



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:21 PM GMT

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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

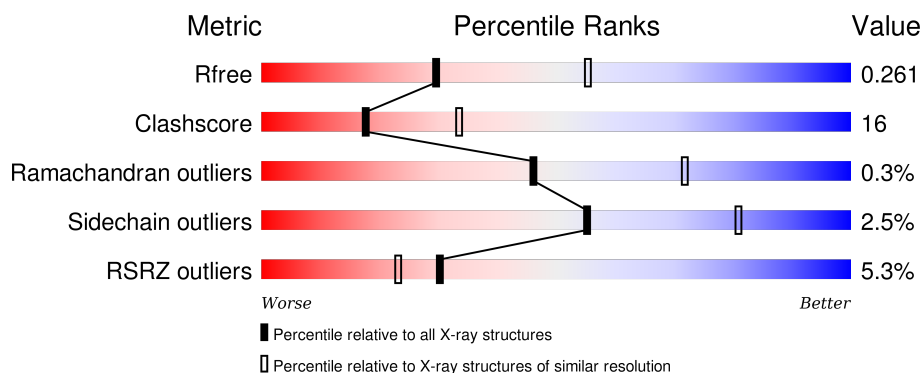
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	224	<div> <div>7%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div> </div>
1	B	224	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
1	C	224	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>14%</div> <div>7%</div> </div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NEX	A	303	-	-	-	X
3	NEX	B	303	-	-	-	X
4	LHG	A	304	-	-	-	X
4	LHG	B	304	-	-	-	X
4	LHG	C	304	-	-	-	X
5	CHL	C	311	-	-	-	X
5	CHL	C	313	-	-	-	X
6	CLA	A	306	X	-	-	X
6	CLA	A	307	X	-	-	X
6	CLA	A	308	X	-	-	-
6	CLA	A	314	X	-	-	-
6	CLA	A	315	X	-	-	-
6	CLA	A	316	X	-	-	-
6	CLA	A	317	X	-	-	-
6	CLA	A	318	X	-	-	-
6	CLA	B	306	X	-	-	-
6	CLA	B	307	X	-	-	X
6	CLA	B	308	X	-	-	-
6	CLA	B	314	X	-	-	-
6	CLA	B	315	X	-	-	-
6	CLA	B	316	X	-	-	X
6	CLA	B	317	X	-	-	-
6	CLA	B	318	X	-	-	-
6	CLA	C	306	X	-	-	X
6	CLA	C	307	X	-	X	X
6	CLA	C	308	X	-	-	-
6	CLA	C	314	X	-	-	-
6	CLA	C	315	X	-	-	-
6	CLA	C	316	X	-	-	-
6	CLA	C	317	X	-	-	-
6	CLA	C	318	X	-	-	-

## 2 Entry composition [i](#)

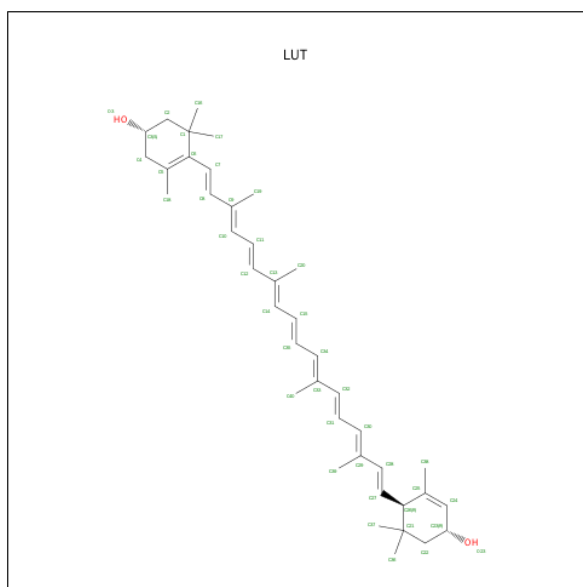
There are 10 unique types of molecules in this entry. The entry contains 8016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



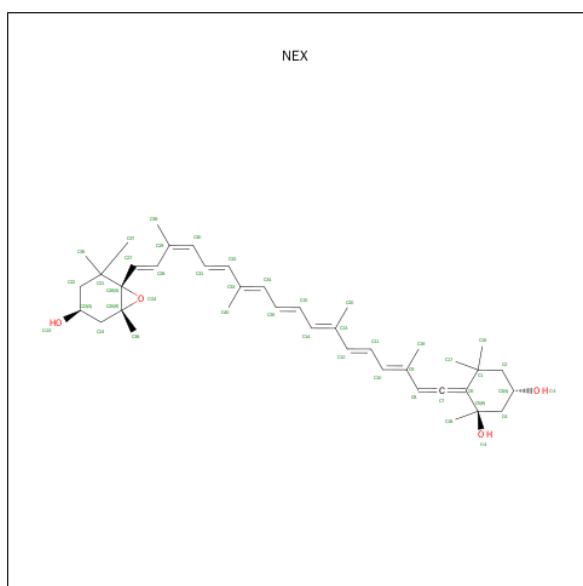
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			42	40	2		
2	A	1	Total	C	O	0	0
			42	40	2		
2	B	1	Total	C	O	0	0
			42	40	2		

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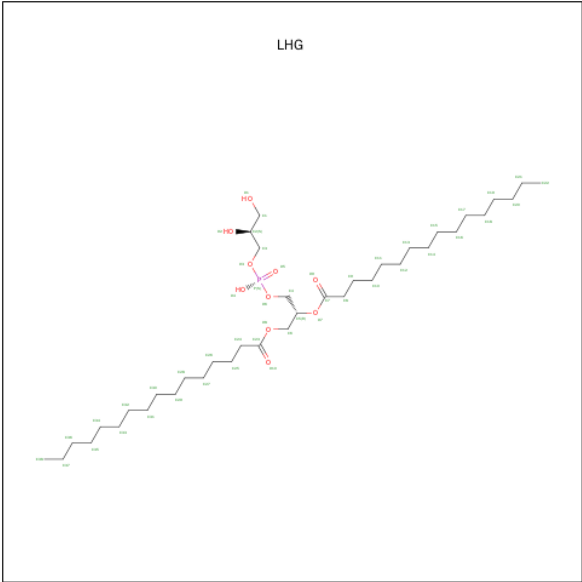
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		

- 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



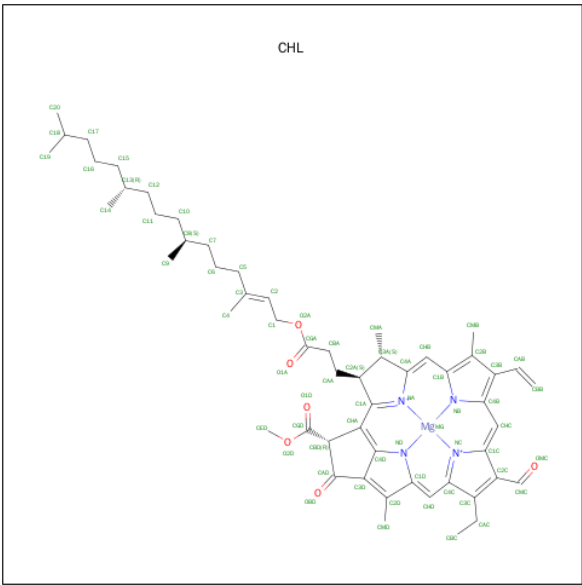
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			44	40	4		
3	B	1	Total	C	O	0	0
			44	40	4		
3	C	1	Total	C	O	0	0
			44	40	4		

- Molecule 4 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



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<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



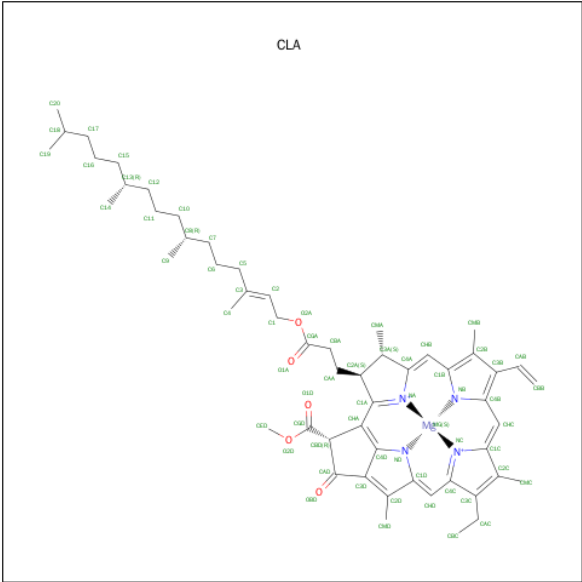
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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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: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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		

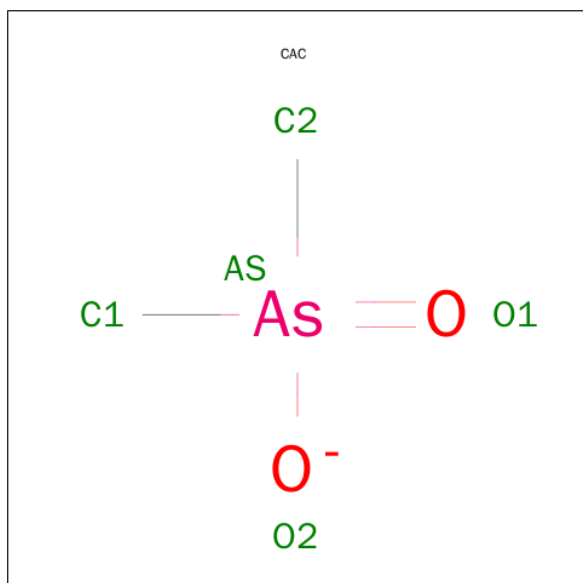
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			62	52	1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

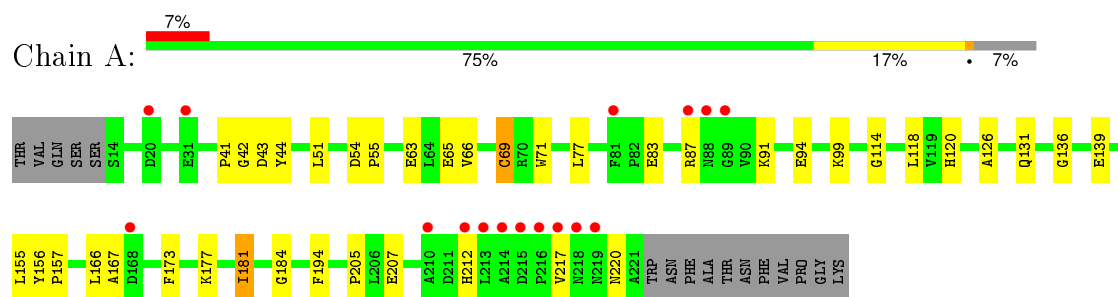
- Molecule 10 is water.

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		

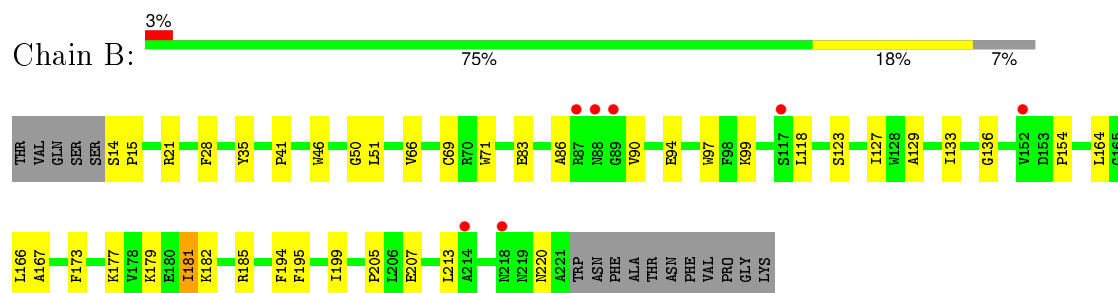
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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.

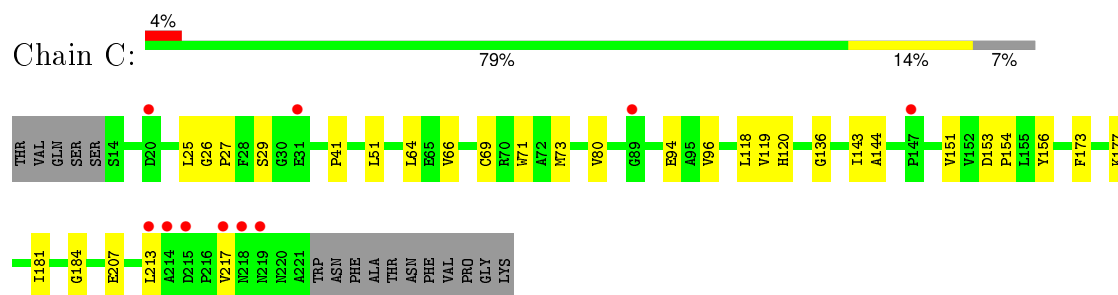
- Molecule 1: Major chlorophyll a/b binding protein LHCb1.3



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



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.3_928)	Depositor
R, $R_{free}$	0.250 , 0.258 0.242 , 0.261	Depositor DCC
$R_{free}$ test set	3045 reflections (5.48%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.6	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 75.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
2	C	84	0	112	7	0
3	A	44	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (250) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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:C:306:CLA:H92	6:C:307:CLA:CMA	2.10	0.75
6:B:315:CLA:HBD	6:B:315:CLA:HBA1	1.69	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:HBB1	5:B:312:CHL:HHC	1.81	0.62
6:C:315:CLA:HBA1	6:C:315:CLA:HBD	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
6:B:307:CLA:C9	6:C:307:CLA:H93	2.32	0.59
1:B:66:VAL:O	1:B:69:CYS:HB2	2.02	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:B:99:LYS:HA	5:B:311:CHL:HED2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:LUT:H34	6:B:314:CLA:CBB	2.32	0.59
1:A:66:VAL:O	1:A:69:CYS:HB2	2.03	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:HHB	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:HBA1	6:A:315:CLA:HBD	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
6:C:306:CLA:HHC	6:C:306:CLA:HBB1	1.92	0.52
1:A:194:PHE:HE2	2:A:301:LUT:H41	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
6:C:314:CLA:H12	6:C:314:CLA:HMB2	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
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
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:B:21:ARG:HG2	1:B:21:ARG:HH11	1.78	0.47
1:A:139:GLU:HG3	5:A:313:CHL:NB	2.30	0.47
2:B:301:LUT:H34	6:B:314:CLA:HBB2	1.95	0.47
5:A:312:CHL:O1A	6:A:314:CLA:HMD2	2.14	0.47
1:B:71:TRP:CD1	5:B:313:CHL:HMD3	2.50	0.47
2:C:302:LUT:H191	2:C:302:LUT:H11	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
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
1:B:118:LEU:HD23	5:B:309:CHL:HED2	1.96	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:B:314:CLA:HAB	6:B:314:CLA:HMB1	1.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:314:CLA:H43	6:C:316:CLA:HBA1	1.97	0.46
5:A:311:CHL:H152	5:A:313:CHL:H71	1.98	0.46
2:A:301:LUT:C33	6:A:316:CLA:HMB2	2.46	0.46
1:A:91:LYS:O	1:A:114:GLY:HA3	2.15	0.46
1:B:83:GLU:OE1	1:B:205:PRO:HD2	2.16	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
1:B:179:LYS:HD3	6:B:316:CLA:HAA2	1.99	0.45
2:A:301:LUT:C31	6:A:314:CLA:HMC2	2.47	0.45
2:B:301:LUT:C34	6:B:316:CLA:HMB2	2.47	0.45
1:A:94:GLU:HG2	1:A:99:LYS:CB	2.45	0.45
1:A:77:LEU:O	1:A:77:LEU:HD12	2.16	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
1:B:136:GLY:CA	5:B:313:CHL:HAB	2.43	0.44
2:A:301:LUT:H34	6:A:314:CLA:CBB	2.47	0.44
3:C:303:NEX:H402	5:C:312:CHL:H152	2.00	0.44
1:A:173:PHE:CZ	6:A:314:CLA:HED3	2.52	0.44
2:C:302:LUT:H32	6:C:306:CLA:HBB1	1.99	0.44
3:C:303:NEX:H191	3:C:303:NEX:H11	1.76	0.44
1:B:35:TYR:HH	1:B:50:GLY:HA2	1.83	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
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
1:C:73:MET:SD	6:C:314:CLA:HBB1	2.58	0.43
5:C:305:CHL:HBA1	5:C:305:CHL:H3A	1.47	0.43
2:A:301:LUT:H11	2:A:301:LUT:H191	1.81	0.43
6:A:307:CLA:H61	6:A:307:CLA:H41	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:B:314:CLA:HHC	6:B:314:CLA:HBB1	2.00	0.43
6:A:314:CLA:H93	6:A:316:CLA:H102	2.01	0.43
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:H191	3:B:303:NEX:H11	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
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
1:B:181:ILE:HD12	1:B:185:ARG:NE	2.34	0.43
6:C:306:CLA:HAB	6:C:306:CLA:HMB1	1.73	0.42
3:C:303:NEX:H401	3:C:303:NEX:H35	1.78	0.42
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
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
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
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
6:C:307:CLA:HMA2	6:C:307:CLA:H42	2.00	0.42
6:B:314:CLA:H51	6:B:316:CLA:HMA1	2.01	0.42
3:A:303:NEX:H35	3:A:303:NEX:H401	1.73	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
5:C:305:CHL:HMA2	5:C:305:CHL:H43	2.01	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
1:A:118:LEU:O	1:A:120:HIS:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:305:CHL:H143	5:A:305:CHL:H111	1.73	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
2:B:301:LUT:H201	2:B:301:LUT:H15	1.93	0.41
6:C:315:CLA:HBB1	6:C:315:CLA:HHC	2.01	0.41
3:B:303:NEX:H201	3:B:303:NEX:H15	1.90	0.41
1:A:212:HIS:CG	6:A:317:CLA:HAA2	2.56	0.41
5:B:312:CHL:CAD	6:B:314:CLA:HMD3	2.50	0.41
1:B:154:PRO:HG2	10:B:437:HOH:O	2.20	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
6:C:307:CLA:HAC2	5:C:311:CHL:H162	2.03	0.41
5:C:305:CHL:H111	5:C:305:CHL:H143	1.65	0.41
1:C:120:HIS:HE1	10:C:409:HOH:O	2.03	0.41
1:C:213:LEU:HD21	6:C:318:CLA:HHC	2.03	0.41
3:A:303:NEX:H183	3:A:303:NEX:H192	2.03	0.41
1:B:97:TRP:O	2:B:302:LUT:O3	2.39	0.41
4:B:304:LHG:H151	4:B:304:LHG:H182	1.77	0.40
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
6:A:306:CLA:C9	6:A:307:CLA:HBB	2.49	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
1:B:195:PHE:O	1:B:199:ILE:HG13	2.21	0.40
4:A:304:LHG:H141	6:A:317:CLA:C9	2.45	0.40
4:C:304:LHG:H151	4:C:304:LHG:H182	1.81	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
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
5:B:305:CHL:HMB1	5:B:305:CHL:HAB	1.79	0.40
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	34	60
1	B	206/224 (92%)	199 (97%)	7 (3%)	0	100	100
1	C	206/224 (92%)	198 (96%)	7 (3%)	1 (0%)	34	60
All	All	618/672 (92%)	596 (96%)	20 (3%)	2 (0%)	46	72

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%)	65	86
1	B	160/174 (92%)	157 (98%)	3 (2%)	65	86
1	C	160/174 (92%)	154 (96%)	6 (4%)	40	68
All	All	480/522 (92%)	468 (98%)	12 (2%)	55	81

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

Mol	Chain	Res	Type
1	A	181	ILE

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Mol	Chain	Res	Type
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 [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	-	41,43,43	0.90	1 (2%)	51,60,60	1.60	8 (15%)
2	LUT	A	302	-	41,43,43	0.91	1 (2%)	51,60,60	1.62	10 (19%)
3	NEX	A	303	-	39,46,46	0.90	1 (2%)	48,70,70	1.97	12 (25%)
4	LHG	A	304	6	48,48,48	0.90	2 (4%)	49,54,54	1.04	3 (6%)
5	CHL	A	305	1	57,74,74	1.79	12 (21%)	56,114,114	1.93	14 (25%)
6	CLA	A	306	1	55,73,73	1.71	10 (18%)	61,113,113	2.15	16 (26%)
6	CLA	A	307	1	55,73,73	1.73	10 (18%)	61,113,113	1.94	18 (29%)
6	CLA	A	308	10	52,70,73	1.71	9 (17%)	56,109,113	2.01	14 (25%)
5	CHL	A	309	1	39,56,74	2.39	12 (30%)	37,92,114	2.28	12 (32%)
5	CHL	A	310	10	42,59,74	2.07	10 (23%)	39,96,114	2.21	15 (38%)
5	CHL	A	311	10	57,74,74	1.84	11 (19%)	56,114,114	1.76	12 (21%)
5	CHL	A	312	10	57,74,74	1.92	11 (19%)	56,114,114	1.86	13 (23%)
5	CHL	A	313	1	57,74,74	1.80	12 (21%)	56,114,114	1.61	11 (19%)
6	CLA	A	314	1	55,73,73	1.93	10 (18%)	61,113,113	1.62	12 (19%)
6	CLA	A	315	4	55,73,73	1.68	11 (20%)	61,113,113	1.99	17 (27%)
6	CLA	A	316	1	55,73,73	1.62	9 (16%)	61,113,113	1.78	12 (19%)
6	CLA	A	317	1	55,73,73	1.61	9 (16%)	61,113,113	1.74	15 (24%)
6	CLA	A	318	1	30,49,73	2.16	10 (33%)	34,84,113	2.17	9 (26%)
7	CAC	A	319	8	0,4,4	0.00	-	0,6,6	0.00	-
2	LUT	B	301	-	41,43,43	0.89	2 (4%)	51,60,60	1.73	16 (31%)
2	LUT	B	302	-	41,43,43	1.05	3 (7%)	51,60,60	1.83	15 (29%)
3	NEX	B	303	-	39,46,46	0.90	2 (5%)	48,70,70	1.78	12 (25%)
4	LHG	B	304	6	48,48,48	0.95	2 (4%)	49,54,54	1.12	3 (6%)
5	CHL	B	305	1	57,74,74	2.15	11 (19%)	56,114,114	1.90	15 (26%)
6	CLA	B	306	1	55,73,73	1.76	9 (16%)	61,113,113	2.13	18 (29%)
6	CLA	B	307	1	55,73,73	1.96	11 (20%)	61,113,113	2.02	14 (22%)
6	CLA	B	308	10	52,70,73	2.06	9 (17%)	56,109,113	2.14	13 (23%)
5	CHL	B	309	1	39,56,74	2.20	12 (30%)	37,92,114	2.21	11 (29%)
5	CHL	B	310	10	42,59,74	2.03	10 (23%)	39,96,114	2.42	13 (33%)
5	CHL	B	311	10	57,74,74	1.84	11 (19%)	56,114,114	1.96	10 (17%)
5	CHL	B	312	10	57,74,74	1.87	12 (21%)	56,114,114	1.87	14 (25%)
5	CHL	B	313	1	57,74,74	1.65	9 (15%)	56,114,114	1.76	12 (21%)
6	CLA	B	314	1	55,73,73	1.94	9 (16%)	61,113,113	1.78	13 (21%)
6	CLA	B	315	4	55,73,73	1.60	7 (12%)	61,113,113	2.10	15 (24%)
6	CLA	B	316	1	55,73,73	1.62	10 (18%)	61,113,113	1.98	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CLA	B	317	1	55,73,73	1.59	7 (12%)	61,113,113	1.75	12 (19%)
6	CLA	B	318	1	30,49,73	2.15	10 (33%)	34,84,113	2.32	10 (29%)
7	CAC	B	319	8	0,4,4	0.00	-	0,6,6	0.00	-
2	LUT	C	301	-	41,43,43	1.03	1 (2%)	51,60,60	2.03	15 (29%)
2	LUT	C	302	-	41,43,43	0.84	2 (4%)	51,60,60	2.00	11 (21%)
3	NEX	C	303	-	39,46,46	0.95	1 (2%)	48,70,70	1.94	12 (25%)
4	LHG	C	304	6	48,48,48	0.91	2 (4%)	49,54,54	1.06	3 (6%)
5	CHL	C	305	1	57,74,74	1.77	11 (19%)	56,114,114	1.81	13 (23%)
6	CLA	C	306	1	55,73,73	1.89	9 (16%)	61,113,113	2.06	20 (32%)
6	CLA	C	307	1	55,73,73	1.69	10 (18%)	61,113,113	1.99	19 (31%)
6	CLA	C	308	10	52,70,73	1.76	9 (17%)	56,109,113	1.96	14 (25%)
5	CHL	C	309	1	39,56,74	2.28	12 (30%)	37,92,114	2.14	10 (27%)
5	CHL	C	310	10	42,59,74	2.07	11 (26%)	39,96,114	2.38	15 (38%)
5	CHL	C	311	10	57,74,74	1.88	12 (21%)	56,114,114	1.96	11 (19%)
5	CHL	C	312	10	57,74,74	2.19	11 (19%)	56,114,114	2.12	15 (26%)
5	CHL	C	313	1	57,74,74	1.74	12 (21%)	56,114,114	1.82	10 (17%)
6	CLA	C	314	1	55,73,73	1.84	10 (18%)	61,113,113	1.74	13 (21%)
6	CLA	C	315	4	55,73,73	1.78	11 (20%)	61,113,113	1.86	15 (24%)
6	CLA	C	316	1	55,73,73	1.69	10 (18%)	61,113,113	1.90	13 (21%)
6	CLA	C	317	1	55,73,73	1.75	10 (18%)	61,113,113	1.77	16 (26%)
6	CLA	C	318	1	29,48,73	2.13	10 (34%)	34,82,113	2.16	8 (23%)
7	CAC	C	319	8	0,4,4	0.00	-	0,6,6	0.00	-

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	-	0/39/137/137	0/0/9/9
6	CLA	A	306	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	A	307	1	3/3/20/25	0/37/135/135	0/0/9/9
6	CLA	A	308	10	2/2/19/25	0/34/132/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHL	A	309	1	-	0/18/116/137	0/0/9/9
5	CHL	A	310	10	-	0/21/119/137	0/0/9/9
5	CHL	A	311	10	-	0/39/137/137	0/0/9/9
5	CHL	A	312	10	-	0/39/137/137	0/0/9/9
5	CHL	A	313	1	-	0/39/137/137	0/0/9/9
6	CLA	A	314	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	A	315	4	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	A	316	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	A	317	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	A	318	1	2/2/15/25	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
4	LHG	B	304	6	-	0/53/53/53	0/0/0/0
5	CHL	B	305	1	-	0/39/137/137	0/0/9/9
6	CLA	B	306	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	B	307	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	B	308	10	2/2/19/25	0/34/132/135	0/0/9/9
5	CHL	B	309	1	-	0/18/116/137	0/0/9/9
5	CHL	B	310	10	-	0/21/119/137	0/0/9/9
5	CHL	B	311	10	-	0/39/137/137	0/0/9/9
5	CHL	B	312	10	-	0/39/137/137	0/0/9/9
5	CHL	B	313	1	-	0/39/137/137	0/0/9/9
6	CLA	B	314	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	B	315	4	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	B	316	1	3/3/20/25	0/37/135/135	0/0/9/9
6	CLA	B	317	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	B	318	1	2/2/15/25	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	-	0/39/137/137	0/0/9/9
6	CLA	C	306	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	C	307	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	C	308	10	2/2/19/25	0/34/132/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHL	C	309	1	-	0/18/116/137	0/0/9/9
5	CHL	C	310	10	-	0/21/119/137	0/0/9/9
5	CHL	C	311	10	-	0/39/137/137	0/0/9/9
5	CHL	C	312	10	-	0/39/137/137	0/0/9/9
5	CHL	C	313	1	-	0/39/137/137	0/0/9/9
6	CLA	C	314	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	C	315	4	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	C	316	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	C	317	1	2/2/20/25	0/37/135/135	0/0/9/9
6	CLA	C	318	1	2/2/14/25	0/8/102/135	0/0/9/9
7	CAC	C	319	8	-	0/0/0/0	0/0/0/0

All (451) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	312	CHL	C3B-C2B	-9.92	1.27	1.40
5	B	305	CHL	C3B-C2B	-9.07	1.28	1.40
6	B	307	CLA	C3B-C2B	-8.49	1.29	1.40
6	B	308	CLA	C3B-C2B	-8.43	1.29	1.40
5	A	309	CHL	C3B-C2B	-7.27	1.30	1.40
6	B	314	CLA	C3B-C2B	-6.95	1.31	1.40
6	A	314	CLA	C3B-C2B	-6.78	1.31	1.40
5	C	309	CHL	C3B-C2B	-6.14	1.32	1.40
6	C	306	CLA	C3B-C2B	-5.91	1.32	1.40
5	A	312	CHL	C3B-C2B	-5.86	1.32	1.40
5	B	309	CHL	C3B-C2B	-5.83	1.32	1.40
6	C	315	CLA	C3B-C2B	-5.44	1.33	1.40
6	C	308	CLA	C3B-C2B	-5.32	1.33	1.40
6	C	317	CLA	C3B-C2B	-5.31	1.33	1.40
6	C	314	CLA	C3B-C2B	-5.29	1.33	1.40
5	B	312	CHL	C3B-C2B	-4.96	1.33	1.40
6	B	306	CLA	C3B-C2B	-4.90	1.33	1.40
5	C	311	CHL	C3B-C2B	-4.86	1.33	1.40
6	C	316	CLA	C3B-C2B	-4.47	1.34	1.40
6	A	307	CLA	C3B-C2B	-4.28	1.34	1.40
6	A	308	CLA	C3B-C2B	-4.05	1.35	1.40
2	C	301	LUT	C22-C21	-3.91	1.50	1.54
6	A	318	CLA	C3B-C2B	-3.81	1.35	1.40
6	A	306	CLA	C3B-C2B	-3.81	1.35	1.40
5	C	305	CHL	C3B-C2B	-3.67	1.35	1.40
6	B	318	CLA	C3B-C2B	-3.63	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	318	CLA	C3B-C2B	-3.58	1.35	1.40
2	A	301	LUT	C22-C21	-3.22	1.51	1.54
6	A	315	CLA	C3B-C2B	-3.21	1.36	1.40
5	B	311	CHL	C3B-C2B	-3.21	1.36	1.40
5	C	305	CHL	C1C-NC	-3.12	1.32	1.37
6	A	317	CLA	C3B-C2B	-3.01	1.36	1.40
6	A	316	CLA	C1C-NC	-2.98	1.32	1.37
5	C	312	CHL	C1C-NC	-2.97	1.33	1.37
5	B	310	CHL	C3B-C2B	-2.88	1.36	1.40
3	C	303	NEX	C7-C8	-2.85	1.26	1.32
3	A	303	NEX	C7-C8	-2.80	1.26	1.32
5	C	313	CHL	C3B-C2B	-2.68	1.36	1.40
5	A	309	CHL	C1C-NC	-2.66	1.33	1.37
3	B	303	NEX	C7-C8	-2.64	1.27	1.32
5	A	305	CHL	C3B-C2B	-2.63	1.36	1.40
6	A	318	CLA	C1C-NC	-2.53	1.33	1.37
6	B	316	CLA	C1C-NC	-2.52	1.33	1.37
5	C	313	CHL	CHB-C4A	-2.51	1.34	1.41
2	C	302	LUT	C1-C6	-2.50	1.50	1.53
5	A	305	CHL	C1C-NC	-2.45	1.33	1.37
6	C	316	CLA	C1C-NC	-2.44	1.33	1.37
5	B	309	CHL	C1C-NC	-2.42	1.33	1.37
5	B	305	CHL	C1C-NC	-2.39	1.33	1.37
5	C	313	CHL	C4C-NC	-2.37	1.33	1.37
6	B	318	CLA	C1C-NC	-2.33	1.33	1.37
6	A	306	CLA	C1C-NC	-2.33	1.33	1.37
5	A	305	CHL	CHB-C4A	-2.29	1.34	1.41
5	B	305	CHL	CHB-C4A	-2.29	1.34	1.41
6	C	307	CLA	C3B-C2B	-2.27	1.37	1.40
5	C	313	CHL	C1C-NC	-2.26	1.34	1.37
5	C	310	CHL	C3B-C2B	-2.26	1.37	1.40
5	A	313	CHL	CHB-C4A	-2.25	1.34	1.41
5	B	311	CHL	C1C-NC	-2.23	1.34	1.37
5	B	309	CHL	CHB-C4A	-2.22	1.34	1.41
5	C	309	CHL	C1C-NC	-2.21	1.34	1.37
5	C	312	CHL	CHB-C4A	-2.20	1.34	1.41
5	B	312	CHL	CHB-C4A	-2.20	1.34	1.41
6	C	318	CLA	C1C-NC	-2.17	1.34	1.37
5	B	311	CHL	CHB-C4A	-2.17	1.35	1.41
5	A	312	CHL	CHB-C4A	-2.17	1.35	1.41
5	A	309	CHL	CHB-C4A	-2.15	1.35	1.41
5	B	313	CHL	CHB-C4A	-2.15	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	311	CHL	CHB-C4A	-2.15	1.35	1.41
6	A	316	CLA	C4C-NC	-2.14	1.34	1.37
5	B	312	CHL	C1C-NC	-2.14	1.34	1.37
6	C	308	CLA	C1C-NC	-2.12	1.34	1.37
6	B	307	CLA	C1C-NC	-2.11	1.34	1.37
3	B	303	NEX	O24-C25	-2.11	1.42	1.46
6	C	315	CLA	C1C-NC	-2.09	1.34	1.37
5	A	313	CHL	C4C-NC	-2.09	1.34	1.37
2	B	301	LUT	C22-C21	-2.08	1.52	1.54
5	C	311	CHL	CHB-C4A	-2.05	1.35	1.41
5	C	309	CHL	CHB-C4A	-2.04	1.35	1.41
6	A	315	CLA	C1C-NC	-2.03	1.34	1.37
5	C	310	CHL	CHB-C4A	-2.03	1.35	1.41
5	A	312	CHL	C1C-NC	-2.03	1.34	1.37
5	C	305	CHL	CHB-C4A	-2.02	1.35	1.41
2	B	302	LUT	C1-C6	-2.01	1.50	1.53
5	C	311	CHL	C2-C3	2.00	1.36	1.33
6	B	316	CLA	C1C-C2C	2.02	1.48	1.44
5	B	309	CHL	C2C-C1C	2.04	1.48	1.44
6	C	318	CLA	C1C-C2C	2.07	1.48	1.44
5	A	305	CHL	CMC-C2C	2.09	1.49	1.45
6	A	315	CLA	C3D-CAD	2.10	1.51	1.45
6	A	315	CLA	C4C-C3C	2.11	1.48	1.45
2	B	301	LUT	C23-C24	2.11	1.52	1.50
5	B	309	CHL	C4C-C3C	2.12	1.48	1.45
6	B	316	CLA	C4C-C3C	2.12	1.48	1.45
6	A	308	CLA	C1C-C2C	2.15	1.48	1.44
6	A	317	CLA	C4C-C3C	2.15	1.48	1.45
5	A	310	CHL	CMC-C2C	2.16	1.49	1.45
2	C	302	LUT	C23-C24	2.17	1.52	1.50
5	A	311	CHL	OBD-CAD	2.19	1.25	1.22
5	C	311	CHL	C4C-C3C	2.25	1.49	1.45
2	B	302	LUT	C26-C27	2.25	1.54	1.50
5	A	309	CHL	C2C-C1C	2.25	1.49	1.44
6	A	306	CLA	C1C-C2C	2.26	1.49	1.44
5	A	313	CHL	CMC-C2C	2.30	1.49	1.45
5	C	305	CHL	C2C-C1C	2.31	1.49	1.44
5	B	305	CHL	C2C-C1C	2.31	1.49	1.44
6	B	318	CLA	C1C-C2C	2.33	1.49	1.44
6	A	318	CLA	C1C-C2C	2.34	1.49	1.44
5	C	311	CHL	C2C-C1C	2.36	1.49	1.44
5	B	310	CHL	C4C-C3C	2.36	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	312	CHL	C4C-C3C	2.37	1.49	1.45
6	C	316	CLA	C1C-C2C	2.40	1.49	1.44
5	A	311	CHL	C2C-C1C	2.40	1.49	1.44
5	C	309	CHL	C4C-C3C	2.41	1.49	1.45
5	A	311	CHL	C4C-C3C	2.46	1.49	1.45
5	C	310	CHL	C2C-C1C	2.47	1.49	1.44
6	B	307	CLA	C4C-C3C	2.48	1.49	1.45
6	B	307	CLA	C1C-C2C	2.51	1.49	1.44
5	B	312	CHL	C4D-CHA	2.51	1.48	1.45
6	C	317	CLA	C1C-C2C	2.53	1.49	1.44
5	B	312	CHL	C2C-C1C	2.54	1.49	1.44
5	C	310	CHL	C4C-C3C	2.60	1.49	1.45
6	C	317	CLA	C4C-C3C	2.61	1.49	1.45
6	A	314	CLA	C1C-C2C	2.61	1.49	1.44
5	A	310	CHL	C4C-C3C	2.61	1.49	1.45
6	C	318	CLA	C4C-C3C	2.63	1.49	1.45
6	C	306	CLA	C1C-C2C	2.63	1.49	1.44
6	B	314	CLA	C4B-CHC	2.65	1.47	1.39
6	C	315	CLA	C1C-C2C	2.66	1.49	1.44
5	B	313	CHL	C4D-CHA	2.66	1.48	1.45
6	A	318	CLA	C4C-C3C	2.67	1.49	1.45
5	C	312	CHL	C2C-C1C	2.67	1.50	1.44
5	C	309	CHL	C2C-C1C	2.68	1.50	1.44
5	B	311	CHL	C2C-C1C	2.69	1.50	1.44
5	A	309	CHL	C4C-C3C	2.70	1.49	1.45
6	B	318	CLA	C4C-C3C	2.70	1.49	1.45
6	A	314	CLA	C4B-CHC	2.71	1.47	1.39
5	B	311	CHL	C4D-CHA	2.72	1.48	1.45
6	B	306	CLA	C1C-C2C	2.73	1.50	1.44
6	A	314	CLA	C4C-C3C	2.73	1.50	1.45
6	C	315	CLA	C4C-C3C	2.74	1.50	1.45
6	B	314	CLA	C4C-C3C	2.75	1.50	1.45
5	A	313	CHL	C4C-C3C	2.75	1.50	1.45
6	A	317	CLA	C1B-CHB	2.75	1.47	1.39
5	C	313	CHL	C3D-C2D	2.76	1.46	1.40
2	A	302	LUT	C23-C24	2.77	1.52	1.50
5	C	305	CHL	C4D-CHA	2.78	1.48	1.45
6	C	317	CLA	C4B-CHC	2.78	1.47	1.39
6	C	307	CLA	C4B-CHC	2.80	1.47	1.39
6	B	307	CLA	C4B-CHC	2.82	1.47	1.39
5	B	305	CHL	CHC-C1C	2.83	1.47	1.41
6	A	317	CLA	C4B-CHC	2.84	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	305	CHL	C2C-C1C	2.86	1.50	1.44
6	C	314	CLA	C4B-CHC	2.86	1.47	1.39
6	C	314	CLA	C4C-C3C	2.87	1.50	1.45
6	B	307	CLA	C1B-CHB	2.87	1.47	1.39
6	A	307	CLA	C1B-CHB	2.89	1.47	1.39
5	A	313	CHL	C2C-C1C	2.90	1.50	1.44
6	B	316	CLA	C4B-CHC	2.90	1.47	1.39
6	C	308	CLA	C1C-C2C	2.94	1.50	1.44
6	C	307	CLA	C1C-C2C	2.94	1.50	1.44
6	A	307	CLA	C4B-CHC	2.95	1.48	1.39
5	A	309	CHL	C4D-CHA	2.95	1.48	1.45
5	C	311	CHL	C4D-CHA	2.95	1.48	1.45
5	A	305	CHL	CHC-C1C	2.96	1.48	1.41
5	B	310	CHL	C2C-C1C	2.97	1.50	1.44
5	C	312	CHL	CHC-C1C	3.00	1.48	1.41
5	A	310	CHL	C2C-C1C	3.01	1.50	1.44
6	A	307	CLA	C1C-C2C	3.01	1.50	1.44
5	B	309	CHL	CHC-C1C	3.02	1.48	1.41
5	B	309	CHL	C4D-CHA	3.02	1.48	1.45
6	B	315	CLA	CHD-C4C	3.02	1.48	1.41
6	C	315	CLA	C1B-CHB	3.04	1.48	1.39
6	C	308	CLA	C1B-CHB	3.04	1.48	1.39
6	A	306	CLA	CHD-C4C	3.05	1.48	1.41
6	C	318	CLA	C4B-CHC	3.07	1.48	1.39
5	B	313	CHL	C2C-C1C	3.08	1.51	1.44
5	A	313	CHL	C3D-C2D	3.09	1.47	1.40
6	B	308	CLA	C1B-CHB	3.09	1.48	1.39
5	A	312	CHL	C2C-C1C	3.09	1.51	1.44
5	B	311	CHL	CHC-C1C	3.09	1.48	1.41
6	C	314	CLA	C1B-CHB	3.09	1.48	1.39
5	A	309	CHL	CHC-C1C	3.10	1.48	1.41
6	A	308	CLA	CHD-C4C	3.11	1.48	1.41
6	C	317	CLA	C1B-CHB	3.13	1.48	1.39
5	C	311	CHL	CHC-C1C	3.13	1.48	1.41
6	B	314	CLA	C1B-CHB	3.14	1.48	1.39
6	C	307	CLA	C1B-CHB	3.17	1.48	1.39
6	A	308	CLA	C4B-CHC	3.17	1.48	1.39
5	B	312	CHL	CHC-C1C	3.17	1.48	1.41
6	C	307	CLA	CHD-C4C	3.18	1.48	1.41
6	B	317	CLA	C1B-CHB	3.18	1.48	1.39
6	B	306	CLA	CHD-C4C	3.19	1.48	1.41
6	C	308	CLA	C4B-CHC	3.19	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	307	CLA	C4C-C3C	3.19	1.50	1.45
5	C	313	CHL	C2C-C1C	3.19	1.51	1.44
5	C	313	CHL	C4D-CHA	3.21	1.49	1.45
6	B	308	CLA	C1C-C2C	3.21	1.51	1.44
6	B	316	CLA	CHD-C4C	3.22	1.48	1.41
5	C	309	CHL	C4D-CHA	3.22	1.49	1.45
6	B	315	CLA	C1B-CHB	3.23	1.48	1.39
6	B	314	CLA	CHD-C4C	3.24	1.48	1.41
6	C	315	CLA	C4B-CHC	3.25	1.48	1.39
6	B	318	CLA	C4B-CHC	3.25	1.48	1.39
5	A	311	CHL	C4D-CHA	3.25	1.49	1.45
5	C	312	CHL	C4D-CHA	3.28	1.49	1.45
6	A	318	CLA	C1B-CHB	3.29	1.48	1.39
6	A	315	CLA	C4B-CHC	3.29	1.48	1.39
5	C	309	CHL	CHC-C1C	3.29	1.48	1.41
6	A	308	CLA	C1B-CHB	3.30	1.48	1.39
6	B	317	CLA	C4B-CHC	3.31	1.49	1.39
6	B	307	CLA	C3D-C2D	3.33	1.48	1.40
6	A	314	CLA	CHD-C4C	3.35	1.49	1.41
6	A	307	CLA	C4C-C3C	3.35	1.51	1.45
6	B	308	CLA	CHD-C4C	3.38	1.49	1.41
5	A	313	CHL	C4D-CHA	3.38	1.49	1.45
5	A	313	CHL	CHC-C1C	3.39	1.49	1.41
6	C	316	CLA	CHD-C4C	3.41	1.49	1.41
6	B	318	CLA	C1B-CHB	3.41	1.49	1.39
6	C	306	CLA	O2A-CGA	3.43	1.43	1.33
5	C	305	CHL	CHC-C1C	3.44	1.49	1.41
6	A	315	CLA	C1B-CHB	3.44	1.49	1.39
6	A	316	CLA	C1B-CHB	3.44	1.49	1.39
4	A	304	LHG	O7-C7	3.45	1.44	1.34
5	A	310	CHL	C3D-C2D	3.46	1.48	1.40
6	B	315	CLA	C4B-CHC	3.46	1.49	1.39
6	C	314	CLA	CHD-C4C	3.47	1.49	1.41
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	C	316	CLA	C4B-CHC	3.48	1.49	1.39
6	C	318	CLA	C1B-CHB	3.49	1.49	1.39
5	B	310	CHL	C4D-CHA	3.51	1.49	1.45
6	B	318	CLA	CHD-C4C	3.51	1.49	1.41
5	A	310	CHL	CHC-C1C	3.51	1.49	1.41
6	A	306	CLA	O2A-CGA	3.52	1.43	1.33
5	A	312	CHL	CHC-C1C	3.53	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	306	CLA	O2A-CGA	3.53	1.43	1.33
2	B	302	LUT	C23-C24	3.55	1.53	1.50
6	A	306	CLA	C1B-CHB	3.56	1.49	1.39
6	A	316	CLA	C4B-CHC	3.57	1.49	1.39
4	B	304	LHG	O7-C7	3.58	1.45	1.34
5	C	310	CHL	CHC-C1C	3.59	1.49	1.41
5	B	311	CHL	C3D-C2D	3.60	1.48	1.40
5	B	313	CHL	CHC-C1C	3.60	1.49	1.41
5	C	309	CHL	C3D-C2D	3.63	1.48	1.40
5	C	313	CHL	CHC-C1C	3.64	1.49	1.41
5	B	312	CHL	C3D-C2D	3.64	1.48	1.40
6	C	318	CLA	CHD-C4C	3.64	1.49	1.41
5	C	311	CHL	C3D-C2D	3.65	1.48	1.40
5	C	313	CHL	O2A-CGA	3.66	1.44	1.33
6	C	314	CLA	C1C-C2C	3.67	1.51	1.44
5	B	313	CHL	C3D-C2D	3.67	1.48	1.40
6	A	315	CLA	CHD-C4C	3.68	1.49	1.41
6	A	316	CLA	CHD-C4C	3.69	1.49	1.41
5	A	305	CHL	C4D-CHA	3.70	1.49	1.45
6	A	307	CLA	CHD-C4C	3.71	1.49	1.41
6	A	314	CLA	C1B-CHB	3.72	1.50	1.39
5	B	309	CHL	C3D-C2D	3.74	1.49	1.40
6	A	317	CLA	CHD-C4C	3.74	1.50	1.41
5	B	311	CHL	CHD-C4C	3.75	1.47	1.35
6	C	317	CLA	C3D-C2D	3.76	1.49	1.40
6	C	316	CLA	C3D-C2D	3.76	1.49	1.40
6	A	318	CLA	CHD-C4C	3.77	1.50	1.41
6	B	308	CLA	C4B-CHC	3.78	1.50	1.39
5	A	311	CHL	CHC-C1C	3.81	1.50	1.41
6	B	317	CLA	CHD-C4C	3.82	1.50	1.41
5	C	305	CHL	C3D-C2D	3.82	1.49	1.40
6	A	308	CLA	C3D-C2D	3.82	1.49	1.40
5	B	305	CHL	CHD-C4C	3.83	1.47	1.35
6	C	308	CLA	C3D-C2D	3.83	1.49	1.40
6	B	316	CLA	C1B-CHB	3.84	1.50	1.39
6	C	315	CLA	CHD-C4C	3.85	1.50	1.41
5	C	312	CHL	C3D-C2D	3.85	1.49	1.40
4	C	304	LHG	O7-C7	3.85	1.45	1.34
5	A	309	CHL	C3D-C2D	3.87	1.49	1.40
5	A	312	CHL	C3D-C2D	3.88	1.49	1.40
6	B	317	CLA	O2A-CGA	3.89	1.45	1.33
6	A	307	CLA	CHC-C1C	3.89	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	306	CLA	C1B-CHB	3.89	1.50	1.39
6	C	317	CLA	O2A-CGA	3.90	1.45	1.33
6	C	316	CLA	C1B-CHB	3.90	1.50	1.39
6	B	307	CLA	CHD-C4C	3.91	1.50	1.41
5	B	312	CHL	O2A-CGA	3.91	1.45	1.33
5	C	310	CHL	C3D-C2D	3.92	1.49	1.40
6	A	307	CLA	C3D-C2D	3.93	1.49	1.40
6	C	318	CLA	C3D-C2D	3.94	1.49	1.40
5	C	313	CHL	CHD-C4C	3.94	1.47	1.35
6	C	315	CLA	C3D-C2D	3.95	1.49	1.40
5	B	313	CHL	CHD-C4C	3.96	1.47	1.35
5	C	305	CHL	O2A-CGA	3.96	1.45	1.33
6	C	307	CLA	C3D-C2D	3.96	1.49	1.40
5	B	310	CHL	CHD-C4C	3.97	1.47	1.35
6	A	306	CLA	C4B-CHC	3.97	1.50	1.39
5	A	310	CHL	C4D-CHA	3.98	1.50	1.45
5	B	310	CHL	C3D-C2D	3.98	1.49	1.40
6	B	318	CLA	CHC-C1C	3.99	1.47	1.35
5	A	311	CHL	C3D-C2D	4.00	1.49	1.40
5	B	310	CHL	CHC-C1C	4.01	1.50	1.41
6	B	316	CLA	CHC-C1C	4.04	1.48	1.35
5	C	305	CHL	CHD-C4C	4.04	1.48	1.35
6	A	316	CLA	C3D-C2D	4.04	1.49	1.40
5	C	311	CHL	CHD-C4C	4.05	1.48	1.35
5	C	312	CHL	O2A-CGA	4.06	1.45	1.33
6	B	316	CLA	O2A-CGA	4.06	1.45	1.33
5	C	309	CHL	CHD-C4C	4.08	1.48	1.35
6	A	317	CLA	O2A-CGA	4.08	1.45	1.33
6	C	306	CLA	CHD-C4C	4.10	1.50	1.41
6	B	315	CLA	O2A-CGA	4.10	1.45	1.33
6	C	307	CLA	CHC-C1C	4.11	1.48	1.35
5	B	313	CHL	O2A-CGA	4.11	1.45	1.33
5	A	305	CHL	O2A-CGA	4.11	1.45	1.33
6	B	316	CLA	C3D-C2D	4.12	1.50	1.40
6	C	318	CLA	CHC-C1C	4.13	1.48	1.35
6	C	308	CLA	CHC-C1C	4.13	1.48	1.35
6	A	316	CLA	CHC-C1C	4.13	1.48	1.35
5	C	310	CHL	C4D-CHA	4.13	1.50	1.45
6	A	318	CLA	C3D-C2D	4.14	1.50	1.40
5	A	305	CHL	C3D-C2D	4.14	1.50	1.40
5	A	312	CHL	CHD-C4C	4.16	1.48	1.35
6	A	317	CLA	C3D-C2D	4.16	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	316	CLA	O2A-CGA	4.17	1.45	1.33
6	A	318	CLA	CHC-C1C	4.17	1.48	1.35
5	C	310	CHL	CHD-C4C	4.19	1.48	1.35
5	A	312	CHL	C4D-CHA	4.19	1.50	1.45
5	B	309	CHL	CHD-C4C	4.20	1.48	1.35
6	A	316	CLA	O2A-CGA	4.21	1.46	1.33
5	A	313	CHL	CHD-C4C	4.22	1.48	1.35
6	C	315	CLA	O2A-CGA	4.23	1.46	1.33
5	C	310	CHL	O2A-CGA	4.23	1.46	1.33
6	B	306	CLA	C3D-C2D	4.23	1.50	1.40
5	A	309	CHL	CHD-C4C	4.24	1.48	1.35
5	B	310	CHL	O2D-CGD	4.24	1.44	1.33
6	A	315	CLA	O2D-CGD	4.26	1.44	1.33
6	A	315	CLA	O2A-CGA	4.26	1.46	1.33
6	B	317	CLA	C3D-C2D	4.26	1.50	1.40
4	C	304	LHG	O8-C23	4.27	1.46	1.33
6	B	307	CLA	CHC-C1C	4.27	1.48	1.35
5	A	312	CHL	O2A-CGA	4.27	1.46	1.33
5	A	309	CHL	O2A-CGA	4.28	1.46	1.33
6	A	314	CLA	C3D-C2D	4.29	1.50	1.40
6	B	308	CLA	O2D-CGD	4.30	1.44	1.33
6	C	314	CLA	C3D-C2D	4.30	1.50	1.40
6	C	316	CLA	CHC-C1C	4.30	1.48	1.35
5	A	313	CHL	O2A-CGA	4.31	1.46	1.33
6	C	317	CLA	CHC-C1C	4.31	1.48	1.35
5	A	310	CHL	CHD-C4C	4.31	1.48	1.35
5	B	310	CHL	O2A-CGA	4.32	1.46	1.33
6	A	307	CLA	O2A-CGA	4.32	1.46	1.33
6	C	315	CLA	CHC-C1C	4.32	1.48	1.35
5	A	305	CHL	O2D-CGD	4.33	1.44	1.33
6	C	317	CLA	CHD-C4C	4.34	1.51	1.41
5	B	305	CHL	C3D-C2D	4.34	1.50	1.40
6	C	306	CLA	C3D-C2D	4.34	1.50	1.40
5	A	310	CHL	O2A-CGA	4.35	1.46	1.33
4	A	304	LHG	O8-C23	4.35	1.46	1.33
5	B	309	CHL	O2D-CGD	4.36	1.44	1.33
5	B	309	CHL	O2A-CGA	4.36	1.46	1.33
6	A	308	CLA	O2A-CGA	4.37	1.46	1.33
6	B	315	CLA	C3D-C2D	4.37	1.50	1.40
5	B	305	CHL	O2A-CGA	4.37	1.46	1.33
6	C	308	CLA	O2A-CGA	4.38	1.46	1.33
6	C	315	CLA	O2D-CGD	4.38	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	306	CLA	C4B-CHC	4.39	1.51	1.39
6	C	316	CLA	O2D-CGD	4.39	1.44	1.33
6	A	308	CLA	CHC-C1C	4.39	1.49	1.35
6	A	314	CLA	CHC-C1C	4.39	1.49	1.35
6	B	308	CLA	O2A-CGA	4.41	1.46	1.33
6	B	314	CLA	CHC-C1C	4.41	1.49	1.35
6	A	317	CLA	CHC-C1C	4.42	1.49	1.35
5	C	309	CHL	O2A-CGA	4.42	1.46	1.33
6	C	306	CLA	C4B-CHC	4.43	1.52	1.39
6	B	308	CLA	C3D-C2D	4.43	1.50	1.40
5	A	311	CHL	CHD-C4C	4.43	1.49	1.35
6	B	318	CLA	C3D-C2D	4.47	1.50	1.40
6	A	316	CLA	O2D-CGD	4.49	1.44	1.33
5	A	305	CHL	CHD-C4C	4.50	1.49	1.35
6	A	315	CLA	CHC-C1C	4.50	1.49	1.35
6	A	315	CLA	C3D-C2D	4.51	1.51	1.40
5	C	309	CHL	O2D-CGD	4.53	1.44	1.33
6	B	315	CLA	CHC-C1C	4.53	1.49	1.35
6	A	306	CLA	C3D-C2D	4.54	1.51	1.40
6	B	317	CLA	CHC-C1C	4.55	1.49	1.35
6	B	307	CLA	O2A-CGA	4.56	1.47	1.33
5	B	313	CHL	O2D-CGD	4.57	1.44	1.33
4	B	304	LHG	O8-C23	4.58	1.47	1.33
6	C	314	CLA	O2A-CGA	4.61	1.47	1.33
6	C	307	CLA	O2A-CGA	4.62	1.47	1.33
5	B	312	CHL	CHD-C4C	4.62	1.49	1.35
6	A	306	CLA	CHC-C1C	4.63	1.49	1.35
6	B	314	CLA	C3D-C2D	4.65	1.51	1.40
6	C	314	CLA	CHC-C1C	4.66	1.49	1.35
5	C	312	CHL	CHD-C4C	4.68	1.50	1.35
5	C	305	CHL	O2D-CGD	4.69	1.45	1.33
6	C	307	CLA	O2D-CGD	4.72	1.45	1.33
5	A	312	CHL	O2D-CGD	4.72	1.45	1.33
6	B	308	CLA	CHC-C1C	4.75	1.50	1.35
6	C	306	CLA	CHC-C1C	4.76	1.50	1.35
5	C	312	CHL	O2D-CGD	4.77	1.45	1.33
5	C	313	CHL	O2D-CGD	4.78	1.45	1.33
5	A	311	CHL	O2A-CGA	4.79	1.47	1.33
6	B	317	CLA	O2D-CGD	4.80	1.45	1.33
6	B	315	CLA	O2D-CGD	4.80	1.45	1.33
6	B	306	CLA	O2D-CGD	4.82	1.45	1.33
6	A	317	CLA	O2D-CGD	4.82	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	311	CHL	O2D-CGD	4.82	1.45	1.33
6	A	318	CLA	O2D-CGD	4.83	1.45	1.33
6	A	306	CLA	O2D-CGD	4.83	1.45	1.33
6	A	314	CLA	O2A-CGA	4.83	1.47	1.33
6	B	306	CLA	CHC-C1C	4.84	1.50	1.35
5	A	309	CHL	O2D-CGD	4.84	1.45	1.33
5	B	311	CHL	O2A-CGA	4.85	1.47	1.33
5	B	305	CHL	O2D-CGD	4.86	1.45	1.33
6	C	308	CLA	O2D-CGD	4.87	1.45	1.33
6	B	314	CLA	O2A-CGA	4.91	1.48	1.33
5	A	311	CHL	O2D-CGD	4.92	1.45	1.33
6	A	308	CLA	O2D-CGD	4.92	1.45	1.33
6	C	314	CLA	O2D-CGD	4.93	1.45	1.33
6	C	306	CLA	O2D-CGD	4.93	1.45	1.33
6	C	318	CLA	O2D-CGD	4.97	1.45	1.33
5	B	311	CHL	O2D-CGD	5.00	1.46	1.33
6	B	307	CLA	O2D-CGD	5.02	1.46	1.33
6	B	318	CLA	O2D-CGD	5.02	1.46	1.33
5	A	313	CHL	O2D-CGD	5.03	1.46	1.33
5	C	311	CHL	O2A-CGA	5.03	1.48	1.33
5	C	310	CHL	O2D-CGD	5.06	1.46	1.33
6	B	316	CLA	O2D-CGD	5.15	1.46	1.33
6	A	314	CLA	O2D-CGD	5.17	1.46	1.33
6	A	307	CLA	O2D-CGD	5.17	1.46	1.33
6	C	317	CLA	O2D-CGD	5.20	1.46	1.33
5	B	305	CHL	C4D-CHA	5.24	1.51	1.45
5	B	313	CHL	C1A-CHA	5.24	1.48	1.37
5	A	310	CHL	O2D-CGD	5.25	1.46	1.33
5	B	312	CHL	O2D-CGD	5.62	1.47	1.33
5	B	309	CHL	C1A-CHA	5.69	1.49	1.37
5	C	310	CHL	C1A-CHA	5.74	1.49	1.37
5	B	310	CHL	C1A-CHA	5.80	1.49	1.37
5	B	305	CHL	C1A-CHA	5.85	1.49	1.37
6	B	314	CLA	O2D-CGD	5.86	1.48	1.33
5	A	310	CHL	C1A-CHA	5.87	1.49	1.37
5	B	312	CHL	C1A-CHA	5.93	1.49	1.37
5	C	313	CHL	C1A-CHA	5.97	1.49	1.37
5	C	309	CHL	C1A-CHA	6.11	1.49	1.37
5	A	312	CHL	C1A-CHA	6.21	1.50	1.37
5	C	305	CHL	C1A-CHA	6.22	1.50	1.37
5	A	309	CHL	C1A-CHA	6.23	1.50	1.37
5	A	311	CHL	C1A-CHA	6.26	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	311	CHL	C1A-CHA	6.31	1.50	1.37
5	C	312	CHL	C1A-CHA	6.33	1.50	1.37
5	A	313	CHL	C1A-CHA	6.39	1.50	1.37
5	A	305	CHL	C1A-CHA	6.51	1.50	1.37
5	B	311	CHL	C1A-CHA	6.85	1.51	1.37

All (686) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	305	CHL	C1D-CHD-C4C	-6.46	115.38	129.26
3	A	303	NEX	C35-C34-C33	-6.41	117.94	127.20
3	C	303	NEX	C35-C34-C33	-5.80	118.82	127.20
5	C	312	CHL	C1D-CHD-C4C	-5.78	116.85	129.26
5	B	311	CHL	C1D-CHD-C4C	-5.68	117.05	129.26
5	A	305	CHL	C1D-CHD-C4C	-5.66	117.11	129.26
5	C	305	CHL	C1D-CHD-C4C	-5.64	117.15	129.26
2	C	301	LUT	C18-C5-C6	-5.60	119.11	124.61
6	C	317	CLA	C4B-CHC-C1C	-5.55	117.34	129.26
5	C	311	CHL	C1D-CHD-C4C	-5.41	117.63	129.26
6	B	317	CLA	C4B-CHC-C1C	-5.26	117.95	129.26
6	B	314	CLA	C4B-CHC-C1C	-5.24	118.00	129.26
6	A	308	CLA	C4B-CHC-C1C	-5.21	118.07	129.26
6	C	318	CLA	C4B-CHC-C1C	-5.21	118.07	129.26
5	A	309	CHL	C1D-CHD-C4C	-5.20	118.09	129.26
5	B	313	CHL	C1D-CHD-C4C	-5.19	118.11	129.26
5	B	310	CHL	C1D-CHD-C4C	-5.12	118.27	129.26
5	C	313	CHL	C1D-CHD-C4C	-5.11	118.28	129.26
5	A	312	CHL	C1D-CHD-C4C	-5.11	118.28	129.26
6	B	307	CLA	C4B-CHC-C1C	-5.10	118.30	129.26
6	B	308	CLA	C4B-CHC-C1C	-5.10	118.31	129.26
5	C	310	CHL	C1D-CHD-C4C	-5.03	118.44	129.26
5	C	309	CHL	C1D-CHD-C4C	-5.03	118.47	129.26
3	B	303	NEX	C35-C34-C33	-4.99	119.98	127.20
6	A	317	CLA	C4B-CHC-C1C	-4.98	118.57	129.26
6	C	308	CLA	CHD-C4C-C3C	-4.97	117.25	124.94
6	B	318	CLA	C4B-CHC-C1C	-4.91	118.71	129.26
5	A	310	CHL	C1D-CHD-C4C	-4.90	118.73	129.26
5	B	309	CHL	C1D-CHD-C4C	-4.87	118.79	129.26
6	A	315	CLA	OBD-CAD-CBD	-4.85	118.61	125.94
6	A	314	CLA	C4B-CHC-C1C	-4.84	118.85	129.26
6	A	315	CLA	C4B-CHC-C1C	-4.83	118.88	129.26
5	A	313	CHL	C1D-CHD-C4C	-4.79	118.97	129.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	315	CLA	C4B-CHC-C1C	-4.76	119.05	129.26
5	B	310	CHL	O2D-CGD-O1D	-4.73	114.01	123.79
5	B	312	CHL	C1D-CHD-C4C	-4.73	119.10	129.26
5	A	311	CHL	C1D-CHD-C4C	-4.65	119.26	129.26
2	C	302	LUT	C11-C10-C9	-4.65	120.47	127.20
6	A	308	CLA	C1D-CHD-C4C	-4.64	115.58	122.60
6	B	314	CLA	C1D-CHD-C4C	-4.63	115.60	122.60
6	B	316	CLA	O1D-CGD-CBD	-4.59	118.05	124.62
6	C	308	CLA	C4B-CHC-C1C	-4.57	119.44	129.26
6	C	306	CLA	C4B-CHC-C1C	-4.57	119.45	129.26
6	A	307	CLA	C4B-CHC-C1C	-4.53	119.52	129.26
6	B	308	CLA	CHD-C4C-C3C	-4.53	117.94	124.94
2	B	301	LUT	C11-C10-C9	-4.52	120.67	127.20
6	A	306	CLA	C6-C5-C3	-4.49	102.62	112.48
6	B	306	CLA	CHD-C4C-C3C	-4.48	118.01	124.94
6	C	308	CLA	C1D-CHD-C4C	-4.44	115.88	122.60
6	B	307	CLA	O2D-CGD-O1D	-4.41	114.68	123.79
6	B	315	CLA	C4B-CHC-C1C	-4.39	119.83	129.26
6	A	308	CLA	CHD-C4C-C3C	-4.39	118.16	124.94
5	C	311	CHL	CAA-CBA-CGA	-4.36	100.56	113.32
6	B	306	CLA	C4B-CHC-C1C	-4.35	119.93	129.26
6	C	314	CLA	C4B-CHC-C1C	-4.32	119.98	129.26
3	A	303	NEX	C25-C24-C23	-4.32	106.01	113.03
6	B	308	CLA	O2D-CGD-O1D	-4.31	114.89	123.79
2	B	302	LUT	C11-C10-C9	-4.28	121.01	127.20
6	A	306	CLA	C4B-CHC-C1C	-4.28	120.06	129.26
6	B	315	CLA	O2D-CGD-O1D	-4.27	114.97	123.79
6	B	316	CLA	C1D-CHD-C4C	-4.25	116.17	122.60
6	C	307	CLA	C4B-CHC-C1C	-4.24	120.15	129.26
6	B	314	CLA	CHD-C4C-C3C	-4.21	118.44	124.94
6	A	316	CLA	C4B-CHC-C1C	-4.19	120.25	129.26
6	A	318	CLA	C4B-CHC-C1C	-4.17	120.30	129.26
5	C	310	CHL	C1-C2-C3	-4.16	119.89	126.71
6	A	306	CLA	CHD-C4C-C3C	-4.16	118.51	124.94
6	A	316	CLA	CHD-C4C-C3C	-4.14	118.54	124.94
6	A	306	CLA	O2D-CGD-O1D	-4.13	115.26	123.79
3	B	303	NEX	C39-C29-C30	-4.08	116.87	122.90
6	A	315	CLA	O2D-CGD-O1D	-4.08	115.38	123.79
6	B	315	CLA	CAA-C2A-C3A	-4.04	101.60	113.22
6	C	315	CLA	OBd-CAD-CBD	-4.02	119.87	125.94
2	C	301	LUT	C15-C35-C34	-4.01	114.53	123.39
5	C	313	CHL	CHD-C4C-C3C	-3.99	117.47	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	312	CHL	O1D-CGD-CBD	-3.99	118.90	124.62
5	A	305	CHL	CHD-C4C-C3C	-3.95	117.55	125.42
6	C	316	CLA	O2D-CGD-O1D	-3.95	115.64	123.79
5	C	310	CHL	OBD-CAD-CBD	-3.95	119.98	125.94
5	B	310	CHL	OBD-CAD-CBD	-3.94	120.00	125.94
5	C	313	CHL	O1D-CGD-CBD	-3.92	119.00	124.62
6	B	316	CLA	CHD-C4C-C3C	-3.91	118.89	124.94
6	B	315	CLA	OBD-CAD-CBD	-3.91	120.04	125.94
6	B	318	CLA	O2D-CGD-O1D	-3.90	115.73	123.79
5	B	311	CHL	CAA-CBA-CGA	-3.90	101.90	113.32
6	B	308	CLA	C1D-CHD-C4C	-3.89	116.72	122.60
5	B	305	CHL	CHD-C4C-C3C	-3.88	117.70	125.42
6	C	314	CLA	O2D-CGD-O1D	-3.87	115.80	123.79
6	B	316	CLA	C4B-CHC-C1C	-3.86	120.96	129.26
6	A	318	CLA	O2D-CGD-O1D	-3.82	115.90	123.79
2	A	302	LUT	C23-C24-C25	-3.82	121.65	125.22
6	C	307	CLA	C1D-CHD-C4C	-3.81	116.83	122.60
3	C	303	NEX	C39-C29-C30	-3.81	117.27	122.90
6	B	308	CLA	OBD-CAD-CBD	-3.81	120.19	125.94
6	C	314	CLA	CHD-C4C-C3C	-3.78	119.09	124.94
5	B	309	CHL	O2D-CGD-O1D	-3.78	115.98	123.79
5	B	310	CHL	CHD-C4C-C3C	-3.75	117.94	125.42
6	A	315	CLA	C1D-CHD-C4C	-3.75	116.92	122.60
2	C	302	LUT	C16-C1-C6	-3.74	104.43	110.30
2	A	302	LUT	C16-C1-C6	-3.72	104.47	110.30
5	B	305	CHL	C3B-CAB-CBB	-3.72	118.71	126.32
5	C	305	CHL	C3B-CAB-CBB	-3.72	118.72	126.32
6	B	315	CLA	C3B-CAB-CBB	-3.70	118.74	126.32
3	C	303	NEX	C25-C24-C23	-3.69	107.03	113.03
2	C	301	LUT	C40-C33-C34	-3.69	117.45	122.90
5	A	312	CHL	C3B-CAB-CBB	-3.69	118.77	126.32
6	C	316	CLA	C1D-CHD-C4C	-3.69	117.02	122.60
5	A	311	CHL	CAA-CBA-CGA	-3.66	102.59	113.32
5	A	310	CHL	C1-C2-C3	-3.66	120.72	126.71
2	B	301	LUT	C20-C13-C14	-3.65	117.51	122.90
6	C	316	CLA	CHD-C4C-C3C	-3.65	119.30	124.94
6	A	314	CLA	CHD-C4C-C3C	-3.62	119.35	124.94
6	C	316	CLA	C3B-CAB-CBB	-3.61	118.93	126.32
6	C	316	CLA	C4B-CHC-C1C	-3.61	121.51	129.26
6	A	316	CLA	C1D-CHD-C4C	-3.61	117.14	122.60
6	B	306	CLA	C6-C5-C3	-3.61	104.57	112.48
6	B	317	CLA	C1D-CHD-C4C	-3.59	117.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	314	CLA	OBD-CAD-CBD	-3.58	120.53	125.94
6	C	317	CLA	C3B-CAB-CBB	-3.58	118.98	126.32
2	B	302	LUT	C20-C13-C14	-3.58	117.61	122.90
5	B	311	CHL	O2D-CGD-O1D	-3.57	116.43	123.79
3	C	303	NEX	C11-C10-C9	-3.55	122.07	127.20
6	A	314	CLA	C1D-CHD-C4C	-3.55	117.23	122.60
5	B	311	CHL	CHD-C4C-C3C	-3.54	118.38	125.42
6	B	306	CLA	O2D-CGD-O1D	-3.53	116.49	123.79
6	B	317	CLA	CHD-C4C-C3C	-3.52	119.50	124.94
6	A	317	CLA	OBD-CAD-CBD	-3.52	120.63	125.94
5	C	312	CHL	O1D-CGD-CBD	-3.47	119.65	124.62
6	C	306	CLA	OBD-CAD-CBD	-3.45	120.73	125.94
5	C	312	CHL	C3B-CAB-CBB	-3.44	119.27	126.32
6	A	307	CLA	C1D-CHD-C4C	-3.43	117.41	122.60
6	A	307	CLA	C3B-CAB-CBB	-3.42	119.31	126.32
6	C	307	CLA	CAA-C2A-C3A	-3.39	103.48	113.22
6	B	306	CLA	C6-C7-C8	-3.39	104.26	115.49
6	C	315	CLA	C3B-CAB-CBB	-3.38	119.40	126.32
2	C	301	LUT	C16-C1-C6	-3.38	105.01	110.30
5	A	305	CHL	C3B-CAB-CBB	-3.37	119.43	126.32
5	B	313	CHL	CHD-C4C-C3C	-3.36	118.72	125.42
2	C	302	LUT	C18-C5-C6	-3.36	121.31	124.61
5	B	310	CHL	C1-C2-C3	-3.34	121.24	126.71
5	B	309	CHL	OBD-CAD-CBD	-3.33	120.91	125.94
6	A	317	CLA	C1D-CHD-C4C	-3.33	117.56	122.60
5	A	309	CHL	C3B-CAB-CBB	-3.33	119.51	126.32
5	B	312	CHL	C3B-CAB-CBB	-3.32	119.52	126.32
6	B	315	CLA	C1D-CHD-C4C	-3.32	117.58	122.60
6	C	318	CLA	O2D-CGD-O1D	-3.31	116.96	123.79
6	B	318	CLA	C3B-CAB-CBB	-3.30	119.58	126.32
6	C	308	CLA	O1D-CGD-CBD	-3.28	119.92	124.62
2	A	301	LUT	C16-C1-C6	-3.28	105.17	110.30
6	B	317	CLA	OBD-CAD-CBD	-3.27	121.00	125.94
3	A	303	NEX	C24-C23-C22	-3.26	103.20	110.41
3	A	303	NEX	C21-C22-C23	-3.26	109.53	115.02
5	C	309	CHL	O2D-CGD-O1D	-3.24	117.09	123.79
6	A	315	CLA	C3B-CAB-CBB	-3.22	119.73	126.32
6	A	317	CLA	CHD-C4C-C3C	-3.21	119.98	124.94
6	A	308	CLA	OBD-CAD-CBD	-3.21	121.10	125.94
6	A	307	CLA	CHD-C4C-C3C	-3.20	119.99	124.94
6	C	315	CLA	C1D-CHD-C4C	-3.20	117.76	122.60
6	C	315	CLA	CAA-C2A-C3A	-3.20	104.02	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	316	CLA	O1D-CGD-CBD	-3.19	120.05	124.62
5	A	312	CHL	CHD-C4C-C3C	-3.18	119.08	125.42
5	C	305	CHL	OMC-CMC-C2C	-3.18	117.41	125.58
5	A	309	CHL	O2D-CGD-O1D	-3.17	117.25	123.79
5	C	311	CHL	CHD-C4C-C3C	-3.16	119.13	125.42
6	C	307	CLA	CHD-C4C-C3C	-3.16	120.06	124.94
5	C	311	CHL	O2D-CGD-O1D	-3.15	117.28	123.79
6	B	307	CLA	C3B-CAB-CBB	-3.15	119.88	126.32
3	B	303	NEX	C11-C10-C9	-3.14	122.66	127.20
6	C	306	CLA	O1D-CGD-CBD	-3.14	120.12	124.62
2	A	302	LUT	C18-C5-C6	-3.14	121.52	124.61
6	A	307	CLA	O2D-CGD-O1D	-3.14	117.31	123.79
5	A	310	CHL	OBD-CAD-CBD	-3.13	121.21	125.94
2	C	301	LUT	C35-C34-C33	-3.13	122.67	127.20
5	A	310	CHL	CHD-C4C-C3C	-3.13	119.18	125.42
3	A	303	NEX	C39-C29-C30	-3.13	118.28	122.90
6	B	317	CLA	C3B-CAB-CBB	-3.13	119.92	126.32
6	B	307	CLA	CHD-C4C-C3C	-3.13	120.11	124.94
5	B	309	CHL	C3B-CAB-CBB	-3.12	119.92	126.32
5	C	310	CHL	O2D-CGD-O1D	-3.11	117.36	123.79
6	B	318	CLA	OBD-CAD-CBD	-3.11	121.25	125.94
6	A	315	CLA	CAA-C2A-C3A	-3.10	104.31	113.22
5	C	309	CHL	C3B-CAB-CBB	-3.08	120.02	126.32
6	A	308	CLA	C9-C8-C10	-3.07	99.26	111.08
6	A	308	CLA	O2D-CGD-O1D	-3.07	117.45	123.79
6	B	307	CLA	C1D-CHD-C4C	-3.05	117.98	122.60
6	C	315	CLA	CHD-C4C-C3C	-3.05	120.23	124.94
2	A	301	LUT	C18-C5-C6	-3.05	121.61	124.61
6	C	314	CLA	C1D-CHD-C4C	-3.05	117.99	122.60
6	B	306	CLA	O2A-CGA-O1A	-3.05	115.63	123.49
6	C	306	CLA	O2D-CGD-O1D	-3.04	117.51	123.79
5	C	309	CHL	CHD-C4C-C3C	-3.04	119.37	125.42
5	A	305	CHL	O2D-CGD-O1D	-3.03	117.53	123.79
6	A	318	CLA	C3B-CAB-CBB	-3.03	120.12	126.32
5	C	312	CHL	CHD-C4C-C3C	-3.01	119.42	125.42
2	A	301	LUT	C11-C10-C9	-3.01	122.84	127.20
6	A	318	CLA	C1D-CHD-C4C	-3.00	118.06	122.60
6	C	318	CLA	C1D-CHD-C4C	-2.98	118.09	122.60
5	C	305	CHL	CHD-C4C-C3C	-2.97	119.50	125.42
5	A	310	CHL	O1D-CGD-CBD	-2.97	120.36	124.62
6	C	307	CLA	O1D-CGD-CBD	-2.96	120.39	124.62
6	C	306	CLA	CHD-C4C-C3C	-2.94	120.41	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	312	CHL	O2D-CGD-O1D	-2.93	117.73	123.79
3	C	303	NEX	C24-C23-C22	-2.93	103.93	110.41
5	B	309	CHL	CHD-C4C-C3C	-2.93	119.59	125.42
6	B	306	CLA	OBD-CAD-CBD	-2.92	121.52	125.94
5	C	310	CHL	CHD-C4C-C3C	-2.92	119.61	125.42
5	A	311	CHL	O2D-CGD-O1D	-2.91	117.79	123.79
6	C	306	CLA	O2A-CGA-O1A	-2.90	116.01	123.49
5	A	311	CHL	CHD-C4C-C3C	-2.89	119.66	125.42
6	B	318	CLA	C1D-CHD-C4C	-2.89	118.23	122.60
3	C	303	NEX	C11-C12-C13	-2.88	117.83	126.32
5	C	311	CHL	O1D-CGD-CBD	-2.88	120.49	124.62
2	A	302	LUT	C8-C7-C6	-2.88	118.67	127.32
6	C	307	CLA	O2D-CGD-O1D	-2.88	117.85	123.79
3	C	303	NEX	C30-C31-C32	-2.87	114.38	123.13
6	C	306	CLA	C6-C5-C3	-2.87	106.19	112.48
6	B	306	CLA	C1D-CHD-C4C	-2.87	118.27	122.60
5	A	312	CHL	O1D-CGD-CBD	-2.86	120.52	124.62
5	A	312	CHL	C6-C5-C3	-2.86	106.22	112.48
6	C	307	CLA	CBC-CAC-C3C	-2.86	103.67	112.39
6	C	318	CLA	CHD-C4C-C3C	-2.85	120.54	124.94
3	B	303	NEX	C15-C14-C13	-2.84	123.09	127.20
4	C	304	LHG	C5-O7-C7	-2.82	111.13	117.89
5	A	305	CHL	CAA-CBA-CGA	-2.81	105.08	113.32
2	B	301	LUT	C35-C34-C33	-2.80	123.16	127.20
2	A	302	LUT	C11-C10-C9	-2.79	123.17	127.20
6	B	306	CLA	C3B-CAB-CBB	-2.78	120.62	126.32
5	A	312	CHL	OMC-CMC-C2C	-2.77	118.45	125.58
5	C	313	CHL	CAA-C2A-C3A	-2.76	105.27	113.22
5	A	313	CHL	O1D-CGD-CBD	-2.75	120.69	124.62
6	B	306	CLA	O1D-CGD-CBD	-2.74	120.69	124.62
5	A	309	CHL	O1D-CGD-CBD	-2.74	120.69	124.62
6	A	318	CLA	CHD-C4C-C3C	-2.73	120.72	124.94
3	A	303	NEX	C15-C14-C13	-2.73	123.26	127.20
5	C	305	CHL	CAA-CBA-CGA	-2.73	105.33	113.32
5	B	309	CHL	OMC-CMC-C2C	-2.69	118.67	125.58
6	B	315	CLA	CHD-C4C-C3C	-2.68	120.80	124.94
3	C	303	NEX	C21-C22-C23	-2.68	110.50	115.02
6	A	306	CLA	OBD-CAD-CBD	-2.67	121.91	125.94
4	B	304	LHG	O8-C23-O10	-2.67	116.61	123.49
6	C	307	CLA	OBD-CAD-CBD	-2.66	121.93	125.94
2	B	302	LUT	C38-C25-C24	-2.65	117.74	123.59
2	C	302	LUT	C38-C25-C24	-2.65	117.74	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	312	CHL	OBD-CAD-CBD	-2.65	121.94	125.94
6	A	306	CLA	C1D-CHD-C4C	-2.64	118.60	122.60
6	B	306	CLA	C2C-C1C-NC	-2.64	108.28	110.24
2	C	301	LUT	C36-C21-C22	-2.64	104.69	109.35
6	C	315	CLA	O2D-CGD-O1D	-2.63	118.35	123.79
6	C	308	CLA	O2D-CGD-O1D	-2.63	118.36	123.79
5	A	305	CHL	CBC-CAC-C3C	-2.63	104.37	112.39
2	B	302	LUT	C8-C7-C6	-2.63	119.43	127.32
6	B	315	CLA	CGD-CBD-CAD	-2.62	101.74	110.62
6	A	308	CLA	CHC-C1C-C2C	-2.62	119.46	126.35
5	B	305	CHL	C4B-CHC-C1C	-2.62	118.64	122.60
2	B	302	LUT	C18-C5-C6	-2.61	122.04	124.61
6	C	307	CLA	C1C-C2C-C3C	-2.61	103.79	106.91
6	C	317	CLA	CHD-C4C-C3C	-2.61	120.91	124.94
5	A	309	CHL	CHD-C4C-C3C	-2.61	120.23	125.42
6	A	308	CLA	C9-C8-C7	-2.60	101.07	111.08
3	B	303	NEX	C15-C35-C34	-2.60	117.65	123.39
5	B	312	CHL	C4B-CHC-C1C	-2.58	118.69	122.60
6	A	317	CLA	C3B-CAB-CBB	-2.58	121.04	126.32
5	B	312	CHL	CHD-C4C-C3C	-2.58	120.29	125.42
6	A	307	CLA	O1D-CGD-CBD	-2.58	120.93	124.62
6	B	314	CLA	CHC-C1C-C2C	-2.57	119.58	126.35
2	A	302	LUT	C31-C32-C33	-2.57	118.76	126.32
5	B	313	CHL	O2D-CGD-O1D	-2.57	118.49	123.79
5	A	310	CHL	C4B-CHC-C1C	-2.56	118.72	122.60
5	A	309	CHL	OMC-CMC-C2C	-2.55	119.03	125.58
2	B	302	LUT	C35-C34-C33	-2.54	123.53	127.20
2	B	302	LUT	C23-C24-C25	-2.54	122.85	125.22
6	A	307	CLA	C6-C7-C8	-2.52	107.12	115.49
5	C	313	CHL	O2A-CGA-O1A	-2.52	116.98	123.49
6	B	318	CLA	CHD-C4C-C3C	-2.51	121.06	124.94
5	C	312	CHL	C6-C5-C3	-2.51	106.98	112.48
6	C	307	CLA	C3B-CAB-CBB	-2.51	121.19	126.32
6	B	307	CLA	CHC-C1C-C2C	-2.50	119.78	126.35
6	A	314	CLA	O2D-CGD-O1D	-2.49	118.64	123.79
5	A	305	CHL	OBD-CAD-CBD	-2.49	122.18	125.94
5	B	310	CHL	C4B-CHC-C1C	-2.49	118.84	122.60
5	C	312	CHL	O2A-CGA-O1A	-2.48	117.10	123.49
5	B	305	CHL	CHC-C1C-C2C	-2.48	120.59	125.64
3	B	303	NEX	C19-C9-C10	-2.47	119.25	122.90
6	C	317	CLA	O2D-CGD-O1D	-2.47	118.69	123.79
3	B	303	NEX	C25-C24-C23	-2.47	109.01	113.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	LUT	C15-C35-C34	-2.47	117.93	123.39
6	C	314	CLA	O2A-CGA-O1A	-2.47	117.12	123.49
5	C	312	CHL	CAA-CBA-CGA	-2.46	106.12	113.32
5	A	313	CHL	CHD-C4C-C3C	-2.46	120.53	125.42
5	C	312	CHL	OBD-CAD-CBD	-2.44	122.26	125.94
6	B	307	CLA	O1D-CGD-CBD	-2.44	121.13	124.62
5	C	310	CHL	O1D-CGD-CBD	-2.43	121.14	124.62
6	C	318	CLA	C3B-CAB-CBB	-2.41	121.39	126.32
6	B	316	CLA	OBD-CAD-CBD	-2.40	122.32	125.94
6	B	316	CLA	O2D-CGD-O1D	-2.39	118.85	123.79
3	A	303	NEX	C19-C9-C10	-2.39	119.37	122.90
6	C	316	CLA	CAA-CBA-CGA	-2.39	106.32	113.32
5	B	312	CHL	C6-C5-C3	-2.39	107.24	112.48
5	B	313	CHL	C4B-CHC-C1C	-2.38	119.00	122.60
6	A	307	CLA	CAA-C2A-C3A	-2.38	106.38	113.22
2	C	301	LUT	C38-C25-C24	-2.36	118.37	123.59
6	B	315	CLA	CAA-CBA-CGA	-2.36	106.40	113.32
5	C	312	CHL	C11-C10-C8	-2.36	107.66	115.49
6	A	317	CLA	C4-C3-C2	-2.36	118.87	123.50
6	A	306	CLA	O1D-CGD-CBD	-2.34	121.26	124.62
6	B	317	CLA	O2A-CGA-O1A	-2.34	117.45	123.49
3	C	303	NEX	C19-C9-C10	-2.34	119.45	122.90
6	C	307	CLA	CHC-C1C-C2C	-2.34	120.20	126.35
6	B	316	CLA	O2A-CGA-O1A	-2.34	117.46	123.49
6	A	306	CLA	O2A-CGA-O1A	-2.33	117.48	123.49
5	B	313	CHL	C3B-CAB-CBB	-2.33	121.56	126.32
6	C	317	CLA	C1D-CHD-C4C	-2.32	119.09	122.60
6	C	308	CLA	OBD-CAD-CBD	-2.31	122.45	125.94
5	A	305	CHL	C4B-CHC-C1C	-2.31	119.11	122.60
6	B	317	CLA	C4-C3-C2	-2.30	118.98	123.50
5	C	309	CHL	OMC-CMC-C2C	-2.30	119.67	125.58
6	C	317	CLA	CHC-C1C-C2C	-2.29	120.34	126.35
5	C	311	CHL	CHC-C1C-C2C	-2.28	120.99	125.64
6	A	315	CLA	CHC-C1C-C2C	-2.28	120.36	126.35
5	A	310	CHL	OMC-CMC-C2C	-2.28	119.73	125.58
6	A	317	CLA	C6-C5-C3	-2.27	107.51	112.48
6	B	307	CLA	CBC-CAC-C3C	-2.27	105.48	112.39
6	B	308	CLA	C3B-CAB-CBB	-2.26	121.68	126.32
6	B	308	CLA	C4-C3-C2	-2.26	119.06	123.50
6	C	306	CLA	C6-C7-C8	-2.26	107.99	115.49
2	C	302	LUT	C8-C7-C6	-2.26	120.54	127.32
6	C	317	CLA	O2A-CGA-O1A	-2.26	117.67	123.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	305	CHL	O2A-CGA-O1A	-2.25	117.68	123.49
6	B	314	CLA	CBC-CAC-C3C	-2.24	105.56	112.39
5	A	311	CHL	C4B-CHC-C1C	-2.23	119.22	122.60
6	A	316	CLA	O2A-CGA-O1A	-2.23	117.73	123.49
6	A	317	CLA	C6-C7-C8	-2.23	108.09	115.49
5	A	310	CHL	CGD-CBD-CAD	-2.23	103.06	110.62
6	A	307	CLA	CHC-C1C-C2C	-2.23	120.49	126.35
6	C	306	CLA	C5-C3-C2	-2.22	116.83	121.05
3	A	303	NEX	C11-C10-C9	-2.22	123.99	127.20
6	C	314	CLA	C3B-CAB-CBB	-2.22	121.78	126.32
2	B	301	LUT	C8-C7-C6	-2.22	120.66	127.32
5	A	309	CHL	CHC-C1C-C2C	-2.20	121.16	125.64
6	C	306	CLA	C7-C6-C5	-2.18	106.61	113.06
5	B	305	CHL	CBC-CAC-C3C	-2.18	105.73	112.39
2	A	301	LUT	C8-C7-C6	-2.18	120.78	127.32
6	A	317	CLA	O2A-CGA-O1A	-2.18	117.88	123.49
3	B	303	NEX	C24-C23-C22	-2.18	105.60	110.41
3	C	303	NEX	C15-C35-C34	-2.17	118.59	123.39
2	B	301	LUT	C30-C31-C32	-2.17	116.51	123.13
6	A	308	CLA	CBC-CAC-C3C	-2.17	105.78	112.39
6	A	317	CLA	CHC-C1C-C2C	-2.17	120.66	126.35
2	C	301	LUT	O3-C3-C2	-2.16	105.48	109.91
6	A	315	CLA	CHD-C4C-C3C	-2.16	121.61	124.94
6	B	314	CLA	O1D-CGD-CBD	-2.15	121.53	124.62
6	B	307	CLA	CMB-C2B-C1B	-2.15	124.80	128.36
2	C	301	LUT	C8-C7-C6	-2.15	120.87	127.32
5	B	310	CHL	OMC-CMC-C2C	-2.14	120.09	125.58
6	C	318	CLA	CHC-C1C-C2C	-2.14	120.73	126.35
2	C	301	LUT	C20-C13-C14	-2.13	119.75	122.90
5	B	313	CHL	O2A-CGA-O1A	-2.13	117.99	123.49
5	B	311	CHL	O1D-CGD-CBD	-2.13	121.57	124.62
6	A	307	CLA	OBD-CAD-CBD	-2.12	122.73	125.94
6	C	306	CLA	C3B-CAB-CBB	-2.12	121.99	126.32
6	C	317	CLA	C4-C3-C2	-2.12	119.35	123.50
3	B	303	NEX	C31-C32-C33	-2.12	120.09	126.32
2	B	301	LUT	C16-C1-C6	-2.11	106.99	110.30
6	B	317	CLA	O2D-CGD-O1D	-2.11	119.43	123.79
6	C	308	CLA	CBC-CAC-C3C	-2.11	105.95	112.39
6	A	308	CLA	O1D-CGD-CBD	-2.11	121.60	124.62
5	C	310	CHL	O2A-CGA-O1A	-2.11	118.05	123.49
6	A	306	CLA	C2C-C1C-NC	-2.10	108.68	110.24
5	A	313	CHL	C4B-CHC-C1C	-2.10	119.42	122.60

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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
2	B	301	LUT	C19-C9-C10	-2.10	119.80	122.90
2	B	302	LUT	C19-C9-C10	-2.10	119.80	122.90
6	C	315	CLA	O1D-CGD-CBD	-2.09	121.63	124.62
5	A	313	CHL	C3B-CAB-CBB	-2.08	122.06	126.32
6	A	306	CLA	C6-C7-C8	-2.08	108.59	115.49
5	C	310	CHL	OMC-CMC-C2C	-2.07	120.26	125.58
6	B	314	CLA	C4-C3-C2	-2.07	119.44	123.50
5	B	305	CHL	OBD-CAD-CBD	-2.07	122.82	125.94
6	B	307	CLA	C1C-C2C-C3C	-2.06	104.44	106.91
5	B	305	CHL	OMC-CMC-C2C	-2.05	120.31	125.58
5	A	312	CHL	CBC-CAC-C3C	-2.05	106.15	112.39
6	C	308	CLA	O2A-CGA-O1A	-2.04	118.22	123.49
5	B	312	CHL	C11-C10-C8	-2.04	108.73	115.49
6	A	307	CLA	C1C-C2C-C3C	-2.04	104.47	106.91
6	B	316	CLA	C3B-CAB-CBB	-2.04	122.15	126.32
5	C	310	CHL	C4B-CHC-C1C	-2.03	119.53	122.60
6	B	308	CLA	O1D-CGD-CBD	-2.03	121.71	124.62
6	B	306	CLA	C11-C10-C8	-2.03	108.75	115.49
6	A	314	CLA	C4-C3-C2	-2.03	119.51	123.50
5	A	311	CHL	CHC-C1C-C2C	-2.02	121.52	125.64
5	A	311	CHL	OMC-CMC-C2C	-2.02	120.39	125.58
6	A	318	CLA	OBD-CAD-CBD	-2.02	122.89	125.94
2	B	301	LUT	C22-C23-C24	-2.02	109.38	111.75
5	B	313	CHL	C4-C3-C2	-2.02	119.55	123.50
6	C	317	CLA	CBC-CAC-C3C	-2.01	106.25	112.39
5	C	305	CHL	O2D-CGD-O1D	-2.01	119.64	123.79
5	A	312	CHL	O2A-CGA-O1A	-2.01	118.31	123.49
5	B	309	CHL	CHC-C1C-C2C	-2.00	121.56	125.64
5	A	313	CHL	O2A-CGA-O1A	-2.00	118.32	123.49
5	A	310	CHL	O2D-CGD-O1D	-2.00	119.66	123.79
2	B	302	LUT	C40-C33-C34	-2.00	119.94	122.90
6	A	318	CLA	CHC-C1C-NC	2.00	127.44	123.67
6	C	315	CLA	OBD-CAD-C3D	2.01	132.45	128.35
6	B	318	CLA	CHC-C1C-NC	2.01	127.45	123.67
6	A	317	CLA	CMD-C2D-C3D	2.02	129.04	125.09
2	B	301	LUT	C8-C9-C10	2.02	122.24	118.98
6	B	316	CLA	C1C-NC-C4C	2.04	108.75	106.27
3	B	303	NEX	C28-C29-C30	2.04	122.27	118.98
6	B	307	CLA	C4-C3-C5	2.04	118.53	115.41
6	C	306	CLA	CMD-C2D-C3D	2.05	129.10	125.09
5	B	310	CHL	C5-C3-C4	2.05	119.69	114.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	318	CLA	CAC-C3C-C4C	2.06	127.82	124.83
6	C	316	CLA	CAC-C3C-C2C	2.06	131.12	127.51
6	C	306	CLA	C4A-NA-C1A	2.06	109.03	106.36
6	C	307	CLA	C9-C8-C7	2.08	119.06	111.08
6	C	308	CLA	C4A-NA-C1A	2.09	109.05	106.36
5	C	312	CHL	CMD-C2D-C3D	2.09	129.17	125.09
2	A	302	LUT	C18-C5-C4	2.09	118.05	114.24
5	C	305	CHL	CMD-C2D-C3D	2.09	129.18	125.09
2	C	302	LUT	C31-C30-C29	2.09	130.22	127.20
2	B	301	LUT	C11-C12-C13	2.10	132.49	126.32
2	B	302	LUT	C11-C12-C13	2.10	132.49	126.32
5	A	310	CHL	CED-O2D-CGD	2.10	120.91	115.99
6	A	307	CLA	CHC-C1C-NC	2.10	127.63	123.67
6	B	306	CLA	CMD-C2D-C3D	2.11	129.21	125.09
5	B	312	CHL	C4C-NC-C1C	2.11	108.83	106.27
6	C	306	CLA	CHC-C1C-NC	2.11	127.64	123.67
6	A	316	CLA	CMD-C2D-C3D	2.12	129.22	125.09
5	A	311	CHL	C4C-NC-C1C	2.12	108.84	106.27
5	A	309	CHL	CAC-C3C-C4C	2.12	127.90	124.83
5	A	310	CHL	C5-C3-C4	2.12	119.86	114.64
6	A	306	CLA	CHC-C1C-NC	2.13	127.68	123.67
3	A	303	NEX	C20-C13-C12	2.13	121.64	118.10
2	C	302	LUT	C19-C9-C8	2.14	121.65	118.10
5	C	309	CHL	C4C-NC-C1C	2.14	108.86	106.27
3	B	303	NEX	C19-C9-C8	2.14	124.22	118.62
6	B	306	CLA	CAA-C2A-C3A	2.15	119.38	113.22
2	B	302	LUT	C31-C30-C29	2.15	130.30	127.20
6	C	316	CLA	CHC-C1C-NC	2.15	127.72	123.67
6	C	314	CLA	CMC-C2C-C1C	2.16	128.36	125.02
6	A	307	CLA	CMC-C2C-C1C	2.16	128.36	125.02
6	A	308	CLA	C4A-NA-C1A	2.18	109.18	106.36
6	A	307	CLA	C2C-C1C-NC	2.19	111.88	110.24
6	B	308	CLA	CHC-C1C-NC	2.19	127.80	123.67
2	B	301	LUT	C20-C13-C12	2.19	121.75	118.10
6	A	315	CLA	C4-C3-C5	2.20	118.76	115.41
6	C	307	CLA	C4-C3-C5	2.22	118.79	115.41
6	C	314	CLA	CMD-C2D-C3D	2.22	129.43	125.09
6	C	315	CLA	CHC-C1C-NC	2.22	127.85	123.67
6	C	307	CLA	C2C-C1C-NC	2.24	111.91	110.24
6	C	307	CLA	CHC-C1C-NC	2.24	127.88	123.67
6	C	308	CLA	O2A-CGA-CBA	2.25	118.75	111.90
6	C	315	CLA	C4A-NA-C1A	2.25	109.27	106.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	315	CLA	C4A-NA-C1A	2.25	109.27	106.36
6	A	307	CLA	C4A-NA-C1A	2.26	109.27	106.36
3	C	303	NEX	C37-C21-C36	2.26	110.72	107.35
6	A	306	CLA	O2A-CGA-CBA	2.26	118.79	111.90
5	A	305	CHL	CMB-C2B-C3B	2.26	129.51	125.09
5	C	313	CHL	C4-C3-C5	2.27	118.87	115.41
5	C	311	CHL	CHB-C4A-NA	2.27	127.69	125.06
5	B	313	CHL	CMD-C2D-C3D	2.27	129.53	125.09
5	A	311	CHL	O2A-CGA-CBA	2.28	118.85	111.90
6	A	314	CLA	CMD-C2D-C3D	2.28	129.55	125.09
5	C	309	CHL	C4A-NA-C1A	2.29	108.74	106.04
6	A	306	CLA	CMD-C2D-C3D	2.29	129.57	125.09
6	C	317	CLA	C1C-NC-C4C	2.30	109.06	106.27
2	C	301	LUT	C20-C13-C12	2.30	121.92	118.10
4	A	304	LHG	C6-O8-C23	2.32	123.33	116.85
5	C	305	CHL	C4-C3-C5	2.32	118.95	115.41
5	C	305	CHL	CED-O2D-CGD	2.32	121.43	115.99
5	A	312	CHL	CMD-C2D-C3D	2.33	129.64	125.09
6	A	314	CLA	C4-C3-C5	2.33	118.97	115.41
2	B	301	LUT	C18-C5-C4	2.33	118.50	114.24
6	A	314	CLA	CHC-C1C-NC	2.34	128.07	123.67
2	C	301	LUT	C7-C8-C9	2.34	129.78	126.22
6	C	314	CLA	C4A-NA-C1A	2.34	109.39	106.36
6	A	315	CLA	OBD-CAD-C3D	2.35	133.14	128.35
6	A	318	CLA	C4A-NA-C1A	2.35	109.39	106.36
6	C	308	CLA	C4-C3-C5	2.35	118.99	115.41
6	C	317	CLA	C4A-NA-C1A	2.35	109.40	106.36
6	C	307	CLA	CMC-C2C-C1C	2.37	128.68	125.02
5	C	310	CHL	C5-C3-C4	2.38	120.49	114.64
2	B	302	LUT	C7-C8-C9	2.38	129.84	126.22
6	A	316	CLA	CHC-C1C-NC	2.38	128.15	123.67
6	A	315	CLA	O2A-CGA-CBA	2.39	119.17	111.90
6	B	315	CLA	O2A-CGA-CBA	2.41	119.23	111.90
6	A	315	CLA	CAA-C2A-C1A	2.43	121.04	112.47
6	B	318	CLA	C4A-NA-C1A	2.44	109.51	106.36
6	C	307	CLA	C9-C8-C10	2.44	120.45	111.08
5	B	312	CHL	C4A-NA-C1A	2.45	108.93	106.04
6	B	314	CLA	O2A-CGA-CBA	2.45	119.36	111.90
3	A	303	NEX	O24-C25-C38	2.45	117.85	114.99
6	C	314	CLA	CHC-C1C-NC	2.45	128.29	123.67
6	B	314	CLA	CMD-C2D-C3D	2.45	129.89	125.09
5	B	311	CHL	CMD-C2D-C3D	2.46	129.89	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	305	CHL	CMD-C2D-C3D	2.47	129.92	125.09
2	A	302	LUT	C31-C30-C29	2.48	130.77	127.20
6	B	315	CLA	C4A-NA-C1A	2.48	109.57	106.36
6	C	306	CLA	C1C-NC-C4C	2.48	109.29	106.27
6	C	316	CLA	C1C-NC-C4C	2.49	109.29	106.27
6	A	315	CLA	C9-C8-C10	2.49	120.65	111.08
5	C	313	CHL	C4A-NA-C1A	2.50	108.98	106.04
6	B	308	CLA	CMD-C2D-C3D	2.51	130.00	125.09
6	C	315	CLA	O2A-CGA-CBA	2.53	119.61	111.90
5	B	305	CHL	CED-O2D-CGD	2.54	121.94	115.99
6	B	306	CLA	C1C-NC-C4C	2.54	109.36	106.27
6	C	318	CLA	CHC-C1C-NC	2.55	128.46	123.67
6	A	314	CLA	CGD-CBD-CAD	2.55	119.28	110.62
2	A	301	LUT	C1-C2-C3	2.57	119.44	113.41
2	B	301	LUT	C38-C25-C26	2.57	117.96	116.04
6	A	316	CLA	C1C-NC-C4C	2.58	109.40	106.27
5	B	305	CHL	CMD-C2D-C3D	2.58	130.14	125.09
6	C	315	CLA	C4-C3-C5	2.59	119.36	115.41
6	C	308	CLA	CHC-C1C-NC	2.59	128.54	123.67
6	B	316	CLA	CHC-C1C-NC	2.60	128.56	123.67
5	B	309	CHL	C4A-NA-C1A	2.63	109.14	106.04
5	A	313	CHL	C4-C3-C5	2.64	119.43	115.41
2	C	301	LUT	C1-C2-C3	2.64	119.60	113.41
6	C	306	CLA	O2A-CGA-CBA	2.65	119.98	111.90
5	B	312	CHL	C4-C3-C5	2.66	119.47	115.41
6	B	317	CLA	CHC-C1C-NC	2.67	128.70	123.67
6	B	317	CLA	O2A-CGA-CBA	2.68	120.06	111.90
6	B	317	CLA	C4-C3-C5	2.68	119.50	115.41
2	B	301	LUT	C2-C1-C6	2.68	114.77	110.49
6	C	316	CLA	C4-C3-C5	2.69	119.51	115.41
5	A	313	CHL	O2A-CGA-CBA	2.69	120.09	111.90
6	C	316	CLA	C4A-NA-C1A	2.69	109.84	106.36
5	A	305	CHL	C4A-NA-C1A	2.71	109.23	106.04
4	A	304	LHG	O7-C7-C8	2.72	117.43	111.53
5	B	312	CHL	O2A-CGA-CBA	2.73	120.20	111.90
6	C	315	CLA	CAA-C2A-C1A	2.74	122.12	112.47
4	C	304	LHG	O7-C7-C8	2.74	117.48	111.53
6	C	308	CLA	CMD-C2D-C3D	2.75	130.46	125.09
6	B	316	CLA	C4A-NA-C1A	2.75	109.92	106.36
6	A	316	CLA	C4A-NA-C1A	2.79	109.97	106.36
4	C	304	LHG	O8-C23-C24	2.80	120.43	111.90
6	A	317	CLA	CHC-C1C-NC	2.80	128.94	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	314	CLA	CED-O2D-CGD	2.82	122.59	115.99
6	C	306	CLA	CMC-C2C-C1C	2.82	129.38	125.02
5	B	310	CHL	C4A-NA-C1A	2.82	109.37	106.04
5	B	309	CHL	O2A-CGA-CBA	2.82	120.51	111.90
6	B	315	CLA	CHC-C1C-NC	2.83	129.00	123.67
6	B	315	CLA	C1C-NC-C4C	2.83	109.71	106.27
5	A	309	CHL	CHD-C4C-NC	2.84	129.02	123.67
5	C	312	CHL	C4A-NA-C1A	2.85	109.40	106.04
5	B	311	CHL	O2A-CGA-CBA	2.85	120.59	111.90
6	A	306	CLA	C1C-NC-C4C	2.86	109.74	106.27
6	C	314	CLA	CGD-CBD-CAD	2.87	120.36	110.62
5	C	311	CHL	O2A-CGA-CBA	2.88	120.66	111.90
5	A	311	CHL	C4A-NA-C1A	2.88	109.44	106.04
6	A	315	CLA	C1C-NC-C4C	2.89	109.78	106.27
6	A	314	CLA	C4A-NA-C1A	2.90	110.10	106.36
6	B	307	CLA	O2A-CGA-CBA	2.90	120.73	111.90
6	A	316	CLA	O2A-CGA-CBA	2.91	120.77	111.90
6	B	308	CLA	C4-C3-C5	2.91	119.86	115.41
5	C	309	CHL	O2A-CGA-CBA	2.92	120.78	111.90
6	B	307	CLA	CHC-C1C-NC	2.92	129.17	123.67
6	B	306	CLA	O2A-CGA-CBA	2.94	120.86	111.90
5	C	310	CHL	C4A-NA-C1A	2.95	109.52	106.04
5	A	313	CHL	CHD-C4C-NC	2.96	129.25	123.67
5	B	310	CHL	O2A-CGA-CBA	2.97	120.94	111.90
6	A	314	CLA	O2A-CGA-CBA	2.98	120.97	111.90
5	B	310	CHL	CMD-C2D-C3D	2.99	130.93	125.09
4	A	304	LHG	O8-C23-C24	3.00	121.03	111.90
6	B	315	CLA	C4-C3-C5	3.00	119.99	115.41
2	B	301	LUT	C1-C2-C3	3.01	120.46	113.41
5	B	311	CHL	C4A-NA-C1A	3.01	109.59	106.04
2	A	302	LUT	C12-C13-C14	3.01	123.84	118.98
2	A	301	LUT	C2-C1-C6	3.02	115.30	110.49
5	A	309	CHL	O2A-CGA-CBA	3.02	121.10	111.90
6	B	316	CLA	C4-C3-C5	3.03	120.03	115.41
6	C	317	CLA	O2A-CGA-CBA	3.03	121.14	111.90
6	B	306	CLA	C4-C3-C5	3.03	120.04	115.41
5	C	310	CHL	CMD-C2D-C3D	3.03	131.02	125.09
5	C	311	CHL	C4A-NA-C1A	3.04	109.62	106.04
6	A	307	CLA	O2A-CGA-CBA	3.04	121.16	111.90
3	A	303	NEX	C37-C21-C36	3.04	111.89	107.35
5	A	309	CHL	C4A-NA-C1A	3.05	109.63	106.04
6	C	317	CLA	CHC-C1C-NC	3.06	129.42	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	317	CLA	C4-C3-C5	3.06	120.08	115.41
5	B	305	CHL	C4A-NA-C1A	3.06	109.65	106.04
6	B	316	CLA	O2A-CGA-CBA	3.09	121.32	111.90
6	A	308	CLA	C4-C3-C5	3.10	120.14	115.41
5	B	313	CHL	O2A-CGA-CBA	3.10	121.34	111.90
5	C	305	CHL	C4A-NA-C1A	3.13	109.73	106.04
6	C	317	CLA	C4-C3-C5	3.14	120.20	115.41
5	A	310	CHL	C4A-NA-C1A	3.15	109.75	106.04
6	C	307	CLA	O2A-CGA-CBA	3.16	121.52	111.90
5	A	313	CHL	C4A-NA-C1A	3.17	109.78	106.04
5	A	310	CHL	O2A-CGA-CBA	3.19	121.62	111.90
5	C	305	CHL	CHD-C4C-NC	3.20	129.69	123.67
5	A	312	CHL	O2A-CGA-CBA	3.20	121.66	111.90
5	C	310	CHL	CHD-C4C-NC	3.21	129.71	123.67
5	C	310	CHL	O2A-CGA-CBA	3.25	121.79	111.90
6	B	308	CLA	C9-C8-C10	3.28	123.67	111.08
6	A	316	CLA	C4-C3-C5	3.28	120.42	115.41
3	C	303	NEX	C26-O24-C25	3.31	65.15	61.25
5	C	309	CHL	CHD-C4C-NC	3.31	129.91	123.67
6	A	317	CLA	O2A-CGA-CBA	3.32	122.01	111.90
5	B	309	CHL	CHD-C4C-NC	3.36	130.00	123.67
6	A	307	CLA	C4-C3-C5	3.37	120.56	115.41
5	B	313	CHL	C4-C3-C5	3.38	120.56	115.41
5	B	312	CHL	CHD-C4C-NC	3.39	130.06	123.67
5	C	311	CHL	CHD-C4C-NC	3.40	130.07	123.67
2	A	301	LUT	C38-C25-C26	3.41	118.59	116.04
5	A	312	CHL	C4A-NA-C1A	3.41	110.06	106.04
6	B	314	CLA	CHC-C1C-NC	3.42	130.10	123.67
5	A	311	CHL	CHD-C4C-NC	3.42	130.11	123.67
4	B	304	LHG	O7-C7-C8	3.42	118.96	111.53
6	C	316	CLA	O2A-CGA-CBA	3.43	122.36	111.90
3	A	303	NEX	C26-O24-C25	3.44	65.31	61.25
5	A	310	CHL	CHD-C4C-NC	3.48	130.22	123.67
5	B	313	CHL	CHD-C4C-NC	3.50	130.25	123.67
6	A	315	CLA	CHC-C1C-NC	3.54	130.32	123.67
6	C	314	CLA	O2A-CGA-CBA	3.55	122.71	111.90
5	C	313	CHL	O2A-CGA-CBA	3.58	122.80	111.90
5	A	312	CHL	CHD-C4C-NC	3.61	130.46	123.67
5	C	312	CHL	CHD-C4C-NC	3.66	130.55	123.67
6	A	308	CLA	CHC-C1C-NC	3.66	130.56	123.67
5	A	305	CHL	O2A-CGA-CBA	3.66	123.06	111.90
2	C	302	LUT	C1-C2-C3	3.67	122.03	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	LUT	C40-C33-C32	3.69	124.23	118.10
5	B	311	CHL	CHD-C4C-NC	3.69	130.62	123.67
2	A	302	LUT	C1-C2-C3	3.73	122.17	113.41
5	B	310	CHL	CHD-C4C-NC	3.80	130.81	123.67
2	C	302	LUT	C15-C14-C13	3.80	132.69	127.20
5	B	305	CHL	O2D-CGD-CBD	3.81	116.52	111.30
3	B	303	NEX	C26-O24-C25	3.87	65.81	61.25
5	C	305	CHL	O2A-CGA-CBA	3.88	123.74	111.90
5	C	312	CHL	O2A-CGA-CBA	3.89	123.76	111.90
6	C	306	CLA	C4-C3-C5	3.89	121.35	115.41
5	C	313	CHL	CHD-C4C-NC	3.91	131.02	123.67
2	B	302	LUT	C1-C2-C3	3.92	122.62	113.41
6	C	306	CLA	C9-C8-C7	3.97	126.34	111.08
5	B	305	CHL	O2A-CGA-CBA	3.99	124.07	111.90
2	C	302	LUT	C7-C8-C9	4.01	132.32	126.22
4	B	304	LHG	O8-C23-C24	4.02	124.14	111.90
2	A	301	LUT	C31-C30-C29	4.23	133.31	127.20
2	B	301	LUT	C31-C30-C29	4.24	133.31	127.20
5	B	305	CHL	CHD-C4C-NC	4.33	131.82	123.67
5	A	305	CHL	CHD-C4C-NC	4.58	132.28	123.67
5	C	305	CHL	O2D-CGD-CBD	4.81	117.90	111.30
6	A	317	CLA	O2D-CGD-CBD	4.88	117.99	111.30
6	B	314	CLA	O2D-CGD-CBD	5.01	118.18	111.30
5	A	313	CHL	O2D-CGD-CBD	5.17	118.39	111.30
6	A	306	CLA	C9-C8-C7	5.28	131.39	111.08
2	B	302	LUT	C38-C25-C26	5.31	120.01	116.04
6	B	317	CLA	O2D-CGD-CBD	5.34	118.63	111.30
6	A	314	CLA	O2D-CGD-CBD	5.36	118.66	111.30
5	A	305	CHL	O2D-CGD-CBD	5.42	118.74	111.30
2	C	301	LUT	C38-C25-C26	5.60	120.23	116.04
6	C	317	CLA	O2D-CGD-CBD	5.67	119.08	111.30
5	A	312	CHL	O2D-CGD-CBD	5.75	119.19	111.30
5	B	313	CHL	O2D-CGD-CBD	5.80	119.26	111.30
5	C	313	CHL	O2D-CGD-CBD	6.01	119.54	111.30
6	C	314	CLA	O2D-CGD-CBD	6.25	119.87	111.30
5	B	312	CHL	O2D-CGD-CBD	6.27	119.90	111.30
5	A	310	CHL	O2D-CGD-CBD	6.29	119.93	111.30
6	A	316	CLA	O2D-CGD-CBD	6.33	119.98	111.30
6	C	315	CLA	O2D-CGD-CBD	6.35	120.01	111.30
6	A	315	CLA	O2D-CGD-CBD	6.57	120.31	111.30
5	A	311	CHL	O2D-CGD-CBD	6.63	120.40	111.30
5	C	309	CHL	O2D-CGD-CBD	6.79	120.61	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	308	CLA	O2D-CGD-CBD	7.03	120.95	111.30
5	B	309	CHL	O2D-CGD-CBD	7.19	121.17	111.30
6	C	318	CLA	O2D-CGD-CBD	7.23	121.22	111.30
5	C	310	CHL	O2D-CGD-CBD	7.42	121.48	111.30
5	B	310	CHL	O2D-CGD-CBD	7.53	121.63	111.30
6	C	308	CLA	O2D-CGD-CBD	7.58	121.71	111.30
6	A	307	CLA	O2D-CGD-CBD	7.59	121.72	111.30
6	C	307	CLA	O2D-CGD-CBD	7.62	121.75	111.30
2	C	302	LUT	C38-C25-C26	7.76	121.84	116.04
5	B	311	CHL	O2D-CGD-CBD	7.80	122.00	111.30
6	B	318	CLA	O2D-CGD-CBD	7.82	122.02	111.30
6	A	318	CLA	O2D-CGD-CBD	7.84	122.05	111.30
5	A	309	CHL	O2D-CGD-CBD	7.84	122.06	111.30
5	C	311	CHL	O2D-CGD-CBD	7.96	122.22	111.30
6	C	316	CLA	O2D-CGD-CBD	7.98	122.24	111.30
6	C	306	CLA	O2D-CGD-CBD	8.05	122.35	111.30
5	C	312	CHL	O2D-CGD-CBD	8.25	122.62	111.30
6	B	315	CLA	O2D-CGD-CBD	8.26	122.64	111.30
6	B	306	CLA	O2D-CGD-CBD	8.34	122.74	111.30
6	B	316	CLA	O2D-CGD-CBD	8.60	123.09	111.30
6	A	306	CLA	O2D-CGD-CBD	8.81	123.38	111.30
6	B	308	CLA	O2D-CGD-CBD	8.81	123.39	111.30
6	B	307	CLA	O2D-CGD-CBD	9.39	124.18	111.30

All (50) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	314	CLA	NC
6	C	314	CLA	NA
6	B	316	CLA	NC
6	B	316	CLA	ND
6	B	316	CLA	NA
6	A	308	CLA	NC
6	A	308	CLA	NA
6	A	318	CLA	NC
6	A	318	CLA	NA
6	B	314	CLA	NC
6	B	314	CLA	NA
6	B	315	CLA	NC
6	B	315	CLA	NA
6	C	306	CLA	NC
6	C	306	CLA	NA

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Mol	Chain	Res	Type	Atom
6	B	306	CLA	NC
6	B	306	CLA	NA
6	A	314	CLA	NC
6	A	314	CLA	NA
6	C	316	CLA	NC
6	C	316	CLA	NA
6	C	307	CLA	NC
6	C	307	CLA	NA
6	C	317	CLA	NC
6	C	317	CLA	NA
6	B	308	CLA	NC
6	B	308	CLA	NA
6	B	317	CLA	NC
6	B	317	CLA	NA
6	C	318	CLA	NC
6	C	318	CLA	NA
6	B	307	CLA	NC
6	B	307	CLA	NA
6	C	315	CLA	NC
6	C	315	CLA	NA
6	A	317	CLA	NC
6	A	317	CLA	NA
6	A	307	CLA	NC
6	A	307	CLA	ND
6	A	307	CLA	NA
6	B	318	CLA	NC
6	B	318	CLA	NA
6	A	306	CLA	NC
6	A	306	CLA	NA
6	A	316	CLA	NC
6	A	316	CLA	NA
6	C	308	CLA	NC
6	C	308	CLA	NA
6	A	315	CLA	NC
6	A	315	CLA	NA

There are no torsion outliers.

There are no ring outliers.

51 monomers are involved in 204 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	LUT	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	302	LUT	1	0
3	A	303	NEX	3	0
4	A	304	LHG	9	0
5	A	305	CHL	7	0
6	A	306	CLA	7	0
6	A	307	CLA	18	0
5	A	309	CHL	2	0
5	A	310	CHL	2	0
5	A	311	CHL	3	0
5	A	312	CHL	5	0
5	A	313	CHL	6	0
6	A	314	CLA	10	0
6	A	315	CLA	3	0
6	A	316	CLA	4	0
6	A	317	CLA	7	0
6	A	318	CLA	1	0
2	B	301	LUT	9	0
2	B	302	LUT	6	0
3	B	303	NEX	3	0
4	B	304	LHG	5	0
5	B	305	CHL	10	0
6	B	306	CLA	12	0
6	B	307	CLA	16	0
6	B	308	CLA	1	0
5	B	309	CHL	1	0
5	B	310	CHL	2	0
5	B	311	CHL	4	0
5	B	312	CHL	3	0
5	B	313	CHL	3	0
6	B	314	CLA	9	0
6	B	315	CLA	5	0
6	B	316	CLA	7	0
6	B	317	CLA	3	0
6	B	318	CLA	1	0
2	C	301	LUT	2	0
2	C	302	LUT	5	0
3	C	303	NEX	3	0
4	C	304	LHG	5	0
5	C	305	CHL	8	0
6	C	306	CLA	15	0
6	C	307	CLA	23	0
5	C	310	CHL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	311	CHL	3	0
5	C	312	CHL	5	0
5	C	313	CHL	5	0
6	C	314	CLA	7	0
6	C	315	CLA	2	0
6	C	316	CLA	2	0
6	C	317	CLA	4	0
6	C	318	CLA	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	208/224 (92%)	0.04	16 (7%) 16 11	6, 39, 77, 97	0
1	B	208/224 (92%)	-0.14	7 (3%) 49 41	8, 34, 67, 94	0
1	C	208/224 (92%)	-0.17	10 (4%) 34 27	6, 33, 69, 107	0
All	All	624/672 (92%)	-0.09	33 (5%) 30 23	6, 35, 70, 107	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	GLY	4.5
1	B	88	ASN	4.5
1	C	217	VAL	4.5
1	B	89	GLY	4.5
1	A	213	LEU	4.2
1	A	88	ASN	4.0
1	A	214	ALA	3.8
1	C	213	LEU	3.3
1	C	214	ALA	3.3
1	C	219	ASN	3.1
1	C	147	PRO	3.1
1	B	214	ALA	3.1
1	C	218	ASN	3.1
1	A	216	PRO	3.0
1	B	152	VAL	2.9
1	A	81	PHE	2.8
1	A	212	HIS	2.8
1	A	31	GLU	2.8
1	A	87	ARG	2.7
1	A	168	ASP	2.6
1	B	87	ARG	2.6
1	A	219	ASN	2.4
1	A	217	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	218	ASN	2.3
1	B	117	SER	2.3
1	A	210	ALA	2.2
1	B	218	ASN	2.2
1	C	31	GLU	2.2
1	C	20	ASP	2.2
1	C	215	ASP	2.2
1	C	89	GLY	2.1
1	A	215	ASP	2.1
1	A	20	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	LHG	B	304	49/49	0.94	0.20	4.69	14,40,98,107	0
3	NEX	A	303	44/44	0.91	0.22	3.62	26,39,94,96	0
6	CLA	A	307	65/65	0.97	0.21	3.50	10,20,81,93	0
6	CLA	B	307	65/65	0.96	0.20	3.39	9,20,82,94	0
3	NEX	B	303	44/44	0.88	0.23	3.33	26,42,94,97	0
6	CLA	C	307	65/65	0.97	0.21	2.99	6,18,80,92	0
6	CLA	C	306	65/65	0.97	0.17	2.72	7,19,41,60	0
4	LHG	A	304	49/49	0.94	0.18	2.56	19,42,98,108	0
4	LHG	C	304	49/49	0.96	0.18	2.43	16,42,96,107	0
6	CLA	B	316	65/65	0.93	0.25	2.27	28,41,89,99	0
6	CLA	A	306	65/65	0.96	0.17	2.15	13,21,43,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CHL	C	311	66/66	0.92	0.19	2.14	11,31,94,115	0
5	CHL	C	313	66/66	0.95	0.18	2.06	5,21,66,80	0
5	CHL	B	313	66/66	0.96	0.17	1.95	14,28,69,85	0
6	CLA	B	306	65/65	0.97	0.16	1.71	9,19,39,58	0
5	CHL	A	313	66/66	0.96	0.16	1.62	14,25,68,82	0
2	LUT	B	302	42/42	0.96	0.16	1.38	6,19,32,35	0
5	CHL	B	311	66/66	0.93	0.18	1.38	21,38,99,119	0
6	CLA	B	315	65/65	0.92	0.23	1.33	20,43,74,83	0
6	CLA	C	314	65/65	0.94	0.19	1.14	15,27,79,93	0
5	CHL	A	309	48/66	0.94	0.26	1.09	32,48,95,101	0
2	LUT	C	302	42/42	0.98	0.15	1.07	6,16,30,35	0
6	CLA	B	314	65/65	0.94	0.20	1.06	24,31,80,96	0
5	CHL	A	305	66/66	0.93	0.18	1.06	17,32,86,104	0
5	CHL	A	311	66/66	0.92	0.18	1.06	19,37,99,119	0
5	CHL	C	309	48/66	0.92	0.22	0.98	26,43,97,104	0
6	CLA	C	315	65/65	0.93	0.20	0.94	21,45,74,87	0
2	LUT	A	302	42/42	0.96	0.16	0.73	7,21,31,37	0
5	CHL	B	309	48/66	0.93	0.23	0.63	35,52,99,105	0
6	CLA	B	318	41/65	0.88	0.24	0.61	44,76,92,115	0
5	CHL	C	305	66/66	0.95	0.16	0.61	14,34,87,104	0
3	NEX	C	303	44/44	0.91	0.20	0.57	14,32,90,92	0
5	CHL	B	305	66/66	0.95	0.16	0.53	8,26,81,100	0
5	CHL	A	310	51/66	0.95	0.16	0.52	21,36,94,100	0
6	CLA	C	316	65/65	0.93	0.20	0.50	22,37,84,97	0
6	CLA	A	314	65/65	0.94	0.18	0.43	23,34,78,93	0
6	CLA	A	315	65/65	0.91	0.21	0.37	28,48,76,86	0
2	LUT	C	301	42/42	0.95	0.17	0.35	15,22,35,57	0
6	CLA	A	318	41/65	0.85	0.31	0.28	44,79,96,119	0
6	CLA	C	308	62/65	0.94	0.16	0.09	12,28,80,87	0
5	CHL	B	312	66/66	0.95	0.15	0.08	22,40,71,83	0
6	CLA	B	317	65/65	0.95	0.17	0.05	14,30,85,94	0
6	CLA	C	317	65/65	0.95	0.16	-0.00	16,31,87,95	0
6	CLA	A	316	65/65	0.92	0.21	-0.01	30,41,88,98	0
6	CLA	B	308	62/65	0.94	0.18	-0.03	21,37,83,91	0
6	CLA	A	317	65/65	0.94	0.18	-0.06	21,37,90,99	0
6	CLA	C	318	40/65	0.90	0.23	-0.08	36,69,91,110	0
5	CHL	C	312	66/66	0.94	0.16	-0.11	9,32,66,79	0
5	CHL	A	312	66/66	0.95	0.14	-0.16	19,36,68,81	0
2	LUT	B	301	42/42	0.96	0.14	-0.18	18,26,42,62	0
5	CHL	C	310	51/66	0.96	0.13	-0.22	13,27,89,94	0
6	CLA	A	308	62/65	0.93	0.17	-0.26	20,35,82,89	0
5	CHL	B	310	51/66	0.96	0.13	-0.27	20,32,92,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	LUT	A	301	42/42	0.96	0.15	-0.51	20,25,39,61	0
7	CAC	A	319	5/5	0.98	0.17	-0.82	57,59,68,81	0
7	CAC	B	319	5/5	0.98	0.17	-0.94	59,62,68,97	0
9	NA	C	323	1/1	0.96	0.23	-	68,68,68,68	0
8	ZN	B	321	1/1	0.98	0.12	-	66,66,66,66	0
9	NA	C	322	1/1	-0.08	0.40	-	80,80,80,80	1
9	NA	B	320	1/1	0.99	0.05	-	42,42,42,42	0
8	ZN	A	320	1/1	0.98	0.09	-	98,98,98,98	0
9	NA	C	320	1/1	0.84	0.22	-	60,60,60,60	0
7	CAC	C	319	5/5	0.97	0.18	-	57,62,79,156	0
9	NA	B	322	1/1	0.91	0.17	-	47,47,47,47	0
8	ZN	A	322	1/1	0.92	0.21	-	122,122,122,122	0
8	ZN	C	321	1/1	0.96	0.13	-	64,64,64,64	0
8	ZN	A	321	1/1	0.98	0.09	-	56,56,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.