



wwPDB EM Validation Summary Report ⓘ

Nov 8, 2022 – 05:21 AM JST

PDB ID : 5XYU
EMDB ID : EMD-6790
Title : Small subunit of Mycobacterium smegmatis ribosome
Authors : Li, Z.; Zhang, Y.; Zheng, L.; Ge, X.; Sanyal, S.; Gao, N.
Deposited on : 2017-07-10
Resolution : 3.45 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:

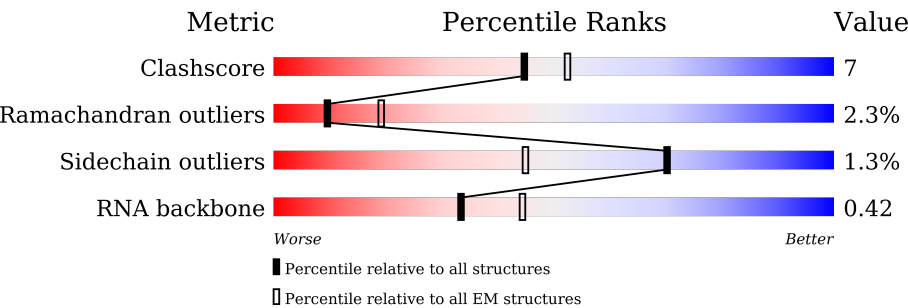
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.45 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	1528	
2	C	275	
3	D	201	
4	E	214	
5	F	90	
6	G	156	
7	H	132	

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Mol	Chain	Length	Quality of chain
8	I	150	
9	J	101	
10	K	138	
11	L	124	
12	M	124	
13	N	61	
14	O	89	
15	P	156	
16	Q	98	
17	R	84	
18	S	93	
19	T	86	
20	U	33	

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 45157 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 16S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1379	Total	C	N	O	P	0	0
			29639	13201	5457	9602	1379		

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	185	Total	C	N	O	S	0	0
			1498	939	287	268	4		

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	138	Total	C	N	O	S	0	0
			1156	721	226	207	2		

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	159	Total	C	N	O	S	0	0
			1147	724	214	206	3		

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	67	Total	C	N	O	S	0	0
			530	335	92	102	1		

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	144	Total	C	N	O	S	0	0
			1141	708	226	205	2		

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	129	Total	C	N	O	S	0	0
			990	622	184	183	1		

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	124	Total	C	N	O		0	0
			974	618	188	168			

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	97	Total	C	N	O	S	0	0
			778	490	144	141	3		

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	115	Total	C	N	O	S	0	0
			853	527	169	156	1		

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	123	Total	C	N	O	S	0	0
			964	597	198	167	2		

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	112	Total	C	N	O	S	0	0
			868	529	176	160	3		

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	60	Total	C	N	O	S	0	0
			477	302	97	73	5		

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	86	Total	C	N	O	0	0
			698	437	139	122		

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	P	94	Total	C	N	O	0	0
			745	477	138	130		

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	91	Total	C	N	O	S	0	0
			721	453	137	129	2		

- Molecule 17 is a protein called 30S ribosomal protein S18 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	55	Total	C	N	O	S	0	0
			432	267	86	78	1		

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	79	Total	C	N	O	S	0	0
			634	408	116	109	1		

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	T	83	Total	C	N	O	0	0
			647	393	137	117		

- Molecule 20 is a protein called Conserved domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	25	Total	C	N	O	S	0	0
			217	133	55	28	1		

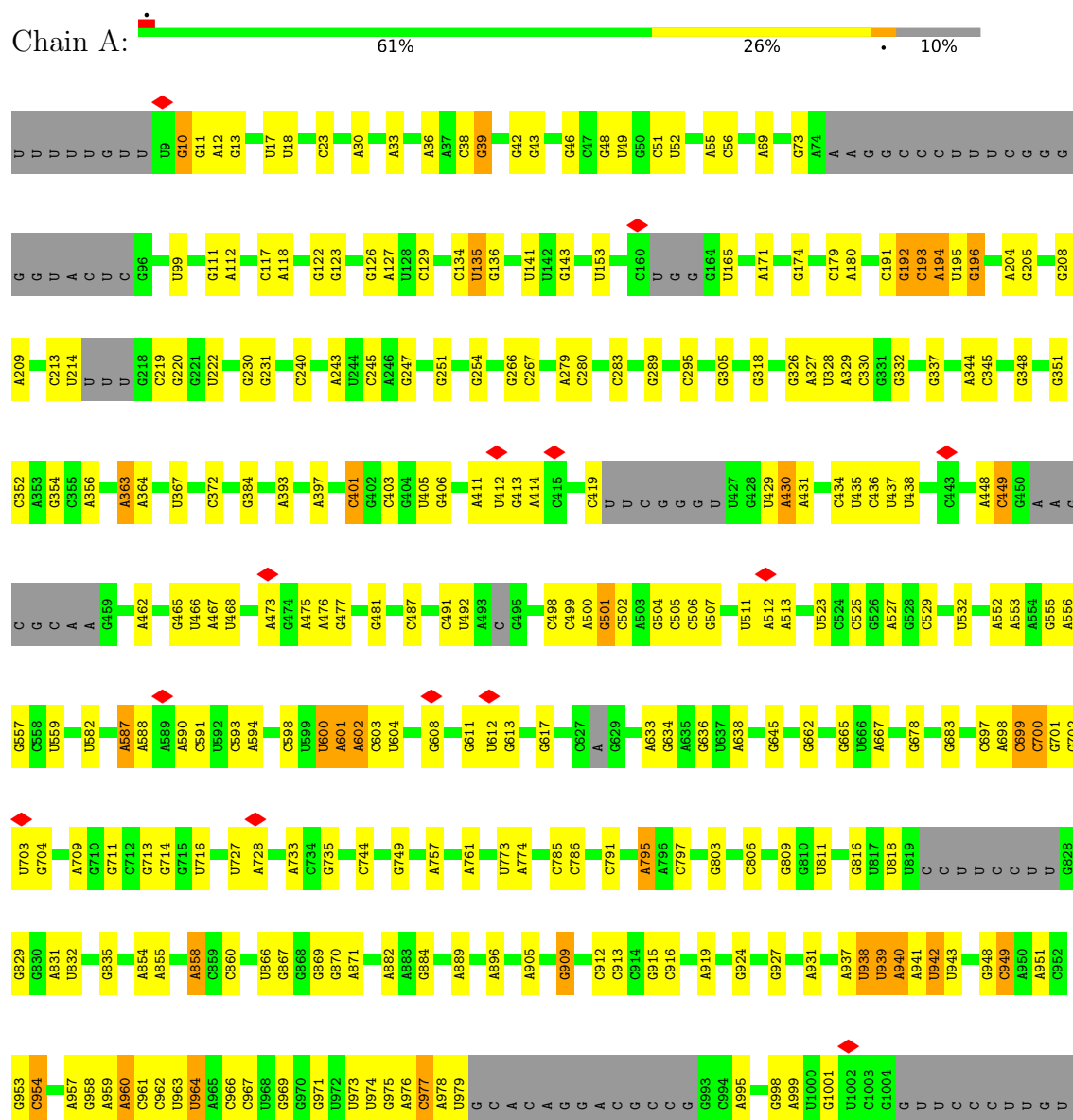
- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

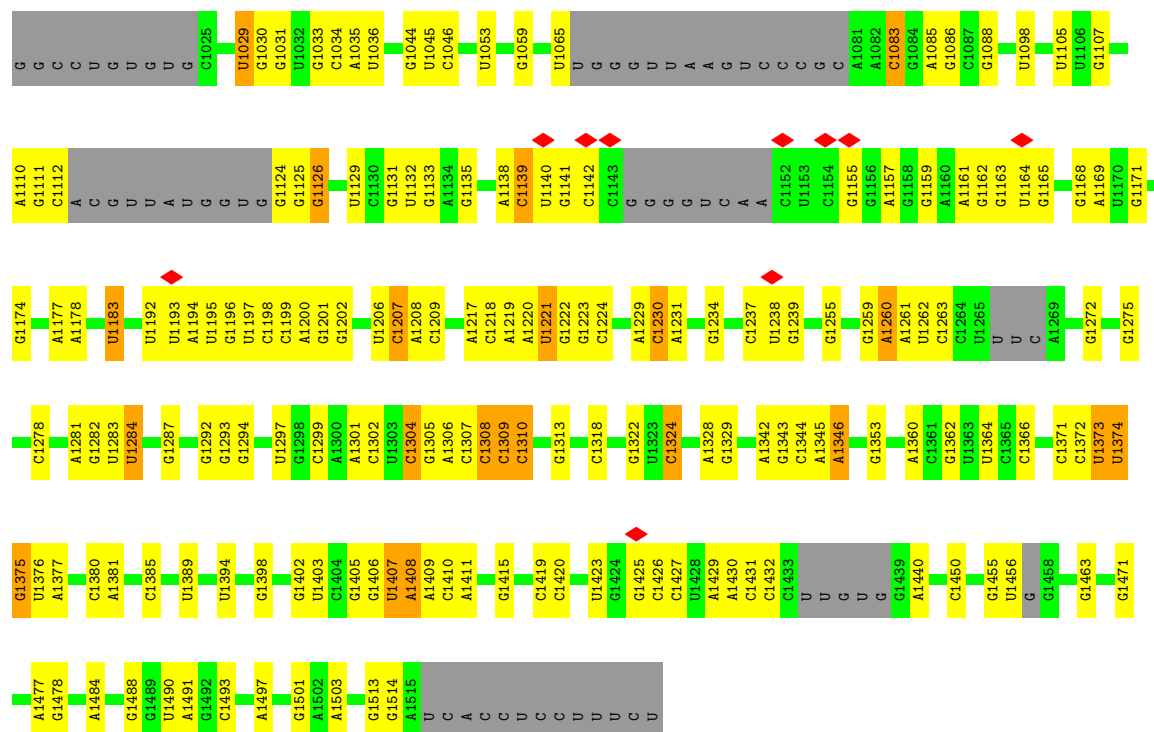
Mol	Chain	Residues	Atoms		AltConf
21	A	47	Total 47	Mg 47	0
21	C	1	Total 1	Mg 1	0

3 Residue-property plots

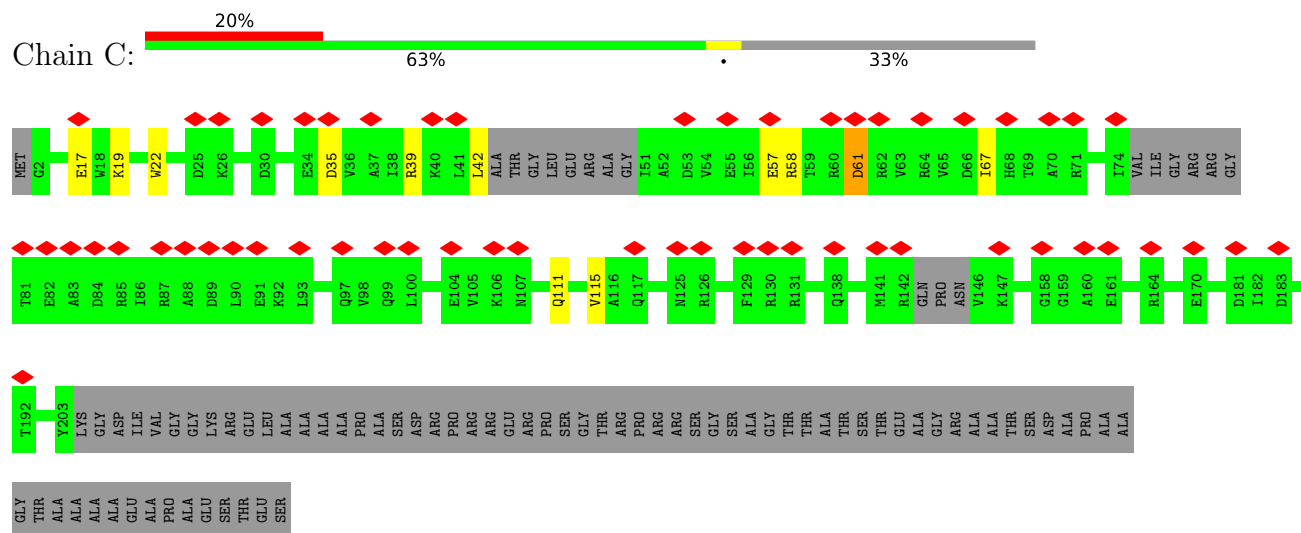
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S RNA

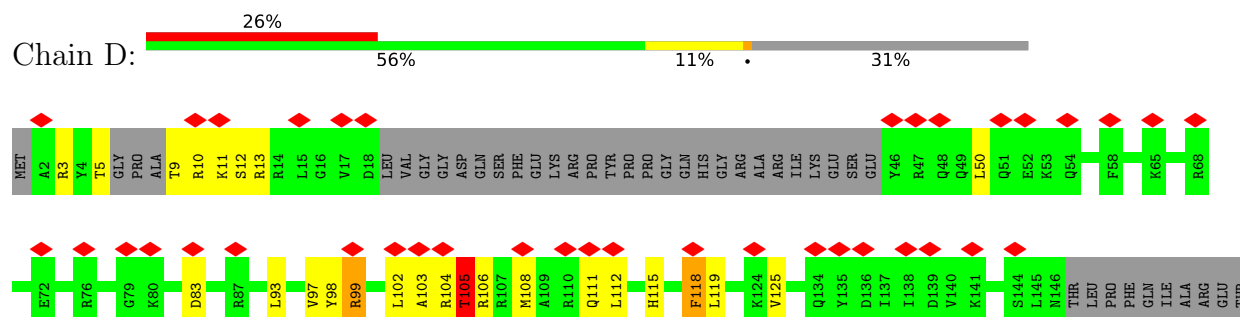


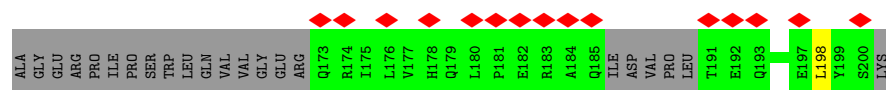


• Molecule 2: 30S ribosomal protein S3

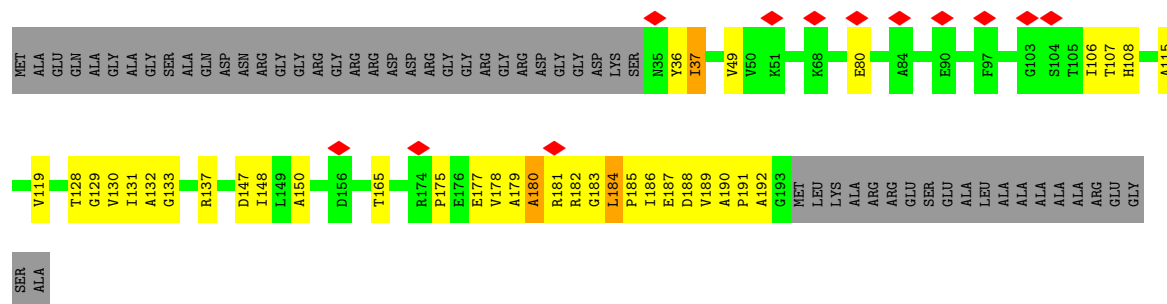


• Molecule 3: 30S ribosomal protein S4

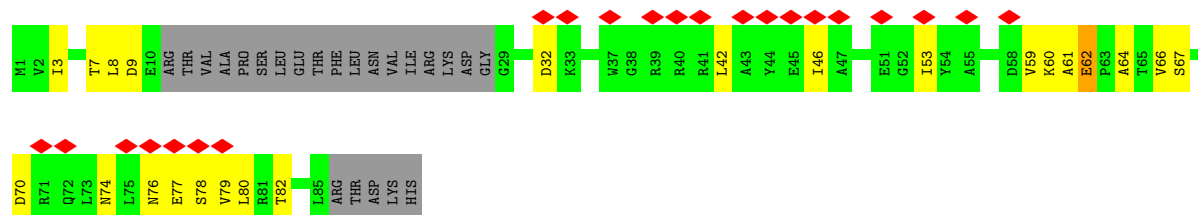




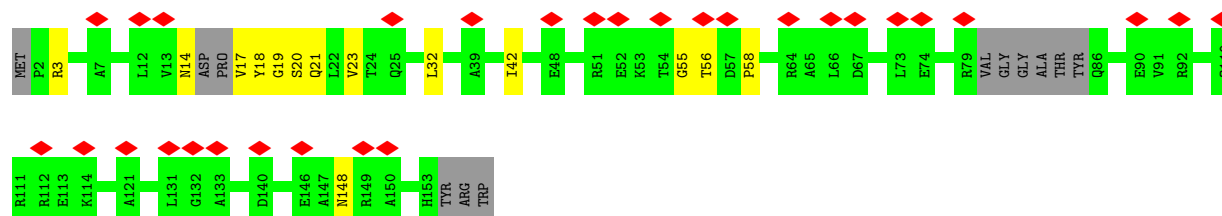
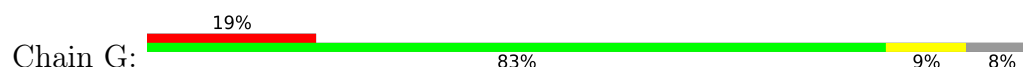
• Molecule 4: 30S ribosomal protein S5



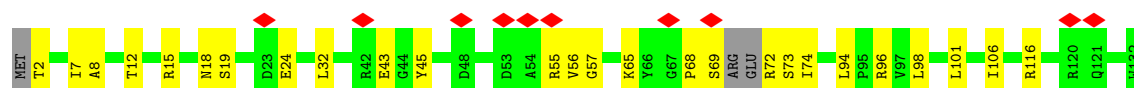
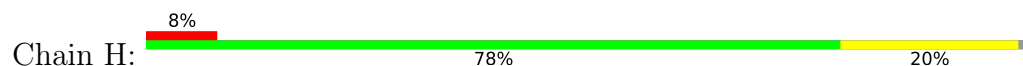
• Molecule 5: 30S ribosomal protein S6



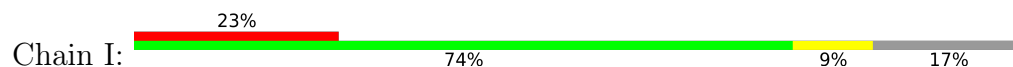
• Molecule 6: 30S ribosomal protein S7

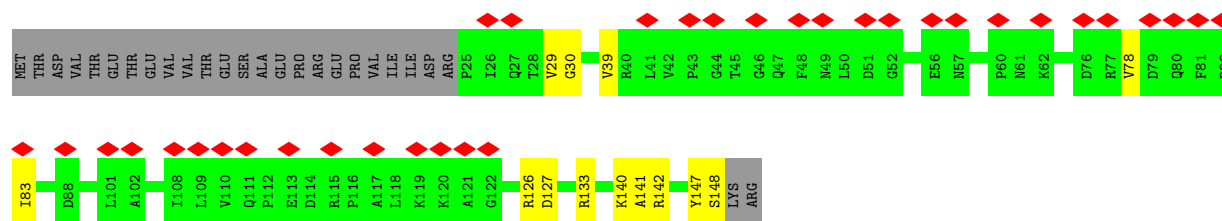


• Molecule 7: 30S ribosomal protein S8

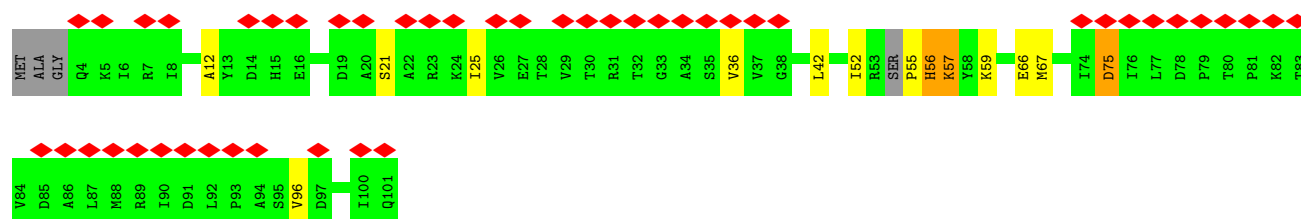
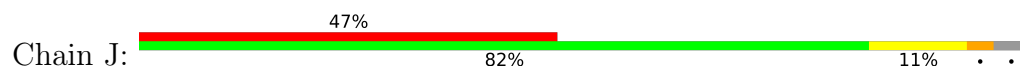


• Molecule 8: 30S ribosomal protein S9

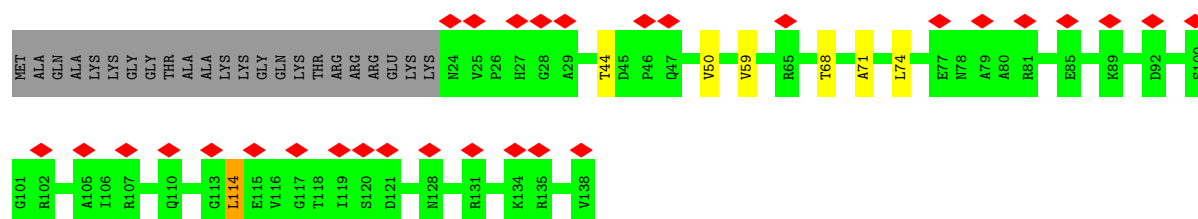
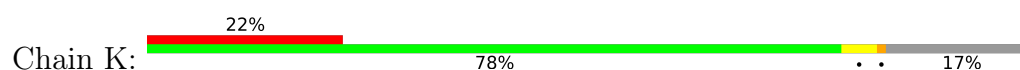




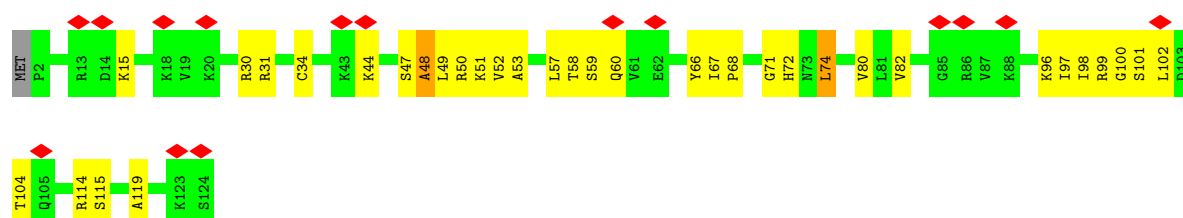
• Molecule 9: 30S ribosomal protein S10



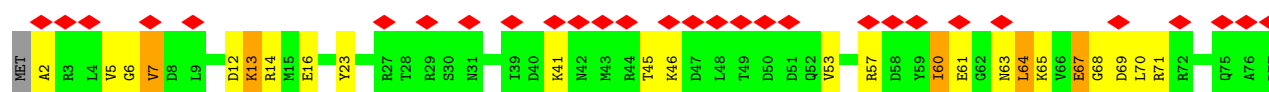
• Molecule 10: 30S ribosomal protein S11

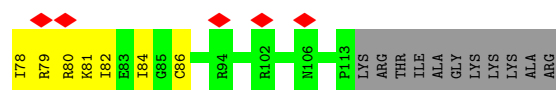


• Molecule 11: 30S ribosomal protein S12



• Molecule 12: 30S ribosomal protein S13





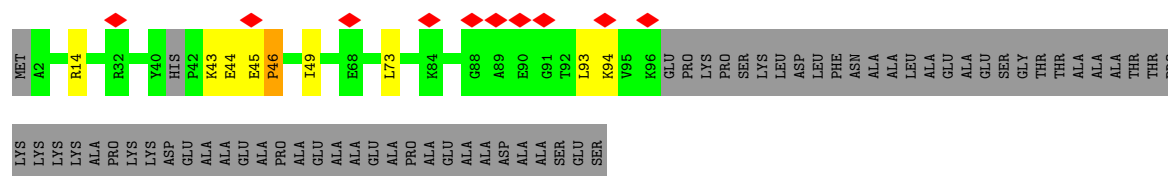
- Molecule 13: 30S ribosomal protein S14 type Z



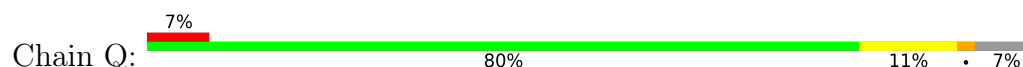
- Molecule 14: 30S ribosomal protein S15



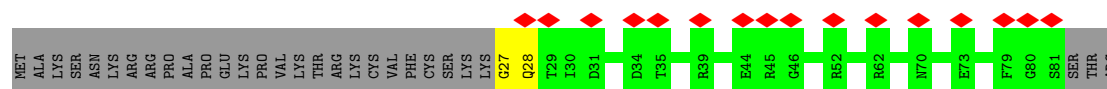
- Molecule 15: 30S ribosomal protein S16



- Molecule 16: 30S ribosomal protein S17

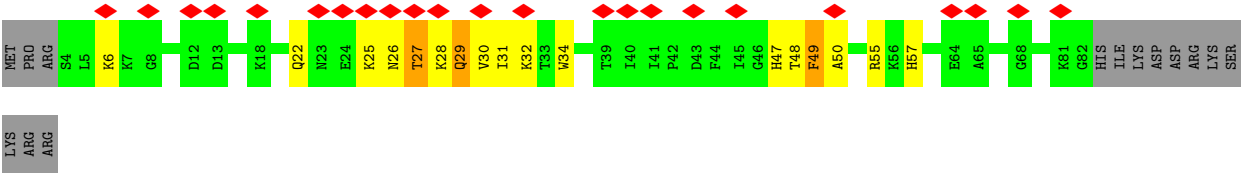


- Molecule 17: 30S ribosomal protein S18 2

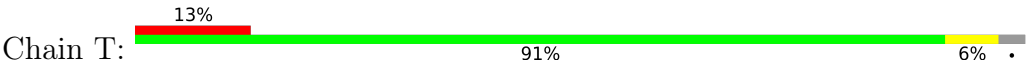


- Molecule 18: 30S ribosomal protein S19

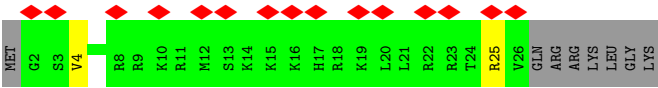
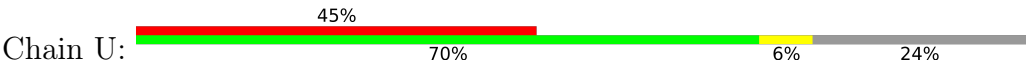




● Molecule 19: 30S ribosomal protein S20



● Molecule 20: Conserved domain protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47338	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 ($e^-/\text{\AA}^2$)	2	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	0.262	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0446	Depositor
Map size (Å)	369.6, 369.6, 369.6	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.32, 1.32, 1.32	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.20	0/33170	0.67	0/51726
2	C	0.35	0/1518	0.56	0/2034
3	D	0.35	0/1169	0.57	0/1561
4	E	0.40	0/1163	0.63	0/1574
5	F	0.39	0/535	0.62	0/724
6	G	0.37	0/1154	0.58	0/1551
7	H	0.38	0/1004	0.59	0/1356
8	I	0.36	0/992	0.55	0/1337
9	J	0.39	0/791	0.59	0/1069
10	K	0.35	0/871	0.51	0/1179
11	L	0.38	0/975	0.62	0/1302
12	M	0.38	0/875	0.65	0/1174
13	N	0.42	0/488	0.65	0/650
14	O	0.35	0/707	0.58	0/949
15	P	0.42	0/757	0.60	0/1018
16	Q	0.33	0/731	0.61	0/977
17	R	0.34	0/436	0.59	0/586
18	S	0.36	0/650	0.57	0/875
19	T	0.37	0/650	0.58	0/864
20	U	0.41	0/217	0.67	0/278
All	All	0.27	0/48853	0.65	0/72784

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	29639	0	14926	127	0
2	C	1498	0	1535	15	0
3	D	1156	0	1177	41	0
4	E	1147	0	1206	65	0
5	F	530	0	548	33	0
6	G	1141	0	1201	18	0
7	H	990	0	1026	38	0
8	I	974	0	1024	7	0
9	J	778	0	811	9	0
10	K	853	0	859	2	0
11	L	964	0	1050	43	0
12	M	868	0	873	63	0
13	N	477	0	500	35	0
14	O	698	0	734	3	0
15	P	745	0	793	8	0
16	Q	721	0	768	26	0
17	R	432	0	448	4	0
18	S	634	0	649	41	0
19	T	647	0	696	1	0
20	U	217	0	261	1	0
21	A	47	0	0	0	0
21	C	1	0	0	0	0
All	All	45157	0	31085	514	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 7.

The worst 5 of 514 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:E:182:ARG:NH1	7:H:45:TYR:CZ	1.78	1.42
12:M:81:LYS:HA	12:M:84:ILE:CD1	1.56	1.36
12:M:80:ARG:O	12:M:84:ILE:CG1	1.71	1.35
12:M:80:ARG:C	12:M:84:ILE:HG13	1.47	1.33
5:F:70:ASP:O	5:F:74:ASN:ND2	1.63	1.31

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	C	177/275 (64%)	161 (91%)	15 (8%)	1 (1%)	25	62
3	D	128/201 (64%)	124 (97%)	3 (2%)	1 (1%)	19	57
4	E	157/214 (73%)	138 (88%)	13 (8%)	6 (4%)	3	24
5	F	63/90 (70%)	58 (92%)	5 (8%)	0	100	100
6	G	138/156 (88%)	132 (96%)	4 (3%)	2 (1%)	11	44
7	H	125/132 (95%)	114 (91%)	10 (8%)	1 (1%)	19	57
8	I	122/150 (81%)	113 (93%)	5 (4%)	4 (3%)	4	27
9	J	93/101 (92%)	82 (88%)	8 (9%)	3 (3%)	4	28
10	K	113/138 (82%)	101 (89%)	10 (9%)	2 (2%)	8	39
11	L	121/124 (98%)	111 (92%)	5 (4%)	5 (4%)	3	23
12	M	110/124 (89%)	101 (92%)	6 (6%)	3 (3%)	5	31
13	N	58/61 (95%)	50 (86%)	6 (10%)	2 (3%)	3	27
14	O	84/89 (94%)	79 (94%)	4 (5%)	1 (1%)	13	48
15	P	90/156 (58%)	78 (87%)	9 (10%)	3 (3%)	4	27
16	Q	87/98 (89%)	78 (90%)	6 (7%)	3 (3%)	3	27
17	R	53/84 (63%)	52 (98%)	1 (2%)	0	100	100
18	S	77/93 (83%)	69 (90%)	5 (6%)	3 (4%)	3	24
19	T	81/86 (94%)	78 (96%)	1 (1%)	2 (2%)	5	32
20	U	23/33 (70%)	22 (96%)	0	1 (4%)	2	21
All	All	1900/2405 (79%)	1741 (92%)	116 (6%)	43 (2%)	9	34

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	180	ALA
8	I	141	ALA
9	J	36	VAL
10	K	71	ALA
11	L	74	LEU

5.3.2 Protein sidechains ⓘ

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	C	155/212 (73%)	154 (99%)	1 (1%)	86	95
3	D	124/176 (70%)	120 (97%)	4 (3%)	39	69
4	E	115/147 (78%)	115 (100%)	0	100	100
5	F	58/79 (73%)	56 (97%)	2 (3%)	37	67
6	G	123/132 (93%)	123 (100%)	0	100	100
7	H	105/108 (97%)	104 (99%)	1 (1%)	76	89
8	I	100/125 (80%)	100 (100%)	0	100	100
9	J	88/90 (98%)	85 (97%)	3 (3%)	37	67
10	K	89/105 (85%)	87 (98%)	2 (2%)	52	77
11	L	104/105 (99%)	102 (98%)	2 (2%)	57	80
12	M	86/104 (83%)	84 (98%)	2 (2%)	50	76
13	N	49/50 (98%)	48 (98%)	1 (2%)	55	79
14	O	74/77 (96%)	74 (100%)	0	100	100
15	P	77/118 (65%)	77 (100%)	0	100	100
16	Q	77/83 (93%)	77 (100%)	0	100	100
17	R	45/72 (62%)	45 (100%)	0	100	100
18	S	70/84 (83%)	67 (96%)	3 (4%)	29	61
19	T	68/70 (97%)	67 (98%)	1 (2%)	65	84
20	U	23/31 (74%)	23 (100%)	0	100	100
All	All	1630/1968 (83%)	1608 (99%)	22 (1%)	70	86

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	L	49	LEU
13	N	39	LEU
12	M	64	LEU
18	S	29	GLN
5	F	62	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
18	S	29	GLN
17	R	59	GLN
11	L	72	HIS
5	F	74	ASN
14	O	28	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1362/1528 (89%)	407 (29%)	41 (3%)

5 of 407 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	G
1	A	11	G
1	A	12	A
1	A	13	G
1	A	17	U

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1132	U
1	A	1346	A
1	A	1193	U
1	A	1259	G
1	A	1374	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](#)

Of 48 ligands modelled in this entry, 48 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

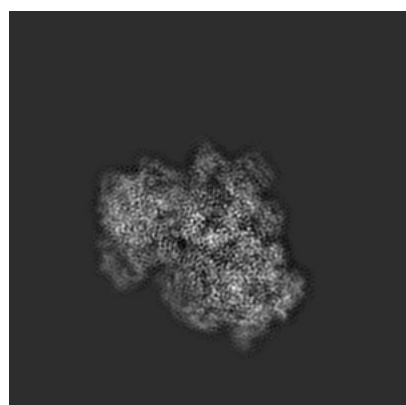
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6790. These allow visual inspection of the internal detail of the map and identification of artifacts.

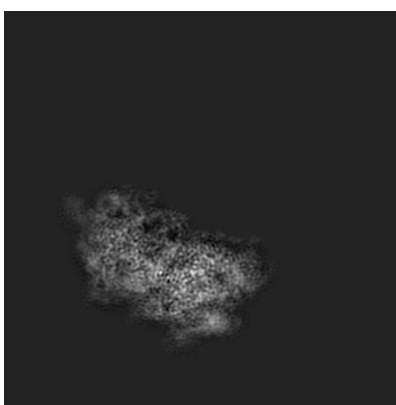
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

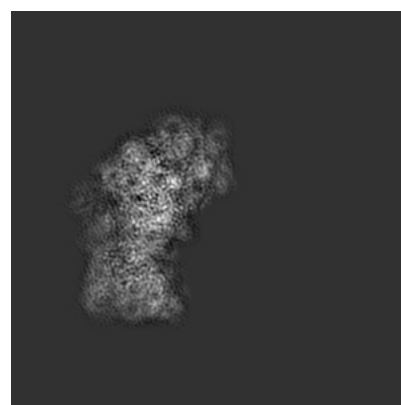
6.1.1 Primary map



X



Y

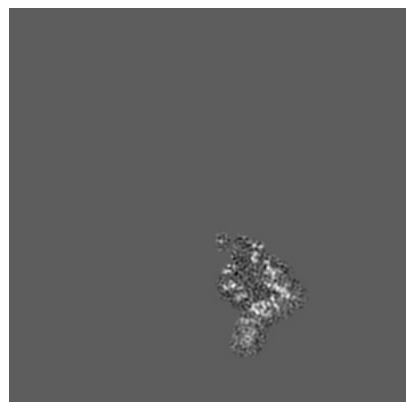


Z

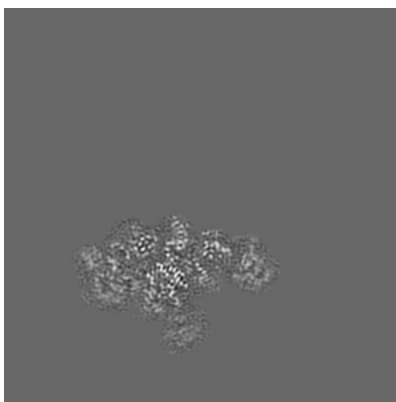
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

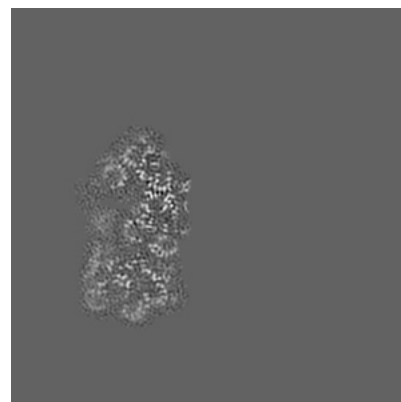
6.2.1 Primary map



X Index: 140



Y Index: 140

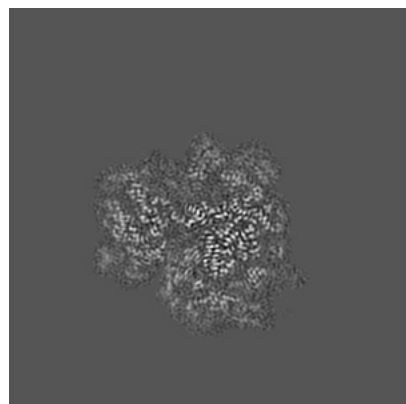


Z Index: 140

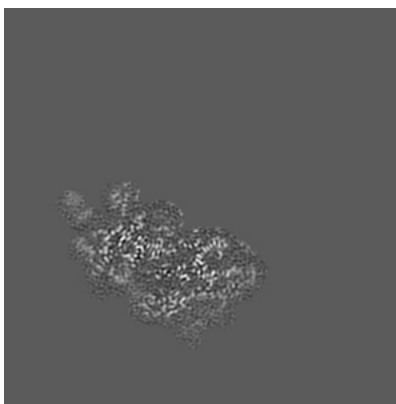
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 96



Y Index: 160

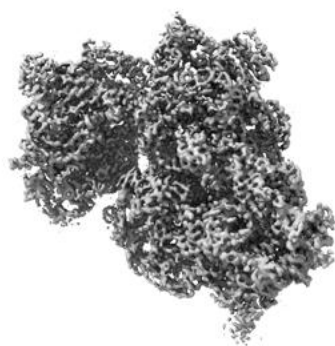


Z Index: 120

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 0.0446. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

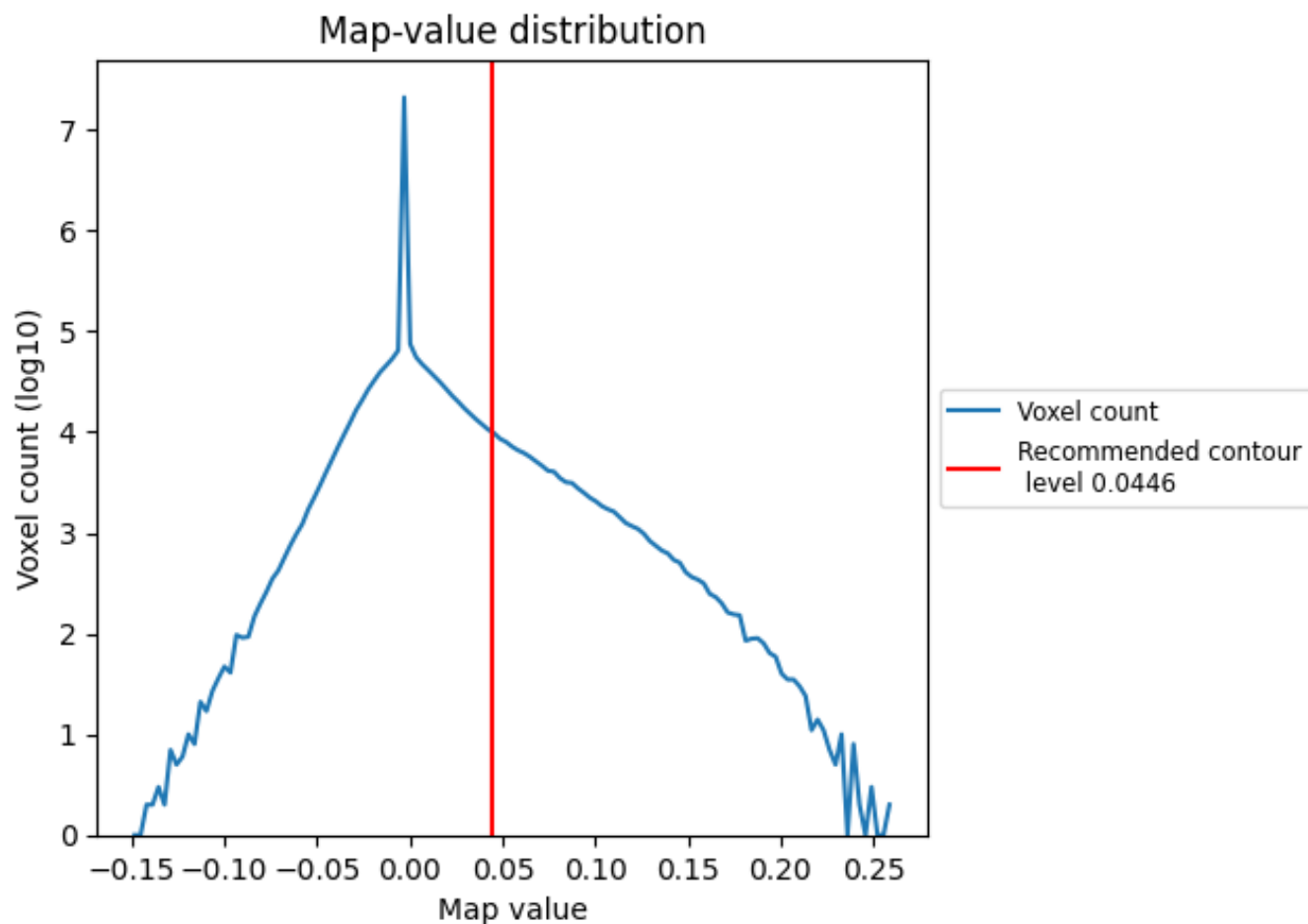
6.5 Mask visualisation

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

7 Map analysis [i](#)

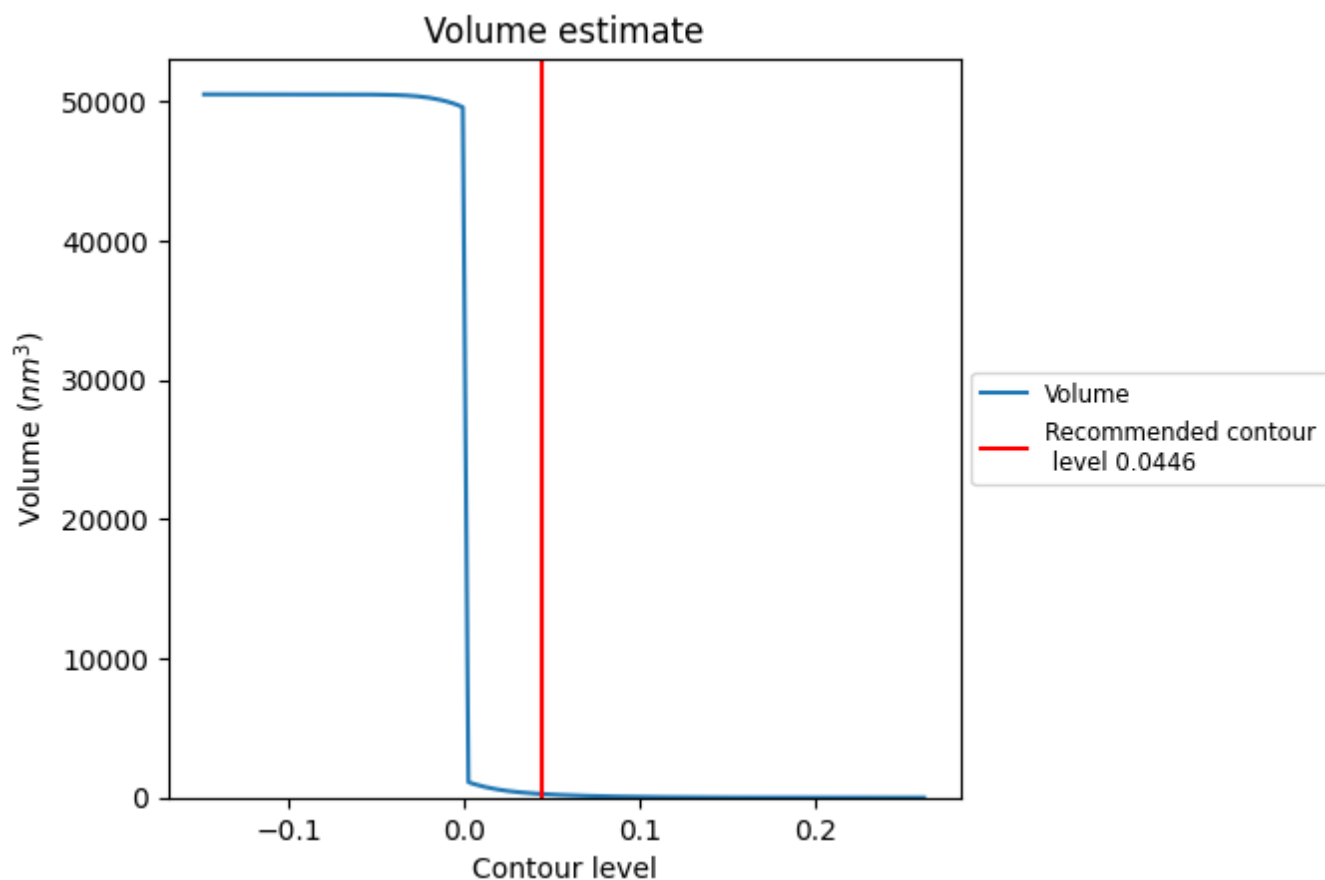
This section contains the results of statistical analysis of the map.

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.

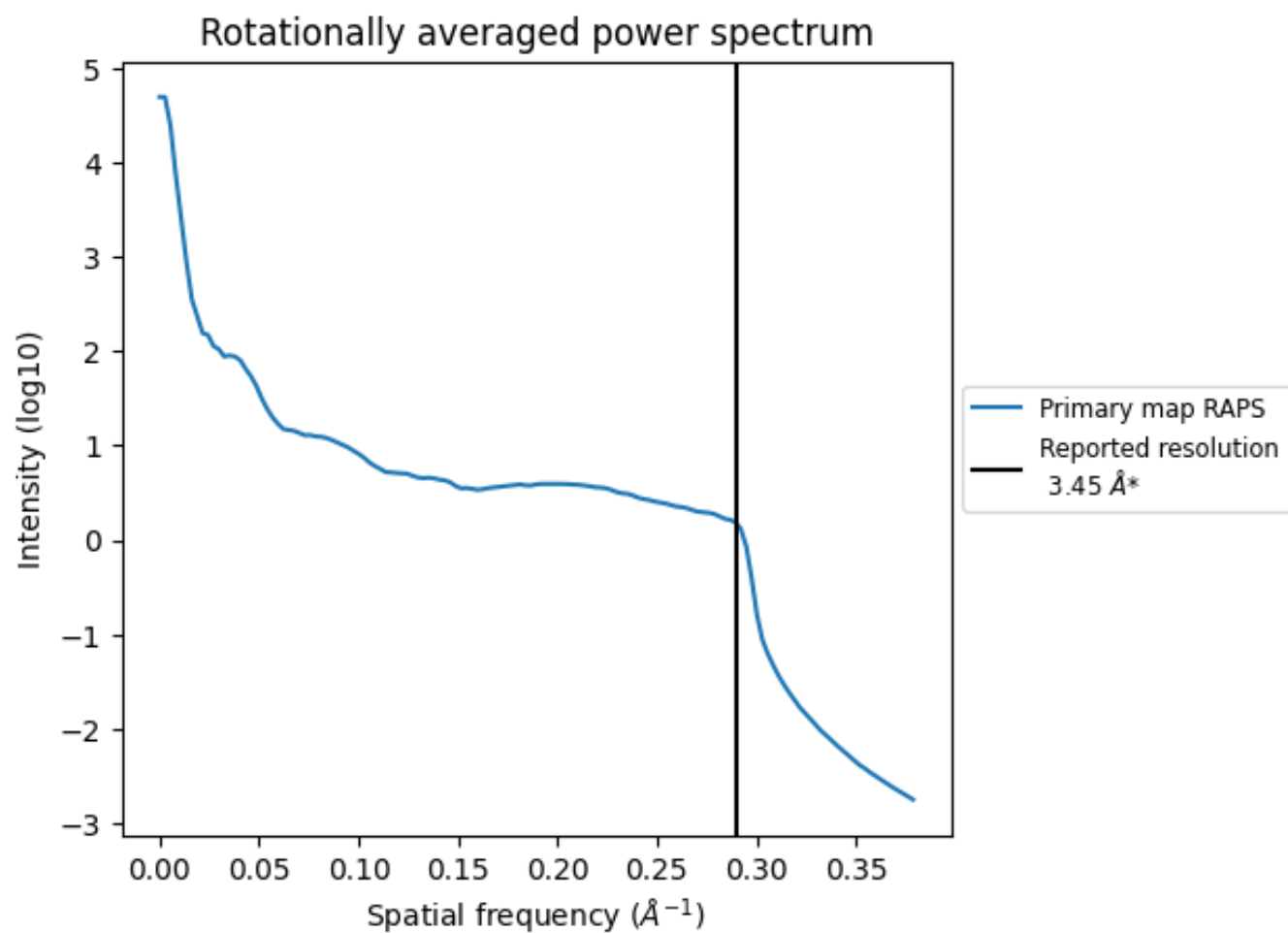
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 254 nm³; this corresponds to an approximate mass of 229 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 ⓘ

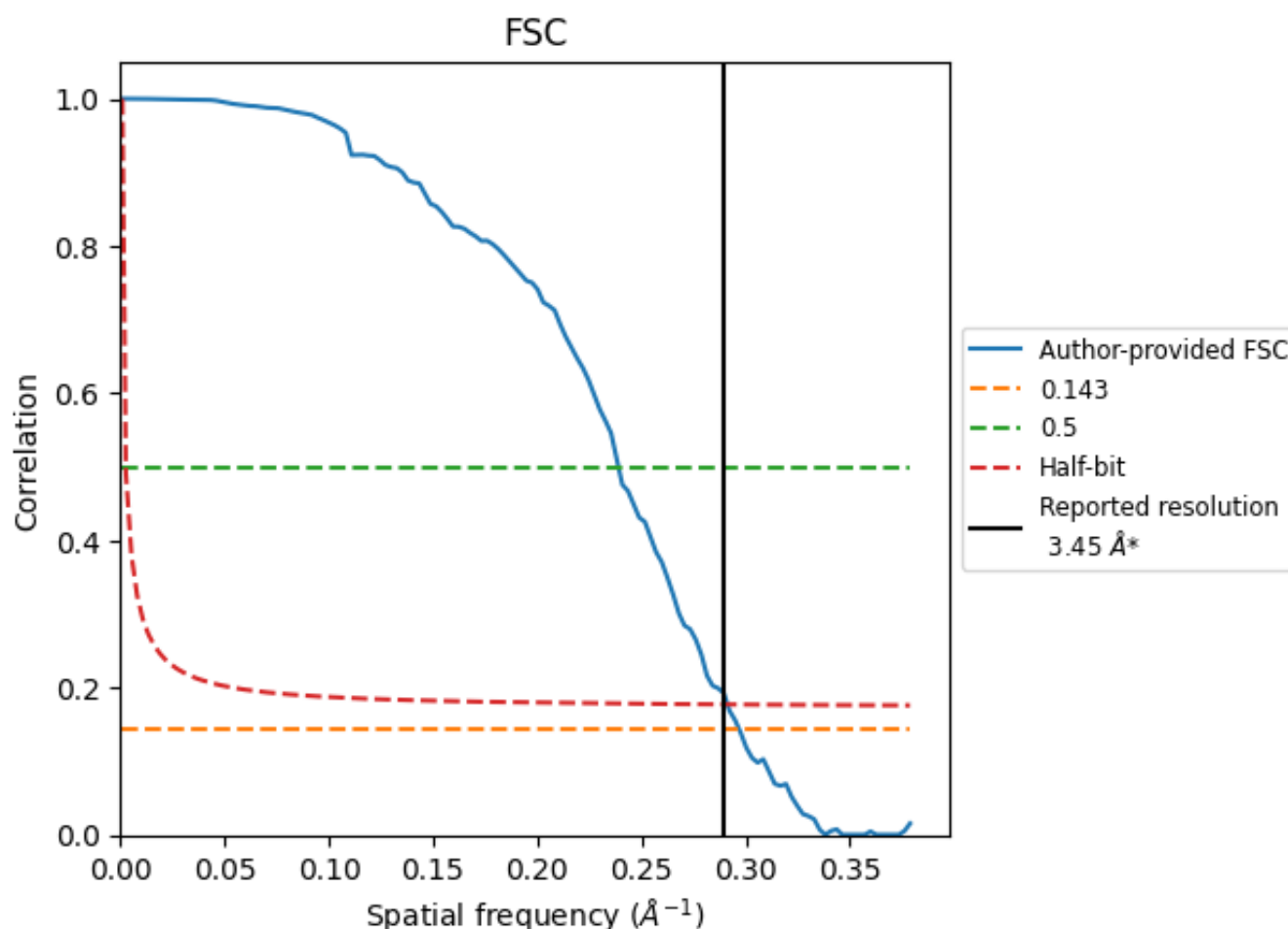


*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.290 Å⁻¹

8.2 Resolution estimates [i](#)

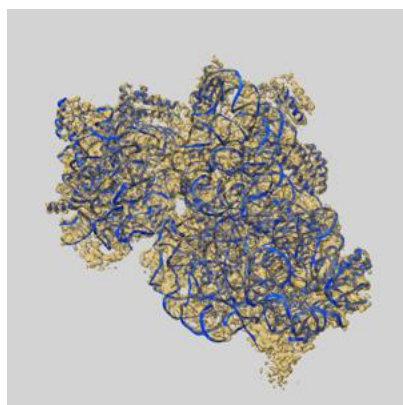
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.45	-	-
Author-provided FSC curve	3.37	4.19	3.43
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

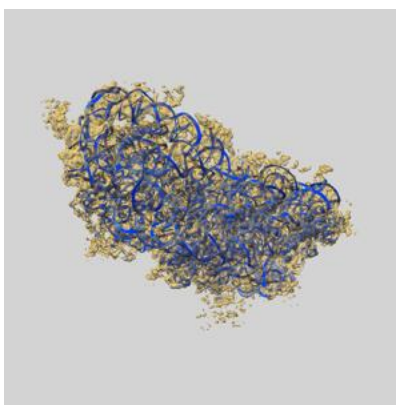
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6790 and PDB model 5XYU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

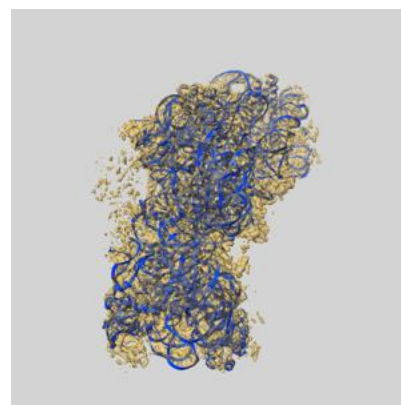
9.1 Map-model overlay [i](#)



X



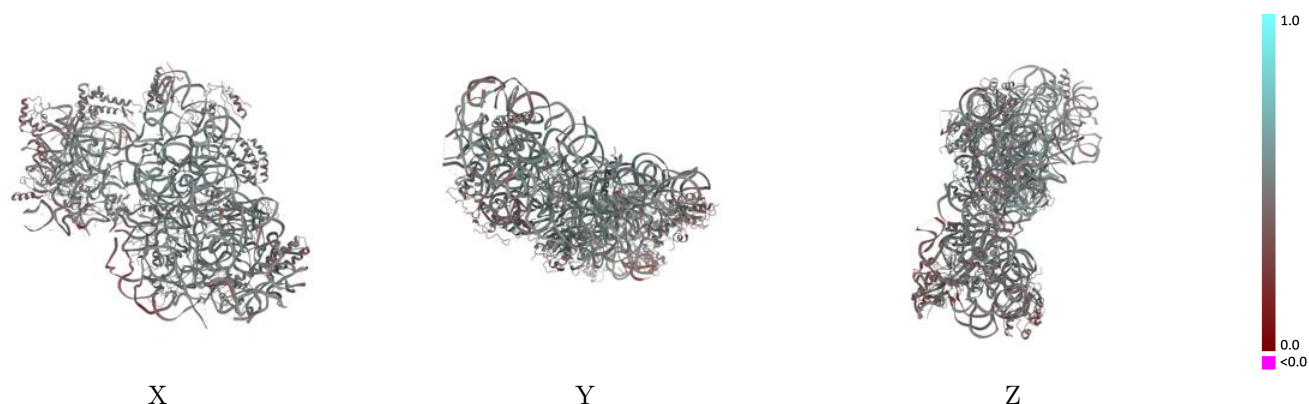
Y



Z

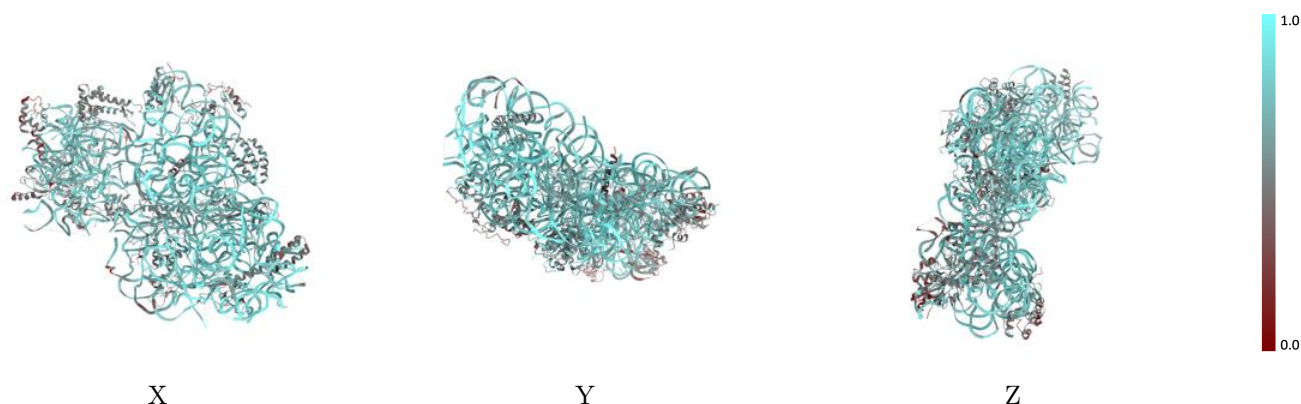
The images above show the 3D surface view of the map at the recommended contour level 0.0446 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



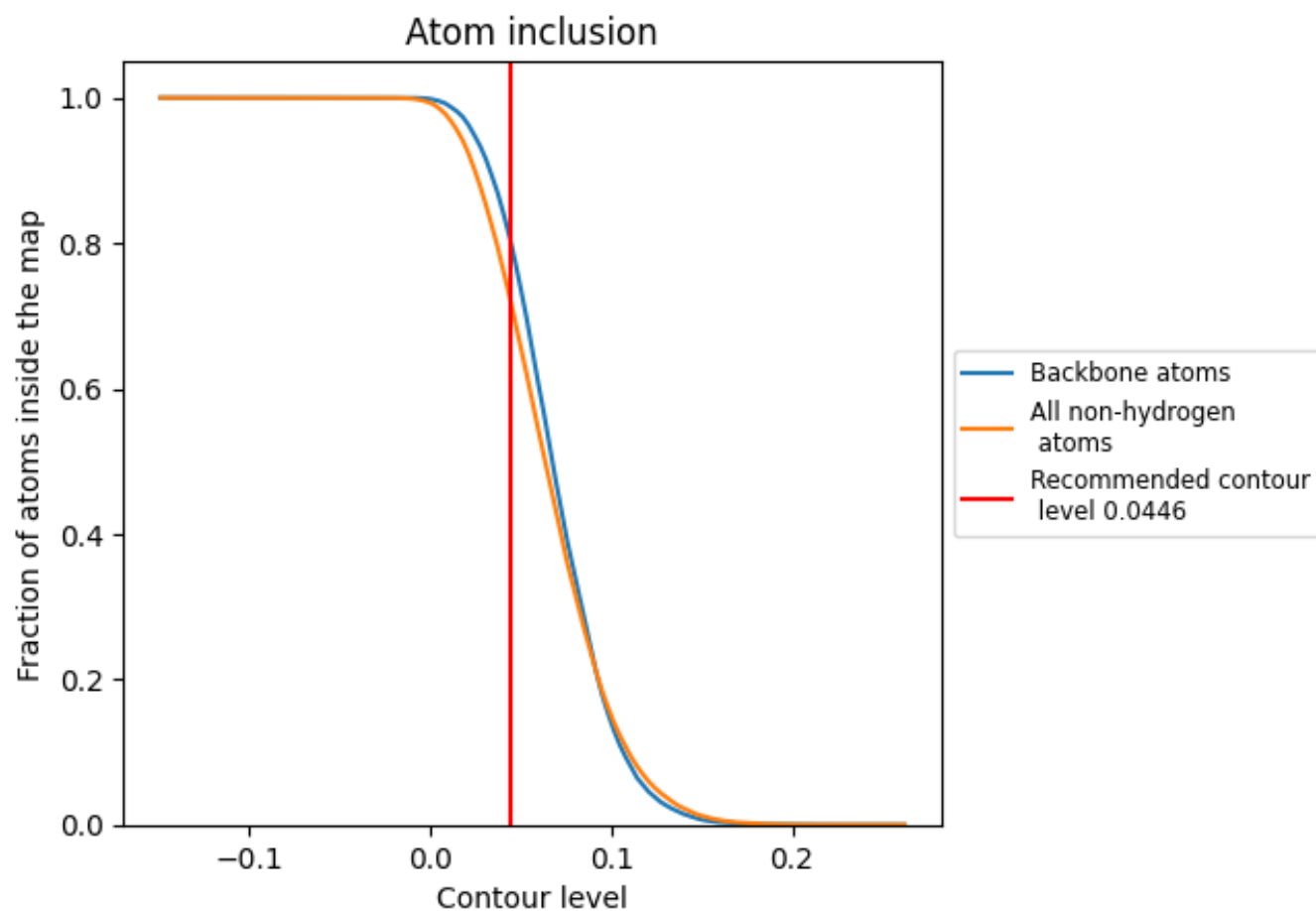
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0446).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.0446) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7213	 0.4820
A	 0.8004	 0.4940
C	 0.5343	 0.4610
D	 0.4860	 0.4330
E	 0.6367	 0.4860
F	 0.4720	 0.4120
G	 0.5426	 0.4500
H	 0.6809	 0.4990
I	 0.5212	 0.4290
J	 0.4333	 0.4210
K	 0.5060	 0.4290
L	 0.6333	 0.5040
M	 0.4940	 0.4120
N	 0.6926	 0.5000
O	 0.6296	 0.4790
P	 0.6468	 0.4950
Q	 0.6538	 0.4950
R	 0.5385	 0.4520
S	 0.5392	 0.4400
T	 0.6045	 0.4670
U	 0.4187	 0.4990

