



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2017 – 12:44 AM EDT

PDB ID : 5X7R
Title : Crystal structure of Paenibacillus sp. 598K alpha-1,6-glucosyltransferase complexed with isomaltohexaose
Authors : Fujimoto, Z.; Kishine, N.; Suzuki, N.; Momma, M.; Ichinose, H.; Kimura, A.; Funane, K.
Deposited on : unknown
Resolution : 1.95 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

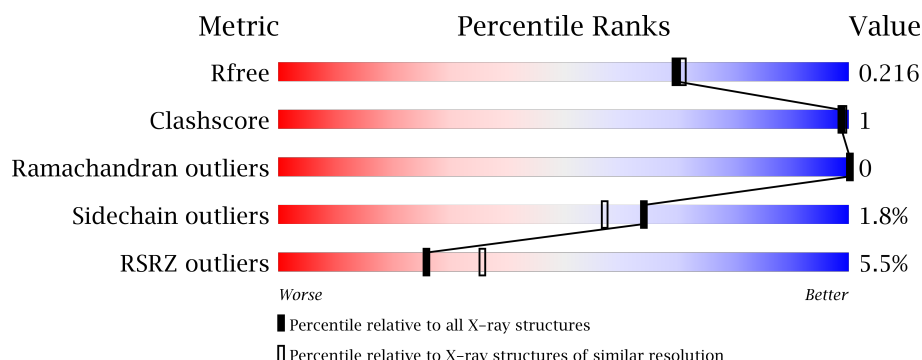
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	100719	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	1263	<div> <div>6%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>
1	B	1263	<div> <div>5%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>

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
10	EDO	A	1802	-	-	-	X
10	EDO	A	1803	-	-	-	X
10	EDO	A	1804	-	-	-	X
10	EDO	B	1801	-	-	-	X
10	EDO	B	1803	-	-	-	X
10	EDO	B	1804	-	-	-	X
4	GLC	A	1461	-	-	-	X
4	GLC	B	1461	-	-	-	X
5	ACR	A	1481	-	-	-	X
8	SO4	A	1707	-	-	-	X
9	MES	A	1704	-	-	-	X
9	MES	A	1705	-	-	-	X
9	MES	A	1706	-	-	-	X
9	MES	A	1709	-	-	-	X
9	MES	A	1711	-	-	-	X
9	MES	B	1706	-	-	-	X
9	MES	B	1707	-	-	-	X
9	MES	B	1708	-	-	-	X
9	MES	B	1711	-	-	-	X
9	MES	B	1712	-	-	-	X
9	MES	B	1716	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 21450 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 Glycoside hydrolase family 31 alpha-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1247	Total	C	N	O	S	0	0	0
			9601	6023	1633	1923	22			
1	B	1247	Total	C	N	O	S	0	0	0
			9601	6023	1633	1923	22			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	HIS	-	expression tag	UNP A0A193PKW5
A	20	HIS	-	expression tag	UNP A0A193PKW5
A	21	HIS	-	expression tag	UNP A0A193PKW5
A	22	HIS	-	expression tag	UNP A0A193PKW5
A	23	HIS	-	expression tag	UNP A0A193PKW5
A	24	HIS	-	expression tag	UNP A0A193PKW5
A	25	SER	-	expression tag	UNP A0A193PKW5
A	26	SER	-	expression tag	UNP A0A193PKW5
A	27	GLY	-	expression tag	UNP A0A193PKW5
A	28	LEU	-	expression tag	UNP A0A193PKW5
A	29	VAL	-	expression tag	UNP A0A193PKW5
A	30	PRO	-	expression tag	UNP A0A193PKW5
A	31	ARG	-	expression tag	UNP A0A193PKW5
A	32	GLY	-	expression tag	UNP A0A193PKW5
A	33	SER	-	expression tag	UNP A0A193PKW5
A	34	HIS	-	expression tag	UNP A0A193PKW5
A	35	MET	-	expression tag	UNP A0A193PKW5
B	19	HIS	-	expression tag	UNP A0A193PKW5
B	20	HIS	-	expression tag	UNP A0A193PKW5
B	21	HIS	-	expression tag	UNP A0A193PKW5
B	22	HIS	-	expression tag	UNP A0A193PKW5
B	23	HIS	-	expression tag	UNP A0A193PKW5
B	24	HIS	-	expression tag	UNP A0A193PKW5
B	25	SER	-	expression tag	UNP A0A193PKW5
B	26	SER	-	expression tag	UNP A0A193PKW5

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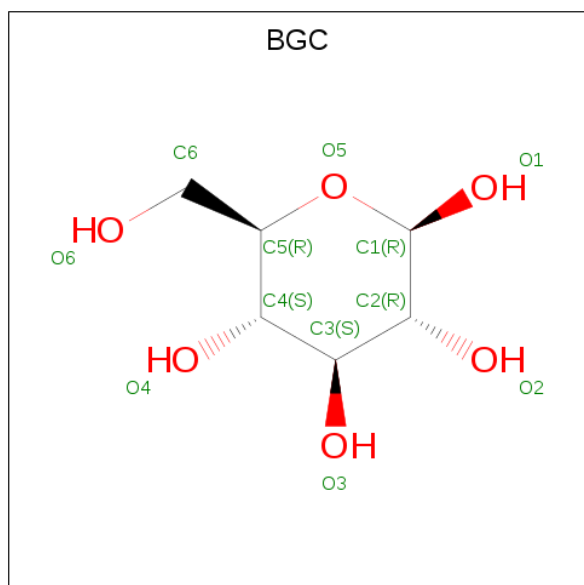
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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLY	-	expression tag	UNP A0A193PKW5
B	28	LEU	-	expression tag	UNP A0A193PKW5
B	29	VAL	-	expression tag	UNP A0A193PKW5
B	30	PRO	-	expression tag	UNP A0A193PKW5
B	31	ARG	-	expression tag	UNP A0A193PKW5
B	32	GLY	-	expression tag	UNP A0A193PKW5
B	33	SER	-	expression tag	UNP A0A193PKW5
B	34	HIS	-	expression tag	UNP A0A193PKW5
B	35	MET	-	expression tag	UNP A0A193PKW5

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Ca 3 3	0	0
2	A	3	Total Ca 3 3	0	0

- Molecule 3 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: C₆H₁₂O₆).



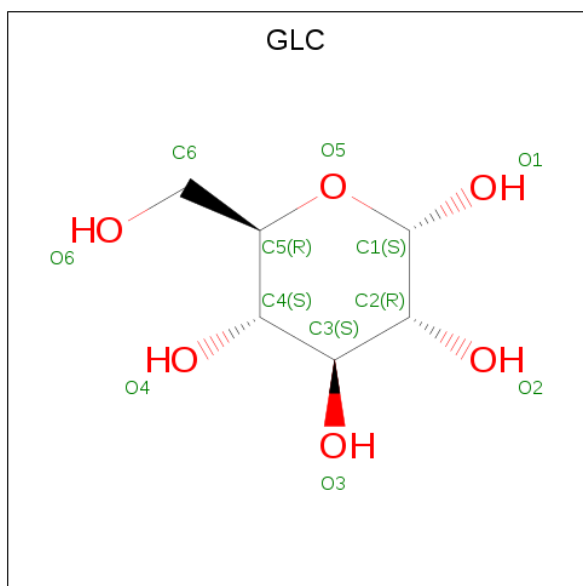
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 6 6	0	0
3	A	1	Total C O 12 6 6	0	0

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

- Molecule 4 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C₆H₁₂O₆).



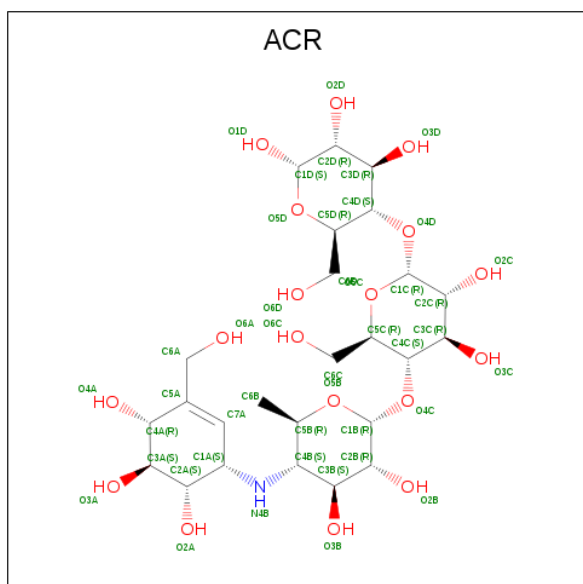
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			12	6	6		
4	A	1	Total	C	O	0	0
			12	6	6		
4	A	1	Total	C	O	0	0
			11	6	5		
4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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			12	6	6		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is ALPHA-ACARBOSE (three-letter code: ACR) (formula: $C_{25}H_{43}NO_{18}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	13	1	8		
5	B	1	Total	C	N	O	0	0
			22	13	1	8		

- Molecule 6 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ni	0	0
			2	2		

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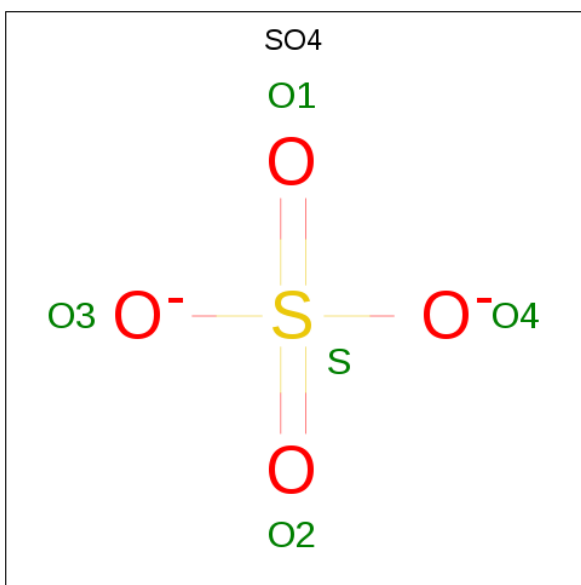
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Ni	0	0
			2	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	10	Total	Mg	0	0
			10	10		
7	A	10	Total	Mg	0	0
			10	10		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



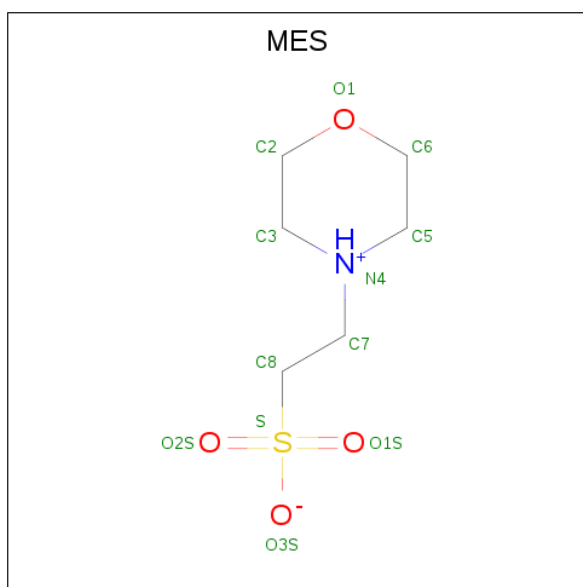
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	O	S		0	0
			5	4	1			
8	B	1	Total	O	S		0	0
			5	4	1			
8	B	1	Total	O	S		0	0
			5	4	1			
8	B	1	Total	O	S		0	0
			5	4	1			
8	B	1	Total	O	S		0	0
			5	4	1			
8	B	1	Total	O	S		0	0
			5	4	1			
8	B	1	Total	O	S		0	0
			5	4	1			

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



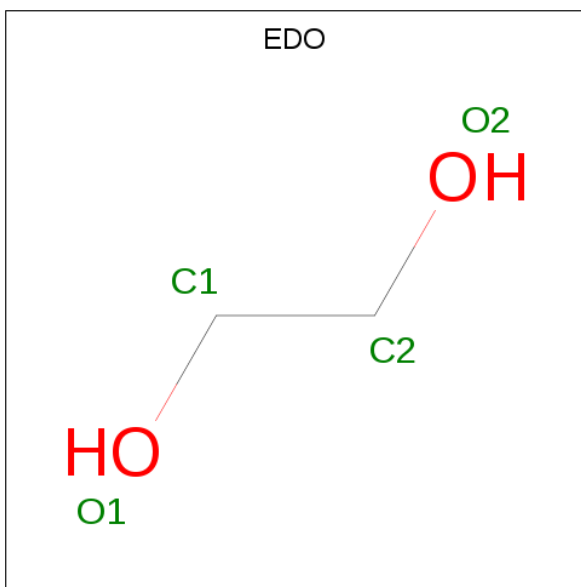
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

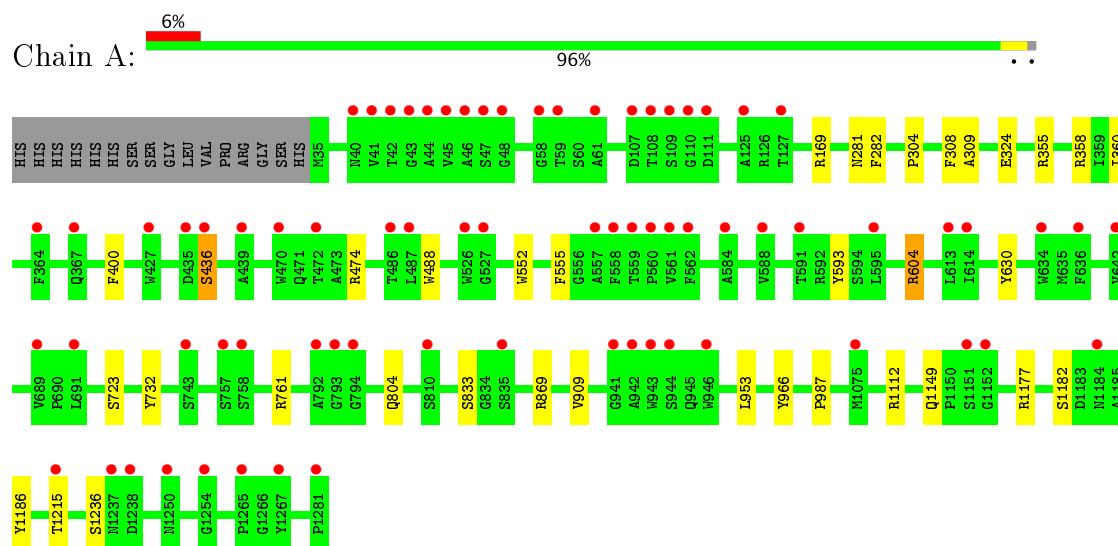
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	828	Total	O	0	0
			828	828		
11	B	824	Total	O	0	0
			824	824		

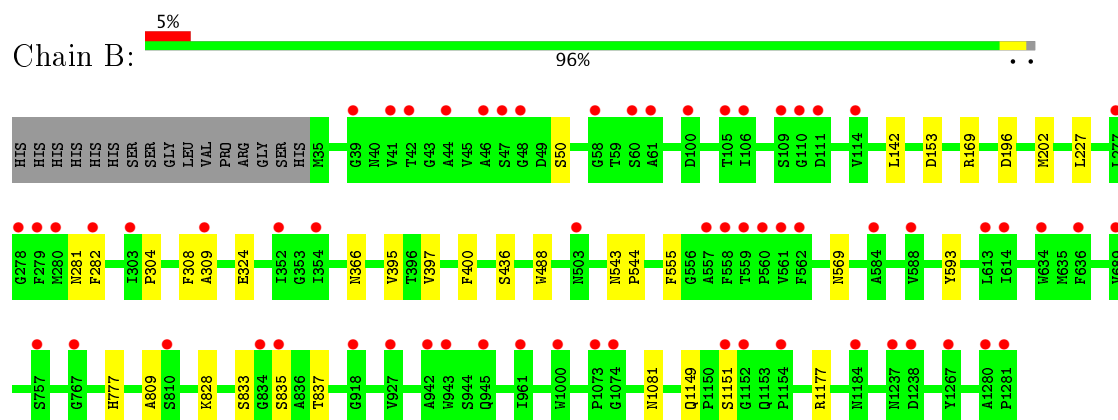
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Glycoside hydrolase family 31 alpha-glucosidase



- Molecule 1: Glycoside hydrolase family 31 alpha-glucosidase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	184.33Å 271.26Å 133.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	152.46 – 1.95 47.51 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.4 (152.46-1.95) 96.8 (47.51-1.94)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.82 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.178 , 0.208 0.188 , 0.216	Depositor DCC
R_{free} test set	11854 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	26.9	Xtriage
Anisotropy	0.710	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21450	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% 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: NI, MG, BGC, CA, GLC, EDO, ACR, SO4, MES

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	0.45	0/9863	0.68	5/13473 (0.0%)
1	B	0.46	0/9863	0.68	2/13473 (0.0%)
All	All	0.46	0/19726	0.68	7/26946 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	196	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	355	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	474	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	A	869	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	1112	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	B	196	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	358	ARG	NE-CZ-NH1	5.02	122.81	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	9601	0	8954	14	1
1	B	9601	0	8954	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	24	0	23	0	0
3	B	12	0	12	0	0
4	A	113	0	100	1	0
4	B	69	0	63	0	0
5	A	22	0	22	0	0
5	B	22	0	22	0	1
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	10	0	0	0	0
7	B	10	0	0	0	0
8	A	30	0	0	0	0
8	B	50	0	0	0	0
9	A	96	0	104	1	0
9	B	96	0	104	1	0
10	A	16	0	24	0	0
10	B	16	0	24	0	0
11	A	828	0	0	2	0
11	B	824	0	0	2	0
All	All	21450	0	18406	21	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 1.

All (21) 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:360:ILE:HD13	1:B:397:VAL:HG12	1.67	0.76
1:B:777:HIS:CD2	11:B:2387:HOH:O	2.49	0.64
9:B:1711:MES:O1S	11:B:2001:HOH:O	2.12	0.63
1:A:761:ARG:NH1	11:A:2006:HOH:O	2.33	0.62
1:A:604:ARG:HD3	1:A:732:TYR:CD1	2.36	0.61
1:A:436:SER:HA	4:A:1413:GLC:O2	2.05	0.57
1:B:366:ASN:HB2	1:B:569:ASN:ND2	2.24	0.52
1:A:360:ILE:HD12	1:B:395:VAL:CG1	2.40	0.50
1:A:630:TYR:OH	11:A:2001:HOH:O	2.20	0.48
1:A:909:VAL:HG21	1:A:953:LEU:HD12	1.95	0.47
1:A:987:PRO:HG2	9:A:1711:MES:H51	1.96	0.47
1:A:282:PHE:CG	1:A:309:ALA:HB3	2.53	0.44
1:A:304:PRO:HB2	1:B:593:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:PHE:CG	1:B:309:ALA:HB3	2.52	0.44
1:A:360:ILE:HD12	1:B:395:VAL:HG11	1.98	0.44
1:B:543:ASN:HB3	1:B:544:PRO:HD2	2.01	0.43
1:A:593:TYR:CE1	1:B:304:PRO:HB2	2.55	0.41
1:B:809:ALA:O	1:B:828:LYS:NZ	2.40	0.41
1:A:604:ARG:HD3	1:A:732:TYR:CE1	2.54	0.41
1:A:1182:SER:HB3	1:A:1186:TYR:CD1	2.56	0.41
1:B:142:LEU:N	1:B:142:LEU:HD23	2.36	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)
1:A:1215:THR:OG1	5:B:1481:ACR:O6A[6_555]	1.99	0.21

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	1245/1263 (99%)	1215 (98%)	30 (2%)	0	100	100
1	B	1245/1263 (99%)	1215 (98%)	30 (2%)	0	100	100
All	All	2490/2526 (99%)	2430 (98%)	60 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	997/1011 (99%)	980 (98%)	17 (2%)	66	60
1	B	997/1011 (99%)	978 (98%)	19 (2%)	62	55
All	All	1994/2022 (99%)	1958 (98%)	36 (2%)	64	57

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	ARG
1	A	281	ASN
1	A	308	PHE
1	A	324	GLU
1	A	400	PHE
1	A	436	SER
1	A	488	TRP
1	A	552	TRP
1	A	555	PHE
1	A	604	ARG
1	A	723	SER
1	A	804	GLN
1	A	833	SER
1	A	966	TYR
1	A	1149	GLN
1	A	1177	ARG
1	A	1236	SER
1	B	50	SER
1	B	153	ASP
1	B	169	ARG
1	B	202	MET
1	B	227	LEU
1	B	281	ASN
1	B	308	PHE
1	B	324	GLU
1	B	400	PHE
1	B	436	SER
1	B	488	TRP
1	B	555	PHE
1	B	833	SER
1	B	835	SER
1	B	837	THR
1	B	1081	ASN

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Mol	Chain	Res	Type
1	B	1149	GLN
1	B	1151	SER
1	B	1177	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	949	GLN
1	A	1226	HIS
1	B	440	GLN
1	B	777	HIS
1	B	1213	ASN
1	B	1226	HIS
1	B	1250	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 91 ligands modelled in this entry, 30 are monoatomic - leaving 61 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	BGC	A	1401	-	12,12,12	0.49	0	17,17,17	0.67	0
4	GLC	A	1411	4	11,11,12	0.72	0	13,15,17	0.88	1 (7%)
4	GLC	A	1412	4	11,11,12	0.52	0	13,15,17	1.08	1 (7%)
4	GLC	A	1413	4	11,11,12	0.48	0	13,15,17	1.01	1 (7%)
4	GLC	A	1414	3,4	11,11,12	0.38	0	13,15,17	0.58	0
3	BGC	A	1415	4	12,12,12	0.47	0	17,17,17	1.06	1 (5%)
4	GLC	A	1431	4	11,11,12	0.50	0	13,15,17	0.93	0
4	GLC	A	1432	4	11,11,12	0.39	0	13,15,17	1.19	2 (15%)
4	GLC	A	1433	4	12,12,12	0.65	0	17,17,17	0.63	0
4	GLC	A	1461	-	12,12,12	0.70	0	17,17,17	0.74	0
4	GLC	A	1471	4	11,11,12	0.44	0	13,15,17	1.15	1 (7%)
4	GLC	A	1472	4	12,12,12	0.59	0	17,17,17	1.22	1 (5%)
5	ACR	A	1481	-	21,23,47	0.66	0	22,34,70	0.83	1 (4%)
8	SO4	A	1701	-	4,4,4	0.40	0	6,6,6	0.12	0
8	SO4	A	1702	-	4,4,4	0.44	0	6,6,6	0.26	0
8	SO4	A	1703	-	4,4,4	0.35	0	6,6,6	0.17	0
9	MES	A	1704	-	12,12,12	1.89	1 (8%)	14,16,16	1.77	2 (14%)
9	MES	A	1705	-	12,12,12	1.87	1 (8%)	14,16,16	2.67	2 (14%)
9	MES	A	1706	-	12,12,12	2.03	1 (8%)	14,16,16	1.85	2 (14%)
8	SO4	A	1707	-	4,4,4	0.39	0	6,6,6	0.22	0
9	MES	A	1708	-	12,12,12	2.20	1 (8%)	14,16,16	1.71	3 (21%)
9	MES	A	1709	-	12,12,12	1.98	1 (8%)	14,16,16	2.33	1 (7%)
8	SO4	A	1710	-	4,4,4	0.42	0	6,6,6	0.40	0
9	MES	A	1711	-	12,12,12	2.02	1 (8%)	14,16,16	2.05	5 (35%)
9	MES	A	1712	-	12,12,12	2.19	1 (8%)	14,16,16	1.37	1 (7%)
9	MES	A	1713	-	12,12,12	2.15	1 (8%)	14,16,16	2.21	2 (14%)
8	SO4	A	1714	-	4,4,4	0.40	0	6,6,6	0.13	0
10	EDO	A	1801	-	3,3,3	0.44	0	2,2,2	0.27	0
10	EDO	A	1802	-	3,3,3	0.40	0	2,2,2	0.44	0
10	EDO	A	1803	-	3,3,3	0.33	0	2,2,2	0.49	0
10	EDO	A	1804	-	3,3,3	0.62	0	2,2,2	0.79	0
3	BGC	B	1401	-	12,12,12	0.45	0	17,17,17	0.61	0
4	GLC	B	1431	4	11,11,12	0.37	0	13,15,17	1.04	1 (7%)
4	GLC	B	1432	4	11,11,12	0.41	0	13,15,17	1.16	1 (7%)
4	GLC	B	1433	4	12,12,12	0.54	0	17,17,17	0.92	1 (5%)
4	GLC	B	1461	-	12,12,12	0.59	0	17,17,17	0.77	0
4	GLC	B	1471	4	11,11,12	0.38	0	13,15,17	0.81	1 (7%)
4	GLC	B	1472	4	12,12,12	0.51	0	17,17,17	0.74	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACR	B	1481	-	21,23,47	0.75	0	22,34,70	0.99	1 (4%)
9	MES	B	1701	-	12,12,12	2.22	1 (8%)	14,16,16	1.59	3 (21%)
8	SO4	B	1702	-	4,4,4	0.42	0	6,6,6	0.32	0
8	SO4	B	1703	-	4,4,4	0.37	0	6,6,6	0.17	0
8	SO4	B	1704	-	4,4,4	0.42	0	6,6,6	0.14	0
8	SO4	B	1705	-	4,4,4	0.41	0	6,6,6	0.17	0
9	MES	B	1706	-	12,12,12	2.06	1 (8%)	14,16,16	2.01	3 (21%)
9	MES	B	1707	-	12,12,12	1.97	1 (8%)	14,16,16	2.02	3 (21%)
9	MES	B	1708	-	12,12,12	1.84	1 (8%)	14,16,16	2.49	5 (35%)
8	SO4	B	1709	-	4,4,4	0.43	0	6,6,6	0.15	0
8	SO4	B	1710	-	4,4,4	0.40	0	6,6,6	0.28	0
9	MES	B	1711	-	12,12,12	1.97	1 (8%)	14,16,16	1.68	3 (21%)
9	MES	B	1712	-	12,12,12	2.11	1 (8%)	14,16,16	1.29	2 (14%)
8	SO4	B	1713	-	4,4,4	0.54	0	6,6,6	0.23	0
9	MES	B	1714	-	12,12,12	2.05	1 (8%)	14,16,16	1.42	2 (14%)
8	SO4	B	1715	-	4,4,4	0.48	0	6,6,6	0.23	0
9	MES	B	1716	-	12,12,12	2.04	1 (8%)	14,16,16	1.95	2 (14%)
8	SO4	B	1717	-	4,4,4	0.44	0	6,6,6	0.12	0
8	SO4	B	1718	-	4,4,4	0.47	0	6,6,6	0.22	0
10	EDO	B	1801	-	3,3,3	0.46	0	2,2,2	0.02	0
10	EDO	B	1802	-	3,3,3	0.37	0	2,2,2	0.25	0
10	EDO	B	1803	-	3,3,3	0.27	0	2,2,2	0.70	0
10	EDO	B	1804	-	3,3,3	0.39	0	2,2,2	0.66	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	BGC	A	1401	-	-	0/2/22/22	0/1/1/1
4	GLC	A	1411	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1412	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1413	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1414	3,4	-	0/2/19/22	0/1/1/1
3	BGC	A	1415	4	-	0/2/22/22	0/1/1/1
4	GLC	A	1431	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1432	4	-	0/2/19/22	0/1/1/1
4	GLC	A	1433	4	-	0/2/22/22	0/1/1/1
4	GLC	A	1461	-	-	0/2/22/22	0/1/1/1
4	GLC	A	1471	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLC	A	1472	4	-	0/2/22/22	0/1/1/1
5	ACR	A	1481	-	-	0/6/46/98	0/2/2/4
8	SO4	A	1701	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1702	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1703	-	-	0/0/0/0	0/0/0/0
9	MES	A	1704	-	-	0/6/14/14	0/1/1/1
9	MES	A	1705	-	-	0/6/14/14	0/1/1/1
9	MES	A	1706	-	-	0/6/14/14	0/1/1/1
8	SO4	A	1707	-	-	0/0/0/0	0/0/0/0
9	MES	A	1708	-	-	0/6/14/14	0/1/1/1
9	MES	A	1709	-	-	0/6/14/14	0/1/1/1
8	SO4	A	1710	-	-	0/0/0/0	0/0/0/0
9	MES	A	1711	-	-	0/6/14/14	0/1/1/1
9	MES	A	1712	-	-	0/6/14/14	0/1/1/1
9	MES	A	1713	-	-	0/6/14/14	0/1/1/1
8	SO4	A	1714	-	-	0/0/0/0	0/0/0/0
10	EDO	A	1801	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1802	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1803	-	-	0/1/1/1	0/0/0/0
10	EDO	A	1804	-	-	0/1/1/1	0/0/0/0
3	BGC	B	1401	-	-	0/2/22/22	0/1/1/1
4	GLC	B	1431	4	-	0/2/19/22	0/1/1/1
4	GLC	B	1432	4	-	0/2/19/22	0/1/1/1
4	GLC	B	1433	4	-	0/2/22/22	0/1/1/1
4	GLC	B	1461	-	-	0/2/22/22	0/1/1/1
4	GLC	B	1471	4	-	0/2/19/22	0/1/1/1
4	GLC	B	1472	4	-	0/2/22/22	0/1/1/1
5	ACR	B	1481	-	-	0/6/46/98	0/2/2/4
9	MES	B	1701	-	-	0/6/14/14	0/1/1/1
8	SO4	B	1702	-	-	0/0/0/0	0/0/0/0
8	SO4	B	1703	-	-	0/0/0/0	0/0/0/0
8	SO4	B	1704	-	-	0/0/0/0	0/0/0/0
8	SO4	B	1705	-	-	0/0/0/0	0/0/0/0
9	MES	B	1706	-	-	0/6/14/14	0/1/1/1
9	MES	B	1707	-	-	0/6/14/14	0/1/1/1
9	MES	B	1708	-	-	0/6/14/14	0/1/1/1
8	SO4	B	1709	-	-	0/0/0/0	0/0/0/0
8	SO4	B	1710	-	-	0/0/0/0	0/0/0/0
9	MES	B	1711	-	-	0/6/14/14	0/1/1/1
9	MES	B	1712	-	-	0/6/14/14	0/1/1/1
8	SO4	B	1713	-	-	0/0/0/0	0/0/0/0
9	MES	B	1714	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	SO4	B	1715	-	-	0/0/0/0	0/0/0/0
9	MES	B	1716	-	-	0/6/14/14	0/1/1/1
8	SO4	B	1717	-	-	0/0/0/0	0/0/0/0
8	SO4	B	1718	-	-	0/0/0/0	0/0/0/0
10	EDO	B	1801	-	-	0/1/1/1	0/0/0/0
10	EDO	B	1802	-	-	0/1/1/1	0/0/0/0
10	EDO	B	1803	-	-	0/1/1/1	0/0/0/0
10	EDO	B	1804	-	-	0/1/1/1	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1708	MES	C8-S	-7.31	1.66	1.77
9	B	1701	MES	C8-S	-7.28	1.66	1.77
9	A	1712	MES	C8-S	-7.21	1.66	1.77
9	A	1713	MES	C8-S	-7.13	1.66	1.77
9	B	1712	MES	C8-S	-6.98	1.67	1.77
9	B	1706	MES	C8-S	-6.77	1.67	1.77
9	A	1706	MES	C8-S	-6.73	1.67	1.77
9	B	1714	MES	C8-S	-6.71	1.67	1.77
9	A	1711	MES	C8-S	-6.64	1.67	1.77
9	B	1716	MES	C8-S	-6.59	1.67	1.77
9	B	1711	MES	C8-S	-6.54	1.67	1.77
9	A	1709	MES	C8-S	-6.44	1.67	1.77
9	B	1707	MES	C8-S	-6.40	1.67	1.77
9	A	1704	MES	C8-S	-6.10	1.68	1.77
9	A	1705	MES	C8-S	-5.97	1.68	1.77
9	B	1708	MES	C8-S	-5.76	1.68	1.77

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1481	ACR	C7A-C1A-N4B	-3.28	106.13	110.88
5	A	1481	ACR	C7A-C1A-N4B	-2.35	107.48	110.88
3	A	1415	BGC	O2-C2-C3	-2.26	105.44	110.36
9	A	1711	MES	O1-C2-C3	-2.22	106.87	111.83
9	B	1708	MES	O3S-S-O1S	-2.07	106.64	111.37
4	A	1412	GLC	O6-C6-C5	-2.05	104.46	111.34
4	A	1411	GLC	C1-O5-C5	2.06	115.00	112.17
9	B	1701	MES	O2S-S-C8	2.08	108.58	106.79
4	B	1433	GLC	C3-C4-C5	2.08	113.89	110.22
9	A	1713	MES	O1S-S-C8	2.14	108.63	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1471	GLC	C1-O5-C5	2.14	115.11	112.17
4	B	1472	GLC	C1-O5-C5	2.14	117.26	113.39
9	B	1708	MES	C2-C3-N4	2.15	113.12	110.11
4	A	1432	GLC	C1-C2-C3	2.18	112.41	109.65
4	A	1413	GLC	C1-O5-C5	2.27	115.29	112.17
9	B	1714	MES	O2S-S-C8	2.32	108.79	106.79
4	B	1431	GLC	C1-O5-C5	2.34	115.39	112.17
9	B	1706	MES	O1S-S-C8	2.36	108.82	106.79
4	A	1432	GLC	C1-O5-C5	2.42	115.50	112.17
4	B	1432	GLC	C1-O5-C5	2.43	115.51	112.17
9	B	1712	MES	O2S-S-C8	2.43	108.88	106.79
9	B	1701	MES	O3S-S-C8	2.45	109.08	106.06
9	B	1712	MES	O1S-S-C8	2.51	108.95	106.79
9	B	1711	MES	O2S-S-C8	2.55	108.98	106.79
9	A	1708	MES	O3S-S-C8	2.57	109.22	106.06
9	A	1711	MES	O3S-S-C8	2.84	109.55	106.06
9	B	1707	MES	O1S-S-C8	2.86	109.25	106.79
4	A	1471	GLC	C1-O5-C5	2.87	116.12	112.17
9	A	1711	MES	O2S-S-C8	3.00	109.37	106.79
9	A	1708	MES	O1S-S-C8	3.23	109.57	106.79
9	B	1711	MES	O1S-S-C8	3.27	109.60	106.79
9	A	1708	MES	O2S-S-C8	3.29	109.62	106.79
9	B	1708	MES	O2S-S-C8	3.38	109.70	106.79
9	A	1704	MES	O3S-S-C8	3.40	110.23	106.06
9	A	1705	MES	O3S-S-C8	3.47	110.32	106.06
9	B	1707	MES	O3S-S-C8	3.47	110.32	106.06
9	A	1706	MES	O1S-S-C8	3.48	109.78	106.79
9	B	1716	MES	O3S-S-C8	3.48	110.34	106.06
9	B	1714	MES	O1S-S-C8	3.58	109.87	106.79
9	B	1711	MES	O3S-S-C8	3.60	110.49	106.06
9	A	1711	MES	C6-C5-N4	3.63	115.19	110.11
9	B	1708	MES	O3S-S-C8	3.86	110.80	106.06
9	A	1711	MES	O1S-S-C8	3.92	110.16	106.79
4	A	1472	GLC	C1-O5-C5	3.94	120.50	113.39
9	A	1712	MES	O3S-S-C8	3.99	110.97	106.06
9	B	1701	MES	O1S-S-C8	4.00	110.23	106.79
9	B	1706	MES	O2S-S-C8	4.18	110.39	106.79
9	B	1706	MES	O3S-S-C8	4.27	111.31	106.06
9	A	1704	MES	O2S-S-C8	4.60	110.74	106.79
9	B	1707	MES	O2S-S-C8	5.12	111.19	106.79
9	A	1706	MES	O3S-S-C8	5.15	112.39	106.06
9	B	1716	MES	O2S-S-C8	5.73	111.71	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
9	B	1708	MES	O1S-S-C8	6.29	112.19	106.79
9	A	1713	MES	O2S-S-C8	7.05	112.85	106.79
9	A	1709	MES	O2S-S-C8	7.81	113.50	106.79
9	A	1705	MES	O2S-S-C8	8.77	114.33	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1413	GLC	1	0
9	A	1711	MES	1	0
5	B	1481	ACR	0	1
9	B	1711	MES	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	1247/1263 (98%)	0.35	73 (5%) 23 32	22, 32, 48, 79	0
1	B	1247/1263 (98%)	0.30	63 (5%) 29 39	21, 31, 48, 80	0
All	All	2494/2526 (98%)	0.32	136 (5%) 26 36	21, 32, 48, 80	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1237	ASN	5.3
1	B	1281	PRO	5.1
1	A	1237	ASN	4.8
1	A	58	GLY	4.7
1	B	61	ALA	4.7
1	B	60	SER	3.9
1	A	1152	GLY	3.9
1	A	439	ALA	3.8
1	A	42	THR	3.8
1	A	588	VAL	3.8
1	A	108	THR	3.8
1	A	109	SER	3.7
1	A	561	VAL	3.6
1	B	58	GLY	3.6
1	A	364	PHE	3.5
1	A	943	TRP	3.5
1	B	110	GLY	3.4
1	B	1151	SER	3.4
1	A	743	SER	3.4
1	A	46	ALA	3.3
1	A	1267	TYR	3.3
1	A	557	ALA	3.2
1	A	1281	PRO	3.2
1	A	793	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1152	GLY	3.1
1	A	43	GLY	3.1
1	A	562	PHE	3.1
1	B	106	ILE	3.1
1	B	114	VAL	3.0
1	A	794	GLY	3.0
1	B	109	SER	3.0
1	A	613	LEU	3.0
1	A	560	PRO	3.0
1	A	486	THR	2.9
1	B	834	GLY	2.9
1	B	41	VAL	2.9
1	B	767	GLY	2.9
1	A	1151	SER	2.8
1	A	946	TRP	2.8
1	B	282	PHE	2.8
1	B	613	LEU	2.8
1	A	584	ALA	2.8
1	B	835	SER	2.7
1	B	354	ILE	2.7
1	B	1074	GLY	2.7
1	A	48	GLY	2.7
1	B	48	GLY	2.7
1	B	503	ASN	2.6
1	A	559	THR	2.6
1	A	41	VAL	2.6
1	A	944	SER	2.6
1	B	557	ALA	2.6
1	B	614	ILE	2.6
1	B	1073	PRO	2.6
1	B	927	VAL	2.6
1	B	943	TRP	2.5
1	B	918	GLY	2.5
1	A	758	SER	2.5
1	B	942	ALA	2.5
1	A	595	LEU	2.5
1	A	107	ASP	2.5
1	B	1238	ASP	2.5
1	A	941	GLY	2.5
1	A	614	ILE	2.5
1	A	436	SER	2.5
1	B	689	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	44	ALA	2.5
1	B	279	PHE	2.5
1	B	39	GLY	2.5
1	A	427	TRP	2.5
1	B	46	ALA	2.5
1	B	561	VAL	2.5
1	A	691	LEU	2.5
1	B	1267	TYR	2.5
1	A	1250	ASN	2.5
1	B	757	SER	2.5
1	A	1238	ASP	2.5
1	A	127	THR	2.4
1	B	810	SER	2.4
1	B	584	ALA	2.4
1	A	835	SER	2.4
1	B	588	VAL	2.4
1	A	636	PHE	2.4
1	B	558	PHE	2.4
1	B	280	MET	2.4
1	A	1215	THR	2.4
1	A	689	VAL	2.4
1	A	487	LEU	2.4
1	B	111	ASP	2.4
1	A	558	PHE	2.3
1	A	45	VAL	2.3
1	B	1184	ASN	2.3
1	B	42	THR	2.3
1	A	111	ASP	2.3
1	A	435	ASP	2.3
1	B	105	THR	2.3
1	A	1184	ASN	2.3
1	B	1000	TRP	2.3
1	B	277	LEU	2.3
1	A	40	ASN	2.3
1	B	303	ILE	2.3
1	A	942	ALA	2.2
1	A	470	TRP	2.2
1	A	757	SER	2.2
1	B	636	PHE	2.2
1	B	352	ILE	2.2
1	B	278	GLY	2.2
1	B	1280	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1254	GLY	2.2
1	B	634	TRP	2.2
1	A	47	SER	2.2
1	A	1265	PRO	2.2
1	A	125	ALA	2.2
1	A	367	GLN	2.2
1	A	110	GLY	2.2
1	B	309	ALA	2.1
1	B	1154	PRO	2.1
1	A	1075	MET	2.1
1	A	527	GLY	2.1
1	B	945	GLN	2.1
1	A	526	TRP	2.1
1	A	642	VAL	2.1
1	B	100	ASP	2.1
1	A	472	THR	2.1
1	A	591	THR	2.1
1	A	810	SER	2.1
1	A	44	ALA	2.1
1	B	961	ILE	2.1
1	A	634	TRP	2.0
1	B	560	PRO	2.0
1	A	61	ALA	2.0
1	A	792	ALA	2.0
1	B	562	PHE	2.0
1	A	59	THR	2.0
1	B	47	SER	2.0
1	B	559	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 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
4	GLC	B	1461	12/12	0.67	0.40	22.07	52,71,77,77	0
4	GLC	A	1461	12/12	0.71	0.41	13.83	52,63,64,65	0
9	MES	A	1706	12/12	0.86	0.22	9.05	81,86,89,90	0
9	MES	A	1704	12/12	0.79	0.24	7.04	78,82,84,87	0
9	MES	B	1707	12/12	0.86	0.17	6.65	75,77,79,81	0
9	MES	A	1709	12/12	0.90	0.25	6.58	48,56,70,70	0
9	MES	B	1711	12/12	0.86	0.24	5.90	58,66,68,69	0
9	MES	A	1705	12/12	0.82	0.27	4.77	54,66,77,79	0
9	MES	A	1711	12/12	0.87	0.22	4.34	59,64,68,71	0
5	ACR	A	1481	22/44	0.86	0.23	4.29	35,47,67,72	0
9	MES	B	1716	12/12	0.85	0.24	4.07	70,74,77,78	0
10	EDO	A	1804	4/4	0.81	0.19	4.02	30,36,36,43	0
10	EDO	B	1803	4/4	0.90	0.19	3.61	49,52,52,54	0
9	MES	B	1706	12/12	0.89	0.27	3.56	72,74,77,80	0
9	MES	B	1708	12/12	0.93	0.15	3.27	44,56,60,63	0
9	MES	B	1712	12/12	0.92	0.16	3.02	52,57,58,58	0
10	EDO	A	1803	4/4	0.92	0.15	2.46	46,47,49,50	0
8	SO4	A	1707	5/5	0.93	0.30	2.36	66,67,75,77	0
10	EDO	B	1801	4/4	0.95	0.12	2.29	35,38,38,38	0
10	EDO	B	1804	4/4	0.93	0.14	2.16	31,35,35,43	0
10	EDO	A	1802	4/4	0.93	0.16	2.09	45,46,46,47	0
8	SO4	B	1702	5/5	0.91	0.17	1.92	58,60,64,66	0
4	GLC	A	1472	12/12	0.85	0.18	1.46	48,58,64,66	0
4	GLC	B	1472	12/12	0.86	0.19	1.38	53,66,68,70	0
9	MES	A	1713	12/12	0.90	0.23	1.32	68,70,74,75	0
4	GLC	A	1471	11/12	0.90	0.14	1.19	39,46,50,51	0
5	ACR	B	1481	22/44	0.82	0.25	1.13	40,53,68,70	0
10	EDO	B	1802	4/4	0.96	0.14	0.91	41,42,42,42	0
4	GLC	B	1431	11/12	0.96	0.17	0.67	31,33,35,36	0
4	GLC	A	1431	11/12	0.94	0.20	0.62	33,38,40,40	0
4	GLC	B	1471	11/12	0.94	0.11	0.55	45,52,56,61	0
4	GLC	A	1411	11/12	0.90	0.13	0.45	38,40,41,42	0
4	GLC	A	1414	11/12	0.85	0.17	-0.13	40,43,45,47	0
9	MES	B	1714	12/12	0.97	0.10	-0.23	30,32,35,37	0
3	BGC	A	1415	12/12	0.88	0.12	-0.23	36,38,39,40	0
2	CA	A	1303	1/1	0.96	0.10	-0.35	33,33,33,33	0
7	MG	B	1601	1/1	0.99	0.10	-0.49	25,25,25,25	0
10	EDO	A	1801	4/4	0.95	0.10	-0.51	33,36,36,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	BGC	A	1401	12/12	0.98	0.12	-0.58	24,26,26,27	0
2	CA	A	1302	1/1	0.98	0.08	-0.59	28,28,28,28	0
4	GLC	A	1413	11/12	0.86	0.13	-0.78	37,42,44,46	0
4	GLC	A	1412	11/12	0.89	0.11	-0.89	37,40,41,41	0
2	CA	B	1303	1/1	0.99	0.09	-0.91	33,33,33,33	0
3	BGC	B	1401	12/12	0.97	0.11	-0.92	23,25,26,27	0
7	MG	B	1603	1/1	0.92	0.11	-1.06	47,47,47,47	0
9	MES	A	1712	12/12	0.99	0.08	-1.07	31,36,38,38	0
7	MG	A	1607	1/1	0.97	0.09	-1.11	34,34,34,34	0
8	SO4	B	1704	5/5	0.94	0.17	-1.15	58,58,64,69	0
2	CA	B	1301	1/1	1.00	0.07	-1.57	30,30,30,30	0
7	MG	A	1603	1/1	0.96	0.07	-1.64	43,43,43,43	0
7	MG	B	1607	1/1	0.96	0.04	-1.87	36,36,36,36	0
7	MG	A	1601	1/1	0.98	0.08	-2.14	31,31,31,31	0
6	NI	A	1501	1/1	1.00	0.06	-2.23	30,30,30,30	0
8	SO4	A	1702	5/5	0.92	0.18	-2.26	54,57,59,68	0
2	CA	A	1301	1/1	0.98	0.05	-2.30	33,33,33,33	0
6	NI	B	1501	1/1	1.00	0.05	-2.57	30,30,30,30	0
2	CA	B	1302	1/1	0.99	0.07	-3.43	30,30,30,30	0
8	SO4	B	1710	5/5	0.97	0.15	-	51,51,53,54	0
7	MG	A	1610	1/1	0.87	0.24	-	58,58,58,58	0
7	MG	A	1606	1/1	0.88	0.15	-	67,67,67,67	0
8	SO4	A	1701	5/5	0.81	0.26	-	78,81,84,88	0
7	MG	B	1609	1/1	0.97	0.05	-	34,34,34,34	0
9	MES	A	1708	12/12	0.76	0.25	-	78,84,108,113	0
8	SO4	B	1717	5/5	0.90	0.31	-	88,89,92,92	0
8	SO4	A	1714	5/5	0.91	0.40	-	91,92,95,95	0
9	MES	B	1701	12/12	0.67	0.26	-	74,78,86,89	0
8	SO4	A	1710	5/5	0.96	0.12	-	50,51,54,54	0
4	GLC	A	1433	12/12	0.71	0.40	-	53,70,73,74	0
7	MG	A	1608	1/1	0.97	0.07	-	39,39,39,39	0
7	MG	B	1604	1/1	0.89	0.08	-	64,64,64,64	0
6	NI	B	1502	1/1	0.98	0.05	-	54,54,54,54	0
8	SO4	A	1703	5/5	0.97	0.27	-	60,64,65,68	0
7	MG	B	1610	1/1	0.74	0.27	-	48,48,48,48	0
7	MG	A	1609	1/1	0.98	0.04	-	33,33,33,33	0
8	SO4	B	1718	5/5	0.91	0.30	-	75,78,81,82	0
7	MG	A	1602	1/1	0.99	0.07	-	28,28,28,28	0
4	GLC	A	1432	11/12	0.93	0.26	-	40,44,49,52	0
8	SO4	B	1703	5/5	0.86	0.32	-	84,87,90,91	0
8	SO4	B	1713	5/5	0.88	0.19	-	57,61,67,67	0
7	MG	B	1602	1/1	0.97	0.05	-	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	MG	A	1604	1/1	0.88	0.07	-	57,57,57,57	0
7	MG	B	1608	1/1	0.77	0.08	-	50,50,50,50	0
4	GLC	B	1433	12/12	0.81	0.41	-	51,76,79,84	0
4	GLC	B	1432	11/12	0.94	0.20	-	36,40,46,46	0
7	MG	A	1605	1/1	0.94	0.14	-	53,53,53,53	0
7	MG	B	1605	1/1	0.95	0.18	-	48,48,48,48	0
7	MG	B	1606	1/1	0.84	0.21	-	67,67,67,67	0
8	SO4	B	1709	5/5	0.88	0.30	-	78,80,87,87	0
8	SO4	B	1715	5/5	0.92	0.28	-	64,66,67,71	0
8	SO4	B	1705	5/5	0.97	0.26	-	58,58,60,61	0
6	NI	A	1502	1/1	0.95	0.07	-	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.