

# wwPDB EM Validation Summary Report (i)

Nov 30, 2021 – 05:35 pm GMT

PDB ID	:	7OHU
EMDB ID	:	EMD-12909
Title	:	Nog1-TAP associated immature ribosomal particles from S. cerevisiae after
		rpL2 expression shut down, population B
Authors	:	Milkereit, P.; Poell, G.
Deposited on	:	2021-05-11
Resolution	:	3.70  Å(reported)
Based on initial model	:	6EM1

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

EMDB validation analysis	:	$0.0.0.{ m dev}97$
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

# 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 3.70 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$
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 >=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 <=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	3396	38% 11%	50%
2	2	158	77%	17% 6%
3	В	387	84%	• 15%
4	С	362	92%	• 7%
5	Е	176	81%	• 18%
6	F	244	<b>•</b> 92%	8%
7	G	256	8% 60%	39%
8	Н	191	6% 98%	••

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Mol	Chain	Length	Quality of chain
9	L	199	53% • 46%
10	М	138	96% ••
11	Ν	204	5% 86% · 13%
12	О	199	98%
13	Р	184	<b>5</b> 9% 41%
14	Q	186	70% • 30%
15	S	172	97%
16	V	137	9% 90% • 9%
17	W	236	97%
18	Y	127	95%
19	b	647	61% • 36%
20	е	130	95% • •
21	f	107	98%
22	h	120	94% • 5%
23	i	100	<sup>6%</sup> 74% 26%
24	j	88	6% 
25	r	261	6%           28%           72%
26	u	199	<b>5</b> 5% •• 42%
27	у	245	91% • 8%

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# 2 Entry composition (i)

There are 28 unique types of molecules in this entry. The entry contains 127652 atoms, of which 54773 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 25S rRNA.

Mol	Chain	Residues			AltConf	Trace				
1	1	1692	Total 54436	C 16178	H 18197	N 6560	O 11809	Р 1692	0	0

• Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues			AltConf	Trace				
2	2	148	Total 4737	C 1407	H 1591	N 557	O 1034	Р 148	0	0

• Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues			AltConf	Trace				
3	В	330	Total 5336	C 1669	Н 2709	N 487	0 466	${f S}{5}$	0	0

• Molecule 4 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues			AltConf	Trace				
4	С	336	Total 5260	C 1622	Н 2688	N 489	0 458	${ m S} { m 3}$	0	0

• Molecule 5 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues			AltConf	Trace				
5	Е	144	Total 2376	C 736	Н 1235	N 206	0 198	S 1	0	0

• Molecule 6 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues			AltConf	Trace				
6	F	225	Total	С	Н	Ν	Ο	$\mathbf{S}$	0	0
0	T	220	3700	1166	1891	329	313	1	0	0



• Molecule 7 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues			AltConf	Trace				
7	G	156	Total 2488	C 784	Н 1275	N 206	0 221	${ m S} { m 2}$	0	0

• Molecule 8 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues			AltConf	Trace				
8	Н	190	Total 3086	$\begin{array}{c} \mathrm{C} \\ 957 \end{array}$	H 1576	N 273	0 276	${S \over 4}$	0	0

• Molecule 9 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues		Α	toms			AltConf	Trace
9	L	108	Total 1782	C 541	H 918	N 180	0 143	0	0

• Molecule 10 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues			AltConf	Trace				
10	М	134	Total	C 668	H 1128	N 107	$0_{174}$	S 2	0	0
			2179	000	1190	197	114	Z		

• Molecule 11 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues			AltConf	Trace				
11	N	177	Total 3079	C 948	Н 1566	N 320	0 244	S 1	0	0

• Molecule 12 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
12	О	197	Total 3215	C 1003	Н 1660	N 289	O 262	S 1	0	0

• Molecule 13 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues		Α	AltConf	Trace			
13	Р	108	Total 1694	C 533	Н 850	N 152	O 159	0	0

• Molecule 14 is a protein called 60S ribosomal protein L18-A.



Mol	Chain	Residues			Atom	IS			AltConf	Trace
14	Q	131	Total 2101	C 645	H 1092	N 190	O 173	S 1	0	0

• Molecule 15 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues			AltConf	Trace				
15	S	170	Total 2904	C 922	Н 1472	N 265	O 242	${ m S} { m 3}$	0	0

• Molecule 16 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues			AltConf	Trace				
16	V	124	Total 1890	C 578	Н 970	N 173	O 162	S 7	0	0

• Molecule 17 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues			Atoms	5			AltConf	Trace
17	W	232	Total 3773	C 1184	Н 1903	N 321	O 360	${ m S}{ m 5}$	0	0

• Molecule 18 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues		A	Atoms			AltConf	Trace
18	Y	125	Total 2060	C 620	Н 1076	N 191	0 173	0	0

• Molecule 19 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
19	h	411	Total	С	Η	Ν	0	$\mathbf{S}$	0	0
10	~		6718	2131	3385	573	612	17		0

• Molecule 20 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues			Atom	.s			AltConf	Trace
20	е	125	Total 2090	C 641	Н 1081	N 203	0 164	S 1	0	0

• Molecule 21 is a protein called 60S ribosomal protein L33-A.



Mol	Chain	Residues			Aton	ns			AltConf	Trace
21	f	106	Total 1731	$\begin{array}{c} \mathrm{C} \\ 540 \end{array}$	Н 881	N 165	0 144	S 1	0	0

• Molecule 22 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues			Atom	S			AltConf	Trace
22	h	114	Total 1969	C 592	Н 1038	N 178	O 160	S 1	0	0

• Molecule 23 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues			Aton	ıs			AltConf	Trace
23	i	74	Total 1236	C 367	Н 642	N 125	O 101	S 1	0	0

• Molecule 24 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	j	71	Total 1137	С 344	Н 571	N 123	0 94	${ m S}{ m 5}$	0	0

• Molecule 25 is a protein called Ribosome biogenesis protein NSA2.

Mol	Chain	Residues			Aton	ns			AltConf	Trace
25	r	73	Total 1288	C 388	Н 660	N 133	O 106	S 1	0	0

• Molecule 26 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues			Atom	IS			AltConf	Trace
26	u	116	Total 1987	C 612	Н 1011	N 200	0 155	S 9	0	0

• Molecule 27 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues			Atom	5			AltConf	Trace
27	У	225	Total 3398	C 1056	Н 1697	N 295	0 343	${f S}{7}$	0	0

• Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).



Mol	Chain	Residues	Atoms	AltConf
28	j	1	Total Zn 1 1	0
28	u	1	Total Zn 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: 25S rRNA











MET KIG5 S2 S2 HS8 HS8 HS8 HS8 HS8 HS8 HS8 HS8
GLU THR HIS HIS ASP
• Molecule 5: 60S ribosomal protein L6-A
Chain E: 81% · 18%
MET SER ALLA ALLA ALLA ALLA CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU
$\bullet$ Molecule 6: 60S ribosomal protein L7-A
Chain F: 92% 8%
MET ALA ALA ALA ALA CUU CUU CUU CUU CUU CUN CUN CUN CUN CUN
$\bullet$ Molecule 7: 60S ribosomal protein L8-A
8% Chain G: 60% • 39%
MET ALA PRO CUYS CUYS CUYS CUYS CUYS ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
CLN LVS LVS LVS LLSU ARG LEU K70 K70 K70 K70 K70 K70 K70 K70 K70 K70
GLY ILE LEU GLY GLY GLY ALA ALA ARF LYS ALA ARF LYS ARS ASP ASP ASP ASP ALA
• Molecule 8: 60S ribosomal protein L9-A
Chain H: 98%
E144         E144         B107         G108         H153         N1533         N157         N157         LEU
• Molecule 9: 60S ribosomal protein L13-A
Chain L: 53% · 46%
MET ALA ALA SER SER ALSN ALA ALA ALA ALA ALA ALA ALA ALA ALA AL
GLN ASP ASP ASP ALS SER ALS ALS ALS ALS ALS ALS ALS ALS ALS ALS
WORLDWIDE PROTEIN DATA BANK

• Molecule 10: 60	0S ribosomal protein L14-A		
Chain M:	96%		I
MET SER THR A A A A A A A A A A A A A A A A A A A	АГА		
• Molecule 11: 60	0S ribosomal protein L15-A		
Chain N:	86%	• 13%	
MET 43 43 43 83 8 44 6 9 6 9 4 8 1 7 8 8 1 7 8 8 1 7 8 8 1 7 8 1 7 8 1 7 8 1 8 1	PRO PRO PRO LYS PRO GLY ALA ALY CLYS PRO CLN CLN CLU CLU CLU	LTR CLN R109 R109 R117 R183 K184 R185 R185 R185 R185 R185 R193 R193 R193 R193 R193 R193	I
• Molecule 12: 60	0S ribosomal protein L16-A		
Chain O:	98%		
MET SER 43 46 76 46 76 76 76 86 86 86 86 86 86 80 80 80 80 80 80 80 80 80 80 80 80 80	F71 F71 K91 V167 V199		
• Molecule 13: 60	0S ribosomal protein L17-A		
Chain P:	59%	41%	
MET ALA ARG ARG GLY ALA ALA ALA THR THR MIO NIO NIO	F60 ARG ARG ARG ARG ARG ASN ASN SER ASN SER ASN ALA ALA ALA GLV GLV GLV GLV CLV CLV CLV CLV CLV CLV CLV CLV CLV C	LINK LYS ALA ARG ARG W83 K124 CLN ARG ARG ARG ARG ARG ARG ARG ARG ARG ARG	E154 GLU ALA VAL
ALA LYS ALA ALA ALA GLU GLU CYS LYS VAL VAL VAL VAL VAL CEU	ARA ARA GLN GLN CLY CLY CLY CLY CLY ARG ARG ARG ARA ALA ALA ALA ALA ALA		
• Molecule 14: 60	0S ribosomal protein L18-A		
Chain Q:	70%	• 30%	•
MET GLY TILE ASP ASE SER CIN CIN CIN ARC ARC	CLA CLA HI5 H15 N145 SER ARG CLY ALA ALA ALA ALA ALA ALA ALA ALA ALA A	ALA ALA ARG ARG LLEU SER SER THR ARG ALA ARG ALA ARG ARG ARG ARG ARG ARG ARG ARG ARG AR	PHE LYS VAL
• Molecule 15: 60	0S ribosomal protein L20-A		
Chain S:	97%		
MET ALA H3 R12 E17 E21 K50	R84		
• Molecule 16: 60	0S ribosomal protein L23-A		
Chain V:	90%	• 9%	
	W P R	ORLDWIDE OTEIN DATA BANK	





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#### VAL GLY LYS THR ASP PHE ARG



#### LUPUS LUPUS CLU LUPUS CLU LUPUS CLU LUPUS SERRA SERRA SERRA SERRA CLU LUPUS CLU LUPUS CLU LUPUS CLU LUPUS SERRA CLU LUPUS CLU

#### 

#### 

• Molecule 26: Ribosome biogenesis protein RLP24

Chain u:	55%	••	42%
M1 C6 E28 E163 E163 E100 R100 R100 R103 R113	K116 GLU LYS LYS ASP PHE LEU ASP LVS LEU VAL VAL CLU SER ASW	PRO GLU LEU LEU LEU ARG ARG GLU VAL GLU	ILE ALA ARG LYS ARG LEU ALA GLU GLU GLU SER SER SER SER SER SER SER SER
GLN GLU GLU SER GLU GLU GLU GLU MSP SER ASP SER ASP SER ASP SCU GLU GLU	GLU GLU GLU GLU GLU CLEU CLYS CLN GLN CLYS CLN CLYS CLN CLYS CLN CLYS CLN CLU CLU CLU CLU CLU CLU CLU CLU CLU CLU	ARG ARG ASN THR LYS LYS TLE ALA PHE	
• Molecule 27: Eukaryotic	e translation initiatio	on factor 6	

Chain y:	91%	• 8%
M1 630 078 A100 A123	Q225 ASP ALA PRO PRO CLU SER CLU SER ASP ASP ASP LEU LEU CLU THR THR THR THR THR SER	



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	86.45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.031	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.021	Depositor
Map size (Å)	425.40002, 425.40002, 425.40002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor



# 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: ZN

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		Bo	Bond lengths		Bond angles		
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	1	0.16	0/40546	0.75	43/63168~(0.1%)		
2	2	0.16	0/3514	0.76	4/5467~(0.1%)		
3	В	0.24	0/2679	0.43	0/3598		
4	С	0.24	0/2619	0.41	0/3544		
5	Е	0.24	0/1157	0.40	0/1553		
6	F	0.24	0/1846	0.39	0/2484		
7	G	0.24	0/1234	0.41	0/1671		
8	Н	0.23	0/1531	0.42	0/2062		
9	L	0.24	0/877	0.40	0/1179		
10	М	0.23	0/1056	0.39	0/1421		
11	Ν	0.23	0/1544	0.39	0/2065		
12	0	0.24	0/1585	0.39	0/2128		
13	Р	0.24	0/859	0.37	0/1160		
14	Q	0.25	0/1024	0.41	0/1385		
15	S	0.24	0/1468	0.41	0/1973		
16	V	0.24	0/933	0.42	0/1254		
17	W	0.23	0/1902	0.42	0/2564		
18	Y	0.24	0/995	0.41	0/1329		
19	b	2.02	6/3395~(0.2%)	0.42	1/4575~(0.0%)		
20	е	0.23	0/1030	0.41	0/1379		
21	f	0.25	0/868	0.43	0/1168		
22	h	0.24	0/938	0.37	0/1245		
23	i	0.24	0/599	0.38	0/793		
24	j	0.24	0/578	0.42	0/767		
25	r	0.23	0/638	0.36	0/837		
26	u	0.38	1/996~(0.1%)	0.80	5/1324~(0.4%)		
27	У	0.23	0/1722	0.44	0/2343		
All	All	0.46	$7/78133\ (0.0\%)$	0.64	$53/\overline{114436}\ (0.0\%)$		

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
8	Н	0	1
26	u	0	1
All	All	0	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	b	469	TYR	CD2-CE2	65.71	2.38	1.39
19	b	469	TYR	CD1-CE1	62.55	2.33	1.39
19	b	469	TYR	CE2-CZ	43.94	1.95	1.38
19	b	469	TYR	CE1-CZ	40.76	1.91	1.38
19	b	469	TYR	CG-CD2	30.58	1.78	1.39

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
26	u	106	ALA	N-CA-CB	-16.41	87.12	110.10
26	u	106	ALA	CB-CA-C	12.52	128.88	110.10
26	u	106	ALA	O-C-N	-10.85	105.35	122.70
1	1	988	U	N3-C4-O4	-8.72	113.30	119.40
1	1	988	U	C5-C4-O4	7.25	130.25	125.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	Н	22	SER	Peptide
26	u	106	ALA	Peptide

#### 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	ntiles
3	В	324/387~(84%)	307~(95%)	17~(5%)	0	100	100
4	$\mathbf{C}$	330/362~(91%)	310 (94%)	20~(6%)	0	100	100
5	Ε	140/176~(80%)	137 (98%)	3~(2%)	0	100	100
6	F	223/244~(91%)	214 (96%)	9~(4%)	0	100	100
7	G	152/256~(59%)	147 (97%)	5(3%)	0	100	100
8	Н	188/191 (98%)	181 (96%)	7 (4%)	0	100	100
9	L	106/199~(53%)	100 (94%)	6~(6%)	0	100	100
10	М	132/138~(96%)	131 (99%)	1 (1%)	0	100	100
11	Ν	173/204~(85%)	171 (99%)	2(1%)	0	100	100
12	Ο	195/199~(98%)	192 (98%)	3(2%)	0	100	100
13	Р	102/184~(55%)	102 (100%)	0	0	100	100
14	Q	129/186~(69%)	129 (100%)	0	0	100	100
15	S	168/172~(98%)	157 (94%)	11 (6%)	0	100	100
16	V	120/137~(88%)	118 (98%)	2(2%)	0	100	100
17	W	230/236~(98%)	224 (97%)	6 (3%)	0	100	100
18	Y	123/127~(97%)	123 (100%)	0	0	100	100
19	b	401/647~(62%)	383 (96%)	18 (4%)	0	100	100
20	е	123/130~(95%)	121 (98%)	2(2%)	0	100	100
21	f	104/107~(97%)	102 (98%)	2(2%)	0	100	100
22	h	110/120 (92%)	107 (97%)	3(3%)	0	100	100
23	i	72/100~(72%)	67 (93%)	5 (7%)	0	100	100
24	j	69/88~(78%)	69 (100%)	0	0	100	100
25	r	71/261~(27%)	63 (89%)	8 (11%)	0	100	100
26	u	114/199~(57%)	105 (92%)	9~(8%)	0	100	100
27	У	223/245~(91%)	217 (97%)	6(3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
All	All	4122/5295~(78%)	3977~(96%)	145 (4%)	0	100	100

There are no Ramachandran outliers to report.

#### 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	Perce	ntiles
3	В	278/323~(86%)	272~(98%)	6(2%)	52	72
4	С	271/289~(94%)	267~(98%)	4 (2%)	65	81
5	Ε	124/153~(81%)	123~(99%)	1 (1%)	81	89
6	F	189/205~(92%)	188 (100%)	1 (0%)	88	94
7	G	127/208~(61%)	125~(98%)	2(2%)	62	80
8	Н	170/171~(99%)	169~(99%)	1 (1%)	86	93
9	L	87/159~(55%)	84 (97%)	3~(3%)	37	64
10	М	106/109~(97%)	105 (99%)	1 (1%)	78	88
11	Ν	153/176~(87%)	151 (99%)	2(1%)	69	83
12	Ο	160/162~(99%)	158 (99%)	2(1%)	69	83
13	Р	89/146~(61%)	89 (100%)	0	100	100
14	Q	107/151~(71%)	106 (99%)	1 (1%)	78	88
15	S	155/156~(99%)	151~(97%)	4(3%)	46	69
16	V	96/105~(91%)	95~(99%)	1 (1%)	76	86
17	W	209/213~(98%)	205~(98%)	4(2%)	57	76
18	Y	108/110~(98%)	104 (96%)	4 (4%)	34	61
19	b	368/573~(64%)	352~(96%)	16 (4%)	29	58
20	е	$10\overline{8}/111~(97\%)$	107~(99%)	1 (1%)	78	88
21	f	90/91~(99%)	89~(99%)	1 (1%)	73	85
22	h	99/105~(94%)	98~(99%)	1 (1%)	76	86
23	i	61/82~(74%)	61 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
24	j	59/71~(83%)	58~(98%)	1 (2%)	60	79
25	r	65/229~(28%)	65~(100%)	0	100	100
26	u	101/180~(56%)	96~(95%)	5 (5%)	24	55
27	у	193/211~(92%)	191~(99%)	2(1%)	76	86
All	All	3573/4489~(80%)	3509~(98%)	64 (2%)	61	77

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 $5~{\rm of}~64$  residues with a non-rotameric side chain are listed below:

Mol	Chain	$\mathbf{Res}$	Type
26	u	6	CYS
26	u	100	ARG
15	S	12	ARG
14	Q	145	ASN
26	u	103	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such side chains are listed below:

Mol	Chain	Res	Type
19	b	217	GLN
27	у	83	HIS
8	Н	51	GLN
11	Ν	182	ASN
11	Ν	195	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1669/3396~(49%)	337 (20%)	35~(2%)
2	2	145/158~(91%)	24 (16%)	0
All	All	1814/3554~(51%)	361 (19%)	35~(1%)

5 of 361 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	U
1	1	3	U
1	1	7	С
1	1	14	U
1	1	20	А



5 of 35 RNA pucker outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
1	1	2857	С
1	1	2986	U
1	1	3218	А
1	1	649	А
1	1	644	G

#### 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)

Of 2 ligands modelled in this entry, 2 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)

There are no chain breaks in this entry.



# 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-12909. 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



6.1.2 Raw map



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



# 6.2 Central slices (i)

## 6.2.1 Primary map



X Index: 200



Y Index: 200



Z Index: 200

#### 6.2.2 Raw map



X Index: 200

Y Index: 200

Z Index: 200  $\,$ 

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: 169



Y Index: 184



Z Index: 150

#### 6.3.2 Raw map



X Index: 169

Y Index: 184



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



#### 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.021. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

#### 6.4.2 Raw map



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.

#### 6.5 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  $1023 \text{ nm}^3$ ; this corresponds to an approximate mass of 924 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 0.270  ${\rm \AA^{-1}}$ 



# 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)



\*Reported resolution corresponds to spatial frequency of 0.270  ${\rm \AA^{-1}}$ 



## 8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estimation criterion (FSC cut-off)		
Resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.68	4.24	3.74
Unmasked-calculated*	4.50	8.16	4.64

\*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 4.50 differs from the reported value 3.7 by more than 10 %



# 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12909 and PDB model 7OHU. Per-residue inclusion information can be found in section 3 on page 9.

## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.021 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 Atom inclusion (i)



At the recommended contour level, 96% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

