



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:30 AM UTC

PDB ID : 4BIR / pdb_00004bir
Title : RIBONUCLEASE T1: FREE HIS92GLN MUTANT
Authors : Doumen, J.; Steyaert, J.
Deposited on : 1998-01-13
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

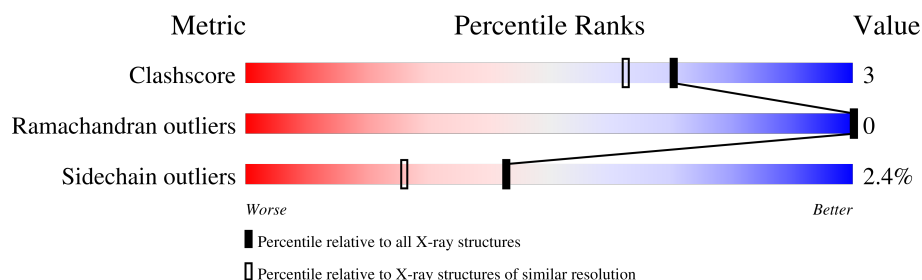
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	104	12% 84% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 933 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 GUANYL-SPECIFIC RIBONUCLEASE T1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	2	0
			785	485	126	170	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	LYS	GLN	conflict	UNP P00651
A	92	GLN	HIS	engineered mutation	UNP P00651

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is water.

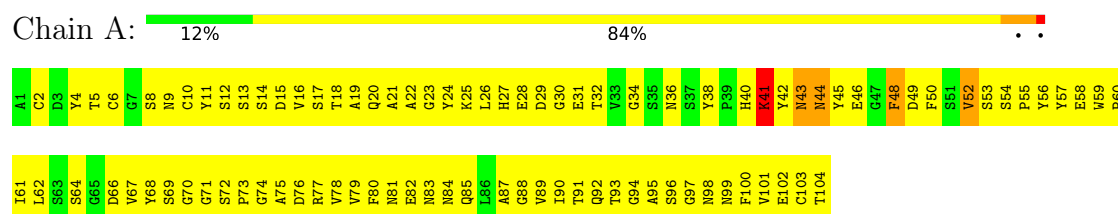
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	147	Total	O	0	0
			147	147		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: GUANYL-SPECIFIC RIBONUCLEASE T1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.82Å 46.53Å 41.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70	Depositor
% Data completeness (in resolution range)	94.5 (10.00-1.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	933	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

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: CA

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	3.43	116/813 (14.3%)	3.25	136/1106 (12.3%)

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	88	GLY	C-N	-11.26	1.19	1.33
1	A	70	GLY	N-CA	9.61	1.57	1.45
1	A	12	SER	CA-C	-9.31	1.40	1.52
1	A	30	GLY	C-N	-9.07	1.20	1.33
1	A	60	PRO	N-CA	-8.77	1.36	1.47
1	A	45	TYR	C-O	8.76	1.35	1.24
1	A	40	HIS	CD2-NE2	-8.69	1.28	1.37
1	A	19	ALA	CA-C	-8.66	1.41	1.52
1	A	48	PHE	C-O	-8.62	1.13	1.23
1	A	5	THR	C-O	8.61	1.33	1.24
1	A	27	HIS	CD2-NE2	-8.59	1.28	1.37
1	A	57	TYR	CA-C	-8.57	1.42	1.52
1	A	8	SER	C-N	-8.46	1.21	1.33
1	A	15	ASP	N-CA	8.45	1.56	1.46
1	A	103	CYS	C-N	-8.34	1.21	1.33
1	A	78[A]	VAL	CA-C	-8.32	1.42	1.52
1	A	78[B]	VAL	CA-C	-8.32	1.42	1.52
1	A	18	THR	N-CA	8.25	1.56	1.46
1	A	11	TYR	N-CA	-8.16	1.35	1.46
1	A	58	GLU	N-CA	-8.13	1.36	1.45
1	A	59	TRP	CA-C	-8.12	1.43	1.52
1	A	77	ARG	CZ-NH2	8.02	1.43	1.33
1	A	85	GLN	C-N	-7.94	1.22	1.33
1	A	81	ASN	C-N	-7.88	1.23	1.34
1	A	62	LEU	CA-C	-7.86	1.43	1.52
1	A	76	ASP	N-CA	7.85	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	GLY	CA-C	-7.85	1.43	1.52
1	A	101	VAL	C-O	7.82	1.32	1.23
1	A	26	LEU	CA-C	-7.74	1.42	1.52
1	A	67	VAL	N-CA	-7.72	1.37	1.46
1	A	61	ILE	CA-CB	7.69	1.64	1.54
1	A	76	ASP	CA-C	-7.64	1.43	1.52
1	A	80	PHE	CA-C	-7.59	1.43	1.52
1	A	95	ALA	N-CA	-7.49	1.36	1.45
1	A	58	GLU	C-N	-7.35	1.23	1.33
1	A	87	ALA	N-CA	7.24	1.55	1.46
1	A	12	SER	N-CA	7.16	1.54	1.45
1	A	28	GLU	C-O	-7.12	1.15	1.24
1	A	56	TYR	N-CA	-7.03	1.37	1.45
1	A	87	ALA	CA-C	-6.98	1.44	1.52
1	A	22	ALA	C-N	6.91	1.43	1.33
1	A	92	GLN	CA-C	-6.88	1.43	1.52
1	A	24	TYR	CA-CB	6.83	1.64	1.53
1	A	40	HIS	ND1-CE1	-6.77	1.25	1.32
1	A	13	SER	N-CA	-6.69	1.38	1.46
1	A	60	PRO	CA-CB	6.52	1.62	1.53
1	A	6	CYS	C-O	6.46	1.31	1.24
1	A	91	THR	CB-OG1	6.45	1.54	1.43
1	A	102	GLU	CA-C	-6.44	1.44	1.52
1	A	27	HIS	CE1-NE2	6.40	1.39	1.32
1	A	31	GLU	CD-OE1	-6.37	1.13	1.25
1	A	52	VAL	C-N	-6.37	1.24	1.33
1	A	53	SER	CA-CB	-6.36	1.43	1.53
1	A	19	ALA	C-N	6.34	1.42	1.33
1	A	34	GLY	C-O	-6.34	1.15	1.23
1	A	101	VAL	CA-CB	-6.33	1.44	1.55
1	A	62	LEU	C-N	-6.31	1.25	1.34
1	A	46	GLU	C-N	-6.28	1.25	1.33
1	A	83	ASN	CA-C	-6.27	1.43	1.52
1	A	49	ASP	C-N	-6.22	1.24	1.33
1	A	41	LYS	CA-C	-6.22	1.45	1.52
1	A	79	VAL	N-CA	-6.17	1.39	1.46
1	A	79	VAL	C-N	-6.16	1.25	1.33
1	A	41	LYS	N-CA	6.16	1.53	1.46
1	A	97	GLY	C-N	-6.14	1.25	1.33
1	A	32	THR	CB-OG1	6.09	1.53	1.43
1	A	32	THR	C-N	-6.06	1.25	1.33
1	A	10	CYS	N-CA	6.06	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	ALA	N-CA	6.04	1.54	1.45
1	A	68	TYR	N-CA	5.96	1.53	1.46
1	A	10	CYS	CA-CB	-5.94	1.45	1.53
1	A	17	SER	C-O	-5.93	1.17	1.24
1	A	17	SER	CA-C	5.91	1.60	1.52
1	A	40	HIS	C-N	-5.84	1.25	1.33
1	A	46	GLU	CA-C	5.83	1.60	1.52
1	A	14	SER	N-CA	5.73	1.53	1.46
1	A	57	TYR	CZ-OH	-5.71	1.26	1.38
1	A	71	GLY	CA-C	5.70	1.59	1.52
1	A	62	LEU	CA-CB	5.69	1.63	1.53
1	A	82	GLU	CA-CB	-5.69	1.43	1.53
1	A	96	SER	CA-C	-5.69	1.45	1.53
1	A	19	ALA	C-O	-5.65	1.17	1.24
1	A	73	PRO	C-O	5.62	1.31	1.24
1	A	50	PHE	CG-CD1	-5.57	1.27	1.38
1	A	28	GLU	N-CA	-5.54	1.39	1.46
1	A	40	HIS	CA-C	5.54	1.59	1.52
1	A	68	TYR	CA-CB	5.53	1.61	1.53
1	A	88	GLY	N-CA	-5.51	1.39	1.45
1	A	22	ALA	N-CA	5.46	1.52	1.46
1	A	62	LEU	N-CA	-5.46	1.39	1.46
1	A	54	SER	CB-OG	-5.44	1.31	1.42
1	A	24	TYR	CZ-OH	-5.43	1.26	1.38
1	A	4	TYR	CA-C	-5.41	1.46	1.52
1	A	98	ASN	C-N	-5.41	1.25	1.33
1	A	25[A]	LYS	C-O	-5.39	1.17	1.24
1	A	25[B]	LYS	C-O	-5.39	1.17	1.24
1	A	67	VAL	CA-C	5.39	1.58	1.52
1	A	98	ASN	CA-CB	-5.39	1.45	1.53
1	A	75	ALA	C-O	5.39	1.31	1.24
1	A	46	GLU	N-CA	-5.36	1.39	1.46
1	A	81	ASN	N-CA	-5.35	1.38	1.45
1	A	38	TYR	CA-CB	-5.24	1.45	1.53
1	A	69	SER	CB-OG	-5.24	1.31	1.42
1	A	8	SER	CA-CB	-5.23	1.45	1.53
1	A	93	THR	N-CA	-5.20	1.39	1.46
1	A	96	SER	N-CA	5.19	1.52	1.45
1	A	24	TYR	C-O	-5.16	1.18	1.24
1	A	18	THR	CA-CB	-5.15	1.45	1.53
1	A	60	PRO	C-N	-5.08	1.27	1.33
1	A	44	ASN	CA-CB	5.07	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	VAL	CA-C	5.05	1.58	1.52
1	A	66	ASP	CA-C	-5.05	1.46	1.52
1	A	18	THR	C-O	-5.04	1.18	1.24
1	A	93	THR	CA-C	5.02	1.59	1.52
1	A	2	CYS	N-CA	-5.01	1.40	1.46
1	A	82	GLU	N-CA	-5.01	1.40	1.46

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ARG	NE-CZ-NH1	16.18	137.69	121.50
1	A	88	GLY	CA-C-O	-15.02	107.36	121.63
1	A	15	ASP	CA-CB-CG	13.12	125.72	112.60
1	A	48	PHE	CZ-CE2-CD2	12.31	142.16	120.00
1	A	89	VAL	CA-C-O	12.11	132.98	120.39
1	A	72	SER	O-C-N	10.55	131.00	121.18
1	A	90	ILE	CA-CB-CG1	9.97	127.35	110.40
1	A	17	SER	O-C-N	9.80	133.33	122.15
1	A	75	ALA	O-C-N	9.76	134.35	122.35
1	A	30	GLY	O-C-N	9.28	131.01	122.57
1	A	70	GLY	O-C-N	-9.24	114.28	123.06
1	A	104	THR	CA-CB-CG2	9.10	125.97	110.50
1	A	9	ASN	OD1-CG-ND2	8.87	131.47	122.60
1	A	49	ASP	CA-CB-CG	8.79	121.39	112.60
1	A	89	VAL	O-C-N	-8.76	113.92	123.20
1	A	10	CYS	CA-C-N	8.73	136.03	122.94
1	A	10	CYS	C-N-CA	8.73	136.03	122.94
1	A	77	ARG	NH1-CZ-NH2	-8.70	108.00	119.30
1	A	92	GLN	OE1-CD-NE2	-8.69	113.91	122.60
1	A	48	PHE	CE1-CZ-CE2	-8.69	104.37	120.00
1	A	34	GLY	CA-C-N	8.68	131.91	120.28
1	A	34	GLY	C-N-CA	8.68	131.91	120.28
1	A	36	ASN	CA-CB-CG	-8.66	103.94	112.60
1	A	50	PHE	CA-CB-CG	8.46	122.26	113.80
1	A	100	PHE	CA-CB-CG	8.38	122.18	113.80
1	A	50	PHE	CA-C-O	-8.23	111.67	120.80
1	A	17	SER	CA-C-O	-8.16	111.77	120.42
1	A	84	ASN	CA-CB-CG	8.05	120.65	112.60
1	A	34	GLY	CA-C-O	8.01	129.84	122.39
1	A	82	GLU	CB-CG-CD	7.83	125.91	112.60
1	A	67	VAL	CA-CB-CG1	7.82	123.69	110.40
1	A	24	TYR	N-CA-CB	7.80	121.70	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ALA	CA-C-N	-7.78	109.41	122.64
1	A	75	ALA	C-N-CA	-7.78	109.41	122.64
1	A	13	SER	CA-CB-OG	-7.67	95.76	111.10
1	A	16	VAL	CA-C-O	-7.65	112.74	120.85
1	A	93	THR	CA-CB-OG1	-7.46	98.41	109.60
1	A	42	TYR	CA-C-O	-7.45	112.26	120.38
1	A	85	GLN	OE1-CD-NE2	-7.45	115.16	122.60
1	A	94	GLY	CA-C-O	-7.34	110.87	119.02
1	A	93	THR	CA-C-O	-7.30	112.30	120.70
1	A	85	GLN	CA-C-O	-7.27	112.50	120.43
1	A	75	ALA	CA-C-O	-7.27	111.05	119.05
1	A	48	PHE	CG-CD2-CE2	-7.27	108.34	120.70
1	A	52	VAL	CB-CA-C	7.27	122.32	110.69
1	A	34	GLY	O-C-N	-7.23	115.04	122.70
1	A	77	ARG	CA-C-O	-7.17	112.96	120.99
1	A	93	THR	CA-CB-CG2	7.12	122.61	110.50
1	A	87	ALA	CA-C-O	-7.07	110.23	120.13
1	A	81	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	4	TYR	O-C-N	-6.83	115.02	123.36
1	A	61	ILE	O-C-N	-6.80	115.91	123.26
1	A	55	PRO	N-CD-CG	-6.77	95.67	103.80
1	A	84	ASN	CA-C-O	6.75	129.31	121.28
1	A	11	TYR	CB-CG-CD2	6.73	130.89	120.80
1	A	103	CYS	N-CA-CB	6.70	120.18	110.06
1	A	10	CYS	O-C-N	-6.64	115.76	123.27
1	A	70	GLY	CA-C-O	-6.62	116.73	122.16
1	A	103	CYS	CA-CB-SG	-6.62	99.18	114.40
1	A	31	GLU	CA-CB-CG	6.60	127.31	114.10
1	A	72	SER	CA-C-O	-6.50	113.05	119.49
1	A	90	ILE	O-C-N	6.44	129.86	122.97
1	A	2	CYS	CA-C-O	-6.44	113.41	120.43
1	A	85	GLN	CB-CG-CD	-6.37	101.77	112.60
1	A	92	GLN	N-CA-C	-6.32	105.57	113.28
1	A	74	GLY	CA-C-O	6.32	131.56	122.58
1	A	90	ILE	N-CA-C	6.24	118.72	108.99
1	A	92	GLN	CA-C-O	-6.23	111.77	119.18
1	A	84	ASN	O-C-N	-6.14	114.19	122.41
1	A	10	CYS	N-CA-CB	-6.12	100.46	110.43
1	A	82	GLU	CG-CD-OE2	6.10	132.42	118.40
1	A	77	ARG	CD-NE-CZ	-6.10	115.87	124.40
1	A	5	THR	CA-C-O	-6.05	113.82	120.30
1	A	80	PHE	O-C-N	-6.04	114.67	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	LYS	CA-C-O	6.02	127.77	121.15
1	A	38	TYR	CA-C-O	5.99	126.80	120.63
1	A	99	ASN	CA-C-O	5.99	128.90	121.89
1	A	95	ALA	CA-C-O	-5.98	114.35	121.11
1	A	27	HIS	CG-CD2-NE2	5.97	113.17	107.20
1	A	11	TYR	CE1-CZ-OH	5.96	137.79	119.90
1	A	41	LYS	O-C-N	-5.95	115.72	122.97
1	A	77	ARG	CB-CA-C	-5.90	97.38	109.94
1	A	77	ARG	CG-CD-NE	5.88	124.95	112.00
1	A	30	GLY	CA-C-O	-5.81	113.05	120.03
1	A	4	TYR	N-CA-CB	5.78	120.51	110.81
1	A	19	ALA	CA-C-O	5.77	127.42	121.07
1	A	103	CYS	N-CA-C	-5.75	101.11	110.20
1	A	43	ASN	CA-C-N	-5.74	113.56	122.05
1	A	43	ASN	C-N-CA	-5.74	113.56	122.05
1	A	43	ASN	CB-CA-C	5.65	119.50	109.72
1	A	18	THR	N-CA-C	-5.63	105.04	111.07
1	A	82	GLU	CA-C-N	5.63	132.25	122.56
1	A	82	GLU	C-N-CA	5.63	132.25	122.56
1	A	4	TYR	CA-C-O	5.61	127.18	120.28
1	A	5	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	89	VAL	CA-C-N	5.56	131.75	122.57
1	A	89	VAL	C-N-CA	5.56	131.75	122.57
1	A	77	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	A	78[A]	VAL	CA-CB-CG1	5.54	119.81	110.40
1	A	78[B]	VAL	CA-CB-CG1	5.54	119.81	110.40
1	A	11	TYR	CB-CG-CD1	-5.51	112.53	120.80
1	A	99	ASN	CB-CG-ND2	-5.50	108.14	116.40
1	A	44	ASN	N-CA-CB	-5.48	103.84	110.53
1	A	52	VAL	N-CA-C	-5.46	99.96	108.86
1	A	97	GLY	CA-C-O	5.44	130.04	120.57
1	A	68	TYR	O-C-N	5.43	129.61	122.93
1	A	52	VAL	CG1-CB-CG2	5.39	122.65	110.80
1	A	29	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	64	SER	CA-C-O	-5.36	112.08	119.05
1	A	62	LEU	N-CA-C	5.35	118.20	109.59
1	A	85	GLN	O-C-N	5.33	129.29	123.27
1	A	92	GLN	CG-CD-OE1	5.32	131.44	120.80
1	A	20	GLN	CA-C-O	-5.30	114.90	120.63
1	A	11	TYR	N-CA-CB	5.28	120.02	110.83
1	A	11	TYR	CD1-CE1-CZ	5.25	129.05	119.60
1	A	60	PRO	N-CA-C	5.24	119.42	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ALA	CA-C-N	5.22	127.23	120.44
1	A	21	ALA	C-N-CA	5.22	127.23	120.44
1	A	18	THR	CA-C-N	5.21	128.03	120.79
1	A	18	THR	C-N-CA	5.21	128.03	120.79
1	A	82	GLU	OE1-CD-OE2	-5.19	110.44	122.90
1	A	78[A]	VAL	CG1-CB-CG2	-5.17	99.42	110.80
1	A	78[B]	VAL	CG1-CB-CG2	-5.17	99.42	110.80
1	A	91	THR	CA-CB-OG1	-5.17	101.84	109.60
1	A	41	LYS	CB-CA-C	5.14	117.97	109.70
1	A	99	ASN	OD1-CG-ND2	5.12	127.72	122.60
1	A	102	GLU	OE1-CD-OE2	5.10	135.15	122.90
1	A	10	CYS	CA-C-O	5.09	125.98	120.43
1	A	31	GLU	N-CA-CB	-5.05	103.02	111.20
1	A	90	ILE	CA-C-O	-5.03	115.81	121.75
1	A	25[A]	LYS	CA-C-N	5.03	127.02	120.28
1	A	25[A]	LYS	C-N-CA	5.03	127.02	120.28
1	A	25[B]	LYS	CA-C-N	5.03	127.02	120.28
1	A	25[B]	LYS	C-N-CA	5.03	127.02	120.28
1	A	93	THR	CB-CA-C	-5.03	102.92	110.16
1	A	77	ARG	CA-CB-CG	5.01	124.13	114.10

There are no chirality outliers.

There are no planarity outliers.

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	785	0	689	5	0
2	A	1	0	0	0	0
3	A	147	0	0	0	2
All	All	933	0	689	5	2

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 3.

All (5) 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:41:LYS:NZ	1:A:43:ASN:HD21	1.82	0.77
1:A:41:LYS:HZ3	1:A:43:ASN:HD21	1.43	0.65
1:A:44:ASN:HD21	1:A:48:PHE:H	1.47	0.61
1:A:41:LYS:HZ1	1:A:43:ASN:HD21	1.62	0.47
1:A:41:LYS:HZ3	1:A:41:LYS:HG2	1.68	0.42

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:147:HOH:O	3:A:197:HOH:O[3_645]	0.06	2.14
3:A:144:HOH:O	3:A:170:HOH:O[4_456]	0.07	2.13

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	104/104 (100%)	101 (97%)	3 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	86/85 (101%)	84 (98%)	2 (2%)	44	27

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	52	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	36	ASN
1	A	43	ASN
1	A	44	ASN
1	A	84	ASN
1	A	99	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 1 ligands modelled in this entry, 1 is 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	88:GLY	C	89:VAL	N	1.19

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.