wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 03:17 pm GMT

PDB ID	:	2WWA
EMDB ID	:	EMD-1669
Title	:	Cryo-EM structure of idle yeast Ssh1 complex bound to the yeast 80S ribosome
Authors	:	Becker, T.; Mandon, E.; Bhushan, S.; Jarasch, A.; Armache, J.P.; Funes, S.; Jossinet, F.; Gumbart, J.; Mielke, T.; Berninghausen, O.; Schulten, K.; Westhof, E.; Gilmore, R.; Beckmann, R.
Deposited on	:	2009-10-22
Resolution	:	8.90 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

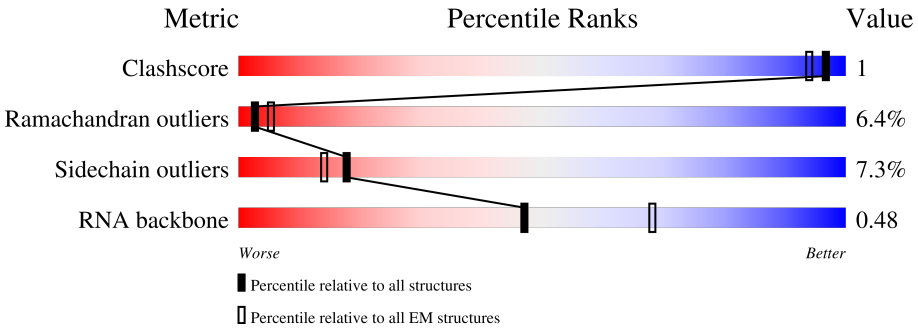
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 8.90 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	A	490	63%, 91%, 8%
2	B	80	55%, 72%, 25%
3	C	87	23%, 22%, 76%
4	D	63	8%, 54%, 44%
5	E	34	6%, 71%, 29%
6	F	25	100%
7	G	18	94%, 6%

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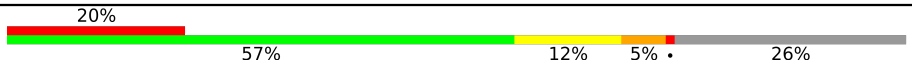
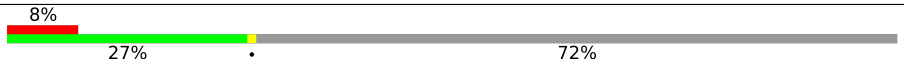
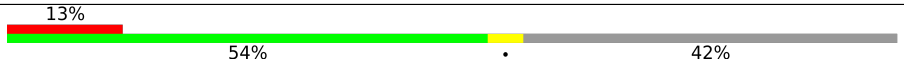
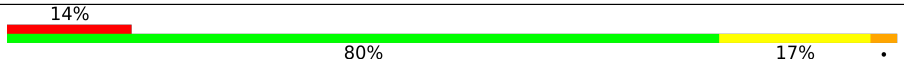
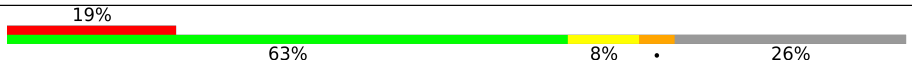
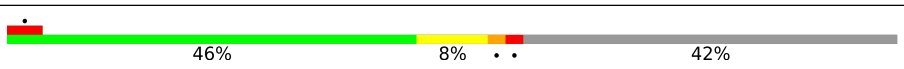
Mol	Chain	Length	Quality of chain
8	H	362	
9	I	184	
10	J	189	
11	K	142	
12	L	127	
13	M	113	
14	N	120	
15	O	51	

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 14301 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 SEC SIXTY-ONE PROTEIN HOMOLOG.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	490	3770	2487	603	671	9	0	0

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	60	472	318	76	77	1	0	0

- Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEB2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	C	21	162	112	24	26	0	0

- Molecule 4 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	D	63	1347	603	245	436	63	0	0

- Molecule 5 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	E	34	740	332	148	226	34	0	0

- Molecule 6 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	F	25	536	239	99	173	25	0	0

- Molecule 7 is a RNA chain called 25S RRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	18	Total	C	N	O	P	0	0
			379	169	64	128	18		

- Molecule 8 is a protein called 60S RIBOSOMAL PROTEIN L4-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	269	Total	C	N	O	S	0	0
			2039	1281	391	363	4		

- Molecule 9 is a protein called 60S RIBOSOMAL PROTEIN L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	153	Total	C	N	O	S	0	0
			1212	756	236	219	1		

- Molecule 10 is a protein called 60S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	53	Total	C	N	O	S	0	0
			410	254	83	72	1		

- Molecule 11 is a protein called 60S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	83	Total	C	N	O	S	0	0
			663	424	111	126	2		

- Molecule 12 is a protein called 60S RIBOSOMAL PROTEIN L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	127	Total	C	N	O	S	0	0
			1002	630	193	178	1		

- Molecule 13 is a protein called 60S RIBOSOMAL PROTEIN L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	84	Total	C	N	O	S	0	0
			706	447	140	118	1		

- Molecule 14 is a protein called 60S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	69	Total	C	N	O	S	0	0
			547	345	101	99	2		

- Molecule 15 is a protein called 60S RIBOSOMAL PROTEIN L39.

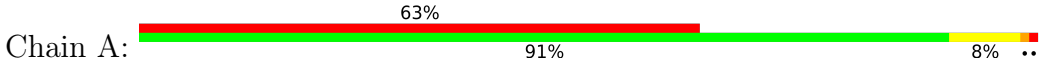
Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	37	Total	C	N	O	S	0	0
			316	200	66	48	2		

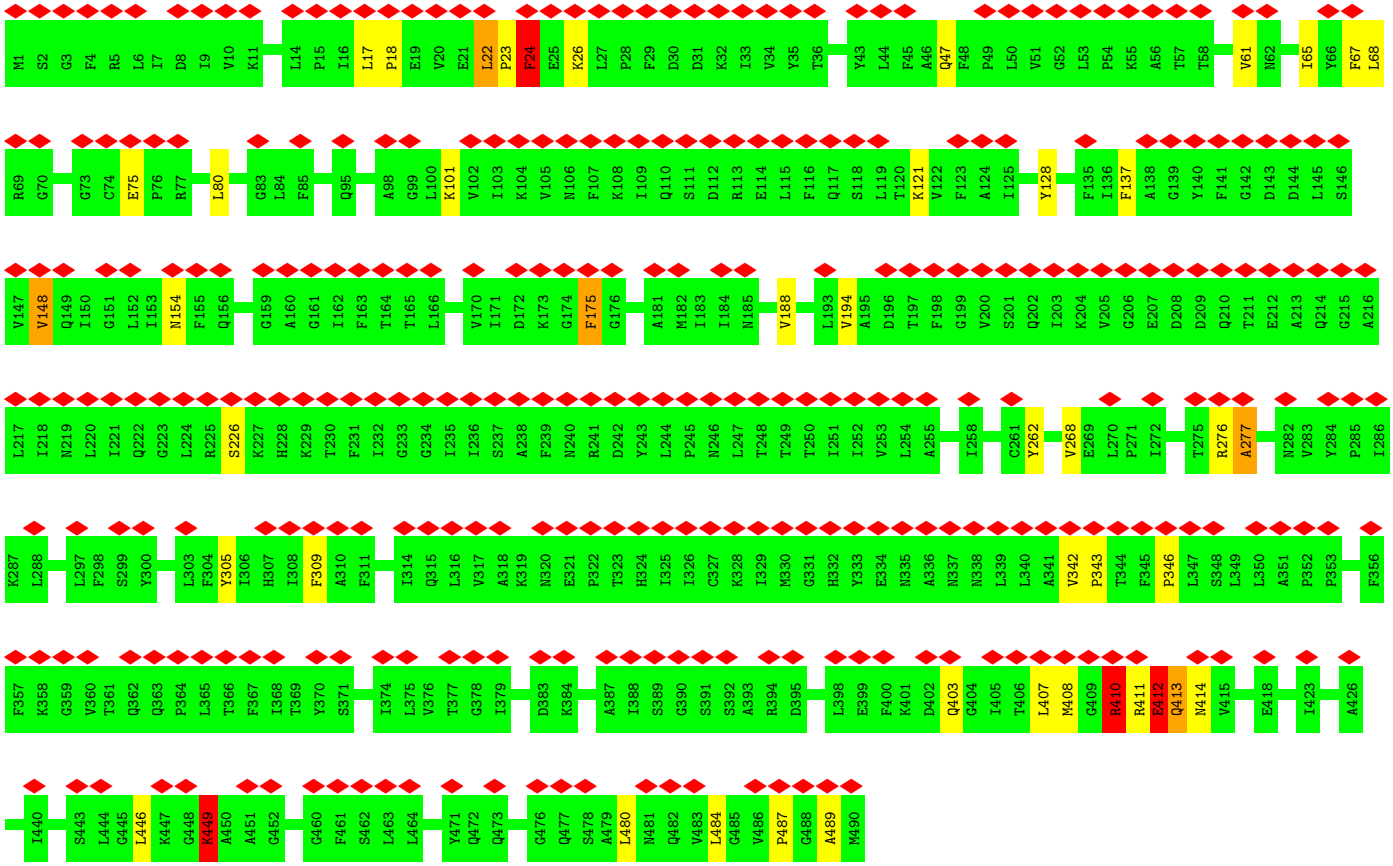
3 Residue-property plots (i)

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: SEC SIXTY-ONE PROTEIN HOMOLOG

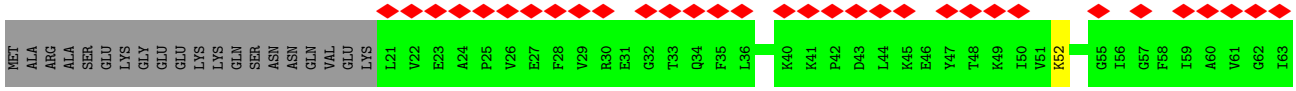
Chain A:

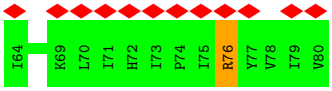




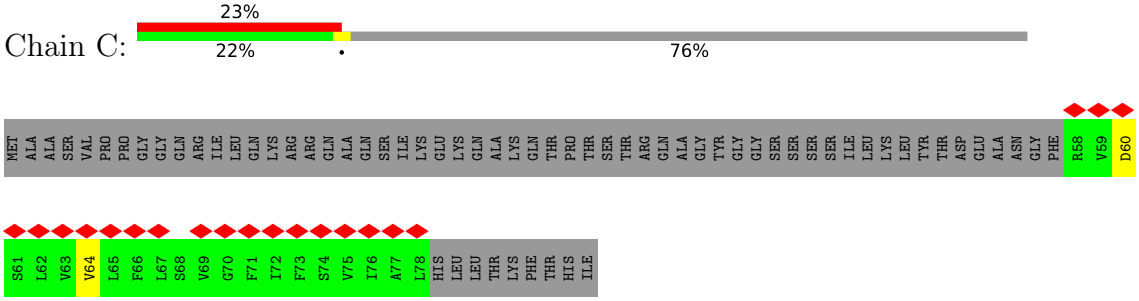
• Molecule 2: PROTEIN TRANSPORT PROTEIN SSS1

Chain B:

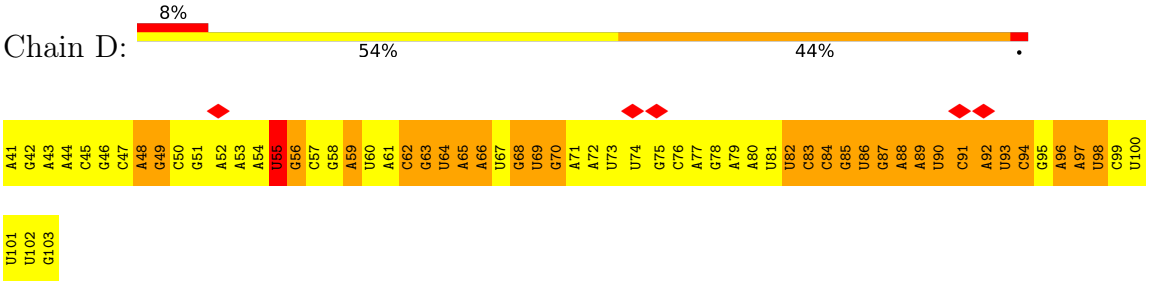




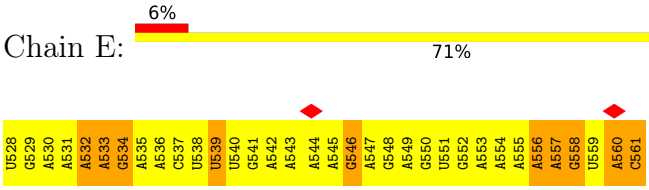
• Molecule 3: PROTEIN TRANSPORT PROTEIN SEB2



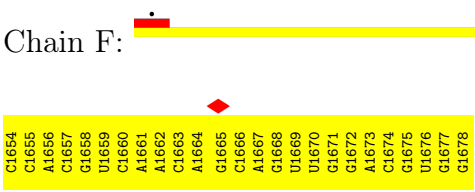
• Molecule 4: 25S RRNA



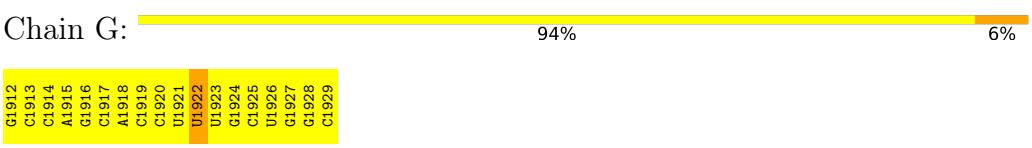
• Molecule 5: 25S RRNA



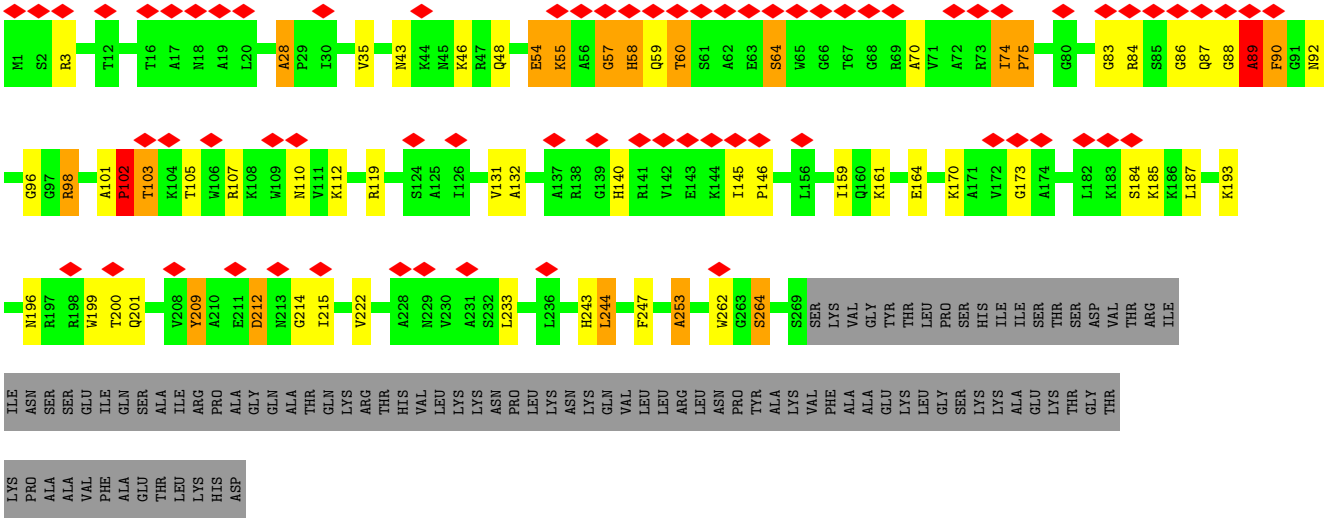
• Molecule 6: 25S RRNA



• Molecule 7: 25S RRNA

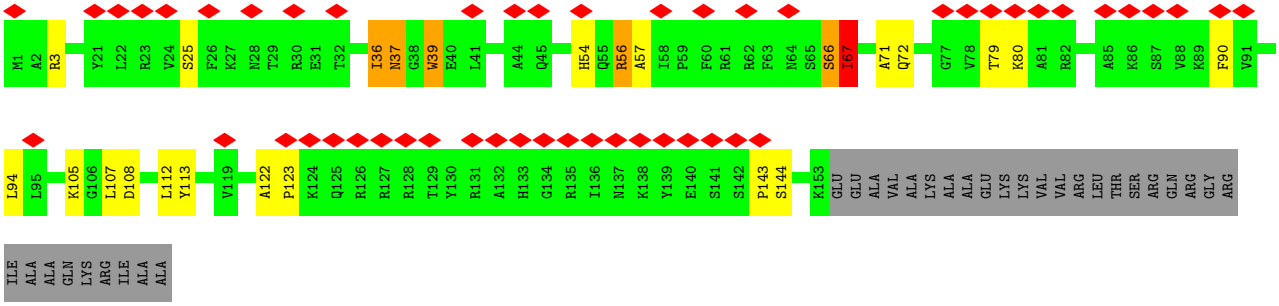


• Molecule 8: 60S RIBOSOMAL PROTEIN L4-B



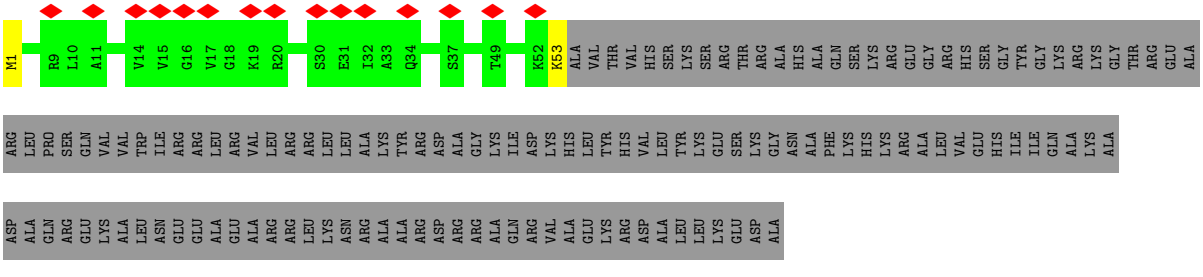
• Molecule 9: 60S RIBOSOMAL PROTEIN L17-A

Chain I:



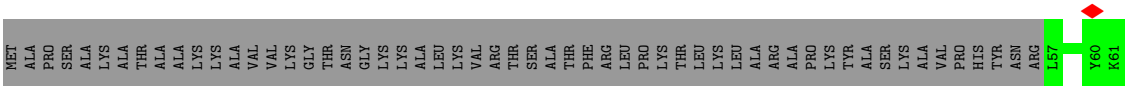
• Molecule 10: 60S RIBOSOMAL PROTEIN L19

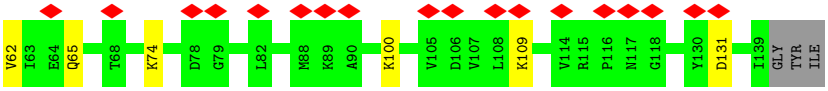
Chain J:



• Molecule 11: 60S RIBOSOMAL PROTEIN L25

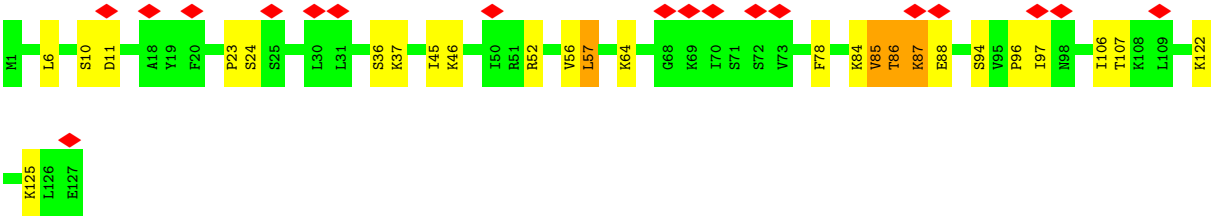
Chain K:





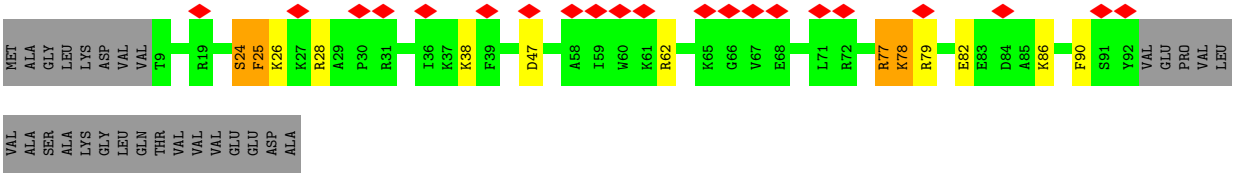
• Molecule 12: 60S RIBOSOMAL PROTEIN L26-A

Chain L:



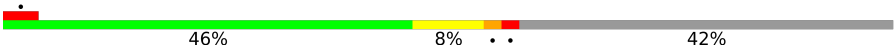
• Molecule 13: 60S RIBOSOMAL PROTEIN L31-A

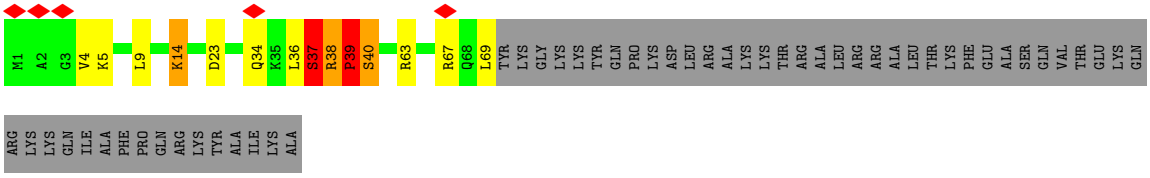
Chain M:



• Molecule 14: 60S RIBOSOMAL PROTEIN L35

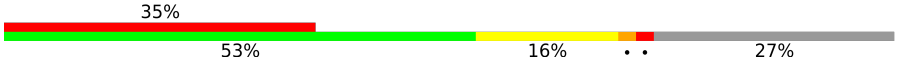
Chain N:

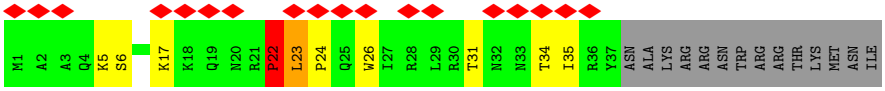




• Molecule 15: 60S RIBOSOMAL PROTEIN L39

Chain O:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	20400	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUP VOLUMES	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	38000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	7.747	Depositor
Minimum map value	-3.672	Depositor
Average map value	0.049	Depositor
Map value standard deviation	0.609	Depositor
Recommended contour level	1.75	Depositor
Map size (Å)	455.4, 455.4, 455.4	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2375, 1.2375, 1.2375	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.90	0/3848	1.03	10/5234 (0.2%)
2	B	0.89	0/481	0.91	0/648
3	C	0.96	0/164	0.89	0/222
4	D	1.59	0/1508	2.60	196/2348 (8.3%)
5	E	1.59	0/833	2.65	118/1298 (9.1%)
6	F	1.60	0/599	2.41	71/932 (7.6%)
7	G	1.54	0/421	2.27	50/653 (7.7%)
8	H	0.99	0/2079	1.31	22/2817 (0.8%)
9	I	1.03	0/1235	1.27	9/1662 (0.5%)
10	J	1.01	0/412	0.90	0/551
11	K	0.90	0/670	0.96	0/903
12	L	1.01	0/1013	1.17	3/1351 (0.2%)
13	M	1.09	0/719	1.19	5/959 (0.5%)
14	N	1.06	1/549 (0.2%)	1.33	9/733 (1.2%)
15	O	1.08	0/321	1.31	3/426 (0.7%)
All	All	1.14	1/14852 (0.0%)	1.61	496/20737 (2.4%)

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
1	A	0	3
4	D	0	2
8	H	0	2
9	I	0	1
12	L	0	1
14	N	0	2
15	O	0	2
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	69	LEU	C-O	-12.06	1.00	1.23

The worst 5 of 496 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	532	A	P-O3'-C3'	18.42	141.80	119.70
4	D	69	U	P-O3'-C3'	14.68	137.31	119.70
4	D	65	A	P-O3'-C3'	13.79	136.25	119.70
4	D	90	U	P-O3'-C3'	13.58	136.00	119.70
5	E	555	A	N1-C6-N6	13.40	126.64	118.60

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	LEU	Peptide
1	A	262	TYR	Sidechain
1	A	407	LEU	Peptide
4	D	55	U	Sidechain
4	D	60	U	Sidechain

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	A	3770	0	3941	4	0
2	B	472	0	519	1	0
3	C	162	0	177	0	0
4	D	1347	0	678	0	0
5	E	740	0	369	1	0
6	F	536	0	272	0	0
7	G	379	0	195	0	0
8	H	2039	0	2106	7	0
9	I	1212	0	1231	2	0
10	J	410	0	452	0	0
11	K	663	0	699	0	0
12	L	1002	0	1093	2	0
13	M	706	0	741	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	N	547	0	613	2	0
15	O	316	0	349	0	0
All	All	14301	0	13435	19	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 1.

The worst 5 of 19 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)
5:E:539:U:H3	5:E:546:G:H1	1.46	0.61
8:H:88:GLY:HA3	8:H:89:ALA:HB3	1.86	0.57
8:H:74:ILE:H	8:H:75:PRO:HA	1.76	0.50
1:A:410:ARG:HH22	1:A:412:GLU:HG3	1.79	0.48
2:B:76:ARG:HE	2:B:76:ARG:HA	1.81	0.46

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	A	488/490 (100%)	434 (89%)	37 (8%)	17 (4%)	3 25
2	B	58/80 (72%)	55 (95%)	3 (5%)	0	100 100
3	C	19/87 (22%)	17 (90%)	1 (5%)	1 (5%)	2 19
8	H	267/362 (74%)	187 (70%)	47 (18%)	33 (12%)	0 5
9	I	151/184 (82%)	114 (76%)	27 (18%)	10 (7%)	1 16
10	J	51/189 (27%)	49 (96%)	2 (4%)	0	100 100
11	K	81/142 (57%)	72 (89%)	6 (7%)	3 (4%)	3 24
12	L	125/127 (98%)	101 (81%)	12 (10%)	12 (10%)	0 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	M	82/113 (73%)	65 (79%)	11 (13%)	6 (7%)	1 14
14	N	67/120 (56%)	61 (91%)	2 (3%)	4 (6%)	1 17
15	O	35/51 (69%)	25 (71%)	5 (14%)	5 (14%)	0 4
All	All	1424/1945 (73%)	1180 (83%)	153 (11%)	91 (6%)	3 16

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	PRO
1	A	148	VAL
1	A	277	ALA
1	A	411	ARG
1	A	413	GLN

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	A	412/412 (100%)	388 (94%)	24 (6%)	20 45
2	B	50/67 (75%)	48 (96%)	2 (4%)	31 55
3	C	19/73 (26%)	18 (95%)	1 (5%)	22 47
8	H	209/288 (73%)	188 (90%)	21 (10%)	7 26
9	I	124/146 (85%)	113 (91%)	11 (9%)	9 30
10	J	44/154 (29%)	42 (96%)	2 (4%)	27 52
11	K	74/118 (63%)	71 (96%)	3 (4%)	30 55
12	L	110/110 (100%)	100 (91%)	10 (9%)	9 29
13	M	74/97 (76%)	67 (90%)	7 (10%)	8 27
14	N	62/105 (59%)	57 (92%)	5 (8%)	11 35
15	O	33/46 (72%)	30 (91%)	3 (9%)	9 29
All	All	1211/1616 (75%)	1122 (93%)	89 (7%)	18 39

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	I	112	LEU
12	L	88	GLU
10	J	1	MET
12	L	52	ARG
13	M	38	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	87	GLN
11	K	111	ASN
12	L	42	GLN
11	K	117	ASN
1	A	414	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	D	62/63 (98%)	22 (35%)	9 (14%)
5	E	33/34 (97%)	7 (21%)	2 (6%)
6	F	24/25 (96%)	0	0
7	G	17/18 (94%)	1 (5%)	0
All	All	136/140 (97%)	30 (22%)	11 (8%)

5 of 30 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	D	49	G
4	D	56	G
4	D	59	A
4	D	62	C
4	D	63	G

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	D	93	U
4	D	96	A
5	E	560	A

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Mol	Chain	Res	Type
5	E	532	A
4	D	69	U

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)

There are no chain breaks in this entry.

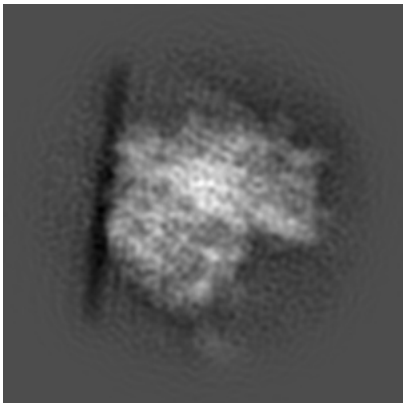
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1669. These allow visual inspection of the internal detail of the map and identification of artifacts.

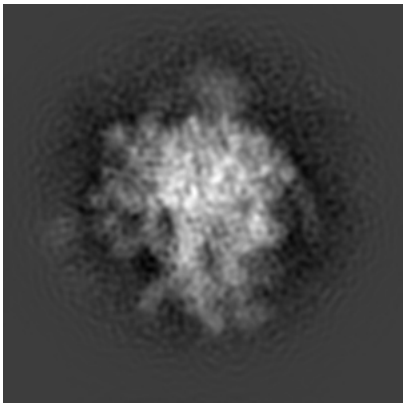
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

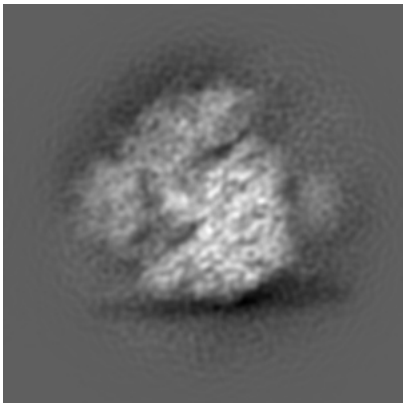
6.1.1 Primary map



X



Y

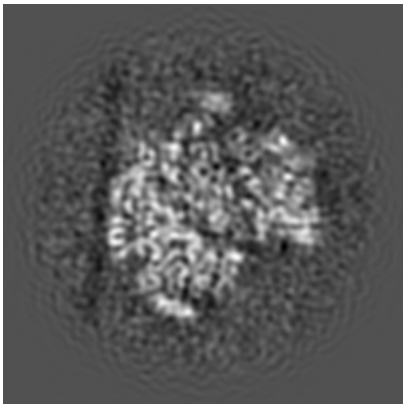


Z

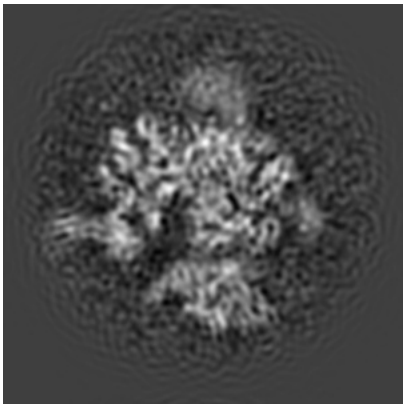
The images above show the map projected in three orthogonal directions.

6.2 Central slices

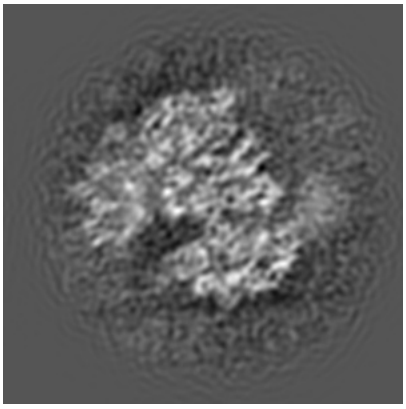
6.2.1 Primary map



X Index: 184



Y Index: 184

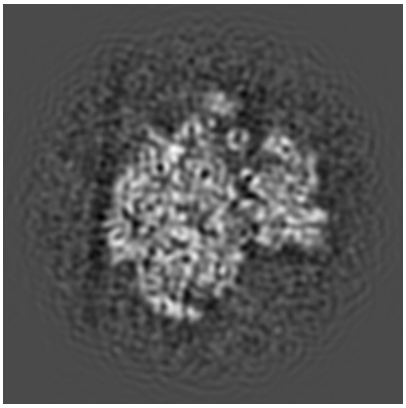


Z Index: 184

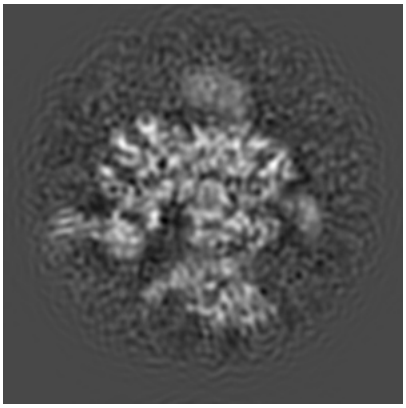
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

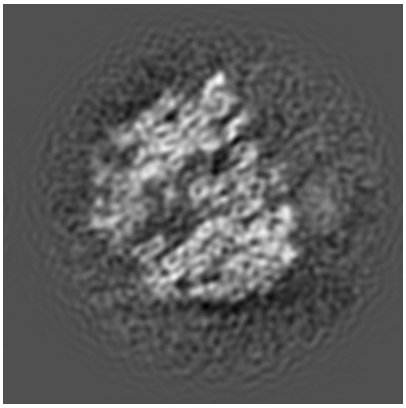
6.3.1 Primary map



X Index: 188



Y Index: 187

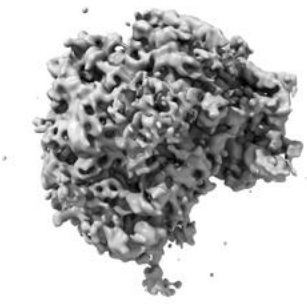


Z Index: 172

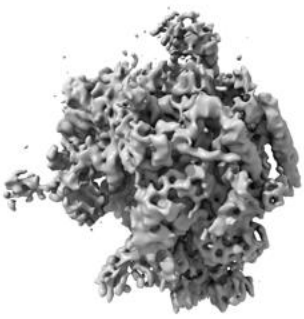
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

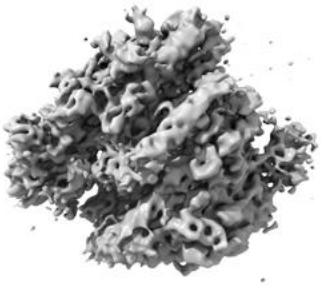
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.75. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

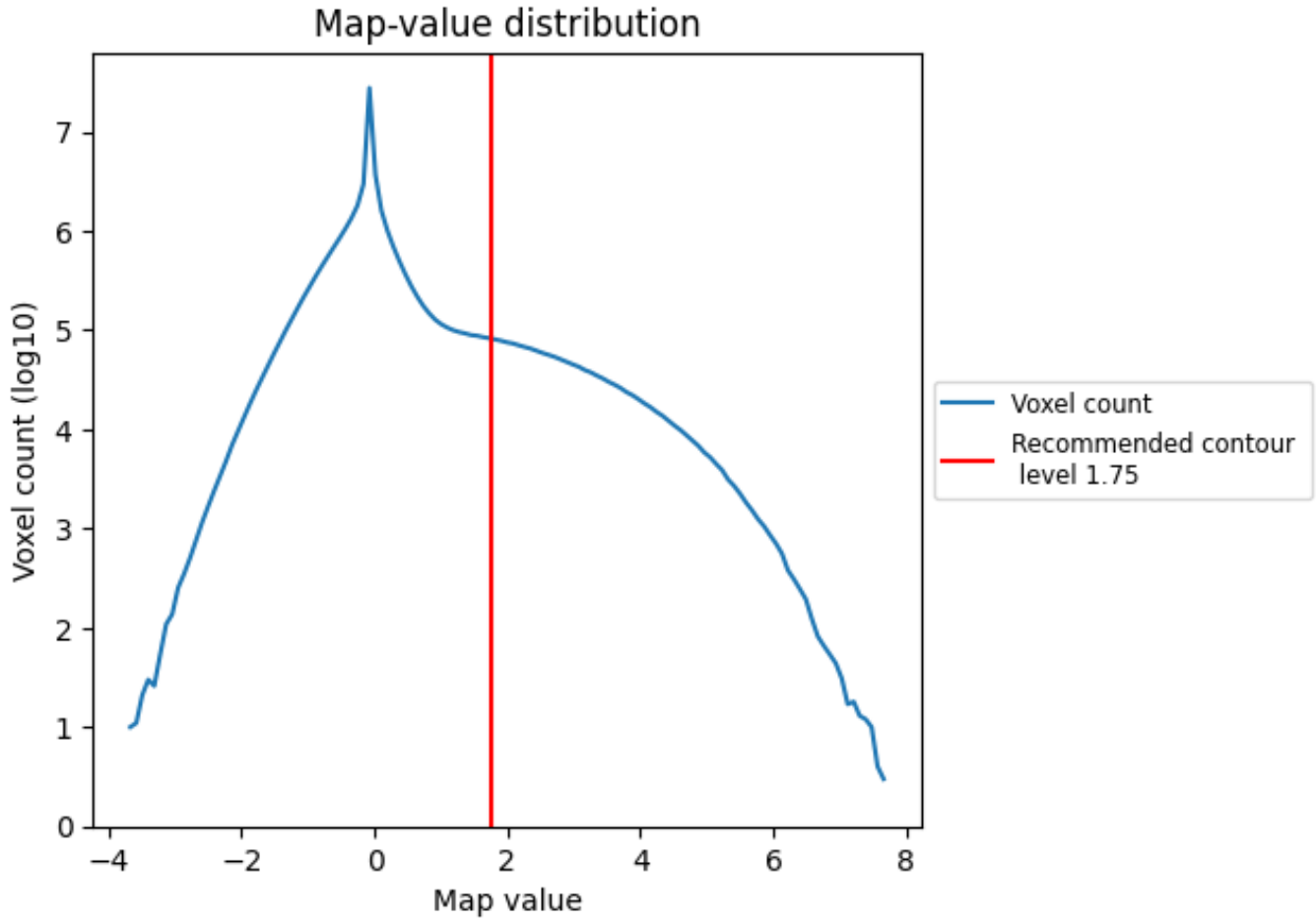
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

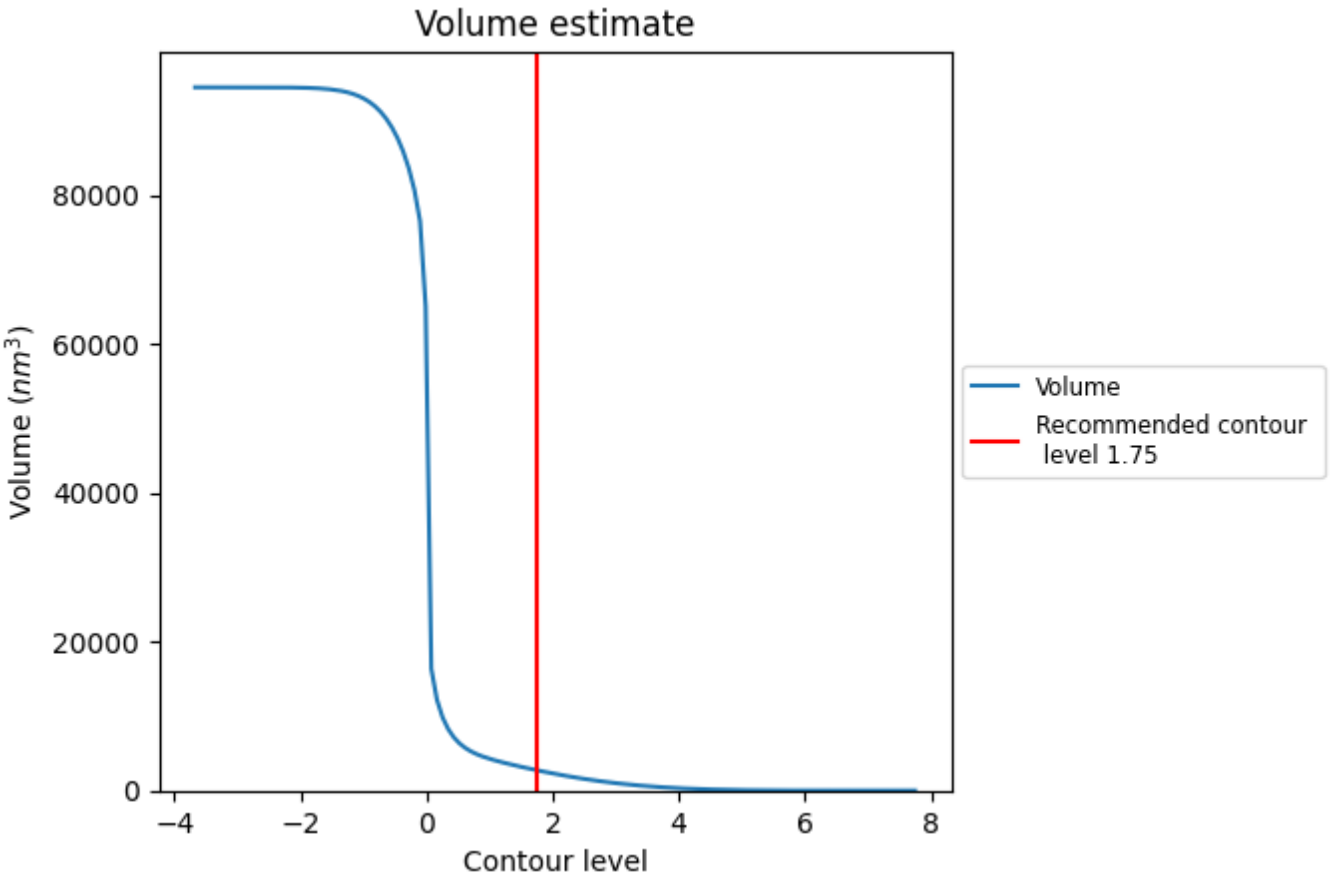
This section contains the results of statistical analysis of the map.

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.

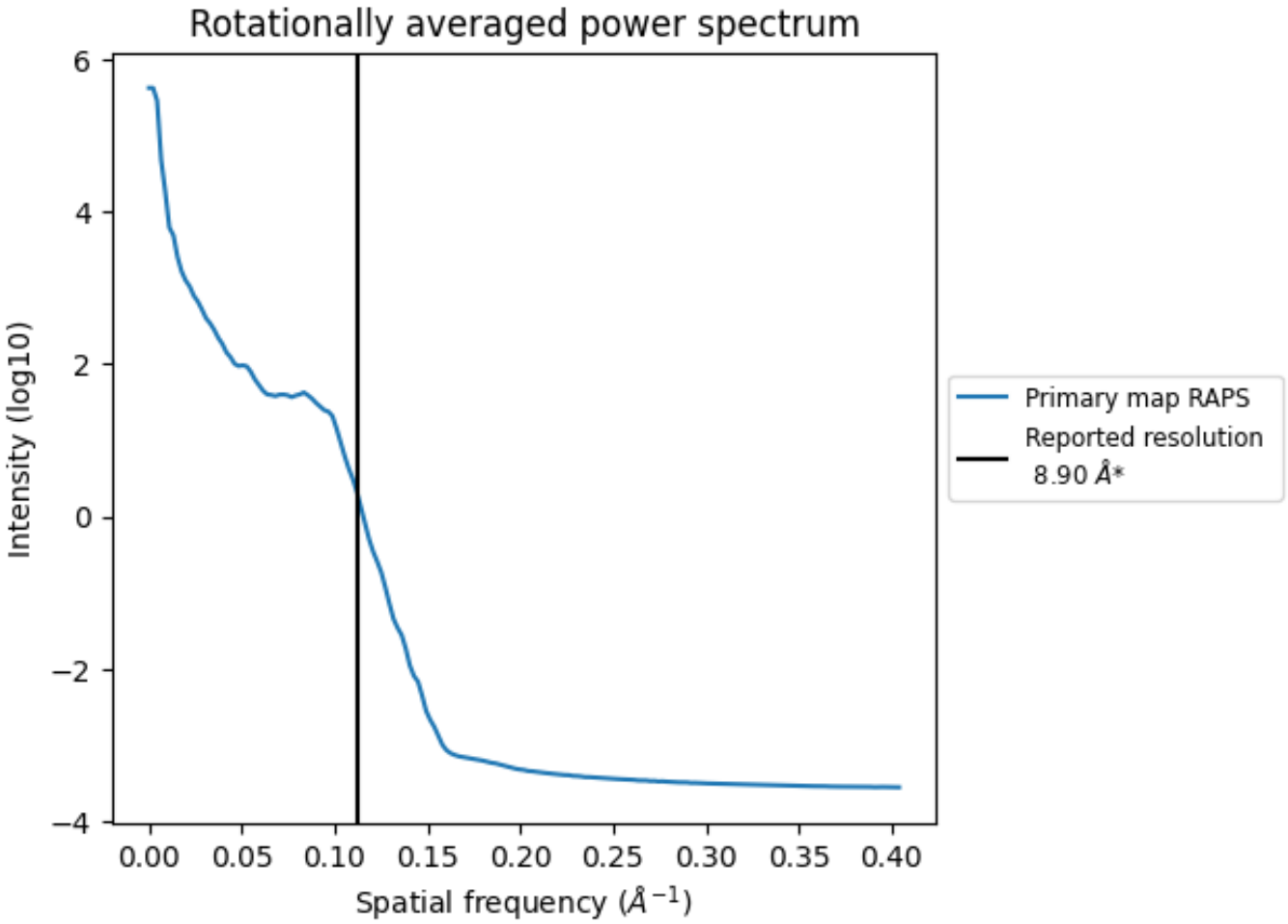
7.2 Volume estimate (i)



The volume at the recommended contour level is 2728 nm^3; this corresponds to an approximate mass of 2464 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 0.112 Å^{-1}

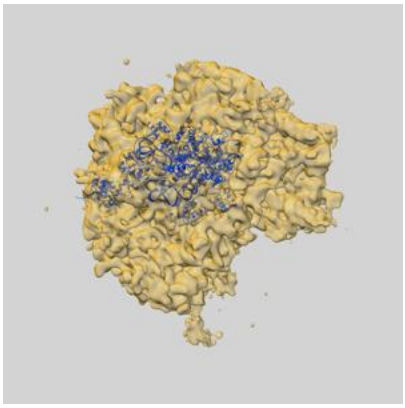
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

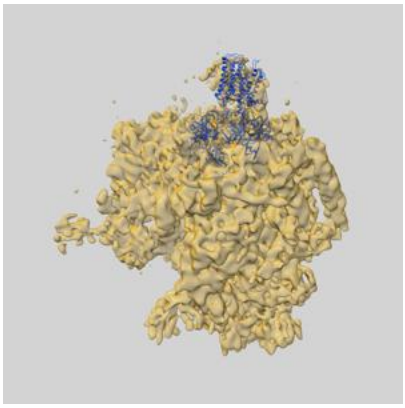
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1669 and PDB model 2WWA. Per-residue inclusion information can be found in section 3 on page 7.

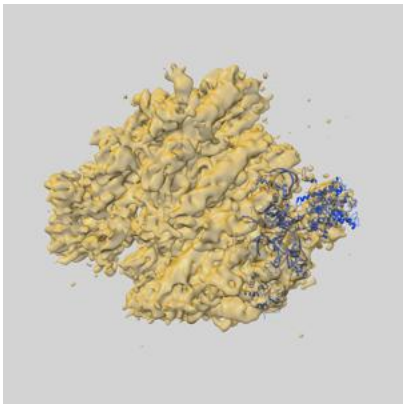
9.1 Map-model overlay



X



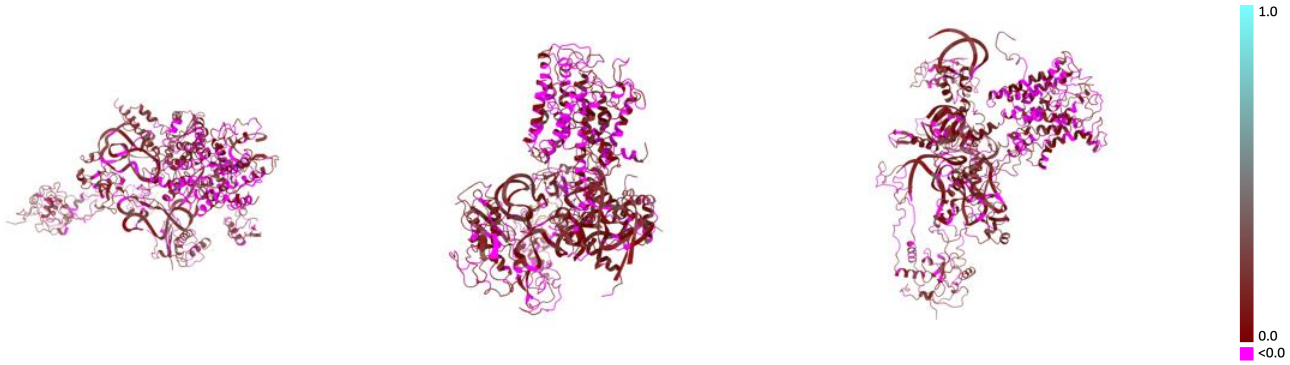
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.75 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.

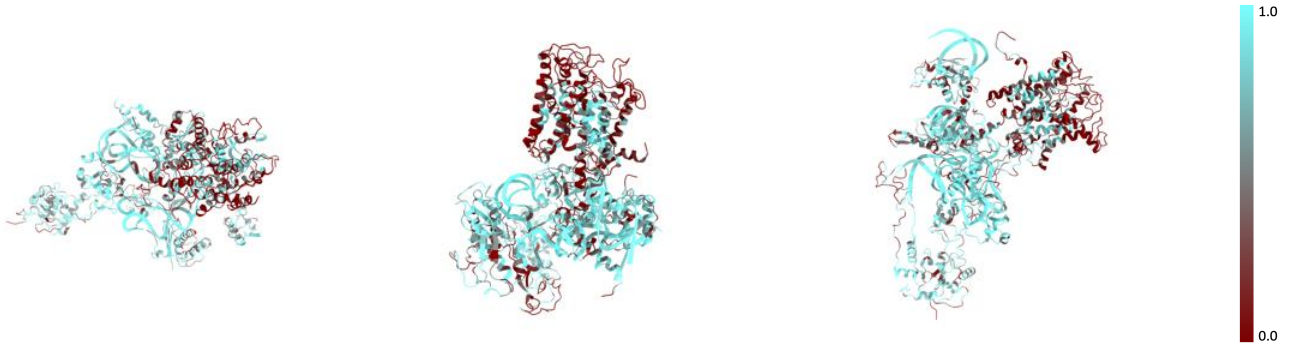
9.2 Q-score mapped to coordinate model (i)



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.

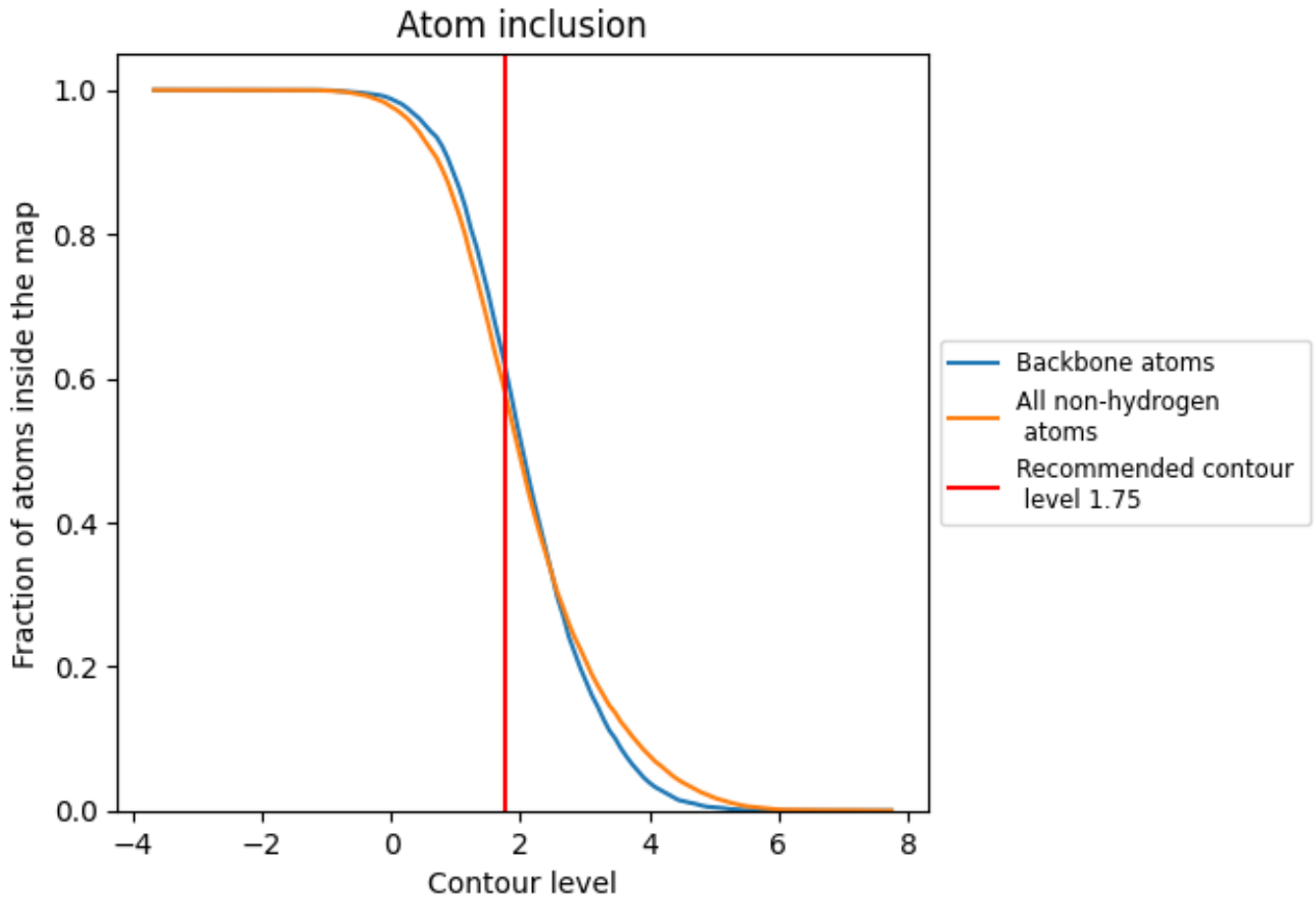
9.3 Atom inclusion mapped to coordinate model (i)



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 (1.75).

9.4 Atom inclusion (i)



At the recommended contour level, 62% of all backbone atoms, 58% 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 (1.75) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5845	0.0690
A	0.3307	0.0200
B	0.2366	-0.0190
C	0.0813	-0.0380
D	0.8426	0.0880
E	0.9000	0.1320
F	0.8731	0.1230
G	0.8628	0.1460
H	0.6351	0.0780
I	0.5587	0.0630
J	0.6266	0.1170
K	0.6258	0.0860
L	0.7487	0.0990
M	0.6265	0.0860
N	0.7537	0.1180
O	0.4309	0.0690