



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:14 PM UTC

PDB ID : 9FYL / pdb_00009fyl
Title : Lacto-N-biosidase from *Treponema denticola* ATCC 35405, HisTag bound in active site
Authors : Vuillemin, M.; Siebenhaar, S.; Zeuner, B.; Morth, J.P.
Deposited on : 2024-07-03
Resolution : 2.24 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
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

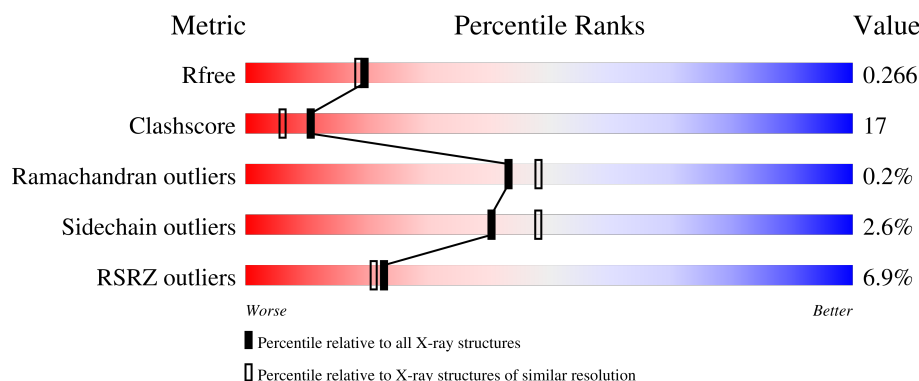
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.24 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	329	8% 74% 23% ..
1	B	329	5% 73% 22% ...

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
2	ZN	B	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10481 atoms, of which 5172 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 Glycoside hydrolase family 20 catalytic domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	H	N	O	S	0	0	0
			5223	1693	2586	439	491	14			
1	B	325	Total	C	H	N	O	S	0	0	0
			5223	1693	2586	439	491	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	355	LEU	-	expression tag	UNP Q73LY9
A	356	GLU	-	expression tag	UNP Q73LY9
A	357	HIS	-	expression tag	UNP Q73LY9
A	358	HIS	-	expression tag	UNP Q73LY9
A	359	HIS	-	expression tag	UNP Q73LY9
A	360	HIS	-	expression tag	UNP Q73LY9
A	361	HIS	-	expression tag	UNP Q73LY9
A	362	HIS	-	expression tag	UNP Q73LY9
B	355	LEU	-	expression tag	UNP Q73LY9
B	356	GLU	-	expression tag	UNP Q73LY9
B	357	HIS	-	expression tag	UNP Q73LY9
B	358	HIS	-	expression tag	UNP Q73LY9
B	359	HIS	-	expression tag	UNP Q73LY9
B	360	HIS	-	expression tag	UNP Q73LY9
B	361	HIS	-	expression tag	UNP Q73LY9
B	362	HIS	-	expression tag	UNP Q73LY9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Zn 1	0	0

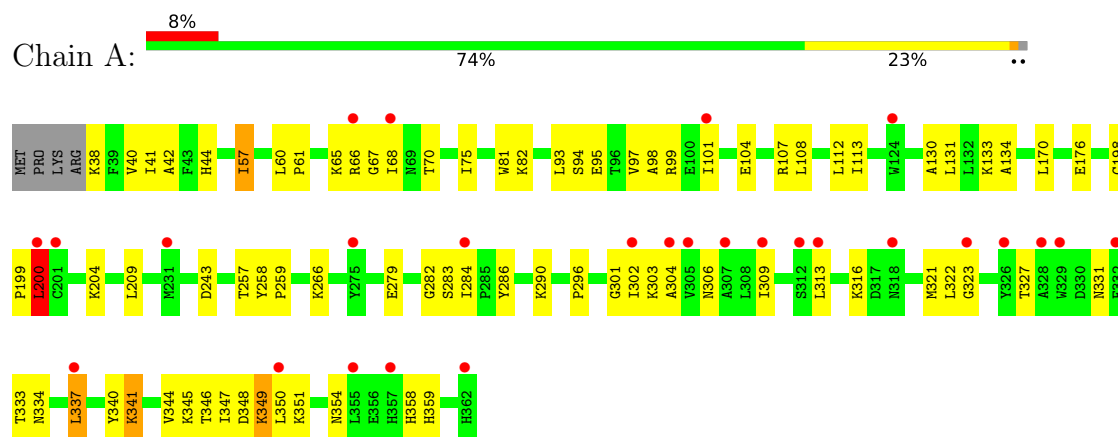
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	13	Total 13	O 13	0	0

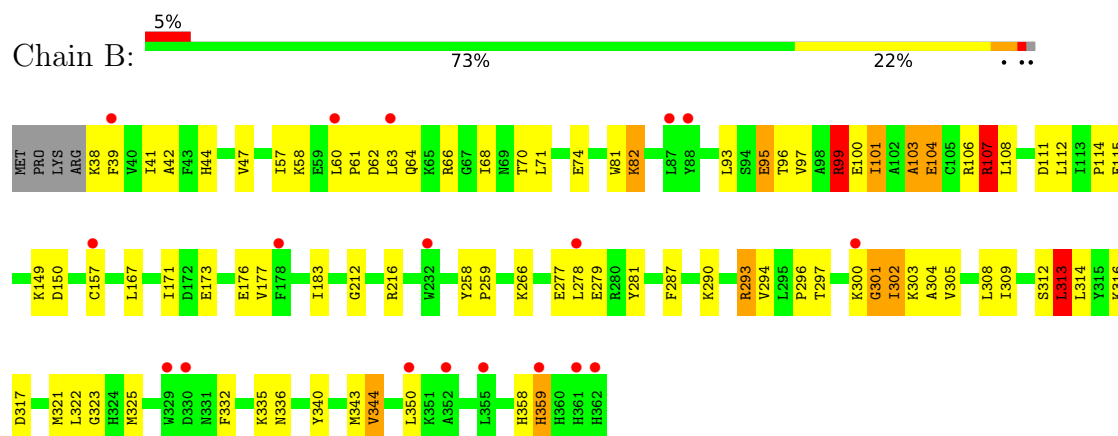
3 Residue-property plots [i](#)

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: Glycoside hydrolase family 20 catalytic domain-containing protein



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	128.92Å 89.47Å 93.76Å 90.00° 127.00° 90.00°	Depositor
Resolution (Å)	46.31 – 2.24 46.31 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.31-2.24) 99.6 (46.31-2.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.232 , 0.269 0.235 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	71.7	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10481	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.68% 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: ZN

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	0.55	5/2704 (0.2%)	0.70	11/3657 (0.3%)
1	B	0.62	11/2704 (0.4%)	0.83	20/3657 (0.5%)
All	All	0.59	16/5408 (0.3%)	0.77	31/7314 (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	B	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	LYS	CD-CE	12.68	1.90	1.52
1	B	82	LYS	CD-CE	12.39	1.89	1.52
1	A	200	LEU	CG-CD2	11.18	1.89	1.52
1	A	284	ILE	CA-C	-10.71	1.43	1.52
1	B	313	LEU	CG-CD2	8.17	1.79	1.52
1	B	82	LYS	CE-NZ	8.07	1.73	1.49
1	A	284	ILE	CA-CB	-7.99	1.50	1.54
1	B	99	ARG	CB-CG	7.59	1.75	1.52
1	A	349	LYS	CE-NZ	7.44	1.71	1.49
1	B	82	LYS	CG-CD	7.43	1.74	1.52
1	B	104	GLU	CD-OE2	7.32	1.39	1.25
1	B	104	GLU	CB-CG	7.17	1.74	1.52
1	B	107	ARG	CB-CG	6.90	1.73	1.52
1	B	99	ARG	CG-CD	6.75	1.72	1.52
1	B	95	GLU	CG-CD	6.45	1.68	1.52
1	B	95	GLU	CD-OE1	6.31	1.37	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	LYS	CG-CD-CE	-15.62	75.38	111.30
1	A	349	LYS	CD-CE-NZ	-13.91	67.37	111.90
1	A	284	ILE	O-C-N	-11.92	112.79	120.42
1	B	95	GLU	CA-CB-CG	9.13	132.37	114.10
1	A	200	LEU	CB-CG-CD2	-9.10	83.39	110.70
1	B	313	LEU	CD1-CG-CD2	8.53	129.57	110.80
1	B	103	ALA	CA-C-N	8.36	131.81	120.44
1	B	103	ALA	C-N-CA	8.36	131.81	120.44
1	B	312	SER	CA-C-N	-8.31	107.33	122.38
1	B	312	SER	C-N-CA	-8.31	107.33	122.38
1	B	95	GLU	CB-CA-C	8.27	126.56	110.67
1	B	104	GLU	CG-CD-OE1	-8.02	99.95	118.40
1	B	107	ARG	CG-CD-NE	7.80	129.16	112.00
1	A	349	LYS	CA-CB-CG	-7.63	98.84	114.10
1	A	284	ILE	CA-C-O	7.40	123.65	118.69
1	B	95	GLU	N-CA-CB	-7.34	98.90	110.28
1	B	82	LYS	CD-CE-NZ	-7.18	88.94	111.90
1	A	349	LYS	CA-C-N	7.01	134.63	122.09
1	A	349	LYS	C-N-CA	7.01	134.63	122.09
1	A	200	LEU	CB-CG-CD1	6.81	131.13	110.70
1	B	99	ARG	CG-CD-NE	6.66	126.64	112.00
1	B	104	GLU	CA-CB-CG	6.57	127.23	114.10
1	B	107	ARG	NE-CZ-NH2	6.46	125.02	119.20
1	B	107	ARG	CD-NE-CZ	-6.16	115.78	124.40
1	A	199	PRO	CA-C-N	5.68	133.73	121.64
1	A	199	PRO	C-N-CA	5.68	133.73	121.64
1	B	81	TRP	CA-C-N	5.58	130.16	120.68
1	B	81	TRP	C-N-CA	5.58	130.16	120.68
1	B	99	ARG	N-CA-C	-5.42	106.74	113.19
1	A	75	ILE	N-CA-C	-5.06	107.87	112.12
1	B	82	LYS	CA-CB-CG	-5.01	104.08	114.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	107	ARG	Sidechain
1	B	99	ARG	Sidechain

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	2637	2586	2585	78	0
1	B	2637	2586	2586	95	0
2	A	1	0	0	0	0
2	B	1	0	0	2	0
3	A	20	0	0	0	0
3	B	13	0	0	0	0
All	All	5309	5172	5171	173	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 17.

All (173) 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:99:ARG:CG	1:B:99:ARG:CB	1.75	1.60
1:B:313:LEU:CD2	1:B:313:LEU:CG	1.79	1.58
1:B:82:LYS:CD	1:B:82:LYS:CG	1.74	1.57
1:A:200:LEU:CG	1:A:200:LEU:CD2	1.89	1.50
1:A:349:LYS:CE	1:A:349:LYS:NZ	1.71	1.50
1:A:349:LYS:CE	1:A:349:LYS:CD	1.90	1.50
1:B:82:LYS:CE	1:B:82:LYS:NZ	1.73	1.48
1:B:82:LYS:CD	1:B:82:LYS:CE	1.89	1.47
1:A:349:LYS:NZ	1:A:349:LYS:CD	2.01	1.24
1:B:82:LYS:CG	1:B:82:LYS:CE	2.23	1.16
1:B:313:LEU:CD2	1:B:313:LEU:HG	1.81	1.10
1:A:200:LEU:CD2	1:A:200:LEU:CB	2.30	1.09
1:A:346:THR:O	1:A:349:LYS:HB2	1.56	1.03
1:B:82:LYS:CE	1:B:82:LYS:HG3	1.88	1.03
1:B:57:ILE:HG23	1:B:104:GLU:HG2	1.56	0.86
1:A:349:LYS:NZ	1:A:349:LYS:HD2	1.89	0.85
1:A:349:LYS:CD	1:A:349:LYS:HZ3	1.92	0.82
1:A:334:ASN:HA	1:A:337:LEU:HD23	1.65	0.77
1:B:99:ARG:NH1	1:B:176:GLU:OE2	2.18	0.76
1:A:112:LEU:HD23	1:A:113:ILE:N	2.01	0.76
1:A:341:LYS:HD2	1:A:341:LYS:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ALA:HA	1:B:106:ARG:CZ	2.16	0.75
1:A:200:LEU:HD22	1:A:200:LEU:HA	1.69	0.75
1:A:200:LEU:CD2	1:A:200:LEU:CA	2.64	0.75
1:A:349:LYS:CE	1:A:349:LYS:CG	2.64	0.74
1:A:41:ILE:HG22	1:A:68:ILE:HA	1.69	0.74
1:A:296:PRO:HD2	1:A:321:MET:HE1	1.70	0.73
1:A:358:HIS:O	1:A:359:HIS:ND1	2.20	0.73
1:B:82:LYS:HZ3	1:B:95:GLU:HG3	1.54	0.73
1:B:82:LYS:CG	1:B:82:LYS:HE2	2.16	0.73
1:B:358:HIS:O	1:B:358:HIS:ND1	2.23	0.71
1:B:82:LYS:CD	1:B:82:LYS:NZ	2.54	0.71
1:B:82:LYS:HG3	1:B:82:LYS:HE2	1.69	0.70
1:B:70:THR:HG22	1:B:111:ASP:HB3	1.74	0.69
1:A:130:ALA:HA	1:A:133:LYS:HE3	1.74	0.69
1:A:349:LYS:CD	1:A:349:LYS:HZ2	2.05	0.69
1:B:278:LEU:HD12	1:B:281:TYR:CE1	2.28	0.69
1:A:349:LYS:HD2	1:A:349:LYS:HZ2	1.56	0.68
1:A:200:LEU:HD22	1:A:200:LEU:CA	2.23	0.68
1:B:82:LYS:NZ	1:B:95:GLU:OE1	2.26	0.67
1:B:358:HIS:O	1:B:359:HIS:ND1	2.27	0.67
1:B:279:GLU:OE1	1:B:279:GLU:N	2.25	0.67
1:B:157:CYS:SG	2:B:401:ZN:ZN	1.84	0.66
1:B:82:LYS:NZ	1:B:95:GLU:HG3	2.11	0.65
1:B:47:VAL:CG1	1:B:93:LEU:HD13	2.27	0.65
1:B:297:THR:HG23	1:B:325:MET:CG	2.27	0.64
1:B:104:GLU:O	1:B:108:LEU:HD12	1.97	0.64
1:B:41:ILE:HG22	1:B:68:ILE:HA	1.78	0.64
1:A:309:ILE:O	1:A:313:LEU:HD23	1.98	0.61
1:A:303:LYS:C	1:A:303:LYS:HD3	2.25	0.61
1:B:104:GLU:OE2	1:B:107:ARG:NH2	2.34	0.61
1:B:82:LYS:HZ3	1:B:95:GLU:CG	2.15	0.59
1:B:82:LYS:HZ1	1:B:95:GLU:CD	2.11	0.59
1:B:293:ARG:HB3	1:B:322:LEU:HD11	1.85	0.59
1:B:321:MET:HE1	1:B:323:GLY:HA2	1.84	0.59
1:B:303:LYS:C	1:B:303:LYS:HD3	2.28	0.58
1:A:82:LYS:NZ	1:A:95:GLU:OE1	2.31	0.58
1:A:345:LYS:HG3	1:A:346:THR:HG23	1.86	0.57
1:B:104:GLU:CD	1:B:107:ARG:HH21	2.13	0.57
1:B:97:VAL:O	1:B:101:ILE:HD12	2.04	0.57
1:A:303:LYS:HD3	1:A:303:LYS:O	2.05	0.56
1:A:97:VAL:O	1:A:101:ILE:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:HIS:HB2	1:B:325:MET:HE2	1.87	0.55
1:B:300:LYS:O	1:B:302:ILE:N	2.39	0.55
1:B:71:LEU:HD23	1:B:112:LEU:HD13	1.88	0.55
1:B:297:THR:HG23	1:B:325:MET:HG3	1.88	0.55
1:A:44:HIS:HB3	1:A:327:THR:HG22	1.89	0.55
1:A:98:ALA:HA	1:A:101:ILE:CD1	2.37	0.54
1:A:333:THR:O	1:A:334:ASN:HB2	2.07	0.54
1:A:93:LEU:HD12	1:A:94:SER:N	2.23	0.54
1:A:38:LYS:HG3	1:A:354:ASN:OD1	2.07	0.54
1:B:277:GLU:HB2	1:B:303:LYS:HG3	1.91	0.53
1:B:313:LEU:CD2	1:B:313:LEU:CB	2.77	0.52
1:B:60:LEU:HB2	1:B:61:PRO:HD3	1.91	0.52
1:A:346:THR:O	1:A:349:LYS:CB	2.46	0.52
1:B:313:LEU:HD13	1:B:313:LEU:N	2.25	0.52
1:B:82:LYS:NZ	1:B:95:GLU:CG	2.73	0.52
1:B:82:LYS:NZ	1:B:95:GLU:CD	2.68	0.52
1:A:348:ASP:HA	1:A:351:LYS:HB2	1.90	0.52
1:B:97:VAL:O	1:B:100:GLU:HB2	2.09	0.52
1:A:198:CYS:SG	1:A:200:LEU:HB2	2.50	0.52
1:B:70:THR:HG22	1:B:111:ASP:CB	2.40	0.51
1:B:157:CYS:HG	2:B:401:ZN:ZN	1.22	0.51
1:A:347:ILE:C	1:A:349:LYS:H	2.19	0.51
1:B:294:VAL:O	1:B:322:LEU:HD12	2.10	0.51
1:B:171:ILE:HG23	1:B:183:ILE:HG12	1.91	0.51
1:A:301:GLY:C	1:A:302:ILE:HD12	2.35	0.51
1:B:41:ILE:CG2	1:B:68:ILE:HD13	2.41	0.50
1:A:204:LYS:HB2	1:A:209:LEU:HD11	1.93	0.50
1:B:173:GLU:O	1:B:177:VAL:HG13	2.10	0.50
1:B:62:ASP:OD2	1:B:66:ARG:NH2	2.45	0.50
1:B:104:GLU:O	1:B:107:ARG:HB3	2.12	0.50
1:B:321:MET:HE3	1:B:321:MET:C	2.36	0.50
1:A:57:ILE:HG23	1:A:104:GLU:HG3	1.94	0.49
1:A:321:MET:HE3	1:A:322:LEU:N	2.27	0.49
1:B:300:LYS:O	1:B:301:GLY:C	2.54	0.49
1:B:97:VAL:HG12	1:B:101:ILE:CD1	2.43	0.49
1:A:112:LEU:HD23	1:A:112:LEU:C	2.37	0.49
1:B:41:ILE:HG22	1:B:68:ILE:HD13	1.94	0.49
1:B:278:LEU:HD12	1:B:281:TYR:CD1	2.48	0.49
1:B:281:TYR:CE2	1:B:308:LEU:HA	2.48	0.49
1:A:95:GLU:OE2	1:A:99:ARG:NH1	2.45	0.49
1:A:303:LYS:HA	1:A:306:ASN:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:GLY:O	1:B:304:ALA:N	2.45	0.49
1:B:314:LEU:HD23	1:B:314:LEU:N	2.28	0.48
1:A:266:LYS:HD3	1:A:290:LYS:O	2.14	0.48
1:A:243:ASP:O	1:A:282:GLY:HA3	2.14	0.48
1:B:103:ALA:HA	1:B:106:ARG:NH2	2.29	0.48
1:A:104:GLU:O	1:A:108:LEU:HD12	2.13	0.48
1:A:301:GLY:O	1:A:303:LYS:N	2.46	0.48
1:A:303:LYS:O	1:A:306:ASN:N	2.47	0.48
1:B:212:GLY:O	1:B:216:ARG:HG3	2.14	0.48
1:B:340:TYR:O	1:B:344:VAL:HG13	2.14	0.48
1:A:67:GLY:HA2	1:A:351:LYS:HE2	1.95	0.47
1:A:313:LEU:O	1:A:316:LYS:HG2	2.13	0.47
1:B:64:GLN:OE1	1:B:64:GLN:C	2.57	0.47
1:A:93:LEU:CD1	1:A:97:VAL:HB	2.44	0.47
1:A:296:PRO:CD	1:A:321:MET:HE1	2.42	0.47
1:A:340:TYR:O	1:A:344:VAL:HG22	2.15	0.47
1:A:257:THR:C	1:A:259:PRO:HD2	2.40	0.46
1:B:258:TYR:CG	1:B:259:PRO:HD3	2.50	0.46
1:B:303:LYS:HD3	1:B:303:LYS:O	2.15	0.46
1:A:258:TYR:N	1:A:259:PRO:CD	2.79	0.46
1:A:341:LYS:H	1:A:341:LYS:CD	2.19	0.46
1:A:66:ARG:HD2	1:A:344:VAL:HG12	1.98	0.46
1:A:61:PRO:HA	1:A:108:LEU:HD21	1.97	0.45
1:B:63:LEU:HD23	1:B:343:MET:HE2	1.99	0.45
1:A:345:LYS:HD2	1:A:345:LYS:C	2.41	0.45
1:B:287:PHE:HB2	1:B:294:VAL:HG21	1.98	0.45
1:B:57:ILE:CG2	1:B:104:GLU:HG2	2.39	0.45
1:B:293:ARG:CB	1:B:322:LEU:HD11	2.46	0.45
1:B:82:LYS:CD	1:B:82:LYS:HZ2	2.26	0.45
1:A:347:ILE:C	1:A:349:LYS:N	2.74	0.45
1:A:60:LEU:HB2	1:A:61:PRO:HD3	1.99	0.44
1:A:258:TYR:CG	1:A:259:PRO:HD3	2.53	0.44
1:A:101:ILE:HD12	1:A:101:ILE:H	1.82	0.44
1:B:294:VAL:HG12	1:B:296:PRO:HD3	2.00	0.44
1:A:176:GLU:C	1:A:176:GLU:OE2	2.61	0.43
1:A:131:LEU:C	1:A:131:LEU:HD23	2.44	0.43
1:A:81:TRP:CD2	1:A:170:LEU:HD22	2.53	0.43
1:A:130:ALA:O	1:A:133:LYS:HD2	2.18	0.43
1:A:99:ARG:NH2	1:A:176:GLU:OE2	2.51	0.43
1:B:114:PRO:O	1:B:183:ILE:HD12	2.19	0.43
1:B:42:ALA:HA	1:B:70:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LYS:HG3	1:A:346:THR:N	2.34	0.43
1:B:38:LYS:O	1:B:39:PHE:HD2	2.02	0.43
1:B:99:ARG:HH12	1:B:176:GLU:CD	2.25	0.43
1:B:313:LEU:N	1:B:313:LEU:CD1	2.81	0.43
1:A:41:ILE:HD11	1:A:350:LEU:HB2	2.00	0.42
1:A:279:GLU:OE2	1:A:279:GLU:N	2.36	0.42
1:B:305:VAL:O	1:B:309:ILE:HG13	2.19	0.42
1:A:65:LYS:HA	1:A:65:LYS:CE	2.49	0.42
1:B:71:LEU:HD23	1:B:112:LEU:CD1	2.47	0.42
1:B:332:PHE:CD1	1:B:332:PHE:N	2.87	0.42
1:B:61:PRO:HA	1:B:108:LEU:HD21	2.00	0.42
1:B:313:LEU:O	1:B:316:LYS:HD3	2.19	0.42
1:B:321:MET:HE1	1:B:323:GLY:CA	2.49	0.42
1:B:266:LYS:HD2	1:B:290:LYS:O	2.20	0.42
1:A:42:ALA:HB2	1:A:70:THR:HB	2.01	0.41
1:A:331:ASN:ND2	1:A:337:LEU:HD22	2.35	0.41
1:B:258:TYR:N	1:B:259:PRO:CD	2.83	0.41
1:B:57:ILE:HG23	1:B:104:GLU:CG	2.39	0.41
1:A:133:LYS:HD2	1:A:134:ALA:N	2.35	0.41
1:B:58:LYS:O	1:B:61:PRO:HD2	2.20	0.41
1:B:74:GLU:HA	1:B:115:GLU:HB3	2.02	0.41
1:B:335:LYS:HD2	1:B:336:ASN:N	2.34	0.41
1:A:303:LYS:O	1:A:304:ALA:C	2.61	0.41
1:B:167:LEU:O	1:B:171:ILE:HG13	2.19	0.41
1:A:40:VAL:O	1:A:323:GLY:HA3	2.20	0.41
1:A:283:SER:HA	1:A:286:TYR:HB3	2.02	0.41
1:B:42:ALA:HB2	1:B:70:THR:OG1	2.20	0.41
1:B:303:LYS:C	1:B:303:LYS:CD	2.92	0.41
1:B:149:LYS:O	1:B:150:ASP:HB2	2.21	0.41

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	323/329 (98%)	299 (93%)	24 (7%)	0	100	100
1	B	323/329 (98%)	303 (94%)	19 (6%)	1 (0%)	36	38
All	All	646/658 (98%)	602 (93%)	43 (7%)	1 (0%)	43	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	GLY

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	288/292 (99%)	283 (98%)	5 (2%)	53	63
1	B	288/292 (99%)	278 (96%)	10 (4%)	32	37
All	All	576/584 (99%)	561 (97%)	15 (3%)	40	48

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	107	ARG
1	A	200	LEU
1	A	337	LEU
1	A	341	LYS
1	B	96	THR
1	B	99	ARG
1	B	101	ILE
1	B	293	ARG
1	B	302	ILE
1	B	313	LEU
1	B	317	ASP
1	B	344	VAL
1	B	350	LEU
1	B	359	HIS

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	215	ASN
1	A	360	HIS
1	A	362	HIS
1	B	306	ASN

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](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

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	325/329 (98%)	0.69	27 (8%) 17 15	65, 103, 162, 206	0
1	B	325/329 (98%)	0.63	18 (5%) 30 29	72, 113, 166, 201	0
All	All	650/658 (98%)	0.66	45 (6%) 23 21	65, 109, 164, 206	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	305	VAL	5.6
1	A	201	CYS	5.2
1	B	329	TRP	4.7
1	A	231	MET	4.6
1	A	304	ALA	4.4
1	A	329	TRP	4.3
1	B	87	LEU	3.7
1	A	302	ILE	3.4
1	A	313	LEU	3.4
1	B	350	LEU	3.4
1	A	312	SER	3.3
1	A	318	ASN	3.2
1	A	355	LEU	3.1
1	A	332	PHE	2.9
1	A	362	HIS	2.9
1	B	362	HIS	2.9
1	A	200	LEU	2.8
1	B	157	CYS	2.7
1	A	350	LEU	2.7
1	A	275	TYR	2.6
1	B	178	PHE	2.6
1	A	323	GLY	2.5
1	B	63	LEU	2.5
1	B	355	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	124	TRP	2.5
1	A	66	ARG	2.4
1	A	337	LEU	2.3
1	A	326	TYR	2.2
1	A	284	ILE	2.2
1	B	330	ASP	2.2
1	B	359	HIS	2.2
1	B	88	TYR	2.2
1	A	328	ALA	2.2
1	A	309	ILE	2.1
1	B	278	LEU	2.1
1	B	232	TRP	2.1
1	B	39	PHE	2.1
1	B	60	LEU	2.1
1	B	361	HIS	2.1
1	A	357	HIS	2.1
1	B	300	LYS	2.0
1	A	307	ALA	2.0
1	B	352	ALA	2.0
1	A	101	ILE	2.0
1	A	68	ILE	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 oligosaccharides 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	ZN	B	401	1/1	0.89	0.20	183,183,183,183	0
2	ZN	A	401	1/1	0.95	0.07	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.