



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 9, 2017 – 11:50 AM EST

PDB ID : 5JBE
Title : 4,6-alpha-glucanotransferase GTFB from *Lactobacillus reuteri* 121 complexed with an isomalto-maltopentasaccharide
Authors : Pijning, T.; Dijkstra, B.W.; Bai, Y.; Gangoiti-Munecas, J.; Dijkhuizen, L.
Deposited on : 2016-04-13
Resolution : 2.10 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-20028442
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-20028442

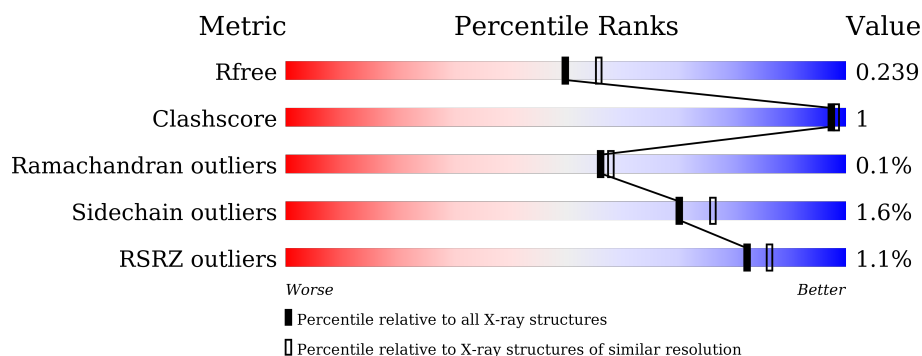
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 $\leq 5\%$. 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	854	<div> <div></div> <div>96%</div> <div>.</div> </div>
1	B	854	<div> <div></div> <div>95%</div> <div>5%</div> </div>

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
6	GLC	A	1712	-	-	-	X
6	GLC	B	1708	-	-	-	X
6	GLC	B	1711	-	-	-	X
6	GLC	B	1712	-	-	-	X
7	MAL	B	1707	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14172 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 Inactive glucansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	854	Total	C	N	O	S	0	0	0
			6678	4151	1146	1355	26			
1	B	854	Total	C	N	O	S	0	0	0
			6678	4151	1146	1355	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	761	MET	-	initiating methionine	UNP Q5SBM0
B	761	MET	-	initiating methionine	UNP Q5SBM0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

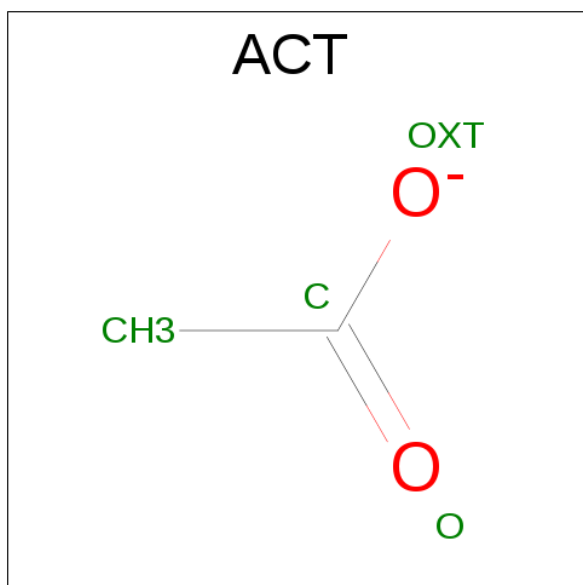
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



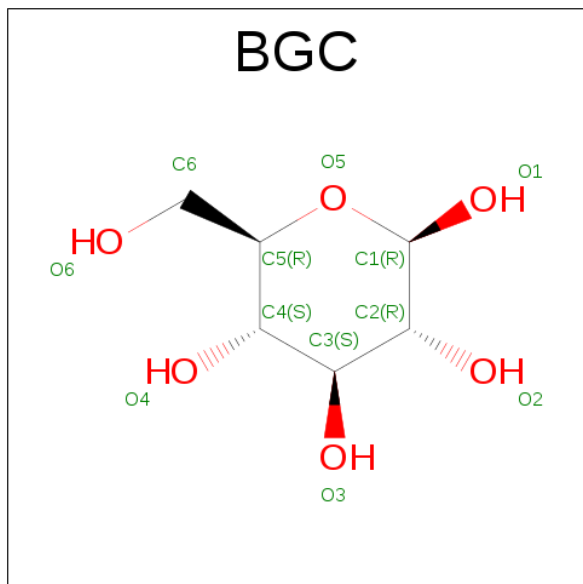
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



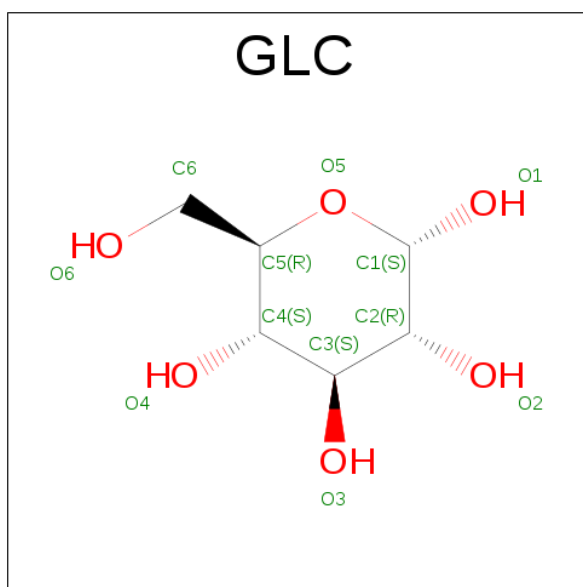
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is BETA-D-GLUCOSE (three-letter code: BGC) (formula: $C_6H_{12}O_6$).



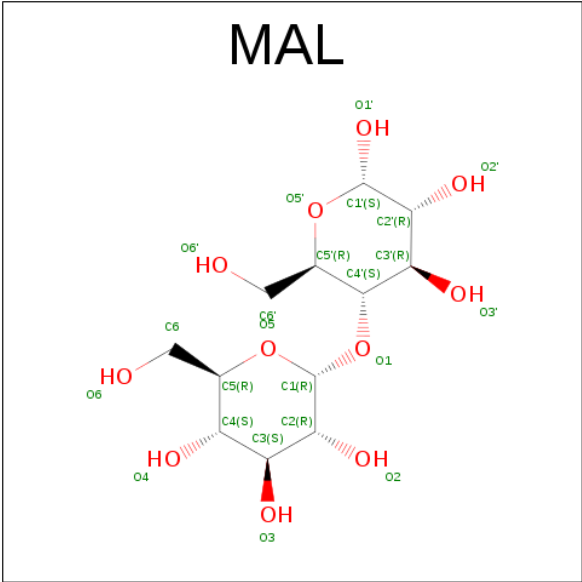
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			12	6	6		

- Molecule 6 is ALPHA-D-GLUCOSE (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



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

- Molecule 7 is MALTOSE (three-letter code: MAL) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			23	12	11		

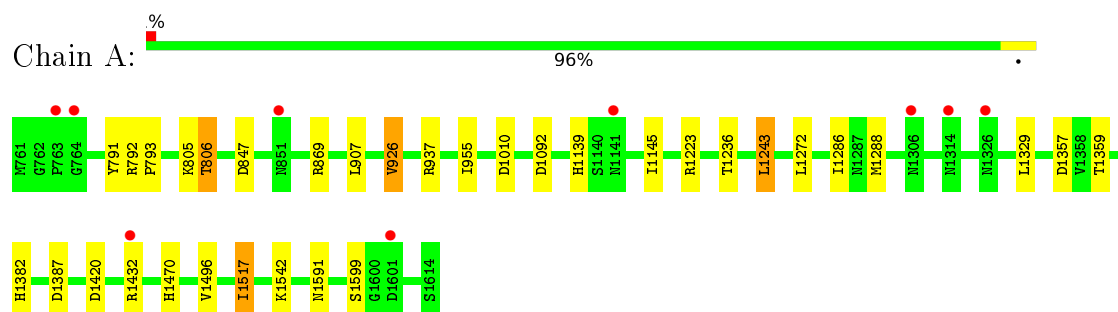
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	312	Total	O	0	0
			312	312		
8	B	311	Total	O	0	0
			311	311		

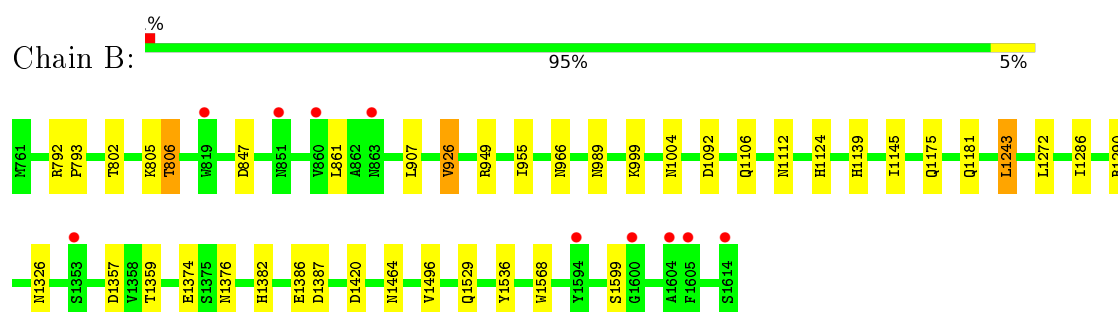
3 Residue-property plots [i](#)

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: Inactive glucansucrase



- Molecule 1: Inactive glucansucrase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.44Å 58.32Å 151.41Å 90.00° 114.25° 90.00°	Depositor
Resolution (Å)	46.16 – 2.10 46.16 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.16-2.10) 99.2 (46.16-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.238 0.208 , 0.239	Depositor DCC
R_{free} test set	5150 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	1.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14172	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, CA, GLC, SO4, ACT, MAL

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	0.50	0/6815	0.66	3/9268 (0.0%)
1	B	0.51	0/6815	0.66	2/9268 (0.0%)
All	All	0.51	0/13630	0.66	5/18536 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1517	ILE	CG1-CB-CG2	-6.23	97.70	111.40
1	A	1432	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	1243	LEU	CA-CB-CG	5.11	127.04	115.30
1	B	1243	LEU	CA-CB-CG	5.07	126.95	115.30
1	B	949	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	6678	0	6329	14	0
1	B	6678	0	6329	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	A	8	0	6	0	0
4	B	16	0	12	0	0
5	A	12	0	12	0	0
6	A	56	0	48	0	0
6	B	56	0	48	0	0
7	B	23	0	22	0	0
8	A	312	0	0	2	0
8	B	311	0	0	0	0
All	All	14172	0	12806	31	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 1.

All (31) 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:A:1357:ASP:OD1	1:A:1359:THR:HG23	1.79	0.82
1:B:1357:ASP:OD1	1:B:1359:THR:HG23	1.81	0.80
1:B:989:ASN:HD21	1:B:1536:TYR:H	1.38	0.71
1:A:792:ARG:HE	1:A:806:THR:CG2	2.10	0.65
1:B:792:ARG:HE	1:B:806:THR:CG2	2.11	0.63
1:B:1124:HIS:HD2	1:B:1386:GLU:OE2	1.82	0.61
1:B:1112:ASN:HD21	1:B:1376:ASN:HD22	1.46	0.61
1:A:937:ARG:NH1	1:A:1591:ASN:O	2.38	0.57
1:A:869:ARG:NH2	8:A:1802:HOH:O	2.38	0.57
1:A:1272:LEU:HD11	1:A:1286:ILE:HD11	1.88	0.54
1:B:1272:LEU:HD21	1:B:1286:ILE:HD11	1.90	0.54
1:B:1004:ASN:HD22	1:B:1464:ASN:HD22	1.57	0.53
1:B:1124:HIS:CD2	1:B:1386:GLU:OE2	2.62	0.52
1:B:1112:ASN:HD22	1:B:1374:GLU:HB3	1.76	0.50
1:A:1010:ASP:OD2	1:A:1470:HIS:HE1	1.96	0.48
1:A:1223:ARG:NH2	8:A:1804:HOH:O	2.46	0.47
1:B:1112:ASN:ND2	1:B:1374:GLU:HB3	2.30	0.47
1:A:1288:MET:HE2	1:A:1329:LEU:HB3	1.97	0.46
1:B:1139:HIS:HB2	1:B:1145:ILE:CD1	2.46	0.45
1:A:926:VAL:HG13	1:A:1496:VAL:HB	1.99	0.45
1:A:1139:HIS:HB2	1:A:1145:ILE:CD1	2.48	0.44
1:B:926:VAL:HG13	1:B:1496:VAL:HB	2.00	0.43
1:A:1236:THR:CG2	1:B:966:ASN:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:793:PRO:O	1:B:806:THR:HG21	2.19	0.43
1:A:793:PRO:O	1:A:806:THR:HG21	2.19	0.42
1:B:1290:ARG:HH12	1:B:1326:ASN:HD22	1.67	0.42
1:B:1175:GLN:HE21	1:B:1181:GLN:HE22	1.68	0.41
1:A:1092:ASP:OD2	1:B:1092:ASP:OD2	2.39	0.41
1:B:1529:GLN:NE2	1:B:1568:TRP:HE1	2.19	0.41
1:A:1382:HIS:HD2	1:A:1420:ASP:OD2	2.04	0.41
1:B:1382:HIS:HD2	1:B:1420:ASP:OD2	2.03	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	852/854 (100%)	831 (98%)	20 (2%)	1 (0%)	56	58
1	B	852/854 (100%)	831 (98%)	20 (2%)	1 (0%)	56	58
All	All	1704/1708 (100%)	1662 (98%)	40 (2%)	2 (0%)	56	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	955	ILE
1	B	955	ILE

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	720/720 (100%)	709 (98%)	11 (2%)	72	78
1	B	720/720 (100%)	708 (98%)	12 (2%)	68	74
All	All	1440/1440 (100%)	1417 (98%)	23 (2%)	70	76

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	791	TYR
1	A	805	LYS
1	A	806	THR
1	A	847	ASP
1	A	907	LEU
1	A	926	VAL
1	A	1243	LEU
1	A	1387	ASP
1	A	1517	ILE
1	A	1542	LYS
1	A	1599	SER
1	B	802	THR
1	B	805	LYS
1	B	806	THR
1	B	847	ASP
1	B	861	LEU
1	B	907	LEU
1	B	926	VAL
1	B	999	LYS
1	B	1106	GLN
1	B	1243	LEU
1	B	1387	ASP
1	B	1599	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	825	GLN
1	A	867	ASN
1	A	947	ASN
1	A	1107	ASN
1	A	1382	HIS

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Mol	Chain	Res	Type
1	A	1470	HIS
1	A	1606	ASN
1	B	867	ASN
1	B	952	ASN
1	B	956	ASN
1	B	974	ASN
1	B	989	ASN
1	B	1043	GLN
1	B	1056	HIS
1	B	1068	ASN
1	B	1106	GLN
1	B	1112	ASN
1	B	1117	ASN
1	B	1124	HIS
1	B	1175	GLN
1	B	1177	ASN
1	B	1256	ASN
1	B	1282	GLN
1	B	1326	ASN
1	B	1382	HIS
1	B	1404	ASN
1	B	1464	ASN
1	B	1529	GLN
1	B	1543	ASN
1	B	1606	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 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	$\# Z > 2$
3	SO4	A	1702	-	4,4,4	0.34	0	6,6,6	0.26	0
3	SO4	A	1703	-	4,4,4	0.31	0	6,6,6	0.19	0
3	SO4	A	1704	-	4,4,4	0.36	0	6,6,6	0.10	0
4	ACT	A	1705	-	0,3,3	0.00	-	0,3,3	0.00	-
4	ACT	A	1706	-	0,3,3	0.00	-	0,3,3	0.00	-
5	BGC	A	1707	-	12,12,12	0.61	0	17,17,17	0.88	1 (5%)
6	GLC	A	1708	6	11,11,12	1.00	1 (9%)	15,15,17	0.89	0
6	GLC	A	1709	6	11,11,12	0.89	0	15,15,17	0.79	0
6	GLC	A	1710	6	11,11,12	0.95	0	15,15,17	0.73	0
6	GLC	A	1711	6	12,12,12	0.91	0	17,17,17	0.74	0
6	GLC	A	1712	6	11,11,12	0.64	0	15,15,17	0.94	1 (6%)
3	SO4	B	1702	-	4,4,4	0.25	0	6,6,6	0.23	0
4	ACT	B	1703	-	0,3,3	0.00	-	0,3,3	0.00	-
4	ACT	B	1704	-	0,3,3	0.00	-	0,3,3	0.00	-
4	ACT	B	1705	-	0,3,3	0.00	-	0,3,3	0.00	-
4	ACT	B	1706	-	0,3,3	0.00	-	0,3,3	0.00	-
7	MAL	B	1707	-	24,24,24	0.52	0	35,35,35	0.76	1 (2%)
6	GLC	B	1708	6	11,11,12	1.22	1 (9%)	15,15,17	1.14	1 (6%)
6	GLC	B	1709	6	11,11,12	0.70	0	15,15,17	0.66	0
6	GLC	B	1710	6	11,11,12	0.91	0	15,15,17	0.66	0
6	GLC	B	1711	6	12,12,12	0.85	0	17,17,17	0.63	0
6	GLC	B	1712	6	11,11,12	0.76	0	15,15,17	1.10	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
3	SO4	A	1702	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1703	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1704	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1705	-	-	0/0/0/0	0/0/0/0
4	ACT	A	1706	-	-	0/0/0/0	0/0/0/0
5	BGC	A	1707	-	-	0/2/22/22	0/1/1/1
6	GLC	A	1708	6	-	0/2/19/22	0/1/1/1
6	GLC	A	1709	6	-	0/2/19/22	0/1/1/1
6	GLC	A	1710	6	-	0/2/19/22	0/1/1/1
6	GLC	A	1711	6	-	0/2/22/22	0/1/1/1
6	GLC	A	1712	6	-	0/2/19/22	0/1/1/1
3	SO4	B	1702	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1703	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1704	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1705	-	-	0/0/0/0	0/0/0/0
4	ACT	B	1706	-	-	0/0/0/0	0/0/0/0
7	MAL	B	1707	-	-	0/8/48/48	0/2/2/2
6	GLC	B	1708	6	-	0/2/19/22	0/1/1/1
6	GLC	B	1709	6	-	0/2/19/22	0/1/1/1
6	GLC	B	1710	6	-	0/2/19/22	0/1/1/1
6	GLC	B	1711	6	-	0/2/22/22	0/1/1/1
6	GLC	B	1712	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1708	GLC	O5-C1	2.08	1.47	1.43
6	B	1708	GLC	O5-C1	3.03	1.48	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1707	BGC	C4-C3-C2	-2.04	107.04	110.79
6	A	1712	GLC	C1-C2-C3	2.09	112.08	109.55
7	B	1707	MAL	C1-C2-C3	2.28	114.51	109.98
6	B	1708	GLC	C1-O5-C5	2.88	116.38	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	854/854 (100%)	0.01	9 (1%) 82 86	25, 37, 55, 75	0
1	B	854/854 (100%)	0.01	10 (1%) 81 85	27, 38, 56, 81	0
All	All	1708/1708 (100%)	0.01	19 (1%) 82 86	25, 37, 56, 81	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1614	SER	3.0
1	B	851	ASN	2.9
1	B	1353	SER	2.8
1	A	851	ASN	2.8
1	A	1326	ASN	2.8
1	B	1605	PHE	2.8
1	B	1594	TYR	2.5
1	A	763	PRO	2.4
1	B	1600	GLY	2.4
1	A	1306	ASN	2.3
1	B	863	ASN	2.3
1	B	819	TRP	2.2
1	A	1432	ARG	2.2
1	A	1314	ASN	2.2
1	A	1141	ASN	2.1
1	A	764	GLY	2.1
1	B	1604	ALA	2.1
1	A	1601	ASP	2.0
1	B	860	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 ⓘ

There are no carbohydrates in this entry.

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, 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
7	MAL	B	1707	23/23	0.85	0.23	3.67	50,55,59,60	0
6	GLC	B	1708	11/12	0.76	0.16	3.04	50,54,65,74	0
6	GLC	B	1712	11/12	0.67	0.28	2.32	70,77,88,90	0
6	GLC	B	1711	12/12	0.85	0.20	2.24	43,44,47,49	0
6	GLC	A	1712	11/12	0.86	0.29	2.16	65,69,76,79	0
4	ACT	B	1704	4/4	0.82	0.15	1.31	46,47,48,51	0
6	GLC	A	1711	12/12	0.88	0.14	1.30	35,38,39,39	0
5	BGC	A	1707	12/12	0.53	0.19	1.01	53,60,61,63	0
6	GLC	A	1708	11/12	0.72	0.15	0.69	51,54,60,66	0
6	GLC	B	1709	11/12	0.85	0.15	0.44	51,53,58,61	0
6	GLC	B	1710	11/12	0.87	0.14	-0.16	39,45,49,50	0
6	GLC	A	1709	11/12	0.90	0.11	-0.32	43,47,51,52	0
2	CA	A	1701	1/1	0.96	0.13	-0.33	25,25,25,25	0
6	GLC	A	1710	11/12	0.91	0.11	-0.37	40,42,43,44	0
2	CA	B	1701	1/1	0.96	0.11	-0.67	32,32,32,32	0
3	SO4	A	1703	5/5	0.93	0.11	-0.83	65,66,66,66	0
4	ACT	B	1706	4/4	0.82	0.23	-	53,57,58,58	0
4	ACT	B	1703	4/4	0.92	0.14	-	41,41,43,43	0
4	ACT	A	1706	4/4	0.93	0.17	-	50,52,53,55	0
3	SO4	B	1702	5/5	0.93	0.17	-	57,62,64,67	0
4	ACT	A	1705	4/4	0.96	0.10	-	32,32,33,35	0
3	SO4	A	1704	5/5	0.89	0.16	-	86,88,89,89	0
3	SO4	A	1702	5/5	0.88	0.15	-	46,52,55,55	0
4	ACT	B	1705	4/4	0.76	0.20	-	59,61,62,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.