



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 09:19 AM UTC

PDB ID : 8K2N / pdb_00008k2n
Title : Crystal structure of Group 4 Monosaccharide-releasing beta-N-acetylgalactosaminidase NgaLy from *Lactacaseibacillus yichunensis*, apo form
Authors : Sumida, T.; Fushinobu, S.
Deposited on : 2023-07-12
Resolution : 2.50 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

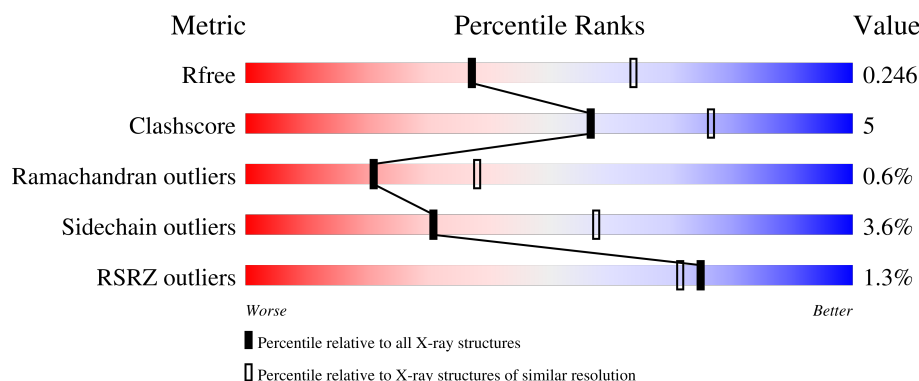
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

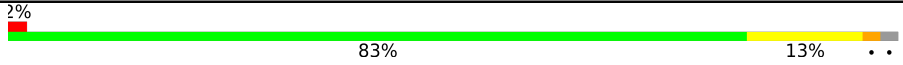
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	552	
1	B	552	
1	C	552	
1	D	552	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17554 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 Monosaccharide-releasing beta-N-acetylgalactosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	544	Total	C	N	O	S	0	0	0
			4266	2759	711	785	11			
1	C	543	Total	C	N	O	S	0	0	0
			4257	2752	710	784	11			
1	A	543	Total	C	N	O	S	0	0	0
			4259	2754	710	784	11			
1	B	543	Total	C	N	O	S	0	0	0
			4258	2754	710	784	10			

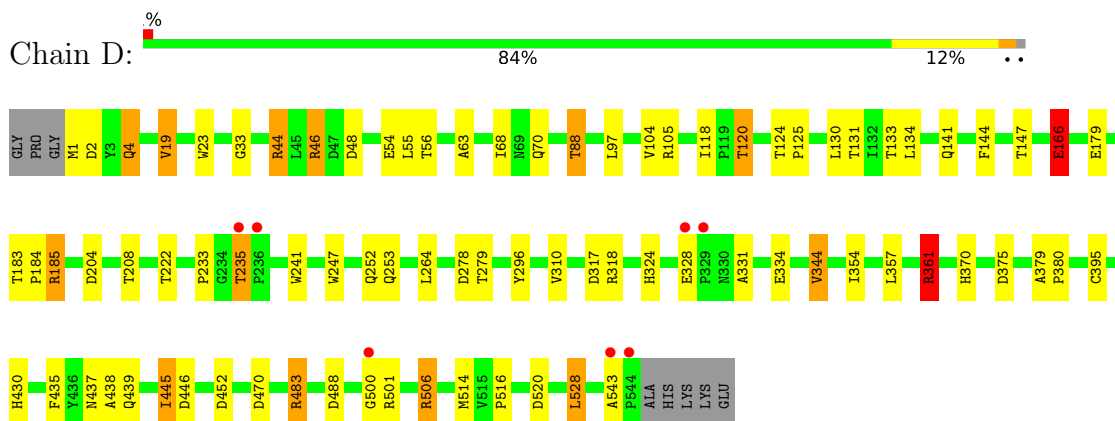
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	139	Total	O	0	0
			139	139		
2	C	103	Total	O	0	0
			103	103		
2	A	133	Total	O	0	0
			133	133		
2	B	139	Total	O	0	0
			139	139		

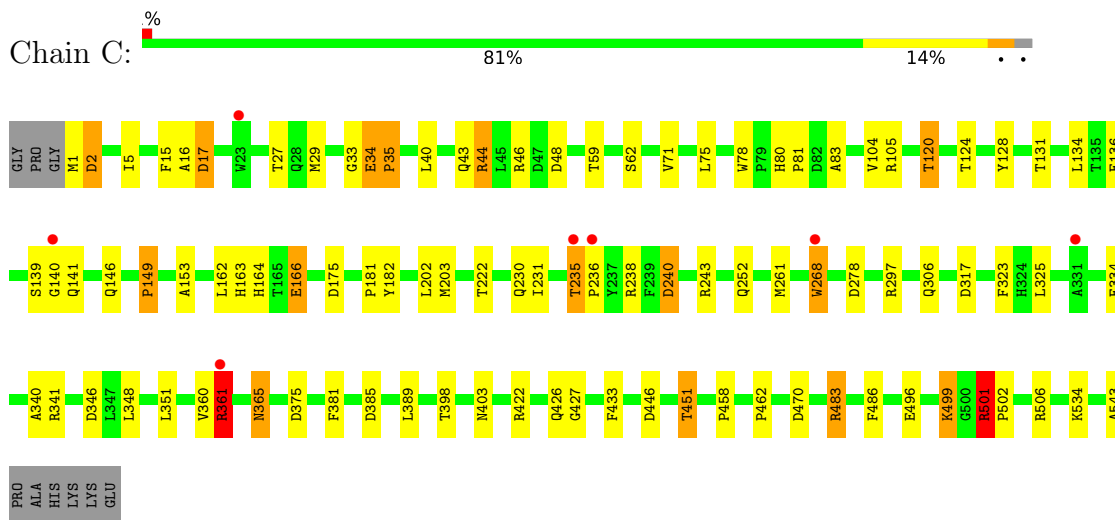
3 Residue-property plots [i](#)

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.

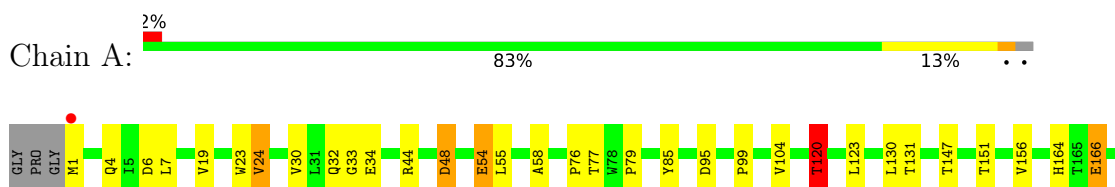
- Molecule 1: Monosaccharide-releasing beta-N-acetylgalactosaminidase

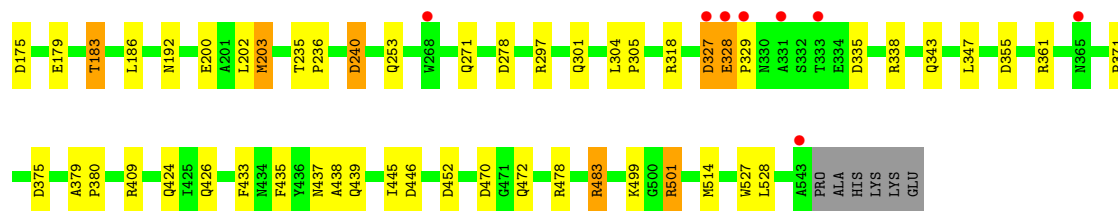


- Molecule 1: Monosaccharide-releasing beta-N-acetylgalactosaminidase

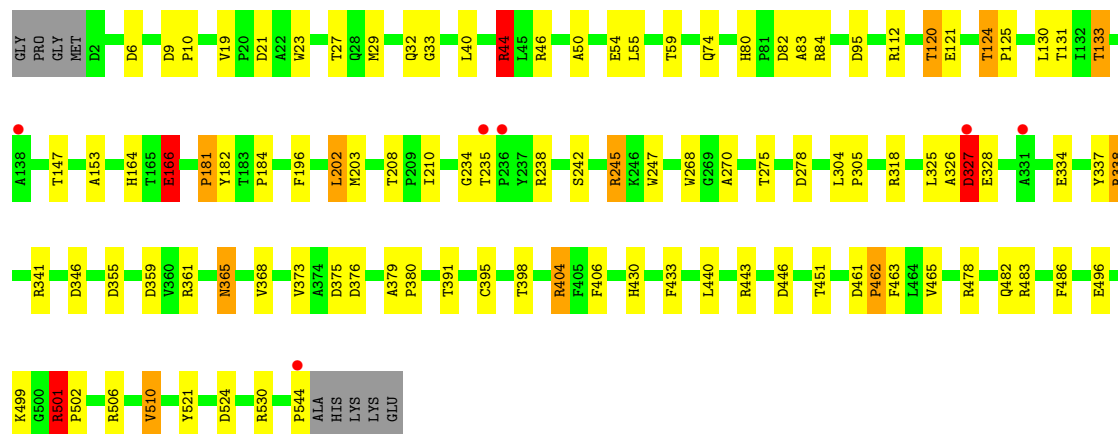
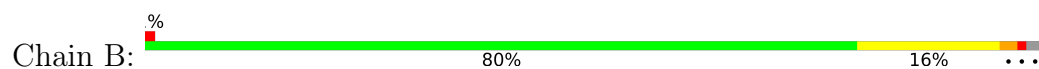


- Molecule 1: Monosaccharide-releasing beta-N-acetylgalactosaminidase





● Molecule 1: Monosaccharide-releasing beta-N-acetylgalactosaminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.93Å 94.62Å 116.18Å 70.93° 73.81° 72.43°	Depositor
Resolution (Å)	48.79 – 2.50 48.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.79-2.50) 100.0 (48.79-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.183 , 0.241 0.190 , 0.246	Depositor DCC
R_{free} test set	5287 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17554	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.96	0/4390	1.42	26/6033 (0.4%)
1	B	0.99	5/4390 (0.1%)	1.47	30/6035 (0.5%)
1	C	0.97	0/4387	1.45	22/6028 (0.4%)
1	D	0.98	3/4398 (0.1%)	1.43	19/6045 (0.3%)
All	All	0.98	8/17565 (0.0%)	1.44	97/24141 (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	5
1	B	0	11
1	C	0	8
1	D	0	9
All	All	0	33

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	452	ASP	CG-OD2	6.36	1.37	1.25
1	D	235	THR	C-N	5.89	1.39	1.33
1	B	355	ASP	CG-OD1	5.56	1.35	1.25
1	B	80	HIS	CG-CD2	5.51	1.42	1.35
1	B	80	HIS	CE1-NE2	5.37	1.38	1.32
1	B	496	GLU	CD-OE1	-5.34	1.15	1.25
1	B	166	GLU	CD-OE1	-5.09	1.15	1.25
1	D	324	HIS	CG-CD2	5.01	1.41	1.35

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	LYS	CA-C-N	-15.72	108.44	122.43
1	A	499	LYS	C-N-CA	-15.72	108.44	122.43
1	C	499	LYS	CA-C-N	-12.38	110.02	122.27
1	C	499	LYS	C-N-CA	-12.38	110.02	122.27
1	A	375	ASP	CA-CB-CG	9.55	122.15	112.60
1	C	278	ASP	CA-CB-CG	9.25	121.85	112.60
1	C	375	ASP	CA-CB-CG	8.72	121.33	112.60
1	B	19	VAL	CA-C-O	8.41	124.11	119.15
1	C	365	ASN	CB-CA-C	-8.38	93.27	109.95
1	C	501	ARG	NE-CZ-NH2	-8.35	111.69	119.20
1	B	124	THR	CB-CA-C	8.34	121.62	109.11
1	D	375	ASP	CA-CB-CG	8.11	120.71	112.60
1	B	499	LYS	CA-C-N	-8.01	113.16	122.85
1	B	499	LYS	C-N-CA	-8.01	113.16	122.85
1	B	365	ASN	CB-CA-C	-7.89	94.71	110.42
1	B	278	ASP	CA-CB-CG	7.86	120.46	112.60
1	A	278	ASP	CA-CB-CG	7.78	120.38	112.60
1	B	501	ARG	NE-CZ-NH2	-7.69	112.28	119.20
1	B	6	ASP	CA-CB-CG	7.58	120.18	112.60
1	B	21	ASP	CA-CB-CG	-7.44	105.16	112.60
1	D	48	ASP	CA-CB-CG	7.40	120.00	112.60
1	A	19	VAL	O-C-N	-7.26	115.25	121.57
1	C	34	GLU	CB-CA-C	7.24	121.10	109.51
1	C	48	ASP	CA-CB-CG	7.22	119.82	112.60
1	C	17	ASP	CA-CB-CG	-7.20	105.40	112.60
1	C	462	PRO	N-CA-C	7.07	122.84	113.57
1	D	235	THR	CA-CB-OG1	-6.96	99.17	109.60
1	B	121	GLU	CB-CG-CD	6.93	124.38	112.60
1	A	120	THR	CB-CA-C	6.81	120.77	109.80
1	B	404	ARG	N-CA-CB	-6.77	100.44	111.01
1	C	317	ASP	CA-CB-CG	6.62	119.22	112.60
1	D	4	GLN	CB-CA-C	6.47	120.39	110.62
1	A	44	ARG	CB-CG-CD	6.45	126.13	111.30
1	A	76	PRO	CB-CA-C	-6.44	102.71	112.11
1	B	346	ASP	CA-CB-CG	6.43	119.03	112.60
1	D	278	ASP	CA-CB-CG	6.34	118.94	112.60
1	A	79	PRO	N-CA-CB	-6.29	98.04	103.32
1	A	355	ASP	CA-CB-CG	6.26	118.86	112.60
1	B	32	GLN	CB-CG-CD	-6.23	102.00	112.60
1	B	275	THR	CB-CA-C	6.17	121.48	111.05
1	D	131	THR	CA-CB-OG1	-6.16	100.37	109.60
1	B	270	ALA	CA-C-N	6.10	128.95	120.29
1	B	270	ALA	C-N-CA	6.10	128.95	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	CB-CA-C	-6.08	98.15	111.71
1	D	204	ASP	CA-CB-CG	6.06	118.66	112.60
1	D	19	VAL	CA-C-O	5.96	124.36	119.47
1	B	404	ARG	CG-CD-NE	-5.92	98.97	112.00
1	A	452	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	58	ALA	CA-C-O	-5.86	113.57	120.60
1	A	203	MET	CG-SD-CE	-5.79	88.17	100.90
1	C	268	TRP	CA-C-N	5.75	127.52	120.22
1	C	268	TRP	C-N-CA	5.75	127.52	120.22
1	D	2	ASP	CA-CB-CG	5.75	118.34	112.60
1	C	175	ASP	CB-CA-C	-5.75	101.82	110.90
1	D	483	ARG	CB-CG-CD	-5.74	98.09	111.30
1	A	355	ASP	CA-C-N	5.70	128.93	120.95
1	A	355	ASP	C-N-CA	5.70	128.93	120.95
1	A	470	ASP	CA-CB-CG	5.69	118.29	112.60
1	C	499	LYS	O-C-N	-5.69	114.91	122.59
1	B	82	ASP	CA-CB-CG	5.63	118.23	112.60
1	D	88	THR	CA-CB-OG1	-5.61	101.18	109.60
1	D	124	THR	CB-CA-C	5.60	118.37	109.52
1	B	245	ARG	CB-CA-C	-5.60	101.50	110.79
1	B	462	PRO	CB-CA-C	-5.54	104.03	112.11
1	D	506	ARG	CB-CA-C	-5.53	101.62	110.79
1	A	131	THR	CA-CB-OG1	-5.52	101.32	109.60
1	A	156	VAL	CB-CA-C	5.51	118.75	110.98
1	A	329	PRO	N-CA-C	5.49	119.12	110.50
1	D	222	THR	CA-CB-OG1	-5.49	101.37	109.60
1	D	328	GLU	CB-CG-CD	5.46	121.88	112.60
1	D	166	GLU	CB-CA-C	5.44	119.50	110.74
1	A	151	THR	CA-CB-OG1	-5.41	101.48	109.60
1	D	317	ASP	CA-CB-CG	5.41	118.01	112.60
1	B	376	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	451	THR	CA-CB-OG1	-5.38	101.54	109.60
1	C	470	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	133	THR	CA-CB-OG1	-5.34	101.59	109.60
1	B	181	PRO	CA-C-O	-5.33	115.52	121.23
1	C	230	GLN	CB-CA-C	5.32	118.42	109.48
1	B	375	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	451	THR	CA-CB-OG1	-5.29	101.67	109.60
1	C	35	PRO	CB-CA-C	-5.28	104.65	111.46
1	D	470	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	54	GLU	CA-C-O	-5.24	114.90	120.92
1	B	44	ARG	CB-CA-C	5.20	118.62	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	327	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	521	TYR	CB-CA-C	5.14	116.95	109.08
1	A	499	LYS	O-C-N	-5.14	115.56	122.14
1	C	252	GLN	N-CA-CB	-5.11	102.60	110.16
1	B	406	PHE	CB-CA-C	-5.09	102.28	110.74
1	A	99	PRO	N-CA-CB	5.09	107.73	103.25
1	D	252	GLN	N-CA-CB	-5.08	102.70	110.07
1	A	175	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	403	ASN	CA-CB-CG	5.04	117.64	112.60
1	C	149	PRO	CB-CA-C	5.03	117.56	110.98
1	A	99	PRO	CB-CA-C	-5.00	105.20	111.56

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	361	ARG	Sidechain
1	A	409	ARG	Sidechain
1	A	478	ARG	Sidechain
1	A	483	ARG	Sidechain
1	A	501	ARG	Sidechain
1	B	112	ARG	Sidechain
1	B	234	GLY	Peptide
1	B	238	ARG	Sidechain
1	B	318	ARG	Sidechain
1	B	338	ARG	Sidechain
1	B	361	ARG	Sidechain
1	B	443	ARG	Sidechain
1	B	483	ARG	Sidechain
1	B	501	ARG	Sidechain
1	B	530	ARG	Sidechain
1	B	84	ARG	Sidechain
1	C	105	ARG	Sidechain
1	C	16	ALA	Mainchain
1	C	238	ARG	Sidechain
1	C	243	ARG	Sidechain
1	C	361	ARG	Sidechain
1	C	422	ARG	Sidechain
1	C	483	ARG	Sidechain
1	C	501	ARG	Sidechain
1	D	105	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	D	185	ARG	Sidechain
1	D	361	ARG	Sidechain
1	D	46	ARG	Sidechain
1	D	483	ARG	Sidechain
1	D	500	GLY	Peptide
1	D	501	ARG	Sidechain
1	D	506	ARG	Sidechain
1	D	543	ALA	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	4259	0	4140	36	0
1	B	4258	0	4135	50	0
1	C	4257	0	4134	45	0
1	D	4266	0	4147	32	0
2	A	133	0	0	2	0
2	B	139	0	0	5	0
2	C	103	0	0	3	0
2	D	139	0	0	3	0
All	All	17554	0	16556	155	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 (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:OE1	1:A:183:THR:HG21	1.79	0.81
1:D:33:GLY:H	1:D:120:THR:HG22	1.51	0.74
1:B:44:ARG:NH1	1:B:46:ARG:O	2.23	0.71
1:C:506:ARG:HH12	1:A:1:MET:HB3	1.59	0.68
1:B:33:GLY:H	1:B:120:THR:HG22	1.59	0.68
1:B:44:ARG:NH2	1:B:50:ALA:O	2.26	0.67
1:B:463:PHE:O	1:B:478:ARG:NH2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:ALA:O	1:D:334:GLU:HG2	1.95	0.65
1:D:133:THR:HG22	2:D:676:HOH:O	1.95	0.65
1:A:24:VAL:HG23	2:A:676:HOH:O	1.95	0.65
1:A:301:GLN:HG2	1:A:347:LEU:HD21	1.77	0.65
1:D:395:CYS:SG	2:D:630:HOH:O	2.42	0.64
1:D:334:GLU:HB2	1:D:361:ARG:NH2	2.12	0.64
1:A:200:GLU:HA	1:A:483:ARG:NH1	2.13	0.63
1:C:398:THR:HB	2:C:699:HOH:O	1.98	0.63
1:D:166:GLU:HG3	1:D:430:HIS:HB3	1.82	0.62
1:A:33:GLY:H	1:A:120:THR:HG22	1.64	0.62
1:B:95:ASP:OD2	1:B:478:ARG:NH1	2.33	0.62
1:B:164:HIS:NE2	1:B:166:GLU:OE1	2.33	0.61
1:A:183:THR:HG22	1:A:186:LEU:H	1.66	0.61
1:B:327:ASP:HB3	2:B:650:HOH:O	2.00	0.60
1:C:543:ALA:HA	2:C:670:HOH:O	2.00	0.60
1:A:164:HIS:NE2	1:A:166:GLU:OE1	2.34	0.60
1:B:379:ALA:HB3	1:B:380:PRO:HD3	1.83	0.60
1:C:506:ARG:NH1	1:A:1:MET:HB3	2.16	0.60
1:B:404:ARG:O	1:B:478:ARG:HD2	2.01	0.60
1:B:166:GLU:HG3	1:B:430:HIS:HB3	1.83	0.59
1:C:334:GLU:OE2	1:C:365:ASN:ND2	2.36	0.58
1:C:164:HIS:NE2	1:C:166:GLU:OE1	2.34	0.58
1:B:501:ARG:HB3	1:B:502:PRO:HD3	1.86	0.57
1:C:15:PHE:C	1:C:17:ASP:H	2.13	0.57
1:D:208:THR:HG23	1:D:247:TRP:NE1	2.20	0.56
1:A:30:VAL:HB	1:A:34:GLU:HB3	1.87	0.56
1:C:203:MET:HE1	1:C:433:PHE:CD1	2.41	0.55
1:A:203:MET:HE1	1:A:433:PHE:CD1	2.40	0.55
1:C:29:MET:HE2	1:C:153:ALA:HB2	1.87	0.55
1:C:361:ARG:CB	1:C:361:ARG:CZ	2.84	0.55
1:D:435:PHE:CZ	1:D:437:ASN:HB2	2.42	0.55
1:C:202:LEU:HD12	1:C:486:PHE:HD2	1.72	0.55
1:D:264:LEU:O	1:D:296:TYR:OH	2.23	0.54
1:B:95:ASP:CG	1:B:478:ARG:HH11	2.15	0.54
1:D:379:ALA:HB3	1:D:380:PRO:HD3	1.89	0.54
1:A:424:GLN:O	1:A:426:GLN:NE2	2.42	0.53
1:B:95:ASP:CG	1:B:478:ARG:NH1	2.67	0.53
1:C:240:ASP:OD1	1:C:240:ASP:C	2.52	0.53
1:B:203:MET:HE1	1:B:433:PHE:CD1	2.44	0.53
1:C:136:GLU:OE1	1:C:139:SER:OG	2.17	0.52
1:B:202:LEU:HD23	1:B:486:PHE:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ARG:HH11	1:B:482:GLN:HE22	1.58	0.51
1:B:40:LEU:C	1:B:40:LEU:HD23	2.36	0.51
1:D:446:ASP:OD2	1:C:446:ASP:OD2	2.29	0.51
1:C:33:GLY:H	1:C:120:THR:CG2	2.24	0.51
1:B:326:ALA:O	1:B:337:TYR:HE2	1.94	0.50
1:C:5:ILE:HG23	1:C:40:LEU:HD11	1.93	0.50
1:A:527:TRP:CE2	1:A:528:LEU:HD12	2.47	0.50
1:C:5:ILE:CG2	1:C:40:LEU:HD11	2.42	0.49
1:D:354:ILE:HG22	1:D:370:HIS:HB3	1.95	0.49
1:C:501:ARG:HB3	1:C:502:PRO:HD3	1.93	0.49
1:A:446:ASP:OD2	1:B:446:ASP:OD2	2.30	0.49
1:A:32:GLN:NE2	1:A:123:LEU:O	2.46	0.49
1:A:192:ASN:CG	1:A:472:GLN:OE1	2.55	0.49
1:A:379:ALA:HB3	1:A:380:PRO:HD3	1.94	0.49
1:C:496:GLU:O	1:C:499:LYS:O	2.32	0.48
1:C:27:THR:HG23	1:C:149:PRO:HB2	1.96	0.48
1:B:334:GLU:OE2	1:B:338:ARG:NH1	2.47	0.47
1:B:398:THR:HB	2:B:722:HOH:O	2.13	0.47
1:C:44:ARG:NH1	1:C:46:ARG:O	2.44	0.47
1:A:438:ALA:O	1:A:439:GLN:C	2.58	0.47
1:C:80:HIS:N	1:C:81:PRO:CD	2.78	0.47
1:C:543:ALA:C	2:C:670:HOH:O	2.58	0.47
1:A:202:LEU:HD13	1:A:483:ARG:HH11	1.80	0.47
1:B:327:ASP:OD1	1:B:327:ASP:N	2.47	0.47
1:B:196:PHE:CE1	1:B:465:VAL:HG11	2.50	0.46
1:C:348:LEU:HD22	1:C:351:LEU:HD12	1.97	0.46
1:B:23:TRP:HH2	2:B:731:HOH:O	1.98	0.46
1:B:59:THR:HA	1:B:131:THR:O	2.15	0.46
1:A:297:ARG:NH1	1:A:343:GLN:O	2.43	0.46
1:A:166:GLU:HB2	1:A:203:MET:HE2	1.97	0.46
1:D:1:MET:HA	1:B:506:ARG:HH12	1.81	0.46
1:D:514:MET:O	1:D:516:PRO:HD3	2.15	0.46
1:B:208:THR:HG23	1:B:247:TRP:CD1	2.51	0.46
1:D:19:VAL:HG21	1:B:510:VAL:HG13	1.98	0.45
1:C:71:VAL:HG12	1:C:451:THR:HG21	1.98	0.45
1:C:83:ALA:HB3	1:B:83:ALA:HB3	1.98	0.45
1:C:506:ARG:NH1	1:A:1:MET:CB	2.78	0.45
1:D:208:THR:HG23	1:D:247:TRP:CD1	2.51	0.45
1:A:200:GLU:HA	1:A:483:ARG:HH12	1.80	0.45
1:C:78:TRP:CD1	1:C:458:PRO:HD3	2.52	0.45
1:C:360:VAL:HA	1:C:381:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:THR:HG23	1:B:247:TRP:NE1	2.32	0.45
1:A:54:GLU:O	1:A:55:LEU:HD23	2.18	0.44
1:D:334:GLU:CB	1:D:361:ARG:NH2	2.79	0.44
1:B:29:MET:HE2	1:B:153:ALA:HB2	1.99	0.44
1:D:183:THR:HB	1:D:184:PRO:HD2	1.99	0.44
1:D:179:GLU:OE2	1:D:185:ARG:HD3	2.18	0.44
1:A:338:ARG:HG3	1:A:338:ARG:HH11	1.83	0.44
1:B:325:LEU:HD21	1:B:341:ARG:HG3	2.00	0.44
1:B:368:VAL:O	1:B:368:VAL:HG12	2.17	0.44
1:C:124:THR:O	1:C:128:TYR:OH	2.32	0.44
1:C:297:ARG:NH2	1:C:346:ASP:OD1	2.51	0.44
1:B:54:GLU:C	1:B:55:LEU:HD23	2.43	0.44
1:D:445:ILE:C	1:D:445:ILE:HD12	2.42	0.44
1:C:34:GLU:HA	1:C:35:PRO:HD2	1.92	0.44
1:C:235:THR:N	1:C:236:PRO:CD	2.81	0.43
1:C:261:MET:HG3	1:C:323:PHE:CE2	2.53	0.43
1:D:130:LEU:O	1:D:147:THR:HA	2.18	0.43
1:A:304:LEU:HB2	1:A:305:PRO:HD3	1.99	0.43
1:C:501:ARG:N	1:C:502:PRO:CD	2.82	0.43
1:A:379:ALA:N	1:A:380:PRO:CD	2.81	0.43
1:A:435:PHE:CZ	1:A:437:ASN:HB2	2.54	0.43
1:A:235:THR:HA	1:A:236:PRO:C	2.44	0.43
1:A:240:ASP:OD1	1:A:240:ASP:C	2.62	0.43
1:A:77:THR:HG22	1:A:85:TYR:CD2	2.53	0.43
1:B:181:PRO:HA	1:B:182:TYR:HA	1.79	0.43
1:D:233:PRO:HD3	1:D:279:THR:OG1	2.19	0.42
1:B:184:PRO:HD3	2:B:682:HOH:O	2.19	0.42
1:A:130:LEU:O	1:A:147:THR:HA	2.19	0.42
1:C:59:THR:HA	1:C:131:THR:O	2.19	0.42
1:A:327:ASP:O	1:A:328:GLU:CB	2.66	0.42
1:C:361:ARG:CZ	1:C:361:ARG:HB3	2.49	0.42
1:B:446:ASP:OD1	1:B:446:ASP:C	2.62	0.42
1:D:63:ALA:HB2	1:D:118:ILE:CD1	2.49	0.42
1:B:166:GLU:HA	1:B:430:HIS:O	2.19	0.42
1:D:438:ALA:O	1:D:439:GLN:C	2.63	0.42
1:C:75:LEU:O	1:C:458:PRO:HA	2.19	0.42
1:C:235:THR:N	1:C:236:PRO:HD2	2.35	0.42
1:B:40:LEU:C	1:B:40:LEU:CD2	2.93	0.42
1:B:54:GLU:O	1:B:55:LEU:HD23	2.20	0.42
1:D:488:ASP:OD2	1:D:528:LEU:HD23	2.20	0.41
1:A:4:GLN:NE2	1:A:6:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:THR:O	1:D:134:LEU:HA	2.20	0.41
1:D:253:GLN:NE2	2:D:605:HOH:O	2.34	0.41
1:C:340:ALA:O	1:C:341:ARG:C	2.63	0.41
1:B:130:LEU:O	1:B:147:THR:HA	2.21	0.41
1:B:245:ARG:HG3	1:B:245:ARG:HH11	1.85	0.41
1:D:133:THR:HA	1:D:144:PHE:O	2.21	0.41
1:B:304:LEU:HB2	1:B:305:PRO:HD3	2.03	0.41
1:C:163:HIS:O	1:C:427:GLY:HA2	2.20	0.41
1:A:501:ARG:NH1	2:A:621:HOH:O	2.53	0.41
1:A:527:TRP:CZ2	1:A:528:LEU:CD1	3.04	0.41
1:D:44:ARG:HD3	1:D:46:ARG:HB3	2.03	0.41
1:D:54:GLU:O	1:D:55:LEU:HD23	2.21	0.41
1:B:328:GLU:HA	1:B:328:GLU:OE1	2.20	0.41
1:B:268:TRP:CH2	1:B:440:LEU:HD21	2.56	0.41
1:B:461:ASP:HB3	1:B:462:PRO:HD3	2.01	0.41
1:D:68:ILE:HG12	1:D:97:LEU:CD2	2.51	0.41
1:D:241:TRP:CD2	1:D:310:VAL:HG21	2.56	0.40
1:C:1:MET:O	1:C:2:ASP:HB2	2.19	0.40
1:C:5:ILE:HG21	1:C:134:LEU:HD12	2.03	0.40
1:B:395:CYS:SG	2:B:689:HOH:O	2.36	0.40
1:C:202:LEU:HD21	1:C:483:ARG:NH1	2.37	0.40
1:B:373:VAL:O	1:B:391:THR:HA	2.20	0.40
1:B:124:THR:HA	1:B:125:PRO:HD3	1.87	0.40
1:C:181:PRO:HA	1:C:182:TYR:HA	1.91	0.40
1:B:9:ASP:HA	1:B:10:PRO:HD3	1.97	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	541/552 (98%)	509 (94%)	30 (6%)	2 (0%)	30 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	541/552 (98%)	509 (94%)	30 (6%)	2 (0%)	30	49
1	C	541/552 (98%)	509 (94%)	27 (5%)	5 (1%)	14	27
1	D	542/552 (98%)	508 (94%)	31 (6%)	3 (1%)	21	38
All	All	2165/2208 (98%)	2035 (94%)	118 (6%)	12 (1%)	21	38

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	385	ASP
1	A	328	GLU
1	C	140	GLY
1	C	268	TRP
1	D	520	ASP
1	C	2	ASP
1	C	162	LEU
1	B	365	ASN
1	D	344	VAL
1	A	95	ASP
1	B	210	ILE
1	D	125	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	447/453 (99%)	430 (96%)	17 (4%)	29	56
1	B	447/453 (99%)	434 (97%)	13 (3%)	37	65
1	C	446/453 (98%)	428 (96%)	18 (4%)	28	54
1	D	448/453 (99%)	432 (96%)	16 (4%)	31	58
All	All	1788/1812 (99%)	1724 (96%)	64 (4%)	31	58

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4	GLN
1	D	23	TRP
1	D	44	ARG
1	D	70	GLN
1	D	88	THR
1	D	104	VAL
1	D	120	THR
1	D	141	GLN
1	D	166	GLU
1	D	235	THR
1	D	318	ARG
1	D	344	VAL
1	D	357	LEU
1	D	361	ARG
1	D	445	ILE
1	D	528	LEU
1	C	43	GLN
1	C	44	ARG
1	C	62	SER
1	C	104	VAL
1	C	120	THR
1	C	141	GLN
1	C	146	GLN
1	C	166	GLU
1	C	222	THR
1	C	231	ILE
1	C	235	THR
1	C	240	ASP
1	C	306	GLN
1	C	325	LEU
1	C	361	ARG
1	C	389	LEU
1	C	426	GLN
1	C	534	LYS
1	A	7	LEU
1	A	23	TRP
1	A	24	VAL
1	A	48	ASP
1	A	104	VAL
1	A	120	THR
1	A	166	GLU
1	A	183	THR
1	A	240	ASP

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Mol	Chain	Res	Type
1	A	253	GLN
1	A	271	GLN
1	A	318	ARG
1	A	327	ASP
1	A	335	ASP
1	A	371	PRO
1	A	445	ILE
1	A	514	MET
1	B	27	THR
1	B	44	ARG
1	B	74	GLN
1	B	120	THR
1	B	133	THR
1	B	166	GLU
1	B	202	LEU
1	B	235	THR
1	B	242	SER
1	B	327	ASP
1	B	510	VAL
1	B	524	ASP
1	B	544	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	28	GLN
1	D	32	GLN
1	D	80	HIS
1	D	424	GLN
1	C	146	GLN
1	C	158	GLN
1	C	178	HIS
1	C	306	GLN
1	A	28	GLN
1	A	43	GLN
1	A	80	HIS
1	A	108	HIS
1	A	158	GLN
1	A	252	GLN
1	A	320	HIS
1	B	4	GLN
1	B	28	GLN

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Mol	Chain	Res	Type
1	B	70	GLN
1	B	252	GLN
1	B	306	GLN
1	B	482	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](#)

There are no ligands in this entry.

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	543/552 (98%)	-0.25	9 (1%) 69 65	11, 23, 43, 81	0
1	B	543/552 (98%)	-0.24	6 (1%) 78 75	9, 22, 46, 76	0
1	C	543/552 (98%)	-0.18	7 (1%) 75 71	10, 23, 50, 82	0
1	D	544/552 (98%)	-0.24	7 (1%) 75 71	10, 23, 44, 83	0
All	All	2173/2208 (98%)	-0.23	29 (1%) 75 71	9, 23, 46, 83	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	544	PRO	6.6
1	D	235	THR	5.4
1	C	235	THR	4.9
1	B	235	THR	4.7
1	C	236	PRO	3.7
1	A	543	ALA	3.6
1	A	327	ASP	3.6
1	A	268	TRP	3.5
1	B	236	PRO	3.4
1	C	268	TRP	3.4
1	D	329	PRO	3.2
1	B	138	ALA	3.1
1	A	365	ASN	3.1
1	D	236	PRO	3.0
1	A	328	GLU	2.6
1	A	333	THR	2.5
1	D	500	GLY	2.4
1	C	361	ARG	2.4
1	A	331	ALA	2.4
1	C	23	TRP	2.3
1	A	329	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	331	ALA	2.2
1	C	140	GLY	2.2
1	A	1	MET	2.2
1	B	331	ALA	2.2
1	B	327	ASP	2.1
1	D	328	GLU	2.1
1	B	544	PRO	2.1
1	D	543	ALA	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.