wwPDB EM Validation Summary Report

Dec 18, 2022 – 07:02 pm GMT

PDB ID	:	7AS8
EMDB ID	:	EMD-11889
Title	:	Bacillus subtilis ribosome quality control complex state B. Ribosomal 50S subunit with P-tRNA, RqcH, and RqcP/YabO
Authors	:	Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on	:	2020-10-27
Resolution	:	2.90 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 ⓘ 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 ⓘ) were used in the production of this report:

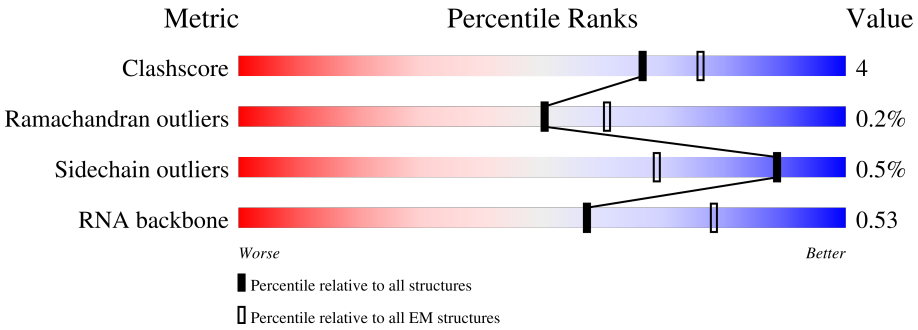
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 2.90 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	Whole archive (#Entries)	EM structures (#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 >=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	0	597	27% 80% 10% 10%
2	1	86	8% 70% 27%
3	2	76	54% 24% 18%
4	A	2926	63% 27% 6%
5	B	119	61% 27% 6% 6%
6	E	277	83% 14%
7	F	209	87% 11%

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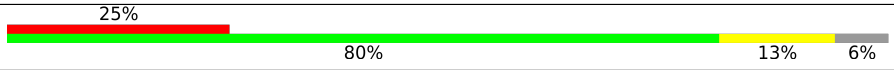
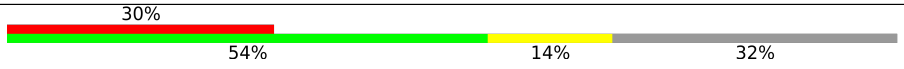
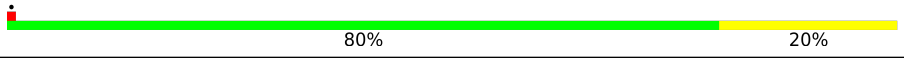
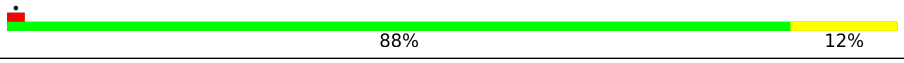
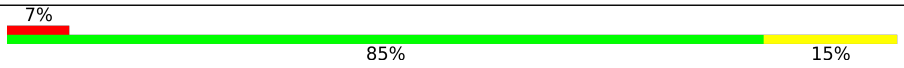
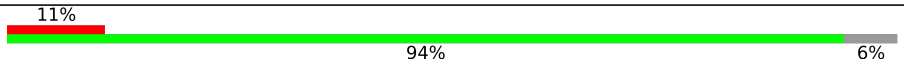
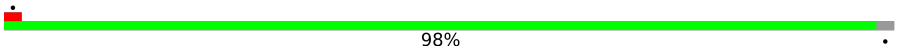
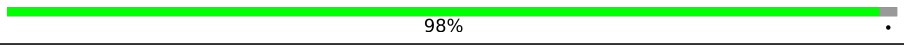
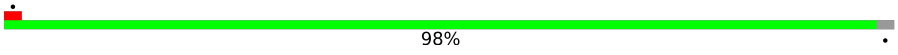
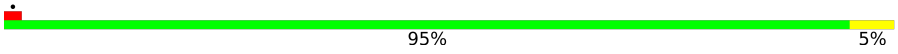
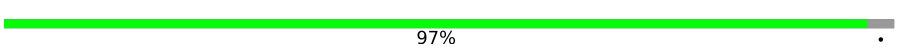
Mol	Chain	Length	Quality of chain
8	G	207	
9	H	179	
10	I	179	
11	K	141	
12	L	166	
13	N	145	
14	O	122	
15	P	146	
16	Q	144	
17	R	120	
18	S	120	
19	T	115	
20	U	119	
21	V	102	
22	W	113	
23	X	95	
24	Y	103	
25	a	94	
26	b	62	
27	c	66	
28	d	59	
29	f	59	
30	g	49	
31	h	44	
32	i	66	

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Mol	Chain	Length	Quality of chain
33	j	37	100%

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 93801 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 Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	536	3993	2520	713	750	10	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	571	GLY	-	expression tag	UNP O34693
0	572	SER	-	expression tag	UNP O34693
0	573	GLY	-	expression tag	UNP O34693
0	574	GLY	-	expression tag	UNP O34693
0	575	ASP	-	expression tag	UNP O34693
0	576	TYR	-	expression tag	UNP O34693
0	577	LYS	-	expression tag	UNP O34693
0	578	ASP	-	expression tag	UNP O34693
0	579	HIS	-	expression tag	UNP O34693
0	580	ASP	-	expression tag	UNP O34693
0	581	GLY	-	expression tag	UNP O34693
0	582	ASP	-	expression tag	UNP O34693
0	583	TYR	-	expression tag	UNP O34693
0	584	LYS	-	expression tag	UNP O34693
0	585	ASP	-	expression tag	UNP O34693
0	586	HIS	-	expression tag	UNP O34693
0	587	ASP	-	expression tag	UNP O34693
0	588	ILE	-	expression tag	UNP O34693
0	589	ASP	-	expression tag	UNP O34693
0	590	TYR	-	expression tag	UNP O34693
0	591	LYS	-	expression tag	UNP O34693
0	592	ASP	-	expression tag	UNP O34693
0	593	ASP	-	expression tag	UNP O34693
0	594	ASP	-	expression tag	UNP O34693
0	595	ASP	-	expression tag	UNP O34693
0	596	LYS	-	expression tag	UNP O34693
0	597	GLY	-	expression tag	UNP O34693

- Molecule 2 is a protein called Uncharacterized protein YabO.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	83	Total	C	N	O	S	0	0
			659	410	121	126	2		

- Molecule 3 is a RNA chain called tRNA-Ala-1-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	73	Total	C	N	O	P	0	0
			1563	695	283	512	73		

- Molecule 4 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	2812	Total	C	N	O	P	0	0
			60389	26942	11160	19477	2810		

- Molecule 5 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 6 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 7 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 8 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	G	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 9 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	H	164	Total 1284	C 813	N 228	O 236	S 7	0	0

- Molecule 10 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	175	Total 1342	C 835	N 248	O 257	S 2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	132	Total 974	C 612	N 172	O 184	S 6	0	0

- Molecule 12 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	113	Total 886	C 559	N 152	O 174	S 1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	142	Total 1123	C 710	N 206	O 202	S 5	0	0

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	122	Total 920	C 571	N 173	O 172	S 4	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	146	Total 1081	C 671	N 207	O 201	S 2	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	135	Total 1076	C 690	N 205	O 176	S 5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	119	Total 953	C 583	N 186	O 180	S 4	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	120	Total 912	C 564	N 176	O 171	S 1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	115	Total 944	C 600	N 185	O 158	S 1	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	117	Total 940	C 591	N 189	O 156	S 4	0	0

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	100	Total 781	C 498	N 138	O 145	0	0

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	109	Total 842	C 525	N 164	O 150	S 3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	a	81	Total	C	N	O	0	0
			624	387	122	115		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 30 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 33 is a protein called 50S ribosomal protein L36.

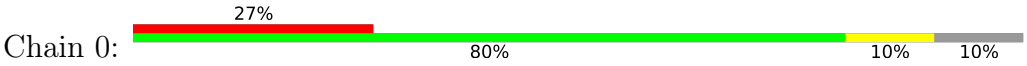
Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

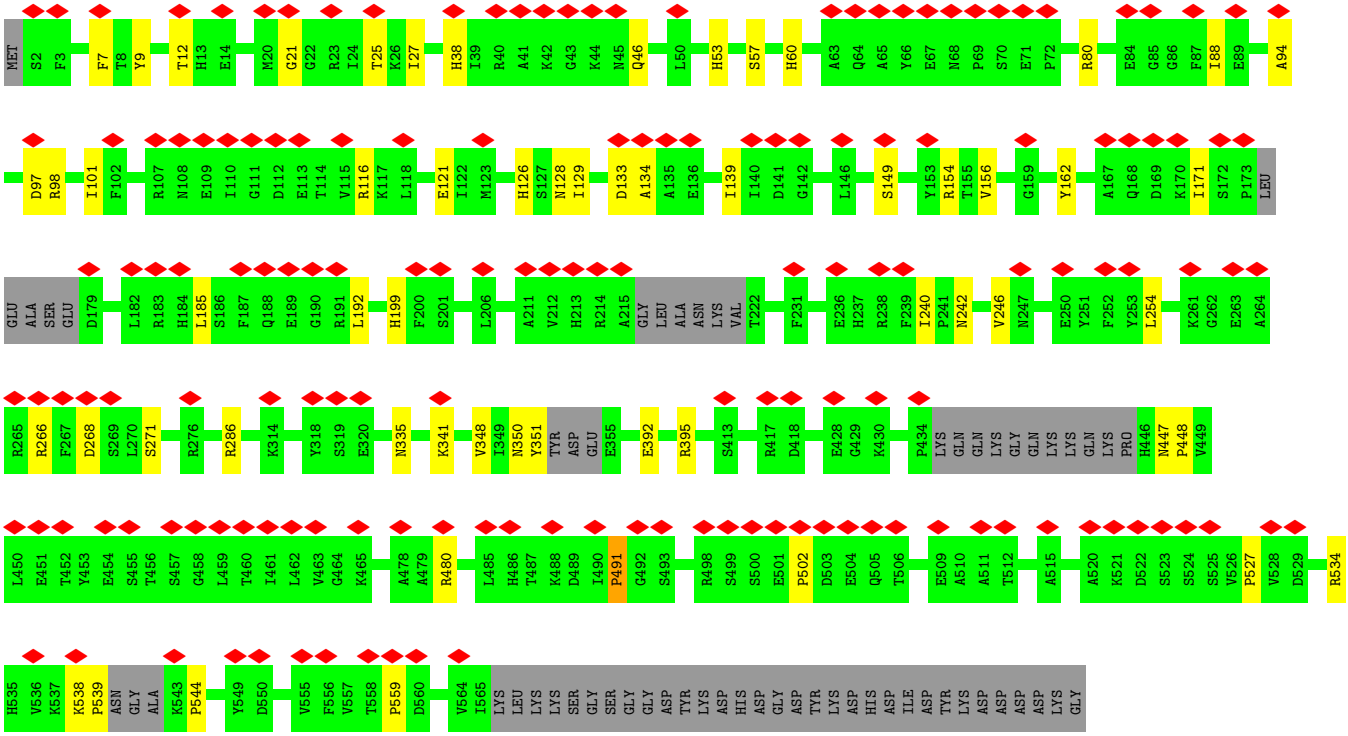
3 Residue-property plots (i)

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: Rqc2 homolog RqcH

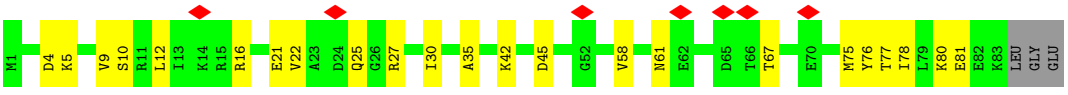
Chain 0:





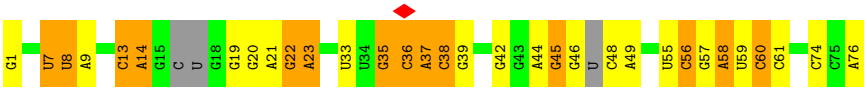
• Molecule 2: Uncharacterized protein YabO

Chain 1:



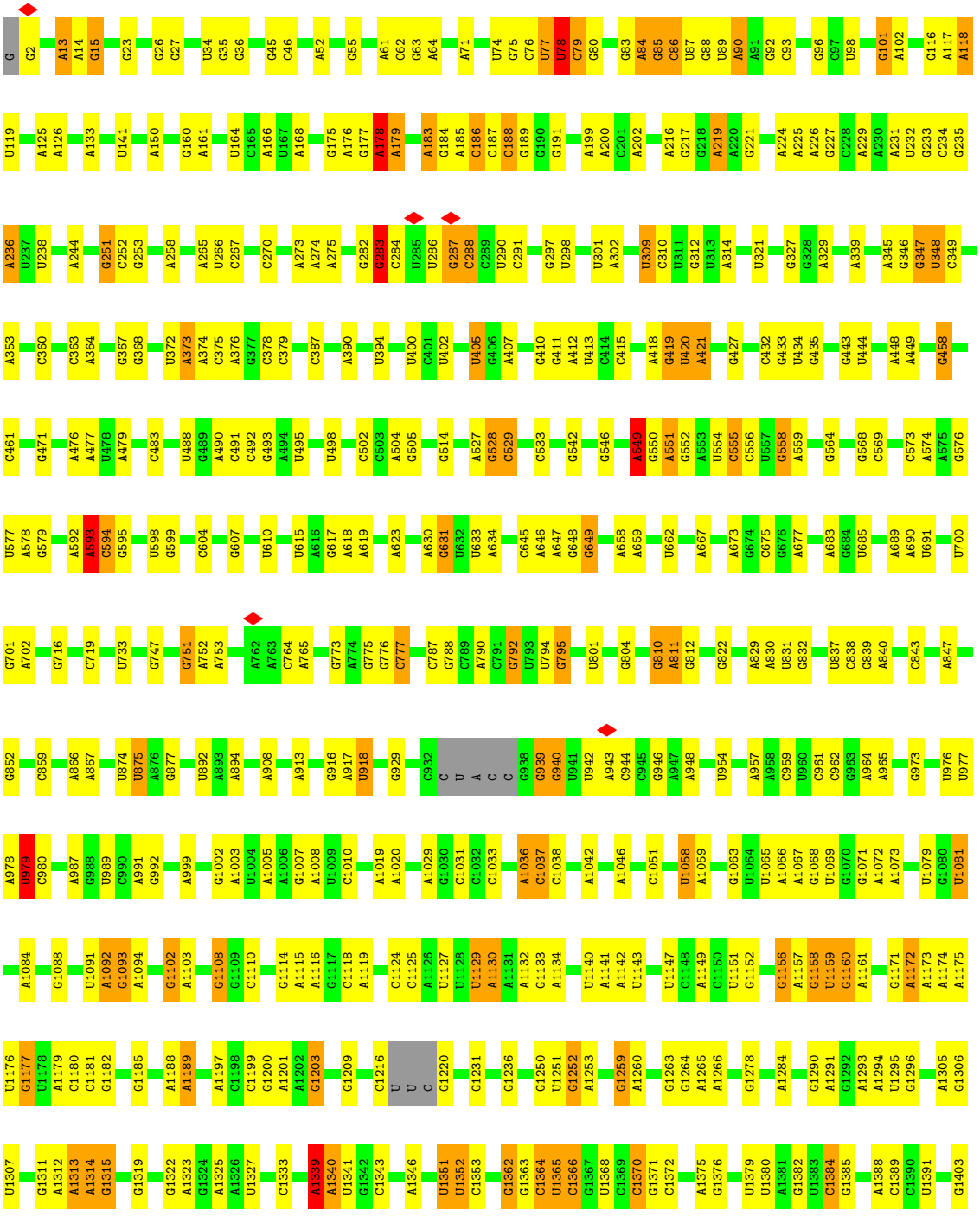
• Molecule 3: tRNA-Ala-1-1

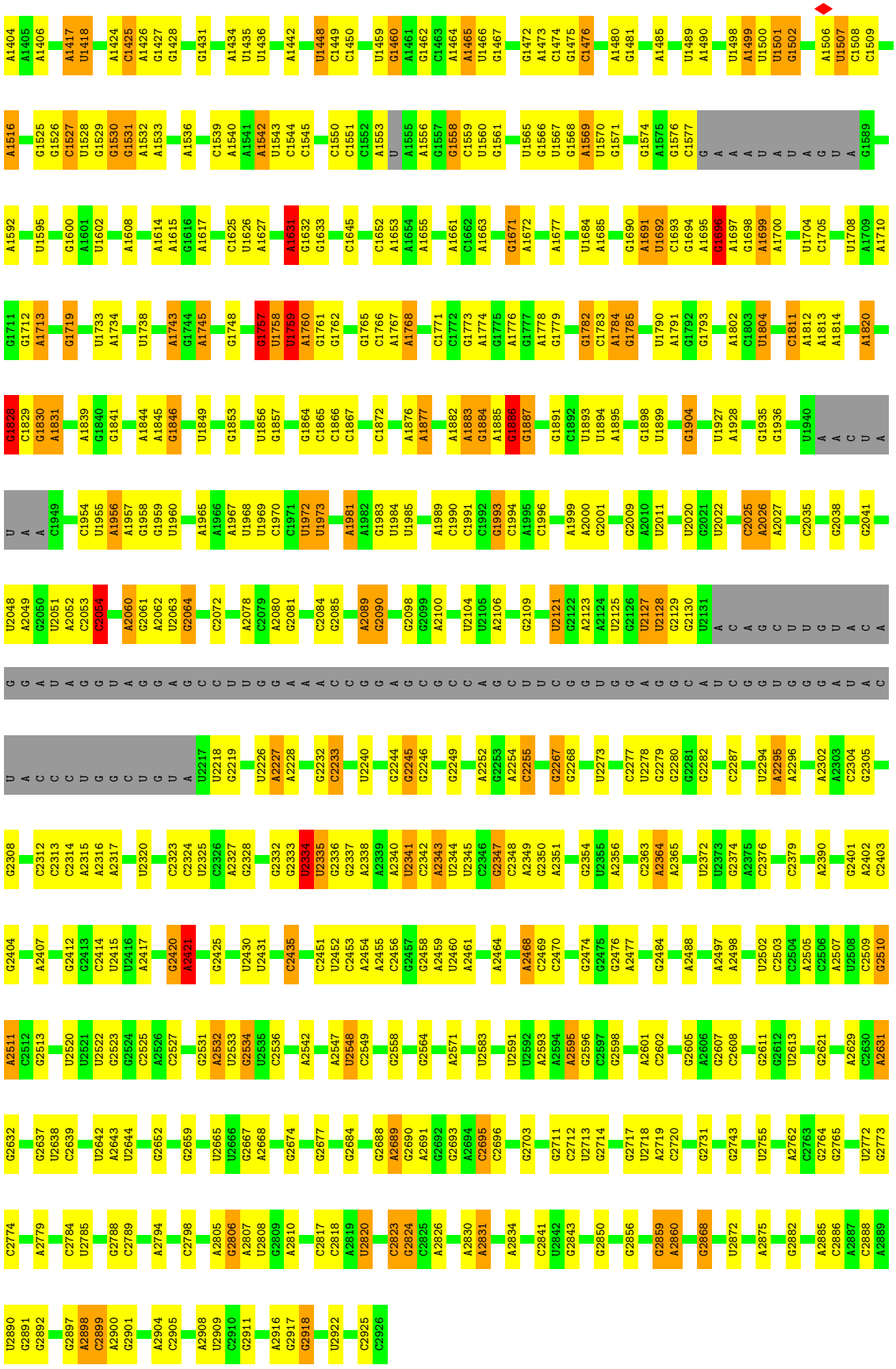
Chain 2:



• Molecule 4: 23S rRNA

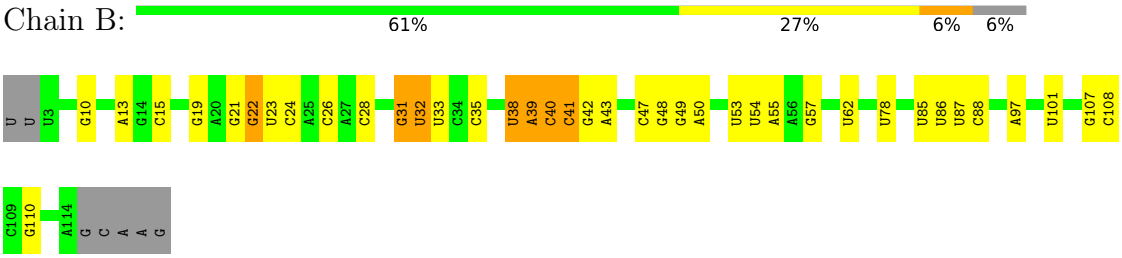
Chain A:





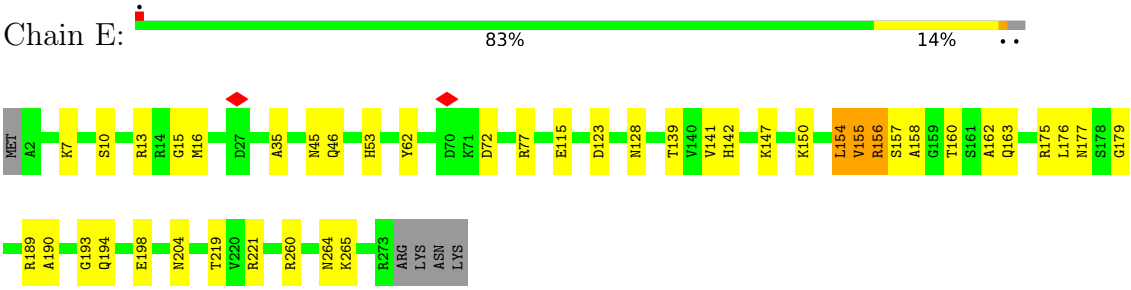
• Molecule 5: 5s rRNA

Chain B:



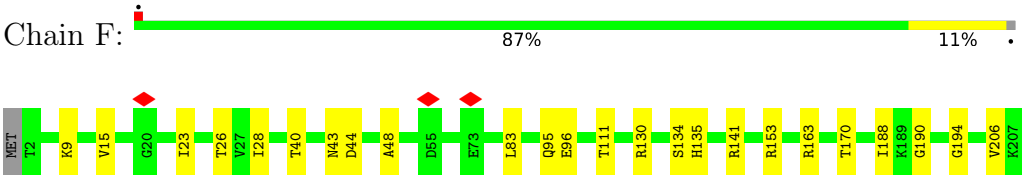
• Molecule 6: 50S ribosomal protein L2

Chain E:



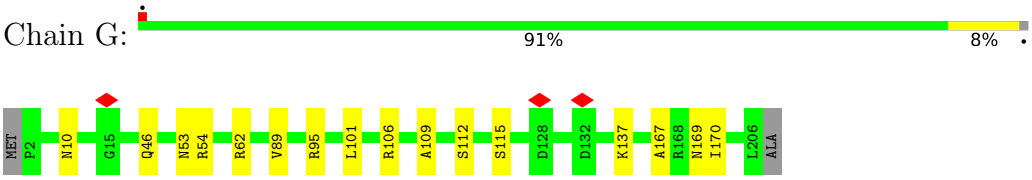
• Molecule 7: 50S ribosomal protein L3

Chain F:



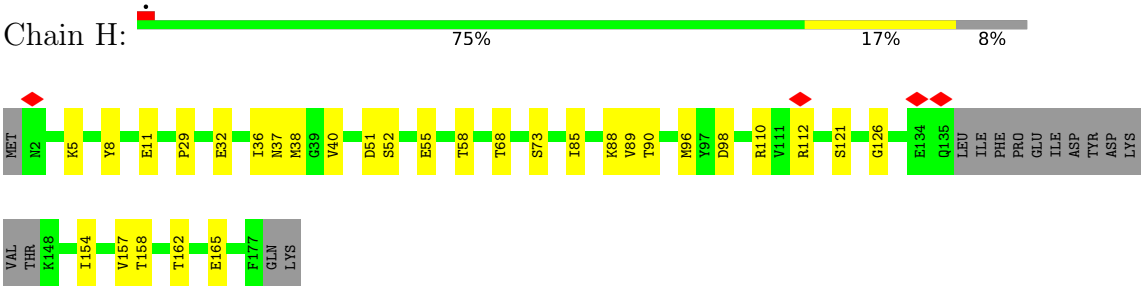
• Molecule 8: 50S ribosomal protein L4

Chain G:



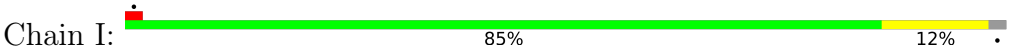
• Molecule 9: 50S ribosomal protein L5

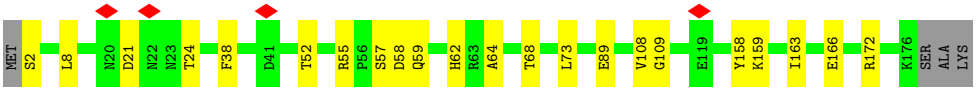
Chain H:



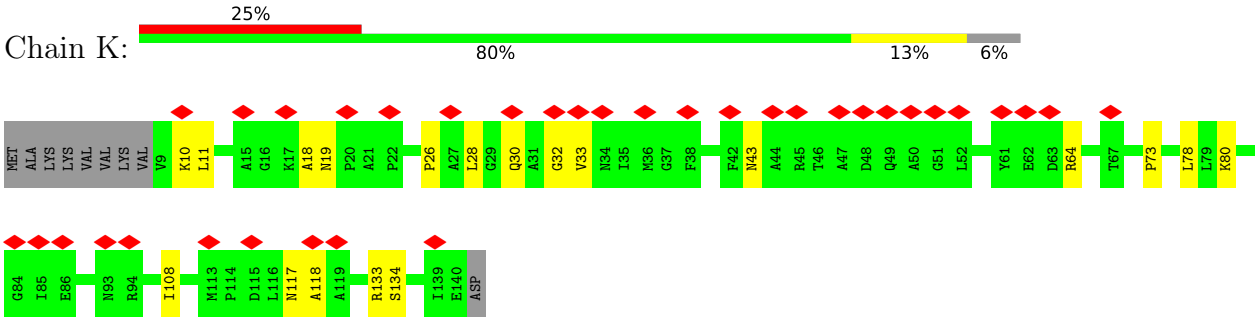
• Molecule 10: 50S ribosomal protein L6

Chain I:

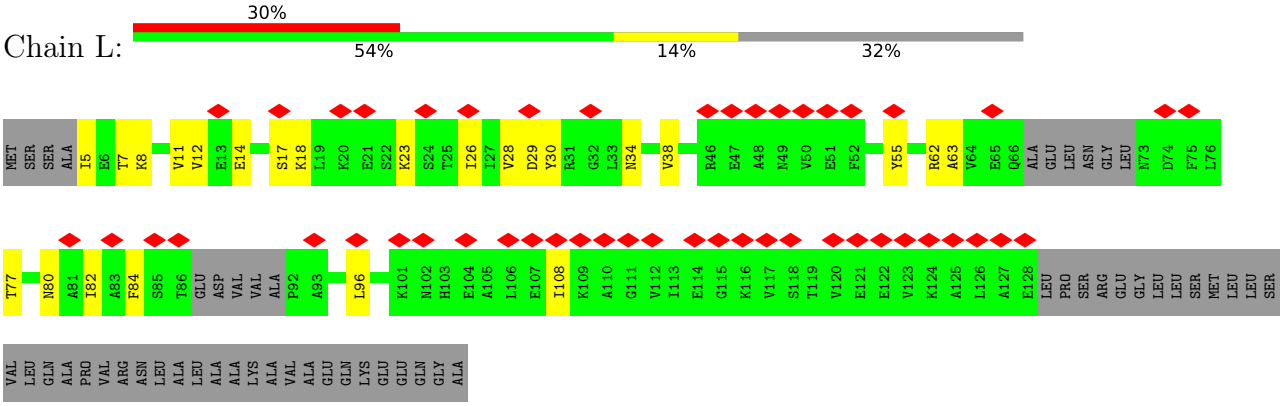




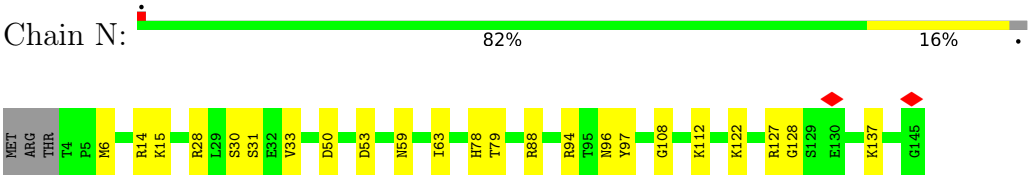
• Molecule 11: 50S ribosomal protein L11



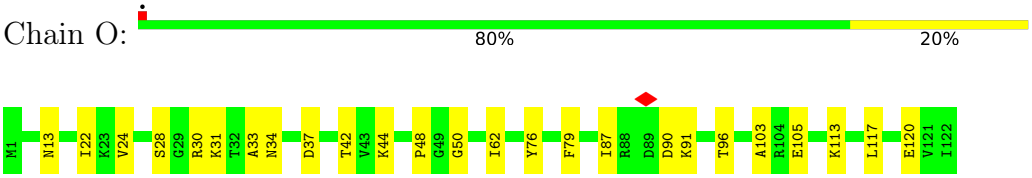
• Molecule 12: 50S ribosomal protein L10



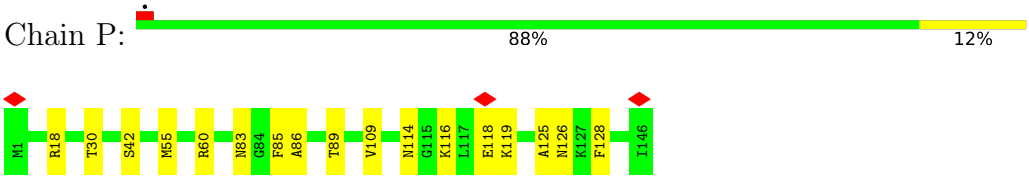
• Molecule 13: 50S ribosomal protein L13



• Molecule 14: 50S ribosomal protein L14

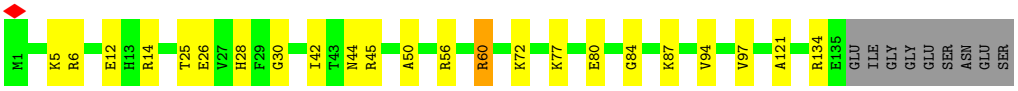


• Molecule 15: 50S ribosomal protein L15



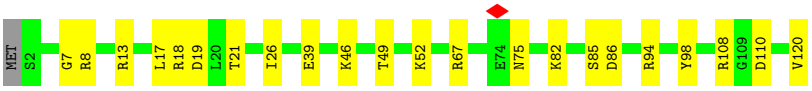
• Molecule 16: 50S ribosomal protein L16

Chain Q:



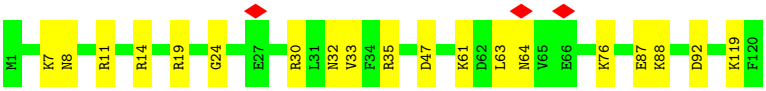
• Molecule 17: 50S ribosomal protein L17

Chain R:



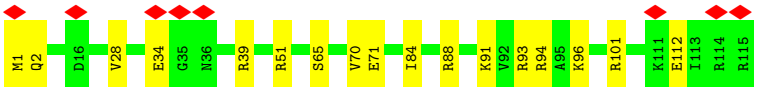
• Molecule 18: 50S ribosomal protein L18

Chain S:



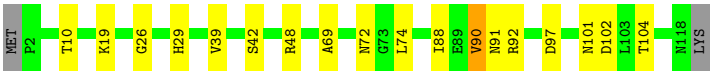
• Molecule 19: 50S ribosomal protein L19

Chain T:



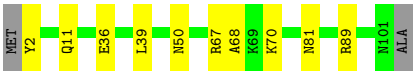
• Molecule 20: 50S ribosomal protein L20

Chain U:



• Molecule 21: 50S ribosomal protein L21

Chain V:

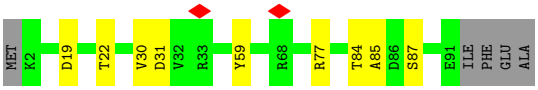


• Molecule 22: 50S ribosomal protein L22

Chain W:

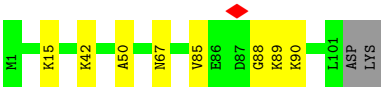
• Molecule 23: 50S ribosomal protein L23

Chain X:



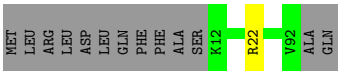
• Molecule 24: 50S ribosomal protein L24

Chain Y:



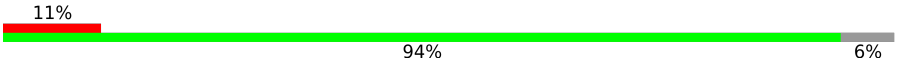
• Molecule 25: 50S ribosomal protein L27

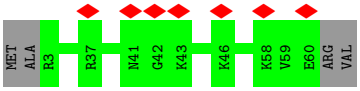
Chain a:



• Molecule 26: 50S ribosomal protein L28

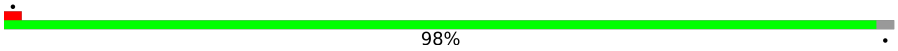
Chain b:

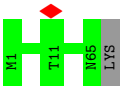




• Molecule 27: 50S ribosomal protein L29

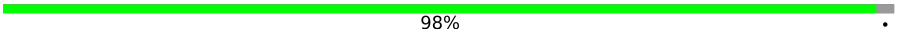
Chain c:





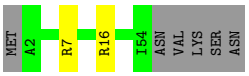
• Molecule 28: 50S ribosomal protein L30

Chain d:



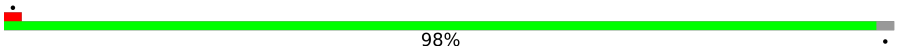
• Molecule 29: 50S ribosomal protein L32

Chain f:



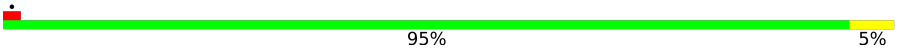
• Molecule 30: 50S ribosomal protein L33 1

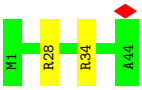
Chain g:



• Molecule 31: 50S ribosomal protein L34

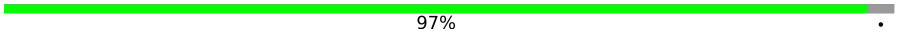
Chain h:





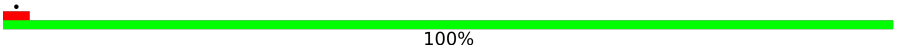
• Molecule 32: 50S ribosomal protein L35

Chain i:



• Molecule 33: 50S ribosomal protein L36

Chain j:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74210	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	29	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	0.044	Depositor
Minimum map value	-0.015	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.33	0/4058	0.59	8/5485 (0.1%)
2	1	0.43	0/662	0.59	0/882
3	2	0.82	1/1744 (0.1%)	1.07	2/2712 (0.1%)
4	A	1.19	2/67639 (0.0%)	1.13	105/105512 (0.1%)
5	B	0.92	0/2675	1.01	0/4170
6	E	0.70	0/2120	0.68	0/2845
7	F	0.71	0/1591	0.65	0/2132
8	G	0.68	0/1580	0.63	0/2132
9	H	0.44	0/1299	0.64	0/1740
10	I	0.51	0/1360	0.63	0/1832
11	K	0.32	0/988	0.57	0/1336
12	L	0.34	0/892	0.59	0/1196
13	N	0.70	0/1146	0.62	0/1542
14	O	0.65	0/927	0.75	0/1245
15	P	0.64	0/1093	0.66	0/1457
16	Q	0.70	0/1099	0.70	0/1468
17	R	0.65	0/960	0.70	0/1284
18	S	0.56	0/921	0.68	0/1236
19	T	0.67	0/957	0.76	0/1279
20	U	0.74	0/952	0.70	0/1266
21	V	0.76	0/792	0.68	0/1063
22	W	0.64	0/851	0.72	0/1146
23	X	0.65	0/731	0.69	0/974
24	Y	0.62	0/772	0.67	1/1032 (0.1%)
25	a	0.76	0/632	0.72	0/839
26	b	0.46	0/448	0.70	0/596
27	c	0.54	0/531	0.71	0/707
28	d	0.63	0/457	0.69	0/613
29	f	0.67	0/425	0.71	1/563 (0.2%)
30	g	0.64	0/406	0.62	0/540
31	h	0.72	0/370	0.78	1/483 (0.2%)
32	i	0.66	0/519	0.68	0/680
33	j	0.75	0/299	0.62	0/393
All	All	1.04	3/101896 (0.0%)	1.02	118/152380 (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
6	E	0	1
11	K	0	1
16	Q	0	1
21	V	0	1
All	All	0	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	1	G	OP3-P	-10.80	1.48	1.61
4	A	574	A	N9-C4	-5.53	1.34	1.37
4	A	1467	G	C8-N7	-5.10	1.27	1.30

The worst 5 of 118 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1757	G	O4'-C1'-N9	9.07	115.45	108.20
4	A	2898	A	N1-C6-N6	-8.59	113.44	118.60
4	A	593	A	N1-C6-N6	-8.05	113.77	118.60
4	A	2503	C	C6-N1-C2	-7.83	117.17	120.30
4	A	555	C	C6-N1-C2	-7.82	117.17	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	E	154	LEU	Peptide
11	K	19	ASN	Peptide
16	Q	60	ARG	Peptide
21	V	50	ASN	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	0	3993	0	3689	27	0
2	1	659	0	705	14	0
3	2	1563	0	794	14	0
4	A	60389	0	30398	290	0
5	B	2392	0	1213	10	0
6	E	2083	0	2168	27	0
7	F	1569	0	1637	16	0
8	G	1561	0	1647	12	0
9	H	1284	0	1344	20	0
10	I	1342	0	1388	17	0
11	K	974	0	1011	14	0
12	L	886	0	920	15	0
13	N	1123	0	1162	16	0
14	O	920	0	977	21	0
15	P	1081	0	1132	11	0
16	Q	1076	0	1145	16	0
17	R	953	0	983	14	0
18	S	912	0	947	12	0
19	T	944	0	1020	12	0
20	U	940	0	1005	15	0
21	V	781	0	821	9	0
22	W	842	0	899	7	0
23	X	725	0	770	6	0
24	Y	762	0	821	5	0
25	a	624	0	639	0	0
26	b	444	0	487	0	0
27	c	530	0	568	0	0
28	d	455	0	491	0	0
29	f	418	0	435	0	0
30	g	401	0	413	0	0
31	h	367	0	410	0	0
32	i	512	0	564	0	0
33	j	296	0	342	0	0
All	All	93801	0	62945	524	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 4.

The worst 5 of 524 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)
4:A:312:G:N2	4:A:405:U:C5	2.33	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:36:C:H2'	3:2:36:C:O2	1.70	0.92
4:A:327:G:H1	4:A:400:U:H3	1.18	0.86
4:A:810:G:O2'	4:A:811:A:O5'	1.95	0.84
4:A:1216:C:O2	4:A:1220:G:N2	2.12	0.82

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	Percentiles
1	0	524/597 (88%)	480 (92%)	41 (8%)	3 (1%)	25 58
2	1	81/86 (94%)	76 (94%)	5 (6%)	0	100 100
6	E	270/277 (98%)	257 (95%)	11 (4%)	2 (1%)	22 54
7	F	204/209 (98%)	187 (92%)	17 (8%)	0	100 100
8	G	203/207 (98%)	184 (91%)	19 (9%)	0	100 100
9	H	160/179 (89%)	141 (88%)	19 (12%)	0	100 100
10	I	173/179 (97%)	153 (88%)	20 (12%)	0	100 100
11	K	130/141 (92%)	115 (88%)	15 (12%)	0	100 100
12	L	107/166 (64%)	106 (99%)	1 (1%)	0	100 100
13	N	140/145 (97%)	127 (91%)	13 (9%)	0	100 100
14	O	120/122 (98%)	105 (88%)	15 (12%)	0	100 100
15	P	144/146 (99%)	136 (94%)	8 (6%)	0	100 100
16	Q	133/144 (92%)	117 (88%)	16 (12%)	0	100 100
17	R	117/120 (98%)	106 (91%)	11 (9%)	0	100 100
18	S	118/120 (98%)	105 (89%)	13 (11%)	0	100 100
19	T	113/115 (98%)	105 (93%)	8 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	U	115/119 (97%)	106 (92%)	8 (7%)	1 (1%)	17 48
21	V	98/102 (96%)	80 (82%)	18 (18%)	0	100 100
22	W	107/113 (95%)	94 (88%)	13 (12%)	0	100 100
23	X	88/95 (93%)	83 (94%)	5 (6%)	0	100 100
24	Y	99/103 (96%)	84 (85%)	15 (15%)	0	100 100
25	a	79/94 (84%)	71 (90%)	8 (10%)	0	100 100
26	b	56/62 (90%)	50 (89%)	6 (11%)	0	100 100
27	c	63/66 (96%)	61 (97%)	2 (3%)	0	100 100
28	d	56/59 (95%)	54 (96%)	2 (4%)	0	100 100
29	f	51/59 (86%)	47 (92%)	4 (8%)	0	100 100
30	g	46/49 (94%)	41 (89%)	5 (11%)	0	100 100
31	h	42/44 (96%)	41 (98%)	1 (2%)	0	100 100
32	i	62/66 (94%)	59 (95%)	3 (5%)	0	100 100
33	j	35/37 (95%)	33 (94%)	2 (6%)	0	100 100
All	All	3734/4021 (93%)	3404 (91%)	324 (9%)	6 (0%)	50 78

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	0	491	PRO
6	E	156	ARG
6	E	155	VAL
1	0	447	ASN
1	0	538	LYS

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain 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	0	372/527 (71%)	370 (100%)	2 (0%)	88 96
2	1	73/75 (97%)	73 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	E	220/225 (98%)	220 (100%)	0	100	100
7	F	167/170 (98%)	167 (100%)	0	100	100
8	G	169/170 (99%)	168 (99%)	1 (1%)	86	96
9	H	139/154 (90%)	137 (99%)	2 (1%)	67	89
10	I	148/151 (98%)	148 (100%)	0	100	100
11	K	102/110 (93%)	102 (100%)	0	100	100
12	L	98/138 (71%)	97 (99%)	1 (1%)	76	92
13	N	120/123 (98%)	120 (100%)	0	100	100
14	O	101/101 (100%)	101 (100%)	0	100	100
15	P	110/110 (100%)	109 (99%)	1 (1%)	78	93
16	Q	109/116 (94%)	108 (99%)	1 (1%)	78	93
17	R	99/100 (99%)	98 (99%)	1 (1%)	76	92
18	S	93/93 (100%)	93 (100%)	0	100	100
19	T	100/100 (100%)	99 (99%)	1 (1%)	76	92
20	U	96/98 (98%)	95 (99%)	1 (1%)	76	92
21	V	83/84 (99%)	83 (100%)	0	100	100
22	W	90/93 (97%)	88 (98%)	2 (2%)	52	81
23	X	81/85 (95%)	81 (100%)	0	100	100
24	Y	85/87 (98%)	84 (99%)	1 (1%)	71	91
25	a	63/74 (85%)	62 (98%)	1 (2%)	62	86
26	b	47/50 (94%)	47 (100%)	0	100	100
27	c	56/57 (98%)	56 (100%)	0	100	100
28	d	52/53 (98%)	52 (100%)	0	100	100
29	f	47/53 (89%)	46 (98%)	1 (2%)	53	81
30	g	46/47 (98%)	46 (100%)	0	100	100
31	h	39/39 (100%)	38 (97%)	1 (3%)	46	77
32	i	54/56 (96%)	54 (100%)	0	100	100
33	j	35/35 (100%)	35 (100%)	0	100	100
All	All	3094/3374 (92%)	3077 (100%)	17 (0%)	89	96

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	a	22	ARG
31	h	28	ARG
16	Q	60	ARG
17	R	75	ASN
19	T	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	335	ASN
1	0	385	ASN
20	U	101	ASN
24	Y	67	ASN
32	i	60	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	2	71/76 (93%)	22 (30%)	5 (7%)
4	A	2804/2926 (95%)	665 (23%)	59 (2%)
5	B	111/119 (93%)	31 (27%)	3 (2%)
All	All	2986/3121 (95%)	718 (24%)	67 (2%)

5 of 718 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	2	8	U
3	2	14	A
3	2	19	G
3	2	21	A
3	2	23	A

5 of 67 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	A	2452	U
4	A	2468	A
5	B	48	G
4	A	1172	A
4	A	1066	A

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
4	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1451:U	O3'	1452:C	P	3.09

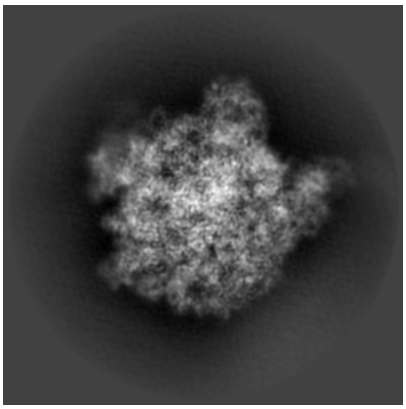
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11889. These allow visual inspection of the internal detail of the map and identification of artifacts.

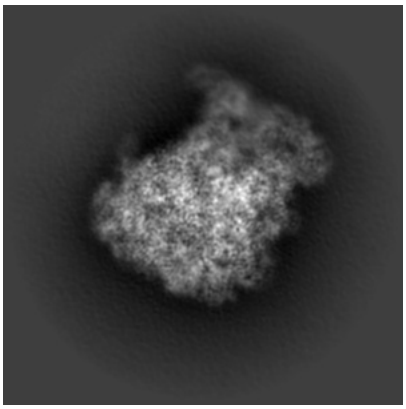
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

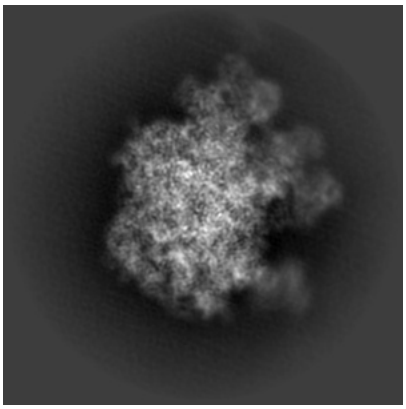
6.1.1 Primary map



X

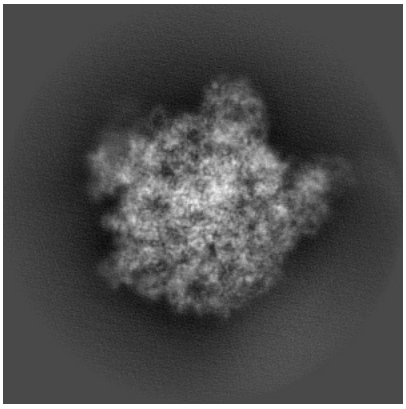


Y

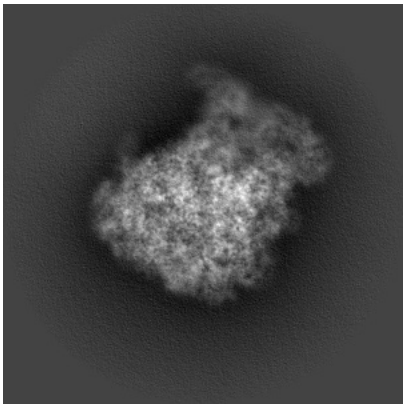


Z

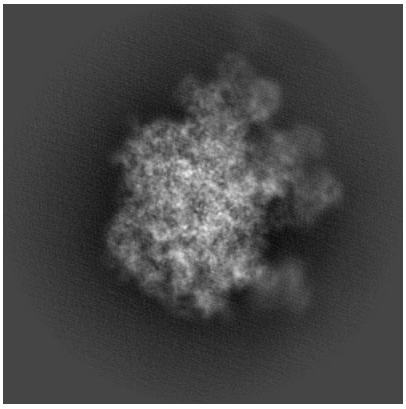
6.1.2 Raw map



X



Y

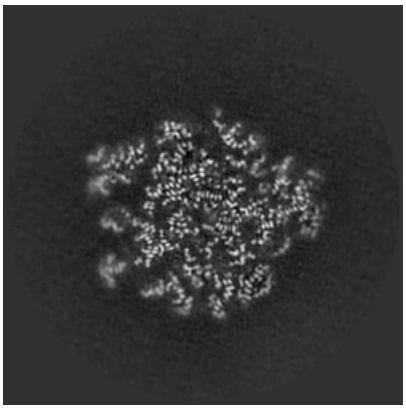


Z

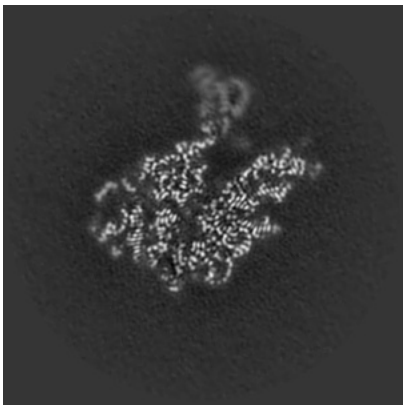
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

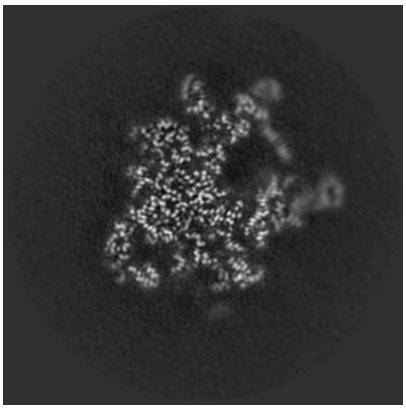
6.2.1 Primary map



X Index: 210

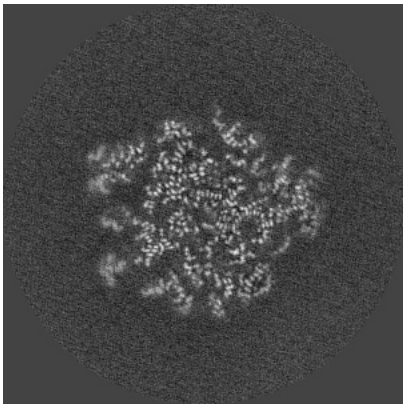


Y Index: 210

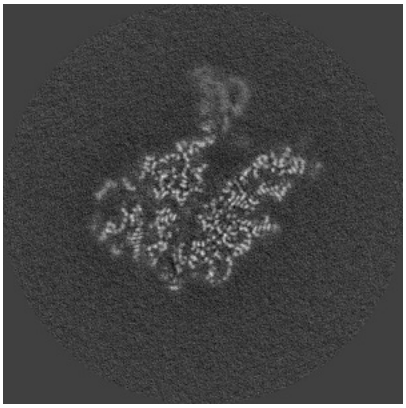


Z Index: 210

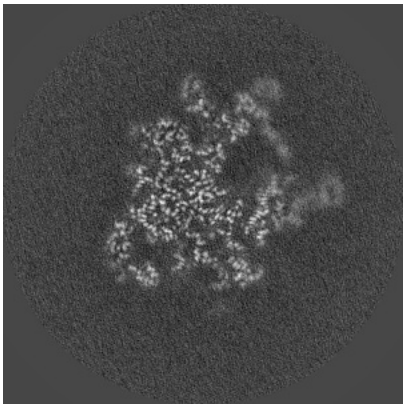
6.2.2 Raw map



X Index: 210



Y Index: 210

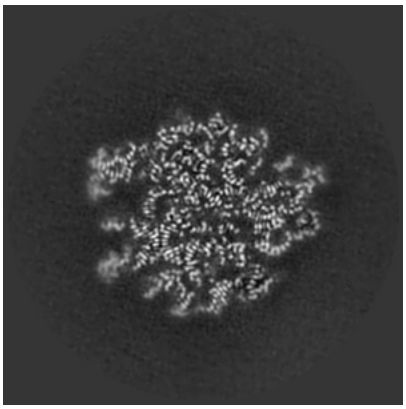


Z Index: 210

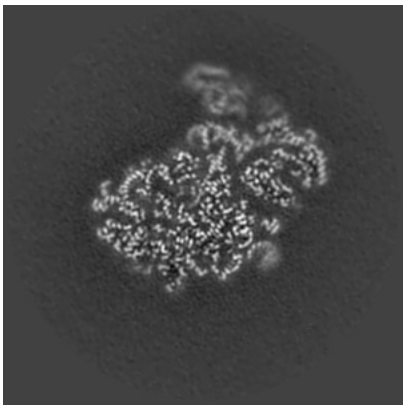
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

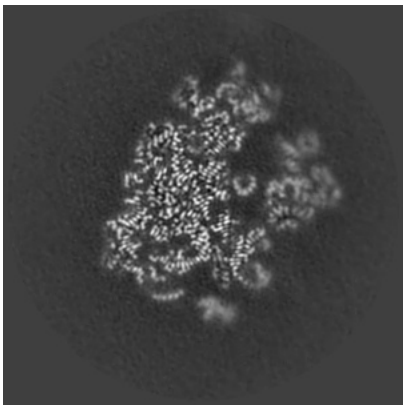
6.3.1 Primary map



X Index: 215

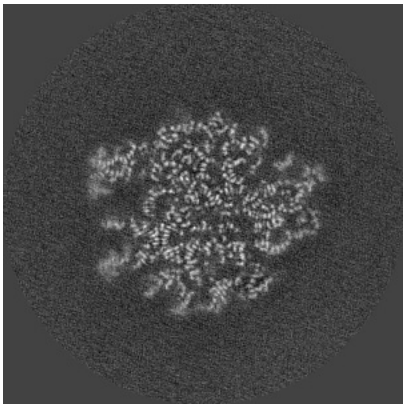


Y Index: 223

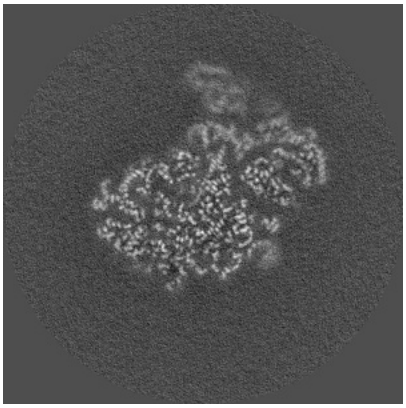


Z Index: 222

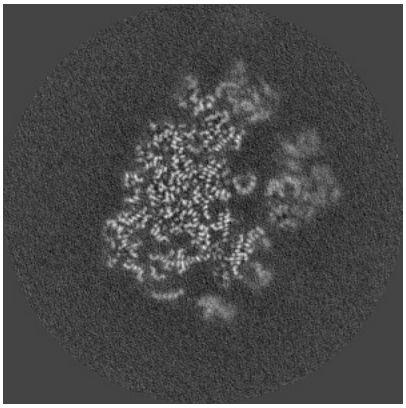
6.3.2 Raw map



X Index: 215



Y Index: 223



Z Index: 223

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

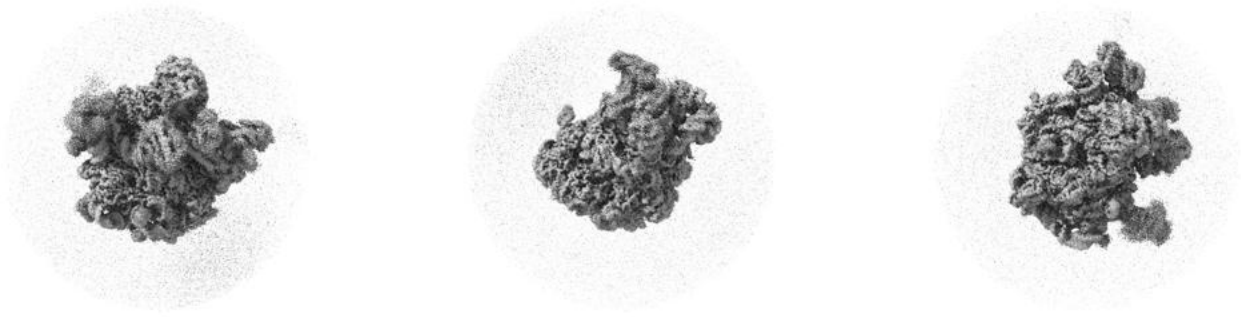
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. 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



X Y Z

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.

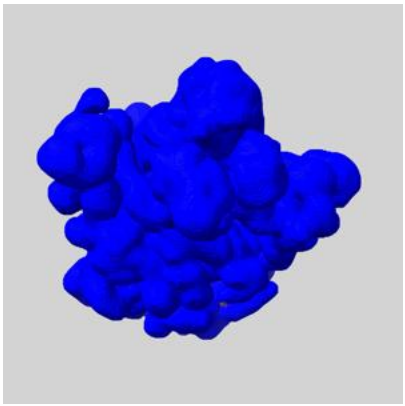
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

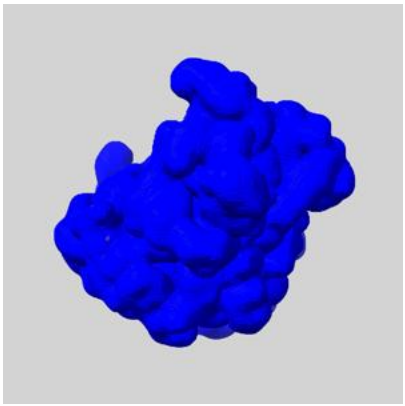
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

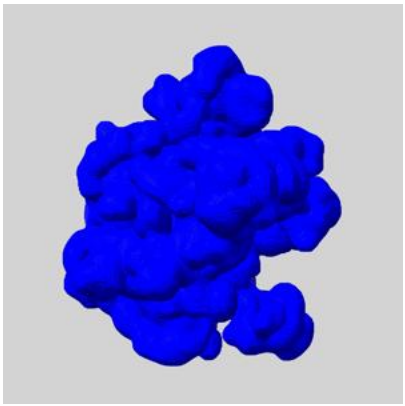
6.5.1 emd_11889_msk_1.map (i)



X



Y

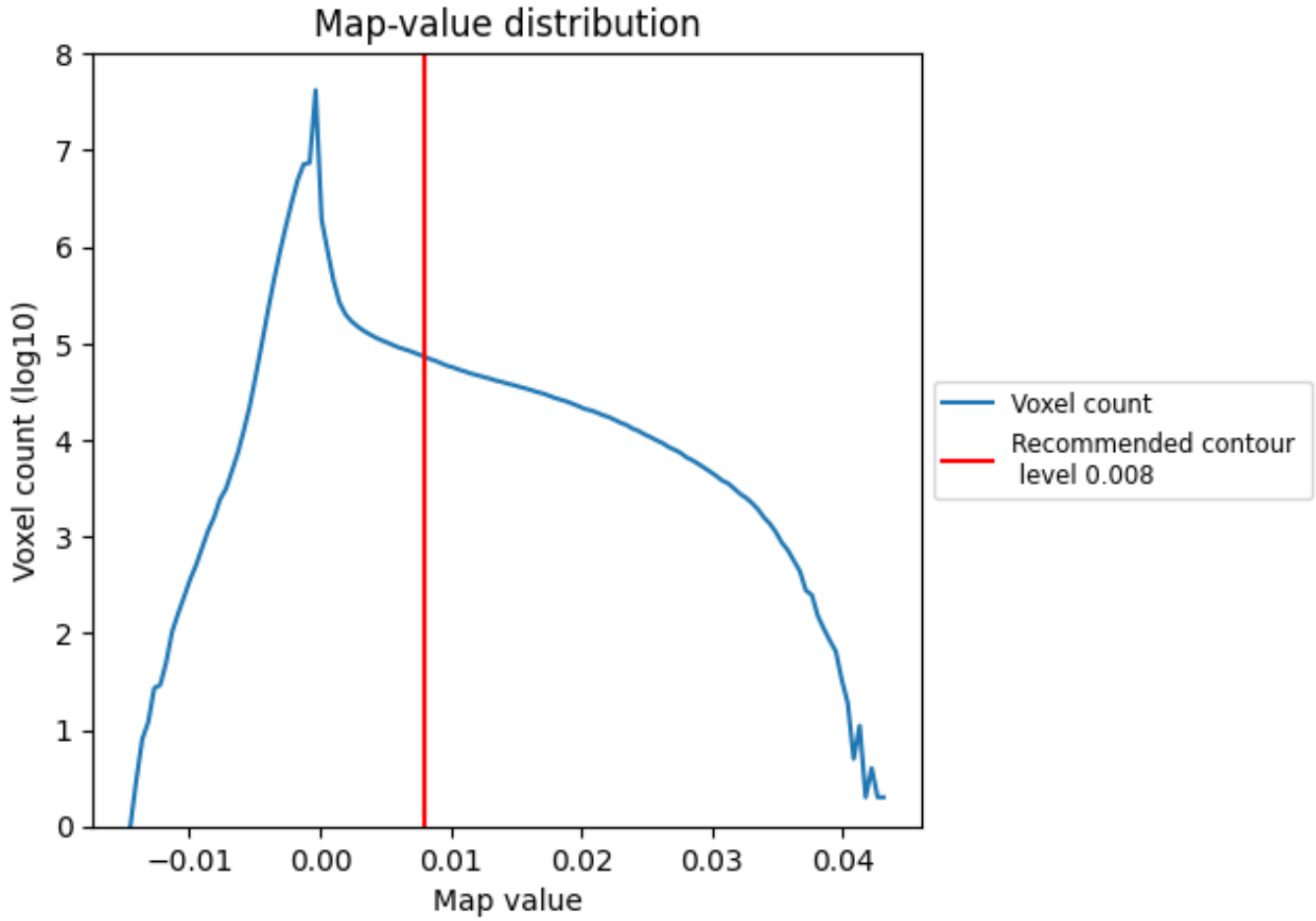


Z

7 Map analysis

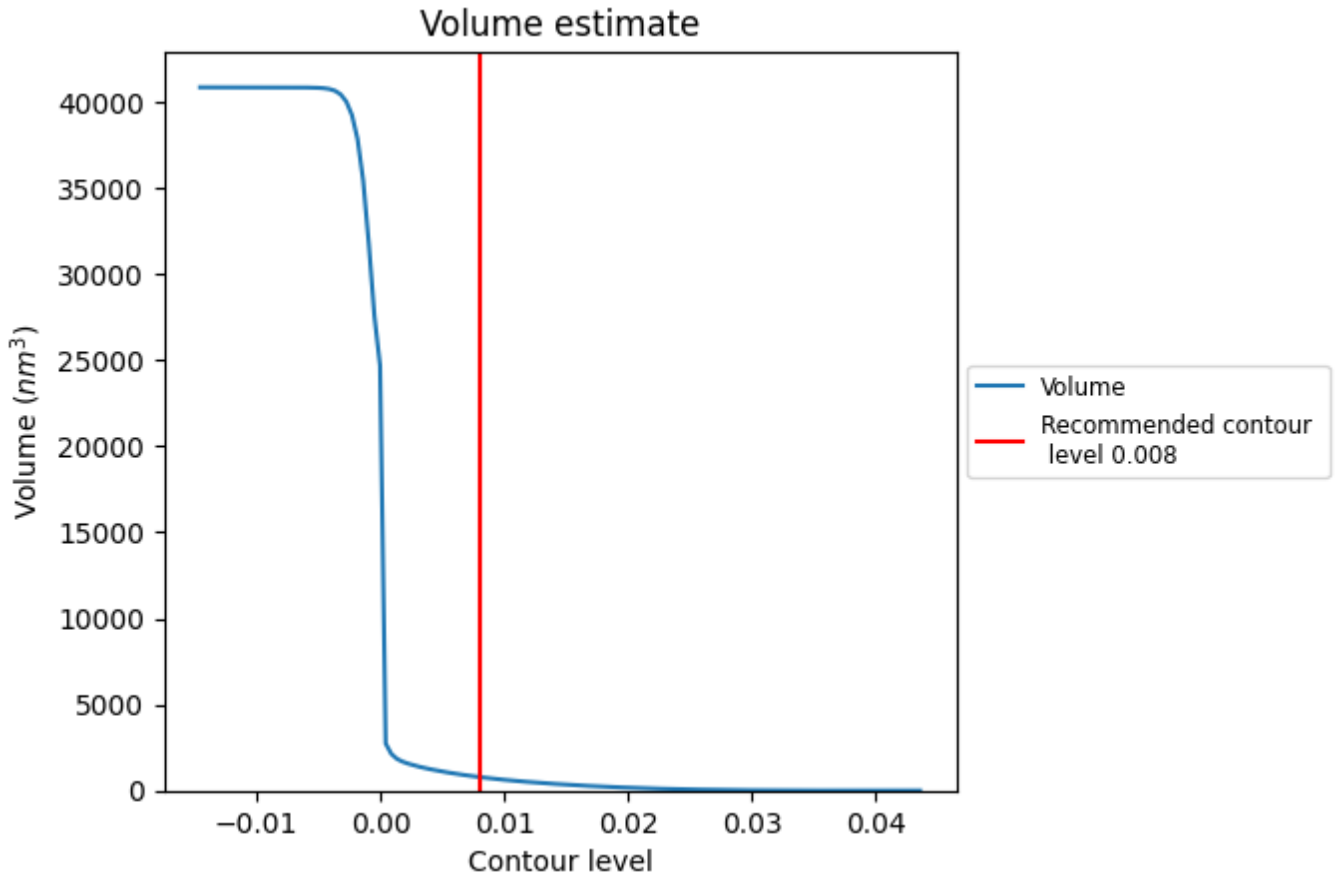
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

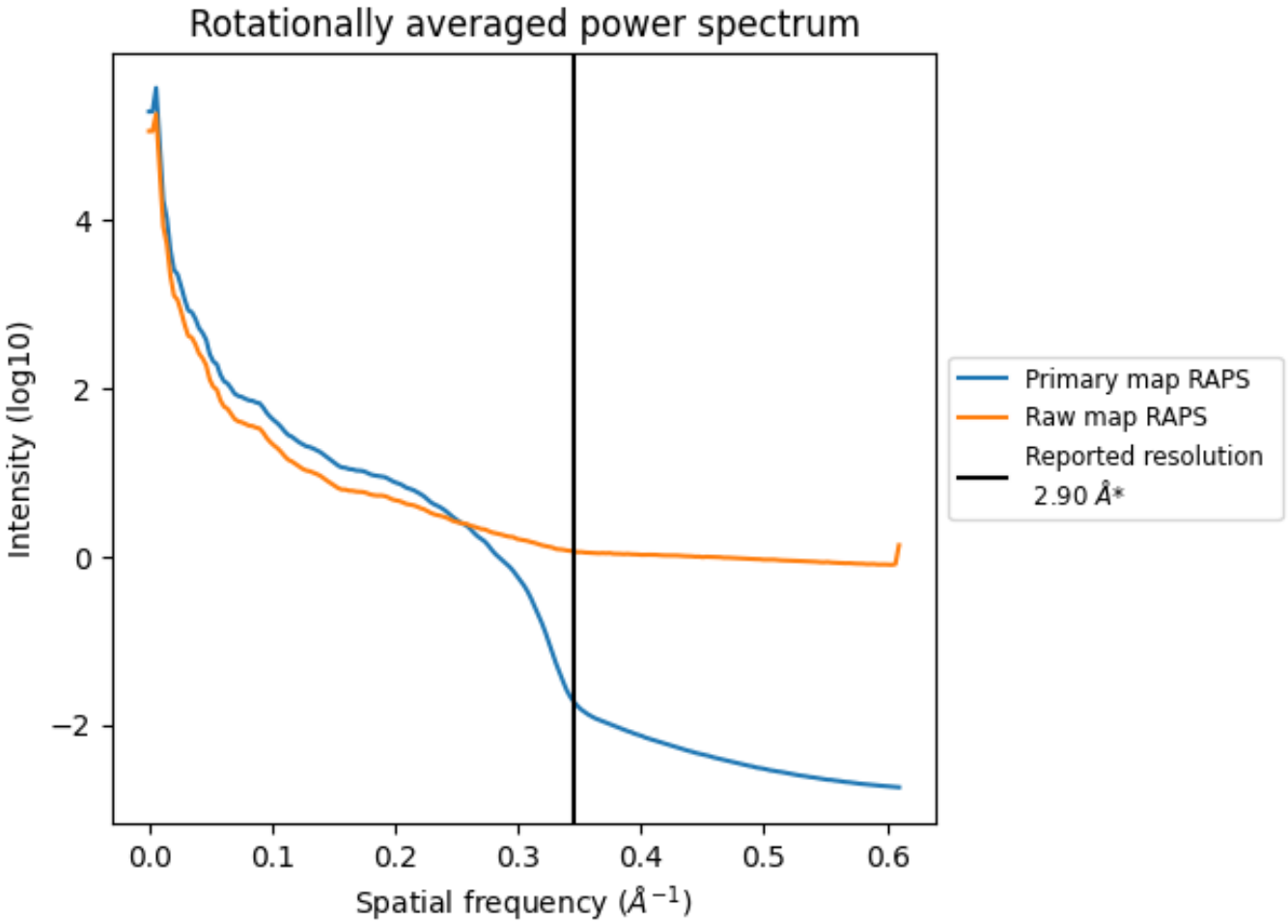
7.2 Volume estimate (i)



The volume at the recommended contour level is 786 nm^3; this corresponds to an approximate mass of 710 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)

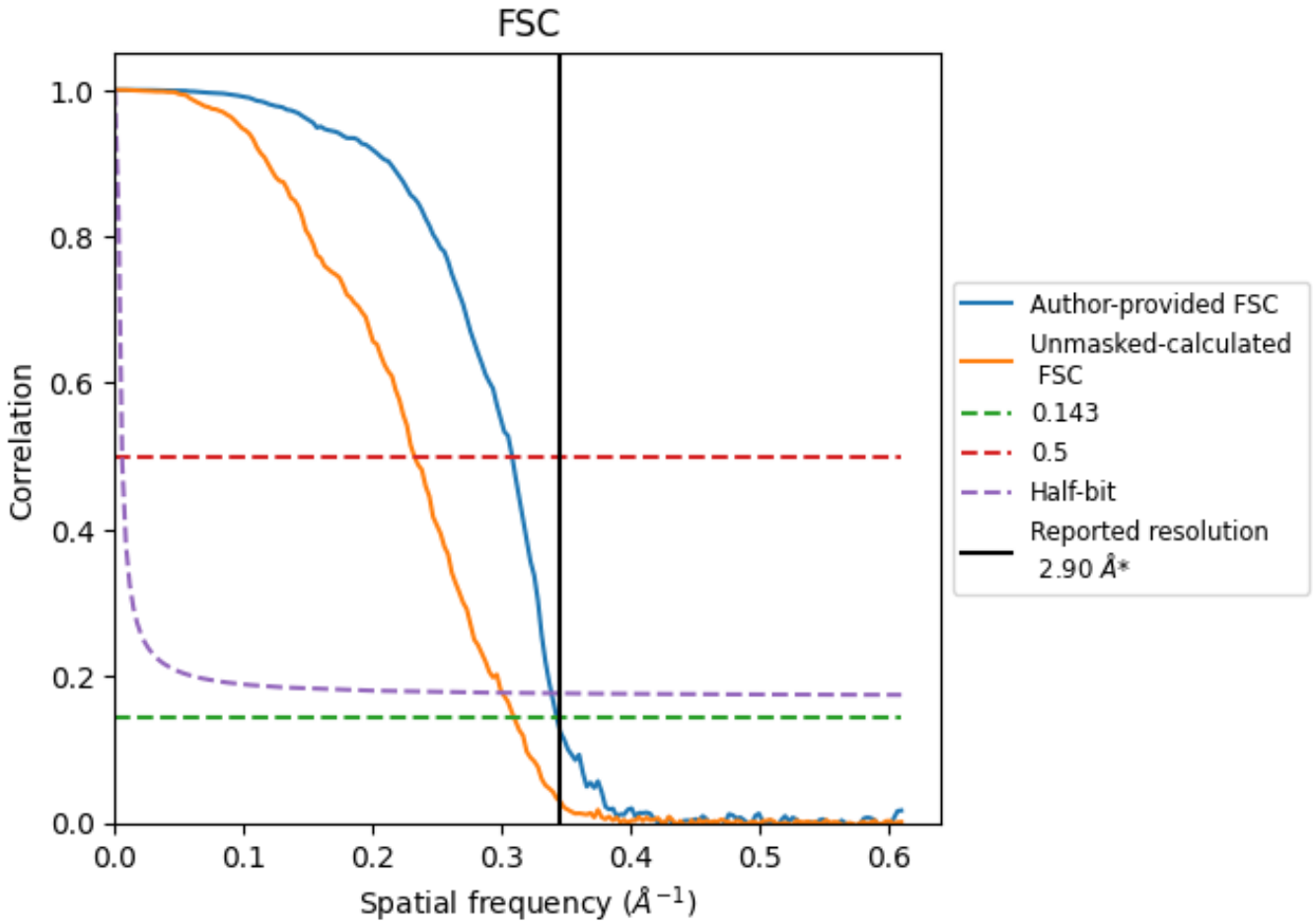


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.345 $Å^{-1}$

8.2 Resolution estimates (i)

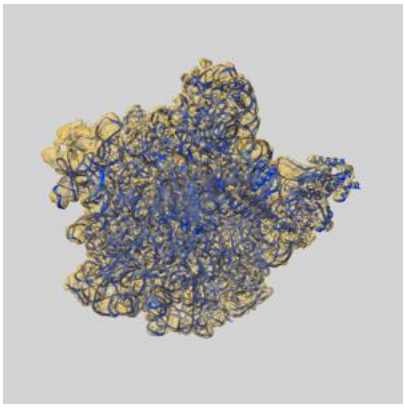
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.92	3.25	2.95
Unmasked-calculated*	3.23	4.30	3.33

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.23 differs from the reported value 2.9 by more than 10 %

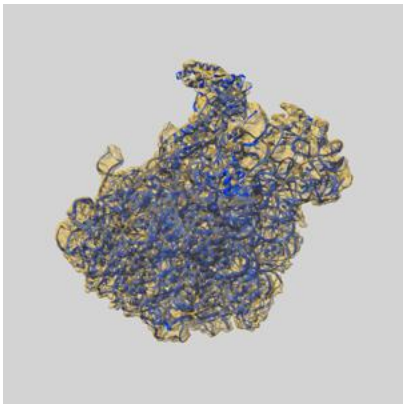
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11889 and PDB model 7AS8. Per-residue inclusion information can be found in section 3 on page 11.

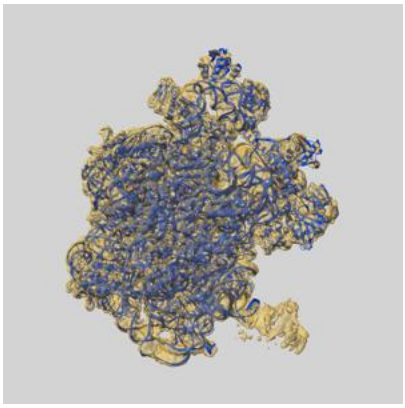
9.1 Map-model overlay



X



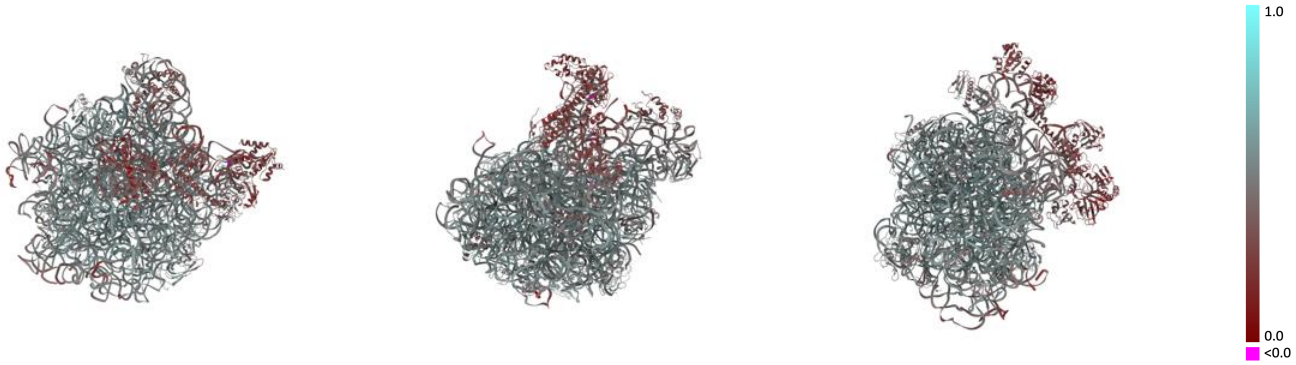
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

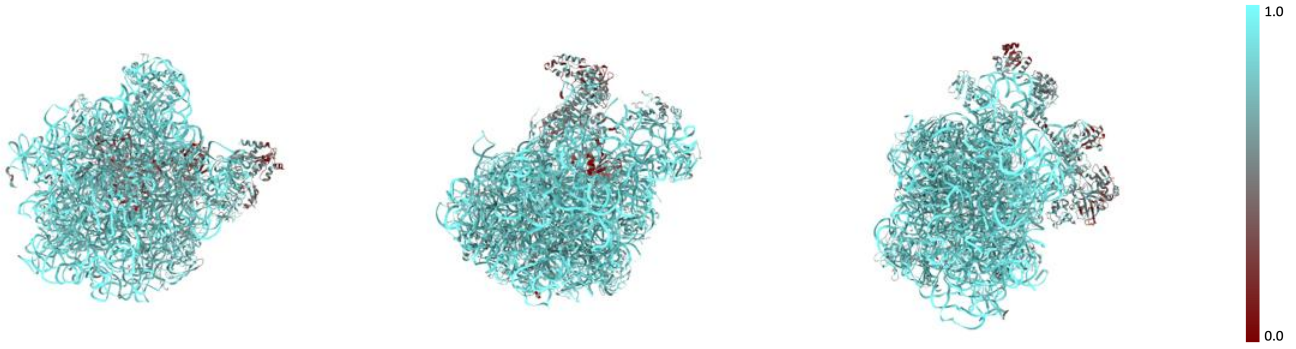
9.2 Q-score mapped to coordinate model



X Y Z

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.

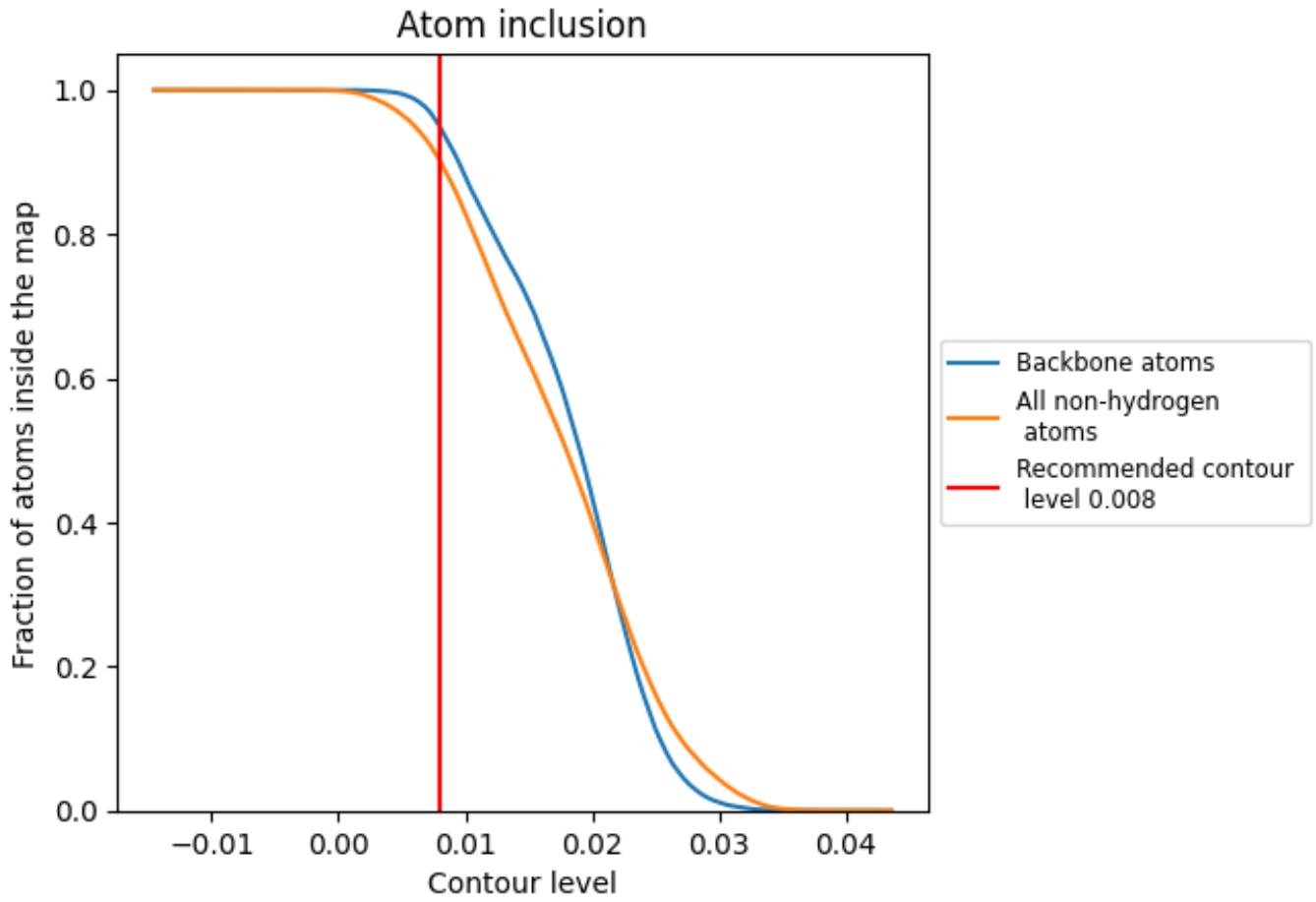
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.008).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9017	0.4970
0	0.5309	0.2700
1	0.6594	0.4060
2	0.9200	0.4260
A	0.9725	0.5250
B	0.9703	0.4700
E	0.8576	0.5290
F	0.8243	0.5220
G	0.8285	0.4960
H	0.7261	0.3620
I	0.7721	0.4410
K	0.5308	0.2540
L	0.4279	0.2840
N	0.8324	0.5040
O	0.7670	0.4930
P	0.8277	0.5090
Q	0.8244	0.5060
R	0.8113	0.4940
S	0.8061	0.4390
T	0.7539	0.4880
U	0.8647	0.5110
V	0.8340	0.5150
W	0.8120	0.5110
X	0.7784	0.4830
Y	0.8026	0.4840
a	0.8491	0.5240
b	0.6088	0.4870
c	0.7568	0.4190
d	0.8180	0.4800
f	0.8198	0.5190
g	0.8165	0.4960
h	0.8696	0.5390
i	0.8497	0.5420
j	0.8276	0.5240