



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:36 AM UTC

PDB ID : 5BXR / pdb_00005bxr
Title : LNBase in complex with LNB-NHAcDNJ
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Deposited on : 2015-06-09
Resolution : 1.60 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

<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

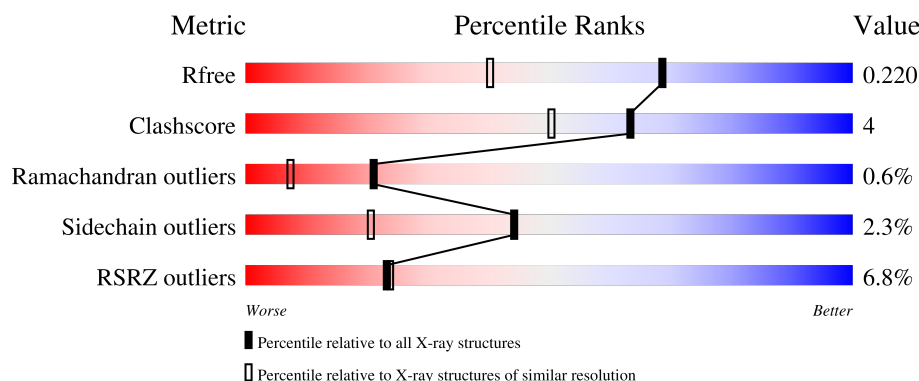
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (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 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	7% 84% 12% ...
1	B	644	7% 87% 10% ..

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:

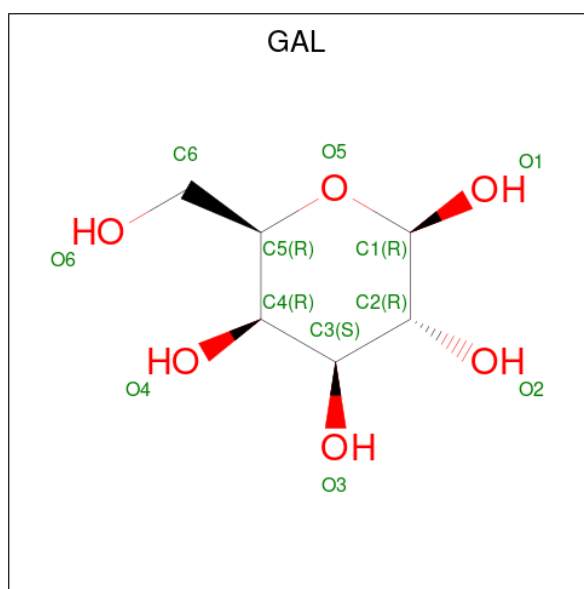
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP B3TLD6
A	21	GLY	-	expression tag	UNP B3TLD6
A	22	SER	-	expression tag	UNP B3TLD6
A	23	SER	-	expression tag	UNP B3TLD6
A	24	HIS	-	expression tag	UNP B3TLD6
A	25	HIS	-	expression tag	UNP B3TLD6
A	26	HIS	-	expression tag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

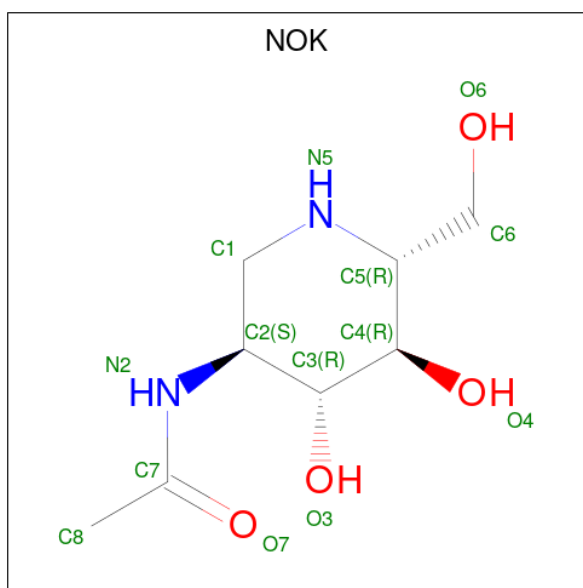
- Molecule 2 is beta-D-galactopyranose (CCD ID: GAL) (formula: $C_6H_{12}O_6$).



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		

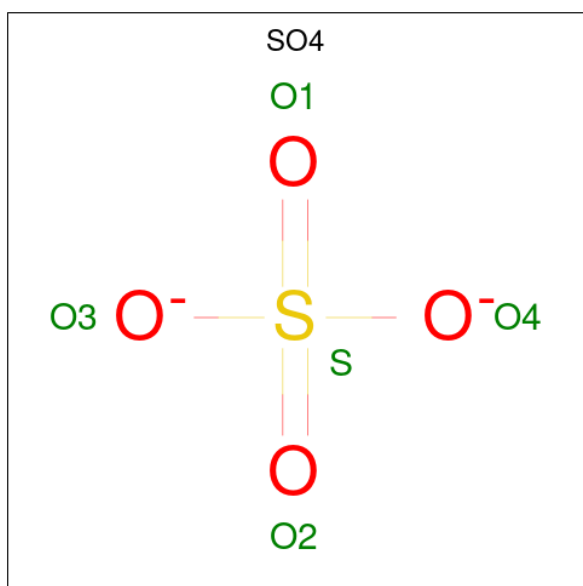
- Molecule 3 is 2-ACETAMIDO-1,2-DIDEOXYNOJIRMYCIN (CCD ID: NOK) (formula:

$C_8H_{16}N_2O_4$).



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 (CCD ID: 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		

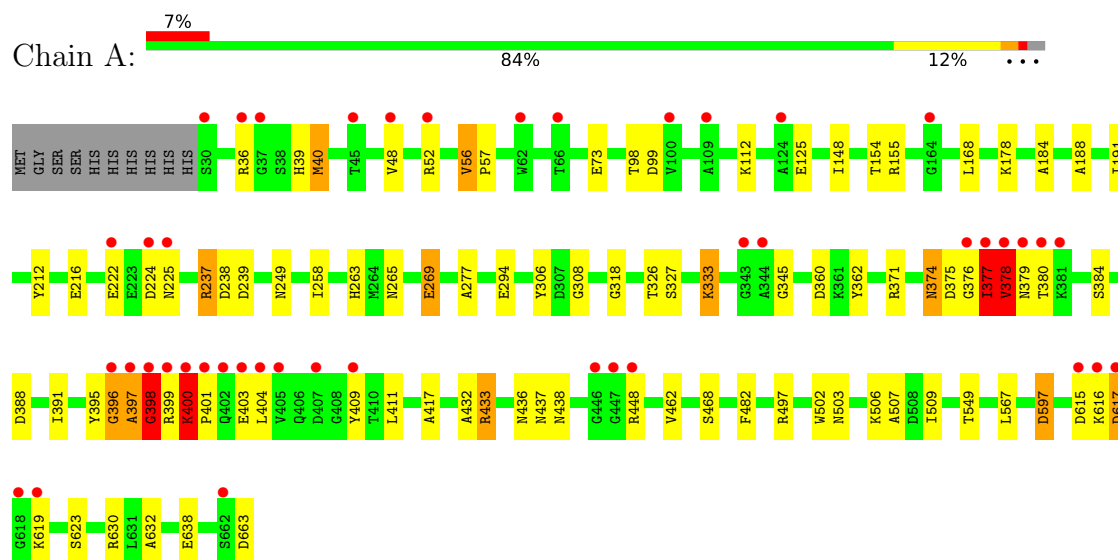
- Molecule 5 is water.

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

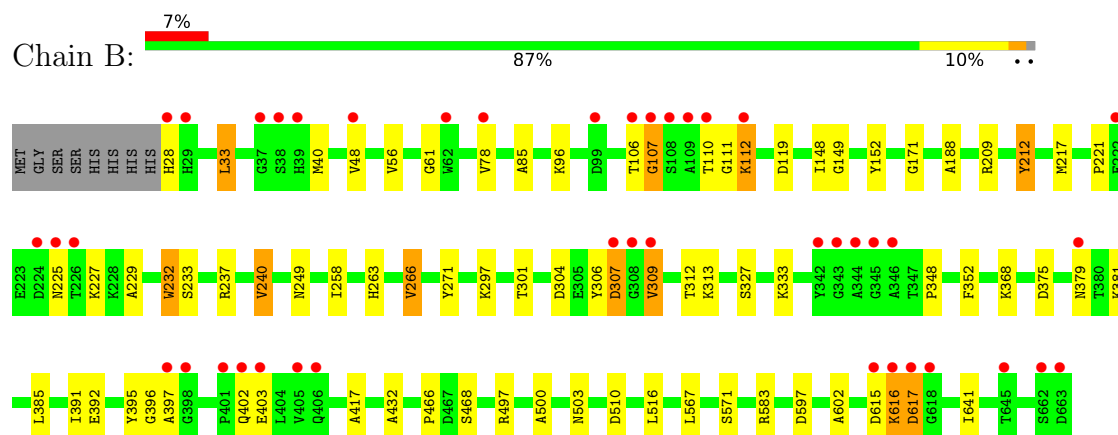
3 Residue-property plots [i](#)

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 21 21 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) 90.0 (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 (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	14.5	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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, 0.333 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, 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	1.57	33/5086 (0.6%)	1.39	21/6902 (0.3%)
1	B	1.55	31/5108 (0.6%)	1.34	17/6932 (0.2%)
All	All	1.56	64/10194 (0.6%)	1.36	38/13834 (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	2
1	B	0	2
All	All	0	4

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	VAL	N-CA	-9.50	1.38	1.45
1	A	377	ILE	CA-C	-8.12	1.43	1.53
1	B	352	PHE	C-O	-7.50	1.15	1.24
1	A	125	GLU	N-CA	-7.27	1.37	1.46
1	B	397	ALA	N-CA	7.21	1.54	1.46
1	A	396	GLY	N-CA	6.94	1.55	1.45
1	B	309	VAL	N-CA	-6.88	1.38	1.46
1	A	237	ARG	CD-NE	-6.78	1.36	1.46
1	A	263	HIS	CA-C	-6.68	1.44	1.53
1	B	503	ASN	N-CA	-6.40	1.38	1.46
1	B	56	VAL	CA-CB	6.36	1.59	1.54
1	A	433	ARG	CD-NE	-6.32	1.37	1.46
1	B	497	ARG	CZ-NH2	6.29	1.41	1.33
1	B	221	PRO	C-O	-6.27	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	GLY	C-O	-6.11	1.15	1.23
1	A	225	ASN	CA-C	6.10	1.61	1.52
1	B	497	ARG	CD-NE	-6.00	1.37	1.46
1	A	503	ASN	CA-C	5.98	1.60	1.52
1	B	119	ASP	CA-C	-5.97	1.45	1.53
1	A	362	TYR	N-CA	-5.96	1.39	1.46
1	A	371	ARG	CA-C	5.95	1.59	1.52
1	B	395	TYR	CA-C	-5.85	1.46	1.52
1	A	326	THR	C-O	-5.83	1.19	1.24
1	B	348	PRO	N-CA	-5.76	1.40	1.47
1	A	417	ALA	CA-C	5.75	1.60	1.52
1	B	240	VAL	CA-CB	-5.64	1.47	1.54
1	B	417	ALA	CA-C	5.60	1.60	1.52
1	B	432	ALA	N-CA	5.58	1.53	1.46
1	A	437	ASN	C-O	-5.57	1.16	1.24
1	B	381	LYS	N-CA	5.55	1.53	1.45
1	A	318	GLY	CA-C	-5.54	1.44	1.51
1	B	61	GLY	N-CA	5.54	1.52	1.45
1	A	155	ARG	N-CA	5.47	1.52	1.46
1	A	224	ASP	C-O	-5.45	1.17	1.24
1	B	309	VAL	C-O	-5.45	1.17	1.24
1	A	269	GLU	CD-OE2	-5.42	1.15	1.25
1	A	597	ASP	CB-CG	5.41	1.65	1.52
1	B	385	LEU	C-O	5.41	1.30	1.23
1	A	294	GLU	C-O	5.40	1.30	1.24
1	B	297	LYS	N-CA	-5.40	1.39	1.46
1	B	392	GLU	CA-CB	-5.39	1.46	1.53
1	B	309	VAL	CA-C	5.39	1.57	1.52
1	A	380	THR	C-O	-5.37	1.17	1.23
1	A	549	THR	C-O	5.36	1.29	1.24
1	B	307	ASP	CB-CG	-5.33	1.38	1.52
1	B	271	TYR	N-CA	5.30	1.52	1.46
1	A	216	GLU	CD-OE1	5.28	1.35	1.25
1	B	229	ALA	N-CA	5.27	1.52	1.46
1	A	239	ASP	CG-OD2	-5.27	1.15	1.25
1	B	313	LYS	C-O	-5.25	1.17	1.24
1	A	345	GLY	CA-C	5.24	1.58	1.51
1	A	398	GLY	N-CA	5.20	1.52	1.45
1	A	168	LEU	CA-C	-5.19	1.45	1.52
1	A	178	LYS	N-CA	-5.13	1.40	1.46
1	A	632	ALA	CA-C	-5.12	1.46	1.52
1	A	148	ILE	C-O	5.11	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	497	ARG	N-CA	-5.10	1.41	1.46
1	B	571	SER	C-O	5.09	1.30	1.23
1	B	391	ILE	CA-CB	-5.09	1.48	1.54
1	B	148	ILE	C-O	5.07	1.30	1.24
1	B	149	GLY	N-CA	5.06	1.52	1.45
1	A	52	ARG	CZ-NH1	5.03	1.39	1.32
1	A	374	ASN	CA-CB	-5.03	1.45	1.53
1	A	507	ALA	CA-C	5.02	1.59	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ILE	CB-CA-C	-16.51	93.35	111.35
1	A	375	ASP	N-CA-C	13.33	128.81	112.54
1	A	377	ILE	N-CA-CB	13.24	125.63	111.46
1	B	375	ASP	N-CA-C	10.21	124.83	112.38
1	B	266	VAL	CG1-CB-CG2	9.23	131.11	110.80
1	A	237	ARG	NE-CZ-NH2	-9.00	111.10	119.20
1	A	237	ARG	CG-CD-NE	-7.63	95.22	112.00
1	A	237	ARG	CD-NE-CZ	7.11	134.35	124.40
1	B	56	VAL	CA-C-O	-6.93	116.34	119.94
1	A	438	ASN	N-CA-C	6.84	120.93	112.58
1	B	307	ASP	CB-CA-C	-6.24	98.00	110.42
1	A	188	ALA	N-CA-C	-6.20	102.84	110.65
1	A	400	LYS	N-CA-C	-6.11	101.14	110.01
1	A	497	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	B	312	THR	N-CA-C	6.01	118.05	110.24
1	A	436	ASN	N-CA-C	5.77	118.51	111.82
1	A	56	VAL	O-C-N	5.76	126.24	120.59
1	A	154	THR	N-CA-CB	5.75	119.07	110.22
1	A	225	ASN	N-CA-CB	-5.74	100.77	110.41
1	A	308	GLY	N-CA-C	5.72	120.96	114.67
1	B	48	VAL	N-CA-C	5.69	116.42	110.62
1	B	500	ALA	N-CA-C	5.62	117.40	111.28
1	B	188	ALA	N-CA-C	-5.60	103.59	110.65
1	B	85	ALA	N-CA-C	-5.54	105.32	111.36
1	B	263	HIS	N-CA-C	5.46	119.10	111.90
1	A	378	VAL	O-C-N	5.42	129.35	122.57
1	B	641	ILE	N-CA-C	5.41	116.03	110.36
1	B	309	VAL	N-CA-C	5.33	116.59	112.12
1	B	510	ASP	N-CA-C	5.33	117.08	111.28
1	B	217	MET	O-C-N	5.32	128.84	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	VAL	CA-C-O	-5.30	117.19	119.94
1	B	602	ALA	N-CA-C	5.28	117.03	111.28
1	A	125	GLU	N-CA-C	-5.20	105.29	111.69
1	A	482	PHE	N-CA-C	5.18	117.34	111.02
1	B	232	TRP	O-C-N	-5.17	117.26	123.06
1	B	237	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	A	237	ARG	NE-CZ-NH1	5.09	126.59	121.50
1	A	433	ARG	N-CA-C	5.03	117.14	111.11

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	53	0
1	B	4997	0	4861	28	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	79	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.

All (79) 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
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
1:B:33:LEU:C	1:B:33:LEU:HD23	2.09	0.77
1:A:395:TYR:HD1	5:A:1188:HOH:O	1.66	0.77
1:A:597:ASP:HB3	5:A:1189:HOH:O	1.85	0.75
1:A:399:ARG:CD	5:A:909:HOH:O	2.35	0.73
1:A:400:LYS:CD	1:A:448:ARG:HE	2.01	0.72
1:A:397:ALA:HA	5:A:857:HOH:O	1.90	0.71
1:B:225:ASN:HD21	1:B:301:THR:HG21	1.57	0.70
1:A:663:ASP:OD1	1:B:28:HIS:HD2	1.80	0.65
1:A:378:VAL:HG13	5:A:855:HOH:O	1.96	0.64
1:A:378:VAL:CG1	5:A:855:HOH:O	2.45	0.64
1:A:377:ILE:HG22	5:A:829:HOH:O	1.98	0.64
1:A:40:MET:CG	1:A:112:LYS:HE2	2.29	0.63
1:A:40:MET:HG2	1:A:112:LYS:HE2	1.80	0.63
1:A:399:ARG:HB3	1:A:403:GLU:HB2	1.80	0.63
1:B:225:ASN:ND2	1:B:301:THR:HG21	2.16	0.61
1:A:398:GLY:HA3	5:A:808:HOH:O	2.00	0.60
1:B:583:ARG:HD2	5:B:1160:HOH:O	2.01	0.60
1:A:48:VAL:HG23	5:A:1108:HOH:O	2.01	0.59
1:B:597:ASP:HB3	5:B:1213:HOH:O	2.04	0.57
1:B:258:ILE:HD11	1:B:306:TYR:CE1	2.40	0.57
1:A:374:ASN:O	1:A:377:ILE:HG12	2.05	0.57
1:B:110:THR:HG22	1:B:111:GLY:N	2.20	0.56
1:A:400:LYS:HD2	1:A:448:ARG:NE	2.16	0.55
1:A:265:ASN:O	1:A:269:GLU:HG3	2.06	0.54
1:A:398:GLY:CA	5:A:808:HOH:O	2.55	0.54
1:B:96:LYS:HD2	1:B:516:LEU:HD21	1.90	0.54
1:A:623:SER:OG	1:A:630:ARG:HD3	2.07	0.53
1:A:395:TYR:CE1	5:A:1188:HOH:O	2.57	0.53
1:A:401:PRO:CD	1:A:448:ARG:HD3	2.40	0.51
1:B:33:LEU:C	1:B:33:LEU:CD2	2.80	0.50
1:A:391:ILE:HB	1:A:411:LEU:HD23	1.92	0.50
1:A:401:PRO:HD3	1:A:448:ARG:HD3	1.94	0.50
1:B:616:LYS:O	1:B:617:ASP:CB	2.58	0.50
1:A:615:ASP:O	1:A:617:ASP:HA	2.12	0.50
1:A:374:ASN:O	1:A:377:ILE:CG1	2.60	0.49
1:B:249:ASN:HB3	5:B:1047:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:ASP:O	1:B:307:ASP:HB2	2.12	0.48
1:A:39:HIS:CE1	1:A:40:MET:SD	3.06	0.48
1:A:663:ASP:OD1	1:A:663:ASP:C	2.55	0.48
1:A:615:ASP:OD2	1:A:619:LYS:HB2	2.14	0.48
1:B:227:LYS:CE	5:B:1185:HOH:O	2.62	0.48
1:A:258:ILE:HD11	1:A:306:TYR:CE1	2.49	0.48
1:A:378:VAL:HB	1:A:379:ASN:H	1.31	0.47
1:A:506:LYS:HA	1:A:509:ILE:HG12	1.96	0.47
1:B:33:LEU:HD23	1:B:33:LEU:O	2.15	0.47
1:A:404:LEU:HD22	1:A:409:TYR:CD2	2.49	0.46
1:A:212:TYR:C	1:A:212:TYR:CD1	2.93	0.46
1:A:238:ASP:HB3	5:A:962:HOH:O	2.16	0.45
1:A:400:LYS:HG3	1:A:448:ARG:HD3	1.97	0.45
1:B:240:VAL:CG1	1:B:309:VAL:CG1	2.94	0.45
1:A:638:GLU:OE2	1:B:28:HIS:HE1	2.00	0.45
1:B:110:THR:CG2	1:B:111:GLY:N	2.80	0.45
1:B:616:LYS:O	1:B:617:ASP:HB2	2.17	0.45
1:B:152:TYR:CG	1:B:209:ARG:HG3	2.53	0.44
1:A:191:ILE:C	1:A:191:ILE:HD12	2.42	0.44
1:A:399:ARG:C	1:A:400:LYS:O	2.58	0.44
1:B:232:TRP:CG	1:B:233:SER:HA	2.52	0.44
1:B:78:VAL:CG1	1:B:107:GLY:HA2	2.48	0.43
1:A:395:TYR:O	1:A:397:ALA:N	2.51	0.43
1:A:98:THR:O	1:A:99:ASP:HB2	2.18	0.43
1:A:399:ARG:N	5:A:808:HOH:O	2.52	0.43
1:B:225:ASN:OD1	1:B:225:ASN:N	2.45	0.42
1:A:360:ASP:OD2	1:A:388:ASP:OD1	2.37	0.42
1:A:40:MET:HG3	1:A:73:GLU:O	2.20	0.42
1:B:212:TYR:CD1	1:B:212:TYR:C	2.97	0.42
1:A:277:ALA:O	1:A:333:LYS:HE2	2.20	0.42
1:A:432:ALA:HA	1:A:502:TRP:CG	2.55	0.42
1:B:40:MET:SD	1:B:112:LYS:HB3	2.60	0.42
1:B:402:GLN:NE2	1:B:402:GLN:HA	2.35	0.42
1:B:106:THR:O	1:B:107:GLY:O	2.38	0.41
1:B:232:TRP:CD2	1:B:233:SER:HA	2.56	0.41
1:A:249:ASN:HB3	5:A:934:HOH:O	2.21	0.40
1:A:56:VAL:HA	1:A:57:PRO:C	2.46	0.40
1:A:184:ALA:HA	1:A:462:VAL:O	2.21	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	632/644 (98%)	613 (97%)	16 (2%)	3 (0%)	24	10
1	B	634/644 (98%)	618 (98%)	12 (2%)	4 (1%)	21	7
All	All	1266/1288 (98%)	1231 (97%)	28 (2%)	7 (1%)	21	7

All (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
1	A	398	GLY
1	B	466	PRO

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%)	518 (98%)	13 (2%)	43	19
1	B	533/540 (99%)	522 (98%)	11 (2%)	47	23
All	All	1064/1080 (98%)	1040 (98%)	24 (2%)	44	20

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	40	MET
1	A	222	GLU
1	A	327	SER
1	A	333	LYS
1	A	377	ILE
1	A	378	VAL
1	A	384	SER
1	A	400	LYS
1	A	433	ARG
1	A	567	LEU
1	A	616	LYS
1	A	617	ASP
1	B	33	LEU
1	B	112	LYS
1	B	212	TYR
1	B	266	VAL
1	B	327	SER
1	B	333	LYS
1	B	368	LYS
1	B	379	ASN
1	B	403	GLU
1	B	567	LEU
1	B	616	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	225	ASN
1	A	402	GLN
1	A	555	GLN
1	B	28	HIS
1	B	349	ASN
1	B	369	GLN
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	1.02	0	15,15,17	1.06	1 (6%)
2	GAL	B	701	3	11,11,12	1.11	0	15,15,17	1.17	1 (6%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GAL	O5-C5-C6	2.49	112.51	107.66
2	B	701	GAL	C3-C4-C5	-2.01	106.58	110.23

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 oligosaccharides 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$
4	SO4	A	705	-	4,4,4	0.92	0	6,6,6	0.24	0
4	SO4	A	703	-	4,4,4	0.92	0	6,6,6	0.54	0
4	SO4	B	703	-	4,4,4	0.71	0	6,6,6	0.49	0
4	SO4	A	704	-	4,4,4	0.72	0	6,6,6	0.73	0
3	NOK	A	702	2	14,14,14	1.04	0	15,19,19	1.96	5 (33%)
4	SO4	B	704	-	4,4,4	0.70	0	6,6,6	0.33	0
2	GAL	A	701	3	11,11,12	1.02	0	15,15,17	1.06	1 (6%)
3	NOK	B	702	2	14,14,14	0.99	0	15,19,19	1.94	4 (26%)
2	GAL	B	701	3	11,11,12	1.11	0	15,15,17	1.17	1 (6%)

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	NOK	B	702	2	-	1/6/23/23	1/1/1/1
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
3	NOK	A	702	2	-	1/6/23/23	1/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	NOK	C1-N5-C5	4.87	120.41	109.71
3	B	702	NOK	C1-N5-C5	4.75	120.15	109.71
3	B	702	NOK	C2-C1-N5	-3.45	105.25	112.47
3	A	702	NOK	C2-N2-C7	-3.08	118.77	122.90
2	A	701	GAL	O5-C5-C6	2.49	112.51	107.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NOK	C3-C4-C5	-2.46	107.42	111.02
3	A	702	NOK	C2-C1-N5	-2.39	107.47	112.47
3	A	702	NOK	C3-C4-C5	-2.29	107.66	111.02
3	B	702	NOK	O6-C6-C5	2.28	116.63	111.10
3	A	702	NOK	O3-C3-C4	2.24	115.66	110.38
2	B	701	GAL	C3-C4-C5	-2.01	106.58	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	NOK	C1-C2-N2-C7
3	B	702	NOK	C1-C2-N2-C7

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

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, 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%)	0.12	44 (6%) 23 23	8, 15, 32, 71	0
1	B	636/644 (98%)	0.15	42 (6%) 24 25	8, 16, 34, 65	0
All	All	1270/1288 (98%)	0.13	86 (6%) 23 24	8, 15, 33, 71	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	109	ALA	7.7
1	A	398	GLY	7.2
1	A	397	ALA	5.7
1	A	399	ARG	5.0
1	A	62	TRP	5.0
1	B	107	GLY	4.9
1	B	29	HIS	4.7
1	B	110	THR	4.6
1	B	662	SER	4.6
1	B	618	GLY	4.5
1	B	108	SER	4.2
1	A	377	ILE	4.2
1	A	378	VAL	4.1
1	B	397	ALA	4.1
1	A	402	GLN	4.1
1	A	617	ASP	4.0
1	A	401	PRO	3.9
1	B	224	ASP	3.8
1	B	663	ASP	3.8
1	B	62	TRP	3.8
1	A	409	TYR	3.7
1	A	404	LEU	3.6
1	A	616	LYS	3.5
1	A	615	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	379	ASN	3.5
1	B	37	GLY	3.4
1	A	109	ALA	3.3
1	B	112	LYS	3.3
1	A	66	THR	3.3
1	A	618	GLY	3.2
1	B	345	GLY	3.2
1	B	343	GLY	3.2
1	B	616	LYS	3.2
1	A	381	LYS	3.2
1	A	376	GLY	3.2
1	A	30	SER	3.1
1	A	379	ASN	3.1
1	A	380	THR	3.1
1	A	619	LYS	3.0
1	A	48	VAL	3.0
1	B	106	THR	3.0
1	A	447	GLY	3.0
1	B	398	GLY	3.0
1	A	224	ASP	2.9
1	B	225	ASN	2.9
1	A	407	ASP	2.8
1	B	226	THR	2.8
1	B	615	ASP	2.8
1	B	645	THR	2.8
1	B	28	HIS	2.8
1	B	346	ALA	2.8
1	A	344	ALA	2.7
1	A	405	VAL	2.7
1	B	405	VAL	2.7
1	A	225	ASN	2.7
1	A	396	GLY	2.7
1	B	308	GLY	2.7
1	A	124	ALA	2.7
1	B	344	ALA	2.7
1	A	662	SER	2.6
1	B	309	VAL	2.6
1	A	164	GLY	2.5
1	A	446	GLY	2.5
1	A	403	GLU	2.5
1	A	36	ARG	2.4
1	A	400	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	37	GLY	2.3
1	B	401	PRO	2.3
1	B	222	GLU	2.3
1	A	222	GLU	2.3
1	B	403	GLU	2.3
1	A	45	THR	2.3
1	A	52	ARG	2.3
1	B	307	ASP	2.3
1	A	100	VAL	2.3
1	B	99	ASP	2.1
1	B	617	ASP	2.1
1	B	342	TYR	2.1
1	B	406	GLN	2.1
1	B	48	VAL	2.1
1	B	78	VAL	2.1
1	A	343	GLY	2.1
1	B	38	SER	2.1
1	B	402	GLN	2.1
1	A	448	ARG	2.1
1	B	39	HIS	2.0

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. 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(Å ²)	Q<0.9
2	GAL	A	701	11/12	0.96	0.07	14,15,16,16	0
2	GAL	B	701	11/12	0.97	0.06	13,14,15,15	0

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(Å ²)	Q<0.9
2	GAL	A	701	11/12	0.96	0.07	14,15,16,16	0
3	NOK	A	702	14/14	0.96	0.07	14,15,17,17	0
3	NOK	B	702	14/14	0.96	0.06	13,14,15,16	0
4	SO4	A	703	5/5	0.96	0.11	26,29,31,34	0
4	SO4	B	703	5/5	0.96	0.09	21,24,25,27	0
4	SO4	A	704	5/5	0.97	0.10	22,24,27,31	0
2	GAL	B	701	11/12	0.97	0.06	13,14,15,15	0
4	SO4	A	705	5/5	0.99	0.07	18,19,20,21	0
4	SO4	B	704	5/5	0.99	0.07	17,17,18,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.