



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:11 PM UTC

PDB ID : 6VYT / pdb_00006vyt
EMDB ID : EMD-21471
Title : Escherichia coli transcription-translation complex A2 (TTC-A2) containing a 15 nt long mRNA spacer, NusG, and fMet-tRNAs at P-site and E-site
Authors : Molodtsov, V.; Wang, C.; Ebright, R.H.; Su, M.
Deposited on : 2020-02-27
Resolution : 14.00 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.dev132
MolProbity : **FAILED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

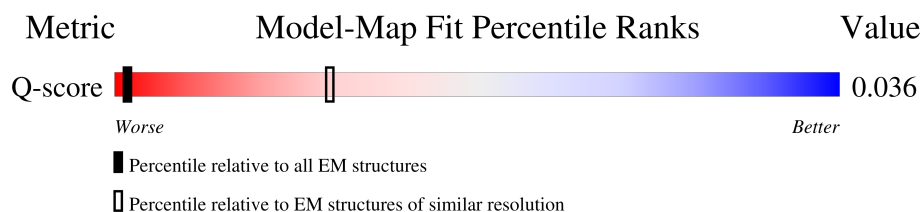
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 14.00 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	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Q-score	25397	61 (13.50 - 14.50)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 298128 atoms, of which 124824 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 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	0	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 2 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	1	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 3 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	2	94	Total	C	H	N	O	S	0	0
			1557	470	811	140	134	2		

- Molecule 4 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	103	Total	C	H	N	O	0	0
			1632	498	844	148	142		

- Molecule 5 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	4	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 6 is a DNA chain called NT DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	5	23	Total	C	H	N	O	P	0	0
			732	225	260	87	137	23		

- Molecule 7 is a DNA chain called T DNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	6	27	Total	C	H	N	O	P	0	0
			847	259	305	89	167	27		

- Molecule 8 is a RNA chain called mRNA with a 15 nt long spacer.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	7	16	Total	C	H	N	O	P	0	0
			515	154	168	62	115	16		

- Molecule 9 is a RNA chain called E-site and P-site tRNA (fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
9	A	76	Total	C	H	N	O	P	0	0
			2446	723	826	295	527	75		
9	B	76	Total	C	H	N	O	P	0	0
			2433	723	813	295	527	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	U	deletion	GB 1847035720
B	?	-	U	deletion	GB 1847035720

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	AA	1322	Total	C	H	N	O	S	0	0
			20851	6539	10426	1817	2026	43		

- Molecule 11 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	AB	98	Total	C	H	N	O	S	0	0
			1573	505	783	139	140	6		

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	AC	230	Total	C	H	N	O	S	0	0
			3599	1112	1813	317	351	6		

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Mol	Chain	Residues	Atoms						AltConf	Trace
12	AD	228	Total	C	H	N	O	S	0	0
			3556	1100	1789	312	349	6		

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	AE	1335	Total	C	H	N	O	S	0	0
			21000	6526	10612	1854	1958	50		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	1384	VAL	MET	variant	UNP A0A4S1NBU2

- Molecule 14 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	C	66	Total	C	H	N	O	S	0	0
			1103	344	559	102	97	1		

- Molecule 15 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	D	1524	Total	C	H	N	O	P	0	0
			49126	14585	16423	6003	10591	1524		

- Molecule 16 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	E	86	Total	C	H	N	O	S	0	0
			1388	414	719	138	114	3		

- Molecule 17 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	F	70	Total	C	H	N	O	S	0	0
			1218	366	629	125	97	1		

- Molecule 18 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	G	225	Total	C	H	N	O	S	0	0
			3545	1113	1785	316	323	8		

- Molecule 19 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	H	259	Total	C	H	N	O	S	0	0
			3184	1073	1454	305	349	3		

- Molecule 20 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	I	208	Total	C	H	N	O	S	0	0
			3346	1036	1710	307	290	3		

- Molecule 21 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	J	205	Total	C	H	N	O	S	0	0
			3350	1026	1707	315	298	4		

- Molecule 22 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	K	156	Total	C	H	N	O	S	0	0
			2348	717	1196	217	212	6		

- Molecule 23 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	L	104	Total	C	H	N	O	S	0	0
			1694	536	846	153	152	7		

- Molecule 24 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	M	151	Total	C	H	N	O	S	0	0
			2416	735	1235	227	215	4		

- Molecule 25 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	N	129	Total	C	H	N	O	S	0	0
			2010	616	1031	173	184	6		

- Molecule 26 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	O	127	Total	C	H	N	O	S	0	0
			2092	634	1070	206	179	3		

- Molecule 27 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	P	99	Total	C	H	N	O	S	0	0
			1621	495	831	151	143	1		

- Molecule 28 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	Q	117	Total	C	H	N	O	S	0	0
			1764	540	887	174	160	3		

- Molecule 29 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	R	121	Total	C	H	N	O	S	0	0
			1940	580	1001	194	161	4		

- Molecule 30 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	S	100	Total	C	H	N	O	S	0	0
			1649	499	844	164	139	3		

- Molecule 31 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	T	88	Total	C	H	N	O	S	0	0
			1448	439	734	144	130	1		

- Molecule 32 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	U	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 33 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	V	80	Total	C	H	N	O	S	0	0
			1339	411	691	121	113	3		

- Molecule 34 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	W	83	Total	C	H	N	O	S	0	0
			1351	424	688	126	111	2		

- Molecule 35 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	X	116	Total	C	H	N	O	S	0	0
			1864	558	964	181	158	3		

- Molecule 36 is a RNA chain called mRNA in the ribosomal RNA entrance pore.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	Y	3	Total	C	H	N	O	P	0	0
			90	27	30	6	24	3		

- Molecule 37 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	a	2880	Total	C	H	N	O	P	0	0
			92918	27587	31077	11398	19976	2880		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	887	A	U	variant	GB 937521852

- Molecule 38 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	b	76	Total	C	H	N	O	S	0	0
			1181	360	599	117	104	1		

- Molecule 39 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	c	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 40 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	d	120	Total	C	H	N	O	P	0	0
			3870	1144	1301	468	837	120		

- Molecule 41 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	e	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 42 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	f	58	Total	C	H	N	O	S	0	0
			936	281	488	87	78	2		

- Molecule 43 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	g	66	Total	C	H	N	O	S	0	0
			1042	323	520	99	94	6		

- Molecule 44 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	h	271	Total	C	H	N	O	S	0	0
			4236	1288	2154	423	364	7		

- Molecule 45 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	i	56	Total	C	H	N	O	S	0	0
			903	269	459	94	80	1		

- Molecule 46 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	j	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

- Molecule 47 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	k	52	Total	C	H	N	O		0	0
			890	275	464	78	73			

- Molecule 48 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	l	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	m	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
50	n	177	Total	C	H	N	O	S	0	0
			2853	899	1443	249	256	6		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	o	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	p	175	Total	C	H	N	O	S	0	0
			2671	826	1358	241	244	2		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	q	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 54 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	r	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 55 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	s	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 56 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
56	t	123	Total	C	H	N	O	S	0	0
			1969	593	1023	181	166	6		

- Molecule 57 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	u	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 58 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
58	v	136	Total	C	H	N	O	S	0	0
			2231	686	1157	205	177	6		

- Molecule 59 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
59	w	119	Total	C	H	N	O	S	0	0
			1945	588	994	195	163	5		

- Molecule 60 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms						AltConf	Trace
60	x	116	Total	C	H	N	O		0	0
			1815	552	923	178	162			

- Molecule 61 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
61	y	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 62 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms						AltConf	Trace
62	z	117	Total	C	H	N	O		0	0
			1967	604	1020	192	151			

- Molecule 63 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
63	7	1	Total	Mg	0
			1	1	

- Molecule 64 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	AA	2	Total	Zn	0
			2	2	

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	6188	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 ($e^-/\text{\AA}^2$)	45	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	0.136	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0168	Depositor
Map size ($\text{\AA}$)	562.56, 562.56, 562.56	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.93, 2.93, 2.93	Depositor

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

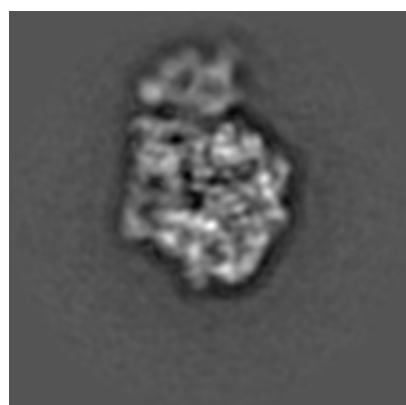
5 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21471. These allow visual inspection of the internal detail of the map and identification of artifacts.

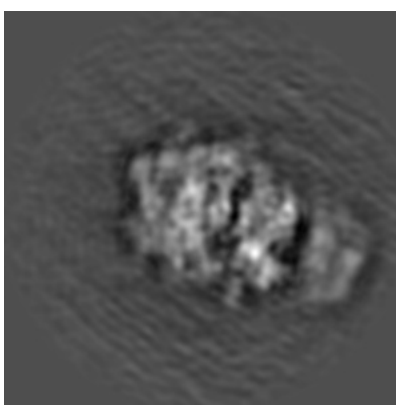
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

5.1 Orthogonal projections [i](#)

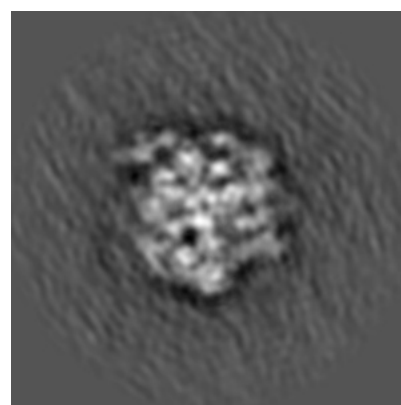
5.1.1 Primary map



X



Y

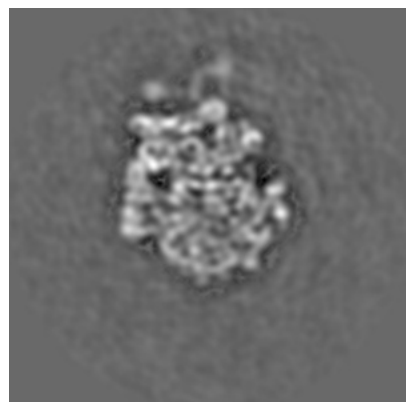


Z

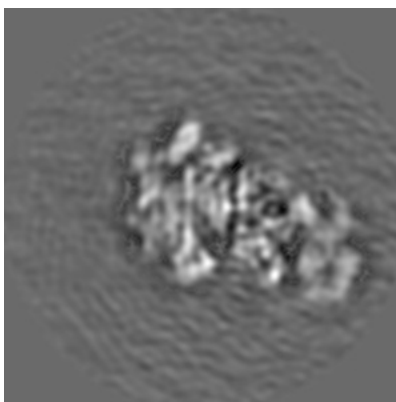
The images above show the map projected in three orthogonal directions.

5.2 Central slices [i](#)

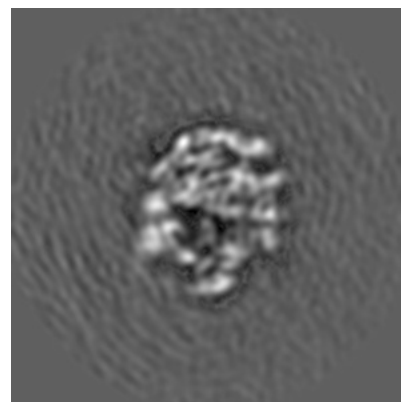
5.2.1 Primary map



X Index: 96



Y Index: 96

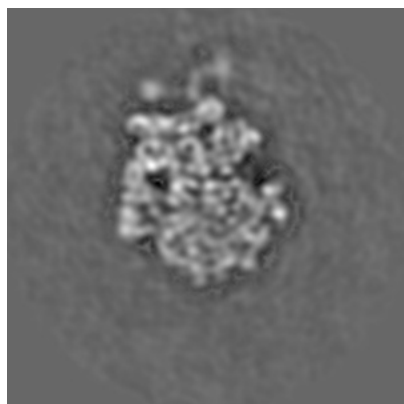


Z Index: 96

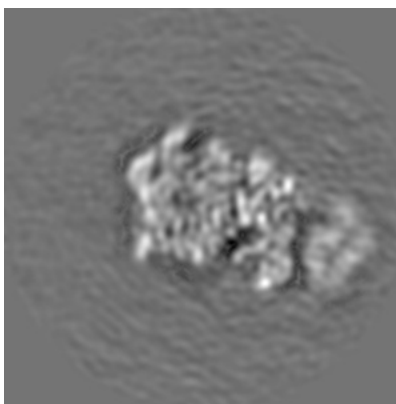
The images above show central slices of the map in three orthogonal directions.

5.3 Largest variance slices [i](#)

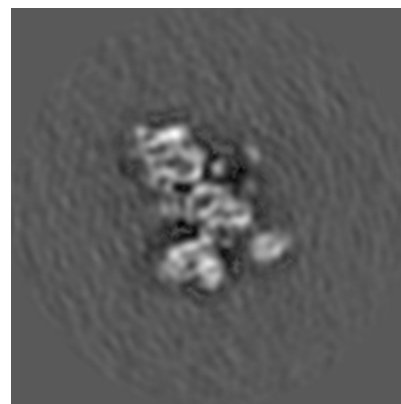
5.3.1 Primary map



X Index: 95



Y Index: 104

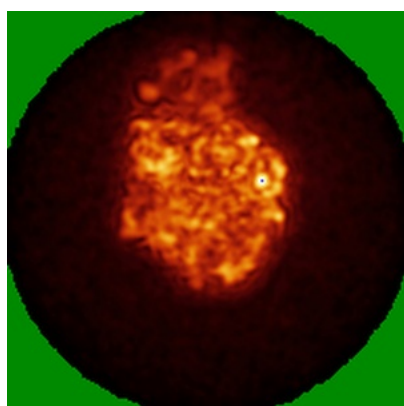


Z Index: 115

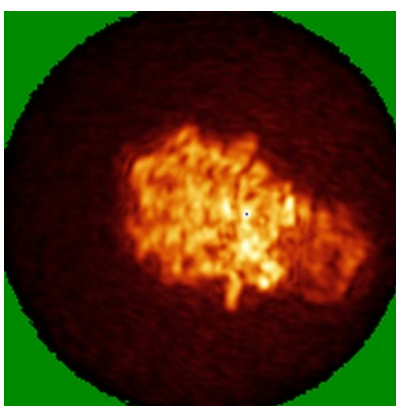
The images above show the largest variance slices of the map in three orthogonal directions.

5.4 Orthogonal standard-deviation projections (False-color) [i](#)

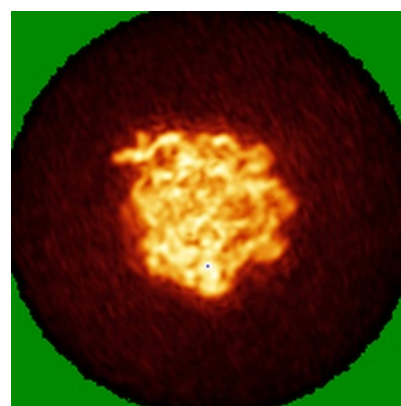
5.4.1 Primary map



X



Y

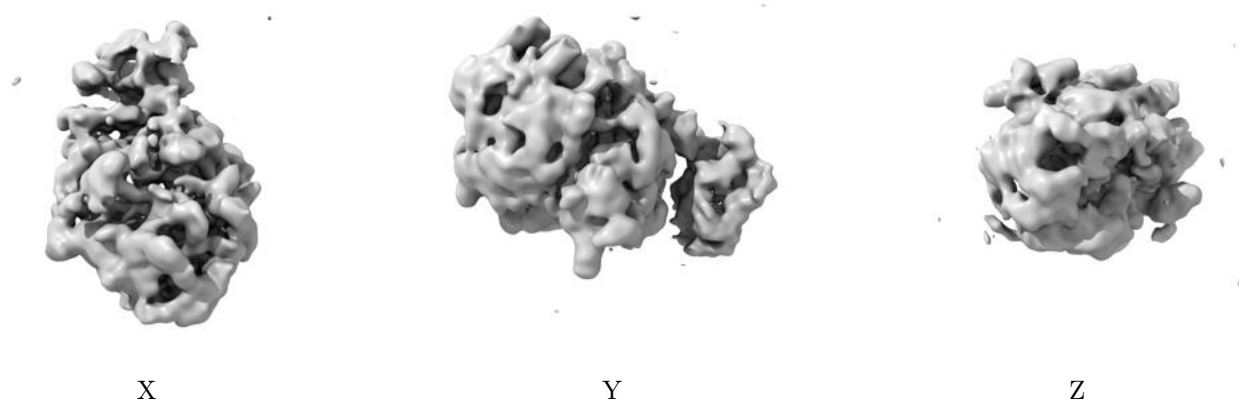


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

5.5 Orthogonal surface views [i](#)

5.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0168. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

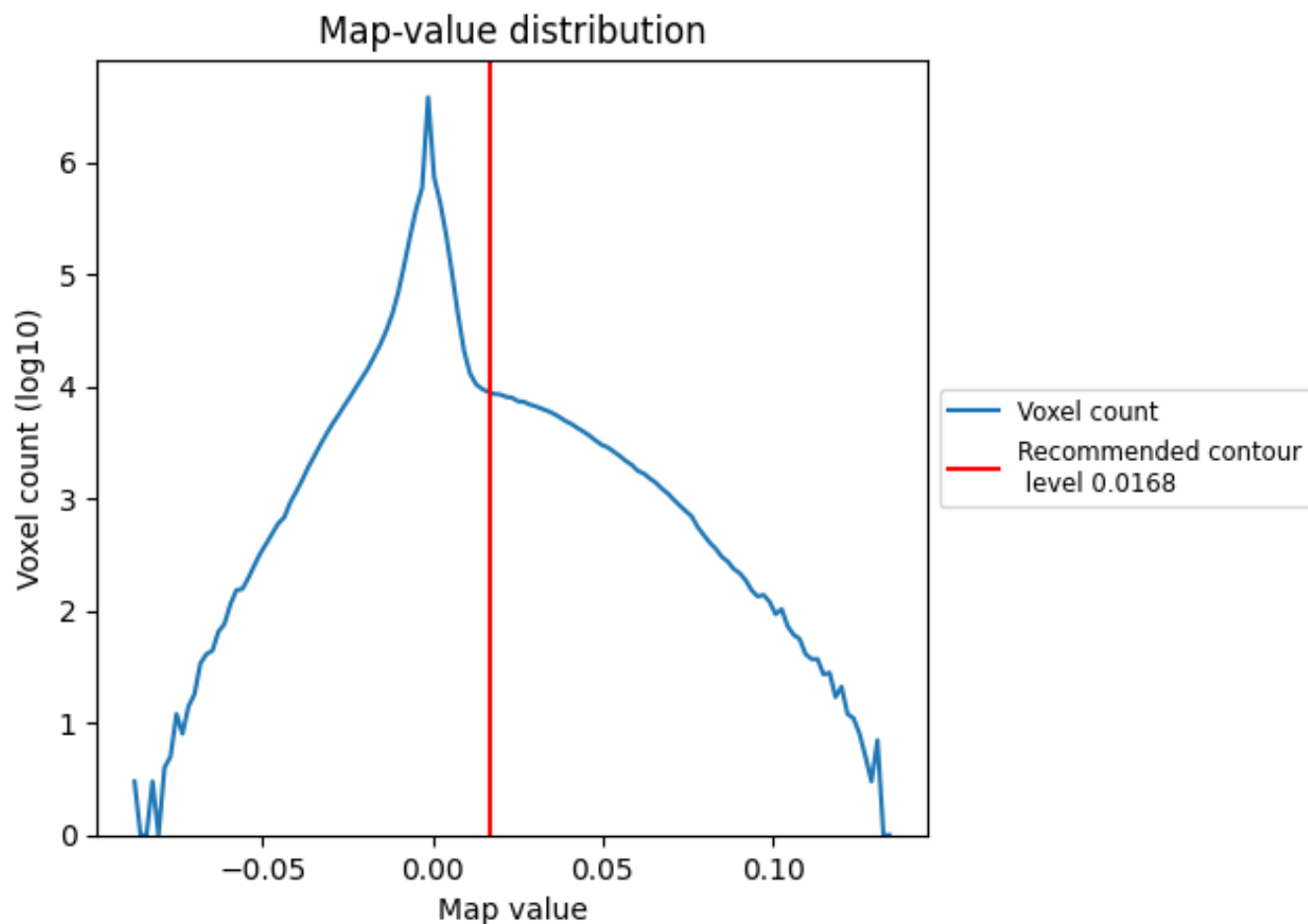
5.6 Mask visualisation [i](#)

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

6 Map analysis [i](#)

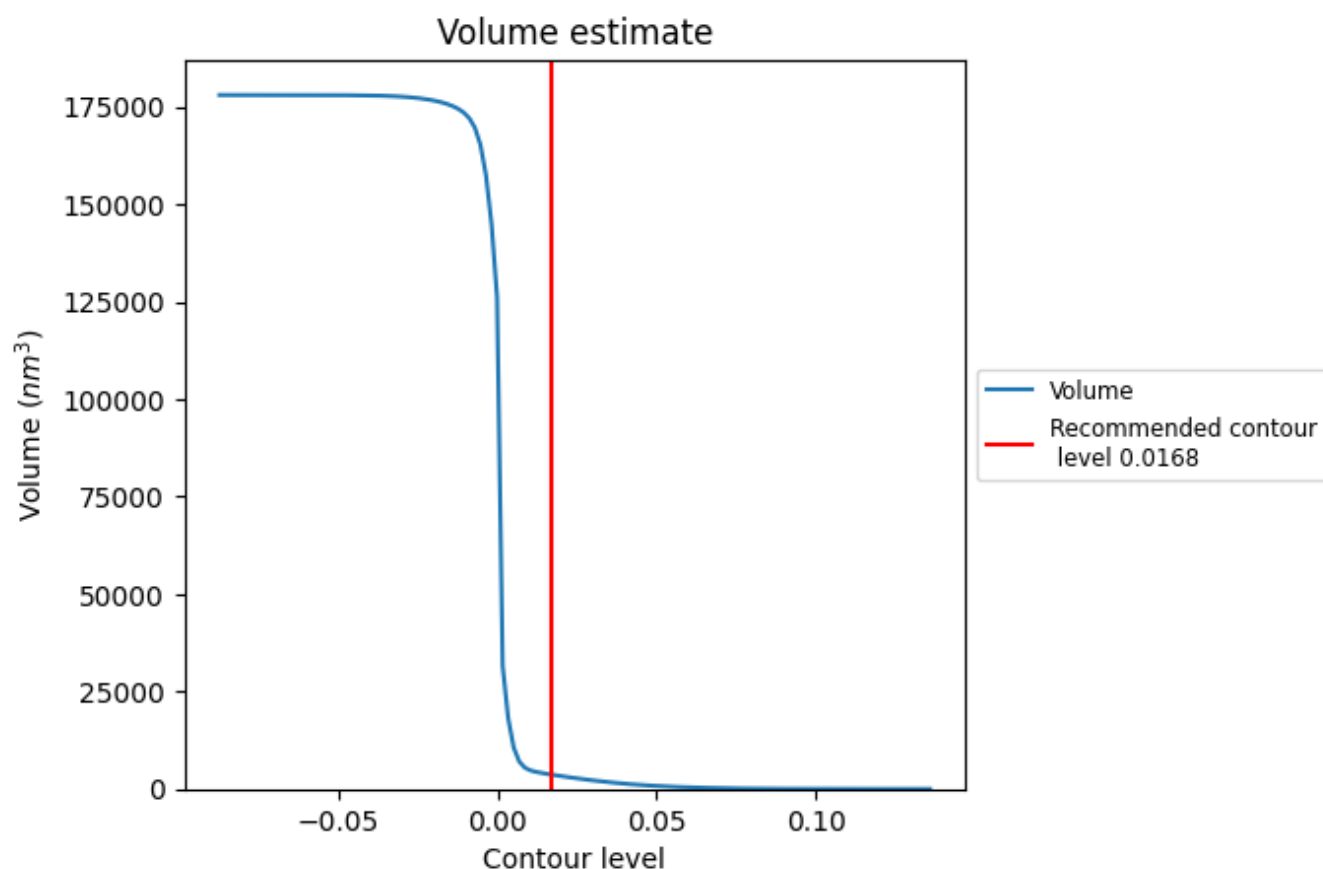
This section contains the results of statistical analysis of the map.

6.1 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.

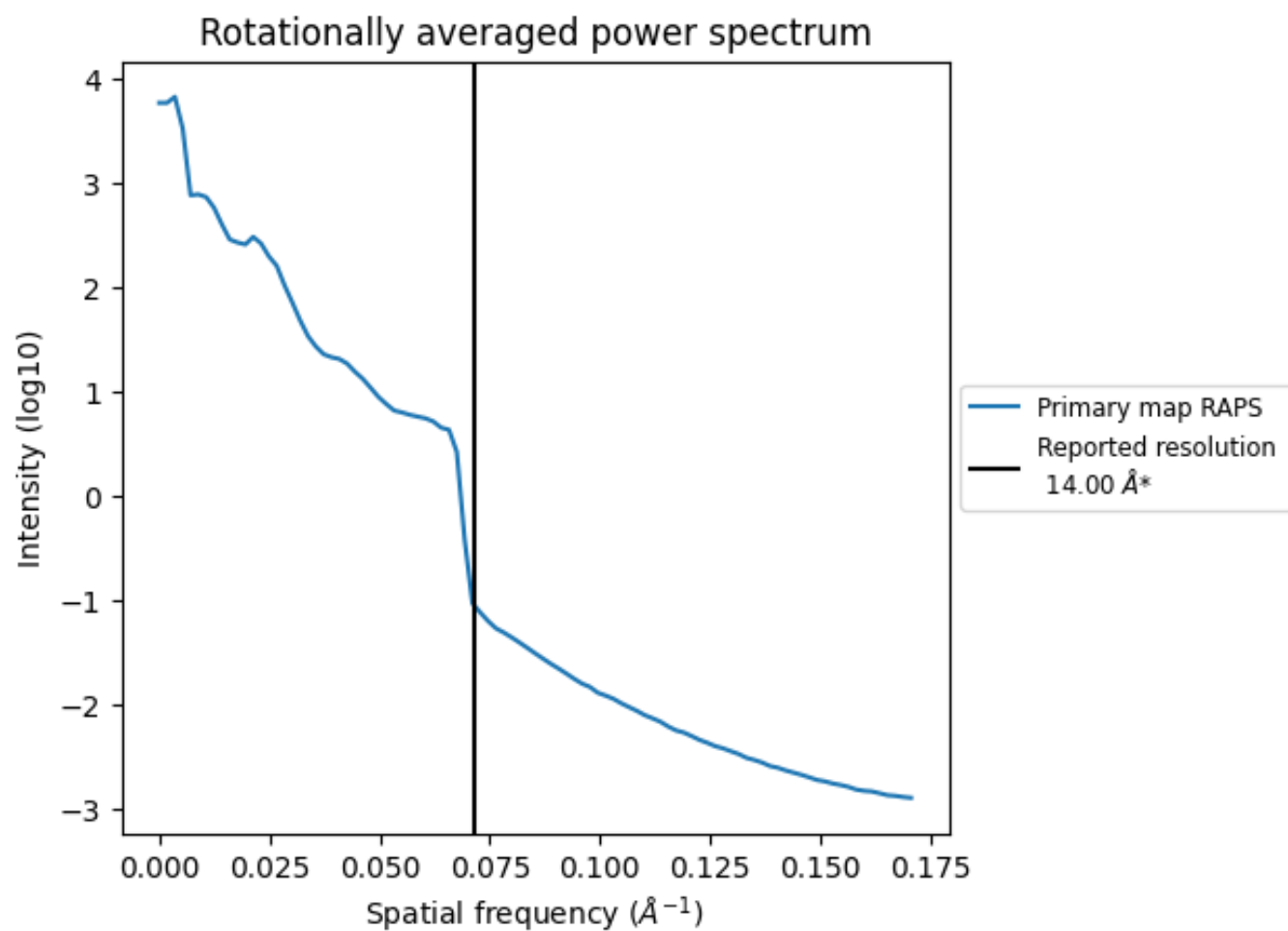
6.2 Volume estimate [i](#)



The volume at the recommended contour level is 3685 nm^3 ; this corresponds to an approximate mass of 3329 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.

6.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.071 Å⁻¹

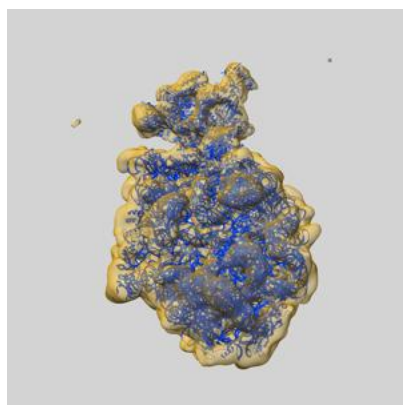
7 Fourier-Shell correlation ⓘ

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

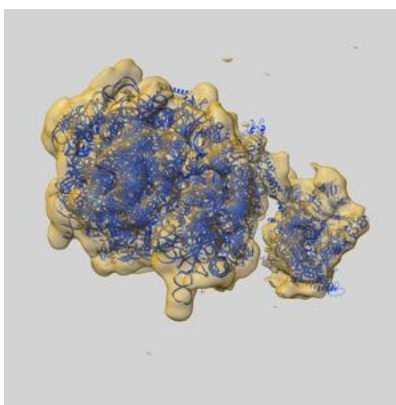
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21471 and PDB model 6VYT. Per-residue inclusion information can be found in section ?? on page ??.

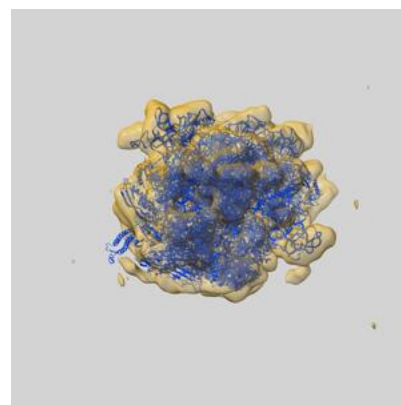
8.1 Map-model overlay [i](#)



X



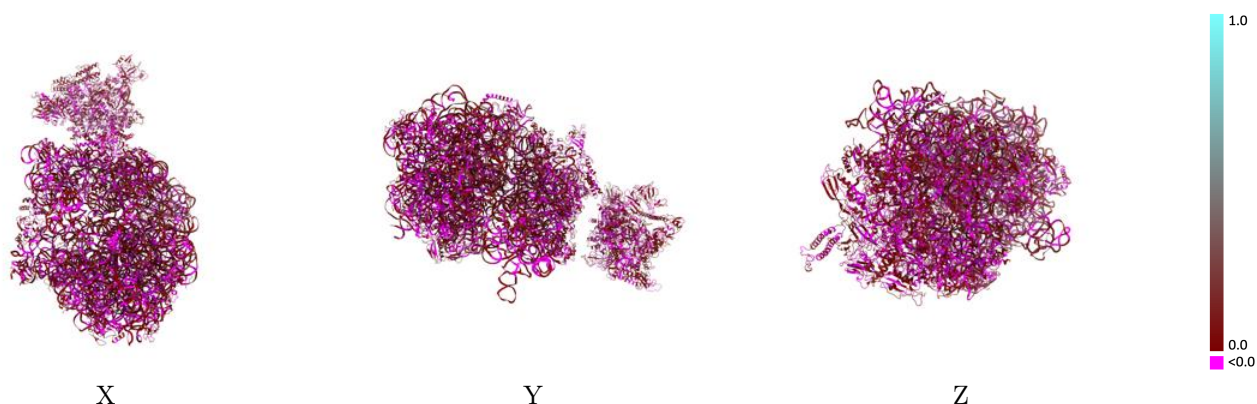
Y



Z

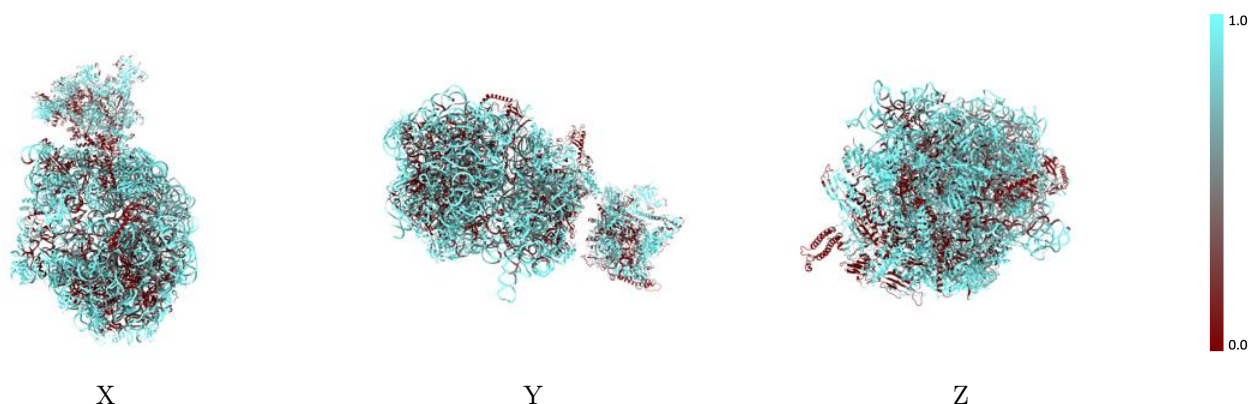
The images above show the 3D surface view of the map at the recommended contour level 0.0168 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



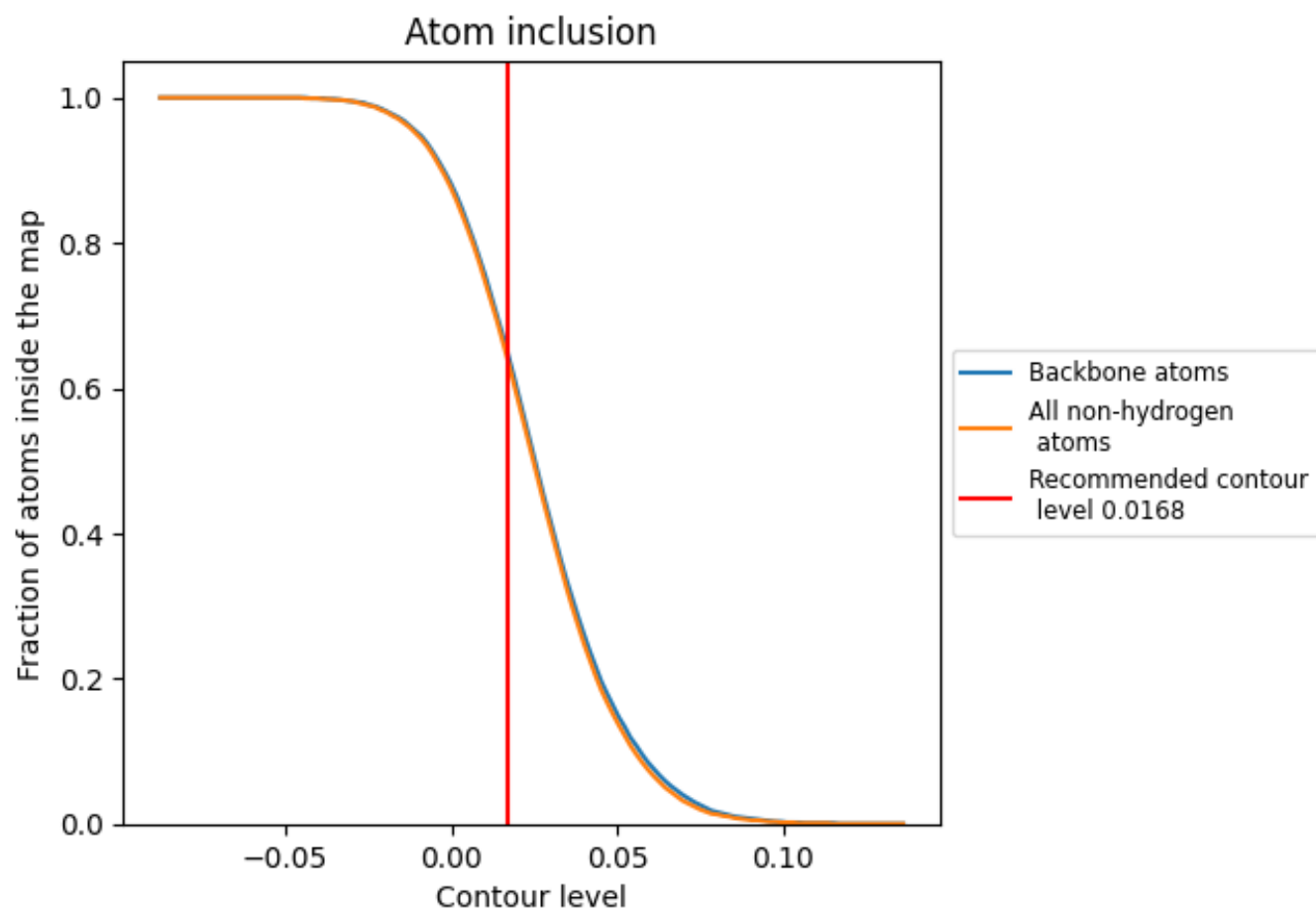
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 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 (0.0168).

8.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0168) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6430	 0.0360
0	 0.7880	 0.0110
1	 0.3040	 -0.0030
2	 0.5820	 -0.0040
3	 0.8330	 0.0340
4	 0.7860	 0.0510
5	 0.4000	 0.0600
6	 0.3100	 0.0170
7	 0.0140	 -0.0160
A	 0.4230	 0.0400
AA	 0.5920	 0.0400
AB	 0.6800	 0.0570
AC	 0.3500	 0.0090
AD	 0.6830	 0.0230
AE	 0.6510	 0.0440
B	 0.5540	 0.0340
C	 0.9100	 0.0520
D	 0.7460	 0.0470
E	 0.6020	 0.0000
F	 0.2220	 0.0340
G	 0.6610	 0.0300
H	 0.2280	 0.0170
I	 0.3690	 0.0120
J	 0.5640	 0.0150
K	 0.5570	 0.0270
L	 0.9100	 0.0660
M	 0.6940	 0.0280
N	 0.6590	 0.0100
O	 0.5690	 -0.0210
P	 0.4220	 -0.0130
Q	 0.7610	 0.0430
R	 0.3910	 0.0010
S	 0.6420	 0.0210
T	 0.8520	 0.0500
U	 0.6540	 0.0100



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Chain	Atom inclusion	Q-score
V	 0.5900	 0.0600
W	 0.7970	 0.0170
X	 0.7030	 0.0150
Y	 0.0000	 -0.0080
a	 0.6870	 0.0450
b	 0.6930	 -0.0050
c	 0.4310	 0.0150
d	 0.6090	 0.0080
e	 0.7440	 0.0170
f	 0.3140	 -0.0320
g	 0.6440	 0.0260
h	 0.3930	 0.0250
i	 0.6870	 0.0040
j	 0.5870	 0.0030
k	 0.7030	 0.0040
l	 0.4870	 0.0150
m	 0.5130	 0.0500
n	 0.6310	 0.0410
o	 0.2690	 -0.0210
p	 0.9000	 0.0390
q	 0.6440	 -0.0420
r	 0.1550	 -0.0140
s	 0.3290	 -0.0150
t	 0.3750	 0.0300
u	 0.7120	 0.0010
v	 0.5630	 0.0140
w	 0.5510	 -0.0190
x	 0.8420	 0.0090
y	 0.4340	 -0.0080
z	 0.6530	 -0.0080