



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:21 PM BST

PDB ID : 6QNJ
Title : Liquid Application Method for time-resolved Analyses (LAMA) by serial synchrotron crystallography, Xylose Isomerase 4.5 s timepoint
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Deposited on : 2019-02-11
Resolution : 1.85 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 ⓘ symbol.

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 : 2.13.1
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) : 2.13.1

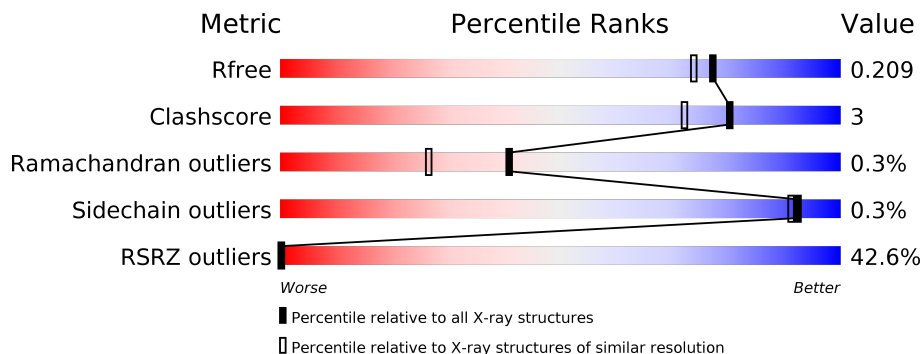
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 ≥ 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	388	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3349 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.

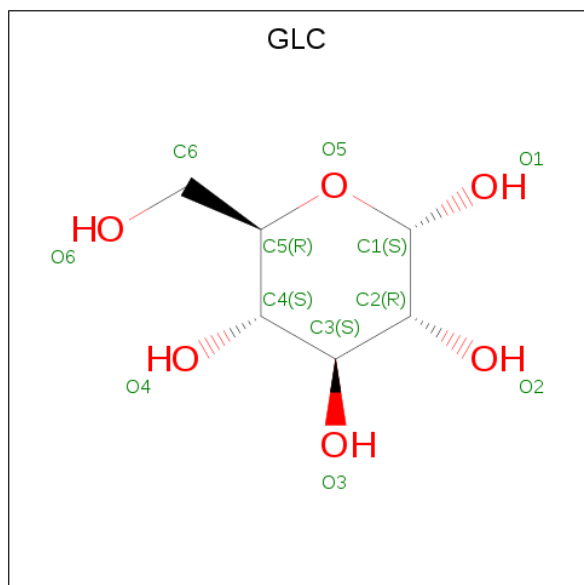
- Molecule 1 is a protein called Xylose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	3063	1923	552	579	9	0	2	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0

- Molecule 3 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	12	6	6	0	0

- Molecule 4 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Co	0	0
			1	1		

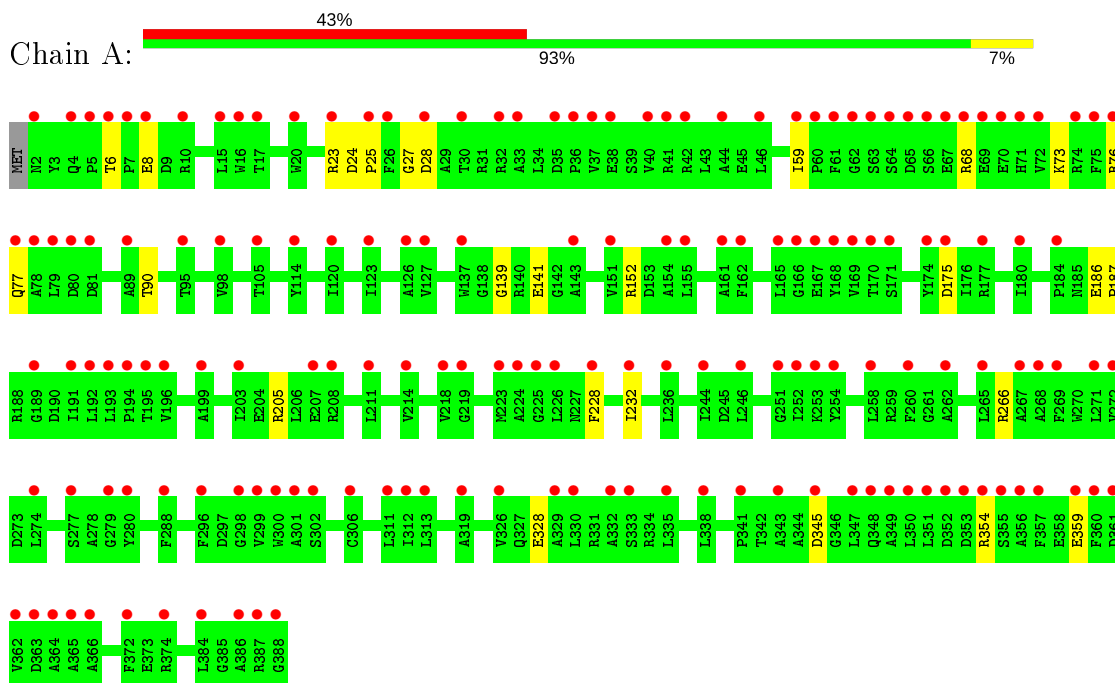
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	272	Total	O	0	0
			272	272		

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: Xylose isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	94.62Å 99.38Å 87.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.69 – 1.85 49.69 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.69-1.85) 99.6 (49.69-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 1.86Å)	Xtrriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.180 , 0.209 0.180 , 0.209	Depositor DCC
R_{free} test set	1733 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtrriage
Anisotropy	0.191	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	0.046 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3349	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, GLC, CO

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	0.37	0/3135	0.55	0/4241

There are no bond length outliers.

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	3063	0	2927	16	2
2	A	1	0	0	0	0
3	A	12	0	11	1	0
4	A	1	0	0	0	0
5	A	272	0	0	7	1
All	All	3349	0	2938	16	2

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 3.

All (16) 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:141:GLU:OE2	5:A:502:HOH:O	2.12	0.66
1:A:354:ARG:NH1	1:A:359:GLU:OE2	2.30	0.65
1:A:28:ASP:OD2	5:A:503:HOH:O	2.14	0.64
1:A:24:ASP:HB2	1:A:25:PRO:HD2	1.79	0.64
1:A:328[A]:GLU:OE1	5:A:504:HOH:O	2.17	0.59
1:A:205:ARG:NH1	5:A:511:HOH:O	2.38	0.56
1:A:90:THR:HG21	3:A:402:GLC:H62	1.91	0.52
1:A:152:ARG:NH1	5:A:505:HOH:O	2.26	0.49
1:A:73:LYS:NZ	1:A:77:GLN:HB2	2.33	0.44
1:A:59:ILE:HD13	1:A:68:ARG:NH1	2.33	0.43
1:A:6:THR:OG1	1:A:8:GLU:OE1	2.36	0.41
1:A:266:ARG:HG3	5:A:551:HOH:O	2.20	0.41
1:A:76:ARG:NH2	5:A:516:HOH:O	2.45	0.41
1:A:139:GLY:O	1:A:187:PRO:HD2	2.21	0.41
1:A:228:PHE:CZ	1:A:232:ILE:HD11	2.56	0.41
1:A:345:ASP:OD1	1:A:345:ASP:N	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:NH1	1:A:23:ARG:NH1[2_655]	1.40	0.80
1:A:27:GLY:O	5:A:501:HOH:O[2_655]	1.96	0.24

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	387/388 (100%)	373 (96%)	13 (3%)	1 (0%)	41 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	186	GLU

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	305/304 (100%)	304 (100%)	1 (0%)	92 91

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	ASP

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are 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
3	GLC	A	402	2	12,12,12	0.51	0	17,17,17	0.82	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
3	GLC	A	402	2	-	0/2/22/22	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	GLC	1	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, 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	387/388 (99%)	1.92	165 (42%) 0 0	5, 12, 31, 54	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	GLY	8.3
1	A	65	ASP	6.5
1	A	62	GLY	6.3
1	A	64	SER	5.6
1	A	175	ASP	5.2
1	A	2	ASN	5.1
1	A	66	SER	4.9
1	A	252	ILE	4.8
1	A	296	PHE	4.6
1	A	59	ILE	4.6
1	A	63	SER	4.2
1	A	67	GLU	4.0
1	A	226	LEU	3.9
1	A	70	GLU	3.9
1	A	357	PHE	3.8
1	A	69	GLU	3.7
1	A	61	PHE	3.6
1	A	174	TYR	3.4
1	A	258	LEU	3.4
1	A	254	TYR	3.4
1	A	218	VAL	3.3
1	A	352	ASP	3.3
1	A	363	ASP	3.3
1	A	25	PRO	3.3
1	A	170	THR	3.3
1	A	77	GLN	3.3
1	A	362	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	3.2
1	A	349	ALA	3.2
1	A	191	ILE	3.2
1	A	386	ALA	3.1
1	A	123	ILE	3.1
1	A	366	ALA	3.1
1	A	260	PHE	3.1
1	A	301	ALA	3.1
1	A	98	VAL	3.1
1	A	224	ALA	3.1
1	A	171	SER	3.0
1	A	37	VAL	3.0
1	A	32	ARG	3.0
1	A	326	VAL	3.0
1	A	274	LEU	3.0
1	A	330	LEU	3.0
1	A	38	GLU	3.0
1	A	6	THR	3.0
1	A	169	VAL	3.0
1	A	80	ASP	2.9
1	A	165	LEU	2.9
1	A	195	THR	2.9
1	A	312	ILE	2.9
1	A	348	GLN	2.9
1	A	72	VAL	2.9
1	A	35	ASP	2.9
1	A	5	PRO	2.8
1	A	192	LEU	2.8
1	A	120	ILE	2.8
1	A	143	ALA	2.8
1	A	8	GLU	2.8
1	A	180	ILE	2.8
1	A	184	PRO	2.8
1	A	151	VAL	2.8
1	A	78	ALA	2.7
1	A	208	ARG	2.7
1	A	353	ASP	2.7
1	A	268	ALA	2.7
1	A	4	GLN	2.7
1	A	364	ALA	2.7
1	A	36	PRO	2.7
1	A	228	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	199	ALA	2.6
1	A	350	LEU	2.6
1	A	359	GLU	2.6
1	A	271	LEU	2.6
1	A	161	ALA	2.6
1	A	60	PRO	2.6
1	A	17	THR	2.6
1	A	168	TYR	2.6
1	A	194	PRO	2.6
1	A	306	CYS	2.6
1	A	81	ASP	2.6
1	A	300	TRP	2.5
1	A	355	SER	2.5
1	A	15	LEU	2.5
1	A	126	ALA	2.5
1	A	360	PHE	2.5
1	A	105	THR	2.5
1	A	265	LEU	2.5
1	A	356	ALA	2.4
1	A	223	MET	2.4
1	A	272	VAL	2.4
1	A	137	TRP	2.4
1	A	343	ALA	2.4
1	A	76	ARG	2.4
1	A	347	LEU	2.4
1	A	244	ILE	2.4
1	A	40	VAL	2.4
1	A	68	ARG	2.4
1	A	177	ARG	2.4
1	A	189	GLY	2.4
1	A	20	TRP	2.4
1	A	351	LEU	2.4
1	A	372	PHE	2.4
1	A	44	ALA	2.4
1	A	338	LEU	2.4
1	A	384	LEU	2.4
1	A	71	HIS	2.4
1	A	46	LEU	2.3
1	A	329	ALA	2.3
1	A	262	ALA	2.3
1	A	280	TYR	2.3
1	A	341	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	74	ARG	2.3
1	A	196	VAL	2.3
1	A	267	ALA	2.3
1	A	335	LEU	2.3
1	A	28	ASP	2.3
1	A	319	ALA	2.3
1	A	79	LEU	2.3
1	A	298	GLY	2.2
1	A	207	GLU	2.2
1	A	33	ALA	2.2
1	A	299	VAL	2.2
1	A	277	SER	2.2
1	A	246	LEU	2.2
1	A	302	SER	2.2
1	A	193	LEU	2.2
1	A	162	PHE	2.2
1	A	365	ALA	2.2
1	A	253	LYS	2.2
1	A	345	ASP	2.2
1	A	225	GLY	2.2
1	A	127	VAL	2.2
1	A	387	ARG	2.2
1	A	155	LEU	2.2
1	A	211	LEU	2.2
1	A	30	THR	2.2
1	A	10	ARG	2.2
1	A	41	ARG	2.2
1	A	269	PHE	2.2
1	A	167	GLU	2.1
1	A	114	TYR	2.1
1	A	354	ARG	2.1
1	A	75	PHE	2.1
1	A	214	VAL	2.1
1	A	166	GLY	2.1
1	A	219	GLY	2.1
1	A	232	ILE	2.1
1	A	236	LEU	2.1
1	A	313	LEU	2.1
1	A	16	TRP	2.1
1	A	42	ARG	2.1
1	A	333	SER	2.1
1	A	374	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	26	PHE	2.1
1	A	154	ALA	2.1
1	A	7	PRO	2.1
1	A	203	ILE	2.1
1	A	89	ALA	2.0
1	A	311	LEU	2.0
1	A	361	ASP	2.0
1	A	23	ARG	2.0
1	A	251	GLY	2.0
1	A	288	PHE	2.0
1	A	332	ALA	2.0
1	A	95	THR	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
3	GLC	A	402	12/12	0.77	0.29	8,13,22,23	12
2	MG	A	401	1/1	0.99	0.10	9,9,9,9	0
4	CO	A	403	1/1	0.99	0.10	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.