



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:46 PM UTC

PDB ID : 5BXT / pdb_00005bxt
Title : LNBase in complex with LNB-NHAcAUS
Authors : Ito, T.; Arakawa, T.; Fushinobu, S.
Deposited on : 2015-06-09
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

<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

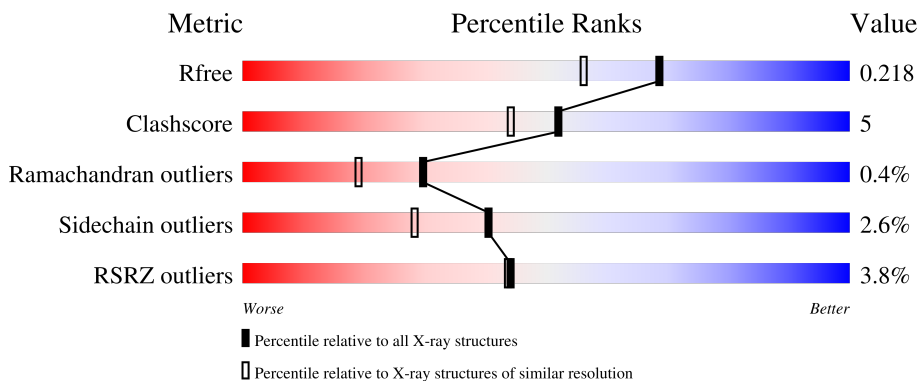
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (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 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	 2% 90% 8% ...
1	B	644	 5% 85% 11% ...

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10926 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	633	4969	3132	846	974	17	0	0	0
1	B	634	4983	3141	851	974	17	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

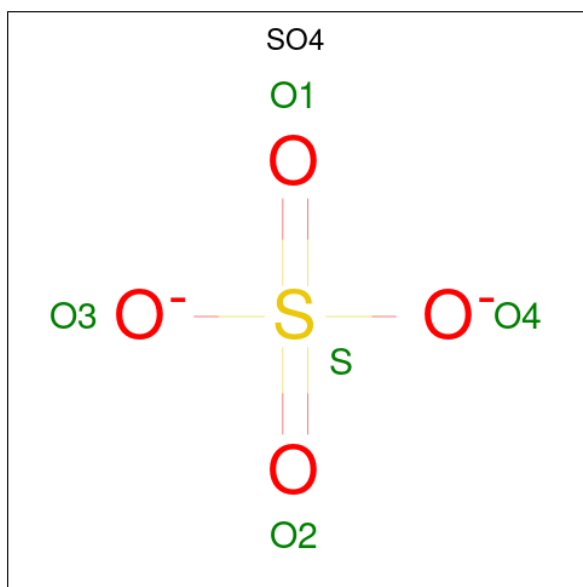
Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP B3TLD6
A	21	GLY	-	expression tag	UNP B3TLD6
A	22	SER	-	expression tag	UNP B3TLD6
A	23	SER	-	expression tag	UNP B3TLD6
A	24	HIS	-	expression tag	UNP B3TLD6
A	25	HIS	-	expression tag	UNP B3TLD6
A	26	HIS	-	expression tag	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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



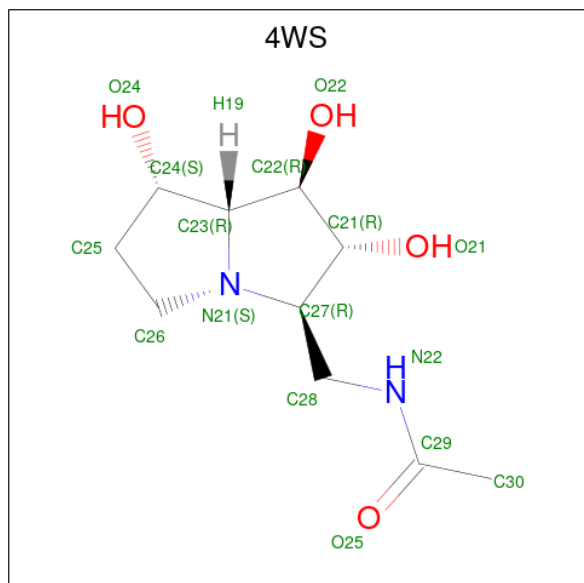
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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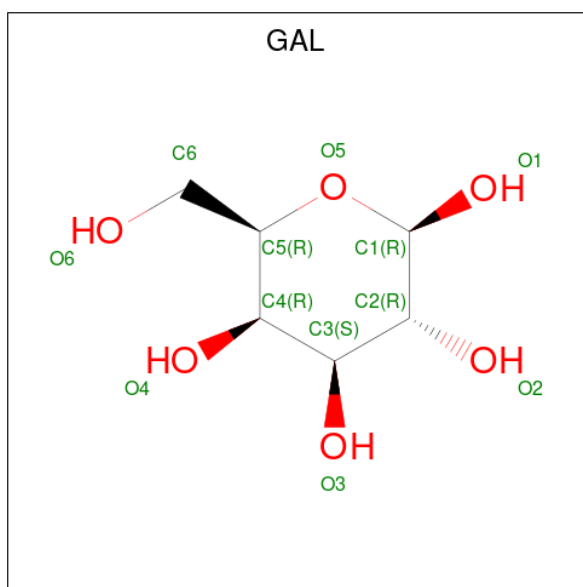
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is N-[[[(1R,2R,3R,7S,7aR)-1,2,7-trihydroxyhexahydro-1H-pyrrolizin-3-yl]methyl]acetamide (CCD ID: 4WS) (formula: C₁₀H₁₈N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	10	2	4		
3	B	1	Total	C	N	O	0	0
			16	10	2	4		

- Molecule 4 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



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

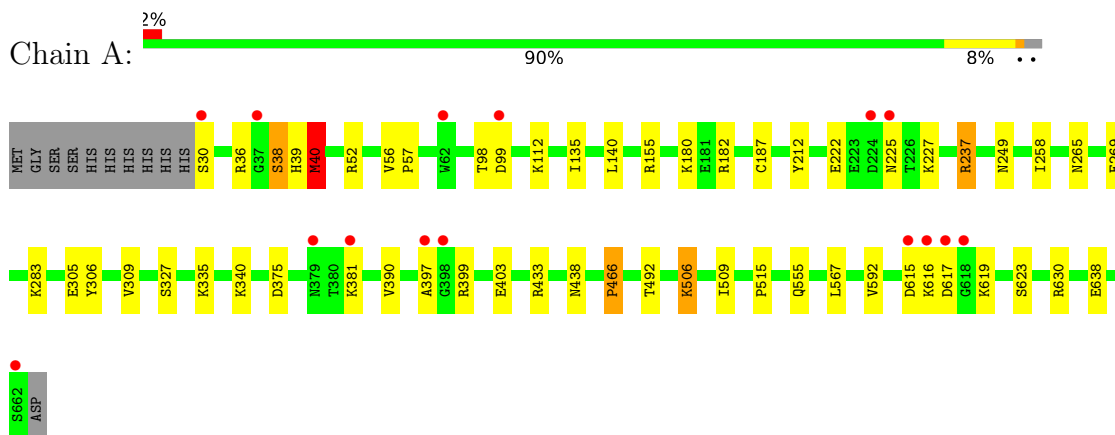
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	456	Total O 456 456	0	0
5	B	439	Total O 439 439	0	0

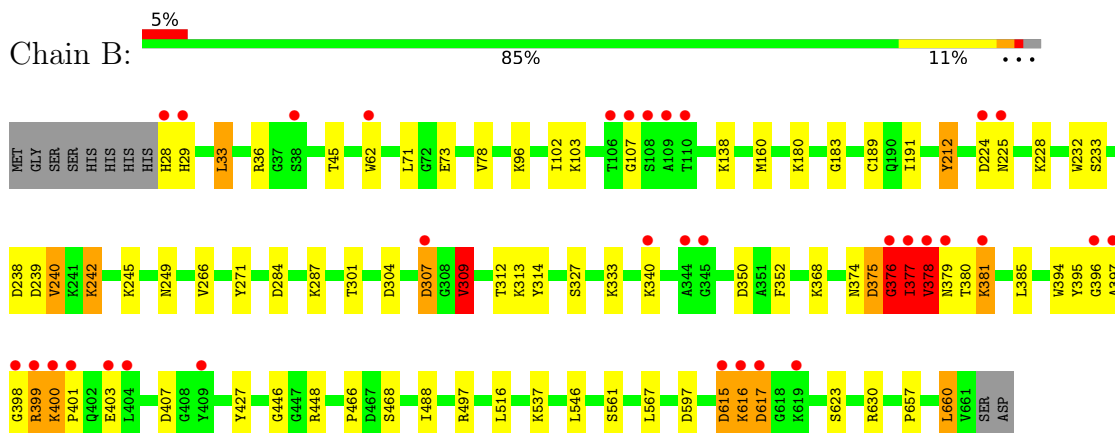
3 Residue-property plots [i](#)

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



- 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	116.98Å 131.51Å 104.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.42 – 1.80 30.42 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.42-1.80) 99.9 (30.42-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.177 , 0.209 0.187 , 0.218	Depositor DCC
R_{free} test set	7449 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtrriage
Anisotropy	0.033	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10926	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: GAL, SO4, 4WS

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	1.34	8/5078 (0.2%)	1.14	7/6891 (0.1%)
1	B	1.37	11/5094 (0.2%)	1.19	15/6913 (0.2%)
All	All	1.36	19/10172 (0.2%)	1.17	22/13804 (0.2%)

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	3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	ASN	CA-C	6.58	1.61	1.52
1	A	390	VAL	C-O	-6.39	1.17	1.24
1	B	400	LYS	CA-C	6.39	1.61	1.52
1	B	497	ARG	CZ-NH2	6.20	1.41	1.33
1	B	352	PHE	C-O	-6.08	1.17	1.24
1	B	309	VAL	C-O	-6.01	1.17	1.23
1	A	340	LYS	C-O	-5.94	1.17	1.24
1	A	155	ARG	N-CA	5.85	1.53	1.46
1	B	400	LYS	C-N	5.74	1.41	1.34
1	B	397	ALA	CA-C	5.71	1.59	1.52
1	A	309	VAL	N-CA	5.70	1.51	1.46
1	A	515	PRO	C-O	5.67	1.30	1.23
1	B	561	SER	C-O	-5.43	1.16	1.24
1	B	399	ARG	C-O	5.37	1.30	1.23
1	B	240	VAL	CA-CB	-5.11	1.48	1.54
1	B	546	LEU	C-O	5.11	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	ARG	CD-NE	-5.06	1.39	1.46
1	B	397	ALA	N-CA	5.04	1.51	1.46
1	A	375	ASP	C-O	-5.01	1.16	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	ASP	N-CA-C	11.19	126.44	113.01
1	B	377	ILE	N-CA-C	8.71	135.40	111.00
1	A	237	ARG	NE-CZ-NH2	-7.99	112.01	119.20
1	B	378	VAL	N-CA-C	6.56	116.83	108.82
1	A	438	ASN	N-CA-C	6.39	120.38	112.58
1	B	307	ASP	N-CA-C	6.33	121.81	111.37
1	A	237	ARG	CG-CD-NE	-6.27	98.20	112.00
1	A	38	SER	N-CA-C	5.85	118.72	110.23
1	B	312	THR	N-CA-C	5.69	117.64	110.24
1	A	397	ALA	N-CA-C	-5.66	102.91	110.55
1	B	397	ALA	N-CA-C	5.45	116.69	108.46
1	B	376	GLY	N-CA-C	-5.31	97.90	113.30
1	B	376	GLY	CA-C-O	-5.22	109.83	120.80
1	B	537	LYS	N-CA-C	5.17	117.65	111.71
1	B	242	LYS	N-CA-C	5.15	116.58	111.07
1	A	40	MET	CG-SD-CE	5.05	112.02	100.90
1	B	376	GLY	CA-C-N	5.05	130.80	121.70
1	B	376	GLY	C-N-CA	5.05	130.80	121.70
1	B	224	ASP	N-CA-C	5.03	116.77	111.28
1	B	400	LYS	N-CA-CB	-5.02	102.75	109.88
1	A	506	LYS	N-CA-C	5.02	116.75	111.28
1	B	307	ASP	CB-CA-C	-5.01	102.43	110.74

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	376	GLY	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	4969	0	4843	30	0
1	B	4983	0	4852	70	0
2	A	15	0	0	0	0
2	B	10	0	0	0	0
3	A	16	0	17	1	0
3	B	16	0	17	1	0
4	A	11	0	10	0	0
4	B	11	0	10	0	0
5	A	456	0	0	8	0
5	B	439	0	0	15	0
All	All	10926	0	9749	100	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 5.

All (100) 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:374:ASN:O	1:B:376:GLY:HA3	1.53	1.07
1:B:160:MET:HE3	5:B:802:HOH:O	1.67	0.91
1:B:374:ASN:C	1:B:376:GLY:HA3	1.96	0.90
1:B:400:LYS:HG3	1:B:401:PRO:HD3	1.55	0.88
1:A:222:GLU:HB3	5:A:970:HOH:O	1.73	0.86
1:B:399:ARG:NH2	1:B:407:ASP:OD2	2.10	0.83
1:B:597:ASP:HB3	5:B:1177:HOH:O	1.80	0.81
1:B:374:ASN:C	1:B:376:GLY:CA	2.55	0.80
1:B:400:LYS:HG3	1:B:401:PRO:CD	2.12	0.80
1:B:375:ASP:N	1:B:376:GLY:CA	2.48	0.77
1:B:33:LEU:C	1:B:33:LEU:HD23	2.10	0.77
1:B:180:LYS:HE3	5:B:1021:HOH:O	1.84	0.77
1:B:238:ASP:HB3	5:B:829:HOH:O	1.84	0.77
1:B:375:ASP:N	1:B:376:GLY:HA2	2.02	0.74
1:A:38:SER:HA	5:A:808:HOH:O	1.90	0.72
1:B:377:ILE:N	1:B:377:ILE:HD13	2.05	0.70
1:A:283:LYS:HE2	5:A:837:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:VAL:HG23	1:B:379:ASN:O	1.95	0.67
1:B:249:ASN:HB3	5:B:928:HOH:O	1.97	0.65
1:B:96:LYS:HD2	1:B:516:LEU:HD21	1.79	0.63
1:A:249:ASN:HB3	5:A:836:HOH:O	1.99	0.62
1:B:78:VAL:CG1	1:B:107:GLY:C	2.73	0.61
1:B:400:LYS:CG	1:B:401:PRO:CD	2.80	0.60
1:B:616:LYS:O	1:B:617:ASP:CB	2.50	0.60
1:B:304:ASP:O	1:B:307:ASP:HB2	2.02	0.59
1:A:40:MET:CE	1:A:40:MET:H	2.17	0.57
1:A:615:ASP:O	1:A:617:ASP:HA	2.03	0.57
1:B:78:VAL:HG12	1:B:107:GLY:C	2.28	0.57
1:A:98:THR:O	1:A:99:ASP:HB2	2.04	0.57
1:B:33:LEU:C	1:B:33:LEU:CD2	2.77	0.56
1:B:615:ASP:HB3	1:B:616:LYS:O	2.06	0.56
1:B:62:TRP:HB2	5:B:941:HOH:O	2.04	0.56
1:A:638:GLU:OE2	1:B:28:HIS:HE1	1.91	0.54
1:B:616:LYS:O	1:B:617:ASP:HB2	2.09	0.53
1:B:374:ASN:O	1:B:377:ILE:HB	2.09	0.53
1:B:377:ILE:HD12	1:B:385:LEU:HD22	1.91	0.53
1:A:506:LYS:HA	1:A:509:ILE:HG12	1.91	0.52
1:A:40:MET:HG3	1:A:112:LYS:HD3	1.90	0.52
1:B:400:LYS:HB2	5:B:805:HOH:O	2.10	0.52
1:B:225:ASN:HD21	1:B:301:THR:HG21	1.73	0.52
1:A:623:SER:OG	1:A:630:ARG:HD3	2.10	0.52
1:B:374:ASN:C	1:B:376:GLY:HA2	2.31	0.52
1:B:287:LYS:HE3	5:B:907:HOH:O	2.10	0.52
1:B:313:LYS:HE3	1:B:314:TYR:CE1	2.44	0.52
1:A:39:HIS:CD2	1:A:40:MET:HE3	2.45	0.51
1:B:657:PRO:HD2	1:B:660:LEU:HD22	1.92	0.51
1:B:597:ASP:CB	5:B:1177:HOH:O	2.51	0.51
1:B:284:ASP:OD2	1:B:287:LYS:NZ	2.40	0.51
1:B:377:ILE:N	1:B:377:ILE:CD1	2.72	0.49
1:B:446:GLY:HA3	1:B:448:ARG:NH1	2.28	0.48
1:B:377:ILE:CD1	1:B:385:LEU:HD22	2.43	0.48
1:B:427:TYR:CE2	3:B:703:4WS:H14	2.49	0.48
1:B:394:TRP:CD2	1:B:395:TYR:HB2	2.49	0.47
1:A:52:ARG:CZ	5:A:938:HOH:O	2.62	0.47
1:A:56:VAL:HA	1:A:57:PRO:C	2.38	0.47
1:B:29:HIS:HB2	5:B:825:HOH:O	2.14	0.47
1:B:398:GLY:O	1:B:399:ARG:C	2.58	0.46
1:B:239:ASP:CG	5:B:808:HOH:O	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:SER:OG	1:B:630:ARG:HD3	2.16	0.46
1:A:237:ARG:NH2	1:A:305:GLU:O	2.44	0.46
3:A:704:4WS:N21	3:A:704:4WS:O25	2.48	0.46
1:B:394:TRP:CE3	1:B:395:TYR:HB2	2.52	0.45
1:B:189:CYS:HB2	5:B:1155:HOH:O	2.16	0.45
1:A:40:MET:H	1:A:40:MET:HE3	1.81	0.45
1:B:45:THR:HA	5:B:1148:HOH:O	2.17	0.44
1:B:242:LYS:HE2	5:B:834:HOH:O	2.18	0.44
1:B:71:LEU:HD21	1:B:102:ILE:HD11	1.99	0.44
1:B:240:VAL:CG1	1:B:309:VAL:CG1	2.95	0.44
1:B:313:LYS:HE3	1:B:314:TYR:CZ	2.53	0.43
1:B:488:ILE:HD12	1:B:488:ILE:HA	1.88	0.43
1:A:38:SER:CA	5:A:808:HOH:O	2.60	0.43
1:B:36:ARG:HH21	1:B:36:ARG:HG3	1.84	0.43
1:B:380:THR:O	1:B:381:LYS:HG3	2.19	0.43
1:A:258:ILE:HD11	1:A:306:TYR:CE1	2.54	0.43
1:A:222:GLU:CB	5:A:970:HOH:O	2.46	0.43
1:A:615:ASP:OD2	1:A:619:LYS:HB2	2.18	0.43
1:A:212:TYR:C	1:A:212:TYR:CD1	2.96	0.42
1:B:242:LYS:CE	5:B:834:HOH:O	2.67	0.42
1:A:39:HIS:CG	1:A:40:MET:HE3	2.55	0.42
1:B:378:VAL:HG23	1:B:379:ASN:N	2.34	0.42
1:B:616:LYS:O	1:B:617:ASP:CG	2.63	0.42
1:A:182:ARG:HG2	1:A:492:THR:HB	2.02	0.42
1:B:78:VAL:HG12	1:B:107:GLY:O	2.20	0.42
1:B:225:ASN:OD1	1:B:225:ASN:N	2.33	0.42
1:B:350:ASP:OD1	1:B:380:THR:HB	2.19	0.42
1:A:180:LYS:HE3	5:A:1219:HOH:O	2.19	0.42
1:B:228:LYS:HB2	1:B:271:TYR:CZ	2.55	0.42
1:B:232:TRP:CG	1:B:233:SER:HA	2.55	0.41
1:B:616:LYS:CD	1:B:616:LYS:H	2.32	0.41
1:A:135:ILE:HG12	1:A:140:LEU:HG	2.02	0.41
1:B:183:GLY:HA3	1:B:212:TYR:O	2.21	0.41
1:B:313:LYS:O	1:B:313:LYS:HD2	2.21	0.41
1:B:616:LYS:N	1:B:616:LYS:HD2	2.35	0.41
1:A:399:ARG:NH2	1:A:403:GLU:OE2	2.53	0.41
1:A:555:GLN:HB2	1:A:592:VAL:HG21	2.03	0.41
1:A:265:ASN:O	1:A:269:GLU:HG3	2.21	0.41
1:B:191:ILE:C	1:B:191:ILE:HD12	2.46	0.41
1:A:187:CYS:HB3	1:A:466:PRO:HD3	2.01	0.40
1:A:615:ASP:HB2	1:A:619:LYS:H	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:GLY:HA3	1:B:377:ILE:HB	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%)	617 (98%)	13 (2%)	1 (0%)	43 31
1	B	632/644 (98%)	615 (97%)	13 (2%)	4 (1%)	21 11
All	All	1263/1288 (98%)	1232 (98%)	26 (2%)	5 (0%)	30 19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	377	ILE
1	B	396	GLY
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%)	521 (98%)	9 (2%)	53	45
1	B	531/540 (98%)	512 (96%)	19 (4%)	31	18
All	All	1061/1080 (98%)	1033 (97%)	28 (3%)	40	28

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	SER
1	A	36	ARG
1	A	40	MET
1	A	227	LYS
1	A	327	SER
1	A	335	LYS
1	A	381	LYS
1	A	567	LEU
1	A	616	LYS
1	B	33	LEU
1	B	73	GLU
1	B	103	LYS
1	B	138	LYS
1	B	212	TYR
1	B	245	LYS
1	B	266	VAL
1	B	309	VAL
1	B	327	SER
1	B	333	LYS
1	B	340	LYS
1	B	368	LYS
1	B	377	ILE
1	B	378	VAL
1	B	381	LYS
1	B	403	GLU
1	B	567	LEU
1	B	616	LYS
1	B	660	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	ASN
1	A	402	GLN
1	B	28	HIS
1	B	406	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
2	SO4	B	701	-	4,4,4	1.04	0	6,6,6	0.50	0
3	4WS	A	704	4	16,17,17	2.43	4 (25%)	21,25,25	2.28	8 (38%)
4	GAL	A	705	3	11,11,12	0.95	0	15,15,17	1.20	1 (6%)
2	SO4	B	702	-	4,4,4	1.33	0	6,6,6	0.30	0
2	SO4	A	703	-	4,4,4	1.31	0	6,6,6	0.61	0
2	SO4	A	702	-	4,4,4	1.25	0	6,6,6	0.34	0
4	GAL	B	704	3	11,11,12	0.88	0	15,15,17	1.24	1 (6%)
3	4WS	B	703	4	16,17,17	2.29	3 (18%)	21,25,25	2.28	7 (33%)
2	SO4	A	701	-	4,4,4	1.03	0	6,6,6	0.80	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
3	4WS	B	703	4	-	2/5/34/34	0/2/2/2
3	4WS	A	704	4	-	2/5/34/34	0/2/2/2
4	GAL	A	705	3	-	0/2/19/22	0/1/1/1
4	GAL	B	704	3	-	0/2/19/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	4WS	O25-C29	6.90	1.38	1.23
3	B	703	4WS	O25-C29	6.51	1.37	1.23
3	B	703	4WS	C24-C23	-4.49	1.49	1.54
3	A	704	4WS	C29-N22	4.17	1.45	1.34
3	A	704	4WS	C24-C23	-4.06	1.50	1.54
3	B	703	4WS	C29-N22	3.19	1.42	1.34
3	A	704	4WS	C23-N21	2.01	1.53	1.49

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	703	4WS	C26-C25-C24	5.78	113.19	103.95
3	A	704	4WS	O25-C29-C30	-4.26	114.47	122.05
3	A	704	4WS	C26-C25-C24	4.21	110.68	103.95
3	A	704	4WS	C24-C23-N21	4.11	111.37	104.72
3	B	703	4WS	O25-C29-C30	-4.11	114.73	122.05
3	B	703	4WS	C26-N21-C23	3.46	112.14	106.06
3	A	704	4WS	C21-C22-C23	-3.36	98.37	102.79
3	B	703	4WS	C21-C22-C23	-3.10	98.71	102.79
3	A	704	4WS	C28-N22-C29	-2.90	118.42	122.64
3	B	703	4WS	C30-C29-N22	-2.71	111.49	116.12
3	B	703	4WS	O25-C29-N22	-2.63	114.88	121.78
3	A	704	4WS	C30-C29-N22	-2.59	111.69	116.12
3	A	704	4WS	O24-C24-C25	-2.52	105.53	111.43
3	A	704	4WS	O25-C29-N22	-2.51	115.20	121.78
3	B	703	4WS	O24-C24-C25	-2.39	105.84	111.43
4	B	704	GAL	O5-C5-C6	-2.33	103.14	107.66
4	A	705	GAL	O3-C3-C2	-2.24	105.48	110.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	4WS	C27-C28-N22-C29
3	B	703	4WS	C27-C28-N22-C29
3	A	704	4WS	C30-C29-N22-C28
3	B	703	4WS	C30-C29-N22-C28

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	704	4WS	1	0
3	B	703	4WS	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, 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%)	-0.23	15 (2%) 59 60	8, 16, 32, 70	0
1	B	634/644 (98%)	-0.10	33 (5%) 33 31	7, 16, 35, 60	0
All	All	1267/1288 (98%)	-0.16	48 (3%) 44 44	7, 16, 34, 70	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	397	ALA	6.8
1	B	379	ASN	6.1
1	B	376	GLY	5.3
1	B	109	ALA	4.9
1	A	398	GLY	4.7
1	A	616	LYS	4.5
1	B	377	ILE	4.5
1	B	616	LYS	4.3
1	B	29	HIS	4.2
1	B	398	GLY	4.2
1	A	617	ASP	4.1
1	B	107	GLY	3.9
1	A	62	TRP	3.8
1	B	378	VAL	3.8
1	B	399	ARG	3.5
1	A	615	ASP	3.5
1	B	224	ASP	3.4
1	A	224	ASP	3.3
1	B	110	THR	3.3
1	B	225	ASN	3.2
1	B	400	LYS	3.1
1	B	108	SER	2.9
1	A	225	ASN	2.9
1	A	397	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	409	TYR	2.8
1	A	30	SER	2.8
1	B	62	TRP	2.8
1	A	618	GLY	2.7
1	B	28	HIS	2.5
1	A	379	ASN	2.5
1	B	617	ASP	2.5
1	B	106	THR	2.4
1	A	99	ASP	2.4
1	B	615	ASP	2.4
1	B	344	ALA	2.4
1	A	662	SER	2.4
1	B	403	GLU	2.3
1	B	38	SER	2.3
1	B	307	ASP	2.3
1	B	340	LYS	2.2
1	B	401	PRO	2.2
1	B	404	LEU	2.1
1	B	381	LYS	2.1
1	B	619	LYS	2.1
1	B	345	GLY	2.1
1	B	396	GLY	2.1
1	A	381	LYS	2.0
1	A	37	GLY	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 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(\AA^2)	Q<0.9
2	SO4	A	701	5/5	0.95	0.18	27,29,35,35	0
2	SO4	B	701	5/5	0.95	0.13	25,28,34,34	0
3	4WS	B	703	16/16	0.95	0.07	14,16,19,20	0
4	GAL	A	705	11/12	0.95	0.06	17,17,18,19	0
2	SO4	A	703	5/5	0.96	0.13	41,46,47,51	0
3	4WS	A	704	16/16	0.96	0.06	14,17,23,23	0
4	GAL	B	704	11/12	0.97	0.05	14,15,18,19	0
2	SO4	A	702	5/5	0.98	0.13	25,26,28,29	0
2	SO4	B	702	5/5	0.98	0.14	23,24,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.