



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 07:58 am BST

PDB ID : 3WRF  
Title : The crystal structure of native HypBA1 from Bifidobacterium longum JCM 1217  
Authors : Huang, C.H.; Zhu, Z.; Cheng, Y.S.; Chan, H.C.; Ko, T.P.; Chen, C.C.; Wang, I.; Ho, M.R.; Hsu, S.T.; Zeng, Y.F.; Huang, Y.N.; Liu, J.R.; Guo, R.T.  
Deposited on : 2014-02-25  
Resolution : 2.25 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

<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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

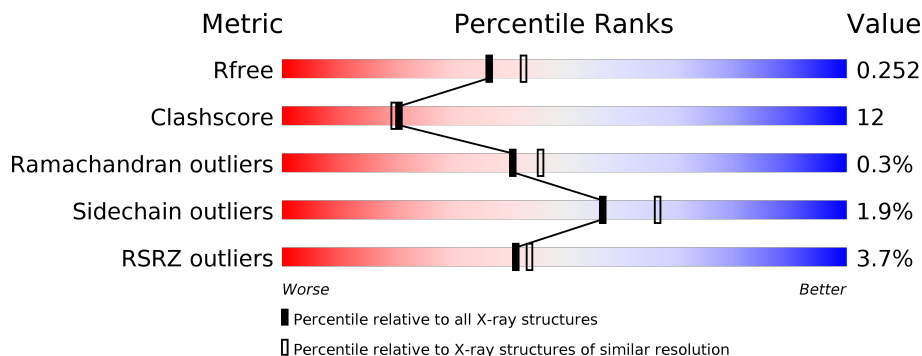
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	658	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5297 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 Non-reducing end beta-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	639	5018	3162	862	972	7	15	0	0	0

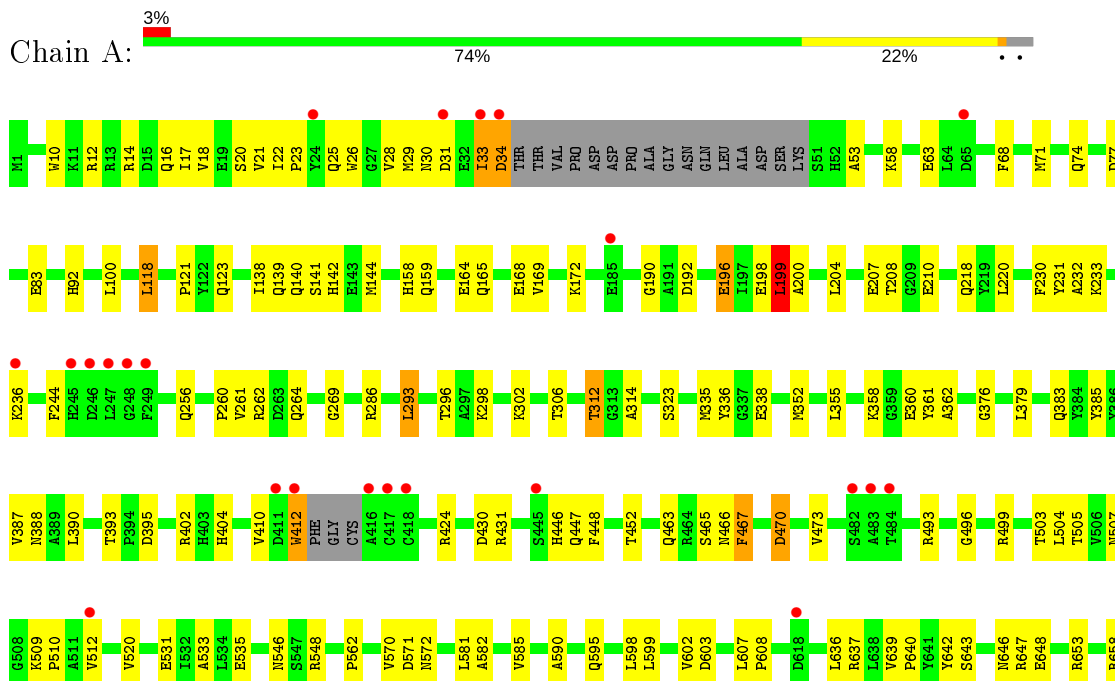
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	279	Total	O	0	0
			279	279		

### 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: Non-reducing end beta-L-arabinofuranosidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.87Å 75.87Å 254.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.25 24.84 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.6 (25.00-2.25) 96.5 (24.84-2.25)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.89 (at 2.24Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.215 , 0.252 0.215 , 0.252	Depositor DCC
$R_{free}$ test set	2066 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.0	Xtrriage
Anisotropy	0.467	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5297	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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](#)

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	0.26	0/5121	0.53	1/6937 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LEU	CA-CB-CG	5.27	127.42	115.30

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	5018	0	4793	121	0
2	A	279	0	0	7	0
All	All	5297	0	4793	121	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 12.

All (121) 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)
1:A:208:THR:HG23	1:A:210:GLU:H	1.26	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LEU:HD21	1:A:647:ARG:HD2	1.57	0.87
1:A:159:GLN:HE22	1:A:431:ARG:HH12	1.28	0.80
1:A:10:TRP:O	1:A:14:ARG:HG3	1.83	0.78
1:A:379:LEU:H	1:A:646:ASN:HD21	1.32	0.76
1:A:393:THR:HB	1:A:402:ARG:HH22	1.52	0.75
1:A:507:ASN:ND2	1:A:531:GLU:H	1.87	0.72
1:A:232:ALA:O	1:A:236:LYS:HG3	1.91	0.71
1:A:362:ALA:HB3	1:A:493:ARG:HD3	1.75	0.69
1:A:393:THR:HB	1:A:402:ARG:NH2	2.10	0.65
1:A:71:MSE:HA	1:A:71:MSE:HE2	1.79	0.64
1:A:58:LYS:HG2	1:A:63:GLU:OE1	1.98	0.64
1:A:572:ASN:HD21	1:A:637:ARG:H	1.46	0.64
1:A:546:ASN:OD1	1:A:548:ARG:HG2	1.98	0.64
1:A:262:ARG:CZ	1:A:293:LEU:HD13	2.28	0.63
1:A:379:LEU:H	1:A:646:ASN:ND2	1.96	0.63
1:A:503:THR:HB	1:A:535:GLU:HB2	1.83	0.60
1:A:639:VAL:HG13	1:A:640:PRO:HD2	1.82	0.60
1:A:507:ASN:HD21	1:A:531:GLU:H	1.48	0.59
1:A:336:TYR:O	1:A:387:VAL:HG13	2.03	0.59
1:A:14:ARG:HD3	2:A:877:HOH:O	2.04	0.57
1:A:335:MSE:O	1:A:404:HIS:HE1	1.87	0.57
1:A:196:GLU:O	1:A:199:LEU:HD13	2.03	0.57
1:A:29:MSE:HB2	1:A:53:ALA:HB3	1.87	0.57
1:A:647:ARG:HD3	2:A:711:HOH:O	2.05	0.56
1:A:139:GLN:HB2	1:A:231:TYR:CD1	2.39	0.56
1:A:83:GLU:CD	1:A:424:ARG:HD2	2.25	0.56
1:A:144:MSE:HB2	1:A:192:ASP:HB2	1.87	0.56
1:A:22:ILE:HB	1:A:23:PRO:HD3	1.88	0.55
1:A:302:LYS:O	1:A:306:THR:HB	2.06	0.54
1:A:585:VAL:HG11	1:A:608:PRO:HG2	1.88	0.54
1:A:570:VAL:HG13	1:A:648:GLU:HB3	1.89	0.54
1:A:582:ALA:HB3	1:A:585:VAL:HG11	1.90	0.54
1:A:383:GLN:HA	1:A:410:VAL:O	2.08	0.53
1:A:204:LEU:O	1:A:208:THR:HG22	2.08	0.53
1:A:25:GLN:O	1:A:28:VAL:HG22	2.09	0.53
1:A:168:GLU:O	1:A:172:LYS:HG3	2.08	0.53
1:A:29:MSE:HE1	1:A:77:ASP:O	2.09	0.53
1:A:26:TRP:CZ2	1:A:100:LEU:HD11	2.44	0.52
1:A:30:ASN:O	1:A:31:ASP:HB3	2.09	0.52
1:A:335:MSE:SE	1:A:390:LEU:HD13	2.59	0.52
1:A:338:GLU:HG2	2:A:797:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:VAL:HG22	1:A:512:VAL:O	2.09	0.52
1:A:466:ASN:HB3	1:A:470:ASP:HB2	1.92	0.52
1:A:25:GLN:O	1:A:29:MSE:HG2	2.10	0.52
1:A:572:ASN:ND2	1:A:636:LEU:HD12	2.25	0.51
1:A:581:LEU:HB3	1:A:585:VAL:HG21	1.92	0.51
1:A:582:ALA:HB3	1:A:585:VAL:CG1	2.41	0.51
1:A:269:GLY:O	1:A:323:SER:HB2	2.10	0.50
1:A:144:MSE:HE1	1:A:220:LEU:HD11	1.93	0.50
1:A:12:ARG:HG3	1:A:12:ARG:HH11	1.76	0.50
1:A:362:ALA:CB	1:A:493:ARG:HD3	2.42	0.49
1:A:159:GLN:NE2	1:A:431:ARG:HH12	2.04	0.49
1:A:71:MSE:H	1:A:74:GLN:NE2	2.10	0.49
1:A:590:ALA:HB2	1:A:607:LEU:HD21	1.93	0.49
1:A:68:PHE:CE2	1:A:121:PRO:HB3	2.48	0.49
1:A:504:LEU:CD2	1:A:520:VAL:HG11	2.42	0.49
1:A:467:PHE:CE2	1:A:562:PRO:HG3	2.48	0.49
1:A:198:GLU:HB2	2:A:726:HOH:O	2.13	0.49
1:A:140:GLN:HB3	1:A:244:PHE:HD1	1.78	0.49
1:A:582:ALA:O	1:A:585:VAL:HG22	2.13	0.49
1:A:393:THR:HG22	1:A:395:ASP:N	2.28	0.48
1:A:571:ASP:CG	1:A:647:ARG:HH22	2.16	0.48
1:A:158:HIS:HE1	1:A:164:GLU:OE2	1.96	0.48
1:A:595:GLN:HB2	1:A:598:LEU:HB3	1.94	0.48
1:A:571:ASP:OD1	1:A:647:ARG:NH2	2.47	0.48
1:A:20:SER:O	1:A:23:PRO:HD2	2.13	0.48
1:A:404:HIS:HD2	2:A:783:HOH:O	1.96	0.47
1:A:261:VAL:HG12	1:A:296:THR:HG21	1.95	0.47
1:A:190:GLY:HA3	1:A:230:PHE:CZ	2.50	0.47
1:A:33:ILE:HG22	1:A:34:ASP:N	2.30	0.46
1:A:190:GLY:HA3	1:A:230:PHE:CE2	2.50	0.46
1:A:260:PRO:O	1:A:264:GLN:HG3	2.15	0.46
1:A:448:PHE:HA	1:A:463:GLN:HE22	1.80	0.46
1:A:640:PRO:HG2	1:A:643:SER:OG	2.16	0.46
1:A:141:SER:O	1:A:142:HIS:HB2	2.15	0.45
1:A:83:GLU:OE1	1:A:424:ARG:HD2	2.16	0.45
1:A:505:THR:OG1	1:A:533:ALA:HB3	2.17	0.45
1:A:358:LYS:HB3	1:A:360:GLU:HG2	1.98	0.45
1:A:298:LYS:HG2	1:A:352:MSE:HE1	1.99	0.45
1:A:256:GLN:HA	2:A:740:HOH:O	2.16	0.44
1:A:358:LYS:HB2	1:A:361:TYR:CD2	2.52	0.44
1:A:362:ALA:HB3	1:A:493:ARG:CD	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:HIS:ND1	1:A:447:GLN:HG2	2.32	0.44
1:A:335:MSE:HE2	1:A:388:ASN:O	2.18	0.44
1:A:602:VAL:CG1	1:A:603:ASP:N	2.80	0.44
1:A:390:LEU:O	1:A:653:ARG:HA	2.18	0.44
1:A:138:ILE:HA	1:A:141:SER:OG	2.18	0.44
1:A:18:VAL:HG11	1:A:92:HIS:CD2	2.52	0.43
1:A:199:LEU:HD22	1:A:199:LEU:C	2.39	0.43
1:A:312:THR:HG22	1:A:314:ALA:H	1.83	0.43
1:A:140:GLN:HB3	1:A:244:PHE:CD1	2.54	0.43
1:A:412:TRP:N	1:A:412:TRP:CE3	2.86	0.43
1:A:465:SER:HB3	1:A:473:VAL:HG13	2.00	0.42
1:A:393:THR:HG22	1:A:395:ASP:H	1.83	0.42
1:A:20:SER:C	1:A:23:PRO:HD2	2.39	0.42
1:A:14:ARG:NH2	1:A:430:ASP:OD1	2.51	0.42
1:A:496:GLY:O	1:A:499:ARG:HG2	2.19	0.42
1:A:642:TYR:C	1:A:642:TYR:CD1	2.92	0.42
1:A:172:LYS:NZ	1:A:172:LYS:HB3	2.35	0.42
1:A:199:LEU:HD22	1:A:200:ALA:N	2.34	0.42
1:A:262:ARG:NH2	1:A:293:LEU:HD13	2.35	0.42
1:A:158:HIS:HD2	1:A:207:GLU:OE2	2.03	0.42
1:A:118:LEU:HA	1:A:123:GLN:OE1	2.20	0.41
1:A:286:ARG:NH1	1:A:286:ARG:HB3	2.36	0.41
1:A:448:PHE:HB2	1:A:467:PHE:CD2	2.56	0.41
1:A:17:ILE:HA	1:A:21:VAL:HB	2.03	0.41
1:A:358:LYS:HB2	1:A:361:TYR:CE2	2.56	0.41
1:A:376:GLY:HA2	1:A:385:TYR:HB2	2.01	0.41
1:A:496:GLY:O	1:A:499:ARG:NH1	2.54	0.41
1:A:12:ARG:O	1:A:16:GLN:HG3	2.21	0.41
1:A:138:ILE:HD11	1:A:230:PHE:CE2	2.56	0.41
1:A:286:ARG:HG3	1:A:355:LEU:HD23	2.03	0.40
1:A:504:LEU:HD23	1:A:520:VAL:HG11	2.03	0.40
1:A:572:ASN:ND2	1:A:636:LEU:HA	2.37	0.40
1:A:233:LYS:HA	1:A:236:LYS:HD2	2.03	0.40
1:A:28:VAL:HG23	1:A:29:MSE:N	2.37	0.40
1:A:509:LYS:HA	1:A:510:PRO:HD3	1.87	0.40
1:A:602:VAL:HG11	1:A:640:PRO:CD	2.51	0.40
1:A:165:GLN:O	1:A:169:VAL:HG23	2.22	0.40
1:A:452:THR:HG23	2:A:968:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	633/658 (96%)	601 (95%)	30 (5%)	2 (0%)	41 46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLU
1	A	33	ILE

### 5.3.2 Protein sidechains [i](#)

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	523/523 (100%)	513 (98%)	10 (2%)	57 66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	118	LEU
1	A	199	LEU
1	A	218	GLN
1	A	293	LEU
1	A	312	THR
1	A	412	TRP
1	A	467	PHE
1	A	470	ASP

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Mol	Chain	Res	Type
1	A	658	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	25	GLN
1	A	30	ASN
1	A	52	HIS
1	A	74	GLN
1	A	92	HIS
1	A	142	HIS
1	A	158	HIS
1	A	159	GLN
1	A	180	ASN
1	A	194	HIS
1	A	218	GLN
1	A	229	GLN
1	A	239	ASN
1	A	264	GLN
1	A	265	GLN
1	A	270	HIS
1	A	291	GLN
1	A	351	GLN
1	A	404	HIS
1	A	421	ASN
1	A	447	GLN
1	A	451	ASN
1	A	463	GLN
1	A	507	ASN
1	A	572	ASN
1	A	646	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	624/658 (94%)	-0.03	23 (3%) 41 44	28, 42, 64, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	LEU	12.4
1	A	412	TRP	7.9
1	A	249	PHE	6.3
1	A	417	CYS	6.0
1	A	34	ASP	5.3
1	A	246	ASP	5.2
1	A	65	ASP	4.5
1	A	33	ILE	4.5
1	A	512	VAL	4.4
1	A	31	ASP	3.8
1	A	245	HIS	3.5
1	A	483	ALA	3.3
1	A	484	THR	3.3
1	A	248	GLY	3.2
1	A	418	CYS	3.1
1	A	482	SER	2.8
1	A	416	ALA	2.4
1	A	24	TYR	2.3
1	A	185	GLU	2.3
1	A	445	SER	2.2
1	A	236	LYS	2.2
1	A	618	ASP	2.1
1	A	411	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.