Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:48 PM GMT

PDB ID	:	1VB9
Title	:	Crystal structure of Thermoactinomyces vulgaris R-47 alpha-amylase II (TVA II) complexed with transglycosylated product
Authors	:	Mizuno, M.; Tonozuka, T.; Uechi, A.; Ohtaki, A.; Ichikawa, K.; Kamitori, S.; Nishikawa, A.; Sakano, Y.
Deposited on	:	2004-02-25
Resolution	:	2.20 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 (1)) were used in the production of this report:

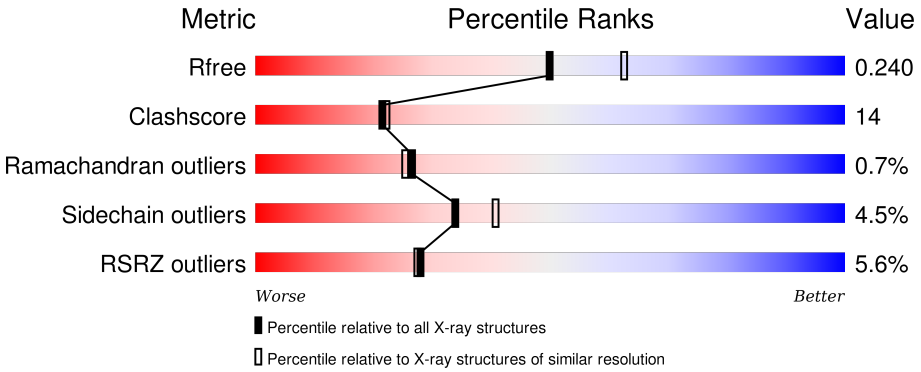
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	585	5% 72% 25%
1	B	585	6% 75% 22%

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	701	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10196 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 alpha-amylase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	0	0
			4776	3056	832	873	15			
1	B	585	Total	C	N	O	S	0	0	0
			4776	3056	832	873	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	325	ASN	ASP	ENGINEERED	UNP Q08751
B	325	ASN	ASP	ENGINEERED	UNP Q08751

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	6	Total	C	O	0	0
			67	36	31		
2	B	6	Total	C	O	0	0
			67	36	31		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	249	Total	O	0	0
			249	249		

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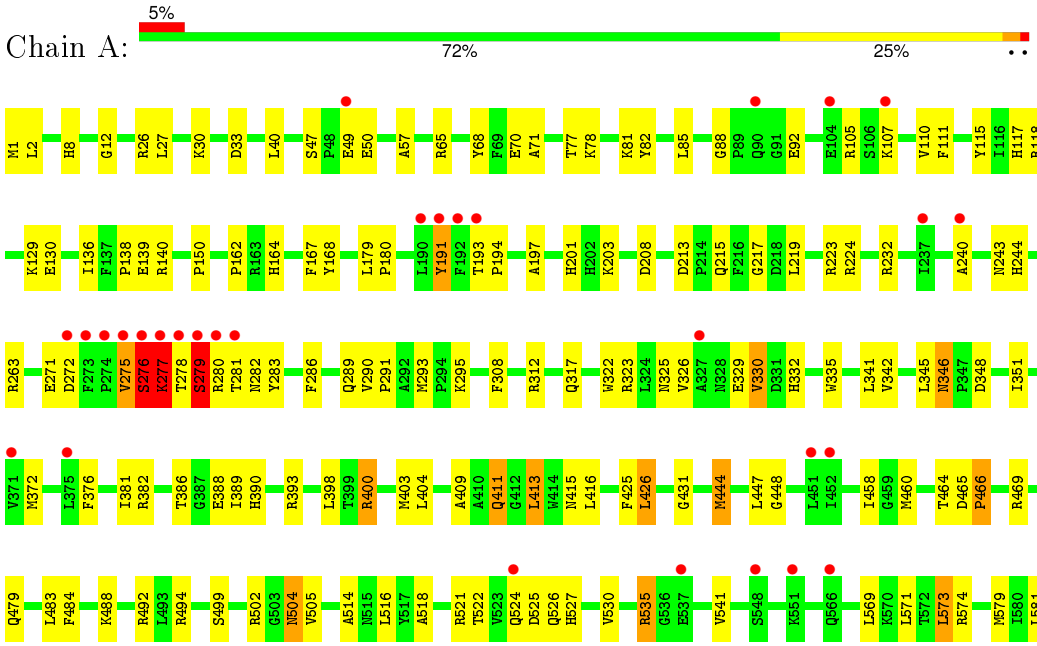
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	259	Total	O	0	0
			259	259		

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.

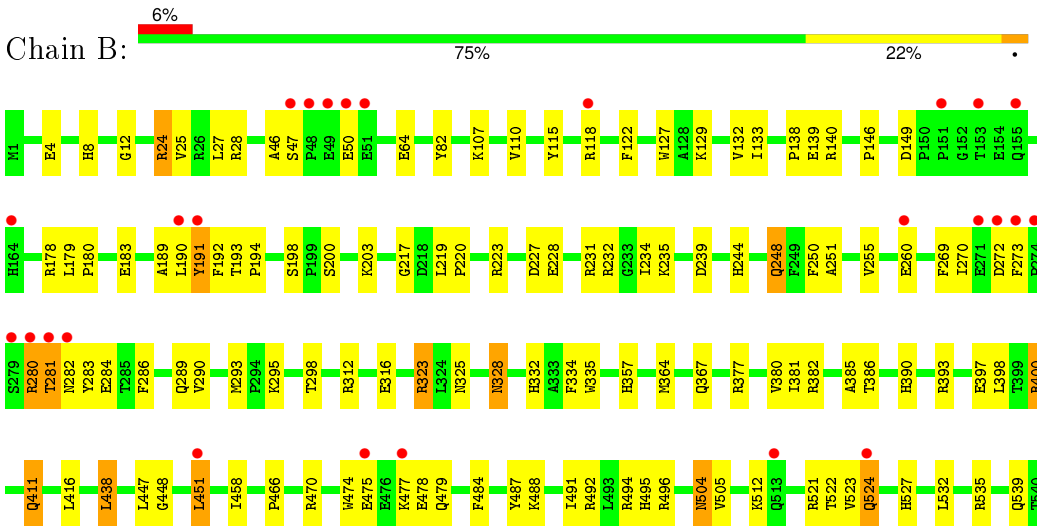
- Molecule 1: alpha-amylase II

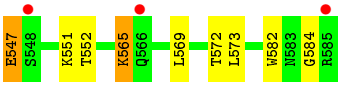
Chain A:



- Molecule 1: alpha-amylase II

Chain B:




E547
S548
K551
T552
K565
Q566
L569
T572
L573
W582
N583
G584
R585

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.05Å 118.27Å 112.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.99 – 2.20 33.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (33.99-2.20) 99.9 (33.98-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.29 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.194 , 0.233 0.202 , 0.240	Depositor DCC
R_{free} test set	7736 reflections (10.08%)	DCC
Wilson B-factor (Å^2)	29.2	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.5	EDS
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 76732 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10196	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/4906	0.62	3/6641 (0.0%)
1	B	0.35	0/4906	0.60	1/6641 (0.0%)
All	All	0.35	0/9812	0.61	4/13282 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	LYS	N-CA-C	-7.84	89.83	111.00
1	A	276	SER	N-CA-C	5.99	127.18	111.00
1	A	279	SER	N-CA-C	-5.39	96.45	111.00
1	B	323	ARG	N-CA-C	-5.08	97.29	111.00

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	4776	0	4609	143	0
1	B	4776	0	4609	129	0
2	A	67	0	57	4	0
2	B	67	0	57	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	249	0	0	6	0
4	B	259	0	0	14	0
All	All	10196	0	9332	269	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 14.

All (269) 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:342:VAL:HG11	1:A:351:ILE:HD11	1.46	0.97
1:B:293:MET:HE1	2:B:702:GLC:H62	1.45	0.97
1:A:293:MET:HE1	2:A:702:GLC:H62	1.48	0.94
1:A:585:ARG:HH11	1:A:585:ARG:HB3	1.35	0.89
1:B:198:SER:HB3	1:B:203:LYS:HG3	1.57	0.87
1:B:293:MET:CE	2:B:702:GLC:H62	2.05	0.86
1:A:140:ARG:HG2	1:A:469:ARG:O	1.77	0.84
1:A:290:VAL:HG11	1:A:293:MET:CE	2.06	0.84
1:A:293:MET:CE	2:A:702:GLC:H62	2.07	0.84
1:A:280:ARG:HA	1:A:289:GLN:OE1	1.79	0.81
1:B:290:VAL:HG11	1:B:293:MET:HE3	1.64	0.80
1:B:46:ALA:HB1	1:B:50:GLU:HG3	1.63	0.80
1:B:523:VAL:HG22	1:B:524:GLN:NE2	1.97	0.79
1:A:290:VAL:HG11	1:A:293:MET:HE2	1.65	0.78
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.32	0.76
1:A:447:LEU:HB2	1:A:505:VAL:HG21	1.66	0.76
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.21	0.76
1:B:470:ARG:HG3	4:B:741:HOH:O	1.85	0.75
1:A:504:ASN:C	1:A:504:ASN:HD22	1.91	0.73
1:B:505:VAL:HG12	1:B:521:ARG:CD	2.18	0.73
1:A:191:TYR:CZ	1:A:323:ARG:HD3	2.22	0.73
1:B:275:VAL:O	1:B:282:ASN:ND2	2.23	0.72
1:B:290:VAL:HG11	1:B:293:MET:CE	2.20	0.72
1:B:139:GLU:HB3	1:B:140:ARG:HH11	1.56	0.71
1:A:341:LEU:O	1:A:345:LEU:HD13	1.90	0.71
1:A:569:LEU:HG	1:A:571:LEU:HD13	1.72	0.71
1:A:390:HIS:HD2	1:A:393:ARG:H	1.39	0.71
1:A:277:LYS:HG3	1:A:277:LYS:O	1.91	0.70
1:B:328:ASN:HD22	1:B:328:ASN:N	1.89	0.70
1:A:194:PRO:HB2	1:A:203:LYS:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:487:TYR:O	1:B:491:ILE:HG12	1.93	0.69
1:A:516:LEU:HD13	1:A:541:VAL:HG11	1.74	0.69
1:A:330:VAL:HG22	1:A:335:TRP:NE1	2.08	0.69
1:A:447:LEU:HB2	1:A:505:VAL:CG2	2.23	0.68
1:A:271:GLU:HG3	1:A:272:ASP:H	1.58	0.68
1:A:400:ARG:HH21	1:A:400:ARG:CB	2.07	0.68
1:B:547:GLU:HG2	1:B:551:LYS:HE2	1.76	0.67
1:B:139:GLU:HB3	1:B:140:ARG:NH1	2.09	0.66
1:A:290:VAL:HG11	1:A:293:MET:HE3	1.76	0.66
1:A:224:ARG:HA	1:A:224:ARG:HE	1.59	0.66
1:A:477:LYS:HD2	1:A:477:LYS:N	2.11	0.65
1:B:492:ARG:O	1:B:496:ARG:HG3	1.98	0.64
1:A:275:VAL:O	1:A:275:VAL:HG12	1.97	0.64
1:B:400:ARG:O	1:B:404:LEU:HD13	1.98	0.63
1:B:255:VAL:HG11	1:B:270:ILE:HD11	1.78	0.63
1:B:504:ASN:HD22	1:B:504:ASN:C	2.02	0.62
1:B:523:VAL:HG22	1:B:524:GLN:HE22	1.64	0.62
1:A:386:THR:OG1	1:A:388:GLU:HG3	2.00	0.62
1:B:183:GLU:OE2	1:B:232:ARG:HD2	2.00	0.62
1:B:328:ASN:HD22	1:B:328:ASN:H	1.47	0.61
1:A:118:ARG:HG2	4:B:727:HOH:O	1.99	0.61
1:A:271:GLU:HG3	1:A:272:ASP:N	2.14	0.61
1:A:129:LYS:HD2	1:A:502:ARG:HH12	1.66	0.60
1:A:390:HIS:CD2	1:A:393:ARG:H	2.19	0.60
1:B:64:GLU:HB2	4:B:816:HOH:O	2.00	0.60
1:A:224:ARG:NE	1:A:224:ARG:HA	2.17	0.60
1:B:484:PHE:CE1	1:B:488:LYS:HD2	2.36	0.60
1:A:129:LYS:HB3	1:A:411:GLN:OE1	2.02	0.59
1:B:260:GLU:HB2	1:B:273:PHE:CD2	2.38	0.59
1:B:133:ILE:HB	1:B:451:LEU:HD23	1.85	0.59
1:A:129:LYS:HD2	1:A:502:ARG:NH1	2.17	0.59
1:A:409:ALA:O	1:A:413:LEU:HD13	2.04	0.58
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.39	0.58
1:B:390:HIS:NE2	1:B:512:LYS:HE2	2.19	0.57
1:B:447:LEU:HB2	1:B:505:VAL:CG1	2.34	0.57
1:A:382:ARG:HG2	1:A:389:ILE:HG23	1.86	0.57
1:B:505:VAL:HG12	1:B:521:ARG:HD2	1.86	0.56
1:B:312:ARG:O	1:B:316:GLU:HG3	2.04	0.56
1:B:448:GLY:O	1:B:494:ARG:NH2	2.38	0.56
1:B:328:ASN:H	1:B:328:ASN:ND2	2.03	0.56
1:B:28:ARG:HD2	4:B:819:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:VAL:HG22	1:A:521:ARG:NE	2.21	0.55
1:B:416:LEU:H	1:B:416:LEU:HD23	1.70	0.55
1:B:190:LEU:HD13	1:B:234:ILE:CG2	2.36	0.55
1:A:26:ARG:HD3	1:A:70:GLU:OE2	2.05	0.55
1:A:254:ASP:OD2	1:A:262:SER:HB2	2.06	0.55
1:A:201:HIS:HE1	1:A:469:ARG:HH11	1.53	0.55
1:A:411:GLN:HG2	4:A:909:HOH:O	2.06	0.55
1:B:382:ARG:NH1	1:B:397:GLU:OE1	2.39	0.55
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.88	0.55
1:B:129:LYS:HG2	1:B:411:GLN:NE2	2.22	0.54
1:A:115:TYR:CZ	1:B:295:LYS:HE2	2.43	0.54
1:B:277:LYS:O	1:B:278:THR:OG1	2.23	0.54
1:A:139:GLU:OE2	1:A:140:ARG:NH1	2.41	0.54
1:A:504:ASN:ND2	1:A:504:ASN:C	2.59	0.54
1:A:514:ALA:O	1:A:535:ARG:HG3	2.08	0.54
1:B:572:THR:C	1:B:573:LEU:HD23	2.27	0.53
1:B:522:THR:OG1	1:B:527:HIS:HD2	1.90	0.53
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.42	0.53
1:A:275:VAL:O	1:A:276:SER:CB	2.56	0.53
1:B:328:ASN:ND2	1:B:328:ASN:N	2.56	0.53
1:B:255:VAL:HG11	1:B:270:ILE:CD1	2.38	0.52
1:B:541:VAL:HG22	1:B:543:LEU:HD12	1.91	0.52
1:B:190:LEU:HD13	1:B:234:ILE:HG21	1.91	0.52
1:A:162:PRO:HB3	1:A:168:TYR:HE2	1.75	0.52
1:B:193:THR:HB	1:B:194:PRO:HD2	1.91	0.52
1:A:281:THR:HG23	1:A:283:TYR:CE2	2.44	0.52
1:A:416:LEU:HD23	1:A:416:LEU:H	1.73	0.52
1:A:8:HIS:HD2	1:A:26:ARG:O	1.93	0.52
1:B:393:ARG:HH21	1:B:393:ARG:HG3	1.75	0.52
1:B:280:ARG:NH2	1:B:289:GLN:NE2	2.58	0.51
1:A:400:ARG:HH21	1:A:400:ARG:HB3	1.75	0.51
1:A:65:ARG:HB2	1:B:4:GLU:HG3	1.92	0.51
1:B:325:ASN:HD21	2:B:703:GLC:C1	2.24	0.51
1:B:447:LEU:HB2	1:B:505:VAL:HG11	1.92	0.51
1:A:275:VAL:O	1:A:276:SER:HB2	2.10	0.51
1:A:129:LYS:HG2	1:A:411:GLN:NE2	2.26	0.51
1:A:201:HIS:CE1	1:A:469:ARG:HH11	2.29	0.51
1:B:107:LYS:HE3	4:B:845:HOH:O	2.10	0.51
1:B:200:SER:O	1:B:203:LYS:HD2	2.11	0.50
1:B:504:ASN:HB2	4:B:751:HOH:O	2.11	0.50
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:GLU:O	1:B:232:ARG:HG2	2.12	0.50
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.93	0.50
1:B:47:SER:HB3	1:B:50:GLU:HG2	1.93	0.50
1:A:574:ARG:HB2	1:A:574:ARG:NH1	2.27	0.50
1:B:357:HIS:HD2	4:B:719:HOH:O	1.94	0.50
1:A:458:ILE:CD1	1:A:460:MET:HG3	2.42	0.50
1:A:522:THR:OG1	1:A:527:HIS:HD2	1.95	0.50
1:B:12:GLY:O	1:B:364:MET:HE1	2.12	0.50
1:A:213:ASP:OD1	1:A:215:GLN:HG2	2.12	0.49
1:A:346:ASN:ND2	1:A:348:ASP:H	2.10	0.49
1:A:488:LYS:O	1:A:492:ARG:HG3	2.12	0.49
1:A:140:ARG:HH12	1:A:201:HIS:HB2	1.78	0.49
1:A:346:ASN:HD22	1:A:346:ASN:C	2.15	0.49
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.95	0.49
1:A:382:ARG:HG3	1:A:388:GLU:HB2	1.95	0.49
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.78	0.49
1:B:275:VAL:O	1:B:282:ASN:CG	2.51	0.48
1:B:504:ASN:ND2	1:B:504:ASN:C	2.66	0.48
1:A:281:THR:HG22	1:A:283:TYR:H	1.77	0.48
1:A:82:TYR:N	1:A:110:VAL:CG2	2.76	0.48
1:A:323:ARG:HD2	1:A:372:MET:SD	2.54	0.48
1:A:162:PRO:HB3	1:A:168:TYR:CE2	2.48	0.48
1:B:248:GLN:HB2	4:B:783:HOH:O	2.12	0.48
1:A:448:GLY:O	1:A:494:ARG:NH2	2.47	0.48
1:A:255:VAL:HG12	1:A:275:VAL:HG21	1.95	0.48
1:A:68:TYR:CD2	1:A:403:MET:HG3	2.49	0.48
1:B:535:ARG:HD3	1:B:539:GLN:CD	2.34	0.48
1:A:585:ARG:NH1	1:A:585:ARG:HB3	2.17	0.48
1:B:158:LYS:HG2	1:B:478:GLU:OE2	2.14	0.47
1:B:82:TYR:N	1:B:110:VAL:HG22	2.29	0.47
1:A:505:VAL:HG22	1:A:521:ARG:CD	2.44	0.47
1:A:193:THR:HB	1:A:194:PRO:CD	2.45	0.47
1:B:277:LYS:O	1:B:277:LYS:HD3	2.14	0.47
1:A:179:LEU:N	1:A:180:PRO:CD	2.78	0.47
1:A:326:VAL:HG12	1:A:329:GLU:HB2	1.97	0.47
1:A:293:MET:HE2	2:A:702:GLC:H62	1.95	0.47
1:B:547:GLU:CG	1:B:551:LYS:HE2	2.45	0.47
1:B:393:ARG:HG3	1:B:393:ARG:NH2	2.29	0.47
1:B:477:LYS:NZ	1:B:477:LYS:HB3	2.30	0.47
1:A:275:VAL:O	1:A:275:VAL:CG1	2.63	0.47
1:B:223:ARG:HH21	1:B:223:ARG:HG3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:VAL:C	1:A:282:ASN:OD1	2.54	0.46
1:A:140:ARG:NH2	4:A:751:HOH:O	2.48	0.46
1:B:276:SER:HB2	1:B:283:TYR:HE2	1.80	0.46
1:A:2:LEU:HD12	1:A:30:LYS:CD	2.45	0.46
1:A:77:THR:O	1:A:78:LYS:HB2	2.16	0.46
1:B:127:TRP:CG	1:B:235:LYS:HE3	2.51	0.46
1:A:217:GLY:HA2	4:A:745:HOH:O	2.16	0.46
1:B:504:ASN:HD21	1:B:522:THR:HB	1.80	0.46
1:A:197:ALA:HB3	1:A:208:ASP:HB3	1.97	0.46
1:B:277:LYS:O	1:B:278:THR:HG23	2.16	0.46
1:B:381:ILE:O	1:B:385:ALA:HB3	2.16	0.46
1:A:40:LEU:HD22	1:A:40:LEU:N	2.31	0.46
1:A:488:LYS:HB3	1:A:488:LYS:NZ	2.30	0.45
1:A:330:VAL:HG22	1:A:335:TRP:CE2	2.51	0.45
1:A:475:GLU:O	1:A:479:GLN:HG3	2.16	0.45
1:B:377:ARG:O	1:B:380:VAL:HG22	2.17	0.45
1:A:232:ARG:NE	4:A:896:HOH:O	2.41	0.45
1:B:293:MET:HE2	2:B:702:GLC:H62	1.96	0.45
1:A:244:HIS:CD2	1:A:286:PHE:HB2	2.51	0.45
1:A:416:LEU:H	1:A:416:LEU:CD2	2.29	0.45
1:B:118:ARG:NH1	4:B:786:HOH:O	2.49	0.45
1:A:136:ILE:O	1:A:138:PRO:HD3	2.16	0.45
1:A:569:LEU:HG	1:A:571:LEU:CD1	2.42	0.45
1:A:271:GLU:HG2	1:A:282:ASN:O	2.17	0.45
1:A:444:MET:O	1:A:494:ARG:NH1	2.45	0.45
1:B:191:TYR:CE1	1:B:323:ARG:HG3	2.52	0.45
1:B:132:VAL:HG11	1:B:491:ILE:HD12	1.99	0.45
1:A:223:ARG:HD3	1:A:317:GLN:OE1	2.17	0.45
1:A:585:ARG:CB	1:A:585:ARG:HH11	2.18	0.45
1:B:133:ILE:HD13	1:B:189:ALA:HB3	1.99	0.45
1:B:223:ARG:HB3	1:B:223:ARG:CZ	2.46	0.45
1:B:535:ARG:HD3	1:B:539:GLN:NE2	2.32	0.45
1:A:129:LYS:CB	1:A:411:GLN:OE1	2.65	0.44
1:B:133:ILE:CD1	1:B:189:ALA:HB3	2.47	0.44
1:B:416:LEU:CD2	1:B:416:LEU:H	2.31	0.44
1:B:447:LEU:HB2	1:B:505:VAL:HG13	2.00	0.44
1:B:138:PRO:HD2	1:B:193:THR:OG1	2.18	0.44
1:B:251:ALA:O	1:B:255:VAL:HG23	2.17	0.44
1:B:298:THR:HB	1:B:334:PHE:CD2	2.52	0.44
1:A:323:ARG:HH12	1:A:325:ASN:HD22	1.65	0.44
1:B:232:ARG:HG3	1:B:232:ARG:NH1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:ASP:OD2	1:B:282:ASN:ND2	2.50	0.44
1:B:280:ARG:HA	1:B:280:ARG:HD2	1.87	0.44
1:A:280:ARG:HG3	1:A:280:ARG:O	2.18	0.43
1:B:491:ILE:O	1:B:495:HIS:ND1	2.51	0.43
1:A:504:ASN:HD21	1:A:522:THR:HB	1.83	0.43
1:A:524:GLN:HB3	1:A:525:ASP:H	1.58	0.43
1:B:582:TRP:CZ2	1:B:584:GLY:HA2	2.53	0.43
1:B:382:ARG:HA	1:B:386:THR:OG1	2.19	0.43
1:A:81:LYS:HB2	1:A:110:VAL:HG21	1.99	0.43
1:B:438:LEU:CD2	1:B:532:LEU:HD22	2.48	0.43
1:A:223:ARG:NE	1:A:223:ARG:HA	2.33	0.43
1:A:381:ILE:HD13	1:A:425:PHE:CE1	2.53	0.43
1:A:105:ARG:HH21	1:A:105:ARG:HG2	1.83	0.43
1:A:332:HIS:HE1	4:B:906:HOH:O	2.02	0.43
1:A:477:LYS:CD	1:A:477:LYS:N	2.81	0.43
1:B:227:ASP:O	1:B:231:ARG:HG2	2.18	0.43
1:B:275:VAL:HG12	1:B:276:SER:N	2.34	0.43
1:B:277:LYS:C	1:B:277:LYS:HD3	2.39	0.43
1:A:107:LYS:HD3	4:A:947:HOH:O	2.18	0.43
1:A:110:VAL:HG22	1:A:111:PHE:O	2.19	0.42
1:A:478:GLU:HA	1:A:478:GLU:OE2	2.20	0.42
1:B:269:PHE:HB2	1:B:284:GLU:HB3	2.01	0.42
1:B:565:LYS:HE3	4:B:831:HOH:O	2.19	0.42
1:A:518:ALA:HA	1:A:530:VAL:O	2.19	0.42
1:A:330:VAL:CG2	1:A:335:TRP:CE2	3.03	0.42
1:A:82:TYR:C	1:A:110:VAL:HG23	2.40	0.42
1:B:8:HIS:CE1	1:B:25:VAL:HG13	2.55	0.42
1:B:178:ARG:HG3	1:B:474:TRP:CZ2	2.55	0.42
1:A:82:TYR:O	1:A:110:VAL:HG23	2.19	0.42
1:A:499:SER:OG	1:A:526:GLN:HG2	2.20	0.42
1:B:458:ILE:HD12	1:B:479:GLN:HG2	2.01	0.42
1:B:523:VAL:HG13	1:B:523:VAL:O	2.19	0.42
1:A:325:ASN:HD21	2:A:703:GLC:C1	2.33	0.42
1:B:217:GLY:HA2	4:B:867:HOH:O	2.20	0.42
1:A:308:PHE:O	1:A:312:ARG:HG3	2.20	0.42
1:B:24:ARG:HG3	1:B:407:GLU:OE1	2.19	0.42
1:A:464:THR:O	1:A:465:ASP:C	2.59	0.42
1:B:477:LYS:HZ3	1:B:477:LYS:HB3	1.85	0.42
1:A:107:LYS:HE2	1:A:107:LYS:HB3	1.86	0.42
1:A:240:ALA:HB2	1:A:322:TRP:CE3	2.55	0.42
1:A:12:GLY:HA2	1:A:364:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:TRP:CE3	1:A:335:TRP:HA	2.56	0.41
1:A:275:VAL:O	1:A:282:ASN:OD1	2.38	0.41
1:A:278:THR:HG23	1:A:291:PRO:CG	2.50	0.41
1:A:426:LEU:HD22	1:A:431:GLY:HA2	2.01	0.41
1:A:164:HIS:CE1	1:A:466:PRO:HD3	2.56	0.41
1:B:541:VAL:HG22	1:B:542:LEU:N	2.36	0.41
1:A:117:HIS:HB2	1:A:120:GLU:HG3	2.02	0.41
1:A:88:GLY:HA3	1:A:92:GLU:OE1	2.21	0.41
1:A:330:VAL:HG22	1:A:335:TRP:HE1	1.83	0.41
1:B:543:LEU:N	1:B:543:LEU:HD12	2.35	0.41
1:B:163:ARG:HH11	1:B:163:ARG:HG3	1.86	0.41
1:B:179:LEU:N	1:B:180:PRO:CD	2.83	0.41
1:B:280:ARG:HG3	1:B:280:ARG:O	2.21	0.41
1:B:27:LEU:C	1:B:27:LEU:HD23	2.41	0.41
1:B:192:PHE:O	1:B:239:ASP:HB2	2.21	0.41
1:A:574:ARG:HH11	1:A:574:ARG:CB	2.34	0.41
1:B:477:LYS:NZ	1:B:477:LYS:CB	2.84	0.41
1:A:332:HIS:HD2	1:A:367:GLN:OE1	2.04	0.41
1:B:277:LYS:O	1:B:278:THR:CB	2.69	0.41
1:A:1:MET:HB3	4:A:846:HOH:O	2.20	0.41
1:A:150:PRO:HG2	1:A:167:PHE:CD2	2.56	0.41
1:B:244:HIS:CD2	1:B:286:PHE:HB2	2.56	0.41
1:B:146:PRO:HA	1:B:149:ASP:OD1	2.21	0.40
1:A:27:LEU:C	1:A:27:LEU:HD23	2.41	0.40
1:B:400:ARG:NH2	1:B:400:ARG:HG3	2.37	0.40
1:B:250:PHE:CG	1:B:251:ALA:N	2.89	0.40
1:B:325:ASN:HB3	4:B:728:HOH:O	2.20	0.40
1:A:130:GLU:HG2	1:A:130:GLU:H	1.81	0.40
1:B:335:TRP:HA	1:B:335:TRP:CE3	2.56	0.40
1:A:376:PHE:CE1	1:A:415:ASN:HB3	2.56	0.40
1:B:282:ASN:O	1:B:282:ASN:OD1	2.39	0.40
1:A:30:LYS:O	1:A:33:ASP:HB2	2.22	0.40
1:A:573:LEU:CD1	1:A:579:MET:HG3	2.51	0.40
1:B:475:GLU:HG2	4:B:846:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	583/585 (100%)	556 (95%)	24 (4%)	3 (0%)	34	35
1	B	583/585 (100%)	556 (95%)	22 (4%)	5 (1%)	21	19
All	All	1166/1170 (100%)	1112 (95%)	46 (4%)	8 (1%)	26	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	SER
1	B	275	VAL
1	B	278	THR
1	A	275	VAL
1	B	281	THR
1	B	547	GLU
1	B	280	ARG
1	A	276	SER

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/493 (100%)	468 (95%)	25 (5%)	29	34
1	B	493/493 (100%)	474 (96%)	19 (4%)	39	48
All	All	986/986 (100%)	942 (96%)	44 (4%)	34	41

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLU
1	A	85	LEU
1	A	122	PHE
1	A	191	TYR
1	A	219	LEU
1	A	263	ARG
1	A	276	SER
1	A	277	LYS
1	A	279	SER
1	A	330	VAL
1	A	346	ASN
1	A	398	LEU
1	A	400	ARG
1	A	404	LEU
1	A	411	GLN
1	A	413	LEU
1	A	426	LEU
1	A	444	MET
1	A	466	PRO
1	A	483	LEU
1	A	504	ASN
1	A	535	ARG
1	A	573	LEU
1	A	581	LEU
1	A	585	ARG
1	B	24	ARG
1	B	122	PHE
1	B	158	LYS
1	B	191	TYR
1	B	248	GLN
1	B	281	THR
1	B	328	ASN
1	B	398	LEU
1	B	400	ARG
1	B	411	GLN
1	B	438	LEU
1	B	451	LEU
1	B	466	PRO
1	B	504	ASN
1	B	524	GLN
1	B	542	LEU
1	B	552	THR
1	B	565	LYS

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Mol	Chain	Res	Type
1	B	569	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	90	GLN
1	A	135	GLN
1	A	164	HIS
1	A	201	HIS
1	A	244	HIS
1	A	261	GLN
1	A	325	ASN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	504	ASN
1	A	527	HIS
1	A	563	HIS
1	B	135	GLN
1	B	243	ASN
1	B	244	HIS
1	B	257	GLN
1	B	261	GLN
1	B	289	GLN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	367	GLN
1	B	411	GLN
1	B	504	ASN
1	B	509	HIS
1	B	524	GLN
1	B	527	HIS
1	B	568	GLN

5.3.3 RNA

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)

12 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	701	2	11,11,12	0.46	0	14,15,17	0.60	0
2	GLC	A	702	2	11,11,12	0.49	0	14,15,17	0.72	0
2	GLC	A	703	2	11,11,12	0.68	0	14,15,17	1.62	2 (14%)
2	GLC	A	704	2	11,11,12	0.65	0	14,15,17	0.73	1 (7%)
2	GLC	A	705	2	12,12,12	0.43	0	17,17,17	0.38	0
2	GLC	A	706	2	11,11,12	0.48	0	14,15,17	0.58	0
2	GLC	B	701	2	11,11,12	0.46	0	14,15,17	0.54	0
2	GLC	B	702	2	11,11,12	0.53	0	14,15,17	0.64	0
2	GLC	B	703	2	11,11,12	0.48	0	14,15,17	1.21	2 (14%)
2	GLC	B	704	2	11,11,12	0.57	0	14,15,17	0.77	1 (7%)
2	GLC	B	705	2	12,12,12	0.37	0	17,17,17	0.34	0
2	GLC	B	706	2	11,11,12	0.48	0	14,15,17	0.64	1 (7%)

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	701	2	-	0/2/19/22	0/1/1/1
2	GLC	A	702	2	-	0/2/19/22	0/1/1/1
2	GLC	A	703	2	-	0/2/19/22	0/1/1/1
2	GLC	A	704	2	-	0/2/19/22	0/1/1/1
2	GLC	A	705	2	-	0/2/22/22	0/1/1/1
2	GLC	A	706	2	-	0/2/19/22	0/1/1/1
2	GLC	B	701	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	702	2	-	0/2/19/22	0/1/1/1
2	GLC	B	703	2	-	0/2/19/22	0/1/1/1
2	GLC	B	704	2	-	0/2/19/22	0/1/1/1
2	GLC	B	705	2	-	0/2/22/22	0/1/1/1
2	GLC	B	706	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	703	GLC	C1-C2-C3	-2.83	106.19	109.54
2	B	703	GLC	C1-C2-C3	-2.41	106.69	109.54
2	B	706	GLC	C1-O5-C5	2.09	114.90	112.25
2	B	704	GLC	C1-O5-C5	2.22	115.07	112.25
2	A	704	GLC	C1-O5-C5	2.27	115.13	112.25
2	B	703	GLC	C1-O5-C5	2.75	115.74	112.25
2	A	703	GLC	C1-O5-C5	4.06	117.41	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	702	GLC	3	0
2	A	703	GLC	1	0
2	B	702	GLC	3	0
2	B	703	GLC	1	0

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	585/585 (100%)	0.04	31 (5%)	30	29	18, 28, 48, 96	0
1	B	585/585 (100%)	0.08	35 (5%)	25	25	19, 29, 51, 106	0
All	All	1170/1170 (100%)	0.06	66 (5%)	28	27	18, 28, 49, 106	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	SER	16.6
1	B	279	SER	14.8
1	B	273	PHE	11.8
1	B	280	ARG	9.6
1	B	272	ASP	9.1
1	B	277	LYS	9.0
1	B	274	PRO	8.4
1	A	280	ARG	7.9
1	B	275	VAL	7.8
1	B	278	THR	7.8
1	B	276	SER	7.4
1	A	278	THR	7.4
1	A	272	ASP	6.7
1	A	273	PHE	5.7
1	A	274	PRO	5.5
1	A	275	VAL	4.2
1	B	513	GLN	4.1
1	B	477	LYS	4.0
1	B	48	PRO	4.0
1	A	277	LYS	3.8
1	B	281	THR	3.3
1	B	51	GLU	3.3
1	A	49	GLU	3.3
1	A	281	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	49	GLU	3.1
1	A	451	LEU	3.0
1	A	107	LYS	3.0
1	B	282	ASN	3.0
1	B	548	SER	2.9
1	A	551	LYS	2.9
1	A	566	GLN	2.8
1	B	164	HIS	2.8
1	B	158	LYS	2.6
1	A	237	ILE	2.6
1	A	276	SER	2.6
1	B	155	GLN	2.6
1	B	566	GLN	2.6
1	B	585	ARG	2.6
1	A	548	SER	2.5
1	A	477	LYS	2.5
1	B	159	ASP	2.5
1	A	191	TYR	2.5
1	B	47	SER	2.5
1	A	524	GLN	2.4
1	A	375	LEU	2.4
1	A	371	VAL	2.4
1	A	452	ILE	2.4
1	B	153	THR	2.4
1	B	50	GLU	2.3
1	A	537	GLU	2.3
1	A	104	GLU	2.3
1	A	190	LEU	2.3
1	B	190	LEU	2.3
1	B	191	TYR	2.2
1	B	271	GLU	2.2
1	B	118	ARG	2.2
1	A	90	GLN	2.2
1	B	524	GLN	2.2
1	A	327	ALA	2.2
1	B	260	GLU	2.1
1	B	451	LEU	2.1
1	A	193	THR	2.1
1	A	192	PHE	2.0
1	A	240	ALA	2.0
1	B	475	GLU	2.0
1	B	151	PRO	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GLC	A	701	11/12	0.91	0.15	6.09	30,35,40,46	0
2	GLC	A	703	11/12	0.86	0.18	0.48	24,28,31,42	0
2	GLC	B	704	11/12	0.87	0.16	0.44	37,43,47,52	0
2	GLC	B	703	11/12	0.89	0.16	0.19	28,32,36,46	0
2	GLC	B	701	11/12	0.93	0.14	-0.00	37,39,42,43	0
2	GLC	A	702	11/12	0.97	0.08	-1.07	26,28,30,31	0
2	GLC	A	704	11/12	0.94	0.10	-1.42	31,34,37,43	0
2	GLC	B	702	11/12	0.95	0.09	-1.46	30,30,32,36	0
2	GLC	B	706	11/12	0.68	0.26	-	56,59,60,61	0
2	GLC	A	706	11/12	0.84	0.23	-	48,52,54,55	0
2	GLC	A	705	12/12	0.86	0.17	-	36,42,45,47	0
2	GLC	B	705	12/12	0.76	0.20	-	46,51,54,54	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, 95^{th} 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
3	CA	A	601	1/1	0.99	0.06	-2.03	26,26,26,26	0
3	CA	B	602	1/1	0.99	0.04	-3.11	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.