



Full wwPDB X-ray Structure Validation Report

Jun 16, 2014 – 03:58 PM EDT

PDB ID : 4LCZ
Title : Crystal structure of a multilayer-packed major light-harvesting complex
Authors : Wan, T.; Li, M.; Chang, W.R.
Deposited on : 2013-06-24
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

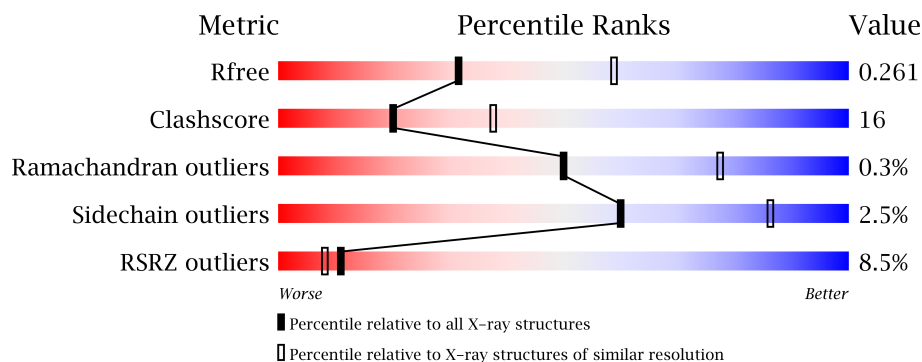
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	
1	C	224	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NEX	A	303	-	X
3	NEX	B	303	-	X
4	LHG	A	304	-	X
4	LHG	B	304	-	X
5	CHL	A	309	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
6	CLA	A	306	-	X
6	CLA	A	307	-	X
6	CLA	B	307	-	X
6	CLA	B	316	-	X
6	CLA	C	307	-	X
7	CAC	A	319	X	-
7	CAC	B	319	X	-
7	CAC	C	319	X	-
9	NA	C	320	-	X
9	NA	C	323	-	X

2 Entry composition i

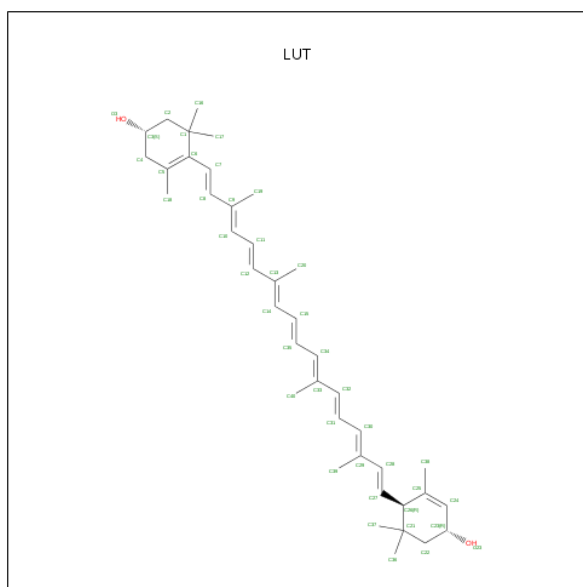
There are 10 unique types of molecules in this entry. The entry contains 8016 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Major chlorophyll a/b binding protein LHCb1.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1579	1023	257	292	7			
1	B	208	Total	C	N	O	S	0	0	0
			1579	1023	257	292	7			
1	C	208	Total	C	N	O	S	0	0	0
			1579	1023	257	292	7			

- Molecule 2 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



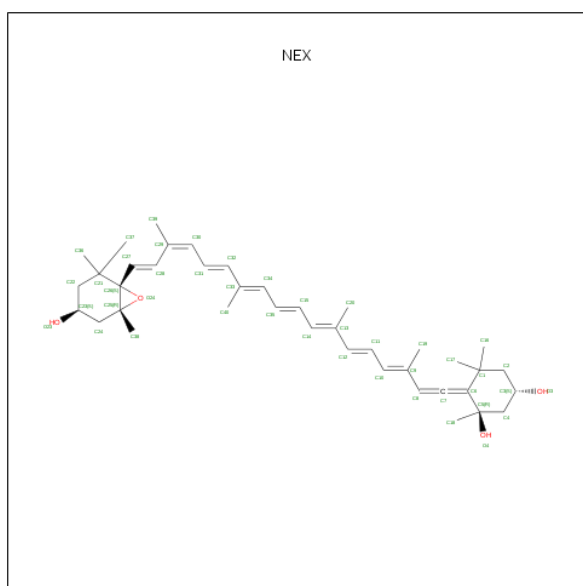
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			42	40	2		
2	A	1	Total	C	O	0	0
			42	40	2		
2	B	1	Total	C	O	0	0
			42	40	2		

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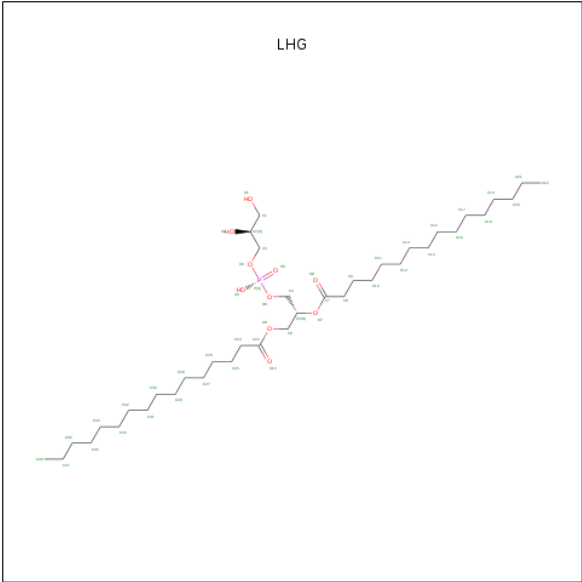
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		

- Molecule 3 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



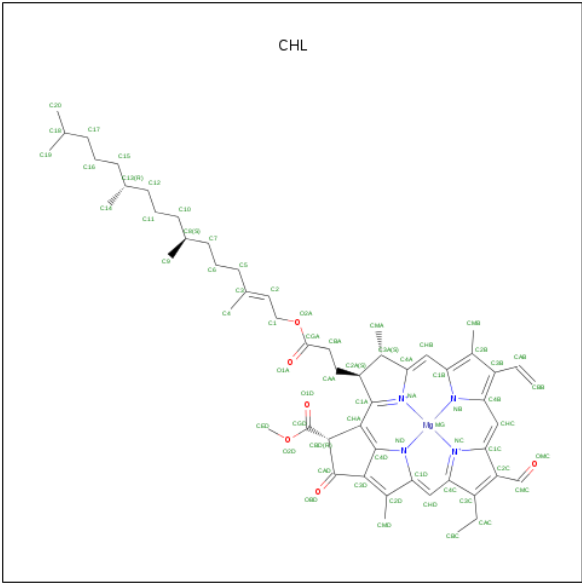
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			44	40	4		
3	B	1	Total	C	O	0	0
			44	40	4		
3	C	1	Total	C	O	0	0
			44	40	4		

- Molecule 4 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			49	38	10	1		
4	B	1	Total	C	O	P	0	0
			49	38	10	1		
4	C	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 5 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



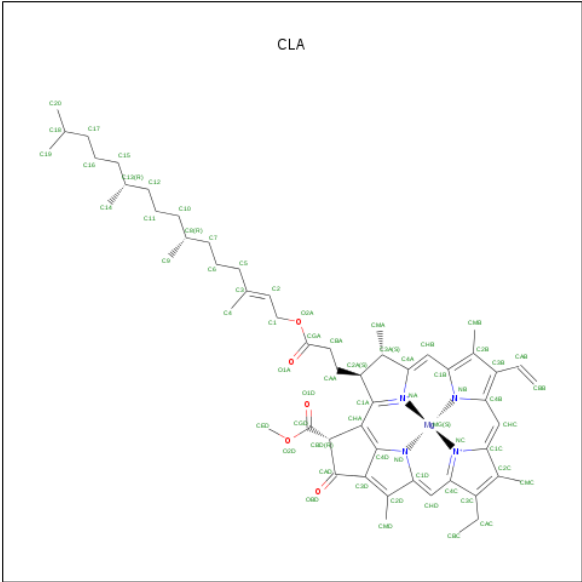
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	B	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			48	37	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			51	40	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		
5	C	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

- Molecule 6 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



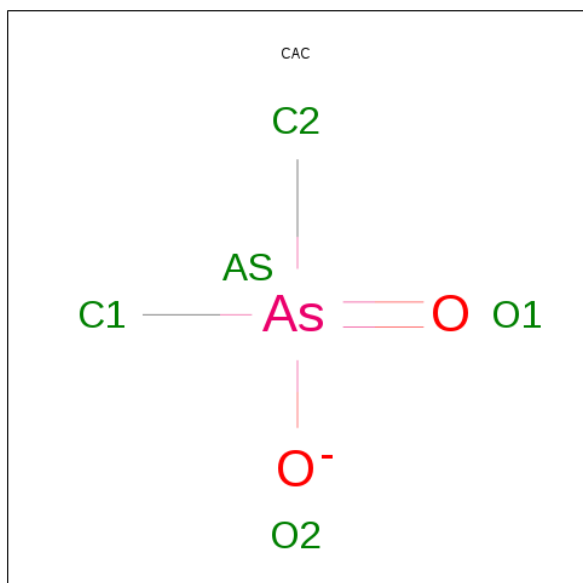
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	A	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			62	52	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			40	32	1	4	3		

- Molecule 7 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	As	C	O	0	0
			5	1	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	As	C	O	0	0
			5	1	2	2		
7	C	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Zn	0	0
			1	1		
8	A	3	Total	Zn	0	0
			3	3		
8	C	1	Total	Zn	0	0
			1	1		

- Molecule 9 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	Na	0	0
			2	2		
9	C	3	Total	Na	0	0
			3	3		

- Molecule 10 is water.

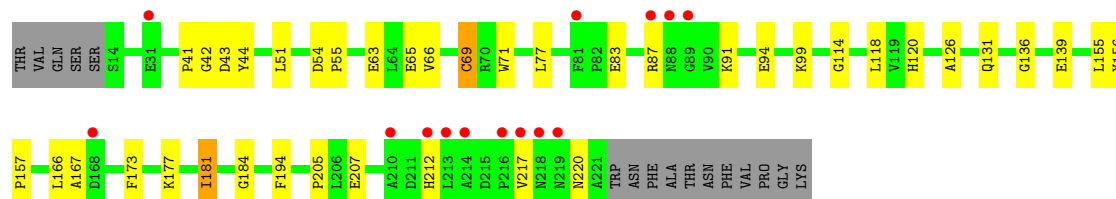
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	58	Total	O	0	0
			58	58		
10	B	46	Total	O	0	0
			46	46		
10	C	52	Total	O	0	0
			52	52		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

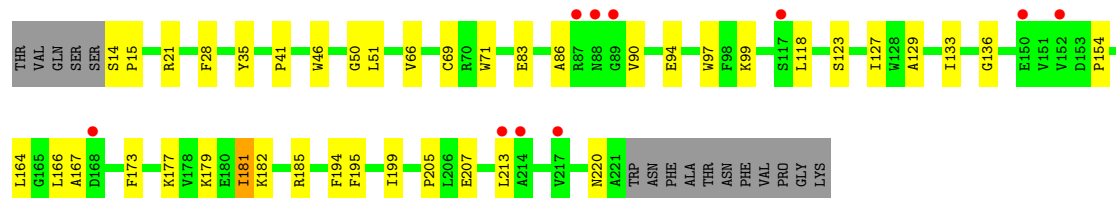
- Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain A: 



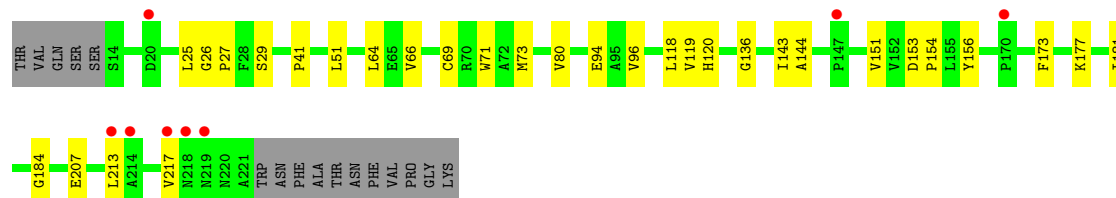
- Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain B: 



- Molecule 1: Major chlorophyll a/b binding protein LHCb1.3

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.19Å 115.10Å 109.60Å 90.00° 113.23° 90.00°	Depositor
Resolution (Å)	43.45 – 2.60 49.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.4 (43.45-2.60) 83.4 (49.97-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3.928)	Depositor
R, R_{free}	0.250 , 0.258 0.239 , 0.261	Depositor DCC
R_{free} test set	2945 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 60677 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8016	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, ZN, LUT, NA, CHL, CLA, NEX, CAC

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	0.51	1/1626 (0.1%)	0.60	0/2212
1	B	0.53	0/1626	0.60	0/2212
1	C	0.53	0/1626	0.64	0/2212
All	All	0.52	1/4878 (0.0%)	0.61	0/6636

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	CYS	CB-SG	-5.30	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1579	0	1520	33	0
1	B	1579	0	1521	31	0
1	C	1579	0	1521	20	0
2	A	84	0	112	6	0
2	B	84	0	112	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	84	0	112	7	0
3	A	44	0	56	3	0
3	B	44	0	56	3	0
3	C	44	0	56	3	0
4	A	49	0	74	9	0
4	B	49	0	74	5	0
4	C	49	0	74	5	0
5	A	363	0	350	23	0
5	B	363	0	350	22	0
5	C	363	0	350	21	0
6	A	493	0	522	43	0
6	B	493	0	524	43	0
6	C	492	0	521	47	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
7	C	5	0	0	0	0
8	A	3	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
9	B	2	0	0	0	0
9	C	3	0	0	0	0
10	A	58	0	0	1	0
10	B	46	0	0	2	0
10	C	52	0	0	2	0
All	All	8016	0	7905	250	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (250) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:C:304:LHG:C14	6:C:317:CLA:H93	1.72	1.19
6:C:306:CLA:H92	6:C:307:CLA:HMA1	1.20	1.14
4:A:304:LHG:H142	6:A:317:CLA:H93	1.22	1.12
4:A:304:LHG:C14	6:A:317:CLA:H93	1.83	1.08
6:B:306:CLA:H92	6:B:307:CLA:HMA1	1.32	1.08
4:B:304:LHG:H142	6:B:317:CLA:H93	1.37	1.06
6:A:307:CLA:C9	6:C:307:CLA:H92	1.85	1.06
4:C:304:LHG:H142	6:C:317:CLA:H93	1.05	1.03
6:A:307:CLA:H92	6:C:307:CLA:H92	1.40	1.03
4:C:304:LHG:H142	6:C:317:CLA:C9	1.96	0.95
6:A:306:CLA:H92	6:A:307:CLA:HMA1	1.56	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:A:307:CLA:C9	6:C:307:CLA:C9	2.52	0.87
6:B:306:CLA:C9	6:B:307:CLA:HMA1	2.03	0.87
4:B:304:LHG:C14	6:B:317:CLA:H93	2.03	0.87
6:C:306:CLA:C9	6:C:307:CLA:HMA1	2.05	0.85
2:C:301:LUT:H30	6:C:314:CLA:H52	1.65	0.78
6:A:306:CLA:H93	6:A:307:CLA:HMB3	1.67	0.77
6:B:306:CLA:H92	6:B:307:CLA:CMA	2.15	0.76
6:B:315:CLA:HBD	6:B:315:CLA:HBA1	1.69	0.75
6:C:306:CLA:H92	6:C:307:CLA:CMA	2.10	0.75
6:A:307:CLA:HBB1	6:A:307:CLA:HHC	1.69	0.75
6:B:307:CLA:H92	6:C:307:CLA:H93	1.70	0.73
1:B:136:GLY:HA2	5:B:313:CHL:HAB	1.72	0.70
6:B:306:CLA:C9	6:B:307:CLA:HHB	2.22	0.70
5:A:310:CHL:HBA2	5:A:310:CHL:HBD	1.72	0.69
5:B:311:CHL:O1A	10:B:446:HOH:O	2.11	0.69
6:C:316:CLA:HBB1	6:C:316:CLA:HHC	1.73	0.68
5:B:305:CHL:HHC	5:B:305:CHL:HBB1	1.76	0.67
6:A:306:CLA:H93	6:A:307:CLA:CMB	2.25	0.66
1:A:136:GLY:HA2	5:A:313:CHL:HAB	1.77	0.66
5:B:305:CHL:H2	5:C:311:CHL:H201	1.78	0.65
5:B:310:CHL:HBA2	5:B:310:CHL:HBD	1.77	0.65
1:C:41:PRO:HG3	1:C:177:LYS:HB3	1.78	0.65
4:A:304:LHG:H141	6:A:317:CLA:H93	1.76	0.65
1:B:28:PHE:O	1:C:144:ALA:HB2	1.97	0.64
1:C:136:GLY:HA2	5:C:313:CHL:HAB	1.79	0.64
6:A:307:CLA:H92	6:C:307:CLA:C9	2.22	0.63
6:B:307:CLA:HHC	6:B:307:CLA:HBB1	1.80	0.63
6:A:318:CLA:HBB1	6:A:318:CLA:HHC	1.81	0.63
5:A:305:CHL:HBB1	5:A:305:CHL:HHC	1.80	0.62
5:B:312:CHL:HHC	5:B:312:CHL:HBB1	1.81	0.62
6:C:315:CLA:HBD	6:C:315:CLA:HBA1	1.82	0.61
1:A:41:PRO:HG3	1:A:177:LYS:HB3	1.82	0.61
5:A:312:CHL:HHC	5:A:312:CHL:HBB1	1.82	0.60
6:A:315:CLA:H18	6:A:316:CLA:H193	1.83	0.60
1:A:156:TYR:CE2	1:A:177:LYS:HE2	2.36	0.60
6:C:307:CLA:HHC	6:C:307:CLA:HBB1	1.83	0.59
1:B:66:VAL:O	1:B:69:CYS:HB2	2.02	0.59
6:B:307:CLA:C9	6:C:307:CLA:H93	2.32	0.59
5:C:312:CHL:HBB1	5:C:312:CHL:HHC	1.83	0.59
4:C:304:LHG:H141	6:C:317:CLA:H93	1.80	0.59
1:A:66:VAL:O	1:A:69:CYS:HB2	2.03	0.59
1:B:99:LYS:HA	5:B:311:CHL:HED2	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:301:LUT:H34	6:B:314:CLA:CBB	2.32	0.59
5:B:305:CHL:H142	5:B:305:CHL:H91	1.84	0.58
5:C:310:CHL:HBD	5:C:310:CHL:HBA2	1.84	0.58
2:B:301:LUT:C31	6:B:314:CLA:HMC2	2.33	0.58
5:C:305:CHL:HHC	5:C:305:CHL:HBB1	1.84	0.58
1:A:156:TYR:CD2	1:A:177:LYS:HE2	2.39	0.58
1:A:51:LEU:HD12	2:A:302:LUT:H221	1.86	0.58
1:C:173:PHE:CZ	1:C:177:LYS:HE3	2.39	0.58
6:B:306:CLA:H93	6:B:307:CLA:HHB	1.85	0.57
1:A:71:TRP:CD1	5:A:313:CHL:HMD3	2.38	0.57
5:B:310:CHL:HBB2	5:B:311:CHL:HBB1	1.85	0.57
6:C:306:CLA:H93	6:C:307:CLA:HHB	1.87	0.57
1:C:71:TRP:CD1	5:C:313:CHL:HMD3	2.39	0.57
5:A:309:CHL:HHD	5:A:310:CHL:OBD	2.05	0.56
6:A:316:CLA:HBB1	6:A:316:CLA:HHC	1.87	0.56
1:B:46:TRP:CE3	2:B:302:LUT:H383	2.41	0.56
6:C:306:CLA:H93	6:C:307:CLA:HMB3	1.88	0.55
6:B:307:CLA:H92	6:C:307:CLA:C9	2.36	0.55
1:A:139:GLU:HG3	5:A:313:CHL:C4B	2.38	0.54
6:C:306:CLA:C9	6:C:307:CLA:HHB	2.38	0.54
5:C:305:CHL:H141	5:C:305:CHL:H193	1.89	0.54
4:A:304:LHG:C14	6:A:317:CLA:C9	2.73	0.53
6:A:315:CLA:HBD	6:A:315:CLA:HBA1	1.90	0.53
6:A:306:CLA:H92	6:A:307:CLA:HHB	1.90	0.53
6:B:315:CLA:H18	6:B:316:CLA:H193	1.91	0.53
5:A:313:CHL:HBB1	5:C:305:CHL:H51	1.89	0.53
6:B:316:CLA:HBB1	6:B:316:CLA:HHC	1.92	0.52
4:A:304:LHG:H222	6:B:307:CLA:H201	1.91	0.52
1:A:194:PHE:HE2	2:A:301:LUT:H41	1.73	0.52
6:C:306:CLA:HHC	6:C:306:CLA:HBB1	1.92	0.52
5:A:305:CHL:H141	5:A:305:CHL:H193	1.92	0.52
6:A:307:CLA:H93	6:C:307:CLA:H92	1.86	0.52
1:B:166:LEU:HD12	6:B:314:CLA:CGA	2.39	0.51
2:C:302:LUT:H32	6:C:306:CLA:CBB	2.40	0.51
1:C:118:LEU:O	1:C:120:HIS:N	2.44	0.51
1:A:131:GLN:OE1	5:A:311:CHL:HMC	2.10	0.50
6:A:314:CLA:HBB1	6:A:314:CLA:HHC	1.93	0.50
5:C:312:CHL:O1A	6:C:314:CLA:HMD2	2.11	0.50
1:A:99:LYS:HA	5:A:311:CHL:HED2	1.92	0.50
6:B:307:CLA:HAC2	5:B:311:CHL:H162	1.93	0.50
5:B:305:CHL:H141	5:B:305:CHL:H193	1.94	0.50
6:B:306:CLA:H92	6:B:307:CLA:HHB	1.94	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:182:LYS:HE2	6:B:315:CLA:O1D	2.11	0.50
1:A:166:LEU:HD12	6:A:314:CLA:CGA	2.40	0.49
1:B:41:PRO:HG3	1:B:177:LYS:HB3	1.92	0.49
1:B:164:LEU:HD12	2:B:301:LUT:H222	1.95	0.49
6:A:307:CLA:H91	6:C:307:CLA:C9	2.41	0.49
1:A:173:PHE:CZ	1:A:177:LYS:HE3	2.48	0.49
1:B:167:ALA:HB1	1:B:173:PHE:CD1	2.48	0.49
2:C:302:LUT:H382	6:C:306:CLA:HBA1	1.95	0.48
1:A:42:GLY:O	1:A:44:TYR:HD1	1.96	0.48
1:A:65:GLU:HG2	1:A:181:ILE:HD11	1.95	0.48
6:C:314:CLA:H12	6:C:314:CLA:HMB2	1.95	0.48
1:C:25:LEU:HB2	1:C:29:SER:HA	1.96	0.48
4:A:304:LHG:H281	4:A:304:LHG:HC91	1.96	0.48
1:A:51:LEU:HD13	6:A:306:CLA:H42	1.96	0.48
1:C:173:PHE:CE1	6:C:314:CLA:HED3	2.48	0.48
1:A:220:ASN:HB2	6:A:317:CLA:O1A	2.14	0.48
1:B:173:PHE:CZ	1:B:177:LYS:HE3	2.48	0.48
3:B:303:NEX:H183	3:B:303:NEX:H192	1.95	0.48
1:A:63:GLU:HA	1:A:155:LEU:HD21	1.96	0.47
1:B:21:ARG:HG2	1:B:21:ARG:HH11	1.78	0.47
4:B:304:LHG:H142	6:B:317:CLA:C9	2.27	0.47
5:B:305:CHL:H172	5:B:305:CHL:H13	1.47	0.47
1:A:139:GLU:HG3	5:A:313:CHL:NB	2.30	0.47
5:A:312:CHL:O1A	6:A:314:CLA:HMD2	2.14	0.47
2:B:301:LUT:H34	6:B:314:CLA:HBB2	1.95	0.47
1:B:71:TRP:CD1	5:B:313:CHL:HMD3	2.50	0.47
2:C:302:LUT:H11	2:C:302:LUT:H191	1.78	0.47
1:C:69:CYS:SG	1:C:184:GLY:HA3	2.55	0.47
6:B:306:CLA:H93	6:B:307:CLA:CMB	2.45	0.47
1:B:118:LEU:HD23	5:B:309:CHL:HED2	1.96	0.46
6:B:307:CLA:H62	6:B:307:CLA:H92	1.78	0.46
1:C:64:LEU:HD23	5:C:313:CHL:OBD	2.15	0.46
1:C:66:VAL:O	1:C:69:CYS:HB2	2.15	0.46
5:A:305:CHL:H41	5:A:305:CHL:H62	1.70	0.46
6:A:307:CLA:C9	6:C:307:CLA:H91	2.44	0.46
6:B:306:CLA:H41	6:B:306:CLA:H61	1.71	0.46
6:A:314:CLA:H12	6:A:314:CLA:HMB2	1.96	0.46
1:A:83:GLU:OE1	1:A:205:PRO:HD2	2.14	0.46
6:B:314:CLA:HAB	6:B:314:CLA:HMB1	1.55	0.46
1:A:91:LYS:O	1:A:114:GLY:HA3	2.15	0.46
2:A:301:LUT:C33	6:A:316:CLA:HMB2	2.46	0.46
5:A:311:CHL:H152	5:A:313:CHL:H71	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:83:GLU:OE1	1:B:205:PRO:HD2	2.16	0.46
6:C:314:CLA:H43	6:C:316:CLA:HBA1	1.97	0.46
1:B:14:SER:HA	1:B:15:PRO:HD3	1.83	0.46
6:A:307:CLA:H62	6:A:307:CLA:H92	1.67	0.46
5:A:305:CHL:HBA1	5:A:305:CHL:H3A	1.53	0.45
1:C:156:TYR:CE1	1:C:177:LYS:HG2	2.51	0.45
5:C:312:CHL:HMB1	5:C:312:CHL:HAB	1.60	0.45
1:C:51:LEU:HD13	6:C:306:CLA:H42	1.98	0.45
6:C:318:CLA:HBB1	6:C:318:CLA:HHC	1.98	0.45
2:C:302:LUT:C31	6:C:306:CLA:HMC2	2.47	0.45
2:A:301:LUT:C31	6:A:314:CLA:HMC2	2.47	0.45
1:B:179:LYS:HD3	6:B:316:CLA:HAA2	1.99	0.45
1:A:77:LEU:O	1:A:77:LEU:HD12	2.16	0.45
1:A:94:GLU:HG2	1:A:99:LYS:CB	2.45	0.45
2:B:301:LUT:C34	6:B:316:CLA:HMB2	2.47	0.45
5:B:305:CHL:H3A	5:B:305:CHL:HBA1	1.65	0.45
2:B:301:LUT:H31	6:B:314:CLA:HMC2	1.99	0.45
1:A:69:CYS:SG	1:A:184:GLY:HA3	2.57	0.44
2:A:301:LUT:H34	6:A:314:CLA:CBB	2.47	0.44
1:B:136:GLY:CA	5:B:313:CHL:HAB	2.43	0.44
1:A:173:PHE:CZ	6:A:314:CLA:HED3	2.52	0.44
3:C:303:NEX:H402	5:C:312:CHL:H152	2.00	0.44
1:B:35:TYR:HH	1:B:50:GLY:HA2	1.83	0.44
3:C:303:NEX:H191	3:C:303:NEX:H11	1.76	0.44
2:C:302:LUT:H32	6:C:306:CLA:HBB1	1.99	0.44
2:B:301:LUT:H11	2:B:301:LUT:H191	1.75	0.44
6:B:308:CLA:HAB	6:B:308:CLA:HMB1	1.68	0.44
5:A:312:CHL:CAD	6:A:314:CLA:HMD3	2.48	0.44
5:A:305:CHL:H172	5:A:305:CHL:H13	1.57	0.44
1:C:151:VAL:HG11	10:C:406:HOH:O	2.18	0.44
6:B:307:CLA:H41	6:C:307:CLA:H51	1.99	0.44
6:B:315:CLA:C1D	6:B:316:CLA:HMD2	2.48	0.43
2:A:301:LUT:H11	2:A:301:LUT:H191	1.81	0.43
5:B:305:CHL:H41	5:B:305:CHL:H62	1.78	0.43
5:B:305:CHL:H61	5:B:305:CHL:H101	1.46	0.43
5:C:305:CHL:HBA1	5:C:305:CHL:H3A	1.47	0.43
1:C:73:MET:SD	6:C:314:CLA:HBB1	2.58	0.43
6:A:307:CLA:H61	6:A:307:CLA:H41	1.80	0.43
6:A:314:CLA:H93	6:A:316:CLA:H102	2.01	0.43
6:B:314:CLA:HHC	6:B:314:CLA:HBB1	2.00	0.43
6:C:306:CLA:H93	6:C:307:CLA:CMB	2.48	0.43
1:C:143:ILE:HD11	5:C:313:CHL:HMA3	2.00	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:GLU:HG2	1:A:99:LYS:HB3	1.99	0.43
6:B:315:CLA:HBD	6:B:316:CLA:OBD	2.18	0.43
4:A:304:LHG:H151	4:A:304:LHG:H182	1.80	0.43
3:B:303:NEX:H11	3:B:303:NEX:H191	1.78	0.43
1:B:86:ALA:HA	1:B:90:VAL:O	2.19	0.43
4:A:304:LHG:H171	5:A:305:CHL:H42	2.00	0.43
1:B:181:ILE:HD12	1:B:185:ARG:NE	2.34	0.43
2:B:302:LUT:C31	6:B:306:CLA:HMC2	2.49	0.43
5:C:312:CHL:OMC	5:C:312:CHL:HHC	2.17	0.43
5:B:312:CHL:C4A	5:B:312:CHL:HBA2	2.49	0.42
1:B:35:TYR:OH	1:B:50:GLY:HA2	2.19	0.42
3:C:303:NEX:H401	3:C:303:NEX:H35	1.78	0.42
6:C:306:CLA:HAB	6:C:306:CLA:HMB1	1.73	0.42
5:A:312:CHL:H143	5:A:312:CHL:H161	1.74	0.42
6:A:314:CLA:HAB	6:A:314:CLA:HMB1	1.65	0.42
1:B:129:ALA:O	1:B:133:ILE:HG12	2.19	0.42
2:B:302:LUT:H11	2:B:302:LUT:H191	1.84	0.42
6:C:306:CLA:H141	6:C:306:CLA:H161	1.80	0.42
6:A:307:CLA:HBB1	6:A:307:CLA:CHC	2.46	0.42
6:A:307:CLA:HMA2	6:A:307:CLA:H42	2.01	0.42
1:A:87:ARG:NH1	10:A:402:HOH:O	2.53	0.42
6:A:306:CLA:HAB	6:A:306:CLA:HMB1	1.81	0.42
2:B:302:LUT:H401	2:B:302:LUT:H35	1.88	0.42
1:B:213:LEU:HD21	6:B:318:CLA:HHC	2.00	0.42
1:C:153:ASP:HA	1:C:154:PRO:HD2	1.86	0.42
3:A:303:NEX:H35	3:A:303:NEX:H401	1.73	0.42
6:B:314:CLA:H51	6:B:316:CLA:HMA1	2.01	0.42
6:C:307:CLA:HMA2	6:C:307:CLA:H42	2.00	0.42
6:B:306:CLA:H141	6:B:306:CLA:H161	1.73	0.42
1:A:157:PRO:HD3	5:A:312:CHL:HMD2	2.02	0.42
1:B:194:PHE:HE2	2:B:301:LUT:H41	1.85	0.41
5:C:305:CHL:HAB	5:C:305:CHL:HMB1	1.78	0.41
1:A:167:ALA:HB1	1:A:173:PHE:CD1	2.54	0.41
1:A:118:LEU:O	1:A:120:HIS:N	2.52	0.41
6:A:315:CLA:HBA1	6:A:315:CLA:CHA	2.50	0.41
1:B:123:SER:O	1:B:127:ILE:HG13	2.21	0.41
5:C:305:CHL:HMA2	5:C:305:CHL:H43	2.01	0.41
5:A:305:CHL:H143	5:A:305:CHL:H111	1.73	0.41
2:B:301:LUT:H15	2:B:301:LUT:H201	1.93	0.41
1:B:51:LEU:HD13	6:B:306:CLA:H42	2.02	0.41
6:B:306:CLA:H62	6:B:306:CLA:H92	1.66	0.41
5:C:311:CHL:H152	5:C:313:CHL:H71	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:303:NEX:H201	3:B:303:NEX:H15	1.90	0.41
6:C:315:CLA:HBB1	6:C:315:CLA:HHC	2.01	0.41
1:A:212:HIS:CG	6:A:317:CLA:HAA2	2.56	0.41
1:B:154:PRO:HG2	10:B:437:HOH:O	2.20	0.41
5:B:312:CHL:CAD	6:B:314:CLA:HMD3	2.50	0.41
1:C:26:GLY:HA3	1:C:27:PRO:HD2	1.93	0.41
2:B:302:LUT:H201	2:B:302:LUT:H15	1.94	0.41
1:B:94:GLU:HG2	1:B:99:LYS:CB	2.50	0.41
1:C:213:LEU:HD21	6:C:318:CLA:HHC	2.03	0.41
5:C:305:CHL:H111	5:C:305:CHL:H143	1.65	0.41
6:C:307:CLA:HAC2	5:C:311:CHL:H162	2.03	0.41
3:A:303:NEX:H183	3:A:303:NEX:H192	2.03	0.41
1:C:120:HIS:HE1	10:C:409:HOH:O	2.03	0.41
1:B:97:TRP:O	2:B:302:LUT:O3	2.39	0.41
1:A:126:ALA:HB3	5:A:309:CHL:HMC	2.03	0.40
3:A:303:NEX:H191	3:A:303:NEX:H11	1.87	0.40
4:B:304:LHG:H151	4:B:304:LHG:H182	1.77	0.40
6:A:306:CLA:C9	6:A:307:CLA:HHB	2.49	0.40
1:B:195:PHE:O	1:B:199:ILE:HG13	2.21	0.40
4:B:304:LHG:H171	5:B:305:CHL:H42	2.04	0.40
6:C:314:CLA:HBB1	6:C:314:CLA:HHC	2.01	0.40
4:A:304:LHG:H141	6:A:317:CLA:C9	2.45	0.40
6:B:307:CLA:C9	6:C:307:CLA:C9	2.97	0.40
2:C:301:LUT:H35	2:C:301:LUT:H401	1.75	0.40
4:C:304:LHG:H151	4:C:304:LHG:H182	1.81	0.40
5:C:305:CHL:H13	5:C:305:CHL:H172	1.51	0.40
6:A:307:CLA:H91	6:C:307:CLA:H91	2.03	0.40
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.87	0.40
5:B:305:CHL:HAB	5:B:305:CHL:HMB1	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. 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	206/224 (92%)	199 (97%)	6 (3%)	1 (0%)	38	67
1	B	206/224 (92%)	199 (97%)	7 (3%)	0	100	100
1	C	206/224 (92%)	198 (96%)	7 (3%)	1 (0%)	38	67
All	All	618/672 (92%)	596 (96%)	20 (3%)	2 (0%)	50	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	C	119	VAL

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 X-ray entries followed by that with respect to entries of similar resolution. 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	160/174 (92%)	157 (98%)	3 (2%)	69	91
1	B	160/174 (92%)	157 (98%)	3 (2%)	69	91
1	C	160/174 (92%)	154 (96%)	6 (4%)	44	74
All	All	480/522 (92%)	468 (98%)	12 (2%)	60	86

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	ILE
1	A	207	GLU
1	A	217	VAL
1	B	181	ILE
1	B	207	GLU
1	B	220	ASN
1	C	80	VAL
1	C	94	GLU
1	C	96	VAL
1	C	181	ILE
1	C	207	GLU
1	C	217	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 67 ligands modelled in this entry, 10 are monoatomic - leaving 57 for Mogul analysis.

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	$\# Z > 2$
2	LUT	A	301	-	43,43,43	0.95	2 (4%)	60,60,60	1.57	11 (18%)
2	LUT	A	302	-	43,43,43	0.97	2 (4%)	60,60,60	1.56	12 (20%)
3	NEX	A	303	-	46,46,46	1.13	3 (6%)	70,70,70	2.93	22 (31%)
4	LHG	A	304	6	48,48,48	0.89	2 (4%)	54,54,54	1.04	4 (7%)
5	CHL	A	305	1	62,74,74	4.03	17 (27%)	52,114,114	1.79	11 (21%)
6	CLA	A	306	1	73,73,73	2.00	18 (24%)	96,113,113	2.34	27 (28%)
6	CLA	A	307	1	73,73,73	2.03	18 (24%)	96,113,113	2.21	34 (35%)
6	CLA	A	308	10	70,70,73	2.52	18 (25%)	92,109,113	2.43	24 (26%)
5	CHL	A	309	1	43,56,74	5.29	19 (44%)	29,92,114	2.27	9 (31%)
5	CHL	A	310	10	47,59,74	4.43	20 (42%)	32,96,114	2.11	9 (28%)
5	CHL	A	311	10	62,74,74	3.96	20 (32%)	52,114,114	1.68	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHL	A	312	10	62,74,74	4.28	21 (33%)	52,114,114	1.64	9 (17%)
5	CHL	A	313	1	62,74,74	3.90	19 (30%)	52,114,114	1.60	8 (15%)
6	CLA	A	314	1	73,73,73	2.24	19 (26%)	96,113,113	2.12	28 (29%)
6	CLA	A	315	4	73,73,73	2.26	19 (26%)	96,113,113	2.20	31 (32%)
6	CLA	A	316	1	73,73,73	2.44	15 (20%)	96,113,113	2.23	29 (30%)
6	CLA	A	317	1	73,73,73	2.00	17 (23%)	96,113,113	2.21	31 (32%)
6	CLA	A	318	1	48,49,73	2.69	21 (43%)	65,84,113	2.27	23 (35%)
7	CAC	A	319	8	4,4,4	5.33	3 (75%)	6,6,6	18.37	5 (83%)
2	LUT	B	301	-	43,43,43	0.94	2 (4%)	60,60,60	1.70	16 (26%)
2	LUT	B	302	-	43,43,43	1.05	2 (4%)	60,60,60	1.77	15 (25%)
3	NEX	B	303	-	46,46,46	1.14	4 (8%)	70,70,70	2.93	23 (32%)
4	LHG	B	304	6	48,48,48	0.94	2 (4%)	54,54,54	1.10	3 (5%)
5	CHL	B	305	1	62,74,74	4.48	16 (25%)	52,114,114	1.64	9 (17%)
6	CLA	B	306	1	73,73,73	2.15	17 (23%)	96,113,113	2.34	35 (36%)
6	CLA	B	307	1	73,73,73	2.23	17 (23%)	96,113,113	2.33	30 (31%)
6	CLA	B	308	10	70,70,73	2.62	19 (27%)	92,109,113	2.42	23 (25%)
5	CHL	B	309	1	43,56,74	4.82	21 (48%)	29,92,114	2.35	9 (31%)
5	CHL	B	310	10	47,59,74	4.42	21 (44%)	32,96,114	2.47	10 (31%)
5	CHL	B	311	10	62,74,74	4.25	17 (27%)	52,114,114	1.73	9 (17%)
5	CHL	B	312	10	62,74,74	4.10	21 (33%)	52,114,114	1.59	8 (15%)
5	CHL	B	313	1	62,74,74	3.58	18 (29%)	52,114,114	1.73	11 (21%)
6	CLA	B	314	1	73,73,73	2.15	15 (20%)	96,113,113	2.29	27 (28%)
6	CLA	B	315	4	73,73,73	2.14	15 (20%)	96,113,113	2.25	31 (32%)
6	CLA	B	316	1	73,73,73	2.28	16 (21%)	96,113,113	2.17	30 (31%)
6	CLA	B	317	1	73,73,73	2.04	15 (20%)	96,113,113	2.27	28 (29%)
6	CLA	B	318	1	48,49,73	2.71	19 (39%)	65,84,113	2.33	20 (30%)
7	CAC	B	319	8	4,4,4	5.78	3 (75%)	6,6,6	24.59	5 (83%)
2	LUT	C	301	-	43,43,43	1.03	1 (2%)	60,60,60	1.96	18 (30%)
2	LUT	C	302	-	43,43,43	0.86	2 (4%)	60,60,60	1.92	13 (21%)
3	NEX	C	303	-	46,46,46	1.20	3 (6%)	70,70,70	3.06	22 (31%)
4	LHG	C	304	6	48,48,48	0.90	2 (4%)	54,54,54	1.01	3 (5%)
5	CHL	C	305	1	62,74,74	4.07	17 (27%)	52,114,114	1.76	12 (23%)
6	CLA	C	306	1	73,73,73	2.34	17 (23%)	96,113,113	2.23	31 (32%)
6	CLA	C	307	1	73,73,73	2.02	17 (23%)	96,113,113	2.25	39 (40%)
6	CLA	C	308	10	70,70,73	2.23	18 (25%)	92,109,113	2.34	25 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	CHL	C	309	1	43,56,74	5.09	20 (46%)	29,92,114	2.29	7 (24%)
5	CHL	C	310	10	47,59,74	4.38	23 (48%)	32,96,114	2.28	9 (28%)
5	CHL	C	311	10	62,74,74	4.20	18 (29%)	52,114,114	1.74	9 (17%)
5	CHL	C	312	10	62,74,74	4.78	20 (32%)	52,114,114	1.68	12 (23%)
5	CHL	C	313	1	62,74,74	3.87	17 (27%)	52,114,114	1.84	13 (25%)
6	CLA	C	314	1	73,73,73	2.21	17 (23%)	96,113,113	2.23	28 (29%)
6	CLA	C	315	4	73,73,73	2.33	18 (24%)	96,113,113	2.19	26 (27%)
6	CLA	C	316	1	73,73,73	2.27	17 (23%)	96,113,113	2.08	27 (28%)
6	CLA	C	317	1	73,73,73	2.17	18 (24%)	96,113,113	2.19	30 (31%)
6	CLA	C	318	1	48,48,73	4.19	21 (43%)	60,82,113	2.42	20 (33%)
7	CAC	C	319	8	4,4,4	4.67	3 (75%)	6,6,6	25.36	4 (66%)

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
2	LUT	A	301	-	-	0/29/67/67	0/2/2/2
2	LUT	A	302	-	-	0/29/67/67	0/2/2/2
3	NEX	A	303	-	-	0/27/83/83	0/2/3/3
4	LHG	A	304	6	-	0/53/53/53	0/0/0/0
5	CHL	A	305	1	-	0/41/177/177	0/0/9/9
6	CLA	A	306	1	-	0/37/135/135	0/0/9/9
6	CLA	A	307	1	-	0/37/135/135	0/0/9/9
6	CLA	A	308	10	-	0/34/132/135	0/0/9/9
5	CHL	A	309	1	-	0/20/156/177	0/0/9/9
5	CHL	A	310	10	-	0/23/159/177	0/0/9/9
5	CHL	A	311	10	-	0/41/177/177	0/0/9/9
5	CHL	A	312	10	-	0/41/177/177	0/0/9/9
5	CHL	A	313	1	-	0/41/177/177	0/0/9/9
6	CLA	A	314	1	-	0/37/135/135	0/0/9/9
6	CLA	A	315	4	-	0/37/135/135	0/0/9/9
6	CLA	A	316	1	-	0/37/135/135	0/0/9/9
6	CLA	A	317	1	-	0/37/135/135	0/0/9/9
6	CLA	A	318	1	-	0/8/106/135	0/0/9/9
7	CAC	A	319	8	-	0/0/0/0	0/0/0/0
2	LUT	B	301	-	-	0/29/67/67	0/2/2/2
2	LUT	B	302	-	-	0/29/67/67	0/2/2/2
3	NEX	B	303	-	-	0/27/83/83	0/2/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LHG	B	304	6	-	0/53/53/53	0/0/0/0
5	CHL	B	305	1	-	0/41/177/177	0/0/9/9
6	CLA	B	306	1	-	0/37/135/135	0/0/9/9
6	CLA	B	307	1	-	0/37/135/135	0/0/9/9
6	CLA	B	308	10	-	0/34/132/135	0/0/9/9
5	CHL	B	309	1	-	0/20/156/177	0/0/9/9
5	CHL	B	310	10	-	0/23/159/177	0/0/9/9
5	CHL	B	311	10	-	0/41/177/177	0/0/9/9
5	CHL	B	312	10	-	0/41/177/177	0/0/9/9
5	CHL	B	313	1	-	0/41/177/177	0/0/9/9
6	CLA	B	314	1	-	0/37/135/135	0/0/9/9
6	CLA	B	315	4	-	0/37/135/135	0/0/9/9
6	CLA	B	316	1	-	0/37/135/135	0/0/9/9
6	CLA	B	317	1	-	0/37/135/135	0/0/9/9
6	CLA	B	318	1	-	0/8/106/135	0/0/9/9
7	CAC	B	319	8	-	0/0/0/0	0/0/0/0
2	LUT	C	301	-	-	0/29/67/67	0/2/2/2
2	LUT	C	302	-	-	0/29/67/67	0/2/2/2
3	NEX	C	303	-	-	0/27/83/83	0/2/3/3
4	LHG	C	304	6	-	0/53/53/53	0/0/0/0
5	CHL	C	305	1	-	0/41/177/177	0/0/9/9
6	CLA	C	306	1	-	0/37/135/135	0/0/9/9
6	CLA	C	307	1	-	0/37/135/135	0/0/9/9
6	CLA	C	308	10	-	0/34/132/135	0/0/9/9
5	CHL	C	309	1	-	0/20/156/177	0/0/9/9
5	CHL	C	310	10	-	0/23/159/177	0/0/9/9
5	CHL	C	311	10	-	0/41/177/177	0/0/9/9
5	CHL	C	312	10	-	0/41/177/177	0/0/9/9
5	CHL	C	313	1	-	0/41/177/177	0/0/9/9
6	CLA	C	314	1	-	0/37/135/135	0/0/9/9
6	CLA	C	315	4	-	0/37/135/135	0/0/9/9
6	CLA	C	316	1	-	0/37/135/135	0/0/9/9
6	CLA	C	317	1	-	0/37/135/135	0/0/9/9
6	CLA	C	318	1	-	0/8/102/135	0/0/9/9
7	CAC	C	319	8	-	0/0/0/0	0/0/0/0

All (802) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	311	CHL	C1A-CHA	25.24	1.51	1.39
5	A	305	CHL	C1A-CHA	23.87	1.50	1.39
5	A	313	CHL	C1A-CHA	23.39	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	312	CHL	C3B-C2B	-23.28	1.27	1.45
5	C	312	CHL	C1A-CHA	23.14	1.50	1.39
5	C	311	CHL	C1A-CHA	23.08	1.50	1.39
5	A	311	CHL	C1A-CHA	22.88	1.50	1.39
5	A	309	CHL	C1A-CHA	22.75	1.50	1.39
5	C	305	CHL	C1A-CHA	22.70	1.50	1.39
5	A	312	CHL	C1A-CHA	22.66	1.50	1.39
5	C	309	CHL	C1A-CHA	22.28	1.49	1.39
5	B	305	CHL	C3B-C2B	-21.84	1.28	1.45
6	C	318	CLA	C2A-C1A	21.75	1.50	1.39
5	C	313	CHL	C1A-CHA	21.69	1.49	1.39
5	B	312	CHL	C1A-CHA	21.56	1.49	1.39
5	A	310	CHL	C1A-CHA	21.32	1.49	1.39
5	B	305	CHL	C1A-CHA	21.25	1.49	1.39
5	B	310	CHL	C1A-CHA	21.01	1.49	1.39
5	C	310	CHL	C1A-CHA	20.79	1.49	1.39
5	B	309	CHL	C1A-CHA	20.60	1.49	1.39
5	B	313	CHL	C1A-CHA	18.79	1.48	1.39
5	A	309	CHL	C3B-C2B	-18.78	1.30	1.45
5	C	309	CHL	C3B-C2B	-16.86	1.32	1.45
5	A	312	CHL	C3B-C2B	-16.38	1.32	1.45
5	B	309	CHL	C3B-C2B	-16.34	1.32	1.45
5	B	312	CHL	C3B-C2B	-14.86	1.33	1.45
5	C	311	CHL	C3B-C2B	-14.69	1.33	1.45
6	A	316	CLA	MG-NA	14.14	2.49	2.07
5	C	305	CHL	C3B-C2B	-12.67	1.35	1.45
6	A	308	CLA	MG-NA	12.08	2.43	2.07
5	B	311	CHL	C3B-C2B	-11.89	1.36	1.45
6	B	316	CLA	MG-NA	11.76	2.42	2.07
5	B	310	CHL	C3B-C2B	-11.32	1.36	1.45
5	C	313	CHL	C3B-C2B	-10.99	1.36	1.45
6	C	316	CLA	MG-NA	10.94	2.39	2.07
5	A	305	CHL	C3B-C2B	-10.91	1.36	1.45
6	C	315	CLA	MG-NA	10.38	2.38	2.07
5	C	310	CHL	C3B-C2B	-10.27	1.37	1.45
5	A	310	CHL	MG-NA	9.92	2.38	2.02
6	B	308	CLA	MG-NA	9.90	2.36	2.07
6	A	315	CLA	MG-NA	9.74	2.36	2.07
6	B	315	CLA	MG-NA	9.62	2.35	2.07
6	C	306	CLA	MG-NA	9.62	2.35	2.07
6	B	318	CLA	MG-NA	9.25	2.34	2.07
6	B	307	CLA	C3B-C2B	-8.86	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	313	CHL	MG-NA	8.85	2.34	2.02
6	B	308	CLA	C3B-C2B	-8.80	1.29	1.40
6	A	318	CLA	MG-NA	8.68	2.32	2.07
5	B	310	CHL	MG-NA	8.54	2.33	2.02
6	C	318	CLA	MG-NA	8.52	2.32	2.07
5	B	311	CHL	C3D-C4D	-8.42	1.38	1.45
5	A	309	CHL	C3D-C4D	-8.27	1.38	1.45
5	A	310	CHL	C3B-C2B	-8.24	1.38	1.45
5	A	311	CHL	C3B-C2B	-8.22	1.38	1.45
6	C	308	CLA	C3B-C4B	8.21	1.51	1.41
6	C	314	CLA	C3B-C4B	8.20	1.51	1.41
6	A	314	CLA	MG-NA	8.19	2.31	2.07
5	A	312	CHL	MG-NA	8.17	2.31	2.02
6	B	306	CLA	C3B-C4B	8.17	1.51	1.41
5	B	313	CHL	C3B-C2B	-8.16	1.39	1.45
6	B	308	CLA	C3B-C4B	8.08	1.51	1.41
6	C	317	CLA	MG-NA	8.05	2.31	2.07
5	A	311	CHL	MG-NA	8.03	2.31	2.02
6	C	314	CLA	MG-NA	7.99	2.30	2.07
6	A	308	CLA	C3B-C4B	7.98	1.50	1.41
5	A	313	CHL	MG-NA	7.95	2.31	2.02
5	B	305	CHL	MG-NA	7.82	2.30	2.02
6	C	315	CLA	C3B-C4B	7.73	1.50	1.41
6	C	306	CLA	C3B-C4B	7.70	1.50	1.41
5	C	310	CHL	MG-NA	7.68	2.30	2.02
7	B	319	CAC	AS-C2	7.67	2.01	1.91
5	C	311	CHL	C3D-C4D	-7.66	1.39	1.45
6	B	307	CLA	MG-NA	7.59	2.29	2.07
5	C	305	CHL	C3D-C4D	-7.58	1.39	1.45
5	B	312	CHL	C3D-C4D	-7.56	1.39	1.45
5	C	309	CHL	MG-NA	7.51	2.29	2.02
6	B	317	CLA	C3B-C4B	7.50	1.50	1.41
5	C	305	CHL	MG-NA	7.50	2.29	2.02
6	C	307	CLA	MG-NA	7.50	2.29	2.07
5	C	309	CHL	C3D-C4D	-7.48	1.39	1.45
7	B	319	CAC	O2-AS	7.40	1.76	1.68
5	B	309	CHL	MG-NA	7.39	2.29	2.02
5	C	313	CHL	MG-NA	7.37	2.29	2.02
7	A	319	CAC	AS-C2	7.36	2.00	1.91
6	A	315	CLA	C3B-C4B	7.34	1.50	1.41
6	B	317	CLA	MG-NA	7.29	2.28	2.07
6	B	314	CLA	C3B-C2B	-7.26	1.31	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	310	CHL	CHC-C1C	7.23	1.50	1.41
5	B	309	CHL	C3D-C4D	-7.21	1.39	1.45
5	A	313	CHL	C3B-C2B	-7.16	1.39	1.45
5	C	311	CHL	C3B-C4B	7.14	1.50	1.45
6	A	318	CLA	C3B-C4B	7.09	1.49	1.41
6	A	314	CLA	C3B-C2B	-7.08	1.31	1.40
6	A	317	CLA	C3B-C4B	7.07	1.49	1.41
6	C	316	CLA	C3B-C4B	7.06	1.49	1.41
5	A	309	CHL	MG-NA	7.06	2.27	2.02
5	B	313	CHL	C3D-C4D	-7.05	1.39	1.45
6	B	318	CLA	C3B-C4B	6.94	1.49	1.41
6	B	306	CLA	MG-NA	6.94	2.27	2.07
5	C	310	CHL	C3D-C4D	-6.88	1.40	1.45
5	A	311	CHL	CHC-C1C	6.86	1.50	1.41
6	A	306	CLA	C3B-C4B	6.77	1.49	1.41
6	A	307	CLA	C3B-C4B	6.76	1.49	1.41
5	C	312	CHL	CHD-C4C	6.73	1.50	1.41
5	C	312	CHL	MG-NA	6.71	2.26	2.02
6	C	318	CLA	C3B-C4B	6.70	1.49	1.41
6	B	316	CLA	C3B-C4B	6.70	1.49	1.41
6	C	308	CLA	MG-NA	6.69	2.27	2.07
5	A	310	CHL	C3D-C4D	-6.69	1.40	1.45
5	A	305	CHL	MG-NA	6.64	2.26	2.02
6	B	307	CLA	C3B-C4B	6.64	1.49	1.41
5	A	311	CHL	C3B-C4B	6.62	1.50	1.45
5	B	312	CHL	CHD-C4C	6.59	1.49	1.41
6	C	317	CLA	C3B-C4B	6.56	1.49	1.41
5	C	313	CHL	CHC-C1C	6.55	1.49	1.41
6	A	317	CLA	MG-NA	6.55	2.26	2.07
5	B	313	CHL	CHC-C1C	6.48	1.49	1.41
5	C	310	CHL	CHC-C1C	6.46	1.49	1.41
6	C	307	CLA	C3B-C4B	6.43	1.48	1.41
5	C	313	CHL	C3B-C4B	6.43	1.50	1.45
5	A	313	CHL	C3D-C4D	-6.42	1.40	1.45
5	B	305	CHL	C3B-C4B	6.40	1.50	1.45
5	B	311	CHL	C3B-C4B	6.40	1.50	1.45
6	A	316	CLA	C3B-C4B	6.39	1.48	1.41
5	B	313	CHL	C3B-C4B	6.38	1.50	1.45
5	C	305	CHL	C3B-C4B	6.38	1.50	1.45
5	A	305	CHL	C3D-C4D	-6.37	1.40	1.45
5	A	312	CHL	CHC-C1C	6.35	1.49	1.41
7	A	319	CAC	O2-AS	6.35	1.75	1.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	310	CHL	CHC-C1C	6.33	1.49	1.41
5	A	305	CHL	CHD-C4C	6.30	1.49	1.41
6	A	314	CLA	C3B-C4B	6.30	1.48	1.41
6	B	314	CLA	MG-NA	6.27	2.25	2.07
5	A	305	CHL	C3B-C4B	6.27	1.50	1.45
6	B	314	CLA	C3B-C4B	6.26	1.48	1.41
5	B	305	CHL	C3D-C4D	-6.20	1.40	1.45
5	C	305	CHL	CHC-C1C	6.19	1.49	1.41
5	B	310	CHL	C3D-C4D	-6.19	1.40	1.45
6	C	306	CLA	C3B-C2B	-6.17	1.32	1.40
5	A	311	CHL	CHD-C4C	6.15	1.49	1.41
6	B	308	CLA	C17-C16	-6.14	1.52	1.55
5	B	312	CHL	C3B-C4B	6.14	1.50	1.45
5	A	313	CHL	CHC-C1C	6.10	1.49	1.41
5	C	313	CHL	C3D-C4D	-6.08	1.40	1.45
6	B	315	CLA	C3B-C4B	6.07	1.48	1.41
5	B	312	CHL	MG-NA	6.04	2.24	2.02
5	A	311	CHL	C3D-C4D	-6.03	1.40	1.45
5	C	312	CHL	C3B-C4B	6.01	1.50	1.45
5	C	309	CHL	CHC-C1C	5.93	1.48	1.41
5	A	310	CHL	CHD-C4C	5.87	1.48	1.41
6	A	306	CLA	MG-NA	5.80	2.24	2.07
6	B	314	CLA	O2D-CGD	5.78	1.48	1.33
5	A	312	CHL	C3D-C4D	-5.75	1.40	1.45
5	A	312	CHL	C3B-C4B	5.74	1.49	1.45
5	B	312	CHL	CHC-C1C	5.72	1.48	1.41
5	A	309	CHL	CHD-C4C	5.69	1.48	1.41
6	C	315	CLA	C3B-C2B	-5.68	1.33	1.40
5	A	313	CHL	CHD-C4C	5.66	1.48	1.41
5	A	310	CHL	C3B-C4B	5.65	1.49	1.45
5	C	311	CHL	CHC-C1C	5.63	1.48	1.41
7	C	319	CAC	AS-C1	5.62	1.98	1.91
5	A	309	CHL	CHC-C1C	5.59	1.48	1.41
5	B	309	CHL	CHD-C4C	5.59	1.48	1.41
5	B	311	CHL	CHC-C1C	5.57	1.48	1.41
5	C	310	CHL	CHD-C4C	5.57	1.48	1.41
6	C	308	CLA	C3B-C2B	-5.56	1.33	1.40
7	C	319	CAC	AS-C2	5.55	1.98	1.91
6	C	317	CLA	C3B-C2B	-5.54	1.33	1.40
5	B	312	CHL	O2D-CGD	5.54	1.47	1.33
5	C	312	CHL	C3D-C4D	-5.54	1.41	1.45
6	C	318	CLA	C1A-NA	-5.54	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	314	CLA	C3B-C2B	-5.52	1.33	1.40
5	C	310	CHL	C3B-C4B	5.52	1.49	1.45
6	A	308	CLA	C17-C16	-5.51	1.53	1.55
5	A	312	CHL	CHD-C4C	5.49	1.48	1.41
5	B	311	CHL	MG-NA	5.45	2.22	2.02
5	C	311	CHL	MG-NA	5.44	2.22	2.02
5	B	309	CHL	CHC-C1C	5.43	1.48	1.41
5	C	312	CHL	CHC-C1C	5.40	1.48	1.41
5	A	305	CHL	CHC-C1C	5.34	1.48	1.41
6	C	308	CLA	C17-C16	-5.33	1.53	1.55
5	C	309	CHL	CHD-C4C	5.31	1.48	1.41
5	C	311	CHL	CHD-C4C	5.23	1.48	1.41
5	C	305	CHL	CHD-C4C	5.22	1.48	1.41
5	A	310	CHL	O2D-CGD	5.17	1.46	1.33
6	C	317	CLA	O2D-CGD	5.13	1.46	1.33
6	B	306	CLA	C3B-C2B	-5.11	1.33	1.40
6	C	318	CLA	C1A-CHA	5.10	1.49	1.40
6	A	307	CLA	O2D-CGD	5.10	1.46	1.33
6	A	314	CLA	O2D-CGD	5.10	1.46	1.33
5	B	305	CHL	CHC-C1C	5.09	1.47	1.41
6	B	316	CLA	O2D-CGD	5.08	1.46	1.33
5	B	310	CHL	CHD-C4C	5.04	1.47	1.41
5	B	313	CHL	CHD-C4C	5.02	1.47	1.41
5	C	310	CHL	O2D-CGD	4.99	1.46	1.33
5	C	313	CHL	CHD-C4C	4.98	1.47	1.41
5	C	311	CHL	O2A-CGA	4.96	1.48	1.33
5	A	313	CHL	O2D-CGD	4.96	1.46	1.33
6	B	318	CLA	O2D-CGD	4.95	1.46	1.33
6	B	307	CLA	O2D-CGD	4.95	1.46	1.33
5	B	311	CHL	O2D-CGD	4.93	1.46	1.33
6	C	318	CLA	O2D-CGD	4.90	1.45	1.33
6	C	306	CLA	O2D-CGD	4.87	1.45	1.33
6	C	314	CLA	O2D-CGD	4.86	1.45	1.33
6	A	308	CLA	O2D-CGD	4.86	1.45	1.33
5	A	311	CHL	O2D-CGD	4.85	1.45	1.33
6	B	314	CLA	O2A-CGA	4.84	1.48	1.33
6	C	308	CLA	O2D-CGD	4.81	1.45	1.33
5	B	305	CHL	O2D-CGD	4.79	1.45	1.33
5	B	311	CHL	O2A-CGA	4.78	1.47	1.33
5	A	309	CHL	O2D-CGD	4.78	1.45	1.33
6	A	314	CLA	O2A-CGA	4.76	1.47	1.33
6	A	306	CLA	O2D-CGD	4.76	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	318	CLA	O2D-CGD	4.76	1.45	1.33
5	A	313	CHL	C3B-C4B	4.76	1.49	1.45
5	C	311	CHL	O2D-CGD	4.75	1.45	1.33
6	A	317	CLA	O2D-CGD	4.75	1.45	1.33
6	B	306	CLA	O2D-CGD	4.75	1.45	1.33
6	A	307	CLA	MG-NA	4.75	2.21	2.07
7	C	319	CAC	O2-AS	4.73	1.73	1.68
6	B	315	CLA	O2D-CGD	4.73	1.45	1.33
6	B	317	CLA	O2D-CGD	4.73	1.45	1.33
5	A	311	CHL	O2A-CGA	4.72	1.47	1.33
5	B	305	CHL	CHD-C4C	4.71	1.47	1.41
5	C	313	CHL	O2D-CGD	4.71	1.45	1.33
5	C	312	CHL	O2D-CGD	4.70	1.45	1.33
6	C	316	CLA	C3B-C2B	-4.67	1.34	1.40
5	A	312	CHL	O2D-CGD	4.66	1.45	1.33
6	C	307	CLA	O2D-CGD	4.66	1.45	1.33
5	B	310	CHL	C3B-C4B	4.64	1.48	1.45
6	B	314	CLA	C3D-C2D	4.64	1.51	1.40
5	C	305	CHL	O2D-CGD	4.62	1.45	1.33
5	C	309	CHL	C3B-C4B	4.61	1.48	1.45
6	B	306	CLA	CHC-C1C	4.58	1.50	1.35
6	C	307	CLA	O2A-CGA	4.55	1.47	1.33
6	C	314	CLA	O2A-CGA	4.54	1.47	1.33
6	A	318	CLA	MG-NC	4.54	2.20	2.07
5	B	311	CHL	CHD-C4C	4.54	1.47	1.41
6	A	306	CLA	C3D-C2D	4.53	1.51	1.40
4	B	304	LHG	O8-C23	4.52	1.47	1.33
5	B	313	CHL	O2D-CGD	4.51	1.44	1.33
6	A	315	CLA	C3D-C2D	4.50	1.51	1.40
6	C	306	CLA	CHC-C1C	4.50	1.50	1.35
6	B	308	CLA	CHC-C1C	4.49	1.50	1.35
6	B	307	CLA	O2A-CGA	4.49	1.47	1.33
6	A	307	CLA	C3B-C2B	-4.47	1.34	1.40
6	B	318	CLA	C3D-C2D	4.46	1.50	1.40
5	C	309	CHL	O2D-CGD	4.46	1.44	1.33
6	A	316	CLA	O2D-CGD	4.43	1.44	1.33
6	C	306	CLA	C4B-CHC	4.43	1.52	1.39
6	B	308	CLA	C3D-C2D	4.42	1.50	1.40
6	C	314	CLA	CHC-C1C	4.41	1.49	1.35
6	B	306	CLA	C4B-CHC	4.39	1.51	1.39
6	A	306	CLA	CHC-C1C	4.38	1.49	1.35
6	B	315	CLA	C3D-C2D	4.36	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	309	CHL	O2A-CGA	4.36	1.46	1.33
6	B	318	CLA	MG-NC	4.36	2.20	2.07
6	B	308	CLA	O2A-CGA	4.35	1.46	1.33
6	C	306	CLA	C3D-C2D	4.33	1.50	1.40
6	C	316	CLA	O2D-CGD	4.33	1.44	1.33
6	C	315	CLA	O2D-CGD	4.32	1.44	1.33
6	C	308	CLA	O2A-CGA	4.32	1.46	1.33
5	B	305	CHL	O2A-CGA	4.31	1.46	1.33
6	A	308	CLA	O2A-CGA	4.31	1.46	1.33
5	B	309	CHL	O2A-CGA	4.30	1.46	1.33
7	B	319	CAC	AS-C1	4.30	1.96	1.91
5	B	309	CHL	O2D-CGD	4.30	1.44	1.33
6	B	317	CLA	CHC-C1C	4.30	1.49	1.35
5	A	310	CHL	O2A-CGA	4.30	1.46	1.33
4	A	304	LHG	O8-C23	4.30	1.46	1.33
6	C	314	CLA	C3D-C2D	4.29	1.50	1.40
6	B	315	CLA	CHC-C1C	4.28	1.49	1.35
6	A	314	CLA	C3D-C2D	4.28	1.50	1.40
5	A	305	CHL	O2D-CGD	4.27	1.44	1.33
6	A	307	CLA	O2A-CGA	4.26	1.46	1.33
5	B	310	CHL	O2A-CGA	4.26	1.46	1.33
5	C	312	CHL	C3A-C2A	-4.26	1.50	1.54
6	B	317	CLA	C3D-C2D	4.26	1.50	1.40
6	A	315	CLA	CHC-C1C	4.26	1.49	1.35
6	C	317	CLA	CHD-C4C	4.25	1.51	1.41
5	A	313	CHL	O2A-CGA	4.25	1.46	1.33
6	A	315	CLA	C1B-C2B	4.25	1.50	1.43
3	B	303	NEX	C26-C25	4.25	1.55	1.48
6	B	308	CLA	O2D-CGD	4.24	1.44	1.33
6	A	308	CLA	C3B-C2B	-4.23	1.35	1.40
6	B	306	CLA	C3D-C2D	4.22	1.50	1.40
5	A	309	CHL	C3B-C4B	4.22	1.48	1.45
5	A	309	CHL	O2A-CGA	4.22	1.46	1.33
5	A	312	CHL	O2A-CGA	4.22	1.46	1.33
4	C	304	LHG	O8-C23	4.21	1.46	1.33
6	A	315	CLA	O2A-CGA	4.20	1.46	1.33
6	A	315	CLA	O2D-CGD	4.20	1.44	1.33
6	A	317	CLA	CHC-C1C	4.18	1.49	1.35
5	B	310	CHL	O2D-CGD	4.18	1.44	1.33
6	B	314	CLA	CHC-C1C	4.17	1.49	1.35
5	C	310	CHL	O2A-CGA	4.17	1.46	1.33
6	C	315	CLA	O2A-CGA	4.17	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	317	CLA	C3D-C2D	4.16	1.50	1.40
6	A	316	CLA	O2A-CGA	4.16	1.46	1.33
6	A	314	CLA	CHC-C1C	4.16	1.49	1.35
6	A	308	CLA	CHC-C1C	4.15	1.49	1.35
6	A	318	CLA	C3D-C2D	4.13	1.50	1.40
7	A	319	CAC	AS-C1	4.13	1.96	1.91
6	B	316	CLA	C3D-C2D	4.12	1.50	1.40
6	C	316	CLA	O2A-CGA	4.11	1.45	1.33
6	C	315	CLA	CHC-C1C	4.09	1.48	1.35
6	C	317	CLA	CHC-C1C	4.08	1.48	1.35
6	B	315	CLA	MG-NC	4.07	2.19	2.07
6	C	316	CLA	CHC-C1C	4.06	1.48	1.35
5	A	305	CHL	O2A-CGA	4.06	1.45	1.33
6	B	318	CLA	C1B-C2B	4.06	1.50	1.43
5	B	313	CHL	O2A-CGA	4.05	1.45	1.33
6	B	315	CLA	O2A-CGA	4.05	1.45	1.33
5	A	312	CHL	CMB-C2B	4.05	1.52	1.45
6	C	317	CLA	C1B-C2B	4.05	1.50	1.43
6	B	307	CLA	CHC-C1C	4.04	1.48	1.35
6	A	316	CLA	C3D-C2D	4.04	1.49	1.40
6	A	317	CLA	O2A-CGA	4.03	1.45	1.33
6	B	314	CLA	C1B-C2B	4.02	1.50	1.43
6	C	306	CLA	CHD-C4C	4.01	1.50	1.41
6	B	316	CLA	O2A-CGA	4.01	1.45	1.33
5	C	312	CHL	O2A-CGA	4.00	1.45	1.33
6	C	307	CLA	C1B-C2B	3.99	1.49	1.43
6	A	318	CLA	C3B-C2B	-3.98	1.35	1.40
6	A	306	CLA	C3B-C2B	-3.98	1.35	1.40
6	A	306	CLA	C4B-CHC	3.97	1.50	1.39
6	B	316	CLA	C1B-C2B	3.97	1.49	1.43
6	C	307	CLA	C3D-C2D	3.96	1.49	1.40
5	C	310	CHL	CMB-C2B	3.95	1.52	1.45
6	C	318	CLA	MG-NC	3.95	2.18	2.07
6	C	315	CLA	C3D-C2D	3.95	1.49	1.40
6	A	318	CLA	CHC-C1C	3.94	1.48	1.35
6	C	318	CLA	C3D-C2D	3.93	1.49	1.40
6	A	307	CLA	C3D-C2D	3.93	1.49	1.40
6	A	308	CLA	C1B-C2B	3.91	1.49	1.43
5	C	305	CHL	O2A-CGA	3.91	1.45	1.33
6	A	316	CLA	CHC-C1C	3.91	1.48	1.35
6	C	308	CLA	CHC-C1C	3.91	1.48	1.35
6	C	316	CLA	C1B-CHB	3.90	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	318	CLA	CHC-C1C	3.90	1.48	1.35
6	C	306	CLA	C1B-CHB	3.89	1.50	1.39
2	C	301	LUT	C22-C21	-3.89	1.50	1.54
6	C	307	CLA	CHC-C1C	3.88	1.48	1.35
5	B	311	CHL	CMB-C2B	3.86	1.51	1.45
5	B	312	CHL	O2A-CGA	3.86	1.45	1.33
5	C	305	CHL	CMB-C2B	3.85	1.51	1.45
6	C	317	CLA	O2A-CGA	3.85	1.45	1.33
6	B	316	CLA	C1B-CHB	3.84	1.50	1.39
6	B	317	CLA	O2A-CGA	3.84	1.45	1.33
6	B	307	CLA	CHD-C4C	3.83	1.50	1.41
6	C	308	CLA	C3D-C2D	3.83	1.49	1.40
5	A	311	CHL	CMB-C2B	3.83	1.51	1.45
5	C	312	CHL	CMB-C2B	3.82	1.51	1.45
4	C	304	LHG	O7-C7	3.82	1.45	1.34
6	B	316	CLA	CHC-C1C	3.82	1.48	1.35
6	A	308	CLA	C3D-C2D	3.82	1.49	1.40
6	A	318	CLA	C1B-C2B	3.81	1.49	1.43
6	B	318	CLA	C3B-C2B	-3.79	1.35	1.40
6	A	314	CLA	C1B-C2B	3.79	1.49	1.43
5	B	309	CHL	CMB-C2B	3.79	1.51	1.45
6	B	308	CLA	C4B-CHC	3.78	1.50	1.39
6	B	317	CLA	C1B-C2B	3.77	1.49	1.43
6	C	315	CLA	CHD-C4C	3.77	1.50	1.41
6	A	306	CLA	MG-NC	3.78	2.18	2.07
6	B	318	CLA	CHC-C1C	3.77	1.47	1.35
6	A	317	CLA	C1B-C2B	3.76	1.49	1.43
5	A	313	CHL	C4C-C3C	3.76	1.50	1.43
6	A	307	CLA	C1B-C2B	3.76	1.49	1.43
6	C	316	CLA	C3D-C2D	3.76	1.49	1.40
6	C	317	CLA	C3D-C2D	3.76	1.49	1.40
6	B	317	CLA	CHD-C4C	3.75	1.50	1.41
6	C	318	CLA	C3B-C2B	-3.74	1.35	1.40
5	C	313	CHL	C3A-C2A	-3.73	1.50	1.54
5	C	312	CHL	CMD-C2D	3.72	1.51	1.45
6	A	314	CLA	C1B-CHB	3.72	1.50	1.39
3	C	303	NEX	C7-C6	-3.72	1.26	1.30
5	A	309	CHL	C4C-C3C	3.71	1.49	1.43
6	A	318	CLA	CHD-C4C	3.69	1.50	1.41
6	A	307	CLA	MG-NC	3.68	2.18	2.07
6	A	307	CLA	CHC-C1C	3.68	1.47	1.35
6	A	317	CLA	CHD-C4C	3.67	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	314	CLA	C1C-C2C	3.65	1.51	1.44
6	A	307	CLA	CHD-C4C	3.64	1.49	1.41
5	B	305	CHL	CMD-C2D	3.64	1.51	1.45
5	A	310	CHL	C4C-C3C	3.62	1.49	1.43
6	A	316	CLA	CHD-C4C	3.62	1.49	1.41
5	C	313	CHL	O2A-CGA	3.61	1.44	1.33
6	A	315	CLA	CHD-C4C	3.61	1.49	1.41
5	C	311	CHL	CMB-C2B	3.61	1.51	1.45
5	C	310	CHL	C4C-C3C	3.61	1.49	1.43
2	B	302	LUT	C23-C24	3.60	1.53	1.50
6	A	315	CLA	MG-NC	3.59	2.17	2.07
5	A	312	CHL	CMD-C2D	3.59	1.51	1.45
3	C	303	NEX	C26-C25	3.58	1.54	1.48
5	B	313	CHL	C3A-C2A	-3.58	1.51	1.54
6	C	318	CLA	CHD-C4C	3.57	1.49	1.41
6	A	316	CLA	C4B-CHC	3.57	1.49	1.39
6	A	306	CLA	C1B-CHB	3.56	1.49	1.39
5	C	305	CHL	CMD-C2D	3.55	1.51	1.45
4	B	304	LHG	O7-C7	3.55	1.45	1.34
5	C	309	CHL	CMB-C2B	3.54	1.51	1.45
5	B	313	CHL	CMD-C2D	3.54	1.51	1.45
5	A	311	CHL	CMD-C2D	3.52	1.51	1.45
5	B	310	CHL	CMB-C2B	3.51	1.51	1.45
6	B	308	CLA	C1B-C2B	3.50	1.49	1.43
6	B	315	CLA	C1B-C2B	3.50	1.49	1.43
5	A	309	CHL	CMB-C2B	3.49	1.51	1.45
6	C	318	CLA	C1B-CHB	3.49	1.49	1.39
6	B	306	CLA	MG-NC	3.49	2.17	2.07
6	B	306	CLA	O2A-CGA	3.49	1.43	1.33
6	A	316	CLA	C1B-C2B	3.48	1.49	1.43
6	C	316	CLA	C4B-CHC	3.48	1.49	1.39
6	A	318	CLA	C4B-CHC	3.48	1.49	1.39
6	B	306	CLA	C1B-CHB	3.48	1.49	1.39
6	A	306	CLA	O2A-CGA	3.48	1.43	1.33
6	C	318	CLA	C1B-C2B	3.48	1.49	1.43
5	A	311	CHL	C4C-C3C	3.47	1.49	1.43
5	C	311	CHL	CMD-C2D	3.47	1.51	1.45
3	A	303	NEX	C26-C25	3.47	1.54	1.48
6	B	315	CLA	C4B-CHC	3.46	1.49	1.39
6	C	306	CLA	C1B-C2B	3.46	1.49	1.43
6	A	317	CLA	MG-NC	3.46	2.17	2.07
6	C	316	CLA	C1B-C2B	3.45	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	318	CLA	CHD-C4C	3.44	1.49	1.41
6	A	316	CLA	C1B-CHB	3.44	1.49	1.39
6	A	315	CLA	C1B-CHB	3.44	1.49	1.39
5	C	309	CHL	C4C-C3C	3.42	1.49	1.43
4	A	304	LHG	O7-C7	3.42	1.44	1.34
5	B	311	CHL	MG-NC	3.42	2.14	2.02
6	C	314	CLA	CHD-C4C	3.41	1.49	1.41
6	B	318	CLA	C1B-CHB	3.41	1.49	1.39
6	B	317	CLA	MG-NC	3.40	2.17	2.07
5	A	310	CHL	CMB-C2B	3.40	1.51	1.45
5	B	309	CHL	CMD-C2D	3.39	1.51	1.45
6	C	315	CLA	C1B-C2B	3.39	1.49	1.43
6	C	306	CLA	O2A-CGA	3.39	1.43	1.33
5	B	312	CHL	C4C-C3C	3.39	1.49	1.43
5	B	310	CHL	C4C-C3C	3.37	1.49	1.43
6	A	315	CLA	C3B-C2B	-3.35	1.36	1.40
6	C	316	CLA	CHD-C4C	3.34	1.49	1.41
5	A	309	CHL	CMD-C2D	3.34	1.51	1.45
6	B	307	CLA	C3D-C2D	3.32	1.48	1.40
5	B	310	CHL	CMD-C2D	3.31	1.51	1.45
6	B	308	CLA	CHD-C4C	3.31	1.49	1.41
5	B	311	CHL	CMD-C2D	3.31	1.51	1.45
6	B	317	CLA	C4B-CHC	3.31	1.49	1.39
5	C	313	CHL	CMB-C2B	3.30	1.51	1.45
6	A	307	CLA	C4C-C3C	3.30	1.51	1.45
6	A	308	CLA	C1B-CHB	3.30	1.48	1.39
5	B	313	CHL	CMB-C2B	3.29	1.51	1.45
6	A	318	CLA	C1B-CHB	3.29	1.48	1.39
5	A	313	CHL	CMB-C2B	3.29	1.50	1.45
6	A	315	CLA	C4B-CHC	3.29	1.48	1.39
6	A	314	CLA	CHD-C4C	3.28	1.49	1.41
5	B	309	CHL	C3B-C4B	3.28	1.47	1.45
5	C	311	CHL	C4C-C3C	3.26	1.49	1.43
6	B	318	CLA	C4B-CHC	3.25	1.48	1.39
6	C	315	CLA	C4B-CHC	3.25	1.48	1.39
6	B	315	CLA	C1B-CHB	3.23	1.48	1.39
6	C	317	CLA	MG-NC	3.21	2.16	2.07
5	C	313	CHL	C1C-C2C	3.21	1.51	1.44
2	A	301	LUT	C22-C21	-3.21	1.51	1.54
6	B	308	CLA	C1C-C2C	3.20	1.51	1.44
6	C	308	CLA	C4B-CHC	3.19	1.48	1.39
6	B	314	CLA	CHD-C4C	3.18	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	312	CHL	CMB-C2B	3.18	1.50	1.45
6	B	317	CLA	C1B-CHB	3.18	1.48	1.39
5	C	310	CHL	CMD-C2D	3.18	1.50	1.45
6	A	308	CLA	C4B-CHC	3.17	1.48	1.39
6	C	307	CLA	C1B-CHB	3.17	1.48	1.39
5	A	305	CHL	CMB-C2B	3.17	1.50	1.45
6	B	316	CLA	CHD-C4C	3.16	1.48	1.41
5	A	313	CHL	CMC-C2C	3.16	1.49	1.44
5	B	312	CHL	CMD-C2D	3.14	1.50	1.45
6	C	307	CLA	C4C-C3C	3.14	1.50	1.45
6	A	317	CLA	C3B-C2B	-3.14	1.36	1.40
6	B	314	CLA	C1B-CHB	3.14	1.48	1.39
5	B	309	CHL	C4C-C3C	3.14	1.48	1.43
6	B	306	CLA	CHD-C4C	3.13	1.48	1.41
6	C	317	CLA	C1B-CHB	3.13	1.48	1.39
5	A	305	CHL	CMD-C2D	3.13	1.50	1.45
6	C	307	CLA	CHD-C4C	3.12	1.48	1.41
5	A	312	CHL	C1C-C2C	3.11	1.51	1.44
5	B	313	CHL	C1C-C2C	3.11	1.51	1.44
6	C	314	CLA	C1B-CHB	3.09	1.48	1.39
5	C	309	CHL	CMD-C2D	3.09	1.50	1.45
6	B	308	CLA	C1B-CHB	3.09	1.48	1.39
5	B	305	CHL	C4D-CHA	3.08	1.51	1.43
6	C	318	CLA	C4B-CHC	3.07	1.48	1.39
6	A	308	CLA	CHD-C4C	3.05	1.48	1.41
5	A	310	CHL	C1C-C2C	3.04	1.50	1.44
6	C	308	CLA	C1B-C2B	3.04	1.48	1.43
6	C	308	CLA	C1B-CHB	3.04	1.48	1.39
6	C	315	CLA	C1B-CHB	3.04	1.48	1.39
6	B	307	CLA	C1D-ND	3.03	1.45	1.38
6	B	316	CLA	C1D-ND	3.01	1.45	1.38
6	B	307	CLA	C1D-C2D	3.01	1.50	1.42
5	C	310	CHL	C1B-C2B	3.00	1.51	1.43
5	B	310	CHL	C1C-C2C	3.00	1.50	1.44
6	A	307	CLA	C1C-C2C	3.00	1.50	1.44
6	A	306	CLA	CHD-C4C	2.99	1.48	1.41
5	A	310	CHL	CMC-C2C	2.98	1.49	1.44
6	B	315	CLA	CHD-C4C	2.97	1.48	1.41
6	B	306	CLA	C4A-NA	-2.97	1.33	1.38
5	A	313	CHL	MG-NC	2.96	2.13	2.02
5	C	313	CHL	CMD-C2D	2.96	1.50	1.45
6	A	307	CLA	C1D-ND	2.96	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	303	NEX	C7-C6	-2.95	1.27	1.30
6	A	307	CLA	C4B-CHC	2.95	1.48	1.39
5	A	313	CHL	C1C-C2C	2.94	1.50	1.44
6	C	315	CLA	C1D-ND	2.93	1.45	1.38
6	C	316	CLA	C1D-ND	2.93	1.45	1.38
6	C	307	CLA	C1C-C2C	2.93	1.50	1.44
6	C	308	CLA	C1C-C2C	2.92	1.50	1.44
6	A	318	CLA	C1D-ND	2.92	1.45	1.38
6	C	318	CLA	C1D-C2D	2.92	1.49	1.42
5	C	313	CHL	MG-NC	2.91	2.12	2.02
6	B	316	CLA	C4B-CHC	2.90	1.47	1.39
6	C	308	CLA	MG-NC	2.90	2.15	2.07
5	A	311	CHL	C3B-CAB	2.90	1.49	1.40
5	A	305	CHL	C1C-C2C	2.90	1.50	1.44
6	C	316	CLA	C4D-CHA	2.89	1.50	1.38
6	A	307	CLA	C1B-CHB	2.89	1.47	1.39
5	C	312	CHL	C4C-C3C	2.89	1.48	1.43
6	A	315	CLA	C1D-ND	2.89	1.45	1.38
5	A	310	CHL	C3B-CAB	2.89	1.49	1.40
3	C	303	NEX	C7-C8	-2.88	1.26	1.32
5	A	305	CHL	CMC-C2C	2.88	1.49	1.44
6	A	316	CLA	MG-NC	-2.88	1.98	2.07
6	C	317	CLA	C1D-ND	2.87	1.45	1.38
6	B	307	CLA	C1B-CHB	2.87	1.47	1.39
5	C	313	CHL	C3B-CAB	2.87	1.49	1.40
5	B	311	CHL	C4C-C3C	2.87	1.48	1.43
6	C	317	CLA	C1D-C2D	2.86	1.49	1.42
6	C	314	CLA	C4B-CHC	2.86	1.47	1.39
5	C	311	CHL	C3B-CAB	2.86	1.49	1.40
6	B	314	CLA	C4A-NA	-2.86	1.33	1.38
6	A	315	CLA	C4D-CHA	2.86	1.50	1.38
6	C	318	CLA	C1D-ND	2.86	1.45	1.38
6	B	318	CLA	C1D-ND	2.86	1.45	1.38
6	C	314	CLA	C1B-C2B	2.85	1.48	1.43
6	C	317	CLA	C4A-NA	-2.85	1.33	1.38
6	B	315	CLA	C1D-ND	2.84	1.45	1.38
6	A	317	CLA	C4B-CHC	2.84	1.47	1.39
5	A	313	CHL	CMD-C2D	2.84	1.50	1.45
5	A	310	CHL	CMD-C2D	2.84	1.50	1.45
3	A	303	NEX	C7-C8	-2.84	1.26	1.32
2	A	302	LUT	C23-C24	2.83	1.52	1.50
6	C	314	CLA	C4C-C3C	2.82	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	306	CLA	C1D-C2D	2.82	1.49	1.42
6	B	307	CLA	C4B-CHC	2.82	1.47	1.39
5	B	313	CHL	C4C-C3C	2.81	1.48	1.43
6	C	307	CLA	C4B-CHC	2.80	1.47	1.39
6	A	318	CLA	C1D-C2D	2.79	1.49	1.42
6	C	317	CLA	C4B-CHC	2.78	1.47	1.39
6	B	317	CLA	C1D-ND	2.78	1.44	1.38
6	B	315	CLA	C1D-C2D	2.77	1.49	1.42
6	C	314	CLA	C4A-NA	-2.75	1.33	1.38
6	A	317	CLA	C1B-CHB	2.75	1.47	1.39
6	A	316	CLA	C1C-NC	-2.75	1.32	1.37
5	B	310	CHL	C3B-CAB	2.75	1.49	1.40
5	B	305	CHL	CMB-C2B	2.75	1.50	1.45
6	B	318	CLA	C1D-C2D	2.74	1.49	1.42
5	B	311	CHL	C3B-CAB	2.74	1.49	1.40
6	A	308	CLA	C4A-NA	-2.74	1.33	1.38
5	C	312	CHL	C1D-C2D	2.74	1.50	1.43
5	B	311	CHL	C1C-C2C	2.74	1.50	1.44
6	C	318	CLA	C4A-NA	-2.74	1.33	1.38
6	A	306	CLA	C1B-C2B	2.74	1.48	1.43
5	B	305	CHL	C3D-C2D	2.74	1.50	1.43
6	C	314	CLA	C4D-CHA	2.73	1.50	1.38
5	C	312	CHL	C1C-C2C	2.73	1.50	1.44
5	C	309	CHL	C1C-C2C	2.73	1.50	1.44
6	A	314	CLA	MG-NC	2.72	2.15	2.07
5	B	312	CHL	MG-NC	2.72	2.12	2.02
6	A	317	CLA	C1D-ND	2.72	1.44	1.38
5	A	312	CHL	C4C-C3C	2.71	1.48	1.43
6	B	306	CLA	C1C-C2C	2.71	1.50	1.44
6	A	314	CLA	C4B-CHC	2.71	1.47	1.39
5	B	312	CHL	C3A-C2A	-2.71	1.51	1.54
6	B	314	CLA	C4C-C3C	2.70	1.50	1.45
6	C	307	CLA	C1D-ND	2.71	1.44	1.38
6	C	315	CLA	C4C-C3C	2.70	1.50	1.45
6	A	314	CLA	C4C-C3C	2.69	1.50	1.45
5	B	310	CHL	C3A-C2A	-2.69	1.51	1.54
5	C	309	CHL	CMC-C2C	2.69	1.49	1.44
3	B	303	NEX	C7-C8	-2.68	1.27	1.32
6	B	306	CLA	C1B-C2B	2.67	1.48	1.43
3	B	303	NEX	C7-C6	-2.66	1.27	1.30
5	C	310	CHL	C3B-CAB	2.66	1.49	1.40
6	B	318	CLA	C4C-C3C	2.66	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	312	CHL	C1D-C2D	2.66	1.50	1.43
6	B	314	CLA	C4B-CHC	2.65	1.47	1.39
6	C	315	CLA	C1C-C2C	2.65	1.49	1.44
5	A	313	CHL	C3B-CAB	2.65	1.49	1.40
6	A	318	CLA	C4C-C3C	2.63	1.49	1.45
5	C	310	CHL	MG-NC	2.63	2.11	2.02
6	A	315	CLA	C4A-NA	-2.63	1.33	1.38
5	B	305	CHL	C4C-C3C	2.63	1.47	1.43
6	C	306	CLA	C1C-C2C	2.62	1.49	1.44
6	C	315	CLA	C4D-CHA	2.62	1.49	1.38
5	A	312	CHL	CBD-CGD	-2.61	1.48	1.53
6	B	315	CLA	C4D-CHA	2.61	1.49	1.38
5	B	313	CHL	C3B-CAB	2.60	1.48	1.40
5	C	305	CHL	C4C-C3C	2.60	1.47	1.43
6	C	315	CLA	C1D-C2D	2.60	1.49	1.42
6	A	314	CLA	C1C-C2C	2.60	1.49	1.44
5	B	312	CHL	C1C-C2C	2.60	1.49	1.44
6	B	317	CLA	C4A-NA	-2.60	1.33	1.38
6	C	318	CLA	C4C-C3C	2.59	1.49	1.45
6	A	317	CLA	C4A-NA	-2.59	1.34	1.38
6	B	318	CLA	C4A-NA	-2.59	1.34	1.38
5	C	311	CHL	C1B-C2B	2.58	1.50	1.43
5	A	312	CHL	C4D-CHA	2.58	1.50	1.43
6	C	317	CLA	C4C-C3C	2.57	1.49	1.45
6	A	315	CLA	C1D-C2D	2.56	1.49	1.42
5	C	305	CHL	C1B-C2B	2.56	1.50	1.43
6	B	308	CLA	MG-NC	2.56	2.14	2.07
6	C	317	CLA	C4D-CHA	2.56	1.49	1.38
6	A	308	CLA	C4D-CHA	2.55	1.49	1.38
5	A	312	CHL	C1B-C2B	2.55	1.50	1.43
5	C	310	CHL	C4D-CHA	2.55	1.50	1.43
5	A	305	CHL	C3D-C2D	2.55	1.50	1.43
5	A	305	CHL	C4C-C3C	2.55	1.47	1.43
5	B	312	CHL	C3B-CAB	2.54	1.48	1.40
5	A	312	CHL	C3A-C2A	-2.53	1.52	1.54
5	C	310	CHL	C1C-C2C	2.53	1.49	1.44
5	A	310	CHL	C3A-C2A	-2.52	1.52	1.54
6	C	317	CLA	C1C-C2C	2.52	1.49	1.44
6	A	307	CLA	C1D-C2D	2.52	1.48	1.42
6	A	314	CLA	CHB-C4A	2.52	1.36	1.33
5	B	309	CHL	C3A-C2A	-2.51	1.52	1.54
6	B	317	CLA	C4D-CHA	2.51	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	316	CLA	C4A-NA	-2.51	1.34	1.38
5	C	309	CHL	C3A-C2A	-2.51	1.52	1.54
6	C	315	CLA	MG-NC	2.50	2.14	2.07
5	C	309	CHL	C1D-C2D	2.50	1.50	1.43
6	B	307	CLA	C1C-C2C	2.50	1.49	1.44
5	C	305	CHL	MG-NC	2.49	2.11	2.02
6	B	318	CLA	C4D-CHA	2.49	1.49	1.38
6	A	318	CLA	C4D-CHA	2.49	1.49	1.38
6	A	306	CLA	C4A-NA	-2.49	1.34	1.38
6	B	308	CLA	C4A-NA	-2.49	1.34	1.38
6	B	315	CLA	C4A-NA	-2.49	1.34	1.38
5	B	311	CHL	CMC-C2C	2.49	1.48	1.44
6	B	316	CLA	C4D-CHA	2.48	1.49	1.38
5	A	310	CHL	C4D-CHA	2.47	1.50	1.43
6	A	308	CLA	C1D-C2D	2.47	1.48	1.42
5	C	305	CHL	C3B-CAB	2.47	1.48	1.40
2	C	302	LUT	C1-C6	-2.48	1.50	1.53
6	C	308	CLA	C4A-NA	-2.48	1.34	1.38
6	C	306	CLA	C1D-ND	2.47	1.44	1.38
5	A	311	CHL	C1C-C2C	2.47	1.49	1.44
5	B	309	CHL	C3B-CAB	2.46	1.48	1.40
6	B	306	CLA	C1A-NA	-2.46	1.26	1.32
6	B	308	CLA	C4D-CHA	2.45	1.49	1.38
6	A	307	CLA	C4A-NA	-2.45	1.34	1.38
6	C	315	CLA	C4A-NA	-2.44	1.34	1.38
6	B	307	CLA	C4C-C3C	2.44	1.49	1.45
6	A	307	CLA	C4D-CHA	2.44	1.49	1.38
6	A	306	CLA	C1D-C2D	2.44	1.48	1.42
5	C	311	CHL	CMC-C2C	2.43	1.48	1.44
6	C	307	CLA	C4D-CHA	2.43	1.48	1.38
5	A	313	CHL	C1B-C2B	2.43	1.49	1.43
5	C	311	CHL	C1C-C2C	2.43	1.49	1.44
5	A	312	CHL	C3B-CAB	2.43	1.48	1.40
6	A	314	CLA	C4D-CHA	2.42	1.48	1.38
6	C	314	CLA	C1D-C2D	2.42	1.48	1.42
6	C	318	CLA	C4D-CHA	2.42	1.48	1.38
5	A	311	CHL	C3D-C2D	2.42	1.49	1.43
6	A	318	CLA	C4A-NA	-2.41	1.34	1.38
6	B	314	CLA	C4D-CHA	2.41	1.48	1.38
6	A	314	CLA	C1D-C2D	2.41	1.48	1.42
5	B	312	CHL	CMC-C2C	2.40	1.48	1.44
5	B	310	CHL	C3D-C2D	2.39	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	305	CHL	C3B-CAB	2.39	1.48	1.40
5	B	305	CHL	C3B-CAB	2.39	1.48	1.40
5	C	312	CHL	C1B-C2B	2.39	1.49	1.43
6	B	307	CLA	C4A-NA	-2.39	1.34	1.38
6	B	307	CLA	C1B-C2B	2.39	1.47	1.43
5	A	310	CHL	C5-C3	2.39	1.51	1.39
6	C	316	CLA	C1C-C2C	2.39	1.49	1.44
5	B	305	CHL	C1C-C2C	2.39	1.49	1.44
5	C	305	CHL	C1C-C2C	2.38	1.49	1.44
5	A	311	CHL	C3A-C2A	-2.38	1.52	1.54
5	C	311	CHL	MG-NC	2.38	2.10	2.02
6	B	308	CLA	C1D-C2D	2.37	1.48	1.42
6	C	307	CLA	C3B-C2B	-2.37	1.37	1.40
5	C	309	CHL	C3B-CAB	2.36	1.48	1.40
5	B	313	CHL	CMC-C2C	2.35	1.48	1.44
6	A	318	CLA	C1C-NC	-2.35	1.33	1.37
6	C	306	CLA	C4D-CHA	2.34	1.48	1.38
5	A	309	CHL	C3B-CAB	2.34	1.48	1.40
5	A	305	CHL	C4D-CHA	2.34	1.49	1.43
6	B	307	CLA	C4D-CHA	2.34	1.48	1.38
6	B	316	CLA	C1C-NC	-2.34	1.33	1.37
5	B	310	CHL	C5-C3	2.34	1.51	1.39
6	B	316	CLA	C4A-NA	-2.34	1.34	1.38
5	C	310	CHL	C3D-C2D	2.33	1.49	1.43
5	A	309	CHL	C1C-C2C	2.33	1.49	1.44
6	C	314	CLA	C1D-ND	2.33	1.43	1.38
6	A	317	CLA	C4D-CHA	2.33	1.48	1.38
6	A	318	CLA	C1C-C2C	2.33	1.49	1.44
6	A	316	CLA	C4D-CHA	2.33	1.48	1.38
5	C	310	CHL	C5-C3	2.32	1.51	1.39
5	A	311	CHL	C3D-CAD	2.32	1.50	1.44
6	B	318	CLA	C1C-C2C	2.32	1.49	1.44
6	C	307	CLA	C1D-C2D	2.31	1.48	1.42
6	B	314	CLA	C1D-C2D	2.31	1.48	1.42
6	B	308	CLA	C1D-ND	2.31	1.43	1.38
5	B	312	CHL	C1B-C2B	2.30	1.49	1.43
5	A	312	CHL	C3D-C2D	2.30	1.49	1.43
6	B	306	CLA	C1D-C2D	2.29	1.48	1.42
6	C	316	CLA	C4A-NA	-2.29	1.34	1.38
6	A	317	CLA	C1D-C2D	2.29	1.48	1.42
5	A	309	CHL	C3D-C2D	2.29	1.49	1.43
6	C	316	CLA	C1D-C2D	2.28	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	309	CHL	C1B-C2B	2.28	1.49	1.43
5	C	312	CHL	C3D-C2D	2.27	1.49	1.43
6	A	318	CLA	C3A-C2A	-2.27	1.51	1.55
6	C	316	CLA	C1C-NC	-2.27	1.33	1.37
6	C	306	CLA	C4A-NA	-2.26	1.34	1.38
5	B	310	CHL	C4D-CHA	2.25	1.49	1.43
6	A	306	CLA	C1C-C2C	2.25	1.49	1.44
5	C	310	CHL	CMC-C2C	2.25	1.48	1.44
5	C	312	CHL	C3B-CAB	2.25	1.47	1.40
5	C	305	CHL	C3D-C2D	2.24	1.49	1.43
2	C	302	LUT	C23-C24	2.23	1.52	1.50
6	B	306	CLA	C4D-CHA	2.21	1.47	1.38
6	C	306	CLA	MG-NC	2.21	2.13	2.07
5	B	310	CHL	CMC-C2C	2.20	1.48	1.44
6	A	318	CLA	C1A-NA	-2.20	1.27	1.32
5	B	310	CHL	C1B-C2B	2.19	1.49	1.43
5	A	313	CHL	C4D-CHA	2.19	1.49	1.43
5	C	312	CHL	CMC-C2C	2.18	1.48	1.44
6	C	308	CLA	C4D-CHA	2.18	1.47	1.38
2	B	301	LUT	C23-C24	2.17	1.52	1.50
5	B	309	CHL	C3D-C2D	2.16	1.49	1.43
5	A	309	CHL	C3A-C2A	-2.16	1.52	1.54
6	B	318	CLA	C1C-NC	-2.16	1.33	1.37
6	A	306	CLA	C1C-NC	-2.16	1.33	1.37
6	A	308	CLA	C1D-ND	2.16	1.43	1.38
6	C	308	CLA	C1D-ND	2.15	1.43	1.38
5	B	309	CHL	CMC-C2C	2.14	1.48	1.44
6	A	308	CLA	C1C-C2C	2.14	1.48	1.44
5	C	312	CHL	C4D-CHA	2.14	1.49	1.43
6	B	318	CLA	C3A-C2A	-2.13	1.52	1.55
5	A	311	CHL	C1D-C2D	2.13	1.49	1.43
2	B	302	LUT	C26-C27	2.13	1.54	1.50
5	B	309	CHL	C1C-C2C	2.13	1.48	1.44
6	A	314	CLA	C1D-ND	2.13	1.43	1.38
5	A	311	CHL	C4D-CHA	2.13	1.49	1.43
6	B	308	CLA	C1A-NA	-2.13	1.27	1.32
6	A	306	CLA	C4D-CHA	2.13	1.47	1.38
6	C	307	CLA	CAA-C2A	-2.12	1.50	1.54
6	A	317	CLA	C4C-C3C	2.12	1.48	1.45
6	A	306	CLA	C1D-ND	2.12	1.43	1.38
5	A	311	CHL	CMC-C2C	2.11	1.48	1.44
5	C	310	CHL	C3A-C2A	-2.11	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	309	CHL	C4D-CHA	2.11	1.49	1.43
5	A	310	CHL	C1D-C2D	2.10	1.49	1.43
5	C	313	CHL	C4D-CHA	2.10	1.49	1.43
6	A	315	CLA	OBD-CAD	2.10	1.25	1.22
5	B	313	CHL	C3D-C2D	2.10	1.48	1.43
6	A	316	CLA	C1D-ND	2.10	1.43	1.38
5	A	309	CHL	MG-NC	2.10	2.09	2.02
6	C	308	CLA	C1A-NA	-2.10	1.27	1.32
5	A	312	CHL	CMC-C2C	2.10	1.48	1.44
5	B	312	CHL	C1D-C2D	2.10	1.49	1.43
5	A	313	CHL	CBD-CGD	-2.10	1.49	1.53
6	B	316	CLA	C4C-C3C	2.09	1.48	1.45
2	B	301	LUT	C22-C21	-2.09	1.52	1.54
6	B	317	CLA	C1D-C2D	2.09	1.47	1.42
5	C	311	CHL	C3D-C2D	2.08	1.48	1.43
5	C	313	CHL	C4C-C3C	2.08	1.46	1.43
6	A	315	CLA	C4C-C3C	2.08	1.48	1.45
5	C	309	CHL	C1B-C2B	2.08	1.49	1.43
5	B	312	CHL	C3D-C2D	2.07	1.48	1.43
6	C	308	CLA	C1D-C2D	2.07	1.47	1.42
5	A	310	CHL	C1B-C2B	2.06	1.48	1.43
5	B	313	CHL	C3D-CAD	2.06	1.50	1.44
5	B	309	CHL	C1B-C2B	2.06	1.48	1.43
5	C	309	CHL	C3D-C2D	2.06	1.48	1.43
5	B	309	CHL	C1D-C2D	2.06	1.48	1.43
6	C	318	CLA	C1C-C2C	2.06	1.48	1.44
5	B	309	CHL	CBD-CAD	-2.05	1.47	1.56
6	A	318	CLA	C2A-C1A	-2.03	1.50	1.51
5	B	311	CHL	C3D-C2D	2.03	1.48	1.43
2	A	301	LUT	C26-C25	-2.02	1.50	1.53
6	C	318	CLA	C1C-NC	-2.02	1.34	1.37
5	B	310	CHL	C3D-CAD	2.02	1.49	1.44
3	B	303	NEX	O24-C25	-2.02	1.42	1.46
6	A	314	CLA	C4A-NA	-2.02	1.34	1.38
5	C	310	CHL	CBD-CAD	-2.02	1.47	1.56
6	A	315	CLA	C3D-CAD	2.01	1.51	1.45
5	B	309	CHL	C4D-CHA	2.01	1.48	1.43
2	A	302	LUT	C21-C26	-2.01	1.53	1.56
6	B	316	CLA	C1C-C2C	2.01	1.48	1.44
5	C	310	CHL	C3D-CAD	2.01	1.49	1.44
6	A	308	CLA	C1A-NA	-2.01	1.27	1.32
5	A	309	CHL	CMC-C2C	2.00	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	312	CHL	C3D-CAD	2.00	1.49	1.44

All (1025) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	319	CAC	O2-AS-O1	-56.08	100.44	112.54
7	B	319	CAC	O2-AS-O1	-53.64	100.97	112.54
7	A	319	CAC	O2-AS-O1	-35.35	104.91	112.54
7	A	319	CAC	O2-AS-C2	-27.19	86.90	109.15
7	C	319	CAC	O2-AS-C2	-26.21	87.70	109.15
7	B	319	CAC	O2-AS-C2	-25.95	87.92	109.15
3	C	303	NEX	O24-C25-C24	16.64	125.68	113.33
3	B	303	NEX	O24-C25-C24	16.11	125.29	113.33
3	A	303	NEX	O24-C25-C24	15.00	124.46	113.33
6	A	316	CLA	CHD-C4C-NC	11.04	131.99	124.28
6	A	308	CLA	CHD-C4C-NC	10.61	131.70	124.28
6	B	306	CLA	CHD-C4C-NC	10.55	131.65	124.28
6	A	306	CLA	CHD-C4C-NC	10.35	131.51	124.28
6	B	314	CLA	CHD-C4C-NC	9.87	131.18	124.28
6	B	308	CLA	CHD-C4C-NC	9.87	131.18	124.28
6	C	308	CLA	CHD-C4C-NC	9.86	131.17	124.28
6	B	317	CLA	CHD-C4C-NC	9.79	131.12	124.28
6	C	316	CLA	CHD-C4C-NC	9.55	130.96	124.28
6	B	316	CLA	CHD-C4C-NC	9.53	130.94	124.28
6	B	307	CLA	CHD-C4C-NC	9.19	130.70	124.28
6	C	314	CLA	CHD-C4C-NC	9.09	130.63	124.28
6	C	306	CLA	CHD-C4C-NC	8.65	130.32	124.28
6	C	315	CLA	CHD-C4C-NC	8.61	130.30	124.28
6	C	317	CLA	CHD-C4C-NC	8.50	130.22	124.28
6	A	317	CLA	CHD-C4C-NC	8.49	130.21	124.28
6	C	307	CLA	CHD-C4C-NC	8.47	130.20	124.28
6	B	315	CLA	CHD-C4C-NC	8.36	130.12	124.28
6	A	307	CLA	CHD-C4C-NC	8.31	130.09	124.28
6	A	315	CLA	CHD-C4C-NC	8.19	130.00	124.28
6	A	314	CLA	CHD-C4C-NC	8.18	130.00	124.28
6	C	317	CLA	C4B-CHC-C1C	-7.70	117.34	127.47
6	C	318	CLA	CHD-C4C-NC	7.69	129.65	124.28
2	C	302	LUT	C38-C25-C26	7.66	121.84	116.05
6	A	318	CLA	CHD-C4C-NC	7.30	129.39	124.28
6	A	308	CLA	C4B-C3B-CAB	7.30	141.96	127.18
6	B	317	CLA	C4B-CHC-C1C	-7.23	117.95	127.47
6	B	314	CLA	C4B-CHC-C1C	-7.20	118.00	127.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	308	CLA	C4B-CHC-C1C	-7.15	118.07	127.47
6	C	318	CLA	C4B-CHC-C1C	-7.14	118.07	127.47
6	B	308	CLA	C2B-C3B-CAB	-7.02	112.96	127.33
6	B	314	CLA	C2B-C3B-CAB	-6.98	113.03	127.33
6	B	307	CLA	C4B-CHC-C1C	-6.97	118.30	127.47
6	B	308	CLA	C4B-CHC-C1C	-6.96	118.31	127.47
6	B	314	CLA	C4B-C3B-CAB	6.94	141.24	127.18
6	B	318	CLA	CHD-C4C-NC	6.94	129.13	124.28
6	A	308	CLA	C2B-C3B-CAB	-6.93	113.14	127.33
6	B	308	CLA	C4B-C3B-CAB	6.92	141.20	127.18
6	C	308	CLA	C2B-C3B-CAB	-6.83	113.35	127.33
6	A	317	CLA	C4B-CHC-C1C	-6.77	118.57	127.47
6	C	308	CLA	C4B-C3B-CAB	6.76	140.87	127.18
6	B	318	CLA	C4B-CHC-C1C	-6.66	118.71	127.47
7	B	319	CAC	C2-AS-C1	6.58	124.46	109.43
6	A	314	CLA	C4B-CHC-C1C	-6.55	118.85	127.47
3	B	303	NEX	C38-C25-C26	-6.54	112.03	122.50
6	A	315	CLA	C4B-CHC-C1C	-6.53	118.88	127.47
3	A	303	NEX	C22-C21-C26	6.52	116.82	110.08
6	A	306	CLA	C2B-C3B-CAB	-6.47	114.08	127.33
3	A	303	NEX	C35-C34-C33	-6.47	117.94	127.29
5	C	309	CHL	C1-O2A-CGA	6.46	122.86	115.30
6	C	315	CLA	C4B-CHC-C1C	-6.40	119.05	127.47
6	B	307	CLA	O2D-CGD-CBD	6.36	124.18	111.34
6	C	314	CLA	C4B-C3B-CAB	6.33	140.00	127.18
5	A	311	CHL	C4D-C3D-C2D	-6.19	105.69	108.16
6	A	317	CLA	C4B-C3B-CAB	6.12	139.56	127.18
6	C	308	CLA	C4B-CHC-C1C	-6.10	119.44	127.47
6	C	306	CLA	C4B-CHC-C1C	-6.10	119.45	127.47
5	C	313	CHL	C3C-C4C-NC	6.07	111.48	109.67
3	C	303	NEX	C22-C21-C26	6.07	116.36	110.08
3	C	303	NEX	C21-C26-C27	6.06	122.06	115.88
6	A	307	CLA	C4B-CHC-C1C	-6.04	119.52	127.47
6	A	314	CLA	C2B-C3B-CAB	-6.03	114.98	127.33
6	C	314	CLA	C2B-C3B-CAB	-6.03	114.99	127.33
5	A	313	CHL	C4D-C3D-C2D	-6.03	105.76	108.16
6	A	314	CLA	C4B-C3B-CAB	6.00	139.33	127.18
6	A	317	CLA	C2B-C3B-CAB	-5.99	115.06	127.33
6	B	317	CLA	C4B-C3B-CAB	5.97	139.27	127.18
6	B	308	CLA	O2D-CGD-CBD	5.97	123.39	111.34
6	A	306	CLA	O2D-CGD-CBD	5.96	123.38	111.34
6	C	306	CLA	C2B-C3B-CAB	-5.90	115.25	127.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	306	CLA	C4B-C3B-CAB	5.90	139.13	127.18
6	C	317	CLA	C2B-C3B-CAB	-5.90	115.26	127.33
3	C	303	NEX	C35-C34-C33	-5.86	118.82	127.29
3	B	303	NEX	C22-C21-C26	5.86	116.14	110.08
6	B	316	CLA	O2D-CGD-CBD	5.82	123.09	111.34
6	B	315	CLA	C4B-CHC-C1C	-5.81	119.83	127.47
3	A	303	NEX	C38-C25-C26	-5.80	113.22	122.50
5	C	312	CHL	O2D-CGD-CBD	5.78	122.62	111.36
3	C	303	NEX	C38-C25-C26	-5.74	113.32	122.50
6	B	306	CLA	C4B-CHC-C1C	-5.73	119.93	127.47
6	B	307	CLA	C2B-C3B-CAB	-5.70	115.67	127.33
6	C	314	CLA	C4B-CHC-C1C	-5.70	119.98	127.47
6	B	306	CLA	O2D-CGD-CBD	5.64	122.74	111.34
6	A	306	CLA	C4B-CHC-C1C	-5.63	120.06	127.47
6	B	315	CLA	O2D-CGD-CBD	5.59	122.64	111.34
5	C	311	CHL	O2D-CGD-CBD	5.58	122.22	111.36
3	A	303	NEX	C21-C26-C27	5.57	121.57	115.88
6	C	307	CLA	C4B-CHC-C1C	-5.56	120.15	127.47
2	C	301	LUT	C38-C25-C26	5.52	120.23	116.05
5	C	305	CHL	OMC-CMC-C2C	-5.52	117.41	124.79
6	C	317	CLA	C4B-C3B-CAB	5.50	138.31	127.18
5	A	309	CHL	O2D-CGD-CBD	5.49	122.06	111.36
6	A	316	CLA	C4B-CHC-C1C	-5.49	120.25	127.47
6	A	307	CLA	C2B-C3B-CAB	-5.46	116.15	127.33
5	B	311	CHL	O2D-CGD-CBD	5.46	122.00	111.36
6	A	318	CLA	C4B-CHC-C1C	-5.45	120.30	127.47
5	A	309	CHL	C1-O2A-CGA	5.45	121.68	115.30
6	C	306	CLA	O2D-CGD-CBD	5.45	122.35	111.34
6	B	317	CLA	C2B-C3B-CAB	-5.43	116.21	127.33
6	C	316	CLA	O2D-CGD-CBD	5.40	122.24	111.34
5	B	310	CHL	C4D-C3D-C2D	-5.38	106.02	108.16
6	B	306	CLA	C2B-C3B-CAB	-5.37	116.34	127.33
6	C	315	CLA	C2B-C3B-CAB	-5.36	116.35	127.33
5	B	309	CHL	C4D-C3D-C2D	-5.33	106.04	108.16
5	A	305	CHL	CBC-CAC-C3C	-5.31	104.37	113.04
6	A	318	CLA	O2D-CGD-CBD	5.30	122.05	111.34
6	B	318	CLA	O2D-CGD-CBD	5.29	122.02	111.34
6	C	306	CLA	C4B-C3B-CAB	5.27	137.85	127.18
5	B	310	CHL	C3C-C4C-NC	5.27	111.24	109.67
5	B	310	CHL	O2D-CGD-CBD	5.27	121.63	111.36
2	B	302	LUT	C38-C25-C26	5.24	120.01	116.05
6	C	315	CLA	C4B-C3B-CAB	5.23	137.77	127.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	310	CHL	C4D-C3D-C2D	-5.23	106.08	108.16
6	A	306	CLA	C9-C8-C7	5.21	131.39	111.05
5	C	310	CHL	O2D-CGD-CBD	5.19	121.48	111.36
3	C	303	NEX	C24-C25-C26	-5.19	115.64	120.12
3	A	303	NEX	C27-C28-C29	-5.18	117.47	125.59
6	B	307	CLA	C4B-C3B-CAB	5.18	137.66	127.18
6	C	307	CLA	O2D-CGD-CBD	5.15	121.75	111.34
6	A	307	CLA	O2D-CGD-CBD	5.14	121.72	111.34
6	C	308	CLA	O2D-CGD-CBD	5.13	121.71	111.34
7	B	319	CAC	O2-AS-C1	-5.12	104.96	109.15
3	B	303	NEX	C35-C34-C33	-5.05	119.98	127.29
5	B	309	CHL	O2D-CGD-CBD	5.04	121.17	111.36
6	C	308	CLA	CHD-C4C-C3C	-5.02	117.25	124.97
6	C	307	CLA	CBD-CHA-C1A	5.01	135.32	128.77
6	B	316	CLA	C4B-C3B-CAB	4.97	137.25	127.18
6	A	307	CLA	C4B-C3B-CAB	4.96	137.22	127.18
6	B	316	CLA	C4B-CHC-C1C	-4.95	120.96	127.47
5	C	310	CHL	C1-C2-C3	-4.94	119.89	126.05
6	C	318	CLA	O2D-CGD-CBD	4.89	121.22	111.34
6	C	318	CLA	C4B-C3B-CAB	4.88	137.06	127.18
5	B	310	CHL	O2D-CGD-O1D	-4.87	114.01	123.79
5	B	313	CHL	C4D-C3D-C2D	-4.86	106.22	108.16
6	A	315	CLA	OBD-CAD-CBD	-4.85	118.61	125.94
5	A	310	CHL	C4D-C3D-C2D	-4.83	106.24	108.16
5	B	309	CHL	C1-O2A-CGA	4.81	120.93	115.30
6	A	316	CLA	C4B-C3B-CAB	4.81	136.91	127.18
6	A	318	CLA	C2B-C3B-CAB	-4.80	117.51	127.33
6	B	306	CLA	C4B-C3B-CAB	4.80	136.89	127.18
2	C	301	LUT	C18-C5-C6	-4.77	119.11	124.50
6	A	308	CLA	O2D-CGD-CBD	4.75	120.95	111.34
5	C	309	CHL	O2D-CGD-CBD	4.75	120.61	111.36
6	A	315	CLA	C2B-C3B-CAB	-4.75	117.60	127.33
5	A	312	CHL	OMC-CMC-C2C	-4.73	118.45	124.79
6	C	318	CLA	C2B-C3B-CAB	-4.72	117.67	127.33
2	C	302	LUT	C11-C10-C9	-4.71	120.47	127.29
6	B	315	CLA	CAA-C2A-C3A	-4.68	101.60	113.32
3	A	303	NEX	C25-C24-C23	-4.66	106.01	113.19
5	A	305	CHL	C1-C2-C3	-4.66	118.15	126.23
6	C	316	CLA	C2B-C3B-CAB	-4.65	117.82	127.33
3	B	303	NEX	C21-C26-C27	4.64	120.62	115.88
5	A	311	CHL	O2D-CGD-CBD	4.64	120.40	111.36
7	A	319	CAC	C2-AS-C1	4.63	120.01	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	318	CLA	C2B-C3B-CAB	-4.61	117.89	127.33
6	B	308	CLA	CHD-C4C-C3C	-4.58	117.94	124.97
2	B	301	LUT	C11-C10-C9	-4.58	120.67	127.29
5	B	309	CHL	OMC-CMC-C2C	-4.57	118.67	124.79
6	B	315	CLA	C2B-C3B-CAB	-4.56	118.00	127.33
6	A	315	CLA	C4B-C3B-CAB	4.56	136.40	127.18
6	B	307	CLA	O2D-CGD-O1D	-4.54	114.68	123.79
6	C	316	CLA	C4B-CHC-C1C	-4.53	121.51	127.47
6	B	306	CLA	CHD-C4C-C3C	-4.53	118.01	124.97
6	A	318	CLA	C4B-C3B-CAB	4.53	136.34	127.18
6	A	308	CLA	C1D-CHD-C4C	-4.52	115.58	122.60
6	B	314	CLA	C1D-CHD-C4C	-4.51	115.60	122.60
5	B	305	CHL	C1-C2-C3	-4.48	118.46	126.23
5	B	305	CHL	CBC-CAC-C3C	-4.47	105.73	113.04
5	C	311	CHL	C4D-C3D-C2D	-4.46	106.38	108.16
6	B	316	CLA	C2B-C3B-CAB	-4.46	118.20	127.33
5	B	311	CHL	C3C-C4C-NC	4.45	111.00	109.67
5	B	313	CHL	C3C-C4C-NC	4.45	111.00	109.67
6	A	315	CLA	O2D-CGD-CBD	4.44	120.31	111.34
6	A	308	CLA	CHD-C4C-C3C	-4.43	118.16	124.97
6	B	308	CLA	O2D-CGD-O1D	-4.43	114.89	123.79
6	A	317	CLA	C1-C2-C3	-4.43	118.54	126.23
6	A	316	CLA	CHB-C1B-NB	4.43	132.23	124.70
6	B	318	CLA	C4B-C3B-CAB	4.43	136.14	127.18
5	A	310	CHL	O2D-CGD-CBD	4.40	119.93	111.36
5	B	312	CHL	C4D-C3D-C2D	-4.39	106.41	108.16
6	B	315	CLA	O2D-CGD-O1D	-4.39	114.97	123.79
6	B	317	CLA	C1-C2-C3	-4.39	118.62	126.23
5	B	312	CHL	O2D-CGD-CBD	4.38	119.90	111.36
6	C	315	CLA	C2B-C1B-CHB	-4.38	117.69	126.00
6	A	306	CLA	C6-C5-C3	-4.38	102.62	112.62
3	A	303	NEX	C24-C25-C26	-4.34	116.37	120.12
2	B	302	LUT	C11-C10-C9	-4.34	121.01	127.29
6	C	308	CLA	C1D-CHD-C4C	-4.34	115.88	122.60
6	B	308	CLA	CHB-C1B-NB	4.33	132.06	124.70
3	B	303	NEX	C8-C7-C6	-4.33	171.98	177.63
6	A	308	CLA	CHB-C1B-NB	4.31	132.03	124.70
5	C	311	CHL	CAA-CBA-CGA	-4.30	100.56	113.24
5	A	309	CHL	OMC-CMC-C2C	-4.30	119.03	124.79
6	C	315	CLA	O2D-CGD-CBD	4.29	120.01	111.34
6	A	316	CLA	O2D-CGD-CBD	4.28	119.98	111.34
5	A	310	CHL	C1-C2-C3	-4.27	120.72	126.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	305	CHL	C1-C2-C3	-4.27	118.82	126.23
2	B	302	LUT	C1-C2-C3	4.26	122.62	113.40
6	B	307	CLA	CBD-CHA-C1A	4.26	134.34	128.77
6	B	314	CLA	CHD-C4C-C3C	-4.25	118.44	124.97
6	A	306	CLA	O2D-CGD-O1D	-4.25	115.26	123.79
3	B	303	NEX	C39-C29-C30	-4.25	116.87	122.92
6	C	317	CLA	C1-C2-C3	-4.25	118.86	126.23
6	A	316	CLA	C2B-C3B-CAB	-4.24	118.65	127.33
5	C	309	CHL	C4D-C3D-C2D	-4.22	106.48	108.16
6	C	314	CLA	O2D-CGD-CBD	4.22	119.87	111.34
5	A	312	CHL	CBC-CAC-C3C	-4.22	106.15	113.04
6	C	307	CLA	C4B-C3B-CAB	4.22	135.72	127.18
6	A	314	CLA	CBD-CHA-C1A	4.21	134.27	128.77
6	A	306	CLA	CHD-C4C-C3C	-4.20	118.51	124.97
5	C	313	CHL	O2D-CGD-CBD	4.20	119.54	111.36
6	A	315	CLA	O2D-CGD-O1D	-4.19	115.38	123.79
6	A	316	CLA	CHD-C4C-C3C	-4.19	118.54	124.97
6	B	315	CLA	C4B-C3B-CAB	4.18	135.63	127.18
6	C	314	CLA	CBD-CHA-C1A	4.17	134.22	128.77
2	B	301	LUT	C31-C30-C29	4.17	133.31	127.29
2	A	301	LUT	C31-C30-C29	4.16	133.31	127.29
6	A	308	CLA	C2B-C1B-CHB	-4.15	118.12	126.00
6	B	316	CLA	C1D-CHD-C4C	-4.15	116.17	122.60
6	B	306	CLA	CHB-C1B-NB	4.13	131.72	124.70
6	C	314	CLA	C2B-C1B-CHB	-4.10	118.23	126.00
6	C	315	CLA	CHB-C1B-NB	4.09	131.65	124.70
2	C	302	LUT	C7-C8-C9	4.08	132.32	126.22
6	C	308	CLA	C2B-C1B-CHB	-4.08	118.26	126.00
6	B	307	CLA	C2B-C1B-CHB	-4.07	118.27	126.00
6	C	316	CLA	C4B-C3B-CAB	4.07	135.41	127.18
6	C	316	CLA	O2D-CGD-O1D	-4.06	115.64	123.79
5	B	313	CHL	O2D-CGD-CBD	4.06	119.26	111.36
6	B	315	CLA	C2B-C1B-CHB	-4.06	118.31	126.00
2	A	302	LUT	C1-C2-C3	4.06	122.17	113.40
2	C	301	LUT	C15-C35-C34	-4.05	114.53	123.45
6	C	318	CLA	CHB-C1B-NB	4.03	131.54	124.70
5	A	312	CHL	O2D-CGD-CBD	4.02	119.19	111.36
6	C	315	CLA	OBD-CAD-CBD	-4.02	119.87	125.94
6	B	318	CLA	O2D-CGD-O1D	-4.01	115.73	123.79
3	C	303	NEX	C25-C24-C23	-4.01	107.03	113.19
4	B	304	LHG	O8-C23-C24	4.00	124.14	111.90
2	C	302	LUT	C1-C2-C3	3.99	122.03	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	314	CLA	O2D-CGD-O1D	-3.98	115.80	123.79
5	B	305	CHL	O2A-CGA-CBA	3.97	124.07	111.90
3	C	303	NEX	C39-C29-C30	-3.97	117.27	122.92
6	C	318	CLA	C2B-C1B-CHB	-3.97	118.48	126.00
6	C	314	CLA	CHB-C1B-NB	3.96	131.42	124.70
6	B	316	CLA	CHD-C4C-C3C	-3.96	118.89	124.97
6	A	317	CLA	CBD-CHA-C1A	3.95	133.93	128.77
6	C	307	CLA	CAA-C2A-C3A	-3.93	103.48	113.32
3	C	303	NEX	C1-C6-C7	-3.93	117.82	120.77
6	C	306	CLA	C4-C3-C5	3.93	121.35	115.39
6	A	318	CLA	O2D-CGD-O1D	-3.93	115.90	123.79
6	B	306	CLA	C2B-C1B-CHB	-3.93	118.56	126.00
6	B	317	CLA	C2B-C1B-CHB	-3.92	118.57	126.00
6	C	306	CLA	C9-C8-C7	3.92	126.34	111.05
6	B	315	CLA	CHB-C1B-NB	3.91	131.35	124.70
6	B	315	CLA	OBD-CAD-CBD	-3.91	120.04	125.94
6	A	307	CLA	CBD-CHA-C1A	3.90	133.86	128.77
5	B	309	CHL	O2D-CGD-O1D	-3.89	115.98	123.79
6	B	307	CLA	CHB-C1B-NB	3.88	131.29	124.70
6	C	308	CLA	CBD-CHA-C1A	3.88	133.84	128.77
6	C	307	CLA	C2B-C3B-CAB	-3.88	119.39	127.33
5	C	312	CHL	O2A-CGA-CBA	3.88	123.76	111.90
6	C	317	CLA	CBD-CHA-C1A	3.87	133.83	128.77
5	C	305	CHL	O2A-CGA-CBA	3.87	123.74	111.90
6	C	306	CLA	CHB-C1B-NB	3.86	131.26	124.70
5	B	310	CHL	C1-C2-C3	-3.85	121.24	126.05
5	B	311	CHL	CAA-CBA-CGA	-3.85	101.90	113.24
2	C	301	LUT	C40-C33-C34	-3.84	117.45	122.92
5	C	305	CHL	C3C-C4C-NC	3.84	110.82	109.67
6	C	317	CLA	O2D-CGD-CBD	3.83	119.08	111.34
6	B	308	CLA	C2B-C1B-CHB	-3.83	118.73	126.00
6	B	317	CLA	CHB-C1B-NB	3.83	131.21	124.70
6	C	314	CLA	CHD-C4C-C3C	-3.83	119.09	124.97
5	C	309	CHL	OMC-CMC-C2C	-3.82	119.67	124.79
6	B	308	CLA	OBD-CAD-CBD	-3.81	120.19	125.94
3	B	303	NEX	C24-C25-C26	-3.81	116.84	120.12
6	A	315	CLA	C2B-C1B-CHB	-3.80	118.79	126.00
5	C	313	CHL	C4D-C3D-C2D	-3.80	106.65	108.16
2	C	301	LUT	C40-C33-C32	3.80	124.23	118.09
2	B	301	LUT	C20-C13-C14	-3.80	117.51	122.92
6	B	308	CLA	C1D-CHD-C4C	-3.79	116.72	122.60
5	A	305	CHL	O2D-CGD-CBD	3.79	118.74	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	315	CLA	C1-C2-C3	-3.78	119.67	126.23
5	A	310	CHL	OMC-CMC-C2C	-3.78	119.73	124.79
6	B	318	CLA	CHB-C1B-NB	3.78	131.11	124.70
6	C	307	CLA	C3B-C4B-CHC	-3.77	118.84	126.00
3	C	303	NEX	C26-C27-C28	-3.77	118.00	126.06
6	B	318	CLA	C2B-C1B-CHB	-3.77	118.86	126.00
6	A	316	CLA	C1D-C2D-C3D	-3.76	103.29	106.97
2	A	302	LUT	C23-C24-C25	-3.74	121.65	125.23
2	C	302	LUT	C15-C14-C13	3.74	132.69	127.29
2	B	302	LUT	C20-C13-C14	-3.73	117.61	122.92
6	C	307	CLA	C1D-CHD-C4C	-3.72	116.83	122.60
6	C	315	CLA	CAA-C2A-C3A	-3.71	104.02	113.32
6	A	318	CLA	C2B-C1B-CHB	-3.71	118.97	126.00
6	A	308	CLA	C1-C2-C3	-3.70	119.81	126.23
5	C	311	CHL	C3C-C4C-NC	3.70	110.77	109.67
6	C	316	CLA	CHD-C4C-C3C	-3.69	119.30	124.97
6	B	316	CLA	CHB-C1B-NB	3.69	130.96	124.70
6	A	318	CLA	CHB-C1B-NB	3.67	130.93	124.70
5	B	311	CHL	O2D-CGD-O1D	-3.67	116.43	123.79
6	A	314	CLA	CHD-C4C-C3C	-3.66	119.35	124.97
6	A	315	CLA	C1D-CHD-C4C	-3.66	116.92	122.60
3	A	303	NEX	C24-C23-C22	-3.65	103.20	110.42
5	A	305	CHL	O2A-CGA-CBA	3.65	123.06	111.90
6	B	306	CLA	O2D-CGD-O1D	-3.63	116.49	123.79
5	A	309	CHL	C3C-C4C-NC	3.63	110.75	109.67
6	C	315	CLA	CAA-C2A-C1A	3.62	122.12	112.51
6	A	314	CLA	O2D-CGD-CBD	3.62	118.66	111.34
6	C	317	CLA	CHB-C1B-NB	3.62	130.85	124.70
6	A	314	CLA	C1-O2A-CGA	3.62	127.51	117.00
5	A	311	CHL	CAA-CBA-CGA	-3.61	102.59	113.24
3	C	303	NEX	C11-C10-C9	-3.61	122.07	127.29
5	A	313	CHL	O2D-CGD-CBD	3.61	118.39	111.36
3	B	303	NEX	C1-C6-C7	-3.61	118.06	120.77
6	B	317	CLA	O2D-CGD-CBD	3.61	118.63	111.34
6	A	315	CLA	CAA-C2A-C3A	-3.60	104.31	113.32
6	A	308	CLA	CHC-C1C-NC	3.60	130.56	123.42
6	C	316	CLA	C1D-CHD-C4C	-3.60	117.02	122.60
6	B	306	CLA	C6-C7-C8	-3.59	104.26	115.44
6	C	306	CLA	C2B-C1B-CHB	-3.59	119.19	126.00
6	B	314	CLA	OBD-CAD-CBD	-3.58	120.53	125.94
6	B	317	CLA	CHD-C4C-C3C	-3.56	119.50	124.97
5	C	313	CHL	O2A-CGA-CBA	3.56	122.80	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	302	LUT	C16-C1-C6	-3.56	104.43	110.33
6	A	307	CLA	C2D-C1D-ND	-3.54	105.52	109.56
6	A	317	CLA	C2B-C1B-CHB	-3.54	119.29	126.00
2	A	302	LUT	C16-C1-C6	-3.54	104.47	110.33
6	B	307	CLA	C3A-C4A-NA	3.54	115.09	110.81
6	C	308	CLA	C1D-C2D-C3D	-3.54	103.51	106.97
6	C	314	CLA	O2A-CGA-CBA	3.53	122.71	111.90
6	B	306	CLA	C6-C5-C3	-3.53	104.57	112.62
6	A	316	CLA	C1D-CHD-C4C	-3.52	117.14	122.60
6	A	317	CLA	OBD-CAD-CBD	-3.52	120.63	125.94
6	A	314	CLA	CHB-C1B-NB	3.51	130.67	124.70
6	B	314	CLA	C1-O2A-CGA	3.51	127.21	117.00
5	B	310	CHL	OMC-CMC-C2C	-3.51	120.09	124.79
5	C	309	CHL	C3C-C4C-NC	3.51	110.72	109.67
6	B	317	CLA	C1D-CHD-C4C	-3.50	117.17	122.60
6	C	306	CLA	C1-C2-C3	-3.49	120.17	126.23
3	B	303	NEX	C27-C28-C29	-3.49	120.11	125.59
4	B	304	LHG	O7-C7-C8	3.48	118.96	111.54
6	B	315	CLA	C3B-CAB-CBB	-3.48	118.74	125.95
6	A	315	CLA	CHC-C1C-NC	3.48	130.32	123.42
6	B	317	CLA	CBD-CHA-C1A	3.47	133.30	128.77
7	C	319	CAC	C2-AS-C1	3.47	117.35	109.43
6	A	314	CLA	C1D-CHD-C4C	-3.46	117.23	122.60
2	C	301	LUT	C36-C21-C26	3.46	114.26	109.68
5	C	310	CHL	CMD-C2D-C3D	3.46	131.02	124.28
5	B	313	CHL	C1-C2-C3	-3.46	120.23	126.23
6	C	308	CLA	CHB-C1B-NB	3.45	130.57	124.70
6	B	315	CLA	C1-C2-C3	-3.45	120.24	126.23
6	C	306	CLA	OBD-CAD-CBD	-3.45	120.73	125.94
6	A	306	CLA	CBD-CHA-C1A	3.42	133.25	128.77
6	C	316	CLA	O2A-CGA-CBA	3.42	122.36	111.90
5	A	313	CHL	CBC-CAC-C3C	-3.42	107.46	113.04
5	B	310	CHL	CMD-C2D-C3D	3.41	130.93	124.28
5	B	313	CHL	C4-C3-C5	3.41	120.56	115.39
5	B	312	CHL	CBC-CAC-C3C	-3.40	107.48	113.04
3	B	303	NEX	C26-O24-C25	3.40	65.81	61.17
6	C	318	CLA	O2D-CGD-O1D	-3.40	116.96	123.79
6	A	307	CLA	C4-C3-C5	3.40	120.56	115.39
6	A	315	CLA	CHB-C1B-NB	3.40	130.47	124.70
6	C	316	CLA	C3B-CAB-CBB	-3.39	118.93	125.95
6	B	314	CLA	O2D-CGD-CBD	3.38	118.18	111.34
5	C	310	CHL	OMC-CMC-C2C	-3.38	120.26	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	307	CLA	C2D-C1D-ND	-3.37	105.72	109.56
6	B	314	CLA	CHC-C1C-NC	3.37	130.10	123.42
6	C	317	CLA	C3B-CAB-CBB	-3.36	118.98	125.95
5	C	305	CHL	O2D-CGD-CBD	3.36	117.90	111.36
2	A	301	LUT	C38-C25-C26	3.35	118.59	116.05
6	C	316	CLA	CHB-C1B-NB	3.35	130.40	124.70
6	A	307	CLA	C1D-CHD-C4C	-3.35	117.41	122.60
5	B	305	CHL	OMC-CMC-C2C	-3.35	120.31	124.79
5	C	309	CHL	O2D-CGD-O1D	-3.34	117.09	123.79
5	C	310	CHL	C3C-C4C-NC	3.33	110.67	109.67
3	C	303	NEX	C27-C28-C29	-3.33	120.37	125.59
3	A	303	NEX	C26-C27-C28	-3.32	118.96	126.06
6	A	316	CLA	C4-C3-C5	3.31	120.42	115.39
6	A	306	CLA	CHB-C1B-NB	3.31	130.32	124.70
3	A	303	NEX	C21-C22-C23	-3.30	109.53	115.25
6	A	317	CLA	O2A-CGA-CBA	3.30	122.01	111.90
6	C	314	CLA	C1D-C2D-C3D	-3.30	103.74	106.97
6	A	317	CLA	O2D-CGD-CBD	3.29	117.99	111.34
5	A	311	CHL	OMC-CMC-C2C	-3.29	120.39	124.79
5	C	305	CHL	C4D-C3D-C2D	-3.29	106.85	108.16
3	C	303	NEX	C24-C23-C22	-3.28	103.93	110.42
6	A	317	CLA	CHB-C1B-NB	3.28	130.27	124.70
5	A	313	CHL	C1-C2-C3	-3.28	120.53	126.23
6	A	307	CLA	C2B-C1B-CHB	-3.27	119.80	126.00
6	C	317	CLA	C2B-C1B-CHB	-3.27	119.80	126.00
6	B	317	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
5	A	305	CHL	C4D-C3D-C2D	-3.27	106.86	108.16
2	B	301	LUT	C1-C2-C3	3.27	120.46	113.40
3	A	303	NEX	C39-C29-C30	-3.26	118.28	122.92
5	A	309	CHL	O2D-CGD-O1D	-3.26	117.25	123.79
6	A	317	CLA	C1D-CHD-C4C	-3.25	117.56	122.60
6	A	317	CLA	CHD-C4C-C3C	-3.25	119.98	124.97
5	C	311	CHL	O2D-CGD-O1D	-3.24	117.28	123.79
6	A	307	CLA	CHD-C4C-C3C	-3.24	119.99	124.97
6	B	315	CLA	C1D-CHD-C4C	-3.24	117.58	122.60
5	C	310	CHL	O2A-CGA-CBA	3.23	121.79	111.90
6	B	308	CLA	C9-C8-C10	3.23	123.67	111.05
6	A	307	CLA	O2D-CGD-O1D	-3.23	117.31	123.79
6	A	307	CLA	C4D-ND-C1D	3.22	110.46	106.57
6	A	315	CLA	CAA-C2A-C1A	3.22	121.04	112.51
5	C	313	CHL	CAA-C2A-C3A	-3.22	105.27	113.32
2	C	301	LUT	C16-C1-C6	-3.21	105.01	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	314	CLA	C3D-C4D-CHA	3.20	113.30	108.16
6	A	308	CLA	OBD-CAD-CBD	-3.21	121.10	125.94
6	B	314	CLA	CBD-CHA-C1A	3.20	132.96	128.77
6	C	307	CLA	CHC-C4B-NB	3.21	130.15	124.70
6	A	307	CLA	C3B-CAB-CBB	-3.21	119.31	125.95
3	B	303	NEX	C11-C10-C9	-3.20	122.66	127.29
5	C	310	CHL	O2D-CGD-O1D	-3.20	117.36	123.79
2	C	301	LUT	C35-C34-C33	-3.19	122.67	127.29
6	C	307	CLA	CHD-C4C-C3C	-3.19	120.06	124.97
6	C	314	CLA	C1-C2-C3	-3.19	120.70	126.23
5	A	312	CHL	O2A-CGA-CBA	3.19	121.66	111.90
6	C	307	CLA	C1-C2-C3	-3.19	120.70	126.23
6	A	315	CLA	C1-C2-C3	-3.19	120.70	126.23
6	A	307	CLA	CHC-C4B-NB	3.18	130.10	124.70
5	A	310	CHL	O2A-CGA-CBA	3.18	121.62	111.90
6	C	318	CLA	CBD-CHA-C1A	3.18	132.92	128.77
6	B	307	CLA	C1-C2-C3	-3.17	120.72	126.23
6	C	317	CLA	C4-C3-C5	3.17	120.20	115.39
6	B	307	CLA	CHD-C4C-C3C	-3.17	120.11	124.97
6	C	315	CLA	C3B-CAB-CBB	-3.16	119.40	125.95
2	A	302	LUT	C12-C13-C14	3.16	123.84	118.98
5	A	305	CHL	OMC-CMC-C2C	-3.16	120.56	124.79
6	A	308	CLA	O2D-CGD-O1D	-3.16	117.45	123.79
6	A	315	CLA	CBD-CHA-C1A	3.15	132.89	128.77
5	C	313	CHL	CBC-CAC-C3C	-3.15	107.89	113.04
6	C	307	CLA	O2A-CGA-CBA	3.14	121.52	111.90
6	B	316	CLA	O1D-CGD-CBD	-3.14	118.05	124.45
6	C	316	CLA	C2B-C1B-CHB	-3.13	120.06	126.00
6	A	308	CLA	C4-C3-C5	3.13	120.14	115.39
6	C	306	CLA	O2D-CGD-O1D	-3.13	117.51	123.79
6	C	315	CLA	C1D-CHD-C4C	-3.12	117.76	122.60
6	A	307	CLA	CHB-C1B-NB	3.12	130.00	124.70
2	A	301	LUT	C16-C1-C6	-3.12	105.17	110.33
5	A	305	CHL	O2D-CGD-O1D	-3.12	117.53	123.79
5	A	310	CHL	C3C-C4C-NC	3.11	110.60	109.67
6	A	316	CLA	C2B-C1B-CHB	-3.11	120.11	126.00
6	C	306	CLA	CMC-C2C-C1C	3.11	129.38	124.95
6	C	307	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
6	B	318	CLA	OBD-CAD-CBD	-3.11	121.25	125.94
6	A	306	CLA	C2B-C1B-CHB	-3.10	120.12	126.00
5	A	309	CHL	C4D-C3D-C2D	-3.09	106.93	108.16
6	A	308	CLA	C1-O2A-CGA	3.09	125.99	117.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	317	CLA	C4-C3-C5	3.09	120.08	115.39
6	C	315	CLA	CHD-C4C-C3C	-3.09	120.23	124.97
5	B	313	CHL	O2A-CGA-CBA	3.08	121.34	111.90
6	B	318	CLA	C3B-CAB-CBB	-3.08	119.58	125.95
6	B	316	CLA	O2A-CGA-CBA	3.08	121.32	111.90
2	A	301	LUT	C11-C10-C9	-3.07	122.84	127.29
6	A	318	CLA	CBD-CHA-C1A	3.07	132.78	128.77
6	B	317	CLA	C2A-C1A-NA	3.07	115.26	111.33
6	B	306	CLA	C4-C3-C5	3.06	120.04	115.39
6	B	314	CLA	CHB-C1B-NB	3.06	129.90	124.70
6	B	308	CLA	C1-C2-C3	-3.06	120.92	126.23
6	B	316	CLA	C4D-ND-C1D	3.06	110.26	106.57
6	B	316	CLA	C4-C3-C5	3.06	120.03	115.39
7	C	319	CAC	O1-AS-C1	3.05	119.56	109.18
3	A	303	NEX	C26-O24-C25	3.03	65.31	61.17
6	B	315	CLA	C4-C3-C5	3.03	119.99	115.39
6	A	307	CLA	O2A-CGA-CBA	3.02	121.16	111.90
6	A	316	CLA	C4B-NB-C1B	3.03	110.03	107.12
6	C	317	CLA	CHC-C1C-NC	3.02	129.42	123.42
6	B	318	CLA	CBD-CHA-C1A	3.02	132.72	128.77
6	A	308	CLA	C9-C8-C10	-3.02	99.26	111.05
6	C	317	CLA	O2A-CGA-CBA	3.02	121.14	111.90
6	C	317	CLA	CHC-C4B-NB	3.02	129.83	124.70
5	C	312	CHL	O2D-CGD-O1D	-3.02	117.73	123.79
6	B	317	CLA	C3B-C4B-CHC	-3.01	120.29	126.00
5	C	311	CHL	OMC-CMC-C2C	-3.01	120.76	124.79
5	B	305	CHL	CMD-C2D-C3D	3.01	130.14	124.28
5	A	309	CHL	O2A-CGA-CBA	3.01	121.10	111.90
6	A	315	CLA	C3B-CAB-CBB	-3.00	119.73	125.95
5	B	313	CHL	OMC-CMC-C2C	-3.00	120.77	124.79
6	B	306	CLA	O2A-CGA-O1A	-3.00	115.63	123.48
6	B	318	CLA	C3B-C4B-CHC	-3.00	120.32	126.00
2	A	301	LUT	C22-C21-C26	2.99	112.53	107.34
5	A	311	CHL	O2D-CGD-O1D	-2.99	117.79	123.79
5	B	311	CHL	C1-O2A-CGA	2.99	125.69	117.00
6	B	306	CLA	C1D-C2D-C3D	-2.99	104.05	106.97
4	A	304	LHG	O8-C23-C24	2.98	121.03	111.90
3	C	303	NEX	C11-C12-C13	-2.98	117.83	126.37
6	B	307	CLA	C1D-CHD-C4C	-2.98	117.98	122.60
6	C	314	CLA	C1D-CHD-C4C	-2.97	117.99	122.60
6	C	306	CLA	CHD-C4C-C3C	-2.97	120.41	124.97
6	B	306	CLA	C1-C2-C3	-2.97	121.07	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	314	CLA	O2A-CGA-CBA	2.96	120.97	111.90
6	C	316	CLA	C1D-C2D-C3D	-2.96	104.07	106.97
6	C	307	CLA	O2D-CGD-O1D	-2.96	117.85	123.79
6	C	308	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
5	B	310	CHL	O2A-CGA-CBA	2.96	120.94	111.90
6	B	316	CLA	C2B-C1B-CHB	-2.95	120.41	126.00
6	B	308	CLA	C4-C3-C5	2.94	119.86	115.39
5	B	312	CHL	OMC-CMC-C2C	-2.94	120.86	124.79
6	A	314	CLA	C3B-C4B-CHC	-2.94	120.43	126.00
6	A	314	CLA	C3D-C4D-CHA	2.94	112.87	108.16
6	B	315	CLA	C4D-ND-C1D	2.93	110.11	106.57
6	A	318	CLA	C1D-CHD-C4C	-2.93	118.06	122.60
6	B	307	CLA	C3B-CAB-CBB	-2.93	119.88	125.95
6	A	314	CLA	C1D-C2D-C3D	-2.93	104.10	106.97
6	B	306	CLA	O2A-CGA-CBA	2.93	120.86	111.90
6	C	307	CLA	C2B-C1B-CHB	-2.93	120.45	126.00
6	B	306	CLA	OBD-CAD-CBD	-2.92	121.52	125.94
6	B	316	CLA	C4B-NB-C1B	2.92	109.93	107.12
3	C	303	NEX	C26-O24-C25	2.92	65.15	61.17
6	B	314	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
6	B	317	CLA	C3B-CAB-CBB	-2.91	119.92	125.95
3	B	303	NEX	C25-C26-C27	-2.91	111.42	121.01
6	C	318	CLA	C1D-CHD-C4C	-2.91	118.09	122.60
3	B	303	NEX	C15-C14-C13	-2.91	123.09	127.29
3	C	303	NEX	C25-C26-C27	-2.90	111.46	121.01
5	C	309	CHL	O2A-CGA-CBA	2.90	120.78	111.90
2	A	302	LUT	C8-C7-C6	-2.90	118.67	127.23
6	B	307	CLA	CHC-C1C-NC	2.90	129.17	123.42
6	C	316	CLA	CBD-CHA-C1A	2.90	132.56	128.77
5	A	305	CHL	CMD-C2D-C3D	2.90	129.92	124.28
6	A	316	CLA	O2A-CGA-CBA	2.90	120.77	111.90
6	B	307	CLA	O2A-CGA-CBA	2.88	120.73	111.90
6	C	318	CLA	CHD-C4C-C3C	-2.88	120.54	124.97
6	A	317	CLA	C1D-C2D-C3D	-2.88	104.15	106.97
5	B	311	CHL	CMD-C2D-C3D	2.88	129.89	124.28
6	C	307	CLA	CHB-C1B-NB	2.88	129.59	124.70
6	C	307	CLA	CBC-CAC-C3C	-2.87	103.67	112.37
6	C	306	CLA	O2A-C1-C2	-2.87	101.55	108.12
2	C	301	LUT	C1-C2-C3	2.87	119.60	113.40
6	C	317	CLA	C3B-C4B-CHC	-2.87	120.56	126.00
2	B	301	LUT	C22-C21-C26	2.87	112.31	107.34
6	B	315	CLA	CBD-CHA-C1A	2.87	132.51	128.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	311	CHL	O2A-CGA-CBA	2.86	120.66	111.90
4	C	304	LHG	C5-O7-C7	-2.86	111.13	117.86
2	B	301	LUT	C35-C34-C33	-2.86	123.16	127.29
6	C	306	CLA	O2A-CGA-O1A	-2.86	116.01	123.48
6	A	314	CLA	CHC-C4B-NB	2.86	129.55	124.70
6	B	314	CLA	C1-C2-C3	-2.85	121.28	126.23
2	A	302	LUT	C11-C10-C9	-2.85	123.17	127.29
6	C	314	CLA	CGD-CBD-CAD	2.85	120.36	110.79
6	A	314	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
6	B	308	CLA	C1-O2A-CGA	2.84	125.27	117.00
3	A	303	NEX	C25-C26-C27	-2.84	111.66	121.01
2	C	301	LUT	C22-C21-C26	2.84	112.27	107.34
6	C	315	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
5	B	311	CHL	O2A-CGA-CBA	2.84	120.59	111.90
3	B	303	NEX	C26-C27-C28	-2.84	119.99	126.06
6	A	317	CLA	C3B-C4B-CHC	-2.83	120.64	126.00
2	C	302	LUT	C18-C5-C6	-2.83	121.31	124.50
6	B	307	CLA	C4D-ND-C1D	2.82	109.97	106.57
3	A	303	NEX	C37-C21-C36	2.82	111.89	107.47
6	C	306	CLA	C6-C5-C3	-2.82	106.19	112.62
6	B	318	CLA	C1D-CHD-C4C	-2.82	118.23	122.60
6	A	318	CLA	C3B-CAB-CBB	-2.82	120.12	125.95
6	C	308	CLA	CMD-C2D-C3D	2.81	130.46	125.16
5	B	309	CHL	O2A-CGA-CBA	2.81	120.51	111.90
6	B	315	CLA	CHC-C1C-NC	2.81	129.00	123.42
5	A	312	CHL	C6-C5-C3	-2.81	106.22	112.62
6	C	318	CLA	C3B-C4B-CHC	-2.81	120.68	126.00
6	B	318	CLA	CHC-C4B-NB	2.80	129.45	124.70
6	C	314	CLA	C1-O2A-CGA	2.80	125.13	117.00
6	B	306	CLA	C1D-CHD-C4C	-2.80	118.27	122.60
2	A	301	LUT	C1-C2-C3	2.79	119.44	113.40
3	A	303	NEX	C15-C14-C13	-2.79	123.26	127.29
6	A	316	CLA	CBD-CHA-C1A	2.79	132.42	128.77
4	C	304	LHG	O7-C7-C8	2.79	117.48	111.54
4	C	304	LHG	O8-C23-C24	2.79	120.43	111.90
6	B	317	CLA	C3A-C4A-NA	2.78	114.18	110.81
6	A	317	CLA	CHC-C1C-NC	2.78	128.94	123.42
6	A	307	CLA	CAA-C2A-C3A	-2.77	106.38	113.32
6	A	318	CLA	CHD-C4C-C3C	-2.77	120.72	124.97
6	B	314	CLA	CED-O2D-CGD	2.77	122.59	116.00
5	C	313	CHL	OMC-CMC-C2C	-2.77	121.08	124.79
5	A	305	CHL	CAA-CBA-CGA	-2.77	105.08	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	318	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
4	A	304	LHG	O7-C7-C8	2.76	117.43	111.54
5	C	312	CHL	OMC-CMC-C2C	-2.76	121.09	124.79
6	A	306	CLA	C2D-C3D-CAD	2.76	146.20	134.94
6	A	316	CLA	C2B-C1B-NB	-2.76	107.65	109.50
6	C	306	CLA	C2A-C1A-NA	2.76	114.86	111.33
6	C	307	CLA	C3D-C4D-CHA	2.76	112.58	108.16
5	A	312	CHL	CMD-C2D-C3D	2.75	129.64	124.28
6	B	316	CLA	C2D-C1D-ND	-2.75	106.42	109.56
6	A	318	CLA	C3B-C4B-CHC	-2.75	120.79	126.00
3	C	303	NEX	C21-C22-C23	-2.74	110.50	115.25
6	B	314	CLA	C2D-C3D-CAD	2.74	146.11	134.94
6	C	306	CLA	C2D-C3D-CAD	2.73	146.08	134.94
6	A	306	CLA	C1-C2-C3	-2.73	121.49	126.23
6	B	314	CLA	C2B-C1B-CHB	-2.73	120.83	126.00
6	C	315	CLA	CBD-CHA-C1A	2.73	132.34	128.77
6	A	318	CLA	CHC-C4B-NB	2.72	129.32	124.70
6	B	315	CLA	CHD-C4C-C3C	-2.72	120.80	124.97
6	B	315	CLA	CHC-C4B-NB	2.72	129.31	124.70
6	B	306	CLA	C2A-C1A-NA	2.71	114.81	111.33
5	B	312	CHL	O2A-CGA-CBA	2.71	120.20	111.90
3	B	303	NEX	C25-C24-C23	-2.71	109.01	113.19
6	C	316	CLA	C4-C3-C5	2.71	119.51	115.39
6	B	307	CLA	C3D-C4D-CHA	2.71	112.51	108.16
6	A	314	CLA	C2B-C1B-CHB	-2.71	120.86	126.00
6	B	317	CLA	C4-C3-C5	2.71	119.50	115.39
6	C	315	CLA	O2D-CGD-O1D	-2.71	118.35	123.79
6	C	308	CLA	O2D-CGD-O1D	-2.71	118.36	123.79
5	B	313	CHL	CMD-C2D-C3D	2.70	129.53	124.28
6	B	315	CLA	CGD-CBD-CAD	-2.70	101.74	110.79
5	B	312	CHL	C4-C3-C5	2.69	119.47	115.39
6	B	316	CLA	CBD-CHA-C1A	2.69	132.28	128.77
5	C	305	CHL	CAA-CBA-CGA	-2.68	105.33	113.24
6	B	308	CLA	C2D-C3D-CAD	2.68	145.88	134.94
6	B	306	CLA	C2D-C3D-CAD	2.68	145.86	134.94
5	A	313	CHL	O2A-CGA-CBA	2.68	120.09	111.90
6	A	307	CLA	C6-C7-C8	-2.68	107.12	115.44
6	C	314	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
6	A	318	CLA	C1D-C2D-C3D	-2.67	104.36	106.97
6	A	306	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
6	B	317	CLA	O2A-CGA-CBA	2.67	120.06	111.90
5	A	313	CHL	C4-C3-C5	2.66	119.43	115.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	316	CLA	C1B-CHB-C4A	-2.66	124.85	130.12
5	B	305	CHL	C3C-C4C-NC	2.66	110.47	109.67
6	C	307	CLA	OBD-CAD-CBD	-2.66	121.93	125.94
6	B	307	CLA	C1D-C2D-C3D	-2.66	104.37	106.97
6	B	317	CLA	CHC-C1C-NC	2.66	128.70	123.42
2	A	302	LUT	C31-C32-C33	-2.65	118.76	126.37
6	C	307	CLA	C4D-ND-C1D	2.65	109.77	106.57
5	B	305	CHL	O2D-CGD-CBD	2.65	116.52	111.36
2	B	302	LUT	C8-C7-C6	-2.64	119.43	127.23
6	C	317	CLA	CHD-C4C-C3C	-2.64	120.91	124.97
5	B	313	CHL	O2D-CGD-O1D	-2.64	118.49	123.79
6	C	306	CLA	O2A-CGA-CBA	2.64	119.98	111.90
6	A	314	CLA	C4A-NA-C1A	2.64	110.10	106.38
5	A	312	CHL	C3C-C4C-NC	2.64	110.46	109.67
3	C	303	NEX	C30-C31-C32	-2.64	114.38	123.23
6	B	317	CLA	C1D-C2D-C3D	-2.64	104.39	106.97
2	A	302	LUT	C18-C5-C6	-2.64	121.52	124.50
6	B	315	CLA	C2D-C1D-ND	-2.63	106.56	109.56
3	B	303	NEX	C15-C35-C34	-2.63	117.65	123.45
4	B	304	LHG	O8-C23-O10	-2.63	116.61	123.48
6	A	308	CLA	CHC-C1C-C2C	-2.62	119.46	126.51
6	B	317	CLA	CHC-C4B-NB	2.62	129.15	124.70
6	C	307	CLA	CMC-C2C-C1C	2.62	128.68	124.95
6	A	317	CLA	C2A-C1A-NA	2.62	114.68	111.33
6	C	315	CLA	C4-C3-C5	2.61	119.36	115.39
6	A	315	CLA	C1C-NC-C4C	2.61	109.78	106.26
7	A	319	CAC	O2-AS-C1	-2.61	107.02	109.15
6	B	315	CLA	CAA-C2A-C1A	2.61	119.43	112.51
2	B	302	LUT	C35-C34-C33	-2.60	123.53	127.29
6	C	315	CLA	C1D-C2D-C3D	-2.60	104.42	106.97
6	C	307	CLA	C2D-C1D-ND	-2.59	106.60	109.56
6	A	316	CLA	C3D-C4D-CHA	2.59	112.32	108.16
6	B	316	CLA	CHC-C1C-NC	2.59	128.56	123.42
6	B	316	CLA	C3D-C4D-CHA	2.59	112.32	108.16
6	C	317	CLA	C2A-C1A-NA	2.59	114.65	111.33
7	B	319	CAC	O1-AS-C2	2.59	118.00	109.18
2	A	301	LUT	C2-C1-C6	2.58	115.30	109.60
6	A	307	CLA	C3B-C4B-CHC	-2.59	121.10	126.00
5	B	311	CHL	OMC-CMC-C2C	-2.58	121.33	124.79
6	A	306	CLA	C1D-CHD-C4C	-2.58	118.60	122.60
6	B	314	CLA	CHC-C1C-C2C	-2.58	119.58	126.51
6	A	306	CLA	C1C-NC-C4C	2.58	109.74	106.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	308	CLA	CHC-C1C-NC	2.58	128.54	123.42
3	B	303	NEX	C19-C9-C10	-2.58	119.25	122.92
6	A	315	CLA	C2D-C3D-CAD	2.58	145.45	134.94
6	B	306	CLA	C3B-CAB-CBB	-2.57	120.62	125.95
2	C	301	LUT	C36-C21-C22	-2.57	104.69	109.50
6	C	317	CLA	C1D-C2D-C3D	-2.57	104.45	106.97
6	B	308	CLA	CMD-C2D-C3D	2.57	130.00	125.16
6	B	315	CLA	C3B-C4B-CHC	-2.57	121.13	126.00
6	B	318	CLA	C1D-C2D-C3D	-2.57	104.45	106.97
6	B	315	CLA	C1D-C2D-C3D	-2.57	104.46	106.97
6	A	314	CLA	O2D-CGD-O1D	-2.56	118.64	123.79
6	A	307	CLA	C3A-C4A-NA	2.56	113.91	110.81
2	A	301	LUT	C18-C5-C6	-2.56	121.61	124.50
6	B	315	CLA	C1C-NC-C4C	2.55	109.71	106.26
6	A	308	CLA	C9-C8-C7	-2.55	101.07	111.05
6	B	318	CLA	CHD-C4C-C3C	-2.55	121.06	124.97
6	A	316	CLA	C4A-NA-C1A	2.54	109.97	106.38
5	C	311	CHL	C1-O2A-CGA	2.54	124.39	117.00
6	C	317	CLA	O2D-CGD-O1D	-2.54	118.69	123.79
6	C	318	CLA	CHC-C1C-NC	2.54	128.46	123.42
2	B	302	LUT	C38-C25-C24	-2.53	117.74	123.43
6	A	316	CLA	C4B-C3B-C2B	-2.53	104.44	107.04
6	A	314	CLA	CGD-CBD-CAD	2.53	119.28	110.79
2	C	302	LUT	C38-C25-C24	-2.53	117.74	123.43
2	B	301	LUT	C38-C25-C26	2.53	117.96	116.05
6	C	307	CLA	C1C-C2C-C3C	-2.52	103.79	106.96
6	C	315	CLA	O2A-CGA-CBA	2.52	119.61	111.90
6	B	317	CLA	C2D-C3D-CAD	2.52	145.21	134.94
5	C	305	CHL	CMD-C2D-C3D	2.52	129.18	124.28
6	C	307	CLA	C1D-C2D-C3D	-2.51	104.51	106.97
6	B	316	CLA	C4A-NA-C1A	2.51	109.92	106.38
6	B	308	CLA	CBD-CHA-C1A	2.51	132.05	128.77
5	C	312	CHL	CMD-C2D-C3D	2.51	129.17	124.28
6	B	314	CLA	CMD-C2D-C3D	2.51	129.89	125.16
6	A	317	CLA	C3D-C4D-CHA	2.51	112.19	108.16
6	B	307	CLA	CHC-C1C-C2C	-2.50	119.78	126.51
2	B	302	LUT	C15-C35-C34	-2.50	117.93	123.45
5	C	312	CHL	C11-C10-C8	-2.50	107.66	115.44
6	B	317	CLA	C4B-C3B-C2B	-2.50	104.47	107.04
5	C	312	CHL	C3D-C4D-CHA	2.50	113.14	108.32
6	B	318	CLA	C2D-C3D-CAD	2.50	145.13	134.94
5	B	305	CHL	CED-O2D-CGD	2.50	121.94	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	LUT	C23-C24-C25	-2.49	122.85	125.23
6	A	317	CLA	C2D-C3D-CAD	2.49	145.10	134.94
3	A	303	NEX	C19-C9-C10	-2.49	119.37	122.92
6	C	308	CLA	C2B-C1B-NB	2.49	111.16	109.50
5	C	313	CHL	O2A-CGA-O1A	-2.49	116.98	123.48
6	A	317	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
5	C	312	CHL	C6-C5-C3	-2.48	106.98	112.62
6	A	307	CLA	C1-C2-C3	-2.47	121.94	126.23
6	B	314	CLA	C3B-C4B-CHC	-2.47	121.32	126.00
6	A	315	CLA	OBD-CAD-C3D	2.47	133.14	128.15
6	C	307	CLA	C3A-C4A-NA	2.47	113.79	110.81
5	A	312	CHL	C3D-C2D-C1D	-2.47	101.60	107.73
6	B	316	CLA	O2D-CGD-O1D	-2.46	118.85	123.79
6	A	307	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
6	A	315	CLA	C4D-ND-C1D	2.46	109.54	106.57
6	A	315	CLA	C9-C8-C10	2.46	120.65	111.05
5	B	309	CHL	C3C-C4C-NC	2.46	110.41	109.67
6	C	316	CLA	C4A-NA-C1A	2.45	109.84	106.38
6	C	314	CLA	CHC-C1C-NC	2.45	128.29	123.42
6	A	315	CLA	C3B-C4B-CHC	-2.45	121.36	126.00
6	C	306	CLA	CBD-CHA-C1A	2.45	131.97	128.77
5	C	312	CHL	O2A-CGA-O1A	-2.44	117.10	123.48
3	B	303	NEX	C24-C23-C22	-2.44	105.60	110.42
6	B	314	CLA	O2A-CGA-CBA	2.44	119.36	111.90
6	B	314	CLA	C1D-C2D-C3D	-2.44	104.58	106.97
3	C	303	NEX	C19-C9-C10	-2.44	119.45	122.92
6	B	307	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
6	A	316	CLA	C1-C2-C3	-2.44	122.00	126.23
5	C	313	CHL	CAC-C3C-C4C	-2.43	123.73	127.01
6	C	314	CLA	O2A-CGA-O1A	-2.43	117.12	123.48
6	B	306	CLA	C4B-NB-C1B	2.43	109.46	107.12
6	A	314	CLA	CMA-C3A-C4A	-2.43	104.64	112.40
5	C	305	CHL	CBC-CAC-C3C	-2.43	109.08	113.04
2	B	302	LUT	C7-C8-C9	2.42	129.84	126.22
6	C	318	CLA	CHC-C4B-NB	2.43	128.82	124.70
6	B	306	CLA	CAA-C2A-C3A	2.42	119.38	113.32
6	B	316	CLA	C4B-C3B-C2B	-2.42	104.55	107.04
3	A	303	NEX	O24-C25-C38	2.42	117.85	114.99
6	C	317	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
5	C	312	CHL	CAA-CBA-CGA	-2.42	106.12	113.24
6	B	307	CLA	CHC-C4B-NB	2.42	128.81	124.70
6	B	308	CLA	C1D-C2D-C3D	-2.42	104.61	106.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	306	CLA	C2C-C1C-NC	-2.41	108.28	110.22
6	C	318	CLA	C1D-C2D-C3D	-2.41	104.61	106.97
2	A	302	LUT	C31-C30-C29	2.41	130.77	127.29
6	C	307	CLA	C9-C8-C10	2.41	120.45	111.05
6	A	308	CLA	C1D-C2D-C3D	-2.40	104.62	106.97
6	A	317	CLA	CHC-C4B-NB	2.40	128.78	124.70
6	B	316	CLA	OBD-CAD-CBD	-2.40	122.32	125.94
6	B	315	CLA	O2A-CGA-CBA	2.40	119.23	111.90
6	C	306	CLA	C6-C7-C8	-2.40	107.99	115.44
6	B	316	CLA	C1-C2-C3	-2.39	122.08	126.23
6	A	307	CLA	CMC-C2C-C1C	2.39	128.36	124.95
6	A	315	CLA	C2D-C1D-ND	-2.39	106.83	109.56
6	A	317	CLA	C3A-C4A-NA	2.39	113.70	110.81
6	C	314	CLA	CMC-C2C-C1C	2.39	128.36	124.95
2	C	301	LUT	C7-C8-C9	2.38	129.78	126.22
6	A	316	CLA	CHC-C1C-NC	2.38	128.15	123.42
6	B	307	CLA	CMB-C2B-C1B	-2.38	124.80	128.46
6	A	316	CLA	C3B-C4B-CHC	-2.38	121.49	126.00
6	A	307	CLA	C3D-C4D-CHA	2.38	111.98	108.16
6	C	317	CLA	C2D-C3D-CAD	2.38	144.62	134.94
5	C	312	CHL	C3D-C2D-C1D	-2.37	101.83	107.73
6	A	315	CLA	O2A-CGA-CBA	2.38	119.17	111.90
6	C	308	CLA	C4-C3-C5	2.37	118.99	115.39
2	C	301	LUT	C20-C13-C12	2.37	121.92	118.09
6	A	317	CLA	C3B-CAB-CBB	-2.37	121.04	125.95
6	B	314	CLA	C3D-C4D-CHA	2.37	111.96	108.16
6	C	308	CLA	C1-C2-C3	-2.37	122.12	126.23
6	A	308	CLA	C2D-C3D-CAD	2.37	144.59	134.94
6	A	317	CLA	C6-C7-C8	-2.36	108.09	115.44
6	A	306	CLA	CHC-C4B-NB	2.36	128.72	124.70
6	B	314	CLA	C2A-C1A-NA	2.36	114.35	111.33
5	B	312	CHL	C6-C5-C3	-2.36	107.24	112.62
6	B	306	CLA	CHC-C4B-NB	2.36	128.70	124.70
6	A	314	CLA	C4-C3-C5	2.36	118.97	115.39
6	B	316	CLA	C2D-C3D-CAD	2.35	144.54	134.94
6	C	316	CLA	CAA-CBA-CGA	-2.35	106.32	113.24
6	C	307	CLA	CHC-C1C-C2C	-2.35	120.20	126.51
2	B	301	LUT	C2-C1-C6	2.35	114.77	109.60
6	C	314	CLA	C2D-C3D-CAD	2.34	144.49	134.94
5	C	305	CHL	C4-C3-C5	2.34	118.95	115.39
6	A	314	CLA	CHC-C1C-NC	2.34	128.07	123.42
6	A	307	CLA	C2D-C3D-CAD	2.34	144.49	134.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	306	CLA	CMD-C2D-C3D	2.34	129.57	125.16
2	C	302	LUT	C36-C21-C26	2.34	112.77	109.68
6	C	308	CLA	C2D-C3D-CAD	2.34	144.48	134.94
6	B	316	CLA	CHC-C4B-NB	2.33	128.67	124.70
6	A	317	CLA	C4-C3-C2	-2.33	118.87	123.52
6	A	306	CLA	C2A-C1A-NA	2.33	114.32	111.33
6	A	314	CLA	CMD-C2D-C3D	2.33	129.55	125.16
6	C	307	CLA	C4D-CHA-CBD	-2.33	103.98	109.45
6	A	316	CLA	C1C-NC-C4C	2.33	109.40	106.26
6	C	306	CLA	CHC-C4B-NB	2.32	128.65	124.70
6	B	315	CLA	CAA-CBA-CGA	-2.32	106.40	113.24
6	B	316	CLA	C3B-C4B-CHC	-2.32	121.61	126.00
5	C	312	CHL	CAA-C2A-C3A	-2.32	107.52	113.32
6	A	318	CLA	C2D-C3D-CAD	2.31	144.37	134.94
6	C	318	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
6	C	308	CLA	OBD-CAD-CBD	-2.31	122.45	125.94
6	B	317	CLA	O2A-CGA-O1A	-2.31	117.45	123.48
6	B	316	CLA	O2A-CGA-O1A	-2.30	117.46	123.48
6	C	307	CLA	C3B-CAB-CBB	-2.30	121.19	125.95
5	A	310	CHL	CGD-CBD-CAD	-2.30	103.06	110.79
6	C	317	CLA	CHC-C1C-C2C	-2.30	120.34	126.51
6	B	306	CLA	C1C-NC-C4C	2.30	109.36	106.26
6	A	306	CLA	O2A-CGA-O1A	-2.29	117.48	123.48
5	C	313	CHL	C4-C3-C5	2.29	118.87	115.39
6	A	315	CLA	CHC-C1C-C2C	-2.29	120.36	126.51
6	C	316	CLA	CHC-C4B-NB	2.29	128.59	124.70
5	A	311	CHL	C1-O2A-CGA	2.28	123.64	117.00
3	A	303	NEX	C11-C10-C9	-2.28	123.99	127.29
6	C	315	CLA	C2D-C3D-CAD	2.28	144.24	134.94
5	C	305	CHL	CED-O2D-CGD	2.28	121.43	116.00
5	B	309	CHL	CMD-C2D-C3D	2.28	128.72	124.28
6	B	317	CLA	C4-C3-C2	-2.28	118.98	123.52
6	A	306	CLA	C3D-C4D-CHA	2.28	111.81	108.16
6	A	318	CLA	CGD-CBD-CHA	-2.28	108.37	113.65
6	B	307	CLA	CBC-CAC-C3C	-2.28	105.48	112.37
6	A	315	CLA	C3D-C4D-CHA	2.28	111.81	108.16
6	C	314	CLA	CMA-C3A-C4A	-2.27	105.13	112.40
6	A	314	CLA	C2D-C3D-CAD	2.27	144.21	134.94
5	A	309	CHL	CMD-C2D-C3D	2.27	128.71	124.28
6	B	307	CLA	C3A-C4A-CHB	-2.27	119.60	124.33
5	A	311	CHL	O2A-CGA-CBA	2.27	118.85	111.90
2	C	302	LUT	C8-C7-C6	-2.27	120.54	127.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	311	CHL	CMD-C2D-C3D	2.27	128.69	124.28
6	C	314	CLA	CMD-C2D-C3D	2.26	129.43	125.16
2	B	301	LUT	C18-C5-C4	2.27	118.50	114.25
6	C	317	CLA	C1D-CHD-C4C	-2.26	119.09	122.60
6	B	307	CLA	C4D-CHA-CBD	-2.26	104.14	109.45
2	B	301	LUT	C20-C13-C12	2.26	121.75	118.09
6	B	315	CLA	C4A-NA-C1A	2.26	109.57	106.38
6	C	308	CLA	CMA-C3A-C4A	-2.26	105.17	112.40
5	A	313	CHL	CMD-C2D-C3D	2.25	128.67	124.28
5	B	310	CHL	CAA-C2A-C3A	-2.25	107.68	113.32
6	B	314	CLA	CBC-CAC-C3C	-2.25	105.56	112.37
2	C	301	LUT	C38-C25-C24	-2.25	118.37	123.43
7	A	319	CAC	O1-AS-C2	2.25	116.85	109.18
6	A	306	CLA	O2A-CGA-CBA	2.25	118.79	111.90
6	A	314	CLA	C4D-CHA-CBD	-2.25	104.17	109.45
6	C	307	CLA	CHC-C1C-NC	2.25	127.88	123.42
6	C	316	CLA	C1C-NC-C4C	2.25	109.29	106.26
5	B	311	CHL	C4D-C3D-C2D	-2.25	107.27	108.16
6	C	306	CLA	C1C-NC-C4C	2.24	109.29	106.26
2	C	301	LUT	O3-C3-C2	-2.24	105.48	109.92
6	C	307	CLA	C4-C3-C5	2.24	118.79	115.39
6	B	308	CLA	C4-C3-C2	-2.24	119.06	123.52
6	A	317	CLA	C6-C5-C3	-2.24	107.51	112.62
6	A	307	CLA	CHC-C1C-C2C	-2.24	120.49	126.51
6	A	306	CLA	C4B-NB-C1B	2.24	109.28	107.12
2	A	302	LUT	C27-C28-C29	-2.24	119.01	125.53
6	C	308	CLA	O2A-CGA-CBA	2.24	118.75	111.90
6	B	308	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
5	C	313	CHL	CMD-C2D-C3D	2.23	128.62	124.28
6	C	315	CLA	CHC-C1C-NC	2.23	127.85	123.42
6	B	315	CLA	C2D-C3D-CAD	2.23	144.03	134.94
2	B	301	LUT	C8-C7-C6	-2.23	120.66	127.23
2	C	301	LUT	C20-C13-C14	-2.23	119.75	122.92
6	C	307	CLA	C2D-C3D-CAD	2.23	144.02	134.94
6	B	315	CLA	C3D-C4D-CHA	2.22	111.73	108.16
6	C	317	CLA	O2A-CGA-O1A	-2.22	117.67	123.48
5	A	305	CHL	CMB-C2B-C3B	2.22	129.51	124.26
6	A	315	CLA	C4-C3-C5	2.22	118.76	115.39
5	B	305	CHL	O2A-CGA-O1A	-2.22	117.68	123.48
6	C	315	CLA	C3D-C4D-CHA	2.22	111.72	108.16
6	B	318	CLA	C4A-NA-C1A	2.22	109.51	106.38
4	A	304	LHG	C6-O8-C23	2.22	123.33	116.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	308	CLA	O1D-CGD-CBD	-2.22	119.92	124.45
4	A	304	LHG	O6-P-O3	-2.22	98.36	104.68
6	B	314	CLA	CHC-C4B-NB	2.21	128.46	124.70
6	A	318	CLA	C3D-C4D-CHA	2.21	111.71	108.16
2	A	302	LUT	C21-C22-C23	-2.21	106.69	112.66
6	C	315	CLA	C3B-C4B-CHC	-2.21	121.81	126.00
3	C	303	NEX	C15-C35-C34	-2.21	118.59	123.45
6	B	308	CLA	CHC-C1C-NC	2.20	127.80	123.42
2	C	302	LUT	C19-C9-C8	2.20	121.65	118.09
6	C	318	CLA	C3B-CAB-CBB	-2.20	121.39	125.95
6	A	307	CLA	CMA-C3A-C4A	-2.20	105.36	112.40
6	A	306	CLA	C6-C7-C8	-2.20	108.59	115.44
3	A	303	NEX	C20-C13-C12	2.20	121.64	118.09
6	C	306	CLA	C5-C3-C2	-2.20	116.83	121.06
6	A	316	CLA	O2A-CGA-O1A	-2.20	117.73	123.48
6	B	306	CLA	C3D-C4D-CHA	2.20	111.68	108.16
6	B	306	CLA	CGD-CBD-CHA	-2.20	108.56	113.65
3	B	303	NEX	C31-C32-C33	-2.19	120.09	126.37
2	B	301	LUT	C19-C9-C10	-2.19	119.80	122.92
6	A	315	CLA	CHD-C4C-C3C	-2.19	121.61	124.97
2	A	301	LUT	C8-C7-C6	-2.19	120.78	127.23
2	B	302	LUT	C19-C9-C10	-2.19	119.80	122.92
6	B	306	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
6	A	317	CLA	CHC-C1C-C2C	-2.18	120.66	126.51
6	B	306	CLA	C3A-C4A-NA	2.18	113.44	110.81
6	A	306	CLA	C1D-C2D-C3D	-2.18	104.84	106.97
6	C	318	CLA	C2D-C3D-CAD	2.18	143.82	134.94
6	A	316	CLA	C4D-CHA-CBD	-2.18	104.33	109.45
2	B	302	LUT	C18-C5-C6	-2.18	122.04	124.50
6	A	308	CLA	CBC-CAC-C3C	-2.18	105.78	112.37
6	C	306	CLA	C7-C6-C5	-2.18	106.61	112.97
6	C	316	CLA	C4B-NB-C1B	2.17	109.21	107.12
6	B	317	CLA	O2D-CGD-O1D	-2.17	119.43	123.79
6	A	316	CLA	C4D-C3D-C2D	2.17	109.80	107.17
6	C	314	CLA	C4D-CHA-CBD	-2.17	104.36	109.45
6	C	316	CLA	CHC-C1C-NC	2.17	127.72	123.42
5	C	313	CHL	CBD-CAD-C3D	-2.17	105.76	113.44
6	B	318	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
5	A	311	CHL	CBD-CAD-C3D	-2.16	105.78	113.44
6	B	307	CLA	C2D-C3D-CAD	2.16	143.76	134.94
6	A	318	CLA	C2A-C3A-C4A	-2.16	100.99	104.51
2	A	301	LUT	C21-C26-C27	-2.16	109.83	112.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	312	CHL	C11-C10-C8	-2.16	108.73	115.44
6	A	316	CLA	CMD-C2D-C3D	2.16	129.22	125.16
2	C	301	LUT	C8-C7-C6	-2.16	120.87	127.23
6	A	316	CLA	O1D-CGD-CBD	-2.16	120.05	124.45
6	B	306	CLA	CMD-C2D-C3D	2.15	129.21	125.16
6	B	306	CLA	C11-C10-C8	-2.15	108.75	115.44
5	A	313	CHL	CBD-CAD-C3D	-2.15	105.81	113.44
6	C	318	CLA	CHC-C1C-C2C	-2.15	120.73	126.51
6	A	308	CLA	C2A-C1A-NA	2.15	114.08	111.33
6	A	306	CLA	CHC-C1C-NC	2.15	127.68	123.42
6	A	317	CLA	O2A-CGA-O1A	-2.14	117.88	123.48
6	C	317	CLA	C4A-NA-C1A	2.14	109.40	106.38
3	B	303	NEX	C28-C29-C30	2.14	122.27	118.98
2	B	302	LUT	C11-C12-C13	2.14	132.49	126.37
6	A	318	CLA	C4A-NA-C1A	2.14	109.39	106.38
2	B	301	LUT	C11-C12-C13	2.14	132.49	126.37
3	A	303	NEX	O24-C25-C26	-2.14	57.06	58.90
6	C	314	CLA	C4A-NA-C1A	2.13	109.39	106.38
6	B	316	CLA	C1D-C2D-C3D	-2.13	104.88	106.97
6	C	316	CLA	C4D-ND-C1D	2.13	109.14	106.57
6	A	307	CLA	C3A-C4A-CHB	-2.13	119.90	124.33
6	A	314	CLA	C1-C2-C3	-2.13	122.53	126.23
5	C	313	CHL	C1-O2A-CGA	2.13	123.19	117.00
6	B	306	CLA	CBD-CHA-C1A	2.13	131.55	128.77
6	C	314	CLA	CMB-C2B-C1B	-2.13	125.19	128.46
6	C	316	CLA	C1-C2-C3	-2.13	122.54	126.23
6	C	306	CLA	CHC-C1C-NC	2.13	127.64	123.42
6	C	315	CLA	OBD-CAD-C3D	2.13	132.45	128.15
6	C	318	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
6	A	307	CLA	OBD-CAD-CBD	-2.12	122.73	125.94
2	B	301	LUT	C8-C9-C10	2.12	122.24	118.98
6	C	306	CLA	O1D-CGD-CBD	-2.12	120.12	124.45
6	C	317	CLA	C3D-C4D-CHA	2.12	111.56	108.16
6	A	307	CLA	CHC-C1C-NC	2.12	127.63	123.42
6	C	308	CLA	CBC-CAC-C3C	-2.12	105.95	112.37
3	B	303	NEX	C19-C9-C8	2.12	124.22	118.46
6	B	316	CLA	C2A-C1A-NA	2.11	114.04	111.33
6	A	308	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
6	A	315	CLA	CHC-C4B-NB	2.11	128.29	124.70
5	B	309	CHL	CMC-C2C-C3C	2.11	129.16	125.94
5	A	305	CHL	C3D-C4D-CHA	2.11	112.39	108.32
5	B	313	CHL	O2A-CGA-O1A	-2.10	117.99	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	317	CLA	OBD-CAD-CBD	-2.10	122.77	125.94
6	C	306	CLA	C3D-C4D-CHA	2.10	111.53	108.16
6	C	307	CLA	C4B-C3B-C2B	-2.10	104.88	107.04
6	B	316	CLA	C4D-CHA-CBD	-2.10	104.53	109.45
6	C	317	CLA	C4-C3-C2	-2.10	119.35	123.52
2	B	302	LUT	C40-C33-C34	-2.09	119.94	122.92
6	C	306	CLA	CMD-C2D-C3D	2.09	129.10	125.16
2	C	301	LUT	O23-C23-C22	-2.09	106.30	110.95
6	C	307	CLA	C2C-C1C-NC	2.09	111.91	110.22
6	A	308	CLA	C4B-C3B-C2B	-2.09	104.90	107.04
6	C	316	CLA	C2D-C3D-CAD	2.08	143.44	134.94
2	B	302	LUT	C31-C30-C29	2.08	130.30	127.29
3	A	303	NEX	C20-C13-C14	-2.08	119.96	122.92
2	A	301	LUT	C19-C9-C10	-2.08	119.96	122.92
5	C	310	CHL	O2A-CGA-O1A	-2.08	118.05	123.48
6	C	307	CLA	O2A-C1-C2	2.08	112.87	108.12
6	A	316	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
6	C	317	CLA	C1C-NC-C4C	2.07	109.06	106.26
3	C	303	NEX	C37-C21-C36	2.07	110.72	107.47
5	C	305	CHL	O2D-CGD-O1D	-2.07	119.64	123.79
6	B	307	CLA	C4-C3-C5	2.07	118.53	115.39
5	A	310	CHL	CED-O2D-CGD	2.06	120.91	116.00
6	B	308	CLA	C3B-CAB-CBB	-2.06	121.68	125.95
6	A	317	CLA	CMD-C2D-C3D	2.06	129.04	125.16
5	A	310	CHL	O2D-CGD-O1D	-2.06	119.66	123.79
6	A	316	CLA	CHC-C4B-NB	2.06	128.19	124.70
6	C	316	CLA	C2A-C1A-NA	2.05	113.96	111.33
6	A	307	CLA	C4A-NA-C1A	2.05	109.27	106.38
6	A	315	CLA	C4A-NA-C1A	2.05	109.27	106.38
6	C	307	CLA	C9-C8-C7	2.05	119.06	111.05
6	C	315	CLA	C4A-NA-C1A	2.05	109.27	106.38
6	B	314	CLA	C4-C3-C2	-2.05	119.44	123.52
6	A	307	CLA	C2C-C1C-NC	2.05	111.88	110.22
3	C	303	NEX	C28-C29-C30	2.04	122.12	118.98
6	C	306	CLA	C2D-C1D-ND	-2.04	107.23	109.56
6	A	307	CLA	CBA-CAA-C2A	-2.04	108.96	113.95
6	B	315	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
6	C	307	CLA	C6-C7-C8	-2.04	109.11	115.44
5	A	309	CHL	CBC-CAC-C3C	2.03	116.36	113.04
6	B	318	CLA	CHC-C1C-NC	2.03	127.45	123.42
6	B	306	CLA	CMC-C2C-C1C	2.03	127.84	124.95
5	A	312	CHL	C3D-C4D-CHA	2.03	112.24	108.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	303	NEX	C40-C33-C34	-2.03	120.03	122.92
2	C	302	LUT	C31-C30-C29	2.03	130.22	127.29
5	B	310	CHL	CBC-CAC-C3C	-2.03	109.73	113.04
6	A	315	CLA	CGD-CBD-CAD	-2.03	103.97	110.79
6	A	318	CLA	CHC-C1C-NC	2.03	127.44	123.42
2	A	302	LUT	C18-C5-C4	2.03	118.05	114.25
6	C	307	CLA	C3A-C4A-CHB	-2.02	120.12	124.33
6	A	317	CLA	C4D-CHA-CBD	-2.02	104.70	109.45
6	C	317	CLA	CBC-CAC-C3C	-2.02	106.25	112.37
6	A	318	CLA	OBD-CAD-CBD	-2.02	122.89	125.94
2	C	302	LUT	C27-C28-C29	-2.02	119.65	125.53
6	C	314	CLA	C3B-CAB-CBB	-2.02	121.78	125.95
2	B	301	LUT	C16-C1-C6	-2.02	106.99	110.33
6	B	317	CLA	CHC-C1C-C2C	-2.01	121.10	126.51
6	A	314	CLA	C4-C3-C2	-2.01	119.51	123.52
6	B	317	CLA	C3D-C4D-CHA	2.01	111.39	108.16
6	C	308	CLA	O2A-CGA-O1A	-2.01	118.22	123.48
6	C	316	CLA	CAC-C3C-C2C	2.01	131.12	127.50
6	B	306	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
2	B	301	LUT	C30-C31-C32	-2.00	116.51	123.23
5	B	313	CHL	CBC-CAC-C3C	-2.00	109.77	113.04
6	B	307	CLA	C1C-C2C-C3C	-2.00	104.44	106.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	208/224 (92%)	0.02	14 (6%) 17 15	6, 39, 77, 97	0
1	B	208/224 (92%)	-0.15	10 (4%) 29 26	8, 34, 67, 94	0
1	C	208/224 (92%)	-0.18	8 (3%) 38 35	6, 33, 69, 107	0
All	All	624/672 (92%)	-0.10	32 (5%) 11 23	6, 35, 70, 107	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	217	VAL	5.0
1	A	89	GLY	4.9
1	A	213	LEU	4.7
1	A	88	ASN	4.0
1	A	214	ALA	4.0
1	B	88	ASN	3.8
1	B	89	GLY	3.6
1	A	87	ARG	3.6
1	A	216	PRO	3.5
1	C	147	PRO	3.2
1	C	214	ALA	3.2
1	C	213	LEU	3.1
1	A	81	PHE	3.1
1	B	152	VAL	2.9
1	B	214	ALA	2.9
1	A	217	VAL	2.9
1	A	31	GLU	2.8
1	C	20	ASP	2.7
1	A	210	ALA	2.6
1	B	87	ARG	2.6
1	B	168	ASP	2.5
1	C	218	ASN	2.5
1	C	219	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	212	HIS	2.5
1	A	168	ASP	2.5
1	A	219	ASN	2.5
1	B	117	SER	2.3
1	B	217	VAL	2.1
1	B	213	LEU	2.1
1	A	218	ASN	2.1
1	C	170	PRO	2.1
1	B	150	GLU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q < 0.9
4	LHG	B	304	49/49	0.19	5.40	14,40,98,107	0
3	NEX	B	303	44/44	0.27	3.91	26,42,94,97	0
3	NEX	A	303	44/44	0.25	3.77	26,39,94,96	0
6	CLA	B	307	65/65	0.19	3.74	9,20,82,94	0
9	NA	C	323	1/1	0.29	3.67	68,68,68,68	0
9	NA	C	320	1/1	0.23	3.18	60,60,60,60	0
6	CLA	B	316	65/65	0.27	2.91	28,41,89,99	0
6	CLA	C	307	65/65	0.20	2.74	6,18,80,92	0
4	LHG	A	304	49/49	0.17	2.55	19,42,98,108	0
6	CLA	A	307	65/65	0.20	2.30	10,20,81,93	0
6	CLA	A	306	65/65	0.17	2.20	13,21,43,63	0
5	CHL	A	309	48/66	0.27	2.16	32,48,95,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	CHL	A	311	66/66	0.19	1.92	19,37,99,119	0
4	LHG	C	304	49/49	0.18	1.77	16,42,96,107	0
5	CHL	C	313	66/66	0.17	1.77	5,21,66,80	0
6	CLA	C	306	65/65	0.16	1.76	7,19,41,60	0
5	CHL	B	313	66/66	0.16	1.70	14,28,69,85	0
5	CHL	B	311	66/66	0.18	1.69	21,38,99,119	0
6	CLA	B	315	65/65	0.23	1.57	20,43,74,83	0
6	CLA	B	306	65/65	0.16	1.53	9,19,39,58	0
5	CHL	C	311	66/66	0.18	1.42	11,31,94,115	0
5	CHL	C	309	48/66	0.21	1.41	26,43,97,104	0
5	CHL	A	313	66/66	0.15	1.33	14,25,68,82	0
2	LUT	B	302	42/42	0.15	1.21	6,19,32,35	0
6	CLA	C	314	65/65	0.19	1.15	15,27,79,93	0
5	CHL	A	305	66/66	0.18	1.09	17,32,86,104	0
5	CHL	A	310	51/66	0.17	1.03	21,36,94,100	0
6	CLA	B	314	65/65	0.20	0.98	24,31,80,96	0
6	CLA	C	316	65/65	0.23	0.97	22,37,84,97	0
6	CLA	C	315	65/65	0.20	0.96	21,45,74,87	0
6	CLA	B	318	41/65	0.29	0.78	44,76,92,115	0
7	CAC	C	319	5/5	0.16	0.75	57,62,79,156	0
3	NEX	C	303	44/44	0.21	0.71	14,32,90,92	0
5	CHL	B	309	48/66	0.22	0.69	35,52,99,105	0
6	CLA	A	314	65/65	0.19	0.61	23,34,78,93	0
5	CHL	B	305	66/66	0.16	0.56	8,26,81,100	0
2	LUT	A	302	42/42	0.15	0.55	7,21,31,37	0
2	LUT	C	301	42/42	0.17	0.45	15,22,35,57	0
2	LUT	C	302	42/42	0.14	0.44	6,16,30,35	0
5	CHL	C	305	66/66	0.15	0.37	14,34,87,104	0
6	CLA	A	318	41/65	0.34	0.34	44,79,96,119	0
6	CLA	A	315	65/65	0.20	0.20	28,48,76,86	0
6	CLA	A	316	65/65	0.22	0.18	30,41,88,98	0
5	CHL	B	312	66/66	0.16	0.13	22,40,71,83	0
6	CLA	B	308	62/65	0.17	0.08	21,37,83,91	0
6	CLA	C	317	65/65	0.15	0.08	16,31,87,95	0
5	CHL	C	312	66/66	0.17	0.05	9,32,66,79	0
6	CLA	C	308	62/65	0.15	0.02	12,28,80,87	0
6	CLA	C	318	40/65	0.24	0.01	36,69,91,110	0
5	CHL	A	312	66/66	0.14	-0.06	19,36,68,81	0
5	CHL	B	310	51/66	0.13	-0.07	20,32,92,97	0
6	CLA	B	317	65/65	0.16	-0.07	14,30,85,94	0
6	CLA	A	317	65/65	0.18	-0.10	21,37,90,99	0
6	CLA	A	308	62/65	0.17	-0.20	20,35,82,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	LUT	B	301	42/42	0.14	-0.23	18,26,42,62	0
5	CHL	C	310	51/66	0.12	-0.23	13,27,89,94	0
2	LUT	A	301	42/42	0.16	-0.33	20,25,39,61	0
8	ZN	C	321	1/1	0.13	-0.48	64,64,64,64	0
7	CAC	A	319	5/5	0.15	-0.49	57,59,68,81	0
9	NA	B	322	1/1	0.14	-0.63	47,47,47,47	0
7	CAC	B	319	5/5	0.13	-0.84	59,62,68,97	0
8	ZN	A	320	1/1	0.12	-0.86	98,98,98,98	0
8	ZN	B	321	1/1	0.10	-1.19	66,66,66,66	0
8	ZN	A	321	1/1	0.08	-1.45	56,56,56,56	0
8	ZN	A	322	1/1	0.23	-3.34	122,122,122,122	0
9	NA	B	320	1/1	0.07	-3.81	42,42,42,42	0
9	NA	C	322	1/1	0.39	-	80,80,80,80	1

6.5 Other polymers ⓘ

There are no such residues in this entry.