



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 PM UTC

PDB ID : 1TFR / pdb_00001tfr
Title : RNASE H FROM BACTERIOPHAGE T4
Authors : Mueser, T.C.; Nossal, N.G.; Hyde, C.C.
Deposited on : 1996-04-27
Resolution : 2.06 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

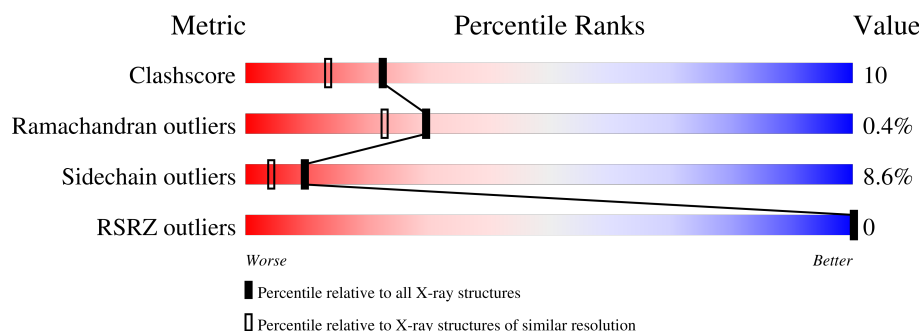
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	305	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2506 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 T4 RNASE H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2325	1507	382	427	9			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total	O	0	0
			179	179		

- Molecule 1: T4 RNASE H

W212	T98	MET
T213	W101	LEU
T214	E102	GLU
R215		GLU
V216		MET
E217	F105	MET
G218	E106	LEU
E219	S107	GLU
R220	S108	GLU
	H109	ASP
M224	K110	TVR
K225	V111	K112
T226	I112	E113
S227	D113	G14
I228	E114	
V229		F20
E230	Y118	
	H119	N31
E237	P120	F32
	Y121	
V241	I122	K37
		I38
T244	D127	N39
	K128	L40
M254		S41
L255	A136	M42
		V43
I258	S143	R44
I263	K148	I47
	I149	L48
N273		
K279	S154	I51
		K52
P281	L161	F53
P282	K163	
R283	Y164	K57
G284	P165	L61
K285	K286	
I286	V167	G69
Y287	K168	I70
		D71
F290	P172	
V291		R80
K292	K175	
	K176	A83
L295		Y84
S296	K179	Y85
K297	I180	
L298	L183	K88
T299	SER	ASN
N300	G183	ARG
S301		GLY
I302	D188	
N303	I303	ALA
F304	I193	ARG
		GLU
F305	K198	GLU
		ASP

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.47Å 87.58Å 54.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.06 6.00 – 2.06	Depositor EDS
% Data completeness (in resolution range)	90.3 (6.00-2.06) 89.2 (6.00-2.06)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.06Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.205 , 0.290 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.61 , 114.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	2506	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.83% 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: MG

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	0.93	1/2378 (0.0%)	1.77	32/3204 (1.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	149	ILE	CA-CB	5.39	1.61	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	GLU	CA-CB-CG	8.14	130.38	114.10
1	A	32	PHE	CA-CB-CG	7.52	121.32	113.80
1	A	80	ARG	CD-NE-CZ	-7.43	114.00	124.40
1	A	113	ASP	O-C-N	6.70	129.79	122.15
1	A	263	ILE	N-CA-C	-6.65	102.43	108.95
1	A	149	ILE	N-CA-C	6.57	117.94	108.48
1	A	118	TYR	CA-C-O	-6.54	111.86	119.64
1	A	273	ASN	CA-CB-CG	6.44	119.04	112.60
1	A	118	TYR	N-CA-C	6.37	121.45	113.43
1	A	219	GLU	N-CA-C	6.35	119.29	109.07
1	A	263	ILE	N-CA-CB	6.32	115.95	110.08
1	A	283	ARG	NE-CZ-NH2	-6.20	113.62	119.20
1	A	283	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	A	71	ASP	CA-CB-CG	5.82	118.42	112.60
1	A	258	ILE	N-CA-C	5.79	117.17	111.67
1	A	290	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	31	ASN	N-CA-C	5.72	120.39	112.90
1	A	48	LEU	O-C-N	5.67	128.61	122.15
1	A	226	THR	O-C-N	5.65	128.11	122.12
1	A	109	HIS	CA-CB-CG	-5.62	108.17	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	N-CA-C	-5.62	105.07	111.14
1	A	188	ASP	O-C-N	5.61	128.55	122.15
1	A	148	LYS	N-CA-C	-5.48	100.76	109.96
1	A	214	THR	N-CA-C	5.41	120.57	112.94
1	A	176	LYS	O-C-N	5.24	128.53	123.29
1	A	244	THR	N-CA-C	-5.17	103.57	110.55
1	A	172	PRO	N-CA-C	5.15	120.36	114.03
1	A	254	ASN	CA-C-O	-5.10	114.11	119.97
1	A	14	GLY	N-CA-C	-5.09	103.90	111.03
1	A	114	GLU	CG-CD-OE1	5.08	130.09	118.40
1	A	48	LEU	CA-C-O	-5.04	115.08	120.42
1	A	69	CYS	CB-CA-C	5.02	118.42	110.19

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	2325	0	2340	49	0
2	A	2	0	0	0	0
3	A	179	0	0	5	0
All	All	2506	0	2340	49	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 10.

All (49) 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:57:LYS:HZ3	1:A:61:LEU:HD11	1.38	0.88
1:A:176:LYS:NZ	1:A:176:LYS:HB3	1.99	0.78
1:A:216:VAL:HG12	1:A:218:GLY:H	1.52	0.74
1:A:281:PRO:HB2	1:A:285:LYS:HD3	1.72	0.71
1:A:57:LYS:NZ	1:A:61:LEU:HD11	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:PRO:HD2	1:A:285:LYS:HD2	1.76	0.66
1:A:44:ARG:HD3	1:A:295:LEU:HD11	1.84	0.59
1:A:37:LYS:HE3	1:A:39:ASN:HB3	1.85	0.58
1:A:53:PHE:CZ	1:A:175:LYS:HE2	2.39	0.57
1:A:216:VAL:O	1:A:219:GLU:HB2	2.05	0.56
1:A:215:ARG:NH2	1:A:219:GLU:O	2.38	0.55
1:A:20:PHE:HZ	1:A:47:ILE:HG23	1.72	0.54
1:A:43:VAL:O	1:A:47:ILE:HG13	2.08	0.53
1:A:281:PRO:HB2	1:A:285:LYS:CD	2.38	0.53
1:A:40:LEU:HA	1:A:107:SER:HB3	1.90	0.53
1:A:198:LYS:HD2	1:A:212:TRP:CH2	2.44	0.53
1:A:224:MET:HE2	1:A:228:ILE:HB	1.90	0.53
1:A:297:LYS:O	1:A:300:ASN:ND2	2.43	0.52
1:A:224:MET:HE3	3:A:517:HOH:O	2.10	0.51
1:A:290:PHE:HA	1:A:295:LEU:HD12	1.94	0.49
1:A:120:PRO:HD3	1:A:286:ILE:HD11	1.93	0.49
1:A:110:LYS:HZ2	1:A:113:ASP:HB2	1.78	0.48
1:A:226:THR:O	1:A:230:GLU:HG3	2.12	0.48
1:A:88:LYS:HE2	3:A:446:HOH:O	2.13	0.48
1:A:70:ILE:HD12	1:A:112:ILE:HD12	1.95	0.47
1:A:110:LYS:NZ	1:A:113:ASP:HB2	2.29	0.47
1:A:224:MET:HE3	1:A:224:MET:HA	1.96	0.46
1:A:193:ILE:HD13	1:A:255:LEU:HD23	1.97	0.46
1:A:47:ILE:O	1:A:51:ILE:HG13	2.14	0.46
1:A:127:ASP:O	1:A:128:LYS:HB2	2.16	0.46
1:A:122:ILE:HG13	3:A:557:HOH:O	2.16	0.45
1:A:282:PRO:CD	1:A:285:LYS:HD2	2.43	0.45
1:A:176:LYS:HB3	1:A:176:LYS:HZ2	1.80	0.45
1:A:20:PHE:CE2	1:A:112:ILE:HD11	2.51	0.45
1:A:88:LYS:HE2	3:A:503:HOH:O	2.17	0.44
1:A:101:TRP:HE3	1:A:105:PHE:HE2	1.66	0.44
1:A:287:TYR:O	1:A:291:VAL:HG23	2.17	0.43
1:A:287:TYR:HA	1:A:302:ILE:HD11	2.00	0.43
1:A:110:LYS:O	1:A:113:ASP:HB2	2.19	0.42
1:A:143:SER:OG	1:A:164:TYR:HB3	2.19	0.42
1:A:136:ALA:HA	1:A:161:LEU:HD11	2.01	0.42
1:A:168:LYS:HG3	3:A:423:HOH:O	2.19	0.41
1:A:287:TYR:CE1	1:A:299:THR:HB	2.55	0.41
1:A:83:ALA:HB1	1:A:85:TYR:CZ	2.54	0.41
1:A:39:ASN:O	1:A:42:MET:HB2	2.20	0.41
1:A:290:PHE:CD2	1:A:298:LEU:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:SER:HB3	1:A:304:GLU:OE2	2.21	0.41
1:A:44:ARG:NH2	1:A:114:GLU:OE2	2.37	0.41
1:A:179:LYS:O	1:A:180:ILE:HD12	2.21	0.40

There are no symmetry-related clashes.

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	277/305 (91%)	266 (96%)	10 (4%)	1 (0%)	30 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	LYS

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	257/277 (93%)	235 (91%)	22 (9%)	10 4

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LYS
1	A	47	ILE
1	A	57	LYS
1	A	80	ARG
1	A	88	LYS
1	A	102	GLU
1	A	110	LYS
1	A	154	SER
1	A	163	LYS
1	A	166	ASN
1	A	176	LYS
1	A	179	LYS
1	A	180	ILE
1	A	220	ARG
1	A	225	LYS
1	A	241	VAL
1	A	279	LYS
1	A	283	ARG
1	A	292	LYS
1	A	295	LEU
1	A	300	ASN
1	A	301	SER

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	45	HIS
1	A	300	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

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	283/305 (92%)	-0.83	0 100 100	17, 28, 52, 74	0

There are no RSRZ outliers to report.

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](#)

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	MG	A	351	1/1	0.90	0.09	38,38,38,38	0
2	MG	A	350	1/1	0.94	0.05	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.