

wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 05:17 pm GMT

PDB ID		6SWA
EMDB ID	:	EMD_10321
	·	EMID-10521
Title	:	Mus musculus brain neocortex ribosome 60S bound to Ebp1
Authors	:	Kraushar, M.L.; Sprink, T.
Deposited on	:	2019-09-20
Resolution	:	3.10 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 (1)) were used in the production of this report:

:	0.0.1. dev 43
:	4.02b-467
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	1.9.9
:	Engh & Huber (2001)
:	Parkinson et al. (1996)
:	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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM\ structures}\ (\#{ m Entries})$
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	А	252	99%
2	В	394	99% ·
3	С	363	9%
4	D	294	11%
5	Е	194	99%
6	F	234	11%
7	G	234	99%
8	Н	191	6%100%

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33

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Chain Length Quality of chain Mol 11% 9 Ι 21199% 21% 10 J 16999% 17% 11 Κ 205100% 5% 12L 139100% 13М 203100% • 14Ν 19599% 5% Ο 15153100% 6% Р 16185100% ÷ Q 1717599% 6% 18R 15799% 17% \mathbf{S} 1910199% 6% Т 2012999% 11% 21U 62100% 12% 22V 11898% 5% W 127 2399% 10% 24Х 13498% 5% Υ 25147100% 18% Ζ 2668100% 6% 2797 \mathbf{a} 100% 10% 28b 10699% 8% 29129 \mathbf{c} 99% 5% 30 109d 100% 8% 31 114е 98% 10% 32f 122100% 17%

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100%

Mol	Chain	Length	Quality of chain	
34	h	84	100%	
35	i	69	23%	
36	j	50	14%	
37	k	50	8%	
38	1	25	16%	
39	m	105	16%	
40	n	91	11%	
41	О	184	15% 99%	·
42	р	122	6% 99%	•
43	q	3612	9% 84%	16%
44	r	157	11% 79%	21%
45	s	119	87%	13%
46	t	353	58% 92%	7%

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2 Entry composition (i)

There are 48 unique types of molecules in this entry. The entry contains 138160 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 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	А	252	Total 1930	C 1209	N 395	O 320	S 6	0	0

• Molecule 2 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues		At	AltConf	Trace			
2	В	394	Total 3178	C 2024	N 597	0 543	S 14	0	0

• Molecule 3 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues		At	AltConf	Trace			
3	С	363	Total 2897	C 1822	N 578	0 482	S 15	0	0

• Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues		At	AltConf	Trace			
4	D	294	Total 2395	C 1509	N 442	0 430	S 14	0	0

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

Mol	Chain	Residues		Ate		AltConf	Trace		
5	Е	194	Total 1576	C 1008	N 296	O 270	${ m S} { m 2}$	0	0

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

Mol	Chain	Residues		Ate		AltConf	Trace		
6	F	234	Total 1947	C 1251	N 375	O 313	S 8	0	0



• Molecule 7 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues		Ate	AltConf	Trace			
7	G	234	Total 1879	C 1197	N 361	0 317	${f S}$ 4	0	0

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

Mol	Chain	Residues		At	oms			AltConf	Trace
8	Н	191	Total 1527	C 960	N 285	0 276	S 6	0	0

• Molecule 9 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues		At	AltConf	Trace			
9	Ι	208	Total 1692	C 1074	N 327	0 278	S 13	0	0

• Molecule 10 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues		At	oms	AltConf	Trace		
10	J	169	Total 1353	C 855	N 252	0 240	S 6	0	0

• Molecule 11 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues		Ate	AltConf	Trace			
11	K	205	Total 1660	C 1038	N 342	0 276	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 12 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues		At	oms			AltConf	Trace
12	L	139	Total 1143	C 732	N 221	0 183	${f S}7$	0	0

• Molecule 13 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues		Ate	oms			AltConf	Trace
13	М	203	Total 1701	C 1072	N 359	O 266	${S \atop 4}$	0	0

• Molecule 14 is a protein called 60S ribosomal protein L13a.



Mol	Chain	Residues		At	\mathbf{oms}			AltConf	Trace
14	Ν	195	Total 1599	C 1029	N 314	O 250	S 6	0	0

• Molecule 15 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues		At	oms	AltConf	Trace		
15	0	153	Total 1242	C 777	N 241	0 215	S 9	0	0

• Molecule 16 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues		At	oms	AltConf	Trace		
16	Р	185	Total 1504	C 941	N 312	0 247	$\frac{S}{4}$	0	0

• Molecule 17 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues		\mathbf{A}	toms			AltConf	Trace
17	Q	175	Total 1447	C 920	N 283	O 233	S 11	0	0

• Molecule 18 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues		At	oms	AltConf	Trace		
18	R	157	Total 1284	C 815	N 251	O 213	${ m S}{ m 5}$	0	0

• Molecule 19 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues		At	oms	AltConf	Trace		
19	S	101	Total 826	C 529	N 145	O 150	${S \over 2}$	0	0

• Molecule 20 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues		At	oms			AltConf	Trace
20	Т	129	Total 969	C 613	N 182	O 169	${S \atop 5}$	0	0

• Molecule 21 is a protein called 60S ribosomal protein L24.



Mol	Chain	Residues		Ate	oms			AltConf	Trace
21	U	62	Total 520	C 332	N 102	0 84	${ m S} { m 2}$	0	0

• Molecule 22 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
22	V	118	Total 966	C 618	N 181	0 166	S 1	0	0

• Molecule 23 is a protein called Ribosomal protein L26.

Mol	Chain	Residues		At	oms			AltConf	Trace
23	W	127	Total 1064	C 668	N 216	0 177	${ m S} { m 3}$	0	0

• Molecule 24 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues		At	oms			AltConf	Trace
24	Х	134	Total 1103	С 712	N 207	0 181	${ m S} { m 3}$	0	0

• Molecule 25 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues		At	oms			AltConf	Trace
25	Y	147	Total 1164	C 736	N 239	0 185	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0

• Molecule 26 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues		At	oms			AltConf	Trace
26	Z	68	Total 558	C 344	N 122	O 90	${ m S} { m 2}$	0	0

• Molecule 27 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues		At	oms			AltConf	Trace
27	a	97	Total 753	C 478	N 133	0 135	${f S}{7}$	0	0

• Molecule 28 is a protein called 60S ribosomal protein L31.



Mol	Chain	Residues		At	oms			AltConf	Trace
28	b	106	Total 879	C 555	N 170	O 152	${ m S} { m 2}$	0	0

• Molecule 29 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues		At	oms			AltConf	Trace
29	с	129	Total 1064	C 673	N 220	O 166	${ m S}{ m 5}$	0	0

• Molecule 30 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues		At	oms	AltConf	Trace		
30	d	109	Total 876	C 555	N 174	0 143	$\frac{S}{4}$	0	0

• Molecule 31 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues		At	oms	AltConf	Trace		
31	е	114	Total 906	C 565	N 187	0 148	S 6	0	0

• Molecule 32 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues		At	oms	AltConf	Trace		
32	f	122	Total 1015	C 643	N 204	0 167	S 1	0	0

• Molecule 33 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues		At	oms			AltConf	Trace
33	g	98	Total 802	C 499	N 168	O 130	${ m S}{ m 5}$	0	0

• Molecule 34 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues		At	oms	AltConf	Trace		
34	h	84	Total 689	C 423	N 152	O 109	${f S}{5}$	0	0

• Molecule 35 is a protein called 60S ribosomal protein L38.



Mol	Chain	Residues		At	oms			AltConf	Trace
35	i	69	Total 568	$\begin{array}{c} \mathrm{C} \\ 365 \end{array}$	N 103	O 99	S 1	0	0

• Molecule 36 is a protein called Ribosomal protein L39.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
36	j	50	Total 443	C 281	N 98	O 63	S 1	0	0

• Molecule 37 is a protein called 60S ribosomal protein L40.

Mol	Chain	Residues		Atc	\mathbf{ms}	AltConf	Trace		
37	k	50	Total 411	C 254	N 87	O 64	S 6	0	0

• Molecule 38 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues		Ato	\mathbf{ms}	AltConf	Trace		
38	1	25	Total	С	Ν	Ο	S	0	0
00	1	20	240	145	64	28	3	0	0

• Molecule 39 is a protein called Ribosomal protein L36A.

Mol	Chain	Residues		At	oms	AltConf	Trace		
39	m	105	Total 863	C 542	N 175	O 140	S 6	0	0

• Molecule 40 is a protein called Ribosomal protein L37a.

Mol	Chain	Residues		At	oms			AltConf	Trace
40	n	91	Total 708	С 445	N 136	O 120	${ m S} 7$	0	0

• Molecule 41 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues		At	oms			AltConf	Trace
41	О	184	Total 1542	C 955	N 332	0 246	S 9	0	0

• Molecule 42 is a protein called 60S ribosomal protein L28.



Mol	Chain	Residues		At	oms			AltConf	Trace
42	р	122	Total 980	C 606	N 204	O 165	${f S}{5}$	0	0

• Molecule 43 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues			Atoms			AltConf	Trace
43	q	3612	Total 77430	C 34484	N 14158	O 25176	Р 3612	0	0

• Molecule 44 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	r	157	Total 3337	C 1489	N 587	0 1104	Р 157	0	0

• Molecule 45 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	s	119	Total 2541	C 1132	N 454	O 836	Р 119	0	0

• Molecule 46 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms				AltConf	Trace	
46	t	353	Total 2739	C 1729	N 470	O 523	S 17	0	0

• Molecule 47 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
47	В	1	Total Mg 1 1	0
47	K	1	Total Mg 1 1	0
47	М	1	Total Mg 1 1	0
47	Р	1	Total Mg 1 1	0
47	W	1	Total Mg 1 1	0
47	b	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms	AltConf
47	С	1	Total Mg 1 1	0
47	1	1	Total Mg 1 1	0
47	q	223	Total Mg 223 223	0
47	r	7	Total Mg 7 7	0
47	s	9	TotalMg99	0

• Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
48	h	1	Total Zn 1 1	0
48	m	1	Total Zn 1 1	0
48	n	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: 60S ribosomal protein L8



•	Molecule 6:	60S	ribosomal	protein	L7
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• Molecule 18: 60S ribosomal protein L21



Chain R:	99% .
T2 K6 K1 K102 K103 K107 C113 C123 C123 C123	E1 12
• Molecule 19: 60S ribosom	nal protein L22
Chain S:	99%
K16 q17 E30 D31 G32 B35 C45 E45 C51 K52 A53 C54 C54 C54 C54 C54 C54	CG58 CG59 E111 C116
• Molecule 20: 60S riboson	nal protein L23
Chain T:	99%
412 815 815 815 899 899 8138 8138 8138 8138 1139	
• Molecule 21: 60S riboson	nal protein L24
Chain U:	100%
K2 V3 E4 R23 T24 D25 B37 L41 L41 C41 C41 C41 C41 C41 C41 C41 C41 C41 C	
• Molecule 22: 60S riboson	nal protein L23a
Chain V:	98%
K39 140 855 867 867 867 867 868 872 872 872 872 872 872 872 872 872 87	1147 148 148 156 156
• Molecule 23: Ribosomal	protein L26
Chain W:	99%
M1 R17 E37 D52 D52 E83 E83 E88 E88 E88 E88 C111	
• Molecule 24: 60S riboson	nal protein L27
Chain X:	98%
K3 K6 B35 A56 M57 G58 G58 G58 B88 B192 D103 D103	K107 R112 B113 K126 K128 K128 K128 F136 F136









• Molecule 38: 60S ribosomal protein L41



Chain l:	100%	
MI K8 R18 R18 S24 K25		
• Molecule 39:	Ribosomal protein L36A	
Chain m:	100%	•
V2 K6 Q25 V26 K27 K27 B31	Q36 R57 R2 R2 P96 K397 K397 K397 K100 G101 Q102 F106 F106	
• Molecule 40:	Ribosomal protein L37a	
Chain n:	100%	
A2 K3 K6 K7 K48 R485	E88 8.3 1.6 2.3 1.6 2.3 1.6 2.4 4 5.0 1.6 2.4 5.0 1.6 2.5 1.6 5.0 1.6 5.0 5.0 1.6 5.0 5.0 1.6 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0 5.0	
• Molecule 41:	60S ribosomal protein L19	
Chain o:	99%	
22 D25 D47 D148 X149 A150 A150 A150	D157 E160 A161 A161 A163 A163 A163 A163 A163 A163	
• Molecule 42:	60S ribosomal protein L28	
Chain p:	99%	
22 A55 D56 R71 R79 K79	<mark>1123 → ●</mark>	
• Molecule 43:	28S ribosomal RNA	
Chain q:	84% 16%	
C1 U8 A10 A25 G32 A39	A42 648 A65 A65 A65 A65 A65 A65 A65 A16 C72 C72 A16 C72 C72 C72 A16 C72 C72 A16 C72 C72 A15 C72 C72 A15 C72 C72 A15 C72 C72 A15 C72 C72 C72 C72 C72 C72 C72 C72	C170 C173 C173 C174 C177 C177 C177 C177
C178 C179 C180 C180 C182 C182 C183 C183 C183 C185 C185 C185	U205 U206 U206 A209 A209 C212 C213 C214 A215 C213 C214 A215 C213 C214 A215 C214 A215 C213 C214 A215 C223 C224 C250 C250 C250 C250 C250 C250 C255 C256 C251	C334 U351 C367 C367 A370
A380 A380 A390 A390 A390 C407 C407 C407 C425 C425	C443 6444 6445 6445 6445 6449 6465 6465 6465	C511 G512 C513 C513 C514 C515 C515 C515 C516 C517 G620 G630 G630













4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	208206	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 $(e^-/\text{\AA}^2)$	31.78	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	20.986	Depositor
Minimum map value	-10.475	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.898	Depositor
Recommended contour level	4.0	Depositor
Map size (Å)	477.612, 477.612, 477.612	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3267, 1.3267, 1.3267	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, MG

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	Bond	lengths	Bond angles		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.24	0/1968	0.44	0/2639	
2	В	0.24	0/3245	0.42	0/4343	
3	С	0.23	0/2951	0.39	0/3961	
4	D	0.24	0/2440	0.39	0/3266	
5	Е	0.24	0/1607	0.43	0/2159	
6	F	0.24	0/1983	0.38	0/2641	
7	G	0.24	0/1913	0.42	0/2577	
8	Н	0.25	0/1545	0.44	0/2076	
9	Ι	0.24	0/1730	0.40	0/2311	
10	J	0.24	0/1376	0.41	0/1841	
11	K	0.24	0/1691	0.41	0/2264	
12	L	0.24	0/1165	0.39	0/1558	
13	М	0.23	0/1746	0.39	0/2338	
14	N	0.24	0/1629	0.39	0/2178	
15	0	0.23	0/1268	0.41	0/1700	
16	Р	0.23	0/1528	0.40	0/2038	
17	Q	0.24	0/1486	0.42	0/1994	
18	R	0.24	0/1312	0.41	0/1752	
19	S	0.25	0/840	0.43	0/1126	
20	Т	0.25	0/983	0.42	0/1319	
21	U	0.24	0/533	0.37	0/710	
22	V	0.24	0/983	0.41	0/1323	
23	W	0.26	0/1081	0.42	0/1439	
24	Х	0.25	0/1126	0.39	0/1502	
25	Y	0.24	0/1193	0.40	0/1593	
26	Z	0.23	0/568	0.37	0/750	
27	a	0.24	0/764	0.41	0/1026	
28	b	0.23	0/894	0.43	0/1204	
29	с	0.23	0/1082	0.40	0/1443	
30	d	0.25	0/895	0.43	0/1198	
31	e	0.24	0/916	0.42	0/1221	
32	f	0.23	0/1023	0.38	0/1350	



Mal	Mol Chain		lengths	Bond angles		
MOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5	
33	g	0.23	0/813	0.38	0/1078	
34	h	0.26	0/703	0.44	0/929	
35	i	0.24	0/574	0.41	0/760	
36	j	0.22	0/453	0.39	0/599	
37	k	0.30	0/417	0.46	0/553	
38	1	0.21	0/241	0.32	0/305	
39	m	0.24	0/877	0.40	0/1156	
40	n	0.24	0/718	0.40	0/953	
41	0	0.22	0/1558	0.36	0/2059	
42	р	0.23	0/995	0.45	1/1333~(0.1%)	
43	q	0.17	0/86618	0.74	13/135116~(0.0%)	
44	r	0.16	0/3726	0.74	0/5804	
45	s	0.19	0/2839	0.76	1/4425~(0.0%)	
46	t	0.28	0/2786	0.51	0/3753	
All	All	0.20	0/148782	0.65	15/219663~(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
2	В	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
43	q	909	С	N1-C2-O2	10.02	124.91	118.90
43	q	909	C	N3-C2-O2	-9.96	114.93	121.90
43	q	2650	С	N3-C2-O2	-6.87	117.09	121.90
43	q	667	С	N3-C2-O2	-6.85	117.11	121.90
43	q	2388	U	C2-N1-C1'	6.76	125.81	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	258	HIS	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
1	А	250/252~(99%)	234 (94%)	16 (6%)	0	100	100
2	В	392/394~(100%)	377~(96%)	15 (4%)	0	100	100
3	С	361/363~(99%)	344 (95%)	17 (5%)	0	100	100
4	D	292/294~(99%)	283 (97%)	9(3%)	0	100	100
5	Е	192/194 (99%)	178 (93%)	14 (7%)	0	100	100
6	F	232/234~(99%)	223 (96%)	9 (4%)	0	100	100
7	G	232/234~(99%)	228 (98%)	4 (2%)	0	100	100
8	Н	189/191 (99%)	181 (96%)	8 (4%)	0	100	100
9	Ι	204/211~(97%)	200 (98%)	4 (2%)	0	100	100
10	J	167/169~(99%)	161 (96%)	6 (4%)	0	100	100
11	К	203/205~(99%)	185 (91%)	18 (9%)	0	100	100
12	L	137/139~(99%)	128 (93%)	9(7%)	0	100	100
13	М	201/203~(99%)	197 (98%)	4 (2%)	0	100	100
14	N	193/195~(99%)	186 (96%)	7 (4%)	0	100	100
15	Ο	151/153~(99%)	147 (97%)	4 (3%)	0	100	100
16	Р	183/185~(99%)	173 (94%)	10 (6%)	0	100	100
17	Q	173/175~(99%)	166 (96%)	7 (4%)	0	100	100
18	R	155/157~(99%)	149 (96%)	6 (4%)	0	100	100
19	S	99/101~(98%)	96 (97%)	3 (3%)	0	100	100
20	Т	127/129~(98%)	127 (100%)	0	0	100	100
21	U	60/62~(97%)	60 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
22	V	116/118 (98%)	113 (97%)	2 (2%)	1 (1%)	17	52
23	W	125/127~(98%)	124 (99%)	1 (1%)	0	100	100
24	X	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
25	Y	145/147~(99%)	140 (97%)	5 (3%)	0	100	100
26	Z	66/68~(97%)	61 (92%)	5 (8%)	0	100	100
27	a	95/97~(98%)	95 (100%)	0	0	100	100
28	b	104/106~(98%)	101 (97%)	3 (3%)	0	100	100
29	с	127/129~(98%)	121 (95%)	6 (5%)	0	100	100
30	d	107/109~(98%)	105 (98%)	2 (2%)	0	100	100
31	e	112/114 (98%)	108 (96%)	4 (4%)	0	100	100
32	f	120/122~(98%)	117 (98%)	3 (2%)	0	100	100
33	g	96/98~(98%)	91 (95%)	5 (5%)	0	100	100
34	h	82/84~(98%)	79~(96%)	3 (4%)	0	100	100
35	i	67/69~(97%)	65~(97%)	2 (3%)	0	100	100
36	j	48/50~(96%)	47 (98%)	1 (2%)	0	100	100
37	k	48/50~(96%)	46 (96%)	2 (4%)	0	100	100
38	1	23/25~(92%)	23 (100%)	0	0	100	100
39	m	103/105~(98%)	95 (92%)	8 (8%)	0	100	100
40	n	89/91~(98%)	87 (98%)	2 (2%)	0	100	100
41	0	182/184~(99%)	181 (100%)	1 (0%)	0	100	100
42	р	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
46	t	351/353~(99%)	296 (84%)	43 (12%)	12 (3%)	3	21
All	All	6651/6742 (99%)	6356 (96%)	282 (4%)	13 (0%)	50	79

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5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	\mathbf{t}	96	GLN
46	\mathbf{t}	153	ALA
46	t	294	VAL
46	t	32	LEU
46	\mathbf{t}	152	ALA



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers Percer		ntiles
1	А	194/194~(100%)	192~(99%)	2(1%)	76	90
2	В	342/342~(100%)	340~(99%)	2(1%)	86	94
3	С	305/305~(100%)	304 (100%)	1 (0%)	92	96
4	D	247/247~(100%)	246 (100%)	1 (0%)	91	96
5	Е	176/176~(100%)	174 (99%)	2 (1%)	73	89
6	F	204/204~(100%)	203 (100%)	1 (0%)	88	94
7	G	199/199~(100%)	197~(99%)	2 (1%)	76	90
8	Н	170/170~(100%)	170 (100%)	0	100	100
9	Ι	178/179~(99%)	178 (100%)	0	100	100
10	J	142/142~(100%)	140 (99%)	2 (1%)	67	86
11	К	172/172~(100%)	172 (100%)	0	100	100
12	L	118/118 (100%)	118 (100%)	0	100	100
13	М	171/171 (100%)	171 (100%)	0	100	100
14	Ν	168/168~(100%)	167~(99%)	1 (1%)	86	94
15	О	134/134~(100%)	134 (100%)	0	100	100
16	Р	163/163~(100%)	163 (100%)	0	100	100
17	Q	155/155~(100%)	154 (99%)	1 (1%)	86	94
18	R	137/137~(100%)	136 (99%)	1 (1%)	84	93
19	S	91/91~(100%)	90~(99%)	1 (1%)	73	89
20	Т	100/100~(100%)	99~(99%)	1 (1%)	76	90
21	U	54/54~(100%)	54 (100%)	0	100	100
22	V	$106/106 \ (100\%)$	105 (99%)	1 (1%)	78	91
23	W	119/119~(100%)	118 (99%)	1 (1%)	81	92
24	X	$\overline{117/117}\ (100\%)$	114 (97%)	3 (3%)	46	74
25	Y	120/120~(100%)	120 (100%)	0	100	100
26	Z	58/58~(100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
27	a	82/82~(100%)	82 (100%)	0	100	100
28	b	97/97~(100%)	96~(99%)	1 (1%)	76	90
29	с	115/115~(100%)	114 (99%)	1 (1%)	78	91
30	d	88/88~(100%)	88 (100%)	0	100	100
31	е	98/98~(100%)	96~(98%)	2(2%)	55	80
32	f	109/109~(100%)	109 (100%)	0	100	100
33	g	85/85~(100%)	85 (100%)	0	100	100
34	h	71/71~(100%)	71~(100%)	0	100	100
35	i	64/64~(100%)	64 (100%)	0	100	100
36	j	47/47~(100%)	47 (100%)	0	100	100
37	k	46/46~(100%)	45 (98%)	1 (2%)	52	78
38	1	24/24~(100%)	24 (100%)	0	100	100
39	m	93/93~(100%)	93~(100%)	0	100	100
40	n	74/74~(100%)	74 (100%)	0	100	100
41	О	163/163~(100%)	162~(99%)	1 (1%)	86	94
42	р	106/106 (100%)	106 (100%)	0	100	100
46	t	297/302~(98%)	281 (95%)	16 (5%)	22	53
All	All	5799/5805~(100%)	5754 (99%)	45 (1%)	82	92

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5 of 45 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	0	176	ARG
46	t	112	VAL
46	t	49	CYS
46	t	101	LYS
46	t	201	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
27	а	51	ASN
42	р	100	ASN
30	d	80	ASN
36	j	25	GLN

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Mol	Chain	Res	Type
46	t	193	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
43	q	3600/3612~(99%)	569~(15%)	0
44	r	156/157~(99%)	33 (21%)	0
45	S	118/119~(99%)	15 (12%)	0
All	All	3874/3888~(99%)	617~(15%)	0

5 of 617 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
43	q	8	U
43	q	9	С
43	q	10	А
43	q	25	А
43	q	32	G

There are no RNA pucker outliers to report.

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 250 ligands modelled in this entry, 250 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
43	q	11

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	q	4734:C	O3'	4818:G	Р	19.70
1	q	3948:C	O3'	4004:G	Р	18.35
1	q	1202:G	O3'	1216:G	Р	17.70
1	q	517:C	O3'	629:G	Р	17.04
1	q	2881:G	O3'	3569:C	Р	16.97



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-10321. 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: 184

Y Index: 206

Z Index: 165

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 4.0. 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 1181 nm^3 ; this corresponds to an approximate mass of 1066 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 0.323 ${\rm \AA}^{-1}$



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-10321 and PDB model 6SWA. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 4.0 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 (4.0).



9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (4.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	$\mathbf{Q} extsf{-score}$
All	0.7150	0.4490
А	0.6636	0.5130
В	0.6899	0.4960
С	0.6604	0.4890
D	0.6308	0.4440
Е	0.5983	0.4340
F	0.6438	0.4610
G	0.5703	0.4360
Н	0.6736	0.4930
Ι	0.6634	0.4830
J	0.5724	0.4320
K	0.6134	0.4400
L	0.7086	0.4760
М	0.7014	0.5120
N	0.7219	0.5030
0	0.6949	0.5040
Р	0.6715	0.4920
Q	0.7168	0.5030
R	0.6709	0.4940
S	0.5743	0.4270
T	0.6642	0.5130
U	0.6587	0.5030
V	0.6294	0.4860
W	0.6839	0.4920
X	0.6314	0.4690
Y	0.6956	0.4970
Z	0.5867	0.4410
a	0.6522	0.4680
b	0.6631	0.5010
С	0.6650	0.5090
d	0.7399	0.5250
е	0.6582	0.4800
f	0.6116	0.4600
g	0.6065	0.4410
h	0.7275	0.5100

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Chain	Atom inclusion	Q-score
i	0.5360	0.4350
j	0.6469	0.4920
k	0.6952	0.5210
1	0.5591	0.4800
m	0.6158	0.4820
n	0.6386	0.4910
0	0.6176	0.4670
р	0.6971	0.4760
q	0.7608	0.4320
r	0.7554	0.4330
S	0.8475	0.4600
t	0.3543	0.3660

