



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:48 am GMT

PDB ID : 5CLW  
Title : Crystal structure of human glycogen branching enzyme (GBE1) in complex with maltoheptaose  
Authors : Krojer, T.; Froese, D.S.; Goubin, S.; Strain-Damerell, C.; Mahajan, P.; Burgess-Brown, N.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Yue, W.; Structural Genomics Consortium (SGC)  
Deposited on : 2015-07-16  
Resolution : 2.80 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

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

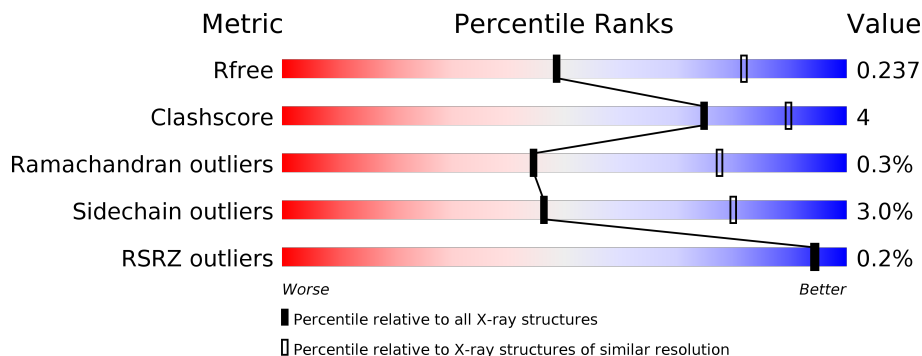
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*




The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	668	 84% 10% • 5%
1	B	668	 87% 9% • •
1	C	668	 84% 10% • 5%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15864 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.

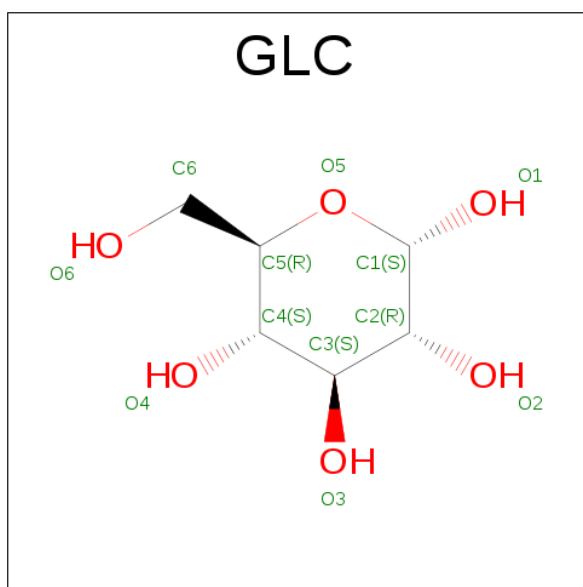
- Molecule 1 is a protein called 1,4-alpha-glucan-branching enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	2	0
			5151	3313	878	938	22			
1	B	645	Total	C	N	O	S	0	1	0
			5225	3366	887	949	23			
1	C	637	Total	C	N	O	S	0	0	0
			5082	3273	855	931	23			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	TYR	-	expression tag	UNP Q04446
A	34	PHE	-	expression tag	UNP Q04446
A	35	GLN	-	expression tag	UNP Q04446
A	36	SER	-	expression tag	UNP Q04446
A	37	MET	-	expression tag	UNP Q04446
A	265	SER	THR	conflict	UNP Q04446
A	334	VAL	ILE	conflict	UNP Q04446
B	33	TYR	-	expression tag	UNP Q04446
B	34	PHE	-	expression tag	UNP Q04446
B	35	GLN	-	expression tag	UNP Q04446
B	36	SER	-	expression tag	UNP Q04446
B	37	MET	-	expression tag	UNP Q04446
B	265	SER	THR	conflict	UNP Q04446
B	334	VAL	ILE	conflict	UNP Q04446
C	33	TYR	-	expression tag	UNP Q04446
C	34	PHE	-	expression tag	UNP Q04446
C	35	GLN	-	expression tag	UNP Q04446
C	36	SER	-	expression tag	UNP Q04446
C	37	MET	-	expression tag	UNP Q04446
C	265	SER	THR	conflict	UNP Q04446
C	334	VAL	ILE	conflict	UNP Q04446

- 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		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			12	6	6		

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0

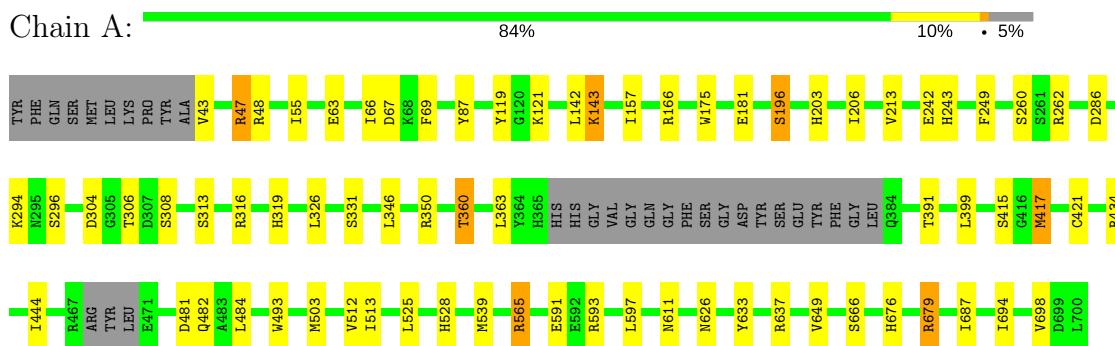
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	107	Total O 107 107	0	0
4	C	32	Total O 32 32	0	0

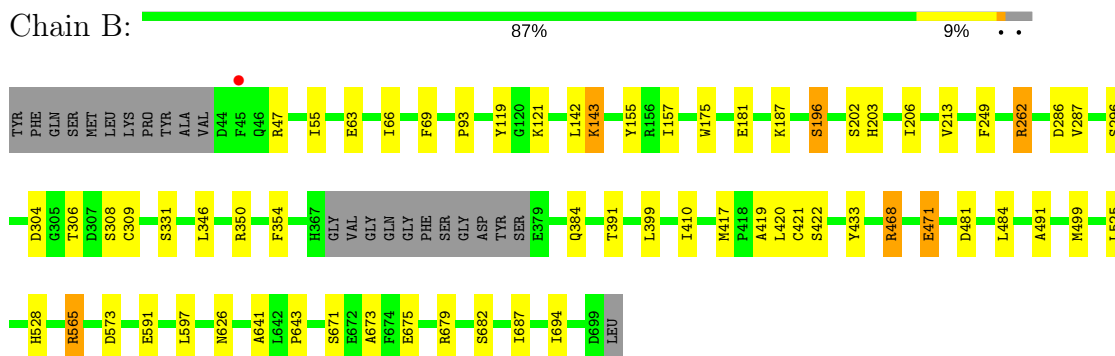
### 3 Residue-property plots

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.

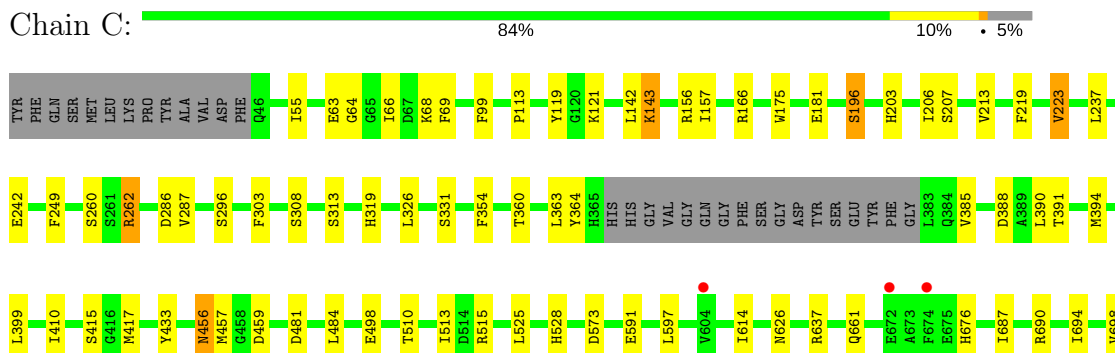
- Molecule 1: 1,4-alpha-glucan-branching enzyme



- Molecule 1: 1,4-alpha-glucan-branching enzyme



- Molecule 1: 1,4-alpha-glucan-branching enzyme





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.69Å 164.54Å 313.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	156.60 – 2.80 156.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (156.60-2.80) 99.7 (156.60-2.80)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.195 , 0.231 0.203 , 0.237	Depositor DCC
$R_{free}$ test set	3710 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.3	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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: NA, 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	0.48	0/5306	0.68	0/7192
1	B	0.53	0/5391	0.70	0/7309
1	C	0.49	0/5238	0.67	0/7112
All	All	0.50	0/15935	0.68	0/21613

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5151	0	4855	38	0
1	B	5225	0	4920	33	0
1	C	5082	0	4735	39	0
2	A	78	0	66	1	0
2	B	78	0	66	1	0
2	C	78	0	66	1	0
3	B	1	0	0	0	0
4	A	32	0	0	1	0
4	B	107	0	0	2	0
4	C	32	0	0	1	0
All	All	15864	0	14708	112	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 4.

All (112) 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:213:VAL:HG11	1:C:262:ARG:HG2	1.44	0.99
1:B:213:VAL:HG11	1:B:262:ARG:HG2	1.42	0.98
1:A:503:MET:HE3	1:A:513:ILE:HD12	1.62	0.80
1:C:55:ILE:HD12	1:C:391:THR:HG21	1.64	0.80
1:B:306:THR:HG22	1:B:308:SER:H	1.53	0.74
1:C:219:PHE:HA	1:C:223:VAL:HG13	1.68	0.74
1:B:420:LEU:HD22	4:B:1143:HOH:O	1.88	0.73
1:B:417:MET:HB3	4:B:1143:HOH:O	1.87	0.73
2:C:1001:GLC:H5	2:C:1002:GLC:H62	1.70	0.72
1:A:213:VAL:HG11	1:A:262:ARG:HG2	1.72	0.72
1:A:503:MET:CE	1:A:513:ILE:HD12	2.21	0.71
1:B:55:ILE:HD12	1:B:391:THR:HG21	1.75	0.69
2:A:1001:GLC:H5	2:A:1002:GLC:H62	1.74	0.68
1:A:421:CYS:SG	1:A:434:ARG:HB3	2.33	0.67
2:B:1001:GLC:H5	2:B:1002:GLC:H62	1.74	0.67
1:A:360:THR:HG23	1:A:415:SER:HB3	1.76	0.67
1:C:457:MET:CE	1:C:614:ILE:HG13	2.26	0.65
1:B:306:THR:HG22	1:B:308:SER:N	2.13	0.63
1:B:491:ALA:HB1	1:B:499:MET:HE3	1.80	0.62
1:B:671:SER:HA	1:B:682:SER:O	2.00	0.62
1:A:444:ILE:HD13	1:A:493:TRP:HE1	1.64	0.61
1:C:63:GLU:HG3	1:C:69:PHE:CD1	2.36	0.61
1:A:63:GLU:HG3	1:A:69:PHE:CD1	2.36	0.61
1:A:87:TYR:CD2	1:C:68:LYS:HE3	2.37	0.60
1:A:55:ILE:HD12	1:A:391:THR:HG21	1.83	0.60
1:C:457:MET:HE3	1:C:614:ILE:HG13	1.84	0.59
1:B:63:GLU:HG3	1:B:69:PHE:CD1	2.37	0.59
1:B:304:ASP:OD1	1:B:306:THR:HB	2.02	0.59
1:C:360:THR:HG23	1:C:415:SER:HB3	1.83	0.58
1:A:243:HIS:O	1:A:262:ARG:NH2	2.36	0.58
1:C:203:HIS:HB3	1:C:206:ILE:HG12	1.85	0.58
1:C:456:ASN:HD22	1:C:459:ASP:H	1.50	0.58
1:B:419:ALA:HA	1:B:422:SER:HB3	1.86	0.57
1:A:304:ASP:OD1	1:A:306:THR:HG22	2.03	0.57
1:B:421:CYS:HB2	1:B:471:GLU:HG3	1.86	0.57
1:A:203:HIS:HB3	1:A:206:ILE:HG12	1.88	0.56
1:A:308:SER:HB3	1:A:313:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:HG12	1:A:399:LEU:HD13	1.89	0.55
1:C:456:ASN:HB3	1:C:459:ASP:HB2	1.88	0.54
1:B:203:HIS:HB3	1:B:206:ILE:HG12	1.90	0.53
1:B:641:ALA:HB2	1:B:679:ARG:NH2	2.24	0.52
1:C:66:ILE:HG12	1:C:399:LEU:HD13	1.91	0.52
1:B:93:PRO:HD2	1:B:309:CYS:SG	2.51	0.50
1:B:468:ARG:HB2	1:B:471:GLU:HB2	1.92	0.50
1:C:457:MET:HE2	1:C:614:ILE:HG13	1.94	0.50
1:B:528:HIS:HE1	1:B:591:GLU:HG3	1.76	0.50
1:A:637:ARG:HG2	1:A:676:HIS:CG	2.46	0.50
1:A:444:ILE:HD13	1:A:493:TRP:NE1	2.26	0.50
1:C:498:GLU:O	1:C:513:ILE:HD11	2.11	0.49
1:B:206:ILE:HD12	1:B:565:ARG:HD3	1.94	0.49
1:C:528:HIS:HE1	1:C:591:GLU:HG3	1.75	0.49
1:C:196:SER:HB3	1:C:597:LEU:HB2	1.94	0.49
1:C:156:ARG:HD2	1:C:303:PHE:HA	1.95	0.48
1:B:66:ILE:HG12	1:B:399:LEU:HD13	1.93	0.48
1:A:157:ILE:HG23	1:A:175:TRP:HB2	1.96	0.48
1:A:528:HIS:HE1	1:A:591:GLU:HG3	1.78	0.47
1:B:410:ILE:HG12	1:B:433:TYR:HB2	1.97	0.47
1:A:679:ARG:HD2	1:A:679:ARG:HA	1.67	0.47
1:B:157:ILE:HG23	1:B:175:TRP:HB2	1.96	0.46
1:A:444:ILE:HD11	1:A:482:GLN:NE2	2.31	0.46
1:B:196:SER:HB3	1:B:597:LEU:HB2	1.98	0.46
1:B:481:ASP:HA	1:B:484:LEU:HD12	1.97	0.46
1:A:196:SER:HB3	1:A:597:LEU:HB2	1.98	0.46
1:C:410:ILE:HG12	1:C:433:TYR:HB2	1.98	0.46
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.80	0.45
1:A:67:ASP:HB3	4:A:1104:HOH:O	2.16	0.45
1:A:525:LEU:HD11	1:A:694:ILE:HD11	1.97	0.45
1:C:119:TYR:HB2	1:C:121:LYS:HE3	1.99	0.45
1:A:203:HIS:H	1:A:539:MET:CE	2.30	0.45
1:C:242:GLU:OE2	1:C:260:SER:HA	2.17	0.45
1:B:143:LYS:HG2	1:B:155:TYR:HB3	1.99	0.45
1:A:43:VAL:HG13	1:A:48[A]:ARG:NH2	2.32	0.44
1:C:308:SER:HB3	1:C:313:SER:HB2	1.98	0.44
1:C:99:PHE:CD1	1:C:113:PRO:HA	2.52	0.44
1:B:643:PRO:HA	1:B:671:SER:HB3	1.99	0.44
1:A:242:GLU:OE2	1:A:260:SER:HA	2.17	0.44
1:A:142:LEU:O	1:A:143:LYS:HD2	2.18	0.43
1:A:319:HIS:HB2	1:A:326:LEU:HD21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:TYR:CE1	1:C:385:VAL:HG22	2.53	0.43
1:C:390:LEU:HG	1:C:394:MET:HE2	1.99	0.43
1:B:119:TYR:HB2	1:B:121:LYS:HE3	2.01	0.43
1:B:142:LEU:O	1:B:143:LYS:HD2	2.19	0.43
1:A:565:ARG:HA	1:A:565:ARG:HD2	1.82	0.43
1:B:626:ASN:HB2	1:B:687:ILE:HG12	2.00	0.43
1:C:390:LEU:HG	1:C:394:MET:CE	2.48	0.43
1:A:119:TYR:HB2	1:A:121:LYS:HE3	2.01	0.42
1:B:525:LEU:HD11	1:B:694:ILE:HD11	2.01	0.42
1:B:565:ARG:HA	1:B:565:ARG:HD2	1.78	0.42
1:A:346:LEU:O	1:A:350:ARG:HA	2.19	0.42
1:C:363:LEU:HD12	4:C:1118:HOH:O	2.18	0.42
1:A:203:HIS:H	1:A:539:MET:HE2	1.84	0.42
1:A:611:ASN:HA	1:A:633:TYR:OH	2.19	0.42
1:C:626:ASN:HB2	1:C:687:ILE:HG12	2.02	0.42
1:C:498:GLU:OE1	1:C:510:THR:HG21	2.20	0.42
1:A:363:LEU:HD13	1:A:417:MET:HG3	2.00	0.42
1:C:142:LEU:O	1:C:143:LYS:HD2	2.20	0.42
1:B:675:GLU:HA	1:B:679:ARG:O	2.20	0.41
1:A:481:ASP:HA	1:A:484:LEU:HD12	2.01	0.41
1:C:637:ARG:HD2	1:C:676:HIS:CD2	2.56	0.41
1:C:157:ILE:HG23	1:C:175:TRP:HB2	2.01	0.41
1:C:287:VAL:HG21	1:C:354:PHE:CD1	2.56	0.41
1:B:287:VAL:HG21	1:B:354:PHE:CD1	2.55	0.41
1:C:525:LEU:HD11	1:C:694:ILE:HD11	2.02	0.41
1:C:207:SER:HB2	1:C:223:VAL:HG11	2.03	0.41
1:B:346:LEU:O	1:B:350:ARG:HA	2.20	0.41
1:C:319:HIS:HB2	1:C:326:LEU:HD21	2.03	0.41
1:A:626:ASN:HB2	1:A:687:ILE:HG12	2.02	0.41
1:A:637:ARG:HG2	1:A:676:HIS:ND1	2.35	0.40
1:C:237:LEU:HA	1:C:237:LEU:HD12	1.98	0.40
1:C:481:ASP:HA	1:C:484:LEU:HD12	2.03	0.40
1:C:64:GLY:HA3	1:C:68:LYS:HD2	2.04	0.40
1:C:515:ARG:HG3	1:C:690:ARG:CZ	2.51	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	633/668 (95%)	615 (97%)	18 (3%)	0	100	100
1	B	642/668 (96%)	625 (97%)	15 (2%)	2 (0%)	44	77
1	C	633/668 (95%)	618 (98%)	12 (2%)	3 (0%)	32	67
All	All	1908/2004 (95%)	1858 (97%)	45 (2%)	5 (0%)	44	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	661	GLN
1	B	673	ALA
1	C	698	VAL
1	B	262	ARG
1	C	262	ARG

### 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	534/575 (93%)	514 (96%)	20 (4%)	39	73
1	B	543/575 (94%)	528 (97%)	15 (3%)	49	82
1	C	521/575 (91%)	508 (98%)	13 (2%)	53	84
All	All	1598/1725 (93%)	1550 (97%)	48 (3%)	46	80

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	143	LYS
1	A	166	ARG
1	A	181	GLU
1	A	196	SER
1	A	249	PHE
1	A	286	ASP
1	A	294	LYS
1	A	296	SER
1	A	316	ARG
1	A	331	SER
1	A	360	THR
1	A	417	MET
1	A	512	VAL
1	A	565	ARG
1	A	593	ARG
1	A	649	VAL
1	A	666	SER
1	A	679	ARG
1	A	698	VAL
1	B	47	ARG
1	B	143	LYS
1	B	181	GLU
1	B	187	LYS
1	B	196	SER
1	B	202	SER
1	B	249	PHE
1	B	286	ASP
1	B	296	SER
1	B	331	SER
1	B	384	GLN
1	B	468	ARG
1	B	471	GLU
1	B	565	ARG
1	B	573	ASP
1	C	143	LYS
1	C	166	ARG
1	C	181	GLU
1	C	196	SER
1	C	223	VAL
1	C	249	PHE
1	C	286	ASP
1	C	296	SER

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Mol	Chain	Res	Type
1	C	331	SER
1	C	388	ASP
1	C	417	MET
1	C	456	ASN
1	C	573	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	A	537	ASN
1	A	601	GLN
1	C	51	GLN
1	C	456	ASN

### 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 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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	1001	2	11,11,12	0.47	0	13,15,17	1.05	1 (7%)
2	GLC	A	1002	2	11,11,12	0.33	0	13,15,17	1.34	1 (7%)
2	GLC	A	1003	2	11,11,12	0.38	0	13,15,17	1.00	1 (7%)
2	GLC	A	1004	2	11,11,12	0.28	0	13,15,17	0.88	1 (7%)
2	GLC	A	1005	2	11,11,12	0.24	0	13,15,17	1.32	1 (7%)
2	GLC	A	1006	2	11,11,12	0.43	0	13,15,17	1.05	1 (7%)
2	GLC	A	1007	2	12,12,12	0.44	0	17,17,17	0.53	0
2	GLC	B	1001	2	11,11,12	0.51	0	13,15,17	1.15	1 (7%)
2	GLC	B	1002	2	11,11,12	0.45	0	13,15,17	1.39	1 (7%)
2	GLC	B	1003	2	11,11,12	0.46	0	13,15,17	0.97	1 (7%)
2	GLC	B	1004	2	11,11,12	0.37	0	13,15,17	1.02	1 (7%)
2	GLC	B	1005	2	11,11,12	0.17	0	13,15,17	1.49	1 (7%)
2	GLC	B	1006	2	11,11,12	0.38	0	13,15,17	1.13	1 (7%)
2	GLC	B	1007	2	12,12,12	0.53	0	17,17,17	0.54	0
2	GLC	C	1001	2	11,11,12	0.47	0	13,15,17	1.16	1 (7%)
2	GLC	C	1002	2	11,11,12	0.32	0	13,15,17	1.27	1 (7%)
2	GLC	C	1003	2	11,11,12	0.41	0	13,15,17	1.06	1 (7%)
2	GLC	C	1004	2	11,11,12	0.37	0	13,15,17	0.90	1 (7%)
2	GLC	C	1005	2	11,11,12	0.46	0	13,15,17	1.40	1 (7%)
2	GLC	C	1006	2	11,11,12	0.55	0	13,15,17	0.98	1 (7%)
2	GLC	C	1007	2	12,12,12	0.40	0	17,17,17	0.53	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	1001	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1002	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1003	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1004	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1005	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1006	2	-	0/2/19/22	0/1/1/1
2	GLC	A	1007	2	-	0/2/22/22	0/1/1/1
2	GLC	B	1001	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1002	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1003	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	B	1004	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1005	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1006	2	-	0/2/19/22	0/1/1/1
2	GLC	B	1007	2	-	0/2/22/22	0/1/1/1
2	GLC	C	1001	2	-	0/2/19/22	0/1/1/1
2	GLC	C	1002	2	-	0/2/19/22	0/1/1/1
2	GLC	C	1003	2	-	0/2/19/22	0/1/1/1
2	GLC	C	1004	2	-	0/2/19/22	0/1/1/1
2	GLC	C	1005	2	-	0/2/19/22	0/1/1/1
2	GLC	C	1006	2	-	0/2/19/22	0/1/1/1
2	GLC	C	1007	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1004	GLC	C1-O5-C5	2.46	115.56	112.17
2	C	1004	GLC	C1-O5-C5	2.51	115.62	112.17
2	B	1003	GLC	C1-O5-C5	2.75	115.96	112.17
2	B	1004	GLC	C1-O5-C5	2.82	116.06	112.17
2	A	1003	GLC	C1-O5-C5	2.90	116.17	112.17
2	C	1006	GLC	C1-O5-C5	3.01	116.32	112.17
2	C	1003	GLC	C1-O5-C5	3.15	116.50	112.17
2	A	1006	GLC	C1-O5-C5	3.23	116.62	112.17
2	A	1001	GLC	C1-O5-C5	3.44	116.91	112.17
2	B	1006	GLC	C1-O5-C5	3.50	117.00	112.17
2	B	1001	GLC	C1-O5-C5	3.72	117.29	112.17
2	C	1001	GLC	C1-O5-C5	3.73	117.31	112.17
2	C	1002	GLC	C1-O5-C5	4.19	117.94	112.17
2	B	1002	GLC	C1-O5-C5	4.46	118.32	112.17
2	A	1002	GLC	C1-O5-C5	4.48	118.34	112.17
2	A	1005	GLC	C1-O5-C5	4.57	118.46	112.17
2	C	1005	GLC	C1-O5-C5	4.91	118.93	112.17
2	B	1005	GLC	C1-O5-C5	5.17	119.29	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GLC	1	0
2	A	1002	GLC	1	0
2	B	1001	GLC	1	0
2	B	1002	GLC	1	0
2	C	1001	GLC	1	0
2	C	1002	GLC	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	637/668 (95%)	-0.06	0	100   100	41, 61, 86, 99	0
1	B	645/668 (96%)	-0.14	1 (0%)	94   94	22, 37, 61, 81	0
1	C	637/668 (95%)	0.07	3 (0%)	90   88	36, 61, 88, 105	0
All	All	1919/2004 (95%)	-0.04	4 (0%)	94   94	22, 55, 84, 105	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	672	GLU	2.9
1	B	45	PHE	2.5
1	C	674	PHE	2.3
1	C	604	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. 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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GLC	C	1005	11/12	0.95	0.21	1.92	63,64,68,72	0
2	GLC	A	1004	11/12	0.96	0.21	0.43	64,65,76,78	0
2	GLC	A	1005	11/12	0.96	0.19	0.11	55,60,68,72	0
2	GLC	C	1004	11/12	0.95	0.18	0.04	65,68,77,81	0
2	GLC	B	1005	11/12	0.98	0.20	-0.04	33,37,40,45	0
2	GLC	A	1007	12/12	0.94	0.15	-0.24	70,78,83,84	0
2	GLC	B	1007	12/12	0.95	0.18	-0.31	40,45,54,58	0
2	GLC	B	1004	11/12	0.97	0.19	-0.84	36,40,44,50	0
2	GLC	C	1007	12/12	0.91	0.15	-0.90	69,78,82,85	0
3	NA	B	1008	1/1	0.99	0.16	-1.68	19,19,19,19	0
2	GLC	B	1006	11/12	0.97	0.17	-	36,39,44,53	0
2	GLC	B	1003	11/12	0.94	0.17	-	44,49,60,60	0
2	GLC	A	1006	11/12	0.97	0.12	-	57,64,68,70	0
2	GLC	C	1003	11/12	0.94	0.17	-	84,89,93,94	0
2	GLC	C	1006	11/12	0.95	0.15	-	58,62,64,65	0
2	GLC	B	1001	11/12	0.87	0.27	-	80,83,90,91	0
2	GLC	A	1001	11/12	0.78	0.38	-	112,114,115,115	0
2	GLC	A	1002	11/12	0.90	0.17	-	92,95,99,106	0
2	GLC	C	1002	11/12	0.82	0.18	-	92,93,96,100	0
2	GLC	C	1001	11/12	0.83	0.18	-	101,102,105,105	0
2	GLC	A	1003	11/12	0.93	0.16	-	85,92,96,97	0
2	GLC	B	1002	11/12	0.91	0.16	-	55,61,66,75	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.