



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 05:56 AM UTC

PDB ID : 2CZJ / pdb_00002czj
Title : Crystal structure of the tRNA domain of tmRNA from *Thermus thermophilus* HB8
Authors : Bessho, Y.; Shibata, R.; Sekine, S.; Murayama, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-07-13
Resolution : 3.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

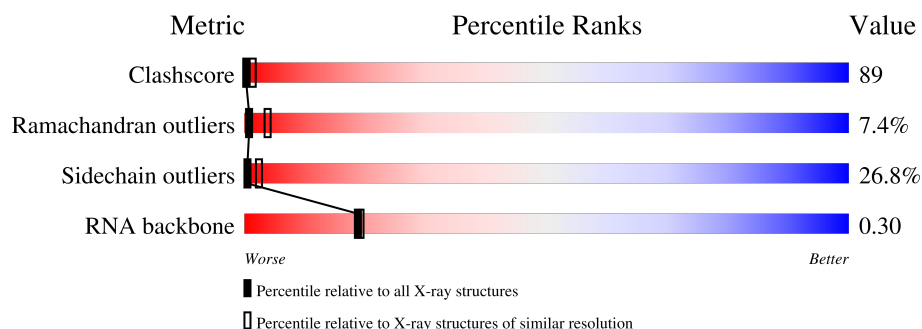
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RNA backbone	3983	1139 (3.24-2.80)

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	123	17% 51% 23% 8% .
1	C	123	14% 48% 30% . .
1	E	123	11% 57% 26% 5% .
1	G	123	6% 52% 33% 7% .
2	B	63	17% 35% 30% 16% .
2	D	63	5% 43% 29% 22% .

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Mol	Chain	Length	Quality of chain
2	F	63	17% 38% 27% 16%
2	H	63	8% 48% 29% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9224 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 SsrA-binding protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	122	Total	C	N	O	0	0	0
			993	637	181	175			
1	C	118	Total	C	N	O	0	0	0
			965	621	176	168			
1	E	122	Total	C	N	O	0	0	0
			993	637	181	175			
1	G	120	Total	C	N	O	0	0	0
			981	629	179	173			

- Molecule 2 is a RNA chain called tmRNA (63-MER).

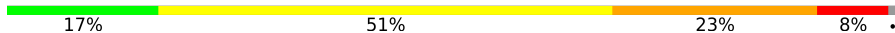
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	62	Total	C	N	O	P	0	0	0
			1323	589	233	439	62			
2	D	62	Total	C	N	O	P	0	0	0
			1323	589	233	439	62			
2	F	62	Total	C	N	O	P	0	0	0
			1323	589	233	439	62			
2	H	62	Total	C	N	O	P	0	0	0
			1323	589	233	439	62			

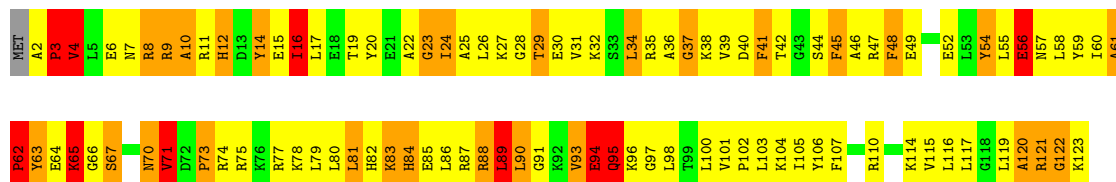
3 Residue-property plots

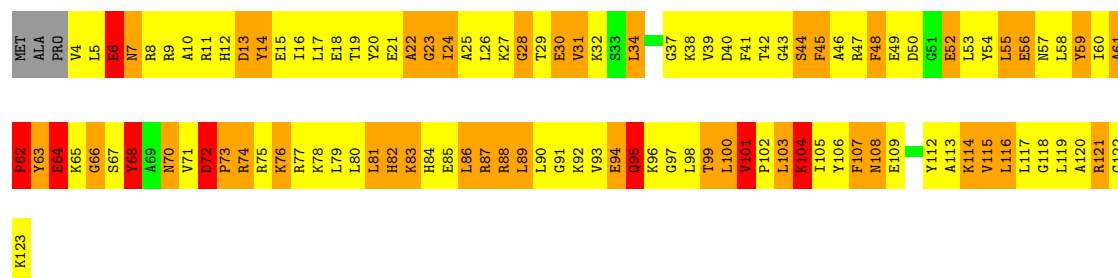
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

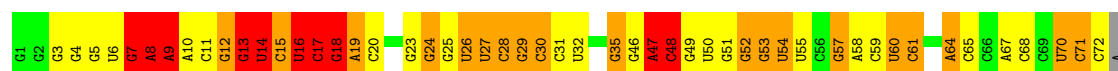
• Molecule 1: SsrA-binding protein

Chain A: 





- Molecule 2: tmRNA (63-MER)



- Molecule 2: tmRNA (63-MER)



- Molecule 2: tmRNA (63-MER)



- Molecule 2: tmRNA (63-MER)



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.78 Å 67.96 Å 178.66 Å 90.00° 90.07° 90.00°	Depositor
Resolution (Å)	48.76 – 3.01	Depositor
% Data completeness (in resolution range)	96.7 (48.76-3.01)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.255 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9224	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU

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	0.78	0/1011	1.36	20/1354 (1.5%)
1	C	1.23	2/982 (0.2%)	1.43	23/1315 (1.7%)
1	E	0.95	1/1011 (0.1%)	1.30	10/1354 (0.7%)
1	G	0.98	2/998 (0.2%)	1.52	22/1335 (1.6%)
2	B	0.73	0/1431	1.32	23/2228 (1.0%)
2	D	0.87	8/1431 (0.6%)	1.46	32/2228 (1.4%)
2	F	0.69	1/1431 (0.1%)	1.21	22/2228 (1.0%)
2	H	0.72	2/1431 (0.1%)	1.24	18/2228 (0.8%)
All	All	0.86	16/9726 (0.2%)	1.35	170/14270 (1.2%)

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	1
1	C	0	2
1	E	0	1
1	G	0	1
2	B	0	2
2	F	0	3
2	H	0	1
All	All	0	11

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	43	GLY	C-O	-30.24	0.83	1.23
2	D	60	U	C3'-O3'	-9.41	1.28	1.42
1	G	43	GLY	C-O	-8.78	1.12	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	24	ILE	CA-CB	8.32	1.66	1.54
2	D	57	G	O3'-P	-7.80	1.49	1.61

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	60	U	C4'-C3'-O3'	-21.06	81.41	113.00
2	D	59	C	C2'-C3'-O3'	-14.72	91.62	113.70
1	G	66	GLY	N-CA-C	-13.63	80.88	113.18
2	H	60	U	C4'-C3'-O3'	-13.49	92.77	113.00
2	D	64	A	C4'-C3'-O3'	-12.92	93.63	113.00

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	TYR	Sidechain
1	C	112	TYR	Sidechain
1	C	20	TYR	Sidechain
1	E	106	TYR	Sidechain
1	G	68	TYR	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	993	0	1030	194	0
1	C	965	0	1002	199	0
1	E	993	0	1030	300	0
1	G	981	0	1018	321	0
2	B	1323	0	672	120	0
2	D	1323	0	672	167	0
2	F	1323	0	672	150	0
2	H	1323	0	672	149	0
All	All	9224	0	6768	1418	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 89.

The worst 5 of 1418 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:C:43:GLY:O	1:C:44:SER:N	1.73	1.21
1:E:21:GLU:O	2:F:18:G:N2	1.73	1.21
1:C:43:GLY:O	1:C:43:GLY:CA	1.89	1.20
2:H:22:G:H2'	2:H:23:G:H5''	1.23	1.18
1:E:55:LEU:HD11	1:E:102:PRO:HG3	1.20	1.17

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	120/123 (98%)	89 (74%)	22 (18%)	9 (8%)	1	3
1	C	114/123 (93%)	91 (80%)	17 (15%)	6 (5%)	1	8
1	E	120/123 (98%)	84 (70%)	24 (20%)	12 (10%)	0	2
1	G	118/123 (96%)	94 (80%)	16 (14%)	8 (7%)	1	4
All	All	472/492 (96%)	358 (76%)	79 (17%)	35 (7%)	1	4

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	4	VAL
1	A	94	GLU
1	C	108	ASN
1	E	3	PRO

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	101/102 (99%)	76 (75%)	25 (25%)	1	3
1	C	98/102 (96%)	77 (79%)	21 (21%)	1	5
1	E	101/102 (99%)	75 (74%)	26 (26%)	0	3
1	G	100/102 (98%)	65 (65%)	35 (35%)	0	1
All	All	400/408 (98%)	293 (73%)	107 (27%)	0	2

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	52	GLU
1	E	105	ILE
1	G	99	THR
1	E	62	PRO
1	E	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	84	HIS
1	E	108	ASN
1	G	70	ASN
1	G	12	HIS
1	C	82	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	61/63 (96%)	21 (34%)	8 (13%)
2	D	61/63 (96%)	25 (40%)	7 (11%)
2	F	61/63 (96%)	21 (34%)	7 (11%)
2	H	61/63 (96%)	20 (32%)	6 (9%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	244/252 (96%)	87 (35%)	28 (11%)

5 of 87 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	7	G
2	B	8	A
2	B	9	A
2	B	11	C
2	B	12	G

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	60	U
2	H	58	A
2	F	12	G
2	H	19	A
2	F	8	A

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5MU	H	54	2	19,22,23	0.97	2 (10%)	27,32,35	2.29	6 (22%)
2	5MU	D	54	2	19,22,23	1.82	5 (26%)	27,32,35	2.44	7 (25%)
2	5MU	F	54	2	19,22,23	1.02	1 (5%)	27,32,35	2.39	7 (25%)
2	5MU	B	54	2	19,22,23	1.62	5 (26%)	27,32,35	2.92	8 (29%)
2	PSU	H	55	2	18,21,22	0.78	0	21,30,33	1.44	3 (14%)
2	PSU	D	55	2	18,21,22	0.80	0	21,30,33	1.39	3 (14%)
2	PSU	F	55	2	18,21,22	0.80	0	21,30,33	1.61	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PSU	B	55	2	18,21,22	0.89	1 (5%)	21,30,33	1.72	4 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5MU	H	54	2	-	0/7/25/26	0/2/2/2
2	5MU	D	54	2	-	0/7/25/26	0/2/2/2
2	5MU	F	54	2	-	0/7/25/26	0/2/2/2
2	5MU	B	54	2	-	0/7/25/26	0/2/2/2
2	PSU	H	55	2	-	0/7/25/26	0/2/2/2
2	PSU	D	55	2	-	0/7/25/26	0/2/2/2
2	PSU	F	55	2	-	1/7/25/26	0/2/2/2
2	PSU	B	55	2	-	1/7/25/26	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	54	5MU	C6-C5	3.90	1.41	1.34
2	D	54	5MU	C6-N1	3.83	1.44	1.38
2	D	54	5MU	C4-C5	3.44	1.50	1.44
2	D	54	5MU	C6-C5	3.36	1.40	1.34
2	B	54	5MU	C6-N1	3.31	1.43	1.38

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54	5MU	C4-N3-C2	-7.54	117.45	127.34
2	B	54	5MU	C5-C4-N3	6.82	121.25	115.32
2	D	54	5MU	C4-N3-C2	-6.08	119.36	127.34
2	F	54	5MU	C5-C4-N3	5.88	120.44	115.32
2	B	54	5MU	O4-C4-C5	-5.74	118.36	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	55	PSU	O4'-C1'-C5-C4
2	F	55	PSU	O4'-C1'-C5-C4

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	54	5MU	2	0
2	D	54	5MU	2	0
2	F	54	5MU	2	0
2	B	54	5MU	3	0
2	H	55	PSU	3	0
2	D	55	PSU	3	0

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 [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.