



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

Mar 2, 2017 – 11:23 am GMT

PDB ID : 3J0D  
EMDB ID: : EMD-1915  
Title : Models for the T. thermophilus ribosome recycling factor bound to the E. coli post-termination complex  
Authors : Yokoyama, T.; Shaikh, T.R.; Iwakura, N.; Kaji, H.; Kaji, A.; Agrawal, R.K.  
Deposited on : 2011-06-29  
Resolution : 11.10 Å(reported)  
Based on PDB ID : PDB ID 2AVY, 2AW4, 1EH1

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.

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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

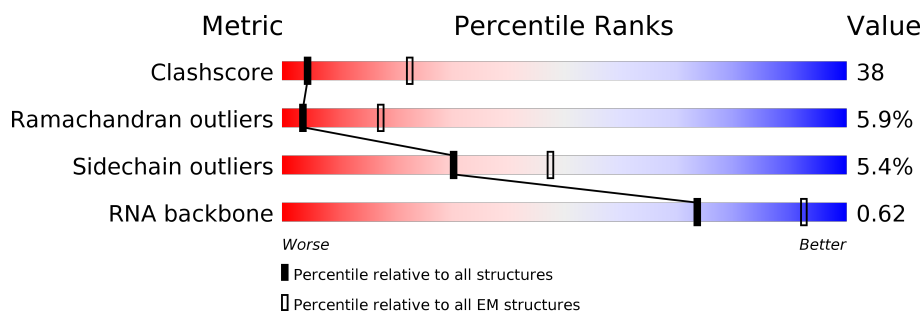
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 11.10 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
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
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	50	<div> <div>36%</div> <div>56%</div> <div>• 6%</div> </div>
2	B	22	<div> <div>36%</div> <div>59%</div> <div>5%</div> </div>
3	C	17	<div> <div>35%</div> <div>65%</div> </div>
4	D	13	<div> <div>54%</div> <div>46%</div> </div>
5	E	19	<div> <div>53%</div> <div>47%</div> </div>
6	F	19	<div> <div>32%</div> <div>63%</div> <div>5%</div> </div>
7	G	141	<div> <div>33%</div> <div>62%</div> <div>•</div> </div>
8	H	18	<div> <div>33%</div> <div>67%</div> </div>

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Mol	Chain	Length	Quality of chain
9	h	19	<div><div></div><div>84%</div><div>16%</div></div>
10	I	123	<div><div></div><div>24%</div><div>58%</div><div>18%</div></div>
11	J	185	<div><div></div><div>96%</div><div></div><div>.</div></div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7260 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 ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	50	Total	C	N	O	P	0	0
			1070	479	196	345	50		

- Molecule 2 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	22	Total	C	N	O	P	0	0
			463	208	81	152	22		

- Molecule 3 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	17	Total	C	N	O	P	0	0
			364	162	65	120	17		

- Molecule 4 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	13	Total	C	N	O	P	0	0
			283	125	53	92	13		

- Molecule 5 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	19	Total	C	N	O	P	0	0
			407	182	75	131	19		

- Molecule 6 is a RNA chain called ribosomal 23S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	19	Total	C	N	O	P	0	0
			411	183	79	130	19		

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 8 is a RNA chain called ribosomal 16S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	18	Total	C	N	O	P	0	0
			386	172	71	125	18		

- Molecule 9 is a RNA chain called ribosomal 16S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	h	19	Total	C	N	O	P	0	0
			412	183	77	133	19		

- Molecule 10 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	123	Total	C	N	O	S	0	0
			954	589	196	165	4		

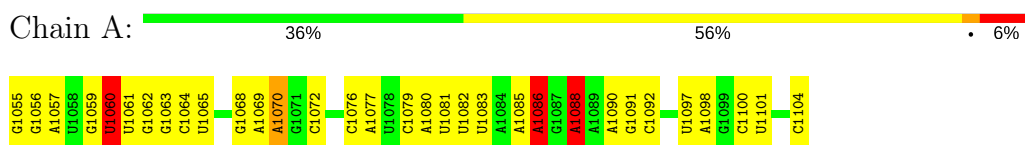
- Molecule 11 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	185	Total	C	N	O	S	0	0
			1478	924	270	282	2		

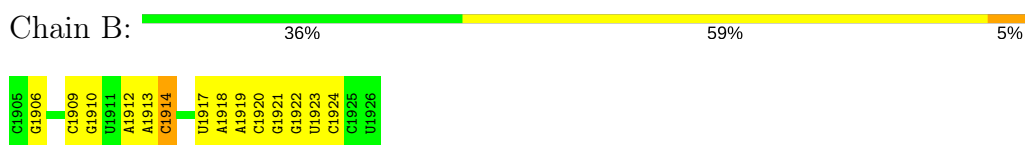
### 3 Residue-property plots

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: ribosomal 23S RNA



- Molecule 2: ribosomal 23S RNA



- Molecule 3: ribosomal 23S RNA



- Molecule 4: ribosomal 23S RNA

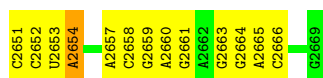


- Molecule 5: ribosomal 23S RNA



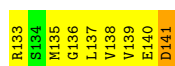
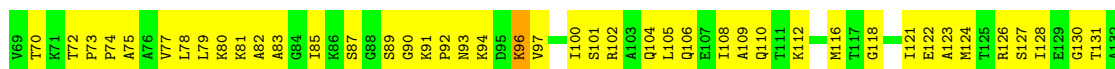
- Molecule 6: ribosomal 23S RNA





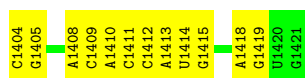
- Molecule 7: 50S ribosomal protein L11

Chain G: 33% 62%



- Molecule 8: ribosomal 16S RNA

Chain H: 33% 67%



- Molecule 9: ribosomal 16S RNA

Chain h: 84% 16%



- Molecule 10: 30S ribosomal protein S12

Chain I: 24% 58% 18%



- Molecule 11: Ribosome-recycling factor

Chain J: 96%



## 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	CTF CORRECTION OF 3D MAPS BY WIENER FILTRATION	Depositor
Microscope	TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	400.00	Depositor
Maximum defocus (nm)	4300.00	Depositor
Magnification	50310	Depositor
Image detector	KODAK S0163 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	0.79	4/1198 (0.3%)	0.86	8/1865 (0.4%)
10	I	0.22	0/966	0.47	0/1295
11	J	0.96	0/1497	0.99	2/2017 (0.1%)
2	B	0.25	0/516	0.74	0/799
3	C	0.25	0/406	0.72	0/631
4	D	0.30	0/316	0.73	0/492
5	E	0.30	0/455	0.76	0/707
6	F	0.24	0/460	0.73	0/716
7	G	0.26	0/1046	0.58	0/1410
8	H	0.29	0/431	0.76	0/670
9	h	0.25	0/461	0.72	0/718
All	All	0.56	4/7752 (0.1%)	0.77	10/11320 (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	3
11	J	1	0
All	All	1	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1086	A	C5-C6	-17.67	1.25	1.41
1	A	1088	A	C6-N1	-10.45	1.28	1.35
1	A	1060	U	C2-N3	8.28	1.43	1.37
1	A	1086	A	N7-C5	-7.29	1.34	1.39

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1088	A	N1-C6-N6	-8.03	113.78	118.60
1	A	1060	U	C5-C4-O4	-7.43	121.44	125.90
1	A	1086	A	C4-C5-C6	6.93	120.47	117.00
1	A	1086	A	C6-C5-N7	-6.89	127.48	132.30
1	A	1088	A	C5-C6-N6	6.18	128.65	123.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	J	103	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1060	U	Sidechain
1	A	1086	A	Sidechain
1	A	1088	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	1070	0	539	54	0
2	B	463	0	236	12	0
3	C	364	0	184	14	0
4	D	283	0	142	8	0
5	E	407	0	206	6	0
6	F	411	0	208	13	0
7	G	1032	0	1088	127	0
8	H	386	0	196	30	0
9	h	412	0	206	0	0
10	I	954	0	1011	111	0
11	J	1478	0	1521	0	0
All	All	7260	0	5537	335	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 38.

The worst 5 of 335 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)
8:H:1411:C:H5'	10:I:53:ARG:NH1	1.62	1.14
8:H:1411:C:H4'	10:I:53:ARG:HD2	1.45	0.98
1:A:1060:U:N3	1:A:1088:A:N7	2.17	0.92
7:G:105:LEU:HD11	7:G:139:VAL:HG11	1.54	0.89
7:G:27:LEU:HD23	7:G:27:LEU:H	1.37	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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	
7	G	139/141 (99%)	124 (89%)	11 (8%)	4 (3%)	5	38
10	I	121/123 (98%)	75 (62%)	29 (24%)	17 (14%)	0	5
11	J	183/185 (99%)	169 (92%)	9 (5%)	5 (3%)	6	40
All	All	443/449 (99%)	368 (83%)	49 (11%)	26 (6%)	4	23

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	18	ASN
10	I	10	PRO
10	I	23	LEU
11	J	84	ARG
10	I	19	ASN

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

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	
7	G	109/109 (100%)	106 (97%)	3 (3%)	49	74
10	I	103/103 (100%)	88 (85%)	15 (15%)	3	21
11	J	157/157 (100%)	155 (99%)	2 (1%)	73	87
All	All	369/369 (100%)	349 (95%)	20 (5%)	30	58

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	I	38	THR
10	I	50	LYS
10	I	107	LYS
10	I	33	CYS
10	I	35	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	33	ASN
10	I	72	ASN
7	G	93	ASN
7	G	29	GLN
10	I	58	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	49/50 (98%)	3 (6%)	0
2	B	20/22 (90%)	2 (10%)	0
3	C	16/17 (94%)	1 (6%)	0
4	D	12/13 (92%)	0	0
5	E	17/19 (89%)	2 (11%)	0
6	F	18/19 (94%)	1 (5%)	0
8	H	17/18 (94%)	2 (11%)	0
9	h	18/19 (94%)	3 (16%)	0
All	All	167/177 (94%)	14 (8%)	0

5 of 14 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1070	A
1	A	1088	A
1	A	1090	A
2	B	1906	G
2	B	1914	C

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.