



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

Jul 11, 2018 – 01:27 PM EDT

PDB ID : 1LU3  
EMDB ID: : EMD-1045  
Title : Separate Fitting of the Anticodon Loop Region of tRNA (nucleotide 26-42) in the Low Resolution Cryo-EM Map of an EF-Tu Ternary Complex (GDP and Kirromycin) Bound to E. coli 70S Ribosome  
Authors : Valle, M.; Sengupta, J.; Swami, N.K.; Grassucci, R.A.; Burkhardt, N.; Nierhaus, K.H.; Agrawal, R.K.; Frank, J.  
Deposited on : 2002-05-21  
Resolution : 16.80 Å (reported)  
Based on PDB ID : 1TTT

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

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

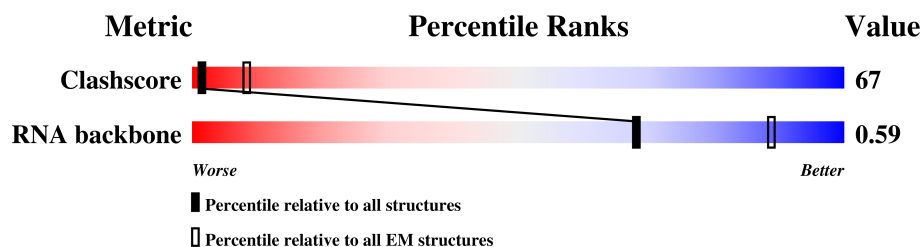
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*


The reported resolution of this entry is 16.80 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	136327	1886
RNA backbone	3747	458

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	17	 6%                      88%                      6%

## 2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 365 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 PHENYLALANINE TRANSFER RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	17	Total	C	N	O	P	0	0
			365	163	68	117	17		

### 3 Residue-property plots [i](#)

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: PHENYLALANINE TRANSFER RNA

Chain A: 

C26	C27	C28	A29	C30	A31	C32	U33	C34	A35	A36	C37	A38	U39	C40	U41	C42
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## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	7985	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction of 3D-maps	Depositor
Microscope	FEI/PHILIPS EM420	Depositor
Voltage (kV)	100	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	52000	Depositor
Image detector	KODAK SO-163 FILM	Depositor

## 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: 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	A	3.82	62/386 (16.1%)	5.73	152/600 (25.3%)

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	G	N3-C4	13.16	1.44	1.35
1	A	34	G	N3-C4	12.95	1.44	1.35
1	A	30	G	N3-C4	12.92	1.44	1.35
1	A	26	G	N3-C4	12.89	1.44	1.35
1	A	37	G	N3-C4	12.71	1.44	1.35

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	37	G	C4-C5-N7	-24.18	101.13	110.80
1	A	42	G	C4-C5-N7	-24.16	101.14	110.80
1	A	26	G	C4-C5-N7	-24.08	101.17	110.80
1	A	34	G	C4-C5-N7	-24.02	101.19	110.80
1	A	30	G	C4-C5-N7	-23.83	101.27	110.80

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	365	0	185	37	0
All	All	365	0	185	37	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 67.

The worst 5 of 37 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:36:A:H2'	1:A:37:G:H5''	1.15	1.12
1:A:36:A:C2'	1:A:37:G:H5''	1.98	0.94
1:A:32:C:H2'	1:A:33:U:C6	2.12	0.85
1:A:32:C:H2'	1:A:33:U:H6	1.51	0.75
1:A:28:C:H2'	1:A:29:A:H8	1.56	0.70

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	16/17 (94%)	1 (6%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	37	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	PSU	A	39	1	16,21,22	1.16	1 (6%)	20,30,33	3.71	7 (35%)

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	PSU	A	39	1	-	0/7/25/26	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	PSU	C6-C5	-3.17	1.34	1.38

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	PSU	N1-C2-N3	-11.50	119.17	128.41
1	A	39	PSU	C5-C4-N3	-5.58	118.17	125.36
1	A	39	PSU	C5-C1'-C2'	-3.23	109.56	115.32
1	A	39	PSU	C5-C6-N1	-3.06	120.52	124.42
1	A	39	PSU	O4'-C1'-C2'	2.16	108.15	104.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	39	PSU	5	0

## 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.