wwPDB EM Validation Summary Report (i)

Oct 8, 2026 – 12:26 PM EDT

PDB ID	:	9PBZ / pdb_00009pbz
EMDB ID	:	EMD-71494
Title	:	PolII/TFIIF of PIC-Med-SWI/SNF-Nucleosome
Authors	:	Yang, C.; Nagai, S.; Chen, D.-H.
Deposited on	:	2025-06-26
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

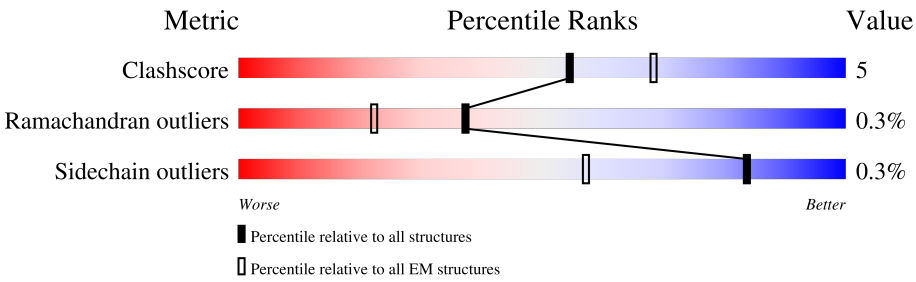
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

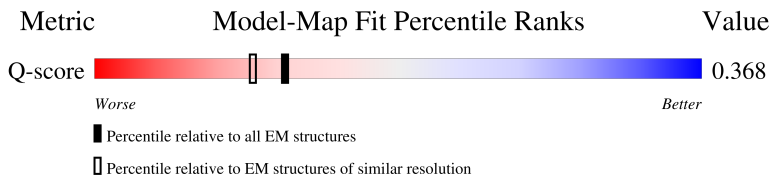
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	C	318	78% • 18%
2	E	215	89% 10% •
3	F	155	48% 5% 46%
4	G	171	22% 89% 9% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	I	122	9% 67% 16% 5% 7% 5%
6	J	70	6% 83% 14%
7	K	120	10% 88% 8%
8	L	70	61% 36%
9	S	309	29% 41% 9% 47%
10	M	345	10% 23% 74%
11	B	1224	9% 87% 6% 6%
12	A	1733	71% 9% 19%
13	D	221	26% 53% 17% 29%
14	H	146	5% 79% 12% 7%
15	Q	735	15% 27% 71%
16	R	400	28% 47% 50%

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 36587 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 DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	262	2061	1299	343	406	13	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	213	1744	1107	308	318	11	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	F	83	670	428	114	125	3	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	171	1340	861	222	249	8	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	116	944	581	172	181	10	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	J	69	569	362	101	100	6	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	K	115	924	593	157	172	2	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	45	359	221	71	63	4	0	0

- Molecule 9 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	S	164	1302	812	230	252	8	0	0

- Molecule 10 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	M	89	679	429	112	129	9	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	1155	9200	5818	1610	1717	55	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	A	1398	10996	6931	1926	2078	61	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	D	157	1253	779	220	252	2	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	H	136	1089	686	184	215	4	0	0

- Molecule 15 is a protein called Transcription initiation factor IIF subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Q	214	1817	1149	337	324	7	0	0

- Molecule 16 is a protein called Transcription initiation factor IIF subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	R	198	1629	1011	293	317	8	0	0

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
17	C	1	1	1	0
17	I	2	2	2	0
17	J	1	1	1	0
17	L	1	1	1	0
17	S	1	1	1	0
17	M	1	1	1	0
17	B	1	1	1	0
17	A	2	2	2	0

- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

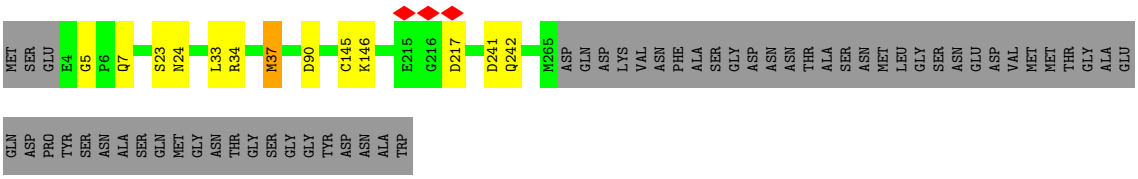
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
18	A	1	1	1	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

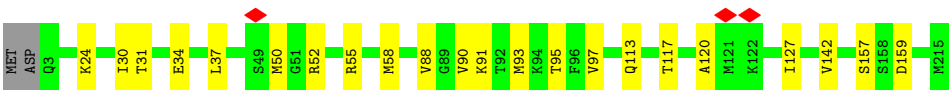
• Molecule 1: DNA-directed RNA polymerase II subunit RPB3

Chain C:



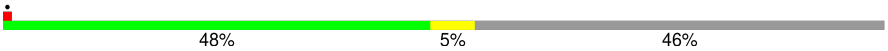
• Molecule 2: DNA-directed RNA polymerases I, II, and III subunit RPABC1

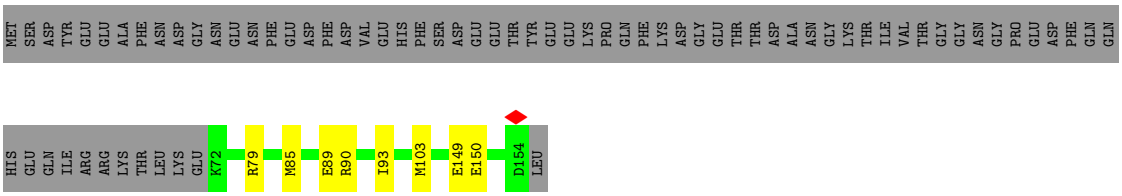
Chain E:



• Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC2

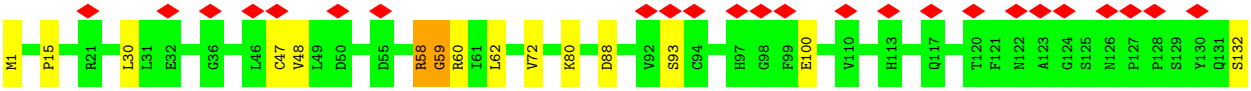
Chain F:

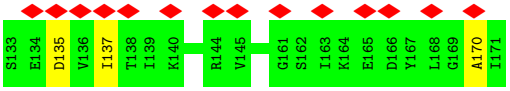




• Molecule 4: DNA-directed RNA polymerase II subunit RPB7

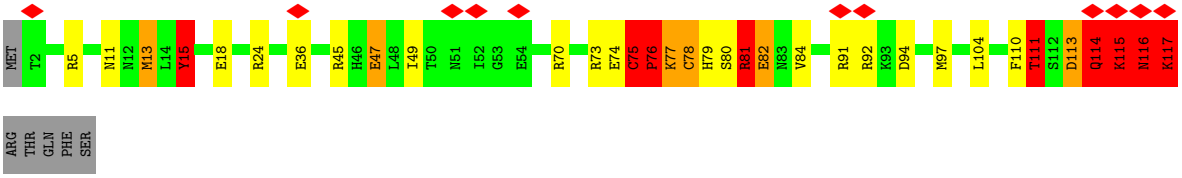
Chain G:





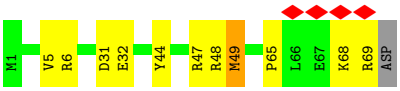
• Molecule 5: DNA-directed RNA polymerase II subunit RPB9

Chain I:



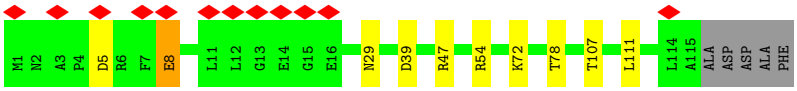
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



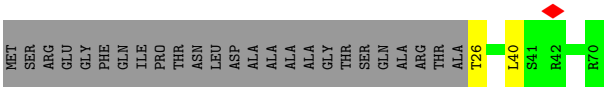
• Molecule 7: DNA-directed RNA polymerase II subunit RPB11

Chain K:



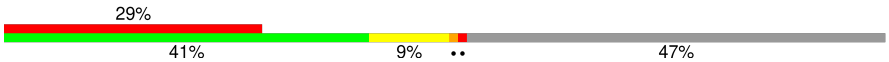
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC4

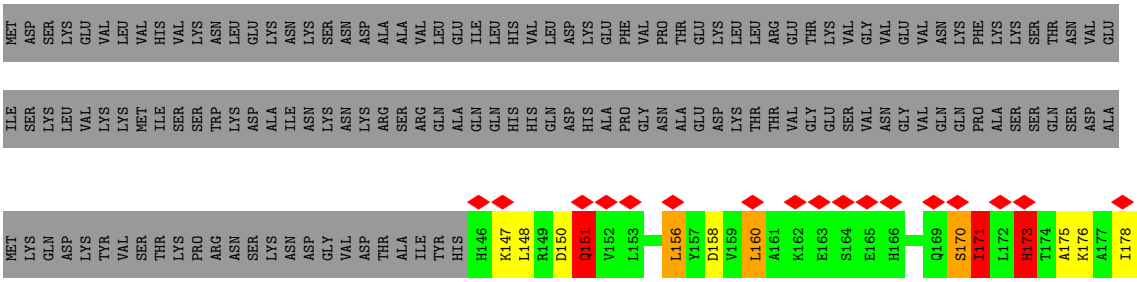
Chain L:

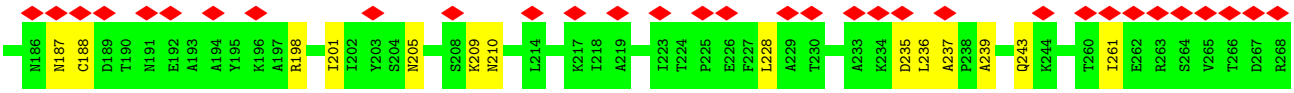


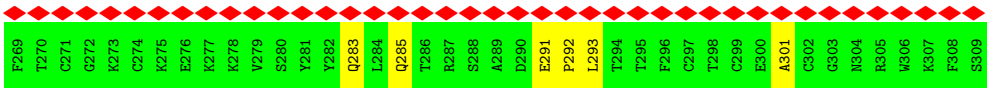
• Molecule 9: Transcription elongation factor S-II

Chain S:



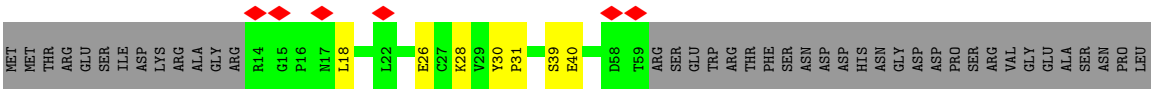


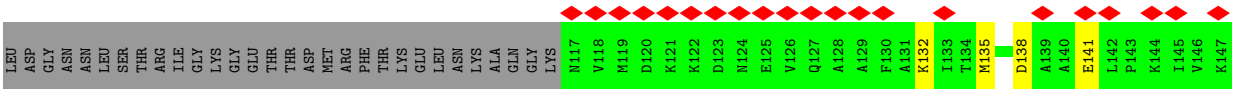


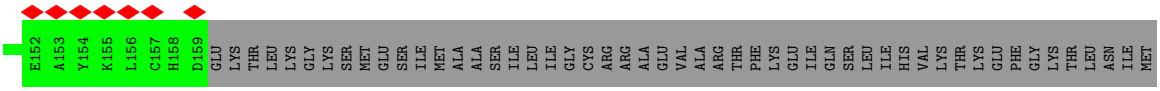


- Molecule 10: Transcription initiation factor IIB

Chain M:

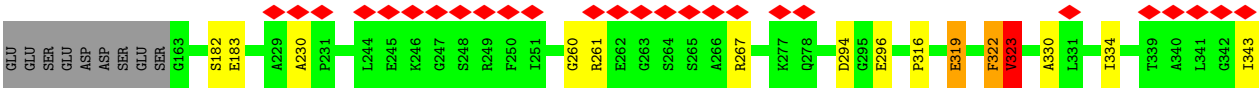


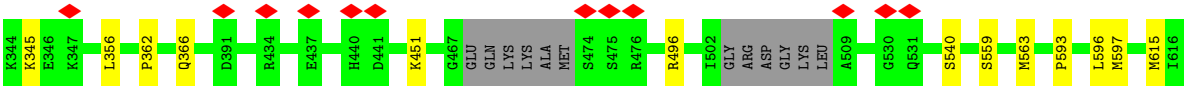


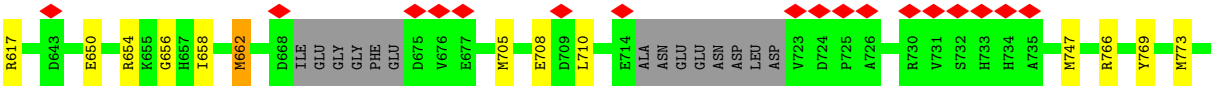


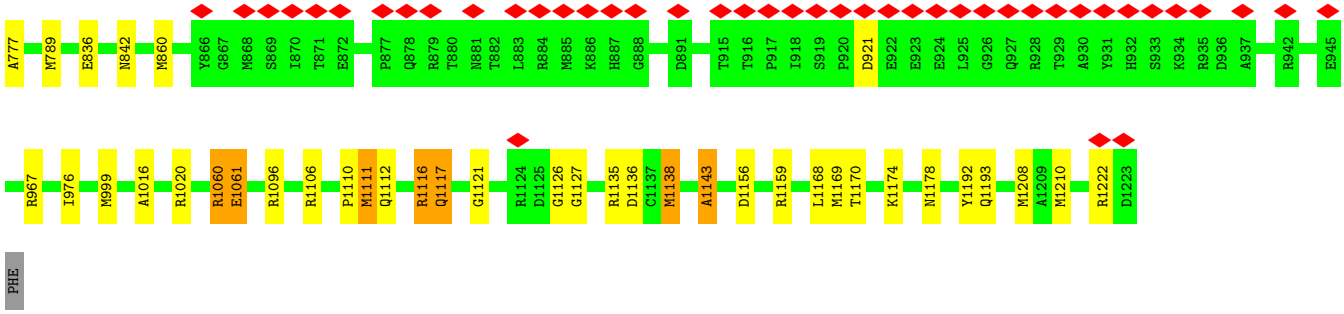
- Molecule 11: DNA-directed RNA polymerase II subunit RPB2

Chain B:



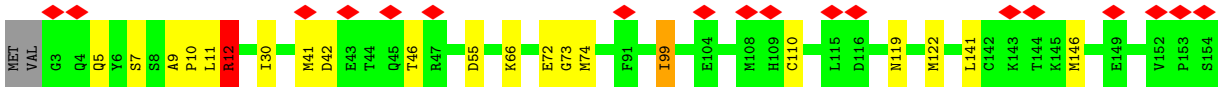


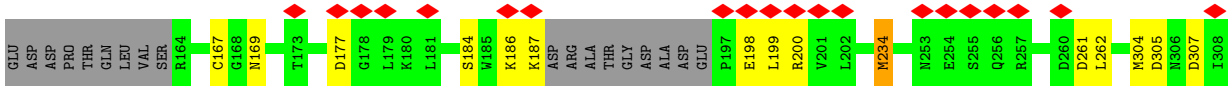


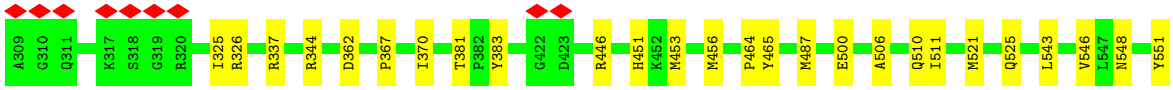


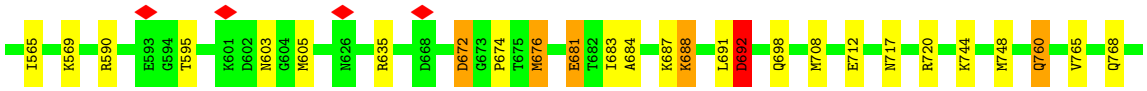
- Molecule 12: DNA-directed RNA polymerase II subunit RPB1

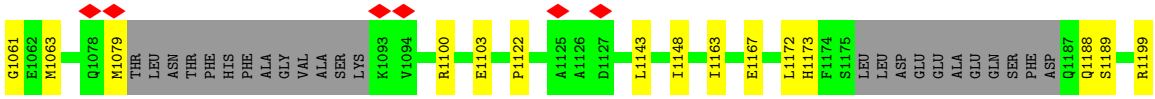
Chain A:

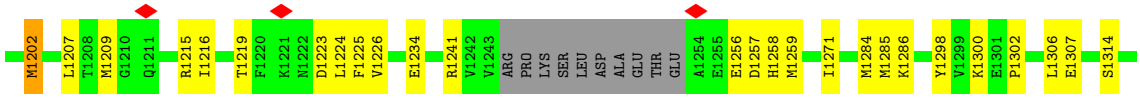


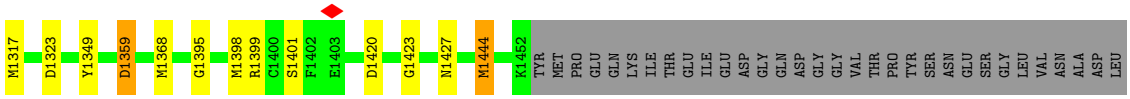


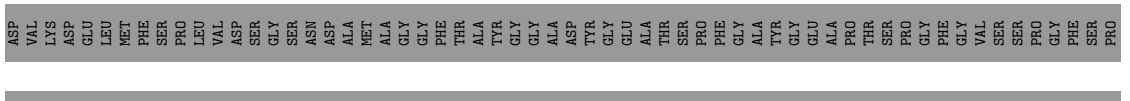


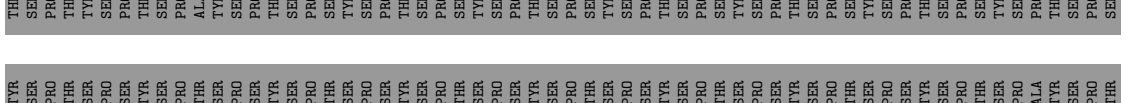


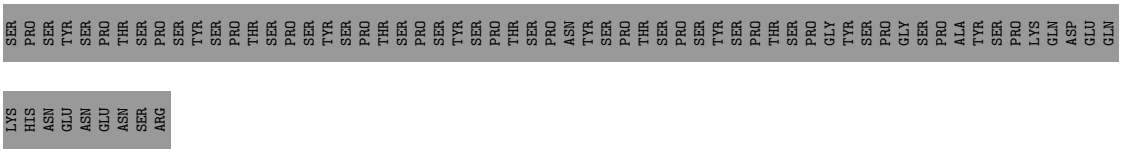






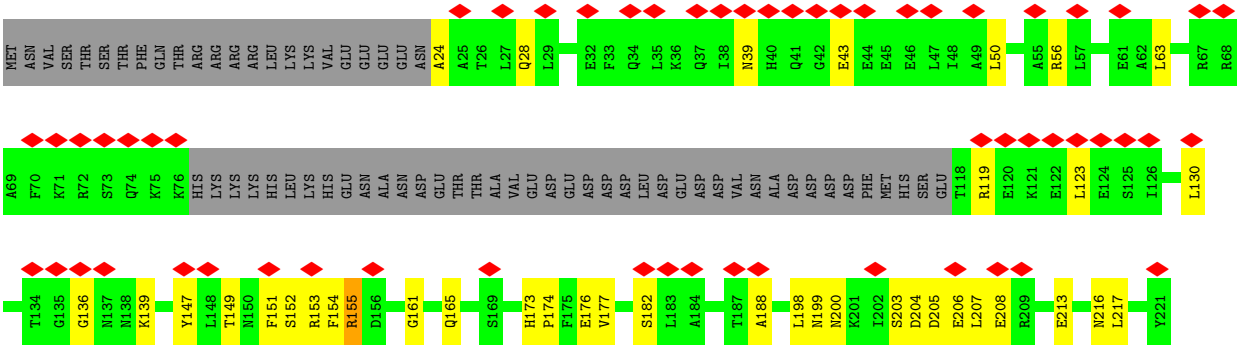






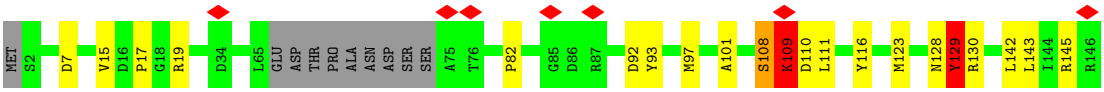
• Molecule 13: DNA-directed RNA polymerase II subunit RPB4

Chain D:



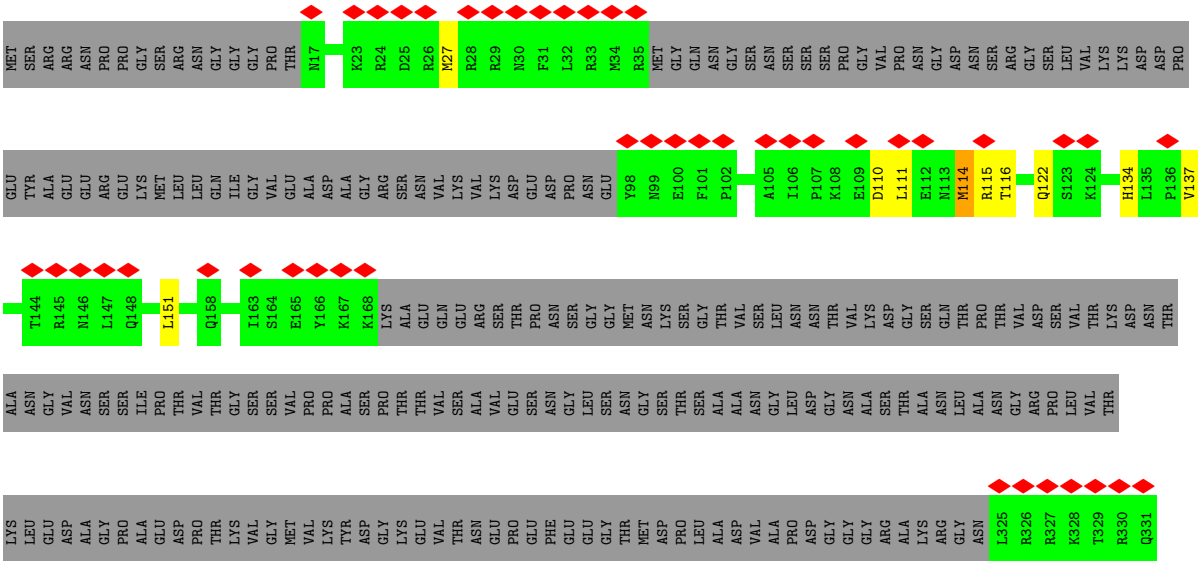
• Molecule 14: DNA-directed RNA polymerases I, II, and III subunit RPABC3

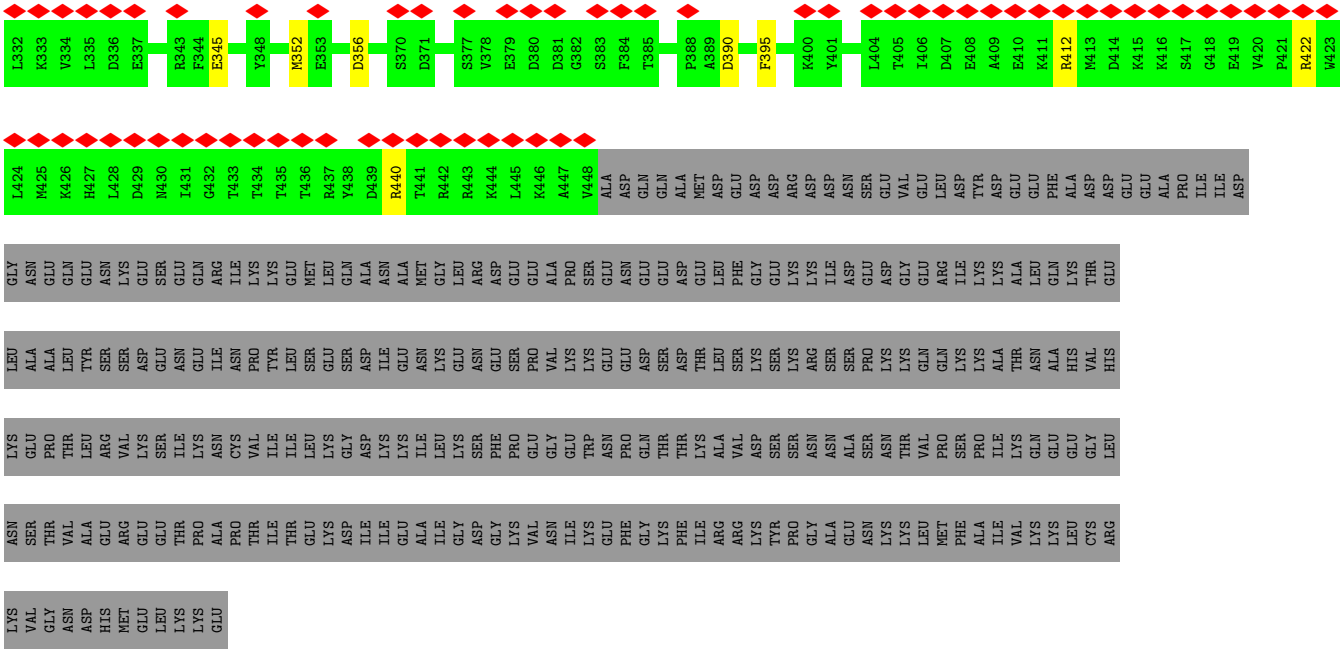
Chain H:



• Molecule 15: Transcription initiation factor IIF subunit alpha

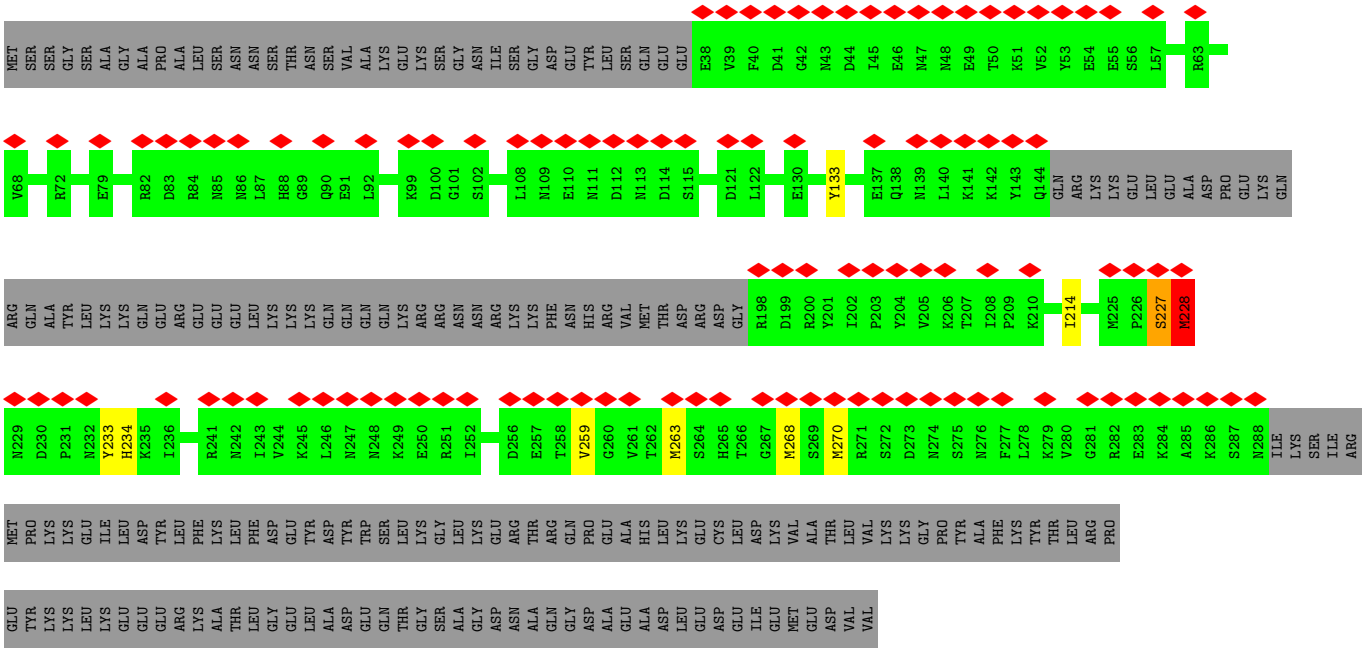
Chain Q:





• Molecule 16: Transcription initiation factor IIF subunit beta

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1102224	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.688	Depositor
Minimum map value	-2.969	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.419	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	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: ZN, MG

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	C	0.45	1/2099 (0.0%)	0.43	1/2845 (0.0%)
2	E	0.31	0/1780	0.47	0/2395
3	F	0.35	0/682	0.49	0/922
4	G	0.46	2/1368 (0.1%)	0.56	0/1844
5	I	2.29	22/962 (2.3%)	2.30	49/1295 (3.8%)
6	J	0.63	2/578 (0.3%)	0.77	2/775 (0.3%)
7	K	0.38	0/942	0.53	1/1272 (0.1%)
8	L	0.19	0/361	0.40	0/478
9	S	1.27	17/1325 (1.3%)	2.17	31/1787 (1.7%)
10	M	0.31	1/687 (0.1%)	0.42	0/927
11	B	0.42	11/9381 (0.1%)	0.63	27/12652 (0.2%)
12	A	0.54	20/11191 (0.2%)	0.72	29/15127 (0.2%)
13	D	0.51	2/1262 (0.2%)	0.63	0/1693
14	H	0.98	10/1107 (0.9%)	1.19	15/1499 (1.0%)
15	Q	0.35	1/1852 (0.1%)	0.43	0/2480
16	R	0.73	5/1652 (0.3%)	0.76	4/2222 (0.2%)
All	All	0.66	94/37229 (0.3%)	0.84	159/50213 (0.3%)

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
5	I	0	10
9	S	1	3
11	B	0	5
12	A	0	7
14	H	1	2
All	All	2	27

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	15	TYR	CZ-OH	46.34	2.35	1.38
5	I	13	MET	SD-CE	28.55	2.50	1.79
12	A	1444	MET	SD-CE	-18.76	1.32	1.79
9	S	173	HIS	CB-CG	-18.67	1.24	1.50
14	H	129	TYR	CA-C	18.10	1.77	1.52

The worst 5 of 159 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	S	173	HIS	CA-CB-CG	66.13	179.93	113.80
5	I	82	GLU	CB-CG-CD	25.76	156.39	112.60
9	S	156	LEU	CB-CG-CD1	20.84	173.21	110.70
14	H	129	TYR	N-CA-C	-19.64	85.15	112.45
11	B	1060	ARG	CG-CD-NE	19.16	154.15	112.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	S	171	ILE	CB
14	H	109	LYS	CA

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	I	15	TYR	Sidechain
5	I	70	ARG	Sidechain
5	I	75	CYS	Mainchain
5	I	81	ARG	Sidechain
5	I	82	GLU	Sidechain

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	C	2061	0	2029	9	0
2	E	1744	0	1772	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	670	0	690	7	0
4	G	1340	0	1357	16	0
5	I	944	0	900	38	0
6	J	569	0	585	8	0
7	K	924	0	934	7	0
8	L	359	0	381	1	0
9	S	1302	0	1295	34	0
10	M	679	0	694	6	0
11	B	9200	0	9193	75	0
12	A	10996	0	11079	120	0
13	D	1253	0	1275	31	0
14	H	1089	0	1062	22	0
15	Q	1817	0	1843	12	0
16	R	1629	0	1619	7	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0
17	M	1	0	0	0	0
17	S	1	0	0	0	0
18	A	1	0	0	0	0
All	All	36587	0	36708	371	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 5.

The worst 5 of 371 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)
5:I:117:LYS:CB	5:I:117:LYS:CG	1.82	1.57
14:H:129:TYR:C	14:H:129:TYR:CA	1.77	1.56
5:I:111:THR:CB	5:I:111:THR:CG2	1.76	1.55
5:I:117:LYS:CB	5:I:117:LYS:HD3	1.30	1.55
5:I:117:LYS:CB	5:I:117:LYS:CD	1.89	1.48

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	C	260/318 (82%)	253 (97%)	6 (2%)	1 (0%)	30	61
2	E	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
3	F	81/155 (52%)	77 (95%)	4 (5%)	0	100	100
4	G	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
5	I	114/122 (93%)	93 (82%)	17 (15%)	4 (4%)	3	23
6	J	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
7	K	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
8	L	43/70 (61%)	41 (95%)	2 (5%)	0	100	100
9	S	162/309 (52%)	147 (91%)	14 (9%)	1 (1%)	21	54
10	M	85/345 (25%)	83 (98%)	2 (2%)	0	100	100
11	B	1139/1224 (93%)	1109 (97%)	28 (2%)	2 (0%)	43	72
12	A	1386/1733 (80%)	1298 (94%)	84 (6%)	4 (0%)	36	65
13	D	153/221 (69%)	142 (93%)	11 (7%)	0	100	100
14	H	132/146 (90%)	127 (96%)	4 (3%)	1 (1%)	16	49
15	Q	208/735 (28%)	203 (98%)	5 (2%)	0	100	100
16	R	192/400 (48%)	186 (97%)	6 (3%)	0	100	100
All	All	4515/6354 (71%)	4304 (95%)	198 (4%)	13 (0%)	37	65

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	I	76	PRO
5	I	113	ASP
9	S	236	LEU
14	H	109	LYS
11	B	22	SER

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	C	230/274 (84%)	230 (100%)	0	100	100
2	E	195/197 (99%)	195 (100%)	0	100	100
3	F	73/137 (53%)	73 (100%)	0	100	100
4	G	152/152 (100%)	152 (100%)	0	100	100
5	I	110/116 (95%)	107 (97%)	3 (3%)	39	61
6	J	64/65 (98%)	64 (100%)	0	100	100
7	K	99/102 (97%)	99 (100%)	0	100	100
8	L	40/57 (70%)	40 (100%)	0	100	100
9	S	143/274 (52%)	140 (98%)	3 (2%)	47	65
10	M	78/299 (26%)	78 (100%)	0	100	100
11	B	1002/1061 (94%)	1001 (100%)	1 (0%)	88	87
12	A	1221/1520 (80%)	1219 (100%)	2 (0%)	87	85
13	D	139/200 (70%)	139 (100%)	0	100	100
14	H	119/128 (93%)	117 (98%)	2 (2%)	53	69
15	Q	198/641 (31%)	198 (100%)	0	100	100
16	R	187/363 (52%)	186 (100%)	1 (0%)	81	80
All	All	4050/5586 (72%)	4038 (100%)	12 (0%)	84	83

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	A	676	MET
12	A	692	ASP
16	R	228	MET
14	H	109	LYS
9	S	151	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
12	A	660	ASN
12	A	1232	ASN
12	A	717	ASN
12	A	862	ASN
13	D	165	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	B	1
16	R	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1155:SER	C	1156:ASP	N	3.18
1	R	227:SER	C	228:MET	N	2.24

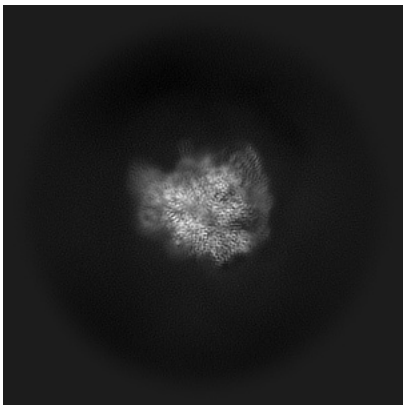
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-71494. These allow visual inspection of the internal detail of the map and identification of artifacts.

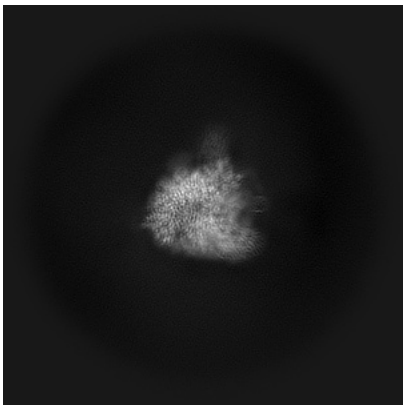
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

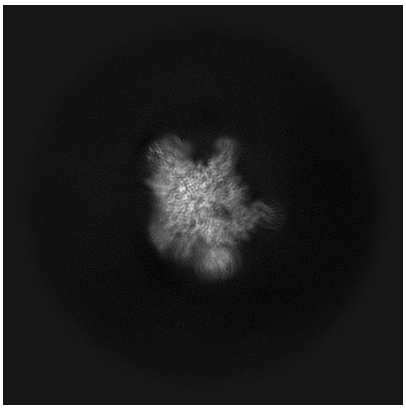
6.1.1 Primary map



X

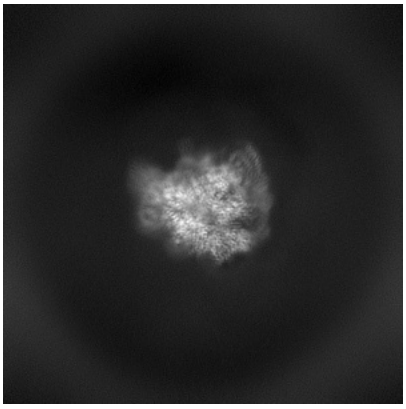


Y

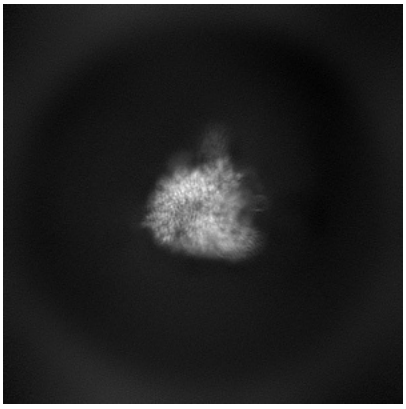


Z

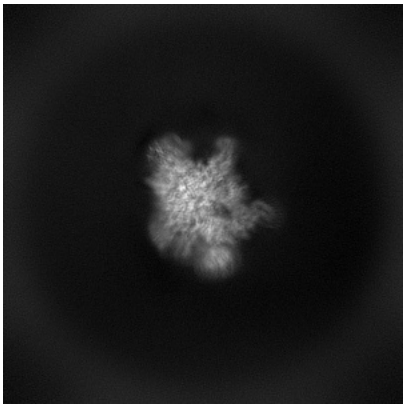
6.1.2 Raw map



X



Y

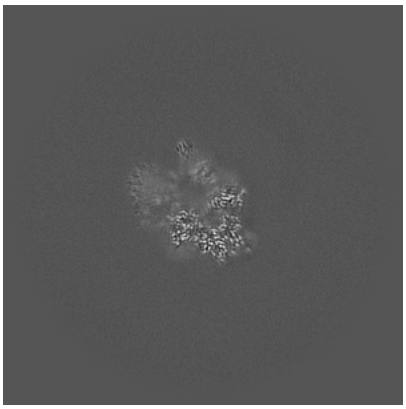


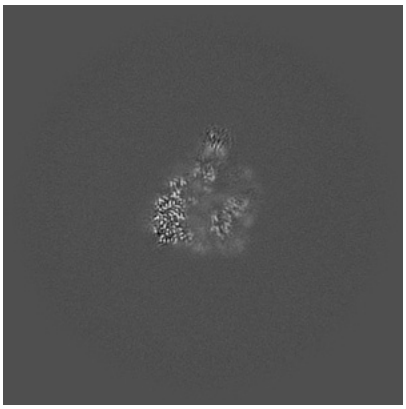
Z

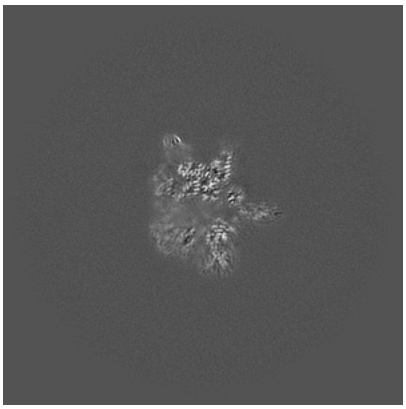
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

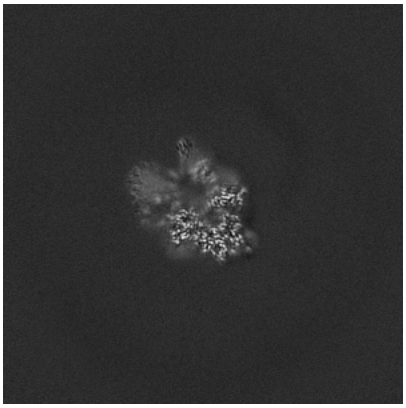
6.2.1 Primary map

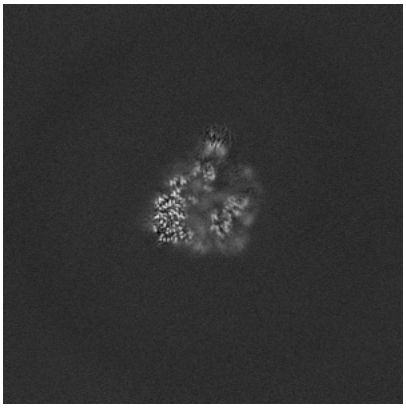

X Index: 192

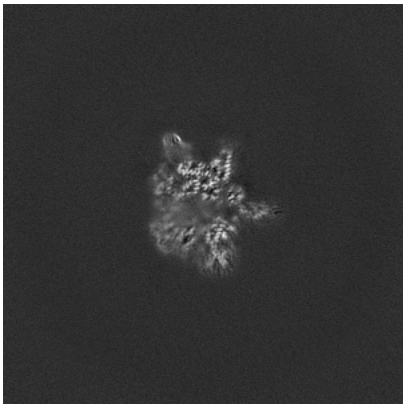

Y Index: 192


Z Index: 192

6.2.2 Raw map


X Index: 192

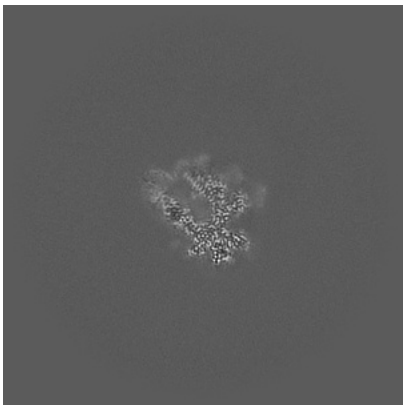

Y Index: 192


Z Index: 192

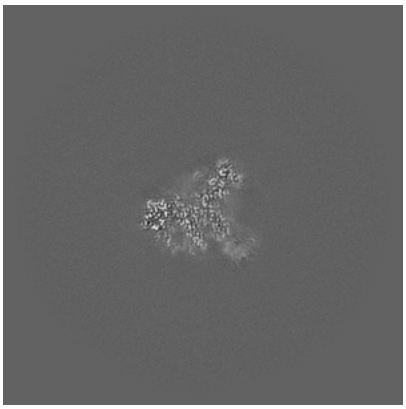
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

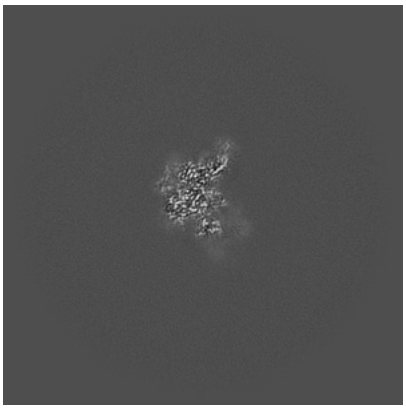
6.3.1 Primary map



X Index: 178

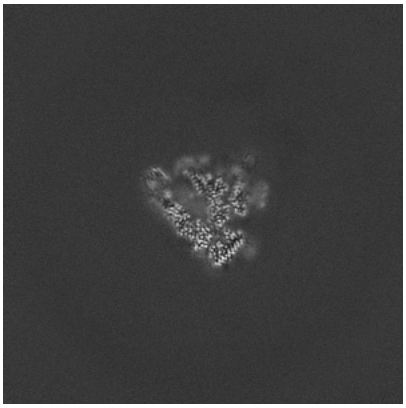


Y Index: 209

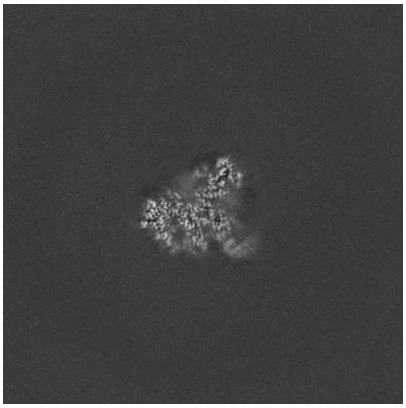


Z Index: 160

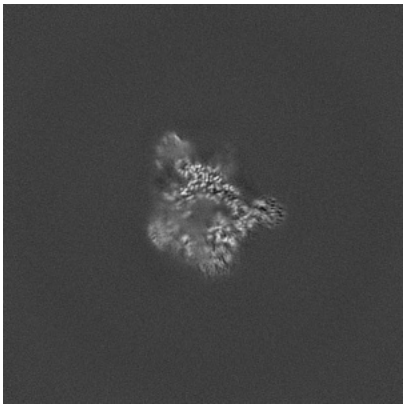
6.3.2 Raw map



X Index: 173



Y Index: 208

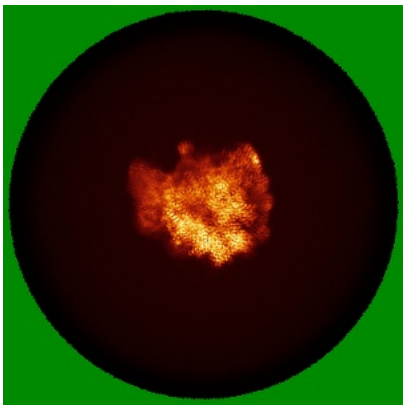


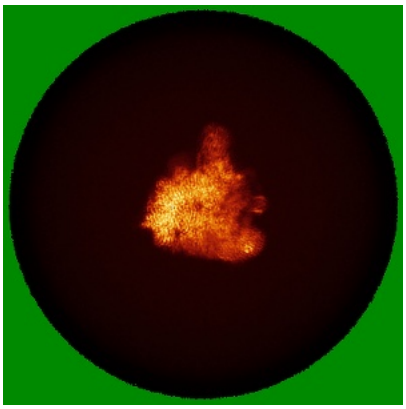
Z Index: 199

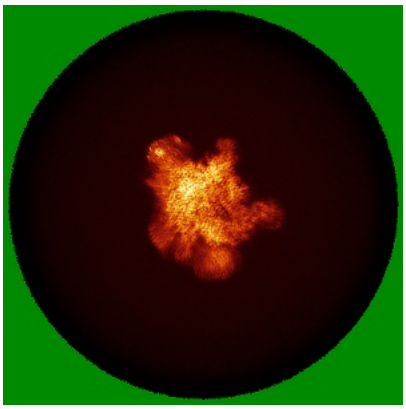
The images above show the largest variance slices of the map in three orthogonal directions.

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

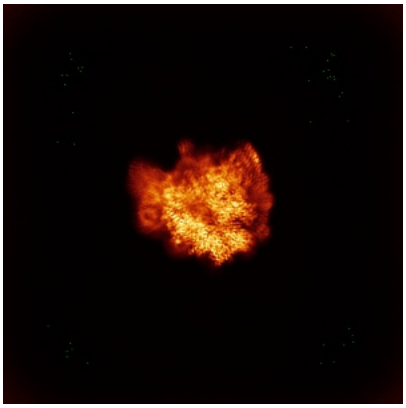
6.4.1 Primary map

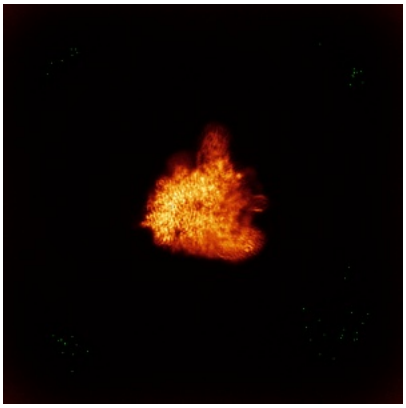

X

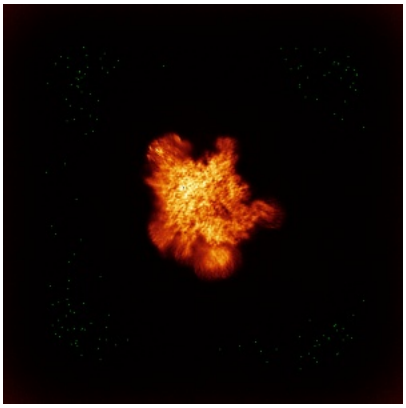

Y


Z

6.4.2 Raw map


X

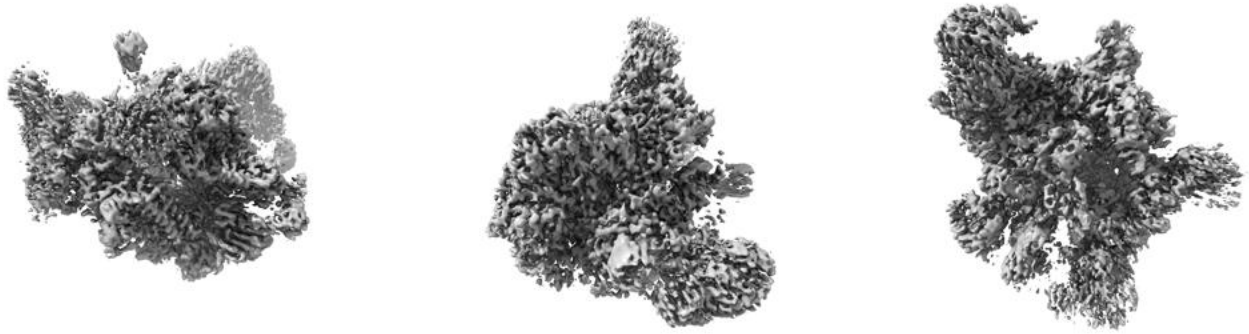

Y


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 0.419. 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.

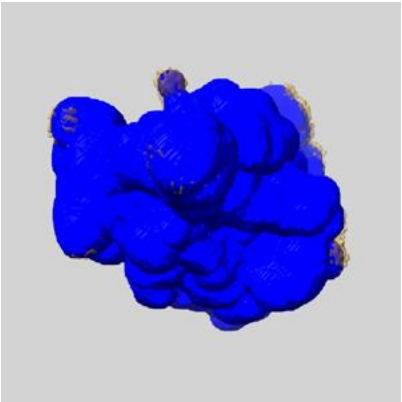
6.6 Mask visualisation (i)

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

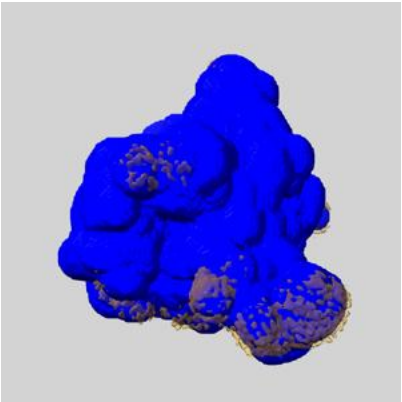
A mask typically either:

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

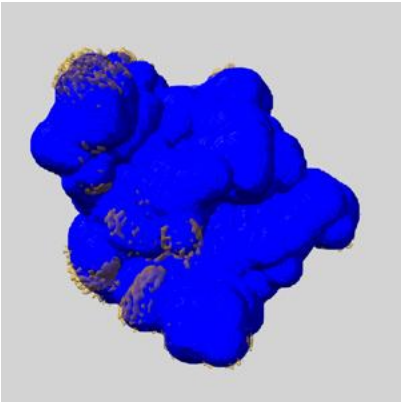
6.6.1 emd_71494_msk_1.map (i)



X



Y

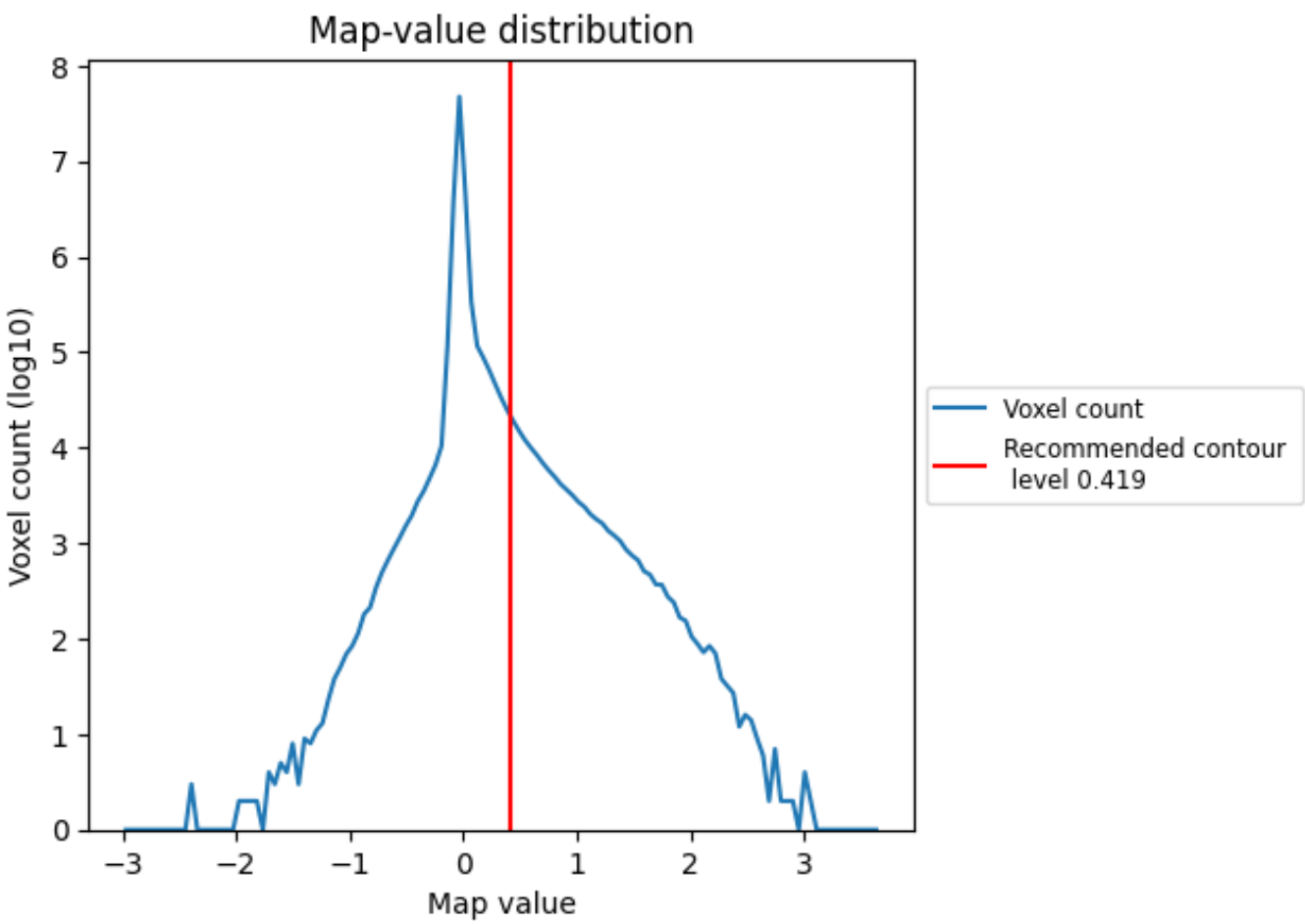


Z

7 Map analysis (i)

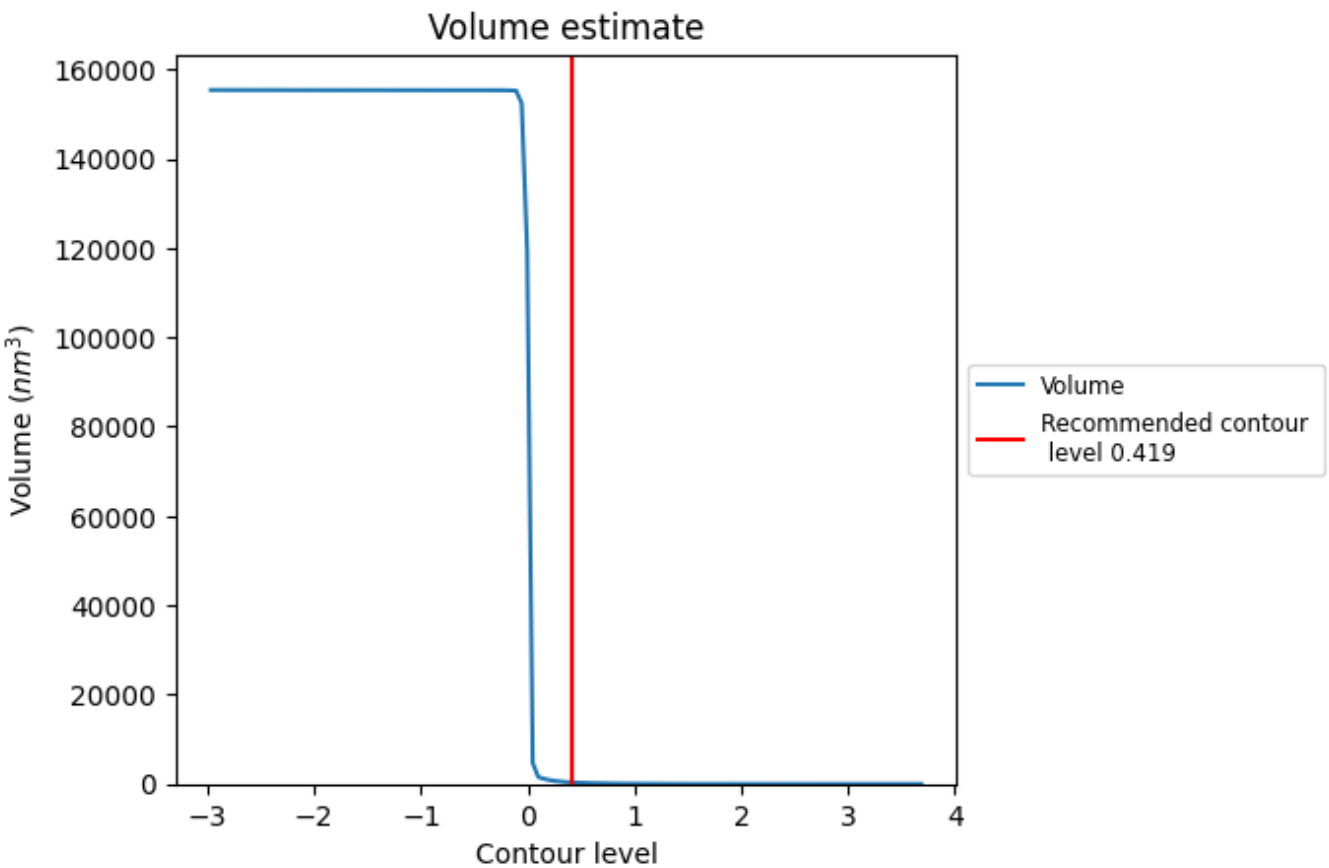
This section contains the results of statistical analysis of the map.

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.

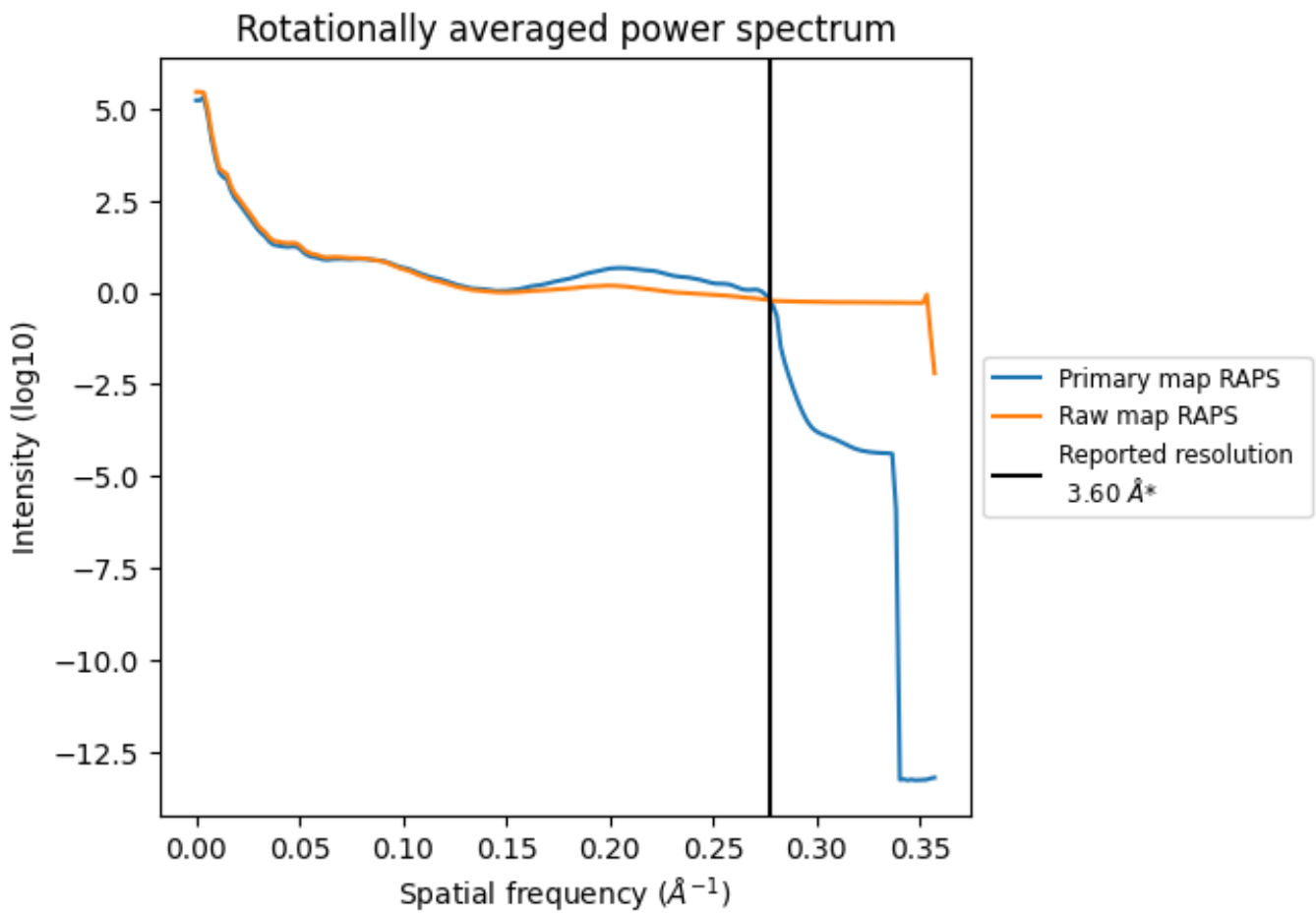
7.2 Volume estimate (i)



The volume at the recommended contour level is 334 nm^3; this corresponds to an approximate mass of 302 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)

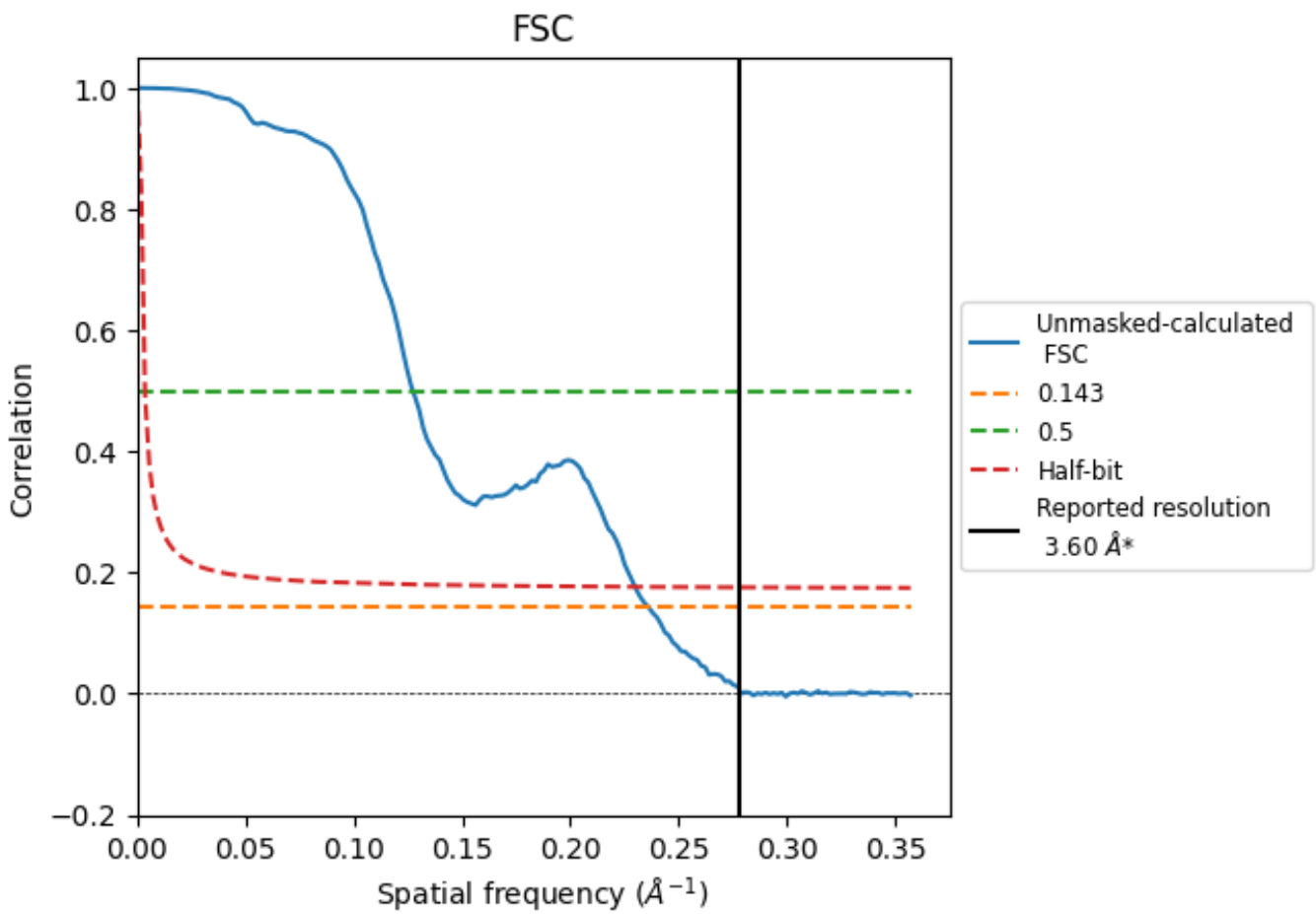


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

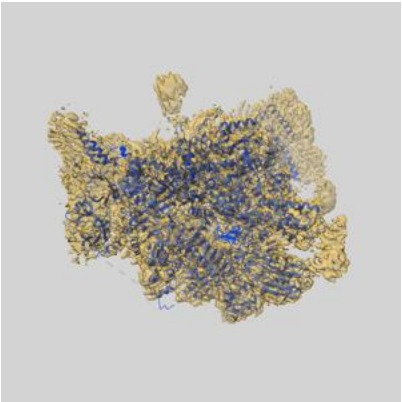
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.24	7.86	4.35

*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 4.24 differs from the reported value 3.6 by more than 10 %

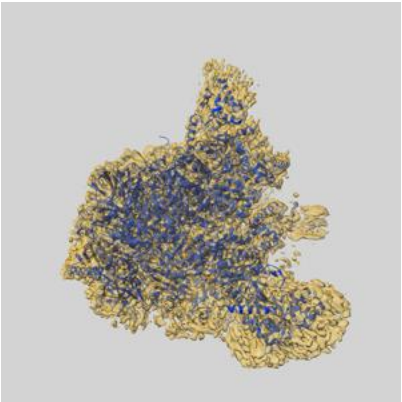
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-71494 and PDB model 9PBZ. Per-residue inclusion information can be found in section 3 on page 7.

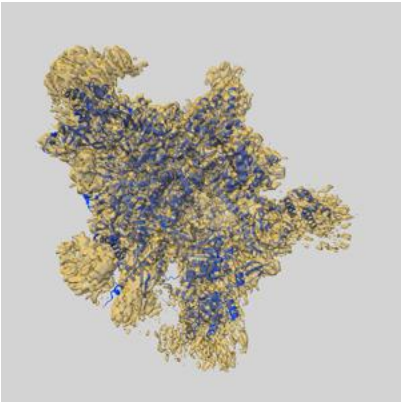
9.1 Map-model overlay (i)



X



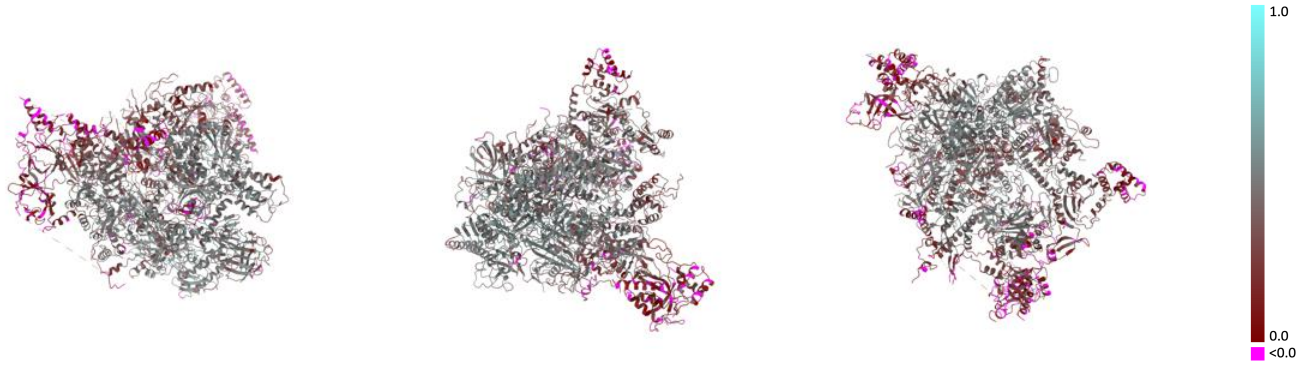
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.419 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.

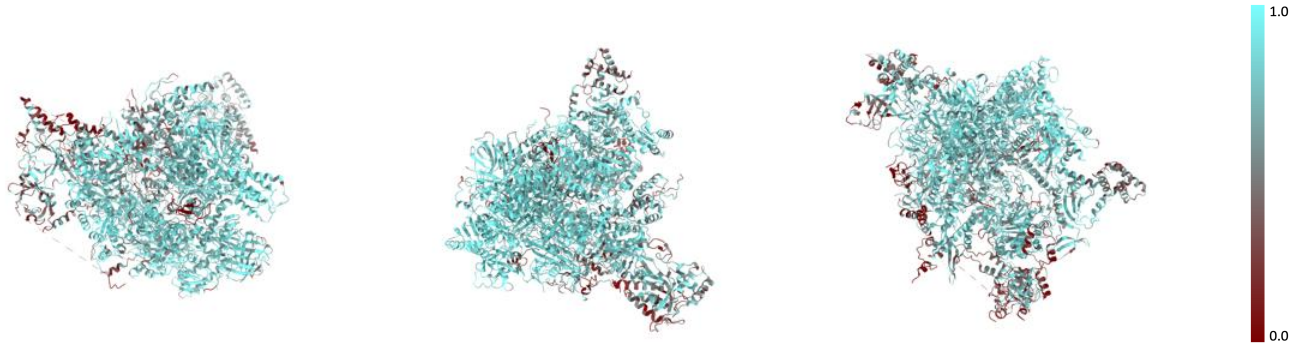
9.2 Q-score mapped to coordinate model (i)



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.

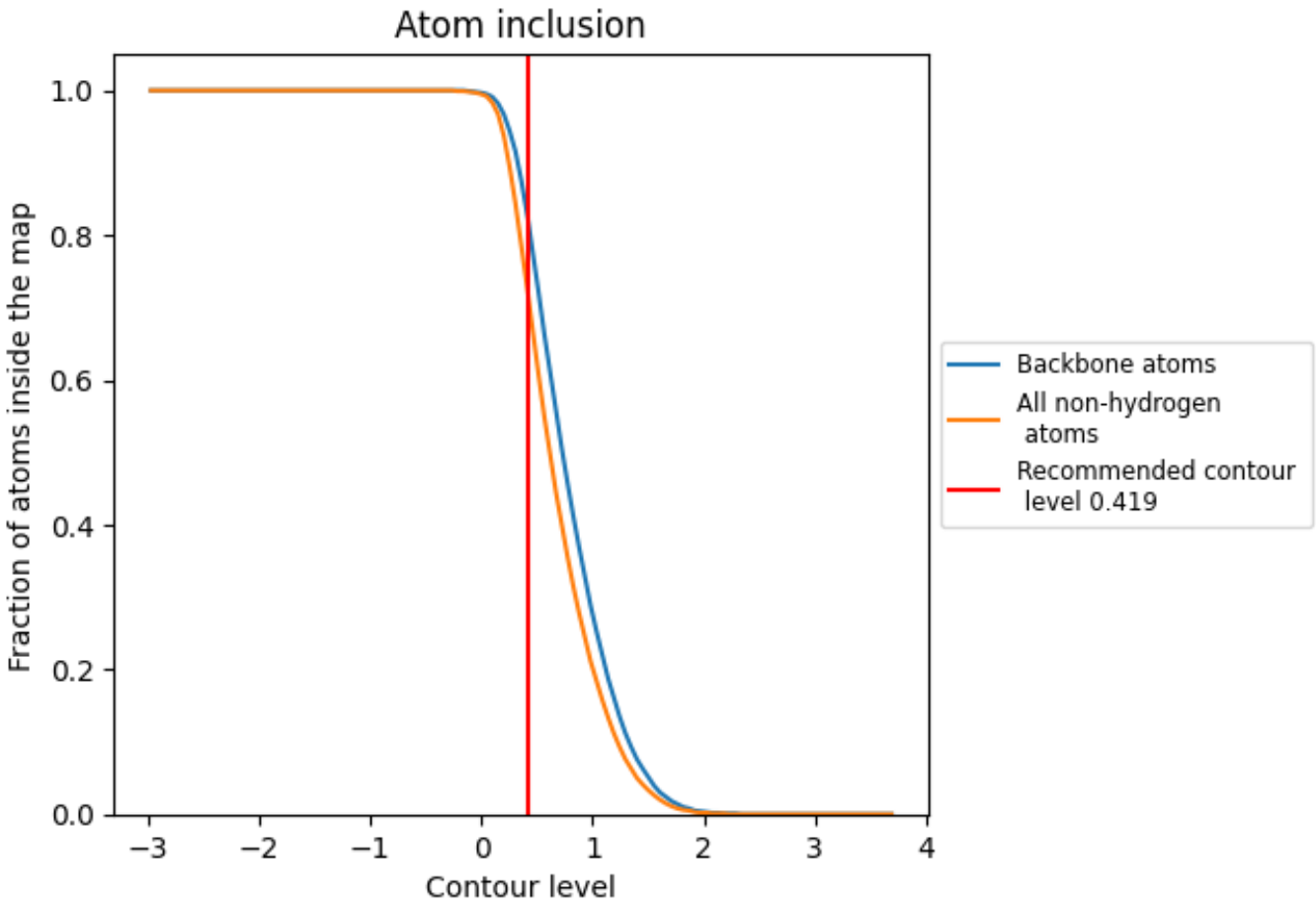
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.419).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.419) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7200	0.3680
A	0.7910	0.4220
B	0.7850	0.4260
C	0.8820	0.4850
D	0.4880	0.1270
E	0.8140	0.4080
F	0.8480	0.4620
G	0.6150	0.2400
H	0.7760	0.4010
I	0.7220	0.3200
J	0.8500	0.4450
K	0.7840	0.4280
L	0.7920	0.4390
M	0.4790	0.2510
Q	0.4260	0.1570
R	0.3610	0.1190
S	0.3480	0.1490