



wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 01:52 am GMT

PDB ID : 6GC7
EMDB ID : EMD-4382
Title : 50S ribosomal subunit assembly intermediate state 1
Authors : Nikolay, R.; Hilal, T.; Qin, B.; Loerke, J.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on : 2018-04-17
Resolution : 4.30 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:

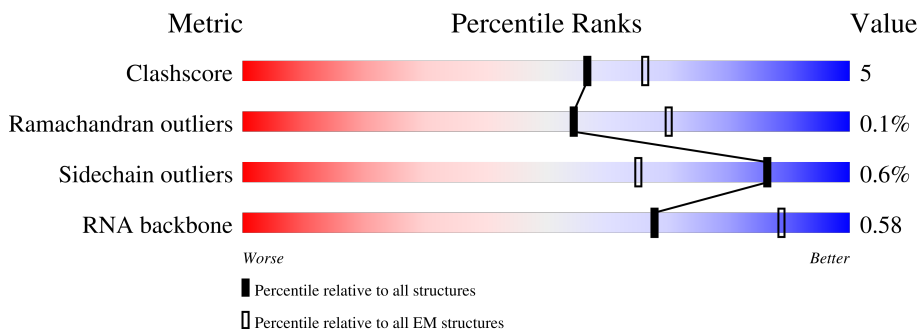
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 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 $\leq 5\%$. 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	A	2904	7% (poor fit), 42% (0 outliers), 21% (1 outlier), 35% (2+ outliers)
2	D	209	8% (poor fit), 74% (0 outliers), 13% (1 outlier), 13% (2+ outliers)
3	E	201	13% (poor fit), 84% (0 outliers), 16% (1 outlier)
4	J	142	11% (poor fit), 87% (0 outliers), 13% (1 outlier)
5	K	122	39% (poor fit), 90% (0 outliers), 10% (1 outlier)
6	L	143	53% (poor fit), 62% (0 outliers), 14% (1 outlier), 24% (2+ outliers)
7	N	120	79% (0 outliers), 20% (1 outlier)

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Mol	Chain	Length	Quality of chain
8	P	114	
9	Q	117	
10	R	103	
11	S	110	
12	T	93	
13	U	102	
14	Y	63	
15	0	56	
16	2	46	
17	Z	58	

2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 54410 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1901	40850	18224	7571	13154	1901	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	D	182	1366	863	245	254	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	201	1552	974	283	290	5	0	0

- Molecule 4 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	J	142	1129	714	212	199	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	122	939	587	180	166	6	0	0

- Molecule 6 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	L	109	778	483	149	146	0	0

- Molecule 7 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	120	961	593	196	167	5	0	0

- Molecule 8 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	P	114	917	574	179	163	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	Q	117	947	604	192	151	0	0

- Molecule 10 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	R	103	816	516	153	145	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	S	110	857	532	166	156	3	0	0

- Molecule 12 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	T	93	739	466	139	132	2	0	0

- Molecule 13 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	U	102	780	492	146	142	0	0

- Molecule 14 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	Y	63	509	313	99	95	2	0	0

- Molecule 15 is a protein called 50S ribosomal protein L32.

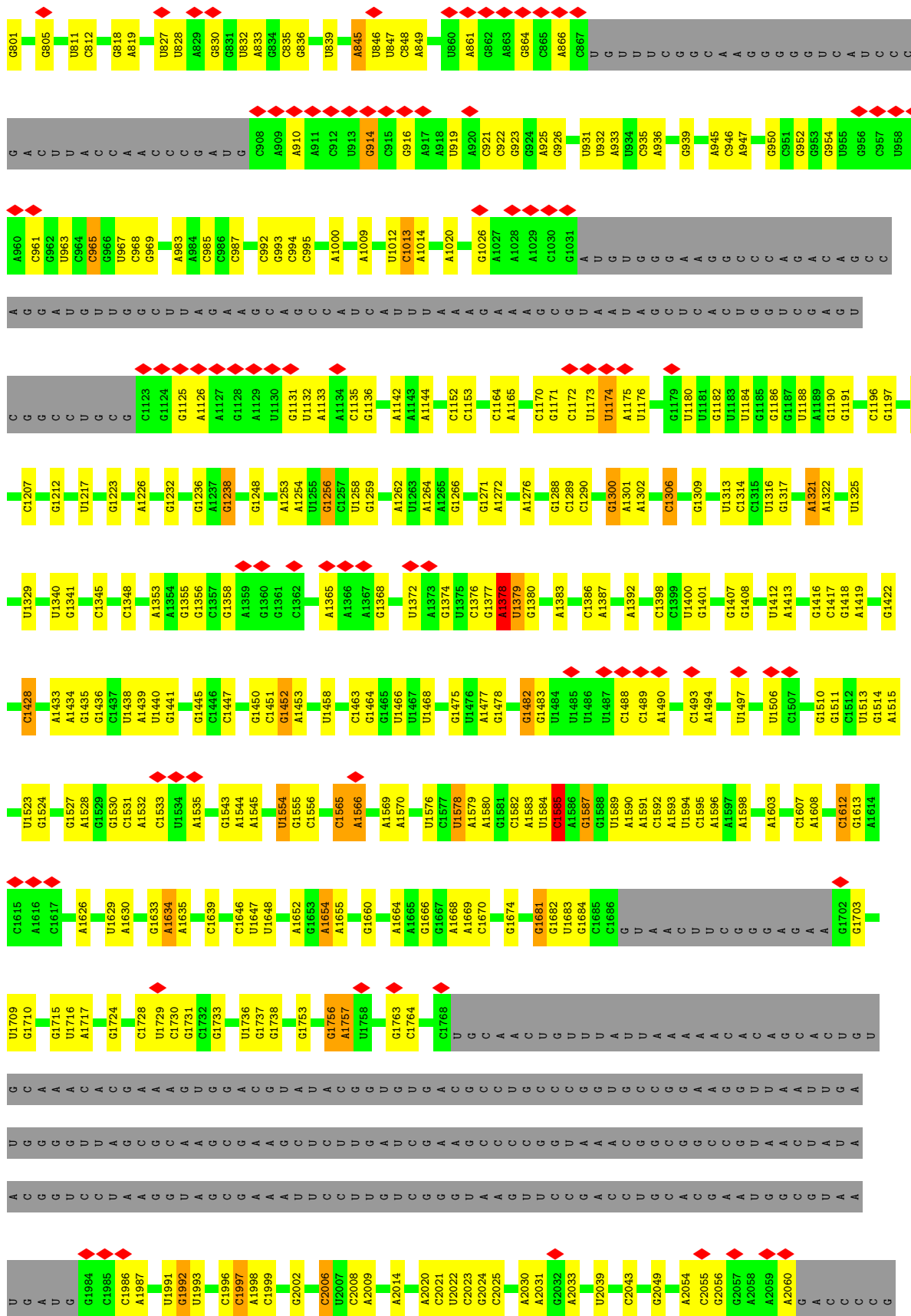
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	0	56	444	269	94	80	1	0	0

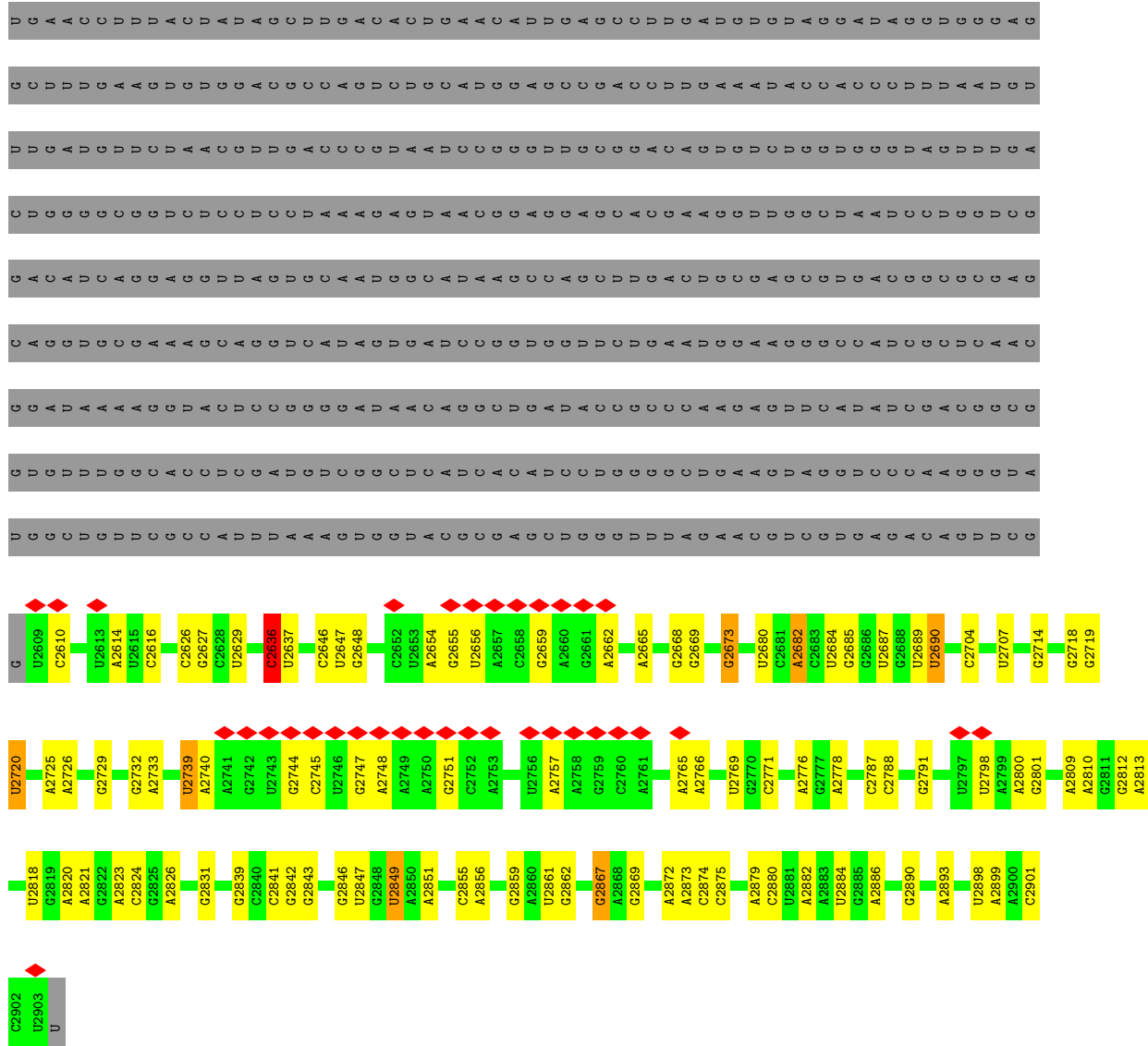
- Molecule 16 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	2	46	377	228	90	57	2	0	0

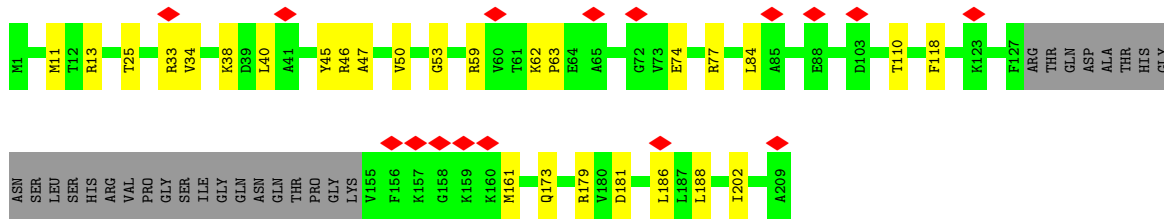
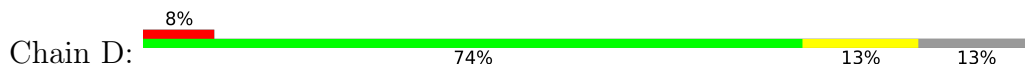
- Molecule 17 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	Z	58	449	281	87	79	2	0	0

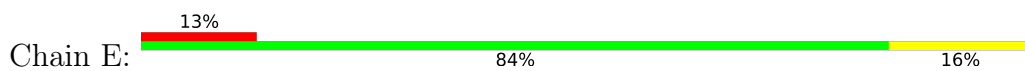


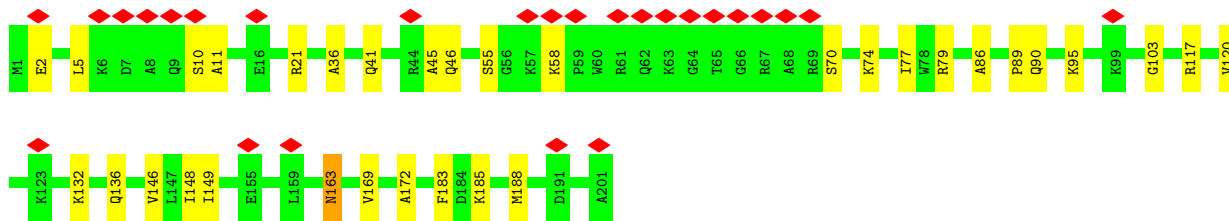


• Molecule 2: 50S ribosomal protein L3

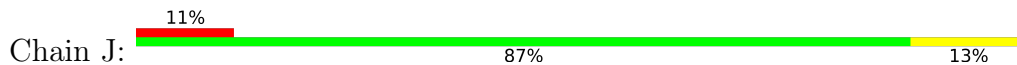


• Molecule 3: 50S ribosomal protein L4

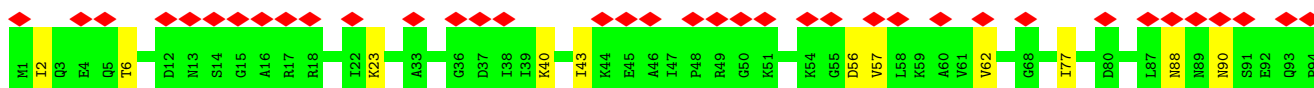
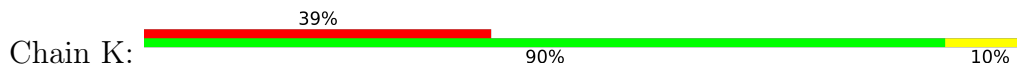




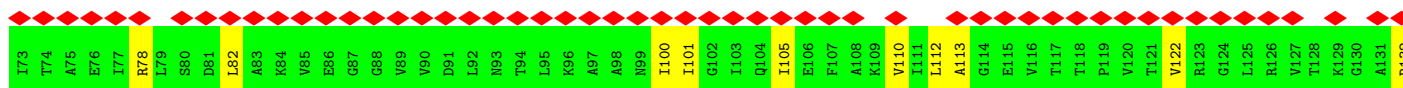
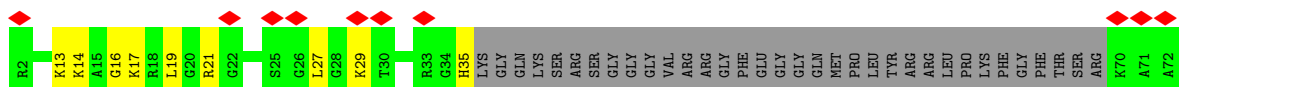
- Molecule 4: 50S ribosomal protein L13



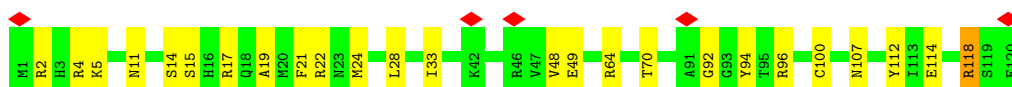
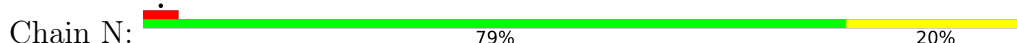
- Molecule 5: 50S ribosomal protein L14



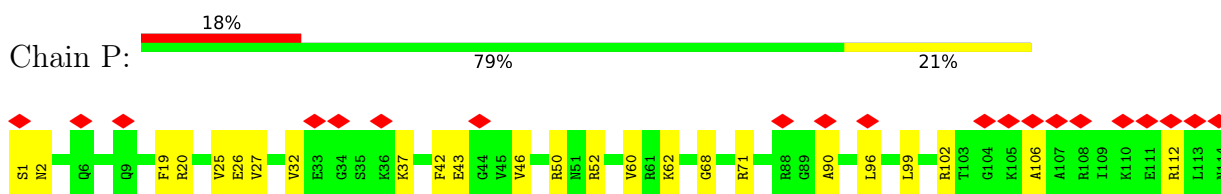
- Molecule 6: 50S ribosomal protein L15



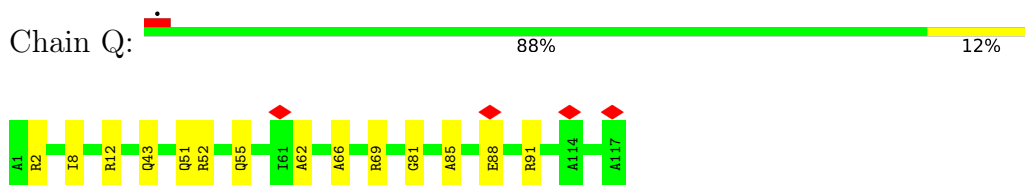
- Molecule 7: 50S ribosomal protein L17



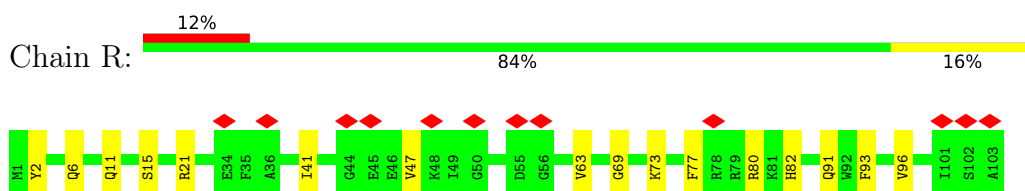
- Molecule 8: 50S ribosomal protein L19



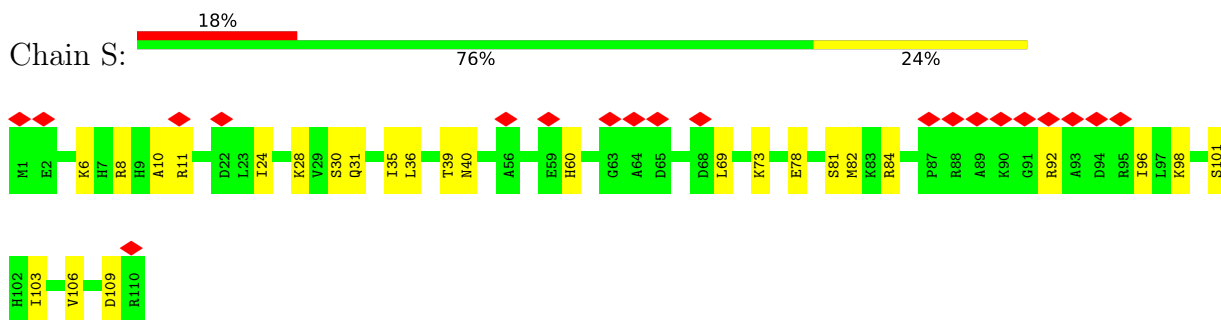
- Molecule 9: 50S ribosomal protein L20



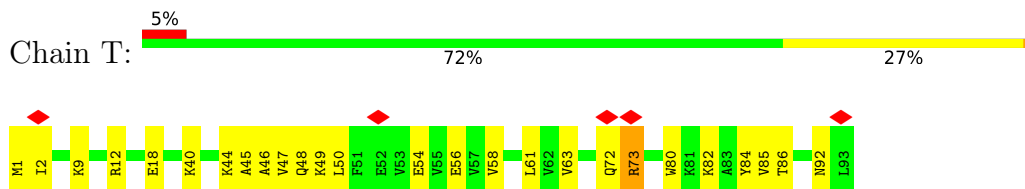
- Molecule 10: 50S ribosomal protein L21



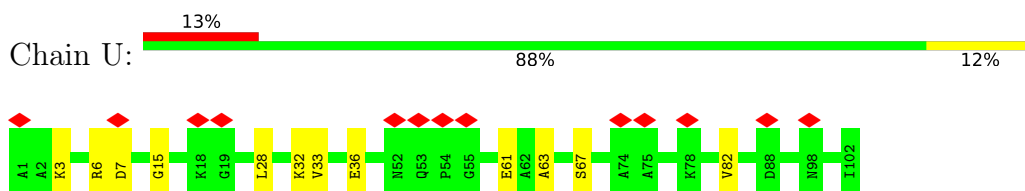
- Molecule 11: 50S ribosomal protein L22



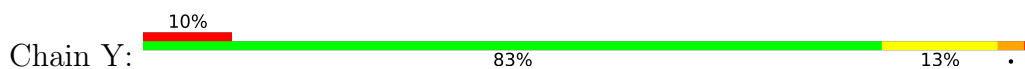
- Molecule 12: 50S ribosomal protein L23

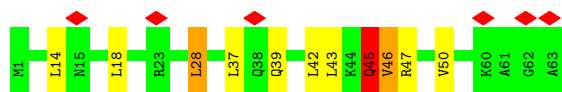


- Molecule 13: 50S ribosomal protein L24

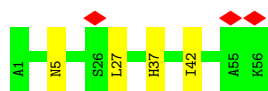
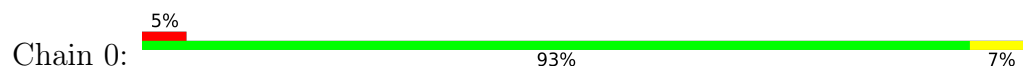


- Molecule 14: 50S ribosomal protein L29

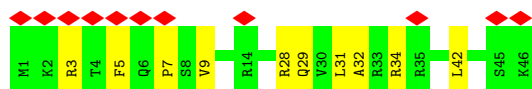
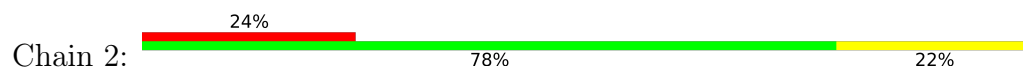




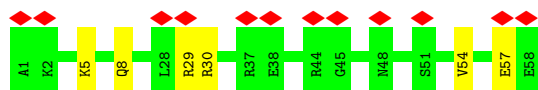
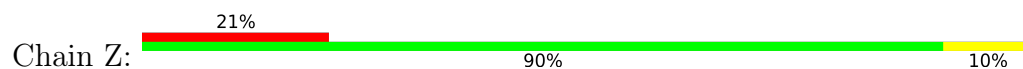
- Molecule 15: 50S ribosomal protein L32



- Molecule 16: 50S ribosomal protein L34



- Molecule 17: 50S ribosomal protein L30



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	17389	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	10.529	Depositor
Minimum map value	-4.245	Depositor
Average map value	0.070	Depositor
Map value standard deviation	0.500	Depositor
Recommended contour level	2.2	Depositor
Map size (\AA)	334.8, 334.8, 334.8	wwPDB
Map dimensions	270, 270, 270	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.24, 1.24, 1.24	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	A	0.26	0/45758	0.95	81/71373 (0.1%)
2	D	0.26	0/1382	0.48	0/1856
3	E	0.25	0/1571	0.47	0/2113
4	J	0.25	0/1152	0.46	0/1551
5	K	0.26	0/948	0.53	0/1268
6	L	0.27	0/780	0.63	1/1041 (0.1%)
7	N	0.27	0/974	0.57	0/1301
8	P	0.26	0/929	0.47	0/1242
9	Q	0.25	0/960	0.41	0/1278
10	R	0.26	0/829	0.51	0/1107
11	S	0.23	0/864	0.48	0/1156
12	T	0.26	0/745	0.52	0/994
13	U	0.29	0/788	0.54	0/1051
14	Y	0.27	0/510	0.62	1/677 (0.1%)
15	0	0.23	0/450	0.52	0/599
16	2	0.24	0/380	0.47	0/498
17	Z	0.25	0/453	0.48	0/605
All	All	0.26	0/59473	0.88	83/89710 (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
14	Y	0	1

There are no bond length outliers.

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	635	C	N3-C2-O2	-9.40	115.32	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1306	C	N3-C2-O2	-9.04	115.57	121.90
1	A	1313	U	C2-N1-C1'	8.89	128.37	117.70
1	A	1313	U	N3-C2-O2	-8.80	116.04	122.20
1	A	1313	U	N1-C2-O2	8.78	128.94	122.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	Y	45	GLN	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	A	40850	0	20558	284	0
2	D	1366	0	1424	21	0
3	E	1552	0	1619	24	0
4	J	1129	0	1162	13	0
5	K	939	0	1012	7	0
6	L	778	0	841	15	0
7	N	961	0	1000	17	0
8	P	917	0	965	19	0
9	Q	947	0	1022	12	0
10	R	816	0	839	11	0
11	S	857	0	922	17	0
12	T	739	0	807	17	0
13	U	780	0	834	7	0
14	Y	509	0	543	7	0
15	0	444	0	461	3	0
16	2	377	0	418	9	0
17	Z	449	0	491	4	0
All	All	54410	0	34918	409	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 409 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:408:G:H1	1:A:419:U:H3	1.17	0.90
1:A:954:G:H1	1:A:963:U:H3	0.95	0.89
1:A:2747:G:H21	1:A:2757:A:H62	1.25	0.85
15:0:27:LEU:HA	15:0:37:HIS:O	1.78	0.84
1:A:78:U:H3	1:A:108:G:H1	1.25	0.84

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	
2	D	178/209 (85%)	170 (96%)	8 (4%)	0	100	100
3	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
4	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
5	K	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
6	L	105/143 (73%)	92 (88%)	13 (12%)	0	100	100
7	N	118/120 (98%)	106 (90%)	12 (10%)	0	100	100
8	P	112/114 (98%)	109 (97%)	3 (3%)	0	100	100
9	Q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
10	R	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
11	S	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
12	T	91/93 (98%)	81 (89%)	10 (11%)	0	100	100
13	U	100/102 (98%)	90 (90%)	10 (10%)	0	100	100
14	Y	61/63 (97%)	54 (88%)	5 (8%)	2 (3%)	4	30
15	0	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
16	2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	Z	56/58 (97%)	56 (100%)	0	0	100	100
All	All	1702/1799 (95%)	1599 (94%)	101 (6%)	2 (0%)	54	85

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	Y	46	VAL
14	Y	45	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	
2	D	142/164 (87%)	142 (100%)	0	100	100
3	E	165/165 (100%)	164 (99%)	1 (1%)	86	92
4	J	116/116 (100%)	115 (99%)	1 (1%)	78	88
5	K	103/103 (100%)	101 (98%)	2 (2%)	57	75
6	L	76/102 (74%)	76 (100%)	0	100	100
7	N	100/100 (100%)	99 (99%)	1 (1%)	76	86
8	P	99/99 (100%)	99 (100%)	0	100	100
9	Q	89/89 (100%)	89 (100%)	0	100	100
10	R	84/84 (100%)	83 (99%)	1 (1%)	71	84
11	S	93/93 (100%)	92 (99%)	1 (1%)	73	85
12	T	80/80 (100%)	78 (98%)	2 (2%)	47	68
13	U	83/83 (100%)	83 (100%)	0	100	100
14	Y	55/55 (100%)	55 (100%)	0	100	100
15	0	47/47 (100%)	47 (100%)	0	100	100
16	2	38/38 (100%)	38 (100%)	0	100	100
17	Z	48/48 (100%)	48 (100%)	0	100	100
All	All	1418/1466 (97%)	1409 (99%)	9 (1%)	86	92

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	T	73	ARG
12	T	92	ASN
5	K	90	ASN
7	N	118	ARG
10	R	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
12	T	92	ASN
13	U	73	ASN
13	U	68	ASN
9	Q	43	GLN
12	T	70	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1892/2904 (65%)	296 (15%)	3 (0%)

5 of 296 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	14	A
1	A	27	G
1	A	45	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	271	G
1	A	479	A
1	A	1378	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
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2045:C	O3'	2046:G	P	3.45
1	A	973:A	O3'	974:G	P	3.31

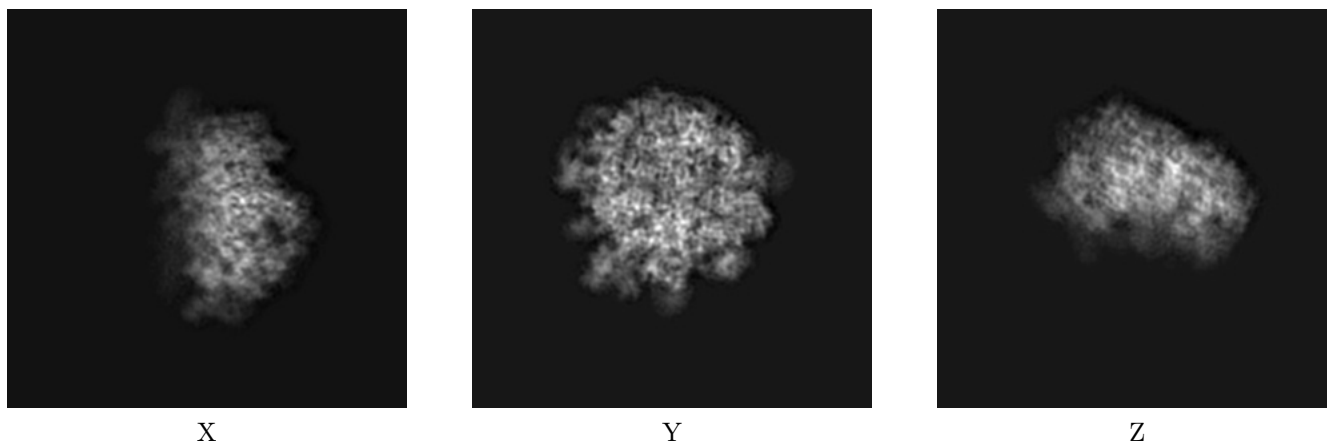
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4382. 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](#)

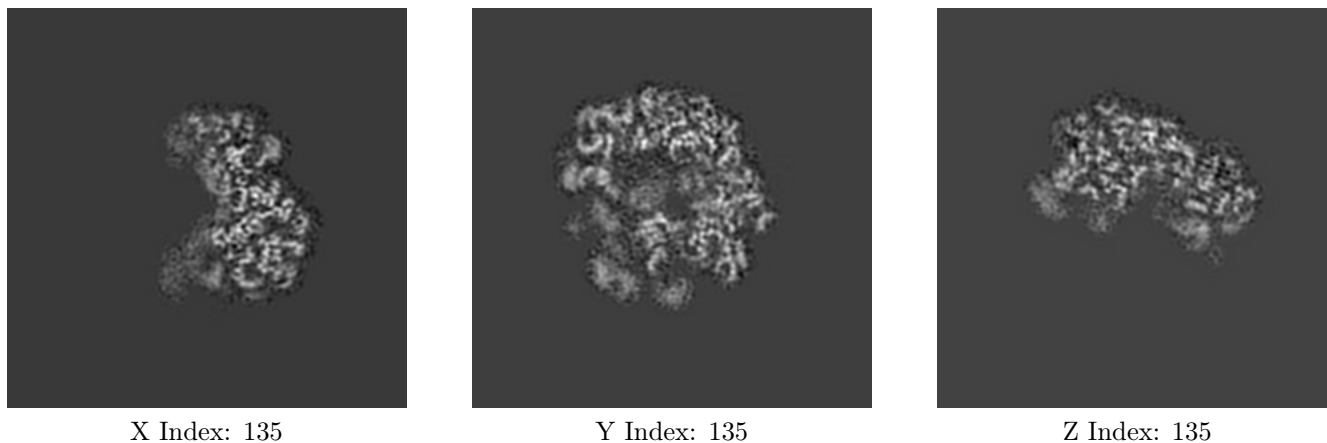
6.1.1 Primary map



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

6.2 Central slices [i](#)

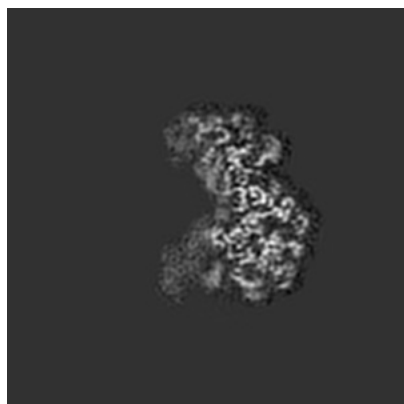
6.2.1 Primary map



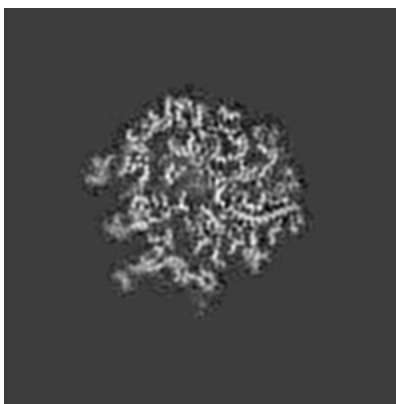
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

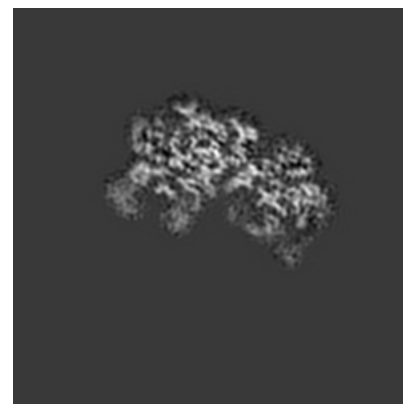
6.3.1 Primary map



X Index: 136



Y Index: 155



Z Index: 139

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

6.4 Orthogonal surface views [i](#)

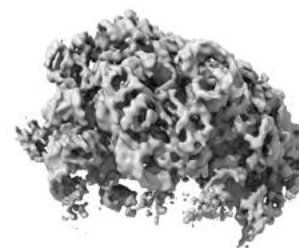
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

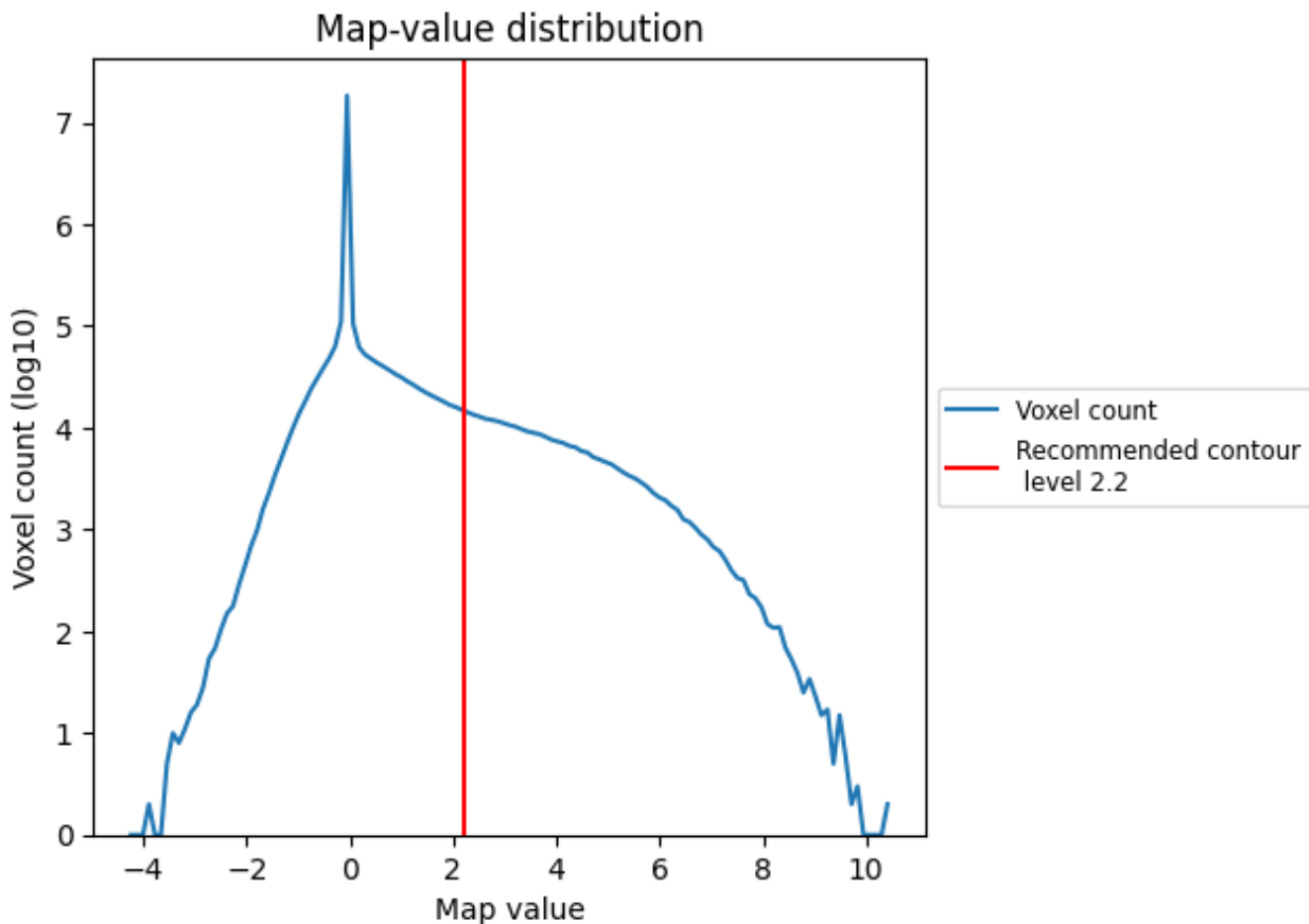
6.5 Mask visualisation

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

7 Map analysis [i](#)

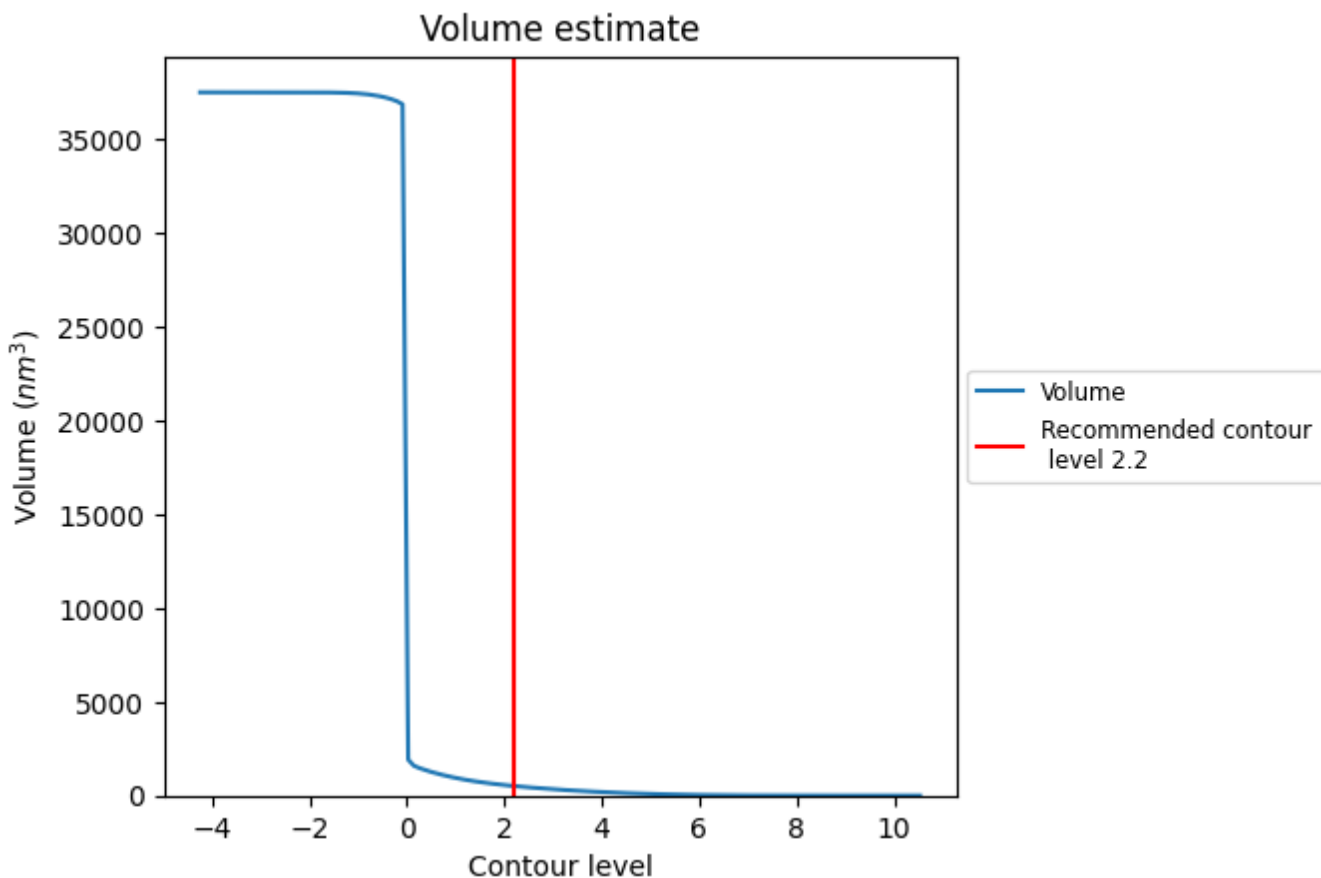
This section contains the results of statistical analysis of the map.

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.

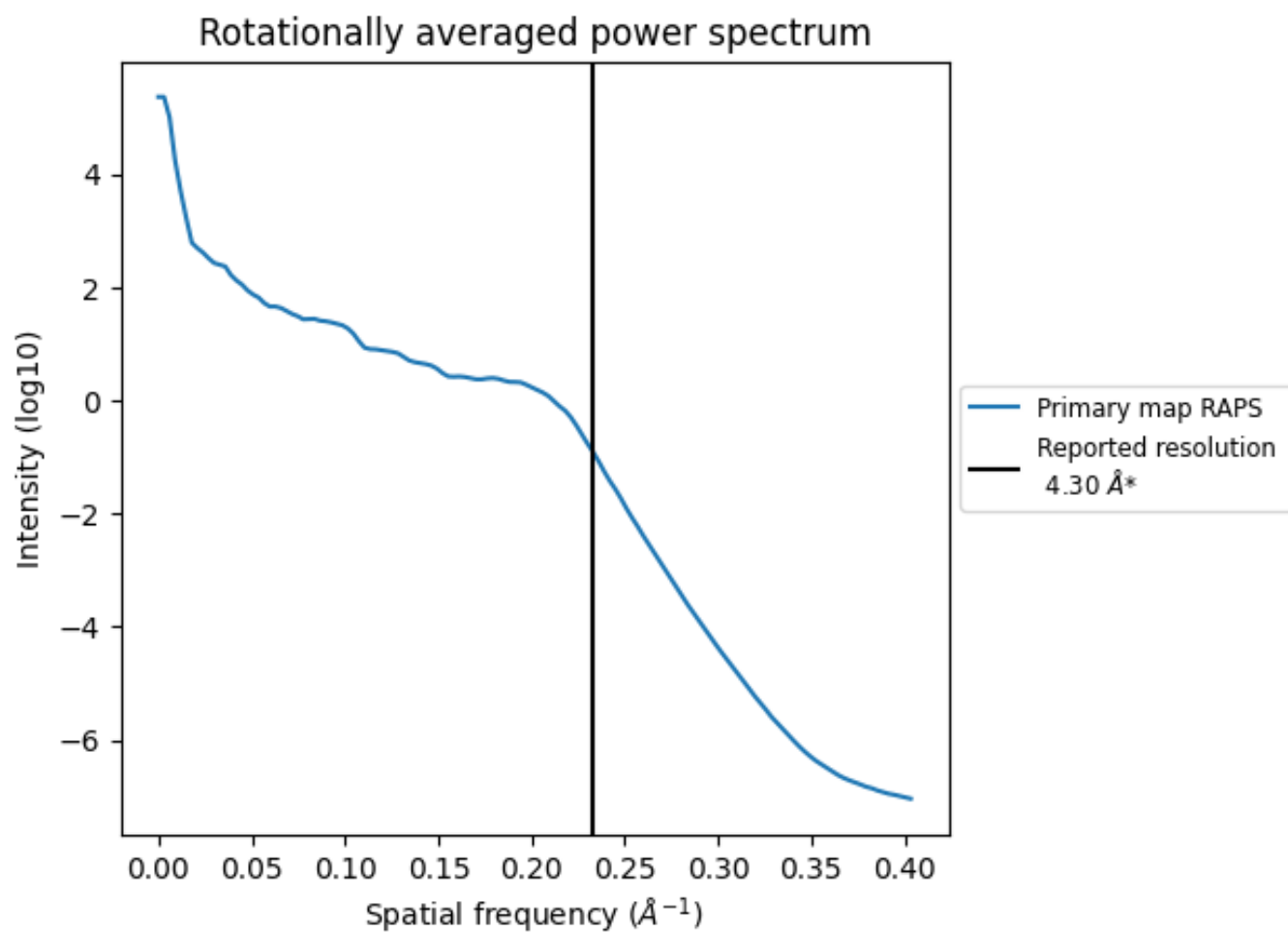
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 508 nm³; this corresponds to an approximate mass of 459 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 0.233 Å⁻¹

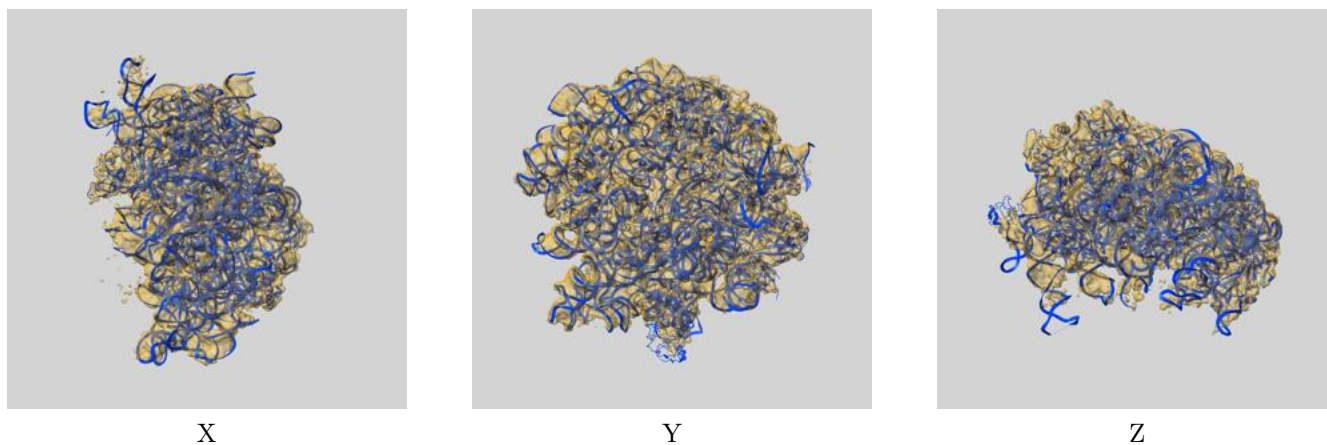
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

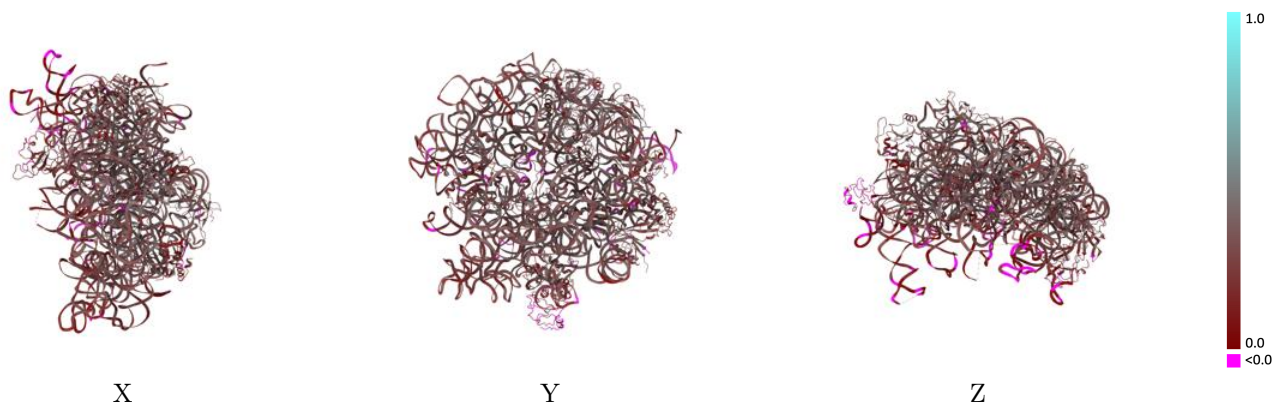
This section contains information regarding the fit between EMDB map EMD-4382 and PDB model 6GC7. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



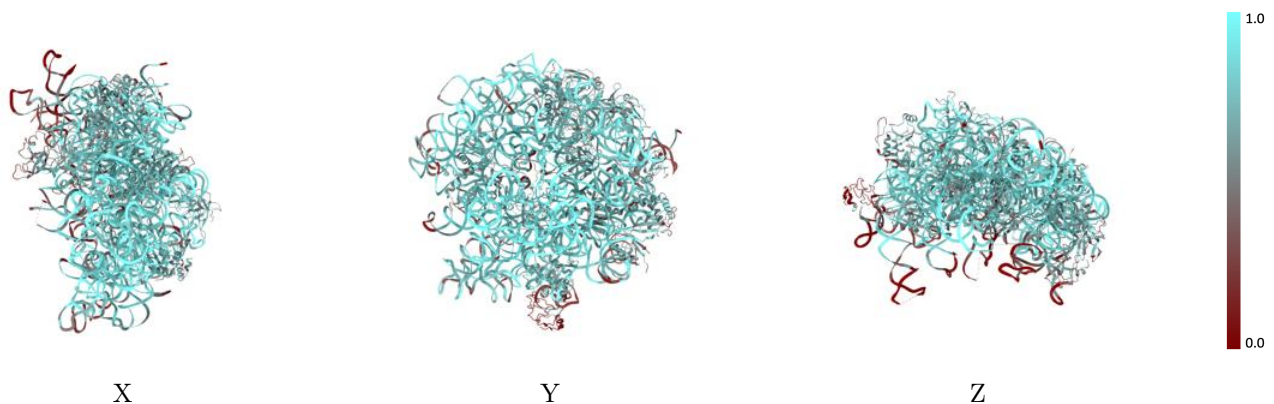
The images above show the 3D surface view of the map at the recommended contour level 2.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



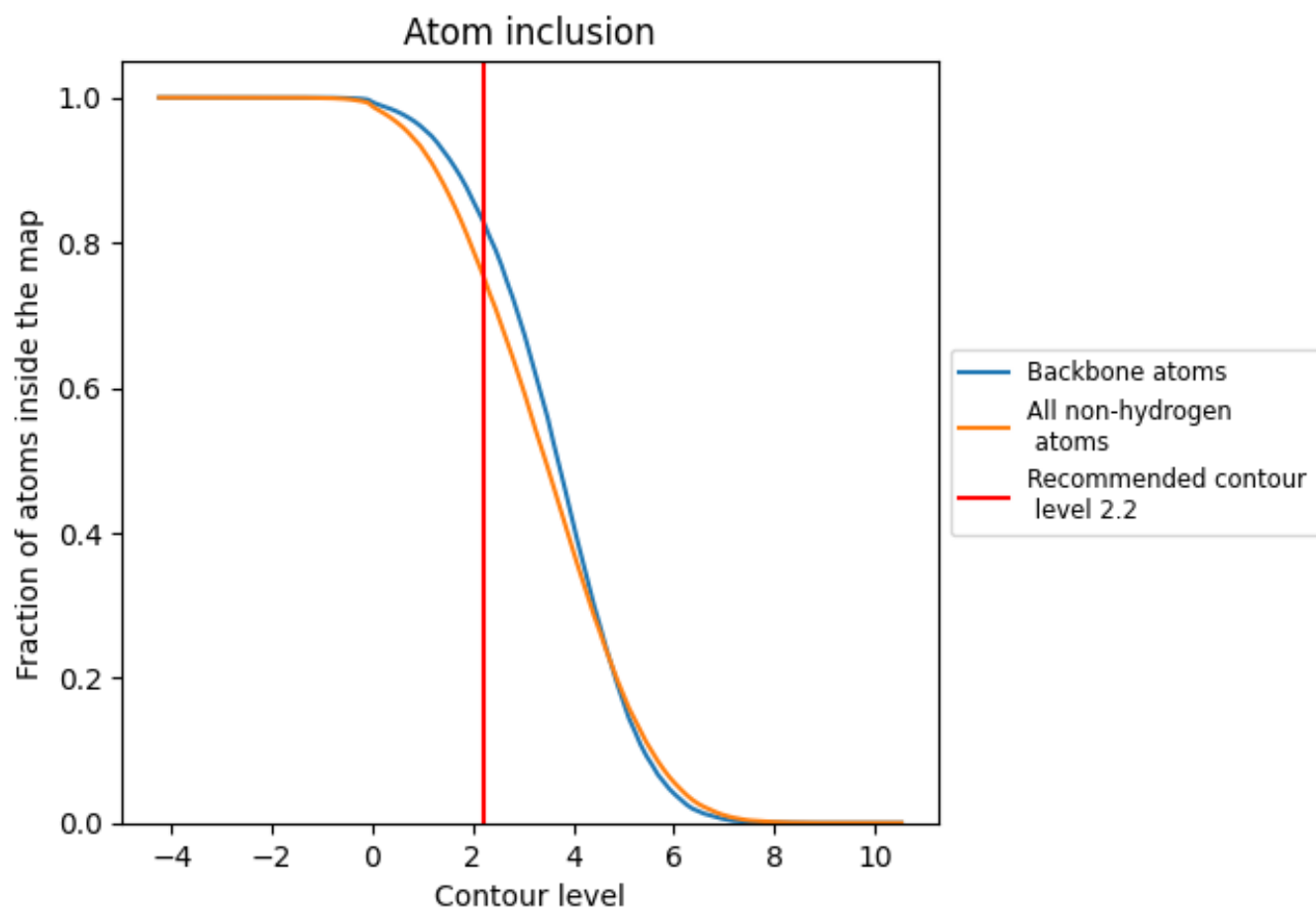
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.2).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 76% 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 (2.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7553	 0.2780
0	 0.6916	 0.2880
2	 0.6056	 0.2320
A	 0.8022	 0.2830
D	 0.6471	 0.3030
E	 0.6270	 0.2640
J	 0.6527	 0.2750
K	 0.4737	 0.2140
L	 0.2402	 0.1090
N	 0.7194	 0.2970
P	 0.5856	 0.2500
Q	 0.7026	 0.2830
R	 0.6324	 0.2950
S	 0.6316	 0.2760
T	 0.6833	 0.2930
U	 0.6393	 0.2840
Y	 0.6117	 0.1940
Z	 0.5515	 0.2480

