



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:40 AM GMT

PDB ID : 2ZYK  
Title : Crystal structure of cyclo/maltodextrin-bindingprotein complexed with gamma-cyclodextrin  
Authors : Tonozuka, T.; Sogawa, A.; Yamada, M.; Matsumoto, N.; Yoshida, H.; Kami-tori, S.; Ichikawa, K.; Mizuno, M.; Nishikawa, A.; Sakano, Y.  
Deposited on : 2009-01-26  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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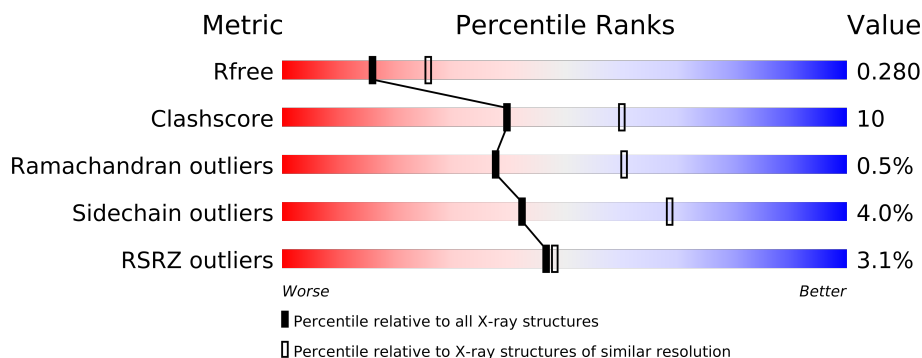
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	397	
1	B	397	
1	C	397	
1	D	397	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12746 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Solute-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2964	1908	490	557	9			
1	B	381	Total	C	N	O	S	0	0	0
			2964	1908	490	557	9			
1	C	381	Total	C	N	O	S	0	0	0
			2964	1908	490	557	9			
1	D	381	Total	C	N	O	S	0	0	0
			2964	1908	490	557	9			

- Molecule 2 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	8	Total	C	O	0	0
			88	48	40		
2	B	8	Total	C	O	0	0
			88	48	40		
2	C	8	Total	C	O	0	0
			88	48	40		
2	D	8	Total	C	O	0	0
			88	48	40		

- Molecule 3 is water.

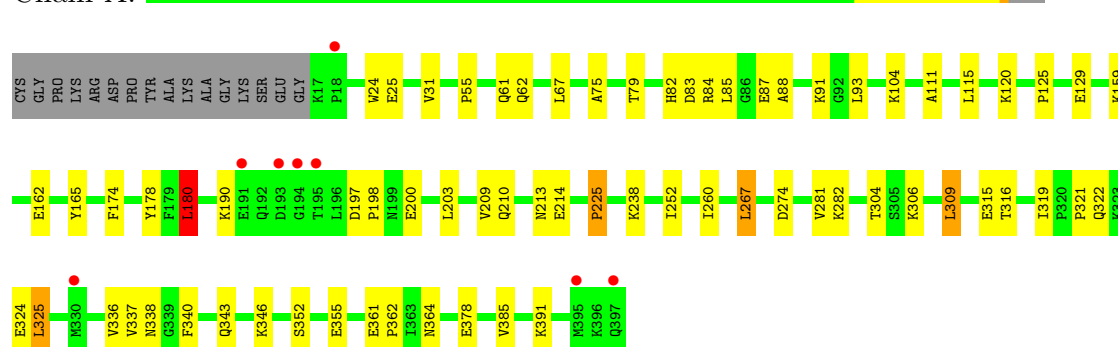
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	113	Total	O	0	0
			113	113		
3	C	146	Total	O	0	0
			146	146		
3	D	134	Total	O	0	0
			134	134		

### 3 Residue-property plots

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

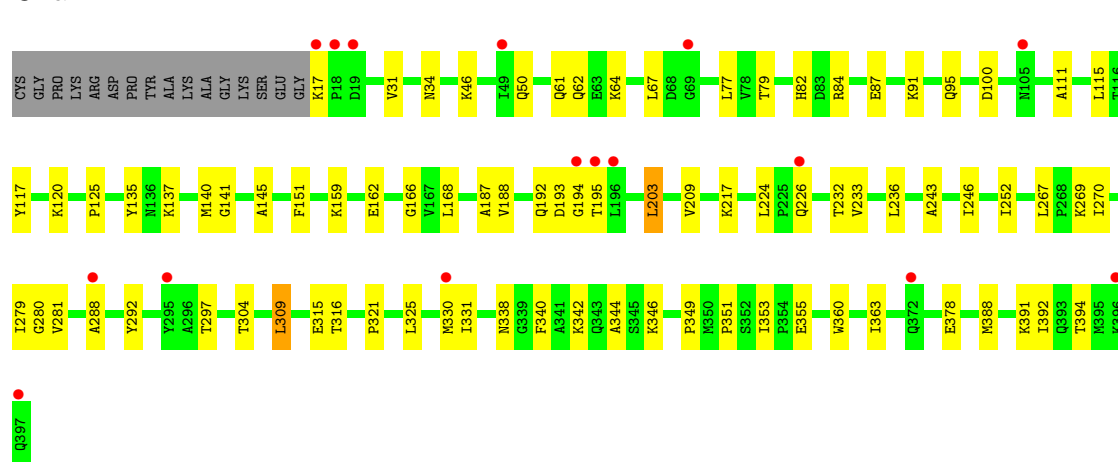
#### • Molecule 1: Solute-binding protein

Chain A:



#### • Molecule 1: Solute-binding protein

Chain B:



#### • Molecule 1: Solute-binding protein

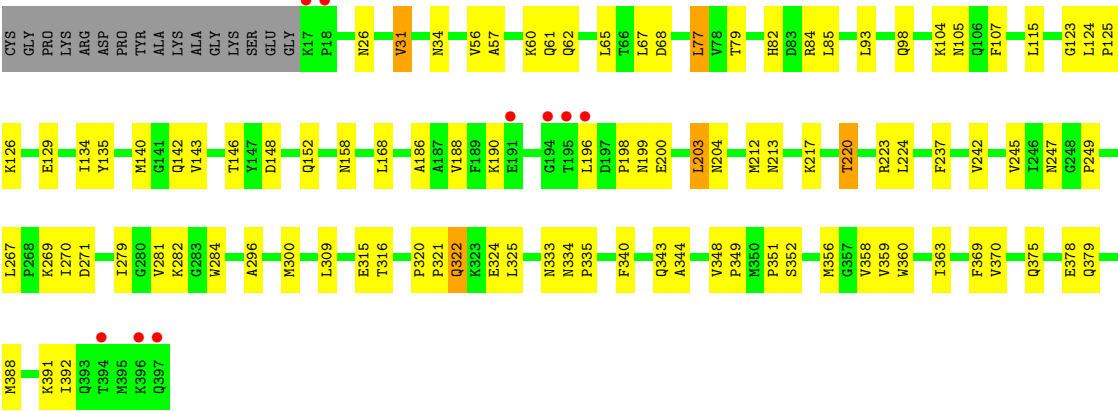
Chain C:





● Molecule 1: Solute-binding protein

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	167.40Å 95.27Å 117.13Å 90.00° 131.56° 90.00°	Depositor
Resolution (Å)	48.51 – 2.50 48.51 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.51-2.50) 99.7 (48.51-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.87 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.285 0.213 , 0.280	Depositor DCC
$R_{free}$ test set	4881 reflections (11.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 20.9	EDS
Estimated twinning fraction	0.000 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 47667 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12746	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.34 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.5579e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

## 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

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	0.44	0/3032	0.57	1/4109 (0.0%)
1	B	0.43	0/3032	0.56	0/4109
1	C	0.43	0/3032	0.55	0/4109
1	D	0.42	0/3032	0.56	0/4109
All	All	0.43	0/12128	0.56	1/16436 (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	180	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2964	0	2986	55	0
1	B	2964	0	2986	56	0
1	C	2964	0	2986	58	0
1	D	2964	0	2986	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	88	0	72	1	0
2	B	88	0	72	1	0
2	C	88	0	72	3	0
2	D	88	0	72	2	0
3	A	145	0	0	6	0
3	B	113	0	0	18	0
3	C	146	0	0	16	0
3	D	134	0	0	11	0
All	All	12746	0	12232	233	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (233) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:210:GLN:HG2	3:C:434:HOH:O	1.09	1.27
1:A:83:ASP:OD2	2:A:903:GLC:O3	1.79	1.00
1:D:125:PRO:HB2	1:D:321:PRO:HG2	1.44	0.96
1:C:25:GLU:OE2	3:C:517:HOH:O	1.88	0.91
1:C:378:GLU:OE1	3:C:498:HOH:O	1.89	0.89
1:B:31:VAL:HG12	1:B:316:THR:HG22	1.58	0.86
1:D:188:VAL:HG22	3:D:452:HOH:O	1.75	0.85
1:D:378:GLU:OE2	3:D:503:HOH:O	1.94	0.84
1:A:252:ILE:HD11	1:A:340:PHE:CE2	2.11	0.84
1:C:82:HIS:HD2	1:C:281:VAL:H	1.26	0.83
1:A:82:HIS:HD2	1:A:281:VAL:H	1.25	0.81
1:D:123:GLY:HA2	1:D:300:MET:HE1	1.62	0.81
1:A:62:GLN:HE22	1:A:84:ARG:HB3	1.45	0.81
1:A:174:PHE:H	1:A:364:ASN:HD21	1.28	0.81
1:D:82:HIS:HD2	1:D:281:VAL:H	1.29	0.80
1:C:61:GLN:HE22	1:C:79:THR:H	1.30	0.80
1:C:97:ILE:HD13	1:C:300:MET:CE	2.12	0.79
1:B:188:VAL:HG21	1:B:351:PRO:HG3	1.64	0.78
1:A:125:PRO:HB2	1:A:321:PRO:HG2	1.65	0.78
1:C:210:GLN:NE2	3:C:434:HOH:O	2.09	0.77
1:B:388:MET:O	1:B:392:ILE:HG12	1.85	0.76
1:D:188:VAL:HG21	1:D:351:PRO:HG3	1.68	0.75
1:C:97:ILE:HD13	1:C:300:MET:HE1	1.67	0.74
1:D:217:LYS:HA	1:D:220:THR:HG22	1.69	0.74
1:A:82:HIS:CD2	1:A:281:VAL:H	2.06	0.74
1:D:62:GLN:HE22	1:D:84:ARG:HB3	1.54	0.73
1:B:232:THR:O	3:B:433:HOH:O	2.06	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:360:TRP:CE3	2:B:903:GLC:H61	2.25	0.72
1:D:26:ASN:ND2	2:D:906:GLC:O3	2.19	0.71
1:B:31:VAL:HG13	1:B:315:GLU:HG2	1.74	0.70
1:A:129:GLU:OE1	1:A:282:LYS:HE2	1.91	0.70
1:A:214:GLU:OE1	3:A:417:HOH:O	2.07	0.70
1:C:61:GLN:NE2	1:C:79:THR:H	1.90	0.70
1:D:388:MET:O	1:D:392:ILE:HG12	1.92	0.70
1:A:338:ASN:HB3	3:A:458:HOH:O	1.93	0.69
1:A:61:GLN:HE22	1:A:79:THR:H	1.40	0.69
1:B:61:GLN:HE22	1:B:79:THR:H	1.39	0.69
1:C:358:VAL:HB	3:C:429:HOH:O	1.90	0.68
1:C:125:PRO:HB2	1:C:321:PRO:HG2	1.75	0.68
1:B:34:ASN:ND2	1:B:315:GLU:OE1	2.27	0.68
1:D:360:TRP:CE3	2:D:903:GLC:H61	2.30	0.67
1:D:126:LYS:HD3	1:D:284:TRP:NE1	2.10	0.66
1:B:61:GLN:NE2	1:B:79:THR:H	1.92	0.66
1:C:388:MET:O	1:C:392:ILE:HG12	1.95	0.66
1:A:174:PHE:H	1:A:364:ASN:ND2	1.94	0.66
1:C:82:HIS:CD2	1:C:281:VAL:H	2.11	0.66
1:D:279:ILE:HB	1:D:349:PRO:HA	1.76	0.66
1:A:252:ILE:HD11	1:A:340:PHE:HE2	1.57	0.65
1:A:252:ILE:HG21	1:A:336:VAL:HG11	1.78	0.65
1:C:360:TRP:CE3	2:C:903:GLC:H61	2.32	0.65
1:C:163:GLN:HG3	3:C:525:HOH:O	1.98	0.64
1:C:66:THR:HA	1:C:93:LEU:HD21	1.78	0.64
1:A:198:PRO:HB3	1:A:355:GLU:HG3	1.79	0.64
1:B:346:LYS:HD2	3:B:525:HOH:O	1.97	0.64
1:D:82:HIS:CD2	1:D:281:VAL:H	2.16	0.63
1:C:38:LYS:HD3	1:D:199:ASN:HB2	1.80	0.63
1:D:146:THR:HG22	1:D:269:LYS:HE2	1.81	0.62
1:C:385:VAL:HG23	3:C:427:HOH:O	2.00	0.62
1:B:125:PRO:HB2	1:B:321:PRO:HG2	1.81	0.62
1:C:210:GLN:CG	3:C:434:HOH:O	1.90	0.61
1:A:306:LYS:HG2	3:A:463:HOH:O	1.98	0.61
1:B:62:GLN:HE22	1:B:84:ARG:HB3	1.65	0.61
1:A:159:LYS:NZ	1:A:162:GLU:HG3	2.16	0.60
1:D:98:GLN:NE2	3:D:481:HOH:O	2.28	0.60
1:B:297:THR:HG21	3:B:474:HOH:O	2.01	0.60
1:C:358:VAL:CG1	1:C:391:LYS:HB2	2.32	0.60
1:D:61:GLN:HE22	1:D:79:THR:H	1.50	0.59
1:B:159:LYS:HD3	3:B:472:HOH:O	2.02	0.59
1:C:97:ILE:HD13	1:C:300:MET:HE3	1.84	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:322:GLN:NE2	3:D:471:HOH:O	2.35	0.59
1:D:77:LEU:HD13	1:D:296:ALA:HB1	1.85	0.59
1:C:126:LYS:HD3	1:C:284:TRP:NE1	2.17	0.59
1:D:135:TYR:HD1	3:D:515:HOH:O	1.86	0.59
1:B:269:LYS:HG2	3:B:466:HOH:O	2.02	0.58
1:A:391:LYS:NZ	1:C:142:GLN:HG3	2.18	0.58
1:B:233:VAL:HA	3:B:433:HOH:O	2.03	0.58
1:D:61:GLN:NE2	1:D:79:THR:H	2.01	0.58
2:C:902:GLC:H62	3:C:538:HOH:O	2.02	0.58
1:A:61:GLN:NE2	1:A:79:THR:H	2.01	0.58
1:B:91:LYS:HD3	3:B:498:HOH:O	2.03	0.58
1:C:323:LYS:O	3:C:422:HOH:O	2.17	0.57
1:D:124:LEU:HG	1:D:300:MET:HE2	1.86	0.57
1:D:188:VAL:HA	1:D:203:LEU:HD13	1.86	0.57
1:D:140:MET:HB3	3:D:515:HOH:O	2.02	0.57
1:C:210:GLN:O	1:C:213:ASN:HB2	2.05	0.56
1:B:137:LYS:HE3	3:B:494:HOH:O	2.04	0.56
1:D:85:LEU:O	1:D:352:SER:O	2.23	0.56
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.86	0.56
1:A:306:LYS:HE2	1:A:325:LEU:HD13	1.87	0.56
1:B:391:LYS:NZ	1:D:142:GLN:HG2	2.21	0.56
1:A:31:VAL:CG1	1:A:316:THR:HA	2.36	0.56
1:D:351:PRO:HG2	1:D:356:MET:SD	2.46	0.56
1:D:134:ILE:HD12	1:D:247:ASN:HB3	1.88	0.55
1:B:159:LYS:NZ	1:B:162:GLU:HG3	2.22	0.55
1:D:267:LEU:H	1:D:343:GLN:HE21	1.54	0.55
1:A:31:VAL:HG11	1:A:316:THR:HA	1.88	0.55
1:D:391:LYS:HD2	3:D:517:HOH:O	2.06	0.54
1:B:209:VAL:HG21	1:B:378:GLU:CD	2.28	0.54
1:A:88:ALA:HA	1:A:93:LEU:HD12	1.89	0.54
1:A:198:PRO:HB3	1:A:355:GLU:CG	2.38	0.54
1:C:396:LYS:H	1:C:396:LYS:HD2	1.72	0.53
1:C:188:VAL:HG21	1:C:351:PRO:HG2	1.91	0.53
1:A:178:TYR:C	1:A:180:LEU:H	2.12	0.53
1:A:336:VAL:O	1:A:336:VAL:HG12	2.08	0.53
1:C:165:TYR:HB2	1:C:242:VAL:HG22	1.90	0.53
1:C:262:VAL:HG22	3:C:450:HOH:O	2.08	0.53
1:B:252:ILE:HD11	1:B:340:PHE:CE2	2.44	0.53
1:A:165:TYR:OH	1:A:225:PRO:HG3	2.09	0.53
1:D:124:LEU:N	1:D:300:MET:CE	2.73	0.52
1:B:84:ARG:NH1	3:B:497:HOH:O	2.42	0.52
1:C:134:ILE:HD12	1:C:247:ASN:HB3	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:274:ASP:CG	1:A:346:LYS:HD2	2.31	0.51
1:A:267:LEU:H	1:A:343:GLN:HE21	1.58	0.51
1:B:338:ASN:O	1:B:342:LYS:HG2	2.10	0.51
1:D:212:MET:SD	1:D:370:VAL:HG21	2.51	0.51
1:D:124:LEU:H	1:D:300:MET:CE	2.23	0.51
1:D:124:LEU:H	1:D:300:MET:HE3	1.75	0.50
1:B:246:ILE:HD12	1:B:267:LEU:HD11	1.93	0.50
1:A:238:LYS:HA	1:A:260:ILE:HD11	1.94	0.50
1:D:190:LYS:HD2	1:D:200:GLU:HB3	1.93	0.50
1:C:212:MET:SD	1:C:370:VAL:HG21	2.52	0.50
1:B:135:TYR:CG	1:B:140:MET:HE2	2.46	0.50
1:B:270:ILE:HD11	3:B:491:HOH:O	2.11	0.50
1:B:203:LEU:HG	1:B:363:ILE:HD12	1.93	0.50
1:A:319:ILE:HD12	1:A:337:VAL:HG13	1.94	0.49
1:B:159:LYS:HG2	1:B:162:GLU:HG2	1.95	0.49
1:D:267:LEU:H	1:D:343:GLN:NE2	2.11	0.49
1:B:330:MET:HB3	1:B:331:ILE:HD12	1.94	0.49
1:B:166:GLY:O	1:B:243:ALA:HB3	2.13	0.49
1:D:115:LEU:HD23	1:D:123:GLY:C	2.32	0.49
1:D:126:LYS:HD3	1:D:284:TRP:CE2	2.47	0.49
1:D:186:ALA:HA	3:D:460:HOH:O	2.12	0.49
1:D:140:MET:HE3	1:D:143:VAL:HA	1.94	0.48
1:D:279:ILE:HD11	1:D:344:ALA:O	2.14	0.48
1:D:105:ASN:ND2	3:D:401:HOH:O	2.46	0.48
1:C:378:GLU:HB3	3:C:498:HOH:O	2.14	0.48
2:C:901:GLC:C1	2:C:902:GLC:O6	2.61	0.48
1:D:107:PHE:CE2	1:D:124:LEU:HD22	2.49	0.48
1:A:306:LYS:HE3	1:A:324:GLU:HB3	1.94	0.48
1:D:57:ALA:HB3	1:D:60:LYS:HD3	1.95	0.48
1:A:209:VAL:HG21	1:A:378:GLU:OE1	2.14	0.48
1:B:82:HIS:CD2	1:B:281:VAL:H	2.30	0.48
1:B:151:PHE:CZ	1:B:217:LYS:HB3	2.49	0.48
1:C:77:LEU:HD13	1:C:296:ALA:HB1	1.96	0.47
1:C:358:VAL:HG11	1:C:391:LYS:HB2	1.96	0.47
1:C:254:ASP:HB3	3:C:539:HOH:O	2.14	0.47
1:D:31:VAL:CG1	1:D:316:THR:HA	2.44	0.47
1:D:379:GLN:NE2	3:D:488:HOH:O	2.47	0.47
1:C:210:GLN:NE2	3:C:482:HOH:O	2.48	0.47
1:B:87:GLU:HG2	1:B:91:LYS:HE2	1.96	0.47
1:C:313:PHE:CZ	1:C:337:VAL:HG21	2.50	0.47
1:A:31:VAL:HG22	1:A:315:GLU:HG2	1.97	0.47
1:D:213:ASN:O	1:D:217:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:304:THR:HA	1:B:309:LEU:HD13	1.96	0.47
1:B:64:LYS:HB2	3:B:457:HOH:O	2.14	0.46
1:A:67:LEU:HD21	3:C:501:HOH:O	2.16	0.46
1:D:65:LEU:HD23	1:D:93:LEU:HB3	1.98	0.46
1:B:279:ILE:HD11	1:B:344:ALA:O	2.15	0.46
1:C:126:LYS:HE3	3:C:480:HOH:O	2.15	0.46
1:A:252:ILE:HG21	1:A:336:VAL:CG1	2.46	0.46
1:A:111:ALA:HA	1:A:281:VAL:HG21	1.96	0.46
1:B:279:ILE:HB	1:B:349:PRO:HA	1.97	0.46
1:B:188:VAL:CG2	1:B:351:PRO:HG3	2.39	0.46
1:B:346:LYS:CD	3:B:525:HOH:O	2.60	0.46
1:C:57:ALA:HB3	1:C:60:LYS:HB2	1.98	0.46
1:A:198:PRO:HB3	1:A:355:GLU:CD	2.36	0.45
1:D:320:PRO:HA	1:D:321:PRO:HD3	1.86	0.45
1:B:168:LEU:HD23	3:B:433:HOH:O	2.15	0.45
1:B:236:LEU:HB2	3:B:433:HOH:O	2.16	0.45
1:A:25:GLU:O	1:A:55:PRO:HA	2.17	0.45
1:C:38:LYS:NZ	1:D:199:ASN:HB2	2.32	0.45
1:A:385:VAL:HG23	3:A:543:HOH:O	2.16	0.45
1:B:100:ASP:HB3	3:B:496:HOH:O	2.17	0.45
1:C:163:GLN:O	1:C:241:LYS:HE3	2.17	0.45
1:D:168:LEU:HD12	1:D:224:LEU:HD22	1.99	0.45
1:B:280:GLY:HA3	3:B:411:HOH:O	2.15	0.45
1:B:188:VAL:HG22	3:B:415:HOH:O	2.17	0.44
1:C:366:ALA:O	1:C:370:VAL:HG22	2.17	0.44
1:D:129:GLU:OE2	1:D:282:LYS:HE3	2.17	0.44
1:A:210:GLN:O	1:A:213:ASN:HB2	2.17	0.44
1:B:111:ALA:HA	1:B:281:VAL:HG21	2.00	0.44
1:C:358:VAL:HG13	1:C:391:LYS:HB2	1.99	0.44
1:C:126:LYS:HD3	1:C:284:TRP:CE2	2.52	0.44
1:C:313:PHE:HB2	1:C:320:PRO:HD3	1.99	0.44
1:C:97:ILE:HG21	1:C:300:MET:HE1	1.99	0.44
1:B:145:ALA:HA	3:B:467:HOH:O	2.18	0.43
1:C:197:ASP:HA	1:C:198:PRO:HD2	1.85	0.43
1:A:62:GLN:HE22	1:A:84:ARG:CB	2.22	0.43
1:B:46:LYS:O	1:B:46:LYS:HG2	2.19	0.43
1:D:34:ASN:ND2	1:D:315:GLU:OE2	2.45	0.43
1:D:56:VAL:HG12	1:D:61:GLN:HG2	1.99	0.43
1:A:267:LEU:HB2	1:A:343:GLN:NE2	2.34	0.43
1:C:194:GLY:O	1:C:196:LEU:N	2.51	0.43
1:A:190:LYS:HB2	1:A:200:GLU:HB2	2.00	0.43
1:D:270:ILE:O	1:D:271:ASP:HB2	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:359:VAL:O	1:D:363:ILE:HG22	2.19	0.42
1:C:218:TRP:HB3	1:C:224:LEU:HD12	2.01	0.42
1:A:85:LEU:O	1:A:352:SER:O	2.36	0.42
1:B:95:GLN:HB3	1:B:288:ALA:HA	2.01	0.42
1:A:197:ASP:HA	1:A:198:PRO:HD2	1.61	0.42
1:C:334:ASN:O	1:C:338:ASN:HB2	2.19	0.42
1:D:123:GLY:CA	1:D:300:MET:HE1	2.42	0.42
1:A:304:THR:HA	1:A:309:LEU:HD13	2.00	0.42
1:D:158:ASN:O	1:D:223:ARG:HD2	2.18	0.42
1:D:356:MET:C	1:D:358:VAL:H	2.22	0.42
1:C:62:GLN:HB2	1:C:62:GLN:HE21	1.65	0.42
1:A:336:VAL:CG1	1:A:336:VAL:O	2.67	0.42
1:A:200:GLU:OE1	3:A:538:HOH:O	2.22	0.42
1:C:355:GLU:HB3	1:C:392:ILE:HD12	2.02	0.41
1:B:159:LYS:HZ1	1:B:162:GLU:HG3	1.85	0.41
1:D:148:ASP:O	1:D:152:GLN:HG2	2.19	0.41
1:D:249:PRO:HG3	1:D:340:PHE:CG	2.54	0.41
1:C:38:LYS:HD3	1:D:199:ASN:CB	2.50	0.41
1:D:237:PHE:HA	1:D:242:VAL:HB	2.02	0.41
1:C:396:LYS:H	1:C:396:LYS:CD	2.32	0.41
1:A:84:ARG:HG2	3:A:524:HOH:O	2.20	0.41
1:C:203:LEU:HD13	1:C:363:ILE:HD13	2.02	0.41
1:D:334:ASN:HA	1:D:335:PRO:HD3	1.97	0.41
1:D:369:PHE:HB3	1:D:375:GLN:HG3	2.03	0.41
1:A:87:GLU:HG2	1:A:91:LYS:HE2	2.02	0.41
1:D:168:LEU:O	1:D:245:VAL:HA	2.21	0.41
1:D:324:GLU:HG3	3:D:471:HOH:O	2.20	0.41
1:A:24:TRP:CD1	1:A:75:ALA:HB2	2.56	0.41
1:B:187:ALA:O	1:B:203:LEU:HD13	2.21	0.40
1:B:168:LEU:HD12	1:B:224:LEU:HD22	2.03	0.40
1:B:226:GLN:OE1	1:B:226:GLN:HA	2.21	0.40
1:B:117:TYR:O	1:B:120:LYS:HE2	2.21	0.40
1:B:31:VAL:HG11	1:B:316:THR:HA	2.04	0.40
1:A:391:LYS:HZ2	1:C:142:GLN:HG3	1.85	0.40
1:C:246:ILE:HG23	1:C:267:LEU:HD11	2.02	0.40
1:C:389:LYS:O	1:C:393:GLN:HG2	2.22	0.40
1:B:353:ILE:HD12	1:B:355:GLU:HG2	2.03	0.40
1:A:120:LYS:HE2	1:A:120:LYS:HB2	1.89	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	379/397 (96%)	364 (96%)	15 (4%)	0	100	100
1	B	379/397 (96%)	361 (95%)	16 (4%)	2 (0%)	38	60
1	C	379/397 (96%)	357 (94%)	18 (5%)	4 (1%)	21	34
1	D	379/397 (96%)	362 (96%)	16 (4%)	1 (0%)	50	73
All	All	1516/1588 (96%)	1444 (95%)	65 (4%)	7 (0%)	38	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	THR
1	B	194	GLY
1	C	396	LYS
1	B	141	GLY
1	C	191	GLU
1	D	198	PRO
1	C	329	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	313/324 (97%)	304 (97%)	9 (3%)	55	81
1	B	313/324 (97%)	300 (96%)	13 (4%)	40	66
1	C	313/324 (97%)	299 (96%)	14 (4%)	38	63
1	D	313/324 (97%)	299 (96%)	14 (4%)	38	63
All	All	1252/1296 (97%)	1202 (96%)	50 (4%)	42	68

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	115	LEU
1	A	180	LEU
1	A	203	LEU
1	A	225	PRO
1	A	267	LEU
1	A	309	LEU
1	A	322	GLN
1	A	325	LEU
1	B	17	LYS
1	B	50	GLN
1	B	67	LEU
1	B	77	LEU
1	B	115	LEU
1	B	192	GLN
1	B	193	ASP
1	B	195	THR
1	B	203	LEU
1	B	292	TYR
1	B	309	LEU
1	B	325	LEU
1	B	394	THR
1	C	31	VAL
1	C	77	LEU
1	C	94	LEU
1	C	98	GLN
1	C	105	ASN
1	C	115	LEU
1	C	124	LEU
1	C	188	VAL
1	C	223	ARG
1	C	231	ASP
1	C	309	LEU
1	C	342	LYS
1	C	355	GLU
1	C	396	LYS
1	D	31	VAL
1	D	67	LEU
1	D	68	ASP
1	D	77	LEU
1	D	104	LYS
1	D	196	LEU

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Mol	Chain	Res	Type
1	D	203	LEU
1	D	204	ASN
1	D	220	THR
1	D	309	LEU
1	D	322	GLN
1	D	325	LEU
1	D	333	ASN
1	D	348	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	62	GLN
1	A	82	HIS
1	A	98	GLN
1	A	199	ASN
1	A	213	ASN
1	A	226	GLN
1	A	301	GLN
1	A	322	GLN
1	A	343	GLN
1	A	364	ASN
1	B	34	ASN
1	B	50	GLN
1	B	61	GLN
1	B	62	GLN
1	B	98	GLN
1	B	105	ASN
1	B	213	ASN
1	B	276	GLN
1	B	333	ASN
1	B	343	GLN
1	B	365	ASN
1	C	61	GLN
1	C	62	GLN
1	C	82	HIS
1	C	105	ASN
1	C	163	GLN
1	C	192	GLN
1	C	199	ASN
1	C	213	ASN

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Mol	Chain	Res	Type
1	C	343	GLN
1	C	365	ASN
1	D	50	GLN
1	D	61	GLN
1	D	62	GLN
1	D	82	HIS
1	D	98	GLN
1	D	105	ASN
1	D	157	ASN
1	D	204	ASN
1	D	213	ASN
1	D	343	GLN
1	D	365	ASN
1	D	379	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

32 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	901	2	10,11,12	0.44	0	11,15,17	0.41	0
2	GLC	A	902	2	10,11,12	0.43	0	11,15,17	0.54	0
2	GLC	A	903	2	10,11,12	0.46	0	11,15,17	0.51	0
2	GLC	A	904	2	10,11,12	0.48	0	11,15,17	0.58	0
2	GLC	A	905	2	10,11,12	0.46	0	11,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLC	A	906	2	10,11,12	0.40	0	11,15,17	0.43	0
2	GLC	A	907	2	10,11,12	0.46	0	11,15,17	0.40	0
2	GLC	A	908	2	10,11,12	0.47	0	11,15,17	0.38	0
2	GLC	B	901	2	10,11,12	0.42	0	11,15,17	0.34	0
2	GLC	B	902	2	10,11,12	0.39	0	11,15,17	0.47	0
2	GLC	B	903	2	10,11,12	0.52	0	11,15,17	0.56	0
2	GLC	B	904	2	10,11,12	0.44	0	11,15,17	0.55	0
2	GLC	B	905	2	10,11,12	0.43	0	11,15,17	0.57	0
2	GLC	B	906	2	10,11,12	0.42	0	11,15,17	0.37	0
2	GLC	B	907	2	10,11,12	0.42	0	11,15,17	0.55	0
2	GLC	B	908	2	10,11,12	0.48	0	11,15,17	0.41	0
2	GLC	C	901	2	10,11,12	0.50	0	11,15,17	0.42	0
2	GLC	C	902	2	10,11,12	0.56	0	11,15,17	0.82	0
2	GLC	C	903	2	10,11,12	0.49	0	11,15,17	0.56	0
2	GLC	C	904	2	10,11,12	0.45	0	11,15,17	0.70	0
2	GLC	C	905	2	10,11,12	0.39	0	11,15,17	0.59	0
2	GLC	C	906	2	10,11,12	0.46	0	11,15,17	0.35	0
2	GLC	C	907	2	10,11,12	0.51	0	11,15,17	0.34	0
2	GLC	C	908	2	10,11,12	0.48	0	11,15,17	0.38	0
2	GLC	D	901	2	10,11,12	0.61	0	11,15,17	0.16	0
2	GLC	D	902	2	10,11,12	0.40	0	11,15,17	0.45	0
2	GLC	D	903	2	10,11,12	0.40	0	11,15,17	0.61	0
2	GLC	D	904	2	10,11,12	0.56	0	11,15,17	0.54	0
2	GLC	D	905	2	10,11,12	0.37	0	11,15,17	0.51	0
2	GLC	D	906	2	10,11,12	0.45	0	11,15,17	0.30	0
2	GLC	D	907	2	10,11,12	0.51	0	11,15,17	0.35	0
2	GLC	D	908	2	10,11,12	0.52	0	11,15,17	0.21	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	901	2	-	0/2/19/22	0/1/1/1
2	GLC	A	902	2	-	0/2/19/22	0/1/1/1
2	GLC	A	903	2	-	0/2/19/22	0/1/1/1
2	GLC	A	904	2	-	0/2/19/22	0/1/1/1
2	GLC	A	905	2	-	0/2/19/22	0/1/1/1
2	GLC	A	906	2	-	0/2/19/22	0/1/1/1
2	GLC	A	907	2	-	0/2/19/22	0/1/1/1
2	GLC	A	908	2	-	0/2/19/22	0/1/1/1
2	GLC	B	901	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	902	2	-	0/2/19/22	0/1/1/1
2	GLC	B	903	2	-	0/2/19/22	0/1/1/1
2	GLC	B	904	2	-	0/2/19/22	0/1/1/1
2	GLC	B	905	2	-	0/2/19/22	0/1/1/1
2	GLC	B	906	2	-	0/2/19/22	0/1/1/1
2	GLC	B	907	2	-	0/2/19/22	0/1/1/1
2	GLC	B	908	2	-	0/2/19/22	0/1/1/1
2	GLC	C	901	2	-	0/2/19/22	0/1/1/1
2	GLC	C	902	2	-	0/2/19/22	0/1/1/1
2	GLC	C	903	2	-	0/2/19/22	0/1/1/1
2	GLC	C	904	2	-	0/2/19/22	0/1/1/1
2	GLC	C	905	2	-	0/2/19/22	0/1/1/1
2	GLC	C	906	2	-	0/2/19/22	0/1/1/1
2	GLC	C	907	2	-	0/2/19/22	0/1/1/1
2	GLC	C	908	2	-	0/2/19/22	0/1/1/1
2	GLC	D	901	2	-	0/2/19/22	0/1/1/1
2	GLC	D	902	2	-	0/2/19/22	0/1/1/1
2	GLC	D	903	2	-	0/2/19/22	0/1/1/1
2	GLC	D	904	2	-	0/2/19/22	0/1/1/1
2	GLC	D	905	2	-	0/2/19/22	0/1/1/1
2	GLC	D	906	2	-	0/2/19/22	0/1/1/1
2	GLC	D	907	2	-	0/2/19/22	0/1/1/1
2	GLC	D	908	2	-	0/2/19/22	0/1/1/1

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.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 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<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	381/397 (95%)	-0.09	8 (2%) 60 63	3, 19, 44, 61	0
1	B	381/397 (95%)	0.18	16 (4%) 35 36	4, 24, 50, 69	0
1	C	381/397 (95%)	0.03	14 (3%) 39 41	6, 22, 47, 69	0
1	D	381/397 (95%)	-0.02	9 (2%) 56 58	6, 22, 40, 63	0
All	All	1524/1588 (95%)	0.03	47 (3%) 47 48	3, 22, 48, 69	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	GLY	10.2
1	D	397	GLN	7.6
1	A	194	GLY	7.3
1	C	195	THR	6.9
1	C	18	PRO	6.7
1	B	195	THR	6.7
1	B	397	GLN	6.2
1	C	396	LYS	6.1
1	C	199	ASN	5.9
1	A	195	THR	4.9
1	C	198	PRO	4.7
1	A	397	GLN	4.6
1	D	18	PRO	4.3
1	D	396	LYS	4.3
1	C	196	LEU	4.2
1	B	18	PRO	4.2
1	C	397	GLN	4.1
1	C	194	GLY	3.8
1	C	395	MET	3.7
1	C	394	THR	3.7
1	D	195	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	194	GLY	3.7
1	A	193	ASP	3.6
1	C	17	LYS	3.6
1	A	18	PRO	3.4
1	A	395	MET	3.3
1	A	191	GLU	3.3
1	C	162	GLU	3.1
1	B	372	GLN	3.1
1	C	192	GLN	3.0
1	B	69	GLY	3.0
1	B	288	ALA	2.9
1	D	17	LYS	2.9
1	B	396	LYS	2.8
1	B	196	LEU	2.7
1	D	191	GLU	2.5
1	B	17	LYS	2.5
1	D	196	LEU	2.5
1	B	295	TYR	2.5
1	B	330	MET	2.4
1	B	49	ILE	2.4
1	B	19	ASP	2.3
1	A	330	MET	2.3
1	D	394	THR	2.3
1	B	226	GLN	2.2
1	B	105	ASN	2.0
1	C	200	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

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<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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	A	907	11/12	0.28	6.55	40,44,46,46	0
2	GLC	B	907	11/12	0.33	6.29	43,49,54,61	0
2	GLC	A	908	11/12	0.26	5.13	47,50,56,60	0
2	GLC	D	906	11/12	0.27	2.26	25,37,43,43	0
2	GLC	C	901	11/12	0.27	2.14	38,42,49,56	0
2	GLC	D	901	11/12	0.30	1.93	37,43,53,58	0
2	GLC	A	901	11/12	0.31	1.32	38,42,45,54	0
2	GLC	B	901	11/12	0.41	1.26	42,44,48,53	0
2	GLC	B	906	11/12	0.20	1.14	27,46,48,53	0
2	GLC	D	908	11/12	0.25	0.97	49,53,56,56	0
2	GLC	C	908	11/12	0.23	0.95	34,47,49,50	0
2	GLC	C	907	11/12	0.21	0.94	33,41,44,50	0
2	GLC	A	906	11/12	0.18	0.87	24,34,38,38	0
2	GLC	A	904	11/12	0.14	0.85	6,11,14,18	0
2	GLC	D	903	11/12	0.14	0.57	13,20,22,24	0
2	GLC	B	903	11/12	0.15	0.49	6,12,14,19	0
2	GLC	B	902	11/12	0.17	0.15	26,29,33,40	0
2	GLC	A	903	11/12	0.14	-0.02	9,14,19,19	0
2	GLC	C	902	11/12	0.16	-0.04	18,24,27,34	0
2	GLC	D	907	11/12	0.22	-0.08	45,51,53,56	0
2	GLC	C	906	11/12	0.15	-0.16	20,26,34,37	0
2	GLC	D	905	11/12	0.14	-0.30	17,21,27,31	0
2	GLC	A	905	11/12	0.12	-0.38	11,18,22,25	0
2	GLC	C	905	11/12	0.12	-0.44	13,21,25,26	0
2	GLC	B	905	11/12	0.13	-0.47	21,22,25,28	0
2	GLC	A	902	11/12	0.14	-0.48	18,24,30,34	0
2	GLC	B	908	11/12	0.21	-0.64	44,47,50,51	0
2	GLC	B	904	11/12	0.10	-0.66	3,11,18,19	0
2	GLC	C	904	11/12	0.10	-0.74	10,13,15,15	0
2	GLC	D	904	11/12	0.10	-0.77	8,11,17,17	0
2	GLC	D	902	11/12	0.12	-1.05	25,27,33,35	0
2	GLC	C	903	11/12	0.10	-1.16	8,16,20,21	0

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.