

# wwPDB EM Validation Summary Report (i)

#### Apr 17, 2024 - 08:46 am BST

:	8P03
:	EMD-17329
:	48S late-stage initiation complex with m6A mRNA
:	Guca, E.; Lima, L.H.F.; Boissier, F.; Hashem, Y.
:	2023-05-09
:	3.04  Å(reported)
	:

This is a wwPDB EM Validation Summary 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
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 3.04 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	$\begin{array}{c} \textbf{Whole archive} \\ \textbf{(\#Entries)} \end{array}$	EM structures (#Entries)
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	1	75	37%		35%	13%					
2	2	1863	8% 60	0%	27%	6% • 6%					
3	3	9	33% 22%	56%		22%					
4	А	284	6:	1% 86%		8% 6%					
5	С	207	<u>.</u>	93%		7%					
6	D	215	<u>.</u>	97%		•					
7	Е	270	<u>-</u>	78%	5%	16%					
8	F	227	6%	94%		5%					



Mol	Chain	Length	Quality of chain	
9	G	263	97%	•
10	Н	191	92%	5% ••
11	Ι	237	9%	5%
12	J	190	42%	6%
13	K	206	91%	9%
14	L	194	6% 93%	· ·
15	М	98	7% 94%	6%
16	Ν	158	96%	•
17	О	132	40% 86%	8% • 6%
18	Р	150	94%	5%•
19	Q	151	83%	7% 10%
20	R	145	86%	9% • •
21	S	141	91%	9%
22	Т	135	87%	6% 7%
23	U	152	89%	7% 5%
24	V	141	95%	5%
25	W	119	8%	6% 13%
26	Х	83	94%	6%
27	Y	130	95%	5% •
28	Ζ	143	95%	
29	a	133	89%	5% • 5%
30	b	115	78%	8% 14%
31	с	84	94%	6%
32	d	69	84%	9% 7%
33	е	56	80%	14% 5%

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Conti		i previous	paye							
Mol	Chain	$\mathbf{Length}$	Quality of chain							
			41%							
34	f	71	96% •							
35	g	313	92%	8%						
			8%							
36	i	133	42% · 56%							
			28%							
37	j	111	86%	10% ••						
			98%							
38	k	595	94%	6%						
			20%							
39	1	25	92%	8%						
			6%							
40	n	124	54% 6% 40%							

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# 2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 86276 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 initiator methionylated tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	75	Total 1614	C 722	N 299	O 519	Р 74	0	0

• Molecule 2 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues		1	AltConf	Trace			
2	2	1743	Total 37193	C 16605	N 6660	O 12186	Р 1742	0	0

• Molecule 3 is a RNA chain called m6A-methylated mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	9	Total 193	C 87	N 36	O 61	Р 9	0	0

• Molecule 4 is a protein called Eukaryotic translation initiation factor 2 subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	А	266	Total 2146	C 1354	N 376	O 405	S 11	0	0

• Molecule 5 is a protein called 40S ribosomal protein SA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	С	207	Total 1637	C 1042	N 288	O 299	S 8	0	0

• Molecule 6 is a protein called ribosomal protein eS1.

Mol	Chain	Residues		At	AltConf	Trace			
6	D	215	Total 1741	C 1107	N 309	O 310	S 15	0	0



• Molecule 7 is a protein called 40S ribosomal protein S2.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	Е	226	Total 1754	C 1139	N 298	O 310	${ m S} 7$	0	0

• Molecule 8 is a protein called Ribosomal protein S3.

Mol	Chain	Residues		Ate	AltConf	Trace			
8	F	227	Total 1764	C 1124	N 317	0 315	S 8	0	0

• Molecule 9 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues		At	AltConf	Trace			
9	G	263	Total 2083	C 1329	N 385	O 359	S 10	0	0

• Molecule 10 is a protein called Ribosomal protein S5.

Mol	Chain	Residues		At	$\mathbf{oms}$			AltConf	Trace
10	Н	187	Total 1482	C 928	N 279	O 268	${f S}7$	0	0

• Molecule 11 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
11	Ι	237	Total 1924	C 1199	N 387	0 331	S 7	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ι	130	THR	PRO	conflict	UNP A0A5K1UJS7

• Molecule 12 is a protein called ribosomal protein eS7.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	J	190	Total 1530	C 975	N 281	0 273	S 1	0	0

• Molecule 13 is a protein called 40S ribosomal protein S8.



Mol	Chain	Residues		At	oms			AltConf	Trace
13	K	206	Total 1680	C 1054	N 329	O 292	${ m S}{ m 5}$	0	0

• Molecule 14 is a protein called 40S ribosomal protein S9.

Mol	Chain	Residues		At	oms			AltConf	Trace
14	L	188	Total	C 070	N 200	0 251	S 2	0	0
			1342	979	309	231	3		

• Molecule 15 is a protein called 40S ribosomal protein eS10.

Mol	Chain	Residues		At	AltConf	Trace			
15	М	98	Total 828	C 539	N 148	0 135	S 6	0	0

• Molecule 16 is a protein called 40S ribosomal protein S11.

Mol	Chain	Residues		At	AltConf	Trace			
16	Ν	158	Total 1296	C 827	N 241	0 221	${ m S} 7$	0	0

• Molecule 17 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues		At	AltConf	Trace			
17	О	124	Total 958	C 600	N 170	0 179	S 9	0	0

• Molecule 18 is a protein called ribosomal protein uS15.

Mol	Chain	Residues		At	oms			AltConf	Trace
18	Р	150	Total 1208	С 773	N 229	O 205	S 1	0	0

• Molecule 19 is a protein called 40S ribosomal protein uS11.

Mol	Chain	Residues		At	oms	Atoms					
19	Q	136	Total 1016	C 621	N 199	0 190	S 6	0	0		

• Molecule 20 is a protein called 40S ribosomal protein uS19.



Mol	Chain	Residues		At	oms			AltConf	Trace
20	R	140	Total 1154	C 733	N 219	O 195	${ m S} 7$	0	0

• Molecule 21 is a protein called 40S ribosomal protein uS9.

Mol	Chain	Residues		Atoms					Trace
21	S	141	Total 1124	C 715	N 212	0 194	${ m S} { m 3}$	0	0

• Molecule 22 is a protein called 40S ribosomal protein eS17.

Mol	Chain	Residues		At	oms			AltConf	Trace
22	Т	126	Total 1019	C 639	N 188	0 187	${ m S}{ m 5}$	0	0

• Molecule 23 is a protein called 40S ribosomal protein uS13.

Mol	Chain	Residues		Atoms					Trace
23	U	145	Total 1194	С 747	N 243	O 203	S 1	0	0

• Molecule 24 is a protein called 40S ribosomal protein eS19.

Mol	Chain	Residues		At	oms	AltConf	Trace		
24	V	141	Total 1113	C 701	N 213	0 196	${ m S} { m 3}$	0	0

• Molecule 25 is a protein called 40S ribosomal protein uS10.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	W	104	Total 822	C 514	N 156	0 148	$\frac{S}{4}$	0	0

• Molecule 26 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues		At	oms			AltConf	Trace
26	Х	83	Total 636	C 393	N 117	0 121	${f S}{5}$	0	0

• Molecule 27 is a protein called Ribosomal protein S15a.



Mol	Chain	Residues		At	oms			AltConf	Trace
27	Y	129	Total 1034	$\begin{array}{c} \mathrm{C} \\ 659 \end{array}$	N 193	O 176	S 6	0	0

• Molecule 28 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues		At	oms	AltConf	Trace		
28	Z	142	Total 1106	C 698	N 220	0 184	$\frac{S}{4}$	0	0

• Molecule 29 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues		Atoms					Trace
29	a	126	Total 1021	C 645	N 198	0 173	${f S}{5}$	0	0

• Molecule 30 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	99	Total 789	C 491	N 162	O 130	S 6	0	0

• Molecule 31 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	с	84	Total 659	C 413	N 122	0 116	S 8	0	0

• Molecule 32 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	64	Total	С	Ν	0	$\mathbf{S}$	0	0
32	u	04	506	308	102	94	2	0	0

• Molecule 33 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	е	53	Total 444	C 278	N 90	0 71	${f S}{5}$	0	0

• Molecule 34 is a protein called ribosomal protein eS31.



Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	71	Total 582	$\begin{array}{c} \mathrm{C} \\ 367 \end{array}$	N 109	O 99	${f S}{7}$	0	0

• Molecule 35 is a protein called Ribosomal protein RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	313	Total 2437	C 1535	N 424	0 466	S 12	0	0

• Molecule 36 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	i	58	Total 464	C 287	N 102	0 74	S 1	0	0

• Molecule 37 is a protein called Eukaryotic translation initiation factor 4C.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	j	108	Total 874	C 543	N 166	0 161	${S \atop 4}$	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	39	ILE	VAL	conflict	UNP G1SYS4
j	76	ILE	VAL	conflict	UNP G1SYS4

• Molecule 38 is a protein called ATP binding cassette subfamily E member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	k	595	Total 4693	C 2995	N 802	O 865	S 31	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	538	ILE	VAL	conflict	UNP G1SG72

• Molecule 39 is a protein called 60S ribosomal protein L41.



Mol	Chain	Residues	Atoms					AltConf	Trace
30	1	25	Total	С	Ν	Ο	S	0	0
- 39	1	20	240	145	64	28	3	0	0

• Molecule 40 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace	
40	n	75	Total 598	C 382	N 111	0 104	S 1	0	0

• Molecule 41 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
41	2	175	Total Mg 175 175	0
41	3	1	Total Mg 1 1	0
41	Ι	1	Total Mg 1 1	0
41	Ζ	1	Total Mg 1 1	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: initiator methionylated tRNA























• Molecule 27: Ribosomal protein S15a



Chain Y:	95%	5%•
MET V2 X12 E51 B55 B55 L104 L104		
• Molecule 28: 40S rib	osomal protein S23	
Chain Z:	95%	
M1 C4 C4 C4 C4 C4 C4 C4 C6 C9 C5 C1 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5 C5		
• Molecule 29: 40S rib	osomal protein S24	
Chain a:	89%	5% • 5%
MET ASN BS R61 R61 R61 R90 R90 R90	RIOT RI18 K122 C126 C126 C128 C128 C128 C128 C128 C128 C128 C128	
• Molecule 30: 40S rib	osomal protein S26	
Chain b:	78%	8% 14%
MET 12 R6 R10 R15 C26 C26 R42 C26 R42 E46	SY6 R96 PHE PHE PHE ARG ALA ALA ALA ALA ALA ALA PRO PRO PRO PRO PRO PRO PRO PRO PRO PRO	
• Molecule 31: 40S rib	osomal protein S27	
Chain c:	94%	6%
M1 P2 G39 F15 F66 F66		
• Molecule 32: 40S rib	osomal protein S28	
Chain d:	84%	9% 7%
MET ASP THR SER V6 V5 V30 V30 V30 V30 V30 V30 V6 V17 V5 V6 V17 V6 V6 V6 V6 V6 V6 V6 V6 V6 V6 V6 V6 V6	RG7 LG8 ARG	
• Molecule 33: 40S rib	osomal protein S29	
Chain e:	80%	14% 5%
MET MET MET MET HI PII 14 R13 F14 R13 F14 R13 F14 C39 C39		







![](_page_18_Picture_5.jpeg)

![](_page_19_Figure_3.jpeg)

 $\bullet$  Molecule 39: 60S ribosomal protein L41

![](_page_19_Figure_5.jpeg)

![](_page_19_Picture_6.jpeg)

![](_page_20_Picture_3.jpeg)

![](_page_20_Picture_4.jpeg)

# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	103050	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{\AA}^2)$	45	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.161	Depositor
Minimum map value	-0.080	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

![](_page_21_Picture_5.jpeg)

# 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: T6A, MG, MA6, I2T  $\,$ 

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).

Mal	Chain	Bo	ond lengths	I	Bond angles
MIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	1	1.02	2/1770~(0.1%)	1.68	37/2759~(1.3%)
2	2	0.87	75/41554~(0.2%)	1.33	662/64761~(1.0%)
3	3	1.28	0/188	1.98	10/288~(3.5%)
4	А	0.47	0/2177	0.85	9/2935~(0.3%)
5	С	0.52	0/1674	0.88	7/2275~(0.3%)
6	D	0.36	0/1769	0.61	0/2367
7	Ε	0.38	0/1794	0.61	1/2430~(0.0%)
8	$\mathbf{F}$	0.31	0/1792	0.51	1/2412~(0.0%)
9	G	0.28	0/2125	0.50	0/2856
10	Н	0.42	0/1503	0.73	6/2020~(0.3%)
11	Ι	0.39	0/1946	0.69	5/2588~(0.2%)
12	J	0.34	0/1553	0.61	1/2079~(0.0%)
13	Κ	0.49	0/1709	0.82	5/2278~(0.2%)
14	L	0.45	0/1567	0.76	4/2092~(0.2%)
15	М	0.45	0/852	0.77	1/1147~(0.1%)
16	Ν	0.39	0/1319	0.59	0/1761
17	0	0.51	0/968	0.84	3/1296~(0.2%)
18	Р	0.42	0/1232	0.72	3/1656~(0.2%)
19	Q	0.53	0/1029	0.91	3/1380~(0.2%)
20	R	0.65	0/1177	1.09	9/1571~(0.6%)
21	S	0.39	0/1142	0.63	3/1528~(0.2%)
22	Т	0.44	0/1031	0.81	3/1383~(0.2%)
23	U	0.38	0/1212	0.64	1/1621~(0.1%)
24	V	0.49	0/1133	0.82	3/1517~(0.2%)
25	W	0.28	0/832	0.51	0/1117
26	Х	0.37	0/643	0.60	0/860
27	Y	0.47	0/1051	0.80	0/1406
28	Ζ	0.36	0/1124	0.59	0/1500
29	а	0.59	0/1038	0.96	4/1380~(0.3%)
30	b	0.54	0/802	0.91	$\overline{6/1076}~(0.6\%)$
31	с	0.46	0/673	0.82	1/902~(0.1%)
32	d	0.32	0/508	0.58	0/680

![](_page_22_Picture_8.jpeg)

Mal	Chain	Bo	ond lengths	I	Bond angles
INIOI	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
33	е	0.54	0/454	0.96	4/603~(0.7%)
34	f	0.41	0/594	0.66	0/786
35	g	0.37	0/2494	0.67	0/3394
36	i	0.62	0/469	0.96	1/617~(0.2%)
37	j	0.39	0/884	0.71	4/1175~(0.3%)
38	k	0.52	0/4780	0.81	10/6452~(0.2%)
39	1	0.25	0/241	0.39	0/305
40	n	0.45	0/604	0.80	3/810~(0.4%)
All	All	0.69	77/91407~(0.1%)	1.10	810/132063~(0.6%)

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	1	0	9
2	2	0	94
3	3	0	1
4	А	0	1
5	С	0	1
10	Н	0	1
11	Ι	0	2
13	Κ	0	2
14	L	0	1
18	Р	0	1
19	Q	0	1
20	R	0	3
22	Т	0	1
36	i	0	1
37	j	0	2
38	k	0	3
All	All	0	124

The worst 5 of 77 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	1	72	U	O3'-P	-15.85	1.42	1.61
2	2	1245	С	O3'-P	-10.77	1.48	1.61
2	2	270	G	P-OP1	7.37	1.61	1.49
2	2	1724	U	P-OP1	7.35	1.61	1.49
2	2	1765	G	P-OP1	7.34	1.61	1.49

![](_page_23_Picture_8.jpeg)

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	1	72	U	OP2-P-O3'	-38.61	20.25	105.20
2	2	71	G	O4'-C1'-N9	12.55	118.24	108.20
1	1	72	U	OP1-P-O3'	12.43	132.54	105.20
2	2	498	А	N1-C6-N6	-12.32	111.21	118.60
2	2	581	U	O4'-C1'-N1	12.25	118.00	108.20

The worst 5 of 810 bond angle outliers are listed below:

There are no chirality outliers.

5 of 124 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	24	G	Sidechain
1	1	26	G	Sidechain
1	1	27	С	Sidechain
1	1	29	G	Sidechain
1	1	32	С	Sidechain

## 5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 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	Perce	$\mathbf{ntiles}$
4	А	264/284~(93%)	237~(90%)	27 (10%)	0	100	100
5	С	205/207~(99%)	184 (90%)	21 (10%)	0	100	100
6	D	213/215~(99%)	188 (88%)	25 (12%)	0	100	100
7	Ε	224/270~(83%)	209~(93%)	14 (6%)	1 (0%)	34	69
8	F	225/227~(99%)	206 (92%)	19 (8%)	0	100	100
9	G	261/263~(99%)	241 (92%)	20 (8%)	0	100	100

![](_page_24_Picture_16.jpeg)

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
10	Η	183/191~(96%)	169~(92%)	14 (8%)	0	100	100
11	Ι	235/237~(99%)	224~(95%)	11 (5%)	0	100	100
12	J	188/190~(99%)	162~(86%)	26 (14%)	0	100	100
13	Κ	204/206~(99%)	182 (89%)	22 (11%)	0	100	100
14	L	186/194~(96%)	174 (94%)	12 (6%)	0	100	100
15	М	96/98~(98%)	89~(93%)	7 (7%)	0	100	100
16	Ν	156/158~(99%)	150 (96%)	6 (4%)	0	100	100
17	Ο	122/132~(92%)	98 (80%)	24 (20%)	0	100	100
18	Р	148/150~(99%)	143 (97%)	5 (3%)	0	100	100
19	Q	134/151~(89%)	118 (88%)	16 (12%)	0	100	100
20	R	138/145~(95%)	122 (88%)	16 (12%)	0	100	100
21	S	139/141~(99%)	130 (94%)	9 (6%)	0	100	100
22	Т	124/135~(92%)	110 (89%)	14 (11%)	0	100	100
23	U	143/152~(94%)	131 (92%)	12 (8%)	0	100	100
24	V	139/141~(99%)	132~(95%)	7 (5%)	0	100	100
25	W	102/119~(86%)	97~(95%)	5 (5%)	0	100	100
26	Х	81/83~(98%)	74 (91%)	7 (9%)	0	100	100
27	Y	127/130~(98%)	122~(96%)	5 (4%)	0	100	100
28	Z	140/143~(98%)	127~(91%)	13 (9%)	0	100	100
29	a	124/133~(93%)	107~(86%)	16 (13%)	1 (1%)	19	54
30	b	97/115~(84%)	91~(94%)	6 (6%)	0	100	100
31	с	82/84~(98%)	70~(85%)	11 (13%)	1 (1%)	13	44
32	d	62/69~(90%)	57~(92%)	5 (8%)	0	100	100
33	е	51/56~(91%)	48 (94%)	3~(6%)	0	100	100
34	f	69/71~(97%)	56~(81%)	13 (19%)	0	100	100
35	g	311/313~(99%)	284 (91%)	26 (8%)	1 (0%)	41	74
36	i	56/133~(42%)	49(88%)	7 (12%)	0	100	100
37	j	106/111 (96%)	98~(92%)	8 (8%)	0	100	100
38	k	593/595~(100%)	516 (87%)	76 (13%)	1 (0%)	47	80
39	1	23/25 (92%)	$23 \ (100\%)$	0	0	100	100
40	n	73/124~(59%)	68~(93%)	5 (7%)	0	100	100

![](_page_25_Picture_6.jpeg)

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	5824/6191 (94%)	5286 (91%)	533 (9%)	5(0%)	54 84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	Е	252	LYS
38	k	439	PRO
35	g	283	PRO
29	a	86	GLU
31	с	39	GLY

#### 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.

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	А	238/255~(93%)	223~(94%)	15~(6%)	18	49	
5	$\mathbf{C}$	173/173~(100%)	164~(95%)	9~(5%)	23	57	
6	D	196/196~(100%)	190~(97%)	6 (3%)	40	73	
7	Ε	190/214~(89%)	176 (93%)	14 (7%)	13	42	
8	F	190/190~(100%)	177 (93%)	13~(7%)	16	46	
9	G	225/225~(100%)	216 (96%)	9~(4%)	31	66	
10	Н	159/161~(99%)	153 (96%)	6 (4%)	33	67	
11	Ι	207/207~(100%)	198 (96%)	9~(4%)	29	63	
12	J	170/170~(100%)	160 (94%)	10 (6%)	19	51	
13	Κ	177/177~(100%)	164 (93%)	13 (7%)	14	42	
14	L	162/168~(96%)	160 (99%)	2(1%)	71	89	
15	М	89/89~(100%)	84 (94%)	5~(6%)	21	54	
16	Ν	142/142~(100%)	135~(95%)	7~(5%)	25	59	
17	О	104/108~(96%)	95 (91%)	9~(9%)	10	34	
18	Р	130/130~(100%)	124 (95%)	6(5%)	27	61	

![](_page_26_Picture_12.jpeg)

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
19	Q	106/119~(89%)	100 (94%)	6 (6%)	20	53
20	R	126/130~(97%)	120~(95%)	6 (5%)	25	60
21	S	117/117~(100%)	105 (90%)	12 (10%)	7	26
22	Т	114/121 (94%)	110 (96%)	4 (4%)	36	69
23	U	125/132~(95%)	116 (93%)	9(7%)	14	43
24	V	113/113~(100%)	109 (96%)	4 (4%)	36	69
25	W	94/107~(88%)	87 (93%)	7 (7%)	13	42
26	Х	67/67~(100%)	62 (92%)	5 (8%)	13	41
27	Y	112/113~(99%)	106 (95%)	6 (5%)	22	55
28	Z	114/115~(99%)	108 (95%)	6 (5%)	22	56
29	a	108/115 (94%)	105~(97%)	3 (3%)	43	75
30	b	87/99~(88%)	84 (97%)	3~(3%)	37	70
31	с	76/76~(100%)	73~(96%)	3 (4%)	32	66
32	d	57/62~(92%)	51 (90%)	6 (10%)	7	25
33	е	47/49~(96%)	42 (89%)	5 (11%)	6	24
34	f	64/64~(100%)	61~(95%)	3~(5%)	26	61
35	g	272/272~(100%)	247~(91%)	25~(9%)	9	31
36	i	48/106~(45%)	48 (100%)	0	100	100
37	j	91/93~(98%)	84 (92%)	7 (8%)	13	40
38	k	523/523~(100%)	498 (95%)	25~(5%)	25	60
39	1	24/24 (100%)	22 (92%)	2 (8%)	11	37
40	n	66/102~(65%)	61 (92%)	5 (8%)	13	41
All	All	5103/5324 (96%)	4818 (94%)	285 (6%)	25	54

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5 of 285 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	g	111	VAL
35	g	199	THR
38	k	354	LYS
13	Κ	105	ASP
13	Κ	86	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

![](_page_27_Picture_8.jpeg)

Mol	Chain	Res	Type
16	Ν	121	GLN
37	j	37	GLN
22	Т	48	ASN
37	j	19	ASN
38	k	549	GLN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	74/75~(98%)	15 (20%)	1 (1%)
2	2	1735/1863~(93%)	319~(18%)	20 (1%)
3	3	7/9~(77%)	2(28%)	0
All	All	1816/1947~(93%)	336~(18%)	21 (1%)

5 of 336 RNA backbone outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	1	13	G
1	1	14	С
1	1	17	С
1	1	18	G
1	1	19	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1427	G
2	2	1472	А
2	2	1855	G
2	2	1548	С
2	2	1471	G

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

3 non-standard protein/DNA/RNA residues are 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.

![](_page_28_Picture_13.jpeg)

Mal	Tune Chain Des Link		Tink	Bond lengths			B	ond ang	les	
1VIOI	туре	Unam	nes		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	T6A	1	37	1	27,34,35	1.28	3 (11%)	29,49,52	1.85	6 (20%)
2	I2T	2	1244	2	24,29,30	0.87	1 (4%)	29,42,45	1.16	2 (6%)
3	MA6	3	49	3	$18,\!25,\!27$	0.96	1(5%)	16,36,41	1.52	2 (12%)

RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

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	T6A	1	37	1	-	5/19/41/42	0/3/3/3
2	I2T	2	1244	2	-	0/16/34/35	0/2/2/2
3	MA6	3	49	3	-	2/5/27/30	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms		Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	1	37	T6A	ODA-C13	4.70	1.36	1.22
2	2	1244	I2T	O36-C34	-2.58	1.22	1.30
1	1	37	T6A	ODB-C13	-2.30	1.23	1.30
3	3	49	MA6	C8-N7	-2.25	1.30	1.34
1	1	37	T6A	C8-N7	-2.20	1.30	1.34

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

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	1	37	T6A	C12-N11-C10	5.27	130.72	121.94
1	1	37	T6A	C2-N1-C6	4.27	120.25	116.59
3	3	49	MA6	C10-N6-C6	4.14	126.44	122.87
2	2	1244	I2T	C3'-C2'-C1'	3.41	105.61	101.64
3	3	49	MA6	C2-N1-C6	3.15	119.29	116.59

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	37	T6A	O10-C10-N6-C6
3	3	49	MA6	O4'-C4'-C5'-O5'

![](_page_29_Picture_15.jpeg)

Mol	Chain	Res	Type	Atoms
3	3	49	MA6	C3'-C4'-C5'-O5'
1	1	37	T6A	C14-C12-N11-C10
1	1	37	T6A	N11-C10-N6-C6

Continued from previous page...

There are no ring outliers.

No monomer is involved in short contacts.

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry (i)

Of 178 ligands modelled in this entry, 178 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers (i)

There are no such residues in this entry.

#### 5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	2	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	2	730:C	O3'	731:C	Р	9.48

![](_page_30_Picture_24.jpeg)

# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-17329. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

## 6.1 Orthogonal projections (i)

#### 6.1.1 Primary map

![](_page_31_Picture_8.jpeg)

6.1.2 Raw map

![](_page_31_Picture_10.jpeg)

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

![](_page_31_Picture_12.jpeg)

## 6.2 Central slices (i)

### 6.2.1 Primary map

![](_page_32_Picture_5.jpeg)

X Index: 192

![](_page_32_Picture_7.jpeg)

Y Index: 192

![](_page_32_Picture_9.jpeg)

Z Index: 192

#### 6.2.2 Raw map

![](_page_32_Picture_12.jpeg)

X Index: 192

Y Index: 192

Z Index: 192

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

![](_page_32_Picture_17.jpeg)

### 6.3 Largest variance slices (i)

### 6.3.1 Primary map

![](_page_33_Picture_5.jpeg)

X Index: 170

![](_page_33_Picture_7.jpeg)

Y Index: 160

![](_page_33_Picture_9.jpeg)

Z Index: 199

#### 6.3.2 Raw map

![](_page_33_Picture_12.jpeg)

X Index: 169

Y Index: 158

![](_page_33_Figure_15.jpeg)

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

![](_page_33_Picture_17.jpeg)

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

### 6.4.1 Primary map

![](_page_34_Picture_5.jpeg)

6.4.2 Raw map

![](_page_34_Picture_7.jpeg)

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.

![](_page_34_Picture_9.jpeg)

### 6.5 Orthogonal surface views (i)

#### 6.5.1 Primary map

![](_page_35_Picture_5.jpeg)

The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.5.2 Raw map

![](_page_35_Picture_8.jpeg)

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

#### 6.6 Mask visualisation (i)

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

![](_page_35_Picture_12.jpeg)

# 7 Map analysis (i)

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

## 7.1 Map-value distribution (i)

![](_page_36_Figure_6.jpeg)

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.

![](_page_36_Picture_8.jpeg)

## 7.2 Volume estimate (i)

![](_page_37_Figure_4.jpeg)

The volume at the recommended contour level is  $603 \text{ nm}^3$ ; this corresponds to an approximate mass of 544 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.

![](_page_37_Picture_7.jpeg)

## 7.3 Rotationally averaged power spectrum (i)

![](_page_38_Figure_4.jpeg)

\*Reported resolution corresponds to spatial frequency of 0.329  ${\rm \AA^{-1}}$ 

![](_page_38_Picture_6.jpeg)

# 8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC (i)

![](_page_39_Figure_6.jpeg)

\*Reported resolution corresponds to spatial frequency of 0.329  $\mathrm{\AA^{-1}}$ 

![](_page_39_Picture_8.jpeg)

## 8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.02	3.37	3.06
Unmasked-calculated*	3.75	6.94	3.88

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.75 differs from the reported value 3.04 by more than 10 %

![](_page_40_Picture_6.jpeg)

# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-17329 and PDB model 8P03. Per-residue inclusion information can be found in section 3 on page 12.

## 9.1 Map-model overlay (i)

![](_page_41_Picture_6.jpeg)

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

![](_page_41_Picture_8.jpeg)

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

![](_page_42_Figure_4.jpeg)

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)

![](_page_42_Figure_7.jpeg)

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 (0.015).

![](_page_42_Picture_9.jpeg)

### 9.4 Atom inclusion (i)

![](_page_43_Figure_4.jpeg)

At the recommended contour level, 79% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.

![](_page_43_Picture_6.jpeg)

## 9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

$\mathbf{Chain}$	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7770	0.5090
1	0.5590	0.2840
2	0.8780	0.5300
3	0.6750	0.4840
А	0.2870	0.3460
С	0.8770	0.5660
D	0.8720	0.5610
Е	0.8640	0.5720
F	0.7900	0.5310
G	0.8780	0.5760
Н	0.8550	0.5580
Ι	0.7760	0.5120
J	0.4800	0.4390
К	0.8050	0.5290
L	0.8560	0.5610
М	0.8420	0.5300
N	0.7750	0.5430
0	0.4710	0.3690
Р	0.8740	0.5650
Q	0.8770	0.5660
R	0.7490	0.5100
S	0.9030	0.5800
Т	0.7090	0.4990
U	0.8020	0.5310
V	0.8780	0.5570
W	0.7530	0.5290
X	0.8730	0.5670
Y	0.9100	0.6000
Z	0.8700	0.5880
a	0.8420	0.5330
b	0.8990	0.5840
c	0.8080	0.5320
d	0.8000	0.5620
e	0.9110	0.5780
f	0.5290	0.3770

0.0 <0.0

1.0

![](_page_44_Picture_8.jpeg)

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Chain	Atom inclusion	Q-score
g	0.8190	0.5210
i	0.7030	0.5160
j	0.5350	0.4920
k	0.0650	0.2560
1	0.7170	0.5250
n	0.7310	0.5130

![](_page_45_Picture_5.jpeg)