Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:12 AM GMT

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

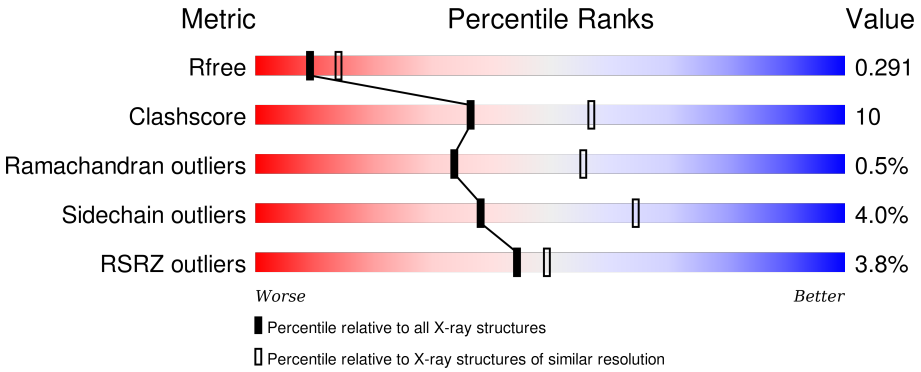
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (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 >=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	397	3% 78% 16%
1	B	397	5% 75% 20%
1	C	397	4% 77% 18%
1	D	397	3% 71% 23%

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	D	906	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12746 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 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.

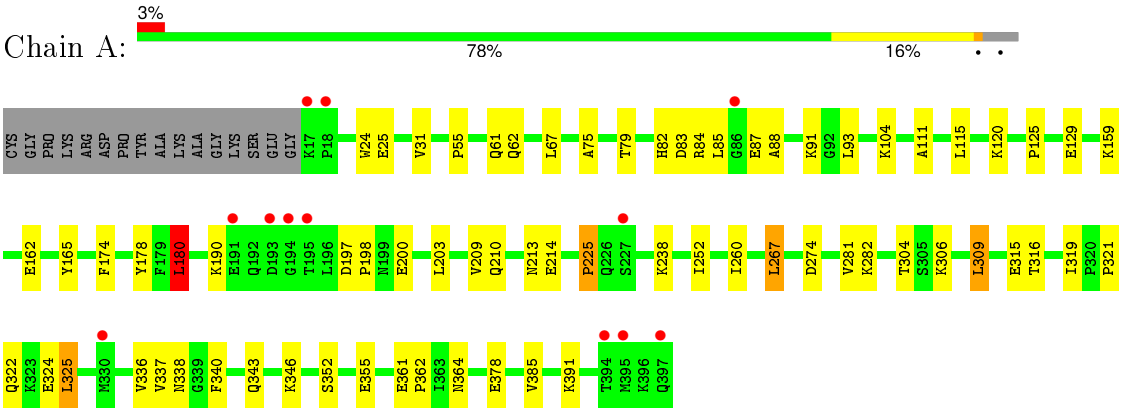
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total	O	0	0
			145	145		
3	B	113	Total	O	0	0
			113	113		
3	C	146	Total	O	0	0
			146	146		
3	D	134	Total	O	0	0
			134	134		

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.

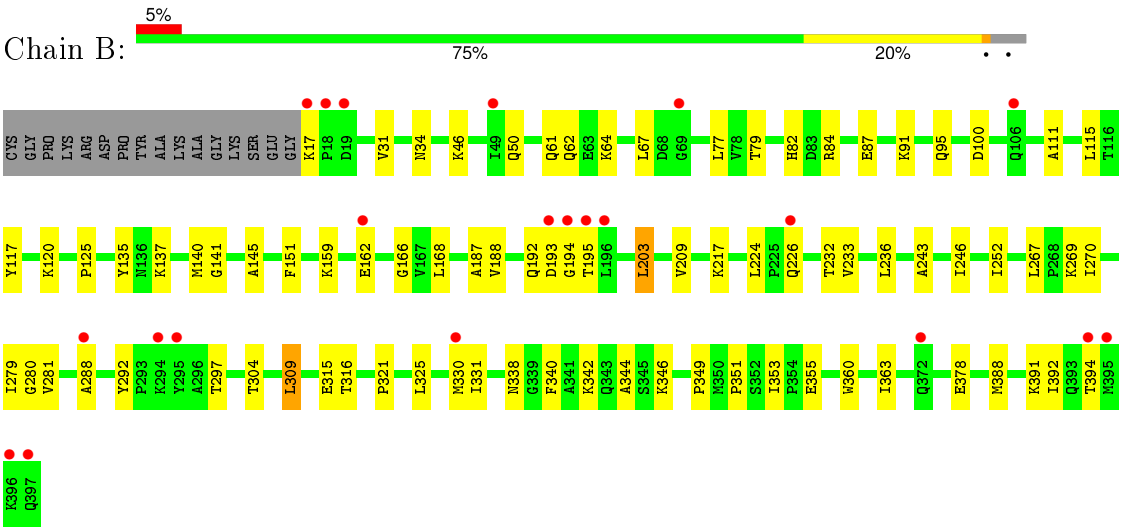
- Molecule 1: Solute-binding protein

Chain A:



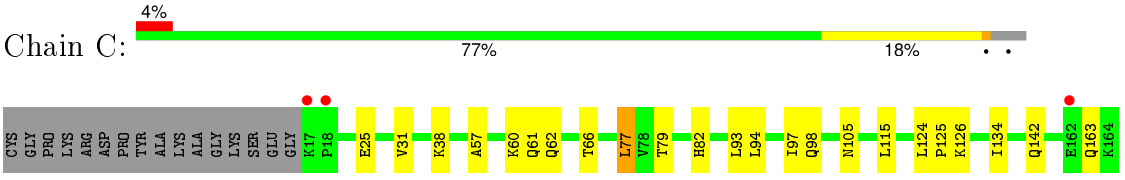
- Molecule 1: Solute-binding protein

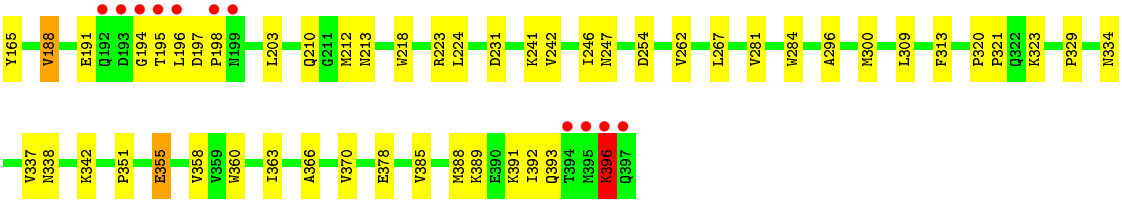
Chain B:



- Molecule 1: Solute-binding protein

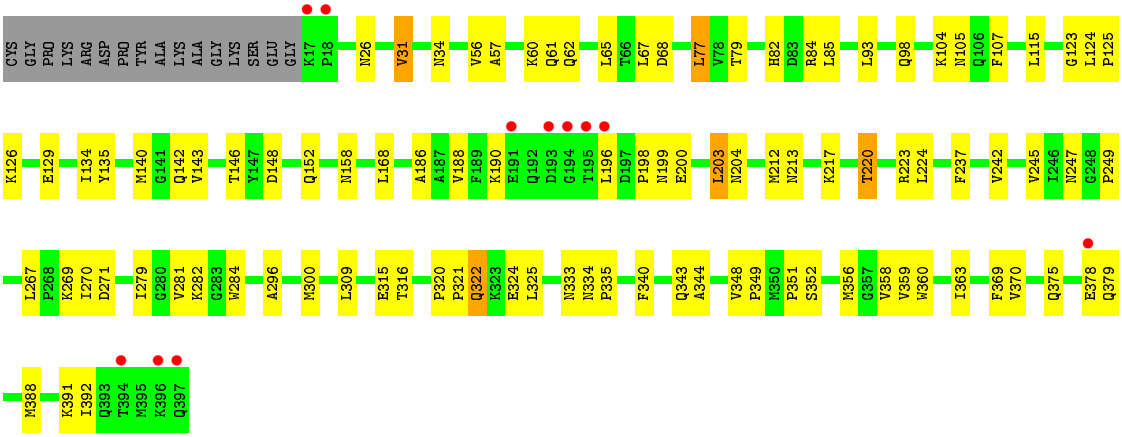
Chain C:





- Molecule 1: Solute-binding protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	7.87 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.285 0.227 , 0.291	Depositor DCC
R_{free} test set	4881 reflections (10.24%)	DCC
Wilson B-factor (Å^2)	21.7	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.4	EDS
Estimated twinning fraction	0.000 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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^2)	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.*

[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: 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(^{o})	Ideal(^{o})
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 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	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
2	A	88	0	72	1	0
2	B	88	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 10.

All (233) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ILE:HD13	1:C:300:MET:HE3	1.84	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	34	55
1	C	379/397 (96%)	357 (94%)	18 (5%)	4 (1%)	17	31
1	D	379/397 (96%)	362 (96%)	16 (4%)	1 (0%)	46	68
All	All	1516/1588 (96%)	1444 (95%)	65 (4%)	7 (0%)	34	55

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%)	50 77
1	B	313/324 (97%)	300 (96%)	13 (4%)	36 62
1	C	313/324 (97%)	299 (96%)	14 (4%)	34 59
1	D	313/324 (97%)	299 (96%)	14 (4%)	34 59
All	All	1252/1296 (97%)	1202 (96%)	50 (4%)	38 64

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates

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	11,11,12	0.54	0	14,15,17	0.51	0
2	GLC	A	902	2	11,11,12	0.43	0	14,15,17	0.76	1 (7%)
2	GLC	A	903	2	11,11,12	0.64	0	14,15,17	0.68	0
2	GLC	A	904	2	11,11,12	0.37	0	14,15,17	0.82	1 (7%)
2	GLC	A	905	2	11,11,12	0.60	0	14,15,17	0.66	0
2	GLC	A	906	2	11,11,12	0.43	0	14,15,17	0.59	0
2	GLC	A	907	2	11,11,12	0.48	0	14,15,17	0.68	1 (7%)
2	GLC	A	908	2	11,11,12	0.50	0	14,15,17	0.55	0
2	GLC	B	901	2	11,11,12	0.52	0	14,15,17	0.48	0
2	GLC	B	902	2	11,11,12	0.52	0	14,15,17	0.63	0
2	GLC	B	903	2	11,11,12	0.61	0	14,15,17	0.73	0
2	GLC	B	904	2	11,11,12	0.51	0	14,15,17	0.67	0
2	GLC	B	905	2	11,11,12	0.46	0	14,15,17	0.61	0
2	GLC	B	906	2	11,11,12	0.40	0	14,15,17	0.53	0
2	GLC	B	907	2	11,11,12	0.47	0	14,15,17	0.74	1 (7%)
2	GLC	B	908	2	11,11,12	0.58	0	14,15,17	0.57	0
2	GLC	C	901	2	11,11,12	0.62	0	14,15,17	0.61	0
2	GLC	C	902	2	11,11,12	0.62	0	14,15,17	1.03	1 (7%)
2	GLC	C	903	2	11,11,12	0.65	0	14,15,17	0.62	0
2	GLC	C	904	2	11,11,12	0.50	0	14,15,17	0.69	0
2	GLC	C	905	2	11,11,12	0.45	0	14,15,17	0.66	0
2	GLC	C	906	2	11,11,12	0.51	0	14,15,17	0.70	0
2	GLC	C	907	2	11,11,12	0.55	0	14,15,17	0.65	1 (7%)
2	GLC	C	908	2	11,11,12	0.57	0	14,15,17	0.61	0
2	GLC	D	901	2	11,11,12	0.65	0	14,15,17	0.55	0
2	GLC	D	902	2	11,11,12	0.45	0	14,15,17	0.50	0
2	GLC	D	903	2	11,11,12	0.50	0	14,15,17	0.63	0
2	GLC	D	904	2	11,11,12	0.51	0	14,15,17	0.62	0
2	GLC	D	905	2	11,11,12	0.54	0	14,15,17	0.52	0
2	GLC	D	906	2	11,11,12	0.54	0	14,15,17	0.67	0
2	GLC	D	907	2	11,11,12	0.55	0	14,15,17	0.67	1 (7%)
2	GLC	D	908	2	11,11,12	0.53	0	14,15,17	0.73	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	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
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.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	907	GLC	C1-O5-C5	2.05	114.86	112.25
2	B	907	GLC	C1-O5-C5	2.10	114.91	112.25
2	A	907	GLC	C1-O5-C5	2.17	115.00	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	907	GLC	C1-O5-C5	2.19	115.03	112.25
2	A	904	GLC	C1-O5-C5	2.20	115.04	112.25
2	A	902	GLC	C1-O5-C5	2.26	115.11	112.25
2	D	908	GLC	C1-O5-C5	2.46	115.37	112.25
2	C	902	GLC	C1-O5-C5	3.01	116.06	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	903	GLC	1	0
2	B	903	GLC	1	0
2	C	901	GLC	1	0
2	C	902	GLC	2	0
2	C	903	GLC	1	0
2	D	903	GLC	1	0
2	D	906	GLC	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{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	381/397 (95%)	-0.06	12 (3%)	52	57	3, 19, 44, 61	0
1	B	381/397 (95%)	0.22	21 (5%)	29	32	4, 24, 50, 69	0
1	C	381/397 (95%)	0.07	14 (3%)	45	50	6, 22, 47, 69	0
1	D	381/397 (95%)	0.01	11 (2%)	55	60	6, 22, 40, 63	0
All	All	1524/1588 (95%)	0.06	58 (3%)	44	49	3, 22, 48, 69	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	194	GLY	11.3
1	A	194	GLY	8.9
1	D	397	GLN	8.6
1	C	195	THR	7.8
1	C	396	LYS	7.7
1	B	195	THR	7.4
1	C	18	PRO	6.5
1	B	397	GLN	6.2
1	C	199	ASN	5.6
1	D	194	GLY	5.6
1	D	195	THR	5.5
1	B	18	PRO	5.5
1	C	194	GLY	5.4
1	A	195	THR	5.1
1	C	198	PRO	4.9
1	D	396	LYS	4.9
1	D	18	PRO	4.9
1	C	397	GLN	4.6
1	A	18	PRO	4.5
1	C	395	MET	4.4
1	A	397	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	191	GLU	4.3
1	A	193	ASP	4.1
1	C	394	THR	3.9
1	A	395	MET	3.8
1	B	17	LYS	3.8
1	C	17	LYS	3.8
1	C	192	GLN	3.8
1	D	191	GLU	3.6
1	C	196	LEU	3.4
1	B	372	GLN	3.4
1	D	17	LYS	3.1
1	C	162	GLU	3.1
1	B	196	LEU	3.0
1	B	295	TYR	3.0
1	B	396	LYS	2.9
1	D	196	LEU	2.9
1	B	69	GLY	2.7
1	B	19	ASP	2.6
1	A	330	MET	2.6
1	B	288	ALA	2.6
1	B	226	GLN	2.6
1	A	17	LYS	2.5
1	D	193	ASP	2.5
1	B	49	ILE	2.4
1	B	162	GLU	2.4
1	D	394	THR	2.4
1	B	294	LYS	2.3
1	C	193	ASP	2.3
1	B	395	MET	2.2
1	A	227	SER	2.2
1	A	86	GLY	2.1
1	B	394	THR	2.1
1	D	378	GLU	2.1
1	B	330	MET	2.1
1	B	106	GLN	2.0
1	B	193	ASP	2.0
1	A	394	THR	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	D	906	11/12	0.83	0.26	3.12	25,37,43,43	0
2	GLC	B	906	11/12	0.91	0.20	1.52	27,46,48,53	0
2	GLC	A	906	11/12	0.93	0.18	1.33	24,34,38,38	0
2	GLC	A	904	11/12	0.95	0.14	1.11	6,11,14,18	0
2	GLC	B	903	11/12	0.95	0.15	0.51	6,12,14,19	0
2	GLC	C	906	11/12	0.93	0.16	0.50	20,26,34,37	0
2	GLC	D	903	11/12	0.94	0.14	0.25	13,20,22,24	0
2	GLC	D	905	11/12	0.93	0.14	-0.11	17,21,27,31	0
2	GLC	A	903	11/12	0.95	0.13	-0.20	9,14,19,19	0
2	GLC	C	905	11/12	0.95	0.12	-0.47	13,21,25,26	0
2	GLC	A	905	11/12	0.95	0.11	-0.63	11,18,22,25	0
2	GLC	C	904	11/12	0.97	0.10	-0.78	10,13,15,15	0
2	GLC	B	905	11/12	0.96	0.12	-0.86	21,22,25,28	0
2	GLC	B	904	11/12	0.97	0.09	-1.00	3,11,18,19	0
2	GLC	D	902	11/12	0.95	0.12	-1.06	25,27,33,35	0
2	GLC	C	903	11/12	0.97	0.11	-1.12	8,16,20,21	0
2	GLC	D	904	11/12	0.95	0.09	-1.45	8,11,17,17	0
2	GLC	D	901	11/12	0.80	0.26	-	37,43,53,58	0
2	GLC	A	908	11/12	0.89	0.21	-	47,50,56,60	0
2	GLC	A	901	11/12	0.78	0.29	-	38,42,45,54	0
2	GLC	B	908	11/12	0.84	0.18	-	44,47,50,51	0
2	GLC	D	907	11/12	0.82	0.18	-	45,51,53,56	0
2	GLC	C	902	11/12	0.91	0.16	-	18,24,27,34	0
2	GLC	B	901	11/12	0.72	0.37	-	42,44,48,53	0
2	GLC	B	902	11/12	0.87	0.18	-	26,29,33,40	0
2	GLC	C	901	11/12	0.84	0.24	-	38,42,49,56	0
2	GLC	D	908	11/12	0.74	0.23	-	49,53,56,56	0
2	GLC	C	908	11/12	0.78	0.19	-	34,47,49,50	0
2	GLC	A	907	11/12	0.84	0.25	-	40,44,46,46	0
2	GLC	B	907	11/12	0.79	0.29	-	43,49,54,61	0
2	GLC	A	902	11/12	0.90	0.15	-	18,24,30,34	0
2	GLC	C	907	11/12	0.87	0.20	-	33,41,44,50	0

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.