



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:57 PM UTC

PDB ID : 4JAW / pdb_00004jaw
Title : Crystal Structure of Lacto-N-Biosidase from Bifidobacterium bifidum complexed with LNB-thiazoline
Authors : Ito, T.; Katayama, T.; Stubbs, K.A.; Fushinobu, S.
Deposited on : 2013-02-19
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

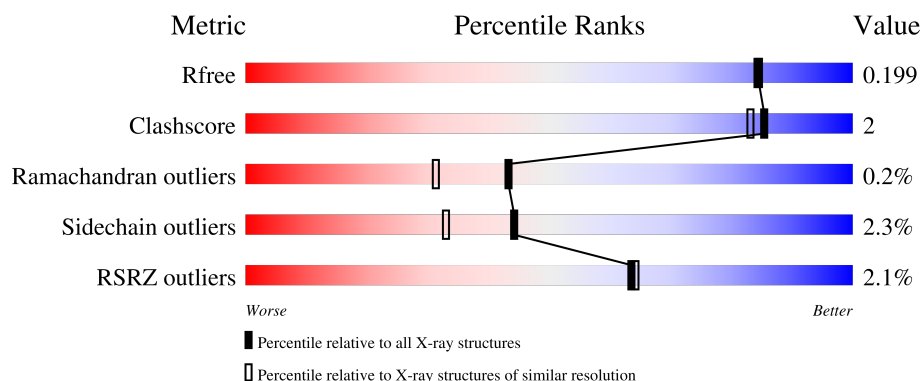
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	644	2% 86% 11% ..
1	B	644	2% 86% 10% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10420 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 Lacto-N-biosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			4969	3132	846	974	17			
1	B	632	Total	C	N	O	S	0	0	0
			4963	3129	845	972	17			

There are 42 discrepancies between the modelled and reference sequences:

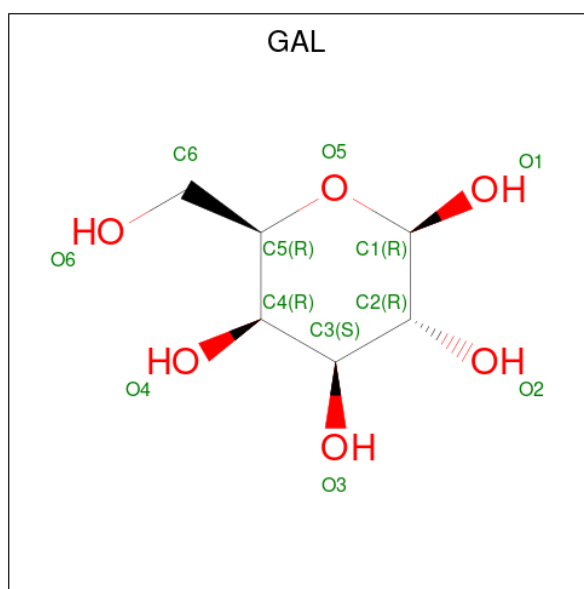
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP B3TLD6
A	21	GLY	-	expression tag	UNP B3TLD6
A	22	SER	-	expression tag	UNP B3TLD6
A	23	SER	-	expression tag	UNP B3TLD6
A	24	HIS	-	expression tag	UNP B3TLD6
A	25	HIS	-	expression tag	UNP B3TLD6
A	26	HIS	-	expression tag	UNP B3TLD6
A	27	HIS	-	expression tag	UNP B3TLD6
A	28	HIS	-	expression tag	UNP B3TLD6
A	29	HIS	-	expression tag	UNP B3TLD6
A	30	SER	-	expression tag	UNP B3TLD6
A	31	SER	-	expression tag	UNP B3TLD6
A	32	GLY	-	expression tag	UNP B3TLD6
A	33	LEU	-	expression tag	UNP B3TLD6
A	34	VAL	-	expression tag	UNP B3TLD6
A	35	PRO	-	expression tag	UNP B3TLD6
A	36	ARG	-	expression tag	UNP B3TLD6
A	37	GLY	-	expression tag	UNP B3TLD6
A	38	SER	-	expression tag	UNP B3TLD6
A	39	HIS	-	expression tag	UNP B3TLD6
A	40	MET	-	expression tag	UNP B3TLD6
B	20	MET	-	expression tag	UNP B3TLD6
B	21	GLY	-	expression tag	UNP B3TLD6
B	22	SER	-	expression tag	UNP B3TLD6
B	23	SER	-	expression tag	UNP B3TLD6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	24	HIS	-	expression tag	UNP B3TLD6
B	25	HIS	-	expression tag	UNP B3TLD6
B	26	HIS	-	expression tag	UNP B3TLD6
B	27	HIS	-	expression tag	UNP B3TLD6
B	28	HIS	-	expression tag	UNP B3TLD6
B	29	HIS	-	expression tag	UNP B3TLD6
B	30	SER	-	expression tag	UNP B3TLD6
B	31	SER	-	expression tag	UNP B3TLD6
B	32	GLY	-	expression tag	UNP B3TLD6
B	33	LEU	-	expression tag	UNP B3TLD6
B	34	VAL	-	expression tag	UNP B3TLD6
B	35	PRO	-	expression tag	UNP B3TLD6
B	36	ARG	-	expression tag	UNP B3TLD6
B	37	GLY	-	expression tag	UNP B3TLD6
B	38	SER	-	expression tag	UNP B3TLD6
B	39	HIS	-	expression tag	UNP B3TLD6
B	40	MET	-	expression tag	UNP B3TLD6

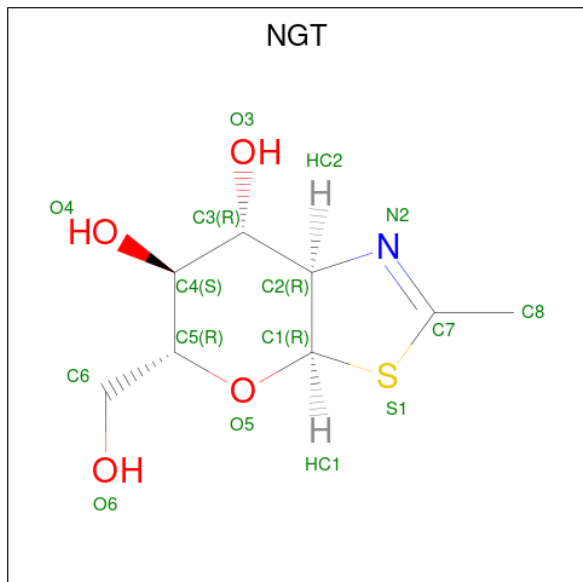
- Molecule 2 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



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

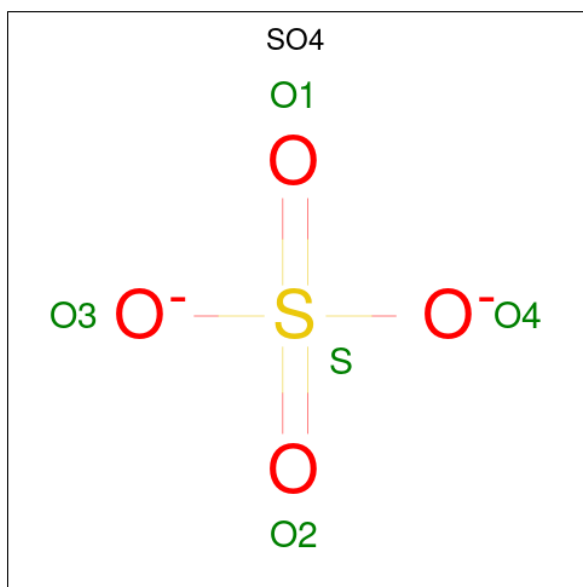
- Molecule 3 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TE

TRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (CCD ID: NGT) (formula: $C_8H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

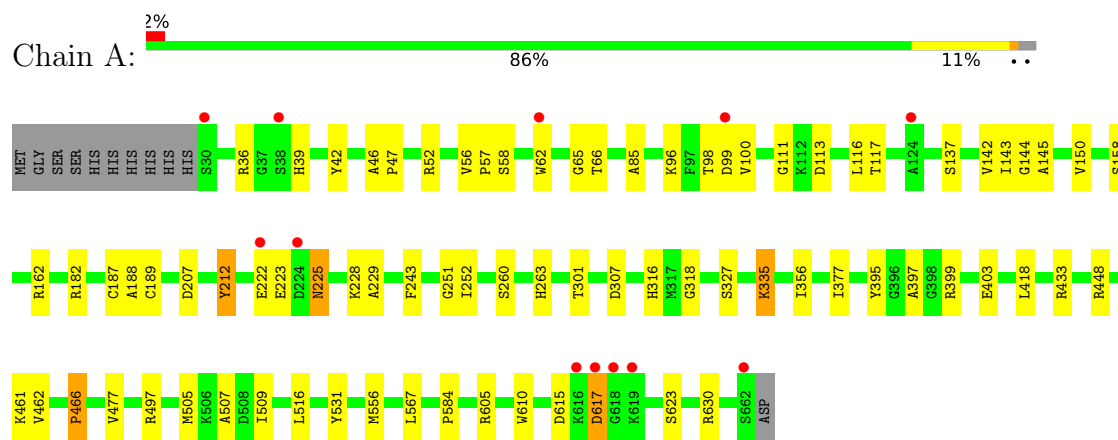
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	197	Total O 197 197	0	0
5	B	206	Total O 206 206	0	0

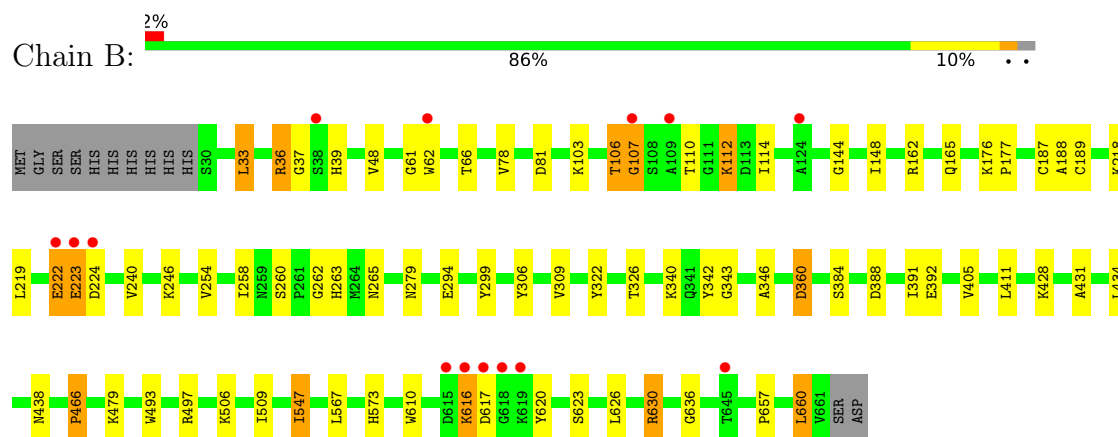
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Lacto-N-biosidase



• Molecule 1: Lacto-N-biosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	116.52Å 131.56Å 104.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.61 – 1.80 43.61 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.61-1.80) 100.0 (43.61-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.62 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.182 , 0.213 (Not available) , 0.199	Depositor DCC
R_{free} test set	7499 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10420	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.63% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GAL, NGT

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	1.63	32/5078 (0.6%)	1.37	13/6891 (0.2%)
1	B	1.68	38/5072 (0.7%)	1.40	22/6883 (0.3%)
All	All	1.65	70/10150 (0.7%)	1.39	35/13774 (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	B	0	1

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	497	ARG	CZ-NH2	8.93	1.45	1.33
1	A	46	ALA	C-O	-8.82	1.14	1.24
1	B	263	HIS	CE1-NE2	7.80	1.40	1.32
1	B	144	GLY	CA-C	7.76	1.58	1.52
1	A	316	HIS	CE1-NE2	7.25	1.39	1.32

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	GLY	N-CA-C	-8.55	100.79	112.25
1	A	52	ARG	NE-CZ-NH1	8.18	129.68	121.50
1	B	224	ASP	N-CA-C	7.88	120.56	111.11
1	B	222	GLU	N-CA-C	-7.78	104.68	114.56
1	B	636	GLY	N-CA-C	-7.38	105.13	115.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	106	THR	Peptide

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	4969	0	4843	24	0
1	B	4963	0	4838	20	0
2	A	11	0	10	0	0
2	B	11	0	10	0	0
3	A	14	0	12	0	0
3	B	14	0	12	0	0
4	A	20	0	0	0	0
4	B	15	0	0	0	0
5	A	197	0	0	1	0
5	B	206	0	0	2	0
All	All	10420	0	9725	43	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 2.

The worst 5 of 43 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:615:ASP:O	1:A:617:ASP:HA	1.61	0.98
1:B:33:LEU:C	1:B:33:LEU:HD23	2.12	0.74
1:A:117:THR:HB	1:A:143:ILE:HD12	1.71	0.72
1:A:98:THR:O	1:A:99:ASP:HB2	1.93	0.68
1:A:117:THR:HB	1:A:143:ILE:CD1	2.27	0.65

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	631/644 (98%)	615 (98%)	15 (2%)	1 (0%)	43	31
1	B	630/644 (98%)	619 (98%)	9 (1%)	2 (0%)	36	25
All	All	1261/1288 (98%)	1234 (98%)	24 (2%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	617	ASP
1	A	466	PRO
1	B	466	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	530/540 (98%)	520 (98%)	10 (2%)	50	41
1	B	529/540 (98%)	515 (97%)	14 (3%)	40	28
All	All	1059/1080 (98%)	1035 (98%)	24 (2%)	44	33

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	112	LYS
1	B	294	GLU
1	B	223	GLU

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Mol	Chain	Res	Type
1	B	340	LYS
1	A	335	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	406	GLN
1	B	192	ASN
1	A	555	GLN
1	A	438	ASN
1	B	134	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	$\# Z > 2$
3	NGT	B	702	2	13,15,15	3.45	4 (30%)	14,22,22	1.90	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	B	701	3	11,11,12	1.49	2 (18%)	15,15,17	1.12	0
4	SO4	A	705	-	4,4,4	0.94	0	6,6,6	0.83	0
4	SO4	A	706	-	4,4,4	1.02	0	6,6,6	0.54	0
4	SO4	B	705	-	4,4,4	0.66	0	6,6,6	0.60	0
2	GAL	A	701	3	11,11,12	1.12	1 (9%)	15,15,17	1.32	2 (13%)
4	SO4	B	704	-	4,4,4	0.89	0	6,6,6	0.98	0
4	SO4	B	703	-	4,4,4	0.41	0	6,6,6	0.60	0
4	SO4	A	704	-	4,4,4	0.56	0	6,6,6	1.98	2 (33%)
4	SO4	A	703	-	4,4,4	0.51	0	6,6,6	0.82	0
3	NGT	A	702	2	13,15,15	2.35	1 (7%)	14,22,22	2.13	6 (42%)

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	GAL	A	701	3	-	0/2/19/22	0/1/1/1
3	NGT	B	702	2	-	1/2/30/30	0/2/2/2
2	GAL	B	701	3	-	0/2/19/22	0/1/1/1
3	NGT	A	702	2	-	0/2/30/30	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NGT	C7-S1	-10.85	1.68	1.77
3	A	702	NGT	C7-S1	-8.33	1.70	1.77
3	B	702	NGT	O5-C1	3.58	1.48	1.42
3	B	702	NGT	C7-N2	3.50	1.30	1.27
2	B	701	GAL	C4-C5	2.53	1.58	1.53

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NGT	C3-C2-N2	-4.67	104.03	110.56
3	B	702	NGT	C3-C4-C5	-3.71	103.50	110.23
2	A	701	GAL	O2-C2-C3	-3.37	103.17	110.15
3	A	702	NGT	O3-C3-C2	-3.15	102.26	109.16
3	A	702	NGT	C8-C7-S1	2.97	123.43	118.96

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	NGT	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	633/644 (98%)	-0.44	12 (1%) 66 66	4, 10, 23, 68	0
1	B	632/644 (98%)	-0.43	14 (2%) 62 62	4, 9, 24, 70	0
All	All	1265/1288 (98%)	-0.44	26 (2%) 63 64	4, 10, 24, 70	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	616	LYS	7.0
1	B	616	LYS	5.9
1	B	107	GLY	5.2
1	B	617	ASP	4.6
1	A	224	ASP	4.1

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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	704	5/5	0.89	0.17	33,37,38,40	0
4	SO4	A	705	5/5	0.92	0.13	33,36,42,43	0
2	GAL	A	701	11/12	0.95	0.08	10,11,12,12	0
2	GAL	B	701	11/12	0.97	0.06	8,9,10,10	0
4	SO4	A	706	5/5	0.97	0.15	21,23,24,30	0
4	SO4	A	704	5/5	0.97	0.10	20,26,27,29	0
3	NGT	A	702	14/14	0.98	0.05	9,11,12,13	0
3	NGT	B	702	14/14	0.98	0.06	7,9,10,10	0
4	SO4	B	705	5/5	0.98	0.08	16,20,22,25	0
4	SO4	A	703	5/5	0.99	0.05	8,9,10,11	0
4	SO4	B	703	5/5	0.99	0.03	6,7,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.