



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:41 PM BST

PDB ID : 3IZZ  
EMDB ID: : EMD-1854  
Title : Models for ribosome components that are nearest neighbors to the bovine mitochondrial initiation factor2 bound to the E. Coli ribosome  
Authors : Yassin, A.S.; Haque, E.; Datta, P.P.; Elmore, K.; Banavali, N.K.; Spremulli, L.L.; Agrawal, R.K.  
Deposited on : 2011-01-20  
Resolution : 10.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

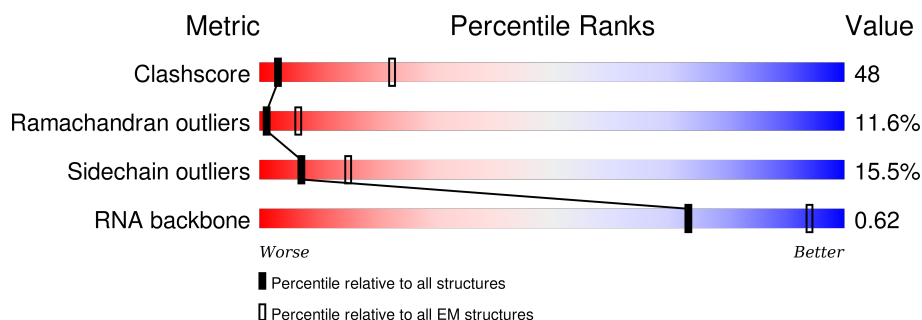
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 10.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	59	41% 51% 8%
2	D	60	30% 52% 13% 5%
3	E	100	21% 66% 12% .
4	F	124	33% 56% 9% .
5	B	118	33% 61% 5% .
6	G	121	21% 55% 21% .

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9118 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 Helix 5, 14, 15 (Small Subunit).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	59	Total	C	N	O	P	0	0
			1262	563	231	409	59		

- Molecule 2 is a RNA chain called Helix 18 (Small Subunit).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	60	Total	C	N	O	P	0	0
			1289	575	241	414	59		

- Molecule 3 is a RNA chain called Helix 44 (Small Subunit).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	100	Total	C	N	O	P	0	0
			2148	956	401	692	99		

- Molecule 4 is a protein called Protein S12 (Small Subunit).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

- Molecule 5 is a RNA chain called Helix 69, 71, 89, 92, 95 (Large Subunit).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	118	Total	C	N	O	P	0	0
			2519	1123	448	830	118		

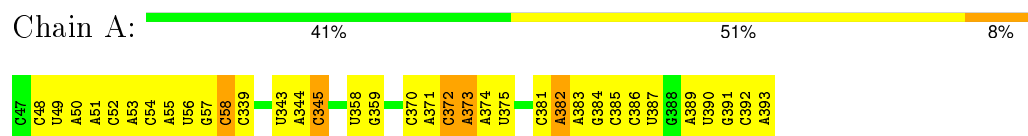
- Molecule 6 is a protein called Protein L14 (Large Subunit).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	121	Total	C	N	O	S	0	0
			930	582	179	164	5		

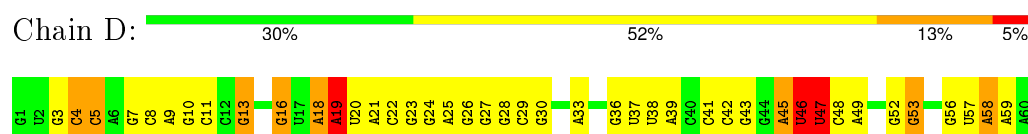
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

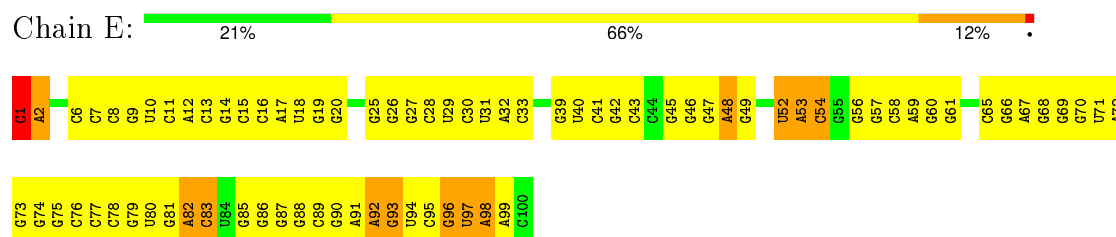
- Molecule 1: Helix 5, 14, 15 (Small Subunit)



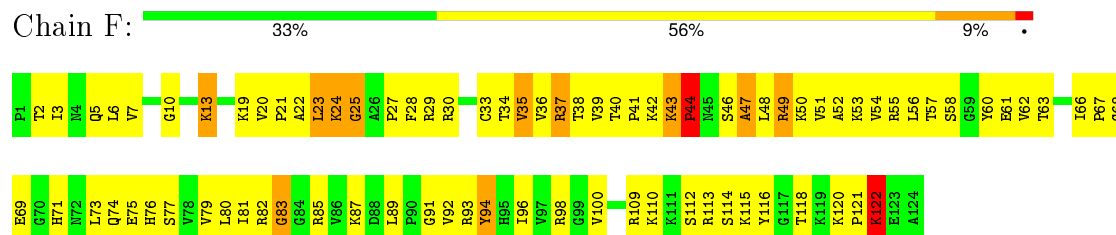
- Molecule 2: Helix 18 (Small Subunit)



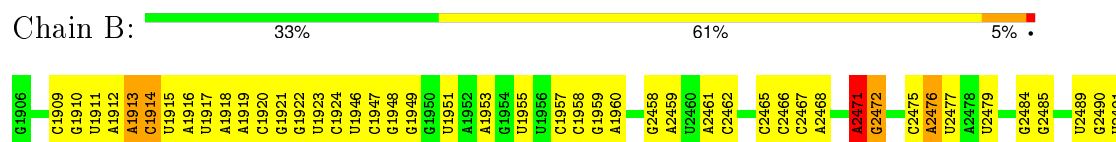
- Molecule 3: Helix 44 (Small Subunit)



- Molecule 4: Protein S12 (Small Subunit)

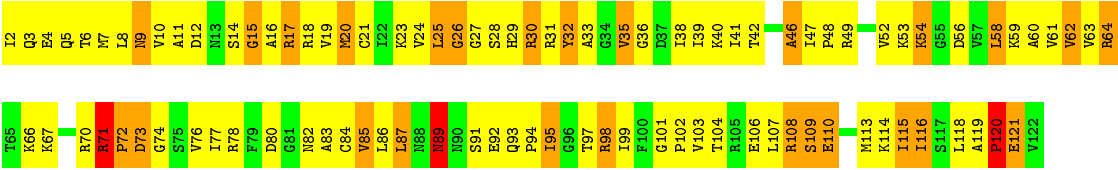


- Molecule 5: Helix 69, 71, 89, 92, 95 (Large Subunit)





● Molecule 6: Protein L14 (Large Subunit)



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	121742	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Every micrograph	Depositor
Microscope	Tecnai F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	50000	Depositor
Image detector	Kodak S0163	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.23	0/1408	0.75	0/2186
2	D	0.57	0/1442	0.84	5/2247 (0.2%)
3	E	0.43	0/2401	0.71	3/3742 (0.1%)
4	F	0.42	0/986	0.75	0/1320
5	B	0.25	0/2811	0.74	1/4371 (0.0%)
6	G	0.35	0/939	1.00	2/1258 (0.2%)
All	All	0.38	0/9987	0.77	11/15124 (0.1%)

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
2	D	1	2
3	E	1	2
5	B	0	1
All	All	2	6

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	45	A	C2'-C3'-O3'	9.71	130.87	109.50
3	E	97	U	C2'-C3'-O3'	8.72	128.68	109.50
2	D	53	G	O5'-C5'-C4'	7.69	126.31	111.70
6	G	91	SER	N-CA-C	-7.10	91.83	111.00
3	E	97	U	C4'-C3'-O3'	5.79	124.59	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	45	A	C3'
3	E	97	U	C3'

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	58	C	Sidechain
2	D	47	U	Sidechain
2	D	58	A	Sidechain
3	E	52	U	Sidechain
3	E	82	A	Sidechain

## 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	1262	0	643	28	0
2	D	1289	0	654	100	0
3	E	2148	0	1075	296	0
4	F	970	0	1056	176	0
5	B	2519	0	1260	271	0
6	G	930	0	998	125	0
All	All	9118	0	5686	709	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 48.

The worst 5 of 709 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)
3:E:26:G:C5'	6:G:48:PRO:HB3	1.38	1.52
3:E:12:A:C2	5:B:1912:A:C5	1.97	1.52
3:E:83:C:C5'	5:B:1959:G:N2	1.79	1.46
3:E:12:A:C2	5:B:1912:A:N7	1.83	1.44
3:E:13:C:H4'	5:B:1915:U:C5	1.54	1.41

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
4	F	122/124 (98%)	91 (75%)	19 (16%)	12 (10%)	1	14
6	G	119/121 (98%)	71 (60%)	32 (27%)	16 (13%)	0	7
All	All	241/245 (98%)	162 (67%)	51 (21%)	28 (12%)	1	9

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	23	LEU
4	F	24	LYS
4	F	76	HIS
6	G	35	VAL
6	G	46	ALA

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
4	F	104/104 (100%)	96 (92%)	8 (8%)	16	52
6	G	102/102 (100%)	78 (76%)	24 (24%)	1	7
All	All	206/206 (100%)	174 (84%)	32 (16%)	7	22

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	G	31	ARG

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Mol	Chain	Res	Type
6	G	58	LEU
6	G	110	GLU
6	G	54	LYS
6	G	62	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
6	G	5	GLN
6	G	88	ASN
6	G	9	ASN
4	F	71	HIS
6	G	82	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	55/59 (93%)	9 (16%)	2 (3%)
2	D	58/60 (96%)	13 (22%)	4 (6%)
3	E	98/100 (98%)	10 (10%)	4 (4%)
5	B	113/118 (95%)	7 (6%)	1 (0%)
All	All	324/337 (96%)	39 (12%)	11 (3%)

5 of 39 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	48	C
1	A	51	A
1	A	52	C
1	A	55	A
1	A	345	C

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	45	A
2	D	46	U
3	E	92	A
2	D	19	A
3	E	53	A

## 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.