



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 05:14 am GMT

PDB ID : 6YHS
EMDB ID : EMD-10809
Title : Acinetobacter baumannii ribosome-amikacin complex - 50S subunit
Authors : Nicholson, D.; Edwards, T.A.; O'Neill, A.J.; Ranson, N.A.
Deposited on : 2020-03-30
Resolution : 2.70 Å(reported)
Based on initial models : 5AFI, 5MDZ

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

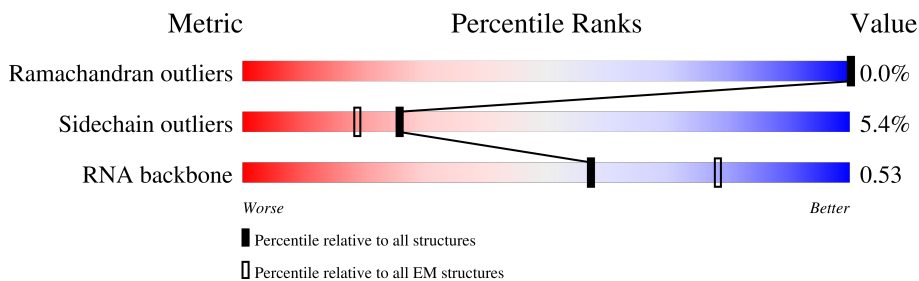
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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)
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	1	2903	
2	5	117	
3	6	77	
3	8	77	
4	A	274	
5	B	212	
6	C	200	
7	D	178	

Continued on next page...

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Mol	Chain	Length	Quality of chain
8	E	177	21% 90% 8%
9	F	142	94% 6%
10	G	122	94% 6%
11	H	146	95% . .
12	I	137	96% .
13	J	125	92% . 5%
14	K	116	10% 94% 5%
15	L	122	6% 91% 5%
16	M	119	97% . .
17	N	103	95% 5%
18	O	110	94% 5%
19	P	106	85% . 13%
20	Q	105	28% 90% 7%
21	R	98	5% 98%
22	S	85	87% . 11%
23	T	78	94% 5%
24	U	65	14% 85% 9% 6%
25	V	58	95% . .
26	X	61	5% 87% . 11%
27	Y	51	6% 96%
28	Z	44	100%
29	a	64	95% . .
30	b	38	97%

2 Entry composition i

There are 32 unique types of molecules in this entry. The entry contains 83514 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
1	1	2672	Total	C	N	O	P	0	0
			57324	25584	10504	18564	2672		

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 3 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	5	Total	C	N	O	P	0	0
			112	49	23	35	5		
3	8	8	Total	C	N	O	P	0	0
			169	76	32	53	8		

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	272	Total	C	N	O	S	0	0
			2109	1301	435	365	8		

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	211	Total	C	N	O	S	0	0
			1571	972	297	299	3		

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	199	1485	933	278	270	4	0	0

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	D	176	865	513	176	176		0	0

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	E	175	1327	838	238	250	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	F	142	1122	717	200	201	4	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	G	122	945	592	180	168	5	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	H	144	1071	663	213	195		0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	I	137	1086	687	210	184	5	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	119	Total	C	N	O	S	1	0
			950	598	187	162	3		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	115	Total	C	N	O	S	0	0
			864	532	175	156	1		

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	L	117	Total	C	N	O	0	0
			919	578	177	164		

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	117	Total	C	N	O	S	0	0
			934	589	197	146	2		

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	103	Total	C	N	O	S	0	0
			806	506	155	142	3		

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	109	Total	C	N	O	S	0	0
			825	514	158	149	4		

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	92	Total	C	N	O	S	0	0
			717	457	129	130	1		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Q	102	Total	C	N	O		
			761	473	141	147	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	96	Total	C	N	O	S		
			753	472	142	138	1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	76	Total	C	N	O	S		
			577	358	111	106	2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	77	Total	C	N	O	S		
			631	395	130	104	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	U	61	Total	C	N	O	S		
			490	304	94	91	1	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	V	57	Total	C	N	O	S		
			453	281	87	81	4	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	54	Total	C	N	O	S		
			447	265	100	81	1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	51	Total	C	N	O	S	0	0
			426	274	77	72	3		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	44	Total	C	N	O	S	0	0
			362	222	85	53	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	63	Total	C	N	O	S	0	0
			508	319	110	75	4		

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	38	Total	C	N	O	S	0	0
			294	179	64	47	4		

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
31	1	157	Total	Mg	0
			157	157	
31	5	3	Total	Mg	0
			3	3	

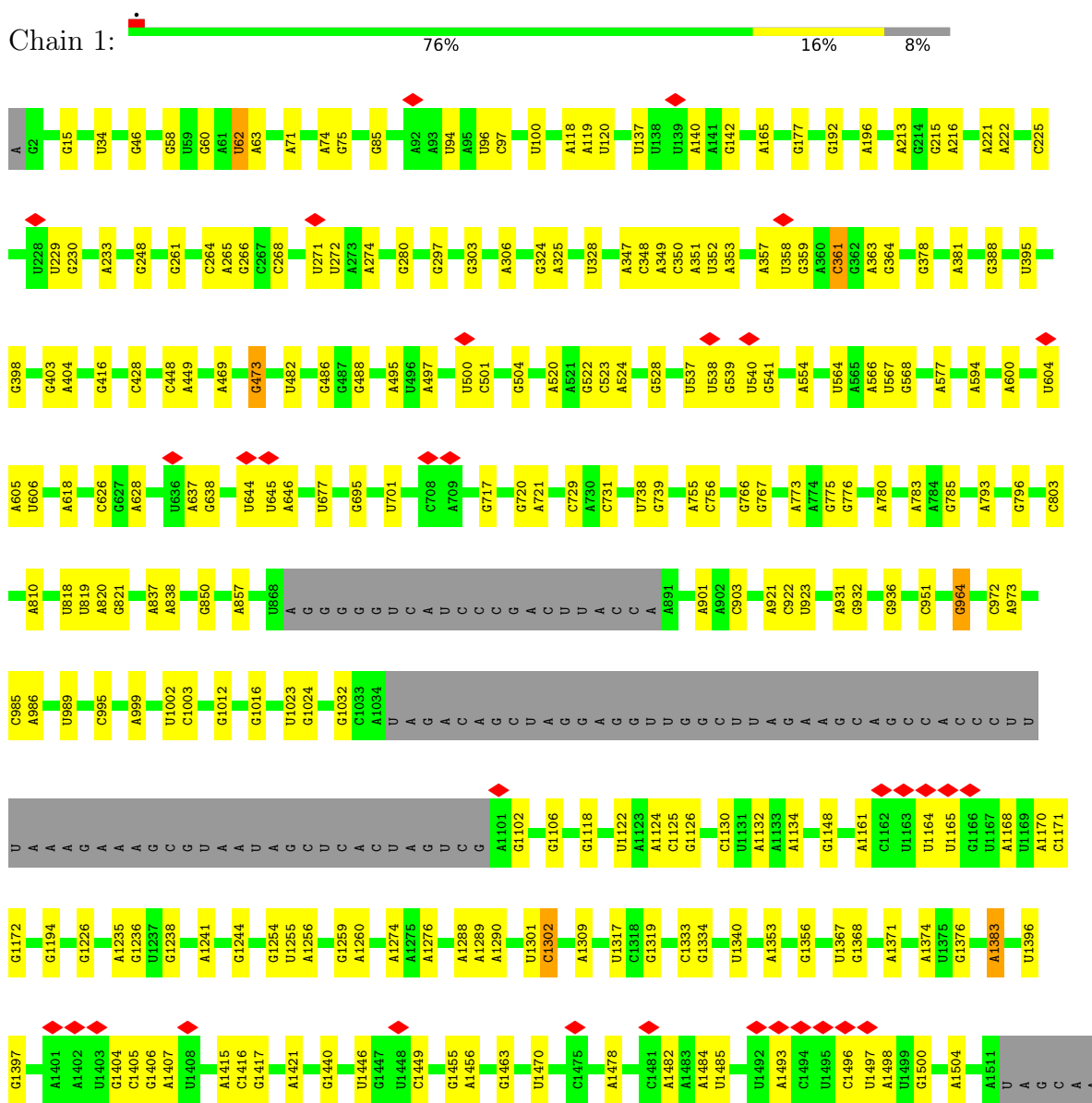
- Molecule 32 is ZINC ION (three-letter code: ZN) (formula: Zn).

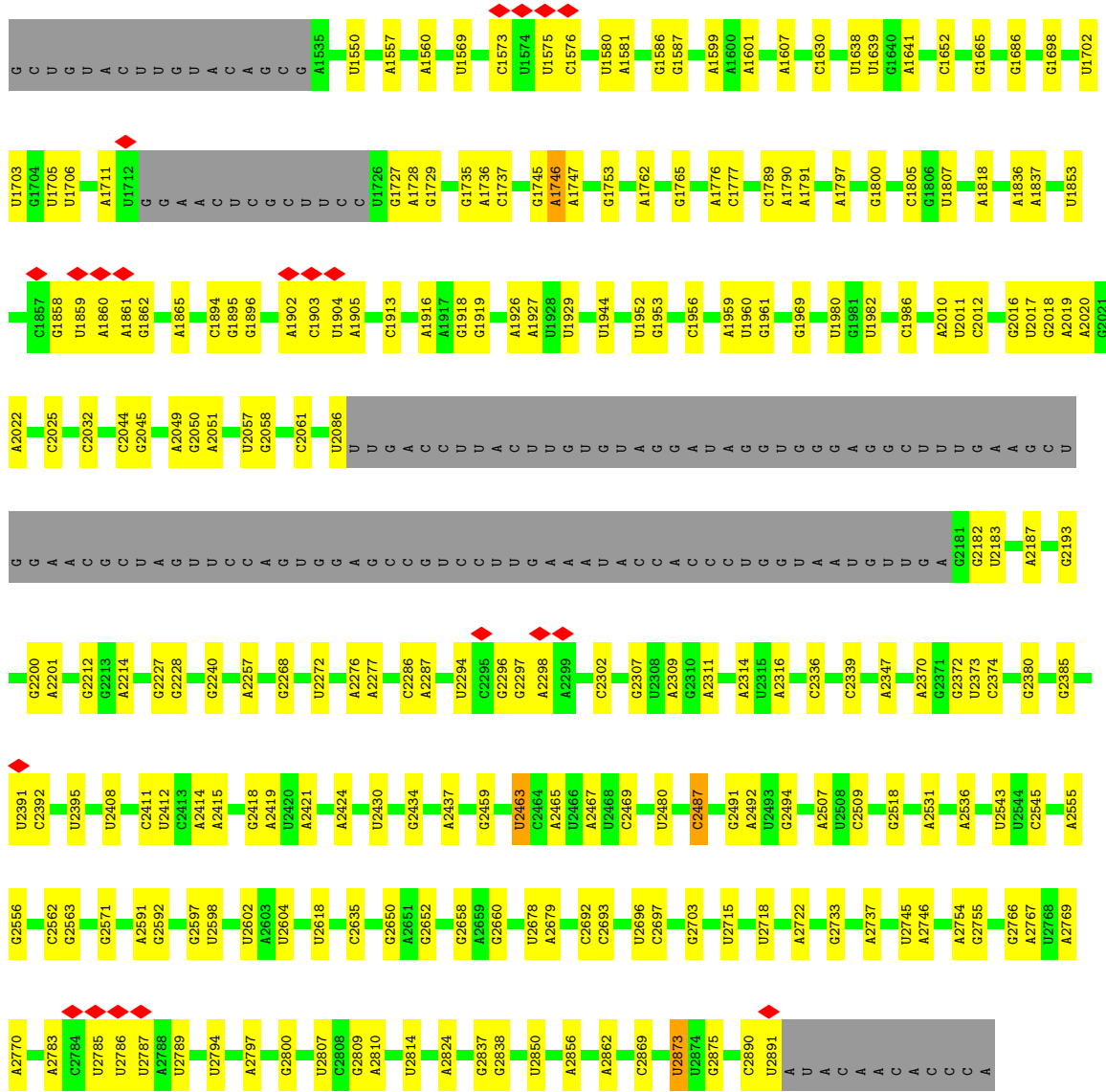
Mol	Chain	Residues	Atoms		AltConf
32	b	1	Total	Zn	0
			1	1	

3 Residue-property plots [i](#)

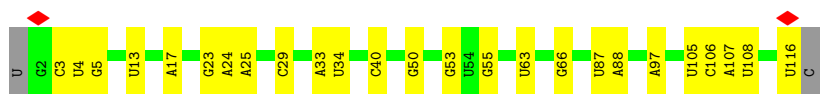
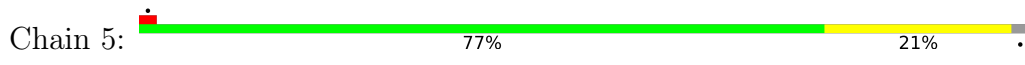
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S ribosomal RNA

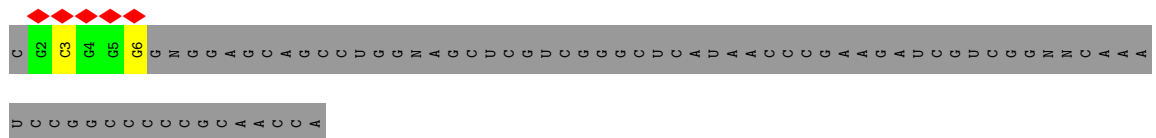




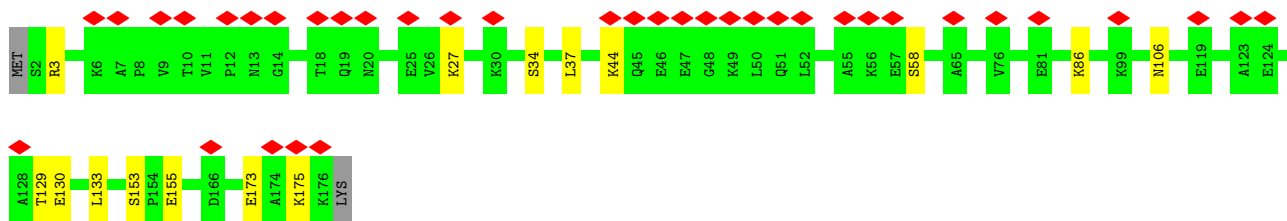
- Molecule 2: 5S ribosomal RNA



- Molecule 3: E-site tRNA



- Molecule 3: E-site tRNA



- Molecule 9: 50S ribosomal protein L13



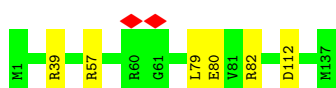
- Molecule 10: 50S ribosomal protein L14



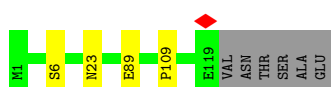
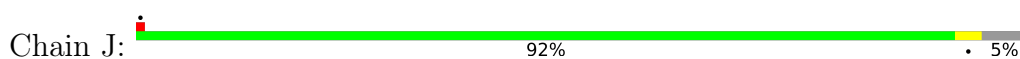
- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16

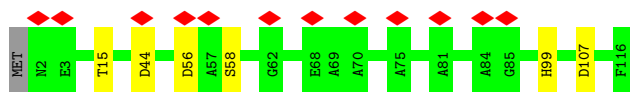


- Molecule 13: 50S ribosomal protein L17

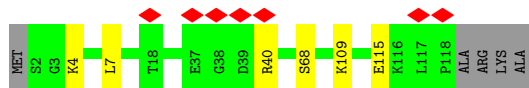
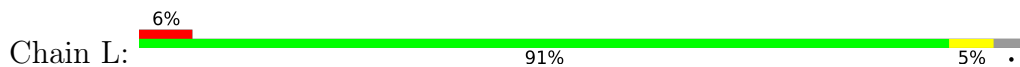


- Molecule 14: 50S ribosomal protein L18





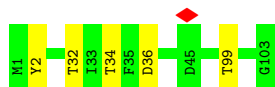
- Molecule 15: 50S ribosomal protein L19



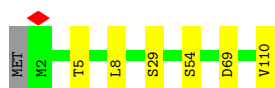
- Molecule 16: 50S ribosomal protein L20



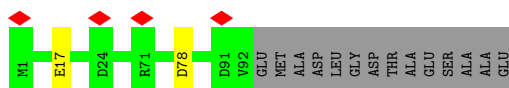
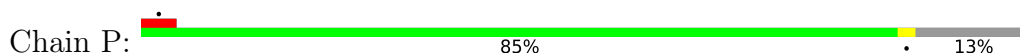
- Molecule 17: 50S ribosomal protein L21



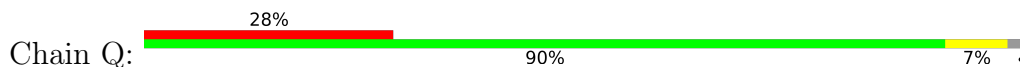
- Molecule 18: 50S ribosomal protein L22



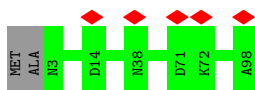
- Molecule 19: 50S ribosomal protein L23



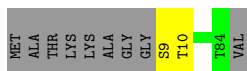
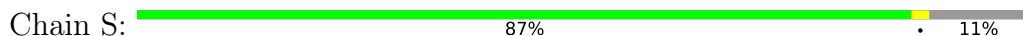
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



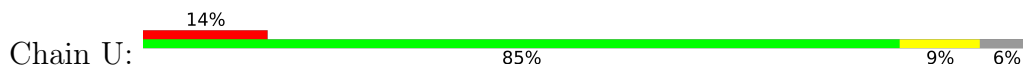
- Molecule 22: 50S ribosomal protein L27



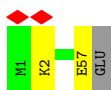
- Molecule 23: 50S ribosomal protein L28



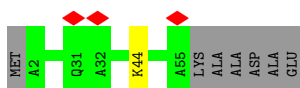
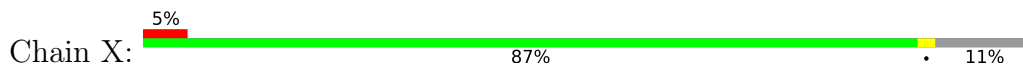
- Molecule 24: 50S ribosomal protein L29



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L32



- Molecule 27: 50S ribosomal protein L33



- Molecule 28: 50S ribosomal protein L34

Chain Z:  100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L35

Chain a:  95%



- Molecule 30: 50S ribosomal protein L36

Chain b:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	51958	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.340	Depositor
Minimum map value	-0.151	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	428.00003, 428.00003, 428.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1	0.87	0/64198	0.94	41/100128 (0.0%)
2	5	0.59	0/2739	0.89	3/4266 (0.1%)
3	6	0.38	0/125	1.02	0/194
3	8	0.36	0/188	0.85	0/290
4	A	0.38	0/2150	0.52	0/2888
5	B	0.38	0/1589	0.53	0/2142
6	C	0.36	0/1506	0.48	0/2035
7	D	0.23	0/864	0.45	0/1199
8	E	0.29	0/1346	0.50	0/1818
9	F	0.40	0/1148	0.50	0/1548
10	G	0.37	0/955	0.52	0/1286
11	H	0.37	0/1079	0.53	0/1439
12	I	0.37	0/1103	0.50	0/1475
13	J	0.39	0/968	0.52	0/1298
14	K	0.30	0/872	0.50	0/1167
15	L	0.36	0/931	0.49	0/1249
16	M	0.45	0/947	0.48	0/1262
17	N	0.36	0/817	0.53	0/1094
18	O	0.36	0/830	0.50	0/1113
19	P	0.37	0/723	0.50	0/967
20	Q	0.30	0/765	0.49	0/1027
21	R	0.33	0/763	0.48	0/1026
22	S	0.40	0/585	0.49	0/783
23	T	0.36	0/641	0.51	0/856
24	U	0.29	0/491	0.49	0/651
25	V	0.37	0/458	0.50	0/612
26	X	0.37	0/453	0.53	0/604
27	Y	0.35	0/433	0.50	0/573
28	Z	0.39	0/366	0.56	0/481
29	a	0.39	0/514	0.52	0/678
30	b	0.36	0/295	0.48	0/389
All	All	0.76	0/90842	0.85	44/136538 (0.0%)

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
5	B	0	1
29	a	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	1	504	G	O4'-C1'-N9	8.62	115.09	108.20
1	1	2302	C	C2-N1-C1'	8.11	127.72	118.80
1	1	1301	U	C2-N1-C1'	8.02	127.32	117.70
1	1	2302	C	C6-N1-C1'	-6.66	112.81	120.80
1	1	2873	U	N3-C2-O2	-6.54	117.62	122.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	B	87	GLU	Peptide
29	a	30	HIS	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
4	A	270/274 (98%)	259 (96%)	11 (4%)	0	100	100
5	B	209/212 (99%)	197 (94%)	12 (6%)	0	100	100
6	C	197/200 (98%)	185 (94%)	12 (6%)	0	100	100
7	D	174/178 (98%)	144 (83%)	30 (17%)	0	100	100
8	E	173/177 (98%)	155 (90%)	18 (10%)	0	100	100
9	F	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
10	G	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
11	H	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
12	I	135/137 (98%)	127 (94%)	8 (6%)	0	100	100
13	J	118/125 (94%)	111 (94%)	7 (6%)	0	100	100
14	K	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
15	L	115/122 (94%)	112 (97%)	3 (3%)	0	100	100
16	M	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
17	N	101/103 (98%)	95 (94%)	6 (6%)	0	100	100
18	O	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
19	P	90/106 (85%)	89 (99%)	1 (1%)	0	100	100
20	Q	100/105 (95%)	86 (86%)	14 (14%)	0	100	100
21	R	94/98 (96%)	89 (95%)	5 (5%)	0	100	100
22	S	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
23	T	75/78 (96%)	75 (100%)	0	0	100	100
24	U	59/65 (91%)	55 (93%)	4 (7%)	0	100	100
25	V	55/58 (95%)	53 (96%)	2 (4%)	0	100	100
26	X	52/61 (85%)	50 (96%)	2 (4%)	0	100	100
27	Y	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
28	Z	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
29	a	61/64 (95%)	58 (95%)	2 (3%)	1 (2%)	9	24
30	b	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3016/3136 (96%)	2849 (94%)	166 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
29	a	31	ILE

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	
4	A	218/220 (99%)	208 (95%)	10 (5%)	27	54
5	B	166/167 (99%)	154 (93%)	12 (7%)	14	34
6	C	145/155 (94%)	140 (97%)	5 (3%)	37	66
8	E	140/142 (99%)	125 (89%)	15 (11%)	6	15
9	F	117/117 (100%)	109 (93%)	8 (7%)	16	36
10	G	103/103 (100%)	96 (93%)	7 (7%)	16	36
11	H	106/108 (98%)	101 (95%)	5 (5%)	26	54
12	I	113/113 (100%)	107 (95%)	6 (5%)	22	48
13	J	97/101 (96%)	93 (96%)	4 (4%)	30	59
14	K	84/85 (99%)	78 (93%)	6 (7%)	14	34
15	L	99/102 (97%)	93 (94%)	6 (6%)	18	41
16	M	85/86 (99%)	83 (98%)	2 (2%)	49	77
17	N	84/84 (100%)	79 (94%)	5 (6%)	19	42
18	O	88/89 (99%)	82 (93%)	6 (7%)	16	36
19	P	78/87 (90%)	76 (97%)	2 (3%)	46	75
20	Q	83/85 (98%)	76 (92%)	7 (8%)	11	25
21	R	78/79 (99%)	78 (100%)	0	100	100
22	S	59/64 (92%)	57 (97%)	2 (3%)	37	66
23	T	69/70 (99%)	65 (94%)	4 (6%)	20	43
24	U	53/56 (95%)	47 (89%)	6 (11%)	6	13
25	V	53/54 (98%)	51 (96%)	2 (4%)	33	62
26	X	46/50 (92%)	45 (98%)	1 (2%)	52	79
27	Y	47/47 (100%)	45 (96%)	2 (4%)	29	57
28	Z	36/36 (100%)	36 (100%)	0	100	100
29	a	52/53 (98%)	50 (96%)	2 (4%)	33	62
30	b	33/33 (100%)	32 (97%)	1 (3%)	41	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2332/2386 (98%)	2206 (95%)	126 (5%)	26 47

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	H	29	VAL
23	T	25	THR
13	J	109	PRO
23	T	22	ASN
25	V	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
29	a	30	HIS
26	X	6	ASN
19	P	90	GLN
24	U	44	GLN
18	O	63	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2666/2903 (91%)	452 (16%)	16 (0%)
2	5	114/117 (97%)	23 (20%)	3 (2%)
3	6	4/77 (5%)	2 (50%)	0
3	8	7/77 (9%)	3 (42%)	0
All	All	2791/3174 (87%)	480 (17%)	19 (0%)

5 of 480 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	15	G
1	1	34	U
1	1	46	G
1	1	58	G
1	1	60	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	2692	C
2	5	33	A
2	5	88	A
2	5	4	U
1	1	1404	G

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 161 ligands modelled in this entry, 161 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.

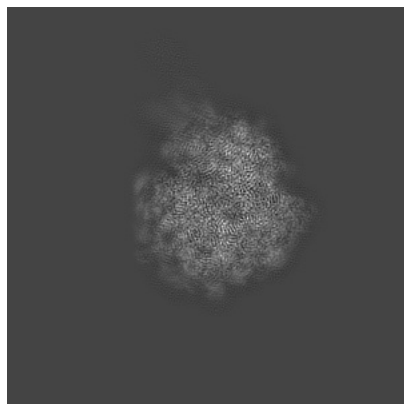
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10809. These allow visual inspection of the internal detail of the map and identification of artifacts.

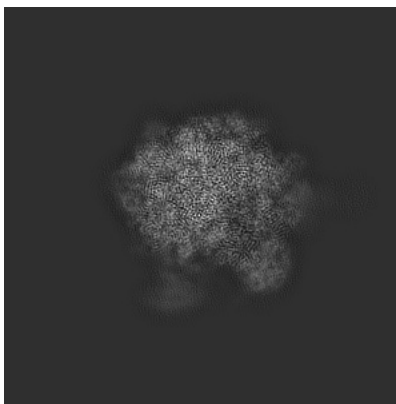
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

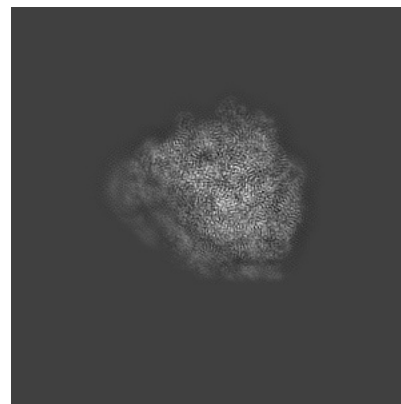
6.1.1 Primary map



X

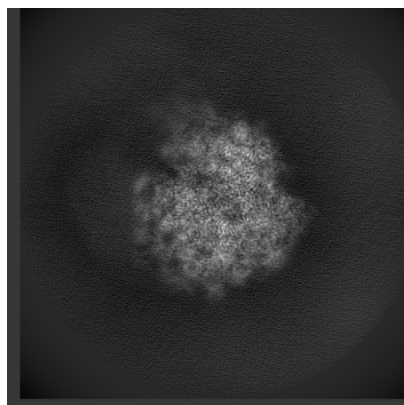


Y

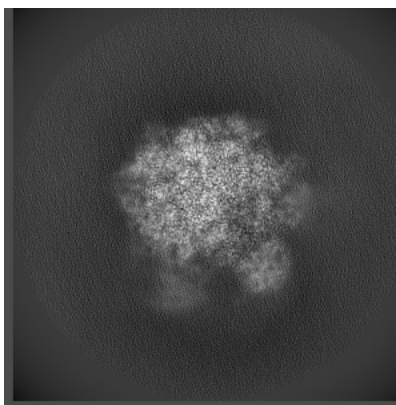


Z

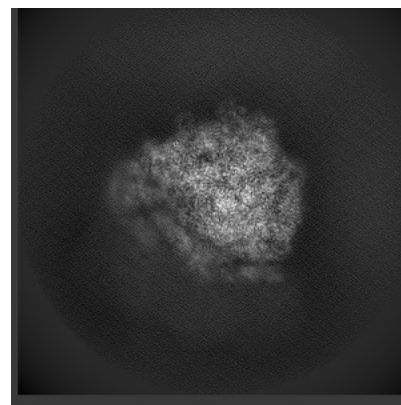
6.1.2 Raw map



X



Y

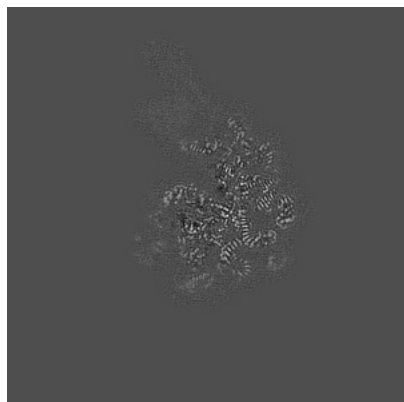


Z

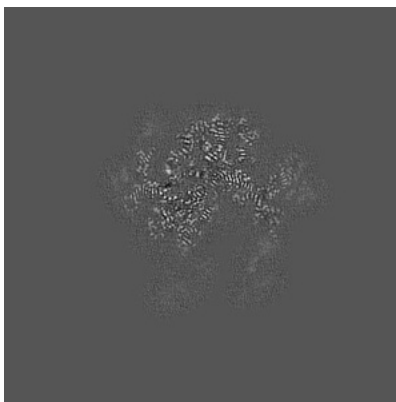
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

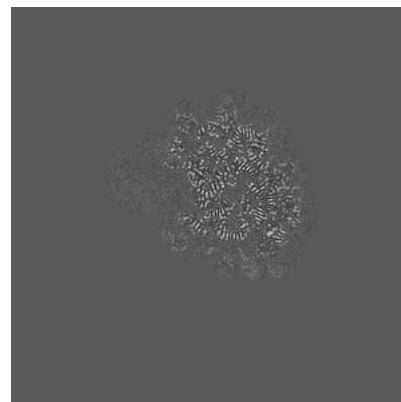
6.2.1 Primary map



X Index: 200

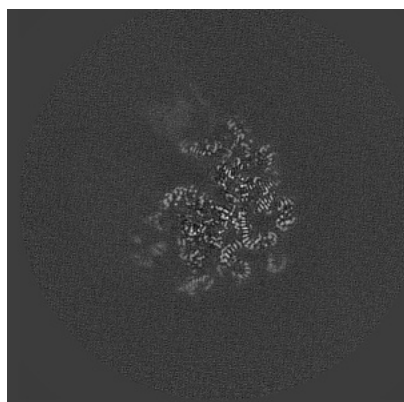


Y Index: 200

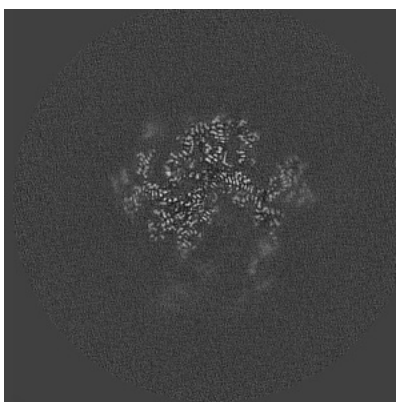


Z Index: 200

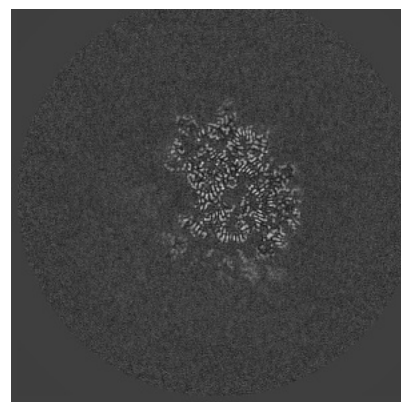
6.2.2 Raw map



X Index: 200



Y Index: 200

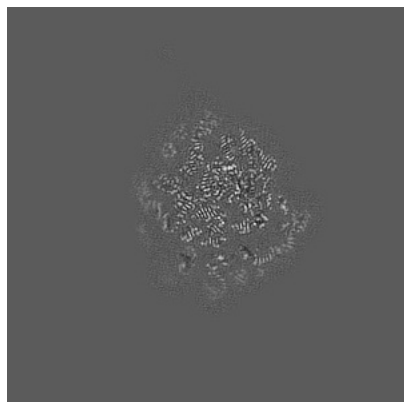


Z Index: 200

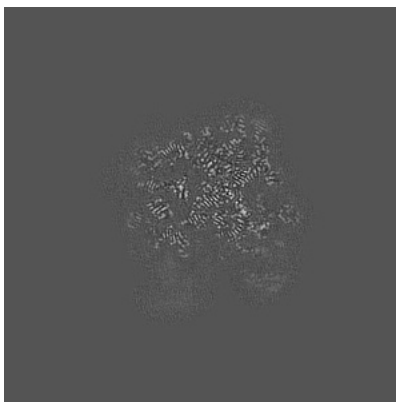
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

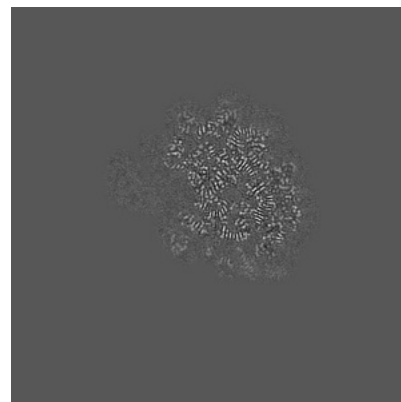
6.3.1 Primary map



X Index: 232

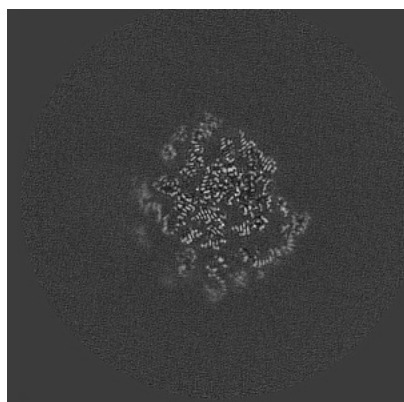


Y Index: 223



Z Index: 201

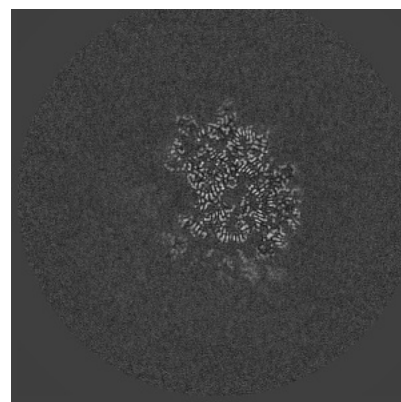
6.3.2 Raw map



X Index: 232



Y Index: 219



Z Index: 200

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

6.4 Orthogonal surface views [i](#)

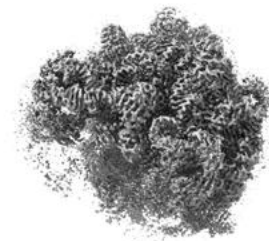
6.4.1 Primary map



X



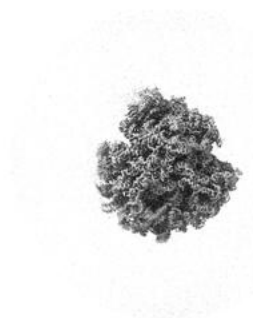
Y



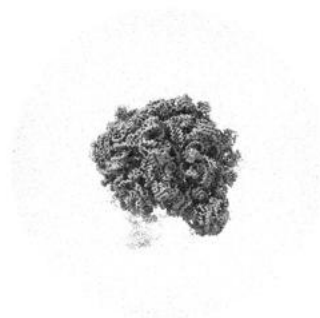
Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

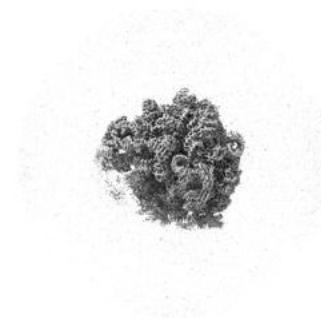
6.4.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

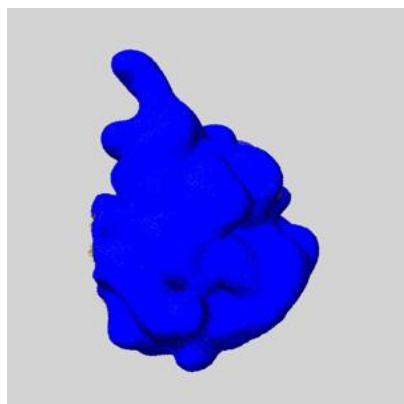
6.5 Mask visualisation [i](#)

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

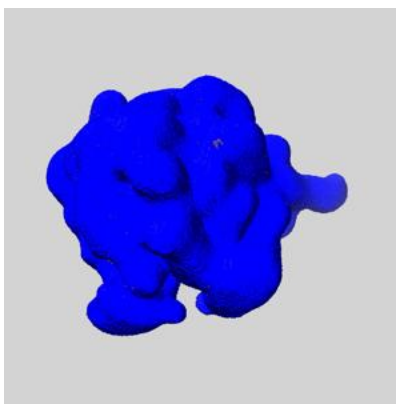
A mask typically either:

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

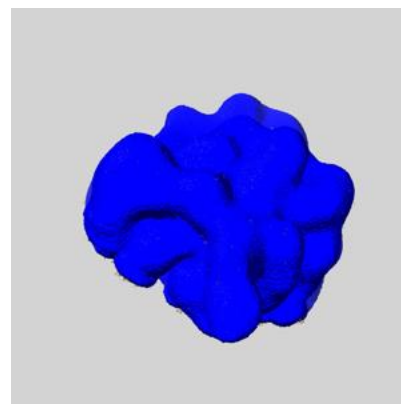
6.5.1 emd_10809_msk_1.map [i](#)



X



Y

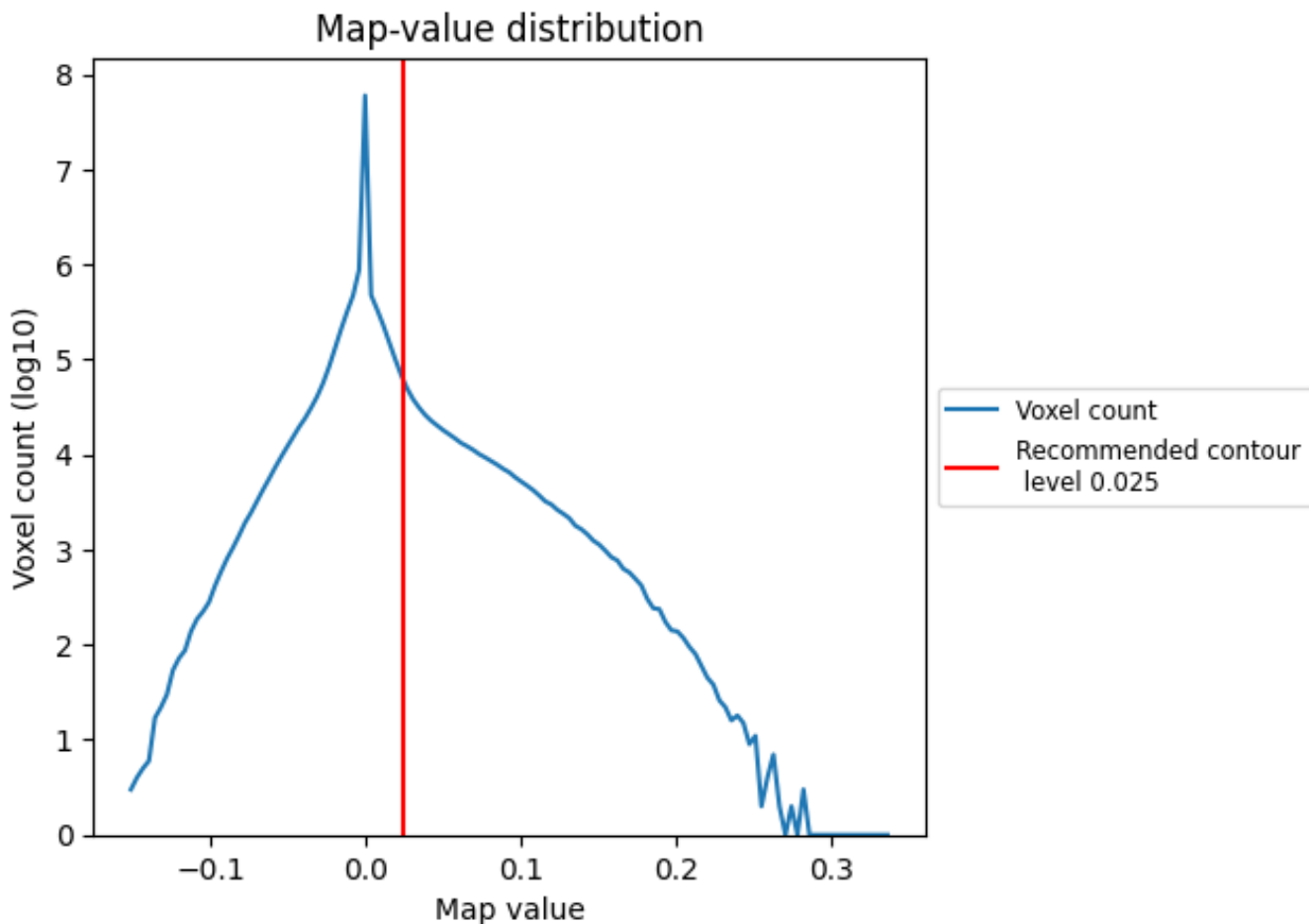


Z

7 Map analysis [i](#)

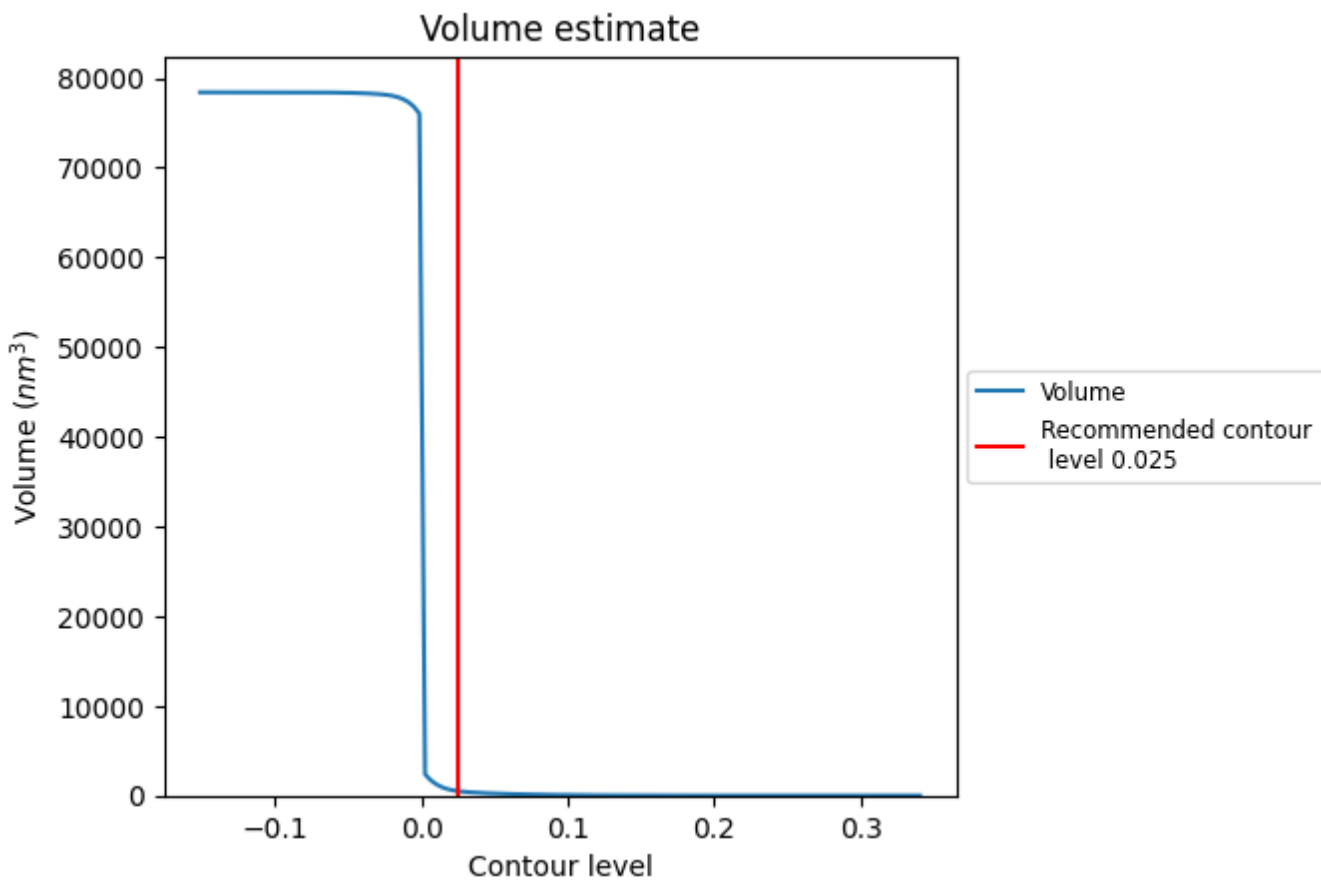
This section contains the results of statistical analysis of the map.

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.

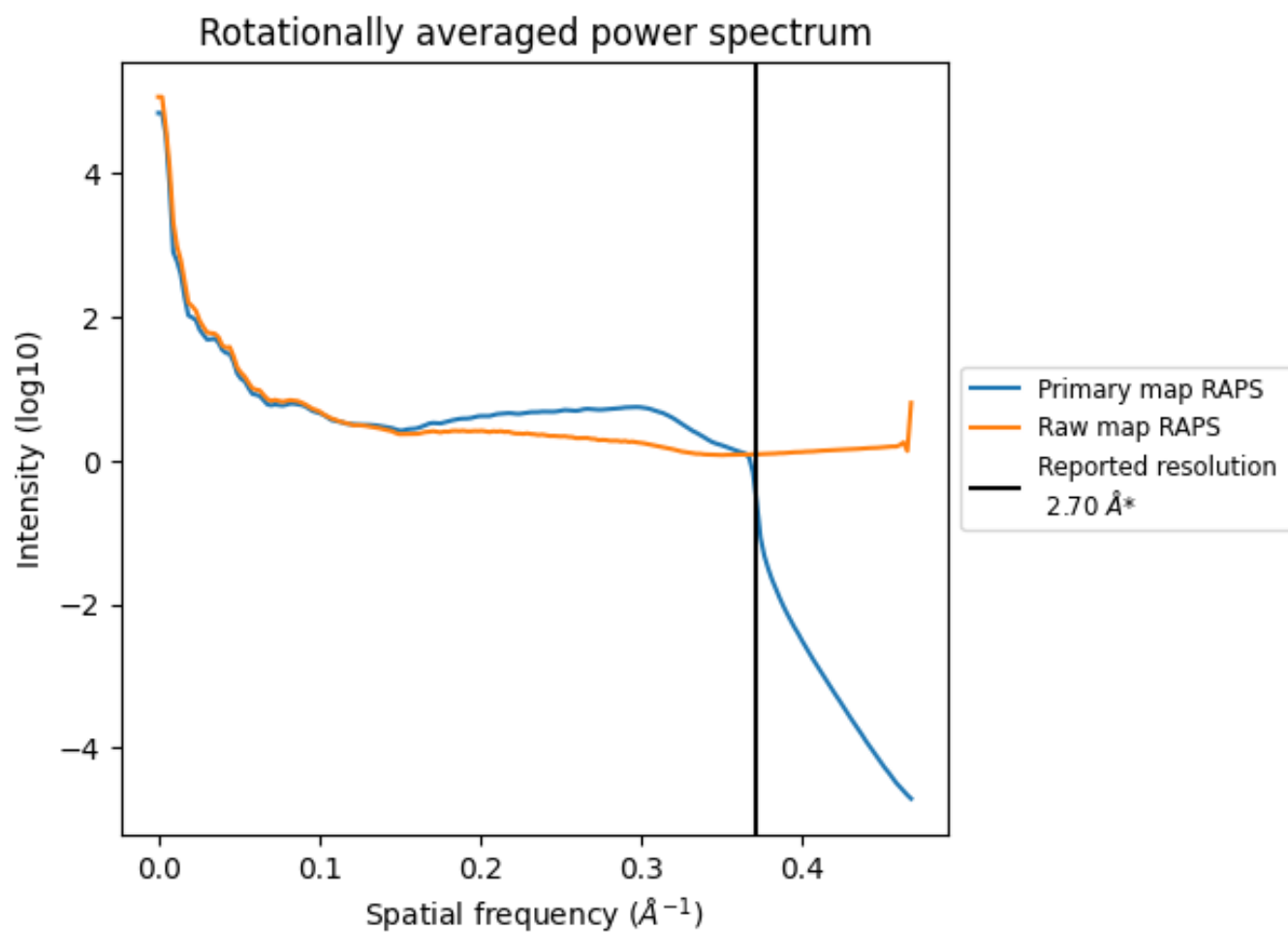
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 500 nm³; this corresponds to an approximate mass of 452 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

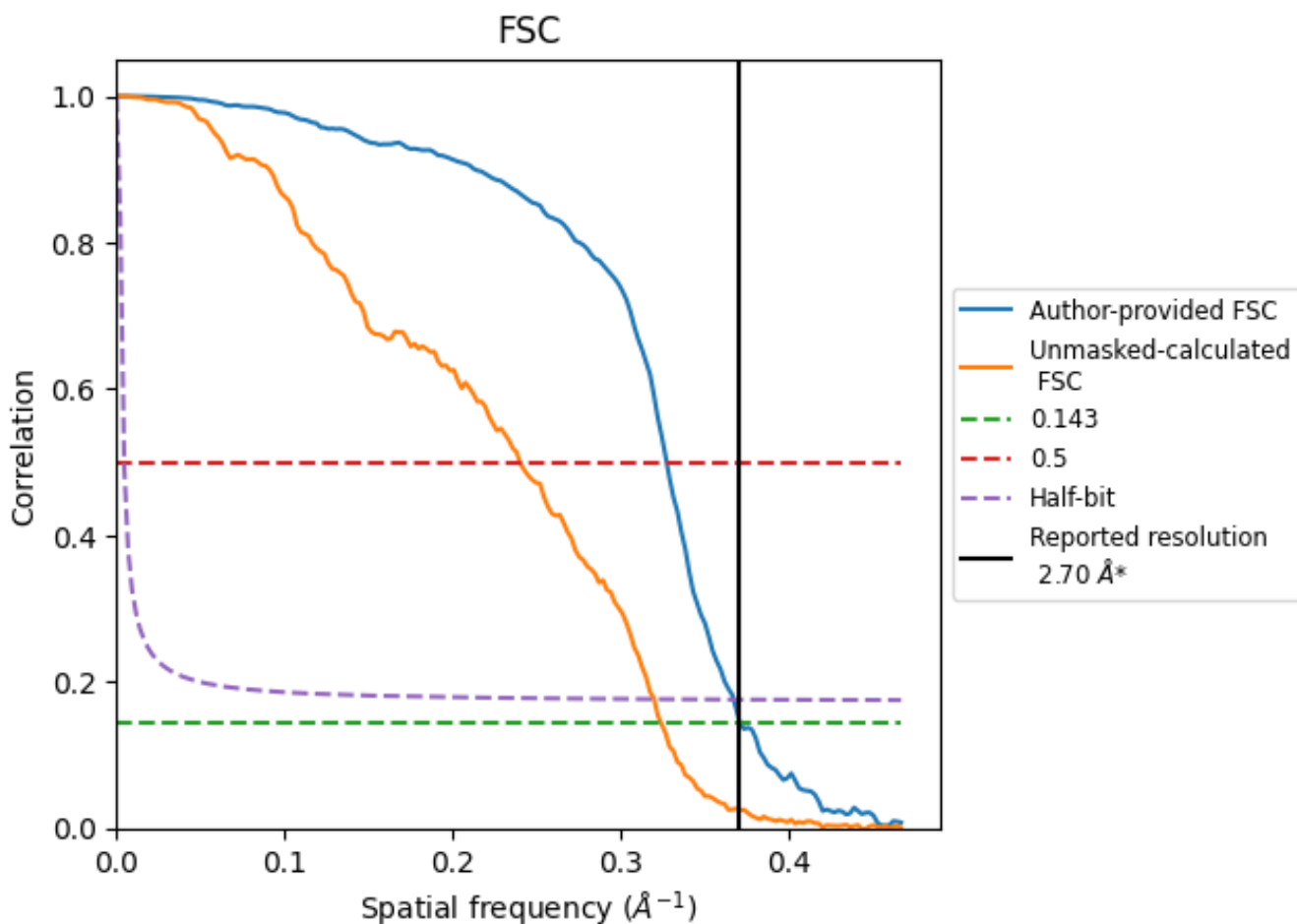


*Reported resolution corresponds to spatial frequency of 0.370 \AA^{-1}

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

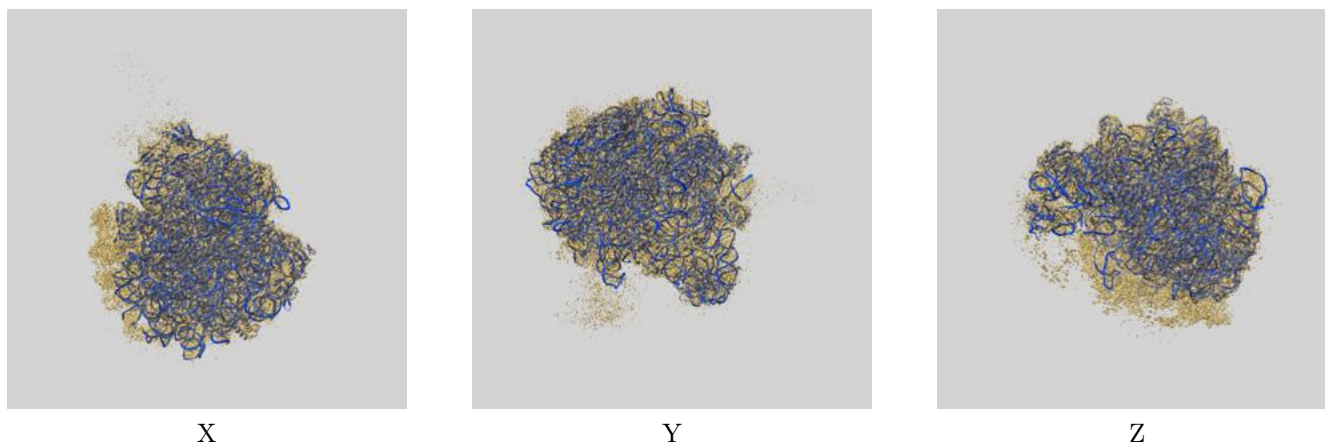
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.69	3.05	2.72
Unmasked-calculated*	3.08	4.16	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.08 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

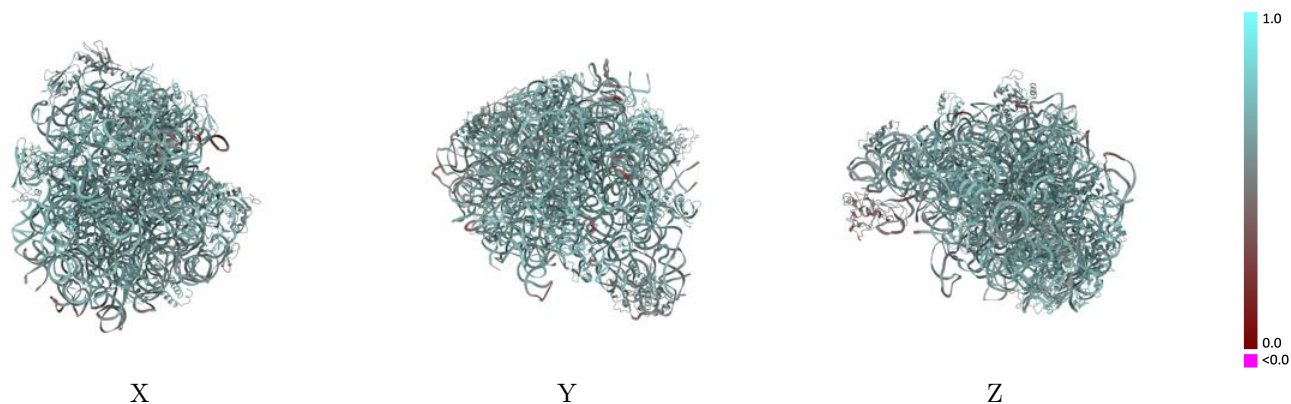
This section contains information regarding the fit between EMDB map EMD-10809 and PDB model 6YHS. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



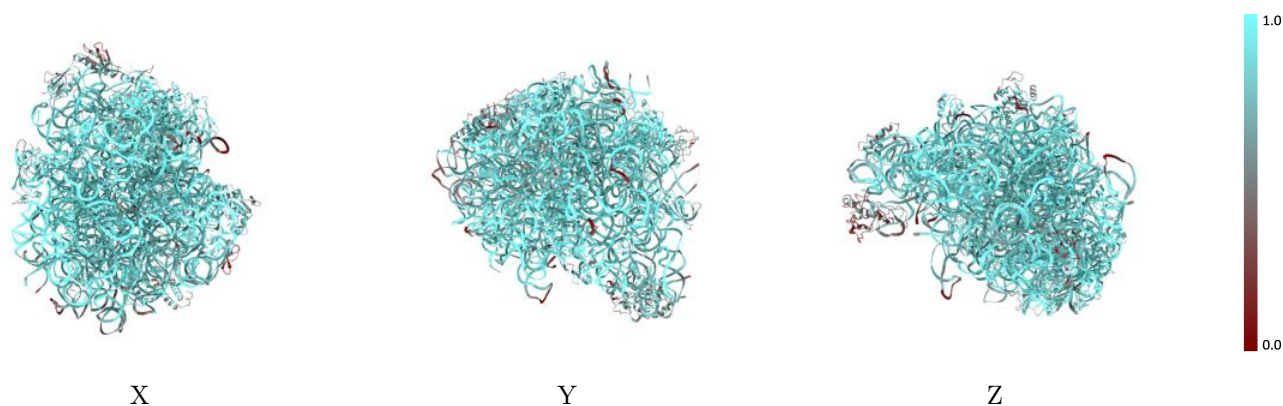
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



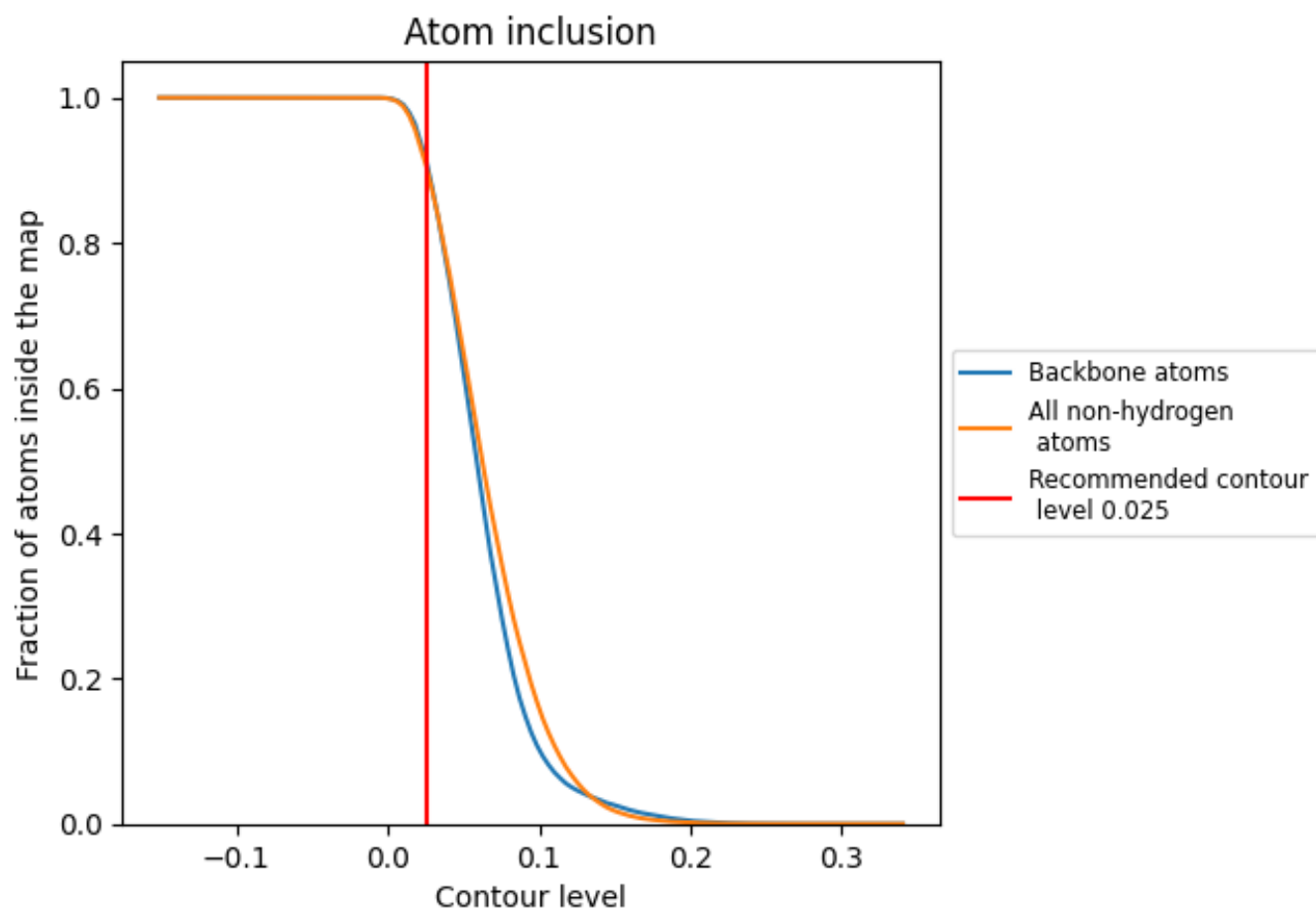
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 91% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9090	 0.6390
1	 0.9412	 0.6430
5	 0.8443	 0.5840
6	 0.1607	 0.4920
8	 0.3373	 0.5070
A	 0.9235	 0.6660
B	 0.9258	 0.6600
C	 0.8462	 0.6350
D	 0.4347	 0.4650
E	 0.5943	 0.5670
F	 0.9248	 0.6610
G	 0.8856	 0.6490
H	 0.8998	 0.6520
I	 0.8944	 0.6480
J	 0.9604	 0.6690
K	 0.7416	 0.5980
L	 0.8533	 0.6470
M	 0.9562	 0.6720
N	 0.8920	 0.6470
O	 0.9109	 0.6630
P	 0.7901	 0.6260
Q	 0.6019	 0.5730
R	 0.8139	 0.6360
S	 0.9396	 0.6750
T	 0.8938	 0.6530
U	 0.6354	 0.5730
V	 0.9120	 0.6470
X	 0.8920	 0.6520
Y	 0.8077	 0.6410
Z	 0.9620	 0.6750
a	 0.9774	 0.6770
b	 0.8877	 0.6480

