WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2023 – 10:49 AM JST

PDB ID	:	5BXT
Title	:	LNBase in complex with LNB-NHAcAUS
Authors	:	Ito, T.; Arakawa, T.; Fushinobu, S.
Deposited on	:	2015-06-09
Resolution	:	1.80 Å(reported)

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

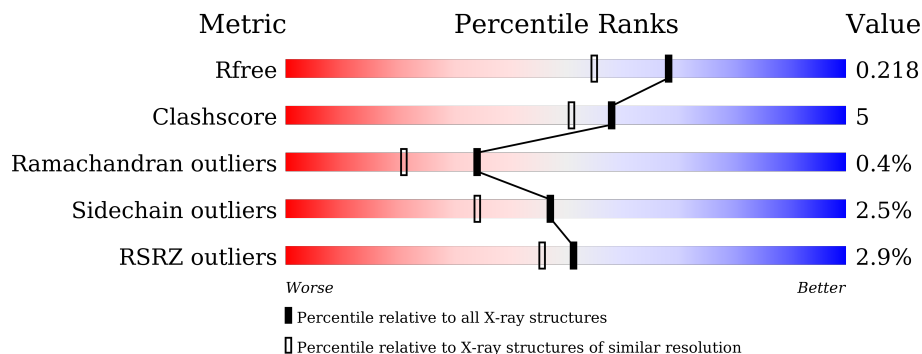|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.218
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		2.5%
RSRZ outliers		2.9%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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 <=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% / 7% ··
1	B	644	3% / 85% / 11% ··

2 Entry composition ⓘ

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
1	A	633	Total	C	N	O	S	0	0	0
			4969	3132	846	974	17			
1	B	634	Total	C	N	O	S	0	0	0
			4983	3141	851	974	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 SULFATE ION (three-letter code: SO4) (formula: O_4S).
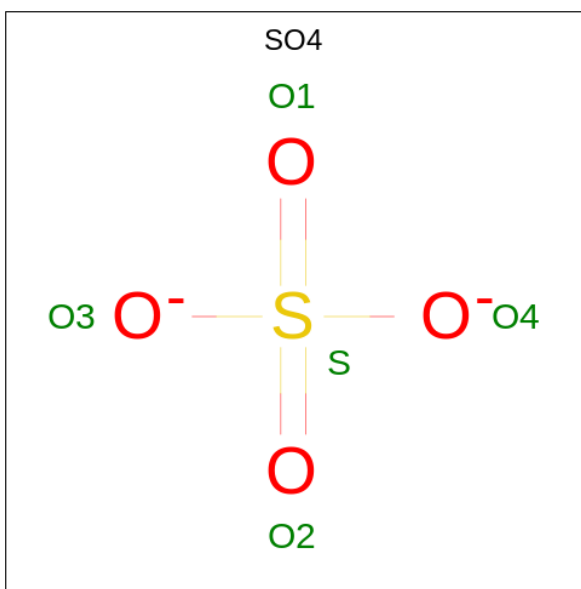
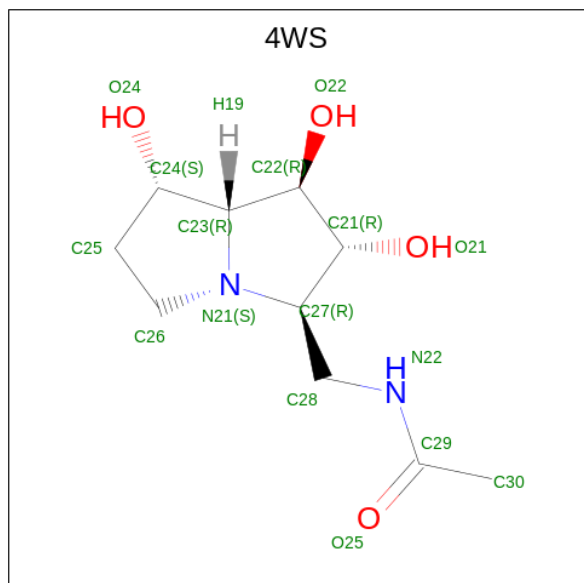
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

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

- Molecule 3 is N-{[(1R,2R,3R,7S,7aR)-1,2,7-trihydroxyhexahydro-1H-pyrrolizin-3-yl]methyl} acetamide (three-letter code: 4WS) (formula: $C_{10}H_{18}N_2O_4$).

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

- Molecule 4 is beta-D-galactopyranose (three-letter code: GAL) (formula: $C_6H_{12}O_6$).

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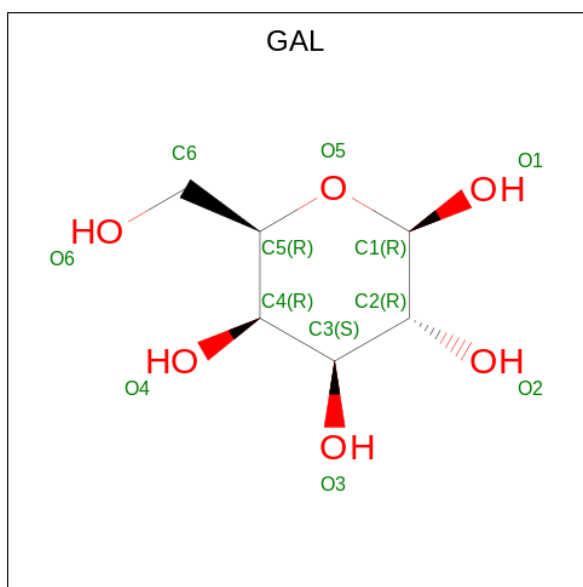
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 11	C 6	O 5	0	0
4	B	1	Total 11	C 6	O 5	0	0

• Molecule 5 is water.

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

3 Residue-property plots ⓘ

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:
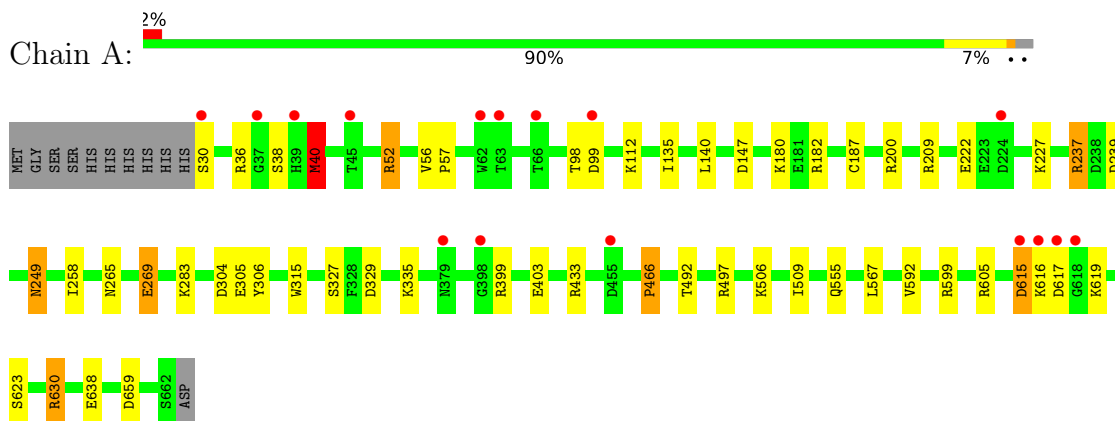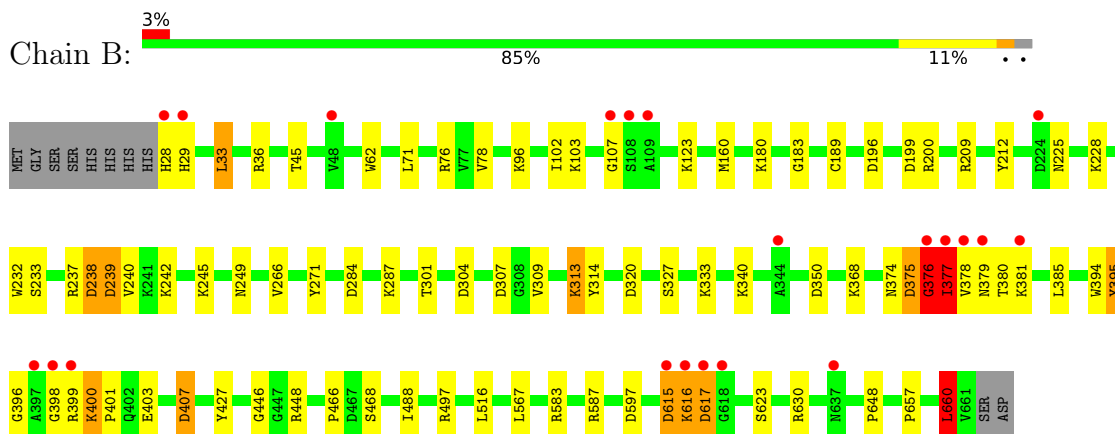
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	116.98Å　131.51Å　104.64Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	30.42　–　1.80 29.96　–　1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.42-1.80) 99.9 (29.96-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.21 (at 1.80Å)	Xtriage
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	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 44.3	EDS
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

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[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: 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	1.06	4/5078 (0.1%)	1.04	20/6891 (0.3%)
1	B	1.07	2/5094 (0.0%)	1.05	15/6913 (0.2%)
All	All	1.07	6/10172 (0.1%)	1.04	35/13804 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	GLU	CD-OE2	-6.72	1.18	1.25
1	B	497	ARG	CZ-NH2	6.51	1.41	1.33
1	B	395	TYR	CG-CD2	-6.04	1.31	1.39
1	A	269	GLU	CB-CG	-5.89	1.41	1.52
1	A	315	TRP	CG-CD1	-5.31	1.29	1.36
1	A	249	ASN	CB-CG	5.03	1.62	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ARG	NE-CZ-NH2	-16.58	112.01	120.30
1	B	587	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	A	237	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	B	377	ILE	N-CA-C	9.04	135.40	111.00
1	A	52	ARG	NE-CZ-NH1	8.45	124.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	433	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	B	239	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	40	MET	CG-SD-CE	7.39	112.02	100.20
1	A	237	ARG	CG-CD-NE	-6.48	98.20	111.80
1	B	266	VAL	CG1-CB-CG2	6.42	121.17	110.90
1	A	605	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	200	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	660	LEU	CB-CG-CD1	6.27	121.65	111.00
1	B	200	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	376	GLY	N-CA-C	-6.08	97.90	113.10
1	B	376	GLY	CA-C-O	-5.98	109.83	120.60
1	A	433	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	239	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	630	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	52	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	238	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	375	ASP	N-CA-C	5.72	126.44	111.00
1	B	237	ARG	NE-CZ-NH2	5.71	123.15	120.30
1	B	583	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	599	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	147	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	329	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	269	GLU	CG-CD-OE2	-5.46	107.39	118.30
1	B	199	ASP	CB-CG-OD1	5.38	123.15	118.30
1	A	304	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	497	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	659	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	615	ASP	CB-CA-C	-5.11	100.17	110.40
1	B	196	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	B	320	ASP	CB-CG-OD2	5.00	122.80	118.30

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 (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	4969	0	4843	27	0
1	B	4983	0	4852	68	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	95	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 (95) 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:400:LYS:HG3	1:B:401:PRO:HD3	1.55	0.88
1:A:40:MET:HE3	1:A:40:MET:H	1.39	0.87
1:A:222:GLU:HB3	5:A:970:HOH:O	1.73	0.86
1:B:374:ASN:C	1:B:376:GLY:HA3	1.96	0.85
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: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: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:374:ASN:C	1:B:376:GLY:CA	2.55	0.75
1:B:375:ASP:N	1:B:376:GLY:HA2	2.02	0.74
1:B:33:LEU:C	1:B:33:LEU:HD23	2.10	0.72
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: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:615:ASP:O	1:A:617:ASP:HA	2.03	0.57
1:A:98:THR:O	1:A:99:ASP:HB2	2.04	0.57
1:B:78:VAL:CG1	1:B:107:GLY:C	2.73	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:B:160:MET:CE	5:B:802:HOH:O	2.53	0.55
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:A:40:MET:H	1:A:40:MET:CE	2.17	0.53
1:B:78:VAL:HG12	1:B:107:GLY:C	2.28	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:33:LEU:C	1:B:33:LEU:CD2	2.77	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: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:374:ASN:C	1:B:376:GLY:HA2	2.31	0.47
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:B:29:HIS:HB2	5:B:825:HOH:O	2.14	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:56:VAL:HA	1:A:57:PRO:C	2.38	0.42
1:B:242:LYS:CE	5:B:834:HOH:O	2.67	0.42
1:B:378:VAL:HG23	1:B:379:ASN:N	2.34	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:398:GLY:O	1:B:399:ARG:C	2.58	0.42
1:B:228:LYS:HB2	1:B:271:TYR:CZ	2.55	0.42
1:B:239:ASP:CG	5:B:808:HOH:O	2.59	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: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
1:B:376:GLY:HA3	1:B:377:ILE:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	47	33
1	B	632/644 (98%)	615 (97%)	13 (2%)	4 (1%)	25	12
All	All	1263/1288 (98%)	1232 (98%)	26 (2%)	5 (0%)	34	21

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 ⓘ

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	530/540 (98%)	521 (98%)	9 (2%)	60	51
1	B	531/540 (98%)	513 (97%)	18 (3%)	37	22
All	All	1061/1080 (98%)	1034 (98%)	27 (2%)	47	34

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

Mol	Chain	Res	Type
1	A	30	SER

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	40	MET
1	A	209	ARG
1	A	227	LYS
1	A	327	SER
1	A	335	LYS
1	A	567	LEU
1	A	616	LYS
1	B	33	LEU
1	B	76	ARG
1	B	103	LYS
1	B	123	LYS
1	B	209	ARG
1	B	245	LYS
1	B	313	LYS
1	B	327	SER
1	B	333	LYS
1	B	340	LYS
1	B	368	LYS
1	B	400	LYS
1	B	403	GLU
1	B	407	ASP
1	B	567	LEU
1	B	616	LYS
1	B	648	PRO
1	B	660	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	HIS
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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	GAL	B	704	3	11,11,12	0.89	0	15,15,17	1.37	2 (13%)
2	SO4	B	702	-	4,4,4	1.31	0	6,6,6	0.29	0
2	SO4	A	701	-	4,4,4	0.98	0	6,6,6	0.83	0
3	4WS	A	704	4	16,17,17	2.39	3 (18%)	22,25,25	2.35	9 (40%)
3	4WS	B	703	4	16,17,17	2.25	3 (18%)	22,25,25	2.37	8 (36%)
2	SO4	B	701	-	4,4,4	1.00	0	6,6,6	0.51	0
4	GAL	A	705	3	11,11,12	0.97	0	15,15,17	1.33	2 (13%)
2	SO4	A	702	-	4,4,4	1.22	0	6,6,6	0.34	0
2	SO4	A	703	-	4,4,4	1.29	0	6,6,6	0.67	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
4	GAL	A	705	3	-	0/2/19/22	0/1/1/1
3	4WS	A	704	4	-	3/5/34/34	0/2/2/2
4	GAL	B	704	3	-	0/2/19/22	0/1/1/1
3	4WS	B	703	4	-	3/5/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	4WS	O25-C29	6.83	1.38	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	4WS	O25-C29	6.44	1.37	1.23
3	B	703	4WS	C24-C23	-4.49	1.49	1.54
3	A	704	4WS	C24-C23	-4.06	1.50	1.54
3	A	704	4WS	C29-N22	3.87	1.45	1.34
3	B	703	4WS	C29-N22	2.95	1.42	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	703	4WS	C26-C25-C24	6.07	113.19	103.74
3	A	704	4WS	C26-C25-C24	4.45	110.68	103.74
3	A	704	4WS	C24-C23-N21	4.11	111.37	104.72
3	A	704	4WS	O25-C29-C30	-4.08	114.47	122.06
3	B	703	4WS	O25-C29-C30	-3.94	114.73	122.06
3	A	704	4WS	C28-C27-C21	3.48	119.62	113.25
3	B	703	4WS	C28-C27-C21	3.44	119.56	113.25
3	B	703	4WS	C26-N21-C23	3.43	112.14	106.10
3	A	704	4WS	C21-C22-C23	-3.33	98.37	102.82
3	B	703	4WS	C21-C22-C23	-3.07	98.71	102.82
3	A	704	4WS	C28-N22-C29	-2.81	118.42	122.75
4	A	705	GAL	O5-C1-C2	2.60	114.78	110.77
3	B	703	4WS	C30-C29-N22	-2.59	111.49	116.09
4	B	704	GAL	O5-C5-C6	-2.59	103.14	107.20
3	A	704	4WS	O24-C24-C25	-2.52	105.53	111.54
3	A	704	4WS	C30-C29-N22	-2.48	111.69	116.09
3	B	703	4WS	O25-C29-N22	-2.44	114.88	121.74
3	B	703	4WS	O24-C24-C25	-2.39	105.84	111.54
4	A	705	GAL	O3-C3-C2	-2.36	105.48	109.99
3	A	704	4WS	O25-C29-N22	-2.32	115.20	121.74
4	B	704	GAL	O5-C1-C2	2.08	113.98	110.77

There are no chirality outliers.

All (6) 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
3	A	704	4WS	N21-C27-C28-N22
3	B	703	4WS	N21-C27-C28-N22

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%)	-0.20	16 (2%)	57	52	8, 16, 32, 70	0
1	B	634/644 (98%)	-0.12	21 (3%)	46	40	7, 16, 35, 60	0
All	All	1267/1288 (98%)	-0.16	37 (2%)	51	46	7, 16, 34, 70	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	616	LYS	6.5
1	B	29	HIS	6.3
1	B	379	ASN	6.2
1	B	397	ALA	5.2
1	A	617	ASP	5.1
1	B	616	LYS	4.9
1	B	617	ASP	4.6
1	A	224	ASP	4.2
1	A	398	GLY	3.9
1	B	109	ALA	3.8
1	B	224	ASP	3.7
1	A	618	GLY	3.6
1	B	376	GLY	3.3
1	B	107	GLY	3.3
1	B	28	HIS	3.0
1	B	377	ILE	2.9
1	B	398	GLY	2.9
1	A	30	SER	2.8
1	B	618	GLY	2.8
1	A	379	ASN	2.7
1	A	63	THR	2.7
1	A	99	ASP	2.6
1	B	381	LYS	2.6
1	B	108	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	48	VAL	2.5
1	B	378	VAL	2.5
1	B	399	ARG	2.4
1	B	344	ALA	2.4
1	B	637	ASN	2.2
1	A	615	ASP	2.2
1	A	66	THR	2.2
1	A	455	ASP	2.2
1	A	62	TRP	2.2
1	A	45	THR	2.1
1	B	615	ASP	2.1
1	A	37	GLY	2.0
1	A	39	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	SO4	B	701	5/5	0.92	0.17	25,28,34,34	0
4	GAL	A	705	11/12	0.94	0.09	17,17,18,19	0
3	4WS	B	703	16/16	0.95	0.09	14,16,19,20	0
2	SO4	A	703	5/5	0.96	0.16	41,46,47,51	0
3	4WS	A	704	16/16	0.96	0.08	14,17,23,23	0
4	GAL	B	704	11/12	0.96	0.08	14,15,18,19	0
2	SO4	A	701	5/5	0.97	0.24	27,29,35,35	0
2	SO4	A	702	5/5	0.99	0.16	25,26,28,29	0
2	SO4	B	702	5/5	0.99	0.16	23,24,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.