



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 11:18 am GMT

PDB ID : 3BBV
EMDB ID: : EMD-1455
Title : The tRNA(phe) fitted into the low resolution Cryo-EM map of the 50S.nc-tRNA.Hsp15 complex
Authors : Jiang, L.; Abrahams, J.P.
Deposited on : 2007-11-11
Resolution : 10.00 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
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
Mogul : 1.7.2 (RC1), CSD as538be (2017)
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

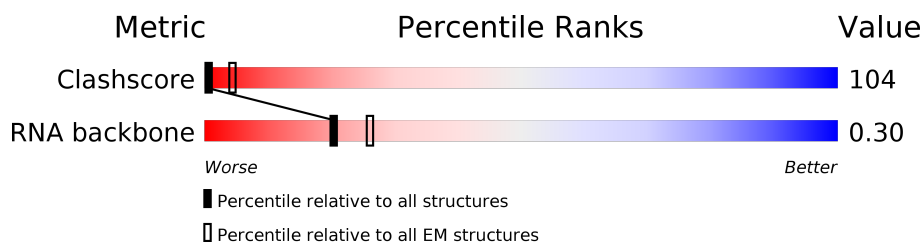
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

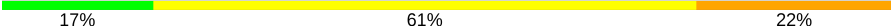
The reported resolution of this entry is 10.00 Å.

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 ≥ 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	z	76	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1628 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(Phe).

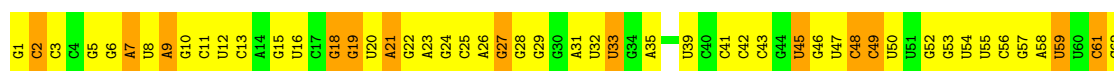
Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
1	z	76	1628	731	290	530	75	2	0	0

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(Phe)

Chain z: 



4 Experimental information

Property	Value	Source
Reconstruction method	Not provided	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction of each particle	Depositor
Microscope	FEI Tecnai F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	3.5	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO-163 film	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, MIA, 4SU, 7MG, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	z	2.66	94/1602 (5.9%)	2.11	76/2493 (3.0%)

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	z	47	U	O3'-P	12.52	1.76	1.61
1	z	26	A	C5-C6	9.54	1.49	1.41
1	z	26	A	N7-C5	7.99	1.44	1.39
1	z	26	A	N9-C4	7.94	1.42	1.37
1	z	12	U	C2-N3	7.84	1.43	1.37

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	z	31	A	C3'-C2'-C1'	-8.56	94.65	101.50
1	z	57	G	C8-N9-C4	7.77	109.51	106.40
1	z	74	C	N3-C4-C5	-7.64	118.84	121.90
1	z	1	G	N9-C4-C5	7.52	108.41	105.40
1	z	61	C	C6-N1-C2	7.51	123.31	120.30

There are no chirality outliers.

There are no planarity outliers.

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	z	1628	0	833	0	0
All	All	1628	0	833	0	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 104.

There are no clashes within the asymmetric unit.

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	z	73/76 (96%)	27 (36%)	0

5 of 27 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	z	2	C
1	z	7	A
1	z	8	4SU
1	z	9	A
1	z	16	H2U

There are no RNA pucker outliers to report.

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

9 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
1	H2U	z	16	1	17,21,22	1.55	3 (17%)	21,30,33	1.45	6 (28%)
1	H2U	z	20	1	17,21,22	1.24	3 (17%)	21,30,33	1.33	2 (9%)
1	PSU	z	32	1	16,21,22	1.28	2 (12%)	20,30,33	3.81	11 (55%)
1	MIA	z	37	1	23,31,32	2.03	6 (26%)	25,44,47	2.11	6 (24%)
1	PSU	z	39	1	16,21,22	2.51	4 (25%)	20,30,33	3.84	8 (40%)
1	7MG	z	46	1	20,26,27	3.14	10 (50%)	22,39,42	2.42	6 (27%)
1	5MU	z	54	1	14,22,23	2.15	6 (42%)	16,32,35	2.86	5 (31%)
1	PSU	z	55	1	16,21,22	2.80	3 (18%)	20,30,33	3.80	9 (45%)
1	4SU	z	8	1	14,21,22	2.75	6 (42%)	15,30,33	2.27	5 (33%)

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
1	H2U	z	16	1	-	0/7/38/39	0/2/2/2
1	H2U	z	20	1	-	0/7/38/39	0/2/2/2
1	PSU	z	32	1	-	0/7/25/26	0/2/2/2
1	MIA	z	37	1	-	0/11/33/34	0/3/3/3
1	PSU	z	39	1	-	0/7/25/26	0/2/2/2
1	7MG	z	46	1	-	0/7/37/38	0/3/3/3
1	5MU	z	54	1	-	0/3/25/26	0/2/2/2
1	PSU	z	55	1	-	0/7/25/26	0/2/2/2
1	4SU	z	8	1	-	0/3/25/26	0/2/2/2

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	z	55	PSU	C5-C1'	-9.32	1.44	1.52
1	z	39	PSU	C5-C1'	-7.66	1.45	1.52
1	z	8	4SU	O5'-C5'	-6.11	1.36	1.44
1	z	39	PSU	O4'-C4'	-4.09	1.35	1.45
1	z	16	H2U	O5'-C5'	-3.76	1.39	1.44

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	z	32	PSU	N1-C2-N3	-12.38	119.49	128.40
1	z	39	PSU	N1-C2-N3	-10.29	121.00	128.40
1	z	55	PSU	N1-C2-N3	-10.06	121.16	128.40
1	z	39	PSU	C5-C4-N3	-8.65	118.33	125.43
1	z	46	7MG	C5-C6-N1	-7.26	111.97	123.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.