wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:43 PM BST

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

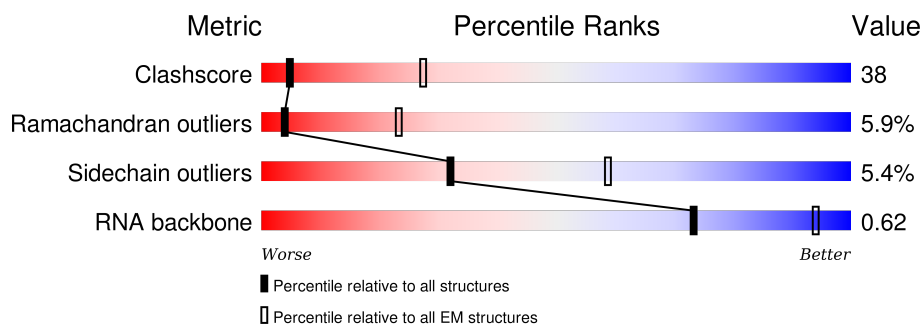|		
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 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	Percentile Ranks	Value
Clashscore		38
Ramachandran outliers		5.9%
Sidechain outliers		5.4%
RNA backbone		0.62

Worse   *Better*

▉ Percentile relative to all structures
▯ Percentile relative to all EM structures

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	50	36% 56% • 6%
2	B	22	36% 55% 9%
3	C	17	35% 65%
4	D	13	54% 46%
5	E	19	53% 47%
6	F	19	32% 63% 5%
7	G	141	33% 62% •
8	H	18	33% 67%

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	h	19	84% — 16%
10	I	123	24% — 58% — 18%
11	J	185	96% — •

2 Entry composition (i)

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
			Total	C	N	O	P		
1	A	50	1070	479	196	345	50	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

| Mol	Chain	Residues	Atoms					AltConf	Trace
11	J	185	Total 1478	C 924	N 270	O 282	S 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 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: ribosomal 23S RNA

Chain A: 36%   56%   ·   6%
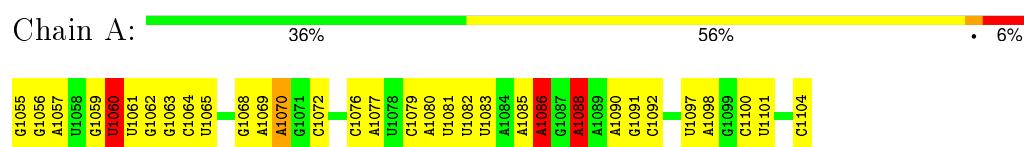
- Molecule 2: ribosomal 23S RNA

Chain B: 36%   55%   9%
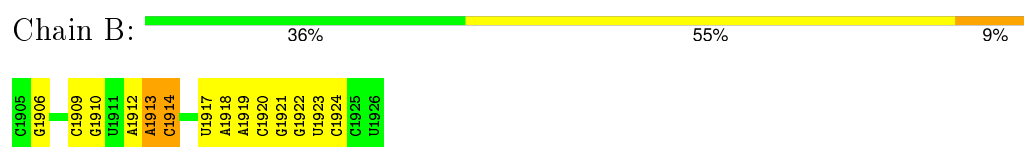
- Molecule 3: ribosomal 23S RNA

Chain C: 35%   65%
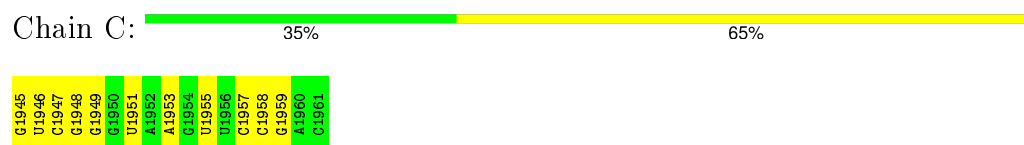
- Molecule 4: ribosomal 23S RNA

Chain D: 54%   46%

- Molecule 5: ribosomal 23S RNA

Chain E: 53%   47%

- Molecule 6: ribosomal 23S RNA

Chain F: 32%   63%   5%

C2651 C2652 U2653 A2654 A2657 C2658 G2659 A2660 G2661 A2662 G2663 G2664 A2665 C2666 G2669
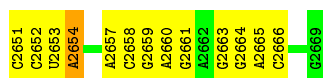
• Molecule 7: 50S ribosomal protein L11

Chain G:

33% 62%

A1 K2 A6 Y7 L10 Q11 V12 A13 A14 G15 M16 A17 N18 P19 S20 P21 P22 V23 G24 P25 A26 L27 G28 Q29 Q30 G31 V32 N33 I34 M35 E36 F37 F41 N42 T45 D46 S47 I48 E49 K50 I54 P55 V56 V57 I58 T59 V60 Y61 A62 D63 R64 S65 F66 T67 F68

V69 T70 K71 T72 P73 P74 A75 A76 V77 L78 L79 K80 K81 A82 A83 G84 I85 K86 S87 G88 S89 G90 K91 P92 N93 K94 D95 K96 V97 I100 S101 R102 A103 Q104 L105 Q106 E107 I108 A109 Q110 T111 K112 M116 T117 G118 I121 E122 A123 M124 T125 R126 S127 I128 E129 G130 T131 A132

R133 S134 M135 G136 L137 V138 V139 E140 D141

• Molecule 8: ribosomal 16S RNA

Chain H:

33% 67%

C1404 G1405 A1408 C1409 A1410 C1411 C1412 A1413 U1414 G1415 A1418 G1419 U1420 G1421
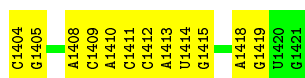
• Molecule 9: ribosomal 16S RNA

Chain h:

84% 16%

C1479 U1490 A1493 G1497
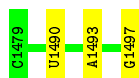
• Molecule 10: 30S ribosomal protein S12

Chain I:

24% 58% 18%

A1 T2 V3 N4 Q5 L6 V7 R8 K9 P10 R13 K14 V15 A16 K17 S18 N19 V20 P21 A22 L23 E24 A25 C26 P27 Q28 K29 R30 G31 V32 C33 T34 R35 V36 Y37 T38 P41 K42 K43 P44 N45 S46 A47 L48 R49 K50 V51 C52 R53 V54 R55 L56 T57 N58 G59 F60 E61 V62

T63 S64 Y65 I66 G67 H71 N72 L73 Q74 E75 V78 I79 L80 I81 R82 G83 G84 R85 V86 K87 D88 L89 P90 G91 V92 R93 Y94 H95 T96 V97 R98 L101 D102 C103 S104 G105 V106 K107 R113 Y116 G117 V118 K119 R120 P121 K122 A123

• Molecule 11: Ribosome-recycling factor

Chain J:

96%

M1 R29 T30 G31 R32 D62 P63 R84 D87 I103 G185

4 Experimental information ⓘ

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	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 $(e^-/\text{Å}^2)$	Not provided	Depositor
Minimum defocus (nm)	400.00	Depositor
Maximum defocus (nm)	4300.00	Depositor
Magnification	50000	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(^{o})	Ideal(^{o})
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 ⓘ

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%)	6	43
10	I	121/123 (98%)	75 (62%)	29 (24%)	17 (14%)	0	6
11	J	183/185 (99%)	169 (92%)	9 (5%)	5 (3%)	6	45
All	All	443/449 (99%)	368 (83%)	49 (11%)	26 (6%)	4	27

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%)	51	78
10	I	103/103 (100%)	88 (85%)	15 (15%)	4	24
11	J	157/157 (100%)	155 (99%)	2 (1%)	76	89
All	All	369/369 (100%)	349 (95%)	20 (5%)	32	64

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%)	1 (5%)
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%)	1 (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

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1913	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.