W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Apr 21, 2025 – 12:12 PM EDT

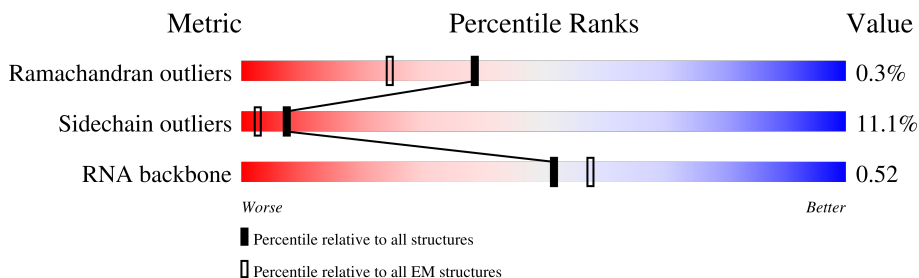|		
PDB ID	:	9AZM / pdb_00009azm
EMDB ID	:	EMD-44016
Title	:	In situ human ribosome (Focused on 40S with SERBP1 CTD)
Authors	:	Wei, Z.; Yong, Z.
Deposited on	:	2024-03-11
Resolution	:	2.68 Å(reported)

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 2.68 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.
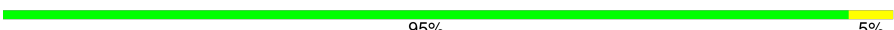
Metric	Percentile Ranks	Value
Ramachandran outliers		0.3%
Sidechain outliers		11.1%
RNA backbone		0.52

Worse   *Better*

▮ Percentile relative to all structures

▯ Percentile relative to all EM structures

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	90% 10%
10	Sc	64	84% 16%
11	Sd	55	95% 5%
12	Sg	313	89% 11%
13	SM	122	12% 85% 14%
14	SZ	75	88% 12%
15	Sf	67	82% 16%
16	S2	1740	21% 7% 72%

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 1198	C 751	N 242	O 203	S 2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

3 Residue-property plots ⓘ

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.
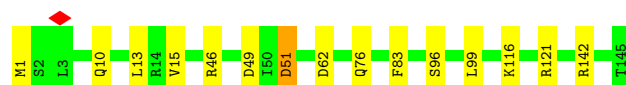
- Molecule 1: Serbp1

Chain CD:
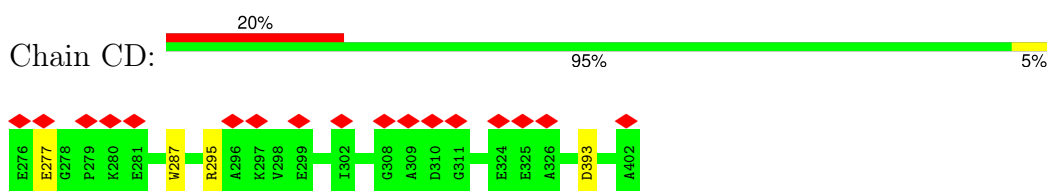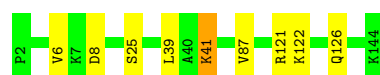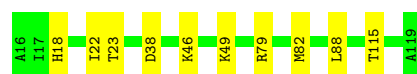
- Molecule 2: Small ribosomal subunit protein uS3
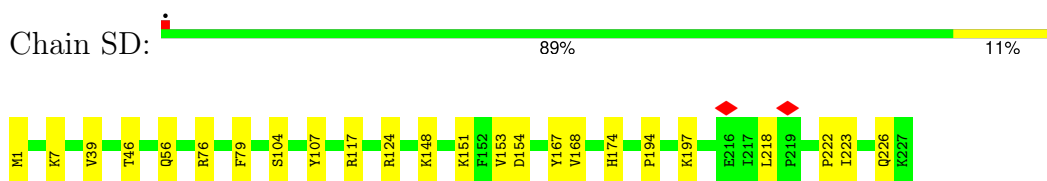
Chain SD:

- Molecule 3: 40S ribosomal protein S5
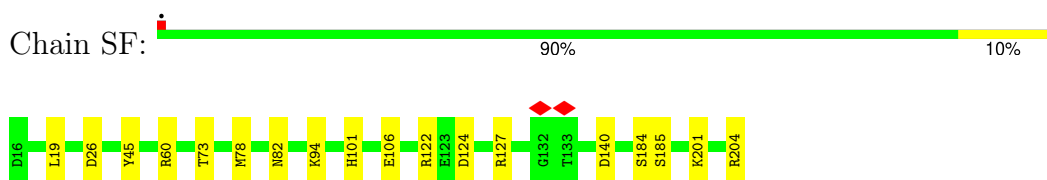
Chain SF:

- Molecule 4: 40S ribosomal protein S10
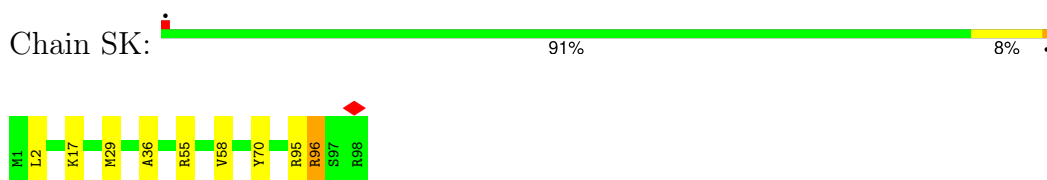
Chain SK:

- Molecule 5: Small ribosomal subunit protein uS19

Chain SP:

• Molecule 6: Small ribosomal subunit protein uS9

Chain SQ:

86%   13%

S3 V10 K17 K26 R27 R37 M41 I42 E43 Y49 L52 L57 D67 V70 Q97 E107 D110 Q114 R125 K131 R138 Y145 R146

• Molecule 7: 40S ribosomal protein S18

Chain SS:

90%   10%

M1 S2 L3 Q10 L13 R14 V15 R46 D49 I50 D51 D62 Q76 F83 S96 L99 K116 R121 R142 T145

• Molecule 8: 40S ribosomal protein S19

Chain ST:

94%   6%

P2 V6 K7 D8 S25 L39 A40 K41 V87 R121 K122 Q126 K144

• Molecule 9: 40S ribosomal protein S20

Chain SU:

90%   10%

A16 I17 H18 I22 T23 D38 K46 K49 R79 M82 L88 T115 A119

• Molecule 10: 40S ribosomal protein S28

Chain Sc:

84%   16%

R5 V6 Q7 V30 E33 F34 M35 D36 R40 S41 V46 S61 R66 R67 L68

• Molecule 11: 40S ribosomal protein S29

Chain Sd:

95%   5%

G2 W8 M38 D56

• Molecule 12: Receptor of activated protein C kinase 1

Chain Sg:

89%   11%

T2 H14 Q26 L32 K38 Y52 H62 S63 H64 F65 R99 R100 D107 F113 R125 C138 K139 Y140 D144 H147 W150 V151 S152 C153 S160 C168 L179 C182 C207 M217 N222 E223 I236 C240 I275 S276

T297 N305 V309 I314

• Molecule 13: Small ribosomal subunit protein eS12

Chain SM:

12%

85% 14%

V11 M12 D13 E20 V21 L22 K23 K44 R45 M60 Y61 V62 K63 E66 E71 D81 C92 K93 I94 D95 R96 E97 G98 K99 P100 R101 V104 S118 K121 Y127 F128 K129 C130 K131 K132

• Molecule 14: Small ribosomal subunit protein eS25

Chain SZ:

88% 12%

R41 N46 F50 D51 K52 K60 K66 R76 L77 K78 L96 I97 K98 K114 G115

• Molecule 15: Ubiquitin-40S ribosomal protein S27a

Chain Sf:

82% 16%

Y85 K89 L103 E110 N111 G112 K113 C121 E125 R138 C141 C145 L146 C149 F150 N151

• Molecule 16: 18S rRNA

Chain S2:

21% 7% 72%

C C C G A A G C G U U U A C U U U G A A A A A U U A G A G U C G U C A A A G A C A G G C C C G A G C C C G C C U G G A U A

C C C G A G C U A G G A A U A A U G A C U A G G A C C C G C G G U C U A U U U G U U U G U U U C G U U U U G A A C U G A G

G C C A U G A U U A A G A U G G A C G G C C C G G G U G C A U U C G U A U U C G C G C C C C U A G A G G U G A A A U U C U U

G G A C C G G C G C A A G A C C G A C C A G A G C C A A A G C C A U U U C G U A A C G A A U G U U U U C A U U A A U C A A G

A A C G A A A A G U C C G A G G U U C G A A A G A C C G A U C A G A U A C C G U C G U A G U U C C G A C C A U A A A C G A U G

C C G A C C G G C G A U G C G G C G G C G U U A U U C C C A U U G A C C C G C C G G C A G C U U C C G G G A A A C C A A

A G U U U U G G G G U U C C G G G G G G A G U A G U A U G G U G C A A A G C U G A A A C U U A A A G G A A U U G A C G G A A

G G1211 G1212 C1215 C1216 A1217 A1220 G1224 G1227 C1237 U1242 U1243 A1251 C1252 A1253 G1256 G1257 A1258 A1259 U1263 C1264 G1274 G1275 C1283 G1286 A1293 G1294 A1295 A1301 G1302 C1303 U1306 U1307 U1308 G1312 G1320 U1342 G1354 U1364

U1371 U1372 C1373 A1376 U1377 A1378 A1401 A1402 G1406 G1411 A1414 C1415 C1416 C1417 C1418 C1419 G1420 A1421 G1422 C1423 C1433 C1434 C1435 C1436 C1437 A1438 U1442 G1449 C1453 A1454 U1463 U1478 A1487 C1488 A1489 G1490 U1494 G1495 U1496 G1497 A1498 A1508 G1520 C1521 A1522

A1533 C1534 U1535 G1536 A1537 C1544 C1552 G1552 U1555 A1556 C1557 C1558 G1570 C1574 U1578 A1579 A1580 C1581 C1582 C1583 G1584 U1585 U1586 G1587 A1588 G1600 A1601 G1604 G1605 G1606 U1621 U1622 A1623 C1629 A1633 A1634 A1637 G1638 G1639 A1640 G1648 G1654 A1663 A1664 G1665

G1671 G1680 U1690 U1691 U1692 G1693 U A C C A C C C G C C C G G U C G C U A C C G A U U G G A U G G U U U A G U G A G G C C C U C C G G

A U C G G C C C C C C G G G U C G C C C A C C G G C C U G G C G G A A C G G C U C G G U U C C G G A A C C U U

G A C U A U C U A G A G G A A G U A U A A A A G U C G G A A C A A G U U U C C G U A G G U G A A C C U G C G G A A G G A U

C A U A

4 Experimental information ⓘ

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 $(e^-/\text{Å}^2)$	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 (i)

5.1   Standard geometry (i)

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.

The worst 5 of 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

There are no chirality outliers.

5 of 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

5.2   Too-close contacts ⓘ

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

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 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

5.3.2　Protein sidechains ⓘ

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

5 of 186 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	Sd	8	TRP
12	Sg	217	MET
12	Sg	26	GLN
12	Sg	125	ARG
12	Sg	309	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
12	Sg	285	GLN
14	SZ	45	ASN
15	Sf	151	ASN
9	SU	92	HIS
12	Sg	62	HIS

5.3.3   RNA ⓘ

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

5 of 111 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	S2	1212	G
16	S2	1215	C

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Mol	Chain	Res	Type
16	S2	1216	C
16	S2	1217	A
16	S2	1220	A

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 ⓘ

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 ⓘ
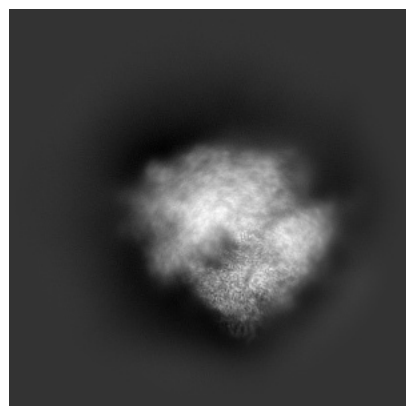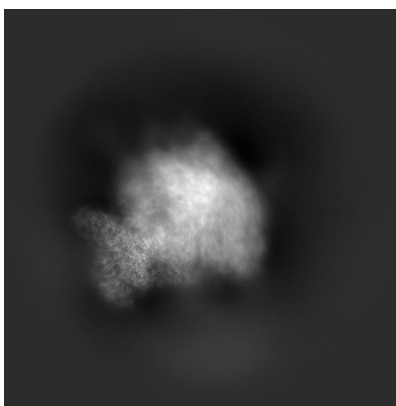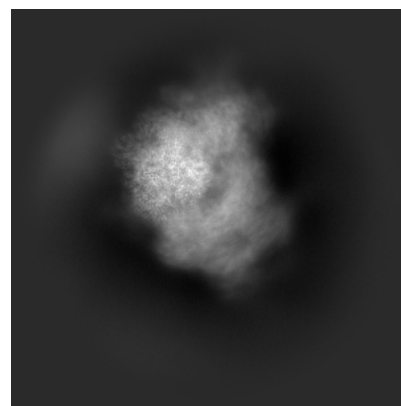
6.1.1 Primary map

| X | Y | Z |

6.1.2 Raw map

| X | Y | Z |
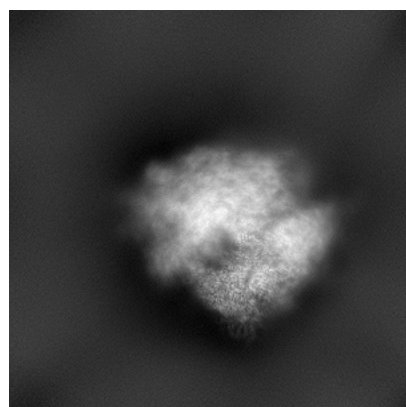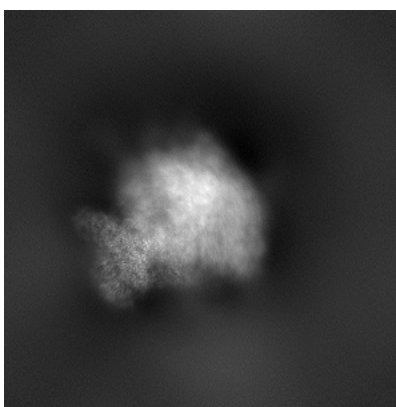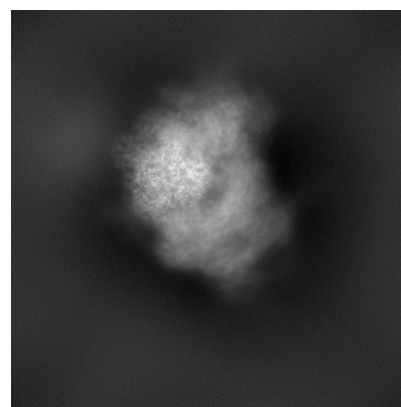
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ
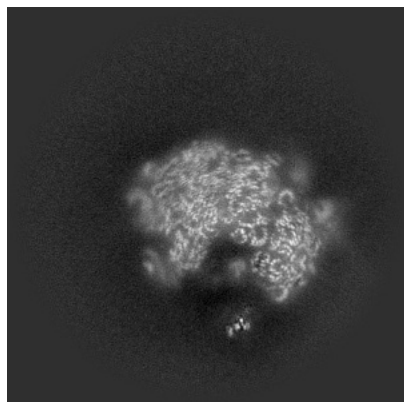
6.2.1 Primary map
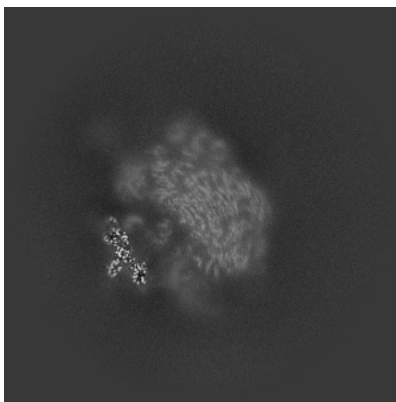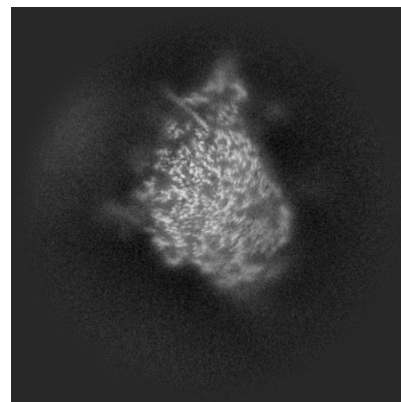
X Index: 256   Y Index: 256   Z Index: 256

6.2.2 Raw map
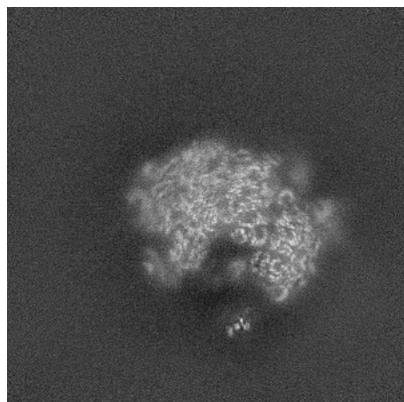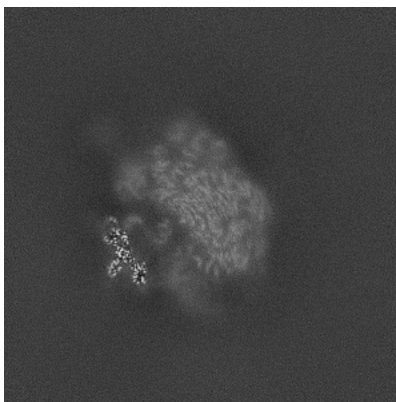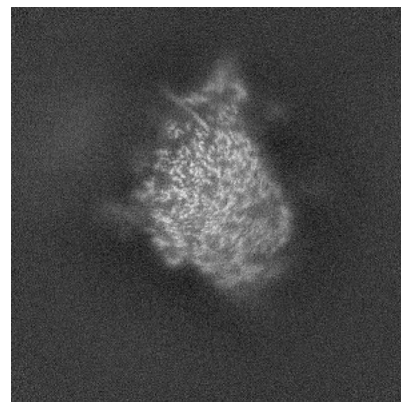
X Index: 256   Y Index: 256   Z Index: 256

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map
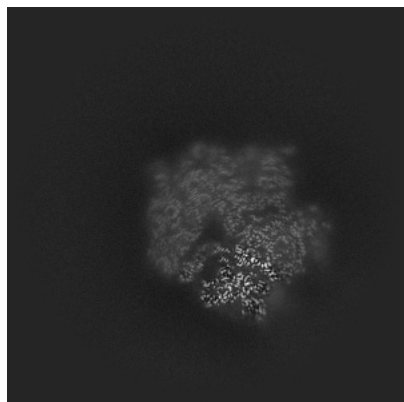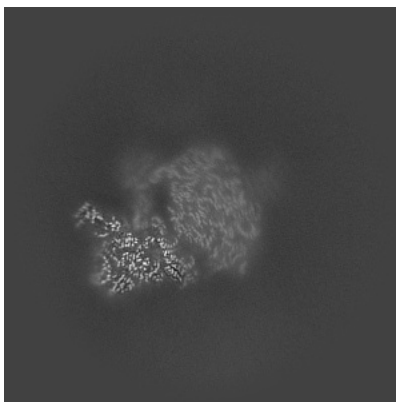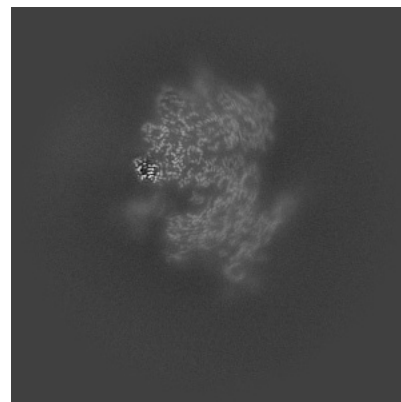
| X Index: 214 | Y Index: 296 | Z Index: 219 |

6.3.2 Raw map
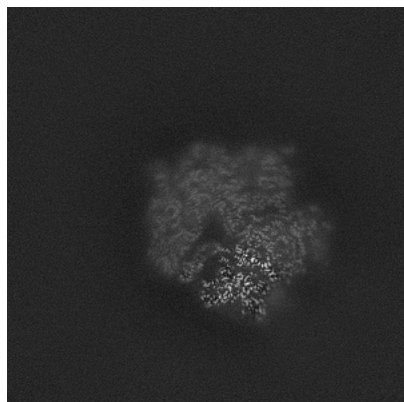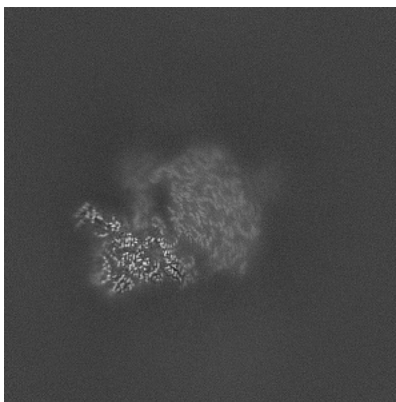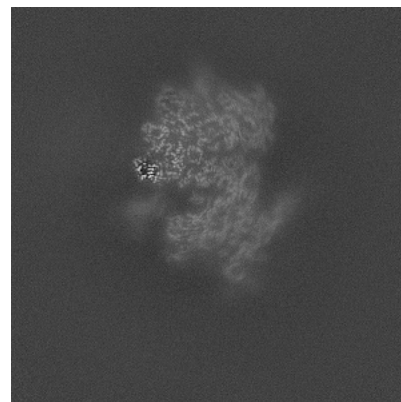
| X Index: 214 | Y Index: 296 | Z Index: 219 |

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

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

6.4.1   Primary map
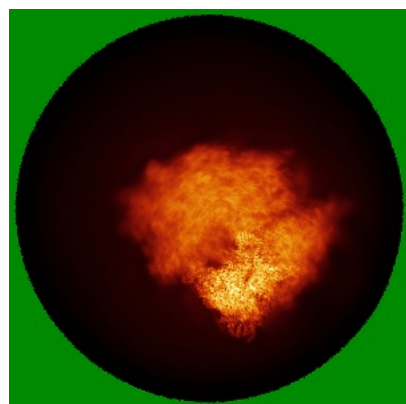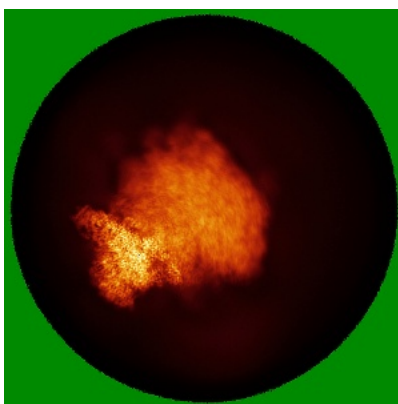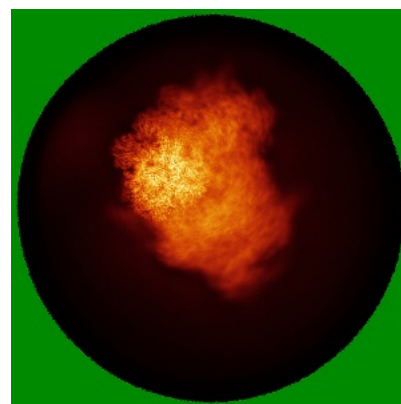
X   Y   Z

6.4.2   Raw map

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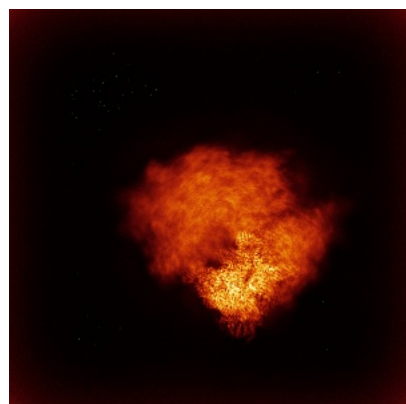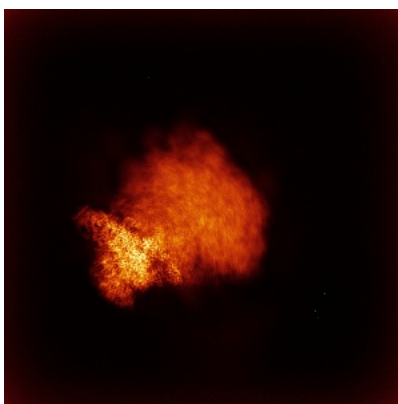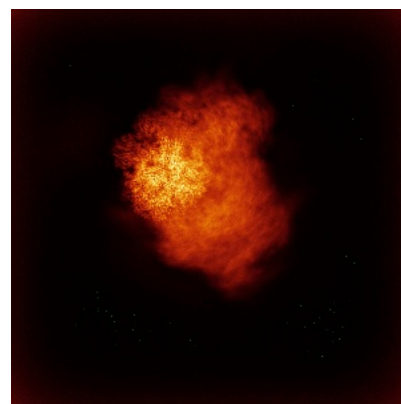
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

| X | Y | Z |
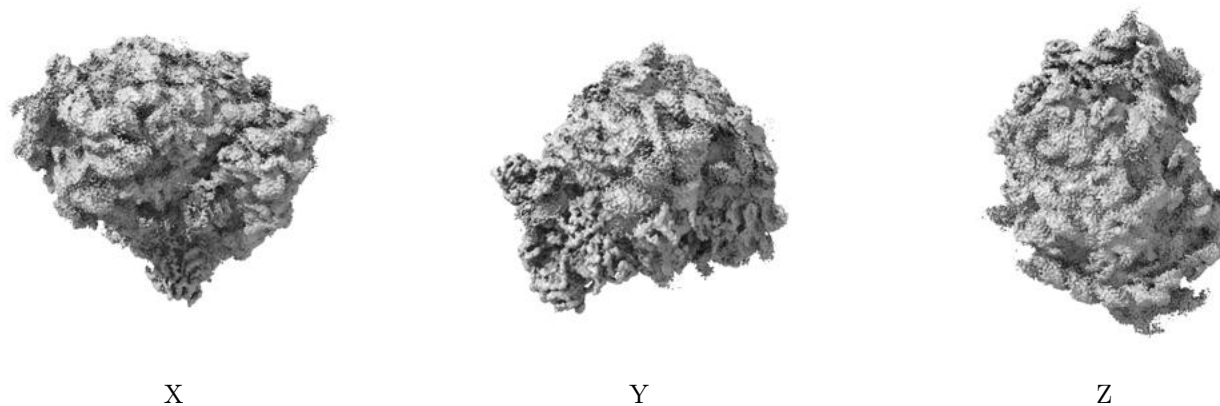
The images above show the 3D surface view of the map at the recommended contour level 0.0146. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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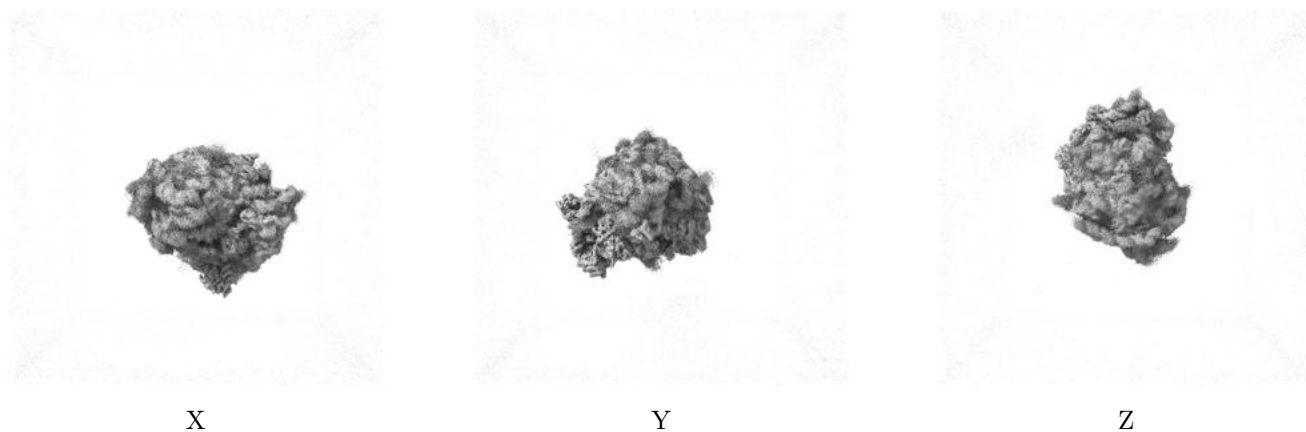
These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

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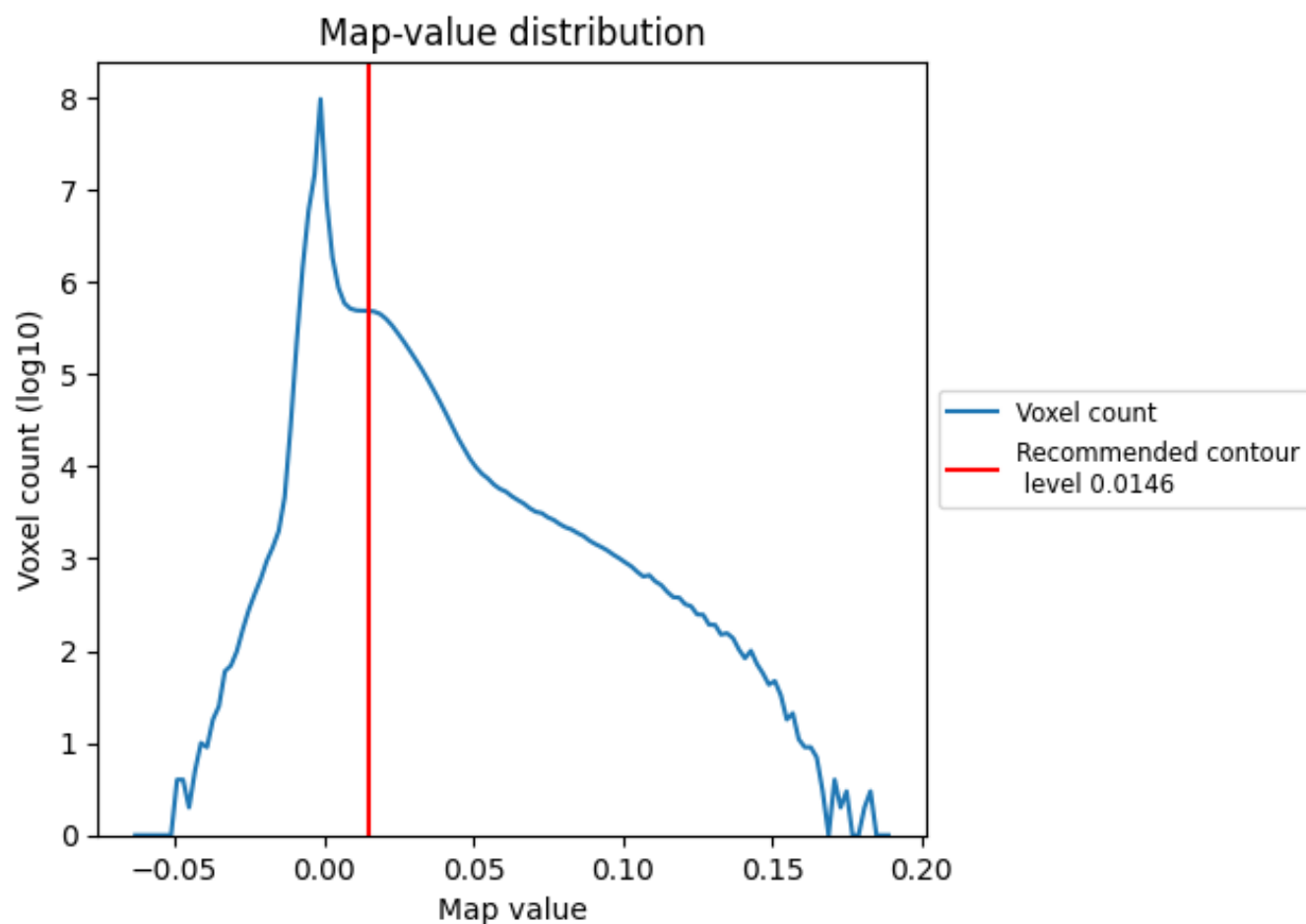
The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2　Volume estimate　ⓘ
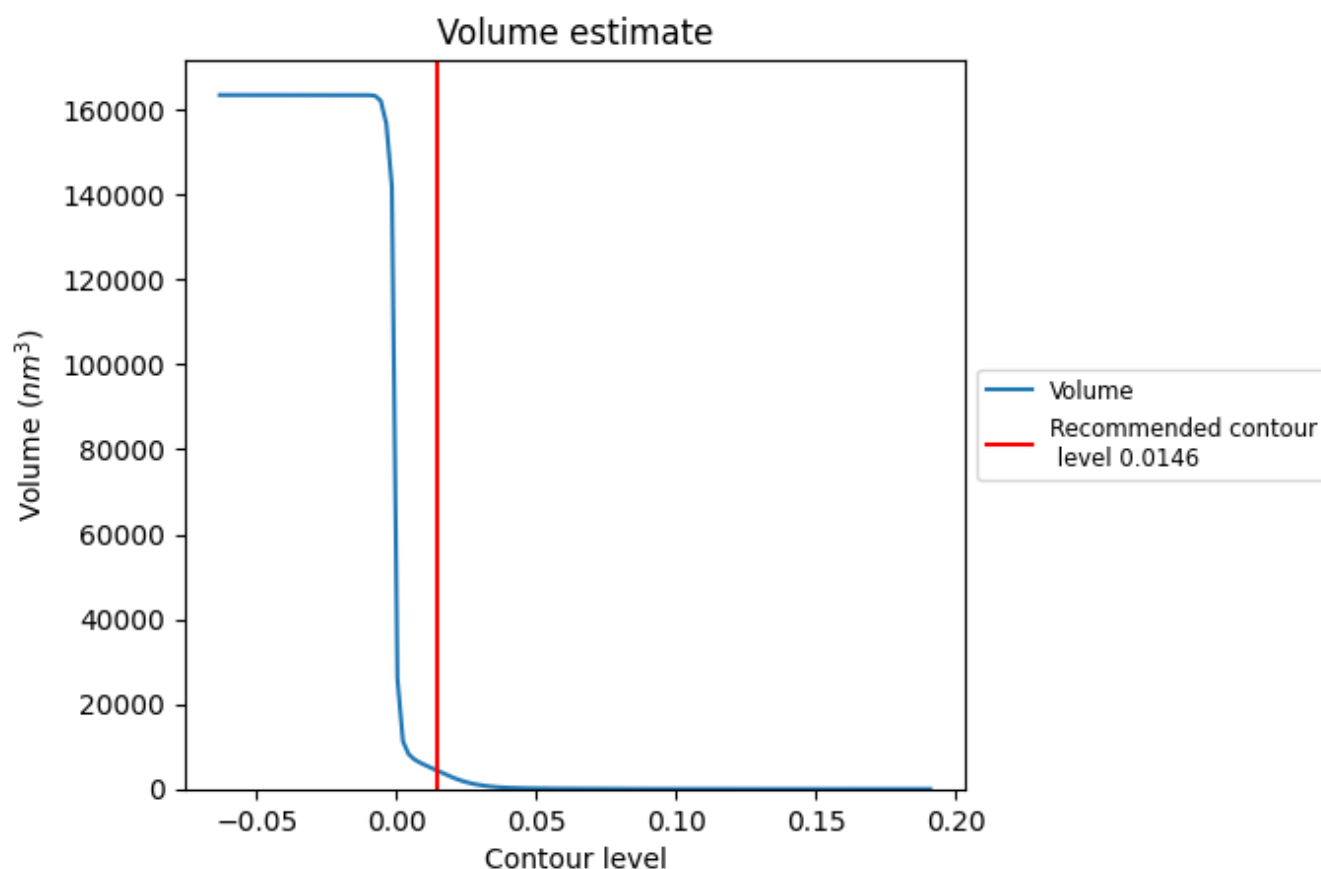
The volume at the recommended contour level is 4308 nm^3; this corresponds to an approximate mass of 3891 kDa.

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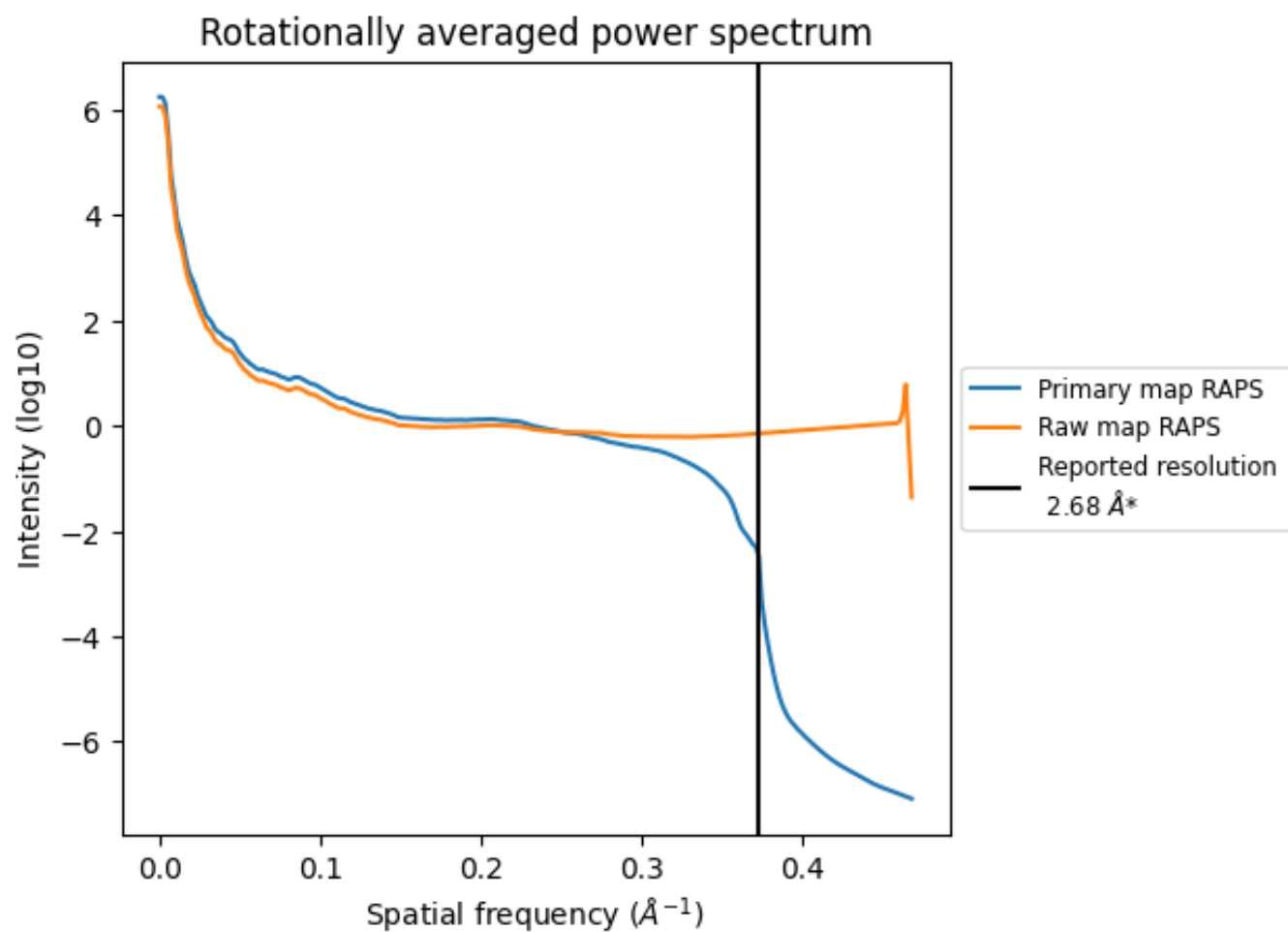
*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

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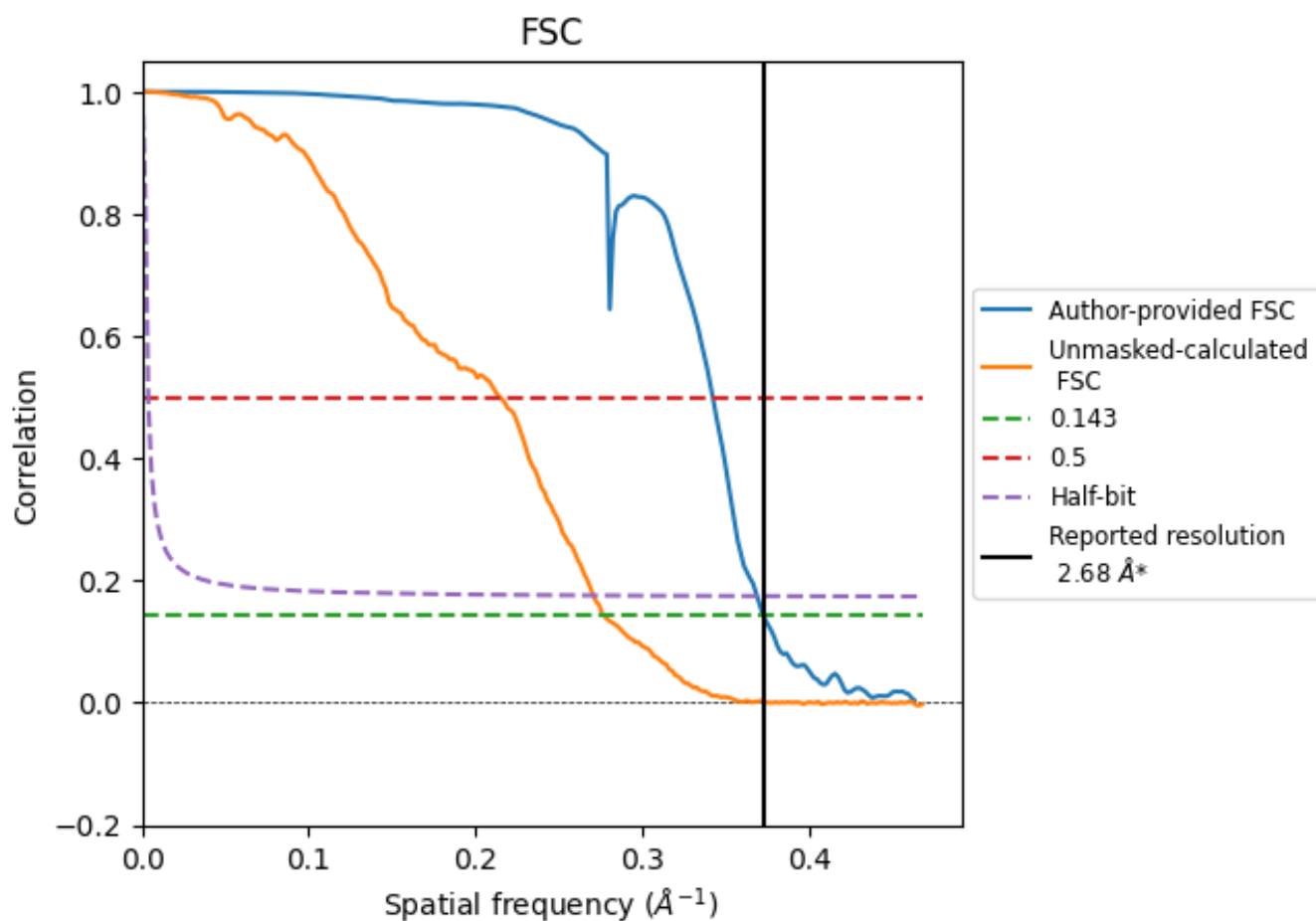
*Reported resolution corresponds to spatial frequency of 0.373 Å^{-1}

8.2 Resolution estimates ⓘ

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 ⓘ
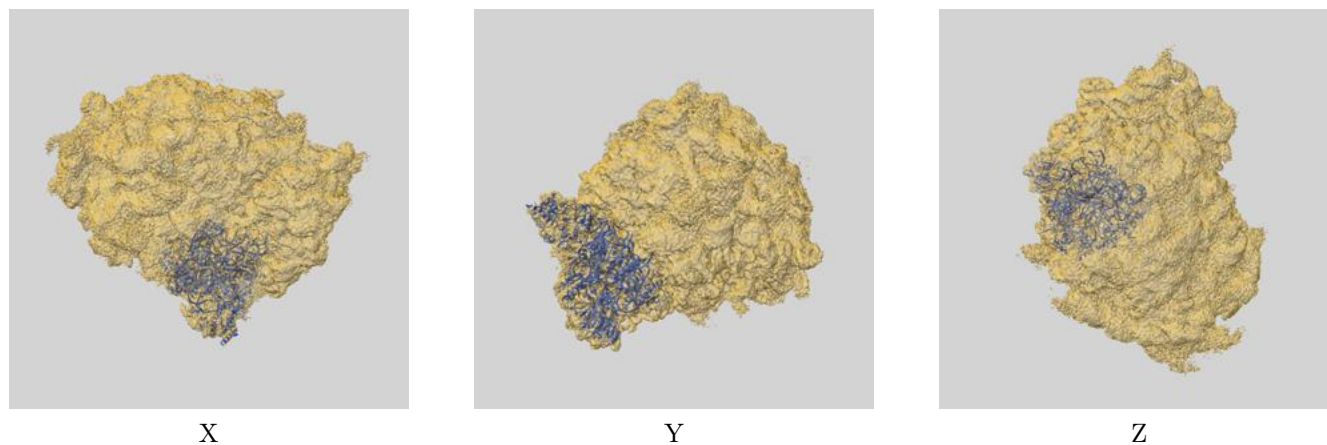
X

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)
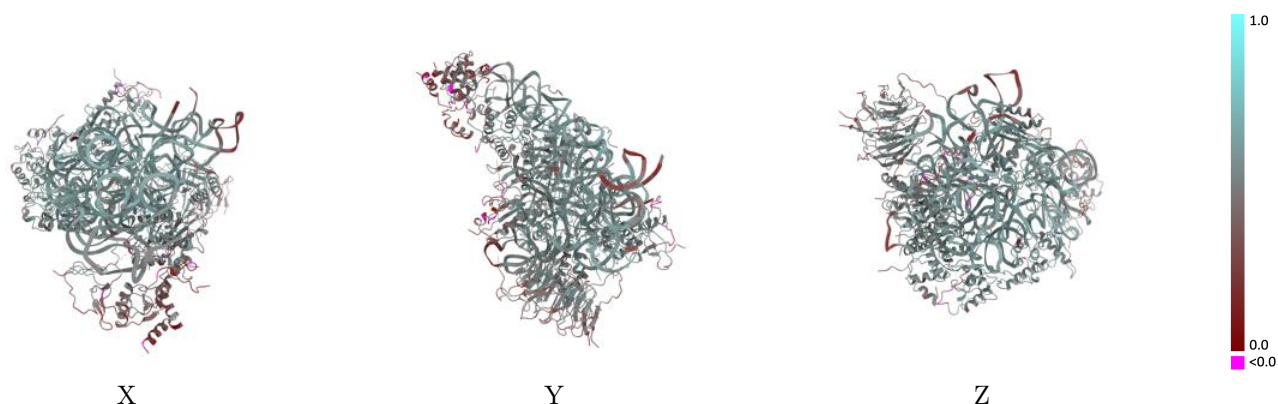
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)
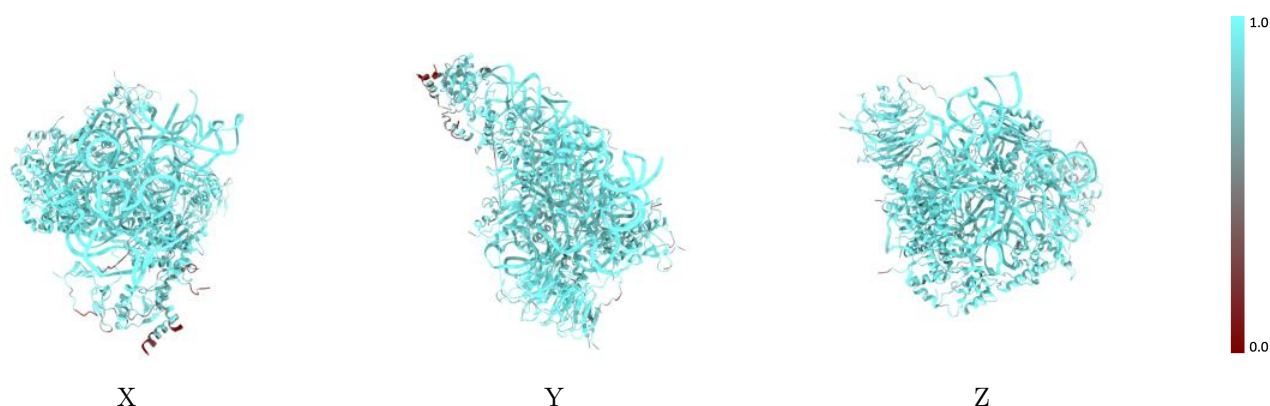
The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0146).

9.4 Atom inclusion ⓘ
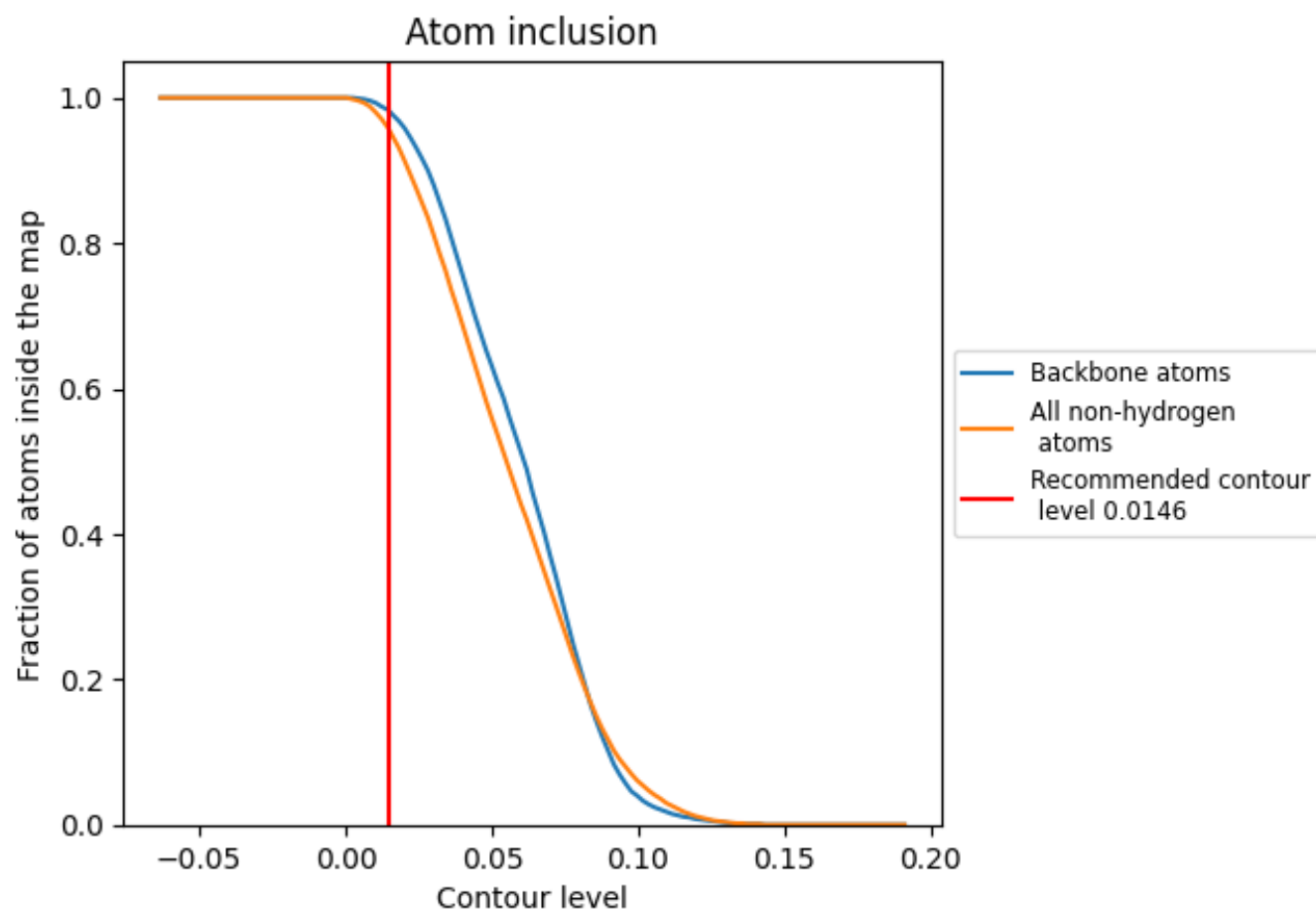
At the recommended contour level, 98% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

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

1.0

0.0
<0.0