



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 03:23 PM UTC

PDB ID : 7DR1 / pdb_00007dr1
EMDB ID : EMD-30821
Title : Structure of Wild-type PSI monomer2 from *Cyanophora paradoxa*
Authors : Kato, K.; Nagao, R.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on : 2020-12-25
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

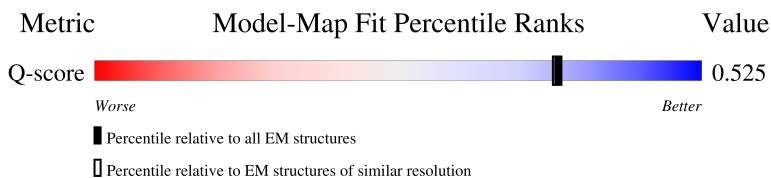
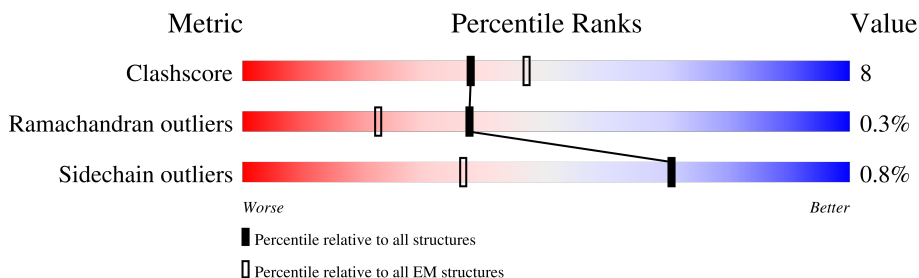
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	752	
2	B	737	
3	C	81	
4	D	220	

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Mol	Chain	Length	Quality of chain
5	E	70	
6	F	186	
7	I	35	
8	J	40	
9	L	146	
10	M	31	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CL0	A	801	X	-	-	-
12	CLA	A	802	X	-	-	-
12	CLA	A	803	X	-	-	-
12	CLA	A	804	X	-	-	-
12	CLA	A	805	X	-	-	-
12	CLA	A	806	X	-	-	-
12	CLA	A	807	X	-	-	-
12	CLA	A	808	X	-	-	-
12	CLA	A	809	X	-	-	-
12	CLA	A	810	X	-	-	-
12	CLA	A	811	X	-	-	-
12	CLA	A	813	X	-	-	-
12	CLA	A	814	X	-	-	-
12	CLA	A	816	X	-	-	-
12	CLA	A	818	X	-	-	-
12	CLA	A	819	X	-	-	-
12	CLA	A	820	X	-	-	-
12	CLA	A	821	X	-	-	-
12	CLA	A	824	X	-	-	-
12	CLA	A	825	X	-	-	-
12	CLA	A	826	X	-	-	-
12	CLA	A	827	X	-	-	-
12	CLA	A	828	X	-	-	-
12	CLA	A	829	X	-	-	-
12	CLA	A	830	X	-	-	-
12	CLA	A	831	X	-	-	-
12	CLA	A	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	833	X	-	-	-
12	CLA	A	835	X	-	-	-
12	CLA	A	836	X	-	-	-
12	CLA	A	837	X	-	-	-
12	CLA	A	838	X	-	-	-
12	CLA	A	840	X	-	-	-
12	CLA	A	841	X	-	-	-
12	CLA	A	842	X	-	-	-
12	CLA	A	854	X	-	-	-
12	CLA	B	801	X	-	-	-
12	CLA	B	802	X	-	-	-
12	CLA	B	803	X	-	-	-
12	CLA	B	804	X	-	-	-
12	CLA	B	805	X	-	-	-
12	CLA	B	806	X	-	-	-
12	CLA	B	807	X	-	-	-
12	CLA	B	808	X	-	-	-
12	CLA	B	809	X	-	-	-
12	CLA	B	810	X	-	-	-
12	CLA	B	811	X	-	-	-
12	CLA	B	812	X	-	-	-
12	CLA	B	813	X	-	-	-
12	CLA	B	814	X	-	-	-
12	CLA	B	815	X	-	-	-
12	CLA	B	817	X	-	-	-
12	CLA	B	818	X	-	-	-
12	CLA	B	819	X	-	-	-
12	CLA	B	820	X	-	-	-
12	CLA	B	821	X	-	-	-
12	CLA	B	822	X	-	-	-
12	CLA	B	823	X	-	-	-
12	CLA	B	825	X	-	-	-
12	CLA	B	826	X	-	-	-
12	CLA	B	828	X	-	-	-
12	CLA	B	829	X	-	-	-
12	CLA	B	830	X	-	-	-
12	CLA	B	832	X	-	-	-
12	CLA	F	203	X	-	-	-
12	CLA	J	101	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 22177 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5803	3794	987	999	23		

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

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

- 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
			601	367	106	117	11		

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

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

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

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

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

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

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

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

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

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

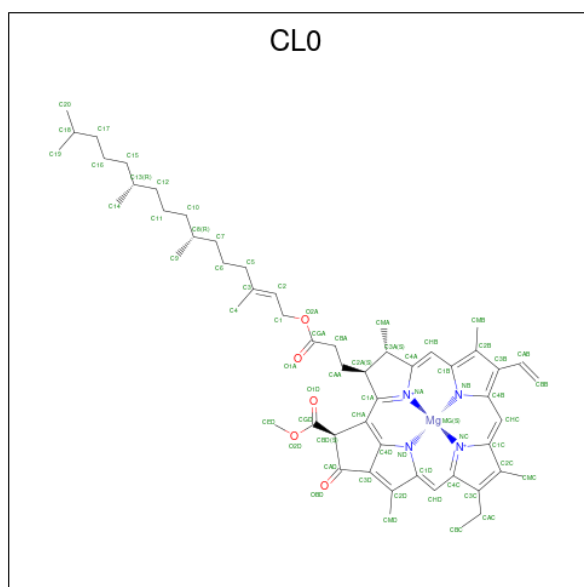
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

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

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

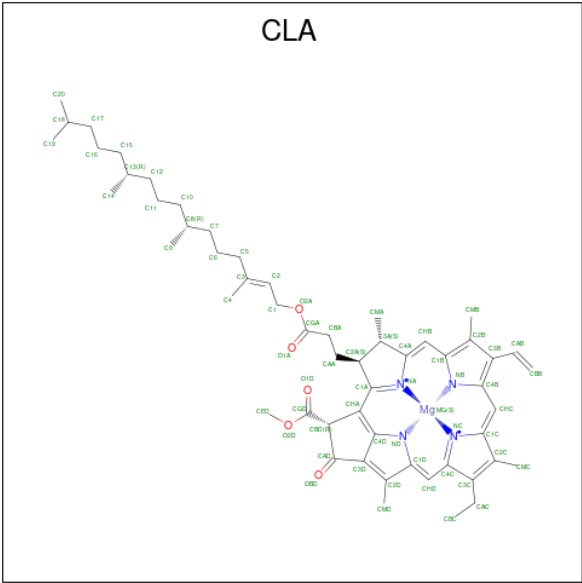
Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	29	Total	C	N	O		0	0
			215	145	34	36			

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



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

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
12	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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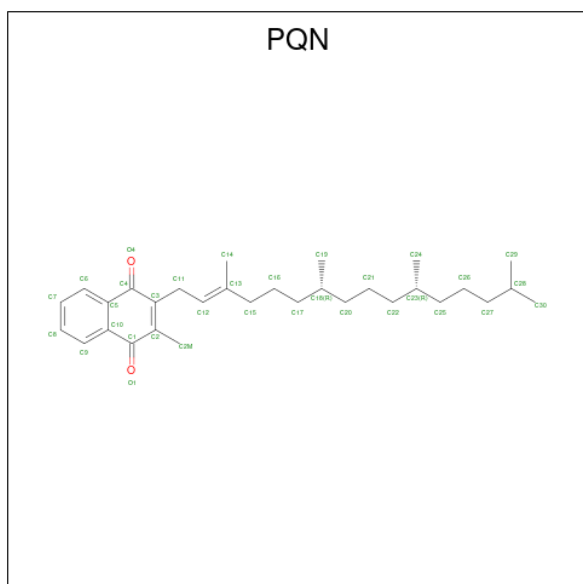
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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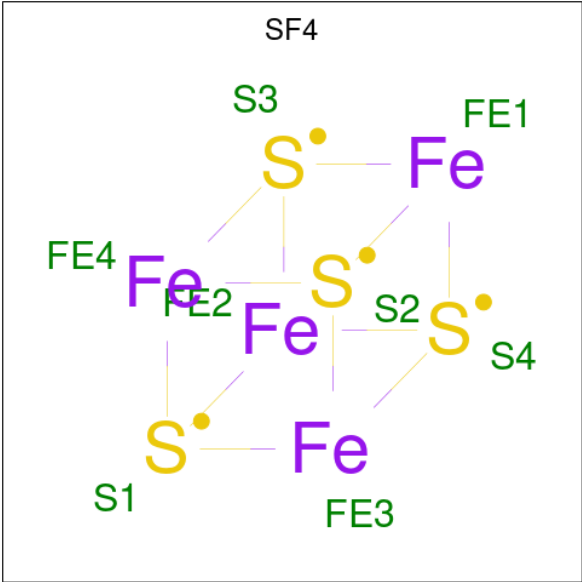
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 13 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



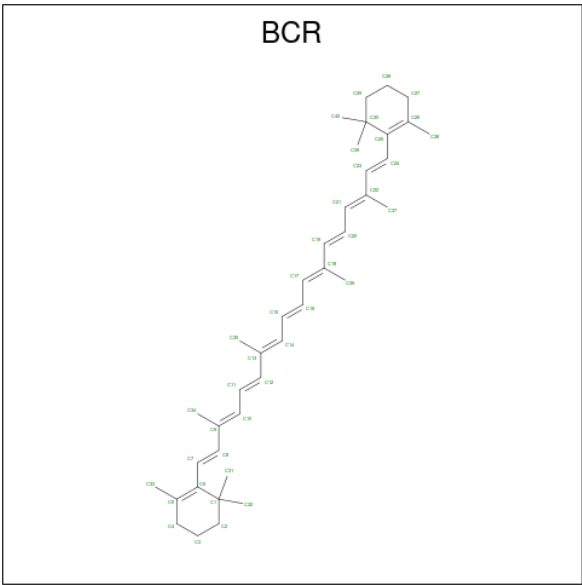
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	C	O	0
			33	31	2	
13	B	1	Total	C	O	0
			33	31	2	

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



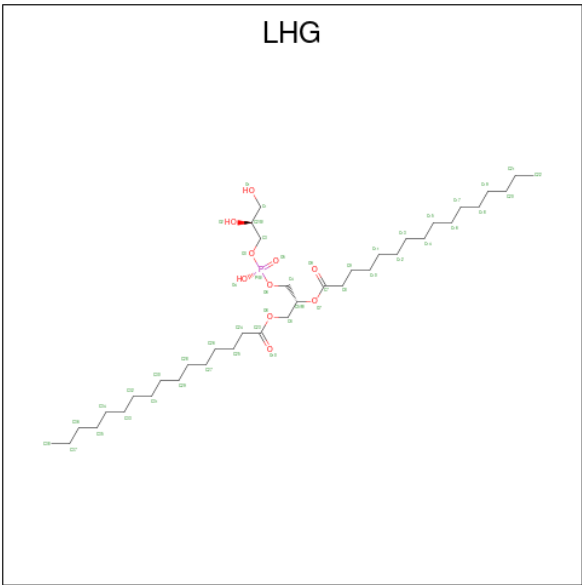
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	

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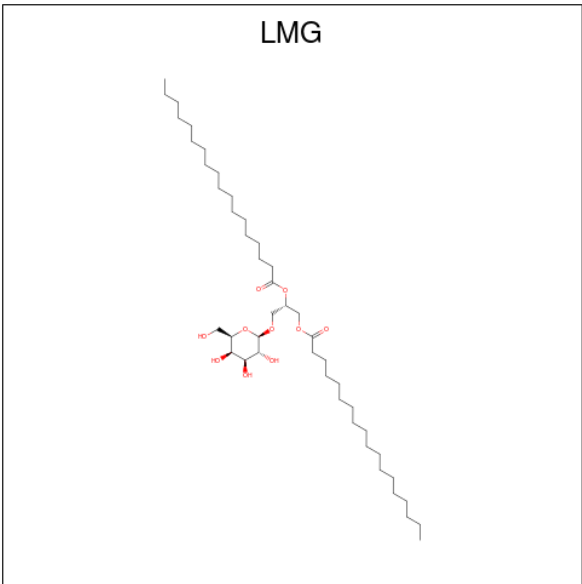
Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C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

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



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

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

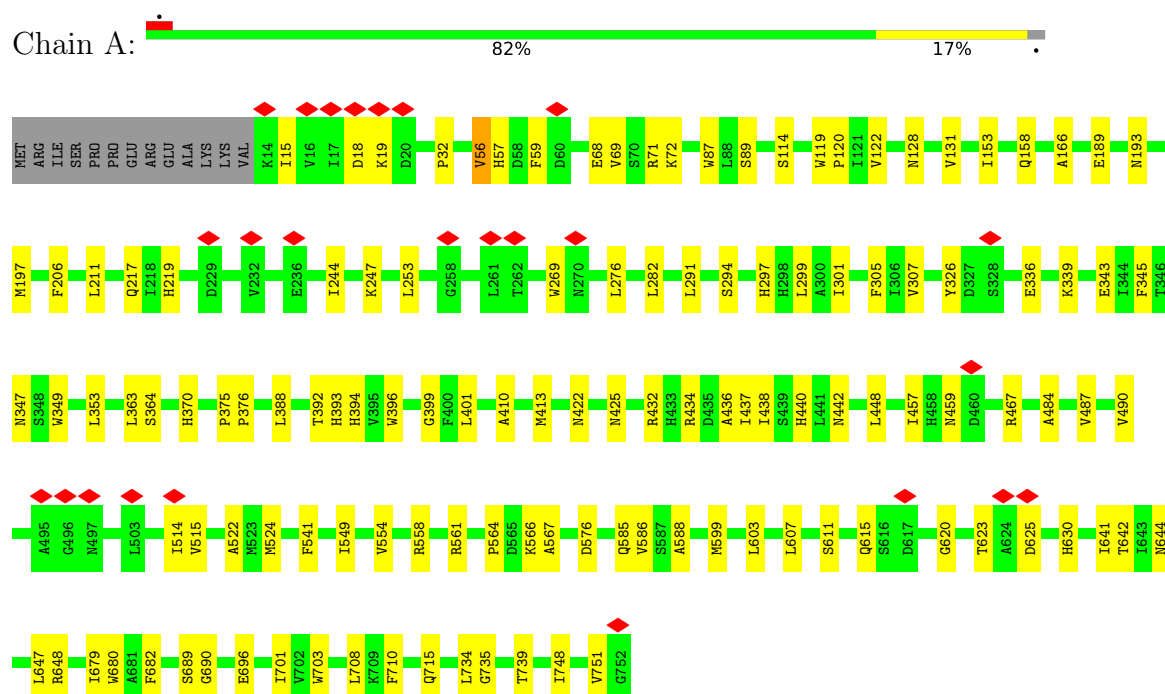


Mol	Chain	Residues	Atoms			AltConf
17	B	1	Total	C	O	0
			55	45	10	

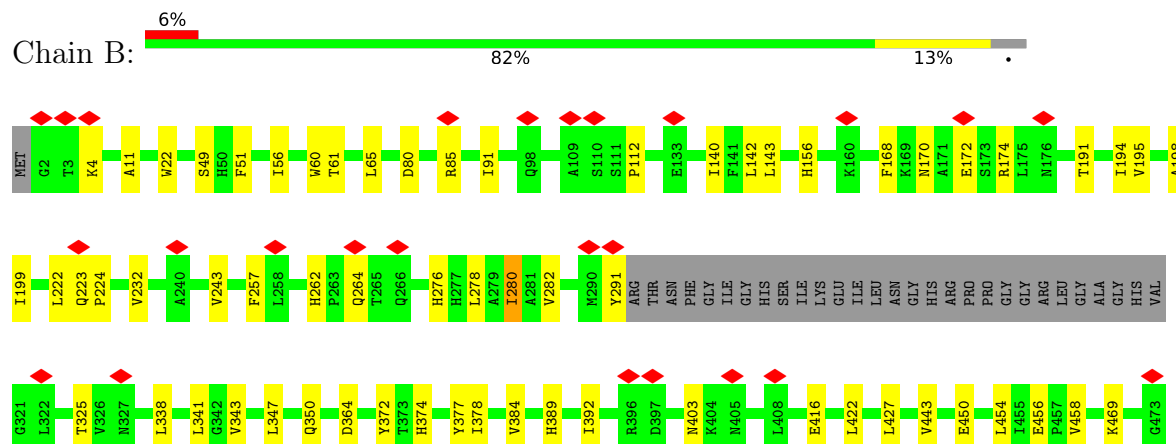
3 Residue-property plots

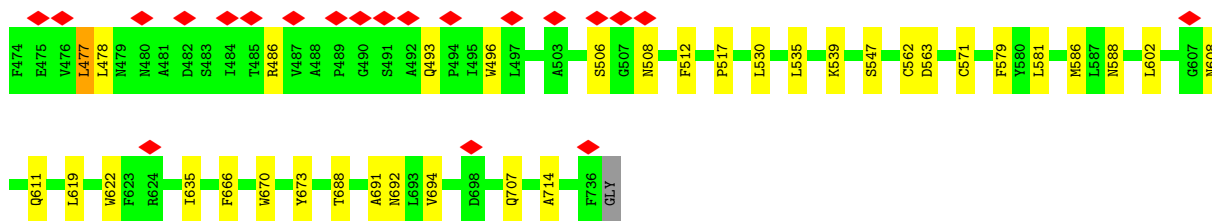
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

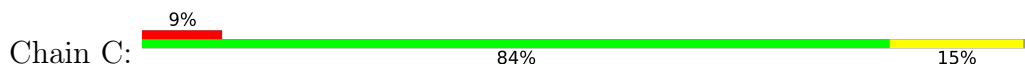


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

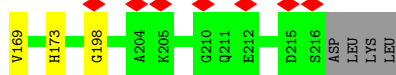




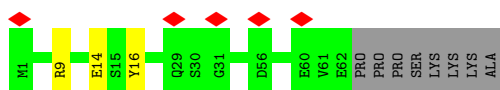
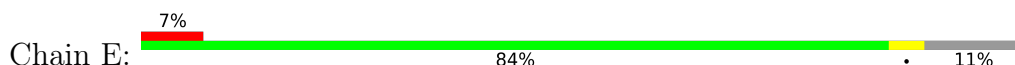
• Molecule 3: Photosystem I iron-sulfur center



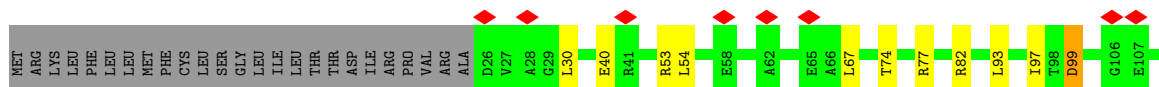
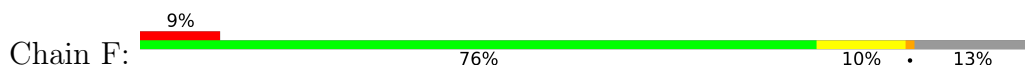
• Molecule 4: Photosystem I reaction center subunit II, cyanelle



• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III

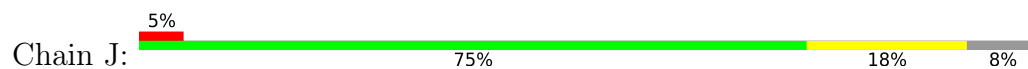


• Molecule 7: Photosystem I reaction center subunit VIII

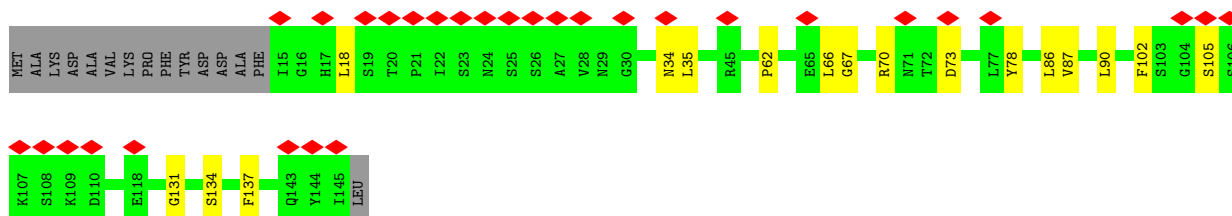
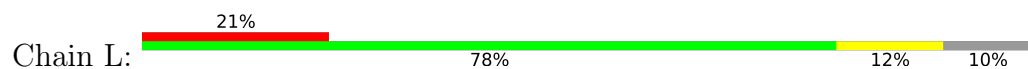




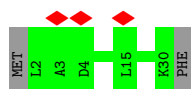
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit XI



- Molecule 10: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	110380	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.376	Depositor
Minimum map value	-0.292	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.06	Depositor
Map size ($\text{\AA}$)	437.2, 437.2, 437.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.093, 1.093, 1.093	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, CL0, SF4, LMG, LHG, BCR, 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	0.22	0/6000	0.46	0/8177
2	B	0.31	0/5820	0.85	2/7955 (0.0%)
3	C	0.31	0/611	1.01	4/828 (0.5%)
4	D	0.24	0/1105	0.82	6/1489 (0.4%)
5	E	0.19	0/516	0.45	0/696
6	F	0.19	0/1281	0.55	2/1733 (0.1%)
7	I	0.27	0/232	0.59	0/319
8	J	0.19	0/300	0.54	0/410
9	L	0.22	0/988	0.60	2/1342 (0.1%)
10	M	0.18	0/217	0.41	0/295
All	All	0.26	0/17070	0.68	16/23244 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
4	D	0	3
6	F	0	1
All	All	0	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	147	ASP	CA-C-N	7.04	124.67	120.24
6	F	147	ASP	C-N-CA	7.04	124.67	120.24
4	D	125	ALA	CA-C-N	6.95	134.47	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	125	ALA	C-N-CA	6.95	134.47	121.97
9	L	73	ASP	CA-C-N	6.26	132.97	121.70
9	L	73	ASP	C-N-CA	6.26	132.97	121.70
4	D	123	GLY	CA-C-N	6.25	133.48	121.54
4	D	123	GLY	C-N-CA	6.25	133.48	121.54
2	B	692	ASN	CA-C-N	6.12	129.31	120.38
2	B	692	ASN	C-N-CA	6.12	129.31	120.38
3	C	62	PHE	CA-C-N	5.96	132.91	121.54
3	C	62	PHE	C-N-CA	5.96	132.91	121.54
4	D	130	GLY	CA-C-N	5.36	131.34	121.70
4	D	130	GLY	C-N-CA	5.36	131.34	121.70
3	C	61	ASP	CA-C-N	5.31	131.68	121.54
3	C	61	ASP	C-N-CA	5.31	131.68	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	493	GLN	Peptide
4	D	124	ALA	Peptide
4	D	125	ALA	Peptide
4	D	164	TYR	Peptide
6	F	99	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5803	0	5621	93	0
2	B	5622	0	5406	64	0
3	C	601	0	576	7	0
4	D	1082	0	1099	16	0
5	E	508	0	507	3	0
6	F	1255	0	1249	14	0
7	I	228	0	247	5	0
8	J	292	0	302	4	0
9	L	965	0	970	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	M	215	0	239	0	0
11	A	65	0	72	3	0
12	A	2407	0	2290	86	0
12	B	1900	0	1927	78	0
12	F	45	0	33	0	0
12	J	45	0	33	0	0
12	L	163	0	148	11	0
13	A	33	0	46	3	0
13	B	33	0	46	5	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
15	A	240	0	336	17	0
15	B	120	0	168	8	0
15	F	80	0	112	6	0
15	I	40	0	56	5	0
15	J	120	0	168	6	0
15	L	120	0	168	11	0
15	M	40	0	56	2	0
16	A	76	0	98	2	0
17	B	55	0	86	7	0
All	All	22177	0	22059	333	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (333) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:807:CLA:H162	12:B:822:CLA:HBB2	1.66	0.78
12:A:819:CLA:HAB	12:A:819:CLA:H8	1.72	0.71
12:B:802:CLA:H203	12:L:203:CLA:HBB1	1.73	0.71
1:A:307:VAL:HG12	15:A:846:BCR:H17C	1.75	0.68
12:B:829:CLA:H71	12:B:829:CLA:HBB1	1.75	0.68
12:A:809:CLA:HAB	15:J:102:BCR:HC7	1.76	0.67
1:A:363:LEU:HD21	12:A:819:CLA:H72	1.75	0.67
2:B:338:LEU:HD21	12:B:823:CLA:HAB	1.76	0.67
12:B:832:CLA:H121	15:I:101:BCR:H21C	1.76	0.66
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.76	0.66
8:J:9:THR:HG22	8:J:11:PRO:HD2	1.77	0.65
12:B:829:CLA:HBC2	15:J:104:BCR:HC7	1.80	0.64
12:B:831:CLA:HBB2	13:B:833:PQN:H141	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:841:CLA:HAB	13:A:844:PQN:H162	1.81	0.62
1:A:353:LEU:HD11	12:A:830:CLA:HBB1	1.81	0.62
12:A:833:CLA:HBB2	9:L:66:LEU:HD13	1.82	0.62
1:A:87:TRP:HA	12:A:807:CLA:HBB2	1.80	0.62
12:B:802:CLA:H192	15:L:205:BCR:H391	1.82	0.61
4:D:162:ARG:HH21	4:D:169:VAL:HB	1.65	0.61
1:A:345:PHE:HB3	12:A:825:CLA:HBC3	1.84	0.60
12:B:820:CLA:H161	15:B:835:BCR:H17C	1.84	0.59
2:B:4:LYS:HD3	7:I:33:GLU:HB2	1.84	0.59
2:B:563:ASP:OD1	3:C:52:LYS:NZ	2.36	0.59
12:B:824:CLA:HAB	12:B:825:CLA:H203	1.85	0.59
12:A:807:CLA:HMB3	12:A:808:CLA:HHB	1.83	0.58
6:F:74:THR:HG22	6:F:77:ARG:HH21	1.69	0.58
2:B:456:GLU:HG3	6:F:30:LEU:HD11	1.85	0.57
7:I:13:VAL:HA	7:I:17:LEU:HB2	1.85	0.57
12:B:832:CLA:HED3	17:B:837:LMG:H162	1.87	0.56
12:A:827:CLA:HED1	12:A:835:CLA:HAB	1.85	0.56
12:B:802:CLA:H143	15:L:201:BCR:H14C	1.86	0.56
12:B:804:CLA:H142	15:I:101:BCR:H393	1.87	0.56
1:A:715:GLN:NE2	5:E:16:TYR:OH	2.39	0.56
1:A:561:ARG:O	4:D:138:ARG:NH1	2.39	0.55
2:B:622:TRP:HB3	12:B:803:CLA:H101	1.87	0.55
12:B:808:CLA:H8	12:B:808:CLA:HBB1	1.88	0.55
12:A:806:CLA:HHB	12:A:830:CLA:HAB	1.87	0.55
1:A:18:ASP:OD2	1:A:71:ARG:NH2	2.40	0.55
1:A:432:ARG:HD2	4:D:90:GLY:HA3	1.88	0.55
12:A:805:CLA:H193	15:A:847:BCR:H10C	1.89	0.55
15:A:846:BCR:HC8	15:A:847:BCR:H382	1.89	0.55
12:B:801:CLA:H13	15:B:836:BCR:H10C	1.88	0.55
12:B:811:CLA:H42	9:L:78:TYR:HB3	1.89	0.55
2:B:56:ILE:HD11	15:M:101:BCR:HC7	1.89	0.54
12:B:807:CLA:H2	12:B:807:CLA:HED3	1.88	0.54
1:A:644:ASN:OD1	1:A:648:ARG:NH1	2.40	0.54
2:B:191:THR:HG21	2:B:278:LEU:HB2	1.88	0.54
1:A:197:MET:HB2	12:A:813:CLA:HBC2	1.90	0.54
1:A:564:PRO:HB3	4:D:120:PRO:HB3	1.89	0.54
12:A:821:CLA:H122	15:A:850:BCR:HC8	1.88	0.54
12:B:808:CLA:HHB	12:B:809:CLA:HMB3	1.89	0.54
2:B:416:GLU:OE1	6:F:186:ARG:NH2	2.40	0.54
2:B:384:VAL:HG21	2:B:586:MET:HG2	1.90	0.54
12:A:819:CLA:H93	12:A:829:CLA:H162	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:807:CLA:H143	12:B:822:CLA:HBB2	1.90	0.53
12:B:808:CLA:H122	15:I:101:BCR:HC41	1.91	0.53
6:F:54:LEU:HD13	6:F:67:LEU:HB2	1.89	0.53
1:A:114:SER:HB2	1:A:131:VAL:HG21	1.90	0.53
9:L:86:LEU:HD21	15:L:201:BCR:H10C	1.91	0.53
12:B:832:CLA:HBA2	13:B:833:PQN:H262	1.90	0.53
9:L:67:GLY:O	9:L:70:ARG:NH1	2.40	0.53
12:B:806:CLA:HBD	12:B:806:CLA:H102	1.91	0.53
1:A:401:LEU:HD21	12:A:806:CLA:H142	1.91	0.53
1:A:708:LEU:O	6:F:127:ARG:NH1	2.41	0.53
1:A:434:ARG:HA	1:A:437:ILE:HD12	1.91	0.52
12:A:834:CLA:H152	15:L:201:BCR:H372	1.90	0.52
12:A:854:CLA:HBC2	2:B:588:ASN:HB2	1.90	0.52
2:B:341:LEU:HD12	12:B:806:CLA:HED3	1.92	0.52
1:A:247:LYS:NZ	12:A:815:CLA:OBD	2.43	0.52
1:A:467:ARG:NH2	12:A:834:CLA:OBD	2.42	0.52
1:A:343:GLU:O	1:A:347:ASN:ND2	2.43	0.52
2:B:350:GLN:NE2	2:B:372:TYR:OH	2.43	0.52
2:B:688:THR:HG23	2:B:691:ALA:HB3	1.92	0.52
1:A:585:GLN:HG3	2:B:670:TRP:HB2	1.92	0.52
4:D:101:VAL:HG23	4:D:102:GLU:HG3	1.92	0.52
12:A:812:CLA:HBB2	12:A:820:CLA:H13	1.90	0.52
2:B:85:ARG:NH1	2:B:364:ASP:OD2	2.41	0.52
2:B:223:GLN:HG2	2:B:224:PRO:HD3	1.90	0.52
4:D:160:ILE:HG12	4:D:173:HIS:HB3	1.91	0.52
5:E:9:ARG:NH1	6:F:180:GLU:OE2	2.43	0.51
12:B:831:CLA:HAB	13:B:833:PQN:H151	1.93	0.51
1:A:680:TRP:HZ3	12:A:854:CLA:HMD3	1.74	0.51
12:A:832:CLA:HMC2	12:L:203:CLA:H152	1.93	0.51
1:A:689:SER:OG	1:A:690:GLY:N	2.43	0.51
1:A:410:ALA:HB1	1:A:588:ALA:HB1	1.92	0.51
1:A:735:GLY:O	1:A:739:THR:OG1	2.28	0.51
15:L:206:BCR:H403	15:L:206:BCR:H371	1.91	0.51
1:A:701:ILE:HD13	12:A:840:CLA:HMD1	1.93	0.51
1:A:388:LEU:HD13	1:A:748:ILE:HG21	1.92	0.51
2:B:195:VAL:HA	2:B:199:ILE:HD12	1.93	0.51
9:L:34:ASN:HB3	12:L:202:CLA:HAC1	1.93	0.51
6:F:99:ASP:OD1	6:F:99:ASP:N	2.43	0.51
1:A:682:PHE:HZ	12:A:842:CLA:HBC2	1.76	0.50
2:B:170:ASN:ND2	2:B:172:GLU:OE1	2.43	0.50
9:L:67:GLY:H	9:L:70:ARG:HD3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:HIS:HE1	12:A:828:CLA:ND	2.09	0.50
2:B:61:THR:HG23	2:B:142:LEU:HD13	1.92	0.50
1:A:457:ILE:HG22	12:A:834:CLA:HBC2	1.94	0.50
2:B:65:LEU:HD11	15:B:834:BCR:H271	1.94	0.50
2:B:325:THR:HG21	2:B:403:ASN:HD21	1.76	0.50
1:A:620:GLY:HA3	1:A:630:HIS:HA	1.94	0.50
1:A:217:GLN:HE22	1:A:294:SER:HB2	1.76	0.50
12:A:806:CLA:HBB2	15:A:848:BCR:H272	1.93	0.50
3:C:75:ARG:NE	4:D:103:GLU:OE2	2.40	0.50
4:D:98:LYS:NZ	4:D:103:GLU:O	2.42	0.50
4:D:120:PRO:HD3	4:D:145:LEU:HD13	1.94	0.50
12:A:821:CLA:H8	15:A:850:BCR:H12C	1.94	0.50
12:B:808:CLA:HMB3	12:B:809:CLA:HHB	1.93	0.50
12:B:826:CLA:H61	15:F:201:BCR:H312	1.94	0.50
12:A:818:CLA:HHC	12:A:818:CLA:HBB1	1.94	0.49
12:A:805:CLA:H72	15:A:848:BCR:H23C	1.93	0.49
2:B:458:VAL:HG11	6:F:97:ILE:HG23	1.95	0.49
2:B:666:PHE:HA	13:B:833:PQN:H9	1.94	0.49
8:J:25:LEU:O	8:J:29:ASN:ND2	2.46	0.49
9:L:102:PHE:HB3	9:L:105:SER:HA	1.93	0.49
12:B:807:CLA:H191	17:B:837:LMG:H272	1.96	0.48
12:A:826:CLA:H42	12:A:838:CLA:HBA1	1.96	0.48
12:B:821:CLA:H161	17:B:837:LMG:H273	1.94	0.48
1:A:326:TYR:OH	12:A:824:CLA:OBD	2.31	0.48
1:A:276:LEU:HD21	1:A:299:LEU:HD23	1.96	0.48
1:A:269:TRP:HZ3	12:A:817:CLA:H51	1.78	0.48
1:A:514:ILE:HG22	1:A:524:MET:HB2	1.96	0.48
2:B:51:PHE:CE2	12:B:812:CLA:HBB1	2.49	0.48
12:A:808:CLA:H42	12:A:828:CLA:H51	1.95	0.47
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.96	0.47
2:B:168:PHE:O	2:B:174:ARG:NH1	2.47	0.47
2:B:422:LEU:HD13	2:B:535:LEU:HA	1.96	0.47
7:I:32:ASP:OD1	7:I:32:ASP:N	2.46	0.47
1:A:128:ASN:O	6:F:53:ARG:NH2	2.47	0.47
12:A:842:CLA:HBA1	16:A:852:LHG:H171	1.96	0.47
13:A:844:PQN:H161	15:F:201:BCR:H382	1.96	0.47
12:A:828:CLA:H62	12:A:828:CLA:H41	1.63	0.47
2:B:172:GLU:HB2	2:B:291:TYR:HB3	1.96	0.47
1:A:153:ILE:HG23	1:A:158:GLN:HB2	1.96	0.47
9:L:134:SER:HA	9:L:137:PHE:HB3	1.96	0.47
1:A:189:GLU:O	1:A:193:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ASN:OD1	1:A:425:ASN:ND2	2.47	0.47
12:B:814:CLA:HMA2	15:B:834:BCR:H282	1.96	0.47
1:A:515:VAL:HG13	1:A:522:ALA:HB3	1.97	0.47
12:B:801:CLA:H201	12:B:810:CLA:H2	1.96	0.47
12:A:854:CLA:HBB	12:B:803:CLA:H202	1.97	0.47
12:B:824:CLA:H42	15:F:202:BCR:H353	1.97	0.47
9:L:62:PRO:HG3	12:L:204:CLA:HBB1	1.97	0.47
12:A:805:CLA:H142	15:A:848:BCR:H372	1.97	0.46
1:A:282:LEU:HD21	1:A:375:PRO:HD2	1.97	0.46
1:A:413:MET:O	1:A:558:ARG:NH1	2.40	0.46
12:A:805:CLA:H41	12:A:829:CLA:H143	1.97	0.46
2:B:343:VAL:HG13	12:B:819:CLA:HED1	1.95	0.46
12:A:832:CLA:H41	12:A:832:CLA:H61	1.56	0.46
2:B:673:TYR:OH	12:B:804:CLA:OBD	2.32	0.46
12:B:801:CLA:H101	12:B:804:CLA:H121	1.97	0.46
12:B:802:CLA:H41	12:B:802:CLA:H61	1.66	0.46
12:A:842:CLA:H191	15:J:102:BCR:H343	1.97	0.46
2:B:378:ILE:HD13	12:B:822:CLA:HBB1	1.98	0.46
1:A:56:VAL:HG11	12:A:804:CLA:HMD2	1.97	0.46
12:B:822:CLA:H3A	12:B:822:CLA:HBA2	1.74	0.46
6:F:169:PHE:HB2	6:F:174:LEU:HD13	1.98	0.46
12:A:840:CLA:H202	6:F:126:GLY:HA2	1.98	0.46
2:B:469:LYS:NZ	2:B:512:PHE:O	2.48	0.46
1:A:219:HIS:HB3	1:A:244:ILE:HD11	1.98	0.46
12:B:804:CLA:H202	12:B:832:CLA:H122	1.97	0.46
1:A:349:TRP:HB3	12:A:805:CLA:HAC1	1.98	0.46
1:A:438:ILE:O	1:A:442:ASN:N	2.46	0.46
12:A:819:CLA:H71	12:A:829:CLA:H91	1.98	0.46
12:B:831:CLA:H8	12:B:832:CLA:H171	1.98	0.45
6:F:171:SER:OG	6:F:173:LYS:NZ	2.49	0.45
8:J:16:LEU:HA	8:J:19:PHE:HB3	1.98	0.45
12:A:808:CLA:HAB	15:J:102:BCR:H363	1.99	0.45
12:A:843:CLA:HBA2	12:A:843:CLA:H3A	1.63	0.45
1:A:392:THR:HG22	1:A:607:LEU:HD22	1.98	0.45
12:A:854:CLA:H61	12:A:854:CLA:H41	1.69	0.45
1:A:679:ILE:HG21	1:A:734:LEU:HD23	1.98	0.45
2:B:194:ILE:HA	2:B:198:ALA:HB3	1.99	0.45
2:B:262:HIS:CD2	2:B:264:GLN:H	2.35	0.45
12:B:825:CLA:H142	15:F:202:BCR:H333	1.98	0.45
11:A:801:CL0:H15	11:A:801:CL0:H2	1.98	0.45
12:A:836:CLA:HHC	12:A:836:CLA:HBB1	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:805:CLA:HBA1	12:A:805:CLA:H3A	1.69	0.45
1:A:370:HIS:ND1	12:A:818:CLA:OBD	2.49	0.45
2:B:224:PRO:HG2	2:B:232:VAL:HG11	1.98	0.45
2:B:608:ASN:HB3	2:B:611:GLN:HE22	1.82	0.45
12:B:807:CLA:H111	12:B:807:CLA:H72	1.80	0.45
1:A:641:ILE:HG13	1:A:642:THR:HG23	1.99	0.45
12:A:830:CLA:H91	16:A:852:LHG:H312	1.99	0.45
12:B:802:CLA:H13	9:L:90:LEU:HD21	1.99	0.45
1:A:375:PRO:HA	1:A:376:PRO:HD3	1.82	0.45
12:B:820:CLA:HED1	12:B:827:CLA:HAB	1.99	0.45
12:B:823:CLA:H142	17:B:837:LMG:H211	1.98	0.45
1:A:211:LEU:HG	12:A:815:CLA:HBB2	1.99	0.44
1:A:703:TRP:HH2	12:B:824:CLA:HED3	1.83	0.44
12:A:804:CLA:HBB1	12:A:811:CLA:H121	2.00	0.44
2:B:280:ILE:HD13	2:B:280:ILE:HA	1.83	0.44
8:J:15:THR:O	8:J:19:PHE:N	2.48	0.44
12:A:808:CLA:HBB2	12:A:828:CLA:H192	1.99	0.44
12:L:202:CLA:H3A	12:L:202:CLA:HBA2	1.69	0.44
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.98	0.44
12:A:832:CLA:HED1	9:L:18:LEU:HD21	1.98	0.44
12:A:854:CLA:H11	2:B:619:LEU:HD12	1.99	0.44
12:A:818:CLA:H3A	12:A:818:CLA:HBA2	1.66	0.44
12:B:806:CLA:HBA1	12:B:806:CLA:H3A	1.75	0.44
15:I:101:BCR:H371	15:I:101:BCR:H24C	1.79	0.44
9:L:87:VAL:HG11	9:L:131:GLY:HA3	1.99	0.44
12:A:842:CLA:H143	13:A:844:PQN:H292	1.99	0.44
12:B:802:CLA:HHD	15:B:836:BCR:H383	1.99	0.44
9:L:35:LEU:HD21	12:L:202:CLA:HBB1	2.00	0.44
1:A:364:SER:OG	1:A:394:HIS:O	2.31	0.44
1:A:599:MET:HE3	1:A:599:MET:HB3	1.87	0.44
2:B:454:LEU:HB3	2:B:517:PRO:HB3	2.00	0.44
2:B:714:ALA:HA	17:B:837:LMG:H392	2.00	0.44
12:A:822:CLA:HBA2	12:A:822:CLA:H3A	1.62	0.43
2:B:60:TRP:HB2	12:B:809:CLA:H192	2.00	0.43
1:A:388:LEU:HD22	1:A:748:ILE:HD13	1.99	0.43
1:A:436:ALA:O	1:A:440:HIS:ND1	2.48	0.43
12:A:828:CLA:H3A	12:A:828:CLA:HBA2	1.64	0.43
12:B:832:CLA:H111	12:B:832:CLA:H91	1.79	0.43
12:B:832:CLA:H112	15:I:101:BCR:H19C	1.99	0.43
3:C:58:CYS:HA	3:C:59:PRO:HD3	1.90	0.43
4:D:198:GLY:N	5:E:14:GLU:OE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:SER:O	1:A:615:GLN:NE2	2.51	0.43
12:B:829:CLA:H142	12:B:829:CLA:H112	1.86	0.43
1:A:696:GLU:OE1	2:B:547:SER:OG	2.34	0.43
1:A:708:LEU:HB2	1:A:710:PHE:HE1	1.83	0.43
2:B:22:TRP:CG	2:B:707:GLN:HE22	2.36	0.43
2:B:478:LEU:O	2:B:486:ARG:NH2	2.46	0.43
12:B:807:CLA:H41	12:B:807:CLA:H61	1.56	0.43
3:C:81:TYR:HB3	4:D:96:LEU:HD11	2.00	0.43
15:L:206:BCR:H15C	15:L:206:BCR:H351	1.89	0.43
1:A:576:ASP:OD1	3:C:53:ARG:NH2	2.44	0.43
1:A:748:ILE:HA	1:A:751:VAL:HG22	2.00	0.43
2:B:4:LYS:NZ	7:I:33:GLU:OE1	2.48	0.43
1:A:487:VAL:HA	1:A:490:VAL:HG22	1.99	0.43
2:B:80:ASP:OD2	2:B:80:ASP:N	2.52	0.43
2:B:377:TYR:CD1	12:B:821:CLA:HAB	2.54	0.43
12:B:820:CLA:H13	15:B:835:BCR:H15C	2.00	0.43
1:A:119:TRP:CD2	12:A:809:CLA:HED3	2.54	0.43
15:A:850:BCR:H15C	15:A:850:BCR:H351	1.85	0.43
6:F:40:GLU:OE1	6:F:82:ARG:NH2	2.52	0.43
12:A:832:CLA:H62	12:L:203:CLA:H72	2.01	0.43
15:A:848:BCR:H20C	15:A:848:BCR:H361	1.82	0.43
4:D:163:VAL:HG23	4:D:167:GLY:HA3	2.00	0.43
2:B:156:HIS:HE1	12:B:812:CLA:NA	2.17	0.42
12:A:808:CLA:H3A	12:A:808:CLA:HBA2	1.59	0.42
2:B:389:HIS:HA	2:B:392:ILE:HD12	2.01	0.42
2:B:506:SER:OG	2:B:508:ASN:OD1	2.36	0.42
1:A:15:ILE:HG21	12:A:810:CLA:HAA2	2.02	0.42
12:A:805:CLA:H162	12:A:805:CLA:H122	1.73	0.42
12:A:828:CLA:O1D	12:A:829:CLA:HHB	2.20	0.42
12:A:830:CLA:H203	12:A:830:CLA:H161	1.86	0.42
12:A:833:CLA:H41	12:B:802:CLA:HBC2	2.01	0.42
12:B:823:CLA:H41	12:B:823:CLA:H61	1.69	0.42
12:B:817:CLA:H122	12:B:817:CLA:HMC1	2.00	0.42
12:A:802:CLA:HMD1	2:B:581:LEU:HB3	2.00	0.42
3:C:11:CYS:HB3	3:C:39:ILE:HG13	2.01	0.42
4:D:103:GLU:OE2	4:D:105:TYR:OH	2.36	0.42
1:A:19:LYS:HD3	1:A:19:LYS:HA	1.93	0.42
1:A:549:ILE:HG12	12:B:804:CLA:HMD3	2.01	0.42
2:B:257:PHE:HE2	2:B:496:TRP:HE3	1.66	0.42
15:B:835:BCR:H15C	15:B:835:BCR:H351	1.89	0.42
1:A:647:LEU:HD23	2:B:635:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:LEU:HA	1:A:647:LEU:HD12	1.83	0.42
15:J:104:BCR:H11C	15:J:104:BCR:H341	1.94	0.42
15:A:851:BCR:H342	15:A:851:BCR:H331	2.02	0.42
15:L:206:BCR:H20C	15:L:206:BCR:H361	1.84	0.42
1:A:438:ILE:HD13	1:A:438:ILE:HA	1.93	0.42
12:B:818:CLA:HBA2	12:B:818:CLA:H3A	1.82	0.42
1:A:119:TRP:HA	1:A:120:PRO:HD3	1.94	0.41
1:A:484:ALA:HA	12:A:837:CLA:HBA1	2.02	0.41
7:I:25:LEU:HD13	15:L:205:BCR:HC8	2.01	0.41
1:A:554:VAL:HG21	15:A:850:BCR:HC31	2.02	0.41
2:B:61:THR:HG21	12:B:822:CLA:H42	2.03	0.41
12:B:802:CLA:H202	12:B:802:CLA:H162	1.83	0.41
1:A:396:TRP:HB3	12:A:828:CLA:HMC3	2.03	0.41
12:A:831:CLA:HMC1	12:A:839:CLA:HAB	2.01	0.41
1:A:434:ARG:NH1	4:D:121:THR:O	2.52	0.41
12:A:832:CLA:HBB1	12:L:203:CLA:H121	2.02	0.41
15:A:848:BCR:H15C	15:A:848:BCR:H351	1.93	0.41
4:D:103:GLU:HG3	4:D:162:ARG:HD2	2.02	0.41
15:L:201:BCR:H24C	15:L:201:BCR:H371	1.93	0.41
1:A:59:PHE:HB2	1:A:69:VAL:HG13	2.01	0.41
1:A:297:HIS:O	1:A:301:ILE:HG12	2.21	0.41
11:A:801:CL0:H72	11:A:801:CL0:H10	1.79	0.41
2:B:374:HIS:HE2	12:B:822:CLA:C1B	2.34	0.41
15:L:205:BCR:H15C	15:L:205:BCR:H351	1.89	0.41
1:A:363:LEU:HD11	12:A:819:CLA:H52	2.02	0.41
2:B:49:SER:HB3	12:B:806:CLA:HBB1	2.03	0.41
2:B:450:GLU:HA	6:F:93:LEU:HD22	2.02	0.41
1:A:89:SER:HB3	1:A:166:ALA:HB3	2.03	0.41
12:A:802:CLA:HBA2	2:B:427:LEU:HD23	2.03	0.41
12:A:820:CLA:H142	12:A:820:CLA:H111	1.95	0.41
12:B:810:CLA:H13	17:B:837:LMG:H212	2.03	0.41
12:B:816:CLA:H3A	12:B:816:CLA:HBA2	1.66	0.41
15:F:202:BCR:H11C	15:F:202:BCR:H341	1.93	0.41
15:J:103:BCR:H15C	15:J:103:BCR:H351	1.94	0.41
1:A:15:ILE:HD11	12:A:812:CLA:HBD	2.01	0.41
1:A:305:PHE:HE1	12:A:821:CLA:HHC	1.85	0.41
12:A:819:CLA:HBA2	12:A:819:CLA:H3A	1.83	0.41
15:A:847:BCR:H361	15:A:847:BCR:H20C	1.82	0.41
15:A:850:BCR:H11C	15:A:850:BCR:H341	1.90	0.41
2:B:282:VAL:HG21	12:B:816:CLA:HAB	2.01	0.41
2:B:530:LEU:HD12	12:B:830:CLA:HED3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:B:835:BCR:H24C	15:B:835:BCR:H371	1.86	0.41
15:L:201:BCR:H15C	15:L:201:BCR:H351	1.93	0.41
12:L:203:CLA:H112	12:L:203:CLA:H142	1.83	0.41
12:L:204:CLA:H62	12:L:204:CLA:H41	1.81	0.41
15:M:101:BCR:H15C	15:M:101:BCR:H351	1.98	0.41
1:A:68:GLU:OE2	1:A:72:LYS:NZ	2.54	0.41
1:A:459:ASN:HD22	1:A:641:ILE:HB	1.85	0.41
1:A:623:THR:HG23	1:A:625:ASP:H	1.85	0.41
2:B:140:ILE:HA	2:B:143:LEU:HD12	2.03	0.41
13:B:833:PQN:H301	17:B:837:LMG:H201	2.03	0.41
12:A:812:CLA:H41	12:A:812:CLA:H62	1.62	0.40
12:B:811:CLA:H203	12:B:811:CLA:H161	1.90	0.40
1:A:32:PRO:HB3	12:A:803:CLA:HAC1	2.03	0.40
2:B:11:ALA:HB1	3:C:71:ALA:HB2	2.03	0.40
12:B:801:CLA:H91	12:B:804:CLA:H8	2.04	0.40
12:B:823:CLA:H143	12:B:823:CLA:H111	1.88	0.40
4:D:128:ARG:H	4:D:132:ASN:HD22	1.68	0.40
15:F:201:BCR:H15C	15:F:201:BCR:H351	1.96	0.40
1:A:57:HIS:HB3	12:A:805:CLA:HAB	2.02	0.40
1:A:206:PHE:HE2	12:A:829:CLA:H13	1.87	0.40
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.94	0.40
1:A:336:GLU:HB3	1:A:339:LYS:HE3	2.03	0.40
1:A:558:ARG:HA	1:A:567:ALA:HB2	2.02	0.40
12:A:831:CLA:HED2	9:L:18:LEU:HD12	2.03	0.40
15:A:849:BCR:H20C	15:A:849:BCR:H361	1.86	0.40
12:B:804:CLA:H143	12:B:804:CLA:H111	1.95	0.40
12:L:203:CLA:H193	12:L:203:CLA:H161	1.85	0.40
11:A:801:CL0:H49	11:A:801:CL0:H41	1.91	0.40
15:A:847:BCR:H15C	15:A:847:BCR:H351	1.88	0.40
1:A:566:LYS:NZ	1:A:586:VAL:O	2.52	0.40
2:B:276:HIS:HE2	12:B:818:CLA:C2B	2.34	0.40
2:B:347:LEU:HD23	12:B:818:CLA:H52	2.03	0.40
12:B:829:CLA:HBA2	12:B:829:CLA:H3A	1.66	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	737/752 (98%)	701 (95%)	35 (5%)	1 (0%)	48	79
2	B	702/737 (95%)	669 (95%)	31 (4%)	2 (0%)	36	68
3	C	78/81 (96%)	72 (92%)	5 (6%)	1 (1%)	9	40
4	D	137/220 (62%)	114 (83%)	21 (15%)	2 (2%)	8	37
5	E	60/70 (86%)	53 (88%)	7 (12%)	0	100	100
6	F	159/186 (86%)	151 (95%)	8 (5%)	0	100	100
7	I	28/35 (80%)	27 (96%)	1 (4%)	0	100	100
8	J	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
9	L	129/146 (88%)	119 (92%)	10 (8%)	0	100	100
10	M	27/31 (87%)	27 (100%)	0	0	100	100
All	All	2092/2298 (91%)	1966 (94%)	120 (6%)	6 (0%)	37	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	63	LEU
1	A	122	VAL
2	B	477	LEU
2	B	562	CYS
4	D	126	ILE
4	D	165	PRO

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	598/610 (98%)	596 (100%)	2 (0%)	86	88
2	B	574/596 (96%)	564 (98%)	10 (2%)	53	75
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	114/171 (67%)	114 (100%)	0	100	100
5	E	58/65 (89%)	58 (100%)	0	100	100
6	F	133/156 (85%)	133 (100%)	0	100	100
7	I	27/31 (87%)	26 (96%)	1 (4%)	30	63
8	J	32/35 (91%)	32 (100%)	0	100	100
9	L	99/111 (89%)	99 (100%)	0	100	100
10	M	21/23 (91%)	21 (100%)	0	100	100
All	All	1723/1866 (92%)	1710 (99%)	13 (1%)	70	82

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	253	LEU
2	B	222	LEU
2	B	243	VAL
2	B	280	ILE
2	B	443	VAL
2	B	477	LEU
2	B	539	LYS
2	B	571	CYS
2	B	579	PHE
2	B	602	LEU
2	B	694	VAL
7	I	31	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	57	HIS
1	A	107	ASN
1	A	193	ASN
1	A	217	GLN
1	A	225	ASN

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Mol	Chain	Res	Type
1	A	350	HIS
1	A	442	ASN
1	A	497	ASN
1	A	505	ASN
1	A	654	GLN
1	A	706	ASN
2	B	29	ASN
2	B	114	ASN
2	B	127	GLN
2	B	156	HIS
2	B	242	HIS
2	B	262	HIS
2	B	350	GLN
2	B	403	ASN
2	B	452	GLN
2	B	606	GLN
2	B	611	GLN
2	B	613	ASN
2	B	636	ASN
2	B	644	ASN
4	D	82	ASN
5	E	3	GLN
5	E	49	ASN
5	E	52	ASN
6	F	35	GLN
6	F	48	GLN
6	F	52	ASN
6	F	131	GLN
8	J	29	ASN
9	L	34	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

108 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	824	-	53,57,73	2.33	20 (37%)	61,93,113	3.17	29 (47%)
12	CLA	B	806	-	69,73,73	1.99	18 (26%)	82,113,113	2.72	32 (39%)
12	CLA	A	806	-	69,73,73	1.97	19 (27%)	82,113,113	2.76	33 (40%)
12	CLA	B	803	-	69,73,73	1.97	18 (26%)	82,113,113	2.74	35 (42%)
12	CLA	B	816	-	59,63,73	2.21	21 (35%)	70,101,113	2.90	30 (42%)
12	CLA	J	101	8	49,53,73	2.40	19 (38%)	58,89,113	3.06	28 (48%)
12	CLA	A	816	-	53,57,73	2.32	20 (37%)	61,93,113	2.94	27 (44%)
12	CLA	A	825	-	69,73,73	1.96	19 (27%)	82,113,113	2.57	32 (39%)
12	CLA	A	834	-	69,73,73	2.01	20 (28%)	82,113,113	2.77	29 (35%)
15	BCR	A	846	-	41,41,41	1.08	2 (4%)	56,56,56	1.33	9 (16%)
12	CLA	L	202	9	50,54,73	2.40	21 (42%)	59,90,113	3.06	28 (47%)
12	CLA	A	804	-	49,53,73	2.38	19 (38%)	58,89,113	3.11	30 (51%)
12	CLA	A	854	-	69,73,73	1.96	21 (30%)	82,113,113	2.73	33 (40%)
12	CLA	A	808	1	69,73,73	2.02	21 (30%)	82,113,113	2.60	31 (37%)
14	SF4	A	845	2,1	0,12,12	-	-	-	-	-
13	PQN	A	844	-	34,34,34	1.57	2 (5%)	43,45,45	1.09	2 (4%)
15	BCR	A	849	-	41,41,41	1.08	2 (4%)	56,56,56	1.34	8 (14%)
12	CLA	B	811	-	69,73,73	2.01	20 (28%)	82,113,113	2.62	36 (43%)
12	CLA	A	811	-	69,73,73	2.01	19 (27%)	82,113,113	2.67	29 (35%)
12	CLA	A	829	-	69,73,73	1.98	19 (27%)	82,113,113	2.57	32 (39%)
12	CLA	A	802	-	49,53,73	2.36	19 (38%)	58,89,113	3.04	29 (50%)
12	CLA	A	842	-	69,73,73	2.02	21 (30%)	82,113,113	2.60	27 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	A	848	-	41,41,41	1.03	2 (4%)	56,56,56	1.44	10 (17%)
15	BCR	F	201	-	41,41,41	1.08	2 (4%)	56,56,56	1.29	5 (8%)
12	CLA	B	807	-	69,73,73	1.99	19 (27%)	82,113,113	2.72	33 (40%)
12	CLA	B	805	2	58,62,73	2.19	21 (36%)	68,99,113	2.91	29 (42%)
12	CLA	B	832	-	69,73,73	2.01	19 (27%)	82,113,113	2.63	31 (37%)
12	CLA	B	821	-	69,73,73	1.98	21 (30%)	82,113,113	2.71	31 (37%)
12	CLA	B	813	-	69,73,73	2.02	20 (28%)	82,113,113	2.68	32 (39%)
12	CLA	A	824	-	51,55,73	2.34	20 (39%)	60,91,113	3.02	30 (50%)
12	CLA	B	828	-	50,54,73	2.34	19 (38%)	59,90,113	3.08	29 (49%)
12	CLA	B	823	-	69,73,73	2.02	19 (27%)	82,113,113	2.69	32 (39%)
12	CLA	A	809	1	49,53,73	2.37	20 (40%)	58,89,113	2.98	28 (48%)
12	CLA	B	809	-	69,73,73	1.95	19 (27%)	82,113,113	2.76	30 (36%)
15	BCR	B	836	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	A	810	-	49,53,73	2.40	20 (40%)	58,89,113	3.05	27 (46%)
12	CLA	B	817	-	63,67,73	2.13	20 (31%)	74,105,113	2.78	29 (39%)
12	CLA	A	833	-	69,73,73	2.00	20 (28%)	82,113,113	2.69	34 (41%)
12	CLA	A	839	-	54,58,73	2.23	21 (38%)	64,95,113	3.07	32 (50%)
12	CLA	A	838	-	60,64,73	2.15	19 (31%)	71,102,113	2.84	31 (43%)
12	CLA	A	814	-	49,53,73	2.40	19 (38%)	58,89,113	3.06	30 (51%)
15	BCR	M	101	-	41,41,41	1.10	2 (4%)	56,56,56	1.26	5 (8%)
12	CLA	A	807	-	55,59,73	2.29	20 (36%)	64,96,113	2.95	32 (50%)
12	CLA	A	805	-	69,73,73	1.99	19 (27%)	82,113,113	2.68	34 (41%)
15	BCR	J	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.29	6 (10%)
12	CLA	A	843	16	56,60,73	2.26	20 (35%)	65,97,113	2.94	29 (44%)
12	CLA	A	826	-	59,63,73	2.19	21 (35%)	70,101,113	2.91	34 (48%)
15	BCR	A	851	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	A	828	-	69,73,73	2.01	22 (31%)	82,113,113	2.64	33 (40%)
12	CLA	B	827	-	49,53,73	2.40	20 (40%)	58,89,113	3.09	27 (46%)
12	CLA	B	825	-	69,73,73	1.98	19 (27%)	82,113,113	2.80	33 (40%)
12	CLA	B	826	-	62,66,73	2.12	18 (29%)	73,104,113	2.84	32 (43%)
12	CLA	L	204	-	56,60,73	2.24	20 (35%)	65,97,113	3.00	29 (44%)
12	CLA	A	822	-	50,54,73	2.36	19 (38%)	59,90,113	3.03	28 (47%)
12	CLA	B	814	-	60,64,73	2.14	21 (35%)	71,102,113	2.79	32 (45%)
12	CLA	B	818	-	64,68,73	2.09	19 (29%)	76,107,113	2.73	32 (42%)
15	BCR	I	101	-	41,41,41	1.08	3 (7%)	56,56,56	1.31	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CL0	A	801	-	58,73,73	3.09	16 (27%)	60,113,113	2.73	18 (30%)
12	CLA	A	823	-	55,59,73	2.27	21 (38%)	64,96,113	2.97	31 (48%)
12	CLA	B	831	-	69,73,73	2.03	20 (28%)	82,113,113	2.63	33 (40%)
12	CLA	B	802	-	69,73,73	2.00	20 (28%)	82,113,113	2.55	31 (37%)
12	CLA	L	203	-	69,73,73	1.98	18 (26%)	82,113,113	2.66	30 (36%)
12	CLA	A	832	-	69,73,73	2.03	20 (28%)	82,113,113	2.69	33 (40%)
12	CLA	A	841	-	55,59,73	2.29	20 (36%)	64,96,113	3.00	31 (48%)
12	CLA	B	820	-	69,73,73	2.02	19 (27%)	82,113,113	2.74	32 (39%)
12	CLA	A	837	-	55,59,73	2.25	18 (32%)	64,96,113	2.97	29 (45%)
12	CLA	B	830	-	51,55,73	2.30	21 (41%)	60,91,113	3.05	27 (45%)
15	BCR	A	850	-	41,41,41	1.11	2 (4%)	56,56,56	1.34	6 (10%)
15	BCR	B	834	-	41,41,41	1.09	2 (4%)	56,56,56	1.23	5 (8%)
15	BCR	J	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.41	8 (14%)
17	LMG	B	837	-	55,55,55	0.79	1 (1%)	63,63,63	1.37	8 (12%)
12	CLA	A	830	-	69,73,73	1.99	18 (26%)	82,113,113	2.63	30 (36%)
12	CLA	B	815	-	49,53,73	2.40	19 (38%)	58,89,113	3.08	27 (46%)
12	CLA	A	827	-	69,73,73	1.98	20 (28%)	82,113,113	2.71	31 (37%)
12	CLA	B	801	-	69,73,73	1.97	19 (27%)	82,113,113	2.75	32 (39%)
14	SF4	C	102	3	0,12,12	-	-	-	-	-
16	LHG	A	852	-	48,48,48	0.68	1 (2%)	51,54,54	1.30	7 (13%)
12	CLA	A	821	-	69,73,73	2.00	19 (27%)	82,113,113	2.60	31 (37%)
16	LHG	A	853	12	26,26,48	0.84	1 (3%)	29,32,54	1.32	3 (10%)
15	BCR	J	104	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	6 (10%)
12	CLA	A	831	-	54,58,73	2.27	20 (37%)	64,95,113	2.93	30 (46%)
14	SF4	C	101	3	0,12,12	-	-	-	-	-
12	CLA	A	815	-	49,53,73	2.41	20 (40%)	58,89,113	3.06	26 (44%)
12	CLA	B	829	-	69,73,73	1.98	19 (27%)	82,113,113	2.67	30 (36%)
15	BCR	B	835	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	B	810	2	69,73,73	1.99	17 (24%)	82,113,113	2.48	30 (36%)
12	CLA	A	817	-	69,73,73	2.01	20 (28%)	82,113,113	2.68	29 (35%)
15	BCR	F	202	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	3 (5%)
15	BCR	L	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	6 (10%)
12	CLA	A	835	1	58,62,73	2.18	19 (32%)	68,99,113	2.89	30 (44%)
12	CLA	A	819	-	69,73,73	2.03	19 (27%)	82,113,113	2.58	32 (39%)
12	CLA	F	203	6	49,53,73	2.42	20 (40%)	58,89,113	3.03	27 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	822	-	69,73,73	1.99	20 (28%)	82,113,113	2.57	33 (40%)
12	CLA	A	803	-	49,53,73	2.39	20 (40%)	58,89,113	3.05	27 (46%)
12	CLA	B	819	-	50,54,73	2.41	21 (42%)	59,90,113	3.16	31 (52%)
15	BCR	L	206	-	41,41,41	1.03	2 (4%)	56,56,56	1.36	9 (16%)
13	PQN	B	833	-	34,34,34	1.54	2 (5%)	43,45,45	1.25	5 (11%)
12	CLA	B	812	-	49,53,73	2.42	20 (40%)	58,89,113	3.03	27 (46%)
12	CLA	A	812	-	58,62,73	2.23	19 (32%)	68,99,113	2.83	31 (45%)
12	CLA	A	818	-	58,62,73	2.21	20 (34%)	68,99,113	2.85	30 (44%)
12	CLA	B	804	-	69,73,73	1.94	20 (28%)	82,113,113	2.56	27 (32%)
12	CLA	A	813	-	49,53,73	2.40	21 (42%)	58,89,113	2.98	27 (46%)
12	CLA	A	836	1	49,53,73	2.42	20 (40%)	58,89,113	3.11	29 (50%)
12	CLA	B	808	-	69,73,73	1.99	18 (26%)	82,113,113	2.67	31 (37%)
12	CLA	A	840	-	69,73,73	2.04	21 (30%)	82,113,113	2.58	33 (40%)
12	CLA	A	820	-	65,69,73	2.10	19 (29%)	77,108,113	2.67	30 (38%)
15	BCR	A	847	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	8 (14%)
15	BCR	L	201	-	41,41,41	1.08	2 (4%)	56,56,56	1.24	5 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	824	-	-	9/20/96/115	-
12	CLA	B	806	-	1/1/15/20	16/39/115/115	-
12	CLA	A	806	-	1/1/15/20	12/39/115/115	-
12	CLA	B	803	-	1/1/15/20	10/39/115/115	-
12	CLA	B	816	-	-	5/27/103/115	-
12	CLA	J	101	8	1/1/11/20	7/15/91/115	-
12	CLA	A	816	-	1/1/11/20	2/20/96/115	-
12	CLA	A	825	-	1/1/15/20	11/39/115/115	-
12	CLA	A	834	-	-	16/39/115/115	-
15	BCR	A	846	-	-	9/29/63/63	0/2/2/2
12	CLA	L	202	9	-	4/17/93/115	-
12	CLA	A	804	-	1/1/11/20	4/15/91/115	-
12	CLA	A	854	-	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	808	1	1/1/15/20	16/39/115/115	-
15	BCR	A	849	-	-	7/29/63/63	0/2/2/2
13	PQN	A	844	-	-	2/23/43/43	0/2/2/2
14	SF4	A	845	2,1	-	-	0/6/5/5
12	CLA	B	811	-	1/1/15/20	11/39/115/115	-
12	CLA	A	811	-	1/1/15/20	11/39/115/115	-
12	CLA	A	829	-	1/1/15/20	10/39/115/115	-
12	CLA	A	802	-	1/1/11/20	3/15/91/115	-
12	CLA	A	842	-	1/1/15/20	6/39/115/115	-
15	BCR	A	848	-	-	9/29/63/63	0/2/2/2
15	BCR	F	201	-	-	11/29/63/63	0/2/2/2
12	CLA	B	807	-	1/1/15/20	13/39/115/115	-
12	CLA	B	805	2	1/1/12/20	3/26/102/115	-
12	CLA	B	832	-	1/1/15/20	15/39/115/115	-
12	CLA	B	821	-	1/1/15/20	17/39/115/115	-
12	CLA	B	813	-	1/1/15/20	19/39/115/115	-
12	CLA	A	824	-	1/1/11/20	4/18/94/115	-
12	CLA	B	828	-	1/1/11/20	6/17/93/115	-
12	CLA	B	823	-	1/1/15/20	13/39/115/115	-
12	CLA	A	809	1	1/1/11/20	4/15/91/115	-
12	CLA	B	809	-	1/1/15/20	9/39/115/115	-
15	BCR	B	836	-	-	10/29/63/63	0/2/2/2
12	CLA	A	810	-	1/1/11/20	4/15/91/115	-
12	CLA	B	817	-	1/1/13/20	9/32/108/115	-
12	CLA	A	833	-	1/1/15/20	9/39/115/115	-
12	CLA	A	839	-	-	5/21/97/115	-
12	CLA	A	838	-	1/1/13/20	11/29/105/115	-
12	CLA	A	814	-	1/1/11/20	2/15/91/115	-
15	BCR	M	101	-	-	14/29/63/63	0/2/2/2
12	CLA	A	807	-	1/1/12/20	8/23/99/115	-
12	CLA	A	805	-	1/1/15/20	17/39/115/115	-
15	BCR	J	102	-	-	14/29/63/63	0/2/2/2
12	CLA	A	843	16	-	13/24/100/115	-
12	CLA	A	826	-	1/1/13/20	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	A	851	-	-	17/29/63/63	0/2/2/2
12	CLA	A	828	-	1/1/15/20	12/39/115/115	-
12	CLA	B	827	-	-	9/15/91/115	-
12	CLA	B	825	-	1/1/15/20	12/39/115/115	-
12	CLA	B	826	-	1/1/13/20	12/31/107/115	-
12	CLA	L	204	-	-	8/24/100/115	-
12	CLA	A	822	-	-	5/17/93/115	-
12	CLA	B	814	-	1/1/13/20	9/29/105/115	-
12	CLA	B	818	-	1/1/14/20	4/33/109/115	-
15	BCR	I	101	-	-	9/29/63/63	0/2/2/2
11	CL0	A	801	-	3/3/20/25	5/37/135/135	-
12	CLA	A	823	-	-	9/23/99/115	-
12	CLA	B	831	-	-	10/39/115/115	-
12	CLA	B	802	-	1/1/15/20	13/39/115/115	-
12	CLA	L	203	-	-	11/39/115/115	-
12	CLA	A	832	-	1/1/15/20	9/39/115/115	-
12	CLA	A	841	-	1/1/12/20	7/23/99/115	-
12	CLA	B	820	-	1/1/15/20	6/39/115/115	-
12	CLA	A	837	-	1/1/12/20	8/23/99/115	-
12	CLA	B	830	-	1/1/11/20	4/18/94/115	-
15	BCR	A	850	-	-	9/29/63/63	0/2/2/2
15	BCR	B	834	-	-	10/29/63/63	0/2/2/2
15	BCR	J	103	-	-	17/29/63/63	0/2/2/2
17	LMG	B	837	-	-	24/50/70/70	0/1/1/1
12	CLA	A	830	-	1/1/15/20	10/39/115/115	-
12	CLA	B	815	-	1/1/11/20	6/15/91/115	-
12	CLA	A	827	-	1/1/15/20	11/39/115/115	-
12	CLA	B	801	-	1/1/15/20	5/39/115/115	-
14	SF4	C	102	3	-	-	0/6/5/5
16	LHG	A	852	-	-	21/53/53/53	-
12	CLA	A	821	-	1/1/15/20	15/39/115/115	-
16	LHG	A	853	12	-	8/31/31/53	-
15	BCR	J	104	-	-	13/29/63/63	0/2/2/2
12	CLA	A	831	-	1/1/12/20	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	C	101	3	-	-	0/6/5/5
12	CLA	A	815	-	-	4/15/91/115	-
12	CLA	B	829	-	1/1/15/20	16/39/115/115	-
15	BCR	B	835	-	-	12/29/63/63	0/2/2/2
12	CLA	B	810	2	1/1/15/20	11/39/115/115	-
12	CLA	A	817	-	-	10/39/115/115	-
15	BCR	F	202	-	-	11/29/63/63	0/2/2/2
15	BCR	L	205	-	-	10/29/63/63	0/2/2/2
12	CLA	A	835	1	1/1/12/20	8/26/102/115	-
12	CLA	A	819	-	1/1/15/20	11/39/115/115	-
12	CLA	F	203	6	1/1/11/20	5/15/91/115	-
12	CLA	B	822	-	1/1/15/20	12/39/115/115	-
12	CLA	A	803	-	1/1/11/20	6/15/91/115	-
12	CLA	B	819	-	1/1/11/20	6/17/93/115	-
15	BCR	L	206	-	-	15/29/63/63	0/2/2/2
13	PQN	B	833	-	-	5/23/43/43	0/2/2/2
12	CLA	B	812	-	1/1/11/20	3/15/91/115	-
12	CLA	A	812	-	-	10/26/102/115	-
12	CLA	A	818	-	1/1/12/20	9/26/102/115	-
12	CLA	B	804	-	1/1/15/20	6/39/115/115	-
12	CLA	A	813	-	1/1/11/20	9/15/91/115	-
12	CLA	A	836	1	1/1/11/20	5/15/91/115	-
12	CLA	B	808	-	1/1/15/20	2/39/115/115	-
12	CLA	A	840	-	1/1/15/20	16/39/115/115	-
12	CLA	A	820	-	1/1/14/20	10/35/111/115	-
15	BCR	A	847	-	-	8/29/63/63	0/2/2/2
15	BCR	L	201	-	-	11/29/63/63	0/2/2/2

All (1635) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	801	CL0	C1A-CHA	9.62	1.50	1.40
11	A	801	CL0	C3B-C4B	8.76	1.49	1.41
11	A	801	CL0	C1B-C2B	7.89	1.48	1.39
13	A	844	PQN	C3-C2	7.65	1.48	1.35
13	B	833	PQN	C3-C2	7.14	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	801	CL0	C1D-C2D	6.82	1.47	1.39
11	A	801	CL0	C3D-C2D	5.48	1.49	1.39
12	B	832	CLA	C3C-C2C	5.43	1.48	1.36
12	L	202	CLA	C3C-C2C	5.40	1.48	1.36
12	B	824	CLA	C3C-C2C	5.38	1.48	1.36
12	A	837	CLA	C3C-C2C	5.36	1.48	1.36
12	B	825	CLA	C3C-C2C	5.34	1.48	1.36
12	A	843	CLA	C3C-C2C	5.31	1.48	1.36
12	B	819	CLA	C3C-C2C	5.31	1.48	1.36
12	A	842	CLA	C3C-C2C	5.30	1.48	1.36
12	B	812	CLA	C3C-C2C	5.28	1.48	1.36
12	A	816	CLA	C3C-C2C	5.26	1.48	1.36
12	A	841	CLA	C3C-C2C	5.24	1.48	1.36
12	A	823	CLA	C3C-C2C	5.24	1.48	1.36
12	A	826	CLA	C3C-C2C	5.24	1.48	1.36
12	A	830	CLA	C3C-C2C	5.23	1.48	1.36
12	B	826	CLA	C3C-C2C	5.23	1.48	1.36
12	B	831	CLA	C3C-C2C	5.23	1.48	1.36
12	B	817	CLA	C3C-C2C	5.22	1.48	1.36
12	A	836	CLA	C3C-C2C	5.21	1.48	1.36
12	B	816	CLA	C3C-C2C	5.21	1.48	1.36
12	B	808	CLA	C3C-C2C	5.21	1.48	1.36
12	A	813	CLA	C3C-C2C	5.20	1.48	1.36
12	L	204	CLA	C3C-C2C	5.20	1.48	1.36
12	L	203	CLA	C3C-C2C	5.20	1.48	1.36
12	A	815	CLA	C3C-C2C	5.19	1.48	1.36
12	A	840	CLA	O2D-CGD	5.19	1.46	1.33
12	B	820	CLA	C3C-C2C	5.19	1.48	1.36
12	A	808	CLA	C3C-C2C	5.18	1.48	1.36
12	B	830	CLA	C3C-C2C	5.18	1.47	1.36
12	A	811	CLA	C3C-C2C	5.18	1.47	1.36
12	F	203	CLA	C3C-C2C	5.18	1.47	1.36
12	A	802	CLA	C3C-C2C	5.18	1.47	1.36
12	A	820	CLA	C3C-C2C	5.18	1.47	1.36
12	B	827	CLA	C3C-C2C	5.17	1.47	1.36
12	B	823	CLA	C3C-C2C	5.16	1.47	1.36
12	A	817	CLA	C3C-C2C	5.16	1.47	1.36
12	A	807	CLA	C3C-C2C	5.15	1.47	1.36
12	A	840	CLA	C3C-C2C	5.13	1.47	1.36
12	B	829	CLA	C3C-C2C	5.13	1.47	1.36
12	A	812	CLA	C3C-C2C	5.13	1.47	1.36
12	B	828	CLA	C3C-C2C	5.13	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	811	CLA	O2D-CGD	5.13	1.45	1.33
12	B	803	CLA	O2D-CGD	5.12	1.45	1.33
12	B	806	CLA	C3C-C2C	5.12	1.47	1.36
12	A	803	CLA	C3C-C2C	5.12	1.47	1.36
12	A	833	CLA	C3C-C2C	5.12	1.47	1.36
12	B	824	CLA	O2D-CGD	5.12	1.45	1.33
12	B	802	CLA	O2D-CGD	5.12	1.45	1.33
12	B	814	CLA	C3C-C2C	5.11	1.47	1.36
12	L	202	CLA	O2D-CGD	5.11	1.45	1.33
12	A	810	CLA	C3C-C2C	5.11	1.47	1.36
12	A	819	CLA	C3C-C2C	5.11	1.47	1.36
12	B	815	CLA	C3C-C2C	5.11	1.47	1.36
11	A	801	CL0	C3B-C2B	5.10	1.47	1.40
12	B	816	CLA	O2D-CGD	5.10	1.45	1.33
12	A	835	CLA	C3C-C2C	5.10	1.47	1.36
12	A	809	CLA	C3C-C2C	5.10	1.47	1.36
12	A	835	CLA	O2D-CGD	5.10	1.45	1.33
12	A	814	CLA	C3C-C2C	5.09	1.47	1.36
12	B	821	CLA	O2D-CGD	5.09	1.45	1.33
12	A	818	CLA	C3C-C2C	5.09	1.47	1.36
12	A	821	CLA	C3C-C2C	5.09	1.47	1.36
12	L	202	CLA	C1D-ND	5.09	1.44	1.37
12	A	829	CLA	C3C-C2C	5.08	1.47	1.36
12	A	831	CLA	C3C-C2C	5.08	1.47	1.36
12	A	822	CLA	C3C-C2C	5.08	1.47	1.36
12	A	816	CLA	O2D-CGD	5.08	1.45	1.33
12	B	822	CLA	C3C-C2C	5.08	1.47	1.36
12	A	834	CLA	C3C-C2C	5.07	1.47	1.36
12	A	827	CLA	C3C-C2C	5.07	1.47	1.36
12	A	804	CLA	CHC-C1C	5.07	1.48	1.38
12	A	828	CLA	O2D-CGD	5.06	1.45	1.33
12	F	203	CLA	O2D-CGD	5.06	1.45	1.33
12	A	839	CLA	C3C-C2C	5.06	1.47	1.36
12	B	831	CLA	O2D-CGD	5.06	1.45	1.33
12	A	838	CLA	C3C-C2C	5.06	1.47	1.36
12	A	832	CLA	C3C-C2C	5.06	1.47	1.36
12	B	818	CLA	O2D-CGD	5.06	1.45	1.33
12	B	809	CLA	C3C-C2C	5.06	1.47	1.36
12	B	818	CLA	C3C-C2C	5.05	1.47	1.36
12	A	854	CLA	C3C-C2C	5.05	1.47	1.36
12	B	828	CLA	O2D-CGD	5.05	1.45	1.33
12	A	807	CLA	O2D-CGD	5.04	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	817	CLA	O2D-CGD	5.04	1.45	1.33
12	A	825	CLA	O2D-CGD	5.04	1.45	1.33
12	B	817	CLA	O2D-CGD	5.04	1.45	1.33
12	A	828	CLA	C3C-C2C	5.04	1.47	1.36
12	B	801	CLA	C3C-C2C	5.03	1.47	1.36
12	J	101	CLA	C3C-C2C	5.03	1.47	1.36
12	B	807	CLA	C3C-C2C	5.03	1.47	1.36
12	A	810	CLA	O2D-CGD	5.03	1.45	1.33
12	B	805	CLA	O2D-CGD	5.03	1.45	1.33
12	A	824	CLA	O2D-CGD	5.02	1.45	1.33
12	A	824	CLA	C3C-C2C	5.02	1.47	1.36
12	B	807	CLA	O2D-CGD	5.01	1.45	1.33
12	A	815	CLA	C1D-ND	5.01	1.44	1.37
12	B	819	CLA	CHC-C1C	5.01	1.48	1.38
12	B	815	CLA	O2D-CGD	5.00	1.45	1.33
12	A	812	CLA	O2D-CGD	5.00	1.45	1.33
12	A	811	CLA	O2D-CGD	5.00	1.45	1.33
12	A	833	CLA	O2D-CGD	5.00	1.45	1.33
12	J	101	CLA	O2D-CGD	4.99	1.45	1.33
12	A	822	CLA	O2D-CGD	4.99	1.45	1.33
12	B	830	CLA	O2D-CGD	4.99	1.45	1.33
12	B	810	CLA	O2D-CGD	4.99	1.45	1.33
12	B	811	CLA	C3C-C2C	4.98	1.47	1.36
12	B	820	CLA	CHC-C1C	4.98	1.48	1.38
12	A	804	CLA	C3C-C2C	4.97	1.47	1.36
12	A	829	CLA	O2D-CGD	4.97	1.45	1.33
12	B	813	CLA	C3C-C2C	4.97	1.47	1.36
12	A	819	CLA	O2D-CGD	4.97	1.45	1.33
12	A	843	CLA	O2D-CGD	4.97	1.45	1.33
12	B	812	CLA	O2D-CGD	4.97	1.45	1.33
12	A	842	CLA	O2D-CGD	4.96	1.45	1.33
12	B	802	CLA	C3C-C2C	4.96	1.47	1.36
12	A	805	CLA	C3C-C2C	4.96	1.47	1.36
12	A	818	CLA	O2D-CGD	4.96	1.45	1.33
12	A	834	CLA	C1D-ND	4.95	1.44	1.37
12	A	820	CLA	C1D-ND	4.95	1.44	1.37
12	B	829	CLA	O2D-CGD	4.95	1.45	1.33
12	A	836	CLA	C1D-ND	4.95	1.44	1.37
11	A	801	CL0	O2D-CGD	4.94	1.45	1.33
12	A	823	CLA	O2D-CGD	4.94	1.45	1.33
12	A	803	CLA	O2D-CGD	4.94	1.45	1.33
12	A	806	CLA	C3C-C2C	4.94	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	816	CLA	C1D-ND	4.93	1.44	1.37
12	A	808	CLA	O2D-CGD	4.93	1.45	1.33
12	A	820	CLA	O2D-CGD	4.93	1.45	1.33
12	A	805	CLA	O2D-CGD	4.92	1.45	1.33
12	B	820	CLA	O2D-CGD	4.92	1.45	1.33
12	B	815	CLA	C1D-ND	4.92	1.44	1.37
12	A	831	CLA	O2D-CGD	4.91	1.45	1.33
12	A	832	CLA	O2D-CGD	4.91	1.45	1.33
12	B	822	CLA	O2D-CGD	4.91	1.45	1.33
12	B	827	CLA	C1D-ND	4.90	1.44	1.37
12	A	815	CLA	O2D-CGD	4.90	1.45	1.33
12	J	101	CLA	C1D-ND	4.90	1.44	1.37
12	A	821	CLA	CHC-C1C	4.90	1.48	1.38
12	A	841	CLA	O2D-CGD	4.90	1.45	1.33
12	A	836	CLA	O2D-CGD	4.89	1.45	1.33
12	A	802	CLA	O2D-CGD	4.89	1.45	1.33
12	B	808	CLA	O2D-CGD	4.89	1.45	1.33
12	B	816	CLA	C1D-ND	4.89	1.44	1.37
12	A	804	CLA	O2D-CGD	4.89	1.45	1.33
12	A	814	CLA	CHC-C1C	4.89	1.48	1.38
12	A	825	CLA	C3C-C2C	4.88	1.47	1.36
12	B	805	CLA	C3C-C2C	4.87	1.47	1.36
12	A	830	CLA	O2D-CGD	4.86	1.45	1.33
12	A	843	CLA	C1D-ND	4.86	1.44	1.37
12	A	812	CLA	C1D-ND	4.85	1.44	1.37
12	A	821	CLA	O2D-CGD	4.85	1.45	1.33
12	B	809	CLA	O2D-CGD	4.85	1.45	1.33
12	A	841	CLA	C1D-ND	4.84	1.44	1.37
12	B	806	CLA	O2D-CGD	4.84	1.45	1.33
12	A	823	CLA	C1D-ND	4.84	1.44	1.37
12	A	807	CLA	C1D-ND	4.84	1.44	1.37
12	B	826	CLA	O2D-CGD	4.84	1.45	1.33
12	A	839	CLA	O2D-CGD	4.83	1.45	1.33
12	L	204	CLA	O2D-CGD	4.83	1.45	1.33
12	A	822	CLA	C1D-ND	4.83	1.44	1.37
12	B	805	CLA	C1D-ND	4.83	1.44	1.37
12	B	827	CLA	O2D-CGD	4.83	1.45	1.33
12	A	803	CLA	C1D-ND	4.83	1.44	1.37
12	A	826	CLA	CHC-C1C	4.83	1.48	1.38
12	L	203	CLA	O2D-CGD	4.82	1.45	1.33
12	A	827	CLA	O2D-CGD	4.82	1.45	1.33
12	A	810	CLA	C1D-ND	4.82	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	826	CLA	O2D-CGD	4.82	1.45	1.33
12	B	832	CLA	O2D-CGD	4.82	1.45	1.33
12	B	817	CLA	C1D-ND	4.82	1.44	1.37
12	A	819	CLA	C1D-ND	4.81	1.44	1.37
13	B	833	PQN	C10-C5	4.81	1.48	1.40
12	B	807	CLA	C1D-ND	4.81	1.44	1.37
12	A	827	CLA	C1D-ND	4.80	1.44	1.37
12	B	810	CLA	C3C-C2C	4.80	1.47	1.36
12	B	813	CLA	CHC-C1C	4.80	1.48	1.38
12	A	818	CLA	C1D-ND	4.79	1.44	1.37
12	B	825	CLA	CHC-C1C	4.79	1.48	1.38
12	B	820	CLA	C1D-ND	4.79	1.44	1.37
12	B	824	CLA	CHC-C1C	4.79	1.48	1.38
12	B	808	CLA	C1D-ND	4.78	1.44	1.37
12	A	806	CLA	O2D-CGD	4.78	1.45	1.33
12	A	838	CLA	O2D-CGD	4.78	1.45	1.33
12	L	204	CLA	CHC-C1C	4.78	1.48	1.38
12	A	814	CLA	C1D-ND	4.77	1.44	1.37
11	A	801	CL0	OBD-CAD	4.76	1.28	1.22
12	A	802	CLA	CHC-C1C	4.76	1.48	1.38
12	B	823	CLA	O2D-CGD	4.76	1.44	1.33
12	A	809	CLA	O2D-CGD	4.76	1.44	1.33
12	B	814	CLA	CHC-C1C	4.75	1.48	1.38
12	F	203	CLA	C1D-ND	4.75	1.44	1.37
11	A	801	CL0	C3A-C2A	-4.75	1.50	1.54
12	B	812	CLA	CHC-C1C	4.74	1.48	1.38
12	B	818	CLA	C1D-ND	4.74	1.44	1.37
12	B	804	CLA	O2D-CGD	4.74	1.44	1.33
12	A	814	CLA	O2D-CGD	4.73	1.44	1.33
12	A	808	CLA	C1D-ND	4.73	1.44	1.37
12	B	811	CLA	C1D-ND	4.73	1.44	1.37
12	B	819	CLA	O2D-CGD	4.73	1.44	1.33
12	B	812	CLA	C1D-ND	4.72	1.44	1.37
12	B	813	CLA	O2D-CGD	4.72	1.44	1.33
12	A	832	CLA	C1D-ND	4.71	1.44	1.37
12	B	817	CLA	CHC-C1C	4.71	1.47	1.38
12	A	813	CLA	CHC-C1C	4.71	1.47	1.38
12	A	817	CLA	C1D-ND	4.71	1.44	1.37
12	A	806	CLA	C1D-ND	4.70	1.44	1.37
12	A	828	CLA	CHC-C1C	4.69	1.47	1.38
12	A	837	CLA	O2D-CGD	4.68	1.44	1.33
12	B	804	CLA	CHC-C1C	4.68	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	803	CLA	C3C-C2C	4.68	1.46	1.36
12	A	829	CLA	CHC-C1C	4.68	1.47	1.38
12	B	829	CLA	CHC-C1C	4.67	1.47	1.38
12	A	854	CLA	CHC-C1C	4.67	1.47	1.38
12	B	819	CLA	C1D-ND	4.67	1.44	1.37
12	A	841	CLA	CHC-C1C	4.67	1.47	1.38
12	B	802	CLA	CHC-C1C	4.67	1.47	1.38
12	B	813	CLA	C1D-ND	4.67	1.44	1.37
12	B	814	CLA	O2D-CGD	4.66	1.44	1.33
12	A	805	CLA	C1D-ND	4.66	1.44	1.37
12	A	824	CLA	C1D-ND	4.66	1.44	1.37
13	A	844	PQN	C10-C5	4.66	1.48	1.40
12	B	832	CLA	C1D-ND	4.65	1.44	1.37
11	A	801	CL0	CHC-C4B	4.65	1.47	1.39
12	A	838	CLA	C1D-ND	4.65	1.44	1.37
12	B	831	CLA	C1D-ND	4.65	1.44	1.37
12	A	840	CLA	CHC-C1C	4.65	1.47	1.38
12	B	828	CLA	C1D-ND	4.65	1.44	1.37
12	A	832	CLA	CHC-C1C	4.65	1.47	1.38
12	A	834	CLA	O2D-CGD	4.65	1.44	1.33
12	B	804	CLA	C3C-C2C	4.64	1.46	1.36
12	A	839	CLA	C1D-ND	4.64	1.44	1.37
12	A	811	CLA	CHC-C1C	4.64	1.47	1.38
12	A	813	CLA	C1D-ND	4.62	1.43	1.37
12	A	807	CLA	CHC-C1C	4.62	1.47	1.38
12	A	831	CLA	C1D-ND	4.62	1.43	1.37
12	A	817	CLA	CHC-C1C	4.62	1.47	1.38
12	A	811	CLA	C1D-ND	4.61	1.43	1.37
12	A	821	CLA	C1D-ND	4.61	1.43	1.37
12	A	854	CLA	O2D-CGD	4.61	1.44	1.33
12	A	842	CLA	CHC-C1C	4.61	1.47	1.38
12	B	826	CLA	C1D-ND	4.60	1.43	1.37
12	A	824	CLA	CHC-C1C	4.60	1.47	1.38
12	J	101	CLA	CHC-C1C	4.60	1.47	1.38
12	A	813	CLA	O2D-CGD	4.60	1.44	1.33
12	A	808	CLA	CHC-C1C	4.60	1.47	1.38
12	B	821	CLA	C3C-C2C	4.60	1.46	1.36
12	A	812	CLA	CHC-C1C	4.60	1.47	1.38
12	A	815	CLA	CHC-C1C	4.60	1.47	1.38
12	B	831	CLA	CHC-C1C	4.59	1.47	1.38
12	A	831	CLA	CHC-C1C	4.59	1.47	1.38
12	B	810	CLA	C1D-ND	4.59	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	827	CLA	CHC-C1C	4.59	1.47	1.38
12	B	828	CLA	CHC-C1C	4.59	1.47	1.38
12	B	824	CLA	C1D-ND	4.59	1.43	1.37
12	B	826	CLA	CHC-C1C	4.59	1.47	1.38
12	L	202	CLA	CHC-C1C	4.58	1.47	1.38
12	B	812	CLA	O2A-CGA	4.57	1.45	1.30
12	J	101	CLA	O2A-CGA	4.57	1.45	1.30
12	A	804	CLA	C1D-ND	4.57	1.43	1.37
12	A	843	CLA	CHC-C1C	4.57	1.47	1.38
12	B	815	CLA	O2A-CGA	4.56	1.45	1.30
12	A	837	CLA	C1D-ND	4.56	1.43	1.37
12	A	805	CLA	CHC-C1C	4.56	1.47	1.38
12	A	826	CLA	C1D-ND	4.55	1.43	1.37
12	B	821	CLA	CHC-C1C	4.55	1.47	1.38
12	A	818	CLA	CHC-C1C	4.55	1.47	1.38
12	A	815	CLA	O2A-CGA	4.55	1.45	1.30
12	A	804	CLA	O2A-CGA	4.54	1.45	1.30
12	A	833	CLA	CHC-C1C	4.54	1.47	1.38
12	B	825	CLA	C1D-ND	4.54	1.43	1.37
12	B	820	CLA	O2A-CGA	4.54	1.46	1.33
12	B	806	CLA	C1D-ND	4.54	1.43	1.37
12	L	203	CLA	CHC-C1C	4.53	1.47	1.38
12	A	814	CLA	O2A-CGA	4.53	1.45	1.30
12	B	805	CLA	CHC-C1C	4.53	1.47	1.38
12	B	827	CLA	O2A-CGA	4.53	1.45	1.30
12	A	822	CLA	CHC-C1C	4.53	1.47	1.38
12	A	840	CLA	C1D-ND	4.53	1.43	1.37
12	A	813	CLA	O2A-CGA	4.52	1.45	1.30
12	L	204	CLA	C1D-ND	4.52	1.43	1.37
12	B	830	CLA	CHC-C1C	4.52	1.47	1.38
12	B	808	CLA	CHC-C1C	4.52	1.47	1.38
12	F	203	CLA	O2A-CGA	4.52	1.45	1.30
12	A	819	CLA	CHC-C1C	4.51	1.47	1.38
12	A	838	CLA	CHC-C1C	4.51	1.47	1.38
12	B	809	CLA	C1D-ND	4.51	1.43	1.37
12	A	828	CLA	C1D-ND	4.51	1.43	1.37
11	A	801	CL0	CHB-C4A	-4.51	1.33	1.38
12	A	809	CLA	C1D-ND	4.51	1.43	1.37
12	A	836	CLA	O2A-CGA	4.51	1.45	1.30
12	B	814	CLA	C1D-ND	4.50	1.43	1.37
12	A	833	CLA	C1D-ND	4.50	1.43	1.37
12	A	803	CLA	O2A-CGA	4.50	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	836	CLA	CHC-C1C	4.50	1.47	1.38
12	A	809	CLA	CHC-C1C	4.49	1.47	1.38
12	A	810	CLA	O2A-CGA	4.49	1.45	1.30
12	B	801	CLA	O2D-CGD	4.49	1.44	1.33
12	A	839	CLA	CHC-C1C	4.49	1.47	1.38
12	A	807	CLA	CHD-C1D	4.49	1.47	1.38
12	B	832	CLA	CHD-C1D	4.49	1.47	1.38
12	A	803	CLA	CHC-C1C	4.49	1.47	1.38
12	A	835	CLA	C1D-ND	4.49	1.43	1.37
12	B	827	CLA	CHC-C1C	4.48	1.47	1.38
12	A	835	CLA	CHC-C1C	4.48	1.47	1.38
12	A	802	CLA	O2A-CGA	4.48	1.45	1.30
12	A	817	CLA	O2A-CGA	4.48	1.46	1.33
12	A	842	CLA	C1D-ND	4.47	1.43	1.37
12	B	816	CLA	CHC-C1C	4.47	1.47	1.38
12	F	203	CLA	CHD-C1D	4.47	1.47	1.38
12	A	809	CLA	O2A-CGA	4.47	1.45	1.30
12	A	825	CLA	CHC-C1C	4.46	1.47	1.38
12	A	819	CLA	CHD-C1D	4.46	1.47	1.38
12	B	823	CLA	CHD-C1D	4.46	1.47	1.38
12	B	829	CLA	C1D-ND	4.46	1.43	1.37
12	B	830	CLA	C1D-ND	4.45	1.43	1.37
12	A	810	CLA	CHC-C1C	4.45	1.47	1.38
12	B	825	CLA	O2D-CGD	4.44	1.44	1.33
12	A	843	CLA	O2A-CGA	4.43	1.46	1.33
12	A	830	CLA	CHC-C1C	4.43	1.47	1.38
12	A	820	CLA	CHD-C1D	4.43	1.47	1.38
12	B	813	CLA	CHD-C1D	4.42	1.47	1.38
12	B	822	CLA	CHC-C1C	4.42	1.47	1.38
12	A	824	CLA	CHD-C1D	4.41	1.47	1.38
12	B	803	CLA	C1D-ND	4.40	1.43	1.37
12	L	203	CLA	C1D-ND	4.40	1.43	1.37
12	B	823	CLA	CHC-C1C	4.40	1.47	1.38
12	B	811	CLA	CHC-C1C	4.40	1.47	1.38
12	B	815	CLA	CHC-C1C	4.40	1.47	1.38
12	F	203	CLA	CHC-C1C	4.40	1.47	1.38
12	A	812	CLA	CHD-C1D	4.40	1.47	1.38
12	A	816	CLA	CHC-C1C	4.39	1.47	1.38
12	B	822	CLA	O2A-CGA	4.39	1.46	1.33
12	B	831	CLA	CHD-C1D	4.38	1.47	1.38
12	B	815	CLA	CHD-C1D	4.38	1.47	1.38
12	B	829	CLA	O2A-CGA	4.38	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	803	CLA	CHC-C1C	4.38	1.47	1.38
12	A	832	CLA	O2A-CGA	4.37	1.46	1.33
12	A	806	CLA	CHC-C1C	4.37	1.47	1.38
12	A	816	CLA	CHD-C1D	4.36	1.46	1.38
12	A	823	CLA	CHD-C1D	4.36	1.46	1.38
12	B	812	CLA	CHD-C1D	4.36	1.46	1.38
12	B	810	CLA	CHD-C1D	4.36	1.46	1.38
12	B	832	CLA	O2A-CGA	4.36	1.46	1.33
12	A	830	CLA	C1D-ND	4.36	1.43	1.37
12	B	821	CLA	O2A-CGA	4.35	1.46	1.33
12	A	834	CLA	CHD-C1D	4.35	1.46	1.38
12	B	824	CLA	O2A-CGA	4.35	1.46	1.33
12	B	819	CLA	CHD-C1D	4.35	1.46	1.38
12	A	837	CLA	O2A-CGA	4.35	1.46	1.33
12	B	801	CLA	CHD-C1D	4.34	1.46	1.38
12	A	837	CLA	CHC-C1C	4.34	1.47	1.38
12	B	826	CLA	CHD-C1D	4.34	1.46	1.38
12	A	840	CLA	O2A-CGA	4.34	1.46	1.33
12	B	807	CLA	CHC-C1C	4.33	1.47	1.38
12	B	827	CLA	CHD-C1D	4.33	1.46	1.38
12	A	836	CLA	CHD-C1D	4.33	1.46	1.38
12	B	811	CLA	CHD-C1D	4.33	1.46	1.38
12	A	802	CLA	C1B-NB	-4.33	1.32	1.37
12	A	823	CLA	CHC-C1C	4.33	1.47	1.38
12	A	835	CLA	O2A-CGA	4.33	1.46	1.33
12	B	802	CLA	C1D-ND	4.32	1.43	1.37
12	A	810	CLA	CHD-C1D	4.32	1.46	1.38
12	L	202	CLA	CHD-C1D	4.32	1.46	1.38
12	A	805	CLA	O2A-CGA	4.32	1.45	1.33
12	A	816	CLA	O2A-CGA	4.31	1.45	1.33
12	A	838	CLA	O2A-CGA	4.31	1.45	1.33
12	B	816	CLA	CHD-C1D	4.31	1.46	1.38
12	A	826	CLA	CHD-C1D	4.30	1.46	1.38
12	A	820	CLA	CHC-C1C	4.30	1.47	1.38
12	A	834	CLA	CHC-C1C	4.30	1.47	1.38
12	B	809	CLA	CHC-C1C	4.30	1.47	1.38
12	B	818	CLA	CHC-C1C	4.30	1.47	1.38
12	A	841	CLA	O2A-CGA	4.30	1.45	1.33
12	A	843	CLA	CHD-C1D	4.30	1.46	1.38
12	B	816	CLA	O2A-CGA	4.29	1.45	1.33
12	B	805	CLA	O2A-CGA	4.29	1.45	1.33
12	A	818	CLA	O2A-CGA	4.29	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	842	CLA	O2A-CGA	4.29	1.45	1.33
12	B	818	CLA	O2A-CGA	4.29	1.45	1.33
12	A	815	CLA	CHD-C1D	4.28	1.46	1.38
12	A	839	CLA	O2A-CGA	4.28	1.45	1.33
12	A	812	CLA	O2A-CGA	4.28	1.45	1.33
12	B	830	CLA	O2A-CGA	4.27	1.45	1.33
12	A	831	CLA	O2A-CGA	4.27	1.45	1.33
12	B	821	CLA	C1D-ND	4.27	1.43	1.37
12	B	823	CLA	C1D-ND	4.27	1.43	1.37
12	A	820	CLA	O2A-CGA	4.27	1.45	1.33
12	A	821	CLA	O2A-CGA	4.26	1.45	1.33
12	A	841	CLA	CHD-C1D	4.26	1.46	1.38
12	B	826	CLA	O2A-CGA	4.26	1.45	1.33
12	B	803	CLA	O2A-CGA	4.26	1.45	1.33
12	B	805	CLA	CHD-C1D	4.26	1.46	1.38
12	A	834	CLA	O2A-CGA	4.26	1.45	1.33
12	L	203	CLA	O2A-CGA	4.26	1.45	1.33
12	L	204	CLA	O2A-CGA	4.25	1.45	1.33
11	A	801	CL0	CHB-C1B	4.25	1.46	1.39
12	B	814	CLA	O2A-CGA	4.25	1.45	1.33
12	B	823	CLA	C1B-NB	-4.24	1.32	1.37
12	A	814	CLA	CHD-C1D	4.24	1.46	1.38
12	A	837	CLA	CHD-C1D	4.23	1.46	1.38
12	A	823	CLA	O2A-CGA	4.23	1.45	1.33
12	B	817	CLA	CHD-C1D	4.23	1.46	1.38
12	B	818	CLA	CHD-C1D	4.23	1.46	1.38
12	A	838	CLA	CHD-C1D	4.23	1.46	1.38
12	A	813	CLA	CHD-C1D	4.23	1.46	1.38
12	A	803	CLA	CHD-C1D	4.22	1.46	1.38
12	A	818	CLA	CHD-C1D	4.22	1.46	1.38
11	A	801	CL0	CHD-C4C	4.22	1.47	1.39
12	A	832	CLA	CHD-C1D	4.22	1.46	1.38
12	B	801	CLA	C1D-ND	4.22	1.43	1.37
12	A	811	CLA	O2A-CGA	4.21	1.45	1.33
12	B	823	CLA	O2A-CGA	4.21	1.45	1.33
12	B	817	CLA	O2A-CGA	4.21	1.45	1.33
12	A	854	CLA	C3D-C2D	4.21	1.50	1.39
12	A	829	CLA	O2A-CGA	4.21	1.45	1.33
12	B	807	CLA	O2A-CGA	4.20	1.45	1.33
12	B	831	CLA	O2A-CGA	4.20	1.45	1.33
12	B	801	CLA	O2A-CGA	4.20	1.45	1.33
12	A	811	CLA	CHD-C1D	4.19	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	819	CLA	CHD-C4C	4.19	1.48	1.39
12	A	831	CLA	CHD-C1D	4.19	1.46	1.38
12	B	809	CLA	O2A-CGA	4.19	1.45	1.33
12	B	828	CLA	O2A-CGA	4.18	1.46	1.33
12	A	825	CLA	O2A-CGA	4.18	1.45	1.33
12	B	825	CLA	O2A-CGA	4.18	1.45	1.33
12	A	807	CLA	O2A-CGA	4.18	1.45	1.33
12	B	810	CLA	C1B-NB	-4.18	1.32	1.37
12	B	802	CLA	CHD-C1D	4.18	1.46	1.38
12	J	101	CLA	CHD-C1D	4.18	1.46	1.38
12	A	833	CLA	CHD-C1D	4.17	1.46	1.38
12	A	805	CLA	CHD-C1D	4.17	1.46	1.38
12	A	808	CLA	CHD-C1D	4.17	1.46	1.38
12	L	202	CLA	O2A-CGA	4.17	1.45	1.33
12	A	819	CLA	O2A-CGA	4.16	1.45	1.33
12	A	822	CLA	O2A-CGA	4.16	1.45	1.33
12	A	808	CLA	O2A-CGA	4.16	1.45	1.33
12	A	835	CLA	CHD-C1D	4.16	1.46	1.38
12	A	830	CLA	CHD-C1D	4.16	1.46	1.38
12	A	854	CLA	O2A-CGA	4.15	1.45	1.33
12	A	826	CLA	O2A-CGA	4.15	1.45	1.33
12	B	806	CLA	O2A-CGA	4.15	1.45	1.33
12	A	824	CLA	CHD-C4C	4.15	1.48	1.39
12	B	806	CLA	CHC-C1C	4.15	1.46	1.38
12	A	822	CLA	CHD-C1D	4.15	1.46	1.38
12	L	204	CLA	CHD-C1D	4.14	1.46	1.38
12	A	827	CLA	O2A-CGA	4.14	1.45	1.33
12	B	822	CLA	C1D-ND	4.14	1.43	1.37
12	A	817	CLA	CHD-C1D	4.14	1.46	1.38
12	B	819	CLA	O2A-CGA	4.14	1.45	1.33
12	A	821	CLA	CHD-C1D	4.13	1.46	1.38
12	F	203	CLA	CHD-C4C	4.13	1.48	1.39
12	A	840	CLA	CHD-C1D	4.13	1.46	1.38
12	A	840	CLA	C3D-C2D	4.13	1.50	1.39
12	A	824	CLA	O2A-CGA	4.13	1.45	1.33
12	B	823	CLA	CHD-C4C	4.12	1.48	1.39
12	A	830	CLA	O2A-CGA	4.12	1.45	1.33
12	A	809	CLA	CHD-C1D	4.12	1.46	1.38
12	A	826	CLA	CHD-C4C	4.12	1.48	1.39
11	A	801	CL0	O2A-CGA	4.11	1.45	1.33
12	B	802	CLA	O2A-CGA	4.11	1.45	1.33
12	B	801	CLA	CHC-C1C	4.11	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	828	CLA	O2A-CGA	4.10	1.45	1.33
12	B	824	CLA	CHD-C4C	4.09	1.48	1.39
11	A	801	CL0	CHC-C1C	4.09	1.47	1.39
12	A	828	CLA	CHD-C1D	4.09	1.46	1.38
12	A	842	CLA	CHD-C1D	4.09	1.46	1.38
12	A	820	CLA	CHD-C4C	4.08	1.48	1.39
12	B	814	CLA	CHD-C1D	4.08	1.46	1.38
12	B	824	CLA	CHD-C1D	4.08	1.46	1.38
12	B	808	CLA	O2A-CGA	4.08	1.45	1.33
12	B	810	CLA	CHC-C1C	4.07	1.46	1.38
12	B	813	CLA	O2A-CGA	4.07	1.45	1.33
12	A	807	CLA	CHD-C4C	4.07	1.48	1.39
12	A	841	CLA	CHD-C4C	4.06	1.48	1.39
12	B	807	CLA	CHD-C1D	4.06	1.46	1.38
12	B	828	CLA	CHD-C1D	4.06	1.46	1.38
12	B	806	CLA	CHD-C1D	4.05	1.46	1.38
12	B	811	CLA	O2A-CGA	4.05	1.45	1.33
11	A	801	CL0	CHD-C1D	4.04	1.46	1.39
12	B	822	CLA	CHD-C1D	4.04	1.46	1.38
12	A	812	CLA	CHD-C4C	4.04	1.48	1.39
12	A	815	CLA	CHD-C4C	4.04	1.48	1.39
12	A	837	CLA	CHD-C4C	4.04	1.48	1.39
12	A	819	CLA	CHD-C4C	4.04	1.48	1.39
12	B	803	CLA	CHD-C1D	4.04	1.46	1.38
12	A	816	CLA	CHD-C4C	4.03	1.48	1.39
12	L	204	CLA	CHD-C4C	4.03	1.48	1.39
12	B	830	CLA	CHD-C4C	4.03	1.48	1.39
12	B	810	CLA	O2A-CGA	4.03	1.45	1.33
12	B	804	CLA	C1D-ND	4.02	1.43	1.37
12	A	804	CLA	CHD-C1D	4.02	1.46	1.38
12	A	806	CLA	CHD-C1D	4.01	1.46	1.38
12	B	813	CLA	CHD-C4C	4.01	1.48	1.39
12	B	816	CLA	CHD-C4C	4.01	1.48	1.39
12	A	836	CLA	CHD-C4C	4.01	1.48	1.39
12	B	831	CLA	CHD-C4C	4.01	1.48	1.39
12	B	827	CLA	CHD-C4C	4.00	1.48	1.39
12	B	808	CLA	CHD-C1D	4.00	1.46	1.38
12	B	829	CLA	CHD-C4C	3.99	1.48	1.39
12	B	830	CLA	CHD-C1D	3.99	1.46	1.38
12	B	811	CLA	CHD-C4C	3.99	1.48	1.39
12	B	826	CLA	CHD-C4C	3.98	1.48	1.39
12	A	839	CLA	CHD-C1D	3.98	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	829	CLA	C1D-ND	3.98	1.43	1.37
12	A	825	CLA	C1D-ND	3.98	1.43	1.37
12	B	832	CLA	CHD-C4C	3.98	1.48	1.39
12	A	806	CLA	O2A-CGA	3.98	1.44	1.33
12	A	805	CLA	CHD-C4C	3.98	1.48	1.39
12	B	815	CLA	CHD-C4C	3.98	1.48	1.39
12	B	812	CLA	CHD-C4C	3.98	1.48	1.39
12	A	821	CLA	CHD-C4C	3.97	1.48	1.39
12	L	202	CLA	CHD-C4C	3.97	1.48	1.39
12	A	843	CLA	CHD-C4C	3.96	1.48	1.39
12	A	833	CLA	O2A-CGA	3.96	1.44	1.33
12	B	804	CLA	O2A-CGA	3.95	1.44	1.33
12	A	833	CLA	CHD-C4C	3.95	1.48	1.39
12	A	813	CLA	CHD-C4C	3.94	1.48	1.39
12	A	838	CLA	CHD-C4C	3.94	1.48	1.39
12	B	810	CLA	CHD-C4C	3.94	1.48	1.39
12	A	834	CLA	CHD-C4C	3.94	1.48	1.39
12	A	832	CLA	CHD-C4C	3.94	1.48	1.39
12	A	823	CLA	CHD-C4C	3.94	1.48	1.39
12	B	825	CLA	CHD-C4C	3.94	1.48	1.39
12	A	808	CLA	CHD-C4C	3.93	1.48	1.39
12	A	814	CLA	CHD-C4C	3.93	1.48	1.39
12	B	817	CLA	CHD-C4C	3.93	1.48	1.39
12	A	830	CLA	C1B-NB	-3.93	1.32	1.37
12	B	832	CLA	CHC-C1C	3.93	1.46	1.38
12	A	810	CLA	CHD-C4C	3.93	1.48	1.39
12	B	818	CLA	C1B-NB	-3.93	1.32	1.37
12	B	802	CLA	C3D-C2D	3.92	1.49	1.39
12	A	804	CLA	CHD-C4C	3.92	1.48	1.39
12	B	806	CLA	CHD-C4C	3.92	1.48	1.39
12	J	101	CLA	CHD-C4C	3.92	1.48	1.39
12	B	820	CLA	CHD-C1D	3.92	1.46	1.38
12	A	831	CLA	CHD-C4C	3.92	1.48	1.39
12	B	814	CLA	CHD-C4C	3.92	1.48	1.39
12	A	829	CLA	CHD-C1D	3.91	1.46	1.38
12	A	808	CLA	C3D-C2D	3.91	1.49	1.39
12	A	827	CLA	CHD-C1D	3.90	1.46	1.38
12	A	817	CLA	CHD-C4C	3.90	1.48	1.39
12	A	811	CLA	CHD-C4C	3.90	1.48	1.39
12	A	840	CLA	CHD-C4C	3.90	1.48	1.39
12	A	830	CLA	CHD-C4C	3.89	1.48	1.39
12	A	842	CLA	CHD-C4C	3.89	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	818	CLA	CHD-C4C	3.89	1.48	1.39
12	A	854	CLA	C1B-NB	-3.89	1.32	1.37
12	B	829	CLA	CHD-C1D	3.89	1.46	1.38
12	L	203	CLA	CHD-C1D	3.88	1.46	1.38
12	B	810	CLA	C3D-C2D	3.88	1.49	1.39
12	B	805	CLA	CHD-C4C	3.88	1.48	1.39
12	A	802	CLA	C3D-C2D	3.88	1.49	1.39
12	L	203	CLA	CHD-C4C	3.87	1.48	1.39
12	A	835	CLA	CHD-C4C	3.87	1.48	1.39
12	A	830	CLA	C3D-C2D	3.87	1.49	1.39
12	A	822	CLA	CHD-C4C	3.87	1.48	1.39
12	A	828	CLA	CHD-C4C	3.87	1.48	1.39
12	F	203	CLA	C3D-C2D	3.87	1.49	1.39
12	B	807	CLA	CHD-C4C	3.86	1.48	1.39
12	A	802	CLA	C1D-ND	3.86	1.42	1.37
12	A	803	CLA	CHD-C4C	3.86	1.48	1.39
12	A	807	CLA	C3D-C2D	3.85	1.49	1.39
12	B	820	CLA	CHC-C4B	3.84	1.48	1.39
12	A	818	CLA	CHD-C4C	3.83	1.47	1.39
12	B	801	CLA	CHD-C4C	3.83	1.47	1.39
12	B	832	CLA	C1B-NB	-3.83	1.32	1.37
12	A	802	CLA	CHD-C4C	3.83	1.47	1.39
12	B	801	CLA	C3D-C2D	3.83	1.49	1.39
12	A	804	CLA	CHC-C4B	3.83	1.48	1.39
12	A	841	CLA	C3D-C2D	3.83	1.49	1.39
12	B	828	CLA	CHD-C4C	3.82	1.47	1.39
12	B	819	CLA	C1B-NB	-3.82	1.32	1.37
12	B	804	CLA	C1B-NB	-3.82	1.32	1.37
12	B	801	CLA	C1B-NB	-3.81	1.32	1.37
12	B	825	CLA	CHC-C4B	3.81	1.48	1.39
12	A	834	CLA	C3D-C2D	3.81	1.49	1.39
12	A	822	CLA	C3D-C2D	3.80	1.49	1.39
12	B	808	CLA	CHD-C4C	3.80	1.47	1.39
12	A	815	CLA	C3D-C2D	3.80	1.49	1.39
12	A	819	CLA	C3D-C2D	3.80	1.49	1.39
12	A	835	CLA	C3D-C2D	3.79	1.49	1.39
12	A	804	CLA	C3D-C2D	3.78	1.49	1.39
12	A	806	CLA	CHD-C4C	3.78	1.47	1.39
12	A	838	CLA	C3D-C2D	3.78	1.49	1.39
12	B	802	CLA	CHD-C4C	3.78	1.47	1.39
12	A	814	CLA	C3D-C2D	3.78	1.49	1.39
12	A	836	CLA	C3D-C2D	3.78	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	820	CLA	CHD-C4C	3.78	1.47	1.39
12	B	817	CLA	CHC-C4B	3.78	1.47	1.39
12	B	827	CLA	OBD-CAD	3.78	1.29	1.22
12	A	843	CLA	C3D-C2D	3.78	1.49	1.39
12	A	828	CLA	C1B-NB	-3.78	1.32	1.37
12	A	809	CLA	CHD-C4C	3.78	1.47	1.39
12	B	832	CLA	C3D-C2D	3.77	1.49	1.39
12	A	824	CLA	C3D-C2D	3.77	1.49	1.39
12	B	815	CLA	C3D-C2D	3.77	1.49	1.39
12	A	819	CLA	C1B-NB	-3.77	1.32	1.37
12	B	805	CLA	C3D-C2D	3.77	1.49	1.39
12	B	804	CLA	C3D-C2D	3.77	1.49	1.39
12	B	827	CLA	C3D-C2D	3.77	1.49	1.39
12	A	829	CLA	C1B-NB	-3.76	1.32	1.37
12	B	817	CLA	C3D-C2D	3.76	1.49	1.39
12	B	821	CLA	CHD-C4C	3.76	1.47	1.39
12	B	813	CLA	C3D-C2D	3.76	1.49	1.39
12	B	821	CLA	CHD-C1D	3.75	1.45	1.38
12	B	808	CLA	C3D-C2D	3.75	1.49	1.39
12	A	839	CLA	CHD-C4C	3.75	1.47	1.39
12	A	821	CLA	CHC-C4B	3.75	1.47	1.39
12	A	814	CLA	OBD-CAD	3.75	1.28	1.22
12	L	203	CLA	C3D-C2D	3.74	1.49	1.39
12	B	821	CLA	C3D-C2D	3.74	1.49	1.39
12	B	822	CLA	CHD-C4C	3.74	1.47	1.39
12	A	810	CLA	C3D-C2D	3.74	1.49	1.39
12	A	811	CLA	C3D-C2D	3.74	1.49	1.39
12	A	821	CLA	C3D-C2D	3.74	1.49	1.39
12	A	827	CLA	CHC-C4B	3.73	1.47	1.39
12	J	101	CLA	C3D-C2D	3.73	1.49	1.39
12	A	831	CLA	C3D-C2D	3.73	1.49	1.39
12	A	818	CLA	C1B-NB	-3.73	1.33	1.37
12	A	816	CLA	OBD-CAD	3.73	1.28	1.22
12	F	203	CLA	OBD-CAD	3.73	1.28	1.22
12	B	818	CLA	C3D-C2D	3.73	1.49	1.39
12	A	818	CLA	CHC-C4B	3.73	1.47	1.39
12	B	807	CLA	C1B-NB	-3.73	1.33	1.37
12	B	816	CLA	C3D-C2D	3.72	1.49	1.39
12	A	812	CLA	C3D-C2D	3.72	1.49	1.39
12	A	816	CLA	C3D-C2D	3.72	1.49	1.39
12	A	813	CLA	C3D-C2D	3.72	1.49	1.39
12	A	843	CLA	OBD-CAD	3.72	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	812	CLA	C3D-C2D	3.72	1.49	1.39
12	A	832	CLA	C3D-C2D	3.72	1.49	1.39
12	L	202	CLA	C3D-C2D	3.72	1.49	1.39
12	A	836	CLA	OBD-CAD	3.71	1.28	1.22
12	A	810	CLA	OBD-CAD	3.71	1.28	1.22
12	A	820	CLA	C3D-C2D	3.71	1.49	1.39
12	A	807	CLA	OBD-CAD	3.70	1.28	1.22
12	A	823	CLA	C3D-C2D	3.70	1.49	1.39
12	B	809	CLA	CHD-C1D	3.70	1.45	1.38
12	A	808	CLA	C1B-NB	-3.70	1.33	1.37
12	B	826	CLA	C3D-C2D	3.69	1.49	1.39
12	B	828	CLA	CHC-C4B	3.69	1.47	1.39
12	A	814	CLA	CHC-C4B	3.69	1.47	1.39
12	A	804	CLA	OBD-CAD	3.69	1.28	1.22
12	A	827	CLA	CHD-C4C	3.69	1.47	1.39
12	A	829	CLA	CHD-C4C	3.69	1.47	1.39
12	A	854	CLA	CHD-C1D	3.69	1.45	1.38
12	A	834	CLA	OBD-CAD	3.68	1.28	1.22
12	L	204	CLA	C3D-C2D	3.68	1.49	1.39
12	A	832	CLA	CHC-C4B	3.68	1.47	1.39
12	A	854	CLA	C1D-ND	3.68	1.42	1.37
12	B	826	CLA	OBD-CAD	3.68	1.28	1.22
12	A	836	CLA	CHC-C4B	3.68	1.47	1.39
12	B	824	CLA	OBD-CAD	3.68	1.28	1.22
12	A	809	CLA	OBD-CAD	3.68	1.28	1.22
12	A	825	CLA	CHD-C1D	3.68	1.45	1.38
12	B	815	CLA	OBD-CAD	3.68	1.28	1.22
12	A	809	CLA	CHC-C4B	3.67	1.47	1.39
12	A	829	CLA	CHC-C4B	3.67	1.47	1.39
12	B	824	CLA	C3D-C2D	3.67	1.49	1.39
12	J	101	CLA	OBD-CAD	3.67	1.28	1.22
12	A	815	CLA	OBD-CAD	3.67	1.28	1.22
12	A	841	CLA	CHC-C4B	3.67	1.47	1.39
12	B	805	CLA	OBD-CAD	3.67	1.28	1.22
12	A	839	CLA	CHC-C4B	3.67	1.47	1.39
12	A	802	CLA	OBD-CAD	3.66	1.28	1.22
12	A	841	CLA	OBD-CAD	3.66	1.28	1.22
12	A	833	CLA	OBD-CAD	3.66	1.28	1.22
12	B	821	CLA	OBD-CAD	3.66	1.28	1.22
12	A	828	CLA	C3D-C2D	3.66	1.49	1.39
12	B	822	CLA	C1B-NB	-3.65	1.33	1.37
12	A	813	CLA	OBD-CAD	3.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	829	CLA	C3D-C2D	3.65	1.48	1.39
12	A	842	CLA	C3D-C2D	3.65	1.48	1.39
12	A	825	CLA	CHD-C4C	3.65	1.47	1.39
12	B	816	CLA	OBD-CAD	3.65	1.28	1.22
12	B	806	CLA	C3D-C2D	3.65	1.48	1.39
12	B	804	CLA	OBD-CAD	3.65	1.28	1.22
12	B	819	CLA	CHC-C4B	3.64	1.47	1.39
12	A	808	CLA	CHC-C4B	3.64	1.47	1.39
12	B	828	CLA	C3D-C2D	3.64	1.48	1.39
12	A	842	CLA	OBD-CAD	3.64	1.28	1.22
12	A	829	CLA	OBD-CAD	3.63	1.28	1.22
12	A	837	CLA	CHB-C1B	3.63	1.47	1.39
12	A	840	CLA	CHC-C4B	3.63	1.47	1.39
12	A	823	CLA	OBD-CAD	3.63	1.28	1.22
12	A	826	CLA	CHC-C4B	3.63	1.47	1.39
12	A	825	CLA	C3D-C2D	3.63	1.48	1.39
12	A	822	CLA	CHC-C4B	3.62	1.47	1.39
12	J	101	CLA	CHC-C4B	3.62	1.47	1.39
12	B	829	CLA	C1B-NB	-3.62	1.33	1.37
12	B	822	CLA	OBD-CAD	3.62	1.28	1.22
12	A	818	CLA	C3D-C2D	3.62	1.48	1.39
12	A	812	CLA	CHC-C4B	3.62	1.47	1.39
12	L	204	CLA	CHC-C4B	3.62	1.47	1.39
12	B	818	CLA	OBD-CAD	3.62	1.28	1.22
12	A	840	CLA	C1B-NB	-3.62	1.33	1.37
12	B	821	CLA	C1B-NB	-3.62	1.33	1.37
12	B	814	CLA	OBD-CAD	3.62	1.28	1.22
12	A	817	CLA	C3D-C2D	3.62	1.48	1.39
12	B	813	CLA	CHC-C4B	3.61	1.47	1.39
12	B	822	CLA	C3D-C2D	3.61	1.48	1.39
12	B	806	CLA	OBD-CAD	3.61	1.28	1.22
12	B	823	CLA	OBD-CAD	3.61	1.28	1.22
12	B	830	CLA	C3D-C2D	3.61	1.48	1.39
12	A	840	CLA	OBD-CAD	3.61	1.28	1.22
12	A	835	CLA	OBD-CAD	3.61	1.28	1.22
12	A	803	CLA	CHC-C4B	3.61	1.47	1.39
12	B	812	CLA	OBD-CAD	3.61	1.28	1.22
12	B	817	CLA	C1B-NB	-3.61	1.33	1.37
12	L	202	CLA	OBD-CAD	3.61	1.28	1.22
12	B	803	CLA	CHD-C4C	3.61	1.47	1.39
12	B	808	CLA	CHC-C4B	3.61	1.47	1.39
12	B	809	CLA	CHD-C4C	3.61	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	803	CLA	C3D-C2D	3.60	1.48	1.39
12	A	802	CLA	CHC-C4B	3.60	1.47	1.39
12	B	807	CLA	C3D-C2D	3.60	1.48	1.39
12	A	820	CLA	C1B-NB	-3.60	1.33	1.37
12	B	802	CLA	C1B-NB	-3.60	1.33	1.37
12	A	806	CLA	CHC-C4B	3.60	1.47	1.39
12	A	802	CLA	CHD-C1D	3.60	1.45	1.38
12	L	203	CLA	OBD-CAD	3.59	1.28	1.22
12	A	818	CLA	OBD-CAD	3.59	1.28	1.22
12	B	819	CLA	OBD-CAD	3.59	1.28	1.22
12	B	802	CLA	CHC-C4B	3.59	1.47	1.39
12	B	820	CLA	C1B-NB	-3.59	1.33	1.37
12	B	804	CLA	CHC-C4B	3.59	1.47	1.39
12	B	803	CLA	CHB-C1B	3.59	1.47	1.39
12	B	831	CLA	C3D-C2D	3.58	1.48	1.39
12	B	832	CLA	OBD-CAD	3.58	1.28	1.22
12	A	826	CLA	C1B-NB	-3.58	1.33	1.37
12	A	833	CLA	C3D-C2D	3.58	1.48	1.39
12	A	822	CLA	C1B-NB	-3.58	1.33	1.37
12	A	819	CLA	OBD-CAD	3.58	1.28	1.22
12	L	204	CLA	OBD-CAD	3.58	1.28	1.22
12	B	809	CLA	C1B-NB	-3.58	1.33	1.37
12	A	825	CLA	OBD-CAD	3.57	1.28	1.22
12	A	838	CLA	C1B-NB	-3.57	1.33	1.37
12	A	827	CLA	C3D-C2D	3.57	1.48	1.39
12	A	822	CLA	OBD-CAD	3.57	1.28	1.22
12	A	820	CLA	OBD-CAD	3.57	1.28	1.22
12	A	803	CLA	C3D-C2D	3.57	1.48	1.39
12	A	809	CLA	CHB-C1B	3.57	1.47	1.39
12	B	829	CLA	C3D-C2D	3.57	1.48	1.39
12	A	812	CLA	OBD-CAD	3.57	1.28	1.22
12	A	831	CLA	CHC-C4B	3.56	1.47	1.39
12	B	812	CLA	CHC-C4B	3.56	1.47	1.39
12	B	831	CLA	OBD-CAD	3.56	1.28	1.22
12	B	803	CLA	OBD-CAD	3.56	1.28	1.22
12	B	824	CLA	CHC-C4B	3.56	1.47	1.39
12	A	824	CLA	OBD-CAD	3.56	1.28	1.22
12	L	202	CLA	CHC-C4B	3.56	1.47	1.39
12	A	837	CLA	C4B-NB	-3.56	1.33	1.37
12	A	803	CLA	C1B-NB	-3.56	1.33	1.37
12	A	854	CLA	CHD-C4C	3.56	1.47	1.39
12	B	828	CLA	C1B-NB	-3.56	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	819	CLA	C3D-C2D	3.56	1.48	1.39
12	A	813	CLA	CHC-C4B	3.56	1.47	1.39
12	B	827	CLA	CHC-C4B	3.55	1.47	1.39
12	A	815	CLA	CHC-C4B	3.55	1.47	1.39
12	F	203	CLA	CHC-C4B	3.55	1.47	1.39
12	A	832	CLA	OBD-CAD	3.55	1.28	1.22
12	B	814	CLA	C3D-C2D	3.55	1.48	1.39
12	A	838	CLA	CHC-C4B	3.54	1.47	1.39
12	A	828	CLA	OBD-CAD	3.54	1.28	1.22
12	B	814	CLA	CHC-C4B	3.54	1.47	1.39
12	B	831	CLA	C1B-NB	-3.54	1.33	1.37
12	B	804	CLA	CHD-C4C	3.53	1.47	1.39
12	B	808	CLA	CHB-C1B	3.53	1.47	1.39
12	B	825	CLA	OBD-CAD	3.53	1.28	1.22
12	A	804	CLA	C1B-NB	-3.53	1.33	1.37
12	A	807	CLA	C1B-NB	-3.53	1.33	1.37
12	B	813	CLA	OBD-CAD	3.53	1.28	1.22
12	B	831	CLA	CHC-C4B	3.53	1.47	1.39
12	A	812	CLA	C1B-NB	-3.52	1.33	1.37
12	A	833	CLA	CHC-C4B	3.52	1.47	1.39
12	B	807	CLA	CHC-C4B	3.52	1.47	1.39
12	B	811	CLA	CHC-C4B	3.52	1.47	1.39
12	A	828	CLA	CHC-C4B	3.52	1.47	1.39
12	B	826	CLA	CHC-C4B	3.52	1.47	1.39
12	A	805	CLA	C3D-C2D	3.52	1.48	1.39
12	B	822	CLA	CHC-C4B	3.52	1.47	1.39
12	A	825	CLA	C1B-NB	-3.52	1.33	1.37
12	A	809	CLA	C3D-C2D	3.52	1.48	1.39
12	A	805	CLA	OBD-CAD	3.51	1.28	1.22
12	B	830	CLA	CHC-C4B	3.51	1.47	1.39
12	A	839	CLA	C3D-C2D	3.50	1.48	1.39
12	B	820	CLA	C3D-C2D	3.50	1.48	1.39
12	B	810	CLA	OBD-CAD	3.49	1.28	1.22
12	A	817	CLA	CHC-C4B	3.49	1.47	1.39
12	A	826	CLA	C3D-C2D	3.49	1.48	1.39
12	A	825	CLA	CHC-C4B	3.49	1.47	1.39
12	A	839	CLA	C1B-NB	-3.49	1.33	1.37
12	A	842	CLA	CHC-C4B	3.49	1.47	1.39
12	A	824	CLA	CHC-C4B	3.48	1.47	1.39
12	B	829	CLA	CHC-C4B	3.48	1.47	1.39
12	A	810	CLA	CHC-C4B	3.48	1.47	1.39
12	B	824	CLA	C1B-NB	-3.48	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	821	CLA	CHC-C4B	3.48	1.47	1.39
12	B	818	CLA	CHC-C4B	3.48	1.47	1.39
12	A	843	CLA	CHC-C4B	3.47	1.47	1.39
12	A	827	CLA	C1B-NB	-3.47	1.33	1.37
12	B	825	CLA	C1B-NB	-3.47	1.33	1.37
12	A	837	CLA	C3D-C2D	3.47	1.48	1.39
12	B	830	CLA	C1B-NB	-3.46	1.33	1.37
12	A	805	CLA	C1B-NB	-3.46	1.33	1.37
12	L	202	CLA	C1B-NB	-3.46	1.33	1.37
12	A	843	CLA	C1B-NB	-3.46	1.33	1.37
12	A	814	CLA	C1B-NB	-3.46	1.33	1.37
12	A	806	CLA	C3D-C2D	3.46	1.48	1.39
12	A	811	CLA	C1B-NB	-3.46	1.33	1.37
12	A	811	CLA	OBD-CAD	3.46	1.28	1.22
12	A	811	CLA	CHC-C4B	3.45	1.47	1.39
12	B	802	CLA	OBD-CAD	3.45	1.28	1.22
12	A	822	CLA	CHB-C1B	3.45	1.47	1.39
12	A	816	CLA	C1B-NB	-3.45	1.33	1.37
12	B	825	CLA	CHD-C1D	3.45	1.45	1.38
12	A	817	CLA	OBD-CAD	3.45	1.28	1.22
12	B	825	CLA	C3D-C2D	3.45	1.48	1.39
12	A	813	CLA	C1B-NB	-3.45	1.33	1.37
12	B	811	CLA	CHB-C1B	3.45	1.47	1.39
12	B	801	CLA	C4B-NB	-3.45	1.33	1.37
12	B	815	CLA	C1B-NB	-3.44	1.33	1.37
12	B	809	CLA	CHC-C4B	3.44	1.47	1.39
12	A	816	CLA	CHC-C4B	3.44	1.47	1.39
12	A	826	CLA	OBD-CAD	3.44	1.28	1.22
12	A	832	CLA	C1B-NB	-3.44	1.33	1.37
12	A	854	CLA	CHC-C4B	3.44	1.47	1.39
12	A	806	CLA	C1B-NB	-3.43	1.33	1.37
12	A	803	CLA	OBD-CAD	3.43	1.28	1.22
12	A	823	CLA	C1B-NB	-3.42	1.33	1.37
15	M	101	BCR	C30-C25	-3.42	1.49	1.53
12	A	836	CLA	C1B-NB	-3.42	1.33	1.37
12	A	807	CLA	CHC-C4B	3.42	1.47	1.39
12	B	805	CLA	CHC-C4B	3.42	1.47	1.39
12	B	811	CLA	C1B-NB	-3.42	1.33	1.37
12	A	837	CLA	CHC-C4B	3.42	1.47	1.39
12	A	831	CLA	OBD-CAD	3.41	1.28	1.22
12	B	808	CLA	C1B-NB	-3.41	1.33	1.37
12	A	831	CLA	C1B-NB	-3.41	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	823	CLA	CHC-C4B	3.41	1.47	1.39
12	B	832	CLA	CHB-C1B	3.41	1.47	1.39
12	A	820	CLA	CHB-C1B	3.41	1.47	1.39
12	A	842	CLA	C1B-NB	-3.40	1.33	1.37
12	A	809	CLA	C1B-NB	-3.40	1.33	1.37
15	B	836	BCR	C30-C25	-3.40	1.49	1.53
12	A	825	CLA	CHB-C1B	3.39	1.47	1.39
12	B	827	CLA	CHB-C1B	3.39	1.47	1.39
12	B	816	CLA	C1B-NB	-3.39	1.33	1.37
12	F	203	CLA	CHB-C1B	3.39	1.47	1.39
12	B	810	CLA	CHB-C1B	3.39	1.47	1.39
12	J	101	CLA	C1B-NB	-3.39	1.33	1.37
15	A	846	BCR	C1-C6	-3.39	1.49	1.53
12	B	811	CLA	OBD-CAD	3.38	1.28	1.22
12	A	835	CLA	CHC-C4B	3.38	1.47	1.39
12	A	816	CLA	CHB-C1B	3.38	1.47	1.39
12	B	806	CLA	C4B-NB	-3.38	1.33	1.37
12	A	806	CLA	CHB-C1B	3.38	1.47	1.39
12	A	834	CLA	CHC-C4B	3.37	1.47	1.39
12	A	820	CLA	CHC-C4B	3.37	1.47	1.39
12	B	812	CLA	CHB-C1B	3.37	1.47	1.39
12	A	843	CLA	CHB-C1B	3.36	1.47	1.39
12	A	854	CLA	CHB-C1B	3.36	1.47	1.39
12	B	809	CLA	OBD-CAD	3.36	1.28	1.22
12	L	203	CLA	C1B-NB	-3.36	1.33	1.37
12	B	814	CLA	C1B-NB	-3.36	1.33	1.37
12	A	810	CLA	C1B-NB	-3.36	1.33	1.37
12	B	809	CLA	C3D-C2D	3.35	1.48	1.39
12	B	815	CLA	CHC-C4B	3.35	1.46	1.39
12	L	203	CLA	CHC-C4B	3.35	1.46	1.39
12	A	834	CLA	C1B-NB	-3.35	1.33	1.37
12	A	836	CLA	CHB-C1B	3.34	1.46	1.39
12	B	806	CLA	CHB-C1B	3.34	1.46	1.39
12	A	834	CLA	C4B-NB	-3.34	1.33	1.37
12	L	204	CLA	C1B-NB	-3.34	1.33	1.37
12	B	813	CLA	C1B-NB	-3.34	1.33	1.37
12	B	817	CLA	OBD-CAD	3.33	1.28	1.22
12	B	811	CLA	C3D-C2D	3.33	1.48	1.39
12	B	804	CLA	CHD-C1D	3.33	1.44	1.38
12	A	838	CLA	OBD-CAD	3.33	1.28	1.22
12	A	821	CLA	OBD-CAD	3.33	1.28	1.22
12	A	805	CLA	CHC-C4B	3.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	821	CLA	C1B-NB	-3.33	1.33	1.37
12	L	203	CLA	CHB-C1B	3.32	1.46	1.39
12	A	817	CLA	C1B-NB	-3.32	1.33	1.37
12	A	803	CLA	CHB-C1B	3.32	1.46	1.39
12	A	841	CLA	CHB-C1B	3.32	1.46	1.39
12	A	830	CLA	OBD-CAD	3.32	1.28	1.22
12	A	842	CLA	CHB-C1B	3.32	1.46	1.39
12	B	812	CLA	C1B-NB	-3.31	1.33	1.37
12	B	828	CLA	OBD-CAD	3.31	1.28	1.22
12	B	820	CLA	CHB-C1B	3.31	1.46	1.39
15	L	205	BCR	C30-C25	-3.31	1.49	1.53
12	A	810	CLA	CHB-C1B	3.31	1.46	1.39
15	B	834	BCR	C30-C25	-3.30	1.49	1.53
12	B	821	CLA	C4B-NB	-3.30	1.33	1.37
12	B	816	CLA	CHC-C4B	3.30	1.46	1.39
12	A	827	CLA	CHB-C1B	3.30	1.46	1.39
12	A	835	CLA	C1B-NB	-3.30	1.33	1.37
12	A	812	CLA	CHB-C1B	3.30	1.46	1.39
12	B	816	CLA	CHB-C1B	3.29	1.46	1.39
12	B	826	CLA	CHB-C1B	3.29	1.46	1.39
12	B	805	CLA	C1B-NB	-3.29	1.33	1.37
12	B	806	CLA	C1B-NB	-3.28	1.33	1.37
12	A	824	CLA	C1B-NB	-3.28	1.33	1.37
12	B	805	CLA	C4B-NB	-3.28	1.33	1.37
12	L	204	CLA	CHB-C1B	3.28	1.46	1.39
12	B	830	CLA	CHB-C1B	3.28	1.46	1.39
12	A	825	CLA	C4B-NB	-3.28	1.33	1.37
12	B	816	CLA	C4B-NB	-3.28	1.33	1.37
12	A	808	CLA	OBD-CAD	3.28	1.28	1.22
12	A	815	CLA	CHB-C1B	3.28	1.46	1.39
12	A	831	CLA	CHB-C1B	3.28	1.46	1.39
12	A	837	CLA	OBD-CAD	3.27	1.28	1.22
12	A	837	CLA	C1B-NB	-3.27	1.33	1.37
12	A	832	CLA	CHB-C1B	3.27	1.46	1.39
12	A	839	CLA	CHB-C1B	3.26	1.46	1.39
12	B	828	CLA	CHB-C1B	3.26	1.46	1.39
12	A	806	CLA	OBD-CAD	3.26	1.28	1.22
12	B	804	CLA	C4B-NB	-3.26	1.33	1.37
12	A	833	CLA	C1B-NB	-3.25	1.33	1.37
12	A	815	CLA	C1B-NB	-3.25	1.33	1.37
12	J	101	CLA	CHB-C1B	3.25	1.46	1.39
12	A	823	CLA	CHB-C1B	3.25	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	833	CLA	CHB-C1B	3.24	1.46	1.39
12	B	807	CLA	CHB-C1B	3.24	1.46	1.39
12	A	830	CLA	CHC-C4B	3.24	1.46	1.39
12	A	802	CLA	C4B-NB	-3.24	1.33	1.37
12	B	823	CLA	CHB-C1B	3.24	1.46	1.39
15	I	101	BCR	C1-C6	-3.24	1.49	1.53
12	B	802	CLA	CHB-C1B	3.24	1.46	1.39
12	B	810	CLA	C4B-NB	-3.23	1.33	1.37
12	B	805	CLA	CHB-C1B	3.23	1.46	1.39
12	A	806	CLA	C4B-NB	-3.23	1.33	1.37
12	A	826	CLA	C4B-NB	-3.23	1.33	1.37
12	B	814	CLA	CHB-C1B	3.23	1.46	1.39
12	B	823	CLA	C4B-NB	-3.23	1.33	1.37
12	B	803	CLA	CHC-C4B	3.22	1.46	1.39
12	B	823	CLA	CHC-C4B	3.22	1.46	1.39
12	B	801	CLA	OBD-CAD	3.22	1.28	1.22
12	B	819	CLA	C4B-NB	-3.22	1.33	1.37
12	B	825	CLA	CHB-C1B	3.21	1.46	1.39
12	A	819	CLA	CHC-C4B	3.21	1.46	1.39
12	A	813	CLA	CHB-C1B	3.21	1.46	1.39
12	B	813	CLA	CHB-C1B	3.21	1.46	1.39
12	B	824	CLA	CHB-C1B	3.21	1.46	1.39
12	B	807	CLA	OBD-CAD	3.21	1.28	1.22
12	B	826	CLA	C1B-NB	-3.21	1.33	1.37
12	B	803	CLA	C1B-NB	-3.20	1.33	1.37
12	A	830	CLA	CHB-C1B	3.20	1.46	1.39
12	A	811	CLA	CHB-C1B	3.19	1.46	1.39
12	A	824	CLA	CHB-C1B	3.19	1.46	1.39
12	A	835	CLA	CHB-C1B	3.19	1.46	1.39
12	A	841	CLA	C1B-NB	-3.19	1.33	1.37
12	A	854	CLA	C4B-NB	-3.19	1.33	1.37
15	J	102	BCR	C1-C6	-3.19	1.49	1.53
12	B	808	CLA	OBD-CAD	3.19	1.28	1.22
12	A	814	CLA	CHB-C1B	3.18	1.46	1.39
12	B	818	CLA	CHB-C1B	3.18	1.46	1.39
12	B	809	CLA	CHB-C1B	3.18	1.46	1.39
15	A	847	BCR	C1-C6	-3.18	1.49	1.53
12	A	817	CLA	CHB-C1B	3.17	1.46	1.39
12	B	831	CLA	CHB-C1B	3.17	1.46	1.39
15	A	850	BCR	C1-C6	-3.17	1.49	1.53
12	B	827	CLA	C1B-NB	-3.17	1.33	1.37
12	A	819	CLA	CHB-C1B	3.16	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	815	CLA	CHB-C1B	3.16	1.46	1.39
12	L	203	CLA	C4B-NB	-3.16	1.33	1.37
12	F	203	CLA	C1B-NB	-3.15	1.33	1.37
12	B	831	CLA	C4B-NB	-3.14	1.33	1.37
12	A	807	CLA	CHB-C1B	3.13	1.46	1.39
12	A	805	CLA	C4B-NB	-3.13	1.33	1.37
12	A	817	CLA	C4B-NB	-3.13	1.33	1.37
12	A	813	CLA	C4B-NB	-3.13	1.33	1.37
12	A	828	CLA	CHB-C1B	3.12	1.46	1.39
12	A	839	CLA	OBD-CAD	3.12	1.27	1.22
12	A	833	CLA	C4B-NB	-3.12	1.33	1.37
15	B	836	BCR	C1-C6	-3.12	1.49	1.53
12	L	202	CLA	CHB-C1B	3.12	1.46	1.39
12	A	829	CLA	CHB-C1B	3.11	1.46	1.39
12	B	822	CLA	CHB-C1B	3.11	1.46	1.39
15	F	201	BCR	C1-C6	-3.11	1.49	1.53
15	L	205	BCR	C1-C6	-3.11	1.49	1.53
12	B	806	CLA	CHC-C4B	3.10	1.46	1.39
12	A	805	CLA	CHB-C1B	3.10	1.46	1.39
12	A	821	CLA	CHB-C1B	3.10	1.46	1.39
12	B	821	CLA	CHB-C1B	3.10	1.46	1.39
12	A	838	CLA	C4B-NB	-3.09	1.33	1.37
12	A	838	CLA	CHB-C1B	3.09	1.46	1.39
12	A	819	CLA	C4B-NB	-3.09	1.33	1.37
12	B	801	CLA	CHC-C4B	3.08	1.46	1.39
12	A	811	CLA	C4B-NB	-3.08	1.33	1.37
12	A	808	CLA	CHB-C1B	3.08	1.46	1.39
12	A	807	CLA	C4B-NB	-3.08	1.33	1.37
15	L	201	BCR	C1-C6	-3.08	1.49	1.53
12	B	822	CLA	C4B-NB	-3.08	1.33	1.37
15	B	834	BCR	C1-C6	-3.07	1.49	1.53
15	J	103	BCR	C30-C25	-3.06	1.49	1.53
15	J	104	BCR	C30-C25	-3.06	1.49	1.53
12	A	827	CLA	OBD-CAD	3.06	1.27	1.22
12	B	817	CLA	CHB-C1B	3.06	1.46	1.39
12	A	828	CLA	C4B-NB	-3.06	1.33	1.37
12	B	824	CLA	C4B-NB	-3.06	1.33	1.37
12	B	803	CLA	C1B-C2B	3.06	1.50	1.43
12	B	829	CLA	CHB-C1B	3.06	1.46	1.39
12	B	813	CLA	C4B-NB	-3.05	1.33	1.37
12	A	840	CLA	CHB-C1B	3.05	1.46	1.39
12	B	829	CLA	C4B-NB	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	803	CLA	C4B-NB	-3.05	1.33	1.37
15	A	849	BCR	C1-C6	-3.05	1.49	1.53
12	A	830	CLA	C4B-NB	-3.04	1.33	1.37
12	A	818	CLA	CHB-C1B	3.04	1.46	1.39
12	B	807	CLA	C4B-NB	-3.03	1.33	1.37
12	A	815	CLA	C4B-NB	-3.03	1.33	1.37
12	A	804	CLA	CHB-C1B	3.03	1.46	1.39
12	A	842	CLA	C4B-NB	-3.03	1.33	1.37
12	B	801	CLA	CHB-C1B	3.03	1.46	1.39
12	A	831	CLA	C4B-NB	-3.02	1.33	1.37
12	A	820	CLA	C4B-NB	-3.02	1.33	1.37
12	B	811	CLA	C4B-NB	-3.02	1.33	1.37
12	B	814	CLA	C4B-NB	-3.02	1.33	1.37
15	B	835	BCR	C30-C25	-3.01	1.49	1.53
12	B	832	CLA	CHC-C4B	3.01	1.46	1.39
12	B	815	CLA	C4B-NB	-3.00	1.33	1.37
12	A	834	CLA	CHB-C1B	3.00	1.46	1.39
15	M	101	BCR	C1-C6	-2.99	1.50	1.53
12	B	820	CLA	OBD-CAD	2.98	1.27	1.22
12	A	821	CLA	C4B-NB	-2.96	1.34	1.37
12	L	204	CLA	C4B-NB	-2.96	1.34	1.37
12	A	824	CLA	C4B-NB	-2.95	1.34	1.37
12	B	826	CLA	C4B-NB	-2.95	1.34	1.37
12	A	812	CLA	C4B-NB	-2.95	1.34	1.37
12	A	814	CLA	C4B-NB	-2.95	1.34	1.37
12	B	829	CLA	OBD-CAD	2.95	1.27	1.22
12	A	835	CLA	C4B-NB	-2.94	1.34	1.37
12	B	832	CLA	C4B-NB	-2.94	1.34	1.37
12	A	827	CLA	C4B-NB	-2.94	1.34	1.37
12	B	817	CLA	C4B-NB	-2.94	1.34	1.37
12	B	810	CLA	CHC-C4B	2.93	1.46	1.39
12	B	823	CLA	C3D-C4D	-2.92	1.37	1.44
12	A	841	CLA	C4B-NB	-2.92	1.34	1.37
12	B	806	CLA	C4C-C3C	2.92	1.50	1.45
12	F	203	CLA	C4B-NB	-2.91	1.34	1.37
12	B	830	CLA	C4B-NB	-2.91	1.34	1.37
12	A	810	CLA	C4B-NB	-2.90	1.34	1.37
12	A	839	CLA	C4B-NB	-2.90	1.34	1.37
12	A	826	CLA	CHB-C1B	2.89	1.45	1.39
12	A	809	CLA	C4B-NB	-2.89	1.34	1.37
15	F	202	BCR	C1-C6	-2.87	1.50	1.53
12	A	808	CLA	C4B-NB	-2.87	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	828	CLA	C4B-NB	-2.87	1.34	1.37
12	B	823	CLA	C3D-C2D	2.87	1.46	1.39
12	J	101	CLA	C4B-NB	-2.86	1.34	1.37
12	B	812	CLA	C4B-NB	-2.85	1.34	1.37
12	B	820	CLA	C4B-NB	-2.85	1.34	1.37
12	A	820	CLA	C4D-CHA	2.84	1.48	1.38
12	A	840	CLA	C4D-CHA	2.84	1.48	1.38
12	A	822	CLA	C4B-NB	-2.83	1.34	1.37
12	A	829	CLA	C4B-NB	-2.83	1.34	1.37
12	A	843	CLA	C4D-CHA	2.82	1.48	1.38
12	B	825	CLA	C3B-C4B	2.82	1.50	1.42
12	A	818	CLA	C3B-C4B	2.82	1.50	1.42
12	B	805	CLA	C4D-CHA	2.82	1.48	1.38
12	A	803	CLA	C4B-NB	-2.82	1.34	1.37
12	A	808	CLA	C4D-CHA	2.82	1.48	1.38
12	B	806	CLA	C1B-C2B	2.82	1.49	1.43
12	L	202	CLA	C4B-NB	-2.82	1.34	1.37
12	A	840	CLA	C4B-NB	-2.82	1.34	1.37
12	A	819	CLA	C4D-CHA	2.81	1.48	1.38
12	B	819	CLA	CHB-C1B	2.81	1.45	1.39
12	B	820	CLA	C4D-CHA	2.81	1.48	1.38
12	A	818	CLA	C4B-NB	-2.80	1.34	1.37
12	B	809	CLA	C4B-NB	-2.80	1.34	1.37
12	B	832	CLA	C4D-CHA	2.80	1.48	1.38
12	B	810	CLA	C4D-CHA	2.79	1.48	1.38
12	A	836	CLA	C4D-CHA	2.79	1.48	1.38
12	A	810	CLA	C4D-CHA	2.79	1.48	1.38
12	A	816	CLA	C4D-CHA	2.78	1.47	1.38
12	A	823	CLA	C4B-NB	-2.78	1.34	1.37
12	L	202	CLA	C4D-CHA	2.78	1.47	1.38
12	J	101	CLA	C4D-CHA	2.78	1.47	1.38
12	A	814	CLA	C4D-CHA	2.77	1.47	1.38
12	A	836	CLA	C3B-C4B	2.77	1.50	1.42
12	B	802	CLA	C4B-NB	-2.77	1.34	1.37
12	A	823	CLA	C4D-CHA	2.77	1.47	1.38
15	B	835	BCR	C1-C6	-2.77	1.50	1.53
12	B	815	CLA	C4D-CHA	2.76	1.47	1.38
12	A	827	CLA	C4D-CHA	2.76	1.47	1.38
12	A	832	CLA	C4B-NB	-2.76	1.34	1.37
12	A	830	CLA	C4D-CHA	2.75	1.47	1.38
12	A	828	CLA	C4D-CHA	2.75	1.47	1.38
12	A	802	CLA	CHB-C1B	2.75	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	L	206	BCR	C1-C6	-2.75	1.50	1.53
12	B	827	CLA	C4D-CHA	2.74	1.47	1.38
12	A	813	CLA	C4D-CHA	2.74	1.47	1.38
12	A	804	CLA	C4B-NB	-2.74	1.34	1.37
12	B	808	CLA	C4D-CHA	2.74	1.47	1.38
12	A	804	CLA	C4D-CHA	2.74	1.47	1.38
12	B	817	CLA	C4D-CHA	2.74	1.47	1.38
12	F	203	CLA	C4D-CHA	2.73	1.47	1.38
12	B	818	CLA	C4D-CHA	2.73	1.47	1.38
12	A	807	CLA	C4D-CHA	2.73	1.47	1.38
12	A	824	CLA	C4D-CHA	2.73	1.47	1.38
12	A	815	CLA	C4D-CHA	2.73	1.47	1.38
12	B	806	CLA	C4D-CHA	2.73	1.47	1.38
12	A	834	CLA	C4D-CHA	2.73	1.47	1.38
12	B	802	CLA	C4D-CHA	2.72	1.47	1.38
12	A	816	CLA	C4B-NB	-2.72	1.34	1.37
12	A	812	CLA	C4D-CHA	2.72	1.47	1.38
15	A	850	BCR	C30-C25	-2.72	1.50	1.53
12	B	804	CLA	C4D-CHA	2.72	1.47	1.38
12	A	831	CLA	C4D-CHA	2.71	1.47	1.38
12	B	816	CLA	C4D-CHA	2.71	1.47	1.38
12	A	841	CLA	C4D-CHA	2.71	1.47	1.38
12	A	843	CLA	C4B-NB	-2.70	1.34	1.37
12	B	807	CLA	C4D-CHA	2.70	1.47	1.38
12	A	818	CLA	C4D-CHA	2.70	1.47	1.38
12	A	842	CLA	C4D-CHA	2.70	1.47	1.38
12	A	837	CLA	C1B-C2B	2.70	1.49	1.43
15	J	103	BCR	C1-C6	-2.70	1.50	1.53
12	B	804	CLA	CHB-C1B	2.70	1.45	1.39
12	B	823	CLA	C4C-C3C	2.70	1.49	1.45
12	B	813	CLA	C4D-CHA	2.69	1.47	1.38
12	B	827	CLA	C4B-NB	-2.69	1.34	1.37
12	B	829	CLA	C4D-CHA	2.69	1.47	1.38
12	A	822	CLA	C4D-CHA	2.68	1.47	1.38
12	B	826	CLA	C4D-CHA	2.68	1.47	1.38
12	B	816	CLA	C1B-C2B	2.68	1.49	1.43
12	A	838	CLA	C4D-CHA	2.68	1.47	1.38
12	B	828	CLA	C4D-CHA	2.68	1.47	1.38
12	B	812	CLA	C4D-CHA	2.68	1.47	1.38
12	A	835	CLA	C4D-CHA	2.67	1.47	1.38
12	A	854	CLA	OBD-CAD	2.67	1.27	1.22
12	A	806	CLA	C4D-CHA	2.67	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	J	104	BCR	C1-C6	-2.67	1.50	1.53
12	A	837	CLA	C3D-C4D	-2.67	1.38	1.44
12	B	808	CLA	C4B-NB	-2.67	1.34	1.37
12	A	803	CLA	C4D-CHA	2.66	1.47	1.38
12	B	830	CLA	C4D-CHA	2.66	1.47	1.38
12	A	811	CLA	C4D-CHA	2.66	1.47	1.38
12	A	805	CLA	C4D-CHA	2.65	1.47	1.38
12	B	811	CLA	C4D-CHA	2.65	1.47	1.38
12	F	203	CLA	C4C-C3C	2.65	1.49	1.45
12	B	821	CLA	C4D-CHA	2.65	1.47	1.38
12	A	829	CLA	C4D-CHA	2.65	1.47	1.38
12	A	839	CLA	C4D-CHA	2.65	1.47	1.38
12	B	824	CLA	C4D-CHA	2.65	1.47	1.38
12	B	831	CLA	C4D-CHA	2.65	1.47	1.38
12	A	809	CLA	C4D-CHA	2.64	1.47	1.38
12	A	827	CLA	C3B-C4B	2.64	1.50	1.42
12	B	822	CLA	C4D-CHA	2.64	1.47	1.38
15	A	851	BCR	C1-C6	-2.63	1.50	1.53
12	B	819	CLA	C4D-CHA	2.63	1.47	1.38
12	B	825	CLA	C4B-NB	-2.63	1.34	1.37
12	A	854	CLA	C4D-CHA	2.62	1.47	1.38
12	A	832	CLA	C4D-CHA	2.62	1.47	1.38
12	A	803	CLA	C3B-C4B	2.62	1.50	1.42
12	A	802	CLA	C4D-CHA	2.62	1.47	1.38
12	A	833	CLA	C4D-CHA	2.62	1.47	1.38
12	A	821	CLA	C4D-CHA	2.62	1.47	1.38
12	A	817	CLA	C4D-CHA	2.62	1.47	1.38
12	A	823	CLA	C4C-C3C	2.61	1.49	1.45
12	A	825	CLA	C4D-CHA	2.61	1.47	1.38
12	B	814	CLA	C4D-CHA	2.61	1.47	1.38
12	A	826	CLA	C4D-CHA	2.60	1.47	1.38
15	L	201	BCR	C30-C25	-2.60	1.50	1.53
12	A	832	CLA	C3B-C4B	2.60	1.50	1.42
15	F	201	BCR	C30-C25	-2.60	1.50	1.53
12	B	818	CLA	C3B-C4B	2.59	1.50	1.42
12	B	811	CLA	C4C-C3C	2.59	1.49	1.45
12	L	204	CLA	C4D-CHA	2.59	1.47	1.38
12	A	837	CLA	C4D-CHA	2.59	1.47	1.38
12	B	832	CLA	C4C-C3C	2.58	1.49	1.45
12	B	809	CLA	C4D-CHA	2.58	1.47	1.38
12	L	203	CLA	C4D-CHA	2.57	1.47	1.38
12	B	803	CLA	C4D-CHA	2.57	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	820	CLA	C1B-C2B	2.57	1.49	1.43
12	B	817	CLA	C3B-C4B	2.56	1.50	1.42
12	A	808	CLA	C3B-C4B	2.56	1.50	1.42
12	A	826	CLA	C3D-C4D	-2.56	1.38	1.44
15	J	102	BCR	C30-C25	-2.56	1.50	1.53
12	B	815	CLA	C1B-C2B	2.56	1.49	1.43
12	B	830	CLA	OBD-CAD	2.56	1.26	1.22
12	A	810	CLA	C1B-C2B	2.55	1.49	1.43
12	B	811	CLA	C1B-C2B	2.54	1.49	1.43
12	A	824	CLA	C1B-C2B	2.53	1.49	1.43
12	A	824	CLA	C4C-C3C	2.53	1.49	1.45
12	L	202	CLA	C3B-C4B	2.52	1.50	1.42
12	B	823	CLA	C4D-CHA	2.52	1.47	1.38
12	A	834	CLA	C1B-C2B	2.52	1.49	1.43
15	A	848	BCR	C1-C6	-2.52	1.50	1.53
12	A	842	CLA	C4C-C3C	2.52	1.49	1.45
12	A	836	CLA	C4B-NB	-2.52	1.34	1.37
12	A	806	CLA	C3D-C4D	-2.51	1.38	1.44
12	B	805	CLA	C1B-C2B	2.51	1.49	1.43
12	B	831	CLA	C3D-C4D	-2.51	1.38	1.44
12	A	829	CLA	C3B-C4B	2.51	1.50	1.42
12	B	801	CLA	C4D-CHA	2.51	1.47	1.38
12	A	841	CLA	C1B-C2B	2.51	1.49	1.43
12	F	203	CLA	C1B-C2B	2.51	1.49	1.43
12	A	842	CLA	C1B-C2B	2.50	1.49	1.43
12	B	807	CLA	C3B-C4B	2.50	1.50	1.42
12	B	827	CLA	C1B-C2B	2.50	1.49	1.43
12	B	812	CLA	C4C-C3C	2.50	1.49	1.45
12	A	804	CLA	C3B-C4B	2.50	1.50	1.42
12	B	814	CLA	C1B-C2B	2.50	1.49	1.43
12	B	819	CLA	C3B-C4B	2.49	1.50	1.42
12	A	812	CLA	C4C-C3C	2.49	1.49	1.45
16	A	852	LHG	O7-C5	-2.49	1.40	1.46
12	B	830	CLA	C3D-C4D	-2.49	1.38	1.44
12	B	826	CLA	C1B-C2B	2.49	1.49	1.43
12	A	807	CLA	C4C-C3C	2.49	1.49	1.45
12	A	819	CLA	C4C-C3C	2.49	1.49	1.45
12	A	843	CLA	C1B-C2B	2.49	1.49	1.43
12	A	816	CLA	C3B-C4B	2.48	1.50	1.42
12	A	816	CLA	C4C-C3C	2.48	1.49	1.45
12	B	820	CLA	C3D-C4D	-2.48	1.38	1.44
12	B	813	CLA	C4C-C3C	2.48	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	827	CLA	C4C-C3C	2.48	1.49	1.45
12	A	836	CLA	C4C-C3C	2.48	1.49	1.45
12	A	817	CLA	C1B-C2B	2.48	1.48	1.43
12	A	833	CLA	C1B-C2B	2.48	1.48	1.43
12	A	835	CLA	C1B-C2B	2.47	1.48	1.43
12	A	813	CLA	C4C-C3C	2.47	1.49	1.45
12	A	803	CLA	C3D-C4D	-2.47	1.38	1.44
12	B	812	CLA	C1B-C2B	2.46	1.48	1.43
12	A	839	CLA	C3D-C4D	-2.46	1.38	1.44
15	A	846	BCR	C30-C25	-2.46	1.50	1.53
12	B	825	CLA	C4D-CHA	2.46	1.46	1.38
12	B	816	CLA	C3B-C2B	2.46	1.49	1.41
12	B	819	CLA	C4C-C3C	2.45	1.49	1.45
12	B	831	CLA	C4C-C3C	2.45	1.49	1.45
12	A	809	CLA	C1B-C2B	2.45	1.48	1.43
12	A	820	CLA	C4C-C3C	2.45	1.49	1.45
12	A	840	CLA	C3B-C4B	2.45	1.49	1.42
12	B	830	CLA	C1B-C2B	2.45	1.48	1.43
12	A	806	CLA	C1B-C2B	2.45	1.48	1.43
12	A	815	CLA	C4C-C3C	2.45	1.49	1.45
12	A	854	CLA	C1B-C2B	2.45	1.48	1.43
12	B	808	CLA	C1B-C2B	2.44	1.48	1.43
12	A	812	CLA	C3B-C4B	2.44	1.49	1.42
17	B	837	LMG	O7-C8	-2.44	1.40	1.46
15	A	848	BCR	C30-C25	-2.44	1.50	1.53
12	B	827	CLA	C3B-C4B	2.44	1.49	1.42
12	A	831	CLA	C4C-C3C	2.44	1.49	1.45
12	B	828	CLA	C3B-C4B	2.44	1.49	1.42
12	A	837	CLA	C4C-C3C	2.44	1.49	1.45
12	A	825	CLA	C1B-C2B	2.44	1.48	1.43
12	A	804	CLA	C1C-C2C	2.44	1.49	1.44
12	A	811	CLA	C1B-C2B	2.43	1.48	1.43
12	B	832	CLA	C1B-C2B	2.43	1.48	1.43
12	L	204	CLA	C1B-C2B	2.43	1.48	1.43
12	B	816	CLA	C4C-C3C	2.43	1.49	1.45
12	A	822	CLA	C1B-C2B	2.43	1.48	1.43
12	J	101	CLA	C3B-C4B	2.43	1.49	1.42
12	A	843	CLA	C3B-C4B	2.42	1.49	1.42
12	A	839	CLA	C3B-C4B	2.42	1.49	1.42
12	A	803	CLA	C4C-C3C	2.42	1.49	1.45
12	B	815	CLA	C4C-C3C	2.42	1.49	1.45
12	B	811	CLA	C3D-C4D	-2.42	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	805	CLA	C1B-C2B	2.42	1.48	1.43
12	B	819	CLA	C3D-C4D	-2.42	1.38	1.44
12	L	204	CLA	C3D-C4D	-2.42	1.38	1.44
12	A	815	CLA	C3B-C4B	2.42	1.49	1.42
15	L	206	BCR	C30-C25	-2.42	1.50	1.53
12	A	813	CLA	C3B-C4B	2.41	1.49	1.42
12	B	808	CLA	C3D-C4D	-2.41	1.38	1.44
12	B	801	CLA	C4C-C3C	2.41	1.49	1.45
12	A	823	CLA	C1B-C2B	2.41	1.48	1.43
12	L	203	CLA	C1B-C2B	2.41	1.48	1.43
15	A	847	BCR	C30-C25	-2.40	1.50	1.53
12	B	817	CLA	C3D-C4D	-2.40	1.38	1.44
12	A	822	CLA	C3B-C4B	2.40	1.49	1.42
12	B	826	CLA	C4C-C3C	2.40	1.49	1.45
12	A	805	CLA	C3D-C4D	-2.40	1.38	1.44
12	A	810	CLA	C3B-C4B	2.40	1.49	1.42
12	A	818	CLA	C3D-C4D	-2.40	1.38	1.44
12	B	812	CLA	C3B-C4B	2.39	1.49	1.42
12	B	813	CLA	C1B-C2B	2.39	1.48	1.43
12	A	830	CLA	C4C-C3C	2.39	1.49	1.45
12	B	807	CLA	C1B-C2B	2.39	1.48	1.43
12	F	203	CLA	C3B-C4B	2.39	1.49	1.42
12	A	843	CLA	C4C-C3C	2.39	1.49	1.45
12	A	803	CLA	C1B-C2B	2.39	1.48	1.43
12	A	832	CLA	C3D-C4D	-2.39	1.38	1.44
12	B	824	CLA	C4C-C3C	2.38	1.49	1.45
12	B	825	CLA	C4C-C3C	2.38	1.49	1.45
12	A	854	CLA	CBD-CAD	-2.38	1.45	1.56
12	B	818	CLA	C4B-NB	-2.38	1.34	1.37
12	A	802	CLA	C3B-C4B	2.38	1.49	1.42
12	A	816	CLA	C1B-C2B	2.38	1.48	1.43
12	B	813	CLA	C3B-C4B	2.38	1.49	1.42
12	A	815	CLA	C1B-C2B	2.38	1.48	1.43
12	L	202	CLA	C1B-C2B	2.38	1.48	1.43
12	A	831	CLA	C3D-C4D	-2.38	1.38	1.44
12	A	809	CLA	C3B-C4B	2.37	1.49	1.42
12	A	836	CLA	C1B-C2B	2.37	1.48	1.43
12	A	821	CLA	C3D-C4D	-2.37	1.38	1.44
12	B	822	CLA	C3D-C4D	-2.37	1.38	1.44
12	A	825	CLA	C3D-C4D	-2.37	1.38	1.44
12	B	802	CLA	C3B-C4B	2.37	1.49	1.42
12	B	822	CLA	C3B-C4B	2.37	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	826	CLA	C3D-C4D	-2.37	1.38	1.44
12	B	808	CLA	C3B-C4B	2.37	1.49	1.42
12	A	817	CLA	C3D-C4D	-2.37	1.38	1.44
12	A	827	CLA	C3D-C4D	-2.37	1.38	1.44
12	J	101	CLA	C1B-C2B	2.37	1.48	1.43
12	A	841	CLA	C3B-C4B	2.36	1.49	1.42
12	A	834	CLA	C3D-C4D	-2.36	1.38	1.44
12	A	834	CLA	C4C-C3C	2.36	1.49	1.45
12	A	835	CLA	C4C-C3C	2.36	1.49	1.45
12	A	840	CLA	C4C-C3C	2.36	1.49	1.45
12	B	809	CLA	C1B-C2B	2.36	1.48	1.43
12	A	821	CLA	C3B-C4B	2.36	1.49	1.42
12	A	833	CLA	C3D-C4D	-2.36	1.38	1.44
12	B	820	CLA	C3B-C4B	2.36	1.49	1.42
12	B	824	CLA	C1B-C2B	2.35	1.48	1.43
12	A	824	CLA	C3D-C4D	-2.35	1.38	1.44
12	J	101	CLA	C4C-C3C	2.35	1.49	1.45
12	B	832	CLA	C3D-C4D	-2.35	1.38	1.44
12	A	814	CLA	C1C-C2C	2.35	1.49	1.44
12	B	809	CLA	C3D-C4D	-2.35	1.38	1.44
12	A	823	CLA	C3B-C4B	2.35	1.49	1.42
12	B	801	CLA	C1B-C2B	2.34	1.48	1.43
12	A	837	CLA	C3B-C2B	2.34	1.49	1.41
12	A	840	CLA	C1C-C2C	2.34	1.49	1.44
12	A	839	CLA	C1B-C2B	2.34	1.48	1.43
12	A	828	CLA	C4C-C3C	2.34	1.49	1.45
12	A	823	CLA	C3D-C4D	-2.34	1.38	1.44
12	B	824	CLA	C3D-C4D	-2.34	1.38	1.44
12	A	841	CLA	C4C-C3C	2.33	1.49	1.45
12	A	831	CLA	C1B-C2B	2.33	1.48	1.43
12	B	828	CLA	C3D-C4D	-2.33	1.38	1.44
12	A	854	CLA	C1C-C2C	2.33	1.49	1.44
12	A	812	CLA	C1B-C2B	2.33	1.48	1.43
12	A	813	CLA	C3D-C4D	-2.33	1.39	1.44
12	F	203	CLA	C3D-C4D	-2.33	1.39	1.44
12	A	814	CLA	C1B-C2B	2.33	1.48	1.43
12	A	838	CLA	C3D-C4D	-2.32	1.39	1.44
12	A	828	CLA	C1B-C2B	2.32	1.48	1.43
12	B	825	CLA	C3D-C4D	-2.32	1.39	1.44
12	B	803	CLA	C3D-C4D	-2.32	1.39	1.44
12	B	815	CLA	C3B-C4B	2.32	1.49	1.42
12	B	809	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	A	851	BCR	C30-C25	-2.32	1.50	1.53
12	A	811	CLA	C4C-C3C	2.32	1.49	1.45
12	B	807	CLA	C3D-C4D	-2.32	1.39	1.44
12	A	835	CLA	C3D-C4D	-2.32	1.39	1.44
12	A	809	CLA	C3D-C4D	-2.32	1.39	1.44
12	A	829	CLA	C3D-C4D	-2.31	1.39	1.44
12	A	810	CLA	C4C-C3C	2.31	1.49	1.45
12	B	805	CLA	C3B-C2B	2.31	1.49	1.41
12	A	811	CLA	C3B-C4B	2.31	1.49	1.42
12	A	817	CLA	C3B-C4B	2.31	1.49	1.42
12	B	810	CLA	C4C-C3C	2.31	1.49	1.45
12	A	838	CLA	C3B-C4B	2.31	1.49	1.42
12	B	802	CLA	C4C-C3C	2.30	1.48	1.45
12	B	812	CLA	C1C-C2C	2.30	1.49	1.44
12	A	807	CLA	C3D-C4D	-2.30	1.39	1.44
12	B	820	CLA	C1B-C2B	2.30	1.48	1.43
12	B	830	CLA	C3B-C4B	2.30	1.49	1.42
12	B	830	CLA	C4C-C3C	2.30	1.48	1.45
12	B	805	CLA	C4C-C3C	2.30	1.48	1.45
12	A	828	CLA	C1C-C2C	2.30	1.49	1.44
12	A	811	CLA	C3D-C4D	-2.30	1.39	1.44
12	A	821	CLA	C1C-C2C	2.29	1.49	1.44
12	L	203	CLA	C3D-C4D	-2.29	1.39	1.44
12	A	838	CLA	C4C-C3C	2.29	1.48	1.45
12	A	830	CLA	C3D-C4D	-2.29	1.39	1.44
12	A	820	CLA	C3B-C4B	2.29	1.49	1.42
12	B	824	CLA	C3B-C4B	2.29	1.49	1.42
12	A	827	CLA	C1B-C2B	2.29	1.48	1.43
12	B	822	CLA	C1B-C2B	2.29	1.48	1.43
12	B	814	CLA	C3B-C4B	2.29	1.49	1.42
12	B	811	CLA	C3B-C4B	2.28	1.49	1.42
12	A	841	CLA	C1C-C2C	2.28	1.49	1.44
12	A	807	CLA	C1B-C2B	2.28	1.48	1.43
12	L	204	CLA	C3B-C4B	2.28	1.49	1.42
12	B	817	CLA	C4C-C3C	2.28	1.48	1.45
12	A	814	CLA	C3B-C4B	2.28	1.49	1.42
12	A	829	CLA	C1C-C2C	2.28	1.49	1.44
12	B	824	CLA	C3B-C2B	2.28	1.48	1.41
12	B	801	CLA	CBD-CAD	-2.27	1.46	1.56
12	J	101	CLA	C3D-C4D	-2.27	1.39	1.44
12	B	829	CLA	C1B-C2B	2.27	1.48	1.43
12	B	819	CLA	C3B-C2B	2.27	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	812	CLA	C3D-C4D	-2.27	1.39	1.44
12	B	804	CLA	C3B-C4B	2.27	1.49	1.42
12	B	826	CLA	C3B-C4B	2.27	1.49	1.42
15	A	849	BCR	C30-C25	-2.27	1.50	1.53
12	L	202	CLA	C4C-C3C	2.27	1.48	1.45
12	A	826	CLA	C3B-C4B	2.26	1.49	1.42
12	A	820	CLA	C3D-C4D	-2.26	1.39	1.44
12	B	815	CLA	C3D-C4D	-2.26	1.39	1.44
12	A	832	CLA	C1B-C2B	2.26	1.48	1.43
12	A	828	CLA	C3D-C4D	-2.26	1.39	1.44
12	B	810	CLA	C3D-C4D	-2.26	1.39	1.44
12	L	202	CLA	C3D-C4D	-2.26	1.39	1.44
12	A	831	CLA	C3B-C4B	2.26	1.49	1.42
12	B	814	CLA	C3D-C4D	-2.26	1.39	1.44
12	A	822	CLA	C3D-C4D	-2.26	1.39	1.44
12	A	825	CLA	C4C-C3C	2.26	1.48	1.45
12	B	821	CLA	C3D-C4D	-2.26	1.39	1.44
12	B	818	CLA	C3D-C4D	-2.25	1.39	1.44
12	A	829	CLA	C1B-C2B	2.25	1.48	1.43
12	B	821	CLA	C3B-C2B	2.25	1.48	1.41
12	A	841	CLA	C3D-C4D	-2.25	1.39	1.44
12	A	814	CLA	C4C-C3C	2.25	1.48	1.45
12	A	840	CLA	C1B-C2B	2.25	1.48	1.43
12	B	821	CLA	C3B-C4B	2.25	1.49	1.42
12	A	818	CLA	C1C-NC	-2.25	1.34	1.37
12	A	828	CLA	C3B-C2B	2.25	1.48	1.41
12	A	832	CLA	C4C-C3C	2.25	1.48	1.45
12	A	842	CLA	C3B-C4B	2.25	1.49	1.42
12	B	813	CLA	C3D-C4D	-2.24	1.39	1.44
12	A	806	CLA	C3B-C4B	2.24	1.49	1.42
12	A	833	CLA	C4C-C3C	2.24	1.48	1.45
12	B	821	CLA	C1B-C2B	2.24	1.48	1.43
12	A	808	CLA	C1B-C2B	2.24	1.48	1.43
12	A	828	CLA	C3B-C4B	2.24	1.49	1.42
12	B	812	CLA	C3D-C4D	-2.24	1.39	1.44
12	A	813	CLA	C1B-C2B	2.24	1.48	1.43
12	A	815	CLA	C3D-C4D	-2.24	1.39	1.44
12	A	816	CLA	C3D-C4D	-2.24	1.39	1.44
12	A	842	CLA	C3D-C4D	-2.24	1.39	1.44
12	A	818	CLA	C4C-C3C	2.24	1.48	1.45
12	A	819	CLA	C3D-C4D	-2.24	1.39	1.44
12	B	801	CLA	C3D-C4D	-2.24	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	828	CLA	C1B-C2B	2.24	1.48	1.43
12	A	804	CLA	C3D-C4D	-2.23	1.39	1.44
12	B	831	CLA	C3B-C4B	2.23	1.49	1.42
12	B	828	CLA	C4C-C3C	2.23	1.48	1.45
12	B	816	CLA	C3D-C4D	-2.23	1.39	1.44
12	B	825	CLA	C1C-C2C	2.23	1.49	1.44
12	A	808	CLA	C4C-C3C	2.23	1.48	1.45
12	B	829	CLA	C3D-C4D	-2.23	1.39	1.44
12	A	807	CLA	C3B-C4B	2.23	1.49	1.42
12	A	826	CLA	C1B-C2B	2.23	1.48	1.43
12	A	802	CLA	C3B-C2B	2.23	1.48	1.41
12	B	814	CLA	C1C-C2C	2.23	1.49	1.44
12	A	808	CLA	C1C-C2C	2.22	1.49	1.44
12	A	854	CLA	C4C-C3C	2.22	1.48	1.45
12	A	810	CLA	C3D-C4D	-2.22	1.39	1.44
12	A	854	CLA	C3B-C2B	2.22	1.48	1.41
12	B	831	CLA	C1B-C2B	2.22	1.48	1.43
12	B	814	CLA	C4C-C3C	2.22	1.48	1.45
12	B	831	CLA	C1C-C2C	2.22	1.49	1.44
12	B	808	CLA	C1C-C2C	2.22	1.49	1.44
12	B	829	CLA	CBD-CAD	-2.22	1.46	1.56
12	A	839	CLA	C1C-C2C	2.21	1.49	1.44
15	F	202	BCR	C30-C25	-2.21	1.51	1.53
12	B	802	CLA	C3D-C4D	-2.21	1.39	1.44
12	B	820	CLA	C1C-C2C	2.20	1.49	1.44
12	A	824	CLA	C3B-C4B	2.20	1.49	1.42
12	A	809	CLA	C4C-C3C	2.20	1.48	1.45
12	L	204	CLA	C4C-C3C	2.20	1.48	1.45
12	B	804	CLA	C4C-C3C	2.20	1.48	1.45
12	A	802	CLA	CHB-C4A	-2.20	1.32	1.37
12	A	817	CLA	C4C-C3C	2.20	1.48	1.45
12	A	805	CLA	C3B-C4B	2.19	1.49	1.42
12	F	203	CLA	C3B-C2B	2.19	1.48	1.41
12	A	841	CLA	C3B-C2B	2.19	1.48	1.41
12	B	829	CLA	C3B-C4B	2.19	1.49	1.42
12	A	835	CLA	C3B-C4B	2.19	1.49	1.42
12	A	834	CLA	C3B-C4B	2.19	1.49	1.42
12	B	825	CLA	C1B-C2B	2.18	1.48	1.43
12	A	820	CLA	C3B-C2B	2.18	1.48	1.41
12	A	809	CLA	C1C-C2C	2.18	1.49	1.44
12	B	809	CLA	C1C-NC	-2.18	1.34	1.37
12	A	805	CLA	C3B-C2B	2.18	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	814	CLA	C3D-C4D	-2.18	1.39	1.44
12	B	822	CLA	C4C-C3C	2.18	1.48	1.45
12	A	836	CLA	C3B-C2B	2.18	1.48	1.41
12	B	804	CLA	C1C-NC	-2.18	1.34	1.37
12	A	836	CLA	C3D-C4D	-2.18	1.39	1.44
12	B	813	CLA	C1C-C2C	2.18	1.48	1.44
12	A	825	CLA	C3B-C2B	2.17	1.48	1.41
12	L	202	CLA	C3B-C2B	2.17	1.48	1.41
12	J	101	CLA	C3B-C2B	2.17	1.48	1.41
12	B	827	CLA	C3D-C4D	-2.17	1.39	1.44
12	A	833	CLA	C3B-C4B	2.17	1.49	1.42
12	A	819	CLA	C3B-C4B	2.17	1.49	1.42
12	B	802	CLA	C1B-C2B	2.17	1.48	1.43
12	B	830	CLA	CBD-CAD	-2.17	1.46	1.56
12	B	832	CLA	C3B-C4B	2.16	1.49	1.42
12	B	806	CLA	C3D-C4D	-2.16	1.39	1.44
12	A	805	CLA	C4C-C3C	2.16	1.48	1.45
12	A	808	CLA	C3D-C4D	-2.16	1.39	1.44
12	B	828	CLA	C1C-C2C	2.16	1.48	1.44
12	A	834	CLA	C1C-NC	-2.16	1.34	1.37
12	B	804	CLA	C3B-C2B	2.16	1.48	1.41
12	B	803	CLA	C1A-CHA	2.16	1.52	1.43
12	B	830	CLA	C3B-C2B	2.16	1.48	1.41
12	B	818	CLA	C1A-CHA	2.16	1.52	1.43
12	B	832	CLA	C1C-NC	-2.16	1.34	1.37
12	B	816	CLA	C3B-C4B	2.16	1.49	1.42
12	A	803	CLA	C3B-C2B	2.16	1.48	1.41
12	A	836	CLA	C1C-C2C	2.15	1.48	1.44
12	A	822	CLA	C3B-C2B	2.15	1.48	1.41
12	B	804	CLA	C1B-C2B	2.15	1.48	1.43
12	A	827	CLA	C1C-NC	-2.15	1.34	1.37
12	A	825	CLA	C3B-C4B	2.15	1.49	1.42
12	A	823	CLA	C3B-C2B	2.15	1.48	1.41
12	B	818	CLA	C4C-C3C	2.15	1.48	1.45
12	A	842	CLA	C1C-C2C	2.15	1.48	1.44
12	B	804	CLA	C1A-CHA	2.15	1.51	1.43
12	B	819	CLA	CHB-C4A	-2.15	1.32	1.37
12	B	811	CLA	C3B-C2B	2.14	1.48	1.41
12	B	817	CLA	C1C-C2C	2.14	1.48	1.44
12	L	203	CLA	C4C-C3C	2.14	1.48	1.45
12	A	819	CLA	C1B-C2B	2.14	1.48	1.43
15	I	101	BCR	C27-C26	-2.13	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	807	CLA	C3B-C2B	2.13	1.48	1.41
12	B	827	CLA	C1C-C2C	2.13	1.48	1.44
12	A	843	CLA	C3D-C4D	-2.13	1.39	1.44
12	A	826	CLA	C1C-C2C	2.13	1.48	1.44
12	A	812	CLA	C3B-C2B	2.12	1.48	1.41
12	A	802	CLA	C1C-C2C	2.12	1.48	1.44
12	B	824	CLA	C1C-C2C	2.12	1.48	1.44
12	L	202	CLA	C1C-C2C	2.12	1.48	1.44
12	B	819	CLA	C1B-C2B	2.12	1.48	1.43
12	A	823	CLA	C1C-C2C	2.12	1.48	1.44
12	A	806	CLA	C3B-C2B	2.12	1.48	1.41
12	A	821	CLA	C4C-C3C	2.12	1.48	1.45
12	A	811	CLA	C3B-C2B	2.12	1.48	1.41
12	A	827	CLA	C1C-C2C	2.11	1.48	1.44
12	L	203	CLA	C3B-C4B	2.11	1.48	1.42
12	A	831	CLA	C1C-C2C	2.11	1.48	1.44
12	B	802	CLA	C1C-C2C	2.11	1.48	1.44
12	B	831	CLA	C3B-C2B	2.11	1.48	1.41
12	A	832	CLA	C3B-C2B	2.11	1.48	1.41
12	A	854	CLA	C3B-C4B	2.10	1.48	1.42
12	A	808	CLA	C3B-C2B	2.10	1.48	1.41
12	B	809	CLA	C3B-C2B	2.10	1.48	1.41
12	A	826	CLA	C4C-C3C	2.10	1.48	1.45
12	L	204	CLA	C3B-C2B	2.10	1.48	1.41
12	A	818	CLA	C1B-C2B	2.10	1.48	1.43
12	A	842	CLA	C3B-C2B	2.10	1.48	1.41
12	A	819	CLA	C1A-CHA	2.10	1.51	1.43
12	A	830	CLA	C3B-C4B	2.10	1.48	1.42
12	B	805	CLA	C1C-C2C	2.10	1.48	1.44
12	B	822	CLA	C1C-C2C	2.10	1.48	1.44
12	A	829	CLA	C4C-C3C	2.10	1.48	1.45
12	A	809	CLA	C3B-C2B	2.10	1.48	1.41
12	F	203	CLA	C1C-C2C	2.10	1.48	1.44
12	A	808	CLA	C1A-CHA	2.09	1.51	1.43
15	I	101	BCR	C30-C25	-2.09	1.51	1.53
12	B	811	CLA	CBD-CAD	-2.09	1.47	1.56
12	B	829	CLA	C4C-C3C	2.09	1.48	1.45
12	B	814	CLA	C3B-C2B	2.09	1.48	1.41
12	A	828	CLA	C1A-CHA	2.09	1.51	1.43
12	B	819	CLA	C1C-C2C	2.09	1.48	1.44
12	A	815	CLA	C3B-C2B	2.09	1.48	1.41
12	A	821	CLA	C1B-C2B	2.09	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	839	CLA	C4C-C3C	2.08	1.48	1.45
12	B	805	CLA	C3D-C4D	-2.08	1.39	1.44
12	B	805	CLA	C1A-CHA	2.08	1.51	1.43
12	B	806	CLA	C3B-C2B	2.08	1.48	1.41
12	A	838	CLA	C3B-C2B	2.08	1.48	1.41
12	A	840	CLA	C3B-C2B	2.08	1.48	1.41
12	A	818	CLA	C3B-C2B	2.08	1.48	1.41
12	B	820	CLA	C3B-C2B	2.08	1.48	1.41
12	A	804	CLA	C1B-C2B	2.08	1.48	1.43
12	A	822	CLA	C1C-C2C	2.08	1.48	1.44
12	A	802	CLA	C3D-C4D	-2.08	1.39	1.44
12	L	204	CLA	C1C-C2C	2.08	1.48	1.44
12	A	833	CLA	C1C-C2C	2.07	1.48	1.44
12	A	839	CLA	C3B-C2B	2.07	1.48	1.41
12	B	822	CLA	C1C-NC	-2.07	1.34	1.37
12	A	843	CLA	C3B-C2B	2.07	1.48	1.41
12	B	827	CLA	C3B-C2B	2.07	1.48	1.41
12	A	816	CLA	C3B-C2B	2.07	1.48	1.41
12	A	839	CLA	C1C-NC	-2.07	1.34	1.37
12	B	812	CLA	C3B-C2B	2.07	1.48	1.41
12	A	838	CLA	C1B-C2B	2.07	1.48	1.43
12	A	843	CLA	C1A-CHA	2.07	1.51	1.43
12	A	842	CLA	C1A-CHA	2.06	1.51	1.43
12	A	813	CLA	C3B-C2B	2.06	1.48	1.41
12	B	823	CLA	C3B-C4B	2.06	1.48	1.42
12	B	816	CLA	C1C-C2C	2.06	1.48	1.44
12	A	804	CLA	C3B-C2B	2.06	1.48	1.41
12	B	802	CLA	C3B-C2B	2.05	1.48	1.41
12	B	816	CLA	C1A-CHA	2.05	1.51	1.43
12	A	806	CLA	C1C-C2C	2.05	1.48	1.44
12	A	832	CLA	C1C-C2C	2.05	1.48	1.44
12	A	813	CLA	C1C-C2C	2.05	1.48	1.44
12	B	813	CLA	C3B-C2B	2.05	1.48	1.41
12	A	810	CLA	C3B-C2B	2.05	1.48	1.41
12	A	835	CLA	C1C-C2C	2.05	1.48	1.44
12	A	854	CLA	C1A-CHA	2.05	1.51	1.43
12	B	815	CLA	C3B-C2B	2.05	1.48	1.41
12	B	823	CLA	C3B-C2B	2.04	1.48	1.41
12	A	813	CLA	C1C-NC	-2.04	1.34	1.37
12	B	810	CLA	C1A-CHA	2.04	1.51	1.43
12	A	817	CLA	C3B-C2B	2.04	1.48	1.41
16	A	853	LHG	O7-C5	-2.04	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	821	CLA	C4C-C3C	2.04	1.48	1.45
12	A	815	CLA	C1C-C2C	2.04	1.48	1.44
12	A	831	CLA	C3B-C2B	2.04	1.48	1.41
12	A	840	CLA	C1A-CHA	2.04	1.51	1.43
12	A	803	CLA	C1C-NC	-2.04	1.34	1.37
12	B	817	CLA	C3B-C2B	2.04	1.48	1.41
12	A	824	CLA	C3B-C2B	2.03	1.48	1.41
12	B	817	CLA	CHB-C4A	-2.03	1.32	1.37
12	A	826	CLA	CHB-C4A	-2.03	1.32	1.37
12	A	840	CLA	C3D-C4D	-2.03	1.39	1.44
12	B	830	CLA	C1C-C2C	2.03	1.48	1.44
12	A	807	CLA	C1C-C2C	2.03	1.48	1.44
12	A	807	CLA	C3B-C2B	2.03	1.48	1.41
12	A	817	CLA	C1C-C2C	2.03	1.48	1.44
12	A	824	CLA	C1C-C2C	2.03	1.48	1.44
12	B	821	CLA	C1C-C2C	2.03	1.48	1.44
12	B	814	CLA	C1A-CHA	2.02	1.51	1.43
12	A	833	CLA	C3B-C2B	2.02	1.48	1.41
12	A	828	CLA	CBD-CAD	-2.02	1.47	1.56
12	B	807	CLA	C1C-NC	-2.02	1.34	1.37
12	B	803	CLA	C4C-C3C	2.02	1.48	1.45
12	B	818	CLA	CHB-C4A	-2.02	1.32	1.37
12	A	834	CLA	C1A-CHA	2.02	1.51	1.43
12	A	827	CLA	C3B-C2B	2.01	1.48	1.41
12	B	801	CLA	C1C-C2C	2.01	1.48	1.44
12	A	823	CLA	C1A-CHA	2.01	1.51	1.43
12	A	826	CLA	C3B-C2B	2.01	1.48	1.41
12	B	821	CLA	C1A-CHA	2.01	1.51	1.43
12	L	202	CLA	C1A-CHA	2.01	1.51	1.43
12	B	823	CLA	CBD-CAD	-2.01	1.47	1.56
12	B	805	CLA	C3B-C4B	2.01	1.48	1.42
12	A	816	CLA	C1A-CHA	2.00	1.51	1.43
12	A	810	CLA	C1A-CHA	2.00	1.51	1.43
12	A	830	CLA	CBD-CAD	-2.00	1.47	1.56

All (2601) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	825	CLA	C1D-ND-C4D	-10.72	98.79	106.31
12	L	203	CLA	C1D-ND-C4D	-9.98	99.31	106.31
12	A	822	CLA	C1D-ND-C4D	-9.75	99.47	106.31
12	A	817	CLA	C1D-ND-C4D	-9.69	99.51	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	801	CL0	O2D-CGD-CBD	9.68	121.58	110.95
12	B	824	CLA	C1D-ND-C4D	-9.61	99.57	106.31
12	L	204	CLA	C1D-ND-C4D	-9.57	99.60	106.31
12	B	816	CLA	C1D-ND-C4D	-9.48	99.66	106.31
12	L	202	CLA	C1D-ND-C4D	-9.47	99.67	106.31
12	B	829	CLA	C1D-ND-C4D	-9.42	99.70	106.31
12	B	809	CLA	C1D-ND-C4D	-9.41	99.71	106.31
12	A	802	CLA	C1D-ND-C4D	-9.41	99.71	106.31
12	B	827	CLA	C1D-ND-C4D	-9.41	99.71	106.31
12	A	815	CLA	C1D-ND-C4D	-9.41	99.71	106.31
12	B	830	CLA	C1D-ND-C4D	-9.40	99.71	106.31
12	A	839	CLA	C1D-ND-C4D	-9.39	99.73	106.31
12	B	803	CLA	C1D-ND-C4D	-9.35	99.75	106.31
12	A	811	CLA	C1D-ND-C4D	-9.33	99.76	106.31
12	A	835	CLA	C1D-ND-C4D	-9.31	99.78	106.31
12	A	832	CLA	C1D-ND-C4D	-9.28	99.80	106.31
12	B	804	CLA	C1D-ND-C4D	-9.28	99.80	106.31
12	B	831	CLA	C1D-ND-C4D	-9.26	99.82	106.31
12	B	807	CLA	C1D-ND-C4D	-9.21	99.85	106.31
12	B	828	CLA	C1D-ND-C4D	-9.20	99.85	106.31
11	A	801	CL0	C1B-CHB-C4A	9.19	127.23	121.32
12	A	804	CLA	C1D-ND-C4D	-9.18	99.87	106.31
12	A	843	CLA	C1D-ND-C4D	-9.18	99.87	106.31
12	A	821	CLA	C1D-ND-C4D	-9.17	99.88	106.31
12	B	821	CLA	C1D-ND-C4D	-9.17	99.88	106.31
12	B	819	CLA	C1D-ND-C4D	-9.16	99.88	106.31
12	A	816	CLA	C1D-ND-C4D	-9.14	99.90	106.31
12	A	841	CLA	C1D-ND-C4D	-9.14	99.90	106.31
12	A	806	CLA	C1D-ND-C4D	-9.12	99.91	106.31
12	A	809	CLA	C1D-ND-C4D	-9.12	99.91	106.31
12	J	101	CLA	C1D-ND-C4D	-9.12	99.92	106.31
12	B	808	CLA	C1D-ND-C4D	-9.10	99.93	106.31
12	A	805	CLA	C1D-ND-C4D	-9.09	99.94	106.31
12	B	814	CLA	C1D-ND-C4D	-9.08	99.94	106.31
12	A	842	CLA	C1D-ND-C4D	-9.06	99.96	106.31
12	A	834	CLA	C1D-ND-C4D	-9.05	99.96	106.31
12	A	823	CLA	C1D-ND-C4D	-9.05	99.96	106.31
12	B	826	CLA	C1D-ND-C4D	-9.04	99.97	106.31
12	B	812	CLA	C1D-ND-C4D	-9.03	99.97	106.31
12	B	817	CLA	C1D-ND-C4D	-9.01	99.99	106.31
12	A	818	CLA	C1D-ND-C4D	-9.00	100.00	106.31
12	A	827	CLA	C1D-ND-C4D	-8.97	100.02	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	810	CLA	C1D-ND-C4D	-8.97	100.02	106.31
12	A	836	CLA	C1D-ND-C4D	-8.96	100.03	106.31
12	A	826	CLA	C1D-ND-C4D	-8.95	100.03	106.31
12	B	806	CLA	C1D-ND-C4D	-8.94	100.04	106.31
12	B	805	CLA	C1D-ND-C4D	-8.93	100.05	106.31
12	A	833	CLA	C1D-ND-C4D	-8.89	100.07	106.31
12	B	822	CLA	C1D-ND-C4D	-8.88	100.08	106.31
12	A	838	CLA	C1D-ND-C4D	-8.88	100.08	106.31
12	A	825	CLA	C1D-ND-C4D	-8.85	100.10	106.31
12	B	815	CLA	C1D-ND-C4D	-8.84	100.11	106.31
12	A	829	CLA	C1D-ND-C4D	-8.84	100.11	106.31
12	A	812	CLA	C1D-ND-C4D	-8.83	100.12	106.31
12	A	831	CLA	C1D-ND-C4D	-8.82	100.12	106.31
12	B	820	CLA	C1D-ND-C4D	-8.77	100.16	106.31
12	A	803	CLA	C1D-ND-C4D	-8.76	100.17	106.31
12	B	802	CLA	C1D-ND-C4D	-8.74	100.18	106.31
12	A	807	CLA	C1D-ND-C4D	-8.74	100.18	106.31
12	A	840	CLA	C1D-ND-C4D	-8.74	100.18	106.31
12	A	808	CLA	C1D-ND-C4D	-8.71	100.20	106.31
12	A	824	CLA	C1D-ND-C4D	-8.71	100.20	106.31
12	A	854	CLA	C1D-ND-C4D	-8.69	100.22	106.31
12	A	814	CLA	C1D-ND-C4D	-8.67	100.23	106.31
12	B	813	CLA	C1D-ND-C4D	-8.66	100.23	106.31
12	A	813	CLA	C1D-ND-C4D	-8.65	100.25	106.31
12	A	828	CLA	C1D-ND-C4D	-8.53	100.33	106.31
12	B	818	CLA	C1D-ND-C4D	-8.51	100.34	106.31
12	B	823	CLA	CMD-C2D-C1D	8.51	139.71	124.73
12	B	832	CLA	C1D-ND-C4D	-8.46	100.37	106.31
12	A	830	CLA	C1D-ND-C4D	-8.43	100.40	106.31
12	A	819	CLA	C1D-ND-C4D	-8.41	100.41	106.31
12	F	203	CLA	C1D-ND-C4D	-8.36	100.44	106.31
12	A	837	CLA	C1D-ND-C4D	-8.28	100.50	106.31
12	B	801	CLA	C1D-ND-C4D	-8.28	100.50	106.31
12	B	811	CLA	C1D-ND-C4D	-8.27	100.51	106.31
12	A	820	CLA	C1D-ND-C4D	-8.25	100.52	106.31
12	B	810	CLA	C1D-ND-C4D	-8.11	100.62	106.31
12	B	823	CLA	C1D-ND-C4D	-7.83	100.82	106.31
12	B	811	CLA	CMD-C2D-C1D	7.64	138.17	124.73
12	A	837	CLA	CMD-C2D-C1D	7.36	137.68	124.73
12	B	819	CLA	CMD-C2D-C1D	7.35	137.68	124.73
12	A	826	CLA	CMD-C2D-C1D	7.31	137.60	124.73
12	B	831	CLA	CMD-C2D-C1D	7.25	137.49	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	829	CLA	CMD-C2D-C1D	7.21	137.42	124.73
12	B	825	CLA	CMD-C2D-C1D	7.21	137.42	124.73
12	B	809	CLA	CHD-C4C-C3C	-7.19	114.29	124.77
12	A	805	CLA	CMD-C2D-C1D	7.16	137.33	124.73
12	B	825	CLA	C2D-C1D-ND	7.11	117.16	110.13
12	B	809	CLA	CMD-C2D-C1D	7.05	137.14	124.73
12	A	806	CLA	CMD-C2D-C1D	7.05	137.14	124.73
12	A	833	CLA	CMD-C2D-C1D	7.04	137.12	124.73
12	A	834	CLA	O2D-CGD-CBD	7.00	123.47	111.23
12	A	839	CLA	O2D-CGD-CBD	6.96	123.39	111.23
12	B	820	CLA	CMD-C2D-C1D	6.95	136.97	124.73
12	A	836	CLA	O2D-CGD-CBD	6.95	123.38	111.23
11	A	801	CL0	C4D-ND-C1D	-6.93	99.96	105.22
12	A	803	CLA	CMD-C2D-C1D	6.90	136.89	124.73
12	B	824	CLA	CMD-C2D-C1D	6.89	136.86	124.73
12	A	836	CLA	CMD-C2D-C1D	6.85	136.79	124.73
12	A	820	CLA	CMD-C2D-C1D	6.84	136.77	124.73
12	A	816	CLA	CMD-C2D-C1D	6.81	136.73	124.73
12	A	814	CLA	CMD-C2D-C1D	6.80	136.71	124.73
12	L	202	CLA	CMD-C2D-C1D	6.80	136.71	124.73
12	A	818	CLA	CMD-C2D-C1D	6.80	136.70	124.73
12	A	830	CLA	O2D-CGD-CBD	6.80	123.11	111.23
12	B	823	CLA	O2D-CGD-CBD	6.79	123.09	111.23
12	A	813	CLA	CMD-C2D-C1D	6.78	136.67	124.73
12	B	816	CLA	CMD-C2D-C1D	6.78	136.66	124.73
12	B	817	CLA	CMD-C2D-C1D	6.78	136.66	124.73
12	J	101	CLA	CMD-C2D-C1D	6.78	136.66	124.73
12	A	832	CLA	CMD-C2D-C1D	6.77	136.66	124.73
12	A	839	CLA	CMD-C2D-C1D	6.77	136.65	124.73
12	A	827	CLA	CMD-C2D-C1D	6.76	136.63	124.73
12	B	828	CLA	CMD-C2D-C1D	6.76	136.63	124.73
12	L	204	CLA	CMD-C2D-C1D	6.76	136.62	124.73
12	A	843	CLA	CMD-C2D-C1D	6.74	136.60	124.73
12	A	817	CLA	CMD-C2D-C1D	6.74	136.59	124.73
12	A	807	CLA	CMD-C2D-C1D	6.74	136.59	124.73
12	B	815	CLA	CMD-C2D-C1D	6.73	136.57	124.73
12	B	804	CLA	C2D-C1D-ND	6.73	116.78	110.13
12	A	838	CLA	O2D-CGD-CBD	6.72	122.98	111.23
12	A	802	CLA	C2D-C1D-ND	6.71	116.77	110.13
12	A	810	CLA	CMD-C2D-C1D	6.70	136.53	124.73
12	A	812	CLA	CMD-C2D-C1D	6.70	136.53	124.73
12	A	815	CLA	CMD-C2D-C1D	6.70	136.53	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	838	CLA	CMD-C2D-C1D	6.70	136.52	124.73
12	B	805	CLA	CMD-C2D-C1D	6.68	136.49	124.73
12	B	813	CLA	CMD-C2D-C1D	6.68	136.49	124.73
12	B	830	CLA	CMD-C2D-C1D	6.68	136.49	124.73
12	B	812	CLA	CMD-C2D-C1D	6.68	136.49	124.73
12	A	827	CLA	O2D-CGD-CBD	6.68	122.91	111.23
12	B	832	CLA	CMD-C2D-C1D	6.67	136.48	124.73
12	B	820	CLA	CHD-C4C-C3C	-6.67	115.05	124.77
12	B	807	CLA	CMD-C2D-C1D	6.66	136.46	124.73
12	A	854	CLA	O2D-CGD-CBD	6.66	122.87	111.23
12	A	834	CLA	CMD-C2D-C1D	6.66	136.45	124.73
12	A	811	CLA	CMD-C2D-C1D	6.65	136.45	124.73
12	F	203	CLA	CMD-C2D-C1D	6.65	136.43	124.73
12	B	818	CLA	CMD-C2D-C1D	6.64	136.42	124.73
12	A	823	CLA	CMD-C2D-C1D	6.64	136.41	124.73
12	A	841	CLA	CMD-C2D-C1D	6.63	136.41	124.73
12	A	854	CLA	C2D-C1D-ND	6.60	116.66	110.13
12	A	819	CLA	CMD-C2D-C1D	6.60	136.36	124.73
12	B	814	CLA	CMD-C2D-C1D	6.60	136.34	124.73
12	B	827	CLA	CMD-C2D-C1D	6.59	136.34	124.73
12	L	203	CLA	C2D-C1D-ND	6.58	116.64	110.13
12	B	826	CLA	CMD-C2D-C1D	6.56	136.28	124.73
12	A	821	CLA	CMD-C2D-C1D	6.52	136.21	124.73
12	B	808	CLA	CMD-C2D-C1D	6.52	136.21	124.73
12	L	203	CLA	CMD-C2D-C1D	6.49	136.16	124.73
12	A	804	CLA	CMD-C2D-C1D	6.49	136.16	124.73
12	A	842	CLA	CMD-C2D-C1D	6.48	136.15	124.73
12	B	803	CLA	CHD-C4C-C3C	-6.46	115.35	124.77
12	A	824	CLA	CMD-C2D-C1D	6.44	136.06	124.73
12	B	806	CLA	CMD-C2D-C1D	6.42	136.03	124.73
12	A	809	CLA	CMD-C2D-C1D	6.41	136.02	124.73
12	B	808	CLA	CHD-C4C-C3C	-6.41	115.43	124.77
12	B	821	CLA	C2D-C1D-ND	6.39	116.45	110.13
12	A	822	CLA	CMD-C2D-C1D	6.38	135.97	124.73
12	A	827	CLA	CHD-C4C-C3C	-6.35	115.52	124.77
12	A	831	CLA	CMD-C2D-C1D	6.32	135.86	124.73
12	B	824	CLA	CAA-C2A-C3A	-6.32	95.93	113.00
12	B	829	CLA	C2D-C1D-ND	6.32	116.38	110.13
12	A	837	CLA	O2D-CGD-CBD	6.26	122.17	111.23
12	A	828	CLA	CMD-C2D-C1D	6.24	135.72	124.73
12	A	806	CLA	CHD-C4C-C3C	-6.23	115.69	124.77
12	A	804	CLA	CHD-C4C-C3C	-6.22	115.70	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	819	CLA	C2B-C1B-NB	6.21	116.77	110.33
12	A	804	CLA	C2D-C1D-ND	6.19	116.25	110.13
12	A	822	CLA	C2D-C1D-ND	6.13	116.19	110.13
12	A	802	CLA	C2B-C1B-NB	6.11	116.66	110.33
12	A	804	CLA	O2D-CGD-CBD	6.11	121.91	111.23
12	B	832	CLA	C2C-C1C-NC	6.10	116.39	109.98
12	B	826	CLA	O2D-CGD-CBD	6.10	121.89	111.23
12	B	808	CLA	C2D-C1D-ND	6.08	116.14	110.13
12	A	831	CLA	O2D-CGD-CBD	6.07	121.84	111.23
12	B	824	CLA	C2D-C1D-ND	6.07	116.13	110.13
12	A	854	CLA	CHD-C4C-C3C	-6.06	115.93	124.77
12	A	827	CLA	C2D-C1D-ND	6.06	116.12	110.13
12	A	835	CLA	CMD-C2D-C1D	6.06	135.39	124.73
12	B	813	CLA	O2D-CGD-CBD	6.05	121.80	111.23
12	B	821	CLA	CMD-C2D-C1D	6.04	135.37	124.73
12	B	820	CLA	C2D-C1D-ND	6.03	116.09	110.13
12	A	840	CLA	C2D-C1D-ND	6.02	116.08	110.13
12	L	204	CLA	C2D-C1D-ND	6.01	116.07	110.13
12	B	809	CLA	C2D-C1D-ND	6.00	116.06	110.13
12	A	829	CLA	CHD-C4C-C3C	-5.98	116.05	124.77
12	B	828	CLA	C2D-C1D-ND	5.98	116.05	110.13
12	B	806	CLA	C2D-C1D-ND	5.98	116.04	110.13
12	B	804	CLA	CHD-C4C-C3C	-5.98	116.06	124.77
12	A	808	CLA	C2D-C1D-ND	5.96	116.02	110.13
12	A	843	CLA	C2D-C1D-ND	5.96	116.02	110.13
12	B	807	CLA	C2D-C1D-ND	5.96	116.02	110.13
12	L	202	CLA	C2D-C1D-ND	5.94	116.01	110.13
12	B	830	CLA	C2D-C1D-ND	5.94	116.00	110.13
12	A	811	CLA	C2D-C1D-ND	5.93	115.99	110.13
12	A	817	CLA	C2D-C1D-ND	5.93	115.99	110.13
12	B	816	CLA	C2D-C1D-ND	5.92	115.98	110.13
12	A	828	CLA	C2B-C1B-NB	5.92	116.46	110.33
12	B	832	CLA	O2D-CGD-CBD	5.90	121.55	111.23
12	B	815	CLA	O2D-CGD-CBD	5.90	121.54	111.23
12	A	828	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
12	A	839	CLA	CHD-C4C-C3C	-5.89	116.19	124.77
12	A	835	CLA	C2D-C1D-ND	5.88	115.95	110.13
12	A	808	CLA	CMD-C2D-C1D	5.88	135.09	124.73
12	B	805	CLA	CHD-C4C-C3C	-5.88	116.20	124.77
12	A	806	CLA	C2D-C1D-ND	5.88	115.95	110.13
12	B	801	CLA	C4A-NA-C1A	-5.88	104.00	106.68
12	A	839	CLA	C2D-C1D-ND	5.88	115.94	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	828	CLA	CHD-C4C-C3C	-5.87	116.21	124.77
12	A	825	CLA	C2D-C1D-ND	5.87	115.94	110.13
12	A	842	CLA	C2D-C1D-ND	5.87	115.93	110.13
12	B	810	CLA	CMD-C2D-C1D	5.86	135.05	124.73
12	A	815	CLA	C2D-C1D-ND	5.86	115.92	110.13
12	B	814	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
12	A	825	CLA	CHD-C4C-C3C	-5.85	116.25	124.77
12	A	814	CLA	CHD-C4C-C3C	-5.84	116.25	124.77
12	B	821	CLA	CHD-C4C-C3C	-5.84	116.27	124.77
12	A	803	CLA	O2D-CGD-CBD	5.83	121.42	111.23
12	B	817	CLA	C2D-C1D-ND	5.83	115.89	110.13
12	A	814	CLA	O2D-CGD-CBD	5.83	121.42	111.23
12	J	101	CLA	C2D-C1D-ND	5.82	115.89	110.13
12	B	801	CLA	C2C-C1C-NC	5.82	116.09	109.98
12	B	801	CLA	CMD-C2D-C1D	5.82	134.97	124.73
12	B	819	CLA	O2D-CGD-CBD	5.82	121.40	111.23
12	B	827	CLA	C2D-C1D-ND	5.81	115.88	110.13
12	A	841	CLA	C2D-C1D-ND	5.81	115.88	110.13
12	B	821	CLA	C2B-C1B-NB	5.81	116.35	110.33
12	B	805	CLA	C2D-C1D-ND	5.81	115.88	110.13
12	B	807	CLA	CHD-C4C-C3C	-5.81	116.30	124.77
12	A	817	CLA	CHD-C4C-C3C	-5.81	116.31	124.77
12	B	809	CLA	O2D-CGD-CBD	5.80	121.38	111.23
12	A	809	CLA	CHD-C4C-C3C	-5.80	116.32	124.77
12	A	830	CLA	CMD-C2D-C1D	5.78	134.90	124.73
12	A	828	CLA	C2D-C1D-ND	5.76	115.83	110.13
12	B	803	CLA	C2D-C1D-ND	5.75	115.82	110.13
12	B	817	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
12	A	820	CLA	O2D-CGD-CBD	5.75	121.28	111.23
12	A	818	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
12	A	810	CLA	C2D-C1D-ND	5.73	115.80	110.13
12	A	834	CLA	C2D-C1D-ND	5.72	115.79	110.13
12	A	836	CLA	C2D-C1D-ND	5.72	115.79	110.13
12	A	821	CLA	CHD-C4C-C3C	-5.72	116.43	124.77
12	A	829	CLA	C2D-C1D-ND	5.72	115.78	110.13
12	A	832	CLA	C2D-C1D-ND	5.71	115.78	110.13
12	B	822	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
12	A	814	CLA	C2D-C1D-ND	5.70	115.77	110.13
12	B	824	CLA	C2B-C1B-NB	5.70	116.24	110.33
12	B	804	CLA	C2B-C1B-NB	5.70	116.24	110.33
12	B	818	CLA	CHD-C4C-C3C	-5.70	116.47	124.77
12	A	818	CLA	C2D-C1D-ND	5.69	115.76	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	805	CLA	O2D-CGD-CBD	5.67	121.15	111.23
12	A	832	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
12	A	804	CLA	C2B-C1B-NB	5.67	116.20	110.33
12	A	840	CLA	CHD-C4C-C3C	-5.67	116.51	124.77
12	A	838	CLA	C2D-C1D-ND	5.66	115.73	110.13
12	A	816	CLA	C2D-C1D-ND	5.66	115.73	110.13
12	A	813	CLA	C2D-C1D-ND	5.66	115.73	110.13
12	A	833	CLA	CHD-C4C-C3C	-5.66	116.53	124.77
12	A	841	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
12	A	802	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
12	A	813	CLA	CHD-C4C-C3C	-5.65	116.53	124.77
12	A	823	CLA	C2B-C1B-NB	5.64	116.18	110.33
12	A	809	CLA	C2D-C1D-ND	5.64	115.71	110.13
12	A	808	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
12	A	822	CLA	CHD-C4C-C3C	-5.64	116.55	124.77
12	A	806	CLA	O2D-CGD-CBD	5.63	121.08	111.23
12	B	822	CLA	CMD-C2D-C1D	5.63	134.64	124.73
12	B	802	CLA	C2D-C1D-ND	5.63	115.70	110.13
12	B	820	CLA	C4A-NA-C1A	-5.62	104.11	106.68
12	A	830	CLA	C2D-C1D-ND	5.62	115.69	110.13
12	A	821	CLA	C2D-C1D-ND	5.62	115.68	110.13
12	J	101	CLA	CHD-C4C-C3C	-5.62	116.58	124.77
12	B	823	CLA	C4A-NA-C1A	-5.61	104.12	106.68
12	L	202	CLA	CHD-C4C-C3C	-5.61	116.59	124.77
12	B	820	CLA	O2D-CGD-CBD	5.61	121.04	111.23
12	B	825	CLA	O2D-CGD-CBD	5.61	121.04	111.23
12	A	837	CLA	C3B-C2B-C1B	-5.60	100.57	107.17
12	B	815	CLA	C2D-C1D-ND	5.59	115.66	110.13
12	B	812	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
12	A	843	CLA	O2D-CGD-CBD	5.58	120.98	111.23
12	L	204	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
12	A	826	CLA	CHD-C4C-C3C	-5.57	116.64	124.77
12	A	843	CLA	CHD-C4C-C3C	-5.57	116.65	124.77
12	B	804	CLA	C3B-C2B-C1B	-5.57	100.61	107.17
12	A	805	CLA	C2B-C1B-NB	5.57	116.10	110.33
12	A	835	CLA	CHD-C4C-C3C	-5.56	116.67	124.77
12	B	805	CLA	C3B-C2B-C1B	-5.56	100.61	107.17
12	B	812	CLA	C2D-C1D-ND	5.56	115.63	110.13
12	A	818	CLA	C2B-C1B-NB	5.56	116.09	110.33
12	A	834	CLA	C2B-C1B-NB	5.56	116.09	110.33
12	B	816	CLA	C2B-C1B-NB	5.55	116.08	110.33
12	B	818	CLA	C2D-C1D-ND	5.55	115.62	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	814	CLA	C2B-C1B-NB	5.55	116.08	110.33
12	B	828	CLA	C4A-NA-C1A	-5.55	104.15	106.68
11	A	801	CL0	CBC-CAC-C3C	-5.54	104.94	112.87
12	A	842	CLA	CHD-C4C-C3C	-5.54	116.69	124.77
12	B	803	CLA	CMD-C2D-C1D	5.53	134.47	124.73
12	B	817	CLA	C2B-C1B-NB	5.52	116.05	110.33
12	A	810	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
12	A	833	CLA	C2D-C1D-ND	5.52	115.59	110.13
12	B	805	CLA	C2B-C1B-NB	5.52	116.05	110.33
12	B	814	CLA	C2D-C1D-ND	5.51	115.58	110.13
12	B	825	CLA	CHD-C4C-C3C	-5.51	116.74	124.77
12	B	819	CLA	C3B-C2B-C1B	-5.51	100.67	107.17
12	B	810	CLA	C2C-C1C-NC	5.51	115.77	109.98
12	B	813	CLA	C2B-C1B-NB	5.51	116.03	110.33
12	A	823	CLA	C2D-C1D-ND	5.50	115.57	110.13
12	B	805	CLA	O2D-CGD-CBD	5.50	120.85	111.23
12	B	802	CLA	CHD-C4C-C3C	-5.50	116.76	124.77
12	A	805	CLA	C2D-C1D-ND	5.49	115.56	110.13
12	A	808	CLA	C2B-C1B-NB	5.48	116.01	110.33
12	B	826	CLA	C2D-C1D-ND	5.48	115.55	110.13
12	B	817	CLA	C4A-NA-C1A	-5.47	104.18	106.68
12	A	824	CLA	O2D-CGD-CBD	5.47	120.79	111.23
12	A	822	CLA	O2D-CGD-CBD	5.47	120.79	111.23
12	A	823	CLA	C2C-C1C-NC	5.47	115.72	109.98
12	B	808	CLA	O2D-CGD-CBD	5.46	120.78	111.23
12	A	807	CLA	C2D-C1D-ND	5.46	115.53	110.13
12	B	816	CLA	CHD-C4C-C3C	-5.45	116.82	124.77
12	A	815	CLA	CHD-C4C-C3C	-5.45	116.83	124.77
12	A	805	CLA	CHD-C4C-C3C	-5.45	116.83	124.77
12	A	812	CLA	C2D-C1D-ND	5.45	115.52	110.13
12	B	829	CLA	CHD-C4C-C3C	-5.45	116.83	124.77
12	B	831	CLA	C2D-C1D-ND	5.45	115.52	110.13
12	B	821	CLA	C3B-C2B-C1B	-5.44	100.75	107.17
12	B	813	CLA	C2D-C1D-ND	5.44	115.51	110.13
12	A	820	CLA	C2C-C1C-NC	5.44	115.69	109.98
12	A	826	CLA	C2B-C1B-NB	5.43	115.96	110.33
12	B	830	CLA	CHD-C4C-C3C	-5.43	116.86	124.77
12	B	826	CLA	C2B-C1B-NB	5.43	115.95	110.33
12	A	814	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
12	B	818	CLA	C4A-NA-C1A	-5.42	104.21	106.68
12	A	836	CLA	CHD-C4C-C3C	-5.42	116.88	124.77
12	A	839	CLA	C2B-C1B-NB	5.42	115.94	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	803	CLA	CHD-C4C-C3C	-5.41	116.88	124.77
12	L	202	CLA	C2B-C1B-NB	5.41	115.94	110.33
12	A	831	CLA	C2D-C1D-ND	5.41	115.48	110.13
12	A	824	CLA	C2B-C1B-NB	5.41	115.93	110.33
12	B	803	CLA	CMB-C2B-C1B	5.41	133.65	125.42
12	A	826	CLA	C3B-C2B-C1B	-5.40	100.80	107.17
12	B	827	CLA	CHD-C4C-C3C	-5.40	116.90	124.77
12	A	824	CLA	C2D-C1D-ND	5.40	115.47	110.13
12	A	840	CLA	C2B-C1B-NB	5.40	115.92	110.33
12	A	834	CLA	C3B-C2B-C1B	-5.39	100.81	107.17
12	B	801	CLA	C2B-C1B-NB	5.39	115.91	110.33
12	J	101	CLA	C2B-C1B-NB	5.38	115.91	110.33
12	F	203	CLA	C2B-C1B-NB	5.38	115.91	110.33
12	B	822	CLA	C2D-C1D-ND	5.38	115.45	110.13
12	B	819	CLA	C4A-NA-C1A	-5.38	104.23	106.68
12	A	823	CLA	CHD-C4C-C3C	-5.38	116.94	124.77
12	B	806	CLA	C2C-C1C-NC	5.38	115.63	109.98
12	B	815	CLA	C2B-C1B-NB	5.37	115.90	110.33
12	B	801	CLA	CHD-C4C-C3C	-5.37	116.94	124.77
12	B	825	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
12	A	831	CLA	CHD-C4C-C3C	-5.37	116.95	124.77
12	B	824	CLA	CHD-C4C-C3C	-5.36	116.95	124.77
12	A	826	CLA	C4A-NA-C1A	-5.36	104.23	106.68
12	A	813	CLA	C2B-C1B-NB	5.36	115.89	110.33
12	A	832	CLA	O2D-CGD-CBD	5.36	120.60	111.23
12	L	203	CLA	CHD-C4C-C3C	-5.35	116.97	124.77
12	A	834	CLA	CHD-C4C-C3C	-5.34	116.98	124.77
12	B	822	CLA	C2B-C1B-NB	5.34	115.86	110.33
12	B	810	CLA	C2D-C1D-ND	5.34	115.41	110.13
12	A	803	CLA	C2D-C1D-ND	5.34	115.41	110.13
12	B	827	CLA	C2B-C1B-NB	5.33	115.85	110.33
12	L	204	CLA	C2B-C1B-NB	5.33	115.85	110.33
12	A	828	CLA	C3B-C2B-C1B	-5.33	100.89	107.17
12	B	813	CLA	CHD-C4C-C3C	-5.33	117.01	124.77
12	J	101	CLA	O2D-CGD-CBD	5.32	120.54	111.23
12	A	838	CLA	CHD-C4C-C3C	-5.32	117.02	124.77
12	B	832	CLA	C2D-C1D-ND	5.32	115.39	110.13
12	B	827	CLA	O2D-CGD-CBD	5.32	120.52	111.23
12	B	819	CLA	C2D-C1D-ND	5.31	115.38	110.13
12	B	831	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
12	A	829	CLA	C2B-C1B-NB	5.31	115.83	110.33
12	B	813	CLA	C3B-C2B-C1B	-5.31	100.91	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	803	CLA	C2B-C1B-NB	5.31	115.83	110.33
12	B	802	CLA	CMD-C2D-C1D	5.30	134.06	124.73
12	A	811	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
12	B	818	CLA	C2C-C1C-NC	5.30	115.55	109.98
12	B	816	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	B	824	CLA	C3B-C2B-C1B	-5.30	100.92	107.17
12	A	836	CLA	C2B-C1B-NB	5.30	115.82	110.33
12	B	823	CLA	C2C-C1C-NC	5.30	115.55	109.98
12	A	837	CLA	CHD-C4C-C3C	-5.30	117.05	124.77
12	A	815	CLA	C2B-C1B-NB	5.29	115.82	110.33
12	B	830	CLA	C2B-C1B-NB	5.29	115.81	110.33
12	A	802	CLA	C3B-C2B-C1B	-5.29	100.94	107.17
12	B	828	CLA	C2B-C1B-NB	5.28	115.81	110.33
12	A	843	CLA	C2B-C1B-NB	5.28	115.80	110.33
12	A	830	CLA	C2C-C1C-NC	5.28	115.53	109.98
12	B	825	CLA	C2B-C1B-NB	5.28	115.80	110.33
12	L	204	CLA	O2D-CGD-CBD	5.28	120.46	111.23
12	A	807	CLA	C2B-C1B-NB	5.27	115.80	110.33
12	B	816	CLA	C2C-C1C-NC	5.27	115.52	109.98
12	B	801	CLA	C2D-C1D-ND	5.27	115.34	110.13
12	A	812	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
12	B	828	CLA	O2D-CGD-CBD	5.27	120.44	111.23
11	A	801	CL0	CMA-C3A-C4A	-5.27	103.27	114.61
12	B	815	CLA	CHD-C4C-C3C	-5.25	117.11	124.77
12	F	203	CLA	C2C-C1C-NC	5.25	115.50	109.98
12	A	817	CLA	C2B-C1B-NB	5.25	115.77	110.33
12	B	814	CLA	C2B-C1B-NB	5.25	115.77	110.33
12	A	805	CLA	C3B-C2B-C1B	-5.24	101.00	107.17
12	B	806	CLA	CHD-C4C-C3C	-5.24	117.14	124.77
12	A	819	CLA	C2D-C1D-ND	5.23	115.31	110.13
12	A	816	CLA	CHD-C4C-C3C	-5.23	117.14	124.77
12	A	816	CLA	C2C-C1C-NC	5.23	115.48	109.98
12	A	826	CLA	C2D-C1D-ND	5.23	115.30	110.13
12	A	835	CLA	C2C-C1C-NC	5.23	115.47	109.98
12	A	811	CLA	C2B-C1B-NB	5.23	115.75	110.33
12	B	807	CLA	O2D-CGD-CBD	5.23	120.36	111.23
12	A	825	CLA	CMD-C2D-C1D	5.23	133.93	124.73
12	A	820	CLA	C2D-C1D-ND	5.22	115.29	110.13
12	A	830	CLA	CHD-C4C-C3C	-5.22	117.16	124.77
12	F	203	CLA	C2D-C1D-ND	5.22	115.29	110.13
12	B	824	CLA	C4A-NA-C1A	-5.21	104.30	106.68
12	A	841	CLA	C2B-C1B-NB	5.21	115.73	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	829	CLA	CMD-C2D-C1D	5.21	133.90	124.73
12	A	812	CLA	C2B-C1B-NB	5.21	115.72	110.33
12	A	810	CLA	C2C-C1C-NC	5.21	115.45	109.98
12	A	807	CLA	CHD-C4C-C3C	-5.20	117.19	124.77
12	A	837	CLA	C2C-C1C-NC	5.20	115.44	109.98
12	L	204	CLA	C3B-C2B-C1B	-5.19	101.05	107.17
12	A	828	CLA	O2D-CGD-CBD	5.19	120.31	111.23
12	A	821	CLA	O2D-CGD-CBD	5.19	120.30	111.23
12	A	841	CLA	C3B-C2B-C1B	-5.19	101.06	107.17
12	B	826	CLA	CHD-C4C-C3C	-5.18	117.21	124.77
12	B	801	CLA	O2D-CGD-CBD	5.17	120.27	111.23
12	B	801	CLA	C3B-C2B-C1B	-5.17	101.08	107.17
12	A	827	CLA	C2B-C1B-NB	5.16	115.68	110.33
12	A	824	CLA	C3B-C2B-C1B	-5.16	101.09	107.17
12	B	813	CLA	C4A-NA-C1A	-5.15	104.33	106.68
12	A	838	CLA	C2B-C1B-NB	5.15	115.67	110.33
12	B	831	CLA	C2B-C1B-NB	5.14	115.66	110.33
12	B	814	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
12	A	804	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
12	B	806	CLA	C3B-C2B-C1B	-5.13	101.12	107.17
12	B	811	CLA	C2C-C1C-NC	5.13	115.37	109.98
12	B	806	CLA	O2D-CGD-CBD	5.12	120.18	111.23
12	A	833	CLA	C3B-C2B-C1B	-5.12	101.14	107.17
12	B	827	CLA	C2C-C1C-NC	5.12	115.36	109.98
12	B	812	CLA	O2D-CGD-CBD	5.11	120.17	111.23
12	B	820	CLA	C3D-C2D-C1D	-5.11	98.86	105.83
12	A	821	CLA	C2B-C1B-NB	5.11	115.62	110.33
12	A	819	CLA	CHD-C4C-C3C	-5.11	117.33	124.77
12	A	813	CLA	C3B-C2B-C1B	-5.10	101.15	107.17
12	A	834	CLA	C2C-C1C-NC	5.10	115.34	109.98
12	B	808	CLA	C2C-C1C-NC	5.10	115.34	109.98
12	B	819	CLA	CHD-C4C-C3C	-5.10	117.34	124.77
12	B	803	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
12	B	807	CLA	C2B-C1B-NB	5.09	115.60	110.33
12	A	806	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
12	B	830	CLA	O2D-CGD-CBD	5.08	120.12	111.23
12	L	202	CLA	O2D-CGD-CBD	5.08	120.11	111.23
12	A	817	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
12	A	824	CLA	CHD-C4C-C3C	-5.07	117.38	124.77
12	A	832	CLA	C2B-C1B-NB	5.07	115.58	110.33
12	A	820	CLA	CHD-C4C-C3C	-5.07	117.38	124.77
12	A	825	CLA	C2B-C1B-NB	5.07	115.58	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	804	CLA	CAC-C3C-C4C	5.07	131.38	124.79
12	B	814	CLA	O2D-CGD-CBD	5.07	120.08	111.23
12	B	816	CLA	O2D-CGD-CBD	5.06	120.08	111.23
12	B	807	CLA	C2C-C1C-NC	5.06	115.30	109.98
12	A	854	CLA	C4A-NA-C1A	-5.06	104.37	106.68
12	F	203	CLA	C4A-NA-C1A	-5.05	104.38	106.68
12	L	203	CLA	O2D-CGD-CBD	5.05	120.05	111.23
12	B	829	CLA	C3D-C2D-C1D	-5.04	98.95	105.83
12	B	811	CLA	CHD-C4C-C3C	-5.04	117.42	124.77
12	A	819	CLA	C2B-C1B-NB	5.04	115.56	110.33
12	A	840	CLA	CMD-C2D-C1D	5.04	133.60	124.73
12	F	203	CLA	O2D-CGD-CBD	5.04	120.04	111.23
12	A	835	CLA	C2B-C1B-NB	5.03	115.55	110.33
12	F	203	CLA	C3B-C2B-C1B	-5.03	101.24	107.17
12	A	841	CLA	C4A-NA-C1A	-5.03	104.38	106.68
12	A	808	CLA	O2D-CGD-CBD	5.03	120.03	111.23
12	B	825	CLA	C4A-NA-C1A	-5.03	104.38	106.68
12	F	203	CLA	CHD-C4C-C3C	-5.03	117.44	124.77
12	B	826	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
12	A	815	CLA	C3B-C2B-C1B	-5.01	101.27	107.17
12	A	836	CLA	C2C-C1C-NC	5.01	115.24	109.98
12	A	833	CLA	C2C-C1C-NC	5.01	115.24	109.98
12	B	808	CLA	C3D-C2D-C1D	-5.00	99.01	105.83
12	A	807	CLA	C3B-C2B-C1B	-5.00	101.28	107.17
12	A	812	CLA	O2D-CGD-CBD	4.99	119.96	111.23
12	B	831	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
12	A	833	CLA	C2B-C1B-NB	4.99	115.50	110.33
12	A	811	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
12	A	842	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
12	B	815	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
12	A	819	CLA	C2C-C1C-NC	4.99	115.22	109.98
12	B	815	CLA	C2C-C1C-NC	4.99	115.22	109.98
12	A	810	CLA	C2B-C1B-NB	4.98	115.49	110.33
12	A	825	CLA	C3B-C2B-C1B	-4.98	101.30	107.17
12	A	843	CLA	C2C-C1C-NC	4.98	115.21	109.98
12	B	830	CLA	C2C-C1C-NC	4.98	115.21	109.98
12	B	830	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
12	A	827	CLA	C3D-C2D-C1D	-4.97	99.04	105.83
12	A	806	CLA	C3D-C2D-C1D	-4.97	99.05	105.83
12	A	822	CLA	C2C-C1C-NC	4.97	115.20	109.98
12	A	829	CLA	C4A-NA-C1A	-4.97	104.41	106.68
12	A	820	CLA	C2B-C1B-NB	4.97	115.48	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	819	CLA	C4A-NA-C1A	-4.96	104.42	106.68
12	A	824	CLA	C2C-C1C-NC	4.96	115.19	109.98
12	L	203	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
12	A	811	CLA	C2C-C1C-NC	4.95	115.18	109.98
12	A	839	CLA	C2C-C1C-NC	4.95	115.18	109.98
12	B	822	CLA	C4A-NA-C1A	-4.95	104.42	106.68
12	B	831	CLA	C2C-C1C-NC	4.95	115.18	109.98
12	B	820	CLA	C2B-C1B-NB	4.95	115.45	110.33
12	B	806	CLA	C2B-C1B-NB	4.94	115.45	110.33
12	A	837	CLA	C2D-C1D-ND	4.94	115.02	110.13
12	A	854	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
12	A	840	CLA	C3B-C2B-C1B	-4.94	101.34	107.17
12	A	832	CLA	C4A-NA-C1A	-4.94	104.42	106.68
12	A	842	CLA	C2B-C1B-NB	4.94	115.45	110.33
12	A	841	CLA	O2D-CGD-CBD	4.94	119.86	111.23
12	A	825	CLA	C2C-C1C-NC	4.94	115.17	109.98
12	B	820	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
12	A	842	CLA	O2D-CGD-CBD	4.93	119.86	111.23
12	B	812	CLA	C2B-C1B-NB	4.93	115.44	110.33
12	B	819	CLA	CAA-C2A-C3A	-4.93	99.67	113.00
12	B	821	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
12	B	831	CLA	C4A-NA-C1A	-4.93	104.43	106.68
12	L	202	CLA	C2C-C1C-NC	4.92	115.15	109.98
12	B	810	CLA	CHD-C4C-C3C	-4.92	117.59	124.77
12	A	802	CLA	CMD-C2D-C1D	4.92	133.40	124.73
12	A	808	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
12	A	839	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
12	A	815	CLA	O2D-CGD-CBD	4.92	119.83	111.23
12	B	817	CLA	C3B-C2B-C1B	-4.92	101.37	107.17
12	B	822	CLA	C2C-C1C-NC	4.91	115.14	109.98
11	A	801	CL0	CHA-C1A-C2A	-4.90	121.79	133.31
12	B	822	CLA	C3B-C2B-C1B	-4.90	101.39	107.17
12	A	807	CLA	C2C-C1C-NC	4.90	115.12	109.98
12	L	202	CLA	C3B-C2B-C1B	-4.89	101.40	107.17
12	B	811	CLA	C2B-C1B-NB	4.89	115.40	110.33
12	L	203	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
12	A	809	CLA	C2C-C1C-NC	4.89	115.12	109.98
12	A	806	CLA	C2B-C1B-NB	4.88	115.39	110.33
12	B	828	CLA	C3B-C2B-C1B	-4.88	101.42	107.17
12	B	817	CLA	O2D-CGD-CBD	4.88	119.76	111.23
12	A	815	CLA	C2C-C1C-NC	4.88	115.10	109.98
12	B	804	CLA	C3D-C2D-C1D	-4.87	99.18	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	813	CLA	C4A-NA-C1A	-4.87	104.46	106.68
12	A	817	CLA	C2C-C1C-NC	4.87	115.10	109.98
12	A	807	CLA	C4A-NA-C1A	-4.87	104.46	106.68
12	A	816	CLA	C2B-C1B-NB	4.87	115.37	110.33
12	A	831	CLA	C2C-C1C-NC	4.87	115.09	109.98
12	B	832	CLA	CHD-C4C-C3C	-4.86	117.68	124.77
12	A	831	CLA	C2B-C1B-NB	4.86	115.37	110.33
12	J	101	CLA	C3B-C2B-C1B	-4.86	101.44	107.17
12	A	804	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
12	A	812	CLA	C2C-C1C-NC	4.85	115.08	109.98
12	B	802	CLA	C2B-C1B-NB	4.85	115.36	110.33
12	B	811	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
12	A	823	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
12	A	811	CLA	O2D-CGD-CBD	4.85	119.70	111.23
12	B	818	CLA	O2D-CGD-CBD	4.84	119.70	111.23
12	A	854	CLA	C2C-C1C-NC	4.84	115.07	109.98
12	B	826	CLA	C2C-C1C-NC	4.84	115.07	109.98
12	A	821	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
12	B	821	CLA	O2D-CGD-CBD	4.84	119.69	111.23
12	A	837	CLA	C2B-C1B-NB	4.83	115.34	110.33
12	B	824	CLA	O2D-CGD-CBD	4.83	119.67	111.23
12	L	203	CLA	C2B-C1B-NB	4.82	115.33	110.33
12	B	825	CLA	CHD-C1D-ND	-4.82	118.02	124.80
12	A	835	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
12	A	831	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
12	A	812	CLA	C3B-C2B-C1B	-4.82	101.49	107.17
12	B	818	CLA	C2B-C1B-NB	4.82	115.32	110.33
12	B	817	CLA	C3D-C2D-C1D	-4.81	99.27	105.83
12	B	828	CLA	C3D-C2D-C1D	-4.80	99.28	105.83
12	A	806	CLA	CAA-C2A-C3A	-4.80	100.03	113.00
12	B	829	CLA	C2B-C1B-NB	4.80	115.30	110.33
12	L	204	CLA	C4A-NA-C1A	-4.80	104.49	106.68
12	A	806	CLA	C2C-C1C-NC	4.79	115.02	109.98
12	B	812	CLA	C4A-NA-C1A	-4.79	104.49	106.68
12	A	842	CLA	C2C-C1C-NC	4.79	115.01	109.98
12	A	820	CLA	C3B-C2B-C1B	-4.78	101.53	107.17
12	A	809	CLA	C2B-C1B-NB	4.78	115.29	110.33
12	A	838	CLA	C3B-C2B-C1B	-4.78	101.54	107.17
12	A	829	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
12	A	837	CLA	C4A-NA-C1A	-4.77	104.50	106.68
12	B	807	CLA	C3D-C2D-C1D	-4.77	99.32	105.83
12	A	808	CLA	C3D-C2D-C1D	-4.76	99.33	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	854	CLA	C2B-C1B-NB	4.76	115.27	110.33
12	L	202	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
12	B	811	CLA	C2D-C1D-ND	4.76	114.84	110.13
12	A	840	CLA	C2C-C1C-NC	4.76	114.98	109.98
12	B	824	CLA	C3D-C2D-C1D	-4.76	99.34	105.83
12	B	821	CLA	C4A-NA-C1A	-4.75	104.51	106.68
12	A	827	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
12	A	843	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
12	L	203	CLA	C2C-C1C-NC	4.74	114.96	109.98
12	A	802	CLA	O2D-CGD-CBD	4.72	119.49	111.23
12	A	813	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
12	B	829	CLA	C3B-C2B-C1B	-4.72	101.60	107.17
12	A	810	CLA	O2D-CGD-CBD	4.72	119.47	111.23
12	A	823	CLA	C4A-NA-C1A	-4.71	104.53	106.68
12	B	812	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
12	A	818	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
12	B	802	CLA	O2D-CGD-CBD	4.71	119.47	111.23
12	A	803	CLA	C3B-C2B-C1B	-4.71	101.61	107.17
12	A	834	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
12	J	101	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
12	B	803	CLA	C1D-CHD-C4C	-4.71	116.01	126.02
12	L	204	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
12	B	827	CLA	C3B-C2B-C1B	-4.70	101.62	107.17
12	B	807	CLA	C3B-C2B-C1B	-4.70	101.63	107.17
12	B	805	CLA	C2C-C1C-NC	4.69	114.91	109.98
12	B	806	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
12	B	809	CLA	C2C-C1C-NC	4.69	114.91	109.98
12	B	830	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
12	B	804	CLA	CMD-C2D-C1D	4.68	132.97	124.73
12	A	829	CLA	C2C-C1C-NC	4.68	114.90	109.98
12	A	841	CLA	C3D-C2D-C1D	-4.68	99.45	105.83
12	A	838	CLA	C2C-C1C-NC	4.67	114.89	109.98
12	A	843	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
12	A	822	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
12	A	817	CLA	O2D-CGD-CBD	4.67	119.39	111.23
12	A	841	CLA	C2C-C1C-NC	4.67	114.88	109.98
12	B	809	CLA	C2B-C1B-NB	4.67	115.17	110.33
12	B	801	CLA	CAA-C2A-C3A	-4.66	100.40	113.00
12	A	810	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
12	B	829	CLA	O2D-CGD-CBD	4.66	119.37	111.23
12	A	802	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
12	A	809	CLA	C3B-C2B-C1B	-4.65	101.69	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	806	CLA	CAC-C3C-C4C	4.65	130.84	124.79
12	A	814	CLA	C3D-C2D-C1D	-4.65	99.49	105.83
12	B	812	CLA	C2C-C1C-NC	4.65	114.86	109.98
12	A	807	CLA	O2D-CGD-CBD	4.64	119.35	111.23
12	B	818	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
12	A	822	CLA	C2B-C1B-NB	4.64	115.14	110.33
12	A	835	CLA	C4A-NA-C1A	-4.64	104.56	106.68
12	A	818	CLA	O2D-CGD-CBD	4.64	119.34	111.23
12	B	816	CLA	C3D-C2D-C1D	-4.64	99.50	105.83
12	A	815	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
12	A	818	CLA	C3D-C2D-C1D	-4.63	99.51	105.83
12	A	840	CLA	C4A-NA-C1A	-4.63	104.57	106.68
12	A	832	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
12	B	803	CLA	C2C-C1C-NC	4.62	114.84	109.98
12	A	819	CLA	O2D-CGD-CBD	4.62	119.31	111.23
12	B	832	CLA	C1C-C2C-C3C	-4.62	102.12	106.98
12	A	808	CLA	C2C-C1C-NC	4.62	114.84	109.98
12	A	838	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
12	B	809	CLA	C3D-C2D-C1D	-4.62	99.53	105.83
12	A	811	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
12	A	828	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
12	A	854	CLA	C3D-C2D-C1D	-4.61	99.54	105.83
12	B	828	CLA	C2C-C1C-NC	4.61	114.82	109.98
12	B	801	CLA	C3B-C4B-NB	4.60	114.64	110.53
12	A	828	CLA	C2C-C1C-NC	4.60	114.81	109.98
12	B	815	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
12	A	836	CLA	C3D-C2D-C1D	-4.59	99.56	105.83
12	A	803	CLA	C2C-C1C-NC	4.59	114.80	109.98
12	A	833	CLA	C4A-NA-C1A	-4.59	104.58	106.68
12	A	823	CLA	O2D-CGD-CBD	4.59	119.25	111.23
12	A	832	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
12	B	809	CLA	C1D-CHD-C4C	-4.58	116.29	126.02
12	B	825	CLA	C3B-C2B-C1B	-4.58	101.78	107.17
12	A	826	CLA	CAA-C2A-C3A	-4.57	100.64	113.00
12	A	830	CLA	C4A-NA-C1A	-4.57	104.59	106.68
12	B	802	CLA	C2C-C1C-NC	4.57	114.78	109.98
12	A	817	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
12	B	816	CLA	C3B-C4B-NB	4.57	114.61	110.53
12	A	810	CLA	C3D-C2D-C1D	-4.57	99.59	105.83
12	A	839	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
12	A	818	CLA	C4A-NA-C1A	-4.56	104.60	106.68
12	A	827	CLA	C4A-NA-C1A	-4.56	104.60	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	806	CLA	C3B-C4B-NB	4.56	114.60	110.53
12	B	819	CLA	CHD-C1D-ND	-4.56	118.39	124.80
12	B	805	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
12	A	803	CLA	C4A-NA-C1A	-4.54	104.61	106.68
12	A	816	CLA	C3D-C2D-C1D	-4.54	99.64	105.83
12	B	823	CLA	C2B-C1B-NB	4.53	115.03	110.33
12	L	203	CLA	C3D-C4D-ND	4.53	117.35	109.99
12	A	832	CLA	C2C-C1C-NC	4.53	114.74	109.98
12	B	825	CLA	C3D-C4D-ND	4.53	117.35	109.99
12	B	829	CLA	CHD-C1D-ND	-4.52	118.44	124.80
12	B	829	CLA	C2C-C1C-NC	4.52	114.73	109.98
12	A	817	CLA	C3D-C4D-ND	4.52	117.33	109.99
12	A	824	CLA	C4A-NA-C1A	-4.51	104.62	106.68
12	A	822	CLA	C3D-C4D-ND	4.51	117.31	109.99
12	A	807	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
12	B	824	CLA	CHD-C1D-ND	-4.50	118.47	124.80
12	A	842	CLA	C3D-C2D-C1D	-4.50	99.69	105.83
12	A	854	CLA	C3C-C4C-NC	4.49	116.19	110.43
12	L	204	CLA	C3D-C4D-ND	4.49	117.29	109.99
12	J	101	CLA	C2C-C1C-NC	4.49	114.70	109.98
12	B	826	CLA	C4A-NA-C1A	-4.49	104.63	106.68
12	A	830	CLA	C2B-C1B-NB	4.49	114.98	110.33
12	B	827	CLA	C3D-C2D-C1D	-4.48	99.71	105.83
12	B	819	CLA	C3D-C4D-ND	4.48	117.28	109.99
12	A	840	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
12	B	831	CLA	O2D-CGD-CBD	4.48	119.06	111.23
12	A	816	CLA	O2D-CGD-CBD	4.48	119.06	111.23
12	A	820	CLA	C3D-C2D-C1D	-4.47	99.73	105.83
12	B	824	CLA	C3D-C4D-ND	4.47	117.25	109.99
12	B	813	CLA	C3D-C2D-C1D	-4.47	99.74	105.83
12	A	833	CLA	C3D-C2D-C1D	-4.46	99.74	105.83
12	L	203	CLA	CHD-C1D-ND	-4.46	118.52	124.80
12	A	829	CLA	O2D-CGD-CBD	4.46	119.03	111.23
12	A	804	CLA	C4A-NA-C1A	-4.46	104.64	106.68
12	A	832	CLA	C3D-C4D-ND	4.46	117.24	109.99
12	A	826	CLA	O2D-CGD-CBD	4.46	119.02	111.23
12	B	809	CLA	C3B-C2B-C1B	-4.45	101.92	107.17
12	A	830	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
12	A	812	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
12	B	824	CLA	C2C-C1C-NC	4.45	114.66	109.98
12	A	835	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
12	B	831	CLA	C3D-C4D-ND	4.45	117.21	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	A	801	CL0	CAA-C2A-C3A	-4.45	100.99	113.00
12	B	814	CLA	C2C-C1C-NC	4.44	114.65	109.98
12	A	822	CLA	C3B-C2B-C1B	-4.44	101.94	107.17
12	A	821	CLA	C3D-C4D-ND	4.44	117.20	109.99
12	A	821	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
12	B	810	CLA	O2D-CGD-CBD	4.44	118.99	111.23
12	B	825	CLA	C2C-C1C-NC	4.43	114.64	109.98
12	F	203	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
12	A	836	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
12	A	803	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
12	B	812	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
12	B	832	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
12	A	835	CLA	C3D-C4D-ND	4.42	117.17	109.99
12	B	807	CLA	C1C-C2C-C3C	-4.42	102.33	106.98
12	B	827	CLA	C3D-C4D-ND	4.42	117.17	109.99
12	B	823	CLA	CHD-C4C-C3C	-4.41	118.34	124.77
12	B	831	CLA	CHD-C1D-ND	-4.41	118.60	124.80
12	A	818	CLA	C2C-C1C-NC	4.41	114.61	109.98
12	A	826	CLA	CHD-C1D-ND	-4.41	118.60	124.80
12	A	819	CLA	C3B-C2B-C1B	-4.40	101.98	107.17
12	A	835	CLA	O2D-CGD-CBD	4.40	118.93	111.23
12	A	805	CLA	C2C-C1C-NC	4.40	114.60	109.98
12	A	805	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
12	A	817	CLA	C4A-NA-C1A	-4.40	104.67	106.68
16	A	852	LHG	O4-P-O5	4.40	132.90	112.44
12	A	824	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
12	B	808	CLA	C4A-NA-C1A	-4.39	104.67	106.68
12	B	830	CLA	C3D-C4D-ND	4.39	117.13	109.99
12	A	825	CLA	C4A-NA-C1A	-4.39	104.68	106.68
12	A	822	CLA	C1C-C2C-C3C	-4.39	102.37	106.98
12	B	816	CLA	C3D-C4D-ND	4.38	117.11	109.99
12	A	815	CLA	C3D-C4D-ND	4.38	117.11	109.99
12	A	823	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
12	L	204	CLA	CHD-C1D-ND	-4.38	118.64	124.80
12	B	817	CLA	C2C-C1C-NC	4.37	114.57	109.98
12	A	826	CLA	C3D-C4D-ND	4.37	117.09	109.99
12	B	826	CLA	C3D-C4D-ND	4.37	117.09	109.99
12	A	832	CLA	CAA-C2A-C3A	-4.37	101.20	113.00
12	A	813	CLA	O2D-CGD-CBD	4.37	118.86	111.23
12	B	810	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
12	A	819	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
12	A	811	CLA	C3D-C4D-ND	4.36	117.08	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	838	CLA	C4A-NA-C1A	-4.36	104.69	106.68
12	A	808	CLA	C4A-NA-C1A	-4.36	104.69	106.68
12	B	832	CLA	C3B-C4B-NB	4.36	114.42	110.53
12	A	827	CLA	C1D-CHD-C4C	-4.35	116.76	126.02
12	B	822	CLA	C3D-C4D-ND	4.35	117.06	109.99
12	B	831	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
12	B	821	CLA	CAC-C3C-C4C	4.34	130.44	124.79
12	A	837	CLA	C3D-C2D-C1D	-4.34	99.90	105.83
12	B	812	CLA	C3D-C4D-ND	4.34	117.04	109.99
12	B	801	CLA	C1C-C2C-C3C	-4.34	102.42	106.98
12	B	802	CLA	C3B-C2B-C1B	-4.33	102.06	107.17
12	B	821	CLA	C2C-C1C-NC	4.33	114.53	109.98
12	A	826	CLA	C2C-C1C-NC	4.33	114.53	109.98
12	A	810	CLA	C4A-NA-C1A	-4.33	104.70	106.68
12	A	821	CLA	C4A-NA-C1A	-4.32	104.71	106.68
12	B	830	CLA	C4A-NA-C1A	-4.32	104.71	106.68
12	B	803	CLA	C4-C3-C5	4.32	122.72	115.23
12	A	814	CLA	C2C-C1C-NC	4.31	114.51	109.98
12	A	817	CLA	CHD-C1D-ND	-4.31	118.73	124.80
12	A	812	CLA	C4A-NA-C1A	-4.31	104.71	106.68
12	A	809	CLA	C1D-CHD-C4C	-4.31	116.86	126.02
12	A	809	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
12	A	811	CLA	CHD-C1D-ND	-4.31	118.74	124.80
12	A	841	CLA	C3D-C4D-ND	4.31	116.99	109.99
12	A	825	CLA	O2D-CGD-CBD	4.30	118.75	111.23
12	A	816	CLA	C3B-C2B-C1B	-4.30	102.10	107.17
16	A	853	LHG	O4-P-O5	4.30	132.46	112.44
12	B	813	CLA	C2C-C1C-NC	4.30	114.50	109.98
12	A	822	CLA	CHD-C1D-ND	-4.30	118.75	124.80
12	A	826	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
12	A	823	CLA	C3D-C4D-ND	4.29	116.97	109.99
12	A	802	CLA	C4A-NA-C1A	-4.29	104.72	106.68
12	A	828	CLA	C4A-NA-C1A	-4.29	104.72	106.68
12	A	806	CLA	C4A-NA-C1A	-4.29	104.72	106.68
12	B	813	CLA	CAC-C3C-C4C	4.29	130.37	124.79
12	A	841	CLA	CHD-C1D-ND	-4.29	118.77	124.80
12	B	803	CLA	C2B-C1B-NB	4.28	114.77	110.33
12	A	816	CLA	C3D-C4D-ND	4.28	116.95	109.99
12	B	814	CLA	C3D-C4D-ND	4.28	116.95	109.99
12	L	202	CLA	C3D-C4D-ND	4.28	116.95	109.99
12	B	819	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
12	A	805	CLA	C3D-C4D-ND	4.27	116.94	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	818	CLA	C1C-C2C-C3C	-4.27	102.49	106.98
12	B	802	CLA	C3D-C4D-ND	4.27	116.93	109.99
12	A	831	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
12	B	826	CLA	C3D-C2D-C1D	-4.27	100.00	105.83
12	B	815	CLA	C4A-NA-C1A	-4.27	104.73	106.68
12	A	811	CLA	C4A-NA-C1A	-4.26	104.73	106.68
12	A	831	CLA	C3D-C4D-ND	4.26	116.92	109.99
12	A	824	CLA	C3D-C4D-ND	4.26	116.91	109.99
12	B	832	CLA	C2B-C1B-NB	4.26	114.74	110.33
12	A	813	CLA	C2C-C1C-NC	4.26	114.45	109.98
12	L	204	CLA	C2C-C1C-NC	4.26	114.45	109.98
12	B	801	CLA	C3D-C2D-C1D	-4.26	100.02	105.83
12	B	816	CLA	CHD-C1D-ND	-4.26	118.81	124.80
12	B	802	CLA	C4A-NA-C1A	-4.25	104.74	106.68
12	F	203	CLA	CHD-C1D-ND	-4.25	118.81	124.80
12	A	806	CLA	C1D-CHD-C4C	-4.25	116.98	126.02
12	B	820	CLA	CAA-C2A-C3A	-4.25	101.51	113.00
12	A	825	CLA	C3D-C2D-C1D	-4.25	100.04	105.83
12	A	838	CLA	C3D-C4D-ND	4.25	116.89	109.99
12	A	807	CLA	C3D-C4D-ND	4.24	116.88	109.99
12	A	827	CLA	C2C-C1C-NC	4.24	114.44	109.98
12	A	834	CLA	C3D-C4D-ND	4.24	116.87	109.99
12	A	809	CLA	C3D-C4D-ND	4.23	116.87	109.99
12	A	824	CLA	CHD-C1D-ND	-4.23	118.84	124.80
12	A	833	CLA	C3D-C4D-ND	4.23	116.86	109.99
12	B	801	CLA	C3D-C4D-ND	4.23	116.86	109.99
12	B	810	CLA	C1C-C2C-C3C	-4.23	102.53	106.98
12	A	812	CLA	C3D-C4D-ND	4.23	116.86	109.99
12	A	814	CLA	C4A-NA-C1A	-4.23	104.75	106.68
12	B	822	CLA	O2D-CGD-CBD	4.23	118.62	111.23
12	B	801	CLA	C1D-CHD-C4C	-4.22	117.04	126.02
12	A	820	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
12	A	839	CLA	C3D-C4D-ND	4.21	116.83	109.99
12	A	815	CLA	CHD-C1D-ND	-4.21	118.88	124.80
12	B	823	CLA	C3D-C4D-ND	4.21	116.83	109.99
12	L	202	CLA	CHD-C1D-ND	-4.21	118.88	124.80
12	A	806	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
12	B	808	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
12	B	813	CLA	C3D-C4D-ND	4.20	116.82	109.99
12	A	833	CLA	O2D-CGD-CBD	4.20	118.57	111.23
12	B	804	CLA	C1D-CHD-C4C	-4.20	117.09	126.02
12	B	813	CLA	CHD-C1D-ND	-4.19	118.90	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	828	CLA	C3D-C4D-ND	4.19	116.80	109.99
12	A	833	CLA	CHD-C1D-ND	-4.19	118.91	124.80
12	B	827	CLA	C4A-NA-C1A	-4.19	104.77	106.68
12	B	811	CLA	CAC-C3C-C4C	4.19	130.24	124.79
12	A	834	CLA	CHD-C1D-ND	-4.18	118.92	124.80
12	B	829	CLA	C3D-C4D-ND	4.18	116.79	109.99
12	A	823	CLA	C3B-C4B-NB	4.18	114.26	110.53
12	A	807	CLA	CHD-C1D-ND	-4.18	118.92	124.80
12	A	804	CLA	CHD-C1D-ND	-4.18	118.92	124.80
12	F	203	CLA	C3D-C4D-ND	4.17	116.77	109.99
12	J	101	CLA	C3D-C4D-ND	4.17	116.77	109.99
12	A	821	CLA	CHD-C1D-ND	-4.17	118.93	124.80
12	A	802	CLA	C3D-C4D-ND	4.17	116.77	109.99
12	A	842	CLA	C3D-C4D-ND	4.17	116.76	109.99
12	A	805	CLA	CHD-C1D-ND	-4.16	118.94	124.80
12	A	836	CLA	C4A-NA-C1A	-4.16	104.78	106.68
12	B	820	CLA	C1-C2-C3	-4.16	119.37	126.20
12	B	815	CLA	C3D-C4D-ND	4.16	116.75	109.99
12	B	802	CLA	C3D-C2D-C1D	-4.16	100.15	105.83
12	B	817	CLA	C3D-C4D-ND	4.16	116.75	109.99
12	A	829	CLA	C3D-C4D-ND	4.16	116.75	109.99
12	B	817	CLA	CHD-C1D-ND	-4.16	118.95	124.80
12	B	812	CLA	CHD-C1D-ND	-4.16	118.95	124.80
12	B	803	CLA	C3D-C2D-C1D	-4.16	100.16	105.83
12	B	810	CLA	C3B-C4B-NB	4.16	114.24	110.53
12	A	832	CLA	CHD-C1D-ND	-4.16	118.95	124.80
12	A	843	CLA	C3D-C4D-ND	4.15	116.74	109.99
12	B	803	CLA	C3D-C4D-ND	4.15	116.74	109.99
12	A	816	CLA	CHD-C1D-ND	-4.15	118.96	124.80
12	A	821	CLA	C2C-C1C-NC	4.15	114.34	109.98
12	B	826	CLA	CHD-C1D-ND	-4.15	118.97	124.80
12	A	818	CLA	C3D-C4D-ND	4.15	116.73	109.99
12	A	840	CLA	C3D-C4D-ND	4.15	116.72	109.99
12	B	830	CLA	CHD-C1D-ND	-4.14	118.97	124.80
12	A	825	CLA	C3C-C4C-NC	4.14	115.74	110.43
12	B	828	CLA	CHD-C1D-ND	-4.14	118.97	124.80
12	A	836	CLA	C3D-C4D-ND	4.14	116.72	109.99
12	B	811	CLA	C3D-C2D-C1D	-4.14	100.18	105.83
12	A	817	CLA	C1D-CHD-C4C	-4.14	117.23	126.02
12	L	202	CLA	C4A-NA-C1A	-4.14	104.79	106.68
12	B	809	CLA	C3D-C4D-ND	4.13	116.70	109.99
12	B	832	CLA	C3D-C4D-ND	4.13	116.70	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	804	CLA	C3D-C4D-ND	4.13	116.70	109.99
12	A	835	CLA	C1D-CHD-C4C	-4.13	117.25	126.02
12	A	810	CLA	C3D-C4D-ND	4.13	116.70	109.99
12	B	807	CLA	C1D-CHD-C4C	-4.13	117.25	126.02
12	B	807	CLA	C3D-C4D-ND	4.13	116.69	109.99
12	A	818	CLA	C1D-CHD-C4C	-4.12	117.25	126.02
12	A	819	CLA	C3D-C4D-ND	4.12	116.69	109.99
12	B	808	CLA	CHD-C1D-ND	-4.12	119.00	124.80
12	B	814	CLA	C3D-C2D-C1D	-4.11	100.22	105.83
12	A	825	CLA	C3D-C4D-ND	4.11	116.67	109.99
12	A	803	CLA	C3D-C4D-ND	4.11	116.67	109.99
12	B	820	CLA	C2C-C1C-NC	4.11	114.30	109.98
12	A	843	CLA	CHD-C1D-ND	-4.11	119.02	124.80
12	A	803	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
12	B	820	CLA	C1D-CHD-C4C	-4.10	117.30	126.02
12	A	834	CLA	O2D-CGD-O1D	-4.10	115.86	123.85
12	A	813	CLA	CHD-C1D-ND	-4.10	119.03	124.80
12	B	822	CLA	C1D-CHD-C4C	-4.10	117.30	126.02
12	B	808	CLA	C2B-C1B-NB	4.10	114.58	110.33
12	A	825	CLA	CAC-C3C-C4C	4.10	130.12	124.79
12	B	805	CLA	C3D-C4D-ND	4.09	116.64	109.99
12	A	838	CLA	CHD-C1D-ND	-4.09	119.04	124.80
12	B	821	CLA	C3D-C4D-ND	4.09	116.64	109.99
12	B	815	CLA	CHD-C1D-ND	-4.09	119.04	124.80
12	A	839	CLA	C1D-CHD-C4C	-4.09	117.32	126.02
12	B	801	CLA	CHD-C1D-ND	-4.09	119.05	124.80
12	A	823	CLA	C1C-C2C-C3C	-4.09	102.68	106.98
12	A	806	CLA	C3D-C4D-ND	4.08	116.63	109.99
12	A	837	CLA	C1D-CHD-C4C	-4.08	117.34	126.02
12	A	829	CLA	C3D-C2D-C1D	-4.08	100.26	105.83
12	A	816	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
12	B	808	CLA	C3B-C2B-C1B	-4.08	102.36	107.17
12	B	815	CLA	C1D-CHD-C4C	-4.08	117.36	126.02
12	A	811	CLA	C1D-CHD-C4C	-4.07	117.36	126.02
12	A	837	CLA	CHD-C1D-ND	-4.07	119.07	124.80
12	A	813	CLA	C3D-C4D-ND	4.07	116.61	109.99
12	B	827	CLA	CHD-C1D-ND	-4.07	119.07	124.80
12	B	806	CLA	C3D-C4D-ND	4.07	116.60	109.99
12	A	830	CLA	C1D-CHD-C4C	-4.06	117.38	126.02
12	A	831	CLA	C4A-NA-C1A	-4.06	104.83	106.68
12	A	810	CLA	C1C-C2C-C3C	-4.06	102.71	106.98
12	A	814	CLA	CHD-C1D-ND	-4.06	119.09	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	825	CLA	C1D-CHD-C4C	-4.05	117.41	126.02
12	A	840	CLA	O2D-CGD-CBD	4.05	118.31	111.23
12	A	829	CLA	C3C-C4C-NC	4.05	115.62	110.43
12	A	834	CLA	C4A-NA-C1A	-4.05	104.83	106.68
12	A	836	CLA	CHD-C1D-ND	-4.04	119.11	124.80
12	L	202	CLA	C1D-CHD-C4C	-4.04	117.42	126.02
12	A	837	CLA	C3D-C4D-ND	4.04	116.56	109.99
12	B	832	CLA	CHD-C1D-ND	-4.04	119.12	124.80
12	B	814	CLA	C1D-CHD-C4C	-4.04	117.44	126.02
12	B	823	CLA	CMD-C2D-C3D	-4.04	118.43	127.69
12	A	822	CLA	C1D-CHD-C4C	-4.04	117.44	126.02
12	A	810	CLA	CHD-C1D-ND	-4.03	119.12	124.80
12	B	808	CLA	C3D-C4D-ND	4.03	116.54	109.99
12	F	203	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
12	A	835	CLA	CHD-C1D-ND	-4.02	119.14	124.80
12	A	830	CLA	C3D-C4D-ND	4.02	116.52	109.99
12	A	806	CLA	CHD-C1D-ND	-4.01	119.16	124.80
12	B	817	CLA	C1D-CHD-C4C	-4.01	117.49	126.02
12	A	812	CLA	CHD-C1D-ND	-4.01	119.16	124.80
12	B	804	CLA	C4C-C3C-C2C	-4.01	101.06	106.89
12	B	811	CLA	CHD-C1D-ND	-4.01	119.16	124.80
12	B	823	CLA	C4B-C3B-C2B	-4.00	102.32	107.30
12	A	839	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
12	A	819	CLA	CHD-C1D-ND	-4.00	119.18	124.80
12	A	802	CLA	C2C-C1C-NC	3.99	114.18	109.98
12	B	818	CLA	CHD-C1D-ND	-3.99	119.18	124.80
12	B	816	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
12	A	842	CLA	C4A-NA-C1A	-3.99	104.86	106.68
12	B	826	CLA	C1D-CHD-C4C	-3.99	117.55	126.02
12	A	810	CLA	C1D-CHD-C4C	-3.98	117.55	126.02
12	A	821	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
12	B	823	CLA	C1C-C2C-C3C	-3.98	102.79	106.98
12	B	811	CLA	C3D-C4D-ND	3.98	116.45	109.99
12	A	814	CLA	C3D-C4D-ND	3.98	116.45	109.99
12	B	805	CLA	C1D-CHD-C4C	-3.97	117.57	126.02
12	A	804	CLA	C2C-C1C-NC	3.97	114.16	109.98
12	A	833	CLA	CAA-C2A-C3A	-3.97	102.26	113.00
12	A	823	CLA	CHD-C1D-ND	-3.97	119.21	124.80
12	A	808	CLA	C3D-C4D-ND	3.97	116.44	109.99
12	B	818	CLA	C3D-C4D-ND	3.97	116.44	109.99
12	A	834	CLA	C1D-CHD-C4C	-3.96	117.59	126.02
12	B	819	CLA	C2C-C1C-NC	3.96	114.14	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	832	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
12	B	810	CLA	C4B-C3B-C2B	-3.96	102.38	107.30
12	J	101	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
12	A	854	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
12	J	101	CLA	CHD-C1D-ND	-3.95	119.25	124.80
12	A	840	CLA	C1D-CHD-C4C	-3.94	117.64	126.02
12	B	809	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
12	F	203	CLA	C1C-C2C-C3C	-3.94	102.84	106.98
12	A	833	CLA	C1C-C2C-C3C	-3.93	102.84	106.98
12	B	821	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
12	A	820	CLA	C1D-CHD-C4C	-3.93	117.66	126.02
12	A	854	CLA	C3D-C4D-ND	3.93	116.38	109.99
12	B	808	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
12	B	807	CLA	CHD-C1D-ND	-3.93	119.28	124.80
12	B	827	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
12	L	202	CLA	C1C-C2C-C3C	-3.93	102.85	106.98
12	B	811	CLA	C1D-CHD-C4C	-3.92	117.68	126.02
12	B	816	CLA	C4A-NA-C1A	-3.92	104.89	106.68
12	B	830	CLA	C1C-C2C-C3C	-3.92	102.86	106.98
12	A	820	CLA	C3D-C4D-ND	3.92	116.36	109.99
12	A	838	CLA	C1D-CHD-C4C	-3.92	117.70	126.02
15	L	206	BCR	C2-C1-C6	3.92	116.13	110.44
12	A	839	CLA	O2D-CGD-O1D	-3.91	116.23	123.85
12	A	814	CLA	C1D-CHD-C4C	-3.91	117.71	126.02
12	B	818	CLA	C1D-CHD-C4C	-3.91	117.72	126.02
12	B	823	CLA	C3B-C4B-NB	3.91	114.02	110.53
12	B	816	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
12	B	814	CLA	C4A-NA-C1A	-3.90	104.90	106.68
12	A	808	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
12	A	829	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
12	A	828	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
12	B	806	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
12	A	815	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
12	A	805	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
12	B	827	CLA	C3B-C4B-NB	3.88	114.00	110.53
12	B	805	CLA	CHD-C1D-ND	-3.88	119.34	124.80
12	A	803	CLA	CHD-C1D-ND	-3.88	119.34	124.80
12	B	810	CLA	C3D-C4D-ND	3.88	116.29	109.99
12	A	820	CLA	C4A-NA-C1A	-3.88	104.91	106.68
12	A	830	CLA	C3B-C2B-C1B	-3.88	102.60	107.17
12	B	832	CLA	C4B-C3B-C2B	-3.88	102.48	107.30
12	A	843	CLA	C4A-NA-C1A	-3.87	104.91	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	802	CLA	C1D-CHD-C4C	-3.87	117.79	126.02
12	B	832	CLA	CHC-C1C-C2C	-3.87	115.95	126.95
12	A	819	CLA	C3B-C4B-NB	3.87	113.98	110.53
12	B	829	CLA	CAA-CBA-CGA	-3.86	102.23	113.21
12	A	830	CLA	C3B-C4B-NB	3.86	113.98	110.53
12	B	828	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
12	B	822	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
12	B	831	CLA	C1C-C2C-C3C	-3.86	102.92	106.98
12	A	830	CLA	CHD-C1D-ND	-3.85	119.38	124.80
12	B	805	CLA	CAC-C3C-C4C	3.85	129.80	124.79
12	A	826	CLA	C1D-CHD-C4C	-3.85	117.83	126.02
12	A	830	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
12	L	203	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
12	B	821	CLA	CHD-C1D-ND	-3.85	119.39	124.80
15	B	835	BCR	C2-C1-C6	3.85	116.03	110.44
12	A	802	CLA	CHD-C1D-ND	-3.85	119.39	124.80
12	A	836	CLA	C1C-C2C-C3C	-3.85	102.93	106.98
12	B	823	CLA	C1D-CHD-C4C	-3.84	117.85	126.02
12	A	843	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
12	A	827	CLA	C3D-C4D-ND	3.84	116.23	109.99
12	B	803	CLA	CAC-C3C-C4C	3.84	129.79	124.79
12	A	854	CLA	CBA-CAA-C2A	3.84	125.21	113.79
12	A	831	CLA	CHD-C1D-ND	-3.84	119.40	124.80
12	A	808	CLA	CHD-C1D-ND	-3.84	119.41	124.80
12	A	807	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
12	B	823	CLA	CHD-C1D-ND	-3.83	119.41	124.80
12	A	816	CLA	C4A-NA-C1A	-3.83	104.93	106.68
12	B	820	CLA	C3C-C4C-NC	3.83	115.33	110.43
12	A	815	CLA	C4A-NA-C1A	-3.82	104.93	106.68
12	A	828	CLA	C3B-C4B-NB	3.82	113.94	110.53
12	A	841	CLA	C1C-C2C-C3C	-3.82	102.97	106.98
12	B	803	CLA	CMA-C3A-C2A	-3.82	99.23	113.98
12	B	818	CLA	C4B-C3B-C2B	-3.82	102.56	107.30
12	A	812	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
12	B	829	CLA	C1C-C2C-C3C	-3.81	102.97	106.98
12	B	811	CLA	C4A-NA-C1A	-3.81	104.94	106.68
12	A	833	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
12	J	101	CLA	C4A-NA-C1A	-3.81	104.94	106.68
12	B	814	CLA	CHD-C1D-ND	-3.81	119.45	124.80
12	A	817	CLA	C3C-C4C-NC	3.81	115.31	110.43
12	A	837	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
12	A	824	CLA	C1C-C2C-C3C	-3.80	102.98	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	816	CLA	C1D-CHD-C4C	-3.80	117.95	126.02
12	B	815	CLA	C3B-C4B-NB	3.80	113.92	110.53
12	B	820	CLA	CHD-C1D-ND	-3.80	119.46	124.80
12	A	802	CLA	CAA-C2A-C3A	-3.80	102.74	113.00
12	A	854	CLA	CMD-C2D-C1D	3.79	131.41	124.73
12	L	204	CLA	CAA-C2A-C3A	-3.79	102.75	113.00
12	B	809	CLA	CHD-C4C-NC	3.79	130.11	124.23
12	B	823	CLA	C3B-C2B-C1B	-3.79	102.70	107.17
12	A	839	CLA	C4A-NA-C1A	-3.79	104.95	106.68
12	A	809	CLA	O2D-CGD-CBD	3.79	117.85	111.23
12	A	842	CLA	CHD-C1D-ND	-3.79	119.47	124.80
12	A	835	CLA	C3C-C4C-NC	3.79	115.28	110.43
12	A	828	CLA	C3C-C4C-NC	3.78	115.28	110.43
12	A	840	CLA	O2A-CGA-CBA	3.78	123.37	111.83
12	B	827	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
12	B	809	CLA	CAA-C2A-C3A	-3.78	102.78	113.00
12	B	805	CLA	C3B-C4B-NB	3.78	113.90	110.53
12	B	813	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
12	A	828	CLA	C3D-C4D-ND	3.77	116.12	109.99
12	A	813	CLA	C1D-CHD-C4C	-3.77	118.00	126.02
12	B	807	CLA	C4A-NA-C1A	-3.77	104.96	106.68
12	B	832	CLA	C3B-C2B-C1B	-3.77	102.72	107.17
12	A	818	CLA	CHD-C1D-ND	-3.77	119.50	124.80
12	A	805	CLA	C3B-C4B-NB	3.77	113.89	110.53
12	A	830	CLA	C4B-C3B-C2B	-3.77	102.62	107.30
12	A	827	CLA	C3C-C4C-NC	3.76	115.25	110.43
12	A	835	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
12	A	831	CLA	C1D-CHD-C4C	-3.76	118.03	126.02
12	A	827	CLA	CHD-C1D-ND	-3.76	119.52	124.80
12	A	820	CLA	CHD-C1D-ND	-3.76	119.52	124.80
12	A	823	CLA	C1D-CHD-C4C	-3.75	118.04	126.02
12	B	804	CLA	C3C-C4C-NC	3.75	115.24	110.43
12	B	811	CLA	C1C-C2C-C3C	-3.75	103.04	106.98
12	A	819	CLA	C1D-CHD-C4C	-3.74	118.06	126.02
12	B	809	CLA	CHD-C1D-ND	-3.74	119.54	124.80
12	A	839	CLA	CHD-C1D-ND	-3.74	119.54	124.80
12	B	826	CLA	CAA-C2A-C3A	-3.74	102.90	113.00
12	B	807	CLA	C1-C2-C3	-3.74	120.08	126.20
12	B	808	CLA	C3C-C4C-NC	3.74	115.22	110.43
12	B	832	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
12	A	809	CLA	C3C-C4C-NC	3.73	115.20	110.43
12	A	807	CLA	C1D-CHD-C4C	-3.73	118.10	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	842	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
12	B	810	CLA	C1D-CHD-C4C	-3.73	118.10	126.02
12	A	836	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
12	A	826	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
12	B	805	CLA	C1C-C2C-C3C	-3.72	103.06	106.98
12	B	823	CLA	CAC-C3C-C4C	3.72	129.63	124.79
12	B	818	CLA	C3B-C2B-C1B	-3.72	102.79	107.17
12	B	826	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
12	A	809	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
12	B	826	CLA	C3B-C4B-NB	3.71	113.84	110.53
12	B	810	CLA	C2B-C1B-NB	3.70	114.17	110.33
12	B	803	CLA	C3C-C4C-NC	3.70	115.17	110.43
12	B	806	CLA	CHD-C1D-ND	-3.70	119.59	124.80
12	A	841	CLA	C1D-CHD-C4C	-3.70	118.16	126.02
12	A	840	CLA	C3C-C4C-NC	3.70	115.17	110.43
12	B	830	CLA	C1D-CHD-C4C	-3.69	118.17	126.02
12	A	828	CLA	CHD-C1D-ND	-3.69	119.61	124.80
12	A	804	CLA	C3C-C4C-NC	3.69	115.15	110.43
12	B	822	CLA	C1C-C2C-C3C	-3.69	103.10	106.98
12	B	825	CLA	C1D-CHD-C4C	-3.68	118.19	126.02
12	B	822	CLA	C3C-C4C-NC	3.68	115.15	110.43
12	B	811	CLA	CAA-C2A-C1A	3.68	124.04	111.97
12	A	805	CLA	C4A-NA-C1A	-3.68	105.00	106.68
12	B	804	CLA	CHD-C1D-ND	-3.68	119.62	124.80
12	A	854	CLA	C4-C3-C5	3.68	121.62	115.23
12	A	842	CLA	C3C-C4C-NC	3.68	115.14	110.43
12	A	825	CLA	C3B-C4B-NB	3.68	113.81	110.53
12	A	820	CLA	C3B-C4B-NB	3.68	113.81	110.53
12	A	804	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
12	B	815	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
12	A	808	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
12	A	811	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
12	A	815	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
12	A	824	CLA	C1D-CHD-C4C	-3.66	118.23	126.02
12	B	806	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
12	B	802	CLA	CAC-C3C-C4C	3.66	129.56	124.79
12	A	831	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
12	A	807	CLA	C4-C3-C5	3.66	120.44	116.13
12	B	810	CLA	CHD-C1D-ND	-3.65	119.66	124.80
12	A	809	CLA	C4A-NA-C1A	-3.65	105.01	106.68
12	A	838	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
12	A	840	CLA	CHD-C1D-ND	-3.64	119.68	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	813	CLA	C3C-C4C-NC	3.64	115.09	110.43
12	A	834	CLA	C1C-C2C-C3C	-3.64	103.15	106.98
12	B	801	CLA	C3C-C4C-NC	3.64	115.09	110.43
12	A	843	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
12	B	810	CLA	CHC-C1C-C2C	-3.63	116.63	126.95
12	A	837	CLA	C3B-C4B-NB	3.63	113.77	110.53
12	B	812	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
15	J	103	BCR	C2-C1-C6	3.63	115.71	110.44
12	B	820	CLA	C3D-C4D-ND	3.63	115.89	109.99
12	A	812	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
12	A	824	CLA	C3B-C4B-NB	3.63	113.77	110.53
12	A	810	CLA	C3B-C4B-NB	3.62	113.77	110.53
12	B	802	CLA	C3C-C4C-NC	3.62	115.07	110.43
12	L	204	CLA	C1D-CHD-C4C	-3.62	118.32	126.02
12	B	825	CLA	C3C-C4C-NC	3.62	115.06	110.43
12	B	809	CLA	C3C-C4C-NC	3.62	115.06	110.43
12	A	840	CLA	C1C-C2C-C3C	-3.62	103.18	106.98
12	B	812	CLA	C1D-CHD-C4C	-3.61	118.34	126.02
12	B	804	CLA	C3D-C4D-ND	3.61	115.86	109.99
12	B	802	CLA	CHD-C1D-ND	-3.60	119.73	124.80
12	A	843	CLA	C3B-C4B-NB	3.60	113.74	110.53
12	F	203	CLA	C3B-C4B-NB	3.60	113.74	110.53
12	B	831	CLA	C1D-CHD-C4C	-3.59	118.38	126.02
12	B	832	CLA	O2D-CGD-O1D	-3.59	116.86	123.85
12	A	809	CLA	CHD-C1D-ND	-3.58	119.76	124.80
12	A	843	CLA	C3C-C4C-NC	3.58	115.02	110.43
12	A	835	CLA	C3B-C4B-NB	3.58	113.72	110.53
12	B	819	CLA	C1D-CHD-C4C	-3.58	118.42	126.02
12	A	834	CLA	CMB-C2B-C1B	3.58	130.86	125.42
12	A	816	CLA	C3B-C4B-NB	3.57	113.72	110.53
12	A	837	CLA	C3C-C4C-NC	3.57	115.00	110.43
12	B	824	CLA	C3B-C4B-NB	3.57	113.71	110.53
12	B	828	CLA	C3C-C4C-NC	3.56	115.00	110.43
12	B	817	CLA	C3C-C4C-NC	3.56	114.99	110.43
12	B	829	CLA	C4A-NA-C1A	-3.55	105.06	106.68
12	A	834	CLA	C3B-C4B-NB	3.55	113.70	110.53
12	B	824	CLA	C1C-C2C-C3C	-3.55	103.25	106.98
12	A	830	CLA	C3C-C4C-NC	3.55	114.97	110.43
12	A	839	CLA	C3C-C4C-NC	3.54	114.96	110.43
12	L	203	CLA	C1D-CHD-C4C	-3.53	118.51	126.02
15	A	848	BCR	C2-C1-C6	3.53	115.56	110.44
12	A	806	CLA	CHD-C4C-NC	3.53	129.70	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	806	CLA	C4A-NA-C1A	-3.52	105.07	106.68
12	B	814	CLA	C3C-C4C-NC	3.52	114.94	110.43
12	B	821	CLA	C3C-C4C-NC	3.52	114.94	110.43
12	A	802	CLA	C3C-C4C-NC	3.52	114.94	110.43
12	A	819	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
12	B	829	CLA	C1D-CHD-C4C	-3.52	118.54	126.02
12	B	828	CLA	C1C-C2C-C3C	-3.52	103.28	106.98
12	A	824	CLA	CAC-C3C-C4C	3.52	129.36	124.79
12	A	842	CLA	O2A-CGA-CBA	3.51	122.55	111.83
12	J	101	CLA	C3B-C4B-NB	3.51	113.66	110.53
12	A	802	CLA	C1D-CHD-C4C	-3.50	118.57	126.02
12	A	806	CLA	C1-C2-C3	-3.50	120.46	126.20
12	A	832	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
12	B	830	CLA	C3B-C4B-NB	3.50	113.65	110.53
12	A	811	CLA	C3C-C4C-NC	3.50	114.91	110.43
12	B	824	CLA	C1D-CHD-C4C	-3.50	118.59	126.02
12	A	817	CLA	C1C-C2C-C3C	-3.50	103.30	106.98
12	A	811	CLA	CAA-C2A-C3A	-3.49	103.56	113.00
12	J	101	CLA	CAC-C3C-C4C	3.49	129.32	124.79
12	B	810	CLA	C3B-C2B-C1B	-3.48	103.06	107.17
12	B	816	CLA	C3C-C4C-NC	3.48	114.89	110.43
12	B	831	CLA	C3C-C4C-NC	3.48	114.89	110.43
15	A	849	BCR	C11-C10-C9	-3.48	122.39	127.28
12	A	829	CLA	C1C-C2C-C3C	-3.48	103.32	106.98
12	A	813	CLA	C4C-C3C-C2C	-3.48	101.82	106.89
12	B	806	CLA	CHC-C1C-C2C	-3.48	117.06	126.95
12	B	832	CLA	C4A-NA-C1A	-3.48	105.09	106.68
12	B	826	CLA	CMB-C2B-C1B	3.47	130.71	125.42
12	A	835	CLA	CAA-C2A-C3A	-3.47	103.61	113.00
12	A	836	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
12	A	814	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
12	B	812	CLA	C3C-C4C-NC	3.46	114.87	110.43
12	A	821	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
12	A	854	CLA	O2D-CGD-O1D	-3.46	117.11	123.85
12	A	823	CLA	C3C-C4C-NC	3.45	114.86	110.43
12	A	808	CLA	C3C-C4C-NC	3.45	114.86	110.43
12	A	818	CLA	C3C-C4C-NC	3.45	114.85	110.43
12	A	841	CLA	CAA-C2A-C3A	-3.45	103.67	113.00
12	A	825	CLA	C4C-C3C-C2C	-3.45	101.87	106.89
12	A	814	CLA	C3C-C4C-NC	3.45	114.84	110.43
12	B	814	CLA	C1C-C2C-C3C	-3.45	103.36	106.98
12	A	820	CLA	CHC-C1C-C2C	-3.44	117.17	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	842	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
12	B	803	CLA	CED-O2D-CGD	3.44	123.72	115.92
12	A	838	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
12	A	854	CLA	C4C-C3C-C2C	-3.43	101.89	106.89
12	A	829	CLA	O2A-CGA-CBA	3.43	122.29	111.83
12	A	822	CLA	C4A-NA-C1A	-3.43	105.11	106.68
12	A	811	CLA	C3B-C4B-NB	3.43	113.59	110.53
12	A	803	CLA	C3C-C4C-NC	3.43	114.82	110.43
12	B	818	CLA	CBA-CAA-C2A	3.42	123.98	113.79
12	B	821	CLA	CMC-C2C-C1C	3.42	130.38	125.03
12	A	819	CLA	CAC-C3C-C4C	3.42	129.24	124.79
12	B	804	CLA	CHB-C4A-NA	3.42	129.34	124.40
12	A	854	CLA	CAC-C3C-C4C	3.42	129.24	124.79
12	B	821	CLA	C3B-C4B-NB	3.42	113.58	110.53
12	A	836	CLA	C4B-C3B-C2B	-3.42	103.06	107.30
12	B	803	CLA	C11-C12-C13	-3.41	104.64	115.97
12	A	833	CLA	C3C-C4C-NC	3.40	114.79	110.43
12	B	810	CLA	CAC-C3C-C4C	3.40	129.21	124.79
12	L	204	CLA	C3C-C4C-NC	3.40	114.78	110.43
12	A	836	CLA	C3B-C4B-NB	3.39	113.56	110.53
12	B	809	CLA	CBC-CAC-C3C	-3.39	103.22	112.42
12	A	816	CLA	C4B-C3B-C2B	-3.39	103.08	107.30
12	B	823	CLA	C2D-C1D-ND	3.39	113.48	110.13
12	B	806	CLA	CMB-C2B-C1B	3.39	130.57	125.42
12	A	831	CLA	C3C-C4C-NC	3.38	114.76	110.43
12	A	808	CLA	C1-C2-C3	-3.38	120.66	126.20
12	A	829	CLA	C1-C2-C3	-3.38	120.66	126.20
12	B	820	CLA	CHD-C4C-NC	3.38	129.47	124.23
12	A	810	CLA	C3C-C4C-NC	3.37	114.75	110.43
12	A	854	CLA	CHD-C1D-ND	-3.37	120.06	124.80
12	B	811	CLA	C3B-C4B-NB	3.37	113.53	110.53
12	B	827	CLA	C3C-C4C-NC	3.37	114.74	110.43
12	A	854	CLA	C1C-C2C-C3C	-3.37	103.44	106.98
12	A	830	CLA	O2D-CGD-O1D	-3.36	117.30	123.85
12	B	802	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
12	L	202	CLA	C3C-C4C-NC	3.36	114.74	110.43
12	A	817	CLA	C3B-C4B-NB	3.36	113.53	110.53
12	A	812	CLA	CAC-C3C-C4C	3.36	129.16	124.79
12	A	819	CLA	C4B-C3B-C2B	-3.36	103.12	107.30
12	A	836	CLA	C3C-C4C-NC	3.36	114.73	110.43
15	J	104	BCR	C2-C1-C6	3.36	115.31	110.44
15	J	103	BCR	C3-C4-C5	-3.35	108.07	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	101	CLA	C3C-C4C-NC	3.35	114.73	110.43
12	A	805	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
12	A	831	CLA	CAC-C3C-C4C	3.35	129.15	124.79
12	A	830	CLA	CHC-C1C-C2C	-3.35	117.44	126.95
12	B	825	CLA	C1C-C2C-C3C	-3.35	103.46	106.98
12	A	819	CLA	CHC-C1C-C2C	-3.34	117.44	126.95
12	B	810	CLA	C4A-NA-C1A	-3.34	105.15	106.68
15	A	848	BCR	C3-C4-C5	-3.34	108.10	114.06
12	B	809	CLA	C3B-C4B-NB	3.34	113.51	110.53
12	A	821	CLA	C3C-C4C-NC	3.34	114.71	110.43
12	B	818	CLA	CHC-C1C-C2C	-3.34	117.46	126.95
12	B	830	CLA	C3C-C4C-NC	3.34	114.70	110.43
12	B	817	CLA	CAA-C2A-C3A	-3.33	104.00	113.00
12	B	811	CLA	CHC-C1C-C2C	-3.33	117.49	126.95
12	B	805	CLA	C4A-NA-C1A	-3.33	105.16	106.68
12	A	818	CLA	C4C-C3C-C2C	-3.33	102.05	106.89
12	B	806	CLA	C1-O2A-CGA	3.33	124.70	116.65
12	A	828	CLA	C1C-C2C-C3C	-3.33	103.48	106.98
12	L	203	CLA	C4A-NA-C1A	-3.33	105.16	106.68
12	B	804	CLA	C2C-C1C-NC	3.32	113.47	109.98
12	A	834	CLA	C3C-C4C-NC	3.32	114.68	110.43
12	A	839	CLA	C3B-C4B-NB	3.31	113.49	110.53
12	A	829	CLA	CHD-C1D-ND	-3.31	120.14	124.80
12	A	831	CLA	C1-C2-C3	-3.31	121.40	126.76
12	A	802	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
12	B	821	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
12	B	818	CLA	C3B-C4B-NB	3.31	113.48	110.53
12	B	818	CLA	C3C-C4C-NC	3.31	114.67	110.43
12	A	823	CLA	C4B-C3B-C2B	-3.31	103.19	107.30
12	A	816	CLA	CHC-C1C-C2C	-3.30	117.57	126.95
12	A	804	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
12	B	813	CLA	C3C-C4C-NC	3.30	114.66	110.43
12	B	807	CLA	CHD-C4C-NC	3.29	129.34	124.23
12	B	815	CLA	C3C-C4C-NC	3.29	114.65	110.43
12	A	815	CLA	C3C-C4C-NC	3.29	114.65	110.43
12	A	841	CLA	C3C-C4C-NC	3.29	114.64	110.43
12	B	826	CLA	C3C-C4C-NC	3.29	114.64	110.43
12	A	842	CLA	CAC-C3C-C4C	3.29	129.07	124.79
15	A	846	BCR	C27-C26-C25	3.29	127.14	122.70
15	L	205	BCR	C24-C23-C22	-3.28	121.38	126.23
12	A	841	CLA	O2A-CGA-CBA	3.28	121.85	111.83
12	B	823	CLA	O2D-CGD-O1D	-3.28	117.46	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	803	CLA	CAC-C3C-C4C	3.28	129.06	124.79
12	B	803	CLA	C1C-C2C-C3C	-3.28	103.53	106.98
15	J	103	BCR	C11-C10-C9	-3.28	122.68	127.28
12	B	823	CLA	CHC-C1C-C2C	-3.28	117.63	126.95
12	A	827	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
12	A	820	CLA	CBC-CAC-C3C	-3.27	103.54	112.42
12	B	811	CLA	C3C-C4C-NC	3.27	114.62	110.43
12	B	802	CLA	C4B-C3B-C2B	-3.27	103.23	107.30
12	L	204	CLA	C1C-C2C-C3C	-3.27	103.54	106.98
12	B	808	CLA	CHD-C4C-NC	3.27	129.31	124.23
12	A	805	CLA	CAC-C3C-C4C	3.27	129.05	124.79
12	A	827	CLA	C4C-C3C-C2C	-3.27	102.14	106.89
12	L	203	CLA	C3C-C4C-NC	3.27	114.61	110.43
12	A	803	CLA	C3B-C4B-NB	3.27	113.44	110.53
12	B	806	CLA	O2A-CGA-CBA	3.26	121.79	111.83
12	A	804	CLA	CMC-C2C-C1C	3.26	130.13	125.03
12	B	816	CLA	C4B-C3B-C2B	-3.26	103.24	107.30
12	B	802	CLA	C3B-C4B-NB	3.26	113.44	110.53
12	B	824	CLA	C3C-C4C-NC	3.26	114.61	110.43
12	L	202	CLA	C3B-C4B-NB	3.26	113.44	110.53
12	F	203	CLA	C3C-C4C-NC	3.26	114.61	110.43
12	A	832	CLA	C3C-C4C-NC	3.26	114.60	110.43
12	A	806	CLA	C3C-C4C-NC	3.26	114.60	110.43
12	B	822	CLA	CHD-C1D-ND	-3.26	120.22	124.80
12	A	807	CLA	C3B-C4B-NB	3.25	113.43	110.53
12	J	101	CLA	C1C-C2C-C3C	-3.25	103.56	106.98
12	B	819	CLA	C1C-C2C-C3C	-3.25	103.57	106.98
12	B	807	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	B	814	CLA	C3B-C4B-NB	3.24	113.42	110.53
12	B	809	CLA	C4B-C3B-C2B	-3.24	103.28	107.30
12	A	808	CLA	O2A-CGA-CBA	3.24	121.70	111.83
12	A	828	CLA	CAC-C3C-C4C	3.24	129.00	124.79
12	B	817	CLA	C1C-C2C-C3C	-3.23	103.58	106.98
12	A	831	CLA	O2A-CGA-CBA	3.23	121.69	111.83
12	A	838	CLA	CAC-C3C-C4C	3.23	129.00	124.79
12	B	825	CLA	CAA-C2A-C3A	-3.23	104.27	113.00
12	L	203	CLA	C3B-C4B-NB	3.23	113.41	110.53
12	A	803	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
12	B	826	CLA	O2A-CGA-CBA	3.23	121.68	111.83
12	B	801	CLA	CHC-C1C-C2C	-3.23	117.77	126.95
12	A	838	CLA	C3C-C4C-NC	3.22	114.56	110.43
12	A	827	CLA	CHD-C4C-NC	3.22	129.23	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	805	CLA	C3C-C4C-NC	3.22	114.56	110.43
12	A	842	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
15	J	103	BCR	C27-C26-C25	3.22	127.06	122.70
12	A	812	CLA	C3C-C4C-NC	3.22	114.56	110.43
12	B	822	CLA	C3B-C4B-NB	3.22	113.40	110.53
12	B	806	CLA	C3C-C4C-NC	3.22	114.55	110.43
12	B	812	CLA	C3B-C4B-NB	3.22	113.40	110.53
12	B	825	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
12	A	824	CLA	CHC-C1C-C2C	-3.21	117.84	126.95
12	B	815	CLA	CHC-C1C-C2C	-3.21	117.84	126.95
12	A	826	CLA	O2A-CGA-CBA	3.21	121.61	111.83
12	B	820	CLA	C4C-C3C-C2C	-3.20	102.23	106.89
12	B	815	CLA	CAC-C3C-C4C	3.20	128.96	124.79
12	A	822	CLA	C4B-C3B-C2B	-3.20	103.32	107.30
12	A	827	CLA	C1C-C2C-C3C	-3.20	103.62	106.98
12	A	854	CLA	O2A-CGA-CBA	3.20	121.58	111.83
12	A	824	CLA	CMB-C2B-C1B	3.19	130.28	125.42
12	A	834	CLA	CHC-C1C-C2C	-3.19	117.88	126.95
12	A	822	CLA	C3B-C4B-NB	3.19	113.38	110.53
12	A	819	CLA	CBA-CAA-C2A	3.18	123.27	113.79
12	A	819	CLA	C3C-C4C-NC	3.18	114.51	110.43
12	A	840	CLA	CAC-C3C-C4C	3.18	128.93	124.79
12	B	820	CLA	C1C-C2C-C3C	-3.18	103.64	106.98
12	B	807	CLA	CHC-C1C-C2C	-3.18	117.91	126.95
12	A	815	CLA	C3B-C4B-NB	3.18	113.37	110.53
12	A	817	CLA	C4C-C3C-C2C	-3.18	102.26	106.89
12	A	803	CLA	C4B-C3B-C2B	-3.18	103.35	107.30
12	B	827	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
12	A	803	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
12	B	817	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
12	A	812	CLA	C3B-C4B-NB	3.17	113.36	110.53
12	A	829	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
12	A	854	CLA	C3B-C4B-NB	3.17	113.36	110.53
12	B	819	CLA	C3B-C4B-NB	3.17	113.36	110.53
12	A	810	CLA	CHC-C1C-C2C	-3.17	117.94	126.95
12	A	825	CLA	C1C-C2C-C3C	-3.17	103.65	106.98
12	A	804	CLA	CHD-C4C-NC	3.17	129.15	124.23
12	B	801	CLA	CAC-C3C-C4C	3.17	128.91	124.79
12	B	803	CLA	CMA-C3A-C4A	-3.17	103.25	111.77
12	B	804	CLA	O2D-CGD-CBD	3.17	116.77	111.23
12	B	807	CLA	C4B-C3B-C2B	-3.17	103.36	107.30
12	F	203	CLA	CHC-C1C-C2C	-3.16	117.95	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	829	CLA	C3B-C4B-NB	3.16	113.35	110.53
13	B	833	PQN	C14-C13-C15	3.16	120.72	115.23
12	B	823	CLA	C4-C3-C5	3.16	120.72	115.23
12	A	816	CLA	C3C-C4C-NC	3.16	114.48	110.43
12	A	820	CLA	C4B-C3B-C2B	-3.16	103.37	107.30
12	A	843	CLA	CHC-C1C-C2C	-3.16	117.97	126.95
12	B	813	CLA	C1C-C2C-C3C	-3.15	103.66	106.98
12	A	825	CLA	CHD-C1D-ND	-3.15	120.36	124.80
12	A	805	CLA	CHB-C4A-NA	3.15	128.95	124.40
12	A	838	CLA	O2A-CGA-CBA	3.15	121.44	111.83
12	A	828	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
12	B	812	CLA	CAA-C2A-C3A	-3.15	104.49	113.00
12	B	823	CLA	C3C-C4C-NC	3.15	114.46	110.43
12	A	834	CLA	CAC-C3C-C4C	3.15	128.88	124.79
12	B	826	CLA	CAC-C3C-C4C	3.15	128.88	124.79
15	J	104	BCR	C7-C8-C9	-3.14	121.58	126.23
12	A	807	CLA	C3C-C4C-NC	3.14	114.46	110.43
12	A	807	CLA	CAC-C3C-C4C	3.14	128.88	124.79
12	B	808	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
12	A	829	CLA	CAC-C3C-C4C	3.14	128.87	124.79
12	B	816	CLA	CHC-C1C-C2C	-3.14	118.03	126.95
12	A	809	CLA	C3B-C4B-NB	3.13	113.33	110.53
12	A	824	CLA	C3C-C4C-NC	3.13	114.44	110.43
12	B	805	CLA	CBC-CAC-C3C	-3.13	103.93	112.42
15	J	102	BCR	C11-C10-C9	-3.13	122.89	127.28
12	A	828	CLA	O2A-CGA-CBA	3.13	121.38	111.83
12	A	822	CLA	CHD-C4C-NC	3.13	129.08	124.23
12	A	802	CLA	CMB-C2B-C3B	3.13	133.91	126.55
12	B	829	CLA	C1-C2-C3	-3.13	121.07	126.20
12	A	834	CLA	O2A-CGA-CBA	3.13	121.37	111.83
15	I	101	BCR	C29-C30-C25	3.13	114.98	110.44
12	A	826	CLA	C3C-C4C-NC	3.12	114.43	110.43
12	A	811	CLA	CHC-C1C-C2C	-3.12	118.08	126.95
12	A	812	CLA	C4-C3-C5	3.12	120.64	115.23
12	A	805	CLA	CHC-C1C-C2C	-3.12	118.08	126.95
12	F	203	CLA	CAC-C3C-C4C	3.12	128.84	124.79
12	A	810	CLA	C4B-C3B-C2B	-3.11	103.43	107.30
12	A	842	CLA	C3B-C4B-NB	3.11	113.31	110.53
12	A	833	CLA	CMB-C2B-C1B	3.11	130.16	125.42
12	A	815	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
15	B	834	BCR	C27-C26-C25	3.11	126.90	122.70
12	A	835	CLA	CMB-C2B-C1B	3.11	130.15	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	843	CLA	C4B-C3B-C2B	-3.10	103.44	107.30
12	B	825	CLA	O2A-CGA-CBA	3.10	121.30	111.83
12	B	832	CLA	C3C-C4C-NC	3.10	114.40	110.43
12	A	803	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
12	B	829	CLA	CHC-C1C-C2C	-3.10	118.14	126.95
13	A	844	PQN	C14-C13-C15	3.10	120.61	115.23
12	A	839	CLA	O2A-CGA-CBA	3.10	121.28	111.83
12	A	802	CLA	CHB-C4A-NA	3.10	128.87	124.40
12	B	803	CLA	C3B-C4B-NB	3.10	113.29	110.53
12	A	835	CLA	CAC-C3C-C4C	3.09	128.82	124.79
12	B	803	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
12	A	836	CLA	CHC-C1C-C2C	-3.09	118.16	126.95
12	A	807	CLA	CHC-C1C-C2C	-3.09	118.17	126.95
12	L	204	CLA	C3B-C4B-NB	3.09	113.29	110.53
12	B	802	CLA	C4C-C3C-C2C	-3.09	102.39	106.89
12	A	836	CLA	CAC-C3C-C4C	3.09	128.81	124.79
15	M	101	BCR	C24-C23-C22	-3.09	121.67	126.23
12	A	843	CLA	C4C-C3C-C2C	-3.09	102.40	106.89
12	B	801	CLA	C4B-C3B-C2B	-3.08	103.47	107.30
12	A	833	CLA	C1-C2-C3	-3.08	121.14	126.20
12	B	821	CLA	O2A-CGA-CBA	3.08	121.24	111.83
12	A	812	CLA	CHC-C1C-C2C	-3.08	118.21	126.95
12	A	833	CLA	C3B-C4B-NB	3.07	113.28	110.53
12	B	826	CLA	CHC-C1C-C2C	-3.07	118.21	126.95
12	A	818	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
12	A	838	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
12	J	101	CLA	C4B-C3B-C2B	-3.07	103.48	107.30
12	A	822	CLA	C3C-C4C-NC	3.07	114.36	110.43
12	A	824	CLA	CAA-C2A-C3A	-3.07	104.71	113.00
12	B	808	CLA	CMB-C2B-C1B	3.07	130.09	125.42
12	A	835	CLA	CHC-C1C-C2C	-3.07	118.23	126.95
12	A	837	CLA	CHC-C1C-C2C	-3.07	118.23	126.95
12	B	821	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
12	A	822	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
11	A	801	CL0	C1-C2-C3	-3.06	121.18	126.20
12	A	835	CLA	C4C-C3C-C2C	-3.06	102.43	106.89
12	B	801	CLA	CHA-C1A-NA	-3.06	119.46	126.39
12	J	101	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
12	B	803	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
12	B	822	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
12	A	833	CLA	CHC-C1C-C2C	-3.05	118.27	126.95
12	B	820	CLA	O2A-CGA-CBA	3.05	121.14	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	807	CLA	C7-C6-C5	-3.05	105.13	113.26
12	A	805	CLA	C3C-C4C-NC	3.05	114.34	110.43
12	L	204	CLA	C4C-C3C-C2C	-3.05	102.45	106.89
12	A	837	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
12	B	803	CLA	CHD-C4C-NC	3.04	128.95	124.23
12	B	806	CLA	C4C-C3C-C2C	-3.04	102.47	106.89
12	B	827	CLA	CAC-C3C-C4C	3.04	128.74	124.79
12	B	803	CLA	CHD-C1D-ND	-3.04	120.53	124.80
12	A	828	CLA	C4B-C3B-C2B	-3.03	103.53	107.30
12	A	823	CLA	C4-C3-C5	3.03	119.70	116.13
12	B	830	CLA	CHC-C1C-C2C	-3.03	118.32	126.95
12	B	825	CLA	CAC-C3C-C4C	3.03	128.74	124.79
12	B	807	CLA	C3C-C4C-NC	3.03	114.32	110.43
12	A	837	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
12	A	834	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
12	J	101	CLA	C4C-C3C-C2C	-3.03	102.48	106.89
12	A	831	CLA	CHC-C1C-C2C	-3.03	118.33	126.95
12	B	829	CLA	C3C-C4C-NC	3.03	114.31	110.43
12	A	841	CLA	C4-C3-C5	3.03	119.69	116.13
12	L	202	CLA	CHC-C1C-C2C	-3.03	118.34	126.95
12	A	809	CLA	C4C-C3C-C2C	-3.03	102.49	106.89
12	A	826	CLA	CHD-C4C-NC	3.02	128.92	124.23
12	L	203	CLA	CMB-C2B-C1B	3.02	130.02	125.42
12	B	811	CLA	C4-C3-C5	3.02	120.48	115.23
12	A	818	CLA	CAC-C3C-C4C	3.02	128.72	124.79
12	L	203	CLA	CHC-C1C-C2C	-3.02	118.36	126.95
12	A	838	CLA	C3B-C4B-NB	3.02	113.23	110.53
12	B	821	CLA	C4C-C3C-C2C	-3.02	102.49	106.89
12	A	820	CLA	C3C-C4C-NC	3.02	114.30	110.43
12	B	828	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
12	B	813	CLA	CMC-C2C-C1C	3.02	129.75	125.03
12	B	805	CLA	CHC-C1C-C2C	-3.02	118.37	126.95
12	A	818	CLA	C1C-C2C-C3C	-3.02	103.81	106.98
12	B	805	CLA	CMC-C2C-C1C	3.02	129.75	125.03
12	A	818	CLA	CHC-C1C-C2C	-3.02	118.38	126.95
12	A	804	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
12	B	810	CLA	C3C-C4C-NC	3.01	114.29	110.43
12	L	203	CLA	C4-C3-C5	3.01	120.46	115.23
12	L	202	CLA	C4B-C3B-C2B	-3.01	103.55	107.30
12	A	811	CLA	O2A-CGA-CBA	3.01	121.02	111.83
12	A	802	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
12	A	814	CLA	CHD-C4C-NC	3.01	128.90	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	840	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
12	A	854	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
12	L	204	CLA	CAC-C3C-C4C	3.01	128.70	124.79
12	B	831	CLA	C3B-C4B-NB	3.01	113.21	110.53
12	A	833	CLA	O2A-CGA-CBA	3.01	121.00	111.83
12	A	811	CLA	C4C-C3C-C2C	-3.01	102.52	106.89
12	A	843	CLA	C4-C3-C5	3.00	120.44	115.23
12	A	811	CLA	CAC-C3C-C4C	3.00	128.70	124.79
12	B	812	CLA	CHC-C1C-C2C	-3.00	118.41	126.95
12	A	832	CLA	CHD-C4C-NC	3.00	128.89	124.23
12	B	813	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
12	A	823	CLA	CHC-C1C-C2C	-3.00	118.42	126.95
12	A	827	CLA	O2A-CGA-CBA	3.00	120.99	111.83
12	A	825	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
12	B	813	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
12	A	834	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
12	A	815	CLA	CAC-C3C-C4C	3.00	128.69	124.79
12	B	805	CLA	CHD-C4C-NC	3.00	128.88	124.23
12	A	830	CLA	C4C-C3C-C2C	-2.99	102.53	106.89
12	A	812	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
12	B	815	CLA	C4B-C3B-C2B	-2.99	103.58	107.30
12	A	821	CLA	CAA-C2A-C3A	-2.99	104.91	113.00
12	B	818	CLA	CHD-C4C-NC	2.99	128.87	124.23
12	A	817	CLA	O2A-CGA-CBA	2.99	120.94	111.83
12	B	801	CLA	C4-C3-C5	2.98	120.41	115.23
12	A	821	CLA	CHD-C4C-NC	2.98	128.86	124.23
12	B	814	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
12	B	809	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
12	B	802	CLA	C4-C3-C5	2.98	120.40	115.23
12	B	808	CLA	CHC-C1C-C2C	-2.98	118.47	126.95
12	B	802	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
12	A	839	CLA	CHD-C4C-NC	2.98	128.85	124.23
15	B	835	BCR	C27-C26-C25	2.98	126.73	122.70
12	B	811	CLA	O2D-CGD-CBD	2.98	116.43	111.23
12	B	807	CLA	C4-C3-C5	2.98	120.39	115.23
12	B	829	CLA	CHD-C4C-NC	2.98	128.84	124.23
12	A	832	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
12	A	842	CLA	CHC-C1C-C2C	-2.97	118.49	126.95
12	A	819	CLA	C4C-C3C-C2C	-2.97	102.56	106.89
12	A	806	CLA	O2A-CGA-CBA	2.97	120.90	111.83
11	A	801	CL0	O1D-CGD-CBD	-2.97	120.22	124.72
12	A	832	CLA	C4B-C3B-C2B	-2.97	103.61	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	808	CLA	C3B-C4B-NB	2.97	113.18	110.53
12	A	814	CLA	CMB-C2B-C1B	2.97	129.94	125.42
12	A	805	CLA	CHD-C4C-NC	2.97	128.84	124.23
12	B	827	CLA	CHC-C1C-C2C	-2.97	118.51	126.95
12	A	817	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
12	B	822	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
15	F	201	BCR	C15-C16-C17	-2.97	117.45	123.52
12	A	802	CLA	C4B-C3B-C2B	-2.97	103.61	107.30
12	A	841	CLA	CHD-C4C-NC	2.96	128.82	124.23
12	A	821	CLA	CMB-C2B-C1B	2.96	129.93	125.42
12	A	809	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
12	B	812	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
12	B	819	CLA	CAC-C3C-C4C	2.96	128.64	124.79
12	B	830	CLA	CAA-C2A-C3A	-2.96	105.01	113.00
12	A	810	CLA	CMB-C2B-C1B	2.96	129.92	125.42
12	A	818	CLA	O2A-CGA-CBA	2.96	120.85	111.83
12	A	814	CLA	CMC-C2C-C1C	2.96	129.65	125.03
12	B	806	CLA	C4B-C3B-C2B	-2.96	103.63	107.30
12	A	841	CLA	C3B-C4B-NB	2.96	113.17	110.53
12	B	814	CLA	CAA-C2A-C3A	-2.95	105.02	113.00
12	B	814	CLA	CHD-C4C-NC	2.95	128.81	124.23
16	A	853	LHG	O8-C23-C24	2.95	120.11	111.15
12	A	831	CLA	C3B-C4B-NB	2.95	113.17	110.53
12	A	823	CLA	CAC-C3C-C4C	2.95	128.63	124.79
12	B	815	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
12	A	838	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
12	A	839	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
12	B	830	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
12	B	813	CLA	O2A-CGA-CBA	2.94	120.81	111.83
12	B	804	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
12	B	821	CLA	CHD-C4C-NC	2.94	128.79	124.23
12	B	828	CLA	CHD-C4C-NC	2.94	128.79	124.23
12	A	808	CLA	CHC-C1C-C2C	-2.94	118.59	126.95
12	B	812	CLA	CAC-C3C-C4C	2.94	128.61	124.79
12	B	824	CLA	C4C-C3C-C2C	-2.94	102.61	106.89
15	A	848	BCR	C27-C26-C25	2.94	126.67	122.70
11	A	801	CL0	CGD-CBD-CAD	-2.94	101.33	110.85
12	B	807	CLA	CAA-C2A-C3A	-2.94	105.06	113.00
12	A	821	CLA	CAC-C3C-C4C	2.94	128.61	124.79
12	B	817	CLA	CAC-C3C-C4C	2.93	128.61	124.79
12	B	812	CLA	C4B-C3B-C2B	-2.93	103.65	107.30
12	B	826	CLA	C4C-C3C-C2C	-2.93	102.62	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	811	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
12	B	831	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
12	A	808	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
12	A	813	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
12	A	806	CLA	CHC-C1C-C2C	-2.92	118.64	126.95
12	F	203	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
12	B	808	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
12	A	815	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
12	A	814	CLA	CAC-C3C-C4C	2.92	128.59	124.79
12	B	825	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
12	B	829	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
12	A	831	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
12	A	804	CLA	C4C-C3C-C2C	-2.92	102.65	106.89
12	B	813	CLA	C3B-C4B-NB	2.91	113.13	110.53
12	B	809	CLA	O2D-CGD-O1D	-2.91	118.17	123.85
12	B	817	CLA	CHC-C1C-C2C	-2.91	118.67	126.95
12	B	823	CLA	C3D-C2D-C1D	-2.91	101.86	105.83
12	A	809	CLA	CHC-C1C-C2C	-2.91	118.68	126.95
12	A	811	CLA	C4B-C3B-C2B	-2.91	103.69	107.30
12	A	805	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
12	A	830	CLA	C1-C2-C3	-2.91	121.43	126.20
12	A	839	CLA	C1-C2-C3	-2.91	122.06	126.76
12	A	819	CLA	C1-C2-C3	-2.91	121.44	126.20
12	A	820	CLA	CAC-C3C-C4C	2.90	128.57	124.79
12	A	818	CLA	CHD-C4C-NC	2.90	128.73	124.23
11	A	801	CL0	O2D-CGD-O1D	-2.90	118.20	123.85
12	B	815	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
12	B	807	CLA	CBC-CAC-C3C	-2.90	104.56	112.42
12	B	819	CLA	CHC-C1C-C2C	-2.90	118.70	126.95
12	B	809	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
12	B	814	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
12	B	805	CLA	CHB-C4A-NA	2.90	128.58	124.40
12	A	832	CLA	C4C-C3C-C2C	-2.90	102.68	106.89
12	B	822	CLA	CAC-C3C-C4C	2.89	128.56	124.79
12	A	840	CLA	CHC-C1C-C2C	-2.89	118.72	126.95
12	A	808	CLA	C3B-C4B-NB	2.89	113.11	110.53
12	B	824	CLA	C4B-C3B-C2B	-2.89	103.70	107.30
12	A	805	CLA	C4B-C3B-C2B	-2.89	103.70	107.30
12	B	822	CLA	C4B-C3B-C2B	-2.89	103.70	107.30
12	B	811	CLA	O2A-CGA-CBA	2.89	120.65	111.83
12	A	821	CLA	CMC-C2C-C1C	2.89	129.55	125.03
12	B	803	CLA	CMC-C2C-C1C	2.89	129.55	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	840	CLA	C1-C2-C3	-2.89	121.46	126.20
12	B	806	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
12	B	816	CLA	CAC-C3C-C4C	2.89	128.55	124.79
12	B	830	CLA	O2A-CGA-CBA	2.89	120.64	111.83
12	A	840	CLA	C3B-C4B-NB	2.89	113.11	110.53
12	A	835	CLA	O2A-CGA-CBA	2.89	120.63	111.83
12	B	819	CLA	C3C-C4C-NC	2.88	114.12	110.43
12	B	803	CLA	O2D-CGD-CBD	2.88	116.27	111.23
12	A	841	CLA	CHC-C1C-C2C	-2.88	118.77	126.95
12	A	831	CLA	C4C-C3C-C2C	-2.88	102.70	106.89
12	J	101	CLA	CHD-C4C-NC	2.87	128.69	124.23
12	A	827	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
12	A	812	CLA	C4C-C3C-C2C	-2.87	102.71	106.89
12	A	824	CLA	O2A-CGA-CBA	2.87	120.59	111.83
12	A	833	CLA	CHD-C4C-NC	2.87	128.68	124.23
12	B	830	CLA	CAC-C3C-C4C	2.87	128.52	124.79
17	B	837	LMG	O6-C1-O1	-2.87	103.27	110.04
12	B	819	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
12	A	808	CLA	C4C-C3C-C2C	-2.86	102.72	106.89
12	L	202	CLA	CHD-C4C-NC	2.86	128.67	124.23
12	A	830	CLA	CAC-C3C-C4C	2.86	128.51	124.79
12	B	804	CLA	CBA-CAA-C2A	2.86	122.31	113.79
12	B	819	CLA	C4B-C3B-C2B	-2.86	103.74	107.30
12	B	831	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
12	A	823	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
12	B	824	CLA	CHC-C1C-C2C	-2.86	118.83	126.95
12	B	818	CLA	C1-C2-C3	-2.86	121.52	126.20
12	B	803	CLA	CAA-C2A-C3A	-2.86	105.28	113.00
12	A	809	CLA	CMB-C2B-C1B	2.86	129.77	125.42
12	A	854	CLA	CHA-C1A-NA	-2.85	119.93	126.39
12	A	814	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
12	B	816	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
12	B	811	CLA	C4C-C3C-C2C	-2.85	102.74	106.89
12	A	835	CLA	C4B-C3B-C2B	-2.85	103.75	107.30
12	A	832	CLA	CAC-C3C-C4C	2.85	128.50	124.79
12	B	813	CLA	CHC-C1C-C2C	-2.85	118.85	126.95
12	B	831	CLA	CAC-C3C-C4C	2.85	128.50	124.79
12	B	801	CLA	CBC-CAC-C3C	-2.85	104.70	112.42
12	A	813	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
12	A	805	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
15	A	850	BCR	C15-C16-C17	-2.85	117.70	123.52
12	A	806	CLA	C3B-C4B-NB	2.84	113.07	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	829	CLA	CMB-C2B-C1B	2.84	129.75	125.42
15	A	848	BCR	C11-C10-C9	-2.84	123.29	127.28
12	A	838	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
12	A	827	CLA	CAA-C2A-C3A	-2.84	105.33	113.00
11	A	801	CL0	CMA-C3A-C2A	-2.84	103.17	114.13
12	B	825	CLA	CMB-C2B-C1B	2.84	129.74	125.42
12	A	836	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
13	B	833	PQN	C2M-C2-C3	-2.84	119.79	124.45
12	A	829	CLA	C4B-C3B-C2B	-2.84	103.78	107.30
12	A	807	CLA	C1-C2-C3	-2.83	121.56	126.20
12	B	817	CLA	CHD-C4C-NC	2.83	128.62	124.23
13	B	833	PQN	C11-C12-C13	-2.83	121.96	126.83
12	A	826	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
12	B	828	CLA	CHC-C1C-C2C	-2.82	118.92	126.95
12	B	814	CLA	O2A-CGA-CBA	2.82	120.44	111.83
12	A	840	CLA	C4B-C3B-C2B	-2.82	103.79	107.30
12	A	821	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
12	L	204	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
12	A	806	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
15	B	834	BCR	C15-C16-C17	-2.82	117.75	123.52
15	L	205	BCR	C27-C26-C25	2.82	126.51	122.70
12	B	827	CLA	CAA-C2A-C3A	-2.82	105.39	113.00
12	A	812	CLA	O2A-CGA-CBA	2.81	120.42	111.83
12	B	814	CLA	CAC-C3C-C4C	2.81	128.45	124.79
12	B	813	CLA	C1-C2-C3	-2.81	121.59	126.20
12	A	820	CLA	O2A-CGA-CBA	2.81	120.41	111.83
12	B	821	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
12	A	808	CLA	CHD-C4C-NC	2.81	128.59	124.23
15	A	850	BCR	C24-C23-C22	-2.81	122.08	126.23
12	A	813	CLA	CAC-C3C-C4C	2.81	128.44	124.79
12	B	817	CLA	O2A-CGA-CBA	2.81	120.39	111.83
12	L	202	CLA	C4C-C3C-C2C	-2.81	102.81	106.89
15	A	850	BCR	C15-C14-C13	-2.81	123.34	127.28
12	A	813	CLA	C3B-C4B-NB	2.80	113.03	110.53
12	A	839	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
12	A	828	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
12	A	842	CLA	CMB-C2B-C1B	2.80	129.69	125.42
12	A	829	CLA	C3B-C4B-NB	2.80	113.03	110.53
12	B	828	CLA	C3B-C4B-NB	2.80	113.03	110.53
12	A	809	CLA	CAC-C3C-C4C	2.80	128.44	124.79
12	L	204	CLA	CHD-C4C-NC	2.80	128.57	124.23
12	B	807	CLA	O2A-CGA-CBA	2.80	120.36	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	807	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
12	B	809	CLA	C4A-NA-C1A	-2.79	105.41	106.68
12	A	807	CLA	O2A-CGA-CBA	2.79	120.35	111.83
12	A	811	CLA	C1-C2-C3	-2.79	121.62	126.20
12	B	805	CLA	O2A-CGA-CBA	2.79	120.34	111.83
12	B	821	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
12	B	826	CLA	C4B-C3B-C2B	-2.79	103.83	107.30
12	F	203	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
12	B	827	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
12	A	825	CLA	CHC-C1C-C2C	-2.79	119.03	126.95
12	L	203	CLA	C4C-C3C-C2C	-2.79	102.84	106.89
12	B	813	CLA	O2D-CGD-O1D	-2.79	118.43	123.85
12	A	826	CLA	CMB-C2B-C1B	2.78	129.66	125.42
12	B	815	CLA	CMB-C2B-C1B	2.78	129.66	125.42
12	A	830	CLA	CAA-C2A-C3A	-2.78	105.48	113.00
12	A	816	CLA	CAC-C3C-C4C	2.78	128.41	124.79
12	B	817	CLA	C1-C2-C3	-2.78	121.64	126.20
12	B	814	CLA	C1-C2-C3	-2.78	121.64	126.20
12	B	820	CLA	CHC-C1C-C2C	-2.78	119.05	126.95
12	A	802	CLA	C3B-C4B-NB	2.78	113.01	110.53
12	A	815	CLA	C4B-C3B-C2B	-2.78	103.85	107.30
12	A	803	CLA	CAA-C2A-C3A	-2.78	105.49	113.00
12	B	828	CLA	CAC-C3C-C4C	2.78	128.40	124.79
12	B	819	CLA	CHD-C4C-NC	2.78	128.53	124.23
12	A	828	CLA	CHD-C4C-NC	2.77	128.53	124.23
12	B	808	CLA	C4C-C3C-C2C	-2.77	102.85	106.89
12	A	829	CLA	CHC-C1C-C2C	-2.77	119.06	126.95
12	A	832	CLA	C3B-C4B-NB	2.77	113.00	110.53
12	B	830	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
12	B	825	CLA	CHC-C1C-C2C	-2.77	119.07	126.95
12	A	810	CLA	CHD-C4C-NC	2.77	128.53	124.23
12	A	815	CLA	CHD-C4C-NC	2.77	128.53	124.23
12	A	808	CLA	CAC-C3C-C4C	2.77	128.39	124.79
12	A	808	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
12	A	802	CLA	CHD-C4C-NC	2.77	128.52	124.23
12	B	827	CLA	CMB-C2B-C1B	2.77	129.63	125.42
12	B	830	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
12	B	808	CLA	CBC-CAC-C3C	-2.77	104.92	112.42
11	A	801	CL0	O2A-CGA-CBA	2.76	120.27	111.83
12	A	803	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
12	B	817	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
12	A	818	CLA	C1-C2-C3	-2.76	121.67	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	831	CLA	C4B-C3B-C2B	-2.76	103.87	107.30
12	A	828	CLA	C4-C3-C5	2.76	120.02	115.23
12	A	829	CLA	CMC-C2C-C1C	2.76	129.35	125.03
12	A	827	CLA	CHC-C1C-C2C	-2.76	119.11	126.95
12	L	204	CLA	O2A-CGA-CBA	2.76	120.24	111.83
15	B	835	BCR	C15-C16-C17	-2.76	117.88	123.52
12	A	833	CLA	C4C-C3C-C2C	-2.76	102.88	106.89
12	A	802	CLA	CHC-C1C-C2C	-2.75	119.12	126.95
12	B	811	CLA	CMB-C2B-C1B	2.75	129.61	125.42
12	A	814	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
12	A	854	CLA	CMC-C2C-C1C	2.75	129.34	125.03
12	A	810	CLA	CAC-C3C-C4C	2.75	128.37	124.79
12	B	822	CLA	O2A-CGA-CBA	2.75	120.22	111.83
12	B	828	CLA	C4B-C3B-C2B	-2.75	103.88	107.30
12	B	803	CLA	O2A-CGA-CBA	2.75	120.22	111.83
12	B	832	CLA	O2A-CGA-CBA	2.75	120.22	111.83
12	B	829	CLA	CHB-C4A-NA	2.75	128.36	124.40
12	A	813	CLA	CAA-C2A-C3A	-2.75	105.58	113.00
12	A	814	CLA	CHC-C1C-C2C	-2.74	119.15	126.95
12	A	841	CLA	C4C-C3C-C2C	-2.74	102.90	106.89
12	B	818	CLA	O2A-CGA-CBA	2.74	120.20	111.83
12	A	831	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
12	A	817	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
12	A	834	CLA	CHB-C4A-NA	2.74	128.36	124.40
12	B	818	CLA	CAC-C3C-C4C	2.74	128.36	124.79
12	B	807	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
12	B	826	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
12	A	809	CLA	CHD-C4C-NC	2.74	128.47	124.23
12	B	823	CLA	C4C-C3C-C2C	-2.74	102.91	106.89
12	A	806	CLA	CMB-C2B-C1B	2.74	129.58	125.42
15	A	848	BCR	C16-C15-C14	-2.73	117.93	123.52
12	B	832	CLA	CMB-C2B-C1B	2.73	129.58	125.42
15	M	101	BCR	C27-C26-C25	2.73	126.39	122.70
12	A	810	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
12	A	837	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
12	B	801	CLA	C4C-C3C-C2C	-2.73	102.92	106.89
12	A	843	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
12	B	820	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
12	L	203	CLA	CBC-CAC-C3C	-2.73	105.03	112.42
12	A	820	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
12	B	810	CLA	O2A-CGA-CBA	2.72	120.14	111.83
12	A	854	CLA	CHC-C1C-C2C	-2.72	119.21	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	801	CLA	O2A-CGA-CBA	2.72	120.13	111.83
12	B	812	CLA	CHD-C4C-NC	2.72	128.45	124.23
12	A	804	CLA	CAC-C3C-C4C	2.72	128.33	124.79
12	A	827	CLA	C3B-C4B-NB	2.72	112.96	110.53
12	A	824	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
12	A	823	CLA	C1-C2-C3	-2.72	121.75	126.20
12	B	804	CLA	C3B-C4B-NB	2.72	112.95	110.53
12	B	823	CLA	O2A-CGA-CBA	2.72	120.11	111.83
12	B	825	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
12	B	824	CLA	CHD-C4C-NC	2.71	128.44	124.23
11	A	801	CL0	C4C-C3C-C2C	-2.71	102.65	113.37
12	B	830	CLA	CHD-C4C-NC	2.71	128.44	124.23
12	A	816	CLA	C4C-C3C-C2C	-2.71	102.94	106.89
12	A	821	CLA	C4-C3-C5	2.71	119.93	115.23
15	B	836	BCR	C27-C26-C25	2.71	126.37	122.70
12	A	807	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
12	A	835	CLA	C1-C2-C3	-2.71	121.76	126.20
12	B	806	CLA	CHB-C4A-NA	2.71	128.31	124.40
12	B	813	CLA	CMB-C2B-C1B	2.71	129.54	125.42
12	B	805	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
12	A	842	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
12	A	838	CLA	CHD-C4C-NC	2.70	128.42	124.23
12	L	203	CLA	CHD-C4C-NC	2.70	128.42	124.23
12	A	831	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
15	A	848	BCR	C40-C30-C25	2.70	114.48	110.24
12	L	203	CLA	C4B-C3B-C2B	-2.70	103.94	107.30
12	A	821	CLA	CHC-C1C-C2C	-2.70	119.28	126.95
12	A	824	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
12	A	837	CLA	O2A-CGA-CBA	2.70	120.06	111.83
12	A	806	CLA	CMC-C2C-C1C	2.69	129.24	125.03
12	A	839	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
12	A	824	CLA	C4C-C3C-C2C	-2.69	102.97	106.89
12	B	822	CLA	CHD-C4C-NC	2.69	128.40	124.23
15	A	846	BCR	C15-C14-C13	-2.69	123.50	127.28
12	B	822	CLA	CMB-C2B-C1B	2.69	129.51	125.42
12	A	821	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
12	B	808	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
12	B	832	CLA	C4C-C3C-C2C	-2.69	102.98	106.89
12	A	827	CLA	CMB-C2B-C1B	2.68	129.51	125.42
12	A	826	CLA	C4C-C3C-C2C	-2.68	102.98	106.89
12	A	828	CLA	C1-C2-C3	-2.68	121.80	126.20
12	A	834	CLA	C1-C2-C3	-2.68	121.80	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	203	CLA	CAA-C2A-C3A	-2.68	105.75	113.00
12	A	837	CLA	CAC-C3C-C4C	2.68	128.28	124.79
12	A	836	CLA	CHD-C4C-NC	2.68	128.39	124.23
12	B	812	CLA	CMB-C2B-C1B	2.68	129.50	125.42
12	A	817	CLA	CHD-C4C-NC	2.68	128.38	124.23
12	B	814	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
15	A	847	BCR	C24-C23-C22	-2.68	122.28	126.23
12	B	811	CLA	CMD-C2D-C3D	-2.67	121.56	127.69
12	A	816	CLA	CHD-C4C-NC	2.67	128.38	124.23
12	A	838	CLA	CAA-C2A-C3A	-2.67	105.77	113.00
15	J	104	BCR	C27-C26-C25	2.67	126.32	122.70
15	B	835	BCR	C11-C10-C9	-2.67	123.53	127.28
12	B	814	CLA	CHB-C4A-NA	2.67	128.25	124.40
12	B	819	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
15	A	849	BCR	C7-C8-C9	-2.67	122.29	126.23
12	A	841	CLA	CAC-C3C-C4C	2.67	128.26	124.79
12	A	813	CLA	CHD-C4C-NC	2.67	128.37	124.23
12	B	805	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
12	B	818	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
12	A	832	CLA	CAA-CBA-CGA	-2.66	105.64	113.21
12	A	825	CLA	O2A-CGA-CBA	2.66	119.96	111.83
12	B	827	CLA	CHD-C4C-NC	2.66	128.36	124.23
12	A	817	CLA	CMB-C2B-C1B	2.66	129.47	125.42
15	A	848	BCR	C30-C25-C26	-2.66	119.00	122.64
12	B	824	CLA	CAC-C3C-C4C	2.66	128.25	124.79
12	A	812	CLA	CHD-C4C-NC	2.66	128.36	124.23
12	A	832	CLA	C1-C2-C3	-2.66	121.84	126.20
12	A	854	CLA	O2A-C1-C2	2.66	118.34	108.11
12	A	822	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
12	A	823	CLA	O2A-CGA-CBA	2.66	119.94	111.83
12	B	819	CLA	CHB-C1B-C2B	-2.66	119.72	127.43
12	A	840	CLA	CMC-C2C-C1C	2.66	129.18	125.03
12	A	807	CLA	CHD-C4C-NC	2.66	128.35	124.23
15	I	101	BCR	C30-C25-C26	-2.65	119.01	122.64
12	A	841	CLA	CMB-C2B-C1B	2.65	129.46	125.42
12	A	839	CLA	CMC-C2C-C1C	2.65	129.18	125.03
12	A	832	CLA	O2A-CGA-CBA	2.65	119.92	111.83
12	A	843	CLA	CMB-C2B-C1B	2.65	129.45	125.42
15	A	851	BCR	C1-C6-C5	-2.65	119.02	122.64
12	F	203	CLA	CAA-C2A-C3A	-2.65	105.84	113.00
12	F	203	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
12	B	805	CLA	C4B-C3B-C2B	-2.65	104.01	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	813	CLA	CHD-C4C-NC	2.65	128.34	124.23
12	A	834	CLA	CHD-C4C-NC	2.65	128.34	124.23
12	A	815	CLA	CAA-C2A-C3A	-2.65	105.85	113.00
15	L	206	BCR	C24-C23-C22	-2.65	122.32	126.23
12	A	832	CLA	C4-C3-C5	2.64	119.82	115.23
12	L	204	CLA	C1-C2-C3	-2.64	121.87	126.20
12	A	829	CLA	CHD-C4C-NC	2.64	128.33	124.23
12	A	843	CLA	CHD-C4C-NC	2.64	128.33	124.23
12	B	829	CLA	C4C-C3C-C2C	-2.64	103.05	106.89
12	B	827	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
12	A	813	CLA	C4B-C3B-C2B	-2.64	104.02	107.30
12	A	818	CLA	C3B-C4B-NB	2.64	112.89	110.53
12	A	820	CLA	CHD-C4C-NC	2.64	128.32	124.23
15	B	836	BCR	C15-C16-C17	-2.64	118.13	123.52
12	A	840	CLA	CHD-C4C-NC	2.63	128.32	124.23
12	A	815	CLA	CHB-C4A-NA	2.63	128.20	124.40
12	B	809	CLA	O2A-CGA-CBA	2.63	119.86	111.83
12	A	802	CLA	CHB-C1B-C2B	-2.63	119.79	127.43
12	B	829	CLA	O2A-CGA-CBA	2.63	119.84	111.83
12	A	816	CLA	CMB-C2B-C1B	2.63	129.42	125.42
12	A	816	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
12	A	826	CLA	C1-C2-C3	-2.63	121.89	126.20
12	A	828	CLA	CMC-C2C-C1C	2.63	129.14	125.03
12	A	825	CLA	CMC-C2C-C1C	2.62	129.14	125.03
12	A	825	CLA	C1-C2-C3	-2.62	121.90	126.20
12	A	803	CLA	CHD-C4C-NC	2.62	128.30	124.23
12	J	101	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
12	A	815	CLA	CMB-C2B-C1B	2.62	129.41	125.42
12	A	831	CLA	CHD-C4C-NC	2.62	128.29	124.23
11	A	801	CL0	C1C-CHC-C4B	2.61	125.42	116.07
12	B	830	CLA	CMB-C2B-C1B	2.61	129.40	125.42
12	B	816	CLA	CHD-C4C-NC	2.61	128.28	124.23
15	B	836	BCR	C10-C11-C12	-2.61	115.63	123.20
12	A	817	CLA	CAC-C3C-C4C	2.61	128.19	124.79
12	B	828	CLA	CAA-C2A-C3A	-2.61	105.95	113.00
12	B	831	CLA	O2A-CGA-CBA	2.61	119.79	111.83
12	A	814	CLA	C3B-C4B-NB	2.61	112.86	110.53
12	L	203	CLA	CAC-C3C-C4C	2.61	128.18	124.79
12	A	830	CLA	O2A-CGA-CBA	2.61	119.78	111.83
12	B	822	CLA	C1-C2-C3	-2.60	121.93	126.20
12	A	839	CLA	CMB-C2B-C1B	2.60	129.38	125.42
12	A	839	CLA	CAC-C3C-C4C	2.60	128.17	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	803	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
12	B	803	CLA	CBC-CAC-C3C	-2.59	105.39	112.42
12	L	204	CLA	C4B-C3B-C2B	-2.59	104.08	107.30
15	L	206	BCR	C15-C16-C17	-2.59	118.22	123.52
15	L	205	BCR	C11-C10-C9	-2.58	123.65	127.28
12	A	820	CLA	C4-C3-C5	2.58	119.71	115.23
15	F	201	BCR	C27-C26-C25	2.58	126.20	122.70
12	A	806	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
12	B	815	CLA	CHD-C4C-NC	2.58	128.24	124.23
12	L	203	CLA	O2A-CGA-CBA	2.58	119.70	111.83
12	A	812	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
12	F	203	CLA	CMB-C2B-C1B	2.58	129.34	125.42
12	A	817	CLA	CHB-C4A-NA	2.58	128.12	124.40
12	B	829	CLA	CMB-C2B-C1B	2.57	129.34	125.42
12	A	837	CLA	C4-C3-C5	2.57	119.16	116.13
12	A	811	CLA	CMB-C2B-C1B	2.57	129.34	125.42
12	B	823	CLA	O1D-CGD-CBD	-2.57	119.45	124.52
12	B	809	CLA	CBA-CAA-C2A	2.57	121.44	113.79
12	A	804	CLA	CHB-C4A-NA	2.57	128.11	124.40
12	B	816	CLA	CHB-C4A-NA	2.57	128.11	124.40
12	A	840	CLA	CAA-C2A-C3A	-2.57	106.06	113.00
12	A	827	CLA	C1-C2-C3	-2.57	121.99	126.20
12	B	825	CLA	C4-C3-C5	2.57	119.68	115.23
12	A	841	CLA	C4B-C3B-C2B	-2.57	104.11	107.30
12	B	815	CLA	CHB-C4A-NA	2.57	128.10	124.40
12	A	823	CLA	CHD-C4C-NC	2.56	128.21	124.23
12	A	804	CLA	CHC-C1C-C2C	-2.56	119.66	126.95
15	B	835	BCR	C15-C14-C13	-2.56	123.68	127.28
15	B	835	BCR	C3-C4-C5	-2.56	109.49	114.06
12	A	820	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
12	B	820	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
12	A	835	CLA	CHB-C4A-NA	2.56	128.09	124.40
12	B	808	CLA	C7-C6-C5	-2.56	106.44	113.26
12	L	203	CLA	CHB-C4A-NA	2.56	128.09	124.40
12	B	813	CLA	C4-C3-C5	2.56	119.67	115.23
12	B	802	CLA	CMA-C3A-C4A	-2.56	104.90	111.77
12	A	832	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
12	A	833	CLA	CAC-C3C-C4C	2.55	128.11	124.79
12	B	825	CLA	CHD-C4C-NC	2.55	128.19	124.23
12	A	816	CLA	CBC-CAC-C3C	-2.55	105.51	112.42
12	B	814	CLA	CMB-C2B-C1B	2.55	129.30	125.42
12	B	811	CLA	O2D-CGD-O1D	-2.55	118.89	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	204	CLA	CMB-C2B-C1B	2.55	129.29	125.42
12	A	804	CLA	C4B-C3B-C2B	-2.55	104.14	107.30
12	A	826	CLA	C3B-C4B-NB	2.55	112.80	110.53
12	B	818	CLA	C4C-C3C-C2C	-2.55	103.19	106.89
12	A	824	CLA	CHD-C4C-NC	2.54	128.18	124.23
12	A	843	CLA	O2A-CGA-CBA	2.54	119.59	111.83
12	A	826	CLA	C4-C3-C5	2.54	119.64	115.23
12	B	808	CLA	O2A-CGA-CBA	2.54	119.59	111.83
12	B	802	CLA	CHD-C4C-NC	2.54	128.17	124.23
12	A	819	CLA	O2A-CGA-CBA	2.54	119.58	111.83
13	B	833	PQN	C16-C15-C13	-2.54	107.28	113.47
12	A	819	CLA	CHD-C4C-NC	2.54	128.16	124.23
12	A	842	CLA	CHD-C4C-NC	2.54	128.16	124.23
12	B	829	CLA	CAC-C3C-C4C	2.54	128.09	124.79
12	A	833	CLA	CBC-CAC-C3C	-2.54	105.55	112.42
12	A	826	CLA	CAA-C2A-C1A	-2.53	103.67	111.97
12	A	810	CLA	CAA-C2A-C3A	-2.53	106.16	113.00
12	B	832	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
12	A	836	CLA	O1D-CGD-CBD	-2.53	119.53	124.52
12	B	804	CLA	C4B-C3B-C2B	-2.53	104.16	107.30
16	A	853	LHG	C11-C10-C9	-2.53	101.59	114.37
15	A	846	BCR	C15-C16-C17	-2.53	118.35	123.52
12	B	803	CLA	C4A-NA-C1A	-2.53	105.53	106.68
12	A	836	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
12	B	802	CLA	CHB-C4A-NA	2.53	128.04	124.40
12	B	824	CLA	O2A-CGA-CBA	2.53	119.53	111.83
12	B	823	CLA	C1-C2-C3	-2.52	122.06	126.20
12	L	204	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
12	B	809	CLA	CHB-C4A-NA	2.52	128.04	124.40
12	A	821	CLA	CHB-C4A-NA	2.52	128.04	124.40
12	B	811	CLA	CHB-C4A-NA	2.52	128.04	124.40
12	B	826	CLA	CHD-C4C-NC	2.52	128.14	124.23
12	A	841	CLA	CMC-C2C-C1C	2.52	128.97	125.03
15	J	104	BCR	C11-C10-C9	-2.52	123.75	127.28
12	B	821	CLA	CHB-C4A-NA	2.51	128.03	124.40
12	A	833	CLA	C4-C3-C5	2.51	119.59	115.23
12	B	819	CLA	CMB-C2B-C3B	2.51	132.46	126.55
17	B	837	LMG	O1-C7-C8	-2.51	104.71	110.82
12	A	842	CLA	C4-C3-C5	2.51	119.58	115.23
15	A	850	BCR	C28-C27-C26	-2.51	109.58	114.06
12	A	821	CLA	C4B-C3B-C2B	-2.51	104.19	107.30
12	A	833	CLA	C4B-C3B-C2B	-2.51	104.19	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	841	CLA	C1-C2-C3	-2.51	122.09	126.20
12	A	821	CLA	C3B-C4B-NB	2.51	112.77	110.53
12	A	805	CLA	CMA-C3A-C4A	-2.50	105.04	111.77
12	B	832	CLA	C1-C2-C3	-2.50	122.09	126.20
12	A	830	CLA	O1D-CGD-CBD	-2.50	119.58	124.52
12	A	822	CLA	CMB-C2B-C1B	2.50	129.23	125.42
12	B	810	CLA	CHD-C4C-NC	2.50	128.11	124.23
12	A	834	CLA	C4B-C3B-C2B	-2.50	104.19	107.30
15	A	846	BCR	C38-C26-C27	-2.50	108.26	113.60
12	L	204	CLA	C4-C3-C5	2.50	119.57	115.23
12	A	824	CLA	CBC-CAC-C3C	-2.50	105.64	112.42
12	A	807	CLA	CBC-CAC-C3C	-2.50	105.64	112.42
12	A	814	CLA	CHB-C4A-NA	2.50	128.01	124.40
12	B	826	CLA	O1D-CGD-CBD	-2.50	119.59	124.52
12	B	817	CLA	C3B-C4B-NB	2.50	112.76	110.53
12	A	820	CLA	CAA-C2A-C3A	-2.50	106.25	113.00
12	A	822	CLA	CMC-C2C-C1C	2.50	128.93	125.03
12	A	818	CLA	CHB-C4A-NA	2.50	128.00	124.40
12	A	805	CLA	C4-C3-C5	2.49	119.56	115.23
12	J	101	CLA	CHB-C4A-NA	2.49	128.00	124.40
12	B	804	CLA	CHD-C4C-NC	2.49	128.09	124.23
15	F	202	BCR	C27-C26-C25	2.49	126.06	122.70
12	A	827	CLA	O1D-CGD-CBD	-2.49	119.61	124.52
12	A	832	CLA	CBC-CAC-C3C	-2.49	105.68	112.42
12	B	822	CLA	CMA-C3A-C4A	-2.49	105.09	111.77
15	A	847	BCR	C15-C14-C13	-2.48	123.79	127.28
12	A	809	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
12	B	831	CLA	CHD-C4C-NC	2.48	128.08	124.23
12	A	833	CLA	CHB-C4A-NA	2.48	127.98	124.40
12	B	813	CLA	C4B-C3B-C2B	-2.48	104.22	107.30
12	B	821	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
12	B	810	CLA	C4C-C3C-C2C	-2.48	103.29	106.89
12	B	810	CLA	CAA-C2A-C3A	-2.47	106.31	113.00
15	L	206	BCR	C3-C4-C5	-2.47	109.64	114.06
12	A	823	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
15	L	206	BCR	C29-C30-C25	2.47	114.03	110.44
12	B	832	CLA	CBC-CAC-C3C	-2.47	105.72	112.42
12	A	819	CLA	C2A-C3A-C4A	-2.47	97.88	101.87
12	A	816	CLA	O2A-CGA-CBA	2.47	119.37	111.83
12	B	820	CLA	OBD-CAD-C3D	-2.47	122.64	128.42
12	A	817	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
15	A	851	BCR	C28-C27-C26	-2.47	109.66	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	816	CLA	CHB-C4A-NA	2.47	127.96	124.40
15	L	205	BCR	C15-C14-C13	-2.47	123.82	127.28
12	A	808	CLA	CMC-C2C-C1C	2.46	128.88	125.03
12	B	806	CLA	C4-C3-C5	2.46	119.50	115.23
12	A	835	CLA	CHD-C4C-NC	2.46	128.05	124.23
15	M	101	BCR	C15-C16-C17	-2.46	118.48	123.52
12	B	801	CLA	CHB-C1B-C2B	-2.46	120.28	127.43
12	B	827	CLA	CBC-CAC-C3C	-2.46	105.75	112.42
15	A	851	BCR	C29-C30-C25	2.46	114.01	110.44
12	A	831	CLA	CHB-C4A-NA	2.46	127.95	124.40
12	A	807	CLA	CHB-C4A-NA	2.46	127.95	124.40
12	A	836	CLA	CHB-C4A-NA	2.46	127.95	124.40
12	A	820	CLA	CMB-C2B-C1B	2.46	129.16	125.42
12	B	823	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
12	B	825	CLA	C3B-C4B-NB	2.46	112.72	110.53
12	A	811	CLA	CHD-C4C-NC	2.46	128.04	124.23
12	A	808	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	B	814	CLA	CMC-C2C-C1C	2.45	128.87	125.03
12	B	802	CLA	O2A-CGA-CBA	2.45	119.31	111.83
12	A	804	CLA	C3B-C4B-NB	2.45	112.72	110.53
12	B	813	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	A	811	CLA	CHB-C4A-NA	2.45	127.94	124.40
12	B	816	CLA	C1-C2-C3	-2.45	122.19	126.20
12	A	806	CLA	C4C-C3C-C2C	-2.45	103.33	106.89
12	A	840	CLA	CHB-C4A-NA	2.45	127.93	124.40
15	A	847	BCR	C15-C16-C17	-2.45	118.51	123.52
12	B	809	CLA	O2A-CGA-O1A	-2.45	117.51	123.63
12	A	805	CLA	C1-C2-C3	-2.45	122.19	126.20
12	B	805	CLA	C4-C3-C5	2.44	119.47	115.23
12	A	803	CLA	CMB-C2B-C1B	2.44	129.14	125.42
12	L	202	CLA	CAC-C3C-C4C	2.44	127.97	124.79
12	A	810	CLA	CBC-CAC-C3C	-2.44	105.79	112.42
12	A	838	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
12	B	807	CLA	CMB-C2B-C1B	2.44	129.14	125.42
12	B	813	CLA	O2A-CGA-O1A	-2.44	117.52	123.63
12	B	820	CLA	CMB-C2B-C1B	2.44	129.14	125.42
12	A	838	CLA	CBC-CAC-C3C	-2.44	105.80	112.42
12	A	826	CLA	CBC-CAC-C3C	-2.44	105.81	112.42
12	A	806	CLA	CBC-CAC-C3C	-2.44	105.81	112.42
12	A	825	CLA	CHD-C4C-NC	2.44	128.01	124.23
12	B	818	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
12	B	803	CLA	CHB-C4A-NA	2.44	127.92	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	827	CLA	CHB-C4A-NA	2.44	127.92	124.40
12	A	813	CLA	O2D-CGD-O1D	-2.44	119.11	123.85
12	A	842	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
15	I	101	BCR	C11-C10-C9	-2.43	123.87	127.28
12	B	828	CLA	CMC-C2C-C1C	2.43	128.83	125.03
15	J	102	BCR	C15-C16-C17	-2.43	118.55	123.52
12	B	806	CLA	O2A-CGA-O1A	-2.42	117.56	123.63
12	A	837	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
11	A	801	CL0	C3D-C4D-ND	2.42	116.82	112.94
12	A	833	CLA	C7-C6-C5	-2.42	106.81	113.26
12	B	818	CLA	CMC-C2C-C1C	2.42	128.81	125.03
12	A	820	CLA	CHB-C4A-NA	2.42	127.89	124.40
12	B	826	CLA	C4-C3-C5	2.42	119.42	115.23
12	A	806	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	A	846	BCR	C11-C10-C9	-2.42	123.89	127.28
12	B	819	CLA	CHB-C4A-NA	2.42	127.89	124.40
12	A	839	CLA	CBC-CAC-C3C	-2.42	105.87	112.42
12	A	812	CLA	C1-C2-C3	-2.41	122.24	126.20
12	A	842	CLA	C1-C2-C3	-2.41	122.24	126.20
12	B	801	CLA	CHD-C4C-NC	2.41	127.97	124.23
12	A	807	CLA	CMB-C2B-C1B	2.41	129.09	125.42
12	B	812	CLA	O2D-CGD-O1D	-2.41	119.16	123.85
12	B	831	CLA	C1-C2-C3	-2.41	122.25	126.20
16	A	852	LHG	C11-C10-C9	-2.41	102.19	114.37
12	B	813	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
12	B	817	CLA	CHB-C4A-NA	2.41	127.87	124.40
12	B	822	CLA	CHB-C4A-NA	2.41	127.87	124.40
12	A	827	CLA	CAC-C3C-C4C	2.41	127.92	124.79
12	A	833	CLA	CMA-C3A-C2A	-2.40	104.69	113.98
12	L	202	CLA	CBC-CAC-C3C	-2.40	105.91	112.42
12	B	806	CLA	CHD-C4C-NC	2.40	127.96	124.23
12	B	811	CLA	CHA-C1A-NA	-2.40	120.95	126.39
12	A	806	CLA	C4-C3-C5	2.40	119.39	115.23
12	F	203	CLA	CHD-C4C-NC	2.40	127.95	124.23
12	B	828	CLA	CMB-C2B-C1B	2.40	129.07	125.42
12	B	802	CLA	CMC-C2C-C1C	2.40	128.78	125.03
12	A	835	CLA	CBC-CAC-C3C	-2.40	105.92	112.42
12	B	801	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
16	A	852	LHG	C20-C19-C18	-2.39	102.27	114.37
12	B	809	CLA	CMB-C2B-C1B	2.39	129.06	125.42
12	A	837	CLA	CHD-C4C-NC	2.39	127.94	124.23
16	A	852	LHG	O8-C23-C24	2.39	119.13	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	811	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
15	A	850	BCR	C29-C30-C25	2.39	113.91	110.44
12	A	821	CLA	C1-C2-C3	-2.39	122.28	126.20
12	A	817	CLA	C4-C3-C5	2.39	119.38	115.23
12	B	808	CLA	CBA-CAA-C2A	2.39	120.90	113.79
12	B	804	CLA	CHC-C1C-NC	2.39	127.91	124.31
12	A	810	CLA	CHB-C4A-NA	2.39	127.84	124.40
11	A	801	CL0	CMC-C2C-C1C	2.39	129.03	124.73
12	A	821	CLA	CBC-CAC-C3C	-2.39	105.95	112.42
12	A	813	CLA	CMB-C2B-C1B	2.38	129.05	125.42
12	A	827	CLA	C4-C3-C5	2.38	119.37	115.23
12	A	827	CLA	CHB-C4A-NA	2.38	127.84	124.40
15	A	847	BCR	C11-C10-C9	-2.38	123.93	127.28
12	B	818	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
15	L	201	BCR	C15-C14-C13	-2.38	123.94	127.28
12	A	831	CLA	CMC-C2C-C1C	2.38	128.76	125.03
12	A	811	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
15	I	101	BCR	C7-C8-C9	-2.38	122.71	126.23
12	A	809	CLA	CMC-C2C-C1C	2.38	128.76	125.03
12	B	820	CLA	C3B-C4B-NB	2.38	112.66	110.53
12	A	824	CLA	CHB-C4A-NA	2.38	127.83	124.40
12	B	832	CLA	CHD-C4C-NC	2.38	127.92	124.23
12	A	813	CLA	CHB-C4A-NA	2.38	127.83	124.40
12	A	843	CLA	CHB-C4A-NA	2.38	127.83	124.40
12	B	810	CLA	C4-C3-C5	2.37	119.34	115.23
12	B	815	CLA	CBC-CAC-C3C	-2.37	106.00	112.42
12	A	817	CLA	C1-C2-C3	-2.37	122.32	126.20
12	A	838	CLA	O1D-CGD-CBD	-2.37	119.85	124.52
12	B	816	CLA	O2A-CGA-CBA	2.37	119.05	111.83
12	A	819	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
12	B	801	CLA	CMC-C2C-C1C	2.36	128.73	125.03
12	A	854	CLA	C4D-C3D-CAD	-2.36	105.54	108.11
12	A	812	CLA	CMB-C2B-C1B	2.36	129.01	125.42
12	B	828	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
15	A	848	BCR	C7-C8-C9	-2.36	122.74	126.23
12	B	811	CLA	CHD-C4C-NC	2.36	127.89	124.23
15	L	206	BCR	C15-C14-C13	-2.36	123.97	127.28
15	L	201	BCR	C27-C26-C25	2.36	125.89	122.70
12	A	831	CLA	CMB-C2B-C1B	2.36	129.01	125.42
12	A	837	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
12	A	838	CLA	CHB-C4A-NA	2.36	127.80	124.40
15	L	206	BCR	C28-C27-C26	-2.36	109.85	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	812	CLA	CMA-C3A-C2A	-2.35	104.88	113.98
12	B	825	CLA	CHB-C4A-NA	2.35	127.79	124.40
12	L	202	CLA	CHB-C4A-NA	2.35	127.79	124.40
12	A	833	CLA	O2A-CGA-O1A	-2.35	117.75	123.63
12	B	807	CLA	C4C-C3C-C2C	-2.35	103.47	106.89
15	F	202	BCR	C16-C15-C14	-2.35	118.71	123.52
12	A	808	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
12	B	802	CLA	CBC-CAC-C3C	-2.35	106.05	112.42
12	B	803	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
12	B	811	CLA	CBA-CAA-C2A	2.35	120.78	113.79
12	A	836	CLA	CBC-CAC-C3C	-2.34	106.06	112.42
12	B	812	CLA	CHB-C4A-NA	2.34	127.78	124.40
16	A	852	LHG	O8-C23-O10	-2.34	117.77	123.63
12	A	854	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
12	A	830	CLA	CHD-C4C-NC	2.34	127.86	124.23
12	B	819	CLA	CAA-C2A-C1A	-2.34	104.31	111.97
12	A	828	CLA	CHA-C1A-NA	-2.34	121.10	126.39
12	A	830	CLA	CHB-C4A-NA	2.34	127.77	124.40
12	B	819	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
12	L	202	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
17	B	837	LMG	O3-C3-C2	-2.34	104.87	110.38
12	B	818	CLA	C2A-C3A-C4A	-2.33	98.10	101.87
12	A	833	CLA	CMA-C3A-C4A	-2.33	105.51	111.77
12	B	826	CLA	CBC-CAC-C3C	-2.33	106.11	112.42
12	A	854	CLA	CHD-C4C-NC	2.33	127.84	124.23
12	A	839	CLA	CHB-C4A-NA	2.33	127.76	124.40
15	L	201	BCR	C24-C23-C22	-2.32	122.80	126.23
12	B	821	CLA	C1-C2-C3	-2.32	122.39	126.20
12	B	802	CLA	C1-C2-C3	-2.32	122.39	126.20
12	A	826	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
12	B	811	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
12	B	819	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
15	B	836	BCR	C21-C20-C19	-2.32	116.48	123.20
12	A	822	CLA	C4C-C3C-C2C	-2.31	103.52	106.89
12	B	816	CLA	O2D-CGD-O1D	-2.31	119.34	123.85
12	A	817	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
12	A	828	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
15	F	201	BCR	C15-C14-C13	-2.31	124.04	127.28
12	L	203	CLA	O2D-CGD-O1D	-2.31	119.36	123.85
15	I	101	BCR	C15-C14-C13	-2.31	124.04	127.28
15	B	834	BCR	C15-C14-C13	-2.31	124.05	127.28
12	A	830	CLA	C6-C5-C3	-2.30	107.86	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	J	101	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
12	J	101	CLA	CMB-C2B-C1B	2.30	128.93	125.42
12	B	803	CLA	C5-C3-C2	-2.30	116.00	121.17
12	A	803	CLA	CHB-C4A-NA	2.30	127.72	124.40
15	F	202	BCR	C11-C10-C9	-2.30	124.05	127.28
12	B	811	CLA	CMC-C2C-C1C	2.30	128.63	125.03
12	A	837	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
13	A	844	PQN	C11-C3-C2	-2.30	120.95	124.89
16	A	852	LHG	C27-C26-C25	-2.30	102.74	114.37
12	A	831	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
12	A	812	CLA	CHB-C4A-NA	2.30	127.72	124.40
13	B	833	PQN	C11-C3-C2	-2.30	120.95	124.89
12	A	842	CLA	CHB-C4A-NA	2.30	127.71	124.40
12	B	832	CLA	CHB-C4A-NA	2.30	127.71	124.40
12	A	826	CLA	O2D-CGD-O1D	-2.30	119.38	123.85
12	B	831	CLA	CHB-C4A-NA	2.30	127.71	124.40
12	B	829	CLA	O2A-CGA-O1A	-2.29	117.89	123.63
12	B	806	CLA	CMA-C3A-C4A	-2.29	105.61	111.77
12	B	824	CLA	CAA-CBA-CGA	-2.29	106.70	113.21
12	A	826	CLA	CMD-C2D-C3D	-2.29	122.43	127.69
12	B	822	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
12	J	101	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
12	F	203	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
12	A	837	CLA	CMB-C2B-C1B	2.29	128.91	125.42
12	B	811	CLA	CAA-C2A-C3A	-2.29	106.81	113.00
12	B	832	CLA	CMC-C2C-C3C	2.29	132.34	126.15
12	B	802	CLA	O2D-CGD-O1D	-2.29	119.39	123.85
12	A	809	CLA	CBC-CAC-C3C	-2.29	106.22	112.42
12	B	805	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
12	B	829	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
12	A	802	CLA	CAC-C3C-C4C	2.29	127.76	124.79
12	B	817	CLA	O2D-CGD-O1D	-2.29	119.40	123.85
12	B	824	CLA	CHB-C1B-C2B	-2.29	120.79	127.43
12	A	811	CLA	C4-C3-C5	2.28	119.19	115.23
12	B	821	CLA	CHA-C1A-NA	-2.28	121.22	126.39
15	A	849	BCR	C15-C16-C17	-2.28	118.85	123.52
15	A	850	BCR	C11-C10-C9	-2.28	124.08	127.28
12	B	804	CLA	O2A-CGA-CBA	2.28	118.79	111.83
12	B	830	CLA	CHB-C4A-NA	2.28	127.69	124.40
15	A	849	BCR	C24-C23-C22	-2.28	122.86	126.23
12	A	828	CLA	CHB-C4A-NA	2.28	127.69	124.40
12	B	816	CLA	C4-C3-C5	2.28	119.18	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	820	CLA	CHA-C1A-NA	-2.28	121.23	126.39
12	A	826	CLA	CHB-C4A-NA	2.27	127.68	124.40
12	B	831	CLA	C1-O2A-CGA	2.27	122.15	116.65
15	L	201	BCR	C16-C15-C14	-2.27	118.87	123.52
12	B	817	CLA	CHB-C1B-C2B	-2.27	120.84	127.43
15	A	846	BCR	C39-C30-C25	2.27	113.80	110.24
12	A	805	CLA	O2A-CGA-CBA	2.27	118.75	111.83
15	J	103	BCR	C15-C16-C17	-2.27	118.88	123.52
12	A	828	CLA	CHB-C1B-C2B	-2.27	120.84	127.43
12	B	820	CLA	O2A-C1-C2	2.27	116.83	108.11
12	B	814	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
12	B	825	CLA	C1-C2-C3	-2.26	122.49	126.20
12	A	815	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
15	A	846	BCR	C30-C25-C26	-2.26	119.55	122.64
12	A	825	CLA	CED-O2D-CGD	2.26	121.04	115.92
12	B	818	CLA	CHA-C1A-NA	-2.26	121.28	126.39
12	B	823	CLA	CMB-C2B-C3B	2.26	131.86	126.55
12	B	831	CLA	CAA-C2A-C3A	-2.26	106.90	113.00
12	A	818	CLA	CHB-C1B-C2B	-2.26	120.88	127.43
17	B	837	LMG	C38-C37-C36	-2.26	102.96	114.37
12	A	818	CLA	CBA-CAA-C2A	2.26	120.50	113.79
12	A	829	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
12	A	815	CLA	CBC-CAC-C3C	-2.25	106.31	112.42
15	B	834	BCR	C11-C10-C9	-2.25	124.12	127.28
12	A	807	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
12	A	814	CLA	C4B-C3B-C2B	-2.25	104.50	107.30
12	A	830	CLA	C6-C7-C8	-2.25	108.49	115.97
12	B	810	CLA	CAA-CBA-CGA	-2.25	106.83	113.21
12	B	824	CLA	CHB-C4A-NA	2.25	127.64	124.40
12	A	819	CLA	CMB-C2B-C1B	2.25	128.84	125.42
12	B	824	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
12	B	809	CLA	C1-C2-C3	-2.25	122.52	126.20
12	A	814	CLA	O1D-CGD-CBD	-2.24	120.09	124.52
15	J	102	BCR	C27-C26-C25	2.24	125.73	122.70
15	B	835	BCR	C24-C23-C22	-2.24	122.92	126.23
12	A	807	CLA	CMC-C2C-C1C	2.24	128.54	125.03
15	B	836	BCR	C16-C15-C14	-2.24	118.93	123.52
12	B	817	CLA	C4-C3-C5	2.24	119.12	115.23
12	A	825	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
12	A	833	CLA	CMC-C2C-C1C	2.24	128.53	125.03
12	A	832	CLA	CMB-C2B-C1B	2.24	128.83	125.42
12	A	854	CLA	C1-O2A-CGA	2.24	122.07	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	841	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
12	A	824	CLA	CMC-C2C-C1C	2.24	128.53	125.03
12	A	804	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
12	A	803	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
12	A	814	CLA	CAA-C2A-C3A	-2.23	106.97	113.00
15	A	848	BCR	C38-C26-C27	-2.23	108.84	113.60
17	B	837	LMG	C42-C41-C40	-2.23	103.10	114.37
12	B	808	CLA	C4-C3-C5	2.23	119.10	115.23
12	J	101	CLA	CMC-C2C-C1C	2.23	128.52	125.03
12	A	804	CLA	CAA-C2A-C3A	-2.23	106.98	113.00
12	B	827	CLA	CMC-C2C-C1C	2.23	128.51	125.03
15	J	103	BCR	C16-C15-C14	-2.23	118.96	123.52
12	L	202	CLA	CBA-CAA-C2A	2.23	120.42	113.79
12	B	832	CLA	CHC-C1C-NC	2.23	127.66	124.31
12	B	810	CLA	O2D-CGD-O1D	-2.23	119.52	123.85
15	I	101	BCR	C28-C27-C26	-2.22	110.09	114.06
12	A	804	CLA	CHB-C1B-C2B	-2.22	120.97	127.43
15	J	102	BCR	C24-C23-C22	-2.22	122.94	126.23
12	B	804	CLA	C4A-NA-C1A	-2.22	105.67	106.68
12	A	808	CLA	CMB-C2B-C1B	2.22	128.80	125.42
12	A	803	CLA	O2A-CGA-CBA	2.22	121.02	114.00
12	A	825	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
12	B	831	CLA	O2D-CGD-O1D	-2.22	119.53	123.85
12	A	818	CLA	C4-C3-C5	2.22	119.08	115.23
12	B	816	CLA	CMB-C2B-C3B	2.22	131.77	126.55
12	A	835	CLA	CMC-C2C-C1C	2.22	128.50	125.03
12	B	831	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
12	L	202	CLA	CMB-C2B-C1B	2.22	128.79	125.42
12	A	836	CLA	CMB-C2B-C1B	2.21	128.79	125.42
12	A	823	CLA	CMB-C2B-C1B	2.21	128.78	125.42
12	B	818	CLA	CHB-C1B-C2B	-2.21	121.01	127.43
12	A	816	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
12	A	841	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
15	A	847	BCR	C29-C30-C25	2.20	113.64	110.44
12	A	820	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
12	B	826	CLA	CHB-C1B-NB	-2.20	120.75	124.05
12	A	829	CLA	CHB-C4A-NA	2.20	127.58	124.40
12	A	807	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
12	A	823	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
12	B	806	CLA	CBA-CAA-C2A	2.20	120.34	113.79
12	A	823	CLA	CHA-C1A-NA	-2.20	121.41	126.39
12	A	826	CLA	CMC-C2C-C1C	2.20	128.47	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	810	CLA	CMC-C2C-C1C	2.20	128.47	125.03
12	B	826	CLA	C1-C2-C3	-2.20	122.60	126.20
12	B	831	CLA	CBC-CAC-C3C	-2.20	106.47	112.42
15	M	101	BCR	C15-C14-C13	-2.20	124.20	127.28
12	A	826	CLA	CAC-C3C-C4C	2.20	127.65	124.79
12	A	819	CLA	CBC-CAC-C3C	-2.19	106.47	112.42
12	A	819	CLA	C4-C3-C5	2.19	119.04	115.23
12	A	825	CLA	C4-C3-C5	2.19	119.03	115.23
12	A	802	CLA	O2D-CGD-O1D	-2.19	119.58	123.85
12	A	839	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
12	B	823	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
17	B	837	LMG	C40-C39-C38	-2.19	103.31	114.37
12	A	825	CLA	CGD-CBD-CAD	-2.18	103.77	110.85
12	B	808	CLA	C1-C2-C3	-2.18	122.62	126.20
12	A	841	CLA	CHB-C4A-NA	2.18	127.55	124.40
12	B	825	CLA	CHB-C1B-C2B	-2.18	121.09	127.43
12	A	826	CLA	CAA-CBA-CGA	-2.18	107.01	113.21
12	B	806	CLA	CHA-C1A-NA	-2.18	121.45	126.39
15	L	206	BCR	C20-C21-C22	-2.18	124.22	127.28
12	B	832	CLA	C4-C3-C5	2.18	119.02	115.23
12	B	810	CLA	CHC-C1C-NC	2.18	127.60	124.31
12	A	836	CLA	CMC-C2C-C1C	2.18	128.44	125.03
12	B	831	CLA	CMC-C2C-C1C	2.18	128.44	125.03
15	A	849	BCR	C27-C26-C25	2.17	125.64	122.70
15	I	101	BCR	C24-C23-C22	-2.17	123.02	126.23
15	A	847	BCR	C28-C27-C26	-2.17	110.18	114.06
15	I	101	BCR	C15-C16-C17	-2.17	119.08	123.52
12	A	838	CLA	CMC-C2C-C1C	2.17	128.43	125.03
12	B	801	CLA	C1-C2-C3	-2.17	122.64	126.20
12	A	810	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
15	J	103	BCR	C38-C26-C25	-2.17	122.12	124.48
12	A	808	CLA	CHA-C1A-NA	-2.16	121.49	126.39
12	B	804	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
12	A	805	CLA	CBA-CAA-C2A	2.16	120.23	113.79
12	L	204	CLA	CHB-C4A-NA	2.16	127.52	124.40
12	A	838	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
12	A	809	CLA	O2A-CGA-CBA	2.16	120.83	114.00
12	A	805	CLA	CMC-C2C-C1C	2.16	128.41	125.03
12	B	826	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
12	A	822	CLA	CHB-C4A-NA	2.16	127.52	124.40
12	A	836	CLA	CHB-C1B-C2B	-2.16	121.16	127.43
15	B	835	BCR	C7-C8-C9	-2.16	123.04	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	B	823	CLA	CHB-C1B-C2B	-2.16	121.17	127.43
12	A	825	CLA	CMB-C2B-C1B	2.16	128.70	125.42
12	A	843	CLA	CAC-C3C-C4C	2.16	127.59	124.79
15	M	101	BCR	C37-C22-C21	-2.15	119.33	122.82
12	A	805	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
12	A	828	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
12	B	819	CLA	C2A-C3A-C4A	-2.15	98.40	101.87
12	B	828	CLA	CHB-C4A-NA	2.15	127.50	124.40
12	A	854	CLA	CMA-C3A-C4A	-2.15	106.00	111.77
12	B	808	CLA	CMC-C2C-C1C	2.15	128.39	125.03
12	A	827	CLA	CMC-C2C-C1C	2.15	128.39	125.03
12	B	807	CLA	CMC-C2C-C1C	2.15	128.39	125.03
12	L	202	CLA	CHB-C1B-C2B	-2.14	121.20	127.43
12	A	832	CLA	CMC-C2C-C1C	2.14	128.38	125.03
12	B	811	CLA	CED-O2D-CGD	2.14	120.77	115.92
12	A	805	CLA	CMB-C2B-C1B	2.14	128.68	125.42
12	A	831	CLA	CBC-CAC-C3C	-2.14	106.62	112.42
12	A	814	CLA	CHA-C1A-NA	-2.14	121.55	126.39
12	A	840	CLA	CBC-CAC-C3C	-2.14	106.62	112.42
12	B	828	CLA	O1D-CGD-CBD	-2.14	120.30	124.52
15	L	205	BCR	C15-C16-C17	-2.14	119.15	123.52
12	A	824	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
15	A	847	BCR	C33-C5-C6	-2.13	122.16	124.48
11	A	801	CL0	C4-C3-C5	2.13	118.93	115.23
15	A	851	BCR	C32-C1-C6	2.13	113.58	110.24
12	B	822	CLA	CMC-C2C-C1C	2.13	128.36	125.03
12	B	831	CLA	C4-C3-C5	2.13	118.92	115.23
12	A	812	CLA	CBC-CAC-C3C	-2.13	106.66	112.42
12	A	835	CLA	C4-C3-C5	2.13	118.92	115.23
12	A	806	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
12	B	814	CLA	CBC-CAC-C3C	-2.12	106.66	112.42
12	A	812	CLA	CMC-C2C-C1C	2.12	128.35	125.03
12	B	812	CLA	CMC-C2C-C1C	2.12	128.35	125.03
12	A	819	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
12	A	826	CLA	CHB-C1B-C2B	-2.12	121.26	127.43
15	A	849	BCR	C15-C14-C13	-2.12	124.30	127.28
12	B	832	CLA	CAC-C3C-C4C	2.12	127.55	124.79
12	B	815	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
12	B	807	CLA	C2A-C3A-C4A	-2.12	98.44	101.87
15	F	201	BCR	C16-C15-C14	-2.12	119.18	123.52
12	A	802	CLA	O2A-CGA-CBA	2.12	120.70	114.00
12	A	809	CLA	CHB-C4A-NA	2.12	127.46	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	A	849	BCR	C28-C27-C26	-2.12	110.28	114.06
12	B	803	CLA	C6-C5-C3	2.12	118.63	113.47
12	A	805	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
12	A	808	CLA	CHB-C1B-C2B	-2.12	121.28	127.43
15	J	104	BCR	C24-C23-C22	-2.12	123.11	126.23
12	B	823	CLA	CMA-C3A-C2A	-2.12	105.80	113.98
12	B	815	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
12	F	203	CLA	CHB-C4A-NA	2.11	127.45	124.40
12	B	829	CLA	CED-O2D-CGD	2.11	120.71	115.92
12	B	826	CLA	CHB-C4A-NA	2.11	127.45	124.40
15	A	846	BCR	C7-C8-C9	-2.11	123.11	126.23
12	B	821	CLA	CHB-C1B-C2B	-2.11	121.30	127.43
12	A	840	CLA	CHA-C1A-NA	-2.11	121.61	126.39
16	A	852	LHG	C18-C17-C16	-2.11	103.70	114.37
12	A	805	CLA	C1-O2A-CGA	2.11	121.76	116.65
12	B	825	CLA	CHA-C1A-NA	-2.11	121.61	126.39
12	L	204	CLA	CMC-C2C-C1C	2.11	128.33	125.03
12	A	829	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
12	A	832	CLA	CHB-C4A-NA	2.11	127.44	124.40
12	A	839	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
12	B	810	CLA	CHA-C1A-NA	-2.11	121.62	126.39
12	A	819	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
15	A	848	BCR	C16-C17-C18	-2.10	124.33	127.28
12	A	804	CLA	CBC-CAC-C3C	-2.10	106.71	112.42
12	B	821	CLA	CMB-C2B-C3B	2.10	131.50	126.55
12	A	818	CLA	CHA-C1A-NA	-2.10	121.63	126.39
17	B	837	LMG	O2-C2-C1	-2.10	105.07	110.08
12	B	809	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
12	A	807	CLA	CED-O2D-CGD	2.10	120.68	115.92
12	A	840	CLA	C11-C10-C8	-2.10	108.98	115.97
12	B	822	CLA	CMA-C3A-C2A	-2.10	105.86	113.98
12	A	804	CLA	CMB-C2B-C1B	2.10	128.62	125.42
12	A	811	CLA	CBC-CAC-C3C	-2.10	106.73	112.42
12	A	839	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
12	A	820	CLA	CHA-C1A-NA	-2.10	121.64	126.39
12	A	825	CLA	CHA-C1A-NA	-2.10	121.64	126.39
12	A	834	CLA	CHB-C1B-C2B	-2.10	121.34	127.43
12	B	804	CLA	C1-O2A-CGA	2.10	121.72	116.65
15	A	851	BCR	C2-C1-C6	2.09	113.48	110.44
12	B	820	CLA	CAC-C3C-C4C	2.09	127.52	124.79
15	A	851	BCR	C16-C15-C14	-2.09	119.23	123.52
12	A	840	CLA	CHB-C1B-C2B	-2.09	121.35	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	829	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
12	A	813	CLA	CHA-C1A-NA	-2.09	121.66	126.39
12	A	830	CLA	CBC-CAC-C3C	-2.09	106.75	112.42
12	B	807	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
12	B	819	CLA	O2A-CGA-CBA	2.09	120.04	112.14
12	B	825	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
12	A	802	CLA	CMC-C2C-C1C	2.09	128.29	125.03
15	B	834	BCR	C24-C23-C22	-2.09	123.15	126.23
12	J	101	CLA	O2A-CGA-CBA	2.09	120.59	114.00
12	B	811	CLA	C1-C2-C3	-2.08	122.78	126.20
15	L	205	BCR	C33-C5-C6	-2.08	122.21	124.48
15	A	849	BCR	C29-C30-C25	2.08	113.46	110.44
12	A	835	CLA	O2D-CGD-O1D	-2.08	119.80	123.85
12	L	202	CLA	CMC-C2C-C1C	2.08	128.28	125.03
12	B	820	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
12	B	828	CLA	CHA-C1A-NA	-2.08	121.69	126.39
15	J	103	BCR	C7-C8-C9	-2.08	123.16	126.23
12	A	823	CLA	CBC-CAC-C3C	-2.08	106.79	112.42
12	A	854	CLA	CHB-C1B-C2B	-2.07	121.40	127.43
12	B	816	CLA	CMC-C2C-C1C	2.07	128.28	125.03
12	A	802	CLA	CBC-CAC-C3C	-2.07	106.80	112.42
12	F	203	CLA	CMC-C2C-C1C	2.07	128.27	125.03
12	A	827	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
12	A	829	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
12	B	822	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
12	B	820	CLA	CHB-C4A-NA	2.07	127.39	124.40
12	A	814	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
15	A	847	BCR	C27-C26-C25	2.07	125.50	122.70
12	B	823	CLA	CHB-C4A-NA	2.07	127.38	124.40
12	B	822	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
12	B	830	CLA	CMC-C2C-C1C	2.07	128.26	125.03
12	A	818	CLA	O2D-CGD-O1D	-2.07	119.83	123.85
12	A	843	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
12	A	822	CLA	CBC-CAC-C3C	-2.06	106.82	112.42
12	B	814	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
15	J	102	BCR	C29-C30-C25	2.06	113.44	110.44
12	B	831	CLA	CMB-C2B-C1B	2.06	128.56	125.42
12	B	801	CLA	C4D-CHA-C1A	2.06	123.70	121.24
12	B	821	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
12	A	843	CLA	C1-C2-C3	-2.06	122.83	126.20
12	B	828	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
12	B	802	CLA	CED-O2D-CGD	2.06	120.58	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	838	CLA	C4-C3-C5	2.06	118.80	115.23
12	A	828	CLA	CMB-C2B-C3B	2.06	131.38	126.55
12	B	814	CLA	C4-C3-C5	2.06	118.80	115.23
12	B	807	CLA	CED-O2D-CGD	2.06	120.58	115.92
15	L	206	BCR	C11-C10-C9	-2.05	124.40	127.28
15	J	104	BCR	C3-C4-C5	-2.05	110.39	114.06
15	J	102	BCR	C15-C14-C13	-2.05	124.40	127.28
12	A	818	CLA	CMB-C2B-C1B	2.05	128.54	125.42
12	A	828	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
12	B	825	CLA	CGD-CBD-CAD	-2.05	104.21	110.85
12	A	806	CLA	C11-C12-C13	-2.05	109.15	115.97
12	L	203	CLA	C1-C2-C3	-2.05	122.84	126.20
15	A	851	BCR	C24-C23-C22	-2.05	123.20	126.23
12	A	807	CLA	CHB-C1B-C2B	-2.05	121.49	127.43
15	F	201	BCR	C40-C30-C25	2.05	113.45	110.24
12	A	822	CLA	CAC-C3C-C4C	2.05	127.45	124.79
12	A	840	CLA	C11-C12-C13	-2.04	109.17	115.97
12	B	822	CLA	O2D-CGD-O1D	-2.04	119.87	123.85
12	A	817	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
12	B	804	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
12	B	825	CLA	C6-C7-C8	-2.04	109.17	115.97
12	A	823	CLA	CMC-C2C-C1C	2.04	128.23	125.03
12	A	804	CLA	CHA-C1A-NA	-2.04	121.77	126.39
12	A	823	CLA	CHB-C4A-NA	2.04	127.35	124.40
12	A	821	CLA	C1-O2A-CGA	2.04	121.59	116.65
12	B	805	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
12	B	807	CLA	C1-O2A-CGA	2.04	121.59	116.65
15	L	201	BCR	C15-C16-C17	-2.04	119.35	123.52
12	A	812	CLA	CHA-C1A-NA	-2.04	121.78	126.39
15	A	846	BCR	C33-C5-C6	-2.04	122.26	124.48
12	A	832	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
12	B	831	CLA	CHB-C1B-C2B	-2.03	121.52	127.43
12	A	809	CLA	CAA-CBA-CGA	-2.03	107.07	112.49
12	A	840	CLA	CED-O2D-CGD	2.03	120.53	115.92
12	B	820	CLA	CMC-C2C-C1C	2.03	128.21	125.03
12	B	816	CLA	CED-O2D-CGD	2.03	120.52	115.92
12	A	832	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
12	B	808	CLA	CHB-C4A-NA	2.03	127.33	124.40
12	B	817	CLA	CMC-C2C-C1C	2.03	128.20	125.03
12	B	824	CLA	CED-O2D-CGD	2.03	120.52	115.92
12	A	822	CLA	CHA-C1A-NA	-2.03	121.80	126.39
12	B	813	CLA	CHB-C1B-C2B	-2.03	121.54	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	833	CLA	CED-O2D-CGD	2.03	120.51	115.92
17	B	837	LMG	O1-C1-C2	-2.02	105.20	108.27
12	B	814	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
12	A	834	CLA	C11-C10-C8	-2.02	109.24	115.97
12	L	203	CLA	CMC-C2C-C1C	2.02	128.20	125.03
12	A	822	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
12	B	810	CLA	CHB-C4A-NA	2.02	127.32	124.40
12	A	839	CLA	C5-C3-C4	2.02	119.24	114.59
12	A	813	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
12	B	806	CLA	CHB-C1B-NB	-2.02	121.02	124.05
12	A	829	CLA	CHA-C1A-NA	-2.02	121.82	126.39
12	B	818	CLA	C4-C3-C5	2.02	118.73	115.23
12	A	812	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
12	B	801	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
12	A	828	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
12	B	802	CLA	CHA-C1A-NA	-2.02	121.83	126.39
12	A	808	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
12	A	841	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
12	B	824	CLA	CMB-C2B-C3B	2.01	131.28	126.55
12	A	806	CLA	CHA-C1A-NA	-2.01	121.83	126.39
12	A	837	CLA	CHA-C1A-NA	-2.01	121.83	126.39
12	A	840	CLA	CMB-C2B-C1B	2.01	128.48	125.42
12	B	816	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
12	A	819	CLA	CHC-C1C-NC	2.01	127.34	124.31
12	A	814	CLA	O2A-CGA-CBA	2.01	120.35	114.00
12	B	822	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
12	B	829	CLA	CBC-CAC-C3C	-2.01	106.98	112.42
12	B	810	CLA	C2A-C3A-C4A	-2.01	98.63	101.87
12	A	806	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
12	A	821	CLA	CHB-C1B-C2B	-2.01	121.60	127.43
12	A	805	CLA	CMA-C3A-C2A	-2.00	106.24	113.98
12	A	829	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
12	A	825	CLA	C7-C6-C5	-2.00	107.93	113.26
12	A	843	CLA	CHA-C1A-NA	-2.00	121.86	126.39
12	A	824	CLA	O1D-CGD-CBD	-2.00	120.57	124.52

All (68) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	801	CL0	NA
11	A	801	CL0	ND
11	A	801	CL0	NC

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Mol	Chain	Res	Type	Atom
12	A	802	CLA	ND
12	A	803	CLA	ND
12	A	804	CLA	ND
12	A	805	CLA	ND
12	A	806	CLA	ND
12	A	807	CLA	ND
12	A	808	CLA	ND
12	A	809	CLA	ND
12	A	810	CLA	ND
12	A	811	CLA	ND
12	A	813	CLA	ND
12	A	814	CLA	ND
12	A	816	CLA	ND
12	A	818	CLA	ND
12	A	819	CLA	ND
12	A	820	CLA	ND
12	A	821	CLA	ND
12	A	824	CLA	ND
12	A	825	CLA	ND
12	A	826	CLA	ND
12	A	827	CLA	ND
12	A	828	CLA	ND
12	A	829	CLA	ND
12	A	830	CLA	ND
12	A	831	CLA	ND
12	A	832	CLA	ND
12	A	833	CLA	ND
12	A	835	CLA	ND
12	A	836	CLA	ND
12	A	837	CLA	ND
12	A	838	CLA	ND
12	A	840	CLA	ND
12	A	841	CLA	ND
12	A	842	CLA	ND
12	A	854	CLA	ND
12	B	801	CLA	ND
12	B	802	CLA	ND
12	B	803	CLA	ND
12	B	804	CLA	ND
12	B	805	CLA	ND
12	B	806	CLA	ND
12	B	807	CLA	ND

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Mol	Chain	Res	Type	Atom
12	B	808	CLA	ND
12	B	809	CLA	ND
12	B	810	CLA	ND
12	B	811	CLA	ND
12	B	812	CLA	ND
12	B	813	CLA	ND
12	B	814	CLA	ND
12	B	815	CLA	ND
12	B	817	CLA	ND
12	B	818	CLA	ND
12	B	819	CLA	ND
12	B	820	CLA	ND
12	B	821	CLA	ND
12	B	822	CLA	ND
12	B	823	CLA	ND
12	B	825	CLA	ND
12	B	826	CLA	ND
12	B	828	CLA	ND
12	B	829	CLA	ND
12	B	830	CLA	ND
12	B	832	CLA	ND
12	F	203	CLA	ND
12	J	101	CLA	ND

All (989) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	803	CLA	CHA-CBD-CGD-O1D
12	A	803	CLA	CHA-CBD-CGD-O2D
12	A	804	CLA	C2B-C3B-CAB-CBB
12	A	804	CLA	C4B-C3B-CAB-CBB
12	A	804	CLA	CHA-CBD-CGD-O1D
12	A	804	CLA	CHA-CBD-CGD-O2D
12	A	805	CLA	C1A-C2A-CAA-CBA
12	A	805	CLA	C3A-C2A-CAA-CBA
12	A	806	CLA	C1A-C2A-CAA-CBA
12	A	807	CLA	C2-C3-C5-C6
12	A	807	CLA	C4-C3-C5-C6
12	A	808	CLA	C1A-C2A-CAA-CBA
12	A	808	CLA	C3A-C2A-CAA-CBA
12	A	813	CLA	C2B-C3B-CAB-CBB
12	A	813	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	A	814	CLA	C4B-C3B-CAB-CBB
12	A	818	CLA	C3A-C2A-CAA-CBA
12	A	819	CLA	C1A-C2A-CAA-CBA
12	A	819	CLA	C3A-C2A-CAA-CBA
12	A	821	CLA	C2B-C3B-CAB-CBB
12	A	821	CLA	C4B-C3B-CAB-CBB
12	A	822	CLA	C1A-C2A-CAA-CBA
12	A	822	CLA	C3A-C2A-CAA-CBA
12	A	823	CLA	C2-C3-C5-C6
12	A	823	CLA	C4-C3-C5-C6
12	A	826	CLA	C2B-C3B-CAB-CBB
12	A	826	CLA	C4B-C3B-CAB-CBB
12	A	828	CLA	C1A-C2A-CAA-CBA
12	A	828	CLA	C3A-C2A-CAA-CBA
12	A	830	CLA	CHA-CBD-CGD-O1D
12	A	830	CLA	CHA-CBD-CGD-O2D
12	A	834	CLA	CHA-CBD-CGD-O1D
12	A	834	CLA	CHA-CBD-CGD-O2D
12	A	836	CLA	CHA-CBD-CGD-O1D
12	A	836	CLA	CHA-CBD-CGD-O2D
12	A	837	CLA	CHA-CBD-CGD-O1D
12	A	837	CLA	CHA-CBD-CGD-O2D
12	A	839	CLA	CHA-CBD-CGD-O1D
12	A	839	CLA	CHA-CBD-CGD-O2D
12	A	840	CLA	CBD-CGD-O2D-CED
12	A	841	CLA	C2-C3-C5-C6
12	A	841	CLA	C4-C3-C5-C6
12	A	842	CLA	C1A-C2A-CAA-CBA
12	A	843	CLA	C1A-C2A-CAA-CBA
12	A	843	CLA	C3A-C2A-CAA-CBA
12	B	803	CLA	C2B-C3B-CAB-CBB
12	B	803	CLA	C4B-C3B-CAB-CBB
12	B	806	CLA	C1A-C2A-CAA-CBA
12	B	806	CLA	C3A-C2A-CAA-CBA
12	B	809	CLA	CHA-CBD-CGD-O1D
12	B	809	CLA	CHA-CBD-CGD-O2D
12	B	810	CLA	C4B-C3B-CAB-CBB
12	B	813	CLA	C1A-C2A-CAA-CBA
12	B	813	CLA	C3A-C2A-CAA-CBA
12	B	815	CLA	CHA-CBD-CGD-O1D
12	B	815	CLA	CHA-CBD-CGD-O2D
12	B	816	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	B	816	CLA	C3A-C2A-CAA-CBA
12	B	818	CLA	C1A-C2A-CAA-CBA
12	B	818	CLA	C3A-C2A-CAA-CBA
12	B	819	CLA	CHA-CBD-CGD-O1D
12	B	819	CLA	CHA-CBD-CGD-O2D
12	B	820	CLA	C2B-C3B-CAB-CBB
12	B	820	CLA	C4B-C3B-CAB-CBB
12	B	822	CLA	C1A-C2A-CAA-CBA
12	B	822	CLA	C3A-C2A-CAA-CBA
12	B	823	CLA	CHA-CBD-CGD-O1D
12	B	823	CLA	CHA-CBD-CGD-O2D
12	B	824	CLA	C1A-C2A-CAA-CBA
12	B	826	CLA	C3A-C2A-CAA-CBA
12	B	828	CLA	CHA-CBD-CGD-O1D
12	B	828	CLA	CHA-CBD-CGD-O2D
12	B	829	CLA	C1A-C2A-CAA-CBA
12	B	829	CLA	C3A-C2A-CAA-CBA
12	B	832	CLA	CAD-CBD-CGD-O1D
12	B	832	CLA	CAD-CBD-CGD-O2D
12	L	202	CLA	C1A-C2A-CAA-CBA
12	L	202	CLA	C3A-C2A-CAA-CBA
12	L	204	CLA	C2B-C3B-CAB-CBB
12	L	204	CLA	C4B-C3B-CAB-CBB
15	A	846	BCR	C7-C8-C9-C10
15	A	846	BCR	C7-C8-C9-C34
15	A	848	BCR	C7-C8-C9-C10
15	A	849	BCR	C37-C22-C23-C24
15	A	850	BCR	C37-C22-C23-C24
15	A	851	BCR	C6-C7-C8-C9
15	A	851	BCR	C18-C19-C20-C21
15	A	851	BCR	C20-C21-C22-C23
15	A	851	BCR	C20-C21-C22-C37
15	B	835	BCR	C7-C8-C9-C10
15	B	835	BCR	C18-C19-C20-C21
15	B	835	BCR	C20-C21-C22-C37
15	B	836	BCR	C11-C10-C9-C34
15	B	836	BCR	C22-C23-C24-C25
15	F	201	BCR	C37-C22-C23-C24
15	F	202	BCR	C21-C22-C23-C24
15	J	102	BCR	C6-C7-C8-C9
15	J	102	BCR	C7-C8-C9-C10
15	J	102	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
15	J	102	BCR	C11-C10-C9-C34
15	J	102	BCR	C21-C22-C23-C24
15	J	102	BCR	C37-C22-C23-C24
15	J	103	BCR	C21-C22-C23-C24
15	J	103	BCR	C22-C23-C24-C25
15	J	103	BCR	C23-C24-C25-C26
15	J	104	BCR	C7-C8-C9-C10
15	J	104	BCR	C16-C17-C18-C36
15	J	104	BCR	C18-C19-C20-C21
15	J	104	BCR	C20-C21-C22-C37
15	L	201	BCR	C7-C8-C9-C34
15	L	201	BCR	C22-C23-C24-C25
15	L	206	BCR	C7-C8-C9-C10
15	L	206	BCR	C7-C8-C9-C34
15	L	206	BCR	C20-C21-C22-C37
15	L	206	BCR	C21-C22-C23-C24
15	L	206	BCR	C22-C23-C24-C25
15	M	101	BCR	C7-C8-C9-C34
15	M	101	BCR	C18-C19-C20-C21
15	M	101	BCR	C20-C21-C22-C23
15	M	101	BCR	C20-C21-C22-C37
15	M	101	BCR	C37-C22-C23-C24
15	M	101	BCR	C22-C23-C24-C25
16	A	853	LHG	C3-O3-P-O4
17	B	837	LMG	C2-C1-O1-C7
12	A	828	CLA	CBD-CGD-O2D-CED
12	A	834	CLA	CBD-CGD-O2D-CED
12	B	803	CLA	CBD-CGD-O2D-CED
12	B	805	CLA	CBD-CGD-O2D-CED
12	B	814	CLA	CBD-CGD-O2D-CED
12	B	821	CLA	CBD-CGD-O2D-CED
12	A	823	CLA	CBA-CGA-O2A-C1
12	A	823	CLA	O1A-CGA-O2A-C1
12	A	826	CLA	O1A-CGA-O2A-C1
12	A	843	CLA	O1A-CGA-O2A-C1
12	A	840	CLA	O1D-CGD-O2D-CED
12	A	810	CLA	CBD-CGD-O2D-CED
12	A	806	CLA	C3-C5-C6-C7
12	A	812	CLA	C3-C5-C6-C7
12	A	842	CLA	C3-C5-C6-C7
12	B	810	CLA	C3-C5-C6-C7
12	B	813	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
12	B	825	CLA	C3-C5-C6-C7
13	A	844	PQN	C13-C15-C16-C17
12	A	806	CLA	CBA-CGA-O2A-C1
12	A	811	CLA	CBA-CGA-O2A-C1
12	A	826	CLA	CBA-CGA-O2A-C1
12	B	818	CLA	CBA-CGA-O2A-C1
12	B	815	CLA	CBD-CGD-O2D-CED
12	B	825	CLA	CBD-CGD-O2D-CED
12	A	828	CLA	C4-C3-C5-C6
12	B	807	CLA	C4-C3-C5-C6
12	A	828	CLA	C2-C3-C5-C6
12	B	803	CLA	O1D-CGD-O2D-CED
12	B	821	CLA	O1D-CGD-O2D-CED
12	A	815	CLA	C2A-CAA-CBA-CGA
12	A	836	CLA	C2A-CAA-CBA-CGA
12	L	204	CLA	C3-C5-C6-C7
12	B	816	CLA	O1A-CGA-O2A-C1
12	A	818	CLA	C3-C5-C6-C7
12	A	821	CLA	C3-C5-C6-C7
12	A	832	CLA	C3-C5-C6-C7
12	A	819	CLA	CBA-CGA-O2A-C1
12	A	843	CLA	CBA-CGA-O2A-C1
12	B	816	CLA	CBA-CGA-O2A-C1
15	A	851	BCR	C13-C14-C15-C16
12	A	811	CLA	O1A-CGA-O2A-C1
12	A	828	CLA	O1D-CGD-O2D-CED
12	B	805	CLA	O1D-CGD-O2D-CED
12	A	805	CLA	C3-C5-C6-C7
12	A	808	CLA	C3-C5-C6-C7
12	A	820	CLA	C3-C5-C6-C7
12	B	823	CLA	C3-C5-C6-C7
12	A	818	CLA	CBD-CGD-O2D-CED
12	A	834	CLA	O1D-CGD-O2D-CED
12	A	820	CLA	CBA-CGA-O2A-C1
12	B	832	CLA	CBA-CGA-O2A-C1
12	A	806	CLA	O1A-CGA-O2A-C1
12	B	818	CLA	O1A-CGA-O2A-C1
12	A	839	CLA	CBD-CGD-O2D-CED
12	B	809	CLA	CBD-CGD-O2D-CED
12	B	819	CLA	CBD-CGD-O2D-CED
12	B	807	CLA	C3-C5-C6-C7
12	B	809	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
17	B	837	LMG	O6-C5-C6-O5
12	A	832	CLA	C4-C3-C5-C6
12	A	854	CLA	C4-C3-C5-C6
12	B	802	CLA	C4-C3-C5-C6
12	A	832	CLA	C2-C3-C5-C6
12	A	854	CLA	C2-C3-C5-C6
12	B	802	CLA	C2-C3-C5-C6
12	B	807	CLA	C2-C3-C5-C6
12	A	819	CLA	O1A-CGA-O2A-C1
12	A	820	CLA	O1A-CGA-O2A-C1
12	B	831	CLA	CBD-CGD-O2D-CED
12	A	825	CLA	C2A-CAA-CBA-CGA
12	B	814	CLA	O1D-CGD-O2D-CED
17	B	837	LMG	O6-C1-O1-C7
12	A	802	CLA	CBD-CGD-O2D-CED
12	A	808	CLA	CBD-CGD-O2D-CED
12	B	806	CLA	CBD-CGD-O2D-CED
12	B	811	CLA	CBD-CGD-O2D-CED
12	B	832	CLA	O1A-CGA-O2A-C1
17	B	837	LMG	C4-C5-C6-O5
12	A	832	CLA	CBA-CGA-O2A-C1
12	B	802	CLA	CBA-CGA-O2A-C1
12	B	826	CLA	CBA-CGA-O2A-C1
12	B	832	CLA	CBD-CGD-O2D-CED
12	A	810	CLA	O1D-CGD-O2D-CED
12	A	812	CLA	C4-C3-C5-C6
12	B	803	CLA	C4-C3-C5-C6
12	B	823	CLA	C4-C3-C5-C6
12	A	812	CLA	C2-C3-C5-C6
12	B	803	CLA	C2-C3-C5-C6
12	B	823	CLA	C2-C3-C5-C6
12	A	821	CLA	C11-C10-C8-C9
12	A	827	CLA	C6-C7-C8-C9
12	B	810	CLA	C14-C13-C15-C16
12	B	823	CLA	C11-C12-C13-C14
12	B	832	CLA	C11-C12-C13-C14
12	B	825	CLA	O1D-CGD-O2D-CED
12	B	802	CLA	O1A-CGA-O2A-C1
15	A	846	BCR	C37-C22-C23-C24
15	A	848	BCR	C11-C12-C13-C35
15	A	848	BCR	C37-C22-C23-C24
15	A	850	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
15	A	850	BCR	C11-C12-C13-C35
15	B	834	BCR	C37-C22-C23-C24
15	B	835	BCR	C7-C8-C9-C34
15	F	202	BCR	C7-C8-C9-C34
15	F	202	BCR	C37-C22-C23-C24
15	J	103	BCR	C11-C12-C13-C35
15	J	103	BCR	C37-C22-C23-C24
15	J	104	BCR	C37-C22-C23-C24
15	L	205	BCR	C37-C22-C23-C24
15	A	849	BCR	C21-C22-C23-C24
15	A	851	BCR	C21-C22-C23-C24
15	F	201	BCR	C7-C8-C9-C10
15	I	101	BCR	C7-C8-C9-C10
15	J	103	BCR	C11-C12-C13-C14
15	L	205	BCR	C7-C8-C9-C10
15	L	205	BCR	C21-C22-C23-C24
12	B	817	CLA	C2A-CAA-CBA-CGA
12	B	821	CLA	C2A-CAA-CBA-CGA
12	B	832	CLA	C2A-CAA-CBA-CGA
12	A	827	CLA	C3-C5-C6-C7
16	A	852	LHG	O7-C5-C6-O8
12	A	832	CLA	O1A-CGA-O2A-C1
12	B	815	CLA	O1D-CGD-O2D-CED
12	A	821	CLA	CBD-CGD-O2D-CED
12	A	805	CLA	C10-C11-C12-C13
12	A	827	CLA	C10-C11-C12-C13
12	B	823	CLA	C10-C11-C12-C13
16	A	853	LHG	C7-C8-C9-C10
12	A	819	CLA	C13-C15-C16-C17
12	B	807	CLA	C13-C15-C16-C17
12	B	825	CLA	C10-C11-C12-C13
12	A	807	CLA	C2A-CAA-CBA-CGA
12	A	824	CLA	C2A-CAA-CBA-CGA
12	A	829	CLA	C2A-CAA-CBA-CGA
12	A	843	CLA	C3-C5-C6-C7
12	B	801	CLA	C2A-CAA-CBA-CGA
12	B	805	CLA	C2A-CAA-CBA-CGA
15	A	848	BCR	C10-C11-C12-C13
15	J	103	BCR	C10-C11-C12-C13
15	L	205	BCR	C18-C19-C20-C21
11	A	801	CL0	C13-C15-C16-C17
12	A	821	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
12	A	821	CLA	C8-C10-C11-C12
12	A	828	CLA	C13-C15-C16-C17
12	B	811	CLA	C15-C16-C17-C18
13	B	833	PQN	C15-C16-C17-C18
17	B	837	LMG	C28-C29-C30-C31
12	B	827	CLA	CBD-CGD-O2D-CED
12	A	805	CLA	C15-C16-C17-C18
12	A	806	CLA	C5-C6-C7-C8
12	B	832	CLA	C8-C10-C11-C12
12	L	203	CLA	C8-C10-C11-C12
13	A	844	PQN	C15-C16-C17-C18
12	B	826	CLA	O1A-CGA-O2A-C1
12	A	826	CLA	C5-C6-C7-C8
12	B	829	CLA	C10-C11-C12-C13
12	A	818	CLA	O1D-CGD-O2D-CED
12	L	203	CLA	CBA-CGA-O2A-C1
12	A	834	CLA	C5-C6-C7-C8
12	B	821	CLA	C5-C6-C7-C8
12	B	824	CLA	CBD-CGD-O2D-CED
12	A	808	CLA	C8-C10-C11-C12
12	B	804	CLA	C8-C10-C11-C12
12	B	809	CLA	C13-C15-C16-C17
12	B	823	CLA	C15-C16-C17-C18
12	B	826	CLA	C5-C6-C7-C8
12	B	829	CLA	C5-C6-C7-C8
12	B	821	CLA	C10-C11-C12-C13
12	L	204	CLA	CBA-CGA-O2A-C1
12	J	101	CLA	CBD-CGD-O2D-CED
16	A	853	LHG	O2-C2-C3-O3
12	A	816	CLA	CBA-CGA-O2A-C1
12	A	831	CLA	CBA-CGA-O2A-C1
12	B	813	CLA	CBA-CGA-O2A-C1
12	B	822	CLA	CBA-CGA-O2A-C1
16	A	853	LHG	C24-C23-O8-C6
15	A	847	BCR	C20-C21-C22-C37
15	A	849	BCR	C20-C21-C22-C37
15	A	851	BCR	C35-C13-C14-C15
15	B	834	BCR	C11-C10-C9-C34
15	F	201	BCR	C35-C13-C14-C15
15	F	201	BCR	C20-C21-C22-C37
15	F	202	BCR	C35-C13-C14-C15
15	J	103	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
15	L	205	BCR	C20-C21-C22-C37
15	L	206	BCR	C16-C17-C18-C36
15	A	851	BCR	C37-C22-C23-C24
15	F	201	BCR	C7-C8-C9-C34
15	I	101	BCR	C7-C8-C9-C34
15	J	103	BCR	C7-C8-C9-C34
15	L	205	BCR	C7-C8-C9-C34
15	L	206	BCR	C37-C22-C23-C24
15	A	846	BCR	C21-C22-C23-C24
15	A	850	BCR	C21-C22-C23-C24
15	I	101	BCR	C17-C18-C19-C20
15	J	103	BCR	C7-C8-C9-C10
12	B	802	CLA	C2A-CAA-CBA-CGA
12	B	831	CLA	C2A-CAA-CBA-CGA
12	B	828	CLA	CBA-CGA-O2A-C1
12	B	807	CLA	C10-C11-C12-C13
16	A	852	LHG	O1-C1-C2-C3
16	A	853	LHG	O1-C1-C2-C3
12	A	839	CLA	O1D-CGD-O2D-CED
12	B	819	CLA	O1D-CGD-O2D-CED
12	B	802	CLA	C3-C5-C6-C7
12	B	803	CLA	C3-C5-C6-C7
15	A	847	BCR	C16-C17-C18-C19
15	A	848	BCR	C11-C10-C9-C8
15	A	848	BCR	C16-C17-C18-C19
15	A	851	BCR	C12-C13-C14-C15
15	B	834	BCR	C11-C10-C9-C8
15	B	835	BCR	C20-C21-C22-C23
15	F	202	BCR	C12-C13-C14-C15
15	I	101	BCR	C20-C21-C22-C23
15	J	103	BCR	C11-C10-C9-C8
15	J	103	BCR	C20-C21-C22-C23
15	J	104	BCR	C16-C17-C18-C19
15	J	104	BCR	C20-C21-C22-C23
12	B	807	CLA	O1D-CGD-O2D-CED
12	A	843	CLA	C2-C1-O2A-CGA
12	B	806	CLA	C2-C1-O2A-CGA
15	F	201	BCR	C14-C15-C16-C17
15	J	102	BCR	C14-C15-C16-C17
16	A	852	LHG	C27-C28-C29-C30
12	L	203	CLA	C15-C16-C17-C18
12	A	805	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	B	837	LMG	C29-C30-C31-C32
12	B	831	CLA	O1D-CGD-O2D-CED
12	A	807	CLA	C4B-C3B-CAB-CBB
12	A	819	CLA	C4B-C3B-CAB-CBB
12	A	824	CLA	C4B-C3B-CAB-CBB
12	A	833	CLA	C4B-C3B-CAB-CBB
12	A	835	CLA	C4B-C3B-CAB-CBB
12	B	813	CLA	C4B-C3B-CAB-CBB
12	B	826	CLA	C4B-C3B-CAB-CBB
12	B	829	CLA	C4B-C3B-CAB-CBB
12	B	831	CLA	C4B-C3B-CAB-CBB
12	L	203	CLA	C4B-C3B-CAB-CBB
12	A	802	CLA	C2A-CAA-CBA-CGA
12	B	820	CLA	C12-C13-C15-C16
17	B	837	LMG	C16-C17-C18-C19
12	A	808	CLA	C5-C6-C7-C8
12	B	806	CLA	C13-C15-C16-C17
17	B	837	LMG	C37-C38-C39-C40
12	L	203	CLA	O1A-CGA-O2A-C1
12	A	854	CLA	C3-C5-C6-C7
12	A	803	CLA	C3A-C2A-CAA-CBA
12	A	806	CLA	C3A-C2A-CAA-CBA
12	A	832	CLA	C3A-C2A-CAA-CBA
12	A	837	CLA	C3A-C2A-CAA-CBA
12	A	842	CLA	C3A-C2A-CAA-CBA
12	B	801	CLA	C3A-C2A-CAA-CBA
12	A	828	CLA	C8-C10-C11-C12
12	A	830	CLA	C13-C15-C16-C17
12	B	809	CLA	O1D-CGD-O2D-CED
15	L	206	BCR	C19-C20-C21-C22
12	A	831	CLA	O1A-CGA-O2A-C1
12	B	813	CLA	O1A-CGA-O2A-C1
12	A	807	CLA	CBA-CGA-O2A-C1
12	A	808	CLA	CBA-CGA-O2A-C1
12	B	832	CLA	C3-C5-C6-C7
12	B	813	CLA	C8-C10-C11-C12
12	A	816	CLA	O1A-CGA-O2A-C1
12	B	822	CLA	O1A-CGA-O2A-C1
12	L	204	CLA	O1A-CGA-O2A-C1
12	A	825	CLA	C10-C11-C12-C13
12	A	807	CLA	C2B-C3B-CAB-CBB
12	A	814	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	A	817	CLA	C2B-C3B-CAB-CBB
12	A	824	CLA	C2B-C3B-CAB-CBB
12	A	831	CLA	C2B-C3B-CAB-CBB
12	A	833	CLA	C2B-C3B-CAB-CBB
12	A	834	CLA	C2B-C3B-CAB-CBB
12	A	835	CLA	C2B-C3B-CAB-CBB
12	A	841	CLA	C2B-C3B-CAB-CBB
12	B	810	CLA	C2B-C3B-CAB-CBB
12	B	812	CLA	C2B-C3B-CAB-CBB
12	B	813	CLA	C2B-C3B-CAB-CBB
12	B	826	CLA	C2B-C3B-CAB-CBB
12	B	829	CLA	C2B-C3B-CAB-CBB
12	B	831	CLA	C2B-C3B-CAB-CBB
12	L	203	CLA	C2B-C3B-CAB-CBB
15	B	835	BCR	C23-C24-C25-C26
15	B	835	BCR	C23-C24-C25-C30
15	I	101	BCR	C1-C6-C7-C8
15	J	103	BCR	C23-C24-C25-C30
15	J	104	BCR	C23-C24-C25-C30
15	L	205	BCR	C23-C24-C25-C26
15	L	205	BCR	C23-C24-C25-C30
15	M	101	BCR	C1-C6-C7-C8
15	M	101	BCR	C23-C24-C25-C26
15	M	101	BCR	C23-C24-C25-C30
12	A	833	CLA	CBA-CGA-O2A-C1
12	B	821	CLA	CBA-CGA-O2A-C1
12	B	821	CLA	C3-C5-C6-C7
17	B	837	LMG	C17-C18-C19-C20
17	B	837	LMG	C36-C37-C38-C39
12	A	812	CLA	C2A-CAA-CBA-CGA
12	A	818	CLA	C2A-CAA-CBA-CGA
12	A	805	CLA	O1A-CGA-O2A-C1
12	A	807	CLA	O1A-CGA-O2A-C1
12	B	811	CLA	O1D-CGD-O2D-CED
17	B	837	LMG	C38-C39-C40-C41
12	B	802	CLA	C13-C15-C16-C17
12	A	818	CLA	CBA-CGA-O2A-C1
12	A	829	CLA	C5-C6-C7-C8
12	B	811	CLA	C13-C15-C16-C17
12	A	811	CLA	C10-C11-C12-C13
12	A	833	CLA	C15-C16-C17-C18
12	B	813	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
15	J	103	BCR	C9-C10-C11-C12
16	A	852	LHG	C8-C7-O7-C5
12	B	810	CLA	C13-C15-C16-C17
12	B	803	CLA	C8-C10-C11-C12
12	A	819	CLA	C3-C5-C6-C7
12	B	831	CLA	C3-C5-C6-C7
12	A	812	CLA	CBA-CGA-O2A-C1
12	A	837	CLA	C2A-CAA-CBA-CGA
12	J	101	CLA	C2A-CAA-CBA-CGA
12	B	817	CLA	CBD-CGD-O2D-CED
12	A	805	CLA	C4-C3-C5-C6
12	B	825	CLA	C4-C3-C5-C6
12	L	204	CLA	C4-C3-C5-C6
12	A	829	CLA	CBD-CGD-O2D-CED
12	A	825	CLA	C3-C5-C6-C7
12	A	840	CLA	C8-C10-C11-C12
12	B	803	CLA	C13-C15-C16-C17
12	A	808	CLA	O1A-CGA-O2A-C1
12	A	833	CLA	O1A-CGA-O2A-C1
12	B	817	CLA	C8-C10-C11-C12
12	B	820	CLA	C10-C11-C12-C13
12	A	827	CLA	CBA-CGA-O2A-C1
12	A	834	CLA	CBA-CGA-O2A-C1
12	A	841	CLA	CBA-CGA-O2A-C1
12	A	818	CLA	O1A-CGA-O2A-C1
17	B	837	LMG	C21-C22-C23-C24
17	B	837	LMG	C11-C12-C13-C14
11	A	801	CL0	C3-C5-C6-C7
12	A	805	CLA	C2-C3-C5-C6
12	B	825	CLA	C2-C3-C5-C6
12	A	813	CLA	C2A-CAA-CBA-CGA
12	B	806	CLA	O1D-CGD-O2D-CED
12	B	821	CLA	O1A-CGA-O2A-C1
12	A	803	CLA	C1A-C2A-CAA-CBA
12	A	811	CLA	C1A-C2A-CAA-CBA
12	A	818	CLA	C1A-C2A-CAA-CBA
12	A	821	CLA	C1A-C2A-CAA-CBA
12	A	824	CLA	C1A-C2A-CAA-CBA
12	A	831	CLA	C1A-C2A-CAA-CBA
12	A	832	CLA	C1A-C2A-CAA-CBA
12	A	834	CLA	C1A-C2A-CAA-CBA
12	A	835	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	837	CLA	C1A-C2A-CAA-CBA
12	B	812	CLA	C1A-C2A-CAA-CBA
12	B	814	CLA	C1A-C2A-CAA-CBA
12	B	823	CLA	C1A-C2A-CAA-CBA
12	B	825	CLA	C1A-C2A-CAA-CBA
12	B	826	CLA	C1A-C2A-CAA-CBA
12	B	827	CLA	C1A-C2A-CAA-CBA
12	B	830	CLA	C1A-C2A-CAA-CBA
12	A	833	CLA	C10-C11-C12-C13
12	A	827	CLA	O1A-CGA-O2A-C1
12	A	830	CLA	C12-C13-C15-C16
12	A	834	CLA	C12-C13-C15-C16
12	B	810	CLA	C12-C13-C15-C16
12	B	822	CLA	C12-C13-C15-C16
12	B	831	CLA	C5-C6-C7-C8
12	B	822	CLA	C3-C5-C6-C7
12	A	830	CLA	C14-C13-C15-C16
12	A	854	CLA	C14-C13-C15-C16
12	B	822	CLA	C14-C13-C15-C16
16	A	852	LHG	C24-C25-C26-C27
12	B	808	CLA	C15-C16-C17-C18
12	A	828	CLA	CBA-CGA-O2A-C1
12	A	812	CLA	O1A-CGA-O2A-C1
15	L	201	BCR	C16-C17-C18-C36
12	A	834	CLA	O1A-CGA-O2A-C1
15	L	206	BCR	C11-C12-C13-C35
15	B	834	BCR	C21-C22-C23-C24
12	A	841	CLA	O1A-CGA-O2A-C1
12	B	820	CLA	C15-C16-C17-C18
12	L	203	CLA	C13-C15-C16-C17
17	B	837	LMG	C15-C16-C17-C18
12	A	808	CLA	C10-C11-C12-C13
15	A	847	BCR	C11-C10-C9-C8
15	A	847	BCR	C20-C21-C22-C23
15	B	836	BCR	C11-C10-C9-C8
15	I	101	BCR	C11-C10-C9-C8
15	M	101	BCR	C11-C10-C9-C8
12	B	814	CLA	CBA-CGA-O2A-C1
17	B	837	LMG	C30-C31-C32-C33
17	B	837	LMG	O1-C7-C8-O7
17	B	837	LMG	C32-C33-C34-C35
17	B	837	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
12	A	838	CLA	CBA-CGA-O2A-C1
16	A	852	LHG	C11-C12-C13-C14
12	B	807	CLA	C15-C16-C17-C18
12	B	817	CLA	C3-C5-C6-C7
12	A	825	CLA	C13-C15-C16-C17
12	A	802	CLA	O1D-CGD-O2D-CED
12	B	828	CLA	O1A-CGA-O2A-C1
12	A	806	CLA	C4-C3-C5-C6
12	A	826	CLA	C4-C3-C5-C6
12	A	843	CLA	C4-C3-C5-C6
12	B	814	CLA	C4-C3-C5-C6
16	A	852	LHG	C29-C30-C31-C32
16	A	852	LHG	O9-C7-O7-C5
12	A	808	CLA	C11-C12-C13-C14
12	A	821	CLA	C14-C13-C15-C16
12	A	829	CLA	C14-C13-C15-C16
12	A	832	CLA	C11-C10-C8-C9
12	A	834	CLA	C14-C13-C15-C16
12	B	807	CLA	C14-C13-C15-C16
12	B	820	CLA	C14-C13-C15-C16
12	A	817	CLA	C4B-C3B-CAB-CBB
12	A	830	CLA	C4B-C3B-CAB-CBB
12	A	831	CLA	C4B-C3B-CAB-CBB
12	A	834	CLA	C4B-C3B-CAB-CBB
12	A	841	CLA	C4B-C3B-CAB-CBB
12	A	842	CLA	C4B-C3B-CAB-CBB
12	B	804	CLA	C4B-C3B-CAB-CBB
12	B	812	CLA	C4B-C3B-CAB-CBB
12	B	814	CLA	C4B-C3B-CAB-CBB
12	A	811	CLA	C2A-CAA-CBA-CGA
12	A	821	CLA	C12-C13-C15-C16
12	A	825	CLA	C12-C13-C15-C16
12	A	829	CLA	C12-C13-C15-C16
12	A	832	CLA	C11-C10-C8-C7
12	A	854	CLA	C12-C13-C15-C16
12	B	802	CLA	C12-C13-C15-C16
12	B	806	CLA	C12-C13-C15-C16
12	L	203	CLA	C12-C13-C15-C16
13	B	833	PQN	C16-C17-C18-C20
12	B	811	CLA	C10-C11-C12-C13
12	A	813	CLA	C3A-C2A-CAA-CBA
12	A	829	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	A	834	CLA	C4-C3-C5-C6
12	B	811	CLA	C4-C3-C5-C6
12	B	822	CLA	C4-C3-C5-C6
13	B	833	PQN	C14-C13-C15-C16
12	A	808	CLA	O1D-CGD-O2D-CED
12	B	813	CLA	C5-C6-C7-C8
12	B	823	CLA	C5-C6-C7-C8
15	A	848	BCR	C9-C10-C11-C12
15	A	851	BCR	C19-C20-C21-C22
15	J	102	BCR	C11-C12-C13-C35
12	B	821	CLA	CAA-CBA-CGA-O2A
12	A	828	CLA	O1A-CGA-O2A-C1
16	A	852	LHG	C4-C5-C6-O8
17	B	837	LMG	O1-C7-C8-C9
12	A	820	CLA	C10-C11-C12-C13
12	A	825	CLA	C8-C10-C11-C12
12	A	812	CLA	C6-C7-C8-C9
12	B	821	CLA	C4-C3-C5-C6
12	A	806	CLA	C2-C3-C5-C6
12	B	811	CLA	C2-C3-C5-C6
12	B	822	CLA	C2-C3-C5-C6
12	B	814	CLA	O1A-CGA-O2A-C1
12	A	842	CLA	C2B-C3B-CAB-CBB
12	B	815	CLA	C2B-C3B-CAB-CBB
15	A	846	BCR	C1-C6-C7-C8
15	A	847	BCR	C1-C6-C7-C8
15	A	847	BCR	C5-C6-C7-C8
15	A	848	BCR	C1-C6-C7-C8
15	A	849	BCR	C1-C6-C7-C8
15	A	849	BCR	C23-C24-C25-C30
15	A	850	BCR	C1-C6-C7-C8
15	A	850	BCR	C23-C24-C25-C30
15	A	851	BCR	C23-C24-C25-C30
15	B	834	BCR	C1-C6-C7-C8
15	B	834	BCR	C23-C24-C25-C30
15	B	835	BCR	C1-C6-C7-C8
15	B	836	BCR	C1-C6-C7-C8
15	B	836	BCR	C23-C24-C25-C30
15	F	201	BCR	C1-C6-C7-C8
15	F	202	BCR	C1-C6-C7-C8
15	J	102	BCR	C1-C6-C7-C8
15	J	103	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
15	L	201	BCR	C1-C6-C7-C8
15	L	205	BCR	C1-C6-C7-C8
15	L	206	BCR	C1-C6-C7-C8
15	L	206	BCR	C23-C24-C25-C30
17	B	837	LMG	C31-C32-C33-C34
12	A	830	CLA	CBA-CGA-O2A-C1
12	B	819	CLA	CBA-CGA-O2A-C1
17	B	837	LMG	C33-C34-C35-C36
12	B	824	CLA	C2A-CAA-CBA-CGA
16	A	852	LHG	C19-C20-C21-C22
12	B	803	CLA	C5-C6-C7-C8
12	A	826	CLA	C2-C3-C5-C6
12	A	834	CLA	C2-C3-C5-C6
12	A	843	CLA	C2-C3-C5-C6
12	B	814	CLA	C2-C3-C5-C6
13	B	833	PQN	C12-C13-C15-C16
12	B	824	CLA	O1D-CGD-O2D-CED
12	A	821	CLA	O1D-CGD-O2D-CED
15	F	201	BCR	C22-C23-C24-C25
12	B	832	CLA	O1D-CGD-O2D-CED
12	B	827	CLA	O1D-CGD-O2D-CED
12	B	825	CLA	C15-C16-C17-C18
12	B	824	CLA	CAA-CBA-CGA-O2A
15	A	846	BCR	C20-C21-C22-C37
15	J	104	BCR	C11-C10-C9-C34
15	L	201	BCR	C35-C13-C14-C15
12	A	817	CLA	C3-C5-C6-C7
15	J	102	BCR	C7-C8-C9-C34
12	A	808	CLA	C6-C7-C8-C10
12	A	819	CLA	C11-C12-C13-C15
12	B	811	CLA	C11-C12-C13-C15
12	B	826	CLA	C6-C7-C8-C10
12	B	829	CLA	C12-C13-C15-C16
16	A	852	LHG	C26-C27-C28-C29
12	A	805	CLA	C13-C15-C16-C17
15	L	201	BCR	C7-C8-C9-C10
15	M	101	BCR	C7-C8-C9-C10
15	M	101	BCR	C21-C22-C23-C24
12	A	817	CLA	CBA-CGA-O2A-C1
12	A	838	CLA	O1A-CGA-O2A-C1
12	A	825	CLA	C4-C3-C5-C6
12	B	813	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
12	B	829	CLA	C3-C5-C6-C7
16	A	852	LHG	C28-C29-C30-C31
16	A	852	LHG	C13-C14-C15-C16
12	A	829	CLA	O1D-CGD-O2D-CED
12	A	830	CLA	O1A-CGA-O2A-C1
15	I	101	BCR	C16-C17-C18-C19
12	A	829	CLA	C2-C3-C5-C6
12	B	821	CLA	C2-C3-C5-C6
12	L	204	CLA	C2-C3-C5-C6
12	B	809	CLA	C14-C13-C15-C16
12	B	826	CLA	C6-C7-C8-C9
12	B	806	CLA	CBA-CGA-O2A-C1
12	A	838	CLA	C4-C3-C5-C6
12	B	829	CLA	C4-C3-C5-C6
12	B	806	CLA	O1A-CGA-O2A-C1
12	A	835	CLA	C6-C7-C8-C9
12	A	817	CLA	O1A-CGA-O2A-C1
12	A	806	CLA	C4B-C3B-CAB-CBB
12	A	810	CLA	C4B-C3B-CAB-CBB
12	A	811	CLA	C4B-C3B-CAB-CBB
12	A	812	CLA	C4B-C3B-CAB-CBB
12	A	815	CLA	C4B-C3B-CAB-CBB
12	A	820	CLA	C4B-C3B-CAB-CBB
12	A	823	CLA	C4B-C3B-CAB-CBB
12	A	838	CLA	C4B-C3B-CAB-CBB
12	A	840	CLA	C4B-C3B-CAB-CBB
12	A	843	CLA	C4B-C3B-CAB-CBB
12	B	802	CLA	C4B-C3B-CAB-CBB
12	B	811	CLA	C4B-C3B-CAB-CBB
12	B	815	CLA	C4B-C3B-CAB-CBB
12	B	821	CLA	C1A-C2A-CAA-CBA
12	B	830	CLA	C4B-C3B-CAB-CBB
12	F	203	CLA	C4B-C3B-CAB-CBB
12	J	101	CLA	C4B-C3B-CAB-CBB
12	L	203	CLA	C1A-C2A-CAA-CBA
15	A	846	BCR	C22-C23-C24-C25
15	B	835	BCR	C22-C23-C24-C25
12	A	806	CLA	C12-C13-C15-C16
12	A	808	CLA	C12-C13-C15-C16
12	A	821	CLA	C11-C10-C8-C7
12	A	827	CLA	C11-C10-C8-C7
12	A	840	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
12	B	813	CLA	C11-C10-C8-C7
12	B	804	CLA	C16-C17-C18-C20
12	B	806	CLA	C16-C17-C18-C20
12	A	818	CLA	CAA-CBA-CGA-O2A
12	B	829	CLA	C2A-CAA-CBA-CGA
12	A	808	CLA	C6-C7-C8-C9
12	A	819	CLA	C11-C12-C13-C14
12	A	825	CLA	C14-C13-C15-C16
12	B	802	CLA	C14-C13-C15-C16
12	B	806	CLA	C14-C13-C15-C16
12	B	811	CLA	C11-C12-C13-C14
12	B	829	CLA	C14-C13-C15-C16
12	L	203	CLA	C14-C13-C15-C16
13	B	833	PQN	C16-C17-C18-C19
15	J	102	BCR	C9-C10-C11-C12
12	B	824	CLA	C1-C2-C3-C4
12	B	801	CLA	C4-C3-C5-C6
12	A	805	CLA	CAD-CBD-CGD-O2D
12	A	813	CLA	CAD-CBD-CGD-O2D
12	A	825	CLA	CAD-CBD-CGD-O2D
12	A	838	CLA	CAD-CBD-CGD-O2D
12	A	843	CLA	CAD-CBD-CGD-O2D
12	B	806	CLA	CAD-CBD-CGD-O2D
12	B	813	CLA	CAD-CBD-CGD-O2D
12	J	101	CLA	CAD-CBD-CGD-O2D
16	A	853	LHG	O10-C23-O8-C6
12	A	805	CLA	CAD-CBD-CGD-O1D
12	A	813	CLA	CAD-CBD-CGD-O1D
12	A	825	CLA	CAD-CBD-CGD-O1D
12	A	838	CLA	CAD-CBD-CGD-O1D
12	A	843	CLA	CAD-CBD-CGD-O1D
12	B	806	CLA	CAD-CBD-CGD-O1D
12	B	813	CLA	CAD-CBD-CGD-O1D
12	B	827	CLA	CHA-CBD-CGD-O1D
12	B	827	CLA	CHA-CBD-CGD-O2D
12	J	101	CLA	CAD-CBD-CGD-O1D
12	A	806	CLA	C2B-C3B-CAB-CBB
12	A	811	CLA	C2B-C3B-CAB-CBB
12	A	819	CLA	C2B-C3B-CAB-CBB
12	A	822	CLA	C2B-C3B-CAB-CBB
12	A	840	CLA	C2B-C3B-CAB-CBB
12	B	802	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	B	811	CLA	C2B-C3B-CAB-CBB
12	B	827	CLA	C2B-C3B-CAB-CBB
12	B	830	CLA	C2B-C3B-CAB-CBB
12	A	825	CLA	C2-C3-C5-C6
12	A	838	CLA	C2-C3-C5-C6
12	B	813	CLA	C2-C3-C5-C6
12	B	807	CLA	C5-C6-C7-C8
12	B	817	CLA	O1D-CGD-O2D-CED
12	B	806	CLA	C15-C16-C17-C18
16	A	852	LHG	C32-C33-C34-C35
16	A	852	LHG	O1-C1-C2-O2
12	B	823	CLA	O1A-CGA-O2A-C1
12	A	805	CLA	C11-C10-C8-C9
12	B	813	CLA	C11-C10-C8-C9
12	J	101	CLA	O1D-CGD-O2D-CED
12	A	805	CLA	C11-C10-C8-C7
12	B	831	CLA	C11-C10-C8-C7
15	B	834	BCR	C20-C21-C22-C23
12	B	832	CLA	C10-C11-C12-C13
12	B	829	CLA	C2-C3-C5-C6
16	A	852	LHG	C17-C18-C19-C20
12	B	823	CLA	CBA-CGA-O2A-C1
12	A	835	CLA	O1A-CGA-O2A-C1
15	F	201	BCR	C21-C22-C23-C24
12	A	835	CLA	CBA-CGA-O2A-C1
12	B	822	CLA	C2A-CAA-CBA-CGA
12	A	820	CLA	C4-C3-C5-C6
12	A	811	CLA	C13-C15-C16-C17
12	A	827	CLA	C11-C10-C8-C9
12	A	837	CLA	CBA-CGA-O2A-C1
12	A	822	CLA	C4B-C3B-CAB-CBB
12	A	854	CLA	C13-C15-C16-C17
12	B	802	CLA	C8-C10-C11-C12
12	B	804	CLA	C10-C11-C12-C13
12	A	833	CLA	C4-C3-C5-C6
16	A	852	LHG	C25-C26-C27-C28
12	A	805	CLA	CAA-CBA-CGA-O2A
12	B	823	CLA	C11-C12-C13-C15
16	A	852	LHG	C18-C19-C20-C21
12	A	837	CLA	O1A-CGA-O2A-C1
17	B	837	LMG	O7-C8-C9-O8
12	A	807	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
12	A	821	CLA	C4-C3-C5-C6
12	A	840	CLA	C3A-C2A-CAA-CBA
12	B	821	CLA	C3A-C2A-CAA-CBA
12	B	824	CLA	C3A-C2A-CAA-CBA
12	B	826	CLA	C4-C3-C5-C6
12	A	820	CLA	C2-C3-C5-C6
12	B	819	CLA	O1A-CGA-O2A-C1
15	A	851	BCR	C11-C10-C9-C34
15	A	851	BCR	C16-C17-C18-C36
15	B	834	BCR	C20-C21-C22-C37
15	B	836	BCR	C6-C7-C8-C9
15	L	201	BCR	C20-C21-C22-C37
12	A	828	CLA	C3-C5-C6-C7
12	A	817	CLA	C2-C1-O2A-CGA
15	B	835	BCR	C9-C10-C11-C12
15	J	104	BCR	C15-C16-C17-C18
12	A	837	CLA	C4-C3-C5-C6
17	B	837	LMG	C13-C14-C15-C16
12	B	831	CLA	C10-C11-C12-C13
12	B	809	CLA	C4-C3-C5-C6
12	B	825	CLA	CAA-CBA-CGA-O2A
12	B	801	CLA	C2-C3-C5-C6
16	A	853	LHG	C1-C2-C3-O3
12	B	804	CLA	C13-C15-C16-C17
12	A	829	CLA	C13-C15-C16-C17
12	A	806	CLA	C14-C13-C15-C16
12	A	811	CLA	C14-C13-C15-C16
12	A	821	CLA	C6-C7-C8-C9
12	B	810	CLA	C6-C7-C8-C9
12	B	807	CLA	CBD-CGD-O2D-CED
12	A	842	CLA	CAA-CBA-CGA-O2A
12	B	826	CLA	CAA-CBA-CGA-O2A
12	A	834	CLA	C10-C11-C12-C13
12	A	823	CLA	C2A-CAA-CBA-CGA
12	A	843	CLA	C2A-CAA-CBA-CGA
12	A	813	CLA	C1A-C2A-CAA-CBA
12	A	815	CLA	C1A-C2A-CAA-CBA
15	A	851	BCR	C16-C17-C18-C19
15	L	206	BCR	C16-C17-C18-C19
12	A	826	CLA	C6-C7-C8-C10
12	A	810	CLA	C2B-C3B-CAB-CBB
12	A	812	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
12	A	815	CLA	C2B-C3B-CAB-CBB
12	A	820	CLA	C2B-C3B-CAB-CBB
12	A	823	CLA	C2B-C3B-CAB-CBB
12	A	830	CLA	C2B-C3B-CAB-CBB
12	A	838	CLA	C2B-C3B-CAB-CBB
12	A	843	CLA	C2B-C3B-CAB-CBB
12	B	806	CLA	C2B-C3B-CAB-CBB
12	B	814	CLA	C2B-C3B-CAB-CBB
12	B	817	CLA	C2B-C3B-CAB-CBB
12	B	822	CLA	C2B-C3B-CAB-CBB
12	F	203	CLA	C2B-C3B-CAB-CBB
12	J	101	CLA	C2B-C3B-CAB-CBB
12	L	202	CLA	C2B-C3B-CAB-CBB
15	A	846	BCR	C5-C6-C7-C8
15	A	847	BCR	C23-C24-C25-C26
15	A	847	BCR	C23-C24-C25-C30
15	A	848	BCR	C5-C6-C7-C8
15	A	849	BCR	C5-C6-C7-C8
15	A	849	BCR	C23-C24-C25-C26
15	A	850	BCR	C5-C6-C7-C8
15	A	850	BCR	C23-C24-C25-C26
15	A	851	BCR	C23-C24-C25-C26
15	B	834	BCR	C5-C6-C7-C8
15	B	834	BCR	C23-C24-C25-C26
15	B	835	BCR	C5-C6-C7-C8
15	B	836	BCR	C5-C6-C7-C8
15	B	836	BCR	C23-C24-C25-C26
15	F	201	BCR	C5-C6-C7-C8
15	F	202	BCR	C5-C6-C7-C8
15	F	202	BCR	C23-C24-C25-C30
15	I	101	BCR	C5-C6-C7-C8
15	J	102	BCR	C5-C6-C7-C8
15	J	103	BCR	C5-C6-C7-C8
15	J	104	BCR	C23-C24-C25-C26
15	L	201	BCR	C5-C6-C7-C8
15	L	201	BCR	C23-C24-C25-C30
15	L	205	BCR	C5-C6-C7-C8
15	L	206	BCR	C5-C6-C7-C8
15	L	206	BCR	C23-C24-C25-C26
15	M	101	BCR	C5-C6-C7-C8
12	A	809	CLA	CAA-CBA-CGA-O2A
12	A	830	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
12	A	813	CLA	CAA-CBA-CGA-O2A
12	A	827	CLA	C4-C3-C5-C6
12	A	835	CLA	C4-C3-C5-C6
12	A	821	CLA	C2-C3-C5-C6
12	B	821	CLA	C11-C12-C13-C15
12	A	826	CLA	C6-C7-C8-C9
12	A	808	CLA	C2A-CAA-CBA-CGA
12	B	810	CLA	C4-C3-C5-C6
12	B	817	CLA	CAA-CBA-CGA-O2A
12	A	827	CLA	C2-C3-C5-C6
12	A	833	CLA	C2-C3-C5-C6
12	B	810	CLA	C2-C3-C5-C6
12	B	826	CLA	C2-C3-C5-C6
12	B	817	CLA	C2-C1-O2A-CGA
12	L	203	CLA	C10-C11-C12-C13
15	A	850	BCR	C7-C8-C9-C10
12	A	817	CLA	C2A-CAA-CBA-CGA
12	A	808	CLA	C14-C13-C15-C16
16	A	852	LHG	C30-C31-C32-C33
12	A	812	CLA	C5-C6-C7-C8
12	A	803	CLA	CAA-CBA-CGA-O2A
12	A	809	CLA	CAA-CBA-CGA-O1A
12	A	813	CLA	CAA-CBA-CGA-O1A
12	A	836	CLA	CAA-CBA-CGA-O2A
12	F	203	CLA	CAA-CBA-CGA-O2A
16	A	853	LHG	O1-C1-C2-O2
12	A	817	CLA	C4-C3-C5-C6
12	A	840	CLA	C4-C3-C5-C6
12	A	829	CLA	CAA-CBA-CGA-O2A
12	B	806	CLA	C4B-C3B-CAB-CBB
12	B	827	CLA	C4B-C3B-CAB-CBB
12	B	825	CLA	O1A-CGA-O2A-C1
11	A	801	CL0	CHA-CBD-CGD-O1D
11	A	801	CL0	CHA-CBD-CGD-O2D
15	F	202	BCR	C20-C21-C22-C37
11	A	801	CL0	CAA-CBA-CGA-O2A
12	B	809	CLA	C2-C3-C5-C6
12	A	819	CLA	C11-C10-C8-C7
12	B	821	CLA	CAA-CBA-CGA-O1A
12	B	808	CLA	C16-C17-C18-C20
12	B	802	CLA	C3A-C2A-CAA-CBA
12	B	824	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
15	B	836	BCR	C18-C19-C20-C21
15	L	206	BCR	C10-C11-C12-C13
12	A	803	CLA	CAA-CBA-CGA-O1A
12	B	827	CLA	CAA-CBA-CGA-O2A
12	F	203	CLA	CAA-CBA-CGA-O1A
12	A	840	CLA	C3-C5-C6-C7
15	A	851	BCR	C11-C10-C9-C8
15	B	835	BCR	C11-C10-C9-C8
15	F	202	BCR	C20-C21-C22-C23
15	L	201	BCR	C20-C21-C22-C23
12	A	836	CLA	CAA-CBA-CGA-O1A
16	A	852	LHG	O6-C4-C5-O7
12	B	825	CLA	CBA-CGA-O2A-C1
12	A	840	CLA	O1A-CGA-O2A-C1
12	B	832	CLA	C4-C3-C5-C6
12	B	829	CLA	CAA-CBA-CGA-O2A
12	A	838	CLA	C5-C6-C7-C8
12	B	827	CLA	CAA-CBA-CGA-O1A
12	A	827	CLA	C6-C7-C8-C10
12	A	805	CLA	C2B-C3B-CAB-CBB
12	B	804	CLA	C2B-C3B-CAB-CBB
12	B	828	CLA	C2B-C3B-CAB-CBB
15	A	851	BCR	C5-C6-C7-C8
15	F	201	BCR	C23-C24-C25-C26
15	F	202	BCR	C23-C24-C25-C26
15	J	102	BCR	C23-C24-C25-C26
15	J	102	BCR	C23-C24-C25-C30
15	J	104	BCR	C1-C6-C7-C8
15	J	104	BCR	C5-C6-C7-C8
15	L	201	BCR	C23-C24-C25-C26
16	A	852	LHG	C11-C10-C9-C8
12	B	810	CLA	C2-C1-O2A-CGA
12	B	825	CLA	C2-C1-O2A-CGA
12	B	821	CLA	C16-C17-C18-C19
12	A	840	CLA	CAA-CBA-CGA-O2A
12	B	831	CLA	C8-C10-C11-C12
12	A	838	CLA	CAA-CBA-CGA-O2A
12	A	822	CLA	C2A-CAA-CBA-CGA
12	A	817	CLA	CAA-CBA-CGA-O2A
12	B	832	CLA	C2C-C3C-CAC-CBC
12	A	840	CLA	CBA-CGA-O2A-C1
12	B	807	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	A	846	BCR	C18-C19-C20-C21
12	A	840	CLA	C11-C10-C8-C9
12	B	821	CLA	C11-C12-C13-C14
12	A	805	CLA	C4B-C3B-CAB-CBB
12	A	809	CLA	C1A-C2A-CAA-CBA
12	A	809	CLA	C4B-C3B-CAB-CBB
12	B	801	CLA	C1A-C2A-CAA-CBA
12	B	817	CLA	C4B-C3B-CAB-CBB
12	B	822	CLA	C4B-C3B-CAB-CBB
12	B	828	CLA	C4B-C3B-CAB-CBB
12	B	832	CLA	C4B-C3B-CAB-CBB
12	L	202	CLA	C4B-C3B-CAB-CBB
12	B	816	CLA	C4-C3-C5-C6
12	A	827	CLA	CAA-CBA-CGA-O2A
12	B	813	CLA	CAA-CBA-CGA-O2A
15	B	836	BCR	C21-C22-C23-C24
15	I	101	BCR	C11-C12-C13-C14
12	A	823	CLA	CAA-CBA-CGA-O2A
12	A	840	CLA	C2A-CAA-CBA-CGA
12	B	824	CLA	C2-C1-O2A-CGA
12	B	832	CLA	C11-C12-C13-C15
12	B	829	CLA	C8-C10-C11-C12
12	B	807	CLA	C16-C17-C18-C19
12	A	817	CLA	CAA-CBA-CGA-O1A
12	L	204	CLA	CAA-CBA-CGA-O2A
12	A	811	CLA	C11-C12-C13-C14
15	J	103	BCR	C19-C20-C21-C22
12	A	838	CLA	CAA-CBA-CGA-O1A
12	B	810	CLA	C8-C10-C11-C12
12	A	840	CLA	CAA-CBA-CGA-O1A
12	B	813	CLA	CAA-CBA-CGA-O1A
12	B	829	CLA	CAA-CBA-CGA-O1A
12	A	823	CLA	CAA-CBA-CGA-O1A
12	A	820	CLA	CAA-CBA-CGA-O2A
12	A	839	CLA	CAA-CBA-CGA-O2A
12	A	835	CLA	C2-C3-C5-C6
15	M	101	BCR	C13-C14-C15-C16
12	A	811	CLA	CAD-CBD-CGD-O2D
12	A	820	CLA	CAD-CBD-CGD-O2D
12	F	203	CLA	CAD-CBD-CGD-O2D
12	A	834	CLA	C2-C1-O2A-CGA
12	B	813	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
12	B	829	CLA	C2-C1-O2A-CGA
12	B	807	CLA	CAA-CBA-CGA-O1A
12	A	828	CLA	CAA-CBA-CGA-O2A
12	B	830	CLA	CAA-CBA-CGA-O2A
17	B	837	LMG	C19-C20-C21-C22
12	A	833	CLA	C13-C15-C16-C17
12	A	841	CLA	O1D-CGD-O2D-CED
12	A	840	CLA	C5-C6-C7-C8

There are no ring outliers.

95 monomers are involved in 205 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	824	CLA	3	0
12	B	806	CLA	4	0
12	A	806	CLA	3	0
12	B	803	CLA	2	0
12	B	816	CLA	2	0
12	A	825	CLA	1	0
12	A	834	CLA	3	0
15	A	846	BCR	2	0
12	L	202	CLA	3	0
12	A	804	CLA	2	0
12	A	854	CLA	5	0
12	A	808	CLA	5	0
13	A	844	PQN	3	0
15	A	849	BCR	1	0
12	B	811	CLA	2	0
12	A	811	CLA	1	0
12	A	829	CLA	5	0
12	A	802	CLA	2	0
12	A	842	CLA	4	0
15	A	848	BCR	5	0
15	F	201	BCR	3	0
12	B	807	CLA	6	0
12	B	832	CLA	7	0
12	B	821	CLA	2	0
12	A	824	CLA	1	0
12	B	823	CLA	4	0
12	A	809	CLA	2	0
12	B	809	CLA	3	0
15	B	836	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	810	CLA	1	0
12	B	817	CLA	1	0
12	A	833	CLA	2	0
12	A	839	CLA	1	0
12	A	838	CLA	1	0
15	M	101	BCR	2	0
12	A	807	CLA	2	0
12	A	805	CLA	8	0
15	J	102	BCR	3	0
12	A	843	CLA	1	0
12	A	826	CLA	1	0
15	A	851	BCR	1	0
12	A	828	CLA	7	0
12	B	827	CLA	1	0
12	B	825	CLA	2	0
12	B	826	CLA	1	0
12	L	204	CLA	2	0
12	A	822	CLA	1	0
12	B	814	CLA	1	0
12	B	818	CLA	3	0
15	I	101	BCR	5	0
11	A	801	CL0	3	0
12	B	831	CLA	3	0
12	B	802	CLA	8	0
12	L	203	CLA	6	0
12	A	832	CLA	5	0
12	A	841	CLA	1	0
12	B	820	CLA	3	0
12	A	837	CLA	1	0
12	B	830	CLA	1	0
15	A	850	BCR	5	0
15	B	834	BCR	2	0
15	J	103	BCR	1	0
17	B	837	LMG	7	0
12	A	830	CLA	4	0
12	A	827	CLA	1	0
12	B	801	CLA	4	0
16	A	852	LHG	2	0
12	A	821	CLA	3	0
15	J	104	BCR	2	0
12	A	831	CLA	2	0
12	A	815	CLA	2	0

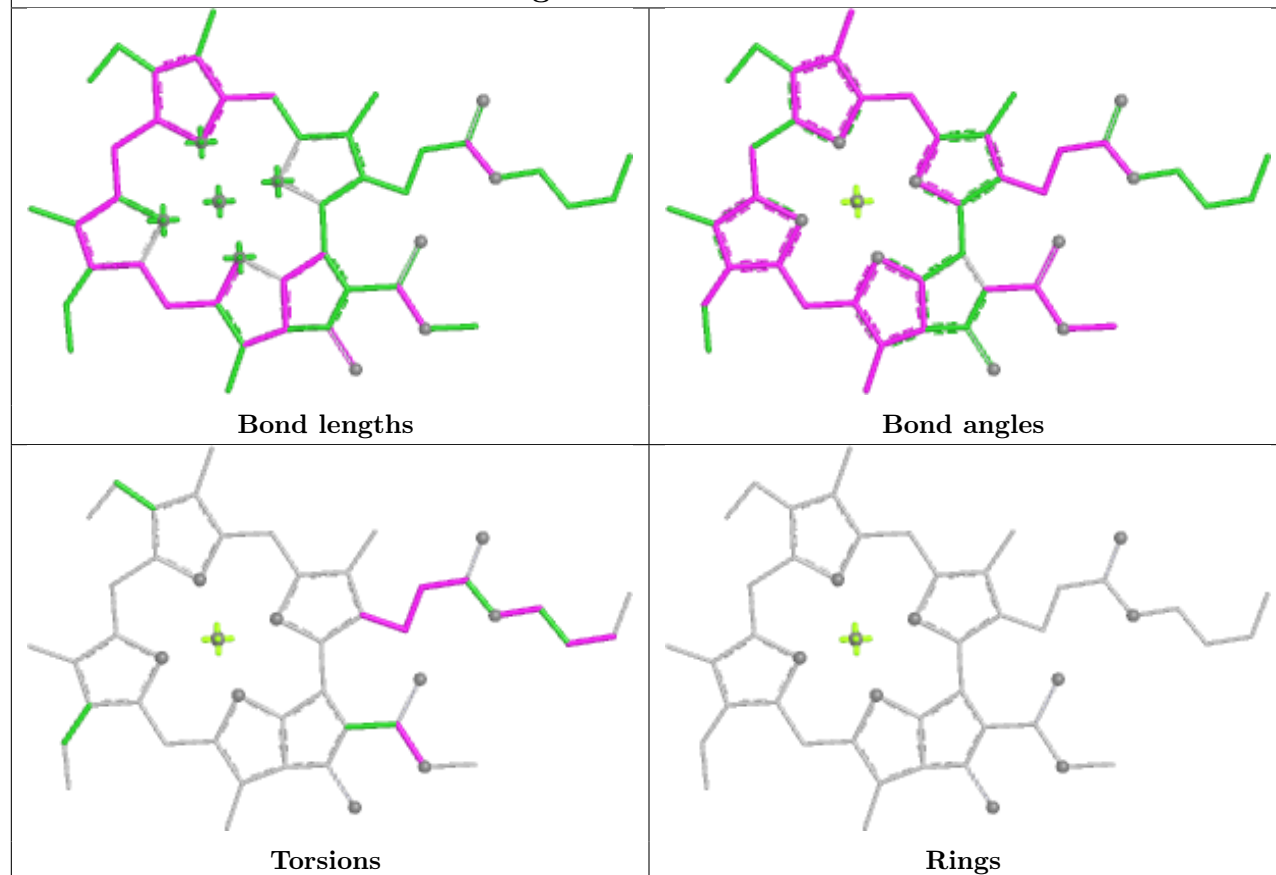
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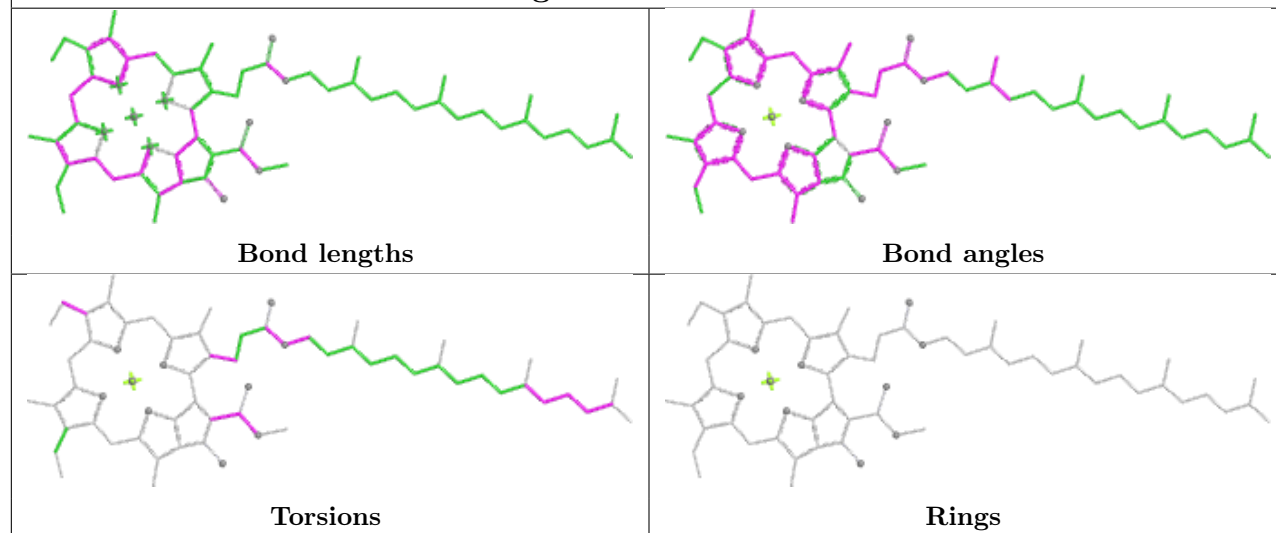
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	829	CLA	4	0
15	B	835	BCR	4	0
12	B	810	CLA	2	0
12	A	817	CLA	1	0
15	F	202	BCR	3	0
15	L	205	BCR	3	0
12	A	835	CLA	1	0
12	A	819	CLA	6	0
12	B	822	CLA	6	0
12	A	803	CLA	1	0
12	B	819	CLA	1	0
15	L	206	BCR	3	0
13	B	833	PQN	5	0
12	B	812	CLA	2	0
12	A	812	CLA	3	0
12	A	818	CLA	3	0
12	B	804	CLA	7	0
12	A	813	CLA	1	0
12	A	836	CLA	1	0
12	B	808	CLA	4	0
12	A	840	CLA	2	0
12	A	820	CLA	2	0
15	A	847	BCR	4	0
15	L	201	BCR	5	0

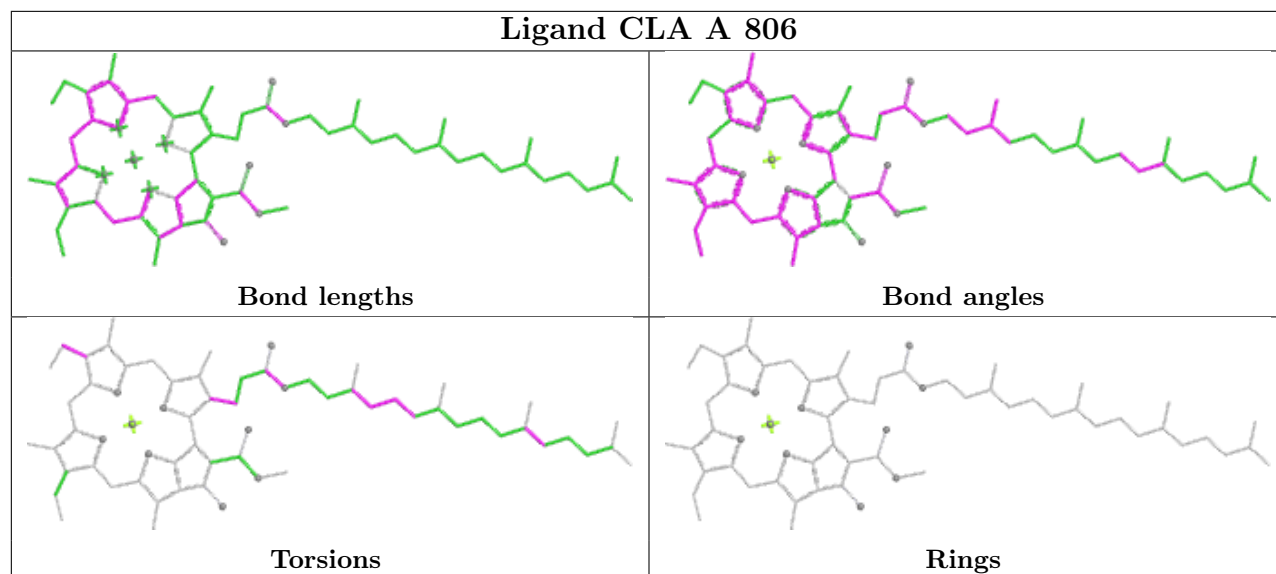
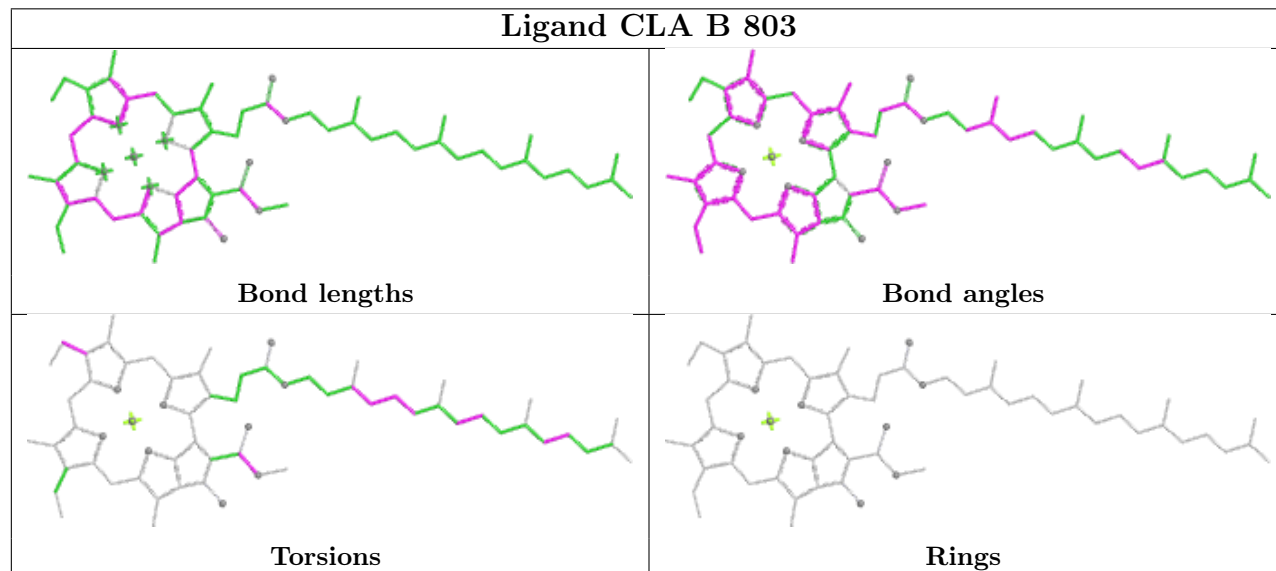
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

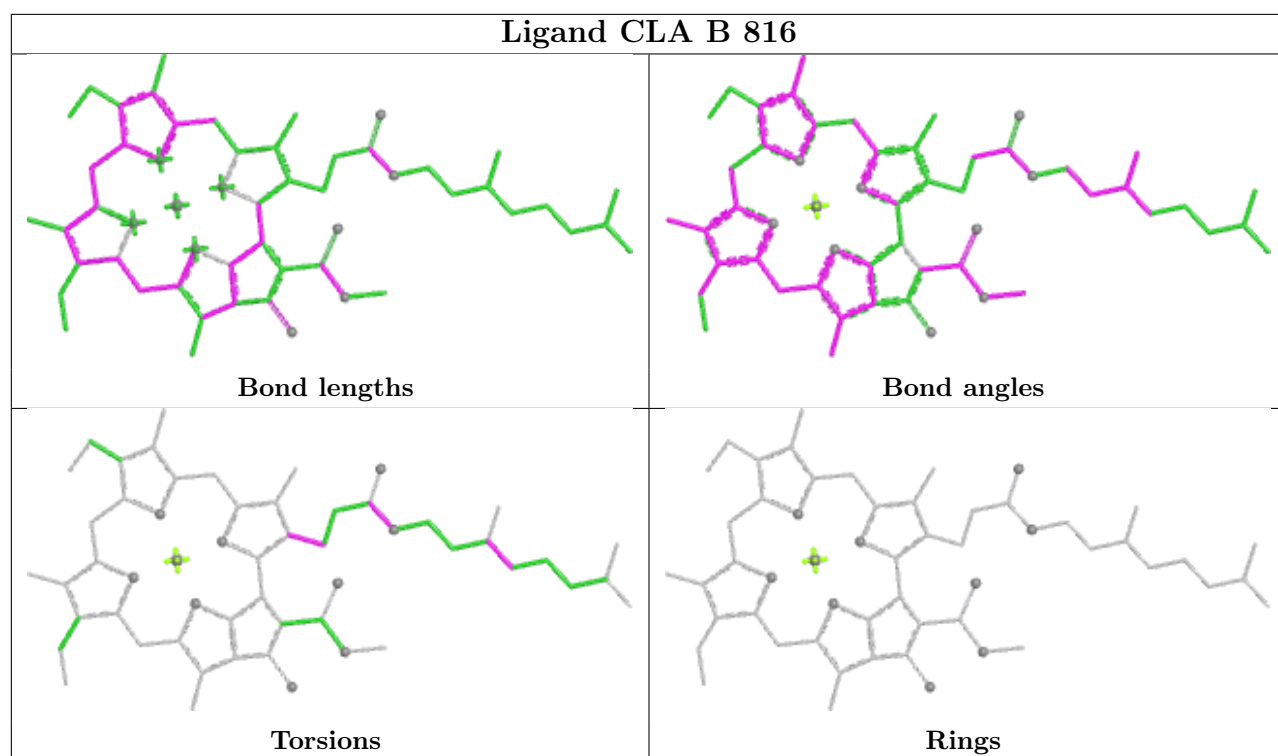
Ligand CLA B 824



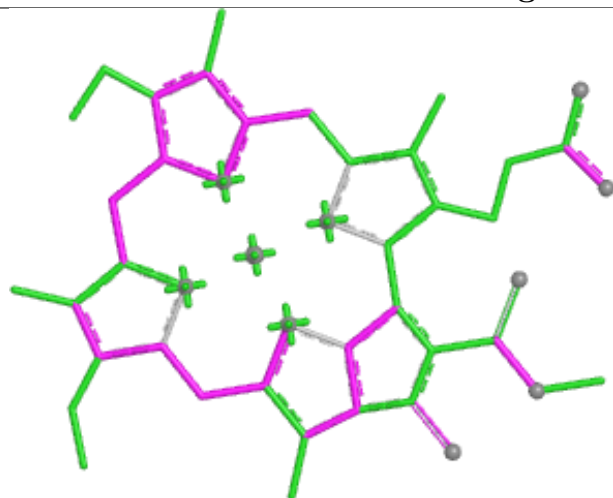
Ligand CLA B 806



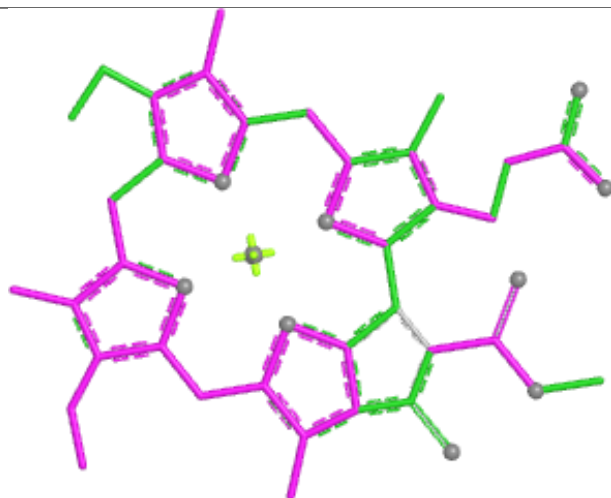
Ligand CLA A 806**Ligand CLA B 803**



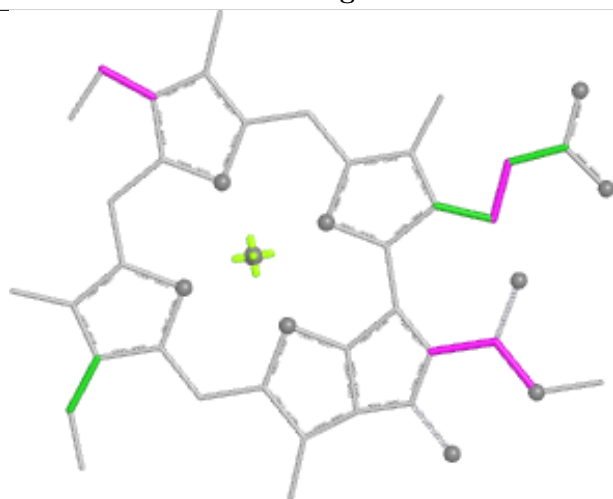
Ligand CLA J 101



Bond lengths



Bond angles

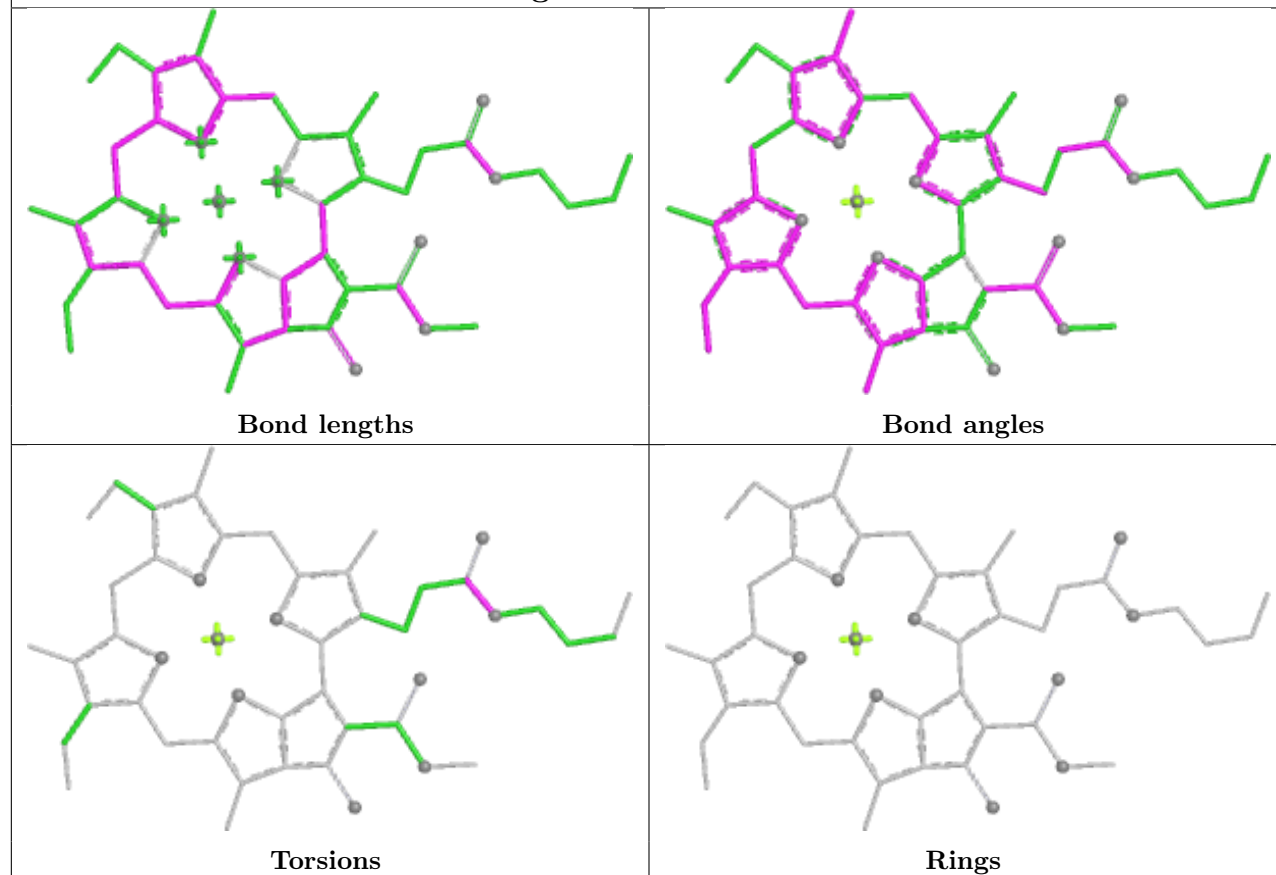


Torsions

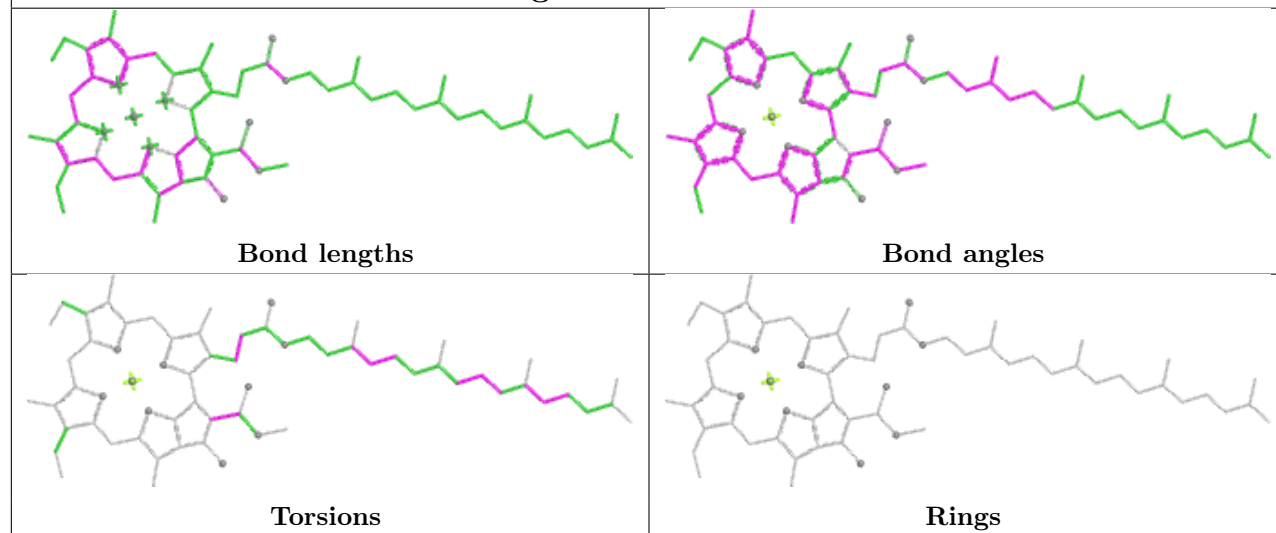


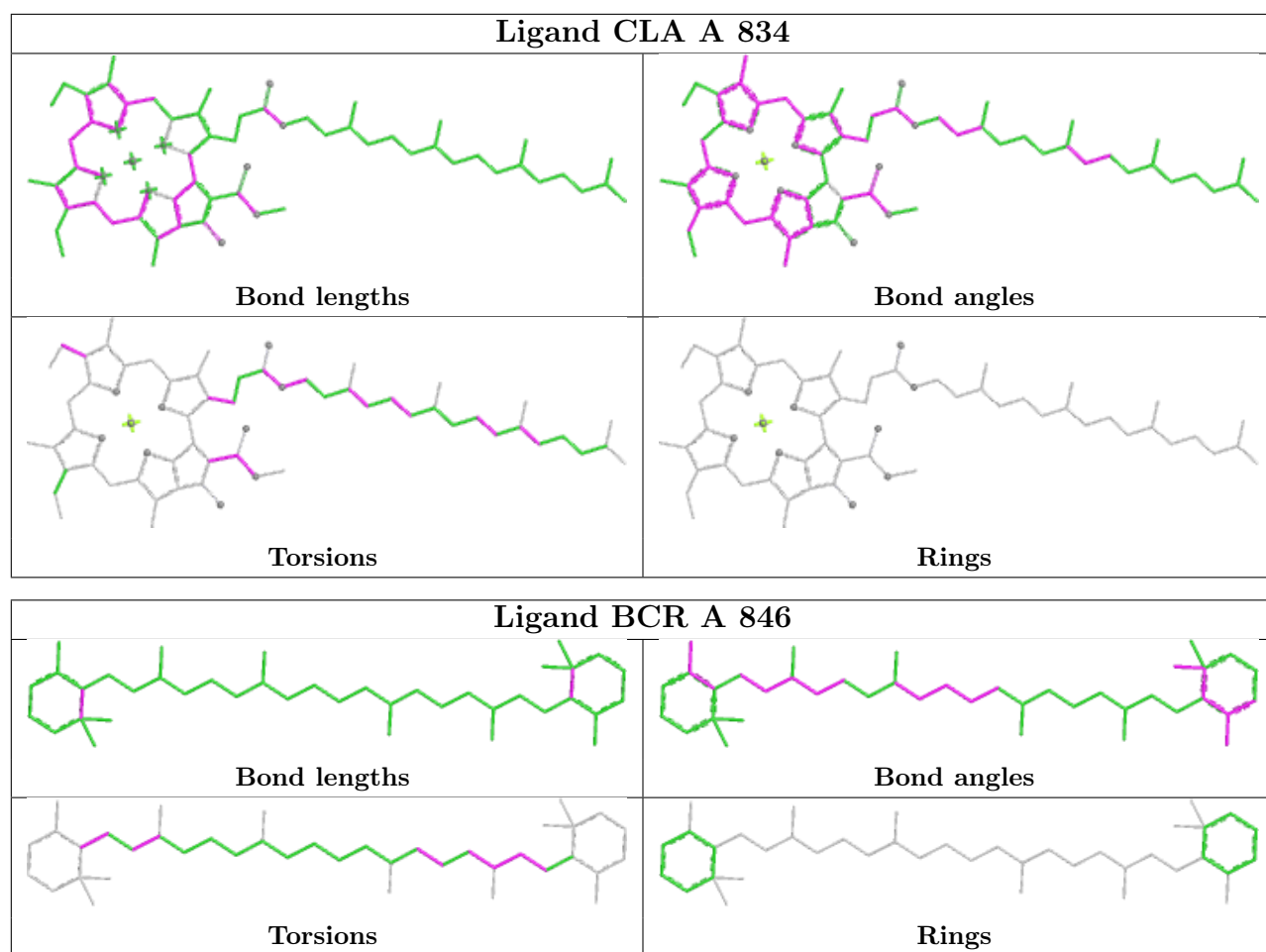
Rings

Ligand CLA A 816

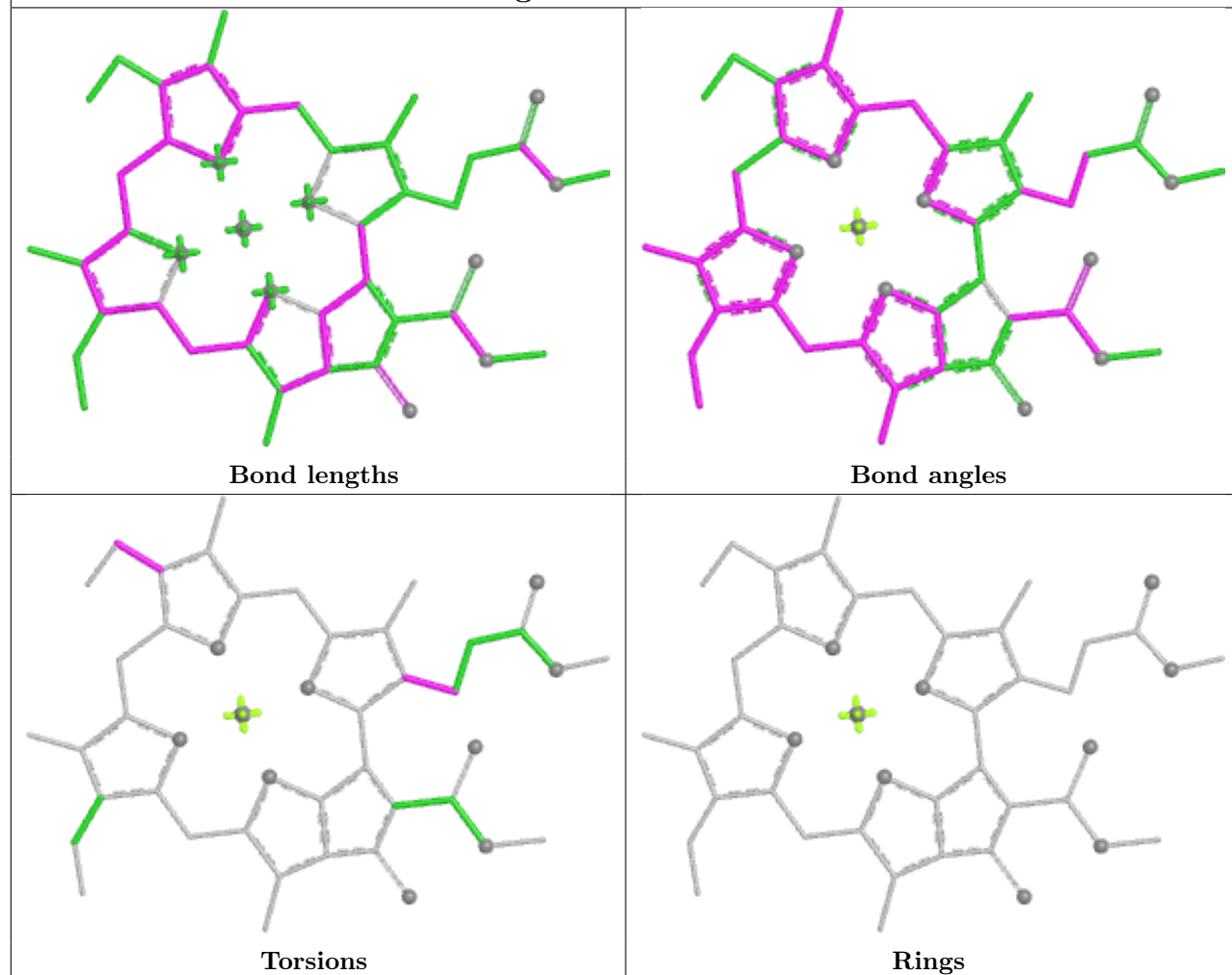


Ligand CLA A 825

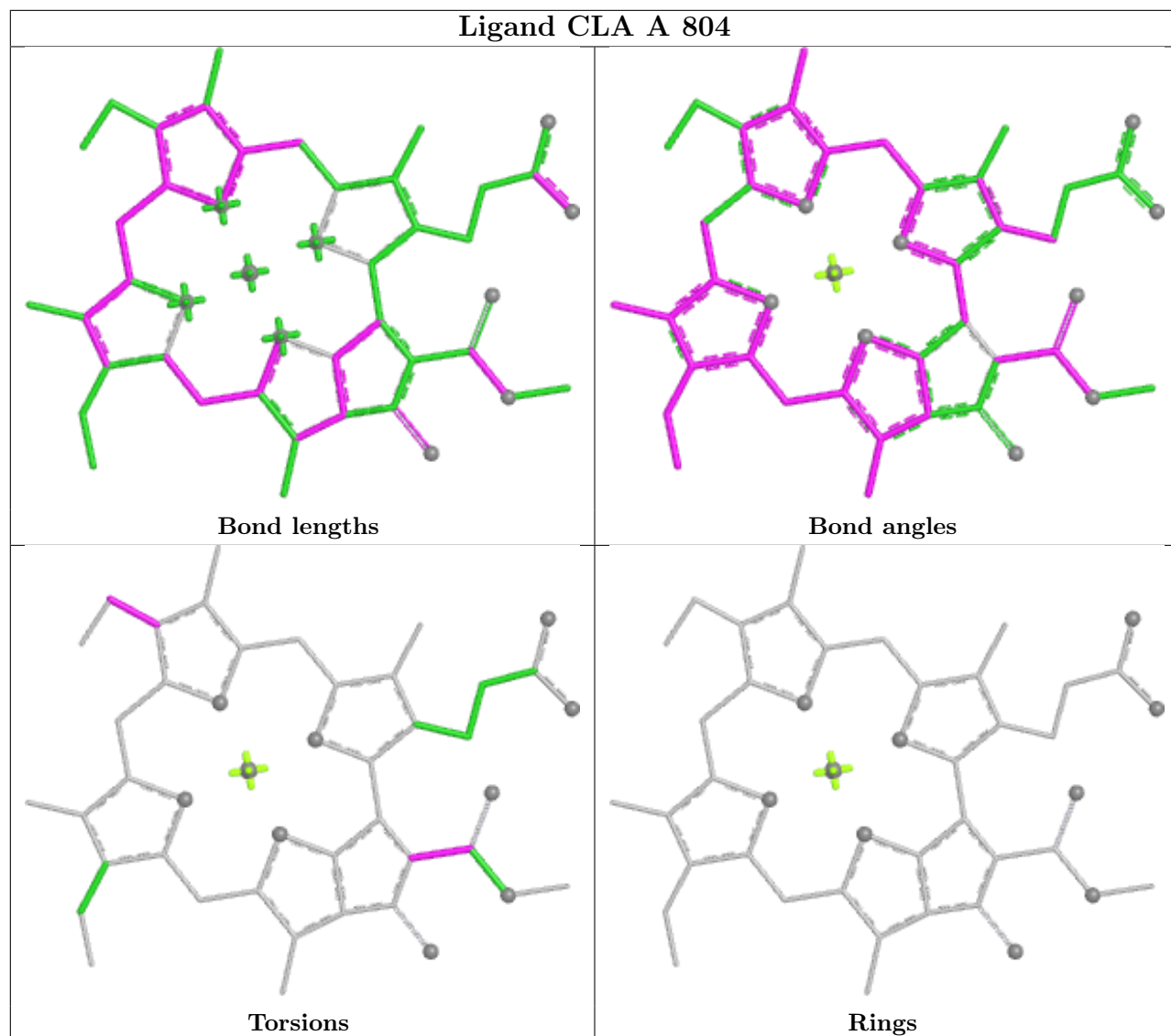




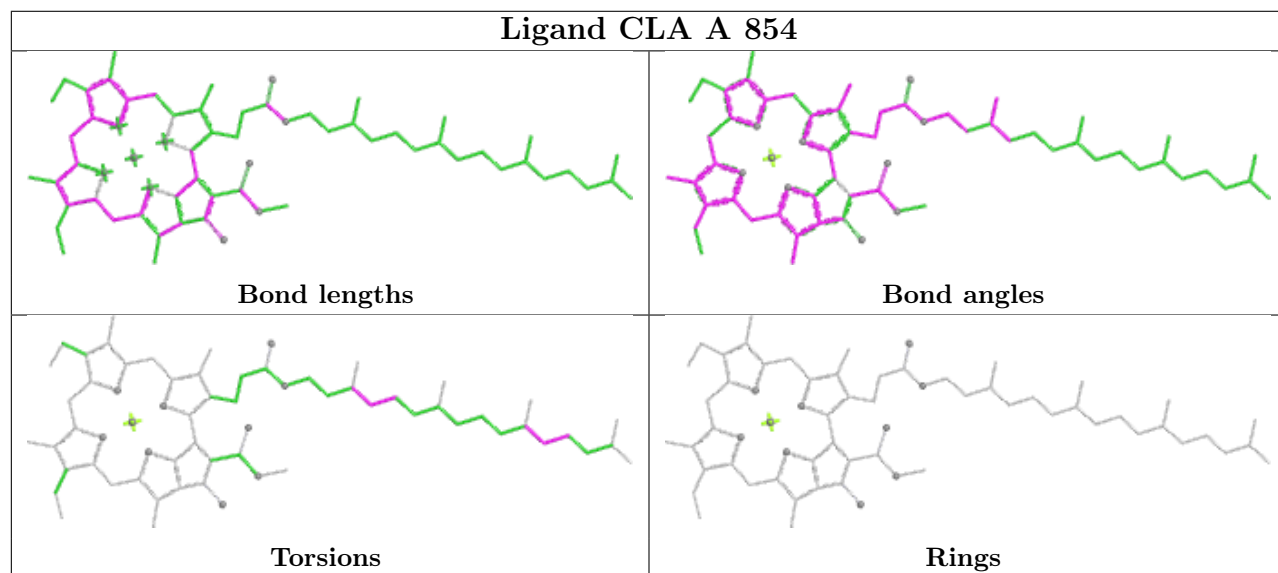
Ligand CLA L 202

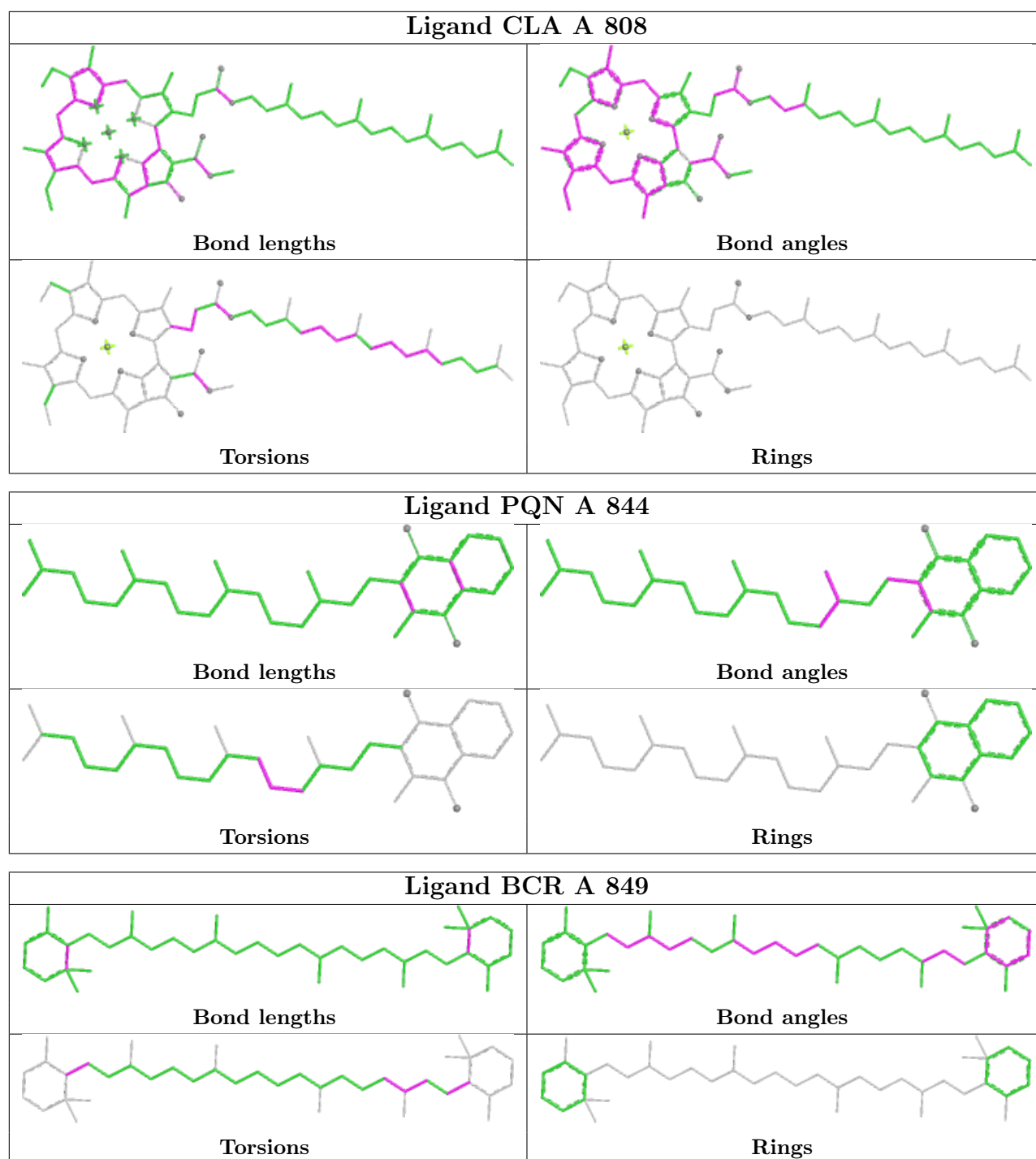


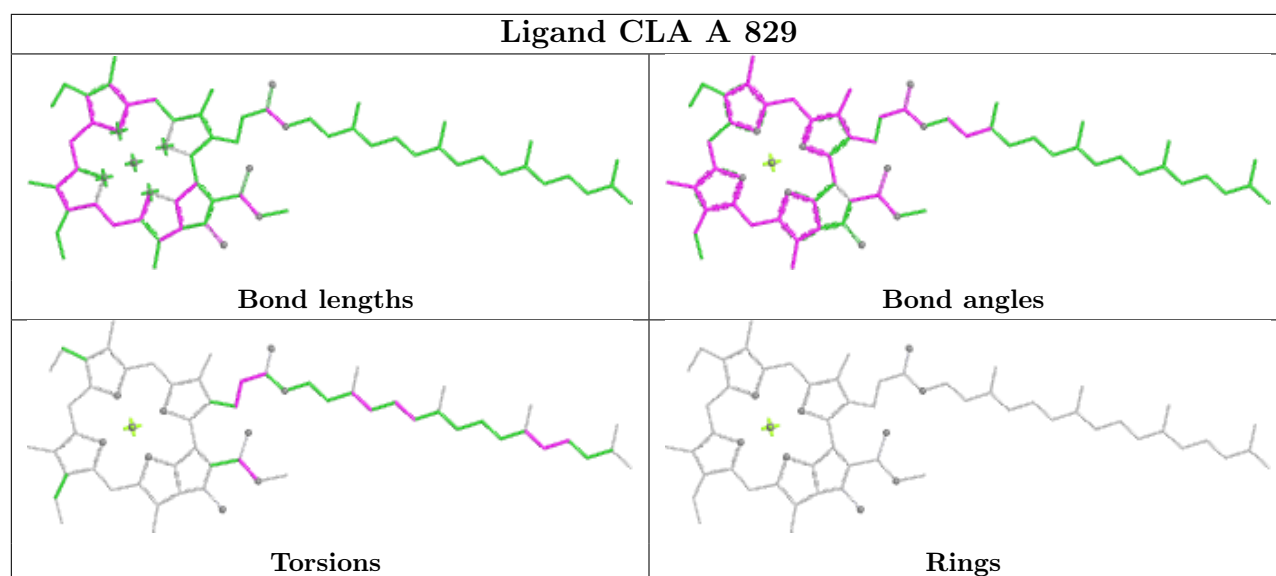
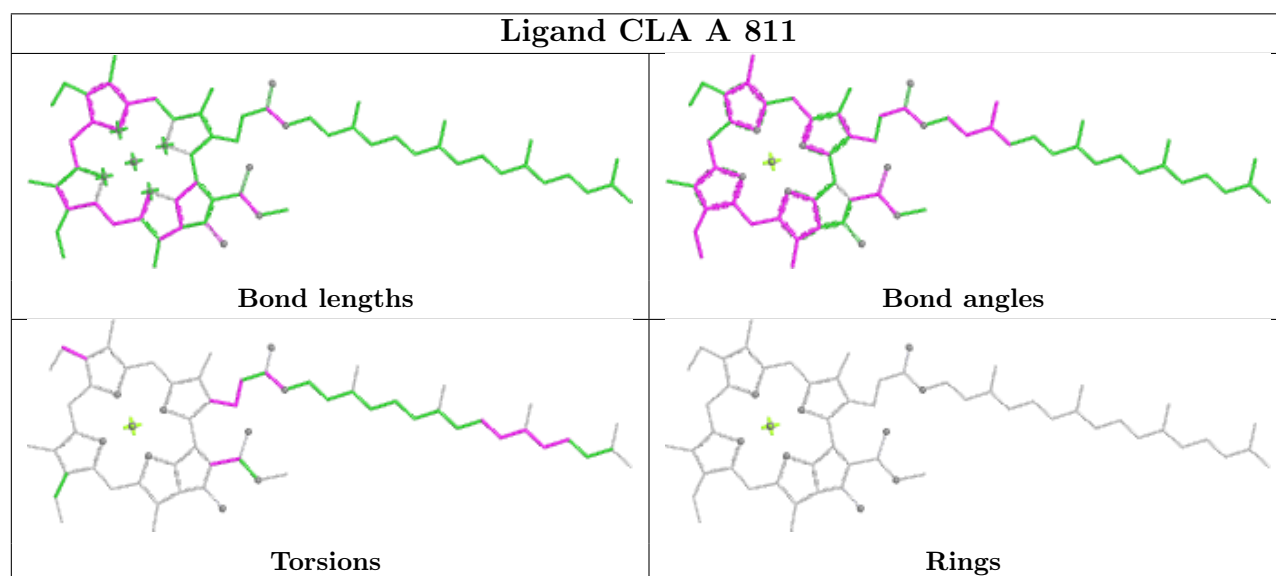
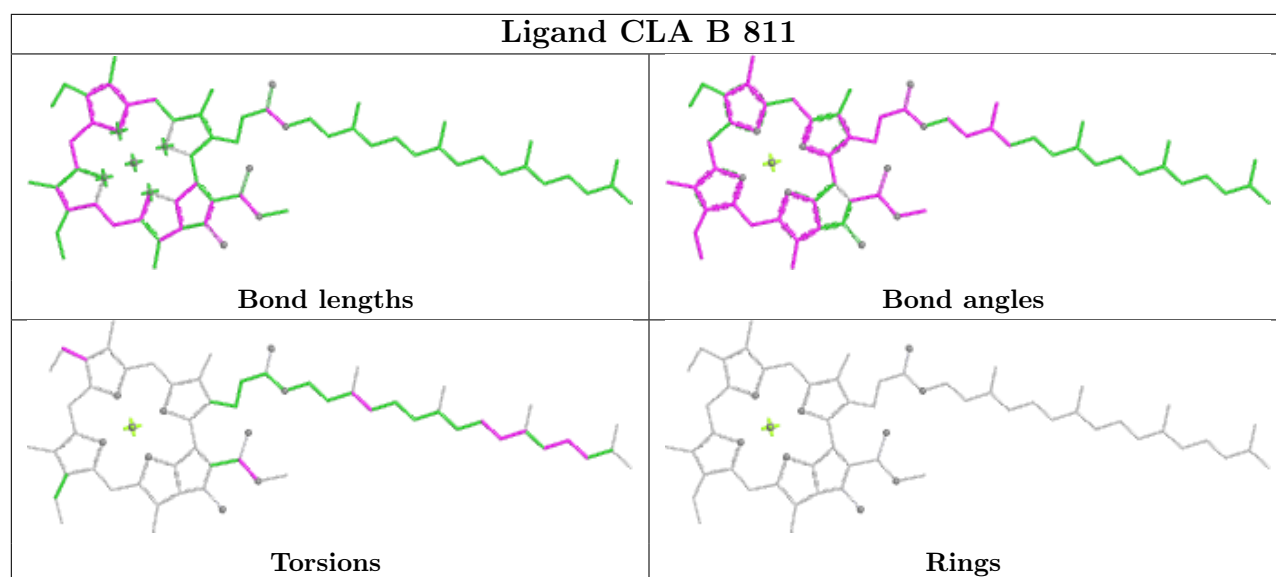
Ligand CLA A 804



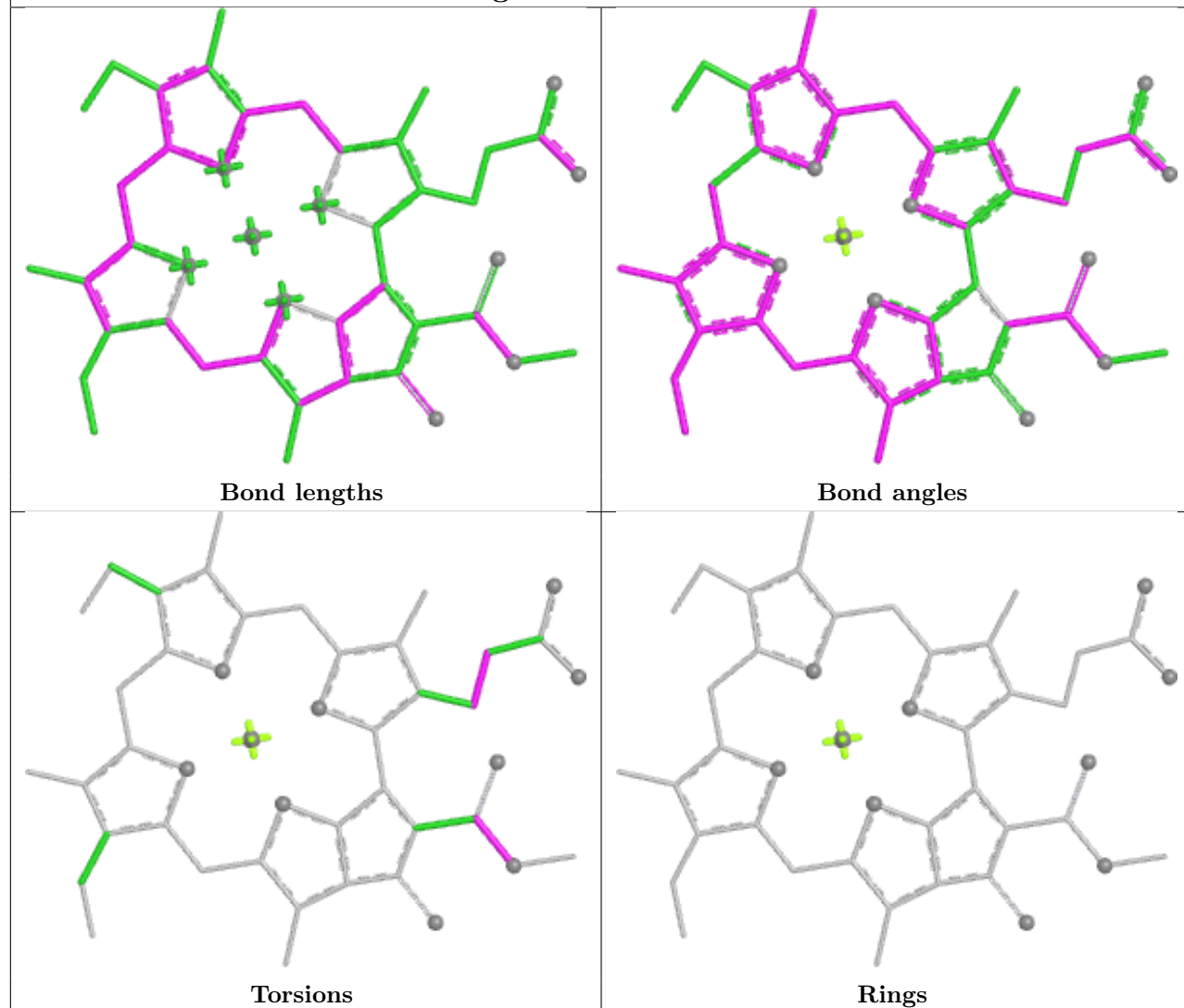
Ligand CLA A 854



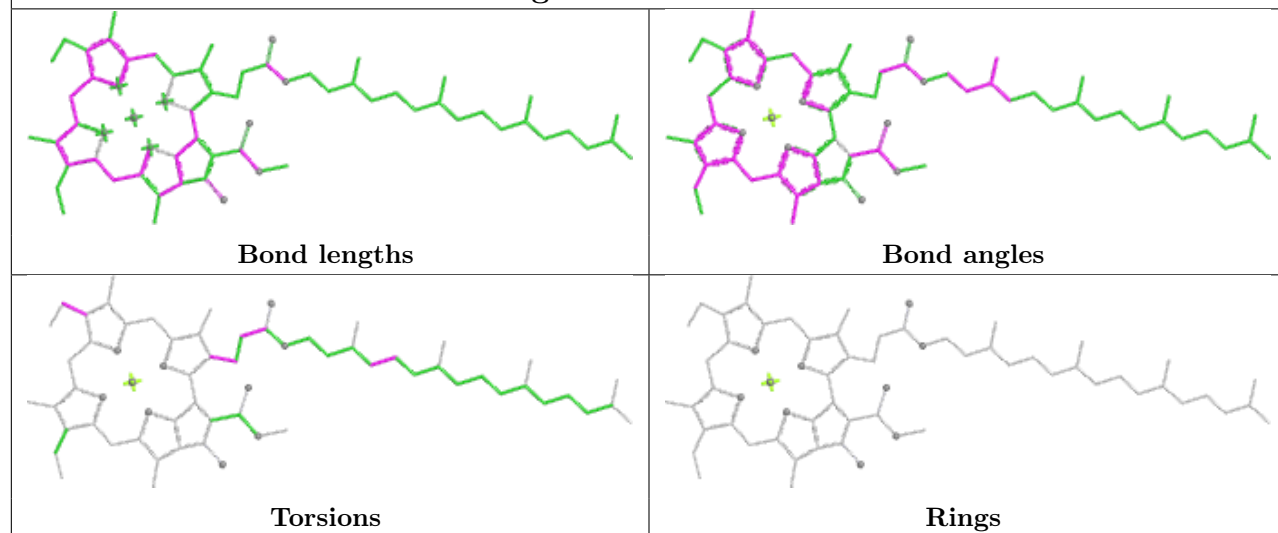


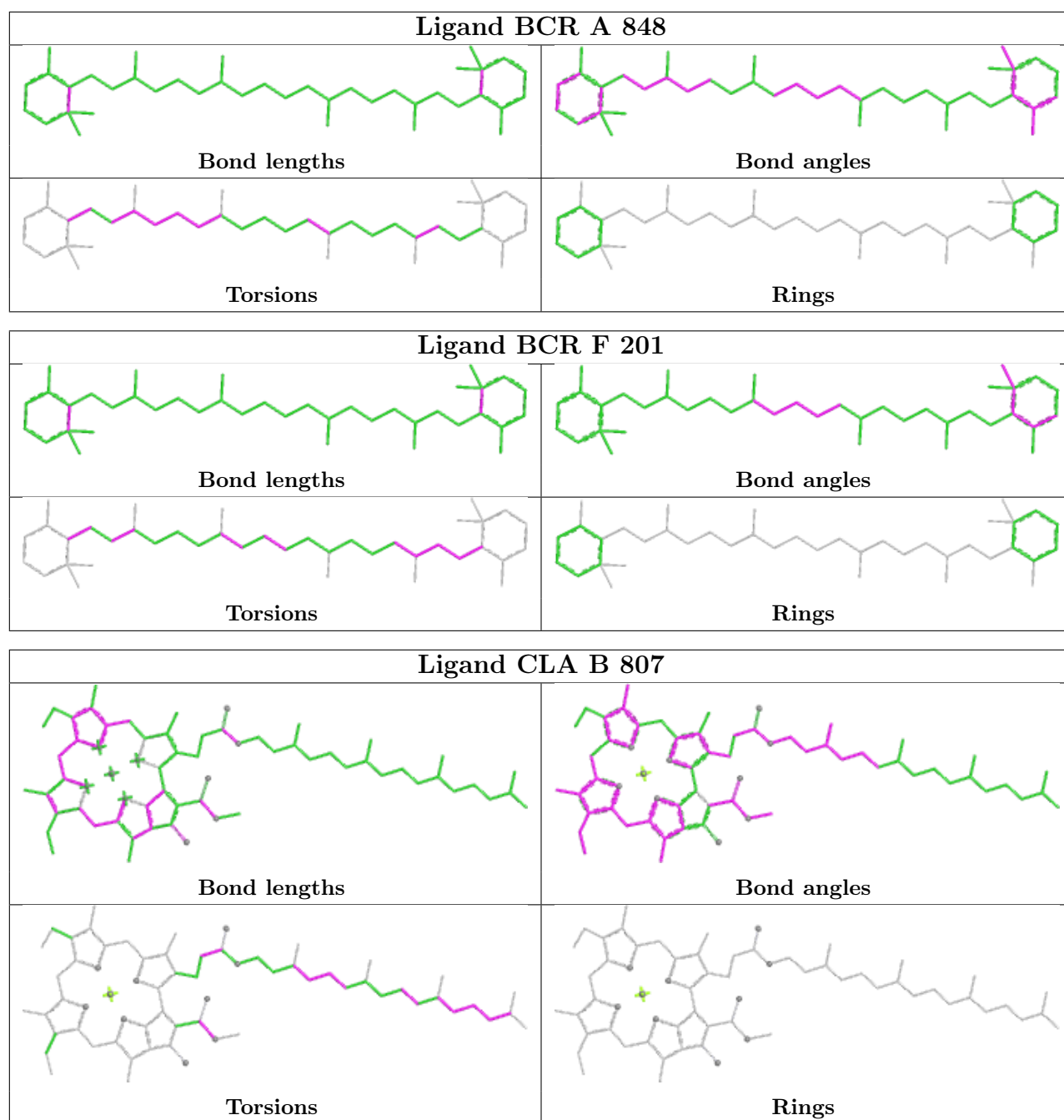


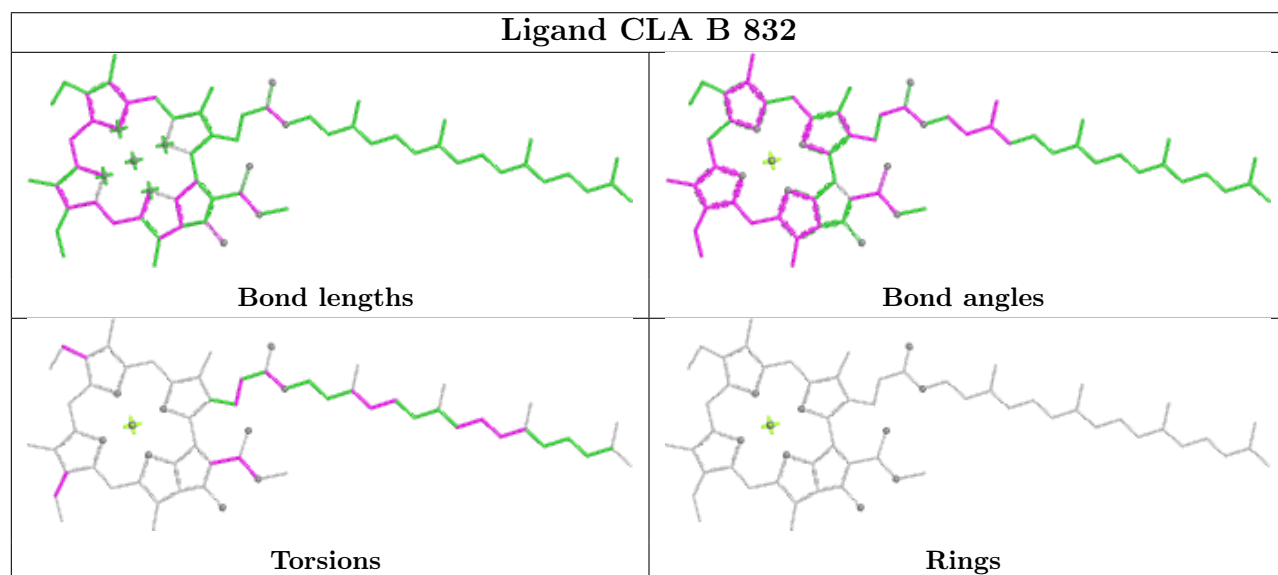
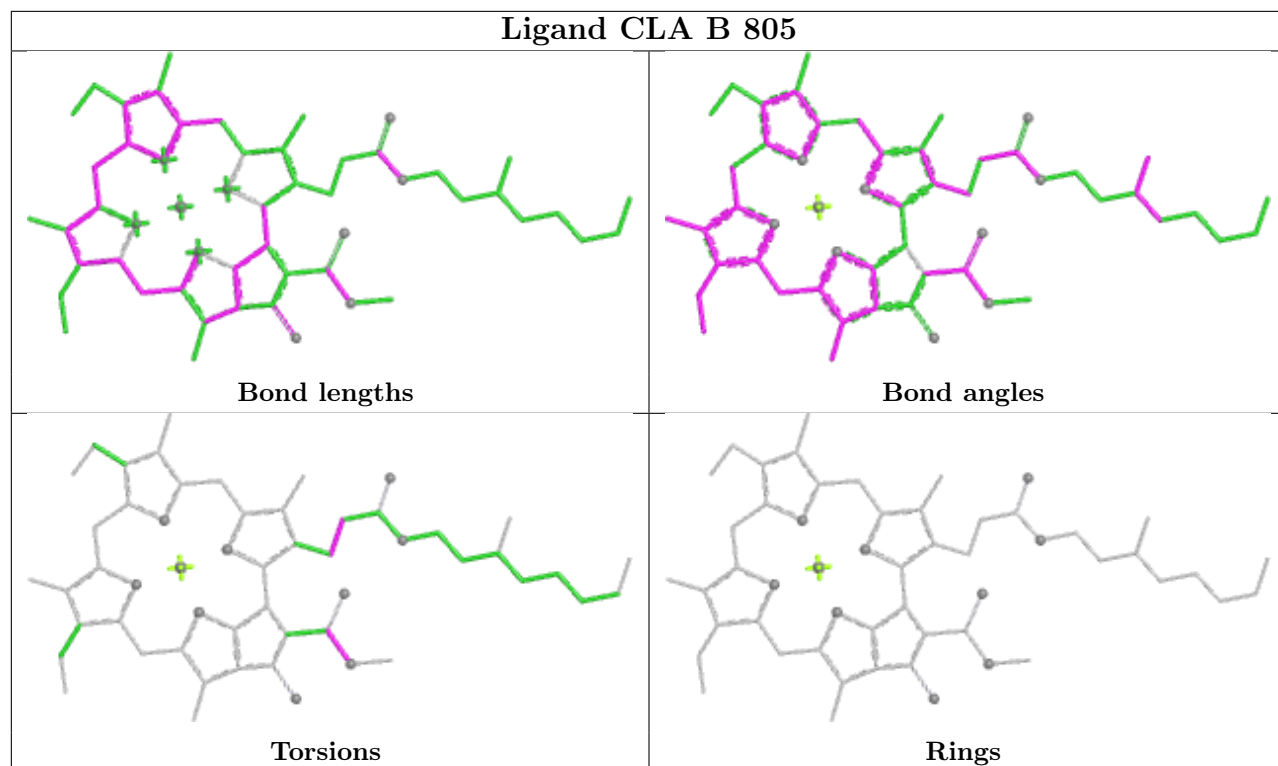
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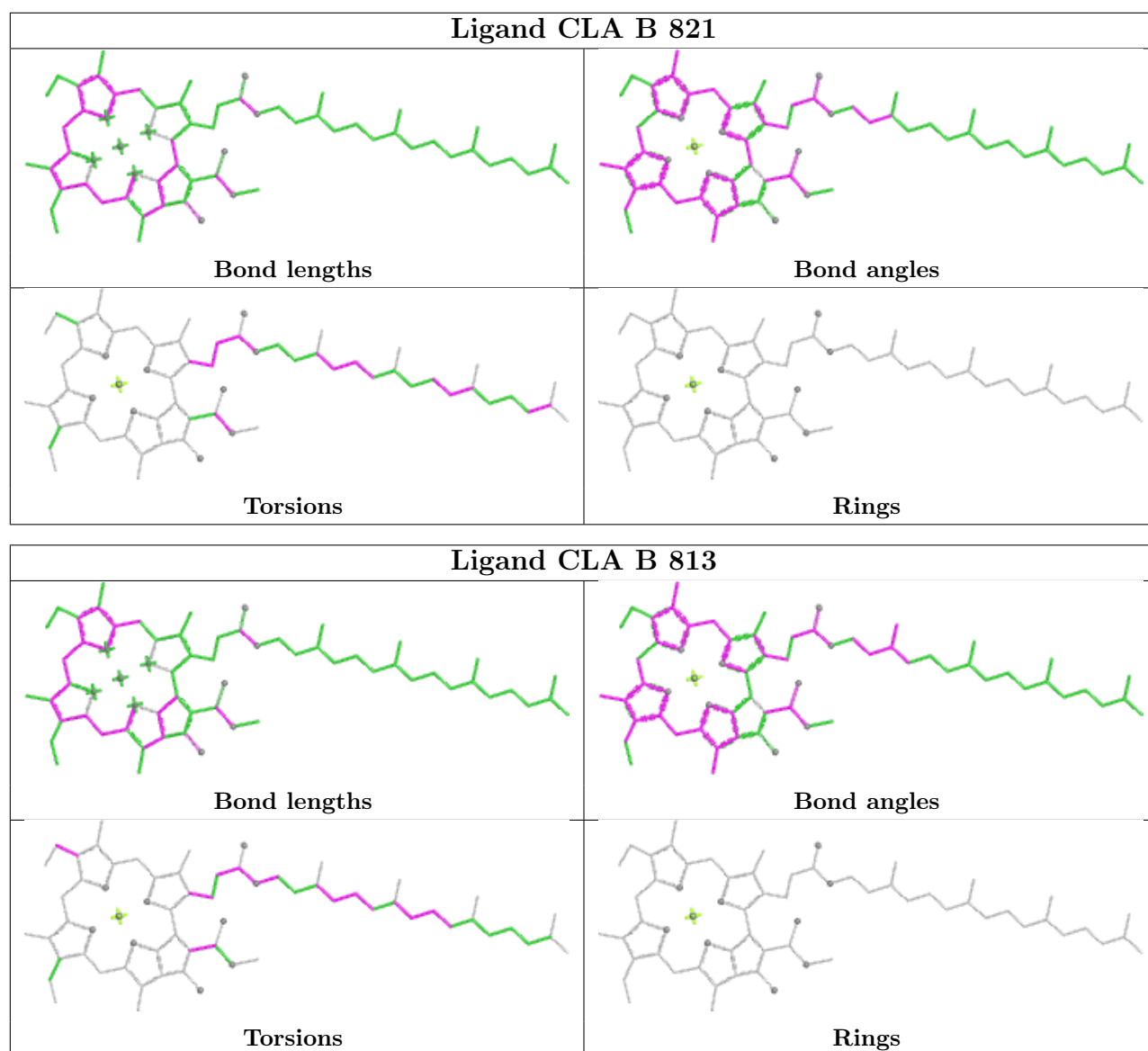


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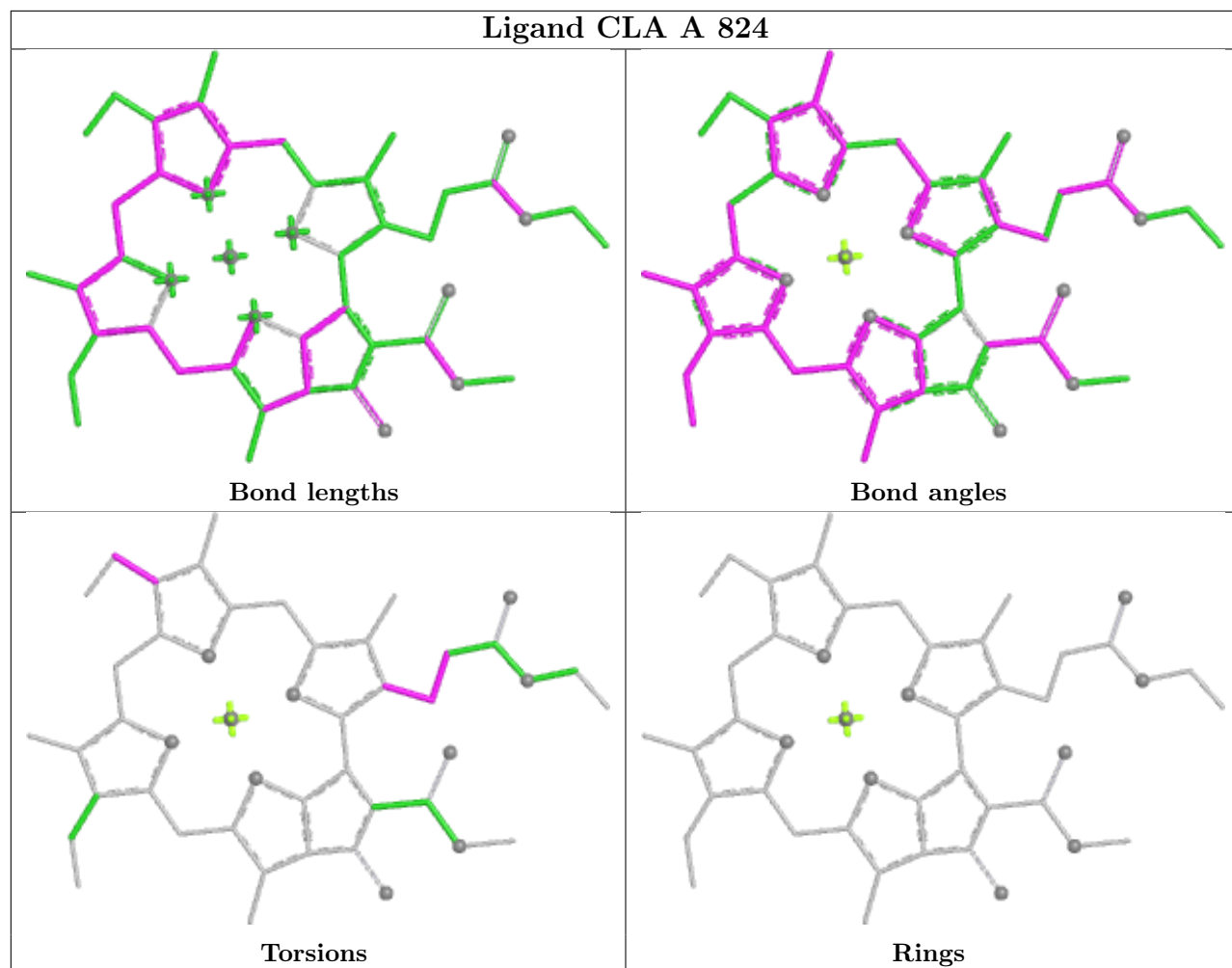




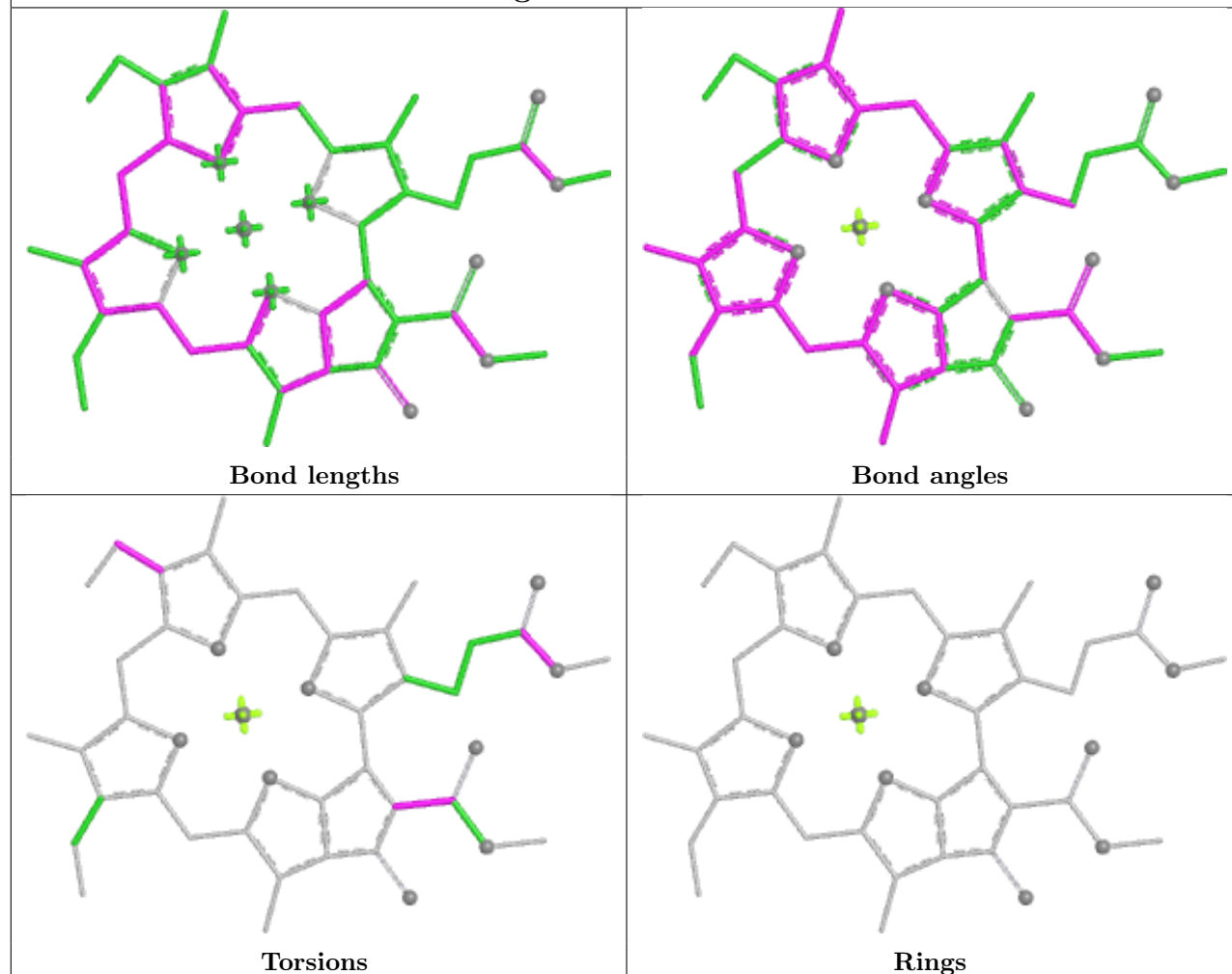




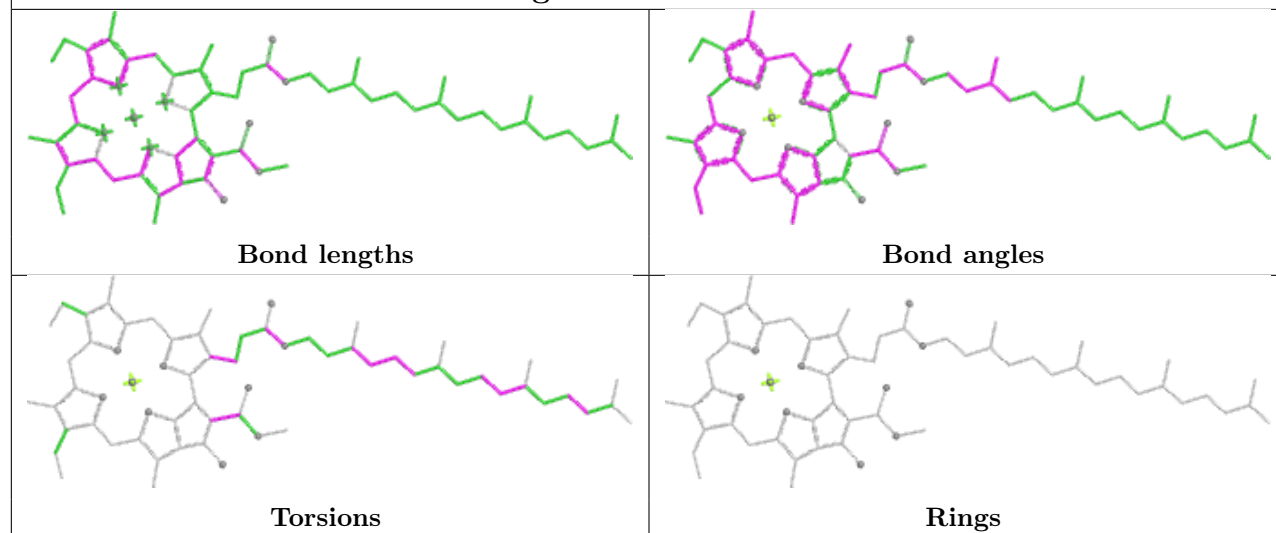
Ligand CLA A 824



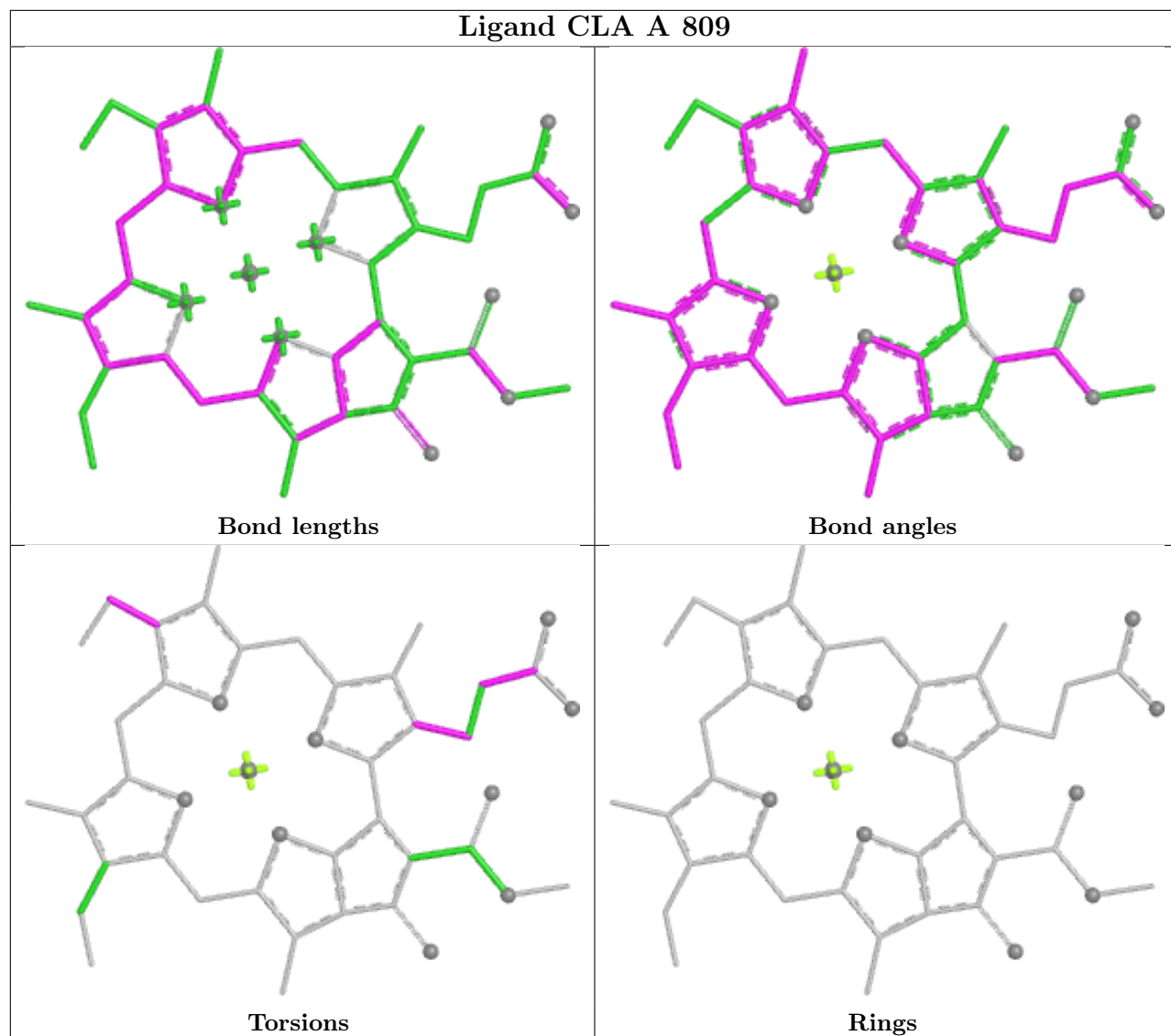
Ligand CLA B 828



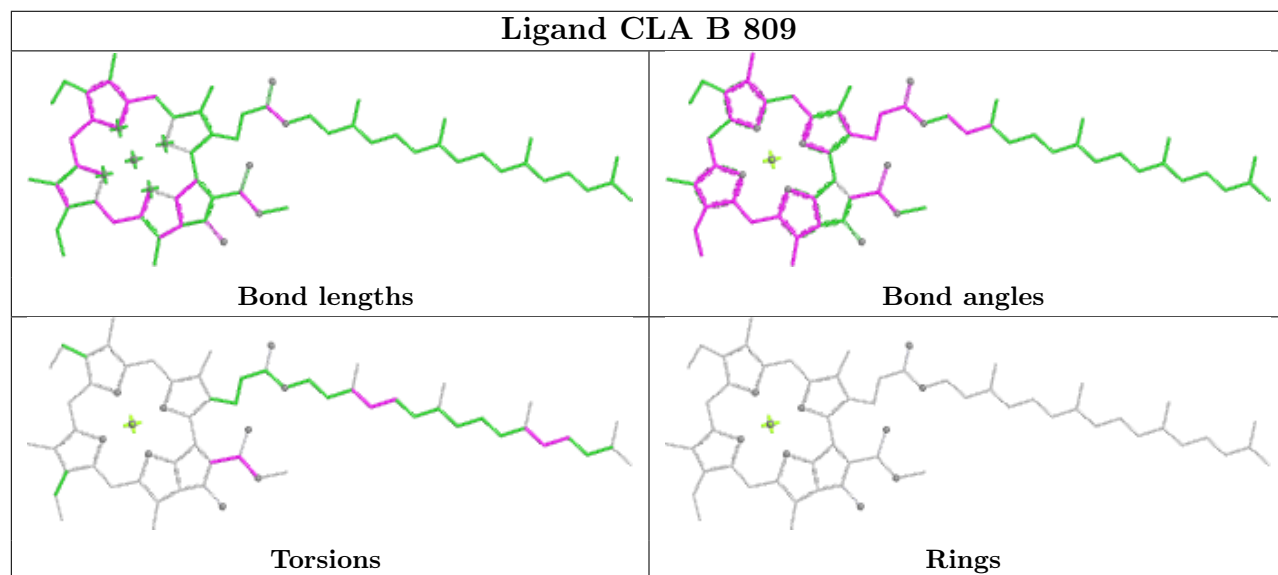
Ligand CLA B 823

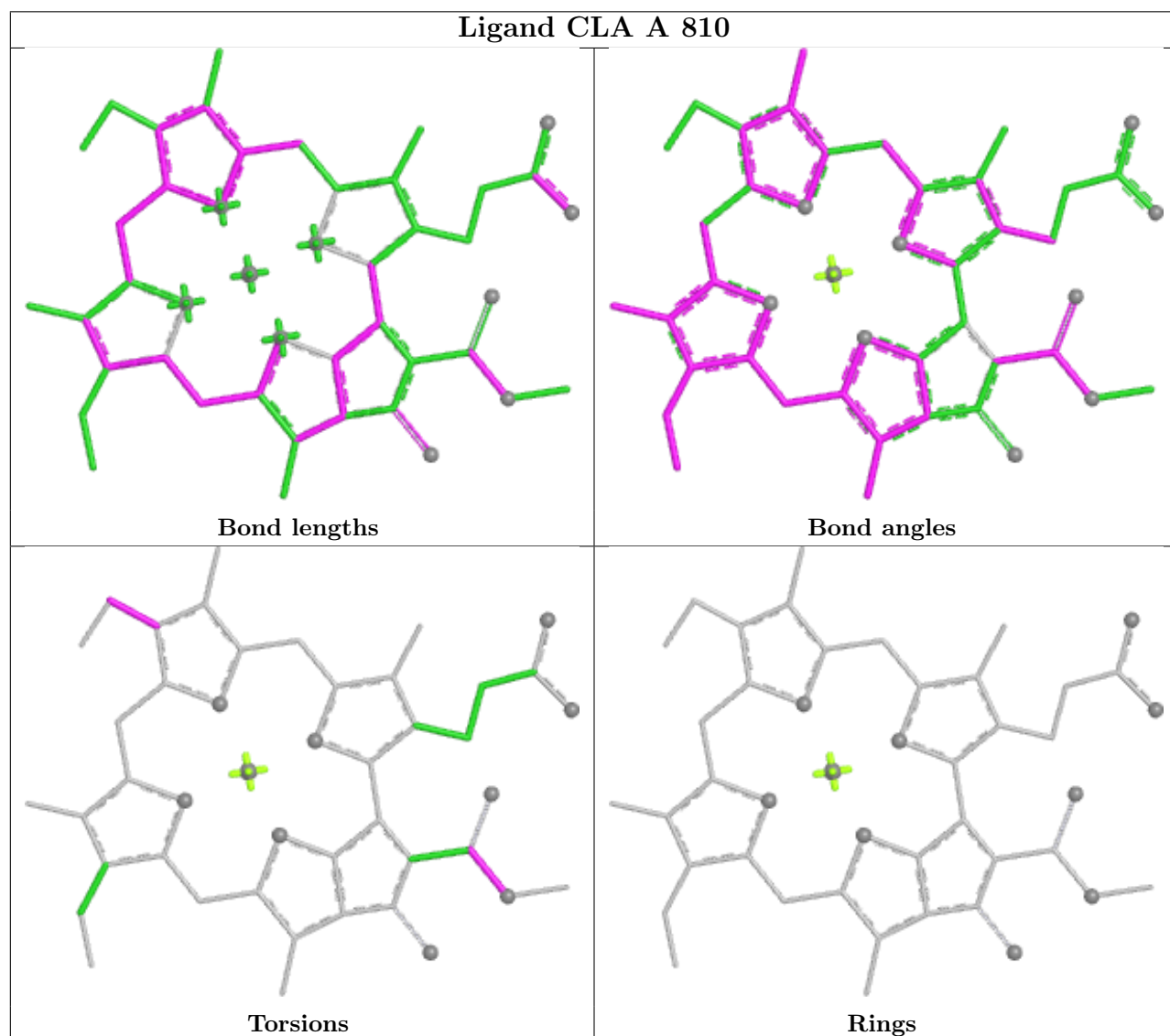
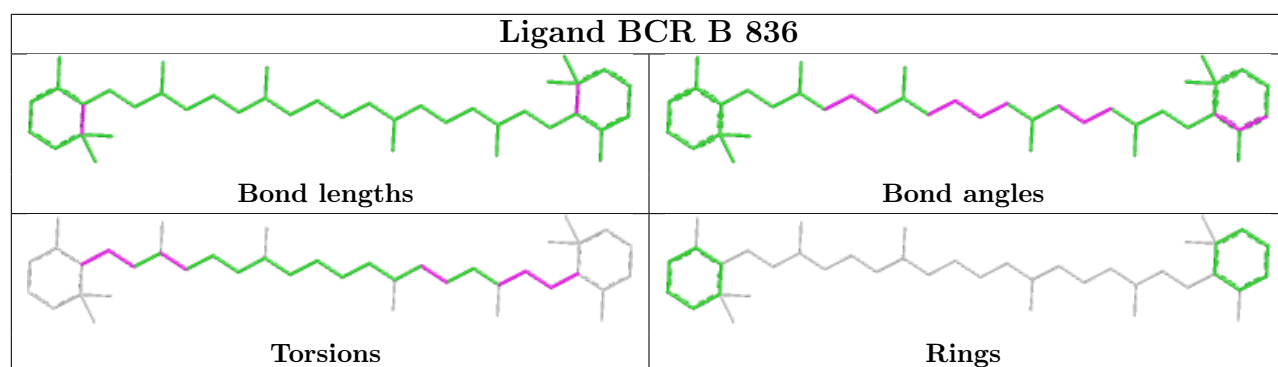


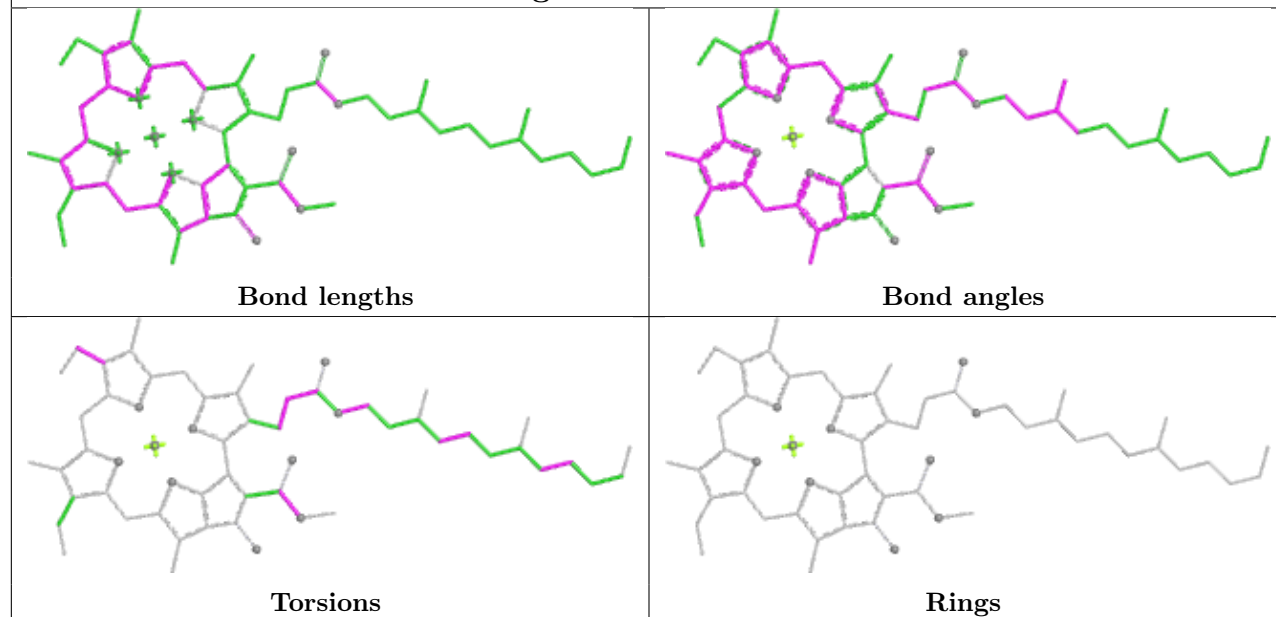
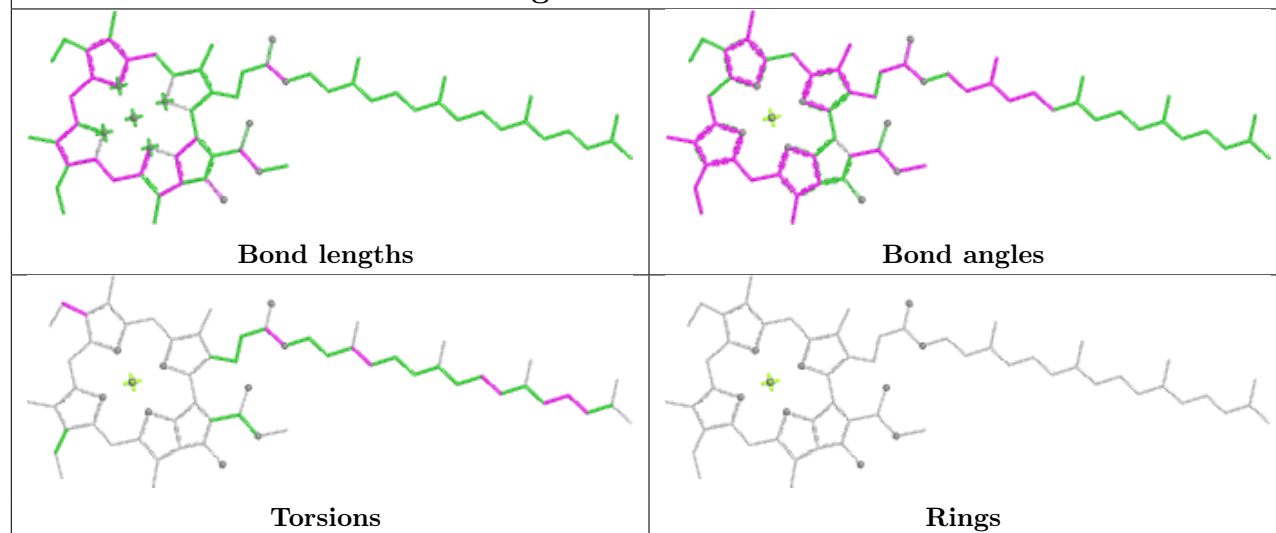
Ligand CLA A 809



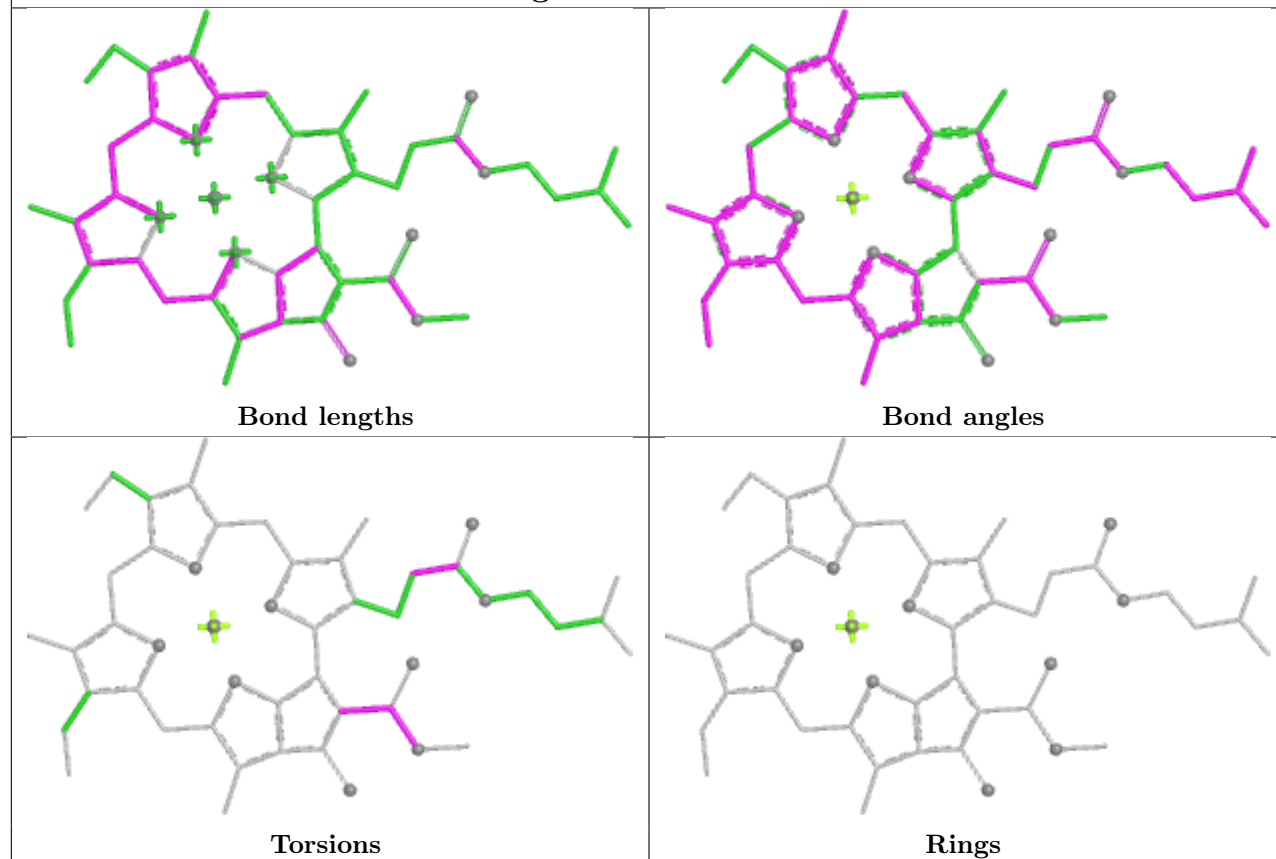
Ligand CLA B 809



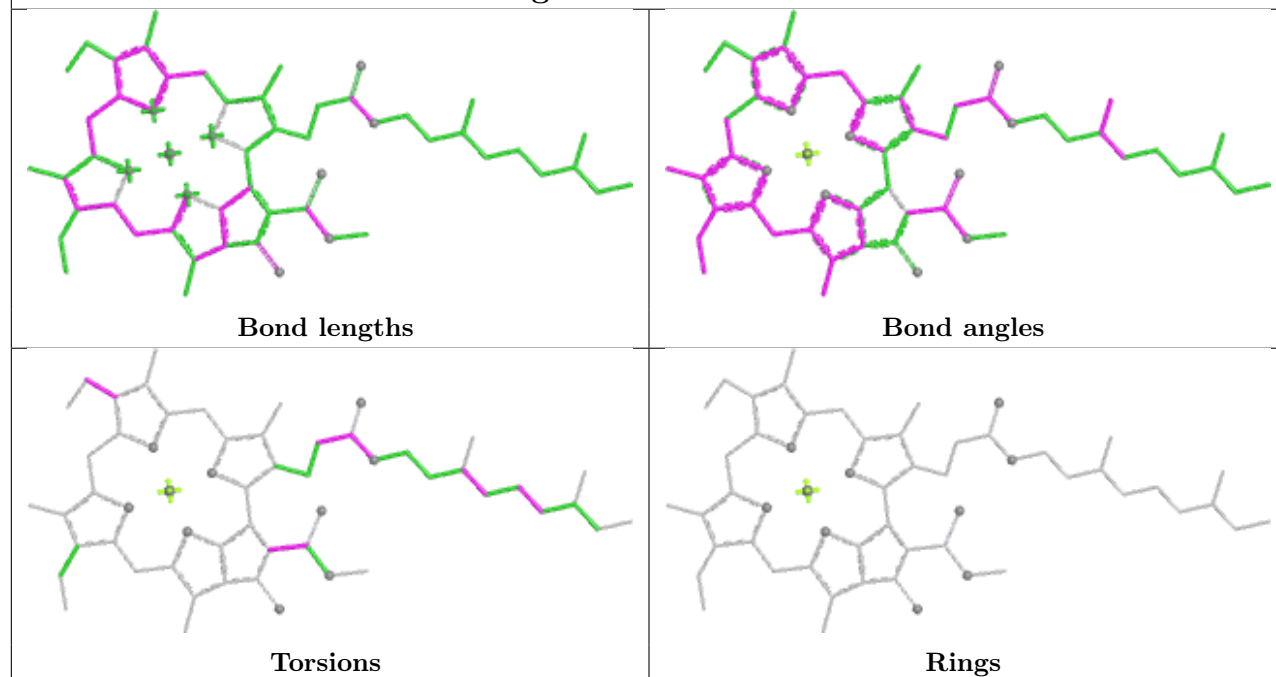


Ligand CLA B 817**Ligand CLA A 833**

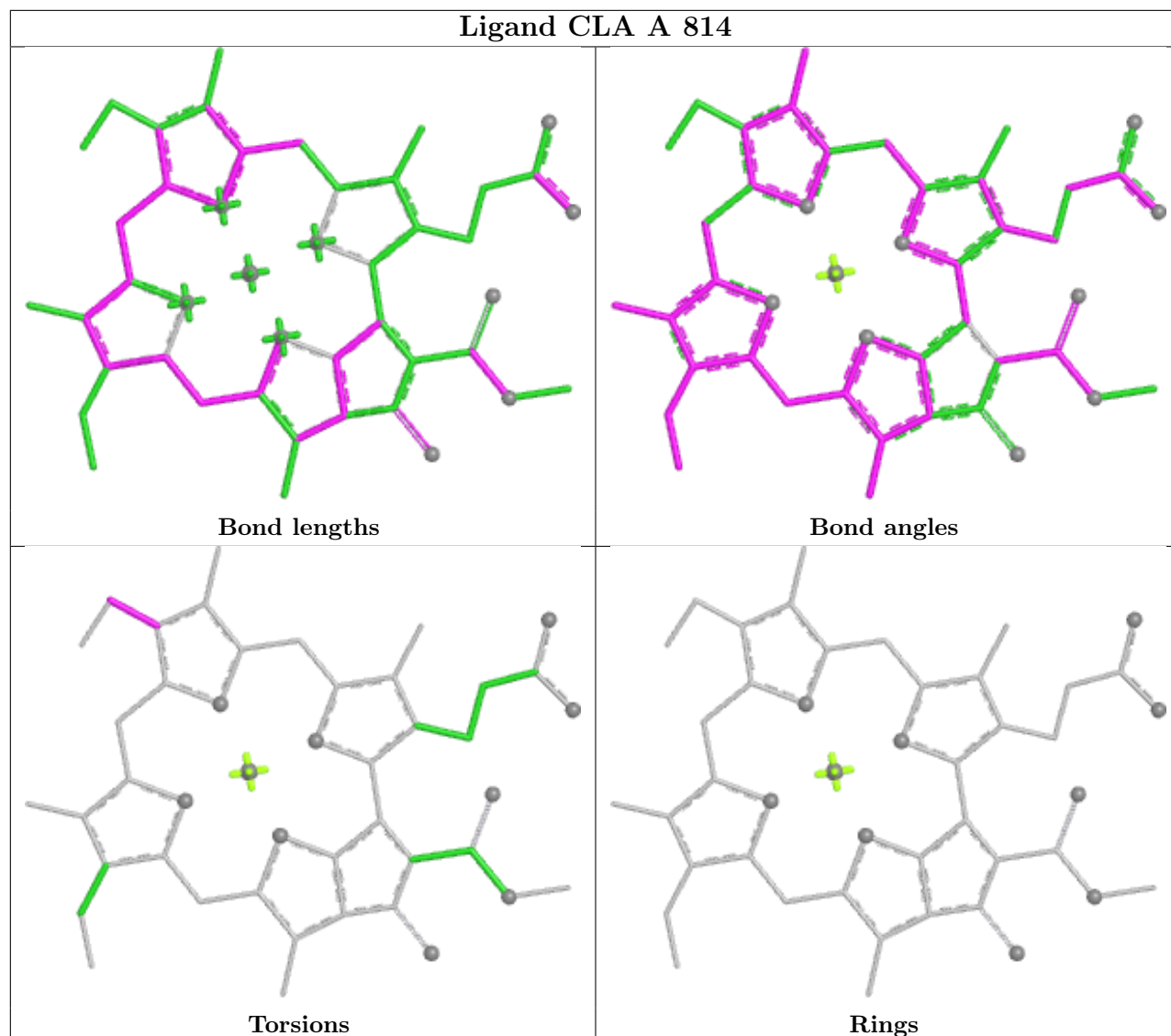
Ligand CLA A 839



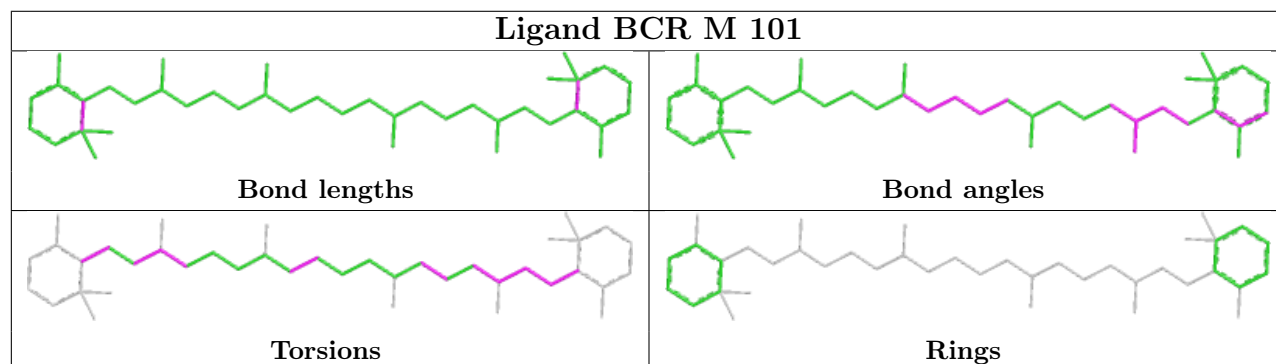
Ligand CLA A 838



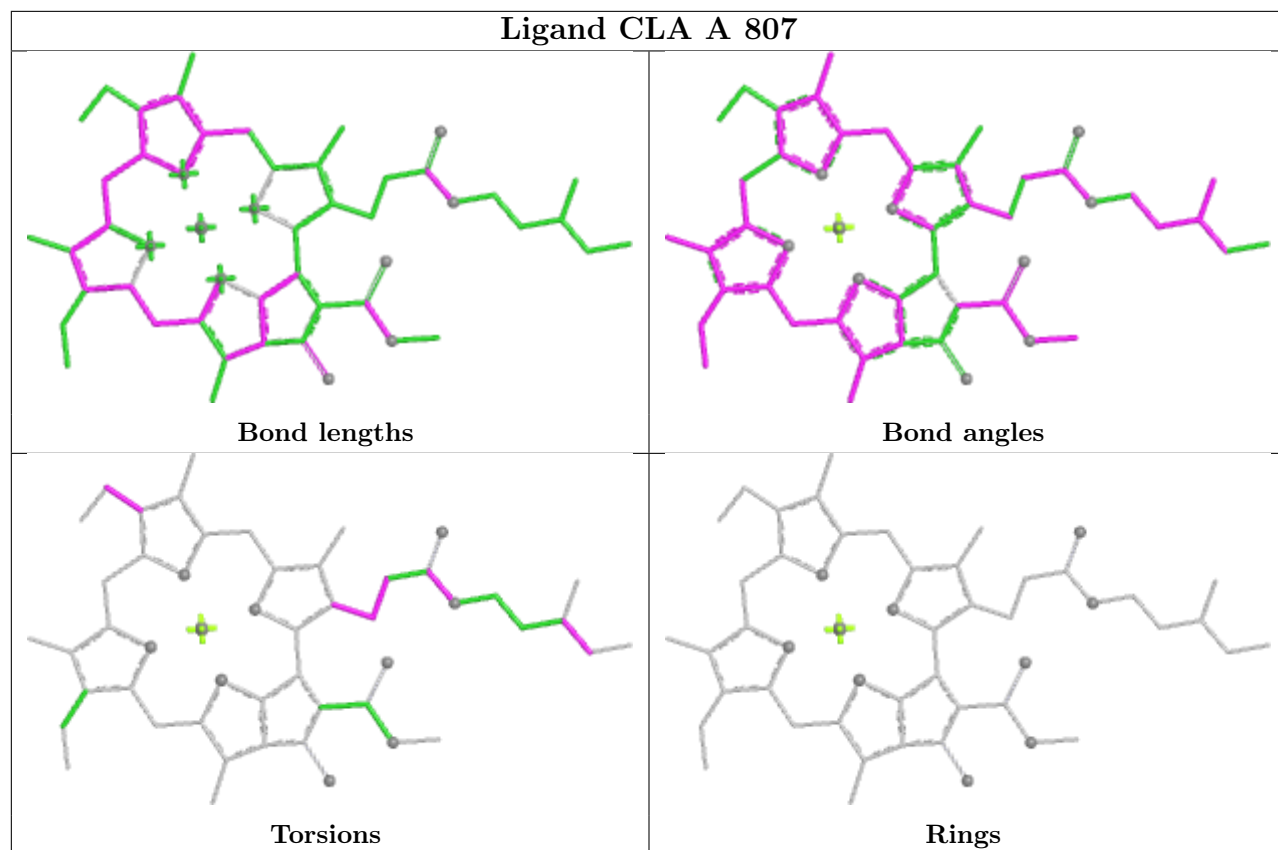
Ligand CLA A 814



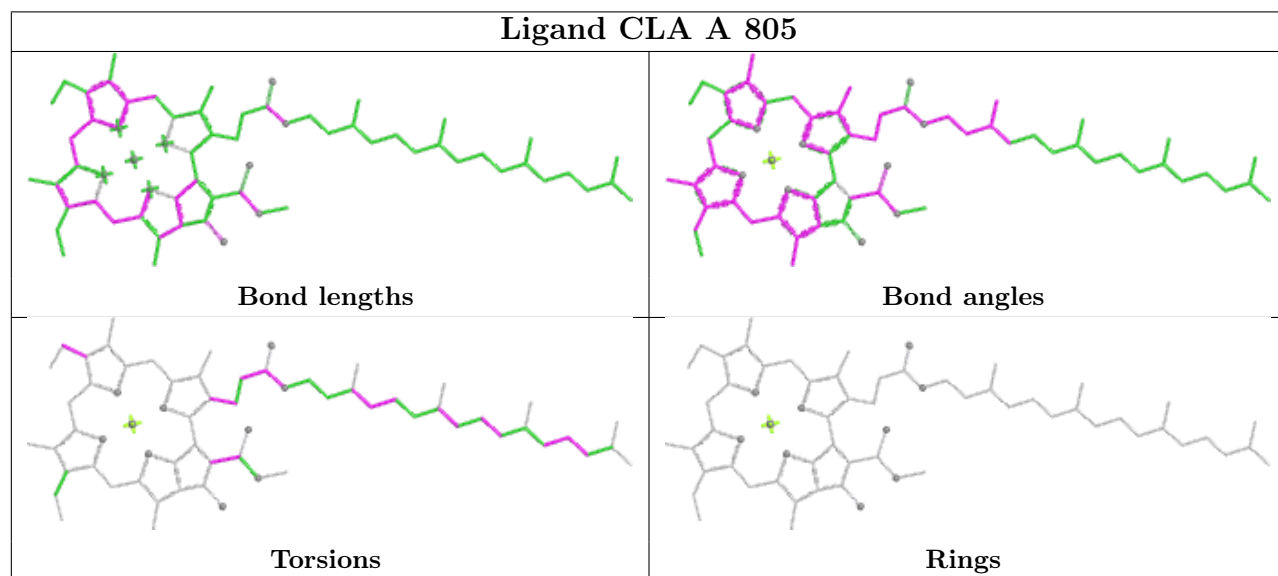
Ligand BCR M 101

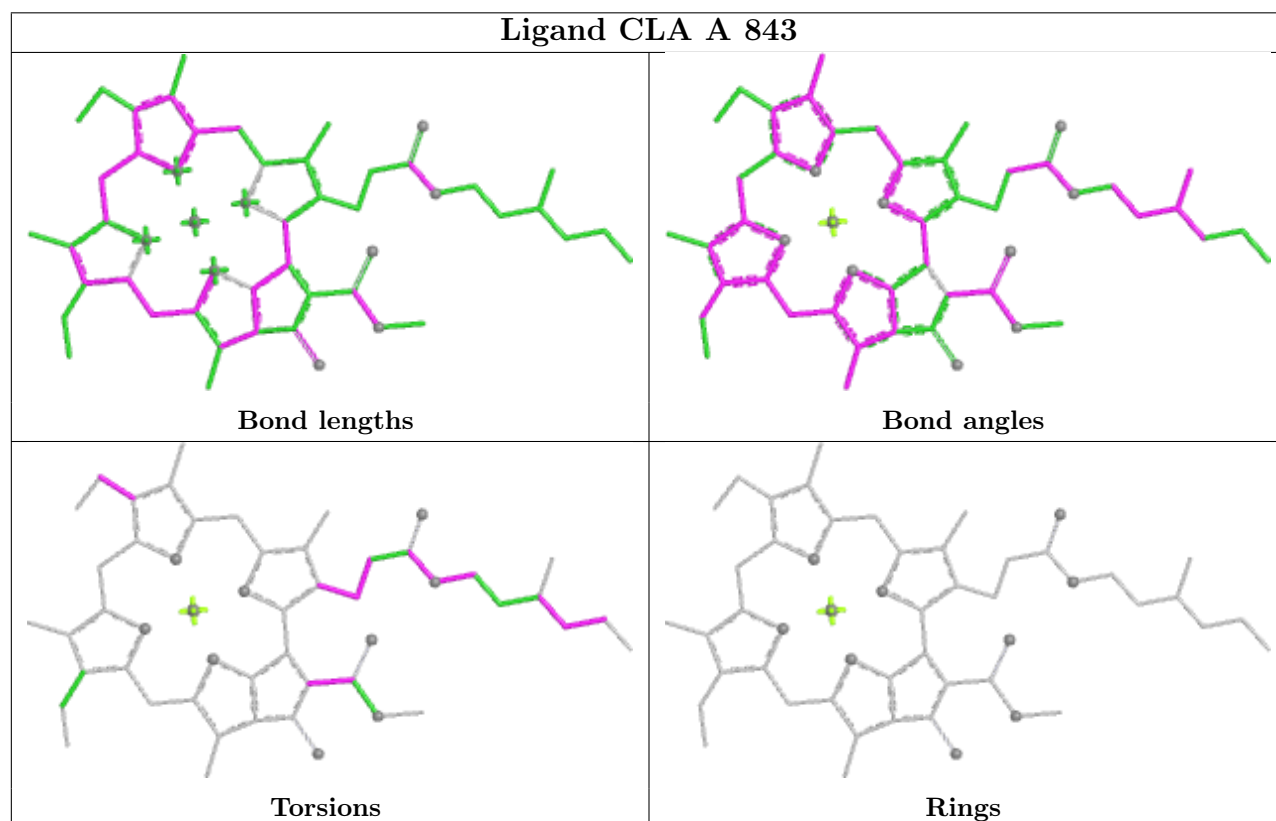
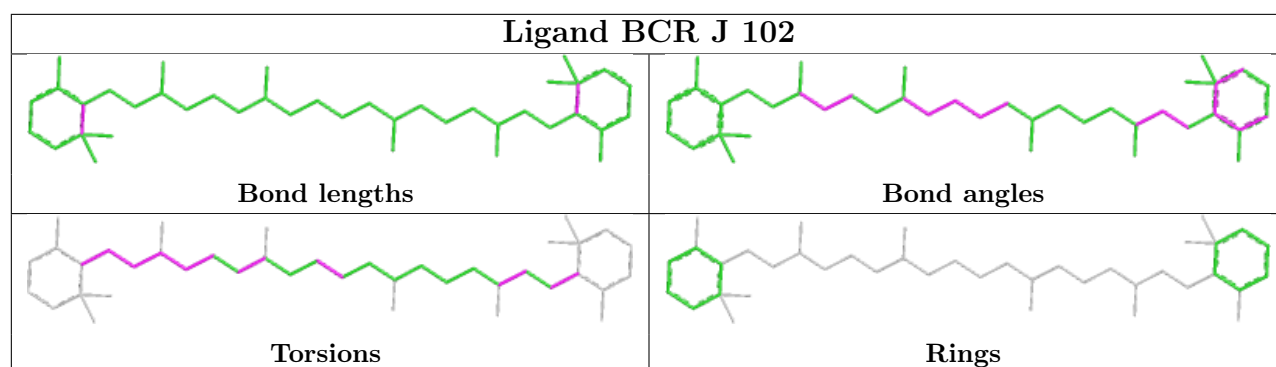


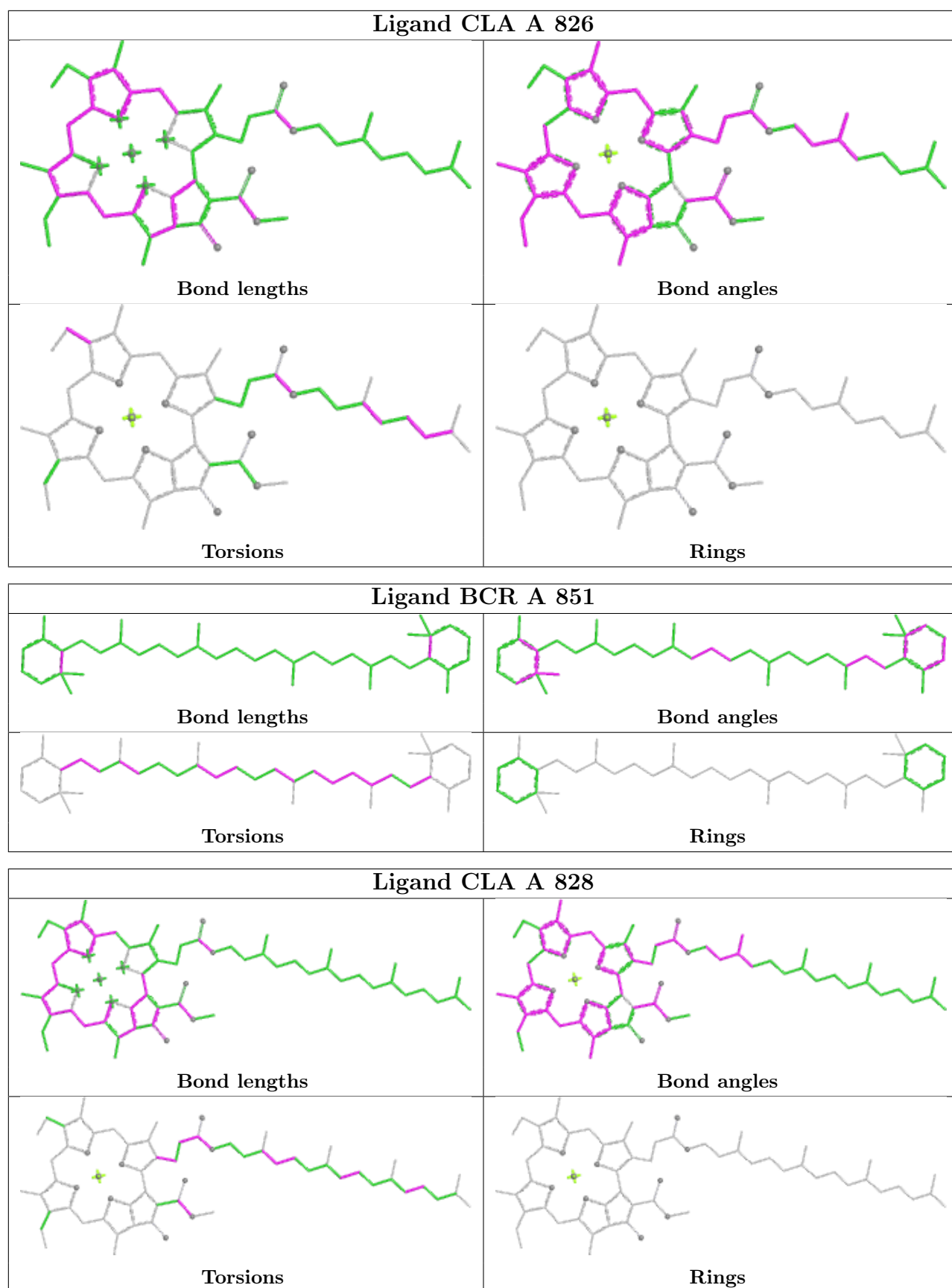
Ligand CLA A 807



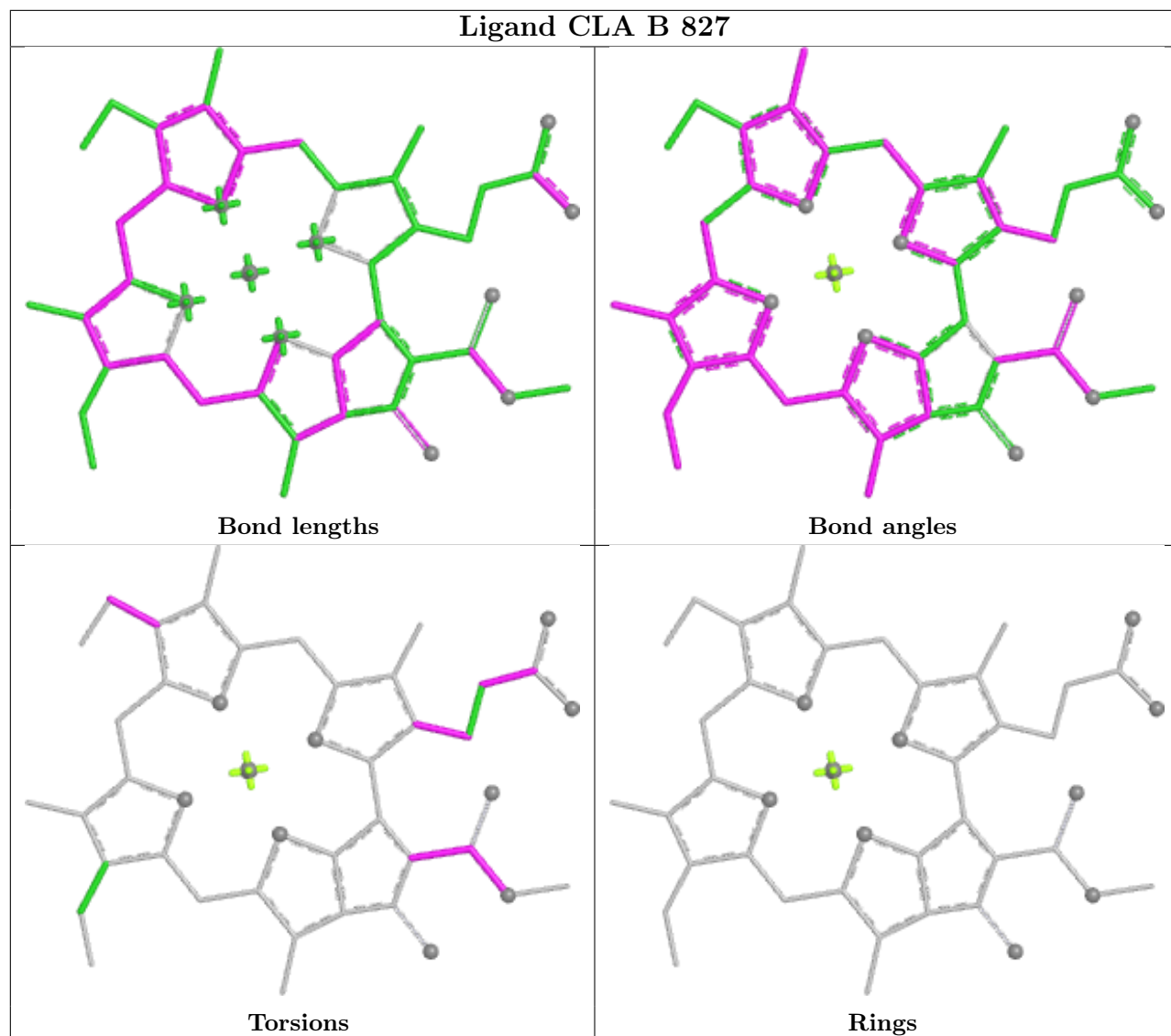
Ligand CLA A 805



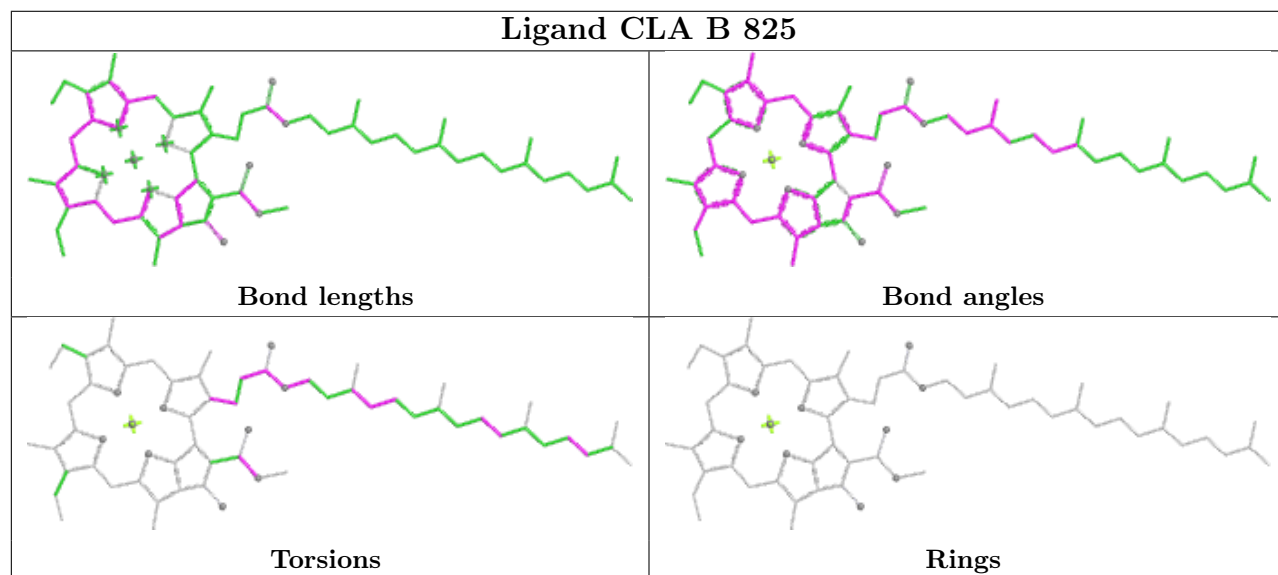




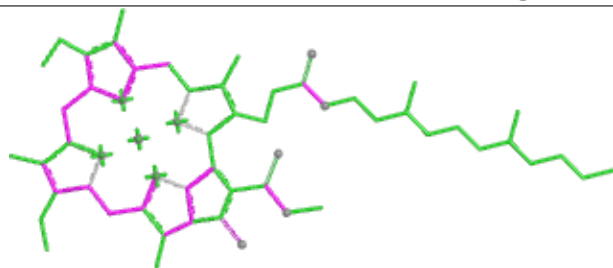
Ligand CLA B 827



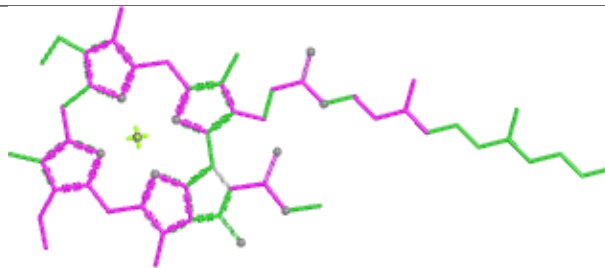
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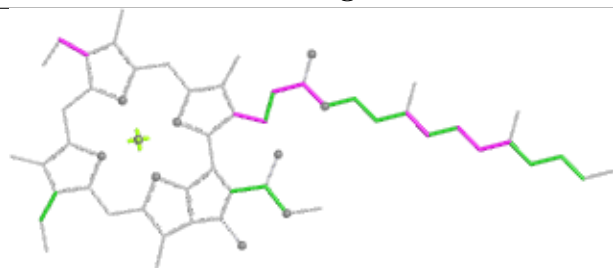
Ligand CLA B 826



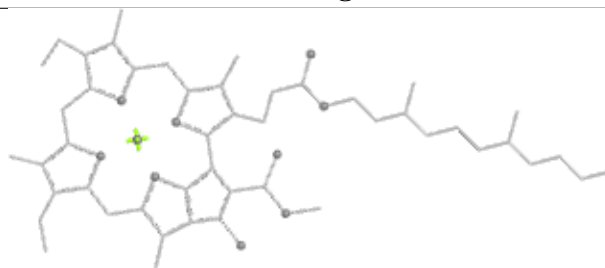
Bond lengths



Bond angles

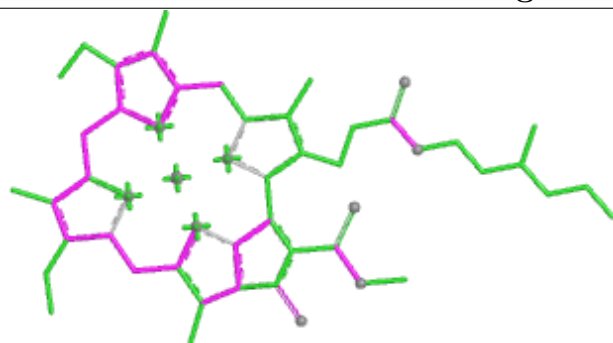


Torsions

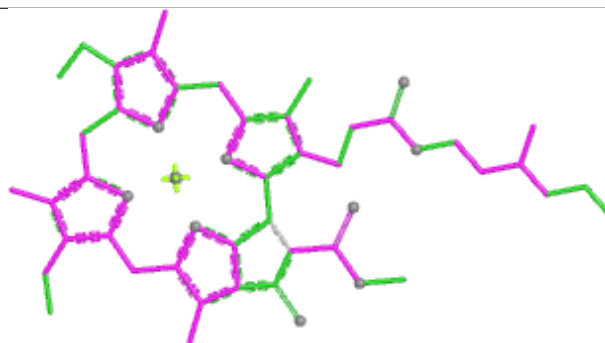


Rings

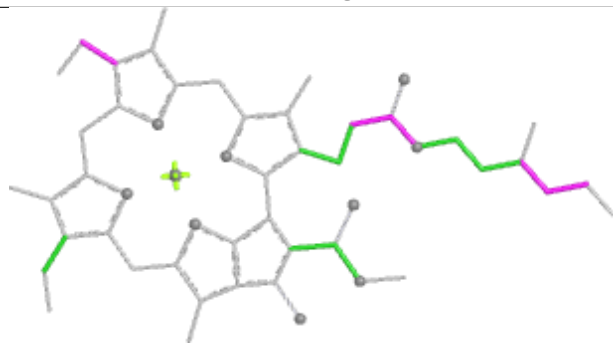
Ligand CLA L 204



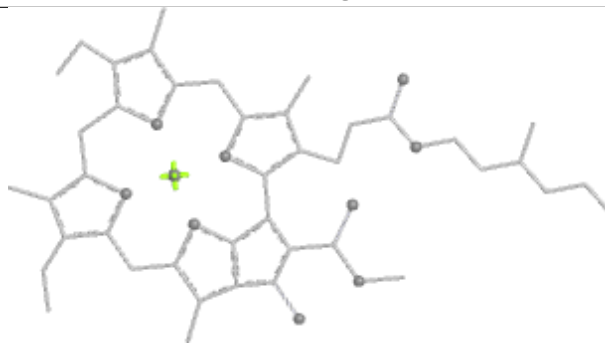
Bond lengths



Bond angles

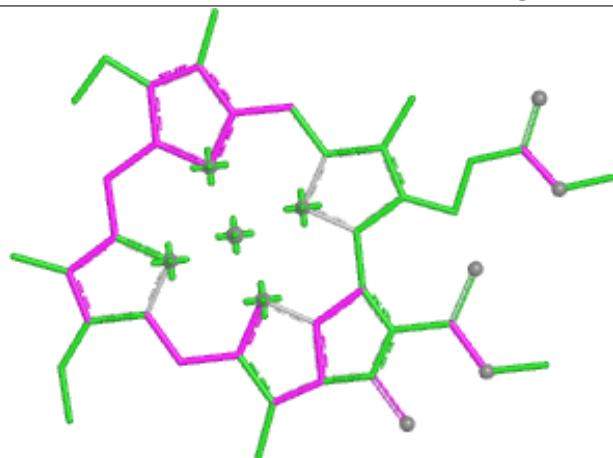


Torsions

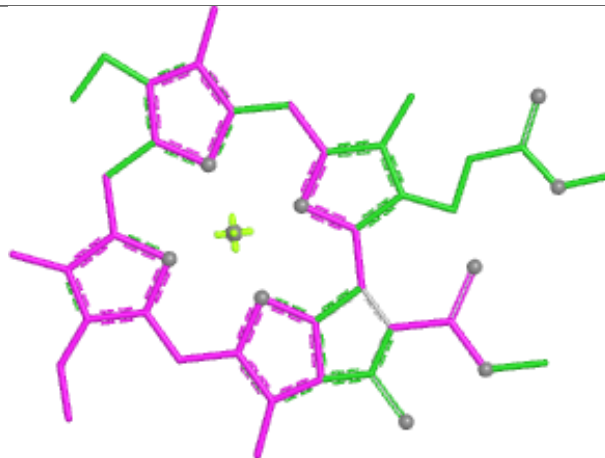


Rings

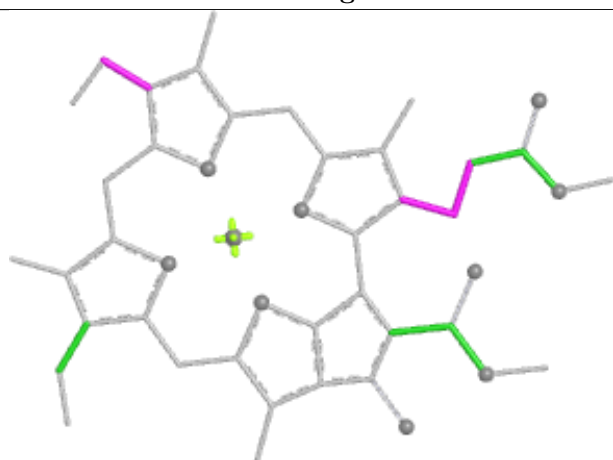
Ligand CLA A 822



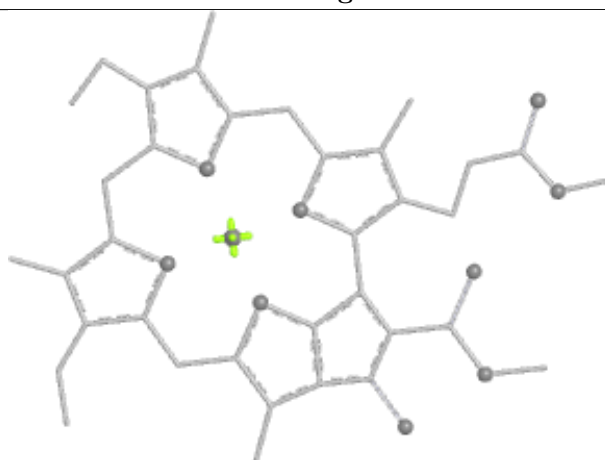
Bond lengths



Bond angles

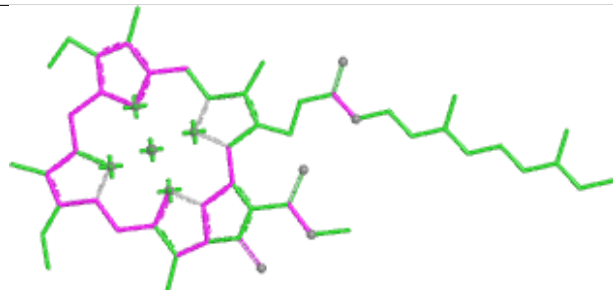


Torsions

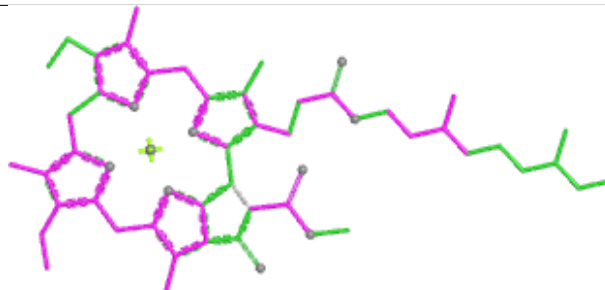


Rings

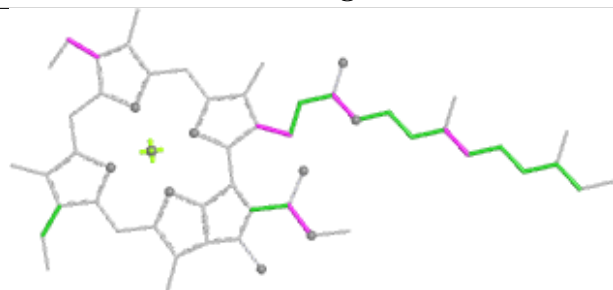
Ligand CLA B 814



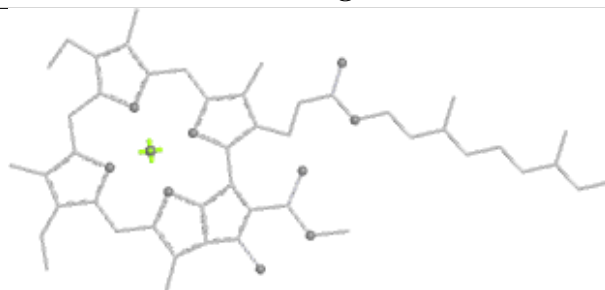
Bond lengths



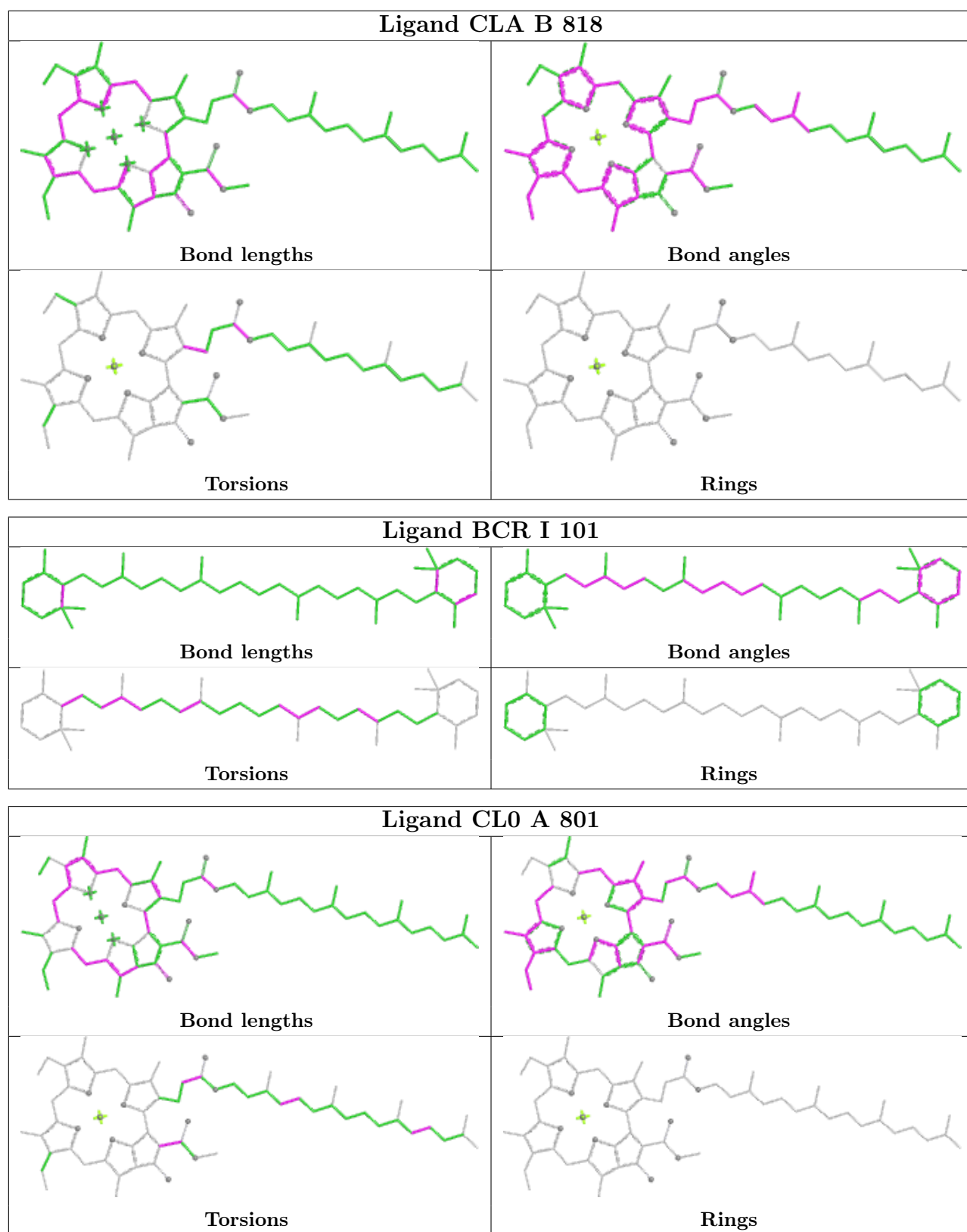
Bond angles



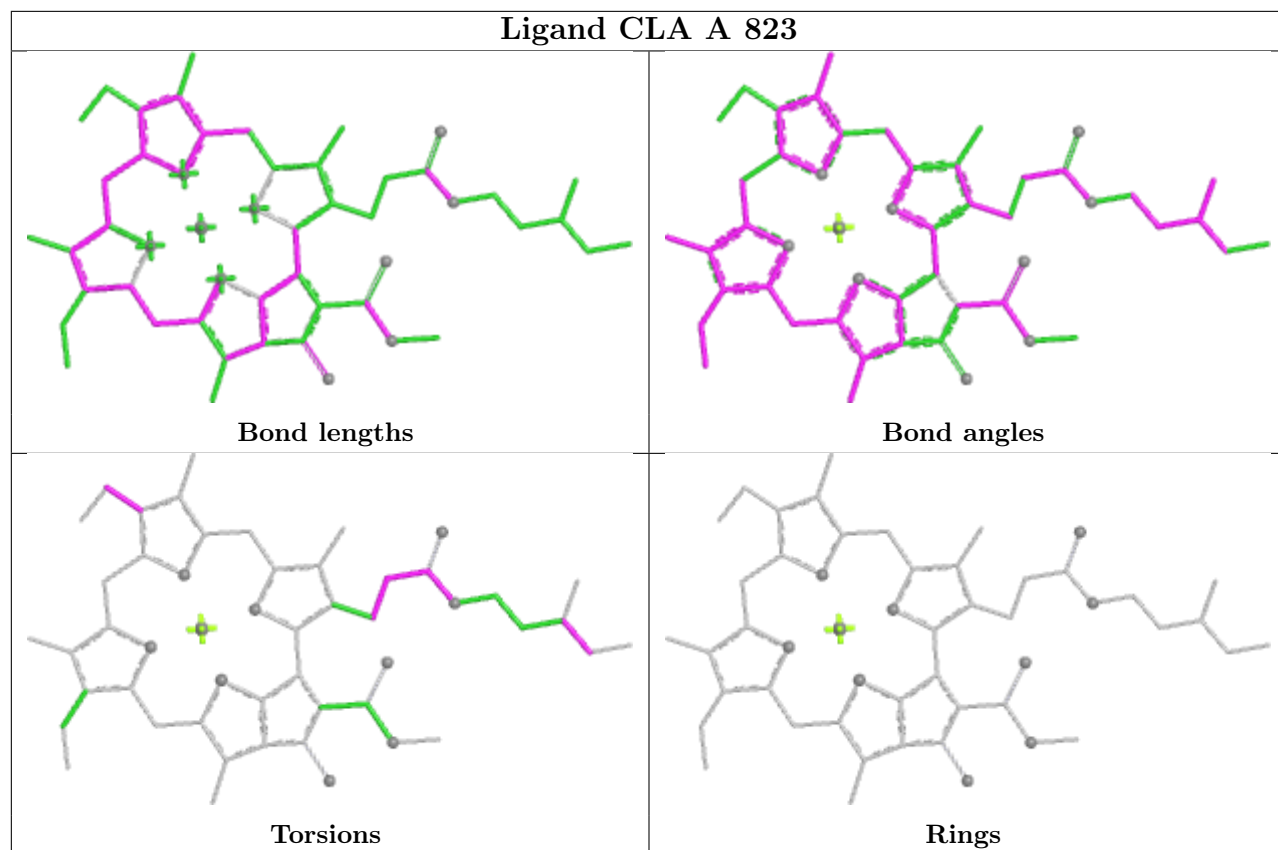
Torsions



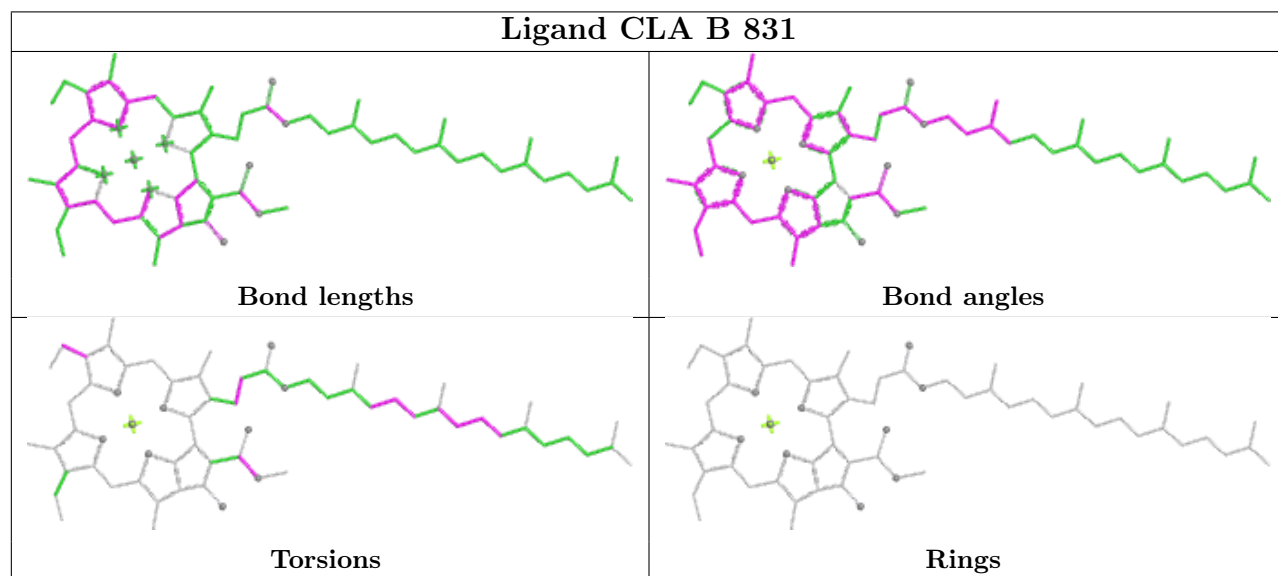
Rings

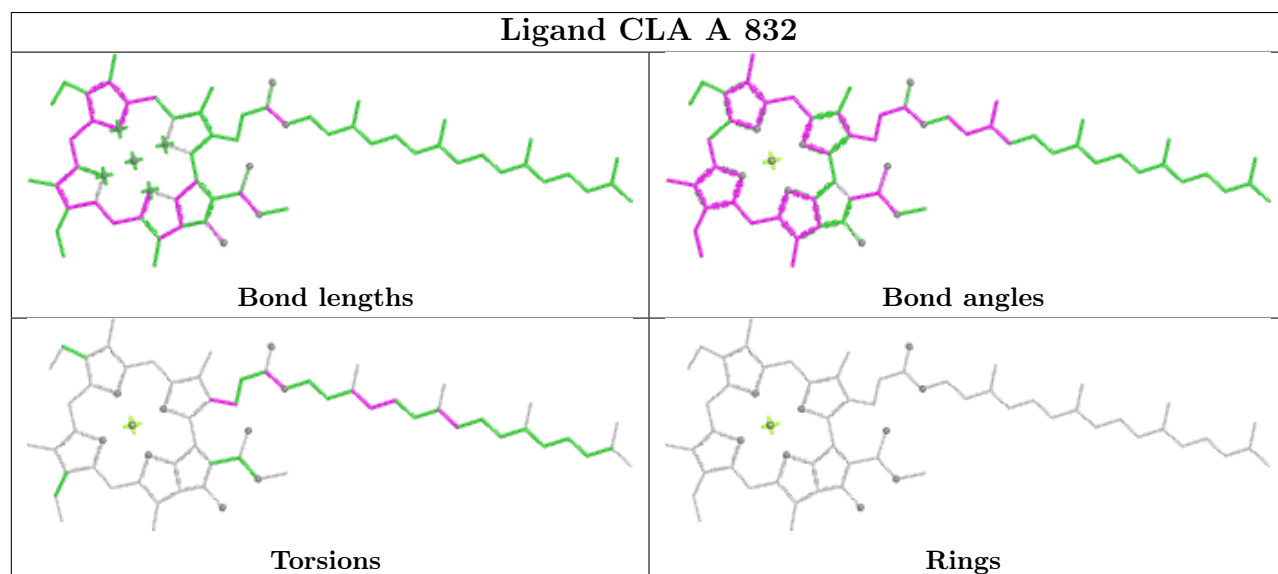
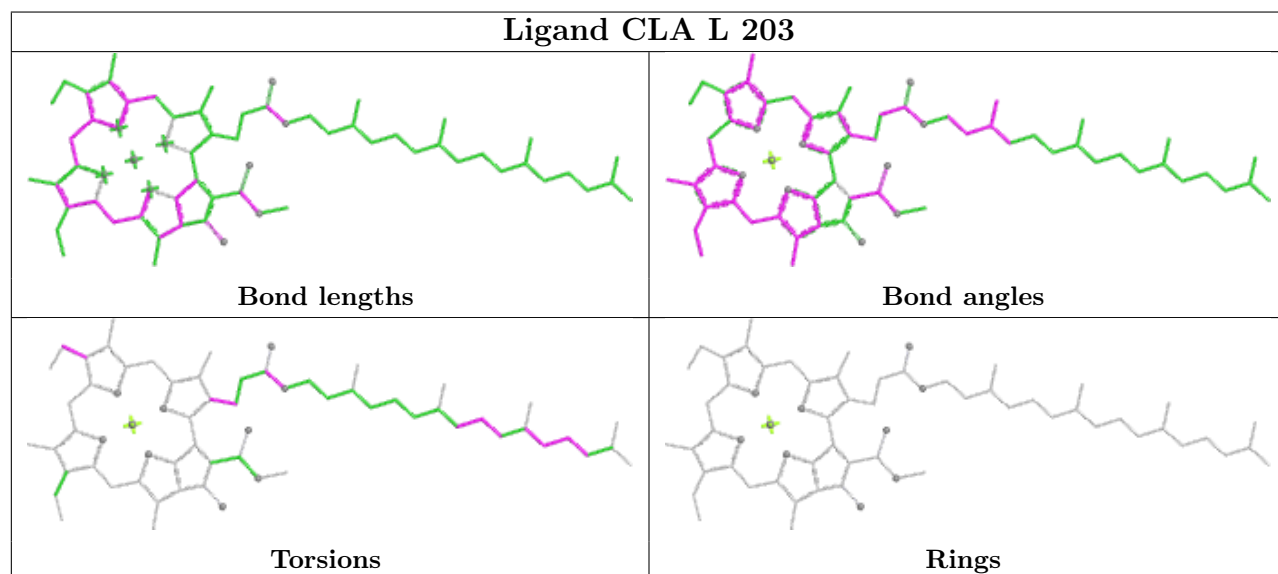
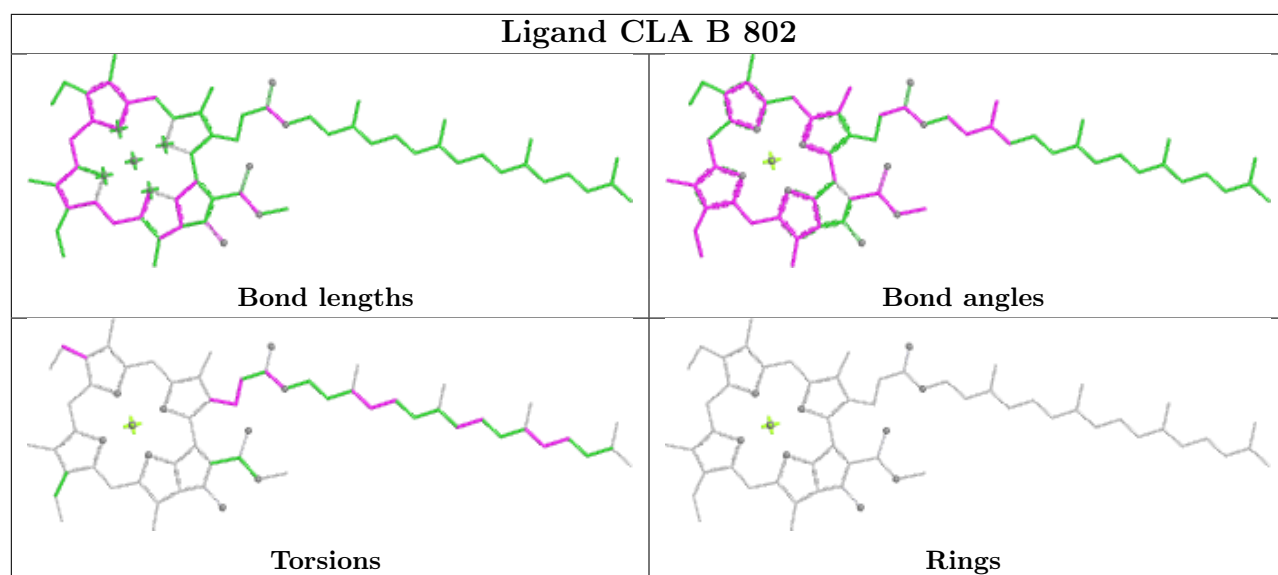


Ligand CLA A 823

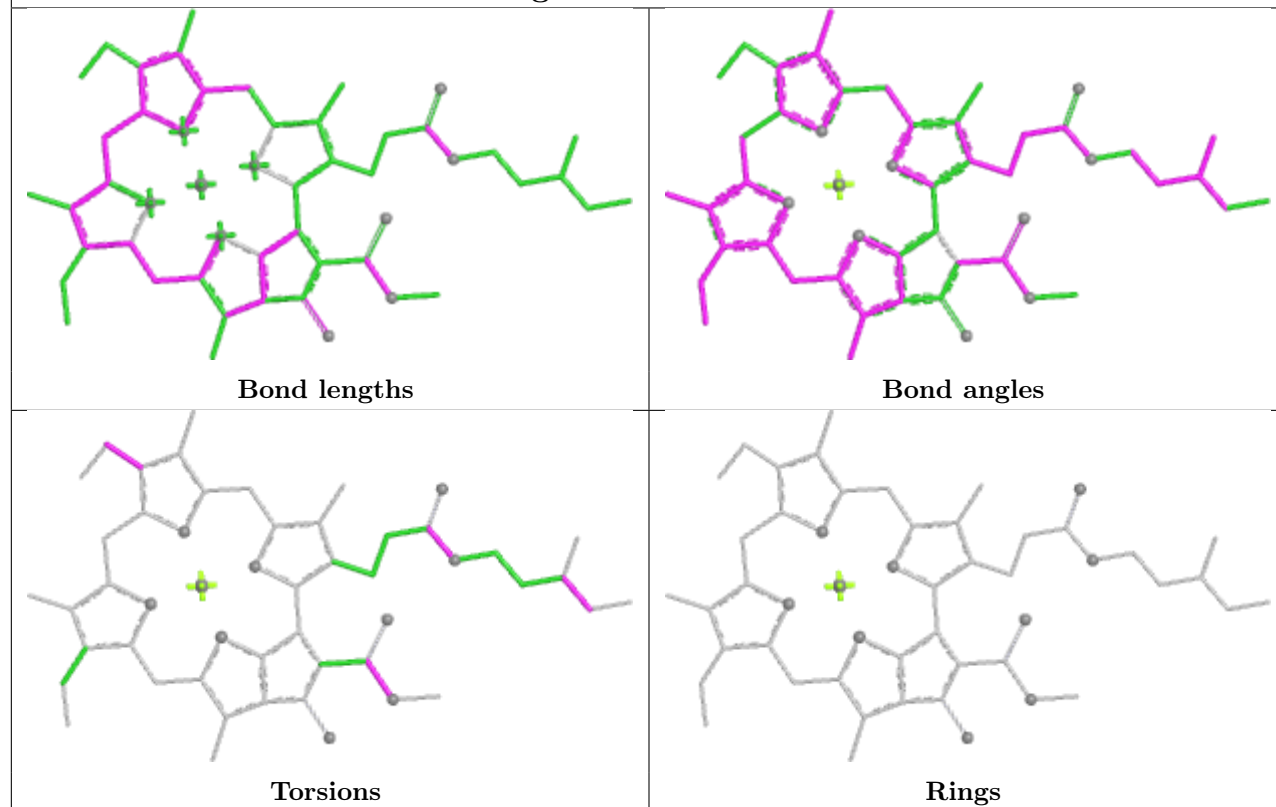


Ligand CLA B 831

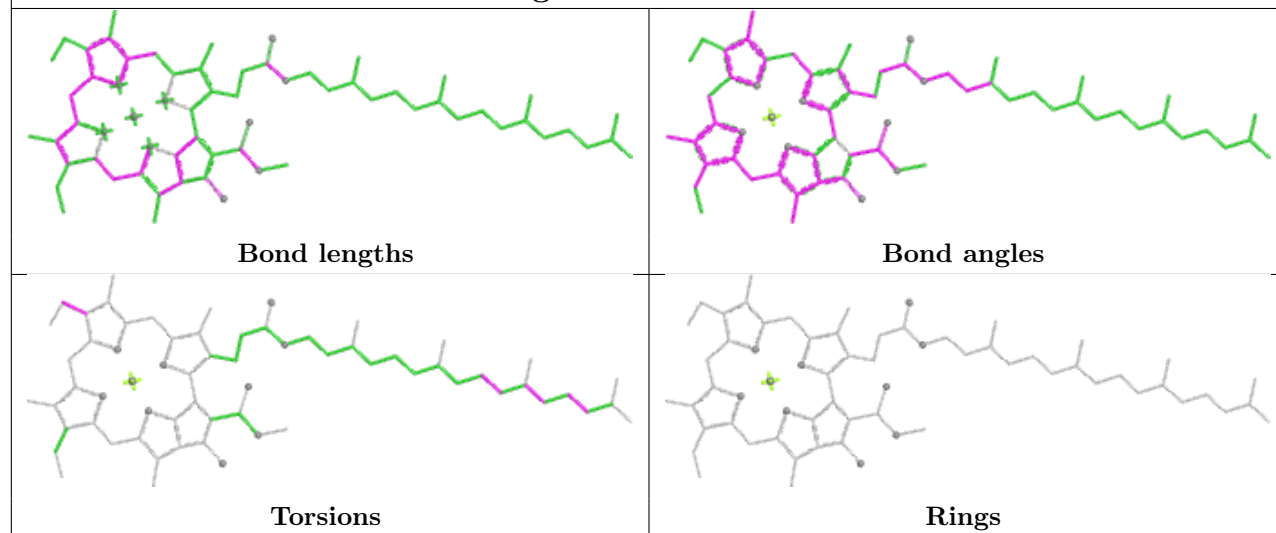


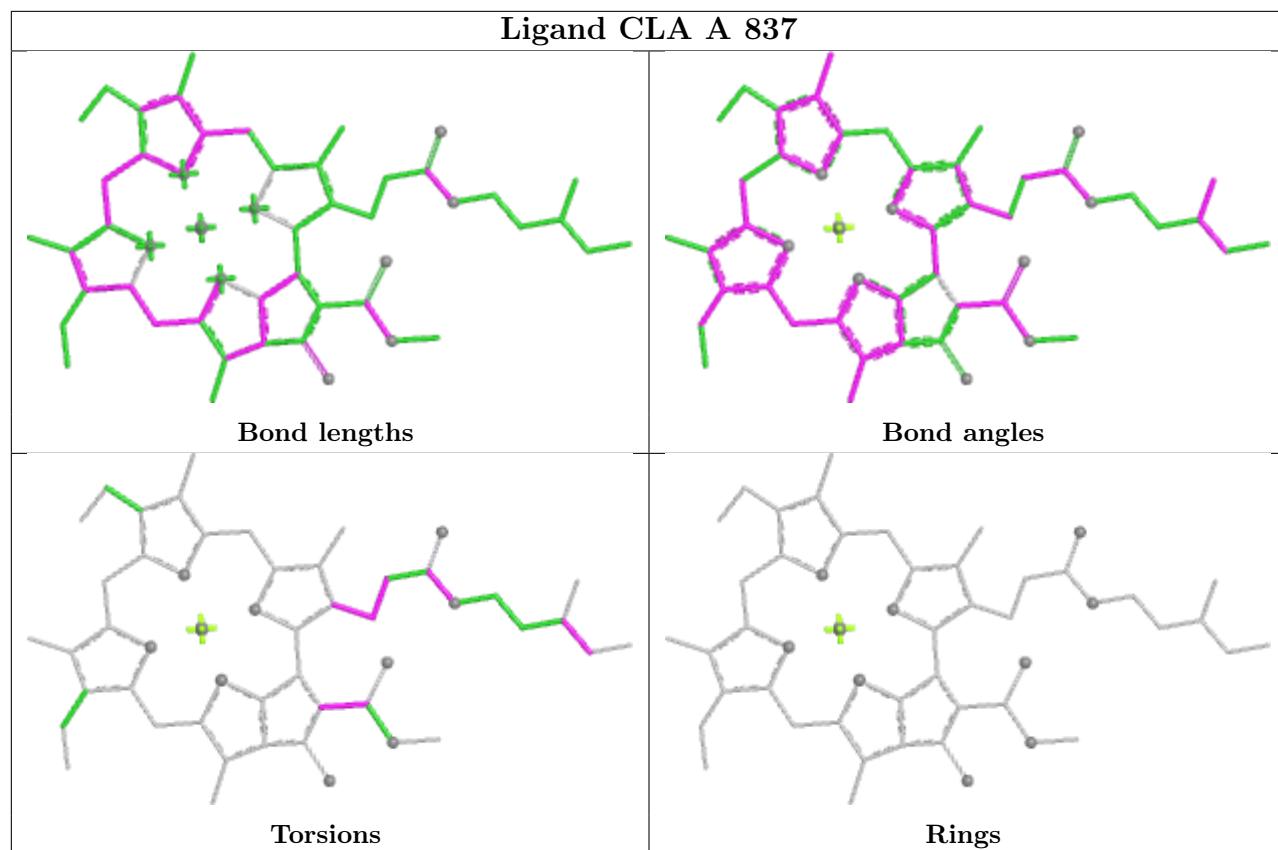


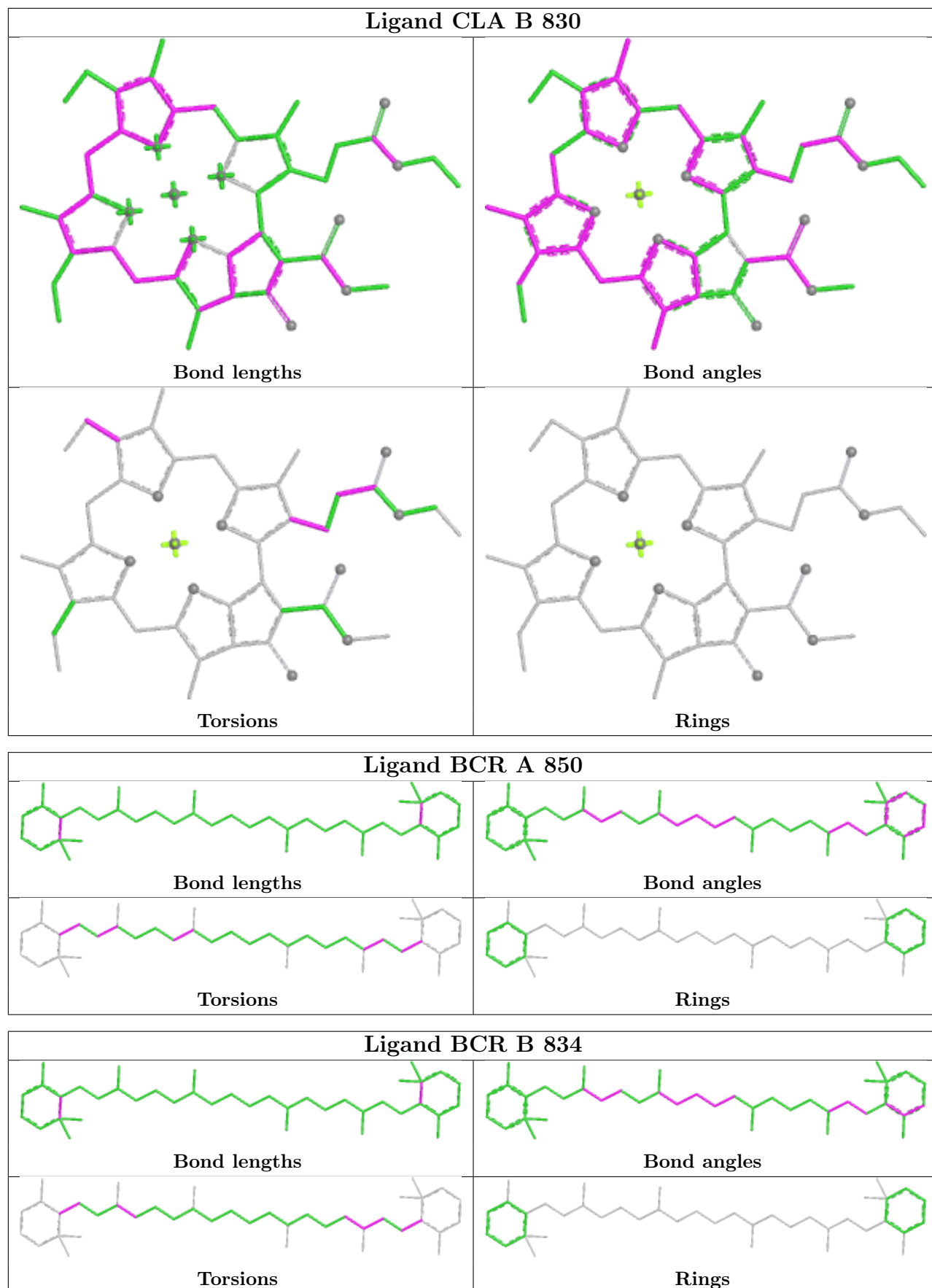
Ligand CLA A 841

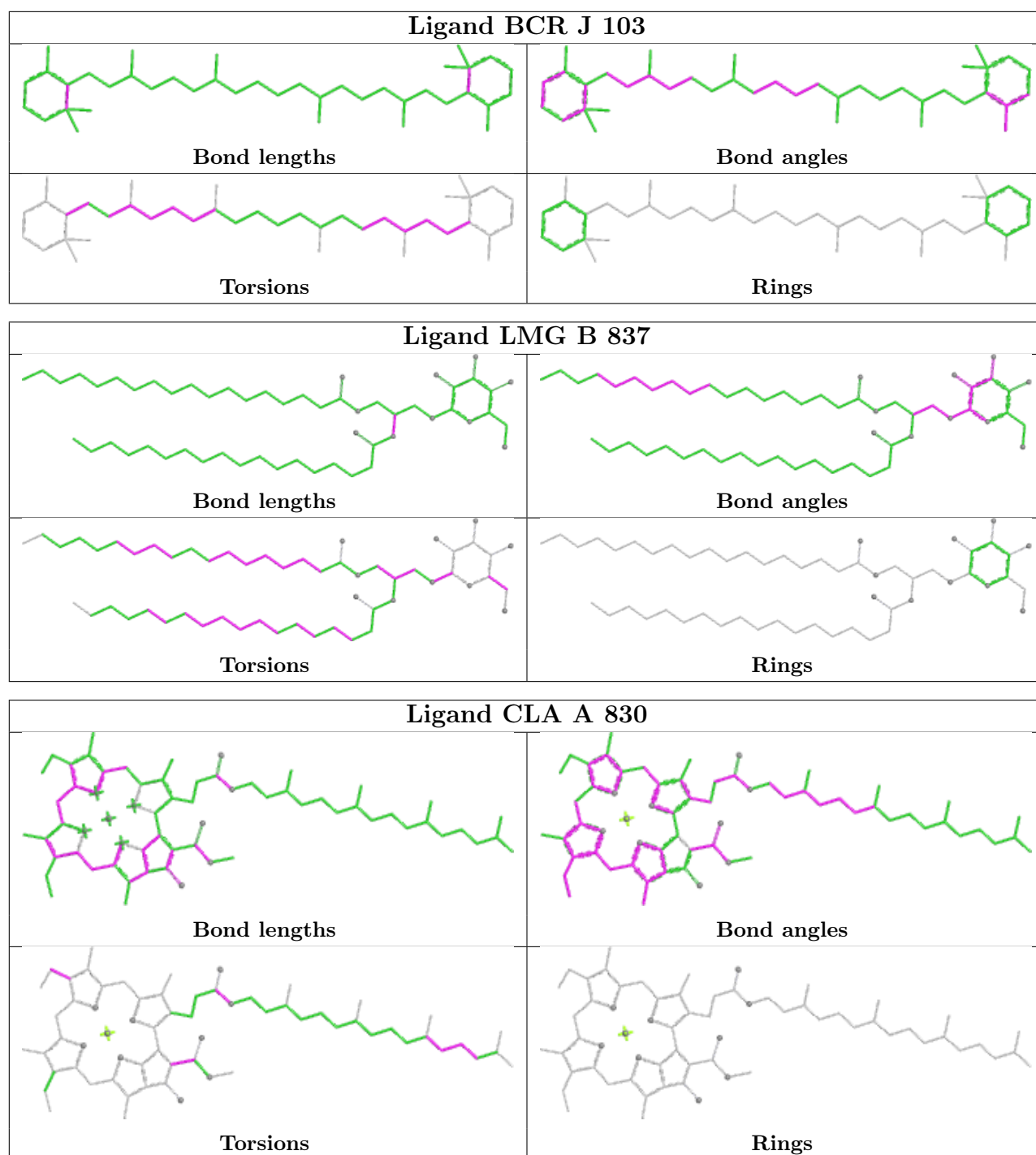


Ligand CLA B 820

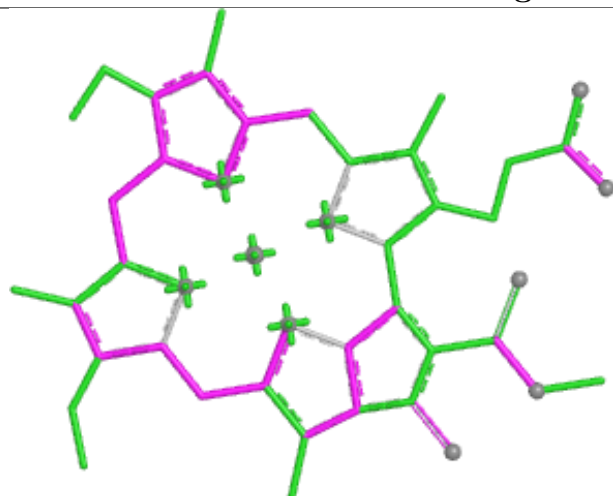




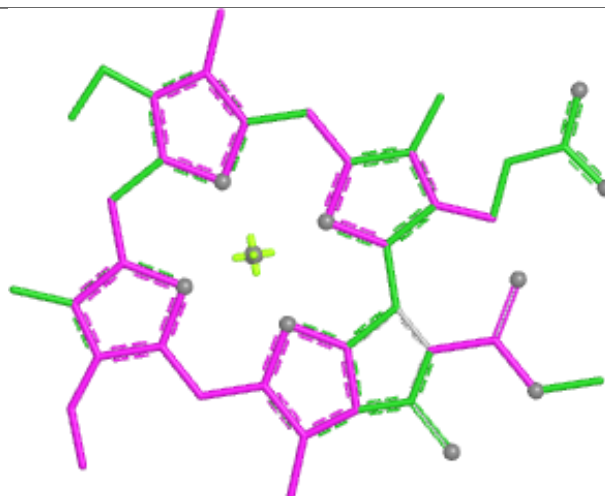




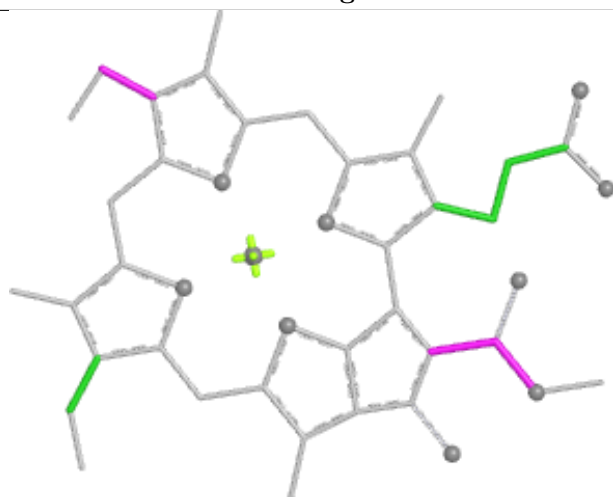
Ligand CLA B 815



Bond lengths



Bond angles

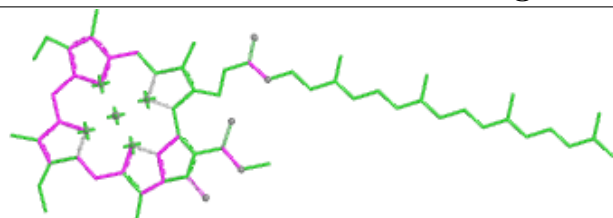


Torsions

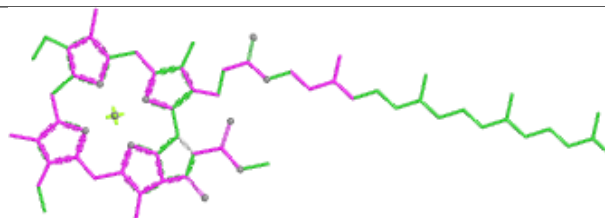


Rings

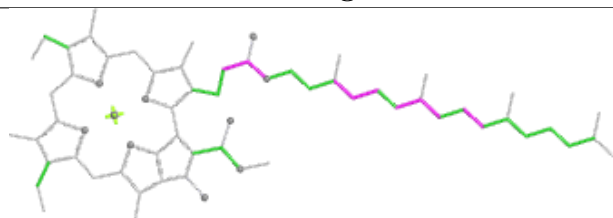
Ligand CLA A 827



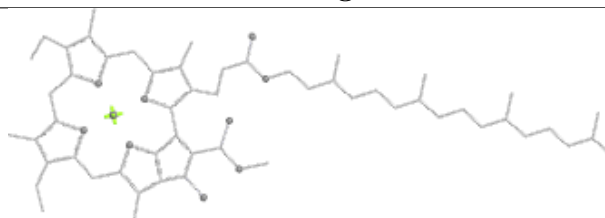
Bond lengths



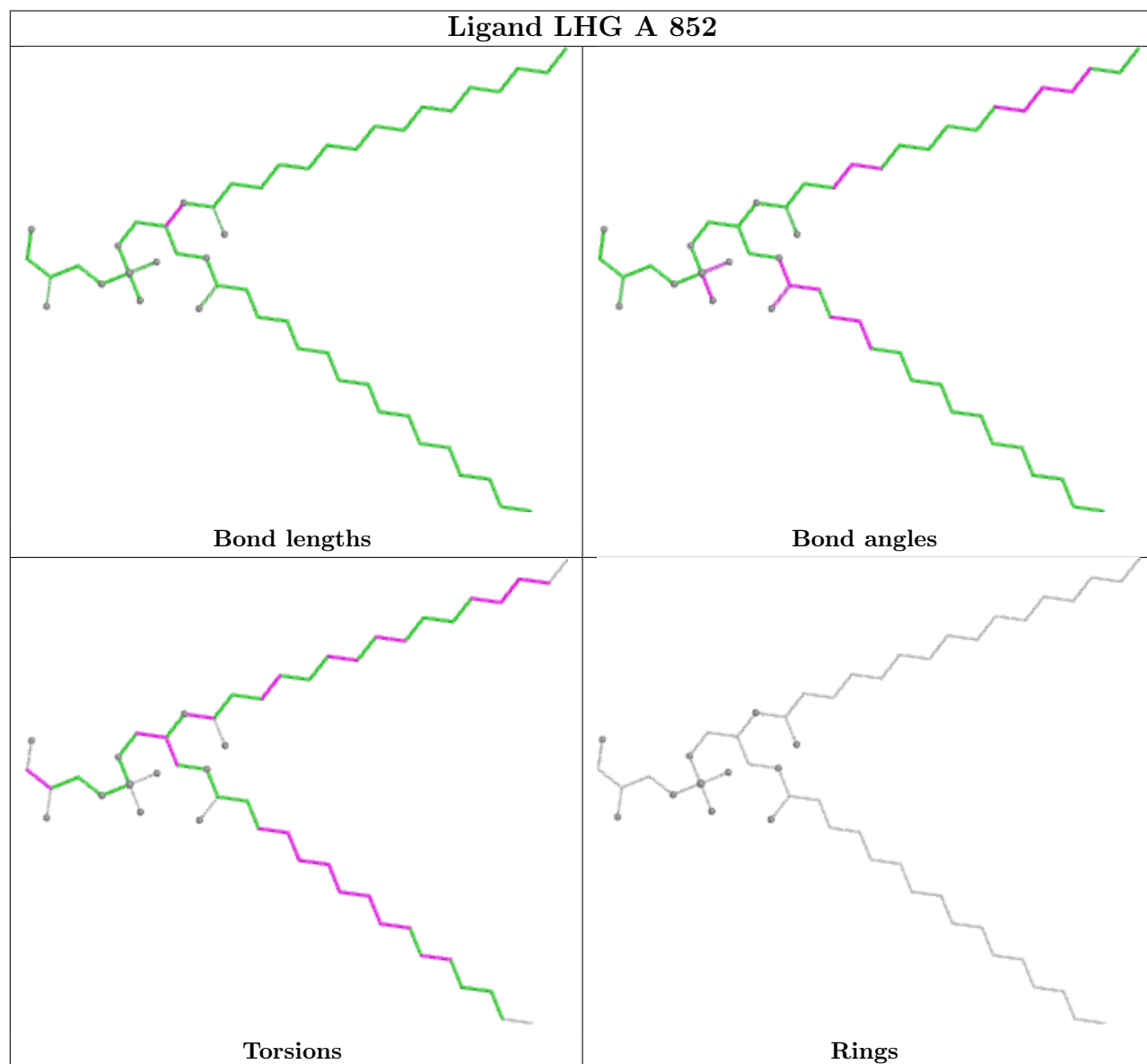
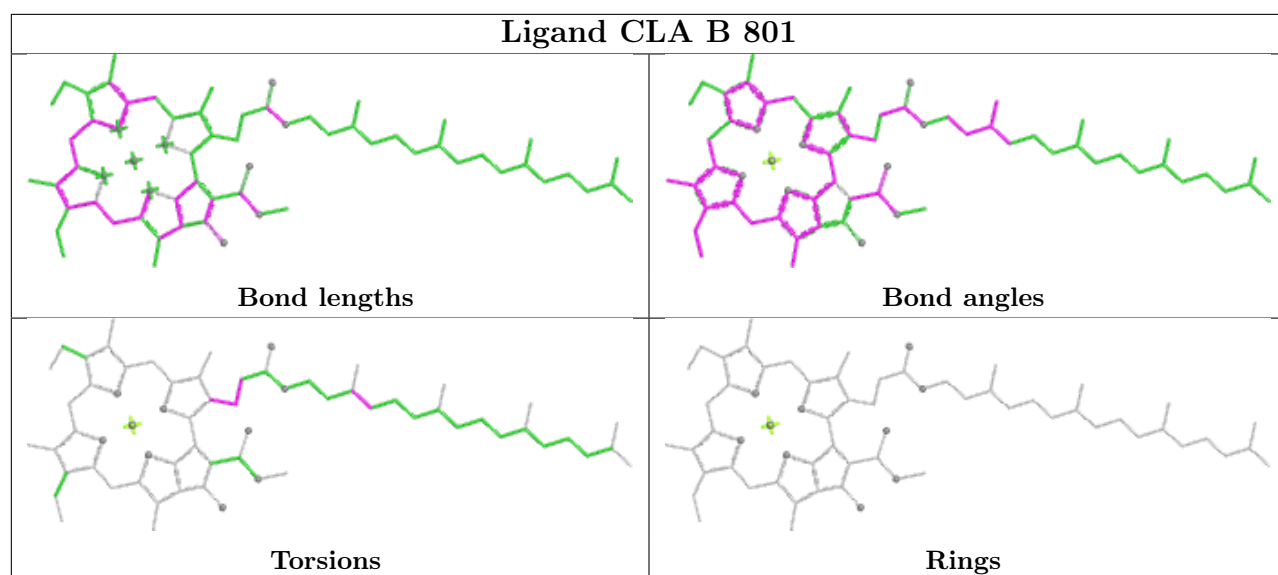
Bond angles

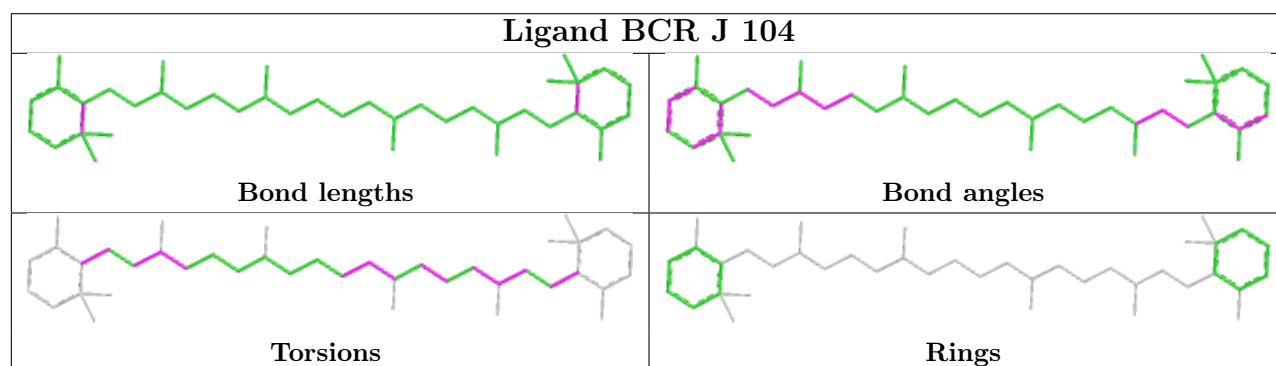
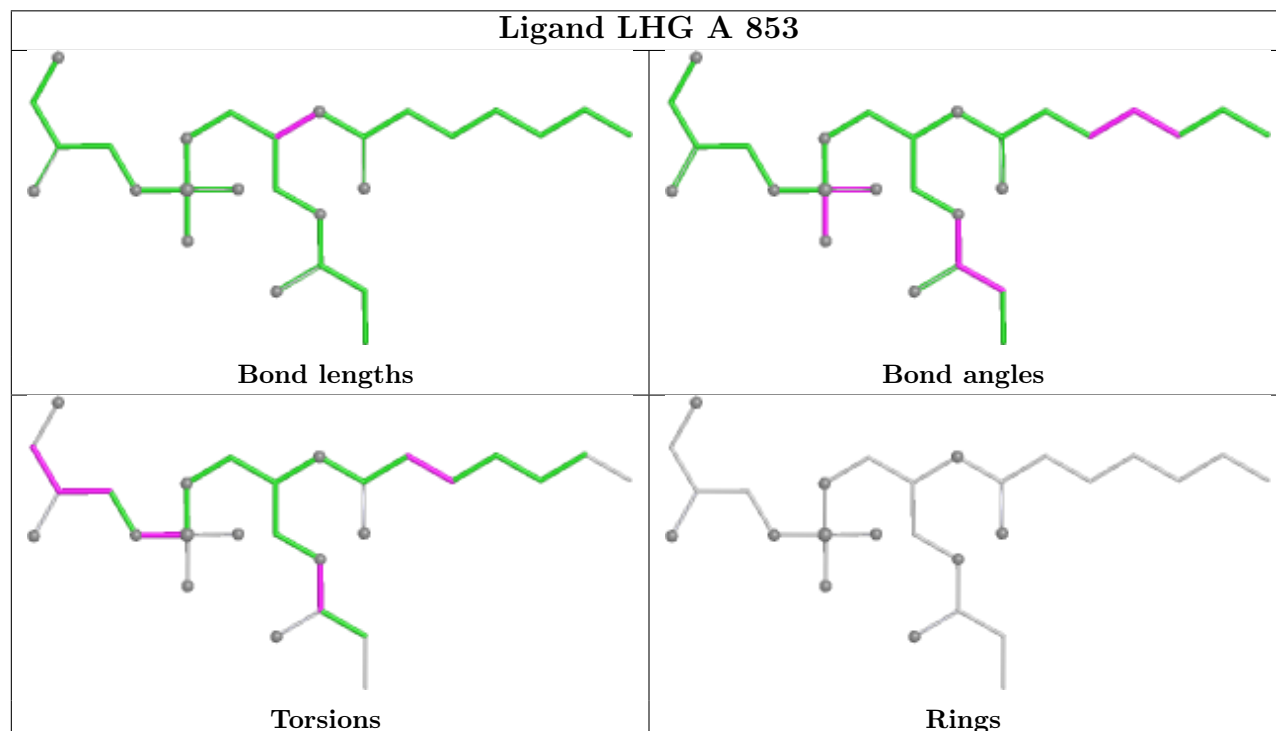
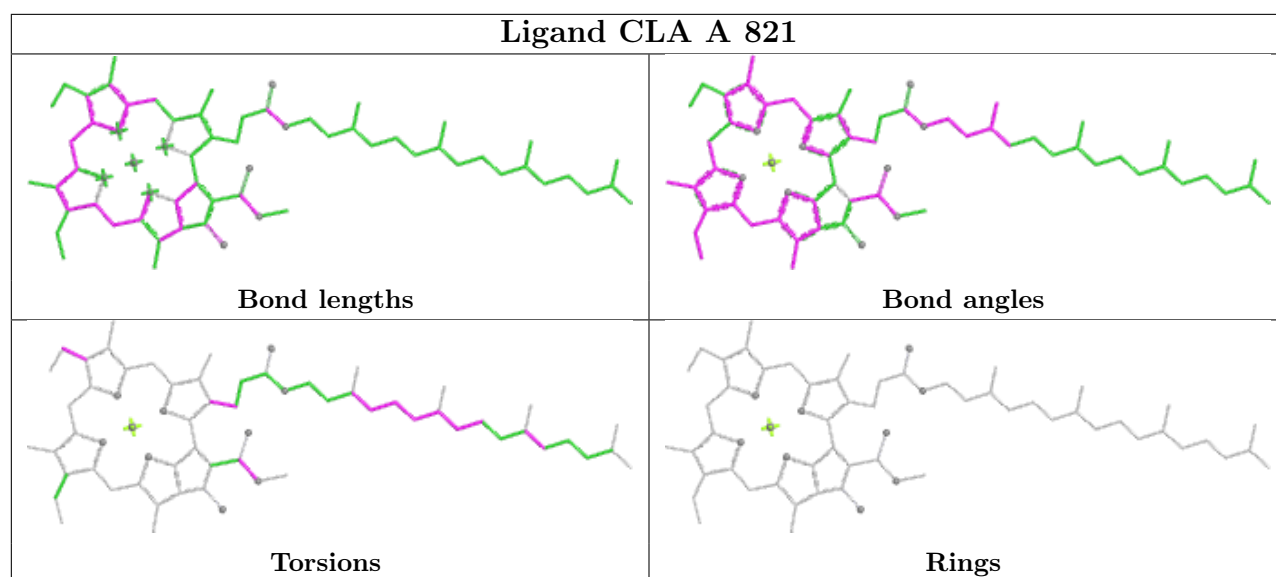


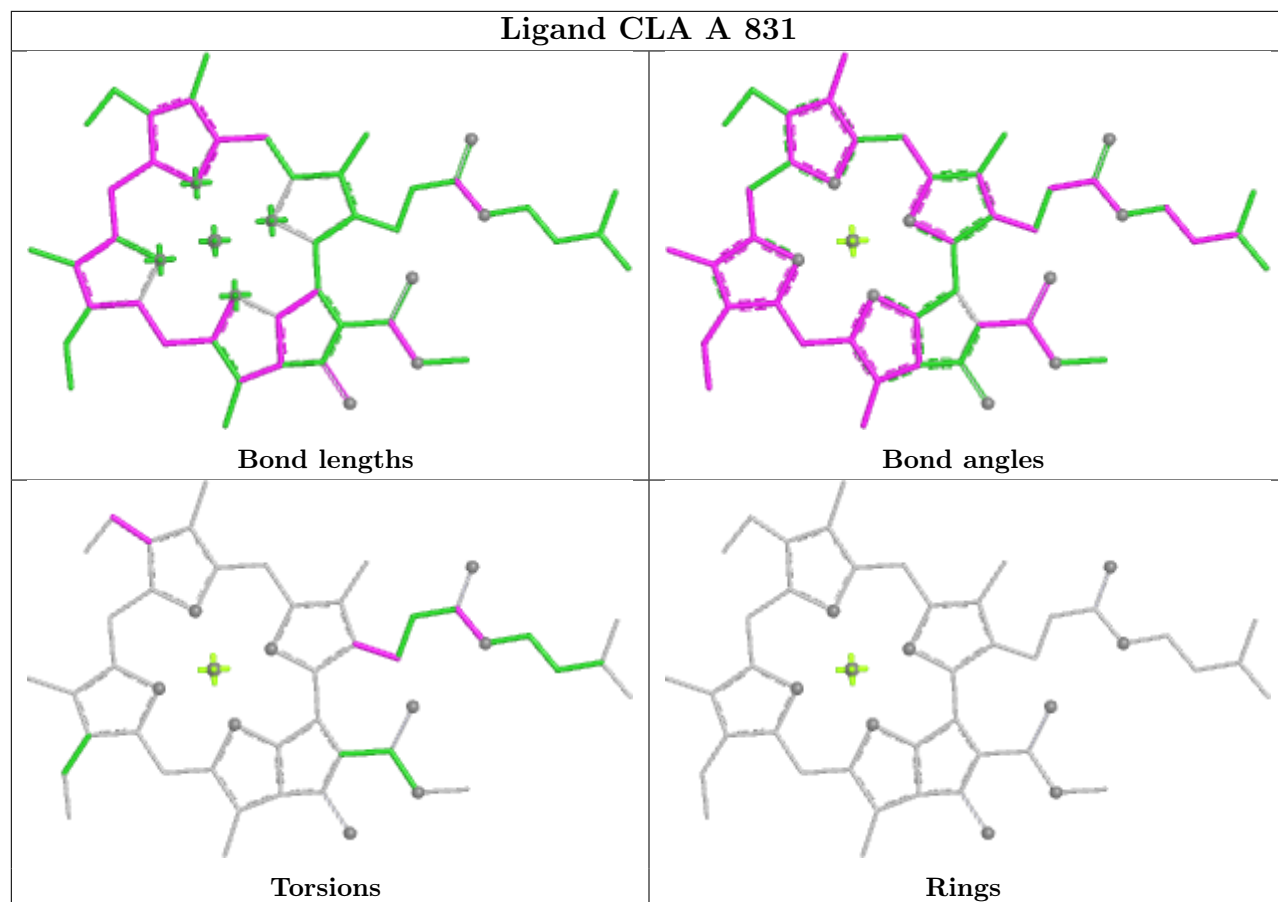
Torsions



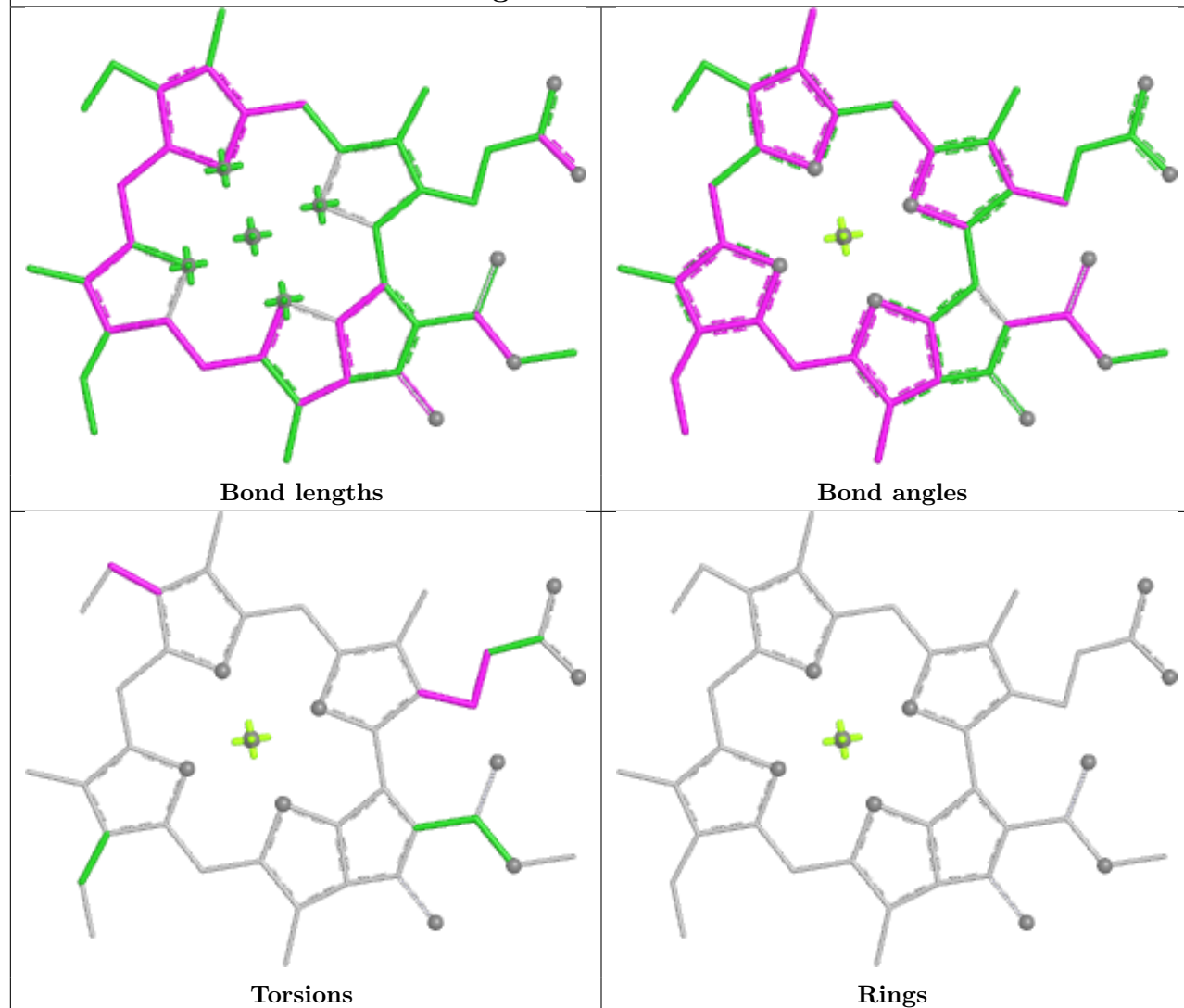
Rings



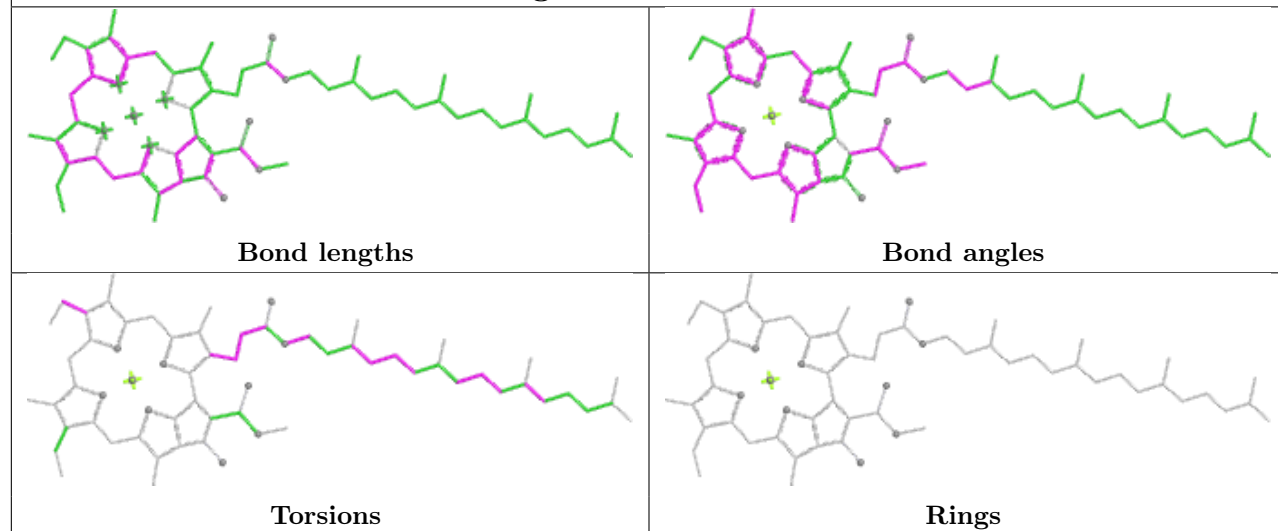


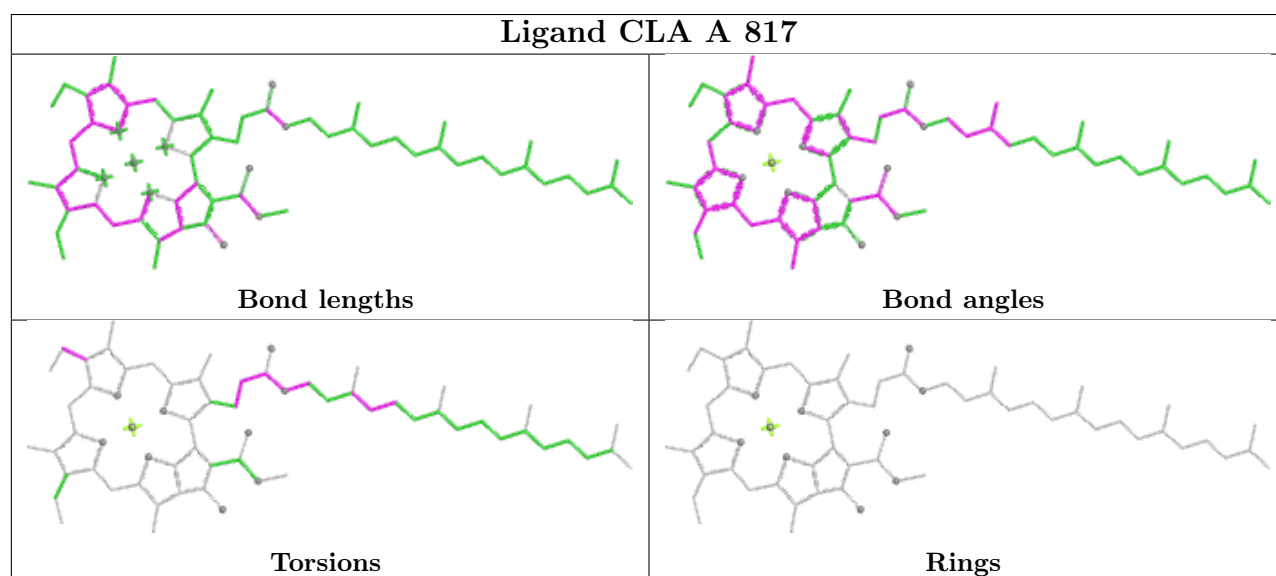
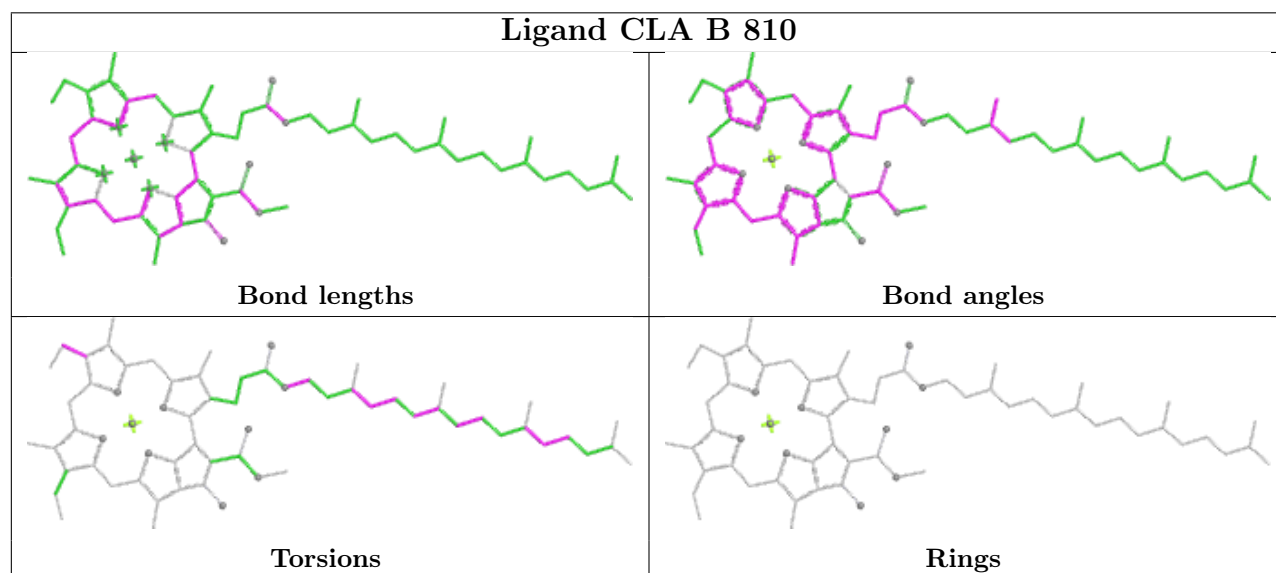
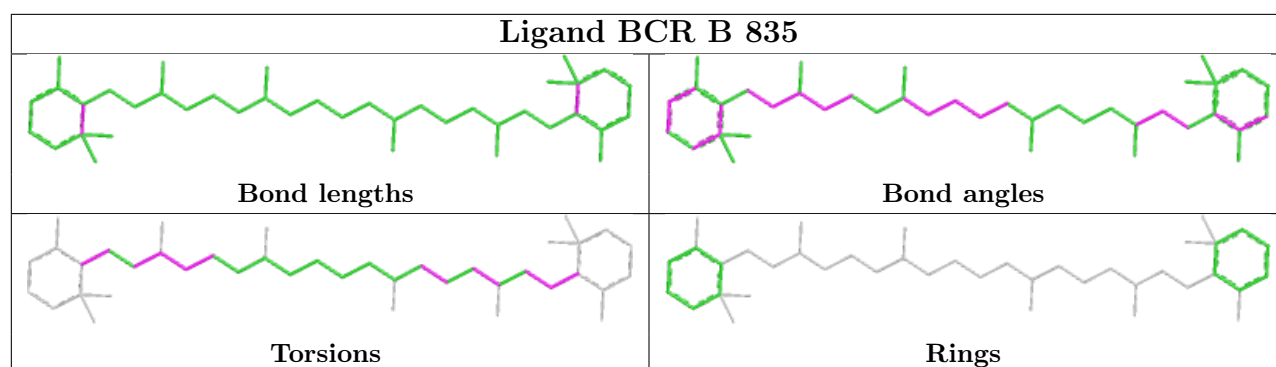


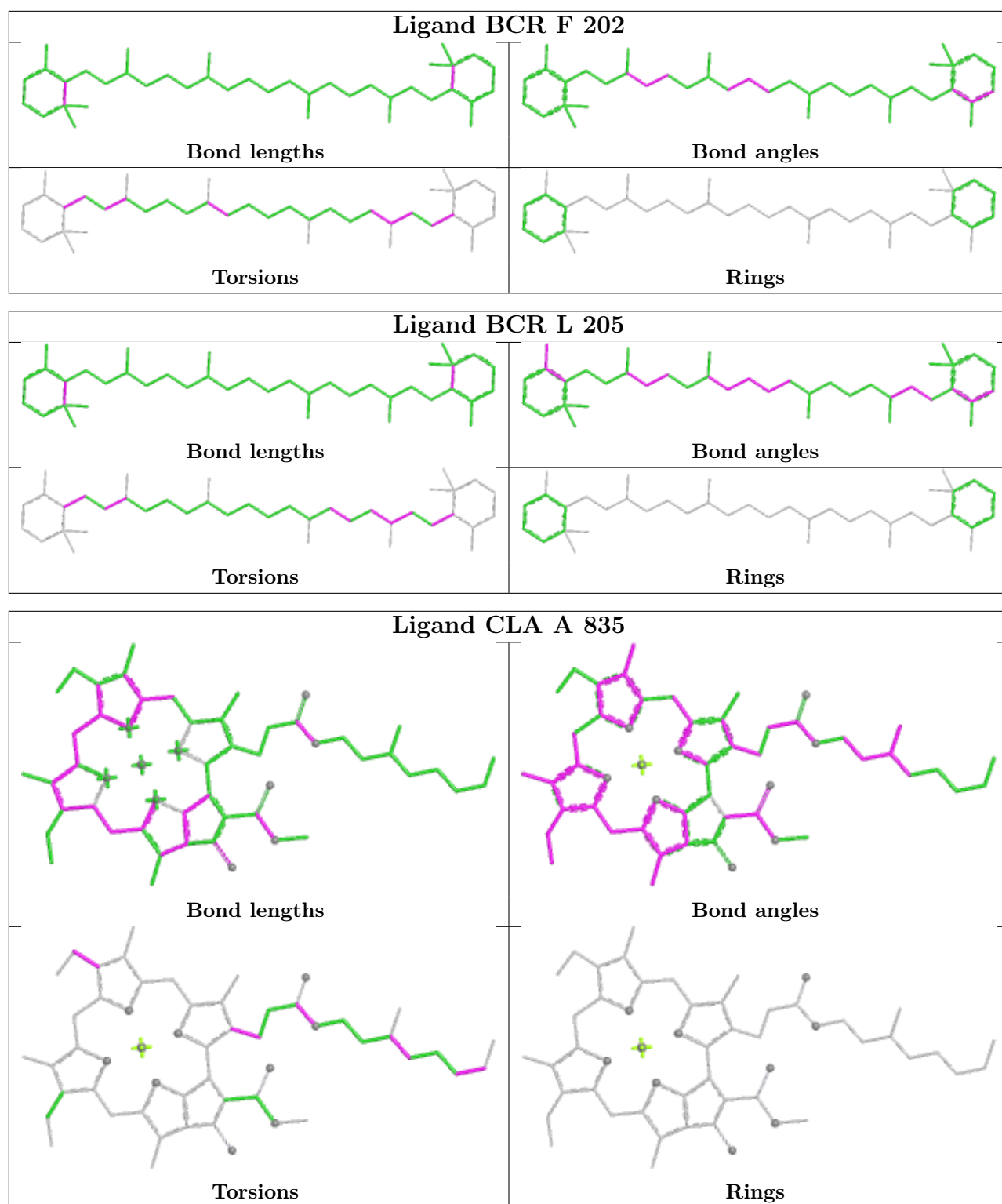
Ligand CLA A 815



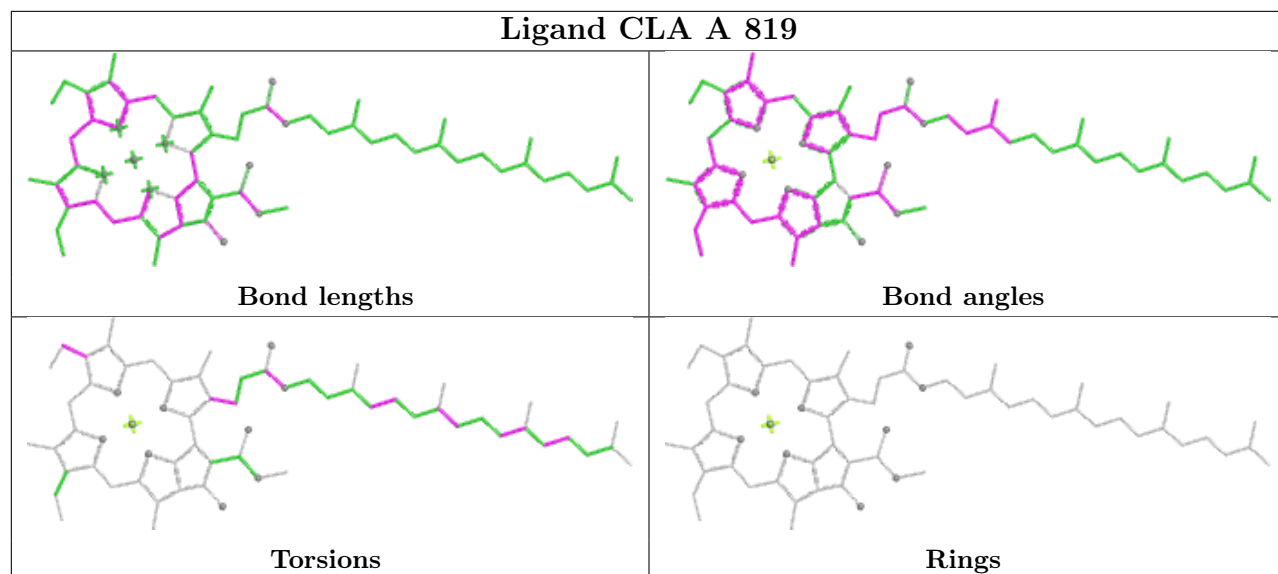
Ligand CLA B 829



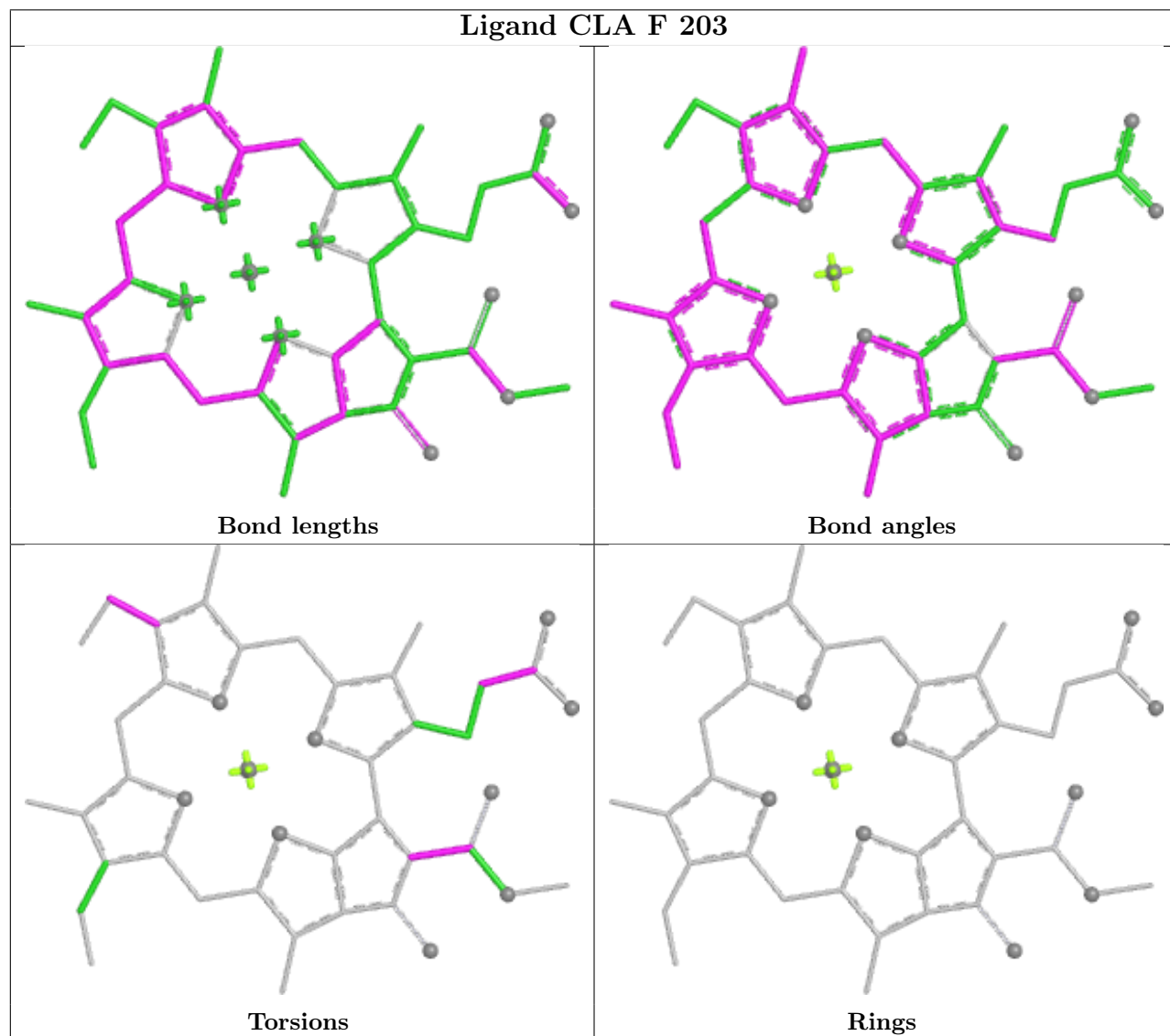


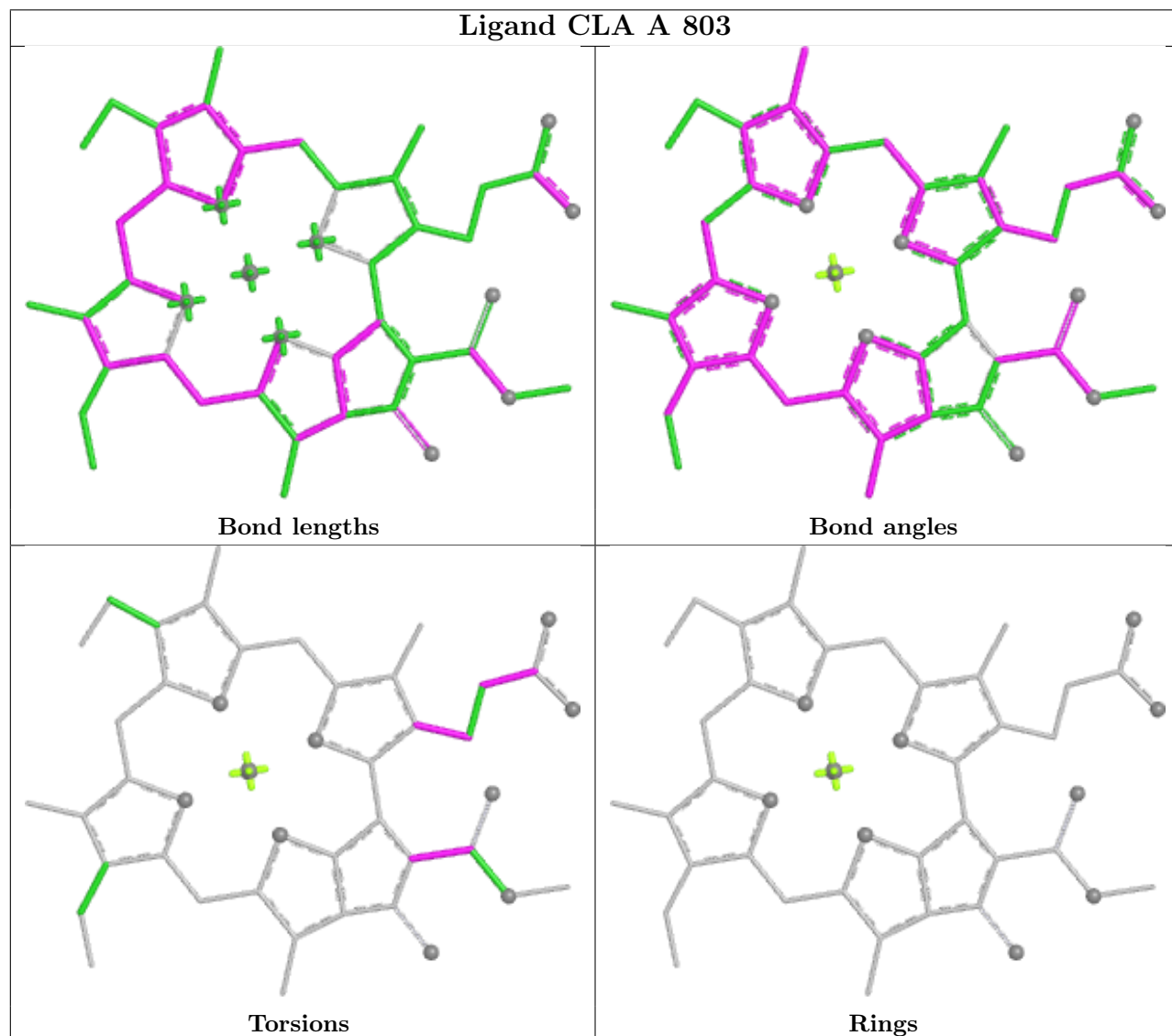
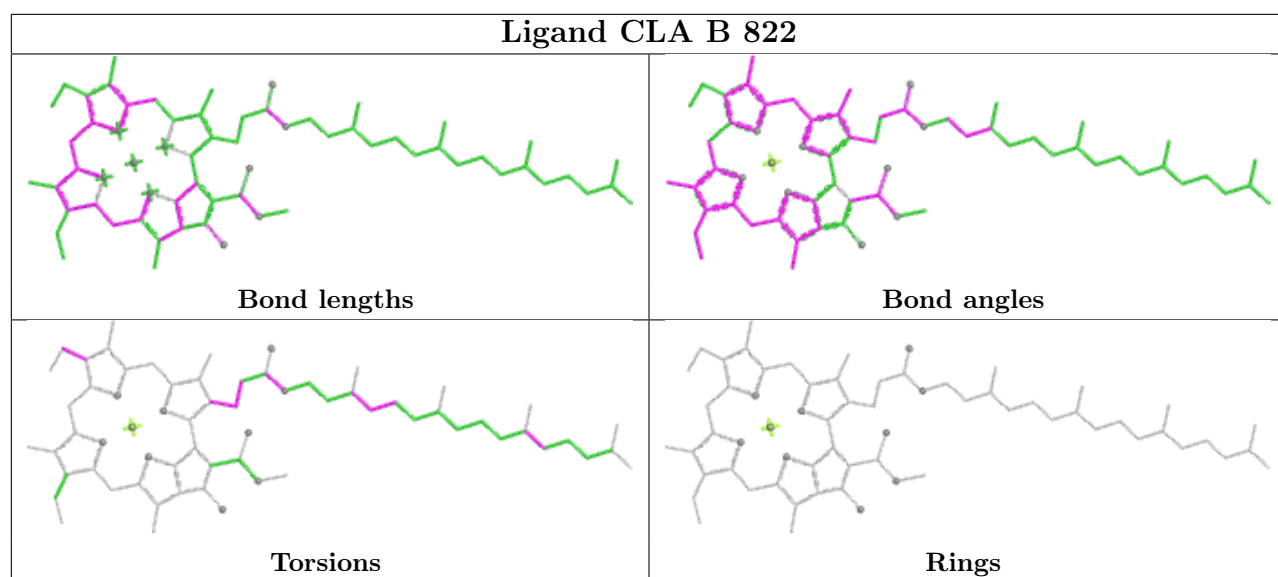


Ligand CLA A 819

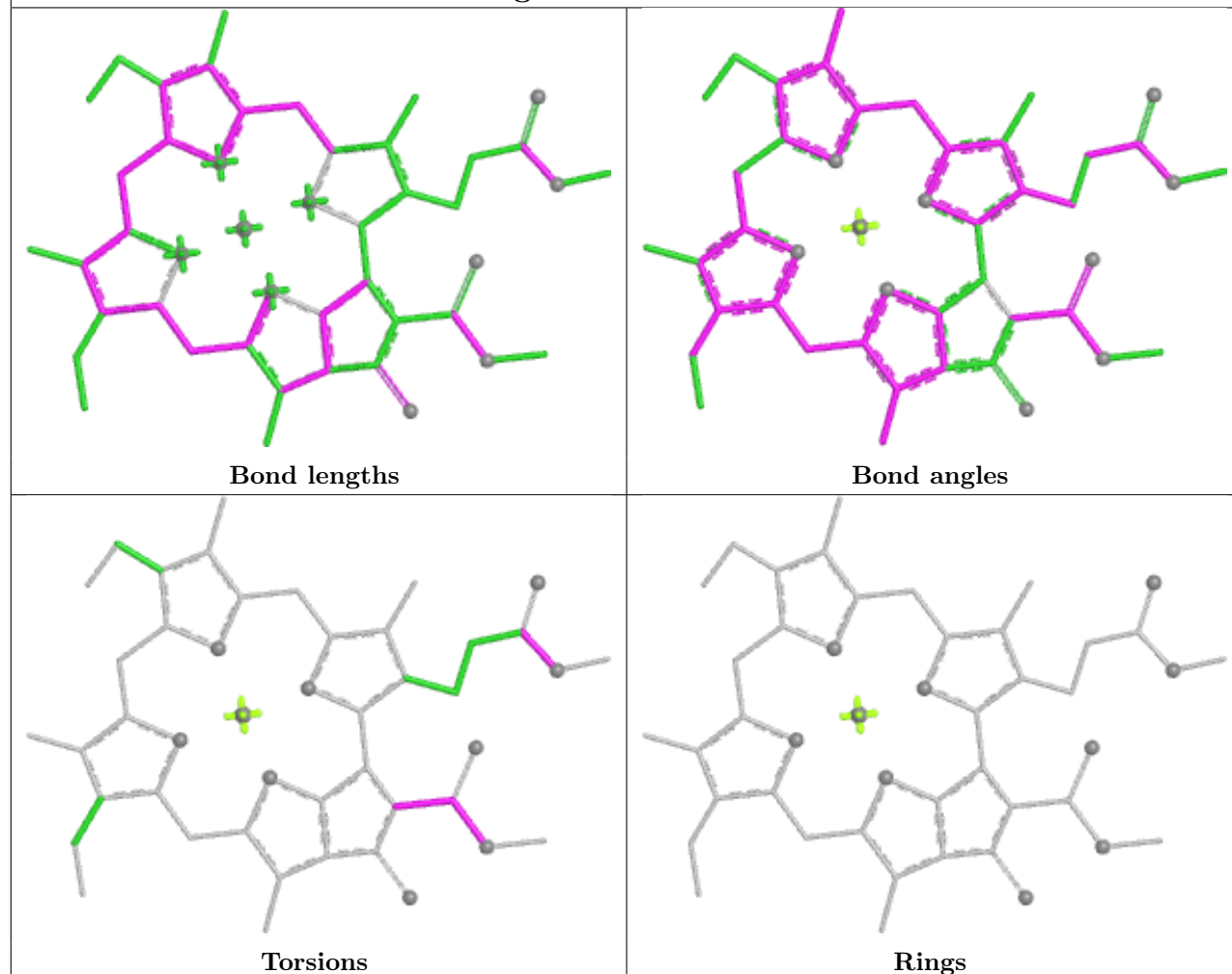


Ligand CLA F 203

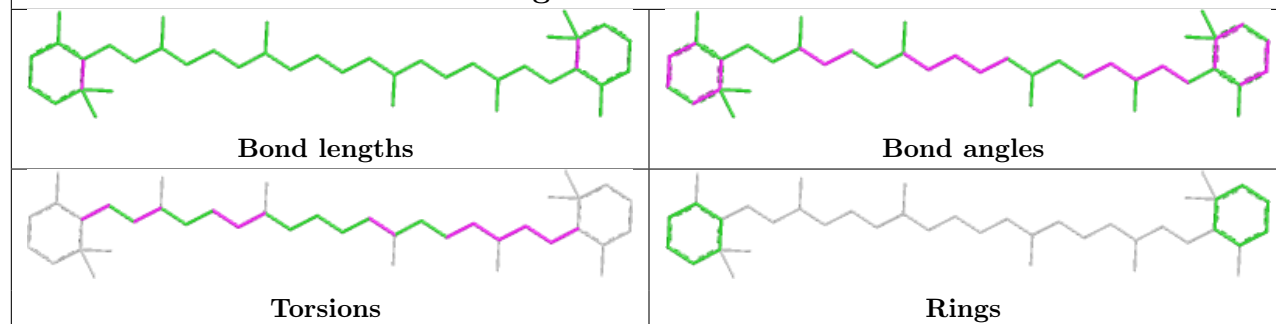


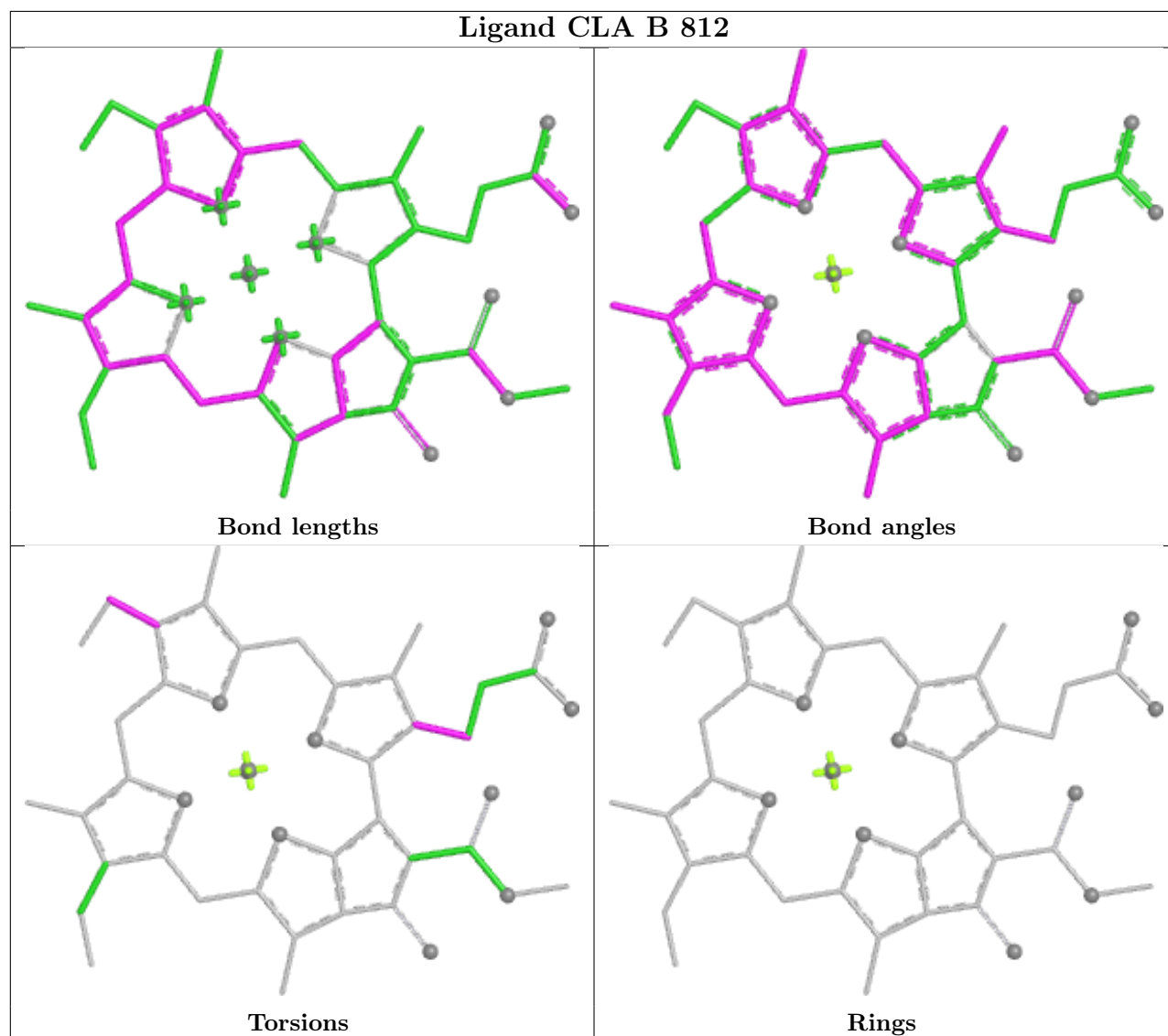
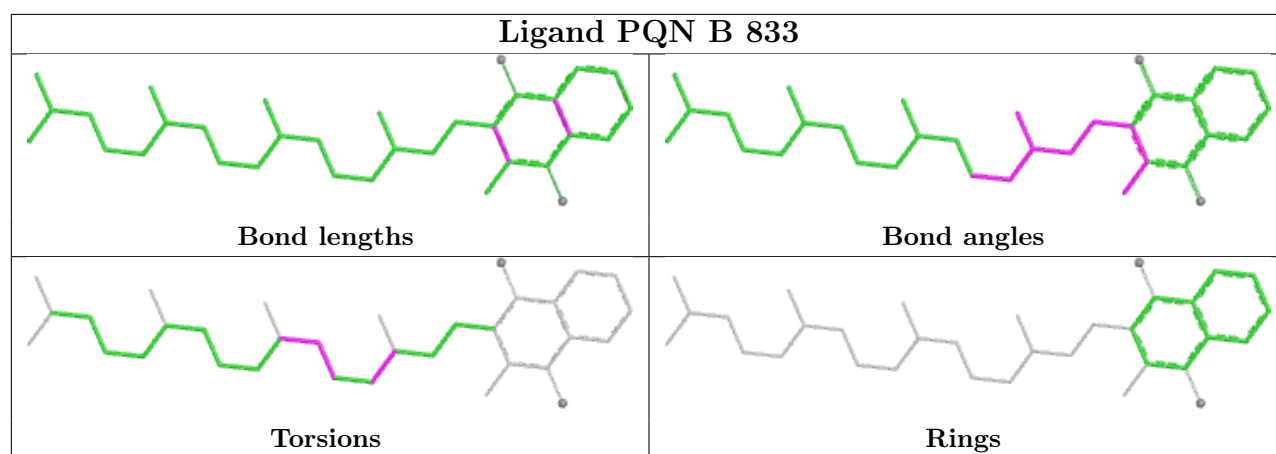


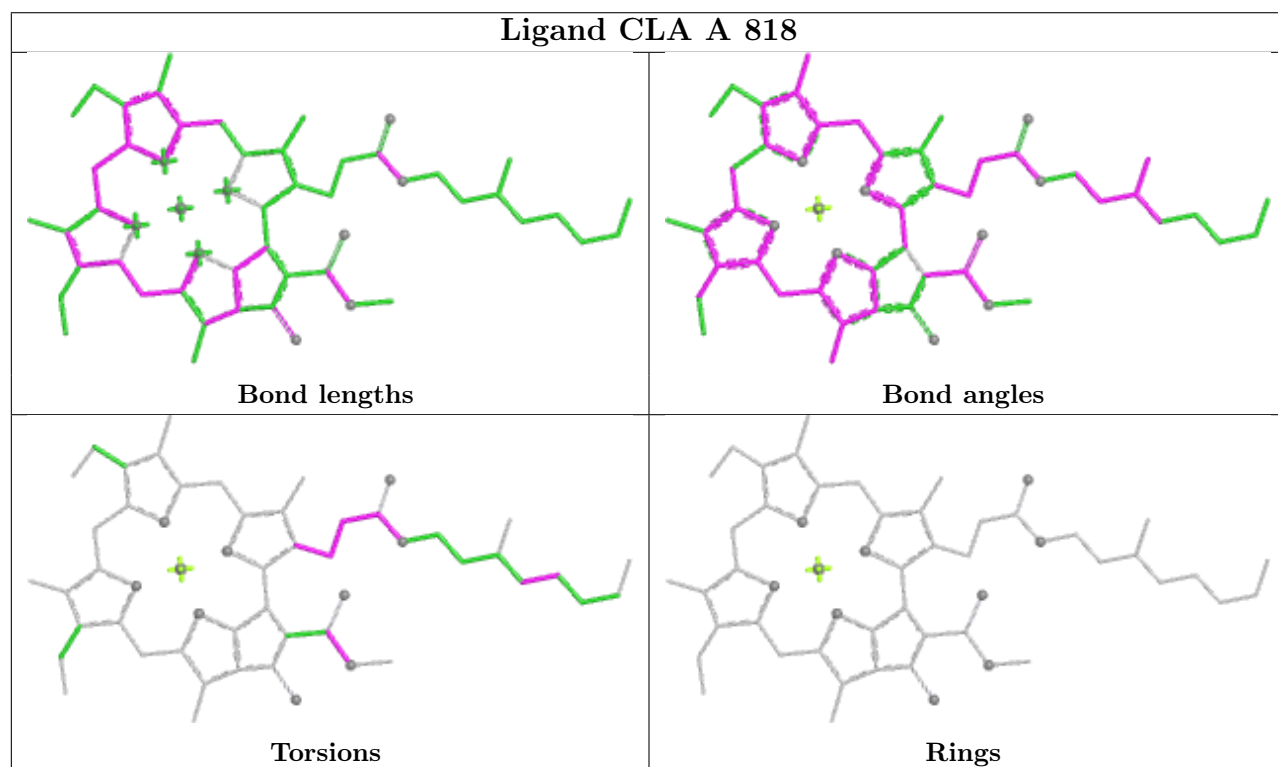
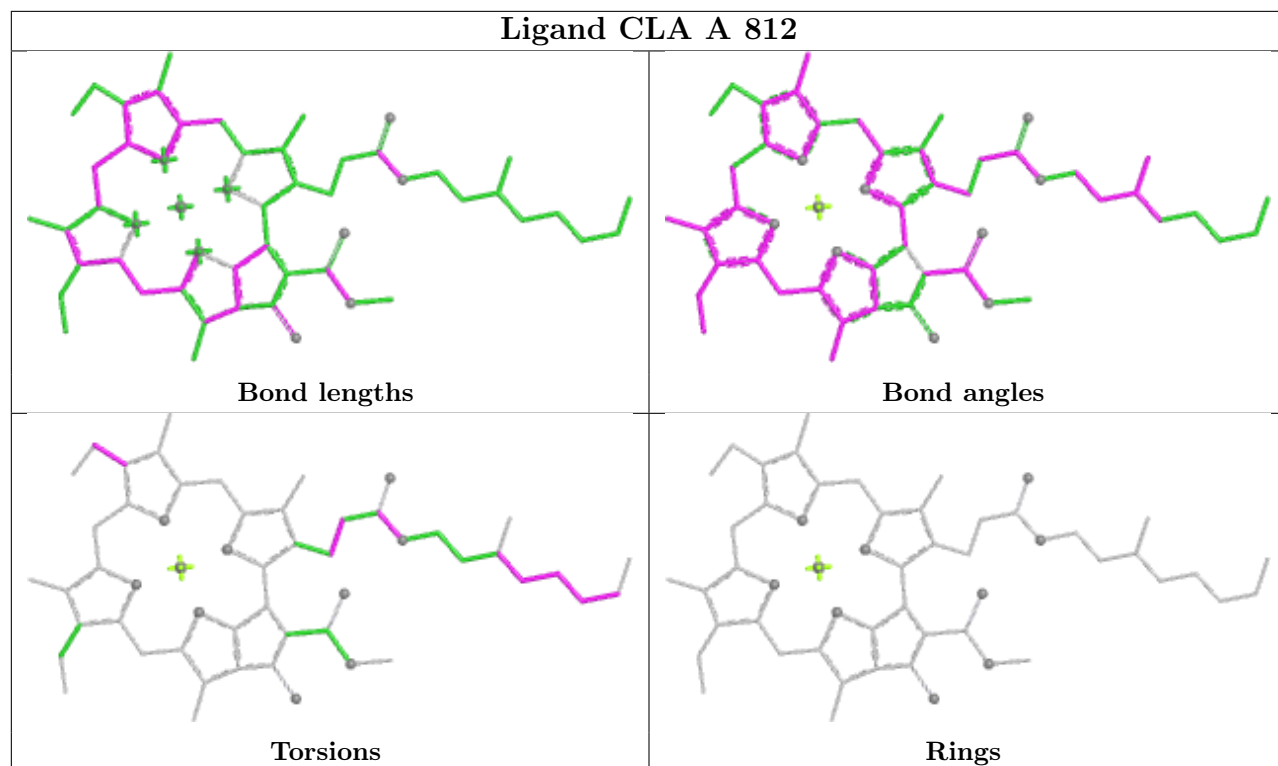
Ligand CLA B 819

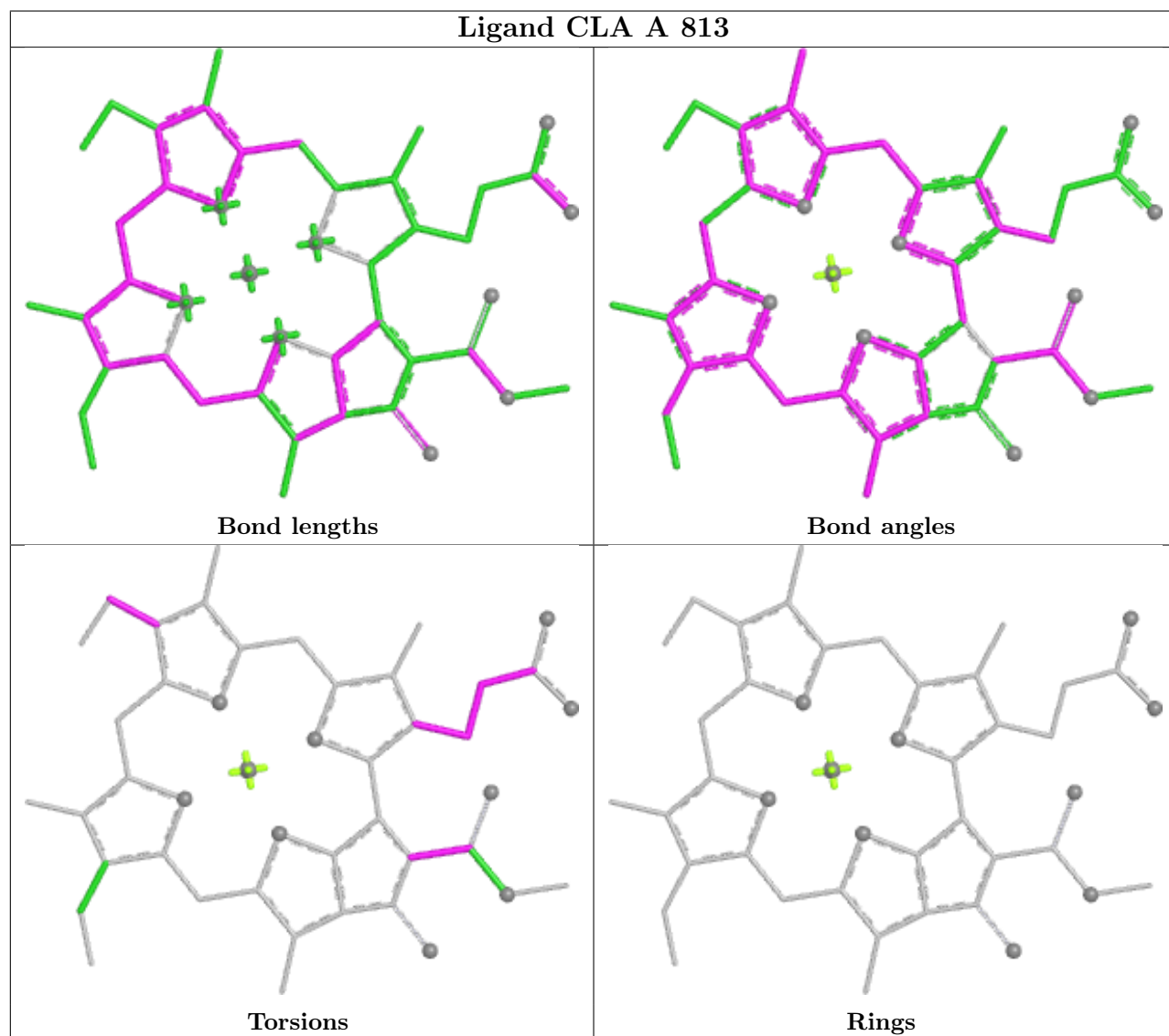
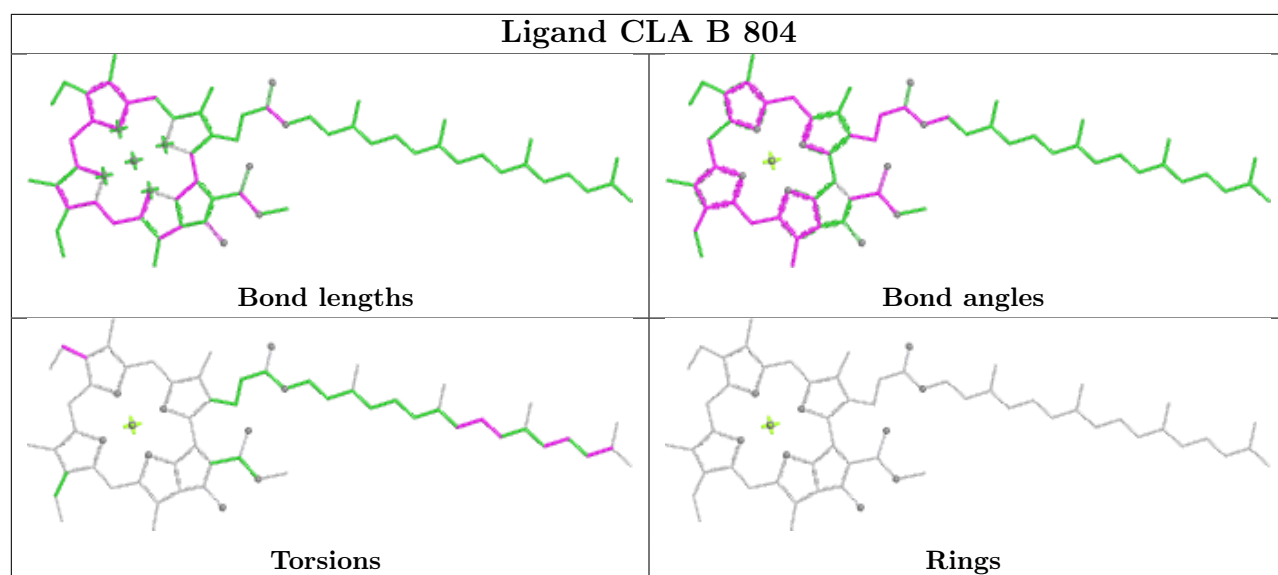


Ligand BCR L 206

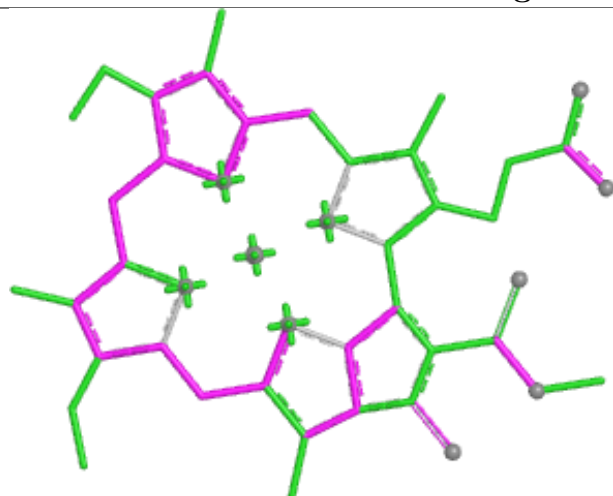




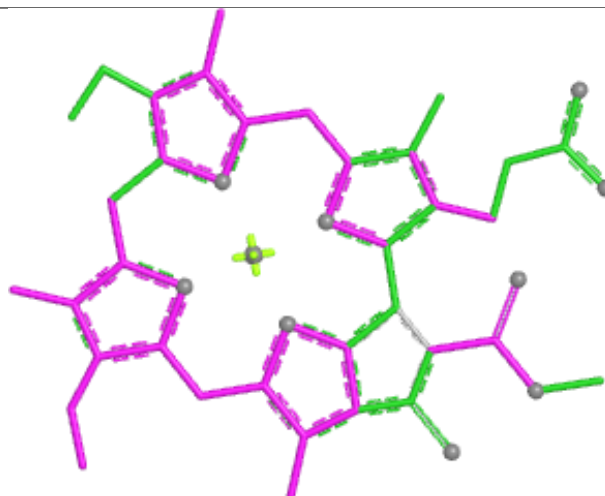




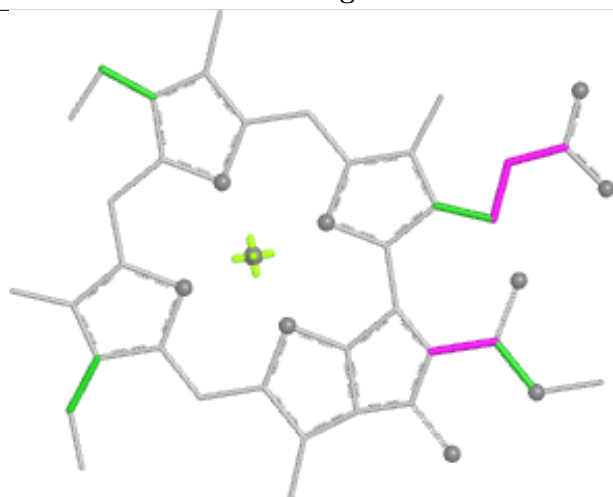
Ligand CLA A 836



Bond lengths



Bond angles

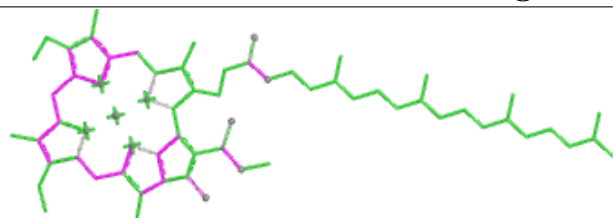


Torsions

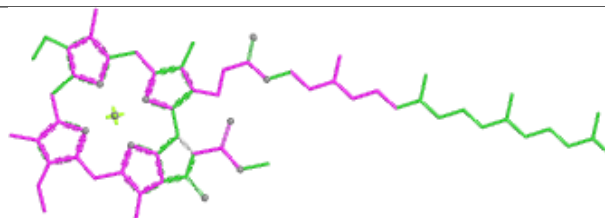


Rings

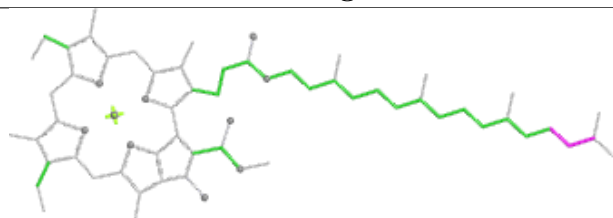
Ligand CLA B 808



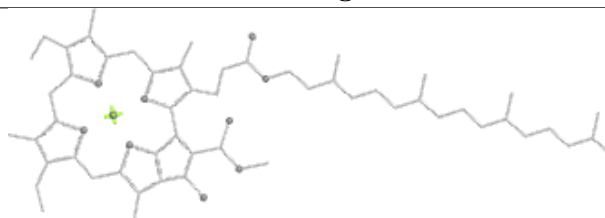
Bond lengths



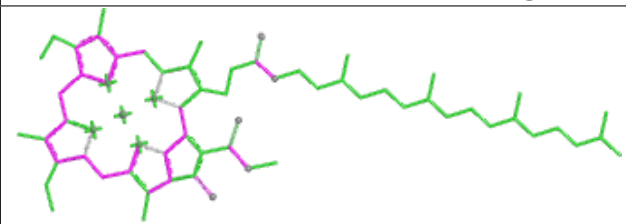
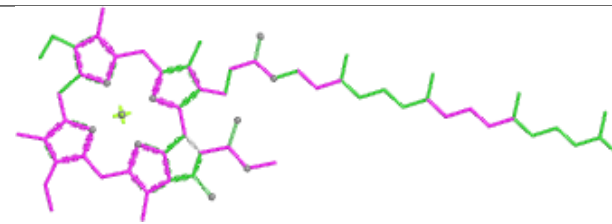
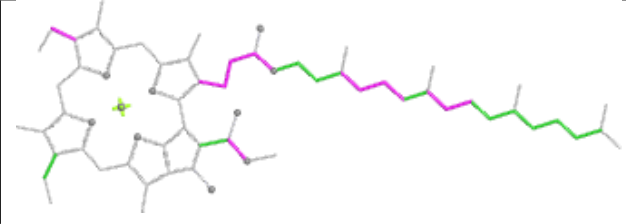
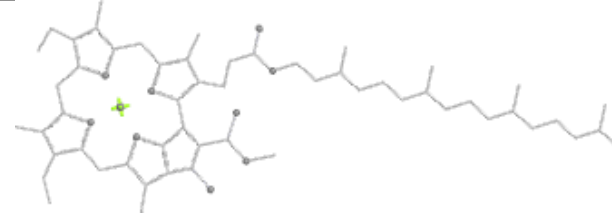
Bond angles

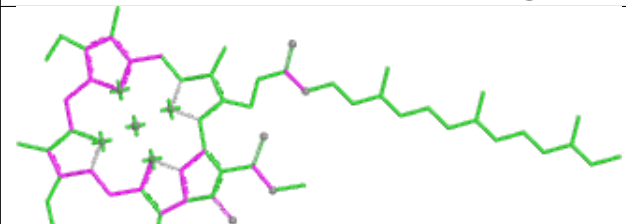
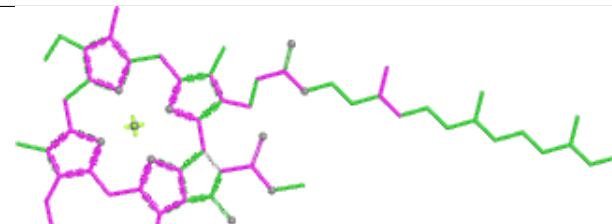
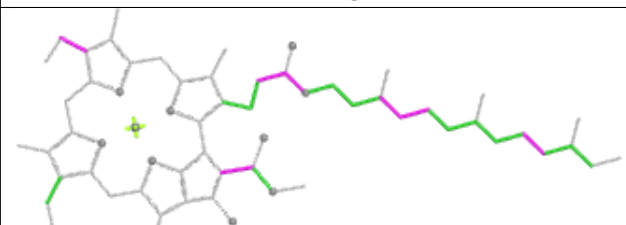
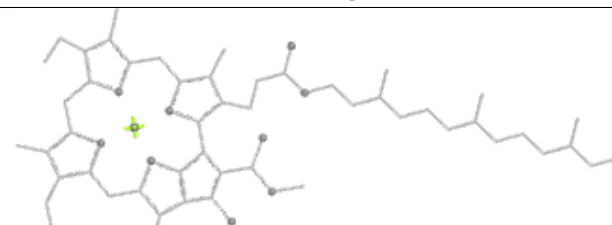


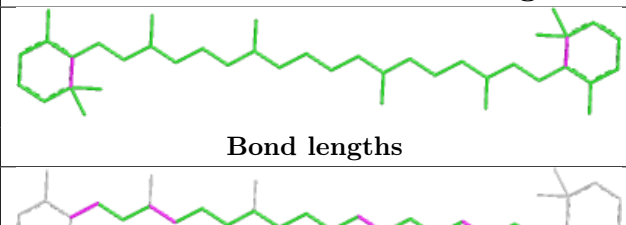
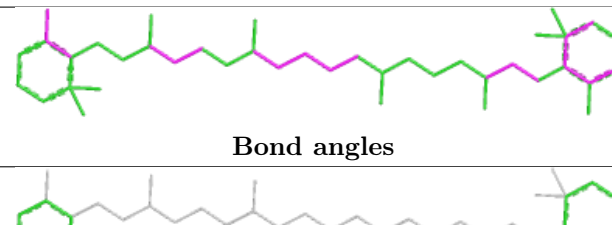
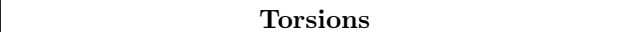
Torsions

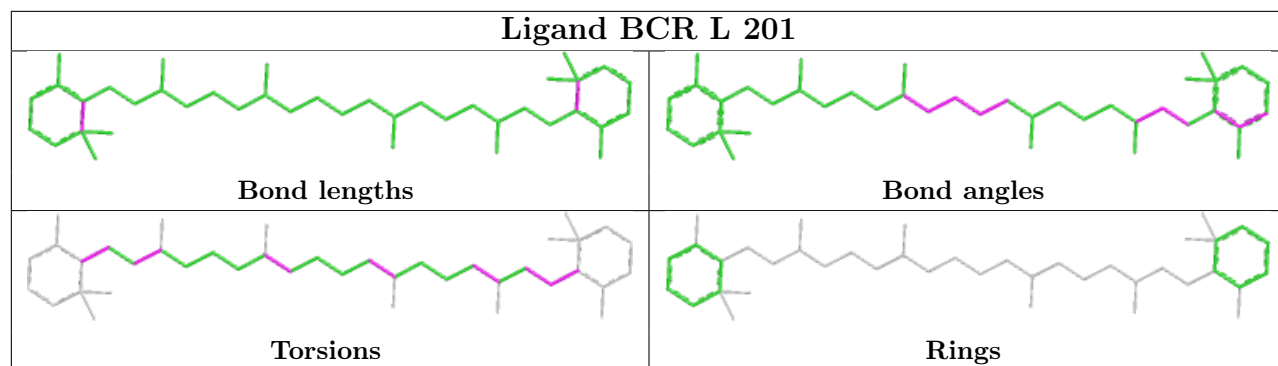


Rings

Ligand CLA A 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 847	
	
Bond lengths	Bond angles
	
Torsions	Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

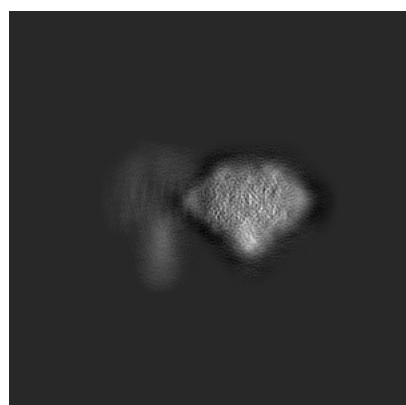
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30821. These allow visual inspection of the internal detail of the map and identification of artifacts.

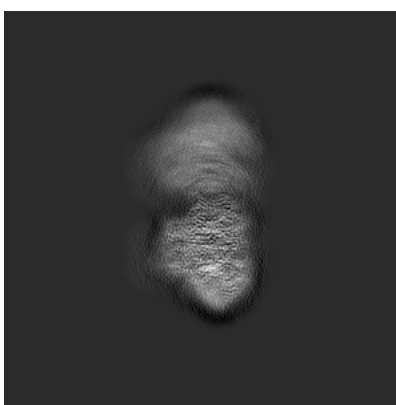
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

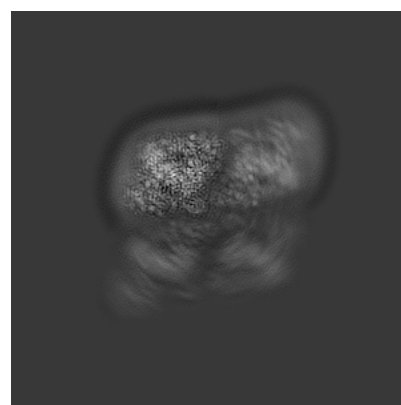
6.1.1 Primary map



X



Y

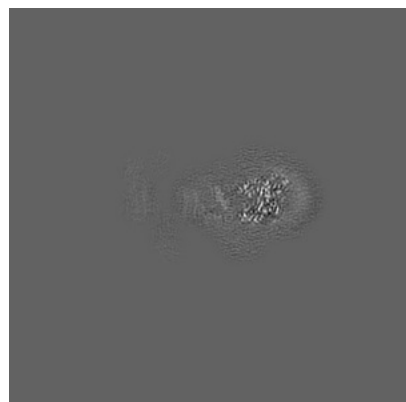


Z

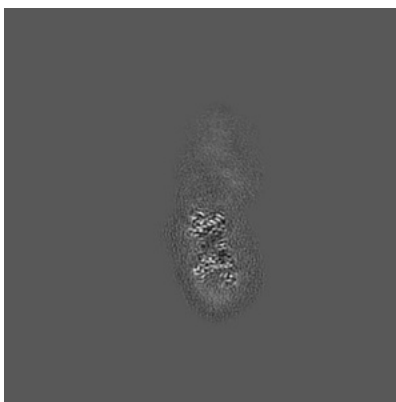
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

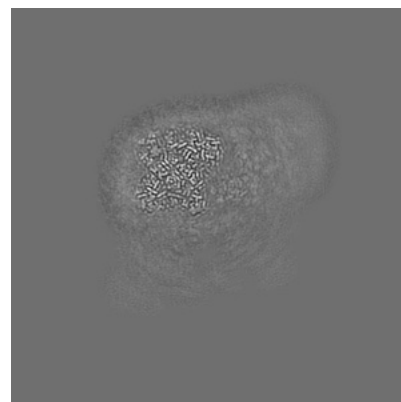
6.2.1 Primary map



X Index: 200



Y Index: 200

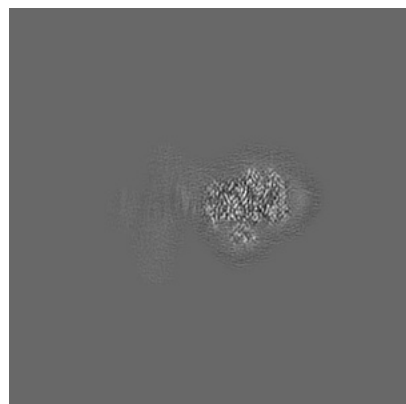


Z Index: 200

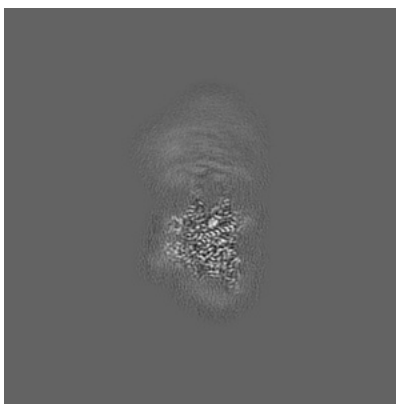
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

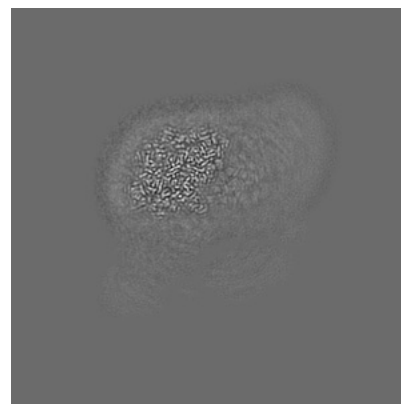
6.3.1 Primary map



X Index: 181



Y Index: 241

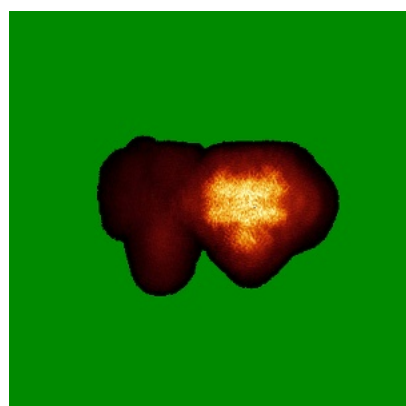


Z Index: 218

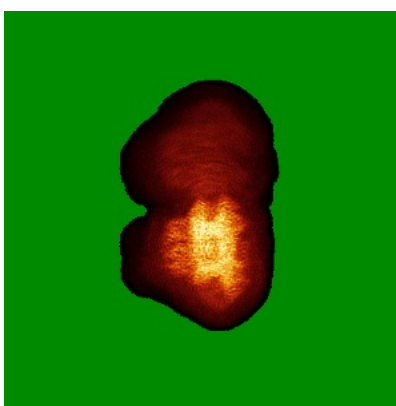
The images above show the largest variance slices of the map in three orthogonal directions.

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

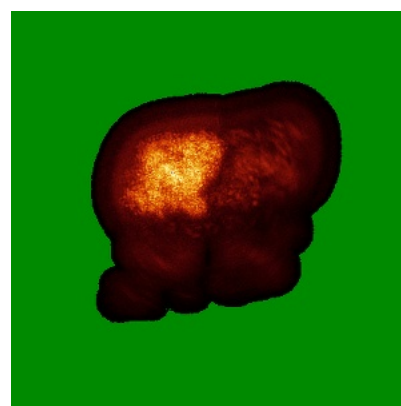
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

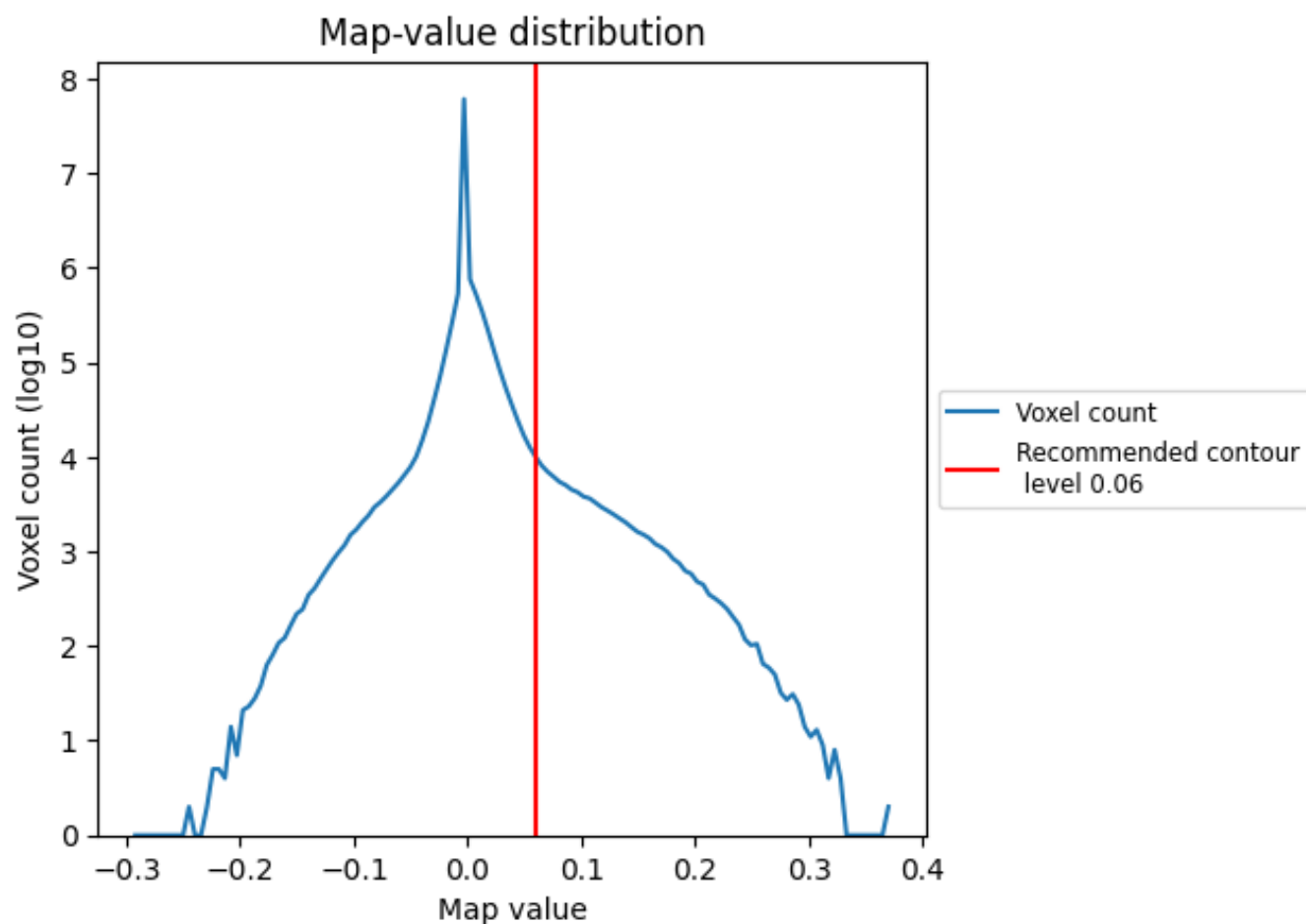
6.6 Mask visualisation

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

7 Map analysis [i](#)

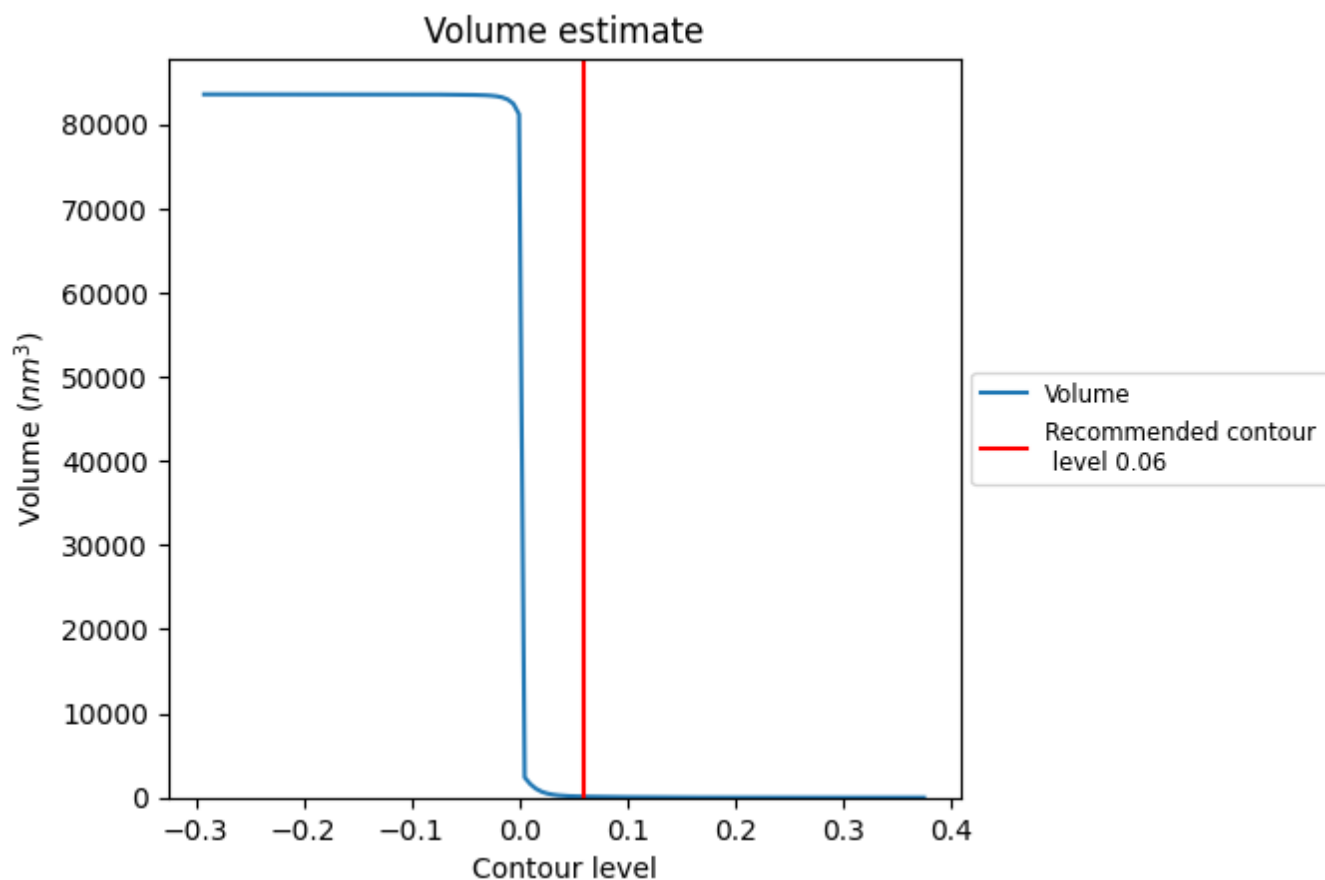
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

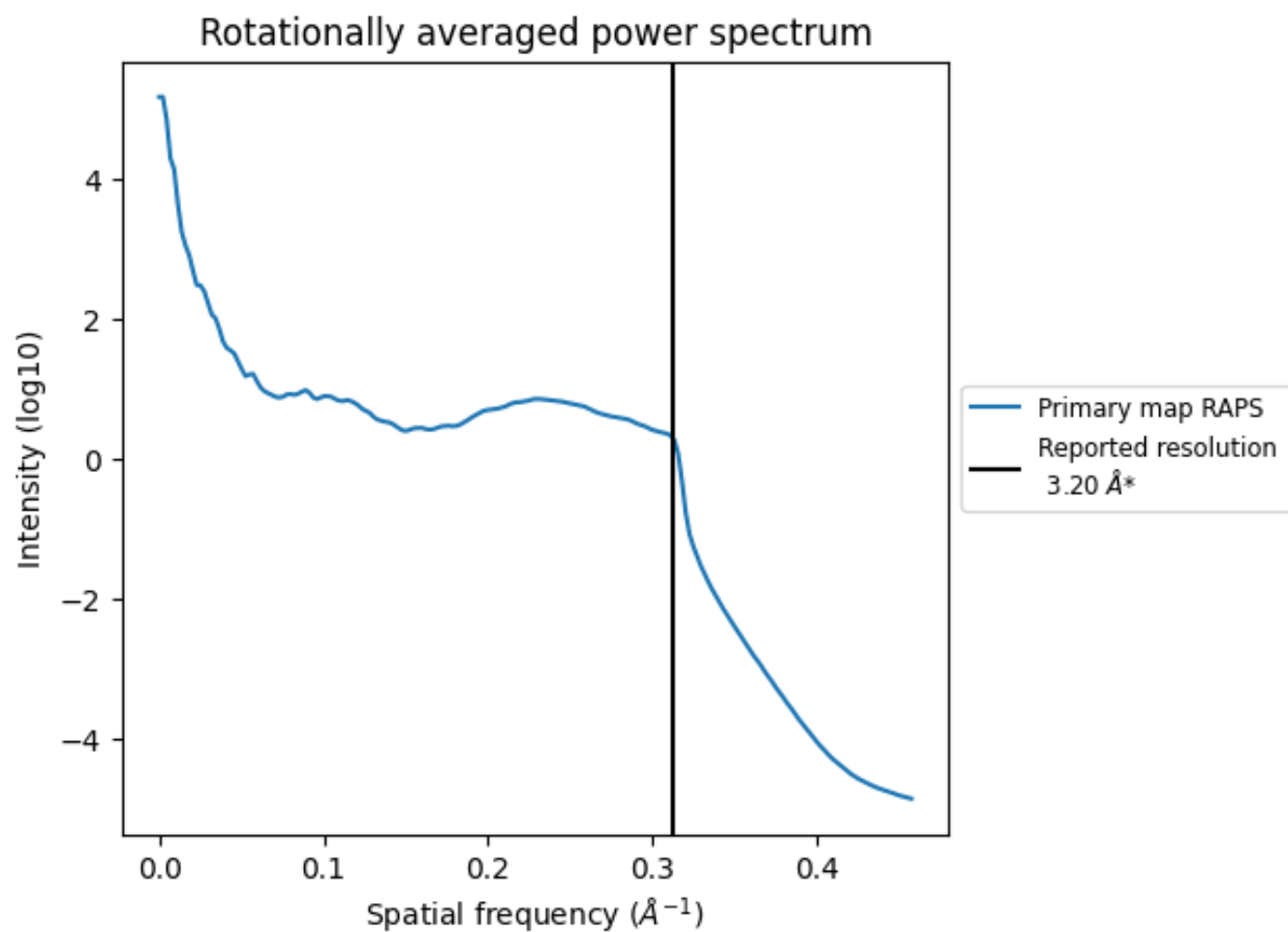
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 117 nm³; this corresponds to an approximate mass of 106 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

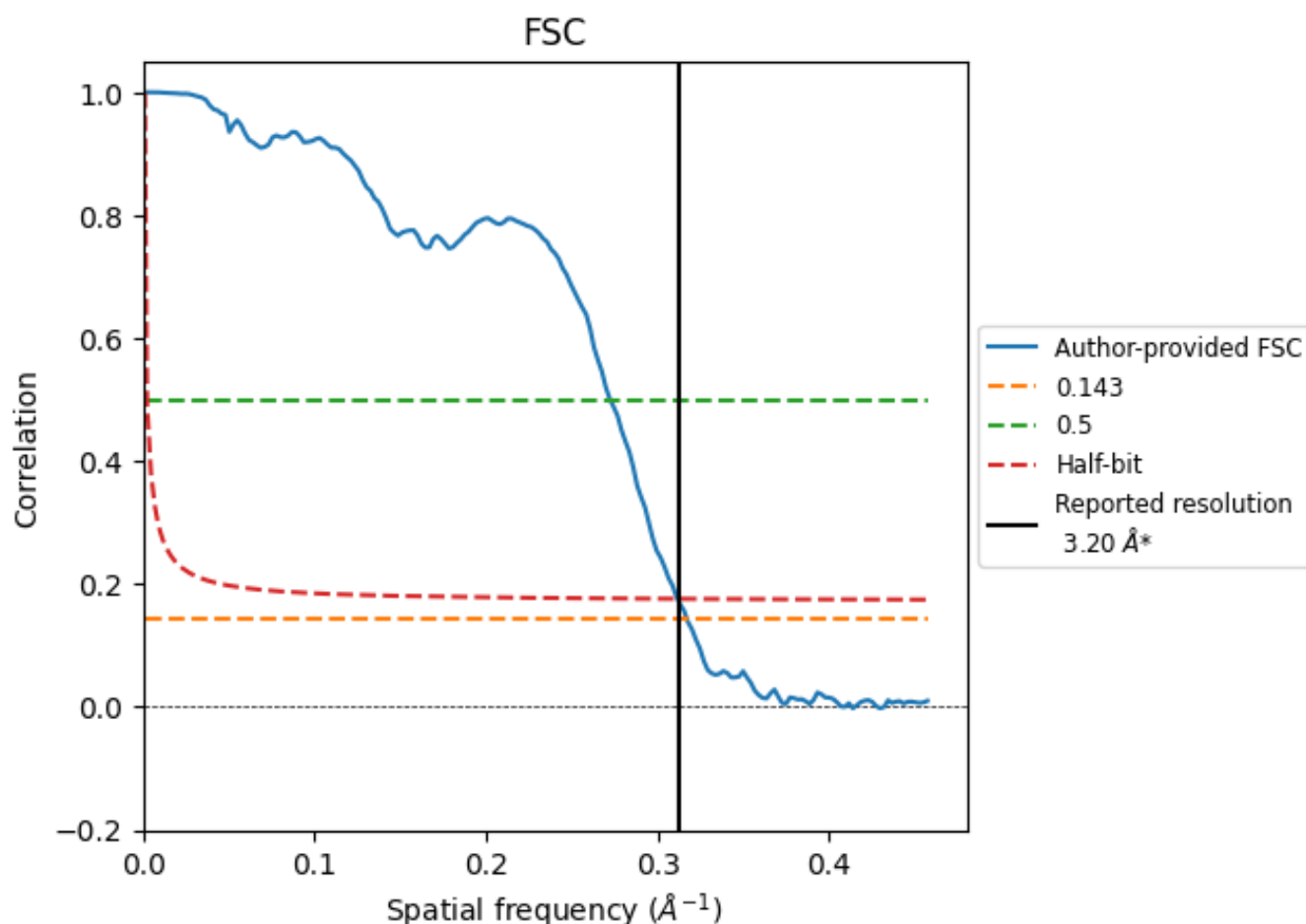


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

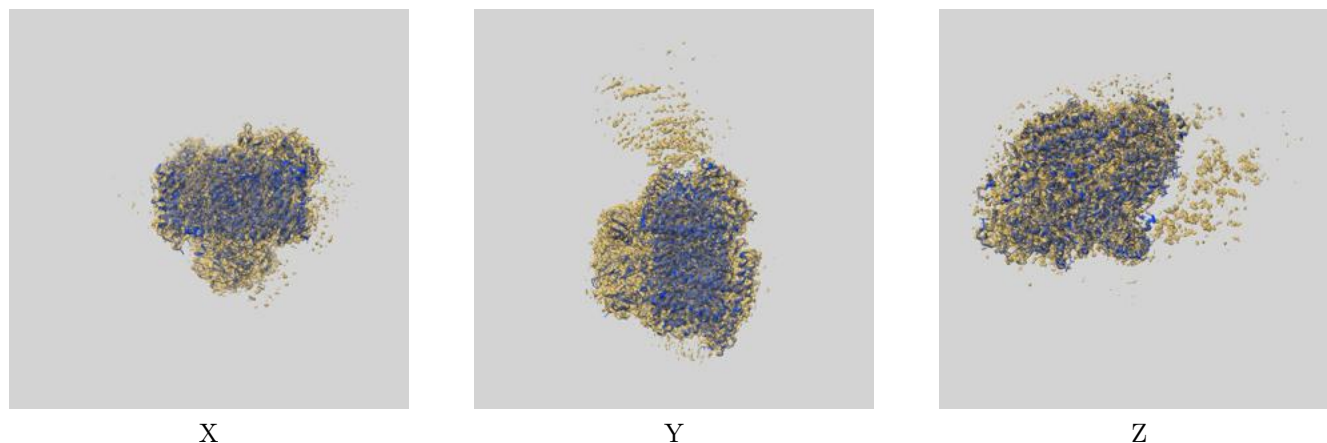
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.15	3.67	3.21
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

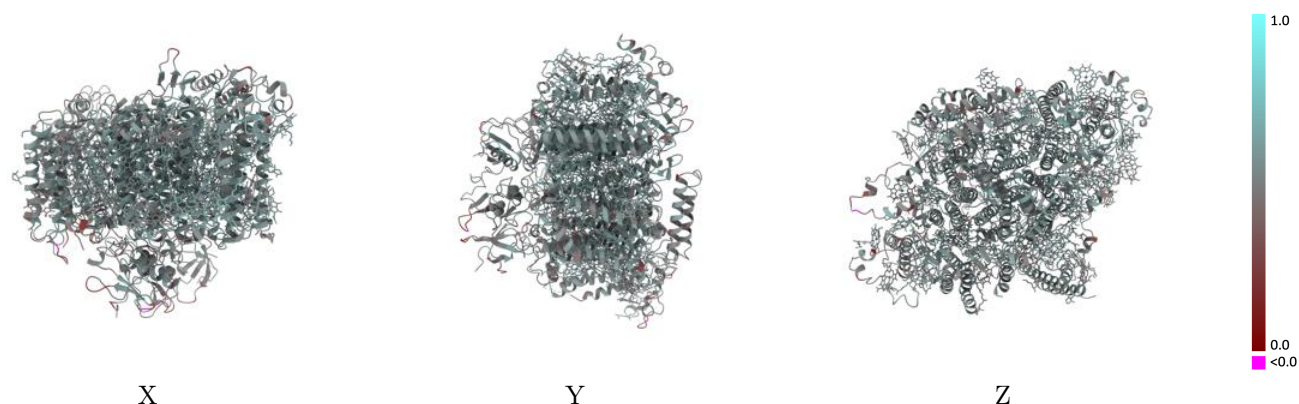
This section contains information regarding the fit between EMDB map EMD-30821 and PDB model 7DR1. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



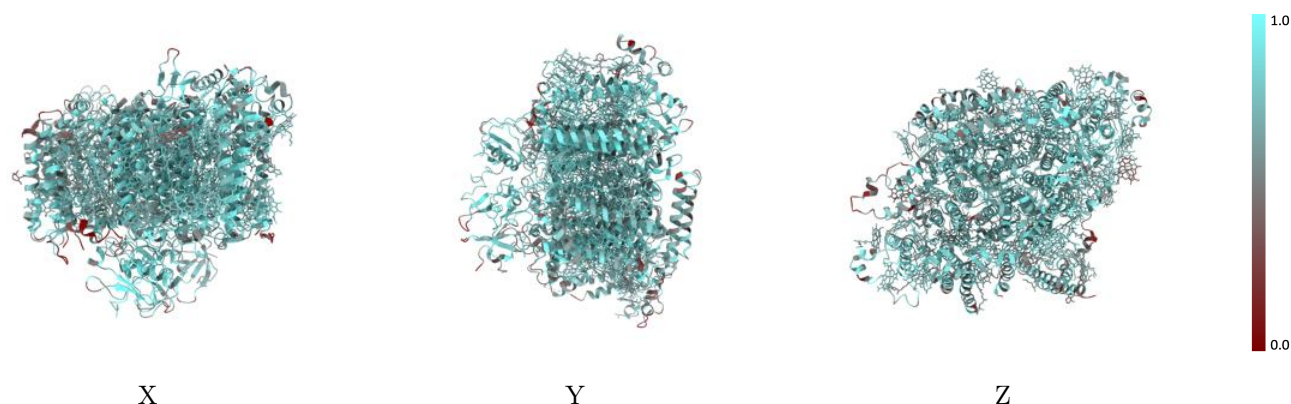
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



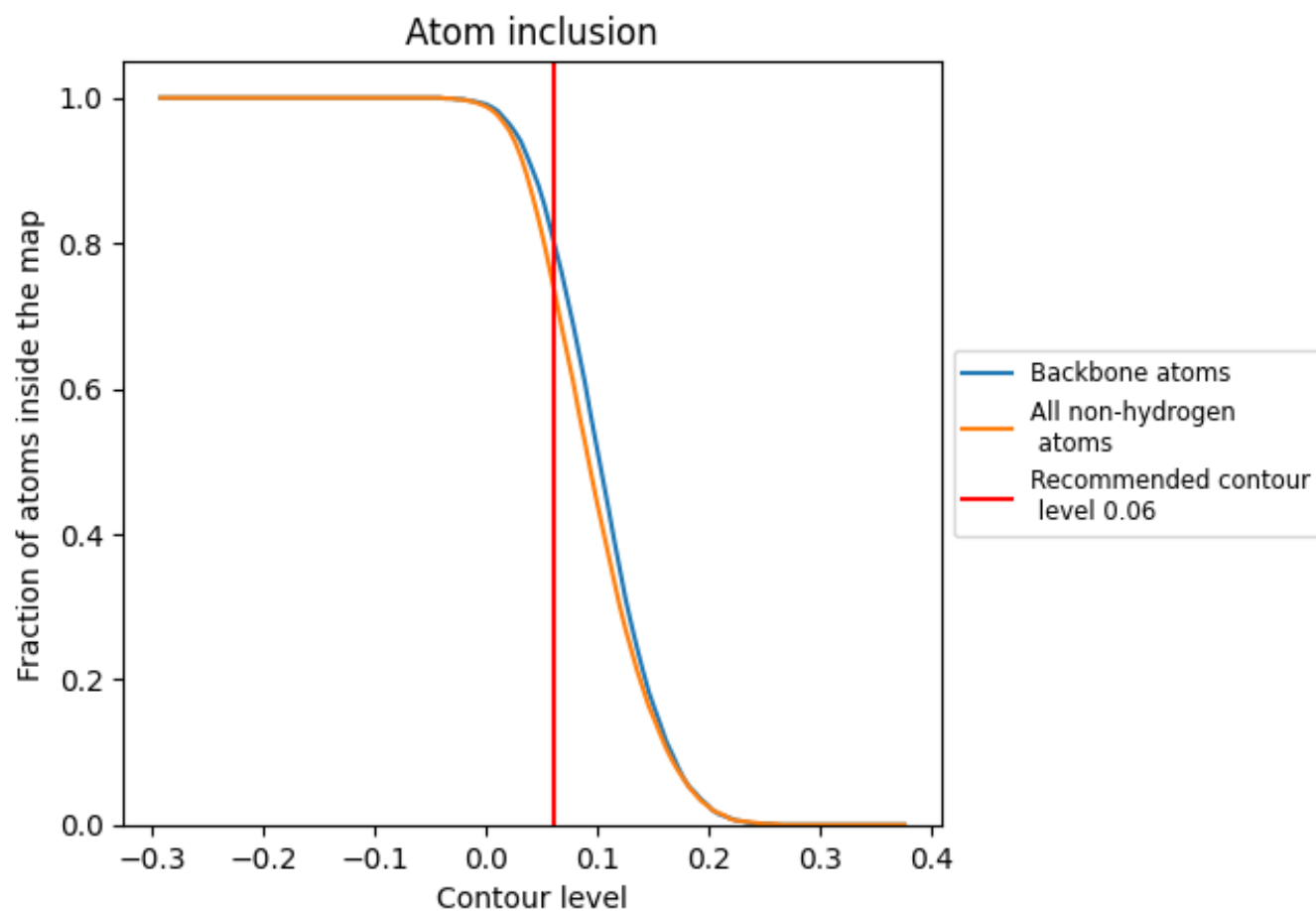
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.5250
A	0.7770	0.5470
B	0.7460	0.5200
C	0.7870	0.4730
D	0.7550	0.4870
E	0.7190	0.4730
F	0.6660	0.5050
I	0.6480	0.5250
J	0.6730	0.5290
L	0.6270	0.5050
M	0.6550	0.5200

