Full wwPDB EM Validation Report ⓘ

May 7, 2024 – 02:52 pm BST

PDB ID	:	8R6W
EMDB ID	:	EMD-18967
Title	:	Structure of the SFTSV L protein in a transcription-priming state with bound capped RNA [TRANSCRIPTION-PRIMING]
Authors	:	Williams, H.M.; Thorkelsson, S.R.; Vogel, D.; Busch, C.; Milewski, M.; Cusack, S.; Grunewald, K.; Quemin, E.R.J.; Rosenthal, M.
Deposited on	:	2023-11-23
Resolution	:	3.35 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:

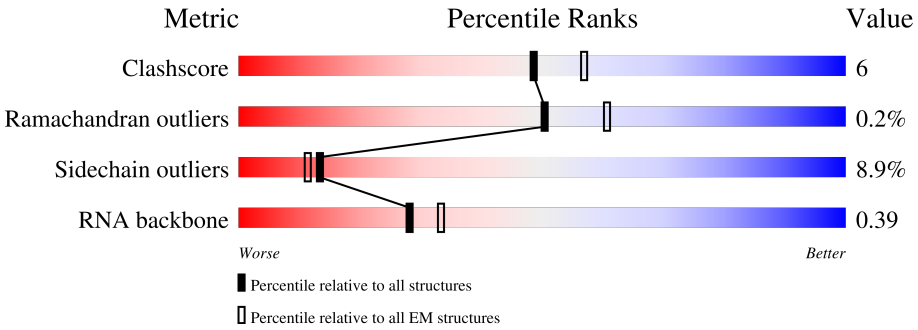
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.35 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	2084	75% 17% · 5%
2	G	16	25% 75%
3	P	20	40% 35% 5% 20%
4	T	26	15% 12% 35% · 35%
5	C	18	17% 6% 78%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16539 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 RNA-directed RNA polymerase L.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1974	15661	9922	2724	2920	95	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	112	ALA	ASP	engineered mutation	UNP U3GU88

- Molecule 2 is a RNA chain called RNA (5'-R(*AP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	G	4	81	38	16	24	3	0	0

- Molecule 3 is a RNA chain called RNA (5'-R(*AP*CP*AP*CP*AP*GP*AP*GP*AP*CP*GP*CP*CP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	P	16	341	154	68	104	15	0	0

- Molecule 4 is a RNA chain called RNA (5'-R(P*CP*UP*GP*GP*GP*CP*GP*GP*UP*CP*UP*UP*UP*GP*UP*GP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	T	17	361	160	58	126	17	0	0

- Molecule 5 is a RNA chain called RNA (5'-R(*(M7G)*AP*AP*A)-3').

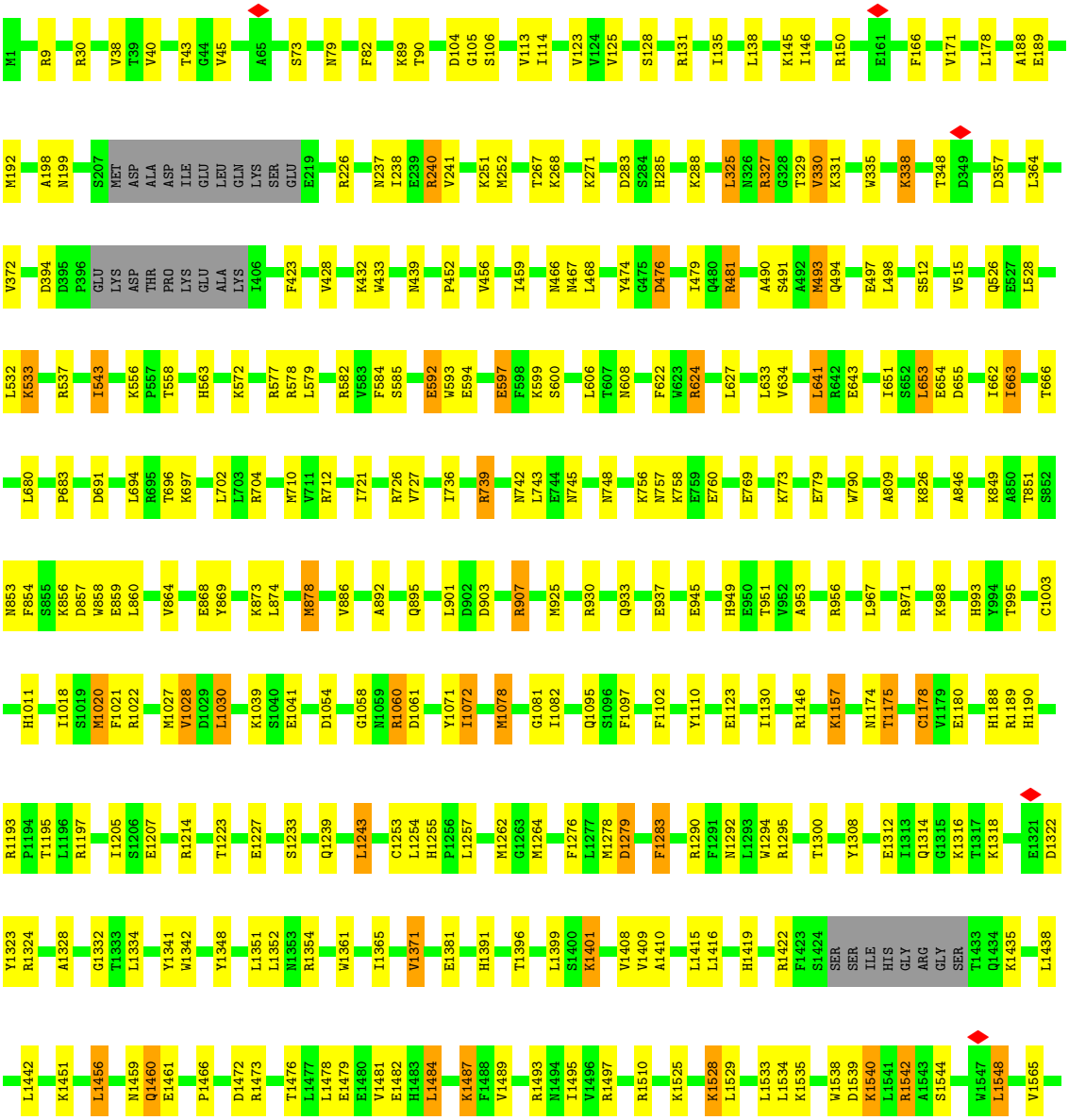
Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	4	Total	C	N	O	P	0	0
			95	41	20	29	5		

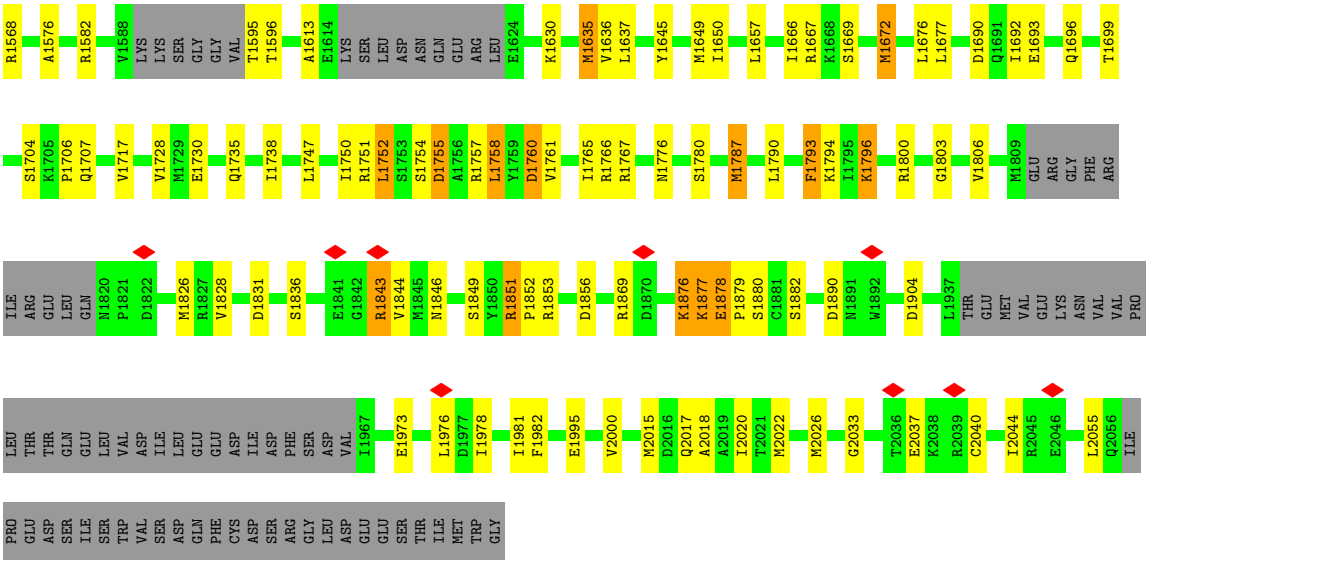
3 Residue-property plots (i)

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: RNA-directed RNA polymerase L

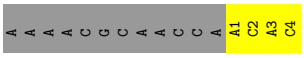
Chain A:





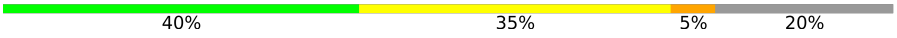
• Molecule 2: RNA (5'-R(*AP*CP*AP*C)-3')

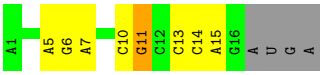
Chain G:



• Molecule 3: RNA (5'-R(*AP*CP*AP*CP*AP*GP*AP*GP*AP*CP*GP*CP*CP*CP*AP*G)-3')

Chain P:





• Molecule 4: RNA (5'-R(P*CP*UP*GP*GP*GP*CP*GP*GP*UP*CP*UP*UP*UP*GP*UP*GP*U)-3')

Chain T:

• Molecule 5: RNA (5'-R(*(M7G)*AP*AP*A)-3')

Chain C:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61698	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.736	Depositor
Minimum map value	-0.235	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	272.0, 272.0, 272.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: M7G

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	A	0.26	0/15980	0.51	0/21562
2	G	0.41	0/90	0.98	0/138
3	P	0.23	0/382	0.79	0/594
4	T	0.34	0/401	1.12	4/623 (0.6%)
5	C	2.40	7/74 (9.5%)	3.95	14/113 (12.4%)
All	All	0.31	7/16927 (0.0%)	0.61	18/23030 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	A	N7-C5	-10.05	1.33	1.39
5	C	2	A	C5-C6	-8.17	1.33	1.41
5	C	2	A	C2-N3	7.18	1.40	1.33
5	C	2	A	C5-C4	-6.88	1.33	1.38
5	C	2	A	N1-C2	6.30	1.40	1.34
5	C	2	A	N9-C4	-6.15	1.34	1.37
5	C	2	A	N9-C8	-5.69	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2	A	N1-C2-N3	-22.26	118.17	129.30
5	C	2	A	C2-N3-C4	19.44	120.32	110.60
5	C	2	A	N7-C8-N9	-10.59	108.50	113.80
5	C	2	A	N3-C4-C5	-9.86	119.90	126.80
5	C	2	A	C5-C6-N6	-9.50	116.10	123.70
5	C	2	A	C5-C6-N1	8.75	122.08	117.70
5	C	2	A	C5-N7-C8	8.25	108.03	103.90
5	C	2	A	C4-C5-C6	8.21	121.11	117.00
5	C	2	A	C3'-C2'-C1'	-6.84	96.03	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	2	A	N3-C4-N9	5.97	132.18	127.40
5	C	2	A	P-O3'-C3'	5.88	126.76	119.70
4	T	20	U	P-O3'-C3'	5.65	126.48	119.70
5	C	2	A	C4-C5-N7	-5.51	107.94	110.70
4	T	19	C	C2-N1-C1'	5.46	124.80	118.80
5	C	2	A	N1-C6-N6	5.37	121.82	118.60
5	C	2	A	N9-C4-C5	5.30	107.92	105.80
4	T	19	C	N1-C2-O2	5.05	121.93	118.90
4	T	19	C	N3-C2-O2	-5.04	118.37	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15661	0	15673	186	0
2	G	81	0	46	4	0
3	P	341	0	178	4	0
4	T	361	0	181	11	0
5	C	95	0	50	2	0
All	All	16539	0	16128	201	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 6.

All (201) 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)
4:T:17:G:H3'	4:T:18:U:H4'	1.68	0.74
1:A:858:TRP:HA	1:A:864:VAL:HG11	1.69	0.73
1:A:1528:LYS:HE3	1:A:1766:ARG:HE	1.57	0.69
1:A:1630:LYS:HB3	1:A:1856:ASP:HB3	1.77	0.67
1:A:1371:VAL:HG11	1:A:1381:GLU:HB3	1.78	0.66
1:A:1239:GLN:HE22	1:A:1279:ASP:HB2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1283:PHE:HB2	1:A:1478:LEU:HD11	1.78	0.63
1:A:849:LYS:HB3	4:T:23:G:H5'	1.80	0.63
1:A:240:ARG:HG2	1:A:901:LEU:HD21	1.79	0.62
1:A:1787:MET:N	1:A:1787:MET:SD	2.72	0.62
1:A:1776:ASN:HD22	1:A:1793:PHE:H	1.49	0.61
3:P:11:G:H22	4:T:16:G:H1	1.49	0.61
1:A:1039:LYS:HE3	1:A:1041:GLU:HB2	1.81	0.61
1:A:348:THR:HG21	1:A:593:TRP:HE1	1.65	0.60
1:A:886:VAL:HG11	1:A:892:ALA:HB2	1.84	0.60
1:A:1878:GLU:HG3	1:A:1879:PRO:HD3	1.82	0.60
1:A:1290:ARG:HD3	1:A:1332:GLY:HA3	1.84	0.59
1:A:1510:ARG:HG2	1:A:1666:ILE:HB	1.83	0.59
1:A:526:GLN:HB3	1:A:1254:LEU:HD11	1.83	0.59
1:A:1003:CYS:O	1:A:1011:HIS:NE2	2.35	0.59
1:A:1481:VAL:HG13	1:A:1613:ALA:HB2	1.85	0.59
1:A:742:ASN:OD1	1:A:745:ASN:ND2	2.36	0.58
1:A:1666:ILE:HG23	1:A:1667:ARG:HG3	1.84	0.58
1:A:859:GLU:OE2	1:A:907:ARG:NH2	2.36	0.58
1:A:433:TRP:O	1:A:439:ASN:ND2	2.36	0.58
1:A:622:PHE:HZ	1:A:748:ASN:HD22	1.51	0.58
1:A:1760:ASP:N	1:A:1760:ASP:OD1	2.34	0.58
2:G:2:C:H2'	2:G:3:A:H8	1.68	0.58
1:A:1264:MET:HB3	1:A:1442:LEU:HD13	1.86	0.57
1:A:1735:GLN:HB2	1:A:1751:ARG:HB3	1.86	0.57
2:G:2:C:H2'	2:G:3:A:C8	2.39	0.57
1:A:608:ASN:ND2	1:A:655:ASP:OD1	2.38	0.57
1:A:756:LYS:NZ	1:A:757:ASN:O	2.37	0.56
1:A:1595:THR:OG1	1:A:1596:THR:N	2.37	0.56
1:A:73:SER:HB3	1:A:226:ARG:HG3	1.86	0.56
1:A:1146:ARG:HD2	1:A:1982:PHE:HE2	1.70	0.56
1:A:171:VAL:HB	1:A:178:LEU:HB3	1.88	0.55
1:A:1704:SER:HB2	1:A:1843:ARG:HG2	1.89	0.54
1:A:423:PHE:HB3	1:A:428:VAL:HB	1.89	0.54
1:A:578:ARG:NH2	1:A:594:GLU:OE2	2.40	0.54
1:A:853:ASN:N	1:A:869:TYR:OH	2.41	0.53
1:A:123:VAL:HG12	1:A:166:PHE:HB3	1.89	0.53
1:A:1877:LYS:HD3	1:A:1879:PRO:HD2	1.89	0.53
1:A:945:GLU:HG2	1:A:953:ALA:HB1	1.91	0.53
1:A:131:ARG:NH2	1:A:199:ASN:OD1	2.42	0.53
1:A:1175:THR:OG1	1:A:1178:CYS:SG	2.66	0.53
1:A:1747:LEU:HD13	1:A:1750:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:C:OP1	3:P:11:G:O2'	2.22	0.52
1:A:285:HIS:HD2	1:A:680:LEU:H	1.57	0.52
3:P:14:C:H2'	3:P:15:A:H8	1.74	0.52
1:A:128:SER:HB3	1:A:145:LYS:HG3	1.91	0.52
1:A:1758:LEU:HD11	1:A:1806:VAL:HG11	1.92	0.52
1:A:1851:ARG:HH21	1:A:1853:ARG:HB3	1.75	0.51
1:A:2033:GLY:O	1:A:2037:GLU:N	2.41	0.51
1:A:452:PRO:O	1:A:704:ARG:NH1	2.43	0.51
1:A:1292:ASN:HD22	1:A:1295:ARG:HH12	1.59	0.51
1:A:1318:LYS:O	1:A:1324:ARG:NH1	2.44	0.50
1:A:558:THR:OG1	1:A:563:HIS:O	2.27	0.50
1:A:662:ILE:HG21	1:A:702:LEU:HB3	1.92	0.50
1:A:1836:SER:HB2	1:A:1844:VAL:HG22	1.93	0.50
1:A:856:LYS:HG2	1:A:907:ARG:HH12	1.77	0.50
1:A:2017:GLN:HA	1:A:2020:ILE:HG12	1.94	0.50
1:A:1054:ASP:HB3	1:A:1060:ARG:HB2	1.94	0.49
1:A:1637:LEU:HD12	1:A:1831:ASP:HA	1.94	0.49
1:A:1836:SER:HA	1:A:1846:ASN:HA	1.94	0.49
1:A:967:LEU:HD22	1:A:971:ARG:HH12	1.76	0.49
1:A:1081:GLY:HA3	4:T:23:G:H21	1.77	0.49
1:A:597:GLU:OE2	1:A:599:LYS:NZ	2.43	0.49
1:A:490:ALA:HB1	1:A:1278:MET:HB2	1.95	0.49
1:A:1904:ASP:OD1	1:A:1904:ASP:N	2.46	0.49
1:A:1978:ILE:HG23	1:A:1981:ILE:HD12	1.93	0.49
1:A:572:LYS:HD3	1:A:594:GLU:HB2	1.94	0.48
1:A:267:THR:O	1:A:271:LYS:HG2	2.14	0.48
1:A:1243:LEU:HD12	1:A:1276:PHE:HB3	1.96	0.48
1:A:949:HIS:ND1	1:A:1123:GLU:OE2	2.47	0.48
1:A:1528:LYS:O	1:A:1767:ARG:NH1	2.41	0.48
4:T:20:U:O2'	4:T:21:U:H3'	2.13	0.48
1:A:1290:ARG:NH2	1:A:1466:PRO:HD2	2.28	0.48
3:P:14:C:H2'	3:P:15:A:C8	2.49	0.47
1:A:1361:TRP:HZ3	1:A:1565:VAL:HG21	1.79	0.47
1:A:40:VAL:HG22	1:A:45:VAL:HG13	1.97	0.47
1:A:1352:LEU:HD21	1:A:1391:HIS:HE1	1.79	0.47
1:A:1422:ARG:HE	1:A:1435:LYS:HE2	1.78	0.47
1:A:1696:GLN:HG3	1:A:1699:THR:HB	1.97	0.47
1:A:330:VAL:HG23	1:A:584:PHE:HA	1.96	0.47
1:A:331:LYS:HB3	1:A:599:LYS:HE2	1.96	0.47
1:A:238:ILE:HA	1:A:241:VAL:HB	1.96	0.47
1:A:372:VAL:HG21	1:A:543:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:THR:HB	1:A:1018:ILE:HG22	1.96	0.47
1:A:188:ALA:O	1:A:192:MET:HG3	2.15	0.46
1:A:1456:LEU:HD12	1:A:1460:GLN:HB3	1.96	0.46
1:A:252:MET:HB3	1:A:790:TRP:CE2	2.51	0.46
1:A:1752:LEU:HD21	1:A:1761:VAL:HG11	1.97	0.46
1:A:1095:GLN:HG3	1:A:1123:GLU:HB3	1.97	0.46
1:A:1487:LYS:H	1:A:1487:LYS:HG3	1.67	0.46
1:A:846:ALA:HB2	1:A:878:MET:HG2	1.98	0.45
1:A:1342:TRP:HH2	1:A:1408:VAL:HG22	1.81	0.45
1:A:1706:PRO:HB3	5:C:1:M7G:HM71	1.97	0.45
1:A:1473:ARG:O	1:A:1476:THR:OG1	2.32	0.45
1:A:1539:ASP:OD1	1:A:1542:ARG:NH2	2.50	0.45
1:A:1880:SER:C	1:A:1882:SER:H	2.20	0.45
1:A:1294:TRP:NE1	1:A:1461:GLU:OE2	2.37	0.45
1:A:82:PHE:HB3	1:A:198:ALA:HB2	1.98	0.45
1:A:988:LYS:HA	1:A:988:LYS:HD3	1.87	0.45
4:T:14:G:H2'	4:T:15:C:H6	1.81	0.45
1:A:1780:SER:OG	1:A:1803:GLY:O	2.26	0.45
1:A:466:ASN:N	1:A:466:ASN:OD1	2.50	0.45
1:A:1497:ARG:NH2	1:A:1582:ARG:HE	2.14	0.45
1:A:1707:GLN:NE2	1:A:1738:ILE:O	2.50	0.45
2:G:1:A:H2'	2:G:2:C:C6	2.52	0.45
1:A:1189:ARG:NH1	1:A:1995:GLU:O	2.50	0.44
1:A:512:SER:HB2	1:A:515:VAL:HG22	2.00	0.44
1:A:903:ASP:OD2	1:A:907:ARG:NH1	2.49	0.44
1:A:1351:LEU:HD23	1:A:1354:ARG:HH12	1.83	0.44
1:A:1637:LEU:HB2	1:A:1852:PRO:HG2	1.99	0.44
1:A:726:ARG:NH1	1:A:1493:ARG:HB3	2.32	0.44
1:A:624:ARG:HG3	1:A:641:LEU:HD21	1.99	0.44
1:A:683:PRO:HB2	1:A:710:MET:SD	2.57	0.44
1:A:38:VAL:HG13	1:A:40:VAL:HG23	1.99	0.44
1:A:1328:ALA:HA	1:A:1334:LEU:HA	1.98	0.44
1:A:1538:TRP:HH2	1:A:1548:LEU:HD12	1.82	0.44
1:A:146:ILE:O	1:A:150:ARG:HB2	2.18	0.44
1:A:1676:LEU:HD13	1:A:1692:ILE:HG12	2.00	0.44
1:A:1796:LYS:HA	1:A:1796:LYS:HD2	1.61	0.44
1:A:113:VAL:HB	1:A:125:VAL:HB	2.00	0.43
1:A:329:THR:HG21	1:A:459:ILE:HD11	2.00	0.43
1:A:467:ASN:HD21	1:A:579:LEU:HA	1.82	0.43
1:A:493:MET:H	1:A:493:MET:HG2	1.55	0.43
1:A:1365:ILE:HG21	1:A:1565:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:THR:OG1	1:A:1022:ARG:NH1	2.51	0.43
1:A:1054:ASP:O	1:A:1058:GLY:N	2.50	0.43
1:A:1157:LYS:HE3	1:A:1157:LYS:HB3	1.88	0.43
1:A:691:ASP:N	1:A:691:ASP:OD1	2.43	0.43
1:A:288:LYS:NZ	1:A:1973:GLU:OE1	2.40	0.43
1:A:592:GLU:HB3	1:A:593:TRP:HD1	1.83	0.43
4:T:16:G:H21	4:T:18:U:H3	1.67	0.43
1:A:338:LYS:HD3	1:A:474:TYR:CE1	2.54	0.43
1:A:79:ASN:HA	1:A:198:ALA:HB1	2.00	0.43
1:A:1540:LYS:H	1:A:1540:LYS:HG2	1.70	0.43
1:A:476:ASP:OD1	1:A:481:ARG:NE	2.51	0.43
1:A:135:ILE:HG23	1:A:138:LEU:HD12	2.00	0.43
1:A:739:ARG:H	1:A:739:ARG:HG2	1.62	0.43
1:A:43:THR:OG1	1:A:895:GLN:OE1	2.37	0.42
1:A:325:LEU:HD21	1:A:327:ARG:HE	1.84	0.42
1:A:357:ASP:OD1	1:A:357:ASP:N	2.50	0.42
1:A:809:ALA:HA	1:A:1097:PHE:HB2	2.01	0.42
1:A:826:LYS:HE3	1:A:826:LYS:HB2	1.89	0.42
1:A:864:VAL:HG23	1:A:1030:LEU:HD11	2.01	0.42
1:A:1876:LYS:HE2	1:A:1876:LYS:HB2	1.72	0.42
1:A:1028:VAL:HG22	1:A:1072:ILE:HG12	1.99	0.42
1:A:1205:ILE:H	1:A:1205:ILE:HG13	1.59	0.42
1:A:2015:MET:HB3	1:A:2018:ALA:HB3	2.02	0.42
1:A:428:VAL:HG13	1:A:556:LYS:HG2	2.01	0.42
1:A:854:PHE:HZ	1:A:1071:TYR:HB3	1.85	0.42
1:A:1020:MET:HG2	1:A:1021:PHE:HD1	1.84	0.42
1:A:1529:LEU:HD22	1:A:1533:LEU:HD23	2.01	0.42
4:T:14:G:H2'	4:T:15:C:C6	2.55	0.42
1:A:653:LEU:HD13	1:A:653:LEU:HA	1.87	0.42
1:A:1766:ARG:HD2	1:A:1793:PHE:HB3	2.01	0.42
5:C:1:M7G:H82	5:C:2:A:OP1	2.20	0.42
1:A:1645:TYR:O	1:A:1649:MET:HG2	2.20	0.42
1:A:2040:CYS:HB2	1:A:2044:ILE:HD11	2.02	0.42
1:A:1438:LEU:HD23	1:A:1438:LEU:HA	1.89	0.42
1:A:1876:LYS:H	1:A:1876:LYS:HG3	1.70	0.42
1:A:104:ASP:OD2	1:A:106:SER:OG	2.37	0.41
1:A:1314:GLN:OE1	1:A:1316:LYS:NZ	2.53	0.41
1:A:1669:SER:HB2	1:A:1672:MET:HG2	2.01	0.41
1:A:663:ILE:O	1:A:666:THR:OG1	2.29	0.41
1:A:993:HIS:HB2	1:A:1078:MET:HG2	2.02	0.41
2:G:1:A:H2'	2:G:2:C:H6	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:HH12	4:T:13:G:H3'	1.86	0.41
1:A:30:ARG:NH1	1:A:189:GLU:OE2	2.52	0.41
1:A:268:LYS:HE2	1:A:268:LYS:HB3	1.90	0.41
1:A:851:THR:HG21	1:A:874:LEU:HD13	2.03	0.41
1:A:1528:LYS:HA	1:A:1528:LYS:HD3	1.74	0.41
1:A:1755:ASP:HA	1:A:1758:LEU:HD23	2.02	0.41
4:T:20:U:O2'	4:T:22:U:OP1	2.39	0.41
1:A:1466:PRO:HB2	1:A:1576:ALA:HB2	2.02	0.41
1:A:89:LYS:NZ	1:A:114:ILE:O	2.42	0.41
1:A:773:LYS:HE2	1:A:773:LYS:HB3	1.84	0.41
1:A:1308:TYR:O	1:A:1312:GLU:HG2	2.20	0.41
1:A:1636:VAL:HG11	1:A:1650:ILE:HG13	2.03	0.41
1:A:1794:LYS:HE3	1:A:1794:LYS:HB2	1.89	0.41
1:A:466:ASN:HB2	1:A:468:LEU:HD13	2.03	0.41
1:A:498:LEU:HD12	1:A:1484:LEU:HD12	2.03	0.41
1:A:597:GLU:H	1:A:597:GLU:HG3	1.62	0.41
1:A:662:ILE:O	1:A:666:THR:HG23	2.20	0.41
1:A:1255:HIS:CD2	1:A:1257:LEU:HB2	2.56	0.41
1:A:1365:ILE:HD13	1:A:1365:ILE:HA	1.94	0.41
1:A:1657:LEU:HD23	1:A:1657:LEU:HA	1.98	0.41
1:A:930:ARG:NH2	4:T:25:G:OP1	2.54	0.40
1:A:1102:PHE:HE2	1:A:1130:ILE:HG21	1.86	0.40
1:A:1188:HIS:CD2	1:A:1189:ARG:HG3	2.56	0.40
1:A:394:ASP:HA	1:A:1419:HIS:CE1	2.56	0.40
1:A:533:LYS:HE2	1:A:1410:ALA:HB1	2.03	0.40
1:A:1223:THR:O	1:A:1227:GLU:HG2	2.21	0.40
1:A:1635:MET:H	1:A:1635:MET:HG2	1.62	0.40
1:A:643:GLU:OE2	1:A:739:ARG:NE	2.55	0.40
1:A:1401:LYS:HZ2	1:A:1401:LYS:HG3	1.80	0.40
1:A:105:GLY:HA2	1:A:1525:LYS:HD3	2.04	0.40
1:A:933:GLN:NE2	1:A:1082:ILE:HG13	2.36	0.40

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	A	1958/2084 (94%)	1801 (92%)	154 (8%)	3 (0%)	47 78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1323	TYR
1	A	1828	VAL
1	A	1495	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1725/1826 (94%)	1572 (91%)	153 (9%)	9 34

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	90	THR
1	A	237	ASN
1	A	240	ARG
1	A	251	LYS
1	A	283	ASP
1	A	325	LEU
1	A	327	ARG
1	A	330	VAL
1	A	335	TRP
1	A	338	LYS
1	A	364	LEU
1	A	432	LYS
1	A	456	VAL
1	A	476	ASP
1	A	479	ILE

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Mol	Chain	Res	Type
1	A	481	ARG
1	A	491	SER
1	A	493	MET
1	A	494	GLN
1	A	497	GLU
1	A	528	LEU
1	A	532	LEU
1	A	533	LYS
1	A	543	ILE
1	A	577	ARG
1	A	582	ARG
1	A	585	SER
1	A	592	GLU
1	A	597	GLU
1	A	600	SER
1	A	606	LEU
1	A	624	ARG
1	A	627	LEU
1	A	633	LEU
1	A	634	VAL
1	A	641	LEU
1	A	651	ILE
1	A	653	LEU
1	A	654	GLU
1	A	663	ILE
1	A	694	LEU
1	A	696	THR
1	A	697	LYS
1	A	712	ARG
1	A	721	ILE
1	A	727	VAL
1	A	736	ILE
1	A	739	ARG
1	A	743	LEU
1	A	758	LYS
1	A	760	GLU
1	A	769	GLU
1	A	779	GLU
1	A	857	ASP
1	A	860	LEU
1	A	868	GLU
1	A	873	LYS

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Mol	Chain	Res	Type
1	A	878	MET
1	A	907	ARG
1	A	925	MET
1	A	937	GLU
1	A	951	THR
1	A	956	ARG
1	A	1020	MET
1	A	1027	MET
1	A	1028	VAL
1	A	1030	LEU
1	A	1060	ARG
1	A	1061	ASP
1	A	1072	ILE
1	A	1078	MET
1	A	1110	TYR
1	A	1157	LYS
1	A	1174	ASN
1	A	1175	THR
1	A	1178	CYS
1	A	1180	GLU
1	A	1190	HIS
1	A	1193	ARG
1	A	1195	THR
1	A	1197	ARG
1	A	1207	GLU
1	A	1214	ARG
1	A	1233	SER
1	A	1243	LEU
1	A	1253	CYS
1	A	1262	MET
1	A	1279	ASP
1	A	1283	PHE
1	A	1300	THR
1	A	1322	ASP
1	A	1341	TYR
1	A	1348	TYR
1	A	1371	VAL
1	A	1396	THR
1	A	1399	LEU
1	A	1401	LYS
1	A	1409	VAL
1	A	1415	LEU

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Mol	Chain	Res	Type
1	A	1416	LEU
1	A	1451	LYS
1	A	1456	LEU
1	A	1459	ASN
1	A	1460	GLN
1	A	1472	ASP
1	A	1479	GLU
1	A	1482	GLU
1	A	1484	LEU
1	A	1487	LYS
1	A	1489	VAL
1	A	1528	LYS
1	A	1534	LEU
1	A	1535	LYS
1	A	1540	LYS
1	A	1542	ARG
1	A	1544	SER
1	A	1548	LEU
1	A	1568	ARG
1	A	1635	MET
1	A	1672	MET
1	A	1677	LEU
1	A	1690	ASP
1	A	1693	GLU
1	A	1717	VAL
1	A	1728	VAL
1	A	1730	GLU
1	A	1752	LEU
1	A	1754	SER
1	A	1755	ASP
1	A	1757	ARG
1	A	1758	LEU
1	A	1760	ASP
1	A	1765	ILE
1	A	1787	MET
1	A	1790	LEU
1	A	1793	PHE
1	A	1796	LYS
1	A	1800	ARG
1	A	1826	MET
1	A	1843	ARG
1	A	1849	SER

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Mol	Chain	Res	Type
1	A	1851	ARG
1	A	1869	ARG
1	A	1876	LYS
1	A	1877	LYS
1	A	1878	GLU
1	A	1890	ASP
1	A	1976	LEU
1	A	2000	VAL
1	A	2022	MET
1	A	2026	MET
1	A	2055	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	285	HIS
1	A	300	ASN
1	A	824	GLN
1	A	828	ASN
1	A	914	ASN
1	A	964	ASN
1	A	1174	ASN
1	A	1188	HIS
1	A	1239	GLN
1	A	1280	ASN
1	A	1292	ASN
1	A	1391	HIS
1	A	1467	GLN
1	A	1679	ASN
1	A	1707	GLN
1	A	1776	ASN
1	A	1820	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	3/16 (18%)	1 (33%)	0
3	P	15/20 (75%)	5 (33%)	0
4	T	16/26 (61%)	9 (56%)	2 (12%)
5	C	3/18 (16%)	2 (66%)	1 (33%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	37/80 (46%)	17 (45%)	3 (8%)

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	4	C
3	P	5	A
3	P	6	G
3	P	7	A
3	P	11	G
3	P	13	C
4	T	14	G
4	T	16	G
4	T	17	G
4	T	18	U
4	T	19	C
4	T	21	U
4	T	23	G
4	T	25	G
4	T	26	U
5	C	3	A
5	C	4	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	T	13	G
4	T	20	U
5	C	2	A

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

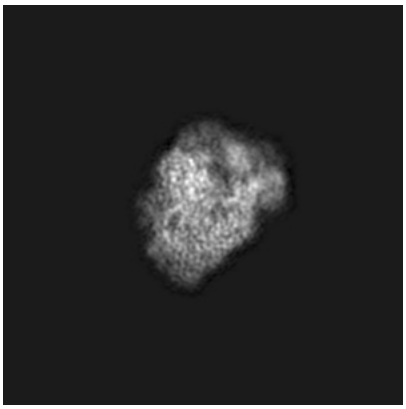
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-18967. These allow visual inspection of the internal detail of the map and identification of artifacts.

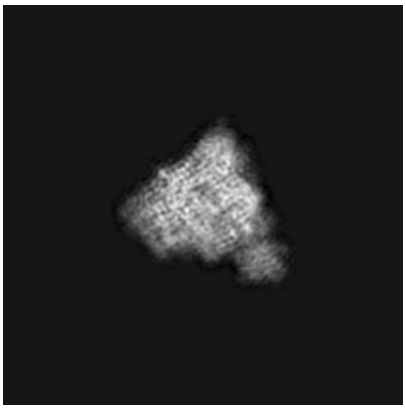
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

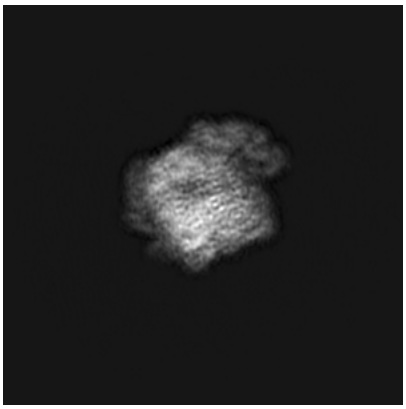
6.1.1 Primary map



X

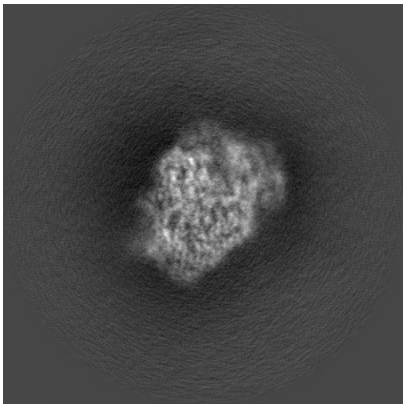


Y

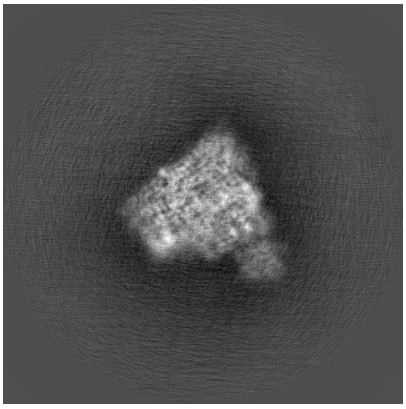


Z

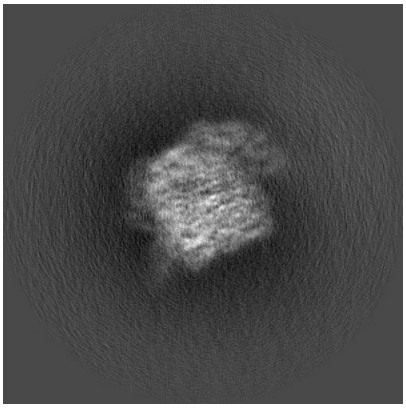
6.1.2 Raw map



X



Y

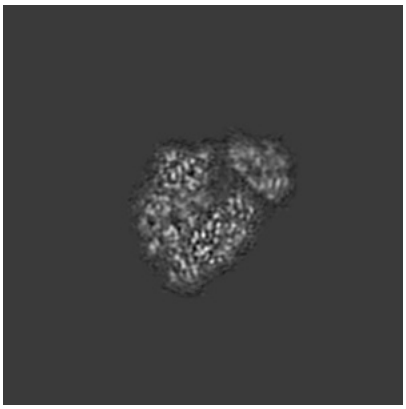


Z

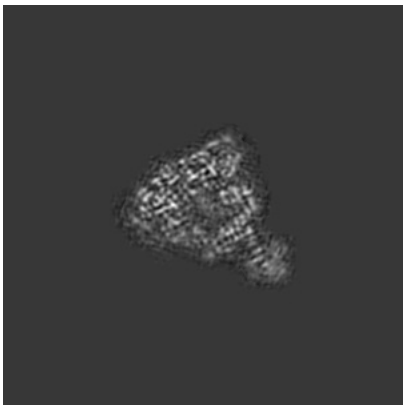
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

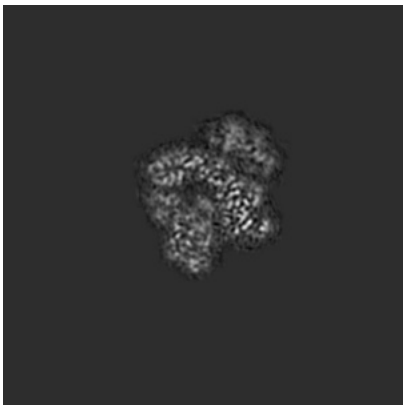
6.2.1 Primary map



X Index: 160

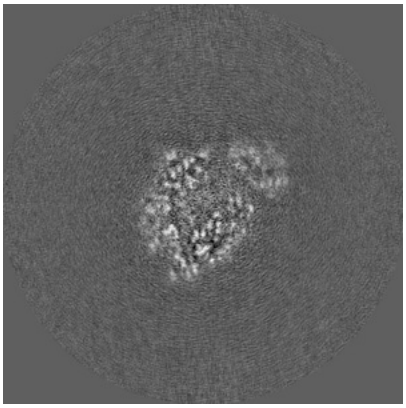


Y Index: 160

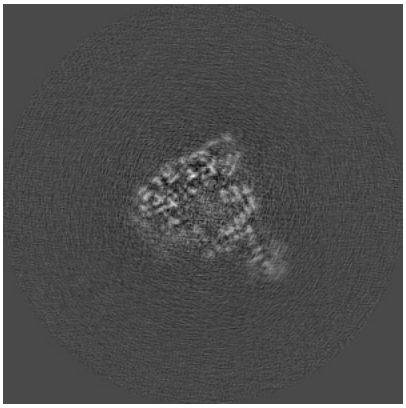


Z Index: 160

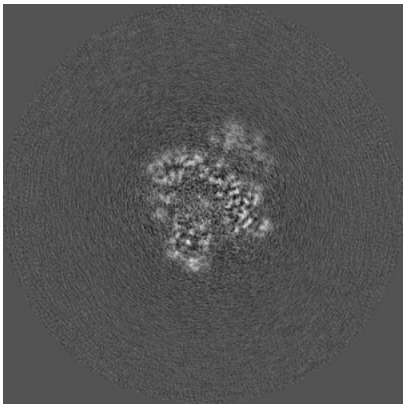
6.2.2 Raw map



X Index: 160



Y Index: 160

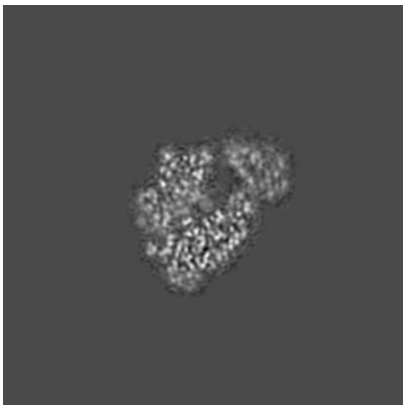


Z Index: 160

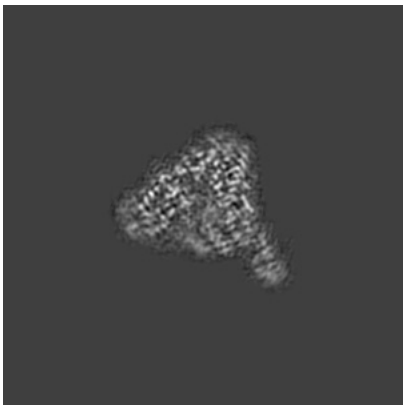
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

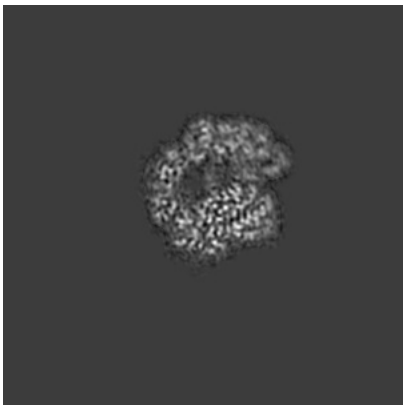
6.3.1 Primary map



X Index: 157

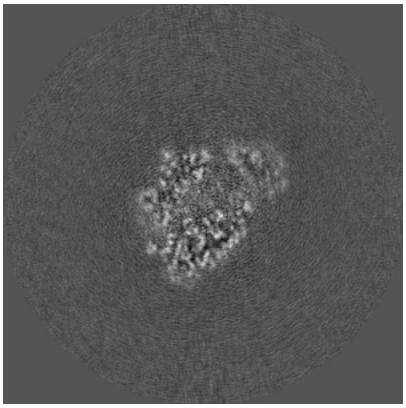


Y Index: 151

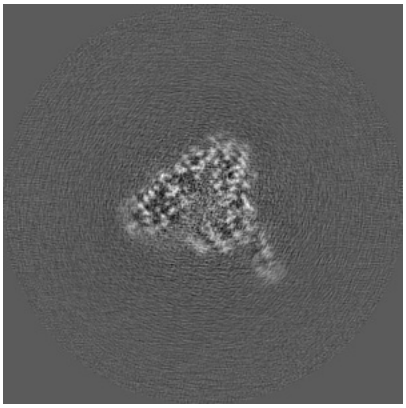


Z Index: 178

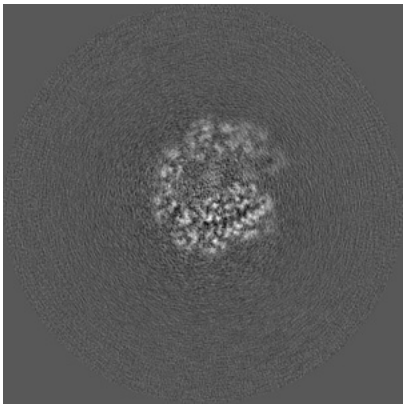
6.3.2 Raw map



X Index: 157



Y Index: 151

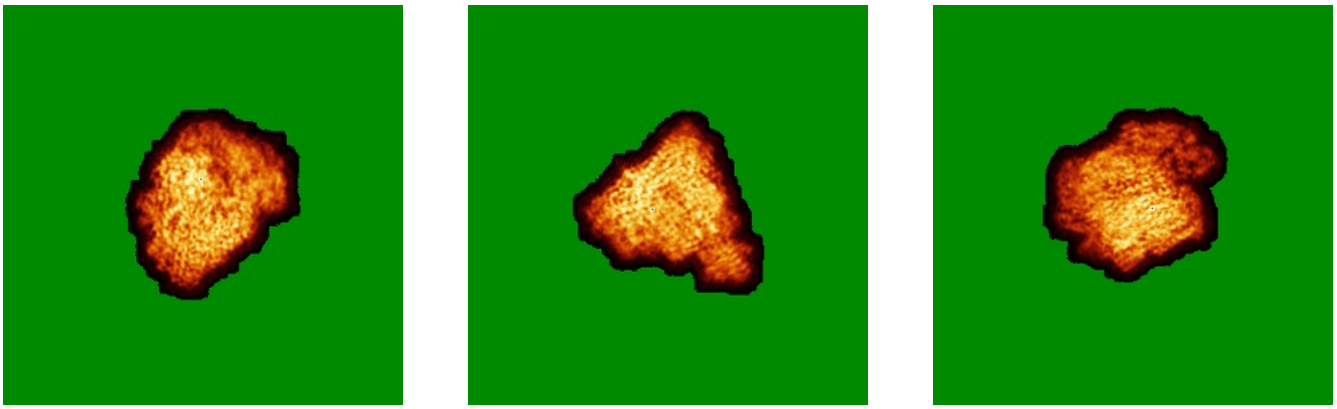


Z Index: 179

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

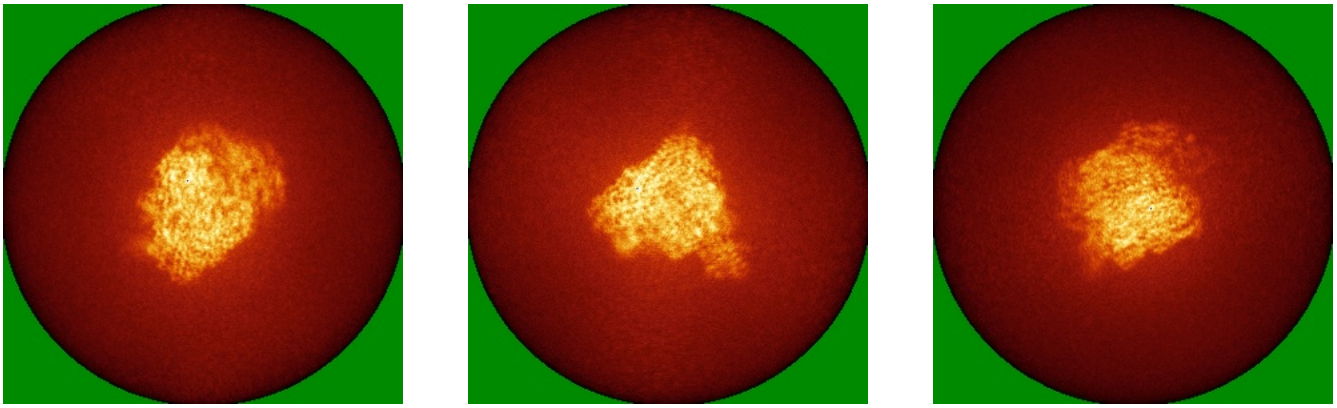
6.4 Orthogonal standard-deviation projections (False-color) (i)

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 0.09. 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.

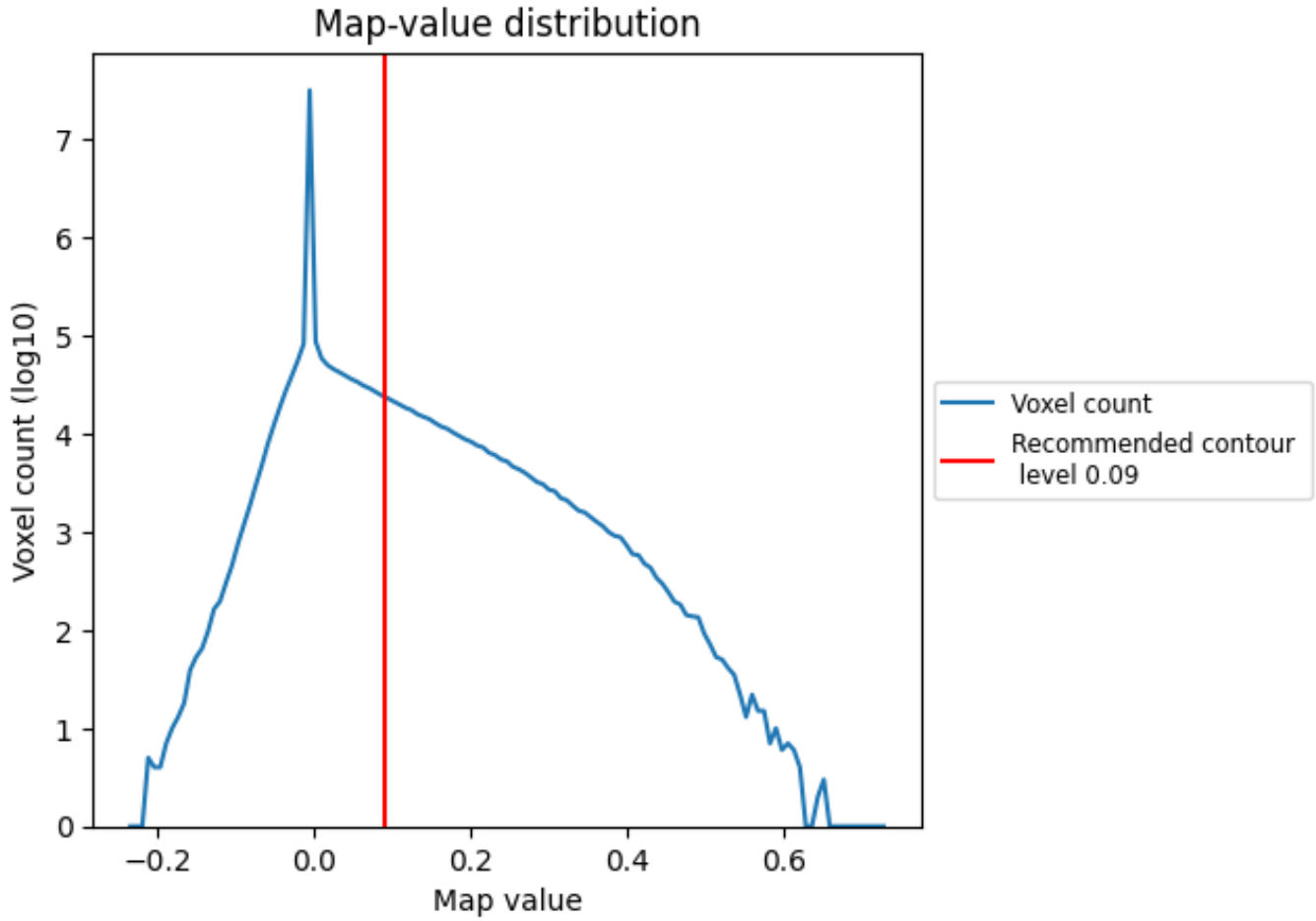
6.6 Mask visualisation (i)

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

7 Map analysis

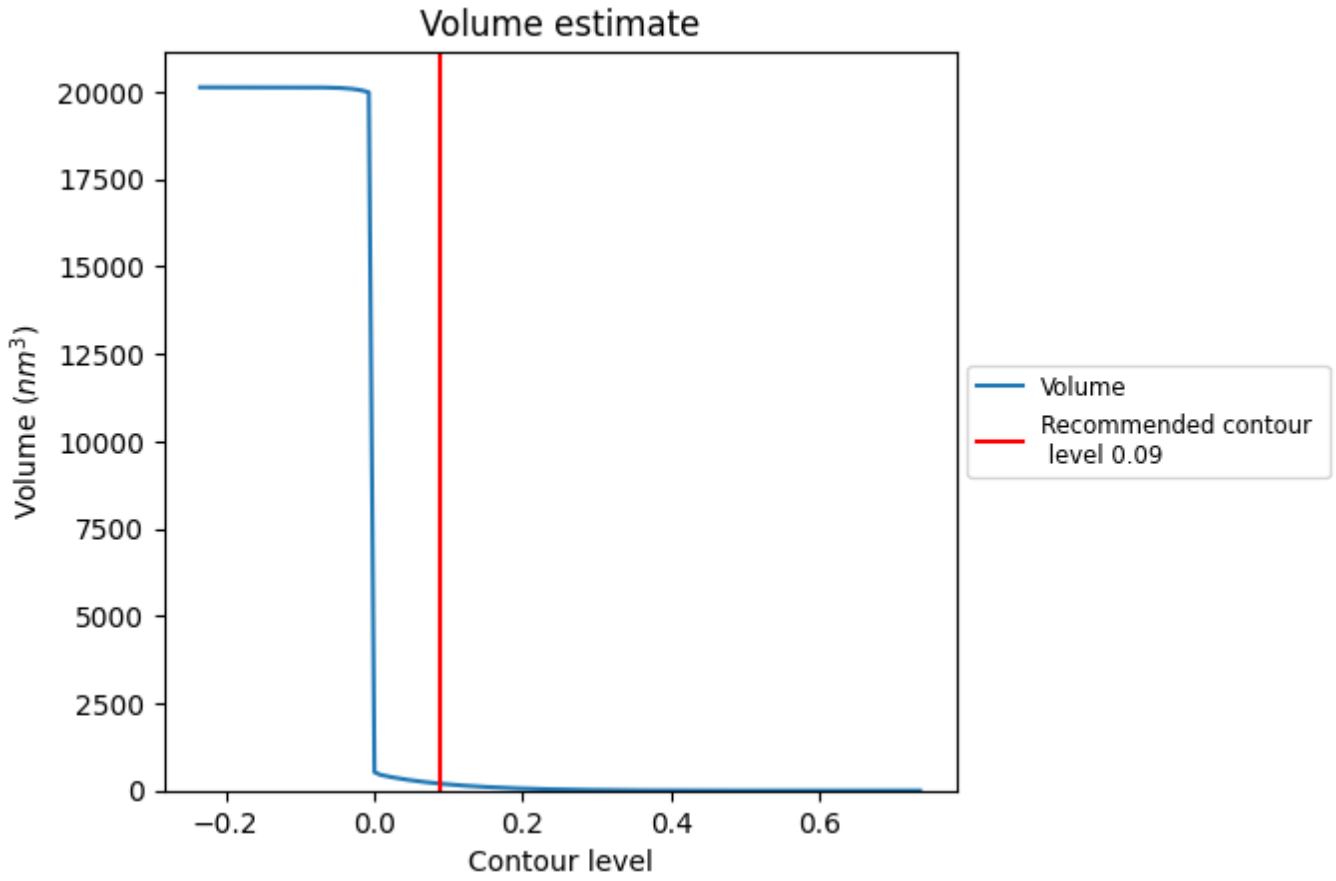
This section contains the results of statistical analysis of the map.

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.

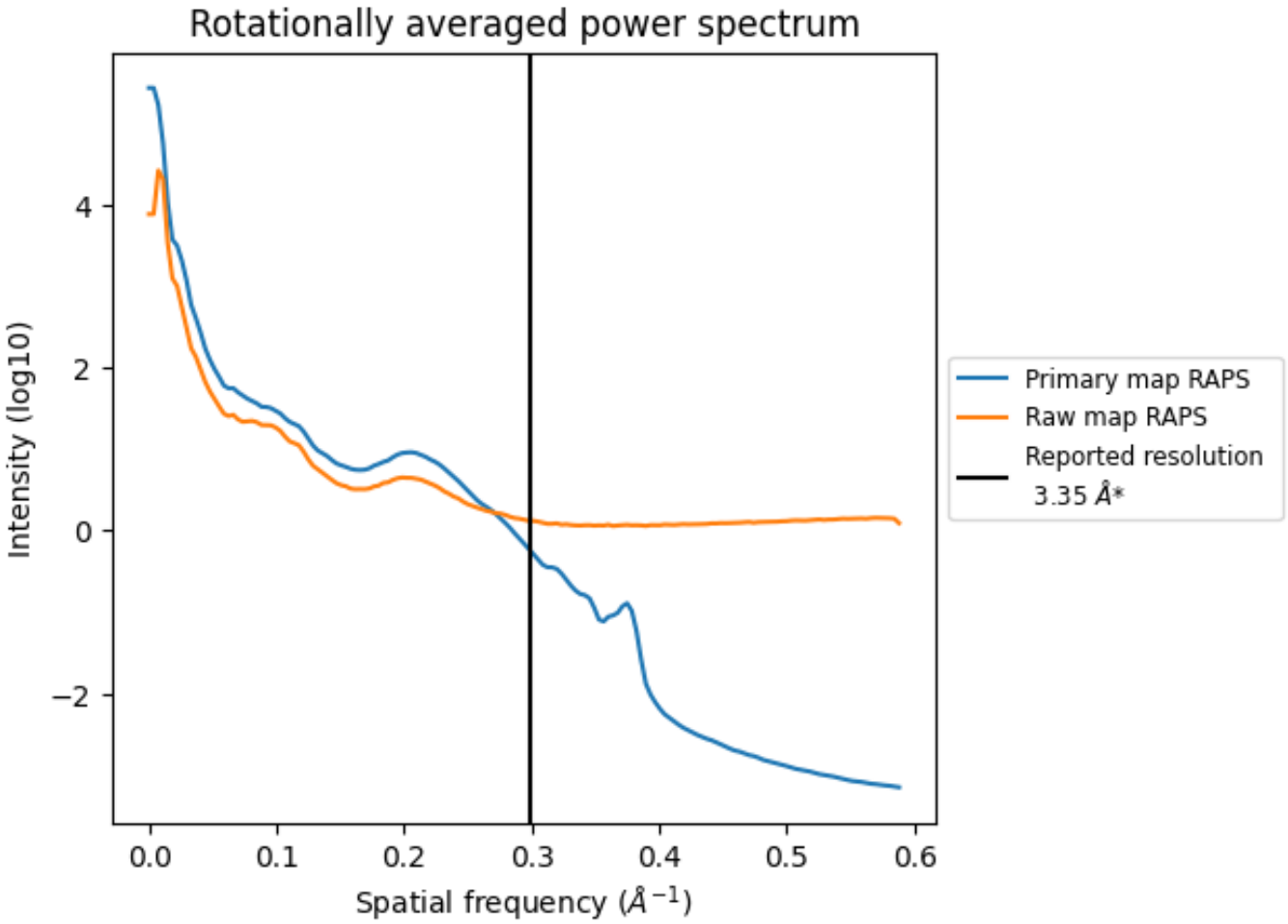
7.2 Volume estimate (i)



The volume at the recommended contour level is 196 nm^3; this corresponds to an approximate mass of 177 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)

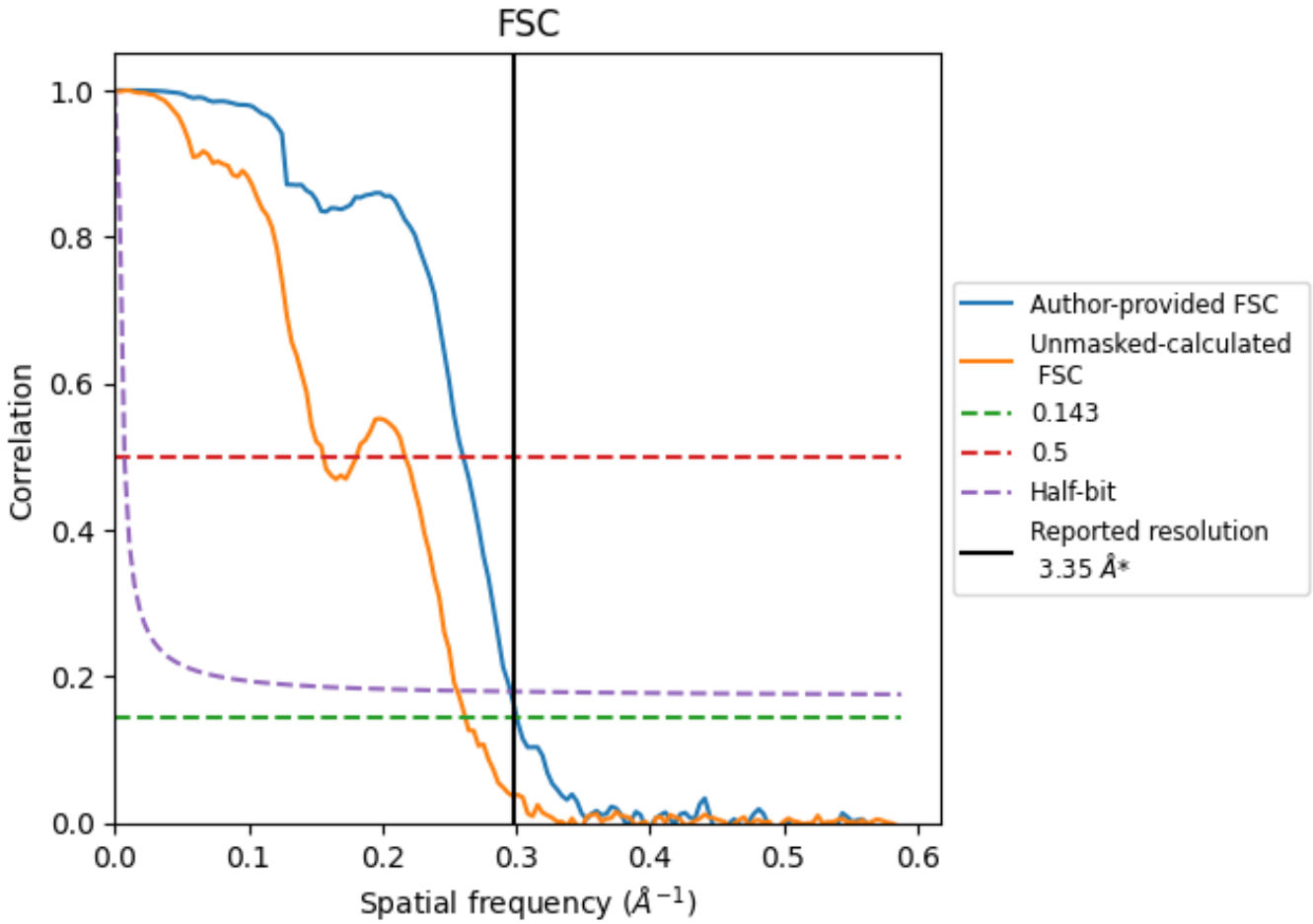


*Reported resolution corresponds to spatial frequency of 0.299 Å^{-1}

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 0.299 Å^{-1}

8.2 Resolution estimates (i)

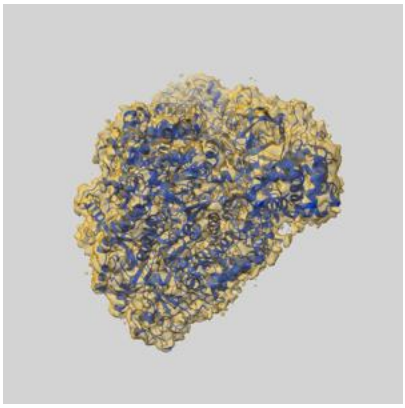
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.35	-	-
Author-provided FSC curve	3.33	3.84	3.38
Unmasked-calculated*	3.81	6.41	3.90

*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 3.81 differs from the reported value 3.35 by more than 10 %

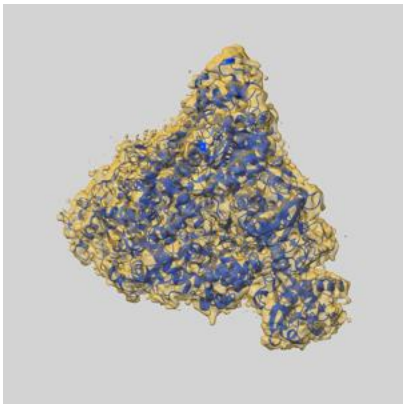
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-18967 and PDB model 8R6W. Per-residue inclusion information can be found in section 3 on page 5.

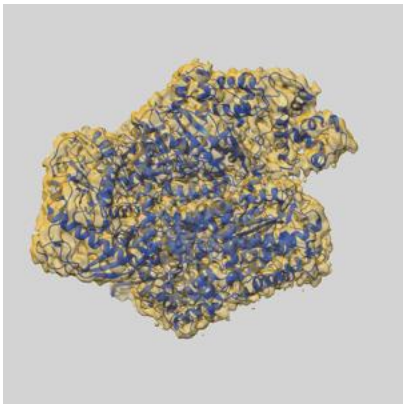
9.1 Map-model overlay



X



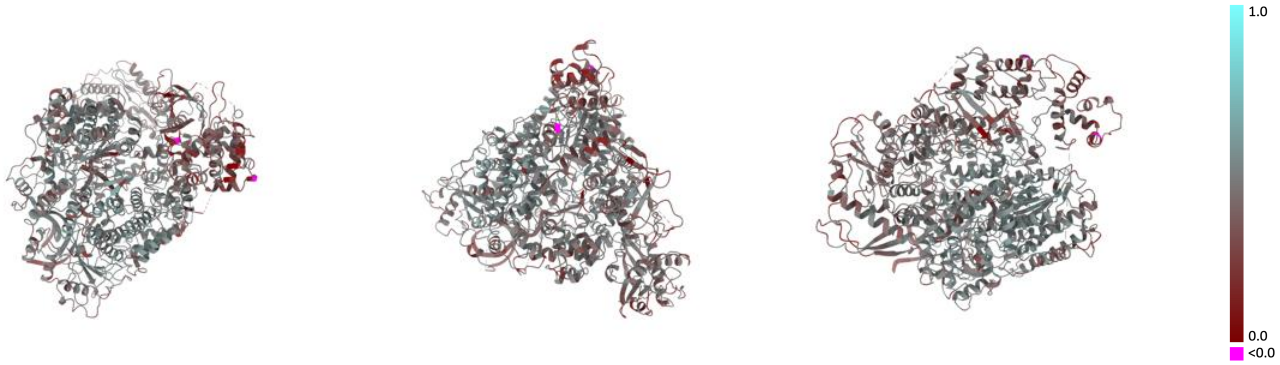
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09 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.

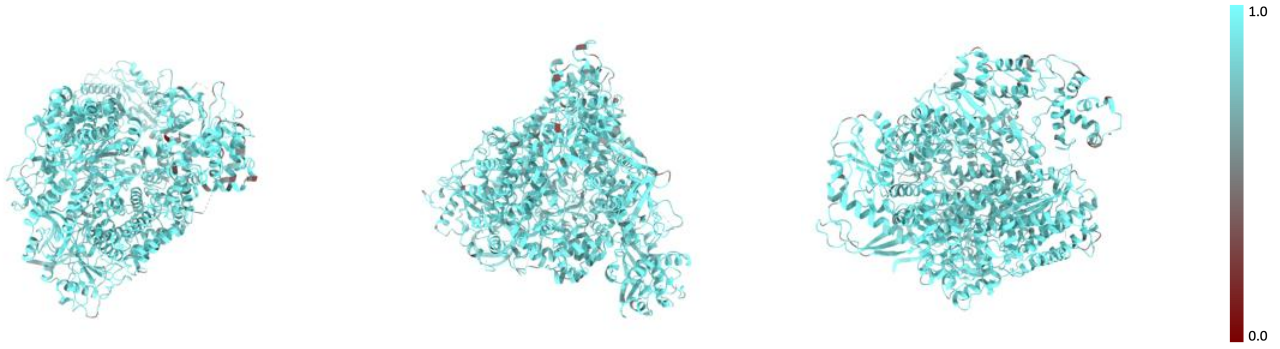
9.2 Q-score mapped to coordinate model (i)



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.

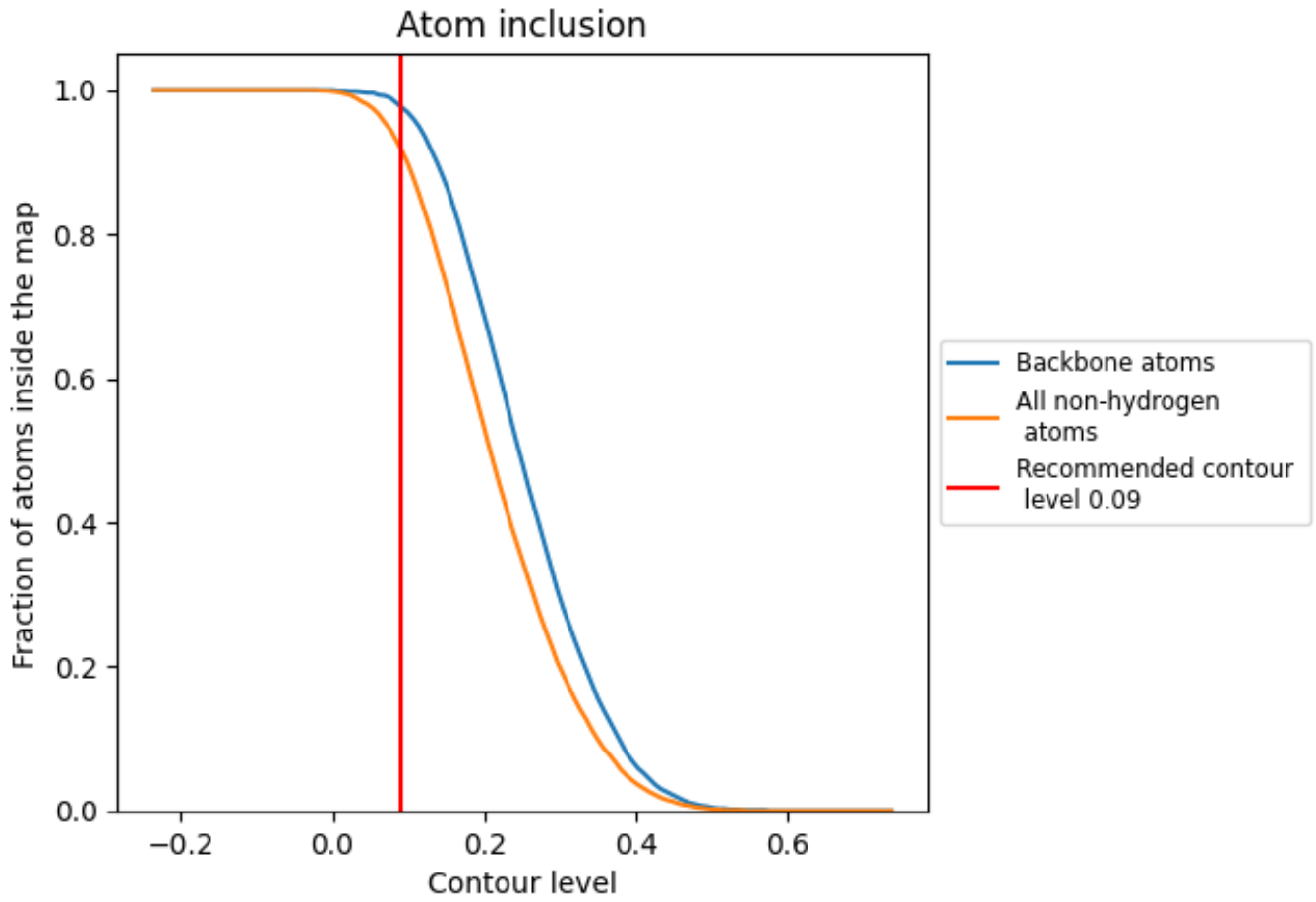
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.09).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 92% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9190	0.4400
A	0.9210	0.4450
C	0.9260	0.3780
G	0.8890	0.2870
P	0.9620	0.4520
T	0.8120	0.2620