wwPDB EM Validation Summary Report (i)

Apr 17, 2024 – 03:03 am BST

PDB ID	:	7AFK
EMDB ID	:	EMD-11768
Title	:	Bacterial 30S ribosomal subunit assembly complex state D (head domain)
Authors	:	Schedlbauer, A.; Iturrioz, I.; Ochoa-Lizarralde, B.; Diercks, T.; Kaminishi, T.; Capuni, R.; Astigarraga, E.; Gil-Carton, D.; Fucini, P.; Connell, S.
Deposited on	:	2020-09-19
Resolution	:	4.90 Å(reported)
Based on initial model	:	4YBB

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

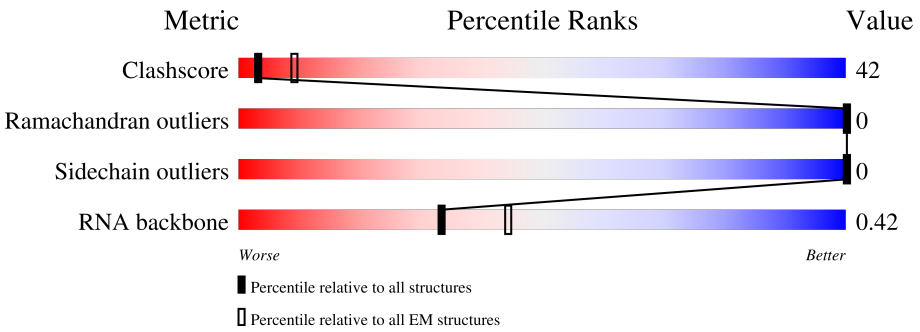
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	1541	· 18% 9% 70%
2	B	241	38% 78% 15% 7%
3	C	233	33% 57% 9%
4	G	179	39% 35% 49% 16%
5	I	130	23% 75% ·
6	J	103	33% 63% ·
7	M	118	42% 55% ·

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Mol	Chain	Length	Quality of chain
8	N	101	40% 59%
9	S	92	17% 72% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	2MG	1	1207	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 18521 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 16SrRNA (head domain of the 30S ribosome).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	456	9758	4357	1772	3173	456	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	224	1753	1109	315	321	8	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	211	1653	1046	310	293	4	0	0

- Molecule 4 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	151	1181	735	227	215	4	0	0

- Molecule 5 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	127	1022	634	206	179	3	0	0

- Molecule 6 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	99	795	498	152	144	1	0	0

- Molecule 7 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	114	883	546	178	156	3	0	0

- Molecule 8 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	100	805	499	164	139	3	0	0

- Molecule 9 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	82	658	421	125	110	2	0	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	1	12	12	12	0

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

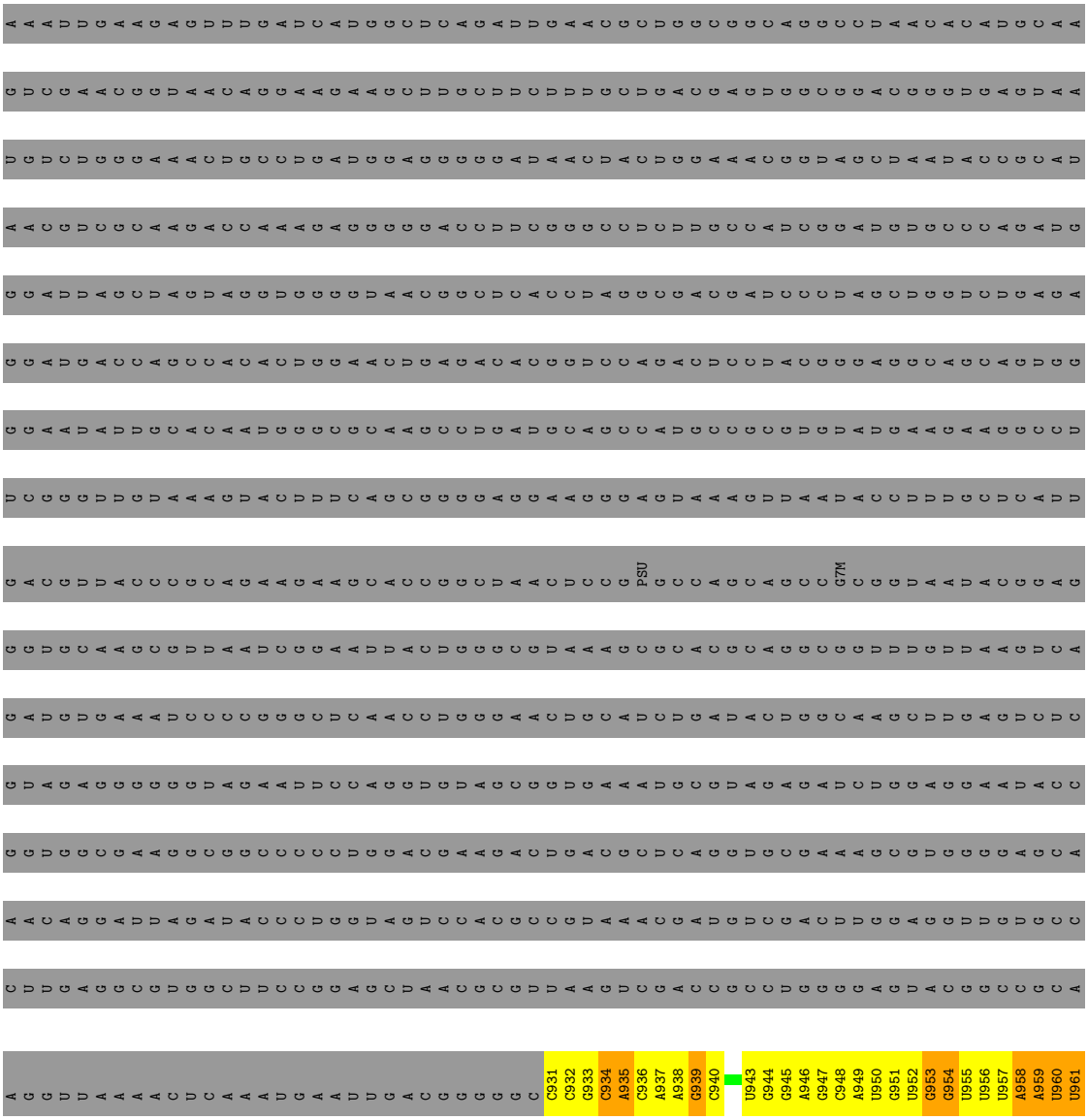
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
11	B	1	1	1	0

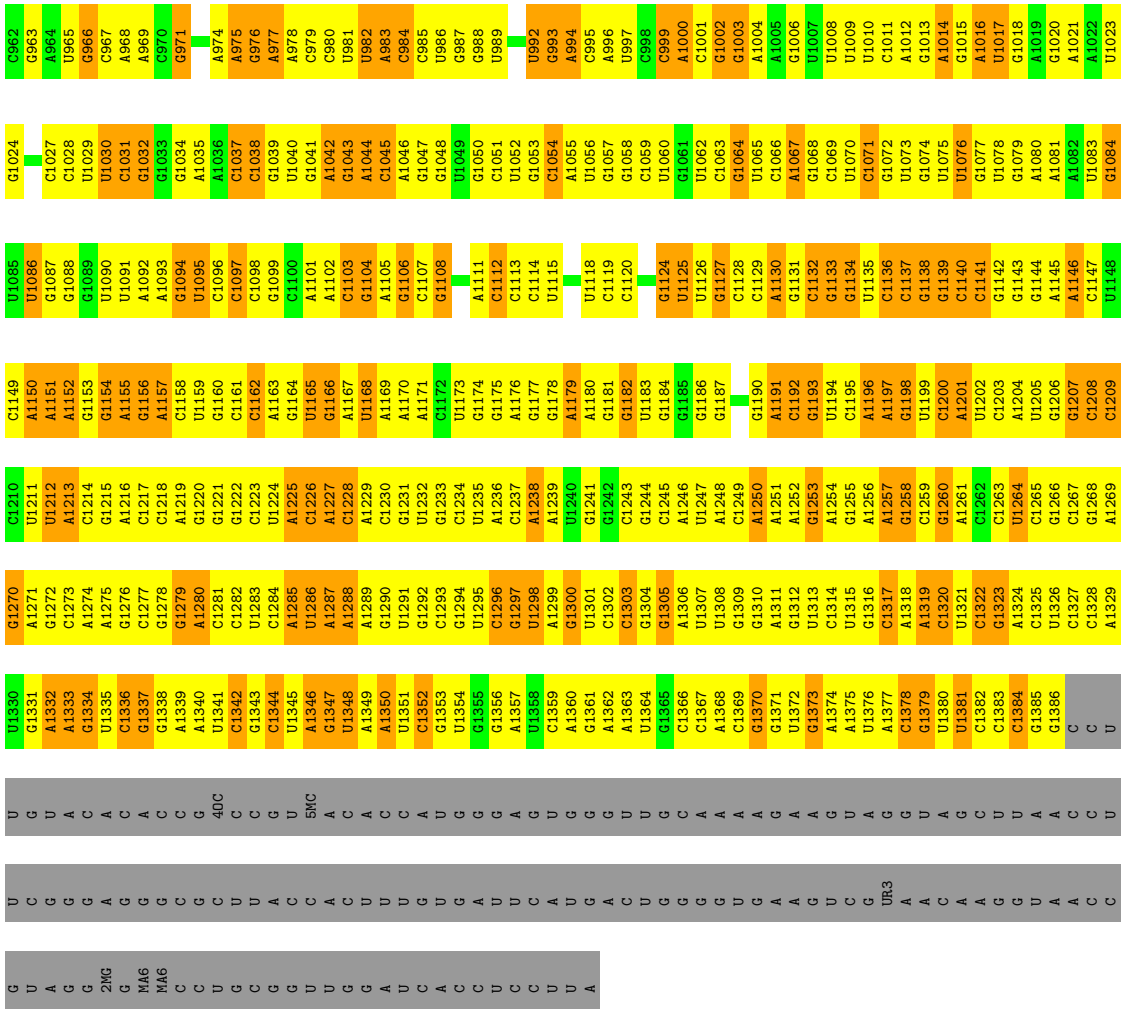
3 Residue-property plots (i)

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: 16SrRNA (head domain of the 30S ribosome)

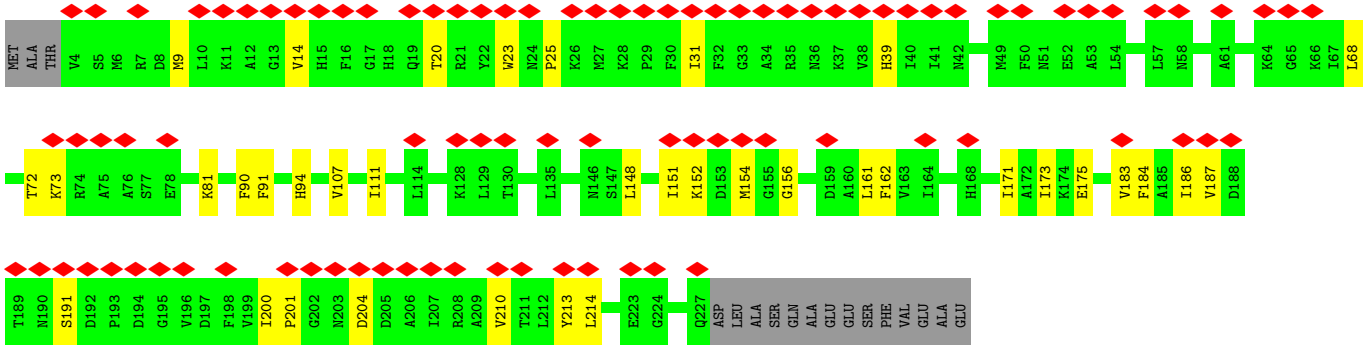
Chain 1:





• Molecule 2: 30S ribosomal protein S2

Chain B:



• Molecule 3: 30S ribosomal protein S3

Chain C:

MET G2 Q3 K4 V5 H6 P7 N8 R11 L12 G13 I14 V15 K16 P17 W18 N19 S20 T21 W22 F23 A24 K27 E28 F29 A30 D31 N32 L33 D34 S35 D36 V39 R40 Q41 Y42 L43 T44 K45 E46 L47 A50 S51 R54 I55 V56 I57 E58 R59 P60 A61 K62 S63 I64 R65

V66 T67 I68 H69 T70 A71 R72 P73 G74 I75 V76 I77 G78 K79 K80 G81 E82 D83 V84 E85 K86 L87 R88 K89 V90 V91 A92 D93 I94 V97 P98 A99 Q100 I101 N102 I103 A104 E105 V106 R107 K108 P109 E110 L111 D112 L115 V116 I120 T121 S122 Q123 L124 E125 R126 R127 V128 M129

F130 R131 R132 A133 M134 K135 R136 A137 V138 Q139 N140 R143 L144 G145 A146 K147 G148 I149 E152 V153 R156 L157 I162 A163 R164 T165 E166 W167 Y168 R169 R172 V173 P174 L175 H176 T177 L178 R179 A180 D181 I182 D183 Y184 T191 G194 I202 F203 K204 G205 E206 A212

ALA VAL GLU GLN PRO GLU LYS PRO ALA ALA GLN PRO LYS LYS GLN GLN ARG LYS GLY ARG LYS

- Molecule 4: 30S ribosomal protein S7

Chain G:

MET P2 R3 R4 R5 V6 I7 G8 Q9 R10 K11 I12 L13 P14 D15 P16 K17 F18 G19 S20 E21 K25 F26 V27 N28 I29 L30 M31 V32 D33 G34 S37 T38 A39 I42 V43 Y44 S45 T49 L50 A51 Q52 R53 S54 G55 K56 S57 E58 L59 E60 A61 F62 E63 V64 A65 L66

E67 N68 V69 R70 P71 T72 V73 E74 V75 K76 S77 R78 R79 V80 G81 G82 S83 T84 Y85 Q86 V87 P88 V89 E90 V91 R92 P93 V94 R95 R96 N97 A98 L99 A100 M101 R102 W103 I104 V105 E106 A107 A108 R109 K110 R111 M116 R119 L120 E123 L124 S125 D126 A127 A128 K131 G132

T133 A134 V135 K136 K137 R138 E139 D140 V141 H142 R143 M144 A145 E146 A147 N148 K149 A150 F151 A152 HIS TYR ARG TRP LEU SER LEU ARG SER PHE SER HIS GLN ALA GLY ALA SER SER LYS GLN PRO ALA LEU GLY TYR LEU ASN

- Molecule 5: 30S ribosomal protein S9

Chain I:

MET ALA GLU N4 Q5 Y6 Y7 G10 R11 R12 K13 S14 S15 A16 A17 R18 V19 F20 I21 K22 P23 G24 N25 G26 K27 I28 V29 I30 N31 Q32 R33 S34 L35 E36 Q37 Y38 F39 G40 R41 E42 T43 A44 R45 M46 V47 V48 R49 Q50 P51 L52 V55 D56 M57 V58 E59 K60 L61 D62

L63 Y64 I65 T66 V67 K68 G69 G70 G71 I72 S73 G74 Q75 I79 R80 H81 G82 I83 T84 R85 A86 L87 M88 E89 Y90 D91 E92 S93 L94 R95 S96 E97 L98 R99 K100 A101 G102 F103 V104 T105 R106 R109 Q110 R113 K114 K115 V116 G117 L118 R119 K120 A121 R122 R123 R124 F127

S128 K129 R130

- Molecule 6: 30S ribosomal protein S10

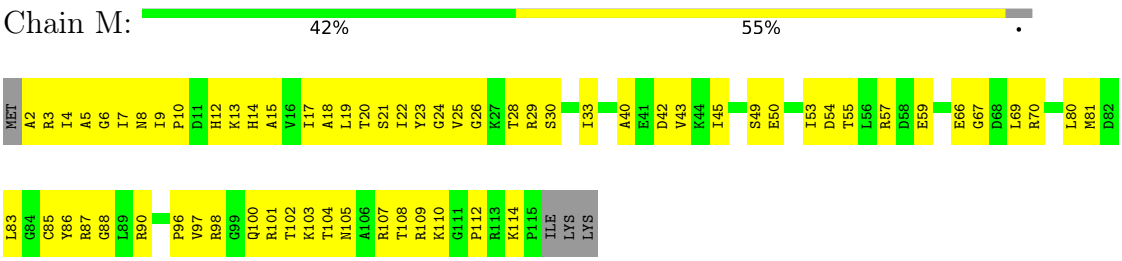
Chain J:

MET GLN ASN Q4 R5 I6 R7 I8 R9 L10 K11 A12 H15 R16 Q20 A21 T22 A23 E24 I25 V26 E27 I28 A29 K30 R31 T32 G33 A34 Q35 V36 R37 G38 P39 I40 P41 L42 P43 T44 R45 K46 E47 R48 F49 T50 V51 L52 I53 H56 V57 R62 D63 Q64 Y65 E66 I67

R68 T69 H70 L71 R72 L73 V74 D75 I76 V77 E78 P79 T80 T83 V84 D85 A86 L87 M88 R89 L90 D91 L92 G95 V96 D97 V98 Q99 I100 S101 L102 GLY

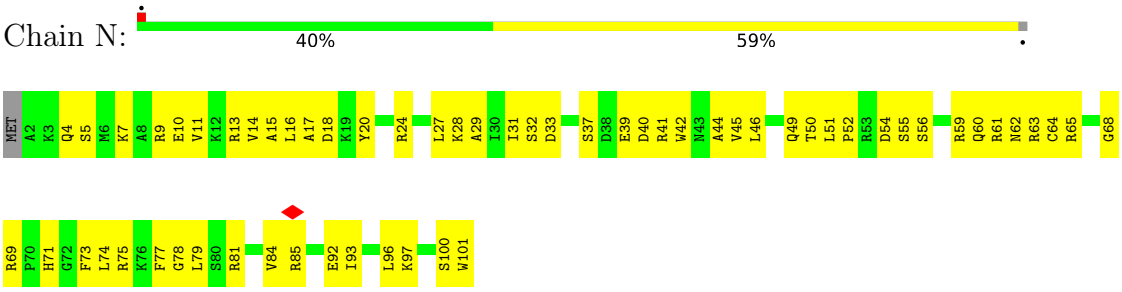
- Molecule 7: 30S ribosomal protein S13

Chain M:



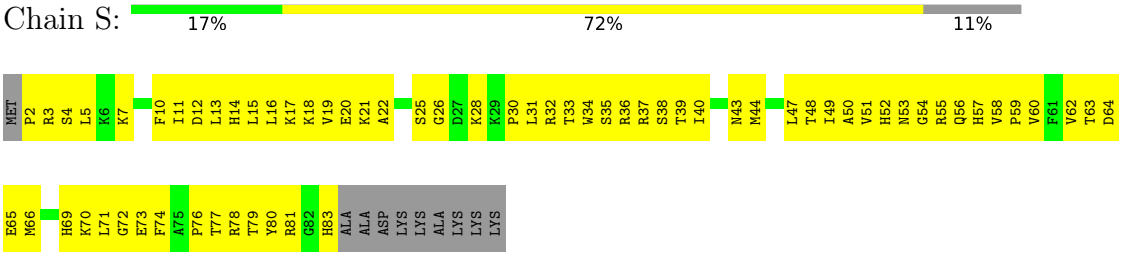
- Molecule 8: 30S ribosomal protein S14

Chain N:



- Molecule 9: 30S ribosomal protein S19

Chain S:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	4573	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 ($e^-/Å^2$)	46.1	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	0.086	Depositor
Minimum map value	-0.026	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	416.64, 416.64, 416.64	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.085, 1.085, 1.085	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, 2MG, ZN, 5MC

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	0.69	0/10842	0.90	0/16904
2	B	0.40	0/1784	0.50	0/2403
3	C	0.37	0/1680	0.51	0/2263
4	G	0.41	0/1195	0.54	0/1602
5	I	0.39	0/1034	0.52	0/1375
6	J	0.43	0/805	0.55	0/1089
7	M	0.48	0/892	0.57	0/1193
8	N	0.41	0/817	0.49	0/1088
9	S	0.36	0/675	0.50	0/908
All	All	0.58	0/19724	0.77	0/28825

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	9758	0	4927	712	0
2	B	1753	0	1780	27	0
3	C	1653	0	1727	146	0
4	G	1181	0	1238	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	I	1022	0	1070	120	0
6	J	795	0	836	79	0
7	M	883	0	941	69	0
8	N	805	0	844	66	0
9	S	658	0	683	76	0
10	1	12	0	0	0	0
11	B	1	0	0	0	0
All	All	18521	0	14046	1209	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 42.

The worst 5 of 1209 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1138:G:H2'	1:1:1140:C:H5'	1.45	0.96
1:1:1055:A:N7	1:1:1200:C:N4	2.17	0.91
3:C:156:ARG:H	3:C:163:ALA:HA	1.35	0.91
6:J:50:THR:HG22	6:J:62:ARG:HE	1.35	0.89
2:B:73:LYS:HE3	2:B:204:ASP:O	1.73	0.88

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	B	222/241 (92%)	217 (98%)	5 (2%)	0	100	100
3	C	209/233 (90%)	190 (91%)	19 (9%)	0	100	100
4	G	149/179 (83%)	137 (92%)	12 (8%)	0	100	100
5	I	125/130 (96%)	109 (87%)	16 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	J	97/103 (94%)	91 (94%)	6 (6%)	0	100	100
7	M	112/118 (95%)	97 (87%)	15 (13%)	0	100	100
8	N	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
9	S	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
All	All	1092/1197 (91%)	1000 (92%)	92 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	172/190 (90%)	172 (100%)	0	100	100
4	G	124/147 (84%)	124 (100%)	0	100	100
5	I	105/107 (98%)	105 (100%)	0	100	100
6	J	87/90 (97%)	87 (100%)	0	100	100
7	M	92/96 (96%)	92 (100%)	0	100	100
8	N	83/84 (99%)	83 (100%)	0	100	100
9	S	72/79 (91%)	72 (100%)	0	100	100
All	All	921/992 (93%)	921 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	122	GLN
4	G	122	ASN
6	J	56	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	455/1541 (29%)	158 (34%)	12 (2%)

5 of 158 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	934	C
1	1	935	A
1	1	939	G
1	1	954	G
1	1	958	A

5 of 12 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1159	U
1	1	1208	C
1	1	1298	U
1	1	1286	U
1	1	999	C

5.4 Non-standard residues in protein, DNA, RNA chains (i)

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	1	967	1	18,22,23	0.98	2 (11%)	26,32,35	1.24	3 (11%)
1	2MG	1	966	1	18,26,27	1.03	1 (5%)	16,38,41	1.43	3 (18%)
1	2MG	1	1207	1	18,26,27	1.05	1 (5%)	16,38,41	1.14	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	1	967	1	-	0/7/25/26	0/2/2/2
1	2MG	1	966	1	-	0/5/27/28	0/3/3/3
1	2MG	1	1207	1	-	1/5/27/28	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1207	2MG	C6-N1	-3.13	1.33	1.37
1	1	967	5MC	C6-C5	2.65	1.39	1.34
1	1	966	2MG	C6-N1	-2.37	1.34	1.37
1	1	967	5MC	C6-N1	-2.34	1.34	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	967	5MC	C5-C6-N1	-3.21	120.04	123.34
1	1	966	2MG	C3'-C2'-C1'	3.04	105.55	100.98
1	1	967	5MC	C5-C4-N3	-2.46	119.02	121.67
1	1	966	2MG	C8-N7-C5	2.38	107.52	102.99
1	1	966	2MG	C5-C6-N1	2.37	118.14	113.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	1207	2MG	N3-C2-N2-CM2

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	1207	2MG	10	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 13 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.

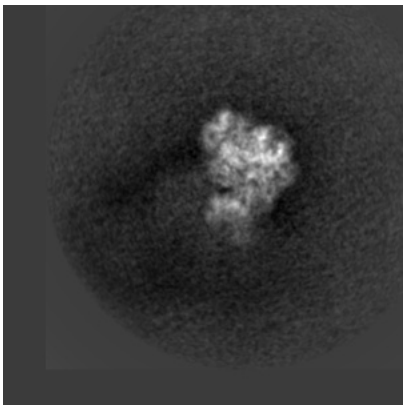
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-11768. These allow visual inspection of the internal detail of the map and identification of artifacts.

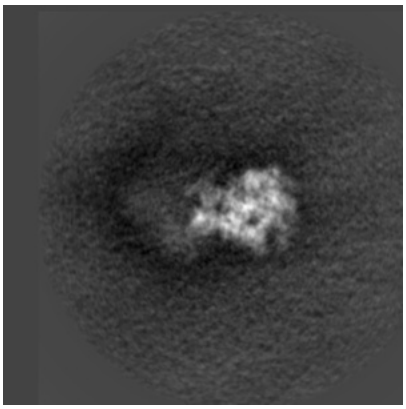
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

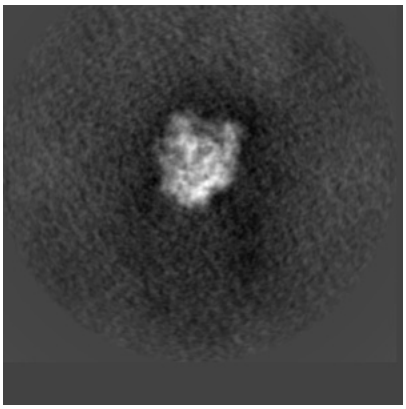
6.1.1 Primary map



X

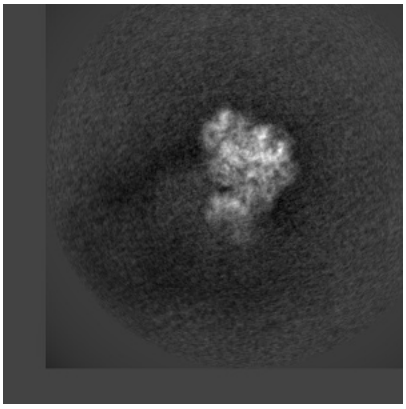


Y

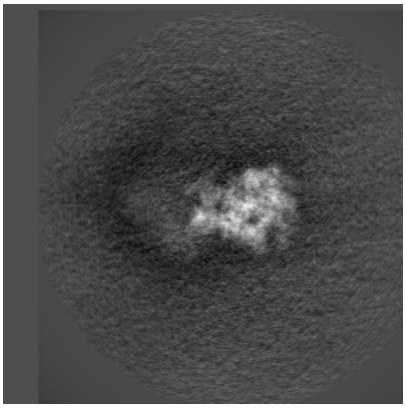


Z

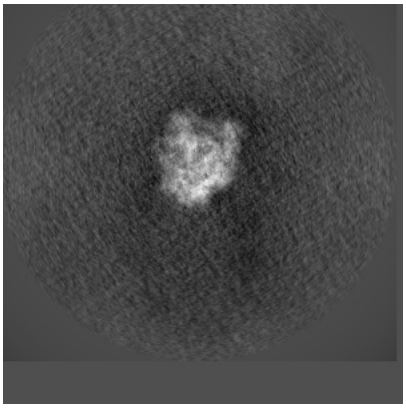
6.1.2 Raw map



X



Y

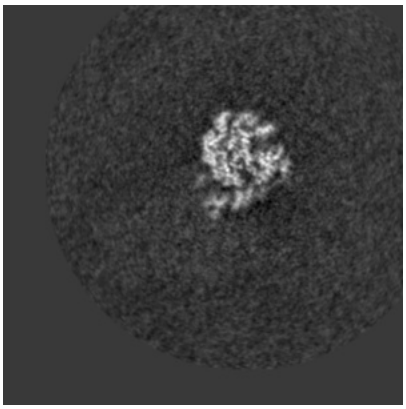


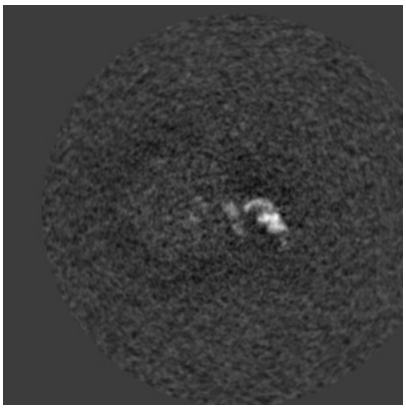
Z

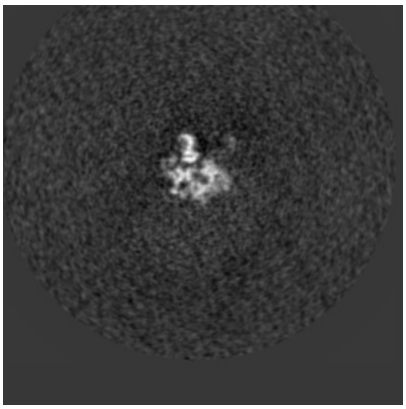
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

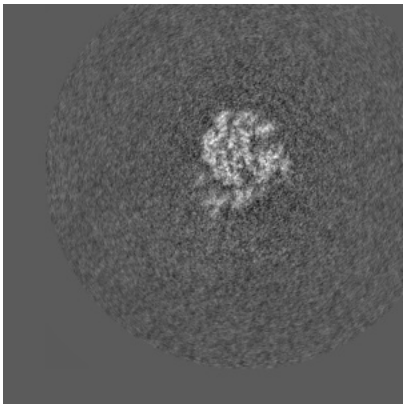
6.2.1 Primary map

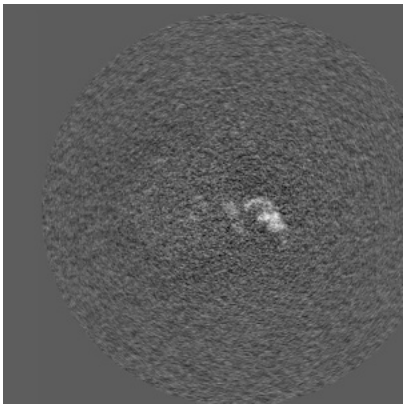

X Index: 192

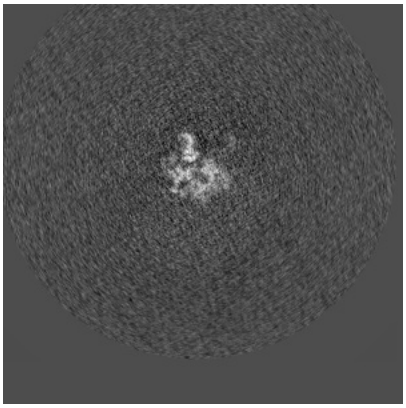

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

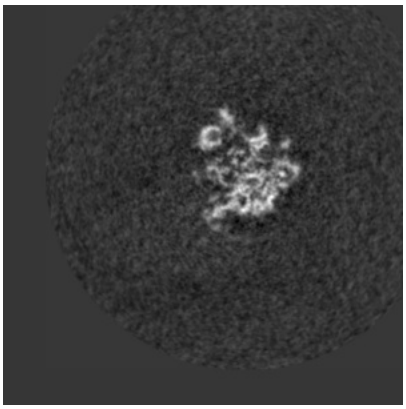

Y Index: 192


Z Index: 192

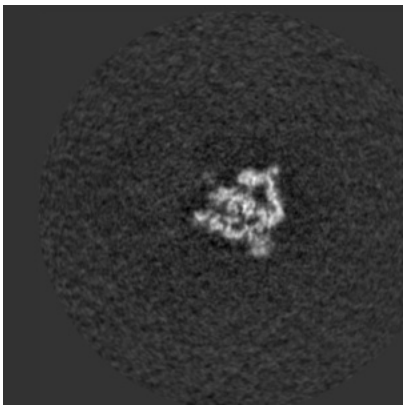
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

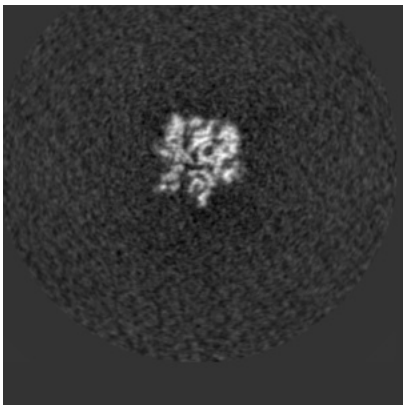
6.3.1 Primary map



X Index: 178

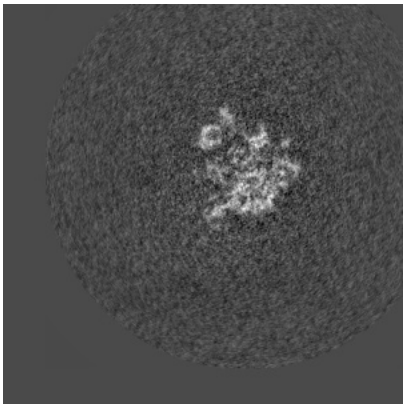


Y Index: 249

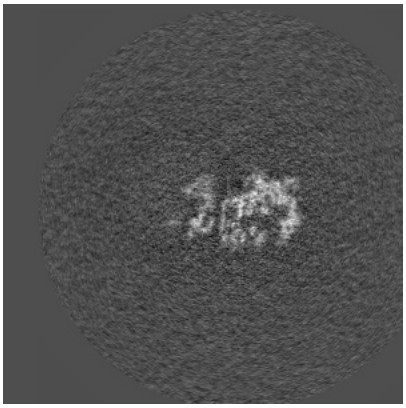


Z Index: 236

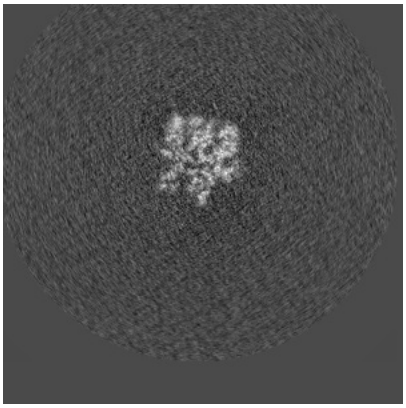
6.3.2 Raw map



X Index: 178



Y Index: 213

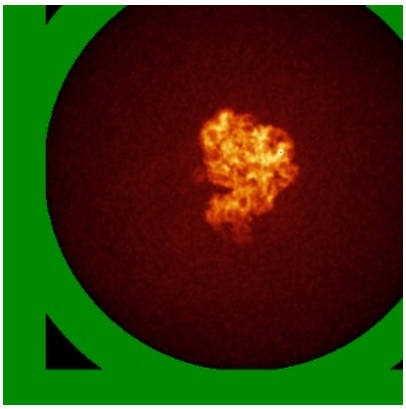


Z Index: 235

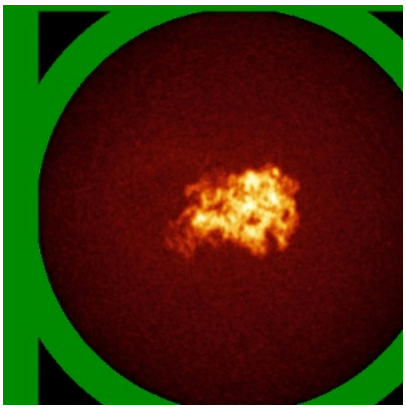
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

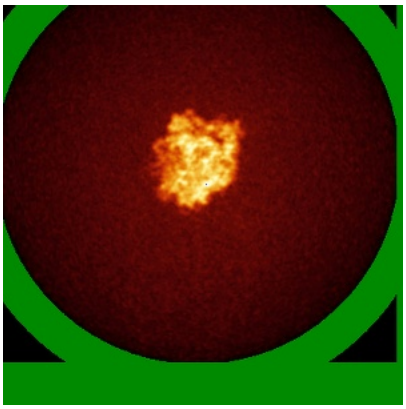
6.4.1 Primary map



X

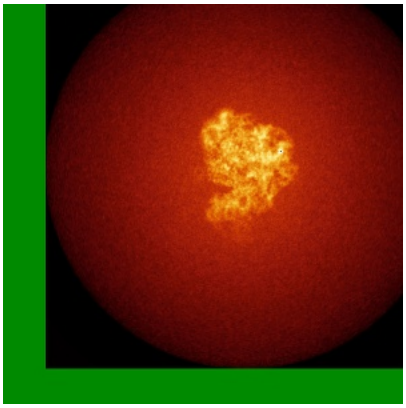


Y

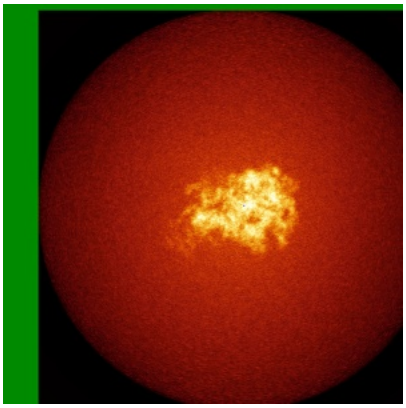


Z

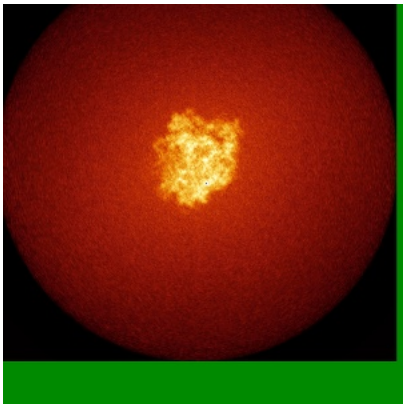
6.4.2 Raw map



X



Y

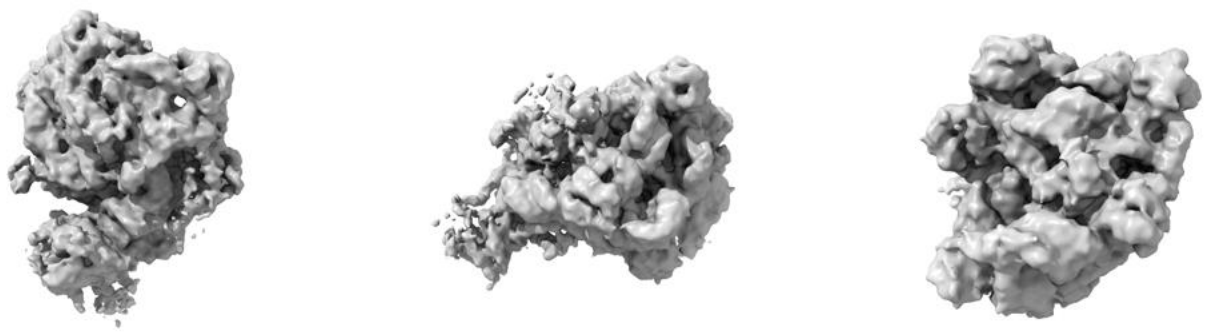


Z

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.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

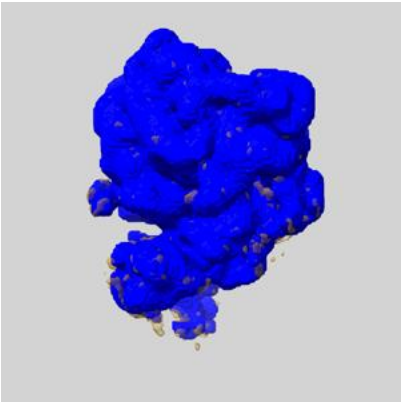
6.6 Mask visualisation (i)

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

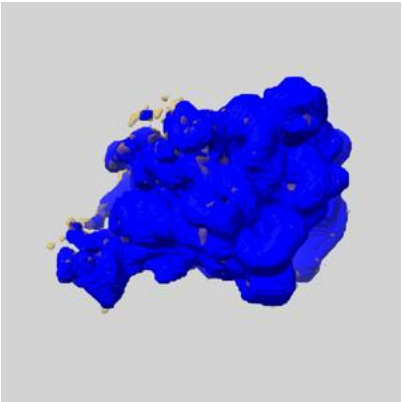
A mask typically either:

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

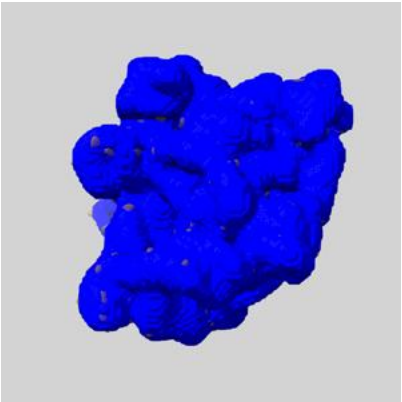
6.6.1 emd_11768_msk_1.map (i)



X



Y

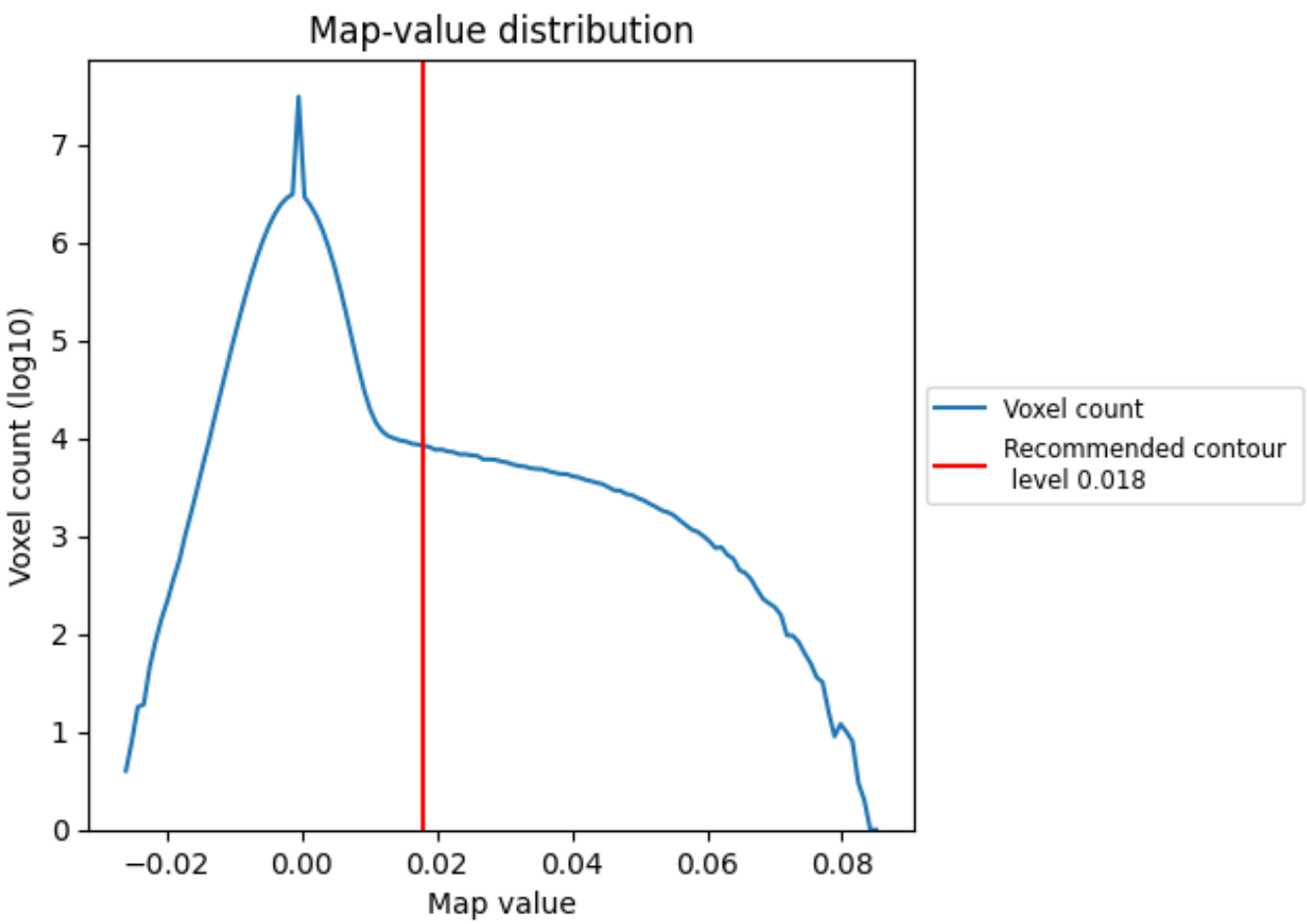


Z

7 Map analysis (i)

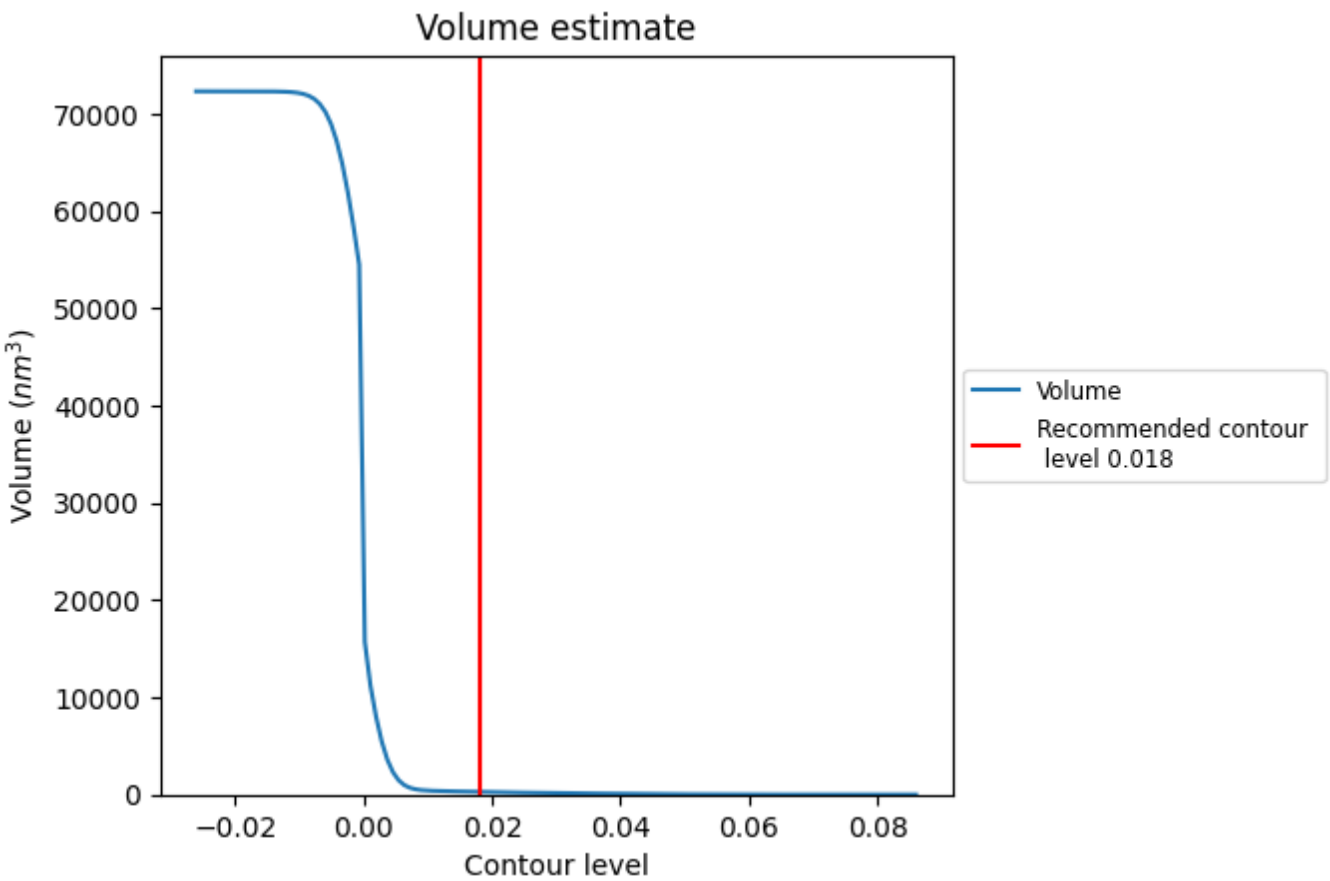
This section contains the results of statistical analysis of the map.

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.

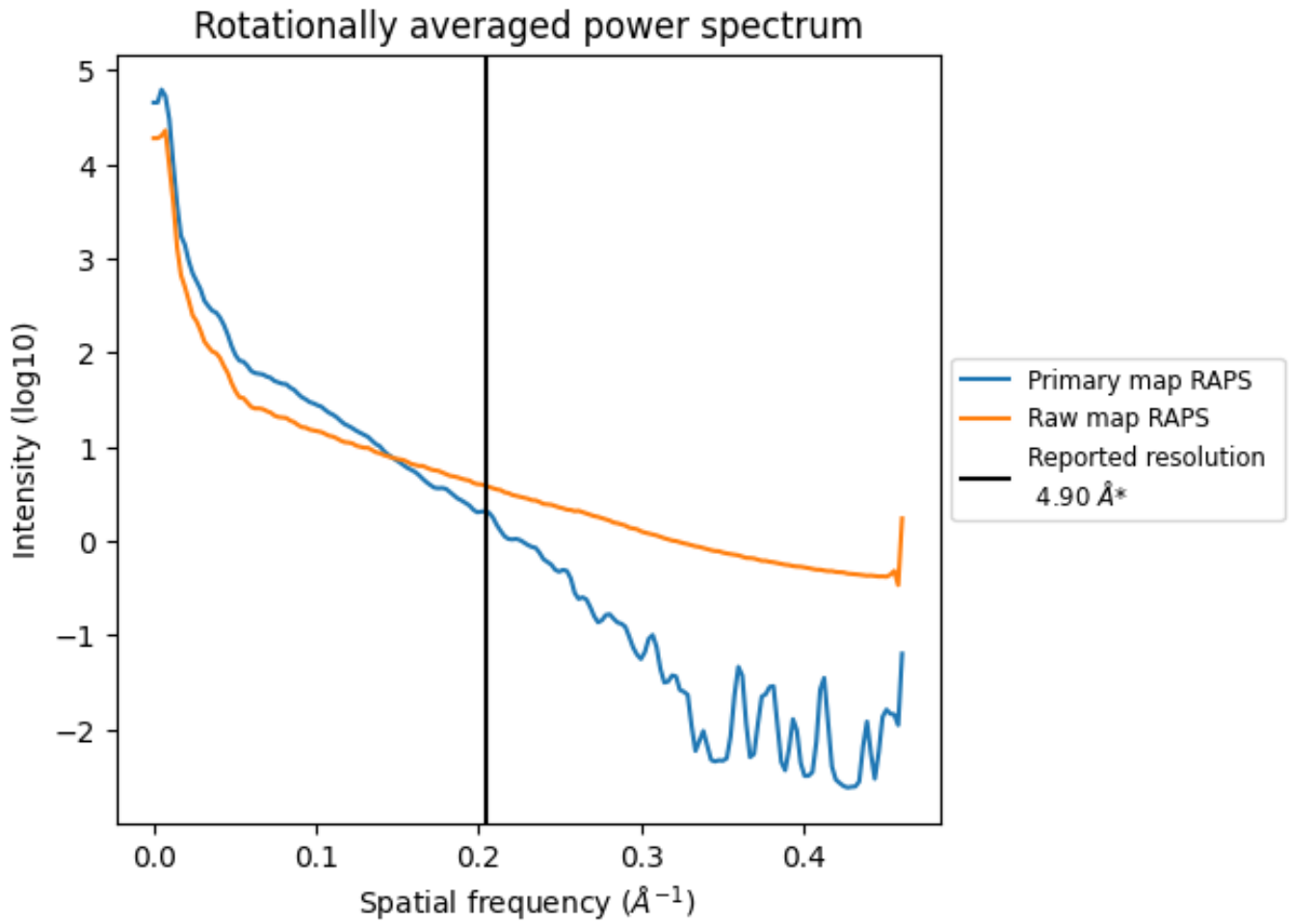
7.2 Volume estimate (i)



The volume at the recommended contour level is 275 nm^3; this corresponds to an approximate mass of 248 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)

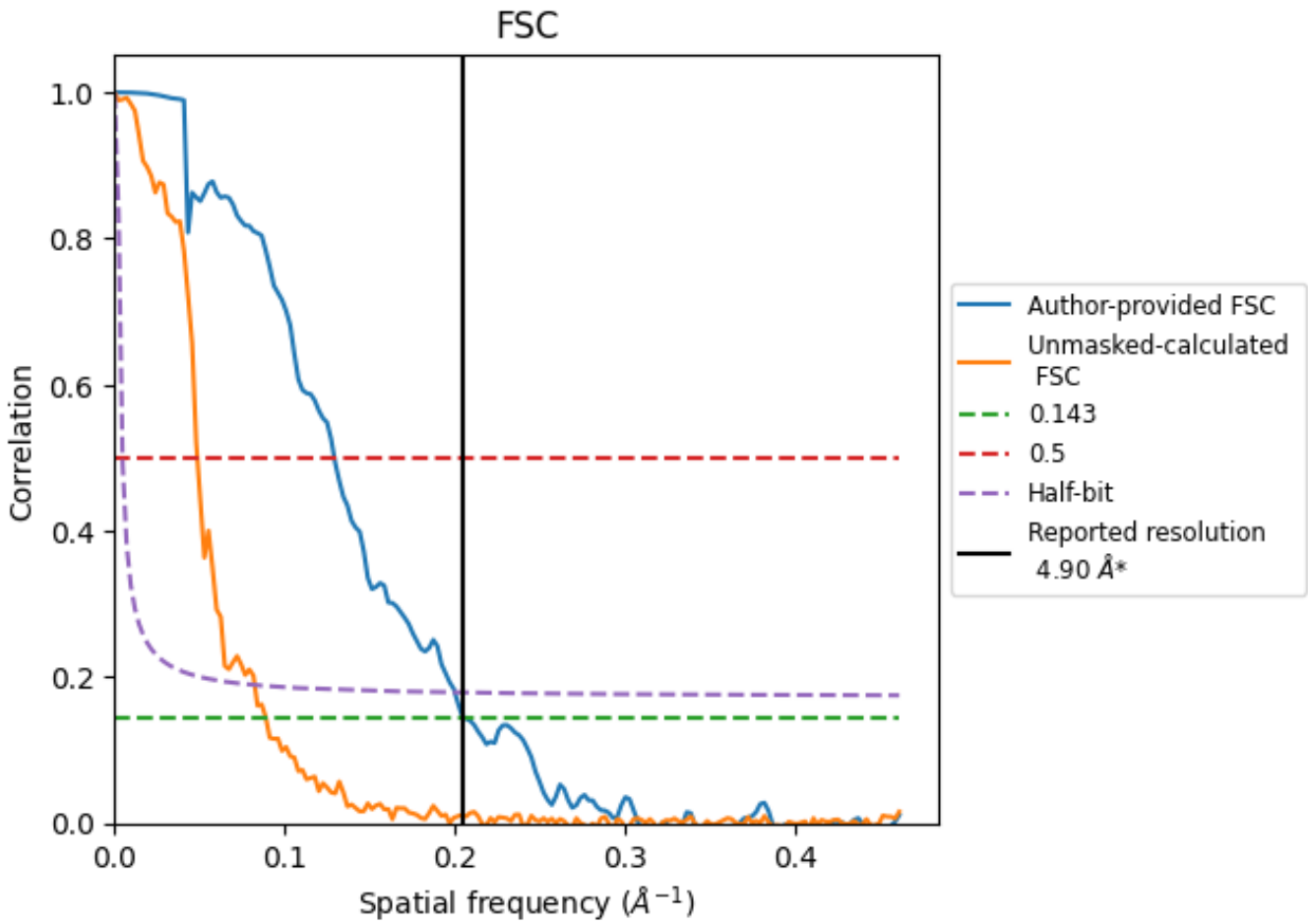


*Reported resolution corresponds to spatial frequency of 0.204 Å^{-1}

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 0.204 Å^{-1}

8.2 Resolution estimates (i)

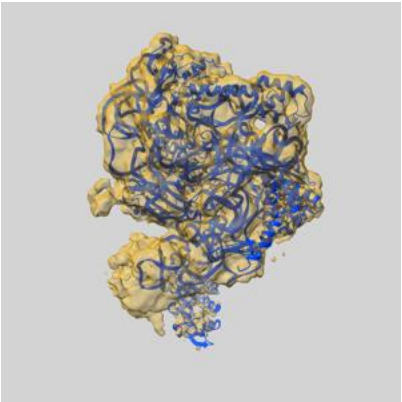
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.90	-	-
Author-provided FSC curve	4.85	7.75	5.01
Unmasked-calculated*	11.24	20.53	12.14

*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 11.24 differs from the reported value 4.9 by more than 10 %

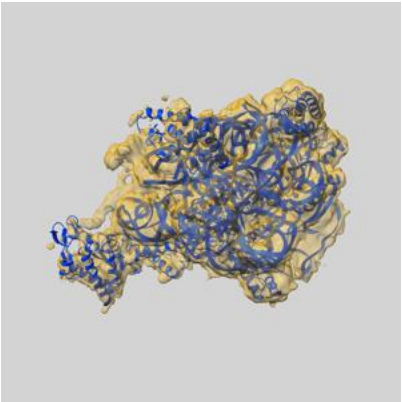
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-11768 and PDB model 7AFK. Per-residue inclusion information can be found in section 3 on page 6.

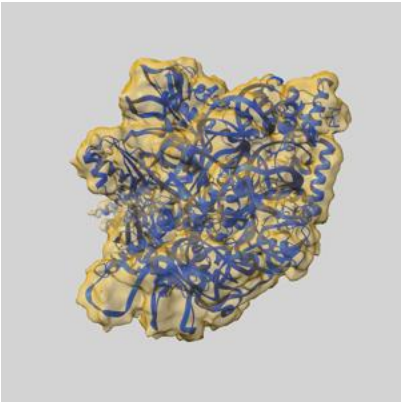
9.1 Map-model overlay (i)



X



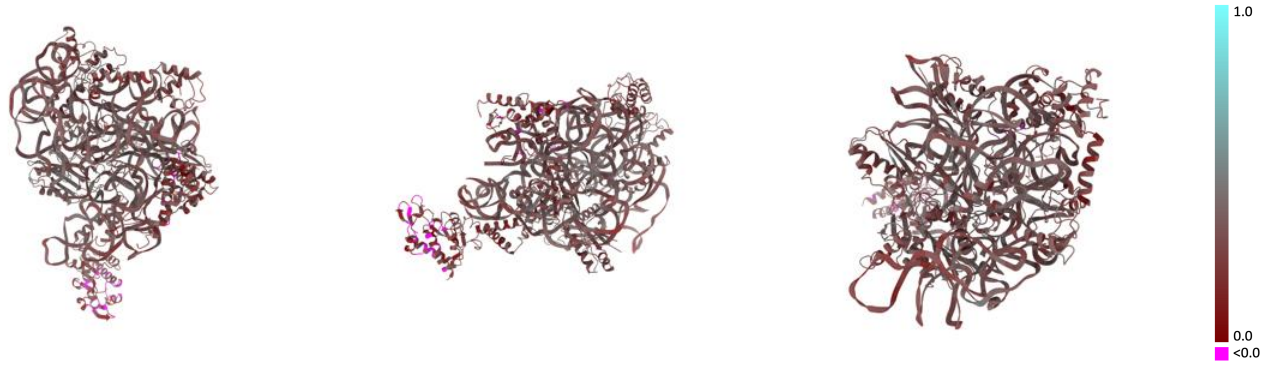
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

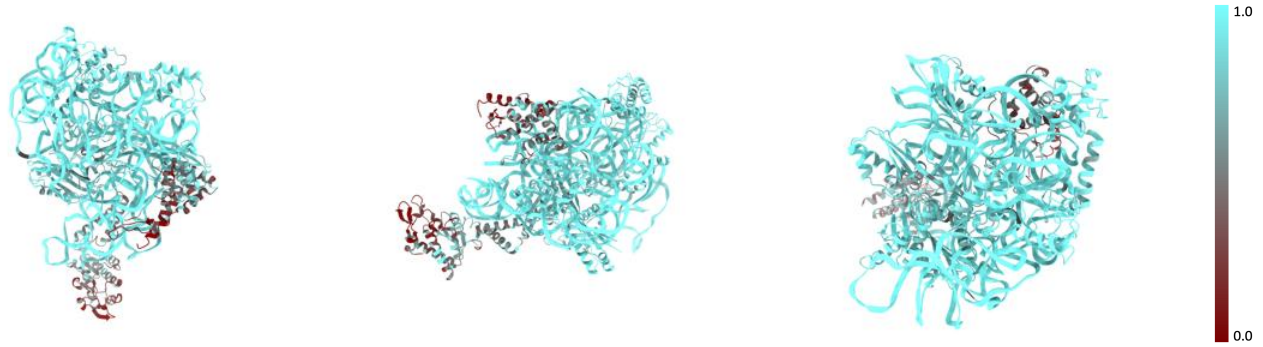
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

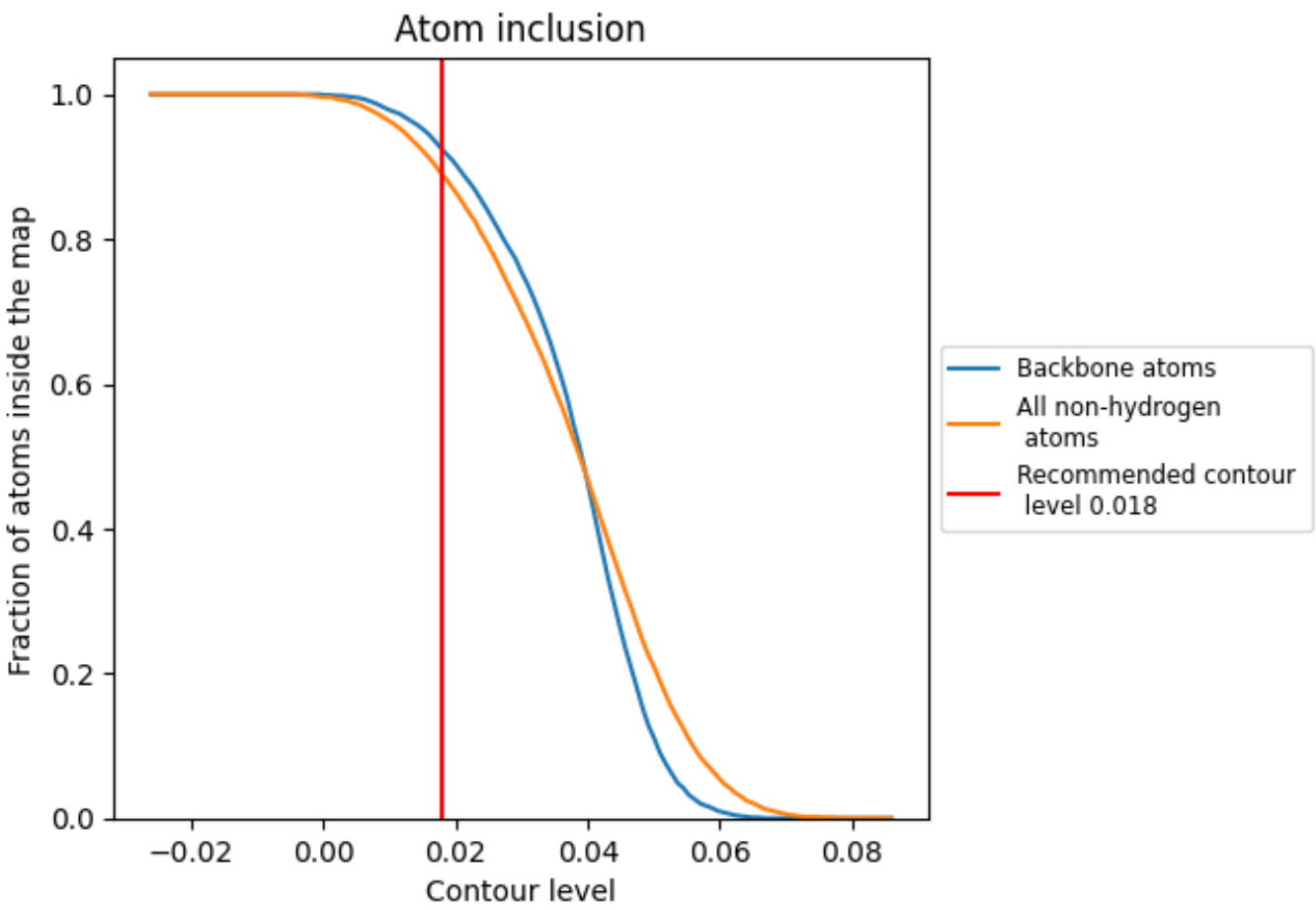
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.018).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.3150
1	0.9970	0.3440
B	0.4600	0.1730
C	0.9210	0.3470
G	0.4290	0.2510
I	0.9300	0.3160
J	0.9190	0.3170
M	0.9260	0.2750
N	0.8990	0.3310
S	0.9840	0.3380