

Feb 12, 2024 – 09:53 AM EST

PDB ID : 3J0E EMDB ID : EMD-1917 Title : Models for the T. thermophilus ribosome recycling factor and the E. coli elongation factor G bound to the E. coli post-termination complex Yokoyama, T.; Shaikh, T.R.; Iwakura, N.; Kaji, H.; Kaji, A.; Agrawal, R.K. Authors : 2011-06-29 Deposited on 9.90 Å(reported) Resolution : Based on initial models 2AW4, 2AVY, 1EH1 :

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

## 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $ELECTRON\ MICROSCOPY$ 

The reported resolution of this entry is 9.90 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq=3, 2, 1$  and 0 types of geometric quality criteria respectively. 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  $\leq=5\%$  The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain	
1	А	22	36%	55%	9%
2	В	17	35%	65%	
3	С	13	15%	46%	
4	D	19	47%	53%	
5	Е	18	33%	67%	
6	е	19		84%	16%
7	F	123	28%	55%	17%



Mol	Chain	Length	Quality of chain		
			58%		
8	G	185	87%	12%	•
			50%		
9	Н	702	88%	10%	•



## 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10187 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	А	22	Total 465	C 208	N 81	0 154	Р 22	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	17	Total 364	C 162	N 65	O 120	Р 17	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	13	Total 283	C 125	N 53	O 92	Р 13	0	0

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

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	D	19	Total 408	C 182	N 75	O 132	Р 19	0	0

• Molecule 5 is a RNA chain called ribosomal 16S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Е	18	Total 386	C 172	N 71	O 125	Р 18	0	0

• Molecule 6 is a RNA chain called ribosomal 16S RNA.

Mol	Chain	Residues		At	$\mathbf{oms}$	AltConf	Trace		
6	е	19	Total 412	C 183	N 77	0 133	Р 19	0	0

• Molecule 7 is a protein called 30S ribosomal protein S12.



Mol	Chain	Residues		At	oms			AltConf	Trace
7	F	123	Total 955	C 590	N 196	O 165	$\frac{S}{4}$	0	0

• Molecule 8 is a protein called Ribosome-recycling factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	185	Total 1478	C 924	N 270	0 282	${ m S} { m 2}$	0	0

• Molecule 9 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms			AltConf	Trace		
9	Н	702	Total 5436	C 3423	N 940	0 1048	S 25	0	0



## 3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 e:		84%	16%	
C1479 U1490 A1493 G1497				
• Molecule 7: 3	30S ribosomal prote	in S12		
Chain F:	28%	55%	17%	
A1 12 12 14 14 16 16 16 16 16 16 16 16 17 18 10	R13 K14 V15 A16 K17 K17 K17 N19 V20 V20 V21 V21 C21 C21 C24	C26 C26 C26 C26 C28 C28 C33 C31 C33 C33 C33 C33 C33 C33 C33 C33	441 641 642 644 844 845 846 846 849 849 849 849 849 849 849 849 849 855 865 865 865 865 865 865 865 865 865	T57 888 659 F60 E61 V62
T63 S64 Y65 G67 G67 G67 G67 H71 H71 H72 H73 Q74 G774	V78 179 181 181 181 882 683 684 788 788 188 188 188 188	(192 (192 (192 (192 (196 (196 (196 (196 (196 (197 (197 (197 (197))))))))))))))))))))))))))))))))))))	V106 K107 K107 N115 N115 N119 N120 P121 K122 M122	
• Molecule 8: 1	Ribosome-recycling	factor		
Chain G:	58%	87%	12% •	
M1 12 L3 K4 E5 L6 K7 X7 A8	R11 812 H13 M14 015 817 L18 E19 E19	H23 N24 L25 A26 C27 C27 T30 C31 C31 C31 C31 C32 C31 C32 C32 C32 C32 C32 C32 C32 C32 C32 C32	N34 P35 L39 H40 L41 K42 V50 P51 F51 F51 N53 N53	155 A56 V58 V58 V58 P61 P61 P61 P63 R64 V67 V67 V68
069 870 072 K77 K77 183 R84	DB5 886 886 886 689 689 891 892 893 893 893 893 893 893	I101 P105 P105 L106 T107 E109 R110 R111 K112	D113	R129 R130 R133 R133 R133 R134 R134 C141 K141 K141 K141 K141
D166 E167 F168 A170 A170 A172 D173	L115 A176 E177 K178 K178 E100 9181 E180 1183 L184 C185			
• Molecule 9: 1	Elongation factor G			
Chain H:	50%	88%	10% •	
A2 R3 T4 T5 P6 R3 R3 R3	113 614 115 816 816 115 115 115 126 126 130 130	Y33           Y36           N37           H38           K39           K41           H44	245       646       A47       A48       A48       A48       A58       M50       M51       M53       656       657	R59 G60 161 162 163 163 865 A66 A66 A67 A67 C68 C73 C73 C74
M75 A76 B80 B80 B81 B81 R83 R83 R83	187 D88 P90 091 H92 H92 H92 H92 H92 H92 H92	N103 N103 N104 V105 L106 D107 V112 V112 V112 C114	Q120 5123 E124 R128 R128 K132 V133 V135 V135	F1400 V141 V141 L152 L152 V159 V156 V165 P166
LI71 LI74 CI74 AI75 EI76 EI77 H178	D184 L185 V186 M187 K187 K189 K189 C199 C199 C199 C199 C199 C199	Y204 E205 D206 A209 W219 W218 H219 H219	1223 E224 E228 E231 E231 E231 C338 C338 C239 C240 E241 E242	E245 A246 C250 1261 1261 1263 V264 V264 V264 C266
G267 G274 G274 Q276 A277 M276 L279 L279	A281 A281 D281 V290 V290 V292 P293 A294 I296 N296 I298	D301 G302 K303 K303 F306 P306 A307 K309 K309 K309	8312 8312 9313 9314 8318 8318 8318 8318 8318 8328 8328 8328	V330 G331 G331 G331 G345 G345 G345 G345 G345 G345 C355 C355 C355 C355 C355 C355 C355 C

WORLDWIDE PROTEIN DATA BANK





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	338823	Depositor
Resolution determination method	Not provided	
CTF correction method	CTF CORRECTION OF 3D MAPS BY	Depositor
	WIENER FILTRATION	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	Not provided	
Minimum defocus (nm)	400.00	Depositor
Maximum defocus (nm)	4000.00	Depositor
Magnification	50310	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	3122.807	Depositor
Minimum map value	-1350.877	Depositor
Average map value	40.613	Depositor
Map value standard deviation	297.310	Depositor
Recommended contour level	272.0	Depositor
Map size (Å)	361.4, 361.4, 361.4	wwPDB
Map dimensions	130, 130, 130	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.78, 2.78, 2.78	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  > 5	RMSZ	# Z  > 5	
1	А	0.25	0/518	0.74	0/804	
2	В	0.25	0/406	0.72	0/631	
3	С	0.30	0/316	0.73	0/492	
4	D	0.29	0/456	0.76	0/709	
5	Е	0.29	0/431	0.76	0/670	
6	е	0.26	0/461	0.72	0/718	
7	F	0.23	0/969	0.47	0/1300	
8	G	0.95	0/1497	1.14	2/2017~(0.1%)	
9	Н	0.95	0/5538	1.14	11/7493~(0.1%)	
All	All	0.79	0/10592	1.00	13/14834~(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
9	Н	1	8

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
9	Н	515	TYR	CB-CG-CD2	8.54	126.12	121.00
9	Н	515	TYR	CB-CG-CD1	-8.30	116.02	121.00
8	G	14	MET	CG-SD-CE	-6.40	89.97	100.20
9	Н	448	TRP	N-CA-C	-6.03	94.71	111.00
9	Н	665	GLY	N-CA-C	-5.87	98.42	113.10
9	Н	160	THR	N-CA-CB	5.69	121.11	110.30
8	G	33	ALA	N-CA-CB	5.55	117.87	110.10
9	Н	583	TYR	N-CA-CB	5.35	120.23	110.60
9	Н	583	TYR	CA-CB-CG	5.31	123.49	113.40



00.000	continuous from process as pagetti								
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$		
9	Н	201	THR	N-CA-CB	5.23	120.23	110.30		
9	Н	204	TYR	CB-CG-CD1	5.04	124.02	121.00		
9	Н	418	ILE	N-CA-C	-5.01	97.47	111.00		
9	Н	318	SER	N-CA-CB	5.00	118.00	110.50		

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	Н	160	THR	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	Н	237	TYR	Sidechain
9	Н	33	TYR	Peptide
9	Н	500	ASP	Peptide
9	Н	533	GLY	Peptide
9	Н	569	TYR	Sidechain
9	Н	583	TYR	Sidechain
9	Н	689	GLU	Peptide
9	Н	80	GLU	Peptide

### 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	А	465	0	238	12	0
2	В	364	0	184	38	0
3	С	283	0	141	8	0
4	D	408	0	206	7	0
5	Е	386	0	196	37	0
6	e	412	0	206	0	0
7	F	955	0	1018	87	0
8	G	1478	0	1526	0	0
9	Н	5436	0	5402	0	0
All	All	10187	0	9117	158	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 34.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom_2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:B:1959:G:C4'	5:E:1418:A:O2'	1.77	1.32	
2:B:1959:G:H4'	5:E:1418:A:C1'	1.64	1.27	
2:B:1959:G:H4'	5:E:1418:A:C2'	1.66	1.23	
2:B:1959:G:C1'	5:E:1418:A:H1'	1.72	1.18	
2:B:1959:G:C4'	5:E:1418:A:C1'	2.21	1.16	
2:B:1959:G:C4'	5:E:1418:A:H1'	1.75	1.15	
2:B:1959:G:C2'	5:E:1418:A:H1'	1.79	1.12	
2:B:1959:G:C5'	5:E:1418:A:O2'	2.03	1.07	
2:B:1959:G:O2'	5:E:1418:A:C1'	2.03	1.05	
2:B:1959:G:H1'	5:E:1418:A:N3	1.71	1.04	
2:B:1959:G:O4'	5:E:1418:A:H1'	1.69	0.91	
2:B:1959:G:H5'	5:E:1418:A:O2'	1.70	0.91	
2:B:1959:G:H4'	5:E:1418:A:O2'	1.50	0.90	
2:B:1959:G:C4'	5:E:1418:A:HO2'	1.68	0.89	
7:F:8:ARG:HG3	7:F:9:LYS:H	1.40	0.87	
1:A:1912:A:N6	5:E:1408:A:O2'	2.09	0.86	
2:B:1959:G:C2'	5:E:1418:A:C1'	2.56	0.84	
7:F:56:LEU:HD11	7:F:81:ILE:HD12	1.61	0.83	
7:F:48:LEU:H	7:F:48:LEU:HD23	1.42	0.83	
1:A:1912:A:N6	5:E:1408:A:HO2'	1.79	0.81	
2:B:1959:G:H4'	5:E:1418:A:C4'	2.12	0.79	
2:B:1959:G:O2'	5:E:1418:A:H1'	1.76	0.77	
7:F:35:ARG:NH2	7:F:75:GLU:HB3	2.00	0.76	
2:B:1959:G:C4'	5:E:1418:A:C2'	2.40	0.74	
2:B:1959:G:H4'	5:E:1418:A:O4'	1.88	0.73	
7:F:66:ILE:HD13	7:F:73:LEU:HD12	1.69	0.73	
7:F:98:ARG:HE	7:F:98:ARG:HA	1.55	0.72	
1:A:1913:A:H1'	1:A:1914:C:OP1	1.90	0.71	
2:B:1959:G:C3'	5:E:1418:A:H1'	2.19	0.71	
7:F:20:VAL:HG13	7:F:94:TYR:HH	1.57	0.70	
7:F:35:ARG:HG3	7:F:36:VAL:H	1.56	0.70	
7:F:28:GLN:HG3	7:F:80:LEU:HD21	1.73	0.69	
7:F:79:ILE:HD13	7:F:96:THR:HG22	1.74	0.69	
2:B:1959:G:O2'	5:E:1418:A:N9	2.25	0.69	
7:F:80:LEU:HD23	7:F:97:VAL:HG21	1.74	0.68	
7:F:24:GLU:HB3	7:F:26:CYS:SG	2.34	0.68	
5:E:1412:C:H2'	5:E:1413:A:C8	2.29	0.67	



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	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:1959:G:HO2'	5:E:1418:A:C1'	2.05	0.65
2:B:1959:G:O2'	5:E:1418:A:O4'	2.17	0.63
7:F:85:ARG:HA	7:F:93:ARG:HA	1.80	0.63
4:D:2591:C:H2'	4:D:2592:G:C8	2.33	0.63
7:F:20:VAL:HG13	7:F:94:TYR:OH	1.98	0.62
4:D:2591:C:H2'	4:D:2592:G:H8	1.64	0.62
2:B:1959:G:C3'	5:E:1418:A:C1'	2.77	0.62
7:F:43:LYS:N	7:F:44:PRO:HD2	2.15	0.62
7:F:64:SER:OG	7:F:96:THR:HG23	2.00	0.61
7:F:78:VAL:HG12	7:F:101:LEU:HD23	1.82	0.60
4:D:2600:A:O2'	4:D:2601:C:H5'	2.01	0.60
7:F:35:ARG:HA	7:F:35:ARG:HE	1.67	0.59
7:F:19:ASN:O	7:F:20:VAL:HG23	2.03	0.59
3:C:2246:G:H2'	3:C:2247:A:C8	2.38	0.58
7:F:19:ASN:HB2	7:F:93:ARG:NH1	2.18	0.58
7:F:22:ALA:HB2	7:F:56:LEU:HD21	1.85	0.57
7:F:42:LYS:HE3	7:F:90:PRO:HD3	1.84	0.57
2:B:1959:G:H4'	5:E:1418:A:C3'	2.33	0.57
7:F:8:ARG:HG3	7:F:9:LYS:N	2.17	0.57
2:B:1951:U:H2'	2:B:1953:A:OP2	2.05	0.56
3:C:2246:G:H2'	3:C:2247:A:H8	1.70	0.56
7:F:105:GLY:HA3	7:F:117:GLY:HA3	1.88	0.56
7:F:37:TYR:HB2	7:F:51:VAL:HG23	1.88	0.55
7:F:3:VAL:O	7:F:7:VAL:HG23	2.06	0.55
7:F:83:GLY:HA2	7:F:94:TYR:HD1	1.70	0.55
3:C:2247:A:H2'	3:C:2248:C:C6	2.41	0.55
7:F:30:ARG:CB	7:F:30:ARG:HH11	2.19	0.55
7:F:20:VAL:O	7:F:23:LEU:HG	2.08	0.54
7:F:58:ASN:ND2	7:F:58:ASN:H	2.05	0.54
2:B:1945:G:H2'	2:B:1946:U:C6	2.43	0.54
4:D:2590:A:H2'	4:D:2591:C:C6	2.43	0.53
7:F:86:VAL:HG11	7:F:89:LEU:HD23	1.90	0.53
5:E:1412:C:H2'	5:E:1413:A:H8	1.73	0.53
7:F:56:LEU:HB3	7:F:58:ASN:ND2	2.24	0.53
7:F:22:ALA:HB2	7:F:56:LEU:CD2	2.39	0.52
7:F:30:ARG:HH11	7:F:30:ARG:HB3	1.74	0.52
7:F:35:ARG:CZ	7:F:75:GLU:HB3	2.39	0.52
7:F:20:VAL:O	7:F:20:VAL:HG12	2.08	0.52
7:F:31:GLY:HA3	7:F:54:VAL:CG1	2.41	0.51
7:F:106:VAL:CG2	7:F:116:TYR:HB3	2.40	0.51
1:A:1909:C:H2'	1:A:1910:G:H8	1.76	0.51



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	to do pago	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
7:F:54:VAL:HG12	7:F:56:LEU:HD12	1.93	0.51
7:F:95:HIS:HD1	7:F:96:THR:N	2.09	0.51
7:F:103:CYS:SG	7:F:104:SER:N	2.83	0.51
7:F:113:ARG:HA	7:F:118:VAL:HG23	1.93	0.50
7:F:20:VAL:HG22	7:F:94:TYR:CE1	2.46	0.50
1:A:1923:U:H2'	1:A:1924:C:C6	2.45	0.50
7:F:3:VAL:HG23	7:F:4:ASN:OD1	2.11	0.50
1:A:1917:U:H2'	1:A:1918:A:H5'	1.93	0.49
2:B:1957:C:H2'	2:B:1958:C:H6	1.77	0.49
7:F:35:ARG:O	7:F:52:CYS:HB2	2.13	0.49
2:B:1957:C:H2'	2:B:1958:C:C6	2.48	0.49
3:C:2247:A:O2'	3:C:2248:C:H5'	2.12	0.49
2:B:1947:C:O2'	2:B:1948:G:H5'	2.13	0.48
2:B:1948:G:O2'	2:B:1949:G:H5'	2.13	0.48
7:F:48:LEU:H	7:F:48:LEU:CD2	2.18	0.48
7:F:90:PRO:C	7:F:92:VAL:H	2.17	0.48
7:F:80:LEU:O	7:F:97:VAL:HG23	2.14	0.47
1:A:1919:A:H2'	1:A:1920:C:H5'	1.95	0.47
7:F:58:ASN:HD22	7:F:58:ASN:N	2.11	0.47
5:E:1414:U:H2'	5:E:1415:G:H8	1.79	0.47
2:B:1959:G:H1'	5:E:1418:A:H1'	1.83	0.47
7:F:106:VAL:HG22	7:F:117:GLY:H	1.79	0.47
7:F:35:ARG:HG3	7:F:36:VAL:N	2.26	0.47
3:C:2250:G:H8	3:C:2250:G:O5'	1.98	0.47
5:E:1410:A:H2'	5:E:1411:C:C6	2.50	0.47
7:F:50:LYS:N	7:F:50:LYS:HE2	2.30	0.47
1:A:1917:U:C2'	1:A:1918:A:H5'	2.45	0.46
1:A:1921:G:O2'	1:A:1922:G:H5'	2.16	0.46
7:F:98:ARG:CB	7:F:116:TYR:HA	2.46	0.46
7:F:121:PRO:C	7:F:123:ALA:H	2.18	0.46
7:F:49:ARG:HH12	7:F:88:ASP:CB	2.28	0.46
2:B:1946:U:H2'	2:B:1947:C:C6	2.52	0.45
7:F:34:THR:HG21	7:F:53:ARG:CZ	2.47	0.45
7:F:43:LYS:N	7:F:44:PRO:CD	2.80	0.45
7:F:8:ARG:CG	7:F:9:LYS:H	2.21	0.45
7:F:119:LYS:O	7:F:119:LYS:HG3	2.16	0.45
5:E:1404:C:H2'	5:E:1405:G:C8	2.52	0.45
7:F:52:CYS:SG	7:F:66:ILE:HD11	2.58	0.44
5:E:1410:A:H2'	5:E:1411:C:H6	1.81	0.44
7:F:106:VAL:CG1	7:F:116:TYR:HB3	2.47	0.44
7:F:71:HIS:CG	7:F:72:ASN:N	$2.\overline{86}$	0.44



EMD-1917,	3J0E
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		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
7:F:80:LEU:HD13	7:F:101:LEU:HD11	1.99	0.44	
2:B:1959:G:C4'	5:E:1418:A:O4'	2.58	0.44	
3:C:2248:C:C2'	3:C:2249:U:H5'	2.47	0.44	
7:F:35:ARG:HH21	7:F:75:GLU:HB3	1.78	0.44	
7:F:58:ASN:ND2	7:F:58:ASN:N	2.64	0.43	
7:F:41:PRO:HG3	7:F:46:SER:O	2.18	0.43	
7:F:41:PRO:HD3	7:F:47:ALA:O	2.19	0.43	
2:B:1958:C:O2'	2:B:1959:G:H5'	2.18	0.43	
7:F:38:THR:HA	7:F:49:ARG:O	2.19	0.43	
7:F:35:ARG:HE	7:F:35:ARG:CA	2.30	0.43	
7:F:22:ALA:HB1	7:F:29:LYS:HG3	2.00	0.43	
2:B:1959:G:O4'	5:E:1418:A:C1'	2.47	0.42	
7:F:14:LYS:NZ	7:F:17:LYS:HE2	2.34	0.42	
7:F:83:GLY:HA2	7:F:94:TYR:CD1	2.52	0.42	
7:F:8:ARG:CZ	7:F:9:LYS:HE3	2.49	0.42	
3:C:2247:A:H2'	3:C:2248:C:H6	1.83	0.42	
7:F:117:GLY:O	7:F:118:VAL:HG13	2.19	0.42	
3:C:2251:G:OP2	3:C:2251:G:H8	2.02	0.42	
7:F:56:LEU:HB2	7:F:60:PHE:O	2.19	0.42	
7:F:21:PRO:HD2	7:F:94:TYR:OH	2.20	0.42	
7:F:98:ARG:HA	7:F:98:ARG:NE	2.29	0.42	
7:F:34:THR:HB	7:F:53:ARG:HB2	2.02	0.42	
7:F:42:LYS:HB3	7:F:43:LYS:H	1.73	0.42	
4:D:2590:A:H2'	4:D:2591:C:H6	1.83	0.42	
4:D:2604:U:O2'	4:D:2605:U:H5'	2.20	0.41	
7:F:4:ASN:O	7:F:8:ARG:HG2	2.19	0.41	
7:F:113:ARG:HD3	7:F:121:PRO:HD3	2.02	0.41	
1:A:1913:A:C1'	1:A:1914:C:OP1	2.65	0.41	
7:F:9:LYS:O	7:F:9:LYS:HG3	2.20	0.41	
1:A:1922:G:H2'	1:A:1923:U:O4'	2.19	0.41	
2:B:1959:G:C3'	5:E:1418:A:O4'	2.67	0.41	
7:F:6:LEU:O	7:F:10:PRO:HG3	2.19	0.41	
7:F:30:ARG:HB3	7:F:57:THR:CG2	2.51	0.41	
2:B:1946:U:H2'	2:B:1947:C:H6	1.86	0.41	
7:F:42:LYS:HB3	7:F:44:PRO:HD2	2.03	0.41	
1:A:1918:A:H1'	1:A:1919:A:N7	2.36	0.41	
7:F:101:LEU:HB3	7:F:102:ASP:H	1.61	0.40	
7:F:80:LEU:HD13	7:F:101:LEU:CD1	2.51	0.40	
4:D:2605:U:H2'	4:D:2606:C:C6	2.57	0.40	

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	Perc	centiles
7	F	121/123~(98%)	74 (61%)	30~(25%)	17 (14%)	0	4
8	G	183/185~(99%)	163 (89%)	10 (6%)	10 (6%)	2	19
9	Н	700/702~(100%)	603 (86%)	64 (9%)	33~(5%)	2	21
All	All	1004/1010 (99%)	840 (84%)	104 (10%)	60 (6%)	3	17

All (60) Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
7	F	10	PRO
7	F	23	LEU
8	G	32	ARG
8	G	33	ALA
8	G	84	ARG
9	Н	65	SER
9	Н	80	GLU
9	Н	81	PRO
9	Н	485	LYS
9	Н	486	PRO
9	Н	534	TYR
9	Н	583	TYR
9	Н	608	ALA
7	F	19	ASN
7	F	72	ASN
7	F	84	GLY
8	G	30	THR
8	G	105	PRO
9	Н	57	GLN
9	Н	197	ASP
9	Н	201	THR
9	Н	312	SER
9	Н	404	ILE
7	F	13	ARG



Mol	Chain	Res	Type
7	F	60	PHE
7	F	122	LYS
8	G	89	GLY
8	G	106	LEU
9	Н	93	VAL
9	Н	461	MET
9	Н	479	VAL
9	Н	496	GLN
9	Н	566	LEU
7	F	14	LYS
7	F	47	ALA
7	F	56	LEU
7	F	67	GLY
7	F	120	ARG
8	G	109	GLU
9	Н	36	VAL
9	Н	134	LYS
9	Н	199	GLY
9	Н	206	ASP
9	Н	390	ASP
9	Н	565	PRO
9	Н	649	VAL
7	F	15	VAL
7	F	42	LYS
7	F	121	PRO
8	G	61	PRO
9	Н	478	ASN
9	Н	68	THR
9	Н	483	VAL
9	Н	40	ILE
9	Н	330	VAL
9	Н	90	PRO
9	Н	402	ALA
9	Н	494	ILE
7	F	62	VAL
8	G	35	PRO

Continued from previous page...

#### 5.3.2 Protein sidechains (i)

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
7	F	103/103~(100%)	88~(85%)	15~(15%)	3 15
8	G	157/157~(100%)	144~(92%)	13 (8%)	11 34
9	Н	576/576~(100%)	533~(92%)	43 (8%)	13 38
All	All	836/836~(100%)	765~(92%)	71 (8%)	14 33

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	F	18	SER
7	F	20	VAL
7	F	28	GLN
7	F	30	ARG
7	F	33	CYS
7	F	35	ARG
7	F	38	THR
7	F	50	LYS
7	F	58	ASN
7	F	71	HIS
7	F	74	GLN
7	F	102	ASP
7	F	103	CYS
7	F	107	LYS
7	F	118	VAL
8	G	15	GLN
8	G	41	LEU
8	G	77	LYS
8	G	83	ILE
8	G	95	LYS
8	G	112	LYS
8	G	120	GLN
8	G	132	ILE
8	G	134	ARG
8	G	137	LEU
8	G	140	LEU
8	G	175	LEU
8	G	180	GLU
9	Н	16	SER
9	Н	53	MET
9	Н	64	THR



Mol	Chain	Res	Type
9	Н	69	THR
9	Н	81	PRO
9	Н	83	ARG
9	Н	106	LEU
9	Н	159	LYS
9	Н	160	THR
9	Н	171	LEU
9	Н	183	VAL
9	Н	197	ASP
9	Н	218	TRP
9	Н	222	LEU
9	Н	298	ILE
9	Н	323	LYS
9	Н	371	ARG
9	Н	375	LYS
9	Н	376	GLU
9	Н	389	LYS
9	Н	399	ASP
9	Н	410	GLU
9	Н	425	LYS
9	Н	445	PHE
9	Н	448	TRP
9	Н	461	MET
9	Н	466	LEU
9	Н	475	ARG
9	Н	479	VAL
9	Н	491	ARG
9	Н	504	LYS
9	Η	515	TYR
9	Н	536	PHE
9	Н	549	TYR
9	Н	557	ILE
9	Н	558	GLN
9	Н	571	VAL
9	Н	574	MET
9	Н	624	PRO
9	Н	626	GLU
9	Н	641	MET
9	Н	664	PHE
9	Н	675	LYS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such side chains are listed below:



Mol	Chain	Res	Type
7	F	58	ASN
7	F	72	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	21/22~(95%)	2 (9%)	1 (4%)
2	В	16/17~(94%)	1 (6%)	0
3	С	12/13~(92%)	0	0
4	D	18/19~(94%)	2 (11%)	0
5	Е	17/18~(94%)	2 (11%)	0
6	е	18/19~(94%)	3(16%)	0
All	All	102/108~(94%)	10 (9%)	1 (0%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	1906	G
1	А	1914	С
2	В	1955	U
4	D	2597	G
4	D	2602	А
5	Е	1409	С
5	Е	1419	G
6	е	1490	U
6	е	1493	А
6	е	1497	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	А	1913	А

### 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 monosaccharides 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.



## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-1917. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

### 6.2 Central slices (i)

#### 6.2.1 Primary map



X Index: 65



Y Index: 65



Z Index: 65



The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices (i)

#### 6.3.1 Primary map



X Index: 68

Y Index: 67

Z Index: 60

The images above show the largest variance slices of the map in three orthogonal directions.

#### 6.4 Orthogonal standard-deviation projections (False-color) (i)

#### 6.4.1 Primary map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



### 6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 272.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

## 6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

This section contains the results of statistical analysis of the map.

## 7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



## 7.2 Volume estimate (i)



The volume at the recommended contour level is  $3343 \text{ nm}^3$ ; this corresponds to an approximate mass of 3020 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



## 7.3 Rotationally averaged power spectrum (i)



\*Reported resolution corresponds to spatial frequency of 0.101  ${\rm \AA^{-1}}$ 



# 8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-1917 and PDB model 3J0E. Per-residue inclusion information can be found in section 3 on page 6.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 272.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



### 9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

#### 9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (272.0).



## 9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (272.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	1.0
All	0.5870	0.0840	
А	0.9720	0.1100	
В	0.9590	0.1140	
С	0.7740	0.0530	
D	0.8770	0.1290	
E	0.8550	0.1050	
F	0.8780	0.0590	
G	0.3610	0.0810	
Н	0.4560	0.0760	0.0 <
e	0.9850	0.1500	

