



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2018 – 06:23 am GMT

PDB ID : 2D2O  
Title : Structure of a complex of Thermoactinomyces vulgaris R-47 alpha-amylase 2 with maltohexaose demonstrates the important role of aromatic residues at the reducing end of the substrate binding cleft  
Authors : Ohtaki, A.; Mizuno, M.; Yoshida, H.; Tonozuka, T.; Sakano, Y.; Kamitori, S.  
Deposited on : 2005-09-13  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

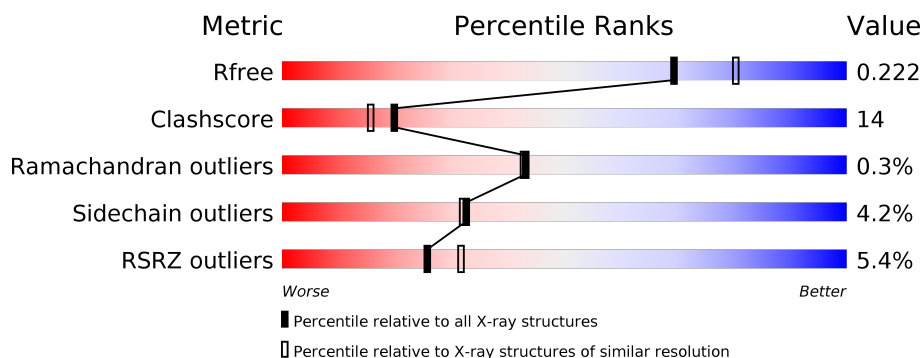
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	111664	4608 (2.10-2.10)
Clashscore	122126	5109 (2.10-2.10)
Ramachandran outliers	120053	5059 (2.10-2.10)
Sidechain outliers	120020	5060 (2.10-2.10)
RSRZ outliers	108989	4497 (2.10-2.10)

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  $\geq 3$ , 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	585	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>22%</div> <div>.</div> </div> </div>
1	B	585	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	A	701	-	-	-	X
2	GLC	A	706	X	-	-	-
2	GLC	B	706	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10668 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.

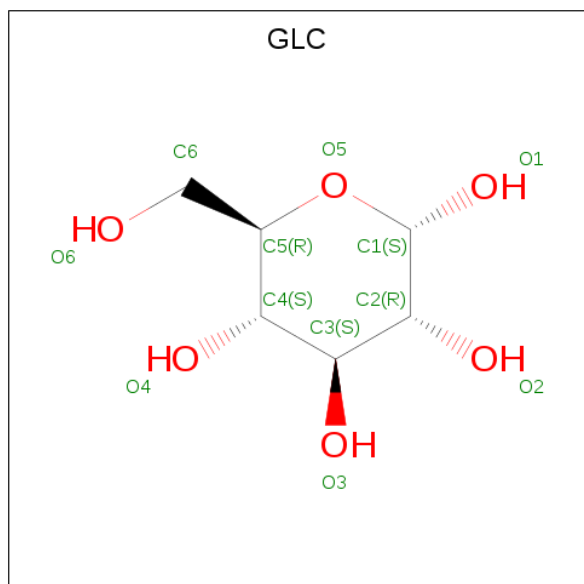
- Molecule 1 is a protein called Neopullulanase 2.

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 ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



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

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

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

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

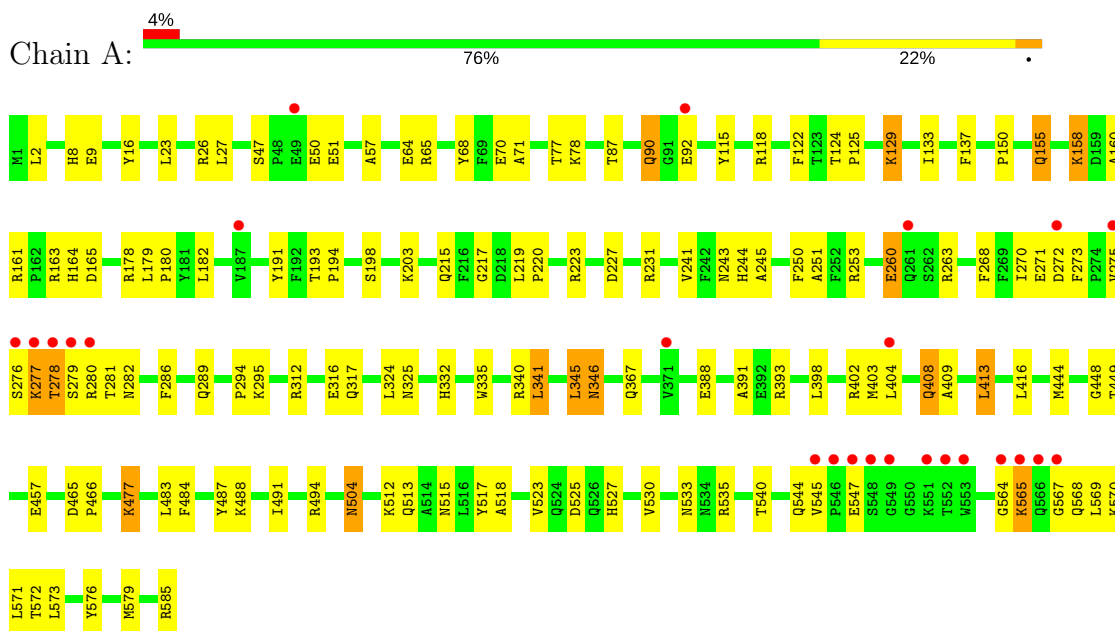
- Molecule 4 is water.

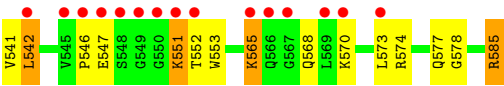
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	498	Total O 498 498	0	0
4	B	482	Total O 482 482	0	0

### 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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Neopullulanase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.69Å 118.71Å 112.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.00 – 2.10 46.37 – 1.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.00-2.10) 93.7 (46.37-1.98)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 1.98Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.184 , 0.217 0.191 , 0.222	Depositor DCC
$R_{free}$ test set	6518 reflections (6.58%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10668	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.59	1/6641 (0.0%)
1	B	0.34	0/4906	0.59	0/6641
All	All	0.35	0/9812	0.59	1/13282 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	PHE	N-CA-C	-5.21	96.92	111.00

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	4776	0	4609	132	0
1	B	4776	0	4609	130	0
2	A	67	0	57	5	0
2	B	67	0	57	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	498	0	0	15	0
4	B	482	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10668	0	9332	259	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 (259) 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:2:LEU:HD21	1:B:2:LEU:HD21	1.25	1.14
1:A:129:LYS:HD2	1:A:129:LYS:H	1.24	1.02
1:A:525:ASP:HB3	1:A:585:ARG:HD3	1.49	0.94
1:A:278:THR:HG22	1:A:279:SER:H	1.35	0.91
1:A:544:GLN:HE22	1:A:568:GLN:HE21	1.20	0.90
1:A:408:GLN:HE21	1:A:408:GLN:H	1.16	0.89
1:B:511:ASP:OD2	1:B:513:GLN:HG2	1.71	0.89
1:A:129:LYS:HD2	1:A:129:LYS:N	1.91	0.83
1:B:28:ARG:HD3	1:B:66:PHE:CD2	2.12	0.83
1:B:552:THR:HB	4:B:1045:HOH:O	1.77	0.83
1:A:565:LYS:HD3	1:A:565:LYS:H	1.44	0.82
1:A:544:GLN:NE2	1:A:568:GLN:HE21	1.79	0.80
1:B:213:ASP:OD1	1:B:215:GLN:HG2	1.83	0.79
1:A:544:GLN:HE22	1:A:568:GLN:NE2	1.80	0.78
1:A:281:THR:H	1:A:289:GLN:HE22	1.32	0.76
1:B:129:LYS:HD2	1:B:502:ARG:NH2	2.00	0.76
1:B:533:ASN:HD21	1:B:539:GLN:HE21	1.31	0.75
1:A:2:LEU:CD2	1:B:2:LEU:HD21	2.13	0.75
1:A:271:GLU:HG2	1:A:282:ASN:O	1.86	0.75
1:A:57:ALA:HB2	1:A:71:ALA:HB2	1.68	0.75
1:B:202:HIS:HD2	1:B:204:TYR:H	1.35	0.74
1:A:223:ARG:HD3	1:A:317:GLN:HE21	1.53	0.74
1:A:408:GLN:NE2	1:A:408:GLN:H	1.87	0.73
1:A:477:LYS:HA	1:A:477:LYS:HE3	1.71	0.72
1:B:585:ARG:HH11	1:B:585:ARG:HB3	1.52	0.72
1:B:140:ARG:HH12	1:B:201:HIS:HB2	1.55	0.71
1:A:26:ARG:HD3	1:A:70:GLU:OE2	1.91	0.70
1:A:243:ASN:HD22	1:A:244:HIS:HD2	1.39	0.70
1:B:140:ARG:HG2	1:B:469:ARG:O	1.91	0.70
1:A:125:PRO:O	1:A:129:LYS:HE2	1.92	0.70
1:B:484:PHE:CE1	1:B:488:LYS:HD2	2.28	0.68
1:A:2:LEU:HD21	1:B:2:LEU:CD2	2.14	0.68
1:B:243:ASN:HD21	1:B:295:LYS:NZ	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LEU:HD21	1:B:570:LYS:HG2	1.76	0.67
1:A:312:ARG:O	1:A:316:GLU:HG3	1.94	0.67
1:B:278:THR:HG23	1:B:280:ARG:H	1.59	0.67
1:A:515:ASN:HB2	1:A:535:ARG:NH2	2.10	0.67
1:B:202:HIS:CD2	1:B:204:TYR:H	2.12	0.67
1:B:328:ASN:N	1:B:328:ASN:HD22	1.93	0.67
1:B:188:THR:HG21	4:B:1454:HOH:O	1.95	0.66
1:A:409:ALA:O	1:A:413:LEU:HD13	1.96	0.66
1:B:47:SER:HB3	1:B:50:GLU:HG3	1.77	0.66
1:A:341:LEU:HD22	1:A:345:LEU:HD22	1.77	0.65
1:A:540:THR:OG1	1:A:572:THR:HG22	1.97	0.64
1:B:256:LEU:HD23	1:B:275:VAL:HB	1.79	0.64
1:B:475:GLU:H	1:B:475:GLU:CD	2.00	0.64
1:B:565:LYS:HE2	1:B:568:GLN:HB2	1.78	0.64
1:B:107:LYS:HG3	4:B:1399:HOH:O	1.98	0.64
1:A:133:ILE:N	1:A:133:ILE:HD12	2.12	0.64
2:A:703:GLC:H5	2:A:704:GLC:H62	1.80	0.63
1:A:388:GLU:OE1	1:B:107:LYS:HE3	1.98	0.63
1:A:525:ASP:HB2	4:A:1289:HOH:O	1.98	0.63
1:B:275:VAL:O	1:B:282:ASN:ND2	2.32	0.63
1:A:340:ARG:NH1	4:A:1365:HOH:O	2.31	0.62
1:A:504:ASN:C	1:A:504:ASN:HD22	2.00	0.62
1:A:465:ASP:OD2	2:A:701:GLC:O2	2.16	0.61
1:B:448:GLY:O	1:B:494:ARG:NH2	2.32	0.61
1:B:279:SER:HB3	4:B:1391:HOH:O	2.01	0.61
1:B:504:ASN:HD22	1:B:504:ASN:C	2.04	0.61
2:B:701:GLC:H61	4:B:1204:HOH:O	2.00	0.61
1:A:8:HIS:HD2	1:A:26:ARG:O	1.84	0.61
1:B:340:ARG:NH2	4:B:1415:HOH:O	2.30	0.61
1:B:328:ASN:H	1:B:328:ASN:HD22	1.49	0.60
1:B:340:ARG:HB3	1:B:340:ARG:HH21	1.66	0.60
1:A:391:ALA:H	1:A:515:ASN:ND2	2.00	0.60
1:B:585:ARG:HH11	1:B:585:ARG:CB	2.15	0.60
2:B:703:GLC:H5	2:B:704:GLC:H62	1.83	0.60
1:B:488:LYS:O	1:B:492:ARG:HG3	2.01	0.60
1:A:276:SER:O	1:A:277:LYS:HB2	2.02	0.59
1:B:173:LYS:HD3	1:B:177:ASP:OD2	2.02	0.59
1:A:408:GLN:HE21	1:A:408:GLN:N	1.96	0.58
1:B:467:ASP:OD1	1:B:470:ARG:HD3	2.03	0.58
1:A:260:GLU:HG3	1:A:273:PHE:CE2	2.38	0.58
1:A:564:GLY:HA2	1:A:568:GLN:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:MET:HE1	1:A:491:ILE:HG12	1.85	0.57
1:B:514:ALA:HB1	1:B:516:LEU:HD13	1.85	0.57
1:A:219:LEU:HB3	1:A:220:PRO:HD3	1.87	0.57
1:B:382:ARG:HH21	1:B:382:ARG:HB2	1.69	0.57
2:A:701:GLC:H61	4:A:1149:HOH:O	2.03	0.57
1:B:525:ASP:HB3	1:B:585:ARG:HD3	1.86	0.57
1:B:57:ALA:HB2	1:B:71:ALA:HB2	1.86	0.56
1:B:164:HIS:CE1	1:B:466:PRO:HD3	2.41	0.56
1:B:547:GLU:HB2	4:B:1369:HOH:O	2.05	0.56
1:A:124:THR:OG1	1:A:129:LYS:HE3	2.06	0.56
1:B:332:HIS:HD2	1:B:367:GLN:OE1	1.89	0.56
1:A:332:HIS:HD2	1:A:367:GLN:OE1	1.90	0.55
1:A:565:LYS:HD3	1:A:565:LYS:N	2.18	0.55
1:A:241:VAL:HG13	1:A:325:ASN:HD22	1.72	0.55
1:A:545:VAL:HA	1:A:569:LEU:HD21	1.89	0.55
1:A:133:ILE:HD13	1:A:449:THR:CG2	2.37	0.55
1:A:160:ALA:O	1:A:161:ARG:HD2	2.06	0.54
1:B:328:ASN:H	1:B:328:ASN:ND2	2.03	0.54
1:B:282:ASN:C	1:B:282:ASN:HD22	2.10	0.54
1:A:164:HIS:CE1	2:A:701:GLC:H2	2.42	0.54
1:A:278:THR:HG22	1:A:279:SER:N	2.14	0.54
1:B:504:ASN:ND2	1:B:504:ASN:C	2.61	0.53
1:B:416:LEU:H	1:B:416:LEU:HD23	1.72	0.53
1:A:115:TYR:CZ	1:B:295:LYS:HE2	2.43	0.53
1:A:90:GLN:HE21	1:A:90:GLN:HA	1.74	0.53
1:A:26:ARG:HG2	1:A:70:GLU:HG3	1.91	0.53
1:B:382:ARG:CB	1:B:382:ARG:HH21	2.22	0.52
1:A:193:THR:HB	1:A:194:PRO:CD	2.40	0.52
1:A:271:GLU:HG3	1:A:272:ASP:OD2	2.10	0.52
1:B:136:ILE:O	1:B:138:PRO:HD3	2.08	0.52
1:B:470:ARG:HG3	4:B:1112:HOH:O	2.09	0.52
1:A:545:VAL:HA	1:A:569:LEU:CD2	2.39	0.52
1:B:153:THR:HG23	1:B:168:TYR:HA	1.90	0.52
1:A:448:GLY:O	1:A:494:ARG:NH2	2.41	0.52
1:B:28:ARG:HD3	1:B:66:PHE:CE2	2.45	0.52
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.74	0.52
1:B:492:ARG:O	1:B:496:ARG:HB2	2.09	0.52
1:B:542:LEU:HD12	1:B:568:GLN:HB3	1.90	0.52
1:A:504:ASN:ND2	1:A:504:ASN:C	2.61	0.52
1:A:515:ASN:HB2	1:A:535:ARG:HH21	1.74	0.52
1:A:268:PHE:HB2	1:A:270:ILE:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:VAL:O	1:B:276:SER:HB3	2.10	0.51
1:A:118:ARG:HG2	4:B:1007:HOH:O	2.10	0.51
1:A:295:LYS:HE2	1:B:115:TYR:CZ	2.46	0.51
1:B:378:GLU:HG3	4:B:1362:HOH:O	2.09	0.51
1:A:158:LYS:HD2	1:A:158:LYS:O	2.11	0.51
1:B:64:GLU:OE1	1:B:393:ARG:HD3	2.11	0.51
1:A:47:SER:HB3	1:A:50:GLU:HG3	1.92	0.51
1:B:164:HIS:CE1	2:B:701:GLC:H2	2.46	0.51
1:B:328:ASN:ND2	1:B:328:ASN:N	2.59	0.50
1:A:484:PHE:CE1	1:A:488:LYS:HD2	2.46	0.50
1:B:524:GLN:HB3	4:B:1430:HOH:O	2.11	0.50
1:B:546:PRO:HG2	1:B:553:TRP:CH2	2.47	0.50
1:A:276:SER:OG	1:A:277:LYS:N	2.44	0.50
1:A:540:THR:HA	1:A:571:LEU:O	2.11	0.50
1:B:219:LEU:HB3	1:B:220:PRO:HD3	1.93	0.50
1:A:281:THR:H	1:A:289:GLN:NE2	2.06	0.50
1:B:243:ASN:ND2	1:B:295:LYS:HZ2	2.10	0.50
1:B:508:TRP:CZ2	1:B:546:PRO:HD3	2.47	0.50
1:B:542:LEU:CD2	1:B:570:LYS:HG2	2.42	0.49
1:A:227:ASP:O	1:A:231:ARG:HG2	2.12	0.49
1:B:139:GLU:OE2	1:B:140:ARG:NH1	2.45	0.49
1:B:507:SER:HB3	4:B:1120:HOH:O	2.13	0.49
1:A:133:ILE:HD13	1:A:449:THR:HG22	1.93	0.49
1:A:253:ARG:HH21	1:A:253:ARG:HG2	1.78	0.49
1:B:210:LEU:HD22	1:B:210:LEU:N	2.28	0.49
1:A:178:ARG:NH2	4:A:1156:HOH:O	2.45	0.49
1:A:393:ARG:HG3	1:A:393:ARG:HH21	1.76	0.49
1:A:512:LYS:HG3	1:A:513:GLN:N	2.27	0.49
1:A:65:ARG:HG2	1:A:65:ARG:HH21	1.78	0.49
1:B:146:PRO:HA	1:B:149:ASP:OD1	2.12	0.49
1:A:215:GLN:HG3	4:A:1300:HOH:O	2.12	0.48
1:A:488:LYS:HB3	4:A:1385:HOH:O	2.13	0.48
1:B:278:THR:OG1	1:B:279:SER:N	2.46	0.48
1:B:551:LYS:HE3	4:B:1045:HOH:O	2.12	0.48
1:A:517:TYR:OH	4:A:1004:HOH:O	2.16	0.48
1:B:477:LYS:NZ	1:B:477:LYS:HB3	2.28	0.48
1:A:268:PHE:HB2	1:A:270:ILE:HD11	1.95	0.47
1:B:273:PHE:HA	1:B:274:PRO:C	2.34	0.47
1:A:565:LYS:CD	1:A:565:LYS:H	2.20	0.47
1:A:155:GLN:HB3	1:A:155:GLN:HE21	1.52	0.47
1:B:282:ASN:C	1:B:282:ASN:ND2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:HD3	4:A:1119:HOH:O	2.14	0.47
1:B:245:ALA:O	1:B:294:PRO:HD2	2.15	0.47
1:B:199:PRO:HG3	1:B:248:GLN:NE2	2.30	0.47
1:A:324:LEU:HD13	1:A:335:TRP:CZ3	2.50	0.46
1:A:87:THR:HA	1:A:92:GLU:O	2.16	0.46
1:B:565:LYS:O	1:B:565:LYS:HD2	2.15	0.46
1:B:312:ARG:O	1:B:316:GLU:HG3	2.14	0.46
1:B:401:ALA:O	1:B:404:LEU:HB2	2.15	0.46
1:A:281:THR:OG1	1:A:289:GLN:NE2	2.49	0.46
1:A:64:GLU:HB2	4:A:1313:HOH:O	2.15	0.46
1:B:340:ARG:HB3	1:B:340:ARG:NH2	2.30	0.46
1:A:150:PRO:HG3	1:A:215:GLN:CD	2.36	0.46
1:A:279:SER:O	1:A:289:GLN:NE2	2.49	0.46
1:A:51:GLU:OE1	1:A:51:GLU:HA	2.16	0.46
1:A:565:LYS:N	1:A:565:LYS:CD	2.79	0.45
1:B:376:PHE:O	1:B:380:VAL:HG23	2.17	0.45
1:A:286:PHE:HZ	2:A:704:GLC:H61	1.80	0.45
1:A:57:ALA:CB	1:A:71:ALA:HB2	2.40	0.45
1:B:140:ARG:NH1	1:B:201:HIS:HB2	2.27	0.45
1:A:163:ARG:NH1	1:A:165:ASP:OD1	2.49	0.45
1:A:272:ASP:O	1:A:282:ASN:ND2	2.50	0.45
1:B:551:LYS:HD2	1:B:551:LYS:O	2.17	0.45
1:A:244:HIS:CD2	1:A:286:PHE:HB2	2.51	0.45
1:B:276:SER:O	1:B:277:LYS:HD2	2.17	0.45
1:A:564:GLY:HA3	1:A:569:LEU:HD13	1.99	0.45
1:B:164:HIS:ND1	4:B:1167:HOH:O	2.36	0.45
1:A:565:LYS:NZ	1:A:570:LYS:HE3	2.32	0.45
1:B:467:ASP:O	1:B:470:ARG:HG3	2.17	0.45
1:B:250:PHE:CG	1:B:251:ALA:N	2.85	0.44
1:B:324:LEU:HD13	1:B:335:TRP:CZ3	2.52	0.44
1:A:402:ARG:HD2	4:A:1261:HOH:O	2.18	0.44
1:B:458:ILE:CD1	1:B:460:MET:HG3	2.47	0.44
1:A:416:LEU:HD23	1:A:416:LEU:H	1.81	0.44
1:A:164:HIS:CE1	1:A:466:PRO:HD3	2.52	0.44
1:A:64:GLU:HG3	4:A:1332:HOH:O	2.17	0.44
1:B:524:GLN:HB3	1:B:525:ASP:H	1.48	0.44
1:B:388:GLU:HB2	4:B:1187:HOH:O	2.17	0.44
1:B:542:LEU:HD11	1:B:565:LYS:NZ	2.32	0.44
1:A:124:THR:OG1	1:A:129:LYS:CE	2.66	0.44
1:B:193:THR:HB	1:B:194:PRO:CD	2.47	0.43
1:A:564:GLY:CA	1:A:568:GLN:O	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:THR:N	1:A:289:GLN:HE22	2.10	0.43
1:A:527:HIS:HD2	4:A:1315:HOH:O	2.00	0.43
1:A:533:ASN:O	1:A:576:TYR:HA	2.17	0.43
1:B:249:PHE:CE2	1:B:251:ALA:HB3	2.53	0.43
1:A:545:VAL:HG23	1:A:567:GLY:C	2.39	0.43
1:A:65:ARG:HB3	1:B:4:GLU:HG3	1.99	0.43
1:B:105:ARG:NH1	1:B:105:ARG:HG2	2.34	0.43
1:B:542:LEU:HD11	1:B:565:LYS:HZ3	1.83	0.43
1:A:245:ALA:O	1:A:294:PRO:HD2	2.19	0.43
1:B:197:ALA:HB3	1:B:208:ASP:HB3	2.01	0.43
1:A:133:ILE:CD1	1:A:449:THR:CG2	2.97	0.43
1:A:518:ALA:HA	1:A:530:VAL:O	2.19	0.43
1:A:27:LEU:C	1:A:27:LEU:HD23	2.39	0.42
1:B:275:VAL:HG12	1:B:275:VAL:O	2.18	0.42
1:A:275:VAL:HG12	1:A:276:SER:N	2.34	0.42
1:B:416:LEU:CD2	1:B:416:LEU:H	2.32	0.42
1:A:270:ILE:HD12	1:A:270:ILE:N	2.34	0.42
1:A:569:LEU:HD22	1:A:569:LEU:N	2.35	0.42
1:A:9:GLU:HA	4:A:1205:HOH:O	2.18	0.42
1:B:190:LEU:HG	1:B:234:ILE:CG2	2.50	0.42
1:B:193:THR:HB	1:B:194:PRO:HD2	2.02	0.42
1:B:516:LEU:HD11	1:B:539:GLN:NE2	2.33	0.42
1:B:162:PRO:HG2	1:B:470:ARG:HA	2.00	0.42
1:B:546:PRO:CG	1:B:553:TRP:CH2	3.02	0.42
1:A:444:MET:CE	1:A:491:ILE:HG12	2.49	0.42
1:A:523:VAL:HG13	1:A:523:VAL:O	2.20	0.42
1:B:424:ARG:HG3	1:B:461:ALA:C	2.39	0.42
1:B:381:ILE:O	1:B:385:ALA:HB3	2.20	0.42
1:B:286:PHE:HZ	2:B:704:GLC:H61	1.83	0.42
1:A:77:THR:O	1:A:78:LYS:HB2	2.20	0.42
1:A:179:LEU:N	1:A:180:PRO:CD	2.83	0.41
1:A:133:ILE:N	1:A:133:ILE:CD1	2.80	0.41
1:A:457:GLU:HA	1:A:487:TYR:CE1	2.55	0.41
1:B:577:GLN:HG2	1:B:578:GLY:N	2.36	0.41
1:A:281:THR:HG22	4:A:1419:HOH:O	2.20	0.41
1:B:264:TYR:O	1:B:267:TRP:HB2	2.20	0.41
1:B:36:ARG:HB3	1:B:87:THR:HB	2.03	0.41
1:A:217:GLY:HA2	4:A:1015:HOH:O	2.19	0.41
1:B:144:GLY:C	1:B:173:LYS:HD2	2.41	0.41
1:B:191:TYR:C	1:B:191:TYR:CD1	2.93	0.41
1:B:465:ASP:HA	1:B:466:PRO:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:PRO:HG2	1:B:553:TRP:CZ2	2.55	0.41
1:A:250:PHE:CG	1:A:251:ALA:N	2.88	0.41
1:A:68:TYR:CD2	1:A:403:MET:HG3	2.55	0.41
1:B:279:SER:O	1:B:281:THR:N	2.54	0.41
1:B:523:VAL:HG13	1:B:523:VAL:O	2.20	0.41
1:B:223:ARG:CZ	1:B:317:GLN:OE1	2.68	0.41
1:B:382:ARG:HG3	1:B:388:GLU:HB3	2.02	0.41
1:B:541:VAL:HG22	1:B:542:LEU:N	2.36	0.41
1:A:198:SER:OG	1:A:203:LYS:HA	2.21	0.41
1:A:345:LEU:HA	1:A:345:LEU:HD12	1.96	0.41
1:A:16:TYR:C	1:A:23:LEU:HD12	2.40	0.41
1:B:179:LEU:N	1:B:180:PRO:CD	2.84	0.41
1:B:574:ARG:HG3	1:B:577:GLN:OE1	2.21	0.41
1:A:346:ASN:HD22	1:A:346:ASN:C	2.23	0.41
1:B:503:GLY:HA2	1:B:523:VAL:HB	2.03	0.41
1:A:573:LEU:HD11	1:A:579:MET:HG3	2.03	0.40
1:B:246:GLY:HA2	1:B:292:ALA:O	2.22	0.40
1:B:382:ARG:HB3	1:B:389:ILE:HG12	2.03	0.40
1:A:223:ARG:HA	1:A:223:ARG:HH11	1.85	0.40
1:A:477:LYS:CA	1:A:477:LYS:HE3	2.47	0.40
1:B:146:PRO:HA	1:B:149:ASP:CG	2.41	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%)	555 (95%)	26 (4%)	2 (0%)	43	43
1	B	583/585 (100%)	551 (94%)	31 (5%)	1 (0%)	49	51
All	All	1166/1170 (100%)	1106 (95%)	57 (5%)	3 (0%)	43	43



All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	LYS
1	A	278	THR
1	B	278	THR

### 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%)	472 (96%)	21 (4%)	32	31
1	B	493/493 (100%)	473 (96%)	20 (4%)	33	33
All	All	986/986 (100%)	945 (96%)	41 (4%)	32	32

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	122	PHE
1	A	129	LYS
1	A	155	GLN
1	A	158	LYS
1	A	182	LEU
1	A	191	TYR
1	A	260	GLU
1	A	280	ARG
1	A	341	LEU
1	A	345	LEU
1	A	346	ASN
1	A	398	LEU
1	A	404	LEU
1	A	408	GLN
1	A	413	LEU
1	A	477	LYS
1	A	483	LEU
1	A	504	ASN
1	A	547	GLU

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Mol	Chain	Res	Type
1	A	565	LYS
1	B	85	LEU
1	B	122	PHE
1	B	155	GLN
1	B	191	TYR
1	B	257	GLN
1	B	282	ASN
1	B	328	ASN
1	B	340	ARG
1	B	373	ASN
1	B	382	ARG
1	B	398	LEU
1	B	404	LEU
1	B	438	LEU
1	B	504	ASN
1	B	524	GLN
1	B	542	LEU
1	B	551	LYS
1	B	565	LYS
1	B	573	LEU
1	B	585	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	90	GLN
1	A	135	GLN
1	A	155	GLN
1	A	244	HIS
1	A	248	GLN
1	A	289	GLN
1	A	317	GLN
1	A	325	ASN
1	A	332	HIS
1	A	346	ASN
1	A	367	GLN
1	A	390	HIS
1	A	408	GLN
1	A	443	GLN
1	A	504	ASN
1	A	509	HIS

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Mol	Chain	Res	Type
1	A	515	ASN
1	A	527	HIS
1	A	539	GLN
1	A	563	HIS
1	A	568	GLN
1	B	135	GLN
1	B	164	HIS
1	B	202	HIS
1	B	243	ASN
1	B	244	HIS
1	B	248	GLN
1	B	282	ASN
1	B	328	ASN
1	B	332	HIS
1	B	357	HIS
1	B	367	GLN
1	B	373	ASN
1	B	504	ASN
1	B	509	HIS
1	B	533	ASN
1	B	539	GLN
1	B	544	GLN
1	B	563	HIS
1	B	566	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	GLC	A	701	2	11,11,12	0.45	0	15,15,17	0.73	1 (6%)
2	GLC	A	702	2	11,11,12	0.63	0	15,15,17	0.63	0
2	GLC	A	703	2	11,11,12	0.61	0	15,15,17	1.19	2 (13%)
2	GLC	A	704	2	11,11,12	0.63	0	15,15,17	0.79	1 (6%)
2	GLC	A	705	2	11,11,12	0.67	0	15,15,17	0.57	0
2	GLC	A	706	2	12,12,12	0.43	0	17,17,17	0.73	0
2	GLC	B	701	2	11,11,12	0.45	0	15,15,17	0.68	1 (6%)
2	GLC	B	702	2	11,11,12	0.57	0	15,15,17	0.61	0
2	GLC	B	703	2	11,11,12	0.56	0	15,15,17	1.06	1 (6%)
2	GLC	B	704	2	11,11,12	0.65	0	15,15,17	0.77	1 (6%)
2	GLC	B	705	2	11,11,12	0.55	0	15,15,17	0.65	0
2	GLC	B	706	2	12,12,12	0.42	0	17,17,17	0.46	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	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	-	0/2/19/22	0/1/1/1
2	GLC	A	706	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	B	701	2	-	0/2/19/22	0/1/1/1
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	-	0/2/19/22	0/1/1/1
2	GLC	B	706	2	1/1/5/5	0/2/22/22	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(°)	Ideal(°)
2	A	703	GLC	C1-C2-C3	-2.36	106.67	109.66
2	B	701	GLC	C1-O5-C5	2.13	115.11	112.19
2	A	701	GLC	C1-O5-C5	2.40	115.49	112.19
2	B	703	GLC	C1-O5-C5	2.44	115.54	112.19
2	B	704	GLC	C1-O5-C5	2.56	115.71	112.19
2	A	704	GLC	C1-O5-C5	2.68	115.87	112.19
2	A	703	GLC	C1-O5-C5	2.78	116.01	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	706	GLC	C1
2	B	706	GLC	C1

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	GLC	3	0
2	A	703	GLC	1	0
2	A	704	GLC	2	0
2	B	701	GLC	2	0
2	B	703	GLC	1	0
2	B	704	GLC	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	585/585 (100%)	-0.00	25 (4%)	35 41	15, 25, 47, 72	0
1	B	585/585 (100%)	0.07	38 (6%)	19 24	17, 27, 50, 83	0
All	All	1170/1170 (100%)	0.03	63 (5%)	26 32	15, 26, 48, 83	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	277	LYS	5.9
1	B	565	LYS	5.7
1	B	279	SER	5.5
1	A	549	GLY	5.1
1	A	277	LYS	5.0
1	B	551	LYS	4.9
1	B	566	GLN	4.7
1	A	280	ARG	4.6
1	B	275	VAL	4.2
1	B	548	SER	4.1
1	B	278	THR	4.1
1	B	552	THR	3.7
1	B	273	PHE	3.7
1	A	551	LYS	3.7
1	B	280	ARG	3.5
1	A	567	GLY	3.4
1	A	276	SER	3.3
1	B	570	LYS	3.2
1	B	542	LEU	3.1
1	A	278	THR	3.1
1	A	547	GLU	3.0
1	A	404	LEU	3.0
1	A	546	PRO	2.9
1	A	548	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	49	GLU	2.8
1	A	552	THR	2.8
1	A	564	GLY	2.8
1	A	279	SER	2.8
1	B	567	GLY	2.7
1	A	275	VAL	2.7
1	A	565	LYS	2.6
1	B	540	THR	2.6
1	B	573	LEU	2.6
1	B	152	GLY	2.5
1	B	153	THR	2.5
1	A	272	ASP	2.5
1	A	545	VAL	2.5
1	B	547	GLU	2.5
1	A	566	GLN	2.5
1	B	51	GLU	2.5
1	B	259	GLY	2.5
1	B	477	LYS	2.3
1	B	516	LEU	2.3
1	B	90	GLN	2.3
1	B	263	ARG	2.3
1	B	272	ASP	2.3
1	A	49	GLU	2.3
1	A	553	TRP	2.3
1	B	224	ARG	2.2
1	B	159	ASP	2.2
1	A	92	GLU	2.2
1	B	545	VAL	2.2
1	B	164	HIS	2.2
1	B	187	VAL	2.1
1	B	546	PRO	2.1
1	A	261	GLN	2.1
1	B	549	GLY	2.1
1	B	569	LEU	2.1
1	A	187	VAL	2.1
1	B	163	ARG	2.1
1	B	550	GLY	2.0
1	B	276	SER	2.0
1	A	371	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	A	706	12/12	0.67	0.32	40,48,52,55	11
2	GLC	B	701	11/12	0.71	0.38	43,47,49,51	11
2	GLC	B	706	12/12	0.72	0.24	51,64,66,67	0
2	GLC	A	701	11/12	0.76	0.41	42,47,50,51	11
2	GLC	B	705	11/12	0.86	0.20	33,38,40,43	11
2	GLC	A	705	11/12	0.92	0.26	23,29,34,37	11
2	GLC	B	703	11/12	0.96	0.09	23,26,27,28	0
2	GLC	B	702	11/12	0.96	0.08	27,29,31,37	0
2	GLC	A	704	11/12	0.96	0.13	20,24,27,33	0
2	GLC	B	704	11/12	0.96	0.10	24,28,31,33	0
2	GLC	A	703	11/12	0.97	0.11	17,21,22,23	0
2	GLC	A	702	11/12	0.97	0.09	21,23,26,33	0
3	CA	B	1002	1/1	0.98	0.04	32,32,32,32	0
3	CA	A	1001	1/1	0.99	0.07	24,24,24,24	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.