Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 10:49 AM JST

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 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 (i) 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 (i)) were used in the production of this report:

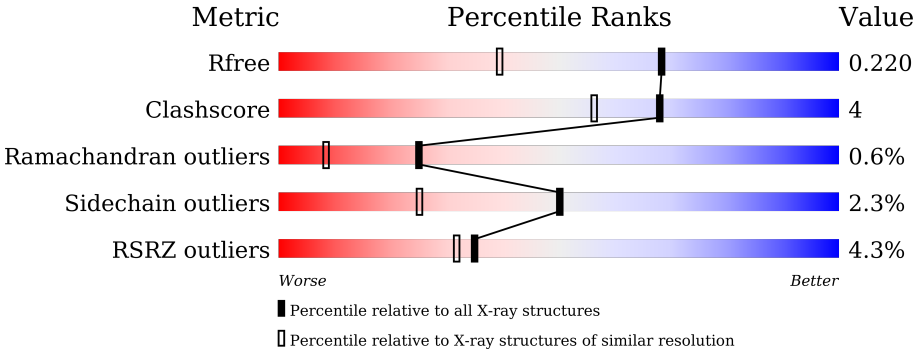
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (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 <=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	4% 84% 12% • •
1	B	644	5% 87% 10% ••

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	634	4977	3136	847	977	17	0	0	0
1	B	636	4997	3148	853	979	17	0	0	0

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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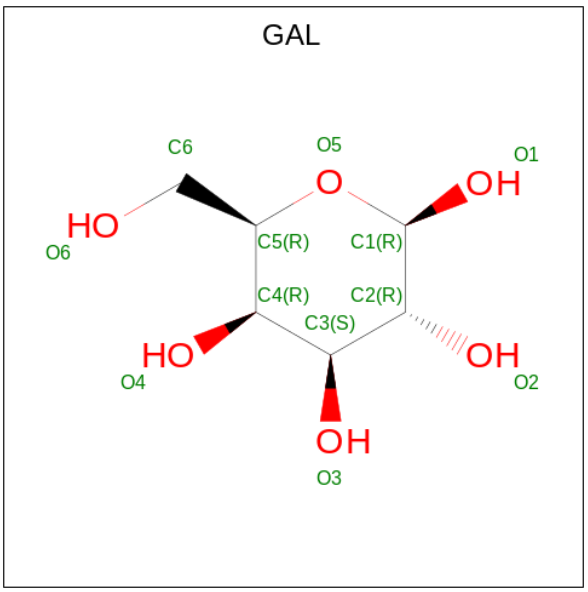
Chain	Residue	Modelled	Actual	Comment	Reference
B	24	HIS	-	expression tag	UNP B3TLD6
B	25	HIS	-	expression tag	UNP B3TLD6
B	26	HIS	-	expression tag	UNP B3TLD6
B	27	HIS	-	expression tag	UNP B3TLD6
B	28	HIS	-	expression tag	UNP B3TLD6
B	29	HIS	-	expression tag	UNP B3TLD6
B	30	SER	-	expression tag	UNP B3TLD6
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

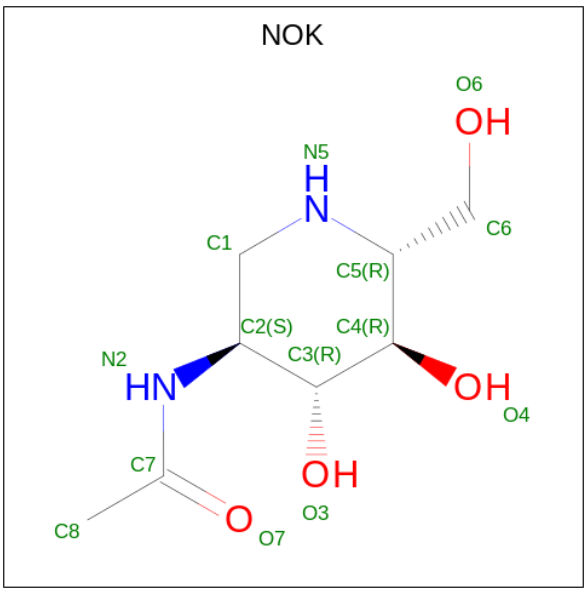
- Molecule 2 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



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			

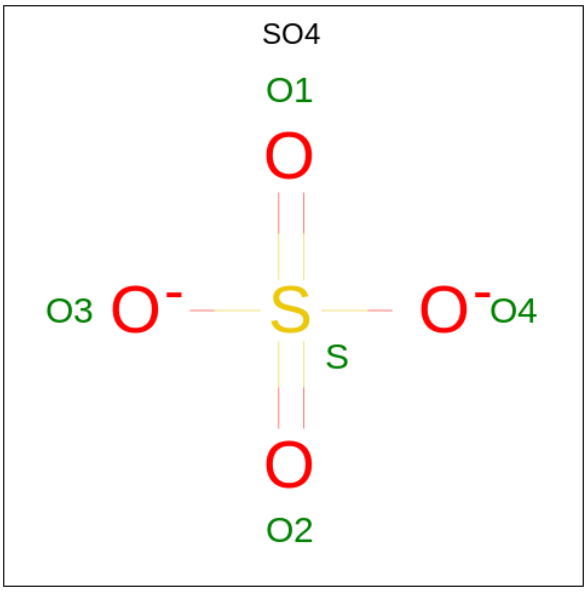
- Molecule 3 is 2-ACETAMIDO-1,2-DIDEOXYNOJIRMYCIN (three-letter code: NOK)

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



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

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



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

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

- Molecule 5 is water.

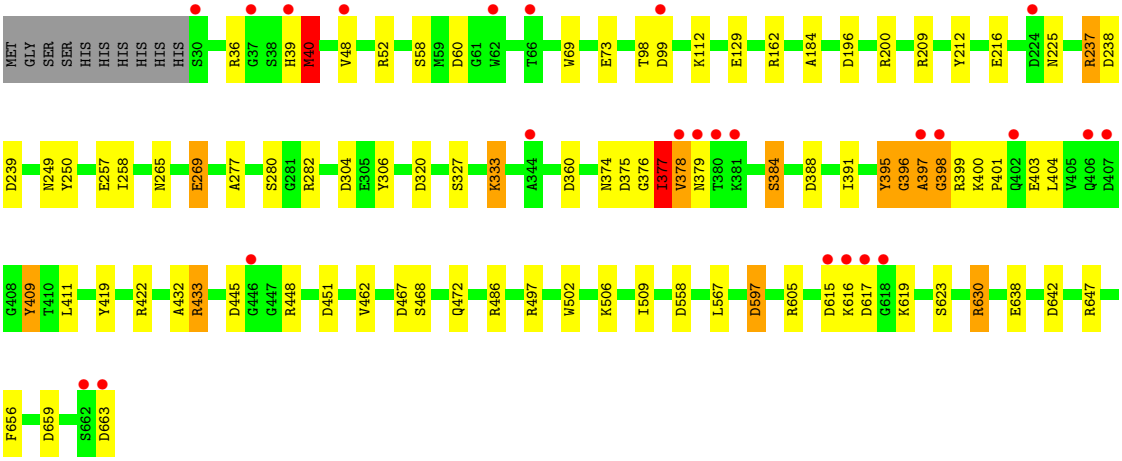
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	471	471	471	0	0
			Total	O		
5	B	476	476	476	0	0

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.

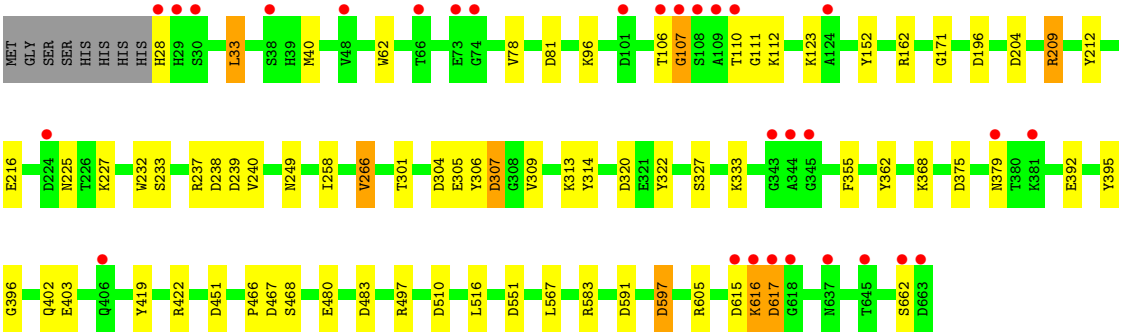
• Molecule 1: Lacto-N-biosidase

Chain A:



• Molecule 1: Lacto-N-biosidase

Chain B:



4 Data and refinement statistics (i)

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) 90.1 (28.19-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.03%)	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)	0.43 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[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: 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	1.26	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

All (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
1	A	597	ASP	CB-CG	6.58	1.65	1.51
1	B	216	GLU	CD-OE1	-6.56	1.18	1.25
1	A	280	SER	CB-OG	-6.30	1.34	1.42
1	A	396	GLY	N-CA	6.25	1.55	1.46
1	A	384	SER	CB-OG	-6.22	1.34	1.42
1	B	307	ASP	CB-CG	-6.20	1.38	1.51
1	A	395	TYR	CG-CD2	-6.05	1.31	1.39
1	A	58	SER	CB-OG	-5.95	1.34	1.42
1	B	62	TRP	CE3-CZ3	5.88	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	TYR	CE1-CZ	5.86	1.46	1.38
1	B	362	TYR	CB-CG	-5.83	1.43	1.51
1	A	69	TRP	CG-CD1	5.82	1.45	1.36
1	A	237	ARG	CD-NE	-5.70	1.36	1.46
1	B	305	GLU	CD-OE1	-5.59	1.19	1.25
1	B	419	TYR	CG-CD1	-5.54	1.31	1.39
1	B	216	GLU	CD-OE2	5.50	1.31	1.25
1	B	597	ASP	CB-CG	5.39	1.63	1.51
1	B	171	GLY	C-O	-5.36	1.15	1.23
1	B	320	ASP	CB-CG	-5.35	1.40	1.51
1	A	433	ARG	CD-NE	-5.33	1.37	1.46
1	B	662	SER	CB-OG	5.23	1.49	1.42
1	B	392	GLU	CD-OE2	5.22	1.31	1.25
1	A	52	ARG	CZ-NH1	5.18	1.39	1.33
1	A	472	GLN	CB-CG	-5.17	1.38	1.52
1	B	497	ARG	CD-NE	-5.06	1.37	1.46
1	B	395	TYR	CG-CD2	-5.00	1.32	1.39

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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
1	B	239	ASP	CB-CG-OD2	-10.02	109.28	118.30
1	B	239	ASP	CB-CG-OD1	9.52	126.86	118.30
1	A	377	ILE	CB-CA-C	-9.12	93.35	111.60
1	B	162	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	A	647	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	A	497	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	A	647	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	A	239	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	237	ARG	CG-CD-NE	-7.89	95.22	111.80
1	A	237	ARG	CD-NE-CZ	7.68	134.35	123.60
1	B	196	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	422	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	238	ASP	CB-CG-OD1	7.32	124.88	118.30
1	A	433	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	B	551	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	630	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	237	ARG	NE-CZ-NH2	7.02	123.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	422	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	419	TYR	CZ-CE2-CD2	6.89	126.00	119.80
1	A	52	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	320	ASP	CB-CG-OD2	6.74	124.37	118.30
1	A	162	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	52	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	375	ASP	N-CA-C	6.59	128.81	111.00
1	A	129	GLU	OE1-CD-OE2	6.59	131.21	123.30
1	A	486	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	A	605	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	422	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	597	ASP	CB-CG-OD2	6.45	124.11	118.30
1	A	377	ILE	N-CA-CB	6.45	125.63	110.80
1	B	204	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	467	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	497	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	B	307	ASP	CB-CA-C	-6.20	98.00	110.40
1	A	196	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	433	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	322	TYR	CB-CG-CD1	6.11	124.67	121.00
1	A	40	MET	CG-SD-CE	6.08	109.92	100.20
1	B	314	TYR	CB-CG-CD1	5.99	124.59	121.00
1	A	257	GLU	OE1-CD-OE2	-5.97	116.13	123.30
1	A	642	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	314	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	304	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	605	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	A	642	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	A	451	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	392	GLU	OE1-CD-OE2	-5.70	116.47	123.30
1	B	480	GLU	OE1-CD-OE2	5.68	130.12	123.30
1	A	445	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	A	282	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	269	GLU	CG-CD-OE2	-5.54	107.23	118.30
1	A	257	GLU	CG-CD-OE1	5.48	129.26	118.30
1	A	225	ASN	N-CA-CB	-5.46	100.77	110.60
1	B	451	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	320	ASP	CB-CG-OD1	5.43	123.18	118.30
1	B	483	ASP	CB-CG-OD1	5.42	123.18	118.30
1	B	320	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	591	ASP	CB-CG-OD2	-5.33	113.51	118.30
1	B	605	ARG	NE-CZ-NH1	5.32	122.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	250	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	B	81	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	60	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	B	510	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	304	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	375	ASP	N-CA-C	5.12	124.83	111.00
1	B	467	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	558	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	A	659	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	320	ASP	OD1-CG-OD2	-5.07	113.67	123.30
1	A	656	PHE	CB-CG-CD2	5.04	124.33	120.80
1	B	355	PHE	CB-CG-CD1	5.03	124.32	120.80

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 (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	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.

All (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
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: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:B:33:LEU:C	1:B:33:LEU:HD23	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:33:LEU:C	1:B:33:LEU:CD2	2.80	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:663:ASP:OD1	1:A:663:ASP:C	2.55	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: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:A:212:TYR:CD1	1:A:212:TYR:C	2.93	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: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%)	29 11
1	B	634/644 (98%)	618 (98%)	12 (2%)	4 (1%)	25 8
All	All	1266/1288 (98%)	1231 (97%)	28 (2%)	7 (1%)	25 8

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%)	520 (98%)	11 (2%)	53 29
1	B	533/540 (99%)	520 (98%)	13 (2%)	49 24
All	All	1064/1080 (98%)	1040 (98%)	24 (2%)	50 25

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	209	ARG
1	A	327	SER
1	A	333	LYS
1	A	377	ILE
1	A	378	VAL
1	A	384	SER
1	A	433	ARG
1	A	567	LEU
1	A	616	LYS
1	B	33	LEU
1	B	123	LYS
1	B	209	ARG
1	B	212	TYR
1	B	266	VAL
1	B	313	LYS
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 (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 (i)

There are no RNA molecules in this entry.

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

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	B	701	3	11,11,12	1.12	0	15,15,17	1.25	2 (13%)
2	GAL	A	701	3	11,11,12	1.03	0	15,15,17	1.27	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	B	701	3	-	0/2/19/22	0/1/1/1
2	GAL	A	701	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	GAL	O5-C5-C6	3.38	112.51	107.20
2	B	701	GAL	C3-C4-C5	-2.05	106.58	110.24
2	B	701	GAL	O5-C5-C6	2.02	110.37	107.20

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	703	-	4,4,4	0.68	0	6,6,6	0.54	0
4	SO4	A	703	-	4,4,4	0.87	0	6,6,6	0.59	0
4	SO4	A	704	-	4,4,4	0.65	0	6,6,6	0.76	0
2	GAL	B	701	3	11,11,12	1.12	0	15,15,17	1.25	2 (13%)
4	SO4	A	705	-	4,4,4	0.88	0	6,6,6	0.22	0
3	NOK	B	702	2	14,14,14	0.98	0	16,19,19	2.36	5 (31%)
4	SO4	B	704	-	4,4,4	0.63	0	6,6,6	0.34	0
3	NOK	A	702	2	14,14,14	1.04	0	16,19,19	2.61	6 (37%)
2	GAL	A	701	3	11,11,12	1.03	0	15,15,17	1.27	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	B	701	3	-	0/2/19/22	0/1/1/1
3	NOK	B	702	2	-	0/6/23/23	1/1/1/1
3	NOK	A	702	2	-	0/6/23/23	1/1/1/1
2	GAL	A	701	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	NOK	C1-C2-N2	7.14	121.00	109.95
3	B	702	NOK	C1-C2-N2	5.58	118.59	109.95
3	A	702	NOK	C1-N5-C5	4.99	120.41	109.61
3	B	702	NOK	C1-N5-C5	4.87	120.15	109.61
3	B	702	NOK	C2-C1-N5	-3.58	105.25	112.33
2	A	701	GAL	O5-C5-C6	3.38	112.51	107.20
3	A	702	NOK	C2-N2-C7	-2.90	118.77	122.90
3	B	702	NOK	C3-C4-C5	-2.46	107.42	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	NOK	C2-C1-N5	-2.45	107.47	112.33
3	A	702	NOK	O3-C3-C4	2.30	115.66	110.35
3	A	702	NOK	C3-C4-C5	-2.29	107.66	111.02
3	B	702	NOK	O6-C6-C5	2.28	116.63	111.09
2	B	701	GAL	C3-C4-C5	-2.05	106.58	110.24
2	B	701	GAL	O5-C5-C6	2.02	110.37	107.20

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%)	39	36	8, 15, 32, 71	0
1	B	636/644 (98%)	0.02	30 (4%)	31	28	8, 16, 34, 65	0
All	All	1270/1288 (98%)	0.00	55 (4%)	35	32	8, 15, 33, 71	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	GLY	7.2
1	B	616	LYS	7.0
1	B	29	HIS	6.7
1	B	663	ASP	6.7
1	A	617	ASP	6.4
1	A	616	LYS	5.8
1	B	108	SER	5.6
1	B	617	ASP	5.4
1	B	662	SER	5.2
1	B	109	ALA	5.1
1	A	618	GLY	4.7
1	A	663	ASP	4.3
1	B	618	GLY	4.0
1	B	345	GLY	3.9
1	B	379	ASN	3.9
1	B	224	ASP	3.8
1	A	379	ASN	3.7
1	A	224	ASP	3.4
1	A	398	GLY	3.2
1	A	381	LYS	2.9
1	B	28	HIS	2.9
1	B	343	GLY	2.9
1	B	344	ALA	2.9
1	B	110	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	30	SER	2.8
1	A	662	SER	2.7
1	A	66	THR	2.7
1	B	637	ASN	2.7
1	A	37	GLY	2.6
1	B	615	ASP	2.6
1	A	378	VAL	2.5
1	B	48	VAL	2.5
1	B	38	SER	2.5
1	A	344	ALA	2.4
1	A	62	TRP	2.4
1	B	66	THR	2.4
1	B	124	ALA	2.4
1	A	406	GLN	2.3
1	A	99	ASP	2.3
1	B	106	THR	2.2
1	A	402	GLN	2.2
1	B	30	SER	2.2
1	A	615	ASP	2.2
1	A	380	THR	2.2
1	A	407	ASP	2.2
1	B	73	GLU	2.2
1	B	645	THR	2.2
1	B	406	GLN	2.2
1	B	101	ASP	2.2
1	A	397	ALA	2.2
1	A	446	GLY	2.1
1	B	74	GLY	2.1
1	A	48	VAL	2.1
1	A	39	HIS	2.1
1	B	381	LYS	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	0.94	0.07	14,15,16,16	0
2	GAL	B	701	11/12	0.95	0.09	13,14,15,15	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	0.94	0.07	14,15,16,16	0
3	NOK	A	702	14/14	0.94	0.08	14,15,17,17	0
3	NOK	B	702	14/14	0.94	0.08	13,14,15,16	0
4	SO4	A	703	5/5	0.94	0.11	26,29,31,34	0
2	GAL	B	701	11/12	0.95	0.09	13,14,15,15	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
4	SO4	A	705	5/5	0.99	0.07	18,19,20,21	0
4	SO4	B	704	5/5	0.99	0.10	17,17,18,19	0

6.5 Other polymers (i)

There are no such residues in this entry.