



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:02 PM GMT

PDB ID : 5BXP  
Title : LNBase in complex with LNB-LOGNAc  
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Deposited on : 2015-06-09  
Resolution : 1.70 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](mailto: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.

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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

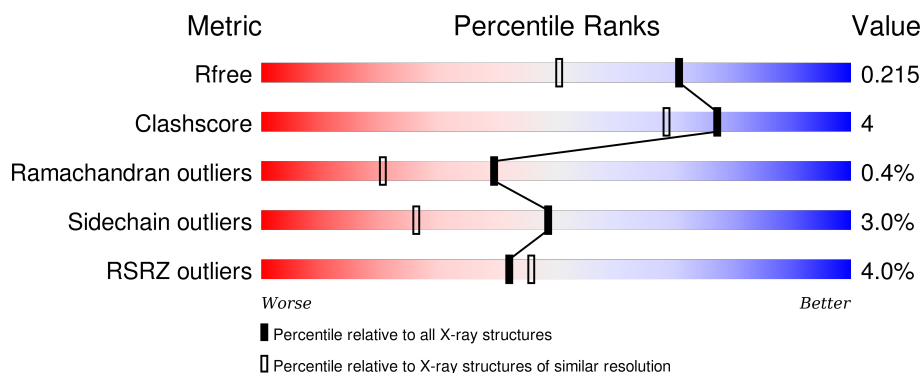
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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  $\geq 3$ , 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>87%</div> <div>10% ..</div> </div>
1	B	644	<div> <div>4%</div> <div>86%</div> <div>10% ...</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	703	-	-	-	X
4	SO4	B	704	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11012 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	636	Total	C	N	O	S	0	0	0
			4997	3148	853	979	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:

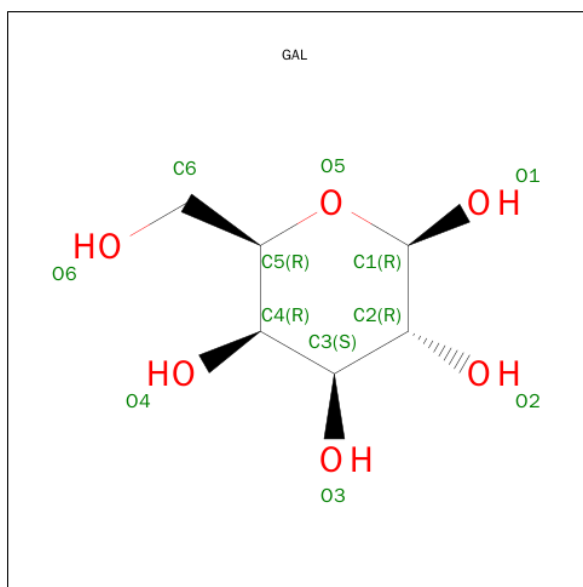
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP B3TLD6
A	21	GLY	-	expression tag	UNP B3TLD6
A	22	SER	-	expression tag	UNP B3TLD6
A	23	SER	-	expression tag	UNP B3TLD6
A	24	HIS	-	expression tag	UNP B3TLD6
A	25	HIS	-	expression tag	UNP B3TLD6
A	26	HIS	-	expression tag	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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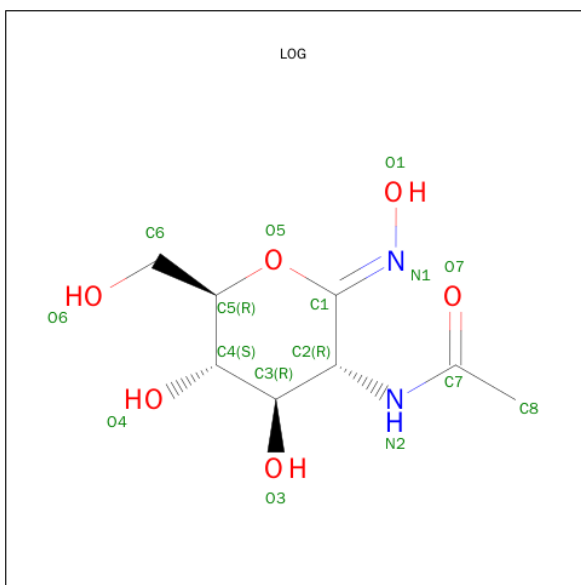
Chain	Residue	Modelled	Actual	Comment	Reference
B	24	HIS	-	expression tag	UNP B3TLD6
B	25	HIS	-	expression tag	UNP B3TLD6
B	26	HIS	-	expression tag	UNP B3TLD6
B	27	HIS	-	expression tag	UNP B3TLD6
B	28	HIS	-	expression tag	UNP B3TLD6
B	29	HIS	-	expression tag	UNP B3TLD6
B	30	SER	-	expression tag	UNP B3TLD6
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:  $C_6H_{12}O_6$ ).



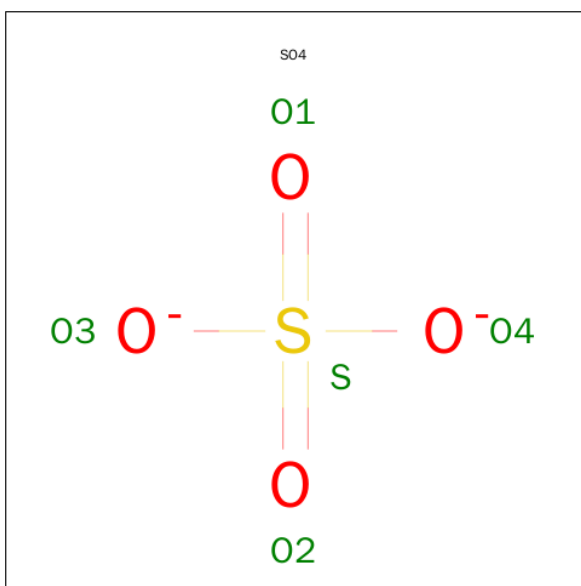
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 3 is LOGNAC (three-letter code: LOG) (formula:  $C_8H_{14}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	8	2	6		
3	B	1	Total	C	N	O	0	0
			16	8	2	6		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

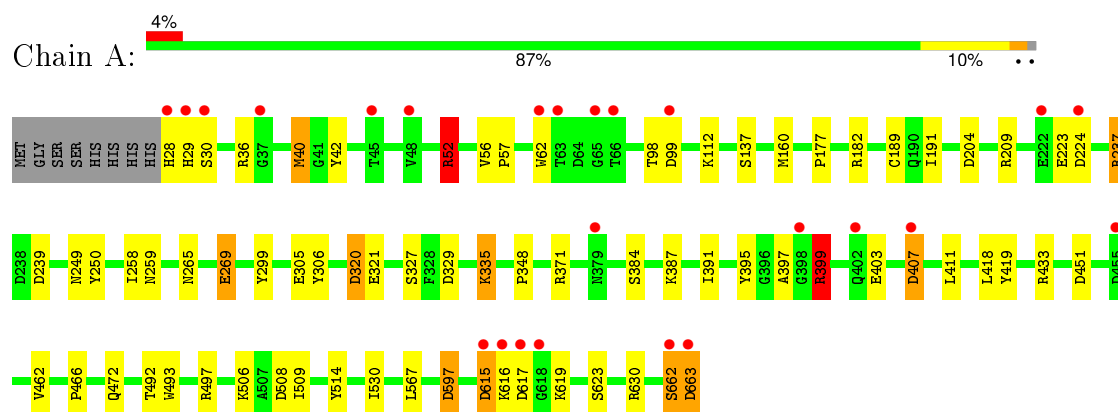
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	460	Total	O	0	0
			460	460		
5	B	479	Total	O	0	0
			479	479		

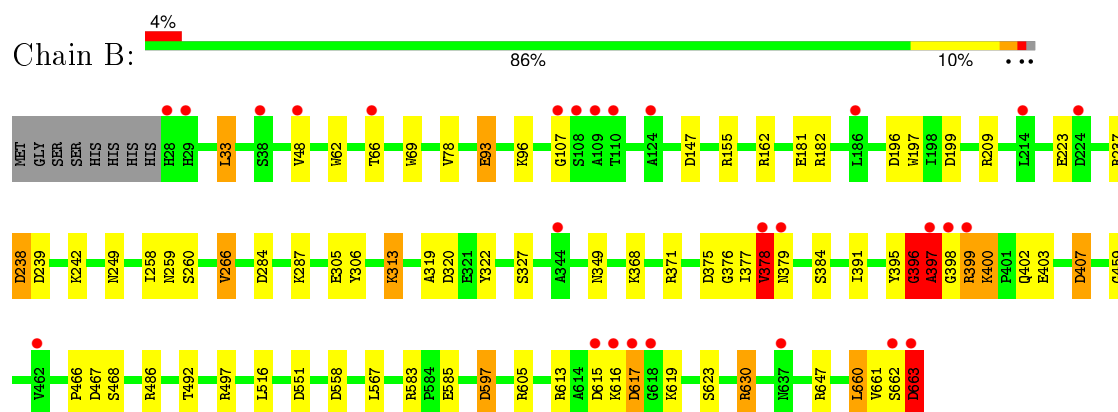
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Lacto-N-biosidase



#### • Molecule 1: Lacto-N-biosidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.76Å 131.62Å 104.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 1.70 29.94 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.94-1.70) 99.6 (29.94-1.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.35 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.175 , 0.206 0.186 , 0.215	Depositor DCC
$R_{free}$ test set	8805 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.6	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 44.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 175883 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11012	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.33% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, LOG, 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	1.25	13/5108 (0.3%)	1.21	24/6932 (0.3%)
1	B	1.27	12/5108 (0.2%)	1.22	32/6932 (0.5%)
All	All	1.26	25/10216 (0.2%)	1.21	56/13864 (0.4%)

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	1
1	B	0	4
All	All	0	5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	376	GLY	N-CA	11.55	1.63	1.46
1	A	597	ASP	CB-CG	8.35	1.69	1.51
1	A	269	GLU	CB-CG	-7.27	1.38	1.52
1	B	497	ARG	CZ-NH2	7.20	1.42	1.33
1	B	62	TRP	CB-CG	-7.10	1.37	1.50
1	B	376	GLY	CA-C	7.04	1.63	1.51
1	A	269	GLU	CD-OE2	-6.94	1.18	1.25
1	A	223	GLU	CD-OE2	-6.85	1.18	1.25
1	A	237	ARG	CD-NE	-6.71	1.35	1.46
1	A	269	GLU	CD-OE1	6.57	1.32	1.25
1	B	223	GLU	CG-CD	-6.45	1.42	1.51
1	B	93	GLU	CB-CG	-6.02	1.40	1.52
1	A	299	TYR	CE2-CZ	-5.65	1.31	1.38
1	A	321	GLU	CD-OE1	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	597	ASP	CB-CG	5.61	1.63	1.51
1	B	69	TRP	CG-CD1	5.58	1.44	1.36
1	A	371	ARG	CZ-NH1	5.50	1.40	1.33
1	B	319	ALA	C-O	-5.46	1.12	1.23
1	A	62	TRP	CG-CD1	5.41	1.44	1.36
1	B	260	SER	CB-OG	5.38	1.49	1.42
1	A	472	GLN	CB-CG	-5.28	1.38	1.52
1	A	514	TYR	CE1-CZ	-5.26	1.31	1.38
1	B	585	GLU	CD-OE2	5.18	1.31	1.25
1	B	197	TRP	CG-CD1	-5.04	1.29	1.36
1	A	399	ARG	CB-CG	-5.00	1.39	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ARG	NE-CZ-NH2	-27.40	106.60	120.30
1	A	237	ARG	CD-NE-CZ	12.86	141.60	123.60
1	A	237	ARG	NE-CZ-NH1	12.44	126.52	120.30
1	A	52	ARG	NE-CZ-NH2	12.13	126.36	120.30
1	B	266	VAL	CG1-CB-CG2	10.24	127.28	110.90
1	B	239	ASP	CB-CG-OD1	9.57	126.92	118.30
1	A	433	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	A	497	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	B	322	TYR	CB-CG-CD1	8.00	125.80	121.00
1	B	237	ARG	NE-CZ-NH2	7.65	124.12	120.30
1	A	305	GLU	OE1-CD-OE2	-7.54	114.25	123.30
1	B	162	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	239	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	419	TYR	CB-CG-CD1	6.93	125.16	121.00
1	B	558	ASP	CB-CG-OD1	-6.89	112.10	118.30
1	A	269	GLU	CG-CD-OE2	-6.80	104.70	118.30
1	B	375	ASP	N-CA-C	6.70	129.09	111.00
1	A	320	ASP	CB-CG-OD2	6.67	124.31	118.30
1	B	155	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	B	239	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	B	663	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	A	52	ARG	CD-NE-CZ	6.34	132.47	123.60
1	B	660	LEU	CB-CG-CD1	6.32	121.75	111.00
1	B	647	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	486	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	A	52	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	A	451	ASP	CB-CG-OD2	-5.90	112.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	583	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	147	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	615	ASP	CB-CA-C	-5.73	98.95	110.40
1	A	419	TYR	CB-CG-CD2	-5.69	117.59	121.00
1	A	52	ARG	CG-CD-NE	5.63	123.64	111.80
1	B	378	VAL	N-CA-CB	5.61	123.85	111.50
1	B	613	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	196	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	A	329	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	204	ASP	CB-CG-OD1	5.54	123.28	118.30
1	B	399	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	238	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	597	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	269	GLU	CG-CD-OE1	5.35	129.00	118.30
1	B	467	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	B	400	LYS	N-CA-CB	-5.32	101.03	110.60
1	B	597	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	250	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	B	375	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	223	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	A	508	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	B	583	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	199	ASP	CB-CG-OD1	5.13	122.91	118.30
1	B	371	ARG	NE-CZ-NH1	-5.13	117.74	120.30
1	B	630	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	399	ARG	CB-CA-C	-5.07	100.27	110.40
1	B	605	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	B	551	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	376	GLY	CA-C-O	5.01	129.62	120.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	ARG	Sidechain
1	B	396	GLY	Peptide
1	B	397	ALA	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	4997	0	4861	31	0
1	B	4997	0	4861	44	0
2	A	11	0	10	0	0
2	B	11	0	10	0	0
3	A	16	0	13	1	0
3	B	16	0	13	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
5	A	460	0	0	6	0
5	B	479	0	0	9	0
All	All	11012	0	9768	74	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 (74) 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:B:377:ILE:HD11	1:B:391:ILE:HD13	1.34	1.04
1:B:378:VAL:HG23	1:B:379:ASN:N	1.71	1.01
1:B:378:VAL:HG23	1:B:379:ASN:H	1.32	0.93
1:B:399:ARG:NH2	1:B:407:ASP:OD2	2.04	0.90
1:B:378:VAL:CG2	1:B:379:ASN:N	2.42	0.79
1:B:597:ASP:HB3	5:B:1205:HOH:O	1.85	0.77
1:B:238:ASP:HB3	5:B:1057:HOH:O	1.86	0.74
1:B:661:VAL:C	1:B:663:ASP:HB3	2.09	0.73
1:B:33:LEU:HD23	1:B:33:LEU:C	2.09	0.73
1:B:377:ILE:HD11	1:B:391:ILE:CD1	2.17	0.72
1:B:313:LYS:O	1:B:313:LYS:HG2	1.92	0.67
1:B:78:VAL:CG1	1:B:107:GLY:C	2.63	0.66
1:B:377:ILE:CG2	1:B:399:ARG:HD3	2.26	0.65
1:A:265:ASN:O	1:A:269:GLU:HG3	1.96	0.64
1:A:615:ASP:O	1:A:617:ASP:HA	1.99	0.63
1:B:662:SER:N	1:B:663:ASP:HB3	2.14	0.63
1:B:305:GLU:CD	5:B:898:HOH:O	2.38	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ILE:HG22	1:B:399:ARG:HG3	1.81	0.61
1:A:662:SER:O	1:A:663:ASP:C	2.39	0.60
1:A:335:LYS:HG2	1:A:348:PRO:HD3	1.83	0.59
1:A:399:ARG:NH1	1:A:403:GLU:OE1	2.36	0.58
1:B:48:VAL:HG12	5:B:1077:HOH:O	2.04	0.57
1:B:78:VAL:HG12	1:B:107:GLY:O	2.06	0.56
1:B:399:ARG:HH22	1:B:407:ASP:CG	2.09	0.54
1:B:378:VAL:CG2	1:B:379:ASN:H	2.04	0.54
1:A:623:SER:OG	1:A:630:ARG:HD3	2.09	0.53
1:B:395:TYR:O	1:B:397:ALA:N	2.42	0.51
1:B:597:ASP:CB	5:B:1205:HOH:O	2.52	0.51
1:A:42:TYR:CG	1:A:137:SER:HA	2.46	0.51
1:A:40:MET:HG2	1:A:112:LYS:HE2	1.94	0.50
1:B:33:LEU:C	1:B:33:LEU:CD2	2.80	0.49
1:B:377:ILE:HG22	1:B:399:ARG:CG	2.42	0.49
1:A:506:LYS:HA	1:A:509:ILE:HG12	1.95	0.49
1:A:160:MET:CE	5:A:806:HOH:O	2.59	0.49
1:A:182:ARG:HG2	1:A:492:THR:HB	1.95	0.49
1:B:258:ILE:HD11	1:B:306:TYR:CE1	2.48	0.48
1:A:40:MET:CG	1:A:112:LYS:HE2	2.43	0.48
1:A:28:HIS:HB2	1:B:663:ASP:OD2	2.13	0.48
1:B:284:ASP:OD2	1:B:287:LYS:NZ	2.42	0.48
1:B:33:LEU:HD23	1:B:33:LEU:O	2.14	0.48
1:B:616:LYS:O	1:B:617:ASP:CB	2.61	0.48
1:B:398:GLY:HA3	5:B:804:HOH:O	2.13	0.47
1:B:349:ASN:ND2	1:B:378:VAL:CG2	2.79	0.46
1:A:249:ASN:HB3	5:A:825:HOH:O	2.15	0.46
1:A:615:ASP:HB2	1:A:619:LYS:H	1.79	0.46
1:B:259:ASN:ND2	1:B:320:ASP:OD1	2.38	0.46
1:B:242:LYS:HE3	5:B:1057:HOH:O	2.16	0.46
1:A:530:ILE:HD11	5:A:1139:HOH:O	2.16	0.46
1:A:395:TYR:CZ	1:A:397:ALA:HB3	2.50	0.46
1:A:615:ASP:OD2	1:A:619:LYS:HB2	2.16	0.45
1:A:399:ARG:HB2	5:A:1099:HOH:O	2.16	0.45
1:B:396:GLY:O	1:B:397:ALA:CB	2.64	0.45
1:A:259:ASN:ND2	1:A:320:ASP:OD1	2.45	0.45
1:A:30:SER:CB	1:B:619:LYS:HB3	2.47	0.45
1:A:177:PRO:HD3	1:A:493:TRP:CH2	2.52	0.45
1:A:387:LYS:HE3	1:A:407:ASP:O	2.18	0.44
1:B:402:GLN:NE2	1:B:402:GLN:HA	2.33	0.44
1:B:182:ARG:HG2	1:B:492:THR:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:LYS:HD2	1:B:516:LEU:HD21	1.98	0.44
1:A:56:VAL:HA	1:A:57:PRO:C	2.37	0.43
1:B:287:LYS:HE3	5:B:903:HOH:O	2.19	0.43
1:B:623:SER:OG	1:B:630:ARG:HD3	2.18	0.43
1:B:249:ASN:HB3	5:B:1037:HOH:O	2.18	0.43
1:A:418:LEU:HB3	1:A:462:VAL:HA	2.00	0.42
1:B:78:VAL:HG12	1:B:107:GLY:C	2.37	0.42
1:A:191:ILE:HD12	1:A:191:ILE:C	2.40	0.42
1:A:391:ILE:HB	1:A:411:LEU:HD23	2.02	0.41
3:A:702:LOG:O7	3:A:702:LOG:C1	2.67	0.41
1:A:52:ARG:CZ	5:A:850:HOH:O	2.67	0.41
1:B:313:LYS:CG	1:B:313:LYS:O	2.66	0.41
1:A:98:THR:O	1:A:99:ASP:HB2	2.20	0.41
1:A:258:ILE:HD11	1:A:306:TYR:CE1	2.56	0.41
1:A:189:CYS:HB2	5:A:1132:HOH:O	2.21	0.41
1:B:181:GLU:O	1:B:459:GLY:HA3	2.21	0.41

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	634/644 (98%)	619 (98%)	14 (2%)	1 (0%)	52	32
1	B	634/644 (98%)	615 (97%)	15 (2%)	4 (1%)	30	12
All	All	1268/1288 (98%)	1234 (97%)	29 (2%)	5 (0%)	39	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	GLY
1	B	397	ALA

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/540 (99%)	517 (97%)	16 (3%)	48	26
1	B	533/540 (99%)	517 (97%)	16 (3%)	48	26
All	All	1066/1080 (99%)	1034 (97%)	32 (3%)	48	26

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	36	ARG
1	A	40	MET
1	A	52	ARG
1	A	209	ARG
1	A	224	ASP
1	A	327	SER
1	A	335	LYS
1	A	384	SER
1	A	399	ARG
1	A	407	ASP
1	A	567	LEU
1	A	597	ASP
1	A	616	LYS
1	A	662	SER
1	A	663	ASP
1	B	33	LEU
1	B	66	THR
1	B	93	GLU
1	B	209	ARG

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Mol	Chain	Res	Type
1	B	266	VAL
1	B	313	LYS
1	B	327	SER
1	B	368	LYS
1	B	378	VAL
1	B	384	SER
1	B	400	LYS
1	B	403	GLU
1	B	407	ASP
1	B	567	LEU
1	B	660	LEU
1	B	663	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
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 ⓘ

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 ⓘ

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	1.36	2 (18%)	15,15,17	2.07	3 (20%)
3	LOG	A	702	2	12,16,16	1.51	2 (16%)	12,22,22	2.24	3 (25%)
4	SO4	A	703	-	4,4,4	0.99	0	6,6,6	0.75	0
4	SO4	A	704	-	4,4,4	1.65	1 (25%)	6,6,6	0.57	0
4	SO4	A	705	-	4,4,4	1.26	0	6,6,6	0.23	0
2	GAL	B	701	3	11,11,12	1.16	0	15,15,17	1.45	2 (13%)
3	LOG	B	702	2	12,16,16	1.37	2 (16%)	12,22,22	1.48	2 (16%)
4	SO4	B	703	-	4,4,4	2.26	2 (50%)	6,6,6	0.93	0
4	SO4	B	704	-	4,4,4	0.62	0	6,6,6	0.25	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	LOG	A	702	2	-	0/6/28/28	0/1/1/1
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	LOG	B	702	2	-	0/6/28/28	0/1/1/1
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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	GAL	C2-C3	-3.27	1.48	1.52
3	B	702	LOG	C8-C7	2.04	1.54	1.50
2	A	701	GAL	C4-C5	2.10	1.57	1.53
3	A	702	LOG	O7-C7	2.10	1.28	1.23
4	A	704	SO4	O1-S	2.26	1.55	1.47
4	B	703	SO4	O1-S	2.61	1.56	1.47
3	B	702	LOG	O1-N1	2.77	1.48	1.40
4	B	703	SO4	O3-S	3.45	1.59	1.47
3	A	702	LOG	O1-N1	4.06	1.52	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	GAL	O3-C3-C2	-5.97	99.06	110.01
3	A	702	LOG	C2-N2-C7	-5.03	115.37	122.06
3	B	702	LOG	C3-C4-C5	-3.90	103.26	110.23
3	A	702	LOG	C3-C4-C5	-3.74	103.56	110.23
2	B	701	GAL	O2-C2-C3	-3.18	103.77	110.19
3	B	702	LOG	C2-N2-C7	-2.50	118.74	122.06
2	A	701	GAL	O5-C1-C2	2.84	115.44	110.89
3	A	702	LOG	O4-C4-C3	2.96	117.03	110.36
2	B	701	GAL	O5-C5-C4	3.03	115.16	110.13
2	A	701	GAL	O3-C3-C4	3.25	117.70	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	LOG	1	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	636/644 (98%)	0.07	24 (3%) 44 49	11, 18, 35, 76	0
1	B	636/644 (98%)	0.09	27 (4%) 40 44	10, 18, 36, 68	0
All	All	1272/1288 (98%)	0.08	51 (4%) 42 46	10, 18, 36, 76	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	HIS	7.3
1	B	29	HIS	6.8
1	B	663	ASP	6.7
1	A	616	LYS	6.3
1	B	398	GLY	5.9
1	B	616	LYS	5.8
1	A	663	ASP	5.7
1	A	617	ASP	5.5
1	B	617	ASP	5.5
1	B	662	SER	4.8
1	B	379	ASN	4.4
1	B	107	GLY	4.3
1	A	618	GLY	4.2
1	B	399	ARG	4.1
1	B	28	HIS	4.0
1	A	224	ASP	4.0
1	A	662	SER	3.9
1	B	378	VAL	3.8
1	A	28	HIS	3.8
1	B	397	ALA	3.6
1	A	379	ASN	3.6
1	A	398	GLY	3.3
1	A	45	THR	3.2
1	B	109	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	66	THR	3.1
1	A	37	GLY	3.0
1	B	618	GLY	2.9
1	A	99	ASP	2.9
1	A	30	SER	2.8
1	A	63	THR	2.8
1	A	62	TRP	2.8
1	A	222	GLU	2.7
1	B	110	THR	2.7
1	B	344	ALA	2.7
1	A	407	ASP	2.7
1	B	224	ASP	2.6
1	B	66	THR	2.4
1	A	48	VAL	2.4
1	B	615	ASP	2.4
1	B	108	SER	2.3
1	B	124	ALA	2.2
1	A	615	ASP	2.2
1	B	38	SER	2.2
1	A	402	GLN	2.2
1	B	462	VAL	2.2
1	B	48	VAL	2.1
1	B	637	ASN	2.1
1	B	186	LEU	2.1
1	A	65	GLY	2.1
1	A	455	ASP	2.0
1	B	214	LEU	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	A	703	5/5	0.97	0.18	2.84	26,32,35,37	0
4	SO4	B	704	5/5	1.00	0.08	2.26	16,17,18,18	0
4	SO4	A	705	5/5	0.99	0.07	1.36	17,18,19,22	0
3	LOG	B	702	16/16	0.90	0.11	1.29	16,19,21,28	0
3	LOG	A	702	16/16	0.91	0.11	0.97	17,21,23,34	0
2	GAL	A	701	11/12	0.91	0.10	0.38	18,21,23,24	0
2	GAL	B	701	11/12	0.93	0.09	-0.51	17,18,22,22	0
4	SO4	B	703	5/5	0.89	0.22	-	26,30,36,41	0
4	SO4	A	704	5/5	0.95	0.28	-	28,30,35,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.