wwPDB EM Validation Summary Report

Jan 22, 2024 – 10:25 pm GMT

PDB ID	:	8C8H
EMDB ID	:	EMD-16476
Title	:	Cryo EM structure of the vaccinia complete RNA polymerase complex lacking the capping enzyme
Authors	:	Grimm, G.; Bartuli, J.; Fischer, U.
Deposited on	:	2023-01-20
Resolution	:	3.84 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 ⓘ 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:

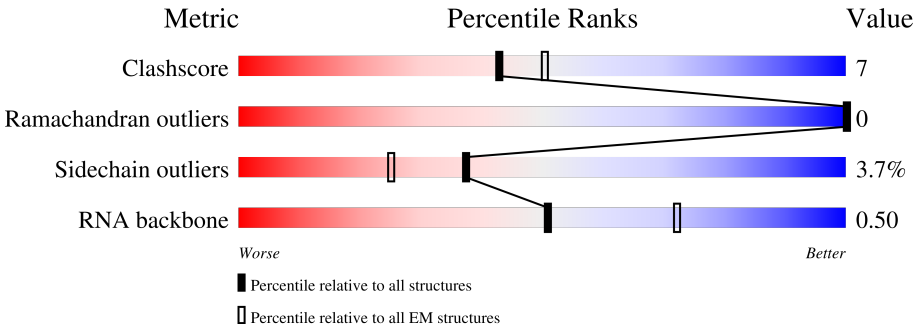
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.84 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	B	1164	5% 77% 19%
2	E	185	8% 79% 20%
3	F	164	51% 12% 37%
4	G	161	13% 75% 19% 5%
5	I	795	16% 68% 16% 16%
6	J	63	67% 27%
7	Q	129	91% 77% 17%

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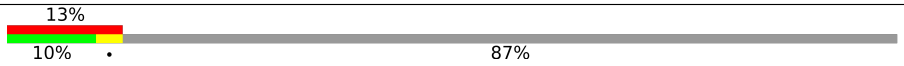
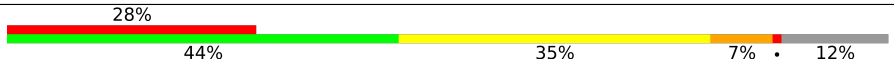
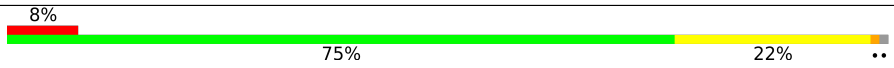
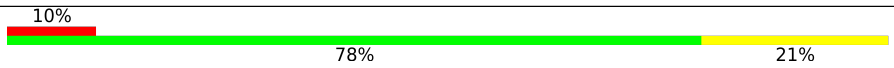
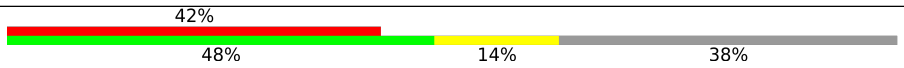
Mol	Chain	Length	Quality of chain
7	R	129	
8	K	710	
9	U	72	
10	A	1286	
11	Y	631	
12	C	305	
13	S	259	

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 41296 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 133 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1129	Total	C	N	O	S	0	0
			9091	5794	1554	1695	48		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	ASN	ASP	conflict	UNP Q76ZP7
B	343	PHE	TYR	variant	UNP Q76ZP7

- Molecule 2 is a protein called DNA-directed RNA polymerase 22 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	184	Total	C	N	O	S	0	0
			1495	966	248	276	5		

- Molecule 3 is a protein called DNA-directed RNA polymerase 19 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	103	Total	C	N	O	S	0	0
			849	545	148	153	3		

- Molecule 4 is a protein called DNA-directed RNA polymerase 18 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	153	Total	C	N	O	S	0	0
			1192	753	198	235	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	11	SER	PRO	variant	UNP P04310

- Molecule 5 is a protein called RNA polymerase-associated transcription-specificity factor

RAP94.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	669	Total	C	N	O	S	0	0
			5603	3669	896	1017	21		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	623	CYS	TYR	variant	UNP P68438
I	624	VAL	ILE	variant	UNP P68438

- Molecule 6 is a protein called DNA-directed RNA polymerase 7 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	61	Total	C	N	O	S	0	0
			490	310	88	88	4		

- Molecule 7 is a protein called Core protein E11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	129	Total	C	N	O	S	1	0
			1056	689	165	197	5		
7	Q	124	Total	C	N	O	S	0	0
			1013	660	158	190	5		

- Molecule 8 is a protein called Early transcription factor 82 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	91	Total	C	N	O	S	0	0
			749	476	131	133	9		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	401	ARG	LYS	variant	UNP P20636

- Molecule 9 is a RNA chain called chr17.trna16-GlnTTG.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	U	63	Total	C	N	O	P	1	0
			1362	608	238	452	64		

- Molecule 10 is a protein called DNA-directed RNA polymerase 147 kDa polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	1268	Total	C	N	O	S	0	0
			10188	6556	1679	1908	45		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	THR	SER	variant	UNP P07392
A	1006	ASN	ASP	variant	UNP P07392
A	1007	ILE	HIS	variant	UNP P07392
A	1008	THR	SER	variant	UNP P07392
A	?	-	PHE	deletion	UNP P07392
A	1010	ARG	GLU	variant	UNP P07392
A	1012	GLU	LYS	variant	UNP P07392
A	1013	THR	GLN	variant	UNP P07392
A	1015	LYS	ARG	variant	UNP P07392
A	1024	ARG	LYS	variant	UNP P07392
A	1113	ASP	CYS	variant	UNP P07392

- Molecule 11 is a protein called Nucleoside triphosphatase I.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	539	Total	C	N	O	S	0	0
			4347	2789	738	797	23		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	342	LYS	ARG	variant	UNP P05807
Y	347	LYS	GLY	variant	UNP P05807
Y	568	LYS	ASN	variant	UNP P05807

- Molecule 12 is a protein called DNA-directed RNA polymerase 35 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	C	304	Total	C	N	O	S	0	0
			2484	1608	399	464	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	212	PHE	LEU	variant	UNP P24757

- Molecule 13 is a protein called DNA-directed RNA polymerase 30 kDa polypeptide.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	S	161	Total	C	N	O	P	S	0	0
			1311	820	211	273	3	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	20	ALA	THR	variant	UNP P21603

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
14	B	1	Total	Zn	0
			1	1	
14	I	1	Total	Zn	0
			1	1	
14	A	2	Total	Zn	0
			2	2	

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	B	26	Total	O	0
			26	26	
16	E	2	Total	O	0
			2	2	
16	F	1	Total	O	0
			1	1	
16	G	3	Total	O	0
			3	3	
16	I	4	Total	O	0
			4	4	
16	J	4	Total	O	0
			4	4	
16	K	1	Total	O	0
			1	1	

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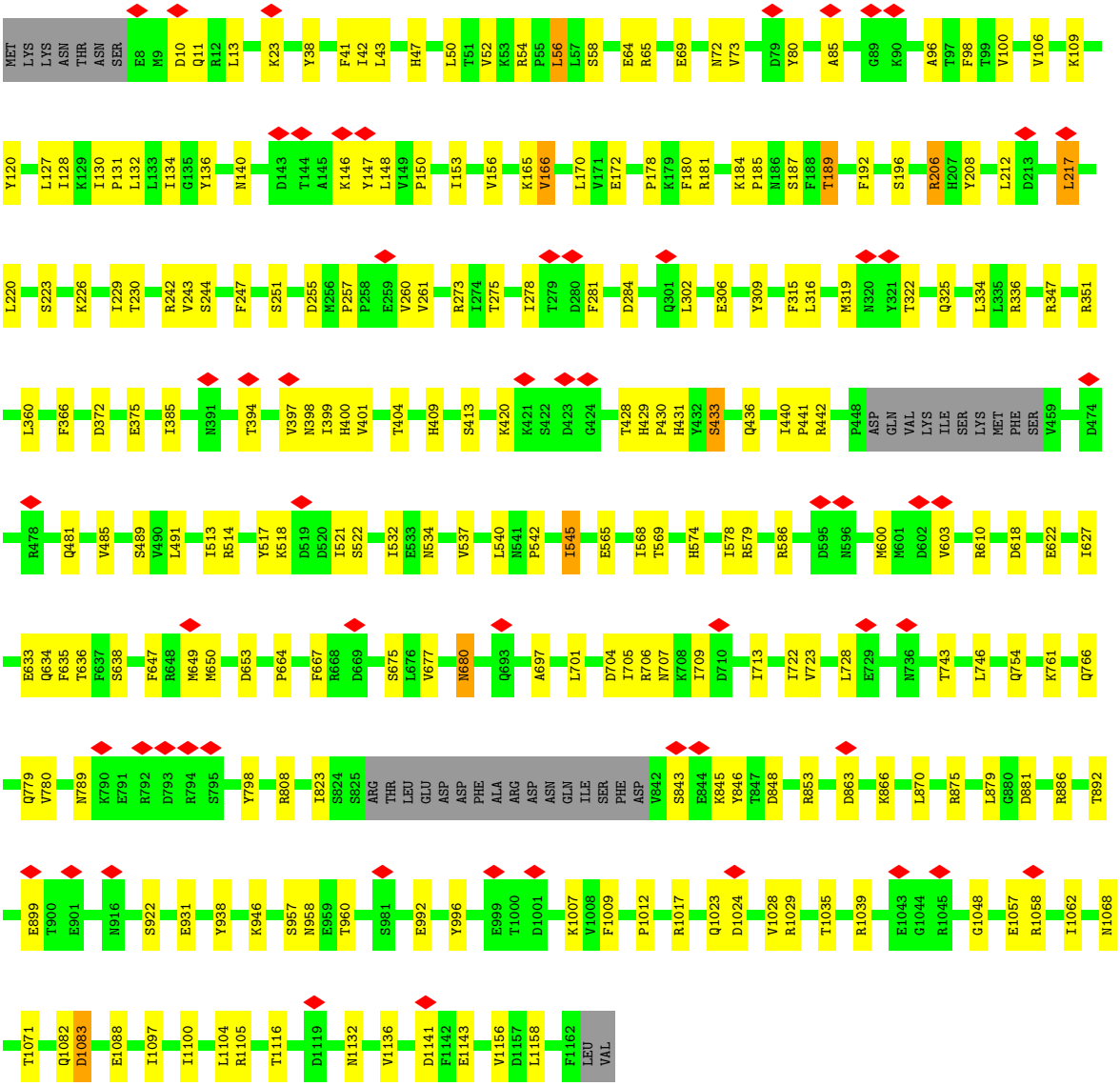
Mol	Chain	Residues	Atoms	AltConf
16	A	17	Total O 17 17	0
16	Y	1	Total O 1 1	0
16	C	2	Total O 2 2	0

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.

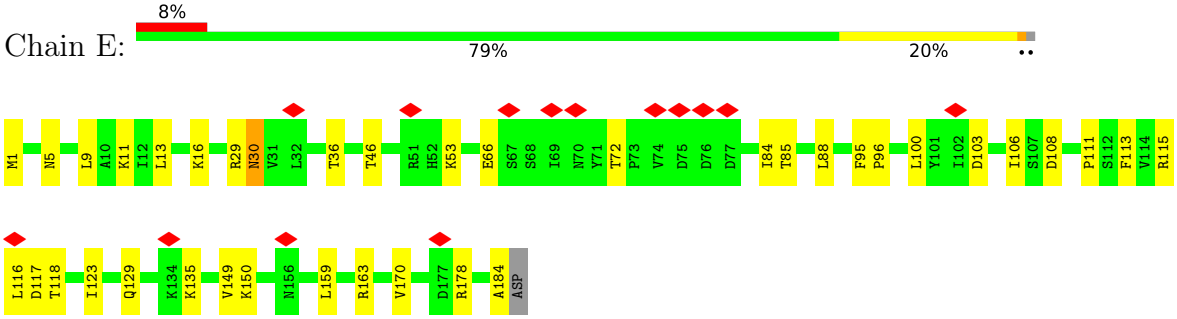
- Molecule 1: DNA-directed RNA polymerase 133 kDa polypeptide

Chain B:



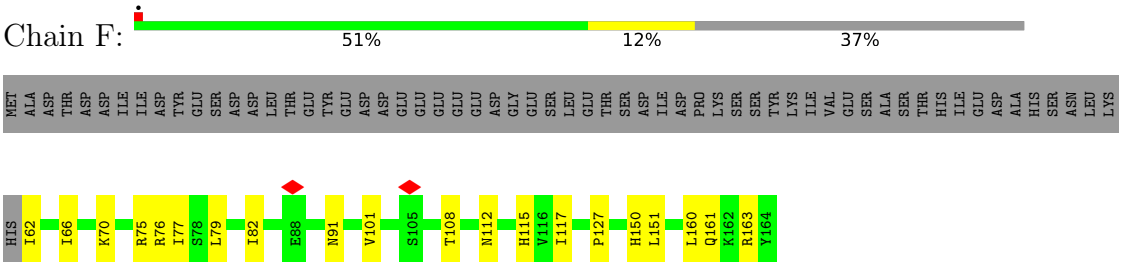
• Molecule 2: DNA-directed RNA polymerase 22 kDa subunit

Chain E:



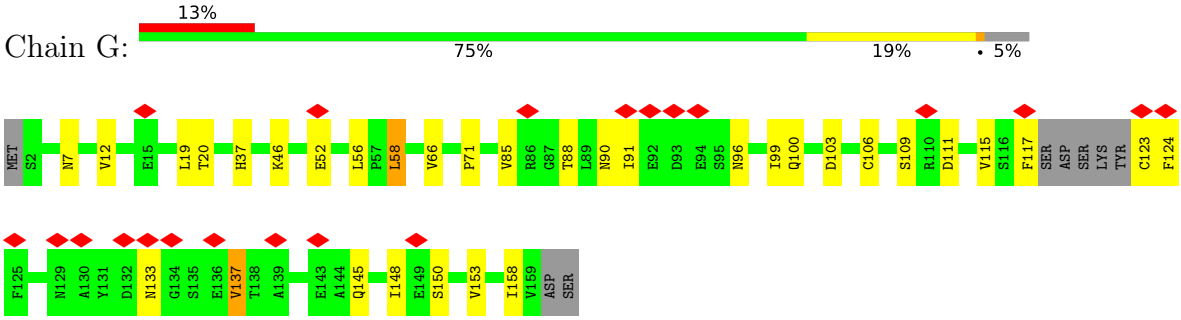
• Molecule 3: DNA-directed RNA polymerase 19 kDa subunit

Chain F:



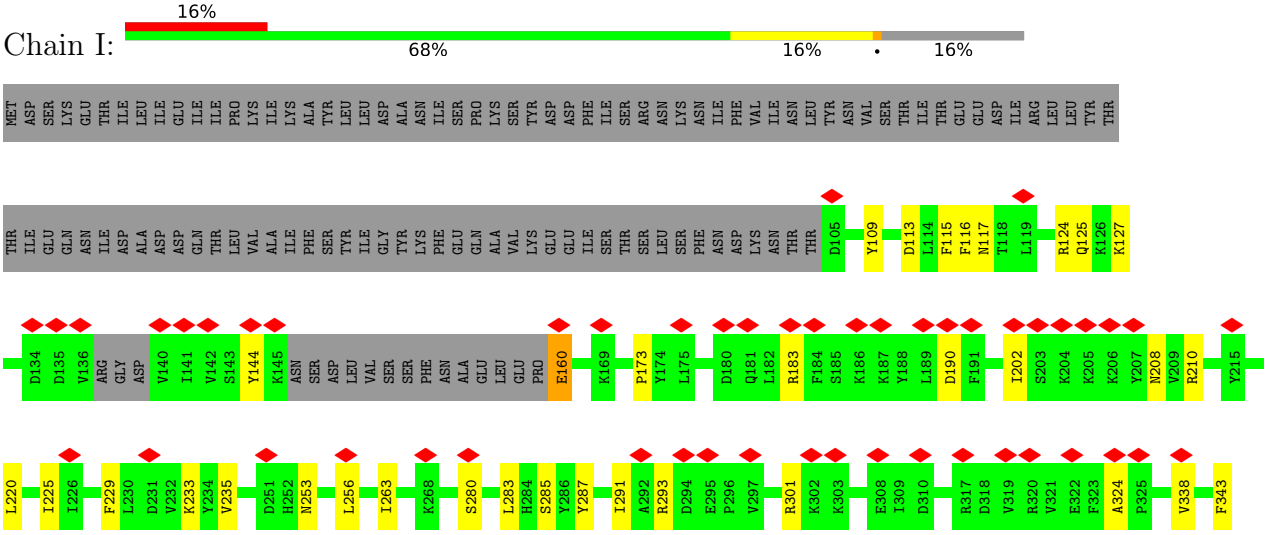
• Molecule 4: DNA-directed RNA polymerase 18 kDa subunit

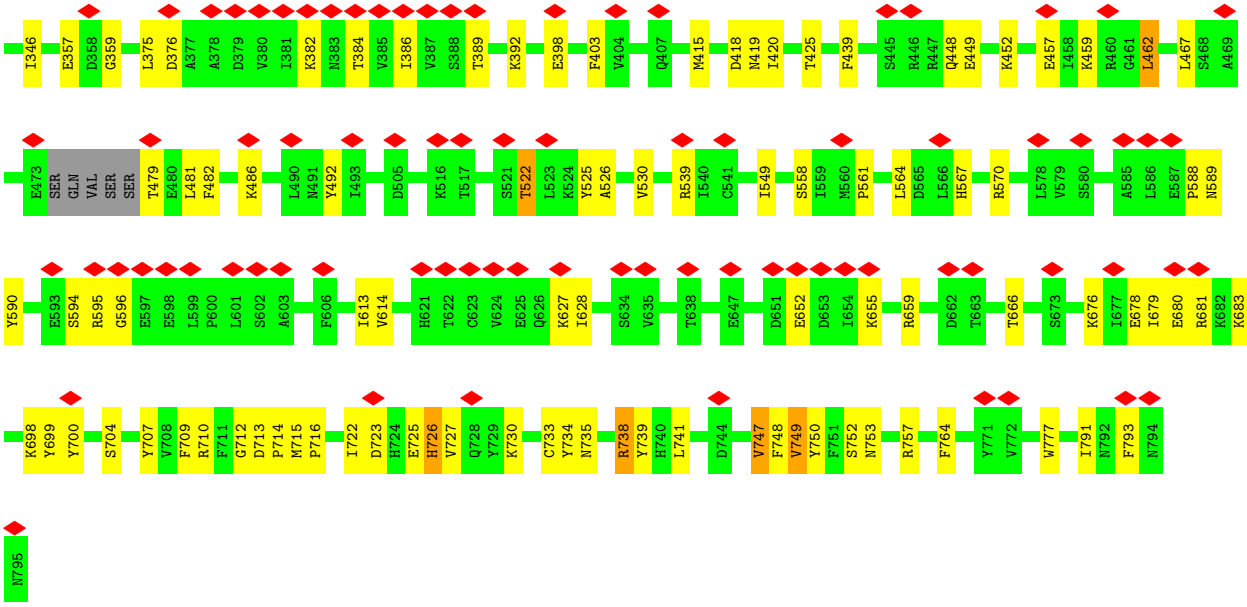
Chain G:



• Molecule 5: RNA polymerase-associated transcription-specificity factor RAP94

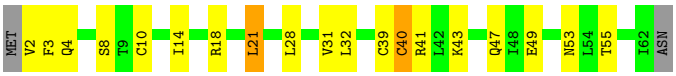
Chain I:





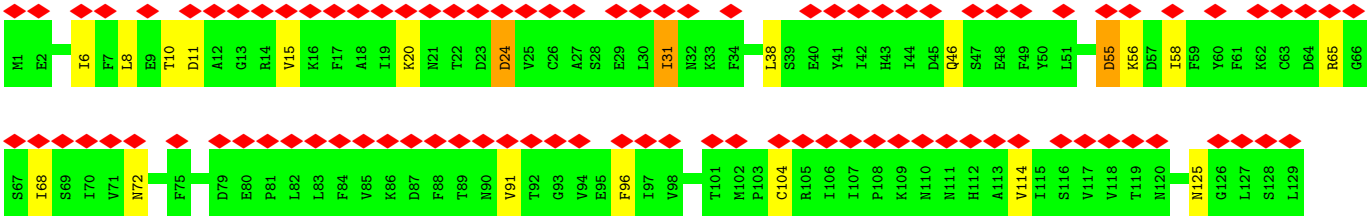
• Molecule 6: DNA-directed RNA polymerase 7 kDa subunit

Chain J:



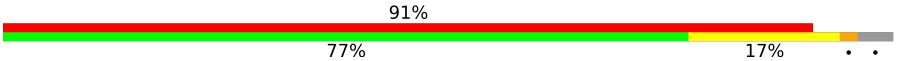
• Molecule 7: Core protein E11

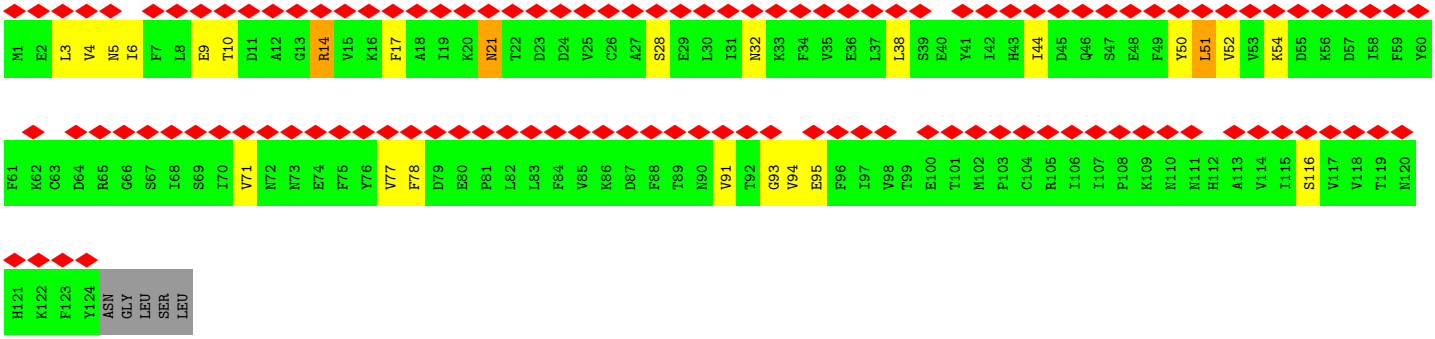
Chain R:



• Molecule 7: Core protein E11

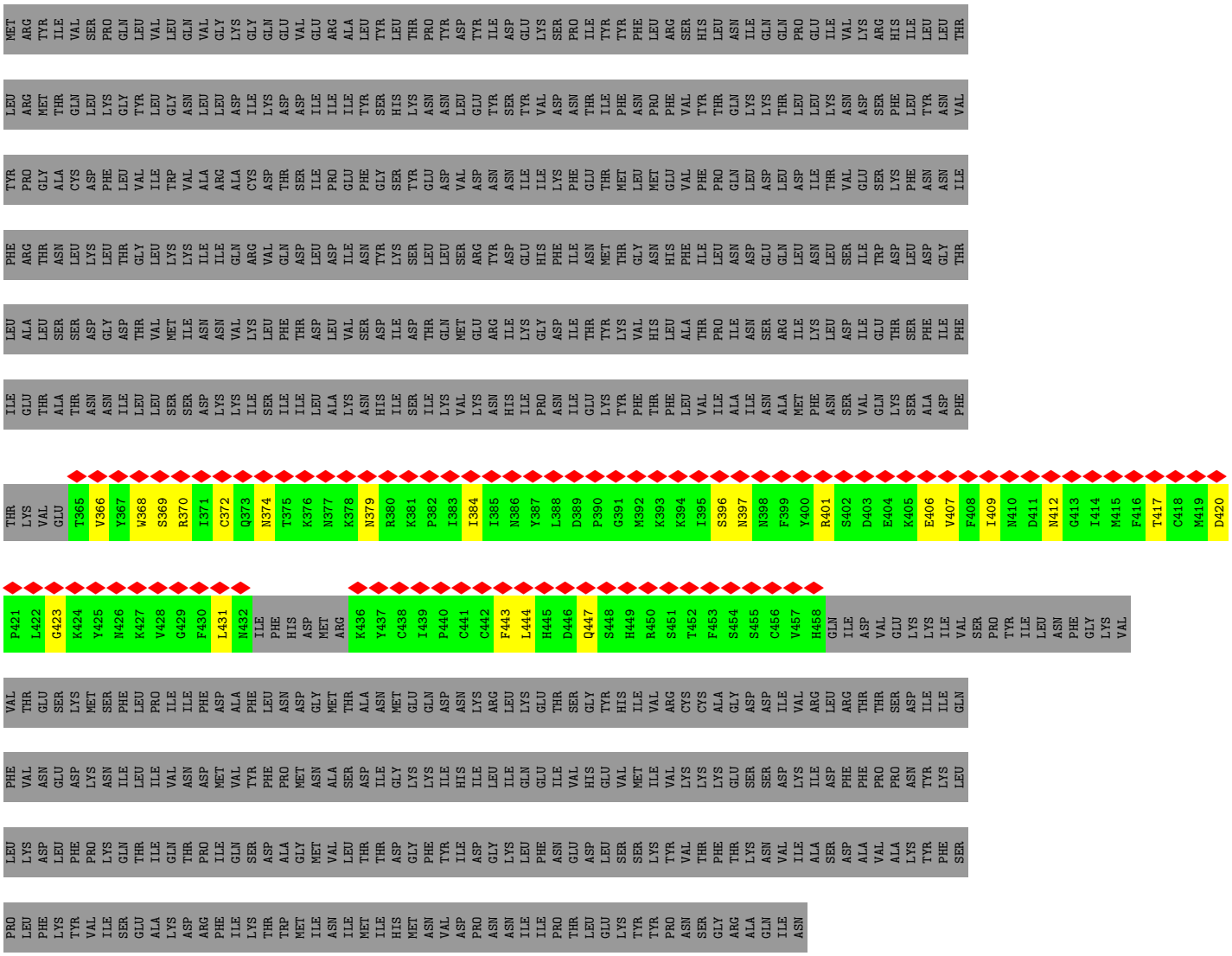
Chain Q:





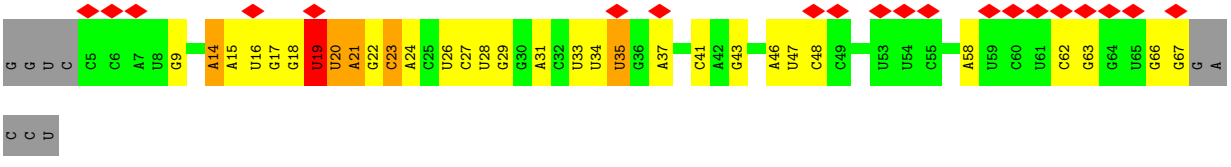
• Molecule 8: Early transcription factor 82 kDa subunit

Chain K:



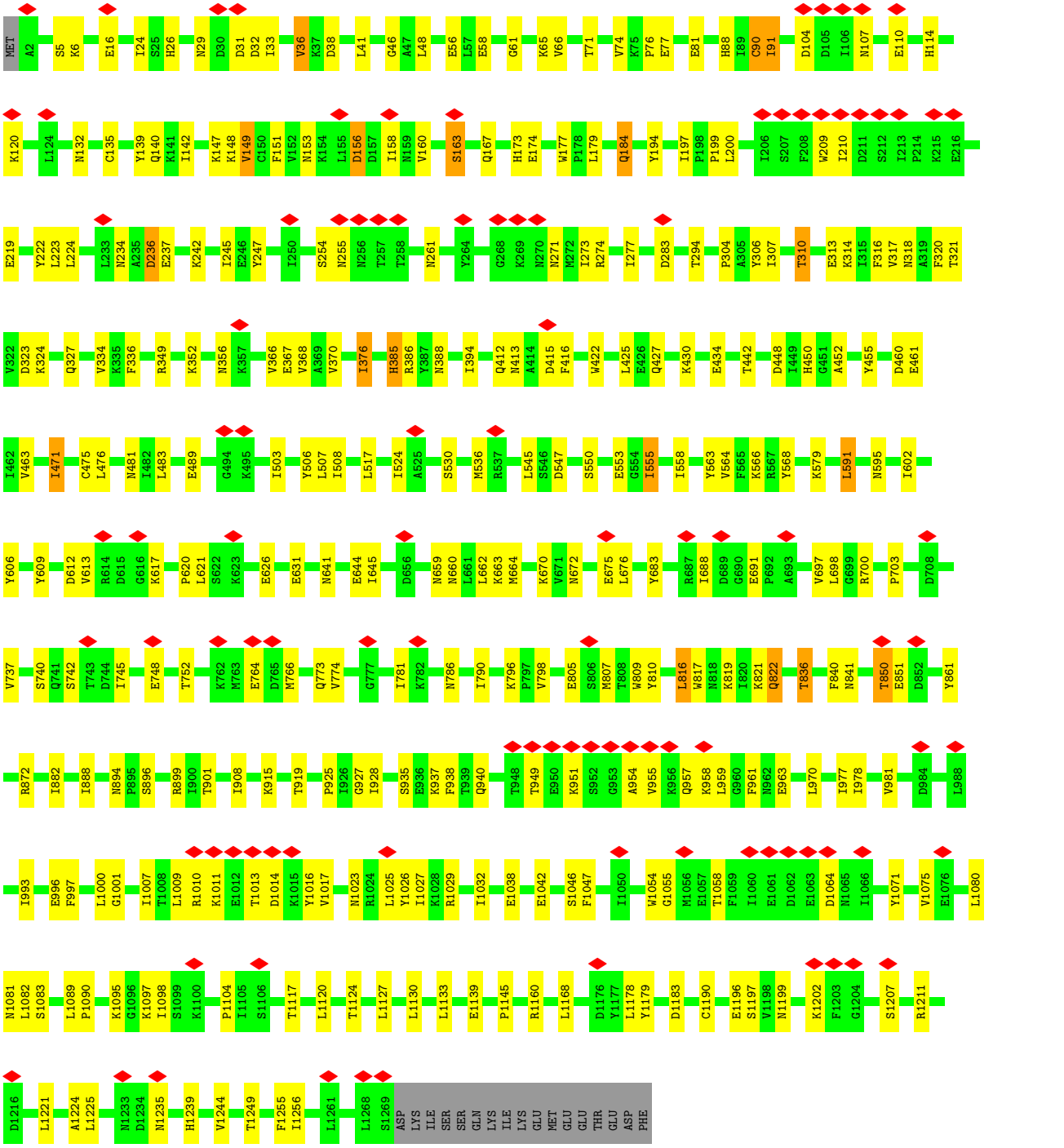
• Molecule 9: chr17.trna16-GlnTTG

Chain U:

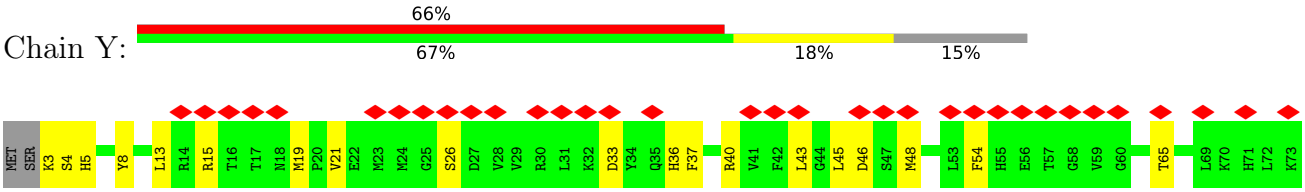


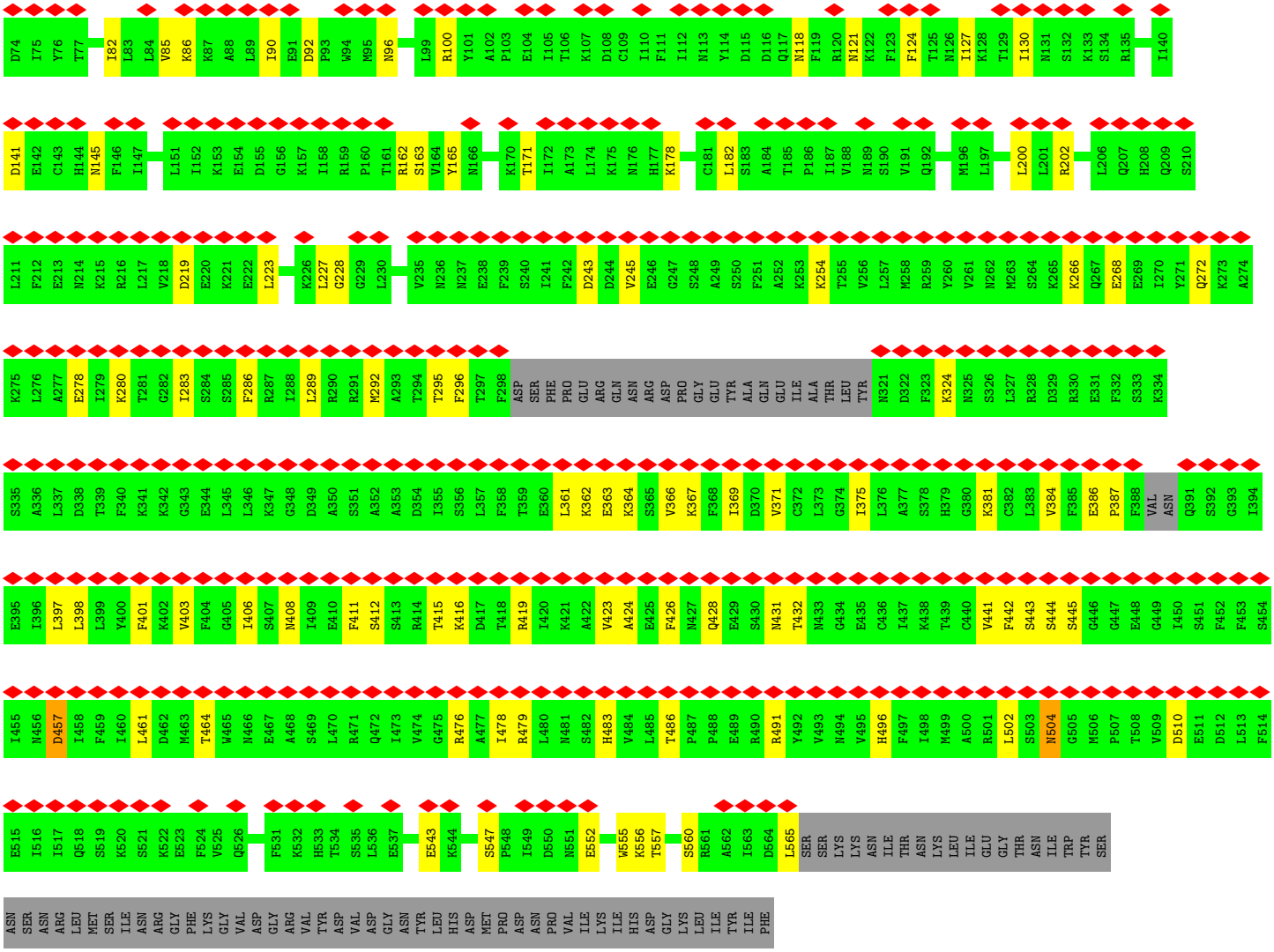
• Molecule 10: DNA-directed RNA polymerase 147 kDa polypeptide

Chain A:



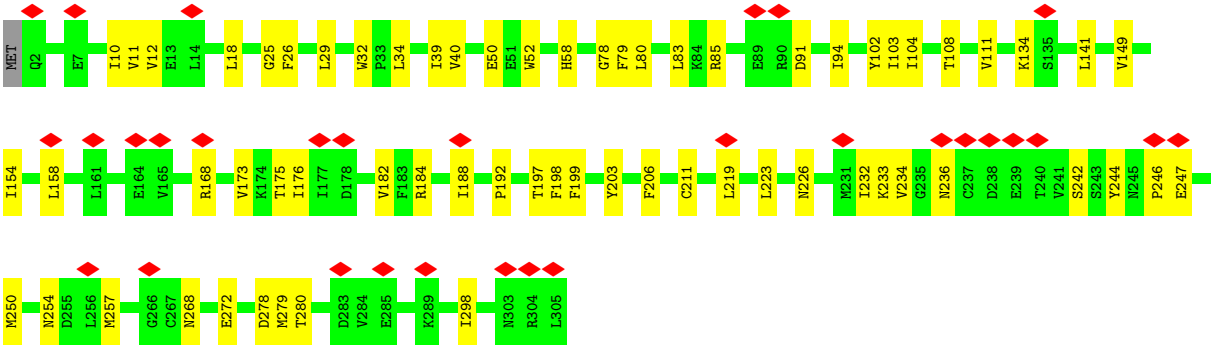
• Molecule 11: Nucleoside triphosphatase I





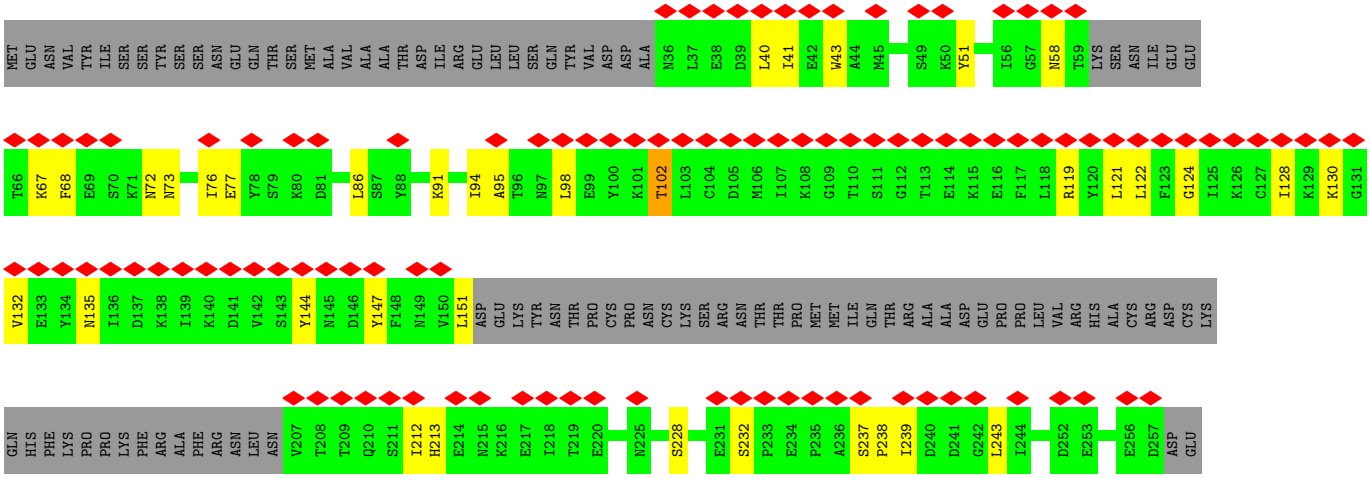
• Molecule 12: DNA-directed RNA polymerase 35 kDa subunit

Chain C:



• Molecule 13: DNA-directed RNA polymerase 30 kDa polypeptide

Chain S:


MET GLU ASN VAL TYR ILE SER SER TYR SER SER ASN GLU GLN THR SER MET ALA VAL ALA ALA THR ASP ILE ARG GLU LEU LEU SER GLN TYR VAL ASP ASP ALA N36 L37 E38 D39 L40 I41 E42 W43 A44 M45 S49 K50 Y51 I56 G57 N58 T59 LYS SER ASN ILE GLU GLU
T66 K67 F68 E69 S70 K71 N72 N73 I76 E77 Y78 S79 K80 D81 L86 S87 Y88 K91 I94 A95 T96 N97 L98 E99 Y100 K101 T102 L103 C104 D105 M106 I107 K108 G109 T110 S111 G112 T113 E114 K115 E116 F117 L118 R119 Y120 L121 L122 F123 G124 I125 K126 C127 I128 K129 K130 G131
V132 E133 Y134 N135 I136 D137 K138 I139 K140 D141 V142 S143 Y144 N145 D146 Y147 F148 N149 V150 L151 ASP GLU LYS TYR ASN THR PRO CYS PRO ASN CYS LYS SER ARG ASN THR THR PRO MET MET ILE GLN THR ARG ALA ALA ASP GLU PRO PRO LEU VAL ARG HIS ALA CYS ARG ASP CYS LYS
GLN HIS PHE LYS PRO PRO LYS PHE ARG ALA PHE ARG ASN LEU ASN V207 T208 T209 Q210 S211 I212 H213 E214 N215 K216 E217 I218 T219 E220 N225 S228 E231 S232 P233 E234 P235 A236 S237 P238 I239 D240 D241 G242 L243 I244 D252 E253 E256 D257 ASP GLU

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	21338	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.345	Depositor
Minimum map value	-0.815	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	382.86002, 382.86002, 382.86002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0635, 1.0635, 1.0635	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SEP, ZN

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	B	0.26	0/9281	0.50	1/12537 (0.0%)
2	E	0.26	0/1522	0.52	0/2069
3	F	0.26	0/863	0.50	0/1158
4	G	0.26	0/1209	0.50	0/1639
5	I	0.25	0/5733	0.46	0/7754
6	J	0.25	0/494	0.52	0/663
7	Q	0.25	0/1035	0.46	0/1402
7	R	0.25	0/1081	0.46	0/1463
8	K	0.24	0/767	0.48	0/1030
9	U	0.24	0/1521	0.91	3/2368 (0.1%)
10	A	0.26	0/10394	0.48	0/14052
11	Y	0.25	0/4429	0.47	0/5960
12	C	0.26	0/2540	0.47	0/3440
13	S	0.23	0/1302	0.47	0/1749
All	All	0.25	0/42171	0.51	4/57284 (0.0%)

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
10	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	U	23	C	O4'-C1'-N1	5.55	112.64	108.20
9	U	19	U	C2-N1-C1'	5.52	124.33	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	347	ARG	C-N-CA	5.45	135.32	121.70
9	U	19	U	N1-C2-O2	5.23	126.46	122.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	147	LYS	Peptide

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	B	9091	0	9146	151	0
2	E	1495	0	1548	26	0
3	F	849	0	874	15	0
4	G	1192	0	1181	18	0
5	I	5603	0	5659	87	0
6	J	490	0	530	12	0
7	Q	1013	0	998	12	0
7	R	1056	0	1056	13	0
8	K	749	0	727	8	0
9	U	1362	0	687	18	0
10	A	10188	0	10312	187	0
11	Y	4347	0	4415	67	0
12	C	2484	0	2470	37	0
13	S	1311	0	1268	30	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	I	1	0	0	0	0
15	A	1	0	0	0	0
16	A	17	0	0	2	0
16	B	26	0	0	0	0
16	C	2	0	0	0	0
16	E	2	0	0	0	0
16	F	1	0	0	0	0
16	G	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	4	0	0	0	0
16	J	4	0	0	0	0
16	K	1	0	0	0	0
16	Y	1	0	0	0	0
All	All	41296	0	40871	584	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 7.

The worst 5 of 584 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:E:88:LEU:HD23	2:E:96:PRO:HG3	1.66	0.78
1:B:1097:ILE:HD12	1:B:1097:ILE:H	1.52	0.73
6:J:32:LEU:HD22	6:J:41:ARG:HG2	1.71	0.73
10:A:336:PHE:HB2	10:A:367:GLU:HB2	1.70	0.73
11:Y:406:ILE:O	11:Y:408:ASN:ND2	2.22	0.72

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	B	1123/1164 (96%)	1047 (93%)	76 (7%)	0	100	100
2	E	182/185 (98%)	165 (91%)	17 (9%)	0	100	100
3	F	101/164 (62%)	95 (94%)	6 (6%)	0	100	100
4	G	149/161 (92%)	139 (93%)	10 (7%)	0	100	100
5	I	661/795 (83%)	615 (93%)	46 (7%)	0	100	100
6	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	Q	122/129 (95%)	118 (97%)	4 (3%)	0	100	100
7	R	128/129 (99%)	121 (94%)	7 (6%)	0	100	100
8	K	87/710 (12%)	81 (93%)	6 (7%)	0	100	100
10	A	1266/1286 (98%)	1190 (94%)	76 (6%)	0	100	100
11	Y	533/631 (84%)	502 (94%)	31 (6%)	0	100	100
12	C	302/305 (99%)	281 (93%)	21 (7%)	0	100	100
13	S	152/259 (59%)	132 (87%)	20 (13%)	0	100	100
All	All	4865/5981 (81%)	4542 (93%)	323 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	B	1030/1064 (97%)	998 (97%)	32 (3%)	40	65
2	E	174/175 (99%)	170 (98%)	4 (2%)	50	71
3	F	94/151 (62%)	92 (98%)	2 (2%)	53	73
4	G	136/144 (94%)	131 (96%)	5 (4%)	34	61
5	I	637/755 (84%)	615 (96%)	22 (4%)	36	63
6	J	60/62 (97%)	55 (92%)	5 (8%)	11	40
7	Q	116/121 (96%)	108 (93%)	8 (7%)	15	46
7	R	122/121 (101%)	116 (95%)	6 (5%)	25	55
8	K	87/665 (13%)	80 (92%)	7 (8%)	12	41
10	A	1139/1157 (98%)	1087 (95%)	52 (5%)	27	56
11	Y	490/573 (86%)	477 (97%)	13 (3%)	44	68
12	C	286/287 (100%)	279 (98%)	7 (2%)	49	71
13	S	146/237 (62%)	143 (98%)	3 (2%)	53	73
All	All	4517/5512 (82%)	4351 (96%)	166 (4%)	37	61

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	A	816	LEU
11	Y	15	ARG
10	A	901	THR
10	A	1083	SER
11	Y	423	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
10	A	513	ASN
10	A	1023	ASN
10	A	548	HIS
10	A	865	HIS
11	Y	5	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	U	61/72 (84%)	17 (27%)	2 (3%)

5 of 17 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	U	9	G
9	U	14	A
9	U	16	U
9	U	17	G
9	U	18	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	U	18	G
9	U	20	U

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

3 non-standard protein/DNA/RNA residues are 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	$\#\|Z\| > 2$
13	SEP	S	237	13	8,9,10	1.56	1 (12%)	8,12,14	1.54	2 (25%)
13	SEP	S	232	13	8,9,10	1.56	1 (12%)	8,12,14	1.82	3 (37%)
13	SEP	S	228	13	8,9,10	1.55	1 (12%)	8,12,14	1.65	2 (25%)

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
13	SEP	S	237	13	-	0/5/8/10	-
13	SEP	S	232	13	-	2/5/8/10	-
13	SEP	S	228	13	-	4/5/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	232	SEP	P-O1P	3.41	1.61	1.50
13	S	237	SEP	P-O1P	3.39	1.61	1.50
13	S	228	SEP	P-O1P	3.36	1.61	1.50

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	S	232	SEP	OG-CB-CA	4.04	112.08	108.14
13	S	228	SEP	P-OG-CB	-3.12	109.71	118.30
13	S	237	SEP	P-OG-CB	-3.08	109.81	118.30
13	S	228	SEP	OG-CB-CA	2.91	110.98	108.14
13	S	237	SEP	OG-CB-CA	2.46	110.54	108.14

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	S	228	SEP	CB-OG-P-O2P
13	S	228	SEP	CB-OG-P-O3P
13	S	228	SEP	CB-OG-P-O1P
13	S	232	SEP	CB-OG-P-O1P
13	S	228	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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)

There are no chain breaks in this entry.

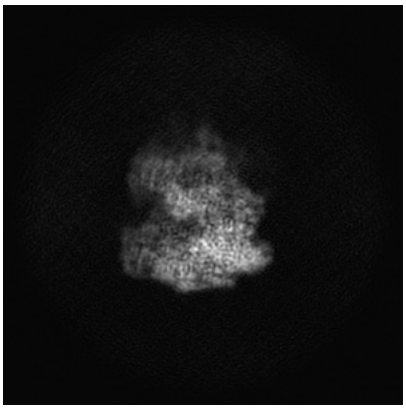
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16476. These allow visual inspection of the internal detail of the map and identification of artifacts.

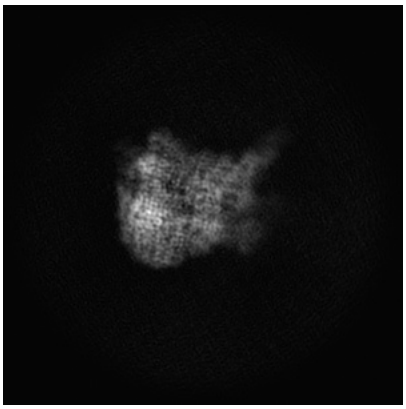
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

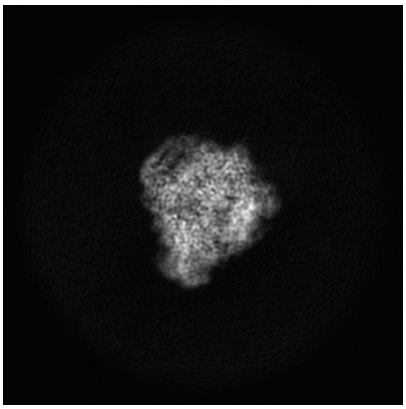
6.1.1 Primary map



X

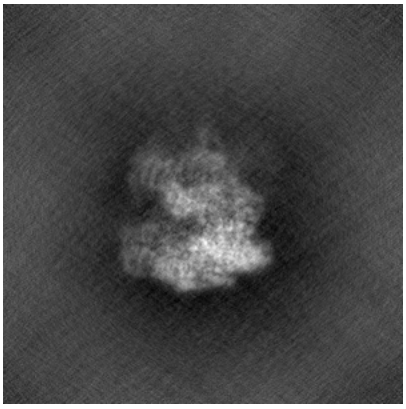


Y

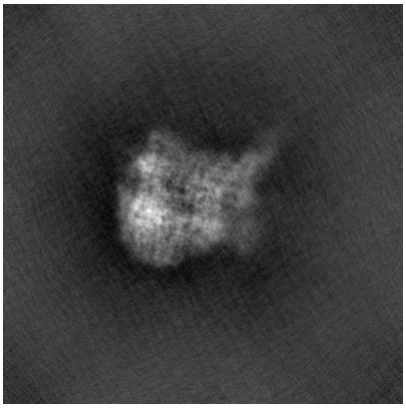


Z

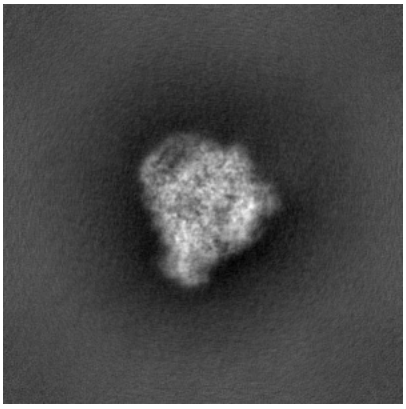
6.1.2 Raw map



X



Y

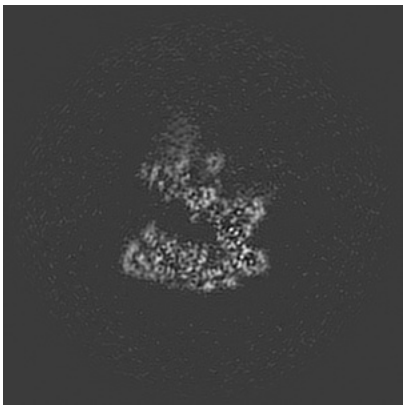


Z

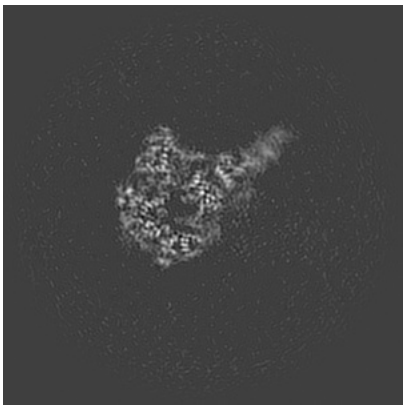
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

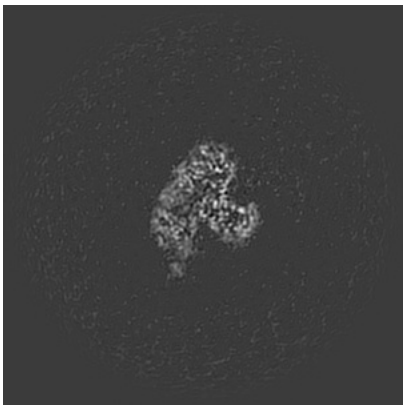
6.2.1 Primary map



X Index: 180

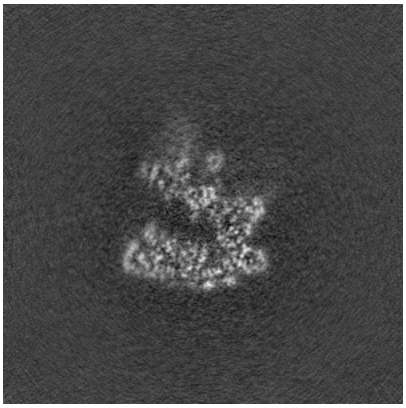


Y Index: 180

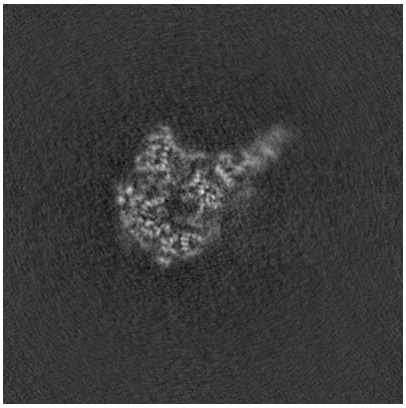


Z Index: 180

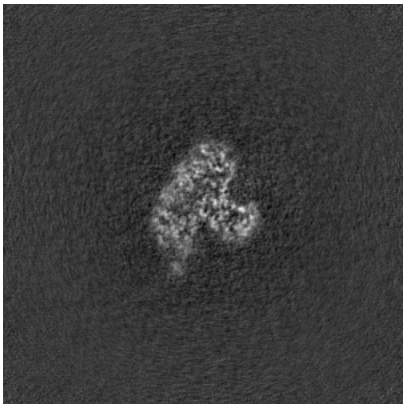
6.2.2 Raw map



X Index: 180



Y Index: 180

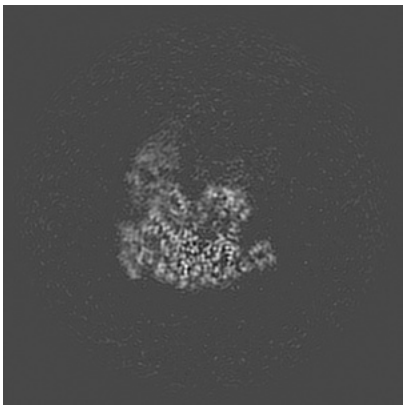


Z Index: 180

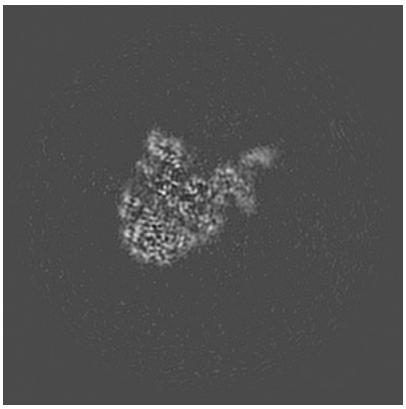
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



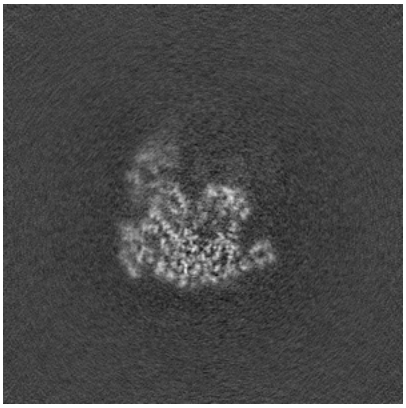
X Index: 163



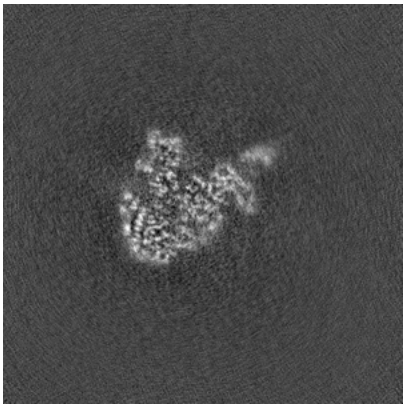
Y Index: 194

Z Index: 137

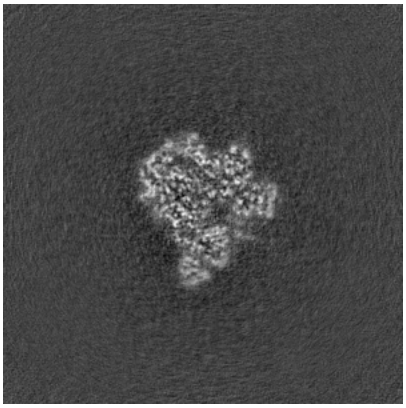
6.3.2 Raw map



X Index: 163



Y Index: 192

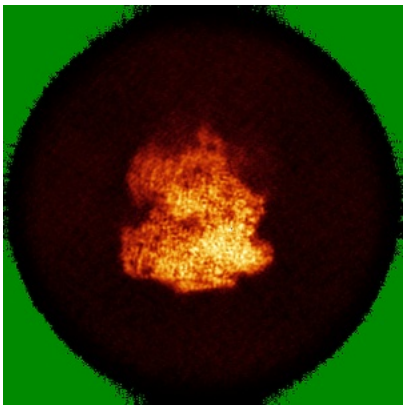


Z Index: 138

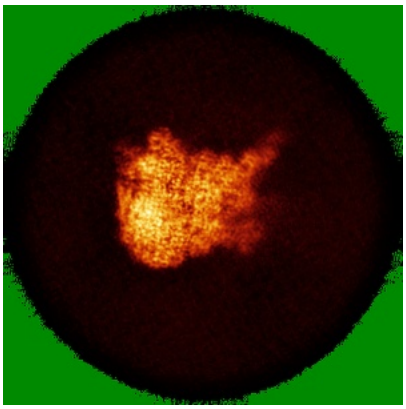
The images above show the largest variance slices of the map in three orthogonal directions.

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

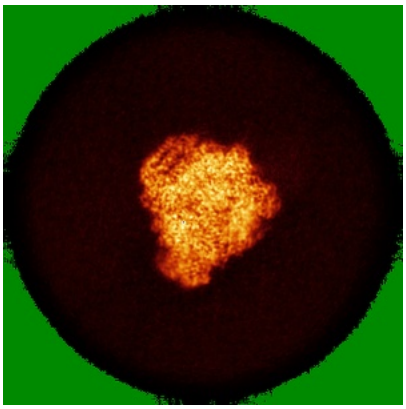
6.4.1 Primary map



X

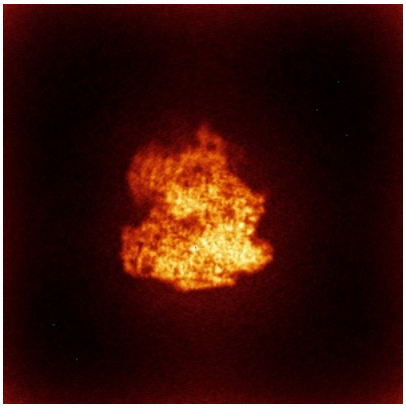


Y

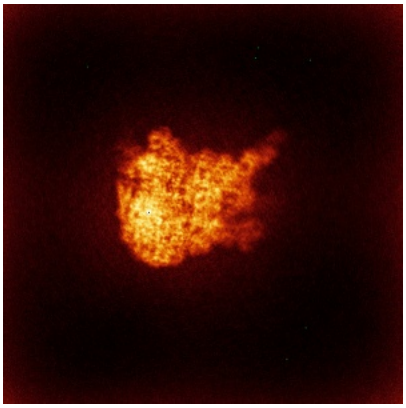


Z

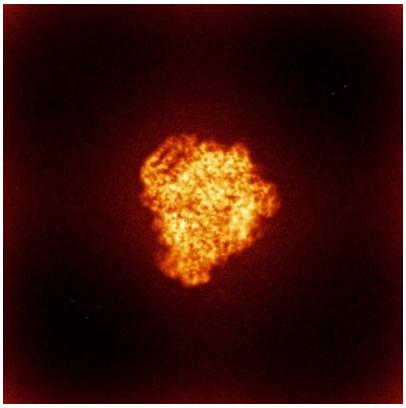
6.4.2 Raw map



X



Y

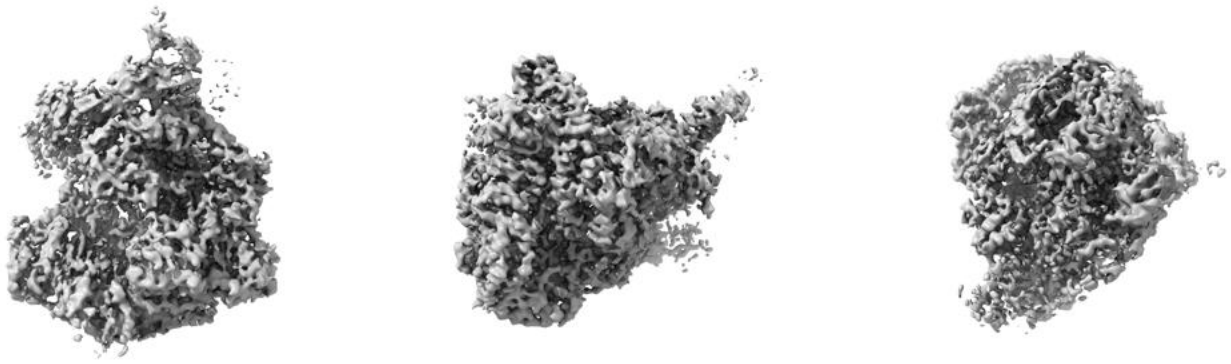


Z

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)

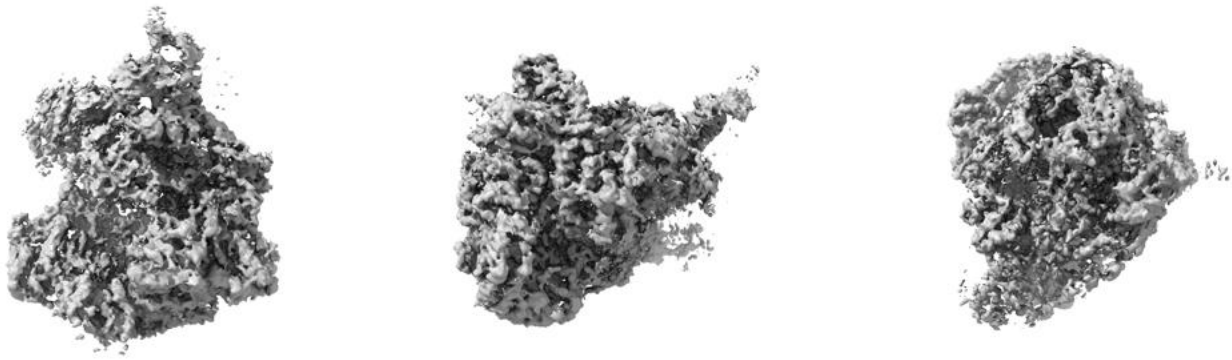
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

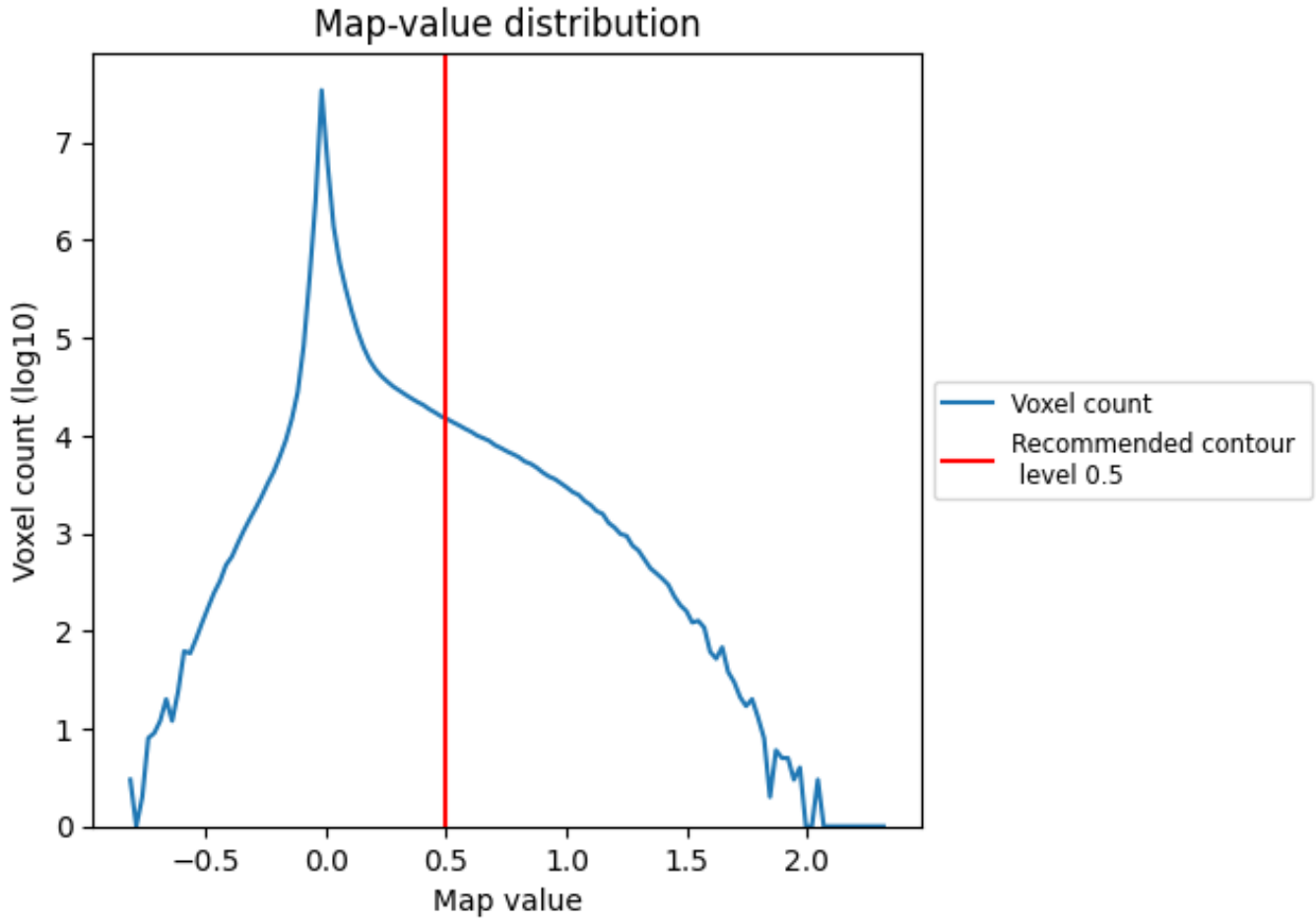
6.6 Mask visualisation (i)

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

7 Map analysis

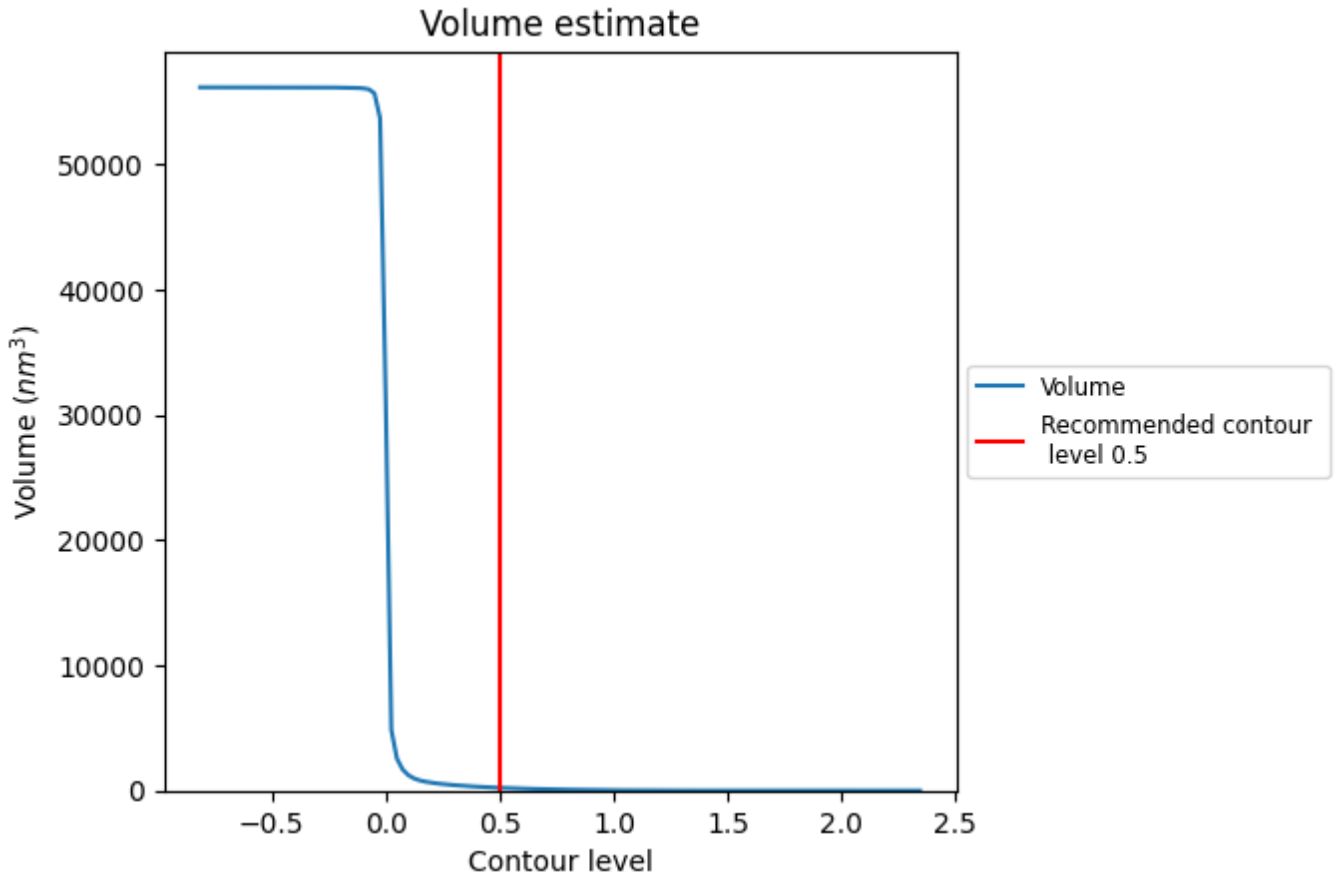
This section contains the results of statistical analysis of the map.

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.

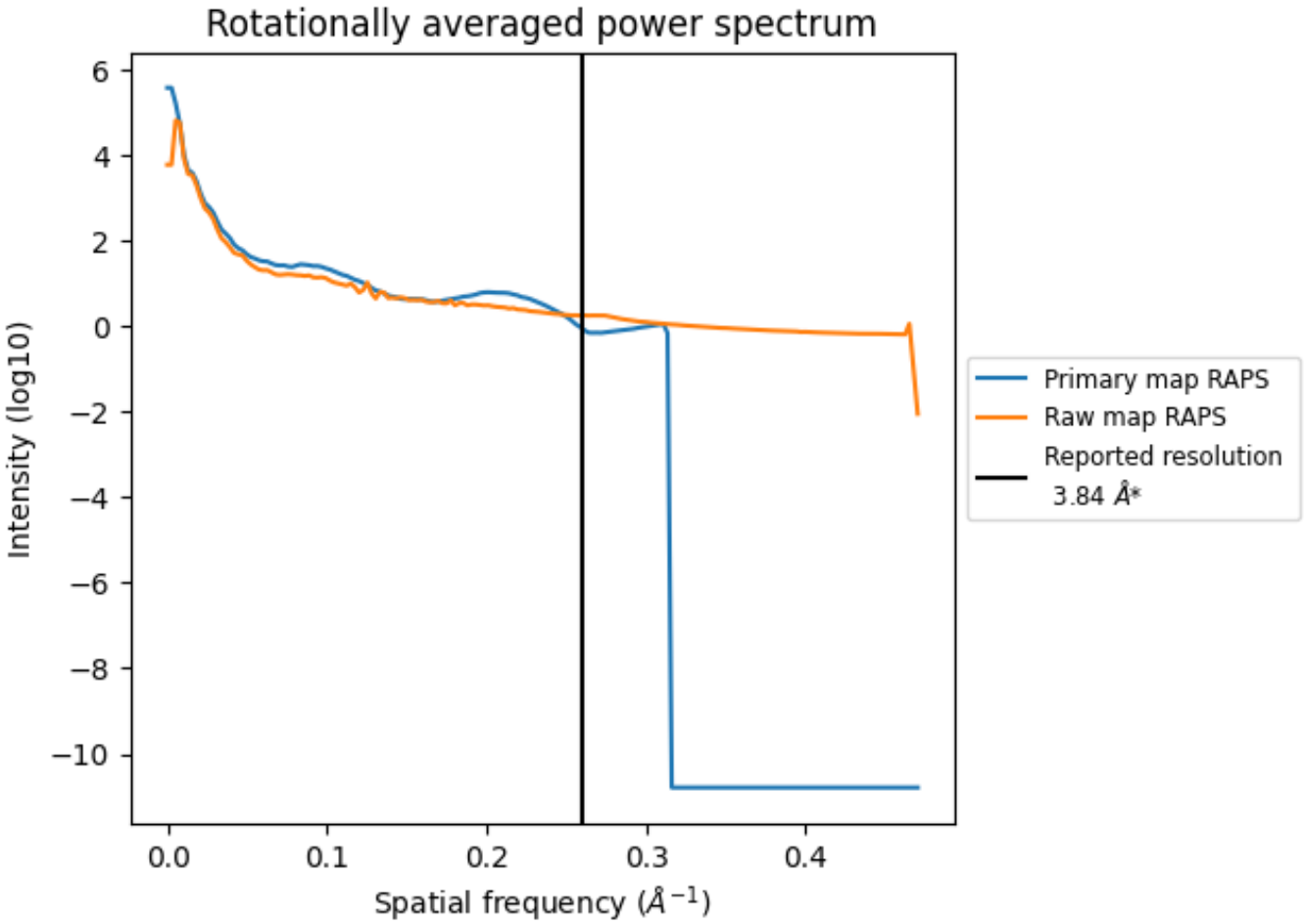
7.2 Volume estimate (i)



The volume at the recommended contour level is 221 nm^3; this corresponds to an approximate mass of 199 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)

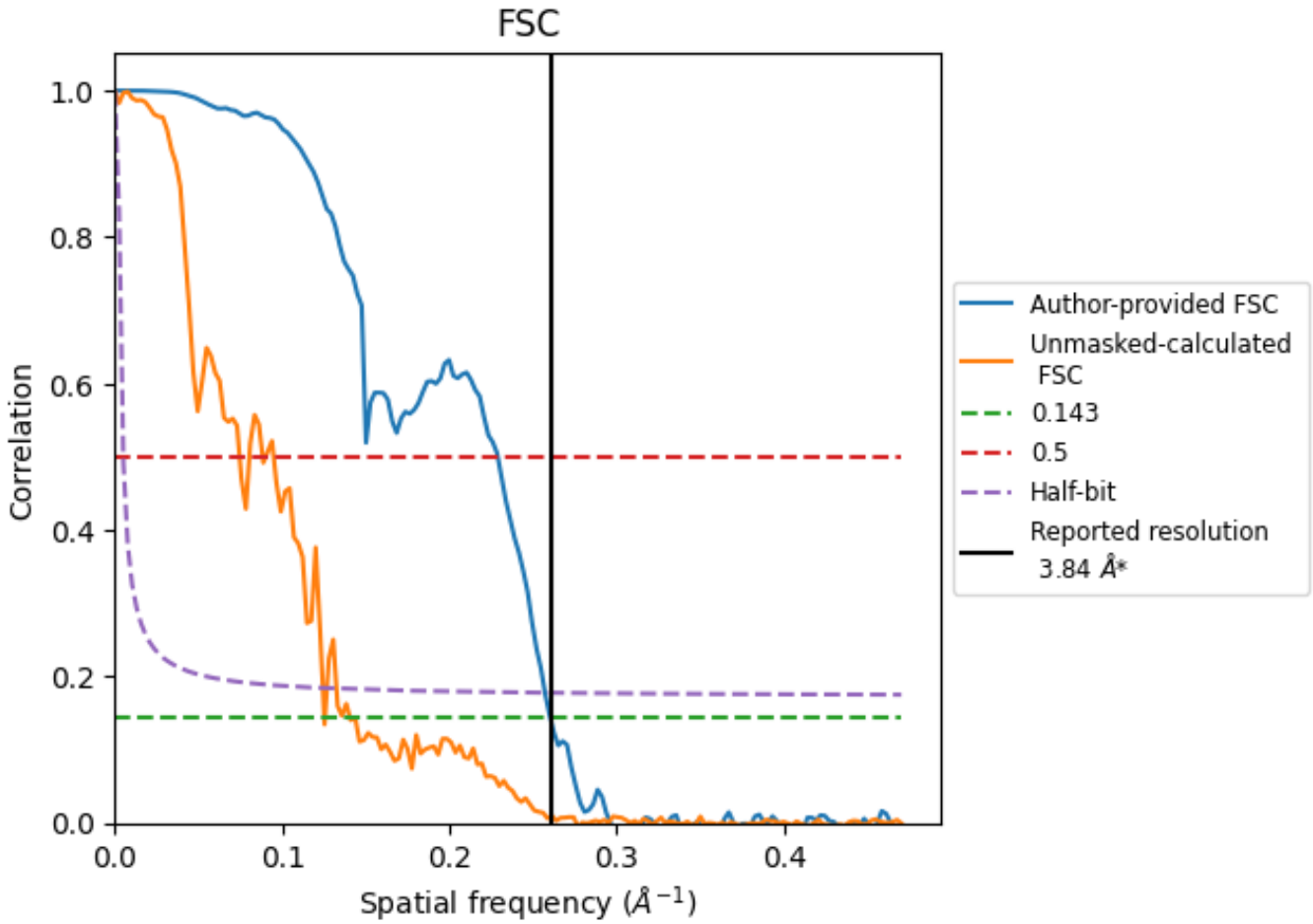


*Reported resolution corresponds to spatial frequency of 0.260 Å^{-1}

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 0.260 Å^{-1}

8.2 Resolution estimates (i)

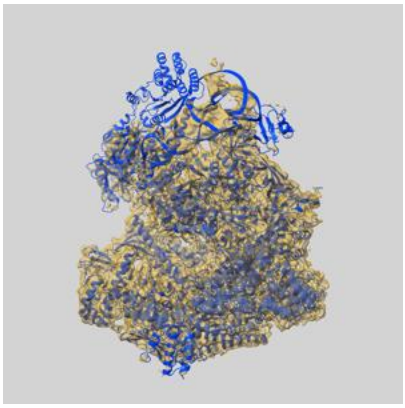
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.84	-	-
Author-provided FSC curve	3.84	4.37	3.89
Unmasked-calculated*	7.99	13.39	8.05

*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 7.99 differs from the reported value 3.84 by more than 10 %

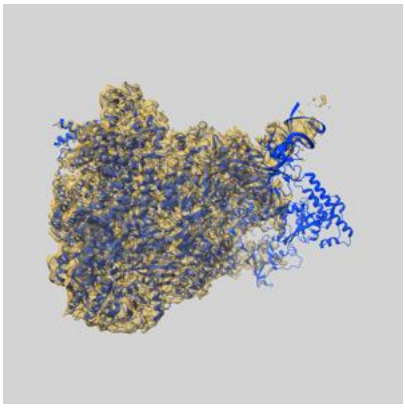
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16476 and PDB model 8C8H. Per-residue inclusion information can be found in section 3 on page 9.

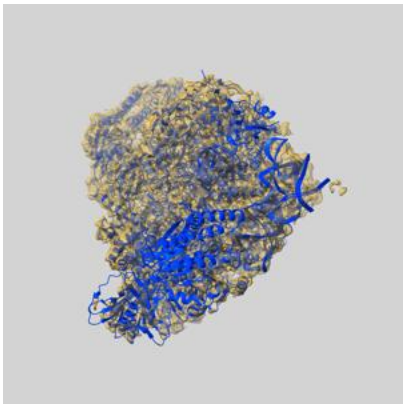
9.1 Map-model overlay



X



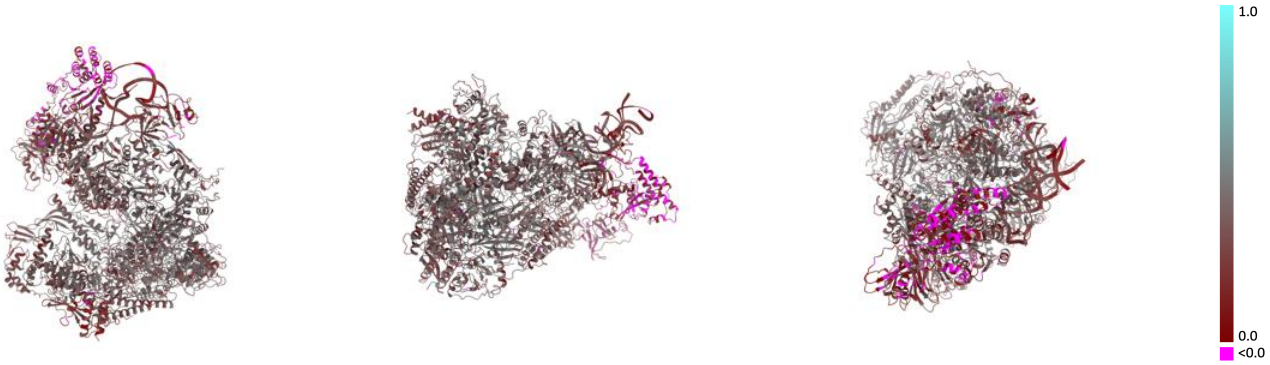
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

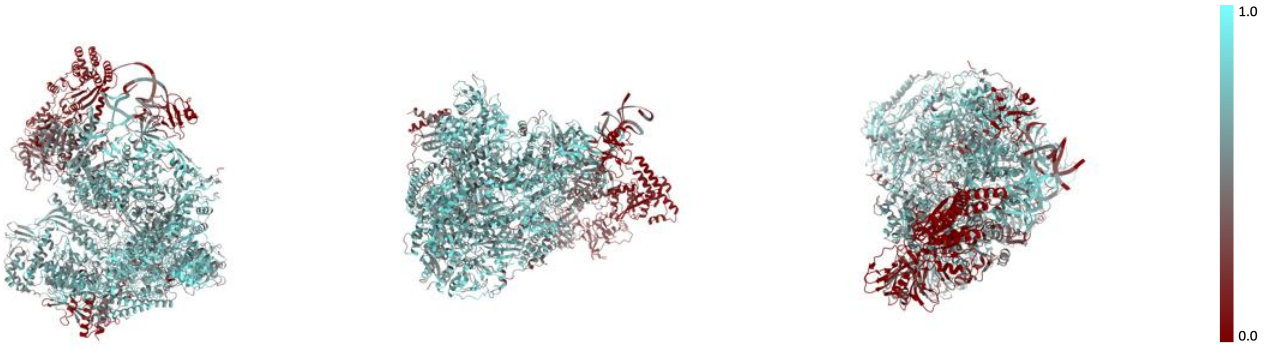
9.2 Q-score mapped to coordinate model



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.

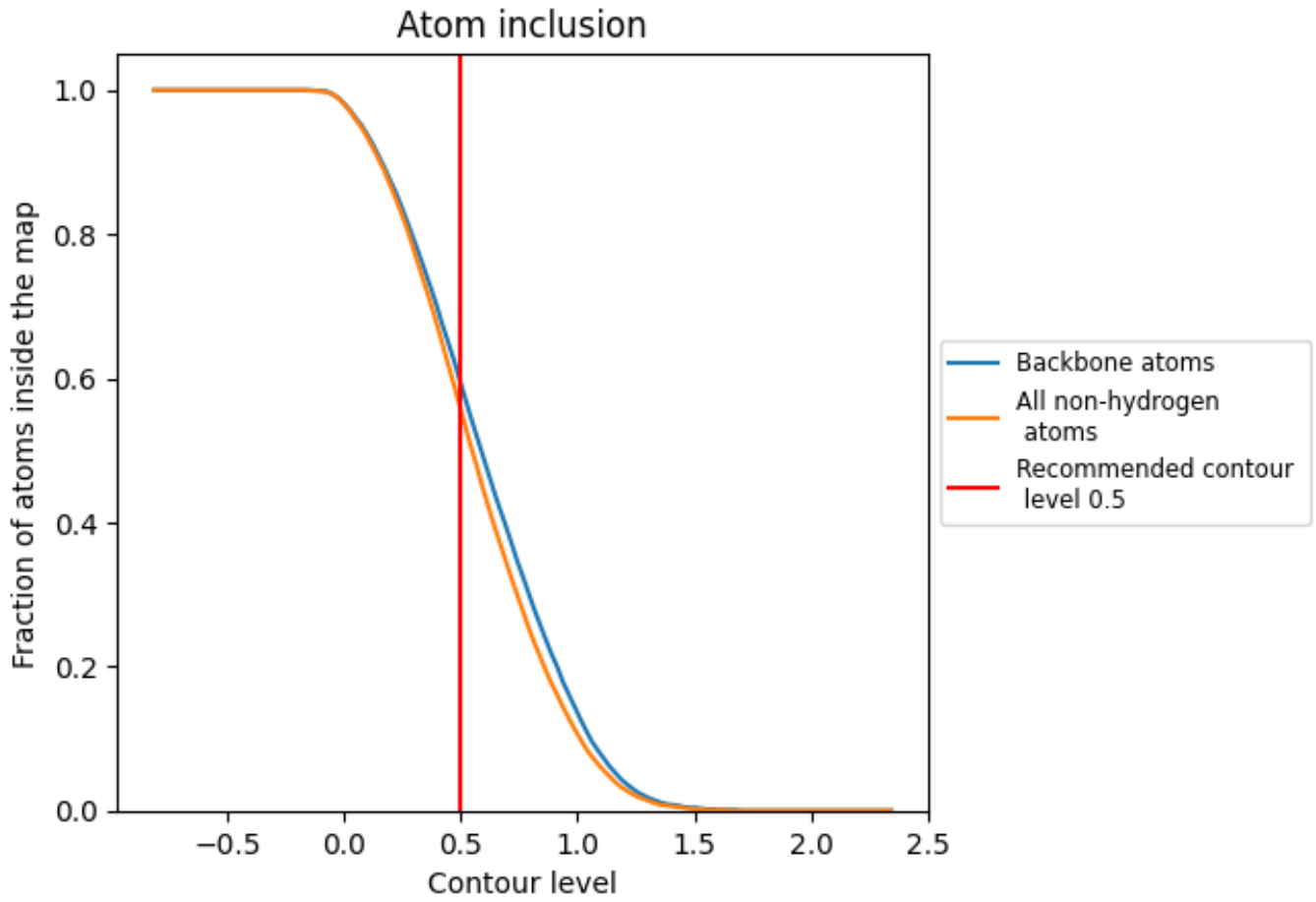
9.3 Atom inclusion mapped to coordinate model



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 59% of all backbone atoms, 56% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5550	0.3330
A	0.6760	0.3790
B	0.6940	0.3930
C	0.6610	0.3610
E	0.6870	0.3790
F	0.7370	0.3870
G	0.6330	0.3450
I	0.5730	0.3320
J	0.6900	0.3770
K	0.0080	0.1850
Q	0.0810	0.1460
R	0.2580	0.2560
S	0.3100	0.2700
U	0.5140	0.2520
Y	0.1930	0.1790