Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:45 AM GMT

PDB ID : 2E9B
Title : Crystal structure of pullulanase type I from Bacillus subtilis str. 168 complexed with maltose
Authors : Mikami, B.; Malle, D.; Utsumi, S.; Iwamoto, H.; Katsuya, Y.
Deposited on : 2007-01-24
Resolution : 2.30 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 (i) symbol.

The following versions of software and data (see references (i)) 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
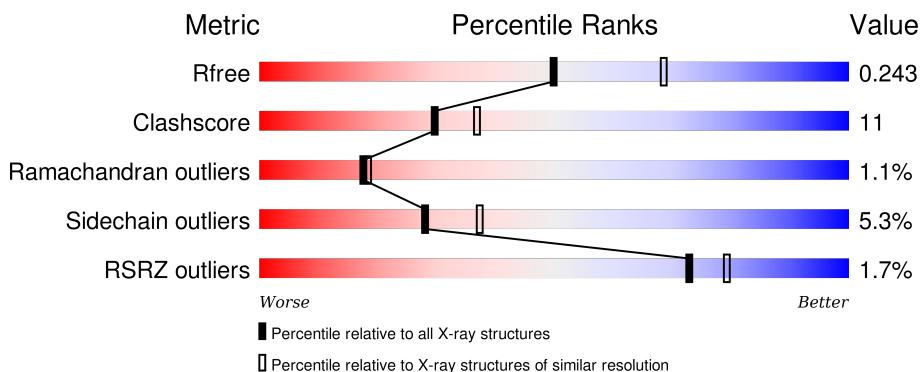
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
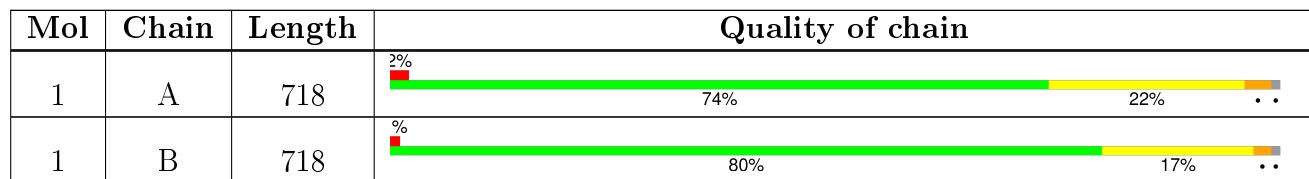
The reported resolution of this entry is 2.30 Å.

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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 <=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	718	
1	B	718	

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	723	-	-	-	X
3	GLC	A	735	-	-	-	X
4	GLC	B	733	-	-	-	X
6	ACT	A	751	-	-	-	X
6	ACT	B	752	-	-	-	X
7	GOL	A	761	-	X	-	X
7	GOL	B	762	-	X	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11961 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 AmyX protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total 5674	C 3617	N 975	O 1060	S 22	0	0	0
1	B	712	Total 5674	C 3617	N 975	O 1060	S 22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	LYS	MET	CONFLICT	UNP O34587
B	365	LYS	MET	CONFLICT	UNP O34587

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total 34	C 18	O 16	0	0

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total 23	C 12	O 11	0	0
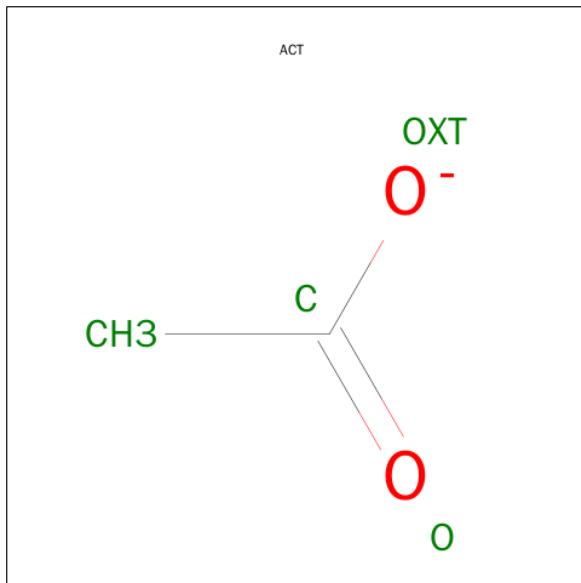
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	3	Total 34	C 18	O 16	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).
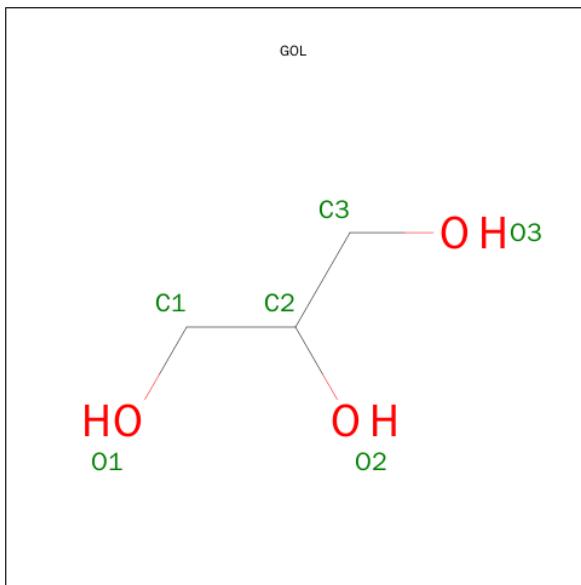
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	Ca 1	0	0
5	A	1	Total 1	Ca 1	0	0

• Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

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

• Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total C O			0	0
			6	3	3		
7	B	1	Total C O			0	0
			6	3	3		
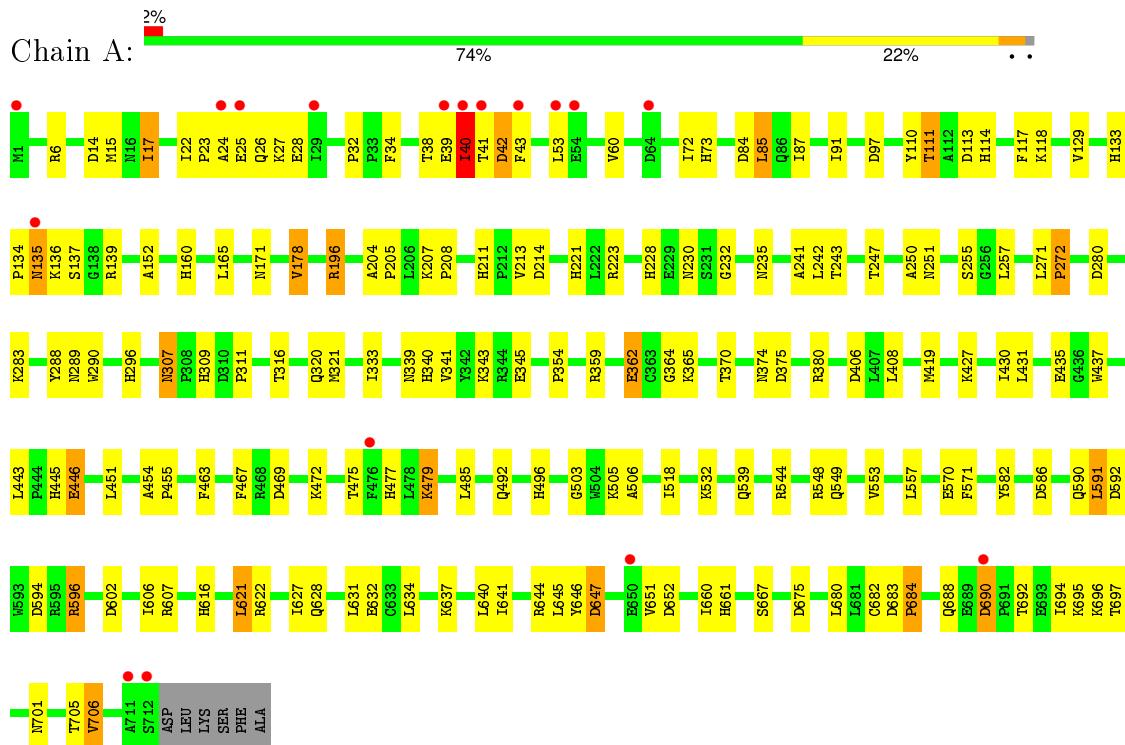
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	236	Total O		0	0
			236	236		
8	B	260	Total O		0	0
			260	260		
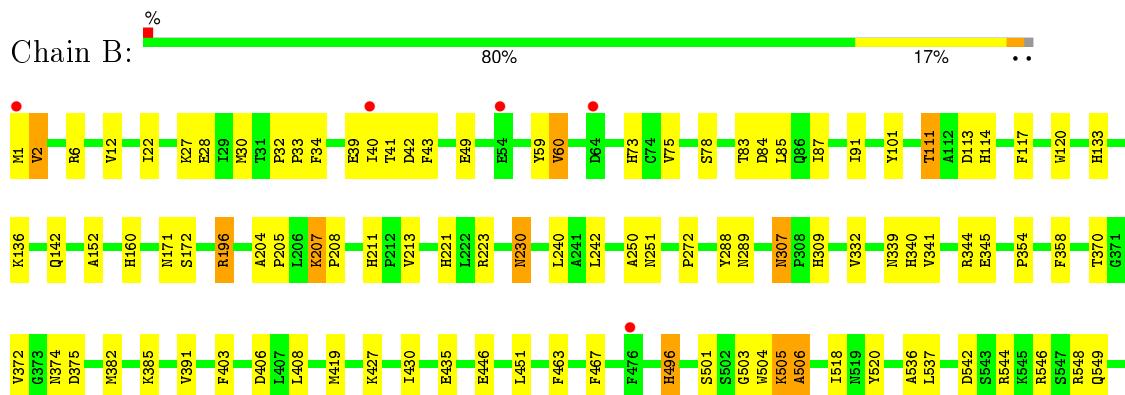
3 Residue-property plots (i)
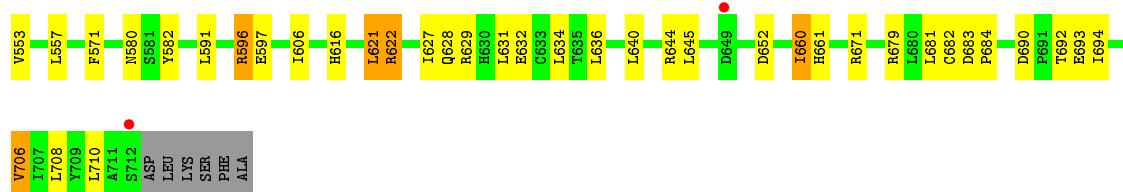
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: AmyX protein

• Molecule 1: AmyX protein

4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.03Å　　129.18Å　　192.06Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	14.97　–　2.30 47.56　–　2.20	Depositor EDS
% Data completeness (in resolution range)	85.1 (14.97-2.30) 83.0 (47.56-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.45 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194　,　0.242 0.196　,　0.243	Depositor DCC
R_{free} test set	6750 reflections (10.04%)	DCC
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49$, $<L^2> = 0.32$	Xtriage
Outliers	0 of 81455 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11961	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, GOL, CA, BGC, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.37	0/5822	0.60	0/7905
1	B	0.37	0/5822	0.61	0/7905
All	All	0.37	0/11644	0.60	0/15810

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5674	0	5528	145	0
1	B	5674	0	5528	109	0
2	A	34	0	30	2	0
3	A	23	0	21	0	0
4	B	34	0	30	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	6	0	0
6	B	4	0	3	0	0
7	A	6	0	3	1	0
7	B	6	0	3	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	236	0	0	8	0
8	B	260	0	0	10	0
All	All	11961	0	11152	254	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 11.

All (254) 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:B:207:LYS:H	1:B:207:LYS:HE2	0.93	1.09
1:A:111:THR:HG22	1:A:114:HIS:H	1.12	1.08
1:B:111:THR:HG22	1:B:114:HIS:H	1.14	1.04
1:B:660:ILE:HG23	1:B:706:VAL:HG13	1.42	1.01
1:B:207:LYS:HE2	1:B:207:LYS:N	1.76	1.01
1:A:247:THR:HG22	1:A:255:SER:OG	1.64	0.95
1:A:14:ASP:HB3	1:A:17:ILE:HG23	1.49	0.94
1:A:87:ILE:H	1:A:171:ASN:HD21	1.05	0.92
1:B:553:VAL:HG11	1:B:606:ILE:HD12	1.52	0.91
1:B:207:LYS:H	1:B:207:LYS:CE	1.84	0.90
1:A:505:LYS:HG2	1:A:506:ALA:H	1.38	0.87
1:A:570:GLU:HB2	1:A:606:ILE:HD13	1.57	0.86
1:B:230:ASN:HD21	1:B:250:ALA:H	1.23	0.84
1:A:505:LYS:CG	1:A:506:ALA:H	1.90	0.84
1:B:87:ILE:H	1:B:171:ASN:HD21	1.25	0.84
1:A:505:LYS:HG2	1:A:506:ALA:N	1.92	0.83
1:B:160:HIS:HD2	1:B:196:ARG:H	1.27	0.82
1:A:406:ASP:OD1	2:A:723:GLC:H1	1.79	0.82
1:A:316:THR:O	1:A:320:GLN:HG3	1.83	0.79
1:B:142:GLN:HG3	8:B:963:HOH:O	1.84	0.77
1:A:87:ILE:H	1:A:171:ASN:ND2	1.82	0.75
1:A:87:ILE:N	1:A:171:ASN:HD21	1.83	0.75
1:A:23:PRO:HG2	1:A:26:GLN:HG3	1.67	0.75
1:A:606:ILE:HG13	8:A:1146:HOH:O	1.86	0.74
1:A:660:ILE:HB	1:A:706:VAL:HG13	1.70	0.74
1:A:479:LYS:H	1:A:479:LYS:HD2	1.52	0.73
1:B:640:LEU:HD21	1:B:660:ILE:HD11	1.71	0.72
1:A:230:ASN:HD21	1:A:250:ALA:H	1.36	0.72
1:A:341:VAL:H	1:A:374:ASN:HD21	1.37	0.72
1:A:496:HIS:HE1	1:A:503:GLY:H	1.38	0.72
1:B:339:ASN:ND2	1:B:340:HIS:HD2	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:HIS:HE1	1:B:503:GLY:H	1.38	0.71
4:B:731:BGC:O5	4:B:732:GLC:H62	1.91	0.70
1:B:111:THR:HG22	1:B:114:HIS:N	1.99	0.69
1:A:135:ASN:N	1:A:135:ASN:HD22	1.90	0.69
1:B:505:LYS:H	1:B:505:LYS:HD2	1.55	0.69
1:A:160:HIS:HD2	1:A:196:ARG:H	1.40	0.69
1:B:87:ILE:H	1:B:171:ASN:ND2	1.92	0.68
1:A:307:ASN:ND2	1:A:309:HIS:H	1.91	0.68
1:A:111:THR:CG2	1:A:114:HIS:H	1.99	0.67
1:A:211:HIS:HD2	1:A:213:VAL:HG22	1.60	0.67
1:B:339:ASN:HD21	1:B:340:HIS:HD2	1.41	0.67
1:B:553:VAL:HG22	8:B:1223:HOH:O	1.95	0.67
1:A:472:LYS:HE3	1:A:475:THR:HG22	1.77	0.67
1:A:39:GLU:O	1:A:40:ILE:HG13	1.95	0.66
1:A:479:LYS:H	1:A:479:LYS:CD	2.07	0.66
1:A:660:ILE:HB	1:A:706:VAL:CG1	2.26	0.66
1:B:22:ILE:HD13	1:B:30:MET:O	1.96	0.66
1:A:111:THR:HG23	1:A:113:ASP:H	1.61	0.66
1:A:40:ILE:O	1:A:40:ILE:HD12	1.97	0.65
1:B:596:ARG:O	1:B:596:ARG:HD2	1.97	0.64
1:A:586:ASP:O	1:A:590:GLN:HG2	1.97	0.64
1:B:370:THR:HG23	1:B:375:ASP:OD2	1.97	0.64
1:B:307:ASN:ND2	1:B:309:HIS:H	1.96	0.64
1:A:505:LYS:HE2	1:A:506:ALA:HB3	1.79	0.64
1:A:602:ASP:O	1:A:606:ILE:HD12	1.97	0.64
1:A:38:THR:HG22	1:A:73:HIS:HA	1.78	0.64
1:B:544:ARG:O	1:B:548:ARG:HG3	1.98	0.64
1:B:211:HIS:HD2	1:B:213:VAL:H	1.46	0.63
1:B:230:ASN:HD21	1:B:250:ALA:N	1.95	0.63
1:A:339:ASN:HD21	1:A:340:HIS:HD2	1.46	0.63
1:A:479:LYS:N	1:A:479:LYS:HD2	2.15	0.62
1:B:211:HIS:CD2	1:B:213:VAL:HG22	2.34	0.62
1:A:505:LYS:CG	1:A:506:ALA:N	2.57	0.62
1:A:339:ASN:ND2	1:A:340:HIS:HD2	1.99	0.61
1:B:505:LYS:O	1:B:506:ALA:CB	2.50	0.60
1:A:111:THR:HG22	1:A:114:HIS:N	1.98	0.60
1:B:120:TRP:CZ2	1:B:382:MET:HG3	2.35	0.60
1:B:111:THR:HG23	1:B:113:ASP:H	1.66	0.60
1:B:39:GLU:HG3	1:B:40:ILE:HG13	1.84	0.59
1:B:133:HIS:HB3	1:B:136:LYS:HB2	1.83	0.59
1:A:628:GLN:HE21	1:A:628:GLN:HA	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:HIS:CD2	1:A:213:VAL:HG22	2.36	0.59
1:B:120:TRP:CH2	1:B:382:MET:HG3	2.38	0.59
1:A:370:THR:HG23	1:A:375:ASP:OD2	2.03	0.58
1:B:22:ILE:HD12	1:B:59:TYR:HE1	1.67	0.58
1:B:406:ASP:OD1	4:B:733:GLC:H1	2.03	0.58
1:B:435:GLU:OE1	4:B:733:GLC:H1	2.03	0.58
1:B:1:MET:HG2	1:B:2:VAL:HG23	1.84	0.58
1:A:606:ILE:HD11	8:A:911:HOH:O	2.02	0.58
1:A:38:THR:OG1	1:A:41:THR:HB	2.04	0.58
1:B:370:THR:OG1	1:B:372:VAL:HG22	2.05	0.57
1:A:223:ARG:HD2	7:A:761:GOL:O3	2.03	0.57
1:A:544:ARG:O	1:A:548:ARG:HG3	2.03	0.57
1:A:695:LYS:O	1:A:697:THR:N	2.36	0.56
1:B:251:ASN:HB2	1:B:597:GLU:OE2	2.06	0.56
1:B:307:ASN:HD21	1:B:309:HIS:HB2	1.71	0.56
1:A:607:ARG:HD3	8:A:1151:HOH:O	2.06	0.56
1:A:553:VAL:HG12	1:A:557:LEU:HD12	1.86	0.56
1:A:549:GLN:O	1:A:553:VAL:HG23	2.06	0.56
1:A:118:LYS:HG2	1:A:152:ALA:HB2	1.88	0.55
1:A:135:ASN:N	1:A:135:ASN:ND2	2.54	0.55
1:B:41:THR:HG22	1:B:42:ASP:N	2.21	0.55
1:B:345:GLU:CD	1:B:345:GLU:H	2.10	0.55
1:A:73:HIS:HB2	1:A:85:LEU:HB2	1.88	0.55
1:B:41:THR:HG21	1:B:43:PHE:CE1	2.42	0.55
1:B:496:HIS:HD2	8:B:1221:HOH:O	1.89	0.55
1:A:247:THR:HG22	1:A:255:SER:HG	1.70	0.54
1:B:73:HIS:HE1	8:B:943:HOH:O	1.89	0.54
1:B:631:LEU:C	1:B:631:LEU:HD23	2.27	0.54
1:A:631:LEU:HD23	1:A:632:GLU:N	2.22	0.54
1:A:87:ILE:HG13	1:A:171:ASN:ND2	2.23	0.54
1:A:640:LEU:HD13	1:A:641:ILE:N	2.23	0.54
1:A:445:HIS:HD2	1:B:632:GLU:OE2	1.91	0.54
1:A:469:ASP:OD2	1:A:475:THR:HG23	2.09	0.53
1:B:536:ALA:O	1:B:537:LEU:HD12	2.08	0.53
1:A:17:ILE:HG13	1:A:17:ILE:O	2.09	0.53
1:A:39:GLU:O	1:A:40:ILE:CG1	2.56	0.53
1:A:570:GLU:CB	1:A:606:ILE:HD13	2.34	0.53
1:A:631:LEU:C	1:A:631:LEU:HD23	2.29	0.53
1:A:571:PHE:CE2	1:A:596:ARG:HB2	2.43	0.53
1:B:341:VAL:H	1:B:374:ASN:HD21	1.56	0.53
1:B:505:LYS:HD2	1:B:505:LYS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLN:NE2	1:A:628:GLN:HA	2.24	0.53
1:B:207:LYS:HB2	1:B:208:PRO:HD2	1.91	0.52
1:A:571:PHE:HZ	1:A:591:LEU:HD22	1.74	0.52
1:B:679:ARG:NH2	1:B:693:GLU:HG3	2.25	0.52
1:B:536:ALA:C	1:B:537:LEU:HD12	2.30	0.52
1:A:427:LYS:O	1:A:430:ILE:HG23	2.09	0.52
1:B:661:HIS:HE1	8:B:1043:HOH:O	1.93	0.52
1:B:692:THR:HG22	8:B:1243:HOH:O	2.08	0.51
1:A:380:ARG:HA	1:A:380:ARG:HE	1.76	0.51
1:B:571:PHE:CE2	1:B:596:ARG:HB2	2.46	0.51
1:A:637:LYS:HE3	8:A:922:HOH:O	2.10	0.50
1:A:6:ARG:HD3	1:A:84:ASP:OD2	2.11	0.50
1:A:178:VAL:HG21	1:A:296:HIS:CE1	2.46	0.50
1:B:101:TYR:CD1	1:B:382:MET:HE3	2.47	0.50
1:A:32:PRO:HG3	1:A:34:PHE:CE1	2.46	0.50
1:B:211:HIS:HD2	1:B:213:VAL:HG22	1.77	0.50
1:B:549:GLN:O	1:B:553:VAL:HG23	2.12	0.49
1:A:87:ILE:HG13	1:A:171:ASN:HD21	1.75	0.49
1:A:230:ASN:HD21	1:A:250:ALA:N	2.09	0.49
1:B:496:HIS:CE1	1:B:503:GLY:H	2.25	0.49
1:B:250:ALA:HB3	8:B:1276:HOH:O	2.12	0.49
1:B:682:CYS:O	1:B:706:VAL:HA	2.12	0.49
1:B:22:ILE:HD12	1:B:59:TYR:CE1	2.48	0.49
1:B:33:PRO:HD2	1:B:78:SER:HB3	1.94	0.49
1:B:32:PRO:HG3	1:B:34:PHE:CE1	2.47	0.48
1:A:41:THR:HG23	1:A:43:PHE:CE1	2.47	0.48
1:B:382:MET:HE2	1:B:385:LYS:HD3	1.96	0.48
1:A:427:LYS:HB3	1:A:430:ILE:CG2	2.44	0.48
1:A:53:LEU:HD12	1:A:53:LEU:N	2.29	0.48
1:A:133:HIS:CD2	1:A:134:PRO:HD2	2.49	0.48
1:A:682:CYS:O	1:A:706:VAL:HA	2.13	0.48
1:A:362:GLU:HG2	1:B:636:LEU:HD13	1.96	0.48
1:A:492:GLN:HE22	1:A:505:LYS:HD2	1.77	0.47
1:B:463:PHE:HA	1:B:518:ILE:HB	1.96	0.47
1:A:406:ASP:OD1	2:A:723:GLC:C1	2.55	0.47
1:A:364:GLY:C	1:A:365:LYS:HD2	2.34	0.47
1:B:504:TRP:O	1:B:505:LYS:C	2.52	0.47
1:A:307:ASN:HD21	1:A:309:HIS:HB2	1.80	0.47
1:A:592:ASP:OD1	1:A:594:ASP:HB2	2.14	0.47
1:B:660:ILE:CG2	1:B:706:VAL:HG13	2.31	0.47
1:A:243:THR:HG22	1:A:321:MET:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ASN:HD22	1:A:307:ASN:C	2.18	0.46
1:B:288:TYR:CD1	1:B:289:ASN:N	2.83	0.46
1:B:427:LYS:HE2	8:B:988:HOH:O	2.15	0.46
1:B:111:THR:CG2	1:B:114:HIS:H	2.05	0.46
1:B:582:TYR:CD2	4:B:732:GLC:H4	2.51	0.46
1:A:39:GLU:C	1:A:40:ILE:HG23	2.35	0.46
1:A:38:THR:HG22	1:A:72:ILE:O	2.15	0.46
1:A:41:THR:HG23	1:A:43:PHE:HE1	1.81	0.46
1:B:406:ASP:OD1	4:B:733:GLC:C1	2.63	0.46
1:A:221:HIS:CD2	1:A:223:ARG:H	2.34	0.46
1:B:221:HIS:CD2	1:B:223:ARG:H	2.34	0.46
1:A:307:ASN:ND2	1:A:307:ASN:C	2.70	0.46
1:A:628:GLN:HE21	1:A:628:GLN:CA	2.25	0.46
1:B:542:ASP:O	1:B:546:ARG:HG3	2.16	0.46
1:A:472:LYS:CE	1:A:475:THR:HG22	2.44	0.45
1:A:41:THR:HG22	1:A:42:ASP:N	2.31	0.45
1:B:382:MET:HA	1:B:382:MET:CE	2.46	0.45
1:A:553:VAL:CG2	8:A:904:HOH:O	2.64	0.45
1:B:616:HIS:HB3	1:B:652:ASP:OD2	2.15	0.45
1:B:683:ASP:HB2	1:B:684:PRO:CD	2.47	0.45
1:B:6:ARG:HD3	1:B:84:ASP:OD2	2.16	0.45
1:A:22:ILE:HD12	1:A:27:LYS:HA	1.97	0.45
1:A:359:ARG:NH2	1:A:443:LEU:HD11	2.32	0.45
1:B:211:HIS:CE1	1:B:622:ARG:HD2	2.52	0.44
1:B:344:ARG:HG3	1:B:358:PHE:CE2	2.53	0.44
1:A:477:HIS:HA	1:A:479:LYS:HZ2	1.83	0.44
1:B:505:LYS:O	1:B:506:ALA:HB3	2.17	0.44
1:A:211:HIS:O	1:A:214:ASP:HB2	2.16	0.44
1:A:232:GLY:O	1:A:247:THR:HG23	2.17	0.44
1:B:596:ARG:HD2	1:B:596:ARG:C	2.37	0.44
1:A:445:HIS:CE1	1:A:446:GLU:HG3	2.53	0.44
1:A:288:TYR:CD1	1:A:289:ASN:N	2.86	0.44
1:A:235:ASN:O	1:A:241:ALA:HB2	2.18	0.44
1:A:485:LEU:HA	1:A:548:ARG:HE	1.82	0.44
1:A:207:LYS:HB3	1:A:208:PRO:HD2	2.00	0.44
1:A:309:HIS:O	1:A:311:PRO:HD3	2.18	0.44
1:A:228:HIS:HD2	1:A:590:GLN:NE2	2.15	0.44
1:A:133:HIS:HD2	1:A:134:PRO:N	2.14	0.44
1:A:14:ASP:HB3	1:A:17:ILE:CG2	2.35	0.43
1:B:553:VAL:HG12	1:B:557:LEU:HD12	2.00	0.43
1:A:680:LEU:HD12	1:A:688:GLN:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:THR:OG1	1:A:41:THR:CB	2.66	0.43
1:A:339:ASN:ND2	1:A:340:HIS:CD2	2.84	0.43
1:B:117:PHE:O	1:B:152:ALA:HA	2.18	0.43
1:A:271:LEU:HB3	1:A:272:PRO:HD2	2.01	0.43
1:B:339:ASN:ND2	1:B:340:HIS:CD2	2.77	0.43
1:A:680:LEU:C	1:A:680:LEU:HD13	2.39	0.43
1:A:380:ARG:HA	1:A:380:ARG:NE	2.34	0.43
1:B:12:VAL:HG13	1:B:12:VAL:O	2.18	0.43
1:A:683:ASP:HB2	1:A:684:PRO:HD2	2.01	0.43
1:B:171:ASN:O	1:B:172:SER:HB2	2.17	0.43
1:B:621:LEU:HD23	1:B:627:ILE:HA	2.00	0.43
1:B:27:LYS:NZ	8:B:1161:HOH:O	2.49	0.43
1:A:91:ILE:HD13	1:A:354:PRO:O	2.19	0.43
1:B:694:ILE:HD11	1:B:708:LEU:CD2	2.48	0.43
1:A:472:LYS:HD2	1:A:532:LYS:HG2	2.01	0.43
1:B:73:HIS:HD2	7:B:762:GOL:H12	1.84	0.43
1:A:435:GLU:HB2	1:A:437:TRP:CE2	2.53	0.42
1:A:621:LEU:HD23	1:A:627:ILE:HA	2.01	0.42
1:A:492:GLN:NE2	1:A:505:LYS:HD2	2.35	0.42
1:B:160:HIS:CD2	1:B:196:ARG:HG2	2.54	0.42
1:A:204:ALA:N	1:A:205:PRO:HD3	2.34	0.42
1:A:661:HIS:HD2	1:A:705:THR:OG1	2.02	0.42
1:B:49:GLU:HG2	1:B:60:VAL:HG22	2.02	0.42
1:A:694:ILE:C	1:A:694:ILE:HD12	2.39	0.42
1:A:160:HIS:CD2	1:A:196:ARG:H	2.28	0.42
1:B:91:ILE:HD13	1:B:354:PRO:O	2.19	0.42
1:B:505:LYS:CD	1:B:505:LYS:N	2.82	0.42
1:B:496:HIS:HE1	1:B:503:GLY:N	2.10	0.42
1:B:75:VAL:CG2	1:B:83:THR:HG22	2.49	0.42
1:A:17:ILE:HD13	1:A:60:VAL:HG13	2.02	0.42
1:A:692:THR:HG22	8:A:929:HOH:O	2.20	0.42
1:B:694:ILE:HD11	1:B:708:LEU:HD22	2.02	0.41
1:B:628:GLN:HA	1:B:628:GLN:HE21	1.84	0.41
1:A:110:TYR:CG	1:A:111:THR:N	2.87	0.41
1:B:496:HIS:CE1	1:B:501:SER:HA	2.55	0.41
1:A:362:GLU:N	1:A:362:GLU:OE1	2.48	0.41
1:B:240:LEU:HG	8:B:1190:HOH:O	2.19	0.41
1:A:280:ASP:OD2	1:A:283:LYS:HE3	2.20	0.41
1:A:129:VAL:HG13	1:A:129:VAL:O	2.20	0.41
1:B:427:LYS:O	1:B:430:ILE:HG23	2.21	0.41
1:B:204:ALA:HA	1:B:205:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:PHE:HA	1:A:518:ILE:HB	2.01	0.41
4:B:731:BGC:C1	4:B:732:GLC:H62	2.51	0.41
1:A:616:HIS:HB3	1:A:652:ASP:OD2	2.21	0.41
1:A:496:HIS:HE1	1:A:503:GLY:N	2.12	0.41
1:A:661:HIS:HE1	8:A:913:HOH:O	2.04	0.41
1:A:333:ILE:HD11	1:A:431:LEU:HD12	2.03	0.41
1:B:391:VAL:HG13	1:B:403:PHE:CE1	2.56	0.41
1:A:646:TYR:CD1	1:A:647:ASP:HB2	2.56	0.41
1:B:690:ASP:N	1:B:690:ASP:OD2	2.51	0.41
1:A:139:ARG:NH1	8:A:838:HOH:O	2.51	0.41
1:A:111:THR:HG21	1:A:114:HIS:CE1	2.57	0.40
1:A:117:PHE:O	1:A:152:ALA:HA	2.21	0.40
1:B:681:LEU:HD22	1:B:681:LEU:O	2.21	0.40
1:B:211:HIS:CD2	1:B:213:VAL:H	2.34	0.40
1:A:667:SER:OG	1:A:701:ASN:OD1	2.40	0.40
1:A:454:ALA:N	1:A:455:PRO:CD	2.84	0.40
1:A:288:TYR:CD1	1:A:288:TYR:C	2.95	0.40
1:A:290:TRP:CD2	1:A:582:TYR:HA	2.57	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	710/718 (99%)	670 (94%)	28 (4%)	12 (2%)	11	10
1	B	710/718 (99%)	675 (95%)	31 (4%)	4 (1%)	30	36
All	All	1420/1436 (99%)	1345 (95%)	59 (4%)	16 (1%)	17	18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	651	VAL
1	B	506	ALA
1	A	42	ASP
1	A	136	LYS
1	A	696	LYS
1	B	505	LYS
1	A	40	ILE
1	A	137	SER
1	A	15	MET
1	A	24	ALA
1	A	343	LYS
1	A	684	PRO
1	B	2	VAL
1	B	272	PRO
1	A	272	PRO
1	A	690	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	609/615 (99%)	574 (94%)	35 (6%)	25	34
1	B	609/615 (99%)	579 (95%)	30 (5%)	31	41
All	All	1218/1230 (99%)	1153 (95%)	65 (5%)	28	37

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ILE
1	A	25	GLU
1	A	28	GLU
1	A	40	ILE
1	A	85	LEU
1	A	97	ASP
1	A	111	THR
1	A	135	ASN

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Mol	Chain	Res	Type
1	A	165	LEU
1	A	178	VAL
1	A	196	ARG
1	A	242	LEU
1	A	251	ASN
1	A	257	LEU
1	A	307	ASN
1	A	345	GLU
1	A	362	GLU
1	A	408	LEU
1	A	419	MET
1	A	446	GLU
1	A	451	LEU
1	A	467	PHE
1	A	479	LYS
1	A	539	GLN
1	A	591	LEU
1	A	596	ARG
1	A	621	LEU
1	A	622	ARG
1	A	634	LEU
1	A	644	ARG
1	A	645	LEU
1	A	647	ASP
1	A	675	ASP
1	A	690	ASP
1	A	706	VAL
1	B	28	GLU
1	B	60	VAL
1	B	85	LEU
1	B	111	THR
1	B	196	ARG
1	B	207	LYS
1	B	230	ASN
1	B	242	LEU
1	B	307	ASN
1	B	332	VAL
1	B	408	LEU
1	B	419	MET
1	B	446	GLU
1	B	451	LEU
1	B	467	PHE

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Mol	Chain	Res	Type
1	B	496	HIS
1	B	520	TYR
1	B	580	ASN
1	B	591	LEU
1	B	596	ARG
1	B	621	LEU
1	B	622	ARG
1	B	629	ARG
1	B	634	LEU
1	B	644	ARG
1	B	645	LEU
1	B	660	ILE
1	B	671	ARG
1	B	706	VAL
1	B	710	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	133	HIS
1	A	135	ASN
1	A	160	HIS
1	A	171	ASN
1	A	180	GLN
1	A	199	GLN
1	A	211	HIS
1	A	221	HIS
1	A	230	ASN
1	A	248	GLN
1	A	274	ASN
1	A	293	ASN
1	A	307	ASN
1	A	309	HIS
1	A	312	GLN
1	A	327	GLN
1	A	328	HIS
1	A	339	ASN
1	A	340	HIS
1	A	374	ASN
1	A	445	HIS
1	A	492	GLN

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Mol	Chain	Res	Type
1	A	496	HIS
1	A	516	GLN
1	A	549	GLN
1	A	580	ASN
1	A	583	GLN
1	A	590	GLN
1	A	628	GLN
1	A	661	HIS
1	B	26	GLN
1	B	73	HIS
1	B	133	HIS
1	B	142	GLN
1	B	160	HIS
1	B	171	ASN
1	B	180	GLN
1	B	211	HIS
1	B	221	HIS
1	B	230	ASN
1	B	248	GLN
1	B	274	ASN
1	B	307	ASN
1	B	309	HIS
1	B	312	GLN
1	B	327	GLN
1	B	328	HIS
1	B	339	ASN
1	B	340	HIS
1	B	374	ASN
1	B	496	HIS
1	B	527	HIS
1	B	549	GLN
1	B	580	ASN
1	B	583	GLN
1	B	628	GLN
1	B	661	HIS

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)

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	GLC	A	721	2	11,11,12	0.55	0	14,15,17	0.61	1 (7%)
2	GLC	A	722	2	11,11,12	0.59	0	14,15,17	0.81	1 (7%)
2	GLC	A	723	2	12,12,12	0.54	0	17,17,17	0.39	0
3	GLC	A	735	3	11,11,12	0.55	0	14,15,17	0.73	1 (7%)
3	GLC	A	736	3	12,12,12	0.53	0	17,17,17	0.46	0
4	BGC	B	731	4	11,11,12	0.51	0	14,15,17	0.58	0
4	GLC	B	732	4	11,11,12	0.60	0	14,15,17	1.26	2 (14%)
4	GLC	B	733	4	12,12,12	0.55	0	17,17,17	0.45	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	721	2	-	0/2/19/22	0/1/1/1
2	GLC	A	722	2	-	0/2/19/22	0/1/1/1
2	GLC	A	723	2	-	0/2/22/22	0/1/1/1
3	GLC	A	735	3	-	0/2/19/22	0/1/1/1
3	GLC	A	736	3	-	0/2/22/22	0/1/1/1
4	BGC	B	731	4	-	0/2/19/22	0/1/1/1
4	GLC	B	732	4	-	0/2/19/22	0/1/1/1
4	GLC	B	733	4	-	0/2/22/22	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(^{o})	Ideal(^{o})
4	B	732	GLC	C2-C3-C4	-2.41	106.95	111.04
2	A	721	GLC	C1-O5-C5	2.10	114.91	112.25
3	A	735	GLC	C1-O5-C5	2.10	114.92	112.25
2	A	722	GLC	C1-O5-C5	2.28	115.15	112.25
4	B	732	GLC	C1-O5-C5	3.10	116.18	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	723	GLC	2	0
4	B	731	BGC	2	0
4	B	732	GLC	3	0
4	B	733	GLC	3	0

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	#$|Z| > 2$
6	ACT	A	751	-	1,3,3	0.32	0	0,3,3	0.00	-
6	ACT	A	753	-	1,3,3	0.86	0	0,3,3	0.00	-
7	GOL	A	761	-	5,5,5	4.48	5 (100%)	5,5,5	5.72	3 (60%)
6	ACT	B	752	-	1,3,3	1.12	0	0,3,3	0.00	-
7	GOL	B	762	-	5,5,5	4.43	5 (100%)	5,5,5	5.76	3 (60%)

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	ACT	A	751	-	-	0/0/0/0	0/0/0/0
6	ACT	A	753	-	-	0/0/0/0	0/0/0/0
7	GOL	A	761	-	-	0/4/4/4	0/0/0/0
6	ACT	B	752	-	-	0/0/0/0	0/0/0/0
7	GOL	B	762	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	761	GOL	C3-C2	-8.21	1.20	1.52
7	B	762	GOL	C3-C2	-8.05	1.21	1.52
7	B	762	GOL	C1-C2	-3.05	1.40	1.52
7	A	761	GOL	C1-C2	-3.02	1.40	1.52
7	A	761	GOL	O2-C2	-2.94	1.34	1.43
7	B	762	GOL	O2-C2	-2.89	1.34	1.43
7	A	761	GOL	O1-C1	-2.30	1.32	1.42
7	B	762	GOL	O1-C1	-2.24	1.32	1.42
7	A	761	GOL	O3-C3	3.13	1.55	1.42
7	B	762	GOL	O3-C3	3.27	1.56	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	762	GOL	O1-C1-C2	3.17	125.54	110.18
7	A	761	GOL	O1-C1-C2	3.27	126.05	110.18
7	B	762	GOL	O2-C2-C3	6.40	137.97	108.65
7	A	761	GOL	O2-C2-C3	6.43	138.12	108.65
7	A	761	GOL	O3-C3-C2	10.55	161.36	110.18
7	B	762	GOL	O3-C3-C2	10.70	162.07	110.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	761	GOL	1	0
7	B	762	GOL	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 (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	712/718 (99%)	-0.27	17 (2%)	62	71	21, 34, 58, 80	0
1	B	712/718 (99%)	-0.38	7 (0%)	84	88	22, 33, 54, 70	0
All	All	1424/1436 (99%)	-0.33	24 (1%)	73	79	21, 34, 56, 80	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.3
1	A	1	MET	6.1
1	A	135	ASN	4.6
1	A	40	ILE	4.6
1	A	712	SER	3.3
1	A	43	PHE	3.1
1	A	24	ALA	3.1
1	A	29	ILE	3.1
1	B	40	ILE	3.1
1	A	25	GLU	2.9
1	A	39	GLU	2.9
1	A	41	THR	2.8
1	A	711	ALA	2.6
1	B	64	ASP	2.3
1	A	690	ASP	2.3
1	A	54	GLU	2.3
1	A	64	ASP	2.2
1	A	476	PHE	2.1
1	B	712	SER	2.1
1	A	650	GLU	2.1
1	B	54	GLU	2.1
1	B	649	ASP	2.0
1	A	53	LEU	2.0
1	B	476	PHE	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
4	GLC	B	733	12/12	0.70	0.30	7.01	69,75,77,77	0
2	GLC	A	723	12/12	0.77	0.20	2.87	57,59,60,62	0
3	GLC	A	735	11/12	0.83	0.17	2.49	50,55,57,58	0
4	GLC	B	732	11/12	0.82	0.18	1.75	69,71,72,72	0
2	GLC	A	722	11/12	0.87	0.13	0.73	51,57,57,58	0
2	GLC	A	721	11/12	0.84	0.21	-	61,61,62,62	0
4	BGC	B	731	11/12	0.66	0.24	-	69,71,72,73	0
3	GLC	A	736	12/12	0.82	0.18	-	58,61,62,62	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
7	GOL	B	762	6/6	0.74	0.22	5.59	40,44,47,48	0
6	ACT	A	751	4/4	0.87	0.18	5.35	53,53,54,55	0
7	GOL	A	761	6/6	0.82	0.15	2.87	49,52,53,54	0
6	ACT	B	752	4/4	0.80	0.17	2.24	51,52,52,53	0
6	ACT	A	753	4/4	0.95	0.08	-0.78	58,59,59,59	0
5	CA	B	742	1/1	0.99	0.07	-1.65	38,38,38,38	0
5	CA	A	741	1/1	0.98	0.08	-2.00	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.