



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:16 pm GMT

PDB ID : 4JAW
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

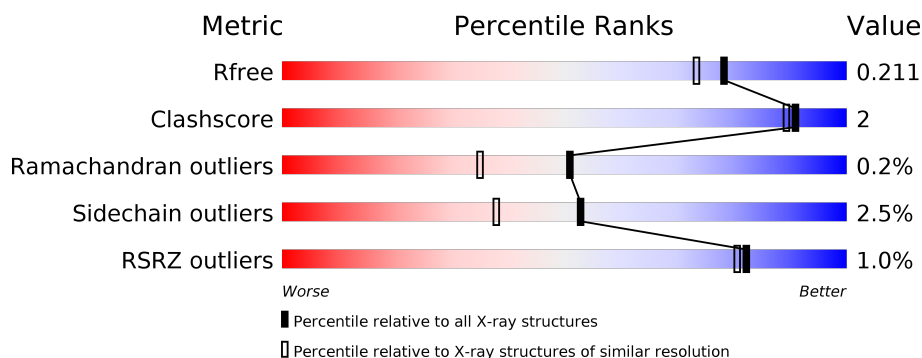
1 Overall quality at a glance

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}	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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 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></div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	B	644	<div> <div></div> <div>85%</div> <div>12%</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	A	705	-	-	-	X
4	SO4	B	704	-	-	-	X

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:

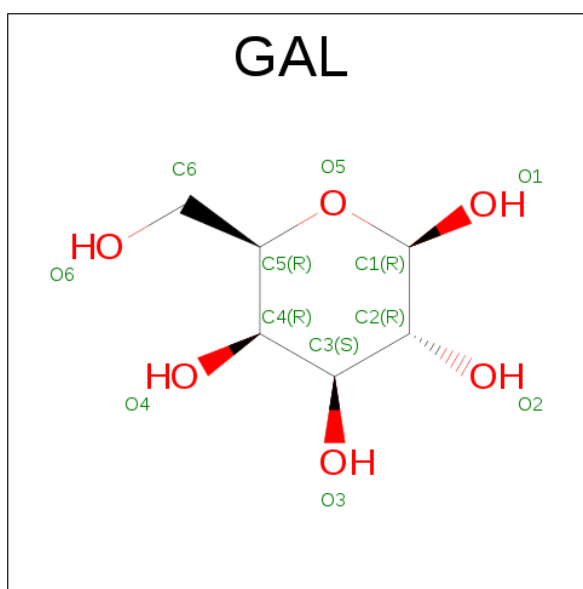
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	EXPRESSION TAG	UNP B3TLD6
A	21	GLY	-	EXPRESSION TAG	UNP B3TLD6
A	22	SER	-	EXPRESSION TAG	UNP B3TLD6
A	23	SER	-	EXPRESSION TAG	UNP B3TLD6
A	24	HIS	-	EXPRESSION TAG	UNP B3TLD6
A	25	HIS	-	EXPRESSION TAG	UNP B3TLD6
A	26	HIS	-	EXPRESSION TAG	UNP B3TLD6
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

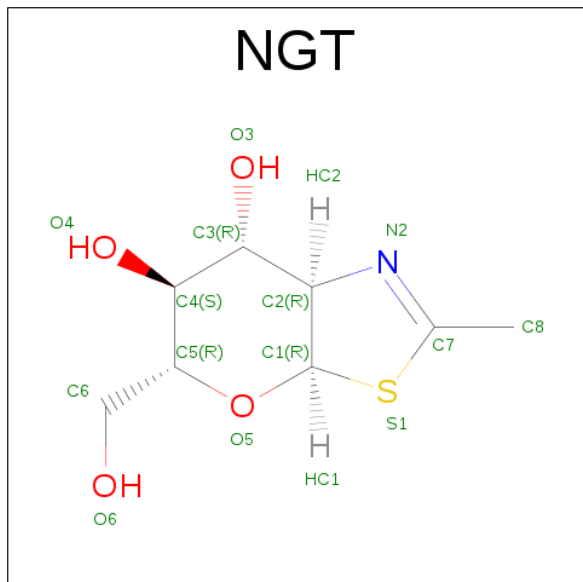
- Molecule 2 is SUGAR (BETA-D-GALACTOSE) (three-letter code: GAL) (formula: C₆H₁₂O₆).



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		

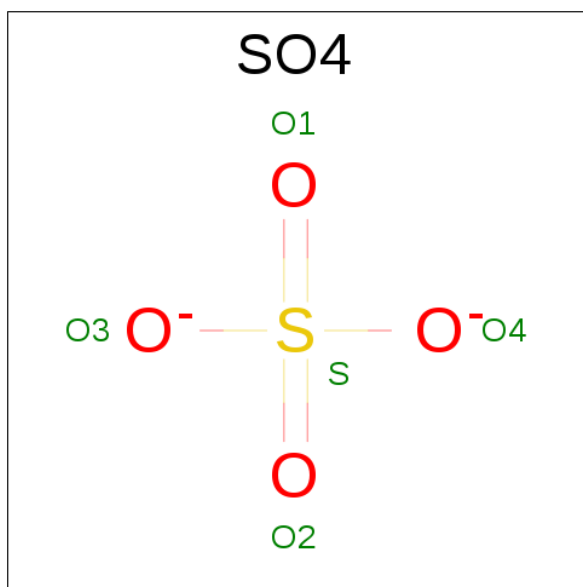
- Molecule 3 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRA

HYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: 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 (three-letter code: 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

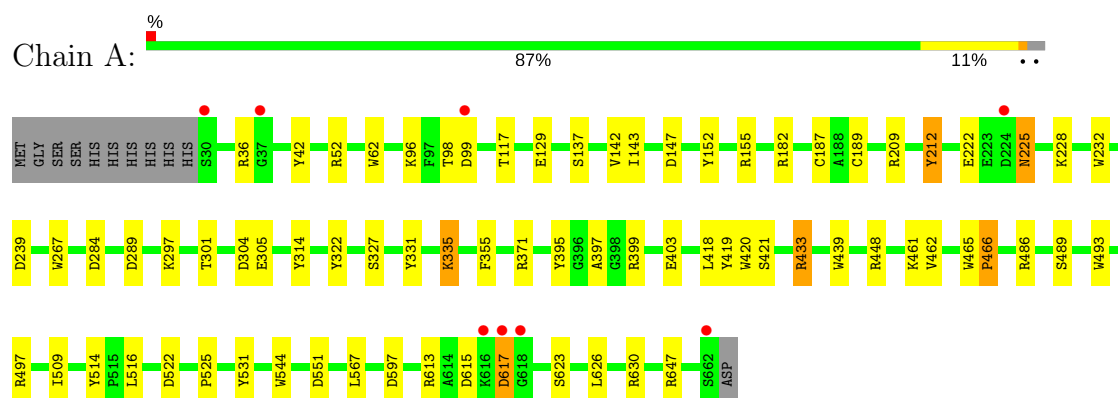
- Molecule 5 is water.

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

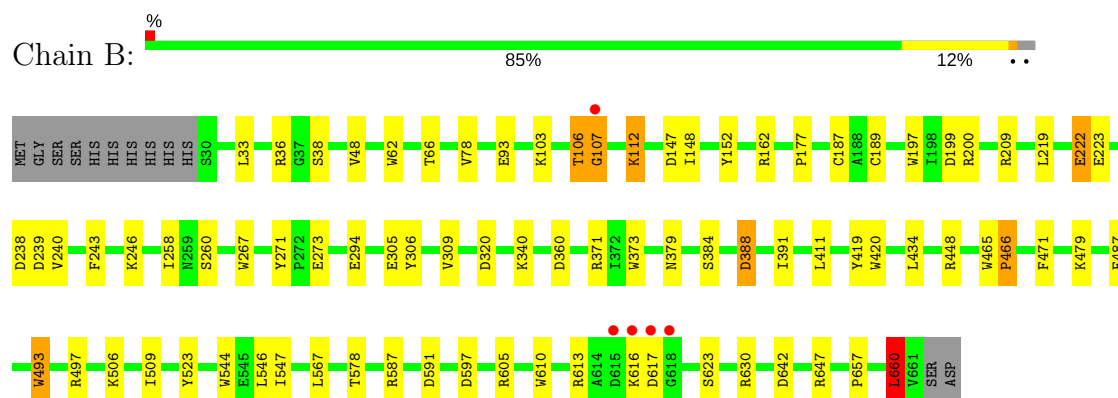
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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	116.52Å 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 0.181 , 0.211	Depositor DCC
R_{free} test set	7499 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	11.1	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 43.3	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

5.1 Standard geometry

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

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	1.36	22/5078 (0.4%)	1.28	33/6891 (0.5%)
1	B	1.37	19/5072 (0.4%)	1.26	36/6883 (0.5%)
All	All	1.36	41/10150 (0.4%)	1.27	69/13774 (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	B	0	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	497	ARG	CZ-NH2	9.24	1.45	1.33
1	B	62	TRP	CD2-CE2	9.23	1.52	1.41
1	A	62	TRP	CD2-CE2	8.23	1.51	1.41
1	A	52	ARG	CZ-NH1	6.99	1.42	1.33
1	B	267	TRP	CD2-CE2	6.96	1.49	1.41
1	B	162	ARG	CZ-NH1	6.87	1.42	1.33
1	B	420	TRP	CD2-CE2	6.60	1.49	1.41
1	A	267	TRP	CD2-CE2	6.45	1.49	1.41
1	A	465	TRP	CD2-CE2	6.19	1.48	1.41
1	B	544	TRP	CG-CD1	6.17	1.45	1.36
1	A	62	TRP	CG-CD1	6.11	1.45	1.36
1	B	93	GLU	CB-CG	-5.92	1.40	1.52
1	A	420	TRP	CD2-CE2	5.87	1.48	1.41
1	B	465	TRP	CD2-CE2	5.86	1.48	1.41
1	A	489	SER	CB-OG	5.83	1.49	1.42
1	A	331	TYR	CE1-CZ	5.73	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	514	TYR	CG-CD1	5.64	1.46	1.39
1	A	465	TRP	CG-CD1	5.62	1.44	1.36
1	B	487	PHE	CG-CD1	5.59	1.47	1.38
1	B	260	SER	CB-OG	5.55	1.49	1.42
1	B	610	TRP	CD2-CE2	5.54	1.48	1.41
1	B	373	TRP	CD2-CE2	5.41	1.47	1.41
1	A	267	TRP	CE3-CZ3	5.37	1.47	1.38
1	A	439	TRP	CD2-CE2	5.37	1.47	1.41
1	A	314	TYR	CE2-CZ	-5.33	1.31	1.38
1	B	465	TRP	CG-CD1	5.33	1.44	1.36
1	A	129	GLU	CG-CD	5.25	1.59	1.51
1	A	232	TRP	CD2-CE2	5.25	1.47	1.41
1	A	52	ARG	NE-CZ	5.25	1.39	1.33
1	A	493	TRP	CD2-CE2	5.24	1.47	1.41
1	A	232	TRP	CE3-CZ3	5.20	1.47	1.38
1	A	355	PHE	CE1-CZ	5.19	1.47	1.37
1	A	597	ASP	CB-CG	5.19	1.62	1.51
1	B	523	TYR	CD2-CE2	5.15	1.47	1.39
1	B	605	ARG	CZ-NH1	5.13	1.39	1.33
1	B	107	GLY	N-CA	5.13	1.53	1.46
1	B	271	TYR	CG-CD1	5.13	1.45	1.39
1	B	197	TRP	CD2-CE2	5.07	1.47	1.41
1	A	544	TRP	CD2-CE2	5.06	1.47	1.41
1	B	493	TRP	CD2-CE2	5.04	1.47	1.41
1	A	421	SER	CB-OG	5.03	1.48	1.42

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ARG	NE-CZ-NH1	18.75	129.68	120.30
1	A	52	ARG	NE-CZ-NH2	-12.88	113.86	120.30
1	A	448	ARG	NE-CZ-NH2	-11.30	114.65	120.30
1	A	448	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	A	433	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	B	200	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	497	ARG	NE-CZ-NH2	9.30	124.95	120.30
1	A	433	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	B	647	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	597	ASP	CB-CG-OD1	7.97	125.47	118.30
1	B	112	LYS	CD-CE-NZ	7.37	128.64	111.70
1	A	182	ARG	NE-CZ-NH2	7.30	123.95	120.30
1	B	200	ARG	NE-CZ-NH2	-7.30	116.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	246	LYS	CD-CE-NZ	-7.21	95.11	111.70
1	A	239	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	B	613	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	B	587	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	239	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	155	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	613	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	A	626	LEU	CB-CG-CD1	-6.67	99.66	111.00
1	B	660	LEU	CB-CG-CD1	6.65	122.30	111.00
1	B	497	ARG	NE-CZ-NH1	-6.63	116.99	120.30
1	B	38	SER	N-CA-CB	6.56	120.34	110.50
1	A	147	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	B	239	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	486	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	371	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	A	297	LYS	CD-CE-NZ	-6.42	96.93	111.70
1	B	434	LEU	CB-CG-CD1	-6.33	100.24	111.00
1	A	304	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	289	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	239	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	182	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	B	613	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	B	147	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	A	371	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	322	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	305	GLU	OE1-CD-OE2	-5.92	116.20	123.30
1	A	647	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	522	ASP	CB-CG-OD1	5.84	123.55	118.30
1	B	305	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	A	52	ARG	CD-NE-CZ	5.72	131.61	123.60
1	B	647	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	419	TYR	CB-CG-CD2	-5.66	117.60	121.00
1	B	591	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	199	ASP	CB-CG-OD1	5.53	123.27	118.30
1	B	222	GLU	CA-CB-CG	5.50	125.51	113.40
1	B	605	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	304	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	B	238	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	371	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	152	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	284	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	B	448	ARG	NE-CZ-NH1	5.29	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	642	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	419	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	551	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	546	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	B	152	TYR	CB-CG-CD2	-5.18	117.89	121.00
1	A	228	LYS	CD-CE-NZ	-5.14	99.87	111.70
1	B	419	TYR	CB-CG-CD1	5.12	124.07	121.00
1	B	471	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	B	273	GLU	OE1-CD-OE2	-5.09	117.20	123.30
1	B	578	THR	CA-CB-CG2	-5.09	105.28	112.40
1	A	433	ARG	CG-CD-NE	-5.08	101.13	111.80
1	B	597	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	320	ASP	CB-CG-OD1	5.04	122.83	118.30
1	B	388	ASP	CB-CG-OD1	5.01	122.81	118.30

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	21	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	40	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.

All (40) 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:A:117:THR:HB	1:A:143:ILE:HD12	1.71	0.72
1:B:33:LEU:HD23	1:B:33:LEU:C	2.12	0.69
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
1:A:96:LYS:HD2	1:A:516:LEU:HD21	1.89	0.54
1:B:657:PRO:HD2	1:B:660:LEU:HD22	1.89	0.54
1:B:78:VAL:CG1	1:B:107:GLY:HA2	2.39	0.52
1:A:615:ASP:C	1:A:617:ASP:HA	2.27	0.52
1:B:623:SER:OG	1:B:630:ARG:HD3	2.10	0.51
1:B:240:VAL:HB	1:B:309:VAL:HG11	1.93	0.50
1:A:225:ASN:HD21	1:A:301:THR:HG21	1.76	0.50
1:A:225:ASN:HD22	1:A:225:ASN:H	1.62	0.48
1:B:187:CYS:HB3	1:B:466:PRO:HD3	1.94	0.48
1:B:36:ARG:HG3	1:B:36:ARG:HH21	1.79	0.47
1:B:479:LYS:HE3	5:B:973:HOH:O	2.14	0.47
1:A:189:CYS:HB2	5:A:996:HOH:O	2.14	0.47
1:B:258:ILE:HD11	1:B:306:TYR:CE1	2.50	0.47
1:A:399:ARG:HG3	1:A:403:GLU:OE1	2.16	0.45
1:B:189:CYS:HB2	5:B:1003:HOH:O	2.16	0.45
1:A:212:TYR:CE2	1:A:461:LYS:HD3	2.53	0.44
1:B:148:ILE:HD12	1:B:148:ILE:HG23	1.81	0.44
1:A:187:CYS:HB3	1:A:466:PRO:HD3	1.99	0.44
1:B:219:LEU:HB3	1:B:306:TYR:CE1	2.53	0.43
1:B:177:PRO:HB3	1:B:493:TRP:CE3	2.53	0.43
1:B:33:LEU:CD2	1:B:33:LEU:C	2.85	0.43
1:A:335:LYS:HG3	1:A:335:LYS:HZ2	1.61	0.43
1:A:395:TYR:CZ	1:A:397:ALA:HB3	2.54	0.43
1:B:106:THR:O	1:B:107:GLY:O	2.37	0.42
1:A:509:ILE:HD13	1:A:509:ILE:HG21	1.83	0.42
1:B:506:LYS:HA	1:B:509:ILE:HG12	2.02	0.42
1:A:623:SER:OG	1:A:630:ARG:HD3	2.19	0.42
1:B:391:ILE:HB	1:B:411:LEU:HD23	2.03	0.41
1:A:615:ASP:C	1:A:615:ASP:OD2	2.58	0.41
1:A:142:VAL:O	1:A:143:ILE:HD13	2.21	0.41
1:A:418:LEU:HB3	1:A:462:VAL:HA	2.02	0.41
1:B:360:ASP:OD2	1:B:388:ASP:OD1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:TYR:CE1	1:B:33:LEU:HD21	2.56	0.40
1:A:42:TYR:CG	1:A:137:SER:HA	2.57	0.40
1:B:78:VAL:HG11	1:B:107:GLY:HA2	2.04	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	631/644 (98%)	615 (98%)	15 (2%)	1 (0%)	51	35
1	B	630/644 (98%)	619 (98%)	9 (1%)	2 (0%)	44	29
All	All	1261/1288 (98%)	1234 (98%)	24 (2%)	3 (0%)	51	35

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 [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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	530/540 (98%)	519 (98%)	11 (2%)	59 46
1	B	529/540 (98%)	513 (97%)	16 (3%)	46 30
All	All	1059/1080 (98%)	1032 (98%)	27 (2%)	53 38

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	209	ARG
1	A	212	TYR
1	A	222	GLU
1	A	225	ASN
1	A	327	SER
1	A	335	LYS
1	A	433	ARG
1	A	525	PRO
1	A	567	LEU
1	A	617	ASP
1	B	48	VAL
1	B	66	THR
1	B	103	LYS
1	B	112	LYS
1	B	209	ARG
1	B	222	GLU
1	B	223	GLU
1	B	243	PHE
1	B	294	GLU
1	B	340	LYS
1	B	379	ASN
1	B	384	SER
1	B	547	ILE
1	B	567	LEU
1	B	616	LYS
1	B	660	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	B	134	ASN
1	B	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	GAL	A	701	3	11,11,12	1.11	0	13,15,17	1.47	2 (15%)
3	NGT	A	702	2	13,15,15	2.35	1 (7%)	11,22,22	1.90	5 (45%)
4	SO4	A	703	-	4,4,4	0.44	0	6,6,6	0.85	0
4	SO4	A	704	-	4,4,4	0.51	0	6,6,6	1.94	2 (33%)
4	SO4	A	705	-	4,4,4	0.93	0	6,6,6	0.94	0
4	SO4	A	706	-	4,4,4	1.05	0	6,6,6	0.50	0
2	GAL	B	701	3	11,11,12	1.49	2 (18%)	13,15,17	1.26	1 (7%)
3	NGT	B	702	2	13,15,15	3.49	4 (30%)	11,22,22	2.02	4 (36%)
4	SO4	B	703	-	4,4,4	0.46	0	6,6,6	0.59	0
4	SO4	B	704	-	4,4,4	0.91	0	6,6,6	0.95	0
4	SO4	B	705	-	4,4,4	0.68	0	6,6,6	0.56	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	NGT	A	702	2	-	0/2/30/30	0/2/2/2
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
4	SO4	A	706	-	-	0/0/0/0	0/0/0/0
2	GAL	B	701	3	-	0/2/19/22	0/1/1/1
3	NGT	B	702	2	-	0/2/30/30	0/2/2/2
4	SO4	B	703	-	-	0/0/0/0	0/0/0/0
4	SO4	B	704	-	-	0/0/0/0	0/0/0/0
4	SO4	B	705	-	-	0/0/0/0	0/0/0/0

All (7) 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	C2-N2	2.12	1.50	1.47
2	B	701	GAL	C4-C3	2.50	1.58	1.52
2	B	701	GAL	C4-C5	2.53	1.58	1.53
3	B	702	NGT	O5-C1	3.45	1.48	1.42
3	B	702	NGT	C7-N2	4.04	1.30	1.27

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NGT	C3-C4-C5	-3.81	103.50	110.22
2	A	701	GAL	O2-C2-C3	-3.57	103.17	110.17
3	A	702	NGT	O3-C3-C2	-2.92	102.26	109.02
4	A	704	SO4	O4-S-O2	-2.57	95.10	109.26
3	A	702	NGT	C3-C4-C5	-2.51	105.80	110.22
4	A	704	SO4	O4-S-O1	-2.32	96.48	109.26
2	A	701	GAL	O4-C4-C3	-2.29	105.38	110.36
3	B	702	NGT	O5-C5-C6	-2.24	101.05	106.41
3	B	702	NGT	O3-C3-C2	-2.02	104.34	109.02
2	B	701	GAL	O5-C1-C2	-2.00	107.66	110.79
3	A	702	NGT	C1-O5-C5	2.09	116.72	112.69
3	A	702	NGT	O4-C4-C3	2.36	115.48	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NGT	C6-C5-C4	2.70	119.33	113.00
3	A	702	NGT	C8-C7-S1	2.97	123.43	118.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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%)	-0.36	8 (1%) 77 74	4, 10, 23, 68	0
1	B	632/644 (98%)	-0.36	5 (0%) 86 84	4, 9, 24, 70	0
All	All	1265/1288 (98%)	-0.36	13 (1%) 82 80	4, 10, 24, 70	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	LYS	6.8
1	B	617	ASP	6.6
1	A	616	LYS	6.3
1	A	618	GLY	6.3
1	A	617	ASP	5.6
1	B	618	GLY	4.2
1	B	107	GLY	3.3
1	A	224	ASP	3.1
1	B	615	ASP	3.1
1	A	662	SER	2.6
1	A	30	SER	2.6
1	A	37	GLY	2.4
1	A	99	ASP	2.2

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 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	0.93	0.17	7.34	33,37,38,40	0
4	SO4	A	705	5/5	0.94	0.14	3.69	33,36,42,43	0
4	SO4	A	704	5/5	0.97	0.11	0.86	20,26,27,29	0
2	GAL	A	701	11/12	0.95	0.09	-0.28	10,11,12,12	0
2	GAL	B	701	11/12	0.96	0.09	-0.31	8,9,10,10	0
3	NGT	B	702	14/14	0.98	0.08	-0.46	7,9,10,10	0
3	NGT	A	702	14/14	0.98	0.07	-1.64	9,11,12,13	0
4	SO4	A	703	5/5	0.99	0.07	-1.88	8,9,10,11	0
4	SO4	B	703	5/5	0.99	0.05	-3.47	6,7,8,8	0
4	SO4	A	706	5/5	0.97	0.15	-	21,23,24,30	0
4	SO4	B	705	5/5	0.97	0.09	-	16,20,22,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.