



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WNN
Title : D308A mutant of Bacillus circulans T-3040 cycloisomaltooligosaccharide glucanotransferase complexed with isomaltooctaose
Authors : Suzuki, N.; Fujimoto, Z.; Kim, Y.M.; Momma, M.; Kishine, N.; Suzuki, R.; Suzuki, S.; Kitamura, S.; Kobayashi, M.; Kimura, A.; Funane, K.
Deposited on : 2013-12-10
Resolution : 2.25 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 (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

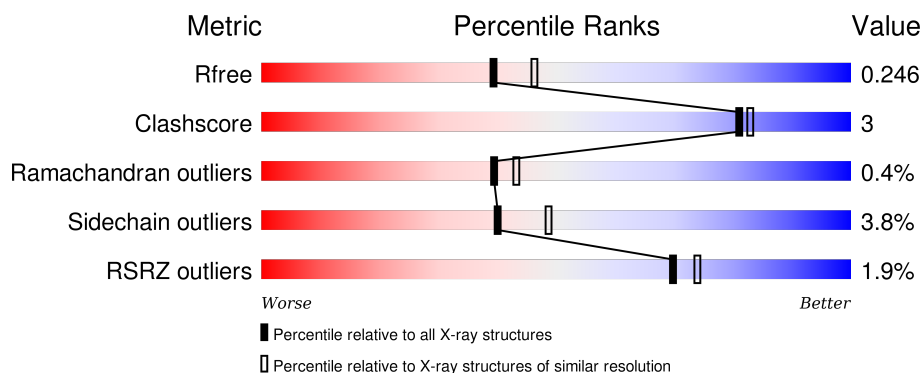
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	710	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>••</div> </div>
1	B	710	<div> <div>2%</div> <div>88%</div> <div>10%</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
4	SO4	A	804	-	-	-	X
4	SO4	B	807	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 11831 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 Cycloisomaltooligosaccharide glucanotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	699	Total	C	N	O	S	0	0	0
			5501	3457	923	1106	15			
1	B	698	Total	C	N	O	S	0	0	0
			5497	3455	922	1105	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	MET	-	EXPRESSION TAG	UNP P94286
A	38	GLY	-	EXPRESSION TAG	UNP P94286
A	278	PHE	SER	SEE REMARK 999	UNP P94286
A	308	ALA	ASP	ENGINEERED MUTATION	UNP P94286
A	739	LEU	-	EXPRESSION TAG	UNP P94286
A	740	GLU	-	EXPRESSION TAG	UNP P94286
A	741	HIS	-	EXPRESSION TAG	UNP P94286
A	742	HIS	-	EXPRESSION TAG	UNP P94286
A	743	HIS	-	EXPRESSION TAG	UNP P94286
A	744	HIS	-	EXPRESSION TAG	UNP P94286
A	745	HIS	-	EXPRESSION TAG	UNP P94286
A	746	HIS	-	EXPRESSION TAG	UNP P94286
B	37	MET	-	EXPRESSION TAG	UNP P94286
B	38	GLY	-	EXPRESSION TAG	UNP P94286
B	278	PHE	SER	SEE REMARK 999	UNP P94286
B	308	ALA	ASP	ENGINEERED MUTATION	UNP P94286
B	739	LEU	-	EXPRESSION TAG	UNP P94286
B	740	GLU	-	EXPRESSION TAG	UNP P94286
B	741	HIS	-	EXPRESSION TAG	UNP P94286
B	742	HIS	-	EXPRESSION TAG	UNP P94286
B	743	HIS	-	EXPRESSION TAG	UNP P94286
B	744	HIS	-	EXPRESSION TAG	UNP P94286
B	745	HIS	-	EXPRESSION TAG	UNP P94286
B	746	HIS	-	EXPRESSION TAG	UNP P94286

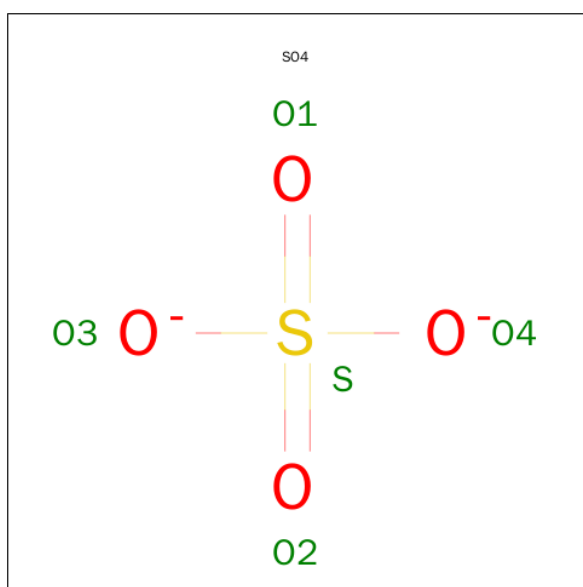
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



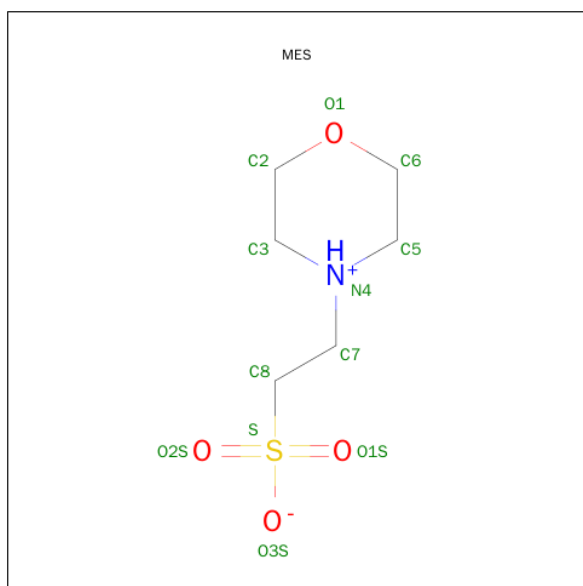
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 6 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	8	Total	C	O	0	0
			89	48	41		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	8	Total	C	O	0	0
			89	48	41		

- Molecule 7 is a polymer of unknown type called SUGAR (4-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	5	Total	C	O	0	0
			56	30	26		

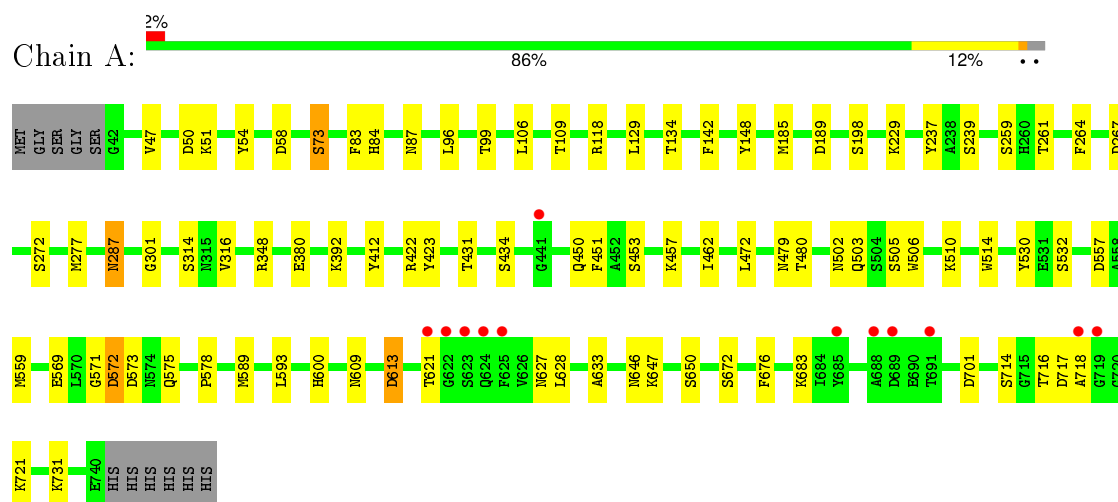
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	204	Total	O	0	0
			204	204		
9	B	267	Total	O	0	0
			267	267		

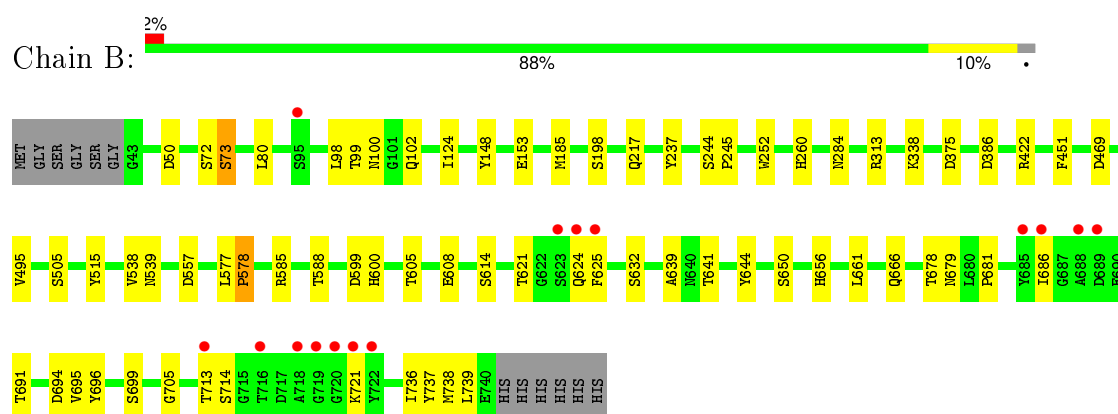
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Cycloisomaltooligosaccharide glucanotransferase



- Molecule 1: Cycloisomaltooligosaccharide glucanotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.03Å 171.26Å 173.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.35 – 2.25 35.32 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.35-2.25) 95.8 (35.32-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.202 , 0.244 0.206 , 0.246	Depositor DCC
R_{free} test set	4326 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.9	EDS
Estimated twinning fraction	0.166 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 86182 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11831	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NA, CA, GLC, 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	0.67	1/5641 (0.0%)	0.78	4/7683 (0.1%)
1	B	0.69	1/5637 (0.0%)	0.79	1/7678 (0.0%)
All	All	0.68	2/11278 (0.0%)	0.78	5/15361 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	50	ASP	CB-CG	6.81	1.66	1.51
1	A	50	ASP	CB-CG	5.19	1.62	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	267	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	58	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	50	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	277	MET	CG-SD-CE	-5.38	91.60	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	5501	0	5106	35	0
1	B	5497	0	5103	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	0	0	0
4	B	25	0	0	0	0
5	A	12	0	13	0	0
5	B	12	0	13	1	0
6	A	89	0	75	2	0
6	B	89	0	75	0	0
7	A	45	0	39	1	0
8	B	56	0	48	1	0
9	A	204	0	0	3	0
9	B	267	0	0	3	0
All	All	11831	0	10472	73	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 3.

All (73) 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)
8:B:823:GLC:H61	9:B:1071:HOH:O	1.88	0.74
1:A:84:HIS:CE1	1:A:118:ARG:HD3	2.31	0.65
1:A:502:ASN:ND2	1:A:503:GLN:O	2.31	0.64
1:A:51:LYS:HB2	1:A:54:TYR:CZ	2.34	0.63
1:A:287:ASN:C	1:A:287:ASN:HD22	2.03	0.62
1:A:301:GLY:O	1:A:348:ARG:NH1	2.34	0.61
1:B:495:VAL:CG1	1:B:515:TYR:CE2	2.84	0.60
1:A:557:ASP:HB3	1:A:600:HIS:CE1	2.38	0.59
1:B:260:HIS:ND1	1:B:260:HIS:O	2.36	0.58
1:A:557:ASP:OD2	1:A:569:GLU:OE2	2.23	0.57
1:A:96:LEU:HD13	1:A:106:LEU:HD21	1.90	0.54
1:B:72:SER:HA	1:B:100:ASN:HB2	1.90	0.53
1:B:313:ARG:NH2	9:B:962:HOH:O	2.41	0.53
1:A:503:GLN:NE2	1:A:510:LYS:HG3	2.24	0.52
1:A:628:LEU:HD12	1:A:633:ALA:HB2	1.91	0.52
6:A:813:GLC:O2	6:A:814:GLC:H61	2.10	0.51
1:B:495:VAL:CG1	1:B:515:TYR:CD2	2.93	0.51
1:B:495:VAL:HG13	1:B:515:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:VAL:HG12	1:A:134:THR:CG2	2.41	0.51
1:B:644:TYR:HA	1:B:656:HIS:O	2.11	0.50
1:B:338:LYS:NZ	1:B:375:ASP:OD2	2.45	0.50
1:B:599:ASP:OD1	5:B:808:MES:N4	2.43	0.49
1:B:696:TYR:O	1:B:736:ILE:HA	2.13	0.48
1:B:72:SER:O	1:B:73:SER:C	2.52	0.47
1:A:422:ARG:HD3	9:A:1109:HOH:O	2.14	0.47
1:A:47:VAL:HG12	1:A:134:THR:HG22	1.97	0.46
1:B:695:VAL:HG22	1:B:738:MET:HG2	1.97	0.46
1:B:639:ALA:O	1:B:641:THR:HG23	2.15	0.46
1:A:609:ASN:O	1:A:613:ASP:HB2	2.16	0.46
1:B:244:SER:HB2	1:B:245:PRO:HD3	1.96	0.46
1:B:699:SER:O	1:B:705:GLY:HA2	2.15	0.46
1:B:98:LEU:HB3	1:B:102:GLN:HB3	1.96	0.45
1:A:380:GLU:OE2	1:A:412:TYR:OH	2.16	0.45
1:A:627:ASN:HB2	1:A:683:LYS:HB3	1.98	0.45
1:B:386:ASP:HB3	1:B:666:GLN:OE1	2.16	0.45
1:A:287:ASN:ND2	1:A:287:ASN:C	2.68	0.45
1:A:589:MET:HG2	1:A:593:LEU:HD23	1.99	0.44
1:A:264:PHE:CE2	1:A:316:VAL:HG22	2.52	0.44
1:B:605:THR:O	1:B:608:GLU:HG2	2.17	0.44
1:A:450:GLN:OE1	7:A:822:GLC:O2	2.36	0.44
1:A:83:PHE:HA	1:A:87:ASN:O	2.17	0.44
1:A:431:THR:HB	1:A:457:LYS:HB2	2.00	0.44
1:A:73:SER:HB3	1:A:99:THR:HA	1.99	0.44
1:A:503:GLN:CD	1:A:510:LYS:HG3	2.39	0.43
1:A:472:LEU:O	1:A:514:TRP:HA	2.18	0.43
1:A:571:GLY:O	1:A:572:ASP:C	2.56	0.43
1:A:676:PHE:CD1	1:A:731:LYS:HA	2.53	0.43
1:A:51:LYS:HB2	1:A:54:TYR:CE1	2.53	0.43
1:B:244:SER:N	1:B:245:PRO:CD	2.81	0.43
1:B:641:THR:CA	1:B:661:LEU:HD23	2.48	0.43
1:B:153:GLU:OE1	1:B:585:ARG:NH2	2.52	0.43
1:B:217:GLN:HA	1:B:217:GLN:NE2	2.34	0.43
1:B:721:LYS:HE2	1:B:721:LYS:HA	2.00	0.43
1:A:480:THR:OG1	9:A:1137:HOH:O	2.21	0.42
6:A:813:GLC:O2	6:A:814:GLC:C6	2.68	0.42
1:B:252:TRP:CE2	1:B:284:ASN:HB3	2.55	0.42
1:A:189:ASP:OD2	1:A:239:SER:HB2	2.19	0.42
1:A:423:TYR:CE1	1:A:462:ILE:HG22	2.55	0.42
1:B:422:ARG:HD3	9:B:983:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:ASN:O	1:B:681:PRO:HD3	2.19	0.41
1:B:577:LEU:HA	1:B:578:PRO:HD3	1.90	0.41
1:A:573:ASP:OD1	1:A:575:GLN:NE2	2.44	0.41
1:A:142:PHE:CD2	1:A:229:LYS:HG3	2.54	0.41
1:B:557:ASP:HB3	1:B:600:HIS:CE1	2.55	0.41
1:B:678:THR:O	1:B:679:ASN:C	2.59	0.41
1:B:694:ASP:HB2	1:B:739:LEU:HB3	2.02	0.41
1:B:713:THR:HG22	1:B:714:SER:N	2.35	0.41
1:B:538:VAL:HG12	1:B:539:ASN:N	2.36	0.41
1:A:109:THR:O	9:A:1142:HOH:O	2.21	0.41
1:B:495:VAL:HG11	1:B:515:TYR:CD2	2.56	0.41
1:B:80:LEU:HD13	1:B:124:ILE:CD1	2.51	0.40
1:A:479:ASN:HB3	1:A:506:TRP:CE2	2.55	0.40
1:B:469:ASP:O	1:B:588:THR:HG21	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	697/710 (98%)	662 (95%)	32 (5%)	3 (0%)	39	43
1	B	696/710 (98%)	657 (94%)	36 (5%)	3 (0%)	39	43
All	All	1393/1420 (98%)	1319 (95%)	68 (5%)	6 (0%)	39	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	73	SER
1	B	686	ILE
1	A	572	ASP
1	A	718	ALA

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Mol	Chain	Res	Type
1	A	272	SER
1	B	578	PRO

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	587/596 (98%)	557 (95%)	30 (5%)	29	32
1	B	587/596 (98%)	572 (97%)	15 (3%)	54	65
All	All	1174/1192 (98%)	1129 (96%)	45 (4%)	40	49

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	SER
1	A	129	LEU
1	A	148	TYR
1	A	185	MET
1	A	198	SER
1	A	237	TYR
1	A	259	SER
1	A	261	THR
1	A	287	ASN
1	A	314	SER
1	A	392	LYS
1	A	434	SER
1	A	451	PHE
1	A	453	SER
1	A	505	SER
1	A	530	TYR
1	A	532	SER
1	A	559	MET
1	A	578	PRO
1	A	613	ASP
1	A	621	THR

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Mol	Chain	Res	Type
1	A	646	ASN
1	A	647	LYS
1	A	650	SER
1	A	672	SER
1	A	701	ASP
1	A	714	SER
1	A	716	THR
1	A	717	ASP
1	A	721	LYS
1	B	99	THR
1	B	148	TYR
1	B	185	MET
1	B	198	SER
1	B	237	TYR
1	B	451	PHE
1	B	505	SER
1	B	614	SER
1	B	621	THR
1	B	624	GLN
1	B	625	PHE
1	B	632	SER
1	B	650	SER
1	B	691	THR
1	B	737	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	287	ASN
1	A	315	ASN
1	A	320	ASN
1	A	371	ASN
1	A	479	ASN
1	A	483	ASN
1	A	521	GLN
1	A	600	HIS
1	A	619	ASN
1	B	242	ASN
1	B	320	ASN
1	B	450	GLN
1	B	496	GLN

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Mol	Chain	Res	Type
1	B	511	HIS
1	B	521	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 ⓘ

25 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	$\# Z > 2$
6	GLC	A	811	6	11,11,12	0.75	0	14,15,17	1.48	2 (14%)
6	GLC	A	812	6	11,11,12	0.62	0	14,15,17	1.27	2 (14%)
6	GLC	A	813	6	11,11,12	0.81	0	14,15,17	1.45	1 (7%)
6	GLC	A	814	6	11,11,12	0.67	0	14,15,17	2.51	2 (14%)
6	GLC	A	815	6	11,11,12	0.60	0	14,15,17	1.50	1 (7%)
6	GLC	A	816	6	11,11,12	0.89	0	14,15,17	1.74	5 (35%)
6	GLC	A	817	6	11,11,12	0.80	0	14,15,17	1.37	3 (21%)
6	BGC	A	818	6	12,12,12	0.68	0	17,17,17	1.48	5 (29%)
7	GLC	A	821	7	11,11,12	0.55	0	14,15,17	1.82	1 (7%)
7	GLC	A	822	7	11,11,12	0.75	0	14,15,17	0.83	0
7	GLC	A	823	7	11,11,12	0.64	0	14,15,17	1.76	4 (28%)
7	GLC	A	824	7	12,12,12	0.63	0	17,17,17	2.45	5 (29%)
6	GLC	B	811	6	11,11,12	0.84	0	14,15,17	1.21	1 (7%)
6	GLC	B	812	6	11,11,12	0.81	0	14,15,17	1.22	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GLC	B	813	6	11,11,12	0.90	1 (9%)	14,15,17	1.92	4 (28%)
6	GLC	B	814	6	11,11,12	1.05	0	14,15,17	2.72	9 (64%)
6	GLC	B	815	6	11,11,12	0.64	0	14,15,17	1.39	2 (14%)
6	GLC	B	816	6	11,11,12	0.85	0	14,15,17	1.48	1 (7%)
6	GLC	B	817	6	11,11,12	0.81	0	14,15,17	1.53	4 (28%)
6	BGC	B	818	6	12,12,12	0.92	1 (8%)	17,17,17	1.27	1 (5%)
8	GLC	B	821	8	11,11,12	0.61	0	14,15,17	1.09	0
8	GLC	B	822	8	11,11,12	0.52	0	14,15,17	2.90	3 (21%)
8	GLC	B	823	8	11,11,12	0.57	0	14,15,17	2.92	2 (14%)
8	GLC	B	824	8	11,11,12	0.72	0	14,15,17	1.41	3 (21%)
8	GLC	B	825	8	12,12,12	0.68	0	17,17,17	1.25	1 (5%)

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
6	GLC	A	811	6	-	0/2/19/22	0/1/1/1
6	GLC	A	812	6	-	0/2/19/22	0/1/1/1
6	GLC	A	813	6	-	0/2/19/22	0/1/1/1
6	GLC	A	814	6	-	0/2/19/22	0/1/1/1
6	GLC	A	815	6	-	0/2/19/22	0/1/1/1
6	GLC	A	816	6	-	0/2/19/22	0/1/1/1
6	GLC	A	817	6	-	0/2/19/22	0/1/1/1
6	BGC	A	818	6	-	0/2/22/22	0/1/1/1
7	GLC	A	821	7	-	0/2/19/22	0/1/1/1
7	GLC	A	822	7	-	0/2/19/22	0/1/1/1
7	GLC	A	823	7	-	0/2/19/22	0/1/1/1
7	GLC	A	824	7	-	0/2/22/22	0/1/1/1
6	GLC	B	811	6	-	0/2/19/22	0/1/1/1
6	GLC	B	812	6	-	0/2/19/22	0/1/1/1
6	GLC	B	813	6	-	0/2/19/22	0/1/1/1
6	GLC	B	814	6	-	0/2/19/22	0/1/1/1
6	GLC	B	815	6	-	0/2/19/22	0/1/1/1
6	GLC	B	816	6	-	0/2/19/22	0/1/1/1
6	GLC	B	817	6	-	0/2/19/22	0/1/1/1
6	BGC	B	818	6	-	0/2/22/22	0/1/1/1
8	GLC	B	821	8	-	0/2/19/22	0/1/1/1
8	GLC	B	822	8	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GLC	B	823	8	-	0/2/19/22	0/1/1/1
8	GLC	B	824	8	-	0/2/19/22	0/1/1/1
8	GLC	B	825	8	-	0/2/22/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	818	BGC	C1-C2	-2.13	1.48	1.52
6	B	813	GLC	O5-C5	-2.02	1.39	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	814	GLC	C6-C5-C4	-6.24	97.62	113.02
6	A	814	GLC	C6-C5-C4	-4.44	102.06	113.02
6	A	811	GLC	O3-C3-C2	-3.57	103.55	110.00
7	A	823	GLC	C2-C3-C4	-3.52	105.06	111.04
6	B	814	GLC	O4-C4-C5	-3.08	101.06	109.24
6	B	814	GLC	C2-C3-C4	-3.06	105.84	111.04
6	A	816	GLC	O5-C1-C2	-3.03	105.94	110.86
6	A	816	GLC	O3-C3-C4	-3.03	103.52	110.34
6	A	818	BGC	O2-C2-C3	-2.71	104.24	110.34
6	B	814	GLC	O6-C6-C5	-2.68	102.47	111.33
6	B	817	GLC	O5-C1-C2	-2.68	106.51	110.86
6	A	816	GLC	C2-C3-C4	-2.63	106.57	111.04
6	A	818	BGC	C1-O5-C5	-2.61	108.64	113.47
8	B	824	GLC	C2-C3-C4	-2.60	106.63	111.04
6	A	818	BGC	C3-C4-C5	-2.57	105.71	110.20
6	A	817	GLC	O5-C1-C2	-2.56	106.71	110.86
6	B	815	GLC	O2-C2-C3	-2.47	105.16	110.12
6	B	814	GLC	O3-C3-C4	-2.35	105.05	110.34
6	B	812	GLC	O4-C4-C3	-2.32	105.10	110.34
8	B	824	GLC	C3-C4-C5	-2.25	106.28	110.20
6	A	817	GLC	O3-C3-C2	-2.22	105.98	110.00
6	B	813	GLC	C3-C4-C5	-2.20	106.36	110.20
6	B	813	GLC	O3-C3-C2	-2.20	106.03	110.00
6	A	816	GLC	C1-C2-C3	-2.12	107.03	109.54
6	A	818	BGC	O5-C1-C2	-2.11	106.44	109.80
7	A	823	GLC	O6-C6-C5	-2.07	104.50	111.33
7	A	823	GLC	C3-C4-C5	-2.04	106.64	110.20
6	B	817	GLC	O2-C2-C1	-2.02	105.15	109.21
8	B	824	GLC	O3-C3-C2	2.04	113.68	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	817	GLC	C3-C4-C5	2.04	113.76	110.20
8	B	825	GLC	O2-C2-C1	2.06	114.36	109.82
6	B	811	GLC	O2-C2-C1	2.09	113.39	109.21
6	A	818	BGC	C4-C3-C2	2.17	114.83	110.79
8	B	822	GLC	C1-C2-C3	2.20	112.15	109.54
6	B	814	GLC	O5-C5-C6	2.22	112.16	107.35
6	B	814	GLC	C1-O5-C5	2.25	115.10	112.25
7	A	824	GLC	O5-C1-C2	2.37	113.58	109.80
6	A	812	GLC	C1-O5-C5	2.39	115.28	112.25
7	A	824	GLC	C1-C2-C3	2.45	114.08	110.43
6	B	818	BGC	C4-C3-C2	2.46	115.38	110.79
6	A	816	GLC	O5-C5-C6	2.46	112.68	107.35
6	B	817	GLC	C1-C2-C3	2.54	112.55	109.54
6	B	814	GLC	O5-C1-C2	2.62	115.11	110.86
6	B	815	GLC	O2-C2-C1	2.64	114.50	109.21
6	B	817	GLC	C1-O5-C5	2.82	115.83	112.25
6	B	813	GLC	C1-C2-C3	3.00	113.09	109.54
6	B	814	GLC	C3-C4-C5	3.08	115.57	110.20
6	A	811	GLC	C1-O5-C5	3.10	116.18	112.25
7	A	823	GLC	O3-C3-C2	3.12	115.63	110.00
6	A	812	GLC	C1-C2-C3	3.12	113.23	109.54
6	A	815	GLC	C1-C2-C3	3.15	113.26	109.54
8	B	822	GLC	O5-C1-C2	3.30	116.21	110.86
6	B	816	GLC	O2-C2-C3	3.62	117.40	110.12
8	B	823	GLC	C3-C4-C5	3.63	116.53	110.20
6	A	813	GLC	O2-C2-C1	3.67	116.56	109.21
7	A	824	GLC	C3-C4-C5	3.88	116.96	110.20
7	A	824	GLC	O5-C5-C4	4.48	118.09	109.68
6	B	813	GLC	O2-C2-C1	4.75	118.74	109.21
7	A	821	GLC	C1-O5-C5	5.96	119.81	112.25
7	A	824	GLC	C1-O5-C5	6.36	125.24	113.47
6	A	814	GLC	C1-O5-C5	7.15	121.32	112.25
8	B	823	GLC	C1-O5-C5	9.59	124.42	112.25
8	B	822	GLC	C1-O5-C5	9.83	124.73	112.25

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
6	A	813	GLC	2	0
6	A	814	GLC	2	0
7	A	822	GLC	1	0
8	B	823	GLC	1	0

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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	$\# Z > 2$
4	SO4	A	803	-	4,4,4	0.11	0	6,6,6	0.82	0
4	SO4	A	804	-	4,4,4	0.77	0	6,6,6	0.39	0
4	SO4	A	805	-	4,4,4	0.53	0	6,6,6	0.23	0
4	SO4	A	806	-	4,4,4	1.13	0	6,6,6	0.66	0
4	SO4	A	807	-	4,4,4	0.59	0	6,6,6	0.51	0
4	SO4	A	808	-	4,4,4	0.49	0	6,6,6	0.34	0
5	MES	A	809	-	11,12,12	0.76	0	14,16,16	1.35	2 (14%)
4	SO4	B	803	-	4,4,4	0.28	0	6,6,6	0.52	0
4	SO4	B	804	-	4,4,4	0.59	0	6,6,6	0.27	0
4	SO4	B	805	-	4,4,4	0.63	0	6,6,6	0.28	0
4	SO4	B	806	-	4,4,4	0.66	0	6,6,6	0.33	0
4	SO4	B	807	-	4,4,4	0.58	0	6,6,6	0.50	0
5	MES	B	808	-	11,12,12	0.74	0	14,16,16	2.72	3 (21%)

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	SO4	A	803	-	-	0/0/0/0	0/0/0/0
4	SO4	A	804	-	-	0/0/0/0	0/0/0/0
4	SO4	A	805	-	-	0/0/0/0	0/0/0/0
4	SO4	A	806	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	807	-	-	0/0/0/0	0/0/0/0
4	SO4	A	808	-	-	0/0/0/0	0/0/0/0
5	MES	A	809	-	-	0/6/14/14	0/1/1/1
4	SO4	B	803	-	-	0/0/0/0	0/0/0/0
4	SO4	B	804	-	-	0/0/0/0	0/0/0/0
4	SO4	B	805	-	-	0/0/0/0	0/0/0/0
4	SO4	B	806	-	-	0/0/0/0	0/0/0/0
4	SO4	B	807	-	-	0/0/0/0	0/0/0/0
5	MES	B	808	-	-	0/6/14/14	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	808	MES	O3S-S-O1S	-2.82	105.04	111.61
5	B	808	MES	C6-C5-N4	2.05	113.24	110.12
5	A	809	MES	C6-C5-N4	2.40	113.76	110.12
5	A	809	MES	O2S-S-C8	2.79	109.28	106.91
5	B	808	MES	O1S-S-C8	8.77	114.38	106.91

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
5	B	808	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	699/710 (98%)	-0.29	12 (1%) 73 77	31, 47, 77, 124	0
1	B	698/710 (98%)	-0.29	15 (2%) 67 71	29, 45, 84, 135	0
All	All	1397/1420 (98%)	-0.29	27 (1%) 70 74	29, 46, 80, 135	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	624	GLN	6.6
1	A	688	ALA	4.6
1	A	718	ALA	4.2
1	A	622	GLY	4.0
1	B	688	ALA	3.7
1	B	722	TYR	3.7
1	A	624	GLN	3.7
1	B	625	PHE	3.7
1	A	625	PHE	3.6
1	A	623	SER	3.4
1	A	621	THR	3.3
1	B	689	ASP	3.3
1	A	691	THR	3.0
1	A	689	ASP	2.8
1	B	623	SER	2.7
1	A	441	GLY	2.7
1	A	719	GLY	2.3
1	B	95	SER	2.3
1	B	686	ILE	2.2
1	B	718	ALA	2.1
1	B	713	THR	2.1
1	B	720	GLY	2.1
1	B	719	GLY	2.1
1	B	721	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	716	THR	2.1
1	B	685	TYR	2.0
1	A	685	TYR	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, 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
6	BGC	A	818	12/12	0.96	0.12	1.03	31,35,37,39	0
6	BGC	B	818	12/12	0.98	0.10	0.25	28,30,34,35	0
6	GLC	B	817	11/12	0.97	0.10	-0.52	30,35,37,42	0
6	GLC	A	817	11/12	0.97	0.10	-0.75	31,34,35,42	0
6	GLC	A	811	11/12	0.97	0.09	-1.04	44,47,53,58	0
8	GLC	B	824	11/12	0.94	0.10	-1.23	49,53,55,55	0
6	GLC	B	815	11/12	0.98	0.09	-1.45	35,39,42,44	0
6	GLC	A	815	11/12	0.94	0.09	-1.45	41,48,52,52	0
7	GLC	A	823	11/12	0.97	0.09	-1.85	58,62,65,66	0
6	GLC	B	811	11/12	0.97	0.08	-2.77	32,36,40,41	0
6	GLC	B	812	11/12	0.96	0.10	-	41,43,53,55	0
7	GLC	A	821	11/12	0.93	0.12	-	57,72,84,85	0
7	GLC	A	822	11/12	0.96	0.17	-	66,73,81,87	0
6	GLC	A	813	11/12	0.91	0.11	-	56,65,69,75	0
6	GLC	B	816	11/12	0.96	0.09	-	39,41,43,43	0
6	GLC	A	816	11/12	0.96	0.09	-	40,44,51,53	0
6	GLC	B	813	11/12	0.95	0.11	-	40,43,47,48	0
7	GLC	A	824	12/12	0.75	0.19	-	69,83,93,94	0
6	GLC	B	814	11/12	0.95	0.12	-	35,42,45,52	0
8	GLC	B	825	12/12	0.92	0.14	-	59,78,83,83	0
6	GLC	A	814	11/12	0.89	0.17	-	47,51,63,64	0
8	GLC	B	823	11/12	0.90	0.11	-	50,58,63,67	0
6	GLC	A	812	11/12	0.91	0.12	-	55,62,65,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	GLC	B	821	11/12	0.86	0.26	-	78,90,94,96	0
8	GLC	B	822	11/12	0.91	0.11	-	64,70,76,84	0

6.4 Ligands

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(\AA^2)	Q<0.9
4	SO4	A	804	5/5	0.85	0.20	6.64	68,77,91,96	0
4	SO4	B	807	5/5	0.96	0.14	2.34	74,75,80,86	0
3	NA	A	802	1/1	0.99	0.11	1.20	44,44,44,44	0
2	CA	B	801	1/1	0.99	0.11	-0.03	44,44,44,44	0
5	MES	A	809	12/12	0.99	0.10	-0.45	44,47,50,51	0
5	MES	B	808	12/12	0.97	0.09	-0.95	43,50,52,53	0
2	CA	A	801	1/1	0.97	0.09	-1.38	49,49,49,49	0
3	NA	B	802	1/1	0.96	0.06	-4.51	49,49,49,49	0
4	SO4	B	803	5/5	0.97	0.14	-	47,48,55,64	0
4	SO4	B	804	5/5	0.92	0.19	-	85,88,98,103	0
4	SO4	B	805	5/5	0.88	0.17	-	83,84,98,101	0
4	SO4	A	803	5/5	0.98	0.09	-	42,50,52,60	0
4	SO4	A	807	5/5	0.90	0.22	-	84,90,94,94	0
4	SO4	A	806	5/5	0.89	0.16	-	56,57,81,83	0
4	SO4	B	806	5/5	0.92	0.20	-	79,91,97,99	0
4	SO4	A	808	5/5	0.94	0.14	-	88,90,93,95	0
4	SO4	A	805	5/5	0.90	0.23	-	93,97,102,106	0

6.5 Other polymers

There are no such residues in this entry.