



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 04:58 AM BST

PDB ID : 6M76  
Title : GH31 alpha-N-acetylgalactosaminidase from *Enterococcus faecalis*  
Authors : Miyazaki, T.  
Deposited on : 2020-03-17  
Resolution : 1.40 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 : 2.14.4.dev1  
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) : 2.14.4.dev1

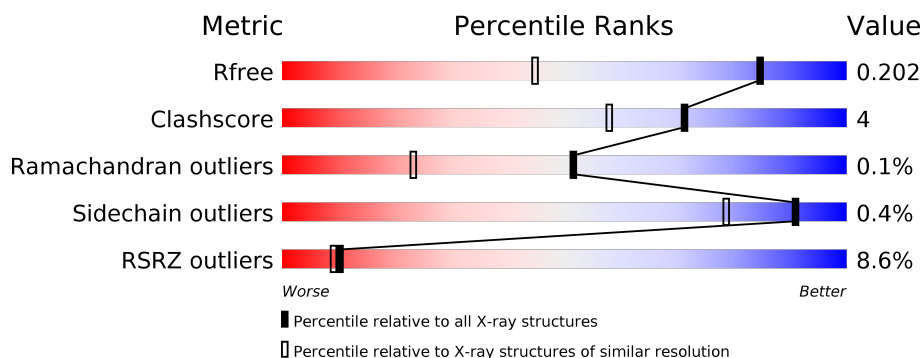
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	963	<div> <div>8%</div> <div>89%</div> <div>7%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8406 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 LPXTG-motif cell wall anchor domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	923	7307	4616	1215	1459	17	0	12	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

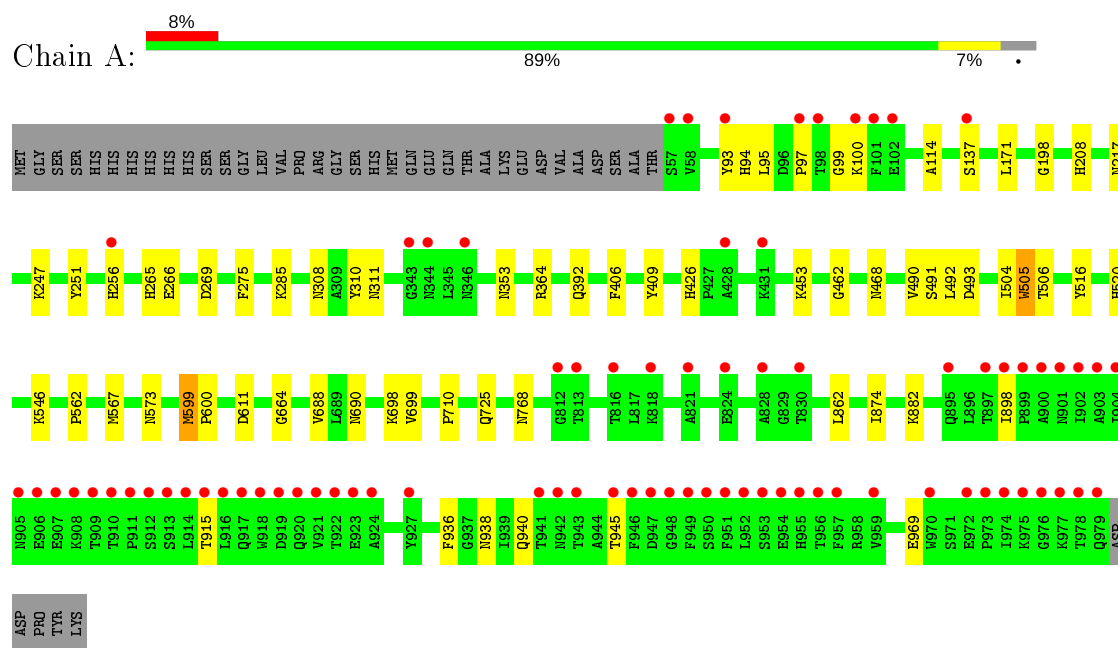
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1063	Total	O	0	0
			1063	1063		

### 3 Residue-property plots

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: LPXTG-motif cell wall anchor domain protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.44Å 82.97Å 149.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.12 – 1.40 46.08 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.12-1.40) 99.7 (46.08-1.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.172 , 0.195 0.181 , 0.202	Depositor DCC
$R_{free}$ test set	9974 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.3	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	8406	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: EDO

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	0.64	0/7479	0.76	1/10151 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	599	MET	CG-SD-CE	-5.13	91.99	100.20

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	7307	0	6986	51	0
2	A	36	0	54	5	0
3	A	1063	0	0	12	0
All	All	8406	0	7040	51	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 4.

All (51) 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:353:ASN:HD22	1:A:364:ARG:HE	1.37	0.71
1:A:768:ASN:HD22	1:A:882:LYS:HA	1.57	0.70
1:A:426:HIS:HD2	3:A:1533:HOH:O	1.77	0.68
1:A:251:TYR:OH	1:A:265:HIS:HE1	1.79	0.66
1:A:506:THR:OG1	1:A:520:HIS:HE1	1.78	0.66
1:A:915:THR:OG1	1:A:945:THR:HG22	1.97	0.64
1:A:256:HIS:CD2	3:A:1641:HOH:O	2.52	0.62
1:A:217:ASN:HD21	1:A:493:ASP:CB	2.14	0.61
1:A:364:ARG:HH11	2:A:1007:EDO:C2	2.14	0.61
1:A:546:LYS:H	1:A:573:ASN:HD21	1.47	0.60
1:A:266:GLU:HG2	3:A:1115:HOH:O	2.02	0.59
1:A:699:VAL:HG23	3:A:1899:HOH:O	2.04	0.57
1:A:256:HIS:CG	3:A:1641:HOH:O	2.57	0.57
1:A:546:LYS:H	1:A:573:ASN:ND2	2.04	0.56
1:A:664:GLY:H	1:A:690:ASN:HD22	1.54	0.55
1:A:453:LYS:HE3	1:A:567:MET:HE3	1.89	0.54
1:A:308:ASN:HB3	1:A:310:TYR:CE2	2.43	0.54
1:A:247:LYS:O	1:A:265:HIS:HD2	1.92	0.53
1:A:409:TYR:CE1	2:A:1007:EDO:H12	2.43	0.52
1:A:862:LEU:HD11	1:A:874:ILE:HD11	1.91	0.51
1:A:353:ASN:ND2	1:A:364:ARG:HE	2.06	0.50
1:A:217:ASN:HD21	1:A:493:ASP:CG	2.15	0.49
1:A:208:HIS:HD2	3:A:1500:HOH:O	1.95	0.49
1:A:490[B]:VAL:HG12	1:A:505:TRP:CE3	2.48	0.48
1:A:94:HIS:HE2	1:A:269:ASP:CG	2.17	0.48
1:A:99:GLY:N	3:A:1102:HOH:O	2.47	0.47
1:A:100:LYS:N	3:A:1102:HOH:O	2.31	0.47
1:A:491:SER:O	1:A:504:ILE:HA	2.14	0.46
1:A:945:THR:HG23	3:A:1936:HOH:O	2.16	0.46
1:A:311:ASN:HD21	1:A:392:GLN:HG3	1.81	0.46
1:A:462:GLY:HA2	3:A:1148:HOH:O	2.14	0.46
1:A:516:TYR:O	1:A:520:HIS:HD2	1.99	0.45
1:A:898:ILE:HD11	1:A:969:GLU:HB2	1.98	0.45
1:A:114:ALA:H	1:A:468:ASN:HD22	1.63	0.45
1:A:698:LYS:HE2	2:A:1008:EDO:H12	1.99	0.45
1:A:426:HIS:HE1	3:A:2002:HOH:O	1.99	0.45
1:A:285:LYS:HE2	1:A:611:ASP:O	2.17	0.45
1:A:938:ASN:ND2	1:A:940:GLN:HE21	2.15	0.45
1:A:688:VAL:O	1:A:936:PHE:HA	2.18	0.44
1:A:137:SER:OG	1:A:137:SER:O	2.35	0.43
1:A:364:ARG:HH11	2:A:1007:EDO:H21	1.82	0.43
1:A:217:ASN:HD21	1:A:493:ASP:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725:GLN:NE2	3:A:1101:HOH:O	2.31	0.43
1:A:93:TYR:OH	1:A:95:LEU:HD12	2.19	0.43
1:A:600:PRO:HB2	1:A:710:PRO:HB2	2.01	0.42
1:A:698:LYS:HE2	2:A:1008:EDO:C1	2.50	0.42
1:A:353:ASN:HD21	1:A:406:PHE:CA	2.34	0.40
1:A:95:LEU:O	1:A:97:PRO:HD3	2.22	0.40
1:A:171:LEU:C	1:A:171:LEU:HD23	2.42	0.40
1:A:599:MET:HE3	1:A:599:MET:HB3	1.84	0.40
1:A:198:GLY:O	1:A:208:HIS:HE1	2.04	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	933/963 (97%)	899 (96%)	33 (4%)	1 (0%)	51 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	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	783/805 (97%)	780 (100%)	3 (0%)	91 78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	275	PHE
1	A	492	LEU
1	A	505	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	ASN
1	A	208	HIS
1	A	214	GLN
1	A	217	ASN
1	A	250	ASN
1	A	256	HIS
1	A	265	HIS
1	A	311	ASN
1	A	353	ASN
1	A	402	ASN
1	A	426	HIS
1	A	468	ASN
1	A	520	HIS
1	A	573	ASN
1	A	690	ASN
1	A	715	ASN
1	A	761	ASN
1	A	768	ASN
1	A	901	ASN
1	A	938	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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	EDO	A	1002	-	3,3,3	0.19	0	2,2,2	0.07	0
2	EDO	A	1007	-	3,3,3	0.43	0	2,2,2	1.01	0
2	EDO	A	1003	-	3,3,3	0.18	0	2,2,2	0.14	0
2	EDO	A	1004	-	3,3,3	0.07	0	2,2,2	0.07	0
2	EDO	A	1005	-	3,3,3	0.34	0	2,2,2	0.14	0
2	EDO	A	1001	-	3,3,3	0.19	0	2,2,2	0.44	0
2	EDO	A	1008	-	3,3,3	0.28	0	2,2,2	0.52	0
2	EDO	A	1006	-	3,3,3	0.29	0	2,2,2	0.17	0
2	EDO	A	1009	-	3,3,3	0.05	0	2,2,2	0.16	0

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	EDO	A	1002	-	-	0/1/1/1	-
2	EDO	A	1007	-	-	1/1/1/1	-
2	EDO	A	1003	-	-	0/1/1/1	-
2	EDO	A	1004	-	-	0/1/1/1	-
2	EDO	A	1005	-	-	0/1/1/1	-
2	EDO	A	1001	-	-	0/1/1/1	-
2	EDO	A	1008	-	-	0/1/1/1	-
2	EDO	A	1006	-	-	1/1/1/1	-
2	EDO	A	1009	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1007	EDO	O1-C1-C2-O2
2	A	1006	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1007	EDO	3	0
2	A	1008	EDO	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	923/963 (95%)	0.30	79 (8%) 10 9	13, 20, 46, 76	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	952	LEU	8.8
1	A	951	PHE	8.8
1	A	903	ALA	7.3
1	A	974	ILE	7.2
1	A	904	ILE	6.8
1	A	922	THR	6.7
1	A	57	SER	6.2
1	A	902	ILE	6.1
1	A	98	THR	5.9
1	A	957	PHE	5.6
1	A	907	GLU	5.3
1	A	914	LEU	5.3
1	A	977	LYS	5.1
1	A	909	THR	5.1
1	A	916	LEU	4.9
1	A	943	THR	4.8
1	A	908	LYS	4.6
1	A	949	PHE	4.5
1	A	918	TRP	4.4
1	A	905	ASN	4.3
1	A	915	THR	4.3
1	A	920	GLN	4.2
1	A	910	THR	4.2
1	A	947	ASP	4.2
1	A	978	THR	4.2
1	A	956	THR	4.0
1	A	100	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	913	SER	3.7
1	A	948	GLY	3.7
1	A	976	GLY	3.6
1	A	942	ASN	3.6
1	A	973	PRO	3.6
1	A	256	HIS	3.5
1	A	917	GLN	3.5
1	A	97	PRO	3.5
1	A	901	ASN	3.5
1	A	954	GLU	3.5
1	A	919	ASP	3.4
1	A	897	THR	3.4
1	A	906	GLU	3.4
1	A	923	GLU	3.4
1	A	346	ASN	3.3
1	A	950	SER	3.3
1	A	979	GLN	3.2
1	A	900	ALA	3.2
1	A	812	GLY	3.1
1	A	912	SER	3.1
1	A	921	VAL	3.0
1	A	927	TYR	3.0
1	A	58	VAL	2.9
1	A	972	GLU	2.9
1	A	955	HIS	2.9
1	A	945	THR	2.8
1	A	924	ALA	2.8
1	A	818	LYS	2.8
1	A	828	ALA	2.8
1	A	946	PHE	2.8
1	A	959	VAL	2.7
1	A	431	LYS	2.7
1	A	898	ILE	2.7
1	A	899	PRO	2.6
1	A	137	SER	2.6
1	A	813	THR	2.6
1	A	821	ALA	2.6
1	A	816	THR	2.6
1	A	101	PHE	2.5
1	A	343	GLY	2.5
1	A	830	THR	2.5
1	A	975	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	941	THR	2.4
1	A	911	PRO	2.3
1	A	344	ASN	2.3
1	A	895	GLN	2.2
1	A	824	GLU	2.2
1	A	953	SER	2.2
1	A	428	ALA	2.1
1	A	93	TYR	2.1
1	A	970	TRP	2.1
1	A	102	GLU	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, 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
2	EDO	A	1007	4/4	0.67	0.23	29,30,30,37	0
2	EDO	A	1009	4/4	0.73	0.17	30,36,39,44	0
2	EDO	A	1006	4/4	0.83	0.15	29,33,34,37	0
2	EDO	A	1008	4/4	0.88	0.17	31,32,33,34	0
2	EDO	A	1004	4/4	0.89	0.13	28,28,29,29	0
2	EDO	A	1003	4/4	0.91	0.08	25,29,29,32	0
2	EDO	A	1001	4/4	0.92	0.09	16,17,19,19	0
2	EDO	A	1002	4/4	0.94	0.08	21,23,23,26	0
2	EDO	A	1005	4/4	0.97	0.11	21,30,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.