Full wwPDB X-ray Structure Validation Report (i)

Aug 17, 2022 – 04:44 PM EDT

PDB ID	:	3WKX
Title	:	Crystal structure of GH127 beta-L-arabinofuranosidase HypBA1 from Bifidobacterium longum arabinose complex form
Authors	:	Ito, T.; Saikawa, K.; Arakawa, T.; Wakagi, T.; Fujita, K.
Deposited on	:	2013-11-01
Resolution	:	2.00 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

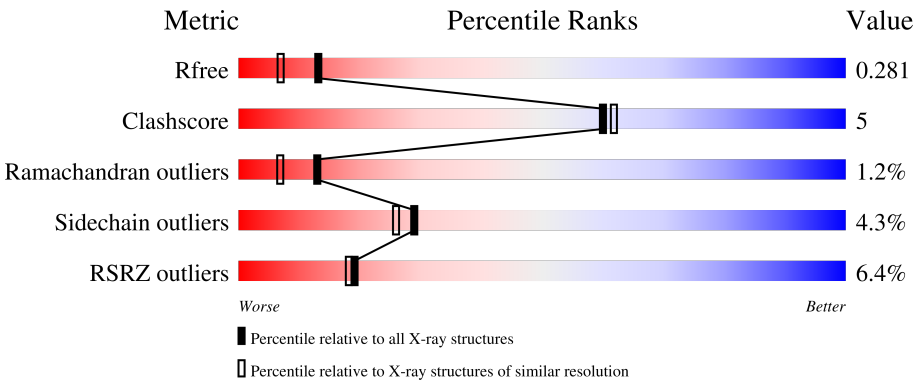
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	669	6% 85% 11% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5413 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.

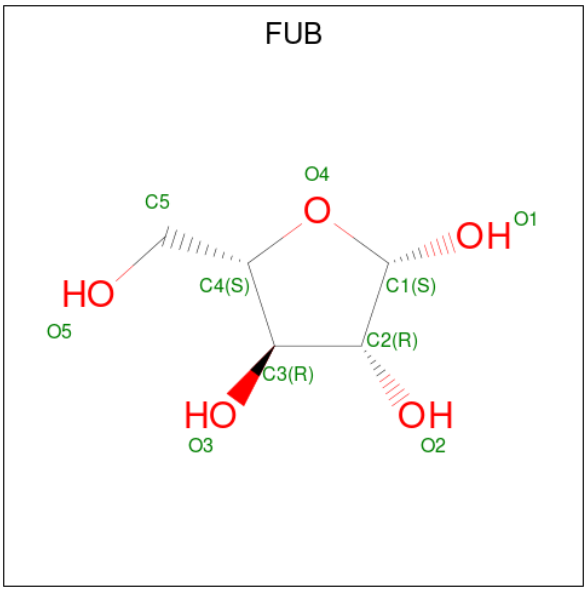
- Molecule 1 is a protein called Non-reducing end beta-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	657	5140	3236	883	998	23	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	659	ALA	-	expression tag	UNP E8MGH8
A	660	ALA	-	expression tag	UNP E8MGH8
A	661	ALA	-	expression tag	UNP E8MGH8
A	662	LEU	-	expression tag	UNP E8MGH8
A	663	GLU	-	expression tag	UNP E8MGH8
A	664	HIS	-	expression tag	UNP E8MGH8
A	665	HIS	-	expression tag	UNP E8MGH8
A	666	HIS	-	expression tag	UNP E8MGH8
A	667	HIS	-	expression tag	UNP E8MGH8
A	668	HIS	-	expression tag	UNP E8MGH8
A	669	HIS	-	expression tag	UNP E8MGH8

- Molecule 2 is beta-L-arabinofuranose (three-letter code: FUB) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

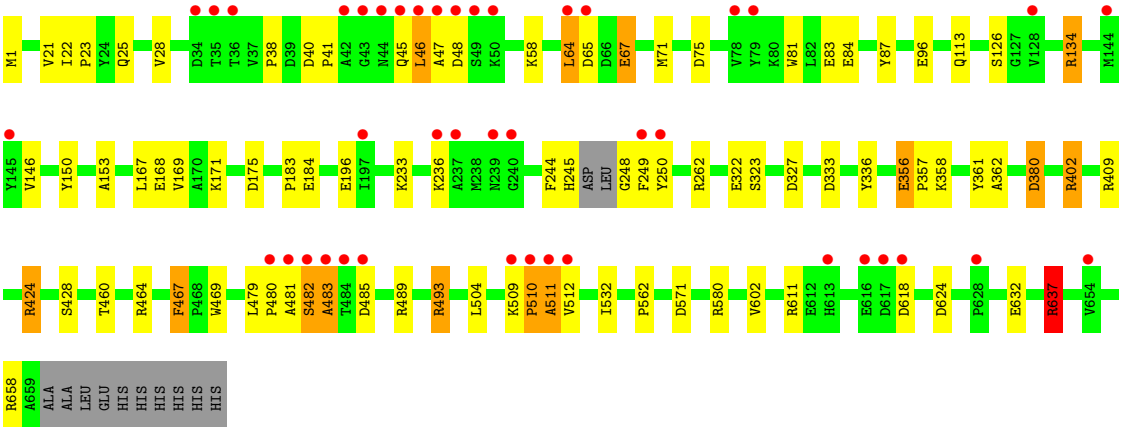
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	262	Total O 262 262	0	0

3 Residue-property plots (i)

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

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	77.73Å 77.73Å 252.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.70 – 2.00 29.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.9 (29.70-2.00) 93.9 (29.70-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.71 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.226 , 0.279 0.233 , 0.281	Depositor DCC
R_{free} test set	2892 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.037 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5413	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: FUB, ZN

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	0.90	1/5261 (0.0%)	1.02	20/7155 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	402	ARG	CD-NE	-5.05	1.37	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	402	ARG	NE-CZ-NH1	13.92	127.26	120.30
1	A	402	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	A	424	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	A	424	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	A	637	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	489	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	A	380	ASP	CB-CG-OD1	7.55	125.10	118.30
1	A	580	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	A	611	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	175	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	327	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	409	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	493	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	262	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	A	464	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	611	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	493	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	175	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	489	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	262	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	5140	0	4903	46	0
2	A	10	0	0	0	0
3	A	1	0	0	0	0
4	A	262	0	0	6	0
All	All	5413	0	4903	46	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 5.

All (46) 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:67:GLU:HG3	1:A:126:SER:HB2	1.38	1.03
1:A:67:GLU:HG3	1:A:126:SER:CB	2.00	0.92
1:A:362:ALA:HB3	1:A:493:ARG:HD3	1.68	0.74
1:A:67:GLU:HG2	4:A:879:HOH:O	1.87	0.73
1:A:510:PRO:O	1:A:511:ALA:C	2.28	0.71
1:A:571:ASP:HB3	1:A:637:ARG:HG2	1.74	0.70
1:A:510:PRO:O	1:A:512:VAL:HG23	1.93	0.68
1:A:113:GLN:OE1	1:A:134:ARG:NH2	2.26	0.67
1:A:67:GLU:CG	1:A:126:SER:HB2	2.21	0.64
1:A:512:VAL:CG2	4:A:996:HOH:O	2.45	0.64
1:A:512:VAL:HG21	4:A:996:HOH:O	2.01	0.60
1:A:333:ASP:HB2	1:A:402:ARG:HD3	1.86	0.57
1:A:150:TYR:CE2	1:A:169:VAL:HG12	2.41	0.56
1:A:481:ALA:O	1:A:483:ALA:N	2.31	0.55
1:A:167:LEU:HG	1:A:171:LYS:HD2	1.90	0.54
1:A:75:ASP:HB2	1:A:146:VAL:CG2	2.39	0.52
1:A:75:ASP:HB2	1:A:146:VAL:HG21	1.92	0.52
1:A:510:PRO:O	1:A:511:ALA:O	2.28	0.51
1:A:21:VAL:O	1:A:25:GLN:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:TRP:CH2	1:A:602:VAL:HG22	2.45	0.51
1:A:87:TYR:CD2	1:A:428:SER:HB3	2.49	0.48
1:A:22:ILE:N	1:A:23:PRO:CD	2.77	0.47
1:A:402:ARG:HD2	4:A:816:HOH:O	2.15	0.47
1:A:467:PHE:CE2	1:A:562:PRO:HG3	2.50	0.47
1:A:479:LEU:HD12	1:A:480:PRO:HD2	1.95	0.47
1:A:1:MET:N	4:A:856:HOH:O	2.46	0.47
1:A:58:LYS:HD3	1:A:64:LEU:HD12	1.95	0.47
1:A:356:GLU:HG3	1:A:357:PRO:HD2	1.97	0.46
1:A:46:LEU:HA	4:A:975:HOH:O	2.15	0.46
1:A:83:GLU:HG2	1:A:87:TYR:CE2	2.50	0.46
1:A:71:MET:HA	1:A:71:MET:HE2	2.00	0.43
1:A:150:TYR:O	1:A:153:ALA:HB3	2.18	0.43
1:A:358:LYS:HD2	1:A:361:TYR:CZ	2.54	0.43
1:A:248:GLY:C	1:A:250:TYR:H	2.22	0.43
1:A:244:PHE:O	1:A:245:HIS:C	2.57	0.42
1:A:81:TRP:O	1:A:84:GLU:HB3	2.18	0.42
1:A:22:ILE:HB	1:A:23:PRO:HD3	2.01	0.42
1:A:362:ALA:CB	1:A:493:ARG:HD3	2.45	0.42
1:A:183:PRO:HD2	1:A:184:GLU:OE2	2.20	0.41
1:A:40:ASP:HA	1:A:41:PRO:HD3	1.90	0.41
1:A:512:VAL:O	1:A:512:VAL:HG12	2.21	0.41
1:A:245:HIS:CD2	1:A:245:HIS:O	2.74	0.41
1:A:38:PRO:O	1:A:47:ALA:HB3	2.22	0.40
1:A:504:LEU:HD11	1:A:532:ILE:CG2	2.51	0.40
1:A:632:GLU:O	1:A:632:GLU:HG2	2.21	0.40
1:A:322:GLU:HG2	1:A:336:TYR:CZ	2.57	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	653/669 (98%)	614 (94%)	31 (5%)	8 (1%)	13 7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLU
1	A	482	SER
1	A	483	ALA
1	A	511	ALA
1	A	45	GLN
1	A	249	PHE
1	A	485	ASP
1	A	510	PRO

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	536/546 (98%)	513 (96%)	23 (4%)	29 26

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	VAL
1	A	46	LEU
1	A	48	ASP
1	A	64	LEU
1	A	65	ASP
1	A	67	GLU
1	A	96	GLU
1	A	134	ARG
1	A	168	GLU
1	A	233	LYS
1	A	236	LYS
1	A	323	SER
1	A	356	GLU

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Mol	Chain	Res	Type
1	A	380	ASP
1	A	424	ARG
1	A	460	THR
1	A	467	PHE
1	A	482	SER
1	A	509	LYS
1	A	618	ASP
1	A	624	ASP
1	A	637	ARG
1	A	658	ARG

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	FUB	A	701	-	10,10,10	2.24	3 (30%)	13,14,14	1.64	2 (15%)

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	FUB	A	701	-	-	0/2/18/18	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FUB	O1-C1	5.58	1.57	1.39
2	A	701	FUB	O2-C2	2.78	1.49	1.43
2	A	701	FUB	C2-C3	-2.38	1.46	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FUB	O1-C1-O4	-3.77	106.30	111.13
2	A	701	FUB	C1-C2-C3	-3.23	98.25	102.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	657/669 (98%)	0.13	42 (6%) 19 18	26, 39, 61, 125	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	LEU	9.4
1	A	47	ALA	7.1
1	A	45	GLN	6.9
1	A	44	ASN	6.0
1	A	49	SER	5.3
1	A	483	ALA	5.0
1	A	48	ASP	4.8
1	A	249	PHE	4.2
1	A	64	LEU	4.0
1	A	43	GLY	3.6
1	A	484	THR	3.6
1	A	65	ASP	3.6
1	A	512	VAL	3.5
1	A	482	SER	3.2
1	A	36	THR	3.2
1	A	616	GLU	3.1
1	A	481	ALA	3.0
1	A	128	VAL	2.9
1	A	509	LYS	2.9
1	A	34	ASP	2.9
1	A	511	ALA	2.7
1	A	510	PRO	2.7
1	A	485	ASP	2.6
1	A	618	ASP	2.6
1	A	145	TYR	2.5
1	A	197	ILE	2.4
1	A	236	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	617	ASP	2.4
1	A	78	VAL	2.3
1	A	240	GLY	2.3
1	A	628	PRO	2.3
1	A	239	ASN	2.3
1	A	237	ALA	2.3
1	A	250	TYR	2.3
1	A	35	THR	2.2
1	A	50	LYS	2.2
1	A	613	HIS	2.2
1	A	79	TYR	2.2
1	A	144	MET	2.1
1	A	480	PRO	2.1
1	A	654	VAL	2.0
1	A	42	ALA	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 monosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FUB	A	701	10/10	0.95	0.14	33,36,40,42	0
3	ZN	A	702	1/1	0.99	0.05	30,30,30,30	1

6.5 Other polymers (i)

There are no such residues in this entry.