



Full wwPDB EM Validation Report ⓘ

Mar 23, 2026 – 07:11 PM UTC

PDB ID : 7DR0 / pdb_00007dr0
EMDB ID : EMD-30820
Title : Structure of Wild-type PSI monomer1 from *Cyanophora paradoxa*
Authors : Kato, K.; Nagao, R.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on : 2020-12-25
Resolution : 3.30 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

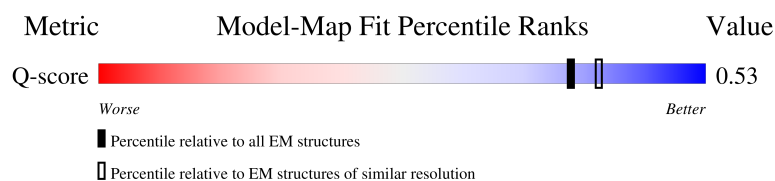
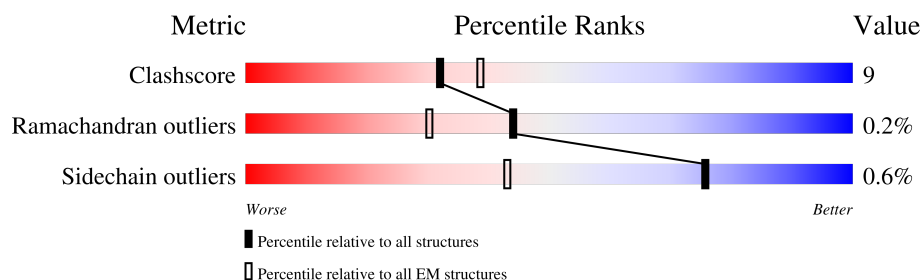
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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.



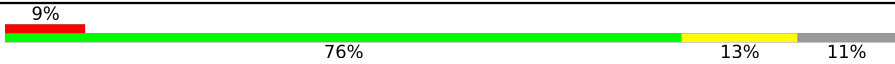
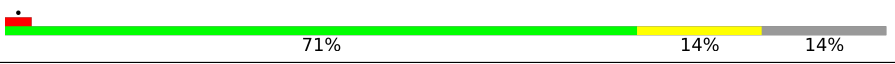
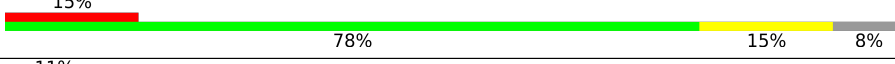
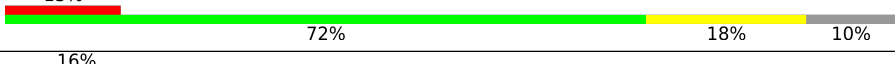
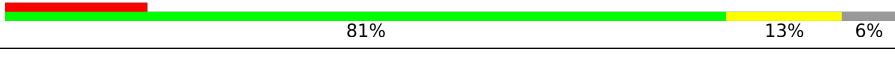
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	K	157	
10	L	146	
11	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
12	CL0	A	801	X	-	-	-
13	CLA	A	802	X	-	-	-
13	CLA	A	803	X	-	-	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	809	X	-	-	-
13	CLA	A	810	X	-	-	-
13	CLA	A	811	X	-	-	-
13	CLA	A	812	X	-	-	-
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	820	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	-
13	CLA	A	825	X	-	-	-
13	CLA	A	826	X	-	-	-
13	CLA	A	827	X	-	-	-
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	831	X	-	-	-
13	CLA	A	833	X	-	-	-
13	CLA	A	834	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	837	X	-	-	-
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	840	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	-	-
13	CLA	A	843	X	-	-	-
13	CLA	A	844	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	803	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	808	X	-	-	-
13	CLA	B	809	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	-
13	CLA	B	813	X	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	821	X	-	-	-
13	CLA	B	822	X	-	-	-
13	CLA	B	823	X	-	-	-
13	CLA	B	825	X	-	-	-
13	CLA	B	826	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	-	-
13	CLA	B	831	X	-	-	-
13	CLA	F	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	J	101	X	-	-	-
13	CLA	K	201	X	-	-	-
13	CLA	K	203	X	-	-	-
13	CLA	L	204	X	-	-	-
15	SF4	A	846	-	-	X	-
15	SF4	C	102	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 22745 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	S	0	0
			292	199	43	50			

- Molecule 9 is a protein called Photosystem I reaction center subunit Psak 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	57	Total	C	N	O	S	0	0
			403	269	65	67	2		

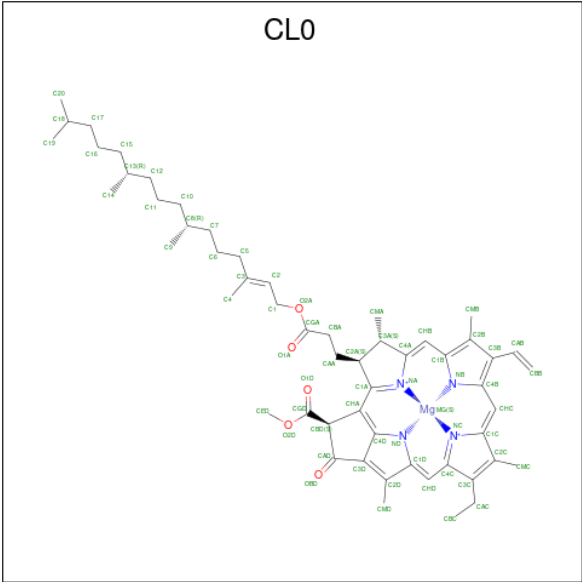
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

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

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

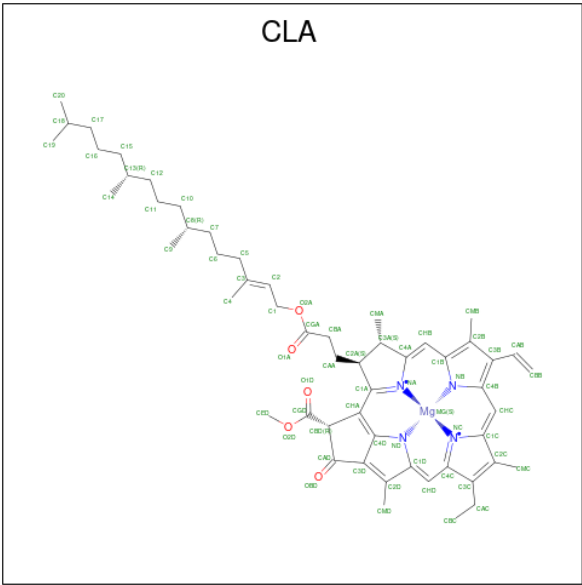
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	29	Total	C	N	O	S	0	0
			215	145	34	36			

- Molecule 12 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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

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



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

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

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

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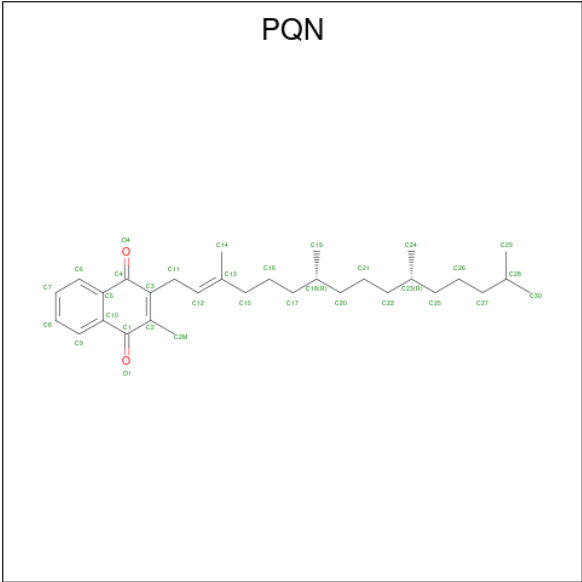
Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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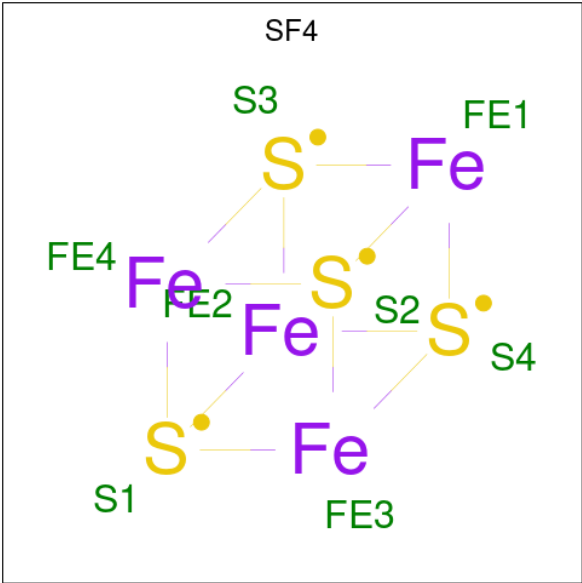
Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

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



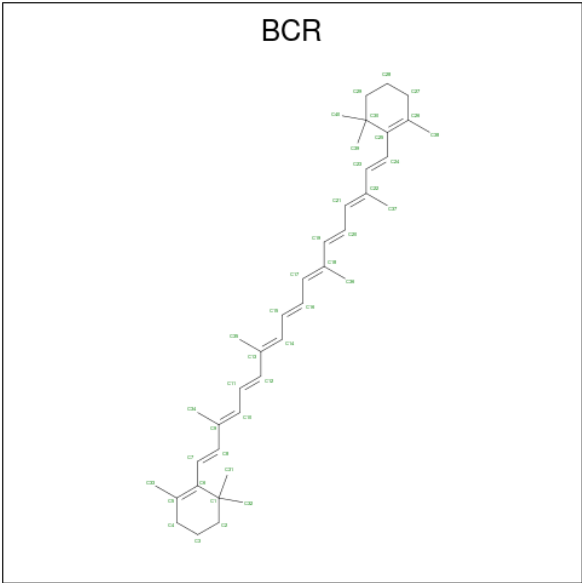
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	

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

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



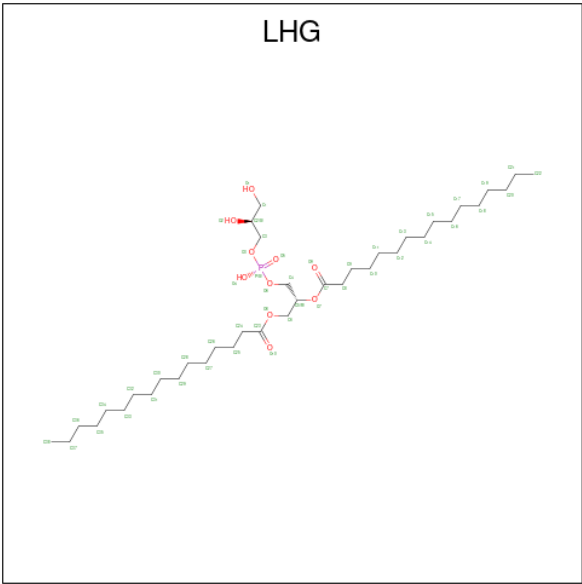
Mol	Chain	Residues	Atoms		AltConf
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	A	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	B	1	Total	C	0
			40	40	
16	F	1	Total	C	0
			40	40	
16	F	1	Total	C	0
			40	40	

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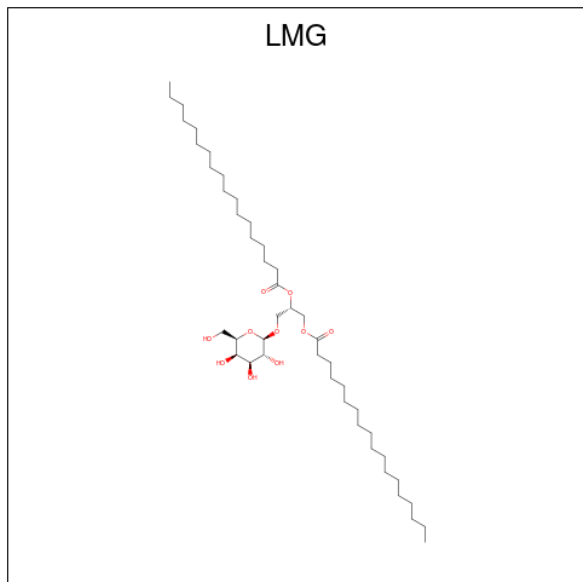
Mol	Chain	Residues	Atoms	AltConf
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



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

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).

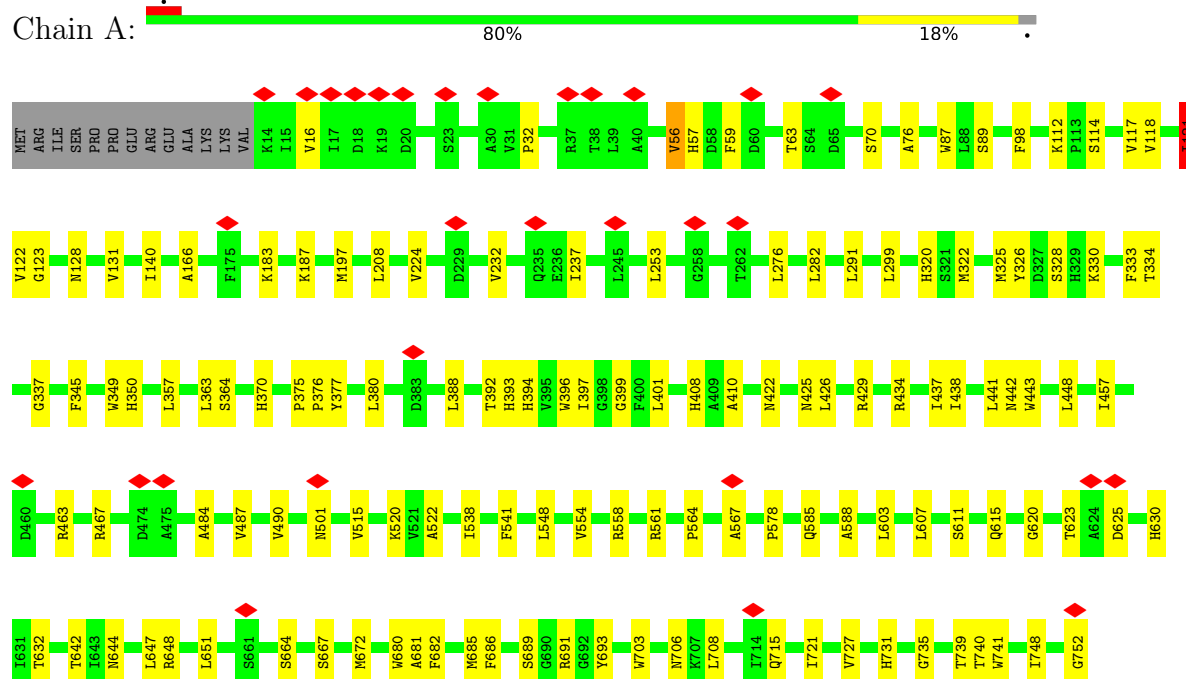


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	B	1	55	45	10	0

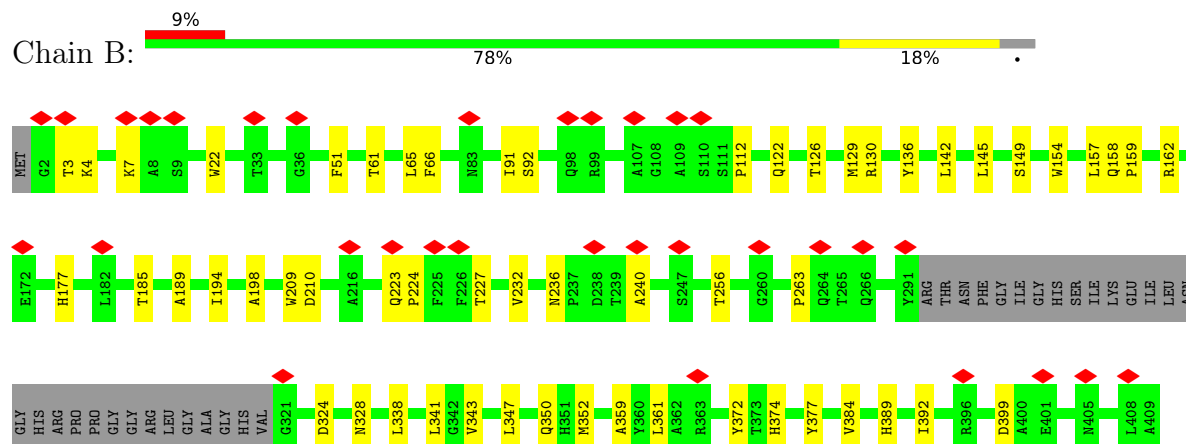
3 Residue-property plots

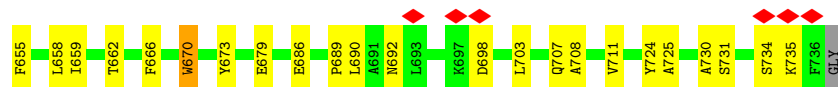
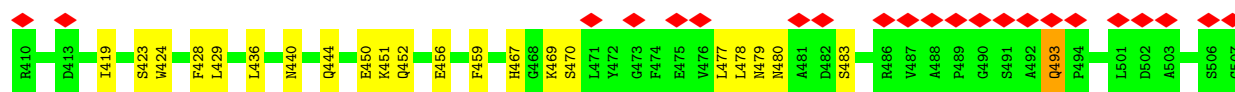
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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

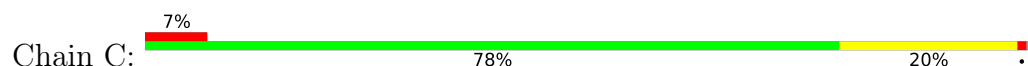


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

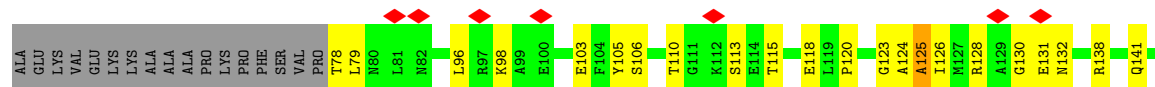
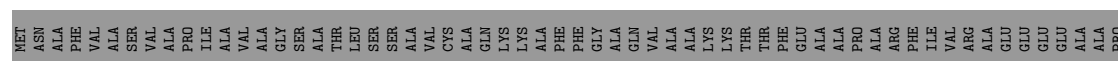




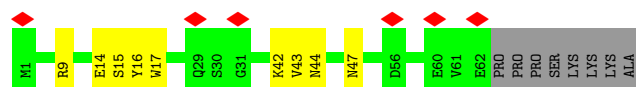
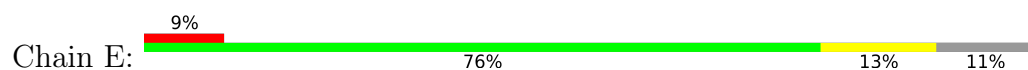
• Molecule 3: Photosystem I iron-sulfur center



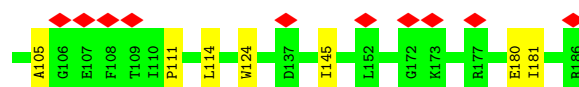
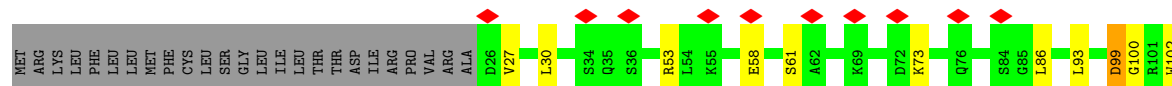
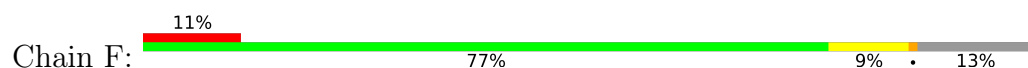
• Molecule 4: Photosystem I reaction center subunit II, cyanelle

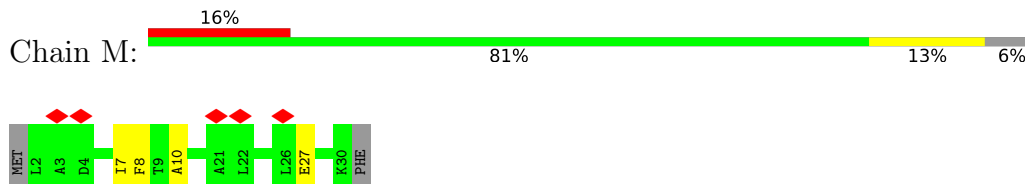


• Molecule 5: Photosystem I reaction center subunit IV



• Molecule 6: Photosystem I reaction center subunit III





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	70920	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	0.396	Depositor
Minimum map value	-0.211	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: SF4, BCR, PQN, CL0, LHG, CLA, LMG

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	0.33	0/6000	0.49	2/8177 (0.0%)
2	B	0.29	0/5820	0.49	1/7955 (0.0%)
3	C	0.27	0/611	0.62	2/828 (0.2%)
4	D	0.28	0/1105	0.85	6/1489 (0.4%)
5	E	0.24	0/516	0.42	0/696
6	F	0.22	0/1281	0.51	0/1733
7	I	0.30	0/232	0.68	0/319
8	J	0.24	0/300	0.53	0/410
9	K	0.23	0/414	0.49	0/564
10	L	0.26	0/988	0.59	2/1342 (0.1%)
11	M	0.21	0/217	0.44	0/295
All	All	0.29	0/17484	0.53	13/23808 (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
1	A	0	1
2	B	0	3
4	D	0	3
6	F	0	1
All	All	0	8

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	125	ALA	CA-C-N	6.97	134.51	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	125	ALA	C-N-CA	6.97	134.51	121.97
4	D	130	GLY	CA-C-N	6.60	133.57	121.70
4	D	130	GLY	C-N-CA	6.60	133.57	121.70
10	L	73	ASP	CA-C-N	6.36	133.15	121.70
10	L	73	ASP	C-N-CA	6.36	133.15	121.70
4	D	123	GLY	CA-C-N	6.32	133.61	121.54
4	D	123	GLY	C-N-CA	6.32	133.61	121.54
2	B	493	GLN	N-CA-C	5.39	121.72	109.81
3	C	62	PHE	CA-C-N	5.18	131.43	121.54
3	C	62	PHE	C-N-CA	5.18	131.43	121.54
1	A	121	ILE	CA-C-N	5.10	131.15	121.97
1	A	121	ILE	C-N-CA	5.10	131.15	121.97

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	SER	Peptide
2	B	478	LEU	Peptide
2	B	493	GLN	Peptide
2	B	670	TRP	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 ⓘ

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	97	0
2	B	5622	0	5406	95	0
3	C	601	0	576	14	0
4	D	1082	0	1099	22	0
5	E	508	0	507	7	0
6	F	1255	0	1249	13	0
7	I	228	0	247	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	292	0	302	5	0
9	K	403	0	421	2	0
10	L	965	0	970	19	0
11	M	215	0	239	4	0
12	A	65	0	72	2	0
13	A	2441	0	2362	87	0
13	B	1945	0	1960	80	0
13	F	45	0	33	0	0
13	J	45	0	33	2	0
13	K	86	0	62	0	0
13	L	163	0	148	5	0
14	A	33	0	46	4	0
14	B	33	0	46	5	0
15	A	8	0	0	2	0
15	C	16	0	0	4	0
16	A	200	0	280	18	0
16	B	120	0	168	8	0
16	F	80	0	112	8	0
16	I	40	0	56	5	0
16	J	120	0	168	12	0
16	K	40	0	56	3	0
16	L	120	0	168	6	0
16	M	40	0	56	4	0
17	A	76	0	98	1	0
18	B	55	0	86	1	0
All	All	22745	0	22647	388	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 9.

All (388) 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)
3:C:17:CYS:HB3	15:C:102:SF4:S4	2.29	0.72
1:A:399:GLY:HA3	1:A:603:LEU:HD11	1.72	0.70
13:B:830:CLA:H71	13:B:830:CLA:HBB1	1.73	0.69
15:A:846:SF4:S3	2:B:562:CYS:CB	2.78	0.69
2:B:338:LEU:HD21	13:B:823:CLA:HAB	1.75	0.68
13:A:830:CLA:H2	16:A:848:BCR:H24C	1.75	0.67
1:A:357:LEU:HD21	13:A:831:CLA:HAB	1.75	0.67
13:B:820:CLA:H13	16:B:836:BCR:H15C	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:820:CLA:HAB	13:A:820:CLA:H8	1.77	0.66
1:A:320:HIS:HB3	1:A:325:MET:HE2	1.79	0.64
13:A:806:CLA:H72	16:A:848:BCR:H23C	1.78	0.64
1:A:87:TRP:HA	13:A:808:CLA:HBB2	1.80	0.63
2:B:374:HIS:HE1	13:B:821:CLA:ND	1.96	0.63
13:A:810:CLA:HAB	16:J:102:BCR:HC7	1.81	0.63
1:A:363:LEU:HD21	13:A:820:CLA:H72	1.81	0.63
13:A:829:CLA:H191	16:J:102:BCR:H14C	1.81	0.63
13:A:842:CLA:HAB	14:A:845:PQN:H162	1.81	0.62
7:I:13:VAL:HA	7:I:17:LEU:HB2	1.82	0.62
1:A:224:VAL:HG23	1:A:237:ILE:HG21	1.81	0.61
13:B:805:CLA:HBB1	16:M:101:BCR:H312	1.82	0.61
15:A:846:SF4:S3	2:B:562:CYS:HB3	2.41	0.61
13:A:809:CLA:HAB	16:J:102:BCR:H363	1.83	0.61
4:D:128:ARG:H	4:D:132:ASN:HD22	1.48	0.60
1:A:401:LEU:HD21	13:A:807:CLA:H142	1.83	0.60
3:C:5:VAL:HG22	3:C:67:VAL:HG22	1.84	0.60
1:A:644:ASN:OD1	1:A:648:ARG:NH1	2.35	0.59
2:B:223:GLN:HG3	2:B:224:PRO:HD3	1.84	0.58
13:A:843:CLA:HBB2	16:A:851:BCR:H19C	1.85	0.58
13:B:807:CLA:H162	13:B:822:CLA:HBB2	1.85	0.58
4:D:110:THR:HG22	4:D:131:GLU:H	1.69	0.58
13:A:804:CLA:HBB2	13:A:812:CLA:H111	1.85	0.57
13:A:833:CLA:HED1	10:L:18:LEU:HD21	1.86	0.57
16:A:851:BCR:H272	16:F:201:BCR:H16C	1.86	0.57
1:A:345:PHE:HB3	13:A:826:CLA:HBC3	1.85	0.57
4:D:163:VAL:HG23	4:D:167:GLY:HA3	1.86	0.57
10:L:35:LEU:HD21	13:L:202:CLA:HBB1	1.86	0.57
1:A:467:ARG:NH2	13:A:835:CLA:OBD	2.37	0.57
4:D:98:LYS:NZ	4:D:103:GLU:O	2.38	0.57
10:L:134:SER:HA	10:L:137:PHE:HB3	1.86	0.57
13:B:802:CLA:H202	13:B:803:CLA:HBB	1.87	0.57
1:A:392:THR:HG22	1:A:607:LEU:HD22	1.87	0.57
2:B:618:TYR:OH	2:B:624:ARG:NH2	2.37	0.57
13:B:833:CLA:H121	16:I:101:BCR:H21C	1.87	0.57
1:A:501:ASN:ND2	13:A:818:CLA:OBD	2.38	0.57
1:A:564:PRO:HB3	4:D:120:PRO:HB3	1.87	0.56
1:A:554:VAL:HG21	16:A:850:BCR:HC31	1.86	0.56
3:C:11:CYS:HB2	15:C:102:SF4:S3	2.45	0.56
7:I:25:LEU:HD13	16:L:205:BCR:HC8	1.86	0.56
2:B:724:TYR:HB2	13:B:802:CLA:HED3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:801:CLA:H111	13:B:832:CLA:H71	1.88	0.56
2:B:679:GLU:HG2	3:C:81:TYR:HE2	1.71	0.55
13:B:833:CLA:H112	16:I:101:BCR:H19C	1.88	0.55
1:A:70:SER:HB3	1:A:349:TRP:HE1	1.72	0.55
1:A:282:LEU:HD12	1:A:515:VAL:HG11	1.89	0.55
1:A:727:VAL:O	1:A:731:HIS:ND1	2.36	0.55
1:A:76:ALA:HB1	13:A:806:CLA:HBB1	1.89	0.54
13:A:812:CLA:H141	16:J:102:BCR:H272	1.88	0.54
13:A:813:CLA:HBB2	13:A:821:CLA:H13	1.88	0.54
4:D:160:ILE:HG12	4:D:173:HIS:HB3	1.90	0.54
1:A:735:GLY:O	1:A:739:THR:OG1	2.26	0.54
2:B:708:ALA:HA	2:B:711:VAL:HB	1.90	0.54
1:A:561:ARG:O	4:D:138:ARG:NH1	2.37	0.54
13:B:830:CLA:HBC2	16:J:104:BCR:HC7	1.90	0.54
1:A:128:ASN:O	6:F:53:ARG:NH2	2.40	0.53
2:B:177:HIS:HB3	13:B:813:CLA:HBB1	1.91	0.53
2:B:725:ALA:HB2	13:B:821:CLA:HBB1	1.91	0.53
2:B:389:HIS:HA	2:B:392:ILE:HD12	1.89	0.53
13:A:841:CLA:HHC	13:A:841:CLA:HBB1	1.90	0.53
10:L:86:LEU:HD21	16:L:201:BCR:H10C	1.91	0.53
1:A:396:TRP:HB3	13:A:829:CLA:HMC3	1.90	0.53
1:A:388:LEU:HD13	1:A:748:ILE:HG21	1.90	0.53
1:A:538:ILE:HG23	12:A:801:CL0:H67	1.91	0.53
3:C:16:GLN:NE2	3:C:57:ALA:O	2.42	0.53
1:A:686:PHE:HA	14:A:845:PQN:H9	1.91	0.52
16:A:847:BCR:H382	16:K:202:BCR:HC8	1.91	0.52
2:B:91:ILE:HB	2:B:112:PRO:HB2	1.91	0.52
2:B:240:ALA:HA	2:B:263:PRO:HG3	1.91	0.52
2:B:652:MET:HA	2:B:655:PHE:HB3	1.91	0.52
1:A:32:PRO:HB3	13:A:804:CLA:HAC1	1.90	0.52
13:A:802:CLA:H101	13:B:804:CLA:H121	1.91	0.52
10:L:67:GLY:O	10:L:70:ARG:NH1	2.41	0.52
1:A:520:LYS:NZ	1:A:752:GLY:O	2.43	0.52
2:B:142:LEU:HD21	16:B:835:BCR:H24C	1.91	0.52
2:B:470:SER:OG	2:B:479:ASN:ND2	2.42	0.52
3:C:19:ARG:HH21	4:D:181:GLU:HB2	1.74	0.52
13:B:808:CLA:H93	16:M:101:BCR:H353	1.91	0.52
5:E:9:ARG:NH1	6:F:180:GLU:OE2	2.43	0.52
4:D:120:PRO:HD3	4:D:145:LEU:HD13	1.91	0.52
2:B:528:LEU:HD21	13:B:803:CLA:HBB1	1.90	0.51
13:B:807:CLA:HAB	13:B:822:CLA:HMC2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:30:GLY:O	10:L:34:ASN:ND2	2.43	0.51
13:A:840:CLA:H61	13:A:840:CLA:H142	1.92	0.51
1:A:691:ARG:NH2	2:B:569:GLY:O	2.41	0.51
13:A:809:CLA:HBB2	13:A:829:CLA:H192	1.92	0.51
2:B:65:LEU:HD11	16:B:835:BCR:H271	1.91	0.51
4:D:138:ARG:HB2	4:D:141:GLN:HG3	1.91	0.51
1:A:118:VAL:O	1:A:128:ASN:ND2	2.38	0.51
13:B:804:CLA:H202	13:B:833:CLA:H122	1.92	0.51
1:A:345:PHE:HE1	16:A:849:BCR:H312	1.75	0.51
1:A:349:TRP:HB3	13:A:806:CLA:HAC1	1.93	0.51
13:A:826:CLA:HBA1	13:A:830:CLA:H193	1.93	0.51
1:A:463:ARG:HE	1:A:642:THR:HG21	1.75	0.51
13:A:805:CLA:HBB1	13:A:812:CLA:H121	1.93	0.51
1:A:715:GLN:NE2	5:E:16:TYR:OH	2.43	0.51
2:B:456:GLU:HG3	6:F:30:LEU:HD11	1.92	0.50
2:B:429:LEU:HD11	13:B:830:CLA:HMB2	1.93	0.50
13:B:807:CLA:H2	13:B:807:CLA:HED3	1.94	0.50
1:A:364:SER:OG	1:A:394:HIS:O	2.29	0.50
2:B:22:TRP:CG	2:B:707:GLN:HE22	2.29	0.50
2:B:343:VAL:HG13	13:B:819:CLA:HED1	1.93	0.50
4:D:78:THR:OG1	4:D:79:LEU:N	2.41	0.50
1:A:59:PHE:O	1:A:63:THR:OG1	2.29	0.50
16:A:851:BCR:H282	16:F:201:BCR:H14C	1.92	0.50
2:B:530:LEU:HD12	13:B:831:CLA:HED3	1.94	0.50
2:B:646:LEU:HA	2:B:649:TRP:HD1	1.77	0.50
2:B:577:ASP:HA	2:B:580:TYR:HB3	1.94	0.50
1:A:422:ASN:OD1	1:A:425:ASN:ND2	2.44	0.50
1:A:578:PRO:HD3	2:B:564:GLY:HA2	1.93	0.50
13:A:843:CLA:HAB	16:A:851:BCR:H16C	1.94	0.50
1:A:623:THR:HG23	1:A:625:ASP:H	1.76	0.49
2:B:666:PHE:HA	14:B:834:PQN:H9	1.93	0.49
2:B:698:ASP:OD1	2:B:698:ASP:N	2.38	0.49
10:L:91:THR:HG21	10:L:128:LEU:HD13	1.93	0.49
1:A:326:TYR:OH	13:A:825:CLA:OBD	2.26	0.49
1:A:620:GLY:HA3	1:A:630:HIS:HA	1.95	0.49
2:B:459:PHE:HE1	13:B:830:CLA:H43	1.78	0.49
3:C:75:ARG:NH2	4:D:168:GLU:OE1	2.46	0.49
1:A:333:PHE:O	1:A:429:ARG:NH2	2.46	0.49
2:B:51:PHE:O	2:B:149:SER:OG	2.28	0.49
2:B:686:GLU:O	2:B:692:ASN:ND2	2.46	0.49
13:A:831:CLA:H91	17:A:852:LHG:H312	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:THR:HB	1:A:426:LEU:HD11	1.94	0.48
2:B:626:TYR:HH	2:B:724:TYR:HH	1.61	0.48
10:L:44:PRO:HA	10:L:47:ARG:HG2	1.95	0.48
13:A:833:CLA:H43	2:B:689:PRO:HG2	1.95	0.48
10:L:107:LYS:HA	10:L:116:SER:HB3	1.94	0.48
1:A:426:LEU:HB3	13:A:825:CLA:HBC2	1.94	0.48
1:A:703:TRP:HH2	13:B:824:CLA:HED3	1.79	0.48
2:B:122:GLN:HG3	2:B:361:LEU:HD13	1.96	0.48
2:B:126:THR:HG21	2:B:359:ALA:H	1.78	0.48
10:L:137:PHE:HB2	16:L:206:BCR:H321	1.95	0.48
1:A:322:MET:HA	1:A:325:MET:HE3	1.94	0.48
1:A:16:VAL:HG22	1:A:187:LYS:HG3	1.95	0.48
1:A:89:SER:HB3	1:A:166:ALA:HB3	1.96	0.48
2:B:469:LYS:NZ	2:B:512:PHE:O	2.36	0.48
1:A:585:GLN:HG3	2:B:670:TRP:HB2	1.96	0.48
2:B:224:PRO:HG2	2:B:232:VAL:HG11	1.94	0.48
3:C:17:CYS:CB	15:C:102:SF4:S4	2.83	0.48
10:L:43:THR:HG22	10:L:46:LEU:HG	1.96	0.48
13:B:801:CLA:H61	13:B:801:CLA:H41	1.62	0.48
4:D:149:LEU:HB3	4:D:155:ILE:HG13	1.95	0.48
2:B:224:PRO:HA	2:B:227:THR:HG22	1.96	0.48
1:A:410:ALA:HB1	1:A:588:ALA:HB1	1.95	0.47
1:A:611:SER:O	1:A:615:GLN:NE2	2.47	0.47
2:B:3:THR:OG1	2:B:4:LYS:N	2.44	0.47
1:A:388:LEU:HD22	1:A:748:ILE:HD13	1.96	0.47
1:A:434:ARG:HA	1:A:437:ILE:HD12	1.95	0.47
13:A:828:CLA:HED1	13:A:836:CLA:HAB	1.96	0.47
2:B:159:PRO:HA	2:B:162:ARG:HD2	1.96	0.47
13:A:843:CLA:H143	14:A:845:PQN:H292	1.96	0.47
1:A:377:TYR:HD1	1:A:380:LEU:HD22	1.79	0.47
16:K:202:BCR:H20C	16:K:202:BCR:H361	1.76	0.47
13:A:809:CLA:HMB2	16:J:102:BCR:H20C	1.96	0.47
13:B:804:CLA:H142	16:I:101:BCR:H393	1.95	0.47
13:B:825:CLA:H62	13:B:825:CLA:H2	1.64	0.47
14:B:834:PQN:H142	16:B:837:BCR:H271	1.95	0.47
1:A:501:ASN:HB2	13:A:837:CLA:HED3	1.96	0.47
1:A:680:TRP:HZ3	13:B:803:CLA:HMD3	1.80	0.47
13:A:818:CLA:CHD	13:A:819:CLA:HBB2	2.45	0.47
2:B:4:LYS:HE3	2:B:7:LYS:HD3	1.97	0.47
16:I:101:BCR:H24C	16:I:101:BCR:H371	1.75	0.47
8:J:30:ARG:HD2	16:J:103:BCR:H312	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:MET:HE2	2:B:352:MET:HB3	1.82	0.47
6:F:102:TRP:HA	6:F:105:ALA:HB2	1.96	0.47
1:A:448:LEU:HB3	1:A:541:PHE:HB2	1.97	0.47
2:B:154:TRP:O	2:B:158:GLN:NE2	2.39	0.46
2:B:350:GLN:NE2	2:B:372:TYR:OH	2.48	0.46
2:B:690:LEU:HB2	16:L:201:BCR:H282	1.97	0.46
13:B:808:CLA:HAA1	7:I:10:VAL:HG12	1.96	0.46
4:D:118:GLU:H	4:D:148:GLN:HE22	1.62	0.46
13:L:204:CLA:H62	13:L:204:CLA:H41	1.72	0.46
1:A:197:MET:HB2	13:A:814:CLA:HBC2	1.97	0.46
2:B:185:THR:O	2:B:189:ALA:N	2.44	0.46
1:A:397:ILE:HD12	13:A:830:CLA:HBB1	1.96	0.46
1:A:457:ILE:HG22	13:A:835:CLA:HBC2	1.96	0.46
2:B:658:LEU:O	2:B:662:THR:OG1	2.32	0.46
10:L:108:SER:OG	10:L:109:LYS:N	2.44	0.46
13:A:822:CLA:H8	16:A:850:BCR:H12C	1.97	0.46
13:A:831:CLA:H203	13:A:831:CLA:H161	1.82	0.46
6:F:111:PRO:HA	6:F:114:LEU:HB3	1.98	0.46
13:A:822:CLA:H91	13:A:822:CLA:H111	1.72	0.46
2:B:424:TRP:O	2:B:428:PHE:N	2.43	0.46
1:A:393:HIS:HE1	13:A:829:CLA:ND	2.10	0.46
13:B:832:CLA:H72	13:B:833:CLA:H141	1.98	0.46
4:D:128:ARG:H	4:D:132:ASN:ND2	2.13	0.46
13:A:809:CLA:H2	16:J:102:BCR:H403	1.98	0.46
2:B:399:ASP:N	2:B:399:ASP:OD1	2.47	0.46
1:A:350:HIS:HD2	1:A:408:HIS:HD1	1.63	0.46
13:A:829:CLA:H62	13:A:829:CLA:H41	1.69	0.46
13:A:844:CLA:H3A	13:A:844:CLA:HBA2	1.68	0.46
2:B:436:LEU:O	2:B:440:ASN:ND2	2.49	0.46
2:B:550:MET:HE2	2:B:563:ASP:HB2	1.98	0.46
13:B:820:CLA:H161	16:B:836:BCR:H17C	1.98	0.46
13:A:819:CLA:HBA2	13:A:819:CLA:H3A	1.78	0.46
13:B:809:CLA:HBA2	13:B:809:CLA:H141	1.97	0.46
13:B:816:CLA:H3A	13:B:816:CLA:HBA2	1.74	0.46
13:B:827:CLA:HHC	13:B:827:CLA:HBB1	1.98	0.46
1:A:558:ARG:HA	1:A:567:ALA:HB2	1.98	0.45
1:A:708:LEU:HD21	13:B:824:CLA:H3A	1.97	0.45
13:A:829:CLA:H112	13:A:829:CLA:H152	1.70	0.45
13:L:202:CLA:H3A	13:L:202:CLA:HBA2	1.69	0.45
13:B:808:CLA:HMB3	13:B:809:CLA:HBB	1.98	0.45
1:A:276:LEU:HD21	1:A:299:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:VAL:HG21	2:B:586:MET:HG2	1.99	0.45
2:B:622:TRP:HB3	13:B:802:CLA:H101	1.98	0.45
4:D:206:LEU:HD22	4:D:211:GLN:HB3	1.99	0.45
16:L:205:BCR:H15C	16:L:205:BCR:H351	1.85	0.45
2:B:384:VAL:HG22	2:B:537:LEU:HD11	1.98	0.45
16:F:202:BCR:H20C	16:F:202:BCR:H361	1.85	0.45
1:A:647:LEU:HD23	2:B:635:ILE:HD11	1.99	0.45
13:A:807:CLA:H151	13:A:830:CLA:HBB2	1.98	0.45
2:B:66:PHE:HZ	11:M:7:ILE:HG23	1.82	0.45
2:B:419:ILE:O	2:B:423:SER:N	2.47	0.45
13:B:832:CLA:H151	13:B:832:CLA:H112	1.83	0.45
13:A:840:CLA:HHC	13:A:840:CLA:HBB1	1.99	0.45
2:B:142:LEU:HD23	2:B:145:LEU:HD12	1.98	0.45
14:B:834:PQN:H301	18:B:838:LMG:H201	1.99	0.45
1:A:114:SER:HB2	1:A:131:VAL:HG21	1.98	0.45
1:A:397:ILE:HG21	13:A:830:CLA:HHC	1.99	0.45
2:B:61:THR:HG21	13:B:822:CLA:H42	1.98	0.45
2:B:444:GLN:OE1	2:B:452:GLN:NE2	2.50	0.45
13:B:824:CLA:HMB2	16:F:202:BCR:HC8	1.99	0.45
16:L:201:BCR:H20C	16:L:201:BCR:H361	1.81	0.45
13:A:833:CLA:H41	13:A:833:CLA:H61	1.66	0.45
2:B:450:GLU:HA	6:F:93:LEU:HD22	1.98	0.45
2:B:703:LEU:HB3	2:B:707:GLN:HG2	1.98	0.45
3:C:55:GLU:OE1	3:C:66:ARG:NH1	2.50	0.45
1:A:682:PHE:HZ	13:A:843:CLA:HBC2	1.81	0.44
13:A:806:CLA:H41	13:A:830:CLA:H143	1.99	0.44
2:B:136:TYR:HE1	11:M:10:ALA:HB2	1.82	0.44
2:B:194:ILE:HA	2:B:198:ALA:HB3	1.99	0.44
2:B:236:ASN:OD1	2:B:236:ASN:N	2.51	0.44
4:D:79:LEU:HD11	4:D:106:SER:HB2	1.98	0.44
4:D:113:SER:HB3	4:D:115:THR:HG22	1.99	0.44
2:B:347:LEU:HD23	13:B:818:CLA:H52	2.00	0.44
13:B:806:CLA:HBA1	13:B:806:CLA:H3A	1.66	0.44
13:B:820:CLA:H203	13:B:820:CLA:H162	1.89	0.44
1:A:672:MET:HE3	1:A:672:MET:HB3	1.80	0.44
13:B:809:CLA:H122	13:B:821:CLA:H122	1.99	0.44
16:A:851:BCR:H342	16:A:851:BCR:H331	2.00	0.44
2:B:673:TYR:OH	13:B:804:CLA:OBD	2.34	0.44
10:L:62:PRO:HB3	13:L:204:CLA:HBB1	2.00	0.44
1:A:438:ILE:O	1:A:442:ASN:N	2.49	0.44
13:B:822:CLA:H3A	13:B:822:CLA:HBA2	1.77	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:822:CLA:H142	13:B:822:CLA:H112	1.86	0.44
13:A:805:CLA:HBA2	13:A:812:CLA:H62	1.99	0.44
2:B:377:TYR:CD1	13:B:821:CLA:HAB	2.53	0.44
13:B:804:CLA:H141	13:B:804:CLA:H161	1.85	0.44
8:J:11:PRO:O	8:J:15:THR:OG1	2.34	0.44
13:A:812:CLA:H111	13:A:812:CLA:H72	1.82	0.44
2:B:210:ASP:N	2:B:210:ASP:OD1	2.48	0.44
13:B:811:CLA:H162	13:B:811:CLA:H122	1.69	0.44
10:L:67:GLY:H	10:L:70:ARG:HD3	1.82	0.44
13:A:832:CLA:HED2	10:L:18:LEU:HD12	2.00	0.44
1:A:370:HIS:ND1	13:A:819:CLA:OBD	2.51	0.44
13:A:823:CLA:H3A	13:A:823:CLA:HBA2	1.66	0.44
13:A:823:CLA:H152	13:A:823:CLA:H111	1.88	0.44
2:B:451:LYS:HB3	13:B:826:CLA:HED1	2.00	0.44
13:B:809:CLA:H2	13:B:809:CLA:H62	1.78	0.44
1:A:330:LYS:HB3	1:A:337:GLY:HA3	2.00	0.43
13:A:821:CLA:H142	13:A:821:CLA:H111	1.89	0.43
2:B:324:ASP:O	2:B:328:ASN:ND2	2.51	0.43
2:B:703:LEU:N	14:B:834:PQN:O4	2.44	0.43
13:B:833:CLA:H91	13:B:833:CLA:H111	1.74	0.43
13:A:809:CLA:H43	13:A:829:CLA:HMD2	1.99	0.43
2:B:92:SER:O	2:B:92:SER:OG	2.35	0.43
13:B:818:CLA:HBA2	13:B:818:CLA:H3A	1.79	0.43
3:C:11:CYS:CB	15:C:102:SF4:S3	3.00	0.43
5:E:43:VAL:HB	5:E:47:ASN:HA	2.01	0.43
1:A:681:ALA:HB3	13:A:803:CLA:HBB2	2.00	0.43
13:B:807:CLA:H72	13:B:807:CLA:H111	1.55	0.43
13:B:823:CLA:H41	13:B:823:CLA:H61	1.61	0.43
13:A:822:CLA:H61	16:A:850:BCR:H14C	2.01	0.43
16:A:847:BCR:H20C	16:A:847:BCR:H361	1.89	0.43
3:C:58:CYS:HA	3:C:59:PRO:HD3	1.91	0.43
1:A:183:LYS:HA	1:A:183:LYS:HD3	1.84	0.43
1:A:644:ASN:HD22	2:B:654:LEU:HD11	1.83	0.43
2:B:157:LEU:HD13	11:M:27:GLU:HG3	2.00	0.43
2:B:522:VAL:HG11	2:B:596:TYR:HB2	2.00	0.43
13:B:804:CLA:H202	13:B:833:CLA:H102	2.00	0.43
13:B:807:CLA:H143	13:B:822:CLA:HBB2	2.00	0.43
4:D:103:GLU:OE2	4:D:105:TYR:OH	2.29	0.43
6:F:86:LEU:HD21	8:J:37:VAL:HG11	1.99	0.43
1:A:721:ILE:HD11	2:B:569:GLY:HA3	2.01	0.43
1:A:741:TRP:NE1	13:A:829:CLA:O1A	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:835:CLA:H192	13:A:835:CLA:H161	1.88	0.43
3:C:55:GLU:HB3	3:C:63:LEU:HD22	2.01	0.43
6:F:58:GLU:O	6:F:61:SER:OG	2.32	0.43
16:J:102:BCR:H15C	16:J:102:BCR:H351	1.87	0.43
13:A:806:CLA:HBA1	13:A:806:CLA:H3A	1.67	0.43
13:A:809:CLA:H3A	13:A:809:CLA:HBA2	1.56	0.43
2:B:730:ALA:O	2:B:734:SER:OG	2.31	0.43
13:B:825:CLA:H61	16:F:202:BCR:HC32	2.00	0.43
13:B:833:CLA:HBA2	14:B:834:PQN:H251	2.00	0.43
4:D:151:ASP:O	4:D:154:LYS:NZ	2.46	0.43
1:A:98:PHE:HB3	1:A:117:VAL:HG23	2.00	0.42
2:B:480:ASN:HB3	2:B:483:SER:HB2	2.01	0.42
13:B:823:CLA:H161	13:B:823:CLA:H192	1.85	0.42
5:E:44:ASN:OD1	5:E:44:ASN:N	2.52	0.42
6:F:99:ASP:OD1	6:F:99:ASP:N	2.50	0.42
1:A:651:LEU:HD11	12:A:801:CL0:H43	2.00	0.42
13:A:807:CLA:HBB2	16:A:848:BCR:H272	2.00	0.42
13:A:820:CLA:H102	13:A:820:CLA:H61	1.80	0.42
2:B:129:MET:O	2:B:130:ARG:NH1	2.47	0.42
2:B:659:ILE:HD12	13:B:833:CLA:HMB3	2.01	0.42
9:K:143:LEU:HB2	16:K:202:BCR:H24C	2.01	0.42
16:A:847:BCR:H362	16:A:848:BCR:H10C	2.01	0.42
3:C:81:TYR:HB3	4:D:96:LEU:HD11	2.02	0.42
5:E:17:TRP:NE1	5:E:42:LYS:O	2.51	0.42
10:L:35:LEU:HD23	10:L:35:LEU:HA	1.93	0.42
14:A:845:PQN:H161	16:F:201:BCR:H382	2.01	0.42
13:B:810:CLA:H141	13:B:810:CLA:H162	1.93	0.42
13:A:815:CLA:HBA1	13:A:815:CLA:H3A	1.96	0.42
6:F:124:TRP:HE3	16:F:202:BCR:HC21	1.85	0.42
9:K:100:MET:HE2	9:K:100:MET:HB2	1.93	0.42
10:L:94:LEU:HB3	10:L:124:VAL:HG22	2.02	0.42
13:B:809:CLA:H71	13:B:809:CLA:HBB1	2.02	0.42
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.94	0.42
2:B:341:LEU:HD21	13:B:806:CLA:H51	2.02	0.42
8:J:28:ILE:HD13	8:J:28:ILE:HA	1.94	0.42
1:A:487:VAL:HA	1:A:490:VAL:HG22	2.02	0.42
13:A:809:CLA:H72	13:A:829:CLA:H92	2.02	0.42
2:B:579:PHE:HE1	13:B:823:CLA:HAC2	1.85	0.42
13:B:802:CLA:H41	13:B:802:CLA:H61	1.75	0.42
4:D:198:GLY:N	5:E:14:GLU:OE1	2.52	0.42
1:A:121:ILE:O	1:A:123:GLY:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HD22	16:A:847:BCR:H361	2.02	0.41
1:A:706:ASN:HB3	6:F:181:ILE:HG23	2.01	0.41
13:A:834:CLA:H2	13:B:833:CLA:H18	2.02	0.41
16:B:836:BCR:H24C	16:B:836:BCR:H371	1.81	0.41
16:A:848:BCR:H361	16:A:848:BCR:H20C	1.83	0.41
2:B:51:PHE:CE2	13:B:812:CLA:HBB1	2.54	0.41
2:B:612:PHE:O	2:B:616:SER:OG	2.26	0.41
1:A:57:HIS:HB3	13:A:806:CLA:HAB	2.01	0.41
16:A:847:BCR:H15C	16:A:847:BCR:H351	1.91	0.41
2:B:467:HIS:CE1	13:B:827:CLA:NB	2.87	0.41
16:B:835:BCR:H20C	16:B:835:BCR:H361	1.85	0.41
1:A:664:SER:O	1:A:667:SER:OG	2.29	0.41
2:B:731:SER:O	2:B:735:LYS:NZ	2.40	0.41
13:B:824:CLA:H42	16:F:202:BCR:H353	2.02	0.41
7:I:32:ASP:OD1	7:I:32:ASP:N	2.52	0.41
13:J:101:CLA:HMC1	16:J:103:BCR:H11C	2.03	0.41
1:A:484:ALA:HA	13:A:838:CLA:HBA1	2.02	0.41
6:F:111:PRO:HB3	16:J:104:BCR:H362	2.03	0.41
13:A:840:CLA:H143	13:A:840:CLA:H203	2.01	0.41
13:B:801:CLA:H143	13:B:801:CLA:H161	1.90	0.41
3:C:11:CYS:HB3	3:C:39:ILE:HG13	2.01	0.41
1:A:693:TYR:CE1	2:B:539:LYS:HD2	2.56	0.41
13:B:804:CLA:H203	13:B:804:CLA:H162	1.80	0.41
1:A:112:LYS:HB2	1:A:131:VAL:HG22	2.02	0.41
1:A:140:ILE:HA	13:A:809:CLA:HMD2	2.02	0.41
2:B:592:TRP:CD1	13:B:802:CLA:H151	2.56	0.41
13:B:817:CLA:H93	13:B:817:CLA:H62	1.80	0.41
1:A:441:LEU:HG	1:A:548:LEU:HB2	2.02	0.41
1:A:443:TRP:NE1	13:A:834:CLA:OBD	2.48	0.41
13:A:840:CLA:H142	13:A:840:CLA:H111	1.84	0.41
13:A:840:CLA:H18	13:A:840:CLA:H151	1.83	0.41
2:B:548:LYS:NZ	5:E:15:SER:O	2.49	0.41
6:F:73:LYS:HE2	8:J:33:PRO:HG3	2.02	0.41
1:A:375:PRO:HA	1:A:376:PRO:HD3	1.89	0.41
1:A:685:MET:O	1:A:689:SER:OG	2.28	0.41
13:B:803:CLA:H201	16:J:102:BCR:H362	2.03	0.41
1:A:515:VAL:HG13	1:A:522:ALA:HB3	2.03	0.40
1:A:615:GLN:HB3	1:A:632:THR:HG23	2.03	0.40
13:B:833:CLA:H121	16:I:101:BCR:H19C	2.02	0.40
13:A:828:CLA:H203	13:A:836:CLA:H62	2.02	0.40
11:M:8:PHE:HD1	16:M:101:BCR:H401	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:TRP:HH2	16:B:835:BCR:H16C	1.87	0.40
13:J:101:CLA:HBB1	13:J:101:CLA:HHC	2.02	0.40
10:L:84:VAL:HB	10:L:135:VAL:HG11	2.01	0.40
16:M:101:BCR:H21C	16:M:101:BCR:H24C	1.87	0.40
1:A:56:VAL:HG11	13:A:805:CLA:HMD2	2.02	0.40
13:A:833:CLA:H122	13:A:833:CLA:H8	1.92	0.40
13:B:820:CLA:H72	13:B:820:CLA:H111	1.91	0.40
13:A:835:CLA:H142	13:A:835:CLA:H112	1.98	0.40
2:B:477:LEU:HD23	2:B:477:LEU:HA	1.94	0.40
13:B:811:CLA:H152	10:L:88:VAL:HG21	2.04	0.40
13:L:203:CLA:H142	13:L:203:CLA:H112	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/752 (98%)	692 (94%)	44 (6%)	1 (0%)	48	75
2	B	702/737 (95%)	670 (95%)	32 (5%)	0	100	100
3	C	78/81 (96%)	75 (96%)	2 (3%)	1 (1%)	9	35
4	D	137/220 (62%)	110 (80%)	25 (18%)	2 (2%)	8	32
5	E	60/70 (86%)	53 (88%)	7 (12%)	0	100	100
6	F	159/186 (86%)	153 (96%)	5 (3%)	1 (1%)	21	52
7	I	28/35 (80%)	27 (96%)	1 (4%)	0	100	100
8	J	35/40 (88%)	34 (97%)	1 (3%)	0	100	100
9	K	55/157 (35%)	53 (96%)	2 (4%)	0	100	100
10	L	129/146 (88%)	116 (90%)	13 (10%)	0	100	100
11	M	27/31 (87%)	27 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2147/2455 (88%)	2010 (94%)	132 (6%)	5 (0%)	44 71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
3	C	63	LEU
4	D	126	ILE
4	D	165	PRO
6	F	100	GLY

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%)	593 (99%)	5 (1%)	73 79
2	B	574/596 (96%)	572 (100%)	2 (0%)	86 86
3	C	67/68 (98%)	65 (97%)	2 (3%)	36 61
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%)	131 (98%)	2 (2%)	57 72
7	I	27/31 (87%)	27 (100%)	0	100 100
8	J	32/35 (91%)	32 (100%)	0	100 100
9	K	40/103 (39%)	40 (100%)	0	100 100
10	L	99/111 (89%)	99 (100%)	0	100 100
11	M	21/23 (91%)	21 (100%)	0	100 100
All	All	1763/1969 (90%)	1752 (99%)	11 (1%)	76 81

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL

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Mol	Chain	Res	Type
1	A	121	ILE
1	A	232	VAL
1	A	253	LEU
1	A	740	THR
2	B	256	THR
2	B	634	LEU
3	C	23	THR
3	C	63	LEU
6	F	27	VAL
6	F	145	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	192	GLN
1	A	225	ASN
1	A	350	HIS
1	A	356	ASN
1	A	442	ASN
1	A	505	ASN
1	A	615	GLN
1	A	621	ASN
1	A	715	GLN
1	A	723	GLN
2	B	98	GLN
2	B	127	GLN
2	B	132	ASN
2	B	262	HIS
2	B	350	GLN
2	B	403	ASN
2	B	440	ASN
2	B	479	ASN
2	B	606	GLN
2	B	613	ASN
2	B	636	ASN
2	B	644	ASN
3	C	16	GLN
4	D	173	HIS
5	E	3	GLN
6	F	83	ASN
6	F	131	GLN

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Mol	Chain	Res	Type
8	J	29	ASN
9	K	120	GLN
10	L	24	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

111 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	$\# Z > 2$
13	CLA	A	842	-	55,59,73	2.24	20 (36%)	64,96,113	3.07	33 (51%)
16	BCR	A	848	-	41,41,41	1.07	2 (4%)	56,56,56	1.51	12 (21%)
13	CLA	A	823	-	69,73,73	1.97	19 (27%)	82,113,113	2.66	30 (36%)
13	CLA	A	836	1	58,62,73	2.14	19 (32%)	68,99,113	2.84	30 (44%)
16	BCR	F	201	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	6 (10%)
13	CLA	B	823	-	69,73,73	2.00	18 (26%)	82,113,113	2.69	31 (37%)
13	CLA	B	825	-	69,73,73	1.93	18 (26%)	82,113,113	2.80	33 (40%)
13	CLA	B	817	-	63,67,73	2.10	18 (28%)	74,105,113	2.77	29 (39%)
13	CLA	A	807	-	69,73,73	1.96	19 (27%)	82,113,113	2.74	33 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	806	-	69,73,73	1.91	19 (27%)	82,113,113	2.76	36 (43%)
13	CLA	B	807	-	69,73,73	1.97	19 (27%)	82,113,113	2.65	31 (37%)
13	CLA	K	201	-	45,49,73	2.33	17 (37%)	54,83,113	3.06	26 (48%)
13	CLA	F	203	6	49,53,73	2.40	20 (40%)	58,89,113	3.02	28 (48%)
13	CLA	A	832	-	54,58,73	2.24	18 (33%)	64,95,113	2.94	33 (51%)
13	CLA	B	813	-	69,73,73	2.00	20 (28%)	82,113,113	2.67	31 (37%)
16	BCR	J	102	-	41,41,41	1.14	3 (7%)	56,56,56	1.30	8 (14%)
13	CLA	B	801	-	69,73,73	1.97	21 (30%)	82,113,113	2.56	33 (40%)
13	CLA	B	808	-	69,73,73	1.97	19 (27%)	82,113,113	2.69	32 (39%)
16	BCR	A	851	-	41,41,41	1.13	4 (9%)	56,56,56	1.29	7 (12%)
13	CLA	A	837	1	49,53,73	2.39	20 (40%)	58,89,113	3.16	28 (48%)
13	CLA	B	831	-	51,55,73	2.28	22 (43%)	60,91,113	3.07	28 (46%)
13	CLA	B	828	-	49,53,73	2.40	20 (40%)	58,89,113	3.17	30 (51%)
16	BCR	J	104	-	41,41,41	1.10	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	B	811	-	69,73,73	2.00	20 (28%)	82,113,113	2.64	31 (37%)
13	CLA	B	805	2	58,62,73	2.15	17 (29%)	68,99,113	2.94	32 (47%)
13	CLA	A	815	-	49,53,73	2.38	20 (40%)	58,89,113	3.04	32 (55%)
13	CLA	B	819	-	50,54,73	2.37	21 (42%)	59,90,113	3.06	29 (49%)
13	CLA	A	827	-	59,63,73	2.12	20 (33%)	70,101,113	2.95	33 (47%)
16	BCR	B	837	-	41,41,41	1.21	4 (9%)	56,56,56	1.24	7 (12%)
13	CLA	A	841	-	69,73,73	2.01	22 (31%)	82,113,113	2.61	32 (39%)
13	CLA	A	813	-	58,62,73	2.15	19 (32%)	68,99,113	2.84	31 (45%)
16	BCR	L	206	-	41,41,41	1.05	2 (4%)	56,56,56	1.39	8 (14%)
16	BCR	I	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.30	5 (8%)
13	CLA	A	824	-	55,59,73	2.22	22 (40%)	64,96,113	2.96	30 (46%)
15	SF4	C	101	3	0,12,12	-	-	-	-	-
13	CLA	A	829	-	69,73,73	1.96	21 (30%)	82,113,113	2.72	32 (39%)
14	PQN	A	845	-	34,34,34	1.55	2 (5%)	43,45,45	1.13	4 (9%)
13	CLA	A	803	-	49,53,73	2.36	18 (36%)	58,89,113	2.98	28 (48%)
13	CLA	B	826	-	62,66,73	2.12	19 (30%)	73,104,113	2.89	33 (45%)
12	CL0	A	801	-	58,73,73	3.01	18 (31%)	60,113,113	2.79	19 (31%)
13	CLA	J	101	8	49,53,73	2.40	21 (42%)	58,89,113	3.04	28 (48%)
13	CLA	A	812	-	69,73,73	1.99	19 (27%)	82,113,113	2.68	31 (37%)
13	CLA	A	821	-	65,69,73	2.02	19 (29%)	77,108,113	2.76	31 (40%)
13	CLA	B	815	-	49,53,73	2.37	19 (38%)	58,89,113	3.08	27 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	814	-	49,53,73	2.38	19 (38%)	58,89,113	2.96	29 (50%)
13	CLA	B	812	-	49,53,73	2.38	19 (38%)	58,89,113	3.06	30 (51%)
13	CLA	A	810	1	49,53,73	2.32	19 (38%)	58,89,113	2.99	30 (51%)
13	CLA	A	818	-	69,73,73	1.96	20 (28%)	82,113,113	2.70	27 (32%)
13	CLA	A	817	-	53,57,73	2.27	19 (35%)	61,93,113	2.93	28 (45%)
13	CLA	A	839	-	60,64,73	2.10	19 (31%)	71,102,113	2.86	30 (42%)
13	CLA	B	818	-	64,68,73	2.05	17 (26%)	76,107,113	2.74	32 (42%)
13	CLA	B	827	-	49,53,73	2.41	21 (42%)	58,89,113	3.04	30 (51%)
16	BCR	B	835	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	5 (8%)
13	CLA	A	825	-	51,55,73	2.34	20 (39%)	60,91,113	3.00	29 (48%)
13	CLA	L	204	-	56,60,73	2.22	19 (33%)	65,97,113	2.98	30 (46%)
13	CLA	A	822	-	69,73,73	1.98	21 (30%)	82,113,113	2.60	29 (35%)
16	BCR	K	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.35	9 (16%)
13	CLA	B	803	-	69,73,73	1.92	21 (30%)	82,113,113	2.80	32 (39%)
16	BCR	M	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	7 (12%)
13	CLA	A	834	-	69,73,73	1.98	19 (27%)	82,113,113	2.68	33 (40%)
13	CLA	A	819	-	58,62,73	2.17	21 (36%)	68,99,113	2.86	34 (50%)
17	LHG	A	853	13	26,26,48	0.86	1 (3%)	29,32,54	1.32	3 (10%)
13	CLA	B	802	-	69,73,73	1.90	18 (26%)	82,113,113	2.84	36 (43%)
16	BCR	F	202	-	41,41,41	1.11	2 (4%)	56,56,56	1.27	7 (12%)
16	BCR	B	836	-	41,41,41	1.12	3 (7%)	56,56,56	1.39	8 (14%)
17	LHG	A	852	-	48,48,48	0.74	1 (2%)	51,54,54	1.32	7 (13%)
13	CLA	A	816	-	49,53,73	2.37	19 (38%)	58,89,113	3.09	26 (44%)
13	CLA	B	824	-	53,57,73	2.29	19 (35%)	61,93,113	3.17	29 (47%)
13	CLA	A	820	-	69,73,73	2.01	18 (26%)	82,113,113	2.63	33 (40%)
14	PQN	B	834	-	34,34,34	1.47	2 (5%)	43,45,45	1.19	6 (13%)
13	CLA	A	826	-	69,73,73	1.92	19 (27%)	82,113,113	2.53	29 (35%)
13	CLA	A	835	-	69,73,73	1.95	20 (28%)	82,113,113	2.81	32 (39%)
13	CLA	A	828	-	69,73,73	1.94	18 (26%)	82,113,113	2.67	31 (37%)
13	CLA	B	814	-	60,64,73	2.12	21 (35%)	71,102,113	2.82	31 (43%)
13	CLA	A	805	-	49,53,73	2.37	19 (38%)	58,89,113	3.08	29 (50%)
16	BCR	L	201	-	41,41,41	1.20	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	B	810	2	69,73,73	1.96	17 (24%)	82,113,113	2.57	30 (36%)
16	BCR	A	847	-	41,41,41	1.14	3 (7%)	56,56,56	1.36	9 (16%)
13	CLA	A	831	-	69,73,73	1.96	19 (27%)	82,113,113	2.70	29 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	844	17	56,60,73	2.21	19 (33%)	65,97,113	3.02	28 (43%)
15	SF4	A	846	2,1	0,12,12	-	-	-		
13	CLA	B	829	-	50,54,73	2.30	19 (38%)	59,90,113	3.05	30 (50%)
13	CLA	B	816	-	59,63,73	2.15	20 (33%)	70,101,113	2.89	30 (42%)
13	CLA	A	840	-	69,73,73	1.96	20 (28%)	82,113,113	2.73	33 (40%)
13	CLA	B	821	-	69,73,73	1.94	20 (28%)	82,113,113	2.69	35 (42%)
16	BCR	A	850	-	41,41,41	1.19	2 (4%)	56,56,56	1.38	6 (10%)
13	CLA	B	809	-	69,73,73	1.95	18 (26%)	82,113,113	2.68	33 (40%)
16	BCR	A	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.34	8 (14%)
13	CLA	A	838	-	55,59,73	2.20	18 (32%)	64,96,113	2.99	31 (48%)
16	BCR	L	205	-	41,41,41	1.15	3 (7%)	56,56,56	1.31	6 (10%)
18	LMG	B	838	-	55,55,55	0.80	1 (1%)	63,63,63	1.42	8 (12%)
13	CLA	B	832	-	69,73,73	2.01	20 (28%)	82,113,113	2.65	31 (37%)
13	CLA	B	822	-	69,73,73	1.97	18 (26%)	82,113,113	2.60	31 (37%)
13	CLA	A	833	-	69,73,73	1.98	19 (27%)	82,113,113	2.65	31 (37%)
13	CLA	L	203	-	69,73,73	1.95	18 (26%)	82,113,113	2.72	29 (35%)
13	CLA	B	820	-	69,73,73	1.99	21 (30%)	82,113,113	2.66	31 (37%)
13	CLA	B	833	-	69,73,73	1.98	18 (26%)	82,113,113	2.62	31 (37%)
13	CLA	K	203	-	49,53,73	2.34	21 (42%)	58,89,113	3.03	30 (51%)
13	CLA	A	830	-	69,73,73	1.95	20 (28%)	82,113,113	2.54	34 (41%)
13	CLA	A	809	1	69,73,73	1.98	20 (28%)	82,113,113	2.63	31 (37%)
13	CLA	A	802	-	69,73,73	1.94	20 (28%)	82,113,113	2.79	34 (41%)
13	CLA	B	804	-	69,73,73	1.94	19 (27%)	82,113,113	2.62	30 (36%)
13	CLA	B	806	-	69,73,73	1.97	19 (27%)	82,113,113	2.63	30 (36%)
13	CLA	B	830	-	69,73,73	1.97	18 (26%)	82,113,113	2.70	32 (39%)
13	CLA	A	804	-	49,53,73	2.34	18 (36%)	58,89,113	3.07	30 (51%)
13	CLA	A	808	-	55,59,73	2.28	20 (36%)	64,96,113	2.91	32 (50%)
15	SF4	C	102	3	0,12,12	-	-	-		
13	CLA	A	811	-	49,53,73	2.36	19 (38%)	58,89,113	3.05	27 (46%)
13	CLA	L	202	10	50,54,73	2.38	20 (40%)	59,90,113	3.12	27 (45%)
16	BCR	J	103	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	10 (17%)
13	CLA	A	843	-	69,73,73	1.99	20 (28%)	82,113,113	2.62	30 (36%)

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
13	CLA	A	842	-	1/1/12/20	8/23/99/115	-
16	BCR	A	848	-	-	8/29/63/63	0/2/2/2
13	CLA	A	823	-	-	16/39/115/115	-
13	CLA	A	836	1	-	11/26/102/115	-
16	BCR	F	201	-	-	12/29/63/63	0/2/2/2
13	CLA	B	823	-	1/1/15/20	16/39/115/115	-
13	CLA	B	825	-	1/1/15/20	12/39/115/115	-
13	CLA	B	817	-	1/1/13/20	15/32/108/115	-
13	CLA	A	807	-	1/1/15/20	13/39/115/115	-
13	CLA	A	806	-	1/1/15/20	13/39/115/115	-
13	CLA	B	807	-	1/1/15/20	11/39/115/115	-
13	CLA	K	201	-	1/1/9/20	3/9/81/115	-
13	CLA	F	203	6	1/1/11/20	4/15/91/115	-
13	CLA	A	832	-	-	7/21/97/115	-
13	CLA	B	813	-	1/1/15/20	19/39/115/115	-
16	BCR	J	102	-	-	13/29/63/63	0/2/2/2
13	CLA	B	801	-	1/1/15/20	11/39/115/115	-
13	CLA	B	808	-	1/1/15/20	9/39/115/115	-
16	BCR	A	851	-	-	19/29/63/63	0/2/2/2
13	CLA	A	837	1	1/1/11/20	8/15/91/115	-
13	CLA	B	831	-	1/1/11/20	4/18/94/115	-
13	CLA	B	828	-	1/1/11/20	4/15/91/115	-
16	BCR	J	104	-	-	9/29/63/63	0/2/2/2
13	CLA	B	811	-	1/1/15/20	12/39/115/115	-
13	CLA	B	805	2	1/1/12/20	11/26/102/115	-
13	CLA	A	815	-	1/1/11/20	6/15/91/115	-
13	CLA	B	819	-	1/1/11/20	6/17/93/115	-
13	CLA	A	827	-	1/1/13/20	8/27/103/115	-
16	BCR	B	837	-	-	9/29/63/63	0/2/2/2
13	CLA	A	841	-	1/1/15/20	10/39/115/115	-
13	CLA	A	813	-	1/1/12/20	7/26/102/115	-
16	BCR	L	206	-	-	18/29/63/63	0/2/2/2
16	BCR	I	101	-	-	7/29/63/63	0/2/2/2
13	CLA	A	824	-	-	11/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SF4	C	101	3	-	-	0/6/5/5
13	CLA	A	829	-	1/1/15/20	14/39/115/115	-
14	PQN	A	845	-	-	2/23/43/43	0/2/2/2
13	CLA	A	803	-	1/1/11/20	3/15/91/115	-
13	CLA	B	826	-	1/1/13/20	14/31/107/115	-
12	CL0	A	801	-	2/2/20/25	6/37/135/135	-
13	CLA	J	101	8	1/1/11/20	7/15/91/115	-
13	CLA	A	812	-	1/1/15/20	11/39/115/115	-
13	CLA	A	821	-	1/1/14/20	8/35/111/115	-
13	CLA	B	815	-	1/1/11/20	8/15/91/115	-
13	CLA	A	814	-	1/1/11/20	11/15/91/115	-
13	CLA	B	812	-	1/1/11/20	2/15/91/115	-
13	CLA	A	810	1	1/1/11/20	4/15/91/115	-
13	CLA	A	818	-	-	12/39/115/115	-
13	CLA	A	817	-	-	2/20/96/115	-
13	CLA	A	839	-	1/1/13/20	8/29/105/115	-
13	CLA	B	818	-	1/1/14/20	5/33/109/115	-
13	CLA	B	827	-	-	2/15/91/115	-
16	BCR	B	835	-	-	10/29/63/63	0/2/2/2
13	CLA	A	825	-	1/1/11/20	5/18/94/115	-
13	CLA	L	204	-	1/1/12/20	9/24/100/115	-
13	CLA	A	822	-	1/1/15/20	12/39/115/115	-
16	BCR	K	202	-	-	7/29/63/63	0/2/2/2
13	CLA	B	803	-	1/1/15/20	11/39/115/115	-
16	BCR	M	101	-	-	15/29/63/63	0/2/2/2
13	CLA	A	834	-	1/1/15/20	15/39/115/115	-
13	CLA	A	819	-	1/1/12/20	10/26/102/115	-
17	LHG	A	853	13	-	12/31/31/53	-
13	CLA	B	802	-	1/1/15/20	16/39/115/115	-
16	BCR	F	202	-	-	13/29/63/63	0/2/2/2
16	BCR	B	836	-	-	11/29/63/63	0/2/2/2
17	LHG	A	852	-	-	17/53/53/53	-
13	CLA	A	816	-	-	8/15/91/115	-
13	CLA	B	824	-	-	11/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	820	-	1/1/15/20	12/39/115/115	-
14	PQN	B	834	-	-	9/23/43/43	0/2/2/2
13	CLA	A	826	-	1/1/15/20	16/39/115/115	-
13	CLA	A	835	-	1/1/15/20	16/39/115/115	-
13	CLA	A	828	-	1/1/15/20	13/39/115/115	-
13	CLA	B	814	-	1/1/13/20	7/29/105/115	-
13	CLA	A	805	-	1/1/11/20	4/15/91/115	-
16	BCR	L	201	-	-	9/29/63/63	0/2/2/2
13	CLA	B	810	2	1/1/15/20	11/39/115/115	-
16	BCR	A	847	-	-	11/29/63/63	0/2/2/2
13	CLA	A	831	-	1/1/15/20	10/39/115/115	-
13	CLA	A	844	17	1/1/12/20	12/24/100/115	-
15	SF4	A	846	2,1	-	-	0/6/5/5
13	CLA	B	829	-	1/1/11/20	8/17/93/115	-
13	CLA	B	816	-	1/1/13/20	7/27/103/115	-
13	CLA	A	840	-	1/1/15/20	15/39/115/115	-
13	CLA	B	821	-	1/1/15/20	17/39/115/115	-
16	BCR	A	850	-	-	14/29/63/63	0/2/2/2
13	CLA	B	809	-	1/1/15/20	9/39/115/115	-
16	BCR	A	849	-	-	10/29/63/63	0/2/2/2
13	CLA	A	838	-	1/1/12/20	7/23/99/115	-
16	BCR	L	205	-	-	11/29/63/63	0/2/2/2
18	LMG	B	838	-	-	27/50/70/70	0/1/1/1
13	CLA	B	832	-	-	9/39/115/115	-
13	CLA	B	822	-	1/1/15/20	13/39/115/115	-
13	CLA	A	833	-	1/1/15/20	10/39/115/115	-
13	CLA	L	203	-	-	15/39/115/115	-
13	CLA	B	820	-	1/1/15/20	9/39/115/115	-
13	CLA	B	833	-	-	16/39/115/115	-
13	CLA	K	203	-	1/1/11/20	5/15/91/115	-
13	CLA	A	830	-	1/1/15/20	13/39/115/115	-
13	CLA	A	809	1	1/1/15/20	17/39/115/115	-
13	CLA	A	802	-	1/1/15/20	6/39/115/115	-
13	CLA	B	804	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	806	-	1/1/15/20	15/39/115/115	-
13	CLA	B	830	-	1/1/15/20	8/39/115/115	-
13	CLA	A	804	-	1/1/11/20	6/15/91/115	-
13	CLA	A	808	-	1/1/12/20	8/23/99/115	-
15	SF4	C	102	3	-	-	0/6/5/5
13	CLA	A	811	-	1/1/11/20	6/15/91/115	-
13	CLA	L	202	10	-	5/17/93/115	-
16	BCR	J	103	-	-	17/29/63/63	0/2/2/2
13	CLA	A	843	-	1/1/15/20	11/39/115/115	-

All (1681) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	801	CL0	C1A-CHA	9.26	1.50	1.40
12	A	801	CL0	C3B-C4B	8.20	1.49	1.41
12	A	801	CL0	C1B-C2B	8.13	1.48	1.39
14	A	845	PQN	C3-C2	7.51	1.48	1.35
14	B	834	PQN	C3-C2	7.10	1.47	1.35
12	A	801	CL0	C1D-C2D	5.63	1.45	1.39
12	A	801	CL0	C3B-C2B	5.60	1.48	1.40
13	L	202	CLA	C3C-C2C	5.57	1.48	1.36
12	A	801	CL0	C3A-C2A	-5.43	1.50	1.54
13	A	844	CLA	C3C-C2C	5.31	1.48	1.36
13	B	806	CLA	C3C-C2C	5.28	1.48	1.36
12	A	801	CL0	C3D-C2D	5.28	1.48	1.39
13	A	814	CLA	C3C-C2C	5.22	1.48	1.36
13	B	828	CLA	C3C-C2C	5.20	1.48	1.36
13	B	833	CLA	C3C-C2C	5.20	1.48	1.36
13	B	829	CLA	C3C-C2C	5.19	1.48	1.36
13	B	825	CLA	C3C-C2C	5.17	1.47	1.36
13	B	819	CLA	C3C-C2C	5.17	1.47	1.36
13	B	827	CLA	C3C-C2C	5.17	1.47	1.36
13	B	824	CLA	C3C-C2C	5.16	1.47	1.36
13	L	203	CLA	C3C-C2C	5.16	1.47	1.36
13	A	812	CLA	C3C-C2C	5.15	1.47	1.36
13	B	832	CLA	C3C-C2C	5.15	1.47	1.36
13	B	817	CLA	C3C-C2C	5.13	1.47	1.36
13	F	203	CLA	C3C-C2C	5.13	1.47	1.36
13	A	830	CLA	C3C-C2C	5.13	1.47	1.36
13	A	837	CLA	C3C-C2C	5.12	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	817	CLA	C3C-C2C	5.12	1.47	1.36
13	A	808	CLA	C3C-C2C	5.12	1.47	1.36
13	B	831	CLA	C3C-C2C	5.11	1.47	1.36
13	A	815	CLA	C3C-C2C	5.11	1.47	1.36
13	B	826	CLA	C3C-C2C	5.11	1.47	1.36
13	A	820	CLA	C3C-C2C	5.11	1.47	1.36
13	A	824	CLA	C3C-C2C	5.11	1.47	1.36
13	B	812	CLA	C3C-C2C	5.11	1.47	1.36
13	B	808	CLA	C3C-C2C	5.10	1.47	1.36
13	A	816	CLA	C3C-C2C	5.10	1.47	1.36
13	B	823	CLA	C3C-C2C	5.09	1.47	1.36
13	A	809	CLA	C3C-C2C	5.08	1.47	1.36
13	A	841	CLA	O2D-CGD	5.08	1.45	1.33
13	B	817	CLA	O2D-CGD	5.07	1.45	1.33
13	B	816	CLA	O2D-CGD	5.07	1.45	1.33
13	A	831	CLA	C3C-C2C	5.06	1.47	1.36
13	A	843	CLA	C3C-C2C	5.06	1.47	1.36
13	K	203	CLA	C3C-C2C	5.06	1.47	1.36
13	A	822	CLA	C3C-C2C	5.06	1.47	1.36
13	J	101	CLA	C3C-C2C	5.05	1.47	1.36
13	A	840	CLA	C3C-C2C	5.05	1.47	1.36
13	A	805	CLA	C3C-C2C	5.04	1.47	1.36
13	A	834	CLA	C3C-C2C	5.04	1.47	1.36
13	B	830	CLA	C3C-C2C	5.04	1.47	1.36
13	F	203	CLA	O2D-CGD	5.04	1.45	1.33
13	A	813	CLA	C3C-C2C	5.03	1.47	1.36
13	B	803	CLA	C3C-C2C	5.02	1.47	1.36
13	A	811	CLA	C3C-C2C	5.02	1.47	1.36
13	L	202	CLA	O2D-CGD	5.02	1.45	1.33
13	K	201	CLA	C3C-C2C	5.01	1.47	1.36
13	A	823	CLA	C3C-C2C	5.01	1.47	1.36
13	B	824	CLA	O2D-CGD	5.01	1.45	1.33
13	B	814	CLA	C3C-C2C	5.01	1.47	1.36
13	A	839	CLA	C3C-C2C	5.00	1.47	1.36
13	A	819	CLA	C3C-C2C	5.00	1.47	1.36
13	A	821	CLA	C3C-C2C	5.00	1.47	1.36
13	B	822	CLA	C3C-C2C	5.00	1.47	1.36
13	A	832	CLA	C3C-C2C	5.00	1.47	1.36
13	B	811	CLA	C3C-C2C	5.00	1.47	1.36
13	A	809	CLA	O2D-CGD	5.00	1.45	1.33
13	B	815	CLA	C3C-C2C	5.00	1.47	1.36
13	B	807	CLA	C3C-C2C	5.00	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	802	CLA	C3C-C2C	4.99	1.47	1.36
13	A	829	CLA	O2D-CGD	4.98	1.45	1.33
13	A	841	CLA	C3C-C2C	4.98	1.47	1.36
13	A	833	CLA	C3C-C2C	4.98	1.47	1.36
13	B	821	CLA	O2D-CGD	4.98	1.45	1.33
13	A	803	CLA	C1B-NB	-4.98	1.31	1.37
13	A	836	CLA	C3C-C2C	4.97	1.47	1.36
13	L	204	CLA	C3C-C2C	4.97	1.47	1.36
13	A	820	CLA	O2D-CGD	4.97	1.45	1.33
13	A	842	CLA	C3C-C2C	4.97	1.47	1.36
13	B	807	CLA	O2D-CGD	4.96	1.45	1.33
13	B	830	CLA	O2D-CGD	4.96	1.45	1.33
13	B	813	CLA	C3C-C2C	4.96	1.47	1.36
13	B	816	CLA	C3C-C2C	4.96	1.47	1.36
13	A	803	CLA	C3C-C2C	4.96	1.47	1.36
13	A	804	CLA	O2D-CGD	4.96	1.45	1.33
13	B	801	CLA	O2D-CGD	4.95	1.45	1.33
13	A	827	CLA	C3C-C2C	4.95	1.47	1.36
13	A	825	CLA	O2D-CGD	4.95	1.45	1.33
13	J	101	CLA	O2D-CGD	4.95	1.45	1.33
13	A	805	CLA	CHC-C1C	4.94	1.48	1.38
13	B	832	CLA	O2D-CGD	4.93	1.45	1.33
13	B	805	CLA	C3C-C2C	4.93	1.47	1.36
13	B	809	CLA	C3C-C2C	4.93	1.47	1.36
13	A	843	CLA	O2D-CGD	4.92	1.45	1.33
13	A	817	CLA	O2D-CGD	4.92	1.45	1.33
13	A	805	CLA	O2D-CGD	4.91	1.45	1.33
13	A	818	CLA	O2D-CGD	4.90	1.45	1.33
13	A	834	CLA	O2D-CGD	4.90	1.45	1.33
13	A	838	CLA	C3C-C2C	4.90	1.47	1.36
13	B	820	CLA	O2D-CGD	4.90	1.45	1.33
13	A	803	CLA	O2D-CGD	4.90	1.45	1.33
13	B	818	CLA	C3C-C2C	4.89	1.47	1.36
13	A	832	CLA	O2D-CGD	4.89	1.45	1.33
13	A	828	CLA	C3C-C2C	4.89	1.47	1.36
13	A	804	CLA	C3C-C2C	4.88	1.47	1.36
13	B	812	CLA	O2D-CGD	4.88	1.45	1.33
13	A	836	CLA	O2D-CGD	4.88	1.45	1.33
13	L	202	CLA	C1D-ND	4.87	1.44	1.37
13	B	827	CLA	C1D-ND	4.87	1.44	1.37
13	B	805	CLA	O2D-CGD	4.86	1.45	1.33
12	A	801	CL0	O2D-CGD	4.86	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	810	CLA	C3C-C2C	4.86	1.47	1.36
13	A	811	CLA	O2D-CGD	4.85	1.45	1.33
13	A	808	CLA	O2D-CGD	4.85	1.45	1.33
13	A	812	CLA	O2D-CGD	4.84	1.45	1.33
13	B	818	CLA	O2D-CGD	4.84	1.45	1.33
13	B	810	CLA	C3C-C2C	4.84	1.47	1.36
13	A	819	CLA	O2D-CGD	4.84	1.45	1.33
13	B	822	CLA	O2D-CGD	4.83	1.45	1.33
13	A	808	CLA	C1D-ND	4.83	1.44	1.37
13	A	826	CLA	O2D-CGD	4.83	1.45	1.33
13	B	804	CLA	C3C-C2C	4.83	1.47	1.36
13	A	837	CLA	O2D-CGD	4.82	1.45	1.33
13	A	824	CLA	O2D-CGD	4.82	1.45	1.33
13	A	835	CLA	C3C-C2C	4.82	1.47	1.36
13	A	807	CLA	C3C-C2C	4.82	1.47	1.36
13	B	819	CLA	O2D-CGD	4.81	1.45	1.33
13	B	815	CLA	O2D-CGD	4.81	1.45	1.33
13	A	844	CLA	O2D-CGD	4.81	1.45	1.33
13	A	813	CLA	O2D-CGD	4.80	1.45	1.33
13	A	818	CLA	C3C-C2C	4.80	1.47	1.36
13	B	820	CLA	C3C-C2C	4.80	1.47	1.36
13	B	806	CLA	O2D-CGD	4.80	1.45	1.33
13	A	821	CLA	O2D-CGD	4.77	1.45	1.33
13	J	101	CLA	C1D-ND	4.77	1.44	1.37
13	A	825	CLA	C3C-C2C	4.77	1.47	1.36
13	B	811	CLA	O2D-CGD	4.76	1.44	1.33
13	A	823	CLA	CHC-C1C	4.76	1.48	1.38
13	A	835	CLA	C1D-ND	4.76	1.44	1.37
13	B	831	CLA	O2D-CGD	4.76	1.44	1.33
13	A	822	CLA	O2D-CGD	4.75	1.44	1.33
13	B	825	CLA	CHC-C1C	4.75	1.48	1.38
13	B	826	CLA	O2D-CGD	4.74	1.44	1.33
13	K	203	CLA	O2D-CGD	4.73	1.44	1.33
13	B	828	CLA	CHC-C1C	4.73	1.48	1.38
13	B	815	CLA	C1D-ND	4.72	1.44	1.37
13	B	809	CLA	O2D-CGD	4.72	1.44	1.33
13	A	803	CLA	CHC-C1C	4.72	1.47	1.38
13	A	833	CLA	O2D-CGD	4.71	1.44	1.33
13	A	827	CLA	CHC-C1C	4.71	1.47	1.38
13	A	842	CLA	O2D-CGD	4.71	1.44	1.33
13	L	204	CLA	O2D-CGD	4.71	1.44	1.33
13	A	840	CLA	O2D-CGD	4.70	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	813	CLA	O2D-CGD	4.70	1.44	1.33
13	B	828	CLA	O2D-CGD	4.70	1.44	1.33
13	B	816	CLA	C1D-ND	4.70	1.44	1.37
13	A	839	CLA	O2D-CGD	4.69	1.44	1.33
13	B	821	CLA	C3C-C2C	4.69	1.46	1.36
13	A	825	CLA	C1D-ND	4.69	1.44	1.37
13	A	819	CLA	C1D-ND	4.69	1.44	1.37
13	A	816	CLA	C1D-ND	4.69	1.44	1.37
13	B	813	CLA	CHC-C1C	4.68	1.47	1.38
13	B	808	CLA	O2D-CGD	4.68	1.44	1.33
13	B	810	CLA	O2D-CGD	4.68	1.44	1.33
13	B	820	CLA	C1D-ND	4.68	1.44	1.37
13	A	817	CLA	C1D-ND	4.67	1.44	1.37
13	A	806	CLA	O2D-CGD	4.67	1.44	1.33
13	B	810	CLA	CHC-C1C	4.67	1.47	1.38
13	B	829	CLA	O2D-CGD	4.67	1.44	1.33
13	A	829	CLA	CHC-C1C	4.66	1.47	1.38
13	B	819	CLA	CHC-C1C	4.66	1.47	1.38
13	A	823	CLA	O2D-CGD	4.66	1.44	1.33
13	A	822	CLA	CHC-C1C	4.66	1.47	1.38
13	B	823	CLA	O2D-CGD	4.66	1.44	1.33
13	B	804	CLA	O2D-CGD	4.65	1.44	1.33
13	B	802	CLA	C3C-C2C	4.65	1.46	1.36
13	A	844	CLA	C1D-ND	4.65	1.44	1.37
13	B	828	CLA	C1D-ND	4.64	1.44	1.37
13	B	829	CLA	CHC-C1C	4.64	1.47	1.38
13	B	805	CLA	CHC-C1C	4.64	1.47	1.38
13	B	830	CLA	CHC-C1C	4.64	1.47	1.38
13	A	842	CLA	C1D-ND	4.63	1.43	1.37
13	B	827	CLA	O2D-CGD	4.63	1.44	1.33
13	B	801	CLA	C3C-C2C	4.63	1.46	1.36
13	K	201	CLA	C1D-ND	4.63	1.43	1.37
13	A	807	CLA	O2D-CGD	4.63	1.44	1.33
13	B	824	CLA	CHC-C1C	4.63	1.47	1.38
13	A	837	CLA	CHC-C1C	4.62	1.47	1.38
13	L	203	CLA	O2D-CGD	4.62	1.44	1.33
13	A	827	CLA	O2D-CGD	4.62	1.44	1.33
13	K	201	CLA	CHC-C1C	4.61	1.47	1.38
13	A	837	CLA	C1D-ND	4.61	1.43	1.37
13	F	203	CLA	C1D-ND	4.61	1.43	1.37
13	A	821	CLA	C1D-ND	4.61	1.43	1.37
13	B	832	CLA	C1D-ND	4.61	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	830	CLA	O2D-CGD	4.60	1.44	1.33
13	B	802	CLA	O2D-CGD	4.60	1.44	1.33
12	A	801	CL0	OBD-CAD	4.60	1.28	1.22
13	B	833	CLA	O2D-CGD	4.60	1.44	1.33
13	A	841	CLA	C1D-ND	4.60	1.43	1.37
13	A	816	CLA	O2D-CGD	4.60	1.44	1.33
13	B	814	CLA	O2D-CGD	4.59	1.44	1.33
13	A	804	CLA	C1D-ND	4.59	1.43	1.37
13	A	815	CLA	CHC-C1C	4.59	1.47	1.38
13	A	815	CLA	C1D-ND	4.59	1.43	1.37
13	B	821	CLA	CHC-C1C	4.58	1.47	1.38
13	L	204	CLA	C1D-ND	4.58	1.43	1.37
13	A	807	CLA	C1D-ND	4.58	1.43	1.37
13	F	203	CLA	O2A-CGA	4.58	1.45	1.30
13	A	808	CLA	CHD-C1D	4.58	1.47	1.38
13	A	837	CLA	O2A-CGA	4.57	1.45	1.30
13	A	806	CLA	C3C-C2C	4.57	1.46	1.36
13	A	816	CLA	O2A-CGA	4.57	1.45	1.30
13	A	814	CLA	CHC-C1C	4.57	1.47	1.38
13	A	815	CLA	O2D-CGD	4.56	1.44	1.33
13	B	817	CLA	CHC-C1C	4.56	1.47	1.38
13	A	828	CLA	C1D-ND	4.55	1.43	1.37
13	B	820	CLA	CHC-C1C	4.55	1.47	1.38
13	B	828	CLA	O2A-CGA	4.55	1.45	1.30
13	L	204	CLA	CHC-C1C	4.55	1.47	1.38
13	B	804	CLA	CHC-C1C	4.55	1.47	1.38
13	A	811	CLA	O2A-CGA	4.54	1.45	1.30
13	A	811	CLA	C1D-ND	4.54	1.43	1.37
13	J	101	CLA	O2A-CGA	4.54	1.45	1.30
13	A	807	CLA	CHC-C1C	4.54	1.47	1.38
13	B	812	CLA	C1D-ND	4.53	1.43	1.37
13	B	808	CLA	CHC-C1C	4.53	1.47	1.38
13	B	826	CLA	CHC-C1C	4.53	1.47	1.38
13	B	812	CLA	O2A-CGA	4.53	1.45	1.30
13	L	202	CLA	CHC-C1C	4.53	1.47	1.38
13	B	813	CLA	C1D-ND	4.53	1.43	1.37
13	A	812	CLA	C1D-ND	4.53	1.43	1.37
13	A	826	CLA	C3C-C2C	4.53	1.46	1.36
13	A	818	CLA	C1D-ND	4.53	1.43	1.37
13	B	827	CLA	CHC-C1C	4.52	1.47	1.38
13	B	815	CLA	O2A-CGA	4.52	1.45	1.30
13	B	825	CLA	O2D-CGD	4.52	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	826	CLA	CHC-C1C	4.52	1.47	1.38
13	B	827	CLA	O2A-CGA	4.52	1.45	1.30
13	A	805	CLA	O2A-CGA	4.52	1.45	1.30
13	B	817	CLA	C1D-ND	4.51	1.43	1.37
13	K	203	CLA	O2A-CGA	4.51	1.45	1.30
13	A	815	CLA	O2A-CGA	4.51	1.45	1.30
13	B	832	CLA	CHC-C1C	4.51	1.47	1.38
13	A	809	CLA	CHC-C1C	4.51	1.47	1.38
13	A	830	CLA	CHC-C1C	4.51	1.47	1.38
13	A	844	CLA	CHC-C1C	4.51	1.47	1.38
14	A	845	PQN	C10-C5	4.50	1.48	1.40
13	A	842	CLA	CHC-C1C	4.50	1.47	1.38
13	B	814	CLA	CHC-C1C	4.49	1.47	1.38
13	A	828	CLA	CHC-C1C	4.49	1.47	1.38
13	A	829	CLA	C3C-C2C	4.49	1.46	1.36
13	B	805	CLA	C1D-ND	4.48	1.43	1.37
13	B	806	CLA	C1D-ND	4.48	1.43	1.37
13	B	826	CLA	C1D-ND	4.48	1.43	1.37
13	B	818	CLA	C1D-ND	4.48	1.43	1.37
13	A	804	CLA	CHC-C1C	4.48	1.47	1.38
13	A	843	CLA	O2A-CGA	4.48	1.46	1.33
13	A	803	CLA	O2A-CGA	4.48	1.45	1.30
13	A	843	CLA	CHC-C1C	4.48	1.47	1.38
13	A	804	CLA	O2A-CGA	4.47	1.45	1.30
13	B	820	CLA	O2A-CGA	4.47	1.46	1.33
13	A	838	CLA	C1D-ND	4.47	1.43	1.37
13	K	201	CLA	O2A-CGA	4.47	1.45	1.30
13	B	831	CLA	CHC-C1C	4.47	1.47	1.38
13	A	808	CLA	CHC-C1C	4.47	1.47	1.38
13	A	810	CLA	O2D-CGD	4.47	1.44	1.33
13	F	203	CLA	CHC-C1C	4.47	1.47	1.38
13	A	820	CLA	CHD-C1D	4.47	1.47	1.38
13	A	843	CLA	C1D-ND	4.47	1.43	1.37
13	L	203	CLA	CHC-C1C	4.47	1.47	1.38
13	A	840	CLA	C1D-ND	4.46	1.43	1.37
13	B	831	CLA	C1D-ND	4.46	1.43	1.37
13	A	835	CLA	O2D-CGD	4.46	1.44	1.33
13	A	814	CLA	O2D-CGD	4.46	1.44	1.33
13	B	803	CLA	CHC-C1C	4.45	1.47	1.38
12	A	801	CL0	CHB-C1B	4.45	1.46	1.39
13	A	825	CLA	CHC-C1C	4.44	1.47	1.38
13	A	814	CLA	O2A-CGA	4.44	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	807	CLA	C1D-ND	4.44	1.43	1.37
12	A	801	CL0	CHC-C4B	4.44	1.46	1.39
13	A	812	CLA	CHC-C1C	4.44	1.47	1.38
13	B	829	CLA	C1D-ND	4.44	1.43	1.37
13	A	834	CLA	CHC-C1C	4.44	1.47	1.38
13	A	836	CLA	O2A-CGA	4.44	1.46	1.33
13	B	816	CLA	CHC-C1C	4.44	1.47	1.38
13	A	838	CLA	O2D-CGD	4.43	1.44	1.33
13	A	828	CLA	O2D-CGD	4.43	1.44	1.33
13	A	833	CLA	C1D-ND	4.43	1.43	1.37
13	J	101	CLA	CHC-C1C	4.43	1.47	1.38
13	A	818	CLA	O2A-CGA	4.42	1.46	1.33
13	B	823	CLA	CHD-C1D	4.42	1.47	1.38
13	A	810	CLA	O2A-CGA	4.42	1.45	1.30
13	A	838	CLA	CHC-C1C	4.42	1.47	1.38
13	B	812	CLA	CHC-C1C	4.42	1.47	1.38
13	B	803	CLA	O2D-CGD	4.41	1.44	1.33
13	A	844	CLA	O2A-CGA	4.41	1.46	1.33
13	K	201	CLA	CHD-C1D	4.40	1.47	1.38
13	A	831	CLA	C1B-NB	-4.40	1.32	1.37
13	B	822	CLA	CHC-C1C	4.40	1.47	1.38
13	B	814	CLA	C1D-ND	4.40	1.43	1.37
13	B	815	CLA	CHC-C1C	4.39	1.47	1.38
13	A	832	CLA	CHC-C1C	4.39	1.47	1.38
13	B	824	CLA	O2A-CGA	4.39	1.46	1.33
13	A	802	CLA	O2D-CGD	4.38	1.44	1.33
13	A	836	CLA	CHC-C1C	4.38	1.47	1.38
13	A	838	CLA	O2A-CGA	4.38	1.46	1.33
13	A	833	CLA	CHC-C1C	4.38	1.47	1.38
13	B	811	CLA	C1D-ND	4.37	1.43	1.37
13	A	825	CLA	CHD-C1D	4.37	1.47	1.38
13	B	824	CLA	C1D-ND	4.37	1.43	1.37
13	A	820	CLA	C1D-ND	4.36	1.43	1.37
13	A	832	CLA	CHD-C1D	4.36	1.46	1.38
13	A	840	CLA	CHC-C1C	4.36	1.47	1.38
13	B	812	CLA	CHD-C1D	4.36	1.46	1.38
13	K	203	CLA	C1D-ND	4.35	1.43	1.37
13	B	801	CLA	C1D-ND	4.35	1.43	1.37
13	A	834	CLA	C1D-ND	4.35	1.43	1.37
13	A	813	CLA	CHC-C1C	4.35	1.47	1.38
13	A	820	CLA	C1B-NB	-4.35	1.32	1.37
13	B	830	CLA	C1D-ND	4.34	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	818	CLA	CHC-C1C	4.34	1.47	1.38
13	A	814	CLA	C1D-ND	4.34	1.43	1.37
13	B	833	CLA	O2A-CGA	4.33	1.46	1.33
13	A	822	CLA	C1D-ND	4.32	1.43	1.37
13	A	839	CLA	CHC-C1C	4.32	1.47	1.38
13	A	823	CLA	O2A-CGA	4.32	1.45	1.33
13	A	819	CLA	O2A-CGA	4.31	1.45	1.33
13	A	835	CLA	CHC-C1C	4.31	1.47	1.38
13	B	811	CLA	CHC-C1C	4.31	1.47	1.38
13	A	831	CLA	O2D-CGD	4.31	1.43	1.33
13	B	822	CLA	O2A-CGA	4.31	1.45	1.33
13	A	806	CLA	CHC-C1C	4.30	1.47	1.38
13	A	805	CLA	C1D-ND	4.30	1.43	1.37
13	A	817	CLA	CHD-C1D	4.30	1.46	1.38
13	A	840	CLA	O2A-CGA	4.30	1.45	1.33
13	A	833	CLA	O2A-CGA	4.30	1.45	1.33
13	B	831	CLA	O2A-CGA	4.29	1.45	1.33
13	B	826	CLA	CHD-C1D	4.29	1.46	1.38
13	A	839	CLA	O2A-CGA	4.29	1.45	1.33
13	A	827	CLA	C1D-ND	4.29	1.43	1.37
13	B	808	CLA	C1D-ND	4.29	1.43	1.37
13	B	832	CLA	CHD-C1D	4.29	1.46	1.38
13	L	204	CLA	O2A-CGA	4.29	1.45	1.33
13	B	823	CLA	C1B-NB	-4.29	1.32	1.37
13	B	807	CLA	CHC-C1C	4.28	1.47	1.38
13	B	806	CLA	O2A-CGA	4.28	1.45	1.33
13	A	839	CLA	C1D-ND	4.28	1.43	1.37
13	A	816	CLA	CHC-C1C	4.28	1.47	1.38
13	A	813	CLA	O2A-CGA	4.27	1.45	1.33
13	A	841	CLA	CHC-C1C	4.27	1.47	1.38
13	L	203	CLA	O2A-CGA	4.27	1.45	1.33
13	B	809	CLA	CHC-C1C	4.27	1.47	1.38
13	A	811	CLA	CHD-C1D	4.26	1.46	1.38
13	A	837	CLA	CHD-C1D	4.26	1.46	1.38
13	A	832	CLA	C1D-ND	4.25	1.43	1.37
13	A	816	CLA	CHD-C1D	4.25	1.46	1.38
13	F	203	CLA	CHD-C1D	4.25	1.46	1.38
13	B	816	CLA	O2A-CGA	4.25	1.45	1.33
13	A	824	CLA	O2A-CGA	4.25	1.45	1.33
13	A	813	CLA	C1D-ND	4.25	1.43	1.37
13	L	203	CLA	C1D-ND	4.25	1.43	1.37
13	B	823	CLA	O2A-CGA	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	809	CLA	O2A-CGA	4.25	1.45	1.33
13	B	811	CLA	O2A-CGA	4.24	1.45	1.33
13	A	818	CLA	CHC-C1C	4.24	1.47	1.38
13	B	819	CLA	CHD-C1D	4.24	1.46	1.38
13	A	825	CLA	O2A-CGA	4.24	1.45	1.33
13	J	101	CLA	CHD-C1D	4.24	1.46	1.38
13	B	833	CLA	C1D-ND	4.24	1.43	1.37
13	B	805	CLA	O2A-CGA	4.24	1.45	1.33
13	K	203	CLA	CHC-C1C	4.24	1.47	1.38
13	B	801	CLA	CHC-C1C	4.23	1.47	1.38
13	A	830	CLA	O2A-CGA	4.23	1.45	1.33
13	B	810	CLA	C1D-ND	4.23	1.43	1.37
13	B	827	CLA	CHD-C1D	4.23	1.46	1.38
13	A	822	CLA	O2A-CGA	4.23	1.45	1.33
13	B	826	CLA	O2A-CGA	4.23	1.45	1.33
13	A	831	CLA	CHC-C1C	4.23	1.47	1.38
13	L	204	CLA	CHD-C1D	4.23	1.46	1.38
13	A	819	CLA	CHD-C1D	4.23	1.46	1.38
13	B	819	CLA	C1D-ND	4.23	1.43	1.37
13	B	823	CLA	C1D-ND	4.21	1.43	1.37
13	A	841	CLA	CHD-C1D	4.21	1.46	1.38
13	A	824	CLA	CHD-C1D	4.21	1.46	1.38
13	B	818	CLA	O2A-CGA	4.21	1.45	1.33
13	A	824	CLA	C1D-ND	4.21	1.43	1.37
13	A	841	CLA	O2A-CGA	4.21	1.45	1.33
13	B	814	CLA	O2A-CGA	4.21	1.45	1.33
13	A	814	CLA	CHD-C1D	4.21	1.46	1.38
13	B	816	CLA	CHD-C1D	4.21	1.46	1.38
13	A	811	CLA	CHC-C1C	4.21	1.46	1.38
13	B	821	CLA	O2A-CGA	4.20	1.45	1.33
13	A	802	CLA	C1B-NB	-4.20	1.32	1.37
13	A	824	CLA	CHC-C1C	4.20	1.46	1.38
13	A	832	CLA	O2A-CGA	4.20	1.45	1.33
13	B	801	CLA	O2A-CGA	4.20	1.45	1.33
13	B	807	CLA	C1B-NB	-4.20	1.32	1.37
13	A	817	CLA	CHC-C1C	4.19	1.46	1.38
13	A	821	CLA	O2A-CGA	4.19	1.45	1.33
13	A	810	CLA	C1D-ND	4.18	1.43	1.37
13	A	842	CLA	O2A-CGA	4.18	1.45	1.33
13	L	202	CLA	O2A-CGA	4.18	1.46	1.33
13	B	829	CLA	O2A-CGA	4.18	1.46	1.33
13	B	819	CLA	O2A-CGA	4.18	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	805	CLA	C1B-NB	-4.17	1.32	1.37
13	B	806	CLA	CHD-C1D	4.17	1.46	1.38
13	B	833	CLA	CHD-C1D	4.17	1.46	1.38
13	B	810	CLA	C1B-NB	-4.17	1.32	1.37
13	A	817	CLA	O2A-CGA	4.17	1.45	1.33
13	B	818	CLA	CHD-C1D	4.17	1.46	1.38
13	A	825	CLA	CHD-C4C	4.16	1.48	1.39
13	B	830	CLA	O2A-CGA	4.16	1.45	1.33
13	B	813	CLA	CHD-C1D	4.16	1.46	1.38
13	A	802	CLA	CHC-C1C	4.16	1.46	1.38
13	B	832	CLA	O2A-CGA	4.16	1.45	1.33
13	B	815	CLA	CHD-C1D	4.16	1.46	1.38
13	A	812	CLA	O2A-CGA	4.15	1.45	1.33
13	A	820	CLA	CHC-C1C	4.15	1.46	1.38
13	A	806	CLA	O2A-CGA	4.15	1.45	1.33
13	A	808	CLA	CHD-C4C	4.15	1.48	1.39
13	A	826	CLA	O2A-CGA	4.15	1.45	1.33
13	A	836	CLA	C1D-ND	4.15	1.43	1.37
13	A	815	CLA	CHD-C1D	4.15	1.46	1.38
13	B	809	CLA	C1D-ND	4.15	1.43	1.37
13	A	834	CLA	CHD-C1D	4.14	1.46	1.38
13	A	820	CLA	O2A-CGA	4.14	1.45	1.33
13	B	811	CLA	CHD-C1D	4.14	1.46	1.38
13	L	202	CLA	CHD-C1D	4.14	1.46	1.38
13	A	831	CLA	C1D-ND	4.13	1.43	1.37
13	B	817	CLA	CHD-C1D	4.13	1.46	1.38
13	B	805	CLA	CHD-C1D	4.13	1.46	1.38
13	B	828	CLA	CHD-C1D	4.13	1.46	1.38
13	B	802	CLA	CHC-C1C	4.13	1.46	1.38
13	A	829	CLA	C1D-ND	4.12	1.43	1.37
13	B	818	CLA	C1B-NB	-4.12	1.32	1.37
13	B	833	CLA	CHC-C1C	4.12	1.46	1.38
13	A	842	CLA	CHD-C1D	4.12	1.46	1.38
13	B	823	CLA	CHC-C1C	4.11	1.46	1.38
13	A	816	CLA	CHD-C4C	4.11	1.48	1.39
13	A	810	CLA	CHC-C1C	4.11	1.46	1.38
13	B	833	CLA	C1B-NB	-4.10	1.32	1.37
13	B	827	CLA	CHD-C4C	4.10	1.48	1.39
13	A	809	CLA	C1D-ND	4.10	1.43	1.37
13	B	808	CLA	O2A-CGA	4.10	1.45	1.33
14	B	834	PQN	C10-C5	4.10	1.47	1.40
13	B	801	CLA	CHD-C1D	4.10	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	201	CLA	CHD-C4C	4.09	1.48	1.39
13	A	810	CLA	CHD-C1D	4.08	1.46	1.38
13	B	832	CLA	CHD-C4C	4.08	1.48	1.39
13	B	822	CLA	CHD-C1D	4.08	1.46	1.38
13	F	203	CLA	CHD-C4C	4.08	1.48	1.39
13	A	827	CLA	O2A-CGA	4.08	1.45	1.33
13	A	831	CLA	O2A-CGA	4.08	1.45	1.33
13	B	806	CLA	CHC-C1C	4.08	1.46	1.38
13	A	821	CLA	CHC-C1C	4.08	1.46	1.38
13	B	817	CLA	O2A-CGA	4.08	1.45	1.33
13	A	809	CLA	O2A-CGA	4.07	1.45	1.33
13	A	812	CLA	CHD-C1D	4.07	1.46	1.38
13	A	808	CLA	O2A-CGA	4.07	1.45	1.33
13	B	825	CLA	C1D-ND	4.07	1.43	1.37
13	A	828	CLA	O2A-CGA	4.07	1.45	1.33
13	A	802	CLA	CHD-C1D	4.06	1.46	1.38
12	A	801	CL0	O2A-CGA	4.06	1.45	1.33
13	B	828	CLA	CHD-C4C	4.05	1.48	1.39
13	B	807	CLA	O2A-CGA	4.05	1.45	1.33
13	A	829	CLA	O2A-CGA	4.04	1.45	1.33
13	A	821	CLA	CHD-C1D	4.04	1.46	1.38
13	A	823	CLA	C1D-ND	4.04	1.43	1.37
13	B	819	CLA	CHD-C4C	4.04	1.48	1.39
13	A	813	CLA	CHD-C1D	4.04	1.46	1.38
13	B	803	CLA	O2A-CGA	4.04	1.45	1.33
13	B	824	CLA	CHD-C1D	4.04	1.46	1.38
13	A	833	CLA	CHD-C1D	4.04	1.46	1.38
13	B	802	CLA	O2A-CGA	4.03	1.45	1.33
13	B	830	CLA	CHD-C4C	4.03	1.48	1.39
13	A	806	CLA	C1D-ND	4.03	1.43	1.37
13	A	835	CLA	CHD-C1D	4.03	1.46	1.38
13	A	836	CLA	CHD-C1D	4.02	1.46	1.38
13	A	835	CLA	O2A-CGA	4.02	1.45	1.33
13	B	814	CLA	CHD-C1D	4.02	1.46	1.38
13	A	841	CLA	C1B-NB	-4.01	1.32	1.37
13	B	808	CLA	CHD-C1D	4.01	1.46	1.38
13	B	819	CLA	C1B-NB	-4.01	1.32	1.37
13	A	842	CLA	CHD-C4C	4.01	1.48	1.39
13	K	203	CLA	CHD-C1D	4.01	1.46	1.38
13	A	844	CLA	CHD-C1D	4.00	1.46	1.38
13	A	804	CLA	CHD-C1D	4.00	1.46	1.38
13	B	803	CLA	C1B-NB	-4.00	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	826	CLA	CHD-C4C	4.00	1.48	1.39
13	B	823	CLA	CHD-C4C	3.99	1.48	1.39
12	A	801	CL0	CHB-C4A	-3.99	1.33	1.38
13	B	804	CLA	O2A-CGA	3.99	1.45	1.33
13	A	843	CLA	CHD-C1D	3.99	1.46	1.38
13	A	839	CLA	C1B-NB	-3.98	1.32	1.37
13	A	819	CLA	CHC-C1C	3.98	1.46	1.38
13	B	809	CLA	C1B-NB	-3.98	1.32	1.37
13	A	832	CLA	CHD-C4C	3.98	1.48	1.39
13	B	810	CLA	CHD-C1D	3.98	1.46	1.38
13	B	822	CLA	C1D-ND	3.97	1.43	1.37
13	B	811	CLA	CHD-C4C	3.97	1.48	1.39
13	A	802	CLA	C1D-ND	3.96	1.43	1.37
13	A	817	CLA	CHD-C4C	3.96	1.48	1.39
13	A	813	CLA	C1B-NB	-3.96	1.32	1.37
13	L	204	CLA	CHD-C4C	3.96	1.48	1.39
13	B	813	CLA	O2A-CGA	3.95	1.44	1.33
13	A	820	CLA	C3D-C2D	3.95	1.49	1.39
13	B	825	CLA	O2A-CGA	3.95	1.44	1.33
13	A	826	CLA	C1D-ND	3.95	1.43	1.37
13	A	837	CLA	CHD-C4C	3.95	1.48	1.39
13	L	202	CLA	CHD-C4C	3.95	1.48	1.39
13	A	807	CLA	O2A-CGA	3.95	1.44	1.33
13	A	822	CLA	CHD-C1D	3.95	1.46	1.38
13	A	820	CLA	CHD-C4C	3.94	1.48	1.39
13	B	817	CLA	CHD-C4C	3.94	1.48	1.39
13	B	813	CLA	CHD-C4C	3.94	1.48	1.39
13	A	814	CLA	CHD-C4C	3.94	1.48	1.39
13	A	840	CLA	C1B-NB	-3.93	1.32	1.37
13	A	839	CLA	CHD-C1D	3.93	1.46	1.38
13	B	820	CLA	CHD-C1D	3.93	1.46	1.38
13	A	802	CLA	O2A-CGA	3.93	1.44	1.33
13	J	101	CLA	CHD-C4C	3.92	1.48	1.39
13	A	815	CLA	CHD-C4C	3.92	1.48	1.39
13	B	810	CLA	O2A-CGA	3.92	1.44	1.33
13	B	815	CLA	CHD-C4C	3.92	1.48	1.39
13	A	823	CLA	C1B-NB	-3.91	1.32	1.37
13	A	827	CLA	CHD-C1D	3.91	1.46	1.38
13	L	203	CLA	CHD-C4C	3.91	1.48	1.39
13	A	840	CLA	CHD-C1D	3.91	1.46	1.38
13	B	802	CLA	C1D-ND	3.91	1.43	1.37
13	B	816	CLA	CHD-C4C	3.91	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	804	CLA	C1B-NB	-3.91	1.32	1.37
13	B	824	CLA	CHD-C4C	3.91	1.48	1.39
13	B	809	CLA	CHD-C1D	3.90	1.46	1.38
13	A	834	CLA	O2A-CGA	3.90	1.44	1.33
13	A	805	CLA	CHD-C4C	3.90	1.48	1.39
13	A	843	CLA	CHD-C4C	3.90	1.48	1.39
13	A	805	CLA	CHD-C1D	3.89	1.46	1.38
13	A	830	CLA	C1D-ND	3.89	1.43	1.37
13	A	807	CLA	CHD-C1D	3.89	1.46	1.38
13	A	828	CLA	CHD-C1D	3.89	1.46	1.38
13	B	812	CLA	CHD-C4C	3.88	1.48	1.39
13	B	804	CLA	C1D-ND	3.88	1.43	1.37
13	A	827	CLA	CHD-C4C	3.88	1.48	1.39
13	B	803	CLA	C3D-C2D	3.88	1.49	1.39
13	A	812	CLA	CHD-C4C	3.88	1.48	1.39
13	A	825	CLA	C3D-C2D	3.88	1.49	1.39
13	A	828	CLA	C1B-NB	-3.88	1.32	1.37
13	A	827	CLA	C1B-NB	-3.88	1.32	1.37
13	A	818	CLA	CHD-C1D	3.88	1.46	1.38
13	A	838	CLA	C4B-NB	-3.87	1.32	1.37
13	B	804	CLA	C3D-C2D	3.87	1.49	1.39
13	A	841	CLA	CHD-C4C	3.87	1.48	1.39
13	B	825	CLA	CHD-C4C	3.87	1.48	1.39
13	A	809	CLA	CHD-C4C	3.87	1.48	1.39
13	A	807	CLA	C1B-NB	-3.87	1.32	1.37
13	A	833	CLA	C1B-NB	-3.87	1.32	1.37
13	B	831	CLA	CHD-C4C	3.87	1.48	1.39
13	J	101	CLA	C1B-NB	-3.86	1.32	1.37
13	A	811	CLA	CHD-C4C	3.85	1.48	1.39
13	A	838	CLA	CHD-C1D	3.85	1.45	1.38
13	B	822	CLA	C1B-NB	-3.85	1.32	1.37
13	B	825	CLA	CHC-C4B	3.85	1.48	1.39
13	A	836	CLA	C3D-C2D	3.84	1.49	1.39
13	A	813	CLA	CHD-C4C	3.84	1.47	1.39
13	B	814	CLA	CHD-C4C	3.84	1.47	1.39
13	A	809	CLA	CHD-C1D	3.84	1.45	1.38
13	B	805	CLA	CHD-C4C	3.83	1.47	1.39
13	A	803	CLA	CHD-C4C	3.83	1.47	1.39
13	A	826	CLA	C1B-NB	-3.83	1.32	1.37
13	A	802	CLA	C4B-NB	-3.83	1.32	1.37
13	A	821	CLA	C1B-NB	-3.83	1.32	1.37
13	A	831	CLA	CHD-C1D	3.83	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	814	CLA	C1B-NB	-3.82	1.32	1.37
13	A	809	CLA	C3D-C2D	3.82	1.49	1.39
13	B	806	CLA	CHD-C4C	3.82	1.47	1.39
13	A	830	CLA	CHD-C1D	3.82	1.45	1.38
13	A	844	CLA	CHD-C4C	3.82	1.47	1.39
13	B	821	CLA	C1D-ND	3.81	1.42	1.37
13	B	821	CLA	C1B-NB	-3.81	1.32	1.37
13	A	806	CLA	C1B-NB	-3.81	1.32	1.37
13	A	829	CLA	C1B-NB	-3.81	1.32	1.37
13	A	806	CLA	CHD-C1D	3.81	1.45	1.38
13	A	819	CLA	C1B-NB	-3.81	1.32	1.37
13	A	836	CLA	CHD-C4C	3.80	1.47	1.39
13	B	817	CLA	C3D-C2D	3.80	1.49	1.39
13	B	820	CLA	CHD-C4C	3.80	1.47	1.39
13	A	808	CLA	C1B-NB	-3.80	1.32	1.37
13	A	808	CLA	C3D-C2D	3.79	1.49	1.39
13	A	824	CLA	CHD-C4C	3.79	1.47	1.39
13	B	830	CLA	CHD-C1D	3.79	1.45	1.38
13	F	203	CLA	C3D-C2D	3.79	1.49	1.39
13	A	824	CLA	C1B-NB	-3.79	1.32	1.37
13	A	839	CLA	CHD-C4C	3.79	1.47	1.39
13	A	832	CLA	C1B-NB	-3.79	1.32	1.37
13	B	818	CLA	CHD-C4C	3.78	1.47	1.39
13	A	809	CLA	C1B-NB	-3.78	1.32	1.37
13	B	808	CLA	C3D-C2D	3.78	1.49	1.39
13	B	806	CLA	C1B-NB	-3.77	1.32	1.37
13	B	833	CLA	CHD-C4C	3.77	1.47	1.39
13	A	828	CLA	CHC-C4B	3.77	1.47	1.39
13	K	201	CLA	C3D-C2D	3.77	1.49	1.39
13	B	829	CLA	CHD-C4C	3.77	1.47	1.39
13	B	801	CLA	C3D-C2D	3.77	1.49	1.39
13	B	810	CLA	CHD-C4C	3.77	1.47	1.39
13	B	808	CLA	CHD-C4C	3.77	1.47	1.39
13	A	807	CLA	CHD-C4C	3.77	1.47	1.39
13	A	815	CLA	C1B-NB	-3.76	1.32	1.37
13	A	812	CLA	C1B-NB	-3.76	1.32	1.37
13	A	823	CLA	C3D-C2D	3.76	1.49	1.39
13	A	821	CLA	CHD-C4C	3.76	1.47	1.39
13	B	832	CLA	C1B-NB	-3.76	1.32	1.37
13	A	802	CLA	CHD-C4C	3.76	1.47	1.39
13	A	806	CLA	CHD-C4C	3.75	1.47	1.39
12	A	801	CL0	CHC-C1C	3.75	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	829	CLA	CHD-C1D	3.75	1.45	1.38
13	A	835	CLA	CHD-C4C	3.75	1.47	1.39
13	A	834	CLA	CHD-C4C	3.75	1.47	1.39
13	J	101	CLA	OBD-CAD	3.75	1.28	1.22
13	B	815	CLA	C3D-C2D	3.74	1.49	1.39
13	B	827	CLA	OBD-CAD	3.74	1.28	1.22
13	A	805	CLA	C3D-C2D	3.73	1.49	1.39
13	B	825	CLA	C1B-NB	-3.73	1.33	1.37
13	B	830	CLA	C1B-NB	-3.73	1.33	1.37
13	A	837	CLA	C3D-C2D	3.73	1.49	1.39
13	A	819	CLA	C4B-NB	-3.73	1.33	1.37
13	K	203	CLA	CHD-C4C	3.73	1.47	1.39
13	A	805	CLA	CHC-C4B	3.73	1.47	1.39
13	J	101	CLA	C3D-C2D	3.73	1.49	1.39
12	A	801	CL0	CHD-C4C	3.72	1.46	1.39
13	B	828	CLA	OBD-CAD	3.72	1.28	1.22
13	B	813	CLA	C3D-C2D	3.72	1.49	1.39
13	A	819	CLA	CHD-C4C	3.72	1.47	1.39
13	B	820	CLA	C1B-NB	-3.72	1.33	1.37
13	K	203	CLA	C1B-NB	-3.72	1.33	1.37
13	A	823	CLA	CHD-C1D	3.72	1.45	1.38
13	A	804	CLA	CHD-C4C	3.72	1.47	1.39
13	A	811	CLA	C1B-NB	-3.72	1.33	1.37
13	A	829	CLA	CHC-C4B	3.72	1.47	1.39
13	A	803	CLA	C3D-C2D	3.72	1.49	1.39
13	A	841	CLA	C3D-C2D	3.71	1.49	1.39
13	B	808	CLA	C1B-NB	-3.71	1.33	1.37
13	L	204	CLA	C3D-C2D	3.71	1.49	1.39
13	L	203	CLA	CHD-C1D	3.71	1.45	1.38
13	A	842	CLA	C3D-C2D	3.71	1.49	1.39
13	B	831	CLA	CHD-C1D	3.71	1.45	1.38
13	A	804	CLA	C1B-NB	-3.70	1.33	1.37
13	A	833	CLA	CHD-C4C	3.70	1.47	1.39
13	B	829	CLA	CHC-C4B	3.70	1.47	1.39
13	B	801	CLA	CHD-C4C	3.70	1.47	1.39
13	A	829	CLA	CHD-C1D	3.70	1.45	1.38
13	A	823	CLA	CHD-C4C	3.70	1.47	1.39
13	L	202	CLA	OBD-CAD	3.70	1.28	1.22
13	A	810	CLA	C1B-NB	-3.69	1.33	1.37
13	A	838	CLA	CHD-C4C	3.69	1.47	1.39
13	A	810	CLA	CHD-C4C	3.69	1.47	1.39
13	A	831	CLA	CHD-C4C	3.68	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	804	CLA	OBD-CAD	3.68	1.28	1.22
13	A	844	CLA	C3D-C2D	3.68	1.49	1.39
13	A	825	CLA	C1B-NB	-3.68	1.33	1.37
13	B	814	CLA	C1B-NB	-3.68	1.33	1.37
13	A	810	CLA	OBD-CAD	3.68	1.28	1.22
13	L	203	CLA	C3D-C2D	3.68	1.49	1.39
13	B	807	CLA	CHD-C1D	3.68	1.45	1.38
13	B	807	CLA	CHD-C4C	3.68	1.47	1.39
13	A	817	CLA	C3D-C2D	3.68	1.49	1.39
13	B	826	CLA	C1B-NB	-3.68	1.33	1.37
13	B	809	CLA	CHD-C4C	3.67	1.47	1.39
13	A	822	CLA	C1B-NB	-3.67	1.33	1.37
13	A	803	CLA	C4B-NB	-3.67	1.33	1.37
13	A	816	CLA	C1B-NB	-3.67	1.33	1.37
13	B	819	CLA	C4B-NB	-3.67	1.33	1.37
13	A	817	CLA	C1B-NB	-3.67	1.33	1.37
13	B	827	CLA	CHC-C4B	3.67	1.47	1.39
13	A	844	CLA	C1B-NB	-3.67	1.33	1.37
13	A	816	CLA	C3D-C2D	3.67	1.49	1.39
13	A	813	CLA	C3D-C2D	3.67	1.49	1.39
13	B	828	CLA	C3D-C2D	3.66	1.49	1.39
13	B	811	CLA	CHC-C4B	3.66	1.47	1.39
13	B	820	CLA	CHC-C4B	3.66	1.47	1.39
13	A	844	CLA	OBD-CAD	3.65	1.28	1.22
13	B	815	CLA	OBD-CAD	3.65	1.28	1.22
13	A	841	CLA	CHC-C4B	3.65	1.47	1.39
13	B	812	CLA	C3D-C2D	3.64	1.48	1.39
13	A	810	CLA	CHB-C1B	3.64	1.47	1.39
13	A	822	CLA	CHC-C4B	3.64	1.47	1.39
13	K	203	CLA	C3D-C2D	3.64	1.48	1.39
13	A	824	CLA	C3D-C2D	3.64	1.48	1.39
13	A	830	CLA	C1B-NB	-3.64	1.33	1.37
13	B	805	CLA	C3D-C2D	3.63	1.48	1.39
13	A	814	CLA	C3D-C2D	3.63	1.48	1.39
16	K	202	BCR	C1-C6	-3.63	1.49	1.53
13	B	822	CLA	CHD-C4C	3.63	1.47	1.39
13	A	835	CLA	C3D-C2D	3.63	1.48	1.39
13	A	837	CLA	C1B-NB	-3.63	1.33	1.37
13	A	829	CLA	CHD-C4C	3.63	1.47	1.39
13	A	815	CLA	C3D-C2D	3.63	1.48	1.39
13	A	842	CLA	CHC-C4B	3.63	1.47	1.39
13	B	810	CLA	C3D-C2D	3.63	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	816	CLA	C3D-C2D	3.63	1.48	1.39
13	B	826	CLA	C3D-C2D	3.63	1.48	1.39
13	B	812	CLA	C1B-NB	-3.62	1.33	1.37
13	A	818	CLA	C1B-NB	-3.62	1.33	1.37
13	B	817	CLA	C1B-NB	-3.62	1.33	1.37
13	A	815	CLA	OBD-CAD	3.62	1.28	1.22
13	B	806	CLA	C3D-C2D	3.62	1.48	1.39
13	A	837	CLA	CHC-C4B	3.61	1.47	1.39
13	B	805	CLA	OBD-CAD	3.61	1.28	1.22
13	A	804	CLA	C3D-C2D	3.61	1.48	1.39
13	A	830	CLA	CHD-C4C	3.61	1.47	1.39
13	A	834	CLA	C1B-NB	-3.61	1.33	1.37
13	B	827	CLA	C3D-C2D	3.61	1.48	1.39
13	B	832	CLA	C3D-C2D	3.61	1.48	1.39
13	A	838	CLA	CHB-C1B	3.61	1.47	1.39
13	B	812	CLA	OBD-CAD	3.61	1.28	1.22
13	B	803	CLA	C1D-ND	3.61	1.42	1.37
13	B	824	CLA	C1B-NB	-3.61	1.33	1.37
13	B	818	CLA	C3D-C2D	3.61	1.48	1.39
13	B	821	CLA	CHD-C4C	3.61	1.47	1.39
13	A	822	CLA	C3D-C2D	3.61	1.48	1.39
13	F	203	CLA	OBD-CAD	3.61	1.28	1.22
13	A	833	CLA	C3D-C2D	3.61	1.48	1.39
13	A	807	CLA	CHC-C4B	3.61	1.47	1.39
13	L	202	CLA	C3D-C2D	3.60	1.48	1.39
13	A	817	CLA	OBD-CAD	3.60	1.28	1.22
13	A	811	CLA	C3D-C2D	3.60	1.48	1.39
13	B	828	CLA	C1B-NB	-3.60	1.33	1.37
13	B	811	CLA	C1B-NB	-3.60	1.33	1.37
13	A	840	CLA	CHD-C4C	3.59	1.47	1.39
13	A	818	CLA	CHD-C4C	3.59	1.47	1.39
13	A	835	CLA	OBD-CAD	3.58	1.28	1.22
13	B	813	CLA	CHC-C4B	3.58	1.47	1.39
13	A	840	CLA	CHC-C4B	3.58	1.47	1.39
13	B	833	CLA	C3D-C2D	3.58	1.48	1.39
13	B	813	CLA	OBD-CAD	3.58	1.28	1.22
13	B	823	CLA	OBD-CAD	3.58	1.28	1.22
13	A	833	CLA	CHC-C4B	3.57	1.47	1.39
13	B	815	CLA	C1B-NB	-3.57	1.33	1.37
13	A	816	CLA	OBD-CAD	3.57	1.28	1.22
13	B	802	CLA	C1B-NB	-3.57	1.33	1.37
13	B	829	CLA	C1B-NB	-3.57	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	821	CLA	CHD-C1D	3.57	1.45	1.38
13	A	808	CLA	OBD-CAD	3.57	1.28	1.22
13	B	826	CLA	OBD-CAD	3.56	1.28	1.22
13	A	837	CLA	OBD-CAD	3.56	1.28	1.22
13	B	829	CLA	C3D-C2D	3.56	1.48	1.39
13	B	801	CLA	C1B-NB	-3.56	1.33	1.37
13	A	831	CLA	C4B-NB	-3.56	1.33	1.37
13	A	809	CLA	CHC-C4B	3.55	1.47	1.39
13	B	801	CLA	CHB-C1B	3.55	1.47	1.39
13	A	822	CLA	CHD-C4C	3.55	1.47	1.39
16	J	103	BCR	C30-C25	-3.55	1.49	1.53
13	B	824	CLA	C3D-C2D	3.55	1.48	1.39
13	A	827	CLA	CHC-C4B	3.55	1.47	1.39
13	B	804	CLA	C4B-NB	-3.55	1.33	1.37
13	A	843	CLA	C1B-NB	-3.55	1.33	1.37
13	L	202	CLA	CHC-C4B	3.55	1.47	1.39
13	B	823	CLA	C4B-NB	-3.55	1.33	1.37
13	A	836	CLA	C1B-NB	-3.54	1.33	1.37
13	A	803	CLA	CHC-C4B	3.54	1.47	1.39
13	A	814	CLA	C4B-NB	-3.54	1.33	1.37
13	A	842	CLA	OBD-CAD	3.54	1.28	1.22
13	B	809	CLA	C3D-C2D	3.54	1.48	1.39
13	A	812	CLA	C3D-C2D	3.54	1.48	1.39
13	A	832	CLA	C3D-C2D	3.54	1.48	1.39
13	A	826	CLA	CHD-C1D	3.54	1.45	1.38
13	L	204	CLA	OBD-CAD	3.54	1.28	1.22
13	B	804	CLA	CHD-C4C	3.54	1.47	1.39
13	A	830	CLA	CHC-C4B	3.54	1.47	1.39
13	A	823	CLA	CHC-C4B	3.54	1.47	1.39
13	J	101	CLA	CHC-C4B	3.54	1.47	1.39
16	B	837	BCR	C30-C25	-3.54	1.49	1.53
13	B	822	CLA	OBD-CAD	3.54	1.28	1.22
13	K	201	CLA	CHC-C4B	3.54	1.47	1.39
13	B	817	CLA	CHC-C4B	3.53	1.47	1.39
13	A	843	CLA	C3D-C2D	3.53	1.48	1.39
13	B	816	CLA	C1B-NB	-3.53	1.33	1.37
13	A	803	CLA	OBD-CAD	3.53	1.28	1.22
13	A	821	CLA	C3D-C2D	3.53	1.48	1.39
13	L	204	CLA	C1B-NB	-3.53	1.33	1.37
13	B	831	CLA	C1B-NB	-3.52	1.33	1.37
13	B	814	CLA	C3D-C2D	3.52	1.48	1.39
13	A	826	CLA	CHC-C4B	3.52	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	815	CLA	CHC-C4B	3.52	1.47	1.39
13	B	805	CLA	C1B-NB	-3.52	1.33	1.37
13	B	822	CLA	C3D-C2D	3.52	1.48	1.39
13	B	819	CLA	C3D-C2D	3.52	1.48	1.39
13	L	202	CLA	C1B-NB	-3.51	1.33	1.37
13	A	834	CLA	OBD-CAD	3.51	1.28	1.22
13	B	802	CLA	CHD-C1D	3.51	1.45	1.38
13	B	830	CLA	C3D-C2D	3.51	1.48	1.39
13	B	821	CLA	CHC-C4B	3.51	1.47	1.39
13	A	834	CLA	C3D-C2D	3.50	1.48	1.39
13	B	803	CLA	CHD-C1D	3.50	1.45	1.38
13	B	809	CLA	C4B-NB	-3.50	1.33	1.37
13	A	828	CLA	CHD-C4C	3.50	1.47	1.39
13	B	830	CLA	CHC-C4B	3.50	1.47	1.39
12	A	801	CL0	CHD-C1D	3.50	1.45	1.39
13	B	831	CLA	C3D-C2D	3.50	1.48	1.39
13	A	813	CLA	OBD-CAD	3.50	1.28	1.22
13	A	839	CLA	C3D-C2D	3.50	1.48	1.39
13	B	809	CLA	OBD-CAD	3.49	1.28	1.22
13	F	203	CLA	CHC-C4B	3.49	1.47	1.39
13	B	814	CLA	OBD-CAD	3.48	1.28	1.22
13	B	821	CLA	OBD-CAD	3.48	1.28	1.22
13	A	838	CLA	C1B-NB	-3.48	1.33	1.37
13	A	818	CLA	C3D-C2D	3.48	1.48	1.39
13	B	819	CLA	CHC-C4B	3.48	1.47	1.39
13	A	839	CLA	CHC-C4B	3.48	1.47	1.39
13	A	831	CLA	C3D-C2D	3.48	1.48	1.39
13	B	803	CLA	C4B-NB	-3.47	1.33	1.37
13	B	806	CLA	OBD-CAD	3.47	1.28	1.22
13	A	827	CLA	C4B-NB	-3.47	1.33	1.37
13	A	834	CLA	CHC-C4B	3.47	1.47	1.39
13	B	824	CLA	OBD-CAD	3.47	1.28	1.22
13	B	828	CLA	CHC-C4B	3.47	1.47	1.39
13	B	818	CLA	OBD-CAD	3.47	1.28	1.22
13	A	843	CLA	CHC-C4B	3.46	1.47	1.39
13	K	203	CLA	OBD-CAD	3.46	1.28	1.22
13	B	807	CLA	CHC-C4B	3.46	1.47	1.39
13	A	830	CLA	C3D-C2D	3.45	1.48	1.39
13	B	821	CLA	C3D-C2D	3.45	1.48	1.39
13	A	807	CLA	C4B-NB	-3.45	1.33	1.37
13	B	804	CLA	CHC-C4B	3.45	1.47	1.39
13	A	829	CLA	C3D-C2D	3.45	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	820	CLA	C3D-C2D	3.45	1.48	1.39
13	B	814	CLA	C4B-NB	-3.44	1.33	1.37
13	A	807	CLA	C3D-C2D	3.44	1.48	1.39
13	B	803	CLA	CHD-C4C	3.44	1.47	1.39
13	A	810	CLA	CHC-C4B	3.44	1.47	1.39
16	M	101	BCR	C30-C25	-3.44	1.49	1.53
13	B	831	CLA	CHC-C4B	3.44	1.47	1.39
13	B	807	CLA	C4B-NB	-3.43	1.33	1.37
13	B	817	CLA	OBD-CAD	3.43	1.28	1.22
13	A	832	CLA	C4B-NB	-3.43	1.33	1.37
13	B	814	CLA	CHC-C4B	3.43	1.47	1.39
13	B	832	CLA	OBD-CAD	3.43	1.28	1.22
13	A	826	CLA	CHB-C1B	3.43	1.47	1.39
13	B	805	CLA	CHC-C4B	3.43	1.47	1.39
13	B	811	CLA	OBD-CAD	3.43	1.28	1.22
13	B	803	CLA	CHC-C4B	3.43	1.47	1.39
13	B	816	CLA	OBD-CAD	3.43	1.28	1.22
13	A	804	CLA	CHC-C4B	3.43	1.47	1.39
13	A	810	CLA	C3D-C2D	3.42	1.48	1.39
13	A	802	CLA	C3D-C2D	3.42	1.48	1.39
13	B	804	CLA	CHD-C1D	3.42	1.45	1.38
13	B	825	CLA	OBD-CAD	3.42	1.28	1.22
13	A	819	CLA	C3D-C2D	3.42	1.48	1.39
13	A	826	CLA	CHD-C4C	3.42	1.47	1.39
13	K	203	CLA	CHC-C4B	3.42	1.47	1.39
13	B	832	CLA	C4B-NB	-3.42	1.33	1.37
13	A	812	CLA	OBD-CAD	3.41	1.28	1.22
13	B	825	CLA	CHD-C1D	3.41	1.45	1.38
13	B	827	CLA	C1B-NB	-3.41	1.33	1.37
13	B	811	CLA	C3D-C2D	3.41	1.48	1.39
13	L	203	CLA	C1B-NB	-3.41	1.33	1.37
13	B	808	CLA	CHC-C4B	3.41	1.47	1.39
13	A	820	CLA	OBD-CAD	3.41	1.28	1.22
13	A	805	CLA	OBD-CAD	3.41	1.28	1.22
13	A	838	CLA	CHC-C4B	3.40	1.47	1.39
13	B	801	CLA	OBD-CAD	3.40	1.28	1.22
13	L	204	CLA	CHC-C4B	3.40	1.47	1.39
13	B	810	CLA	OBD-CAD	3.40	1.28	1.22
13	B	808	CLA	OBD-CAD	3.40	1.28	1.22
13	A	821	CLA	OBD-CAD	3.40	1.28	1.22
13	A	814	CLA	OBD-CAD	3.40	1.28	1.22
16	F	201	BCR	C1-C6	-3.39	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	203	CLA	C1B-NB	-3.39	1.33	1.37
13	B	824	CLA	CHC-C4B	3.39	1.47	1.39
13	B	801	CLA	CHC-C4B	3.38	1.47	1.39
13	A	804	CLA	OBD-CAD	3.38	1.28	1.22
13	B	813	CLA	C1B-NB	-3.38	1.33	1.37
13	A	826	CLA	C3D-C2D	3.38	1.48	1.39
13	A	815	CLA	C4B-NB	-3.38	1.33	1.37
13	A	824	CLA	OBD-CAD	3.38	1.28	1.22
13	A	806	CLA	C4B-NB	-3.37	1.33	1.37
13	A	843	CLA	OBD-CAD	3.37	1.28	1.22
13	A	829	CLA	C4B-NB	-3.37	1.33	1.37
13	A	844	CLA	CHC-C4B	3.37	1.47	1.39
16	F	202	BCR	C1-C6	-3.37	1.49	1.53
13	B	826	CLA	CHC-C4B	3.37	1.47	1.39
13	A	811	CLA	OBD-CAD	3.37	1.28	1.22
16	A	850	BCR	C1-C6	-3.37	1.49	1.53
13	A	841	CLA	OBD-CAD	3.37	1.28	1.22
13	A	825	CLA	CHC-C4B	3.36	1.47	1.39
13	A	818	CLA	C4B-NB	-3.36	1.33	1.37
13	A	813	CLA	CHC-C4B	3.36	1.47	1.39
13	A	806	CLA	OBD-CAD	3.36	1.28	1.22
13	A	831	CLA	OBD-CAD	3.36	1.28	1.22
13	A	842	CLA	C1B-NB	-3.36	1.33	1.37
13	B	811	CLA	CHB-C1B	3.36	1.47	1.39
13	K	201	CLA	C1B-NB	-3.36	1.33	1.37
13	A	814	CLA	CHC-C4B	3.36	1.46	1.39
13	B	832	CLA	CHC-C4B	3.36	1.46	1.39
13	K	203	CLA	CHB-C1B	3.36	1.46	1.39
13	A	830	CLA	OBD-CAD	3.35	1.28	1.22
13	B	802	CLA	OBD-CAD	3.35	1.28	1.22
13	L	203	CLA	OBD-CAD	3.35	1.28	1.22
13	A	803	CLA	CHD-C1D	3.35	1.44	1.38
13	A	823	CLA	OBD-CAD	3.35	1.28	1.22
13	A	812	CLA	CHC-C4B	3.34	1.46	1.39
13	L	203	CLA	C4B-NB	-3.34	1.33	1.37
13	B	831	CLA	CHB-C1B	3.34	1.46	1.39
13	B	802	CLA	CHB-C1B	3.34	1.46	1.39
13	B	812	CLA	CHC-C4B	3.34	1.46	1.39
13	B	819	CLA	OBD-CAD	3.34	1.28	1.22
13	A	825	CLA	OBD-CAD	3.33	1.28	1.22
13	A	806	CLA	C3D-C2D	3.33	1.48	1.39
13	B	802	CLA	C3D-C2D	3.33	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	832	CLA	CHC-C4B	3.33	1.46	1.39
13	A	811	CLA	CHC-C4B	3.33	1.46	1.39
13	A	816	CLA	CHC-C4B	3.33	1.46	1.39
13	B	821	CLA	C4B-NB	-3.32	1.33	1.37
13	A	820	CLA	C4B-NB	-3.32	1.33	1.37
13	B	833	CLA	OBD-CAD	3.32	1.28	1.22
13	A	842	CLA	CHB-C1B	3.32	1.46	1.39
13	B	825	CLA	C3D-C2D	3.32	1.48	1.39
13	A	823	CLA	C4B-NB	-3.32	1.33	1.37
13	A	811	CLA	CHB-C1B	3.32	1.46	1.39
13	A	836	CLA	OBD-CAD	3.31	1.28	1.22
16	B	835	BCR	C30-C25	-3.31	1.49	1.53
16	L	201	BCR	C1-C6	-3.31	1.49	1.53
13	B	807	CLA	C3D-C2D	3.30	1.48	1.39
13	B	802	CLA	CHD-C4C	3.30	1.46	1.39
13	B	802	CLA	C4B-NB	-3.30	1.33	1.37
13	A	840	CLA	C3D-C2D	3.30	1.48	1.39
13	A	809	CLA	C4B-NB	-3.30	1.33	1.37
13	A	821	CLA	C4B-NB	-3.30	1.33	1.37
13	K	201	CLA	CHB-C1B	3.30	1.46	1.39
13	A	819	CLA	OBD-CAD	3.29	1.28	1.22
13	L	203	CLA	CHC-C4B	3.29	1.46	1.39
13	A	836	CLA	CHC-C4B	3.29	1.46	1.39
16	A	847	BCR	C1-C6	-3.29	1.49	1.53
13	B	822	CLA	CHB-C1B	3.29	1.46	1.39
13	A	826	CLA	C4B-NB	-3.28	1.33	1.37
13	A	808	CLA	C4B-NB	-3.28	1.33	1.37
13	A	819	CLA	CHC-C4B	3.28	1.46	1.39
13	B	810	CLA	CHC-C4B	3.28	1.46	1.39
13	A	824	CLA	CHC-C4B	3.28	1.46	1.39
13	A	833	CLA	OBD-CAD	3.28	1.28	1.22
13	B	823	CLA	CHB-C1B	3.28	1.46	1.39
13	A	835	CLA	C4B-NB	-3.28	1.33	1.37
13	A	821	CLA	CHB-C1B	3.28	1.46	1.39
13	B	822	CLA	C4B-NB	-3.27	1.33	1.37
13	A	822	CLA	OBD-CAD	3.27	1.28	1.22
13	A	826	CLA	OBD-CAD	3.27	1.28	1.22
13	A	830	CLA	C4B-NB	-3.26	1.33	1.37
13	B	818	CLA	CHC-C4B	3.26	1.46	1.39
13	A	816	CLA	C4B-NB	-3.26	1.33	1.37
13	A	822	CLA	C4B-NB	-3.26	1.33	1.37
13	F	203	CLA	CHB-C1B	3.26	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	835	CLA	C1B-NB	-3.26	1.33	1.37
13	L	203	CLA	CHB-C1B	3.26	1.46	1.39
16	A	849	BCR	C1-C6	-3.26	1.49	1.53
13	A	818	CLA	OBD-CAD	3.25	1.28	1.22
13	A	828	CLA	C3D-C2D	3.25	1.47	1.39
13	B	822	CLA	CHC-C4B	3.25	1.46	1.39
13	A	817	CLA	CHB-C1B	3.25	1.46	1.39
13	A	808	CLA	CHC-C4B	3.25	1.46	1.39
13	B	815	CLA	CHC-C4B	3.25	1.46	1.39
13	B	809	CLA	CHC-C4B	3.25	1.46	1.39
13	A	835	CLA	CHC-C4B	3.24	1.46	1.39
16	L	205	BCR	C30-C25	-3.24	1.49	1.53
16	B	835	BCR	C1-C6	-3.24	1.49	1.53
13	B	821	CLA	CHB-C1B	3.24	1.46	1.39
13	B	833	CLA	CHB-C1B	3.24	1.46	1.39
13	A	843	CLA	C4B-NB	-3.23	1.33	1.37
16	L	205	BCR	C1-C6	-3.23	1.49	1.53
13	A	809	CLA	OBD-CAD	3.23	1.28	1.22
13	A	838	CLA	C3D-C2D	3.23	1.47	1.39
13	B	806	CLA	CHC-C4B	3.23	1.46	1.39
13	A	844	CLA	CHB-C1B	3.23	1.46	1.39
13	B	829	CLA	C4B-NB	-3.22	1.33	1.37
13	B	829	CLA	CHB-C1B	3.22	1.46	1.39
13	B	828	CLA	CHB-C1B	3.22	1.46	1.39
13	B	816	CLA	CHC-C4B	3.22	1.46	1.39
13	A	823	CLA	CHB-C1B	3.21	1.46	1.39
13	B	810	CLA	CHB-C1B	3.21	1.46	1.39
13	A	825	CLA	C4B-NB	-3.21	1.33	1.37
13	A	840	CLA	CHB-C1B	3.21	1.46	1.39
13	B	813	CLA	C4B-NB	-3.21	1.33	1.37
13	B	833	CLA	C4B-NB	-3.21	1.33	1.37
13	A	832	CLA	OBD-CAD	3.21	1.28	1.22
13	B	813	CLA	CHB-C1B	3.21	1.46	1.39
13	B	827	CLA	CHB-C1B	3.20	1.46	1.39
13	A	818	CLA	CHC-C4B	3.19	1.46	1.39
13	B	818	CLA	CHB-C1B	3.19	1.46	1.39
13	A	827	CLA	C3D-C2D	3.19	1.47	1.39
13	B	816	CLA	CHB-C1B	3.19	1.46	1.39
13	L	204	CLA	C4B-NB	-3.19	1.33	1.37
13	B	820	CLA	CHB-C1B	3.19	1.46	1.39
13	B	826	CLA	C4B-NB	-3.19	1.33	1.37
16	B	837	BCR	C1-C6	-3.19	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	834	CLA	C4B-NB	-3.18	1.33	1.37
13	A	812	CLA	C4B-NB	-3.18	1.33	1.37
13	A	833	CLA	C4B-NB	-3.18	1.33	1.37
13	B	812	CLA	CHB-C1B	3.18	1.46	1.39
13	A	833	CLA	CHB-C1B	3.17	1.46	1.39
13	A	829	CLA	CHB-C1B	3.17	1.46	1.39
13	A	807	CLA	OBD-CAD	3.17	1.27	1.22
13	K	203	CLA	C4B-NB	-3.17	1.33	1.37
16	J	102	BCR	C1-C6	-3.17	1.49	1.53
16	A	850	BCR	C30-C25	-3.17	1.49	1.53
13	A	816	CLA	CHB-C1B	3.17	1.46	1.39
13	A	834	CLA	CHB-C1B	3.17	1.46	1.39
13	A	803	CLA	C1D-ND	3.17	1.42	1.37
13	B	808	CLA	CHB-C1B	3.17	1.46	1.39
13	A	804	CLA	CHB-C1B	3.16	1.46	1.39
13	B	802	CLA	CHC-C4B	3.16	1.46	1.39
13	A	822	CLA	CHB-C1B	3.15	1.46	1.39
13	B	810	CLA	C4B-NB	-3.15	1.33	1.37
13	A	829	CLA	OBD-CAD	3.15	1.27	1.22
13	B	815	CLA	C4B-NB	-3.15	1.33	1.37
13	A	843	CLA	CHB-C1B	3.15	1.46	1.39
13	A	821	CLA	CHC-C4B	3.14	1.46	1.39
13	B	833	CLA	CHC-C4B	3.14	1.46	1.39
16	I	101	BCR	C1-C6	-3.14	1.49	1.53
13	B	815	CLA	CHB-C1B	3.13	1.46	1.39
13	A	839	CLA	CHB-C1B	3.13	1.46	1.39
13	A	831	CLA	CHB-C1B	3.13	1.46	1.39
13	A	812	CLA	CHB-C1B	3.13	1.46	1.39
13	B	805	CLA	C4B-NB	-3.13	1.33	1.37
13	A	806	CLA	CHC-C4B	3.13	1.46	1.39
13	B	831	CLA	C4B-NB	-3.12	1.33	1.37
13	J	101	CLA	CHB-C1B	3.12	1.46	1.39
13	B	811	CLA	C4B-NB	-3.12	1.33	1.37
13	B	828	CLA	C4B-NB	-3.12	1.33	1.37
13	A	817	CLA	CHC-C4B	3.12	1.46	1.39
13	L	204	CLA	CHB-C1B	3.12	1.46	1.39
13	A	805	CLA	C4B-NB	-3.12	1.33	1.37
13	B	824	CLA	C4B-NB	-3.11	1.33	1.37
13	B	823	CLA	C3D-C2D	3.11	1.47	1.39
13	A	839	CLA	C4B-NB	-3.11	1.33	1.37
13	A	824	CLA	C4B-NB	-3.10	1.33	1.37
13	B	816	CLA	C4B-NB	-3.10	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	820	CLA	OBD-CAD	3.10	1.27	1.22
13	B	830	CLA	CHB-C1B	3.09	1.46	1.39
13	A	809	CLA	CHB-C1B	3.09	1.46	1.39
13	B	832	CLA	CHB-C1B	3.09	1.46	1.39
13	A	818	CLA	CHB-C1B	3.09	1.46	1.39
16	L	201	BCR	C30-C25	-3.09	1.49	1.53
13	B	817	CLA	C4B-NB	-3.09	1.33	1.37
13	A	828	CLA	C4B-NB	-3.08	1.33	1.37
13	B	824	CLA	CHB-C1B	3.08	1.46	1.39
13	B	830	CLA	OBD-CAD	3.08	1.27	1.22
13	B	803	CLA	CHB-C1B	3.08	1.46	1.39
13	B	814	CLA	CHB-C1B	3.08	1.46	1.39
13	A	831	CLA	CHC-C4B	3.08	1.46	1.39
13	A	837	CLA	CHB-C1B	3.08	1.46	1.39
13	A	838	CLA	OBD-CAD	3.07	1.27	1.22
17	A	852	LHG	O7-C5	-3.07	1.39	1.46
13	A	832	CLA	CHB-C1B	3.07	1.46	1.39
13	A	802	CLA	CHC-C4B	3.07	1.46	1.39
16	F	201	BCR	C30-C25	-3.07	1.49	1.53
13	B	820	CLA	C4B-NB	-3.07	1.33	1.37
13	A	836	CLA	C4B-NB	-3.06	1.33	1.37
13	B	808	CLA	C4B-NB	-3.06	1.33	1.37
13	B	807	CLA	CHB-C1B	3.06	1.46	1.39
13	B	817	CLA	CHB-C1B	3.05	1.46	1.39
13	B	830	CLA	C4B-NB	-3.04	1.33	1.37
16	M	101	BCR	C1-C6	-3.04	1.49	1.53
13	A	839	CLA	OBD-CAD	3.04	1.27	1.22
13	A	824	CLA	CHB-C1B	3.04	1.46	1.39
13	A	836	CLA	CHB-C1B	3.03	1.46	1.39
13	A	813	CLA	C4B-NB	-3.03	1.33	1.37
13	A	827	CLA	OBD-CAD	3.03	1.27	1.22
13	B	826	CLA	CHB-C1B	3.03	1.46	1.39
13	A	817	CLA	C4B-NB	-3.02	1.33	1.37
13	A	813	CLA	CHB-C1B	3.02	1.46	1.39
13	L	202	CLA	CHB-C1B	3.02	1.46	1.39
13	A	814	CLA	CHB-C1B	3.01	1.46	1.39
13	B	801	CLA	C4B-NB	-3.01	1.33	1.37
13	B	823	CLA	CHC-C4B	3.01	1.46	1.39
13	K	201	CLA	C4B-NB	-3.01	1.33	1.37
13	B	825	CLA	CHB-C1B	3.01	1.46	1.39
13	A	837	CLA	C4B-NB	-3.01	1.33	1.37
13	B	806	CLA	CHB-C1B	3.00	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	828	CLA	CHB-C1B	3.00	1.46	1.39
13	B	829	CLA	OBD-CAD	3.00	1.27	1.22
13	A	820	CLA	CHC-C4B	2.99	1.46	1.39
13	A	830	CLA	CHB-C1B	2.99	1.46	1.39
13	A	825	CLA	CHB-C1B	2.99	1.46	1.39
13	A	820	CLA	CHB-C1B	2.99	1.46	1.39
13	A	804	CLA	C4B-NB	-2.99	1.33	1.37
13	B	806	CLA	C4B-NB	-2.99	1.33	1.37
13	A	828	CLA	OBD-CAD	2.98	1.27	1.22
13	B	831	CLA	OBD-CAD	2.98	1.27	1.22
13	A	840	CLA	C4B-NB	-2.97	1.34	1.37
13	A	842	CLA	C4B-NB	-2.97	1.34	1.37
13	A	835	CLA	CHB-C1B	2.97	1.46	1.39
13	A	811	CLA	C4B-NB	-2.97	1.34	1.37
13	F	203	CLA	C4B-NB	-2.97	1.34	1.37
13	B	823	CLA	C3D-C4D	-2.96	1.37	1.44
13	A	807	CLA	CHB-C1B	2.96	1.46	1.39
13	A	810	CLA	C4B-NB	-2.95	1.34	1.37
13	B	807	CLA	OBD-CAD	2.92	1.27	1.22
13	A	808	CLA	CHB-C1B	2.91	1.45	1.39
13	B	805	CLA	CHB-C1B	2.91	1.45	1.39
16	J	104	BCR	C1-C6	-2.91	1.50	1.53
16	B	836	BCR	C30-C25	-2.90	1.50	1.53
13	A	819	CLA	CHB-C1B	2.90	1.45	1.39
13	A	841	CLA	CHB-C1B	2.88	1.45	1.39
13	L	202	CLA	C4B-NB	-2.88	1.34	1.37
16	J	104	BCR	C30-C25	-2.87	1.50	1.53
13	B	819	CLA	CHB-C1B	2.87	1.45	1.39
13	B	809	CLA	CHB-C1B	2.87	1.45	1.39
13	A	802	CLA	CHB-C1B	2.87	1.45	1.39
16	B	836	BCR	C1-C6	-2.87	1.50	1.53
16	A	851	BCR	C1-C6	-2.87	1.50	1.53
16	L	206	BCR	C1-C6	-2.86	1.50	1.53
13	A	815	CLA	CHB-C1B	2.85	1.45	1.39
13	A	806	CLA	CHB-C1B	2.85	1.45	1.39
13	B	827	CLA	C3B-C4B	2.82	1.50	1.42
16	J	102	BCR	C30-C25	-2.81	1.50	1.53
13	A	841	CLA	C3B-C4B	2.81	1.50	1.42
13	A	817	CLA	C4D-CHA	2.81	1.48	1.38
13	A	844	CLA	C4B-NB	-2.79	1.34	1.37
13	A	827	CLA	C3D-C4D	-2.78	1.37	1.44
13	B	820	CLA	C4D-CHA	2.78	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	818	CLA	C4B-NB	-2.78	1.34	1.37
13	A	835	CLA	C4D-CHA	2.77	1.47	1.38
13	A	837	CLA	C4D-CHA	2.77	1.47	1.38
13	A	802	CLA	OBD-CAD	2.77	1.27	1.22
13	J	101	CLA	C4D-CHA	2.77	1.47	1.38
13	B	812	CLA	C4B-NB	-2.77	1.34	1.37
13	A	808	CLA	C4D-CHA	2.77	1.47	1.38
13	B	815	CLA	C4D-CHA	2.77	1.47	1.38
16	A	847	BCR	C30-C25	-2.76	1.50	1.53
13	A	841	CLA	C4D-CHA	2.76	1.47	1.38
13	A	805	CLA	CHB-C1B	2.75	1.45	1.39
13	B	811	CLA	C4C-C3C	2.75	1.49	1.45
13	K	201	CLA	OBD-CAD	2.75	1.28	1.23
13	B	802	CLA	C1B-C2B	2.74	1.49	1.43
13	B	810	CLA	C4D-CHA	2.74	1.47	1.38
13	A	825	CLA	C4D-CHA	2.74	1.47	1.38
13	B	818	CLA	C4D-CHA	2.74	1.47	1.38
13	A	844	CLA	C4D-CHA	2.73	1.47	1.38
13	A	815	CLA	C4D-CHA	2.72	1.47	1.38
13	B	812	CLA	C4D-CHA	2.72	1.47	1.38
13	B	803	CLA	OBD-CAD	2.72	1.27	1.22
13	A	838	CLA	C3D-C4D	-2.72	1.38	1.44
13	L	202	CLA	C4D-CHA	2.72	1.47	1.38
13	A	816	CLA	C4D-CHA	2.72	1.47	1.38
13	A	820	CLA	C4D-CHA	2.71	1.47	1.38
13	A	842	CLA	C4D-CHA	2.71	1.47	1.38
13	K	203	CLA	C4D-CHA	2.71	1.47	1.38
13	A	805	CLA	C4D-CHA	2.71	1.47	1.38
13	A	821	CLA	C4D-CHA	2.71	1.47	1.38
13	B	823	CLA	C4C-C3C	2.71	1.49	1.45
13	B	827	CLA	C4B-NB	-2.70	1.34	1.37
13	B	816	CLA	C4D-CHA	2.70	1.47	1.38
13	J	101	CLA	C4B-NB	-2.70	1.34	1.37
13	A	814	CLA	C4D-CHA	2.70	1.47	1.38
13	A	832	CLA	C3D-C4D	-2.70	1.38	1.44
13	B	827	CLA	C4D-CHA	2.70	1.47	1.38
13	A	819	CLA	C4D-CHA	2.69	1.47	1.38
13	A	840	CLA	C3D-C4D	-2.69	1.38	1.44
13	B	825	CLA	C3B-C4B	2.69	1.50	1.42
13	A	835	CLA	C1B-C2B	2.69	1.49	1.43
13	A	829	CLA	C4D-CHA	2.69	1.47	1.38
13	A	809	CLA	C4D-CHA	2.69	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	811	CLA	C4D-CHA	2.69	1.47	1.38
13	B	804	CLA	CHB-C1B	2.69	1.45	1.39
13	A	840	CLA	OBD-CAD	2.68	1.27	1.22
16	F	202	BCR	C30-C25	-2.68	1.50	1.53
13	A	810	CLA	C4D-CHA	2.68	1.47	1.38
13	B	817	CLA	C4D-CHA	2.68	1.47	1.38
13	A	813	CLA	C4D-CHA	2.67	1.47	1.38
13	A	827	CLA	CHB-C1B	2.67	1.45	1.39
16	J	103	BCR	C1-C6	-2.67	1.50	1.53
13	B	807	CLA	C4D-CHA	2.67	1.47	1.38
13	A	824	CLA	C4D-CHA	2.67	1.47	1.38
13	F	203	CLA	C4D-CHA	2.67	1.47	1.38
13	A	802	CLA	C3D-C4D	-2.67	1.38	1.44
13	B	801	CLA	C4D-CHA	2.67	1.47	1.38
13	B	811	CLA	C3D-C4D	-2.66	1.38	1.44
16	A	851	BCR	C30-C25	-2.66	1.50	1.53
13	B	833	CLA	C4D-CHA	2.66	1.47	1.38
13	A	836	CLA	C4D-CHA	2.66	1.47	1.38
13	B	813	CLA	C4D-CHA	2.66	1.47	1.38
13	B	833	CLA	C3D-C4D	-2.65	1.38	1.44
13	B	826	CLA	C4D-CHA	2.65	1.47	1.38
13	B	806	CLA	C4D-CHA	2.65	1.47	1.38
13	A	823	CLA	C4D-CHA	2.65	1.47	1.38
13	A	843	CLA	C4D-CHA	2.65	1.47	1.38
13	B	808	CLA	C4D-CHA	2.64	1.47	1.38
13	J	101	CLA	C3B-C4B	2.64	1.50	1.42
13	A	812	CLA	C3D-C4D	-2.64	1.38	1.44
13	A	828	CLA	C4D-CHA	2.64	1.47	1.38
13	B	828	CLA	C4D-CHA	2.64	1.47	1.38
13	A	806	CLA	C3D-C4D	-2.64	1.38	1.44
13	A	834	CLA	C4D-CHA	2.64	1.47	1.38
13	A	819	CLA	C1C-NC	-2.63	1.33	1.37
13	A	841	CLA	C4B-NB	-2.63	1.34	1.37
13	B	829	CLA	C4D-CHA	2.63	1.47	1.38
13	B	813	CLA	C4C-C3C	2.62	1.49	1.45
13	B	814	CLA	C4D-CHA	2.62	1.47	1.38
13	B	807	CLA	C3D-C4D	-2.62	1.38	1.44
13	A	832	CLA	C4D-CHA	2.62	1.47	1.38
13	A	821	CLA	C1B-C2B	2.61	1.49	1.43
13	A	822	CLA	C4D-CHA	2.61	1.47	1.38
13	A	825	CLA	C4C-C3C	2.61	1.49	1.45
13	A	819	CLA	C3D-C4D	-2.60	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	828	CLA	C3B-C4B	2.60	1.50	1.42
13	B	821	CLA	C4D-CHA	2.60	1.47	1.38
13	A	804	CLA	C4D-CHA	2.60	1.47	1.38
13	A	839	CLA	C4D-CHA	2.60	1.47	1.38
13	B	805	CLA	C4D-CHA	2.60	1.47	1.38
13	A	831	CLA	C4D-CHA	2.60	1.47	1.38
13	B	832	CLA	C4D-CHA	2.59	1.47	1.38
13	B	829	CLA	C3D-C4D	-2.59	1.38	1.44
13	L	204	CLA	C4D-CHA	2.59	1.47	1.38
16	A	848	BCR	C1-C6	-2.59	1.50	1.53
13	A	833	CLA	C4D-CHA	2.58	1.47	1.38
13	A	804	CLA	C3B-C4B	2.58	1.50	1.42
13	B	822	CLA	C4D-CHA	2.58	1.47	1.38
13	A	830	CLA	C4D-CHA	2.57	1.47	1.38
13	A	826	CLA	C3D-C4D	-2.57	1.38	1.44
13	B	819	CLA	C3D-C4D	-2.57	1.38	1.44
13	A	807	CLA	C3D-C4D	-2.57	1.38	1.44
13	B	831	CLA	C3D-C4D	-2.56	1.38	1.44
16	I	101	BCR	C30-C25	-2.56	1.50	1.53
13	A	833	CLA	C3D-C4D	-2.56	1.38	1.44
13	A	803	CLA	CHB-C4A	-2.56	1.31	1.37
13	B	809	CLA	C4D-CHA	2.56	1.47	1.38
13	A	840	CLA	C4D-CHA	2.56	1.47	1.38
13	A	828	CLA	C3D-C4D	-2.56	1.38	1.44
13	B	816	CLA	C1B-C2B	2.55	1.49	1.43
13	B	831	CLA	C4D-CHA	2.55	1.47	1.38
13	A	808	CLA	C4C-C3C	2.55	1.49	1.45
13	A	818	CLA	C4D-CHA	2.55	1.47	1.38
13	B	819	CLA	C4D-CHA	2.54	1.47	1.38
13	A	825	CLA	C3D-C4D	-2.54	1.38	1.44
13	A	818	CLA	C3D-C4D	-2.54	1.38	1.44
13	A	812	CLA	C4D-CHA	2.54	1.47	1.38
13	B	824	CLA	C4D-CHA	2.54	1.47	1.38
13	A	803	CLA	C4D-CHA	2.53	1.47	1.38
13	A	830	CLA	C3D-C4D	-2.53	1.38	1.44
13	A	807	CLA	C4D-CHA	2.53	1.47	1.38
13	B	832	CLA	C3D-C4D	-2.53	1.38	1.44
13	A	822	CLA	C3D-C4D	-2.53	1.38	1.44
13	A	806	CLA	C4D-CHA	2.53	1.47	1.38
13	B	830	CLA	C3D-C4D	-2.53	1.38	1.44
13	A	829	CLA	C1C-C2C	2.53	1.49	1.44
13	A	826	CLA	C4D-CHA	2.52	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	838	CLA	C4D-CHA	2.52	1.47	1.38
13	B	820	CLA	C3B-C4B	2.52	1.50	1.42
16	L	206	BCR	C30-C25	-2.52	1.50	1.53
13	B	804	CLA	C4D-CHA	2.51	1.47	1.38
13	B	803	CLA	C4D-CHA	2.51	1.47	1.38
13	B	812	CLA	C3B-C4B	2.51	1.50	1.42
13	A	804	CLA	C3D-C4D	-2.51	1.38	1.44
13	B	815	CLA	C1B-C2B	2.51	1.49	1.43
13	B	811	CLA	C4D-CHA	2.51	1.47	1.38
13	B	824	CLA	C3D-C4D	-2.51	1.38	1.44
13	B	826	CLA	C4C-C3C	2.50	1.49	1.45
13	L	202	CLA	C3B-C4B	2.50	1.50	1.42
13	A	808	CLA	C3D-C4D	-2.50	1.38	1.44
13	A	810	CLA	C3D-C4D	-2.50	1.38	1.44
13	B	827	CLA	C4C-C3C	2.50	1.49	1.45
13	A	828	CLA	C1C-NC	-2.50	1.34	1.37
13	A	838	CLA	C1B-C2B	2.50	1.49	1.43
13	B	823	CLA	C4D-CHA	2.50	1.47	1.38
13	A	827	CLA	C4D-CHA	2.50	1.47	1.38
13	A	814	CLA	C3D-C4D	-2.49	1.38	1.44
13	B	830	CLA	C4D-CHA	2.49	1.46	1.38
13	B	824	CLA	C4C-C3C	2.49	1.49	1.45
13	A	814	CLA	C4C-C3C	2.49	1.49	1.45
13	A	824	CLA	C3D-C4D	-2.49	1.38	1.44
13	B	801	CLA	C1B-C2B	2.48	1.49	1.43
13	A	810	CLA	C1B-C2B	2.48	1.49	1.43
13	F	203	CLA	C4C-C3C	2.47	1.49	1.45
13	A	839	CLA	C3D-C4D	-2.47	1.38	1.44
13	B	826	CLA	C3D-C4D	-2.47	1.38	1.44
13	B	822	CLA	C3D-C4D	-2.47	1.38	1.44
13	K	201	CLA	C3D-C4D	-2.47	1.38	1.44
13	B	817	CLA	C3D-C4D	-2.46	1.38	1.44
13	B	825	CLA	C4B-NB	-2.46	1.34	1.37
13	A	835	CLA	C3D-C4D	-2.46	1.38	1.44
16	K	202	BCR	C30-C25	-2.46	1.50	1.53
13	B	820	CLA	C3D-C4D	-2.46	1.38	1.44
13	L	203	CLA	C3D-C4D	-2.46	1.38	1.44
13	A	831	CLA	C3D-C4D	-2.46	1.38	1.44
13	A	842	CLA	C1B-C2B	2.45	1.48	1.43
13	L	204	CLA	C3D-C4D	-2.45	1.38	1.44
13	A	802	CLA	C4D-CHA	2.45	1.46	1.38
13	A	840	CLA	C3B-C4B	2.45	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	816	CLA	C4C-C3C	2.45	1.49	1.45
13	B	828	CLA	C4C-C3C	2.45	1.49	1.45
13	A	829	CLA	C3D-C4D	-2.45	1.38	1.44
13	B	821	CLA	C3D-C4D	-2.44	1.38	1.44
13	A	844	CLA	C3B-C4B	2.44	1.49	1.42
13	A	834	CLA	C1B-C2B	2.44	1.48	1.43
13	A	837	CLA	C3D-C4D	-2.44	1.38	1.44
13	A	811	CLA	C3D-C4D	-2.44	1.38	1.44
13	A	820	CLA	C3D-C4D	-2.44	1.38	1.44
13	B	818	CLA	C3D-C4D	-2.44	1.38	1.44
16	A	849	BCR	C30-C25	-2.43	1.50	1.53
13	B	812	CLA	C4C-C3C	2.43	1.49	1.45
13	A	813	CLA	C3D-C4D	-2.42	1.38	1.44
13	B	825	CLA	C4D-CHA	2.42	1.46	1.38
13	A	824	CLA	C4C-C3C	2.42	1.49	1.45
13	B	826	CLA	C1B-C2B	2.42	1.48	1.43
13	L	203	CLA	C4D-CHA	2.42	1.46	1.38
13	A	815	CLA	C3D-C4D	-2.42	1.38	1.44
13	A	836	CLA	C3D-C4D	-2.42	1.38	1.44
13	A	832	CLA	C4C-C3C	2.41	1.49	1.45
13	B	825	CLA	C3D-C4D	-2.41	1.38	1.44
13	B	810	CLA	C3D-C4D	-2.41	1.38	1.44
13	F	203	CLA	C1B-C2B	2.41	1.48	1.43
13	A	834	CLA	C3D-C4D	-2.41	1.38	1.44
13	K	203	CLA	C1B-C2B	2.41	1.48	1.43
13	B	802	CLA	C4D-CHA	2.41	1.46	1.38
13	B	806	CLA	C3D-C4D	-2.41	1.38	1.44
13	B	805	CLA	C3D-C4D	-2.41	1.38	1.44
13	B	802	CLA	C1C-NC	-2.40	1.34	1.37
13	J	101	CLA	C4C-C3C	2.40	1.49	1.45
13	B	802	CLA	C3D-C4D	-2.40	1.38	1.44
13	A	844	CLA	C1B-C2B	2.40	1.48	1.43
13	A	811	CLA	C1B-C2B	2.40	1.48	1.43
13	A	814	CLA	C1C-NC	-2.40	1.34	1.37
13	A	821	CLA	C3D-C4D	-2.39	1.38	1.44
13	A	843	CLA	C3D-C4D	-2.39	1.38	1.44
13	B	831	CLA	C1B-C2B	2.39	1.48	1.43
13	B	814	CLA	C1B-C2B	2.39	1.48	1.43
13	A	818	CLA	C1B-C2B	2.38	1.48	1.43
13	A	805	CLA	C3D-C4D	-2.38	1.38	1.44
13	A	803	CLA	C3D-C4D	-2.38	1.38	1.44
13	B	814	CLA	C3D-C4D	-2.38	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	842	CLA	C3D-C4D	-2.38	1.38	1.44
13	B	816	CLA	C3D-C4D	-2.37	1.38	1.44
13	A	843	CLA	C4C-C3C	2.37	1.49	1.45
13	B	803	CLA	CBD-CAD	-2.37	1.45	1.56
13	B	827	CLA	C3D-C4D	-2.37	1.38	1.44
13	A	818	CLA	C1C-NC	-2.37	1.34	1.37
13	B	833	CLA	C1C-NC	-2.37	1.34	1.37
13	A	803	CLA	C3B-C4B	2.37	1.49	1.42
13	B	805	CLA	C1B-C2B	2.36	1.48	1.43
13	A	805	CLA	C3B-C4B	2.36	1.49	1.42
13	B	812	CLA	C3D-C4D	-2.36	1.38	1.44
13	A	802	CLA	CBD-CAD	-2.36	1.46	1.56
13	K	203	CLA	C3D-C4D	-2.36	1.38	1.44
13	L	203	CLA	C1B-C2B	2.36	1.48	1.43
13	A	811	CLA	C3B-C4B	2.36	1.49	1.42
13	A	816	CLA	C3D-C4D	-2.36	1.38	1.44
13	A	813	CLA	C4C-C3C	2.36	1.49	1.45
13	B	809	CLA	C3D-C4D	-2.36	1.38	1.44
13	B	815	CLA	C4C-C3C	2.36	1.49	1.45
13	A	812	CLA	C4C-C3C	2.35	1.49	1.45
13	F	203	CLA	C3D-C4D	-2.35	1.38	1.44
16	A	848	BCR	C30-C25	-2.35	1.50	1.53
13	F	203	CLA	C3B-C4B	2.35	1.49	1.42
13	A	843	CLA	C1B-C2B	2.35	1.48	1.43
13	A	837	CLA	C3B-C4B	2.34	1.49	1.42
13	B	801	CLA	C3D-C4D	-2.34	1.38	1.44
13	B	804	CLA	C1C-NC	-2.34	1.34	1.37
13	A	809	CLA	C3D-C4D	-2.34	1.38	1.44
13	L	202	CLA	C3D-C4D	-2.34	1.38	1.44
13	K	201	CLA	C4C-C3C	2.34	1.49	1.45
13	A	817	CLA	C4C-C3C	2.34	1.49	1.45
13	A	838	CLA	C3B-C2B	2.33	1.49	1.41
13	A	825	CLA	C1B-C2B	2.33	1.48	1.43
13	A	817	CLA	C3B-C4B	2.33	1.49	1.42
13	A	816	CLA	C1B-C2B	2.33	1.48	1.43
13	B	832	CLA	C4C-C3C	2.33	1.49	1.45
13	A	833	CLA	C3B-C4B	2.33	1.49	1.42
13	A	817	CLA	C3D-C4D	-2.33	1.38	1.44
13	B	803	CLA	C1B-C2B	2.33	1.48	1.43
13	A	803	CLA	CHB-C1B	2.33	1.44	1.39
13	L	204	CLA	C1B-C2B	2.33	1.48	1.43
13	K	201	CLA	C3B-C4B	2.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	201	CLA	C1B-C2B	2.32	1.48	1.43
13	B	828	CLA	C3B-C4B	2.32	1.49	1.42
13	B	807	CLA	C3B-C4B	2.32	1.49	1.42
13	A	812	CLA	C3B-C4B	2.32	1.49	1.42
13	B	818	CLA	C3B-C4B	2.32	1.49	1.42
13	A	823	CLA	C3D-C4D	-2.32	1.39	1.44
13	B	813	CLA	C3D-C4D	-2.31	1.39	1.44
13	A	826	CLA	C1B-C2B	2.31	1.48	1.43
13	A	804	CLA	C1C-NC	-2.31	1.34	1.37
13	B	817	CLA	C3B-C4B	2.31	1.49	1.42
13	B	813	CLA	C3B-C4B	2.31	1.49	1.42
13	B	813	CLA	C1B-C2B	2.30	1.48	1.43
13	A	837	CLA	C4C-C3C	2.30	1.48	1.45
13	B	821	CLA	C1B-C2B	2.30	1.48	1.43
13	A	815	CLA	C3B-C4B	2.30	1.49	1.42
13	B	833	CLA	C4C-C3C	2.30	1.48	1.45
13	A	813	CLA	C3B-C4B	2.30	1.49	1.42
13	A	842	CLA	C3B-C4B	2.30	1.49	1.42
13	B	809	CLA	C1C-NC	-2.30	1.34	1.37
13	B	822	CLA	C1B-C2B	2.29	1.48	1.43
13	B	828	CLA	C3D-C4D	-2.29	1.39	1.44
13	A	839	CLA	C3B-C4B	2.29	1.49	1.42
13	A	831	CLA	C4C-C3C	2.29	1.48	1.45
13	B	811	CLA	C3B-C4B	2.28	1.49	1.42
13	B	815	CLA	C3B-C4B	2.28	1.49	1.42
13	A	810	CLA	C3B-C4B	2.28	1.49	1.42
13	B	803	CLA	C3D-C4D	-2.28	1.39	1.44
13	B	829	CLA	C3B-C4B	2.28	1.49	1.42
13	B	823	CLA	C1C-NC	-2.28	1.34	1.37
13	A	841	CLA	C3D-C4D	-2.27	1.39	1.44
13	B	808	CLA	C3D-C4D	-2.27	1.39	1.44
13	A	822	CLA	C3B-C4B	2.27	1.49	1.42
13	B	812	CLA	C1B-C2B	2.27	1.48	1.43
13	A	807	CLA	C3B-C4B	2.27	1.49	1.42
13	B	806	CLA	C3B-C4B	2.26	1.49	1.42
13	A	821	CLA	C1C-NC	-2.26	1.34	1.37
13	A	809	CLA	C4C-C3C	2.26	1.48	1.45
13	B	801	CLA	C4C-C3C	2.26	1.48	1.45
13	A	842	CLA	C1C-C2C	2.26	1.49	1.44
13	A	813	CLA	C1B-C2B	2.26	1.48	1.43
13	B	819	CLA	C3B-C2B	2.25	1.48	1.41
13	A	818	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	K	203	CLA	C3B-C4B	2.25	1.49	1.42
13	L	202	CLA	C1B-C2B	2.25	1.48	1.43
13	A	829	CLA	C3B-C4B	2.25	1.49	1.42
13	B	811	CLA	C1B-C2B	2.25	1.48	1.43
13	B	815	CLA	C3D-C4D	-2.25	1.39	1.44
13	A	843	CLA	C3B-C4B	2.24	1.49	1.42
13	A	836	CLA	C1B-C2B	2.24	1.48	1.43
13	A	806	CLA	C1B-C2B	2.24	1.48	1.43
13	B	827	CLA	C1B-C2B	2.24	1.48	1.43
13	B	833	CLA	C3B-C4B	2.24	1.49	1.42
13	B	830	CLA	C3B-C4B	2.24	1.49	1.42
13	A	802	CLA	C4C-C3C	2.24	1.48	1.45
13	A	840	CLA	C1B-C2B	2.23	1.48	1.43
13	A	810	CLA	C1C-NC	-2.23	1.34	1.37
12	A	801	CL0	C3D-C4D	-2.23	1.38	1.41
13	L	204	CLA	C4C-C3C	2.23	1.48	1.45
13	A	820	CLA	C4C-C3C	2.22	1.48	1.45
13	A	841	CLA	C4C-C3C	2.22	1.48	1.45
13	B	807	CLA	C1C-NC	-2.22	1.34	1.37
13	L	204	CLA	C3B-C4B	2.22	1.49	1.42
13	A	844	CLA	C3D-C4D	-2.22	1.39	1.44
13	A	842	CLA	C3B-C2B	2.22	1.48	1.41
13	A	809	CLA	C3B-C4B	2.22	1.49	1.42
13	B	826	CLA	C3B-C4B	2.22	1.49	1.42
13	A	829	CLA	C3B-C2B	2.21	1.48	1.41
13	A	840	CLA	CBD-CAD	-2.21	1.46	1.56
13	A	811	CLA	C4C-C3C	2.21	1.48	1.45
13	J	101	CLA	C1B-C2B	2.21	1.48	1.43
13	A	812	CLA	C1B-C2B	2.21	1.48	1.43
13	B	806	CLA	C4C-C3C	2.21	1.48	1.45
13	B	824	CLA	C1B-C2B	2.21	1.48	1.43
13	B	829	CLA	C1C-C2C	2.20	1.49	1.44
13	A	816	CLA	C3B-C4B	2.20	1.49	1.42
13	A	827	CLA	C3B-C4B	2.20	1.49	1.42
13	A	840	CLA	C1C-NC	-2.20	1.34	1.37
13	B	803	CLA	C1C-C2C	2.20	1.49	1.44
13	A	831	CLA	C1C-NC	-2.20	1.34	1.37
13	B	806	CLA	C1B-C2B	2.20	1.48	1.43
13	A	834	CLA	C3B-C4B	2.19	1.49	1.42
13	A	812	CLA	C1C-NC	-2.19	1.34	1.37
13	A	814	CLA	C3B-C4B	2.19	1.49	1.42
13	A	829	CLA	CBD-CAD	-2.19	1.46	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	831	CLA	CBD-CAD	-2.18	1.46	1.56
13	B	831	CLA	CBD-CAD	-2.18	1.46	1.56
13	B	806	CLA	C1C-NC	-2.18	1.34	1.37
13	A	838	CLA	C1C-C2C	2.18	1.48	1.44
13	A	816	CLA	C1C-NC	-2.18	1.34	1.37
13	B	819	CLA	C4C-C3C	2.18	1.48	1.45
13	A	803	CLA	C3B-C2B	2.18	1.48	1.41
13	A	815	CLA	C1C-C2C	2.17	1.48	1.44
13	A	837	CLA	C1B-C2B	2.17	1.48	1.43
13	B	817	CLA	C4C-C3C	2.17	1.48	1.45
13	A	842	CLA	C4C-C3C	2.17	1.48	1.45
13	A	836	CLA	C4C-C3C	2.17	1.48	1.45
13	A	839	CLA	CBD-CAD	-2.17	1.46	1.56
13	A	820	CLA	CHB-C4A	-2.17	1.32	1.37
13	A	824	CLA	C3B-C4B	2.16	1.49	1.42
13	A	841	CLA	CHB-C4A	-2.16	1.32	1.37
13	A	835	CLA	C4C-C3C	2.16	1.48	1.45
13	A	823	CLA	C1C-C2C	2.16	1.48	1.44
13	L	202	CLA	C3B-C2B	2.16	1.48	1.41
13	K	203	CLA	C4C-C3C	2.16	1.48	1.45
16	B	837	BCR	C33-C5	-2.16	1.47	1.50
13	B	816	CLA	C4C-C3C	2.16	1.48	1.45
13	A	817	CLA	C1B-C2B	2.16	1.48	1.43
13	A	805	CLA	C1C-C2C	2.15	1.48	1.44
13	A	830	CLA	C1C-C2C	2.15	1.48	1.44
13	A	804	CLA	C1B-C2B	2.15	1.48	1.43
13	A	822	CLA	C1C-C2C	2.15	1.48	1.44
13	B	804	CLA	C3D-C4D	-2.15	1.39	1.44
13	B	803	CLA	C3B-C2B	2.15	1.48	1.41
13	B	824	CLA	C3B-C2B	2.15	1.48	1.41
13	B	807	CLA	C1B-C2B	2.15	1.48	1.43
16	A	851	BCR	C33-C5	-2.15	1.47	1.50
12	A	801	CL0	CBD-CGD	-2.15	1.49	1.52
13	L	202	CLA	C1C-C2C	2.15	1.48	1.44
13	B	819	CLA	C3B-C4B	2.15	1.49	1.42
18	B	838	LMG	O7-C8	-2.14	1.41	1.46
13	A	826	CLA	C1C-NC	-2.14	1.34	1.37
13	L	203	CLA	C4C-C3C	2.14	1.48	1.45
13	B	808	CLA	C1B-C2B	2.14	1.48	1.43
13	A	819	CLA	C3B-C4B	2.14	1.49	1.42
13	B	831	CLA	C3B-C4B	2.14	1.49	1.42
13	B	828	CLA	C1B-C2B	2.14	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	824	CLA	C3B-C4B	2.14	1.49	1.42
13	A	823	CLA	C3B-C2B	2.14	1.48	1.41
13	B	819	CLA	CBD-CAD	-2.14	1.46	1.56
13	A	829	CLA	C1B-C2B	2.14	1.48	1.43
13	B	816	CLA	C3B-C2B	2.14	1.48	1.41
13	A	827	CLA	C1B-C2B	2.13	1.48	1.43
13	A	835	CLA	C1C-NC	-2.13	1.34	1.37
13	B	832	CLA	C3B-C4B	2.13	1.48	1.42
13	A	839	CLA	C1C-NC	-2.13	1.34	1.37
13	B	808	CLA	C4C-C3C	2.13	1.48	1.45
13	B	825	CLA	C1C-C2C	2.13	1.48	1.44
13	B	801	CLA	C3B-C2B	2.13	1.48	1.41
17	A	853	LHG	O7-C5	-2.13	1.41	1.46
13	A	823	CLA	C3B-C4B	2.13	1.48	1.42
13	B	802	CLA	CBD-CAD	-2.13	1.47	1.56
13	A	806	CLA	CBD-CAD	-2.13	1.47	1.56
13	B	830	CLA	C1B-C2B	2.13	1.48	1.43
13	A	837	CLA	C3B-C2B	2.13	1.48	1.41
13	A	810	CLA	C4C-C3C	2.12	1.48	1.45
13	A	811	CLA	C1C-NC	-2.12	1.34	1.37
13	A	827	CLA	CHB-C4A	-2.12	1.32	1.37
13	A	841	CLA	C1C-NC	-2.12	1.34	1.37
13	A	807	CLA	C1C-NC	-2.12	1.34	1.37
13	B	808	CLA	C3B-C4B	2.12	1.48	1.42
13	A	844	CLA	C1C-NC	-2.12	1.34	1.37
13	B	820	CLA	C1B-C2B	2.12	1.48	1.43
13	B	813	CLA	C3B-C2B	2.11	1.48	1.41
13	A	806	CLA	C1C-NC	-2.11	1.34	1.37
13	A	825	CLA	C3B-C4B	2.11	1.48	1.42
13	A	841	CLA	C1A-CHA	2.11	1.51	1.43
13	B	828	CLA	C3B-C2B	2.11	1.48	1.41
13	F	203	CLA	C3B-C2B	2.11	1.48	1.41
13	B	820	CLA	C1C-NC	-2.11	1.34	1.37
13	A	809	CLA	C1B-C2B	2.11	1.48	1.43
13	A	820	CLA	C1C-NC	-2.11	1.34	1.37
13	A	835	CLA	C3B-C4B	2.11	1.48	1.42
13	B	809	CLA	C1B-C2B	2.11	1.48	1.43
13	A	808	CLA	C1B-C2B	2.11	1.48	1.43
13	K	203	CLA	C1C-NC	-2.11	1.34	1.37
13	A	815	CLA	CHB-C4A	-2.11	1.32	1.37
13	A	830	CLA	CBD-CAD	-2.11	1.47	1.56
16	J	103	BCR	C33-C5	-2.11	1.47	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	814	CLA	C3B-C4B	2.11	1.48	1.42
13	A	835	CLA	C1A-CHA	2.11	1.51	1.43
13	A	833	CLA	C1C-NC	-2.11	1.34	1.37
13	J	101	CLA	C3D-C4D	-2.11	1.39	1.44
13	A	843	CLA	CBD-CAD	-2.11	1.47	1.56
16	I	101	BCR	C27-C26	-2.11	1.47	1.51
13	A	824	CLA	CBD-CAD	-2.11	1.47	1.56
13	A	837	CLA	C1C-C2C	2.10	1.48	1.44
13	B	827	CLA	C1C-C2C	2.10	1.48	1.44
13	A	830	CLA	C3B-C4B	2.10	1.48	1.42
13	A	827	CLA	CBD-CAD	-2.10	1.47	1.56
13	A	821	CLA	C3B-C2B	2.10	1.48	1.41
13	A	819	CLA	C4C-C3C	2.10	1.48	1.45
13	L	202	CLA	C4C-C3C	2.10	1.48	1.45
13	B	818	CLA	C1A-CHA	2.10	1.51	1.43
13	A	805	CLA	C4C-C3C	2.10	1.48	1.45
13	B	828	CLA	C1C-C2C	2.10	1.48	1.44
13	K	203	CLA	C3B-C2B	2.10	1.48	1.41
13	K	201	CLA	C3B-C2B	2.10	1.48	1.41
13	A	827	CLA	C1C-C2C	2.10	1.48	1.44
13	B	819	CLA	C1B-C2B	2.10	1.48	1.43
13	A	817	CLA	C1C-NC	-2.09	1.34	1.37
13	B	805	CLA	C3B-C4B	2.09	1.48	1.42
13	A	822	CLA	C4C-C3C	2.09	1.48	1.45
13	A	823	CLA	C1B-C2B	2.09	1.48	1.43
13	B	821	CLA	C3B-C2B	2.09	1.48	1.41
13	A	824	CLA	C1B-C2B	2.09	1.48	1.43
16	L	205	BCR	C33-C5	-2.09	1.47	1.50
16	K	202	BCR	C33-C5	-2.09	1.47	1.50
13	B	801	CLA	C3B-C4B	2.09	1.48	1.42
13	A	809	CLA	C1C-NC	-2.08	1.34	1.37
13	A	822	CLA	CBD-CAD	-2.08	1.47	1.56
13	B	814	CLA	C3B-C2B	2.08	1.48	1.41
13	F	203	CLA	C1C-C2C	2.08	1.48	1.44
13	B	815	CLA	C1C-NC	-2.08	1.34	1.37
13	B	831	CLA	C3B-C2B	2.08	1.48	1.41
13	B	832	CLA	C1B-C2B	2.08	1.48	1.43
13	B	823	CLA	CBD-CAD	-2.08	1.47	1.56
13	B	826	CLA	C1C-NC	-2.08	1.34	1.37
13	B	801	CLA	C1C-NC	-2.07	1.34	1.37
13	A	836	CLA	C3B-C4B	2.07	1.48	1.42
13	A	815	CLA	C1B-C2B	2.07	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	811	CLA	CBD-CAD	-2.07	1.47	1.56
13	A	808	CLA	CHB-C4A	-2.07	1.32	1.37
13	B	832	CLA	C3B-C2B	2.07	1.48	1.41
13	B	831	CLA	C4C-C3C	2.07	1.48	1.45
13	A	802	CLA	CHB-C4A	-2.07	1.32	1.37
16	B	837	BCR	C38-C26	-2.07	1.47	1.50
13	B	811	CLA	C3B-C2B	2.07	1.48	1.41
13	B	820	CLA	C4C-C3C	2.07	1.48	1.45
13	A	834	CLA	C1C-NC	-2.07	1.34	1.37
13	B	821	CLA	C1C-C2C	2.07	1.48	1.44
13	B	831	CLA	C1C-NC	-2.07	1.34	1.37
13	B	813	CLA	C1C-NC	-2.07	1.34	1.37
13	B	804	CLA	C3B-C4B	2.07	1.48	1.42
13	A	805	CLA	CHB-C4A	-2.07	1.32	1.37
13	A	818	CLA	CBD-CAD	-2.06	1.47	1.56
13	A	832	CLA	CBD-CAD	-2.06	1.47	1.56
16	A	847	BCR	C33-C5	-2.06	1.47	1.50
13	A	826	CLA	C3B-C4B	2.06	1.48	1.42
13	B	803	CLA	C4C-C3C	2.06	1.48	1.45
13	A	830	CLA	C1B-C2B	2.06	1.48	1.43
13	B	814	CLA	C1C-C2C	2.06	1.48	1.44
13	B	820	CLA	C1C-C2C	2.06	1.48	1.44
13	J	101	CLA	C3B-C2B	2.06	1.48	1.41
13	B	830	CLA	CBD-CAD	-2.06	1.47	1.56
13	A	826	CLA	C3B-C2B	2.06	1.48	1.41
13	A	824	CLA	C1C-NC	-2.06	1.34	1.37
13	B	810	CLA	C1C-C2C	2.06	1.48	1.44
13	A	832	CLA	C1B-C2B	2.05	1.47	1.43
13	B	832	CLA	C1C-C2C	2.05	1.48	1.44
13	B	821	CLA	C3B-C4B	2.05	1.48	1.42
13	A	824	CLA	C3B-C2B	2.05	1.48	1.41
13	A	828	CLA	CBD-CAD	-2.05	1.47	1.56
13	B	827	CLA	C3B-C2B	2.05	1.48	1.41
13	A	819	CLA	C1B-C2B	2.05	1.47	1.43
13	B	804	CLA	C1A-CHA	2.05	1.51	1.43
13	A	830	CLA	CHB-C4A	-2.05	1.32	1.37
13	A	814	CLA	C1B-C2B	2.05	1.47	1.43
13	A	825	CLA	CBD-CAD	-2.05	1.47	1.56
13	L	203	CLA	C1C-NC	-2.05	1.34	1.37
13	A	802	CLA	C1C-NC	-2.05	1.34	1.37
13	B	816	CLA	C1A-CHA	2.04	1.51	1.43
13	B	821	CLA	CBD-CAD	-2.04	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	841	CLA	C1C-C2C	2.04	1.48	1.44
13	A	808	CLA	C3B-C4B	2.04	1.48	1.42
16	J	102	BCR	C33-C5	-2.04	1.47	1.50
13	A	831	CLA	C3B-C4B	2.04	1.48	1.42
13	B	822	CLA	C1C-NC	-2.04	1.34	1.37
13	A	821	CLA	C3B-C4B	2.04	1.48	1.42
13	A	829	CLA	C1A-CHA	2.04	1.51	1.43
13	A	833	CLA	C1B-C2B	2.04	1.47	1.43
13	A	807	CLA	C1B-C2B	2.04	1.47	1.43
13	A	809	CLA	C3B-C2B	2.04	1.48	1.41
13	B	801	CLA	CBD-CAD	-2.03	1.47	1.56
13	B	825	CLA	C4C-C3C	2.03	1.48	1.45
13	B	827	CLA	C1C-NC	-2.03	1.34	1.37
13	A	815	CLA	C4C-C3C	2.03	1.48	1.45
13	B	803	CLA	C1C-NC	-2.03	1.34	1.37
13	A	808	CLA	CBD-CAD	-2.03	1.47	1.56
13	A	822	CLA	C1C-NC	-2.03	1.34	1.37
13	A	825	CLA	C3B-C2B	2.03	1.48	1.41
13	A	833	CLA	CBD-CAD	-2.03	1.47	1.56
13	A	819	CLA	CHB-C4A	-2.03	1.32	1.37
13	B	819	CLA	CHB-C4A	-2.03	1.32	1.37
13	L	204	CLA	C3B-C2B	2.03	1.48	1.41
13	B	831	CLA	C1C-C2C	2.03	1.48	1.44
16	L	201	BCR	C38-C26	-2.03	1.47	1.50
13	A	824	CLA	CHB-C4A	-2.03	1.32	1.37
13	A	806	CLA	CHB-C4A	-2.02	1.32	1.37
16	B	836	BCR	C33-C5	-2.02	1.47	1.50
13	B	809	CLA	C3B-C4B	2.02	1.48	1.42
13	A	818	CLA	C3B-C2B	2.02	1.48	1.41
16	A	851	BCR	C27-C26	-2.02	1.47	1.51
13	A	822	CLA	C1B-C2B	2.02	1.47	1.43
13	B	816	CLA	C1C-C2C	2.02	1.48	1.44
13	A	834	CLA	C3B-C2B	2.02	1.48	1.41
13	A	841	CLA	C3B-C2B	2.02	1.48	1.41
13	A	843	CLA	C1A-CHA	2.02	1.51	1.43
13	A	839	CLA	C4C-C3C	2.02	1.48	1.45
13	B	810	CLA	CBD-CAD	-2.02	1.47	1.56
13	J	101	CLA	C1C-NC	-2.02	1.34	1.37
13	A	840	CLA	C1C-C2C	2.02	1.48	1.44
13	A	802	CLA	C1B-C2B	2.02	1.47	1.43
13	B	822	CLA	C4C-C3C	2.02	1.48	1.45
13	A	819	CLA	C3B-C2B	2.02	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	844	CLA	C4C-C3C	2.02	1.48	1.45
13	B	829	CLA	C4C-C3C	2.02	1.48	1.45
13	B	814	CLA	CBD-CAD	-2.01	1.47	1.56
13	B	829	CLA	C1B-C2B	2.01	1.47	1.43
13	B	820	CLA	C3B-C2B	2.01	1.48	1.41
13	A	807	CLA	CHB-C4A	-2.01	1.32	1.37
13	B	814	CLA	C1C-NC	-2.01	1.34	1.37
13	B	808	CLA	C1C-C2C	2.01	1.48	1.44
13	J	101	CLA	C1A-CHA	2.01	1.51	1.43
13	B	807	CLA	C3B-C2B	2.01	1.47	1.41
13	K	203	CLA	C1C-C2C	2.01	1.48	1.44
13	B	812	CLA	C1C-C2C	2.01	1.48	1.44
13	B	817	CLA	CHB-C4A	-2.00	1.32	1.37
13	A	836	CLA	C1C-NC	-2.00	1.34	1.37
13	A	813	CLA	C3B-C2B	2.00	1.47	1.41
13	B	804	CLA	C1B-C2B	2.00	1.47	1.43

All (2732) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	825	CLA	C1D-ND-C4D	-10.66	98.84	106.31
13	L	203	CLA	C1D-ND-C4D	-10.28	99.10	106.31
12	A	801	CL0	O2D-CGD-CBD	10.27	122.23	110.95
13	B	802	CLA	C1D-ND-C4D	-9.85	99.40	106.31
13	B	830	CLA	C1D-ND-C4D	-9.77	99.46	106.31
13	L	202	CLA	C1D-ND-C4D	-9.68	99.52	106.31
13	A	818	CLA	C1D-ND-C4D	-9.64	99.54	106.31
13	A	823	CLA	C1D-ND-C4D	-9.64	99.55	106.31
13	B	831	CLA	C1D-ND-C4D	-9.58	99.59	106.31
13	B	828	CLA	C1D-ND-C4D	-9.52	99.63	106.31
13	B	827	CLA	C1D-ND-C4D	-9.47	99.67	106.31
13	A	806	CLA	C1D-ND-C4D	-9.43	99.70	106.31
13	A	844	CLA	C1D-ND-C4D	-9.42	99.70	106.31
13	B	805	CLA	C1D-ND-C4D	-9.41	99.71	106.31
13	B	804	CLA	C1D-ND-C4D	-9.39	99.73	106.31
13	B	824	CLA	C1D-ND-C4D	-9.36	99.75	106.31
13	A	809	CLA	C1D-ND-C4D	-9.34	99.76	106.31
13	A	816	CLA	C1D-ND-C4D	-9.27	99.81	106.31
13	B	808	CLA	C1D-ND-C4D	-9.26	99.81	106.31
13	B	821	CLA	C1D-ND-C4D	-9.17	99.88	106.31
13	A	812	CLA	C1D-ND-C4D	-9.16	99.89	106.31
13	B	803	CLA	C1D-ND-C4D	-9.14	99.90	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	835	CLA	C1D-ND-C4D	-9.13	99.90	106.31
13	A	833	CLA	C1D-ND-C4D	-9.13	99.91	106.31
13	B	832	CLA	C1D-ND-C4D	-9.13	99.91	106.31
13	B	816	CLA	C1D-ND-C4D	-9.11	99.92	106.31
13	A	842	CLA	C1D-ND-C4D	-9.10	99.93	106.31
13	A	827	CLA	C1D-ND-C4D	-9.08	99.94	106.31
13	A	836	CLA	C1D-ND-C4D	-9.08	99.94	106.31
13	L	204	CLA	C1D-ND-C4D	-9.08	99.94	106.31
13	A	824	CLA	C1D-ND-C4D	-9.06	99.95	106.31
13	B	814	CLA	C1D-ND-C4D	-9.05	99.96	106.31
12	A	801	CL0	C1B-CHB-C4A	9.04	127.14	121.32
13	A	840	CLA	C1D-ND-C4D	-9.03	99.98	106.31
13	K	201	CLA	C1D-ND-C4D	-9.02	99.98	106.31
13	A	807	CLA	C1D-ND-C4D	-9.02	99.98	106.31
13	A	822	CLA	C1D-ND-C4D	-9.00	100.00	106.31
13	A	843	CLA	C1D-ND-C4D	-9.00	100.00	106.31
13	B	826	CLA	C1D-ND-C4D	-9.00	100.00	106.31
13	B	817	CLA	C1D-ND-C4D	-8.98	100.01	106.31
13	A	817	CLA	C1D-ND-C4D	-8.96	100.02	106.31
13	A	821	CLA	C1D-ND-C4D	-8.96	100.03	106.31
13	B	807	CLA	C1D-ND-C4D	-8.96	100.03	106.31
13	A	839	CLA	C1D-ND-C4D	-8.95	100.03	106.31
13	B	815	CLA	C1D-ND-C4D	-8.94	100.04	106.31
13	A	826	CLA	C1D-ND-C4D	-8.93	100.04	106.31
13	A	804	CLA	C1D-ND-C4D	-8.93	100.05	106.31
13	B	813	CLA	C1D-ND-C4D	-8.89	100.07	106.31
13	A	834	CLA	C1D-ND-C4D	-8.87	100.08	106.31
13	A	829	CLA	C1D-ND-C4D	-8.87	100.09	106.31
13	B	812	CLA	C1D-ND-C4D	-8.86	100.10	106.31
13	A	831	CLA	C1D-ND-C4D	-8.83	100.11	106.31
13	B	819	CLA	C1D-ND-C4D	-8.83	100.11	106.31
13	A	811	CLA	C1D-ND-C4D	-8.83	100.12	106.31
13	A	828	CLA	C1D-ND-C4D	-8.83	100.12	106.31
13	K	203	CLA	C1D-ND-C4D	-8.81	100.13	106.31
13	A	841	CLA	C1D-ND-C4D	-8.78	100.15	106.31
13	A	805	CLA	C1D-ND-C4D	-8.78	100.15	106.31
13	B	829	CLA	C1D-ND-C4D	-8.78	100.15	106.31
13	A	837	CLA	C1D-ND-C4D	-8.75	100.17	106.31
13	B	801	CLA	C1D-ND-C4D	-8.71	100.20	106.31
13	B	820	CLA	C1D-ND-C4D	-8.67	100.23	106.31
13	B	822	CLA	C1D-ND-C4D	-8.67	100.23	106.31
13	A	810	CLA	C1D-ND-C4D	-8.67	100.23	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	101	CLA	C1D-ND-C4D	-8.65	100.24	106.31
13	A	803	CLA	C1D-ND-C4D	-8.65	100.25	106.31
13	A	815	CLA	C1D-ND-C4D	-8.62	100.26	106.31
13	B	809	CLA	C1D-ND-C4D	-8.62	100.26	106.31
13	F	203	CLA	C1D-ND-C4D	-8.61	100.27	106.31
13	B	833	CLA	C1D-ND-C4D	-8.57	100.30	106.31
13	B	811	CLA	C1D-ND-C4D	-8.56	100.31	106.31
13	A	813	CLA	C1D-ND-C4D	-8.55	100.31	106.31
13	A	832	CLA	C1D-ND-C4D	-8.47	100.37	106.31
13	B	806	CLA	C1D-ND-C4D	-8.41	100.41	106.31
13	B	818	CLA	C1D-ND-C4D	-8.41	100.41	106.31
13	A	814	CLA	C1D-ND-C4D	-8.41	100.41	106.31
13	A	838	CLA	C1D-ND-C4D	-8.32	100.47	106.31
13	B	810	CLA	C1D-ND-C4D	-8.30	100.48	106.31
13	A	819	CLA	C1D-ND-C4D	-8.20	100.56	106.31
13	A	830	CLA	C1D-ND-C4D	-8.18	100.58	106.31
13	A	825	CLA	C1D-ND-C4D	-8.17	100.58	106.31
13	A	802	CLA	C1D-ND-C4D	-8.14	100.60	106.31
13	A	808	CLA	C1D-ND-C4D	-8.08	100.64	106.31
13	B	823	CLA	C1D-ND-C4D	-8.03	100.68	106.31
13	B	823	CLA	CMD-C2D-C1D	8.02	138.85	124.73
13	A	820	CLA	C1D-ND-C4D	-7.95	100.74	106.31
13	A	827	CLA	CMD-C2D-C1D	7.66	138.22	124.73
13	A	837	CLA	O2D-CGD-CBD	7.52	124.37	111.23
13	B	811	CLA	CMD-C2D-C1D	7.48	137.90	124.73
13	A	838	CLA	CMD-C2D-C1D	7.43	137.82	124.73
13	B	826	CLA	O2D-CGD-CBD	7.42	124.21	111.23
13	B	825	CLA	CMD-C2D-C1D	7.25	137.50	124.73
13	B	830	CLA	CMD-C2D-C1D	7.23	137.47	124.73
13	A	840	CLA	CMD-C2D-C1D	7.23	137.46	124.73
13	A	812	CLA	CMD-C2D-C1D	7.23	137.46	124.73
13	A	823	CLA	O2D-CGD-CBD	7.13	123.70	111.23
13	B	823	CLA	O2D-CGD-CBD	7.12	123.67	111.23
13	B	807	CLA	CMD-C2D-C1D	7.06	137.16	124.73
13	A	839	CLA	O2D-CGD-CBD	7.06	123.56	111.23
13	B	832	CLA	CMD-C2D-C1D	7.01	137.08	124.73
13	B	825	CLA	C2D-C1D-ND	7.01	117.06	110.13
13	B	824	CLA	CMD-C2D-C1D	7.01	137.07	124.73
13	A	819	CLA	CMD-C2D-C1D	7.00	137.06	124.73
13	A	806	CLA	CMD-C2D-C1D	7.00	137.05	124.73
13	B	819	CLA	CMD-C2D-C1D	6.99	137.03	124.73
13	A	828	CLA	CMD-C2D-C1D	6.96	136.99	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	202	CLA	CMD-C2D-C1D	6.95	136.96	124.73
13	A	835	CLA	CMD-C2D-C1D	6.95	136.96	124.73
13	A	808	CLA	CMD-C2D-C1D	6.94	136.95	124.73
13	B	804	CLA	C2D-C1D-ND	6.94	116.99	110.13
13	B	833	CLA	CMD-C2D-C1D	6.94	136.94	124.73
13	A	815	CLA	CMD-C2D-C1D	6.93	136.93	124.73
13	B	827	CLA	CMD-C2D-C1D	6.91	136.90	124.73
13	A	831	CLA	CMD-C2D-C1D	6.91	136.90	124.73
13	A	839	CLA	CMD-C2D-C1D	6.91	136.89	124.73
13	B	828	CLA	CMD-C2D-C1D	6.90	136.87	124.73
13	A	807	CLA	CMD-C2D-C1D	6.90	136.87	124.73
13	B	802	CLA	CHD-C4C-C3C	-6.89	114.73	124.77
13	A	802	CLA	CMD-C2D-C1D	6.89	136.85	124.73
13	A	835	CLA	O2D-CGD-CBD	6.86	123.23	111.23
13	B	820	CLA	CMD-C2D-C1D	6.86	136.81	124.73
13	A	832	CLA	CMD-C2D-C1D	6.85	136.79	124.73
13	B	824	CLA	CAA-C2A-C3A	-6.85	94.50	113.00
13	J	101	CLA	CMD-C2D-C1D	6.84	136.78	124.73
13	L	204	CLA	CMD-C2D-C1D	6.82	136.75	124.73
13	A	844	CLA	CMD-C2D-C1D	6.80	136.71	124.73
13	A	843	CLA	CMD-C2D-C1D	6.80	136.71	124.73
13	A	818	CLA	CMD-C2D-C1D	6.80	136.71	124.73
12	A	801	CL0	C4D-ND-C1D	-6.79	100.06	105.22
13	A	842	CLA	CMD-C2D-C1D	6.79	136.69	124.73
13	B	831	CLA	CMD-C2D-C1D	6.79	136.69	124.73
13	B	812	CLA	CMD-C2D-C1D	6.77	136.65	124.73
13	L	203	CLA	C2D-C1D-ND	6.74	116.79	110.13
13	B	802	CLA	C2D-C1D-ND	6.72	116.78	110.13
13	B	816	CLA	CMD-C2D-C1D	6.72	136.56	124.73
13	A	811	CLA	CMD-C2D-C1D	6.71	136.54	124.73
13	B	826	CLA	CMD-C2D-C1D	6.71	136.54	124.73
13	A	817	CLA	CMD-C2D-C1D	6.71	136.54	124.73
13	A	816	CLA	CMD-C2D-C1D	6.70	136.53	124.73
13	A	833	CLA	CMD-C2D-C1D	6.69	136.50	124.73
13	A	803	CLA	C2B-C1B-NB	6.67	117.25	110.33
13	A	834	CLA	CMD-C2D-C1D	6.66	136.46	124.73
13	B	817	CLA	CMD-C2D-C1D	6.66	136.46	124.73
13	F	203	CLA	CMD-C2D-C1D	6.65	136.43	124.73
13	B	818	CLA	CMD-C2D-C1D	6.63	136.40	124.73
13	A	837	CLA	CMD-C2D-C1D	6.62	136.39	124.73
13	K	201	CLA	CMD-C2D-C1D	6.61	136.37	124.73
13	A	805	CLA	CMD-C2D-C1D	6.61	136.37	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	829	CLA	CMD-C2D-C1D	6.60	136.35	124.73
13	B	803	CLA	C2D-C1D-ND	6.60	116.66	110.13
13	A	829	CLA	CHD-C4C-C3C	-6.57	115.20	124.77
13	A	840	CLA	O2D-CGD-CBD	6.55	122.68	111.23
13	B	805	CLA	CMD-C2D-C1D	6.53	136.23	124.73
13	B	813	CLA	CMD-C2D-C1D	6.53	136.23	124.73
13	A	814	CLA	CMD-C2D-C1D	6.53	136.22	124.73
13	L	203	CLA	CMD-C2D-C1D	6.52	136.21	124.73
13	B	806	CLA	CMD-C2D-C1D	6.50	136.17	124.73
13	A	823	CLA	C2D-C1D-ND	6.49	116.55	110.13
13	A	832	CLA	O2D-CGD-CBD	6.48	122.56	111.23
13	B	810	CLA	CMD-C2D-C1D	6.48	136.14	124.73
13	A	838	CLA	O2D-CGD-CBD	6.47	122.55	111.23
13	A	821	CLA	CMD-C2D-C1D	6.46	136.11	124.73
13	A	809	CLA	C2D-C1D-ND	6.46	116.52	110.13
13	B	809	CLA	O2D-CGD-CBD	6.45	122.50	111.23
13	A	804	CLA	O2D-CGD-CBD	6.42	122.45	111.23
13	A	828	CLA	CHD-C4C-C3C	-6.41	115.42	124.77
13	B	809	CLA	CMD-C2D-C1D	6.35	135.92	124.73
13	A	806	CLA	O2D-CGD-CBD	6.34	122.32	111.23
13	A	802	CLA	C4A-NA-C1A	-6.34	103.79	106.68
13	A	829	CLA	C2D-C1D-ND	6.32	116.39	110.13
13	B	803	CLA	O2D-CGD-CBD	6.32	122.28	111.23
13	A	807	CLA	CHD-C4C-C3C	-6.31	115.58	124.77
13	B	821	CLA	C2D-C1D-ND	6.30	116.36	110.13
13	B	821	CLA	CHD-C4C-C3C	-6.30	115.59	124.77
13	B	808	CLA	CMD-C2D-C1D	6.30	135.81	124.73
13	B	830	CLA	C2D-C1D-ND	6.28	116.34	110.13
13	B	808	CLA	C2D-C1D-ND	6.27	116.33	110.13
13	A	844	CLA	C2D-C1D-ND	6.27	116.33	110.13
13	K	203	CLA	O2D-CGD-CBD	6.26	122.18	111.23
13	A	803	CLA	C2D-C1D-ND	6.25	116.31	110.13
13	A	841	CLA	CMD-C2D-C1D	6.23	135.71	124.73
13	B	815	CLA	CMD-C2D-C1D	6.23	135.71	124.73
13	A	805	CLA	O2D-CGD-CBD	6.23	122.12	111.23
13	B	831	CLA	C2D-C1D-ND	6.23	116.29	110.13
13	A	810	CLA	CMD-C2D-C1D	6.22	135.69	124.73
13	A	813	CLA	CMD-C2D-C1D	6.21	135.67	124.73
13	A	822	CLA	CMD-C2D-C1D	6.20	135.65	124.73
13	A	831	CLA	O2D-CGD-CBD	6.20	122.06	111.23
13	A	825	CLA	CMD-C2D-C1D	6.19	135.62	124.73
13	A	838	CLA	CHD-C4C-C3C	-6.16	115.79	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	815	CLA	O2D-CGD-CBD	6.16	121.99	111.23
13	A	828	CLA	O2D-CGD-CBD	6.15	121.99	111.23
13	A	821	CLA	O2D-CGD-CBD	6.15	121.98	111.23
13	B	814	CLA	CMD-C2D-C1D	6.15	135.55	124.73
13	L	202	CLA	C2D-C1D-ND	6.14	116.20	110.13
13	B	807	CLA	CHD-C4C-C3C	-6.12	115.84	124.77
13	B	829	CLA	CHD-C4C-C3C	-6.10	115.88	124.77
13	A	805	CLA	C2D-C1D-ND	6.05	116.12	110.13
13	B	803	CLA	CHD-C4C-C3C	-6.05	115.96	124.77
13	A	818	CLA	CHD-C4C-C3C	-6.04	115.97	124.77
13	A	820	CLA	CMD-C2D-C1D	6.04	135.36	124.73
13	A	830	CLA	CHD-C4C-C3C	-6.03	115.99	124.77
13	B	805	CLA	CHD-C4C-C3C	-6.03	115.99	124.77
13	A	824	CLA	CMD-C2D-C1D	6.02	135.33	124.73
13	B	828	CLA	C2D-C1D-ND	6.02	116.09	110.13
13	A	826	CLA	C2D-C1D-ND	6.02	116.08	110.13
13	B	820	CLA	CHD-C4C-C3C	-6.02	116.00	124.77
13	B	807	CLA	C2D-C1D-ND	6.01	116.08	110.13
13	B	829	CLA	C2D-C1D-ND	6.01	116.07	110.13
13	A	840	CLA	CHD-C4C-C3C	-6.01	116.02	124.77
13	A	822	CLA	CHD-C4C-C3C	-6.00	116.03	124.77
13	A	844	CLA	CHD-C4C-C3C	-6.00	116.03	124.77
13	A	816	CLA	O2D-CGD-CBD	5.98	121.68	111.23
13	B	833	CLA	O2D-CGD-CBD	5.93	121.59	111.23
13	B	801	CLA	CMD-C2D-C1D	5.91	135.14	124.73
13	A	804	CLA	CMD-C2D-C1D	5.91	135.14	124.73
13	L	202	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
13	B	814	CLA	CHD-C4C-C3C	-5.91	116.16	124.77
13	A	820	CLA	O2D-CGD-CBD	5.90	121.55	111.23
13	A	828	CLA	C2D-C1D-ND	5.90	115.96	110.13
13	B	805	CLA	O2D-CGD-CBD	5.89	121.52	111.23
13	B	805	CLA	C2D-C1D-ND	5.89	115.95	110.13
13	B	817	CLA	C2D-C1D-ND	5.87	115.94	110.13
13	A	804	CLA	CHD-C4C-C3C	-5.87	116.21	124.77
13	A	842	CLA	C2D-C1D-ND	5.87	115.94	110.13
13	A	829	CLA	CMD-C2D-C1D	5.87	135.06	124.73
13	A	826	CLA	CHD-C4C-C3C	-5.86	116.23	124.77
13	A	835	CLA	C2D-C1D-ND	5.86	115.93	110.13
13	J	101	CLA	O2D-CGD-CBD	5.86	121.47	111.23
13	A	844	CLA	O2D-CGD-CBD	5.85	121.46	111.23
13	A	805	CLA	CHD-C4C-C3C	-5.85	116.24	124.77
13	A	806	CLA	C2D-C1D-ND	5.85	115.91	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	815	CLA	C2D-C1D-ND	5.85	115.91	110.13
13	A	831	CLA	C2D-C1D-ND	5.84	115.91	110.13
13	B	816	CLA	C2D-C1D-ND	5.84	115.90	110.13
13	B	816	CLA	CHD-C4C-C3C	-5.84	116.26	124.77
13	A	827	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
13	B	809	CLA	CHD-C4C-C3C	-5.83	116.27	124.77
13	A	817	CLA	C2C-C1C-NC	5.83	116.11	109.98
13	B	816	CLA	O2D-CGD-CBD	5.83	121.42	111.23
13	B	828	CLA	O2D-CGD-CBD	5.83	121.42	111.23
13	A	833	CLA	CHD-C4C-C3C	-5.82	116.28	124.77
13	B	804	CLA	C3B-C2B-C1B	-5.82	100.31	107.17
13	B	806	CLA	O2D-CGD-CBD	5.80	121.38	111.23
13	B	810	CLA	CHD-C4C-C3C	-5.80	116.32	124.77
13	B	823	CLA	C2C-C1C-NC	5.80	116.07	109.98
13	A	841	CLA	C2D-C1D-ND	5.79	115.86	110.13
13	A	836	CLA	C2D-C1D-ND	5.79	115.85	110.13
13	B	813	CLA	C2D-C1D-ND	5.79	115.85	110.13
13	A	833	CLA	C2D-C1D-ND	5.78	115.84	110.13
13	B	804	CLA	C2B-C1B-NB	5.78	116.31	110.33
13	B	804	CLA	CHD-C4C-C3C	-5.77	116.35	124.77
13	A	818	CLA	C2D-C1D-ND	5.77	115.84	110.13
13	A	839	CLA	C2D-C1D-ND	5.77	115.84	110.13
13	B	824	CLA	C2D-C1D-ND	5.77	115.84	110.13
13	K	203	CLA	CMD-C2D-C1D	5.77	134.89	124.73
13	B	820	CLA	C2D-C1D-ND	5.77	115.84	110.13
13	A	805	CLA	C2B-C1B-NB	5.76	116.30	110.33
13	B	811	CLA	O2D-CGD-CBD	5.76	121.30	111.23
13	A	830	CLA	C4A-NA-C1A	-5.76	104.05	106.68
13	A	821	CLA	C2D-C1D-ND	5.75	115.82	110.13
13	A	834	CLA	CHD-C4C-C3C	-5.75	116.39	124.77
13	B	818	CLA	CHD-C4C-C3C	-5.75	116.40	124.77
13	B	810	CLA	C2D-C1D-ND	5.74	115.81	110.13
13	L	202	CLA	C2B-C1B-NB	5.74	116.28	110.33
13	L	204	CLA	C2D-C1D-ND	5.74	115.80	110.13
13	B	801	CLA	C2D-C1D-ND	5.74	115.80	110.13
13	B	821	CLA	CMD-C2D-C1D	5.73	134.83	124.73
13	A	807	CLA	C2D-C1D-ND	5.73	115.80	110.13
13	A	815	CLA	CHD-C4C-C3C	-5.73	116.42	124.77
13	A	842	CLA	CHD-C4C-C3C	-5.72	116.43	124.77
13	B	802	CLA	CMD-C2D-C1D	5.71	134.79	124.73
13	J	101	CLA	C2D-C1D-ND	5.71	115.78	110.13
13	B	819	CLA	C2B-C1B-NB	5.71	116.25	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	827	CLA	C2D-C1D-ND	5.71	115.78	110.13
13	B	822	CLA	CHD-C4C-C3C	-5.71	116.45	124.77
13	A	834	CLA	C2D-C1D-ND	5.71	115.77	110.13
13	A	829	CLA	O2D-CGD-CBD	5.70	121.20	111.23
13	B	831	CLA	CHD-C4C-C3C	-5.70	116.46	124.77
13	A	815	CLA	C2B-C1B-NB	5.70	116.24	110.33
13	A	816	CLA	C2D-C1D-ND	5.68	115.75	110.13
13	A	819	CLA	C2B-C1B-NB	5.68	116.22	110.33
13	A	804	CLA	C2D-C1D-ND	5.68	115.75	110.13
13	A	823	CLA	CMD-C2D-C1D	5.67	134.72	124.73
13	A	817	CLA	C2D-C1D-ND	5.67	115.74	110.13
13	B	825	CLA	O2D-CGD-CBD	5.67	121.15	111.23
13	K	203	CLA	C2D-C1D-ND	5.66	115.73	110.13
13	A	806	CLA	CHD-C4C-C3C	-5.66	116.52	124.77
13	A	843	CLA	C2D-C1D-ND	5.66	115.73	110.13
13	B	817	CLA	CHD-C4C-C3C	-5.66	116.53	124.77
13	B	813	CLA	O2D-CGD-CBD	5.65	121.11	111.23
13	A	822	CLA	C2D-C1D-ND	5.64	115.71	110.13
13	A	825	CLA	C2B-C1B-NB	5.63	116.17	110.33
13	B	814	CLA	O2D-CGD-CBD	5.63	121.07	111.23
13	B	822	CLA	CMD-C2D-C1D	5.63	134.64	124.73
13	A	823	CLA	CHD-C4C-C3C	-5.63	116.57	124.77
13	A	802	CLA	C2C-C1C-NC	5.62	115.89	109.98
13	A	813	CLA	O2D-CGD-CBD	5.61	121.03	111.23
13	A	821	CLA	C2C-C1C-NC	5.60	115.87	109.98
13	A	806	CLA	C2B-C1B-NB	5.60	116.14	110.33
13	K	203	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
13	A	837	CLA	C2D-C1D-ND	5.60	115.67	110.13
13	B	825	CLA	CHD-C4C-C3C	-5.60	116.61	124.77
13	A	802	CLA	O2D-CGD-CBD	5.59	121.00	111.23
13	A	802	CLA	CHD-C4C-C3C	-5.58	116.63	124.77
13	A	835	CLA	CHD-C4C-C3C	-5.58	116.64	124.77
13	A	824	CLA	C2B-C1B-NB	5.58	116.11	110.33
13	A	819	CLA	C3B-C2B-C1B	-5.58	100.60	107.17
13	B	829	CLA	O2D-CGD-CBD	5.57	120.97	111.23
13	B	809	CLA	C2D-C1D-ND	5.56	115.63	110.13
13	B	803	CLA	C2B-C1B-NB	5.56	116.09	110.33
13	L	202	CLA	O2D-CGD-CBD	5.56	120.95	111.23
13	A	813	CLA	C2D-C1D-ND	5.56	115.63	110.13
13	B	814	CLA	C2D-C1D-ND	5.55	115.62	110.13
13	A	824	CLA	C2D-C1D-ND	5.55	115.62	110.13
13	B	830	CLA	CHD-C4C-C3C	-5.55	116.68	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	814	CLA	CHD-C4C-C3C	-5.54	116.69	124.77
13	A	824	CLA	C2C-C1C-NC	5.54	115.81	109.98
13	A	825	CLA	O2D-CGD-CBD	5.54	120.92	111.23
13	A	829	CLA	C2B-C1B-NB	5.54	116.07	110.33
13	J	101	CLA	C2B-C1B-NB	5.54	116.07	110.33
13	A	812	CLA	C2D-C1D-ND	5.53	115.60	110.13
13	L	204	CLA	C2B-C1B-NB	5.53	116.06	110.33
13	B	819	CLA	C3B-C2B-C1B	-5.53	100.66	107.17
13	B	801	CLA	CHD-C4C-C3C	-5.52	116.72	124.77
13	A	809	CLA	O2D-CGD-CBD	5.52	120.88	111.23
13	B	831	CLA	O2D-CGD-CBD	5.52	120.88	111.23
13	A	822	CLA	O2D-CGD-CBD	5.51	120.87	111.23
13	B	833	CLA	C2C-C1C-NC	5.51	115.77	109.98
13	A	839	CLA	CHD-C4C-C3C	-5.50	116.75	124.77
13	A	837	CLA	C2B-C1B-NB	5.49	116.02	110.33
13	B	820	CLA	O2D-CGD-CBD	5.49	120.83	111.23
13	A	842	CLA	C4A-NA-C1A	-5.49	104.17	106.68
13	B	829	CLA	C4A-NA-C1A	-5.49	104.17	106.68
13	K	201	CLA	C4A-NA-C1A	-5.49	104.17	106.68
13	A	836	CLA	CHD-C4C-C3C	-5.49	116.77	124.77
13	F	203	CLA	C2D-C1D-ND	5.49	115.56	110.13
13	A	836	CLA	CMD-C2D-C1D	5.48	134.38	124.73
13	A	840	CLA	C2D-C1D-ND	5.48	115.55	110.13
13	B	826	CLA	C2B-C1B-NB	5.48	116.01	110.33
13	A	814	CLA	C2D-C1D-ND	5.48	115.55	110.13
13	B	832	CLA	C2D-C1D-ND	5.48	115.55	110.13
13	B	812	CLA	C2D-C1D-ND	5.47	115.54	110.13
13	B	818	CLA	C2D-C1D-ND	5.47	115.54	110.13
13	A	831	CLA	CHD-C4C-C3C	-5.47	116.80	124.77
13	A	815	CLA	C2D-C1D-ND	5.47	115.54	110.13
13	A	837	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
13	B	803	CLA	C3B-C2B-C1B	-5.46	100.73	107.17
13	A	841	CLA	CHD-C4C-C3C	-5.46	116.81	124.77
13	A	827	CLA	C2D-C1D-ND	5.46	115.53	110.13
13	B	815	CLA	C2B-C1B-NB	5.46	115.98	110.33
13	B	832	CLA	C2B-C1B-NB	5.45	115.98	110.33
13	A	803	CLA	CHD-C4C-C3C	-5.45	116.83	124.77
13	A	829	CLA	C3B-C2B-C1B	-5.45	100.75	107.17
13	A	811	CLA	C2C-C1C-NC	5.45	115.70	109.98
13	L	204	CLA	CHD-C4C-C3C	-5.44	116.84	124.77
13	B	817	CLA	C4A-NA-C1A	-5.44	104.20	106.68
13	B	825	CLA	C2B-C1B-NB	5.43	115.96	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	824	CLA	C4A-NA-C1A	-5.43	104.20	106.68
13	A	815	CLA	O2D-CGD-CBD	5.42	120.71	111.23
13	A	803	CLA	C3B-C2B-C1B	-5.42	100.78	107.17
13	A	813	CLA	CHD-C4C-C3C	-5.42	116.88	124.77
13	A	830	CLA	CMD-C2D-C1D	5.41	134.26	124.73
13	A	838	CLA	C3B-C2B-C1B	-5.41	100.80	107.17
13	A	804	CLA	C2B-C1B-NB	5.41	115.93	110.33
13	K	201	CLA	C2D-C1D-ND	5.39	115.46	110.13
13	A	842	CLA	O2D-CGD-CBD	5.37	120.62	111.23
13	B	806	CLA	C2C-C1C-NC	5.37	115.62	109.98
13	B	815	CLA	CHD-C4C-C3C	-5.37	116.94	124.77
13	B	821	CLA	O2D-CGD-CBD	5.37	120.61	111.23
13	B	821	CLA	C3B-C2B-C1B	-5.37	100.84	107.17
13	A	835	CLA	C2B-C1B-NB	5.37	115.89	110.33
13	B	805	CLA	C2B-C1B-NB	5.36	115.88	110.33
13	B	819	CLA	C4A-NA-C1A	-5.35	104.24	106.68
13	B	806	CLA	C2D-C1D-ND	5.35	115.42	110.13
13	A	807	CLA	C2B-C1B-NB	5.35	115.88	110.33
13	B	818	CLA	C2C-C1C-NC	5.35	115.60	109.98
13	A	811	CLA	C2D-C1D-ND	5.35	115.42	110.13
13	A	844	CLA	C2B-C1B-NB	5.35	115.87	110.33
13	A	809	CLA	C2B-C1B-NB	5.35	115.87	110.33
13	A	821	CLA	CHD-C4C-C3C	-5.35	116.98	124.77
13	A	806	CLA	C3B-C2B-C1B	-5.34	100.87	107.17
13	B	812	CLA	CHD-C4C-C3C	-5.34	116.99	124.77
13	A	809	CLA	CMD-C2D-C1D	5.34	134.13	124.73
13	A	827	CLA	C2B-C1B-NB	5.34	115.86	110.33
13	A	820	CLA	C4A-NA-C1A	-5.34	104.24	106.68
13	L	203	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
13	A	810	CLA	CHD-C4C-C3C	-5.33	117.00	124.77
13	L	203	CLA	O2D-CGD-CBD	5.33	120.55	111.23
13	A	831	CLA	C2C-C1C-NC	5.33	115.58	109.98
13	A	809	CLA	CHD-C4C-C3C	-5.32	117.01	124.77
13	A	843	CLA	CHD-C4C-C3C	-5.32	117.01	124.77
13	A	827	CLA	C3B-C2B-C1B	-5.32	100.90	107.17
12	A	801	CL0	CHA-C1A-C2A	-5.32	120.81	133.31
13	B	808	CLA	CHD-C4C-C3C	-5.32	117.02	124.77
13	B	824	CLA	C2B-C1B-NB	5.31	115.84	110.33
13	J	101	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
13	A	838	CLA	C2D-C1D-ND	5.31	115.38	110.13
13	K	201	CLA	CHD-C4C-C3C	-5.31	117.03	124.77
13	A	815	CLA	C3B-C2B-C1B	-5.31	100.91	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	816	CLA	C2B-C1B-NB	5.30	115.83	110.33
13	A	835	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
13	B	805	CLA	C3B-C2B-C1B	-5.30	100.93	107.17
13	A	802	CLA	C2B-C1B-NB	5.29	115.81	110.33
13	B	806	CLA	C2B-C1B-NB	5.29	115.81	110.33
13	A	833	CLA	O2D-CGD-CBD	5.29	120.48	111.23
13	A	810	CLA	C2C-C1C-NC	5.29	115.54	109.98
13	B	809	CLA	C2B-C1B-NB	5.28	115.80	110.33
13	B	811	CLA	C4A-NA-C1A	-5.27	104.27	106.68
13	A	824	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
13	B	806	CLA	CHD-C4C-C3C	-5.27	117.09	124.77
13	B	814	CLA	C2B-C1B-NB	5.27	115.79	110.33
13	B	822	CLA	C2D-C1D-ND	5.26	115.33	110.13
13	A	810	CLA	C2D-C1D-ND	5.26	115.33	110.13
13	A	841	CLA	C2B-C1B-NB	5.26	115.78	110.33
13	B	833	CLA	C2D-C1D-ND	5.25	115.33	110.13
13	A	811	CLA	CHD-C4C-C3C	-5.25	117.11	124.77
13	B	825	CLA	C3D-C2D-C1D	-5.24	98.68	105.83
13	A	827	CLA	C4A-NA-C1A	-5.24	104.29	106.68
13	K	203	CLA	C2C-C1C-NC	5.24	115.48	109.98
13	B	824	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
13	B	817	CLA	C2B-C1B-NB	5.23	115.75	110.33
13	F	203	CLA	CHD-C4C-C3C	-5.23	117.15	124.77
13	A	819	CLA	CHD-C4C-C3C	-5.22	117.16	124.77
12	A	801	CL0	CBC-CAC-C3C	-5.22	105.40	112.87
13	B	808	CLA	O2D-CGD-CBD	5.22	120.36	111.23
13	B	812	CLA	C2C-C1C-NC	5.21	115.46	109.98
13	A	830	CLA	C2B-C1B-NB	5.21	115.73	110.33
13	B	813	CLA	CHD-C4C-C3C	-5.21	117.17	124.77
13	A	824	CLA	C4A-NA-C1A	-5.21	104.30	106.68
13	B	828	CLA	CHD-C4C-C3C	-5.21	117.18	124.77
13	A	820	CLA	C2C-C1C-NC	5.21	115.45	109.98
13	L	204	CLA	C3B-C2B-C1B	-5.21	101.03	107.17
13	B	832	CLA	CHD-C4C-C3C	-5.20	117.19	124.77
13	B	828	CLA	C4A-NA-C1A	-5.20	104.31	106.68
13	A	808	CLA	C2C-C1C-NC	5.20	115.44	109.98
13	A	825	CLA	C2D-C1D-ND	5.20	115.27	110.13
13	B	812	CLA	C2B-C1B-NB	5.20	115.72	110.33
13	A	809	CLA	C3B-C2B-C1B	-5.20	101.04	107.17
13	A	843	CLA	O2D-CGD-CBD	5.20	120.31	111.23
13	B	820	CLA	C4A-NA-C1A	-5.19	104.31	106.68
13	A	828	CLA	C2B-C1B-NB	5.19	115.71	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	821	CLA	C2B-C1B-NB	5.19	115.71	110.33
13	A	836	CLA	C2C-C1C-NC	5.19	115.43	109.98
13	B	811	CLA	C2C-C1C-NC	5.19	115.43	109.98
13	B	813	CLA	C2B-C1B-NB	5.19	115.71	110.33
13	B	820	CLA	C2B-C1B-NB	5.19	115.71	110.33
13	A	807	CLA	C4A-NA-C1A	-5.19	104.31	106.68
13	A	816	CLA	CHD-C4C-C3C	-5.18	117.22	124.77
13	A	807	CLA	C3B-C2B-C1B	-5.18	101.06	107.17
13	B	830	CLA	O2D-CGD-CBD	5.18	120.28	111.23
13	A	843	CLA	C2B-C1B-NB	5.18	115.69	110.33
13	F	203	CLA	C2B-C1B-NB	5.17	115.69	110.33
13	A	808	CLA	C2B-C1B-NB	5.17	115.69	110.33
13	A	840	CLA	C2C-C1C-NC	5.16	115.41	109.98
13	B	812	CLA	C4A-NA-C1A	-5.16	104.33	106.68
13	B	814	CLA	C3B-C2B-C1B	-5.15	101.09	107.17
13	B	807	CLA	C2B-C1B-NB	5.15	115.67	110.33
13	B	829	CLA	C2B-C1B-NB	5.15	115.67	110.33
13	A	820	CLA	C2D-C1D-ND	5.15	115.22	110.13
13	B	818	CLA	O2D-CGD-CBD	5.14	120.22	111.23
13	B	819	CLA	CHD-C4C-C3C	-5.14	117.28	124.77
13	B	802	CLA	C3B-C2B-C1B	-5.14	101.11	107.17
13	A	825	CLA	C3B-C2B-C1B	-5.14	101.12	107.17
13	B	813	CLA	C4A-NA-C1A	-5.13	104.34	106.68
13	A	819	CLA	C2C-C1C-NC	5.13	115.37	109.98
13	A	813	CLA	C2C-C1C-NC	5.13	115.36	109.98
13	A	802	CLA	C2D-C1D-ND	5.12	115.20	110.13
13	A	812	CLA	CHD-C4C-C3C	-5.12	117.31	124.77
13	L	202	CLA	C3B-C2B-C1B	-5.12	101.13	107.17
13	A	812	CLA	O2D-CGD-CBD	5.12	120.18	111.23
13	B	833	CLA	CHD-C4C-C3C	-5.12	117.31	124.77
13	A	832	CLA	C2C-C1C-NC	5.11	115.35	109.98
13	B	827	CLA	CHD-C4C-C3C	-5.11	117.32	124.77
13	A	811	CLA	O2D-CGD-CBD	5.11	120.16	111.23
13	A	812	CLA	C2C-C1C-NC	5.11	115.34	109.98
13	A	825	CLA	C2C-C1C-NC	5.11	115.34	109.98
13	B	803	CLA	C4A-NA-C1A	-5.10	104.35	106.68
13	B	822	CLA	C2B-C1B-NB	5.10	115.62	110.33
13	B	804	CLA	CMD-C2D-C1D	5.10	133.71	124.73
13	F	203	CLA	C4A-NA-C1A	-5.10	104.35	106.68
13	B	829	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
13	B	816	CLA	C2B-C1B-NB	5.10	115.61	110.33
13	A	802	CLA	C3B-C2B-C1B	-5.10	101.16	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	818	CLA	C2C-C1C-NC	5.10	115.34	109.98
13	A	843	CLA	C3B-C2B-C1B	-5.10	101.16	107.17
13	A	814	CLA	C4A-NA-C1A	-5.09	104.36	106.68
13	B	826	CLA	C2D-C1D-ND	5.09	115.17	110.13
13	B	813	CLA	C3B-C2B-C1B	-5.09	101.17	107.17
13	B	815	CLA	C3B-C2B-C1B	-5.08	101.18	107.17
13	B	816	CLA	C2C-C1C-NC	5.08	115.32	109.98
13	B	828	CLA	C2C-C1C-NC	5.08	115.32	109.98
13	A	842	CLA	C2B-C1B-NB	5.08	115.59	110.33
13	A	841	CLA	C2C-C1C-NC	5.08	115.31	109.98
13	A	814	CLA	C2B-C1B-NB	5.07	115.59	110.33
13	B	827	CLA	C2B-C1B-NB	5.07	115.59	110.33
13	B	828	CLA	C2B-C1B-NB	5.07	115.59	110.33
13	B	832	CLA	C3B-C2B-C1B	-5.07	101.19	107.17
13	B	812	CLA	O2D-CGD-CBD	5.06	120.08	111.23
13	A	818	CLA	C2B-C1B-NB	5.06	115.57	110.33
13	A	830	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
13	A	834	CLA	C3B-C2B-C1B	-5.06	101.21	107.17
13	A	816	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
13	A	842	CLA	C3B-C2B-C1B	-5.05	101.21	107.17
13	B	809	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
13	A	834	CLA	C2C-C1C-NC	5.05	115.28	109.98
13	B	824	CLA	C3B-C2B-C1B	-5.05	101.22	107.17
13	B	830	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
13	A	826	CLA	CMD-C2D-C1D	5.04	133.61	124.73
13	L	204	CLA	O2D-CGD-CBD	5.04	120.05	111.23
13	B	819	CLA	C2D-C1D-ND	5.04	115.11	110.13
13	A	819	CLA	C2D-C1D-ND	5.04	115.11	110.13
13	B	822	CLA	O2D-CGD-CBD	5.04	120.03	111.23
13	B	807	CLA	C3D-C2D-C1D	-5.04	98.96	105.83
13	A	834	CLA	C2B-C1B-NB	5.03	115.54	110.33
13	B	808	CLA	C2B-C1B-NB	5.03	115.54	110.33
13	A	805	CLA	C3B-C2B-C1B	-5.02	101.25	107.17
13	A	812	CLA	C2B-C1B-NB	5.02	115.53	110.33
13	B	813	CLA	CAC-C3C-C4C	5.02	131.32	124.79
13	A	836	CLA	C2B-C1B-NB	5.02	115.53	110.33
13	K	201	CLA	C2B-C1B-NB	5.02	115.53	110.33
13	L	203	CLA	C3D-C2D-C1D	-5.01	98.99	105.83
13	B	829	CLA	C3D-C2D-C1D	-5.01	99.00	105.83
13	F	203	CLA	O2D-CGD-CBD	5.00	119.97	111.23
13	B	801	CLA	C2C-C1C-NC	5.00	115.23	109.98
13	A	826	CLA	O2D-CGD-CBD	5.00	119.97	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	822	CLA	C2C-C1C-NC	5.00	115.23	109.98
13	A	837	CLA	C3B-C2B-C1B	-4.99	101.28	107.17
13	A	842	CLA	C2C-C1C-NC	4.99	115.23	109.98
13	A	830	CLA	C2D-C1D-ND	4.99	115.07	110.13
13	B	815	CLA	C2C-C1C-NC	4.99	115.22	109.98
13	B	826	CLA	C3B-C2B-C1B	-4.99	101.29	107.17
13	A	835	CLA	C2C-C1C-NC	4.98	115.21	109.98
13	A	832	CLA	CHD-C4C-C3C	-4.98	117.51	124.77
13	B	804	CLA	C3D-C2D-C1D	-4.98	99.04	105.83
13	L	203	CLA	C3B-C2B-C1B	-4.97	101.31	107.17
13	A	813	CLA	C2B-C1B-NB	4.97	115.48	110.33
13	B	811	CLA	C2B-C1B-NB	4.97	115.48	110.33
13	A	841	CLA	C4A-NA-C1A	-4.97	104.41	106.68
13	F	203	CLA	C2C-C1C-NC	4.97	115.20	109.98
13	A	807	CLA	O2D-CGD-CBD	4.97	119.91	111.23
13	A	839	CLA	C2C-C1C-NC	4.96	115.20	109.98
13	B	830	CLA	C2B-C1B-NB	4.96	115.47	110.33
13	A	828	CLA	C3D-C2D-C1D	-4.96	99.06	105.83
13	B	832	CLA	C4A-NA-C1A	-4.96	104.42	106.68
13	A	817	CLA	CHD-C4C-C3C	-4.96	117.54	124.77
13	B	832	CLA	C2C-C1C-NC	4.96	115.19	109.98
13	A	826	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
13	B	816	CLA	C3B-C2B-C1B	-4.95	101.34	107.17
12	A	801	CL0	CMA-C3A-C4A	-4.95	103.96	114.61
13	A	820	CLA	C2B-C1B-NB	4.94	115.45	110.33
13	A	810	CLA	O2D-CGD-CBD	4.94	119.87	111.23
13	B	831	CLA	C3D-C2D-C1D	-4.94	99.09	105.83
13	B	831	CLA	C2C-C1C-NC	4.94	115.17	109.98
13	B	810	CLA	C2C-C1C-NC	4.94	115.17	109.98
13	K	201	CLA	C3B-C2B-C1B	-4.94	101.35	107.17
13	A	833	CLA	C2B-C1B-NB	4.93	115.44	110.33
13	A	829	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
13	B	808	CLA	C3D-C2D-C1D	-4.93	99.11	105.83
13	A	836	CLA	O2D-CGD-CBD	4.92	119.83	111.23
13	A	840	CLA	C2B-C1B-NB	4.91	115.42	110.33
13	L	204	CLA	C4A-NA-C1A	-4.91	104.44	106.68
13	B	819	CLA	O2D-CGD-CBD	4.91	119.81	111.23
13	B	808	CLA	C2C-C1C-NC	4.90	115.13	109.98
13	A	808	CLA	CHD-C4C-C3C	-4.90	117.63	124.77
13	A	820	CLA	CHD-C4C-C3C	-4.90	117.63	124.77
13	A	826	CLA	C2B-C1B-NB	4.90	115.40	110.33
13	F	203	CLA	C3B-C2B-C1B	-4.89	101.40	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	816	CLA	C2C-C1C-NC	4.89	115.12	109.98
13	A	832	CLA	C3B-C2B-C1B	-4.89	101.41	107.17
13	B	831	CLA	C2B-C1B-NB	4.88	115.38	110.33
13	A	805	CLA	C3D-C2D-C1D	-4.88	99.18	105.83
13	A	807	CLA	CAA-C2A-C3A	-4.87	99.83	113.00
13	A	831	CLA	C2B-C1B-NB	4.87	115.37	110.33
13	B	818	CLA	C2B-C1B-NB	4.87	115.37	110.33
13	B	807	CLA	C2C-C1C-NC	4.87	115.09	109.98
13	A	844	CLA	C3D-C2D-C1D	-4.86	99.19	105.83
13	B	804	CLA	O2D-CGD-CBD	4.86	119.73	111.23
13	J	101	CLA	C2C-C1C-NC	4.85	115.08	109.98
13	A	814	CLA	C3B-C2B-C1B	-4.85	101.45	107.17
13	B	802	CLA	C1D-CHD-C4C	-4.85	115.71	126.02
13	A	808	CLA	C2D-C1D-ND	4.85	114.93	110.13
13	B	807	CLA	C3B-C2B-C1B	-4.84	101.46	107.17
13	A	823	CLA	C2B-C1B-NB	4.84	115.35	110.33
13	B	831	CLA	C3B-C2B-C1B	-4.84	101.47	107.17
13	L	202	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
13	B	802	CLA	C2B-C1B-NB	4.83	115.34	110.33
13	B	802	CLA	C3D-C2D-C1D	-4.83	99.24	105.83
13	B	827	CLA	C2C-C1C-NC	4.83	115.05	109.98
13	A	818	CLA	O2D-CGD-CBD	4.83	119.67	111.23
13	A	832	CLA	C2B-C1B-NB	4.82	115.33	110.33
13	B	817	CLA	C3D-C2D-C1D	-4.82	99.25	105.83
13	A	822	CLA	C2B-C1B-NB	4.82	115.32	110.33
13	B	820	CLA	C3D-C2D-C1D	-4.82	99.26	105.83
13	K	203	CLA	C2B-C1B-NB	4.82	115.32	110.33
13	A	808	CLA	C3B-C2B-C1B	-4.81	101.50	107.17
13	B	814	CLA	C2C-C1C-NC	4.80	115.03	109.98
13	A	804	CLA	C4A-NA-C1A	-4.80	104.49	106.68
13	A	819	CLA	C4A-NA-C1A	-4.80	104.49	106.68
13	B	817	CLA	C3B-C2B-C1B	-4.80	101.51	107.17
13	B	830	CLA	CHD-C1D-ND	-4.80	118.05	124.80
13	A	809	CLA	C3D-C2D-C1D	-4.79	99.29	105.83
13	A	830	CLA	C2C-C1C-NC	4.79	115.02	109.98
13	B	826	CLA	C2C-C1C-NC	4.78	115.01	109.98
13	A	839	CLA	C2B-C1B-NB	4.78	115.29	110.33
13	A	838	CLA	C2C-C1C-NC	4.78	115.00	109.98
13	A	837	CLA	C2C-C1C-NC	4.78	115.00	109.98
13	A	821	CLA	C3B-C2B-C1B	-4.77	101.54	107.17
13	L	203	CLA	C2B-C1B-NB	4.77	115.28	110.33
13	A	810	CLA	C2B-C1B-NB	4.77	115.27	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	803	CLA	C2C-C1C-NC	4.76	114.99	109.98
13	A	842	CLA	C3D-C2D-C1D	-4.76	99.33	105.83
13	B	824	CLA	O2D-CGD-CBD	4.76	119.55	111.23
13	L	203	CLA	CHD-C1D-ND	-4.76	118.11	124.80
13	A	844	CLA	C3B-C2B-C1B	-4.76	101.56	107.17
13	B	822	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
13	A	823	CLA	C3B-C2B-C1B	-4.75	101.57	107.17
13	B	827	CLA	O2D-CGD-CBD	4.75	119.53	111.23
13	A	825	CLA	C4A-NA-C1A	-4.75	104.51	106.68
13	A	818	CLA	C3B-C2B-C1B	-4.75	101.58	107.17
13	A	835	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
13	B	808	CLA	C3B-C2B-C1B	-4.74	101.58	107.17
13	A	807	CLA	C3D-C2D-C1D	-4.74	99.36	105.83
13	L	203	CLA	C2C-C1C-NC	4.74	114.96	109.98
13	B	810	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
13	B	828	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
13	A	833	CLA	C3D-C2D-C1D	-4.73	99.38	105.83
13	B	811	CLA	CHD-C4C-C3C	-4.72	117.89	124.77
13	A	821	CLA	C2B-C1B-NB	4.72	115.22	110.33
13	K	203	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
13	B	825	CLA	CHD-C1D-ND	-4.72	118.16	124.80
13	A	823	CLA	C3D-C2D-C1D	-4.72	99.39	105.83
13	B	820	CLA	C3B-C2B-C1B	-4.72	101.61	107.17
13	B	825	CLA	C4A-NA-C1A	-4.71	104.53	106.68
13	A	833	CLA	C4A-NA-C1A	-4.71	104.53	106.68
13	B	803	CLA	C3D-C2D-C1D	-4.71	99.40	105.83
13	B	811	CLA	C3B-C2B-C1B	-4.71	101.62	107.17
13	B	821	CLA	C3D-C2D-C1D	-4.70	99.41	105.83
13	A	832	CLA	C2D-C1D-ND	4.70	114.78	110.13
13	L	202	CLA	C2C-C1C-NC	4.70	114.92	109.98
13	A	804	CLA	C3B-C2B-C1B	-4.69	101.64	107.17
13	B	826	CLA	CHD-C4C-C3C	-4.69	117.93	124.77
13	A	819	CLA	O2D-CGD-CBD	4.69	119.43	111.23
13	B	811	CLA	C2D-C1D-ND	4.69	114.77	110.13
13	L	204	CLA	C3D-C2D-C1D	-4.69	99.43	105.83
13	A	824	CLA	C3B-C2B-C1B	-4.68	101.65	107.17
13	B	816	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
13	A	831	CLA	C3D-C2D-C1D	-4.68	99.44	105.83
13	B	813	CLA	C3D-C2D-C1D	-4.67	99.45	105.83
13	A	844	CLA	C2C-C1C-NC	4.67	114.89	109.98
13	A	838	CLA	C3D-C2D-C1D	-4.67	99.46	105.83
13	B	803	CLA	CMD-C2D-C1D	4.67	132.95	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	814	CLA	C2C-C1C-NC	4.66	114.88	109.98
13	B	824	CLA	C2C-C1C-NC	4.66	114.88	109.98
13	A	839	CLA	C3D-C2D-C1D	-4.66	99.47	105.83
13	A	808	CLA	C4A-NA-C1A	-4.66	104.55	106.68
13	B	806	CLA	C3B-C2B-C1B	-4.66	101.68	107.17
13	B	824	CLA	C3D-C2D-C1D	-4.65	99.48	105.83
13	L	203	CLA	C3D-C4D-ND	4.65	117.55	109.99
13	A	835	CLA	O2D-CGD-O1D	-4.65	114.79	123.85
13	B	823	CLA	C4A-NA-C1A	-4.65	104.56	106.68
13	A	843	CLA	C2C-C1C-NC	4.65	114.86	109.98
13	A	814	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
13	A	822	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
13	B	828	CLA	C3B-C2B-C1B	-4.64	101.70	107.17
13	A	821	CLA	C1C-C2C-C3C	-4.64	102.10	106.98
13	B	830	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
13	B	817	CLA	O2D-CGD-CBD	4.63	119.33	111.23
13	B	825	CLA	C3D-C4D-ND	4.63	117.52	109.99
13	J	101	CLA	C3B-C2B-C1B	-4.63	101.71	107.17
13	B	804	CLA	C1D-CHD-C4C	-4.63	116.18	126.02
12	A	801	CL0	CAA-C2A-C3A	-4.63	100.49	113.00
13	J	101	CLA	C3D-C2D-C1D	-4.62	99.52	105.83
13	B	828	CLA	CHD-C1D-ND	-4.62	118.30	124.80
13	B	819	CLA	CAA-C2A-C3A	-4.62	100.52	113.00
13	A	841	CLA	C3D-C2D-C1D	-4.61	99.53	105.83
13	A	818	CLA	C1D-CHD-C4C	-4.61	116.22	126.02
13	A	834	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
13	A	840	CLA	C4A-NA-C1A	-4.60	104.58	106.68
13	A	815	CLA	C3D-C2D-C1D	-4.60	99.55	105.83
13	A	833	CLA	C2C-C1C-NC	4.60	114.81	109.98
13	A	837	CLA	C4A-NA-C1A	-4.59	104.58	106.68
13	B	802	CLA	C2C-C1C-NC	4.59	114.81	109.98
13	A	808	CLA	O2D-CGD-CBD	4.59	119.25	111.23
13	B	822	CLA	C4A-NA-C1A	-4.59	104.59	106.68
13	B	815	CLA	C3D-C2D-C1D	-4.58	99.58	105.83
13	A	827	CLA	CAA-C2A-C3A	-4.58	100.62	113.00
13	A	838	CLA	C2B-C1B-NB	4.58	115.07	110.33
13	A	833	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
13	A	813	CLA	C3B-C2B-C1B	-4.57	101.78	107.17
13	A	803	CLA	CMD-C2D-C1D	4.57	132.78	124.73
13	A	811	CLA	C2B-C1B-NB	4.57	115.06	110.33
13	A	837	CLA	C3D-C2D-C1D	-4.57	99.60	105.83
13	B	820	CLA	C2C-C1C-NC	4.57	114.78	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	809	CLA	C2C-C1C-NC	4.57	114.78	109.98
13	A	812	CLA	C3B-C2B-C1B	-4.57	101.79	107.17
13	A	812	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
13	B	805	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
13	A	827	CLA	C3D-C2D-C1D	-4.56	99.61	105.83
13	B	818	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
13	A	821	CLA	C3D-C2D-C1D	-4.55	99.62	105.83
13	A	812	CLA	C4A-NA-C1A	-4.55	104.60	106.68
13	B	821	CLA	C2C-C1C-NC	4.54	114.75	109.98
13	B	826	CLA	C3D-C4D-ND	4.54	117.37	109.99
13	F	203	CLA	C3D-C2D-C1D	-4.54	99.63	105.83
13	A	809	CLA	C2C-C1C-NC	4.54	114.75	109.98
13	A	825	CLA	CHD-C4C-C3C	-4.53	118.17	124.77
13	A	836	CLA	C3B-C2B-C1B	-4.53	101.83	107.17
13	B	808	CLA	CHD-C1D-ND	-4.53	118.43	124.80
13	K	201	CLA	C3D-C4D-ND	4.52	117.34	109.99
13	A	817	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
13	B	819	CLA	C3D-C4D-ND	4.51	117.32	109.99
13	A	828	CLA	C3B-C2B-C1B	-4.51	101.85	107.17
13	B	825	CLA	C3B-C2B-C1B	-4.51	101.86	107.17
13	A	818	CLA	C3D-C4D-ND	4.50	117.30	109.99
13	A	817	CLA	C2B-C1B-NB	4.49	114.99	110.33
13	B	817	CLA	C2C-C1C-NC	4.49	114.70	109.98
13	A	806	CLA	C3D-C2D-C1D	-4.49	99.71	105.83
13	A	802	CLA	CAA-C2A-C3A	-4.48	100.88	113.00
13	B	802	CLA	CAA-C2A-C3A	-4.48	100.88	113.00
13	A	822	CLA	C2C-C1C-NC	4.48	114.69	109.98
13	A	816	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
13	A	840	CLA	C3D-C2D-C1D	-4.48	99.72	105.83
13	B	832	CLA	O2D-CGD-CBD	4.47	119.04	111.23
13	B	810	CLA	C2B-C1B-NB	4.47	114.96	110.33
13	B	801	CLA	C3B-C2B-C1B	-4.46	101.91	107.17
13	A	830	CLA	O2D-CGD-CBD	4.46	119.03	111.23
13	A	825	CLA	C3D-C2D-C1D	-4.46	99.75	105.83
13	K	201	CLA	C2C-C1C-NC	4.45	114.66	109.98
13	B	824	CLA	CHD-C1D-ND	-4.45	118.53	124.80
13	A	821	CLA	CBC-CAC-C3C	-4.45	100.35	112.42
13	A	827	CLA	CHD-C1D-ND	-4.45	118.53	124.80
13	B	801	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
13	A	836	CLA	C4A-NA-C1A	-4.45	104.65	106.68
13	B	824	CLA	C3D-C4D-ND	4.45	117.22	109.99
17	A	852	LHG	O4-P-O5	4.44	133.12	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	826	CLA	CAC-C3C-C4C	4.44	130.57	124.79
13	A	823	CLA	C2C-C1C-NC	4.44	114.65	109.98
13	K	201	CLA	C3D-C2D-C1D	-4.44	99.77	105.83
13	A	826	CLA	C3D-C2D-C1D	-4.43	99.78	105.83
13	A	824	CLA	O2D-CGD-CBD	4.43	118.98	111.23
13	A	814	CLA	O2D-CGD-CBD	4.43	118.98	111.23
13	B	825	CLA	C2C-C1C-NC	4.43	114.64	109.98
13	B	806	CLA	C3D-C2D-C1D	-4.43	99.79	105.83
13	B	830	CLA	C3D-C4D-ND	4.43	117.19	109.99
13	A	840	CLA	C3B-C2B-C1B	-4.43	101.95	107.17
13	B	828	CLA	C3D-C4D-ND	4.43	117.18	109.99
13	B	801	CLA	O2D-CGD-CBD	4.43	118.97	111.23
13	B	827	CLA	C3D-C2D-C1D	-4.42	99.79	105.83
13	A	836	CLA	C3D-C4D-ND	4.42	117.18	109.99
13	A	831	CLA	C1D-CHD-C4C	-4.42	116.62	126.02
13	A	802	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
13	A	804	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
13	B	832	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
13	B	823	CLA	C2B-C1B-NB	4.41	114.90	110.33
13	A	818	CLA	C3D-C2D-C1D	-4.41	99.81	105.83
13	B	832	CLA	C3D-C4D-ND	4.41	117.16	109.99
13	A	802	CLA	CHD-C1D-ND	-4.41	118.60	124.80
13	B	805	CLA	C3D-C4D-ND	4.41	117.15	109.99
13	A	816	CLA	C3D-C4D-ND	4.41	117.15	109.99
13	A	824	CLA	C3D-C4D-ND	4.40	117.15	109.99
13	A	822	CLA	C3D-C2D-C1D	-4.40	99.82	105.83
13	A	823	CLA	C3D-C4D-ND	4.40	117.14	109.99
13	A	843	CLA	C3D-C2D-C1D	-4.40	99.83	105.83
13	L	204	CLA	C2C-C1C-NC	4.40	114.60	109.98
13	A	819	CLA	C1D-CHD-C4C	-4.39	116.68	126.02
13	A	819	CLA	C3D-C2D-C1D	-4.39	99.84	105.83
17	A	853	LHG	O4-P-O5	4.39	132.85	112.44
13	A	827	CLA	O2D-CGD-CBD	4.39	118.90	111.23
13	B	811	CLA	C3D-C4D-ND	4.39	117.12	109.99
13	B	819	CLA	C2C-C1C-NC	4.38	114.59	109.98
13	B	812	CLA	C3D-C2D-C1D	-4.38	99.85	105.83
13	B	812	CLA	C3B-C2B-C1B	-4.38	102.00	107.17
13	A	811	CLA	C1C-C2C-C3C	-4.38	102.38	106.98
13	B	827	CLA	C3D-C4D-ND	4.38	117.10	109.99
13	B	813	CLA	C2C-C1C-NC	4.38	114.58	109.98
13	A	813	CLA	C3D-C2D-C1D	-4.38	99.86	105.83
13	A	812	CLA	C3D-C4D-ND	4.38	117.10	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	832	CLA	C3D-C4D-ND	4.37	117.10	109.99
13	A	822	CLA	C4A-NA-C1A	-4.37	104.69	106.68
13	A	829	CLA	C3C-C4C-NC	4.37	116.03	110.43
13	A	809	CLA	C4A-NA-C1A	-4.37	104.69	106.68
13	B	807	CLA	C4A-NA-C1A	-4.36	104.69	106.68
13	B	801	CLA	C2B-C1B-NB	4.36	114.85	110.33
13	B	805	CLA	C2C-C1C-NC	4.36	114.56	109.98
13	A	835	CLA	CMB-C2B-C1B	4.36	132.06	125.42
13	B	826	CLA	CAA-C2A-C3A	-4.36	101.22	113.00
13	A	806	CLA	C3D-C4D-ND	4.36	117.07	109.99
13	B	833	CLA	C3D-C2D-C1D	-4.36	99.88	105.83
13	A	804	CLA	C1D-CHD-C4C	-4.36	116.76	126.02
13	A	820	CLA	C3D-C2D-C1D	-4.35	99.89	105.83
13	L	204	CLA	C3D-C4D-ND	4.35	117.06	109.99
13	A	815	CLA	C4A-NA-C1A	-4.35	104.70	106.68
13	A	817	CLA	C1C-C2C-C3C	-4.35	102.41	106.98
13	B	823	CLA	C3B-C4B-NB	4.34	114.41	110.53
13	A	842	CLA	CHD-C1D-ND	-4.34	118.69	124.80
13	B	832	CLA	CHD-C1D-ND	-4.34	118.70	124.80
13	A	810	CLA	C3B-C2B-C1B	-4.34	102.06	107.17
13	A	828	CLA	C1D-CHD-C4C	-4.34	116.81	126.02
13	A	803	CLA	O2D-CGD-CBD	4.33	118.81	111.23
13	K	203	CLA	C4A-NA-C1A	-4.33	104.70	106.68
13	B	802	CLA	CMB-C2B-C1B	4.33	132.01	125.42
13	A	839	CLA	C3B-C2B-C1B	-4.32	102.07	107.17
13	L	202	CLA	C3D-C4D-ND	4.31	117.00	109.99
13	B	810	CLA	C4A-NA-C1A	-4.31	104.71	106.68
13	B	830	CLA	C2C-C1C-NC	4.31	114.51	109.98
13	K	203	CLA	C3D-C2D-C1D	-4.31	99.95	105.83
13	A	833	CLA	C3D-C4D-ND	4.30	116.97	109.99
13	A	829	CLA	C4A-NA-C1A	-4.30	104.72	106.68
13	A	816	CLA	CHD-C1D-ND	-4.30	118.76	124.80
13	A	808	CLA	C3D-C2D-C1D	-4.30	99.97	105.83
13	K	201	CLA	CHD-C1D-ND	-4.29	118.76	124.80
13	B	809	CLA	C3D-C2D-C1D	-4.28	99.99	105.83
13	A	824	CLA	C3B-C4B-NB	4.28	114.35	110.53
13	A	806	CLA	C2C-C1C-NC	4.28	114.48	109.98
13	A	811	CLA	C3D-C2D-C1D	-4.28	100.00	105.83
13	A	822	CLA	C3D-C4D-ND	4.27	116.93	109.99
13	A	836	CLA	C3D-C2D-C1D	-4.27	100.01	105.83
13	A	825	CLA	CAC-C3C-C4C	4.26	130.34	124.79
13	A	803	CLA	C3D-C2D-C1D	-4.26	100.01	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	814	CLA	C3D-C4D-ND	4.26	116.92	109.99
13	B	822	CLA	C3D-C4D-ND	4.26	116.92	109.99
13	B	831	CLA	C3D-C4D-ND	4.26	116.92	109.99
13	B	823	CLA	C3D-C4D-ND	4.26	116.91	109.99
13	B	814	CLA	C1D-CHD-C4C	-4.26	116.97	126.02
13	B	809	CLA	C1D-CHD-C4C	-4.26	116.97	126.02
13	B	817	CLA	C3D-C4D-ND	4.26	116.91	109.99
13	A	831	CLA	CHD-C1D-ND	-4.25	118.81	124.80
13	B	803	CLA	CAA-C2A-C3A	-4.25	101.52	113.00
13	A	815	CLA	C2C-C1C-NC	4.25	114.44	109.98
13	B	806	CLA	C4A-NA-C1A	-4.25	104.74	106.68
13	A	812	CLA	C1D-CHD-C4C	-4.24	117.00	126.02
13	A	831	CLA	C3B-C4B-NB	4.24	114.32	110.53
13	A	840	CLA	C1D-CHD-C4C	-4.24	117.00	126.02
13	B	817	CLA	CHD-C1D-ND	-4.24	118.83	124.80
13	A	842	CLA	C3D-C4D-ND	4.24	116.88	109.99
13	B	812	CLA	C3D-C4D-ND	4.24	116.88	109.99
13	A	811	CLA	C3D-C4D-ND	4.24	116.88	109.99
13	B	808	CLA	C3D-C4D-ND	4.24	116.88	109.99
13	B	829	CLA	C2C-C1C-NC	4.24	114.43	109.98
13	L	202	CLA	CHD-C1D-ND	-4.23	118.84	124.80
13	A	809	CLA	C3D-C4D-ND	4.23	116.87	109.99
13	B	826	CLA	CHD-C1D-ND	-4.23	118.85	124.80
13	B	818	CLA	C1C-C2C-C3C	-4.23	102.53	106.98
13	A	807	CLA	CHD-C1D-ND	-4.23	118.85	124.80
13	A	827	CLA	C2C-C1C-NC	4.23	114.42	109.98
13	A	831	CLA	C4A-NA-C1A	-4.23	104.75	106.68
13	A	826	CLA	C1D-CHD-C4C	-4.22	117.04	126.02
13	A	827	CLA	C3D-C4D-ND	4.22	116.85	109.99
13	B	803	CLA	C1D-CHD-C4C	-4.22	117.04	126.02
13	A	838	CLA	C1D-CHD-C4C	-4.22	117.04	126.02
13	B	833	CLA	C3D-C4D-ND	4.22	116.85	109.99
13	B	818	CLA	C4A-NA-C1A	-4.22	104.75	106.68
13	B	833	CLA	C1C-C2C-C3C	-4.22	102.54	106.98
13	A	828	CLA	C4A-NA-C1A	-4.22	104.76	106.68
13	A	844	CLA	CHD-C1D-ND	-4.21	118.88	124.80
13	A	805	CLA	C2C-C1C-NC	4.21	114.40	109.98
13	A	832	CLA	C4A-NA-C1A	-4.20	104.76	106.68
13	A	839	CLA	C4A-NA-C1A	-4.20	104.76	106.68
13	A	817	CLA	C3D-C4D-ND	4.20	116.82	109.99
13	A	837	CLA	O2D-CGD-O1D	-4.20	115.67	123.85
13	A	810	CLA	C1D-CHD-C4C	-4.20	117.09	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	807	CLA	C2C-C1C-NC	4.20	114.39	109.98
13	A	840	CLA	C1C-C2C-C3C	-4.20	102.56	106.98
13	B	810	CLA	O2D-CGD-CBD	4.20	118.57	111.23
13	L	204	CLA	CHD-C1D-ND	-4.20	118.89	124.80
13	A	812	CLA	CHD-C1D-ND	-4.20	118.89	124.80
13	B	816	CLA	C3B-C4B-NB	4.20	114.28	110.53
13	B	813	CLA	C3D-C4D-ND	4.19	116.80	109.99
13	F	203	CLA	C3D-C4D-ND	4.19	116.80	109.99
13	B	802	CLA	C3C-C4C-NC	4.19	115.80	110.43
13	B	807	CLA	C1D-CHD-C4C	-4.19	117.12	126.02
13	A	811	CLA	C4A-NA-C1A	-4.18	104.77	106.68
13	B	827	CLA	C4A-NA-C1A	-4.18	104.77	106.68
13	A	822	CLA	C1D-CHD-C4C	-4.18	117.13	126.02
13	B	819	CLA	CHD-C1D-ND	-4.18	118.92	124.80
13	A	829	CLA	CMC-C2C-C1C	4.18	131.56	125.03
13	A	838	CLA	C4A-NA-C1A	-4.18	104.77	106.68
13	B	811	CLA	CHD-C1D-ND	-4.17	118.93	124.80
13	A	805	CLA	CHD-C1D-ND	-4.17	118.93	124.80
13	B	814	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
13	A	808	CLA	CHD-C1D-ND	-4.17	118.93	124.80
13	A	824	CLA	C3D-C2D-C1D	-4.17	100.14	105.83
13	A	844	CLA	C3D-C4D-ND	4.17	116.76	109.99
13	B	820	CLA	C1D-CHD-C4C	-4.17	117.16	126.02
13	B	827	CLA	CHD-C1D-ND	-4.16	118.94	124.80
13	B	833	CLA	C2B-C1B-NB	4.16	114.64	110.33
13	A	817	CLA	CHD-C1D-ND	-4.16	118.94	124.80
13	A	808	CLA	C1C-C2C-C3C	-4.16	102.61	106.98
13	B	823	CLA	CHD-C4C-C3C	-4.16	118.71	124.77
13	A	806	CLA	CHD-C1D-ND	-4.16	118.95	124.80
13	B	803	CLA	C3C-C4C-NC	4.16	115.76	110.43
13	B	827	CLA	C3B-C2B-C1B	-4.16	102.27	107.17
13	B	805	CLA	CHD-C1D-ND	-4.16	118.95	124.80
13	A	829	CLA	C2C-C1C-NC	4.15	114.34	109.98
13	A	802	CLA	C3B-C4B-NB	4.15	114.23	110.53
13	B	831	CLA	C4A-NA-C1A	-4.14	104.79	106.68
13	A	837	CLA	CHD-C1D-ND	-4.14	118.97	124.80
13	A	814	CLA	CHD-C1D-ND	-4.14	118.97	124.80
13	A	807	CLA	C1D-CHD-C4C	-4.14	117.22	126.02
13	A	843	CLA	C3D-C4D-ND	4.14	116.72	109.99
13	B	816	CLA	C3D-C4D-ND	4.14	116.72	109.99
13	A	826	CLA	C2C-C1C-NC	4.14	114.33	109.98
13	A	840	CLA	C3D-C4D-ND	4.14	116.72	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	824	CLA	C1C-C2C-C3C	-4.14	102.63	106.98
13	A	810	CLA	C3D-C4D-ND	4.13	116.71	109.99
13	B	815	CLA	C1D-CHD-C4C	-4.13	117.23	126.02
13	B	801	CLA	CAC-C3C-C4C	4.13	130.17	124.79
13	B	821	CLA	C4A-NA-C1A	-4.13	104.79	106.68
13	A	805	CLA	C4A-NA-C1A	-4.13	104.80	106.68
13	A	818	CLA	CHD-C1D-ND	-4.13	118.99	124.80
13	A	811	CLA	C3B-C2B-C1B	-4.13	102.30	107.17
13	A	839	CLA	C3D-C4D-ND	4.13	116.70	109.99
13	A	834	CLA	C4A-NA-C1A	-4.13	104.80	106.68
13	B	801	CLA	C3D-C4D-ND	4.12	116.69	109.99
13	B	826	CLA	C4A-NA-C1A	-4.12	104.80	106.68
13	A	815	CLA	CHD-C1D-ND	-4.12	119.00	124.80
13	B	831	CLA	CHD-C1D-ND	-4.12	119.00	124.80
13	A	833	CLA	CHD-C1D-ND	-4.12	119.00	124.80
13	A	834	CLA	C3D-C4D-ND	4.12	116.68	109.99
13	B	833	CLA	O2D-CGD-O1D	-4.12	115.83	123.85
13	A	835	CLA	C1D-CHD-C4C	-4.12	117.27	126.02
13	A	807	CLA	C3D-C4D-ND	4.11	116.67	109.99
13	K	203	CLA	C3D-C4D-ND	4.11	116.67	109.99
13	A	817	CLA	C3B-C4B-NB	4.11	114.20	110.53
13	A	823	CLA	CHD-C1D-ND	-4.11	119.02	124.80
13	A	841	CLA	C3B-C2B-C1B	-4.11	102.32	107.17
13	F	203	CLA	CHD-C1D-ND	-4.11	119.02	124.80
13	B	816	CLA	CHD-C1D-ND	-4.11	119.02	124.80
13	A	804	CLA	C2C-C1C-NC	4.11	114.30	109.98
13	A	806	CLA	C1D-CHD-C4C	-4.11	117.29	126.02
13	A	808	CLA	C3D-C4D-ND	4.10	116.65	109.99
13	A	837	CLA	C3D-C4D-ND	4.10	116.65	109.99
13	A	831	CLA	C4B-C3B-C2B	-4.10	102.20	107.30
13	A	827	CLA	C1D-CHD-C4C	-4.10	117.31	126.02
13	B	802	CLA	C4A-NA-C1A	-4.10	104.81	106.68
13	B	813	CLA	CHD-C1D-ND	-4.09	119.04	124.80
13	A	820	CLA	C3B-C2B-C1B	-4.09	102.34	107.17
13	A	843	CLA	CHD-C1D-ND	-4.09	119.04	124.80
13	A	835	CLA	CHD-C1D-ND	-4.09	119.05	124.80
13	A	815	CLA	C3D-C4D-ND	4.09	116.63	109.99
13	A	804	CLA	C3D-C4D-ND	4.09	116.63	109.99
13	A	835	CLA	C3D-C4D-ND	4.09	116.63	109.99
13	A	820	CLA	C3D-C4D-ND	4.09	116.63	109.99
13	B	833	CLA	C4A-NA-C1A	-4.09	104.81	106.68
13	L	202	CLA	C1D-CHD-C4C	-4.09	117.34	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	821	CLA	C1D-CHD-C4C	-4.08	117.34	126.02
13	B	822	CLA	C1D-CHD-C4C	-4.08	117.34	126.02
13	B	809	CLA	C3D-C4D-ND	4.08	116.62	109.99
13	A	813	CLA	C4A-NA-C1A	-4.08	104.82	106.68
13	A	817	CLA	C4A-NA-C1A	-4.08	104.82	106.68
13	A	802	CLA	C1C-C2C-C3C	-4.08	102.69	106.98
13	A	839	CLA	CHD-C1D-ND	-4.07	119.07	124.80
13	B	806	CLA	C1D-CHD-C4C	-4.07	117.37	126.02
13	B	821	CLA	C3C-C4C-NC	4.07	115.64	110.43
13	B	802	CLA	C3D-C4D-ND	4.07	116.60	109.99
13	B	823	CLA	C1C-C2C-C3C	-4.07	102.70	106.98
13	A	829	CLA	C1D-CHD-C4C	-4.07	117.38	126.02
13	A	825	CLA	CHD-C1D-ND	-4.07	119.08	124.80
13	A	814	CLA	C3D-C4D-ND	4.06	116.59	109.99
13	B	803	CLA	C3D-C4D-ND	4.06	116.59	109.99
13	A	802	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
13	A	832	CLA	CHD-C1D-ND	-4.06	119.09	124.80
13	B	833	CLA	CHD-C1D-ND	-4.06	119.09	124.80
13	A	825	CLA	C3D-C4D-ND	4.06	116.59	109.99
13	B	811	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
13	B	815	CLA	C3D-C4D-ND	4.06	116.58	109.99
13	A	826	CLA	C3C-C4C-NC	4.06	115.63	110.43
13	B	818	CLA	C1D-CHD-C4C	-4.06	117.39	126.02
13	B	808	CLA	C4A-NA-C1A	-4.06	104.83	106.68
13	A	834	CLA	CHD-C1D-ND	-4.06	119.09	124.80
13	A	821	CLA	C3D-C4D-ND	4.05	116.58	109.99
13	K	203	CLA	C1C-C2C-C3C	-4.05	102.72	106.98
13	A	830	CLA	C3C-C4C-NC	4.05	115.62	110.43
13	A	839	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
13	B	829	CLA	C1D-CHD-C4C	-4.04	117.42	126.02
13	A	841	CLA	CHD-C1D-ND	-4.04	119.11	124.80
13	A	813	CLA	C3D-C4D-ND	4.04	116.56	109.99
13	A	834	CLA	C1C-C2C-C3C	-4.04	102.73	106.98
13	A	828	CLA	C2C-C1C-NC	4.04	114.22	109.98
13	B	821	CLA	C3D-C4D-ND	4.03	116.55	109.99
13	A	830	CLA	C1D-CHD-C4C	-4.03	117.44	126.02
13	B	801	CLA	C1D-CHD-C4C	-4.03	117.45	126.02
13	B	807	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
13	B	805	CLA	C1D-CHD-C4C	-4.03	117.45	126.02
13	A	841	CLA	C3D-C4D-ND	4.03	116.54	109.99
13	A	842	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
13	B	823	CLA	CHD-C1D-ND	-4.03	119.13	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	806	CLA	C1C-C2C-C3C	-4.03	102.74	106.98
13	B	812	CLA	CHD-C1D-ND	-4.03	119.14	124.80
13	K	203	CLA	C1D-CHD-C4C	-4.03	117.46	126.02
13	B	808	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
13	A	830	CLA	C3D-C4D-ND	4.02	116.52	109.99
13	A	831	CLA	C3D-C4D-ND	4.02	116.52	109.99
13	B	828	CLA	C1D-CHD-C4C	-4.02	117.48	126.02
13	L	202	CLA	C4A-NA-C1A	-4.02	104.85	106.68
13	A	820	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
13	A	823	CLA	C1C-C2C-C3C	-4.02	102.75	106.98
13	B	806	CLA	C3D-C4D-ND	4.01	116.50	109.99
13	B	817	CLA	CAA-C2A-C3A	-4.01	102.17	113.00
13	J	101	CLA	CHD-C1D-ND	-4.00	119.17	124.80
13	A	832	CLA	C1C-C2C-C3C	-4.00	102.77	106.98
13	A	825	CLA	C3B-C4B-NB	4.00	114.10	110.53
13	A	836	CLA	C1D-CHD-C4C	-4.00	117.52	126.02
13	A	802	CLA	C3D-C4D-ND	4.00	116.48	109.99
13	B	815	CLA	CHD-C1D-ND	-4.00	119.18	124.80
13	A	820	CLA	CHD-C1D-ND	-3.99	119.18	124.80
13	B	801	CLA	C4A-NA-C1A	-3.99	104.86	106.68
13	B	812	CLA	C1C-C2C-C3C	-3.99	102.78	106.98
13	A	844	CLA	C1D-CHD-C4C	-3.98	117.56	126.02
13	B	819	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
13	B	804	CLA	CHD-C1D-ND	-3.98	119.20	124.80
13	A	810	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
13	A	816	CLA	C4A-NA-C1A	-3.98	104.86	106.68
13	A	834	CLA	CAA-C2A-C3A	-3.97	102.26	113.00
13	A	810	CLA	C1C-C2C-C3C	-3.97	102.80	106.98
13	A	818	CLA	C4A-NA-C1A	-3.97	104.87	106.68
13	A	811	CLA	CHD-C1D-ND	-3.96	119.22	124.80
13	B	802	CLA	O2D-CGD-CBD	3.96	118.16	111.23
13	B	821	CLA	C1D-CHD-C4C	-3.96	117.60	126.02
13	B	822	CLA	C3B-C4B-NB	3.96	114.06	110.53
13	B	816	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
13	B	823	CLA	C2D-C1D-ND	3.96	114.04	110.13
13	A	817	CLA	C1D-CHD-C4C	-3.96	117.61	126.02
13	B	823	CLA	C4B-C3B-C2B	-3.95	102.39	107.30
13	A	841	CLA	C1D-CHD-C4C	-3.95	117.62	126.02
13	A	834	CLA	O2D-CGD-CBD	3.95	118.13	111.23
13	B	816	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
13	A	838	CLA	C3C-C4C-NC	3.95	115.49	110.43
13	B	818	CLA	CHD-C1D-ND	-3.95	119.25	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	814	CLA	C3C-C4C-NC	3.95	115.49	110.43
13	L	202	CLA	C1C-C2C-C3C	-3.95	102.83	106.98
13	A	831	CLA	C3B-C2B-C1B	-3.95	102.52	107.17
13	A	803	CLA	C4A-NA-C1A	-3.94	104.88	106.68
13	B	809	CLA	O2A-CGA-CBA	3.94	123.85	111.83
13	A	803	CLA	C3D-C4D-ND	3.94	116.39	109.99
13	A	805	CLA	C3D-C4D-ND	3.94	116.39	109.99
13	B	811	CLA	CAC-C3C-C4C	3.94	129.92	124.79
13	A	810	CLA	C3B-C4B-NB	3.94	114.05	110.53
13	B	804	CLA	C3D-C4D-ND	3.93	116.38	109.99
13	A	821	CLA	C3B-C4B-NB	3.93	114.04	110.53
13	L	204	CLA	CAA-C2A-C3A	-3.93	102.37	113.00
13	B	810	CLA	C3B-C2B-C1B	-3.93	102.53	107.17
13	J	101	CLA	C3D-C4D-ND	3.93	116.38	109.99
13	A	811	CLA	C1D-CHD-C4C	-3.93	117.67	126.02
13	B	832	CLA	C1C-C2C-C3C	-3.92	102.85	106.98
13	A	836	CLA	C3B-C4B-NB	3.92	114.03	110.53
13	B	818	CLA	C3D-C4D-ND	3.91	116.34	109.99
13	B	818	CLA	C4B-C3B-C2B	-3.91	102.44	107.30
13	B	826	CLA	C3B-C4B-NB	3.91	114.02	110.53
13	A	813	CLA	C1C-C2C-C3C	-3.91	102.87	106.98
13	B	826	CLA	C3D-C2D-C1D	-3.90	100.50	105.83
13	A	803	CLA	CAA-C2A-C3A	-3.90	102.45	113.00
13	A	839	CLA	C1D-CHD-C4C	-3.90	117.73	126.02
13	A	837	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
13	A	826	CLA	C3D-C4D-ND	3.90	116.32	109.99
13	A	816	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
13	B	831	CLA	C1C-C2C-C3C	-3.90	102.88	106.98
13	A	815	CLA	C1D-CHD-C4C	-3.90	117.74	126.02
13	A	819	CLA	C3D-C4D-ND	3.90	116.32	109.99
13	A	817	CLA	O2D-CGD-CBD	3.89	118.04	111.23
13	B	810	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
13	B	812	CLA	C1D-CHD-C4C	-3.89	117.75	126.02
13	B	832	CLA	C1D-CHD-C4C	-3.89	117.76	126.02
13	B	817	CLA	C1D-CHD-C4C	-3.88	117.76	126.02
13	A	822	CLA	C3C-C4C-NC	3.88	115.41	110.43
13	B	833	CLA	C4B-C3B-C2B	-3.88	102.47	107.30
13	A	833	CLA	C1D-CHD-C4C	-3.88	117.77	126.02
13	B	823	CLA	C3B-C2B-C1B	-3.88	102.59	107.17
13	B	811	CLA	C3D-C2D-C1D	-3.88	100.54	105.83
13	K	201	CLA	C1D-CHD-C4C	-3.88	117.77	126.02
13	A	817	CLA	C4B-C3B-C2B	-3.88	102.48	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	807	CLA	CHD-C1D-ND	-3.87	119.35	124.80
13	A	802	CLA	C3C-C4C-NC	3.87	115.38	110.43
16	L	206	BCR	C2-C1-C6	3.87	116.06	110.44
13	B	810	CLA	CHD-C1D-ND	-3.87	119.36	124.80
13	B	829	CLA	C3D-C4D-ND	3.86	116.27	109.99
13	L	203	CLA	C4A-NA-C1A	-3.86	104.92	106.68
13	A	842	CLA	C1D-CHD-C4C	-3.86	117.81	126.02
13	A	832	CLA	C3D-C2D-C1D	-3.86	100.56	105.83
13	B	826	CLA	C1D-CHD-C4C	-3.86	117.82	126.02
13	B	829	CLA	CHD-C1D-ND	-3.86	119.38	124.80
13	B	816	CLA	C4A-NA-C1A	-3.85	104.92	106.68
13	F	203	CLA	C1D-CHD-C4C	-3.84	117.86	126.02
13	A	844	CLA	C4A-NA-C1A	-3.84	104.93	106.68
13	A	818	CLA	C3B-C4B-NB	3.84	113.96	110.53
13	A	821	CLA	CHD-C1D-ND	-3.84	119.40	124.80
13	B	807	CLA	O2D-CGD-CBD	3.84	117.94	111.23
13	A	803	CLA	CMB-C2B-C3B	3.84	135.58	126.55
13	B	822	CLA	C3D-C2D-C1D	-3.84	100.59	105.83
13	A	839	CLA	O2D-CGD-O1D	-3.84	116.38	123.85
13	A	837	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
13	A	814	CLA	C4C-C3C-C2C	-3.83	101.31	106.89
13	B	809	CLA	CAA-C2A-C3A	-3.83	102.65	113.00
13	B	810	CLA	C1C-C2C-C3C	-3.83	102.95	106.98
13	J	101	CLA	C4A-NA-C1A	-3.83	104.93	106.68
13	F	203	CLA	C1C-C2C-C3C	-3.82	102.96	106.98
13	A	820	CLA	C3B-C4B-NB	3.82	113.94	110.53
13	B	822	CLA	C1C-C2C-C3C	-3.82	102.97	106.98
13	B	806	CLA	CHD-C1D-ND	-3.81	119.44	124.80
13	A	809	CLA	CHD-C1D-ND	-3.81	119.44	124.80
13	B	814	CLA	CHD-C1D-ND	-3.81	119.44	124.80
13	B	831	CLA	C1D-CHD-C4C	-3.81	117.92	126.02
13	B	814	CLA	C1C-C2C-C3C	-3.81	102.98	106.98
13	A	834	CLA	C1D-CHD-C4C	-3.81	117.93	126.02
13	B	811	CLA	C1C-C2C-C3C	-3.80	102.98	106.98
13	B	827	CLA	C1D-CHD-C4C	-3.80	117.95	126.02
13	A	818	CLA	C3C-C4C-NC	3.79	115.29	110.43
13	A	829	CLA	CHD-C1D-ND	-3.79	119.47	124.80
13	A	813	CLA	C1D-CHD-C4C	-3.79	117.97	126.02
13	A	841	CLA	C1C-C2C-C3C	-3.78	103.00	106.98
13	A	824	CLA	C1D-CHD-C4C	-3.78	117.98	126.02
13	L	204	CLA	C1D-CHD-C4C	-3.78	117.99	126.02
13	B	823	CLA	O2D-CGD-O1D	-3.78	116.49	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	828	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
13	B	830	CLA	C1C-C2C-C3C	-3.78	103.01	106.98
13	B	810	CLA	C3C-C4C-NC	3.78	115.27	110.43
13	B	807	CLA	C3D-C4D-ND	3.78	116.12	109.99
13	A	838	CLA	CHD-C1D-ND	-3.78	119.49	124.80
13	B	820	CLA	C3D-C4D-ND	3.77	116.12	109.99
13	A	831	CLA	C3C-C4C-NC	3.77	115.26	110.43
13	B	825	CLA	C1C-C2C-C3C	-3.77	103.01	106.98
13	B	809	CLA	CHD-C1D-ND	-3.77	119.50	124.80
13	B	814	CLA	C4A-NA-C1A	-3.77	104.96	106.68
13	A	823	CLA	C4A-NA-C1A	-3.77	104.96	106.68
13	B	810	CLA	C3D-C4D-ND	3.76	116.10	109.99
13	A	827	CLA	C1C-C2C-C3C	-3.76	103.03	106.98
13	A	835	CLA	C3B-C4B-NB	3.75	113.88	110.53
13	B	805	CLA	C4A-NA-C1A	-3.75	104.97	106.68
13	B	815	CLA	C3B-C4B-NB	3.74	113.87	110.53
13	B	827	CLA	C1C-C2C-C3C	-3.74	103.04	106.98
13	A	825	CLA	C1D-CHD-C4C	-3.74	118.07	126.02
13	A	813	CLA	CHD-C1D-ND	-3.74	119.54	124.80
13	A	828	CLA	C3D-C4D-ND	3.74	116.06	109.99
13	A	817	CLA	C3B-C2B-C1B	-3.73	102.77	107.17
13	A	824	CLA	CHD-C1D-ND	-3.73	119.55	124.80
13	B	833	CLA	C1D-CHD-C4C	-3.73	118.09	126.02
13	A	836	CLA	C3C-C4C-NC	3.73	115.21	110.43
13	A	828	CLA	C3C-C4C-NC	3.73	115.21	110.43
13	A	803	CLA	C2C-C1C-NC	3.73	113.90	109.98
13	A	838	CLA	C3D-C4D-ND	3.72	116.04	109.99
13	A	843	CLA	C1D-CHD-C4C	-3.72	118.11	126.02
13	A	836	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
13	B	804	CLA	C4C-C3C-C2C	-3.72	101.48	106.89
13	A	831	CLA	C1C-C2C-C3C	-3.72	103.07	106.98
13	B	820	CLA	CHD-C1D-ND	-3.71	119.58	124.80
13	A	807	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
13	B	818	CLA	C3B-C4B-NB	3.71	113.84	110.53
13	A	823	CLA	C1D-CHD-C4C	-3.71	118.13	126.02
13	B	813	CLA	C1D-CHD-C4C	-3.71	118.13	126.02
13	A	825	CLA	C1C-C2C-C3C	-3.71	103.08	106.98
13	A	836	CLA	CHD-C1D-ND	-3.71	119.58	124.80
13	B	823	CLA	C1D-CHD-C4C	-3.71	118.14	126.02
16	L	205	BCR	C24-C23-C22	-3.71	120.75	126.23
13	L	203	CLA	CMB-C2B-C1B	3.71	131.06	125.42
13	A	844	CLA	C3C-C4C-NC	3.71	115.18	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	828	CLA	CHD-C1D-ND	-3.70	119.59	124.80
13	A	822	CLA	CHD-C1D-ND	-3.70	119.59	124.80
13	B	804	CLA	CAA-C2A-C3A	-3.69	103.03	113.00
13	B	820	CLA	C3C-C4C-NC	3.69	115.16	110.43
13	B	833	CLA	C3B-C4B-NB	3.69	113.82	110.53
13	J	101	CLA	C1D-CHD-C4C	-3.69	118.18	126.02
13	B	823	CLA	CAC-C3C-C4C	3.69	129.59	124.79
13	B	801	CLA	C3C-C4C-NC	3.69	115.15	110.43
13	A	806	CLA	C1C-C2C-C3C	-3.68	103.11	106.98
13	A	830	CLA	C3D-C2D-C1D	-3.68	100.81	105.83
13	A	841	CLA	O2A-CGA-CBA	3.68	123.06	111.83
13	B	808	CLA	C1D-CHD-C4C	-3.68	118.20	126.02
13	A	820	CLA	CBA-CAA-C2A	3.68	124.73	113.79
13	A	843	CLA	C4A-NA-C1A	-3.67	105.00	106.68
13	B	819	CLA	C1D-CHD-C4C	-3.67	118.21	126.02
13	A	808	CLA	C1D-CHD-C4C	-3.67	118.22	126.02
13	B	804	CLA	C3C-C4C-NC	3.67	115.13	110.43
13	A	810	CLA	C4A-NA-C1A	-3.67	105.01	106.68
13	A	838	CLA	C1C-C2C-C3C	-3.67	103.12	106.98
13	B	829	CLA	C3C-C4C-NC	3.67	115.13	110.43
13	L	203	CLA	C1C-C2C-C3C	-3.66	103.13	106.98
13	A	820	CLA	C4B-C3B-C2B	-3.66	102.75	107.30
13	B	801	CLA	CHD-C1D-ND	-3.66	119.66	124.80
13	A	804	CLA	C3C-C4C-NC	3.66	115.11	110.43
13	A	840	CLA	O2D-CGD-O1D	-3.65	116.74	123.85
13	B	814	CLA	C3B-C4B-NB	3.65	113.79	110.53
13	A	829	CLA	CAC-C3C-C4C	3.65	129.54	124.79
13	A	840	CLA	CHD-C1D-ND	-3.65	119.67	124.80
13	B	810	CLA	CAA-C2A-C3A	-3.65	103.14	113.00
13	B	818	CLA	C3B-C2B-C1B	-3.65	102.87	107.17
13	B	822	CLA	C3C-C4C-NC	3.64	115.09	110.43
13	A	841	CLA	C3C-C4C-NC	3.64	115.09	110.43
13	B	802	CLA	CMA-C3A-C2A	-3.64	99.92	113.98
13	A	807	CLA	CHD-C4C-NC	3.63	129.86	124.23
13	A	811	CLA	C3B-C4B-NB	3.63	113.77	110.53
13	A	823	CLA	O2D-CGD-O1D	-3.63	116.78	123.85
13	B	815	CLA	C1C-C2C-C3C	-3.63	103.16	106.98
13	A	820	CLA	C1D-CHD-C4C	-3.63	118.31	126.02
13	B	828	CLA	C3C-C4C-NC	3.63	115.08	110.43
13	A	806	CLA	C3B-C4B-NB	3.63	113.77	110.53
13	A	841	CLA	C4B-C3B-C2B	-3.63	102.79	107.30
13	B	802	CLA	C3B-C4B-NB	3.62	113.76	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	825	CLA	O2A-CGA-CBA	3.62	122.87	111.83
13	A	816	CLA	C1C-C2C-C3C	-3.62	103.18	106.98
13	A	835	CLA	C1C-C2C-C3C	-3.61	103.18	106.98
13	B	830	CLA	C4A-NA-C1A	-3.61	105.03	106.68
13	A	833	CLA	CAA-C2A-C3A	-3.61	103.25	113.00
13	A	805	CLA	C3C-C4C-NC	3.61	115.05	110.43
13	A	814	CLA	C1D-CHD-C4C	-3.61	118.35	126.02
13	B	821	CLA	CHD-C1D-ND	-3.61	119.73	124.80
13	B	812	CLA	C3B-C4B-NB	3.61	113.75	110.53
13	B	814	CLA	C3C-C4C-NC	3.60	115.04	110.43
13	B	824	CLA	C1C-C2C-C3C	-3.60	103.20	106.98
13	A	812	CLA	CAA-C2A-C3A	-3.60	103.28	113.00
13	B	809	CLA	C3C-C4C-NC	3.59	115.03	110.43
13	B	824	CLA	C1D-CHD-C4C	-3.58	118.41	126.02
13	B	823	CLA	CHC-C1C-C2C	-3.58	116.77	126.95
13	B	803	CLA	O2A-CGA-CBA	3.58	122.75	111.83
16	L	206	BCR	C24-C23-C22	-3.58	120.94	126.23
13	A	804	CLA	CHD-C1D-ND	-3.57	119.77	124.80
13	B	806	CLA	CHC-C1C-C2C	-3.57	116.79	126.95
13	A	809	CLA	C3C-C4C-NC	3.57	115.01	110.43
13	A	815	CLA	C1C-C2C-C3C	-3.57	103.22	106.98
13	A	818	CLA	C1C-C2C-C3C	-3.57	103.23	106.98
13	A	829	CLA	O2A-CGA-CBA	3.57	122.71	111.83
13	A	809	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
13	A	803	CLA	C1D-CHD-C4C	-3.57	118.44	126.02
13	A	805	CLA	C1D-CHD-C4C	-3.56	118.44	126.02
13	A	832	CLA	C1D-CHD-C4C	-3.56	118.46	126.02
13	A	812	CLA	C1C-C2C-C3C	-3.56	103.24	106.98
13	A	829	CLA	C3D-C4D-ND	3.56	115.77	109.99
13	B	803	CLA	C3B-C4B-NB	3.56	113.70	110.53
13	B	833	CLA	C3B-C2B-C1B	-3.55	102.98	107.17
13	A	834	CLA	C3C-C4C-NC	3.55	114.98	110.43
13	B	819	CLA	C1C-C2C-C3C	-3.54	103.25	106.98
13	A	803	CLA	CHB-C4A-NA	3.54	129.51	124.40
13	A	826	CLA	C4C-C3C-C2C	-3.54	101.73	106.89
13	K	201	CLA	CAA-C2A-C3A	-3.53	103.45	113.00
13	A	824	CLA	C3C-C4C-NC	3.53	114.96	110.43
13	B	827	CLA	C4B-C3B-C2B	-3.53	102.91	107.30
13	A	820	CLA	CHC-C1C-C2C	-3.53	116.92	126.95
13	A	830	CLA	C1C-C2C-C3C	-3.53	103.27	106.98
13	B	801	CLA	C3B-C4B-NB	3.53	113.68	110.53
13	A	840	CLA	C3C-C4C-NC	3.53	114.95	110.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	203	CLA	C3C-C4C-NC	3.52	114.94	110.43
16	B	836	BCR	C3-C4-C5	-3.52	107.78	114.06
16	A	848	BCR	C2-C1-C6	3.52	115.55	110.44
13	B	803	CLA	O2D-CGD-O1D	-3.52	117.00	123.85
13	B	833	CLA	CHC-C1C-C2C	-3.52	116.96	126.95
13	B	816	CLA	C3C-C4C-NC	3.52	114.93	110.43
13	A	833	CLA	C1C-C2C-C3C	-3.51	103.28	106.98
13	B	805	CLA	C3C-C4C-NC	3.51	114.93	110.43
13	A	838	CLA	C3B-C4B-NB	3.51	113.67	110.53
13	B	802	CLA	C4-C3-C5	3.51	121.32	115.23
13	A	821	CLA	CHC-C1C-C2C	-3.51	116.98	126.95
16	A	848	BCR	C3-C4-C5	-3.50	107.81	114.06
13	B	806	CLA	C3B-C4B-NB	3.50	113.66	110.53
13	A	824	CLA	C4B-C3B-C2B	-3.50	102.95	107.30
16	B	836	BCR	C15-C16-C17	-3.50	116.37	123.52
13	A	842	CLA	CAA-C2A-C3A	-3.49	103.56	113.00
13	B	813	CLA	C3C-C4C-NC	3.49	114.91	110.43
13	B	802	CLA	CHD-C1D-ND	-3.49	119.89	124.80
13	B	822	CLA	O2A-CGA-CBA	3.49	122.48	111.83
13	A	804	CLA	C4C-C3C-C2C	-3.49	101.81	106.89
13	A	842	CLA	C3C-C4C-NC	3.49	114.90	110.43
13	A	835	CLA	C3C-C4C-NC	3.49	114.90	110.43
13	B	826	CLA	C1C-C2C-C3C	-3.49	103.31	106.98
13	A	812	CLA	C3B-C4B-NB	3.49	113.64	110.53
13	B	830	CLA	C1D-CHD-C4C	-3.49	118.61	126.02
13	B	818	CLA	C3C-C4C-NC	3.48	114.89	110.43
13	A	833	CLA	C3C-C4C-NC	3.48	114.89	110.43
13	B	815	CLA	C3C-C4C-NC	3.47	114.88	110.43
13	A	806	CLA	C4A-NA-C1A	-3.47	105.09	106.68
13	A	817	CLA	CHC-C1C-C2C	-3.47	117.08	126.95
13	A	819	CLA	CHD-C1D-ND	-3.47	119.92	124.80
13	B	803	CLA	CHD-C1D-ND	-3.47	119.92	124.80
13	K	203	CLA	CHD-C1D-ND	-3.47	119.92	124.80
13	B	832	CLA	C3B-C4B-NB	3.46	113.62	110.53
13	J	101	CLA	C1C-C2C-C3C	-3.46	103.34	106.98
13	B	826	CLA	CAC-C3C-C4C	3.46	129.29	124.79
13	B	803	CLA	C1C-C2C-C3C	-3.46	103.35	106.98
13	B	823	CLA	C3D-C2D-C1D	-3.45	101.12	105.83
13	B	801	CLA	C1C-C2C-C3C	-3.45	103.35	106.98
16	J	103	BCR	C2-C1-C6	3.45	115.45	110.44
13	A	810	CLA	C3C-C4C-NC	3.44	114.84	110.43
13	B	802	CLA	C1C-C2C-C3C	-3.44	103.36	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	817	CLA	C1C-C2C-C3C	-3.44	103.36	106.98
13	L	204	CLA	C3B-C4B-NB	3.44	113.60	110.53
13	A	806	CLA	O2D-CGD-O1D	-3.44	117.16	123.85
13	A	810	CLA	C4B-C3B-C2B	-3.43	103.03	107.30
13	B	831	CLA	C3C-C4C-NC	3.43	114.82	110.43
13	A	808	CLA	C3B-C4B-NB	3.42	113.59	110.53
13	J	101	CLA	C3C-C4C-NC	3.42	114.81	110.43
13	B	826	CLA	O1D-CGD-CBD	-3.42	117.77	124.52
13	B	826	CLA	CMB-C2B-C1B	3.42	130.63	125.42
13	K	201	CLA	C1C-C2C-C3C	-3.42	103.39	106.98
13	A	832	CLA	CAC-C3C-C4C	3.42	129.23	124.79
13	A	810	CLA	CMB-C2B-C1B	3.42	130.62	125.42
13	A	843	CLA	C3C-C4C-NC	3.41	114.80	110.43
13	A	812	CLA	C3C-C4C-NC	3.41	114.80	110.43
13	B	805	CLA	C1C-C2C-C3C	-3.41	103.39	106.98
13	A	843	CLA	CAC-C3C-C4C	3.41	129.23	124.79
13	A	843	CLA	O2A-CGA-CBA	3.41	122.23	111.83
13	A	811	CLA	C4B-C3B-C2B	-3.41	103.06	107.30
13	B	813	CLA	C4C-C3C-C2C	-3.40	101.94	106.89
13	A	813	CLA	C3C-C4C-NC	3.40	114.78	110.43
13	A	832	CLA	O2A-CGA-CBA	3.40	122.19	111.83
13	A	844	CLA	C3B-C4B-NB	3.40	113.56	110.53
13	J	101	CLA	CAC-C3C-C4C	3.39	129.21	124.79
13	A	841	CLA	O2D-CGD-CBD	3.39	117.16	111.23
13	A	816	CLA	C3B-C4B-NB	3.39	113.56	110.53
13	A	819	CLA	CHC-C1C-C2C	-3.39	117.31	126.95
13	B	809	CLA	C1C-C2C-C3C	-3.39	103.42	106.98
13	B	812	CLA	C4B-C3B-C2B	-3.39	103.09	107.30
13	A	843	CLA	C1C-C2C-C3C	-3.38	103.42	106.98
12	A	801	CL0	CMA-C3A-C2A	-3.38	101.07	114.13
13	A	803	CLA	CHD-C1D-ND	-3.38	120.04	124.80
13	L	203	CLA	C1D-CHD-C4C	-3.38	118.83	126.02
13	B	808	CLA	C3C-C4C-NC	3.38	114.76	110.43
13	B	802	CLA	CHD-C4C-NC	3.38	129.47	124.23
16	B	836	BCR	C2-C1-C6	3.37	115.34	110.44
13	A	835	CLA	C4A-NA-C1A	-3.37	105.14	106.68
13	B	810	CLA	C4B-C3B-C2B	-3.37	103.11	107.30
13	L	203	CLA	C3C-C4C-NC	3.37	114.75	110.43
13	B	807	CLA	CHD-C4C-NC	3.37	129.45	124.23
13	B	818	CLA	CBA-CAA-C2A	3.37	123.81	113.79
13	B	828	CLA	C3B-C4B-NB	3.37	113.53	110.53
13	B	831	CLA	C3B-C4B-NB	3.37	113.53	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	808	CLA	CAC-C3C-C4C	3.36	129.16	124.79
13	A	822	CLA	C1C-C2C-C3C	-3.36	103.44	106.98
13	A	810	CLA	CHD-C1D-ND	-3.36	120.07	124.80
13	L	202	CLA	C3C-C4C-NC	3.36	114.73	110.43
13	A	819	CLA	C1C-C2C-C3C	-3.36	103.45	106.98
13	A	829	CLA	C4C-C3C-C2C	-3.35	102.01	106.89
13	B	824	CLA	C3B-C4B-NB	3.35	113.52	110.53
13	A	803	CLA	C3C-C4C-NC	3.35	114.72	110.43
13	B	818	CLA	CHC-C1C-C2C	-3.35	117.43	126.95
13	B	812	CLA	C3C-C4C-NC	3.34	114.72	110.43
13	B	821	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
13	B	825	CLA	C3C-C4C-NC	3.34	114.71	110.43
13	B	803	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
13	A	819	CLA	CAC-C3C-C4C	3.34	129.13	124.79
13	B	809	CLA	C3B-C4B-NB	3.34	113.51	110.53
13	A	828	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
13	B	807	CLA	C3C-C4C-NC	3.34	114.71	110.43
13	B	817	CLA	C3C-C4C-NC	3.34	114.71	110.43
13	A	841	CLA	CAC-C3C-C4C	3.34	129.13	124.79
13	K	201	CLA	CAC-C3C-C4C	3.34	129.13	124.79
13	A	844	CLA	C4C-C3C-C2C	-3.34	102.03	106.89
13	B	823	CLA	CMD-C2D-C3D	-3.34	120.04	127.69
13	A	827	CLA	CMB-C2B-C1B	3.34	130.50	125.42
13	A	844	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
13	K	203	CLA	C3B-C4B-NB	3.33	113.50	110.53
13	F	203	CLA	C3B-C4B-NB	3.33	113.50	110.53
13	B	815	CLA	C4A-NA-C1A	-3.33	105.16	106.68
13	A	808	CLA	CHC-C1C-C2C	-3.33	117.49	126.95
13	B	804	CLA	C2C-C1C-NC	3.32	113.47	109.98
13	B	827	CLA	C3B-C4B-NB	3.32	113.50	110.53
13	A	804	CLA	CAC-C3C-C4C	3.32	129.11	124.79
13	A	806	CLA	CHD-C4C-NC	3.32	129.38	124.23
13	L	204	CLA	C3C-C4C-NC	3.32	114.68	110.43
13	A	817	CLA	C3C-C4C-NC	3.32	114.68	110.43
14	A	845	PQN	C14-C13-C15	3.32	120.98	115.23
13	B	820	CLA	C1C-C2C-C3C	-3.32	103.49	106.98
13	A	839	CLA	C3C-C4C-NC	3.31	114.68	110.43
13	A	828	CLA	CHD-C4C-NC	3.31	129.37	124.23
13	B	806	CLA	C3C-C4C-NC	3.31	114.67	110.43
13	A	809	CLA	C1C-C2C-C3C	-3.31	103.50	106.98
13	A	813	CLA	C4-C3-C5	3.31	120.97	115.23
13	A	813	CLA	CAC-C3C-C4C	3.31	129.09	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	805	CLA	C1C-C2C-C3C	-3.30	103.50	106.98
13	A	804	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
13	A	835	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
13	A	835	CLA	CAC-C3C-C4C	3.30	129.08	124.79
16	A	850	BCR	C28-C27-C26	-3.30	108.17	114.06
13	A	813	CLA	C3B-C4B-NB	3.30	113.47	110.53
13	B	811	CLA	O2A-CGA-CBA	3.30	121.89	111.83
13	A	820	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
13	A	811	CLA	CHC-C1C-C2C	-3.29	117.59	126.95
13	A	844	CLA	C4-C3-C5	3.29	120.94	115.23
13	A	831	CLA	CHC-C1C-C2C	-3.29	117.60	126.95
13	A	809	CLA	O2A-CGA-CBA	3.29	121.86	111.83
13	A	825	CLA	CHC-C1C-C2C	-3.28	117.62	126.95
13	B	825	CLA	C1D-CHD-C4C	-3.28	119.04	126.02
13	B	833	CLA	C3C-C4C-NC	3.28	114.63	110.43
13	J	101	CLA	CHC-C1C-C2C	-3.28	117.63	126.95
13	A	807	CLA	O2A-CGA-CBA	3.28	121.83	111.83
13	A	842	CLA	O2A-CGA-CBA	3.28	121.83	111.83
13	A	819	CLA	C3C-C4C-NC	3.27	114.62	110.43
13	A	838	CLA	O2D-CGD-O1D	-3.27	117.47	123.85
13	B	813	CLA	CAA-C2A-C3A	-3.27	104.15	113.00
16	B	835	BCR	C15-C16-C17	-3.27	116.83	123.52
13	A	812	CLA	CHC-C1C-C2C	-3.27	117.66	126.95
13	J	101	CLA	C4B-C3B-C2B	-3.27	103.24	107.30
13	B	815	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
13	B	807	CLA	CAA-C2A-C3A	-3.27	104.17	113.00
13	A	832	CLA	CHC-C1C-C2C	-3.27	117.66	126.95
13	A	834	CLA	O2A-CGA-CBA	3.27	121.80	111.83
13	A	822	CLA	C4C-C3C-C2C	-3.27	102.14	106.89
13	A	806	CLA	CHB-C4A-NA	3.26	129.11	124.40
13	A	811	CLA	CAA-C2A-C3A	-3.26	104.20	113.00
13	A	816	CLA	CHC-C1C-C2C	-3.26	117.69	126.95
13	B	811	CLA	C3B-C4B-NB	3.26	113.44	110.53
13	B	821	CLA	CAA-C2A-C3A	-3.26	104.20	113.00
13	A	812	CLA	C4B-C3B-C2B	-3.25	103.26	107.30
13	A	837	CLA	C3C-C4C-NC	3.25	114.59	110.43
13	A	839	CLA	C4B-C3B-C2B	-3.25	103.27	107.30
13	K	203	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
16	A	849	BCR	C11-C10-C9	-3.25	122.73	127.28
13	A	830	CLA	C4C-C3C-C2C	-3.25	102.17	106.89
13	F	203	CLA	C3C-C4C-NC	3.24	114.58	110.43
13	A	831	CLA	C4C-C3C-C2C	-3.24	102.17	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	829	CLA	C1C-C2C-C3C	-3.24	103.57	106.98
13	B	812	CLA	CHC-C1C-C2C	-3.24	117.74	126.95
13	B	821	CLA	CMC-C2C-C1C	3.24	130.09	125.03
13	A	823	CLA	C3C-C4C-NC	3.23	114.57	110.43
13	A	837	CLA	C3B-C4B-NB	3.23	113.42	110.53
13	A	842	CLA	C4-C3-C5	3.23	119.93	116.13
13	A	813	CLA	CHC-C1C-C2C	-3.23	117.76	126.95
13	B	808	CLA	C3B-C4B-NB	3.23	113.42	110.53
13	B	805	CLA	CMB-C2B-C1B	3.23	130.34	125.42
13	A	827	CLA	C3C-C4C-NC	3.23	114.57	110.43
13	B	811	CLA	C3C-C4C-NC	3.23	114.56	110.43
13	B	802	CLA	C4C-C3C-C2C	-3.23	102.19	106.89
12	A	801	CL0	C1-C2-C3	-3.23	120.91	126.20
13	A	840	CLA	C4B-C3B-C2B	-3.22	103.29	107.30
13	A	807	CLA	C3C-C4C-NC	3.22	114.56	110.43
13	B	809	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
13	A	802	CLA	CHC-C1C-C2C	-3.22	117.79	126.95
13	A	819	CLA	C4C-C3C-C2C	-3.22	102.20	106.89
13	A	844	CLA	CHC-C1C-C2C	-3.22	117.79	126.95
13	A	816	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
13	A	827	CLA	O2A-CGA-CBA	3.22	121.64	111.83
13	B	826	CLA	CHC-C1C-C2C	-3.22	117.81	126.95
13	A	818	CLA	C4B-C3B-C2B	-3.22	103.30	107.30
13	L	204	CLA	C1C-C2C-C3C	-3.21	103.60	106.98
13	A	809	CLA	C4C-C3C-C2C	-3.21	102.22	106.89
12	A	801	CL0	O1D-CGD-CBD	-3.20	119.86	124.72
13	B	809	CLA	C4A-NA-C1A	-3.20	105.22	106.68
13	J	101	CLA	C3B-C4B-NB	3.20	113.39	110.53
13	B	819	CLA	C3B-C4B-NB	3.20	113.38	110.53
13	A	811	CLA	CMA-C3A-C2A	-3.20	101.62	113.98
13	B	810	CLA	C3B-C4B-NB	3.20	113.38	110.53
13	B	824	CLA	CAC-C3C-C4C	3.19	128.95	124.79
13	B	832	CLA	C3C-C4C-NC	3.19	114.52	110.43
13	B	815	CLA	CMB-C2B-C1B	3.19	130.28	125.42
13	A	835	CLA	CHC-C1C-C2C	-3.19	117.87	126.95
13	B	808	CLA	C1-C2-C3	-3.19	120.97	126.20
13	B	822	CLA	CHD-C1D-ND	-3.19	120.31	124.80
13	A	813	CLA	C4B-C3B-C2B	-3.19	103.33	107.30
13	B	804	CLA	CHB-C4A-NA	3.19	129.00	124.40
13	A	821	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
13	B	828	CLA	C4B-C3B-C2B	-3.19	103.34	107.30
16	F	201	BCR	C15-C16-C17	-3.19	117.00	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	815	CLA	CHC-C1C-C2C	-3.19	117.89	126.95
13	A	826	CLA	C3B-C4B-NB	3.18	113.37	110.53
13	L	203	CLA	CAA-C2A-C3A	-3.18	104.40	113.00
13	A	827	CLA	CHD-C4C-NC	3.18	129.16	124.23
13	A	803	CLA	C4B-C3B-C2B	-3.18	103.35	107.30
13	A	815	CLA	C3C-C4C-NC	3.18	114.50	110.43
13	A	834	CLA	C1-C2-C3	-3.17	121.00	126.20
13	B	808	CLA	CAA-C2A-C3A	-3.17	104.43	113.00
13	L	204	CLA	CAC-C3C-C4C	3.17	128.91	124.79
13	B	827	CLA	C3C-C4C-NC	3.17	114.48	110.43
13	A	818	CLA	C4C-C3C-C2C	-3.17	102.28	106.89
13	B	801	CLA	C4B-C3B-C2B	-3.17	103.37	107.30
13	B	829	CLA	C4C-C3C-C2C	-3.16	102.29	106.89
17	A	853	LHG	O8-C23-C24	3.16	120.74	111.15
13	B	821	CLA	CAC-C3C-C4C	3.16	128.90	124.79
13	L	202	CLA	C3B-C4B-NB	3.15	113.34	110.53
13	F	203	CLA	CHC-C1C-C2C	-3.15	117.99	126.95
13	A	829	CLA	C1-C2-C3	-3.15	121.03	126.20
13	A	818	CLA	CHC-C1C-C2C	-3.15	117.99	126.95
12	A	801	CL0	O2A-CGA-CBA	3.15	121.45	111.83
13	B	824	CLA	C3C-C4C-NC	3.15	114.47	110.43
13	B	815	CLA	CAC-C3C-C4C	3.15	128.89	124.79
13	B	828	CLA	CAC-C3C-C4C	3.15	128.88	124.79
13	B	827	CLA	CAC-C3C-C4C	3.15	128.88	124.79
13	K	203	CLA	CHC-C1C-C2C	-3.15	118.01	126.95
13	B	809	CLA	C4C-C3C-C2C	-3.15	102.31	106.89
13	B	807	CLA	CHC-C1C-C2C	-3.15	118.01	126.95
13	B	822	CLA	C4B-C3B-C2B	-3.14	103.39	107.30
13	A	811	CLA	C3C-C4C-NC	3.14	114.46	110.43
13	L	202	CLA	CHD-C4C-NC	3.14	129.10	124.23
13	A	810	CLA	CAC-C3C-C4C	3.14	128.88	124.79
13	B	811	CLA	CHC-C1C-C2C	-3.14	118.02	126.95
13	A	836	CLA	C4B-C3B-C2B	-3.14	103.40	107.30
13	A	811	CLA	CMB-C2B-C1B	3.14	130.20	125.42
13	A	812	CLA	C4C-C3C-C2C	-3.14	102.33	106.89
13	B	804	CLA	CAC-C3C-C4C	3.13	128.87	124.79
16	B	835	BCR	C27-C26-C25	3.13	126.94	122.70
13	A	832	CLA	C3B-C4B-NB	3.13	113.33	110.53
13	B	830	CLA	C1-C2-C3	-3.13	121.07	126.20
13	L	203	CLA	C3B-C4B-NB	3.13	113.32	110.53
13	B	820	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
13	B	820	CLA	O2A-CGA-CBA	3.13	121.37	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	815	CLA	CHD-C4C-NC	3.13	129.08	124.23
13	B	821	CLA	C4C-C3C-C2C	-3.13	102.34	106.89
13	B	808	CLA	CHC-C1C-C2C	-3.13	118.06	126.95
13	B	805	CLA	CHD-C4C-NC	3.12	129.07	124.23
13	A	809	CLA	CAC-C3C-C4C	3.12	128.85	124.79
13	B	830	CLA	CHD-C4C-NC	3.12	129.07	124.23
13	B	805	CLA	CAA-C2A-C3A	-3.12	104.57	113.00
13	B	822	CLA	CHC-C1C-C2C	-3.12	118.08	126.95
13	A	832	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
13	A	836	CLA	CAA-C2A-C3A	-3.11	104.58	113.00
13	B	809	CLA	CHC-C1C-C2C	-3.11	118.11	126.95
13	B	802	CLA	CBC-CAC-C3C	-3.11	103.99	112.42
13	B	803	CLA	C4-C3-C5	3.11	120.63	115.23
13	A	827	CLA	CBC-CAC-C3C	-3.11	103.99	112.42
13	B	816	CLA	C4B-C3B-C2B	-3.11	103.44	107.30
13	A	832	CLA	C3C-C4C-NC	3.11	114.41	110.43
13	A	843	CLA	CMB-C2B-C1B	3.10	130.14	125.42
13	A	840	CLA	CHD-C4C-NC	3.10	129.04	124.23
16	A	851	BCR	C28-C27-C26	-3.10	108.53	114.06
13	A	834	CLA	C3B-C4B-NB	3.10	113.30	110.53
13	A	840	CLA	C3B-C4B-NB	3.10	113.30	110.53
13	A	806	CLA	CHC-C1C-C2C	-3.10	118.15	126.95
13	B	806	CLA	CMB-C2B-C1B	3.10	130.13	125.42
13	A	831	CLA	CAC-C3C-C4C	3.09	128.81	124.79
13	A	804	CLA	C4B-C3B-C2B	-3.09	103.46	107.30
13	B	816	CLA	CHC-C1C-C2C	-3.09	118.17	126.95
13	K	201	CLA	C3C-C4C-NC	3.09	114.39	110.43
13	B	833	CLA	C1-C2-C3	-3.09	121.14	126.20
13	B	825	CLA	C1-C2-C3	-3.08	121.14	126.20
13	B	804	CLA	C1-C2-C3	-3.08	121.15	126.20
13	B	809	CLA	O2A-CGA-O1A	-3.08	115.92	123.63
13	B	823	CLA	C4-C3-C5	3.08	120.57	115.23
13	B	803	CLA	C1-C2-C3	-3.08	121.15	126.20
13	B	801	CLA	C4C-C3C-C2C	-3.08	102.41	106.89
13	B	826	CLA	O2A-CGA-CBA	3.08	121.22	111.83
13	A	834	CLA	CHC-C1C-C2C	-3.08	118.21	126.95
13	J	101	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
13	B	806	CLA	O2D-CGD-O1D	-3.07	117.86	123.85
13	B	810	CLA	CHC-C1C-C2C	-3.07	118.22	126.95
13	B	829	CLA	CHD-C4C-NC	3.07	129.00	124.23
13	A	812	CLA	CAC-C3C-C4C	3.07	128.79	124.79
13	B	822	CLA	O2A-CGA-O1A	-3.07	115.94	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	816	CLA	C3C-C4C-NC	3.07	114.36	110.43
13	A	803	CLA	C4C-C3C-C2C	-3.07	102.42	106.89
16	J	103	BCR	C27-C26-C25	3.07	126.85	122.70
13	A	802	CLA	O2A-CGA-CBA	3.07	121.19	111.83
13	A	816	CLA	CAC-C3C-C4C	3.07	128.78	124.79
13	A	840	CLA	O2A-CGA-CBA	3.07	121.19	111.83
13	A	839	CLA	CHC-C1C-C2C	-3.07	118.23	126.95
13	K	203	CLA	C4B-C3B-C2B	-3.07	103.49	107.30
13	A	804	CLA	C3B-C4B-NB	3.07	113.27	110.53
13	L	204	CLA	C4C-C3C-C2C	-3.07	102.43	106.89
13	A	842	CLA	C3B-C4B-NB	3.06	113.27	110.53
13	A	841	CLA	CHC-C1C-C2C	-3.06	118.24	126.95
12	A	801	CL0	O2D-CGD-O1D	-3.06	117.89	123.85
13	A	843	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
13	A	836	CLA	C4C-C3C-C2C	-3.06	102.44	106.89
13	A	802	CLA	CAC-C3C-C4C	3.06	128.77	124.79
16	I	101	BCR	C29-C30-C25	3.06	114.88	110.44
13	A	808	CLA	O2A-CGA-CBA	3.06	121.15	111.83
13	B	806	CLA	C4B-C3B-C2B	-3.06	103.50	107.30
13	B	801	CLA	CHC-C1C-C2C	-3.06	118.26	126.95
13	B	828	CLA	CAA-C2A-C3A	-3.05	104.75	113.00
13	B	819	CLA	C3C-C4C-NC	3.05	114.34	110.43
18	B	838	LMG	O6-C1-O1	-3.05	102.83	110.04
13	A	808	CLA	C1-C2-C3	-3.05	121.20	126.20
13	B	807	CLA	C4B-C3B-C2B	-3.05	103.51	107.30
13	A	825	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	A	826	CLA	C4A-NA-C1A	-3.05	105.29	106.68
13	B	823	CLA	C3C-C4C-NC	3.05	114.33	110.43
13	A	837	CLA	CHC-C1C-C2C	-3.05	118.29	126.95
13	A	822	CLA	CAC-C3C-C4C	3.05	128.75	124.79
13	A	802	CLA	CBC-CAC-C3C	-3.04	104.17	112.42
13	A	810	CLA	CHC-C1C-C2C	-3.04	118.30	126.95
13	A	844	CLA	C4B-C3B-C2B	-3.04	103.52	107.30
13	A	838	CLA	C4C-C3C-C2C	-3.04	102.46	106.89
13	A	825	CLA	O2A-CGA-CBA	3.04	121.11	111.83
13	B	801	CLA	C4-C3-C5	3.04	120.50	115.23
13	A	818	CLA	C4-C3-C5	3.04	120.50	115.23
13	A	803	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
13	B	806	CLA	O2A-CGA-CBA	3.04	121.10	111.83
13	B	818	CLA	C1-C2-C3	-3.04	121.22	126.20
13	B	811	CLA	C4B-C3B-C2B	-3.04	103.53	107.30
13	A	814	CLA	CHC-C1C-C2C	-3.04	118.32	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	850	BCR	C24-C23-C22	-3.04	121.75	126.23
13	A	830	CLA	O2A-CGA-CBA	3.03	121.09	111.83
13	A	843	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
13	A	835	CLA	C1-C2-C3	-3.03	121.23	126.20
13	A	802	CLA	CHA-C1A-NA	-3.03	119.53	126.39
13	A	823	CLA	C3B-C4B-NB	3.03	113.24	110.53
13	B	828	CLA	CHC-C1C-C2C	-3.03	118.35	126.95
16	M	101	BCR	C24-C23-C22	-3.03	121.76	126.23
13	A	828	CLA	CAA-C2A-C3A	-3.03	104.82	113.00
13	B	805	CLA	C3B-C4B-NB	3.03	113.23	110.53
16	B	835	BCR	C15-C14-C13	-3.02	123.04	127.28
13	B	807	CLA	C11-C12-C13	-3.02	105.91	115.97
13	B	805	CLA	CAC-C3C-C4C	3.02	128.72	124.79
13	A	834	CLA	CMB-C2B-C1B	3.02	130.02	125.42
13	A	821	CLA	C3C-C4C-NC	3.02	114.30	110.43
13	A	822	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
12	A	801	CL0	CGD-CBD-CAD	-3.02	101.07	110.85
13	B	811	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
13	B	825	CLA	CAA-C2A-C3A	-3.02	104.84	113.00
13	A	828	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
13	A	833	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
13	B	826	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
13	A	823	CLA	C4B-C3B-C2B	-3.02	103.55	107.30
13	A	802	CLA	C4C-C3C-C2C	-3.02	102.50	106.89
13	B	807	CLA	C3B-C4B-NB	3.02	113.22	110.53
13	A	831	CLA	C1-C2-C3	-3.01	121.26	126.20
13	B	815	CLA	C4C-C3C-C2C	-3.01	102.51	106.89
16	A	847	BCR	C24-C23-C22	-3.01	121.78	126.23
13	B	828	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
13	A	833	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
13	K	201	CLA	CHC-C1C-C2C	-3.01	118.39	126.95
13	B	826	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
13	A	825	CLA	C4B-C3B-C2B	-3.01	103.56	107.30
13	A	824	CLA	C4-C3-C5	3.01	119.67	116.13
13	A	805	CLA	C4C-C3C-C2C	-3.00	102.52	106.89
13	B	832	CLA	CHC-C1C-C2C	-3.00	118.41	126.95
13	A	830	CLA	CMB-C2B-C1B	3.00	129.99	125.42
13	B	813	CLA	C3B-C4B-NB	3.00	113.21	110.53
13	A	814	CLA	CAA-C2A-C3A	-3.00	104.89	113.00
13	A	841	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
13	B	802	CLA	CMA-C3A-C4A	-3.00	103.71	111.77
13	A	821	CLA	O2D-CGD-O1D	-3.00	118.01	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	815	CLA	CMB-C2B-C1B	3.00	129.98	125.42
13	A	802	CLA	C4B-C3B-C2B	-3.00	103.57	107.30
13	B	828	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
13	A	814	CLA	C3B-C4B-NB	3.00	113.21	110.53
13	B	817	CLA	C4C-C3C-C2C	-3.00	102.53	106.89
13	A	836	CLA	CHC-C1C-C2C	-3.00	118.44	126.95
13	A	843	CLA	CHC-C1C-C2C	-3.00	118.44	126.95
13	A	833	CLA	O2A-CGA-CBA	2.99	120.97	111.83
13	B	831	CLA	CHC-C1C-C2C	-2.99	118.44	126.95
13	A	828	CLA	C1C-C2C-C3C	-2.99	103.83	106.98
13	A	835	CLA	CHB-C4A-NA	2.99	128.72	124.40
13	A	830	CLA	CHD-C1D-ND	-2.99	120.59	124.80
13	B	823	CLA	O2A-CGA-CBA	2.99	120.96	111.83
13	A	803	CLA	CHB-C1B-C2B	-2.99	118.75	127.43
16	J	104	BCR	C31-C1-C6	2.99	114.93	110.24
13	A	812	CLA	O2A-CGA-CBA	2.99	120.94	111.83
13	B	825	CLA	C4B-C3B-C2B	-2.99	103.59	107.30
13	A	813	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
13	A	824	CLA	CAC-C3C-C4C	2.99	128.67	124.79
13	F	203	CLA	CAC-C3C-C4C	2.98	128.67	124.79
13	A	823	CLA	CHD-C4C-NC	2.98	128.86	124.23
16	A	848	BCR	C40-C30-C25	2.98	114.92	110.24
13	A	841	CLA	C3B-C4B-NB	2.98	113.19	110.53
13	A	835	CLA	C4C-C3C-C2C	-2.98	102.55	106.89
12	A	801	CL0	C4C-C3C-C2C	-2.98	101.60	113.37
13	B	824	CLA	CHC-C1C-C2C	-2.98	118.48	126.95
13	B	830	CLA	C3B-C4B-NB	2.98	113.19	110.53
13	A	836	CLA	CAC-C3C-C4C	2.98	128.66	124.79
13	B	830	CLA	C3C-C4C-NC	2.98	114.24	110.43
13	B	830	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
13	B	827	CLA	CHC-C1C-C2C	-2.98	118.49	126.95
13	B	808	CLA	CBC-CAC-C3C	-2.97	104.36	112.42
13	A	837	CLA	CAC-C3C-C4C	2.97	128.66	124.79
13	B	826	CLA	C3C-C4C-NC	2.97	114.23	110.43
13	B	820	CLA	CHD-C4C-NC	2.97	128.84	124.23
13	L	203	CLA	C4C-C3C-C2C	-2.97	102.57	106.89
13	L	203	CLA	CHC-C1C-C2C	-2.97	118.52	126.95
13	A	833	CLA	CHD-C4C-NC	2.96	128.83	124.23
13	A	829	CLA	C1C-C2C-C3C	-2.96	103.86	106.98
13	A	831	CLA	CAA-C2A-C3A	-2.96	104.99	113.00
13	B	820	CLA	C4B-C3B-C2B	-2.96	103.62	107.30
13	B	817	CLA	CHC-C1C-C2C	-2.96	118.53	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	805	CLA	C4C-C3C-C2C	-2.96	102.58	106.89
13	A	828	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
16	B	836	BCR	C15-C14-C13	-2.96	123.13	127.28
13	A	811	CLA	CBC-CAC-C3C	-2.96	104.40	112.42
13	B	823	CLA	CMA-C3A-C2A	-2.96	102.56	113.98
16	K	202	BCR	C27-C26-C25	2.95	126.70	122.70
13	B	820	CLA	CAC-C3C-C4C	2.95	128.63	124.79
13	A	836	CLA	O2A-CGA-CBA	2.95	120.84	111.83
13	A	821	CLA	C4A-NA-C1A	-2.95	105.33	106.68
13	B	812	CLA	CAC-C3C-C4C	2.95	128.63	124.79
13	L	204	CLA	CHC-C1C-C2C	-2.95	118.56	126.95
14	B	834	PQN	C2M-C2-C3	-2.95	119.60	124.45
13	A	840	CLA	CHC-C1C-C2C	-2.95	118.57	126.95
13	B	822	CLA	C4C-C3C-C2C	-2.95	102.60	106.89
13	B	832	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
13	A	839	CLA	C3B-C4B-NB	2.95	113.16	110.53
13	B	816	CLA	CHD-C4C-NC	2.95	128.80	124.23
13	A	837	CLA	C4B-C3B-C2B	-2.95	103.64	107.30
13	B	814	CLA	CHD-C4C-NC	2.94	128.80	124.23
13	B	830	CLA	O2A-CGA-CBA	2.94	120.81	111.83
13	A	844	CLA	CHD-C4C-NC	2.94	128.79	124.23
13	B	821	CLA	O2A-CGA-CBA	2.94	120.81	111.83
13	A	808	CLA	C4-C3-C5	2.94	119.59	116.13
13	A	805	CLA	CAC-C3C-C4C	2.94	128.61	124.79
13	A	824	CLA	CHC-C1C-C2C	-2.94	118.60	126.95
13	A	828	CLA	O2A-CGA-CBA	2.94	120.79	111.83
13	A	841	CLA	C1-C2-C3	-2.93	121.39	126.20
13	A	843	CLA	C3B-C4B-NB	2.93	113.15	110.53
13	B	831	CLA	O2A-CGA-CBA	2.93	120.78	111.83
13	A	816	CLA	C4C-C3C-C2C	-2.93	102.63	106.89
13	B	814	CLA	CHC-C1C-C2C	-2.93	118.62	126.95
13	A	829	CLA	CHD-C4C-NC	2.93	128.77	124.23
13	B	818	CLA	O2A-CGA-CBA	2.93	120.76	111.83
13	B	815	CLA	C4B-C3B-C2B	-2.93	103.66	107.30
13	A	809	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
13	B	813	CLA	CHC-C1C-C2C	-2.93	118.63	126.95
13	B	817	CLA	CHD-C4C-NC	2.93	128.77	124.23
13	B	821	CLA	CHD-C4C-NC	2.93	128.77	124.23
13	B	826	CLA	C4C-C3C-C2C	-2.92	102.64	106.89
16	A	848	BCR	C27-C26-C25	2.92	126.66	122.70
13	B	822	CLA	CAC-C3C-C4C	2.92	128.59	124.79
13	A	831	CLA	O2D-CGD-O1D	-2.92	118.16	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	834	CLA	CMA-C3A-C4A	-2.92	103.92	111.77
13	B	814	CLA	CAA-C2A-C3A	-2.92	105.10	113.00
13	B	808	CLA	C4B-C3B-C2B	-2.92	103.67	107.30
13	A	804	CLA	CHC-C1C-C2C	-2.92	118.65	126.95
13	A	804	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
13	A	836	CLA	CMB-C2B-C1B	2.92	129.86	125.42
13	A	820	CLA	C3C-C4C-NC	2.92	114.17	110.43
13	A	824	CLA	O2A-CGA-CBA	2.92	120.72	111.83
13	B	819	CLA	CHC-C1C-C2C	-2.92	118.66	126.95
13	F	203	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
13	B	806	CLA	C4C-C3C-C2C	-2.91	102.65	106.89
13	A	833	CLA	C4B-C3B-C2B	-2.91	103.68	107.30
13	B	809	CLA	CHB-C4A-NA	2.91	128.59	124.40
13	A	818	CLA	CHD-C4C-NC	2.90	128.73	124.23
13	A	842	CLA	CMC-C2C-C1C	2.90	129.57	125.03
13	A	818	CLA	O2A-CGA-CBA	2.90	120.68	111.83
13	B	824	CLA	C4C-C3C-C2C	-2.90	102.67	106.89
13	L	202	CLA	CHC-C1C-C2C	-2.90	118.71	126.95
13	B	831	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	J	101	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	B	831	CLA	C4B-C3B-C2B	-2.90	103.70	107.30
13	A	821	CLA	CHD-C4C-NC	2.90	128.72	124.23
13	B	804	CLA	O2A-CGA-CBA	2.89	120.66	111.83
13	B	831	CLA	CHD-C4C-NC	2.89	128.72	124.23
13	A	838	CLA	CHD-C4C-NC	2.89	128.72	124.23
13	B	814	CLA	C4B-C3B-C2B	-2.89	103.71	107.30
13	B	809	CLA	CBA-CAA-C2A	2.89	122.39	113.79
13	B	802	CLA	C1-C2-C3	-2.89	121.46	126.20
13	A	805	CLA	CHD-C4C-NC	2.89	128.71	124.23
13	B	805	CLA	CHC-C1C-C2C	-2.89	118.74	126.95
13	B	814	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
13	B	823	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
13	B	833	CLA	C4C-C3C-C2C	-2.89	102.69	106.89
13	B	818	CLA	CHD-C4C-NC	2.89	128.71	124.23
13	B	806	CLA	CHB-C4A-NA	2.89	128.56	124.40
13	A	808	CLA	C3C-C4C-NC	2.89	114.13	110.43
16	A	851	BCR	C24-C23-C22	-2.88	121.97	126.23
13	B	830	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
13	B	809	CLA	CHD-C4C-NC	2.88	128.70	124.23
13	B	824	CLA	C4B-C3B-C2B	-2.88	103.72	107.30
13	B	814	CLA	CHB-C4A-NA	2.88	128.55	124.40
13	B	811	CLA	C4C-C3C-C2C	-2.87	102.71	106.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	L	202	CLA	C4B-C3B-C2B	-2.87	103.73	107.30
16	L	205	BCR	C15-C14-C13	-2.87	123.25	127.28
13	A	824	CLA	C4C-C3C-C2C	-2.87	102.72	106.89
13	K	203	CLA	CBC-CAC-C3C	-2.87	104.65	112.42
13	A	808	CLA	C4B-C3B-C2B	-2.87	103.74	107.30
13	B	812	CLA	CAA-C2A-C3A	-2.87	105.26	113.00
13	A	825	CLA	C3C-C4C-NC	2.86	114.10	110.43
13	B	825	CLA	CHD-C4C-NC	2.86	128.67	124.23
13	A	804	CLA	CHD-C4C-NC	2.86	128.67	124.23
13	A	822	CLA	CAA-C2A-C3A	-2.86	105.27	113.00
13	A	832	CLA	C1-C2-C3	-2.86	122.13	126.76
13	A	821	CLA	CMB-C2B-C1B	2.86	129.78	125.42
13	K	201	CLA	C3B-C4B-NB	2.86	113.08	110.53
16	I	101	BCR	C30-C25-C26	-2.86	118.73	122.64
13	A	842	CLA	CHD-C4C-NC	2.86	128.66	124.23
13	A	830	CLA	CAC-C3C-C4C	2.86	128.51	124.79
13	B	814	CLA	C1-C2-C3	-2.86	121.52	126.20
13	K	201	CLA	C4C-C3C-C2C	-2.86	102.73	106.89
13	A	806	CLA	C3C-C4C-NC	2.86	114.09	110.43
16	M	101	BCR	C15-C16-C17	-2.85	117.68	123.52
13	B	801	CLA	CMC-C2C-C1C	2.85	129.49	125.03
13	A	840	CLA	CAA-C2A-C3A	-2.85	105.30	113.00
13	B	805	CLA	CHB-C4A-NA	2.85	128.51	124.40
13	A	805	CLA	CHB-C4A-NA	2.85	128.51	124.40
13	B	827	CLA	C4C-C3C-C2C	-2.85	102.75	106.89
13	A	842	CLA	CBC-CAC-C3C	-2.84	104.71	112.42
13	B	816	CLA	CAC-C3C-C4C	2.84	128.49	124.79
13	A	820	CLA	O2A-CGA-CBA	2.84	120.50	111.83
13	A	810	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
13	A	813	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
16	A	850	BCR	C15-C16-C17	-2.84	117.71	123.52
13	B	802	CLA	CHC-C1C-C2C	-2.84	118.88	126.95
13	A	844	CLA	CMB-C2B-C1B	2.84	129.74	125.42
13	B	805	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
13	A	810	CLA	C4C-C3C-C2C	-2.84	102.76	106.89
13	A	826	CLA	C4B-C3B-C2B	-2.84	103.78	107.30
13	A	834	CLA	CHD-C4C-NC	2.83	128.63	124.23
13	K	203	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
13	A	842	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
13	A	820	CLA	CAC-C3C-C4C	2.83	128.47	124.79
13	A	815	CLA	CHC-C1C-C2C	-2.83	118.90	126.95
13	A	810	CLA	CBC-CAC-C3C	-2.83	104.75	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	A	848	BCR	C11-C10-C9	-2.83	123.31	127.28
13	B	831	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
13	A	839	CLA	O2A-CGA-CBA	2.83	120.46	111.83
13	A	806	CLA	CAC-C3C-C4C	2.83	128.47	124.79
13	A	835	CLA	O2A-CGA-CBA	2.82	120.44	111.83
13	A	803	CLA	C3B-C4B-NB	2.82	113.05	110.53
13	L	202	CLA	C4C-C3C-C2C	-2.82	102.78	106.89
13	K	203	CLA	CAC-C3C-C4C	2.82	128.46	124.79
13	B	819	CLA	C4C-C3C-C2C	-2.82	102.79	106.89
13	A	837	CLA	CHD-C4C-NC	2.82	128.60	124.23
13	A	820	CLA	CAA-C2A-C3A	-2.82	105.38	113.00
13	A	830	CLA	CHC-C1C-C2C	-2.82	118.94	126.95
13	A	841	CLA	CAA-C2A-C3A	-2.81	105.39	113.00
13	A	816	CLA	C4B-C3B-C2B	-2.81	103.80	107.30
13	A	822	CLA	CHC-C1C-C2C	-2.81	118.95	126.95
13	A	823	CLA	CHC-C1C-C2C	-2.81	118.96	126.95
13	B	830	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
13	A	819	CLA	C3B-C4B-NB	2.81	113.04	110.53
13	A	814	CLA	C4B-C3B-C2B	-2.81	103.81	107.30
14	B	834	PQN	C14-C13-C15	2.81	120.11	115.23
13	A	806	CLA	C1-C2-C3	-2.81	121.60	126.20
13	B	820	CLA	C4-C3-C5	2.81	120.10	115.23
13	B	825	CLA	CHC-C1C-C2C	-2.81	118.98	126.95
16	J	103	BCR	C3-C4-C5	-2.80	109.05	114.06
13	B	810	CLA	C4C-C3C-C2C	-2.80	102.81	106.89
13	B	809	CLA	C4B-C3B-C2B	-2.80	103.81	107.30
13	K	201	CLA	CHD-C4C-NC	2.80	128.58	124.23
16	A	850	BCR	C15-C14-C13	-2.80	123.35	127.28
13	A	834	CLA	CHB-C4A-NA	2.80	128.44	124.40
13	A	807	CLA	CHC-C1C-C2C	-2.80	118.98	126.95
13	A	807	CLA	CMC-C2C-C1C	2.80	129.41	125.03
13	A	839	CLA	CHD-C4C-NC	2.80	128.57	124.23
13	B	825	CLA	C4C-C3C-C2C	-2.80	102.82	106.89
13	A	805	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
13	B	813	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
13	A	826	CLA	CMC-C2C-C1C	2.80	129.41	125.03
13	A	809	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
13	A	822	CLA	CHD-C4C-NC	2.80	128.57	124.23
13	B	815	CLA	CHB-C4A-NA	2.79	128.43	124.40
13	A	815	CLA	CAC-C3C-C4C	2.79	128.42	124.79
13	A	840	CLA	CMB-C2B-C1B	2.79	129.67	125.42
13	A	838	CLA	O2A-CGA-CBA	2.79	120.34	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	836	BCR	C27-C26-C25	2.79	126.47	122.70
13	A	828	CLA	CHC-C1C-C2C	-2.79	119.02	126.95
13	B	821	CLA	C3B-C4B-NB	2.79	113.02	110.53
13	A	834	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
13	A	813	CLA	CMB-C2B-C1B	2.79	129.66	125.42
16	A	851	BCR	C1-C6-C5	-2.79	118.83	122.64
13	B	813	CLA	O2A-CGA-CBA	2.79	120.33	111.83
13	B	831	CLA	CAA-C2A-C3A	-2.79	105.47	113.00
13	A	814	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
13	B	819	CLA	C4B-C3B-C2B	-2.78	103.84	107.30
13	L	204	CLA	C4-C3-C5	2.78	120.06	115.23
13	F	203	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
13	B	812	CLA	C4C-C3C-C2C	-2.78	102.84	106.89
13	A	811	CLA	CAC-C3C-C4C	2.78	128.41	124.79
13	B	818	CLA	CAC-C3C-C4C	2.78	128.40	124.79
13	A	816	CLA	CMB-C2B-C1B	2.78	129.65	125.42
13	B	813	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
13	F	203	CLA	CAA-C2A-C3A	-2.77	105.51	113.00
13	B	803	CLA	C4B-C3B-C2B	-2.77	103.86	107.30
13	B	820	CLA	C3B-C4B-NB	2.77	113.00	110.53
13	B	816	CLA	C4C-C3C-C2C	-2.77	102.86	106.89
13	B	820	CLA	CHC-C1C-C2C	-2.77	119.09	126.95
13	B	801	CLA	O2A-CGA-CBA	2.76	120.26	111.83
13	A	818	CLA	CMB-C2B-C1B	2.76	129.63	125.42
13	A	805	CLA	CHC-C1C-C2C	-2.76	119.10	126.95
13	B	804	CLA	CHD-C4C-NC	2.76	128.51	124.23
13	B	803	CLA	CAC-C3C-C4C	2.76	128.38	124.79
16	B	837	BCR	C27-C26-C25	2.76	126.43	122.70
13	A	819	CLA	O2A-CGA-CBA	2.75	120.22	111.83
13	A	840	CLA	C4C-C3C-C2C	-2.75	102.89	106.89
13	B	817	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
13	L	204	CLA	C4B-C3B-C2B	-2.75	103.89	107.30
18	B	838	LMG	O1-C7-C8	-2.75	104.14	110.82
13	B	808	CLA	O2A-CGA-CBA	2.75	120.21	111.83
13	A	805	CLA	C4B-C3B-C2B	-2.74	103.89	107.30
13	A	833	CLA	C3B-C4B-NB	2.74	112.98	110.53
13	B	832	CLA	C1-C2-C3	-2.74	121.71	126.20
13	B	833	CLA	O2A-CGA-CBA	2.74	120.18	111.83
13	L	204	CLA	CHD-C4C-NC	2.74	128.47	124.23
13	A	842	CLA	C4B-C3B-C2B	-2.74	103.90	107.30
13	B	821	CLA	C1-C2-C3	-2.74	121.71	126.20
13	B	804	CLA	CHC-C1C-C2C	-2.73	119.18	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	824	CLA	CAA-CBA-CGA	-2.73	105.45	113.21
16	L	206	BCR	C15-C16-C17	-2.73	117.93	123.52
13	B	819	CLA	CAC-C3C-C4C	2.73	128.34	124.79
13	A	835	CLA	CHD-C4C-NC	2.73	128.46	124.23
13	B	817	CLA	O2A-CGA-CBA	2.73	120.15	111.83
13	A	824	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
13	B	811	CLA	CAA-C2A-C3A	-2.73	105.63	113.00
13	B	822	CLA	CHD-C4C-NC	2.73	128.46	124.23
13	A	826	CLA	CHC-C1C-C2C	-2.72	119.20	126.95
13	B	817	CLA	C1-C2-C3	-2.72	121.73	126.20
13	B	805	CLA	O2A-CGA-CBA	2.72	120.14	111.83
13	A	803	CLA	CHD-C4C-NC	2.72	128.45	124.23
13	A	820	CLA	C2A-C3A-C4A	-2.72	97.47	101.87
13	B	829	CLA	CAC-C3C-C4C	2.72	128.33	124.79
13	A	839	CLA	C4C-C3C-C2C	-2.72	102.93	106.89
13	A	809	CLA	CHB-C4A-NA	2.72	128.32	124.40
13	K	203	CLA	CHD-C4C-NC	2.72	128.45	124.23
13	A	806	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
13	A	822	CLA	C4B-C3B-C2B	-2.72	103.92	107.30
13	A	817	CLA	CAC-C3C-C4C	2.72	128.32	124.79
13	A	809	CLA	C3B-C4B-NB	2.72	112.95	110.53
13	A	837	CLA	C4C-C3C-C2C	-2.72	102.94	106.89
13	B	802	CLA	CMC-C2C-C1C	2.72	129.28	125.03
16	M	101	BCR	C27-C26-C25	2.72	126.37	122.70
13	B	817	CLA	CAC-C3C-C4C	2.71	128.32	124.79
13	B	810	CLA	O2A-CGA-CBA	2.71	120.11	111.83
13	B	807	CLA	C4C-C3C-C2C	-2.71	102.94	106.89
13	A	815	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
13	A	839	CLA	CAC-C3C-C4C	2.71	128.31	124.79
13	B	813	CLA	C4-C3-C5	2.71	119.93	115.23
16	J	103	BCR	C11-C10-C9	-2.71	123.48	127.28
16	J	104	BCR	C7-C8-C9	-2.71	122.23	126.23
13	A	817	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
13	B	808	CLA	C4C-C3C-C2C	-2.71	102.95	106.89
13	A	829	CLA	O1D-CGD-CBD	-2.70	119.19	124.52
13	A	811	CLA	CHD-C4C-NC	2.70	128.42	124.23
13	A	830	CLA	C1-C2-C3	-2.70	121.77	126.20
13	A	816	CLA	CHD-C4C-NC	2.70	128.42	124.23
13	B	803	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
16	F	202	BCR	C27-C26-C25	2.70	126.35	122.70
13	A	827	CLA	CHC-C1C-C2C	-2.70	119.27	126.95
13	B	803	CLA	CHA-C1A-NA	-2.70	120.28	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	810	CLA	CHD-C4C-NC	2.70	128.41	124.23
13	A	838	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
13	B	832	CLA	CAC-C3C-C4C	2.69	128.30	124.79
13	B	816	CLA	C1-C2-C3	-2.69	121.78	126.20
13	B	821	CLA	CHC-C1C-C2C	-2.69	119.29	126.95
16	L	205	BCR	C27-C26-C25	2.69	126.34	122.70
13	A	829	CLA	C3B-C4B-NB	2.69	112.93	110.53
13	B	830	CLA	CMB-C2B-C1B	2.69	129.52	125.42
13	B	832	CLA	C4C-C3C-C2C	-2.69	102.97	106.89
13	B	808	CLA	CAC-C3C-C4C	2.69	128.29	124.79
13	B	813	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
16	A	849	BCR	C7-C8-C9	-2.69	122.26	126.23
13	A	842	CLA	CAC-C3C-C4C	2.69	128.29	124.79
13	K	201	CLA	C4B-C3B-C2B	-2.69	103.96	107.30
16	L	201	BCR	C24-C23-C22	-2.69	122.26	126.23
13	B	807	CLA	C1-C2-C3	-2.69	121.80	126.20
13	A	815	CLA	C3B-C4B-NB	2.69	112.93	110.53
13	A	830	CLA	CHD-C4C-NC	2.68	128.39	124.23
13	A	832	CLA	C4B-C3B-C2B	-2.68	103.97	107.30
14	B	834	PQN	C16-C15-C13	-2.68	106.93	113.47
16	I	101	BCR	C28-C27-C26	-2.68	109.28	114.06
13	A	820	CLA	C4C-C3C-C2C	-2.68	102.99	106.89
13	B	824	CLA	CHD-C4C-NC	2.68	128.38	124.23
13	B	822	CLA	C1-C2-C3	-2.68	121.81	126.20
13	A	833	CLA	C4-C3-C5	2.68	119.88	115.23
13	A	833	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
13	L	203	CLA	CBC-CAC-C3C	-2.68	105.17	112.42
13	B	819	CLA	CHD-C4C-NC	2.67	128.38	124.23
13	A	834	CLA	C4B-C3B-C2B	-2.67	103.98	107.30
16	J	103	BCR	C7-C8-C9	-2.67	122.28	126.23
13	B	811	CLA	CMD-C2D-C3D	-2.67	121.57	127.69
13	A	817	CLA	O2A-CGA-CBA	2.67	119.97	111.83
16	B	835	BCR	C11-C10-C9	-2.67	123.54	127.28
13	L	204	CLA	O2A-CGA-CBA	2.67	119.97	111.83
13	B	820	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
13	B	824	CLA	O2A-CGA-CBA	2.66	119.96	111.83
13	A	823	CLA	O2A-CGA-CBA	2.66	119.96	111.83
13	A	818	CLA	CAA-C2A-C3A	-2.66	105.80	113.00
13	A	819	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	B	819	CLA	CMB-C2B-C3B	2.66	132.81	126.55
13	B	829	CLA	CHC-C1C-C2C	-2.66	119.39	126.95
13	A	827	CLA	C4-C3-C5	2.66	119.84	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	830	CLA	C3B-C4B-NB	2.66	112.90	110.53
13	A	805	CLA	CMA-C3A-C4A	-2.66	104.63	111.77
13	A	816	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	A	843	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	A	803	CLA	CHC-C1C-C2C	-2.66	119.40	126.95
13	B	825	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
13	B	832	CLA	CBC-CAC-C3C	-2.65	105.22	112.42
16	J	104	BCR	C27-C26-C25	2.65	126.29	122.70
13	A	813	CLA	CHD-C4C-NC	2.65	128.34	124.23
13	A	842	CLA	C4C-C3C-C2C	-2.65	103.03	106.89
13	A	839	CLA	CBC-CAC-C3C	-2.65	105.23	112.42
13	B	830	CLA	CHB-C4A-NA	2.65	128.22	124.40
16	K	202	BCR	C15-C14-C13	-2.65	123.57	127.28
13	A	818	CLA	CHB-C4A-NA	2.64	128.22	124.40
13	A	825	CLA	C4C-C3C-C2C	-2.64	103.04	106.89
13	A	833	CLA	CAC-C3C-C4C	2.64	128.23	124.79
13	A	818	CLA	CAC-C3C-C4C	2.64	128.22	124.79
16	F	201	BCR	C27-C26-C25	2.64	126.27	122.70
13	A	826	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
13	B	827	CLA	CHB-C4A-NA	2.64	128.21	124.40
13	A	807	CLA	CMB-C2B-C1B	2.64	129.44	125.42
13	B	831	CLA	CMB-C2B-C1B	2.64	129.43	125.42
13	A	844	CLA	O2D-CGD-O1D	-2.64	118.72	123.85
13	A	822	CLA	C4-C3-C5	2.64	119.80	115.23
13	A	807	CLA	C4C-C3C-C2C	-2.63	103.06	106.89
13	B	818	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
13	A	827	CLA	C4C-C3C-C2C	-2.63	103.07	106.89
13	A	826	CLA	CHD-C1D-ND	-2.63	121.11	124.80
13	A	811	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
13	A	832	CLA	C4C-C3C-C2C	-2.62	103.07	106.89
13	A	822	CLA	CMB-C2B-C1B	2.62	129.41	125.42
13	B	812	CLA	CHD-C4C-NC	2.62	128.29	124.23
13	B	832	CLA	CHD-C4C-NC	2.62	128.29	124.23
13	A	841	CLA	CED-O2D-CGD	2.62	121.86	115.92
16	A	848	BCR	C16-C15-C14	-2.62	118.16	123.52
16	J	102	BCR	C11-C10-C9	-2.62	123.61	127.28
13	A	806	CLA	CMC-C2C-C1C	2.62	129.12	125.03
13	B	817	CLA	C3B-C4B-NB	2.62	112.86	110.53
13	A	815	CLA	CMC-C2C-C1C	2.62	129.12	125.03
13	A	831	CLA	CMB-C2B-C3B	2.61	132.70	126.55
13	B	803	CLA	CHD-C4C-NC	2.61	128.28	124.23
13	B	813	CLA	C1-C2-C3	-2.61	121.92	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	829	CLA	CMB-C2B-C1B	2.61	129.39	125.42
13	A	806	CLA	C4-C3-C5	2.61	119.76	115.23
13	B	813	CLA	CMB-C2B-C1B	2.61	129.39	125.42
13	B	809	CLA	CAC-C3C-C4C	2.61	128.18	124.79
13	A	842	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
13	B	818	CLA	C4C-C3C-C2C	-2.60	103.10	106.89
13	B	814	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
13	B	811	CLA	C1-C2-C3	-2.60	121.93	126.20
13	F	203	CLA	CHD-C4C-NC	2.60	128.26	124.23
13	A	831	CLA	O2A-CGA-CBA	2.60	119.76	111.83
13	A	804	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
17	A	852	LHG	C11-C10-C9	-2.60	101.24	114.37
13	K	201	CLA	CBC-CAC-C3C	-2.60	105.38	112.42
13	A	821	CLA	CHB-C4A-NA	2.60	128.15	124.40
13	A	807	CLA	C1-C2-C3	-2.60	121.94	126.20
13	L	203	CLA	CHD-C4C-NC	2.59	128.25	124.23
13	A	815	CLA	CHB-C4A-NA	2.59	128.14	124.40
16	J	102	BCR	C15-C16-C17	-2.59	118.22	123.52
13	A	808	CLA	CHD-C4C-NC	2.59	128.24	124.23
13	A	822	CLA	C3B-C4B-NB	2.59	112.84	110.53
16	A	847	BCR	C15-C16-C17	-2.58	118.23	123.52
13	B	821	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
13	B	806	CLA	CHD-C4C-NC	2.58	128.23	124.23
13	B	818	CLA	CBC-CAC-C3C	-2.58	105.42	112.42
13	A	838	CLA	C4B-C3B-C2B	-2.58	104.09	107.30
13	A	809	CLA	C4B-C3B-C2B	-2.58	104.10	107.30
13	A	807	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
16	F	202	BCR	C16-C15-C14	-2.57	118.26	123.52
13	B	818	CLA	CAA-C2A-C3A	-2.57	106.05	113.00
13	A	819	CLA	CHD-C4C-NC	2.57	128.22	124.23
13	B	808	CLA	CHD-C4C-NC	2.57	128.22	124.23
13	B	801	CLA	CMB-C2B-C1B	2.57	129.33	125.42
13	B	830	CLA	C4C-C3C-C2C	-2.57	103.15	106.89
13	B	822	CLA	CMB-C2B-C1B	2.57	129.33	125.42
13	B	805	CLA	CBC-CAC-C3C	-2.57	105.46	112.42
13	A	826	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
13	B	810	CLA	CAC-C3C-C4C	2.57	128.13	124.79
13	A	824	CLA	C1-C2-C3	-2.57	121.99	126.20
13	A	807	CLA	C11-C12-C13	-2.56	107.44	115.97
13	A	825	CLA	CAA-C2A-C3A	-2.56	106.07	113.00
13	B	807	CLA	O2A-CGA-CBA	2.56	119.65	111.83
13	A	823	CLA	CMC-C2C-C1C	2.56	129.04	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	K	201	CLA	CMB-C2B-C1B	2.56	129.32	125.42
13	A	812	CLA	C4-C3-C5	2.56	119.67	115.23
13	B	802	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
13	B	816	CLA	CHB-C4A-NA	2.56	128.09	124.40
13	A	811	CLA	C4C-C3C-C2C	-2.56	103.17	106.89
13	A	822	CLA	CMC-C2C-C1C	2.56	129.03	125.03
13	A	829	CLA	C4B-C3B-C2B	-2.56	104.12	107.30
13	A	805	CLA	O1D-CGD-CBD	-2.56	119.47	124.52
13	A	820	CLA	CHD-C4C-NC	2.56	128.20	124.23
13	A	825	CLA	CMB-C2B-C1B	2.55	129.31	125.42
13	B	827	CLA	CHD-C4C-NC	2.55	128.19	124.23
13	B	827	CLA	CMB-C2B-C1B	2.55	129.30	125.42
13	B	806	CLA	C4-C3-C5	2.55	119.66	115.23
13	B	802	CLA	CAA-CBA-CGA	-2.55	105.97	113.21
16	A	848	BCR	C30-C25-C26	-2.55	119.15	122.64
13	A	843	CLA	C4-C3-C5	2.55	119.65	115.23
13	A	843	CLA	CHD-C4C-NC	2.55	128.18	124.23
13	A	821	CLA	C4-C3-C5	2.55	119.65	115.23
13	A	805	CLA	C3B-C4B-NB	2.55	112.80	110.53
13	B	803	CLA	CAA-CBA-CGA	-2.54	105.98	113.21
13	B	831	CLA	CAC-C3C-C4C	2.54	128.10	124.79
13	B	807	CLA	C4-C3-C5	2.54	119.64	115.23
13	B	825	CLA	CMB-C2B-C1B	2.54	129.29	125.42
12	A	801	CL0	C1C-CHC-C4B	2.54	125.17	116.07
13	B	815	CLA	CHD-C4C-NC	2.54	128.17	124.23
13	J	101	CLA	CHB-C4A-NA	2.54	128.06	124.40
16	J	104	BCR	C2-C1-C6	2.54	114.13	110.44
13	B	805	CLA	CMC-C2C-C1C	2.54	129.00	125.03
13	L	204	CLA	CMB-C2B-C1B	2.54	129.28	125.42
13	A	823	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
13	A	815	CLA	CBC-CAC-C3C	-2.54	105.54	112.42
13	A	826	CLA	O2A-CGA-CBA	2.54	119.57	111.83
13	B	814	CLA	O2A-CGA-CBA	2.53	119.56	111.83
13	A	808	CLA	CMB-C2B-C1B	2.53	129.28	125.42
13	J	101	CLA	CHD-C4C-NC	2.53	128.16	124.23
13	L	202	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
13	A	810	CLA	CHD-C4C-NC	2.53	128.15	124.23
13	A	808	CLA	CBC-CAC-C3C	-2.53	105.56	112.42
13	B	822	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
13	L	204	CLA	C1-C2-C3	-2.53	122.06	126.20
13	A	816	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
16	B	837	BCR	C24-C23-C22	-2.53	122.50	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	826	CLA	CMB-C2B-C1B	2.53	129.26	125.42
13	B	816	CLA	O2D-CGD-O1D	-2.52	118.93	123.85
13	A	808	CLA	CHB-C4A-NA	2.52	128.04	124.40
13	A	828	CLA	C3B-C4B-NB	2.52	112.78	110.53
13	A	810	CLA	CAA-CBA-CGA	-2.52	105.77	112.49
13	A	830	CLA	CMA-C3A-C4A	-2.52	105.00	111.77
13	B	829	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
13	A	826	CLA	CHD-C4C-NC	2.52	128.14	124.23
13	B	833	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
13	A	843	CLA	C4B-C3B-C2B	-2.52	104.17	107.30
16	A	847	BCR	C11-C10-C9	-2.52	123.75	127.28
13	B	809	CLA	CMB-C2B-C1B	2.52	129.25	125.42
13	A	819	CLA	CAA-C2A-C3A	-2.52	106.19	113.00
13	L	203	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
13	A	834	CLA	C4-C3-C5	2.52	119.60	115.23
13	A	844	CLA	O2A-CGA-CBA	2.52	119.51	111.83
13	A	838	CLA	CAA-C2A-C3A	-2.52	106.20	113.00
16	A	850	BCR	C29-C30-C25	2.52	114.09	110.44
13	A	808	CLA	C4C-C3C-C2C	-2.52	103.23	106.89
13	B	820	CLA	CMB-C2B-C1B	2.52	129.25	125.42
13	A	828	CLA	CHB-C4A-NA	2.52	128.03	124.40
13	A	806	CLA	CMA-C3A-C4A	-2.52	105.01	111.77
16	L	206	BCR	C28-C27-C26	-2.51	109.57	114.06
16	K	202	BCR	C38-C26-C27	-2.51	108.24	113.60
13	A	828	CLA	C4-C3-C5	2.51	119.59	115.23
13	B	820	CLA	CMC-C2C-C1C	2.51	128.96	125.03
16	L	205	BCR	C11-C10-C9	-2.51	123.76	127.28
13	B	801	CLA	CHD-C4C-NC	2.51	128.12	124.23
16	L	206	BCR	C3-C4-C5	-2.51	109.58	114.06
16	L	201	BCR	C15-C16-C17	-2.51	118.38	123.52
13	B	816	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
13	A	837	CLA	CBC-CAC-C3C	-2.51	105.62	112.42
13	B	825	CLA	C3B-C4B-NB	2.51	112.77	110.53
13	A	836	CLA	C1-C2-C3	-2.51	122.09	126.20
13	B	832	CLA	O2A-CGA-CBA	2.51	119.47	111.83
17	A	852	LHG	O8-C23-C24	2.51	119.47	111.83
13	A	820	CLA	C1-C2-C3	-2.50	122.09	126.20
13	B	814	CLA	CBC-CAC-C3C	-2.50	105.63	112.42
12	A	801	CL0	CMC-C2C-C1C	2.50	129.24	124.73
16	I	101	BCR	C24-C23-C22	-2.50	122.53	126.23
18	B	838	LMG	C40-C39-C38	-2.50	101.73	114.37
13	B	818	CLA	CHB-C1B-C2B	-2.50	120.17	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	823	CLA	C4C-C3C-C2C	-2.50	103.25	106.89
13	A	817	CLA	CBC-CAC-C3C	-2.50	105.65	112.42
13	B	803	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
16	A	851	BCR	C29-C30-C25	2.50	114.06	110.44
13	A	803	CLA	CAC-C3C-C4C	2.50	128.04	124.79
13	B	806	CLA	C1-C2-C3	-2.49	122.11	126.20
13	B	814	CLA	CAC-C3C-C4C	2.49	128.03	124.79
13	A	834	CLA	CMA-C3A-C2A	-2.49	104.34	113.98
13	B	813	CLA	CMC-C2C-C1C	2.49	128.93	125.03
13	B	823	CLA	CAA-C2A-C3A	-2.49	106.27	113.00
13	B	826	CLA	C1-C2-C3	-2.49	122.12	126.20
13	A	841	CLA	CHD-C4C-NC	2.49	128.09	124.23
13	B	812	CLA	CMB-C2B-C1B	2.49	129.21	125.42
13	L	202	CLA	CHB-C4A-NA	2.49	127.99	124.40
16	L	201	BCR	C15-C14-C13	-2.48	123.80	127.28
13	A	814	CLA	CMB-C2B-C1B	2.48	129.20	125.42
13	B	829	CLA	CMC-C2C-C1C	2.48	128.91	125.03
13	A	832	CLA	CHD-C4C-NC	2.48	128.08	124.23
16	F	201	BCR	C11-C10-C9	-2.48	123.80	127.28
13	A	832	CLA	CAA-C2A-C3A	-2.48	106.30	113.00
16	J	104	BCR	C15-C16-C17	-2.48	118.45	123.52
13	B	816	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
13	F	203	CLA	CMB-C2B-C1B	2.48	129.19	125.42
13	B	821	CLA	CHB-C4A-NA	2.48	127.98	124.40
13	A	836	CLA	CHB-C4A-NA	2.48	127.97	124.40
13	A	829	CLA	C4-C3-C5	2.48	119.53	115.23
16	K	202	BCR	C29-C30-C25	2.48	114.04	110.44
13	A	821	CLA	O2A-CGA-CBA	2.48	119.38	111.83
13	B	829	CLA	CAA-C2A-C3A	-2.47	106.31	113.00
13	A	836	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
13	A	807	CLA	C3B-C4B-NB	2.47	112.74	110.53
13	A	812	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
13	L	203	CLA	CHB-C4A-NA	2.47	127.97	124.40
13	B	821	CLA	CMB-C2B-C1B	2.47	129.18	125.42
16	A	848	BCR	C15-C14-C13	-2.47	123.81	127.28
13	B	801	CLA	C1-C2-C3	-2.47	122.15	126.20
13	B	832	CLA	C1-O2A-CGA	2.47	122.63	116.65
13	A	832	CLA	O1D-CGD-CBD	-2.47	119.65	124.52
13	A	827	CLA	CMC-C2C-C1C	2.47	128.89	125.03
13	A	804	CLA	CHB-C4A-NA	2.47	127.96	124.40
13	A	817	CLA	CMB-C2B-C1B	2.46	129.17	125.42
13	B	833	CLA	CHD-C4C-NC	2.46	128.05	124.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	834	PQN	C11-C12-C13	-2.46	122.59	126.83
13	B	801	CLA	CBC-CAC-C3C	-2.46	105.75	112.42
13	A	805	CLA	CMC-C2C-C1C	2.46	128.88	125.03
13	A	828	CLA	CMB-C2B-C1B	2.46	129.16	125.42
13	A	838	CLA	CMC-C2C-C1C	2.46	128.88	125.03
13	A	805	CLA	CAA-C2A-C3A	-2.46	106.36	113.00
13	A	807	CLA	C4B-C3B-C2B	-2.46	104.25	107.30
13	B	808	CLA	CMB-C2B-C1B	2.46	129.16	125.42
13	B	826	CLA	C4-C3-C5	2.46	119.49	115.23
13	B	806	CLA	CAC-C3C-C4C	2.46	127.98	124.79
13	B	802	CLA	C11-C12-C13	-2.46	107.80	115.97
13	A	806	CLA	C4C-C3C-C2C	-2.46	103.32	106.89
16	A	848	BCR	C38-C26-C27	-2.45	108.36	113.60
13	A	827	CLA	C3B-C4B-NB	2.45	112.72	110.53
13	A	802	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
13	A	839	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
13	L	203	CLA	O2A-CGA-CBA	2.45	119.30	111.83
13	B	827	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
13	A	814	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
13	L	204	CLA	O2D-CGD-O1D	-2.45	119.09	123.85
13	A	822	CLA	CHB-C4A-NA	2.45	127.93	124.40
13	A	832	CLA	CMB-C2B-C1B	2.44	129.14	125.42
13	B	804	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
14	A	845	PQN	C16-C15-C13	-2.44	107.52	113.47
13	B	803	CLA	CMC-C2C-C1C	2.44	128.85	125.03
13	A	836	CLA	CHD-C4C-NC	2.44	128.02	124.23
13	B	829	CLA	CBA-CAA-C2A	-2.44	106.53	113.79
13	A	834	CLA	O2A-CGA-O1A	-2.44	117.53	123.63
13	B	810	CLA	C4-C3-C5	2.44	119.46	115.23
13	B	825	CLA	CHB-C4A-NA	2.44	127.92	124.40
13	B	821	CLA	C4B-C3B-C2B	-2.44	104.27	107.30
13	A	834	CLA	CAC-C3C-C4C	2.43	127.96	124.79
13	B	808	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
13	A	808	CLA	CAA-C2A-C3A	-2.43	106.43	113.00
13	K	203	CLA	CMB-C2B-C1B	2.43	129.12	125.42
13	B	816	CLA	CMC-C2C-C1C	2.43	128.83	125.03
13	A	804	CLA	CMB-C2B-C1B	2.43	129.12	125.42
13	B	830	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
13	A	813	CLA	O2A-CGA-CBA	2.43	119.24	111.83
13	A	837	CLA	CHB-C4A-NA	2.42	127.90	124.40
13	B	827	CLA	CMA-C3A-C4A	-2.42	105.26	111.77
13	B	828	CLA	CGD-CBD-CAD	-2.42	103.01	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	835	CLA	C4B-C3B-C2B	-2.42	104.29	107.30
13	A	802	CLA	CHD-C4C-NC	2.42	127.98	124.23
13	A	809	CLA	CHD-C4C-NC	2.42	127.98	124.23
13	B	802	CLA	CAC-C3C-C4C	2.42	127.94	124.79
16	L	206	BCR	C29-C30-C25	2.42	113.95	110.44
13	B	819	CLA	CAA-C2A-C1A	-2.42	104.05	111.97
16	A	847	BCR	C28-C27-C26	-2.42	109.75	114.06
13	A	837	CLA	CMC-C2C-C1C	2.42	128.81	125.03
13	L	203	CLA	C4B-C3B-C2B	-2.41	104.30	107.30
13	A	828	CLA	CAC-C3C-C4C	2.41	127.93	124.79
16	L	206	BCR	C15-C14-C13	-2.41	123.89	127.28
13	A	822	CLA	C1-O2A-CGA	2.41	122.49	116.65
13	A	832	CLA	CHB-C4A-NA	2.41	127.88	124.40
13	B	816	CLA	CMB-C2B-C1B	2.41	129.09	125.42
18	B	838	LMG	C38-C37-C36	-2.41	102.19	114.37
13	A	817	CLA	CAA-C2A-C3A	-2.41	106.49	113.00
13	A	827	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
13	A	819	CLA	C4B-C3B-C2B	-2.41	104.31	107.30
13	A	820	CLA	CHB-C1B-C2B	-2.41	120.44	127.43
13	A	811	CLA	CHB-C4A-NA	2.41	127.87	124.40
13	A	831	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
13	A	826	CLA	C7-C6-C5	-2.40	106.85	113.26
16	F	202	BCR	C11-C10-C9	-2.40	123.91	127.28
13	B	814	CLA	CMC-C2C-C1C	2.40	128.79	125.03
13	A	841	CLA	CMC-C2C-C1C	2.40	128.78	125.03
13	A	824	CLA	CHD-C4C-NC	2.40	127.95	124.23
16	A	849	BCR	C24-C23-C22	-2.40	122.69	126.23
13	A	841	CLA	CHB-C1B-C2B	-2.40	120.47	127.43
13	A	844	CLA	O1D-CGD-CBD	-2.39	119.80	124.52
13	B	823	CLA	CMA-C3A-C4A	-2.39	105.34	111.77
13	L	204	CLA	CHB-C4A-NA	2.39	127.85	124.40
17	A	852	LHG	C20-C19-C18	-2.39	102.27	114.37
13	A	827	CLA	CHB-C4A-NA	2.39	127.85	124.40
13	B	830	CLA	O2A-CGA-O1A	-2.39	117.65	123.63
13	A	834	CLA	CBC-CAC-C3C	-2.39	105.94	112.42
13	B	820	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
13	A	821	CLA	C4C-C3C-C2C	-2.38	103.42	106.89
18	B	838	LMG	O3-C3-C2	-2.38	104.76	110.38
13	B	827	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
13	A	831	CLA	CHD-C4C-NC	2.38	127.93	124.23
13	B	809	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
12	A	801	CL0	C3D-C4D-ND	2.38	116.76	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	L	201	BCR	C27-C26-C25	2.38	125.92	122.70
13	B	805	CLA	C4-C3-C5	2.38	119.36	115.23
13	B	813	CLA	CHD-C4C-NC	2.38	127.92	124.23
13	A	806	CLA	CBA-CAA-C2A	2.38	120.87	113.79
13	B	823	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
13	A	815	CLA	C4B-C3B-C2B	-2.38	104.35	107.30
13	A	837	CLA	CAA-C2A-C3A	-2.38	106.58	113.00
16	B	837	BCR	C10-C11-C12	-2.37	116.32	123.20
13	A	829	CLA	CHB-C1B-C2B	-2.37	120.53	127.43
13	B	802	CLA	C11-C10-C8	-2.37	108.08	115.97
13	A	812	CLA	CMB-C2B-C1B	2.37	129.03	125.42
13	A	815	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
13	B	825	CLA	O2A-CGA-O1A	-2.37	117.70	123.63
13	A	812	CLA	CHB-C4A-NA	2.37	127.82	124.40
13	A	806	CLA	CMB-C2B-C1B	2.37	129.03	125.42
13	A	830	CLA	C4-C3-C5	2.37	119.34	115.23
13	B	811	CLA	C4-C3-C5	2.37	119.34	115.23
13	B	803	CLA	C6-C7-C8	-2.37	108.09	115.97
17	A	853	LHG	C11-C10-C9	-2.37	102.40	114.37
13	A	844	CLA	CHB-C4A-NA	2.37	127.81	124.40
13	A	802	CLA	C4-C3-C5	2.37	119.33	115.23
18	B	838	LMG	C42-C41-C40	-2.36	102.42	114.37
13	B	804	CLA	CMB-C2B-C1B	2.36	129.02	125.42
16	K	202	BCR	C16-C17-C18	-2.36	123.97	127.28
13	A	817	CLA	CHB-C4A-NA	2.36	127.81	124.40
13	A	808	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
13	A	840	CLA	O2A-C1-C2	2.36	117.20	108.11
13	B	802	CLA	CHB-C4A-NA	2.36	127.81	124.40
13	B	812	CLA	CHB-C4A-NA	2.36	127.81	124.40
13	A	819	CLA	C1-C2-C3	-2.36	122.33	126.20
16	J	104	BCR	C15-C14-C13	-2.36	123.97	127.28
13	A	842	CLA	CMB-C2B-C1B	2.36	129.00	125.42
13	A	812	CLA	CHD-C4C-NC	2.35	127.88	124.23
13	A	840	CLA	C6-C5-C3	2.35	119.20	113.47
13	B	825	CLA	CAC-C3C-C4C	2.35	127.85	124.79
13	K	203	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
13	A	827	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
13	A	826	CLA	C1-C2-C3	-2.35	122.34	126.20
13	B	808	CLA	C4-C3-C5	2.35	119.31	115.23
16	A	847	BCR	C15-C14-C13	-2.35	123.98	127.28
13	A	830	CLA	C4B-C3B-C2B	-2.35	104.38	107.30
13	B	810	CLA	O2D-CGD-O1D	-2.35	119.27	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	815	CLA	CAA-C2A-C3A	-2.35	106.65	113.00
13	B	814	CLA	CMB-C2B-C1B	2.35	128.99	125.42
16	L	205	BCR	C15-C16-C17	-2.35	118.72	123.52
13	B	828	CLA	CBC-CAC-C3C	-2.35	106.06	112.42
16	F	201	BCR	C24-C23-C22	-2.35	122.77	126.23
13	F	203	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
13	B	809	CLA	O1D-CGD-CBD	-2.34	119.89	124.52
16	A	849	BCR	C28-C27-C26	-2.34	109.88	114.06
13	A	804	CLA	O2A-CGA-O1A	-2.34	117.31	123.33
13	A	802	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
13	B	805	CLA	C4B-C3B-C2B	-2.34	104.39	107.30
13	A	836	CLA	CBC-CAC-C3C	-2.34	106.07	112.42
13	A	802	CLA	CHB-C1B-C2B	-2.34	120.63	127.43
13	L	203	CLA	C1-C2-C3	-2.34	122.37	126.20
13	A	820	CLA	C4-C3-C5	2.34	119.28	115.23
16	J	102	BCR	C29-C30-C25	2.34	113.83	110.44
13	A	824	CLA	CAA-C2A-C3A	-2.34	106.69	113.00
17	A	852	LHG	O8-C23-O10	-2.34	117.79	123.63
13	A	841	CLA	CBC-CAC-C3C	-2.33	106.09	112.42
13	A	819	CLA	CMB-C2B-C1B	2.33	128.97	125.42
13	A	806	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
13	A	828	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
13	A	829	CLA	CHC-C1C-C2C	-2.33	120.33	126.95
13	A	834	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
13	A	805	CLA	CHB-C1B-C2B	-2.33	120.67	127.43
16	B	837	BCR	C15-C16-C17	-2.33	118.76	123.52
13	A	825	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	A	807	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	B	808	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	B	832	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	A	832	CLA	CBC-CAC-C3C	-2.32	106.12	112.42
16	A	847	BCR	C29-C30-C25	2.32	113.81	110.44
13	B	826	CLA	CHD-C4C-NC	2.32	127.83	124.23
13	A	806	CLA	C6-C7-C8	-2.32	108.25	115.97
13	B	811	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
13	B	829	CLA	C4B-C3B-C2B	-2.32	104.42	107.30
13	A	838	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
13	B	810	CLA	CMC-C2C-C1C	2.32	128.66	125.03
13	A	809	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
13	A	809	CLA	C1-C2-C3	-2.32	122.40	126.20
13	A	814	CLA	CHD-C4C-NC	2.32	127.82	124.23
13	B	832	CLA	CAA-C2A-C3A	-2.32	106.74	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	833	CLA	CHB-C4A-NA	2.32	127.74	124.40
13	A	807	CLA	O2A-CGA-O1A	-2.32	117.84	123.63
13	A	830	CLA	CHA-C1A-NA	-2.31	121.15	126.39
13	B	815	CLA	CBC-CAC-C3C	-2.31	106.15	112.42
17	A	852	LHG	C18-C17-C16	-2.31	102.67	114.37
13	B	816	CLA	O2A-CGA-CBA	2.31	118.89	111.83
13	A	840	CLA	CMC-C2C-C1C	2.31	128.65	125.03
13	A	837	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
13	A	827	CLA	C4B-C3B-C2B	-2.31	104.43	107.30
13	A	833	CLA	C1-C2-C3	-2.31	122.41	126.20
13	B	819	CLA	CHB-C1B-C2B	-2.31	120.72	127.43
13	A	829	CLA	CMB-C2B-C3B	2.31	131.98	126.55
13	B	820	CLA	O1D-CGD-CBD	-2.31	119.97	124.52
13	A	803	CLA	O2A-CGA-CBA	2.31	121.29	114.00
13	B	825	CLA	CMC-C2C-C1C	2.31	128.64	125.03
13	B	807	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
16	J	103	BCR	C15-C16-C17	-2.30	118.81	123.52
13	B	833	CLA	CAC-C3C-C4C	2.30	127.78	124.79
13	B	804	CLA	C3B-C4B-NB	2.30	112.58	110.53
13	F	203	CLA	CBC-CAC-C3C	-2.30	106.18	112.42
13	A	839	CLA	CMC-C2C-C1C	2.30	128.63	125.03
13	A	833	CLA	CMB-C2B-C1B	2.30	128.92	125.42
13	B	811	CLA	CMB-C2B-C1B	2.30	128.92	125.42
13	A	809	CLA	CMB-C2B-C1B	2.30	128.91	125.42
13	L	203	CLA	CAC-C3C-C4C	2.29	127.78	124.79
13	B	810	CLA	CBC-CAC-C3C	-2.29	106.21	112.42
13	A	839	CLA	O1D-CGD-CBD	-2.29	120.00	124.52
13	A	832	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
13	A	813	CLA	CMC-C2C-C1C	2.29	128.61	125.03
13	A	819	CLA	CHA-C1A-NA	-2.29	121.20	126.39
13	A	821	CLA	O1D-CGD-CBD	-2.29	120.01	124.52
16	I	101	BCR	C11-C10-C9	-2.29	124.07	127.28
13	A	813	CLA	CHB-C4A-NA	2.29	127.70	124.40
13	A	822	CLA	C1-C2-C3	-2.28	122.45	126.20
13	A	807	CLA	CBC-CAC-C3C	-2.28	106.23	112.42
13	A	817	CLA	CHD-C4C-NC	2.28	127.77	124.23
13	B	826	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	A	842	CLA	C1-C2-C3	-2.28	122.46	126.20
13	A	819	CLA	C4-C3-C5	2.28	119.19	115.23
13	A	809	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
13	A	830	CLA	CMC-C2C-C1C	2.28	128.60	125.03
13	B	819	CLA	CHB-C4A-NA	2.28	127.69	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	852	LHG	C27-C26-C25	-2.28	102.85	114.37
13	B	828	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	A	835	CLA	OBD-CAD-C3D	-2.28	123.09	128.42
16	F	201	BCR	C15-C14-C13	-2.28	124.08	127.28
13	A	841	CLA	CHB-C4A-NA	2.28	127.69	124.40
16	J	104	BCR	C1-C6-C5	-2.28	119.53	122.64
16	J	102	BCR	C2-C1-C6	2.27	113.74	110.44
13	A	830	CLA	CHB-C4A-NA	2.27	127.68	124.40
13	A	830	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
13	A	807	CLA	C4-C3-C5	2.27	119.17	115.23
13	K	203	CLA	CMC-C2C-C1C	2.27	128.58	125.03
13	A	814	CLA	CHB-C4A-NA	2.27	127.67	124.40
16	J	102	BCR	C24-C23-C22	-2.27	122.88	126.23
14	A	845	PQN	C11-C3-C2	-2.26	121.01	124.89
13	B	823	CLA	C1-C2-C3	-2.26	122.49	126.20
13	A	815	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
13	B	812	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
13	B	829	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
13	B	823	CLA	CHB-C4A-NA	2.26	127.66	124.40
16	J	103	BCR	C15-C14-C13	-2.26	124.11	127.28
13	A	827	CLA	C1-C2-C3	-2.26	122.50	126.20
13	A	825	CLA	CHD-C4C-NC	2.26	127.73	124.23
13	B	820	CLA	CHA-C1A-NA	-2.26	121.28	126.39
13	A	823	CLA	C4-C3-C5	2.26	119.15	115.23
13	B	828	CLA	CHD-C4C-NC	2.26	127.73	124.23
16	J	103	BCR	C16-C15-C14	-2.26	118.90	123.52
16	A	849	BCR	C15-C16-C17	-2.25	118.91	123.52
16	B	836	BCR	C11-C10-C9	-2.25	124.12	127.28
13	B	821	CLA	CBA-CAA-C2A	2.25	120.50	113.79
16	A	848	BCR	C7-C8-C9	-2.25	122.90	126.23
16	F	202	BCR	C40-C30-C25	2.25	113.77	110.24
13	B	822	CLA	CHB-C4A-NA	2.25	127.64	124.40
13	B	827	CLA	CAA-C2A-C3A	-2.25	106.92	113.00
13	B	805	CLA	C1-C2-C3	-2.25	122.51	126.20
13	A	829	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
13	L	202	CLA	CHB-C1B-C2B	-2.25	120.91	127.43
13	A	840	CLA	CHB-C4A-NA	2.24	127.64	124.40
13	A	838	CLA	CGD-CBD-CAD	-2.24	103.59	110.85
13	B	802	CLA	CHA-C1A-NA	-2.24	121.32	126.39
13	A	813	CLA	CBC-CAC-C3C	-2.24	106.35	112.42
13	A	810	CLA	O2A-CGA-CBA	2.24	121.07	114.00
13	B	817	CLA	CHB-C1B-C2B	-2.24	120.93	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	818	CLA	CMC-C2C-C1C	2.24	128.53	125.03
13	L	202	CLA	O1D-CGD-CBD	-2.24	120.11	124.52
13	A	833	CLA	CBC-CAC-C3C	-2.24	106.36	112.42
13	A	831	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	B	829	CLA	CHA-C1A-NA	-2.23	121.33	126.39
13	B	824	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	A	843	CLA	CAA-C2A-C3A	-2.23	106.96	113.00
12	A	801	CL0	O2A-CGA-O1A	-2.23	118.04	123.63
13	B	819	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
13	A	836	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
13	B	810	CLA	CHB-C1B-C2B	-2.23	120.95	127.43
13	B	824	CLA	CHB-C1B-C2B	-2.23	120.96	127.43
13	B	807	CLA	OBD-CAD-C3D	-2.23	123.21	128.42
13	A	804	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
13	A	829	CLA	CHA-C1A-NA	-2.23	121.35	126.39
13	B	814	CLA	O1D-CGD-CBD	-2.23	120.13	124.52
13	A	823	CLA	CAC-C3C-C4C	2.22	127.68	124.79
16	J	103	BCR	C38-C26-C25	-2.22	122.06	124.48
16	A	849	BCR	C29-C30-C25	2.22	113.67	110.44
13	B	811	CLA	CMC-C2C-C1C	2.22	128.51	125.03
13	A	840	CLA	C4-C3-C5	2.22	119.08	115.23
13	B	818	CLA	C2A-C3A-C4A	-2.22	98.28	101.87
13	B	809	CLA	C4-C3-C5	2.22	119.08	115.23
13	A	821	CLA	C1-C2-C3	-2.22	122.57	126.20
13	B	816	CLA	C4-C3-C5	2.22	119.07	115.23
13	B	810	CLA	CHA-C1A-NA	-2.21	121.38	126.39
13	B	813	CLA	CHB-C4A-NA	2.21	127.59	124.40
13	B	805	CLA	O1D-CGD-CBD	-2.21	120.15	124.52
13	B	802	CLA	O2A-CGA-CBA	2.21	118.58	111.83
16	B	836	BCR	C7-C8-C9	-2.21	122.96	126.23
13	A	835	CLA	C11-C10-C8	-2.21	108.62	115.97
13	B	819	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
16	F	202	BCR	C15-C16-C17	-2.21	119.00	123.52
13	A	820	CLA	CHC-C1C-NC	2.20	127.63	124.31
13	A	841	CLA	C11-C10-C8	-2.20	108.64	115.97
13	A	841	CLA	CHA-C1A-NA	-2.20	121.40	126.39
16	B	837	BCR	C16-C15-C14	-2.20	119.01	123.52
13	L	202	CLA	CMB-C2B-C1B	2.20	128.77	125.42
16	K	202	BCR	C11-C10-C9	-2.20	124.19	127.28
13	B	824	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
13	A	832	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
13	B	825	CLA	O1D-CGD-CBD	-2.20	120.18	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	843	CLA	C1-O2A-CGA	2.20	121.98	116.65
13	K	201	CLA	CHB-C4A-NA	2.20	127.58	124.40
13	A	818	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
13	J	101	CLA	CHB-C1B-C2B	-2.20	121.05	127.43
16	A	848	BCR	C15-C16-C17	-2.20	119.03	123.52
13	L	204	CLA	CBC-CAC-C3C	-2.20	106.47	112.42
13	B	830	CLA	CED-O2D-CGD	2.19	120.89	115.92
13	B	807	CLA	CMB-C2B-C1B	2.19	128.76	125.42
16	F	201	BCR	C16-C15-C14	-2.19	119.03	123.52
13	A	840	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
13	A	838	CLA	C4-C3-C5	2.19	118.70	116.13
13	B	831	CLA	CHB-C4A-NA	2.19	127.56	124.40
13	B	818	CLA	C4-C3-C5	2.19	119.02	115.23
13	A	833	CLA	CHB-C4A-NA	2.18	127.55	124.40
13	A	842	CLA	CHA-C1A-NA	-2.18	121.45	126.39
13	A	806	CLA	CBC-CAC-C3C	-2.18	106.50	112.42
13	K	203	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
16	A	849	BCR	C15-C14-C13	-2.18	124.22	127.28
13	J	101	CLA	O1D-CGD-CBD	-2.18	120.23	124.52
13	B	806	CLA	CHC-C1C-NC	2.17	127.58	124.31
13	L	204	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
13	B	811	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
16	M	101	BCR	C15-C14-C13	-2.17	124.23	127.28
13	B	809	CLA	CHB-C1B-C2B	-2.17	121.12	127.43
16	A	849	BCR	C16-C15-C14	-2.17	119.07	123.52
13	B	829	CLA	C3B-C4B-NB	2.17	112.47	110.53
13	B	812	CLA	CBC-CAC-C3C	-2.17	106.53	112.42
13	B	833	CLA	C4-C3-C5	2.17	119.00	115.23
16	A	851	BCR	C32-C1-C6	2.17	113.64	110.24
13	A	815	CLA	CHA-C1A-NA	-2.17	121.48	126.39
13	B	820	CLA	CHB-C4A-NA	2.17	127.53	124.40
13	B	801	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
13	A	838	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
13	A	819	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
13	A	827	CLA	CAA-C2A-C1A	-2.16	104.89	111.97
13	A	844	CLA	CAC-C3C-C2C	2.16	131.53	127.56
13	A	815	CLA	CHB-C1B-C2B	-2.16	121.15	127.43
13	A	823	CLA	CBA-CAA-C2A	2.16	120.22	113.79
13	A	830	CLA	CMA-C3A-C2A	-2.16	105.63	113.98
13	A	825	CLA	CBC-CAC-C3C	-2.16	106.57	112.42
13	A	837	CLA	CHB-C1B-C2B	-2.16	121.16	127.43
13	B	810	CLA	O2A-CGA-O1A	-2.16	118.23	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	826	CLA	CHB-C1B-NB	-2.16	120.82	124.05
13	A	809	CLA	CBA-CAA-C2A	2.16	120.20	113.79
13	B	833	CLA	CBC-CAC-C3C	-2.16	106.58	112.42
13	A	816	CLA	CBC-CAC-C3C	-2.15	106.58	112.42
16	J	102	BCR	C27-C26-C25	2.15	125.61	122.70
13	B	821	CLA	C4-C3-C5	2.15	118.96	115.23
13	B	812	CLA	CHB-C1B-C2B	-2.15	121.18	127.43
13	B	825	CLA	CHA-C1A-NA	-2.15	121.52	126.39
13	A	842	CLA	CGD-CBD-CAD	-2.15	103.89	110.85
13	A	829	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
13	A	821	CLA	CAC-C3C-C4C	2.15	127.58	124.79
13	K	201	CLA	CMC-C2C-C1C	2.15	128.39	125.03
13	B	825	CLA	CHB-C1B-C2B	-2.15	121.19	127.43
13	A	802	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
13	A	823	CLA	CHB-C4A-NA	2.15	127.50	124.40
16	J	102	BCR	C15-C14-C13	-2.14	124.27	127.28
13	A	812	CLA	C11-C12-C13	-2.14	108.84	115.97
13	A	805	CLA	CHA-C1A-NA	-2.14	121.54	126.39
13	A	823	CLA	CBC-CAC-C3C	-2.14	106.61	112.42
13	B	828	CLA	CHA-C1A-NA	-2.14	121.54	126.39
16	A	848	BCR	C16-C17-C18	-2.14	124.27	127.28
13	B	829	CLA	CHB-C4A-NA	2.14	127.49	124.40
13	A	821	CLA	CAA-C2A-C3A	-2.14	107.21	113.00
13	B	819	CLA	O2A-CGA-CBA	2.14	120.23	112.14
13	B	825	CLA	CGD-CBD-CAD	-2.14	103.91	110.85
12	A	801	CL0	C4-C3-C5	2.14	118.94	115.23
13	J	101	CLA	CMB-C2B-C1B	2.14	128.68	125.42
13	A	808	CLA	CHB-C1B-C2B	-2.14	121.21	127.43
16	F	202	BCR	C30-C25-C26	-2.14	119.71	122.64
13	A	824	CLA	CHA-C1A-NA	-2.14	121.55	126.39
13	A	812	CLA	C1-C2-C3	-2.14	122.69	126.20
13	B	833	CLA	CMB-C2B-C1B	2.14	128.67	125.42
13	B	821	CLA	CBC-CAC-C3C	-2.14	106.63	112.42
13	B	811	CLA	CHD-C4C-NC	2.14	127.54	124.23
13	B	812	CLA	CMA-C3A-C2A	-2.13	105.73	113.98
13	B	828	CLA	CHB-C1B-C2B	-2.13	121.23	127.43
13	A	826	CLA	CHA-C1A-NA	-2.13	121.56	126.39
13	A	834	CLA	CMC-C2C-C1C	2.13	128.37	125.03
13	A	838	CLA	CAC-C3C-C4C	2.13	127.56	124.79
16	A	851	BCR	C15-C16-C17	-2.13	119.16	123.52
13	A	820	CLA	CAA-CBA-CGA	2.13	119.25	113.21
13	A	831	CLA	CHB-C1B-C2B	-2.13	121.25	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	840	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
16	M	101	BCR	C33-C5-C6	-2.12	122.17	124.48
13	B	832	CLA	O2D-CGD-O1D	-2.12	119.71	123.85
13	F	203	CLA	CHB-C4A-NA	2.12	127.47	124.40
13	A	807	CLA	CHA-C1A-NA	-2.12	121.59	126.39
13	A	839	CLA	CHB-C4A-NA	2.12	127.46	124.40
13	A	840	CLA	CAC-C3C-C4C	2.12	127.55	124.79
13	A	838	CLA	OBD-CAD-C3D	-2.12	123.47	128.42
14	B	834	PQN	C11-C3-C2	-2.12	121.26	124.89
13	A	802	CLA	CGD-CBD-CAD	-2.12	103.99	110.85
13	A	826	CLA	C4-C3-C5	2.12	118.90	115.23
13	A	810	CLA	CMC-C2C-C1C	2.12	128.34	125.03
13	B	830	CLA	CAC-C3C-C4C	2.12	127.54	124.79
13	A	824	CLA	CMC-C2C-C1C	2.12	128.34	125.03
13	B	817	CLA	CED-O2D-CGD	2.12	120.71	115.92
13	A	839	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
13	B	832	CLA	CMC-C2C-C1C	2.11	128.34	125.03
13	B	826	CLA	CBC-CAC-C3C	-2.11	106.69	112.42
13	A	836	CLA	CMC-C2C-C1C	2.11	128.34	125.03
13	B	804	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
13	B	808	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
13	B	832	CLA	C4-C3-C5	2.11	118.89	115.23
13	A	814	CLA	CHA-C1A-NA	-2.11	121.61	126.39
13	B	832	CLA	CHB-C1B-C2B	-2.11	121.31	127.43
13	K	203	CLA	O2A-CGA-CBA	2.11	120.66	114.00
13	B	827	CLA	CMA-C3A-C2A	-2.11	105.84	113.98
16	K	202	BCR	C20-C21-C22	-2.11	124.33	127.28
13	A	842	CLA	CHB-C4A-NA	2.10	127.43	124.40
16	F	202	BCR	C33-C5-C6	-2.10	122.19	124.48
13	K	203	CLA	CHB-C4A-NA	2.10	127.43	124.40
13	A	825	CLA	CHA-C1A-NA	-2.10	121.64	126.39
13	A	802	CLA	C11-C10-C8	-2.10	108.99	115.97
13	A	810	CLA	O2A-CGA-O1A	-2.10	117.93	123.33
16	K	202	BCR	C15-C16-C17	-2.10	119.22	123.52
13	B	808	CLA	CMC-C2C-C1C	2.10	128.31	125.03
13	B	828	CLA	CMC-C2C-C1C	2.10	128.31	125.03
16	L	206	BCR	C37-C22-C21	-2.10	119.42	122.82
13	A	819	CLA	CHB-C1B-C2B	-2.09	121.35	127.43
13	A	819	CLA	CBA-CAA-C2A	2.09	120.02	113.79
13	A	844	CLA	C1-C2-C3	-2.09	122.77	126.20
13	A	840	CLA	CHA-C1A-NA	-2.09	121.65	126.39
13	A	817	CLA	O2D-CGD-O1D	-2.09	119.78	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	J	101	CLA	CAA-C2A-C3A	-2.09	107.34	113.00
13	B	821	CLA	C11-C10-C8	-2.09	109.01	115.97
13	A	810	CLA	CHA-C1A-NA	-2.09	121.66	126.39
16	A	847	BCR	C7-C8-C9	-2.09	123.14	126.23
13	A	806	CLA	C1-O2A-CGA	2.09	121.71	116.65
16	A	850	BCR	C11-C10-C9	-2.09	124.35	127.28
13	A	819	CLA	C1-O2A-CGA	2.09	121.70	116.65
13	B	826	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
13	B	804	CLA	C1C-C2C-C3C	-2.09	104.79	106.98
13	A	832	CLA	CMC-C2C-C1C	2.08	128.29	125.03
13	B	807	CLA	CHA-C1A-NA	-2.08	121.67	126.39
14	A	845	PQN	C11-C12-C13	-2.08	123.24	126.83
13	B	801	CLA	CHB-C4A-NA	2.08	127.41	124.40
13	B	814	CLA	CMA-C3A-C4A	-2.08	106.17	111.77
13	A	824	CLA	CHB-C1B-C2B	-2.08	121.38	127.43
13	A	815	CLA	CBB-CAB-C3B	-2.08	117.12	127.53
13	B	804	CLA	C4-C3-C5	2.08	118.84	115.23
13	A	828	CLA	C1-C2-C3	-2.08	122.78	126.20
13	B	824	CLA	CBA-CAA-C2A	2.08	119.98	113.79
16	L	201	BCR	C16-C15-C14	-2.08	119.27	123.52
13	B	824	CLA	CMC-C2C-C1C	2.07	128.28	125.03
13	B	821	CLA	CHA-C1A-NA	-2.07	121.69	126.39
13	A	825	CLA	CMC-C2C-C1C	2.07	128.28	125.03
13	B	807	CLA	CHB-C4A-NA	2.07	127.39	124.40
13	A	812	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
13	B	817	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
13	A	813	CLA	C1-C2-C3	-2.07	122.80	126.20
13	B	813	CLA	O1D-CGD-CBD	-2.07	120.43	124.52
13	B	812	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
13	A	819	CLA	CBC-CAC-C3C	-2.07	106.81	112.42
13	B	829	CLA	CHB-C1B-C2B	-2.07	121.42	127.43
13	A	842	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
13	B	830	CLA	CMC-C2C-C1C	2.07	128.27	125.03
13	A	808	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
13	B	817	CLA	C4-C3-C5	2.07	118.82	115.23
13	A	810	CLA	CHB-C1B-NB	-2.07	120.95	124.05
13	B	802	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
13	A	803	CLA	CMC-C2C-C1C	2.07	128.26	125.03
13	B	826	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
18	B	838	LMG	C3-C4-C5	-2.06	106.49	110.23
13	B	827	CLA	CMC-C2C-C1C	2.06	128.26	125.03
16	J	103	BCR	C31-C1-C6	2.06	113.48	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	820	CLA	CBC-CAC-C3C	-2.06	106.83	112.42
13	A	835	CLA	C11-C12-C13	-2.06	109.11	115.97
13	A	807	CLA	CHB-C1B-C2B	-2.06	121.45	127.43
16	L	205	BCR	C33-C5-C6	-2.06	122.24	124.48
13	J	101	CLA	CBC-CAC-C3C	-2.06	106.84	112.42
13	A	830	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	B	821	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	B	807	CLA	O2D-CGD-O1D	-2.05	119.85	123.85
16	B	836	BCR	C24-C23-C22	-2.05	123.19	126.23
18	B	838	LMG	O7-C10-O9	-2.05	118.90	123.70
13	B	812	CLA	CHA-C1A-NA	-2.05	121.74	126.39
13	B	813	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
13	B	804	CLA	CHA-C1A-NA	-2.05	121.74	126.39
16	A	851	BCR	C4-C5-C6	2.05	125.48	122.70
13	B	830	CLA	CBC-CAC-C3C	-2.05	106.86	112.42
13	B	831	CLA	CMC-C2C-C1C	2.05	128.24	125.03
16	A	847	BCR	C27-C26-C25	2.05	125.47	122.70
13	A	827	CLA	CHB-C1B-C2B	-2.05	121.47	127.43
13	B	817	CLA	CHB-C4A-NA	2.05	127.36	124.40
13	B	833	CLA	C1-O2A-CGA	2.05	121.61	116.65
13	B	818	CLA	CHA-C1A-NA	-2.05	121.75	126.39
13	B	820	CLA	OBD-CAD-C3D	-2.05	123.63	128.42
13	A	839	CLA	CHB-C1B-C2B	-2.05	121.48	127.43
13	A	828	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
13	A	806	CLA	CMA-C3A-C2A	-2.05	106.07	113.98
16	B	835	BCR	C24-C23-C22	-2.05	123.21	126.23
16	B	837	BCR	C33-C5-C6	-2.05	122.25	124.48
13	L	202	CLA	CBC-CAC-C3C	-2.05	106.87	112.42
16	M	101	BCR	C37-C22-C21	-2.05	119.50	122.82
13	B	803	CLA	CHB-C1B-C2B	-2.05	121.49	127.43
16	J	102	BCR	C28-C27-C26	-2.05	110.41	114.06
13	B	801	CLA	CHA-C1A-NA	-2.05	121.76	126.39
13	A	828	CLA	CAA-CBA-CGA	-2.05	107.40	113.21
13	A	829	CLA	CHB-C4A-NA	2.04	127.35	124.40
16	L	201	BCR	C21-C20-C19	-2.04	117.28	123.20
13	B	804	CLA	C4B-C3B-C2B	-2.04	104.76	107.30
13	B	831	CLA	CBC-CAC-C3C	-2.04	106.88	112.42
13	B	805	CLA	CHB-C1B-C2B	-2.04	121.50	127.43
13	A	815	CLA	O2A-CGA-CBA	2.04	120.45	114.00
13	L	203	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
13	A	835	CLA	CBC-CAC-C3C	-2.04	106.89	112.42
13	B	833	CLA	C16-C15-C13	-2.04	109.18	115.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	833	CLA	CMC-C2C-C1C	2.04	128.22	125.03
16	K	202	BCR	C7-C8-C9	-2.04	123.22	126.23
13	A	812	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	A	838	CLA	CHA-C1A-NA	-2.04	121.78	126.39
13	A	843	CLA	C1-C2-C3	-2.04	122.86	126.20
13	F	203	CLA	CMC-C2C-C1C	2.04	128.22	125.03
13	B	827	CLA	O2A-CGA-CBA	2.04	120.43	114.00
13	A	806	CLA	CHC-C1C-NC	2.03	127.38	124.31
13	A	827	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
13	A	841	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
13	A	804	CLA	O2A-CGA-CBA	2.03	120.42	114.00
16	A	847	BCR	C33-C5-C6	-2.03	122.27	124.48
13	B	801	CLA	CED-O2D-CGD	2.03	120.53	115.92
13	A	804	CLA	CHB-C1B-C2B	-2.03	121.53	127.43
13	B	822	CLA	CBA-CAA-C2A	2.03	119.84	113.79
13	A	814	CLA	CAC-C3C-C4C	2.03	127.43	124.79
13	A	803	CLA	O2D-CGD-O1D	-2.03	119.90	123.85
13	A	806	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
13	A	814	CLA	CHB-C1B-C2B	-2.03	121.54	127.43
13	B	815	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
13	K	203	CLA	CHA-C1A-NA	-2.03	121.80	126.39
13	A	813	CLA	CHA-C1A-NA	-2.03	121.80	126.39
13	A	814	CLA	O2A-CGA-CBA	2.03	120.40	114.00
13	A	817	CLA	CHA-C1A-NA	-2.03	121.81	126.39
13	B	809	CLA	C1-C2-C3	-2.02	122.88	126.20
13	A	833	CLA	CHB-C1B-C2B	-2.02	121.55	127.43
13	A	843	CLA	CMC-C2C-C1C	2.02	128.19	125.03
13	B	808	CLA	O1D-CGD-CBD	-2.02	120.53	124.52
13	A	802	CLA	C1-C2-C3	-2.02	122.89	126.20
13	A	830	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
13	A	830	CLA	CHB-C1B-C2B	-2.02	121.56	127.43
13	B	821	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
13	F	203	CLA	O2A-CGA-CBA	2.02	120.38	114.00
13	L	202	CLA	CHA-C1A-NA	-2.02	121.82	126.39
13	B	830	CLA	CBA-CAA-C2A	2.02	119.80	113.79
13	A	820	CLA	CAA-C2A-C1A	-2.02	105.36	111.97
13	B	822	CLA	CBC-CAC-C3C	-2.02	106.95	112.42
13	K	201	CLA	O2A-CGA-CBA	2.02	120.38	114.00
13	B	806	CLA	CBC-CAC-C3C	-2.02	106.95	112.42
13	B	801	CLA	CMA-C3A-C2A	-2.02	106.18	113.98
13	A	809	CLA	CBC-CAC-C3C	-2.02	106.95	112.42
13	B	823	CLA	C2A-C1A-CHA	-2.02	120.37	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	822	CLA	CMA-C3A-C2A	-2.02	106.19	113.98
13	B	806	CLA	CHA-C1A-NA	-2.02	121.83	126.39
16	B	837	BCR	C15-C14-C13	-2.02	124.45	127.28
13	A	804	CLA	CMC-C2C-C1C	2.02	128.18	125.03
13	A	824	CLA	CBC-CAC-C3C	-2.01	106.96	112.42
13	A	809	CLA	CHB-C1B-C2B	-2.01	121.58	127.43
13	A	813	CLA	C1-O2A-CGA	2.01	121.52	116.65
13	A	832	CLA	C5-C3-C4	2.01	119.22	114.59
13	B	801	CLA	C11-C12-C13	-2.01	109.28	115.97
14	B	834	PQN	C16-C17-C18	-2.01	109.28	115.97
13	A	808	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
16	M	101	BCR	C10-C11-C12	-2.01	117.38	123.20
13	B	828	CLA	O2A-CGA-CBA	2.01	120.34	114.00
13	A	821	CLA	CHA-C1A-NA	-2.01	121.84	126.39
13	A	802	CLA	CMB-C2B-C3B	2.01	131.27	126.55
13	B	804	CLA	CHC-C1C-NC	2.01	127.33	124.31
13	A	815	CLA	CAA-C2A-C3A	-2.00	107.58	113.00
13	B	822	CLA	CMA-C3A-C4A	-2.00	106.39	111.77
13	A	823	CLA	C1-O2A-CGA	2.00	121.50	116.65
13	A	835	CLA	CHB-C1B-C2B	-2.00	121.61	127.43
13	A	814	CLA	CAC-C3C-C2C	2.00	131.24	127.56
13	A	819	CLA	CMD-C2D-C3D	-2.00	123.10	127.69

All (72) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	801	CL0	ND
12	A	801	CL0	NC
13	A	802	CLA	ND
13	A	803	CLA	ND
13	A	804	CLA	ND
13	A	805	CLA	ND
13	A	806	CLA	ND
13	A	807	CLA	ND
13	A	808	CLA	ND
13	A	809	CLA	ND
13	A	810	CLA	ND
13	A	811	CLA	ND
13	A	812	CLA	ND
13	A	813	CLA	ND
13	A	814	CLA	ND
13	A	815	CLA	ND

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Mol	Chain	Res	Type	Atom
13	A	819	CLA	ND
13	A	820	CLA	ND
13	A	821	CLA	ND
13	A	822	CLA	ND
13	A	825	CLA	ND
13	A	826	CLA	ND
13	A	827	CLA	ND
13	A	828	CLA	ND
13	A	829	CLA	ND
13	A	830	CLA	ND
13	A	831	CLA	ND
13	A	833	CLA	ND
13	A	834	CLA	ND
13	A	835	CLA	ND
13	A	837	CLA	ND
13	A	838	CLA	ND
13	A	839	CLA	ND
13	A	840	CLA	ND
13	A	841	CLA	ND
13	A	842	CLA	ND
13	A	843	CLA	ND
13	A	844	CLA	ND
13	B	801	CLA	ND
13	B	802	CLA	ND
13	B	803	CLA	ND
13	B	804	CLA	ND
13	B	805	CLA	ND
13	B	806	CLA	ND
13	B	807	CLA	ND
13	B	808	CLA	ND
13	B	809	CLA	ND
13	B	810	CLA	ND
13	B	811	CLA	ND
13	B	812	CLA	ND
13	B	813	CLA	ND
13	B	814	CLA	ND
13	B	815	CLA	ND
13	B	816	CLA	ND
13	B	817	CLA	ND
13	B	818	CLA	ND
13	B	819	CLA	ND
13	B	820	CLA	ND

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Mol	Chain	Res	Type	Atom
13	B	821	CLA	ND
13	B	822	CLA	ND
13	B	823	CLA	ND
13	B	825	CLA	ND
13	B	826	CLA	ND
13	B	828	CLA	ND
13	B	829	CLA	ND
13	B	830	CLA	ND
13	B	831	CLA	ND
13	F	203	CLA	ND
13	J	101	CLA	ND
13	K	201	CLA	ND
13	K	203	CLA	ND
13	L	204	CLA	ND

All (1110) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	804	CLA	CHA-CBD-CGD-O1D
13	A	804	CLA	CHA-CBD-CGD-O2D
13	A	805	CLA	C2B-C3B-CAB-CBB
13	A	805	CLA	C4B-C3B-CAB-CBB
13	A	805	CLA	CHA-CBD-CGD-O1D
13	A	805	CLA	CHA-CBD-CGD-O2D
13	A	806	CLA	C3A-C2A-CAA-CBA
13	A	807	CLA	C1A-C2A-CAA-CBA
13	A	808	CLA	C4B-C3B-CAB-CBB
13	A	808	CLA	C2-C3-C5-C6
13	A	809	CLA	C3A-C2A-CAA-CBA
13	A	811	CLA	CBD-CGD-O2D-CED
13	A	814	CLA	C4B-C3B-CAB-CBB
13	A	814	CLA	CAD-CBD-CGD-O2D
13	A	815	CLA	C1A-C2A-CAA-CBA
13	A	815	CLA	C2B-C3B-CAB-CBB
13	A	815	CLA	C4B-C3B-CAB-CBB
13	A	819	CLA	C1A-C2A-CAA-CBA
13	A	820	CLA	C1A-C2A-CAA-CBA
13	A	820	CLA	C3A-C2A-CAA-CBA
13	A	823	CLA	C1A-C2A-CAA-CBA
13	A	823	CLA	C3A-C2A-CAA-CBA
13	A	824	CLA	C2-C3-C5-C6
13	A	824	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	826	CLA	CAD-CBD-CGD-O2D
13	A	827	CLA	C2B-C3B-CAB-CBB
13	A	827	CLA	C4B-C3B-CAB-CBB
13	A	829	CLA	C1A-C2A-CAA-CBA
13	A	829	CLA	C3A-C2A-CAA-CBA
13	A	829	CLA	CBD-CGD-O2D-CED
13	A	829	CLA	C4-C3-C5-C6
13	A	831	CLA	CHA-CBD-CGD-O1D
13	A	831	CLA	CHA-CBD-CGD-O2D
13	A	832	CLA	C2B-C3B-CAB-CBB
13	A	832	CLA	C4B-C3B-CAB-CBB
13	A	835	CLA	CHA-CBD-CGD-O1D
13	A	835	CLA	CHA-CBD-CGD-O2D
13	A	835	CLA	CBD-CGD-O2D-CED
13	A	837	CLA	CHA-CBD-CGD-O1D
13	A	837	CLA	CHA-CBD-CGD-O2D
13	A	838	CLA	CHA-CBD-CGD-O1D
13	A	838	CLA	CHA-CBD-CGD-O2D
13	A	840	CLA	CHA-CBD-CGD-O1D
13	A	840	CLA	CHA-CBD-CGD-O2D
13	A	842	CLA	C2-C3-C5-C6
13	A	842	CLA	C4-C3-C5-C6
13	A	844	CLA	C1A-C2A-CAA-CBA
13	A	844	CLA	C3A-C2A-CAA-CBA
13	B	802	CLA	CBD-CGD-O2D-CED
13	B	804	CLA	CBD-CGD-O2D-CED
13	B	805	CLA	C2B-C3B-CAB-CBB
13	B	805	CLA	C4B-C3B-CAB-CBB
13	B	805	CLA	CHA-CBD-CGD-O1D
13	B	805	CLA	CHA-CBD-CGD-O2D
13	B	806	CLA	C3A-C2A-CAA-CBA
13	B	810	CLA	C2B-C3B-CAB-CBB
13	B	810	CLA	C4B-C3B-CAB-CBB
13	B	815	CLA	CHA-CBD-CGD-O1D
13	B	815	CLA	CHA-CBD-CGD-O2D
13	B	818	CLA	C1A-C2A-CAA-CBA
13	B	818	CLA	C3A-C2A-CAA-CBA
13	B	819	CLA	CHA-CBD-CGD-O1D
13	B	819	CLA	CHA-CBD-CGD-O2D
13	B	821	CLA	C1A-C2A-CAA-CBA
13	B	822	CLA	C1A-C2A-CAA-CBA
13	B	823	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	B	823	CLA	CHA-CBD-CGD-O2D
13	B	824	CLA	C1A-C2A-CAA-CBA
13	B	833	CLA	CAD-CBD-CGD-O1D
13	B	833	CLA	CAD-CBD-CGD-O2D
13	J	101	CLA	C1A-C2A-CAA-CBA
13	L	202	CLA	C1A-C2A-CAA-CBA
13	L	202	CLA	C3A-C2A-CAA-CBA
13	L	203	CLA	C2B-C3B-CAB-CBB
13	L	203	CLA	C4B-C3B-CAB-CBB
16	A	847	BCR	C20-C21-C22-C23
16	A	847	BCR	C20-C21-C22-C37
16	A	848	BCR	C6-C7-C8-C9
16	A	848	BCR	C7-C8-C9-C10
16	A	848	BCR	C21-C22-C23-C24
16	A	849	BCR	C37-C22-C23-C24
16	A	850	BCR	C7-C8-C9-C34
16	A	850	BCR	C11-C12-C13-C35
16	A	851	BCR	C6-C7-C8-C9
16	A	851	BCR	C11-C12-C13-C35
16	A	851	BCR	C12-C13-C14-C15
16	A	851	BCR	C18-C19-C20-C21
16	A	851	BCR	C20-C21-C22-C23
16	A	851	BCR	C20-C21-C22-C37
16	B	836	BCR	C7-C8-C9-C34
16	B	836	BCR	C16-C17-C18-C36
16	B	836	BCR	C18-C19-C20-C21
16	B	837	BCR	C7-C8-C9-C34
16	B	837	BCR	C21-C22-C23-C24
16	F	201	BCR	C21-C22-C23-C24
16	F	202	BCR	C14-C15-C16-C17
16	I	101	BCR	C16-C17-C18-C19
16	I	101	BCR	C16-C17-C18-C36
16	J	102	BCR	C6-C7-C8-C9
16	J	102	BCR	C7-C8-C9-C10
16	J	102	BCR	C7-C8-C9-C34
16	J	102	BCR	C11-C10-C9-C8
16	J	103	BCR	C21-C22-C23-C24
16	J	103	BCR	C37-C22-C23-C24
16	J	104	BCR	C7-C8-C9-C10
16	K	202	BCR	C7-C8-C9-C10
16	K	202	BCR	C7-C8-C9-C34
16	K	202	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
16	K	202	BCR	C37-C22-C23-C24
16	L	201	BCR	C7-C8-C9-C10
16	L	201	BCR	C20-C21-C22-C37
16	L	205	BCR	C18-C19-C20-C21
16	L	205	BCR	C37-C22-C23-C24
16	L	205	BCR	C23-C24-C25-C26
16	L	206	BCR	C11-C12-C13-C14
16	L	206	BCR	C11-C12-C13-C35
16	L	206	BCR	C13-C14-C15-C16
16	L	206	BCR	C17-C18-C19-C20
16	L	206	BCR	C36-C18-C19-C20
16	L	206	BCR	C19-C20-C21-C22
16	L	206	BCR	C20-C21-C22-C37
16	L	206	BCR	C21-C22-C23-C24
16	M	101	BCR	C7-C8-C9-C34
16	M	101	BCR	C18-C19-C20-C21
16	M	101	BCR	C20-C21-C22-C37
17	A	852	LHG	C3-O3-P-O4
17	A	853	LHG	O2-C2-C3-O3
13	A	811	CLA	O1D-CGD-O2D-CED
13	A	810	CLA	CBD-CGD-O2D-CED
13	A	834	CLA	CBD-CGD-O2D-CED
13	B	821	CLA	CBD-CGD-O2D-CED
13	B	816	CLA	O1A-CGA-O2A-C1
13	B	815	CLA	CBD-CGD-O2D-CED
13	A	827	CLA	O1A-CGA-O2A-C1
13	A	829	CLA	O1D-CGD-O2D-CED
13	B	802	CLA	O1D-CGD-O2D-CED
12	A	801	CL0	C3-C5-C6-C7
13	A	807	CLA	C3-C5-C6-C7
13	A	821	CLA	C3-C5-C6-C7
13	A	833	CLA	C3-C5-C6-C7
13	B	807	CLA	C3-C5-C6-C7
13	B	817	CLA	C3-C5-C6-C7
13	B	823	CLA	C3-C5-C6-C7
13	B	825	CLA	C3-C5-C6-C7
13	B	833	CLA	C3-C5-C6-C7
13	A	824	CLA	CBA-CGA-O2A-C1
13	A	827	CLA	CBA-CGA-O2A-C1
13	B	816	CLA	CBA-CGA-O2A-C1
13	B	833	CLA	CBD-CGD-O2D-CED
13	A	835	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	812	CLA	O1A-CGA-O2A-C1
13	A	813	CLA	C4-C3-C5-C6
13	A	833	CLA	C4-C3-C5-C6
13	B	803	CLA	C4-C3-C5-C6
13	L	204	CLA	C4-C3-C5-C6
13	A	813	CLA	C2-C3-C5-C6
13	A	829	CLA	C2-C3-C5-C6
13	A	833	CLA	C2-C3-C5-C6
13	B	803	CLA	C2-C3-C5-C6
13	L	204	CLA	C2-C3-C5-C6
13	B	804	CLA	O1D-CGD-O2D-CED
13	A	822	CLA	C3-C5-C6-C7
13	A	841	CLA	C3-C5-C6-C7
13	B	801	CLA	C3-C5-C6-C7
13	B	804	CLA	C3-C5-C6-C7
13	B	808	CLA	C3-C5-C6-C7
13	B	809	CLA	C3-C5-C6-C7
13	B	813	CLA	C3-C5-C6-C7
14	A	845	PQN	C13-C15-C16-C17
13	A	807	CLA	CBA-CGA-O2A-C1
13	A	809	CLA	CBA-CGA-O2A-C1
13	A	823	CLA	CBA-CGA-O2A-C1
13	A	844	CLA	CBA-CGA-O2A-C1
13	B	813	CLA	CBA-CGA-O2A-C1
13	B	818	CLA	CBA-CGA-O2A-C1
16	J	103	BCR	C9-C10-C11-C12
13	A	821	CLA	O1A-CGA-O2A-C1
13	A	824	CLA	O1A-CGA-O2A-C1
13	A	844	CLA	O1A-CGA-O2A-C1
13	B	829	CLA	CBA-CGA-O2A-C1
13	B	810	CLA	C3-C5-C6-C7
13	B	820	CLA	C3-C5-C6-C7
13	B	829	CLA	CBD-CGD-O2D-CED
13	A	810	CLA	O1D-CGD-O2D-CED
13	A	821	CLA	CBA-CGA-O2A-C1
13	B	801	CLA	CBA-CGA-O2A-C1
13	B	813	CLA	O1A-CGA-O2A-C1
13	A	834	CLA	O1D-CGD-O2D-CED
13	A	809	CLA	C3-C5-C6-C7
13	B	803	CLA	C3-C5-C6-C7
13	B	832	CLA	C3-C5-C6-C7
13	A	812	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	818	CLA	C2-C3-C5-C6
13	B	823	CLA	C2-C3-C5-C6
13	A	807	CLA	O1A-CGA-O2A-C1
13	A	823	CLA	O1A-CGA-O2A-C1
13	B	801	CLA	O1A-CGA-O2A-C1
13	A	830	CLA	C2A-CAA-CBA-CGA
13	A	832	CLA	C2A-CAA-CBA-CGA
13	B	833	CLA	C2A-CAA-CBA-CGA
13	A	809	CLA	O1A-CGA-O2A-C1
13	B	818	CLA	O1A-CGA-O2A-C1
18	B	838	LMG	O6-C1-O1-C7
13	A	825	CLA	CBD-CGD-O2D-CED
13	B	819	CLA	CBD-CGD-O2D-CED
13	K	203	CLA	CBD-CGD-O2D-CED
13	B	829	CLA	O1A-CGA-O2A-C1
18	B	838	LMG	O6-C5-C6-O5
13	A	813	CLA	CBA-CGA-O2A-C1
13	A	820	CLA	CBA-CGA-O2A-C1
13	A	833	CLA	CBA-CGA-O2A-C1
13	A	839	CLA	CBA-CGA-O2A-C1
13	B	833	CLA	CBA-CGA-O2A-C1
18	B	838	LMG	C4-C5-C6-O5
13	B	815	CLA	O1D-CGD-O2D-CED
13	B	821	CLA	O1D-CGD-O2D-CED
13	A	818	CLA	C4-C3-C5-C6
13	B	801	CLA	C4-C3-C5-C6
13	B	802	CLA	C4-C3-C5-C6
13	B	823	CLA	C4-C3-C5-C6
13	B	801	CLA	C2-C3-C5-C6
13	B	802	CLA	C2-C3-C5-C6
13	B	802	CLA	C3-C5-C6-C7
13	A	809	CLA	C11-C12-C13-C14
13	A	812	CLA	C14-C13-C15-C16
13	A	828	CLA	C6-C7-C8-C9
13	A	829	CLA	C11-C10-C8-C9
13	A	831	CLA	C6-C7-C8-C9
13	A	840	CLA	C11-C12-C13-C14
13	A	840	CLA	C14-C13-C15-C16
13	B	804	CLA	C6-C7-C8-C9
13	B	806	CLA	C11-C12-C13-C14
13	B	823	CLA	C11-C12-C13-C14
13	B	833	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
18	B	838	LMG	C2-C1-O1-C7
13	A	820	CLA	O1A-CGA-O2A-C1
13	B	826	CLA	CBD-CGD-O2D-CED
16	A	848	BCR	C7-C8-C9-C34
16	A	848	BCR	C37-C22-C23-C24
16	A	849	BCR	C7-C8-C9-C34
16	A	850	BCR	C37-C22-C23-C24
16	F	201	BCR	C7-C8-C9-C34
16	F	201	BCR	C37-C22-C23-C24
16	F	202	BCR	C7-C8-C9-C34
16	F	202	BCR	C37-C22-C23-C24
16	J	102	BCR	C37-C22-C23-C24
16	J	103	BCR	C11-C12-C13-C35
16	J	104	BCR	C7-C8-C9-C34
16	J	104	BCR	C37-C22-C23-C24
16	L	205	BCR	C7-C8-C9-C34
16	M	101	BCR	C11-C12-C13-C35
16	A	850	BCR	C21-C22-C23-C24
16	A	851	BCR	C21-C22-C23-C24
16	J	102	BCR	C21-C22-C23-C24
16	J	103	BCR	C11-C12-C13-C14
16	L	205	BCR	C7-C8-C9-C10
13	B	803	CLA	C2A-CAA-CBA-CGA
13	A	833	CLA	O1A-CGA-O2A-C1
13	B	833	CLA	O1A-CGA-O2A-C1
13	A	836	CLA	CBA-CGA-O2A-C1
14	A	845	PQN	C15-C16-C17-C18
13	B	825	CLA	CBD-CGD-O2D-CED
16	I	101	BCR	C14-C15-C16-C17
13	B	807	CLA	C8-C10-C11-C12
13	B	807	CLA	C15-C16-C17-C18
13	B	817	CLA	C5-C6-C7-C8
13	B	825	CLA	C8-C10-C11-C12
13	A	826	CLA	C3-C5-C6-C7
13	B	826	CLA	CBA-CGA-O2A-C1
13	B	823	CLA	C10-C11-C12-C13
13	A	831	CLA	C13-C15-C16-C17
13	B	804	CLA	C10-C11-C12-C13
13	B	806	CLA	C10-C11-C12-C13
13	B	809	CLA	C13-C15-C16-C17
13	A	813	CLA	O1A-CGA-O2A-C1
13	A	835	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	B	802	CLA	C8-C10-C11-C12
13	A	802	CLA	C2A-CAA-CBA-CGA
13	A	808	CLA	C2A-CAA-CBA-CGA
13	A	816	CLA	C2A-CAA-CBA-CGA
13	A	825	CLA	C2A-CAA-CBA-CGA
13	B	805	CLA	C2A-CAA-CBA-CGA
13	B	817	CLA	C2A-CAA-CBA-CGA
13	B	821	CLA	C2A-CAA-CBA-CGA
13	A	818	CLA	C8-C10-C11-C12
13	A	822	CLA	C8-C10-C11-C12
13	A	823	CLA	C8-C10-C11-C12
13	A	828	CLA	C10-C11-C12-C13
13	A	841	CLA	C5-C6-C7-C8
13	B	821	CLA	C13-C15-C16-C17
13	B	833	CLA	C8-C10-C11-C12
13	L	203	CLA	C15-C16-C17-C18
18	B	838	LMG	C28-C29-C30-C31
16	J	103	BCR	C22-C23-C24-C25
13	A	812	CLA	C10-C11-C12-C13
13	A	820	CLA	C13-C15-C16-C17
13	A	829	CLA	C13-C15-C16-C17
13	A	840	CLA	C8-C10-C11-C12
13	B	801	CLA	C13-C15-C16-C17
13	B	806	CLA	C13-C15-C16-C17
13	B	823	CLA	C15-C16-C17-C18
13	B	825	CLA	C5-C6-C7-C8
13	A	839	CLA	O1A-CGA-O2A-C1
13	B	804	CLA	C15-C16-C17-C18
13	B	808	CLA	C13-C15-C16-C17
13	B	825	CLA	C15-C16-C17-C18
13	L	203	CLA	C8-C10-C11-C12
13	A	820	CLA	C3-C5-C6-C7
13	A	830	CLA	C5-C6-C7-C8
13	A	842	CLA	CBD-CGD-O2D-CED
13	A	836	CLA	O1A-CGA-O2A-C1
13	B	807	CLA	C5-C6-C7-C8
13	A	806	CLA	CBA-CGA-O2A-C1
13	B	801	CLA	C5-C6-C7-C8
13	A	834	CLA	C3-C5-C6-C7
16	A	851	BCR	C13-C14-C15-C16
13	A	840	CLA	C10-C11-C12-C13
13	B	826	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
17	A	853	LHG	C1-C2-C3-O3
13	A	813	CLA	C2A-CAA-CBA-CGA
13	A	819	CLA	C2A-CAA-CBA-CGA
13	A	817	CLA	CBA-CGA-O2A-C1
13	A	835	CLA	CBA-CGA-O2A-C1
13	A	827	CLA	C5-C6-C7-C8
13	B	820	CLA	C10-C11-C12-C13
13	B	825	CLA	C10-C11-C12-C13
13	A	829	CLA	C10-C11-C12-C13
13	B	813	CLA	C10-C11-C12-C13
13	A	840	CLA	C13-C15-C16-C17
13	B	806	CLA	CBA-CGA-O2A-C1
13	A	819	CLA	C3-C5-C6-C7
13	A	824	CLA	CBD-CGD-O2D-CED
17	A	852	LHG	O9-C7-O7-C5
13	B	804	CLA	C8-C10-C11-C12
13	B	832	CLA	C8-C10-C11-C12
13	B	802	CLA	C5-C6-C7-C8
16	A	850	BCR	C20-C21-C22-C37
16	A	851	BCR	C35-C13-C14-C15
16	B	835	BCR	C16-C17-C18-C36
16	F	201	BCR	C35-C13-C14-C15
16	F	201	BCR	C16-C17-C18-C36
16	F	202	BCR	C16-C17-C18-C36
16	J	102	BCR	C11-C10-C9-C34
16	L	205	BCR	C20-C21-C22-C37
16	L	206	BCR	C16-C17-C18-C36
16	A	851	BCR	C37-C22-C23-C24
16	J	103	BCR	C7-C8-C9-C34
16	L	201	BCR	C7-C8-C9-C34
16	L	206	BCR	C37-C22-C23-C24
16	A	849	BCR	C21-C22-C23-C24
16	A	851	BCR	C11-C12-C13-C14
16	F	201	BCR	C7-C8-C9-C10
16	F	202	BCR	C7-C8-C9-C10
16	J	103	BCR	C7-C8-C9-C10
16	L	205	BCR	C21-C22-C23-C24
16	M	101	BCR	C21-C22-C23-C24
13	A	817	CLA	O1A-CGA-O2A-C1
13	A	838	CLA	C2A-CAA-CBA-CGA
13	B	804	CLA	C2A-CAA-CBA-CGA
13	B	828	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	B	832	CLA	C2A-CAA-CBA-CGA
13	A	807	CLA	C5-C6-C7-C8
17	A	853	LHG	O1-C1-C2-C3
13	B	823	CLA	CBD-CGD-O2D-CED
13	B	833	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	O1A-CGA-O2A-C1
13	A	809	CLA	C8-C10-C11-C12
16	A	847	BCR	C16-C17-C18-C19
16	A	851	BCR	C11-C10-C9-C8
16	B	835	BCR	C11-C10-C9-C8
16	B	837	BCR	C11-C10-C9-C8
16	F	202	BCR	C16-C17-C18-C19
16	J	103	BCR	C11-C10-C9-C8
16	L	201	BCR	C11-C10-C9-C8
16	L	206	BCR	C20-C21-C22-C23
16	M	101	BCR	C11-C10-C9-C8
13	B	829	CLA	O1D-CGD-O2D-CED
14	B	834	PQN	C26-C27-C28-C29
17	A	852	LHG	C27-C28-C29-C30
18	B	838	LMG	C11-C12-C13-C14
13	A	835	CLA	O1A-CGA-O2A-C1
13	B	811	CLA	C10-C11-C12-C13
13	A	806	CLA	C4B-C3B-CAB-CBB
13	A	822	CLA	C4B-C3B-CAB-CBB
13	A	825	CLA	C4B-C3B-CAB-CBB
13	A	826	CLA	C4B-C3B-CAB-CBB
13	A	830	CLA	C4B-C3B-CAB-CBB
13	A	835	CLA	C4B-C3B-CAB-CBB
13	B	804	CLA	C4B-C3B-CAB-CBB
13	B	808	CLA	C4B-C3B-CAB-CBB
13	B	821	CLA	C4B-C3B-CAB-CBB
13	B	822	CLA	C4B-C3B-CAB-CBB
13	B	826	CLA	C4B-C3B-CAB-CBB
13	B	832	CLA	C4B-C3B-CAB-CBB
13	L	204	CLA	C4B-C3B-CAB-CBB
18	B	838	LMG	C29-C30-C31-C32
13	B	806	CLA	O1A-CGA-O2A-C1
13	A	804	CLA	C3A-C2A-CAA-CBA
13	A	807	CLA	C3A-C2A-CAA-CBA
13	A	814	CLA	C3A-C2A-CAA-CBA
13	A	815	CLA	C3A-C2A-CAA-CBA
13	A	819	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	A	833	CLA	C3A-C2A-CAA-CBA
13	A	838	CLA	C3A-C2A-CAA-CBA
13	B	813	CLA	C3A-C2A-CAA-CBA
13	B	822	CLA	C3A-C2A-CAA-CBA
13	B	826	CLA	C3A-C2A-CAA-CBA
13	J	101	CLA	C3A-C2A-CAA-CBA
13	A	814	CLA	C2C-C3C-CAC-CBC
13	B	809	CLA	C8-C10-C11-C12
17	A	853	LHG	C7-C8-C9-C10
16	A	850	BCR	C13-C14-C15-C16
13	A	832	CLA	CBA-CGA-O2A-C1
13	A	834	CLA	CBA-CGA-O2A-C1
13	B	814	CLA	CBA-CGA-O2A-C1
17	A	853	LHG	C24-C23-O8-C6
13	A	828	CLA	C3-C5-C6-C7
17	A	852	LHG	C32-C33-C34-C35
17	A	853	LHG	C9-C10-C11-C12
14	B	834	PQN	C26-C27-C28-C30
13	A	808	CLA	C2B-C3B-CAB-CBB
13	A	814	CLA	C2B-C3B-CAB-CBB
13	A	825	CLA	C2B-C3B-CAB-CBB
13	A	830	CLA	C2B-C3B-CAB-CBB
13	A	835	CLA	C2B-C3B-CAB-CBB
13	A	842	CLA	C2B-C3B-CAB-CBB
13	B	801	CLA	C2B-C3B-CAB-CBB
13	B	808	CLA	C2B-C3B-CAB-CBB
13	B	826	CLA	C2B-C3B-CAB-CBB
13	B	832	CLA	C2B-C3B-CAB-CBB
16	A	851	BCR	C23-C24-C25-C26
16	A	851	BCR	C23-C24-C25-C30
16	B	837	BCR	C1-C6-C7-C8
16	J	103	BCR	C23-C24-C25-C26
16	J	103	BCR	C23-C24-C25-C30
16	L	205	BCR	C1-C6-C7-C8
16	L	205	BCR	C23-C24-C25-C30
16	M	101	BCR	C23-C24-C25-C30
13	B	822	CLA	CBD-CGD-O2D-CED
17	A	852	LHG	C8-C7-O7-C5
13	B	819	CLA	O1D-CGD-O2D-CED
18	B	838	LMG	C16-C17-C18-C19
13	A	809	CLA	C2A-CAA-CBA-CGA
13	A	844	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	A	847	BCR	C18-C19-C20-C21
16	A	850	BCR	C18-C19-C20-C21
16	J	103	BCR	C10-C11-C12-C13
16	J	104	BCR	C18-C19-C20-C21
13	A	826	CLA	C15-C16-C17-C18
13	A	822	CLA	C6-C7-C8-C9
13	A	840	CLA	C6-C7-C8-C9
13	L	203	CLA	C6-C7-C8-C9
13	A	806	CLA	C10-C11-C12-C13
18	B	838	LMG	C17-C18-C19-C20
16	A	849	BCR	C6-C7-C8-C9
16	B	837	BCR	C22-C23-C24-C25
16	L	206	BCR	C22-C23-C24-C25
13	L	204	CLA	CBA-CGA-O2A-C1
13	B	804	CLA	C5-C6-C7-C8
16	M	101	BCR	C37-C22-C23-C24
13	B	819	CLA	CBA-CGA-O2A-C1
16	B	836	BCR	C7-C8-C9-C10
16	I	101	BCR	C7-C8-C9-C10
13	A	837	CLA	C2A-CAA-CBA-CGA
13	B	801	CLA	C2A-CAA-CBA-CGA
13	A	843	CLA	C16-C17-C18-C20
13	J	101	CLA	CBD-CGD-O2D-CED
13	A	809	CLA	C5-C6-C7-C8
13	A	832	CLA	O1A-CGA-O2A-C1
13	A	834	CLA	O1A-CGA-O2A-C1
13	B	814	CLA	O1A-CGA-O2A-C1
13	A	826	CLA	C10-C11-C12-C13
13	A	835	CLA	C5-C6-C7-C8
17	A	852	LHG	C29-C30-C31-C32
13	A	822	CLA	C5-C6-C7-C8
17	A	852	LHG	C24-C25-C26-C27
13	A	844	CLA	C2-C1-O2A-CGA
18	B	838	LMG	C33-C34-C35-C36
13	B	812	CLA	CBD-CGD-O2D-CED
13	A	819	CLA	CBA-CGA-O2A-C1
13	A	840	CLA	C5-C6-C7-C8
13	A	804	CLA	C1A-C2A-CAA-CBA
13	A	806	CLA	C1A-C2A-CAA-CBA
13	A	809	CLA	C1A-C2A-CAA-CBA
13	A	811	CLA	C1A-C2A-CAA-CBA
13	A	812	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	A	814	CLA	C1A-C2A-CAA-CBA
13	A	822	CLA	C1A-C2A-CAA-CBA
13	A	832	CLA	C1A-C2A-CAA-CBA
13	A	833	CLA	C1A-C2A-CAA-CBA
13	A	835	CLA	C1A-C2A-CAA-CBA
13	A	836	CLA	C1A-C2A-CAA-CBA
13	A	838	CLA	C1A-C2A-CAA-CBA
13	A	840	CLA	C1A-C2A-CAA-CBA
13	B	806	CLA	C1A-C2A-CAA-CBA
13	B	813	CLA	C1A-C2A-CAA-CBA
13	B	823	CLA	C1A-C2A-CAA-CBA
13	B	825	CLA	C1A-C2A-CAA-CBA
13	B	826	CLA	C1A-C2A-CAA-CBA
13	B	831	CLA	C1A-C2A-CAA-CBA
13	K	203	CLA	C1A-C2A-CAA-CBA
13	L	203	CLA	C1A-C2A-CAA-CBA
14	B	834	PQN	C15-C16-C17-C18
13	B	807	CLA	C13-C15-C16-C17
13	B	820	CLA	C15-C16-C17-C18
13	A	812	CLA	C11-C12-C13-C15
13	A	822	CLA	C12-C13-C15-C16
13	A	830	CLA	C12-C13-C15-C16
13	B	807	CLA	C11-C10-C8-C7
13	B	820	CLA	C12-C13-C15-C16
13	B	823	CLA	C11-C12-C13-C15
13	B	822	CLA	C4-C3-C5-C6
13	B	809	CLA	C2-C3-C5-C6
13	L	204	CLA	O1A-CGA-O2A-C1
13	A	830	CLA	C14-C13-C15-C16
13	A	841	CLA	C11-C10-C8-C9
13	B	807	CLA	C14-C13-C15-C16
13	B	826	CLA	C6-C7-C8-C9
13	B	832	CLA	C14-C13-C15-C16
14	B	834	PQN	C21-C22-C23-C24
13	K	203	CLA	O1D-CGD-O2D-CED
13	A	842	CLA	CBA-CGA-O2A-C1
18	B	838	LMG	O1-C7-C8-C9
12	A	801	CL0	C13-C15-C16-C17
13	B	825	CLA	O1D-CGD-O2D-CED
13	A	828	CLA	CBA-CGA-O2A-C1
13	B	821	CLA	CBA-CGA-O2A-C1
13	B	823	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	L	203	CLA	CBA-CGA-O2A-C1
16	A	849	BCR	C11-C10-C9-C34
16	A	851	BCR	C16-C17-C18-C36
16	B	835	BCR	C11-C10-C9-C34
16	F	202	BCR	C35-C13-C14-C15
16	J	103	BCR	C11-C10-C9-C34
18	B	838	LMG	C38-C39-C40-C41
13	A	844	CLA	C2-C3-C5-C6
13	B	822	CLA	C2-C3-C5-C6
13	B	809	CLA	C5-C6-C7-C8
13	B	813	CLA	C8-C10-C11-C12
13	B	802	CLA	C16-C17-C18-C19
13	A	819	CLA	O1A-CGA-O2A-C1
13	A	828	CLA	O1A-CGA-O2A-C1
13	B	823	CLA	C5-C6-C7-C8
14	B	834	PQN	C25-C26-C27-C28
16	A	850	BCR	C10-C11-C12-C13
16	A	851	BCR	C10-C11-C12-C13
17	A	852	LHG	C30-C31-C32-C33
13	A	843	CLA	C16-C17-C18-C19
16	F	201	BCR	C11-C10-C9-C8
16	L	206	BCR	C16-C17-C18-C19
13	B	805	CLA	CBA-CGA-O2A-C1
13	B	817	CLA	CBA-CGA-O2A-C1
13	A	807	CLA	C2-C3-C5-C6
13	B	811	CLA	C2-C3-C5-C6
18	B	838	LMG	C39-C40-C41-C42
13	B	802	CLA	C16-C17-C18-C20
17	A	852	LHG	C31-C32-C33-C34
18	B	838	LMG	C41-C42-C43-C44
17	A	852	LHG	O7-C5-C6-O8
13	B	817	CLA	C11-C12-C13-C14
13	B	824	CLA	CAA-CBA-CGA-O2A
18	B	838	LMG	C30-C31-C32-C33
13	B	830	CLA	C3-C5-C6-C7
13	B	817	CLA	CBD-CGD-O2D-CED
13	B	822	CLA	C15-C16-C17-C18
13	A	842	CLA	O1D-CGD-O2D-CED
13	A	806	CLA	C4-C3-C5-C6
13	A	809	CLA	C10-C11-C12-C13
13	A	826	CLA	C13-C15-C16-C17
13	A	809	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	A	812	CLA	C11-C12-C13-C14
13	A	822	CLA	C14-C13-C15-C16
13	A	831	CLA	C14-C13-C15-C16
13	A	834	CLA	C11-C12-C13-C14
13	B	811	CLA	C11-C12-C13-C14
13	B	820	CLA	C14-C13-C15-C16
13	A	825	CLA	O1D-CGD-O2D-CED
13	A	823	CLA	C4B-C3B-CAB-CBB
13	A	834	CLA	C4B-C3B-CAB-CBB
13	B	801	CLA	C4B-C3B-CAB-CBB
13	B	813	CLA	C4B-C3B-CAB-CBB
13	B	815	CLA	C4B-C3B-CAB-CBB
13	B	816	CLA	C4B-C3B-CAB-CBB
13	B	830	CLA	C4B-C3B-CAB-CBB
13	A	814	CLA	C4C-C3C-CAC-CBC
13	A	842	CLA	O1A-CGA-O2A-C1
13	A	821	CLA	C10-C11-C12-C13
17	A	852	LHG	C18-C19-C20-C21
13	A	809	CLA	C6-C7-C8-C10
13	A	820	CLA	C11-C12-C13-C15
13	A	829	CLA	C11-C10-C8-C7
13	A	831	CLA	C12-C13-C15-C16
13	A	834	CLA	C11-C12-C13-C15
13	A	841	CLA	C11-C10-C8-C7
13	B	802	CLA	C11-C10-C8-C7
13	B	803	CLA	C6-C7-C8-C10
13	B	811	CLA	C11-C12-C13-C15
13	B	826	CLA	C6-C7-C8-C10
13	B	821	CLA	O1A-CGA-O2A-C1
13	B	823	CLA	O1A-CGA-O2A-C1
13	L	203	CLA	O1A-CGA-O2A-C1
13	A	837	CLA	C3A-C2A-CAA-CBA
13	A	843	CLA	C3A-C2A-CAA-CBA
13	B	806	CLA	C4-C3-C5-C6
13	B	809	CLA	C4-C3-C5-C6
13	B	811	CLA	C4-C3-C5-C6
13	B	816	CLA	C3A-C2A-CAA-CBA
13	B	821	CLA	C3A-C2A-CAA-CBA
13	B	821	CLA	C4-C3-C5-C6
13	A	826	CLA	C8-C10-C11-C12
16	L	205	BCR	C15-C16-C17-C18
16	A	847	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
13	A	808	CLA	C4-C3-C5-C6
18	B	838	LMG	C35-C36-C37-C38
13	A	807	CLA	C4-C3-C5-C6
13	B	826	CLA	O1D-CGD-O2D-CED
13	A	834	CLA	C2B-C3B-CAB-CBB
13	A	837	CLA	C2B-C3B-CAB-CBB
13	A	843	CLA	C2B-C3B-CAB-CBB
13	B	809	CLA	C2B-C3B-CAB-CBB
13	B	813	CLA	C2B-C3B-CAB-CBB
13	B	815	CLA	C2B-C3B-CAB-CBB
13	B	828	CLA	C2B-C3B-CAB-CBB
13	B	830	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C1-C6-C7-C8
16	A	847	BCR	C23-C24-C25-C30
16	A	848	BCR	C1-C6-C7-C8
16	A	849	BCR	C1-C6-C7-C8
16	A	849	BCR	C23-C24-C25-C30
16	A	850	BCR	C1-C6-C7-C8
16	A	850	BCR	C23-C24-C25-C30
16	B	835	BCR	C1-C6-C7-C8
16	B	835	BCR	C23-C24-C25-C30
16	B	836	BCR	C1-C6-C7-C8
16	B	836	BCR	C23-C24-C25-C30
16	B	837	BCR	C23-C24-C25-C30
16	F	201	BCR	C1-C6-C7-C8
16	F	202	BCR	C1-C6-C7-C8
16	I	101	BCR	C1-C6-C7-C8
16	J	102	BCR	C1-C6-C7-C8
16	J	104	BCR	C23-C24-C25-C30
16	K	202	BCR	C1-C6-C7-C8
16	L	201	BCR	C1-C6-C7-C8
16	L	206	BCR	C1-C6-C7-C8
16	L	206	BCR	C23-C24-C25-C30
16	M	101	BCR	C1-C6-C7-C8
16	M	101	BCR	C23-C24-C25-C26
14	B	834	PQN	C13-C15-C16-C17
17	A	852	LHG	C26-C27-C28-C29
13	B	802	CLA	C15-C16-C17-C18
13	A	819	CLA	CAA-CBA-CGA-O2A
18	B	838	LMG	C21-C22-C23-C24
16	B	836	BCR	C10-C11-C12-C13
16	B	837	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
13	A	806	CLA	C2-C3-C5-C6
13	B	806	CLA	C2-C3-C5-C6
13	A	823	CLA	C3-C5-C6-C7
13	B	802	CLA	C11-C10-C8-C9
13	L	203	CLA	C14-C13-C15-C16
13	B	821	CLA	CAA-CBA-CGA-O2A
16	A	847	BCR	C22-C23-C24-C25
16	M	101	BCR	C22-C23-C24-C25
13	B	805	CLA	C3-C5-C6-C7
13	A	826	CLA	C2A-CAA-CBA-CGA
13	B	806	CLA	C15-C16-C17-C18
13	B	833	CLA	C10-C11-C12-C13
13	A	838	CLA	CBA-CGA-O2A-C1
13	B	813	CLA	C4-C3-C5-C6
13	B	821	CLA	C2-C3-C5-C6
13	B	813	CLA	C5-C6-C7-C8
13	A	824	CLA	O1D-CGD-O2D-CED
13	A	831	CLA	C15-C16-C17-C18
16	A	849	BCR	C16-C17-C18-C36
16	B	836	BCR	C35-C13-C14-C15
16	J	103	BCR	C35-C13-C14-C15
13	A	830	CLA	CBA-CGA-O2A-C1
13	B	822	CLA	CBA-CGA-O2A-C1
14	B	834	PQN	C18-C20-C21-C22
13	A	833	CLA	C5-C6-C7-C8
16	I	101	BCR	C7-C8-C9-C34
13	A	809	CLA	C12-C13-C15-C16
13	A	826	CLA	C12-C13-C15-C16
13	A	828	CLA	C11-C10-C8-C7
13	A	834	CLA	C11-C10-C8-C7
13	B	803	CLA	C12-C13-C15-C16
13	L	203	CLA	C12-C13-C15-C16
14	B	834	PQN	C21-C22-C23-C25
17	A	852	LHG	C28-C29-C30-C31
16	M	101	BCR	C7-C8-C9-C10
13	A	830	CLA	O1A-CGA-O2A-C1
13	B	805	CLA	O1A-CGA-O2A-C1
13	B	817	CLA	O1A-CGA-O2A-C1
13	A	814	CLA	C2A-CAA-CBA-CGA
13	A	836	CLA	C6-C7-C8-C9
13	B	830	CLA	C4-C3-C5-C6
13	B	824	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	843	CLA	CBA-CGA-O2A-C1
14	B	834	PQN	C20-C21-C22-C23
16	M	101	BCR	C20-C21-C22-C23
13	B	805	CLA	C6-C7-C8-C9
18	B	838	LMG	C13-C14-C15-C16
13	A	838	CLA	O1A-CGA-O2A-C1
18	B	838	LMG	O10-C28-O8-C9
13	A	822	CLA	C4-C3-C5-C6
13	B	813	CLA	C2-C3-C5-C6
13	A	822	CLA	C11-C10-C8-C9
13	A	826	CLA	C14-C13-C15-C16
13	A	834	CLA	C11-C10-C8-C9
13	B	801	CLA	C14-C13-C15-C16
13	B	803	CLA	C6-C7-C8-C9
13	A	843	CLA	O1A-CGA-O2A-C1
13	A	837	CLA	CBD-CGD-O2D-CED
13	A	836	CLA	C5-C6-C7-C8
13	B	823	CLA	O1D-CGD-O2D-CED
13	A	821	CLA	C4-C3-C5-C6
13	A	826	CLA	C4-C3-C5-C6
13	B	805	CLA	C4-C3-C5-C6
13	A	807	CLA	C4B-C3B-CAB-CBB
13	A	809	CLA	C4B-C3B-CAB-CBB
13	A	813	CLA	C4B-C3B-CAB-CBB
13	A	816	CLA	C1A-C2A-CAA-CBA
13	A	816	CLA	C4B-C3B-CAB-CBB
13	A	818	CLA	C4B-C3B-CAB-CBB
13	A	819	CLA	C4B-C3B-CAB-CBB
13	A	821	CLA	C4B-C3B-CAB-CBB
13	A	824	CLA	C4B-C3B-CAB-CBB
13	A	836	CLA	C4B-C3B-CAB-CBB
13	A	837	CLA	C4B-C3B-CAB-CBB
13	A	842	CLA	C4B-C3B-CAB-CBB
13	A	843	CLA	C4B-C3B-CAB-CBB
13	B	802	CLA	C4B-C3B-CAB-CBB
13	B	809	CLA	C4B-C3B-CAB-CBB
13	B	814	CLA	C1A-C2A-CAA-CBA
13	B	817	CLA	C4B-C3B-CAB-CBB
13	B	819	CLA	O1A-CGA-O2A-C1
13	B	828	CLA	C1A-C2A-CAA-CBA
13	B	828	CLA	C4B-C3B-CAB-CBB
13	B	829	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	B	831	CLA	C4B-C3B-CAB-CBB
13	B	833	CLA	C1A-C2A-CAA-CBA
13	K	201	CLA	C4B-C3B-CAB-CBB
13	K	203	CLA	C4B-C3B-CAB-CBB
13	A	830	CLA	C4-C3-C5-C6
13	A	802	CLA	C10-C11-C12-C13
16	J	104	BCR	C21-C22-C23-C24
13	B	822	CLA	O1D-CGD-O2D-CED
13	A	840	CLA	CBD-CGD-O2D-CED
13	A	807	CLA	C12-C13-C15-C16
13	A	820	CLA	C11-C10-C8-C7
13	A	840	CLA	C12-C13-C15-C16
13	A	843	CLA	C11-C10-C8-C7
13	B	806	CLA	C11-C12-C13-C15
13	L	203	CLA	C16-C17-C18-C20
13	A	831	CLA	C5-C6-C7-C8
13	B	811	CLA	CBD-CGD-O2D-CED
13	A	802	CLA	C3A-C2A-CAA-CBA
13	A	841	CLA	C4-C3-C5-C6
13	A	820	CLA	C11-C12-C13-C14
13	A	823	CLA	C6-C7-C8-C9
13	A	828	CLA	C11-C10-C8-C9
13	B	803	CLA	C14-C13-C15-C16
13	A	806	CLA	C5-C6-C7-C8
13	B	811	CLA	C8-C10-C11-C12
13	B	824	CLA	C1-C2-C3-C4
13	B	817	CLA	O1D-CGD-O2D-CED
13	L	203	CLA	C16-C17-C18-C19
13	A	829	CLA	C5-C6-C7-C8
13	A	818	CLA	O1A-CGA-O2A-C1
13	A	822	CLA	C2-C3-C5-C6
13	A	806	CLA	CAD-CBD-CGD-O2D
13	A	815	CLA	CAD-CBD-CGD-O2D
13	A	816	CLA	CAD-CBD-CGD-O2D
13	A	823	CLA	CAD-CBD-CGD-O2D
13	A	839	CLA	CAD-CBD-CGD-O2D
13	A	844	CLA	CAD-CBD-CGD-O2D
13	B	813	CLA	CAD-CBD-CGD-O2D
13	B	814	CLA	CAD-CBD-CGD-O2D
13	B	820	CLA	CAD-CBD-CGD-O2D
13	J	101	CLA	CAD-CBD-CGD-O2D
13	B	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	A	812	CLA	C2A-CAA-CBA-CGA
13	B	817	CLA	C8-C10-C11-C12
13	A	818	CLA	CBA-CGA-O2A-C1
13	A	806	CLA	CAD-CBD-CGD-O1D
13	A	814	CLA	CAD-CBD-CGD-O1D
13	A	815	CLA	CAD-CBD-CGD-O1D
13	A	816	CLA	CAD-CBD-CGD-O1D
13	A	823	CLA	CAD-CBD-CGD-O1D
13	A	826	CLA	CAD-CBD-CGD-O1D
13	A	839	CLA	CAD-CBD-CGD-O1D
13	A	844	CLA	CAD-CBD-CGD-O1D
13	B	813	CLA	CAD-CBD-CGD-O1D
13	B	814	CLA	CAD-CBD-CGD-O1D
13	B	820	CLA	CAD-CBD-CGD-O1D
13	B	827	CLA	CHA-CBD-CGD-O1D
13	B	827	CLA	CHA-CBD-CGD-O2D
13	J	101	CLA	CAD-CBD-CGD-O1D
16	A	851	BCR	C15-C16-C17-C18
17	A	853	LHG	C3-O3-P-O4
17	A	853	LHG	C4-O6-P-O3
17	A	853	LHG	C4-O6-P-O5
13	A	806	CLA	C2B-C3B-CAB-CBB
13	A	807	CLA	C2B-C3B-CAB-CBB
13	A	812	CLA	C2B-C3B-CAB-CBB
13	A	816	CLA	C2B-C3B-CAB-CBB
13	A	821	CLA	C2B-C3B-CAB-CBB
13	A	822	CLA	C2B-C3B-CAB-CBB
13	A	826	CLA	C2B-C3B-CAB-CBB
13	A	836	CLA	C2B-C3B-CAB-CBB
13	B	802	CLA	C2B-C3B-CAB-CBB
13	B	804	CLA	C2B-C3B-CAB-CBB
13	B	817	CLA	C2B-C3B-CAB-CBB
13	B	821	CLA	C2B-C3B-CAB-CBB
13	B	822	CLA	C2B-C3B-CAB-CBB
13	B	829	CLA	C2B-C3B-CAB-CBB
13	K	201	CLA	C2B-C3B-CAB-CBB
13	L	204	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C5-C6-C7-C8
16	J	103	BCR	C1-C6-C7-C8
13	A	821	CLA	C2-C3-C5-C6
16	B	835	BCR	C37-C22-C23-C24
18	B	838	LMG	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
13	B	804	CLA	C13-C15-C16-C17
13	A	830	CLA	C8-C10-C11-C12
13	B	830	CLA	C2-C3-C5-C6
13	B	832	CLA	CBA-CGA-O2A-C1
13	A	809	CLA	C14-C13-C15-C16
13	A	835	CLA	C14-C13-C15-C16
13	A	823	CLA	C6-C7-C8-C10
13	A	835	CLA	C12-C13-C15-C16
13	B	813	CLA	C11-C10-C8-C7
13	B	808	CLA	C4-C3-C5-C6
13	B	822	CLA	O1A-CGA-O2A-C1
18	B	838	LMG	O1-C7-C8-O7
12	A	801	CL0	CAA-CBA-CGA-O2A
13	A	806	CLA	CAA-CBA-CGA-O2A
13	L	203	CLA	C13-C15-C16-C17
13	B	825	CLA	CAA-CBA-CGA-O2A
13	A	803	CLA	C2A-CAA-CBA-CGA
13	B	824	CLA	C2A-CAA-CBA-CGA
16	A	848	BCR	C19-C20-C21-C22
13	B	833	CLA	C4-C3-C5-C6
13	A	826	CLA	C2-C3-C5-C6
13	A	829	CLA	CBA-CGA-O2A-C1
13	B	813	CLA	C11-C10-C8-C9
13	A	812	CLA	C4B-C3B-CAB-CBB
13	A	820	CLA	C4B-C3B-CAB-CBB
13	B	814	CLA	C4B-C3B-CAB-CBB
13	B	824	CLA	C4B-C3B-CAB-CBB
13	F	203	CLA	C4B-C3B-CAB-CBB
13	A	840	CLA	O1D-CGD-O2D-CED
13	B	811	CLA	C13-C15-C16-C17
13	A	835	CLA	C4-C3-C5-C6
13	B	810	CLA	C4-C3-C5-C6
13	B	817	CLA	CAA-CBA-CGA-O2A
13	B	808	CLA	C2-C3-C5-C6
13	B	824	CLA	O1D-CGD-O2D-CED
17	A	852	LHG	C10-C11-C12-C13
18	B	838	LMG	C18-C19-C20-C21
13	A	827	CLA	C4-C3-C5-C6
13	A	834	CLA	C4-C3-C5-C6
13	B	820	CLA	C4-C3-C5-C6
13	B	824	CLA	C3A-C2A-CAA-CBA
13	A	830	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
16	A	850	BCR	C35-C13-C14-C15
16	A	851	BCR	C11-C10-C9-C34
16	B	835	BCR	C20-C21-C22-C37
16	F	201	BCR	C6-C7-C8-C9
16	K	202	BCR	C22-C23-C24-C25
13	B	803	CLA	C15-C16-C17-C18
13	B	826	CLA	C2-C1-O2A-CGA
13	A	814	CLA	CAA-CBA-CGA-O1A
12	A	801	CL0	C4-C3-C5-C6
13	A	802	CLA	C4-C3-C5-C6
13	A	836	CLA	C4-C3-C5-C6
13	A	841	CLA	C2-C3-C5-C6
13	A	830	CLA	C16-C17-C18-C19
13	B	816	CLA	C2A-CAA-CBA-CGA
13	L	204	CLA	C3-C5-C6-C7
13	B	806	CLA	C14-C13-C15-C16
13	B	810	CLA	C16-C17-C18-C20
13	A	839	CLA	C5-C6-C7-C8
13	B	825	CLA	C13-C15-C16-C17
13	B	826	CLA	CAA-CBA-CGA-O2A
13	A	837	CLA	O1D-CGD-O2D-CED
12	A	801	CL0	C2-C3-C5-C6
13	A	834	CLA	C2-C3-C5-C6
13	B	833	CLA	C2-C3-C5-C6
17	A	853	LHG	O1-C1-C2-O2
13	B	832	CLA	C10-C11-C12-C13
13	A	834	CLA	C2A-CAA-CBA-CGA
13	A	831	CLA	C1A-C2A-CAA-CBA
13	A	843	CLA	C1A-C2A-CAA-CBA
13	B	816	CLA	C1A-C2A-CAA-CBA
13	B	829	CLA	C1A-C2A-CAA-CBA
16	B	835	BCR	C20-C21-C22-C23
13	A	809	CLA	C2B-C3B-CAB-CBB
13	A	813	CLA	C2B-C3B-CAB-CBB
13	A	818	CLA	C2B-C3B-CAB-CBB
13	A	819	CLA	C2B-C3B-CAB-CBB
13	A	820	CLA	C2B-C3B-CAB-CBB
13	A	824	CLA	C2B-C3B-CAB-CBB
13	B	814	CLA	C2B-C3B-CAB-CBB
13	B	824	CLA	C2B-C3B-CAB-CBB
13	B	831	CLA	C2B-C3B-CAB-CBB
13	F	203	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	K	203	CLA	C2B-C3B-CAB-CBB
13	L	202	CLA	C2B-C3B-CAB-CBB
16	A	847	BCR	C23-C24-C25-C26
16	A	848	BCR	C5-C6-C7-C8
16	A	849	BCR	C5-C6-C7-C8
16	A	849	BCR	C23-C24-C25-C26
16	A	850	BCR	C5-C6-C7-C8
16	A	850	BCR	C23-C24-C25-C26
16	B	835	BCR	C5-C6-C7-C8
16	B	835	BCR	C23-C24-C25-C26
16	B	836	BCR	C5-C6-C7-C8
16	B	836	BCR	C23-C24-C25-C26
16	B	837	BCR	C5-C6-C7-C8
16	B	837	BCR	C23-C24-C25-C26
16	F	201	BCR	C5-C6-C7-C8
16	F	202	BCR	C5-C6-C7-C8
16	I	101	BCR	C5-C6-C7-C8
16	J	102	BCR	C5-C6-C7-C8
16	J	103	BCR	C5-C6-C7-C8
16	J	104	BCR	C23-C24-C25-C26
16	K	202	BCR	C5-C6-C7-C8
16	L	201	BCR	C5-C6-C7-C8
16	L	201	BCR	C23-C24-C25-C26
16	L	201	BCR	C23-C24-C25-C30
16	L	205	BCR	C5-C6-C7-C8
16	L	206	BCR	C5-C6-C7-C8
16	L	206	BCR	C23-C24-C25-C26
16	M	101	BCR	C5-C6-C7-C8
13	B	811	CLA	C5-C6-C7-C8
13	A	808	CLA	O1A-CGA-O2A-C1
13	A	814	CLA	CAA-CBA-CGA-O2A
13	A	802	CLA	C2-C3-C5-C6
13	A	827	CLA	C2-C3-C5-C6
13	A	809	CLA	C11-C12-C13-C15
13	A	840	CLA	C6-C7-C8-C10
13	B	804	CLA	C6-C7-C8-C10
13	B	806	CLA	C12-C13-C15-C16
13	B	810	CLA	C11-C10-C8-C7
13	B	821	CLA	C6-C7-C8-C10
13	B	824	CLA	CAA-CBA-CGA-O1A
17	A	852	LHG	C34-C35-C36-C37
13	A	828	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	A	839	CLA	C4-C3-C5-C6
13	A	835	CLA	C2-C3-C5-C6
13	B	810	CLA	C2-C3-C5-C6
13	B	826	CLA	C5-C6-C7-C8
13	A	810	CLA	CAA-CBA-CGA-O2A
18	B	838	LMG	C31-C32-C33-C34
18	B	838	LMG	C14-C15-C16-C17
16	F	202	BCR	C6-C7-C8-C9
13	A	836	CLA	C2-C3-C5-C6
13	B	805	CLA	C2-C3-C5-C6
13	B	820	CLA	C2-C3-C5-C6
17	A	852	LHG	C4-C5-C6-O8
13	A	811	CLA	CAA-CBA-CGA-O2A
13	A	829	CLA	O1A-CGA-O2A-C1
13	A	831	CLA	C4-C3-C5-C6
13	A	810	CLA	CAA-CBA-CGA-O1A
13	A	808	CLA	CBA-CGA-O2A-C1
17	A	853	LHG	O10-C23-O8-C6
12	A	801	CL0	CHA-CBD-CGD-O2D
16	J	103	BCR	C16-C17-C18-C36
13	B	825	CLA	O1A-CGA-O2A-C1
13	A	807	CLA	C15-C16-C17-C18
13	B	821	CLA	C10-C11-C12-C13
13	L	203	CLA	C3-C5-C6-C7
13	B	811	CLA	O1D-CGD-O2D-CED
13	B	806	CLA	CAA-CBA-CGA-O2A
13	F	203	CLA	CAA-CBA-CGA-O2A
13	B	811	CLA	C6-C7-C8-C9
13	A	832	CLA	C2-C1-O2A-CGA
13	A	834	CLA	C2-C1-O2A-CGA
13	A	836	CLA	C2-C1-O2A-CGA
13	A	840	CLA	C2-C1-O2A-CGA
13	B	830	CLA	C2-C1-O2A-CGA
13	A	808	CLA	C3A-C2A-CAA-CBA
13	B	803	CLA	C3A-C2A-CAA-CBA
13	B	829	CLA	C3A-C2A-CAA-CBA
13	A	843	CLA	CAA-CBA-CGA-O2A
13	A	819	CLA	CAA-CBA-CGA-O1A
13	A	816	CLA	CAA-CBA-CGA-O2A
13	B	825	CLA	CBA-CGA-O2A-C1
16	A	851	BCR	C16-C17-C18-C19
16	F	202	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
16	L	201	BCR	C20-C21-C22-C23
13	A	811	CLA	CAA-CBA-CGA-O1A
13	B	812	CLA	O1D-CGD-O2D-CED
13	B	822	CLA	C3-C5-C6-C7
13	F	203	CLA	CAA-CBA-CGA-O1A
13	A	823	CLA	C15-C16-C17-C18
13	A	816	CLA	CAA-CBA-CGA-O1A
16	A	847	BCR	C15-C16-C17-C18
16	L	206	BCR	C9-C10-C11-C12
13	A	804	CLA	CAA-CBA-CGA-O2A
13	B	821	CLA	CAA-CBA-CGA-O1A
13	A	807	CLA	C14-C13-C15-C16
13	A	820	CLA	C11-C10-C8-C9
13	A	841	CLA	CAA-CBA-CGA-O2A
13	B	802	CLA	CAA-CBA-CGA-O2A
13	B	813	CLA	CAA-CBA-CGA-O2A
16	A	850	BCR	C11-C12-C13-C14
16	J	102	BCR	C11-C12-C13-C14
13	B	810	CLA	CAA-CBA-CGA-O2A
13	A	828	CLA	C2-C3-C5-C6
18	B	838	LMG	C34-C35-C36-C37
13	A	812	CLA	C12-C13-C15-C16
13	A	828	CLA	C6-C7-C8-C10
13	A	829	CLA	C11-C12-C13-C15
13	B	811	CLA	C12-C13-C15-C16
13	A	823	CLA	C2B-C3B-CAB-CBB
13	B	816	CLA	C2B-C3B-CAB-CBB
16	F	201	BCR	C23-C24-C25-C26
16	F	201	BCR	C23-C24-C25-C30
16	F	202	BCR	C23-C24-C25-C26
16	J	102	BCR	C23-C24-C25-C26
16	J	102	BCR	C23-C24-C25-C30
16	J	104	BCR	C1-C6-C7-C8
13	A	818	CLA	C2-C1-O2A-CGA
13	B	802	CLA	C2-C1-O2A-CGA
13	B	808	CLA	C2-C1-O2A-CGA
13	B	813	CLA	C2-C1-O2A-CGA
13	B	822	CLA	C2-C1-O2A-CGA
13	B	824	CLA	C2-C1-O2A-CGA
13	B	804	CLA	CAA-CBA-CGA-O2A
13	B	815	CLA	CAA-CBA-CGA-O2A
13	K	201	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	L	203	CLA	C10-C11-C12-C13
13	A	818	CLA	CAA-CBA-CGA-O2A
13	B	818	CLA	C3-C5-C6-C7
16	J	102	BCR	C18-C19-C20-C21
13	A	824	CLA	CAA-CBA-CGA-O2A
13	A	804	CLA	CAA-CBA-CGA-O1A
13	A	802	CLA	C1A-C2A-CAA-CBA
13	A	811	CLA	C4B-C3B-CAB-CBB
13	A	833	CLA	C4B-C3B-CAB-CBB
13	B	803	CLA	C1A-C2A-CAA-CBA
13	B	806	CLA	C4B-C3B-CAB-CBB
13	B	807	CLA	C4B-C3B-CAB-CBB
13	B	833	CLA	C4B-C3B-CAB-CBB
13	L	202	CLA	C4B-C3B-CAB-CBB
13	B	817	CLA	C4-C3-C5-C6
16	B	836	BCR	C6-C7-C8-C9
13	A	826	CLA	CAA-CBA-CGA-O2A
13	B	808	CLA	CAA-CBA-CGA-O2A
13	A	844	CLA	C4C-C3C-CAC-CBC
13	B	810	CLA	C16-C17-C18-C19
13	A	828	CLA	CAA-CBA-CGA-O2A
13	A	839	CLA	CAA-CBA-CGA-O2A
13	B	807	CLA	CAA-CBA-CGA-O2A
13	A	818	CLA	C2A-CAA-CBA-CGA
13	B	817	CLA	C10-C11-C12-C13
13	B	833	CLA	C13-C15-C16-C17
13	L	204	CLA	CAA-CBA-CGA-O2A
13	A	827	CLA	C2-C1-O2A-CGA
13	A	841	CLA	C2-C1-O2A-CGA
13	B	817	CLA	C2-C1-O2A-CGA
13	A	833	CLA	C11-C10-C8-C7
13	B	807	CLA	C12-C13-C15-C16
13	A	828	CLA	C15-C16-C17-C18
13	A	830	CLA	C16-C17-C18-C20
13	A	803	CLA	CAA-CBA-CGA-O2A
18	B	838	LMG	C29-C28-O8-C9
13	A	823	CLA	C2A-CAA-CBA-CGA
13	A	824	CLA	C2A-CAA-CBA-CGA
13	A	841	CLA	C2A-CAA-CBA-CGA
13	B	815	CLA	CAA-CBA-CGA-O1A
13	J	101	CLA	CAA-CBA-CGA-O1A
13	A	835	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
13	A	839	CLA	C2-C3-C5-C6
16	M	101	BCR	C12-C13-C14-C15
13	B	810	CLA	CAA-CBA-CGA-O1A
13	A	818	CLA	CAA-CBA-CGA-O1A
13	B	804	CLA	CAA-CBA-CGA-O1A
13	A	844	CLA	CBD-CGD-O2D-CED
13	B	809	CLA	C15-C16-C17-C18
13	A	843	CLA	C11-C10-C8-C9
13	B	810	CLA	C11-C10-C8-C9
13	B	821	CLA	C6-C7-C8-C9
13	B	830	CLA	CAA-CBA-CGA-O2A
16	F	202	BCR	C13-C14-C15-C16
13	A	824	CLA	CAA-CBA-CGA-O1A
13	L	204	CLA	CAA-CBA-CGA-O1A
13	A	826	CLA	CAA-CBA-CGA-O1A
13	B	813	CLA	CAA-CBA-CGA-O1A
17	A	852	LHG	C12-C13-C14-C15
17	A	853	LHG	O10-C23-C24-C25
13	A	841	CLA	CAA-CBA-CGA-O1A
13	A	828	CLA	CAA-CBA-CGA-O1A
13	B	807	CLA	CAA-CBA-CGA-O1A
13	B	808	CLA	CAA-CBA-CGA-O1A
13	A	844	CLA	C2C-C3C-CAC-CBC
13	A	803	CLA	CAD-CBD-CGD-O2D
13	A	818	CLA	CAD-CBD-CGD-O2D
13	A	836	CLA	CAD-CBD-CGD-O2D
13	B	826	CLA	CAD-CBD-CGD-O2D
13	B	830	CLA	CAD-CBD-CGD-O2D
13	B	831	CLA	CAD-CBD-CGD-O2D
16	J	104	BCR	C6-C7-C8-C9
13	B	823	CLA	C2-C1-O2A-CGA
13	A	823	CLA	CAA-CBA-CGA-O2A
13	L	202	CLA	CAA-CBA-CGA-O2A
13	J	101	CLA	CAA-CBA-CGA-O2A
18	B	838	LMG	C15-C16-C17-C18
13	A	823	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

96 monomers are involved in 218 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	842	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	848	BCR	5	0
13	A	823	CLA	2	0
13	A	836	CLA	2	0
16	F	201	BCR	3	0
13	B	823	CLA	4	0
13	B	825	CLA	2	0
13	B	817	CLA	1	0
13	A	807	CLA	3	0
13	A	806	CLA	6	0
13	B	807	CLA	5	0
13	A	832	CLA	1	0
13	B	813	CLA	1	0
16	J	102	BCR	8	0
13	B	801	CLA	3	0
13	B	808	CLA	3	0
16	A	851	BCR	5	0
13	A	837	CLA	1	0
13	B	831	CLA	1	0
16	J	104	BCR	2	0
13	B	811	CLA	2	0
13	B	805	CLA	1	0
13	A	815	CLA	1	0
13	B	819	CLA	1	0
16	B	837	BCR	1	0
13	A	841	CLA	1	0
13	A	813	CLA	1	0
16	L	206	BCR	1	0
16	I	101	BCR	5	0
13	A	829	CLA	9	0
14	A	845	PQN	4	0
13	A	803	CLA	1	0
13	B	826	CLA	1	0
12	A	801	CL0	2	0
13	J	101	CLA	2	0
13	A	812	CLA	5	0
13	A	821	CLA	2	0
13	A	814	CLA	1	0
13	B	812	CLA	1	0
13	A	810	CLA	1	0
13	A	818	CLA	2	0
13	B	818	CLA	2	0
13	B	827	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	835	BCR	4	0
13	A	825	CLA	2	0
13	L	204	CLA	2	0
13	A	822	CLA	3	0
16	K	202	BCR	3	0
13	B	803	CLA	4	0
16	M	101	BCR	4	0
13	A	834	CLA	2	0
13	A	819	CLA	3	0
13	B	802	CLA	5	0
16	F	202	BCR	5	0
16	B	836	BCR	3	0
17	A	852	LHG	1	0
13	B	824	CLA	4	0
13	A	820	CLA	3	0
14	B	834	PQN	5	0
13	A	826	CLA	2	0
13	A	835	CLA	4	0
13	A	828	CLA	2	0
13	A	805	CLA	3	0
16	L	201	BCR	3	0
13	B	810	CLA	1	0
16	A	847	BCR	5	0
13	A	831	CLA	3	0
13	A	844	CLA	1	0
15	A	846	SF4	2	0
13	B	816	CLA	1	0
13	A	840	CLA	5	0
13	B	821	CLA	4	0
16	A	850	BCR	3	0
13	B	809	CLA	5	0
16	A	849	BCR	1	0
13	A	838	CLA	1	0
16	L	205	BCR	2	0
18	B	838	LMG	1	0
13	B	832	CLA	3	0
13	B	822	CLA	6	0
13	A	833	CLA	4	0
13	L	203	CLA	1	0
13	B	820	CLA	4	0
13	B	833	CLA	10	0
13	A	830	CLA	6	0

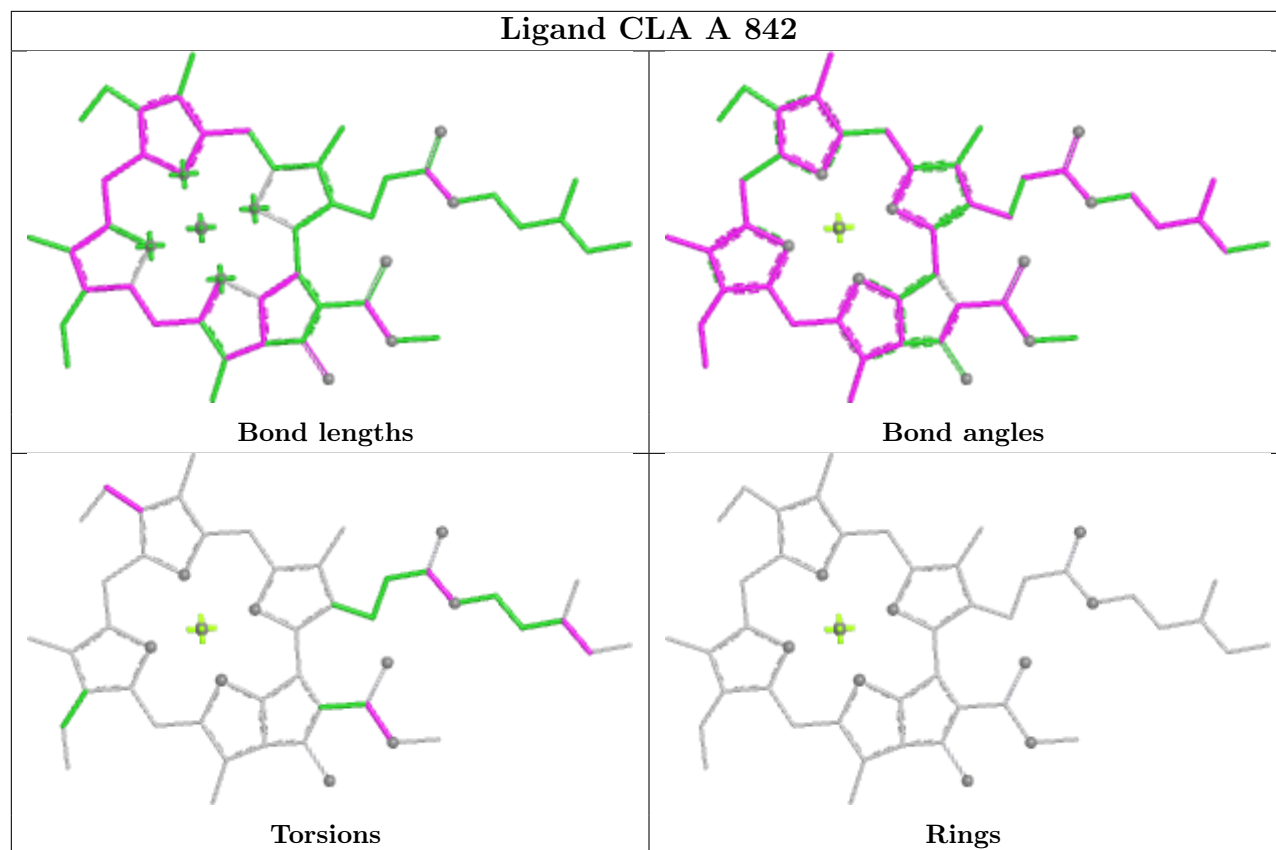
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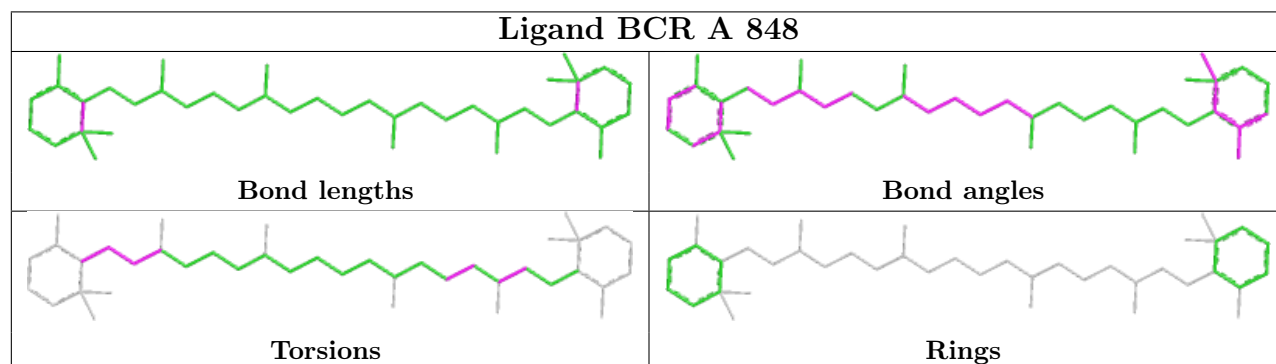
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	809	CLA	8	0
13	A	802	CLA	1	0
13	B	804	CLA	7	0
13	B	806	CLA	2	0
13	B	830	CLA	4	0
13	A	804	CLA	2	0
13	A	808	CLA	1	0
15	C	102	SF4	4	0
13	L	202	CLA	2	0
16	J	103	BCR	2	0
13	A	843	CLA	4	0

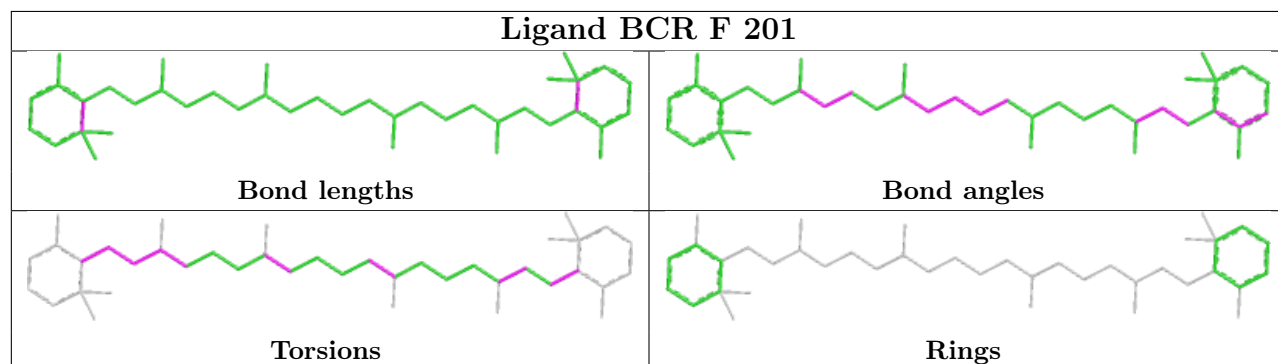
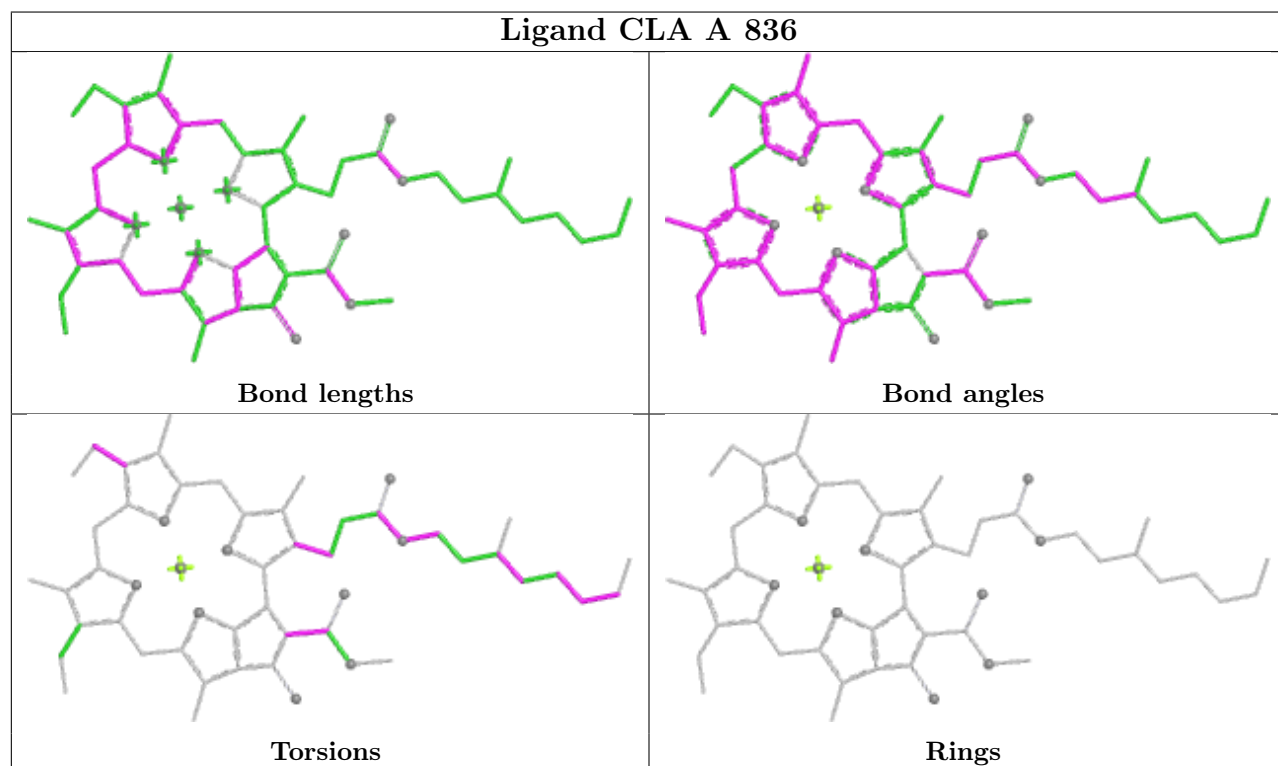
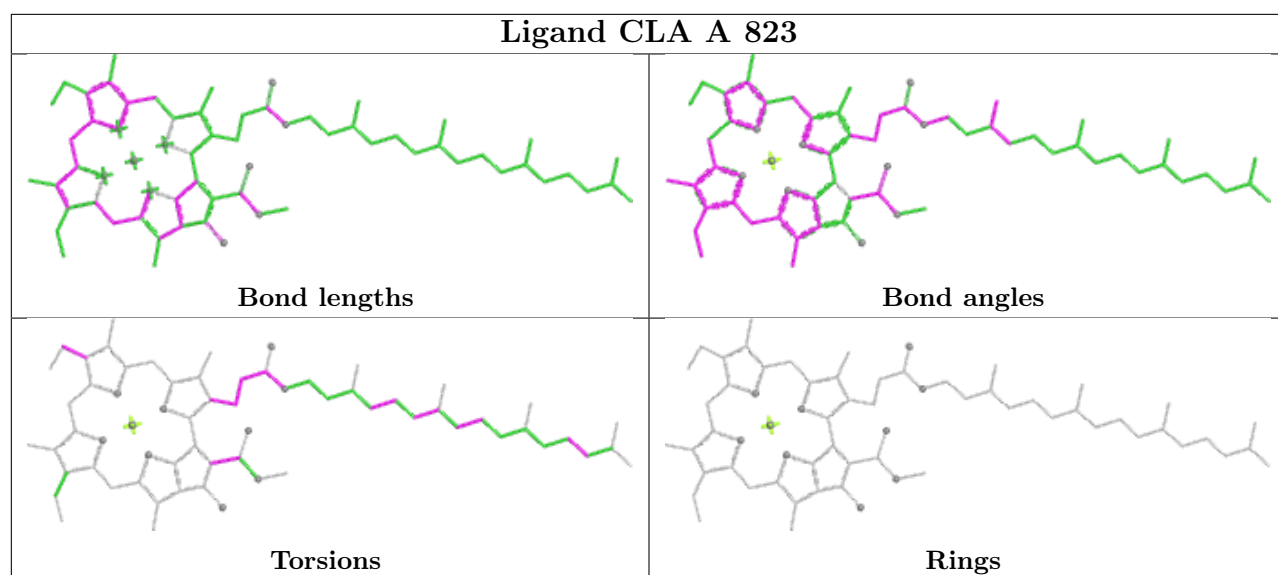
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

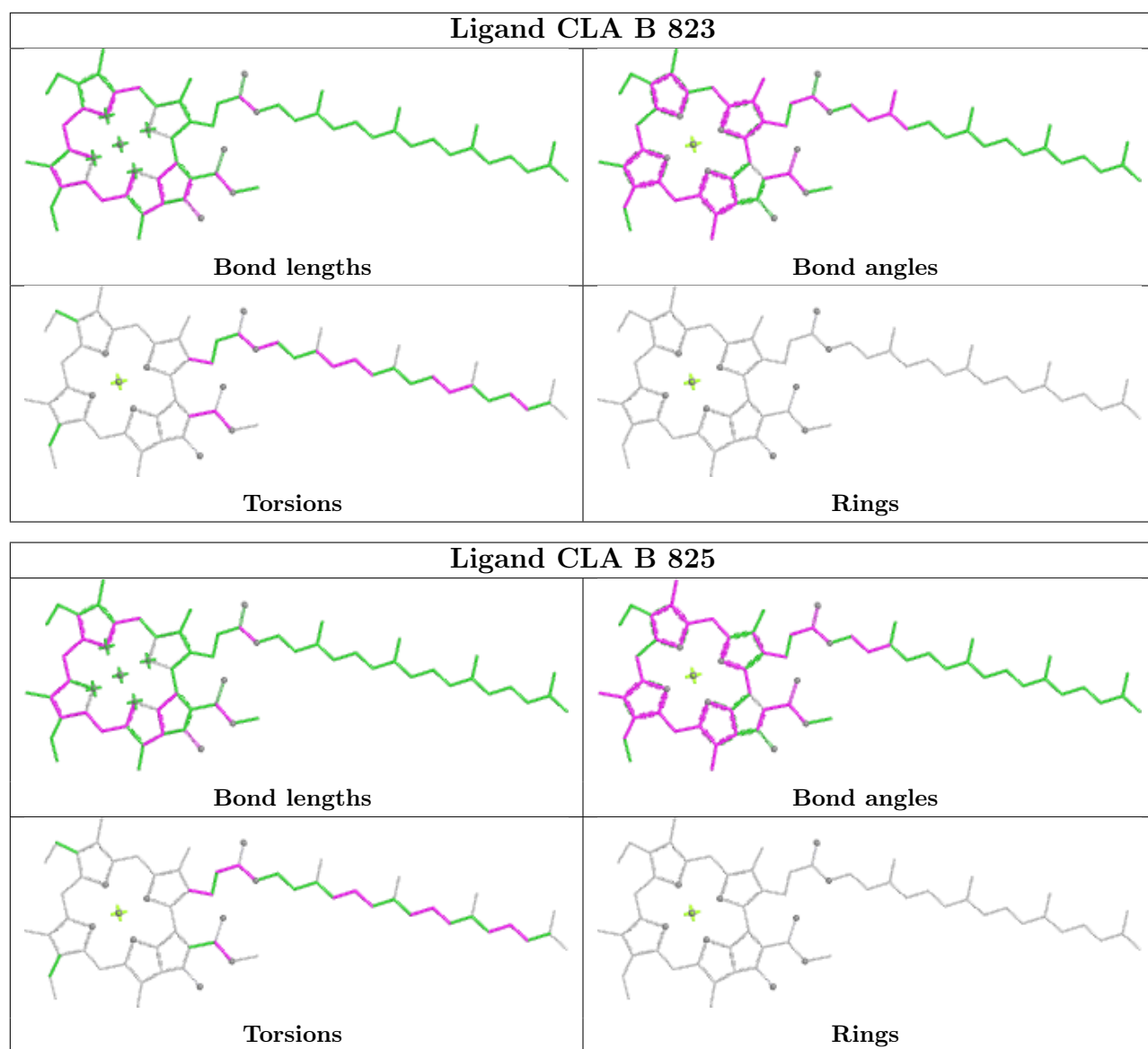
Ligand CLA A 842



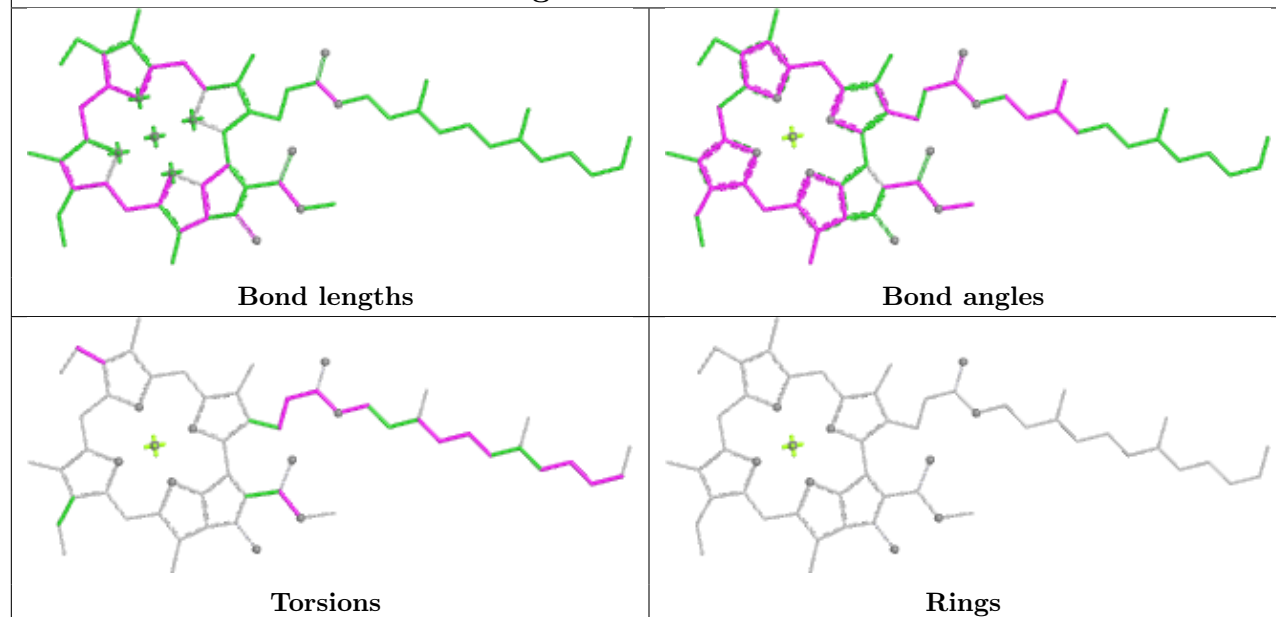
Ligand BCR A 848



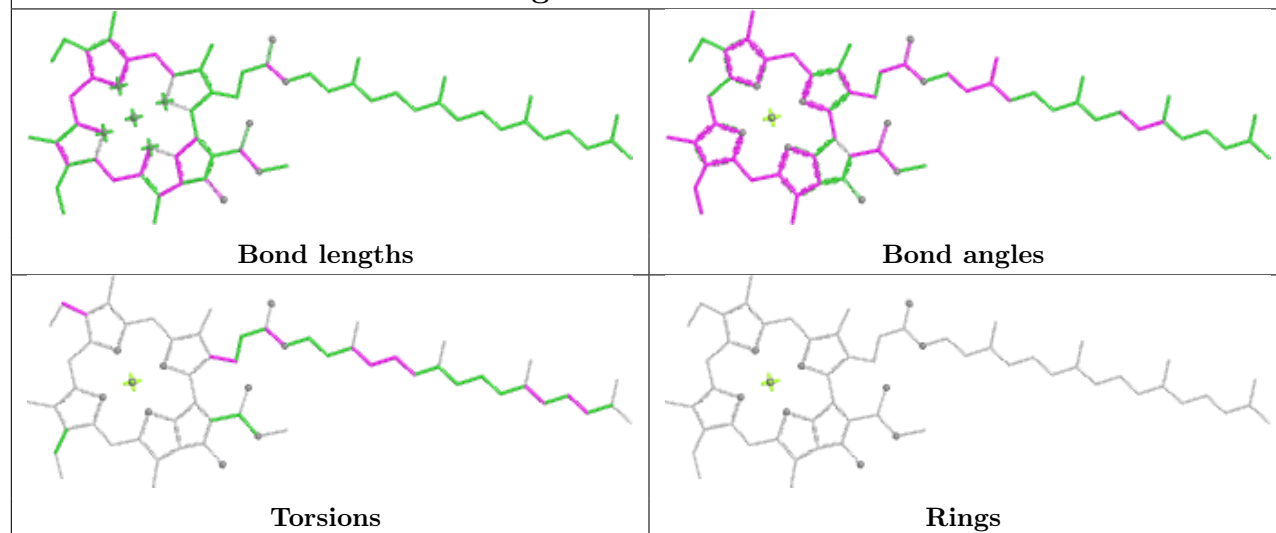


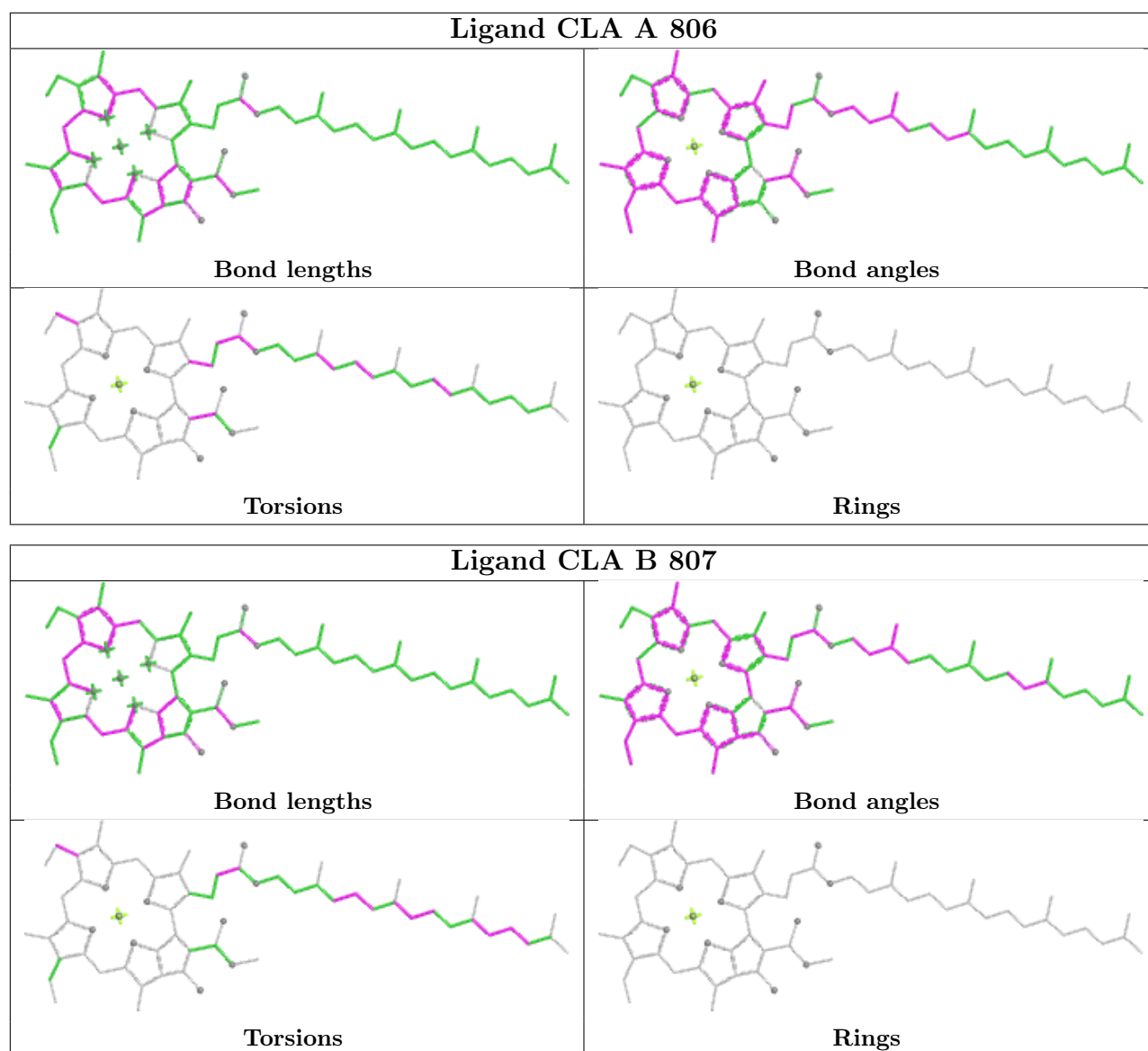


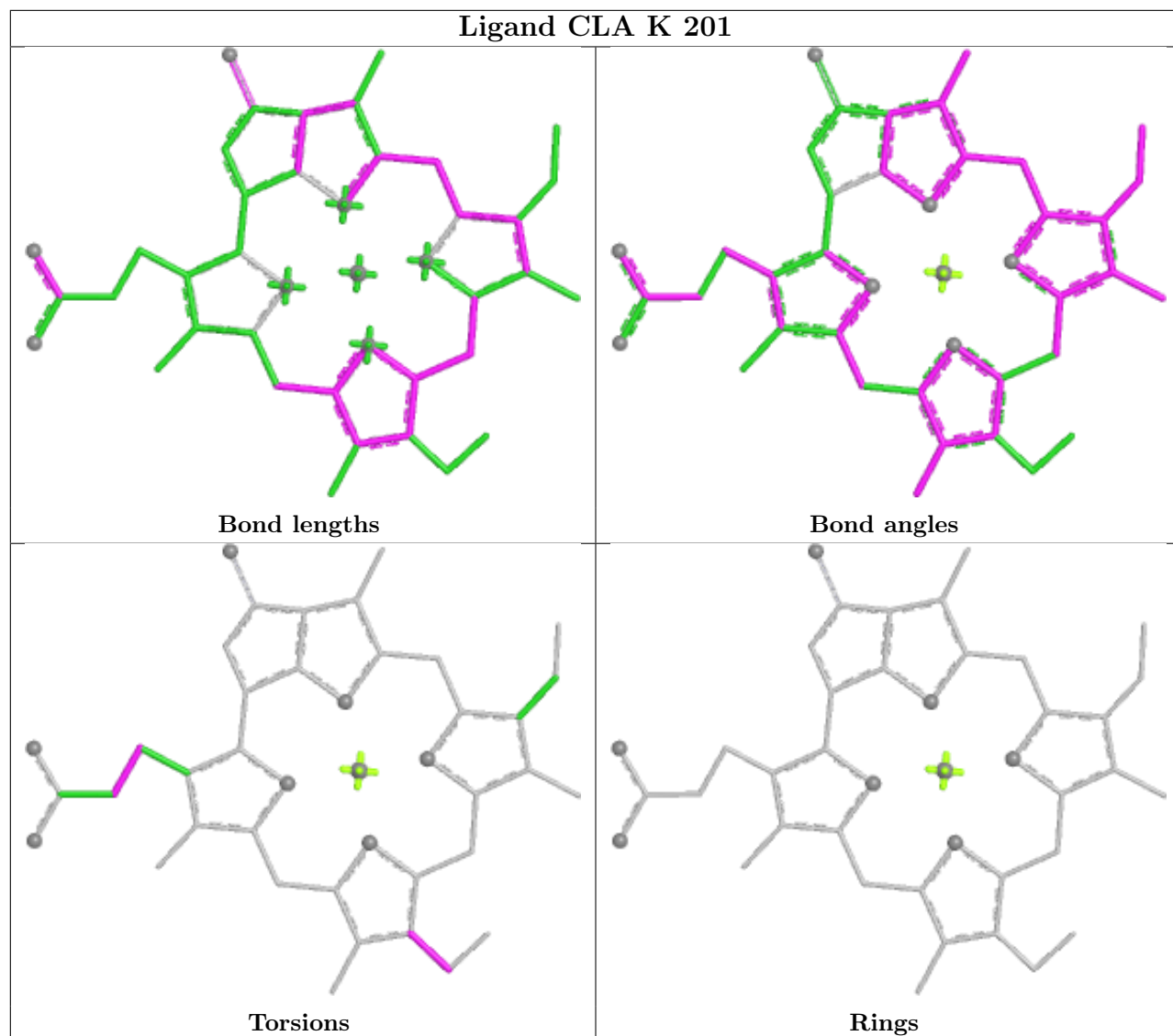
Ligand CLA B 817



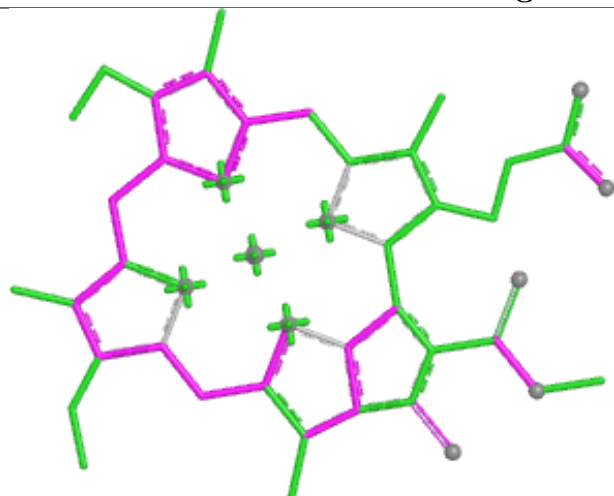
Ligand CLA A 807



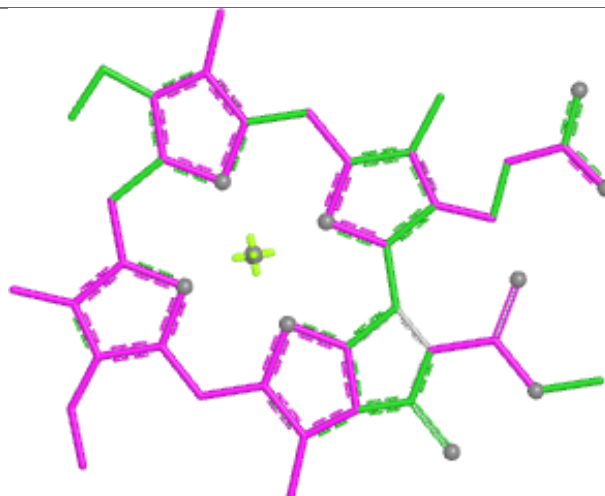




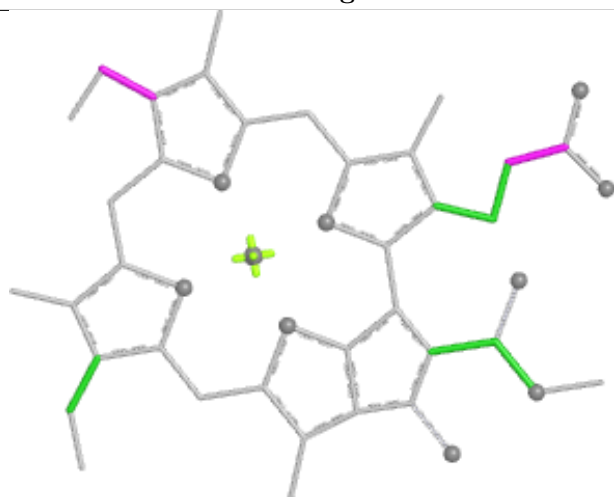
Ligand CLA F 203



Bond lengths



Bond angles

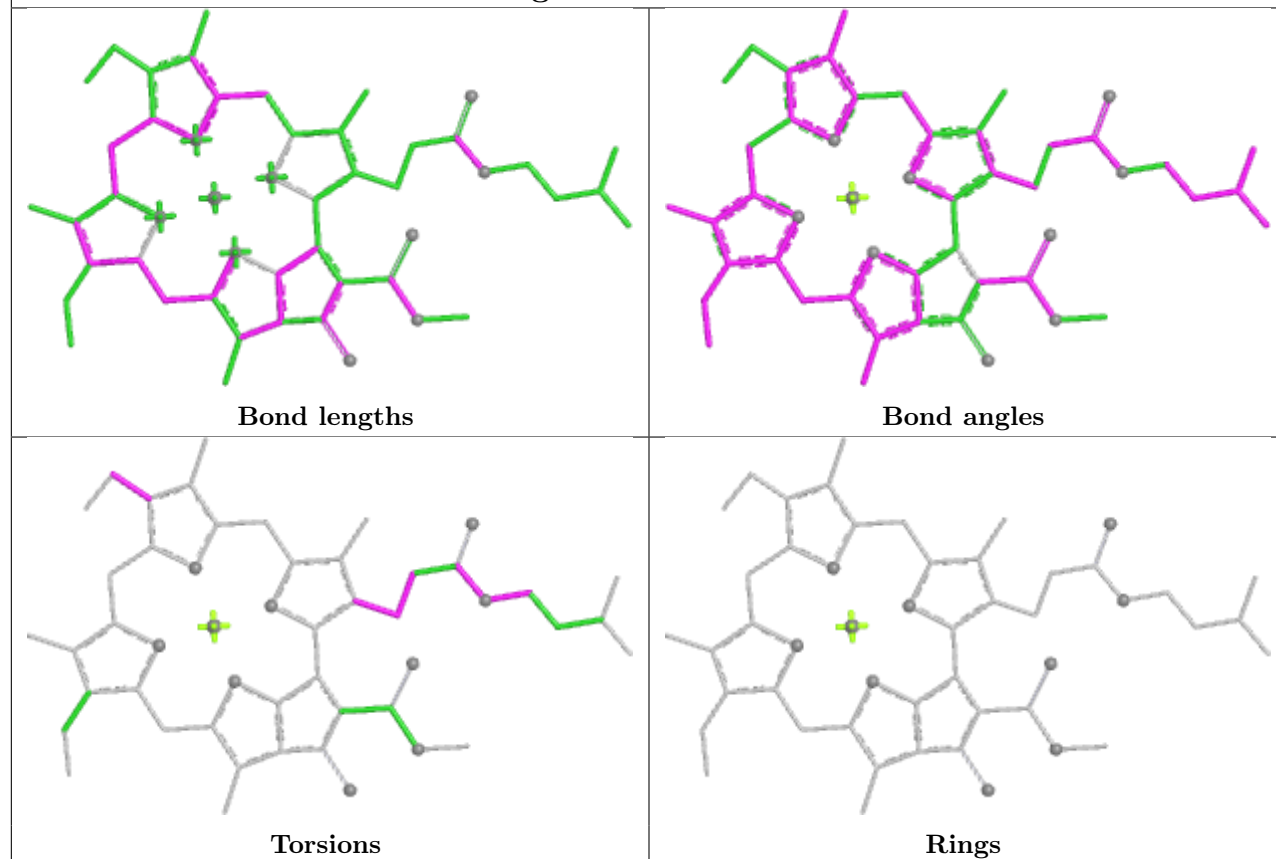


Torsions

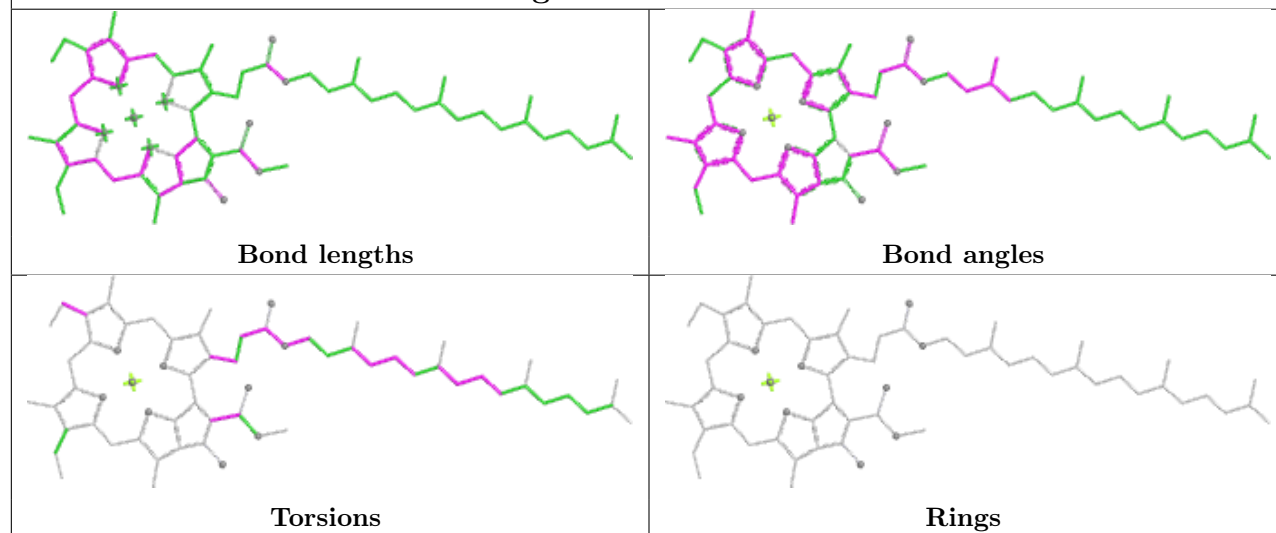


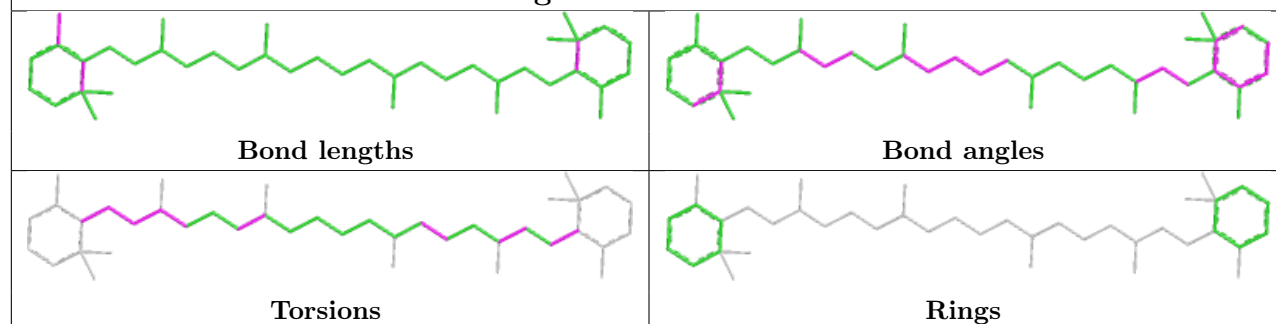
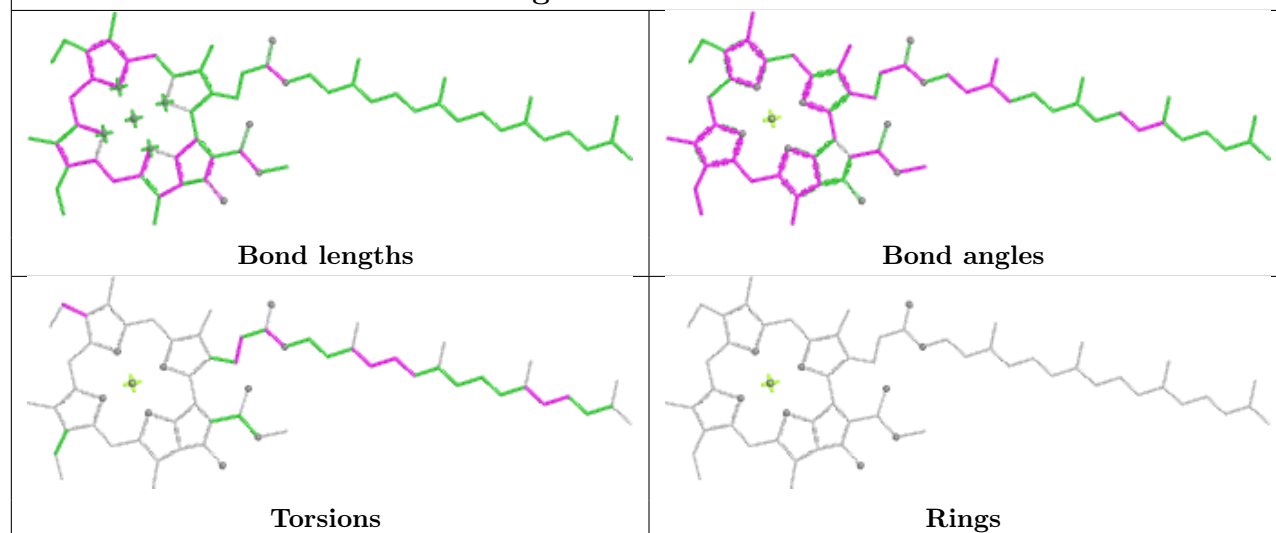
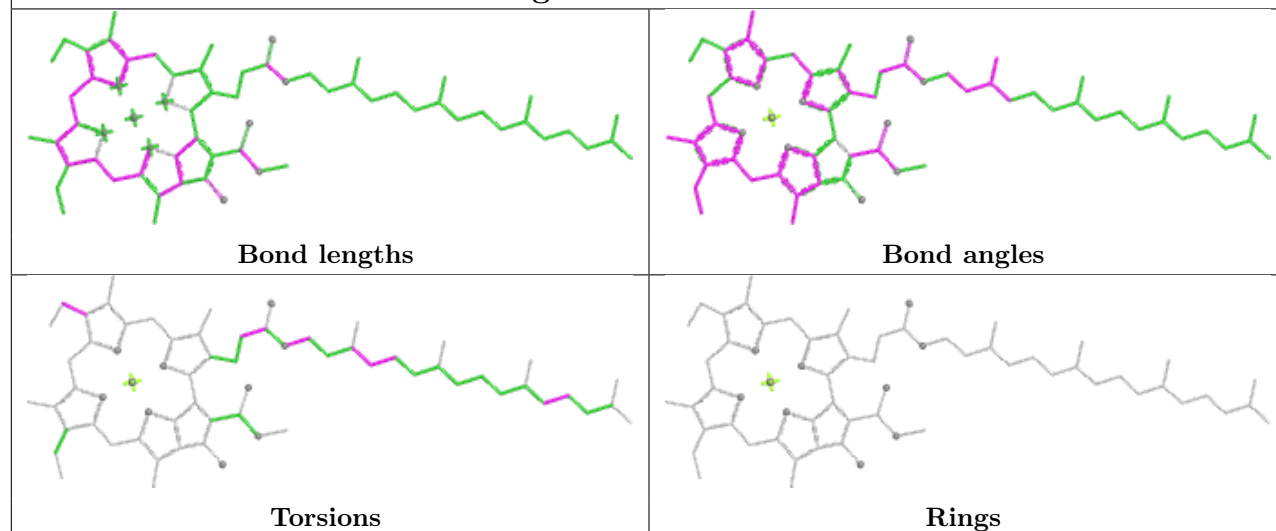
Rings

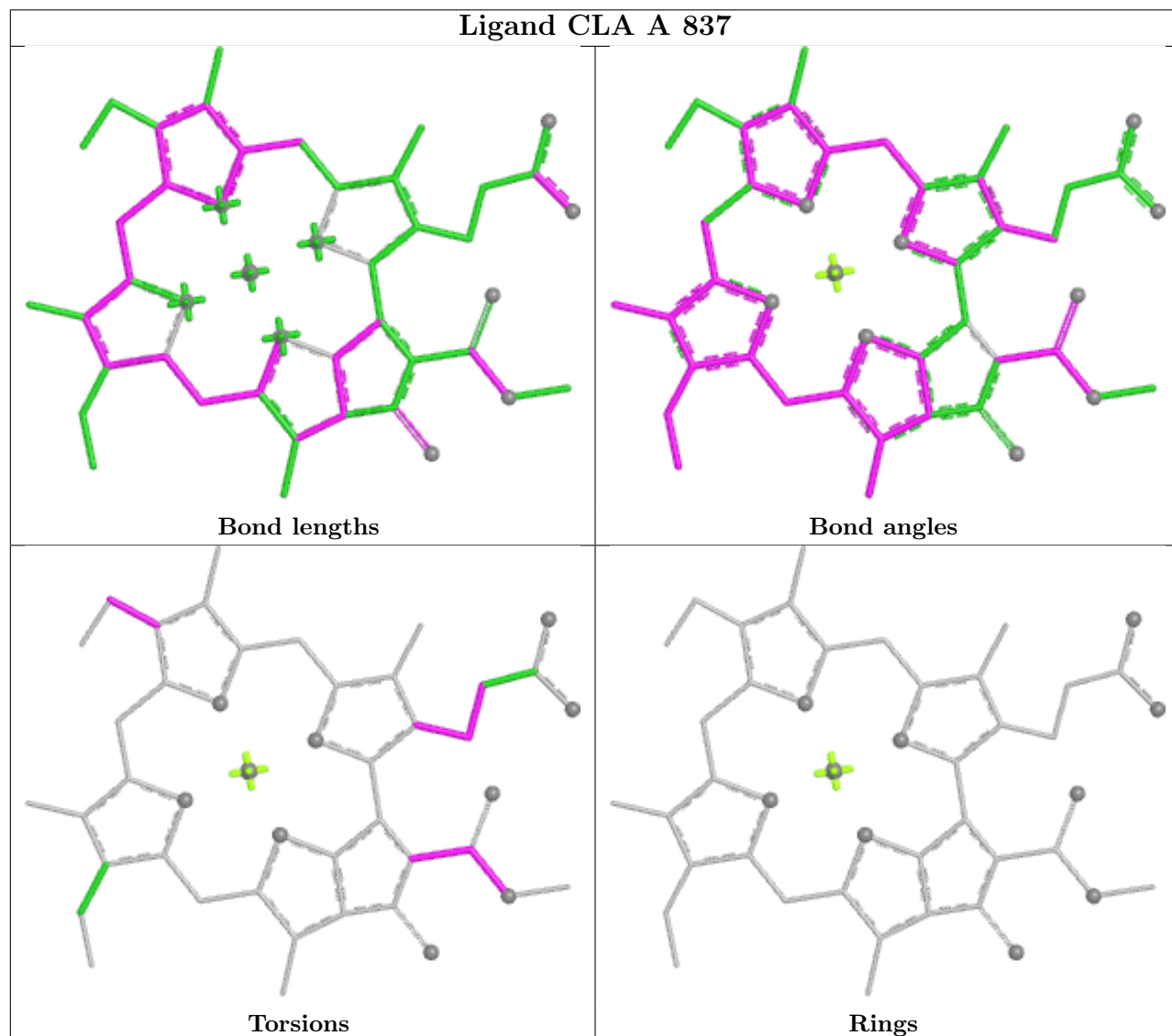
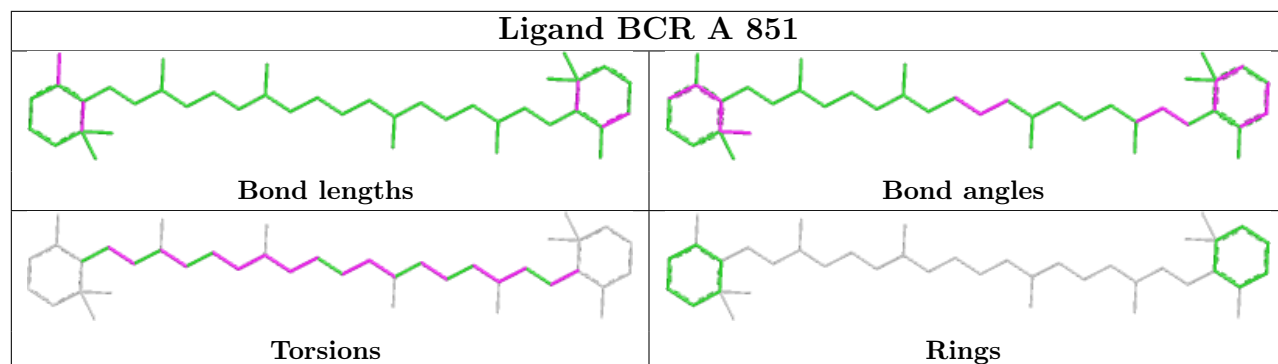
Ligand CLA A 832



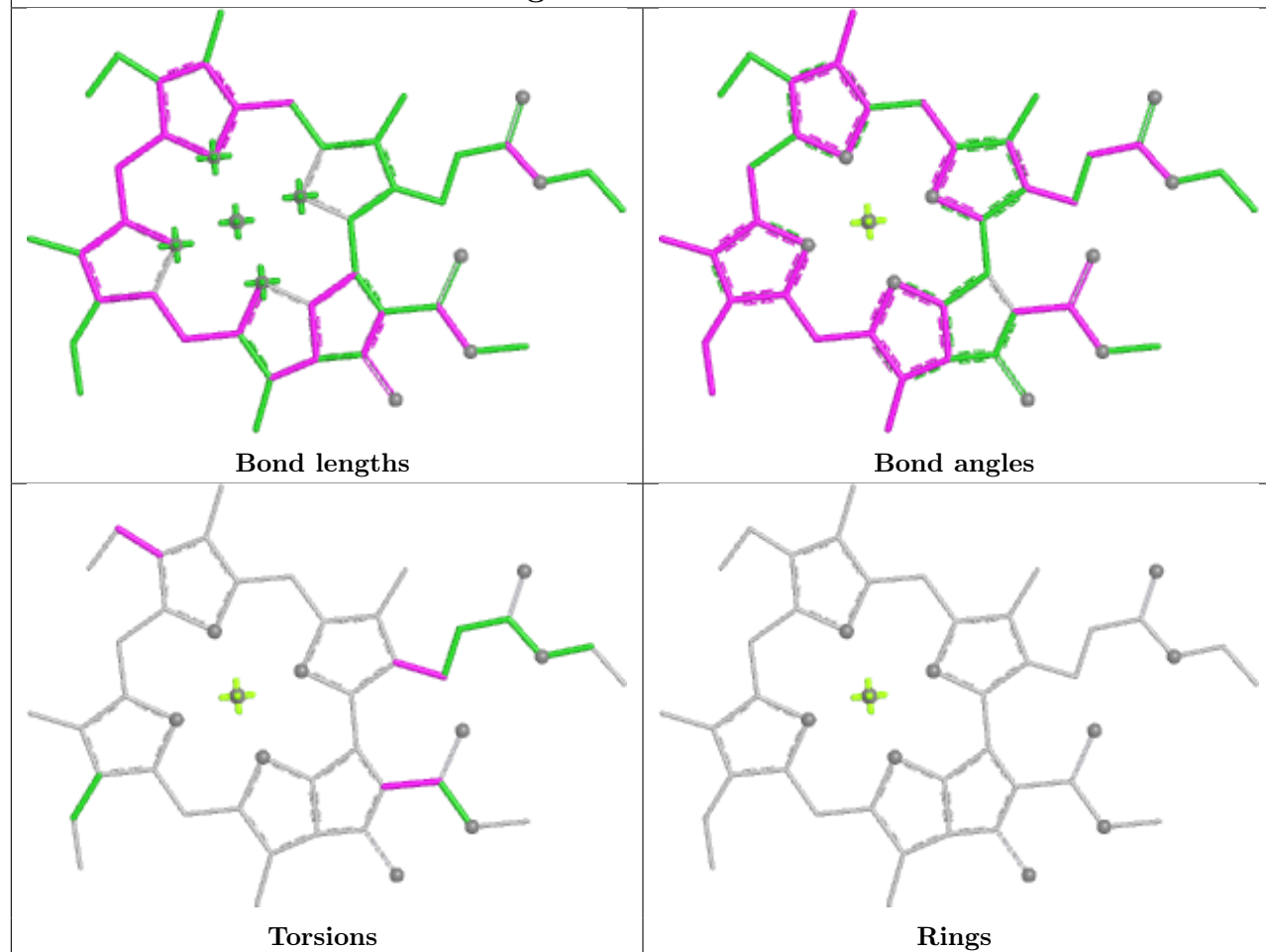
Ligand CLA B 813



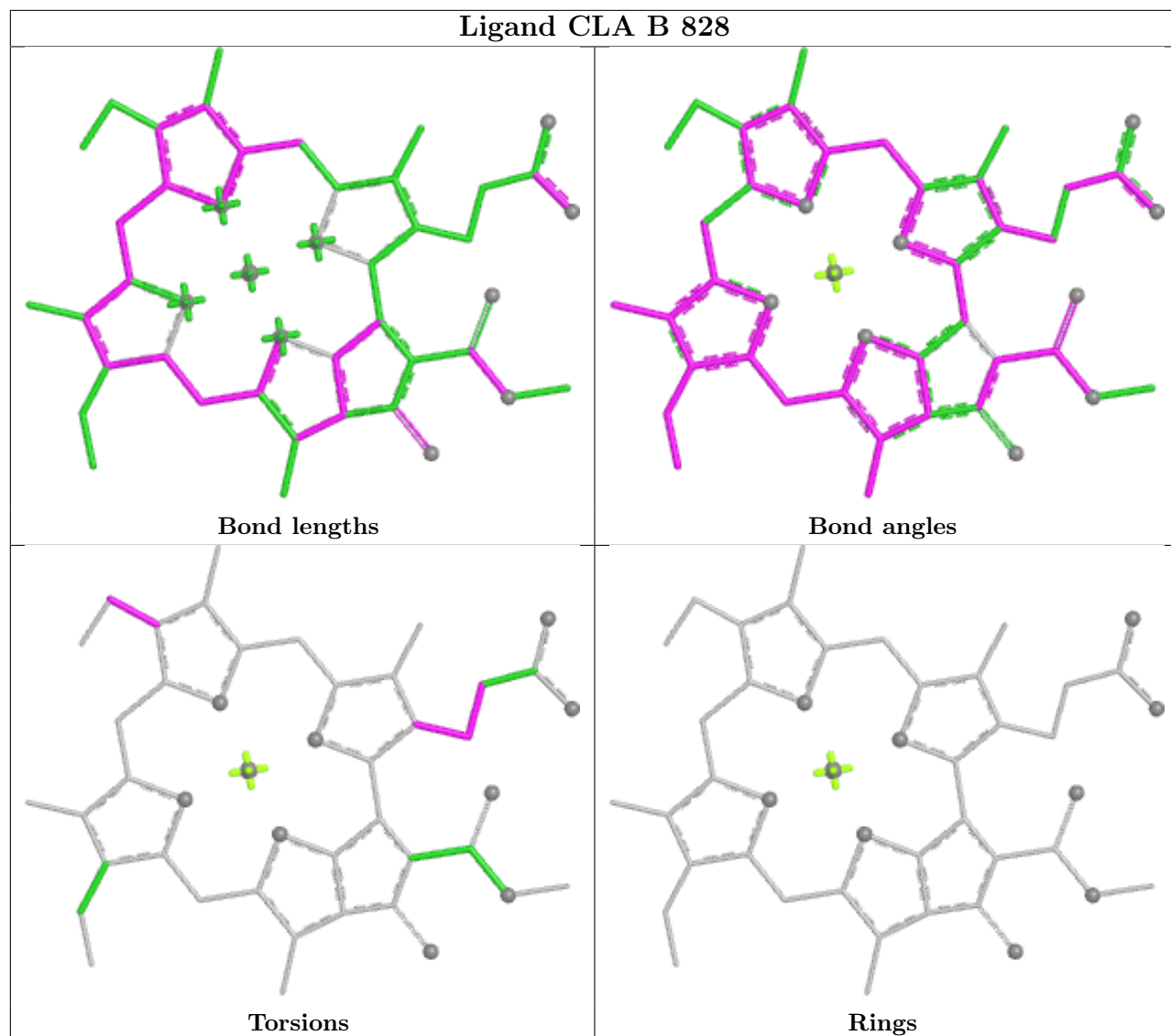
Ligand BCR J 102**Ligand CLA B 801****Ligand CLA B 808**



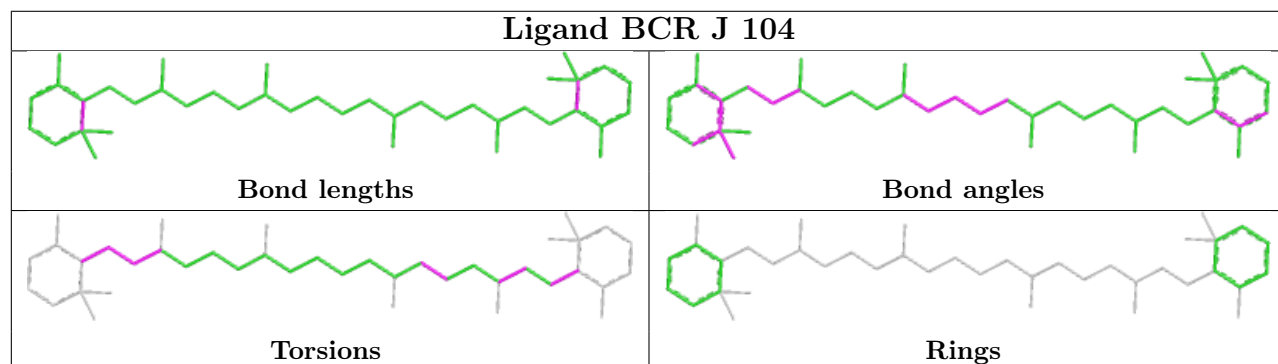
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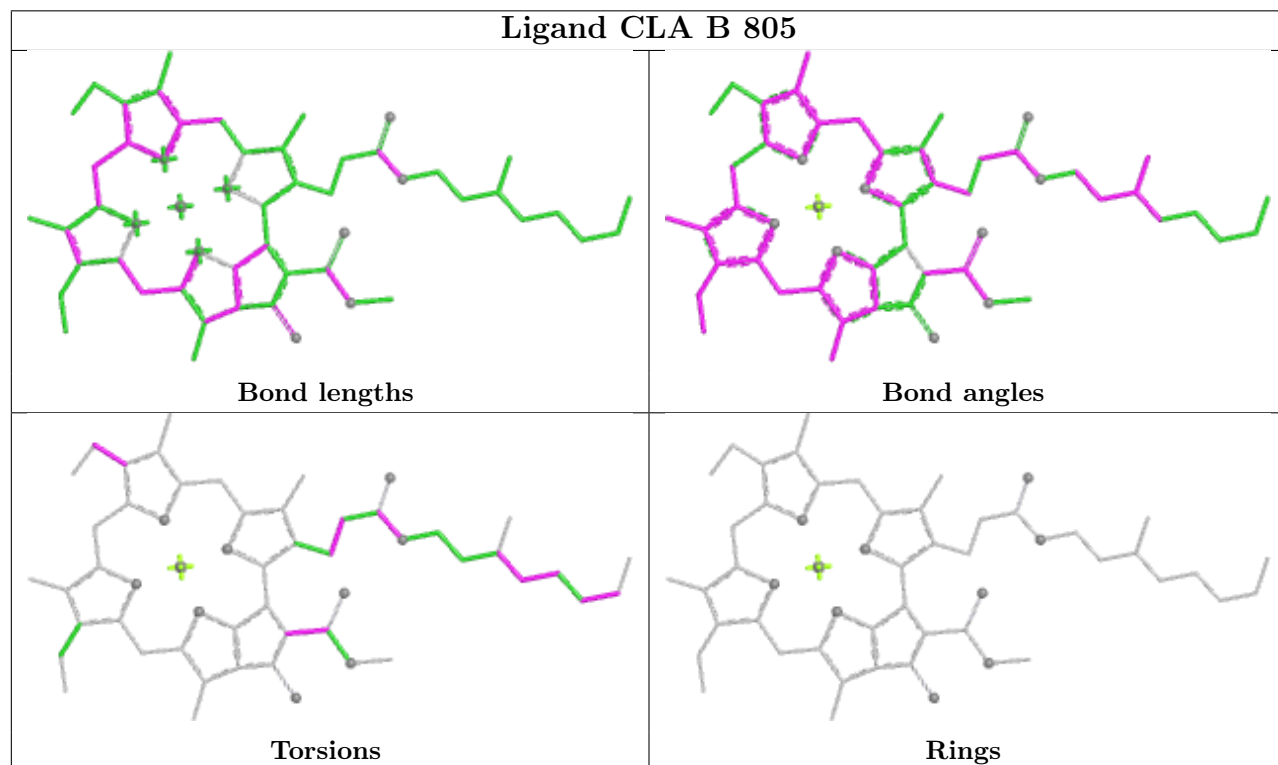
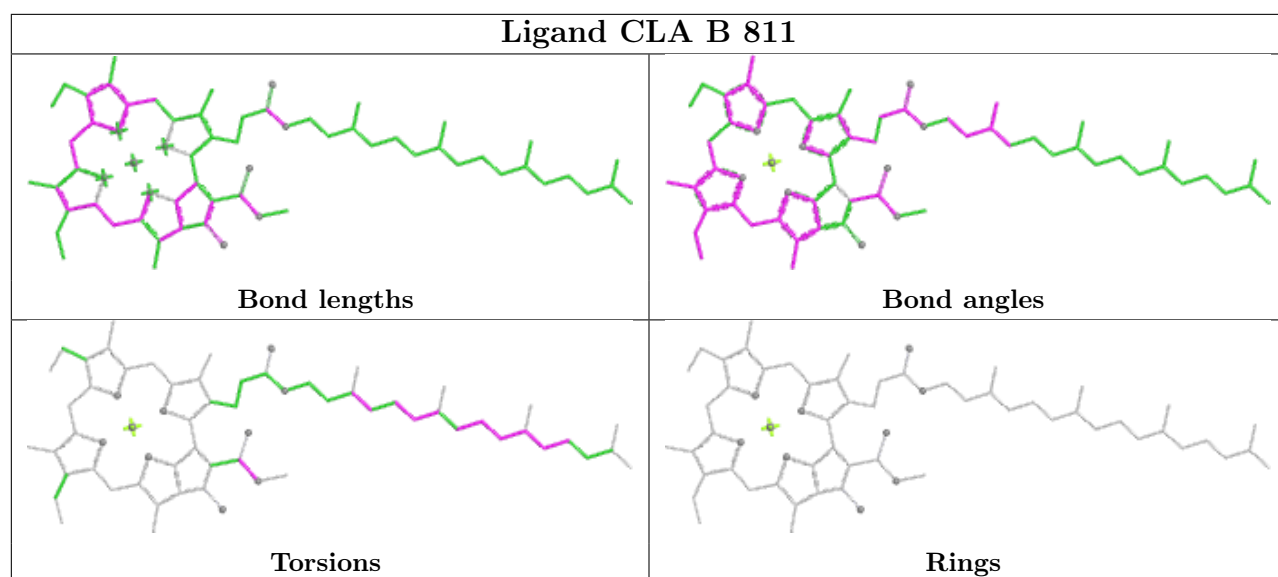


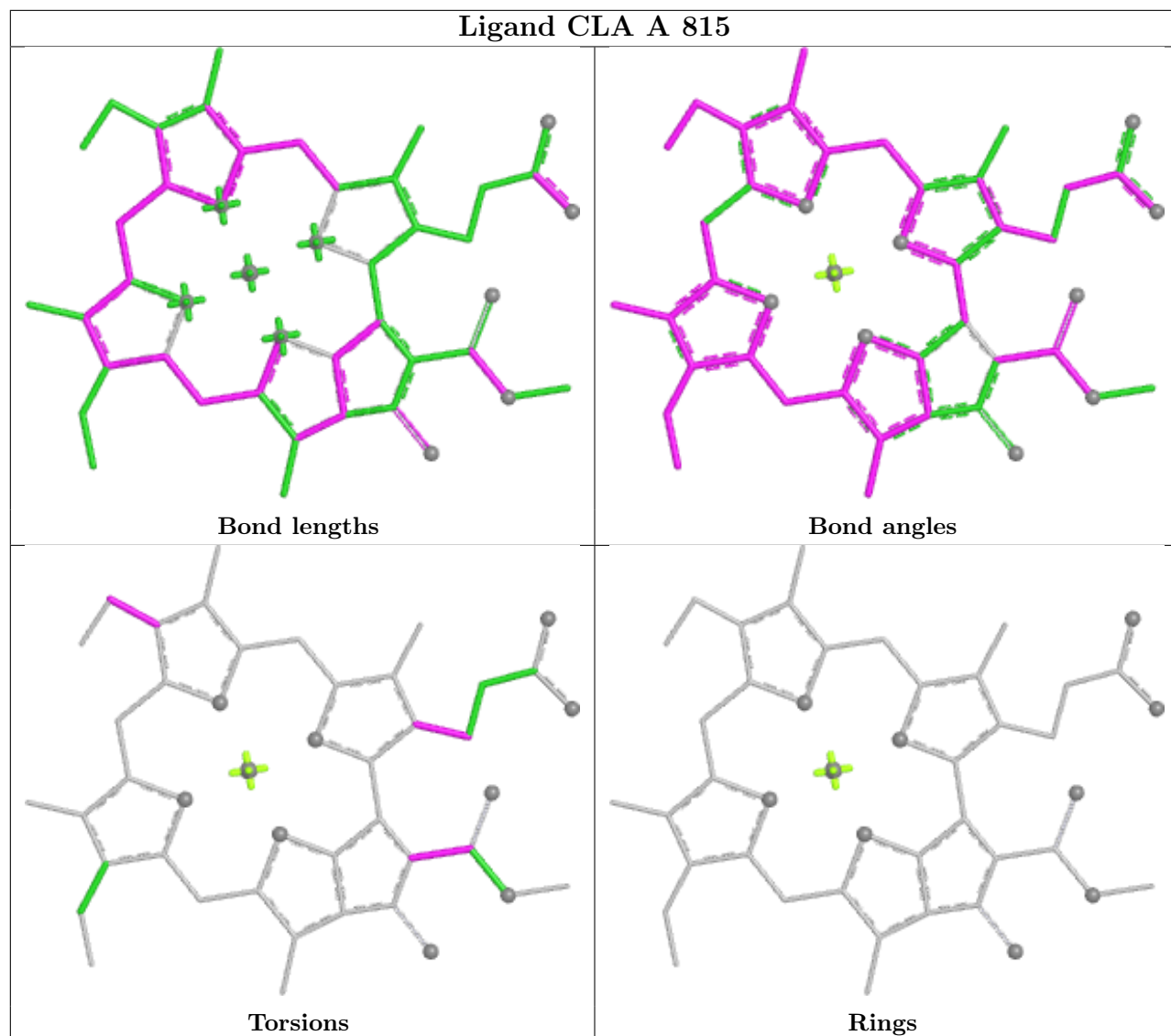
Ligand CLA B 828



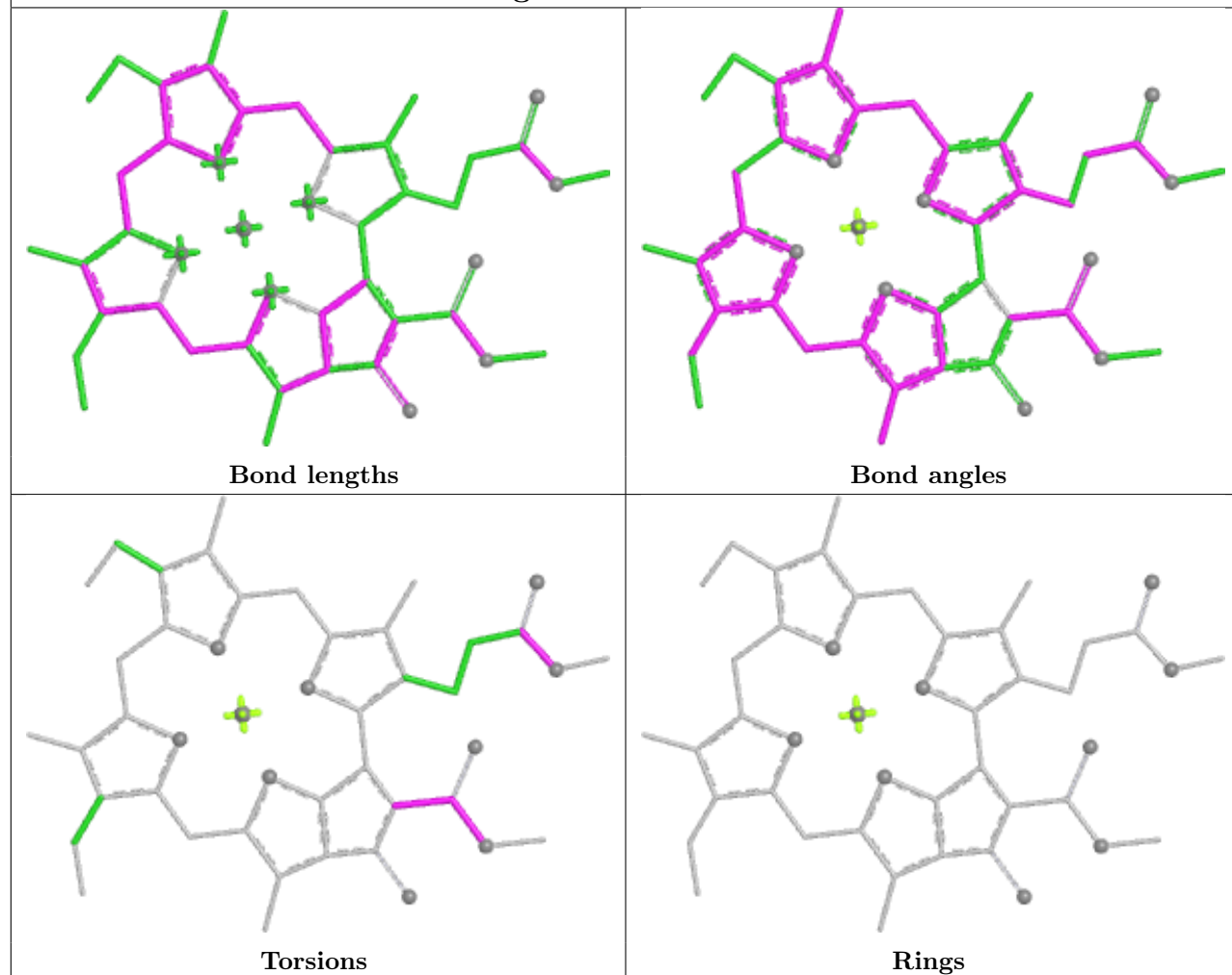
Ligand BCR J 104

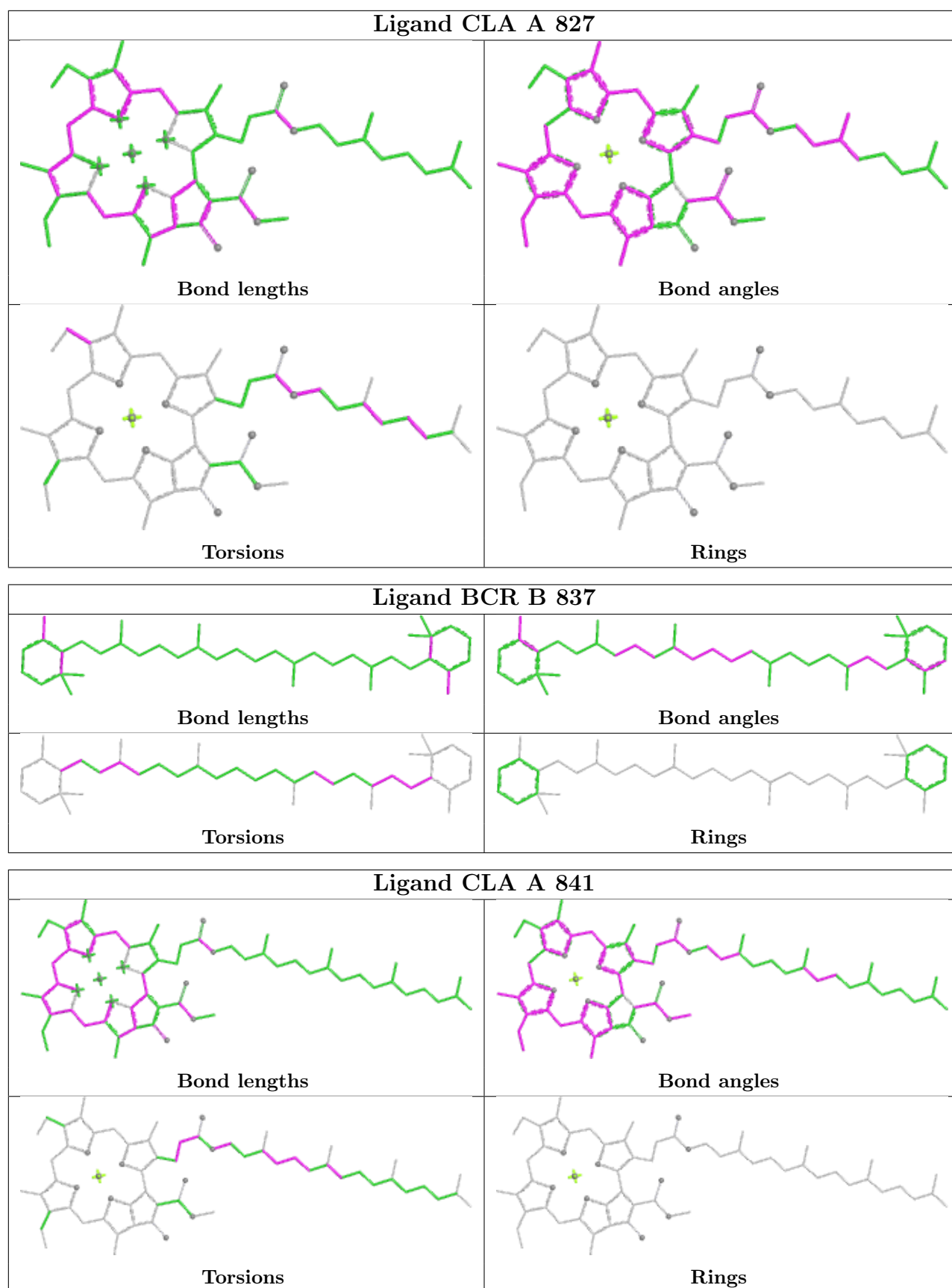


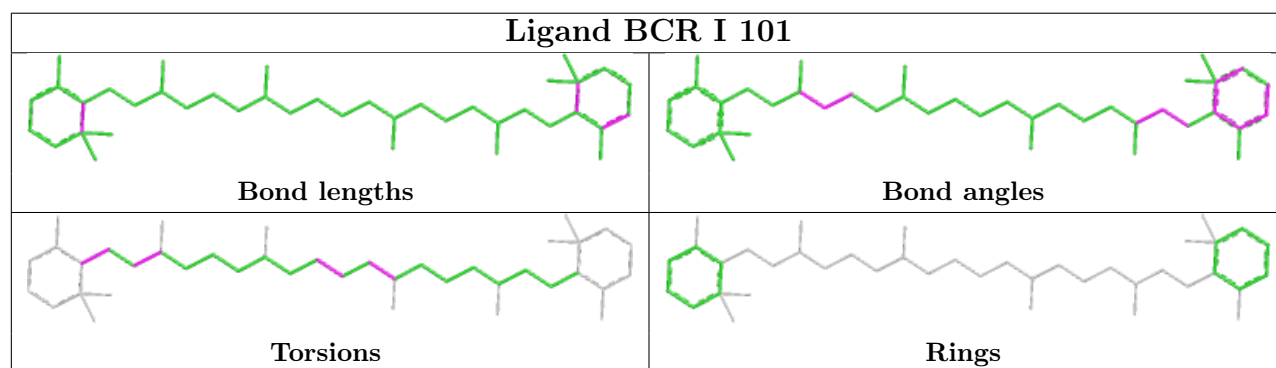
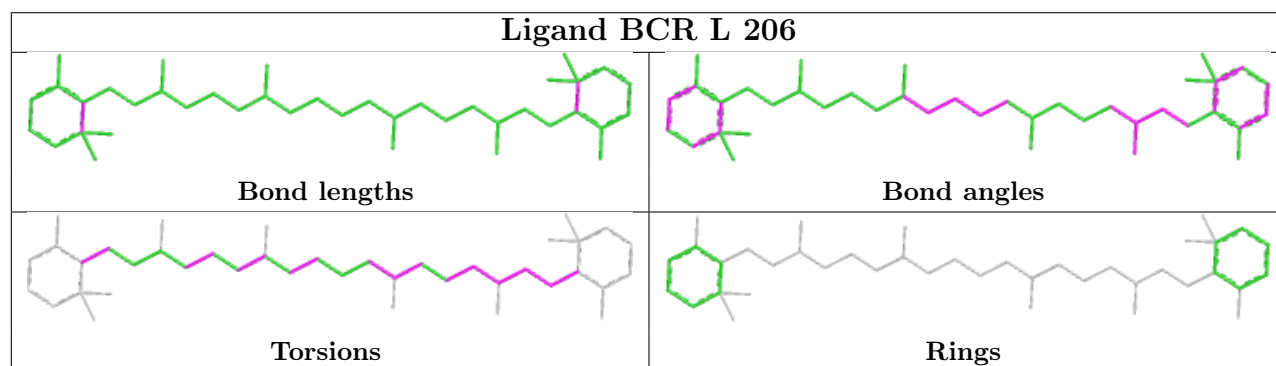
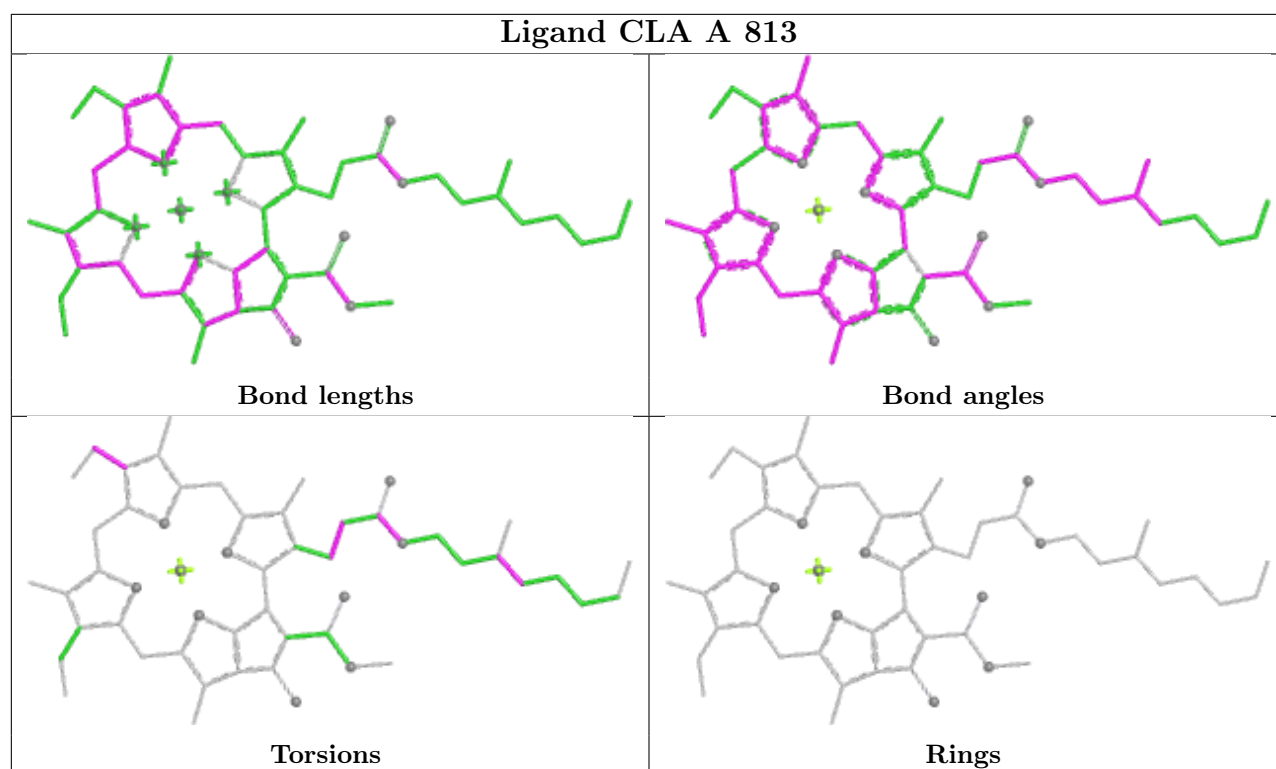




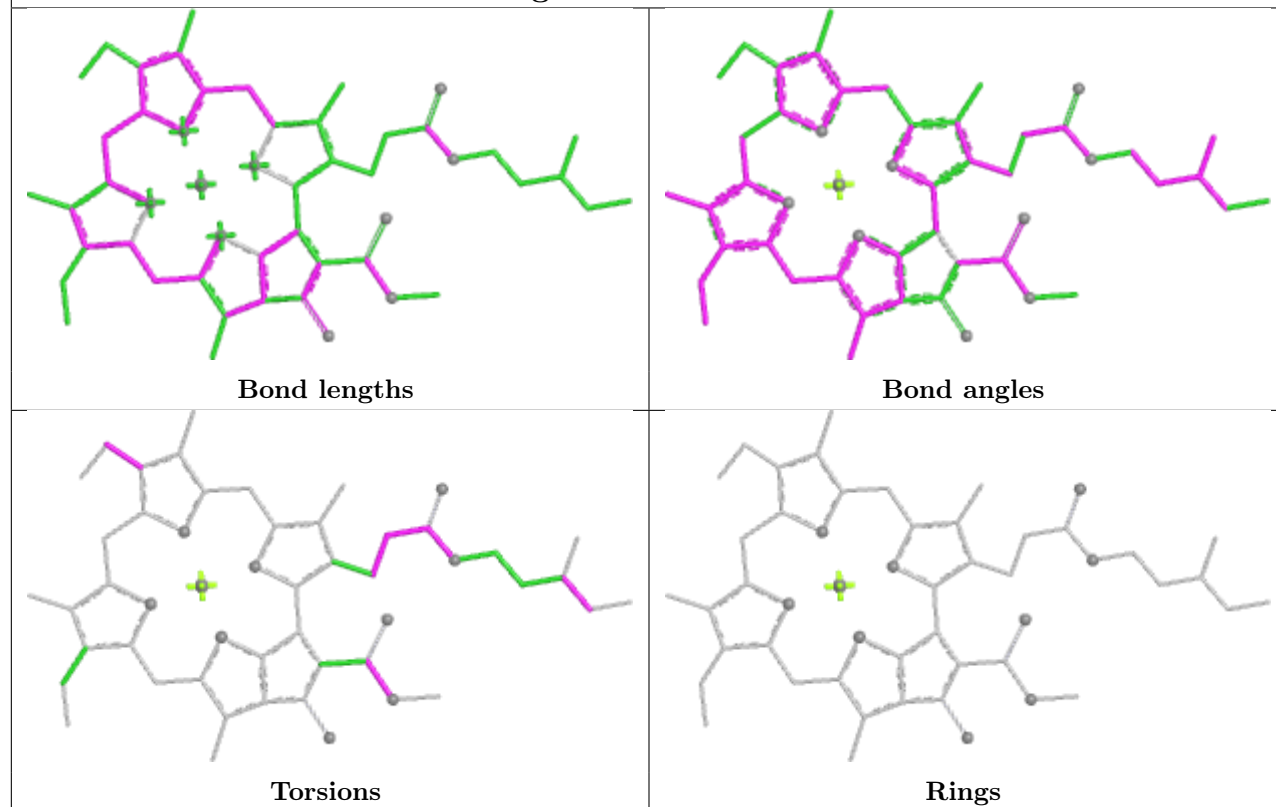
Ligand CLA B 819



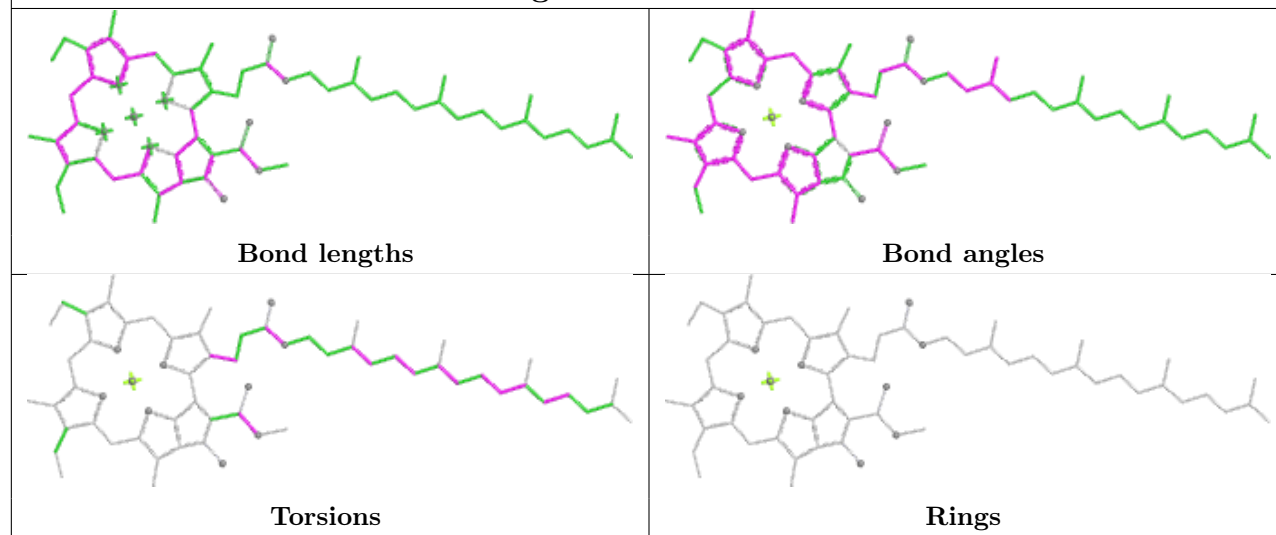


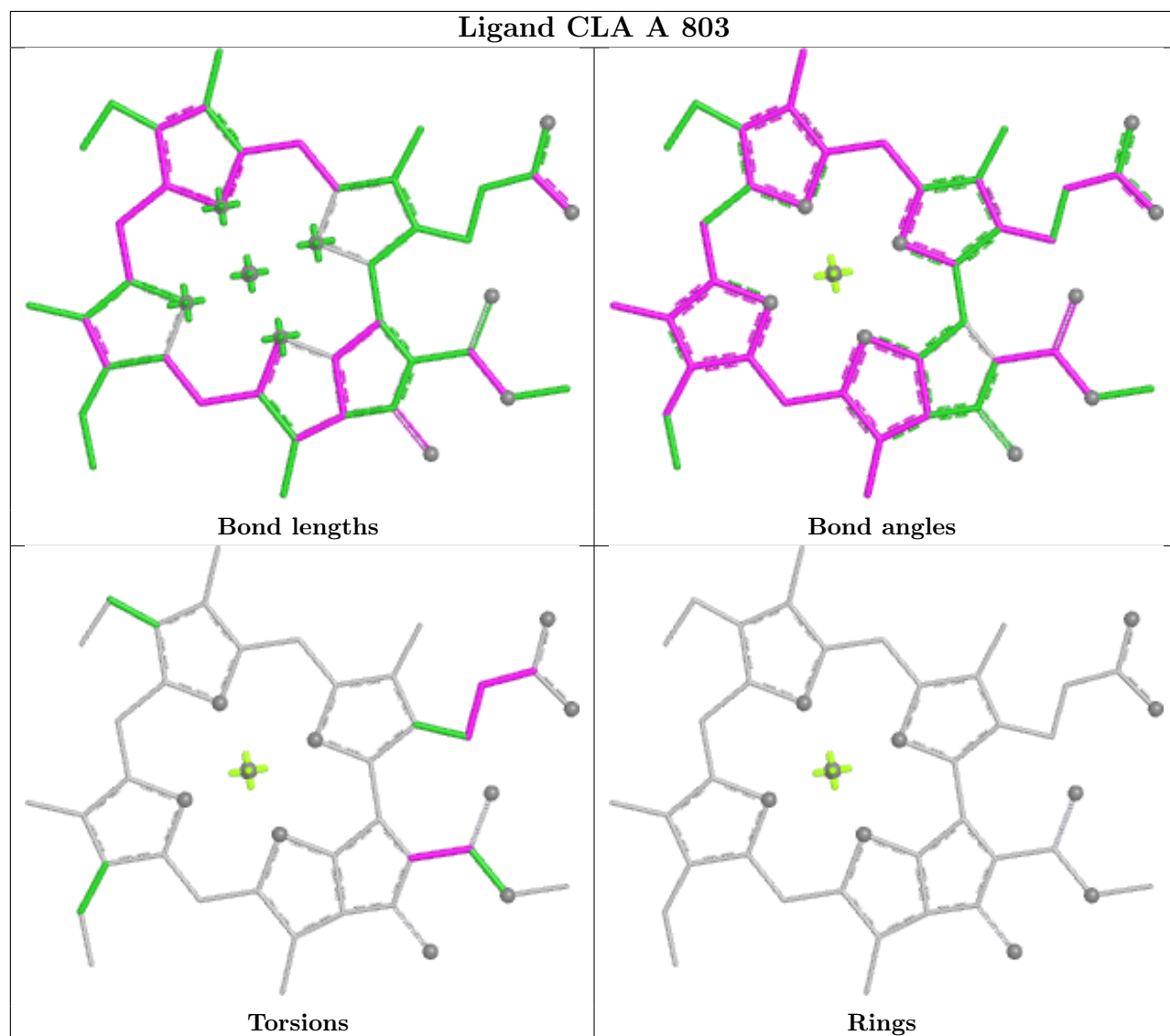
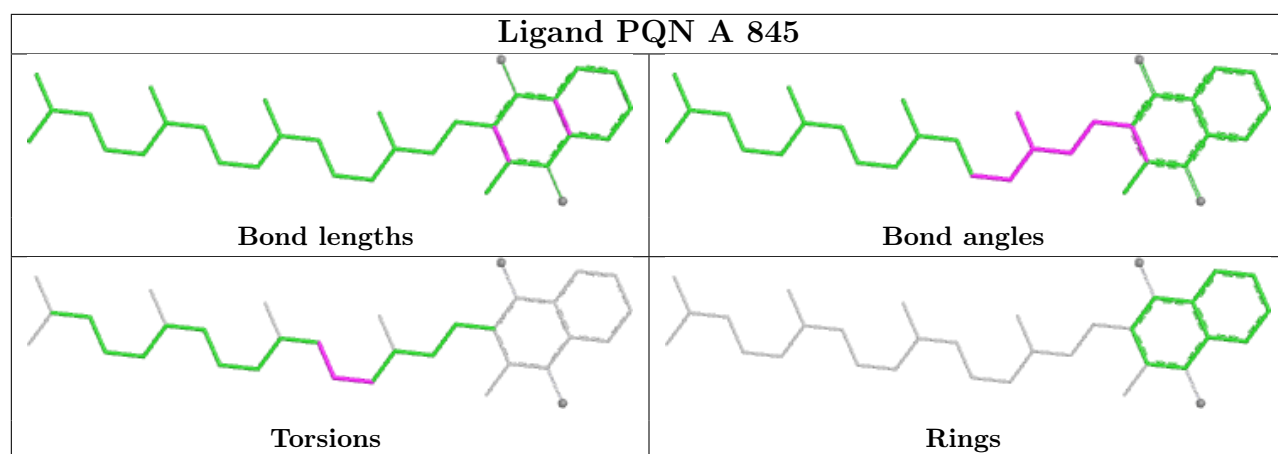


Ligand CLA A 824

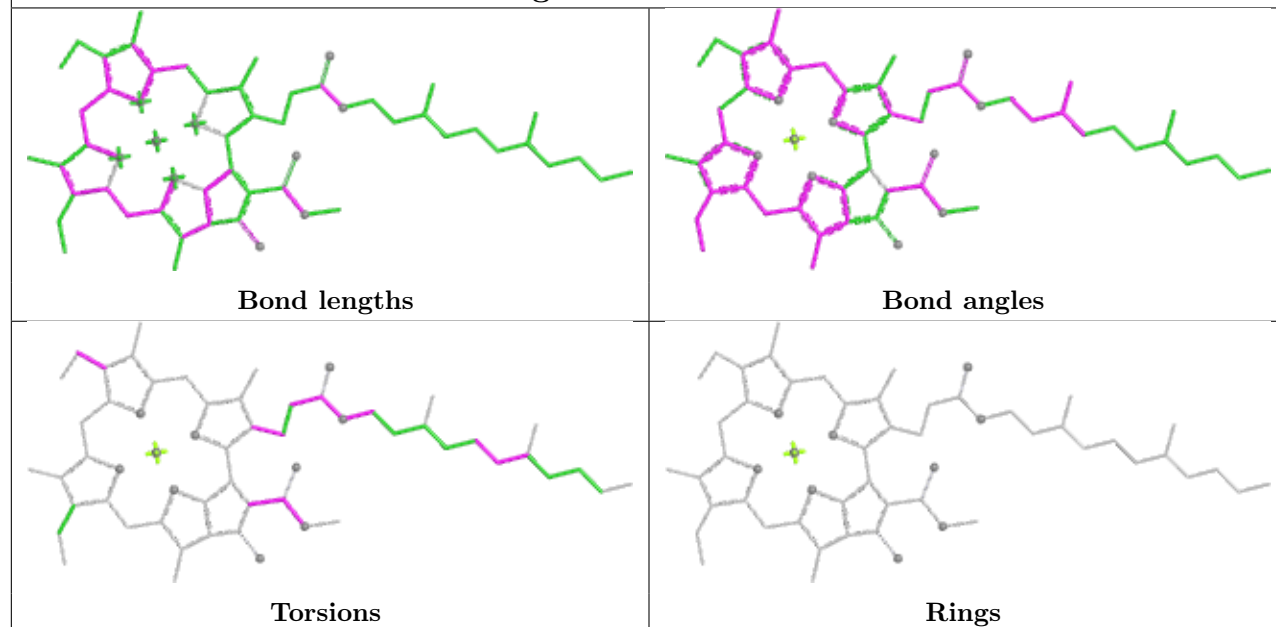


Ligand CLA A 829

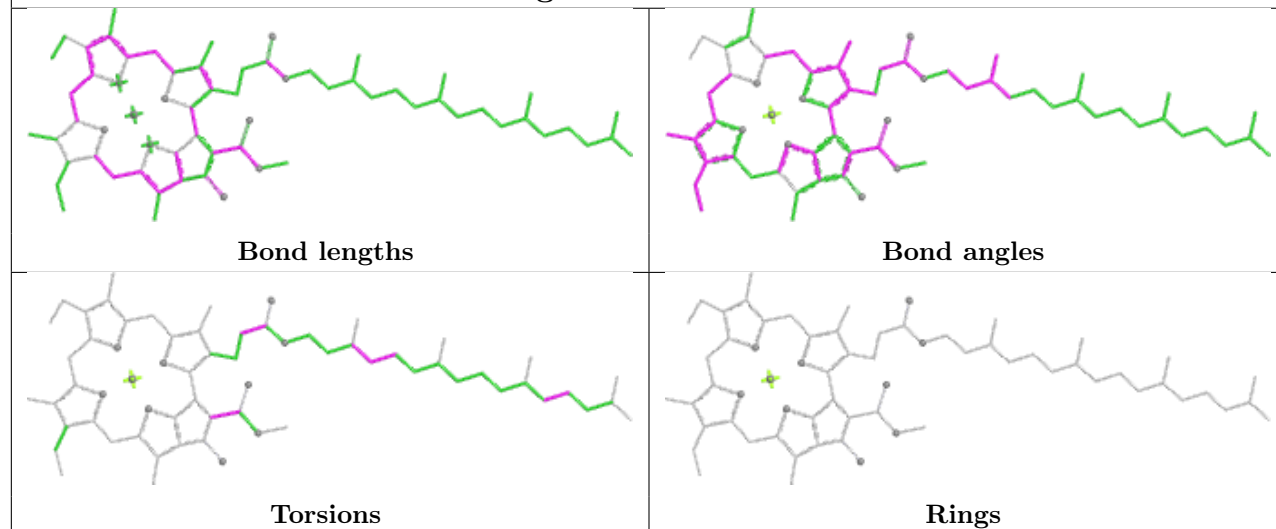




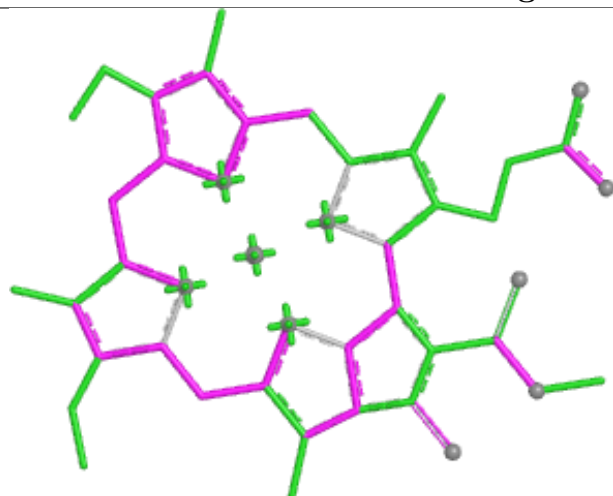
Ligand CLA B 826



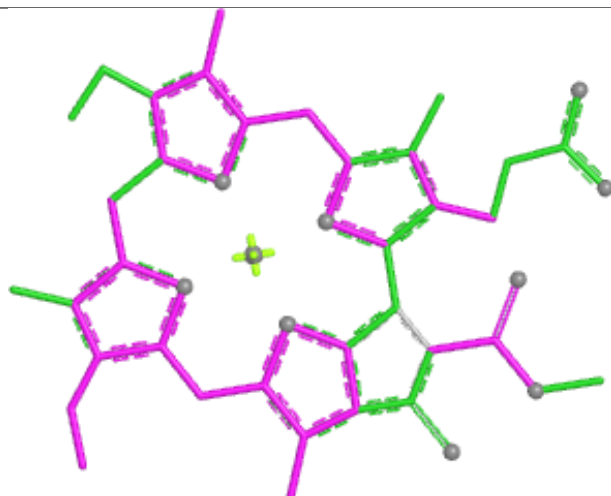
Ligand CL0 A 801



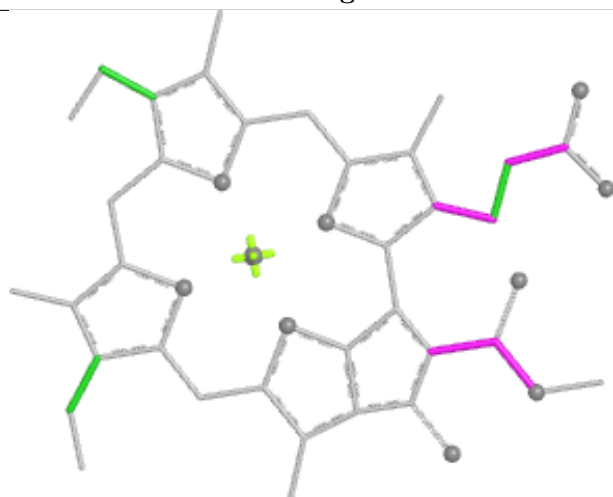
Ligand CLA J 101



Bond lengths



Bond angles

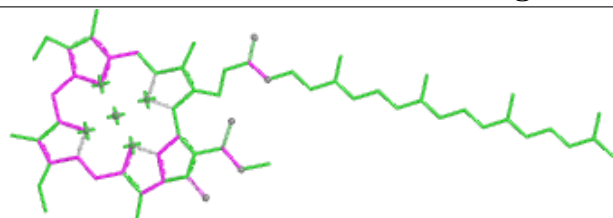


Torsions

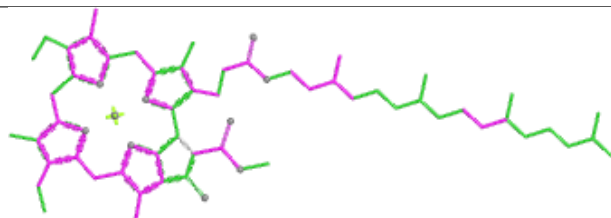


Rings

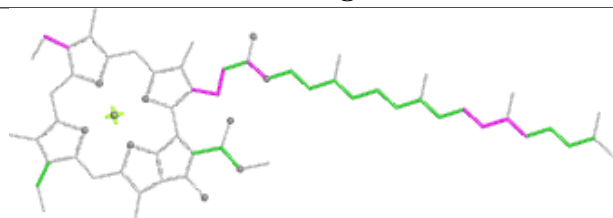
Ligand CLA A 812



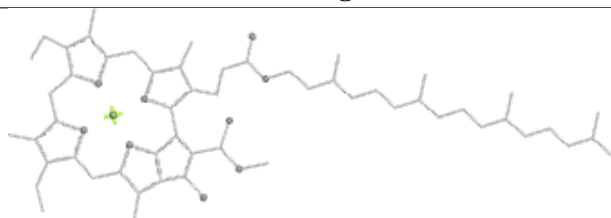
Bond lengths



Bond angles

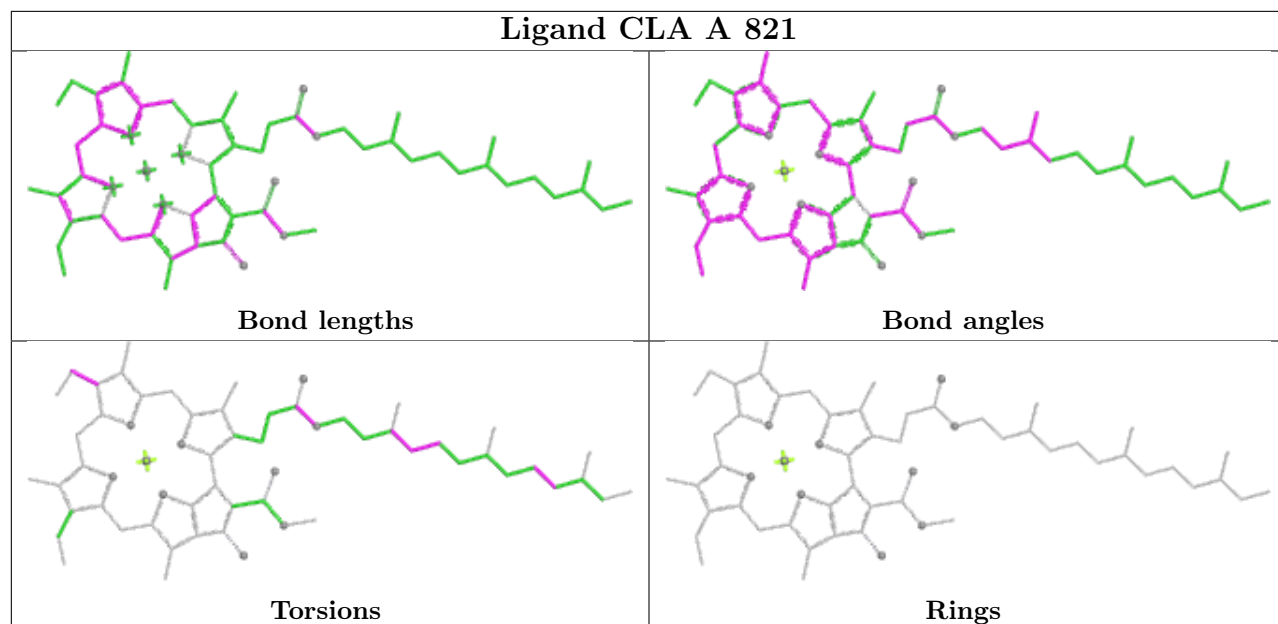


Torsions

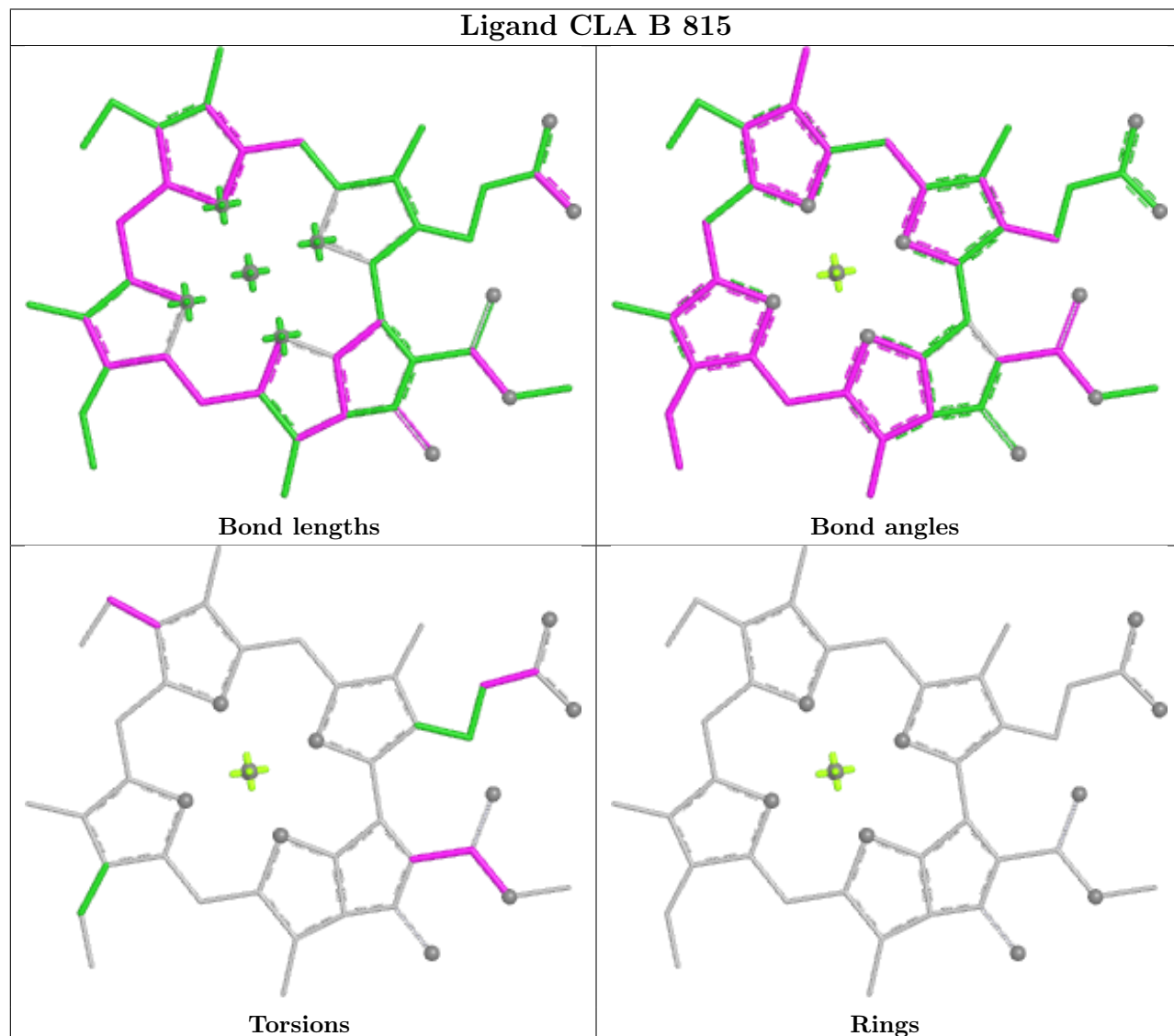


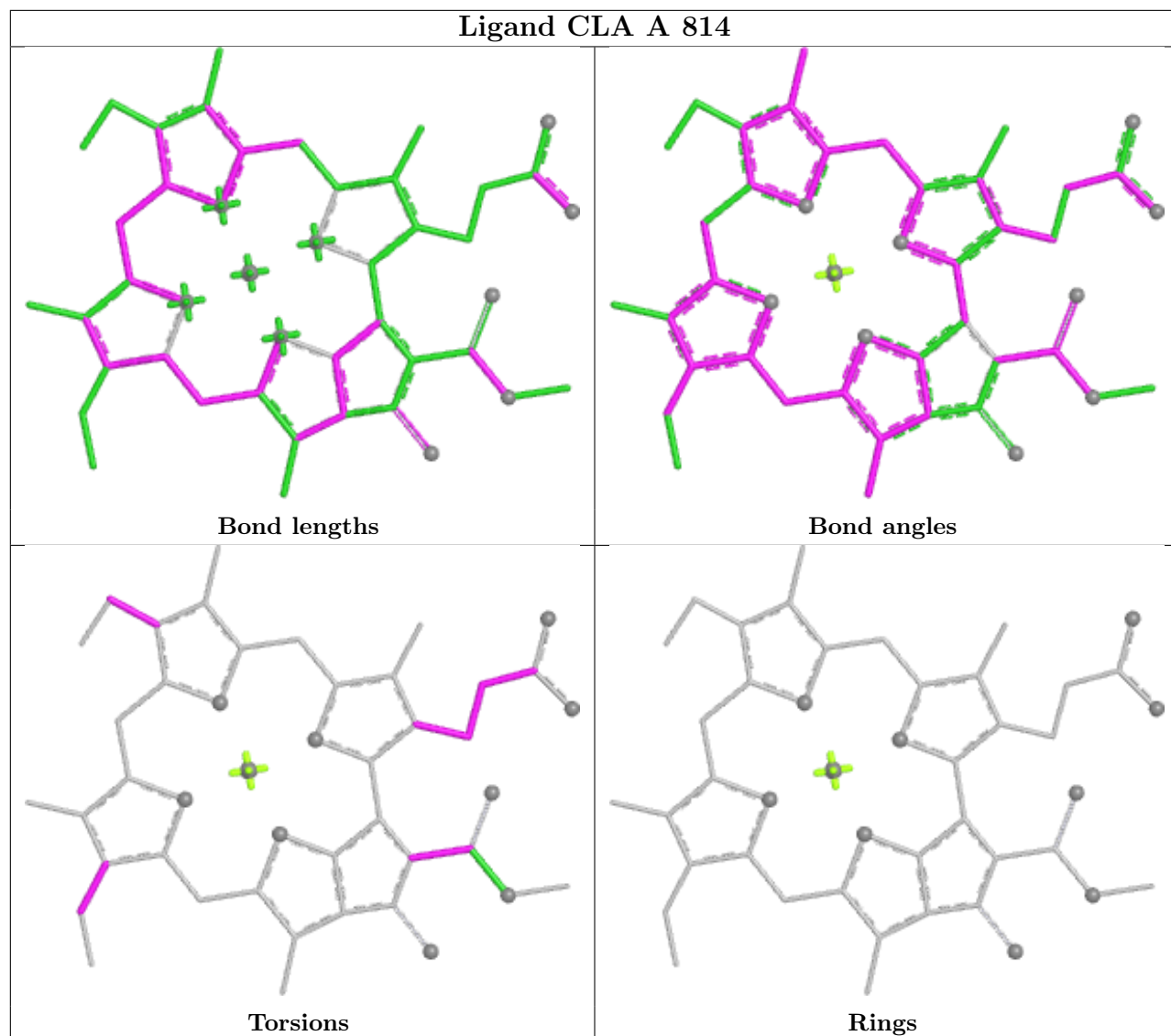
Rings

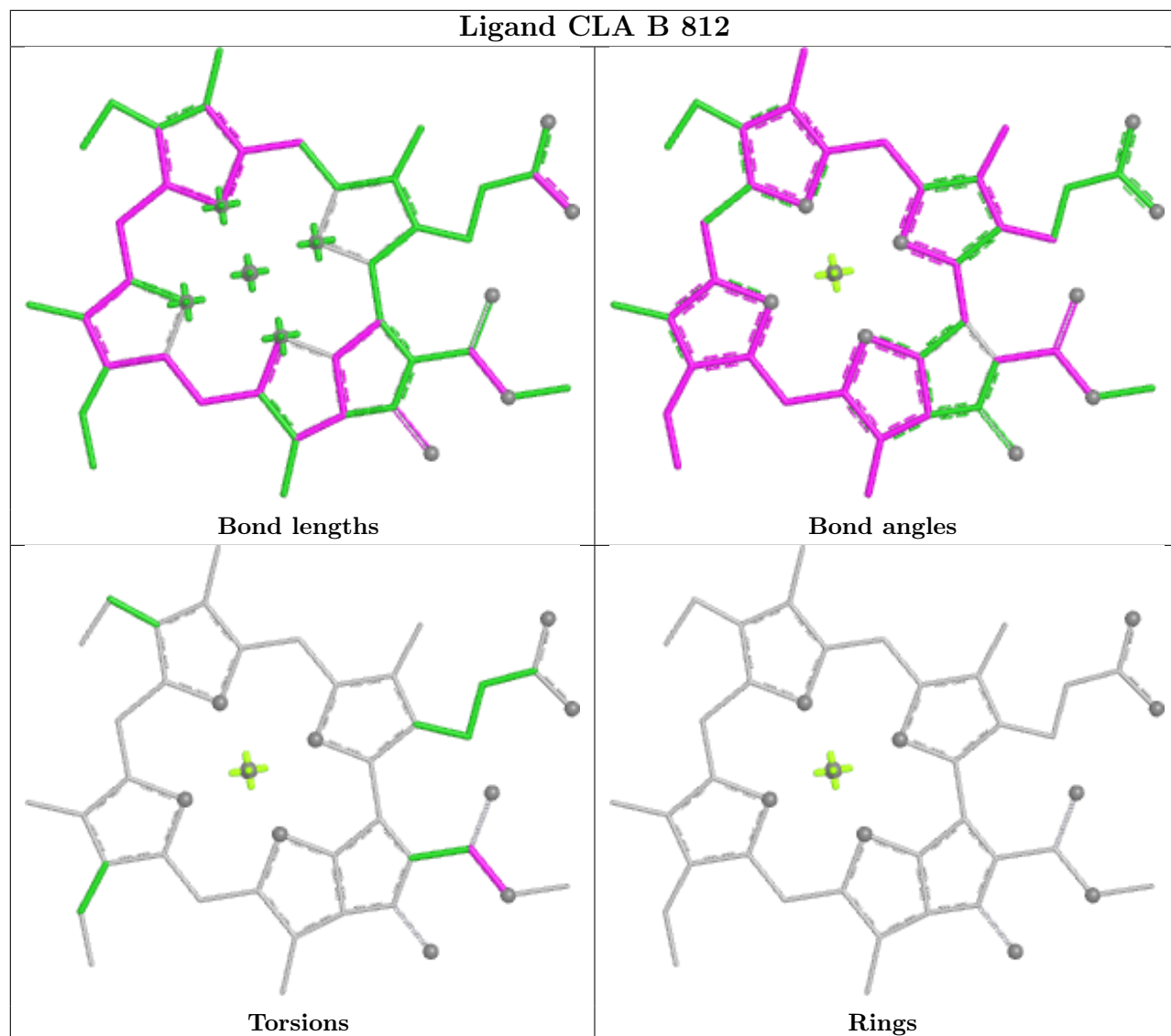
Ligand CLA A 821



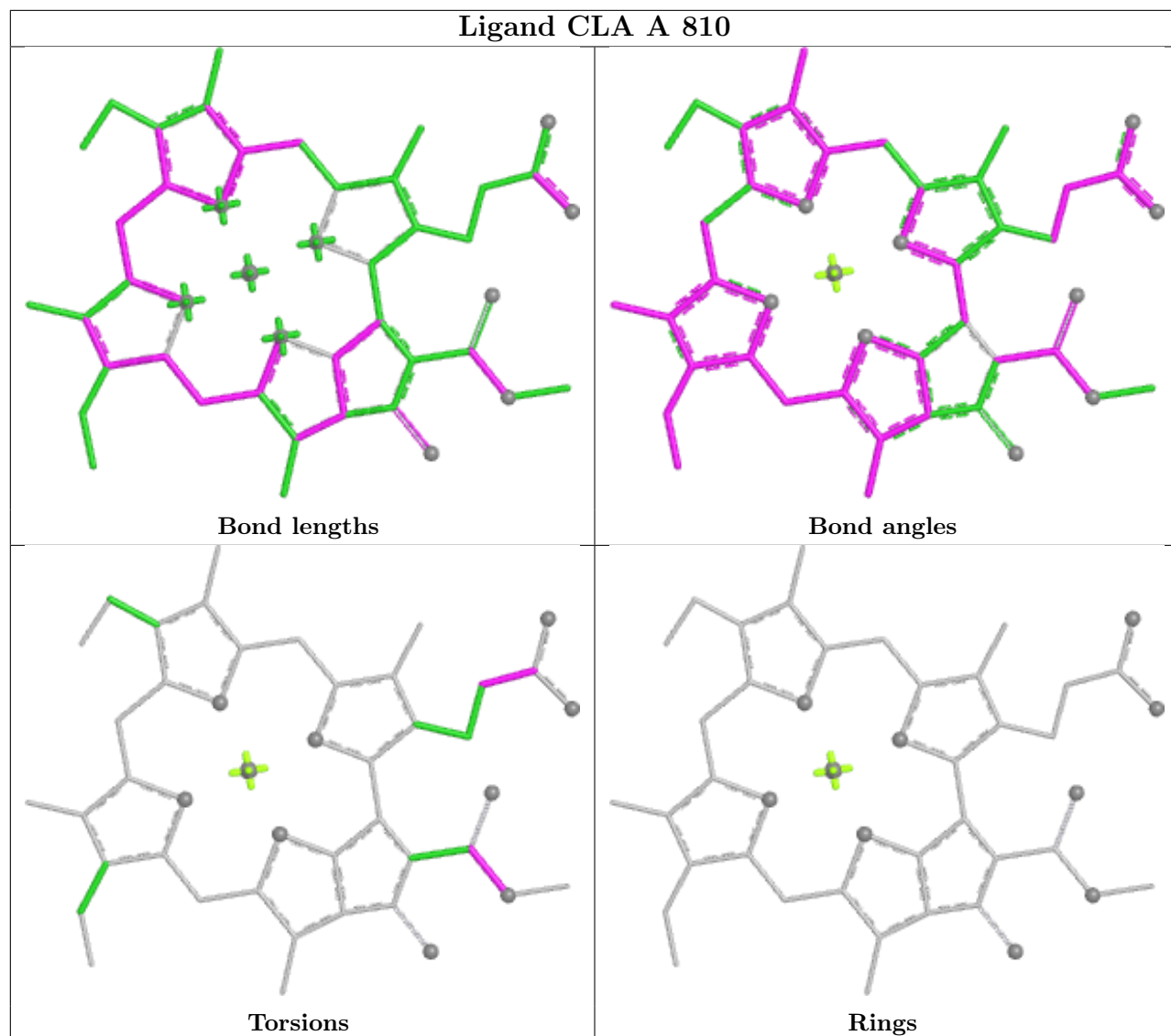
Ligand CLA B 815



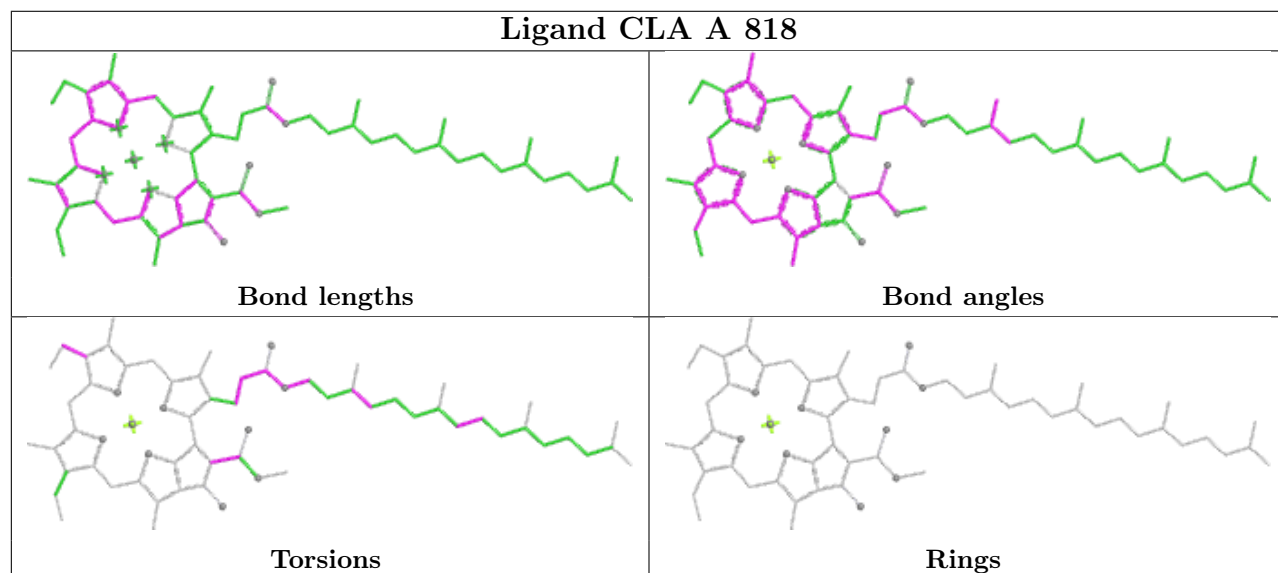




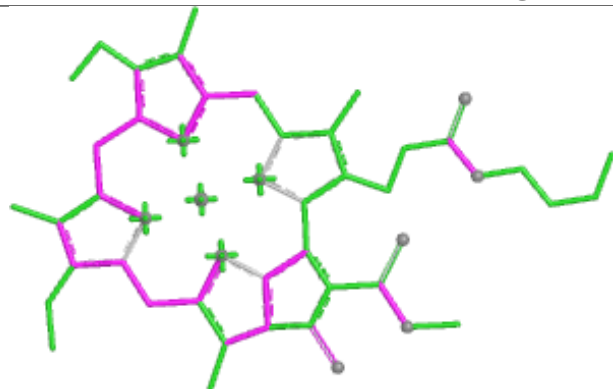
Ligand CLA A 810



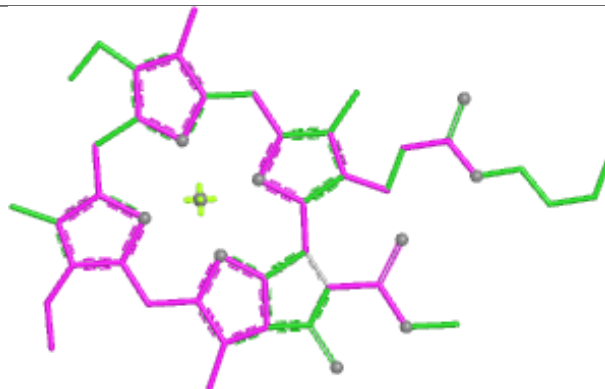
Ligand CLA A 818



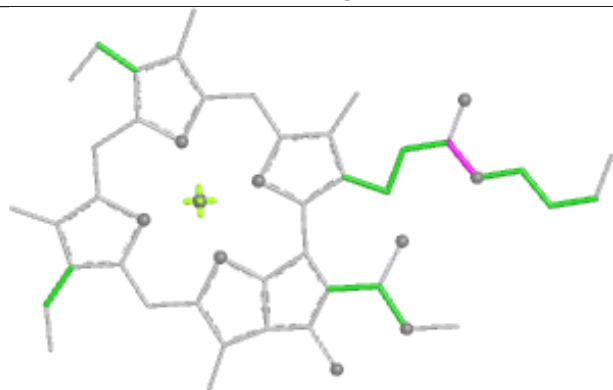
Ligand CLA A 817



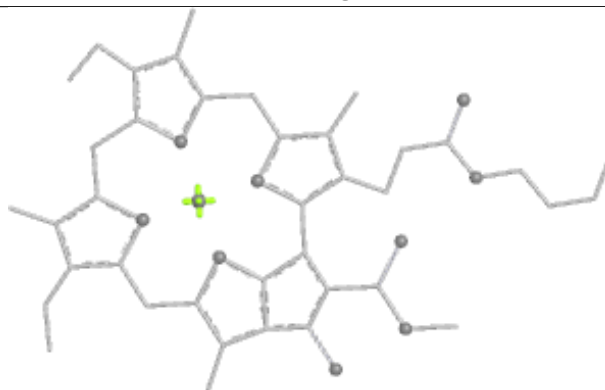
Bond lengths



Bond angles

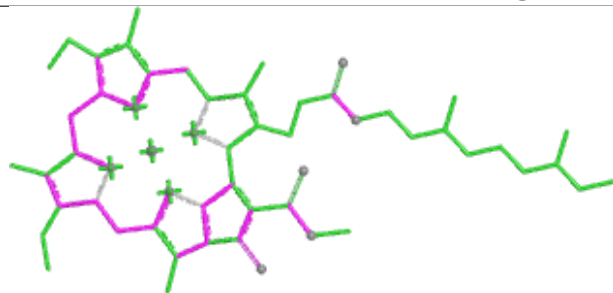


Torsions

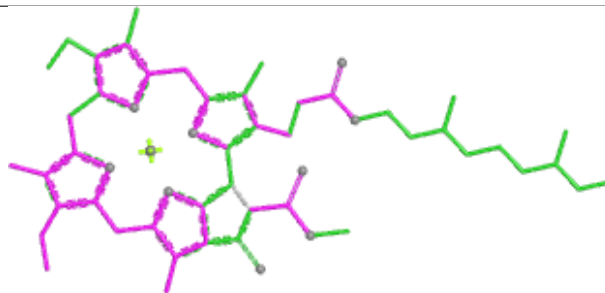


Rings

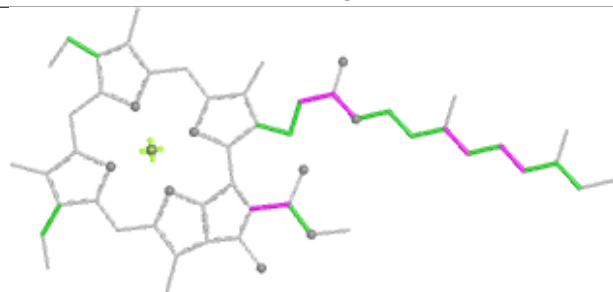
Ligand CLA A 839



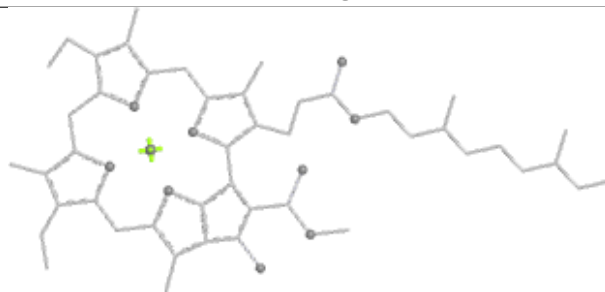
Bond lengths



Bond angles

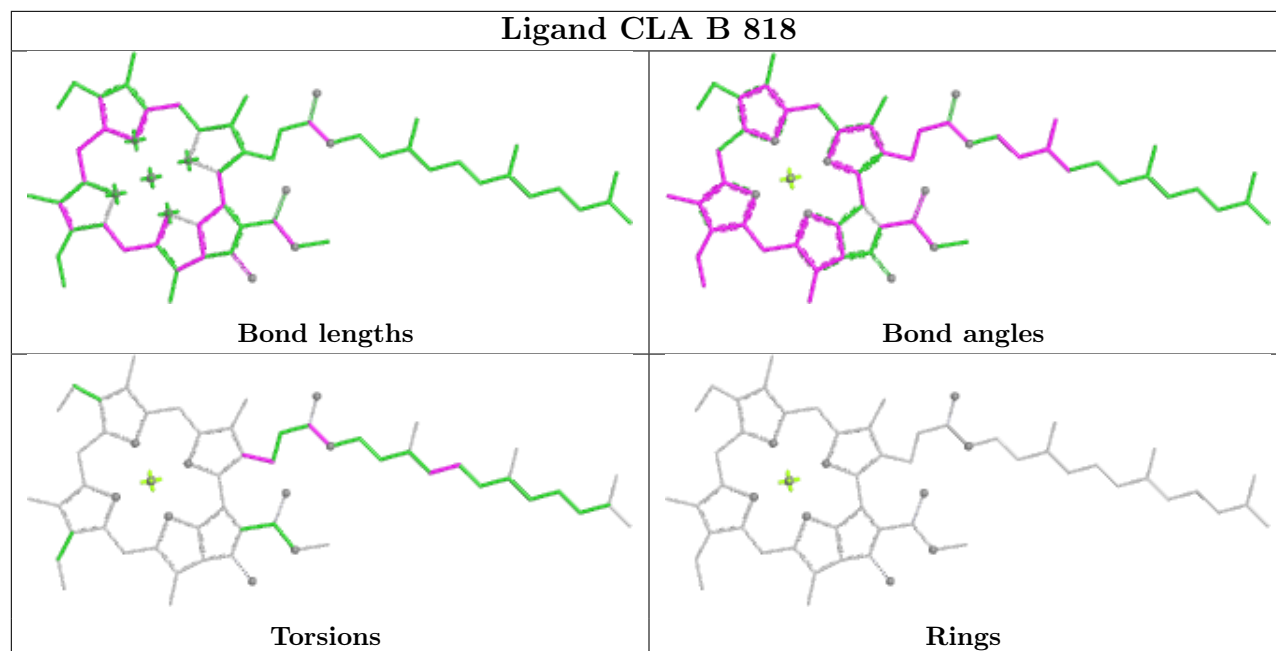


Torsions

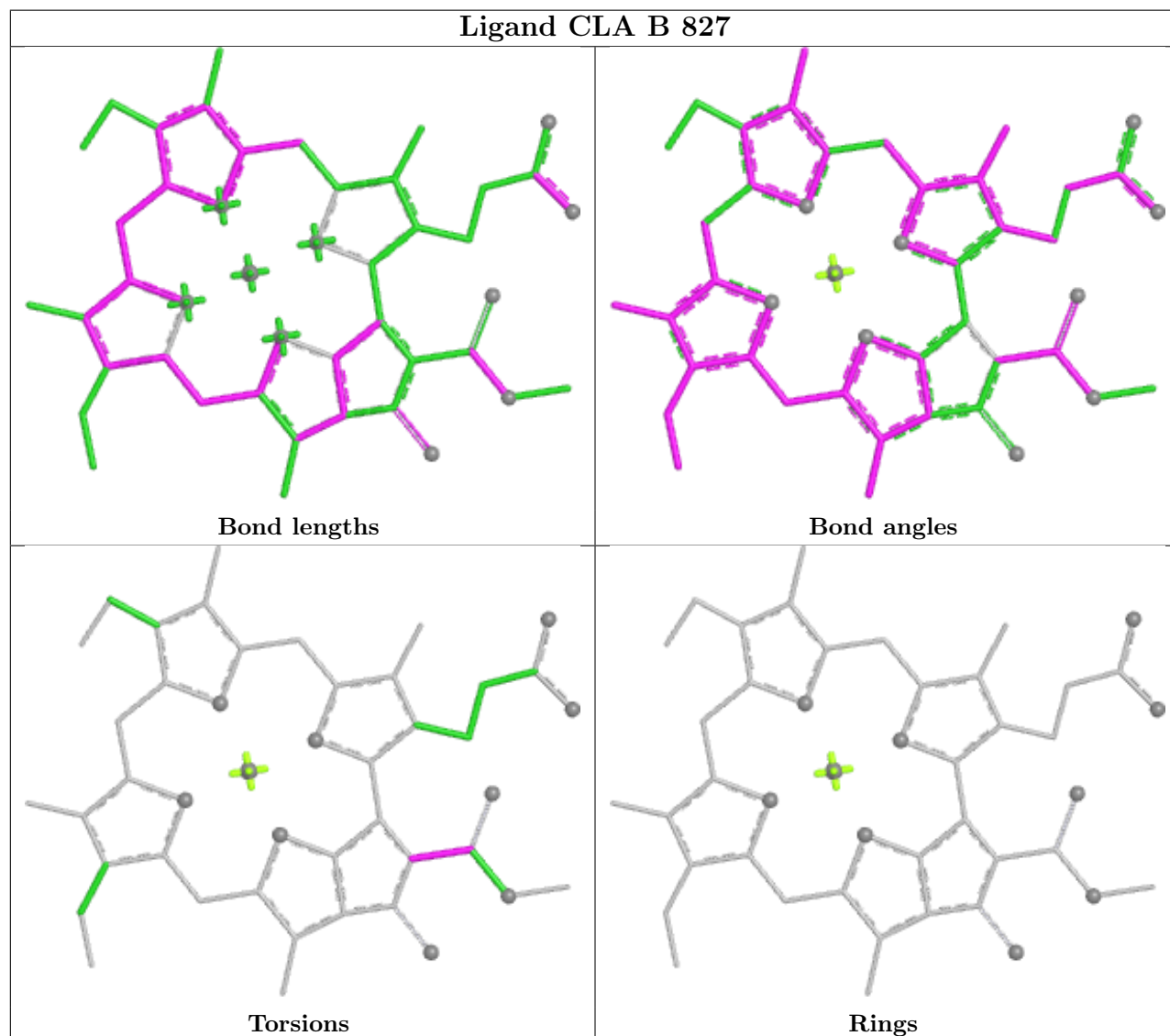


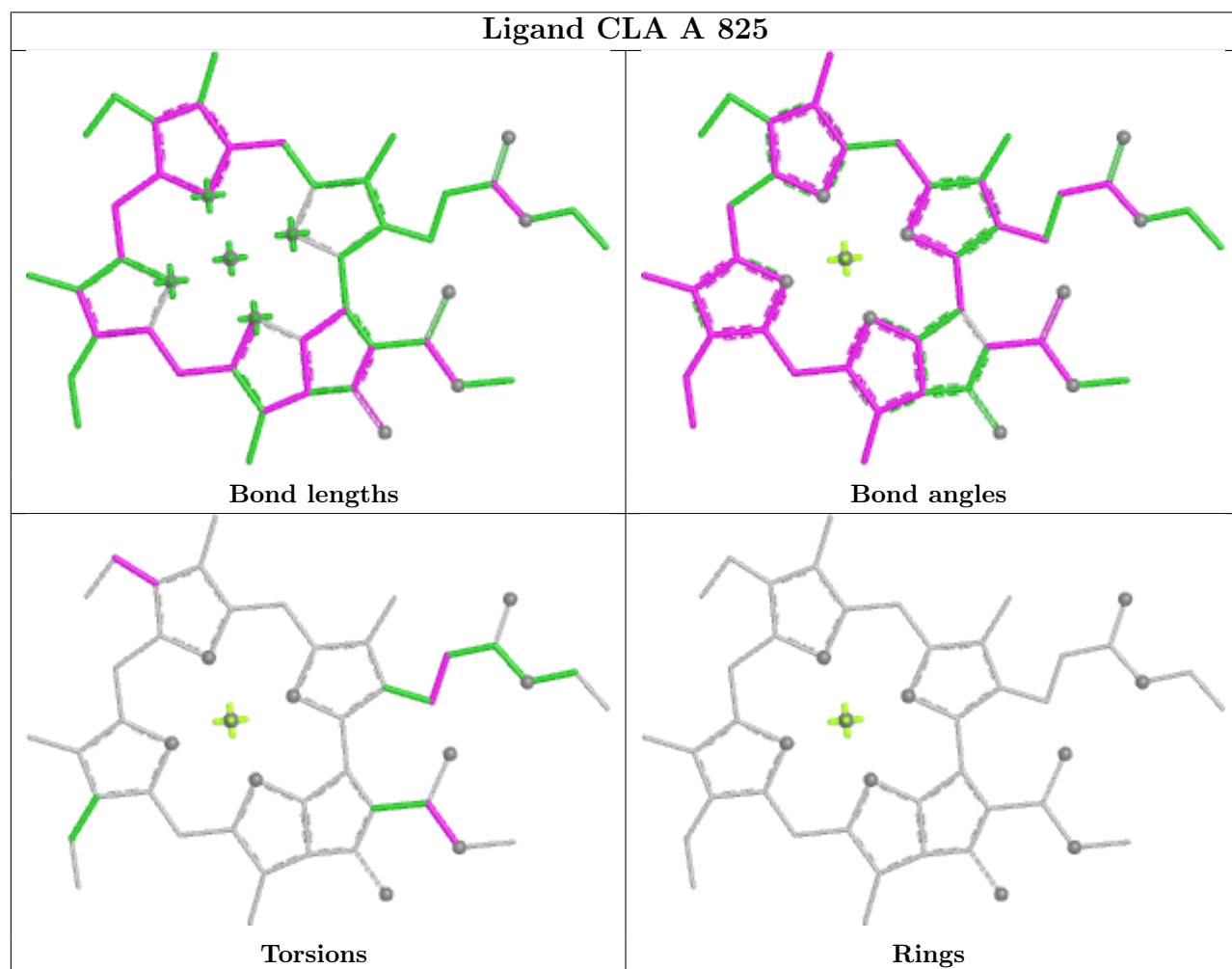
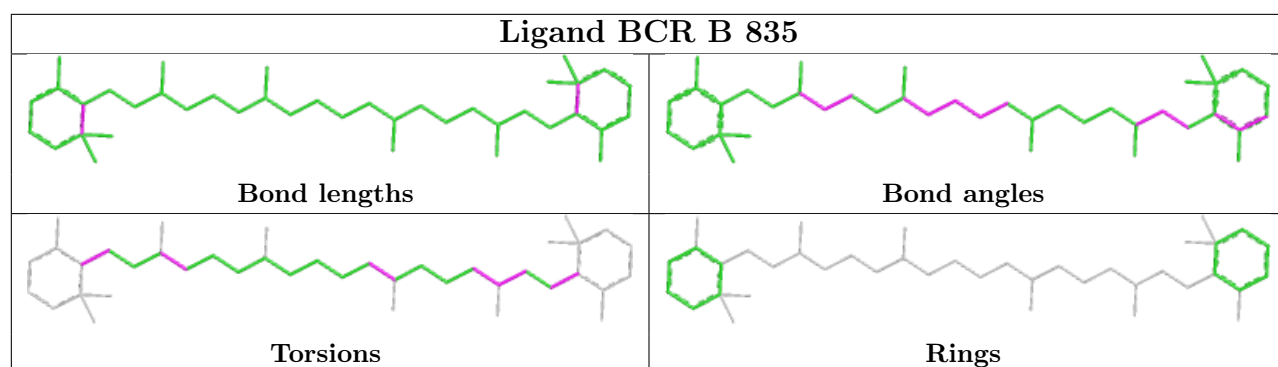
Rings

Ligand CLA B 818

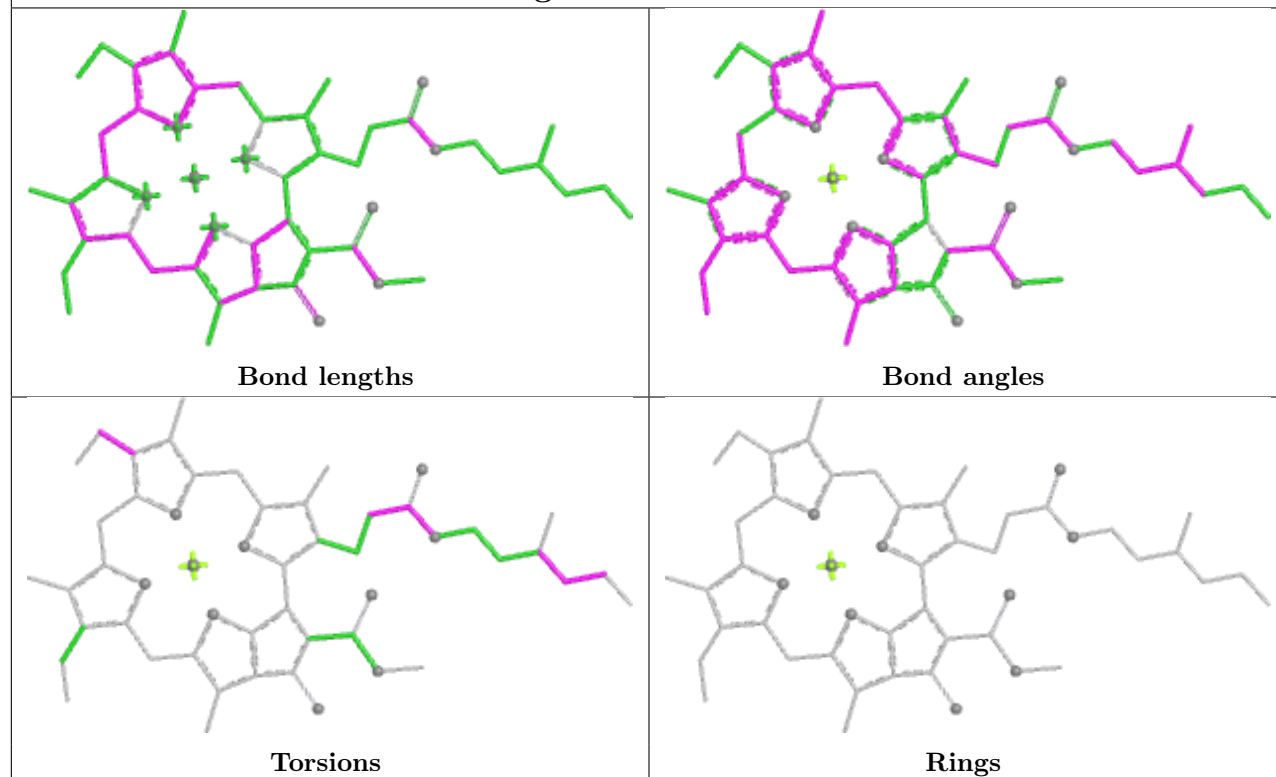


Ligand CLA B 827

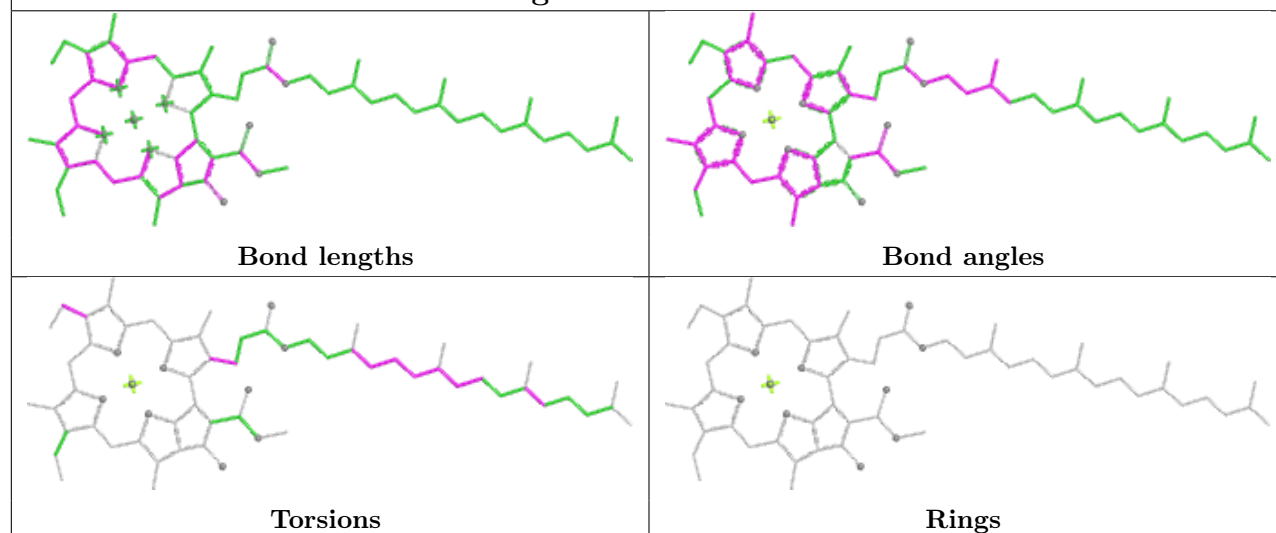




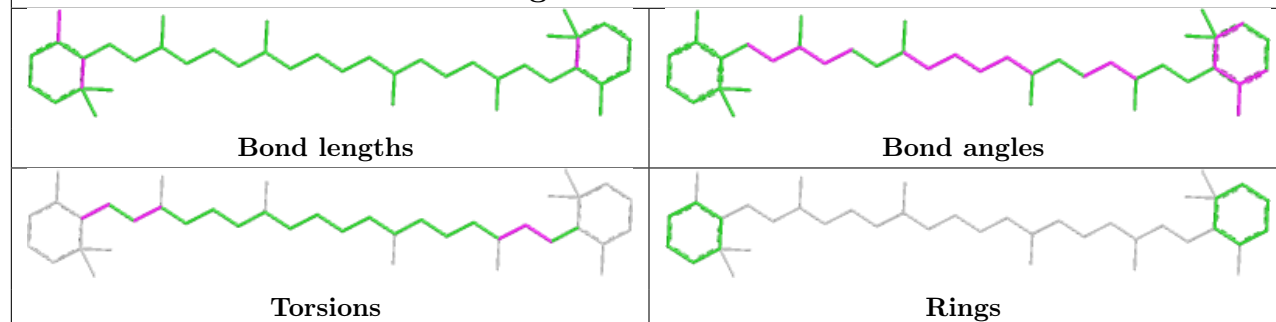
Ligand CLA L 204

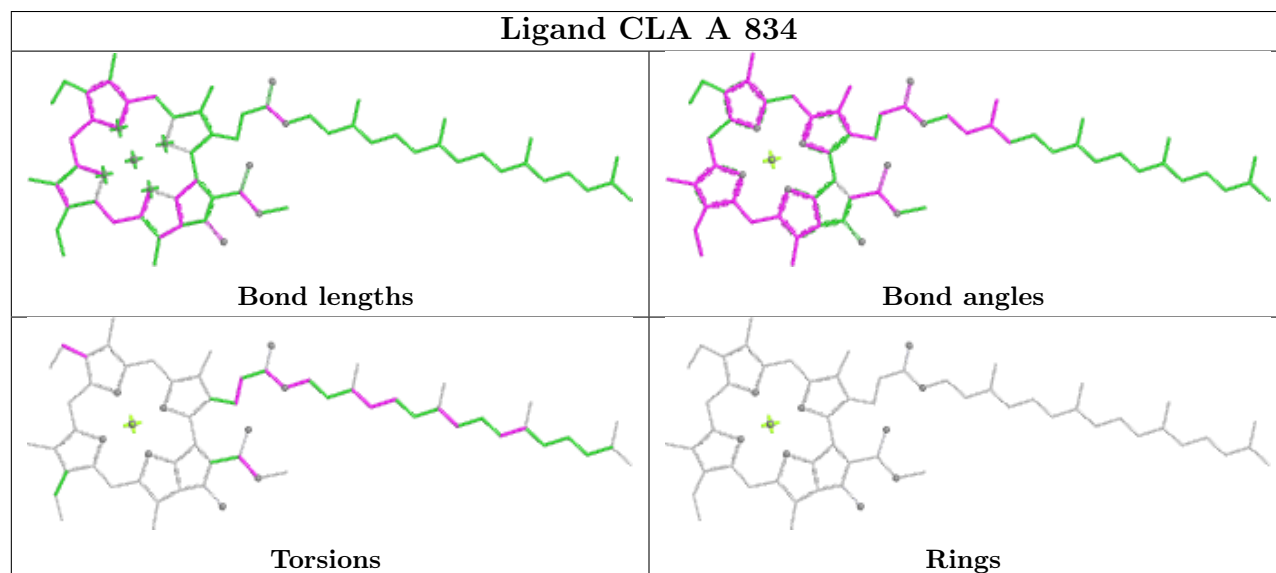
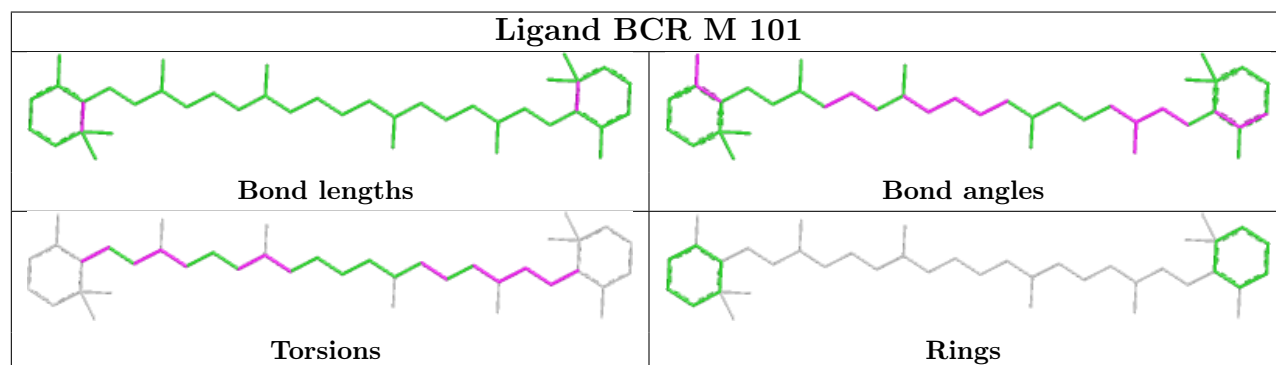
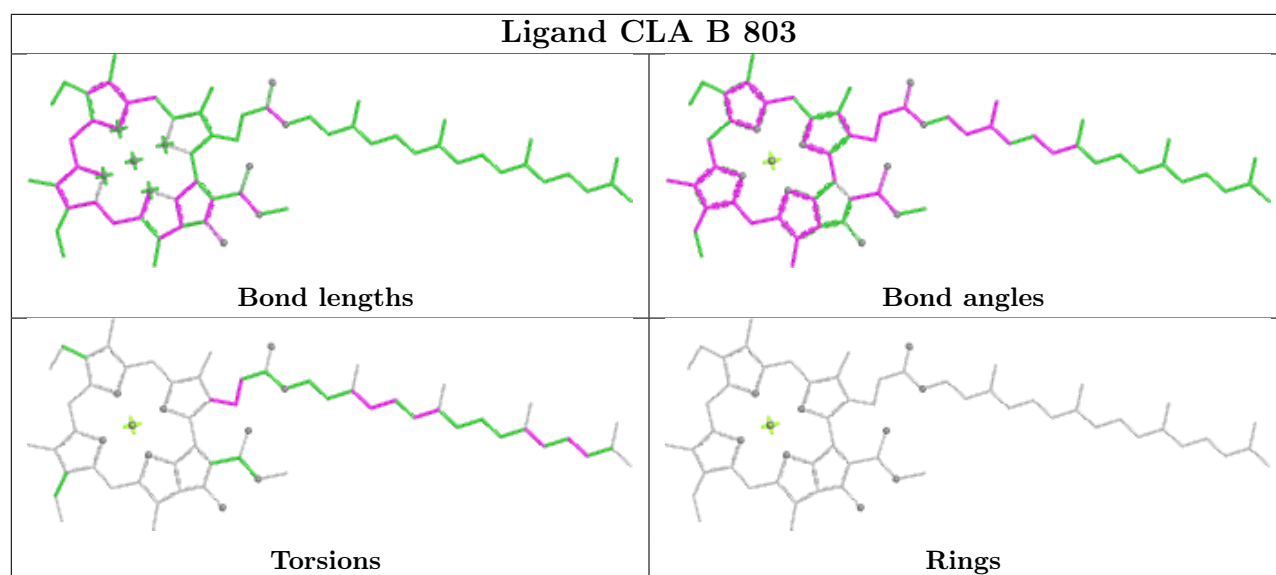


Ligand CLA A 822

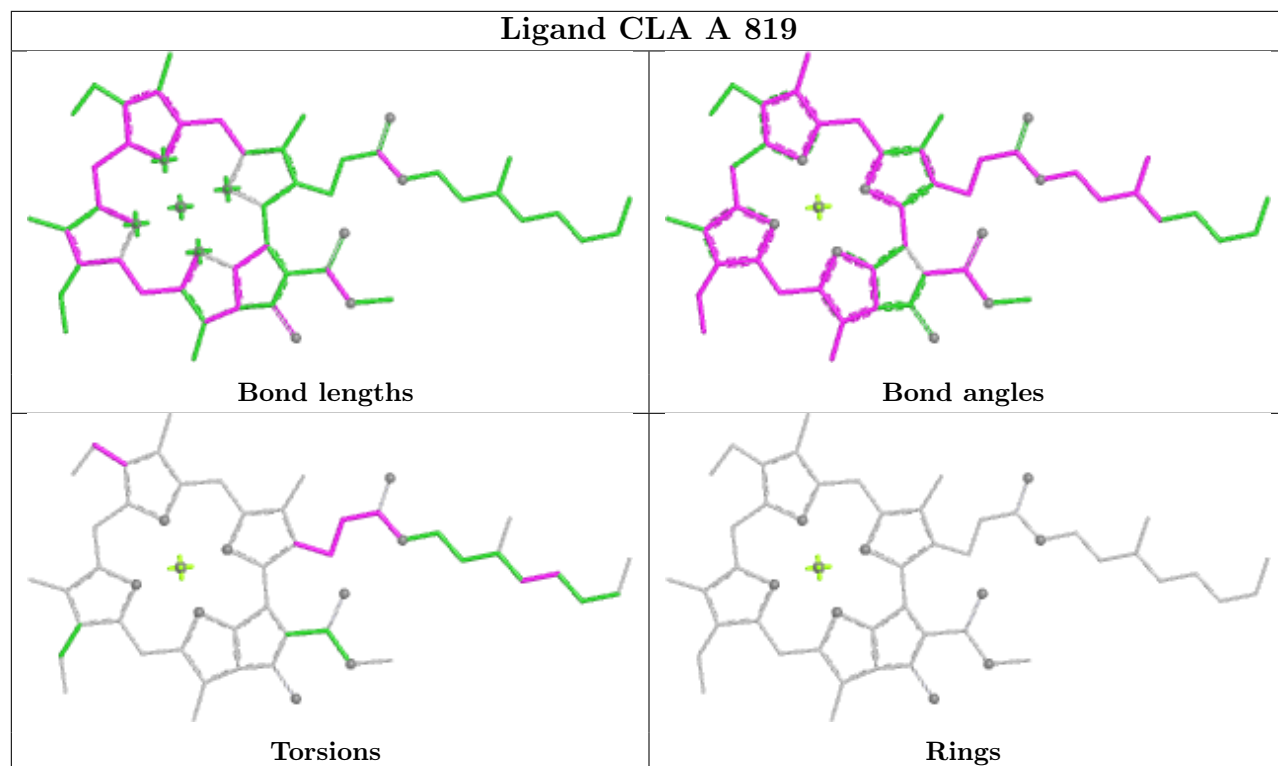


Ligand BCR K 202

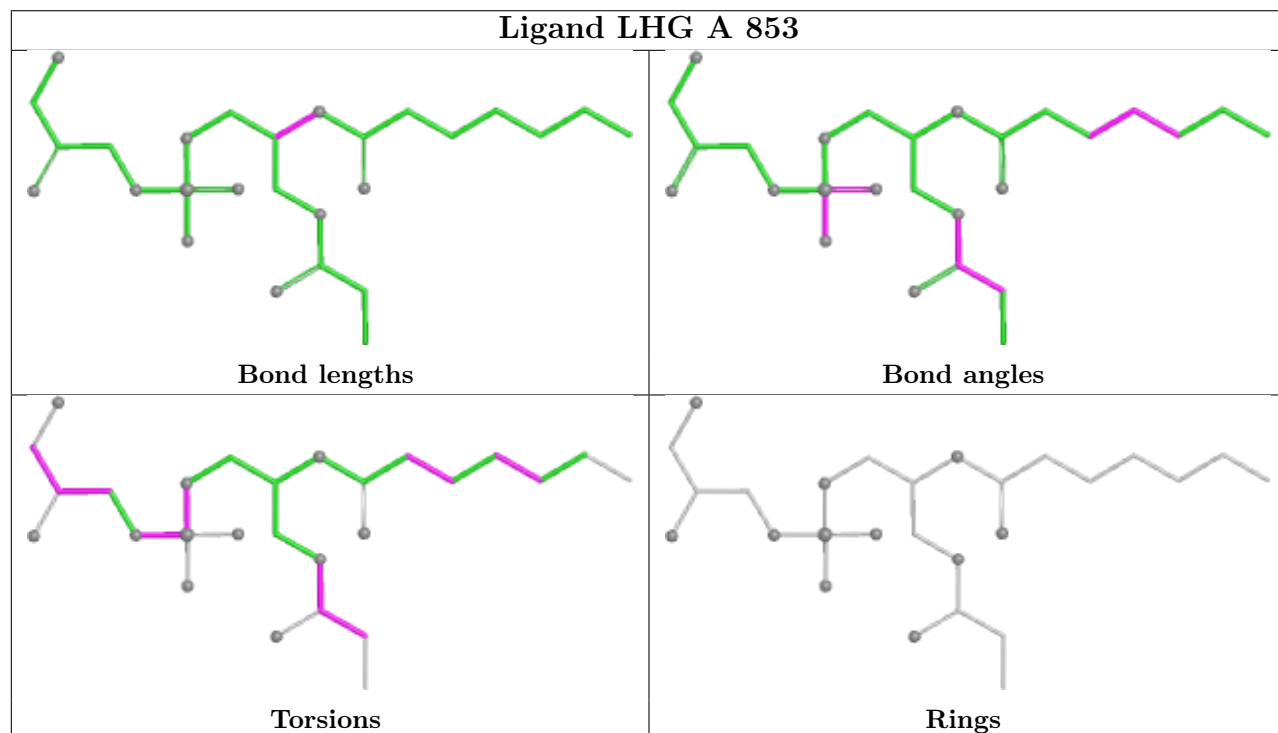


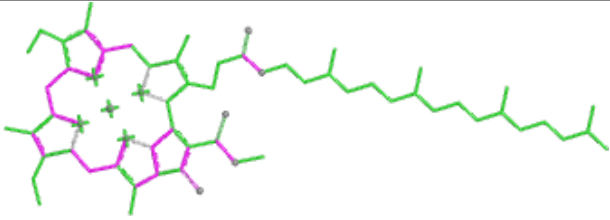
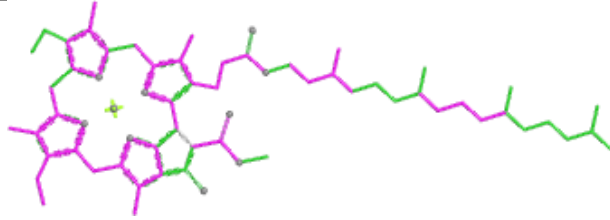
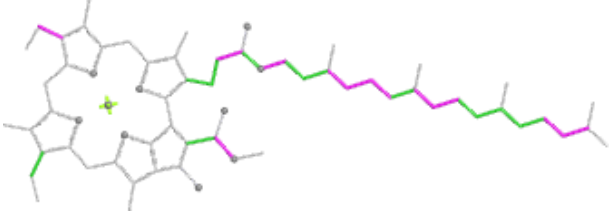
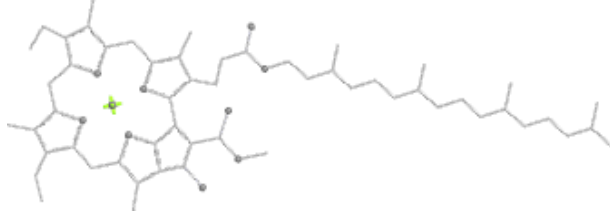
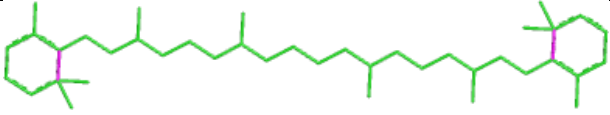
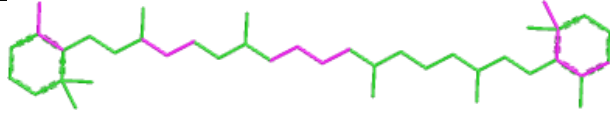
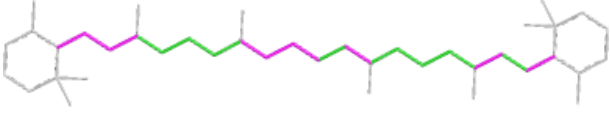
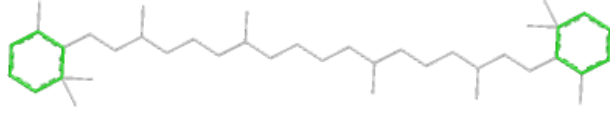
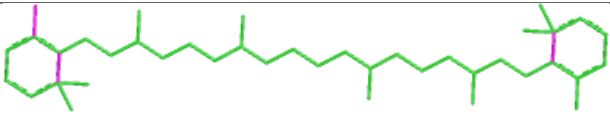
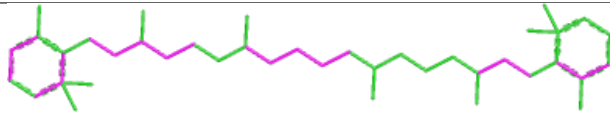
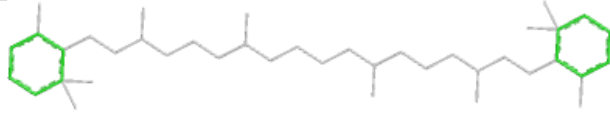


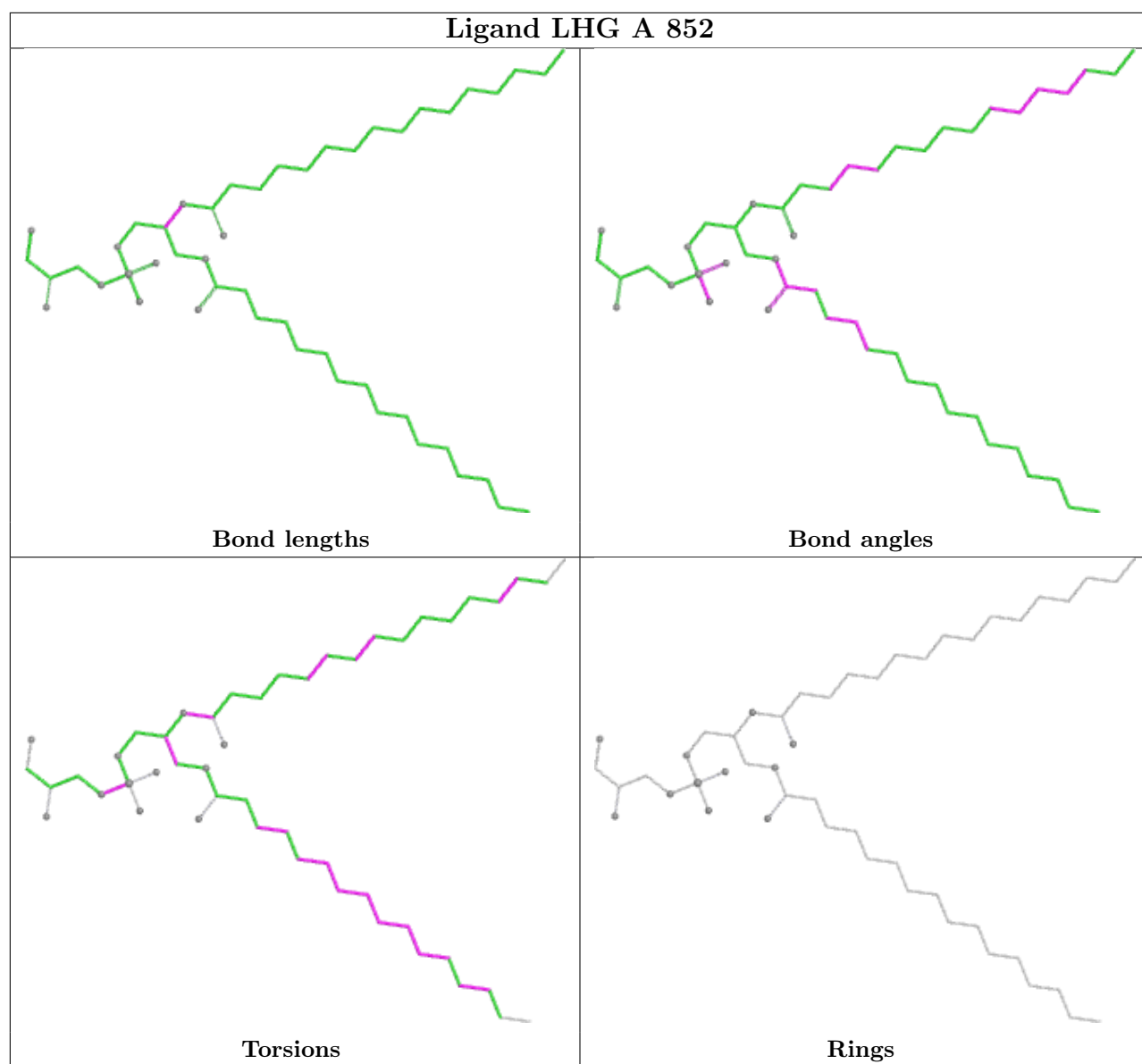
Ligand CLA A 819

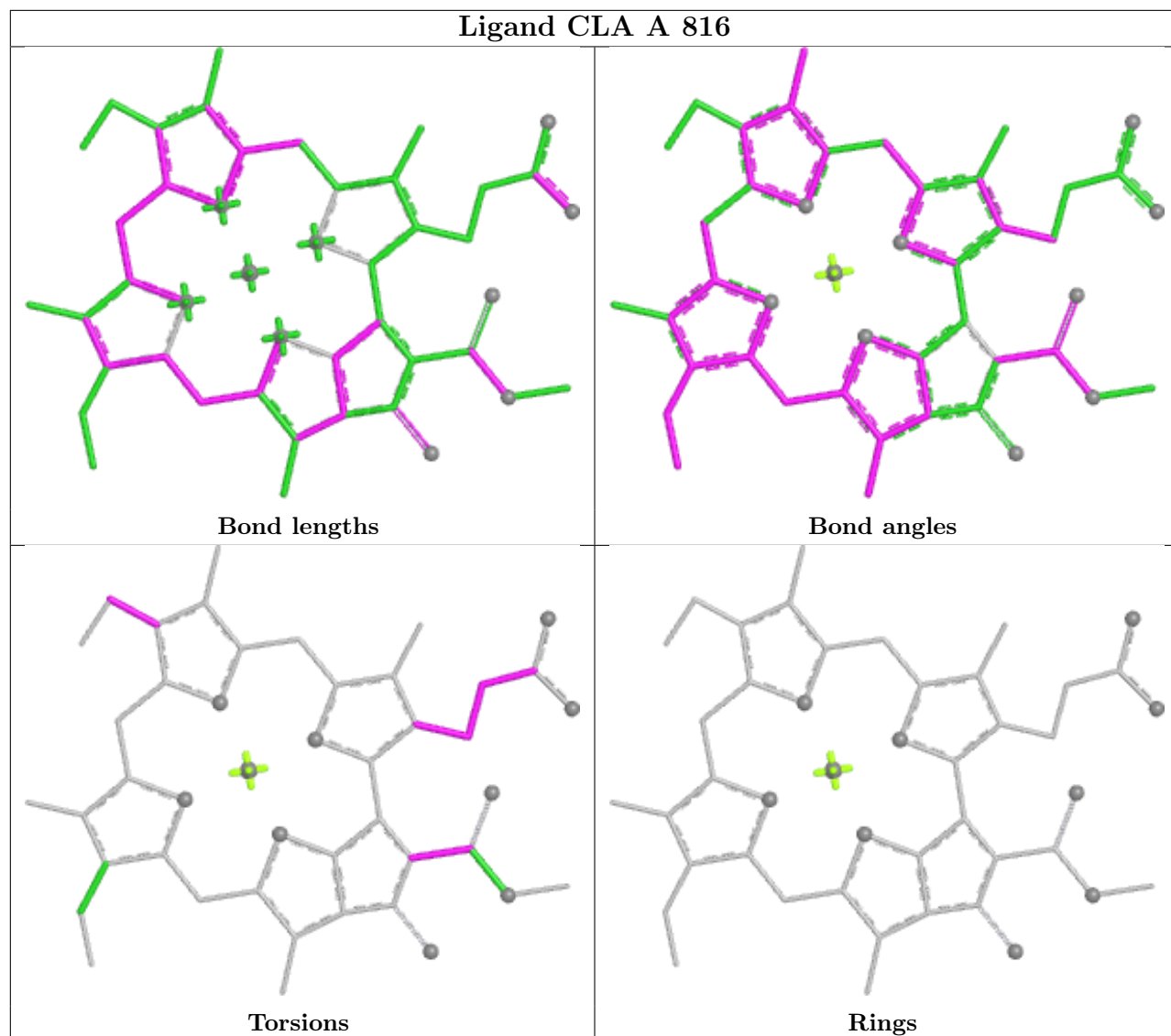


Ligand LHG A 853

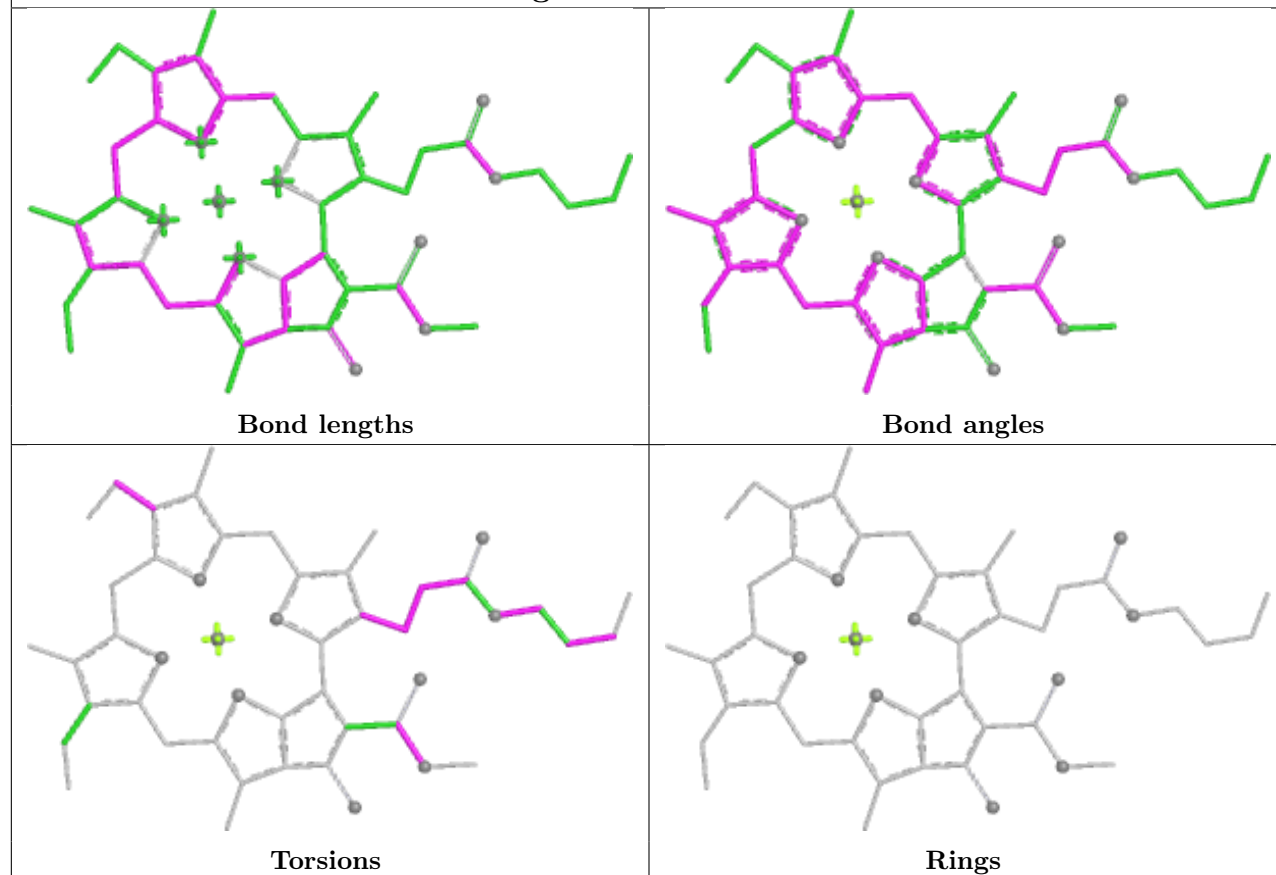


Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR F 202	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 836	
 Bond lengths	 Bond angles
 Torsions	 Rings

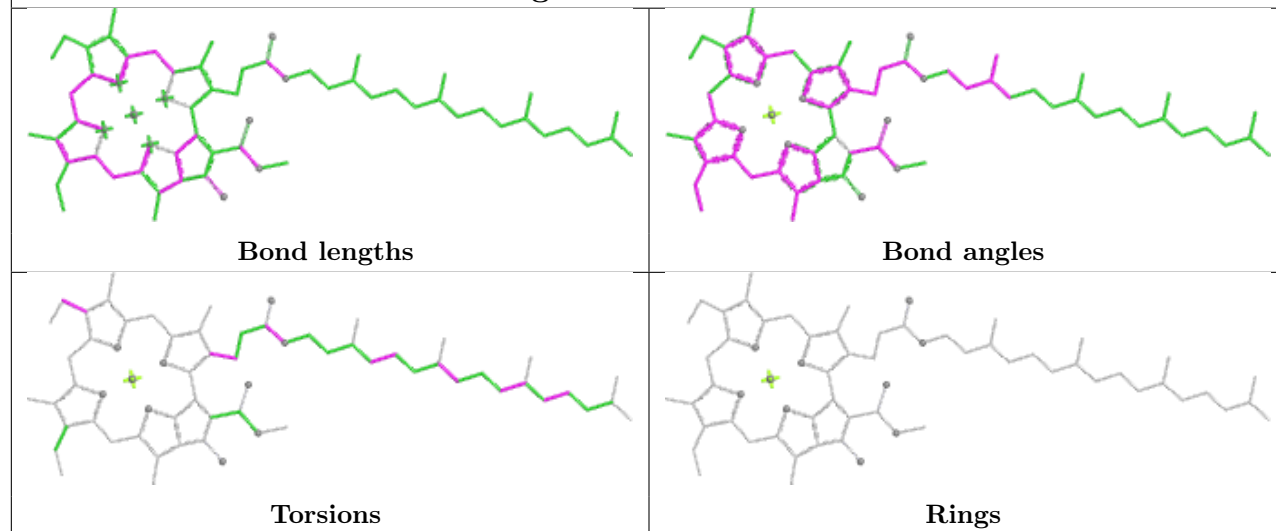


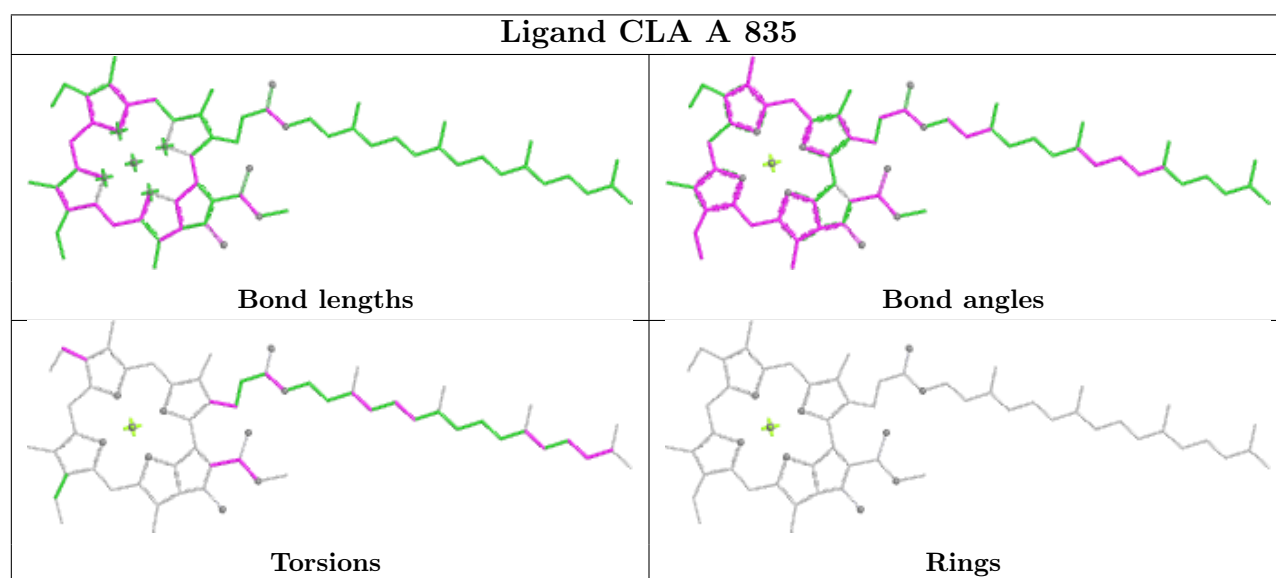
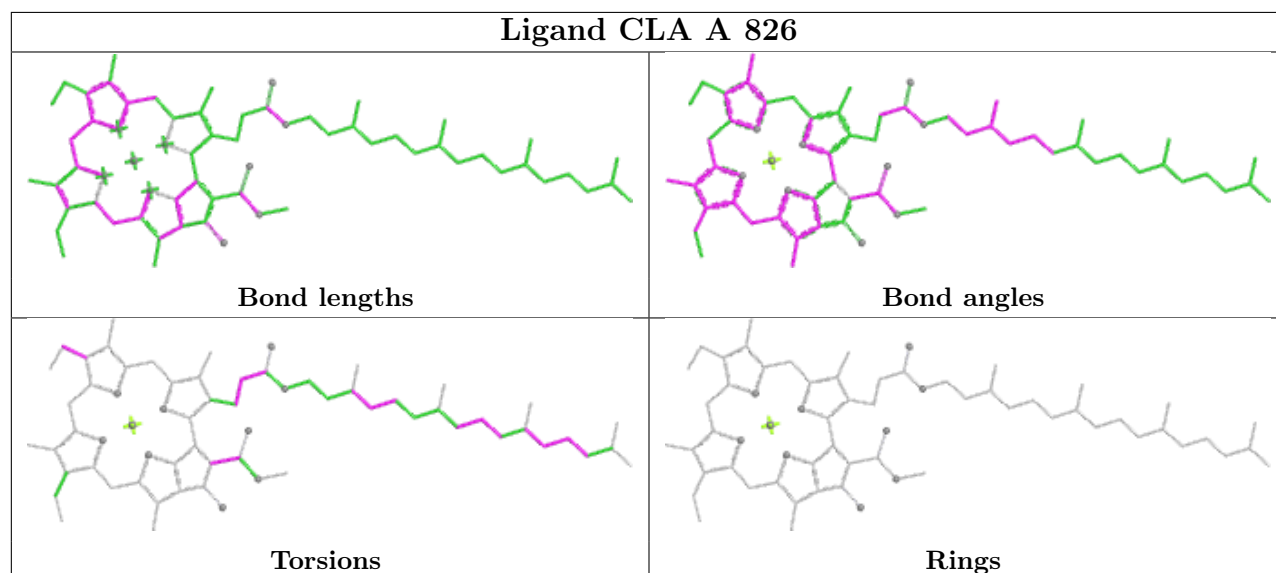
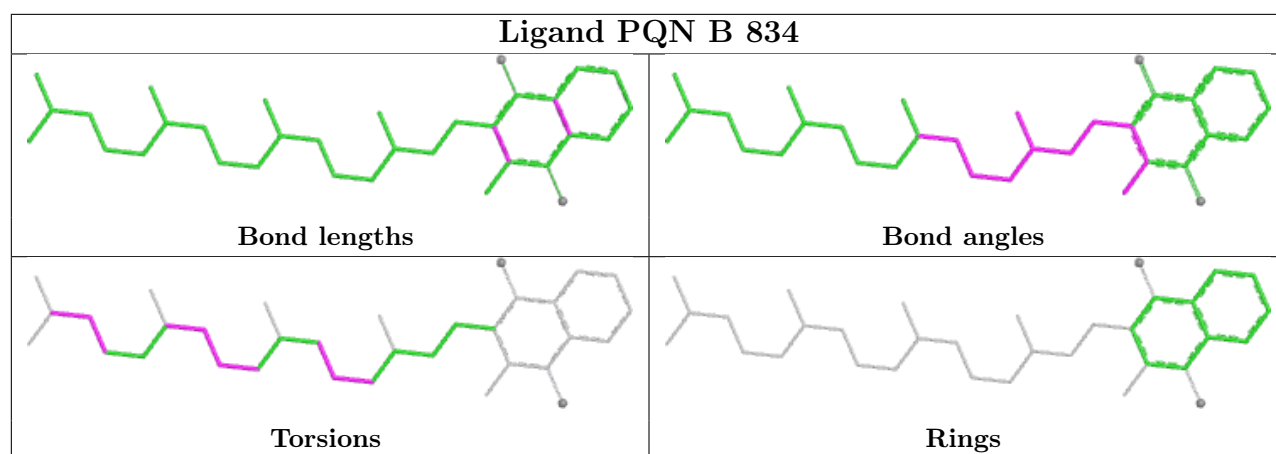


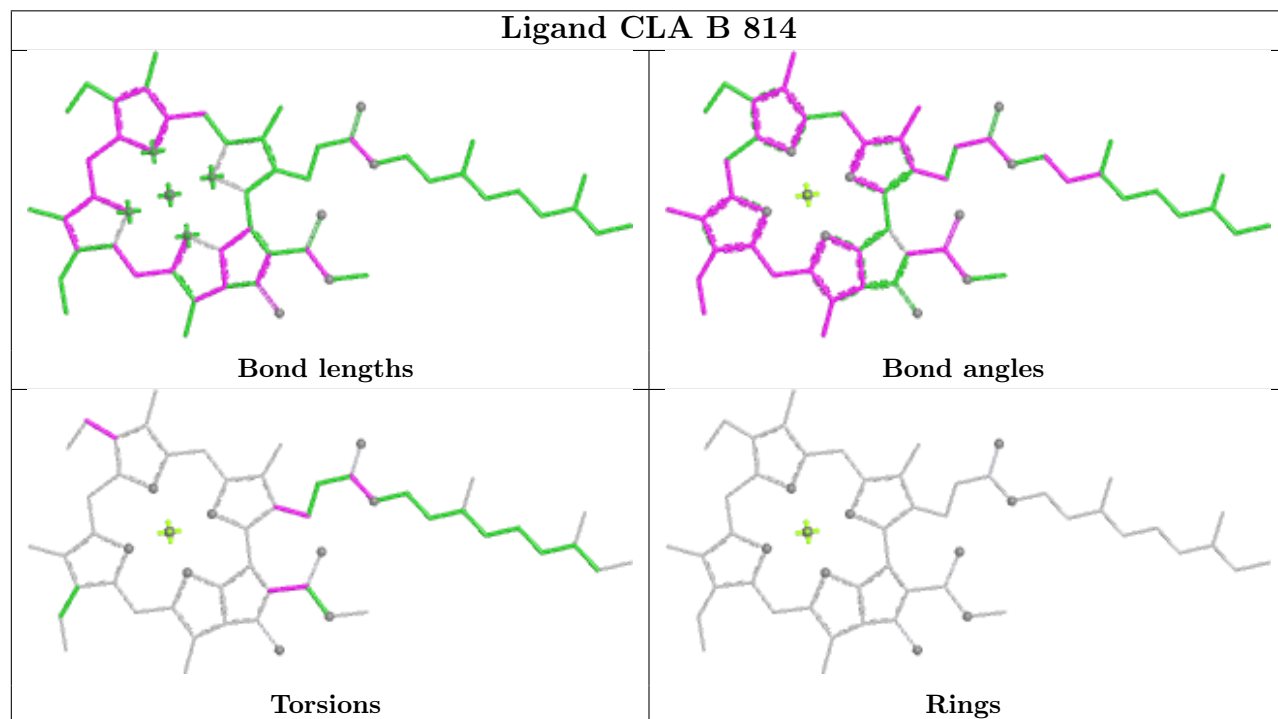
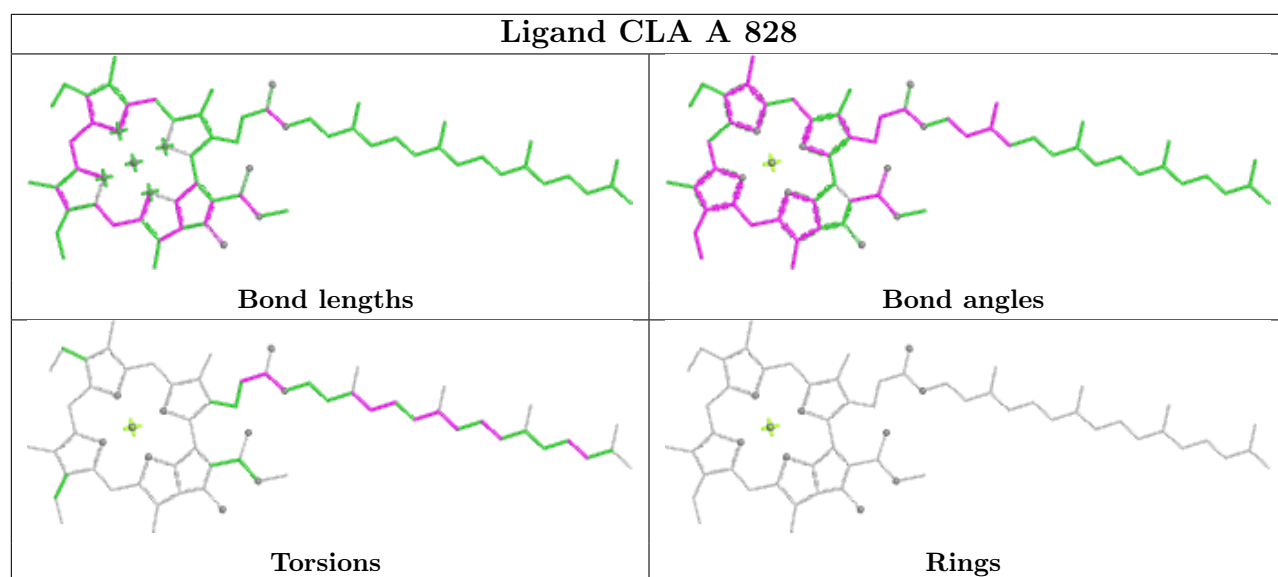
Ligand CLA B 824



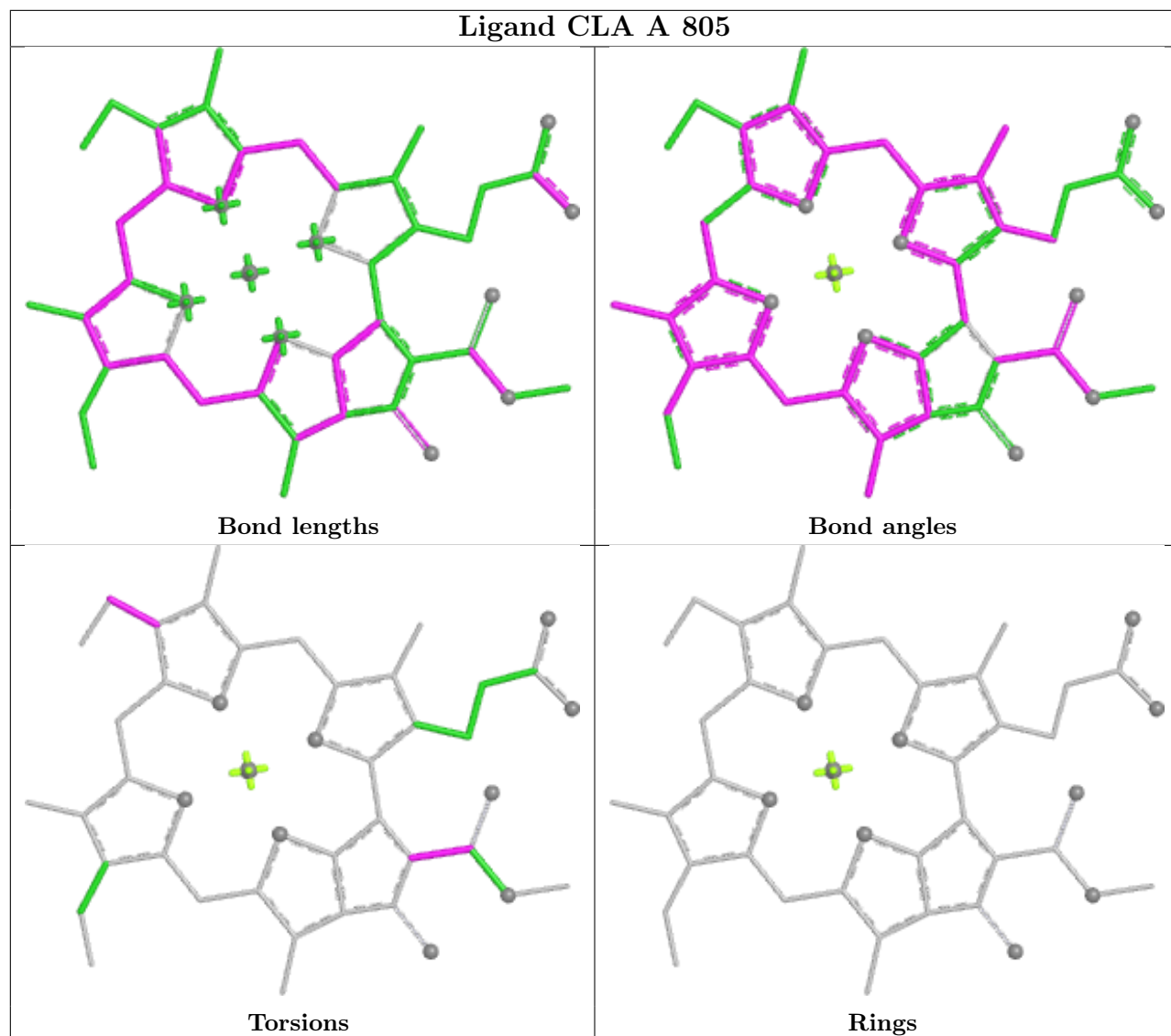
Ligand CLA A 820



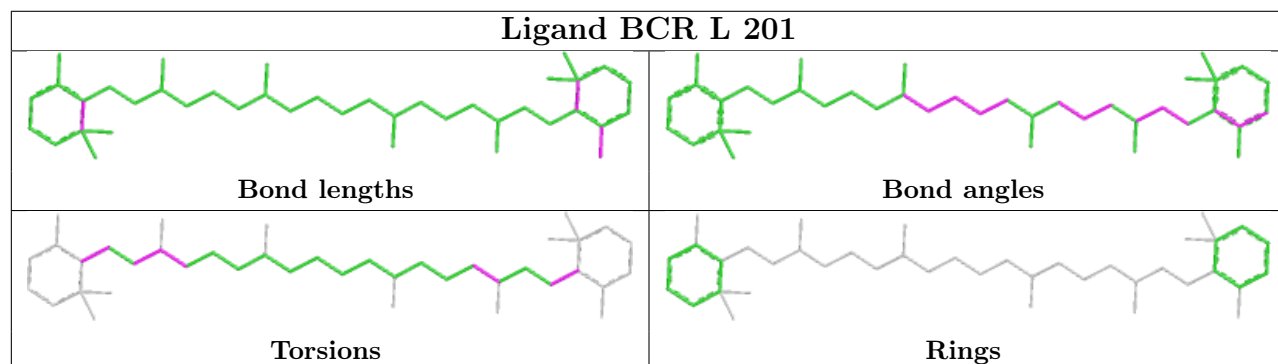


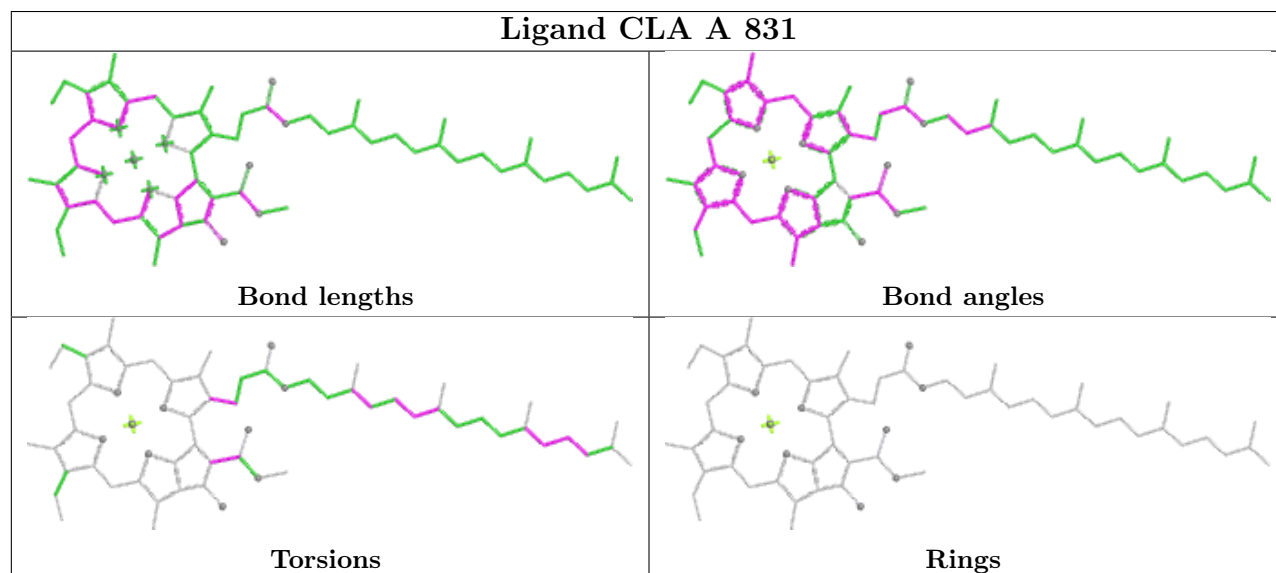
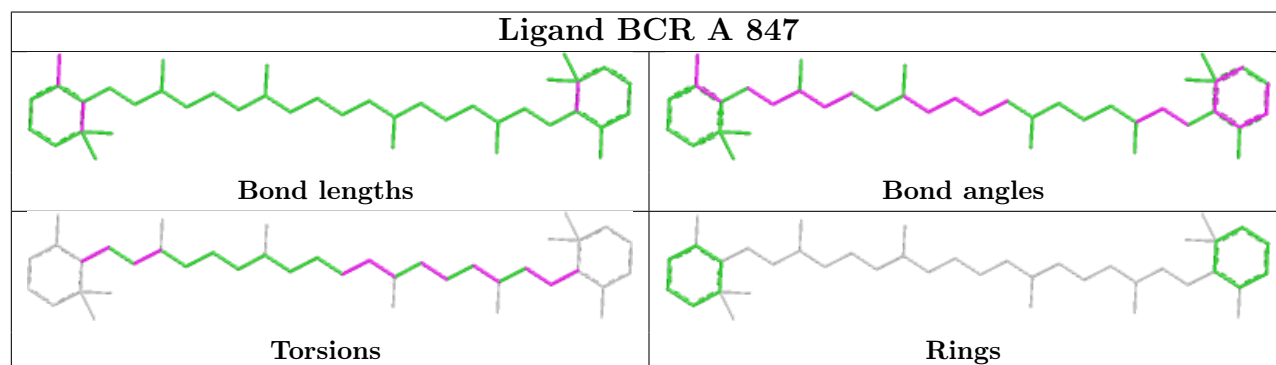
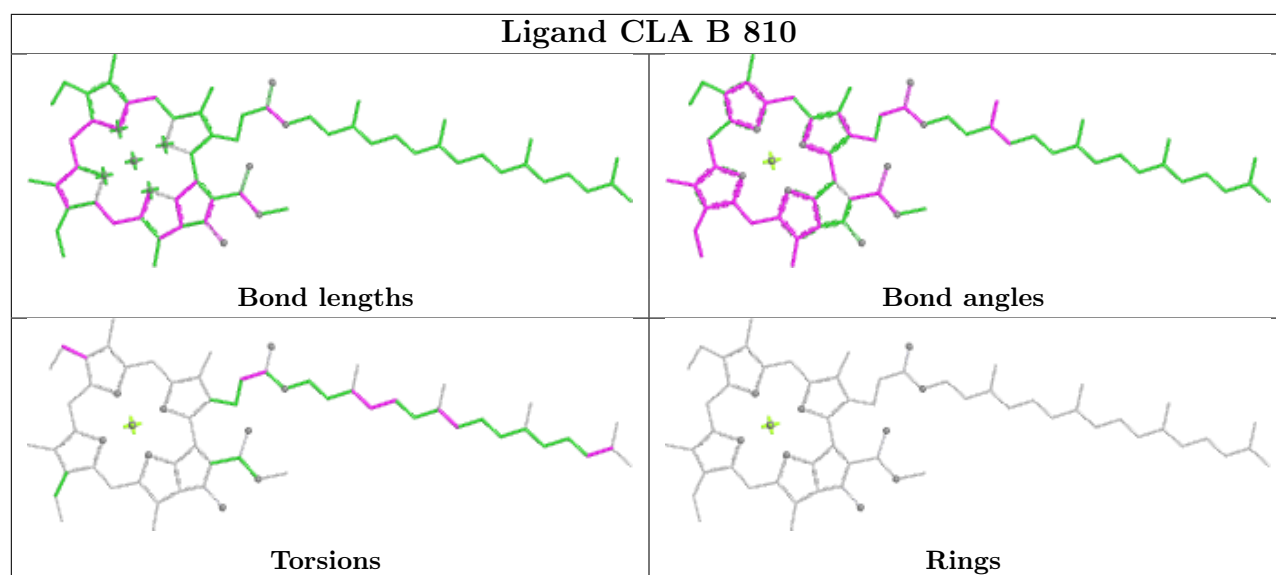


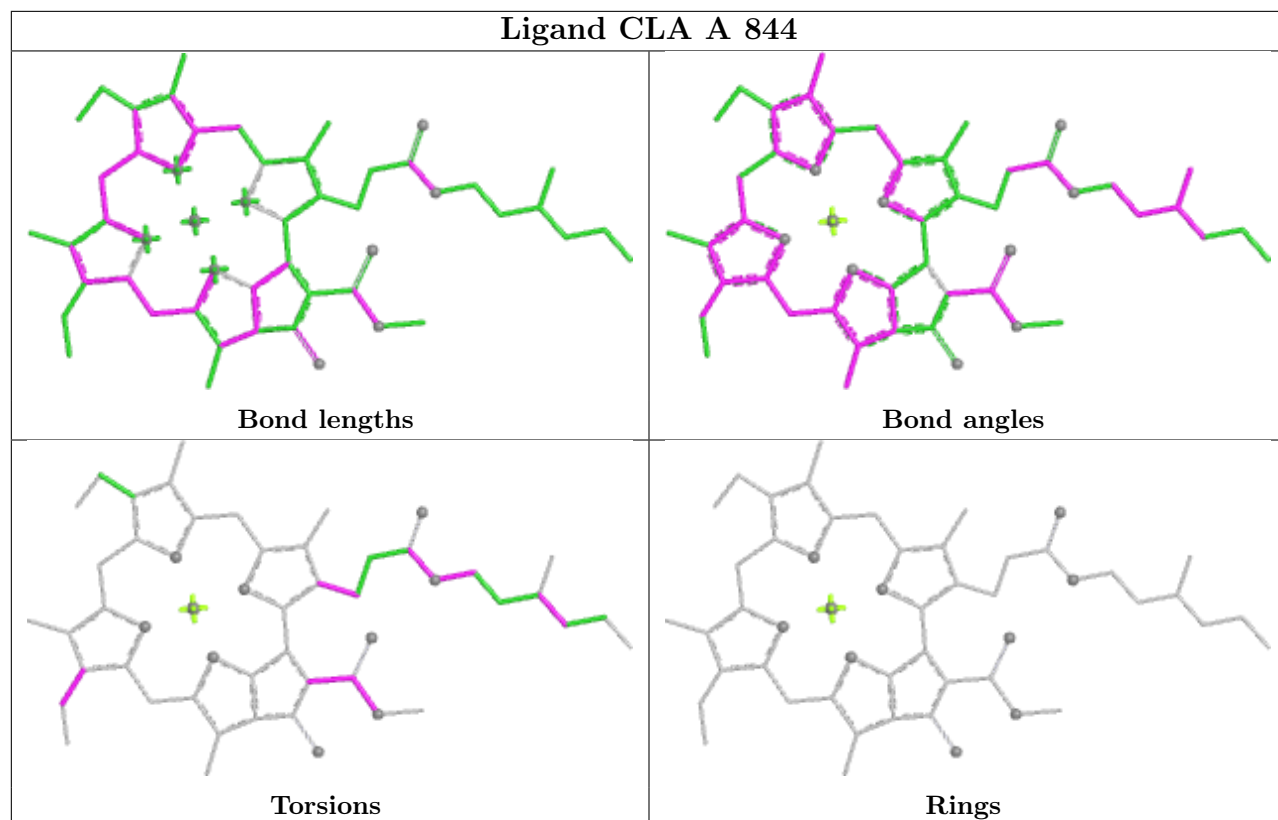
Ligand CLA A 805



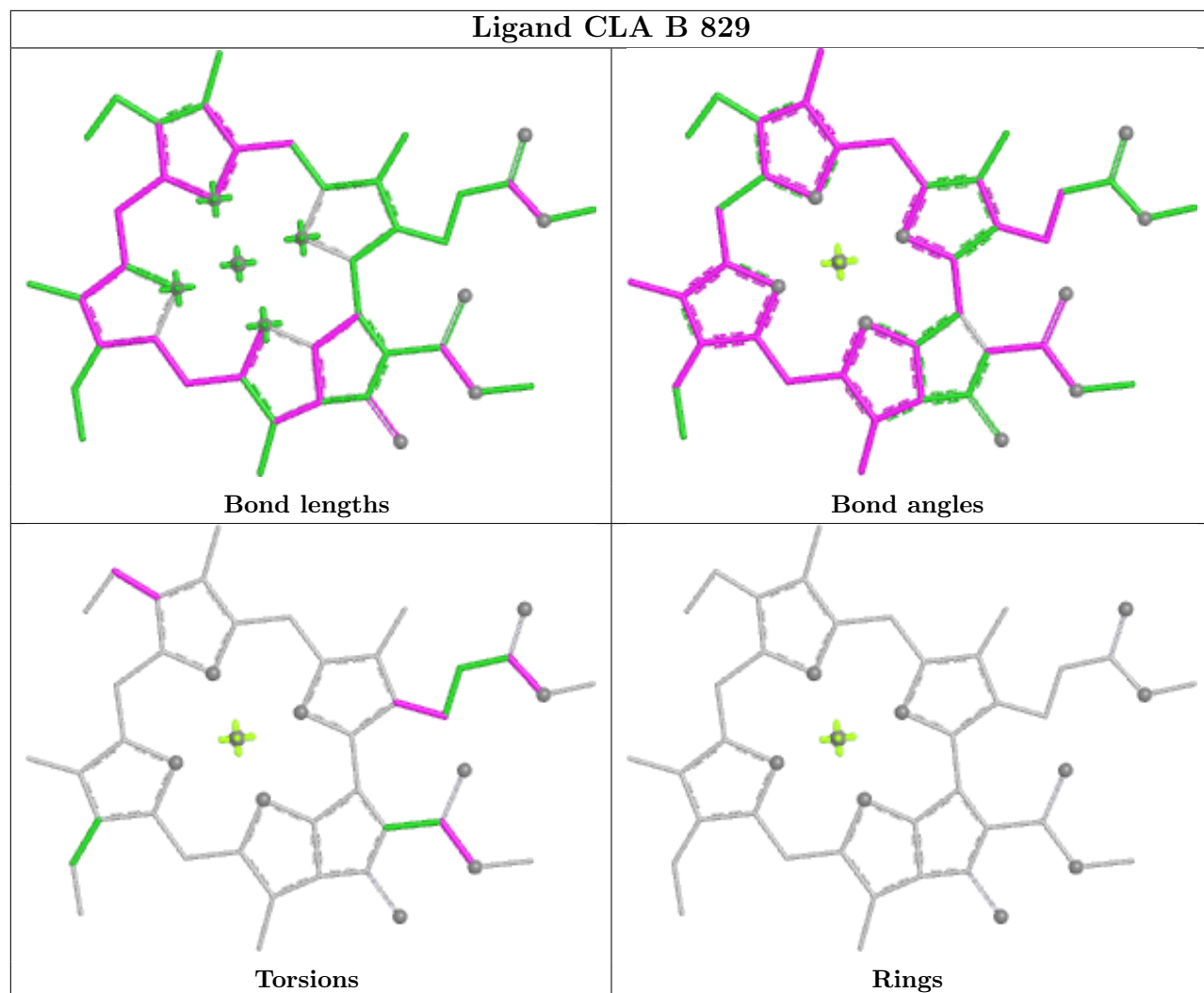
Ligand BCR L 201



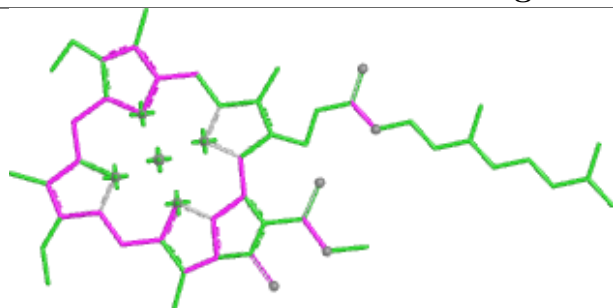




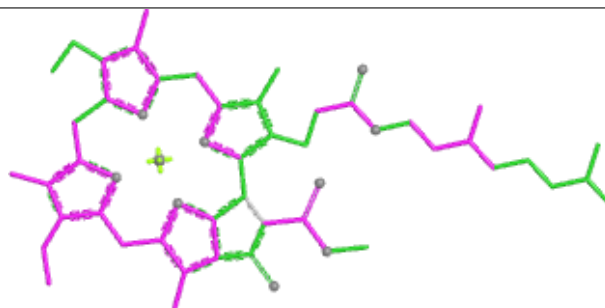
Ligand CLA B 829



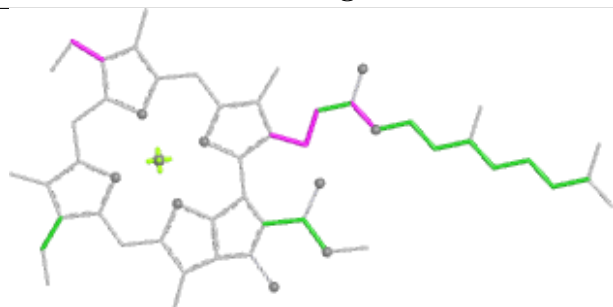
Ligand CLA B 816



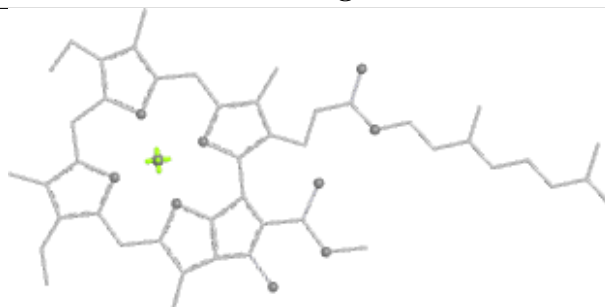
Bond lengths



Bond angles

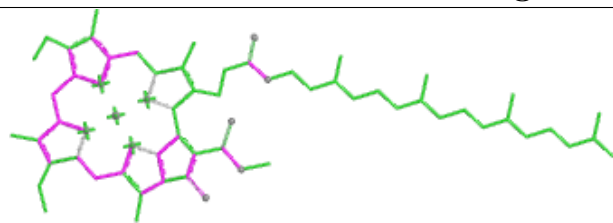


Torsions

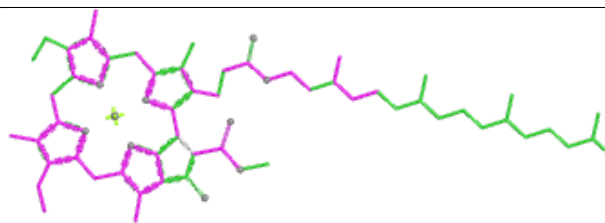


Rings

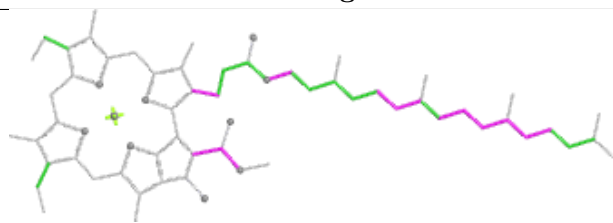
Ligand CLA A 840



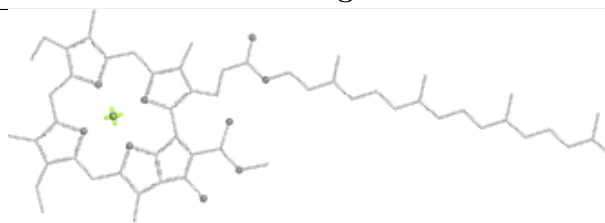
Bond lengths



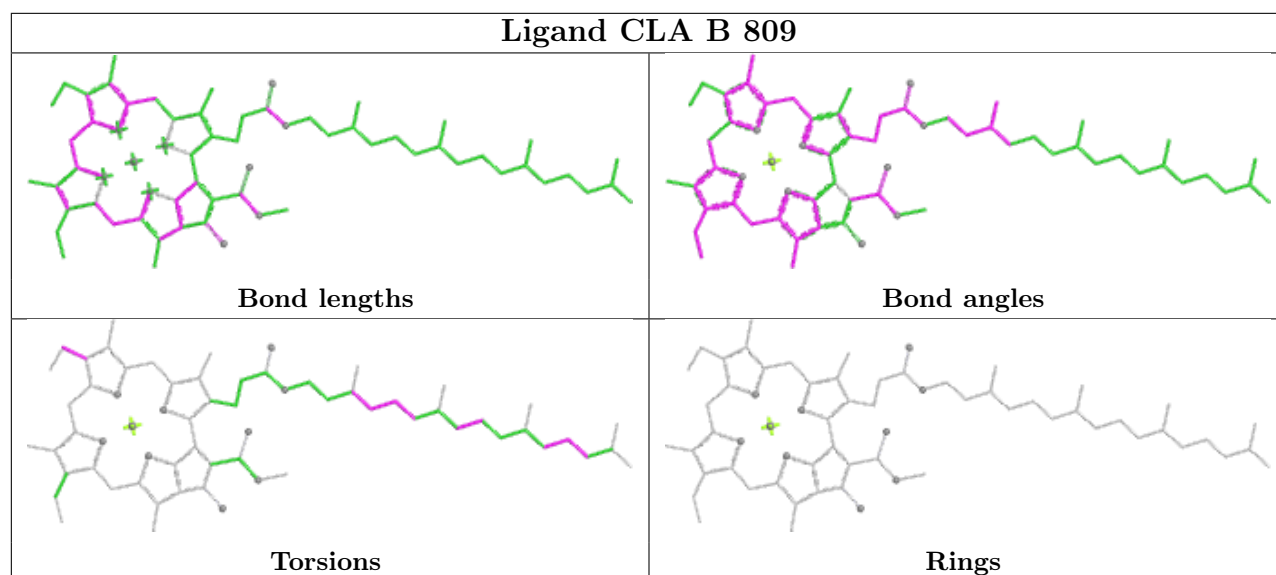
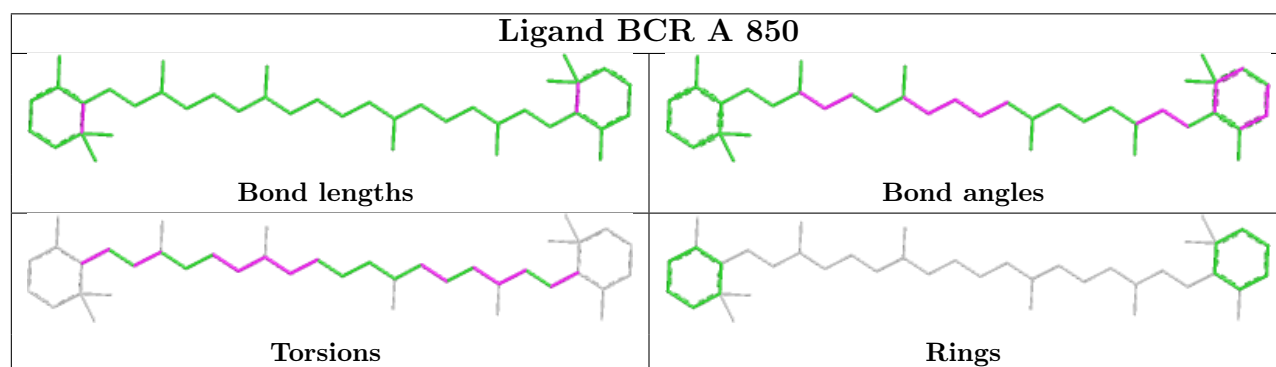
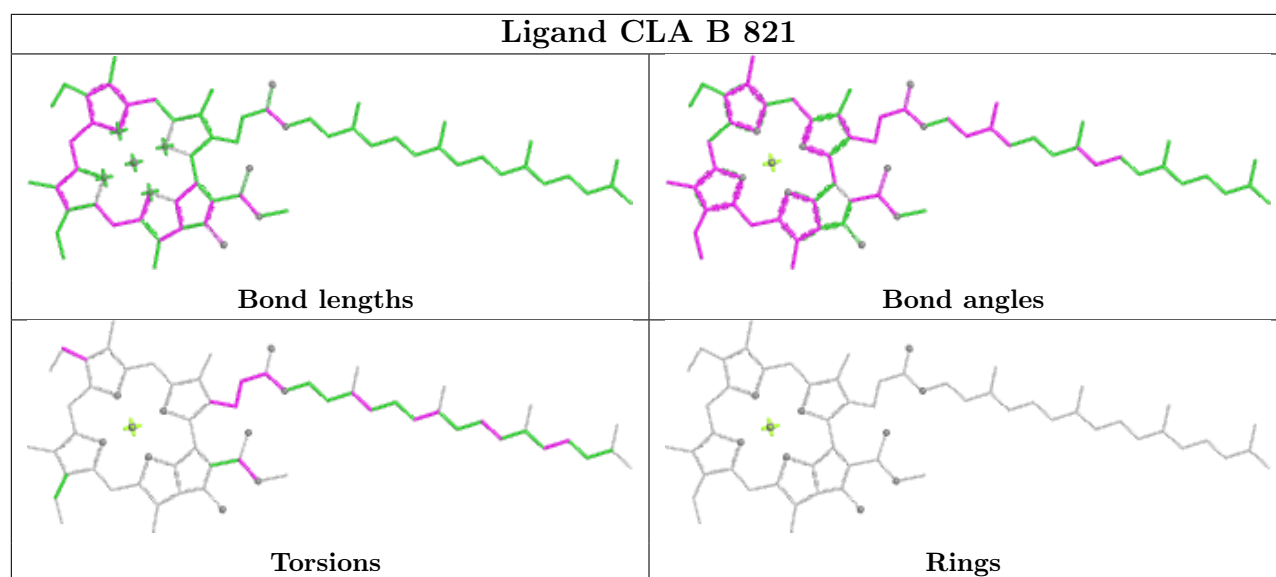
Bond angles

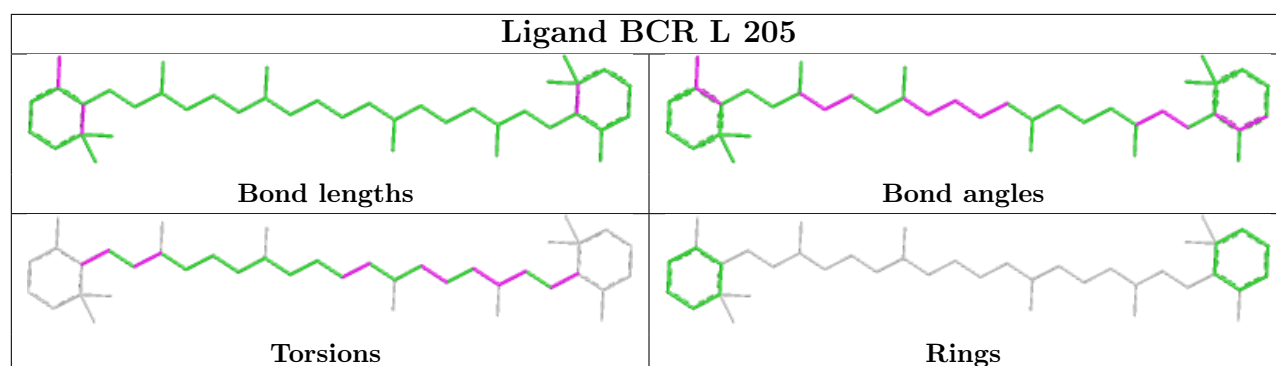
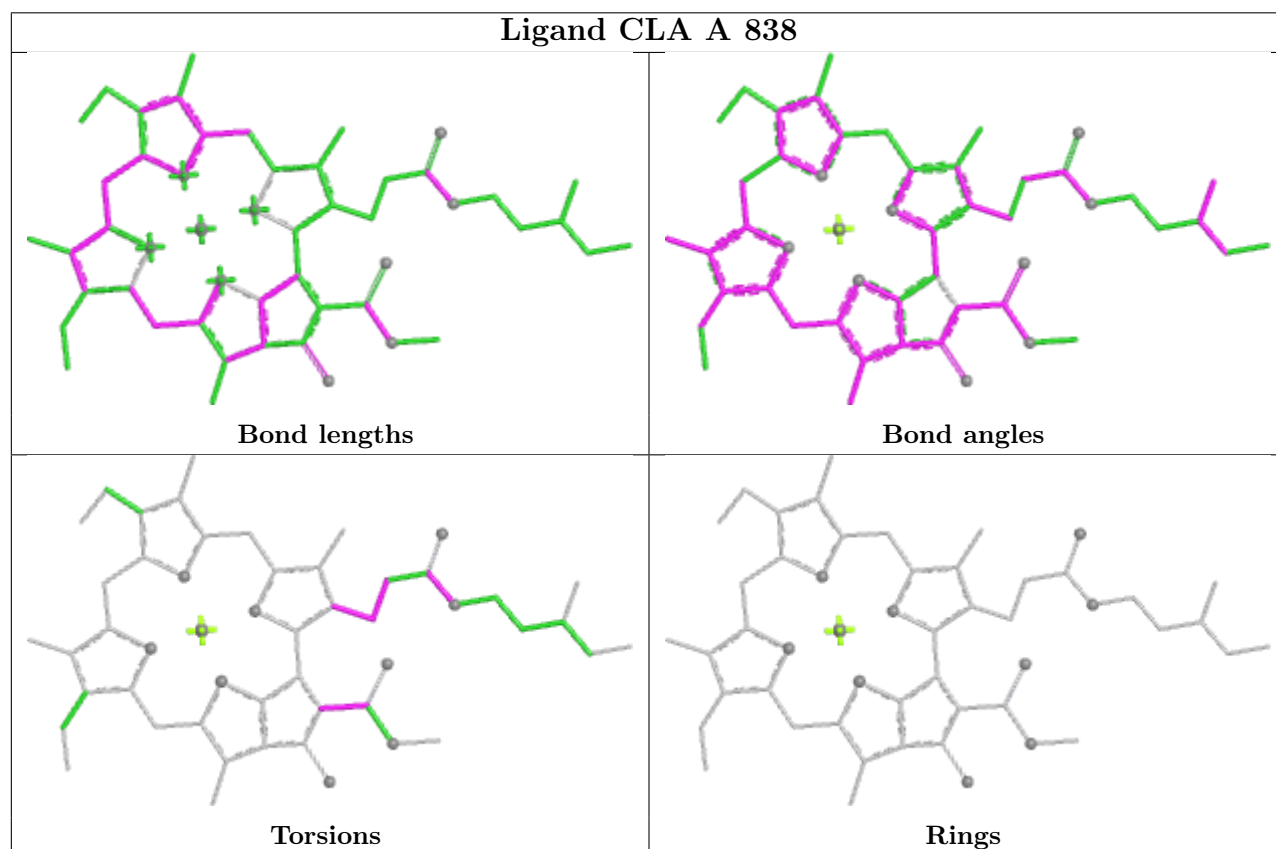
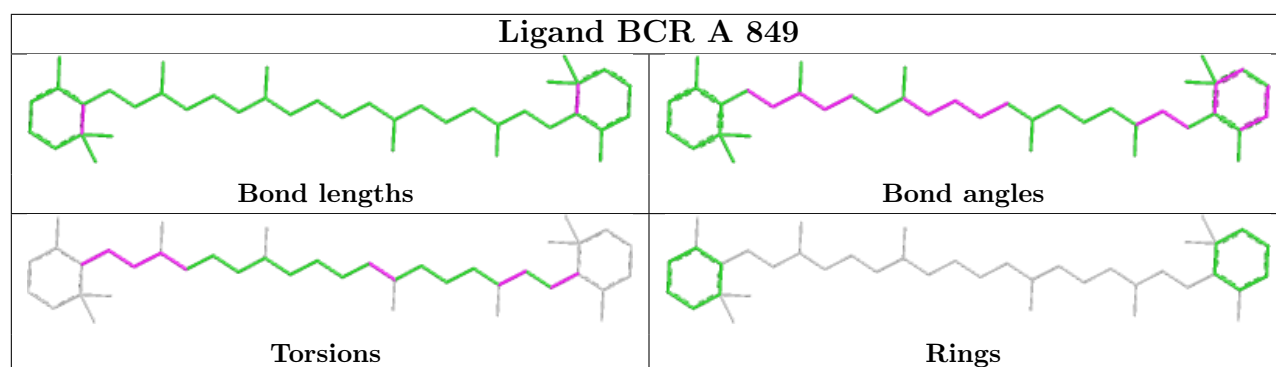


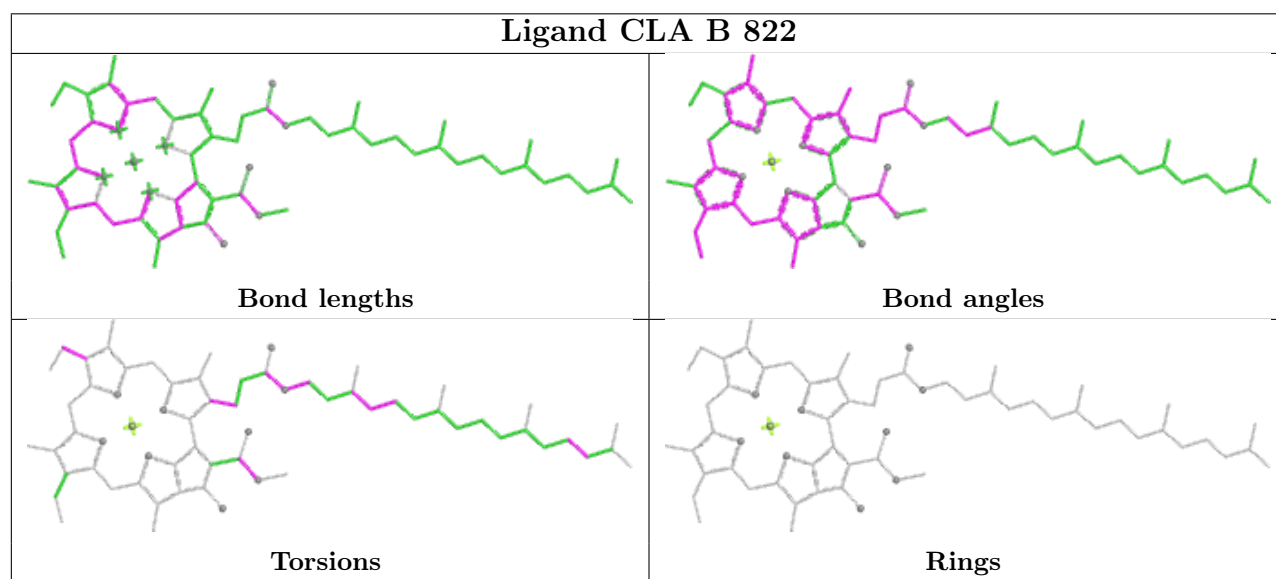
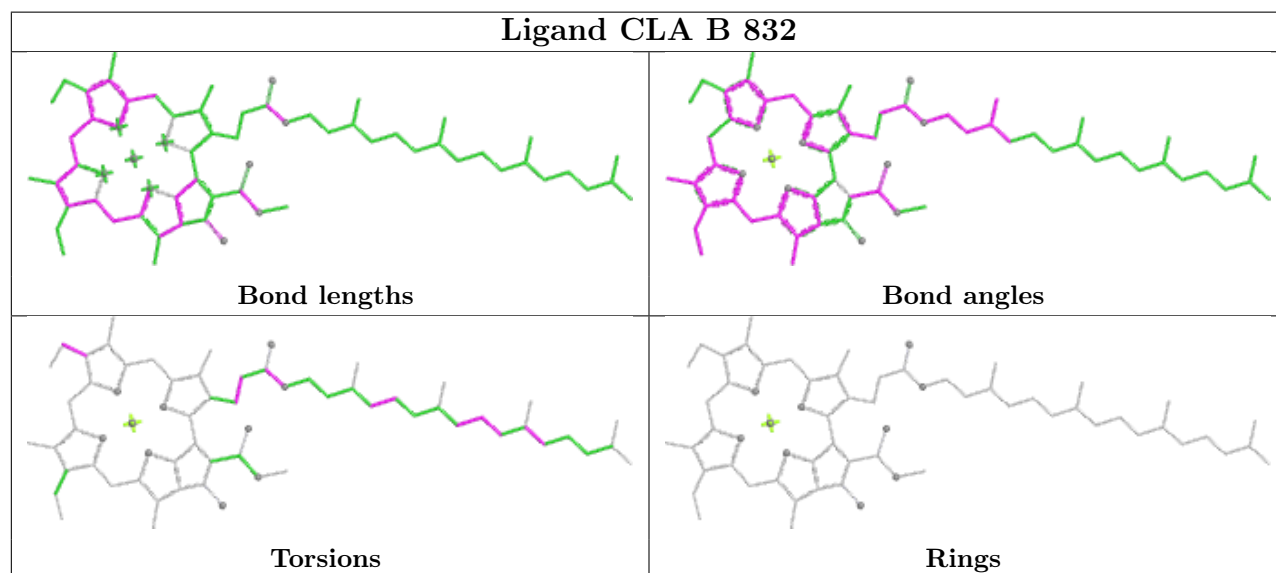
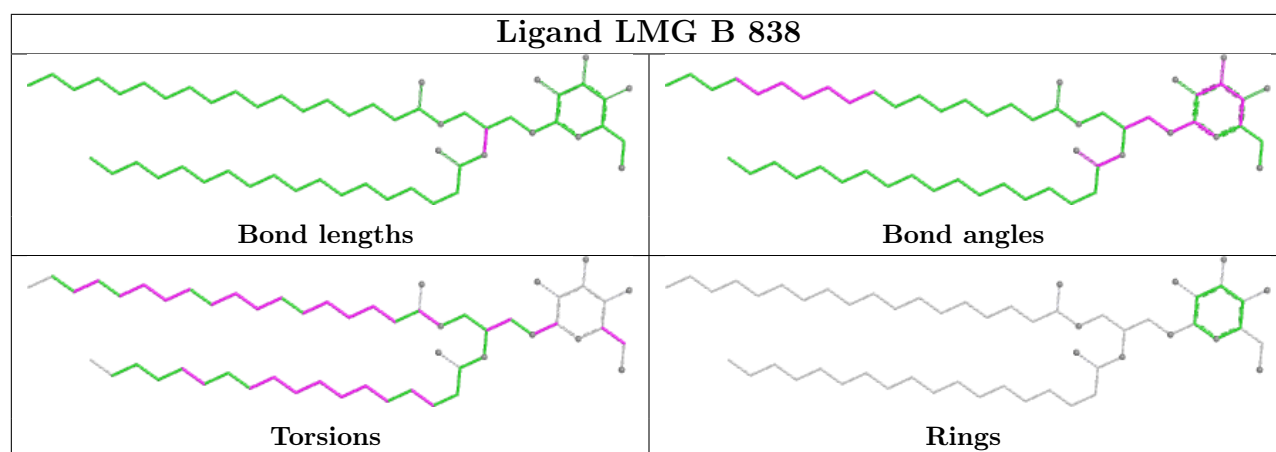
Torsions

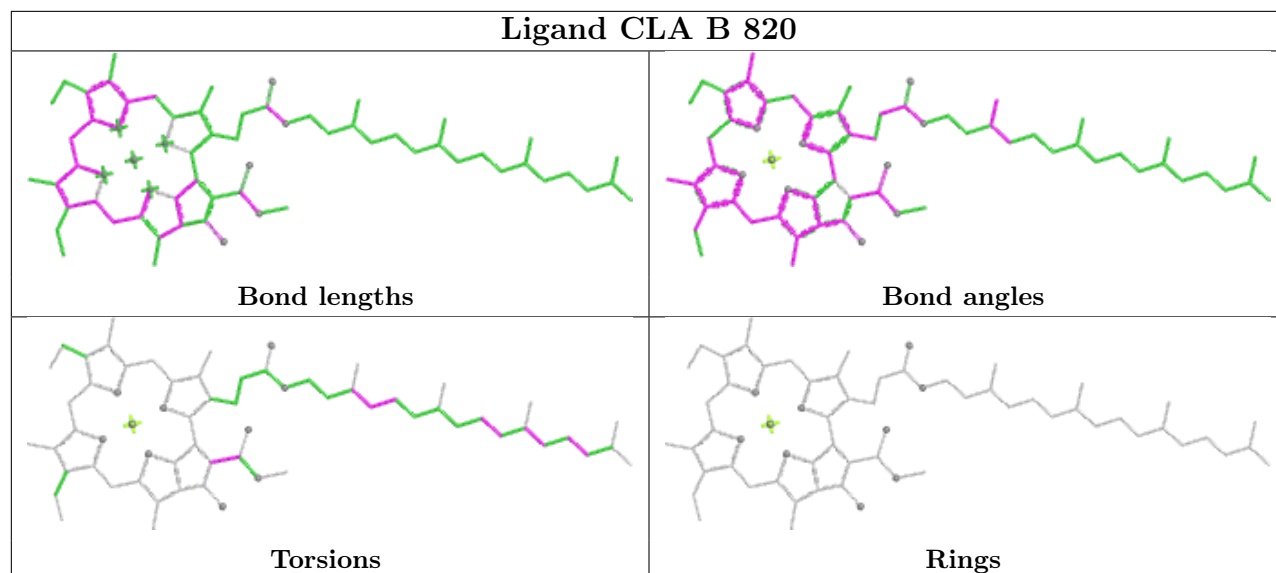
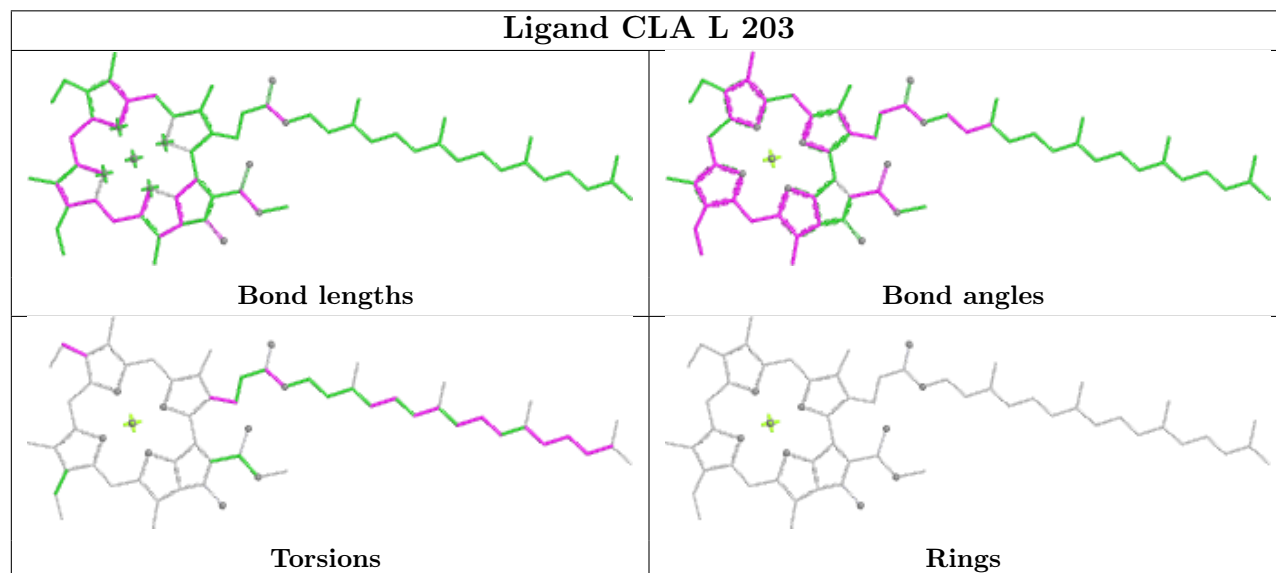
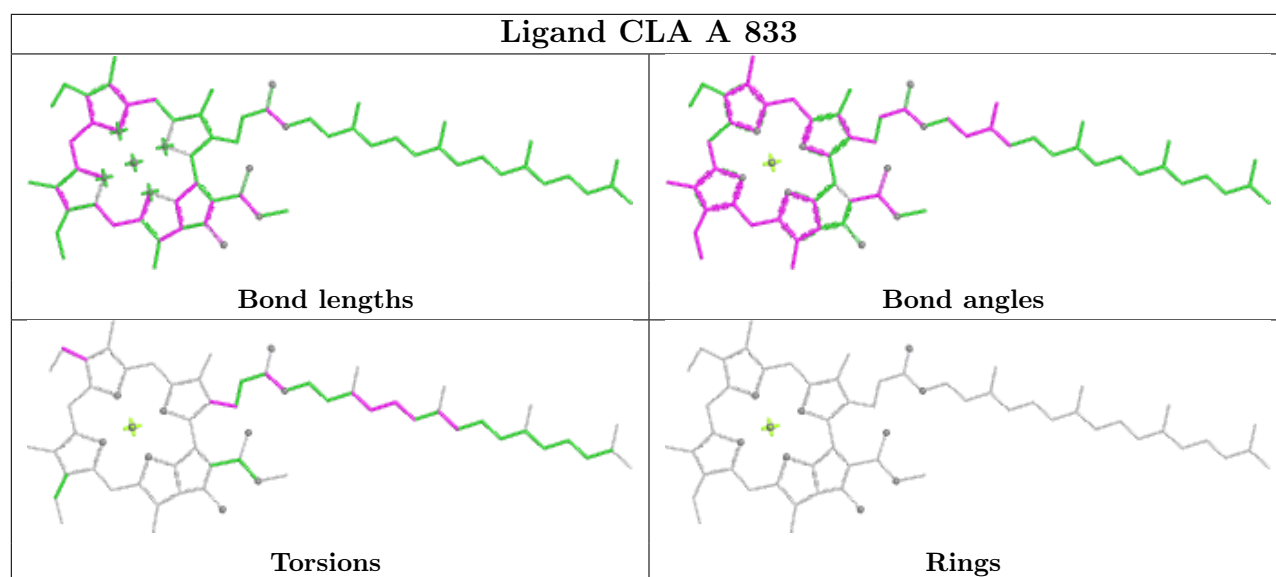


Rings

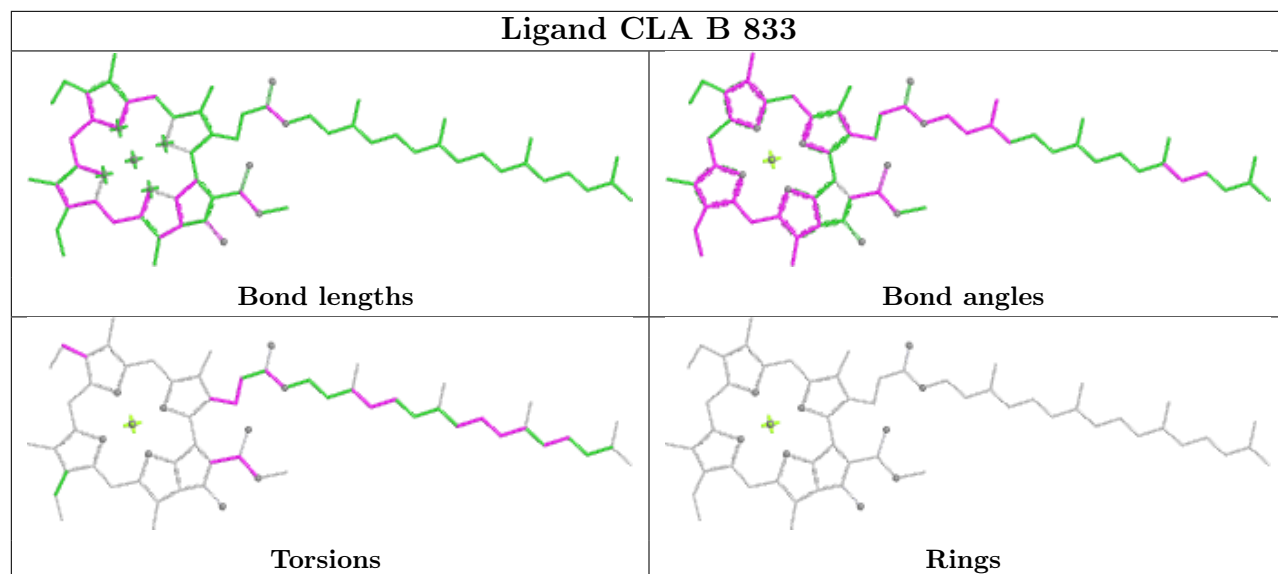




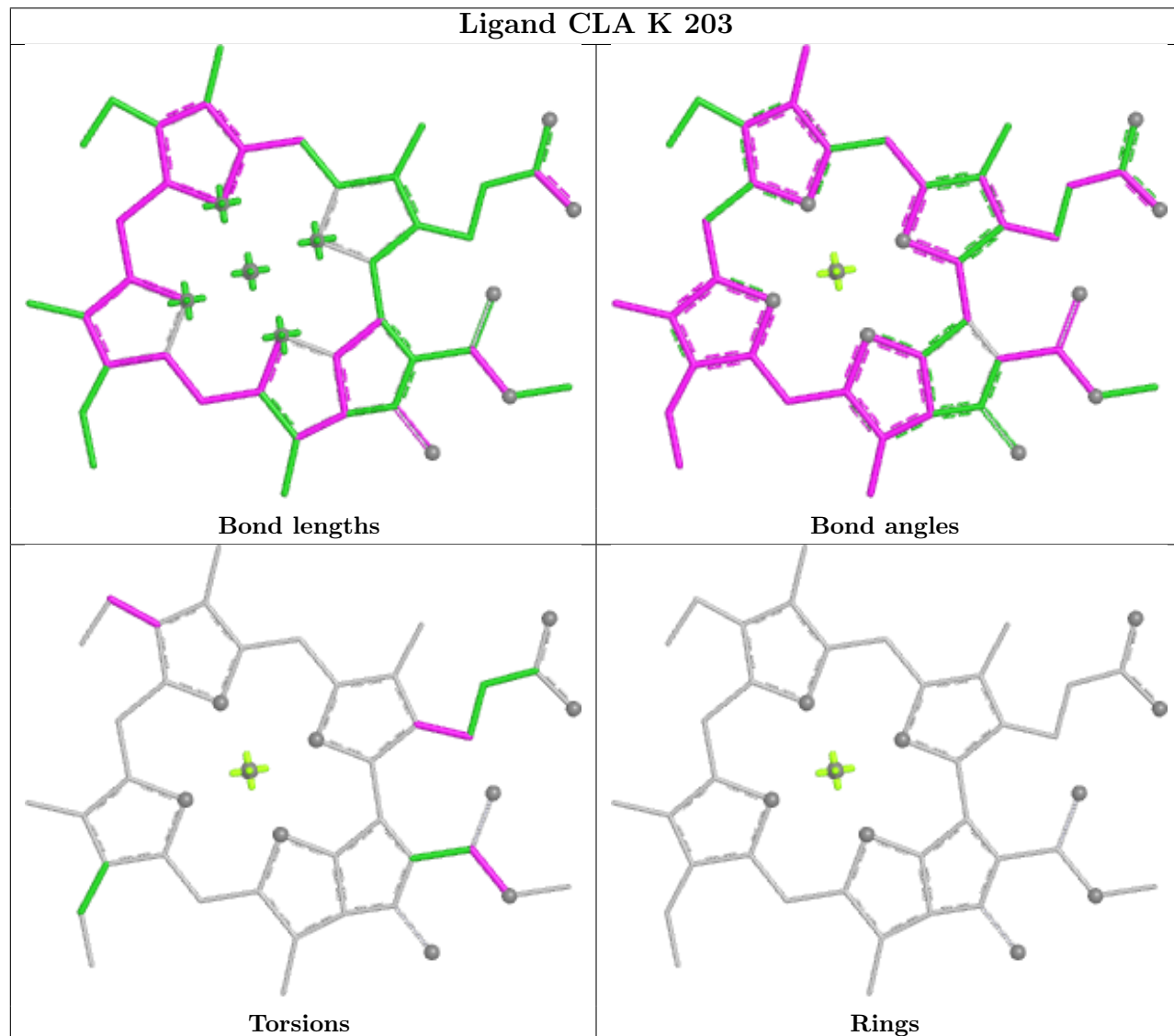


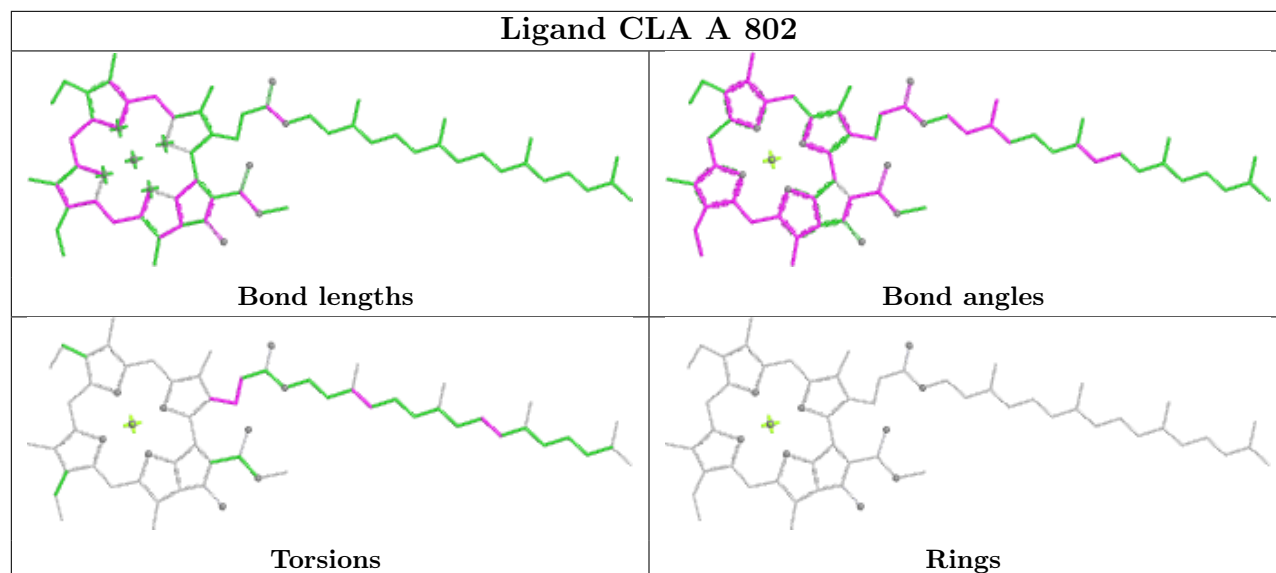
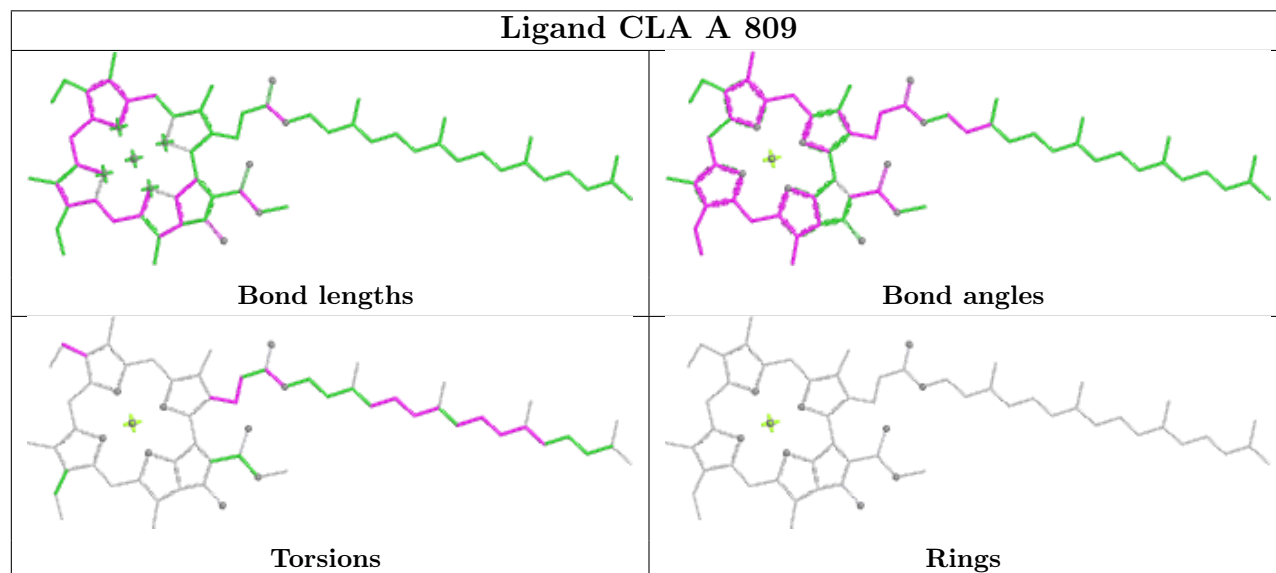
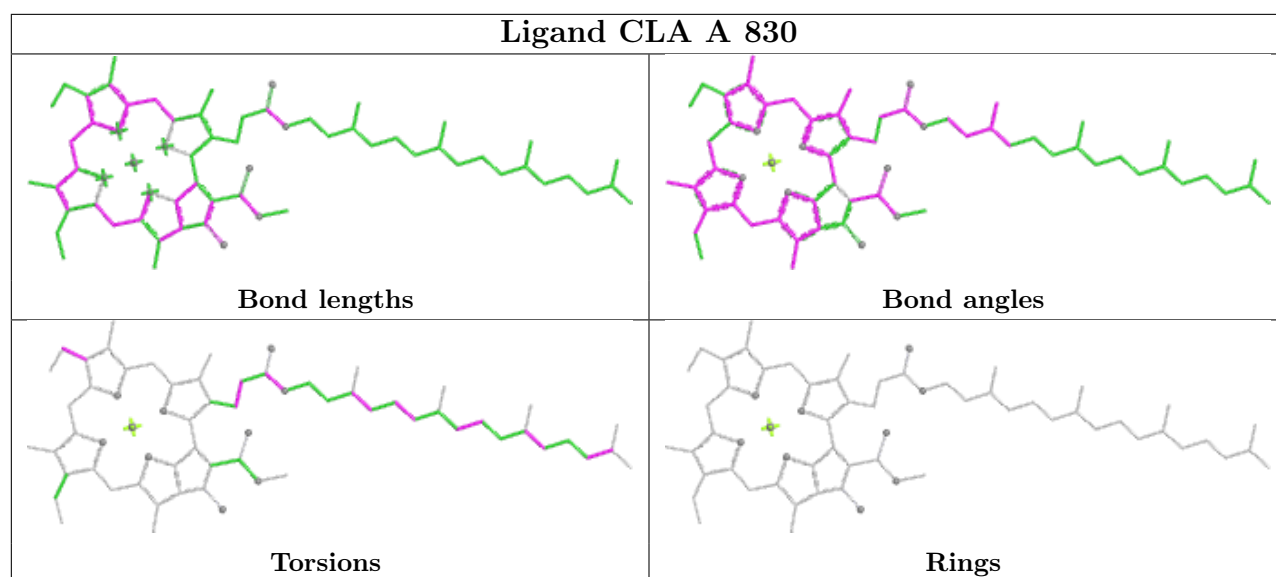


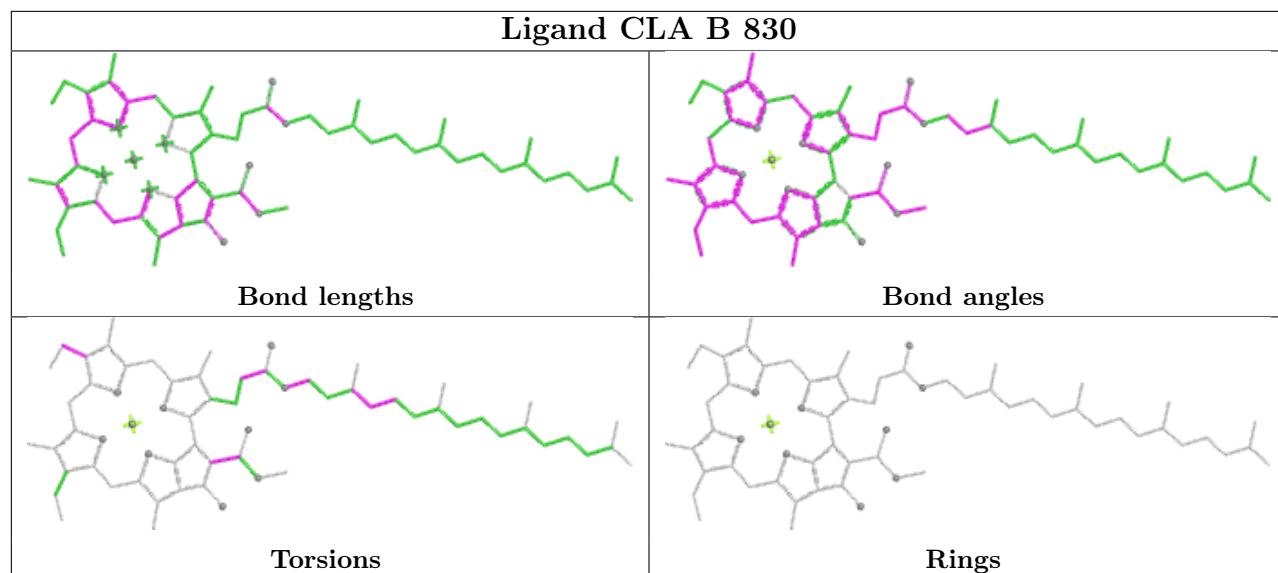
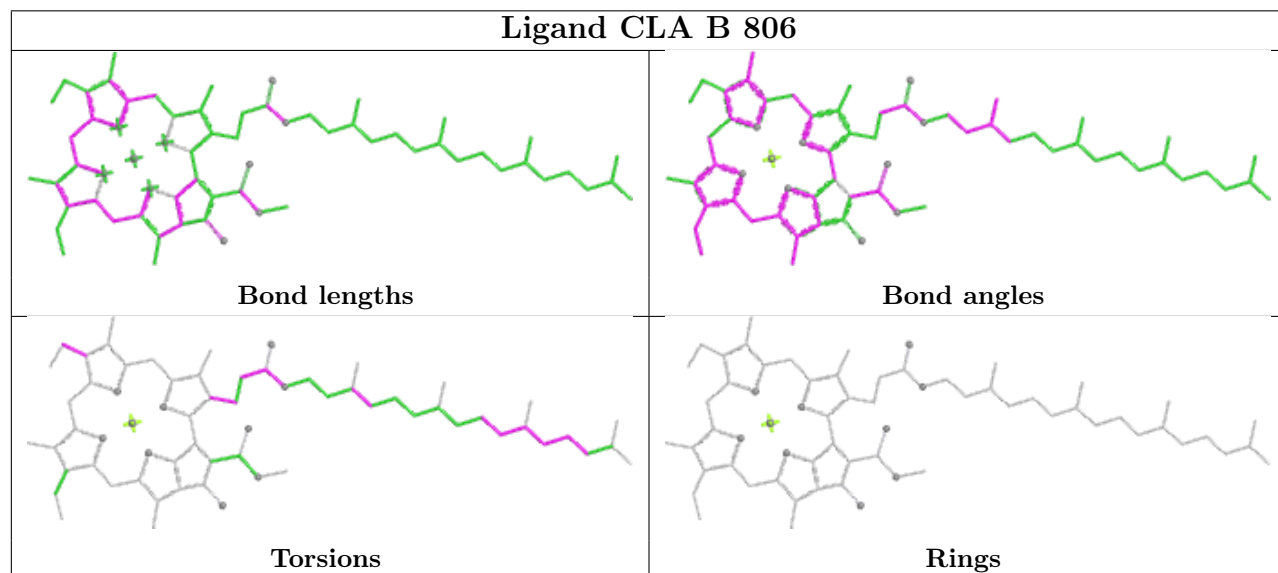
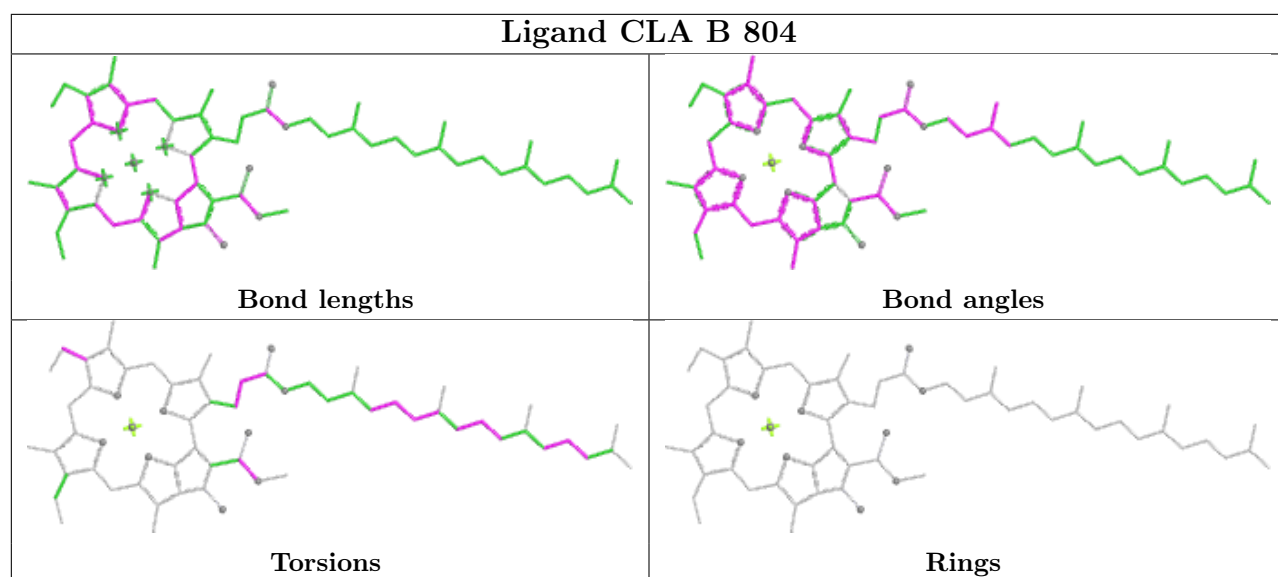
Ligand CLA B 833

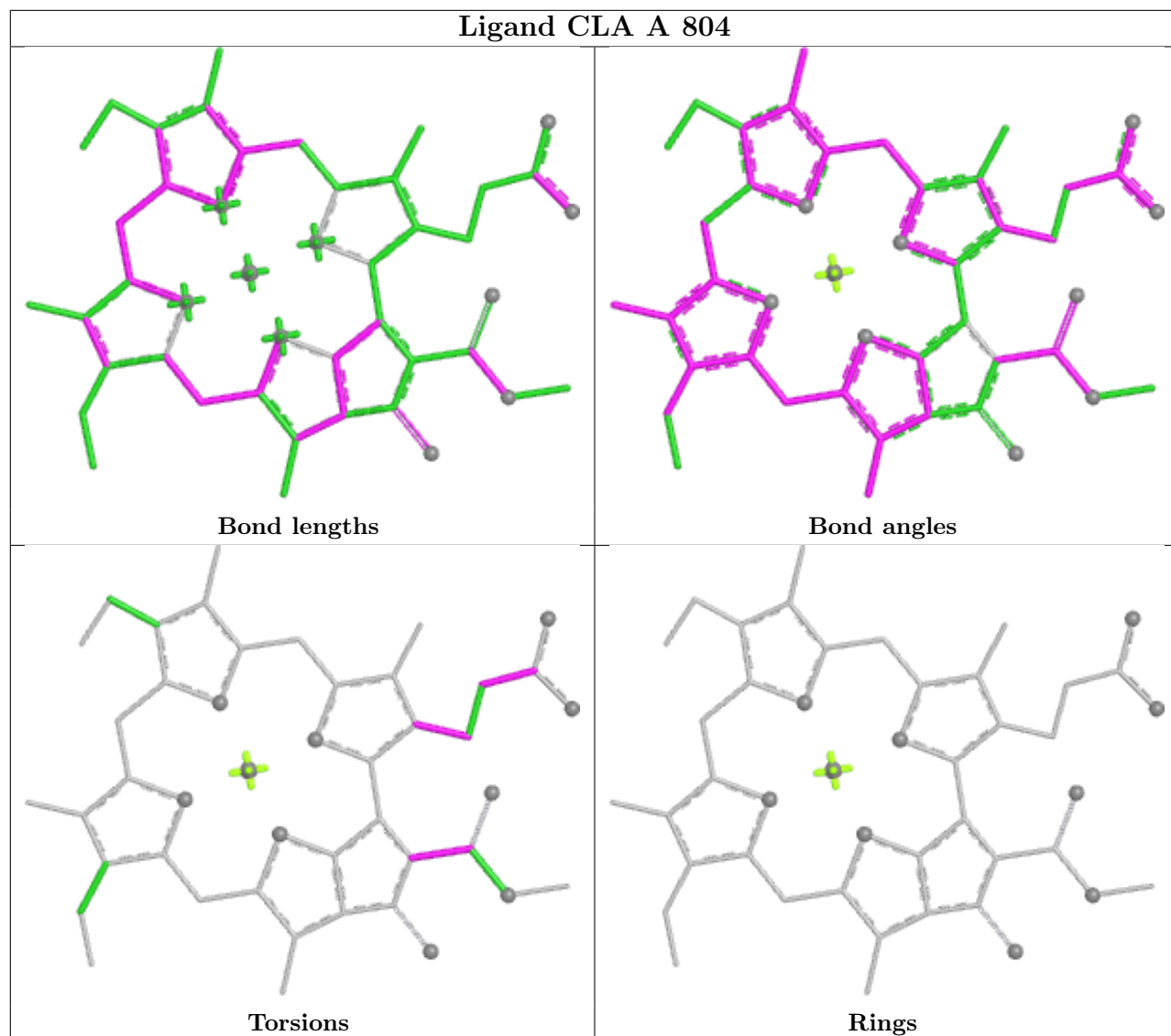


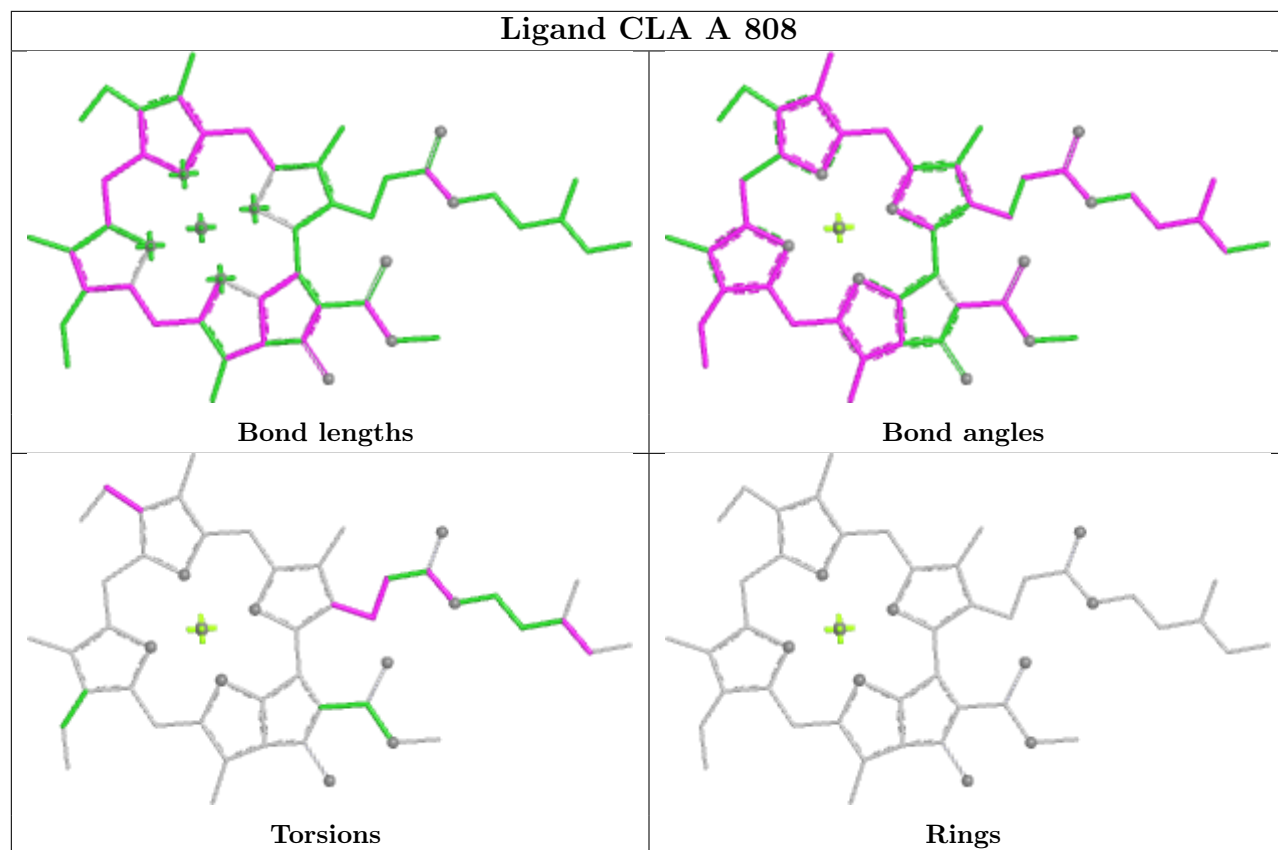
Ligand CLA K 203

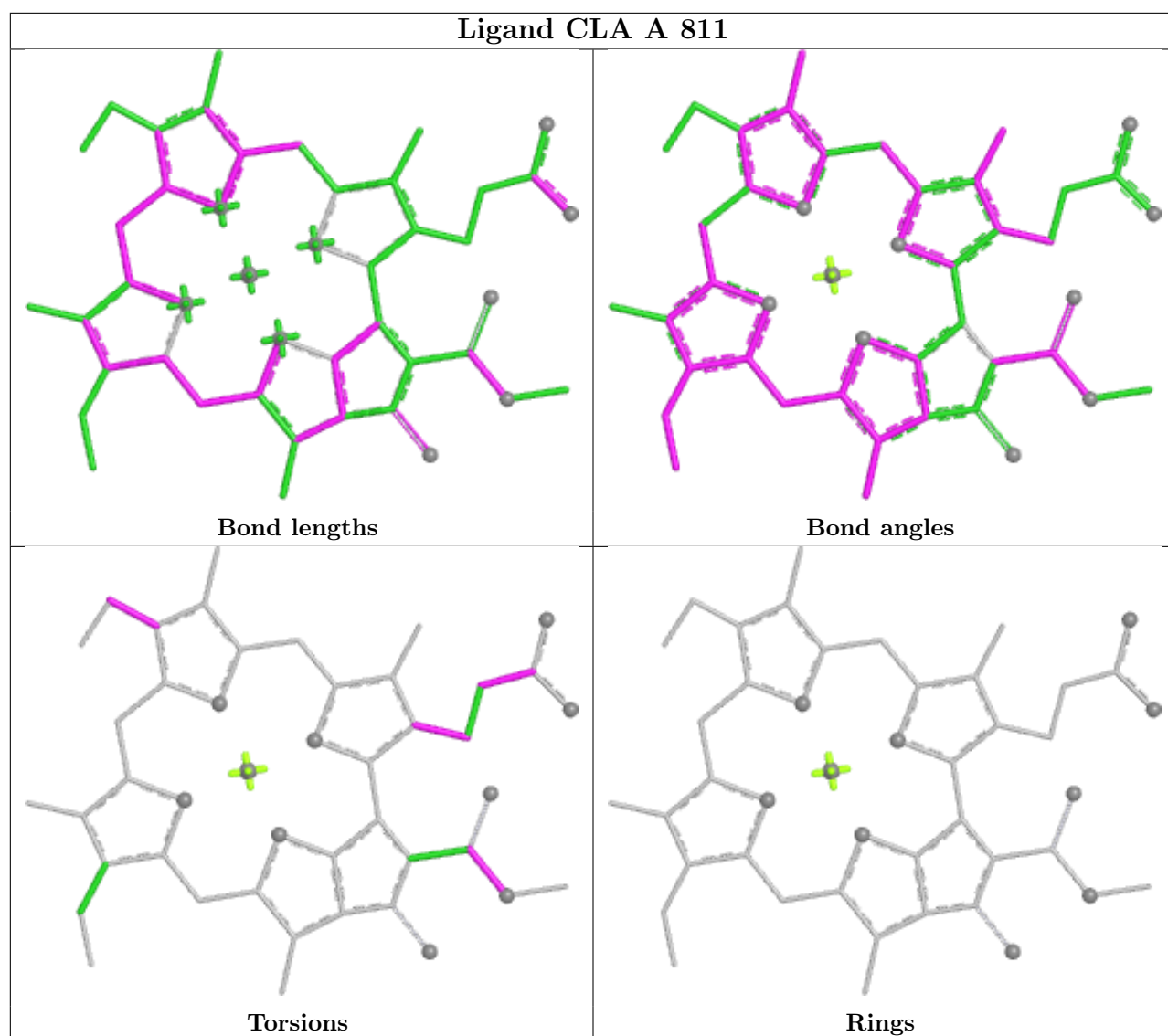




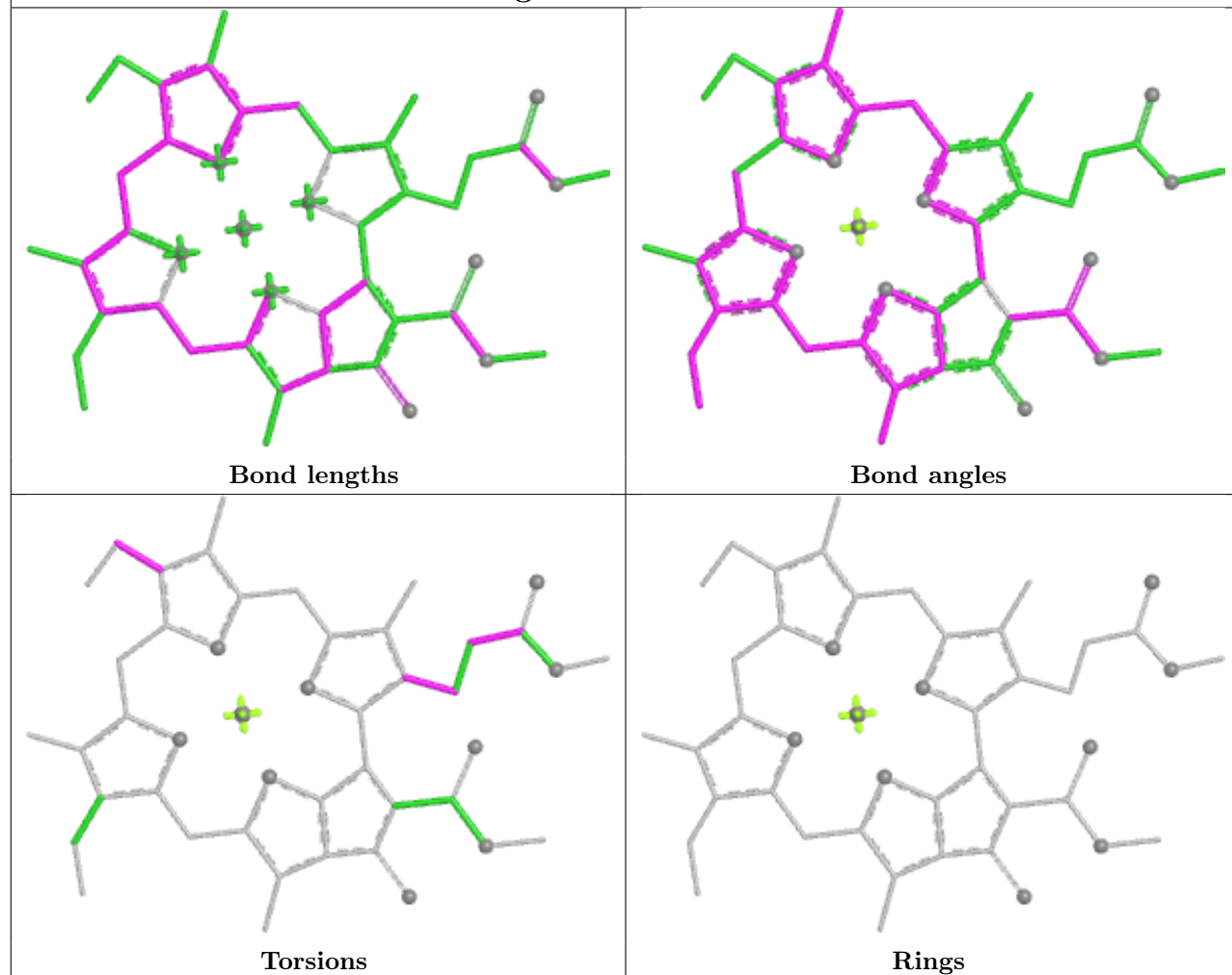




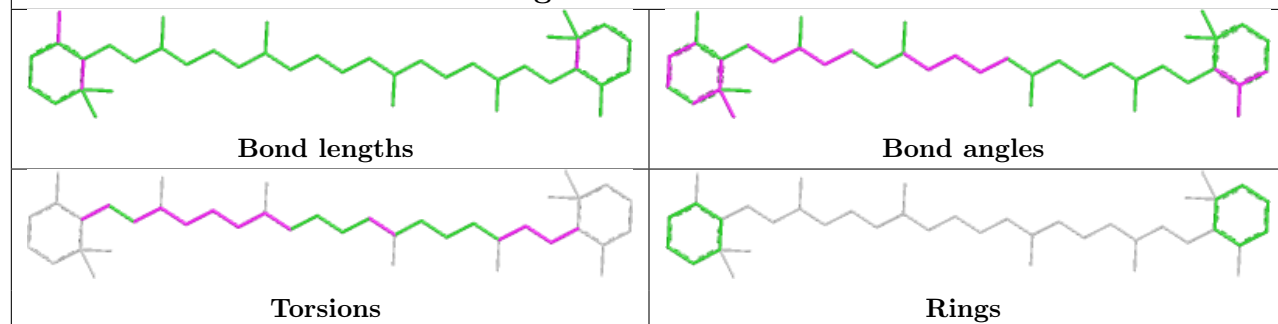


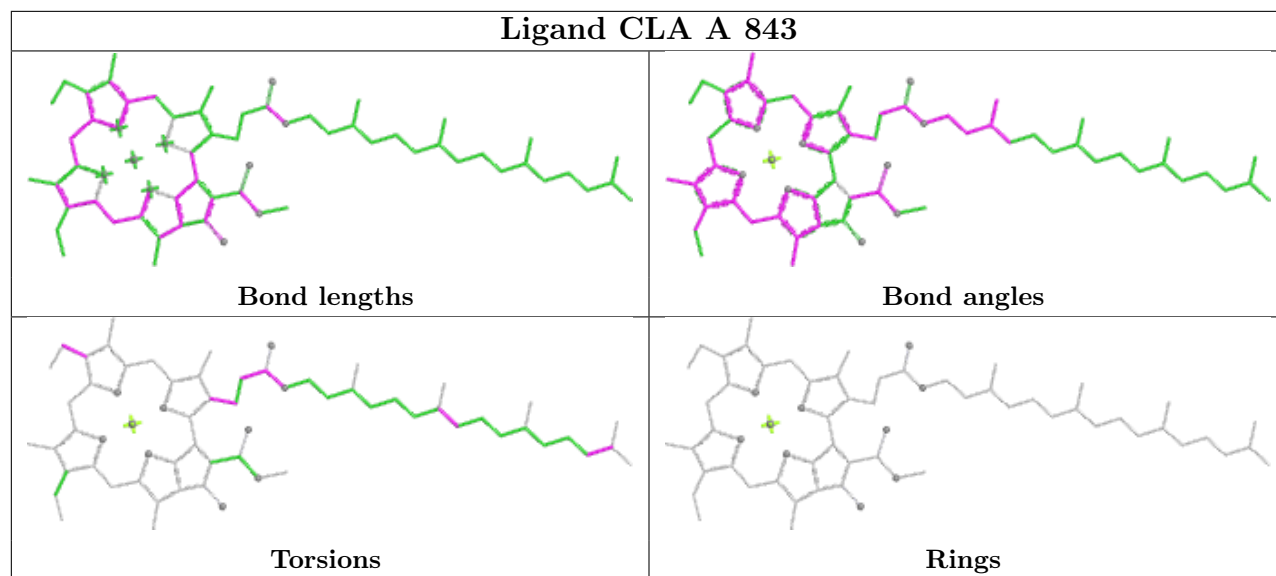


Ligand CLA L 202



Ligand BCR J 103





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.

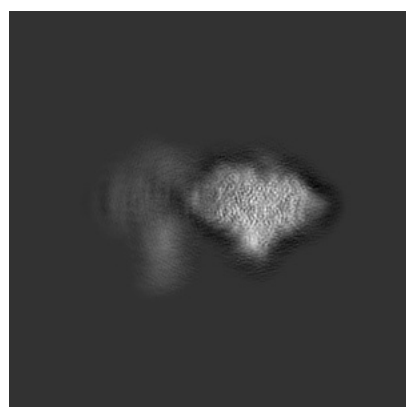
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30820. These allow visual inspection of the internal detail of the map and identification of artifacts.

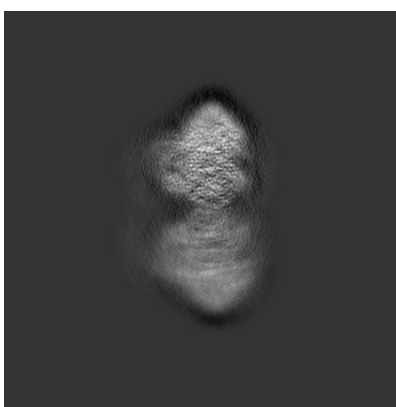
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

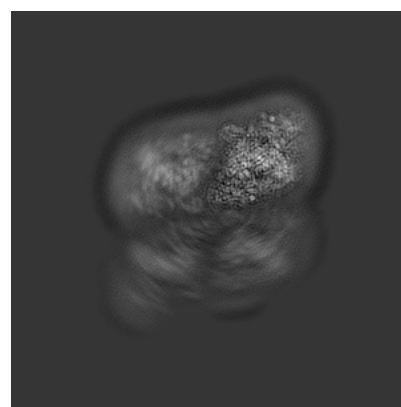
6.1.1 Primary map



X



Y

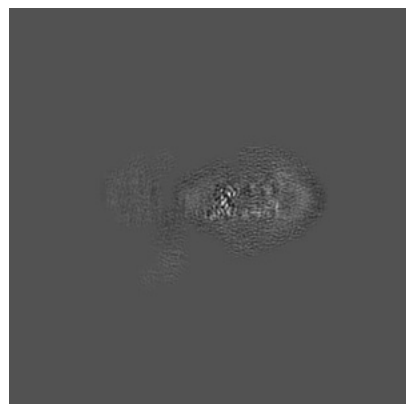


Z

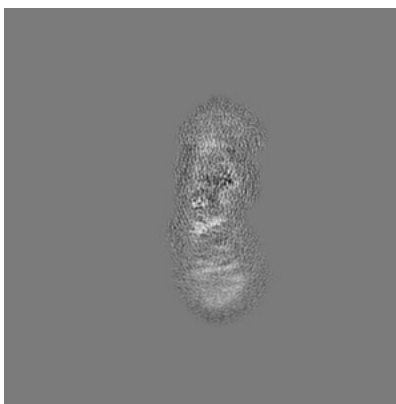
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

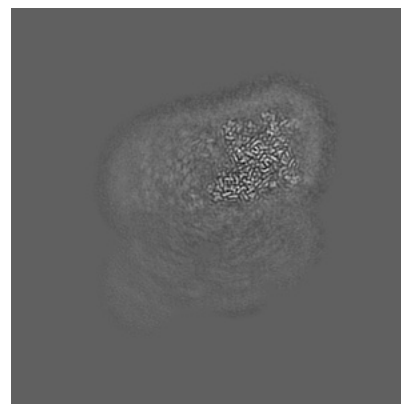
6.2.1 Primary map



X Index: 200



Y Index: 200

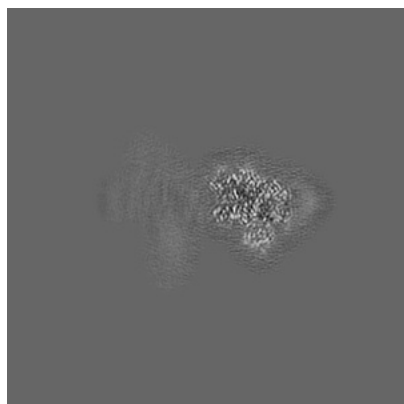


Z Index: 200

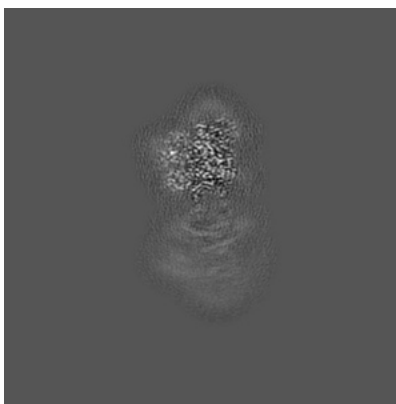
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

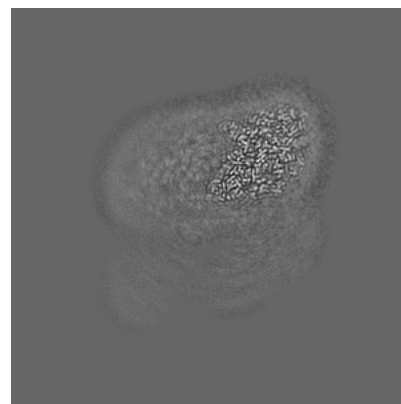
6.3.1 Primary map



X Index: 233



Y Index: 247

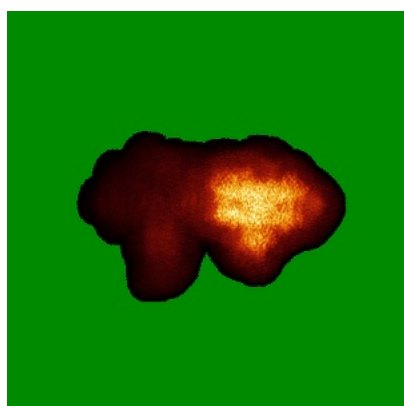


Z Index: 216

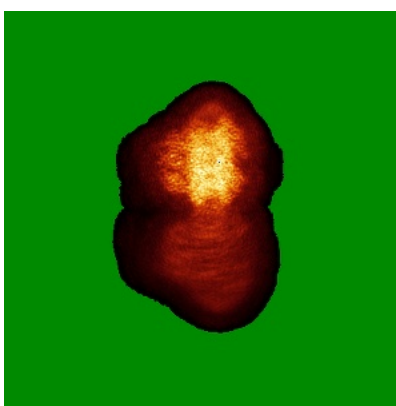
The images above show the largest variance slices of the map in three orthogonal directions.

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

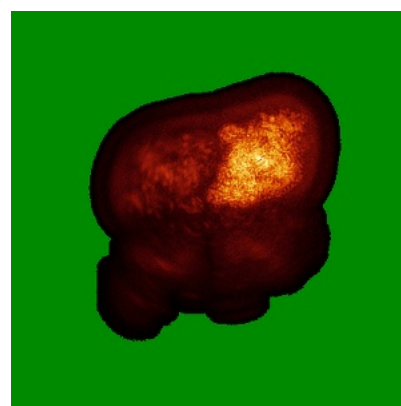
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

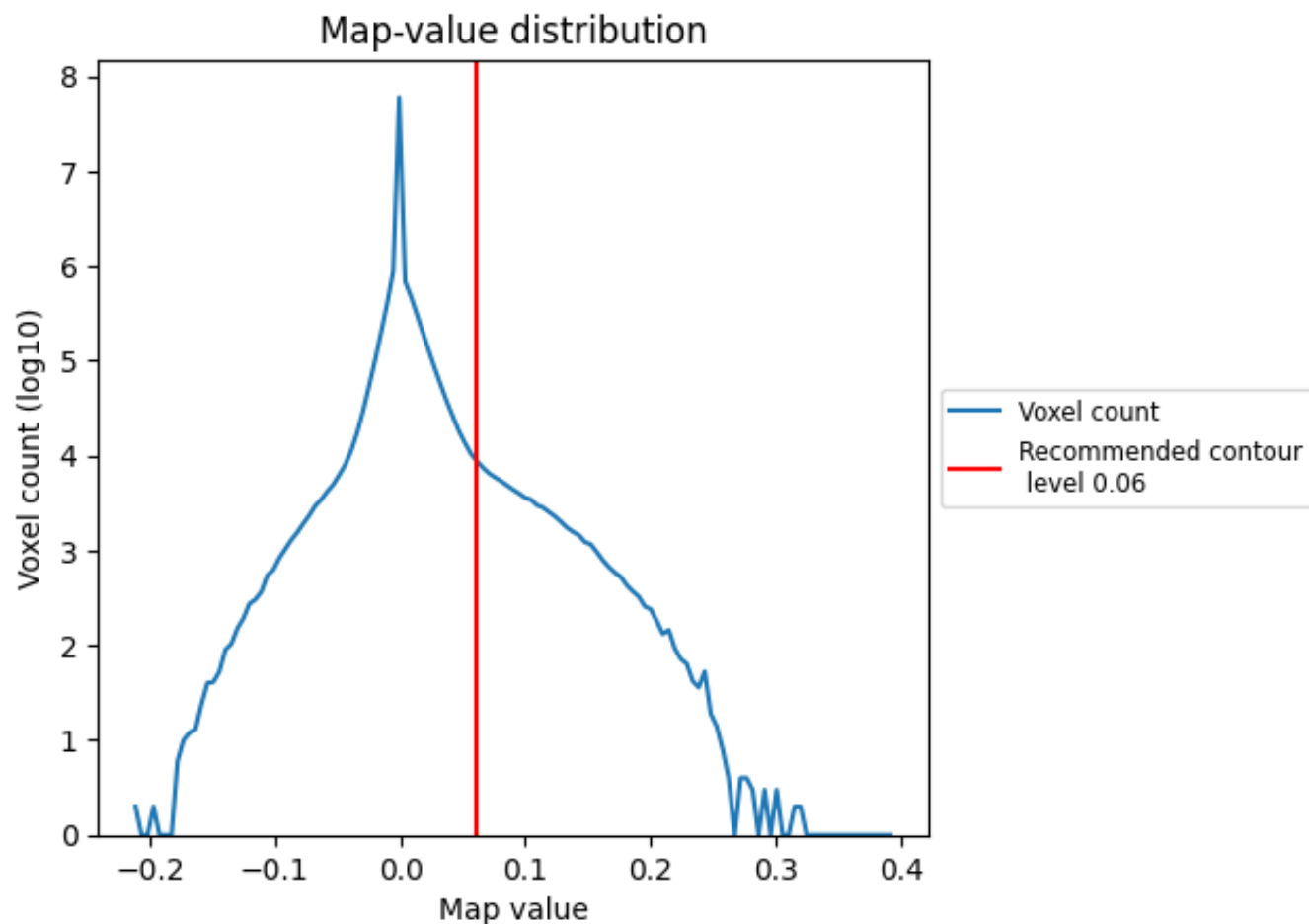
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

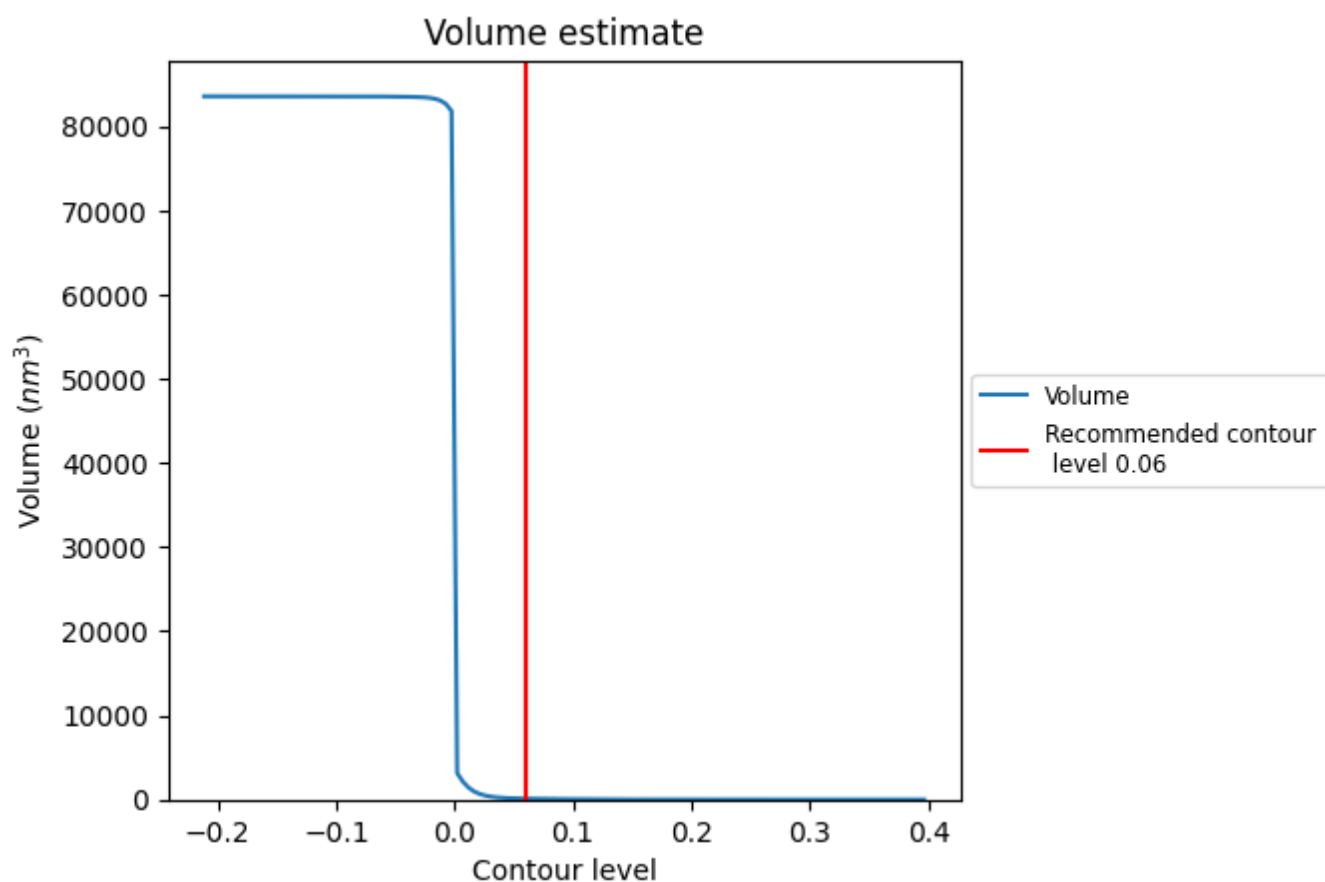
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

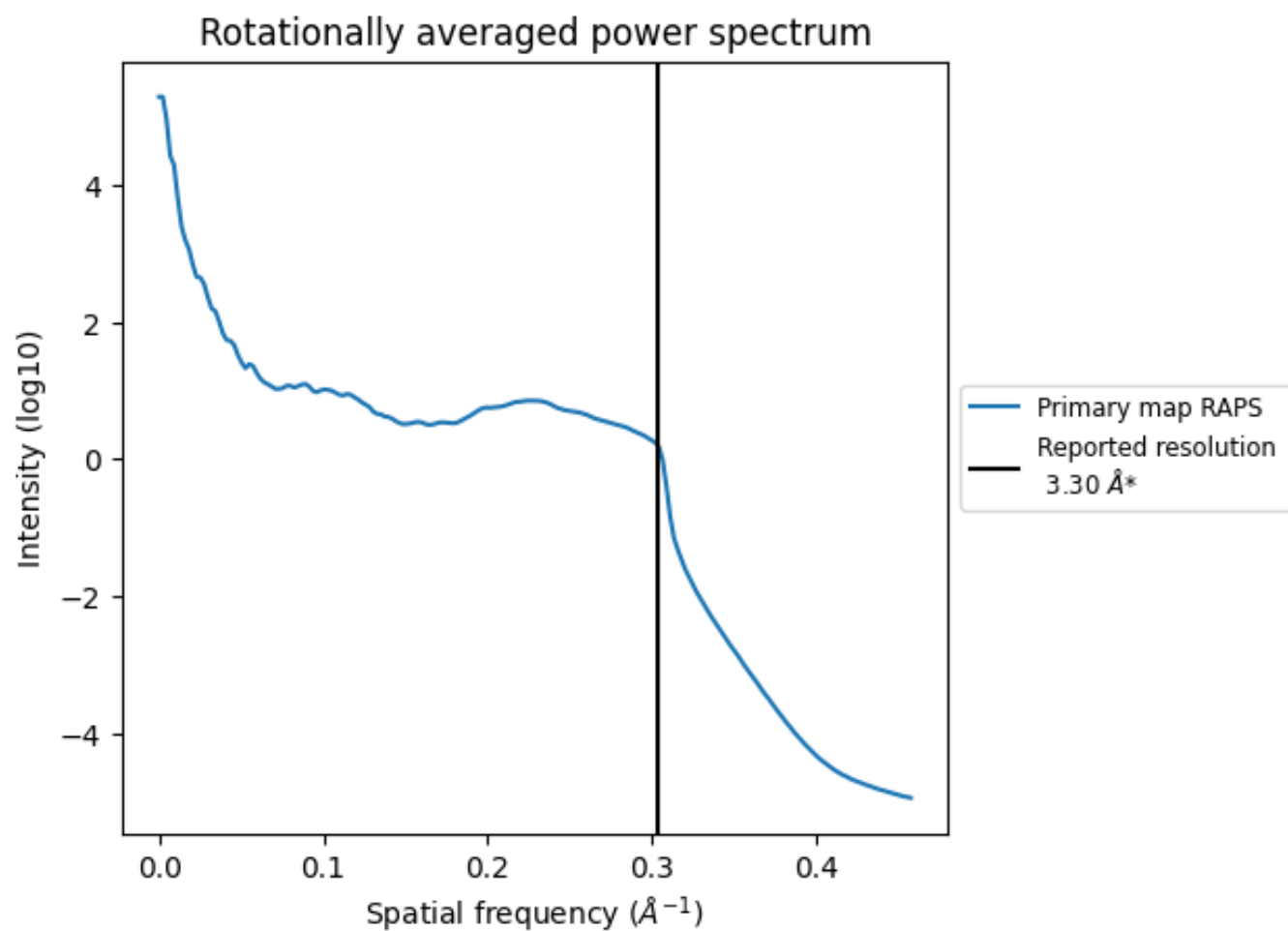
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 108 nm^3 ; this corresponds to an approximate mass of 98 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 ⓘ

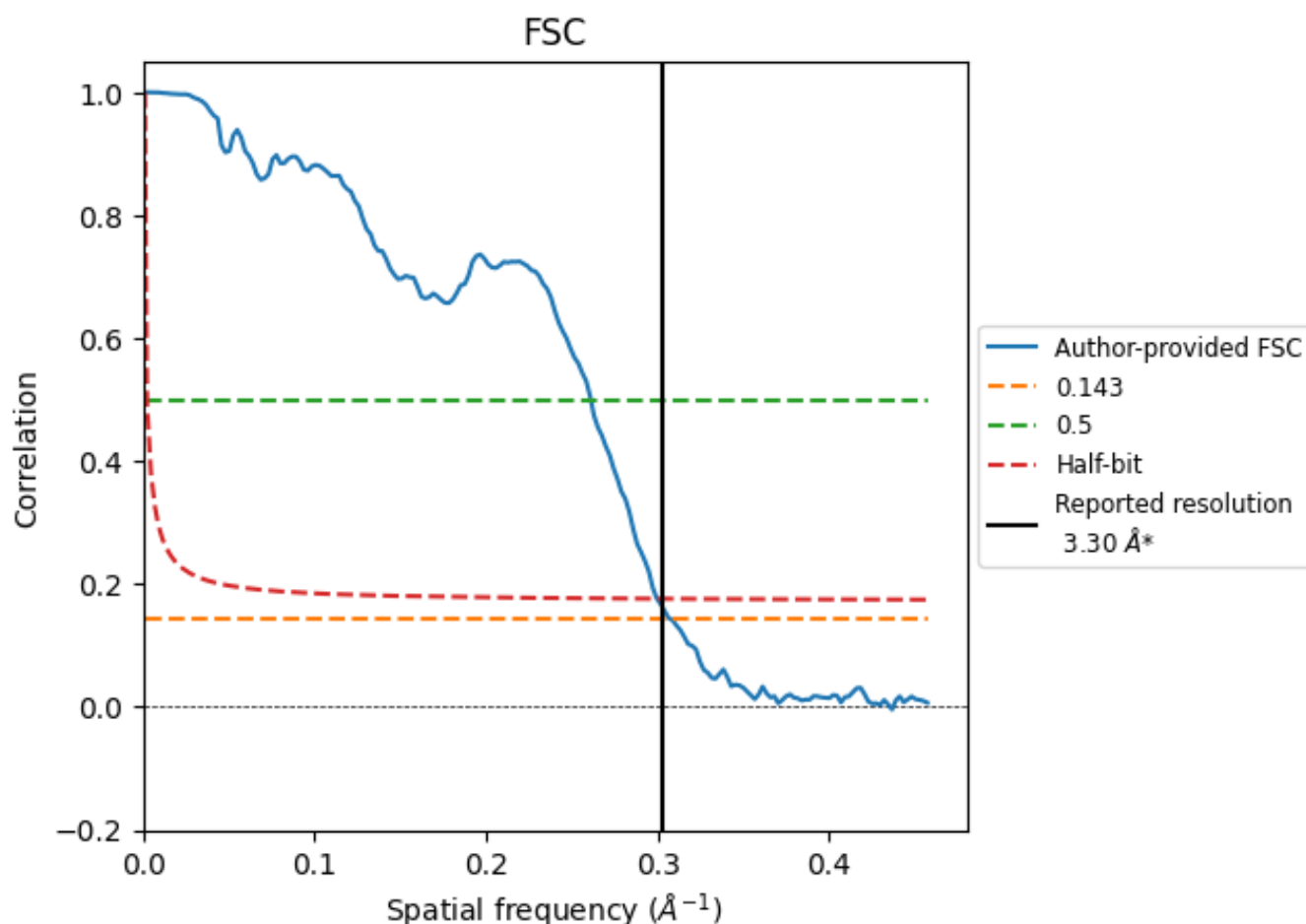


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

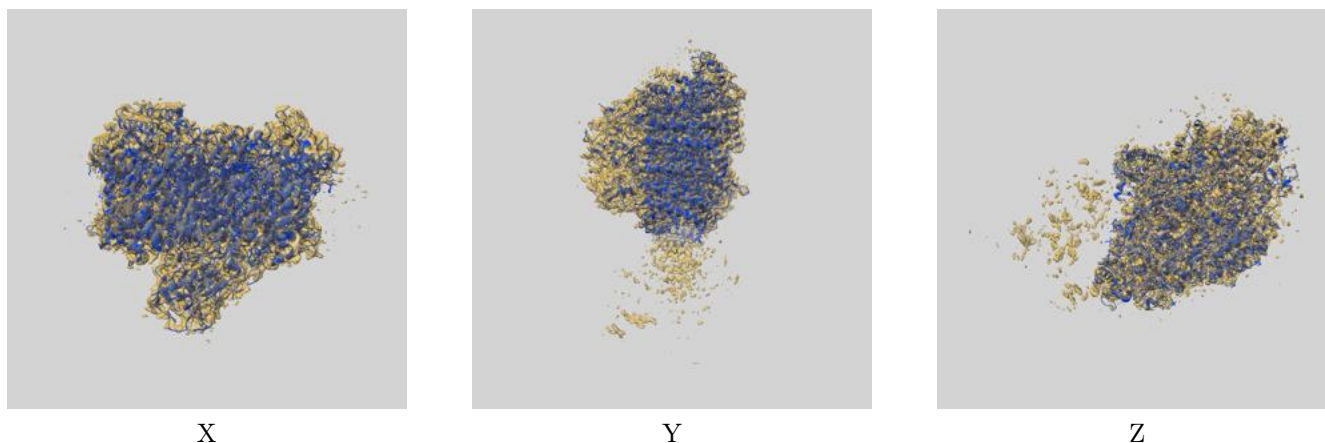
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.25	3.83	3.34
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

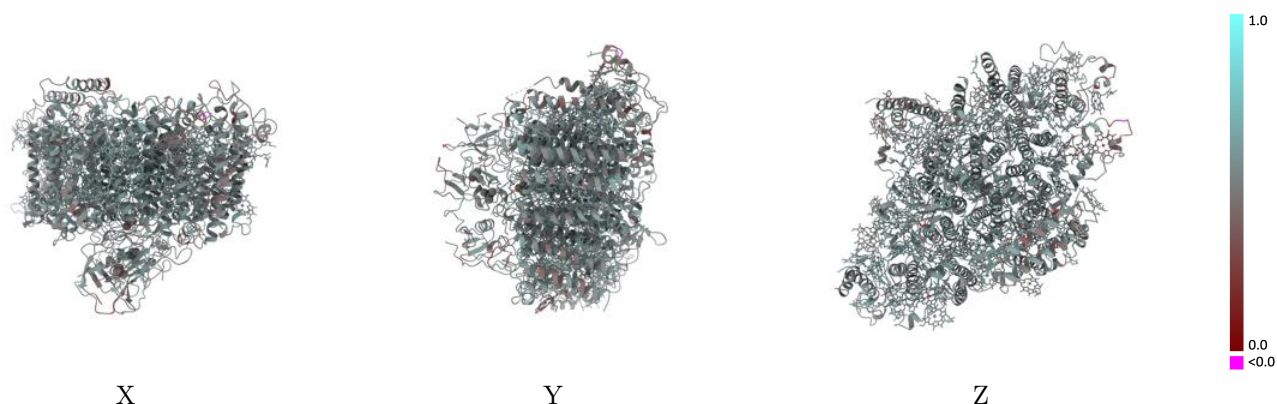
This section contains information regarding the fit between EMDB map EMD-30820 and PDB model 7DR0. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



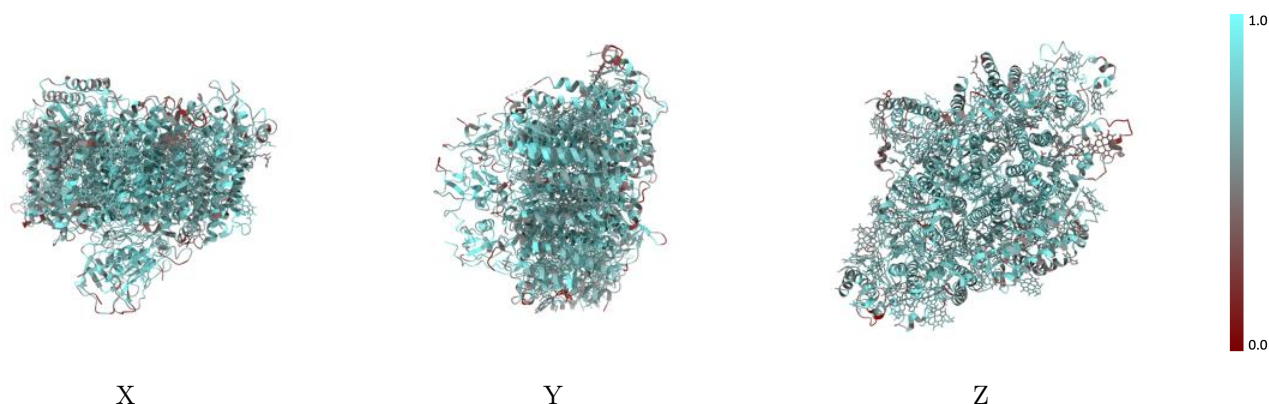
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



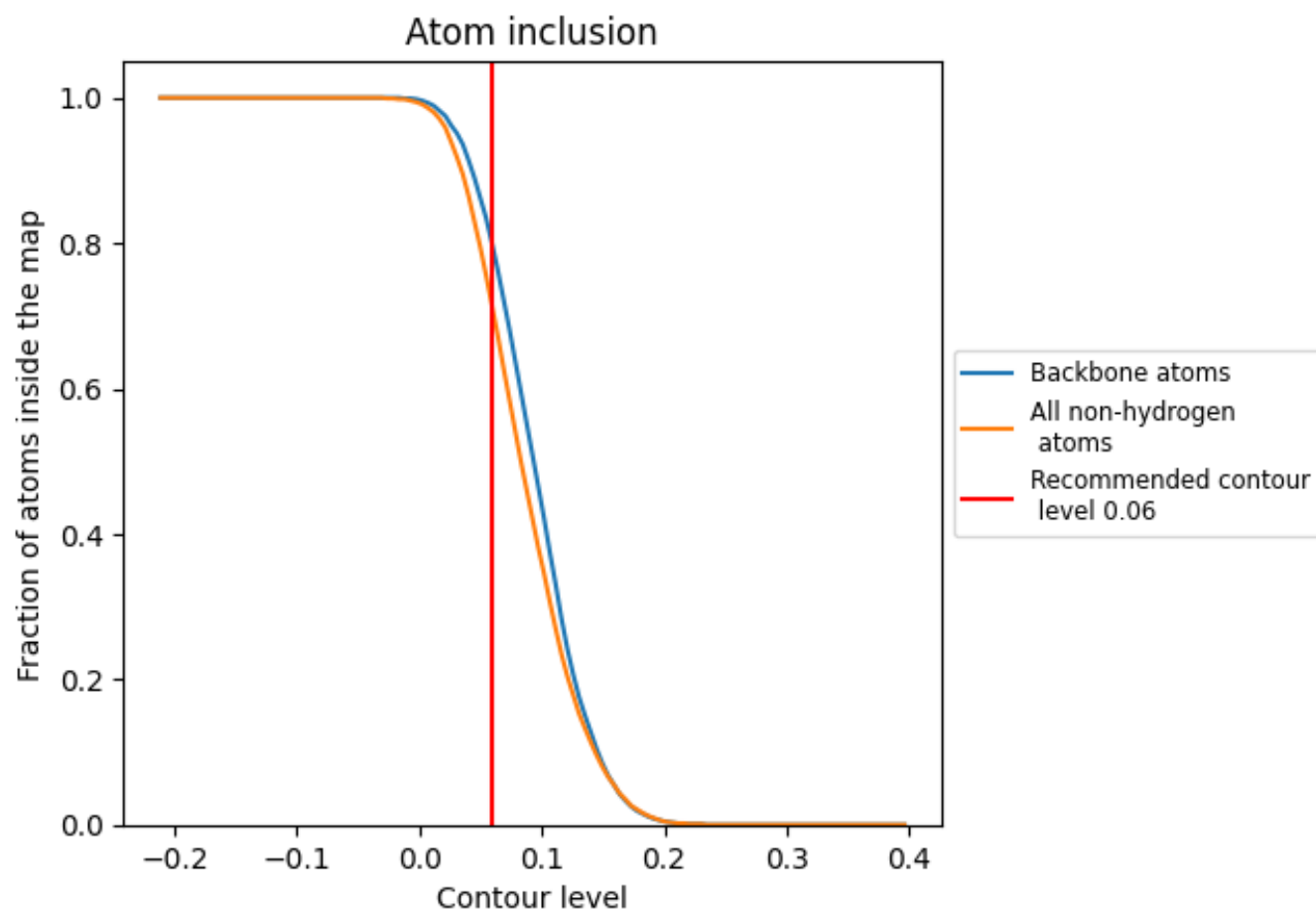
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 80% of all backbone atoms, 71% 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	0.7090	0.5300
A	0.7420	0.5480
B	0.7170	0.5290
C	0.7920	0.5060
D	0.7190	0.5020
E	0.6930	0.4980
F	0.6460	0.5030
I	0.6290	0.5120
J	0.5750	0.5230
K	0.5520	0.5180
L	0.6200	0.5010
M	0.5910	0.5210

1.0

0.0

<0.0