Full wwPDB EM Validation Report

Apr 21, 2025 – 12:13 PM EDT

PDB ID	:	9AZM / pdb_00009azm
EMDB ID	:	EMD-44016
Title	:	In situ human ribosome (Focused on 40S with SERBP1 CTD)
Authors	:	Wei, Z.; Yong, Z.
Deposited on	:	2024-03-11
Resolution	:	2.68 Å(reported)

This is a Full wwPDB EM Validation 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:

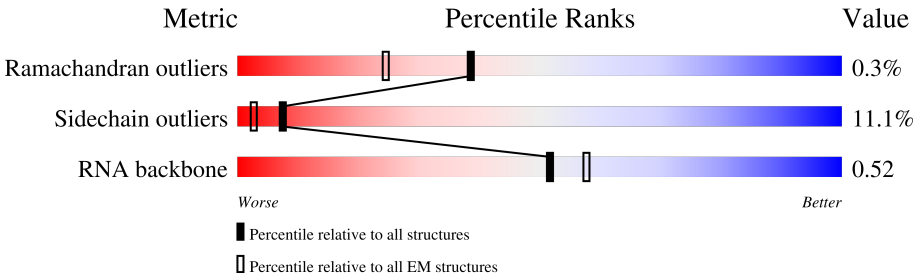
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.68 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	CD	85	20% 95% 5%
2	SD	227	89% 11%
3	SF	189	90% 10%
4	SK	98	91% 8%
5	SP	121	92% 7%
6	SQ	144	86% 13%
7	SS	145	90% 10%
8	ST	143	94% 6%

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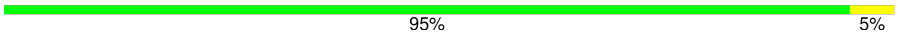
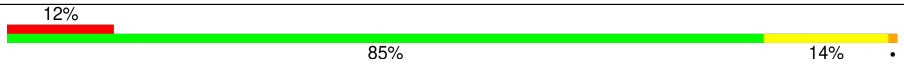
Mol	Chain	Length	Quality of chain
9	SU	104	
10	Sc	64	
11	Sd	55	
12	Sg	313	
13	SM	122	
14	SZ	75	
15	Sf	67	
16	S2	1740	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 25782 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 Serbp1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	CD	85	667	418	115	133	1	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	SD	227	1765	1125	317	315	8	0	0

- Molecule 3 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	SF	189	1495	934	284	270	7	0	0

- Molecule 4 is a protein called 40S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	SK	98	827	539	148	134	6	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	SP	121	985	623	185	170	7	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	SQ	144	1142	726	216	197	3	0	0

- Molecule 7 is a protein called 40S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	SS	145	Total	C	N	O	S	0	0
			1198	751	242	203	2		

- Molecule 8 is a protein called 40S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	ST	143	Total	C	N	O	S	0	0
			1112	697	214	198	3		

- Molecule 9 is a protein called 40S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	SU	104	Total	C	N	O	S	0	0
			821	514	155	148	4		

- Molecule 10 is a protein called 40S ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Sc	64	Total	C	N	O	S	0	0
			506	308	102	94	2		

- Molecule 11 is a protein called 40S ribosomal protein S29.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Sd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 12 is a protein called Receptor of activated protein C kinase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Sg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 13 is a protein called Small ribosomal subunit protein eS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	SM	122	Total	C	N	O	S	0	0
			940	590	164	177	9		

- Molecule 14 is a protein called Small ribosomal subunit protein eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 15 is a protein called Ubiquitin-40S ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Sf	67	Total	C	N	O	S	0	0
			548	346	102	93	7		

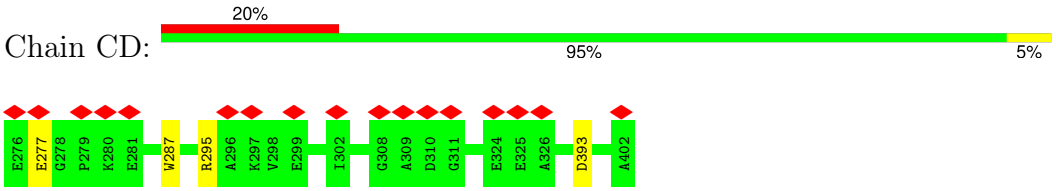
- Molecule 16 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S2	483	Total	C	N	O	P	0	0
			10283	4588	1820	3392	483		

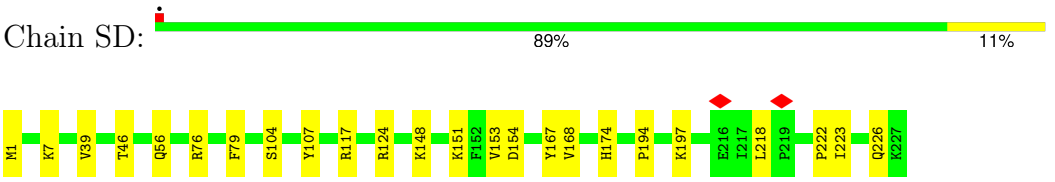
3 Residue-property plots (i)

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.

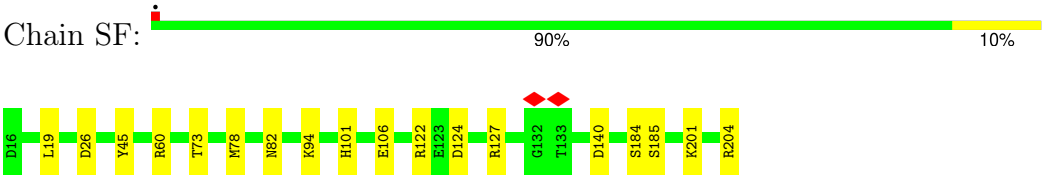
• Molecule 1: Serbp1



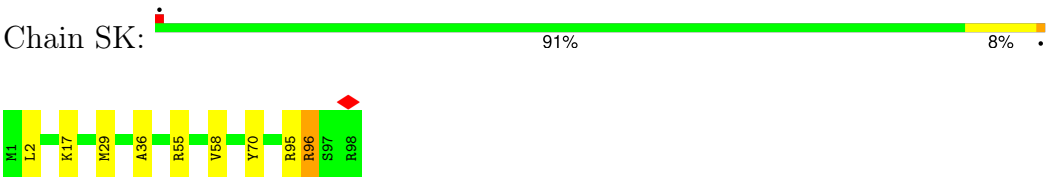
• Molecule 2: Small ribosomal subunit protein uS3



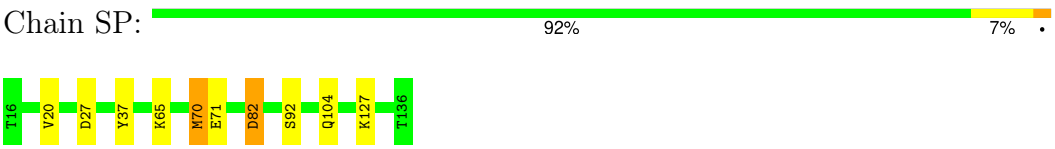
• Molecule 3: 40S ribosomal protein S5



• Molecule 4: 40S ribosomal protein S10

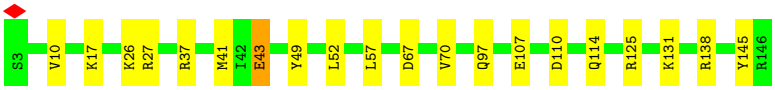


• Molecule 5: Small ribosomal subunit protein uS19



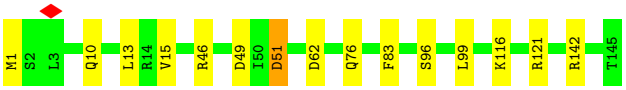
• Molecule 6: Small ribosomal subunit protein uS9

Chain SQ:



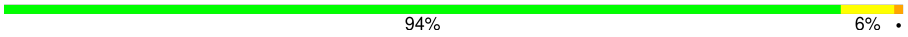
• Molecule 7: 40S ribosomal protein S18

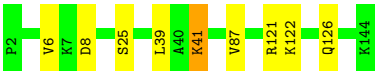
Chain SS:



• Molecule 8: 40S ribosomal protein S19

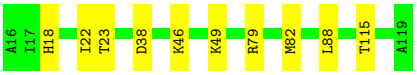
Chain ST:





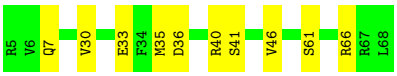
• Molecule 9: 40S ribosomal protein S20

Chain SU:



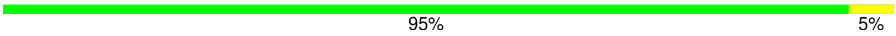
• Molecule 10: 40S ribosomal protein S28

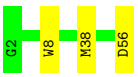
Chain Sc:



• Molecule 11: 40S ribosomal protein S29

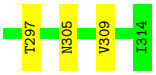
Chain Sd:





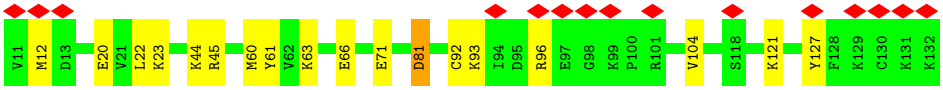
• Molecule 12: Receptor of activated protein C kinase 1

Chain Sg:



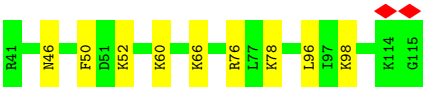
• Molecule 13: Small ribosomal subunit protein eS12

Chain SM:



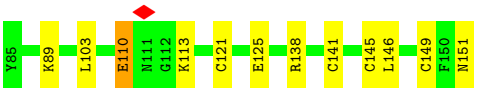
• Molecule 14: Small ribosomal subunit protein eS25

Chain SZ:



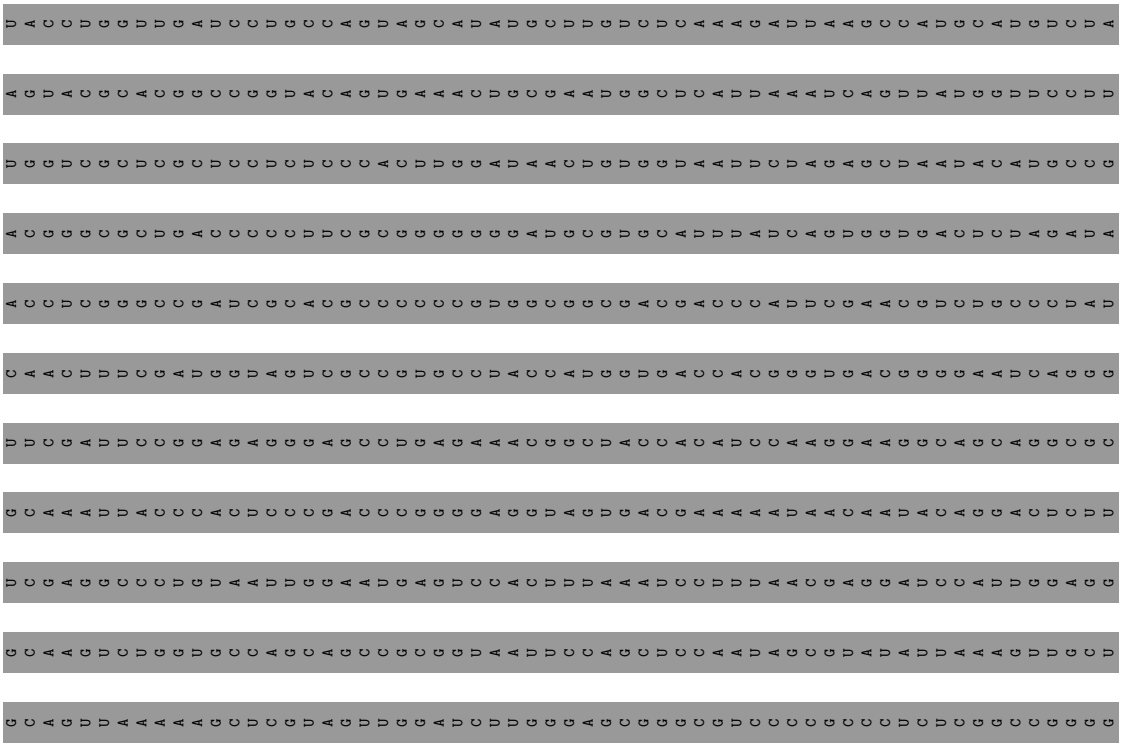
• Molecule 15: Ubiquitin-40S ribosomal protein S27a

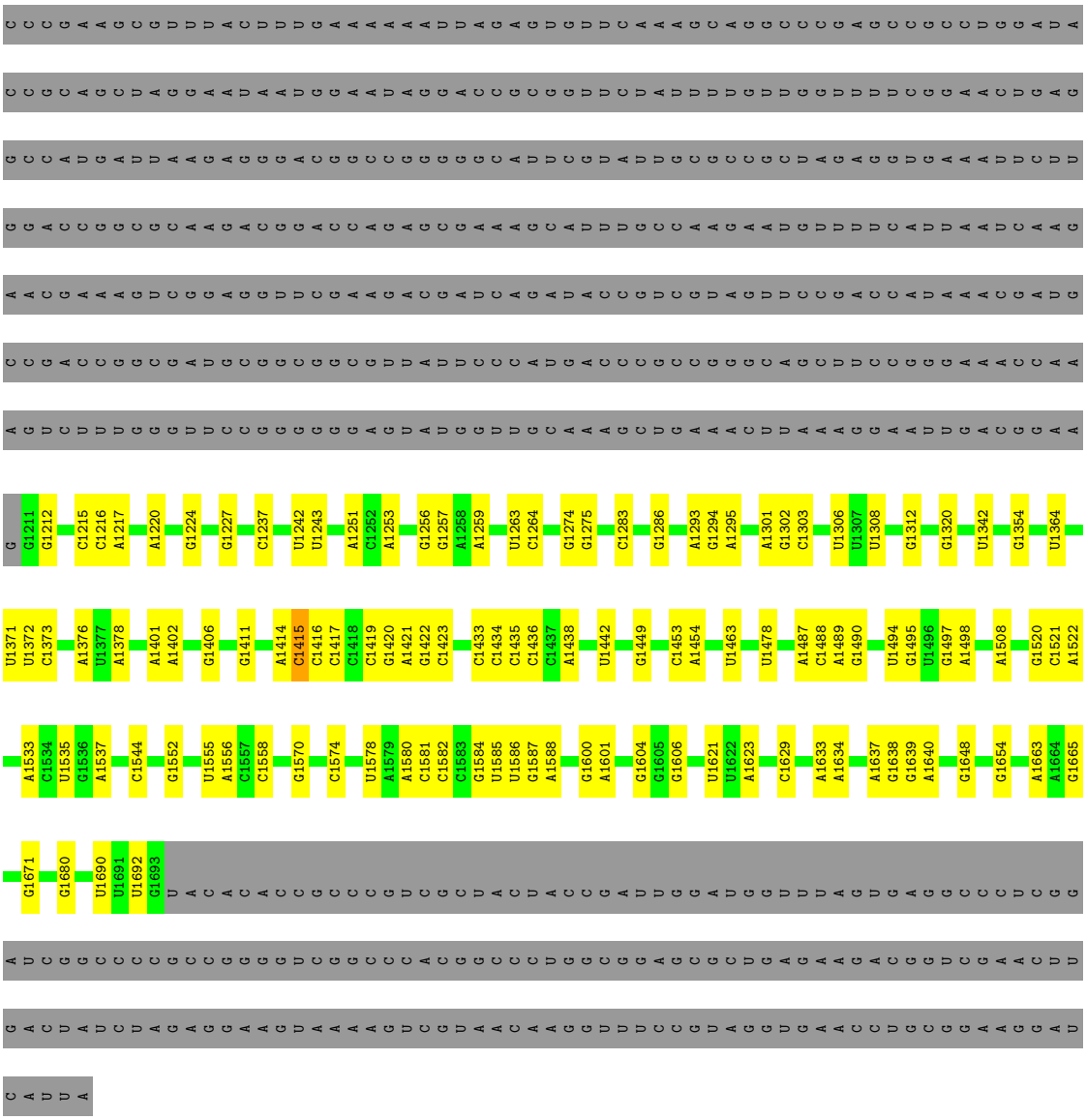
Chain Sf:



• Molecule 16: 18S rRNA

Chain S2:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1754680	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.191	Depositor
Minimum map value	-0.063	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0146	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality

5.1 Standard geometry

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	CD	0.26	0/679	0.55	0/911
2	SD	0.31	0/1793	0.69	3/2414 (0.1%)
3	SF	0.28	0/1516	0.58	1/2037 (0.0%)
4	SK	0.29	0/851	0.59	1/1147 (0.1%)
5	SP	0.30	0/1003	0.67	4/1342 (0.3%)
6	SQ	0.29	0/1160	0.69	1/1553 (0.1%)
7	SS	0.28	0/1216	0.67	1/1628 (0.1%)
8	ST	0.28	0/1131	0.57	0/1515
9	SU	0.26	0/831	0.62	0/1115
10	Sc	0.31	0/508	0.82	0/680
11	Sd	0.27	0/470	0.60	0/623
12	Sg	0.27	0/2493	0.60	0/3394
13	SM	0.28	0/950	0.72	1/1275 (0.1%)
14	SZ	0.32	0/604	0.66	0/810
15	Sf	0.36	0/560	0.85	3/745 (0.4%)
16	S2	0.27	0/11489	0.87	11/17905 (0.1%)
All	All	0.28	0/27254	0.76	26/39094 (0.1%)

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
3	SF	0	2
5	SP	0	1
6	SQ	0	2
14	SZ	0	1
All	All	0	6

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	SD	194	PRO	CA-N-CD	-10.12	97.33	111.50
2	SD	222	PRO	CA-N-CD	-9.23	98.58	111.50
16	S2	1453	C	C2-N1-C1'	7.21	126.74	118.80
16	S2	1415	C	N1-C2-O2	6.90	123.04	118.90
16	S2	1453	C	N1-C2-O2	6.56	122.84	118.90
16	S2	1416	C	N3-C2-O2	-6.48	117.36	121.90
7	SS	51	ASP	CB-CG-OD1	6.31	123.98	118.30
16	S2	1520	G	C4-N9-C1'	6.25	134.63	126.50
15	Sf	103	LEU	CA-CB-CG	6.10	129.32	115.30
5	SP	27	ASP	CB-CG-OD2	6.08	123.78	118.30
5	SP	70	MET	CA-CB-CG	6.02	123.53	113.30
5	SP	70	MET	CB-CG-SD	5.81	129.83	112.40
15	Sf	110	GLU	CA-CB-CG	5.75	126.05	113.40
16	S2	1520	G	N3-C4-N9	5.52	129.31	126.00
5	SP	82	ASP	CB-CG-OD1	5.51	123.26	118.30
16	S2	1520	G	C8-N9-C1'	-5.48	119.88	127.00
16	S2	1416	C	C6-N1-C2	-5.37	118.15	120.30
4	SK	2	LEU	CA-CB-CG	5.35	127.61	115.30
2	SD	218	LEU	CA-CB-CG	5.22	127.30	115.30
16	S2	1453	C	C6-N1-C1'	-5.14	114.63	120.80
3	SF	19	LEU	CA-CB-CG	5.14	127.13	115.30
16	S2	1582	C	N1-C2-O2	5.14	121.98	118.90
6	SQ	43	GLU	CA-CB-CG	5.13	124.69	113.40
13	SM	81	ASP	CB-CG-OD1	5.09	122.88	118.30
16	S2	1415	C	N3-C2-O2	-5.07	118.35	121.90
15	Sf	113	LYS	CA-CB-CG	5.03	124.47	113.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	SF	60	ARG	Peptide
3	SF	78	MET	Peptide
5	SP	127	LYS	Peptide
6	SQ	17	LYS	Peptide
6	SQ	43	GLU	Peptide
14	SZ	46	ASN	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
1	CD	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	10 23
2	SD	225/227 (99%)	210 (93%)	15 (7%)	0	100 100
3	SF	187/189 (99%)	166 (89%)	21 (11%)	0	100 100
4	SK	96/98 (98%)	86 (90%)	8 (8%)	2 (2%)	5 14
5	SP	119/121 (98%)	111 (93%)	8 (7%)	0	100 100
6	SQ	142/144 (99%)	125 (88%)	17 (12%)	0	100 100
7	SS	143/145 (99%)	138 (96%)	5 (4%)	0	100 100
8	ST	141/143 (99%)	129 (92%)	10 (7%)	2 (1%)	9 21
9	SU	102/104 (98%)	92 (90%)	10 (10%)	0	100 100
10	Sc	62/64 (97%)	50 (81%)	12 (19%)	0	100 100
11	Sd	53/55 (96%)	50 (94%)	3 (6%)	0	100 100
12	Sg	311/313 (99%)	275 (88%)	36 (12%)	0	100 100
13	SM	120/122 (98%)	107 (89%)	12 (10%)	1 (1%)	16 35
14	SZ	73/75 (97%)	60 (82%)	13 (18%)	0	100 100
15	Sf	65/67 (97%)	57 (88%)	8 (12%)	0	100 100
All	All	1916/1952 (98%)	1725 (90%)	185 (10%)	6 (0%)	38 59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	SK	96	ARG
8	ST	39	LEU
4	SK	36	ALA
8	ST	41	LYS
1	CD	295	ARG
13	SM	96	ARG

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	CD	69/70 (99%)	66 (96%)	3 (4%)	25 49
2	SD	190/190 (100%)	169 (89%)	21 (11%)	5 11
3	SF	159/159 (100%)	144 (91%)	15 (9%)	7 16
4	SK	89/89 (100%)	82 (92%)	7 (8%)	10 23
5	SP	107/107 (100%)	99 (92%)	8 (8%)	11 25
6	SQ	119/119 (100%)	101 (85%)	18 (15%)	2 5
7	SS	126/126 (100%)	111 (88%)	15 (12%)	4 9
8	ST	113/113 (100%)	105 (93%)	8 (7%)	12 27
9	SU	94/94 (100%)	84 (89%)	10 (11%)	5 12
10	Sc	57/57 (100%)	47 (82%)	10 (18%)	1 3
11	Sd	48/48 (100%)	45 (94%)	3 (6%)	15 32
12	Sg	272/272 (100%)	239 (88%)	33 (12%)	4 8
13	SM	102/104 (98%)	85 (83%)	17 (17%)	2 4
14	SZ	66/66 (100%)	58 (88%)	8 (12%)	4 8
15	Sf	60/60 (100%)	50 (83%)	10 (17%)	2 4
All	All	1671/1674 (100%)	1485 (89%)	186 (11%)	7 11

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CD	277	GLU
1	CD	287	TRP
1	CD	393	ASP
2	SD	1	MET
2	SD	7	LYS
2	SD	39	VAL
2	SD	46	THR
2	SD	56	GLN
2	SD	76	ARG
2	SD	79	PHE

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Mol	Chain	Res	Type
2	SD	104	SER
2	SD	107	TYR
2	SD	117	ARG
2	SD	124	ARG
2	SD	148	LYS
2	SD	151	LYS
2	SD	153	VAL
2	SD	154	ASP
2	SD	167	TYR
2	SD	168	VAL
2	SD	174	HIS
2	SD	197	LYS
2	SD	223	ILE
2	SD	226	GLN
3	SF	26	ASP
3	SF	45	TYR
3	SF	73	THR
3	SF	82	ASN
3	SF	94	LYS
3	SF	101	HIS
3	SF	106	GLU
3	SF	122	ARG
3	SF	124	ASP
3	SF	127	ARG
3	SF	140	ASP
3	SF	184	SER
3	SF	185	SER
3	SF	201	LYS
3	SF	204	ARG
4	SK	17	LYS
4	SK	29	MET
4	SK	55	ARG
4	SK	58	VAL
4	SK	70	TYR
4	SK	95	ARG
4	SK	96	ARG
5	SP	20	VAL
5	SP	37	TYR
5	SP	65	LYS
5	SP	70	MET
5	SP	71	GLU
5	SP	82	ASP

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Mol	Chain	Res	Type
5	SP	92	SER
5	SP	104	GLN
6	SQ	10	VAL
6	SQ	26	LYS
6	SQ	27	ARG
6	SQ	37	ARG
6	SQ	41	MET
6	SQ	49	TYR
6	SQ	52	LEU
6	SQ	57	LEU
6	SQ	67	ASP
6	SQ	70	VAL
6	SQ	97	GLN
6	SQ	107	GLU
6	SQ	110	ASP
6	SQ	114	GLN
6	SQ	125	ARG
6	SQ	131	LYS
6	SQ	138	ARG
6	SQ	145	TYR
7	SS	1	MET
7	SS	10	GLN
7	SS	13	LEU
7	SS	15	VAL
7	SS	46	ARG
7	SS	49	ASP
7	SS	51	ASP
7	SS	62	ASP
7	SS	76	GLN
7	SS	83	PHE
7	SS	96	SER
7	SS	99	LEU
7	SS	116	LYS
7	SS	121	ARG
7	SS	142	ARG
8	ST	6	VAL
8	ST	8	ASP
8	ST	25	SER
8	ST	41	LYS
8	ST	87	VAL
8	ST	121	ARG
8	ST	122	LYS

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Mol	Chain	Res	Type
8	ST	126	GLN
9	SU	18	HIS
9	SU	22	ILE
9	SU	23	THR
9	SU	38	ASP
9	SU	46	LYS
9	SU	49	LYS
9	SU	79	ARG
9	SU	82	MET
9	SU	88	LEU
9	SU	115	THR
10	Sc	7	GLN
10	Sc	30	VAL
10	Sc	33	GLU
10	Sc	35	MET
10	Sc	36	ASP
10	Sc	40	ARG
10	Sc	41	SER
10	Sc	46	VAL
10	Sc	61	SER
10	Sc	66	ARG
11	Sd	8	TRP
11	Sd	38	MET
11	Sd	56	ASP
12	Sg	14	HIS
12	Sg	26	GLN
12	Sg	32	LEU
12	Sg	38	LYS
12	Sg	52	TYR
12	Sg	62	HIS
12	Sg	63	SER
12	Sg	65	PHE
12	Sg	99	ARG
12	Sg	100	ARG
12	Sg	107	ASP
12	Sg	113	PHE
12	Sg	125	ARG
12	Sg	138	CYS
12	Sg	140	TYR
12	Sg	144	ASP
12	Sg	147	HIS
12	Sg	150	TRP

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Mol	Chain	Res	Type
12	Sg	152	SER
12	Sg	153	CYS
12	Sg	160	SER
12	Sg	168	CYS
12	Sg	179	LEU
12	Sg	182	CYS
12	Sg	207	CYS
12	Sg	217	MET
12	Sg	222	ASN
12	Sg	223	GLU
12	Sg	236	ILE
12	Sg	240	CYS
12	Sg	297	THR
12	Sg	305	ASN
12	Sg	309	VAL
13	SM	12	MET
13	SM	20	GLU
13	SM	22	LEU
13	SM	23	LYS
13	SM	44	LYS
13	SM	45	ARG
13	SM	60	MET
13	SM	61	TYR
13	SM	63	LYS
13	SM	66	GLU
13	SM	71	GLU
13	SM	81	ASP
13	SM	92	CYS
13	SM	93	LYS
13	SM	104	VAL
13	SM	121	LYS
13	SM	127	TYR
14	SZ	50	PHE
14	SZ	52	LYS
14	SZ	60	LYS
14	SZ	66	LYS
14	SZ	76	ARG
14	SZ	78	LYS
14	SZ	96	LEU
14	SZ	98	LYS
15	Sf	89	LYS
15	Sf	110	GLU

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Mol	Chain	Res	Type
15	Sf	121	CYS
15	Sf	125	GLU
15	Sf	138	ARG
15	Sf	141	CYS
15	Sf	145	CYS
15	Sf	146	LEU
15	Sf	149	CYS
15	Sf	151	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	CD	344	ASN
5	SP	32	GLN
7	SS	73	ASN
9	SU	92	HIS
12	Sg	62	HIS
12	Sg	181	ASN
12	Sg	191	HIS
12	Sg	285	GLN
14	SZ	45	ASN
15	Sf	151	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	S2	482/1740 (27%)	111 (23%)	1 (0%)

All (111) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	S2	1212	G
16	S2	1215	C
16	S2	1216	C
16	S2	1217	A
16	S2	1220	A
16	S2	1224	G
16	S2	1227	G
16	S2	1237	C
16	S2	1242	U

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Mol	Chain	Res	Type
16	S2	1243	U
16	S2	1251	A
16	S2	1253	A
16	S2	1256	G
16	S2	1257	G
16	S2	1259	A
16	S2	1263	U
16	S2	1264	C
16	S2	1274	G
16	S2	1275	G
16	S2	1283	C
16	S2	1286	G
16	S2	1293	A
16	S2	1294	G
16	S2	1295	A
16	S2	1301	A
16	S2	1302	G
16	S2	1303	C
16	S2	1306	U
16	S2	1308	U
16	S2	1312	G
16	S2	1320	G
16	S2	1342	U
16	S2	1354	G
16	S2	1364	U
16	S2	1371	U
16	S2	1372	U
16	S2	1373	C
16	S2	1376	A
16	S2	1378	A
16	S2	1401	A
16	S2	1402	A
16	S2	1406	G
16	S2	1411	G
16	S2	1414	A
16	S2	1415	C
16	S2	1417	C
16	S2	1419	C
16	S2	1420	G
16	S2	1421	A
16	S2	1422	G
16	S2	1423	C

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Mol	Chain	Res	Type
16	S2	1433	C
16	S2	1434	C
16	S2	1435	C
16	S2	1436	C
16	S2	1438	A
16	S2	1442	U
16	S2	1449	G
16	S2	1454	A
16	S2	1463	U
16	S2	1478	U
16	S2	1487	A
16	S2	1488	C
16	S2	1489	A
16	S2	1490	G
16	S2	1494	U
16	S2	1495	G
16	S2	1497	G
16	S2	1498	A
16	S2	1508	A
16	S2	1521	C
16	S2	1522	A
16	S2	1533	A
16	S2	1535	U
16	S2	1537	A
16	S2	1544	C
16	S2	1552	G
16	S2	1555	U
16	S2	1556	A
16	S2	1558	C
16	S2	1570	G
16	S2	1574	C
16	S2	1578	U
16	S2	1580	A
16	S2	1581	C
16	S2	1584	G
16	S2	1585	U
16	S2	1586	U
16	S2	1587	G
16	S2	1588	A
16	S2	1600	G
16	S2	1601	A
16	S2	1604	G

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Mol	Chain	Res	Type
16	S2	1606	G
16	S2	1621	U
16	S2	1623	A
16	S2	1629	C
16	S2	1633	A
16	S2	1634	A
16	S2	1637	A
16	S2	1638	G
16	S2	1639	G
16	S2	1640	A
16	S2	1648	G
16	S2	1654	G
16	S2	1663	A
16	S2	1665	G
16	S2	1671	G
16	S2	1680	G
16	S2	1690	U
16	S2	1692	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
16	S2	1434	C

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	CD	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	360:PRO	C	389:TYR	N	41.78
1	CD	326:ALA	C	341:PRO	N	40.51
1	CD	309:ALA	C	310:ASP	N	3.29

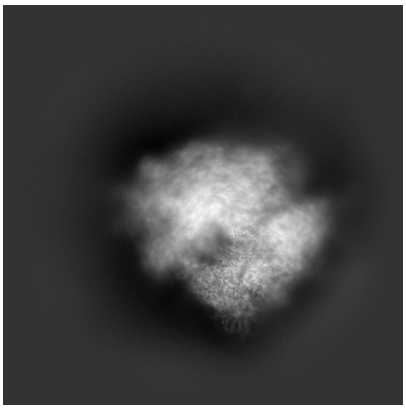
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44016. These allow visual inspection of the internal detail of the map and identification of artifacts.

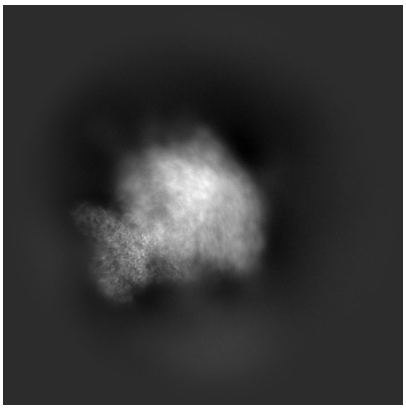
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

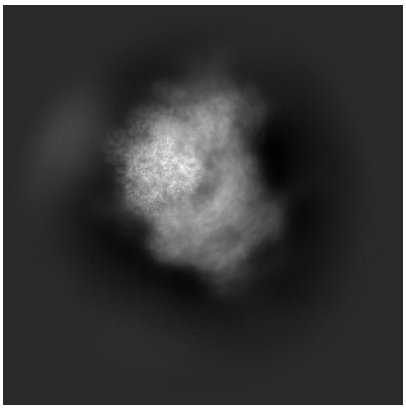
6.1.1 Primary map



X

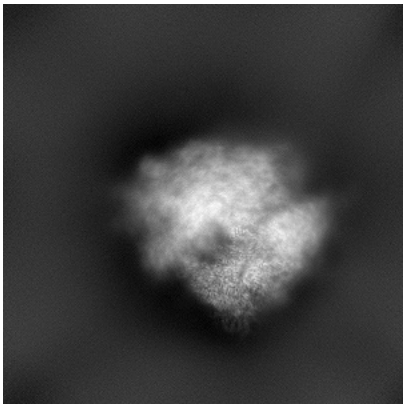


Y

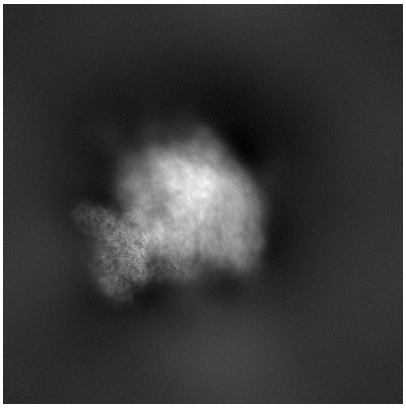


Z

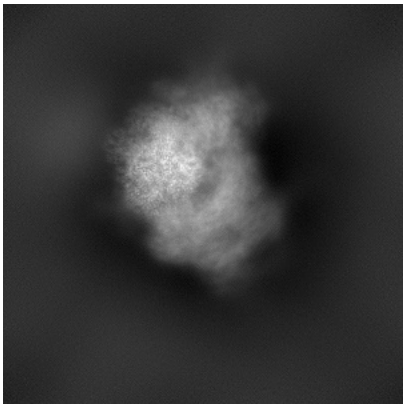
6.1.2 Raw map



X



Y

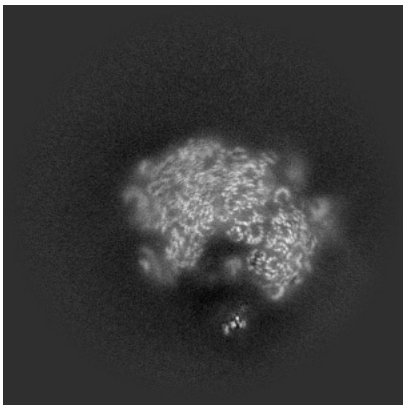


Z

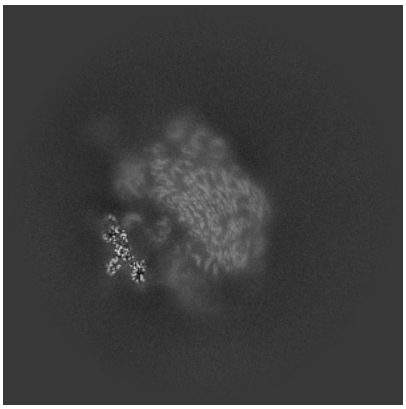
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

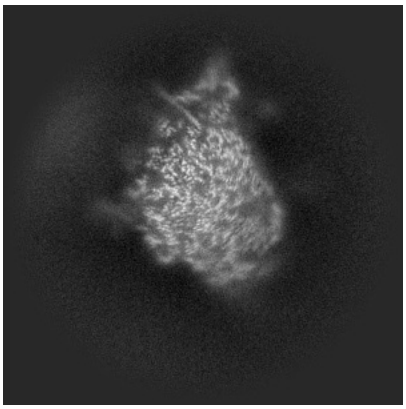
6.2.1 Primary map



X Index: 256

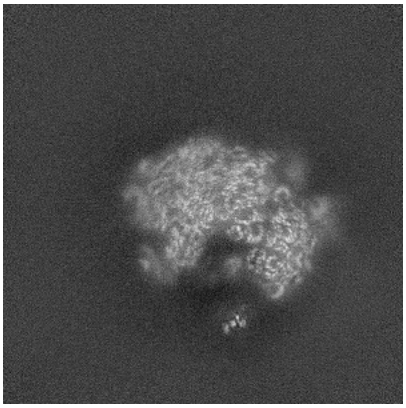


Y Index: 256

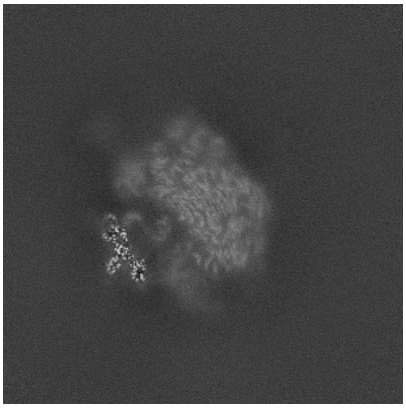


Z Index: 256

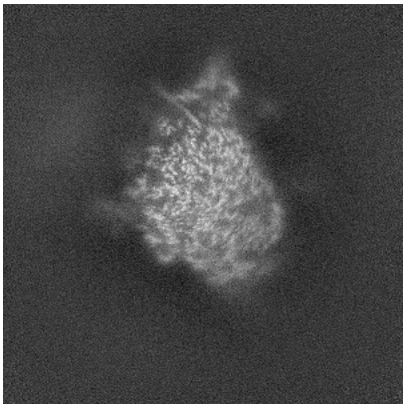
6.2.2 Raw map



X Index: 256



Y Index: 256

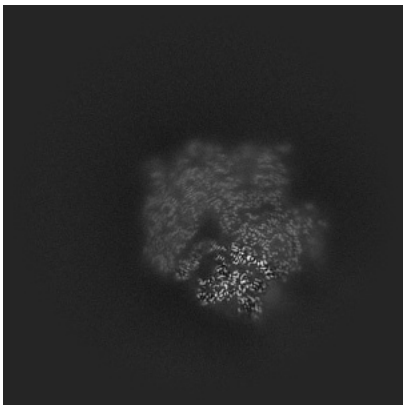


Z Index: 256

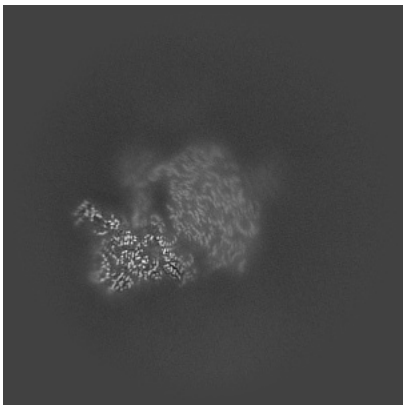
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

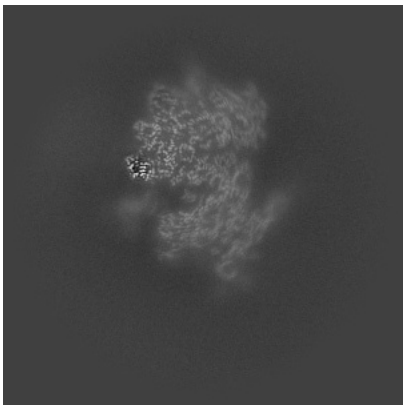
6.3.1 Primary map



X Index: 214

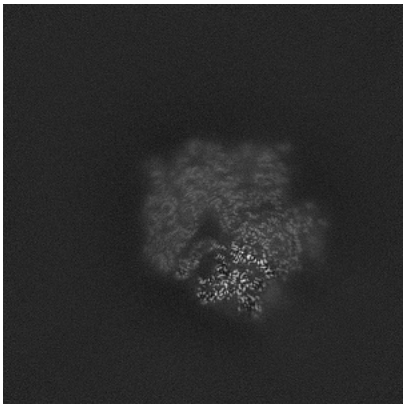


Y Index: 296

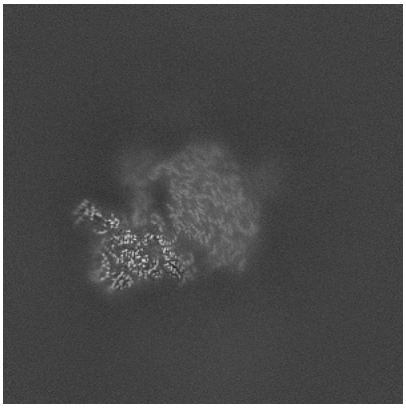


Z Index: 219

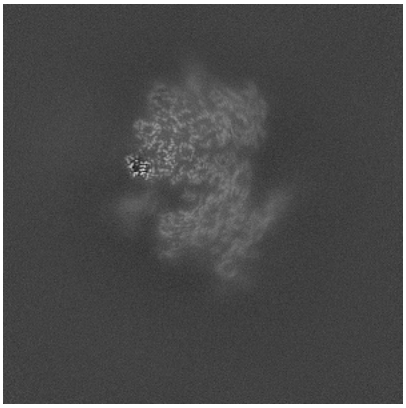
6.3.2 Raw map



X Index: 214



Y Index: 296

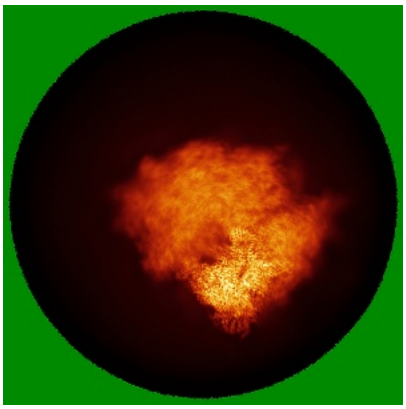


Z Index: 219

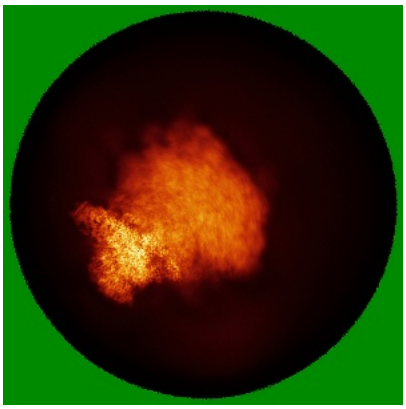
The images above show the largest variance slices of the map in three orthogonal directions.

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

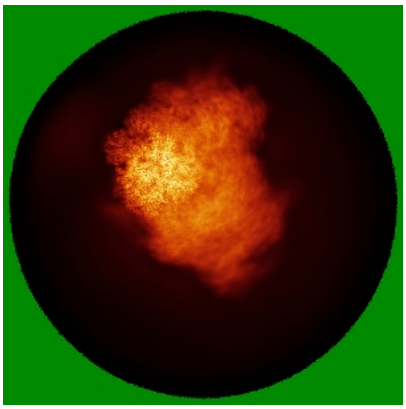
6.4.1 Primary map



X

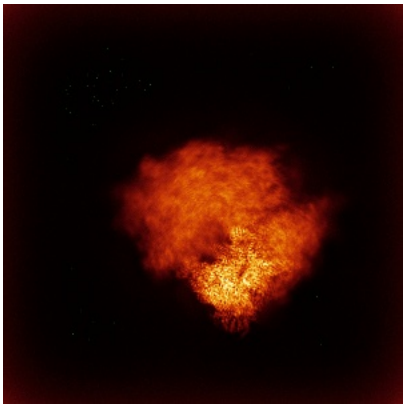


Y

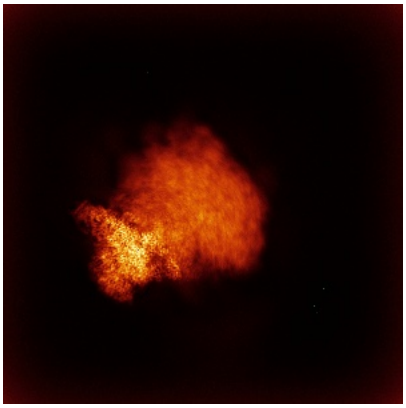


Z

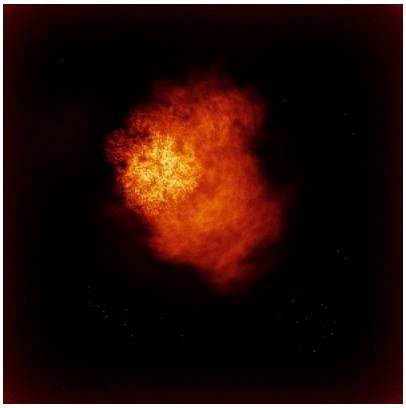
6.4.2 Raw map



X



Y

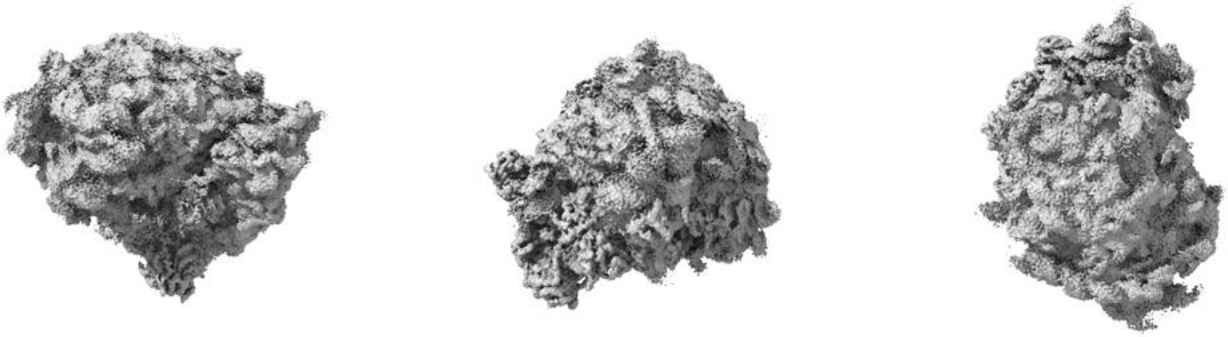


Z

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 0.0146. 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.

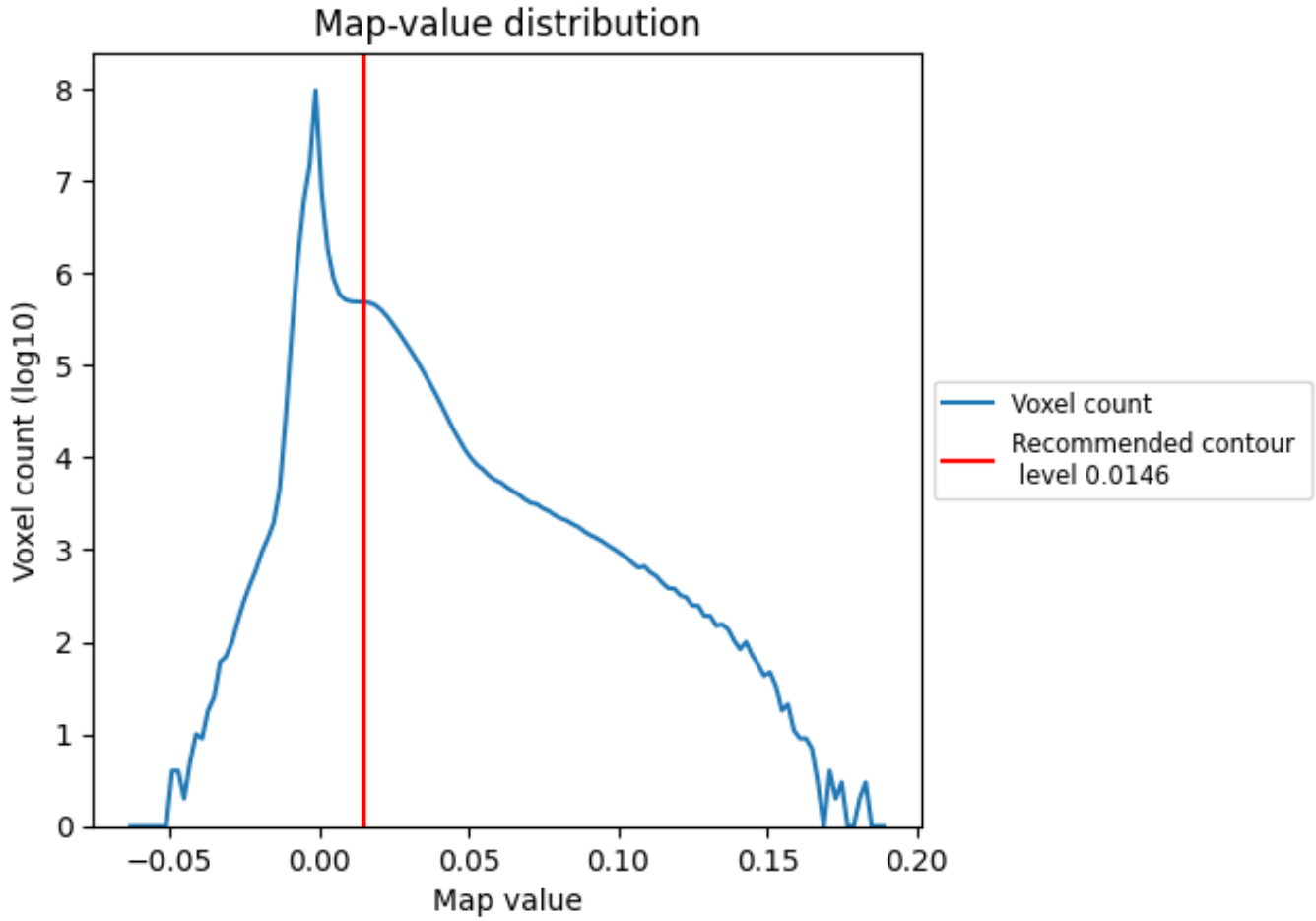
6.6 Mask visualisation (i)

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

7 Map analysis

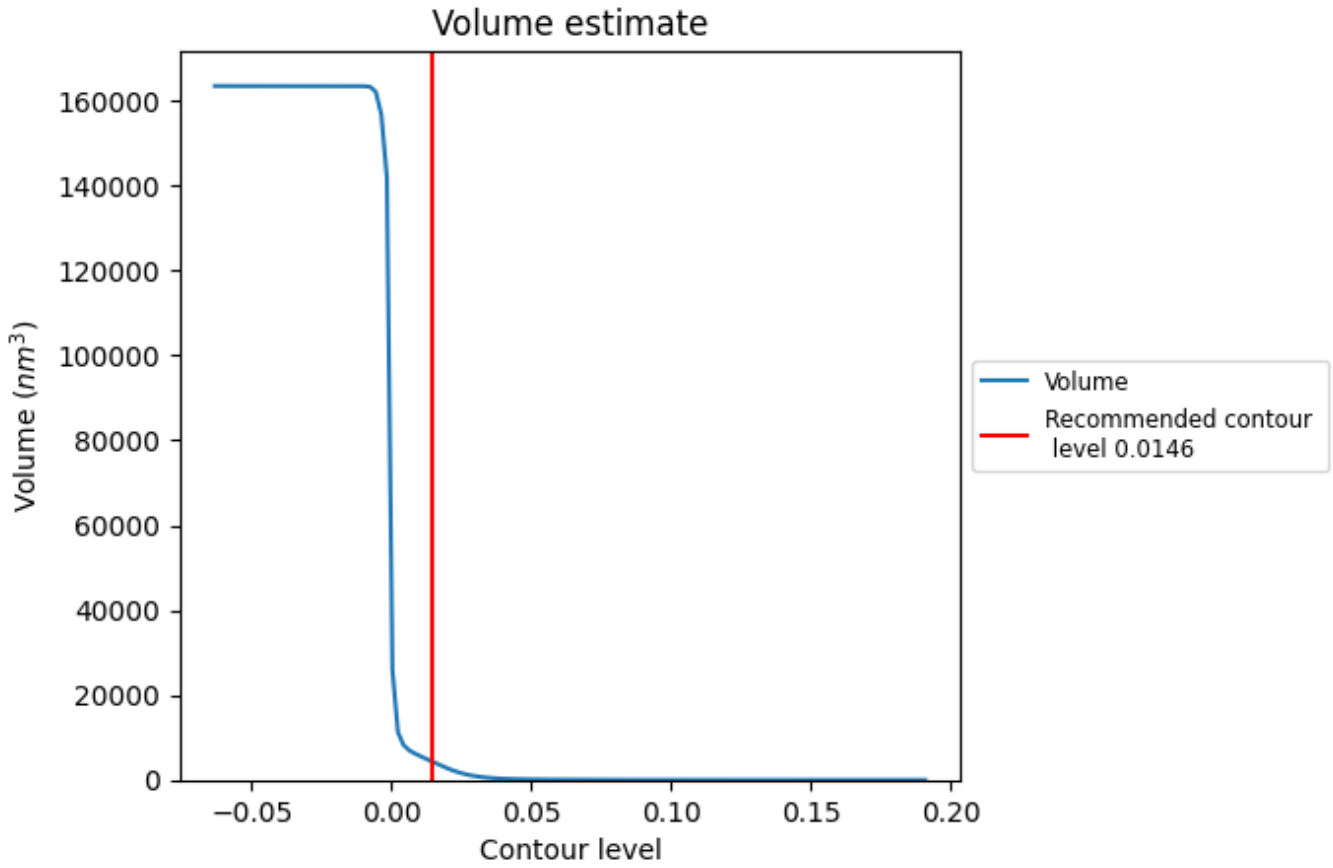
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

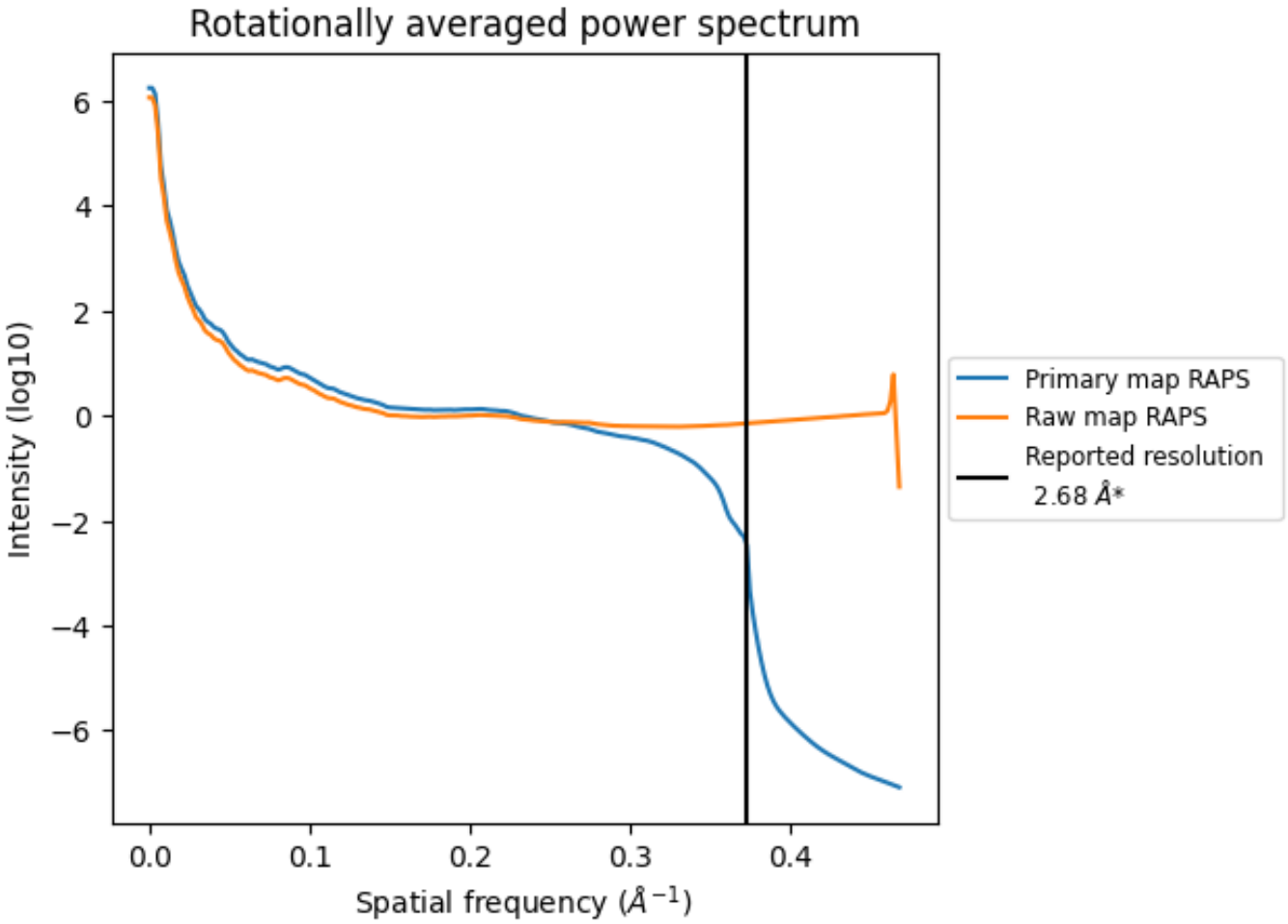
7.2 Volume estimate



The volume at the recommended contour level is 4308 nm^3; this corresponds to an approximate mass of 3891 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)

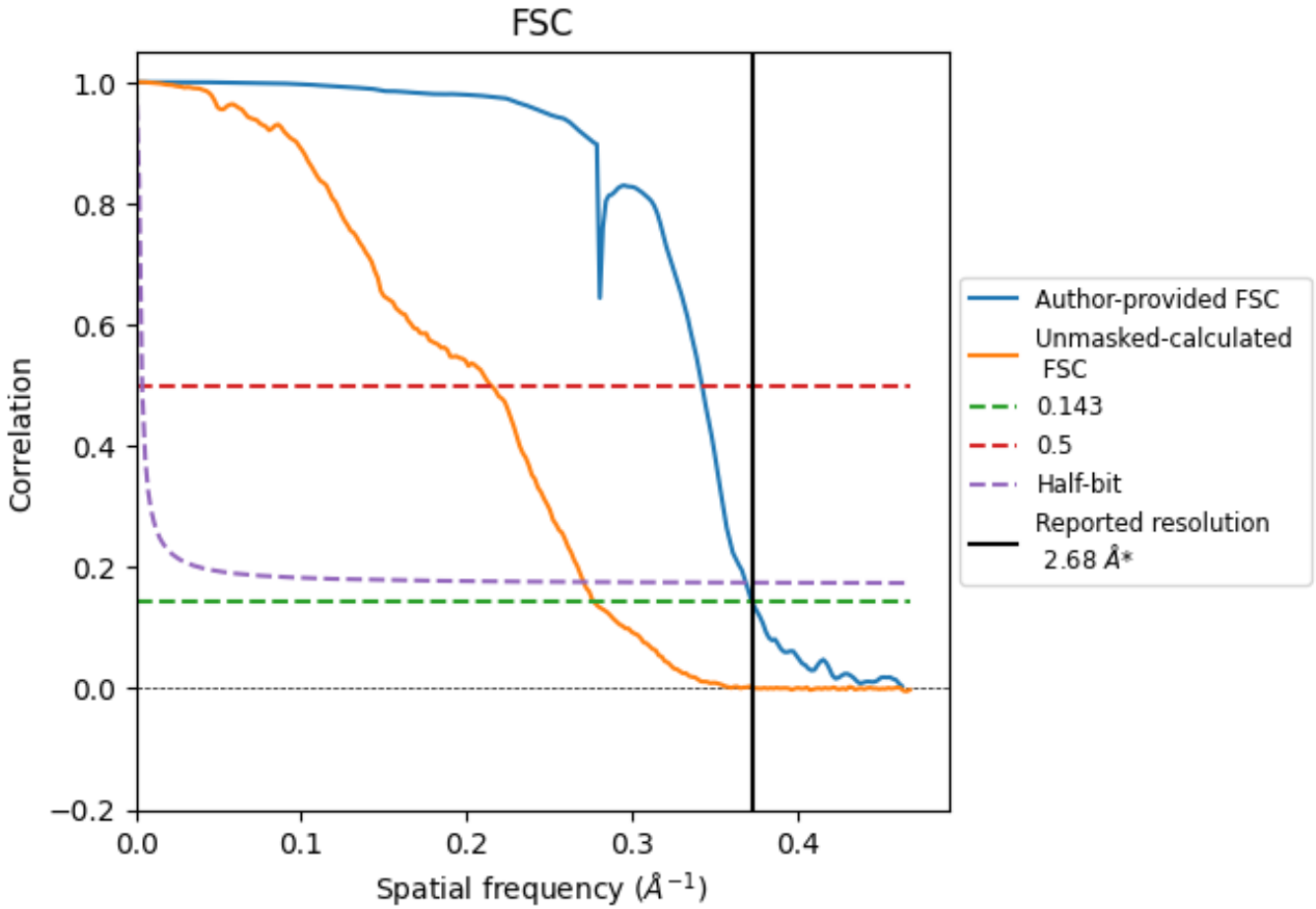


*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8.2 Resolution estimates (i)

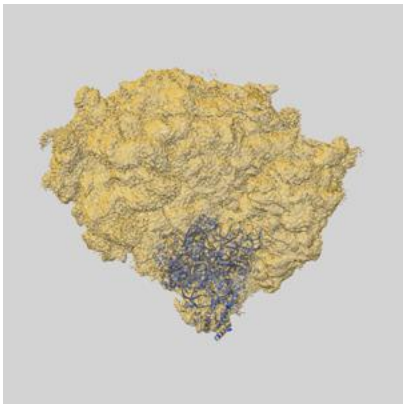
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	2.92	2.71
Unmasked-calculated*	3.61	4.66	3.69

*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 3.61 differs from the reported value 2.68 by more than 10 %

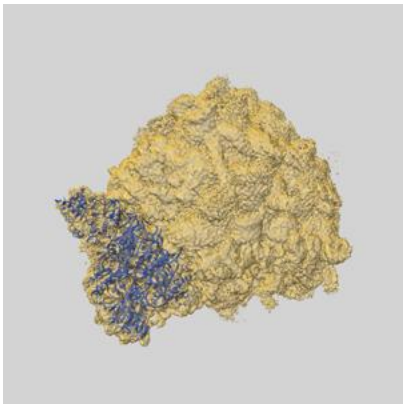
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44016 and PDB model 9AZM. Per-residue inclusion information can be found in section 3 on page 7.

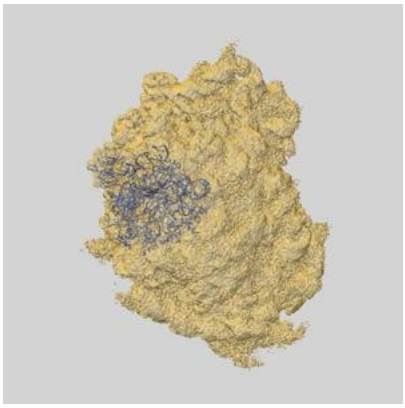
9.1 Map-model overlay



X



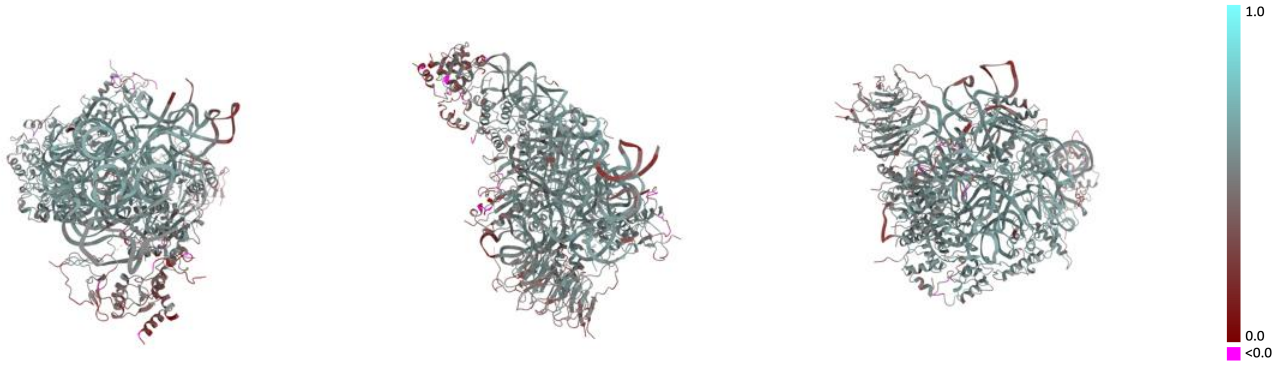
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0146 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.

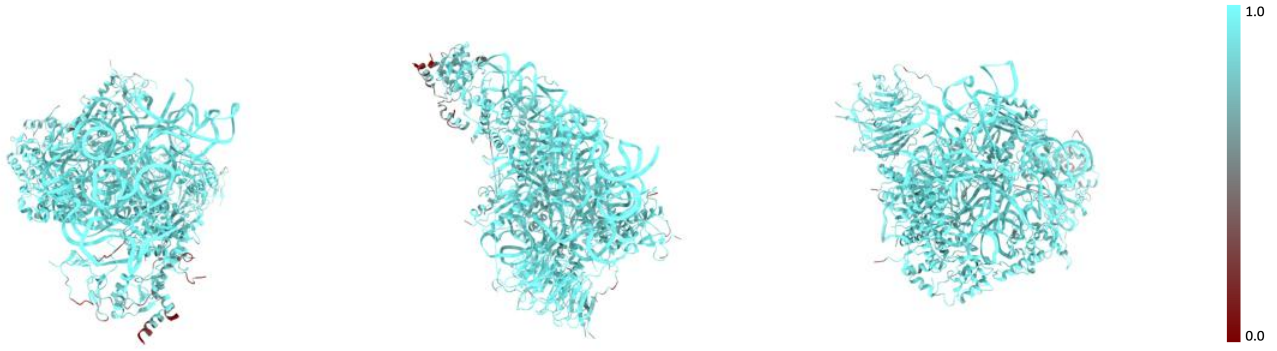
9.2 Q-score mapped to coordinate model (i)



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.

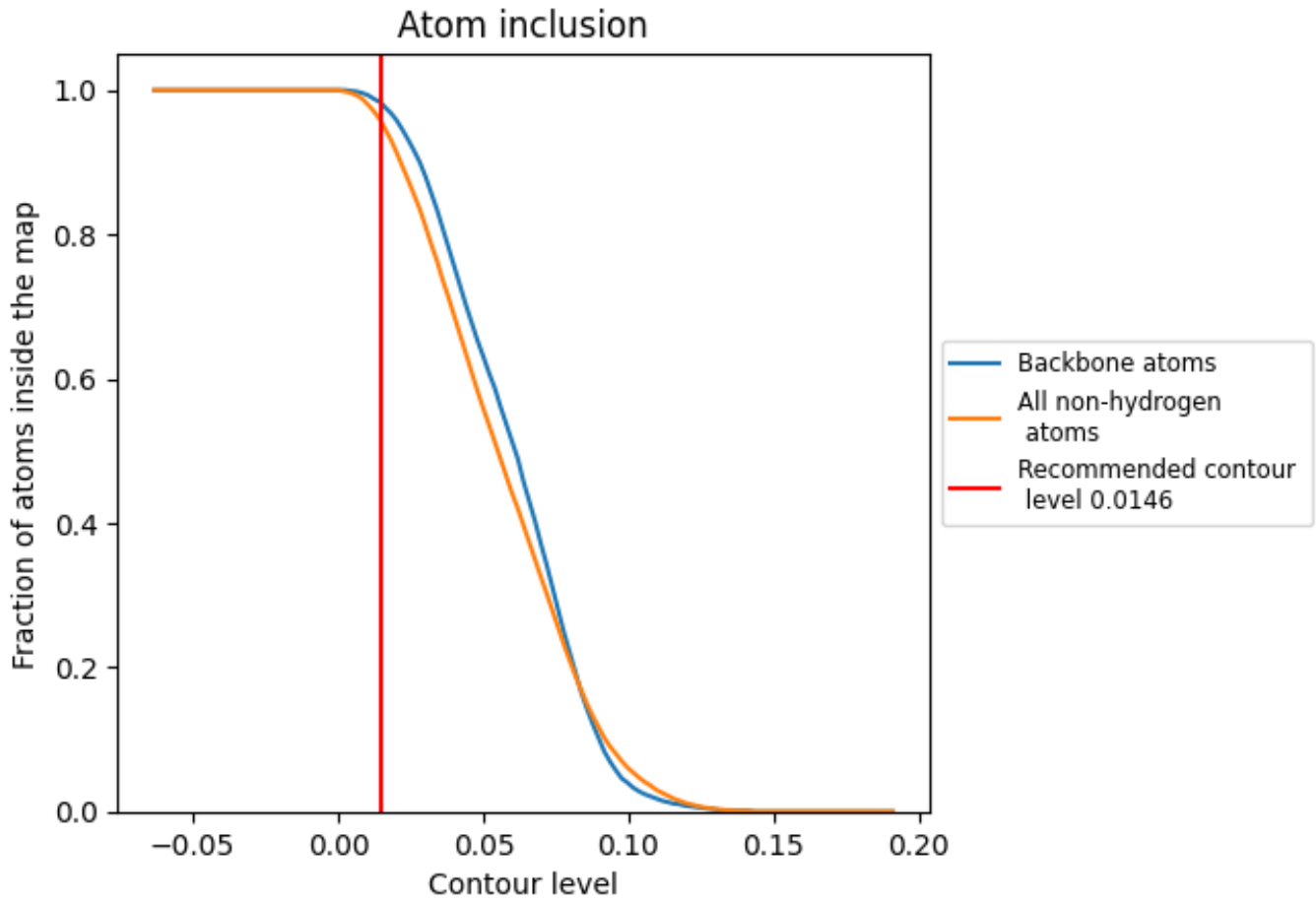
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0146).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.0146) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.5080
CD	0.6770	0.3080
S2	0.9960	0.5520
SD	0.9650	0.4840
SF	0.9760	0.5170
SK	0.9620	0.5170
SM	0.7570	0.3320
SP	0.9750	0.5500
SQ	0.9770	0.5260
SS	0.9650	0.5370
ST	0.9760	0.5340
SU	0.9540	0.4540
SZ	0.9000	0.4790
Sc	0.9240	0.4270
Sd	0.9960	0.5660
Sf	0.9020	0.4000
Sg	0.9320	0.4540