11	A	804	CLA	C1D-ND	3.07	1.41	1.37
11	A	801	CLA	C4D-CHA	-3.06	1.34	1.44
11	A	829	CLA	MG-NC	-3.06	1.99	2.06
11	L	1502	CLA	C1D-ND	3.06	1.41	1.37
11	A	821	CLA	C1D-ND	3.05	1.41	1.37
11	B	827	CLA	C1D-ND	3.04	1.41	1.37
11	B	816	CLA	MG-NC	-3.03	1.99	2.06
11	B	807	CLA	C1D-ND	3.01	1.41	1.37
11	A	826	CLA	C1D-ND	2.99	1.41	1.37
11	B	808	CLA	C1D-ND	2.98	1.41	1.37
11	A	801	CLA	C1D-ND	2.94	1.41	1.37
11	A	836	CLA	C1D-ND	2.92	1.41	1.37
11	B	821	CLA	C1D-ND	2.91	1.41	1.37
11	B	811	CLA	C1D-ND	2.90	1.41	1.37
11	B	817	CLA	C1D-ND	2.83	1.41	1.37
11	A	859	CLA	MG-NC	-2.83	1.99	2.06
11	A	828	CLA	C1D-ND	2.82	1.41	1.37
11	A	808	CLA	C1D-ND	2.82	1.41	1.37
11	B	823	CLA	C1D-ND	2.80	1.41	1.37
11	B	801	CLA	C1D-ND	2.80	1.41	1.37
11	A	859	CLA	C1D-ND	2.79	1.41	1.37
11	A	860	CLA	C1D-ND	2.77	1.41	1.37
11	B	805	CLA	C1D-C2D	-2.76	1.39	1.45
11	A	860	CLA	C1D-C2D	-2.72	1.40	1.45
14	A	850	LHG	O7-C5	-2.70	1.39	1.46
11	B	810	CLA	C1D-C2D	-2.70	1.40	1.45
11	A	816	CLA	C1D-C2D	-2.64	1.40	1.45
11	A	825	CLA	C1D-C2D	-2.64	1.40	1.45
11	A	819	CLA	C1D-ND	2.63	1.41	1.37
11	A	809	CLA	C1D-C2D	-2.61	1.40	1.45
11	A	829	CLA	C1D-C2D	-2.59	1.40	1.45
11	A	827	CLA	C1D-C2D	-2.59	1.40	1.45
11	B	808	CLA	C1D-C2D	-2.58	1.40	1.45
11	A	806	CLA	C1D-C2D	-2.58	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	A	810	CLA	C1D-C2D	-2.57	1.40	1.45
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	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	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	-2.53	1.40	1.45
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	820	CLA	C1D-ND	2.52	1.40	1.37
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	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	A	859	CLA	C1D-C2D	-2.49	1.40	1.45
11	B	810	CLA	C1D-ND	2.49	1.40	1.37
11	A	831	CLA	C3B-C2B	-2.49	1.36	1.40
11	A	822	CLA	C1D-C2D	-2.49	1.40	1.45
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	B	805	CLA	C1D-ND	2.47	1.40	1.37
11	A	804	CLA	C1D-C2D	-2.47	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	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	-2.46	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
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	805	CLA	C1D-C2D	-2.43	1.40	1.45
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
11	B	805	CLA	C3A-C2A	-2.40	1.47	1.54
11	B	811	CLA	C3B-C2B	-2.40	1.37	1.40
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
14	A	851	LHG	O7-C5	-2.37	1.40	1.46
11	B	830	CLA	C1D-C2D	-2.36	1.40	1.45
11	B	827	CLA	C1D-C2D	-2.36	1.40	1.45
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	B	816	CLA	C1C-C2C	2.36	1.49	1.44
11	A	814	CLA	C1D-C2D	-2.36	1.40	1.45
11	A	859	CLA	C3D-C4D	-2.35	1.38	1.44
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	833	CLA	C1D-C2D	-2.32	1.40	1.45
11	A	802	CLA	C1D-ND	2.31	1.40	1.37
11	B	817	CLA	C3B-C2B	-2.29	1.37	1.40
11	B	819	CLA	C1D-C2D	-2.29	1.40	1.45
16	B	843	LMG	O7-C8	-2.27	1.40	1.46
11	B	814	CLA	C1D-C2D	-2.26	1.40	1.45
11	A	823	CLA	C1D-C2D	-2.26	1.40	1.45
11	A	806	CLA	C3A-C2A	-2.26	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	833	CLA	C3A-C2A	-2.25	1.48	1.54
11	A	802	CLA	C3D-C4D	-2.24	1.39	1.44
11	L	1501	CLA	C1D-C2D	-2.24	1.40	1.45
11	B	834	CLA	C3D-C4D	-2.22	1.39	1.44
11	A	811	CLA	C3D-C4D	-2.21	1.39	1.44
11	A	826	CLA	C3D-C4D	-2.20	1.39	1.44
11	A	814	CLA	C3D-C4D	-2.20	1.39	1.44
11	B	823	CLA	C3D-C4D	-2.19	1.39	1.44
11	A	841	CLA	C3D-C4D	-2.18	1.39	1.44
11	A	816	CLA	C4D-CHA	-2.18	1.37	1.44
11	B	821	CLA	C3D-C4D	-2.17	1.39	1.44
11	A	828	CLA	C3D-C4D	-2.17	1.39	1.44
11	A	801	CLA	C3A-C2A	-2.17	1.48	1.54
11	B	810	CLA	C3D-C4D	-2.16	1.39	1.44
11	A	838	CLA	C3D-C4D	-2.16	1.39	1.44
11	A	828	CLA	C1C-C2C	2.15	1.48	1.44
11	B	817	CLA	C3D-C4D	-2.15	1.39	1.44
11	B	821	CLA	C1C-C2C	2.15	1.48	1.44
11	A	829	CLA	C1C-C2C	2.14	1.48	1.44
11	A	837	CLA	C3D-C4D	-2.14	1.39	1.44
11	B	807	CLA	C3D-C4D	-2.14	1.39	1.44
11	A	808	CLA	C3D-C4D	-2.14	1.39	1.44
11	A	809	CLA	C3A-C2A	-2.14	1.48	1.54
11	A	832	CLA	C3D-C4D	-2.14	1.39	1.44
11	B	833	CLA	C3D-C4D	-2.13	1.39	1.44
11	A	834	CLA	C3D-C4D	-2.13	1.39	1.44
11	B	820	CLA	C3D-C4D	-2.13	1.39	1.44
11	A	821	CLA	C3D-C4D	-2.13	1.39	1.44
11	A	819	CLA	C3D-C4D	-2.13	1.39	1.44
11	A	840	CLA	C3D-C4D	-2.12	1.39	1.44
11	A	801	CLA	C3D-C4D	-2.12	1.39	1.44
11	A	839	CLA	C3D-C4D	-2.12	1.39	1.44
11	L	1502	CLA	C1C-C2C	2.11	1.48	1.44
11	B	815	CLA	C3D-C4D	-2.11	1.39	1.44
11	B	809	CLA	C3D-C4D	-2.11	1.39	1.44
11	A	830	CLA	C3D-C4D	-2.11	1.39	1.44
11	A	837	CLA	C3A-C2A	-2.10	1.48	1.54
11	A	839	CLA	C3A-C2A	-2.10	1.48	1.54
11	A	804	CLA	C3D-C4D	-2.10	1.39	1.44
11	A	842	CLA	C2A-C3A	-2.10	1.48	1.53
11	B	818	CLA	C1C-C2C	2.09	1.48	1.44
11	A	833	CLA	C3D-C4D	-2.09	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	826	CLA	C3A-C2A	-2.09	1.48	1.54
11	A	836	CLA	C3D-C4D	-2.09	1.39	1.44
11	B	812	CLA	C3D-C4D	-2.09	1.39	1.44
11	A	803	CLA	C3D-C4D	-2.09	1.39	1.44
11	B	825	CLA	C3D-C4D	-2.09	1.39	1.44
11	B	803	CLA	C3D-C4D	-2.09	1.39	1.44
11	B	811	CLA	C3D-C4D	-2.08	1.39	1.44
11	B	824	CLA	C3D-C4D	-2.08	1.39	1.44
11	B	827	CLA	C3D-C4D	-2.08	1.39	1.44
11	B	819	CLA	C3D-C4D	-2.08	1.39	1.44
11	A	816	CLA	C3A-C2A	-2.07	1.48	1.54
11	A	820	CLA	C3D-C4D	-2.07	1.39	1.44
11	A	829	CLA	C3D-C4D	-2.07	1.39	1.44
11	A	823	CLA	C3D-C4D	-2.06	1.39	1.44
11	A	807	CLA	C3D-C4D	-2.06	1.39	1.44
11	A	835	CLA	C3D-C4D	-2.06	1.39	1.44
11	B	836	CLA	C3D-C4D	-2.06	1.39	1.44
11	A	859	CLA	C1C-C2C	2.06	1.48	1.44
11	A	812	CLA	C3D-C4D	-2.06	1.39	1.44
11	B	805	CLA	CHD-C4C	-2.06	1.34	1.39
11	A	824	CLA	C1C-C2C	2.05	1.48	1.44
11	A	827	CLA	C3D-C4D	-2.05	1.39	1.44
11	B	801	CLA	C3D-C4D	-2.05	1.39	1.44
11	B	813	CLA	C3D-C4D	-2.05	1.39	1.44
11	B	803	CLA	C3A-C2A	-2.05	1.48	1.54
11	A	860	CLA	C3D-C4D	-2.04	1.39	1.44
11	B	814	CLA	C3D-C4D	-2.04	1.39	1.44
11	B	832	CLA	C3D-C4D	-2.04	1.39	1.44
11	L	1502	CLA	C3D-C4D	-2.04	1.39	1.44
11	B	826	CLA	C3D-C4D	-2.04	1.39	1.44
11	B	835	CLA	C3D-C4D	-2.04	1.39	1.44
11	A	825	CLA	CHD-C4C	-2.04	1.34	1.39
11	B	806	CLA	C3D-C4D	-2.03	1.39	1.44
11	A	831	CLA	C3D-C4D	-2.03	1.39	1.44
11	A	813	CLA	C3D-C4D	-2.03	1.39	1.44
11	A	815	CLA	C3B-C2B	-2.03	1.37	1.40
11	A	805	CLA	C3D-C4D	-2.03	1.39	1.44
11	A	818	CLA	C3D-C4D	-2.03	1.39	1.44
11	A	817	CLA	C3D-C4D	-2.02	1.39	1.44
11	B	822	CLA	C3D-C4D	-2.02	1.39	1.44
11	A	806	CLA	C3D-C4D	-2.02	1.39	1.44
11	B	818	CLA	C3D-C4D	-2.02	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	808	CLA	C3D-C4D	-2.02	1.39	1.44
11	A	816	CLA	CHD-C4C	-2.02	1.34	1.39
13	A	849	BCR	C20-C21	2.02	1.49	1.43
16	B	843	LMG	O1-C7	-2.01	1.40	1.43
11	A	815	CLA	C3D-C4D	-2.01	1.39	1.44
11	B	830	CLA	C3B-C2B	-2.01	1.37	1.40
11	A	824	CLA	C3D-C4D	-2.00	1.39	1.44
11	B	802	CLA	C3D-C4D	-2.00	1.39	1.44

All (740) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	1502	CLA	C4A-NA-C1A	-7.42	103.37	106.71
11	A	805	CLA	C4A-NA-C1A	-6.85	103.63	106.71
11	B	824	CLA	C4A-NA-C1A	-6.80	103.65	106.71
11	L	1503	CLA	C4A-NA-C1A	-6.75	103.67	106.71
11	B	803	CLA	C4A-NA-C1A	-6.74	103.67	106.71
11	B	836	CLA	C4A-NA-C1A	-6.66	103.71	106.71
11	L	1501	CLA	C4A-NA-C1A	-6.55	103.76	106.71
13	F	201	BCR	C21-C20-C19	6.50	143.51	123.22
11	B	817	CLA	C4A-NA-C1A	-6.47	103.80	106.71
11	A	823	CLA	C4A-NA-C1A	-6.30	103.87	106.71
11	B	814	CLA	C4A-NA-C1A	-6.27	103.89	106.71
11	A	811	CLA	C4A-NA-C1A	-6.27	103.89	106.71
11	B	812	CLA	C4A-NA-C1A	-6.22	103.91	106.71
11	B	819	CLA	C4A-NA-C1A	-6.15	103.94	106.71
11	A	828	CLA	C4A-NA-C1A	-6.13	103.95	106.71
11	B	822	CLA	C4A-NA-C1A	-6.07	103.98	106.71
11	B	815	CLA	C4A-NA-C1A	-6.04	103.99	106.71
11	B	807	CLA	C4A-NA-C1A	-6.03	104.00	106.71
11	A	808	CLA	C4A-NA-C1A	-5.91	104.05	106.71
11	A	832	CLA	C4A-NA-C1A	-5.85	104.08	106.71
11	B	827	CLA	C4A-NA-C1A	-5.81	104.09	106.71
11	B	821	CLA	C4A-NA-C1A	-5.78	104.11	106.71
11	A	822	CLA	C4A-NA-C1A	-5.76	104.12	106.71
11	A	801	CLA	C4A-NA-C1A	-5.76	104.12	106.71
11	A	813	CLA	C4A-NA-C1A	-5.73	104.13	106.71
11	A	826	CLA	C4A-NA-C1A	-5.70	104.14	106.71
11	B	830	CLA	C4A-NA-C1A	-5.65	104.17	106.71
11	B	823	CLA	C4A-NA-C1A	-5.58	104.20	106.71
11	B	820	CLA	C4A-NA-C1A	-5.51	104.23	106.71
11	A	804	CLA	C4A-NA-C1A	-5.49	104.24	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	814	CLA	C4A-NA-C1A	-5.48	104.24	106.71
11	B	818	CLA	C4A-NA-C1A	-5.45	104.25	106.71
11	B	813	CLA	C4A-NA-C1A	-5.43	104.27	106.71
11	B	809	CLA	C4A-NA-C1A	-5.41	104.28	106.71
11	A	842	CLA	C4A-NA-C1A	-5.36	104.30	106.71
11	A	802	CLA	C4A-NA-C1A	-5.35	104.30	106.71
11	A	836	CLA	C4A-NA-C1A	-5.34	104.31	106.71
11	A	840	CLA	C4A-NA-C1A	-5.31	104.32	106.71
11	A	820	CLA	C4A-NA-C1A	-5.30	104.32	106.71
11	A	819	CLA	C4A-NA-C1A	-5.19	104.37	106.71
11	B	811	CLA	C4A-NA-C1A	-5.14	104.39	106.71
11	A	837	CLA	C4A-NA-C1A	-5.12	104.40	106.71
11	B	828	CLA	C4A-NA-C1A	-5.12	104.40	106.71
11	B	806	CLA	C4A-NA-C1A	-5.12	104.41	106.71
11	B	834	CLA	C4A-NA-C1A	-5.12	104.41	106.71
11	A	833	CLA	C4A-NA-C1A	-5.11	104.41	106.71
11	A	831	CLA	C4A-NA-C1A	-5.09	104.42	106.71
11	A	859	CLA	C4A-NA-C1A	-5.07	104.43	106.71
11	A	818	CLA	C4A-NA-C1A	-5.01	104.45	106.71
11	A	806	CLA	C4A-NA-C1A	-4.99	104.46	106.71
11	A	803	CLA	C4A-NA-C1A	-4.98	104.47	106.71
11	A	829	CLA	C4A-NA-C1A	-4.93	104.49	106.71
11	A	817	CLA	C4A-NA-C1A	-4.91	104.50	106.71
11	B	816	CLA	C4A-NA-C1A	-4.86	104.52	106.71
11	B	801	CLA	C4A-NA-C1A	-4.84	104.53	106.71
11	B	826	CLA	C4A-NA-C1A	-4.78	104.56	106.71
11	B	832	CLA	C4A-NA-C1A	-4.74	104.57	106.71
11	A	838	CLA	C4A-NA-C1A	-4.72	104.58	106.71
11	A	807	CLA	C4A-NA-C1A	-4.71	104.59	106.71
11	B	810	CLA	C4A-NA-C1A	-4.62	104.63	106.71
13	F	202	BCR	C23-C24-C25	4.60	140.11	127.20
11	B	829	CLA	C4A-NA-C1A	-4.59	104.64	106.71
13	F	202	BCR	C24-C23-C22	4.57	133.15	126.23
11	A	824	CLA	C4A-NA-C1A	-4.54	104.67	106.71
11	A	827	CLA	C4A-NA-C1A	-4.52	104.67	106.71
11	A	830	CLA	C4A-NA-C1A	-4.52	104.67	106.71
11	A	834	CLA	C4A-NA-C1A	-4.51	104.68	106.71
11	A	821	CLA	C4A-NA-C1A	-4.42	104.72	106.71
11	A	839	CLA	C4A-NA-C1A	-4.41	104.72	106.71
11	B	805	CLA	C4A-NA-C1A	-4.36	104.75	106.71
11	A	825	CLA	C4A-NA-C1A	-4.26	104.79	106.71
11	A	812	CLA	C4A-NA-C1A	-4.25	104.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	201	BCR	C15-C16-C17	4.22	132.11	123.47
11	A	815	CLA	C4A-NA-C1A	-4.22	104.81	106.71
11	B	831	CLA	C4A-NA-C1A	-4.22	104.81	106.71
11	B	825	CLA	C4A-NA-C1A	-4.18	104.83	106.71
14	A	850	LHG	O4-P-O5	4.17	132.84	112.24
11	B	802	CLA	C4A-NA-C1A	-4.15	104.84	106.71
14	A	851	LHG	O4-P-O5	4.14	132.70	112.24
11	A	809	CLA	C4A-NA-C1A	-4.12	104.85	106.71
11	A	819	CLA	O2A-C1-C2	4.08	119.35	108.64
11	B	808	CLA	C4A-NA-C1A	-4.07	104.88	106.71
11	A	841	CLA	C4A-NA-C1A	-3.98	104.92	106.71
11	B	835	CLA	C4A-NA-C1A	-3.96	104.92	106.71
11	B	833	CLA	CHD-C1D-ND	-3.92	120.85	124.45
11	A	816	CLA	C4A-NA-C1A	-3.90	104.95	106.71
11	L	1502	CLA	CHD-C1D-ND	-3.90	120.87	124.45
11	B	817	CLA	CHD-C1D-ND	-3.88	120.89	124.45
11	B	833	CLA	C4A-NA-C1A	-3.87	104.97	106.71
11	L	1503	CLA	CHD-C1D-ND	-3.86	120.90	124.45
11	A	835	CLA	C4A-NA-C1A	-3.85	104.97	106.71
11	B	813	CLA	CHD-C1D-ND	-3.83	120.94	124.45
11	B	801	CLA	CHD-C1D-ND	-3.79	120.97	124.45
11	B	809	CLA	CHD-C1D-ND	-3.77	120.99	124.45
11	A	823	CLA	CHD-C1D-ND	-3.76	121.00	124.45
11	A	840	CLA	CHD-C1D-ND	-3.75	121.00	124.45
11	B	820	CLA	CAA-C2A-C1A	-3.74	99.72	111.97
11	B	814	CLA	CHD-C1D-ND	-3.73	121.03	124.45
11	A	811	CLA	CHD-C1D-ND	-3.69	121.06	124.45
11	A	836	CLA	CHD-C1D-ND	-3.69	121.06	124.45
11	L	1501	CLA	CHD-C1D-ND	-3.69	121.07	124.45
11	A	826	CLA	CHD-C1D-ND	-3.68	121.07	124.45
11	B	820	CLA	CHD-C1D-ND	-3.68	121.08	124.45
13	A	856	BCR	C16-C15-C14	3.67	131.00	123.47
11	A	822	CLA	CHD-C1D-ND	-3.66	121.09	124.45
11	A	810	CLA	C4A-NA-C1A	-3.66	105.06	106.71
11	B	819	CLA	CHD-C1D-ND	-3.65	121.10	124.45
11	A	803	CLA	CHD-C1D-ND	-3.64	121.11	124.45
11	B	827	CLA	CHD-C1D-ND	-3.64	121.11	124.45
11	B	807	CLA	CHD-C1D-ND	-3.63	121.12	124.45
11	A	820	CLA	CHD-C1D-ND	-3.60	121.14	124.45
11	B	830	CLA	CHD-C1D-ND	-3.60	121.15	124.45
11	B	806	CLA	CHD-C1D-ND	-3.60	121.15	124.45
11	A	832	CLA	CHD-C1D-ND	-3.59	121.15	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	828	CLA	CHD-C1D-ND	-3.59	121.15	124.45
11	A	804	CLA	CHD-C1D-ND	-3.59	121.16	124.45
11	A	838	CLA	CHD-C1D-ND	-3.58	121.16	124.45
13	A	855	BCR	C1-C6-C7	-3.58	112.98	122.42
13	A	852	BCR	C8-C7-C6	3.57	131.59	125.51
11	A	814	CLA	CHD-C1D-ND	-3.57	121.17	124.45
11	A	860	CLA	C4A-NA-C1A	-3.57	105.10	106.71
11	B	802	CLA	CHD-C1D-ND	-3.57	121.18	124.45
11	A	802	CLA	CHD-C1D-ND	-3.55	121.20	124.45
11	A	805	CLA	CHD-C1D-ND	-3.54	121.20	124.45
11	A	810	CLA	CHD-C1D-ND	-3.50	121.23	124.45
11	A	819	CLA	CHD-C1D-ND	-3.50	121.24	124.45
11	B	824	CLA	CHD-C1D-ND	-3.48	121.25	124.45
11	B	823	CLA	CHD-C1D-ND	-3.48	121.26	124.45
11	A	860	CLA	CHD-C1D-ND	-3.47	121.26	124.45
11	A	817	CLA	CHD-C1D-ND	-3.47	121.27	124.45
11	A	837	CLA	CHD-C1D-ND	-3.45	121.28	124.45
13	F	201	BCR	C16-C17-C18	3.45	132.24	127.31
11	B	812	CLA	CHD-C1D-ND	-3.45	121.29	124.45
11	B	818	CLA	CHD-C1D-ND	-3.45	121.29	124.45
11	B	822	CLA	CHD-C1D-ND	-3.44	121.29	124.45
11	A	824	CLA	CHD-C1D-ND	-3.44	121.29	124.45
11	A	834	CLA	CHD-C1D-ND	-3.43	121.30	124.45
11	A	808	CLA	CHD-C1D-ND	-3.43	121.30	124.45
11	B	808	CLA	CHD-C1D-ND	-3.43	121.31	124.45
11	B	829	CLA	CHD-C1D-ND	-3.42	121.31	124.45
11	A	829	CLA	CHD-C1D-ND	-3.42	121.31	124.45
11	B	803	CLA	CHD-C1D-ND	-3.42	121.31	124.45
13	A	849	BCR	C21-C20-C19	3.41	133.86	123.22
11	B	834	CLA	CHD-C1D-ND	-3.40	121.33	124.45
11	A	835	CLA	CHD-C1D-ND	-3.40	121.33	124.45
11	A	815	CLA	CHD-C1D-ND	-3.39	121.34	124.45
11	A	818	CLA	CHD-C1D-ND	-3.38	121.35	124.45
11	A	833	CLA	CHD-C1D-ND	-3.38	121.35	124.45
11	B	826	CLA	CHD-C1D-ND	-3.37	121.35	124.45
11	A	804	CLA	CAA-C2A-C1A	-3.36	100.97	111.97
11	B	811	CLA	CHD-C1D-ND	-3.34	121.38	124.45
11	B	815	CLA	CHD-C1D-ND	-3.34	121.38	124.45
11	A	831	CLA	CHD-C1D-ND	-3.34	121.39	124.45
11	B	836	CLA	CHD-C1D-ND	-3.33	121.39	124.45
11	A	816	CLA	CHD-C1D-ND	-3.32	121.40	124.45
11	B	821	CLA	CHD-C1D-ND	-3.32	121.40	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	808	CLA	CAA-C2A-C1A	-3.31	101.13	111.97
11	A	812	CLA	CHD-C1D-ND	-3.31	121.42	124.45
11	B	828	CLA	CHD-C1D-ND	-3.31	121.42	124.45
11	B	831	CLA	CHD-C1D-ND	-3.30	121.42	124.45
14	A	851	LHG	O8-C23-C24	3.30	120.03	111.38
11	A	859	CLA	CHD-C1D-ND	-3.29	121.43	124.45
13	A	849	BCR	C16-C15-C14	3.28	130.20	123.47
11	A	807	CLA	CHD-C1D-ND	-3.28	121.44	124.45
11	A	821	CLA	CHD-C1D-ND	-3.27	121.45	124.45
11	A	816	CLA	CHA-C1A-NA	-3.24	118.97	126.40
11	B	835	CLA	CHD-C1D-ND	-3.24	121.47	124.45
11	A	841	CLA	CHD-C1D-ND	-3.24	121.48	124.45
13	L	1504	BCR	C23-C24-C25	3.24	136.29	127.20
11	A	827	CLA	CHD-C1D-ND	-3.23	121.48	124.45
11	B	825	CLA	CHD-C1D-ND	-3.23	121.48	124.45
11	A	806	CLA	CHD-C1D-ND	-3.21	121.50	124.45
13	A	856	BCR	C15-C14-C13	3.21	131.89	127.31
11	A	842	CLA	CHD-C1D-ND	-3.20	121.51	124.45
11	B	833	CLA	C1D-ND-C4D	-3.19	104.07	106.33
11	A	816	CLA	C2C-C1C-NC	3.19	112.96	109.97
11	A	820	CLA	C1D-ND-C4D	-3.18	104.08	106.33
11	A	830	CLA	CHD-C1D-ND	-3.18	121.53	124.45
11	A	839	CLA	CHD-C1D-ND	-3.17	121.54	124.45
11	A	809	CLA	CHD-C1D-ND	-3.16	121.55	124.45
11	A	801	CLA	CHD-C1D-ND	-3.16	121.55	124.45
11	B	832	CLA	CHD-C1D-ND	-3.15	121.56	124.45
13	F	201	BCR	C15-C14-C13	3.14	131.80	127.31
11	A	813	CLA	CHD-C1D-ND	-3.12	121.59	124.45
11	A	816	CLA	C2A-C1A-CHA	3.11	129.29	123.86
11	B	805	CLA	CHD-C1D-ND	-3.10	121.61	124.45
11	B	815	CLA	C1D-ND-C4D	-3.08	104.15	106.33
11	B	816	CLA	CHD-C1D-ND	-3.08	121.63	124.45
11	A	838	CLA	C1D-ND-C4D	-3.07	104.15	106.33
11	A	831	CLA	C2C-C1C-NC	3.06	112.84	109.97
13	A	849	BCR	C15-C16-C17	3.02	129.65	123.47
13	A	849	BCR	C20-C21-C22	3.00	131.59	127.31
11	A	819	CLA	CAA-C2A-C1A	-2.99	102.16	111.97
11	A	832	CLA	C1D-ND-C4D	-2.99	104.21	106.33
11	A	813	CLA	C2C-C1C-NC	2.99	112.77	109.97
11	B	828	CLA	C2C-C1C-NC	2.99	112.77	109.97
11	B	809	CLA	C1D-ND-C4D	-2.99	104.21	106.33
11	B	808	CLA	C2C-C1C-NC	2.97	112.75	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	822	CLA	C1D-ND-C4D	-2.95	104.24	106.33
11	A	820	CLA	C2C-C1C-NC	2.94	112.73	109.97
11	B	815	CLA	C2C-C1C-NC	2.94	112.72	109.97
11	A	818	CLA	C2C-C1C-NC	2.93	112.72	109.97
11	B	832	CLA	C2C-C1C-NC	2.93	112.72	109.97
11	A	826	CLA	C1D-ND-C4D	-2.92	104.26	106.33
11	A	837	CLA	C1D-ND-C4D	-2.92	104.26	106.33
11	A	806	CLA	C2C-C1C-NC	2.90	112.69	109.97
11	A	825	CLA	CHD-C1D-ND	-2.89	121.80	124.45
11	A	813	CLA	CHA-C1A-NA	-2.88	119.79	126.40
13	B	840	BCR	C20-C19-C18	2.87	134.49	126.42
11	B	812	CLA	C1D-ND-C4D	-2.87	104.30	106.33
11	A	815	CLA	C1D-ND-C4D	-2.87	104.30	106.33
11	L	1503	CLA	CAA-C2A-C1A	-2.87	105.79	112.14
11	A	825	CLA	CHA-C1A-NA	-2.86	119.84	126.40
13	A	852	BCR	C1-C6-C7	-2.86	114.86	122.42
11	A	836	CLA	C1D-ND-C4D	-2.86	104.30	106.33
11	L	1502	CLA	C1D-ND-C4D	-2.86	104.30	106.33
13	B	840	BCR	C21-C20-C19	2.86	132.14	123.22
11	A	809	CLA	CHA-C1A-NA	-2.85	119.87	126.40
11	B	817	CLA	C1D-ND-C4D	-2.84	104.32	106.33
11	B	810	CLA	CHD-C1D-ND	-2.84	121.84	124.45
16	B	843	LMG	O6-C1-O1	-2.83	103.27	109.97
11	B	820	CLA	C1-C2-C3	-2.83	121.15	126.04
11	A	840	CLA	C1D-ND-C4D	-2.83	104.33	106.33
11	A	816	CLA	CHC-C1C-C2C	-2.81	118.94	126.72
13	F	201	BCR	C20-C21-C22	2.81	131.31	127.31
11	A	826	CLA	CAA-C2A-C1A	-2.80	102.80	111.97
11	B	824	CLA	C1-C2-C3	-2.80	121.20	126.04
11	B	826	CLA	C2C-C1C-NC	2.79	112.59	109.97
11	B	828	CLA	CHC-C1C-C2C	-2.79	119.01	126.72
11	A	803	CLA	C1D-ND-C4D	-2.77	104.36	106.33
11	L	1503	CLA	C1D-ND-C4D	-2.77	104.36	106.33
11	B	828	CLA	C1D-ND-C4D	-2.77	104.37	106.33
11	B	819	CLA	C1D-ND-C4D	-2.77	104.37	106.33
11	B	818	CLA	C1D-ND-C4D	-2.76	104.37	106.33
11	A	827	CLA	C2C-C1C-NC	2.76	112.55	109.97
11	B	802	CLA	C1D-ND-C4D	-2.75	104.38	106.33
11	A	819	CLA	C1-C2-C3	-2.74	121.30	126.04
11	B	836	CLA	C2C-C1C-NC	2.74	112.54	109.97
11	A	820	CLA	CAA-C2A-C1A	-2.74	105.05	111.81
11	A	814	CLA	C1D-ND-C4D	-2.72	104.40	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	834	CLA	C1D-ND-C4D	-2.72	104.40	106.33
11	A	837	CLA	C2C-C1C-NC	2.72	112.52	109.97
11	B	834	CLA	C2C-C1C-NC	2.71	112.52	109.97
11	A	824	CLA	C1D-ND-C4D	-2.71	104.41	106.33
11	A	812	CLA	C1D-ND-C4D	-2.69	104.42	106.33
11	B	823	CLA	CAA-C2A-C1A	-2.69	103.17	111.97
14	A	850	LHG	O8-C23-C24	2.69	120.33	111.91
11	A	817	CLA	C1D-ND-C4D	-2.68	104.43	106.33
11	B	814	CLA	C1D-ND-C4D	-2.67	104.44	106.33
11	A	810	CLA	CHC-C1C-C2C	-2.67	119.33	126.72
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	106.33
11	B	829	CLA	C1D-ND-C4D	-2.66	104.44	106.33
11	A	813	CLA	CHC-C1C-C2C	-2.66	119.36	126.72
11	B	831	CLA	C2C-C1C-NC	2.66	112.47	109.97
11	A	834	CLA	C1D-ND-C4D	-2.66	104.44	106.33
11	A	839	CLA	C2C-C1C-NC	2.66	112.46	109.97
13	F	202	BCR	C8-C7-C6	2.66	134.67	127.20
11	A	828	CLA	C1D-ND-C4D	-2.66	104.45	106.33
11	B	801	CLA	C1D-ND-C4D	-2.66	104.45	106.33
11	B	820	CLA	C1D-ND-C4D	-2.66	104.45	106.33
13	A	849	BCR	C10-C11-C12	2.66	131.51	123.22
11	B	809	CLA	C2C-C1C-NC	2.65	112.46	109.97
11	B	827	CLA	CHC-C1C-C2C	-2.65	119.39	126.72
11	B	827	CLA	C2C-C1C-NC	2.65	112.46	109.97
11	A	805	CLA	C1-C2-C3	-2.65	121.46	126.04
11	B	811	CLA	C2C-C1C-NC	2.65	112.45	109.97
11	B	834	CLA	CHC-C1C-C2C	-2.64	119.41	126.72
11	L	1501	CLA	CHC-C1C-NC	2.64	128.21	124.20
11	A	820	CLA	CHC-C1C-C2C	-2.64	119.42	126.72
11	A	804	CLA	C1D-ND-C4D	-2.64	104.46	106.33
11	A	839	CLA	CHC-C1C-C2C	-2.64	119.43	126.72
11	A	831	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
11	A	827	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
11	A	834	CLA	CHC-C1C-C2C	-2.63	119.44	126.72
11	B	832	CLA	C1D-ND-C4D	-2.63	104.47	106.33
11	A	809	CLA	CHC-C1C-NC	2.63	128.19	124.20
13	B	844	BCR	C23-C24-C25	2.62	134.57	127.20
13	F	201	BCR	C16-C15-C14	2.62	128.84	123.47
11	A	807	CLA	CHC-C1C-NC	2.62	128.18	124.20
11	A	859	CLA	C1-C2-C3	-2.61	121.52	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	832	CLA	CHC-C1C-C2C	-2.61	119.50	126.72
11	B	801	CLA	CAA-C2A-C1A	-2.61	103.42	111.97
11	B	836	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
11	A	807	CLA	C1D-ND-C4D	-2.61	104.48	106.33
11	B	828	CLA	CHC-C1C-NC	2.61	128.16	124.20
11	A	829	CLA	C1D-ND-C4D	-2.61	104.48	106.33
11	B	824	CLA	CHA-C1A-NA	-2.61	120.43	126.40
16	B	843	LMG	O1-C7-C8	-2.61	104.61	110.90
11	B	827	CLA	CHC-C1C-NC	2.61	128.16	124.20
11	B	816	CLA	C1D-ND-C4D	-2.60	104.49	106.33
11	A	818	CLA	C1D-ND-C4D	-2.60	104.49	106.33
11	B	831	CLA	CHC-C1C-C2C	-2.59	119.55	126.72
11	B	806	CLA	C1D-ND-C4D	-2.59	104.50	106.33
11	A	831	CLA	CHA-C1A-NA	-2.58	120.48	126.40
11	A	817	CLA	CHC-C1C-NC	2.58	128.12	124.20
11	A	825	CLA	C2C-C1C-NC	2.58	112.39	109.97
11	B	835	CLA	C1D-ND-C4D	-2.58	104.50	106.33
11	A	812	CLA	CHA-C1A-NA	-2.58	120.49	126.40
11	A	812	CLA	CHC-C1C-C2C	-2.58	119.59	126.72
11	B	826	CLA	C1D-ND-C4D	-2.57	104.51	106.33
11	B	828	CLA	CHA-C1A-NA	-2.57	120.51	126.40
11	A	807	CLA	CHC-C1C-C2C	-2.57	119.62	126.72
11	B	835	CLA	CHC-C1C-C2C	-2.57	119.63	126.72
11	A	834	CLA	CHC-C1C-NC	2.56	128.09	124.20
11	A	812	CLA	CHC-C1C-NC	2.56	128.09	124.20
11	A	806	CLA	CHC-C1C-C2C	-2.56	119.64	126.72
11	A	840	CLA	CHC-C1C-NC	2.56	128.09	124.20
11	A	835	CLA	C1D-ND-C4D	-2.56	104.52	106.33
11	A	806	CLA	CHA-C1A-NA	-2.56	120.54	126.40
11	A	816	CLA	CHC-C1C-NC	2.55	128.08	124.20
11	B	808	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
11	B	801	CLA	CHC-C1C-NC	2.55	128.07	124.20
11	B	833	CLA	CHC-C1C-C2C	-2.55	119.67	126.72
11	A	842	CLA	C2C-C1C-NC	2.55	112.36	109.97
11	A	825	CLA	CHC-C1C-C2C	-2.55	119.68	126.72
11	A	832	CLA	C2C-C1C-NC	2.54	112.36	109.97
11	A	803	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
11	A	837	CLA	CHC-C1C-C2C	-2.54	119.69	126.72
11	A	816	CLA	C1D-ND-C4D	-2.54	104.53	106.33
11	B	825	CLA	C1D-ND-C4D	-2.54	104.53	106.33
11	B	819	CLA	CAA-C2A-C1A	-2.54	103.66	111.97
11	B	814	CLA	CHC-C1C-C2C	-2.54	119.70	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	839	CLA	CHA-C1A-NA	-2.54	120.59	126.40
11	B	826	CLA	CHC-C1C-C2C	-2.54	119.71	126.72
11	A	809	CLA	CHC-C1C-C2C	-2.53	119.71	126.72
11	B	833	CLA	CHC-C1C-NC	2.53	128.05	124.20
11	B	809	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
11	A	835	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
11	A	841	CLA	CHC-C1C-NC	2.53	128.04	124.20
11	B	834	CLA	CHC-C1C-NC	2.53	128.04	124.20
11	A	815	CLA	CHC-C1C-C2C	-2.53	119.72	126.72
11	B	830	CLA	C1D-ND-C4D	-2.53	104.54	106.33
11	A	827	CLA	C1D-ND-C4D	-2.52	104.54	106.33
11	A	831	CLA	C1D-ND-C4D	-2.52	104.54	106.33
11	A	835	CLA	C2C-C1C-NC	2.52	112.33	109.97
11	B	805	CLA	CHA-C1A-NA	-2.52	120.63	126.40
11	A	819	CLA	CHC-C1C-NC	2.52	128.02	124.20
11	A	836	CLA	C2C-C1C-NC	2.52	112.33	109.97
11	A	818	CLA	CHC-C1C-C2C	-2.52	119.76	126.72
11	L	1501	CLA	CHC-C1C-C2C	-2.51	119.77	126.72
11	B	813	CLA	CHC-C1C-NC	2.51	128.02	124.20
11	B	816	CLA	CHA-C1A-NA	-2.51	120.64	126.40
11	B	811	CLA	CHC-C1C-C2C	-2.51	119.78	126.72
11	L	1501	CLA	C1D-ND-C4D	-2.51	104.55	106.33
11	B	807	CLA	C1D-ND-C4D	-2.51	104.55	106.33
11	A	803	CLA	CHC-C1C-NC	2.51	128.01	124.20
11	B	827	CLA	C1D-ND-C4D	-2.51	104.56	106.33
13	F	201	BCR	C24-C25-C26	2.51	127.53	121.46
11	B	815	CLA	CHC-C1C-C2C	-2.50	119.81	126.72
11	B	806	CLA	CHC-C1C-NC	2.50	127.99	124.20
11	A	823	CLA	C1D-ND-C4D	-2.50	104.56	106.33
11	B	820	CLA	CHC-C1C-C2C	-2.50	119.82	126.72
11	A	805	CLA	CHA-C1A-NA	-2.49	120.69	126.40
11	A	839	CLA	CHC-C1C-NC	2.49	127.99	124.20
11	A	842	CLA	CHC-C1C-C2C	-2.49	119.83	126.72
11	A	833	CLA	C1D-ND-C4D	-2.49	104.56	106.33
11	A	841	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
11	B	835	CLA	CHC-C1C-NC	2.49	127.98	124.20
11	L	1503	CLA	CHC-C1C-NC	2.49	127.98	124.20
11	B	801	CLA	CHC-C1C-C2C	-2.49	119.84	126.72
11	B	832	CLA	CHA-C1A-NA	-2.49	120.70	126.40
11	B	836	CLA	CHC-C1C-C2C	-2.48	119.86	126.72
11	A	819	CLA	CHC-C1C-C2C	-2.48	119.87	126.72
11	A	826	CLA	CHC-C1C-NC	2.48	127.96	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	810	CLA	C2C-C1C-NC	2.48	112.29	109.97
11	B	822	CLA	CHA-C1A-NA	-2.47	120.73	126.40
11	B	802	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
11	A	834	CLA	C2C-C1C-NC	2.47	112.29	109.97
11	B	817	CLA	CHC-C1C-C2C	-2.47	119.88	126.72
11	A	822	CLA	CHC-C1C-NC	2.47	127.95	124.20
11	B	803	CLA	CHA-C1A-NA	-2.47	120.74	126.40
11	A	832	CLA	CHC-C1C-C2C	-2.47	119.89	126.72
11	A	825	CLA	C1D-ND-C4D	-2.47	104.58	106.33
11	B	814	CLA	CHC-C1C-NC	2.46	127.94	124.20
11	B	831	CLA	CHC-C1C-NC	2.46	127.94	124.20
11	A	803	CLA	C2C-C1C-NC	2.46	112.28	109.97
11	B	803	CLA	CHC-C1C-C2C	-2.46	119.93	126.72
11	B	813	CLA	CHC-C1C-C2C	-2.46	119.93	126.72
11	A	802	CLA	CHA-C1A-NA	-2.45	120.78	126.40
11	B	812	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
11	A	815	CLA	CHC-C1C-NC	2.45	127.92	124.20
11	A	817	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
11	A	811	CLA	C1D-ND-C4D	-2.45	104.59	106.33
11	A	821	CLA	CHC-C1C-C2C	-2.45	119.94	126.72
11	A	825	CLA	CHC-C1C-NC	2.44	127.91	124.20
11	A	833	CLA	CHC-C1C-C2C	-2.44	119.97	126.72
11	A	810	CLA	CHC-C1C-NC	2.44	127.91	124.20
11	B	829	CLA	CHC-C1C-NC	2.44	127.90	124.20
14	A	850	LHG	C20-C19-C18	-2.44	102.05	114.42
11	B	825	CLA	CHC-C1C-C2C	-2.44	119.98	126.72
11	A	810	CLA	C1D-ND-C4D	-2.44	104.61	106.33
11	A	823	CLA	CHC-C1C-C2C	-2.43	119.99	126.72
11	A	836	CLA	CHC-C1C-C2C	-2.43	119.99	126.72
11	A	827	CLA	CHC-C1C-NC	2.43	127.89	124.20
11	L	1503	CLA	CHC-C1C-C2C	-2.43	120.00	126.72
11	B	820	CLA	CHC-C1C-NC	2.43	127.89	124.20
11	B	812	CLA	C2C-C1C-NC	2.43	112.25	109.97
14	A	851	LHG	C11-C10-C9	-2.43	102.10	114.42
11	B	830	CLA	CHC-C1C-C2C	-2.43	120.01	126.72
11	A	809	CLA	C1D-ND-C4D	-2.43	104.61	106.33
11	B	817	CLA	CHC-C1C-NC	2.43	127.88	124.20
11	B	802	CLA	CHC-C1C-NC	2.43	127.88	124.20
11	A	822	CLA	CHC-C1C-C2C	-2.42	120.02	126.72
11	B	835	CLA	CHA-C1A-NA	-2.42	120.85	126.40
11	B	811	CLA	CHA-C1A-NA	-2.42	120.85	126.40
11	A	808	CLA	C1D-ND-C4D	-2.42	104.62	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	811	CLA	CHC-C1C-NC	2.42	127.87	124.20
11	A	813	CLA	CHC-C1C-NC	2.42	127.87	124.20
11	B	831	CLA	C1D-ND-C4D	-2.41	104.62	106.33
11	B	830	CLA	CHC-C1C-NC	2.41	127.86	124.20
11	A	837	CLA	CHA-C1A-NA	-2.41	120.88	126.40
11	B	826	CLA	CHA-C1A-NA	-2.41	120.89	126.40
11	B	819	CLA	CHC-C1C-C2C	-2.41	120.07	126.72
11	A	840	CLA	CHC-C1C-C2C	-2.40	120.07	126.72
11	B	831	CLA	CHA-C1A-NA	-2.40	120.89	126.40
13	A	852	BCR	C10-C11-C12	2.40	130.72	123.22
11	A	832	CLA	CHA-C1A-NA	-2.40	120.90	126.40
11	A	838	CLA	C1-C2-C3	-2.40	121.89	126.04
11	A	821	CLA	C2C-C1C-NC	2.40	112.22	109.97
11	B	822	CLA	CHC-C1C-C2C	-2.40	120.09	126.72
11	A	836	CLA	CAA-C2A-C1A	-2.40	104.12	111.97
16	B	843	LMG	C38-C37-C36	-2.40	102.26	114.42
11	A	816	CLA	C1-C2-C3	-2.40	122.88	126.75
11	B	803	CLA	CHC-C1C-NC	2.39	127.83	124.20
11	B	829	CLA	CHA-C1A-NA	-2.39	120.93	126.40
11	B	814	CLA	C2C-C1C-NC	2.39	112.21	109.97
11	B	808	CLA	CHA-C1A-NA	-2.39	120.93	126.40
11	B	806	CLA	CHC-C1C-C2C	-2.39	120.12	126.72
11	B	809	CLA	CHC-C1C-NC	2.39	127.82	124.20
11	A	815	CLA	C2C-C1C-NC	2.38	112.20	109.97
11	B	823	CLA	CHC-C1C-C2C	-2.38	120.13	126.72
11	A	859	CLA	CHA-C1A-NA	-2.38	120.94	126.40
11	B	810	CLA	CBA-CAA-C2A	2.38	120.89	113.86
11	A	804	CLA	CHC-C1C-NC	2.38	127.81	124.20
11	L	1501	CLA	C2A-C3A-C4A	-2.38	99.36	103.59
11	A	814	CLA	CHC-C1C-NC	2.38	127.81	124.20
11	B	813	CLA	C1D-ND-C4D	-2.38	104.65	106.33
11	A	801	CLA	CHC-C1C-C2C	-2.38	120.15	126.72
11	A	805	CLA	C1D-ND-C4D	-2.38	104.65	106.33
11	B	820	CLA	C2C-C1C-NC	2.38	112.20	109.97
11	B	805	CLA	CHC-C1C-C2C	-2.37	120.15	126.72
11	B	825	CLA	CHC-C1C-NC	2.37	127.80	124.20
11	A	820	CLA	CHC-C1C-NC	2.37	127.80	124.20
11	B	818	CLA	CHA-C1A-NA	-2.37	120.97	126.40
11	L	1502	CLA	CHA-C1A-NA	-2.37	120.97	126.40
11	B	819	CLA	C2C-C1C-NC	2.37	112.19	109.97
11	A	821	CLA	CHC-C1C-NC	2.37	127.80	124.20
11	A	829	CLA	CHA-C1A-NA	-2.37	120.98	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	830	CLA	CHA-C1A-NA	-2.36	120.98	126.40
11	B	803	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
11	B	823	CLA	CHC-C1C-NC	2.36	127.79	124.20
13	A	855	BCR	C8-C7-C6	2.36	129.53	125.51
11	A	828	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
11	A	842	CLA	CHC-C1C-NC	2.36	127.78	124.20
11	B	836	CLA	CHA-C1A-NA	-2.36	121.00	126.40
11	B	832	CLA	CHC-C1C-NC	2.36	127.78	124.20
11	A	823	CLA	CHC-C1C-NC	2.36	127.78	124.20
11	A	842	CLA	CBD-CHA-C1A	2.36	131.28	128.50
11	A	829	CLA	C1-C2-C3	-2.35	121.97	126.04
11	A	826	CLA	CHC-C1C-C2C	-2.35	120.21	126.72
11	B	829	CLA	CHC-C1C-C2C	-2.35	120.22	126.72
11	A	814	CLA	CHC-C1C-C2C	-2.35	120.22	126.72
11	A	860	CLA	CHC-C1C-NC	2.35	127.77	124.20
11	B	801	CLA	CMB-C2B-C1B	-2.35	124.86	128.46
11	B	810	CLA	CHC-C1C-C2C	-2.35	120.23	126.72
11	A	804	CLA	CHC-C1C-C2C	-2.35	120.23	126.72
11	A	839	CLA	C1D-ND-C4D	-2.35	104.67	106.33
11	A	837	CLA	CHC-C1C-NC	2.34	127.76	124.20
11	B	808	CLA	C1D-ND-C4D	-2.34	104.67	106.33
11	A	811	CLA	CHC-C1C-C2C	-2.34	120.24	126.72
11	L	1501	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
11	A	801	CLA	C2C-C1C-NC	2.34	112.17	109.97
11	A	808	CLA	CHC-C1C-NC	2.34	127.75	124.20
11	A	803	CLA	CAA-C2A-C1A	-2.34	106.96	112.14
11	A	830	CLA	CHC-C1C-C2C	-2.34	120.25	126.72
11	B	822	CLA	C1D-ND-C4D	-2.34	104.67	106.33
11	A	817	CLA	CHA-C1A-NA	-2.34	121.05	126.40
11	B	811	CLA	CHC-C1C-NC	2.33	127.74	124.20
11	B	802	CLA	C1-C2-C3	-2.33	122.01	126.04
11	B	834	CLA	CHA-C1A-NA	-2.33	121.06	126.40
11	B	822	CLA	C2C-C1C-NC	2.32	112.15	109.97
11	A	835	CLA	CHC-C1C-NC	2.32	127.73	124.20
13	A	852	BCR	C23-C24-C25	2.32	133.73	127.20
11	A	823	CLA	C2C-C1C-NC	2.32	112.15	109.97
11	A	833	CLA	CHC-C1C-NC	2.32	127.72	124.20
11	A	812	CLA	C2C-C1C-NC	2.32	112.14	109.97
11	L	1502	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
11	B	821	CLA	C1D-ND-C4D	-2.32	104.69	106.33
11	A	831	CLA	CHC-C1C-NC	2.32	127.72	124.20
11	B	822	CLA	C1B-CHB-C4A	-2.32	125.53	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	807	CLA	CHC-C1C-C2C	-2.32	120.32	126.72
11	B	802	CLA	C2C-C1C-NC	2.31	112.14	109.97
11	L	1501	CLA	C2A-C1A-CHA	2.31	126.30	122.71
11	B	803	CLA	C2C-C1C-NC	2.31	112.14	109.97
14	A	850	LHG	C11-C10-C9	-2.31	102.70	114.42
11	L	1502	CLA	C2A-C1A-CHA	2.31	127.90	123.86
11	A	807	CLA	CHA-C1A-NA	-2.31	121.11	126.40
11	A	824	CLA	CHA-C1A-NA	-2.31	121.12	126.40
11	B	825	CLA	CHA-C1A-NA	-2.31	121.12	126.40
11	A	824	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
11	B	814	CLA	CHA-C1A-NA	-2.30	121.13	126.40
11	A	819	CLA	C1D-ND-C4D	-2.30	104.70	106.33
11	A	821	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
11	B	827	CLA	CAA-C2A-C1A	-2.30	106.13	111.81
11	A	808	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
11	A	805	CLA	CHC-C1C-C2C	-2.30	120.36	126.72
16	B	843	LMG	C40-C39-C38	-2.30	102.76	114.42
11	B	812	CLA	CHC-C1C-NC	2.30	127.69	124.20
11	B	818	CLA	CHC-C1C-NC	2.30	127.69	124.20
11	A	801	CLA	CHA-C1A-NA	-2.29	121.14	126.40
11	A	842	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
11	A	860	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
11	B	824	CLA	CHC-C1C-C2C	-2.29	120.38	126.72
11	A	832	CLA	CHC-C1C-NC	2.29	127.68	124.20
11	B	805	CLA	C2C-C1C-NC	2.29	112.12	109.97
11	B	813	CLA	CAA-C2A-C1A	-2.29	104.47	111.97
11	A	806	CLA	CHC-C1C-NC	2.29	127.68	124.20
11	B	819	CLA	CHC-C1C-NC	2.29	127.67	124.20
11	A	833	CLA	C2C-C1C-NC	2.29	112.11	109.97
11	B	824	CLA	CHC-C1C-NC	2.29	127.67	124.20
11	A	802	CLA	C2C-C1C-NC	2.29	112.11	109.97
11	B	818	CLA	CHC-C1C-C2C	-2.28	120.41	126.72
11	A	830	CLA	CHA-C1A-NA	-2.28	121.18	126.40
11	B	811	CLA	C1-C2-C3	-2.27	122.11	126.04
16	B	843	LMG	O2-C2-C1	-2.27	104.53	110.05
11	B	807	CLA	CHC-C1C-NC	2.27	127.65	124.20
11	B	835	CLA	C2C-C1C-NC	2.27	112.10	109.97
11	B	812	CLA	CHA-C1A-NA	-2.27	121.20	126.40
11	B	821	CLA	CHA-C1A-NA	-2.27	121.20	126.40
11	A	814	CLA	CHA-C1A-NA	-2.27	121.21	126.40
11	A	836	CLA	CHC-C1C-NC	2.27	127.64	124.20
11	A	842	CLA	CHA-C1A-NA	-2.27	121.32	126.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	822	CLA	CHA-C1A-NA	-2.26	121.21	126.40
11	A	824	CLA	CHC-C1C-NC	2.26	127.64	124.20
11	A	818	CLA	C1-C2-C3	-2.26	122.13	126.04
11	A	830	CLA	CHC-C1C-NC	2.26	127.63	124.20
11	A	860	CLA	CMB-C2B-C1B	-2.26	124.99	128.46
11	L	1502	CLA	CHC-C1C-NC	2.26	127.63	124.20
11	B	823	CLA	C1D-ND-C4D	-2.26	104.73	106.33
11	A	833	CLA	CHA-C1A-NA	-2.26	121.23	126.40
11	B	832	CLA	C1-C2-C3	-2.26	123.10	126.75
11	A	838	CLA	CHC-C1C-C2C	-2.25	120.48	126.72
11	A	860	CLA	C1D-ND-C4D	-2.25	104.73	106.33
11	A	811	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
11	B	821	CLA	CHC-C1C-C2C	-2.24	120.51	126.72
11	B	807	CLA	CHA-C1A-NA	-2.24	121.26	126.40
11	L	1501	CLA	CHA-C1A-NA	-2.24	121.36	126.41
11	A	829	CLA	CHC-C1C-NC	2.24	127.61	124.20
11	A	805	CLA	CHC-C1C-NC	2.24	127.60	124.20
11	B	816	CLA	CHC-C1C-C2C	-2.24	120.53	126.72
11	A	823	CLA	CHA-C1A-NA	-2.24	121.28	126.40
11	A	811	CLA	CHA-C1A-NA	-2.24	121.28	126.40
11	A	835	CLA	CHA-C1A-NA	-2.23	121.28	126.40
11	B	823	CLA	CHA-C1A-NA	-2.23	121.29	126.40
14	A	850	LHG	C18-C17-C16	-2.23	103.11	114.42
11	A	821	CLA	C1D-ND-C4D	-2.23	104.75	106.33
11	A	802	CLA	CHC-C1C-C2C	-2.23	120.57	126.72
11	A	805	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
11	A	834	CLA	C1-C2-C3	-2.22	122.20	126.04
11	A	830	CLA	C1D-ND-C4D	-2.22	104.76	106.33
11	B	822	CLA	CHC-C1C-NC	2.22	127.57	124.20
11	B	824	CLA	C1D-ND-C4D	-2.22	104.76	106.33
11	B	808	CLA	CHC-C1C-NC	2.22	127.56	124.20
11	L	1503	CLA	CHA-C1A-NA	-2.22	121.32	126.40
11	A	829	CLA	CHC-C1C-C2C	-2.21	120.60	126.72
11	B	817	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
11	B	810	CLA	CHC-C1C-NC	2.21	127.55	124.20
11	A	833	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
11	A	859	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
11	B	824	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
11	A	805	CLA	C2C-C1C-NC	2.20	112.03	109.97
11	A	834	CLA	CHA-C1A-NA	-2.20	121.36	126.40
11	A	819	CLA	C2C-C1C-NC	2.20	112.03	109.97
13	A	858	BCR	C23-C24-C25	2.20	133.38	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	860	CLA	CHA-C1A-NA	-2.20	121.36	126.40
11	A	825	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
11	B	817	CLA	C2C-C1C-NC	2.20	112.03	109.97
11	A	802	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
11	A	841	CLA	CHA-C1A-NA	-2.19	121.38	126.40
11	B	826	CLA	CHC-C1C-NC	2.19	127.53	124.20
11	B	817	CLA	CAA-C2A-C1A	-2.19	104.79	111.97
11	B	807	CLA	C2C-C1C-NC	2.19	112.02	109.97
11	B	817	CLA	CHA-C1A-NA	-2.19	121.39	126.40
11	B	821	CLA	CHC-C1C-NC	2.19	127.52	124.20
11	A	801	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
11	A	810	CLA	CHA-C1A-NA	-2.19	121.39	126.40
11	A	828	CLA	CHA-C1A-NA	-2.19	121.39	126.40
11	A	818	CLA	CHA-C1A-NA	-2.18	121.40	126.40
11	A	818	CLA	CHC-C1C-NC	2.18	127.52	124.20
11	A	838	CLA	CHC-C1C-NC	2.18	127.51	124.20
11	B	830	CLA	C2C-C1C-NC	2.18	112.02	109.97
11	B	836	CLA	CHC-C1C-NC	2.18	127.51	124.20
11	B	801	CLA	C2C-C1C-NC	2.18	112.01	109.97
11	B	820	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
11	A	806	CLA	C1-C2-C3	-2.17	122.28	126.04
11	A	827	CLA	CHA-C1A-NA	-2.17	121.42	126.40
11	B	833	CLA	C2C-C1C-NC	2.17	112.01	109.97
11	L	1502	CLA	CHC-C1C-C2C	-2.17	120.72	126.72
11	A	819	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
11	B	825	CLA	C2C-C1C-NC	2.17	112.00	109.97
11	A	801	CLA	CHC-C1C-NC	2.16	127.48	124.20
11	A	828	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
11	L	1501	CLA	CBD-CHA-C1A	2.16	130.34	128.06
13	B	844	BCR	C24-C25-C26	2.15	126.68	121.46
11	A	842	CLA	C1D-ND-C4D	-2.15	104.81	106.33
11	A	823	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
11	B	815	CLA	CHC-C1C-NC	2.15	127.47	124.20
11	B	836	CLA	C1D-ND-C4D	-2.15	104.81	106.33
11	B	805	CLA	CHC-C1C-NC	2.15	127.47	124.20
11	A	819	CLA	CHA-C1A-NA	-2.15	121.47	126.40
11	A	859	CLA	CHC-C1C-C2C	-2.15	120.78	126.72
11	A	807	CLA	C2C-C1C-NC	2.15	111.98	109.97
16	B	843	LMG	O3-C3-C2	-2.15	105.38	110.35
11	A	821	CLA	CHA-C1A-NA	-2.15	121.48	126.40
11	B	815	CLA	C1-C2-C3	-2.14	122.33	126.04
13	B	838	BCR	C23-C24-C25	2.14	133.22	127.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	806	CLA	CHA-C1A-NA	-2.14	121.49	126.40
11	A	811	CLA	C2A-C1A-CHA	2.14	127.60	123.86
11	A	820	CLA	CHA-C1A-NA	-2.14	121.49	126.40
11	L	1503	CLA	C2C-C1C-NC	2.14	111.98	109.97
13	F	201	BCR	C30-C25-C24	-2.14	109.73	115.78
13	F	201	BCR	C20-C19-C18	2.14	132.42	126.42
11	A	838	CLA	C2C-C1C-NC	2.14	111.97	109.97
11	B	829	CLA	CMB-C2B-C1B	-2.14	125.18	128.46
11	B	816	CLA	CHC-C1C-NC	2.14	127.44	124.20
11	A	822	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
11	B	823	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
11	A	824	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
11	A	819	CLA	C1B-CHB-C4A	-2.13	125.90	130.12
11	B	810	CLA	C2C-C1C-NC	2.13	111.97	109.97
11	A	801	CLA	C1D-ND-C4D	-2.13	104.82	106.33
11	L	1503	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
11	B	823	CLA	C2C-C1C-NC	2.13	111.96	109.97
11	B	819	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
11	A	827	CLA	C1-C2-C3	-2.12	122.37	126.04
11	B	803	CLA	C1-C2-C3	-2.12	122.37	126.04
11	B	806	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
11	A	813	CLA	C1D-ND-C4D	-2.12	104.83	106.33
11	A	815	CLA	CHA-C1A-NA	-2.12	121.54	126.40
11	B	811	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
11	B	802	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
11	B	816	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
11	A	842	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
11	B	827	CLA	CHA-C1A-NA	-2.11	121.56	126.40
11	A	808	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
11	A	809	CLA	C2C-C1C-NC	2.11	111.95	109.97
11	A	816	CLA	CAA-C2A-C3A	-2.11	107.01	112.78
11	B	803	CLA	C1D-ND-C4D	-2.10	104.84	106.33
11	B	815	CLA	CHA-C1A-NA	-2.10	121.58	126.40
11	L	1502	CLA	C1-C2-C3	-2.10	122.42	126.04
11	A	814	CLA	C2C-C1C-NC	2.10	111.94	109.97
11	B	805	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
11	A	822	CLA	C2C-C1C-NC	2.10	111.94	109.97
11	A	830	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
16	B	843	LMG	C42-C41-C40	-2.09	103.81	114.42
11	A	814	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
13	A	849	BCR	C23-C24-C25	2.09	133.07	127.20
16	B	843	LMG	O1-C1-C2	-2.09	105.04	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	201	BCR	C19-C18-C17	-2.09	115.74	118.94
11	A	838	CLA	CMB-C2B-C1B	-2.08	125.26	128.46
11	B	809	CLA	CHA-C1A-NA	-2.08	121.63	126.40
11	B	807	CLA	CMB-C2B-C1B	-2.08	125.26	128.46
11	B	814	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
11	B	814	CLA	CAA-C2A-C1A	-2.08	105.16	111.97
11	B	803	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
11	A	821	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
11	B	825	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
11	A	817	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
11	A	809	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
11	B	831	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
11	A	828	CLA	CHC-C1C-NC	2.07	127.34	124.20
11	B	801	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
11	A	826	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
11	B	807	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
11	A	825	CLA	C1-C2-C3	-2.07	122.47	126.04
11	B	821	CLA	C2C-C1C-NC	2.07	111.91	109.97
11	B	810	CLA	C1B-CHB-C4A	-2.07	126.03	130.12
11	A	835	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
11	A	808	CLA	C1-C2-C3	-2.06	122.48	126.04
11	A	804	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
11	A	836	CLA	C1B-CHB-C4A	-2.06	126.03	130.12
11	A	807	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
11	A	818	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
11	B	813	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
11	B	820	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
11	B	830	CLA	C1B-CHB-C4A	-2.06	126.04	130.12
11	B	818	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
11	A	841	CLA	C2C-C1C-NC	2.06	111.90	109.97
11	B	824	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
11	A	812	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
11	A	837	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
11	B	805	CLA	C1-C2-C3	-2.05	122.50	126.04
11	A	804	CLA	C2C-C1C-NC	2.05	111.89	109.97
11	A	802	CLA	CHC-C1C-NC	2.05	127.31	124.20
11	L	1502	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
11	A	832	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
11	B	819	CLA	C1-C2-C3	-2.04	122.51	126.04
11	B	832	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
11	A	859	CLA	C1D-ND-C4D	-2.04	104.89	106.33
11	A	808	CLA	CHA-C1A-NA	-2.04	121.73	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	836	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
11	B	831	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
11	A	826	CLA	C1-C2-C3	-2.04	122.52	126.04
11	A	859	CLA	C2C-C1C-NC	2.04	111.88	109.97
11	A	805	CLA	CMB-C2B-C1B	-2.04	125.33	128.46
11	B	821	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
11	A	824	CLA	C2C-C1C-NC	2.03	111.88	109.97
14	A	850	LHG	C27-C26-C25	-2.03	104.10	114.42
11	A	829	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
11	A	838	CLA	CHA-C1A-NA	-2.03	121.74	126.40
11	A	840	CLA	CMB-C2B-C1B	-2.03	125.34	128.46
11	A	828	CLA	CHC-C1C-C2C	-2.03	121.11	126.72
11	A	830	CLA	C2C-C1C-NC	2.03	111.87	109.97
11	B	824	CLA	C2C-C1C-NC	2.03	111.87	109.97
11	A	827	CLA	CMB-C2B-C1B	-2.03	125.35	128.46
11	B	830	CLA	CAA-C2A-C1A	-2.03	106.81	111.81
11	B	829	CLA	C2C-C1C-NC	2.02	111.87	109.97
11	B	835	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
11	A	813	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
11	A	811	CLA	C1-C2-C3	-2.02	122.55	126.04
11	B	811	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
11	B	801	CLA	C1-C2-C3	-2.02	122.55	126.04
11	A	859	CLA	CMB-C2B-C1B	-2.02	125.36	128.46
11	B	810	CLA	C1-C2-C3	-2.01	122.56	126.04
11	B	816	CLA	C2C-C1C-NC	2.01	111.86	109.97
11	B	824	CLA	C2A-C1A-CHA	2.01	127.38	123.86
11	B	816	CLA	O2A-C1-C2	-2.01	103.34	108.64
11	A	802	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
11	A	842	CLA	C2A-C1A-CHA	2.01	125.83	122.71
11	B	810	CLA	C1D-ND-C4D	-2.01	104.91	106.33
11	B	833	CLA	C1B-CHB-C4A	-2.01	126.13	130.12
11	B	819	CLA	CHA-C1A-NA	-2.01	121.79	126.40
11	A	816	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
13	A	856	BCR	C2-C1-C6	2.01	113.57	110.48
11	B	817	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
11	A	803	CLA	CHA-C1A-NA	-2.01	121.81	126.40
11	B	814	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
11	A	839	CLA	CMB-C2B-C1B	-2.00	125.39	128.46

All (82) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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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
11	A	838	CLA	ND
11	A	839	CLA	ND
11	A	840	CLA	ND
11	A	841	CLA	ND

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

All (522) 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	816	CLA	C1A-C2A-CAA-CBA
11	A	818	CLA	C2-C3-C5-C6
11	A	819	CLA	C3A-C2A-CAA-CBA
11	A	819	CLA	CHA-CBD-CGD-O1D
11	A	819	CLA	CHA-CBD-CGD-O2D
11	A	823	CLA	CHA-CBD-CGD-O1D
11	A	823	CLA	CHA-CBD-CGD-O2D
11	A	824	CLA	C1A-C2A-CAA-CBA
11	A	824	CLA	CHA-CBD-CGD-O1D
11	A	824	CLA	CHA-CBD-CGD-O2D
11	A	830	CLA	CHA-CBD-CGD-O1D
11	A	830	CLA	CHA-CBD-CGD-O2D
11	A	834	CLA	CHA-CBD-CGD-O1D
11	A	834	CLA	CHA-CBD-CGD-O2D
11	A	836	CLA	CHA-CBD-CGD-O1D
11	A	836	CLA	CHA-CBD-CGD-O2D
11	A	841	CLA	C1-C2-C3-C4
11	A	842	CLA	CHA-CBD-CGD-O1D
11	A	842	CLA	CHA-CBD-CGD-O2D
11	B	802	CLA	CHA-CBD-CGD-O1D
11	B	802	CLA	CHA-CBD-CGD-O2D
11	B	803	CLA	C1A-C2A-CAA-CBA
11	B	807	CLA	CHA-CBD-CGD-O1D
11	B	807	CLA	CHA-CBD-CGD-O2D
11	B	807	CLA	CAD-CBD-CGD-O1D
11	B	810	CLA	CHA-CBD-CGD-O1D
11	B	810	CLA	CHA-CBD-CGD-O2D
11	B	817	CLA	C1A-C2A-CAA-CBA
11	B	822	CLA	C1A-C2A-CAA-CBA
11	B	822	CLA	CHA-CBD-CGD-O2D
11	B	824	CLA	C2A-CAA-CBA-CGA
11	B	825	CLA	CHA-CBD-CGD-O2D
11	B	830	CLA	CHA-CBD-CGD-O1D
11	B	830	CLA	CHA-CBD-CGD-O2D
11	B	836	CLA	C1A-C2A-CAA-CBA
11	B	836	CLA	CAD-CBD-CGD-O1D
11	B	836	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	A	843	PQN	C12-C13-C15-C16
12	A	843	PQN	C14-C13-C15-C16
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
13	B	842	BCR	C1-C6-C7-C8
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	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
11	A	818	CLA	C2A-CAA-CBA-CGA
11	A	829	CLA	C2A-CAA-CBA-CGA
11	B	835	CLA	C2A-CAA-CBA-CGA
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	A	825	CLA	C13-C15-C16-C17
11	B	810	CLA	C3-C5-C6-C7
11	B	803	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
11	B	831	CLA	C2A-CAA-CBA-CGA
14	A	851	LHG	C1-C2-C3-O3
11	A	806	CLA	C13-C15-C16-C17
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
12	A	843	PQN	C15-C16-C17-C18
11	B	823	CLA	C2A-CAA-CBA-CGA
13	A	856	BCR	C11-C12-C13-C35
13	A	856	BCR	C11-C12-C13-C14
11	B	818	CLA	C5-C6-C7-C8
11	A	859	CLA	C3-C5-C6-C7
11	A	813	CLA	C10-C11-C12-C13
11	A	824	CLA	C13-C15-C16-C17
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	807	CLA	C11-C10-C8-C7
11	A	828	CLA	C2A-CAA-CBA-CGA
11	B	806	CLA	C2A-CAA-CBA-CGA
16	B	843	LMG	O6-C1-O1-C7
11	B	825	CLA	C8-C10-C11-C12
11	B	805	CLA	C13-C15-C16-C17
16	B	843	LMG	O6-C5-C6-O5
11	A	811	CLA	C15-C16-C17-C18
11	A	827	CLA	C13-C15-C16-C17
14	A	850	LHG	C3-O3-P-O6
14	A	851	LHG	C4-O6-P-O3
11	B	807	CLA	C13-C15-C16-C17
14	A	850	LHG	O9-C7-O7-C5
11	B	820	CLA	C4-C3-C5-C6
11	A	860	CLA	C2A-CAA-CBA-CGA
11	B	835	CLA	C13-C15-C16-C17
13	F	201	BCR	C35-C13-C14-C15
14	A	850	LHG	C31-C32-C33-C34
16	B	843	LMG	C29-C30-C31-C32
11	A	828	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
16	B	843	LMG	C40-C41-C42-C43
14	A	850	LHG	C24-C25-C26-C27
16	B	843	LMG	C16-C17-C18-C19
14	A	850	LHG	C27-C28-C29-C30
16	B	843	LMG	C41-C42-C43-C44
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
16	B	843	LMG	C2-C1-O1-C7
16	B	843	LMG	C37-C38-C39-C40
11	A	819	CLA	C16-C17-C18-C20
11	A	834	CLA	C4-C3-C5-C6
11	B	833	CLA	C4-C3-C5-C6
11	B	820	CLA	C2-C3-C5-C6
11	B	807	CLA	C14-C13-C15-C16
11	B	828	CLA	C11-C12-C13-C14
16	B	843	LMG	C32-C33-C34-C35
11	A	817	CLA	C2A-CAA-CBA-CGA
11	A	859	CLA	C2A-CAA-CBA-CGA
16	B	843	LMG	C34-C35-C36-C37
14	A	850	LHG	O1-C1-C2-C3
14	A	851	LHG	O1-C1-C2-C3
11	B	803	CLA	C3-C5-C6-C7
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
13	A	856	BCR	C20-C21-C22-C23
11	A	828	CLA	C16-C17-C18-C19
14	A	851	LHG	C4-C5-C6-O8
11	B	828	CLA	O2A-C1-C2-C3
11	A	825	CLA	C4-C3-C5-C6
11	A	825	CLA	C2-C3-C5-C6
11	B	833	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	852	BCR	C5-C6-C7-C8
14	A	851	LHG	C7-C8-C9-C10
13	A	848	BCR	C1-C6-C7-C8
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	A	861	BCR	C23-C24-C25-C26
13	A	861	BCR	C23-C24-C25-C30
13	B	839	BCR	C1-C6-C7-C8
13	B	839	BCR	C5-C6-C7-C8
13	B	842	BCR	C5-C6-C7-C8
13	F	201	BCR	C1-C6-C7-C8
13	I	102	BCR	C23-C24-C25-C26
13	I	102	BCR	C23-C24-C25-C30
13	L	1504	BCR	C23-C24-C25-C26
12	B	837	PQN	C15-C16-C17-C18
16	B	843	LMG	C33-C34-C35-C36
11	B	816	CLA	C4-C3-C5-C6
11	A	825	CLA	C11-C12-C13-C15
11	A	827	CLA	C2-C3-C5-C6
11	B	807	CLA	C12-C13-C15-C16
11	B	815	CLA	C2-C3-C5-C6
11	B	816	CLA	C2-C3-C5-C6
12	B	837	PQN	C17-C18-C20-C21
12	A	843	PQN	C20-C21-C22-C23
11	A	841	CLA	C2A-CAA-CBA-CGA
11	B	820	CLA	C2A-CAA-CBA-CGA
16	B	843	LMG	C23-C24-C25-C26
14	A	850	LHG	C8-C7-O7-C5
13	A	856	BCR	C10-C11-C12-C13
13	A	849	BCR	C14-C15-C16-C17
11	A	817	CLA	C3-C5-C6-C7
11	A	819	CLA	C16-C17-C18-C19
11	A	827	CLA	C4-C3-C5-C6
11	B	815	CLA	C4-C3-C5-C6
11	A	829	CLA	C14-C13-C15-C16
11	B	807	CLA	C11-C10-C8-C9
12	A	843	PQN	C24-C23-C25-C26
16	B	843	LMG	C31-C32-C33-C34
11	A	802	CLA	C2A-CAA-CBA-CGA
11	A	805	CLA	C1A-C2A-CAA-CBA
11	A	817	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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
11	A	811	CLA	C4-C3-C5-C6
11	B	803	CLA	C4-C3-C5-C6
14	A	851	LHG	O1-C1-C2-O2
12	B	837	PQN	C11-C12-C13-C14
13	A	856	BCR	C35-C13-C14-C15
11	A	811	CLA	C2-C3-C5-C6
11	A	834	CLA	C2-C3-C5-C6
12	A	843	PQN	C12-C11-C3-C4
11	A	815	CLA	C2A-CAA-CBA-CGA
14	A	850	LHG	C29-C30-C31-C32
14	A	850	LHG	O6-C4-C5-O7
14	A	850	LHG	O7-C5-C6-O8
11	A	805	CLA	C11-C12-C13-C15
11	A	813	CLA	C12-C13-C15-C16
11	A	829	CLA	C12-C13-C15-C16
12	A	843	PQN	C16-C17-C18-C20
12	A	843	PQN	C22-C23-C25-C26
12	B	837	PQN	C16-C17-C18-C20
11	A	805	CLA	C11-C12-C13-C14
11	A	811	CLA	C11-C12-C13-C14
11	A	813	CLA	C11-C10-C8-C9
11	A	813	CLA	C14-C13-C15-C16
11	A	824	CLA	C11-C10-C8-C9
11	A	834	CLA	C14-C13-C15-C16
12	B	837	PQN	C19-C18-C20-C21
16	B	843	LMG	C19-C20-C21-C22
11	B	810	CLA	C4-C3-C5-C6
11	B	819	CLA	C4-C3-C5-C6
11	A	806	CLA	C3A-C2A-CAA-CBA
11	A	813	CLA	C3A-C2A-CAA-CBA
11	A	824	CLA	C3A-C2A-CAA-CBA
16	B	843	LMG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
11	A	808	CLA	C4-C3-C5-C6
11	B	803	CLA	C2-C3-C5-C6
11	B	810	CLA	C2-C3-C5-C6
11	A	808	CLA	C2A-CAA-CBA-CGA
11	A	825	CLA	C16-C17-C18-C20
11	B	828	CLA	C10-C11-C12-C13
14	A	850	LHG	C32-C33-C34-C35
11	A	806	CLA	C2-C1-O2A-CGA
11	A	860	CLA	C2-C1-O2A-CGA
11	B	823	CLA	C2-C1-O2A-CGA
11	A	825	CLA	C14-C13-C15-C16
11	A	827	CLA	C14-C13-C15-C16
11	B	815	CLA	C6-C7-C8-C9
13	A	847	BCR	C5-C6-C7-C8
13	A	848	BCR	C5-C6-C7-C8
13	B	841	BCR	C23-C24-C25-C26
13	B	841	BCR	C23-C24-C25-C30
11	A	811	CLA	C11-C12-C13-C15
11	A	813	CLA	C11-C12-C13-C15
11	A	819	CLA	C6-C7-C8-C10
11	A	824	CLA	C11-C10-C8-C7
11	A	825	CLA	C12-C13-C15-C16
11	A	827	CLA	C11-C10-C8-C7
11	A	827	CLA	C12-C13-C15-C16
11	A	834	CLA	C12-C13-C15-C16
13	A	852	BCR	C35-C13-C14-C15
11	A	812	CLA	CAD-CBD-CGD-O2D
11	A	817	CLA	CAD-CBD-CGD-O2D
11	B	812	CLA	CAD-CBD-CGD-O2D
11	B	820	CLA	CAD-CBD-CGD-O2D
11	B	826	CLA	CAD-CBD-CGD-O2D
11	B	834	CLA	CAD-CBD-CGD-O2D
11	A	821	CLA	C4-C3-C5-C6
11	B	811	CLA	C16-C17-C18-C19
11	A	859	CLA	C2-C3-C5-C6
14	A	850	LHG	C11-C10-C9-C8
11	A	805	CLA	CHA-CBD-CGD-O1D
11	A	805	CLA	CHA-CBD-CGD-O2D
11	A	811	CLA	CHA-CBD-CGD-O1D
11	A	815	CLA	CHA-CBD-CGD-O1D
11	A	815	CLA	CHA-CBD-CGD-O2D
11	A	837	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	A	839	CLA	CHA-CBD-CGD-O1D
11	A	839	CLA	CHA-CBD-CGD-O2D
11	B	825	CLA	CHA-CBD-CGD-O1D
11	L	1502	CLA	CHA-CBD-CGD-O1D
11	L	1502	CLA	CHA-CBD-CGD-O2D
11	A	813	CLA	C3-C5-C6-C7
11	A	801	CLA	C3-C5-C6-C7
11	A	859	CLA	C4-C3-C5-C6
11	B	809	CLA	C4-C3-C5-C6
11	A	813	CLA	C11-C12-C13-C14
11	A	805	CLA	C2A-CAA-CBA-CGA
13	A	849	BCR	C11-C12-C13-C14
16	B	843	LMG	C4-C5-C6-O5
11	A	813	CLA	C1A-C2A-CAA-CBA
11	A	818	CLA	C1A-C2A-CAA-CBA
16	B	843	LMG	C18-C19-C20-C21
13	A	855	BCR	C1-C6-C7-C8
14	A	851	LHG	C3-O3-P-O5
14	A	851	LHG	C4-O6-P-O4
11	A	822	CLA	O2A-C1-C2-C3
11	A	819	CLA	CBA-CGA-O2A-C1
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	A	832	CLA	C2-C3-C5-C6
11	B	830	CLA	CAD-CBD-CGD-O1D
11	B	802	CLA	C3-C5-C6-C7
11	A	806	CLA	C11-C12-C13-C15
11	A	826	CLA	C11-C10-C8-C7
11	B	805	CLA	C12-C13-C15-C16
11	B	815	CLA	C6-C7-C8-C10
12	A	843	PQN	C17-C18-C20-C21
12	B	837	PQN	C22-C23-C25-C26
14	A	851	LHG	O7-C5-C6-O8
12	A	843	PQN	C12-C11-C3-C2
11	A	805	CLA	C11-C10-C8-C9
11	A	819	CLA	C6-C7-C8-C9
11	A	827	CLA	C11-C10-C8-C9
11	A	830	CLA	C6-C7-C8-C9
11	A	833	CLA	C14-C13-C15-C16
11	B	811	CLA	C16-C17-C18-C20
13	B	840	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
11	A	821	CLA	C2-C3-C5-C6
11	A	822	CLA	C1-C2-C3-C4
11	A	831	CLA	C1-C2-C3-C4
16	B	843	LMG	C42-C43-C44-C45
14	A	850	LHG	O6-C4-C5-C6
11	A	819	CLA	C2A-CAA-CBA-CGA
11	A	807	CLA	C2-C1-O2A-CGA
11	A	813	CLA	C2-C1-O2A-CGA
11	A	817	CLA	C2-C1-O2A-CGA
11	A	819	CLA	C2-C1-O2A-CGA
11	A	841	CLA	C2-C1-O2A-CGA
11	B	801	CLA	C2-C1-O2A-CGA
13	A	852	BCR	C14-C15-C16-C17
13	A	847	BCR	C1-C6-C7-C8
13	B	840	BCR	C23-C24-C25-C30
13	B	842	BCR	C23-C24-C25-C30
14	A	850	LHG	C35-C36-C37-C38
14	A	850	LHG	C4-C5-C6-O8
11	B	823	CLA	C4-C3-C5-C6
11	B	809	CLA	C2-C3-C5-C6
11	B	828	CLA	C11-C12-C13-C15
11	A	827	CLA	C8-C10-C11-C12
13	L	1504	BCR	C21-C22-C23-C24
16	B	843	LMG	C11-C12-C13-C14
11	A	808	CLA	C2-C3-C5-C6
11	A	819	CLA	O1A-CGA-O2A-C1
12	A	843	PQN	C26-C27-C28-C29
11	B	819	CLA	C2-C3-C5-C6
11	A	837	CLA	C2-C1-O2A-CGA
11	B	802	CLA	C2A-CAA-CBA-CGA
11	B	822	CLA	C3A-C2A-CAA-CBA
11	B	836	CLA	C3A-C2A-CAA-CBA
11	A	804	CLA	C6-C7-C8-C9
11	A	828	CLA	C11-C12-C13-C14
11	B	811	CLA	C11-C10-C8-C9
16	B	843	LMG	C30-C31-C32-C33
11	A	825	CLA	C8-C10-C11-C12
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	812	CLA	C1A-C2A-CAA-CBA
11	B	823	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
11	B	809	CLA	C2A-CAA-CBA-CGA
11	B	815	CLA	C2A-CAA-CBA-CGA
11	A	841	CLA	O2A-C1-C2-C3
11	A	825	CLA	C16-C17-C18-C19
11	B	823	CLA	C2-C3-C5-C6
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
14	A	850	LHG	C10-C11-C12-C13
11	A	836	CLA	CAA-CBA-CGA-O2A
11	A	817	CLA	C4-C3-C5-C6
11	A	811	CLA	C2-C1-O2A-CGA
11	A	821	CLA	C2-C1-O2A-CGA
11	A	834	CLA	C2-C1-O2A-CGA
11	A	834	CLA	C5-C6-C7-C8
11	A	836	CLA	CAA-CBA-CGA-O1A
11	A	832	CLA	C4-C3-C5-C6
11	A	826	CLA	C2A-CAA-CBA-CGA
13	A	847	BCR	C23-C24-C25-C30
13	A	849	BCR	C1-C6-C7-C8
13	A	849	BCR	C5-C6-C7-C8
13	A	861	BCR	C1-C6-C7-C8
13	B	840	BCR	C1-C6-C7-C8
13	B	842	BCR	C23-C24-C25-C26
11	B	805	CLA	CAA-CBA-CGA-O2A
11	A	802	CLA	C4-C3-C5-C6
11	B	802	CLA	C4-C3-C5-C6
11	A	801	CLA	CAA-CBA-CGA-O2A
11	A	818	CLA	CAA-CBA-CGA-O2A
11	B	828	CLA	C3-C5-C6-C7
11	A	829	CLA	C4-C3-C5-C6
11	A	813	CLA	C11-C10-C8-C7
14	A	850	LHG	O1-C1-C2-O2
11	A	811	CLA	CAA-CBA-CGA-O2A
11	B	808	CLA	CAA-CBA-CGA-O2A
11	B	817	CLA	CAA-CBA-CGA-O1A
11	B	815	CLA	C5-C6-C7-C8
11	A	831	CLA	O2A-C1-C2-C3
11	A	804	CLA	CAA-CBA-CGA-O2A
11	B	811	CLA	CAA-CBA-CGA-O2A
13	A	849	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
11	A	804	CLA	C4-C3-C5-C6
11	A	806	CLA	C2-C3-C5-C6
11	A	806	CLA	C11-C12-C13-C14
11	A	826	CLA	C11-C10-C8-C9
11	A	818	CLA	C3A-C2A-CAA-CBA
11	B	819	CLA	CAA-CBA-CGA-O2A
11	A	804	CLA	CAD-CBD-CGD-O2D
11	A	807	CLA	CAD-CBD-CGD-O2D
11	A	811	CLA	CAD-CBD-CGD-O2D
11	A	822	CLA	CAD-CBD-CGD-O2D
11	A	825	CLA	CAD-CBD-CGD-O2D
11	A	826	CLA	CAD-CBD-CGD-O2D
11	A	831	CLA	CAD-CBD-CGD-O2D
11	A	833	CLA	CAD-CBD-CGD-O2D
11	A	838	CLA	CAD-CBD-CGD-O2D
11	A	841	CLA	CAD-CBD-CGD-O2D
11	B	807	CLA	CAD-CBD-CGD-O2D
11	B	814	CLA	CAD-CBD-CGD-O2D
11	B	828	CLA	CAD-CBD-CGD-O2D
14	A	850	LHG	C33-C34-C35-C36
11	A	860	CLA	CAA-CBA-CGA-O2A
11	B	814	CLA	CAA-CBA-CGA-O2A
13	A	852	BCR	C21-C22-C23-C24
11	B	831	CLA	CAA-CBA-CGA-O1A
11	B	814	CLA	CAA-CBA-CGA-O1A
11	B	831	CLA	CAA-CBA-CGA-O2A
11	A	803	CLA	CHA-CBD-CGD-O1D
11	A	803	CLA	CHA-CBD-CGD-O2D
11	A	810	CLA	CHA-CBD-CGD-O1D
11	A	810	CLA	CHA-CBD-CGD-O2D
11	A	811	CLA	CHA-CBD-CGD-O2D
11	A	820	CLA	CHA-CBD-CGD-O1D
11	A	827	CLA	CHA-CBD-CGD-O1D
11	A	827	CLA	CHA-CBD-CGD-O2D
11	A	829	CLA	CHA-CBD-CGD-O2D
11	A	860	CLA	CHA-CBD-CGD-O1D
11	A	860	CLA	CHA-CBD-CGD-O2D
11	B	806	CLA	CHA-CBD-CGD-O1D
11	B	816	CLA	CHA-CBD-CGD-O1D
11	B	816	CLA	CHA-CBD-CGD-O2D
11	B	821	CLA	CHA-CBD-CGD-O1D
11	B	821	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
11	B	824	CLA	CHA-CBD-CGD-O1D
11	B	824	CLA	CHA-CBD-CGD-O2D
11	B	829	CLA	CHA-CBD-CGD-O1D
11	B	832	CLA	CHA-CBD-CGD-O1D
11	B	832	CLA	CHA-CBD-CGD-O2D
11	B	836	CLA	CHA-CBD-CGD-O1D
11	B	836	CLA	CHA-CBD-CGD-O2D
11	B	801	CLA	CAA-CBA-CGA-O2A
11	B	822	CLA	C2A-CAA-CBA-CGA
11	B	822	CLA	CAA-CBA-CGA-O2A
11	B	801	CLA	C11-C10-C8-C7
11	B	811	CLA	C11-C12-C13-C15
11	B	816	CLA	C12-C13-C15-C16
11	B	803	CLA	CAA-CBA-CGA-O2A
14	A	850	LHG	O8-C23-C24-C25
11	B	805	CLA	C14-C13-C15-C16
11	A	804	CLA	CAA-CBA-CGA-O1A
12	A	843	PQN	C26-C27-C28-C30
14	A	850	LHG	O10-C23-C24-C25
14	A	851	LHG	O7-C7-C8-C9
13	A	852	BCR	C17-C18-C19-C20
11	A	808	CLA	C1A-C2A-CAA-CBA
11	B	807	CLA	C1A-C2A-CAA-CBA
11	B	814	CLA	C1A-C2A-CAA-CBA
11	B	808	CLA	CAA-CBA-CGA-O1A
11	B	811	CLA	CAA-CBA-CGA-O1A
14	A	851	LHG	O9-C7-C8-C9
11	B	817	CLA	CAA-CBA-CGA-O2A
12	B	837	PQN	C26-C27-C28-C30
11	B	811	CLA	C5-C6-C7-C8
16	B	843	LMG	C36-C37-C38-C39
11	A	811	CLA	CAA-CBA-CGA-O1A
11	A	860	CLA	CAA-CBA-CGA-O1A
16	B	843	LMG	O7-C10-C11-C12
13	A	852	BCR	C16-C17-C18-C36
13	A	847	BCR	C23-C24-C25-C26
13	B	840	BCR	C23-C24-C25-C26
11	B	803	CLA	CAA-CBA-CGA-O1A
11	B	822	CLA	CAA-CBA-CGA-O1A
11	A	814	CLA	CAD-CBD-CGD-O1D
11	A	838	CLA	CAD-CBD-CGD-O1D
11	B	815	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	B	824	CLA	C13-C15-C16-C17
11	B	802	CLA	C6-C7-C8-C9
11	B	823	CLA	C11-C10-C8-C9
11	A	805	CLA	CAA-CBA-CGA-O2A
16	B	843	LMG	C14-C15-C16-C17
11	B	823	CLA	CAA-CBA-CGA-O2A
11	A	804	CLA	C6-C7-C8-C10
11	A	805	CLA	C11-C10-C8-C7
11	A	833	CLA	C12-C13-C15-C16
11	B	814	CLA	C3A-C2A-CAA-CBA
11	B	817	CLA	C3A-C2A-CAA-CBA
11	B	822	CLA	CHA-CBD-CGD-O1D
11	B	801	CLA	CAA-CBA-CGA-O1A
11	A	805	CLA	CAA-CBA-CGA-O1A
11	A	831	CLA	C2A-CAA-CBA-CGA
11	B	816	CLA	C2A-CAA-CBA-CGA
11	A	830	CLA	C8-C10-C11-C12

There are no ring outliers.

75 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	805	CLA	3	0
14	A	851	LHG	2	0
11	A	830	CLA	1	0
11	B	829	CLA	1	0
13	A	848	BCR	1	0
11	A	824	CLA	2	0
11	B	825	CLA	1	0
13	A	857	BCR	2	0
11	B	812	CLA	1	0
11	A	828	CLA	2	0
11	A	808	CLA	3	0
11	A	840	CLA	1	0
11	A	821	CLA	4	0
11	B	836	CLA	1	0
11	B	815	CLA	4	0
13	A	844	BCR	2	0
12	B	837	PQN	9	0
11	B	820	CLA	1	0
11	B	818	CLA	2	0
11	B	811	CLA	2	0

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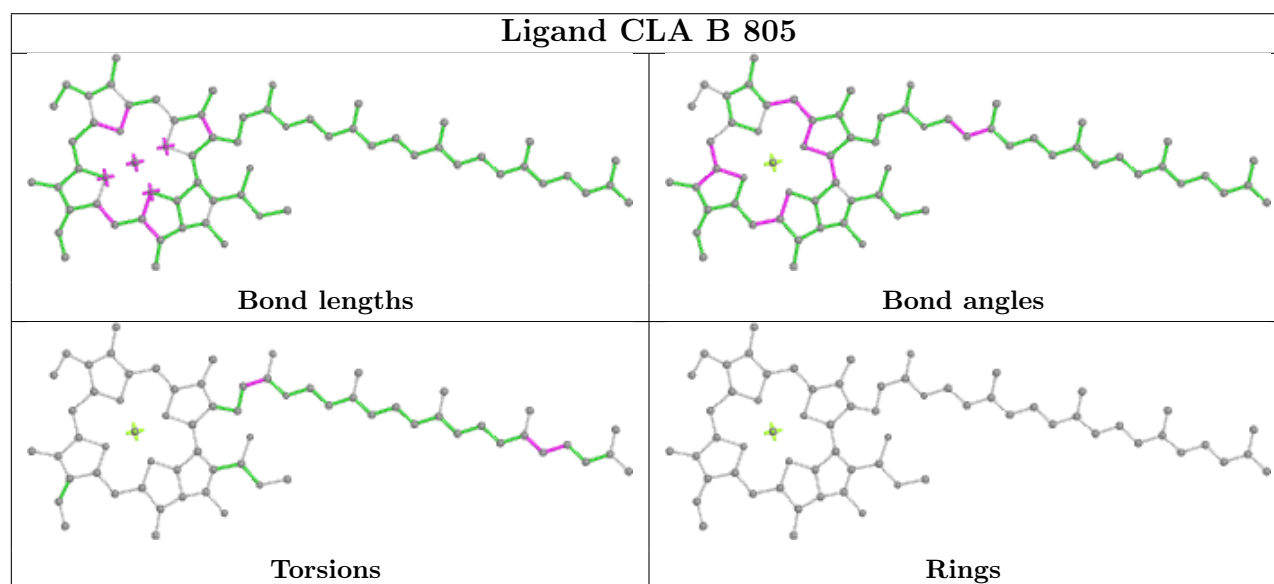
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	860	CLA	1	0
11	A	815	CLA	1	0
12	A	843	PQN	20	0
11	A	813	CLA	2	0
11	A	837	CLA	3	0
13	A	845	BCR	2	0
11	B	807	CLA	2	0
11	B	808	CLA	2	0
11	A	836	CLA	2	0
11	A	842	CLA	1	0
11	B	828	CLA	2	0
13	B	841	BCR	2	0
11	A	805	CLA	3	0
11	B	835	CLA	2	0
11	B	821	CLA	1	0
11	B	802	CLA	4	0
13	I	101	BCR	2	0
11	B	816	CLA	2	0
13	A	852	BCR	2	0
11	A	841	CLA	2	0
11	A	859	CLA	2	0
11	L	1503	CLA	1	0
11	A	838	CLA	2	0
11	A	835	CLA	2	0
11	B	817	CLA	1	0
13	B	844	BCR	2	0
11	A	817	CLA	4	0
11	A	802	CLA	1	0
13	A	846	BCR	1	0
11	B	809	CLA	1	0
11	A	809	CLA	3	0
11	A	825	CLA	2	0
11	A	818	CLA	3	0
11	A	811	CLA	3	0
11	A	819	CLA	1	0
11	B	834	CLA	1	0
11	B	813	CLA	1	0
13	B	842	BCR	1	0
11	A	831	CLA	1	0
13	B	840	BCR	1	0
11	B	803	CLA	1	0
11	A	812	CLA	1	0

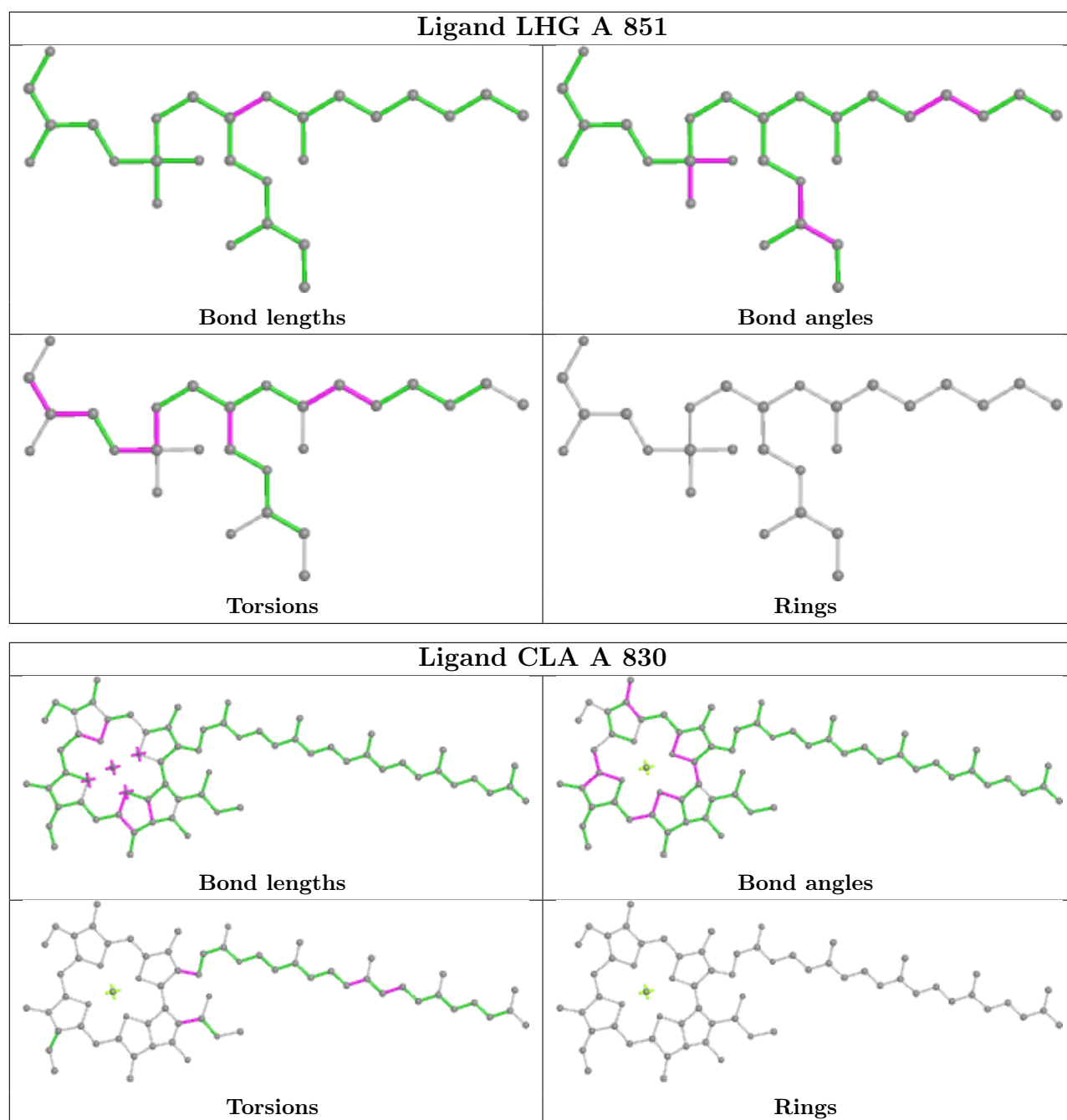
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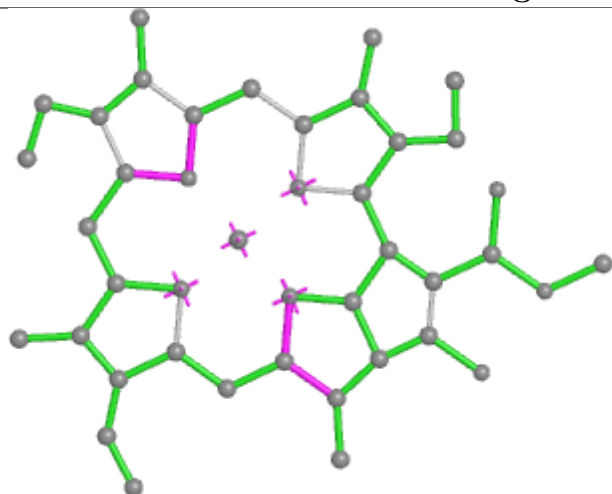
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	806	CLA	2	0
13	B	838	BCR	1	0
11	B	824	CLA	3	0
11	A	810	CLA	2	0
13	F	201	BCR	13	0
11	A	829	CLA	1	0
11	A	820	CLA	1	0
13	A	858	BCR	2	0
13	A	854	BCR	1	0
13	A	855	BCR	2	0
11	A	826	CLA	1	0
13	A	849	BCR	2	0
13	F	202	BCR	2	0

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

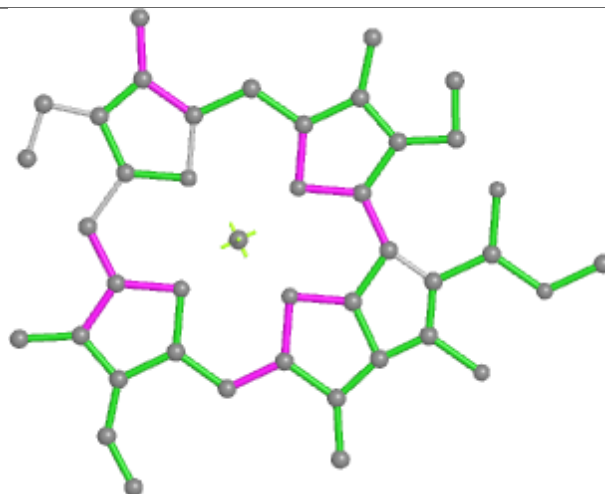




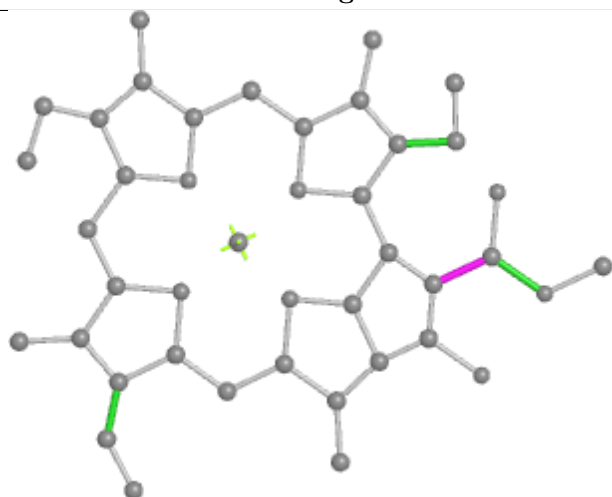
Ligand CLA B 829



Bond lengths



Bond angles

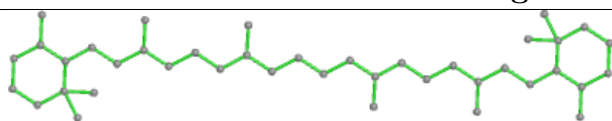


Torsions

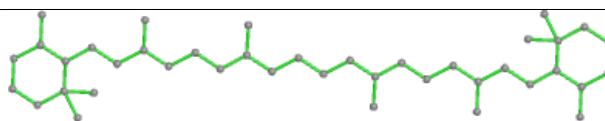


Rings

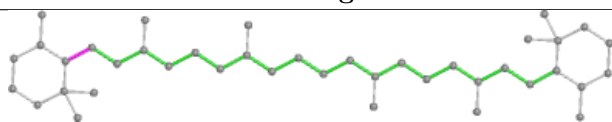
Ligand BCR A 848



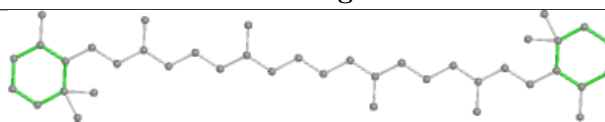
Bond lengths



Bond angles

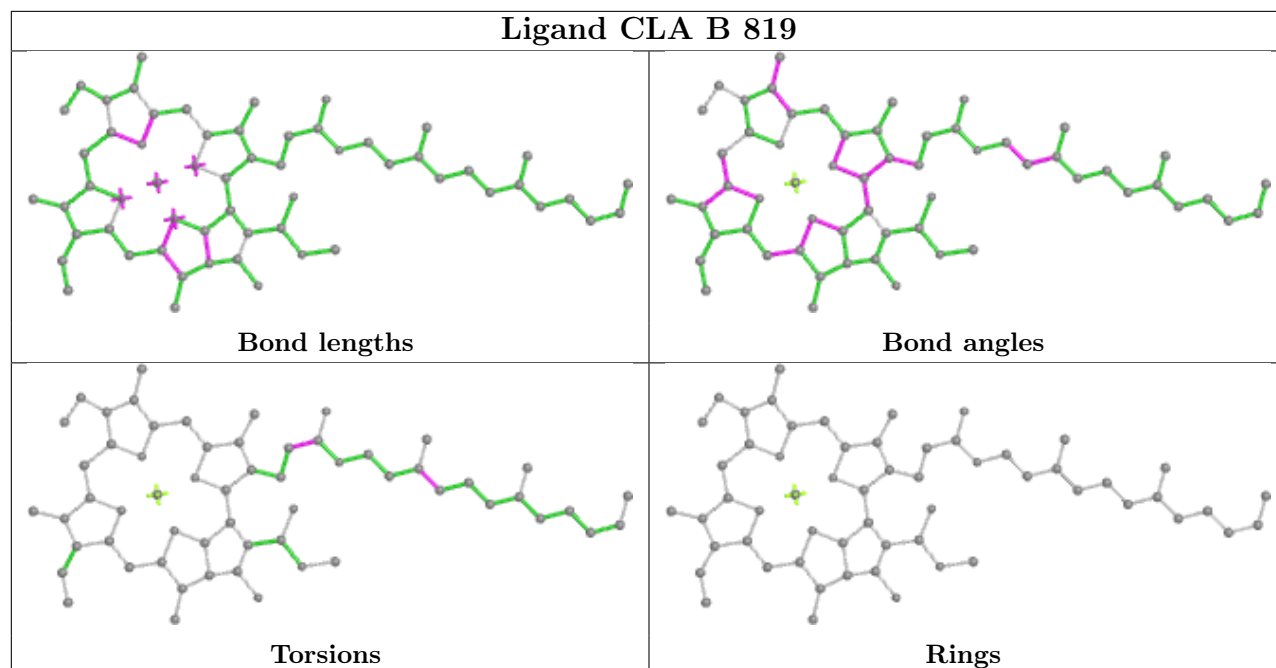


Torsions

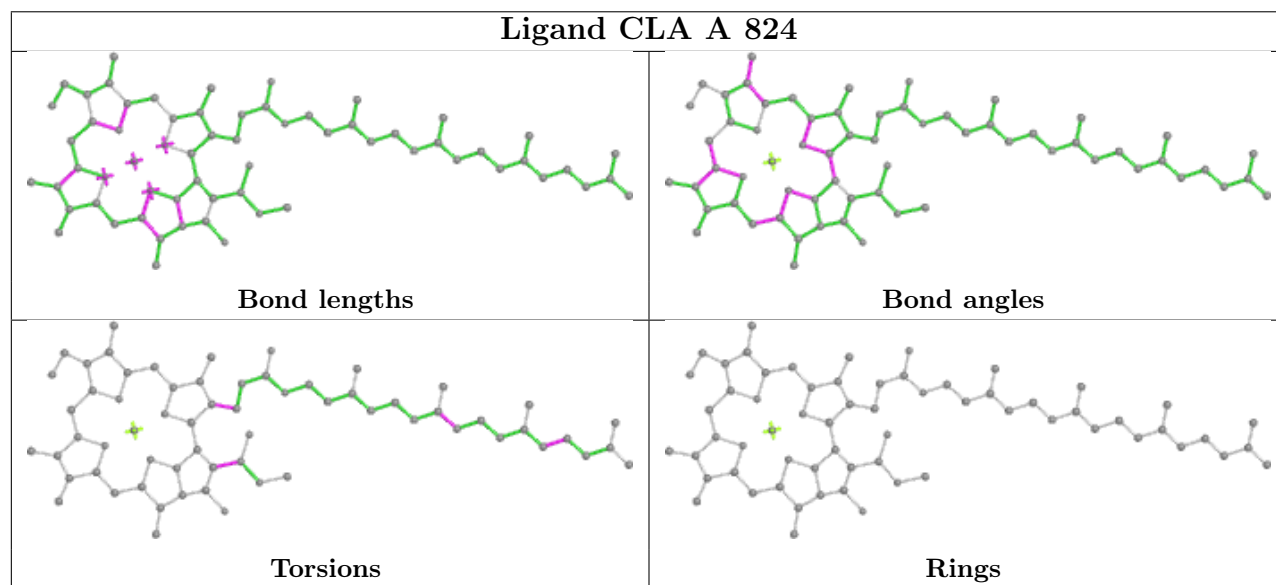


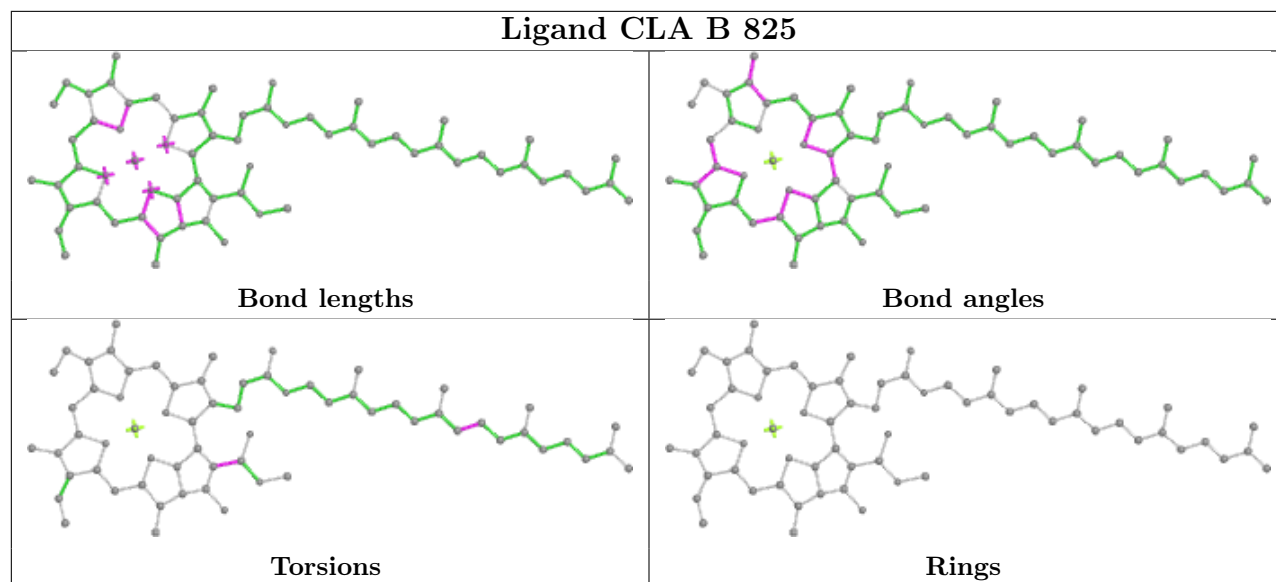
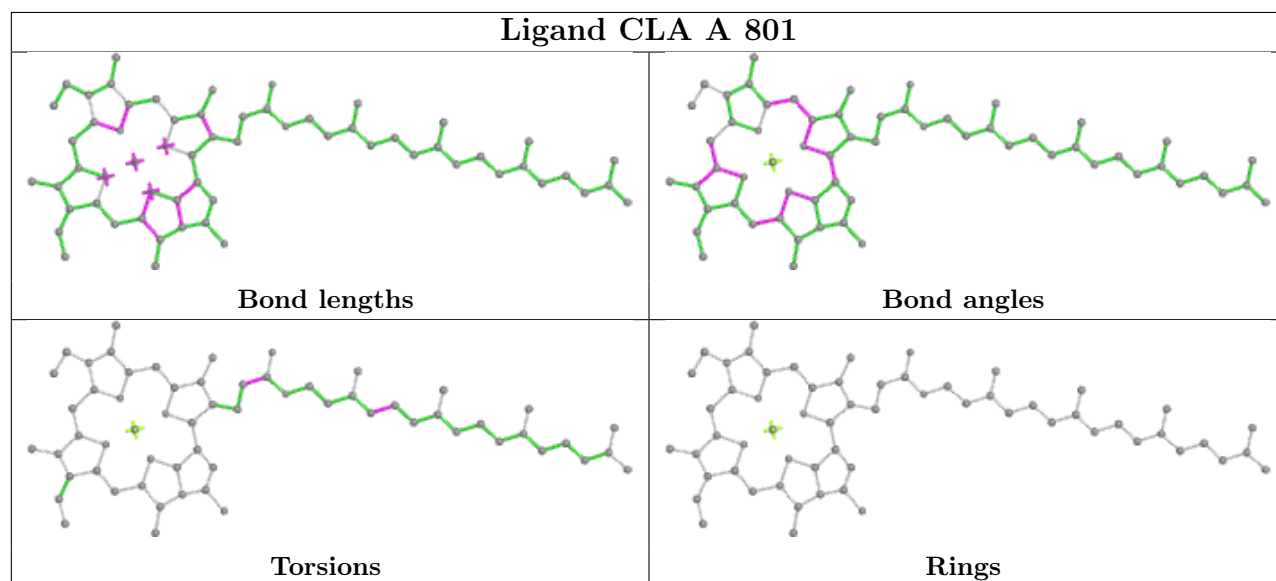
Rings

Ligand CLA B 819

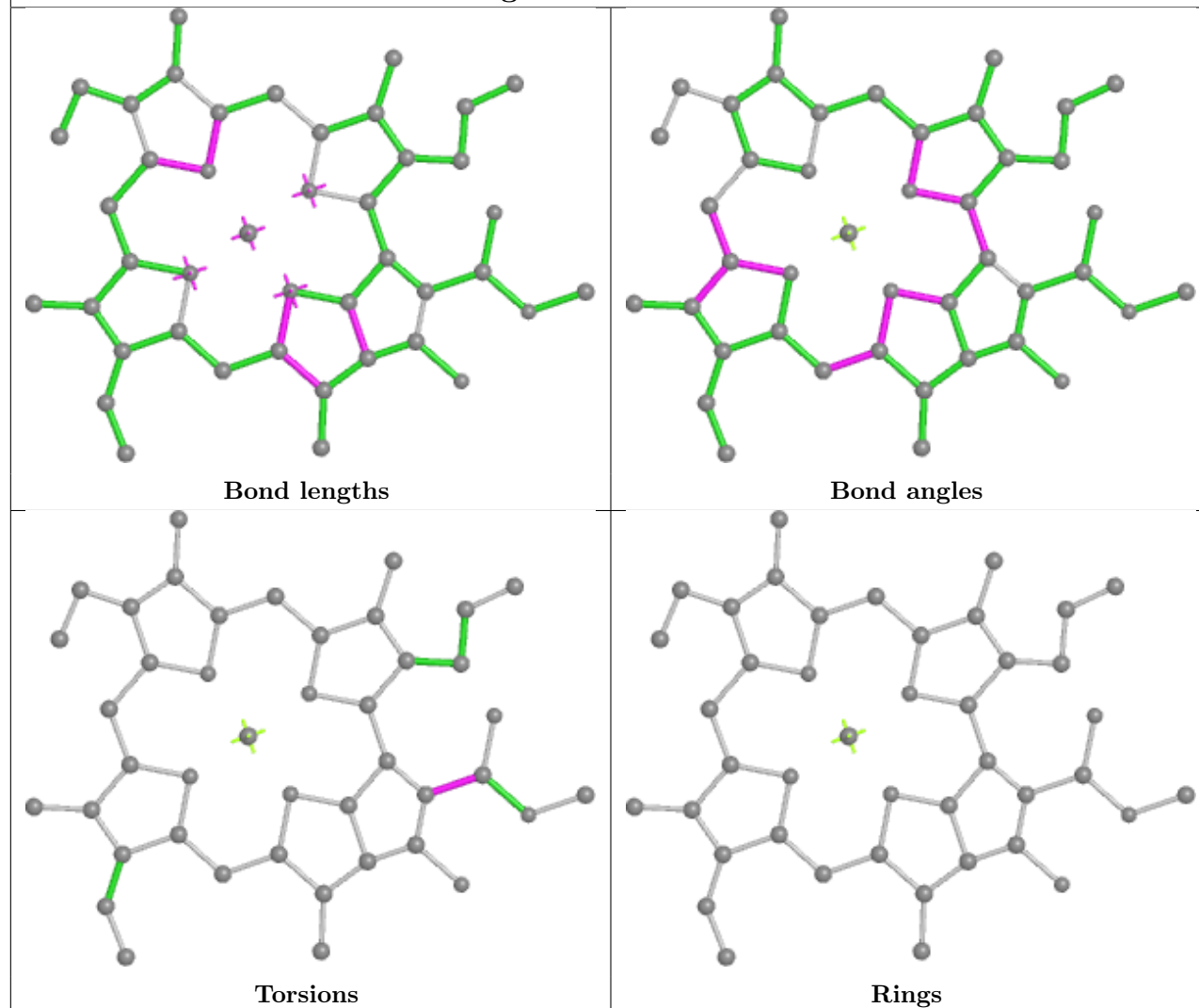


Ligand CLA A 824

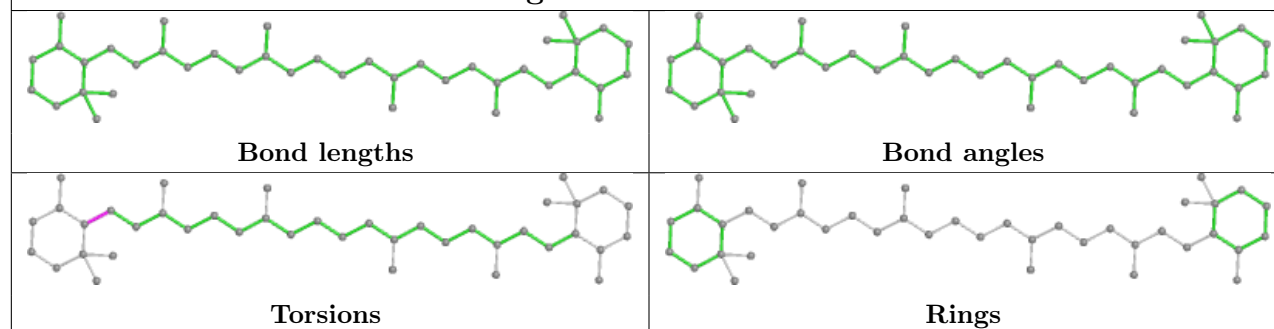


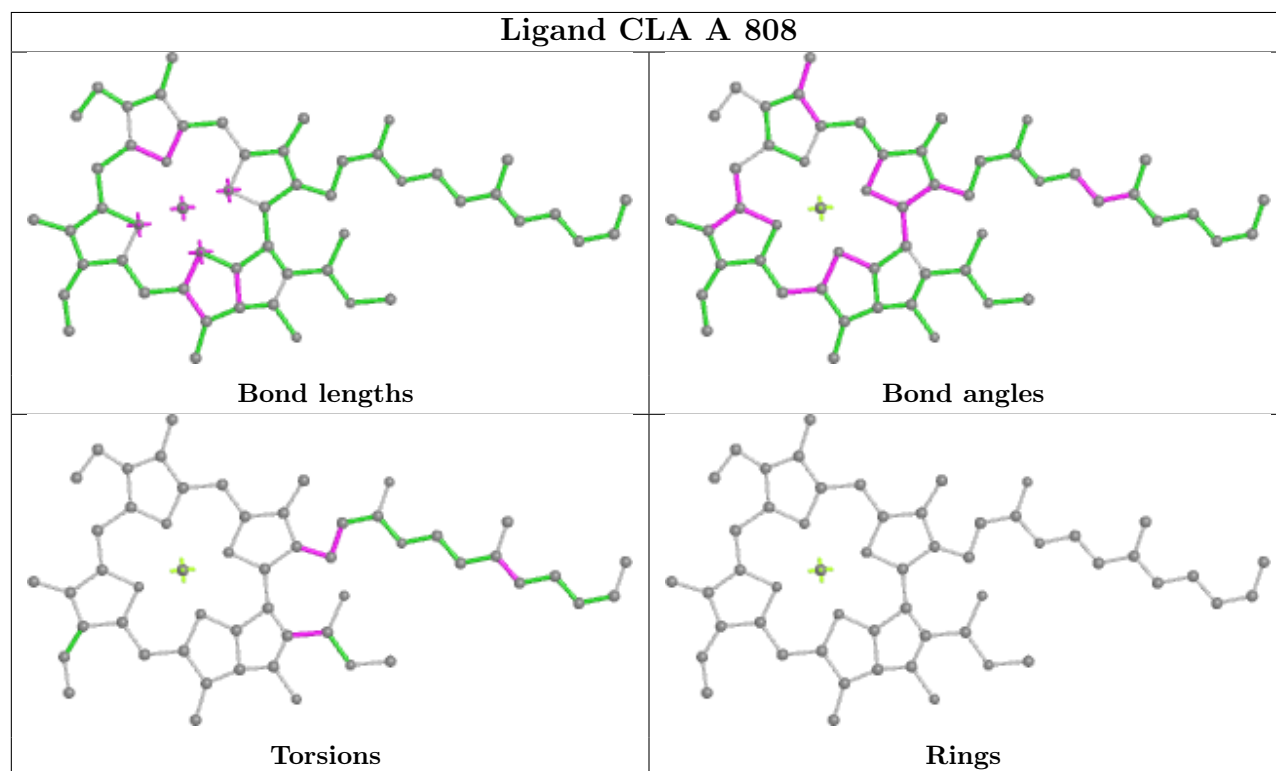
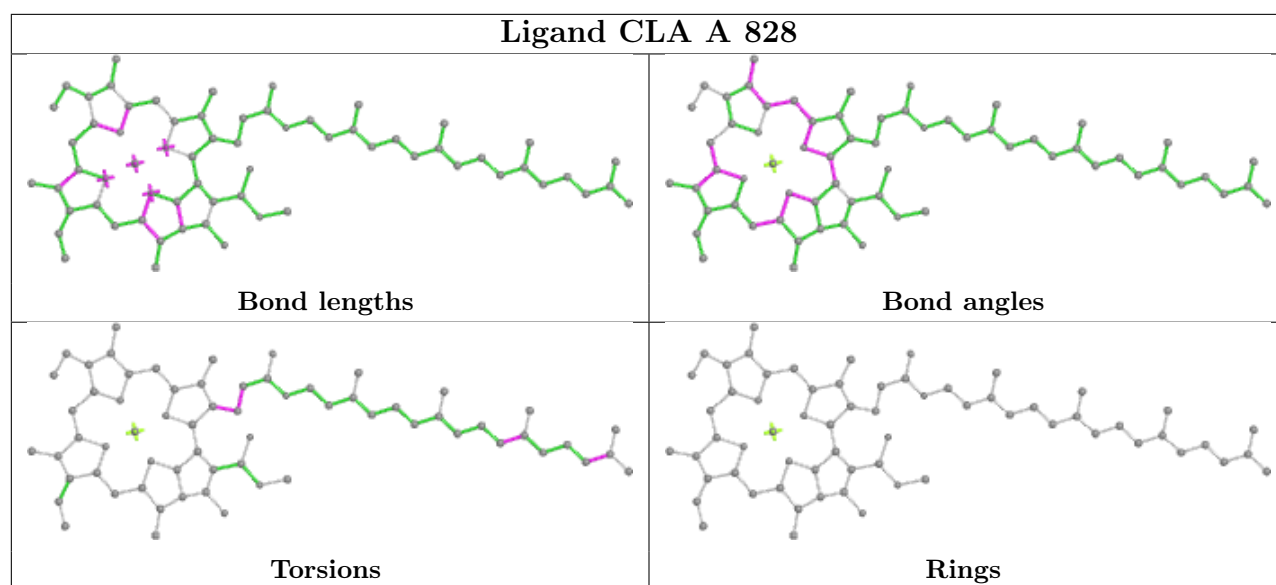
Ligand CLA B 825**Ligand CLA A 801**

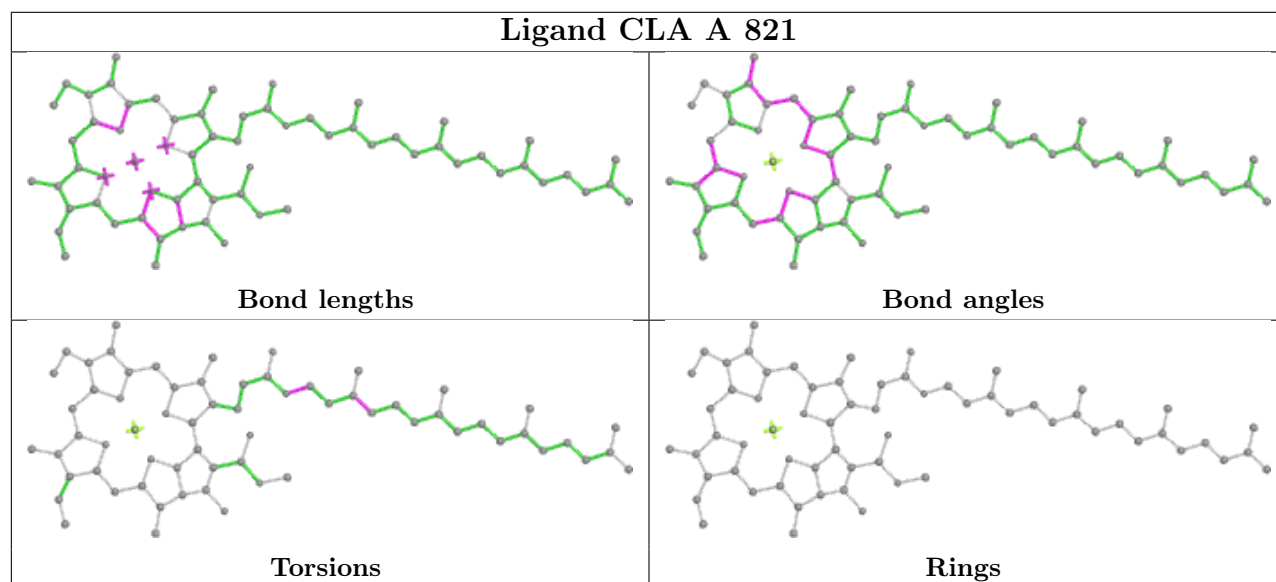
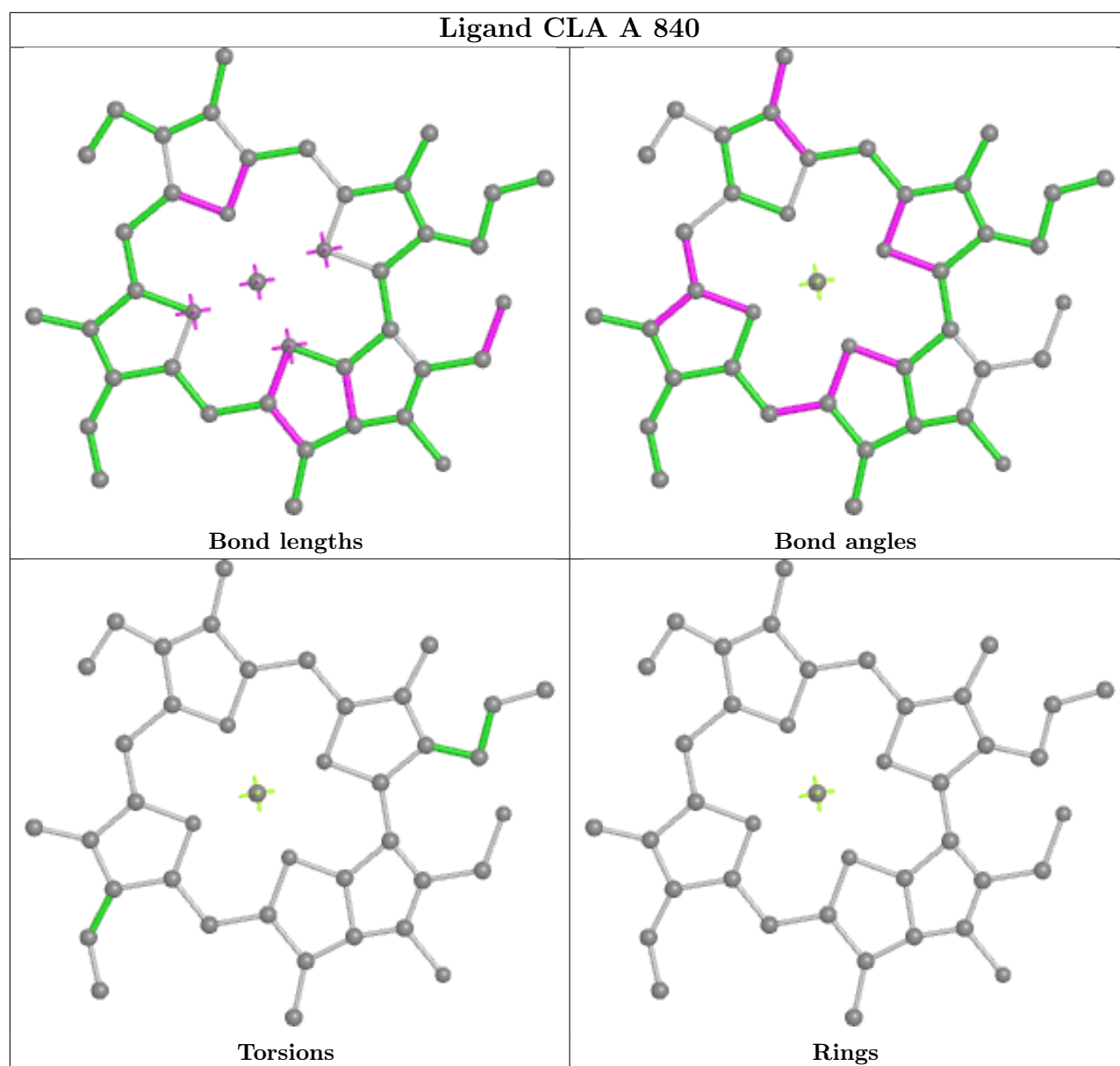
Ligand CLA B 812



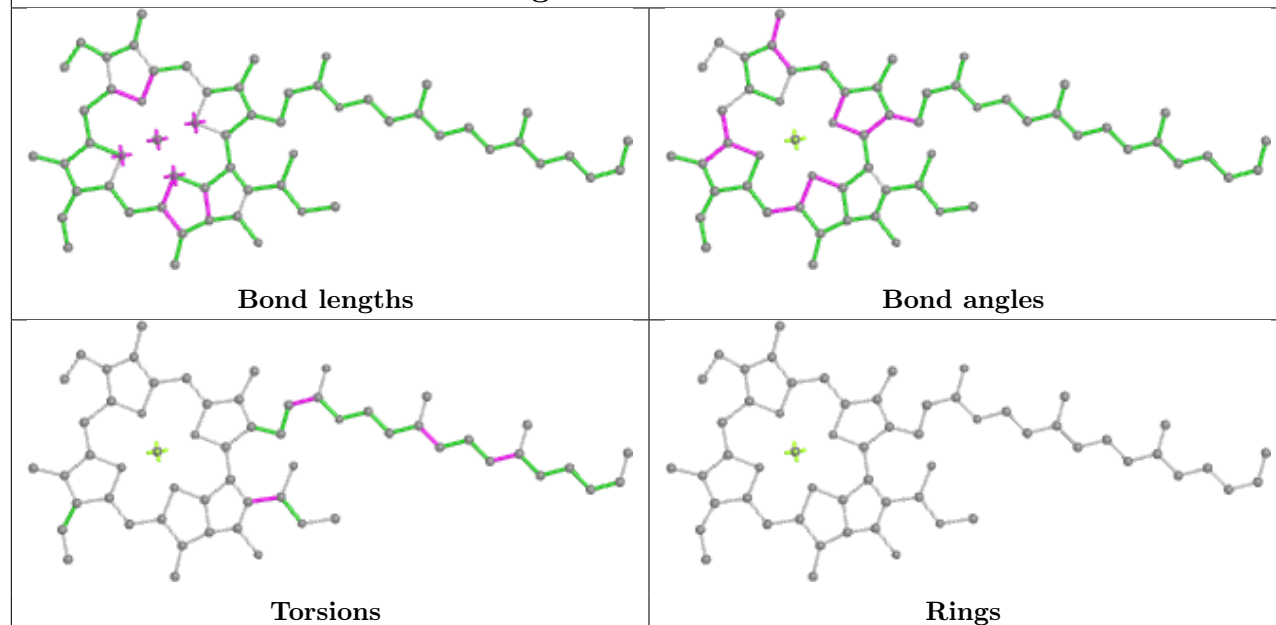
Ligand BCR M 101



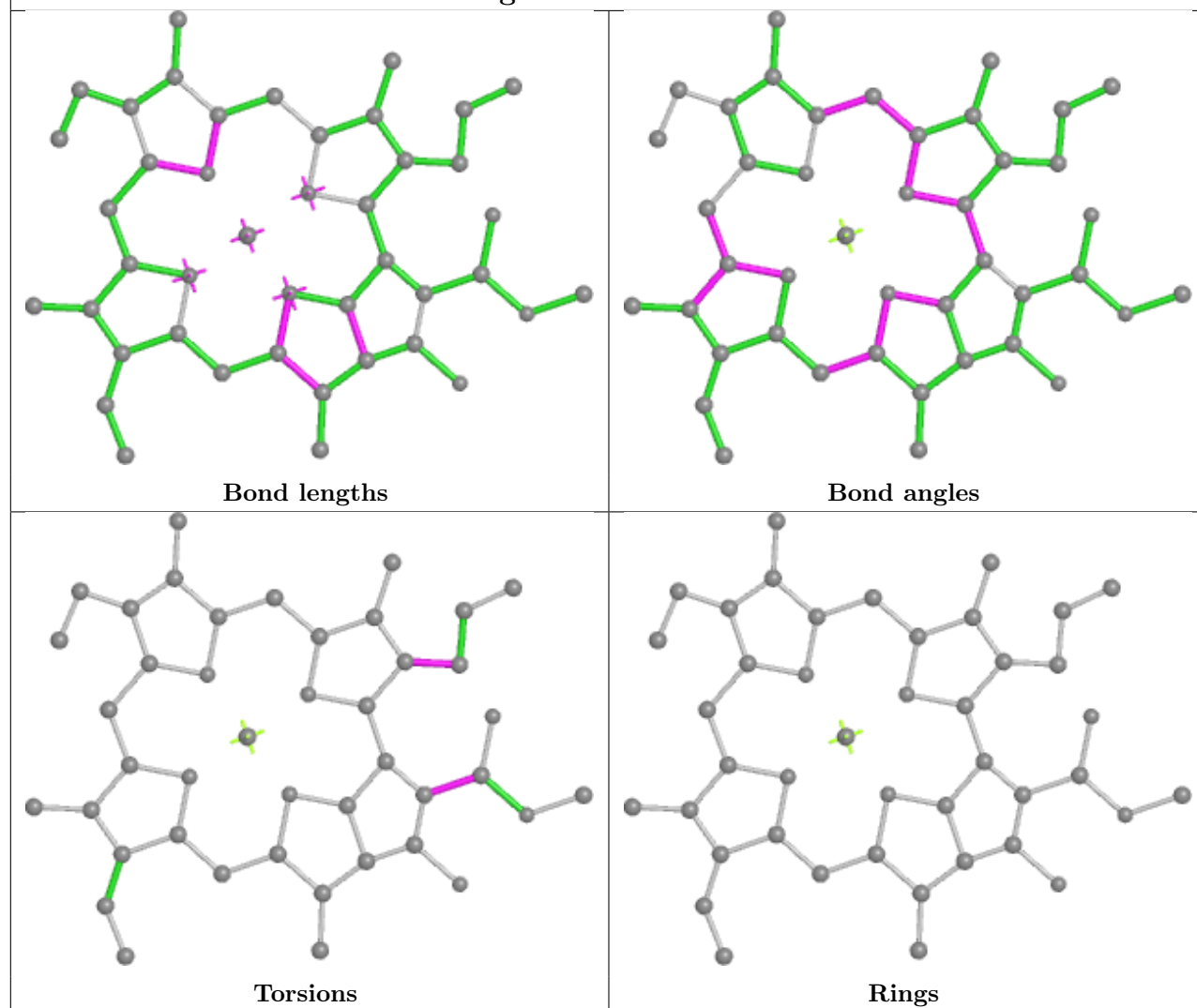


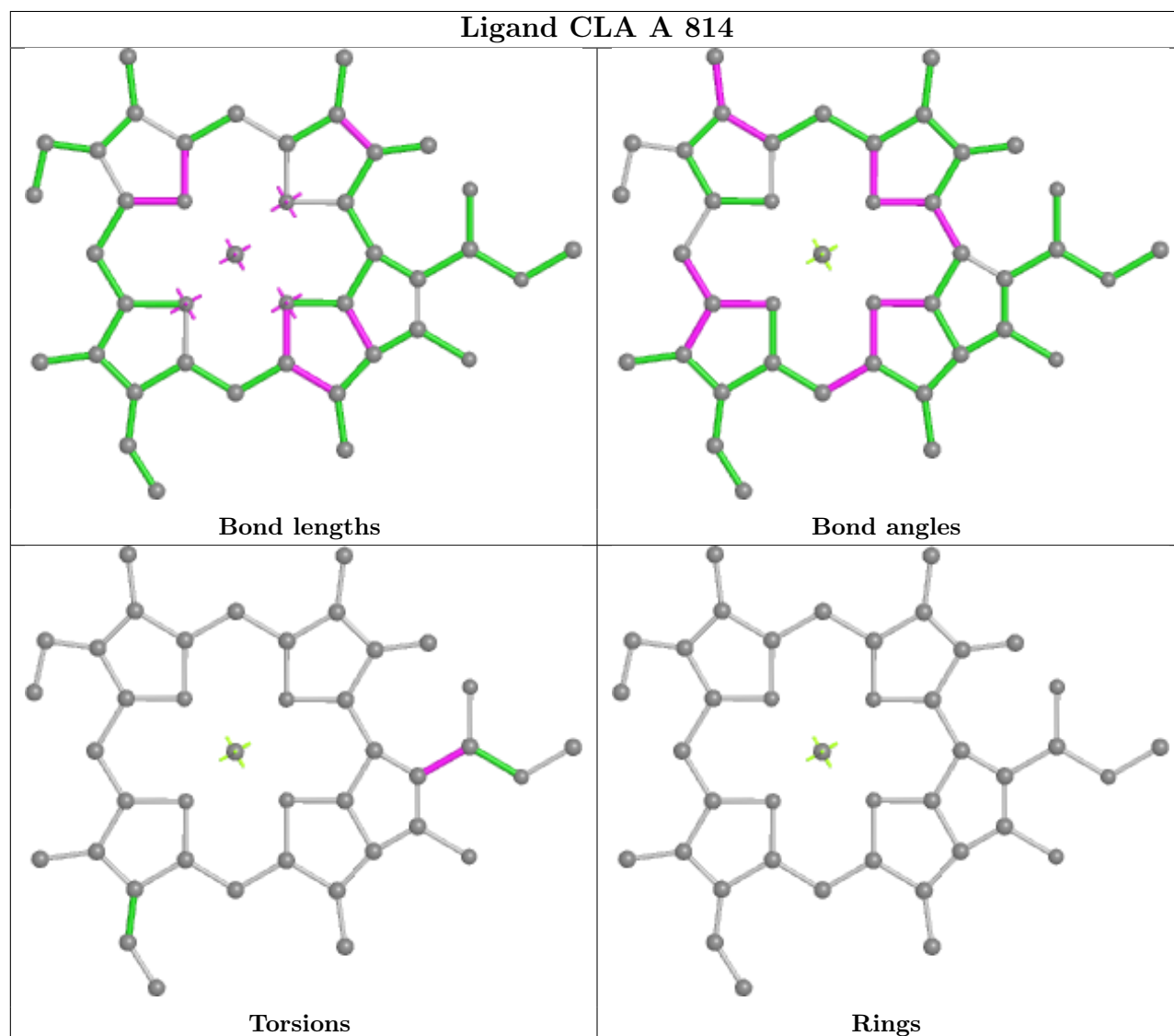
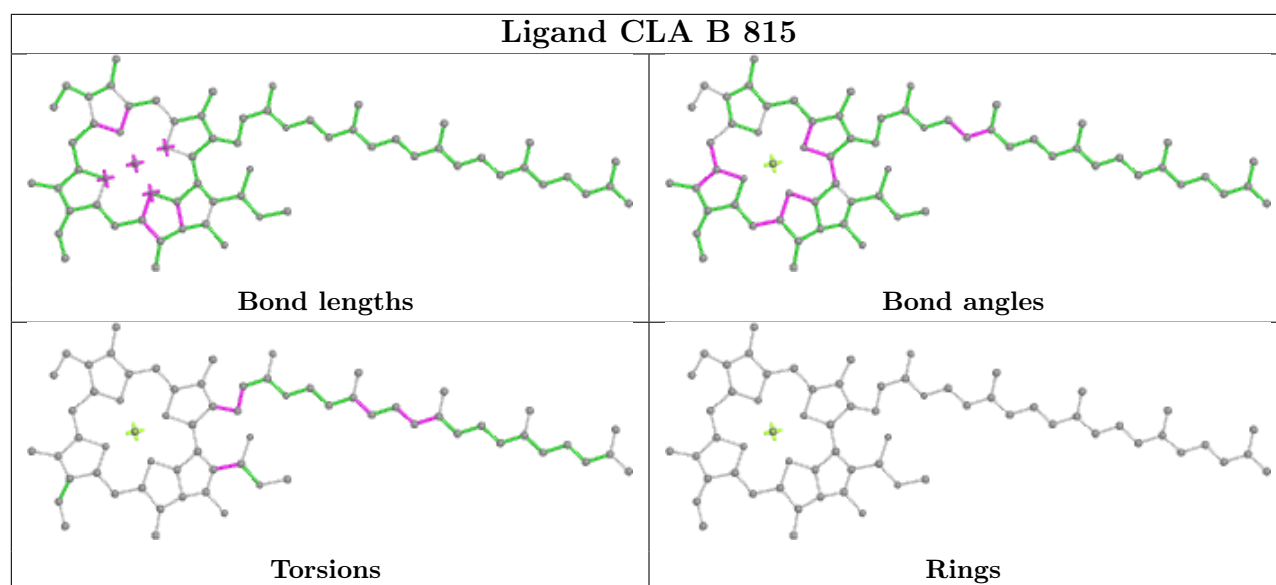


Ligand CLA A 804

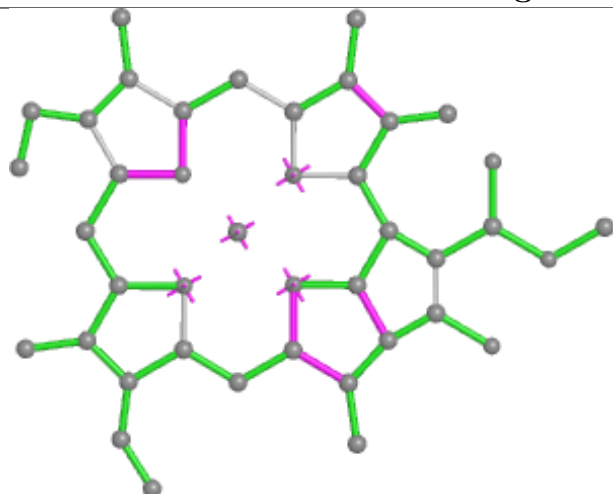


Ligand CLA B 836

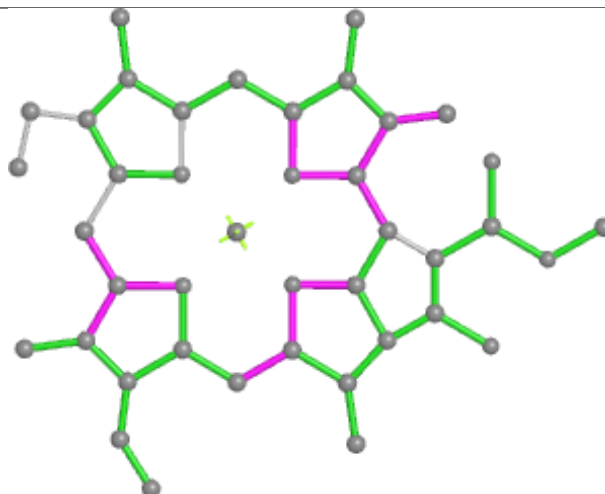




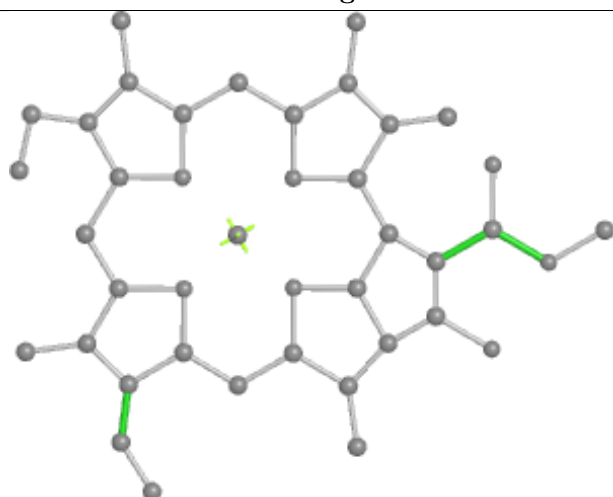
Ligand CLA B 827



Bond lengths



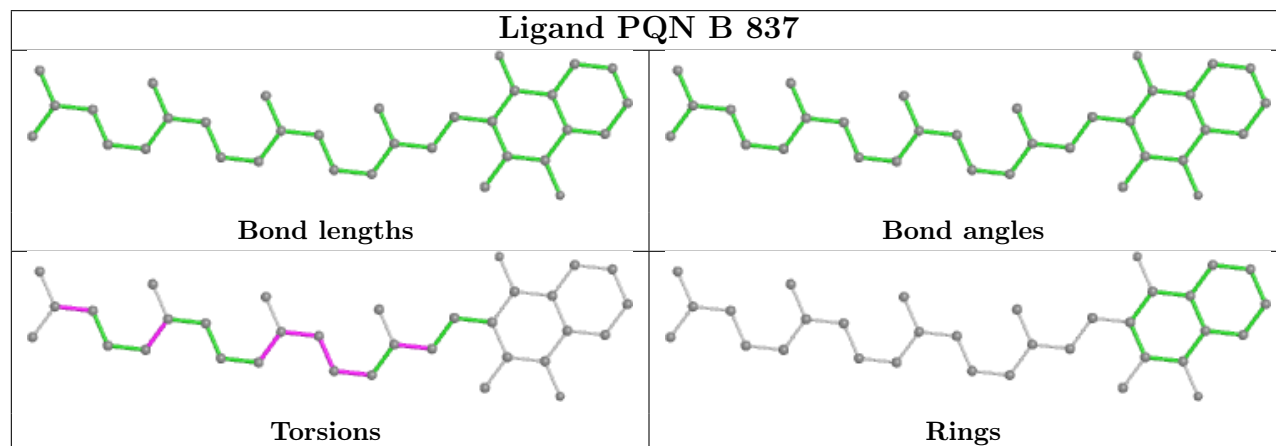
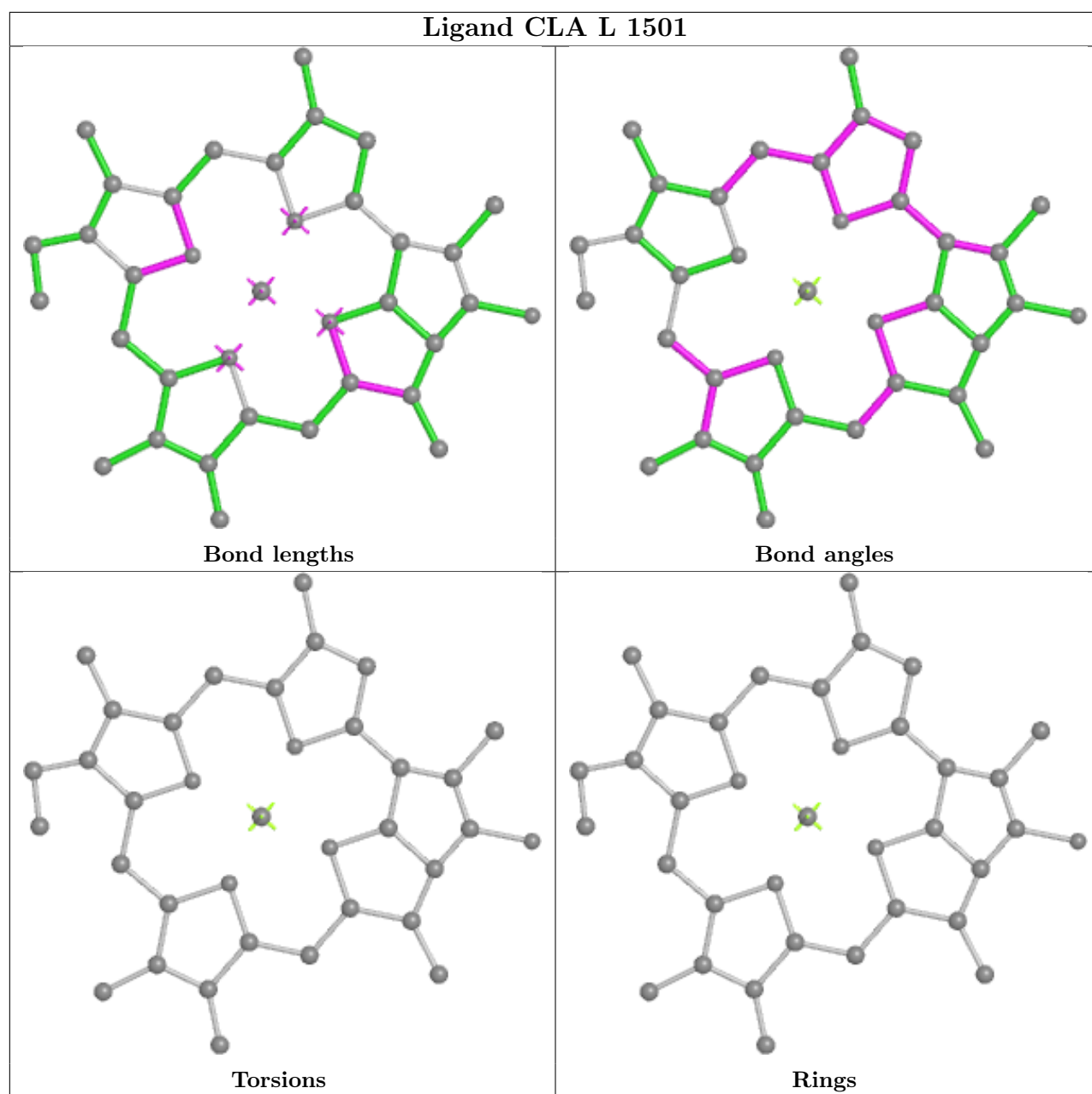
Bond angles



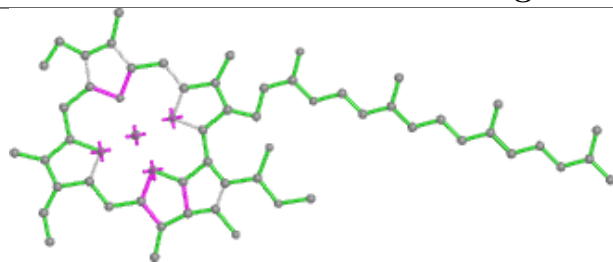
Torsions



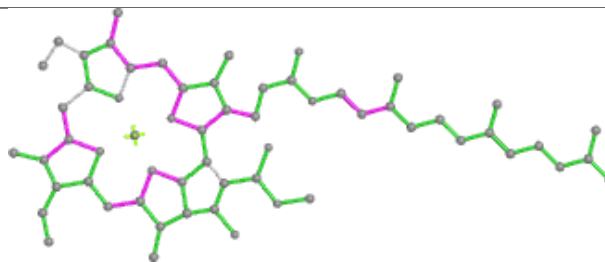
Rings



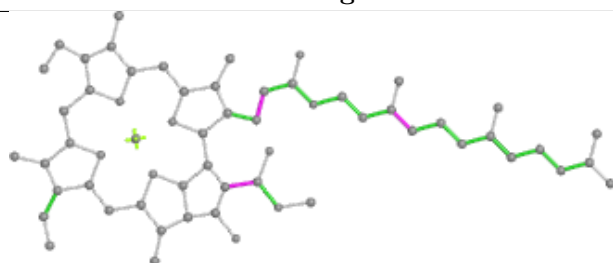
Ligand CLA B 820



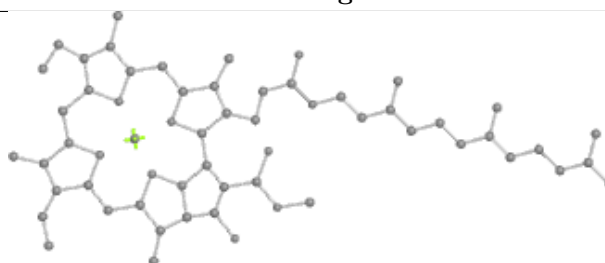
Bond lengths



Bond angles

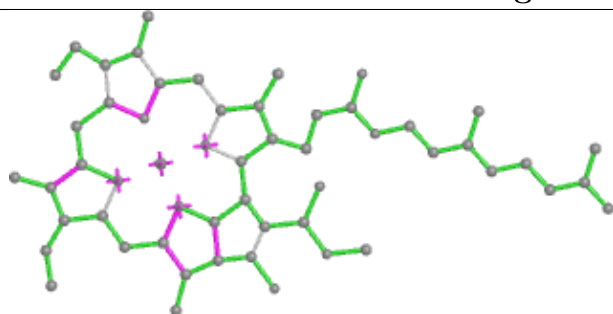


Torsions

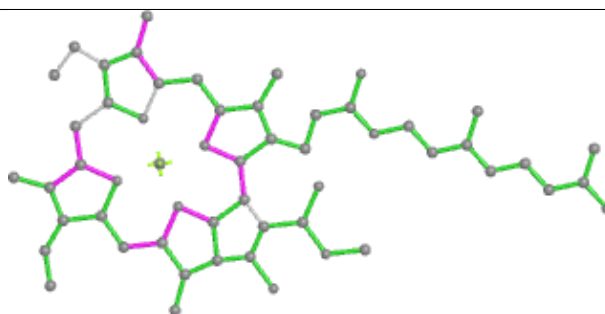


Rings

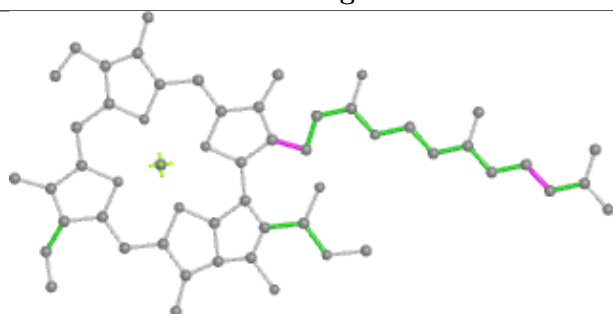
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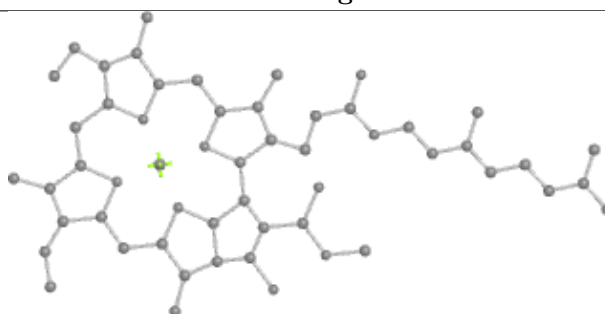
Bond lengths



Bond angles

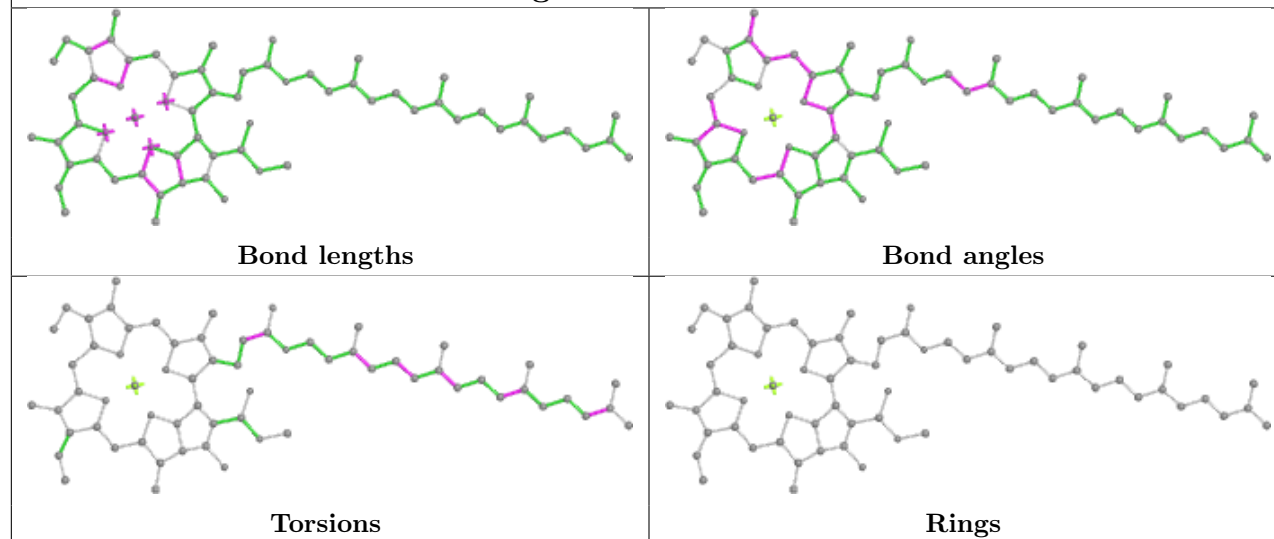


Torsions

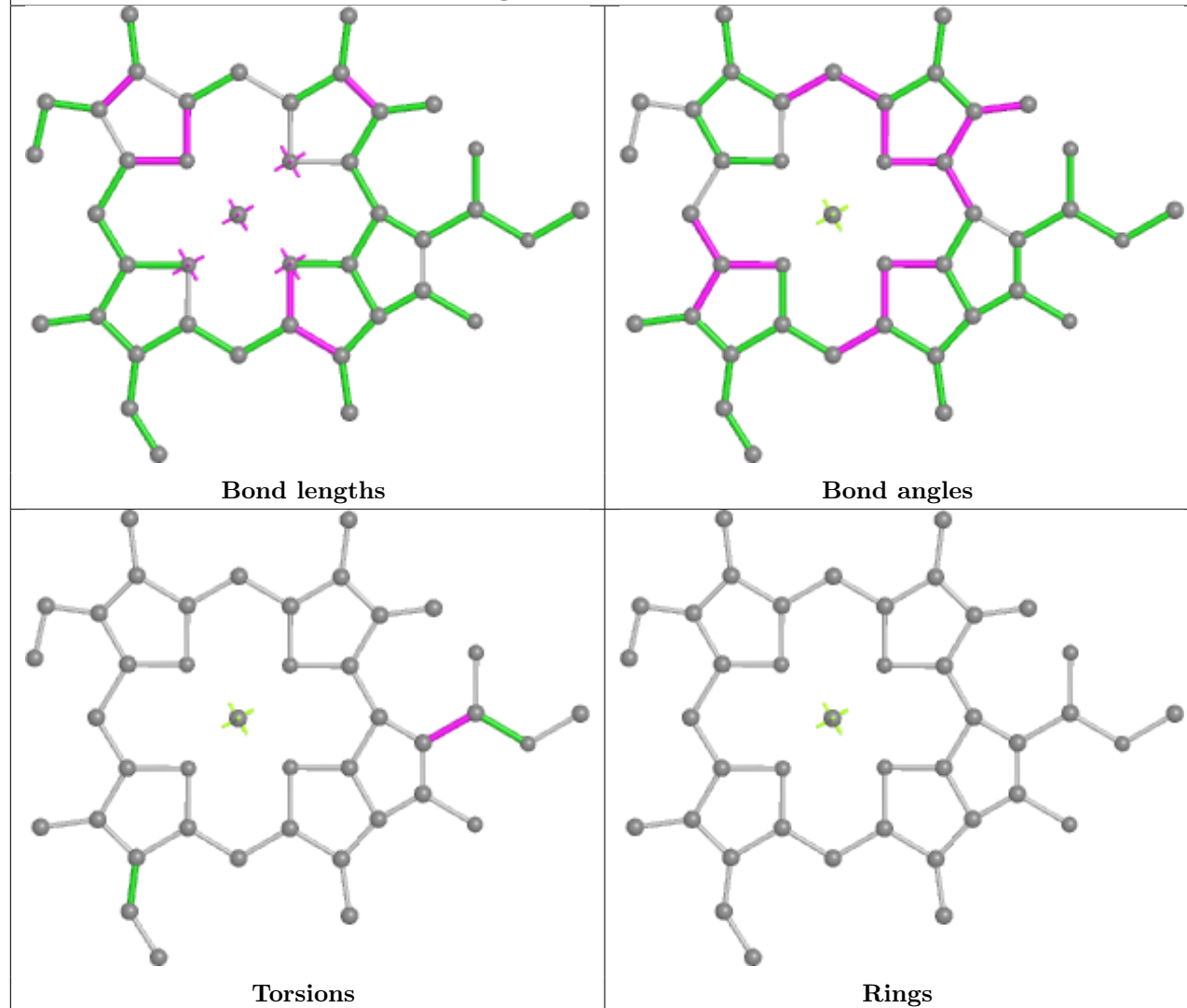


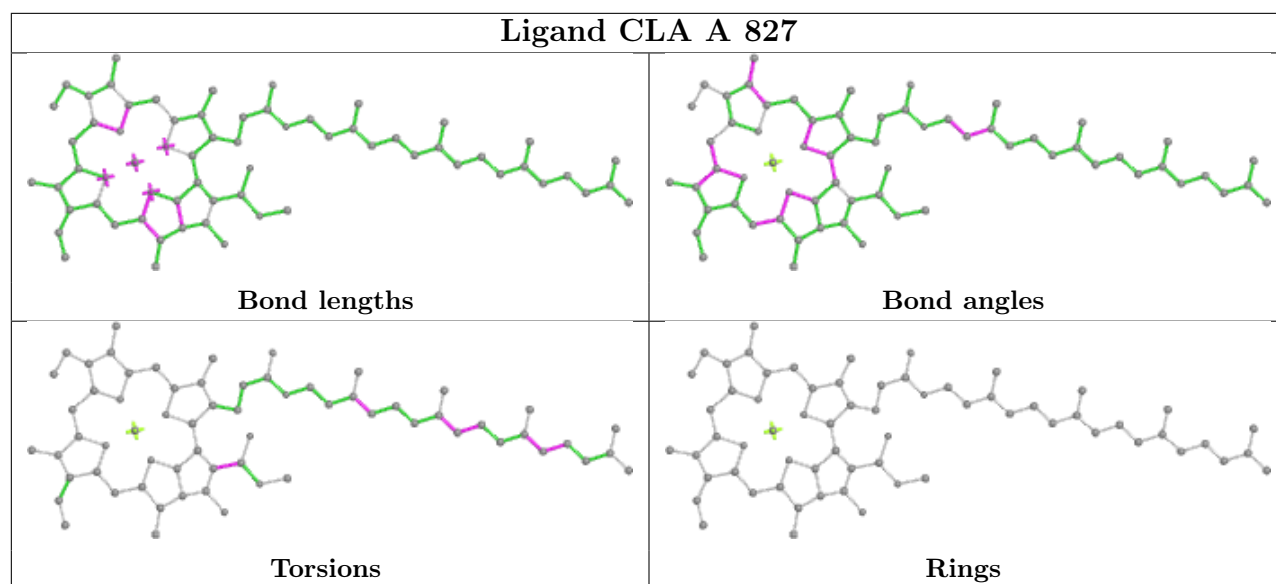
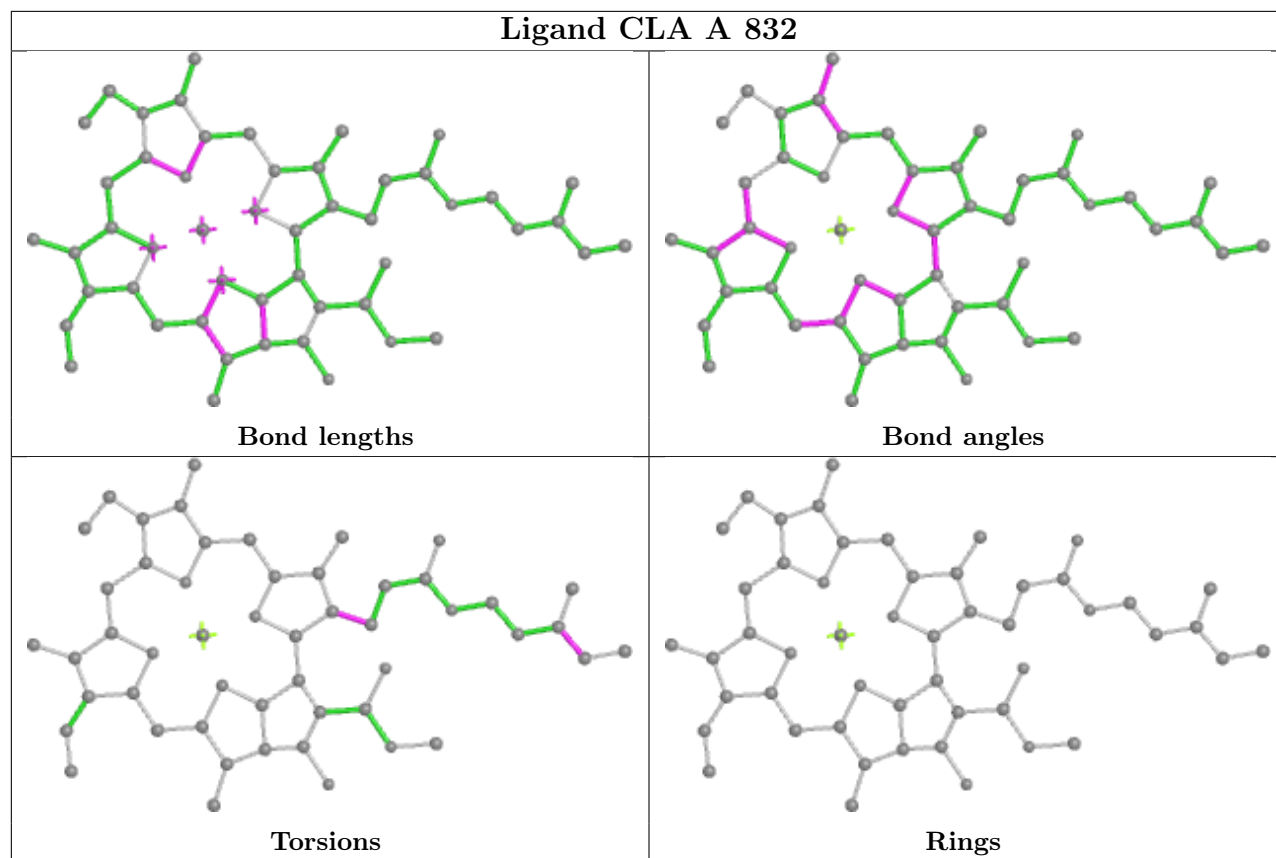
Rings

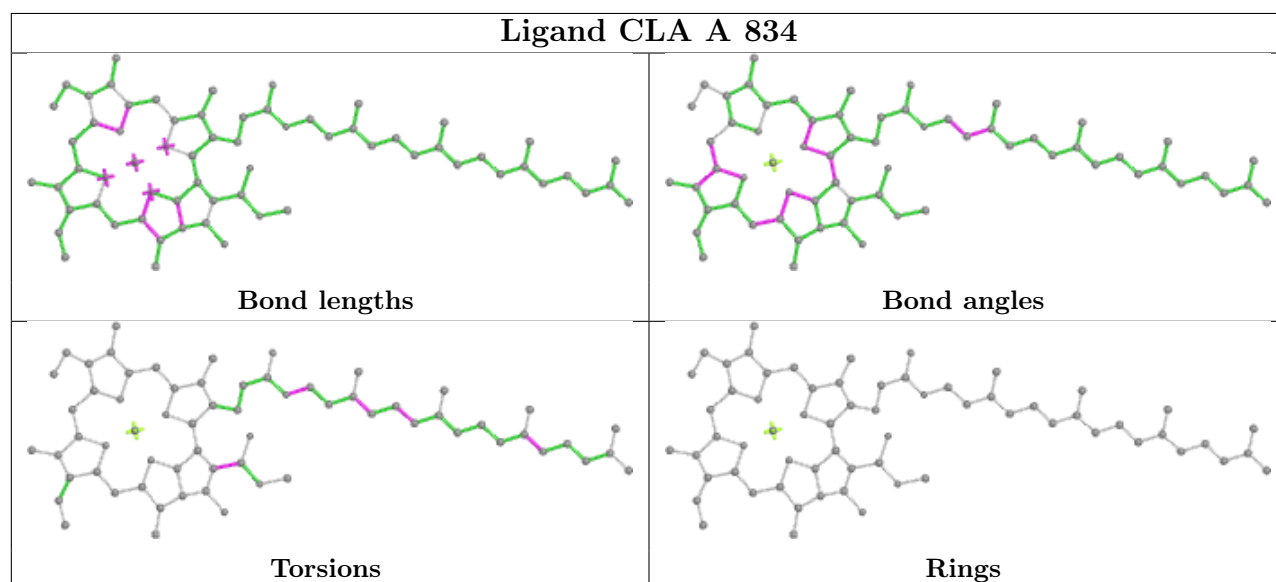
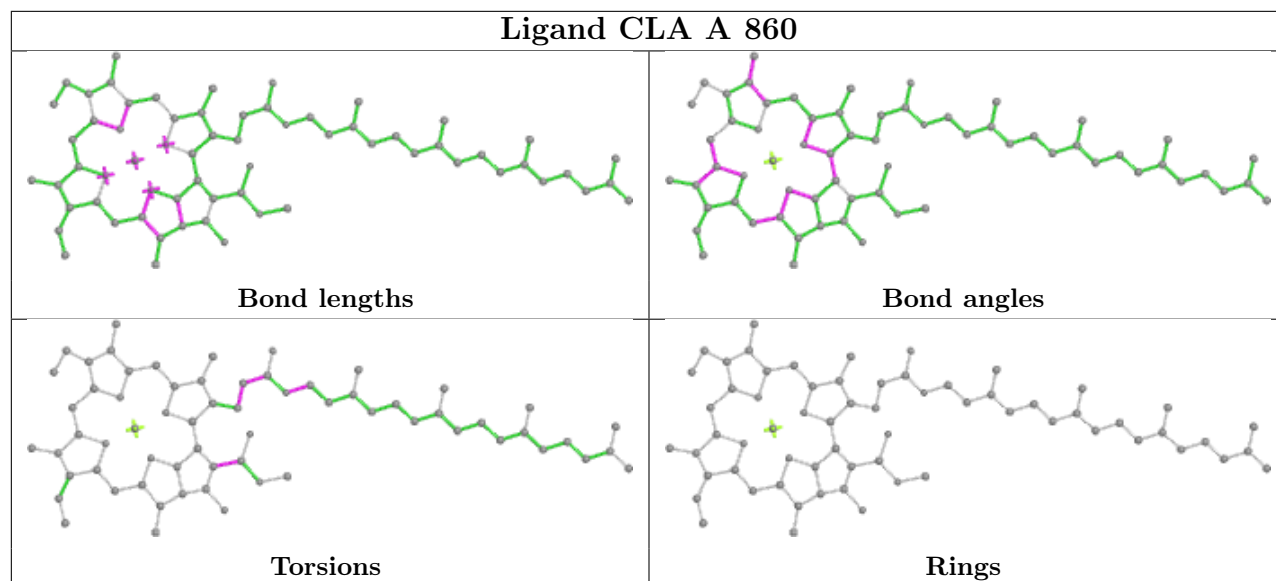
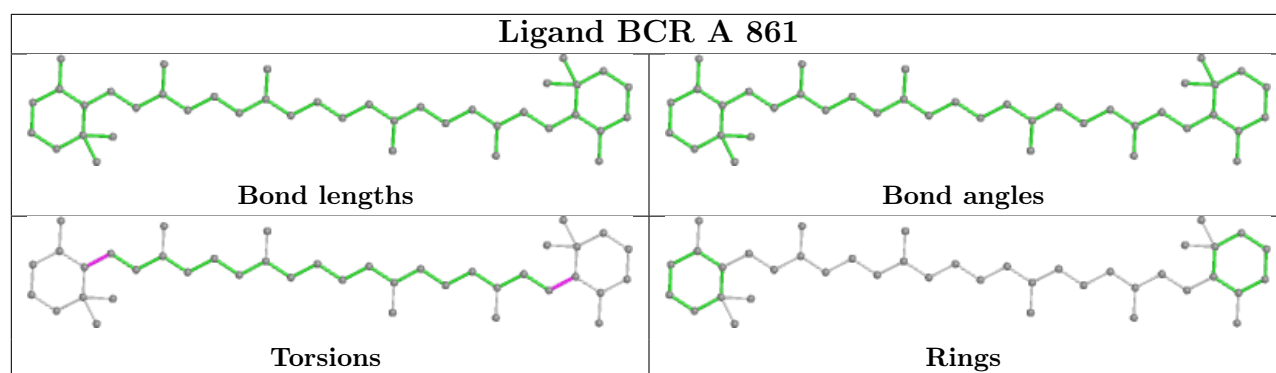
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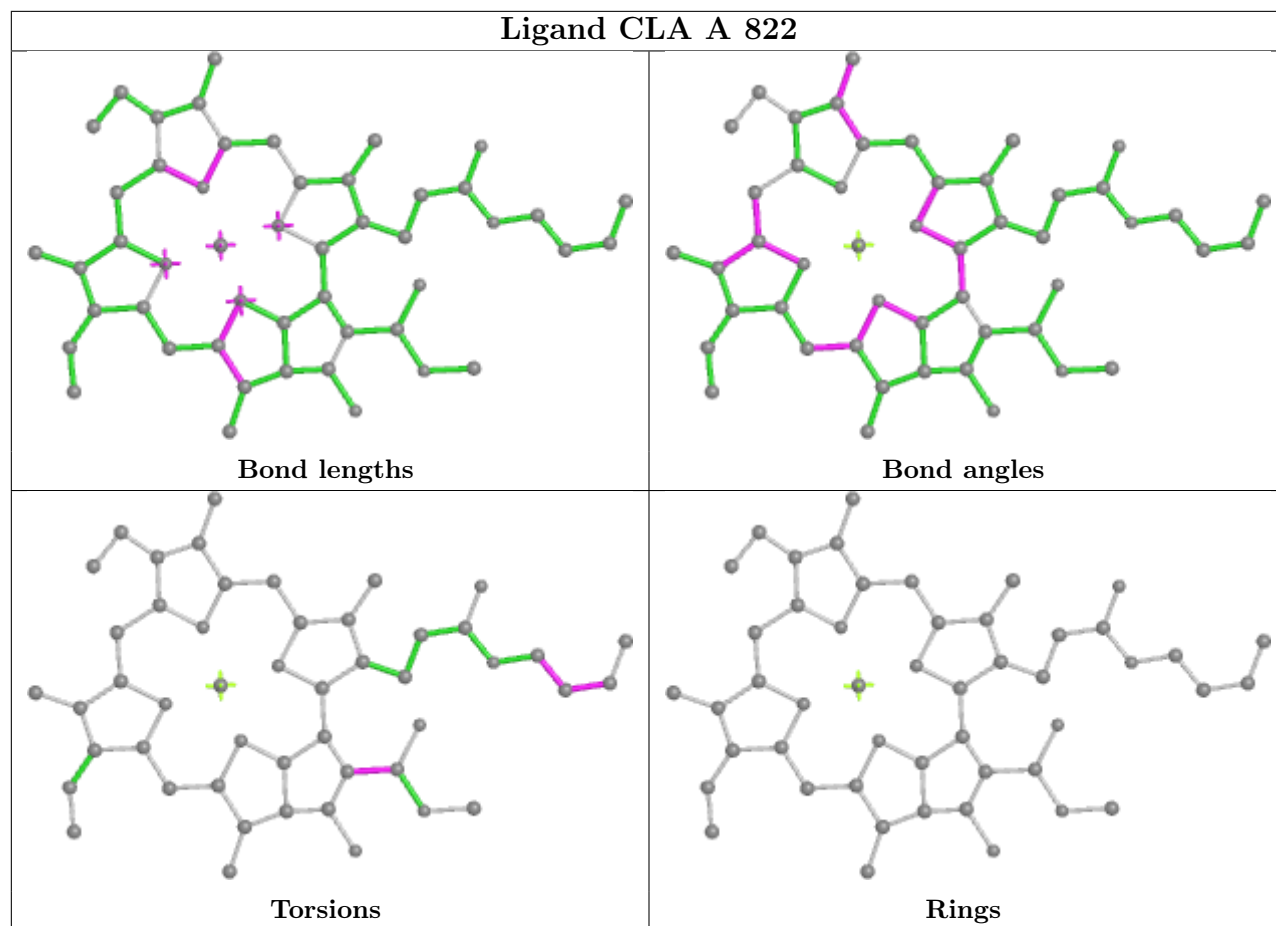


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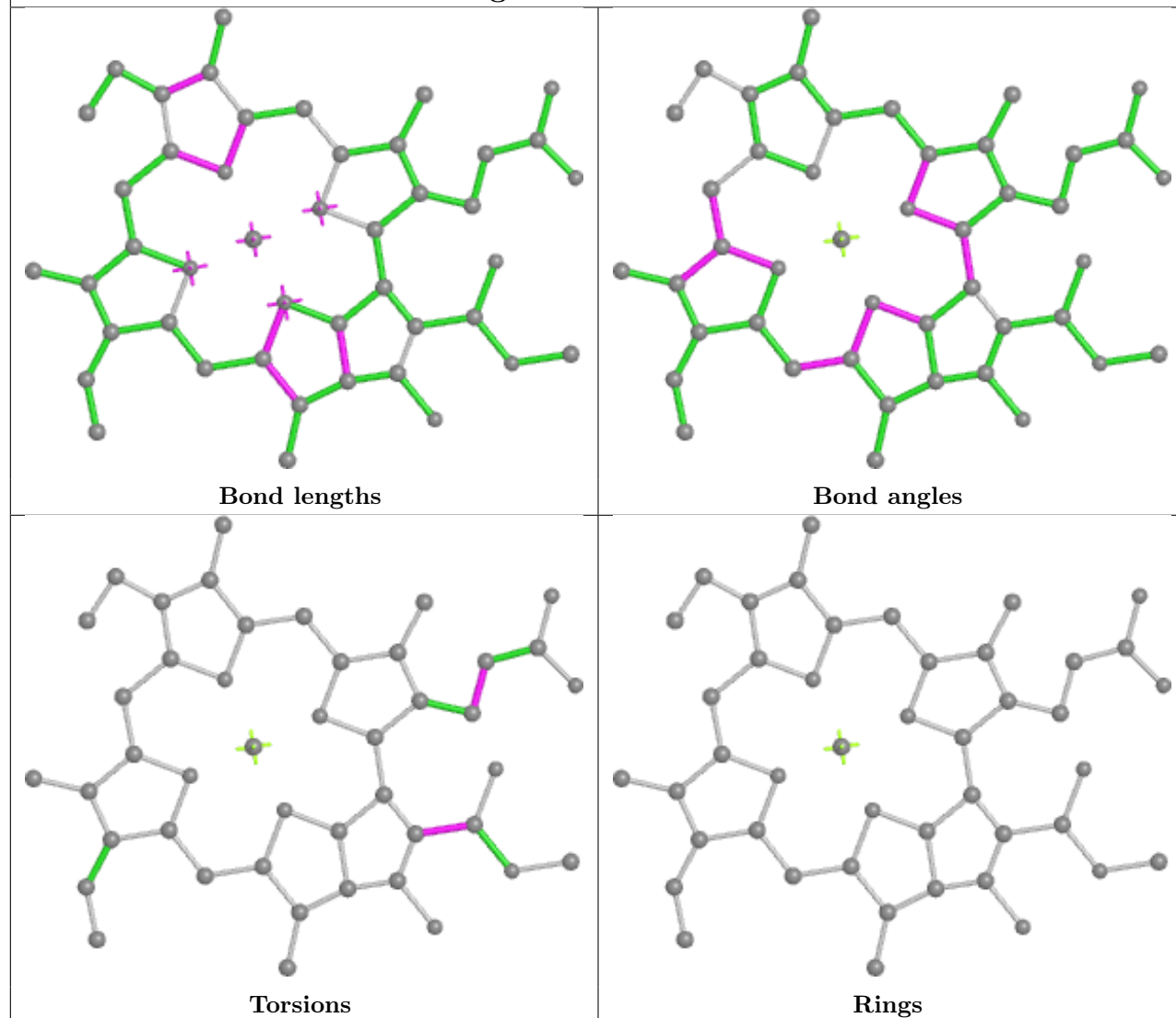




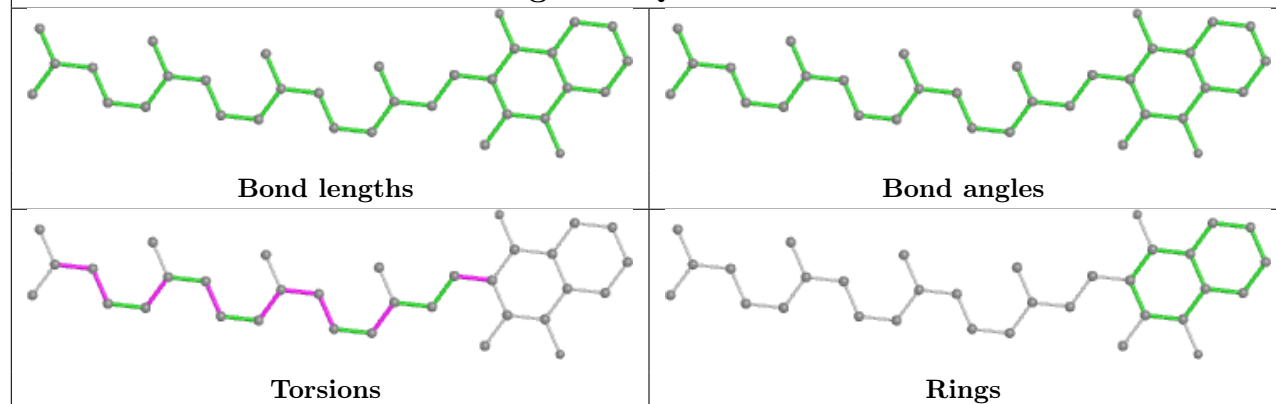


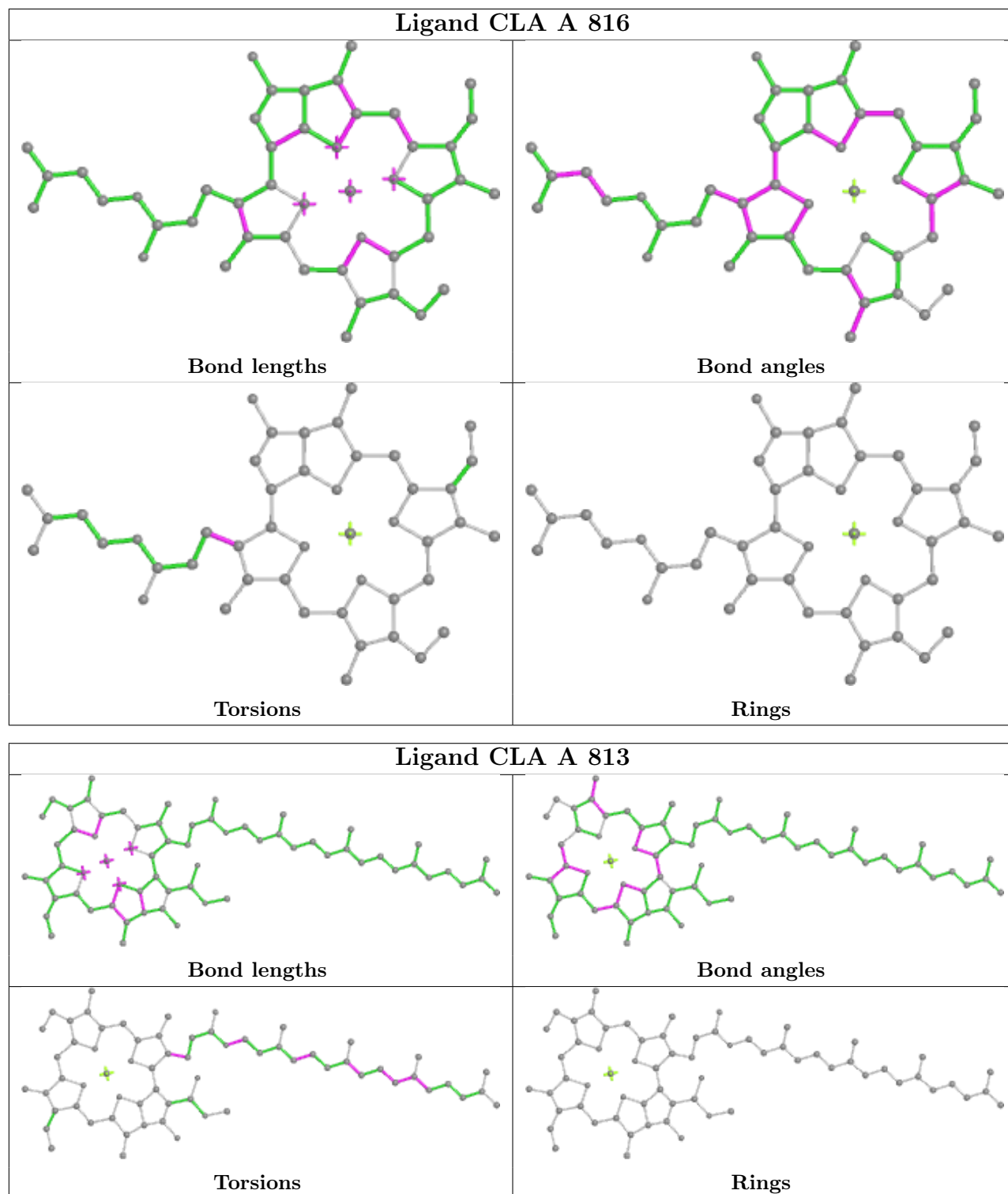


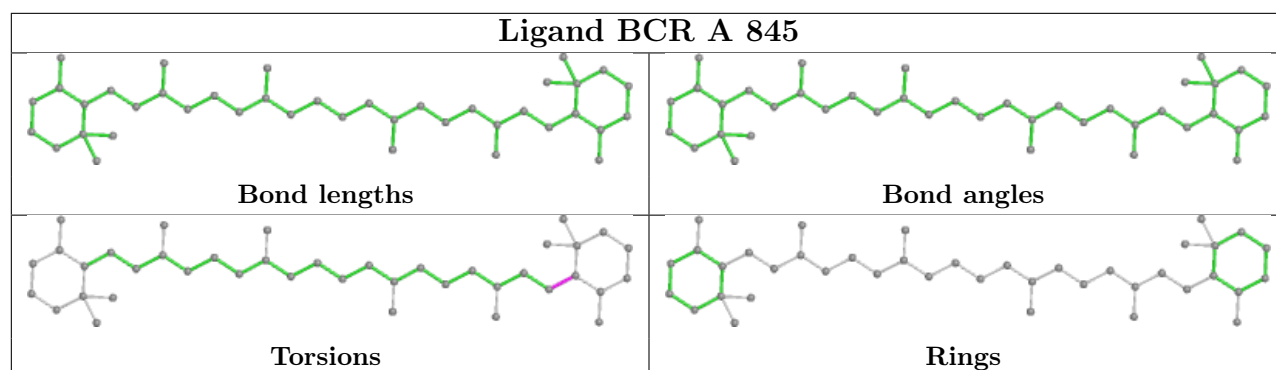
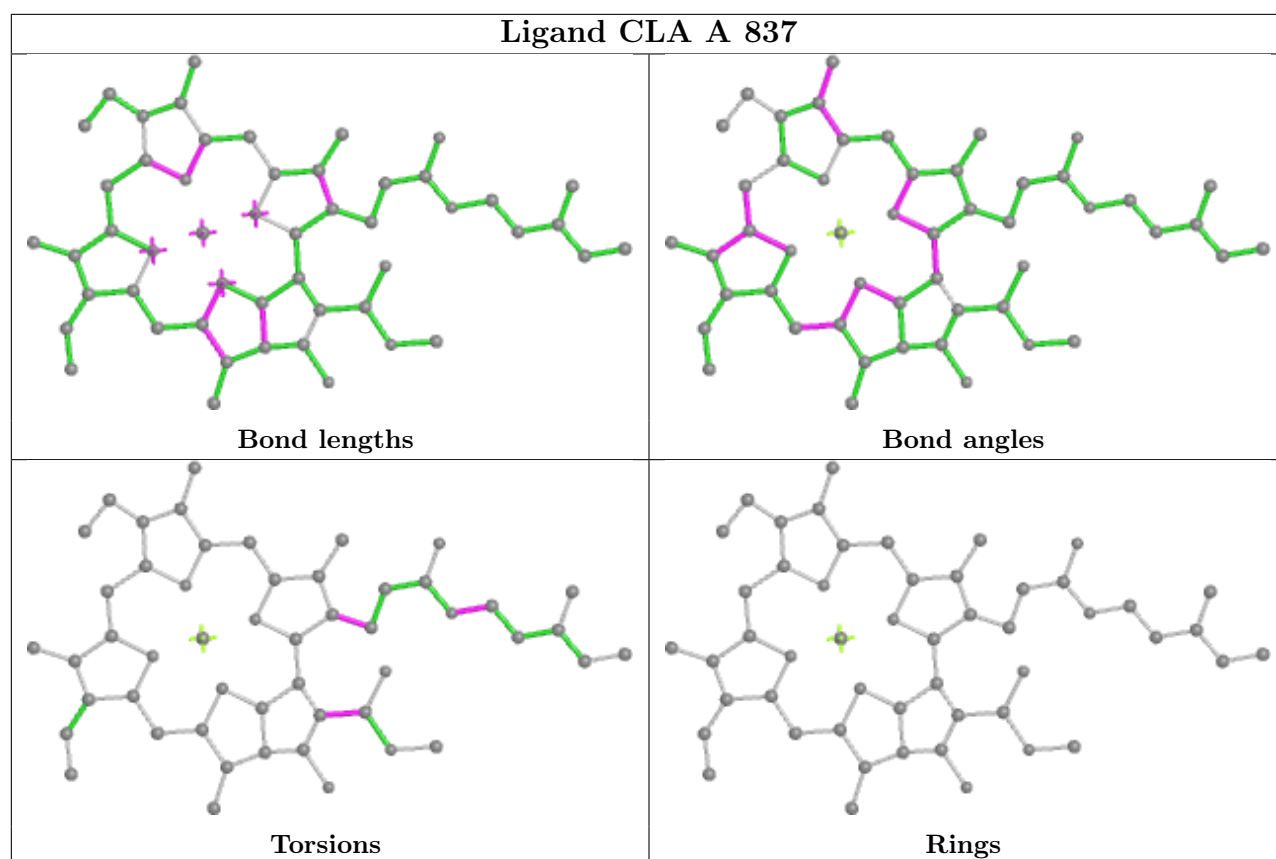
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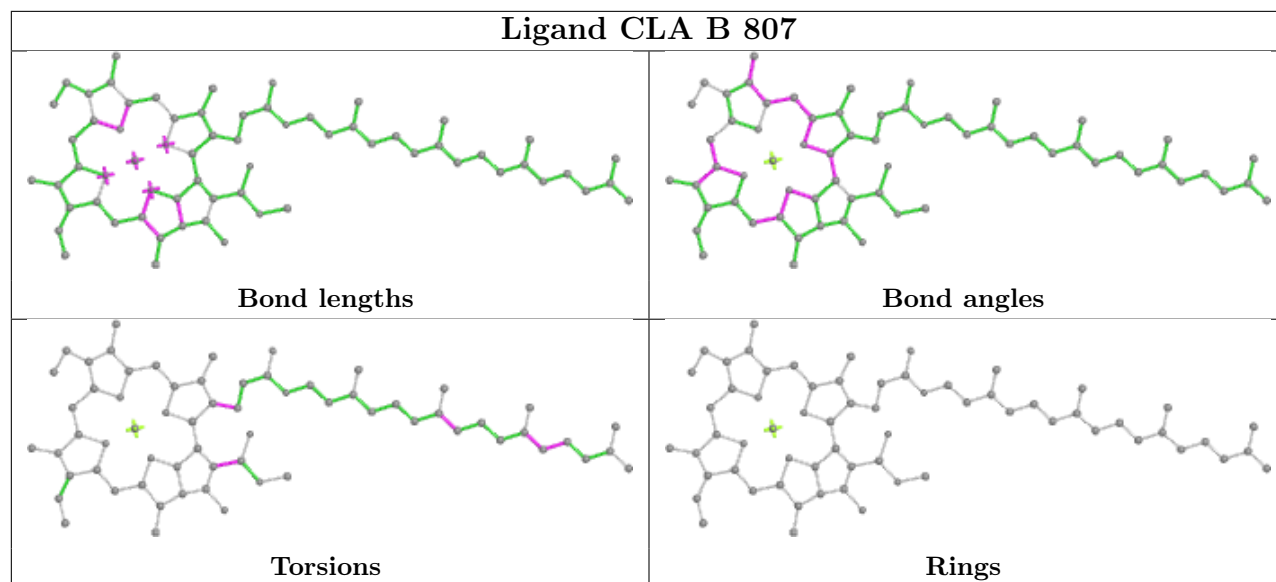
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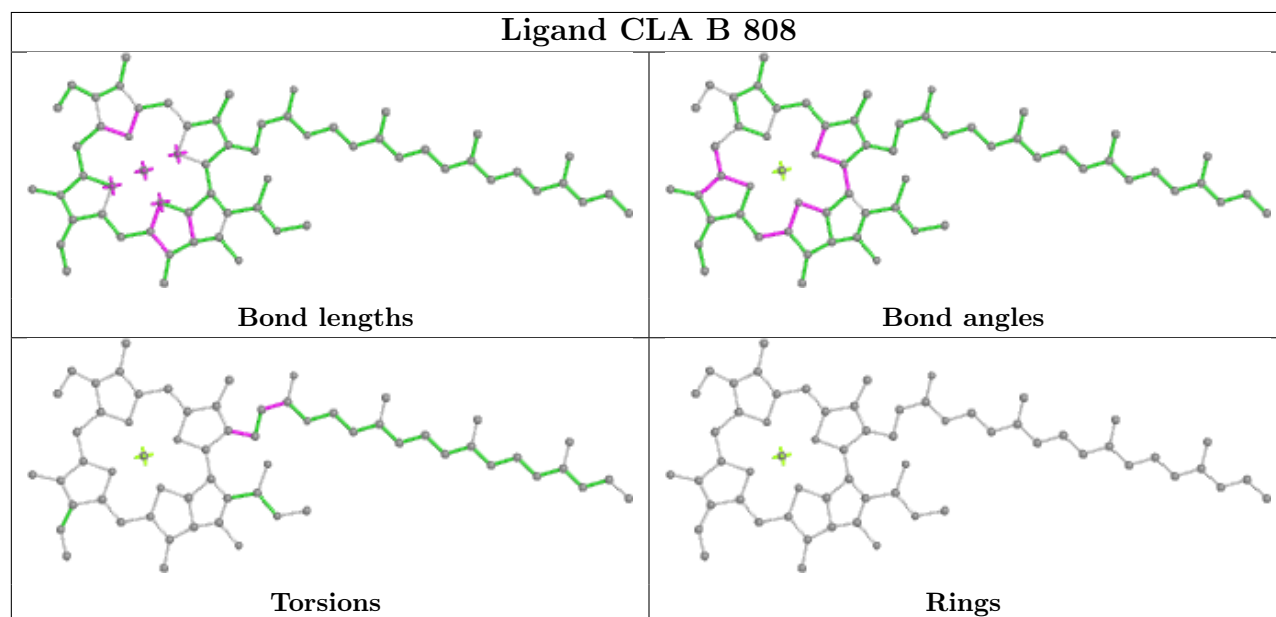




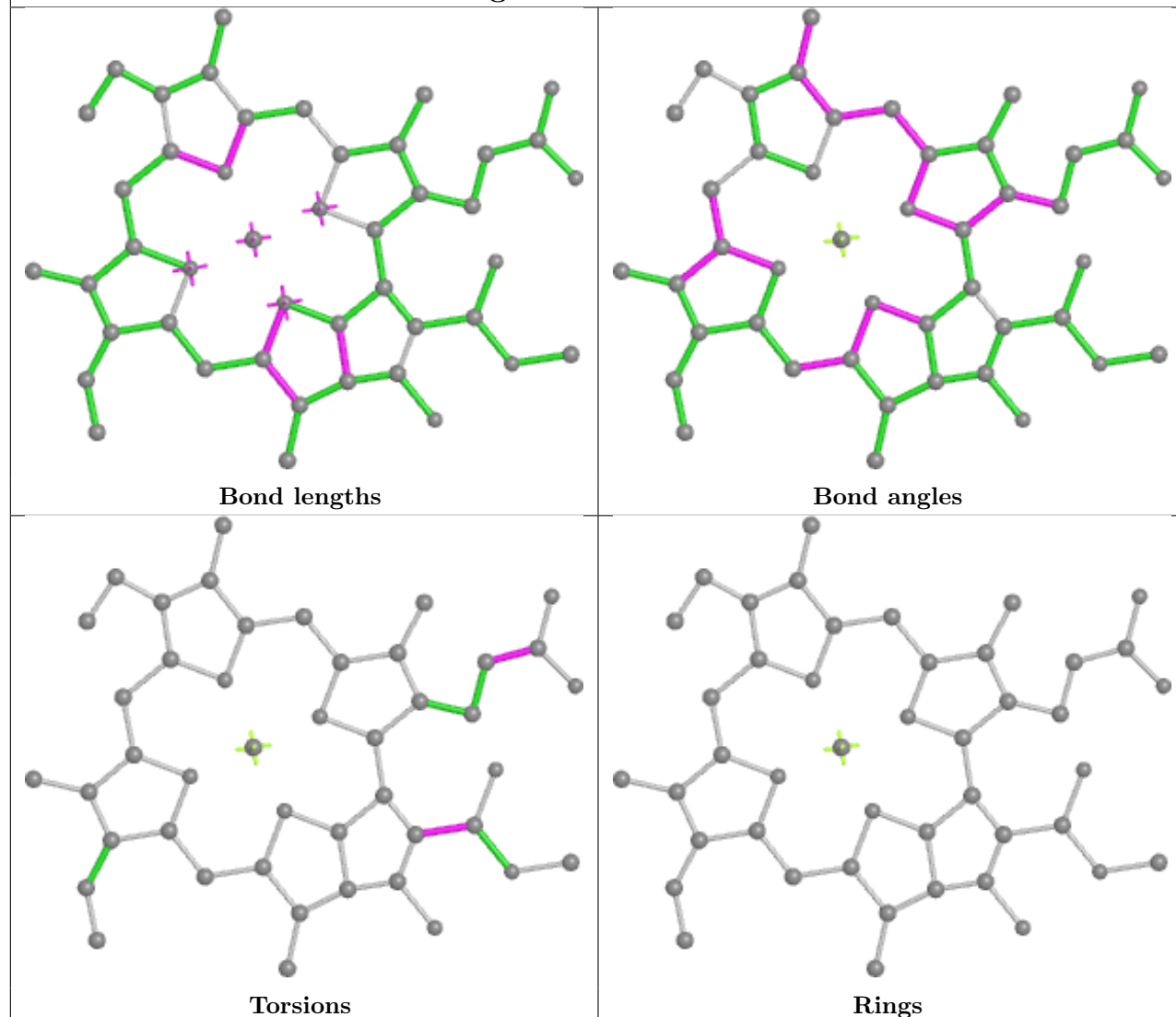
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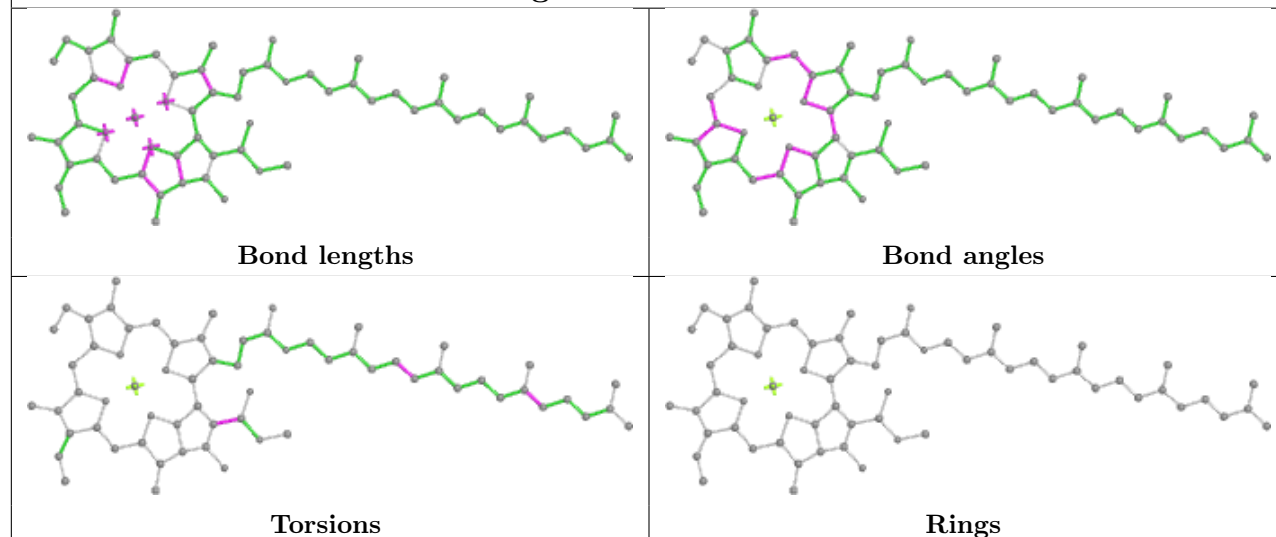
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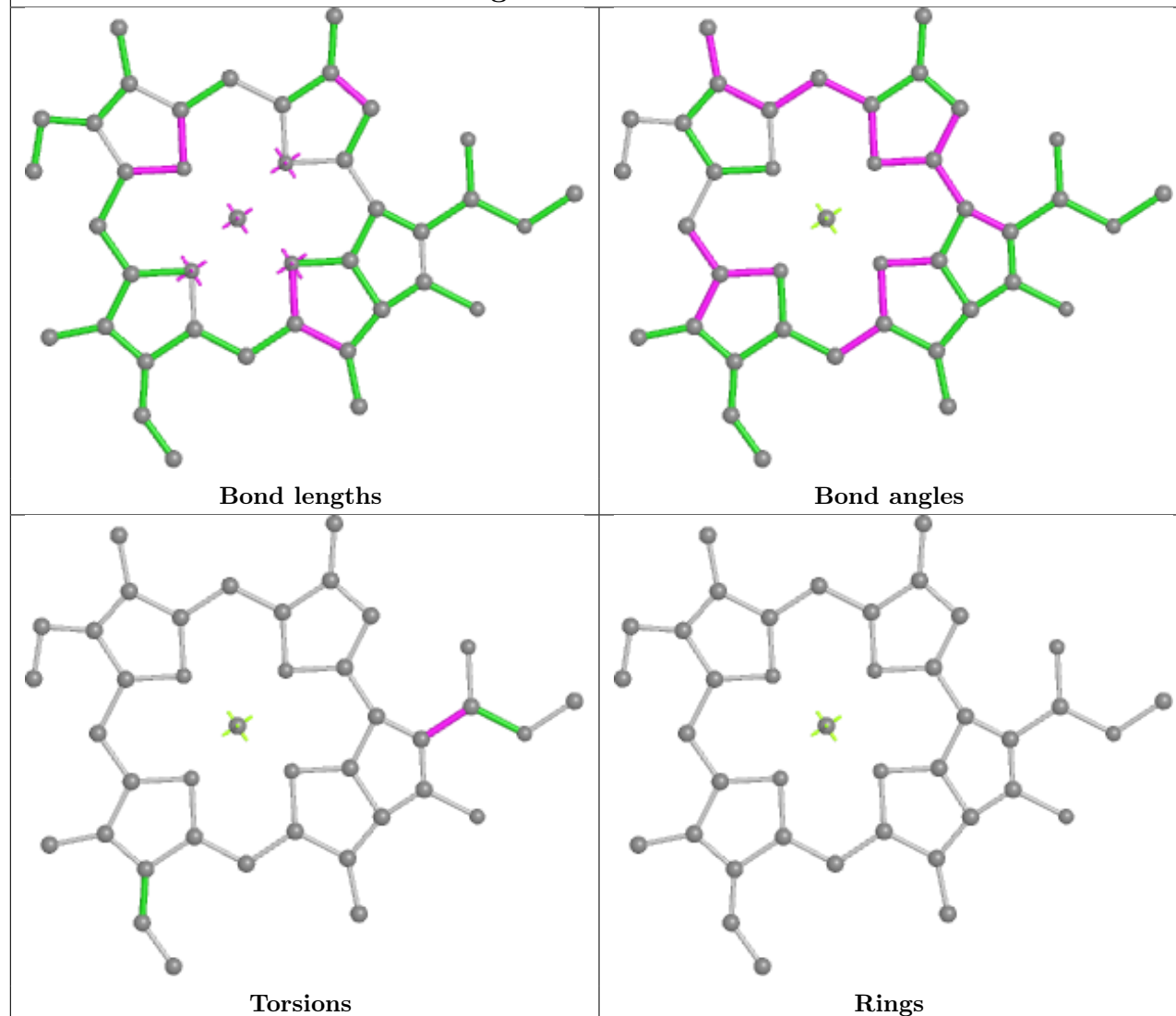
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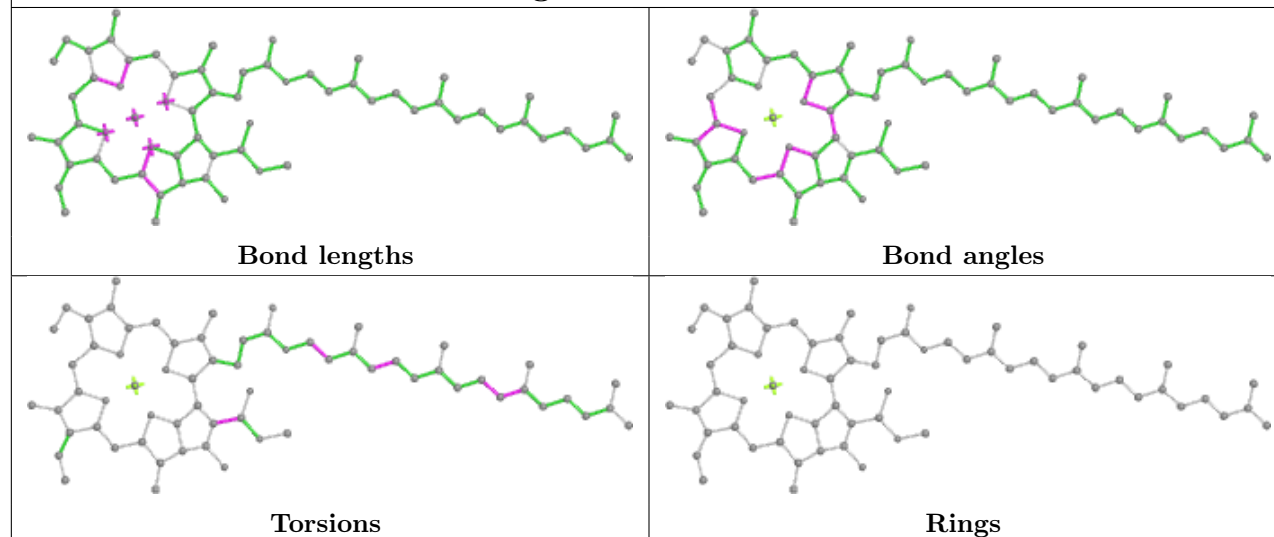
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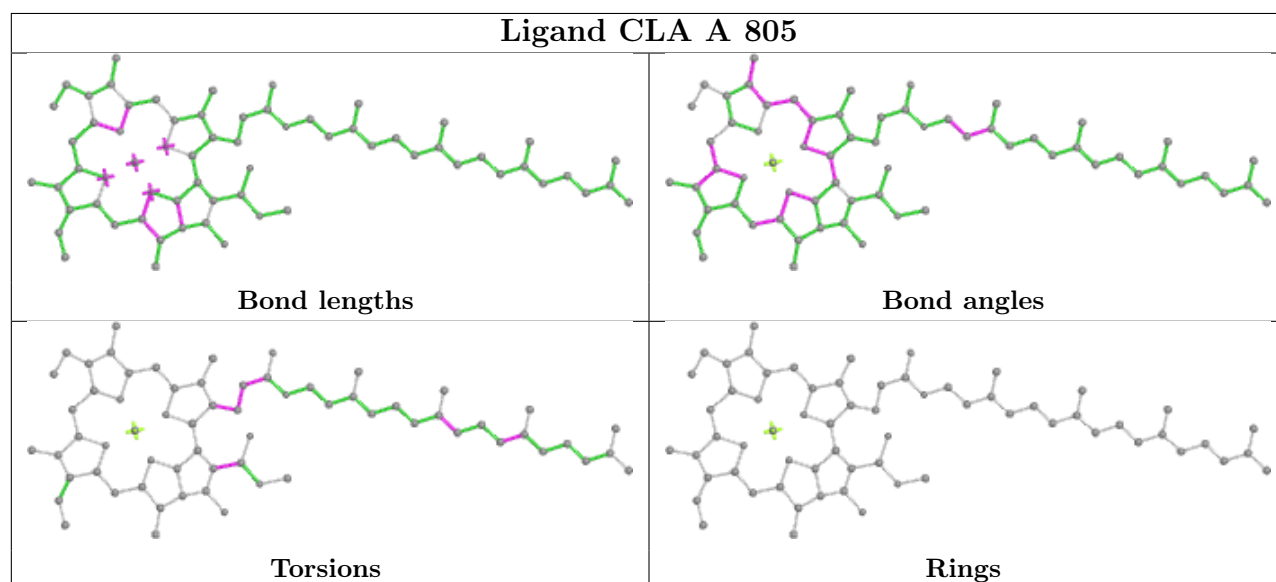
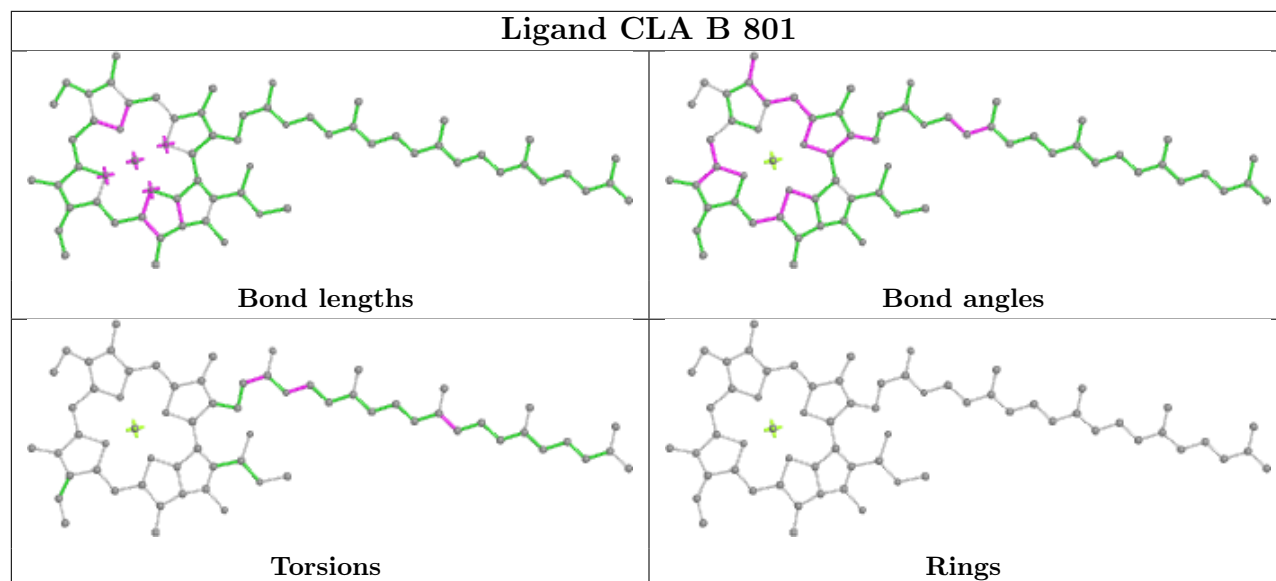
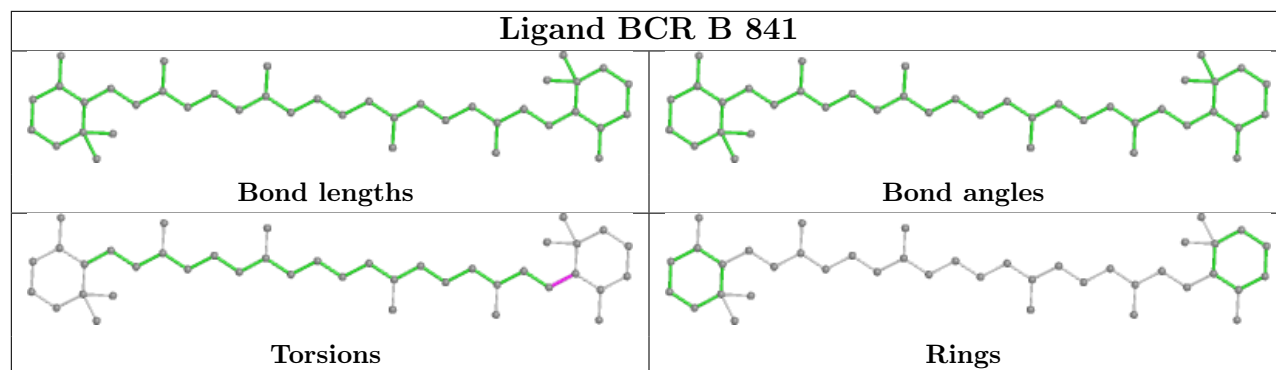


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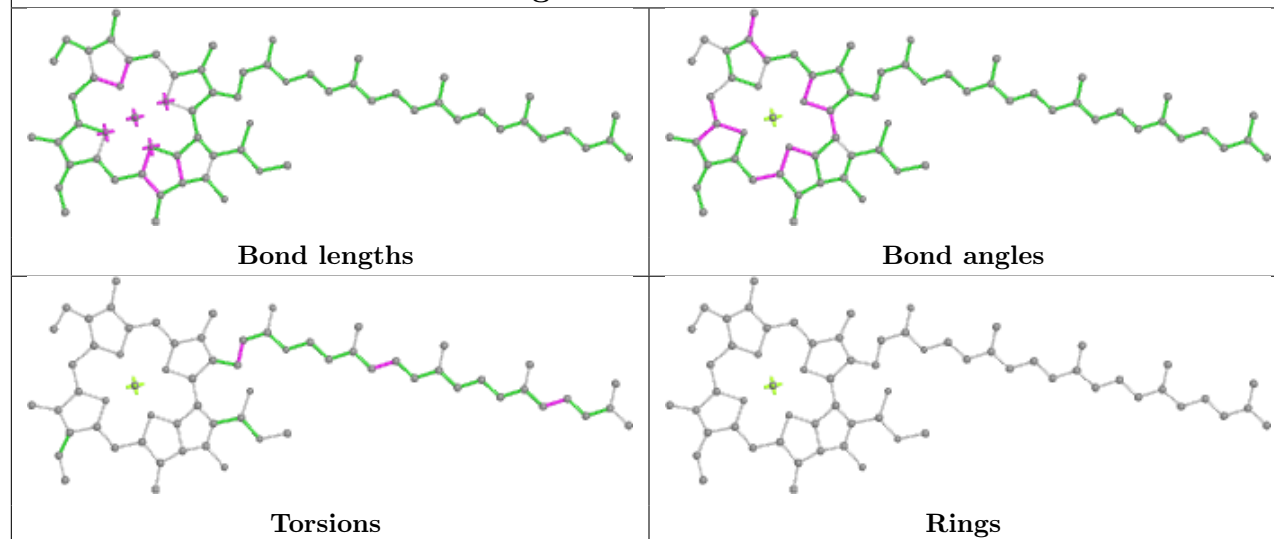


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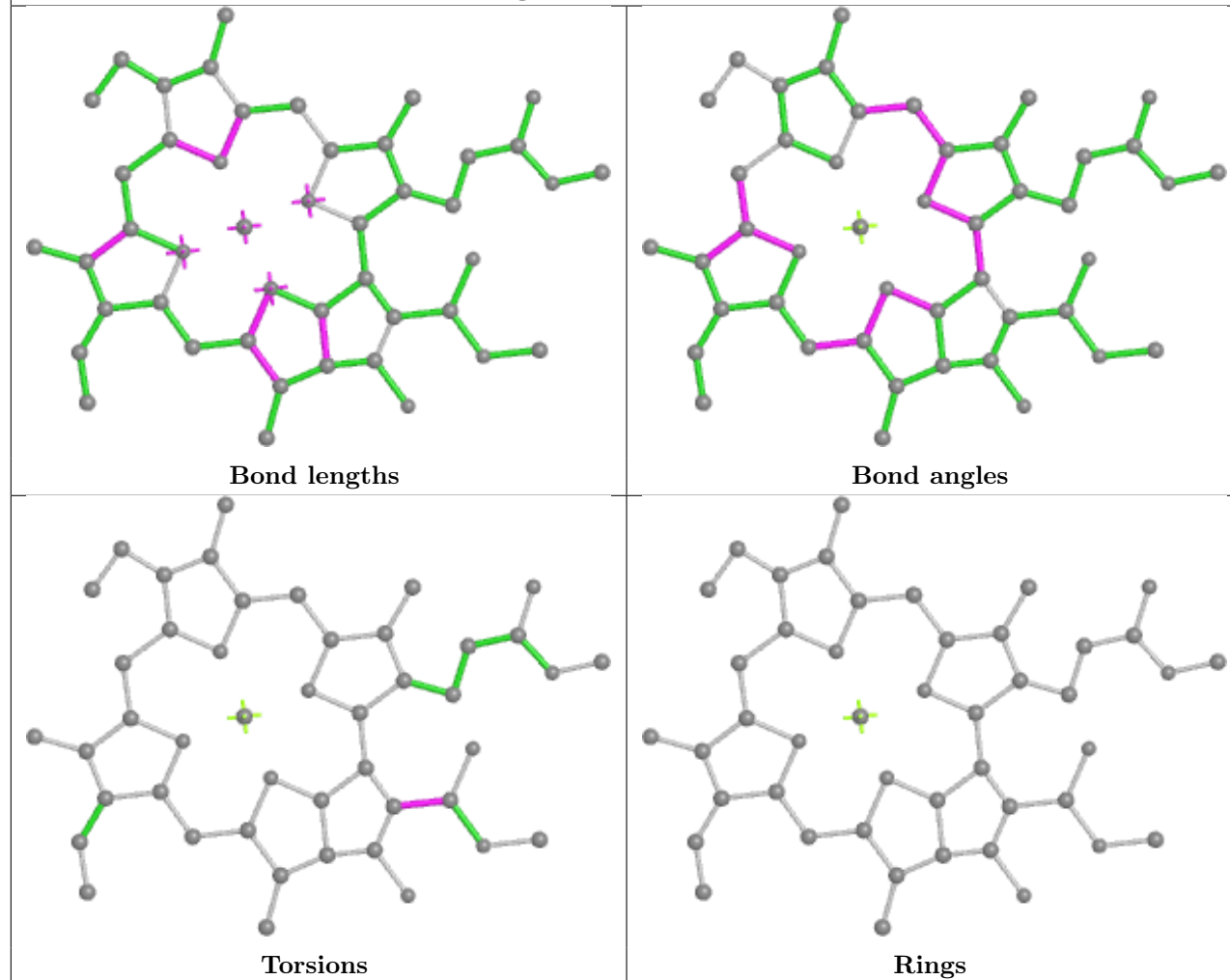


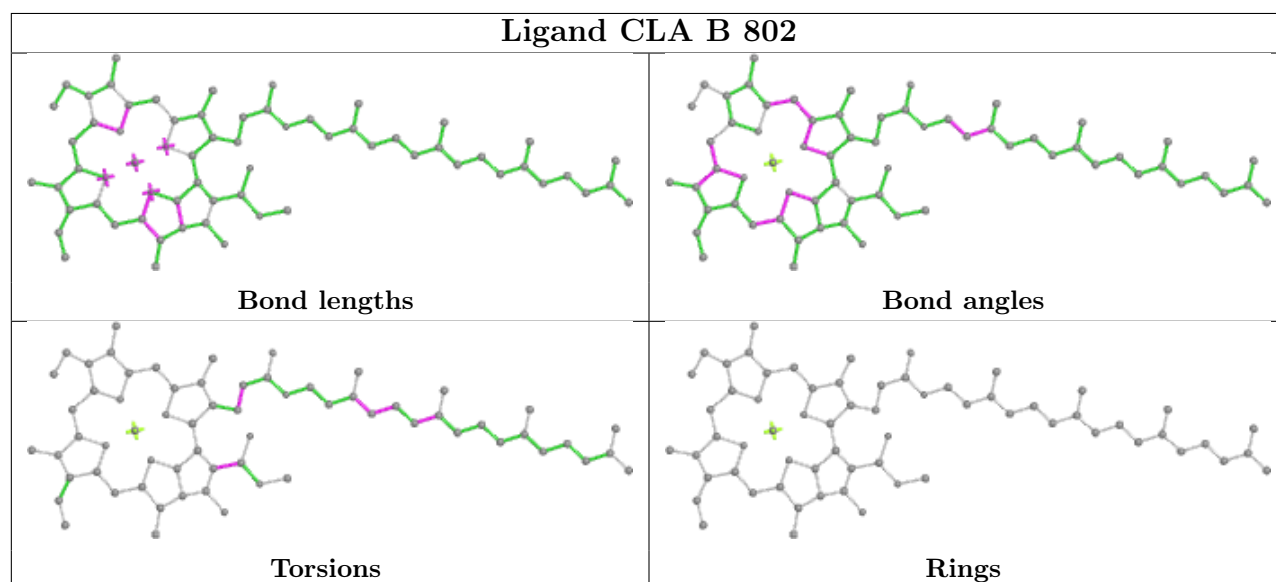
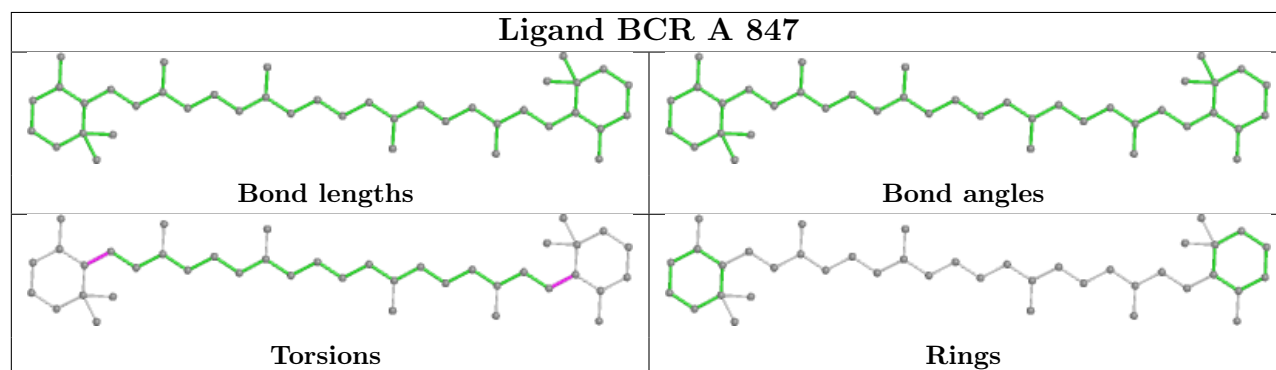
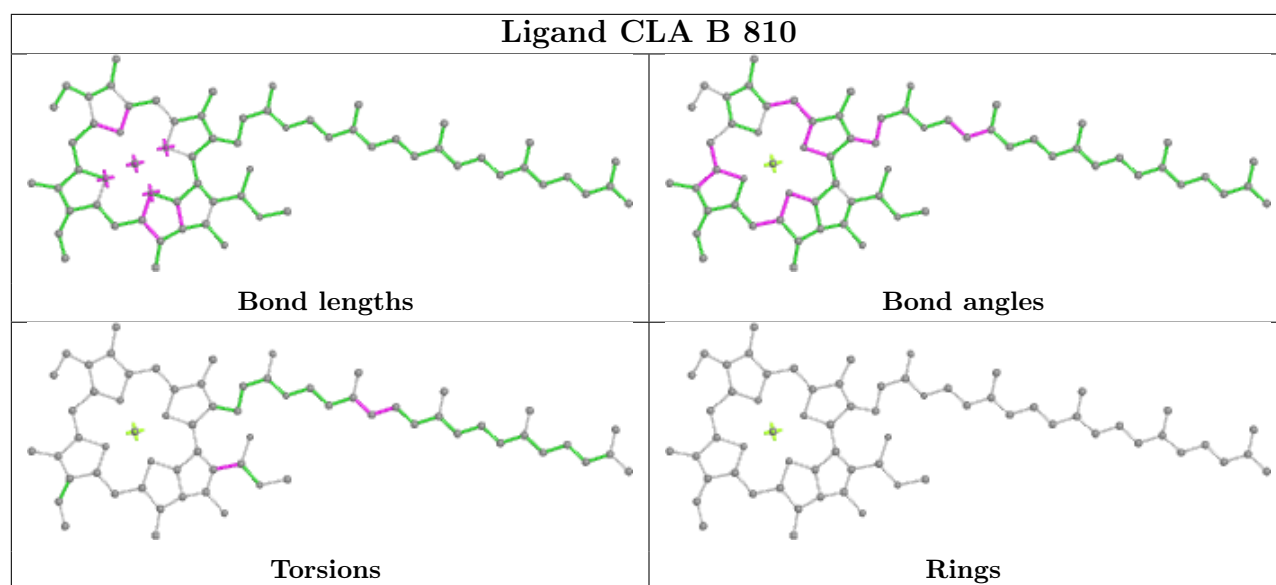


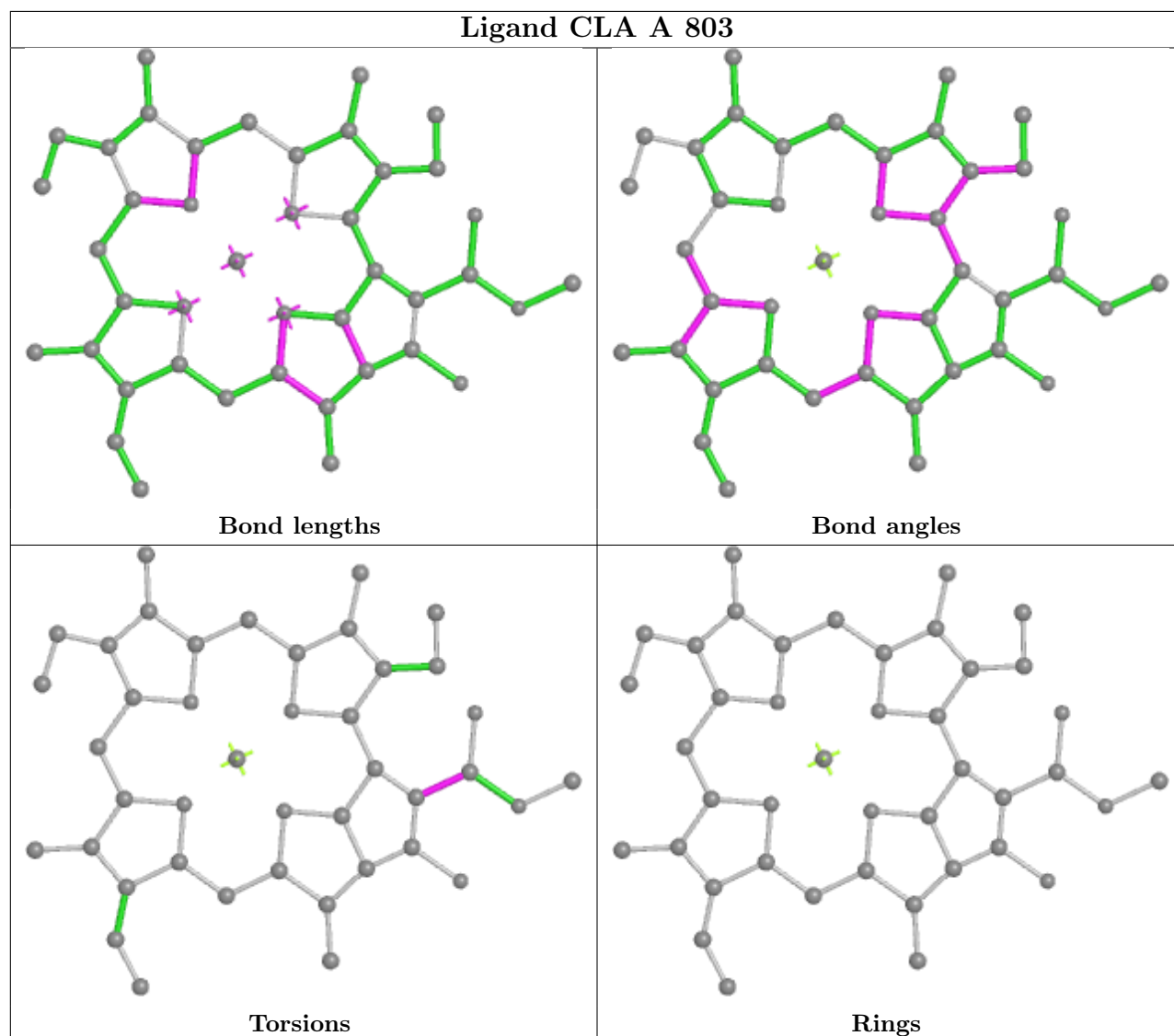
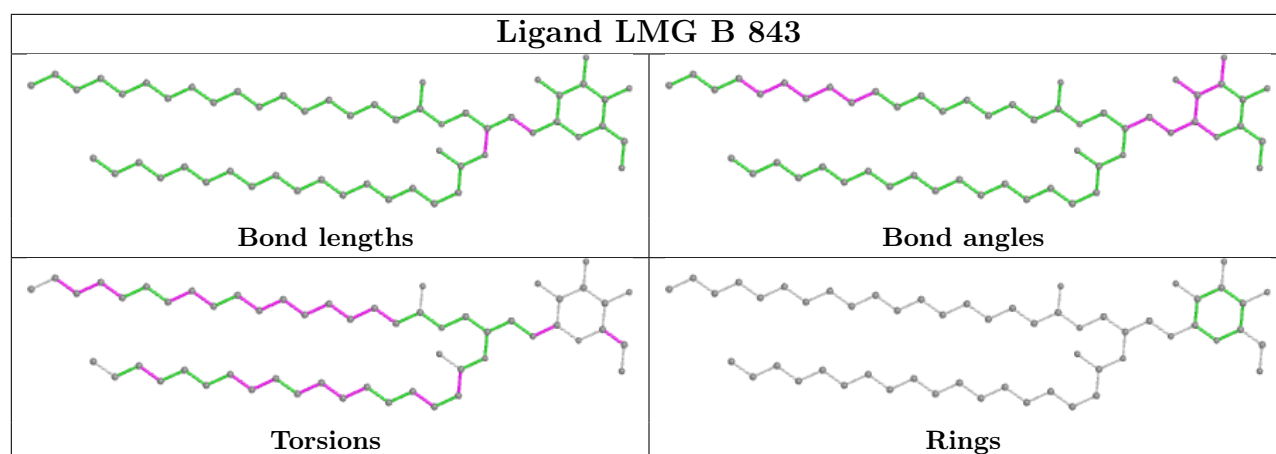
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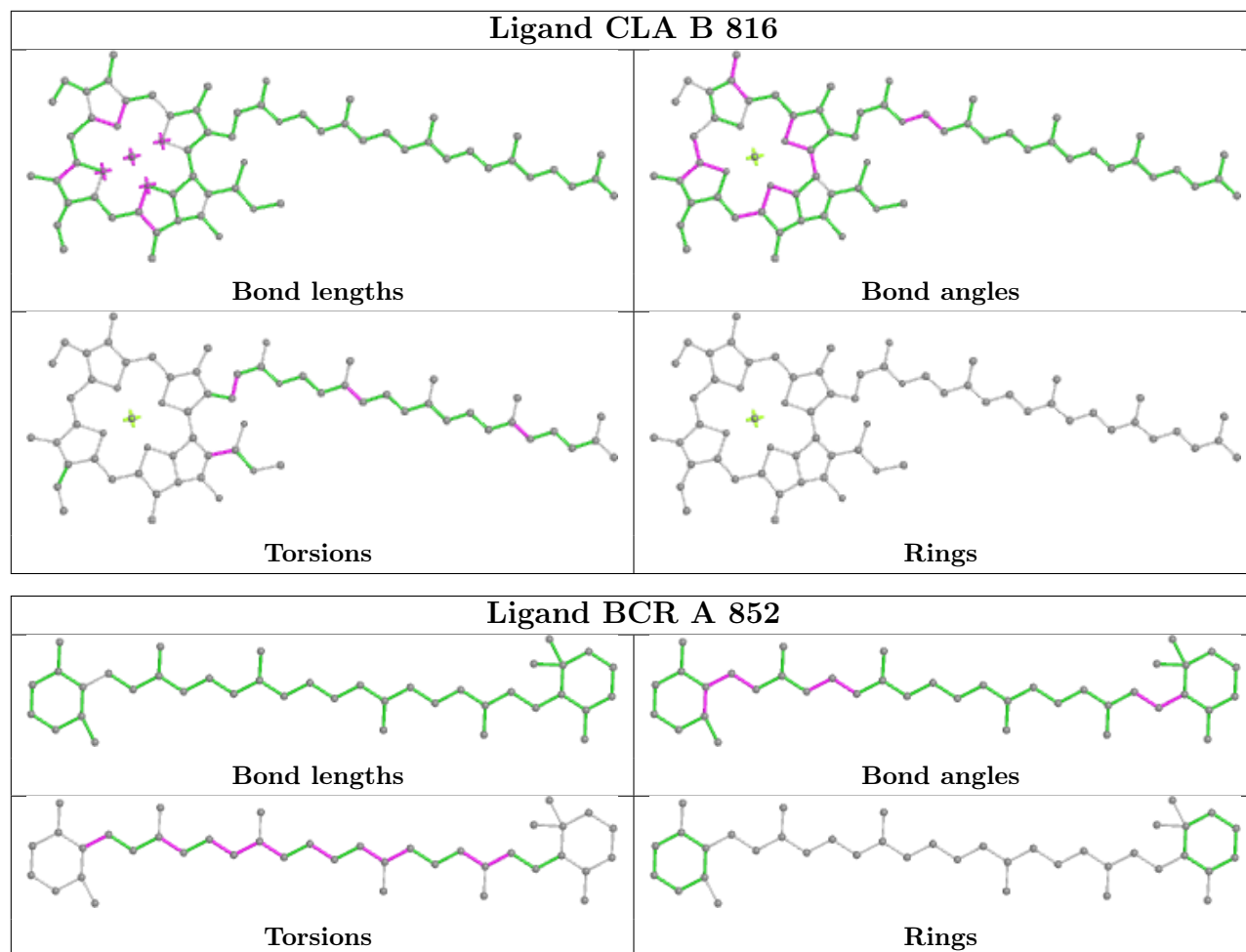


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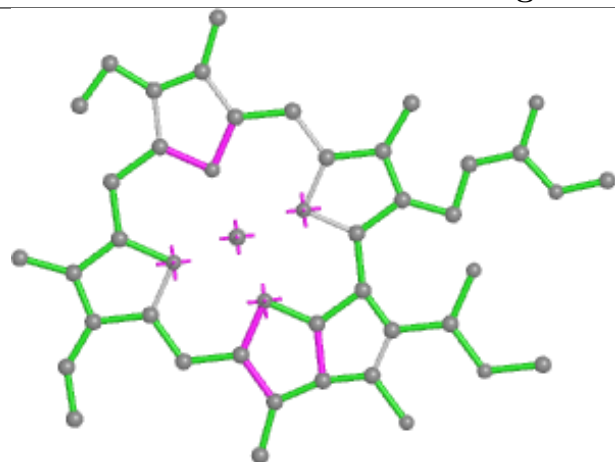




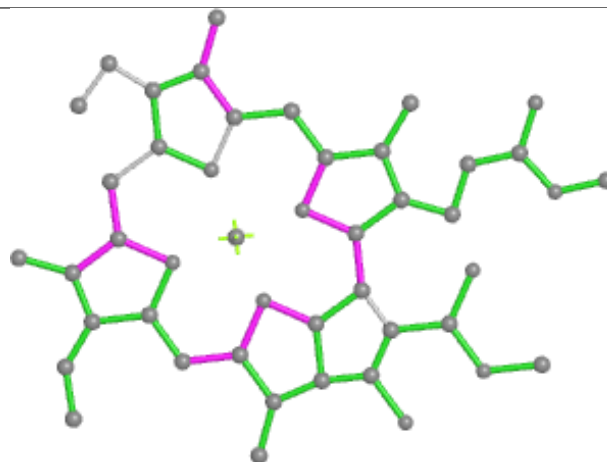




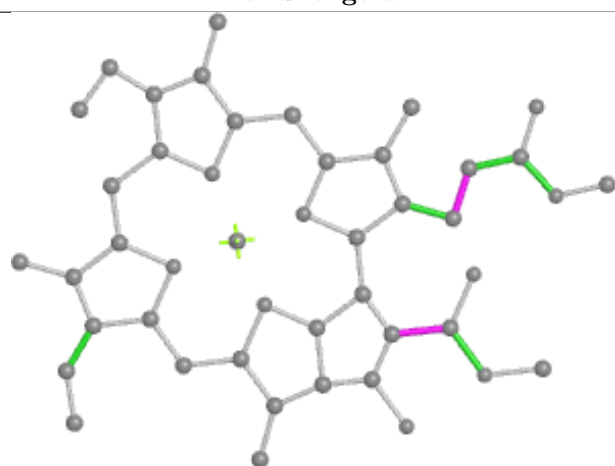
Ligand CLA B 806



Bond lengths



Bond angles

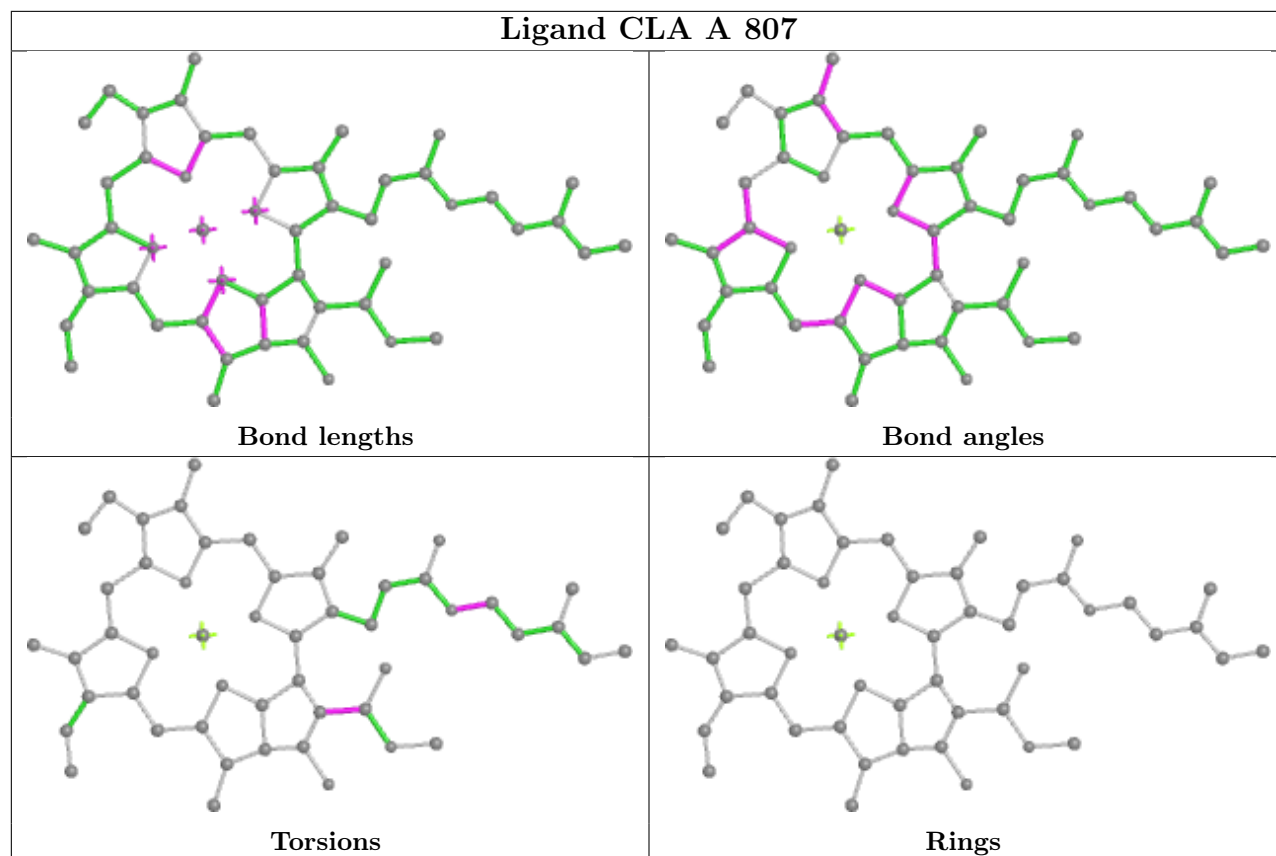


Torsions

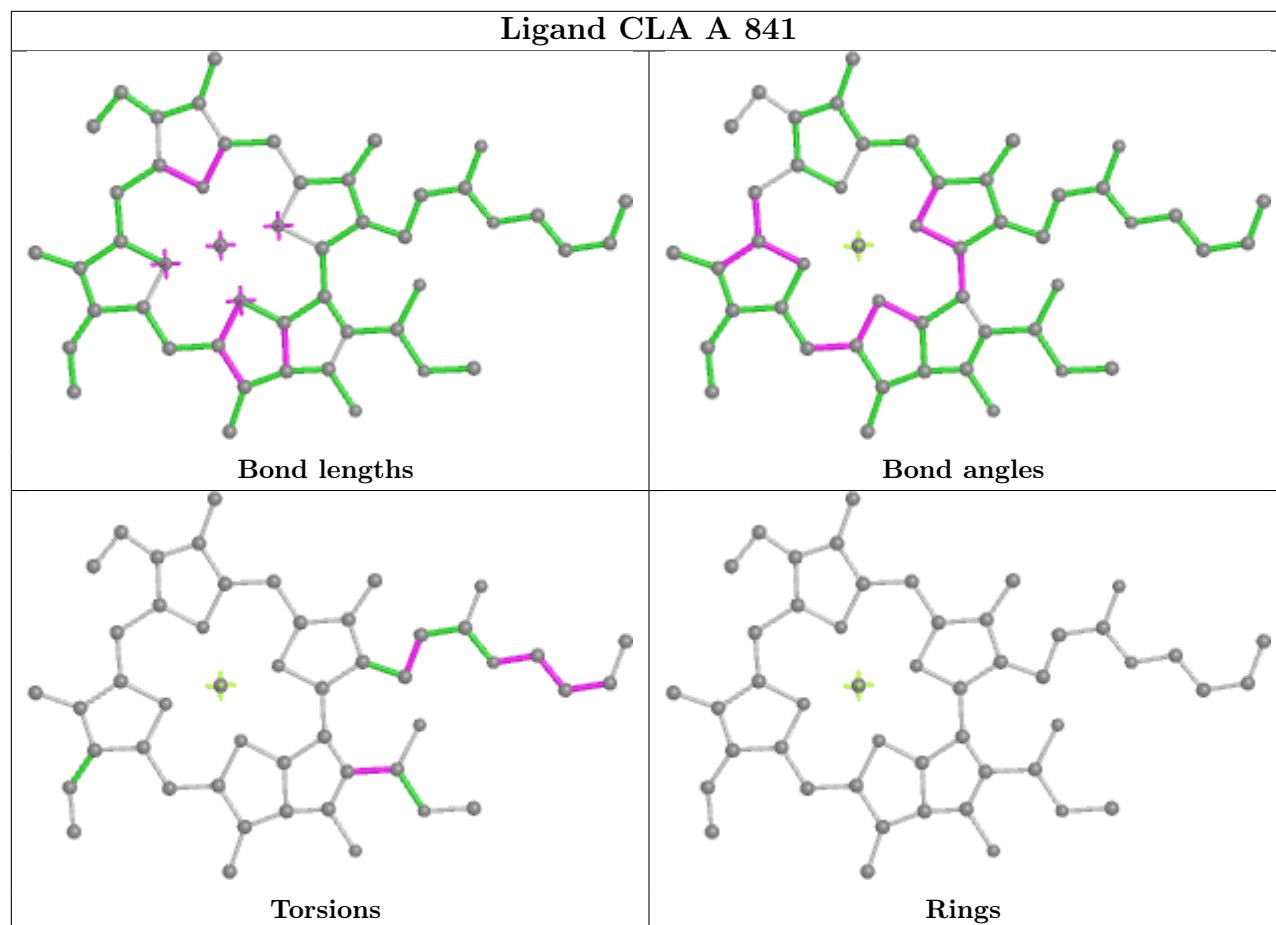


Rings

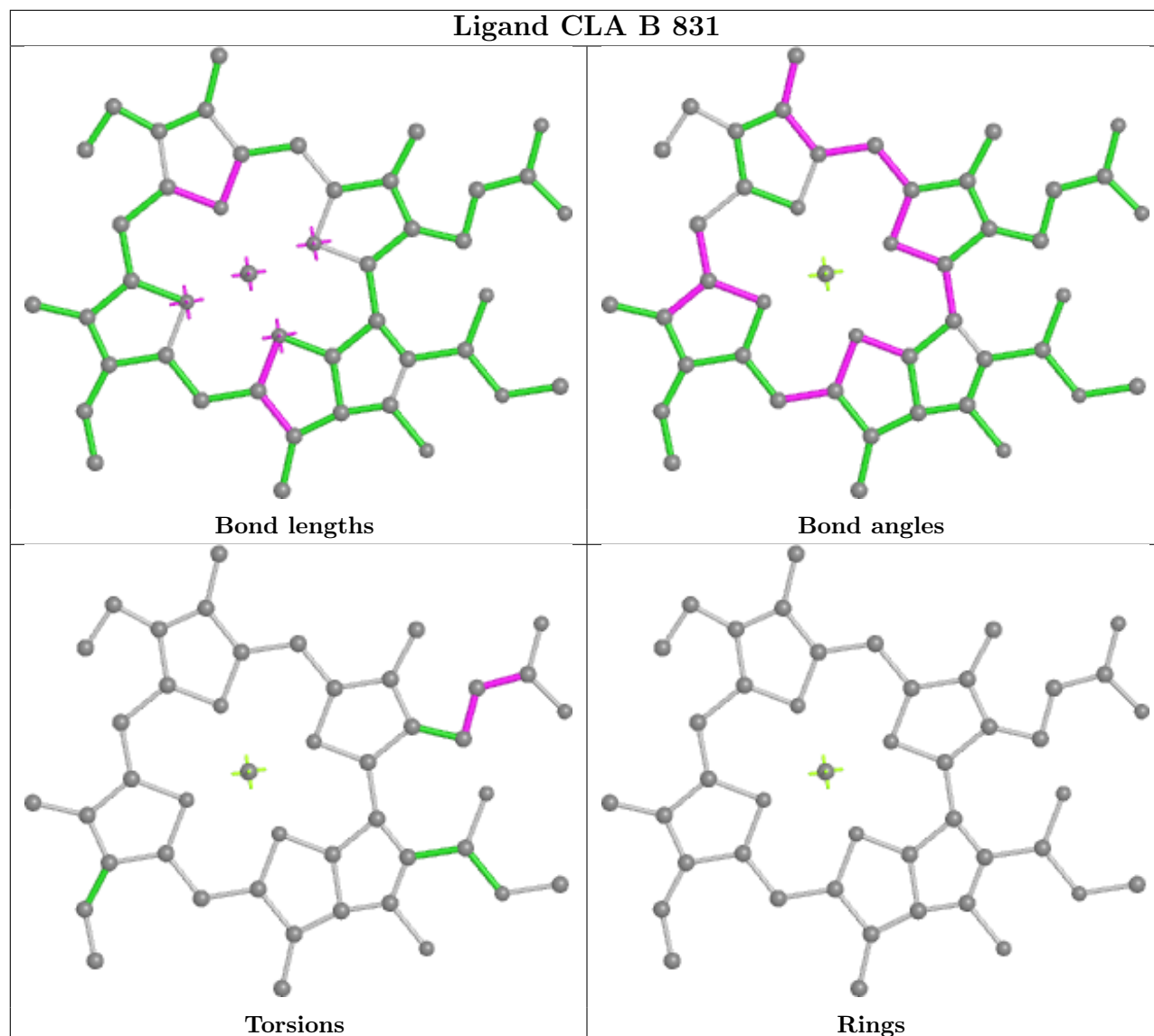
Ligand CLA A 807



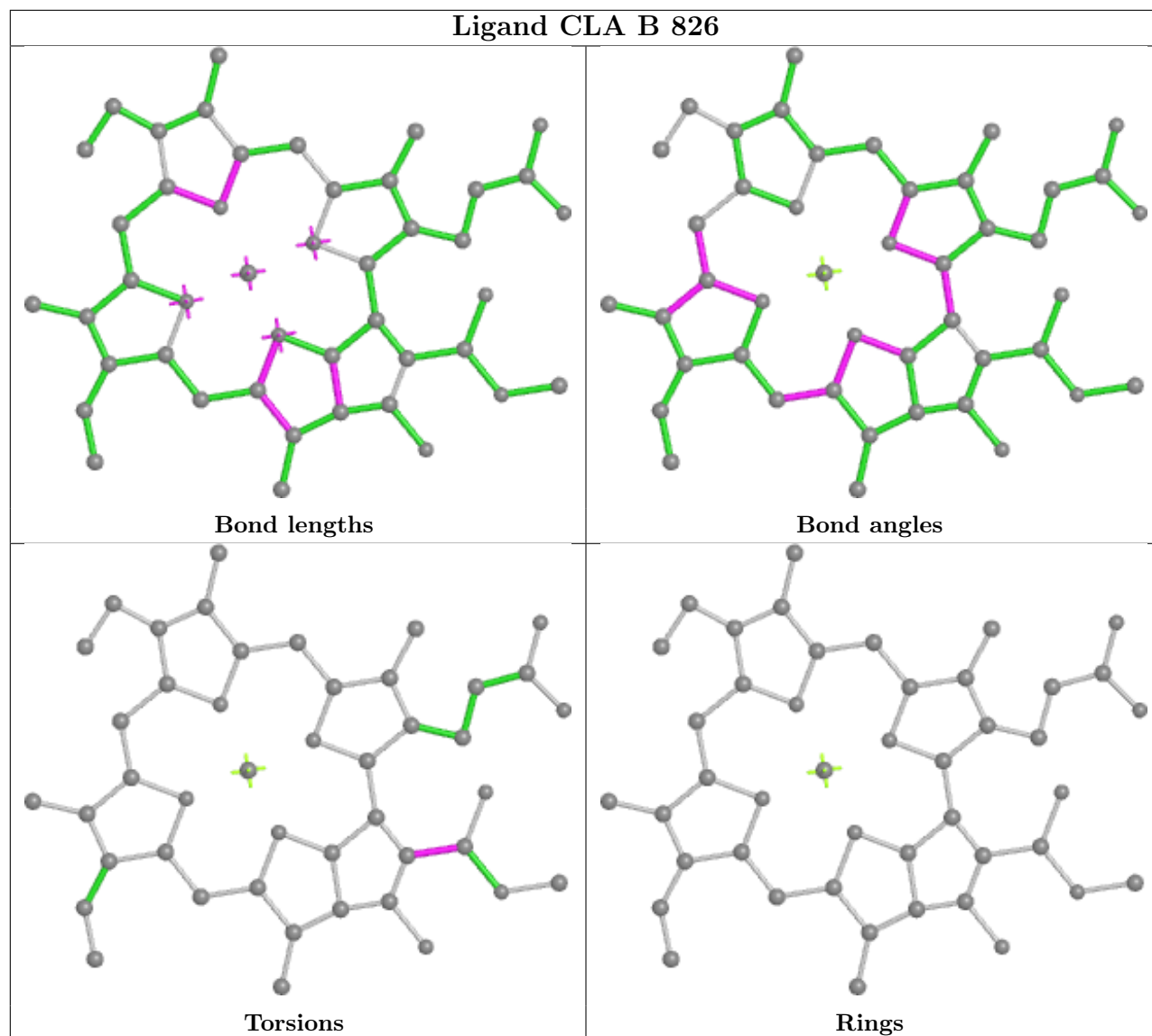
Ligand CLA A 841



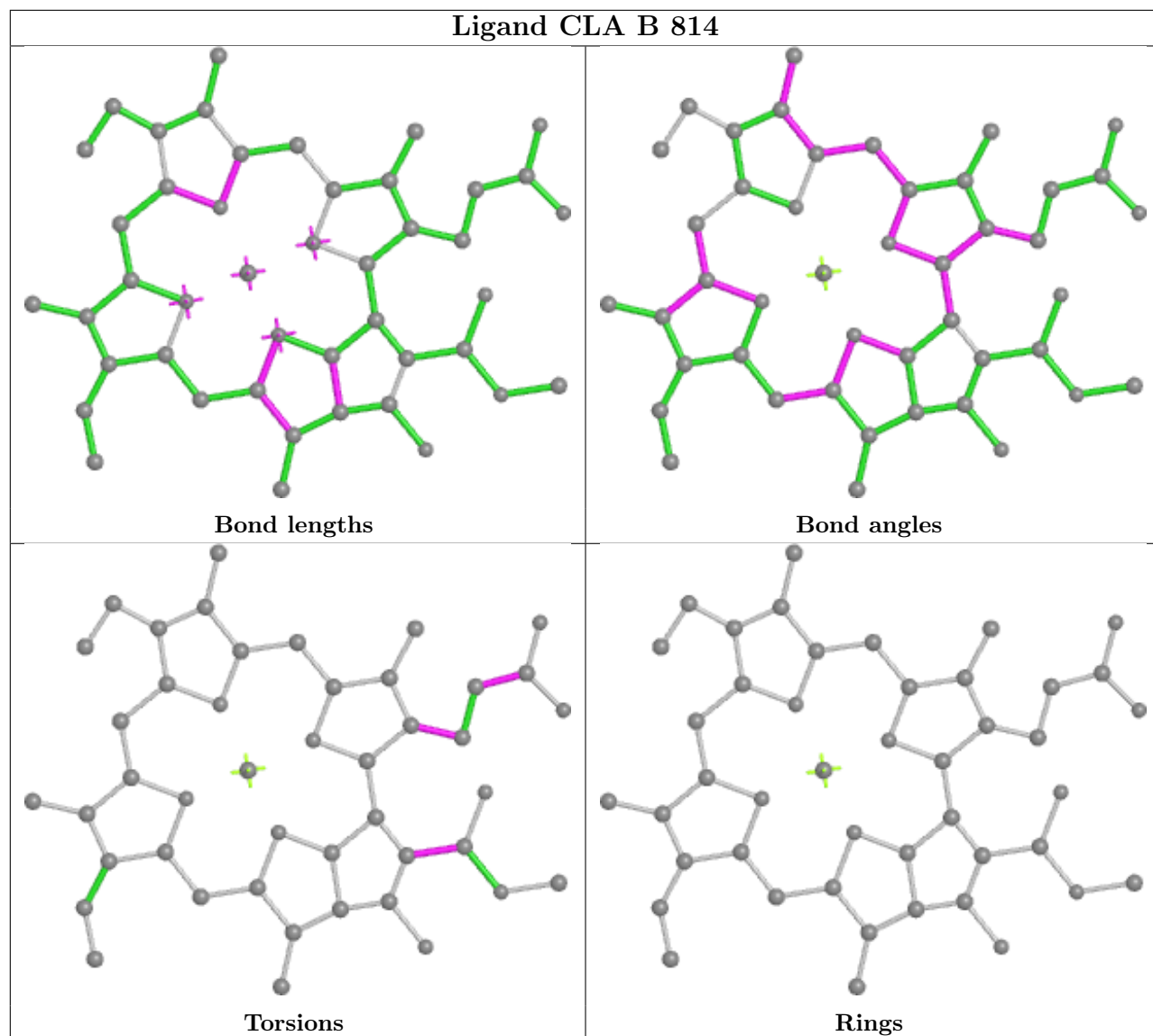
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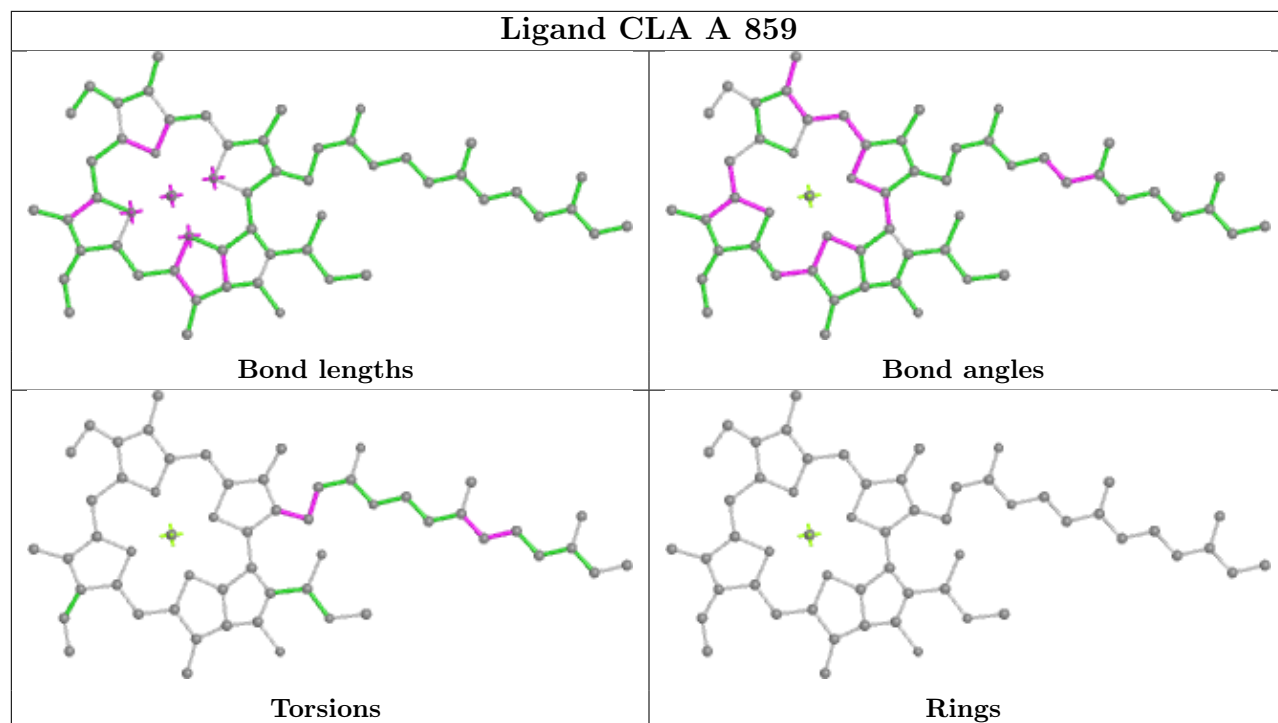


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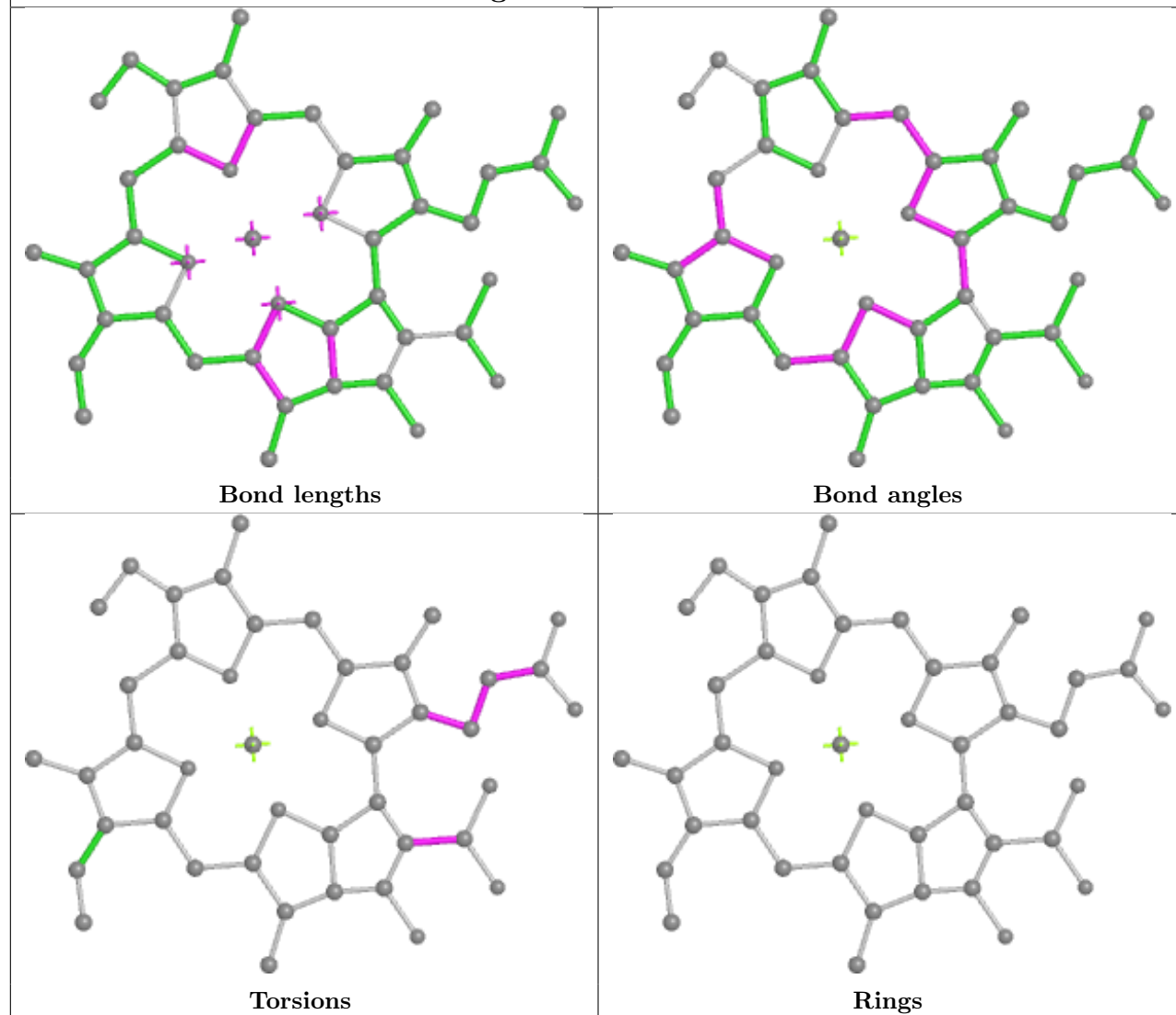


Ligand CLA B 814

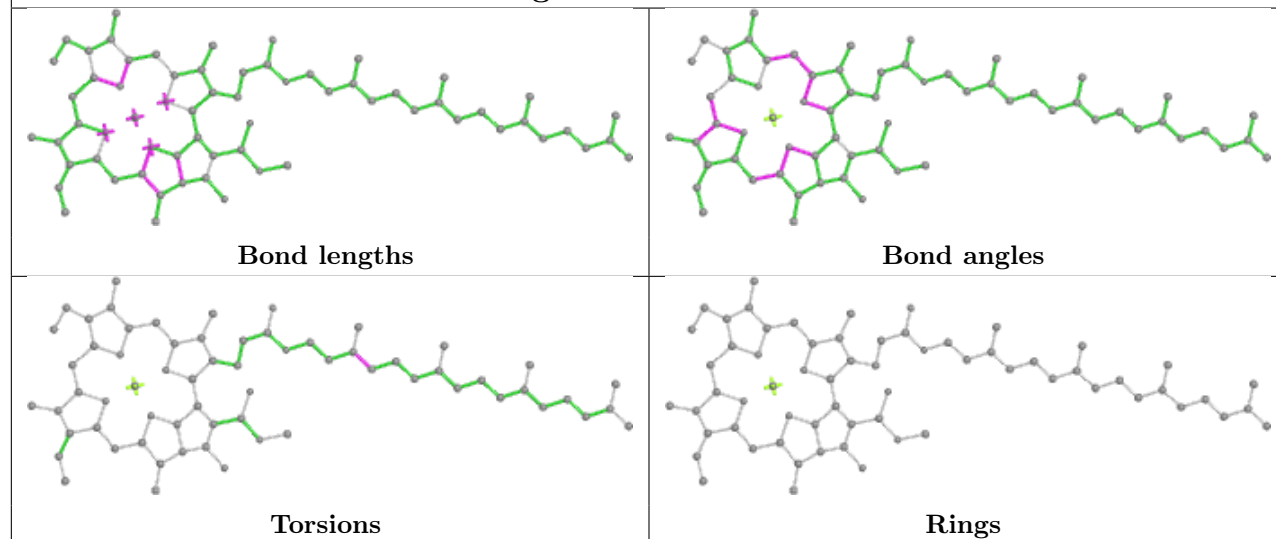


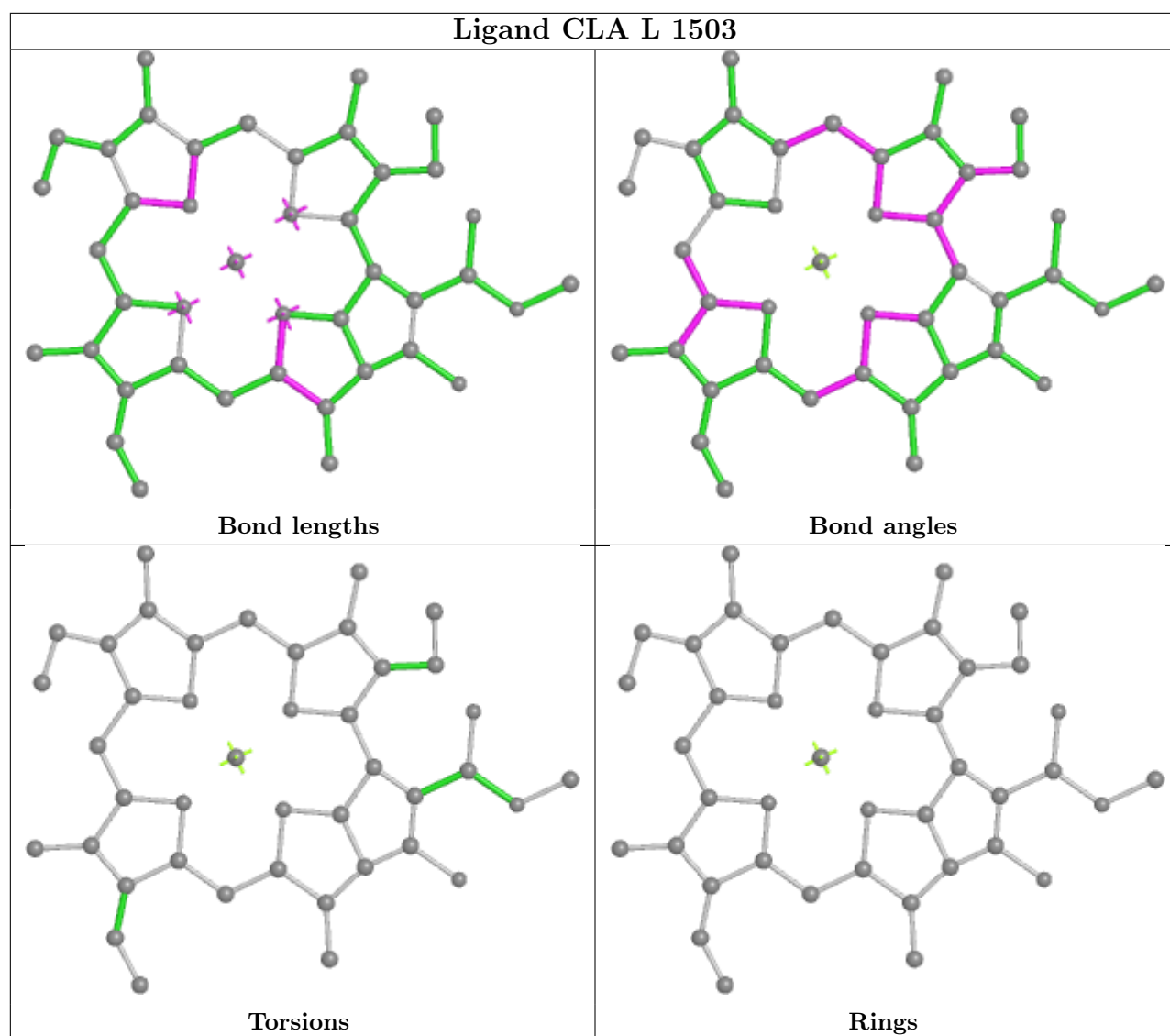


Ligand CLA B 822

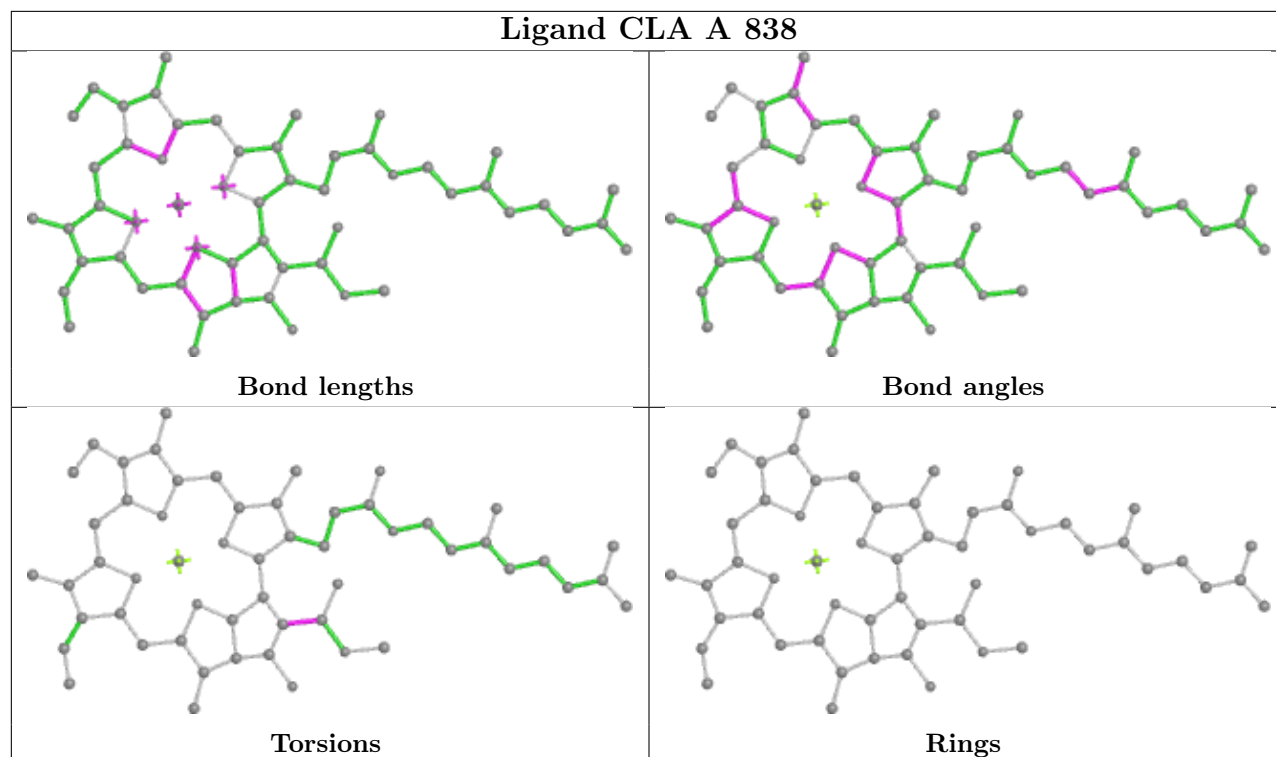


Ligand CLA B 833

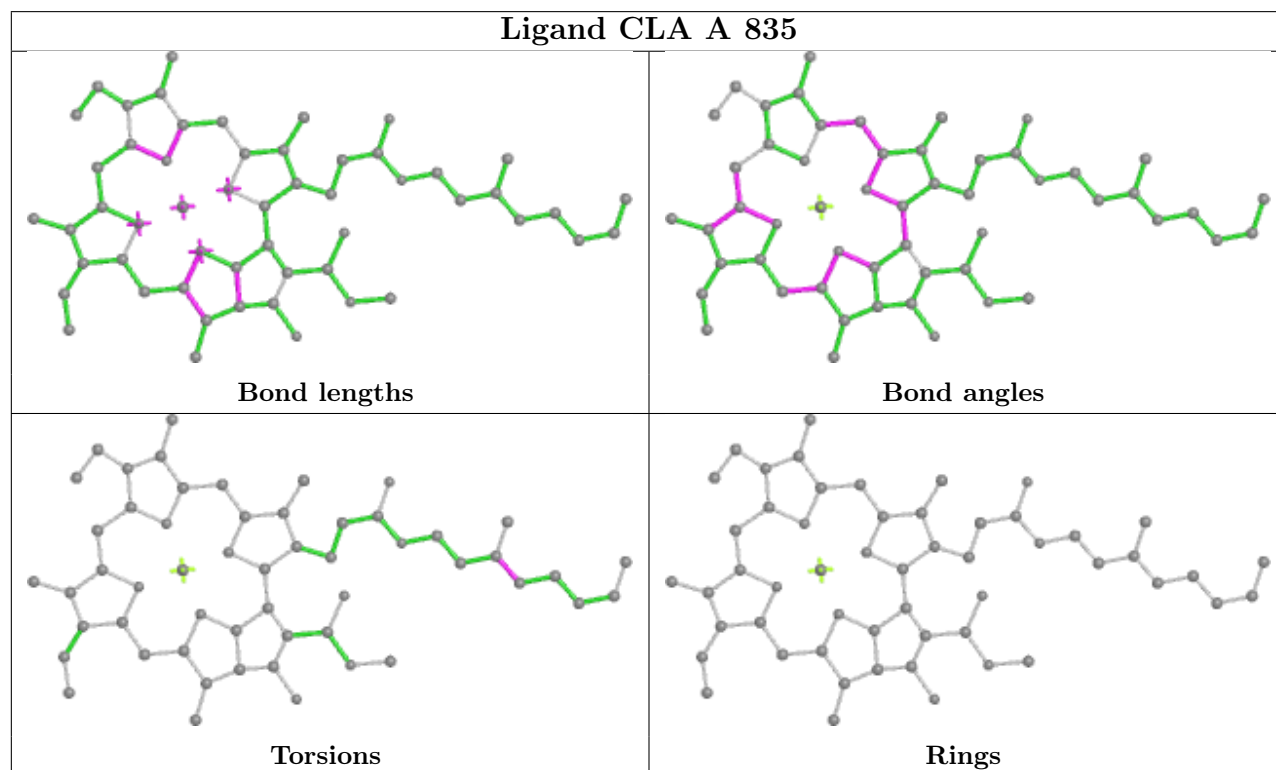




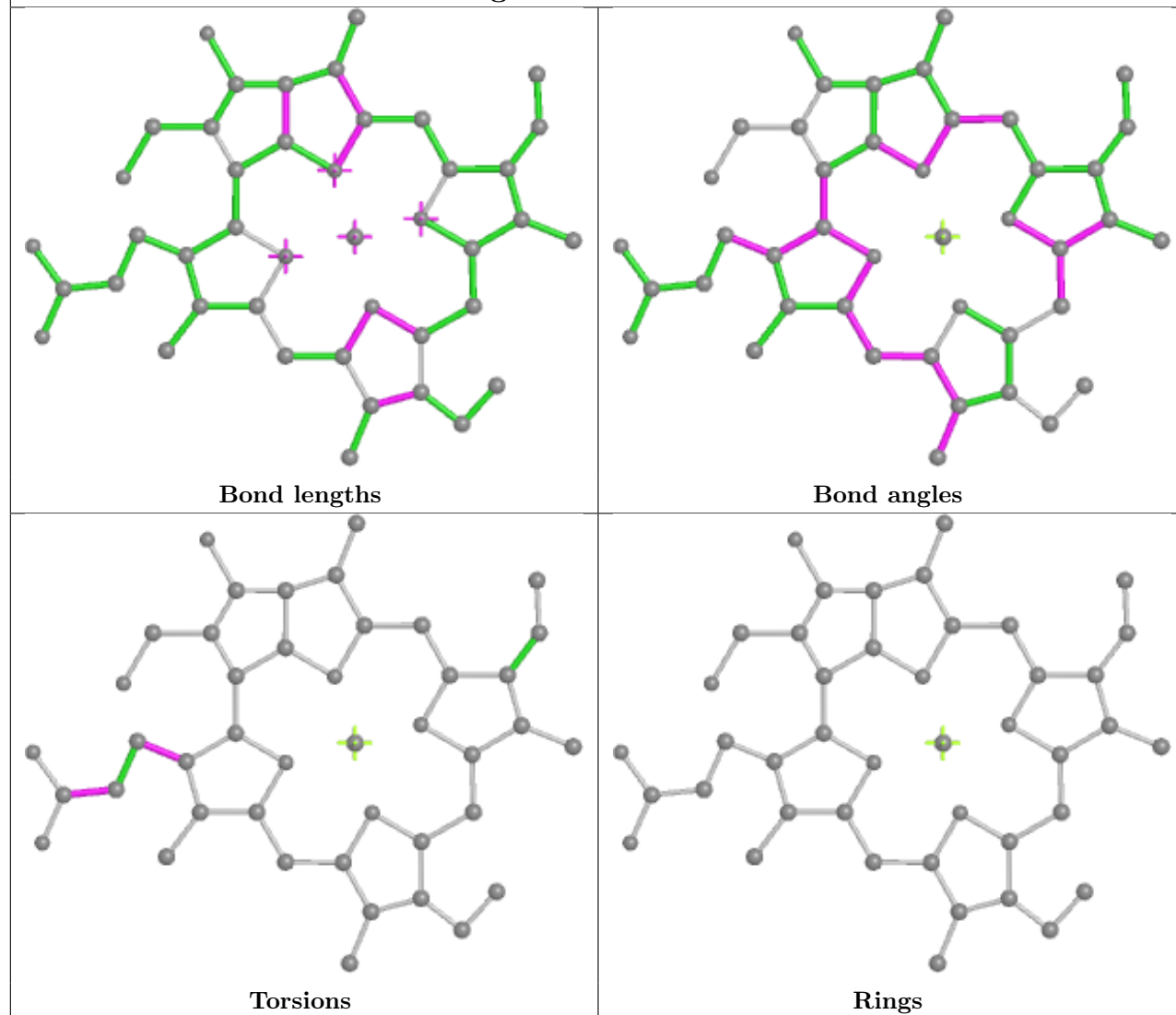
Ligand CLA A 838



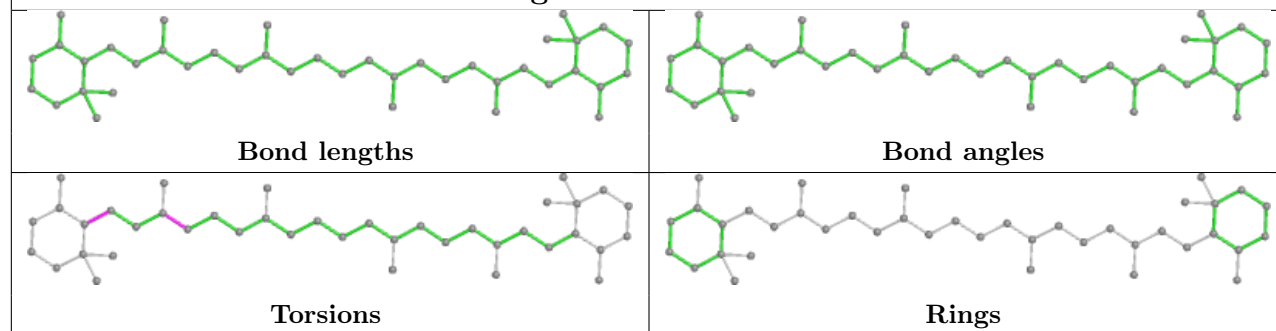
Ligand CLA A 835



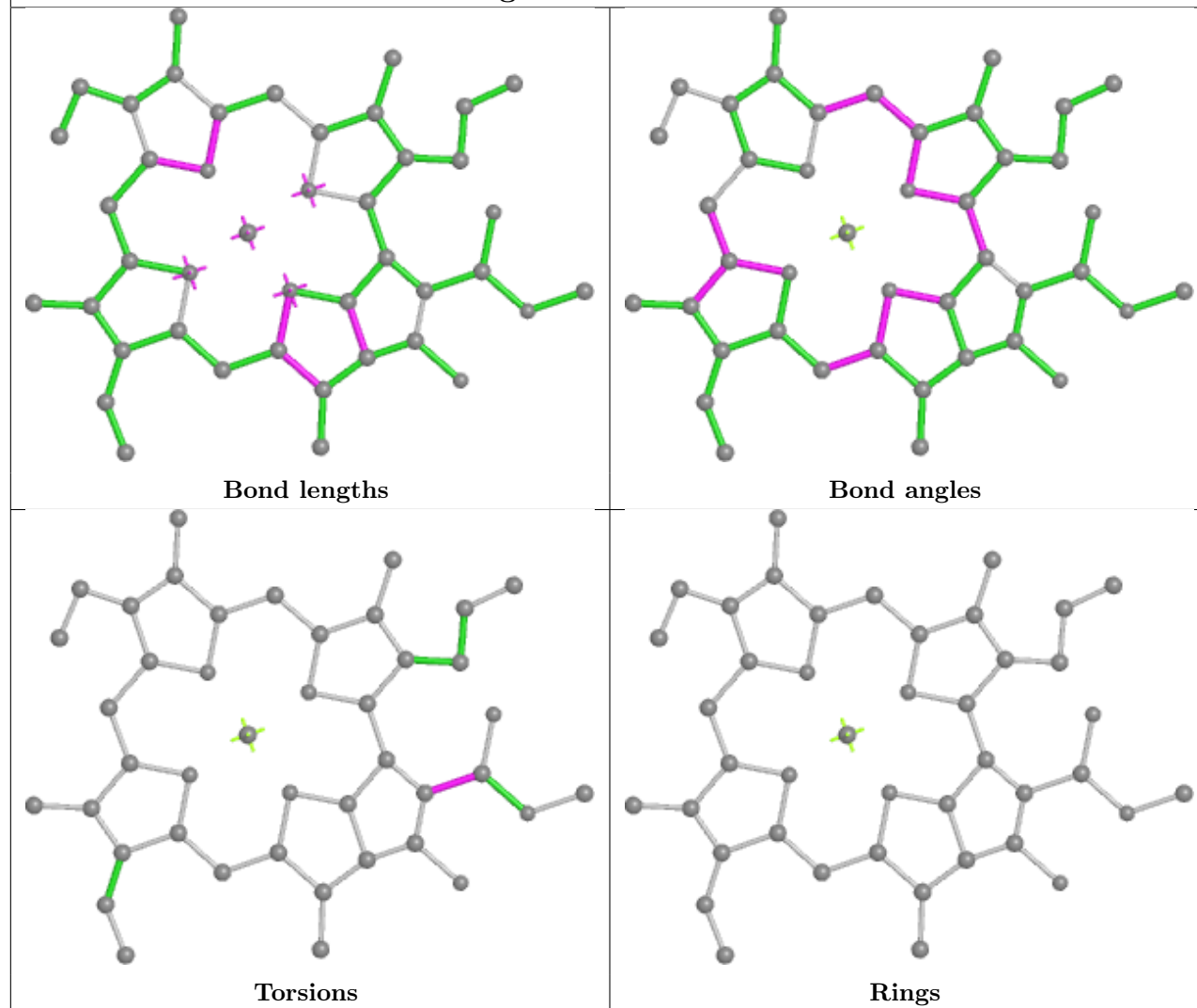
Ligand CLA B 817



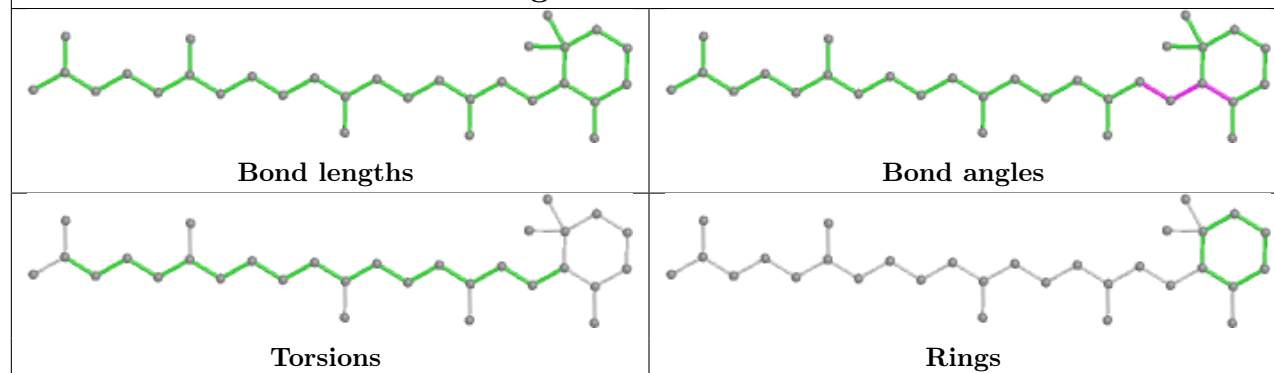
Ligand BCR B 839

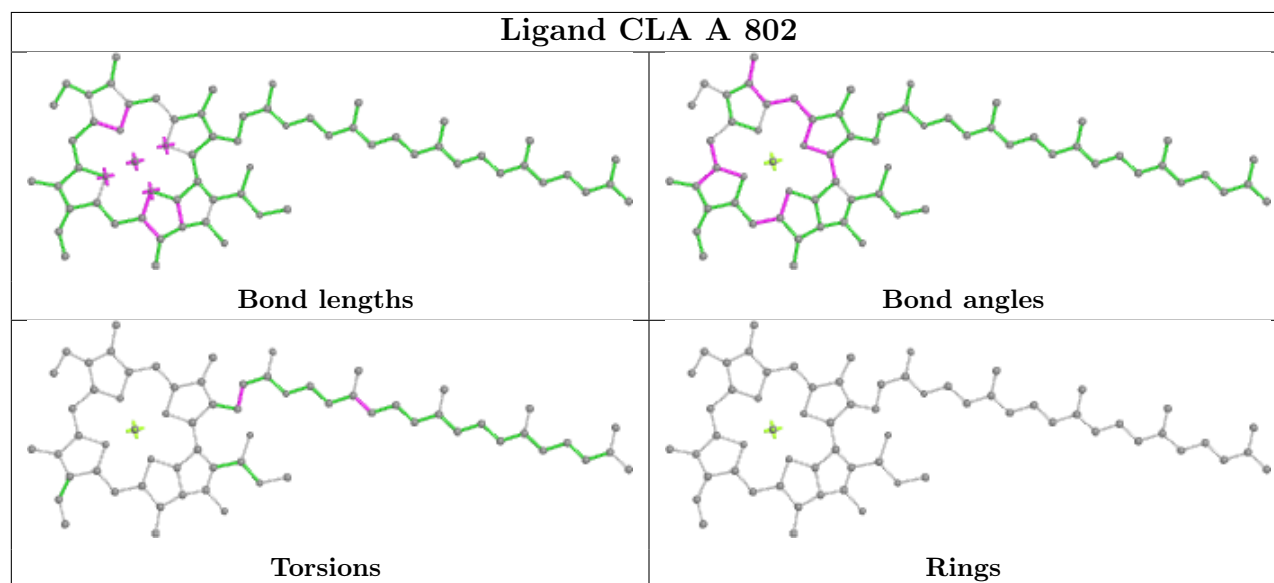
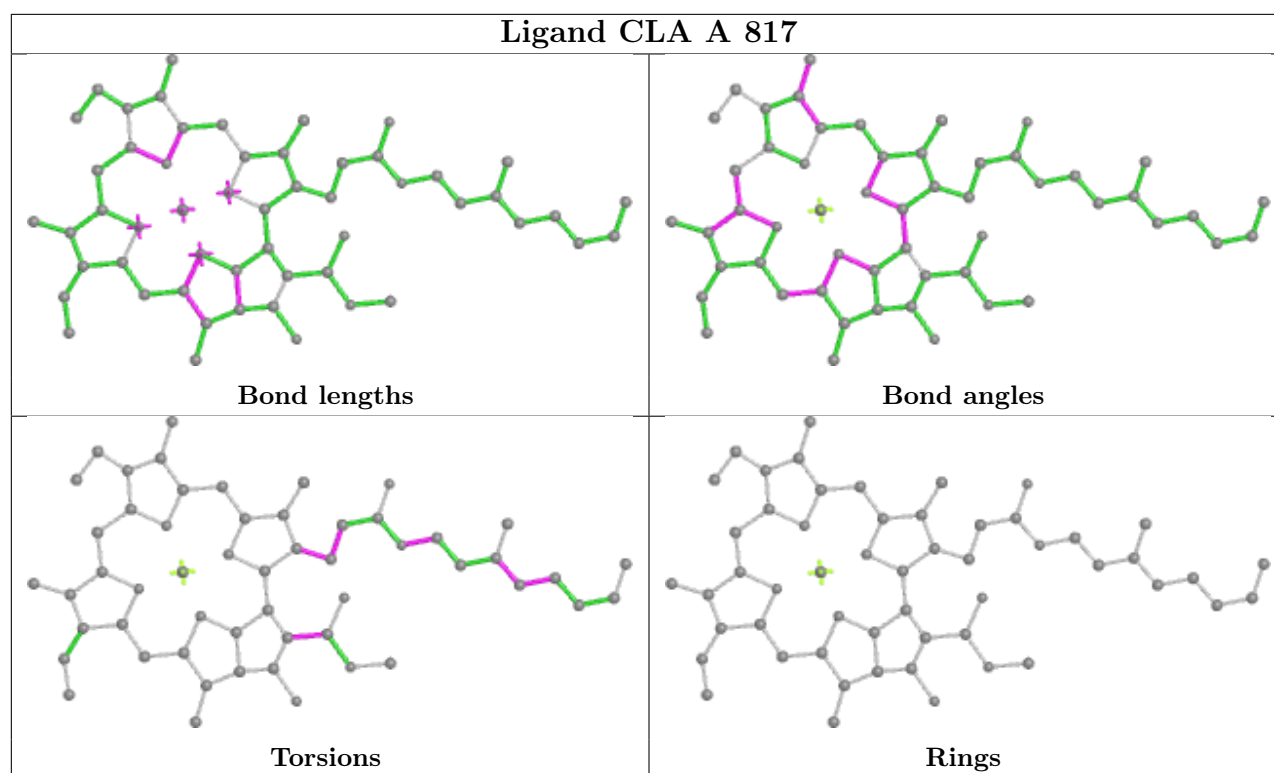


Ligand CLA A 823

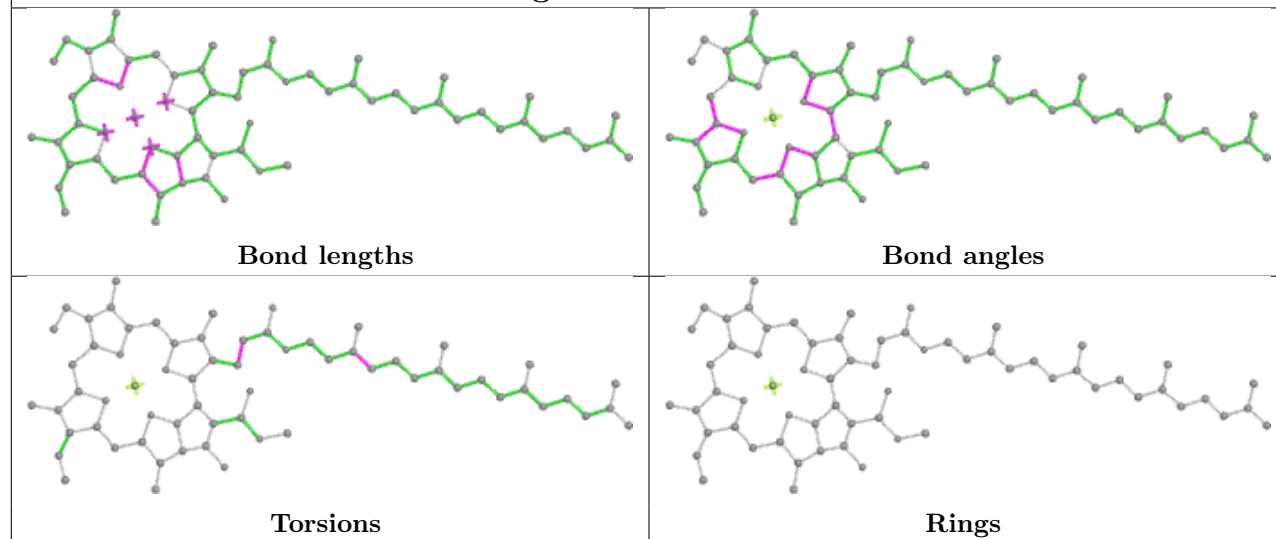


Ligand BCR B 844

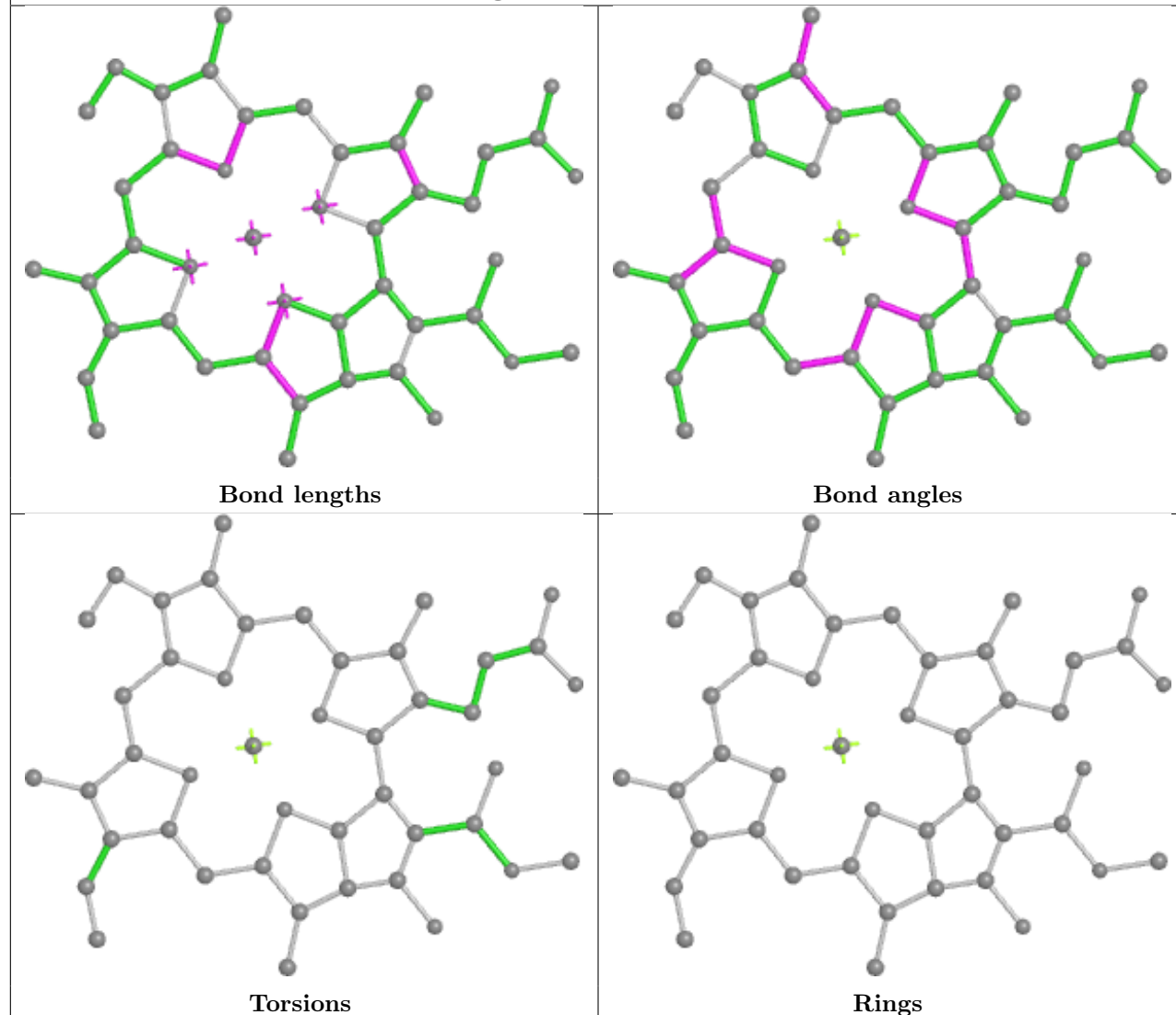


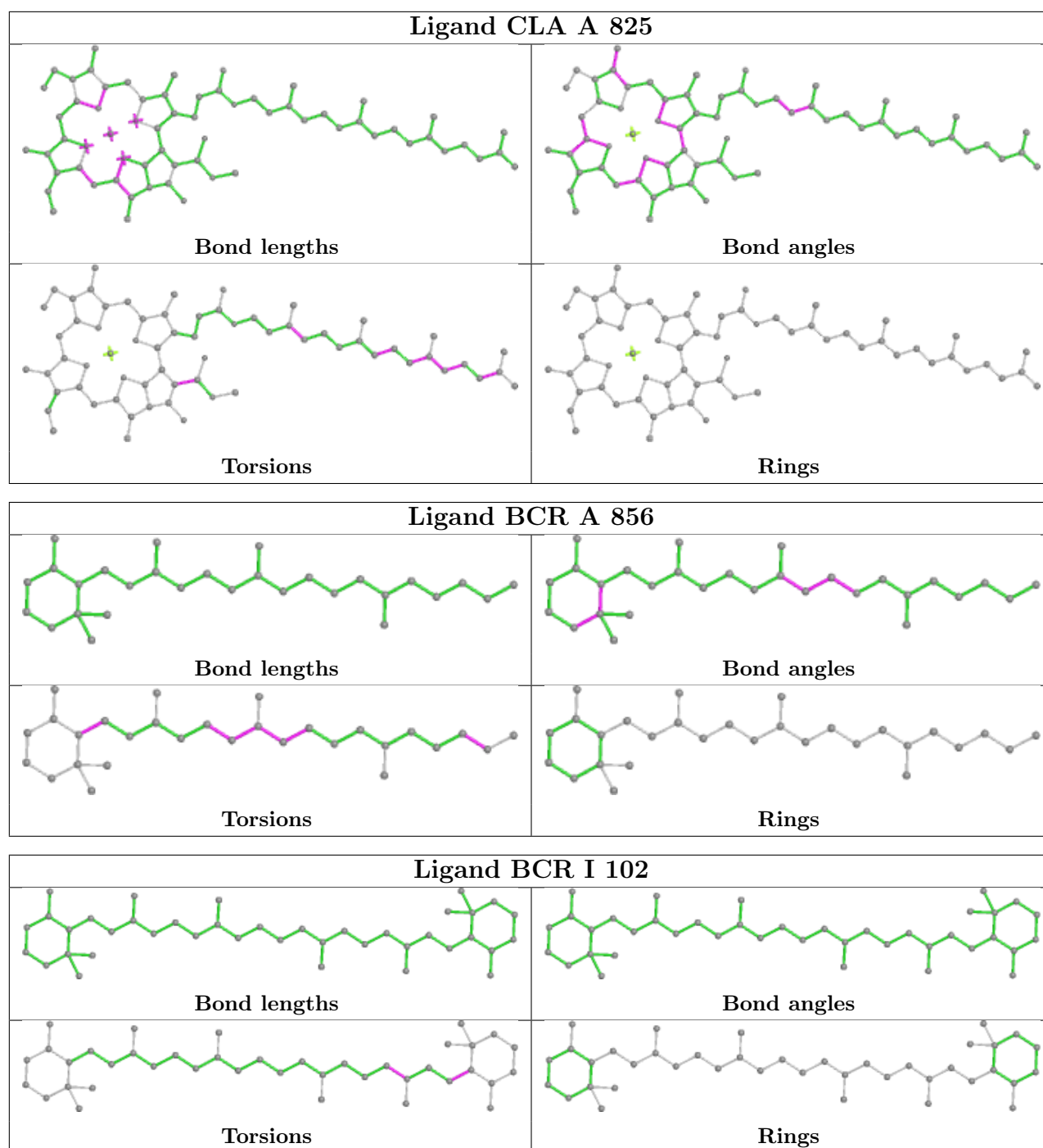


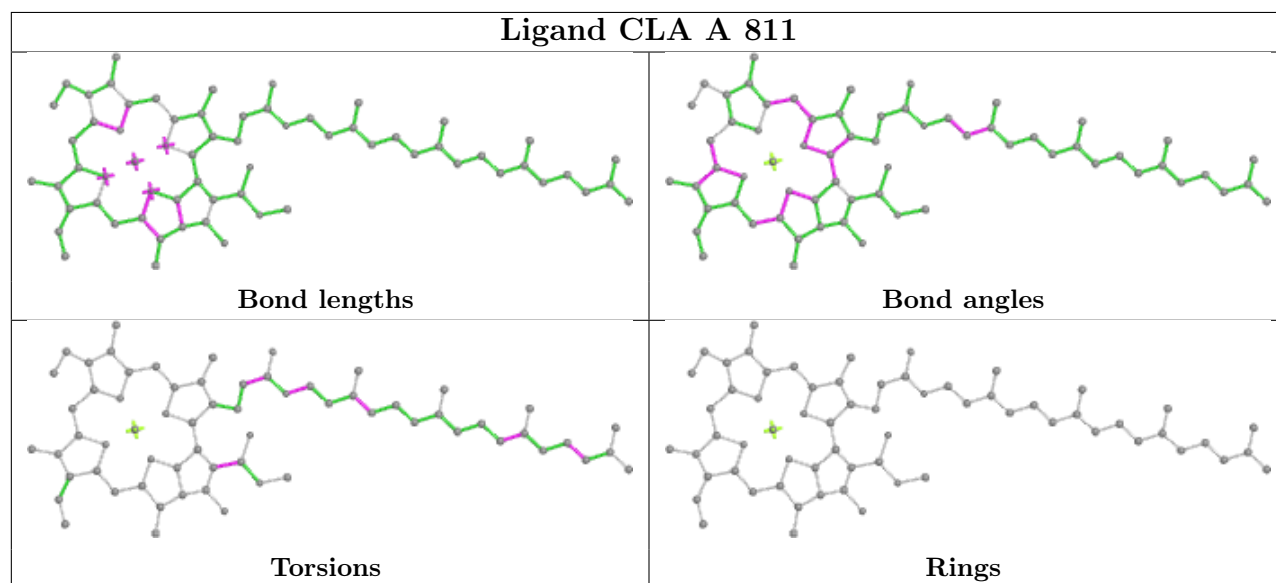
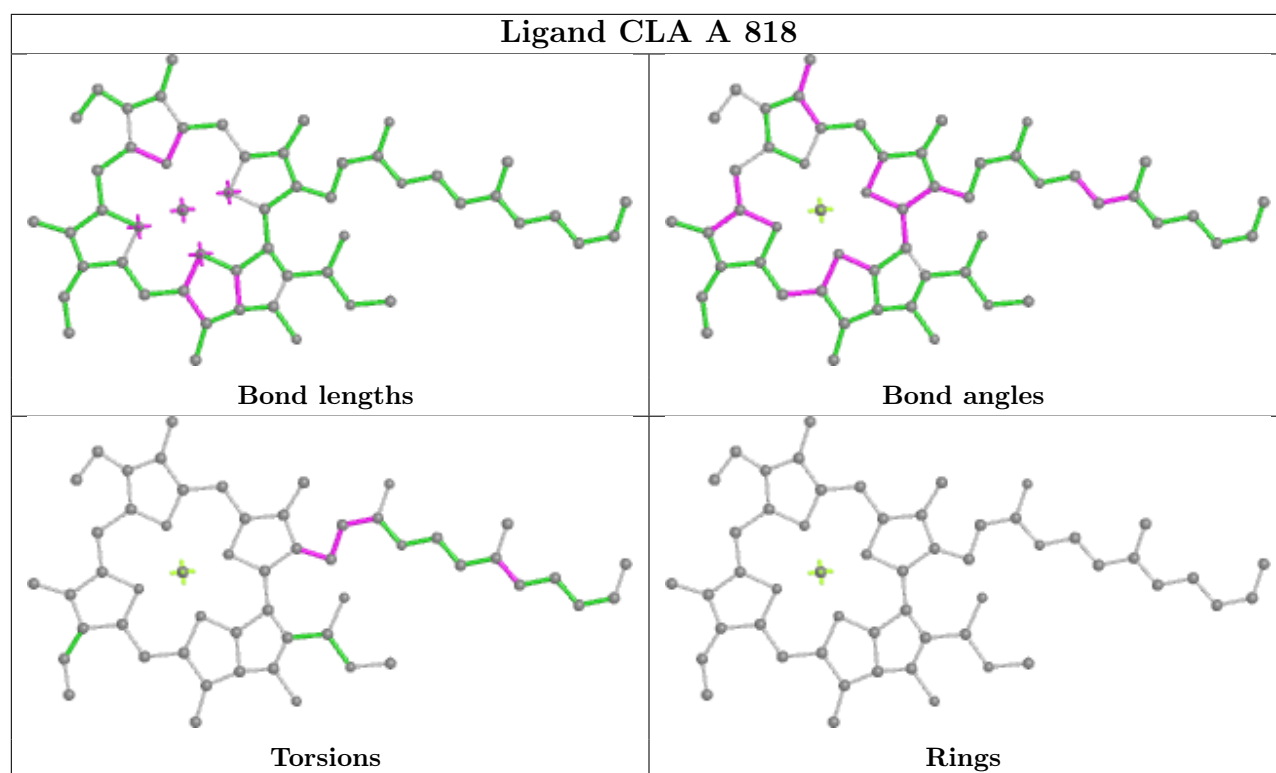
Ligand CLA B 809



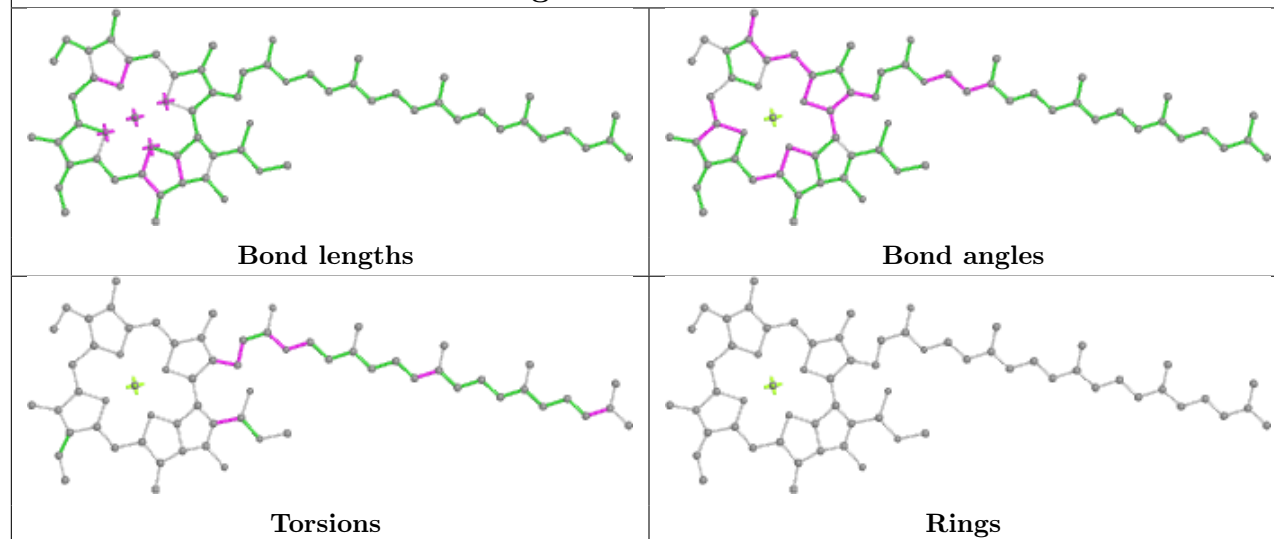
Ligand CLA A 809



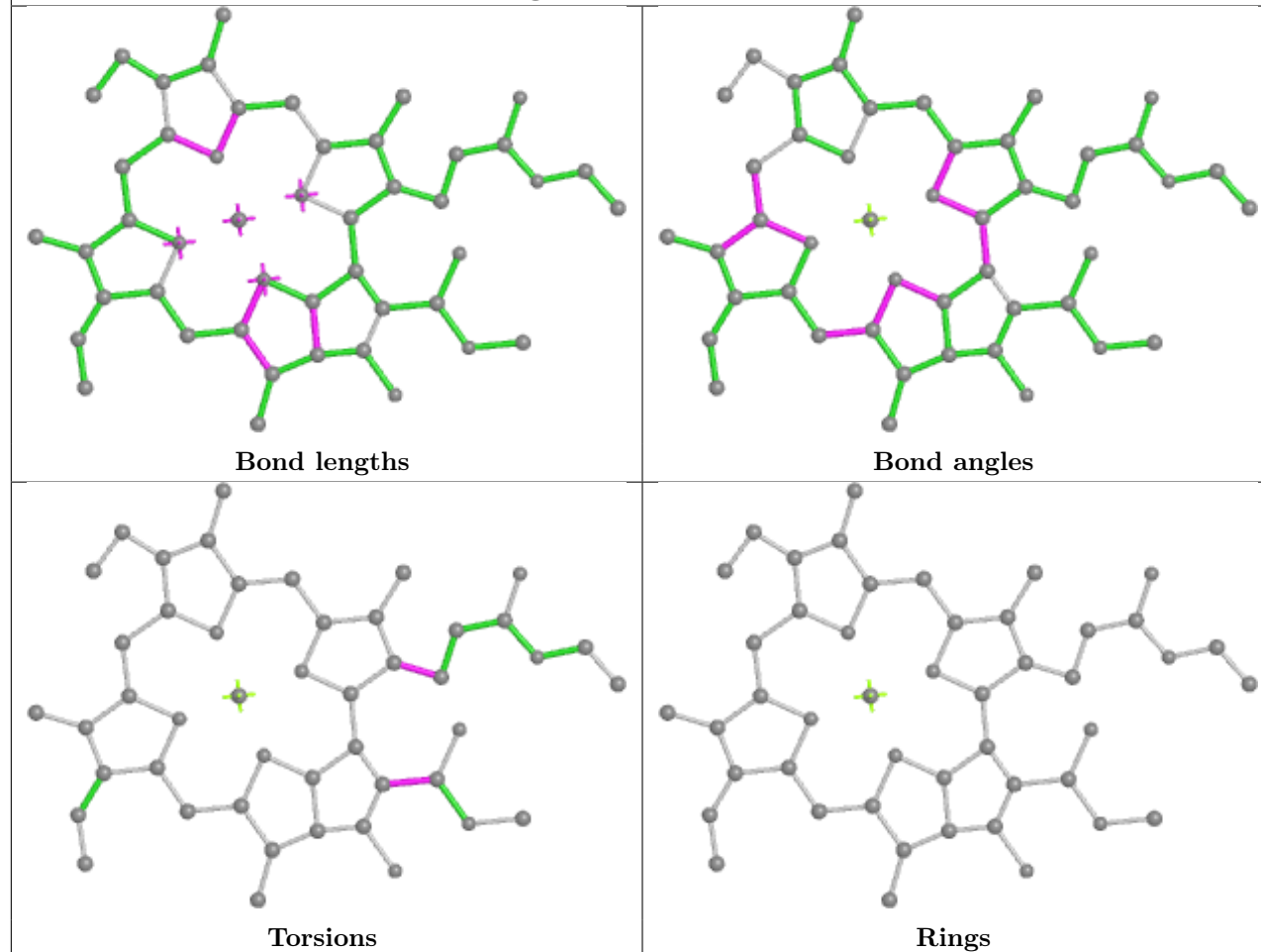




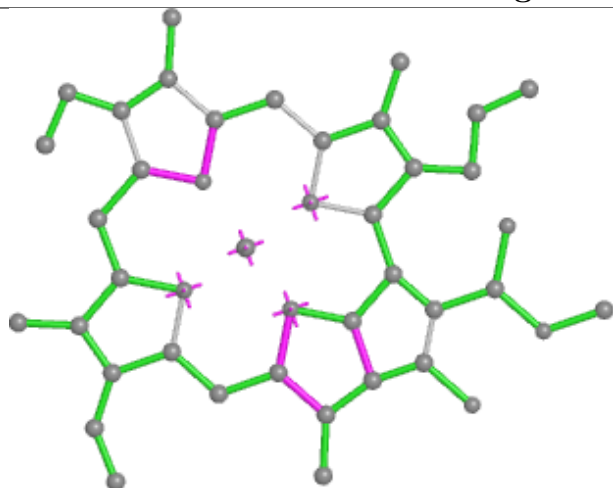
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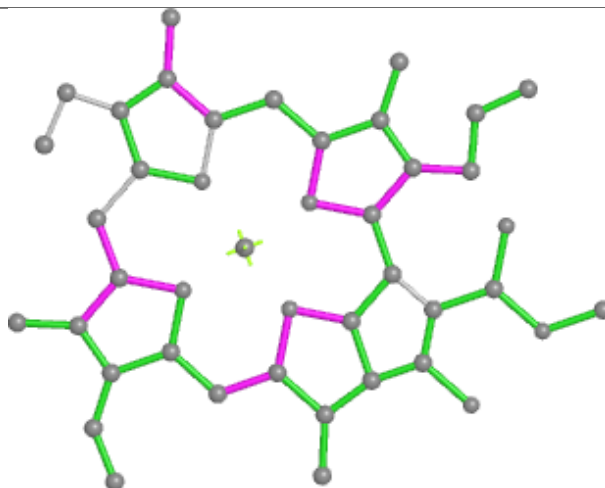
Ligand CLA B 834



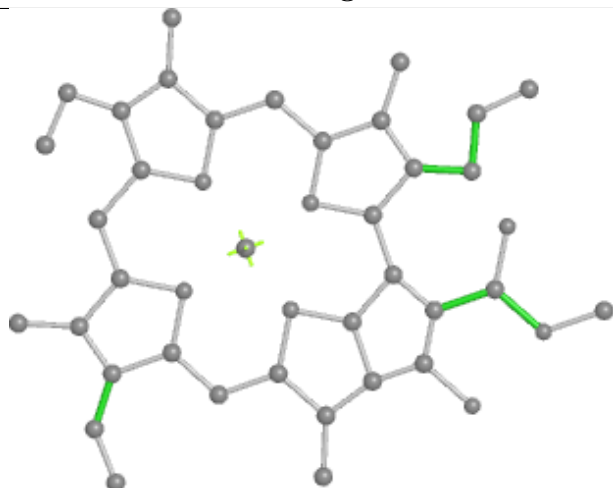
Ligand CLA B 813



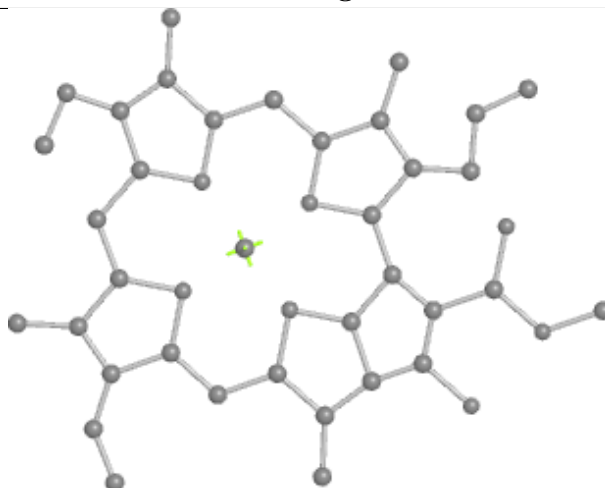
Bond lengths



Bond angles

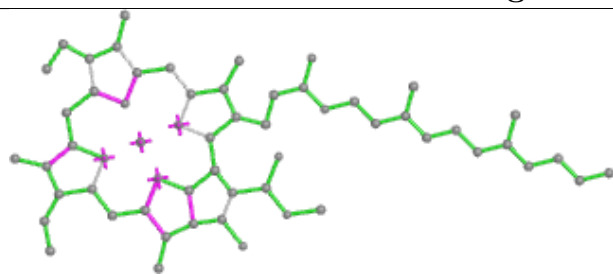


Torsions

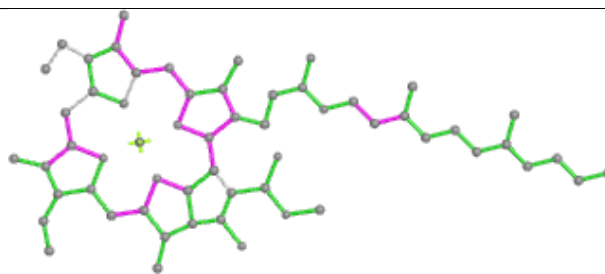


Rings

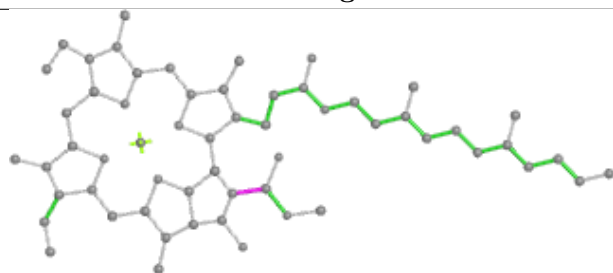
Ligand CLA L 1502



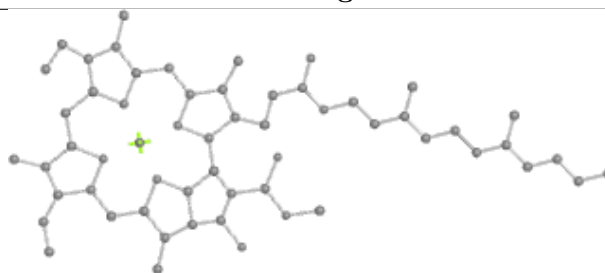
Bond lengths



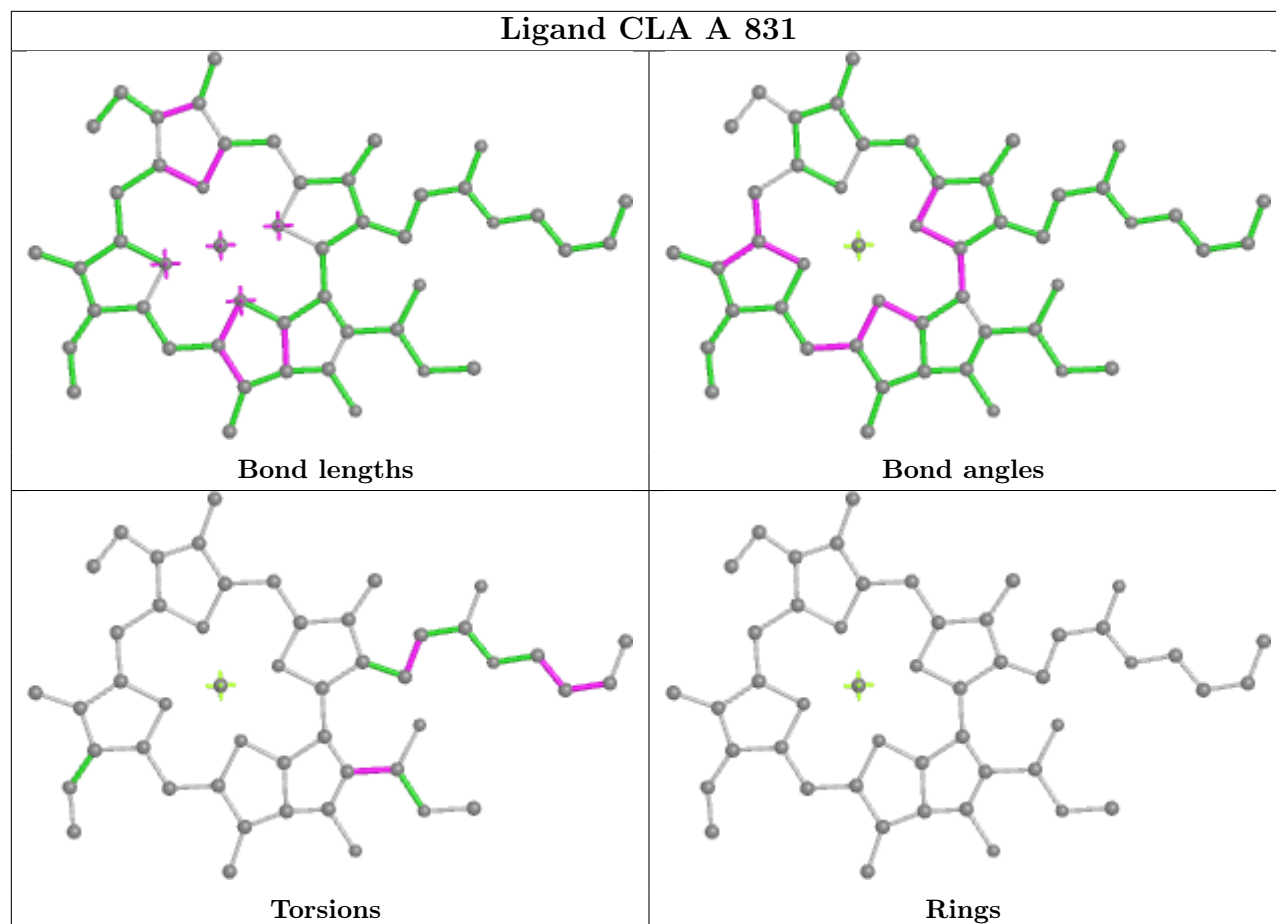
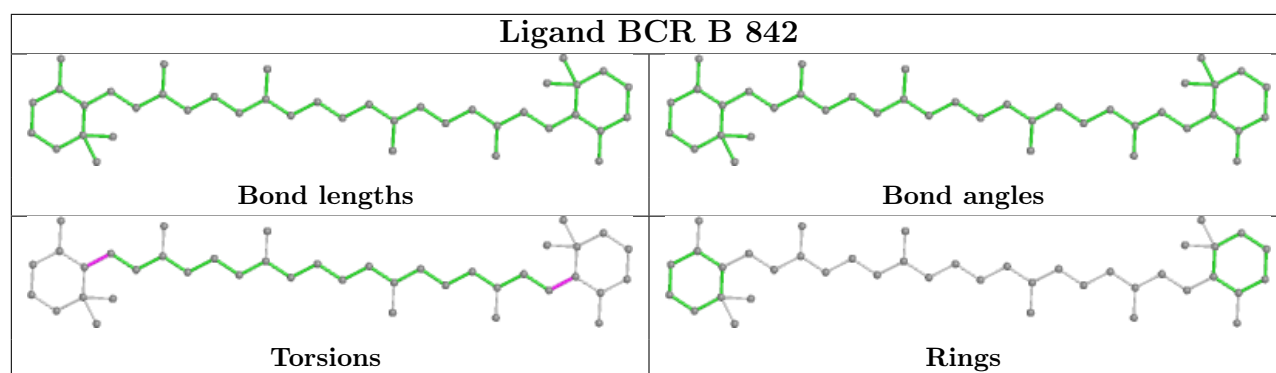
Bond angles



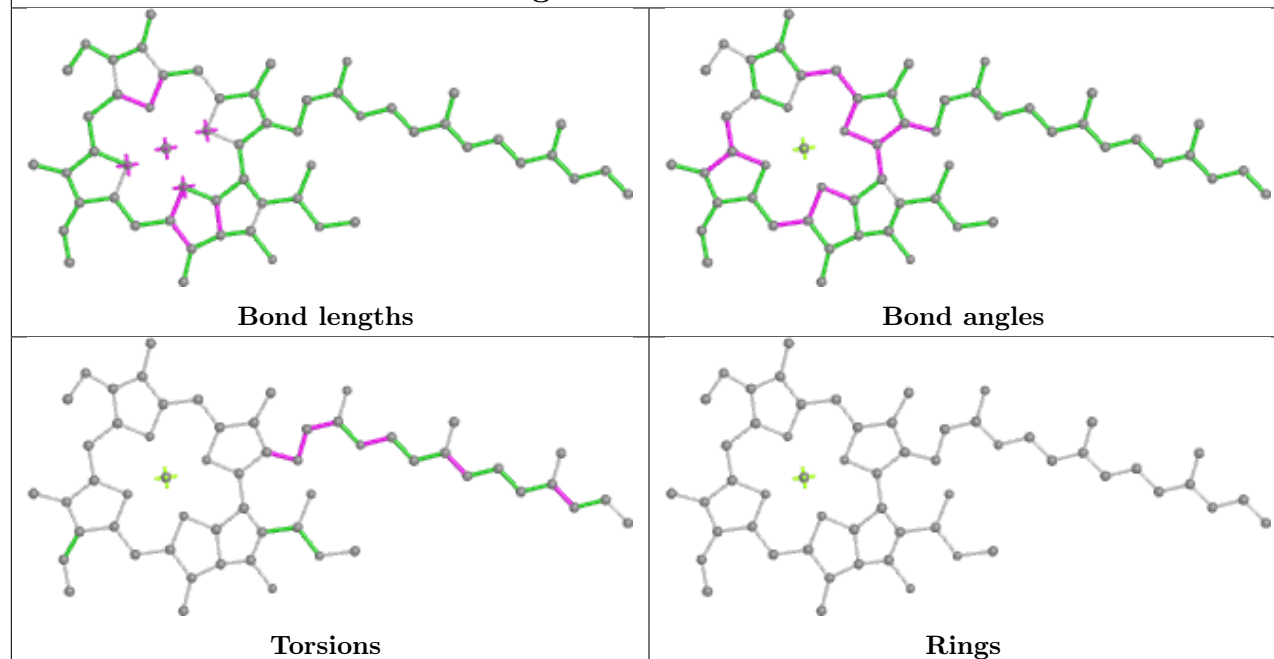
Torsions



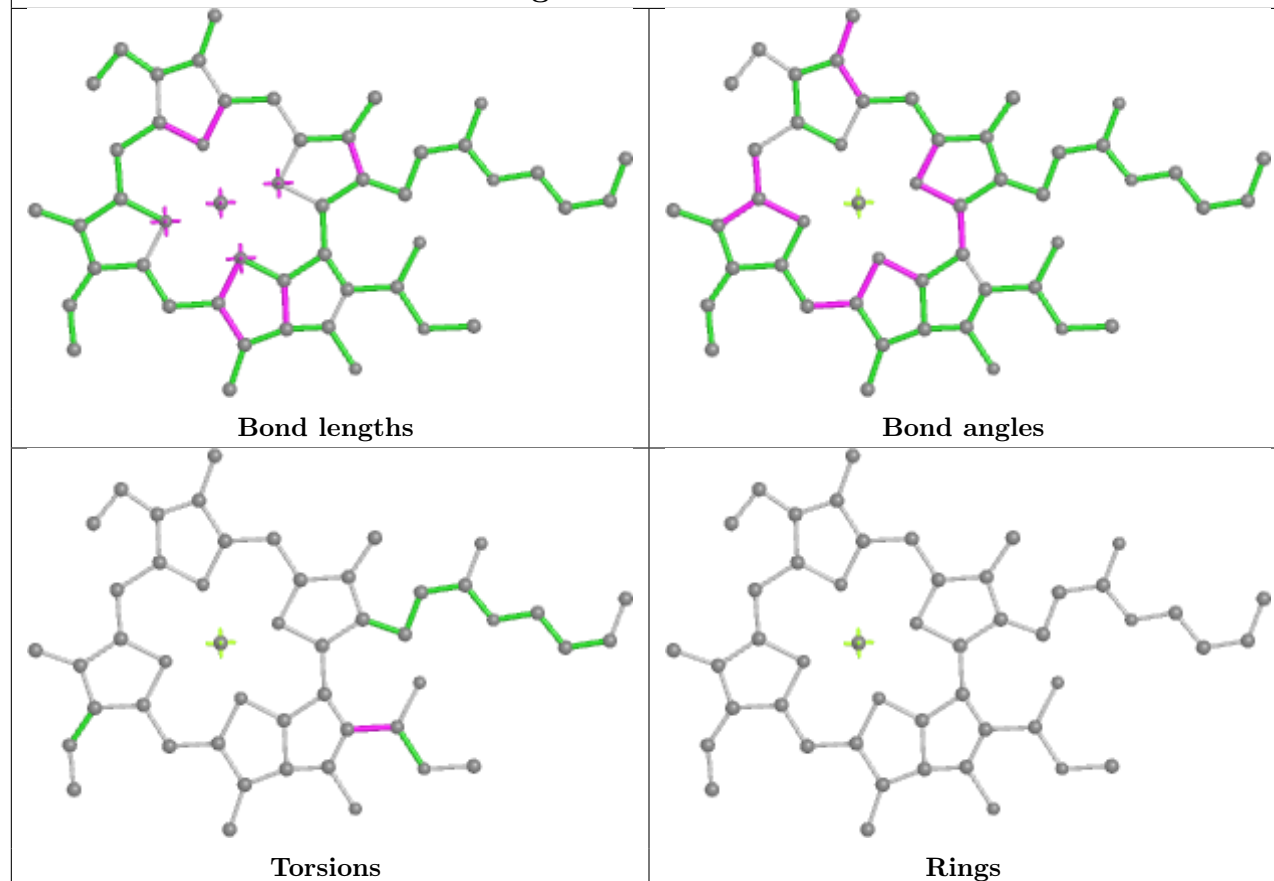
Rings

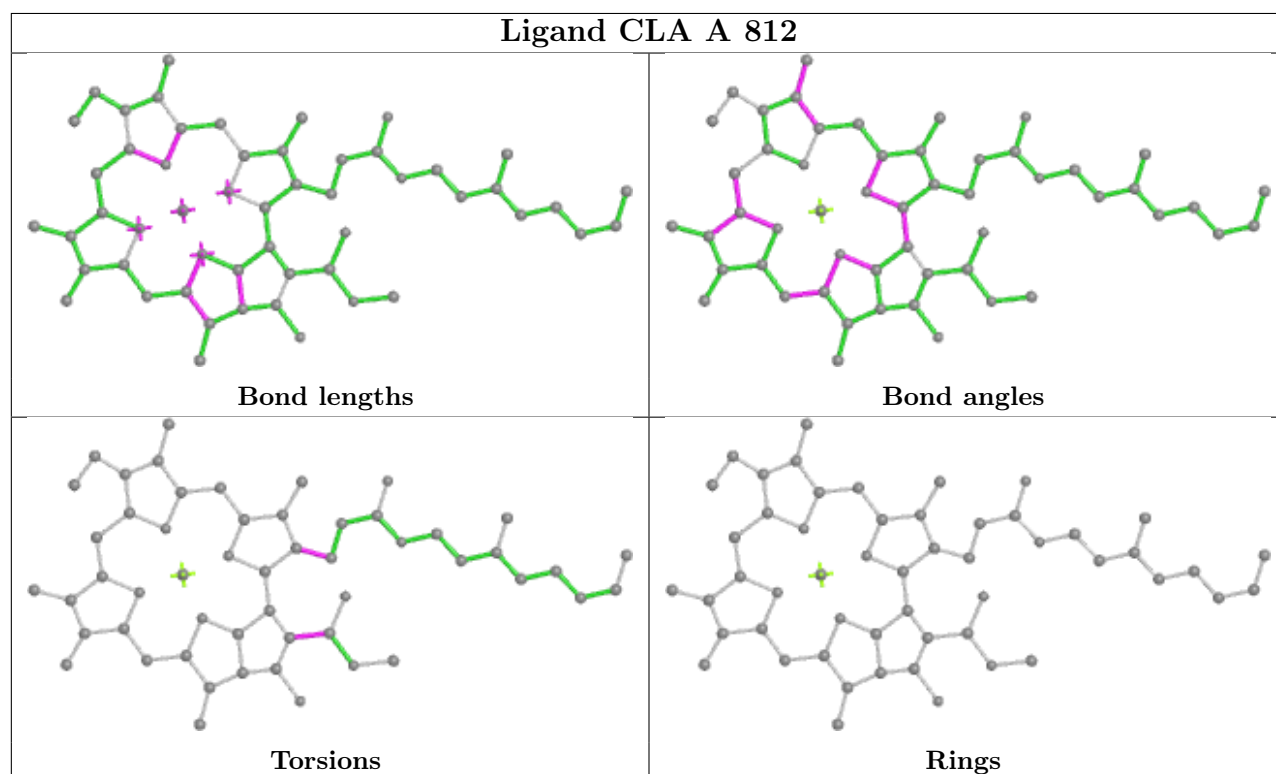
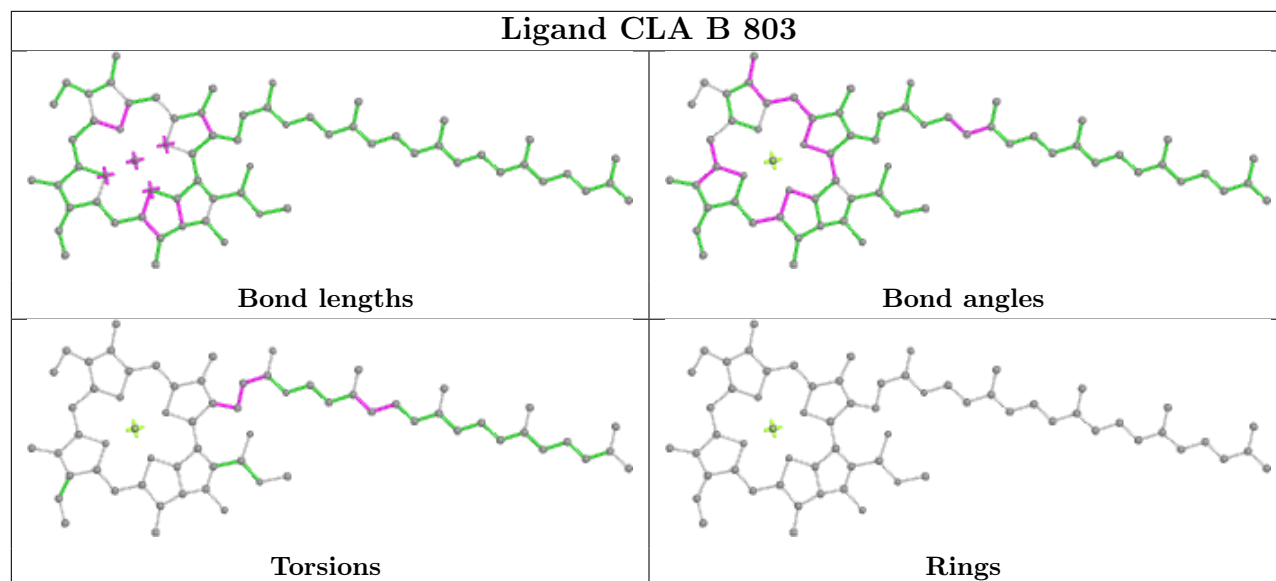
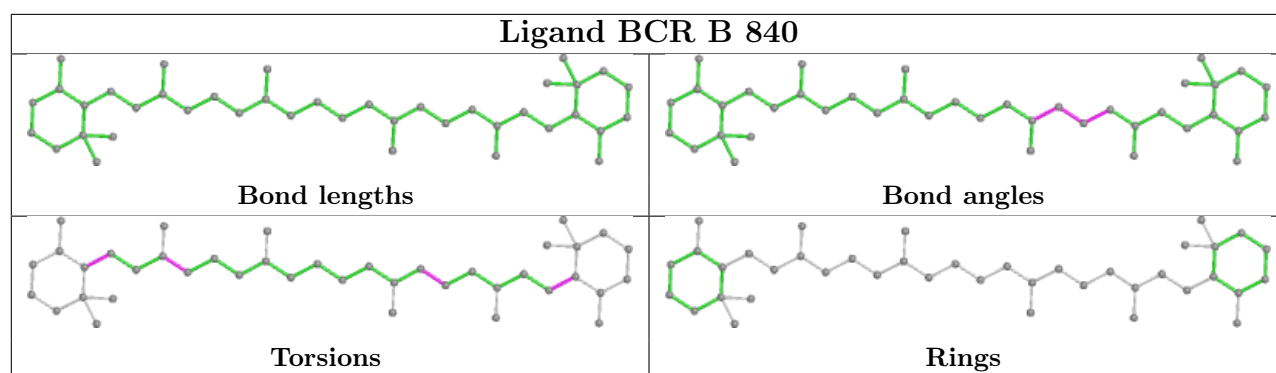


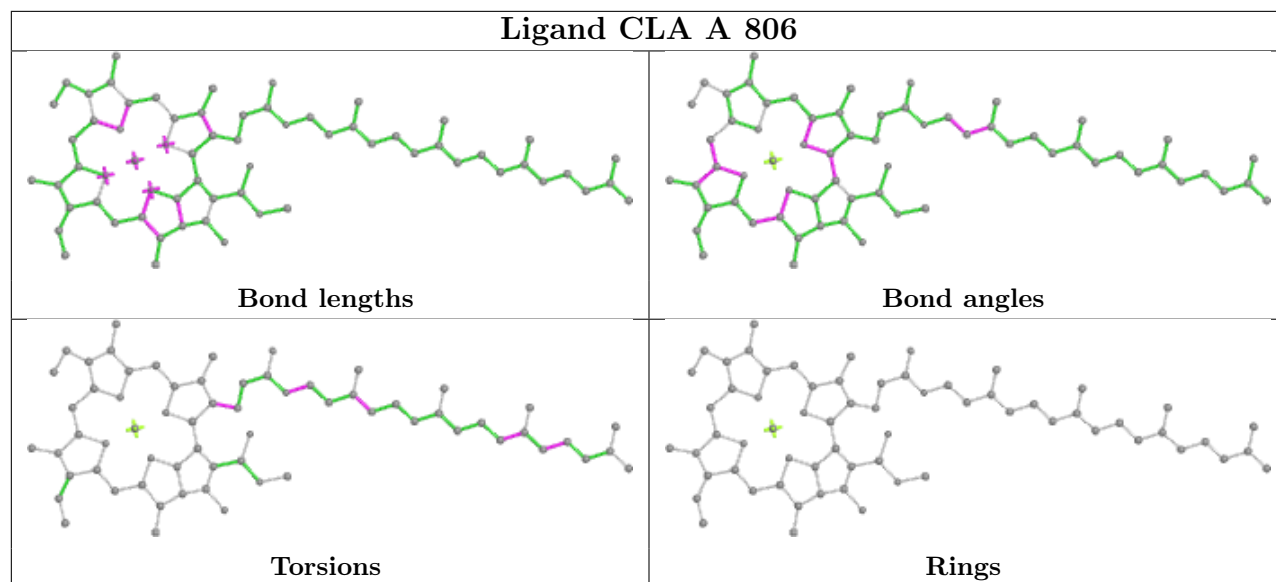
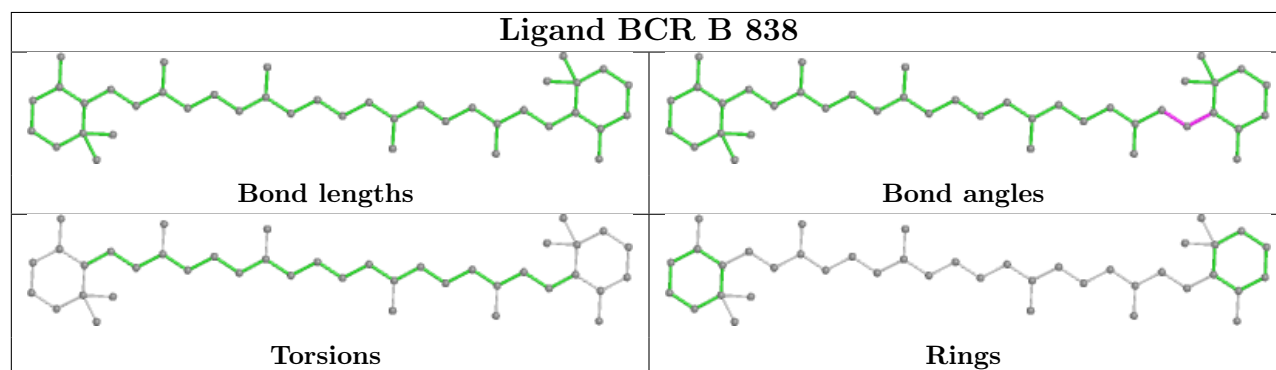
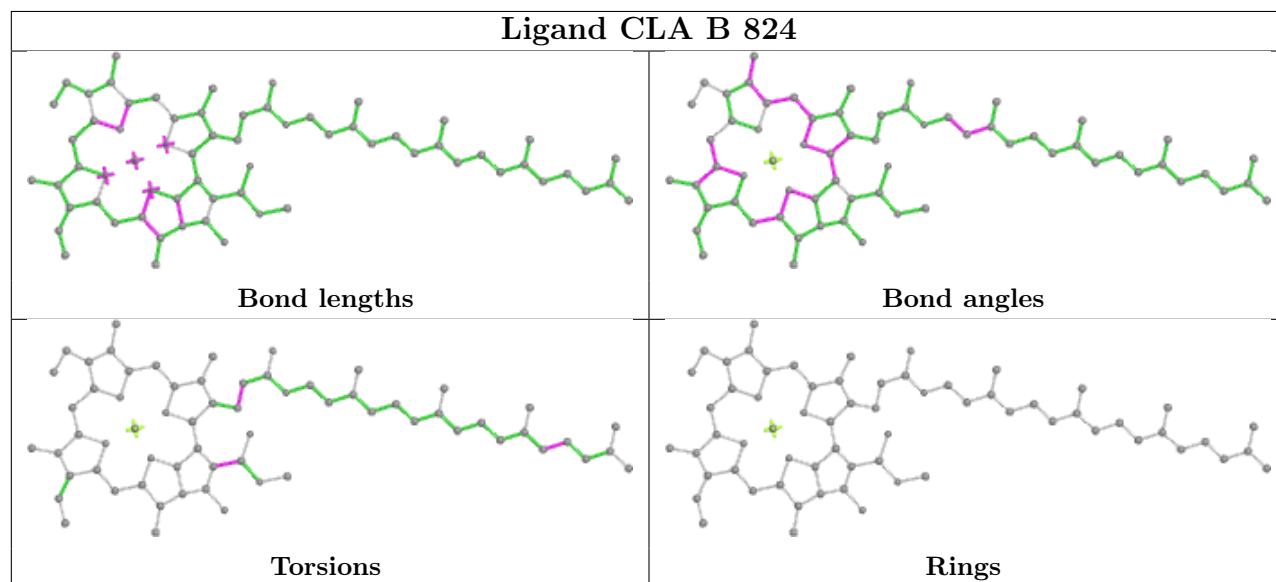
Ligand CLA B 823

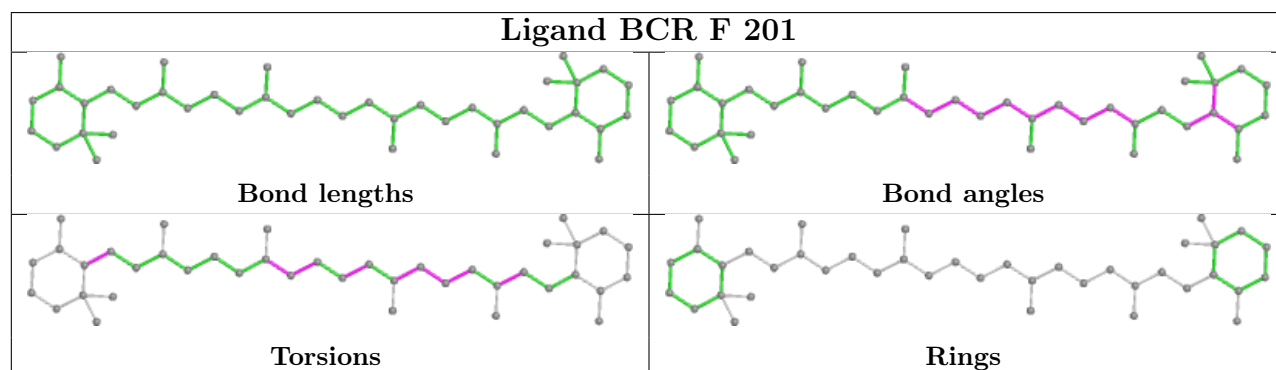
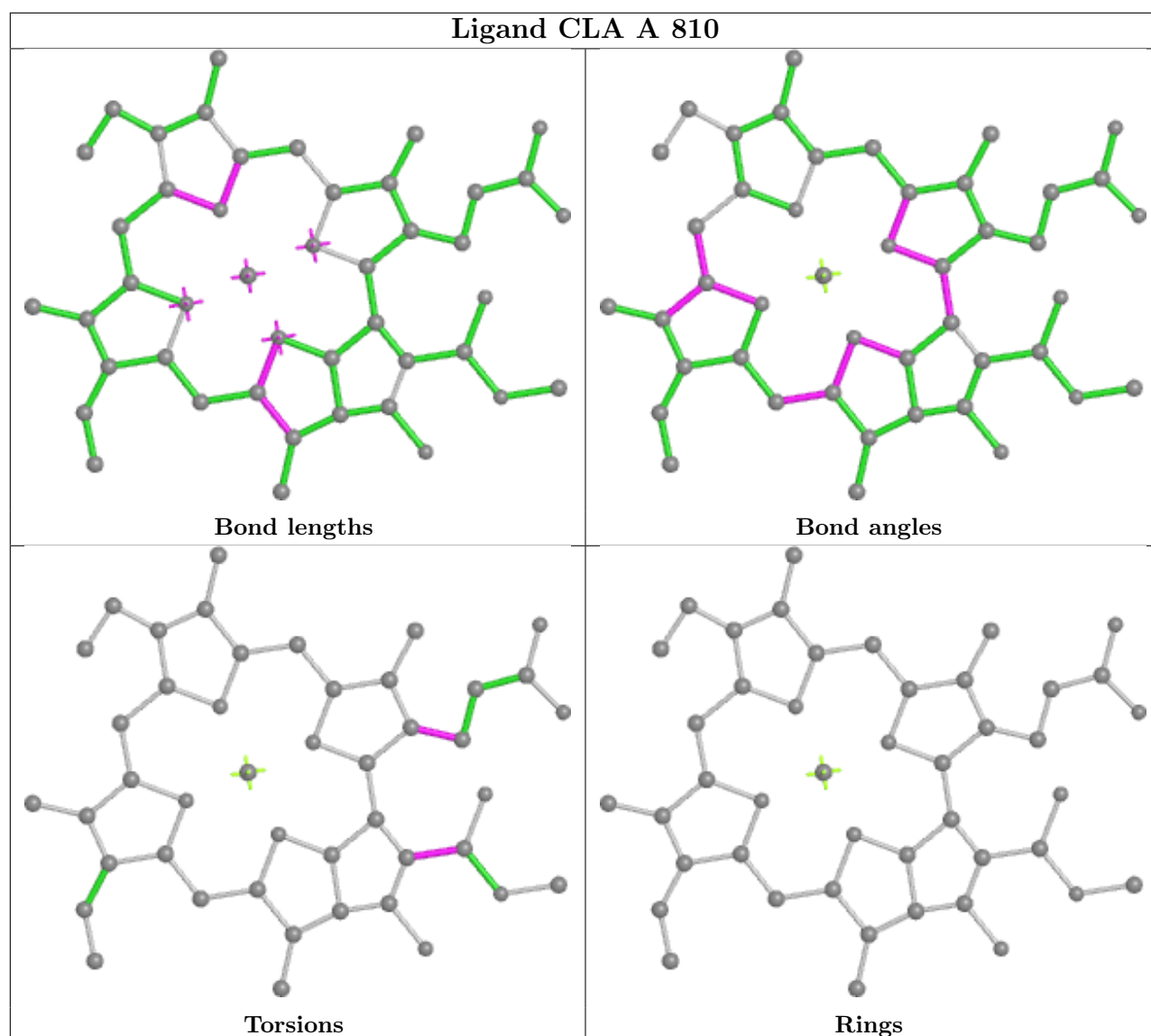


Ligand CLA A 839

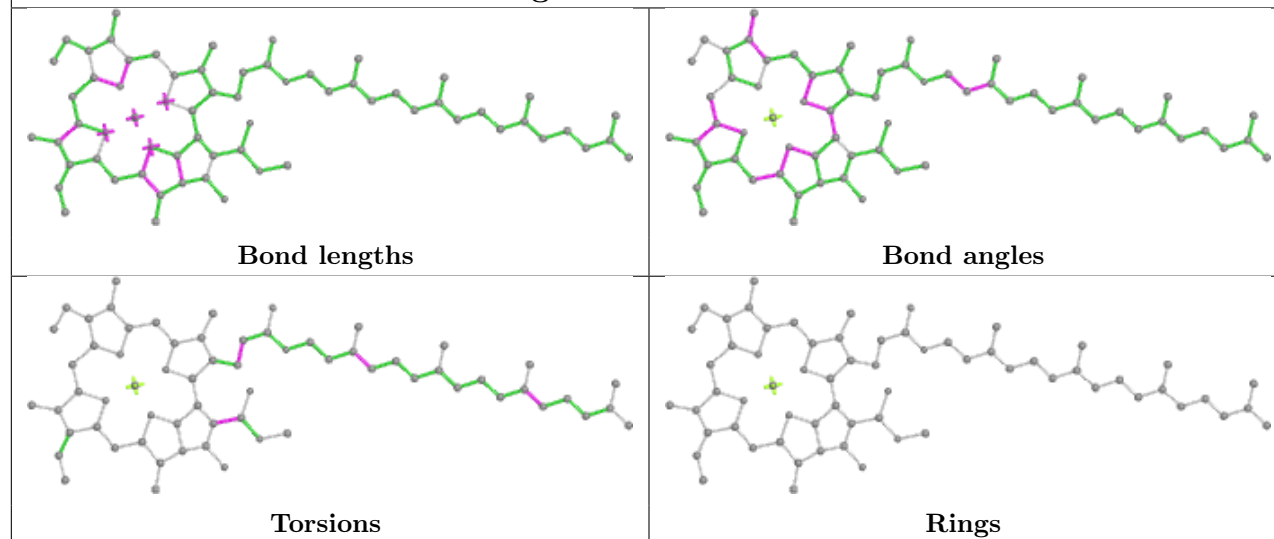




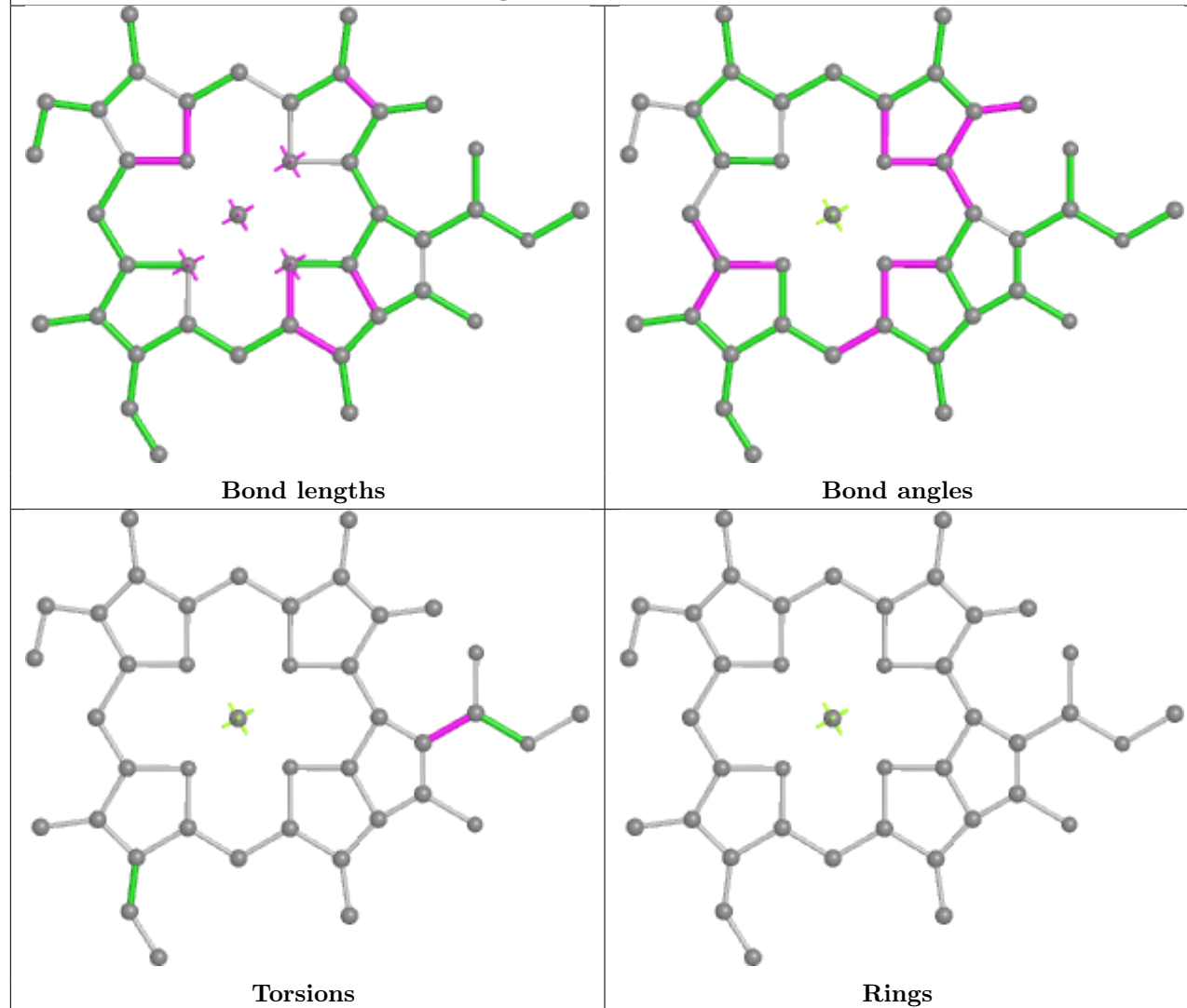
Ligand CLA A 806**Ligand BCR B 838****Ligand CLA B 824**

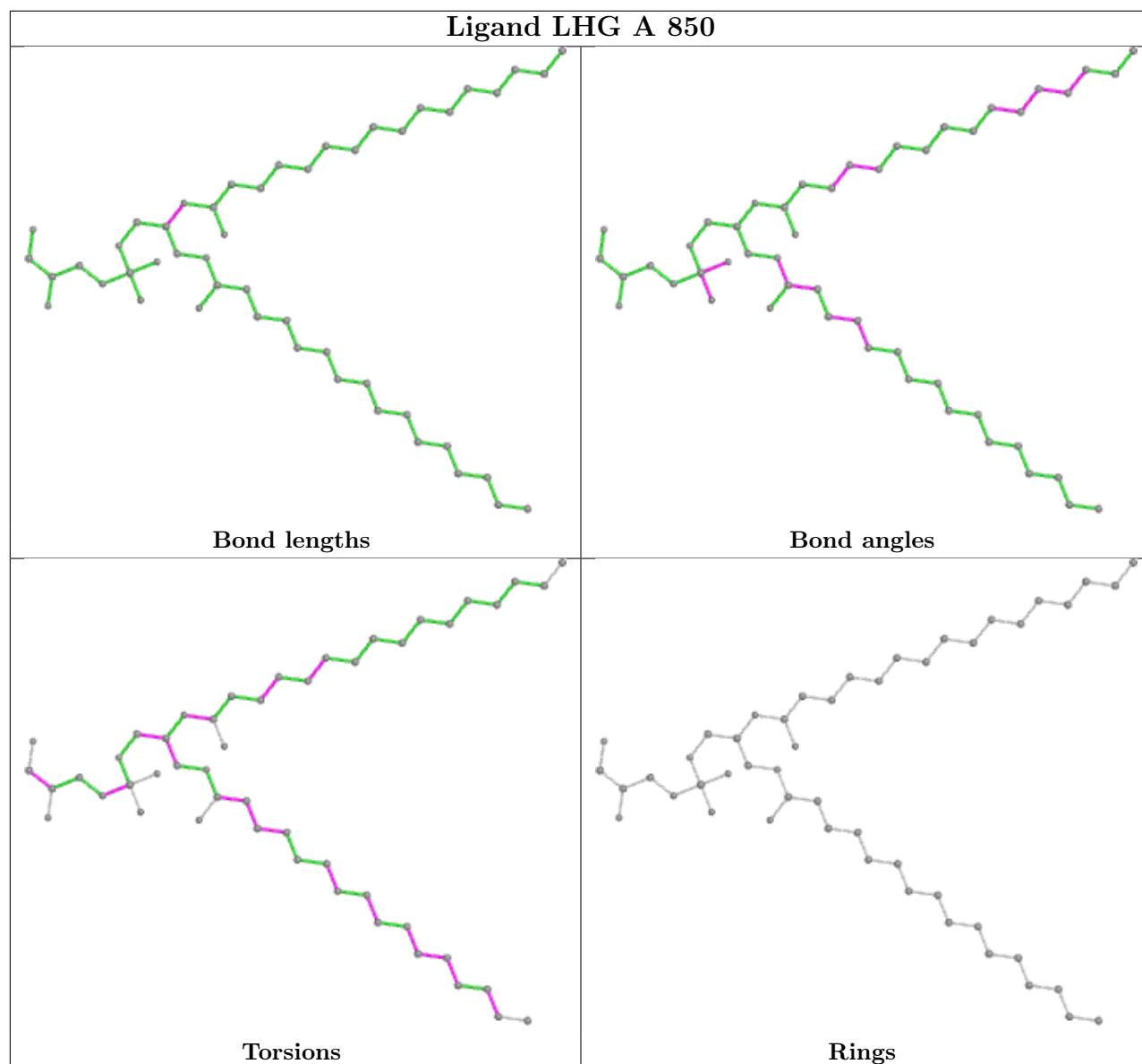
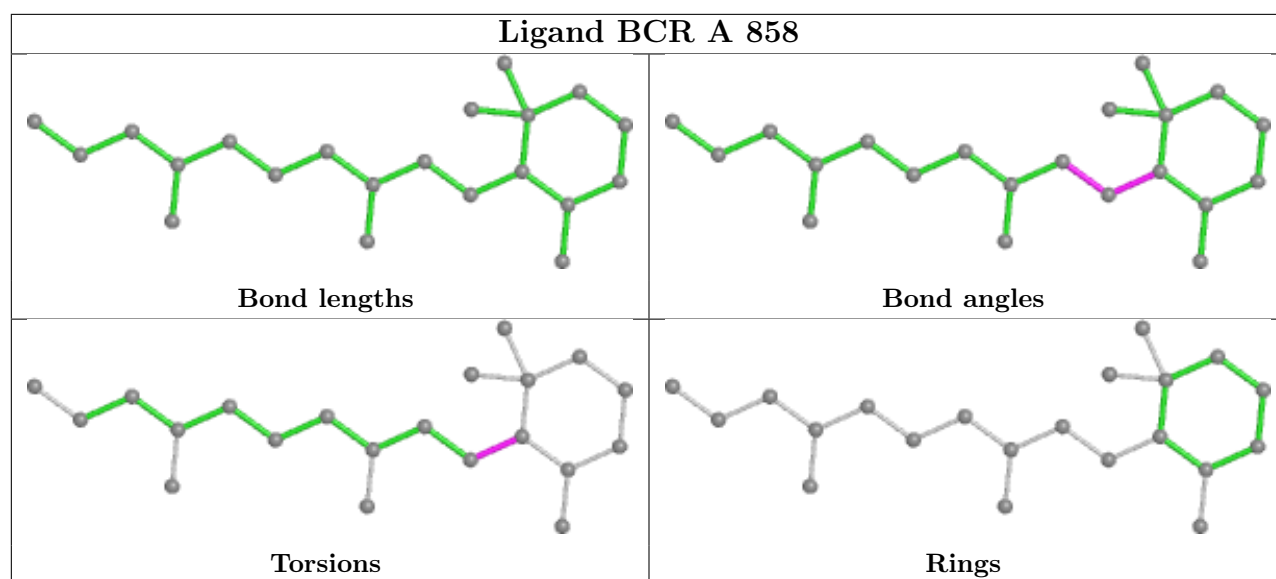


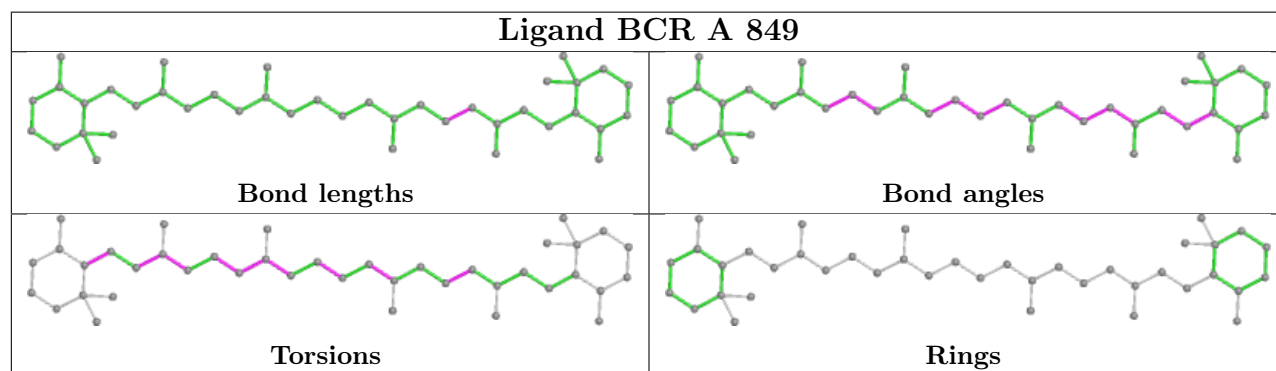
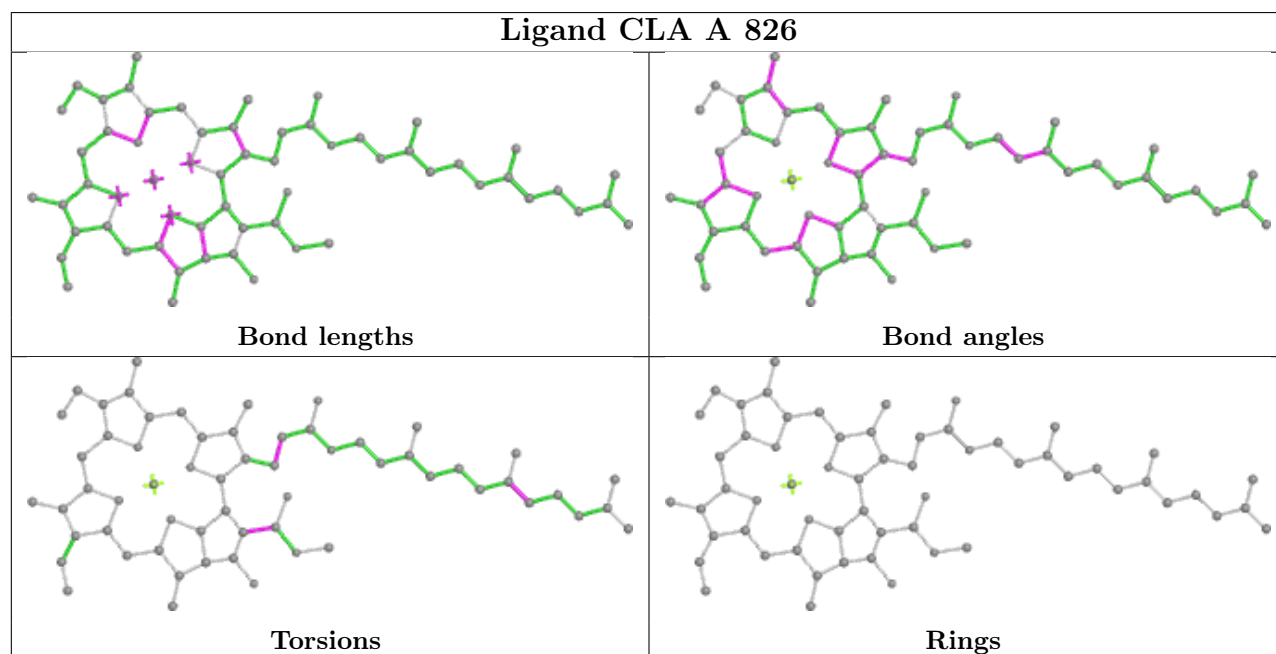
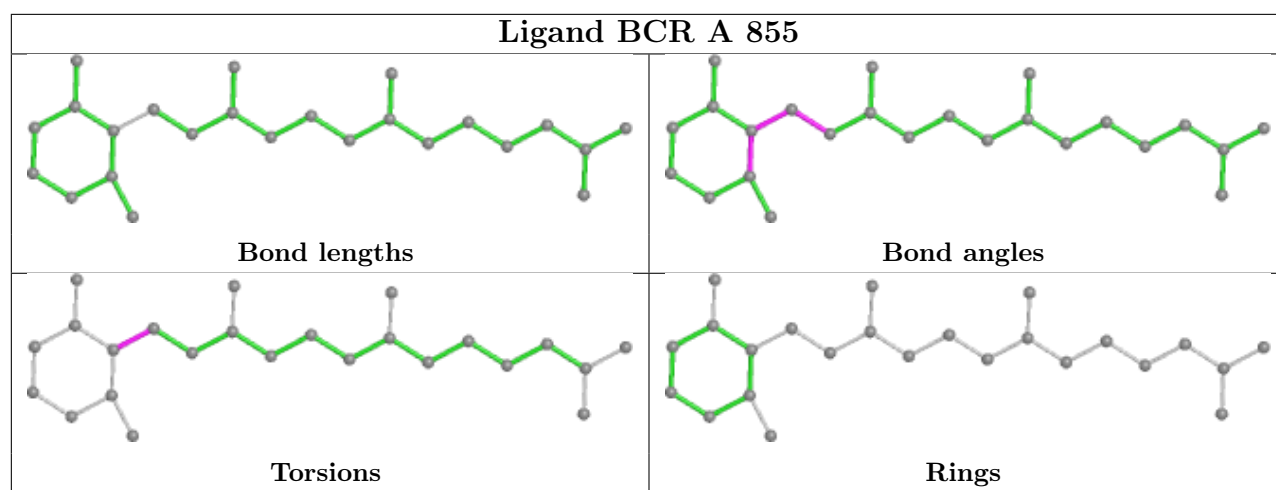
Ligand CLA A 829

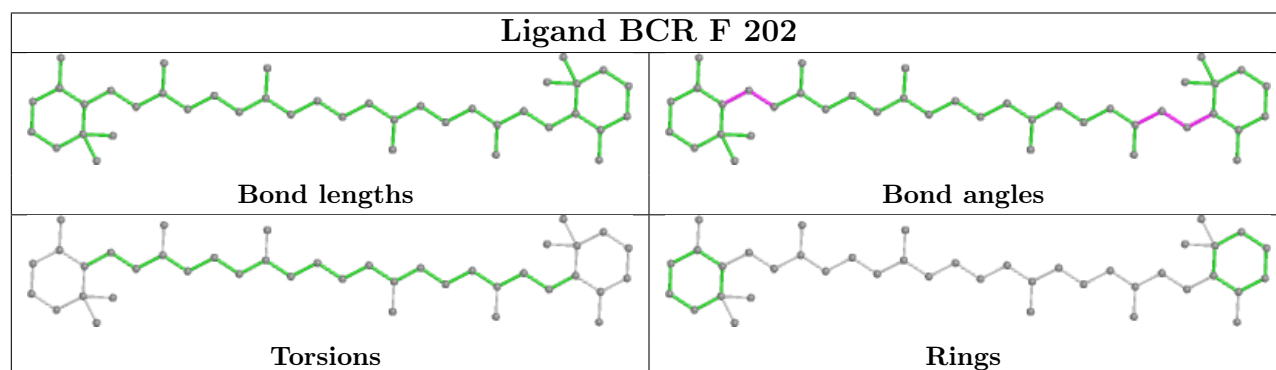
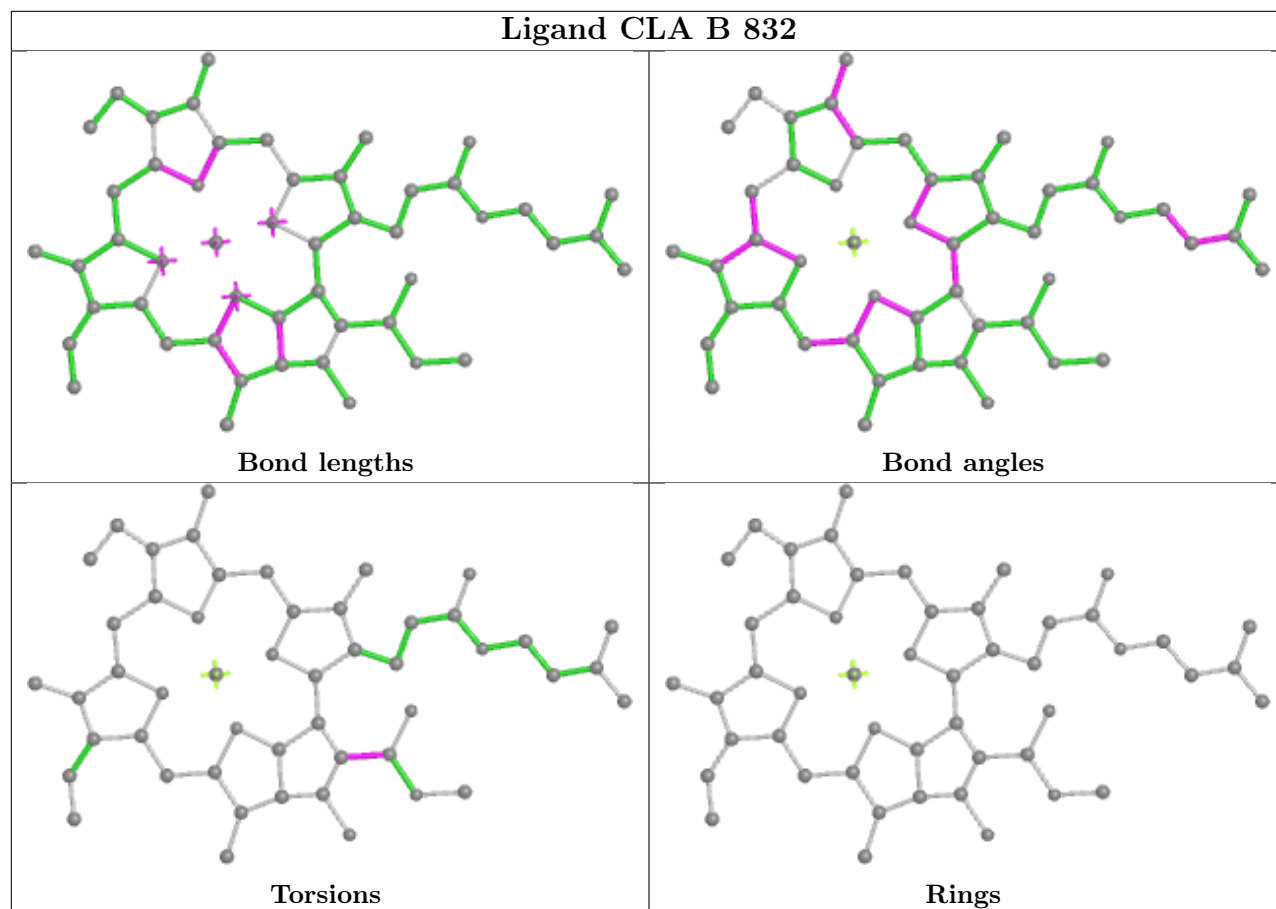
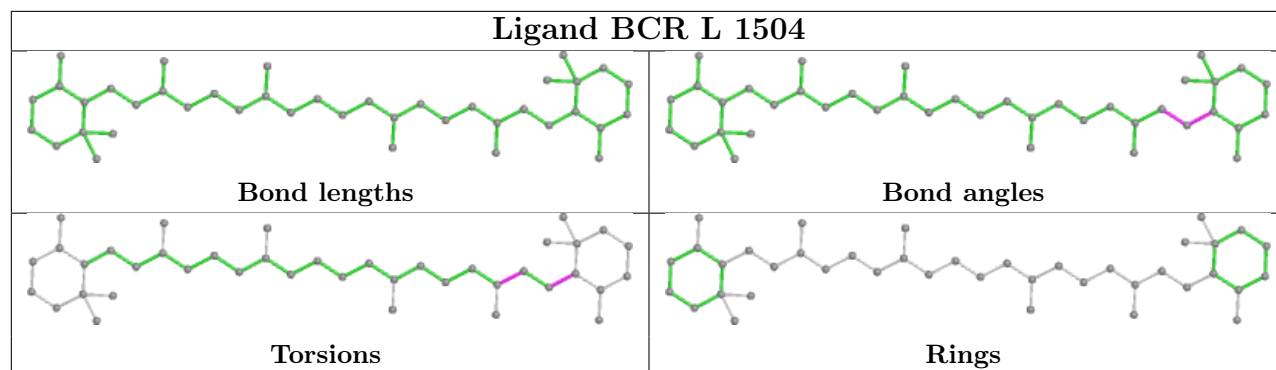


Ligand CLA A 820









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.