



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:57 PM GMT

PDB ID : 3VMO  
Title : Crystal structure of dextranase from Streptococcus mutans in complex with isomaltotriose  
Authors : Suzuki, N.; Fujimoto, Z.; Kim, Y.M.; Momma, M.; Okuyama, M.; Mori, H.; Funane, K.; Kimura, A.  
Deposited on : 2011-12-14  
Resolution : 1.90 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

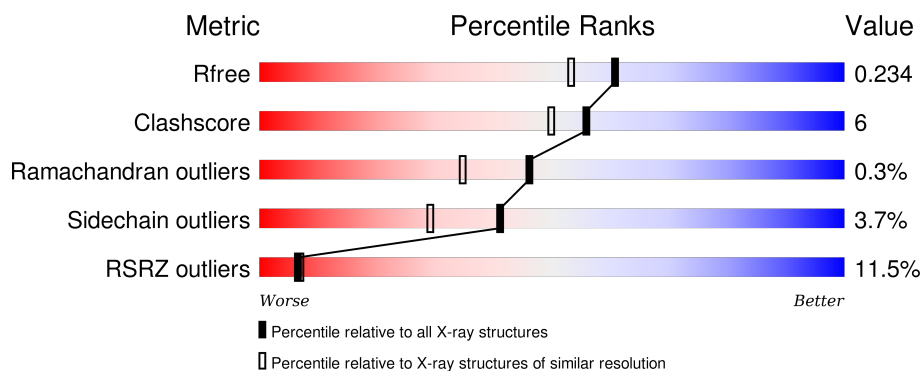
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	643	

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	GLC	A	805	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	A	806	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5333 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 Dextranase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	0
			4985	3137	844	988	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	MET	-	EXPRESSION TAG	UNP F5BA50
A	99	ASP	-	EXPRESSION TAG	UNP F5BA50
A	733	LEU	-	EXPRESSION TAG	UNP F5BA50
A	734	GLU	-	EXPRESSION TAG	UNP F5BA50
A	735	HIS	-	EXPRESSION TAG	UNP F5BA50
A	736	HIS	-	EXPRESSION TAG	UNP F5BA50
A	737	HIS	-	EXPRESSION TAG	UNP F5BA50
A	738	HIS	-	EXPRESSION TAG	UNP F5BA50
A	739	HIS	-	EXPRESSION TAG	UNP F5BA50
A	740	HIS	-	EXPRESSION TAG	UNP F5BA50

- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	4	Total	C	O	0	0
			45	24	21		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			23	12	11		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	275	Total	O	0	0
			275	275		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.03Å 90.34Å 63.00Å 90.00° 100.33° 90.00°	Depositor
Resolution (Å)	29.22 – 1.90 29.22 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.22-1.90) 99.6 (29.22-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.03 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.187 , 0.237 0.186 , 0.234	Depositor DCC
$R_{free}$ test set	2511 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.3	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 49486 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5333	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.93% 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: BGC, PO4, GLC

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	0.83	1/5091 (0.0%)	0.79	2/6927 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	209	GLU	CB-CG	5.73	1.63	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	476	ARG	NE-CZ-NH2	-5.01	117.79	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	4985	0	4804	61	0
2	A	45	0	39	1	0
3	A	23	0	21	0	0
4	A	5	0	0	0	0
5	A	275	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5333	0	4864	61	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 6.

All (61) 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:710:ASN:HB3	1:A:716:VAL:HG21	1.47	0.93
1:A:734:GLU:O	1:A:735:HIS:CG	2.33	0.80
1:A:315:ALA:HB2	1:A:351:LEU:HA	1.65	0.77
1:A:422:GLU:OE1	5:A:1111:HOH:O	2.03	0.76
1:A:683:ILE:HD13	1:A:734:GLU:HG2	1.70	0.72
1:A:326:TYR:CE1	1:A:353:TYR:HD2	2.09	0.70
1:A:395:HIS:O	1:A:398:LYS:HG2	1.91	0.70
1:A:337:GLN:O	1:A:340:GLN:HB3	1.95	0.66
1:A:323:ASP:HA	1:A:326:TYR:HD2	1.61	0.66
1:A:323:ASP:HA	1:A:326:TYR:CD2	2.31	0.65
1:A:315:ALA:HB2	1:A:351:LEU:O	1.97	0.65
1:A:387:ILE:HD12	1:A:388:GLY:H	1.63	0.63
1:A:418:ASN:O	1:A:422:GLU:HG3	2.00	0.61
1:A:190:ASN:ND2	1:A:201:GLN:HG2	2.16	0.61
1:A:702:SER:OG	5:A:1233:HOH:O	2.16	0.60
1:A:386:THR:HG22	5:A:1119:HOH:O	2.02	0.59
1:A:245:GLN:HE22	1:A:552:GLY:HA2	1.68	0.57
1:A:559:ALA:HB1	2:A:801:BGC:H3	1.84	0.57
1:A:128:ASN:OD1	1:A:164:SER:OG	2.17	0.57
1:A:228:ASN:HB3	1:A:281:SER:O	2.04	0.57
1:A:710:ASN:HB3	1:A:716:VAL:CG2	2.31	0.56
1:A:734:GLU:O	1:A:735:HIS:CD2	2.59	0.56
1:A:434:VAL:O	5:A:1200:HOH:O	2.18	0.55
1:A:689:LEU:HB2	1:A:703:LEU:HD11	1.90	0.54
1:A:706:GLN:OE1	5:A:1174:HOH:O	2.18	0.54
1:A:245:GLN:HG3	5:A:1100:HOH:O	2.06	0.54
1:A:315:ALA:HB2	1:A:351:LEU:CA	2.36	0.53
1:A:675:VAL:HG12	1:A:676:SER:O	2.09	0.52
1:A:326:TYR:HE1	1:A:353:TYR:HD2	1.57	0.49
1:A:353:TYR:N	1:A:353:TYR:CD1	2.80	0.49
1:A:315:ALA:HB2	1:A:351:LEU:C	2.35	0.48
1:A:593:LYS:HD2	5:A:1148:HOH:O	2.14	0.47
1:A:228:ASN:O	1:A:229:ASN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PRO:O	1:A:178:SER:OG	2.30	0.46
1:A:332:THR:HA	1:A:336:GLY:O	2.15	0.45
1:A:570:LYS:HD3	1:A:570:LYS:HA	1.83	0.45
1:A:326:TYR:HH	1:A:353:TYR:HE2	1.60	0.45
1:A:710:ASN:C	1:A:710:ASN:HD22	2.20	0.45
1:A:261:LYS:HD3	1:A:273:PHE:HB2	1.98	0.45
1:A:501:ASP:N	1:A:501:ASP:OD1	2.50	0.45
1:A:502:ASN:HB2	5:A:1137:HOH:O	2.17	0.45
1:A:108:LEU:HD22	1:A:189:VAL:HG21	1.98	0.45
1:A:313:GLN:HB2	1:A:355:TYR:HE2	1.82	0.44
1:A:316:ASN:HD22	1:A:316:ASN:N	2.15	0.44
1:A:198:ILE:HG21	1:A:201:GLN:HG3	1.99	0.44
1:A:350:PRO:C	1:A:351:LEU:HD22	2.39	0.43
1:A:679:GLU:O	1:A:683:ILE:HG13	2.19	0.43
1:A:672:LEU:HB3	1:A:675:VAL:HB	2.01	0.43
1:A:505:PRO:HG3	1:A:514:LEU:CD1	2.49	0.43
1:A:327:ILE:HG13	1:A:392:VAL:HB	2.01	0.42
1:A:663:GLN:HB3	1:A:666:LEU:HD21	2.02	0.42
1:A:582:PHE:HB2	1:A:692:PRO:HB3	2.01	0.42
1:A:629:LYS:HE3	1:A:629:LYS:HB2	1.72	0.42
1:A:190:ASN:ND2	1:A:201:GLN:OE1	2.48	0.41
1:A:295:ASN:O	1:A:299:GLN:HG3	2.20	0.41
1:A:332:THR:OG1	1:A:337:GLN:HA	2.21	0.41
1:A:387:ILE:HG13	1:A:387:ILE:H	1.54	0.41
1:A:149:LYS:NZ	5:A:1220:HOH:O	2.53	0.41
1:A:313:GLN:HG2	1:A:353:TYR:CE2	2.56	0.41
1:A:679:GLU:HG2	1:A:682:ARG:HD2	2.03	0.41
1:A:351:LEU:O	1:A:352:GLN:HG2	2.21	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	624/643 (97%)	602 (96%)	20 (3%)	2 (0%)	46 35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	A	464	ASN

### 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	538/552 (98%)	518 (96%)	20 (4%)	41 29

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	169	LYS
1	A	178	SER
1	A	187	LEU
1	A	218	TYR
1	A	255	PHE
1	A	279	TRP
1	A	284	GLN
1	A	316	ASN
1	A	331	GLU
1	A	353	TYR
1	A	386	THR
1	A	387	ILE
1	A	476	ARG
1	A	503	ARG
1	A	570	LYS
1	A	631	ASN
1	A	632	ASP
1	A	702	SER

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Mol	Chain	Res	Type
1	A	710	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	168	GLN
1	A	190	ASN
1	A	201	GLN
1	A	284	GLN
1	A	299	GLN
1	A	338	ASN
1	A	396	ASN
1	A	452	ASN
1	A	607	ASN
1	A	619	ASN
1	A	710	ASN
1	A	720	GLN

### 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 ⓘ

6 carbohydrates 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	BGC	A	801	2	12,12,12	0.61	0	17,17,17	0.84	0
2	GLC	A	802	2	11,11,12	0.67	0	14,15,17	1.36	2 (14%)
2	GLC	A	803	2	11,11,12	0.58	0	14,15,17	0.93	1 (7%)
2	GLC	A	804	2	11,11,12	0.60	0	14,15,17	1.44	4 (28%)
3	GLC	A	805	3	12,12,12	0.63	0	17,17,17	0.90	0
3	GLC	A	806	3	11,11,12	0.60	0	14,15,17	1.62	2 (14%)

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	BGC	A	801	2	-	0/2/22/22	0/1/1/1
2	GLC	A	802	2	-	0/2/19/22	0/1/1/1
2	GLC	A	803	2	-	0/2/19/22	0/1/1/1
2	GLC	A	804	2	-	0/2/19/22	0/1/1/1
3	GLC	A	805	3	-	0/2/22/22	0/1/1/1
3	GLC	A	806	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	802	GLC	O3-C3-C4	-2.02	105.80	110.34
2	A	804	GLC	O5-C5-C6	2.14	111.98	107.35
2	A	804	GLC	C1-C2-C3	2.17	112.11	109.54
3	A	806	GLC	C1-C2-C3	2.48	112.47	109.54
2	A	804	GLC	C3-C4-C5	2.48	114.52	110.20
2	A	804	GLC	C2-C3-C4	2.52	115.32	111.04
2	A	803	GLC	C1-O5-C5	2.55	115.48	112.25
2	A	802	GLC	C1-O5-C5	3.07	116.14	112.25
3	A	806	GLC	C1-O5-C5	4.58	118.06	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BGC	1	0

## 5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z  > 2$
4	PO4	A	807	-	4,4,4	0.34	0	6,6,6	0.28	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
4	PO4	A	807	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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 ⓘ

### 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	628/643 (97%)	0.48	72 (11%) 6 7	17, 32, 58, 66	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	PRO	8.9
1	A	353	TYR	6.0
1	A	711	GLU	5.7
1	A	351	LEU	5.6
1	A	735	HIS	5.1
1	A	279	TRP	5.1
1	A	280	TRP	4.9
1	A	345	SER	4.8
1	A	339	GLY	4.3
1	A	310	ILE	4.2
1	A	169	LYS	4.1
1	A	503	ARG	4.0
1	A	315	ALA	4.0
1	A	322	PRO	3.9
1	A	343	THR	3.7
1	A	344	TYR	3.7
1	A	105	MET	3.7
1	A	340	GLN	3.6
1	A	464	ASN	3.6
1	A	328	TYR	3.4
1	A	337	GLN	3.4
1	A	332	THR	3.3
1	A	457	PHE	3.2
1	A	382	TRP	3.2
1	A	384	GLY	3.2
1	A	270	VAL	3.1
1	A	282	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	338	ASN	3.1
1	A	501	ASP	3.1
1	A	107	ASN	3.0
1	A	395	HIS	2.9
1	A	673	THR	2.9
1	A	326	TYR	2.8
1	A	276	SER	2.8
1	A	277	TRP	2.8
1	A	539	MET	2.8
1	A	323	ASP	2.8
1	A	396	ASN	2.7
1	A	674	GLY	2.7
1	A	255	PHE	2.7
1	A	324	THR	2.6
1	A	399	ASP	2.6
1	A	341	VAL	2.6
1	A	451	TYR	2.6
1	A	490	VAL	2.6
1	A	502	ASN	2.6
1	A	327	ILE	2.6
1	A	168	GLN	2.5
1	A	682	ARG	2.5
1	A	269	ASN	2.4
1	A	352	GLN	2.3
1	A	307	TYR	2.3
1	A	386	THR	2.3
1	A	330	TYR	2.3
1	A	537	TYR	2.3
1	A	489	ILE	2.2
1	A	444	ASN	2.2
1	A	219	ALA	2.2
1	A	393	LEU	2.2
1	A	678	ALA	2.2
1	A	218	TYR	2.2
1	A	366	ILE	2.2
1	A	263	ALA	2.1
1	A	278	ASN	2.1
1	A	319	ALA	2.1
1	A	679	GLU	2.1
1	A	358	LEU	2.1
1	A	631	ASN	2.0
1	A	334	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	316	ASN	2.0
1	A	329	ASN	2.0
1	A	531	ILE	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](#)

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
3	GLC	A	806	11/12	0.92	0.29	11.93	38,43,48,53	0
3	GLC	A	805	12/12	0.91	0.21	4.01	39,43,45,47	0
2	BGC	A	801	12/12	0.86	0.13	-0.66	46,51,54,56	0
2	GLC	A	802	11/12	0.84	0.12	-1.13	43,45,49,51	0
2	GLC	A	803	11/12	0.89	0.13	-	53,57,60,62	0
2	GLC	A	804	11/12	0.65	0.28	-	63,65,66,67	0

## 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	PO4	A	807	5/5	0.94	0.19	0.80	67,68,69,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.