



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 24, 2019 – 06:34 PM EDT

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

This is a wwPDB X-ray Structure Validation Summary 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

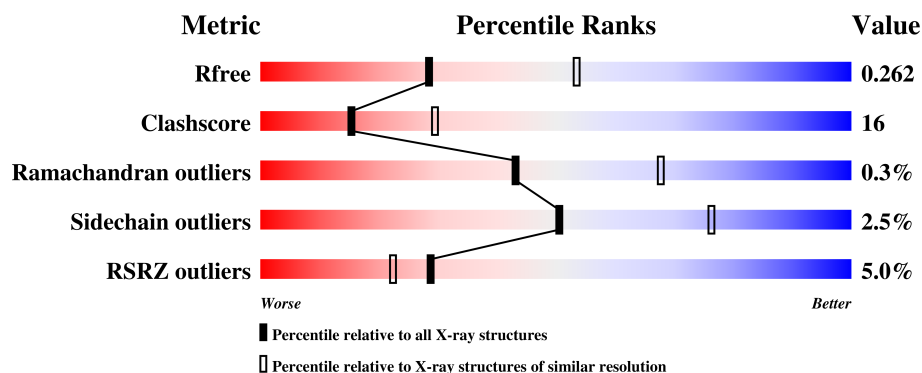
# 1 Overall quality at a glance

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))
$R_{free}$	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (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>6%</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
5	CHL	A	305	X	-	-	-
5	CHL	A	309	X	-	-	-
5	CHL	A	310	X	-	-	-
5	CHL	A	311	X	-	-	-
5	CHL	A	312	X	-	-	-
5	CHL	A	313	X	-	-	-
5	CHL	B	305	X	-	-	-
5	CHL	B	309	X	-	-	-
5	CHL	B	310	X	-	-	-
5	CHL	B	311	X	-	-	-
5	CHL	B	312	X	-	-	-
5	CHL	B	313	X	-	-	-
5	CHL	C	305	X	-	-	-
5	CHL	C	309	X	-	-	-
5	CHL	C	310	X	-	-	-
5	CHL	C	311	X	-	-	-
5	CHL	C	312	X	-	-	-
5	CHL	C	313	X	-	-	-
6	CLA	A	306	X	-	-	-
6	CLA	A	307	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	-	-	-
6	CLA	B	308	X	-	-	-
6	CLA	B	314	X	-	-	-
6	CLA	B	315	X	-	-	-
6	CLA	B	316	X	-	-	-
6	CLA	B	317	X	-	-	-
6	CLA	B	318	X	-	-	-
6	CLA	C	306	X	-	-	-
6	CLA	C	307	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 ⓘ

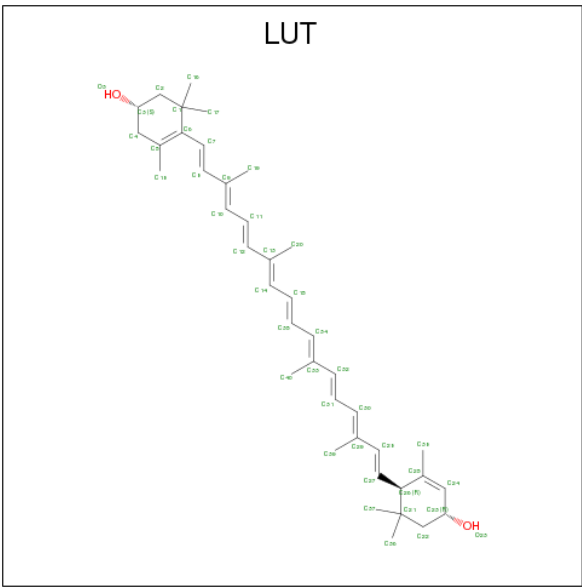
There are 10 unique types of molecules in this entry. The entry contains 8016 atoms, of which 0 are hydrogens and 0 are deuteriums.

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>).



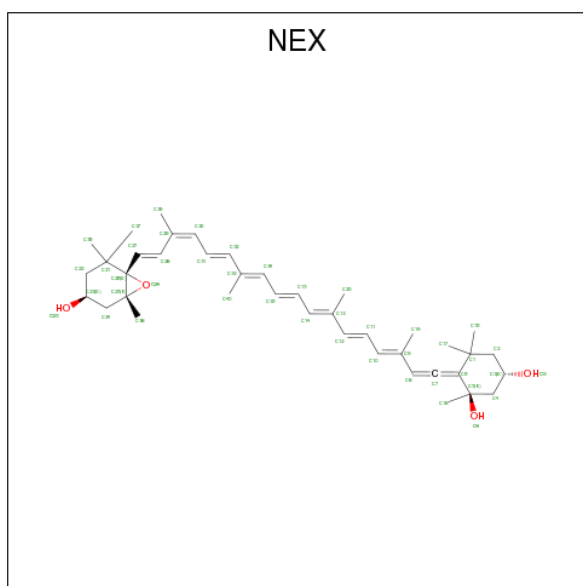
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			42	40	2		
2	A	1	Total	C	O	0	0
			42	40	2		
2	B	1	Total	C	O	0	0
			42	40	2		

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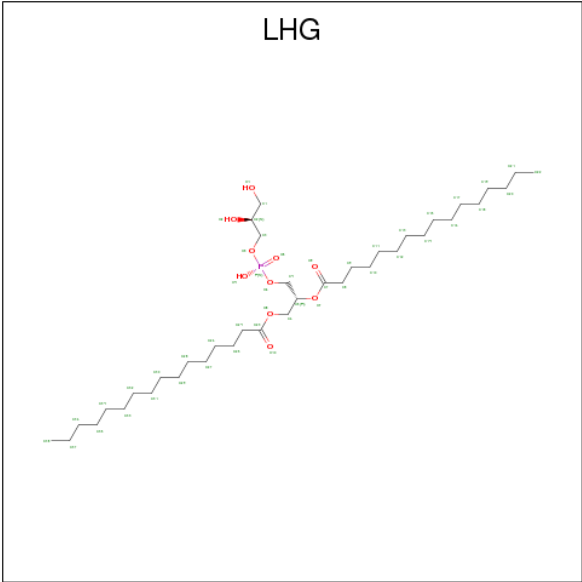
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		
2	C	1	Total	C	O	0	0
			42	40	2		

- 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>).



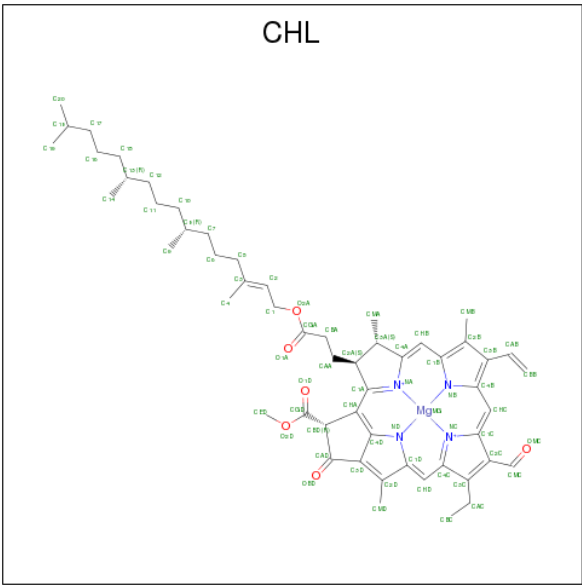
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			44	40	4		
3	B	1	Total	C	O	0	0
			44	40	4		
3	C	1	Total	C	O	0	0
			44	40	4		

- 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>).



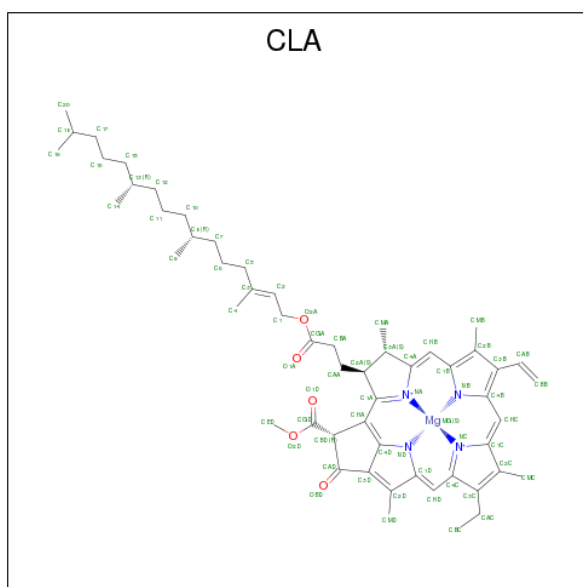
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Mg	N	O	0	0
			66	55	1	4	6		

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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 65	C 55	Mg 1	N 4	O 5	0	0
6	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	A	1	Total 62	C 52	Mg 1	N 4	O 5	0	0
6	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	A	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
6	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	B	1	Total 62	C 52	Mg 1	N 4	O 5	0	0
6	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
6	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

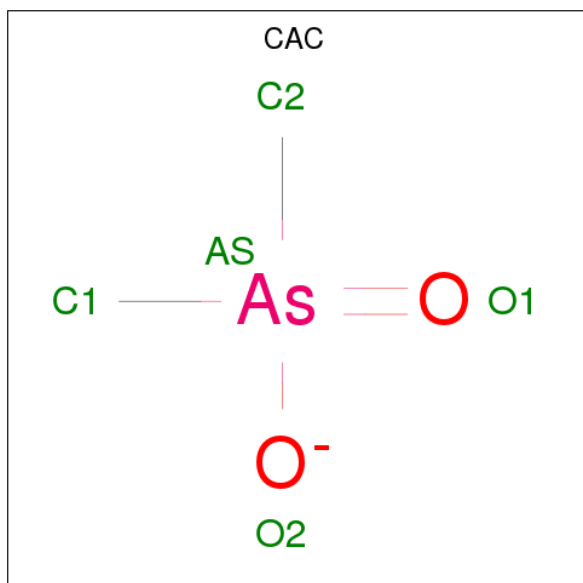
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
6	C	1	Total	C	Mg	N	O	0	0
			62	52	1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

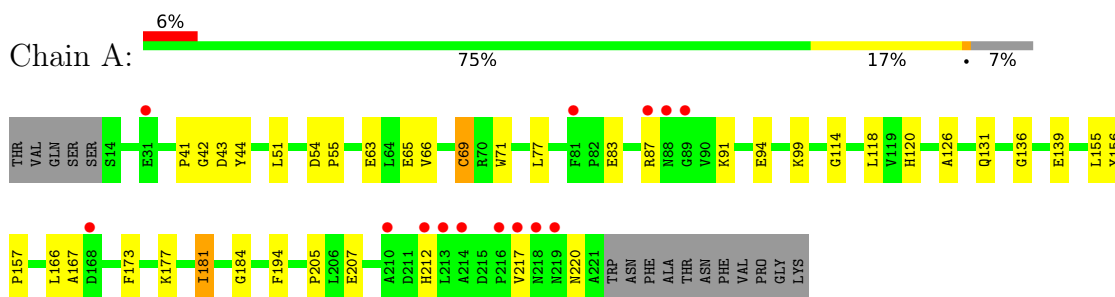
- Molecule 10 is water.

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		

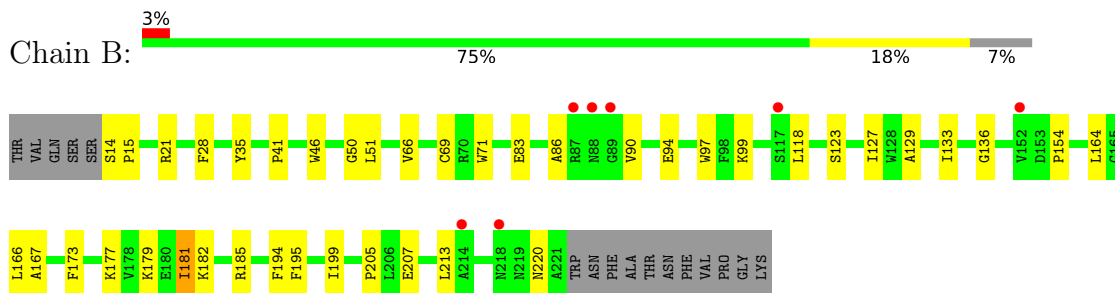
### 3 Residue-property plots [i](#)

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

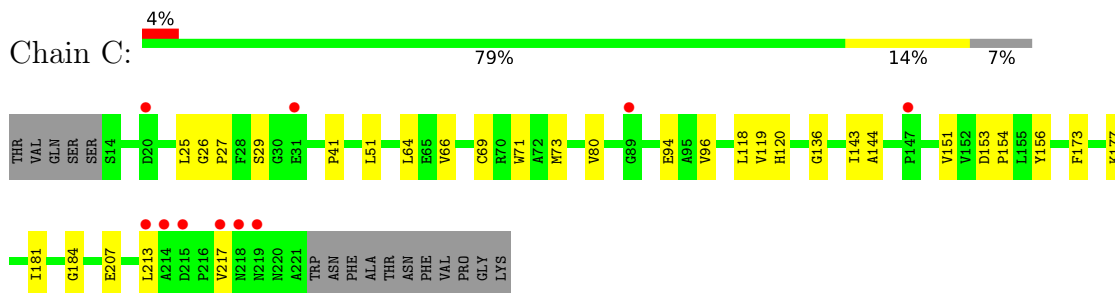
- Molecule 1: Major chlorophyll a/b binding protein LHCb1.3



- 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>	3.69 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.250 , 0.258 0.241 , 0.262	Depositor DCC
$R_{free}$ test set	3046 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 75.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	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 18.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 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.

The worst 5 of 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

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%)	31	56
1	B	206/224 (92%)	199 (97%)	7 (3%)	0	100	100
1	C	206/224 (92%)	198 (96%)	7 (3%)	1 (0%)	31	56
All	All	618/672 (92%)	596 (96%)	20 (3%)	2 (0%)	43	68

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%)	60	82
1	B	160/174 (92%)	157 (98%)	3 (2%)	60	82
1	C	160/174 (92%)	154 (96%)	6 (4%)	36	63
All	All	480/522 (92%)	468 (98%)	12 (2%)	50	76

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	220	ASN

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Mol	Chain	Res	Type
1	C	80	VAL
1	C	181	ILE
1	B	207	GLU
1	C	96	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	-	42,43,43	0.89	1 (2%)	51,60,60	1.54	10 (19%)
2	LUT	A	302	-	42,43,43	0.92	3 (7%)	51,60,60	1.53	8 (15%)
3	NEX	A	303	-	38,46,46	0.96	1 (2%)	50,70,70	3.03	17 (34%)
4	LHG	A	304	6	48,48,48	0.91	2 (4%)	51,54,54	1.00	2 (3%)
5	CHL	A	305	1	57,74,74	2.04	12 (21%)	63,114,114	2.02	18 (28%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	CLA	A	306	1	57,73,73	2.19	13 (22%)	66,113,113	2.06	15 (22%)
6	CLA	A	307	1	57,73,73	2.11	13 (22%)	66,113,113	1.90	20 (30%)
6	CLA	A	308	10	54,70,73	2.78	12 (22%)	62,109,113	2.10	16 (25%)
5	CHL	A	309	1	39,56,74	2.75	13 (33%)	41,92,114	2.24	13 (31%)
5	CHL	A	310	10	42,59,74	2.92	12 (28%)	45,96,114	2.19	14 (31%)
5	CHL	A	311	10	57,74,74	2.30	12 (21%)	63,114,114	1.79	11 (17%)
5	CHL	A	312	10	57,74,74	2.36	12 (21%)	63,114,114	1.87	12 (19%)
5	CHL	A	313	1	57,74,74	2.24	14 (24%)	63,114,114	1.69	12 (19%)
6	CLA	A	314	1	57,73,73	2.49	13 (22%)	66,113,113	1.85	15 (22%)
6	CLA	A	315	4	57,73,73	2.53	15 (26%)	66,113,113	1.99	19 (28%)
6	CLA	A	316	1	57,73,73	2.96	11 (19%)	66,113,113	1.89	13 (19%)
6	CLA	A	317	1	57,73,73	2.14	13 (22%)	66,113,113	1.75	17 (25%)
6	CLA	A	318	1	33,49,73	3.19	14 (42%)	37,84,113	2.10	9 (24%)
7	CAC	A	319	8	0,4,4	0.00	-	0,6,6	0.00	-
2	LUT	B	301	-	42,43,43	0.90	0	51,60,60	1.71	14 (27%)
2	LUT	B	302	-	42,43,43	1.05	3 (7%)	51,60,60	1.69	13 (25%)
3	NEX	B	303	-	38,46,46	0.96	2 (5%)	50,70,70	3.01	17 (34%)
4	LHG	B	304	6	48,48,48	0.97	2 (4%)	51,54,54	1.08	3 (5%)
5	CHL	B	305	1	57,74,74	2.44	12 (21%)	63,114,114	2.03	16 (25%)
6	CLA	B	306	1	57,73,73	2.29	13 (22%)	66,113,113	2.03	19 (28%)
6	CLA	B	307	1	57,73,73	2.39	13 (22%)	66,113,113	1.90	14 (21%)
6	CLA	B	308	10	54,70,73	2.79	13 (24%)	62,109,113	2.09	14 (22%)
5	CHL	B	309	1	39,56,74	2.67	12 (30%)	41,92,114	2.12	13 (31%)
5	CHL	B	310	10	42,59,74	2.68	12 (28%)	45,96,114	2.33	15 (33%)
5	CHL	B	311	10	57,74,74	2.02	13 (22%)	63,114,114	1.98	13 (20%)
5	CHL	B	312	10	57,74,74	2.13	14 (24%)	63,114,114	1.74	16 (25%)
5	CHL	B	313	1	57,74,74	2.30	10 (17%)	63,114,114	1.70	14 (22%)
6	CLA	B	314	1	57,73,73	2.30	12 (21%)	66,113,113	1.86	15 (22%)
6	CLA	B	315	4	57,73,73	2.49	12 (21%)	66,113,113	2.07	17 (25%)
6	CLA	B	316	1	57,73,73	2.63	12 (21%)	66,113,113	1.99	13 (19%)
6	CLA	B	317	1	57,73,73	2.19	10 (17%)	66,113,113	1.71	13 (19%)
6	CLA	B	318	1	33,49,73	3.25	14 (42%)	37,84,113	2.20	11 (29%)
7	CAC	B	319	8	0,4,4	0.00	-	0,6,6	0.00	-
2	LUT	C	301	-	42,43,43	1.02	1 (2%)	51,60,60	1.90	15 (29%)
2	LUT	C	302	-	42,43,43	0.85	1 (2%)	51,60,60	1.70	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NEX	C	303	-	38,46,46	1.01	1 (2%)	50,70,70	3.13	17 (34%)
4	LHG	C	304	6	48,48,48	0.94	2 (4%)	51,54,54	1.02	4 (7%)
5	CHL	C	305	1	57,74,74	2.19	13 (22%)	63,114,114	1.90	17 (26%)
6	CLA	C	306	1	57,73,73	2.60	13 (22%)	66,113,113	2.00	20 (30%)
6	CLA	C	307	1	57,73,73	2.20	14 (24%)	66,113,113	1.98	21 (31%)
6	CLA	C	308	10	54,70,73	2.26	12 (22%)	62,109,113	1.99	18 (29%)
5	CHL	C	309	1	39,56,74	2.77	13 (33%)	41,92,114	2.03	12 (29%)
5	CHL	C	310	10	42,59,74	2.57	14 (33%)	45,96,114	2.26	15 (33%)
5	CHL	C	311	10	57,74,74	2.04	13 (22%)	63,114,114	1.99	17 (26%)
5	CHL	C	312	10	57,74,74	2.40	12 (21%)	63,114,114	1.99	18 (28%)
5	CHL	C	313	1	57,74,74	2.12	13 (22%)	63,114,114	1.79	15 (23%)
6	CLA	C	314	1	57,73,73	2.37	12 (21%)	66,113,113	1.90	18 (27%)
6	CLA	C	315	4	57,73,73	2.61	14 (24%)	66,113,113	1.89	17 (25%)
6	CLA	C	316	1	57,73,73	2.57	12 (21%)	66,113,113	1.93	13 (19%)
6	CLA	C	317	1	57,73,73	2.36	14 (24%)	66,113,113	1.77	16 (24%)
6	CLA	C	318	1	31,48,73	3.14	13 (41%)	35,82,113	2.15	11 (31%)
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	4/4/20/26	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
5	CHL	A	309	1	3/3/16/26	0/18/116/137	0/0/9/9
5	CHL	A	310	10	3/3/17/26	0/21/119/137	0/0/9/9
5	CHL	A	311	10	4/4/20/26	0/39/137/137	0/0/9/9
5	CHL	A	312	10	4/4/20/26	0/39/137/137	0/0/9/9
5	CHL	A	313	1	4/4/20/26	0/39/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	4/4/20/26	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	3/3/16/26	0/18/116/137	0/0/9/9
5	CHL	B	310	10	3/3/17/26	0/21/119/137	0/0/9/9
5	CHL	B	311	10	4/4/20/26	0/39/137/137	0/0/9/9
5	CHL	B	312	10	4/4/20/26	0/39/137/137	0/0/9/9
5	CHL	B	313	1	4/4/20/26	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	4/4/20/26	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
5	CHL	C	309	1	3/3/16/26	0/18/116/137	0/0/9/9
5	CHL	C	310	10	3/3/17/26	0/21/119/137	0/0/9/9
5	CHL	C	311	10	4/4/20/26	0/39/137/137	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHL	C	312	10	4/4/20/26	0/39/137/137	0/0/9/9
5	CHL	C	313	1	4/4/20/26	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

The worst 5 of 552 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	312	CHL	C3B-C2B	-9.44	1.27	1.40
5	B	305	CHL	C3B-C2B	-8.63	1.28	1.40
6	B	307	CLA	C3B-C2B	-8.08	1.29	1.40
6	B	308	CLA	C3B-C2B	-8.03	1.29	1.40
5	A	309	CHL	C3B-C2B	-6.93	1.30	1.40

The worst 5 of 766 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	303	NEX	C35-C34-C33	-6.56	117.94	127.31
3	B	303	NEX	C38-C25-C26	-6.08	112.03	122.31
3	C	303	NEX	C35-C34-C33	-5.95	118.82	127.31
3	A	303	NEX	C38-C25-C26	-5.38	113.22	122.31
3	C	303	NEX	C38-C25-C26	-5.32	113.32	122.31

5 of 116 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	314	CLA	NC
6	C	314	CLA	NA
5	A	310	CHL	NC
5	A	310	CHL	ND
5	A	310	CHL	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
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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	0.01	14 (6%) 18 13	6, 39, 77, 97	0
1	B	208/224 (92%)	-0.17	7 (3%) 45 37	8, 34, 67, 94	0
1	C	208/224 (92%)	-0.20	10 (4%) 30 23	6, 33, 69, 107	0
All	All	624/672 (92%)	-0.12	31 (4%) 29 22	6, 35, 70, 107	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89	GLY	4.5
1	C	217	VAL	4.5
1	B	89	GLY	4.5
1	B	88	ASN	4.4
1	A	213	LEU	4.2

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
9	NA	C	322	1/1	-0.09	0.39	80,80,80,80	1
9	NA	C	320	1/1	0.84	0.21	60,60,60,60	0
6	CLA	A	318	41/65	0.85	0.31	44,79,96,119	0
6	CLA	B	318	41/65	0.88	0.24	44,76,92,115	0
3	NEX	B	303	44/44	0.88	0.23	26,42,94,97	0
3	NEX	C	303	44/44	0.91	0.20	14,32,90,92	0
6	CLA	C	318	40/65	0.91	0.23	36,69,91,110	0
3	NEX	A	303	44/44	0.91	0.22	26,39,94,96	0
9	NA	B	322	1/1	0.91	0.17	47,47,47,47	0
6	CLA	A	315	65/65	0.91	0.21	28,48,76,86	0
6	CLA	B	315	65/65	0.92	0.23	20,43,74,83	0
5	CHL	A	311	66/66	0.92	0.18	19,37,99,119	0
6	CLA	A	316	65/65	0.92	0.21	30,41,88,98	0
8	ZN	A	322	1/1	0.92	0.21	122,122,122,122	0
5	CHL	C	309	48/66	0.92	0.22	26,43,97,104	0
5	CHL	C	311	66/66	0.92	0.19	11,31,94,115	0
6	CLA	C	315	65/65	0.93	0.20	21,45,74,87	0
6	CLA	A	308	62/65	0.93	0.17	20,35,82,89	0
5	CHL	B	311	66/66	0.93	0.18	21,38,99,119	0
6	CLA	C	316	65/65	0.93	0.20	22,37,84,97	0
5	CHL	A	305	66/66	0.93	0.18	17,32,86,104	0
6	CLA	B	316	65/65	0.93	0.25	28,41,89,99	0
5	CHL	B	309	48/66	0.93	0.23	35,52,99,105	0
5	CHL	A	309	48/66	0.94	0.26	32,48,95,101	0
4	LHG	B	304	49/49	0.94	0.20	14,40,98,107	0
6	CLA	A	317	65/65	0.94	0.18	21,37,90,99	0
4	LHG	A	304	49/49	0.94	0.18	19,42,98,108	0
6	CLA	C	314	65/65	0.94	0.19	15,27,79,93	0
6	CLA	A	314	65/65	0.94	0.18	23,34,78,93	0
6	CLA	C	308	62/65	0.94	0.16	12,28,80,87	0
6	CLA	B	308	62/65	0.94	0.18	21,37,83,91	0
6	CLA	B	314	65/65	0.94	0.20	24,31,80,96	0
5	CHL	C	312	66/66	0.94	0.16	9,32,66,79	0
5	CHL	A	312	66/66	0.95	0.14	19,36,68,81	0
5	CHL	B	305	66/66	0.95	0.16	8,26,81,100	0
6	CLA	C	317	65/65	0.95	0.16	16,31,87,95	0
5	CHL	B	312	66/66	0.95	0.15	22,40,71,83	0
6	CLA	B	317	65/65	0.95	0.17	14,30,85,94	0
5	CHL	A	310	51/66	0.95	0.16	21,36,94,100	0
5	CHL	C	305	66/66	0.95	0.16	14,34,87,104	0
2	LUT	C	301	42/42	0.95	0.17	15,22,35,57	0
5	CHL	C	313	66/66	0.95	0.18	5,21,66,80	0
2	LUT	A	301	42/42	0.96	0.15	20,25,39,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	LHG	C	304	49/49	0.96	0.18	16,42,96,107	0
8	ZN	C	321	1/1	0.96	0.13	64,64,64,64	0
2	LUT	B	301	42/42	0.96	0.15	18,26,42,62	0
5	CHL	C	310	51/66	0.96	0.13	13,27,89,94	0
6	CLA	A	306	65/65	0.96	0.17	13,21,43,63	0
2	LUT	A	302	42/42	0.96	0.16	7,21,31,37	0
5	CHL	B	310	51/66	0.96	0.13	20,32,92,97	0
2	LUT	B	302	42/42	0.96	0.16	6,19,32,35	0
6	CLA	B	307	65/65	0.96	0.20	9,20,82,94	0
5	CHL	B	313	66/66	0.96	0.17	14,28,69,85	0
5	CHL	A	313	66/66	0.96	0.16	14,25,68,82	0
9	NA	C	323	1/1	0.96	0.22	68,68,68,68	0
6	CLA	C	307	65/65	0.97	0.21	6,18,80,92	0
6	CLA	B	306	65/65	0.97	0.16	9,19,39,58	0
7	CAC	C	319	5/5	0.97	0.18	57,62,79,156	0
6	CLA	C	306	65/65	0.97	0.17	7,19,41,60	0
6	CLA	A	307	65/65	0.97	0.21	10,20,81,93	0
7	CAC	A	319	5/5	0.98	0.17	57,59,68,81	0
7	CAC	B	319	5/5	0.98	0.17	59,62,68,97	0
8	ZN	B	321	1/1	0.98	0.12	66,66,66,66	0
2	LUT	C	302	42/42	0.98	0.15	6,16,30,35	0
8	ZN	A	321	1/1	0.98	0.09	56,56,56,56	0
8	ZN	A	320	1/1	0.98	0.09	98,98,98,98	0
9	NA	B	320	1/1	0.99	0.05	42,42,42,42	0

## 6.5 Other polymers

There are no such residues in this entry.