



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 03:29 PM UTC

PDB ID : 8Q91 / pdb_00008q91
EMDB ID : EMD-18267
Title : Structure of the human 20S U5 snRNP core
Authors : Schneider, S.; Galej, W.P.
Deposited on : 2023-08-19
Resolution : 3.10 Å(reported)

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

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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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

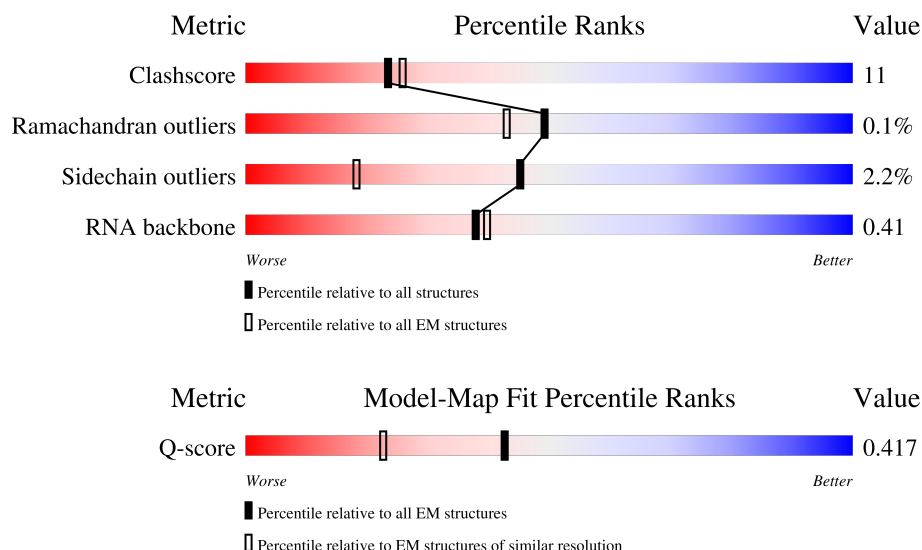
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



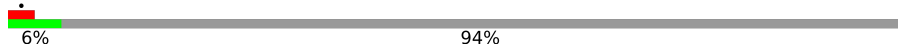
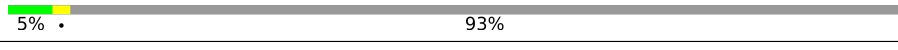
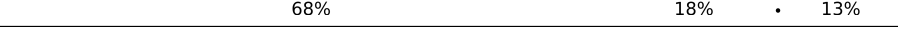
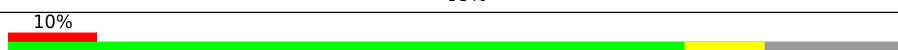
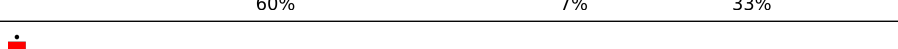
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	F	341	
2	A	2335	
3	5	117	

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Mol	Chain	Length	Quality of chain
4	E	941	 6% 94%
5	D	820	 5% 93%
6	C	972	 68% 18% 13%
7	B	2136	 99%
8	m	86	 10% 76% 9% 15%
9	n	76	 22% 86% 12%
10	i	119	 65% 32%
11	j	118	 16% 80% 17%
12	k	126	 60% 7% 33%
13	h	240	 28% 70%
14	l	92	 5% 75% 8% 16%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 26706 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 CD2 antigen cytoplasmic tail-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	140	Total	C	N	O	S	0	0
			887	552	165	169	1		

- Molecule 2 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1627	Total	C	N	O	S	0	0
			13247	8535	2321	2333	58		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	104	Total	C	N	O	P	0	0
			2192	983	372	734	103		

- Molecule 4 is a protein called Pre-mRNA-processing factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	60	Total	C	N	O	0	0
			300	180	60	60		

- Molecule 5 is a protein called Probable ATP-dependent RNA helicase DDX23.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	54	Total	C	N	O	0	0
			455	294	78	83		

- Molecule 6 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	847	Total	C	N	O	S	0	0
			6629	4238	1108	1250	33		

- Molecule 7 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	27	Total	C	N	O	S	0	0
			201	123	38	39	1		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	m	73	Total	C	N	O	0	0
			356	210	73	73		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	n	74	Total	C	N	O	0	0
			364	215	74	75		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	i	81	Total	C	N	O	0	0
			401	239	81	81		

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	j	98	Total	C	N	O	0	0
			487	291	98	98		

- Molecule 12 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	k	84	Total	C	N	O	0	0
			414	246	84	84		

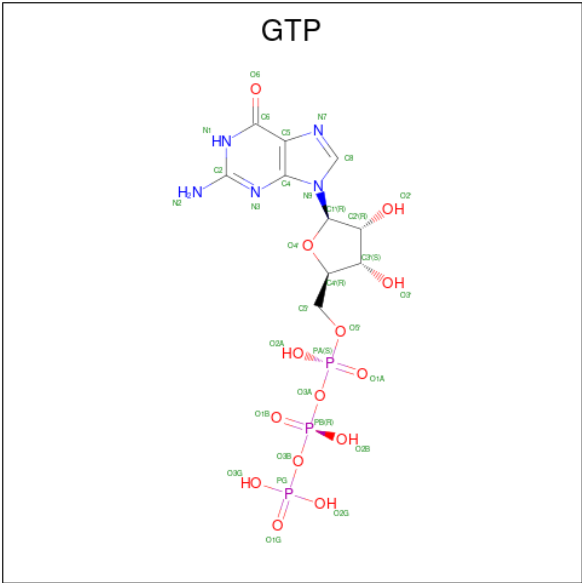
- Molecule 13 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	h	73	Total	C	N	O	0	0
			360	214	73	73		

- Molecule 14 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	1	77	Total	C	N	O	0	0
			381	227	77	77		

- Molecule 15 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).

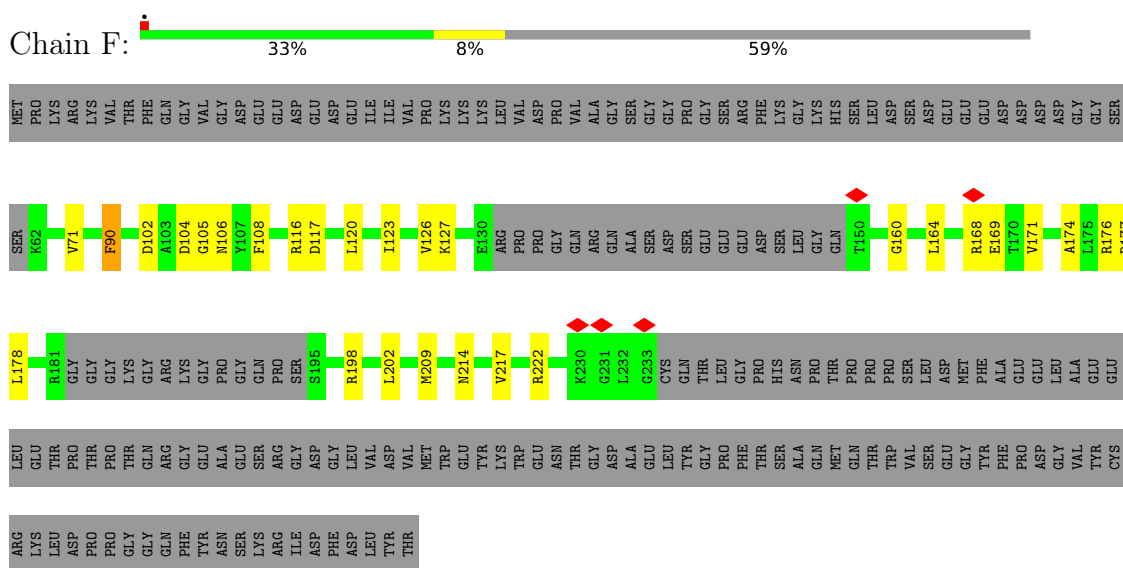


Mol	Chain	Residues	Atoms					AltConf
15	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

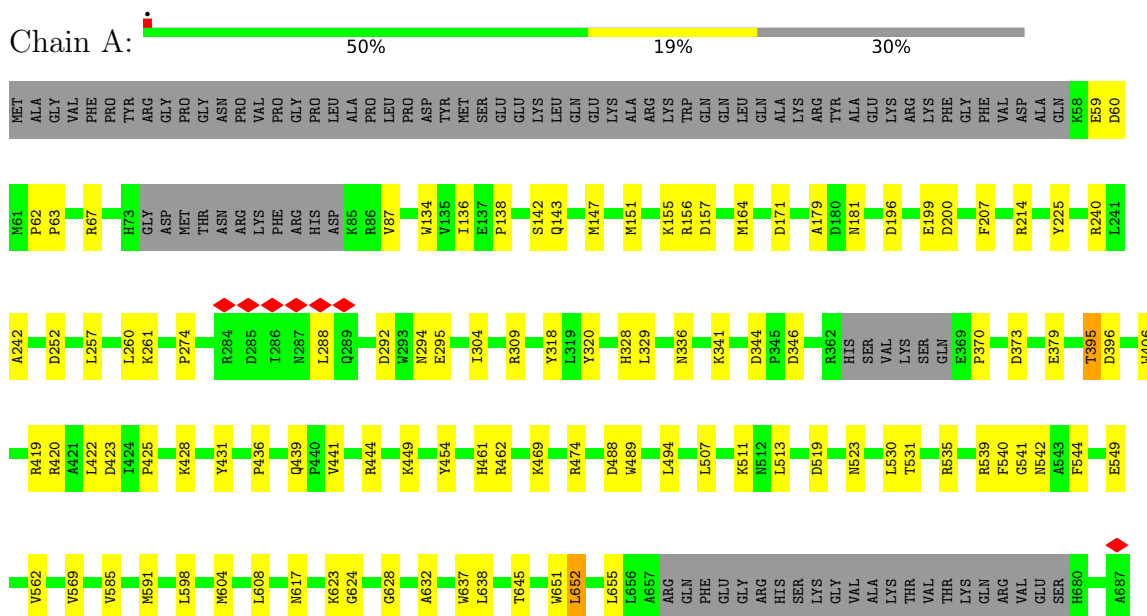
3 Residue-property plots

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: CD2 antigen cytoplasmic tail-binding protein 2



• Molecule 2: Pre-mRNA-processing-splicing factor 8

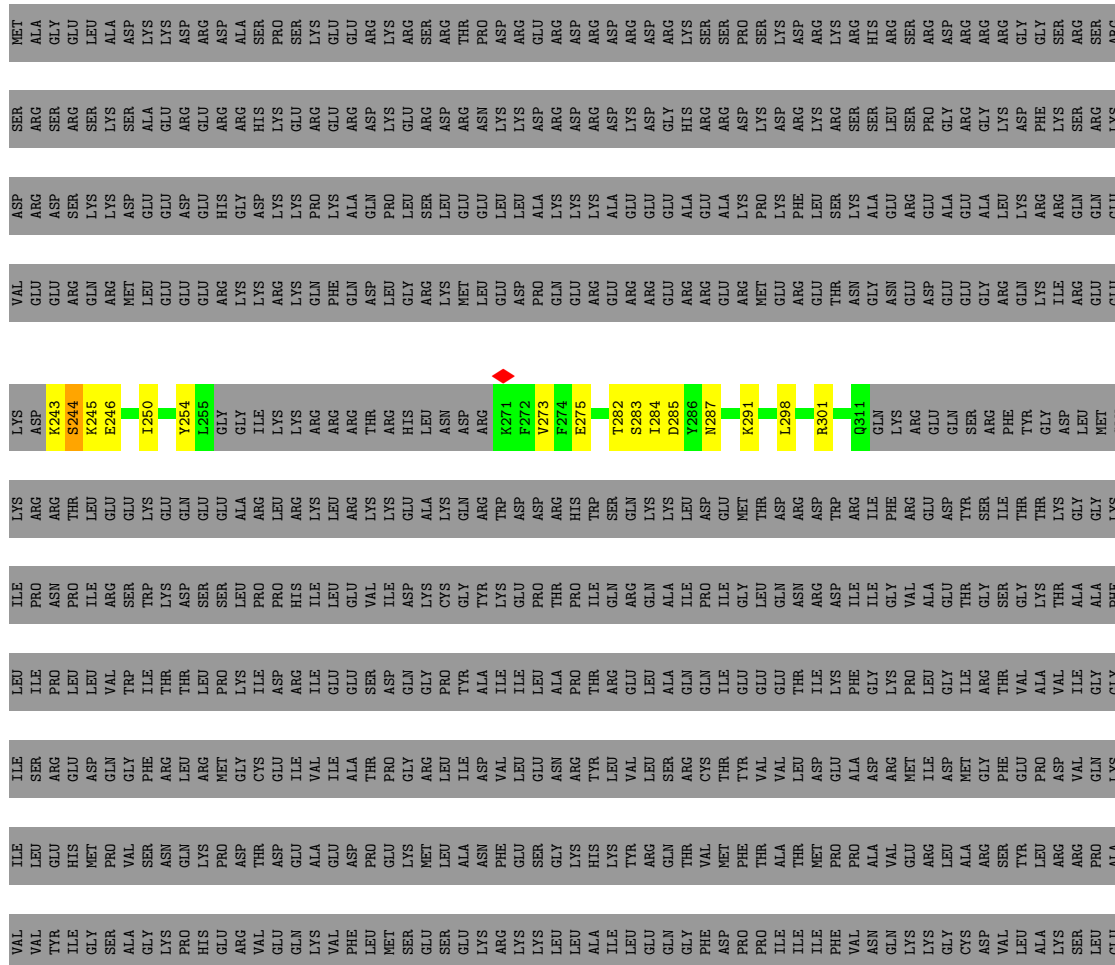


LEU	THR	LYS	ALA	P1738	Y1660	I1585	SER	I1411	E1193	P1065	N974	Q860	P898
ILE	ILE	GLY	ILE	A1739	W1661	H1586	MET	W1412	CL194	Q1066	N976	R861	E899
ALA	THR	MET	PHE	L1740	I1662	D1413	LYS	D1413	R1201	N1069	Y975	L864	G700
ASP	THR	ASP	PHE	R1746	D1663	G1415	TRP	R1414	T1202	F1071	S979	G865	I701
GLY	ALA	PRO	ASN	I1747	W1668	L1593	LYS	I1395	H1205	Q1075	R980	L866	K702
LYS	PHE	LEU	ARG	R1748	W1668	L1593	LEU	P1336	E1205	D1076	L992	L867	Q703
LYS	THR	GLU	ARG	Y1754	Y1671	F1597	THR	R1418	F1207	A1077	N994	E868	N704
ASN	THR	SER	ALA	SER	D1672	E1600	ASN	T1421	E1206	A1082	L996	E876	C719
GLN	THR	SER	GLY	GLN	S1673	E1600	ALA	D1426	F1208	H1083	L997	A877	N723
LEU	THR	PRO	ARG	ARG	I1676	L1604	ARG	R1427	H1209	A1082	R880	R880	N731
LEU	THR	ASP	PHE	SER	E1677	E1605	SER	H1428	H1218	H1083	L881	L885	P732
LEU	THR	PHE	LEU	GLY	E1677	E1605	GLY	T1429	E1219	F1088	V1001	L896	C772
LEU	THR	PRO	ILE	ASN	E1678	E1606	LEU	D1433	W1220	C1089	H1003	D900	L776
LEU	THR	ASN	ILE	GLN	E1679	E1607	ASN	K1434	F1208	R1090	D1002	L901	G777
LEU	THR	ALA	THR	GLN	A1680	E1610	GLN	G1349	H1208	Y1091	N1004	Y902	L778
GLN	THR	LEU	HIS	ILE	R1681	Q1610	ILE	I1386	H1209	I1095	I1005	V906	T780
SER	THR	SER	THR	P1530	Y1687	E1612	P1530	I1386	M1237	I1092	A1006	V908	R781
GLN	SER	SER	SER	N1531	S1697	E1612	N1531	F1353	W1242	R1100	M1012	L908	L782
VAL	GLN	GLN	VAL	R1532	M1615	H1615	R1532	R1354	R1243	A1103	N1013	P913	E804
TRP	TRP	TYR	ALA	L1536	H1616	H1615	L1536	S1355	W1244	R1107	V1016	E805	E806
GLY	GLY	GLY	GLY	W1537	R1617	H1617	W1537	GLY	V1257	R1107	N1017	A806	V807
LEU	LEU	LEU	LEU	S1539	K1621	M1622	S1539	ASP	T1268	I1126	N1018	L917	A808
PRO	ARG	PRO	ARG	M1623	M1622	M1622	M1623	Q1363	I1276	V1126	Y1019	D919	V809
LEU	LEU	LEU	GLN	S1624	S1624	S1624	R1544	L1364	E1283	G1127	K1020	L922	T811
ALA	GLN	GLN	GLN	A1645	S1625	S1625	A1645	I1365	L1284	Y1128	M1021	Q924	T812
LEU	GLN	GLN	LEU	C1626	C1626	C1626	N1546	I1385	E1289	N1129	H1024	Y925	V814
ALA	LEU	LEU	ALA	A1627	A1627	A1627	W1465	L1364	V1297	N1130	T1025	L926	H815
LYS	LYS	LYS	LYS	D1628	D1628	D1628	R1466	L1364	K1300	R1136	N1031	P938	T813
TRP	TRP	TRP	TRP	L1630	L1630	L1630	L1467	I1365	V1297	D1137	G1032	I940	V814
VAL	VAL	VAL	VAL	F1551	F1551	F1551	L1468	I1385	K1300	K1144	G1033	L945	Y832
ASP	ASP	ASP	ASP	Q1552	Q1552	Q1552	N1469	I1369	V1307	V1147	L1034	E946	D835
ASP	ASP	ASP	ASP	L1555	L1555	L1555	M1474	Y1372	P1308	V1153	Y1043	P947	T836
THR	THR	THR	THR	G1559	G1559	G1559	L1478	Q1373	S1309	W1170	Y1044	P948	K837
GLY	GLY	GLY	GLY	I1560	I1560	I1560	E1482	P1374	R1310	G1045	G1045	L950	L841
ASP	ASP	ASP	ASP	H1563	H1563	H1563	G1483	W1375	F1312	E1171	L1046	L961	E848
GLU	GLU	GLU	GLU	P1567	P1567	P1567	I1484	F1379	V1314	W1172	D1049	L962	R855
THR	THR	THR	THR	I1571	I1571	I1571	T1493	S1382	M1307	V1153	Y1043	V965	N857
ASN	ASN	ASN	ASN	S1572	S1572	S1572	W1498	V1385	P1308	W1153	Y1043	L965	
LEU	LEU	LEU	LEU	L1573	L1573	L1573	E1499	L1391	R1310	W1170	G1045	L965	
GLY	GLY	GLY	GLY	I1574	I1574	I1574	G1500	L1391	F1311	E1171	L1046	L965	
ASN	ASN	ASN	ASN	Q1575	Q1575	Q1575	L1501	R1392	P1312	W1172	D1049	L965	
LEU	LEU	LEU	LEU	I1576	I1576	I1576	E1504	R1393	V1314	S1173	L1055	L965	
THR	THR	THR	THR	F1577	F1577	F1577	K1396	E1395	V1315	W1173	L1055	L965	
THR	THR	THR	THR	R1578	R1578	R1578	K1505	E1395	V1315	W1173	L1055	L965	
LYS	LYS	LYS	LYS	A1579	A1579	A1579	ALA	I1397	T1318	K1180	L1055	L965	
GLN	GLN	GLN	GLN	H1580	H1580	H1580	SER	I1397	P1319	W1179	L1055	L965	
ILE	ILE	ILE	ILE	L1581	L1581	L1581	GLY	I1397	K1320	N1188	M1061	L965	
VAL	VAL	VAL	VAL	W1582	W1582	W1582	PHE	L1403	E1321	C1189	A1062	L965	
THR	THR	THR	THR	Q1583	Q1583	Q1583	GLU	L1408	L1322	M1190	G1063	L965	
ARG	ARG	ARG	ARG	K1584	K1584	K1584	GLU	L1409	G1323	C1190	P1064	L965	
								D1410	G1324				

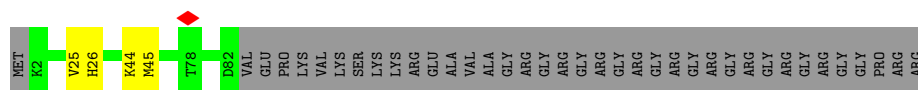


- Molecule 5: Probable ATP-dependent RNA helicase DDX23

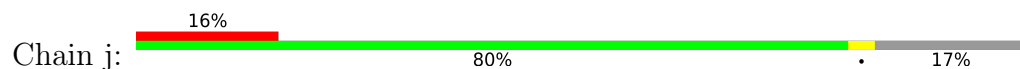
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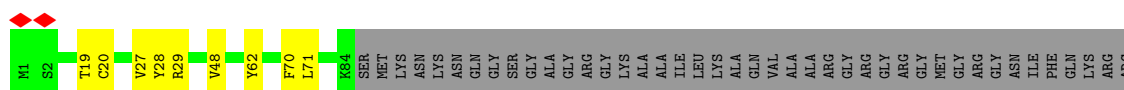




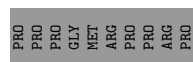
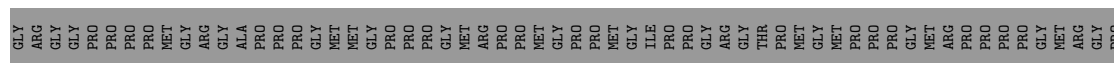
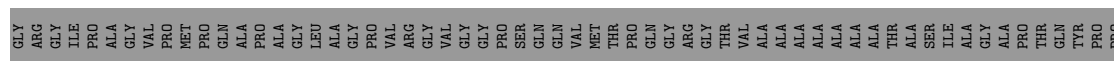
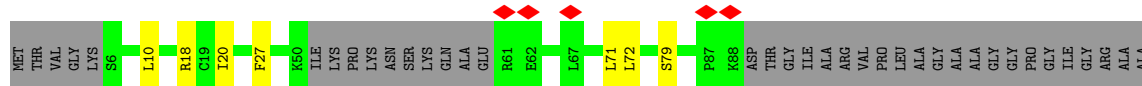
- Molecule 11: Small nuclear ribonucleoprotein Sm D2



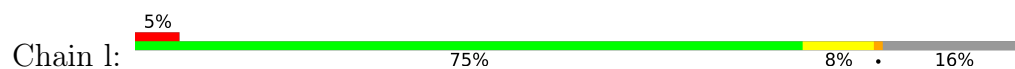
- Molecule 12: Small nuclear ribonucleoprotein Sm D3



- Molecule 13: Small nuclear ribonucleoprotein-associated proteins B and B'



- Molecule 14: Small nuclear ribonucleoprotein E



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76918	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 ($e^-/\text{\AA}^2$)	40.5	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.051	Depositor
Minimum map value	-0.392	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	526.6296, 526.6296, 526.6296	wwPDB
Map dimensions	504, 504, 504	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0449, 1.0449, 1.0449	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	F	0.21	0/896	0.44	0/1224
2	A	0.17	0/13608	0.38	1/18483 (0.0%)
3	5	0.12	0/2444	0.30	0/3798
4	E	0.10	0/298	0.27	0/414
5	D	0.17	0/464	0.44	0/620
6	C	0.18	0/6777	0.39	4/9214 (0.0%)
7	B	0.19	0/202	0.50	0/268
8	m	0.30	0/355	0.63	0/490
9	n	0.19	0/363	0.54	0/501
10	i	0.35	0/400	0.60	0/556
11	j	0.17	0/485	0.47	0/674
12	k	0.23	0/413	0.45	0/573
13	h	0.21	0/358	0.57	1/495 (0.2%)
14	l	0.22	0/380	0.82	2/528 (0.4%)
All	All	0.18	0/27443	0.40	8/37838 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	l	15	VAL	CA-C-N	7.75	135.25	121.76
14	l	15	VAL	C-N-CA	7.75	135.25	121.76
6	C	144	CYS	N-CA-CB	7.07	120.47	109.94
13	h	10	LEU	N-CA-C	-5.82	105.44	112.54
2	A	867	ILE	CA-CB-CG1	5.49	119.73	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	887	0	714	30	0
2	A	13247	0	12877	344	0
3	5	2192	0	1111	42	0
4	E	300	0	132	0	0
5	D	455	0	450	13	0
6	C	6629	0	6607	124	0
7	B	201	0	214	10	0
8	m	356	0	156	5	0
9	n	364	0	160	6	0
10	i	401	0	165	2	0
11	j	487	0	199	2	0
12	k	414	0	185	6	0
13	h	360	0	149	4	0
14	l	381	0	159	5	0
15	C	32	0	12	1	0
All	All	26706	0	23290	552	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 11.

The worst 5 of 552 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)
2:A:1474:MET:HE3	2:A:1474:MET:HA	1.51	0.91
2:A:885:LEU:HD21	2:A:922:LEU:HD21	1.53	0.89
2:A:1365:ILE:HG13	2:A:1474:MET:HE1	1.55	0.86
2:A:1307:MET:HE3	2:A:1307:MET:H	1.39	0.86
2:A:813:THR:HG21	2:A:996:LEU:HD11	1.59	0.84

There are no symmetry-related clashes.

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	F	134/341 (39%)	123 (92%)	10 (8%)	1 (1%)	18	49
2	A	1615/2335 (69%)	1558 (96%)	56 (4%)	1 (0%)	48	78
4	E	56/941 (6%)	56 (100%)	0	0	100	100
5	D	50/820 (6%)	49 (98%)	1 (2%)	0	100	100
6	C	845/972 (87%)	813 (96%)	31 (4%)	1 (0%)	48	78
7	B	25/2136 (1%)	25 (100%)	0	0	100	100
8	m	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
9	n	72/76 (95%)	64 (89%)	8 (11%)	0	100	100
10	i	79/119 (66%)	73 (92%)	6 (8%)	0	100	100
11	j	94/118 (80%)	84 (89%)	10 (11%)	0	100	100
12	k	82/126 (65%)	78 (95%)	4 (5%)	0	100	100
13	h	69/240 (29%)	67 (97%)	2 (3%)	0	100	100
14	l	75/92 (82%)	72 (96%)	3 (4%)	0	100	100
All	All	3267/8402 (39%)	3130 (96%)	134 (4%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1020	LYS
6	C	148	CYS
1	F	126	VAL

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	F	58/281 (21%)	57 (98%)	1 (2%)	53	74
2	A	1384/2108 (66%)	1357 (98%)	27 (2%)	48	72
5	D	48/721 (7%)	44 (92%)	4 (8%)	10	35
6	C	737/866 (85%)	721 (98%)	16 (2%)	45	71
7	B	22/1908 (1%)	21 (96%)	1 (4%)	24	56
All	All	2249/5884 (38%)	2200 (98%)	49 (2%)	45	71

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	D	244	SER
6	C	162	ASP
5	D	246	GLU
6	C	109	LEU
6	C	357	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
6	C	139	HIS
6	C	337	GLN
6	C	571	ASN
6	C	451	HIS
2	A	542	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	5	101/117 (86%)	34 (33%)	4 (3%)

5 of 34 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	5	4	C
3	5	5	U
3	5	6	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	5	9	G
3	5	20	G

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	5	57	G
3	5	58	U
3	5	96	A
3	5	105	U

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	GTP	C	1001	-	33,34,34	0.60	0	50,54,54	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	GTP	C	1001	-	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

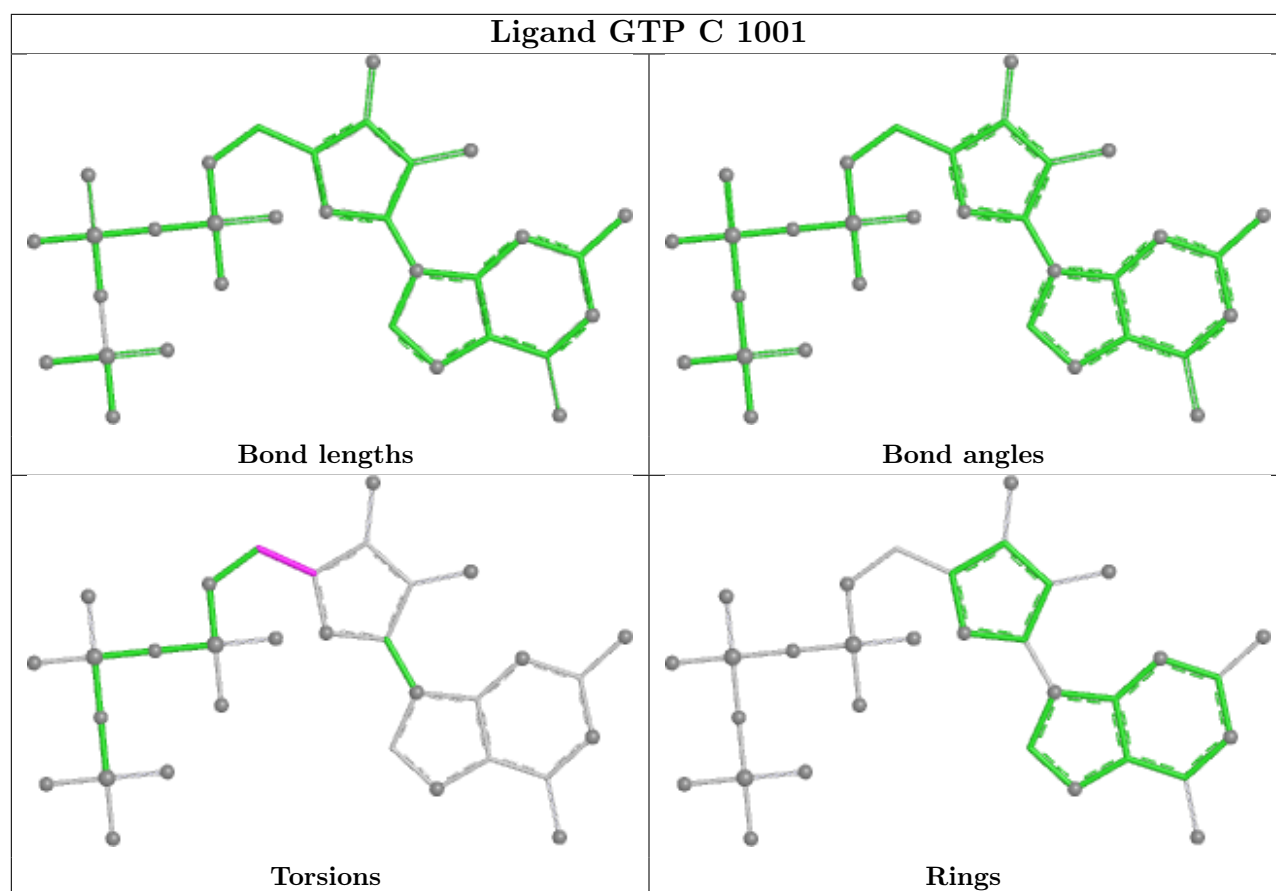
Mol	Chain	Res	Type	Atoms
15	C	1001	GTP	O4'-C4'-C5'-O5'
15	C	1001	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	1001	GTP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

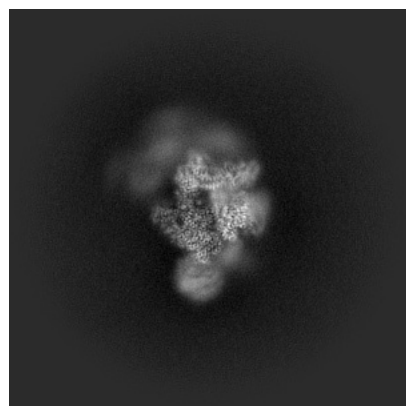
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18267. These allow visual inspection of the internal detail of the map and identification of artifacts.

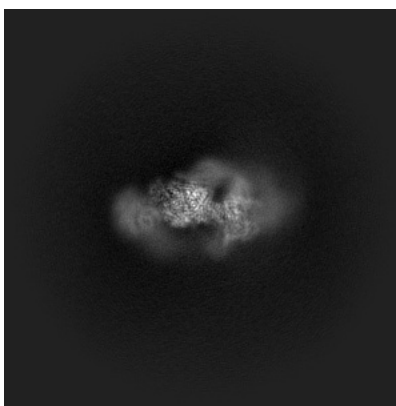
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

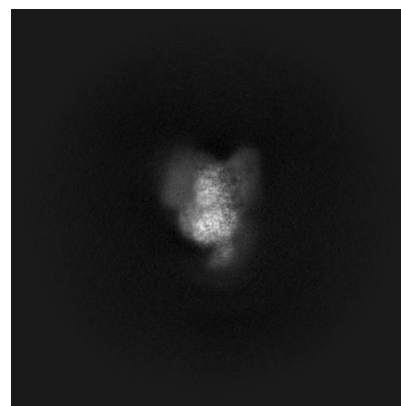
6.1.1 Primary map



X

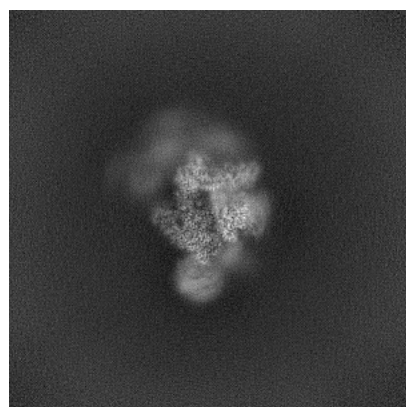


Y

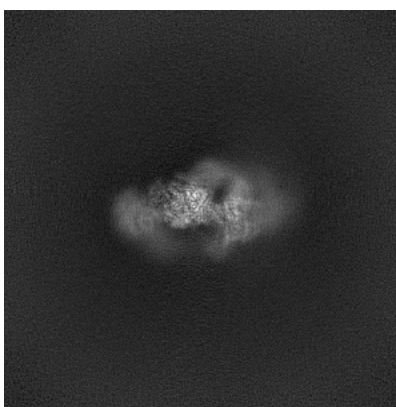


Z

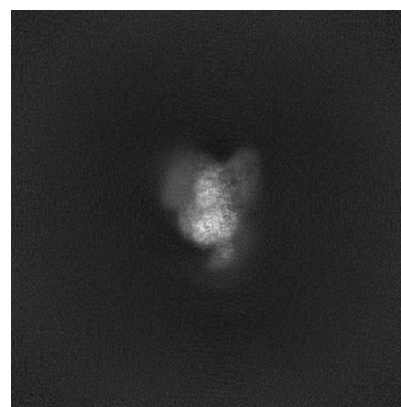
6.1.2 Raw map



X



Y

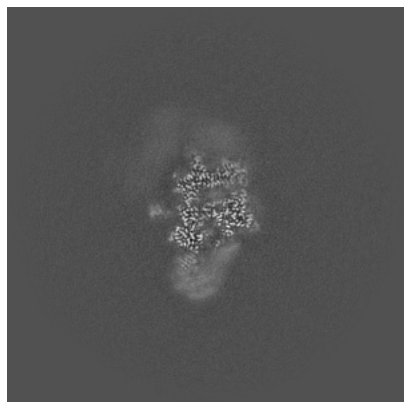


Z

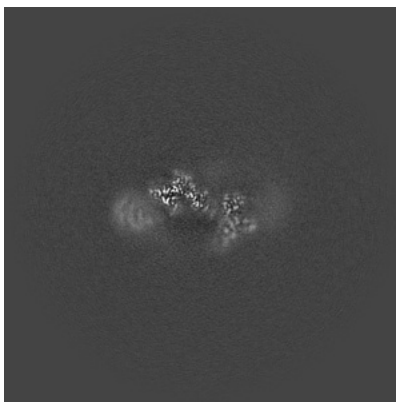
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

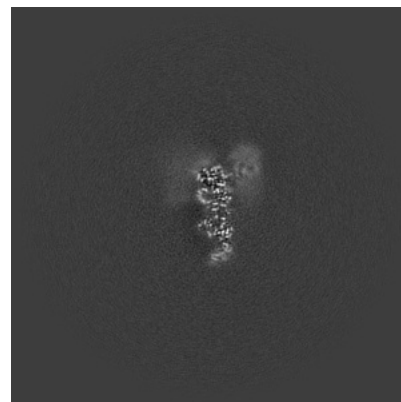
6.2.1 Primary map



X Index: 252

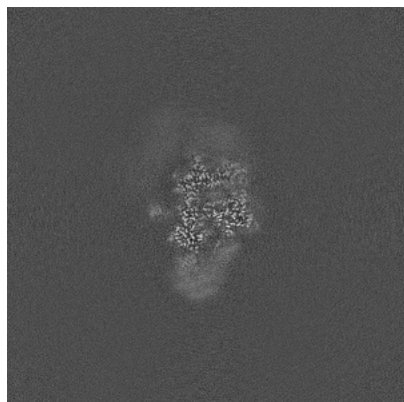


Y Index: 252

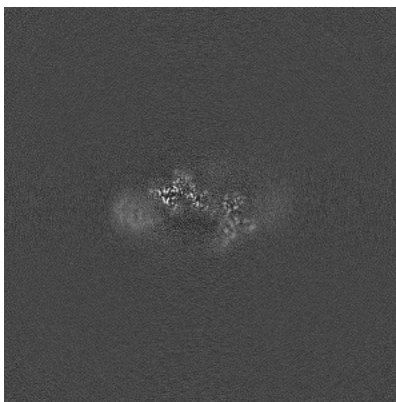


Z Index: 252

6.2.2 Raw map



X Index: 252



Y Index: 252

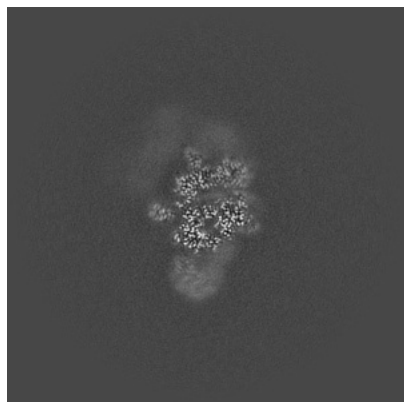


Z Index: 252

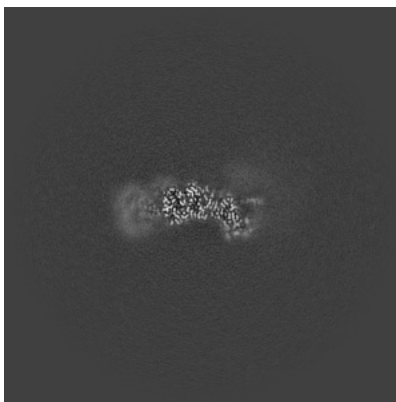
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

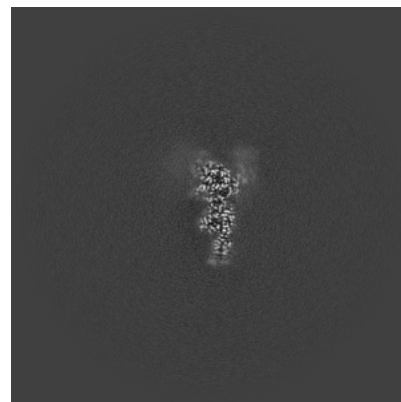
6.3.1 Primary map



X Index: 256

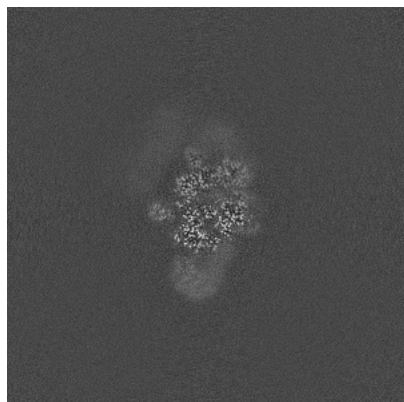


Y Index: 228

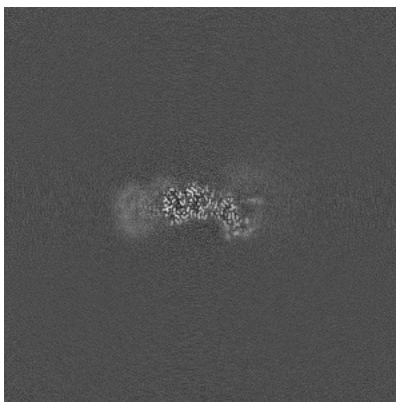


Z Index: 241

6.3.2 Raw map



X Index: 256



Y Index: 228

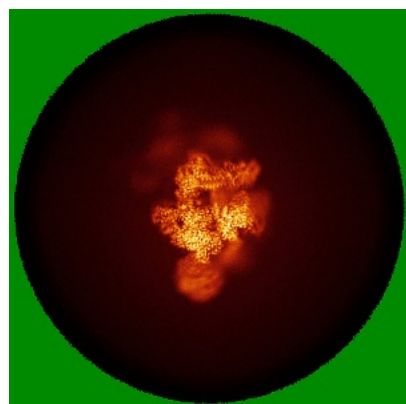


Z Index: 241

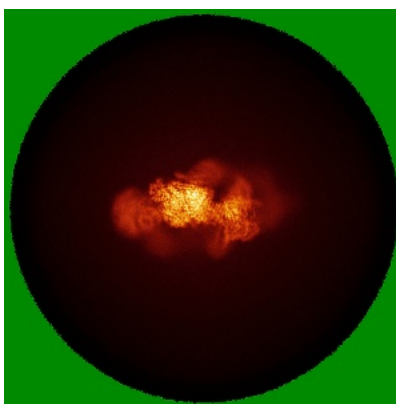
The images above show the largest variance slices of the map in three orthogonal directions.

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

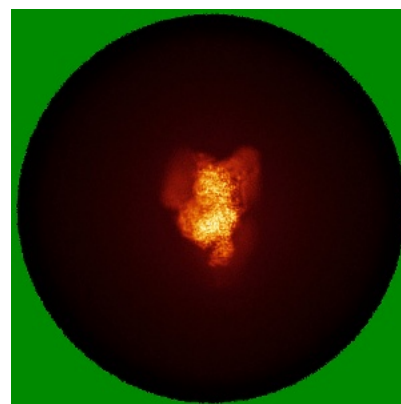
6.4.1 Primary map



X

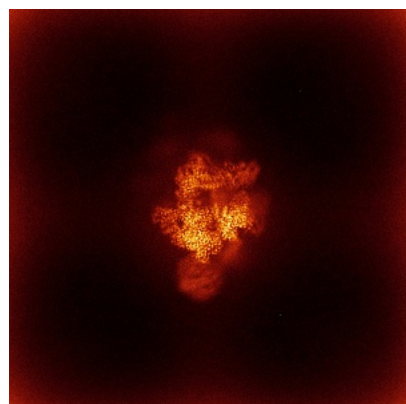


Y

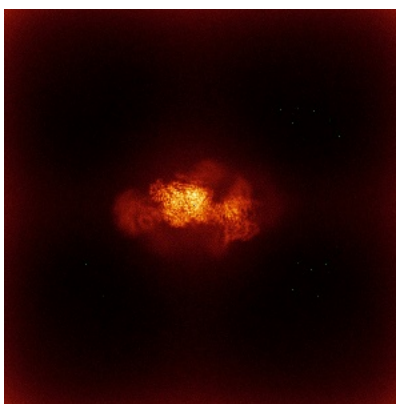


Z

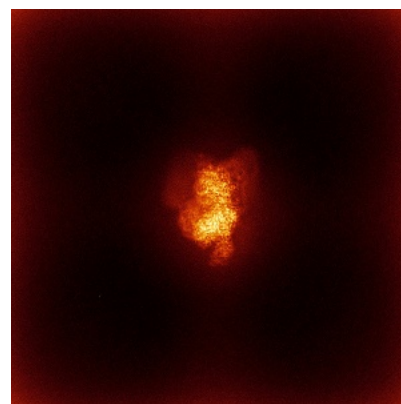
6.4.2 Raw map



X



Y

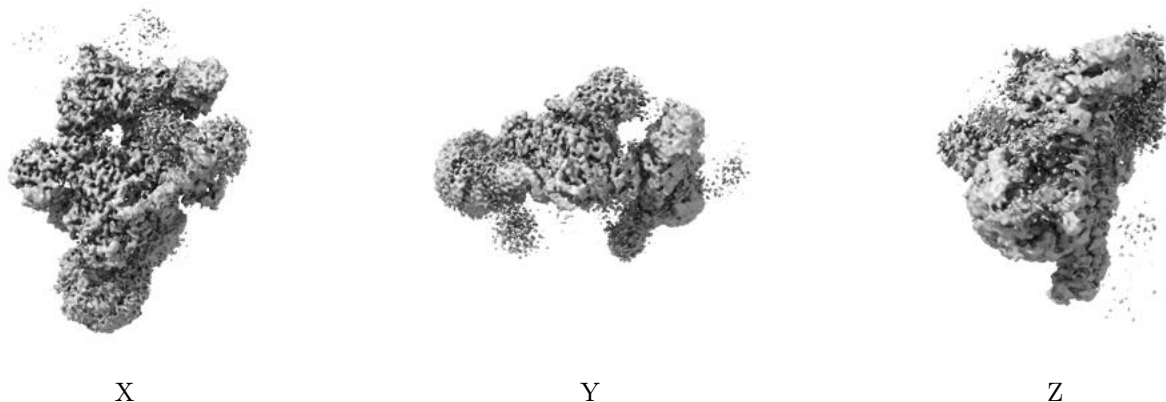


Z

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

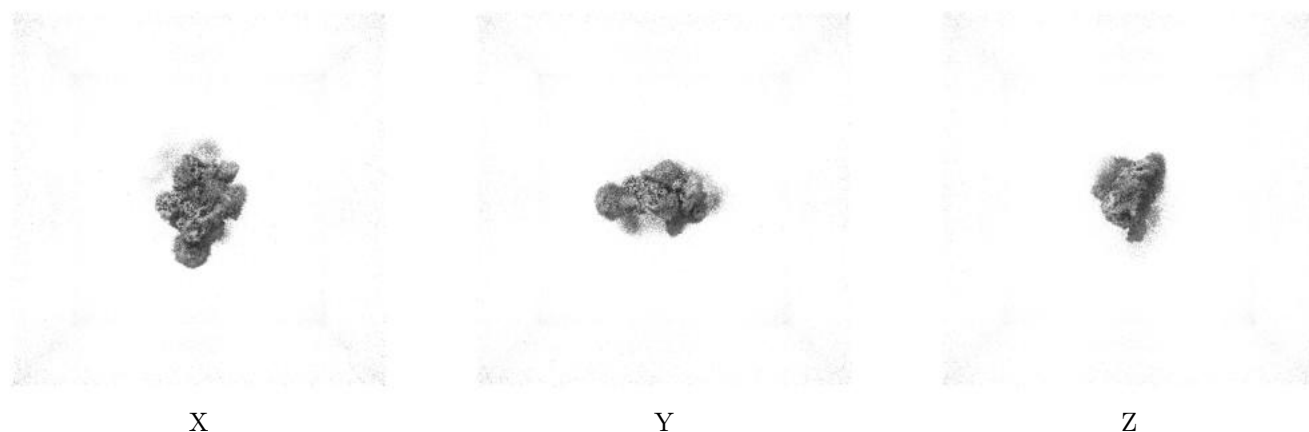
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

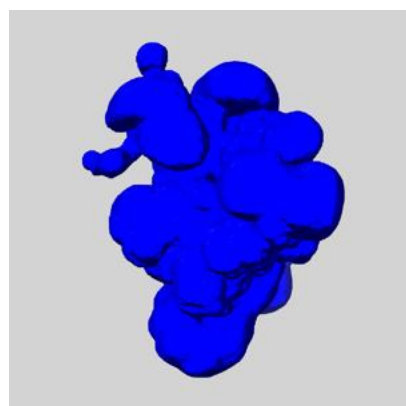
6.6 Mask visualisation [i](#)

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

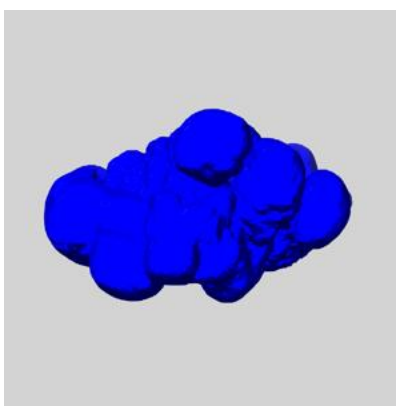
A mask typically either:

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

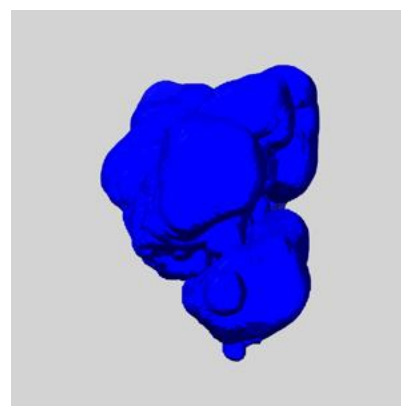
6.6.1 emd_18267_msk_1.map [i](#)



X



Y

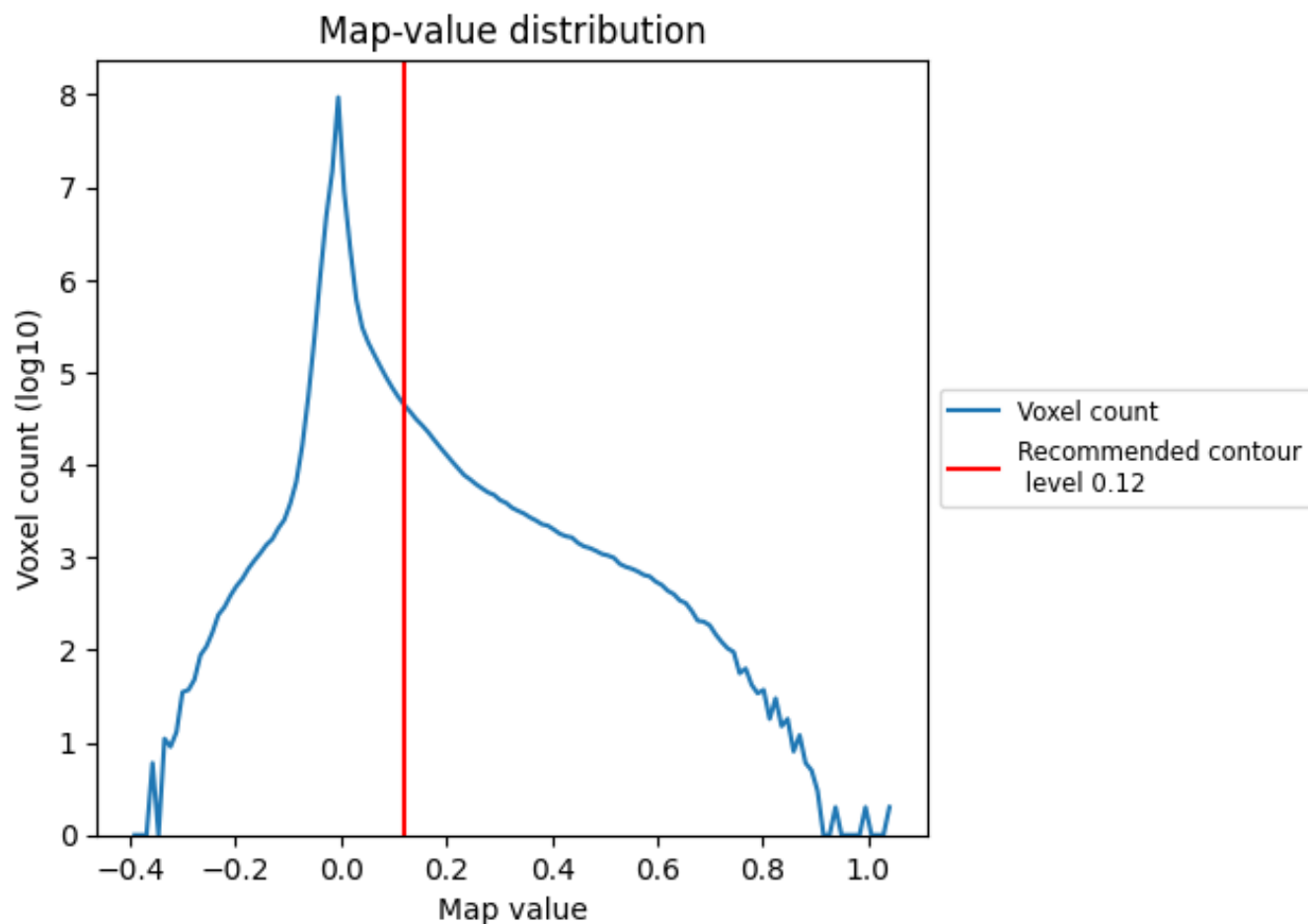


Z

7 Map analysis [i](#)

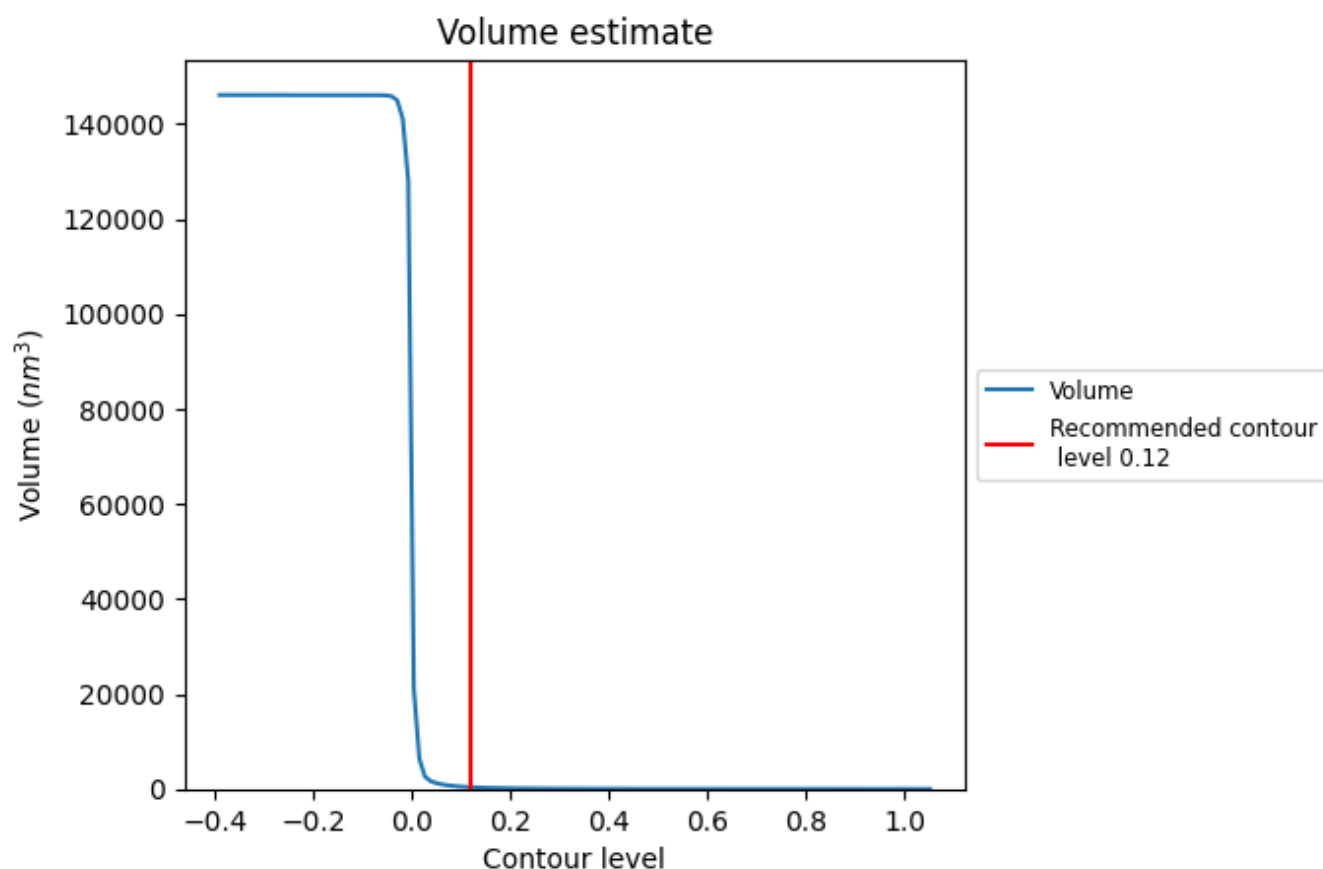
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

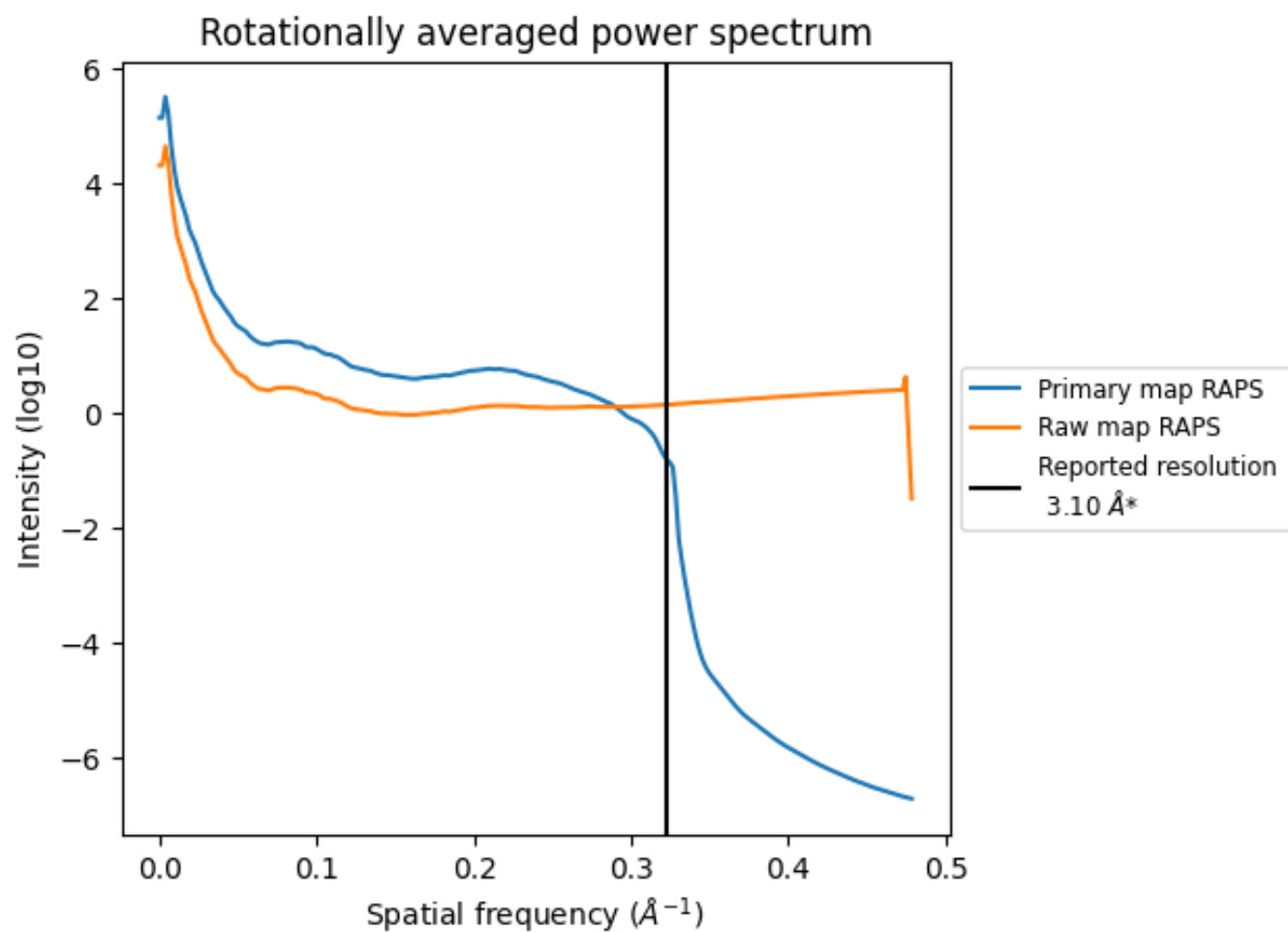
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 362 nm³; this corresponds to an approximate mass of 327 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 ⓘ

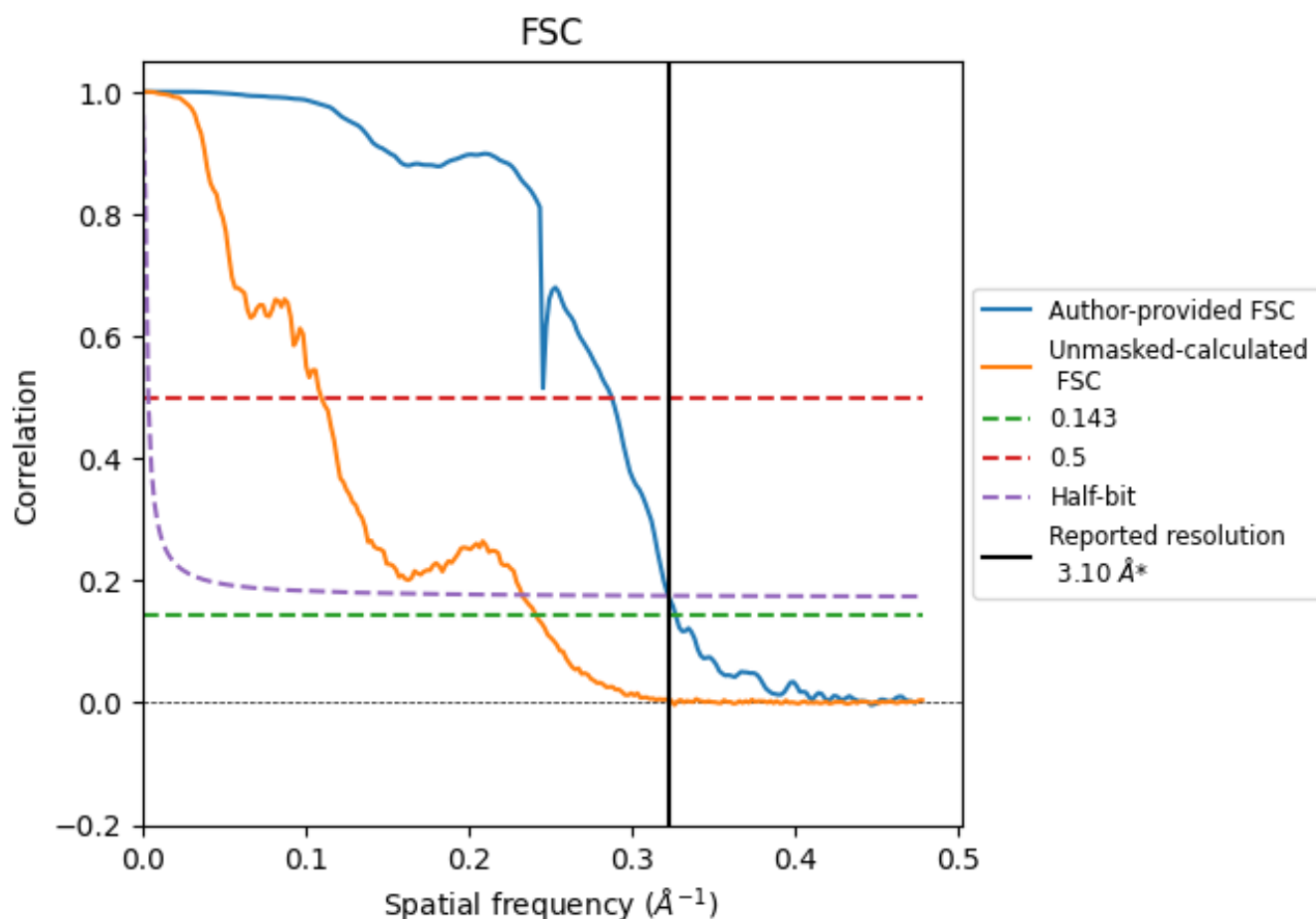


*Reported resolution corresponds to spatial frequency of $0.323 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.323 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

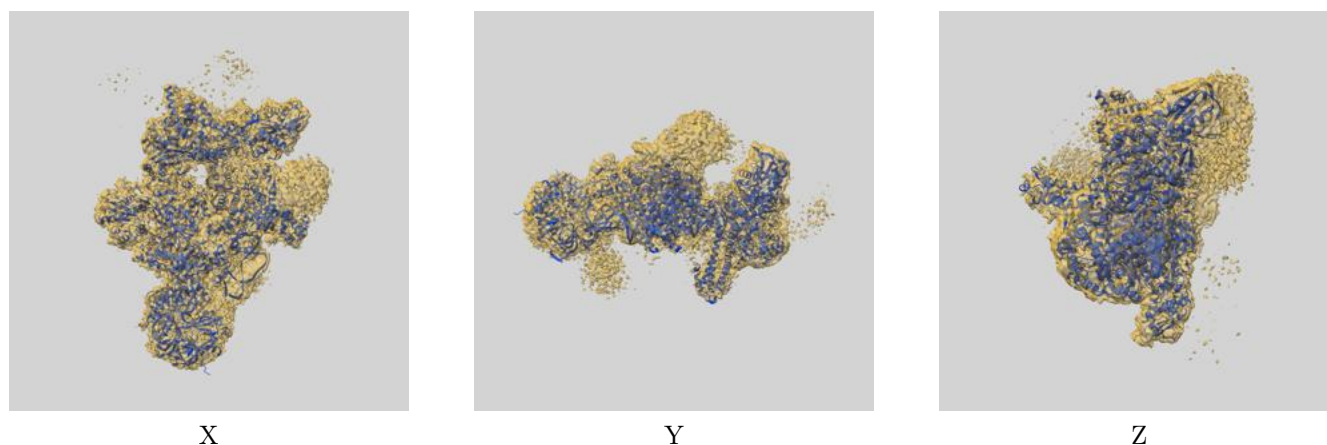
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.47	3.10
Unmasked-calculated*	4.14	9.11	4.29

*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 4.14 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

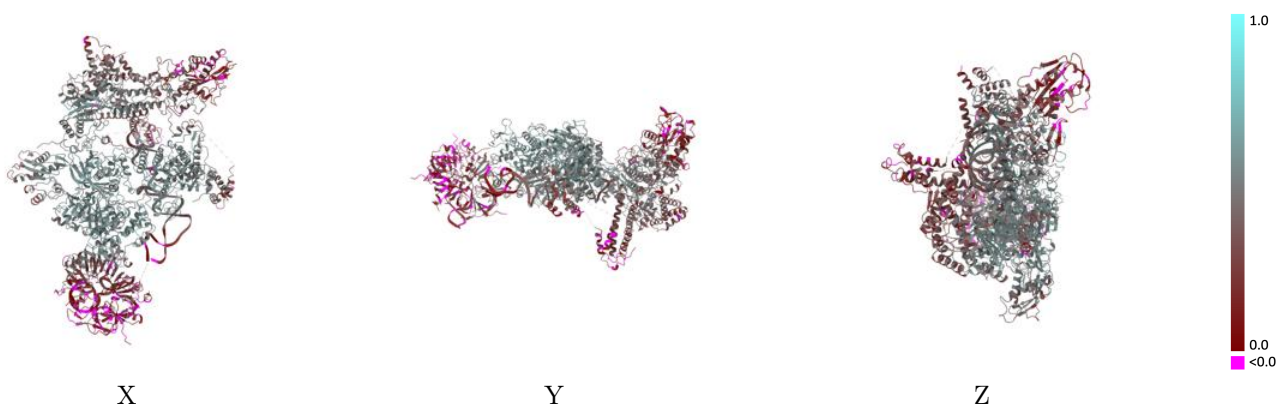
This section contains information regarding the fit between EMDB map EMD-18267 and PDB model 8Q91. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



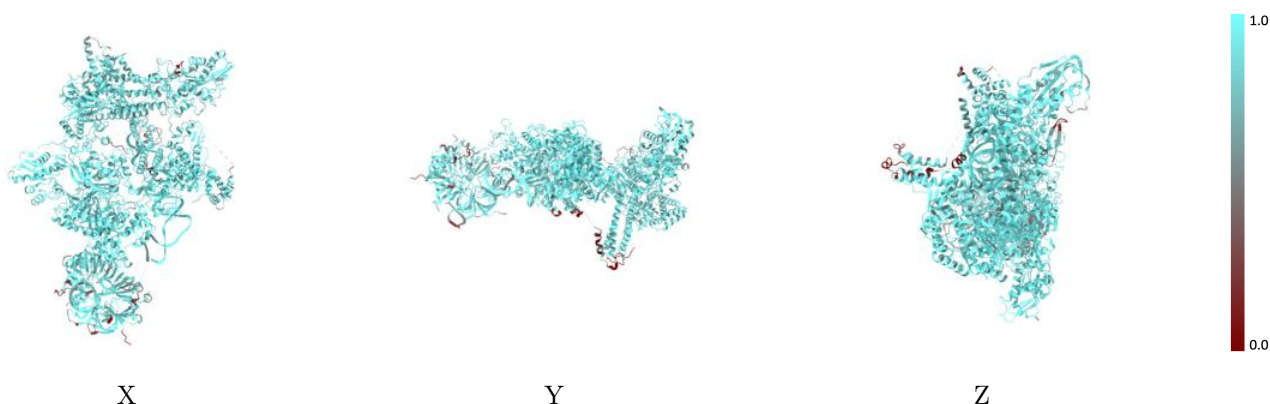
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



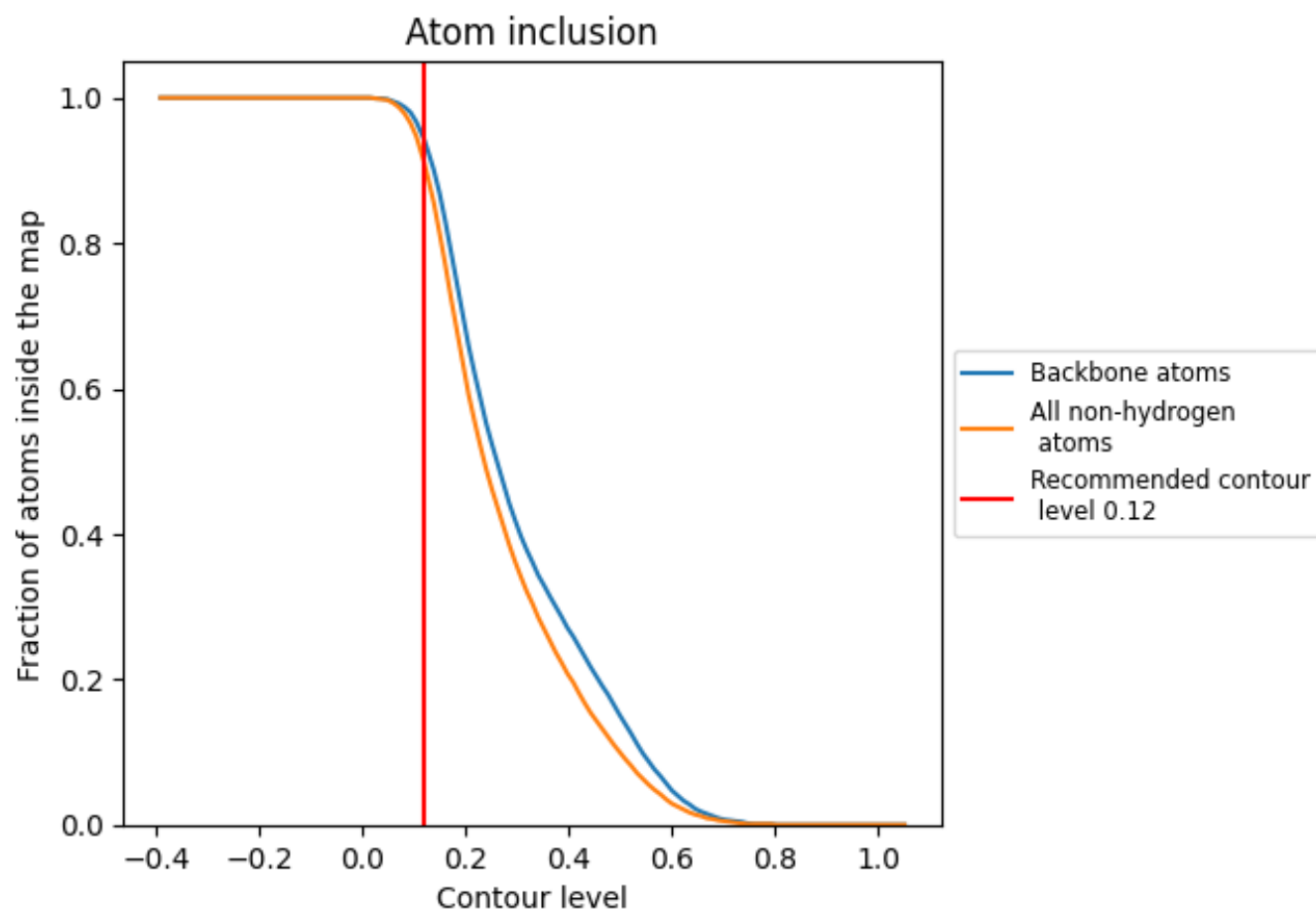
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 91% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9100	 0.4170
5	 0.8850	 0.2720
A	 0.9190	 0.4350
B	 0.7870	 0.4280
C	 0.9590	 0.5270
D	 0.8880	 0.5120
E	 0.4570	 0.2020
F	 0.8490	 0.3660
h	 0.8940	 0.2550
i	 0.9250	 0.1800
j	 0.7700	 0.0980
k	 0.9350	 0.3980
l	 0.8920	 0.1310
m	 0.8480	 0.0930
n	 0.7450	 0.2620

