



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:26 AM EST

PDB ID : 5GQV
Title : Crystal structure of branching enzyme from *Cyanothece* sp. ATCC 51142 in complex with maltohexaose
Authors : Suzuki, R.; Suzuki, E.
Deposited on : 2016-08-08
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

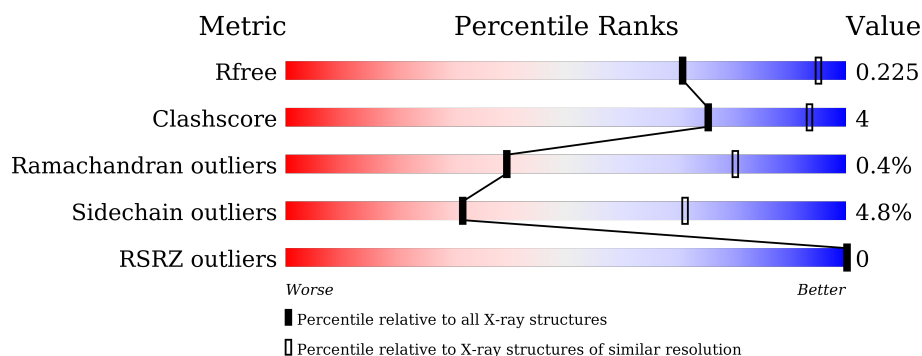
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	793	

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
2	GLC	A	801	-	-	-	X
2	GLC	A	802	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	803	-	-	-	X
2	GLC	A	806	-	-	-	X
2	GLC	A	815	-	-	-	X
2	GLC	A	825	-	-	-	X
3	GOL	A	838	-	-	-	X
3	GOL	A	839	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6863 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.

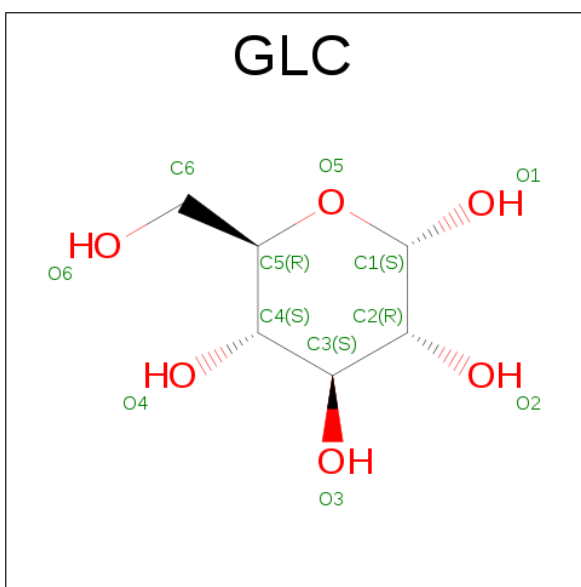
- Molecule 1 is a protein called 1,4-alpha-glucan branching enzyme GlgB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	755	6273	4057	1042	1150	24	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B1WPM8
A	-18	GLY	-	expression tag	UNP B1WPM8
A	-17	SER	-	expression tag	UNP B1WPM8
A	-16	SER	-	expression tag	UNP B1WPM8
A	-15	HIS	-	expression tag	UNP B1WPM8
A	-14	HIS	-	expression tag	UNP B1WPM8
A	-13	HIS	-	expression tag	UNP B1WPM8
A	-12	HIS	-	expression tag	UNP B1WPM8
A	-11	HIS	-	expression tag	UNP B1WPM8
A	-10	HIS	-	expression tag	UNP B1WPM8
A	-9	SER	-	expression tag	UNP B1WPM8
A	-8	SER	-	expression tag	UNP B1WPM8
A	-7	GLY	-	expression tag	UNP B1WPM8
A	-6	LEU	-	expression tag	UNP B1WPM8
A	-5	VAL	-	expression tag	UNP B1WPM8
A	-4	PRO	-	expression tag	UNP B1WPM8
A	-3	ARG	-	expression tag	UNP B1WPM8
A	-2	GLY	-	expression tag	UNP B1WPM8
A	-1	SER	-	expression tag	UNP B1WPM8
A	0	HIS	-	expression tag	UNP B1WPM8

- Molecule 2 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		

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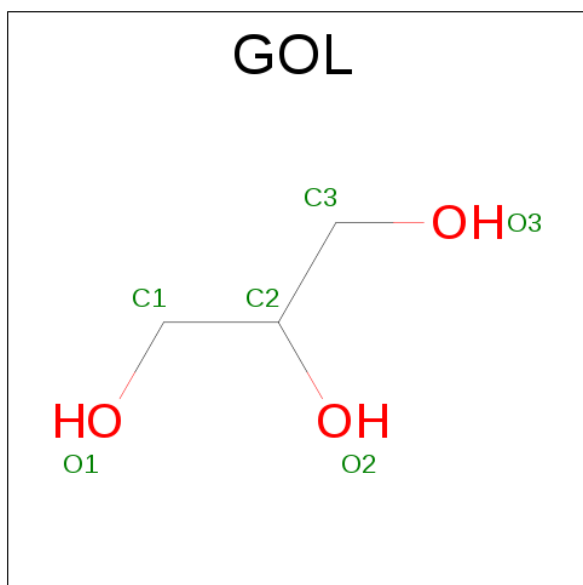
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	166	Total	O	0	0
			166	166		

4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.13Å 134.13Å 184.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.42 – 3.00 42.92 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.42-3.00) 99.8 (42.92-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	13.51 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.163 , 0.224 0.168 , 0.225	Depositor DCC
R_{free} test set	1730 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6863	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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: GOL, MG, 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	0.74	0/6493	0.83	4/8836 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	647	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	A	307	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	647	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	225	ASP	CB-CG-OD2	-5.08	113.73	118.30

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	6273	0	5857	49	0
2	A	411	0	347	6	0
3	A	12	0	16	2	0
4	A	1	0	0	0	1
5	A	166	0	0	0	1
All	All	6863	0	6220	50	1

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 (50) 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:202:ILE:HG22	1:A:202:ILE:O	1.91	0.70
1:A:258:LEU:HD22	1:A:297:LEU:HD13	1.83	0.61
1:A:440:LEU:HD13	1:A:492:TRP:CD2	2.40	0.57
1:A:204:GLU:OE1	2:A:811:GLC:O2	2.21	0.56
1:A:416:VAL:O	1:A:419:VAL:HG12	2.07	0.55
1:A:323:PHE:HB2	2:A:804:GLC:H3	1.90	0.54
1:A:67:VAL:HG11	1:A:74:GLU:HB2	1.91	0.53
1:A:560:GLY:HA2	1:A:606:GLU:OE2	2.10	0.51
1:A:523:ASN:ND2	1:A:567:LYS:O	2.43	0.50
1:A:725:LYS:HE2	1:A:740:ASP:O	2.11	0.50
1:A:240:LYS:O	1:A:244:SER:OG	2.22	0.49
1:A:329:TYR:HB2	2:A:801:GLC:H61	1.95	0.49
1:A:482:ILE:C	1:A:482:ILE:HD12	2.33	0.48
1:A:571:ASP:OD1	1:A:574:GLN:HG3	2.14	0.47
1:A:242:ARG:HG3	1:A:480:PRO:HG2	1.96	0.47
1:A:490:THR:O	1:A:491:GLU:HB2	2.15	0.46
1:A:543:TYR:CZ	1:A:590:PRO:HB2	2.51	0.46
1:A:705:GLU:HA	1:A:751:LEU:HD23	1.98	0.46
1:A:27:CYS:SG	1:A:82:LEU:HD23	2.56	0.45
1:A:617:LEU:HB3	1:A:623:HIS:CD2	2.51	0.45
1:A:706:LEU:HA	1:A:706:LEU:HD12	1.69	0.45
1:A:10:VAL:O	1:A:14:ILE:HG12	2.17	0.45
1:A:211:PHE:C	1:A:336:SER:HB2	2.38	0.45
1:A:618:LEU:HD23	1:A:618:LEU:HA	1.84	0.44
1:A:273:LEU:O	1:A:274:ASN:C	2.56	0.43
1:A:652:GLY:O	1:A:670:ARG:HA	2.18	0.43
1:A:64:MET:HA	1:A:75:CYS:HB2	2.00	0.43
1:A:722:LEU:HD23	2:A:828:GLC:H3	1.98	0.43
1:A:197:ASN:HB2	1:A:382:GLY:HA3	2.01	0.43
1:A:182:VAL:HG11	1:A:185:ILE:HD13	2.00	0.43
1:A:576:TYR:CG	3:A:838:GOL:H12	2.53	0.43
1:A:59:ARG:HA	1:A:59:ARG:NE	2.34	0.43
1:A:704:VAL:O	1:A:751:LEU:HA	2.19	0.43
1:A:701:GLY:HA3	1:A:753:LEU:HD11	2.00	0.42
1:A:732:PHE:O	1:A:733:HIS:C	2.57	0.42
1:A:715:GLY:HA3	3:A:838:GOL:H11	2.02	0.42
1:A:152:ARG:NH2	1:A:198:SER:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ARG:HA	1:A:59:ARG:HE	1.85	0.42
1:A:64:MET:HB3	1:A:73:PHE:HB3	2.01	0.41
1:A:418:ASN:O	1:A:421:PHE:HB3	2.20	0.41
1:A:443:ASN:HB3	1:A:451:TRP:CE2	2.55	0.41
1:A:609:VAL:HG22	1:A:609:VAL:O	2.21	0.41
1:A:443:ASN:HB3	1:A:451:TRP:CD2	2.56	0.41
1:A:270:MET:HG3	1:A:293:SER:HB3	2.03	0.41
1:A:269:LYS:NZ	1:A:278:ASP:OD1	2.53	0.41
1:A:655:TRP:HE1	2:A:837:GLC:H2	1.86	0.41
2:A:831:GLC:H62	2:A:832:GLC:H5	2.03	0.40
1:A:597:MET:HG3	1:A:613:LEU:HD11	2.04	0.40
1:A:419:VAL:HG13	1:A:420:LEU:N	2.37	0.40
1:A:592:LYS:C	1:A:593:LYS:HD3	2.42	0.40

All (1) 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)
4:A:840:MG:MG	5:A:989:HOH:O[3_545]	1.59	0.61

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	753/793 (95%)	711 (94%)	39 (5%)	3 (0%)	39 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	733	HIS
1	A	68	HIS
1	A	598	SER

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	668/700 (95%)	636 (95%)	32 (5%)	31 71

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	38	LYS
1	A	62	ASP
1	A	81	GLU
1	A	155	SER
1	A	192	LYS
1	A	203	TYR
1	A	216	ARG
1	A	244	SER
1	A	283	SER
1	A	307	ASP
1	A	336	SER
1	A	369	HIS
1	A	373	ASP
1	A	413	ASN
1	A	432	ARG
1	A	447	LYS
1	A	466	SER
1	A	525	ASP
1	A	539	SER
1	A	562	SER
1	A	605	SER
1	A	639	GLN
1	A	649	GLU
1	A	667	SER
1	A	672	SER
1	A	686	THR
1	A	691	SER
1	A	706	LEU
1	A	709	SER

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Mol	Chain	Res	Type
1	A	732	PHE
1	A	735	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	35	ASN
1	A	65	ASN
1	A	286	ASN
1	A	634	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](#)

Of 40 ligands modelled in this entry, 1 is monoatomic - leaving 39 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	GLC	A	801	2	11,11,12	1.00	1 (9%)	15,15,17	2.56	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	A	802	2	11,11,12	0.75	0	15,15,17	1.53	2 (13%)
2	GLC	A	803	2	11,11,12	0.62	0	15,15,17	2.36	6 (40%)
2	GLC	A	804	2	11,11,12	0.69	0	15,15,17	1.97	3 (20%)
2	GLC	A	805	2	11,11,12	0.62	0	15,15,17	1.20	2 (13%)
2	GLC	A	806	2	11,11,12	1.14	1 (9%)	15,15,17	2.11	6 (40%)
2	GLC	A	807	2	12,12,12	0.66	0	17,17,17	0.86	0
2	GLC	A	808	2	11,11,12	0.92	1 (9%)	15,15,17	1.70	4 (26%)
2	GLC	A	809	2	11,11,12	0.63	0	15,15,17	2.78	4 (26%)
2	GLC	A	810	2	11,11,12	0.61	0	15,15,17	1.12	1 (6%)
2	GLC	A	811	2	12,12,12	0.83	0	17,17,17	1.83	5 (29%)
2	GLC	A	812	2	11,11,12	1.03	1 (9%)	15,15,17	2.44	6 (40%)
2	GLC	A	813	2	11,11,12	0.74	0	15,15,17	2.11	4 (26%)
2	GLC	A	814	2	11,11,12	0.54	0	15,15,17	2.00	3 (20%)
2	GLC	A	815	2	11,11,12	0.81	0	15,15,17	1.88	4 (26%)
2	GLC	A	816	2	11,11,12	0.62	0	15,15,17	1.54	3 (20%)
2	GLC	A	817	2	11,11,12	0.73	0	15,15,17	1.19	1 (6%)
2	GLC	A	818	2	11,11,12	0.76	0	15,15,17	1.82	4 (26%)
2	GLC	A	819	2	11,11,12	0.49	0	15,15,17	1.92	2 (13%)
2	GLC	A	820	2	11,11,12	0.82	0	15,15,17	1.99	4 (26%)
2	GLC	A	821	2	11,11,12	1.12	1 (9%)	15,15,17	1.99	4 (26%)
2	GLC	A	822	2	11,11,12	0.84	0	15,15,17	1.74	4 (26%)
2	GLC	A	823	2	11,11,12	0.93	1 (9%)	15,15,17	1.57	2 (13%)
2	GLC	A	824	2	11,11,12	0.88	0	15,15,17	2.78	6 (40%)
2	GLC	A	825	2	12,12,12	0.55	0	17,17,17	1.62	3 (17%)
2	GLC	A	826	2	11,11,12	0.49	0	15,15,17	1.56	3 (20%)
2	GLC	A	827	2	11,11,12	0.72	0	15,15,17	1.98	5 (33%)
2	GLC	A	828	2	11,11,12	0.76	0	15,15,17	1.41	3 (20%)
2	GLC	A	829	2	11,11,12	0.69	0	15,15,17	1.76	2 (13%)
2	GLC	A	830	2	11,11,12	0.61	0	15,15,17	1.62	3 (20%)
2	GLC	A	831	2	12,12,12	0.94	1 (8%)	17,17,17	1.73	3 (17%)
2	GLC	A	832	2	11,11,12	0.81	0	15,15,17	2.04	6 (40%)
2	GLC	A	833	2	11,11,12	0.38	0	15,15,17	0.72	0
2	GLC	A	834	2	11,11,12	0.73	0	15,15,17	1.96	3 (20%)
2	GLC	A	835	2	11,11,12	1.04	1 (9%)	15,15,17	2.55	5 (33%)
2	GLC	A	836	2	11,11,12	0.71	0	15,15,17	2.51	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	A	837	2	11,11,12	1.18	1 (9%)	15,15,17	2.81	7 (46%)
3	GOL	A	838	-	5,5,5	0.96	0	5,5,5	1.35	1 (20%)
3	GOL	A	839	-	5,5,5	0.56	0	5,5,5	0.96	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	GLC	A	801	2	-	0/2/19/22	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
2	GLC	A	805	2	-	0/2/19/22	0/1/1/1
2	GLC	A	806	2	-	0/2/19/22	0/1/1/1
2	GLC	A	807	2	-	0/2/22/22	0/1/1/1
2	GLC	A	808	2	-	0/2/19/22	0/1/1/1
2	GLC	A	809	2	-	0/2/19/22	0/1/1/1
2	GLC	A	810	2	-	0/2/19/22	0/1/1/1
2	GLC	A	811	2	-	0/2/22/22	0/1/1/1
2	GLC	A	812	2	-	0/2/19/22	0/1/1/1
2	GLC	A	813	2	-	0/2/19/22	0/1/1/1
2	GLC	A	814	2	-	0/2/19/22	0/1/1/1
2	GLC	A	815	2	-	0/2/19/22	0/1/1/1
2	GLC	A	816	2	-	0/2/19/22	0/1/1/1
2	GLC	A	817	2	-	0/2/19/22	0/1/1/1
2	GLC	A	818	2	-	0/2/19/22	0/1/1/1
2	GLC	A	819	2	-	0/2/19/22	0/1/1/1
2	GLC	A	820	2	-	0/2/19/22	0/1/1/1
2	GLC	A	821	2	-	0/2/19/22	0/1/1/1
2	GLC	A	822	2	-	0/2/19/22	0/1/1/1
2	GLC	A	823	2	-	0/2/19/22	0/1/1/1
2	GLC	A	824	2	-	0/2/19/22	0/1/1/1
2	GLC	A	825	2	-	0/2/22/22	0/1/1/1
2	GLC	A	826	2	-	0/2/19/22	0/1/1/1
2	GLC	A	827	2	-	0/2/19/22	0/1/1/1
2	GLC	A	828	2	-	0/2/19/22	0/1/1/1
2	GLC	A	829	2	-	0/2/19/22	0/1/1/1
2	GLC	A	830	2	-	0/2/19/22	0/1/1/1
2	GLC	A	831	2	-	0/2/22/22	0/1/1/1
2	GLC	A	832	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	833	2	-	0/2/19/22	0/1/1/1
2	GLC	A	834	2	-	0/2/19/22	0/1/1/1
2	GLC	A	835	2	-	0/2/19/22	0/1/1/1
2	GLC	A	836	2	-	0/2/19/22	0/1/1/1
2	GLC	A	837	2	-	0/2/19/22	0/1/1/1
3	GOL	A	838	-	-	0/4/4/4	0/0/0/0
3	GOL	A	839	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	823	GLC	O5-C1	-2.44	1.39	1.43
2	A	835	GLC	O5-C1	-2.19	1.40	1.43
2	A	812	GLC	O5-C1	-2.05	1.40	1.43
2	A	831	GLC	C4-C5	2.00	1.57	1.53
2	A	808	GLC	C2-C3	2.19	1.55	1.52
2	A	801	GLC	C2-C3	2.47	1.55	1.52
2	A	806	GLC	C2-C3	2.51	1.55	1.52
2	A	821	GLC	C2-C3	3.09	1.56	1.52
2	A	837	GLC	C2-C3	3.39	1.57	1.52

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	835	GLC	O5-C1-C2	-5.39	102.28	110.89
2	A	829	GLC	O5-C1-C2	-4.97	102.94	110.89
2	A	834	GLC	O5-C1-C2	-4.74	103.31	110.89
2	A	812	GLC	O3-C3-C2	-4.37	102.00	110.01
2	A	824	GLC	C1-C2-C3	-3.97	104.74	109.55
2	A	818	GLC	O5-C1-C2	-3.96	104.56	110.89
2	A	812	GLC	O5-C5-C4	-3.75	103.93	110.13
2	A	801	GLC	O3-C3-C4	-3.66	102.11	110.36
2	A	825	GLC	C3-C4-C5	-3.63	103.76	110.23
2	A	819	GLC	O4-C4-C3	-3.46	102.56	110.36
2	A	821	GLC	C3-C4-C5	-3.29	104.37	110.23
2	A	821	GLC	O5-C1-C2	-3.20	105.78	110.89
2	A	826	GLC	O5-C1-C2	-3.15	105.85	110.89
2	A	831	GLC	C1-C2-C3	-3.11	105.58	110.68
2	A	830	GLC	O3-C3-C4	-3.08	103.42	110.36
2	A	824	GLC	C2-C3-C4	-3.08	105.68	111.05
2	A	813	GLC	C2-C3-C4	-3.07	105.70	111.05
2	A	803	GLC	C2-C3-C4	-3.02	105.78	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	826	GLC	C3-C4-C5	-3.02	104.84	110.23
2	A	808	GLC	O3-C3-C4	-2.98	103.64	110.36
2	A	831	GLC	O5-C1-C2	-2.97	104.80	110.00
2	A	804	GLC	O3-C3-C4	-2.81	104.02	110.36
2	A	832	GLC	O3-C3-C4	-2.80	104.04	110.36
2	A	834	GLC	O3-C3-C4	-2.77	104.10	110.36
2	A	801	GLC	O5-C1-C2	-2.71	106.57	110.89
2	A	808	GLC	O5-C1-C2	-2.66	106.65	110.89
2	A	829	GLC	O4-C4-C5	-2.65	102.25	109.23
2	A	818	GLC	O4-C4-C3	-2.63	104.42	110.36
2	A	832	GLC	O4-C4-C3	-2.62	104.45	110.36
2	A	803	GLC	C1-C2-C3	-2.58	106.42	109.55
2	A	822	GLC	C6-C5-C4	-2.55	106.60	112.99
2	A	823	GLC	C3-C4-C5	-2.53	105.71	110.23
2	A	830	GLC	O5-C1-C2	-2.40	107.05	110.89
2	A	815	GLC	O5-C1-C2	-2.40	107.05	110.89
2	A	811	GLC	O6-C6-C5	-2.40	103.30	111.30
2	A	809	GLC	C2-C3-C4	-2.36	106.93	111.05
2	A	827	GLC	O4-C4-C3	-2.30	105.17	110.36
2	A	828	GLC	O5-C1-C2	-2.24	107.31	110.89
2	A	837	GLC	C3-C4-C5	-2.24	106.24	110.23
2	A	827	GLC	O3-C3-C4	-2.23	105.33	110.36
2	A	822	GLC	O5-C1-C2	-2.17	107.43	110.89
2	A	816	GLC	O3-C3-C2	-2.16	106.05	110.01
2	A	824	GLC	C6-C5-C4	-2.10	107.72	112.99
2	A	827	GLC	O2-C2-C3	-2.08	106.00	110.19
2	A	832	GLC	C2-C3-C4	-2.08	107.42	111.05
2	A	837	GLC	O5-C1-C2	-2.01	107.68	110.89
2	A	812	GLC	C6-C5-C4	2.01	118.02	112.99
2	A	806	GLC	C3-C4-C5	2.02	113.83	110.23
2	A	813	GLC	O3-C3-C2	2.03	113.73	110.01
2	A	801	GLC	O5-C5-C6	2.09	111.82	107.34
2	A	803	GLC	O5-C5-C4	2.11	113.63	110.13
2	A	814	GLC	O5-C1-C2	2.14	114.31	110.89
2	A	820	GLC	O4-C4-C5	2.14	114.86	109.23
2	A	808	GLC	O5-C5-C6	2.16	111.96	107.34
2	A	832	GLC	O3-C3-C2	2.18	113.99	110.01
2	A	813	GLC	O5-C5-C4	2.21	113.80	110.13
2	A	809	GLC	O2-C2-C1	2.22	113.68	109.23
2	A	805	GLC	C1-O5-C5	2.24	115.43	112.14
2	A	802	GLC	C1-C2-C3	2.26	112.29	109.55
2	A	837	GLC	O3-C3-C2	2.27	114.17	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	835	GLC	C2-C3-C4	2.28	115.02	111.05
2	A	828	GLC	C2-C3-C4	2.29	115.03	111.05
2	A	806	GLC	C1-C2-C3	2.35	112.40	109.55
2	A	822	GLC	O5-C5-C6	2.39	112.45	107.34
2	A	811	GLC	O5-C5-C4	2.39	114.22	109.67
2	A	837	GLC	C1-O5-C5	2.40	115.67	112.14
2	A	806	GLC	O2-C2-C3	2.45	115.12	110.19
3	A	838	GOL	O1-C1-C2	2.51	122.71	109.97
2	A	835	GLC	C1-O5-C5	2.52	115.84	112.14
2	A	810	GLC	C1-O5-C5	2.53	115.86	112.14
2	A	817	GLC	C1-C2-C3	2.53	112.62	109.55
2	A	803	GLC	O3-C3-C2	2.56	114.70	110.01
2	A	806	GLC	O5-C1-C2	2.60	115.05	110.89
2	A	818	GLC	O5-C5-C4	2.60	114.44	110.13
2	A	824	GLC	O3-C3-C2	2.62	114.80	110.01
2	A	815	GLC	O2-C2-C1	2.62	114.48	109.23
2	A	803	GLC	O5-C5-C6	2.72	113.16	107.34
2	A	825	GLC	C1-O5-C5	2.74	118.78	113.54
2	A	801	GLC	C3-C4-C5	2.74	115.11	110.23
2	A	806	GLC	O5-C5-C4	2.74	114.68	110.13
2	A	805	GLC	C1-C2-C3	2.77	112.91	109.55
2	A	834	GLC	O5-C5-C6	2.77	113.27	107.34
2	A	827	GLC	C1-O5-C5	2.84	116.32	112.14
2	A	811	GLC	C1-O5-C5	2.85	118.99	113.54
2	A	826	GLC	C1-O5-C5	2.91	116.42	112.14
2	A	825	GLC	O5-C1-C2	2.92	115.11	110.00
2	A	820	GLC	C6-C5-C4	2.92	120.31	112.99
2	A	837	GLC	C2-C3-C4	2.96	116.20	111.05
2	A	837	GLC	O5-C5-C6	3.07	113.91	107.34
2	A	828	GLC	C1-C2-C3	3.07	113.28	109.55
2	A	816	GLC	C2-C3-C4	3.13	116.51	111.05
2	A	812	GLC	O2-C2-C1	3.16	115.56	109.23
2	A	831	GLC	C3-C4-C5	3.20	115.93	110.23
2	A	818	GLC	C1-O5-C5	3.20	116.85	112.14
2	A	832	GLC	C1-C2-C3	3.24	113.48	109.55
2	A	811	GLC	O2-C2-C1	3.25	116.85	109.74
2	A	811	GLC	O5-C5-C6	3.25	114.80	106.38
2	A	816	GLC	C1-C2-C3	3.39	113.66	109.55
2	A	820	GLC	C1-O5-C5	3.42	117.18	112.14
2	A	815	GLC	O5-C5-C4	3.49	115.92	110.13
2	A	801	GLC	C2-C3-C4	3.58	117.29	111.05
2	A	830	GLC	C1-O5-C5	3.61	117.44	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	812	GLC	C2-C3-C4	3.66	117.43	111.05
2	A	804	GLC	C2-C3-C4	3.70	117.50	111.05
2	A	822	GLC	C1-C2-C3	3.72	114.06	109.55
2	A	821	GLC	O3-C3-C2	3.84	117.04	110.01
2	A	808	GLC	C1-C2-C3	3.91	114.29	109.55
2	A	832	GLC	O5-C5-C4	3.97	116.71	110.13
2	A	823	GLC	C1-O5-C5	3.99	118.01	112.14
2	A	820	GLC	C1-C2-C3	4.00	114.40	109.55
2	A	814	GLC	O5-C5-C4	4.05	116.83	110.13
2	A	821	GLC	C1-C2-C3	4.09	114.51	109.55
2	A	801	GLC	O5-C5-C4	4.14	117.00	110.13
2	A	815	GLC	C1-O5-C5	4.17	118.28	112.14
2	A	836	GLC	O5-C5-C4	4.30	117.26	110.13
2	A	802	GLC	C1-O5-C5	4.40	118.62	112.14
2	A	809	GLC	O5-C5-C4	4.47	117.53	110.13
2	A	804	GLC	C1-O5-C5	4.66	119.00	112.14
2	A	827	GLC	C1-C2-C3	4.89	115.47	109.55
2	A	835	GLC	C1-C2-C3	4.90	115.48	109.55
2	A	814	GLC	C1-O5-C5	4.94	119.40	112.14
2	A	812	GLC	C1-C2-C3	4.95	115.55	109.55
2	A	835	GLC	O5-C5-C4	4.97	118.37	110.13
2	A	806	GLC	C1-O5-C5	5.35	120.01	112.14
2	A	801	GLC	C1-C2-C3	5.42	116.12	109.55
2	A	824	GLC	C1-O5-C5	5.51	120.24	112.14
2	A	813	GLC	C1-O5-C5	5.69	120.50	112.14
2	A	803	GLC	C1-O5-C5	5.95	120.89	112.14
2	A	824	GLC	O5-C5-C4	6.03	120.12	110.13
2	A	819	GLC	C1-O5-C5	6.06	121.05	112.14
2	A	837	GLC	C1-C2-C3	8.14	119.41	109.55
2	A	836	GLC	C1-O5-C5	8.15	124.13	112.14
2	A	809	GLC	C1-O5-C5	8.75	125.01	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GLC	1	0
2	A	804	GLC	1	0
2	A	811	GLC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	828	GLC	1	0
2	A	831	GLC	1	0
2	A	832	GLC	1	0
2	A	837	GLC	1	0
3	A	838	GOL	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 [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	755/793 (95%)	-0.56	0 100 100	21, 36, 60, 109	0

There are no RSRZ outliers to report.

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](#)

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GLC	A	806	11/12	0.60	0.56	9.12	80,105,122,123	0
3	GOL	A	838	6/6	0.87	0.29	8.32	48,53,54,57	0
2	GLC	A	803	11/12	0.90	0.29	6.97	74,102,114,122	0
2	GLC	A	801	11/12	0.68	0.37	6.04	82,101,110,119	0
2	GLC	A	815	11/12	0.94	0.22	3.69	53,60,67,68	0
2	GLC	A	802	11/12	0.87	0.23	2.51	83,103,112,112	0
3	GOL	A	839	6/6	0.95	0.16	2.49	46,49,51,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GLC	A	825	12/12	0.90	0.37	2.15	85,96,103,105	0
2	GLC	A	817	11/12	0.93	0.27	1.98	64,75,98,101	0
2	GLC	A	836	11/12	0.88	0.22	1.56	71,91,99,100	0
2	GLC	A	835	11/12	0.85	0.24	1.44	76,89,90,91	0
2	GLC	A	812	11/12	0.95	0.22	1.41	57,64,70,85	0
2	GLC	A	816	11/12	0.97	0.16	0.65	51,53,59,64	0
2	GLC	A	830	11/12	0.96	0.16	0.65	44,46,47,48	0
2	GLC	A	833	11/12	0.97	0.17	0.62	32,40,50,52	0
2	GLC	A	823	11/12	0.96	0.23	0.13	48,55,61,66	0
2	GLC	A	829	11/12	0.98	0.18	-0.15	36,40,44,45	0
2	GLC	A	822	11/12	0.98	0.16	-0.35	44,47,56,58	0
2	GLC	A	832	11/12	0.98	0.13	-	32,38,41,44	0
2	GLC	A	804	11/12	0.75	0.32	-	88,105,112,122	0
2	GLC	A	828	11/12	0.97	0.28	-	42,49,52,54	0
2	GLC	A	820	11/12	0.89	0.37	-	73,84,95,101	0
4	MG	A	840	1/1	0.98	0.06	-	14,14,14,14	0
2	GLC	A	827	11/12	0.95	0.27	-	56,61,63,64	0
2	GLC	A	821	11/12	0.85	0.29	-	64,71,78,79	0
2	GLC	A	814	11/12	0.89	0.34	-	64,81,92,97	0
2	GLC	A	808	11/12	0.94	0.27	-	52,56,63,64	0
2	GLC	A	809	11/12	0.95	0.36	-	57,67,80,81	0
2	GLC	A	805	11/12	0.77	0.42	-	101,124,130,132	0
2	GLC	A	826	11/12	0.96	0.29	-	60,66,72,74	0
2	GLC	A	837	11/12	0.86	0.34	-	70,82,89,91	0
2	GLC	A	831	12/12	0.88	0.35	-	52,70,78,79	0
2	GLC	A	819	11/12	0.87	0.32	-	84,90,96,97	0
2	GLC	A	824	11/12	0.87	0.31	-	73,77,84,86	0
2	GLC	A	807	12/12	0.88	0.35	-	69,83,92,97	0
2	GLC	A	810	11/12	0.85	0.47	-	77,87,94,95	0
2	GLC	A	834	11/12	0.89	0.32	-	55,59,65,65	0
2	GLC	A	811	12/12	0.88	0.18	-	46,49,57,64	0
2	GLC	A	818	11/12	0.83	0.42	-	93,106,115,122	0
2	GLC	A	813	11/12	0.86	0.34	-	72,83,88,90	0

6.5 Other polymers ⓘ

There are no such residues in this entry.