



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:14 PM GMT

PDB ID : 3BC9  
Title : Alpha-amylase B in complex with acarbose  
Authors : Tan, T.-C.; Mijts, B.N.; Swaminathan, K.; Patel, B.K.C.; Divne, C.  
Deposited on : 2007-11-12  
Resolution : 1.35 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>

---

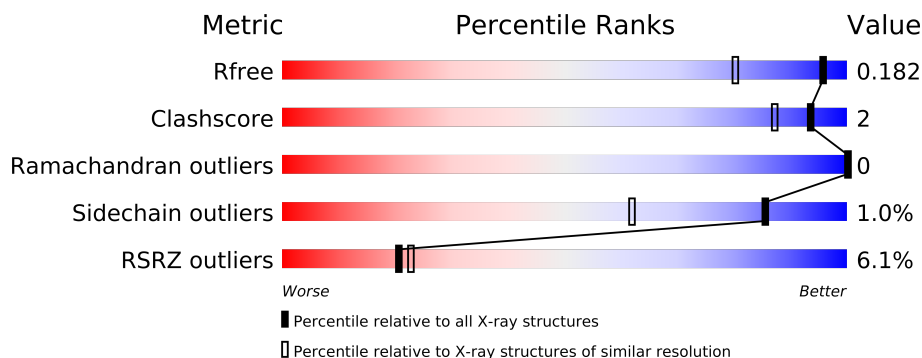
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.35 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	1519 (1.40-1.32)
Clashscore	79885	1707 (1.40-1.32)
Ramachandran outliers	78287	1662 (1.40-1.32)
Sidechain outliers	78261	1661 (1.40-1.32)
RSRZ outliers	66119	1519 (1.40-1.32)

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	599	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GLC	A	1001	-	X
4	GLC	A	1002	-	X
5	CA	A	705	-	X

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5566 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.

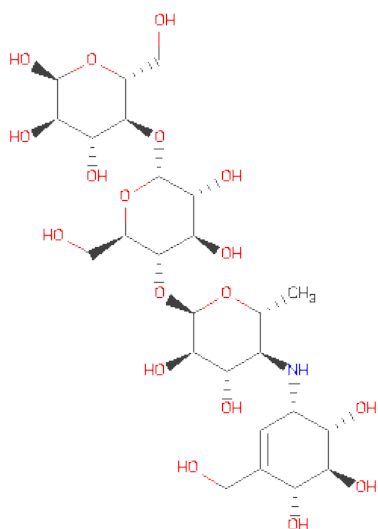
- Molecule 1 is a protein called Alpha amylase, catalytic region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	585	Total	C	N	O	S	0	9	0
			4822	3071	780	959	12			

- Molecule 2 is a polymer of unknown type called SUGAR (9-MER).

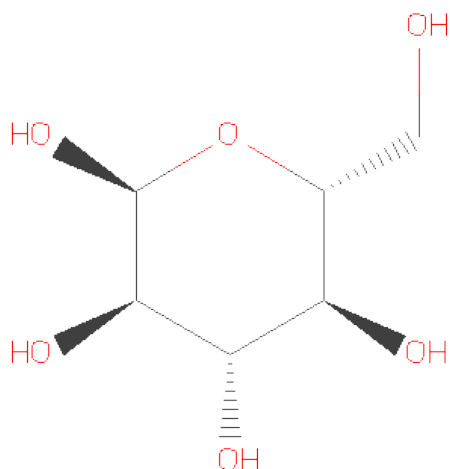
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	9	Total	C	N	O	0	0
			97	56	2	39		

- Molecule 3 is SUGAR (ACARBOSE) (three-letter code: ACR) (formula:  $C_{25}H_{43}NO_{18}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			44	25	1	18		

- Molecule 4 is SUGAR (GLUCOSE) (three-letter code: GLC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	6	6		
4	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	Ca	0	0
			4	4		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is water.

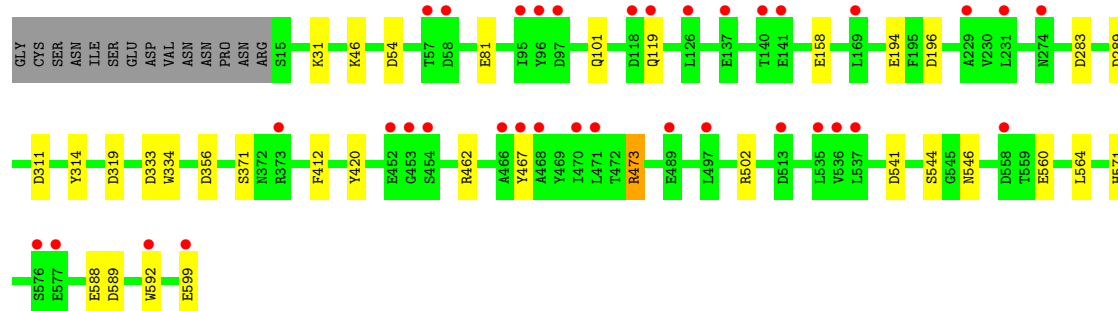
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	574	Total	O	0	0
			574	574		

### 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: Alpha amylase, catalytic region

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	227.85Å 77.24Å 50.38Å 90.00° 98.63° 90.00°	Depositor
Resolution (Å)	30.00 – 1.35 29.71 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-1.35) 99.3 (29.71-1.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.151 , 0.178 0.161 , 0.182	Depositor DCC
$R_{free}$ test set	1877 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.0	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 187593 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5566	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NA, ACI, GLC, GLD, G6D, ACR, CA

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	1.05	5/4955 (0.1%)	1.04	19/6751 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	588	GLU	CB-CG	-5.91	1.41	1.52
1	A	334	TRP	CZ3-CH2	-5.57	1.31	1.40
1	A	158	GLU	CB-CG	-5.51	1.41	1.52
1	A	194	GLU	CB-CG	-5.23	1.42	1.52
1	A	194	GLU	CG-CD	-5.11	1.44	1.51

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	502	ARG	NE-CZ-NH2	10.12	125.36	120.30
1	A	356	ASP	CB-CG-OD2	8.58	126.03	118.30
1	A	502	ARG	NE-CZ-NH1	-8.33	116.13	120.30
1	A	283	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	467	TYR	CB-CG-CD1	7.84	125.70	121.00
1	A	54	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	467	TYR	CB-CG-CD2	-7.03	116.78	121.00
1	A	473	ARG	NE-CZ-NH2	-6.83	116.88	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	A	319	ASP	CB-CG-OD1	-6.12	112.79	118.30
1	A	412	PHE	CB-CG-CD2	6.00	125.00	120.80
1	A	54	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	311	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	462	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	541	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	420	TYR	CB-CG-CD2	5.42	124.25	121.00
1	A	46	LYS	CD-CE-NZ	5.41	124.15	111.70
1	A	31	LYS	CD-CE-NZ	5.31	123.92	111.70
1	A	196	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	314	TYR	Sidechain

## 5.2 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 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	4822	0	0	7	0
2	A	97	0	0	0	0
3	A	44	0	0	0	0
4	A	24	0	0	1	0
5	A	4	0	0	0	0
6	A	1	0	0	0	0
7	A	574	0	0	4	1
All	All	5566	0	0	8	1

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 2.

All (8) close contacts within the same asymmetric unit are listed below.



Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:599:GLU:O	7:A:1558:HOH:O	2.09	0.70
1:A:544:SER:OG	1:A:546:ASN:OD1	2.17	0.62
4:A:1001:GLC:O4	4:A:1001:GLC:O6	2.22	0.54
1:A:101:GLN:NE2	7:A:1314:HOH:O	2.43	0.50
1:A:81:GLU:OE2	7:A:1471:HOH:O	2.19	0.49
1:A:560:GLU:OE2	1:A:571:HIS:ND1	2.48	0.47
1:A:589:ASP:O	1:A:592[A]:TRP:CZ3	2.70	0.45
1:A:333:ASP:OD1	7:A:1461:HOH:O	2.22	0.43

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:A:1384:HOH:O	7:A:1405:HOH:O[4_555]	2.07	0.13

## 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	592/599 (99%)	577 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	513/517 (99%)	508 (99%)	5 (1%)	85	62

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	289	ASP
1	A	371	SER
1	A	473	ARG
1	A	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

9 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	G6D	A	801	2	9,10,11	1.09	1 (11%)	10,14,16	1.82	3 (30%)
2	GLC	A	802	2	10,11,12	1.02	0	11,15,17	1.94	6 (54%)
2	ACI	A	803	2	12,12,12	1.63	2 (16%)	17,17,17	1.73	5 (29%)
2	GLD	A	804	2	8,9,10	0.74	0	8,12,14	2.12	1 (12%)
2	GLC	A	805	2	10,11,12	1.10	0	11,15,17	1.47	2 (18%)
2	ACI	A	806	2	12,12,12	2.21	5 (41%)	17,17,17	2.53	6 (35%)
2	GLD	A	807	2	8,9,10	0.70	0	8,12,14	2.07	4 (50%)
2	GLC	A	808	2	10,11,12	0.93	0	11,15,17	1.55	1 (9%)
2	BGC	A	809	2	12,12,12	1.10	0	17,17,17	1.45	3 (17%)

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	G6D	A	801	2	-	0/0/17/20	0/1/1/1
2	GLC	A	802	2	-	0/2/19/22	0/1/1/1
2	ACI	A	803	2	-	0/2/22/22	0/1/1/1
2	GLD	A	804	2	-	0/0/13/16	0/1/1/1
2	GLC	A	805	2	-	0/2/19/22	0/1/1/1
2	ACI	A	806	2	-	0/2/22/22	0/1/1/1
2	GLD	A	807	2	-	0/0/13/16	0/1/1/1
2	GLC	A	808	2	-	0/2/19/22	0/1/1/1
2	BGC	A	809	2	-	0/2/22/22	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	806	ACI	C3-C4	-3.82	1.48	1.53
2	A	806	ACI	C7-C5	3.48	1.38	1.32
2	A	803	ACI	O4-C4	3.32	1.48	1.42
2	A	806	ACI	O6-C6	2.84	1.50	1.41
2	A	806	ACI	O2-C2	2.75	1.49	1.43
2	A	803	ACI	C7-C5	2.66	1.36	1.32
2	A	806	ACI	C2-C1	2.65	1.58	1.52
2	A	801	G6D	O2-C2	-2.45	1.38	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	804	GLD	O5-C5-C6	5.64	111.75	105.82
2	A	806	ACI	O6-C6-C5	-5.60	96.90	112.40
2	A	806	ACI	C7-C1-N1	5.17	119.03	111.05
2	A	806	ACI	C2-C1-C7	-4.31	101.46	109.53
2	A	801	G6D	O5-C5A-C6A	-4.08	101.48	108.03
2	A	807	GLD	C3-C4-C5	-3.95	101.64	111.26
2	A	808	GLC	C4-C3-C2	-3.71	105.52	110.50
2	A	805	GLC	C4-C3-C2	-3.67	105.58	110.50
2	A	803	ACI	C6-C5-C4	3.47	119.48	114.53
2	A	809	BGC	C3-C4-C5	-3.33	104.26	110.20
2	A	806	ACI	C2-C1-N1	3.19	117.98	111.47
2	A	803	ACI	C7-C1-N1	-3.09	106.29	111.05
2	A	809	BGC	C1-O5-C5	-2.90	108.21	113.40

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	806	ACI	C2-C3-C4	-2.88	106.78	110.62
2	A	802	GLC	C3-C4-C5	-2.85	105.11	110.20
2	A	802	GLC	O4-C4-C3	-2.85	103.95	110.35
2	A	803	ACI	O4-C4-C5	-2.79	104.63	109.69
2	A	802	GLC	O2-C2-C3	-2.71	104.33	110.18
2	A	809	BGC	C1-C2-C3	-2.43	106.68	110.53
2	A	802	GLC	O5-C5-C4	2.29	113.56	110.65
2	A	807	GLD	C6-C5-C4	-2.27	109.64	113.38
2	A	807	GLD	O5-C5-C6	-2.27	103.43	105.82
2	A	803	ACI	O3-C3-C4	-2.24	105.97	109.36
2	A	802	GLC	O3-C3-C2	-2.20	105.91	109.94
2	A	801	G6D	O3A-C3A-C2	-2.18	105.94	109.94
2	A	807	GLD	O5-C5-C4	-2.17	105.16	109.65
2	A	805	GLC	O4-C4-C3	-2.09	105.67	110.35
2	A	803	ACI	O4-C4-C3	2.09	114.61	110.13
2	A	801	G6D	O2-C2-C3A	-2.07	105.71	110.18
2	A	802	GLC	O3-C3-C4	-2.04	105.77	110.35
2	A	806	ACI	O3-C3-C4	2.04	112.45	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\# Z  > 2$
4	GLC	A	1001	-	12,12,12	0.98	0	17,17,17	2.64	5 (29%)
4	GLC	A	1002	-	12,12,12	0.48	0	17,17,17	2.26	7 (41%)
3	ACR	A	901	-	47,47,47	0.67	0	70,70,70	1.38	10 (14%)

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
4	GLC	A	1001	-	-	0/2/22/22	0/1/1/1
4	GLC	A	1002	-	1/1/5/5	0/2/22/22	0/1/1/1
3	ACR	A	901	-	1/1/20/22	0/18/98/98	0/4/4/4

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	GLC	C4-C3-C2	-6.51	98.78	110.82
4	A	1001	GLC	C6-C5-C4	-5.98	98.55	113.00
4	A	1002	GLC	O1-C1-O5	4.95	123.67	110.32
4	A	1002	GLC	O1-C1-C2	4.66	122.65	109.47
3	A	901	ACR	C6A-C5A-C4A	4.39	120.79	114.53
4	A	1001	GLC	O5-C5-C4	4.23	117.58	109.76
3	A	901	ACR	O2D-C2D-C1D	3.08	116.44	109.89
4	A	1002	GLC	O5-C5-C4	2.99	115.30	109.76
4	A	1002	GLC	C4-C3-C2	-2.73	105.77	110.82
4	A	1001	GLC	O3-C3-C4	-2.73	104.23	110.35
3	A	901	ACR	O3A-C3A-C4A	2.71	113.46	109.36
3	A	901	ACR	C2D-C3D-C4D	2.60	115.25	109.61
3	A	901	ACR	C7A-C1A-N4B	-2.59	107.45	111.19
3	A	901	ACR	C2A-C3A-C4A	-2.50	107.29	110.62
3	A	901	ACR	O2D-C2D-C3D	-2.49	104.76	110.35
3	A	901	ACR	O5C-C1C-C2C	-2.49	105.21	110.31
4	A	1002	GLC	O5-C5-C6	2.45	112.36	106.34
4	A	1002	GLC	C1-O5-C5	2.40	117.70	113.40
4	A	1002	GLC	O5-C1-C2	2.37	113.53	109.86
4	A	1001	GLC	O2-C2-C1	2.12	114.40	109.89
3	A	901	ACR	C5B-C4B-N4B	2.05	116.67	111.20
3	A	901	ACR	C1B-C2B-C3B	-2.01	106.09	110.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1002	GLC	C1
3	A	901	ACR	C1D

There are no torsion outliers.

There are no ring outliers.

## 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	585/599 (97%)	0.19	35 (5%) 21 23	10, 17, 28, 39	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	SER	5.0
1	A	452	GLU	4.2
1	A	96	TYR	4.2
1	A	453	GLY	4.1
1	A	97	ASP	3.8
1	A	599	GLU	3.7
1	A	577	GLU	3.5
1	A	119	GLN	3.4
1	A	140	THR	3.3
1	A	537	LEU	3.2
1	A	137	GLU	3.0
1	A	513	ASP	2.8
1	A	118	ASP	2.8
1	A	58	ASP	2.8
1	A	592[A]	TRP	2.7
1	A	169	LEU	2.7
1	A	231	LEU	2.7
1	A	95	ILE	2.5
1	A	471	LEU	2.5
1	A	535	LEU	2.5
1	A	57	THR	2.5
1	A	576	SER	2.5
1	A	141	GLU	2.4
1	A	536	VAL	2.4
1	A	470	ILE	2.3
1	A	126	LEU	2.3
1	A	497	LEU	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	467	TYR	2.3
1	A	558	ASP	2.2
1	A	489	GLU	2.2
1	A	466	ALA	2.2
1	A	229	ALA	2.1
1	A	274	ASN	2.1
1	A	373[A]	ARG	2.1
1	A	468	ALA	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(Å <sup>2</sup> )	Q<0.9
2	G6D	A	801	10/11	0.29	14.70	26,35,41,41	0
2	ACI	A	803	12/12	0.20	6.95	20,22,29,38	0
2	GLC	A	802	11/12	0.19	4.60	25,26,30,35	0
2	BGC	A	809	12/12	0.25	4.06	26,38,43,47	0
2	GLC	A	805	11/12	0.08	1.61	15,17,21,24	0
2	GLD	A	804	9/10	0.10	1.04	21,22,28,28	0
2	ACI	A	806	12/12	0.10	0.53	14,18,24,30	0
2	GLC	A	808	11/12	0.08	0.44	17,20,24,29	0
2	GLD	A	807	9/10	0.06	-0.74	13,14,17,19	0

## 6.4 Ligands ⓘ

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
4	GLC	A	1002	12/12	0.24	18.73	72,74,74,75	0
4	GLC	A	1001	12/12	0.33	13.51	26,40,42,46	0
5	CA	A	705	1/1	0.17	2.70	30,30,30,30	0
3	ACR	A	901	44/44	0.13	1.58	14,23,48,52	0
5	CA	A	702	1/1	0.06	-0.64	10,10,10,10	0
5	CA	A	703	1/1	0.03	-1.19	14,14,14,14	0
6	NA	A	704	1/1	0.03	-1.60	10,10,10,10	0
5	CA	A	701	1/1	0.03	-1.74	11,11,11,11	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.