



wwPDB X-ray Structure Validation Summary Report ⓘ

May 7, 2026 – 12:05 PM EDT

PDB ID : 1N36 / pdb_00001n36
Title : Structure of the *Thermus thermophilus* 30S ribosomal subunit in the presence of crystallographically disordered codon and near-cognate transfer RNA anticodon stem-loop mismatched at the second codon position
Authors : Ogle, J.M.; Murphy IV, F.V.; Tarry, M.J.; Ramakrishnan, V.
Deposited on : 2002-10-25
Resolution : 3.65 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	:	NOT EXECUTED
Xtriage (Phenix)	:	2.0
EDS	:	NOT EXECUTED
Buster-report	:	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

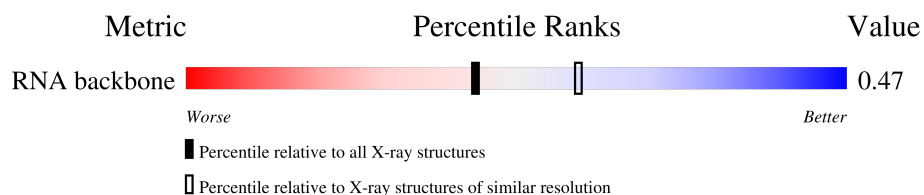
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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))
RNA backbone	3983	1027 (4.26-3.06)

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

2 Data and refinement statistics

EDS was not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.84Å 402.84Å 174.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.42 – 3.65	Depositor
% Data completeness (in resolution range)	92.6 (141.42-3.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.324	Depositor
Wilson B-factor (Å ²)	107.1	Xtriage
Anisotropy	0.426	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	51680	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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.

3 Model quality ⓘ

3.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.52	0/36387	0.77	61/56789 (0.1%)
2	B	0.60	0/1935	1.22	27/2609 (1.0%)
3	C	0.57	0/1636	1.17	13/2205 (0.6%)
4	D	0.56	0/1733	1.03	13/2318 (0.6%)
5	E	0.81	1/1162 (0.1%)	1.23	11/1564 (0.7%)
6	F	0.51	0/856	1.06	8/1154 (0.7%)
7	G	0.52	0/1276	1.22	17/1709 (1.0%)
8	H	0.86	1/1136 (0.1%)	1.32	15/1527 (1.0%)
9	I	0.55	0/1029	1.17	11/1378 (0.8%)
10	J	0.59	0/805	1.32	14/1082 (1.3%)
11	K	0.64	0/900	1.21	11/1213 (0.9%)
12	L	0.64	0/986	1.24	9/1320 (0.7%)
13	M	0.51	0/947	1.24	16/1270 (1.3%)
14	N	0.51	0/501	1.07	5/664 (0.8%)
15	O	0.67	1/745 (0.1%)	1.04	4/992 (0.4%)
16	P	0.67	0/716	1.25	9/963 (0.9%)
17	Q	0.75	0/870	1.34	14/1159 (1.2%)
18	R	0.58	0/603	1.06	2/799 (0.3%)
19	S	0.59	0/661	1.35	13/890 (1.5%)
20	T	0.58	0/765	1.09	5/1007 (0.5%)
21	V	0.56	0/212	0.96	0/277
All	All	0.56	3/55861 (0.0%)	0.93	278/82889 (0.3%)

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	1	63
8	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	1	64

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	109	ILE	CA-CB	-5.76	1.46	1.54
5	E	101	ILE	CA-CB	-5.25	1.47	1.53
15	O	29	VAL	CA-CB	-5.24	1.48	1.54

The worst 5 of 278 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	30	ILE	N-CA-C	-13.09	99.88	112.96
1	A	1498	U	C2'-C3'-O3'	12.81	128.71	109.50
18	R	46	GLU	N-CA-C	-11.68	98.28	111.71
12	L	26	ALA	N-CA-C	-11.66	99.80	113.21
3	C	122	GLU	N-CA-C	-11.49	98.77	111.07

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1498	U	C3'

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	G	Sidechain
1	A	129	U	Sidechain
1	A	156	G	Sidechain
1	A	183	G	Sidechain
1	A	77	G	Sidechain

3.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

3.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

3.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	253 (16%)	0

5 of 253 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

There are no RNA pucker outliers to report.

3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

Mogul was not executed - this section is therefore empty.

3.5 Carbohydrates [i](#)

Mogul was not executed - this section is therefore empty.

3.6 Ligand geometry [i](#)

Mogul was not executed - this section is therefore empty.

3.7 Other polymers [i](#)

Mogul was not executed - this section is therefore empty.

3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data

4.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

4.3 Carbohydrates

EDS was not executed - this section is therefore empty.

4.4 Ligands

EDS was not executed - this section is therefore empty.

4.5 Other polymers

EDS was not executed - this section is therefore empty.