

# wwPDB EM Validation Summary Report (i)

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PDB ID	:	7ASM
EMDB ID	:	EMD-11900
Title	:	Staphylococcus aureus 50S after 30 minutes incubation at $37C$
Authors	:	Cimicata, G.; Bashan, A.; Yonath, A.
Deposited on	:	2020-10-27
Resolution	:	2.48  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 43
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	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

## 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 2.48 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{f Entries})$		
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	Ν	114	91%	9%
2	Е	206	90%	10%
3	А	2923	<b>6</b> 6% 25	5% •
4	В	115	57% 38%	
5	С	274	94%	5%
6	G	175	79%	21%
7	Н	145	81%	18% •

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Mol	Chain	Length	Quality of chain	
8	J	146	88%	12%
9	К	137	93%	7%
10	М	119	80%	19% •
11	О	116	89%	10% •
12	Р	102	87%	12% •
13	R	89	90%	10%
14	S	104	81%	15% •
15	Т	94	84%	16%
16	U	79	96%	•
17	W	67	97%	•
18	3	64	89%	11%
19	1	47	91%	9%
20	2	43	95%	5%
21	4	37	78%	19% •
22	D	215	81%	18% •
23	F	158	97%	•
24	Ι	122	83%	17%
25	Q	112	90%	10%
26	V	49	82%	16% ·
27	Х	58	90%	10%
28	Z	48	98%	•
29	L	120	88%	11% •

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# 2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 86149 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 protein called 50S ribosomal protein L19.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
1	Ν	114	Total 889	C 563	N 175	0 151	0	0

• Molecule 2 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues		At	oms	AltConf	Trace		
2	Е	206	Total 1572	C 986	N 288	O 296	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues				AltConf	Trace		
3	А	2834	Total 60769	C 27128	N 11118	O 19689	Р 2834	0	0

• Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues		A	AltConf	Trace			
4	В	115	Total 2448	C 1094	N 436	O 803	Р 115	0	0

• Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues		Ate	AltConf	Trace			
5	С	274	Total 2094	C 1303	N 415	0 371	${ m S}{ m 5}$	0	0

• Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	G	175	Total 1263	C 791	N 240	O 229	${ m S} { m 3}$	0	0



• Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues		At	oms	AltConf	Trace		
7	Н	145	Total 1149	C 717	N 211	0 218	${ m S} { m 3}$	0	0

• Molecule 8 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues		At	AltConf	Trace			
8	J	146	Total	C 674	N 214	0	S 1	0	0
			1080	074	214	197	T		

• Molecule 9 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues		At	oms			AltConf	Trace
9	K	137	Total 1071	C 689	N 203	0 175	$\frac{S}{4}$	0	0

• Molecule 10 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
10	М	119	Total 882	C 549	N 174	O 159	0	0

• Molecule 11 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues		At	oms	AltConf	Trace		
11	Ο	116	Total 942	C 593	N 189	0 156	${S \atop 4}$	0	0

• Molecule 12 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues		At	AltConf	Trace			
12	Р	102	Total 790	C 503	N 142	0 144	S 1	0	0

• Molecule 13 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues		At	AltConf	Trace			
13	R	89	Total 715	C 453	N 127	0 131	${S \atop 4}$	0	0

• Molecule 14 is a protein called 50S ribosomal protein L24.



Mol	Chain	Residues		At	AltConf	Trace			
14	S	100	Total 755	C 477	N 139	0 138	S 1	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	49	GLN	ARG	conflict	UNP A0A6K7SSC4

• Molecule 15 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues		Ato	$\mathbf{ms}$	AltConf	Trace	
15	Т	94	Total 722	C 463	N 130	O 129	0	0

• Molecule 16 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues		Ato	ms	AltConf	Trace	
16	U	79	Total 597	C 369	N 117	0 111	0	0

• Molecule 17 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues		Ato	ms		AltConf	Trace
17	W	67	Total 541	C 333	N 102	O 106	0	0

• Molecule 18 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues		At	oms			AltConf	Trace
18	3	64	Total 521	C 324	N 113	O 82	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 19 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1	47	Total	С	N 70	0	S	0	0
			390	238	78	70	4		

• Molecule 20 is a protein called 50S ribosomal protein L34.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	2	43	Total 367	C 225	N 89	O 52	S 1	0	0

• Molecule 21 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4	37	Total 295	C 186	N 60	0 44	${ m S}{ m 5}$	0	0

• Molecule 22 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	215	Total 1627	C 1018	N 299	O 305	$\frac{S}{5}$	0	0

• Molecule 23 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	F	158	Total 778	C 462	N 158	O 158	0	0

• Molecule 24 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Ι	122	Total 918	C 572	N 174	0 168	$\frac{S}{4}$	0	0

• Molecule 25 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	112	Total 854	С 534	N 164	0 153	${ m S} { m 3}$	0	0

• Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	V	49	Total 379	C 234	N 82	O 63	0	0

• Molecule 27 is a protein called 50S ribosomal protein L30.



Mol	Chain	Residues	Atoms				AltConf	Trace
27	Х	58	Total 449	C 280	N 85	O 84	0	0

• Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ζ	48	Total 360	C 222	N 77	O 59	${ m S} { m 2}$	0	0

• Molecule 29 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L	120	Total 925	C 573	N 181	0 170	S 1	0	0

• Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
30	А	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: 50S ribosomal protein L19











• Molecule 8: 50S ribosomal protein	L15	
Chain J:	88%	12%
M1 V19 C20 C20 C20 C20 C20 C20 C20 C20 C20 C20	1122 V123 1146	
• Molecule 9: 50S ribosomal protein	L16	
Chain K:	93%	7%
M1 G30 G30 G30 G43 G45 A1 C A1 C A1 C A1 C A1 C A1 C A1 C A1 C A4 A5 A6 A6 A6 A6 A6 A6 A6 A6 A6 A6		
• Molecule 10: 50S ribosomal protein	n L18	
Chain M: 80°	%	19% •
M1 R17 R17 R19 R19 R19 R31 R32 R33 R33 R33 R33 R33 R33 R33	<b>F.1</b> L72 K75 K82 K82 K82 K96 K96 K99 K113 F119	
• Molecule 11: 50S ribosomal protein	n L20	
Chain O:	89%	10% •
P2 N4 N4 N4 N4 N4 N6 N6 N6 N6 N6 N9 N9 N9 N9 N9 N9 N9 N9 N9 N9 N9 N9 N9	2117	
• Molecule 12: 50S ribosomal protein	n L21	
Chain P:	87%	12% •
M1 72 73 73 740 751 752 752 752 752 752 752 752 752 752 752		
• Molecule 13: 50S ribosomal protein	n L23	
Chain R:	90%	10%
E2 E43 E43 F44 F44 F43 F44 F43 F44 F45 F45 F45 F71 F71 F71 F71 F71		
• Molecule 14: 50S ribosomal protein	n L24	
Chain S: 819	6	15% •
MET MET 13 13 14 14 14 14 14 14 14 14 14 14 14 14 14	A 94 K 95 S 97 C 98 N 104	
• Molecule 15: 50S ribosomal protein	n L25	

Chain T:	84%	16%
A2 S3 L4 K12 C25 C25 C25 D44 E45 E47 E47	149 149 151 151 151 194 194 194	
• Molecule 16: 50	OS ribosomal protein L27	
Chain U:	96%	
V15 K19 R22 R22 A93		
• Molecule 17: 50	OS ribosomal protein L29	
Chain W:	97%	•
K2 M68 M68		
• Molecule 18: 50	OS ribosomal protein L35	
Chain 3:	89%	11%
P2 L22 D54 M55 K57 K57 K59 K59	M M M	
• Molecule 19: 50	OS ribosomal protein L33	
Chain 1:	91%	9%
R2 C9 C12 T19 R24 *		
• Molecule 20: 50	OS ribosomal protein L34	
Chain 2:	95%	5%
V2 H17 S44		
• Molecule 21: 50	OS ribosomal protein L36	
Chain 4:	78%	19% ·
M1 611 612 613 614 716 716 716 716 716 716 716 716 716 716		

• Molecule 22: 50S ribosomal protein L3



Chain D:	81%	18% •
12 K3 L6 113 013 013 055 N33 N33 N33 N33 N33 N33 N33	P84 P84 V94 V107 V107 V107 V107 V108 V108 V128 C128 C128 C128 C128 C128 C128 C128 C	5145 H148 4154 4155 1159 5158 1158 7158 7158 717 717 717 7177 717
D189 1194 1194 1194 1194 1194 1194 1194 1		
• Molecule 23: 50S ril	bosomal protein L5	
Chain F:	97%	<del>.</del>
K19 A43 V44 Q45 Q45 K72 S73 A75 A75 T76	F1 F	S147 K148 V149 G151 P176
• Molecule 24: 50S ril	bosomal protein L14	
Chain I:	83%	17%
M1 44 65 85 87 87 87 120 121 121 121 135 041	165 870 876 177 177 177 177 177 179 198 198 111 1117 1117	
• Molecule 25: 50S ril	bosomal protein L22	
Chain Q:	90%	10%
M1 E2 R11 D22 R25 R25 R25 R25 R26 R26 R26 R26 R26 R26 R26 R26 R26 R26	R92 X98 8108 8112	
• Molecule 26: 50S ril	bosomal protein L28	
Chain V:	82%	16% ·
412 819 819 828 827 828 828 828 828 846 846 846 846 846 846 846 846 846 84	200 2	
• Molecule 27: 50S ril	bosomal protein L30	
Chain X:	90%	10%
A2 16 11 12 12 12 12 12 12 12 12 12 12 12 12		
• Molecule 28: 50S ril	bosomal protein L32	
Chain Z:	98%	<del>.</del>





• Molecule 29: 50S ribosomal protein L17

	L:	88%	11% •
S58 T65 L66 R67	V44 L50	K102 K105 V122	



# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.085	Depositor
Minimum map value	-0.030	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0037	Depositor
Map size (Å)	308.88, 308.88, 308.88	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85800004, 0.85800004, 0.85800004	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: 5MU, MG, 2MA  $\,$ 

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	Bond angles	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	Ν	0.52	0/901	0.51	0/1209
2	Е	0.51	0/1595	0.53	0/2154
3	А	1.18	16/67978~(0.0%)	0.96	112/106007~(0.1%)
4	В	0.73	0/2736	0.80	1/4261~(0.0%)
5	С	0.50	0/2129	0.52	0/2858
6	G	0.32	0/1281	0.48	0/1735
7	Н	0.59	0/1171	0.61	1/1577~(0.1%)
8	J	0.50	0/1100	0.54	0/1467
9	Κ	0.52	0/1095	0.50	0/1472
10	М	0.37	0/891	0.50	0/1194
11	0	0.59	0/954	0.51	0/1264
12	Р	0.58	0/800	0.56	0/1070
13	R	0.52	0/723	0.50	0/966
14	S	0.43	0/763	0.51	0/1018
15	Т	0.40	0/730	0.48	0/981
16	U	0.59	0/603	0.52	0/802
17	W	0.44	0/542	0.48	0/722
18	3	0.47	0/526	0.50	0/690
19	1	0.29	0/395	0.43	0/530
20	2	0.60	0/371	0.67	1/484~(0.2%)
21	4	0.40	0/298	0.48	0/392
22	D	0.59	0/1651	0.67	0/2215
23	F	0.25	0/777	0.43	0/1079
24	Ι	0.50	0/925	0.54	0/1242
25	Q	0.53	0/862	0.57	0/1161
26	V	0.41	0/384	0.55	0/515
27	Х	0.48	0/451	0.52	0/606
28	Ζ	0.50	0/366	0.53	0/489
29	L	0.53	0/929	0.61	0/1244
All	All	1.04	16/93927~(0.0%)	0.88	115/141404~(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
5	С	0	1
7	Н	0	1
10	М	0	1
12	Р	0	1
21	4	0	1
22	D	0	3
29	L	0	1
All	All	0	9

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	666	A	N9-C4	-7.23	1.33	1.37
3	А	1228	А	N9-C4	-6.71	1.33	1.37
3	А	650	U	C2-N3	-6.47	1.33	1.37
3	А	1228	А	N3-C4	-6.32	1.31	1.34
3	А	721	А	N9-C4	-6.18	1.34	1.37

The worst 5 of 115 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	576	U	N3-C2-O2	-10.60	114.78	122.20
3	А	1599	G	N3-C2-N2	-10.00	112.90	119.90
3	А	1599	G	N3-C4-N9	-9.88	120.07	126.00
3	А	557	G	O4'-C1'-N9	8.93	115.35	108.20
3	А	2845	G	C2-N3-C4	-8.84	107.48	111.90

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	4	11	CYS	Peptide
5	С	233	GLY	Peptide
7	Н	76	TYR	Peptide
10	М	68	THR	Peptide
12	Р	50	ALA	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	N	889	0	937	7	0
2	Е	1572	0	1619	14	0
3	А	60769	0	30546	501	0
4	В	2448	0	1239	35	0
5	С	2094	0	2205	11	0
6	G	1263	0	1232	25	0
7	Н	1149	0	1145	17	0
8	J	1086	0	1125	10	0
9	Κ	1071	0	1123	7	0
10	М	882	0	900	19	0
11	0	942	0	1014	10	0
12	Р	790	0	830	10	0
13	R	715	0	748	6	0
14	S	755	0	803	10	0
15	Т	722	0	766	9	0
16	U	597	0	604	2	0
17	W	541	0	563	2	0
18	3	521	0	586	5	0
19	1	390	0	394	3	0
20	2	367	0	415	1	0
21	4	295	0	339	7	0
22	D	1627	0	1667	20	0
23	F	778	0	348	3	0
24	Ι	918	0	981	13	0
25	Q	854	0	914	8	0
26	V	379	0	400	6	0
27	Х	449	0	491	4	0
28	Ζ	360	0	358	1	0
29	L	925	0	975	10	0
30	A	1	0	0	0	0
All	All	86149	0	55267	721	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 5.

The worst 5 of 721 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)
3:A:1521:A:N6	3:A:1559:G:H1	1.50	1.10
3:A:1514:A:N1	3:A:1566:G:N2	2.08	1.01
3:A:2128:G:H1	3:A:2215:U:H3	1.00	0.95
3:A:2127:G:H1	3:A:2216:U:H3	1.13	0.94
3:A:1578:A:N6	3:A:1591:G:N7	2.15	0.93

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	Perce	entiles
1	Ν	112/114~(98%)	106 (95%)	6 (5%)	0	100	100
2	Е	204/206~(99%)	197~(97%)	7 (3%)	0	100	100
5	С	272/274~(99%)	259~(95%)	13 (5%)	0	100	100
6	G	173/175~(99%)	155~(90%)	18 (10%)	0	100	100
7	Н	143/145~(99%)	124 (87%)	18 (13%)	1 (1%)	22	36
8	J	144/146~(99%)	135 (94%)	8 (6%)	1 (1%)	22	36
9	Κ	135/137~(98%)	126 (93%)	9 (7%)	0	100	100
10	М	117/119~(98%)	104 (89%)	12 (10%)	1 (1%)	17	29
11	Ο	114/116~(98%)	111 (97%)	3 (3%)	0	100	100
12	Р	100/102~(98%)	92 (92%)	7 (7%)	1 (1%)	15	26
13	R	87/89~(98%)	80 (92%)	7 (8%)	0	100	100
14	S	96/104~(92%)	81 (84%)	15 (16%)	0	100	100
15	Т	92/94~(98%)	87~(95%)	5 (5%)	0	100	100
16	U	77/79~(98%)	73~(95%)	4 (5%)	0	100	100
17	W	65/67~(97%)	61 (94%)	4 (6%)	0	100	100
18	3	62/64~(97%)	58 (94%)	4 (6%)	0	100	100

Continued on next page...



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
19	1	45/47~(96%)	44 (98%)	1 (2%)	0	100	100
20	2	41/43~(95%)	39~(95%)	2(5%)	0	100	100
21	4	35/37~(95%)	35~(100%)	0	0	100	100
22	D	213/215~(99%)	179 (84%)	27 (13%)	7 (3%)	4	4
23	F	156/158~(99%)	141 (90%)	15 (10%)	0	100	100
24	Ι	120/122~(98%)	107 (89%)	13 (11%)	0	100	100
25	Q	110/112~(98%)	107~(97%)	3(3%)	0	100	100
26	V	47/49~(96%)	45~(96%)	2 (4%)	0	100	100
27	Х	56/58~(97%)	55~(98%)	1 (2%)	0	100	100
28	Z	46/48~(96%)	43~(94%)	3~(6%)	0	100	100
29	L	118/120 (98%)	106 (90%)	11 (9%)	1 (1%)	19	33
All	All	2980/3040 (98%)	2750 (92%)	218 (7%)	12 (0%)	38	52

Continued from previous page...

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	$\mathbf{Res}$	Type
22	D	130	ALA
29	L	67	ARG
22	D	158	SER
22	D	164	PHE
8	J	36	LYS

#### 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
1	Ν	93/100~(93%)	93 (100%)	0	100 100
2	Ε	168/168~(100%)	167~(99%)	1 (1%)	86 94
5	С	221/221~(100%)	221 (100%)	0	100 100
6	G	124/153~(81%)	122 (98%)	2(2%)	62 82
7	Н	123/123~(100%)	123 (100%)	0	100 100

Continued on next page...



Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
8	J	109/112~(97%)	109 (100%)	0	100	100
9	Κ	108/114~(95%)	108 (100%)	0	100	100
10	М	83/95~(87%)	82 (99%)	1 (1%)	71	87
11	Ο	96/96~(100%)	95~(99%)	1 (1%)	76	89
12	Р	84/86~(98%)	82 (98%)	2 (2%)	49	72
13	R	78/80~(98%)	78 (100%)	0	100	100
14	S	81/89~(91%)	81 (100%)	0	100	100
15	Т	78/82~(95%)	78 (100%)	0	100	100
16	U	59/62~(95%)	59 (100%)	0	100	100
17	W	58/60~(97%)	58 (100%)	0	100	100
18	3	55/55~(100%)	55 (100%)	0	100	100
19	1	44/45~(98%)	44 (100%)	0	100	100
20	2	39/39~(100%)	39 (100%)	0	100	100
21	4	35/35~(100%)	35 (100%)	0	100	100
22	D	173/173~(100%)	167 (96%)	6 (4%)	36	59
24	Ι	100/100~(100%)	99~(99%)	1 (1%)	76	89
25	Q	89/91~(98%)	89 (100%)	0	100	100
26	V	39/41~(95%)	38~(97%)	1 (3%)	46	70
27	Х	52/52~(100%)	52 (100%)	0	100	100
28	Z	35/44~(80%)	35 (100%)	0	100	100
29	L	94/101~(93%)	93~(99%)	1 (1%)	73	88
All	All	2318/2417~(96%)	2302 (99%)	16 (1%)	84	93

Continued from previous page...

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	V	27	ARG
24	Ι	122	LEU
22	D	107	VAL
22	D	173	MET
22	D	25	VAL

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such side chains are listed below:



Mol	Chain	Res	Type
24	Ι	110	ASN
25	Q	60	HIS
10	М	43	GLN
10	М	15	HIS
26	V	16	ASN

#### 5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	А	2823/2923~(96%)	445 (15%)	12 (0%)
4	В	114/115~(99%)	13 (11%)	0
All	All	2937/3038~(96%)	458 (15%)	12 (0%)

5 of 458 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	А	10	А
3	А	28	А
3	А	34	U
3	А	36	G
3	А	43	А

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	А	2528	С
3	А	2629	А
3	А	2900	С
3	А	2840	А
3	А	872	U

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



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm sths}$	E	ond ang	gles
IVIOI	Moi Type Chain		nes Lilli		Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	2MA	А	2530	3	17,25,26	2.22	5 (29%)	17,37,40	1.47	3 (17%)
3	5MU	А	792	3	19,22,23	4.74	7 (36%)	28,32,35	3.81	11 (39%)
3	5MU	А	1966	3	19,22,23	4.75	7 (36%)	28,32,35	<mark>3.72</mark>	9 (32%)

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
3	2MA	А	2530	3	-	2/3/25/26	0/3/3/3
3	5MU	А	792	3	-	2/7/25/26	0/2/2/2
3	5MU	А	1966	3	-	0/7/25/26	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	А	792	5MU	C2-N1	10.82	1.55	1.38
3	А	1966	5MU	C2-N1	10.55	1.55	1.38
3	А	1966	5MU	C6-N1	10.27	1.55	1.38
3	А	792	5MU	C6-N1	10.06	1.55	1.38
3	А	1966	5MU	C4-C5	9.58	1.60	1.44

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
3	А	792	5MU	C5-C4-N3	12.67	126.12	115.31
3	А	1966	5MU	C5-C4-N3	12.42	125.91	115.31
3	А	792	5MU	C5-C6-N1	-10.70	112.34	123.34
3	А	1966	5MU	C5-C6-N1	-10.55	112.48	123.34
3	А	792	5MU	O4-C4-C5	-5.79	118.19	124.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	792	5MU	C3'-C4'-C5'-O5'
3	А	792	5MU	O4'-C4'-C5'-O5'
3	А	2530	2MA	O4'-C4'-C5'-O5'
3	А	2530	2MA	C3'-C4'-C5'-O5'



There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	2530	2MA	1	0
3	А	792	5MU	1	0

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is 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-11900. 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: 180



Y Index: 180



Z Index: 180

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: 193

Y Index: 176

Z Index: 173

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 0.0037. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 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 916  $\text{nm}^3$ ; this corresponds to an approximate mass of 827 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 0.403  ${\rm \AA^{-1}}$ 



# 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-11900 and PDB model 7ASM. 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 0.0037 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 (0.0037).



#### 9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.0037) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9622	0.6000	
1	0.7787	0.5820	
2	0.9913	0.6820	
3	0.9920	0.6650	
4	0.9792	0.6120	
А	0.9586	0.5980	
В	0.9963	0.5330	
С	0.9882	0.6520	
D	0.9607	0.6240	
Е	0.9851	0.6410	
F	0.8368	0.3580	
G	0.9466	0.5060	
Н	0.9732	0.6380	
Ι	0.9743	0.6290	
J	0.9887	0.6420	
К	0.9884	0.6320	
L	0.9832	0.6360	
М	0.9674	0.5040	
Ν	0.9523	0.6200	
0	0.9857	0.6640	
Р	0.9833	0.6350	
Q	0.9820	0.6610	
R	0.9757	0.6230	
S	0.9759	0.5770	
Т	0.9661	0.5790	
U	0.9810	0.6460	
V	0.9781	0.6060	
W	0.9638	0.5910	
X	0.9773	0.6380	
Z	0.9971	0.6100	



1.0

