Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 10:45 AM EDT

PDB ID	:	4BIR
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 (i) symbol.

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

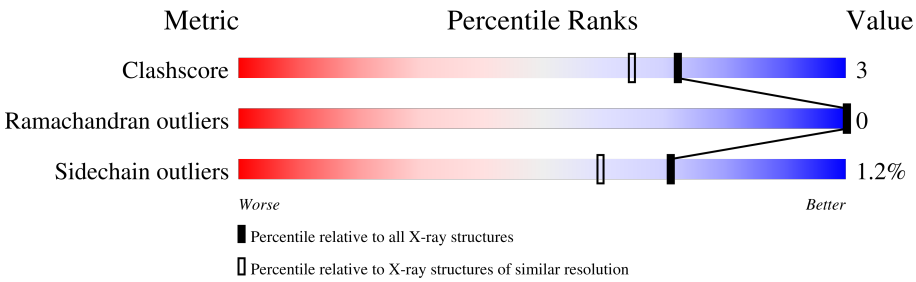
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	104	36% 62% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	104	785	485	126	170	4	0	2	0

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is water.

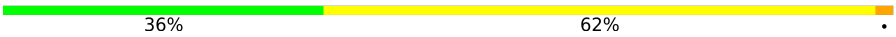
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	147	147	147	0	0

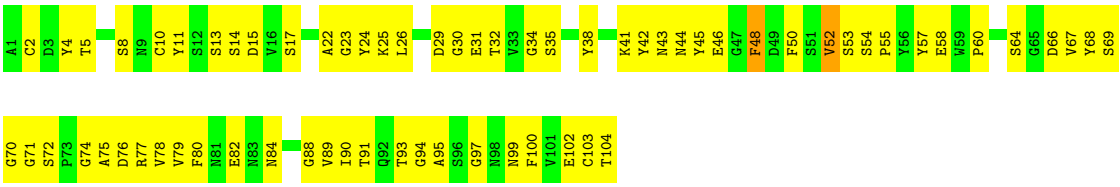
3 Residue-property plots (i)

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. 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

Chain A: 



4 Data and refinement statistics (i)

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	2.75	54/813 (6.6%)	3.02	83/1106 (7.5%)

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	GLU	CD-OE1	-11.28	1.13	1.25
1	A	54	SER	CB-OG	-8.45	1.31	1.42
1	A	77	ARG	CZ-NH2	8.33	1.43	1.33
1	A	69	SER	CB-OG	-8.13	1.31	1.42
1	A	70	GLY	N-CA	7.91	1.57	1.46
1	A	50	PHE	CG-CD1	-7.73	1.27	1.38
1	A	64	SER	CB-OG	-7.62	1.32	1.42
1	A	11	TYR	CG-CD1	7.18	1.48	1.39
1	A	24	TYR	CD2-CE2	-7.17	1.28	1.39
1	A	57	TYR	CD2-CE2	-7.09	1.28	1.39
1	A	45	TYR	CE2-CZ	-7.01	1.29	1.38
1	A	14	SER	CB-OG	-6.98	1.33	1.42
1	A	57	TYR	CZ-OH	-6.93	1.26	1.37
1	A	57	TYR	CD1-CE1	-6.88	1.29	1.39
1	A	45	TYR	CG-CD1	-6.86	1.30	1.39
1	A	68	TYR	CE1-CZ	-6.83	1.29	1.38
1	A	53	SER	CA-CB	-6.66	1.43	1.52
1	A	24	TYR	CZ-OH	-6.59	1.26	1.37
1	A	11	TYR	CD2-CE2	6.57	1.49	1.39
1	A	57	TYR	CB-CG	-6.52	1.41	1.51
1	A	60	PRO	N-CA	-6.30	1.36	1.47
1	A	45	TYR	C-O	6.30	1.35	1.23
1	A	88	GLY	C-N	-6.27	1.19	1.34
1	A	24	TYR	CD1-CE1	-6.22	1.30	1.39
1	A	31	GLU	CD-OE2	-5.97	1.19	1.25
1	A	30	GLY	C-N	-5.83	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	80	PHE	CG-CD1	-5.78	1.30	1.38
1	A	13	SER	CA-CB	5.70	1.61	1.52
1	A	2	CYS	CB-SG	-5.66	1.72	1.81
1	A	17	SER	CB-OG	5.56	1.49	1.42
1	A	35	SER	CB-OG	5.54	1.49	1.42
1	A	5	THR	C-O	5.53	1.33	1.23
1	A	22	ALA	C-N	5.51	1.43	1.33
1	A	38	TYR	CE2-CZ	5.47	1.45	1.38
1	A	8	SER	C-N	-5.43	1.21	1.34
1	A	91	THR	CB-OG1	5.41	1.54	1.43
1	A	103	CYS	C-N	-5.38	1.21	1.34
1	A	23	GLY	CA-C	-5.34	1.43	1.51
1	A	11	TYR	CE2-CZ	5.27	1.45	1.38
1	A	104	THR	C-O	5.26	1.33	1.23
1	A	97	GLY	N-CA	-5.24	1.38	1.46
1	A	34	GLY	C-O	-5.22	1.15	1.23
1	A	100	PHE	CG-CD1	-5.22	1.30	1.38
1	A	11	TYR	N-CA	-5.20	1.35	1.46
1	A	57	TYR	CG-CD2	5.16	1.45	1.39
1	A	48	PHE	C-O	-5.13	1.13	1.23
1	A	32	THR	CB-OG1	5.12	1.53	1.43
1	A	58	GLU	N-CA	-5.09	1.36	1.46
1	A	71	GLY	N-CA	-5.05	1.38	1.46
1	A	15	ASP	N-CA	5.04	1.56	1.46
1	A	8	SER	CA-CB	-5.03	1.45	1.52
1	A	13	SER	CB-OG	5.03	1.48	1.42
1	A	71	GLY	CA-C	5.03	1.59	1.51
1	A	46	GLU	CD-OE2	5.00	1.31	1.25

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	ARG	NE-CZ-NH1	34.77	137.69	120.30
1	A	48	PHE	CZ-CE2-CD2	18.38	142.16	120.10
1	A	11	TYR	CB-CG-CD2	16.49	130.89	121.00
1	A	11	TYR	CB-CG-CD1	-14.11	112.53	121.00
1	A	77	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	A	48	PHE	CG-CD2-CE2	-11.33	108.34	120.80
1	A	57	TYR	CB-CG-CD2	-11.24	114.26	121.00
1	A	82	GLU	OE1-CD-OE2	-10.72	110.44	123.30
1	A	77	ARG	NH1-CZ-NH2	-10.37	108.00	119.40
1	A	11	TYR	CD1-CE1-CZ	10.28	129.05	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	GLU	OE1-CD-OE2	9.87	135.15	123.30
1	A	68	TYR	CB-CG-CD1	9.72	126.83	121.00
1	A	104	THR	CA-CB-CG2	9.69	125.97	112.40
1	A	29	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	A	68	TYR	CB-CG-CD2	-8.73	115.76	121.00
1	A	48	PHE	CE1-CZ-CE2	-8.69	104.37	120.00
1	A	90	ILE	CA-CB-CG1	8.60	127.35	111.00
1	A	42	TYR	CB-CG-CD2	-8.57	115.86	121.00
1	A	67	VAL	CA-CB-CG1	8.53	123.69	110.90
1	A	103	CYS	CA-CB-SG	-8.23	99.18	114.00
1	A	45	TYR	CB-CG-CD1	8.04	125.82	121.00
1	A	45	TYR	CB-CG-CD2	-7.61	116.43	121.00
1	A	57	TYR	CG-CD1-CE1	-7.57	115.24	121.30
1	A	88	GLY	CA-C-O	-7.36	107.36	120.60
1	A	52	VAL	CG1-CB-CG2	7.34	122.65	110.90
1	A	93	THR	CA-CB-CG2	7.29	122.61	112.40
1	A	75	ALA	O-C-N	7.28	134.35	122.70
1	A	78[A]	VAL	CG1-CB-CG2	-7.18	99.42	110.90
1	A	78[B]	VAL	CG1-CB-CG2	-7.18	99.42	110.90
1	A	82	GLU	CG-CD-OE2	7.06	132.42	118.30
1	A	100	PHE	CB-CG-CD2	-6.91	115.96	120.80
1	A	38	TYR	CB-CG-CD2	6.74	125.05	121.00
1	A	17	SER	O-C-N	6.64	133.33	122.70
1	A	11	TYR	CE1-CZ-OH	6.55	137.79	120.10
1	A	77	ARG	CB-CA-C	-6.51	97.38	110.40
1	A	66	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	70	GLY	CA-C-N	6.39	128.97	116.20
1	A	31	GLU	CA-CB-CG	6.32	127.31	113.40
1	A	67	VAL	CG1-CB-CG2	-6.29	100.83	110.90
1	A	77	ARG	CG-CD-NE	6.26	124.95	111.80
1	A	24	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	A	24	TYR	N-CA-CB	6.17	121.70	110.60
1	A	89	VAL	CA-C-O	6.13	132.98	120.10
1	A	74	GLY	CA-C-O	6.09	131.56	120.60
1	A	76	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	76	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	78[A]	VAL	CA-CB-CG1	5.94	119.81	110.90
1	A	78[B]	VAL	CA-CB-CG1	5.94	119.81	110.90
1	A	52	VAL	CB-CA-C	5.75	122.32	111.40
1	A	10	CYS	C-N-CA	5.73	136.03	121.70
1	A	13	SER	CA-CB-OG	-5.72	95.76	111.20
1	A	38	TYR	CB-CG-CD1	-5.71	117.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	ASP	CB-CG-OD1	-5.69	113.17	118.30
1	A	76	ASP	OD1-CG-OD2	-5.67	112.52	123.30
1	A	26	LEU	CB-CG-CD1	-5.66	101.39	111.00
1	A	10	CYS	N-CA-CB	-5.63	100.46	110.60
1	A	15	ASP	CA-CB-CG	5.60	125.72	113.40
1	A	48	PHE	CB-CG-CD2	-5.55	116.92	120.80
1	A	77	ARG	CD-NE-CZ	-5.53	115.87	123.60
1	A	99	ASN	CA-C-N	-5.53	105.05	117.20
1	A	4	TYR	N-CA-CB	5.51	120.51	110.60
1	A	89	VAL	O-C-N	-5.49	113.92	122.70
1	A	94	GLY	CA-C-O	-5.41	110.87	120.60
1	A	11	TYR	CG-CD1-CE1	-5.35	117.02	121.30
1	A	103	CYS	N-CA-CB	5.32	120.18	110.60
1	A	84	ASN	O-C-N	-5.32	114.19	122.70
1	A	95	ALA	CB-CA-C	-5.31	102.14	110.10
1	A	70	GLY	O-C-N	-5.25	114.28	123.20
1	A	97	GLY	CA-C-O	5.24	130.04	120.60
1	A	25[A]	LYS	CB-CG-CD	5.24	125.22	111.60
1	A	25[B]	LYS	CB-CG-CD	5.24	125.22	111.60
1	A	11	TYR	N-CA-CB	5.24	120.02	110.60
1	A	72	SER	O-C-N	5.21	131.00	121.10
1	A	42	TYR	CB-CG-CD1	5.20	124.12	121.00
1	A	30	GLY	O-C-N	5.20	131.01	122.70
1	A	11	TYR	OH-CZ-CE2	-5.17	106.14	120.10
1	A	79	VAL	CA-CB-CG2	5.16	118.63	110.90
1	A	34	GLY	CA-C-O	5.13	129.84	120.60
1	A	66	ASP	OD1-CG-OD2	5.07	132.94	123.30
1	A	42	TYR	CG-CD1-CE1	-5.05	117.26	121.30
1	A	93	THR	CA-CB-OG1	-5.04	98.41	109.00
1	A	80	PHE	O-C-N	-5.02	114.67	122.70
1	A	55	PRO	N-CD-CG	-5.02	95.67	103.20

There are no chirality outliers.

There are no planarity outliers.

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	785	0	684	5	0
2	A	1	0	0	0	0
3	A	147	0	0	0	2
All	All	933	0	684	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	1.42	0.66
1:A:44:ASN:HD21	1:A:48:PHE:H	1.47	0.61
1:A:41:LYS:HZ1	1:A:43:ASN:HD21	1.64	0.45
1:A:41:LYS:HZ3	1:A:41:LYS:HG2	1.68	0.41

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 (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	104/104 (100%)	101 (97%)	3 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	86/85 (101%)	85 (99%)	1 (1%)	71 59

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL

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

Mol	Chain	Res	Type
1	A	43	ASN
1	A	44	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.