Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2016 – 01:39 PM EDT

PDB ID	:	5LGV
Title	:	GlgE isoform 1 from Streptomyces coelicolor E423A mutant soaked in maltooctaose
Authors	:	Syson, K.; Stevenson, C.E.M.; Mia, F.; Barclay, J.E.; Tang, M.; Gorelik, A.; Rashid, A.M.; Lawson, D.M.; Bornemann, S.
Deposited on	:	2016-07-08
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 ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
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)	:	rb-20028320

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	Percentile Ranks	Value
Rfree		0.210
Clashscore		0
Ramachandran outliers		0.1%
Sidechain outliers		1.2%
RSRZ outliers		3.9%

Worse   Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
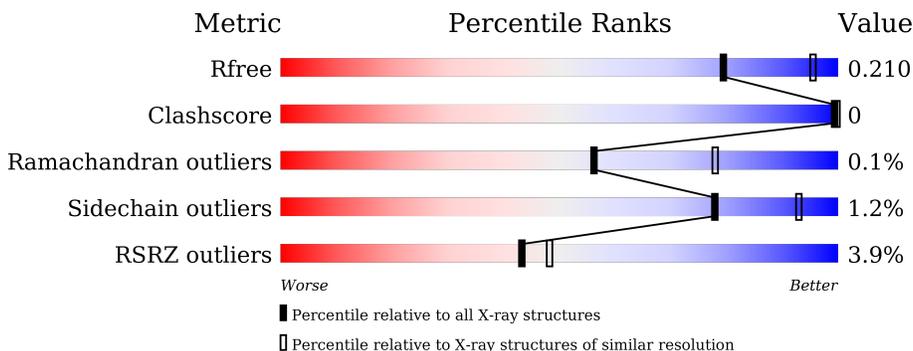
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	695	5% [red bar] 91% · 7%
1	B	695	2% [red bar] 91% · 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10941 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 Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total 5119	C 3242	N 931	O 936	S 10	0	4	0
1	B	649	Total 5085	C 3224	N 911	O 940	S 10	0	5	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9L1K2
A	-18	GLY	-	expression tag	UNP Q9L1K2
A	-17	SER	-	expression tag	UNP Q9L1K2
A	-16	SER	-	expression tag	UNP Q9L1K2
A	-15	HIS	-	expression tag	UNP Q9L1K2
A	-14	HIS	-	expression tag	UNP Q9L1K2
A	-13	HIS	-	expression tag	UNP Q9L1K2
A	-12	HIS	-	expression tag	UNP Q9L1K2
A	-11	HIS	-	expression tag	UNP Q9L1K2
A	-10	HIS	-	expression tag	UNP Q9L1K2
A	-9	SER	-	expression tag	UNP Q9L1K2
A	-8	SER	-	expression tag	UNP Q9L1K2
A	-7	GLY	-	expression tag	UNP Q9L1K2
A	-6	LEU	-	expression tag	UNP Q9L1K2
A	-5	VAL	-	expression tag	UNP Q9L1K2
A	-4	PRO	-	expression tag	UNP Q9L1K2
A	-3	ARG	-	expression tag	UNP Q9L1K2
A	-2	GLY	-	expression tag	UNP Q9L1K2
A	-1	SER	-	expression tag	UNP Q9L1K2
A	0	HIS	-	expression tag	UNP Q9L1K2
A	423	ALA	GLU	conflict	UNP Q9L1K2
B	-19	MET	-	initiating methionine	UNP Q9L1K2
B	-18	GLY	-	expression tag	UNP Q9L1K2
B	-17	SER	-	expression tag	UNP Q9L1K2
B	-16	SER	-	expression tag	UNP Q9L1K2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP Q9L1K2
B	-14	HIS	-	expression tag	UNP Q9L1K2
B	-13	HIS	-	expression tag	UNP Q9L1K2
B	-12	HIS	-	expression tag	UNP Q9L1K2
B	-11	HIS	-	expression tag	UNP Q9L1K2
B	-10	HIS	-	expression tag	UNP Q9L1K2
B	-9	SER	-	expression tag	UNP Q9L1K2
B	-8	SER	-	expression tag	UNP Q9L1K2
B	-7	GLY	-	expression tag	UNP Q9L1K2
B	-6	LEU	-	expression tag	UNP Q9L1K2
B	-5	VAL	-	expression tag	UNP Q9L1K2
B	-4	PRO	-	expression tag	UNP Q9L1K2
B	-3	ARG	-	expression tag	UNP Q9L1K2
B	-2	GLY	-	expression tag	UNP Q9L1K2
B	-1	SER	-	expression tag	UNP Q9L1K2
B	0	HIS	-	expression tag	UNP Q9L1K2
B	423	ALA	GLU	conflict	UNP Q9L1K2

- Molecule 2 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).
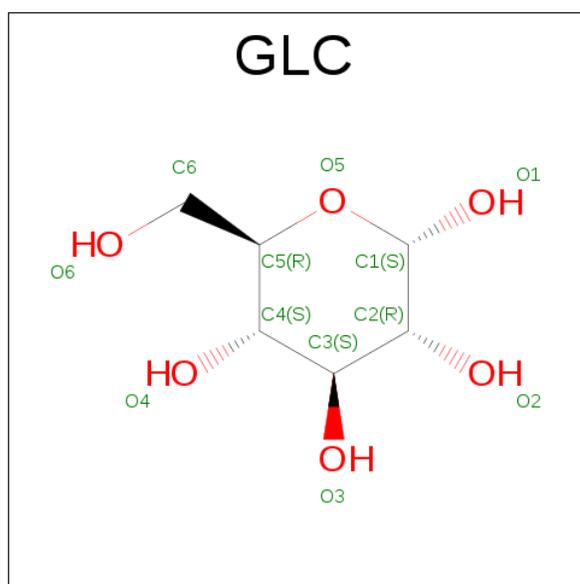
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			11	6	5		

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

• Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	258	Total 258	O 258	0	0
3	B	189	Total 189	O 189	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 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-1,4-glucan:maltose-1-phosphate maltosyltransferase 1
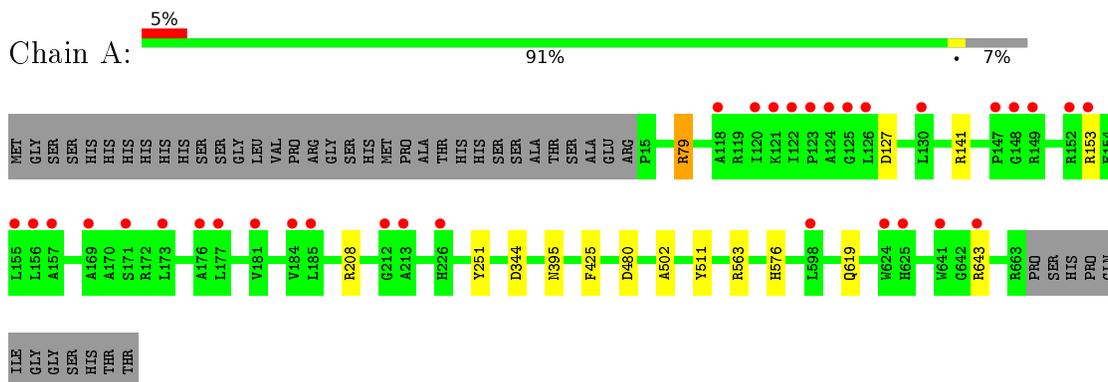
• Molecule 1: Alpha-1,4-glucan:maltose-1-phosphate maltosyltransferase 1
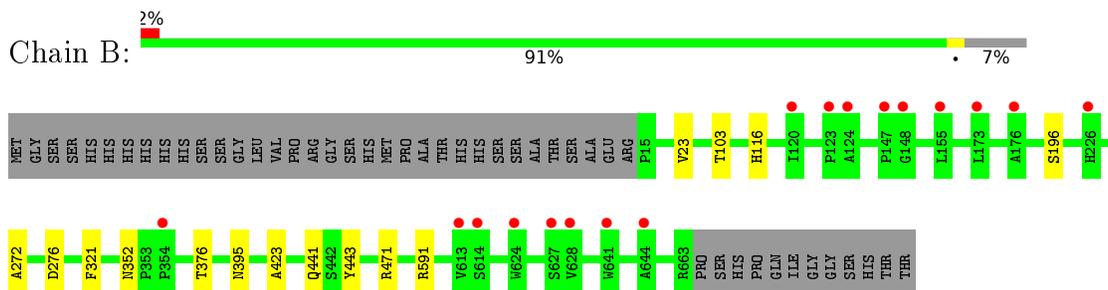
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	113.61Å 113.61Å 313.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.50 49.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.92-2.50) 100.0 (49.92-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.179 , 0.209 0.182 , 0.210	Depositor DCC
R_{free} test set	3560 reflections (5.20%)	DCC
Wilson B-factor (Å^2)	51.1	Xtriage
Anisotropy	0.331	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 35.0	EDS
L-test for twinning[2]	$< |L| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10941	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.74% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.52	0/5285	0.74	5/7232 (0.1%)
1	B	0.48	0/5255	0.71	1/7200 (0.0%)
All	All	0.50	0/10540	0.73	6/14432 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	344	ASP	CB-CG-OD1	6.36	124.02	118.30
1	A	208	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	471	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	344	ASP	CB-CG-OD2	-5.11	113.71	118.30
1	A	141	ARG	NE-CZ-NH1	5.03	122.81	120.30

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	5119	0	4946	4	0
1	B	5085	0	4864	5	0
2	A	145	0	123	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	145	0	123	2	0
3	A	258	0	0	0	0
3	B	189	0	0	0	0
All	All	10941	0	10056	10	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 0.

All (10) 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:B:272:ALA:HB1	1:B:276:ASP:HB2	1.89	0.52
2:A:711:GLC:O3	2:A:712:GLC:O2	2.13	0.46
1:A:395:ASN:ND2	2:A:707:GLC:O5	2.49	0.45
1:B:395:ASN:ND2	2:B:707:GLC:O5	2.49	0.45
1:A:576:HIS:CG	1:A:619:GLN:HG2	2.50	0.45
1:B:321:PHE:CZ	1:B:376:THR:HG23	2.52	0.44
1:B:395:ASN:ND2	2:B:706:GLC:O3	2.51	0.44
1:A:425:PHE:HB3	2:A:704:GLC:O6	2.18	0.44
1:A:502:ALA:HB1	1:A:563:ARG:HD2	1.99	0.43
1:B:423:ALA:HA	1:B:443:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	651/695 (94%)	642 (99%)	8 (1%)	1 (0%)	52	75
1	B	652/695 (94%)	634 (97%)	18 (3%)	0	100	100
All	All	1303/1390 (94%)	1276 (98%)	26 (2%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	ASP

5.3.2 Protein sidechains (i)

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	529/574 (92%)	523 (99%)	6 (1%)	80	94
1	B	523/574 (91%)	515 (98%)	8 (2%)	72	91
All	All	1052/1148 (92%)	1038 (99%)	14 (1%)	78	92

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	153	ARG
1	A	251	TYR
1	A	480	ASP
1	A	511	TYR
1	A	643	ARG
1	B	23	VAL
1	B	103	THR
1	B	116[A]	HIS
1	B	116[B]	HIS
1	B	196	SER
1	B	352	ASN
1	B	441	GLN
1	B	591	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	352	ASN
1	B	395	ASN
1	B	450	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)

26 ligands 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	701	2	12,12,12	0.30	0	17,17,17	0.38	0
2	GLC	A	702	2	11,11,12	0.26	0	15,15,17	0.61	0
2	GLC	A	703	2	11,11,12	0.30	0	15,15,17	0.61	0
2	GLC	A	704	2	11,11,12	0.38	0	15,15,17	0.74	0
2	GLC	A	705	2	11,11,12	0.30	0	15,15,17	0.49	0
2	GLC	A	706	2	11,11,12	0.43	0	15,15,17	0.78	0
2	GLC	A	707	2	11,11,12	0.30	0	15,15,17	1.22	2 (13%)
2	GLC	A	708	2	11,11,12	0.34	0	15,15,17	0.53	0
2	GLC	A	709	2	12,12,12	0.40	0	17,17,17	0.67	0
2	GLC	A	710	2	11,11,12	0.36	0	15,15,17	0.45	0
2	GLC	A	711	2	11,11,12	0.27	0	15,15,17	0.56	0
2	GLC	A	712	2	11,11,12	0.24	0	15,15,17	0.65	0
2	GLC	A	713	2	11,11,12	0.28	0	15,15,17	0.37	0
2	GLC	B	701	2	12,12,12	0.23	0	17,17,17	0.52	0
2	GLC	B	702	2	11,11,12	0.32	0	15,15,17	0.51	0
2	GLC	B	703	2	11,11,12	0.33	0	15,15,17	0.47	0
2	GLC	B	704	2	11,11,12	0.47	0	15,15,17	0.80	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	GLC	B	705	2	11,11,12	0.33	0	15,15,17	0.60	0
2	GLC	B	706	2	11,11,12	0.37	0	15,15,17	0.76	0
2	GLC	B	707	2	11,11,12	0.36	0	15,15,17	1.17	2 (13%)
2	GLC	B	708	2	11,11,12	0.31	0	15,15,17	0.46	0
2	GLC	B	709	2	12,12,12	0.32	0	17,17,17	0.56	0
2	GLC	B	710	2	11,11,12	0.32	0	15,15,17	0.43	0
2	GLC	B	711	2	11,11,12	0.24	0	15,15,17	0.41	0
2	GLC	B	712	2	11,11,12	0.29	0	15,15,17	0.57	0
2	GLC	B	713	2	11,11,12	0.24	0	15,15,17	0.48	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLC	A	701	2	-	0/2/22/22	0/1/1/1
2	GLC	A	702	2	-	0/2/19/22	0/1/1/1
2	GLC	A	703	2	-	0/2/19/22	0/1/1/1
2	GLC	A	704	2	-	0/2/19/22	0/1/1/1
2	GLC	A	705	2	-	0/2/19/22	0/1/1/1
2	GLC	A	706	2	-	0/2/19/22	0/1/1/1
2	GLC	A	707	2	-	0/2/19/22	0/1/1/1
2	GLC	A	708	2	-	0/2/19/22	0/1/1/1
2	GLC	A	709	2	-	0/2/22/22	0/1/1/1
2	GLC	A	710	2	-	0/2/19/22	0/1/1/1
2	GLC	A	711	2	-	0/2/19/22	0/1/1/1
2	GLC	A	712	2	-	0/2/19/22	0/1/1/1
2	GLC	A	713	2	-	0/2/19/22	0/1/1/1
2	GLC	B	701	2	-	0/2/22/22	0/1/1/1
2	GLC	B	702	2	-	0/2/19/22	0/1/1/1
2	GLC	B	703	2	-	0/2/19/22	0/1/1/1
2	GLC	B	704	2	-	0/2/19/22	0/1/1/1
2	GLC	B	705	2	-	0/2/19/22	0/1/1/1
2	GLC	B	706	2	-	0/2/19/22	0/1/1/1
2	GLC	B	707	2	-	0/2/19/22	0/1/1/1
2	GLC	B	708	2	-	0/2/19/22	0/1/1/1
2	GLC	B	709	2	-	0/2/22/22	0/1/1/1
2	GLC	B	710	2	-	0/2/19/22	0/1/1/1
2	GLC	B	711	2	-	0/2/19/22	0/1/1/1
2	GLC	B	712	2	-	0/2/19/22	0/1/1/1
2	GLC	B	713	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	707	GLC	O5-C1-C2	-2.25	107.29	110.89
2	B	707	GLC	O5-C1-C2	-2.10	107.54	110.89
2	B	704	GLC	C1-C2-C3	2.23	112.25	109.55
2	A	707	GLC	O5-C5-C4	2.82	114.81	110.13
2	B	707	GLC	O5-C5-C4	2.93	114.98	110.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	704	GLC	1	0
2	A	707	GLC	1	0
2	A	711	GLC	1	0
2	A	712	GLC	1	0
2	B	706	GLC	1	0
2	B	707	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, 95th 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	649/695 (93%)	-0.03	33 (5%)	32	36	38, 56, 114, 132	0
1	B	649/695 (93%)	-0.12	17 (2%)	59	63	39, 66, 108, 141	0
All	All	1298/1390 (93%)	-0.07	50 (3%)	43	48	38, 61, 110, 141	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	176	ALA	7.2
1	B	155	LEU	5.2
1	A	155	LEU	4.8
1	A	122	ILE	4.5
1	A	177	LEU	4.3
1	A	185	LEU	4.2
1	A	153	ARG	4.2
1	A	173	LEU	4.1
1	B	644	ALA	4.1
1	B	624	TRP	3.8
1	A	148	GLY	3.7
1	B	123	PRO	3.7
1	A	149	ARG	3.6
1	A	181	VAL	3.6
1	A	157	ALA	3.5
1	A	123	PRO	3.4
1	A	641	TRP	3.3
1	A	147	PRO	3.2
1	B	148	GLY	3.1
1	B	628	VAL	3.1
1	A	184	VAL	3.0
1	A	124	ALA	3.0
1	B	124	ALA	3.0
1	A	125	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	152	ARG	2.9
1	A	121	LYS	2.9
1	B	176	ALA	2.9
1	A	120	ILE	2.8
1	A	625	HIS	2.8
1	B	173	LEU	2.8
1	B	613	VAL	2.7
1	B	641	TRP	2.6
1	B	147	PRO	2.6
1	A	171	SER	2.6
1	A	118	ALA	2.5
1	B	354	PRO	2.5
1	A	212	GLY	2.5
1	A	213	ALA	2.5
1	B	226	HIS	2.4
1	A	156	LEU	2.4
1	A	169	ALA	2.4
1	A	598	LEU	2.2
1	A	126	LEU	2.2
1	A	226[A]	HIS	2.1
1	A	624	TRP	2.1
1	A	643	ARG	2.1
1	B	614	SER	2.1
1	B	120	ILE	2.0
1	B	627	SER	2.0
1	A	130	LEU	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, 95th 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	A	709	12/12	0.89	0.23	1.50	70,79,97,98	0
2	GLC	B	705	11/12	0.91	0.22	0.83	81,86,96,99	0
2	GLC	A	705	11/12	0.92	0.16	0.48	64,78,87,90	0
2	GLC	A	707	11/12	0.95	0.14	-0.08	66,74,80,87	0
2	GLC	A	708	11/12	0.97	0.13	-0.16	47,53,57,60	0
2	GLC	A	706	11/12	0.93	0.14	-0.30	74,79,91,97	0
2	GLC	A	713	11/12	0.91	0.16	-0.42	72,86,106,112	0
2	GLC	B	713	11/12	0.91	0.17	-0.57	98,118,125,130	0
2	GLC	B	707	11/12	0.91	0.13	-0.61	68,83,100,102	0
2	GLC	A	703	11/12	0.96	0.12	-0.80	64,74,81,86	0
2	GLC	B	703	11/12	0.93	0.12	-1.00	74,81,90,102	0
2	GLC	B	708	11/12	0.98	0.08	-1.21	59,67,74,74	0
2	GLC	B	706	11/12	0.93	0.10	-1.62	81,90,96,97	0
2	GLC	B	702	11/12	0.93	0.17	-	89,104,112,116	0
2	GLC	B	709	12/12	0.89	0.30	-	92,106,124,135	0
2	GLC	A	712	11/12	0.94	0.15	-	73,97,108,112	0
2	GLC	A	701	12/12	0.85	0.24	-	89,108,115,119	0
2	GLC	B	704	11/12	0.94	0.16	-	81,86,93,96	0
2	GLC	A	704	11/12	0.95	0.14	-	61,68,76,81	0
2	GLC	B	701	12/12	0.87	0.33	-	108,125,131,136	0
2	GLC	B	712	11/12	0.89	0.35	-	113,127,132,132	0
2	GLC	A	711	11/12	0.94	0.10	-	74,80,90,91	0
2	GLC	A	710	11/12	0.89	0.26	-	79,87,91,96	0
2	GLC	A	702	11/12	0.86	0.18	-	88,98,115,117	0
2	GLC	B	711	11/12	0.87	0.24	-	106,113,127,133	0
2	GLC	B	710	11/12	0.86	0.28	-	106,121,131,136	0

6.5 Other polymers (i)

There are no such residues in this entry.