



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:06 am GMT

PDB ID : 1ZO3  
EMDB ID: : EMD-1248  
Title : The P-site and P/E-site tRNA structures fitted to P/I site codon.  
Authors : Allen, G.S.; Zavialov, A.; Gursky, R.; Ehrenberg, M.; Frank, J.  
Deposited on : 2005-05-12  
Resolution : 13.80 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

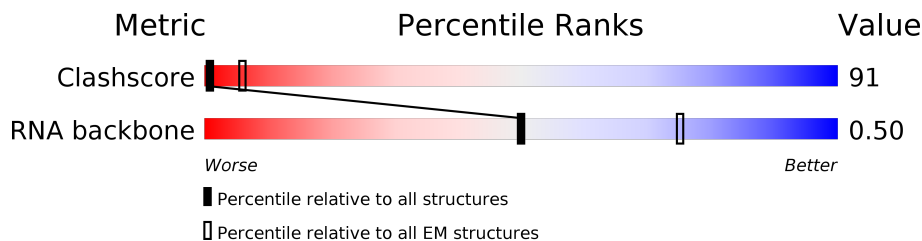
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



The reported resolution of this entry is 13.80 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)	EM structures (#Entries)
Clashscore	125131	1336
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	76	 87% 12%
1	B	76	 87% 12%

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3250 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	76	Total	C	N	O	P	0	0
			1625	725	293	531	76		
1	B	76	Total	C	N	O	P	0	0
			1625	725	293	531	76		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

#### ● Molecule 1: tRNA

Chain A: 

G1	C2	G3	G4	A5	U6	U7	U8	A9	G10	C11	U12	C13	A14	G15	U16	U17	G18	G19	G20	A21	G22	A23	G24	C25	G26	C27	C28	A29	G30	A31	C32	U33	G34	A35	A36	G37	A38	U39	C40	U41	G42	G43	A44	G45	G46	U47	C48	C49	U50	G51	U52	G53	U54	U55	C56	G57	A58	U59	C60
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

C61	A62	C63	A64	G65	A66	A67	U68	U69	C70	G71	C72	A73	C74	C75	A76
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

#### ● Molecule 1: tRNA

Chain B: 

G1	C2	G3	G4	A5	U6	U7	U8	A9	G10	C11	U12	C13	A14	G15	U16	U17	G18	G19	G20	A21	G22	A23	G24	C25	G26	C27	C28	A29	G30	A31	C32	U33	G34	A35	A36	G37	A38	U39	C40	U41	G42	G43	A44	G45	G46	U47	C48	C49	U50	G51	U52	G53	U54	U55	C56	G57	A58	U59	C60
----	----	----	----	----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

C61	A62	C63	A64	G65	A66	A67	U68	U69	C70	G71	C72	A73	C74	C75	A76
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	DEFOCUS GROUPS 0.93-3.93 UM	Depositor
Microscope	TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	-930.00	Depositor
Maximum defocus (nm)	-3930.00	Depositor
Magnification	Not provided	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	5.59	278/1817 (15.3%)	6.10	698/2831 (24.7%)
1	B	6.39	280/1817 (15.4%)	6.28	698/2831 (24.7%)
All	All	6.01	558/3634 (15.4%)	6.19	1396/5662 (24.7%)

The worst 5 of 558 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	U	C1'-N1	148.98	3.72	1.48
1	B	39	U	C1'-N1	148.94	3.72	1.48
1	B	1	G	P-OP2	106.09	3.29	1.49
1	A	55	U	C1'-N1	91.85	2.86	1.48
1	B	55	U	C1'-N1	91.80	2.86	1.48

The worst 5 of 1396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	U	C6-N1-C1'	-83.89	3.75	121.20
1	B	55	U	C6-N1-C1'	-83.89	3.75	121.20
1	B	39	U	C6-N1-C1'	-73.68	18.05	121.20
1	A	39	U	C6-N1-C1'	-73.67	18.06	121.20
1	A	55	U	C5-C6-N1	-50.83	97.29	122.70

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	1625	0	811	298	0
1	B	1625	0	814	296	0
All	All	3250	0	1625	438	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 91.

The worst 5 of 438 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:33:U:C4	1:B:34:G:H2'	1.18	1.64
1:A:37:G:C6	1:B:36:A:C2	2.04	1.45
1:A:33:U:C6	1:B:33:U:O2'	1.70	1.42
1:A:33:U:H1'	1:B:35:A:N6	1.41	1.36
1:A:32:C:C6	1:B:33:U:N3	1.70	1.35

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	75/76 (98%)	9 (12%)	0
1	B	75/76 (98%)	9 (12%)	0
All	All	150/152 (98%)	18 (12%)	0

5 of 18 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	17	U
1	A	18	G
1	A	21	A
1	A	37	G

There are no RNA pucker outliers to report.

#### 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 carbohydrates 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.