



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:02 PM GMT

PDB ID : 5BXR
Title : LNBase in complex with LNB-NHAcDNJ
Authors : Ito, T.; Arakawa, T.; Fushinobu, S.
Deposited on : 2015-06-09
Resolution : 1.60 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
<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-20026982
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-20026982

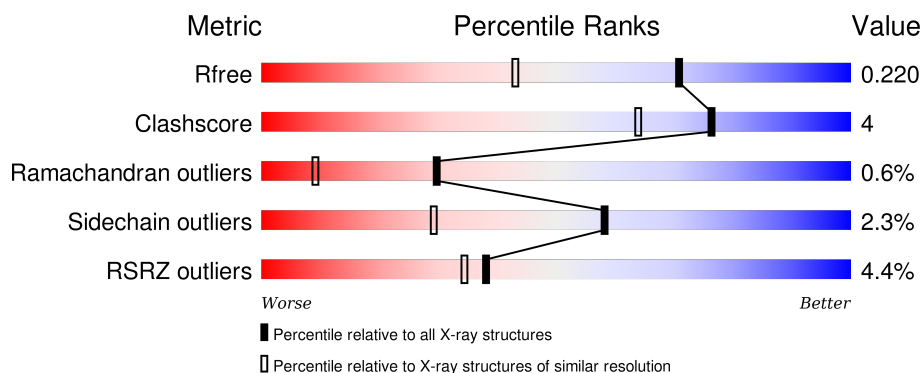
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	644	<div> <div>4%</div> <div>84%</div> <div>12%</div> <div>••</div> </div>
1	B	644	<div> <div>5%</div> <div>87%</div> <div>10%</div> <div>••</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
4	SO4	B	704	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10996 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	634	Total	C	N	O	S	0	0	0
			4977	3136	847	977	17			
1	B	636	Total	C	N	O	S	0	0	0
			4997	3148	853	979	17			

There are 42 discrepancies between the modelled and reference sequences:

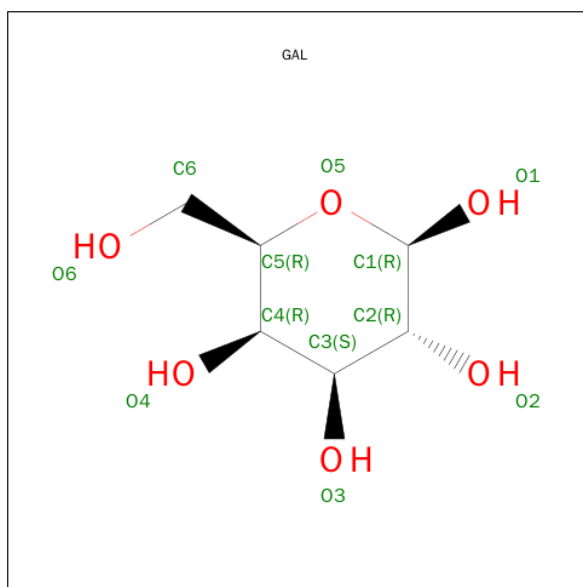
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP B3TLD6
A	21	GLY	-	expression tag	UNP B3TLD6
A	22	SER	-	expression tag	UNP B3TLD6
A	23	SER	-	expression tag	UNP B3TLD6
A	24	HIS	-	expression tag	UNP B3TLD6
A	25	HIS	-	expression tag	UNP B3TLD6
A	26	HIS	-	expression tag	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	-	initiating methionine	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

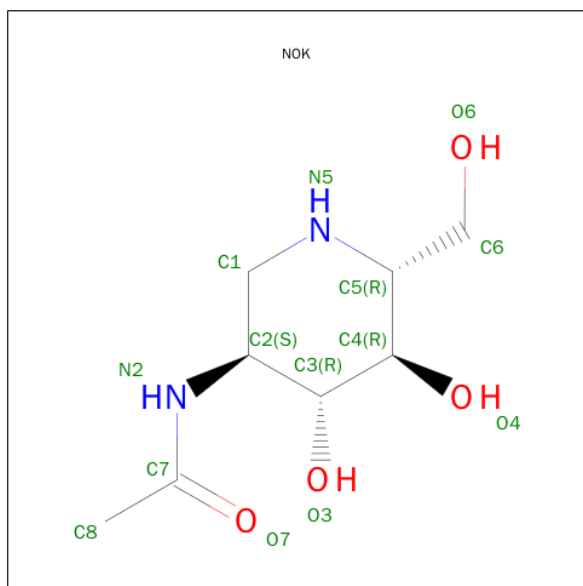
- Molecule 2 is BETA-D-GALACTOSE (three-letter code: GAL) (formula: C₆H₁₂O₆).



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		

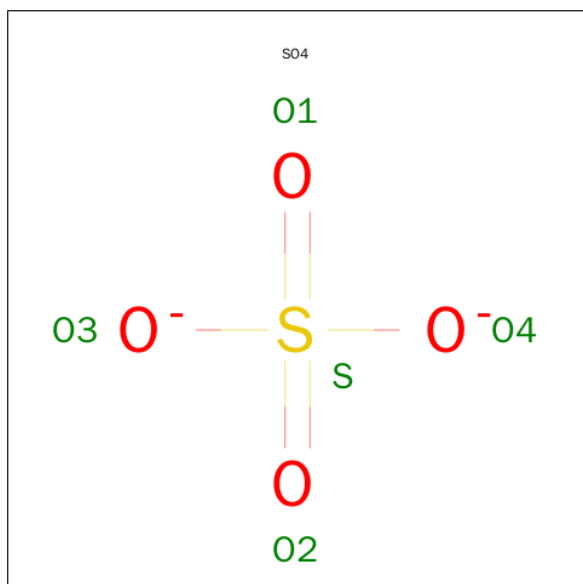
- Molecule 3 is 2-ACETAMIDO-1,2-DIDEOXYNOJIRMYCIN (three-letter code: NOK)

(formula: $C_8H_{16}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	2	4		
3	B	1	Total	C	N	O	0	0
			14	8	2	4		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	471	Total	O	0	0
			471	471		
5	B	476	Total	O	0	0
			476	476		

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	116.87Å 131.27Å 104.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.19 – 1.60 28.19 – 1.60	Depositor EDS
% Data completeness (in resolution range)	90.1 (28.19-1.60) 90.1 (28.19-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.181 , 0.212 0.191 , 0.220	Depositor DCC
R_{free} test set	9542 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 47.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 189853 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10996	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GAL, SO4, NOK

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	1.26	16/5086 (0.3%)	1.29	45/6902 (0.7%)
1	B	1.22	15/5108 (0.3%)	1.22	30/6932 (0.4%)
All	All	1.24	31/10194 (0.3%)	1.25	75/13834 (0.5%)

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	2
1	B	0	2
All	All	0	4

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	GLU	CD-OE2	-9.64	1.15	1.25
1	A	216	GLU	CD-OE1	8.85	1.35	1.25
1	A	269	GLU	CB-CG	-7.53	1.37	1.52
1	A	395	TYR	CE2-CZ	-7.41	1.28	1.38
1	B	497	ARG	CZ-NH2	6.59	1.41	1.33

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ARG	NE-CZ-NH2	-18.40	111.10	120.30
1	B	266	VAL	CG1-CB-CG2	12.63	131.11	110.90
1	A	237	ARG	NE-CZ-NH1	12.59	126.59	120.30
1	A	200	ARG	NE-CZ-NH1	11.74	126.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	239	ASP	CB-CG-OD2	-10.02	109.28	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ARG	Sidechain
1	A	468	SER	Peptide
1	B	468	SER	Peptide
1	B	615	ASP	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	4977	0	4847	50	0
1	B	4997	0	4861	27	0
2	A	11	0	10	0	0
2	B	11	0	10	0	0
3	A	14	0	15	0	0
3	B	14	0	15	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
5	A	471	0	0	17	0
5	B	476	0	0	4	0
All	All	10996	0	9758	75	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.

The worst 5 of 75 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:378:VAL:HG23	5:A:907:HOH:O	1.54	1.04
1:A:400:LYS:HD2	1:A:448:ARG:HE	1.37	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLY:O	1:A:378:VAL:HG22	1.76	0.86
1:A:395:TYR:CD1	5:A:1188:HOH:O	2.32	0.81
1:A:399:ARG:HD2	5:A:909:HOH:O	1.83	0.78

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	632/644 (98%)	613 (97%)	16 (2%)	3 (0%)	34	12
1	B	634/644 (98%)	618 (98%)	12 (2%)	4 (1%)	30	9
All	All	1266/1288 (98%)	1231 (97%)	28 (2%)	7 (1%)	30	9

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	GLY
1	B	107	GLY
1	B	617	ASP
1	A	397	ALA
1	B	396	GLY

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	531/540 (98%)	520 (98%)	11 (2%)	61	33
1	B	533/540 (99%)	520 (98%)	13 (2%)	57	27
All	All	1064/1080 (98%)	1040 (98%)	24 (2%)	58	29

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

Mol	Chain	Res	Type
1	A	616	LYS
1	B	209	ARG
1	B	567	LEU
1	B	33	LEU
1	B	123	LYS

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	28	HIS
1	B	379	ASN
1	B	402	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	GAL	A	701	3	11,11,12	1.03	1 (9%)	15,15,17	1.13	1 (6%)
2	GAL	B	701	3	11,11,12	1.08	0	15,15,17	1.36	2 (13%)

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
2	GAL	B	701	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GAL	C2-C3	-2.18	1.49	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	GAL	C3-C4-C5	-2.05	106.58	110.23
2	A	701	GAL	O5-C5-C6	2.41	112.51	107.34
2	B	701	GAL	O5-C5-C4	3.13	115.31	110.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

9 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	GAL	A	701	3	11,11,12	1.03	1 (9%)	15,15,17	1.13	1 (6%)
3	NOK	A	702	2	13,14,14	1.13	1 (7%)	13,19,19	2.62	4 (30%)
4	SO4	A	703	-	4,4,4	1.17	0	6,6,6	0.81	0
4	SO4	A	704	-	4,4,4	1.01	0	6,6,6	0.59	0
4	SO4	A	705	-	4,4,4	1.34	1 (25%)	6,6,6	0.26	0
2	GAL	B	701	3	11,11,12	1.08	0	15,15,17	1.36	2 (13%)
3	NOK	B	702	2	13,14,14	0.91	0	13,19,19	2.11	3 (23%)
4	SO4	B	703	-	4,4,4	1.24	0	6,6,6	0.68	0
4	SO4	B	704	-	4,4,4	0.87	0	6,6,6	0.38	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	GAL	A	701	3	-	0/2/19/22	0/1/1/1
3	NOK	A	702	2	-	0/6/23/23	1/1/1/1
4	SO4	A	703	-	-	0/0/0/0	0/0/0/0
4	SO4	A	704	-	-	0/0/0/0	0/0/0/0
4	SO4	A	705	-	-	0/0/0/0	0/0/0/0
2	GAL	B	701	3	-	0/2/19/22	0/1/1/1
3	NOK	B	702	2	-	0/6/23/23	1/1/1/1
4	SO4	B	703	-	-	0/0/0/0	0/0/0/0
4	SO4	B	704	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GAL	C2-C3	-2.18	1.49	1.52
4	A	705	SO4	O1-S	2.14	1.54	1.47
3	A	702	NOK	C5-N5	2.66	1.50	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NOK	C2-N2-C7	-3.33	118.77	123.11
3	B	702	NOK	C3-C4-C5	-2.53	107.42	111.34
3	A	702	NOK	C3-C4-C5	-2.37	107.66	111.34
2	B	701	GAL	C3-C4-C5	-2.05	106.58	110.23
3	B	702	NOK	O6-C6-C5	2.04	116.63	111.05

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	NOK	C1-C2-C3-C4-C5-N5
3	B	702	NOK	C1-C2-C3-C4-C5-N5

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	634/644 (98%)	-0.02	25 (3%) 43 40	8, 15, 32, 71	0
1	B	636/644 (98%)	0.02	31 (4%) 33 30	8, 16, 34, 65	0
All	All	1270/1288 (98%)	-0.00	56 (4%) 38 34	8, 15, 33, 71	0

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	GLY	7.3
1	B	616	LYS	7.0
1	B	29	HIS	6.7
1	B	663	ASP	6.6
1	A	617	ASP	6.4

6.2 Non-standard residues in protein, DNA, RNA chains [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	GAL	B	701	11/12	0.95	0.09	0.20	13,14,15,15	0
2	GAL	A	701	11/12	0.94	0.07	-0.63	14,15,16,16	0

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
4	SO4	B	704	5/5	0.99	0.10	6.18	17,17,18,19	0
4	SO4	A	705	5/5	0.99	0.07	1.31	18,19,20,21	0
4	SO4	A	703	5/5	0.94	0.11	1.28	26,29,31,34	0
3	NOK	B	702	14/14	0.94	0.08	0.63	13,14,15,16	0
3	NOK	A	702	14/14	0.94	0.08	0.48	14,15,17,17	0
2	GAL	B	701	11/12	0.95	0.09	0.20	13,14,15,15	0
2	GAL	A	701	11/12	0.94	0.07	-0.63	14,15,16,16	0
4	SO4	B	703	5/5	0.96	0.10	-	21,24,25,27	0
4	SO4	A	704	5/5	0.98	0.12	-	22,24,27,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.