

wwPDB EM Validation Summary Report (i)

Nov 19, 2022 - 09:01 am GMT

PDB ID	:	5LQW
EMDB ID	:	EMD-4099
Title	:	yeast activated spliceosome
Authors	:	Rauhut, R.; Luehrmann, R.
Deposited on	:	2016-08-17
Resolution	:	5.80 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)
:	2.31.2
	: : : : :

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 5.80 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.



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	2413	8%	• 12%			
2	В	1008	5% 82%	• 16%			
3	С	2163	83%	16%			
4	D	364	51%	49%			
5	Е	157	83%	• 12%			
6	F	339	6% 60%	• 36%			
7	Н	577	43% 75%	• 24%			
8	J	148	5% 69%	• 30%			
9	K	451	• 73%	• 25%			

Continued on next page...



Mol	Chain	Length	Quality of chain		
10	т	966	<u></u>		
10	L	200	12% 88% 10%		
11	М	379	41%	55%	
12	Ν	204	53%		22%
13	0	876	20%		200/
10	0	010	5%		2070
14	Р	859	23% • 76%		
15	Q	971	80%	•	19%
16	R	687	32% 68	%	
17	W	590	21% · 78%		
18	Х	1361	5% 79%	•	20%
19	Y	107	5%	•	17%
20	Z	85	80%		20%
21	b	196	5%	59%	
22	d	101	81%		19%
		94	16%		20%
20		51	20%		2076
24	f	86	84%		16%
25	g	77	90%		10%
26	h	146	5%	44%	
27	j	110	85%		15%
28	2	1175	93%		
29	5	179	7%	9%	21%
<u> </u>	0	T10	6%	<i>o / c</i>	Z I /0
30	6	112	39% 43%		7% • 9%
31	9	572	• • 5% • 91%		

Continued from previous page...



2 Entry composition (i)

There are 31 unique types of molecules in this entry. The entry contains 18351 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	А	2130	Total C 2130 2130	0	2130

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	153	ASN	MET	conflict	UNP P33334

• Molecule 2 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	В	843	Total 843 8	C 843	0	843

• Molecule 3 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	С	1811	Total 1811	C 1811	0	1811

• Molecule 4 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	D	187	Total C 187 187	0	187

• Molecule 5 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	Е	138	Total C 138 138	0	138

• Molecule 6 is a protein called Pre-mRNA-splicing factor CWC2.



Mol	Chain	Residues	Atoms	AltConf	Trace
6	F	218	Total C 218 218	0	218

• Molecule 7 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms		AltConf	Trace
7	Н	437	Total 437	С 437	0	437

• Molecule 8 is a protein called U2 snRNP component IST3.

Mol	Chain	Residues	Atoms		AltConf	Trace
8	J	104	Total 104	C 104	0	104

• Molecule 9 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	Κ	338	Total C 338 338	0	338

• Molecule 10 is a protein called Pre-mRNA-splicing factor CWC26.

Mol	Chain	Residues	Atoms	AltConf	Trace
10	L	32	TotalC3232	0	32

• Molecule 11 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms	AltConf	Trace
11	М	169	Total C 169 169	0	169

• Molecule 12 is a protein called Pre-mRNA leakage protein 1.

Mol	Chain	Residues	Atoms	AltConf	Trace
12	Ν	159	Total C 159 159	0	159

• Molecule 13 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase-like protein PRP2.



Mol	Chain	Residues	Atom	\mathbf{S}	AltConf	Trace
13	О	628	Total 628 6	C 528	0	628

• Molecule 14 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Ato	ms	AltConf	Trace
14	Р	202	Total 202	C 202	0	202

• Molecule 15 is a protein called U2 snRNP component HSH155.

Mol	Chain	Residues	Ato	ms	AltConf	Trace
15	Q	791	Total 791	C 791	0	791

• Molecule 16 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms	AltConf	Trace
16	R	219	Total C 219 219	0	219

• Molecule 17 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Aton	ns	AltConf	Trace
17	W	128	Total 128	C 128	0	128

• Molecule 18 is a protein called Pre-mRNA-splicing factor RSE1.

Mol	Chain	Residues	Atoms	AltConf	Trace
18	Х	1095	Total C 1095 1095	0	1095

• Molecule 19 is a protein called Pre-mRNA-splicing factor RDS3.

Mol	Chain	Residues	Atoms	AltConf	Trace
19	Y	89	Total C 89 89	0	89

• Molecule 20 is a protein called RDS3 complex subunit 10.



Mol	Chain	Residues	Atoms	AltConf	Trace
20	Ζ	68	Total C 68 68	0	68

• Molecule 21 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms	AltConf	Trace
21	b	80	Total C 80 80	0	80

• Molecule 22 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Ator	\mathbf{ns}	AltConf	Trace
22	d	82	Total 82	C 82	0	82

• Molecule 23 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms	AltConf	Trace
23	е	75	Total C 75 75	0	75

• Molecule 24 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms	AltConf	Trace
24	f	72	TotalC7272	0	72

• Molecule 25 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms	AltConf	Trace
25	g	69	Total C 69 69	0	69

• Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms	AltConf	Trace
26	h	82	Total C 82 82	0	82

• Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D2.



Mol	Chain	Residues	Atoms	AltConf	Trace
27	j	94	Total C 94 94	0	94

• Molecule 28 is a RNA chain called U2 snRNA.

Mol	Chain	Residues		\mathbf{A}	AltConf	Trace			
28	2	81	Total 1707	С 764	N 285	O 577	Р 81	0	0

• Molecule 29 is a RNA chain called U5 snRNA.

Mol	Chain	Residues		A	AltConf	Trace			
29	5	141	Total 2999	C 1342	N 530	O 986	Р 141	0	0

• Molecule 30 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	102	Total 2170	C 972	N 386	0 710	Р 102	0	0

• Molecule 31 is a RNA chain called actin pre-mRNA.

Mol	Chain	Residues		A	AltConf	Trace			
31	9	54	Total 1135	C 509	N 187	O 385	Р 54	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pre-mRNA-splicing factor 8













• Molecule 9: Pre-mF	RNA-splicing factor P	PRP46		
Chain K:	73%	·	25%	
MET ASP GLY ASP ASP HTS HTS ASP CLU CLU CLU CLU CLU CLU CLU CLU ASP ASP ASP	PHE TYR SER ARG ILE ARG ARG ARD ARC ARD ALA ALA	THR LEU PRO PRO HIS HIS LEU GLU GLU GLU CLY CLY	SER LEU LEU MET MET ARG TYR ARG TYR ARG LYS GLU	SER SER SER
PHE SER GLV GLV GLV CLVS CLVS CLVS LVS LVS LVS CLV HR CLV HIR HR HR	PHE SER GLU ALA ALA CLU ALA CLU ALA ALA ALA ALA ALA ALA ALA ALA ALA A	THR HIS ALA SER ALA PHE CYS LYS LYS LYS LYS CLV GLU	VAL 4107 4146 9149 9149 9151 0151 6172	6180 K204
	⁵ ² ² ⁵⁰ 5 ⁵⁰ 5	36 33 33 34 54 54 54 54 54 54 54 54 54 54 54 54 54	445 6 5 S S S S S S S S S S S S S S S S S S	
13 13<			RIAL SEC ALL LY PH PH	
• Molecule 10: Pre-m	RNA-splicing factor	CWC26		
Chain L: 12%		88%		
MET ALA ALA LEU LEU HTS GLN CLU CLU CLU CLU THR THR THR THR TYS FRO	ASN ASN ASN ASN ASN LYS LYS LYS LYS LYS CLU SER LYS SER AASP AASP	ASN SER ASP LYS THR SER LEU TLEU TLEU VAL LYS GLU ARG CLU SER	THR LEU GLN GLN GLU GLU GLU CLV SER SER SER SEA ALA	PHE SER
LYS PHE ASP LYS GLN LYS GLN LYS SER LYS ASN TLE TRP LYS ASN CLU GLU GLU	ASN ASN GLU LEU SER HIS HIS HIS PRO SER ALA SER SER SER SER	THR GLY ASN GLU SER CLU SER LYS GLU ILE ARG ALA	GLN GLU CLU FRO LEU VAL VAL ALA ASP ASP LYS SER LYS	THR ARG LYS
THR TYR ARG ASP ALA ALA ALA ALA CIN CIN ASP SER SER	L L L L L L L L L L L L L L L L L L L	ALA ALA GLU GLU TYR GLU LYS LEU LEU LEU ASN MET GLY	ASP VAL GGLN LLYS LLEU LLEU ALF ASN ASP HLS	ASP LYS LYS
			•	•
LYS LYS ALN GLN ALA ALA SER SER SER SER LEU TLE GLU ALA ALA TLE TLE	PHE THR HIS ASP LYS GLU ARG CLV VAL LYS THR SER LEU LEU CLV GLY	ARG LYS LEU LEU ASP ASP PRO PRO GLU ASN ARG ALA	ILE MET PRO GLY SER ARG TRP ASP GLY GLY C235 C240	I 252
•• •• ••••				
K255 K256 S259 Y260 Q263 E264 D265 Y266				
• Molecule 11: Pre-m	RNA-processing prot	tein 45		
Chain M:	41% •	55%		
	1 * * * - * * *			
ME SEH AR AR AR PRR AR HIT FRR HIT SEE GLI GLI GLI VAN	AL AL AR ARSS CU ARSS ARSS ARSS ARSS ARSS ARSS ARSS ARS	K44 ARC GLI SS SS SS VS	K8 SEI ASS ARV ARV ALL S99 S99	494 GLI
LLA LLA LLA S.N L.E.U L.E.U L.E.U S.N S.N L12 L12 L12 L12 L12 L12 L12 L12	129 134 135 135 133 133 143 144 144 144 143	149 150 151 152 153 155 155	159	LEU RG AL YS LA
	<mark>и >> « н (ш Z D Ш ></mark>			HU442014
ASP ASN GLU N195 T196 T196 A229 M230 E231 Q232 E233	M234 L2235 L1235 GLU GLU LYS GLU LYS GLU LTS GLU SER ARG ALA	ARG HIS ASN GLY PRO GLN CIN CIN ALA ALA ALA ALA ILE LVS	PR0 LYS LYS LYS SER THR SER ALA ALA ALA LYS LYS	LEU ALA TYR SER GLN
28644398449244888	13328834684388438 133	A S A R A S S S S S A A A A A A	N Q D H J N N A H P H H	斑 怒 鹿
2 A L A L C C C C C C C C C C C C C C C C		A A C A L A H B A C A S A A A S A A A S A A A A S A A A A		



• Molecule 12: Pre-mRNA leakage protein 1











Chain W:

21%

78%

















• Molecule 30: U6 snRNA



	6%				
Chain 6:		39%	43%	7% • 9%	
<mark>13</mark> 13 10 10 10	C14 622 623 623 625 726 826 027	U28 U29 C33 C33 C33 C33 A34 A36 U35 C33 U35 C33 U37 C33 C33 C33 C33 C33 C33 C33 C33 C33 C	A41 A42 A44 A55 A55 A55 A55 A55 A55 C58 A55 C58 C58 C58 C58 C51 C51 C61 C61 C61 C61 C61 C61 C61 C61 C61 C6	A62 663 U64 U65 U65 C66 C66 C66 C7 A75 A75	67.7 67.8 A7.9 U8.0 G8.1
A82 A83 C84 C85 G86 U87	U88 U89 U90 A91 A93 A95 A95	U102 M M M M M M M M M M M M M M M M M M M			
• Molecu	le 31: actin	pre-mRNA			
Chain 9.	. 5% .		91%		
	. 5% .		5170		
0004000		U D D A O A D D D D D O A O A O A O A O A	000040000000000000000000000000000000000	DCCCAAGADC	A A A
A U C2	G4 G4 U7 V7 B9	A10 C11 A12 A12 A13 A13 C15 C15 A17 U18 U18 U18 U18 C20 C20 C20 C22	623 124 1256 126 127 128 127 128 127 128 127 128 127 128 127 128 127 128 128 128 128 128 128 128 128 128 128	0<00<>000	U U U A A U U U
D A A D A <	S S S S S S S S S S S S S S S S S S S	C G G D C C C A A D G C D	C C C C C C C P C P C P C C C	ranana a	A A A
	;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;;	しょ ょ こ こ こ こ こ っ っ っ っ っ っ っ っ っ っ っ っ っ	じょじつじょつじつじつ 4 4 5 4 4 0	U A D G A D A D A	0000
A U A A A A A A A A A A A A A A A A A A		9 4 4 4 D D D 9 9 4 4 4 4	4 4 4 4 4 4 4 0 D 0 4 4 A A A	U N D D D D D N D D D D D D D D D D D D	A G U
0 4 D 4 0 D 0		0 D D D 4 D D 0 0 D 4 0	אין אין מיטטטמא איטטטמא אין מיטטטמא איטטטמא איטטממא מישא	14.96 14.97 14.99 14.99 14.500 14.501 1504 1504 1504 1504	4500 4507 U509
G510 C511 U512 U516 U516	2013 100 100 100 100) D		0 4 4 U U
	D A D O D A D O D A	440000000000000	000000000000000000000000000000000000000	טכבטבטבטטנ	U A C
UD A D U U E)) U U U D A U A U	U < < U < U < U U < C U D	< > U < > U < > U O D U D U D O D O D O D O D O D O D O	D U A A A A G A U	ם ט ט ם
ADQUUQA)) U U A D U A D U A D U A D U A D U A D U A D U A D U A D U A D U A D U A D U A D U A D U A D U A D U A D U A	000440000000040	υ		



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	74000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.343	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	512.0, 512.0, 512.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.0, 2.0, 2.0	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond	lengths	Bo	ond angles
MIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
28	2	0.13	0/1902	0.79	2/2956~(0.1%)
29	5	0.12	0/3350	0.68	0/5209
30	6	0.16	0/2427	0.76	4/3778~(0.1%)
31	9	0.17	0/1264	0.65	0/1961
All	All	0.14	0/8943	0.72	6/13904~(0.0%)

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
28	2	76	A	C2-N3-C4	15.59	118.39	110.60
28	2	76	А	N1-C2-N3	10.07	134.34	129.30
30	6	3	U	C2-N1-C1'	7.71	126.95	117.70
30	6	3	U	N1-C2-O2	7.28	127.90	122.80
30	6	3	U	N3-C2-O2	-6.56	117.61	122.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2130	0	0	48	0
2	В	843	0	0	8	0
3	С	1811	0	0	5	0
4	D	187	0	0	0	0

Continued on next page...



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Е	138	0	0	17	0
6	F	218	0	0	22	0
7	Н	437	0	0	3	0
8	J	104	0	0	1	0
9	Κ	338	0	0	4	0
10	L	32	0	0	0	0
11	М	169	0	0	10	0
12	Ν	159	0	0	1	0
13	0	628	0	0	19	0
14	Р	202	0	0	3	0
15	Q	791	0	0	13	0
16	R	219	0	0	4	0
17	W	128	0	0	3	0
18	Х	1095	0	0	13	0
19	Y	89	0	0	7	0
20	Ζ	68	0	0	0	0
21	b	80	0	0	0	0
22	d	82	0	0	0	0
23	е	75	0	0	0	0
24	f	72	0	0	0	0
25	g	69	0	0	0	0
26	h	82	0	0	0	0
27	j	94	0	0	0	0
28	2	1707	0	860	31	0
29	5	2999	0	1515	50	0
30	6	2170	0	1094	53	0
31	9	1135	0	575	32	0
All	All	18351	0	4044	247	0

Continued from previous page...

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 11.

The worst 5 of 247 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)
1:A:1377:SER:CA	31:9:18:U:C5	1.87	1.56
5:E:98:THR:CA	30:6:4:C:C2	1.88	1.52
15:Q:927:ALA:CA	28:2:57:A:H1'	1.05	1.51
6:F:72:PHE:CA	30:6:34:A:C2	1.94	1.50
6:F:72:PHE:CA	30:6:34:A:H2	1.20	1.49



There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	2	80/1175~(6%)	21 (26%)	2(2%)
29	5	137/179~(76%)	31 (22%)	4 (2%)
30	6	101/112~(90%)	41 (40%)	6(5%)
31	9	52/572~(9%)	27~(51%)	1 (1%)
All	All	370/2038~(18%)	120 (32%)	13 (3%)

5 of 120 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
28	2	12	U
28	2	14	С
28	2	15	С
28	2	18	U
28	2	20	G

5 of 13 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	6	26	А
30	6	42	А
31	9	505	С
30	6	64	U
30	6	86	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	5	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	166:U	O3'	167:A	Р	3.66



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4099. 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: 128

Y Index: 128





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: 135

Y Index: 131

Z Index: 131

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 0.11. 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 1066 $\rm nm^3;$ this corresponds to an approximate mass of 963 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 0.172 ${\rm \AA^{-1}}$



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-4099 and PDB model 5LQW. 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 0.11 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 (0.11).



9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 79% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7884	0.1440
2	0.5237	0.1370
5	0.7706	0.1210
6	0.7700	0.1500
9	0.5894	0.1550
А	0.9131	0.1640
В	0.9454	0.1700
С	0.8774	0.1370
D	0.8770	0.1460
Е	0.8913	0.1170
F	0.9083	0.1660
Н	0.4279	0.0900
J	0.9231	0.1610
K	0.9438	0.1790
L	0.6875	0.1720
М	0.7692	0.2040
N	0.3145	0.1200
0	0.7182	0.0910
Р	0.7921	0.1200
Q	0.9267	0.1570
R	0.9498	0.1360
W	0.8984	0.1540
Х	0.9361	0.1760
Y	0.9438	0.2000
Z	1.0000	0.1760
b	0.8875	0.1220
d	0.8415	0.1380
е	0.8000	0.0960
f	0.7639	0.0760
g	0.8116	0.1070
h	0.9024	0.1480
j	0.7872	0.1020



1.0

0.0 <0.0

