



wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 05:02 pm BST

PDB ID : 8R6F
EMDB ID : EMD-18951
Title : CryoEM structure of wheat 40S ribosomal subunit, body domain
Authors : Kravchenko, O.V.; Baymukhametov, T.N.; Afonina, Z.A.; Vasilenko, K.S.
Deposited on : 2023-11-22
Resolution : 2.34 Å (reported)
Based on initial model : 7qix

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.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

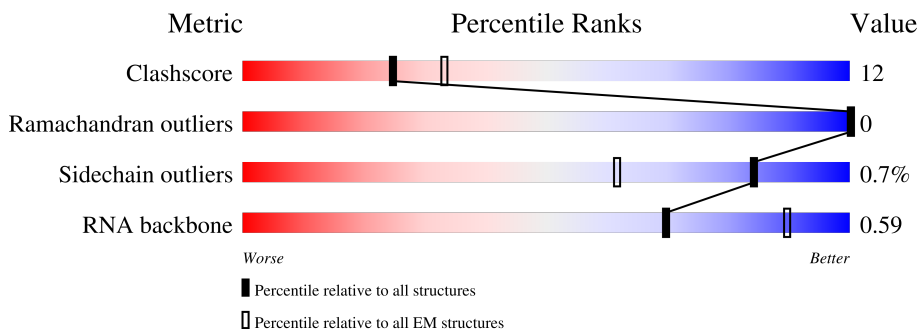
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.34 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	Y	137	
2	X	142	
3	E	265	
4	O	151	
5	W	130	
6	b	86	
7	e	62	

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Mol	Chain	Length	Quality of chain
8	k	308	 64% 35%
9	B	263	 5% 50% 30% 20%
10	V	81	 72% 28%
11	a	139	 70% 29%
12	J	195	 74% 18% 7%
13	C	275	 61% 16% 22%
14	G	250	 70% 22% 8%
15	H	192	 35% 55% 41% 7%
16	h	143	 18% 81%
17	L	159	 74% 18% 8%
18	N	151	 70% 23% 7%
19	n	25	 88% 8%
20	I	224	 66% 17% 17%
21	A	1810	 29% 31% 5% 35%

2 Entry composition

There are 25 unique types of molecules in this entry. The entry contains 49016 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 protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Y	124	1014	648	196	168	2	0	0

- Molecule 2 is a protein called 40S ribosomal protein S23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	X	140	1088	690	212	183	3	0	0

- Molecule 3 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	260	2077	1322	387	361	7	0	0

- Molecule 4 is a protein called 30S ribosomal protein S11, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	130	984	603	195	182	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	138	IAS	ASP	conflict	UNP A0A3B6SS17

- Molecule 5 is a protein called Small ribosomal subunit protein uS8c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	W	129	1032	659	188	180	5	0	0

- Molecule 6 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	83	Total	C	N	O	S	0	0
			645	405	117	116	7		

- Molecule 7 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	e	48	Total	C	N	O	0	0
			383	232	87	64		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	k	199	Total	C	N	O	S	0	0
			1586	1004	285	286	11		

- Molecule 9 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	210	Total	C	N	O	S	0	0
			1716	1094	310	303	9		

- Molecule 10 is a protein called Genome assembly, chromosome: II.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	V	81	Total	C	N	O	S	0	0
			630	389	116	122	3		

- Molecule 11 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	a	98	Total	C	N	O	S	0	0
			794	487	172	128	7		

- Molecule 12 is a protein called 30S ribosomal protein S4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	181	Total	C	N	O	S	0	0
			1494	947	298	245	4		

- Molecule 13 is a protein called S5 DRBM domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	C	214	Total	C	N	O	S	0	0
			1660	1070	294	287	9		

- Molecule 14 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	230	Total	C	N	O	S	0	0
			1856	1157	366	325	8		

- Molecule 15 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	184	Total	C	N	O	S	0	0
			1508	962	278	266	2		

- Molecule 16 is a protein called 40S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	27	Total	C	N	O	S	0	0
			208	129	34	42	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	146	Total	C	N	O	S	0	0
			1167	745	224	193	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS15 N-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	141	Total	C	N	O	S	0	0
			1138	731	215	190	2		

- Molecule 19 is a protein called Large ribosomal subunit protein eL41z/eL41y/eL41x/eL41w/eL41v.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	n	23	Total	C	N	O	S	0	0
			222	136	59	24	3		

- Molecule 20 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	I	186	1510	936	302	268	4	0	0

- Molecule 21 is a RNA chain called RNA (1177-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
21	A	1177	25190	11273	4545	8196	1176	0	0

- Molecule 22 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
22	a	1	1	1	0

- Molecule 23 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
23	G	1	1	1	0
23	A	31	31	31	0

- Molecule 24 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
24	A	14	14	14	0

- Molecule 25 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
25	Y	6	6	6	0
25	X	14	14	14	0
25	E	24	24	24	0
25	O	3	3	3	0

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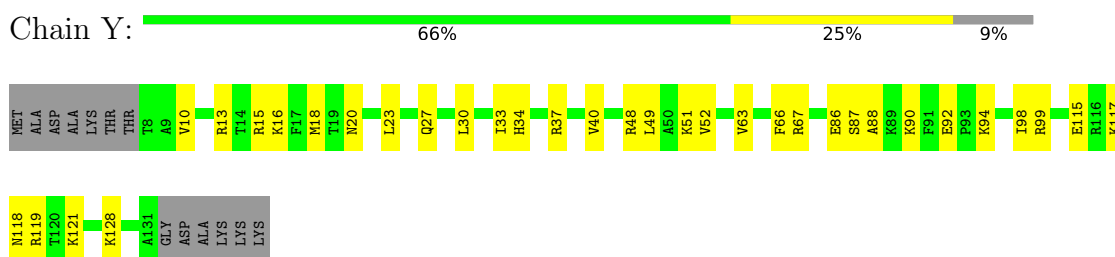
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Mol	Chain	Residues	Atoms		AltConf
25	W	6	Total 6	O 6	0
25	e	3	Total 3	O 3	0
25	B	2	Total 2	O 2	0
25	a	8	Total 8	O 8	0
25	J	14	Total 14	O 14	0
25	C	10	Total 10	O 10	0
25	G	7	Total 7	O 7	0
25	L	24	Total 24	O 24	0
25	N	3	Total 3	O 3	0
25	I	18	Total 18	O 18	0
25	A	925	Total 925	O 925	0

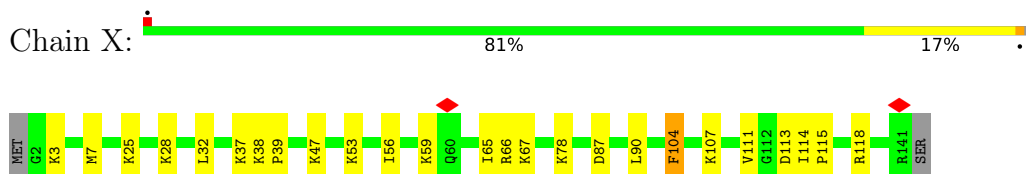
3 Residue-property plots [i](#)

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.

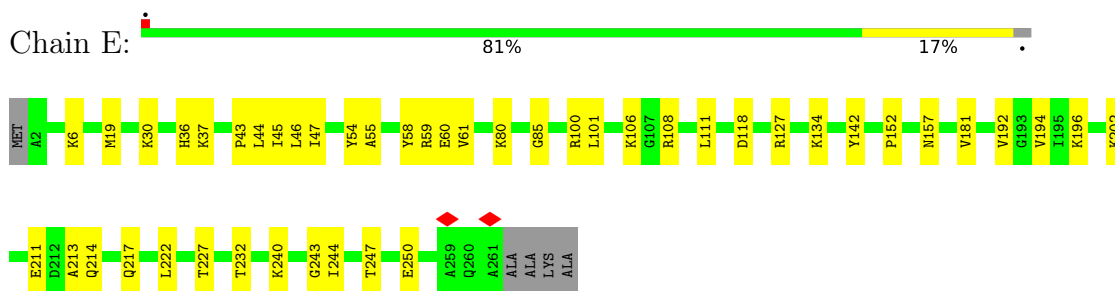
- Molecule 1: 40S ribosomal protein S24



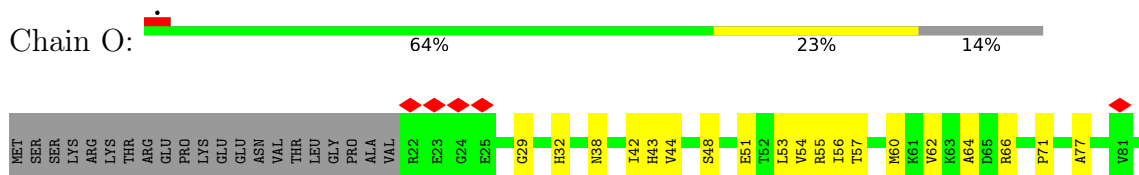
- Molecule 2: 40S ribosomal protein S23



- Molecule 3: 40S ribosomal protein S4

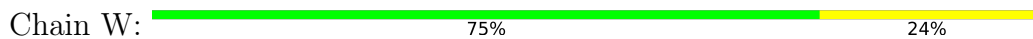


- Molecule 4: 30S ribosomal protein S11, chloroplastic

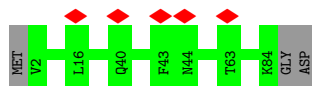




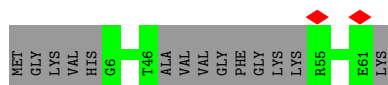
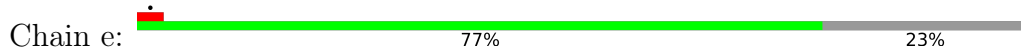
- Molecule 5: Small ribosomal subunit protein uS8c



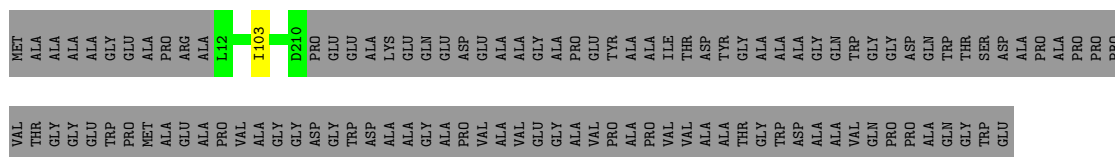
- Molecule 6: 40S ribosomal protein S27



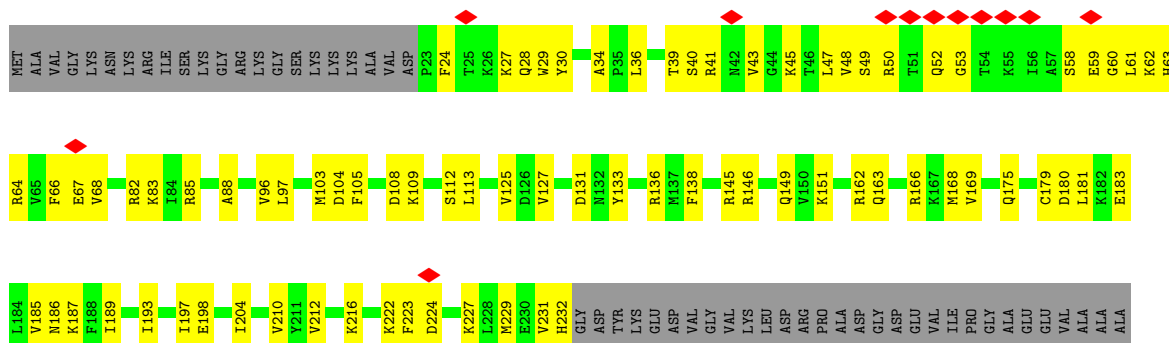
- Molecule 7: 40S ribosomal protein S30



- Molecule 8: Small ribosomal subunit protein uS2



- Molecule 9: Small ribosomal subunit protein eS1



GLU

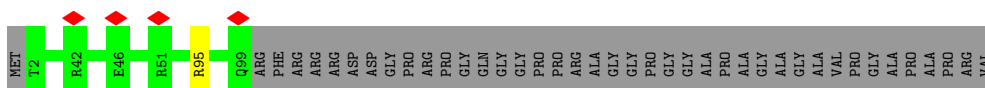
- Molecule 10: Genome assembly, chromosome: II

Chain V: 72% 28%



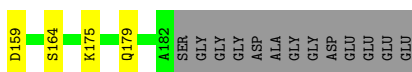
- Molecule 11: 40S ribosomal protein S26

Chain a: 70% 29%



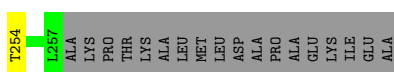
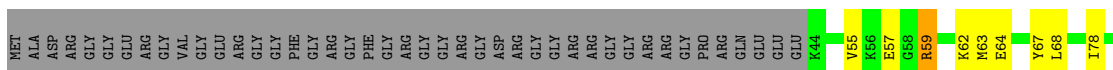
- Molecule 12: 30S ribosomal protein S4, chloroplastic

Chain J: 74% 18% 7%



- Molecule 13: S5 DRBM domain-containing protein

Chain C: 61% 16% 22%



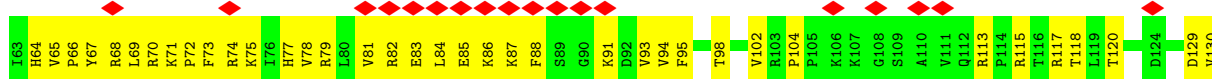
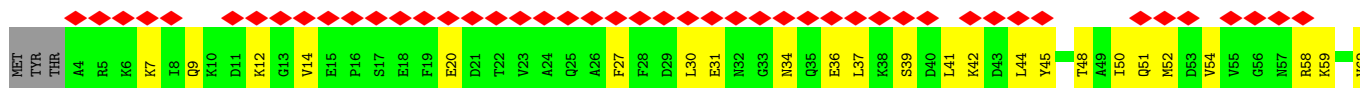
- Molecule 14: 40S ribosomal protein S6

Chain G: 70% 22% 8%

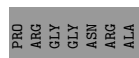
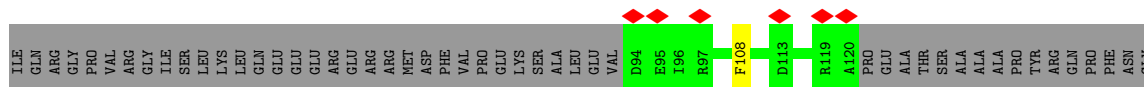




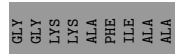
• Molecule 15: 40S ribosomal protein S7



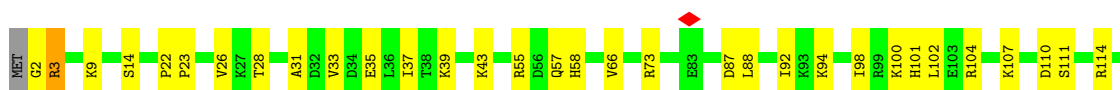
• Molecule 16: 40S ribosomal protein S17

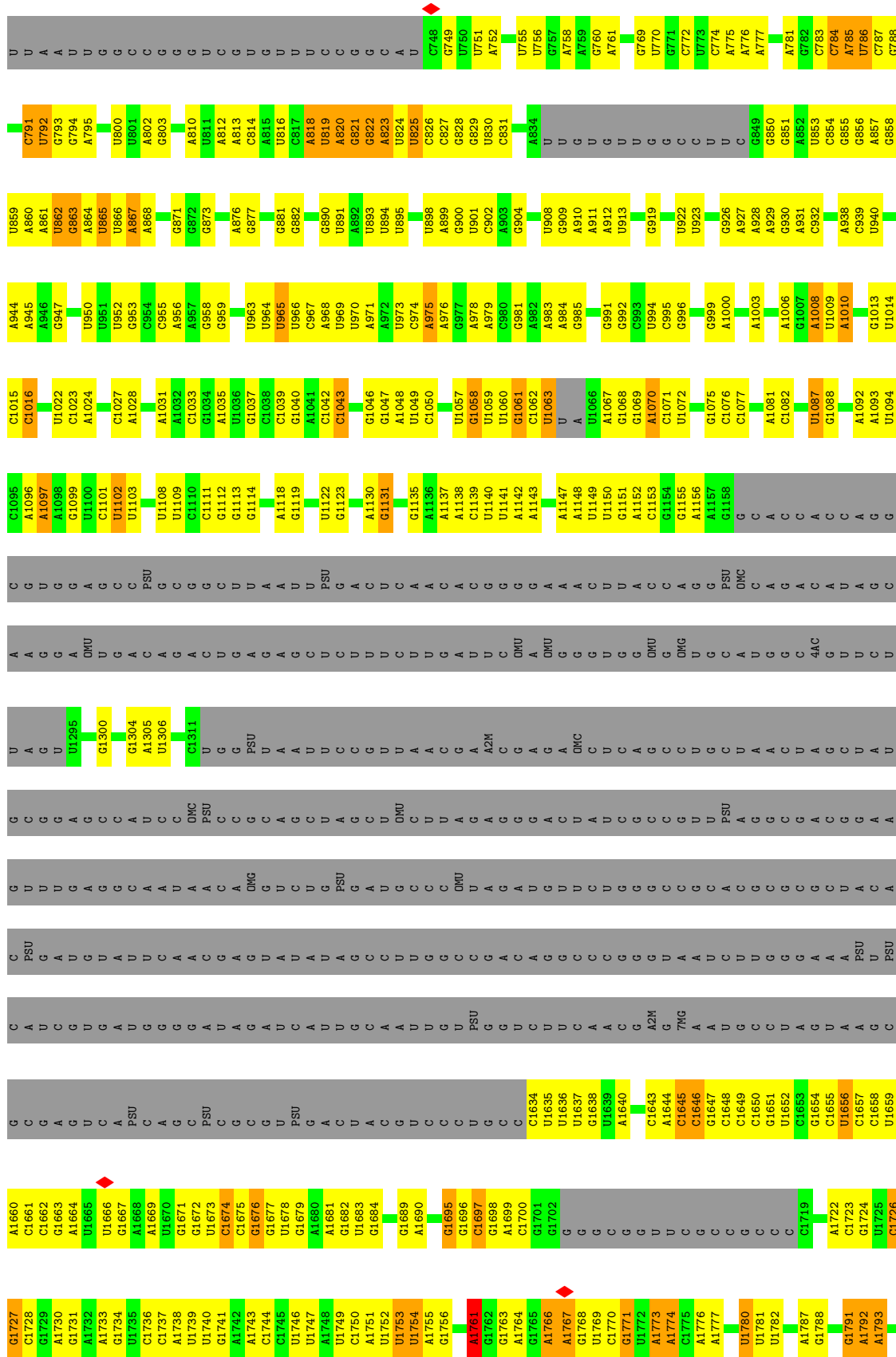


• Molecule 17: Small ribosomal subunit protein uS17 N-terminal domain-containing protein



• Molecule 18: Small ribosomal subunit protein uS15 N-terminal domain-containing protein





U1796
G1797
C1798
G1799
G1803
G1804
A1805
U1806
C1807
A1808
U1809
U1810
G1811

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	256000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	84	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	9.900	Depositor
Minimum map value	-6.521	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.4	Depositor
Map size (\AA)	412.80002, 412.80002, 412.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 6MZ, AME, OMU, K, OMC, MG, 4AC, A2M, OMG, UY1, MA6, IAS, PSU, 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	Y	0.32	0/1029	0.58	0/1366
2	X	0.31	0/1107	0.57	0/1474
3	E	0.28	0/2118	0.56	0/2846
4	O	0.33	0/988	0.60	0/1322
5	W	0.37	0/1050	0.63	0/1405
6	b	0.27	0/656	0.52	0/883
7	e	0.31	0/387	0.63	0/510
8	k	0.32	0/1620	0.56	0/2193
9	B	0.32	0/1745	0.60	0/2344
10	V	0.39	0/628	0.59	0/847
11	a	0.34	0/809	0.57	0/1083
12	J	0.28	0/1522	0.58	0/2037
13	C	0.33	0/1696	0.58	0/2292
14	G	0.29	0/1876	0.60	0/2492
15	H	0.33	0/1535	0.62	0/2065
16	h	0.43	0/209	0.63	0/279
17	L	0.31	0/1193	0.58	0/1599
18	N	0.27	0/1162	0.53	0/1560
19	n	0.39	0/223	0.76	0/283
20	I	0.30	0/1532	0.62	0/2046
21	A	0.30	0/26873	0.78	0/41868
All	All	0.31	0/49958	0.70	0/72794

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	1014	0	1099	29	0
2	X	1088	0	1153	20	0
3	E	2077	0	2166	34	0
4	O	984	0	1011	33	0
5	W	1032	0	1068	23	0
6	b	645	0	664	0	0
7	e	383	0	406	0	0
8	k	1586	0	1590	0	0
9	B	1716	0	1790	67	0
10	V	630	0	614	16	0
11	a	794	0	812	0	0
12	J	1494	0	1563	30	0
13	C	1660	0	1743	34	0
14	G	1856	0	1995	47	0
15	H	1508	0	1573	72	0
16	h	208	0	205	0	0
17	L	1167	0	1228	22	0
18	N	1138	0	1228	30	0
19	n	222	0	271	0	0
20	I	1510	0	1555	31	0
21	A	25190	0	12722	475	0
22	a	1	0	0	0	0
23	A	31	0	0	0	0
23	G	1	0	0	0	0
24	A	14	0	0	0	0
25	A	925	0	0	21	0
25	B	2	0	0	0	0
25	C	10	0	0	0	0
25	E	24	0	0	0	0
25	G	7	0	0	0	0
25	I	18	0	0	1	0
25	J	14	0	0	0	0
25	L	24	0	0	2	0
25	N	3	0	0	0	0
25	O	3	0	0	0	0
25	W	6	0	0	0	0
25	X	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	Y	6	0	0	1	0
25	a	8	0	0	0	0
25	e	3	0	0	0	0
All	All	49016	0	36456	843	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 12.

The worst 5 of 843 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)
21:A:1672:G:H1	21:A:1749:U:H3	1.13	0.94
15:H:88:PHE:HB2	15:H:91:LYS:HD2	1.58	0.85
9:B:34:ALA:O	9:B:41:ARG:HD2	1.76	0.84
9:B:67:GLU:OE1	9:B:85:ARG:HG3	1.78	0.83
20:I:2:GLY:N	21:A:1740:U:HO2'	1.78	0.82

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	
1	Y	122/137 (89%)	121 (99%)	1 (1%)	0	100	100
2	X	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
3	E	258/265 (97%)	253 (98%)	5 (2%)	0	100	100
4	O	126/151 (83%)	123 (98%)	3 (2%)	0	100	100
5	W	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
6	b	81/86 (94%)	72 (89%)	9 (11%)	0	100	100
7	e	44/62 (71%)	42 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	k	197/308 (64%)	192 (98%)	5 (2%)	0	100	100
9	B	208/263 (79%)	203 (98%)	5 (2%)	0	100	100
10	V	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
11	a	96/139 (69%)	94 (98%)	2 (2%)	0	100	100
12	J	179/195 (92%)	177 (99%)	2 (1%)	0	100	100
13	C	212/275 (77%)	206 (97%)	6 (3%)	0	100	100
14	G	228/250 (91%)	225 (99%)	3 (1%)	0	100	100
15	H	182/192 (95%)	170 (93%)	12 (7%)	0	100	100
16	h	25/143 (18%)	23 (92%)	2 (8%)	0	100	100
17	L	144/159 (91%)	143 (99%)	1 (1%)	0	100	100
18	N	139/151 (92%)	136 (98%)	3 (2%)	0	100	100
19	n	21/25 (84%)	21 (100%)	0	0	100	100
20	I	182/224 (81%)	176 (97%)	6 (3%)	0	100	100
All	All	2788/3378 (82%)	2712 (97%)	76 (3%)	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	
1	Y	108/117 (92%)	108 (100%)	0	100	100
2	X	111/113 (98%)	110 (99%)	1 (1%)	78	87
3	E	222/224 (99%)	222 (100%)	0	100	100
4	O	101/120 (84%)	101 (100%)	0	100	100
5	W	111/112 (99%)	111 (100%)	0	100	100
6	b	76/78 (97%)	76 (100%)	0	100	100
7	e	39/49 (80%)	39 (100%)	0	100	100
8	k	170/233 (73%)	169 (99%)	1 (1%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	B	189/228 (83%)	188 (100%)	1 (0%)	88	93
10	V	65/65 (100%)	65 (100%)	0	100	100
11	a	85/108 (79%)	84 (99%)	1 (1%)	71	82
12	J	154/162 (95%)	153 (99%)	1 (1%)	86	92
13	C	181/219 (83%)	178 (98%)	3 (2%)	60	72
14	G	202/215 (94%)	201 (100%)	1 (0%)	88	93
15	H	164/171 (96%)	160 (98%)	4 (2%)	49	59
16	h	22/124 (18%)	21 (96%)	1 (4%)	27	34
17	L	125/132 (95%)	123 (98%)	2 (2%)	62	74
18	N	123/131 (94%)	122 (99%)	1 (1%)	81	89
19	n	22/24 (92%)	21 (96%)	1 (4%)	27	34
20	I	160/179 (89%)	160 (100%)	0	100	100
All	All	2430/2804 (87%)	2412 (99%)	18 (1%)	84	90

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
17	L	47	ARG
19	n	1	MET
18	N	3	ARG
14	G	41	LEU
16	h	108	PHE

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

Mol	Chain	Res	Type
6	b	51	HIS
8	k	81	GLN
18	N	123	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	A	1159/1810 (64%)	205 (17%)	0

5 of 205 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	A	14	C
21	A	25	C
21	A	26	A
21	A	34	G
21	A	42	G

There are no RNA pucker outliers to report.

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

57 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
21	OMG	A	599	21	18,26,27	1.01	3 (16%)	19,38,41	0.69	0
21	PSU	A	1004	21	18,21,22	0.49	0	22,30,33	0.59	0
21	PSU	A	255	21,23	18,21,22	0.50	0	22,30,33	0.60	0
21	OMG	A	1131	21	18,26,27	1.02	3 (16%)	19,38,41	0.62	0
21	OMU	A	168	21	19,22,23	0.41	0	26,31,34	0.88	1 (3%)
21	PSU	A	606	21	18,21,22	0.53	0	22,30,33	0.59	0
10	AME	V	1	10	9,10,11	1.37	1 (11%)	9,11,13	1.62	2 (22%)
21	OMU	A	615	21	19,22,23	1.70	4 (21%)	26,31,34	1.83	6 (23%)
21	PSU	A	1122	21	18,21,22	0.50	0	22,30,33	0.61	0
21	OMG	A	434	21	18,26,27	1.02	3 (16%)	19,38,41	0.63	0
21	A2M	A	979	21	18,25,26	0.73	1 (5%)	18,36,39	1.03	1 (5%)
21	A2M	A	424	21	18,25,26	0.72	1 (5%)	18,36,39	0.97	1 (5%)
21	PSU	A	607	21	18,21,22	0.53	0	22,30,33	0.56	0
21	PSU	A	35	21	18,21,22	0.52	0	22,30,33	0.58	0
21	4AC	A	1784	21	21,24,25	0.43	0	29,34,37	0.60	0
21	PSU	A	103	21	18,21,22	0.52	0	22,30,33	0.56	0
21	PSU	A	306	21	18,21,22	0.54	0	22,30,33	0.57	0
21	PSU	A	308	21	18,21,22	0.56	0	22,30,33	0.57	0
21	MA6	A	1792	21	18,26,27	0.83	1 (5%)	19,38,41	0.71	1 (5%)
21	A2M	A	162	21	18,25,26	0.71	0	18,36,39	0.95	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	PSU	A	1306	21	18,21,22	0.57	0	22,30,33	0.55	0
21	OMC	A	38	21	19,22,23	0.33	0	26,31,34	0.51	0
21	PSU	A	806	21	18,21,22	0.48	0	22,30,33	0.61	0
21	OMU	A	1014	21	19,22,23	0.34	0	26,31,34	0.50	0
21	PSU	A	1108	21	18,21,22	0.53	0	22,30,33	0.57	0
21	PSU	A	1310	21	18,21,22	0.53	0	22,30,33	0.40	0
21	PSU	A	1637	21	18,21,22	0.52	0	22,30,33	0.57	0
21	A2M	A	545	21	18,25,26	0.72	1 (5%)	18,36,39	0.90	1 (5%)
21	A2M	A	1761	21	18,25,26	0.70	0	18,36,39	0.82	1 (5%)
21	PSU	A	636	21	18,21,22	0.55	0	22,30,33	0.58	0
21	PSU	A	121	21	18,21,22	0.50	0	22,30,33	0.76	0
21	A2M	A	440	21	18,25,26	0.70	1 (5%)	18,36,39	0.79	1 (5%)
21	OMG	A	246	21	18,26,27	0.99	2 (11%)	19,38,41	0.61	0
21	UY1	A	604	21	19,22,23	0.50	0	22,31,34	0.61	0
21	PSU	A	765	21	18,21,22	0.48	0	22,30,33	0.59	0
21	PSU	A	208	21	18,21,22	0.50	0	22,30,33	0.59	0
21	MA6	A	1793	21	18,26,27	0.76	1 (5%)	19,38,41	0.95	1 (5%)
21	PSU	A	1100	21	18,21,22	0.54	0	22,30,33	0.55	0
21	A2M	A	28	21	18,25,26	0.73	1 (5%)	18,36,39	0.83	1 (5%)
4	IAS	O	138	4	6,7,8	0.82	0	6,8,10	1.06	0
21	A2M	A	802	21	18,25,26	0.70	0	18,36,39	0.94	1 (5%)
21	OMC	A	418	21	19,22,23	0.30	0	26,31,34	0.47	0
21	OMU	A	123	21	19,22,23	0.36	0	26,31,34	0.46	0
21	PSU	A	1295	21	18,21,22	0.46	0	22,30,33	0.60	0
21	6MZ	A	1774	24,21,23	18,25,26	0.78	1 (5%)	16,36,39	1.12	2 (12%)
21	PSU	A	258	21	18,21,22	0.50	0	22,30,33	0.59	0
21	PSU	A	300	21	18,21,22	0.50	0	22,30,33	0.56	0
21	PSU	A	811	21	18,21,22	0.51	0	22,30,33	0.59	0
21	OMC	A	1648	21	19,22,23	0.33	0	26,31,34	0.50	0
21	A2M	A	468	21	18,25,26	0.70	0	18,36,39	1.04	1 (5%)
21	PSU	A	362	21	18,21,22	0.50	0	22,30,33	0.63	0
21	OMG	A	1300	21	18,26,27	1.00	3 (16%)	19,38,41	0.68	0
21	PSU	A	111	24,21	18,21,22	0.52	0	22,30,33	0.59	0
21	A2M	A	623	21,23	18,25,26	0.72	0	18,36,39	0.82	1 (5%)
21	OMG	A	392	21	18,26,27	1.01	3 (16%)	19,38,41	0.66	0
21	PSU	A	1084	21	18,21,22	0.48	0	22,30,33	0.63	0
21	PSU	A	764	21	18,21,22	0.50	0	22,30,33	0.66	0

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
21	OMG	A	599	21	-	1/5/27/28	0/3/3/3
21	PSU	A	1004	21	-	0/7/25/26	0/2/2/2
21	PSU	A	255	21,23	-	0/7/25/26	0/2/2/2
21	OMG	A	1131	21	-	1/5/27/28	0/3/3/3
21	OMU	A	168	21	-	0/9/27/28	0/2/2/2
21	PSU	A	606	21	-	0/7/25/26	0/2/2/2
10	AME	V	1	10	-	2/9/10/12	-
21	OMU	A	615	21	-	1/9/27/28	0/2/2/2
21	PSU	A	1122	21	-	0/7/25/26	0/2/2/2
21	OMG	A	434	21	-	0/5/27/28	0/3/3/3
21	A2M	A	979	21	-	0/5/27/28	0/3/3/3
21	A2M	A	424	21	-	0/5/27/28	0/3/3/3
21	PSU	A	607	21	-	0/7/25/26	0/2/2/2
21	PSU	A	35	21	-	0/7/25/26	0/2/2/2
21	4AC	A	1784	21	-	0/11/29/30	0/2/2/2
21	PSU	A	103	21	-	0/7/25/26	0/2/2/2
21	PSU	A	306	21	-	0/7/25/26	0/2/2/2
21	PSU	A	308	21	-	0/7/25/26	0/2/2/2
21	MA6	A	1792	21	-	0/7/29/30	0/3/3/3
21	A2M	A	162	21	-	0/5/27/28	0/3/3/3
21	PSU	A	1306	21	-	0/7/25/26	0/2/2/2
21	OMC	A	38	21	-	0/9/27/28	0/2/2/2
21	PSU	A	806	21	-	0/7/25/26	0/2/2/2
21	OMU	A	1014	21	-	0/9/27/28	0/2/2/2
21	PSU	A	1108	21	-	0/7/25/26	0/2/2/2
21	PSU	A	1310	21	-	2/7/25/26	0/2/2/2
21	PSU	A	1637	21	-	0/7/25/26	0/2/2/2
21	A2M	A	545	21	-	0/5/27/28	0/3/3/3
21	A2M	A	1761	21	-	2/5/27/28	0/3/3/3
21	PSU	A	636	21	-	0/7/25/26	0/2/2/2
21	PSU	A	121	21	-	0/7/25/26	0/2/2/2
21	A2M	A	440	21	-	0/5/27/28	0/3/3/3
21	OMG	A	246	21	-	2/5/27/28	0/3/3/3
21	UY1	A	604	21	-	0/9/27/28	0/2/2/2
21	PSU	A	765	21	-	0/7/25/26	0/2/2/2
21	PSU	A	208	21	-	0/7/25/26	0/2/2/2
21	MA6	A	1793	21	-	2/7/29/30	0/3/3/3
21	PSU	A	1100	21	-	0/7/25/26	0/2/2/2
21	A2M	A	28	21	-	0/5/27/28	0/3/3/3
4	IAS	O	138	4	-	1/7/7/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	A2M	A	802	21	-	0/5/27/28	0/3/3/3
21	OMC	A	418	21	-	0/9/27/28	0/2/2/2
21	OMU	A	123	21	-	1/9/27/28	0/2/2/2
21	PSU	A	1295	21	-	0/7/25/26	0/2/2/2
21	6MZ	A	1774	24,21,23	-	0/5/27/28	0/3/3/3
21	PSU	A	258	21	-	0/7/25/26	0/2/2/2
21	PSU	A	300	21	-	0/7/25/26	0/2/2/2
21	PSU	A	811	21	-	0/7/25/26	0/2/2/2
21	OMC	A	1648	21	-	2/9/27/28	0/2/2/2
21	A2M	A	468	21	-	2/5/27/28	0/3/3/3
21	PSU	A	362	21	-	0/7/25/26	0/2/2/2
21	OMG	A	1300	21	-	0/5/27/28	0/3/3/3
21	PSU	A	111	24,21	-	0/7/25/26	0/2/2/2
21	A2M	A	623	21,23	-	2/5/27/28	0/3/3/3
21	OMG	A	392	21	-	2/5/27/28	0/3/3/3
21	PSU	A	1084	21	-	0/7/25/26	0/2/2/2
21	PSU	A	764	21	-	0/7/25/26	0/2/2/2

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	A	615	OMU	C4-N3	-4.31	1.30	1.38
21	A	615	OMU	C2-N3	-4.04	1.30	1.38
10	V	1	AME	CT1-N	3.31	1.45	1.34
21	A	615	OMU	C5-C4	-2.53	1.38	1.43
21	A	1131	OMG	C5-C6	-2.49	1.42	1.47

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	615	OMU	N3-C2-N1	4.45	120.80	114.89
21	A	615	OMU	C4-N3-C2	-4.42	120.75	126.58
21	A	615	OMU	C5-C4-N3	4.33	121.32	114.84
21	A	1793	MA6	N1-C6-N6	-3.32	113.56	117.06
21	A	1774	6MZ	C9-N6-C6	3.27	125.69	122.87

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	246	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
21	A	615	OMU	C1'-C2'-O2'-CM2
21	A	623	A2M	O4'-C4'-C5'-O5'
21	A	1310	PSU	C2'-C1'-C5-C4
21	A	1648	OMC	O4'-C1'-N1-C2

There are no ring outliers.

21 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A	606	PSU	2	0
21	A	615	OMU	1	0
21	A	1122	PSU	2	0
21	A	607	PSU	2	0
21	A	306	PSU	1	0
21	A	308	PSU	2	0
21	A	1792	MA6	1	0
21	A	1306	PSU	1	0
21	A	38	OMC	1	0
21	A	1014	OMU	2	0
21	A	1108	PSU	1	0
21	A	1637	PSU	1	0
21	A	1761	A2M	1	0
21	A	636	PSU	2	0
21	A	208	PSU	2	0
21	A	1793	MA6	1	0
21	A	28	A2M	1	0
21	A	418	OMC	3	0
21	A	123	OMU	1	0
21	A	1774	6MZ	2	0
21	A	1648	OMC	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 47 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

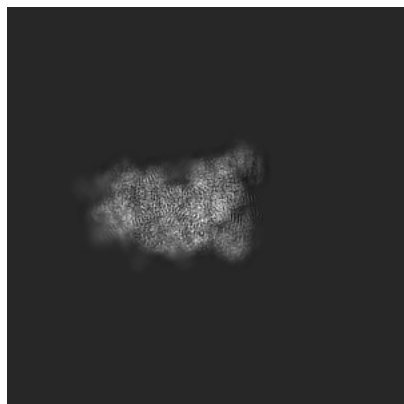
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18951. These allow visual inspection of the internal detail of the map and identification of artifacts.

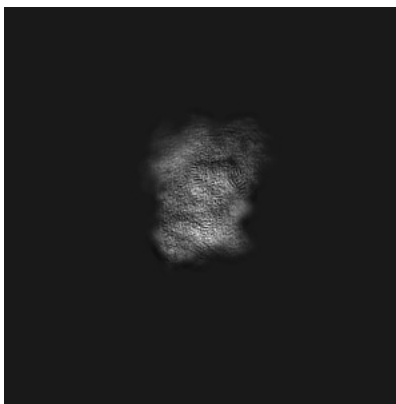
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

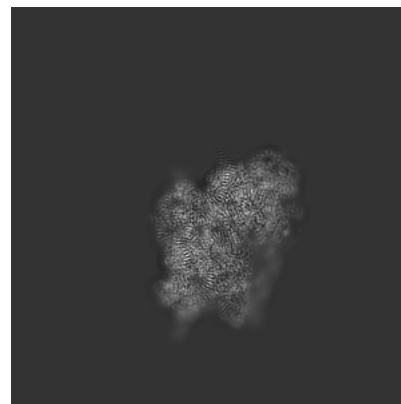
6.1.1 Primary map



X

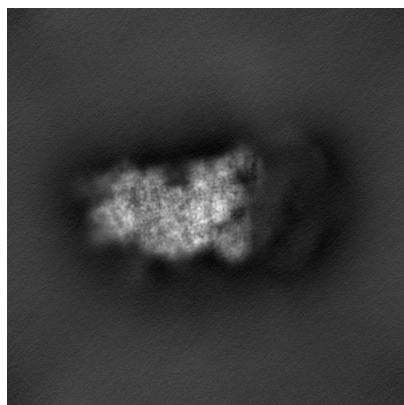


Y

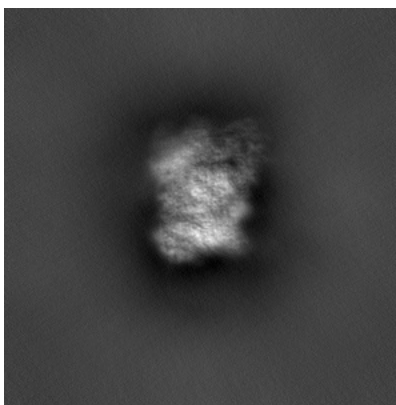


Z

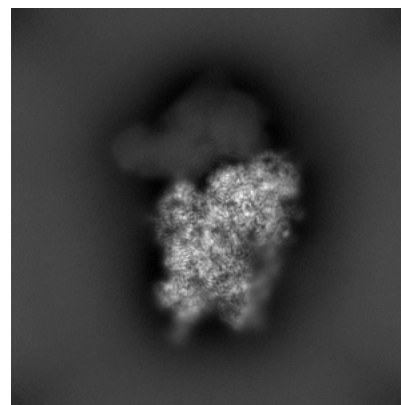
6.1.2 Raw map



X



Y

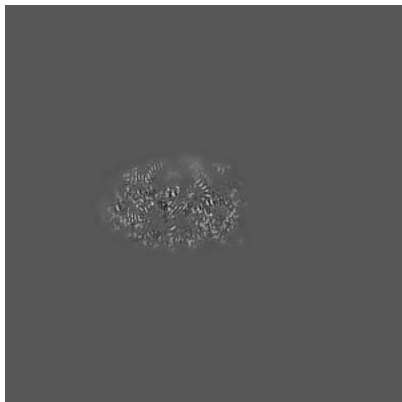


Z

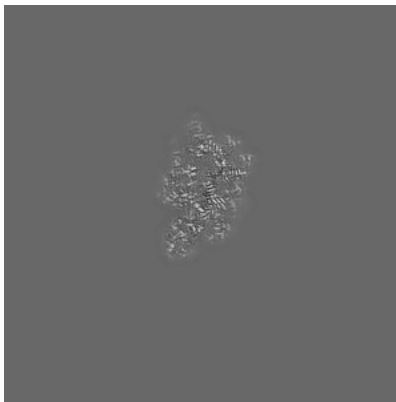
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

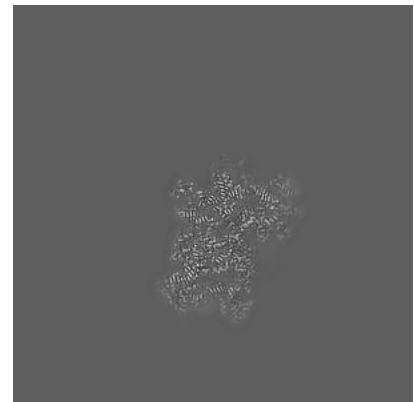
6.2.1 Primary map



X Index: 240

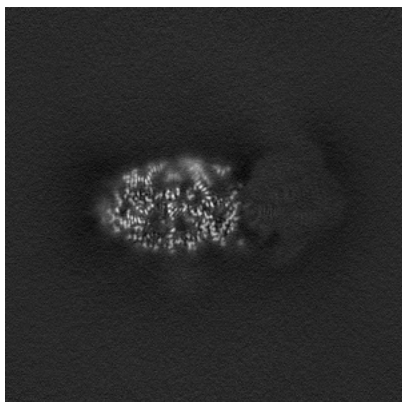


Y Index: 240

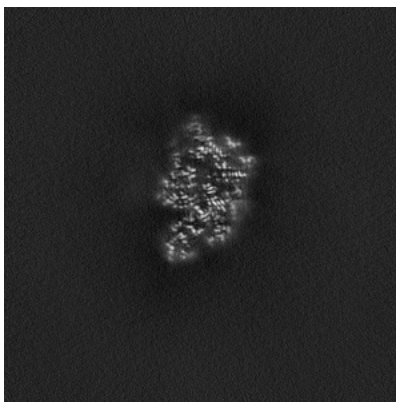


Z Index: 240

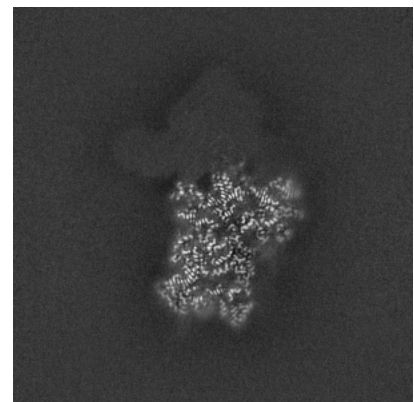
6.2.2 Raw map



X Index: 240



Y Index: 240

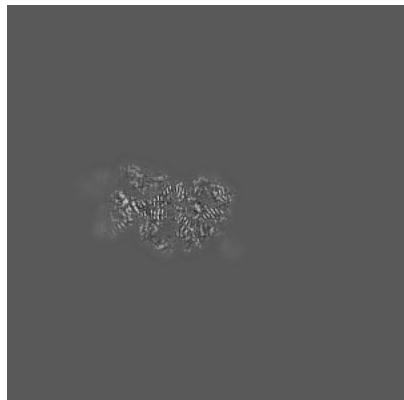


Z Index: 240

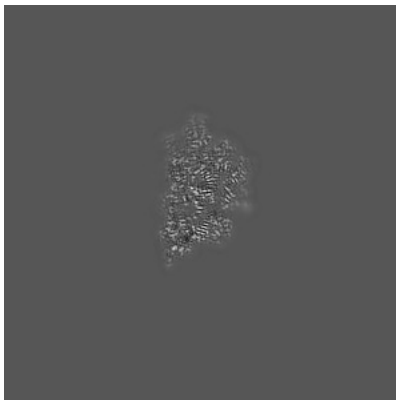
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

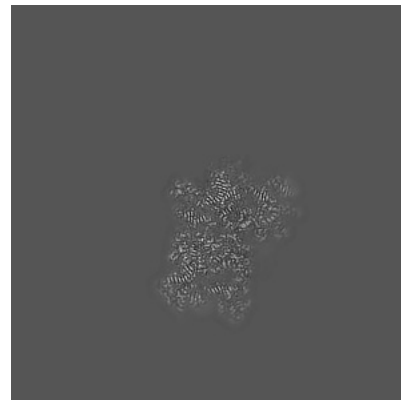
6.3.1 Primary map



X Index: 210

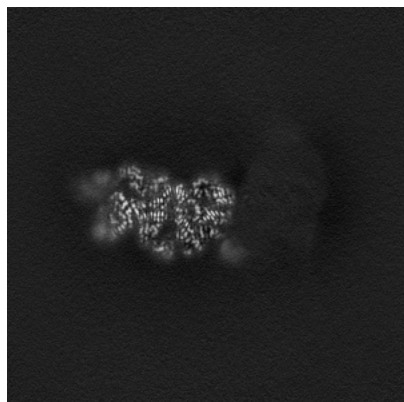


Y Index: 229

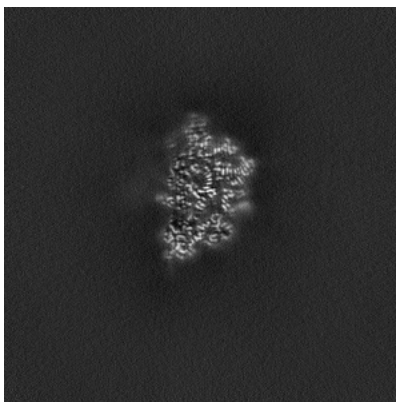


Z Index: 241

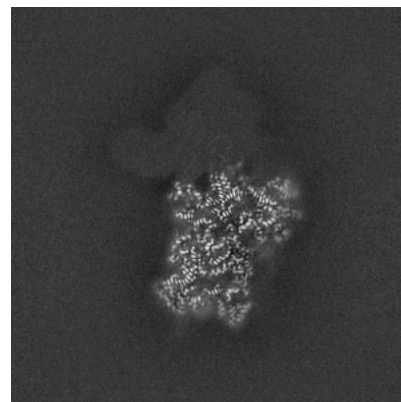
6.3.2 Raw map



X Index: 210



Y Index: 234

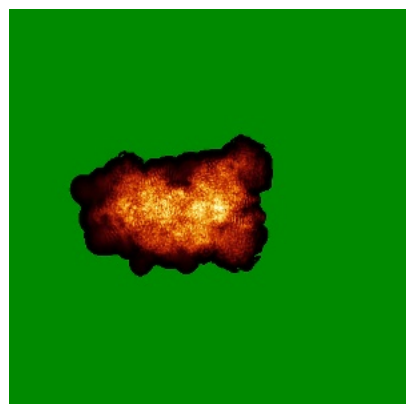


Z Index: 240

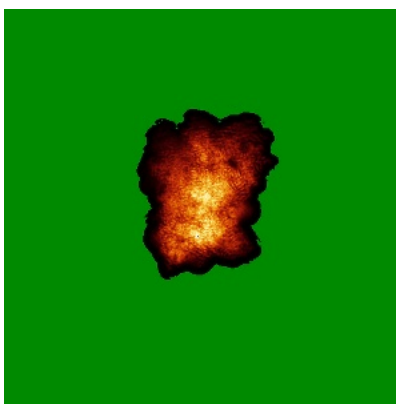
The images above show the largest variance slices of the map in three orthogonal directions.

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

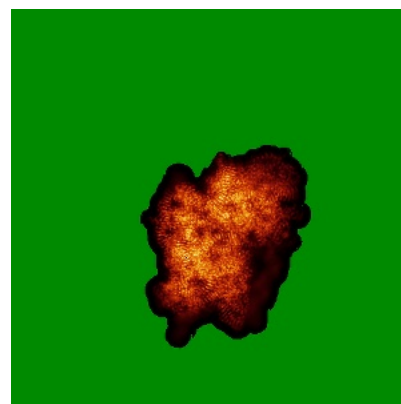
6.4.1 Primary map



X

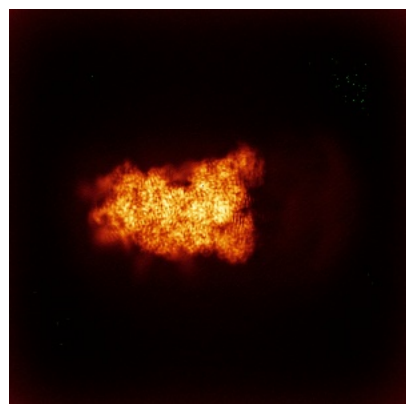


Y

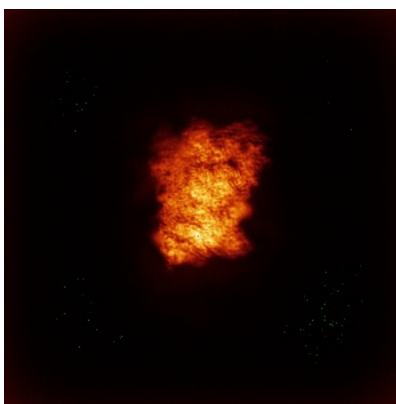


Z

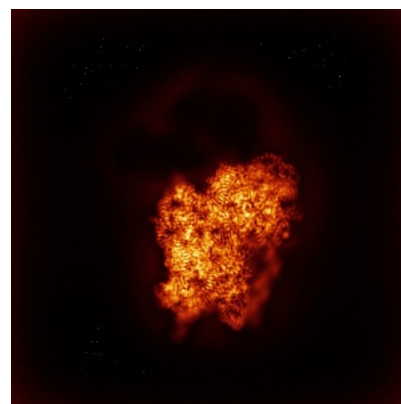
6.4.2 Raw map



X



Y

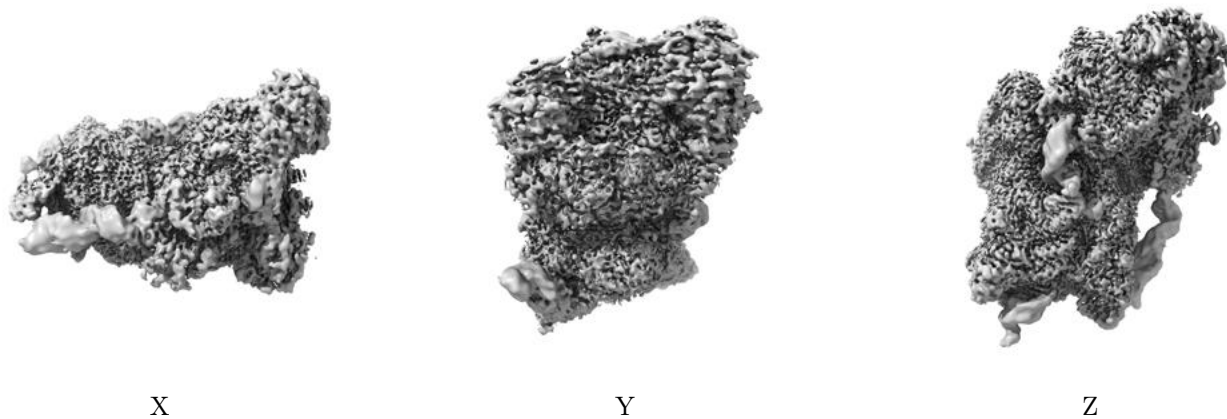


Z

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.

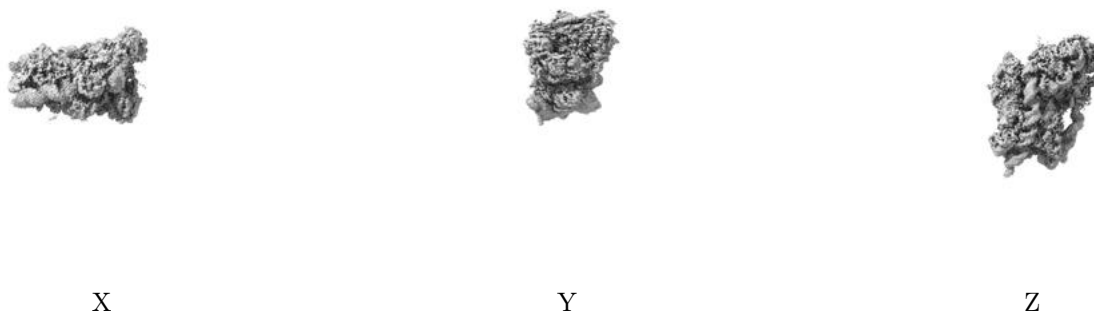
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.4. 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



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.

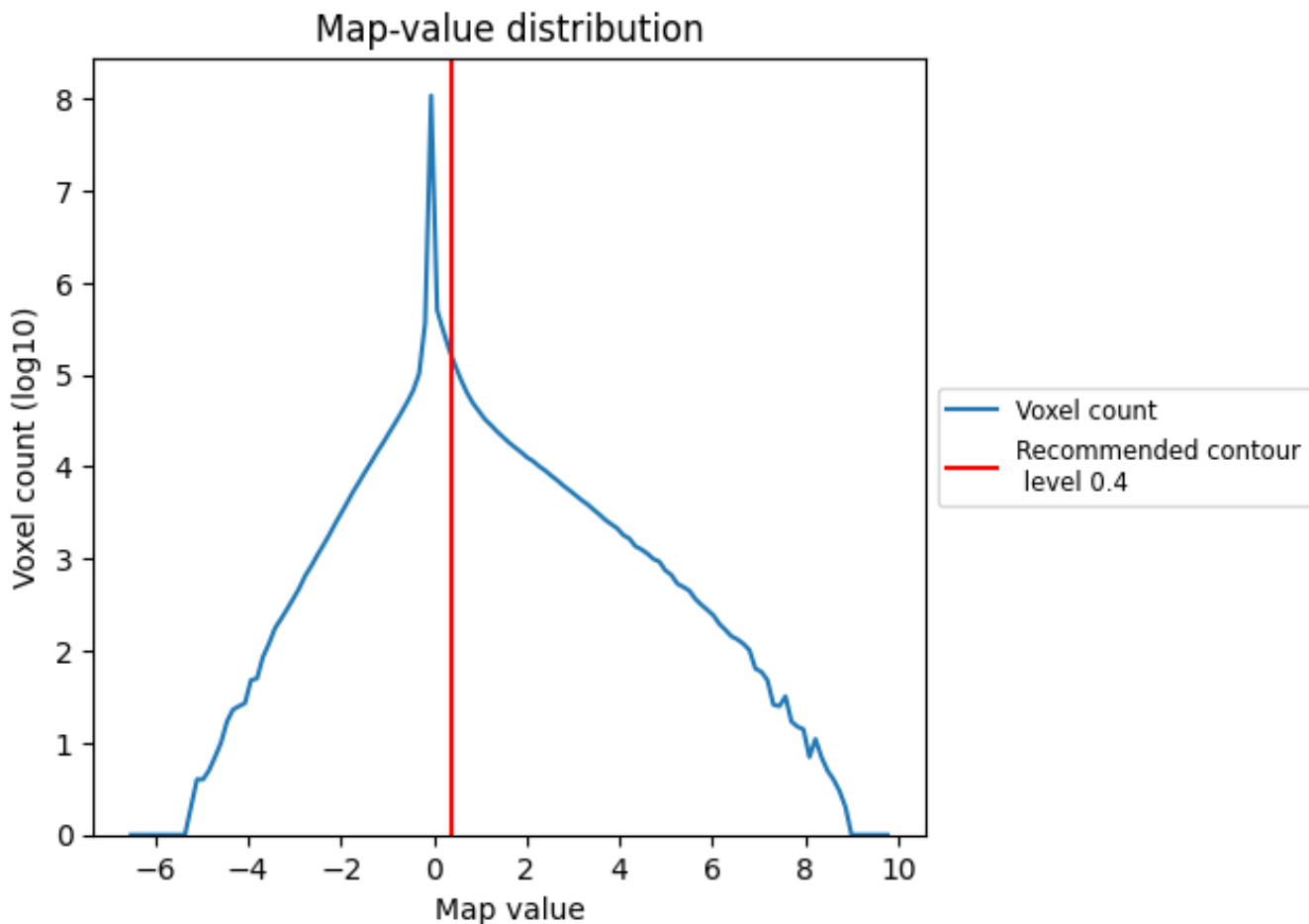
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

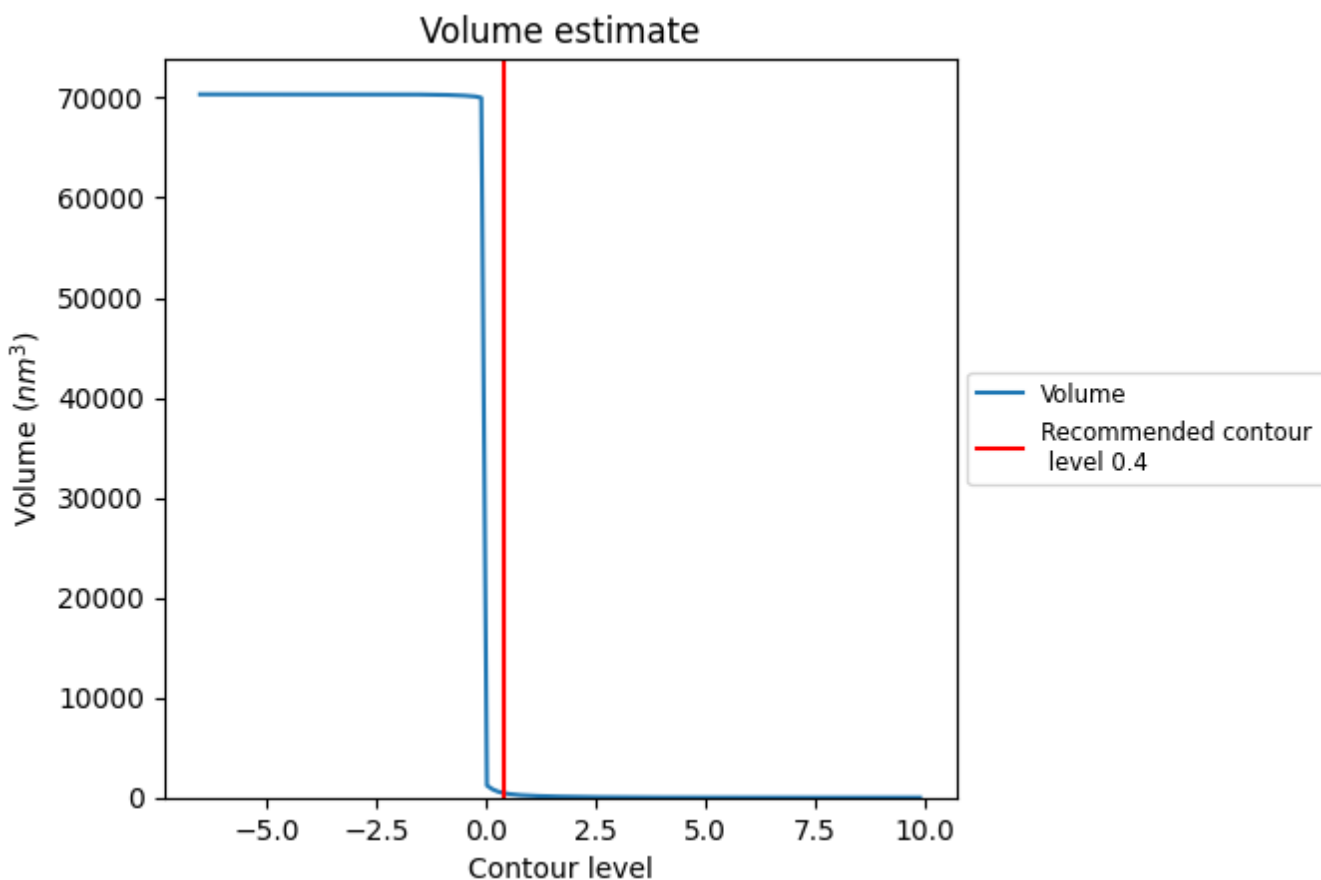
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

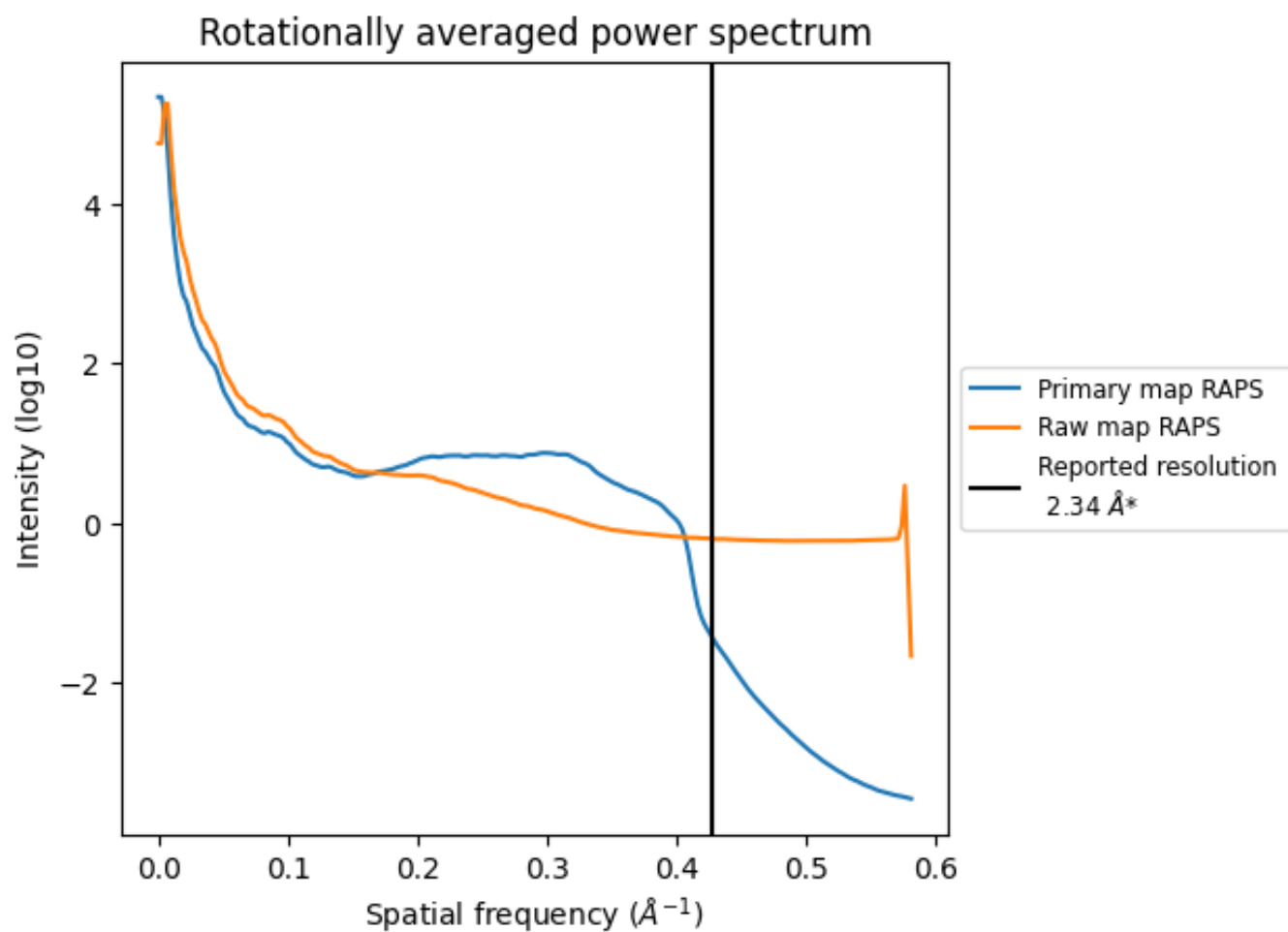
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 453 nm³; this corresponds to an approximate mass of 409 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

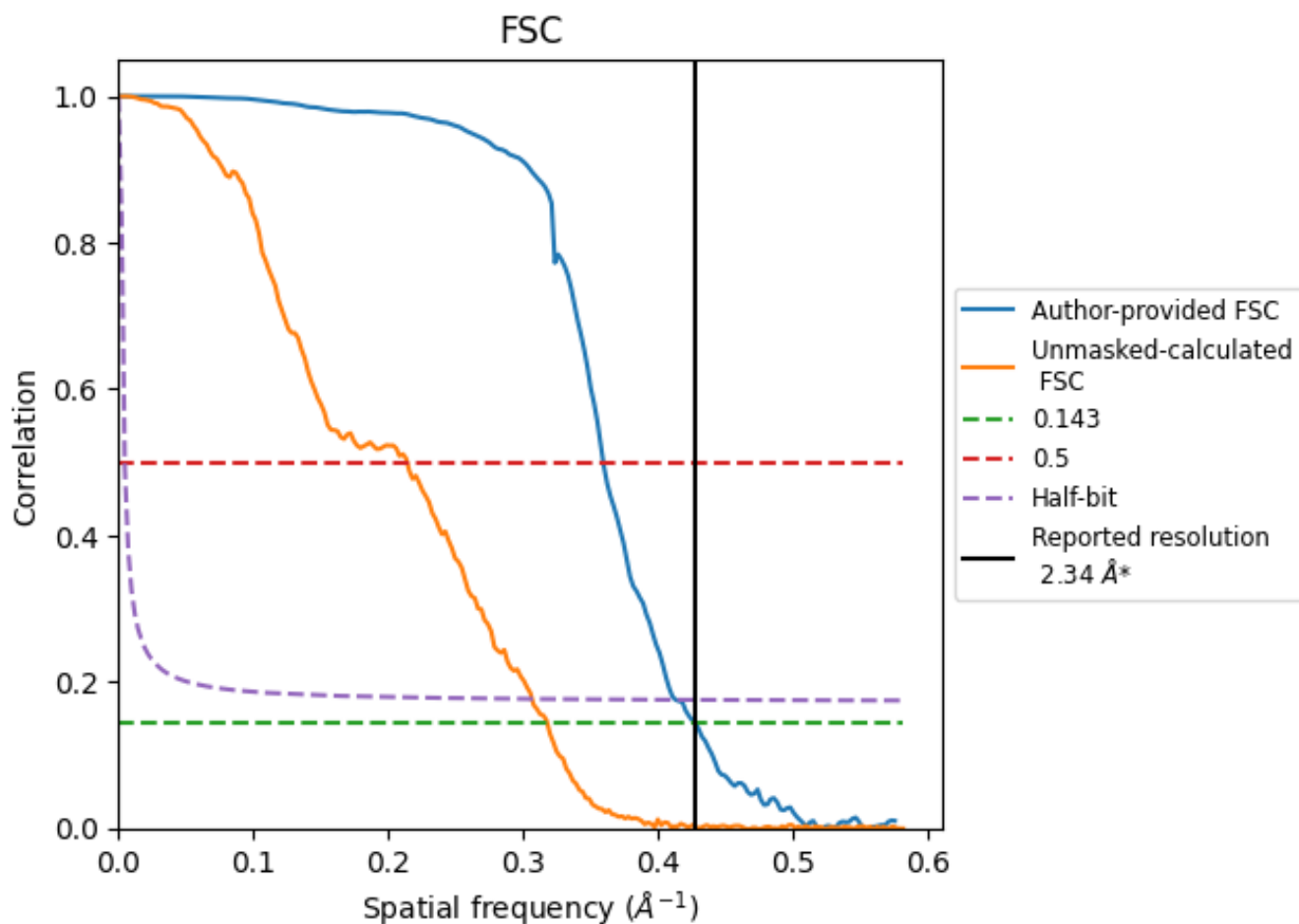


*Reported resolution corresponds to spatial frequency of 0.427 Å⁻¹

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 0.427 Å⁻¹

8.2 Resolution estimates [i](#)

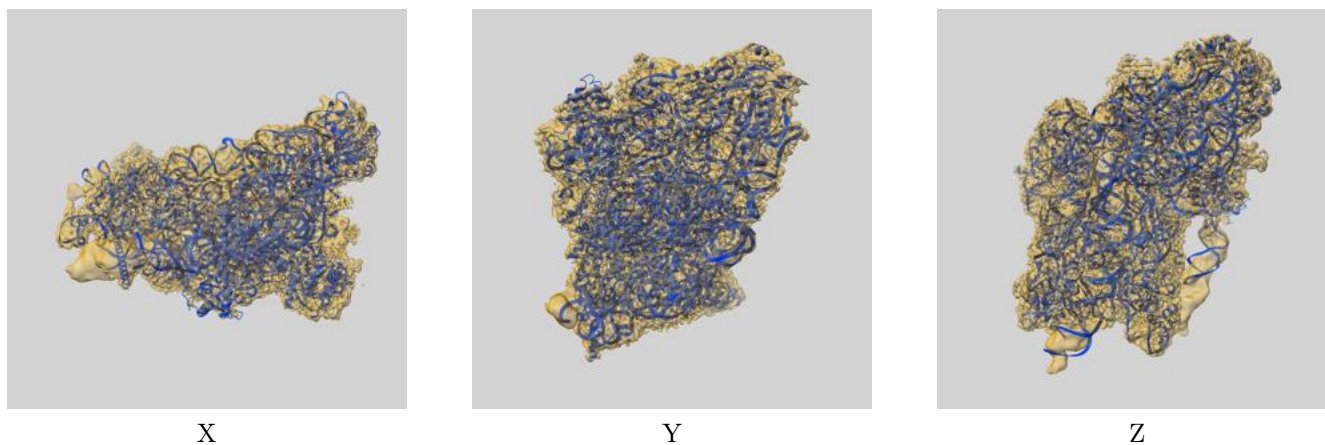
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.34	-	-
Author-provided FSC curve	2.34	2.78	2.42
Unmasked-calculated*	3.15	4.68	3.26

*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 3.15 differs from the reported value 2.34 by more than 10 %

9 Map-model fit [i](#)

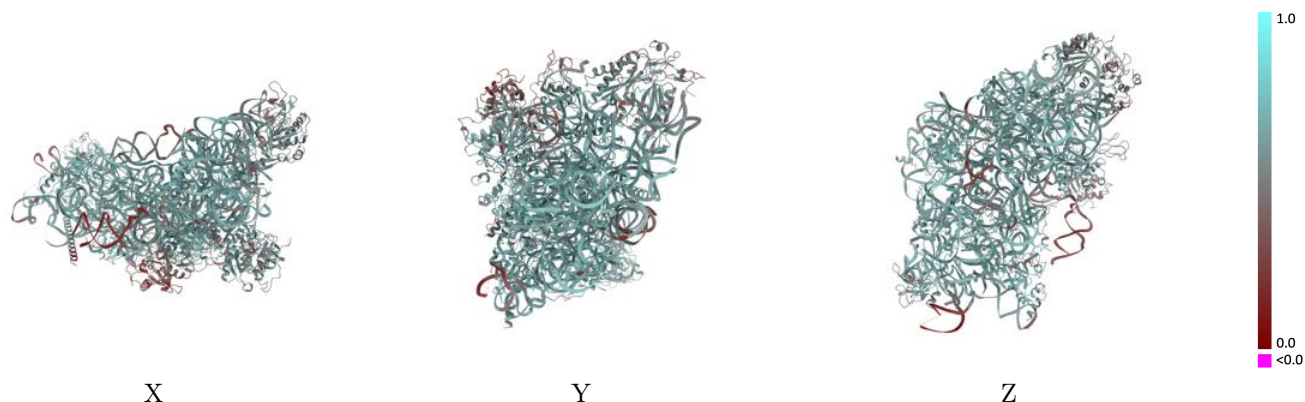
This section contains information regarding the fit between EMDB map EMD-18951 and PDB model 8R6F. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



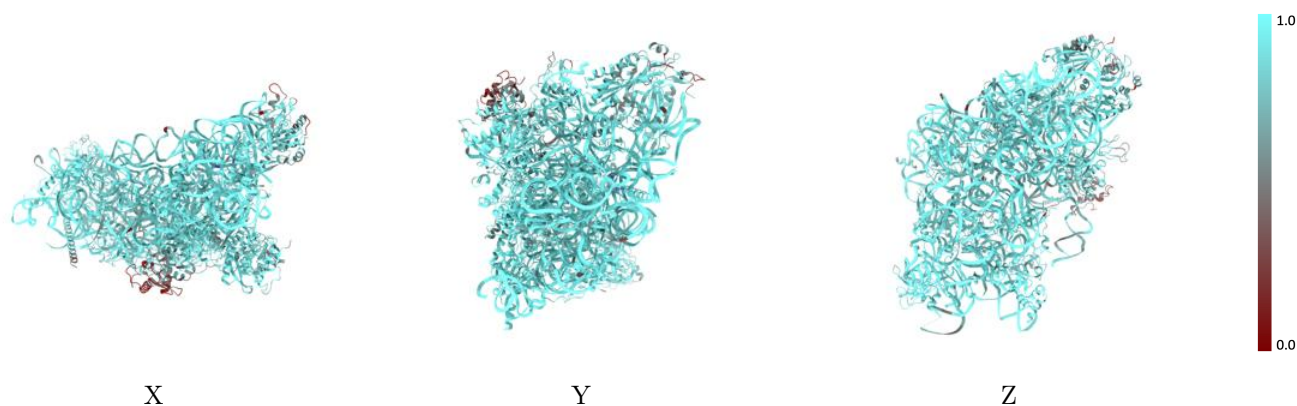
The images above show the 3D surface view of the map at the recommended contour level 0.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



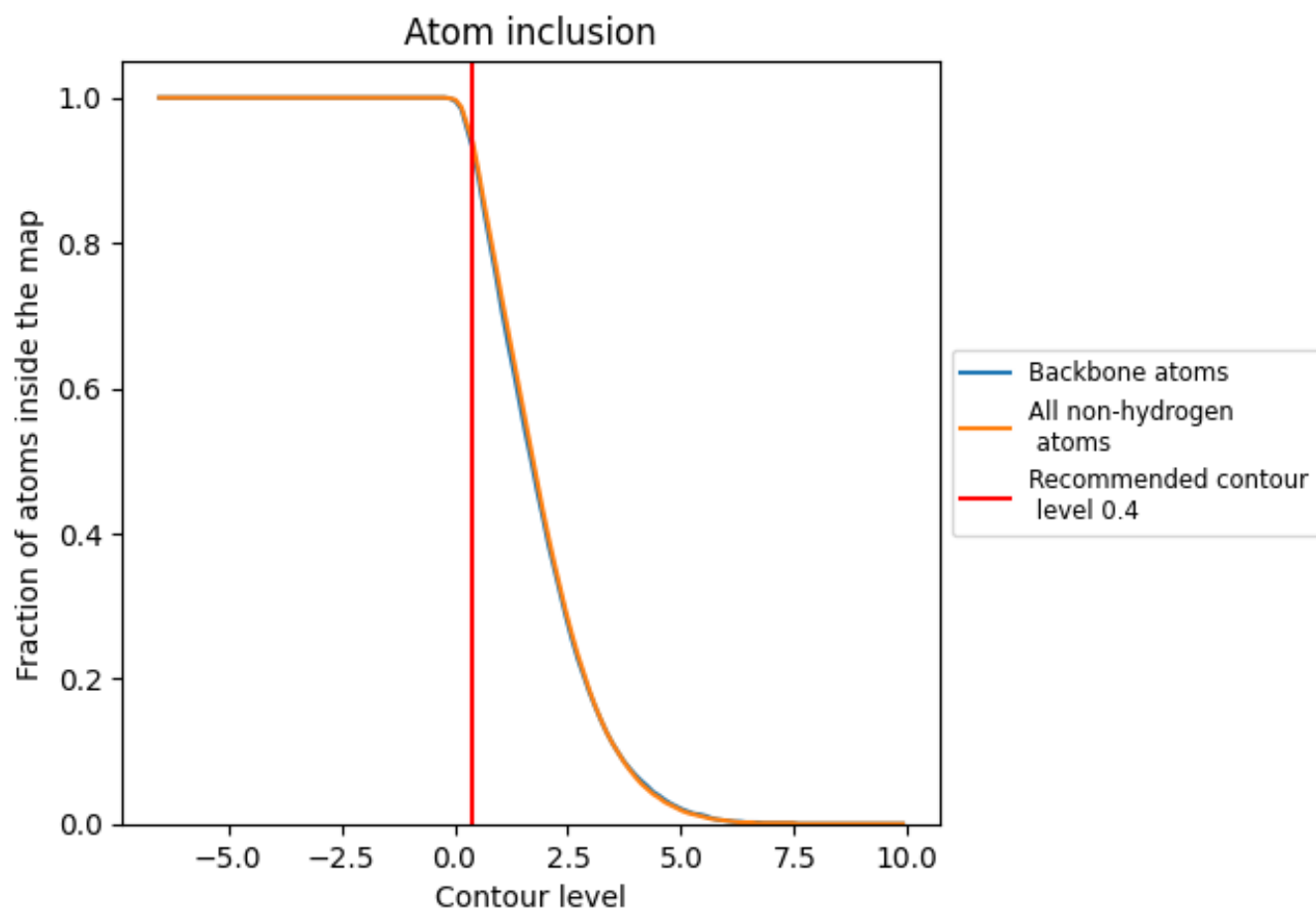
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.4).













































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 94% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.6000
A	 0.9700	 0.6060
B	 0.8370	 0.5260
C	 0.9620	 0.6410
E	 0.9620	 0.6430
G	 0.9280	 0.5700
H	 0.5400	 0.4000
I	 0.9670	 0.6380
J	 0.9670	 0.6490
L	 0.9750	 0.6630
N	 0.9430	 0.5980
O	 0.8410	 0.5460
V	 0.9450	 0.6060
W	 0.9820	 0.6700
X	 0.9710	 0.6460
Y	 0.9610	 0.6320
a	 0.8850	 0.6060
b	 0.8410	 0.5120
e	 0.9180	 0.6070
h	 0.6030	 0.3810
k	 0.9410	 0.5810
n	 0.9310	 0.5990

