wwPDB EM Validation Summary Report

Nov 19, 2022 – 11:35 am GMT

PDB ID	:	5M3M
EMDB ID	:	EMD-4148
Title	:	Free monomeric RNA polymerase I at 4.0A resolution
Authors	:	Neyer, S.; Kunz, M.; Geiss, C.; Hantsche, M.; Hodirnau, V.-V.; Seybert, A.; Engel, C.; Scheffer, M.P.; Cramer, P.; Frangakis, A.S.
Deposited on	:	2016-10-15
Resolution	:	4.00 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:

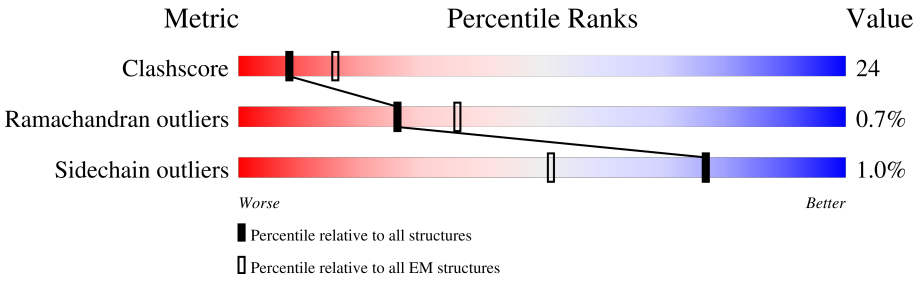
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.00 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

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

Mol	Chain	Length	Quality of chain
1	A	1664	61% 44% 43% 12%
2	B	1203	51% 49% 48% .
3	C	335	52% 41% 49% 9%
4	E	215	87% 44% 54% .
5	F	155	52% 32% 31% 37%
6	H	146	52% 48% 42% 10%
7	I	125	91% 46% 46% 7%
8	J	70	40% 44% 54% .

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Mol	Chain	Length	Quality of chain
9	K	142	35% 33% 38% 29%
10	L	70	40% 37% 26% 37%
11	M	415	23% 18% 5% 77%
12	N	233	56% 43% 13% 44%
13	D	137	42% 31% 9% 58%
14	G	326	59% 45% 13% 41%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SO4	B	1301	-	-	X	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 33233 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 I subunit RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1462	11558	7304	2006	2187	61	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase I subunit RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1166	9266	5864	1617	1734	51	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	305	2423	1539	416	460	8	0	0

- Molecule 4 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		
4	E	212	1735	1102	306	316	11	0	0

- Molecule 5 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		
5	F	98	807	512	142	150	3	0	0

- Molecule 6 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		
6	H	131	1052	664	176	208	4	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase I subunit RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	116	Total	C	N	O	S	0	0
			883	550	148	176	9		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

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

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	44	Total	C	N	O	S	0	0
			352	217	70	61	4		

- Molecule 11 is a protein called DNA-directed RNA polymerase I subunit RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	M	97	Total	C	N	O	0	0
			771	490	124	157		

- Molecule 12 is a protein called DNA-directed RNA polymerase I subunit RPA34.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	131	Total	C	N	O	S	0	0
			1035	660	171	200	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase I subunit RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	D	58	Total	C	N	O	0	0
			459	289	78	92		

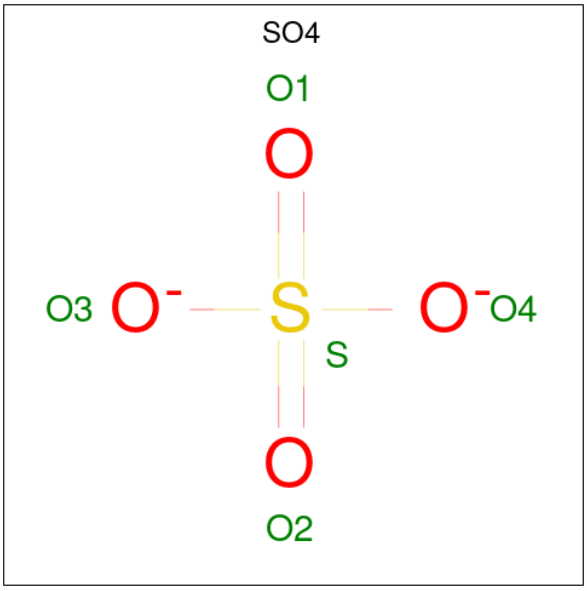
- Molecule 14 is a protein called DNA-directed RNA polymerase I subunit RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	192	Total	C	N	O	S	0	0
			1518	979	261	273	5		

- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
15	A	2	Total	Zn	0
			2	2	
15	B	1	Total	Zn	0
			1	1	
15	I	2	Total	Zn	0
			2	2	
15	J	1	Total	Zn	0
			1	1	
15	L	1	Total	Zn	0
			1	1	

- Molecule 16 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



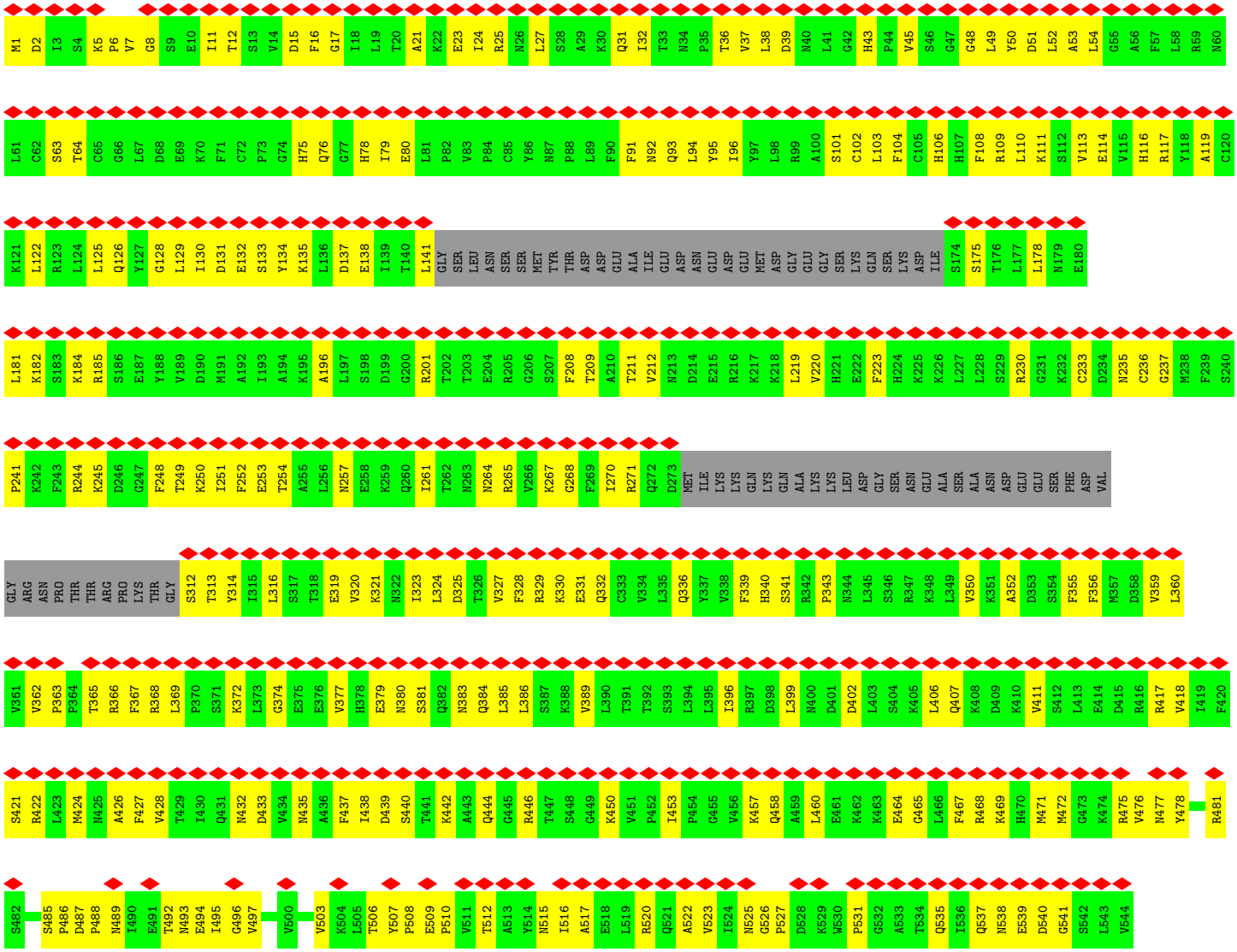
Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	O	S	0
			5	4	1	

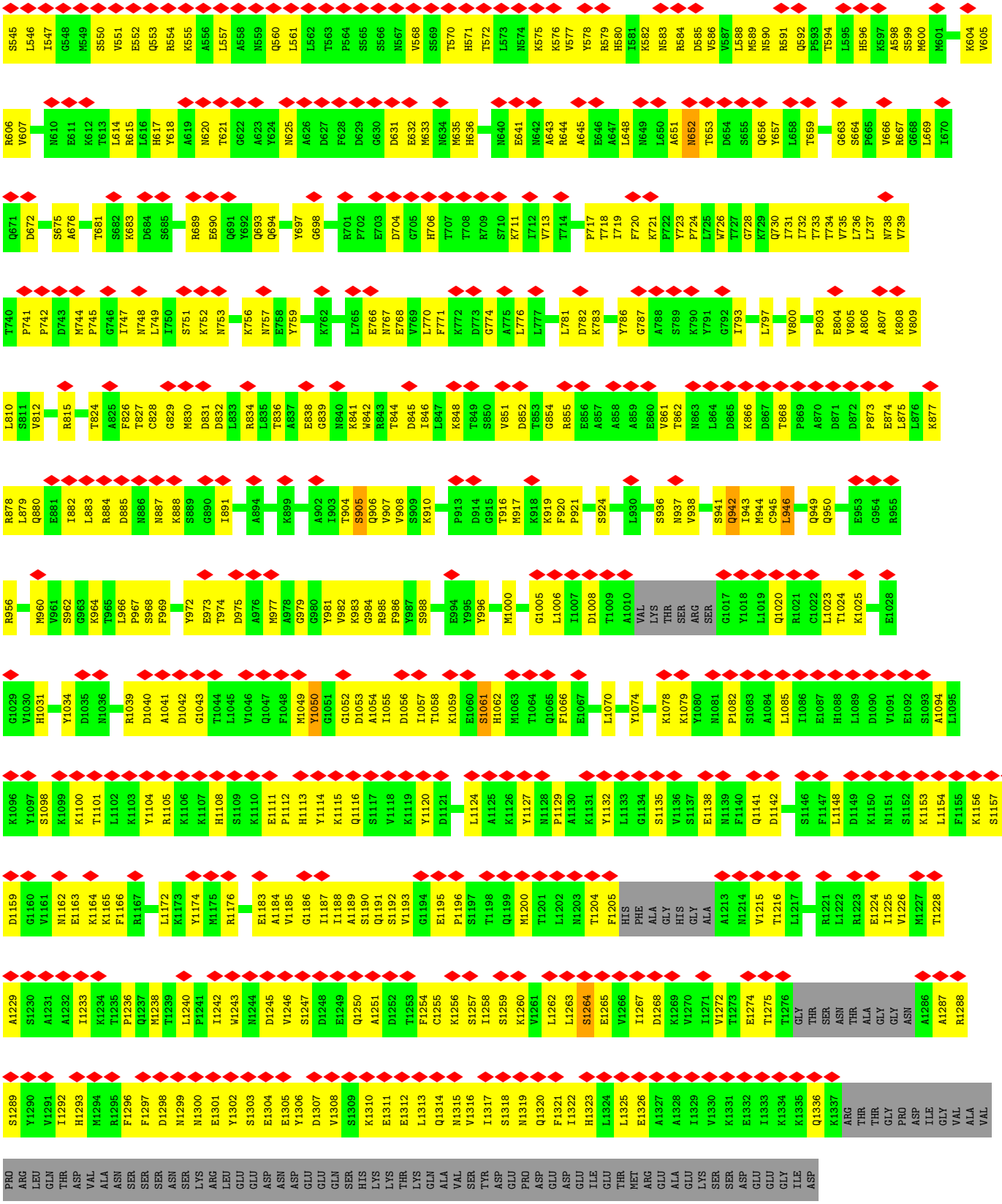
3 Residue-property plots (i)

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 I subunit RPA190

Chain A:

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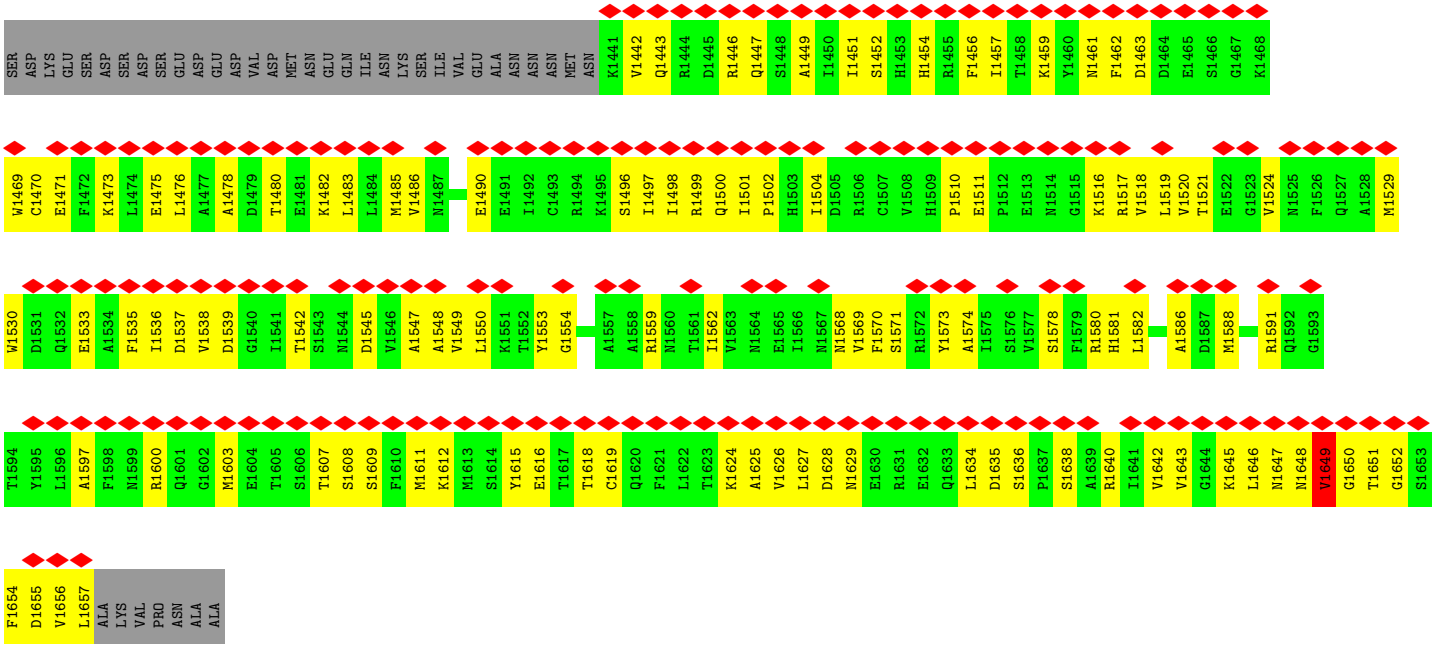
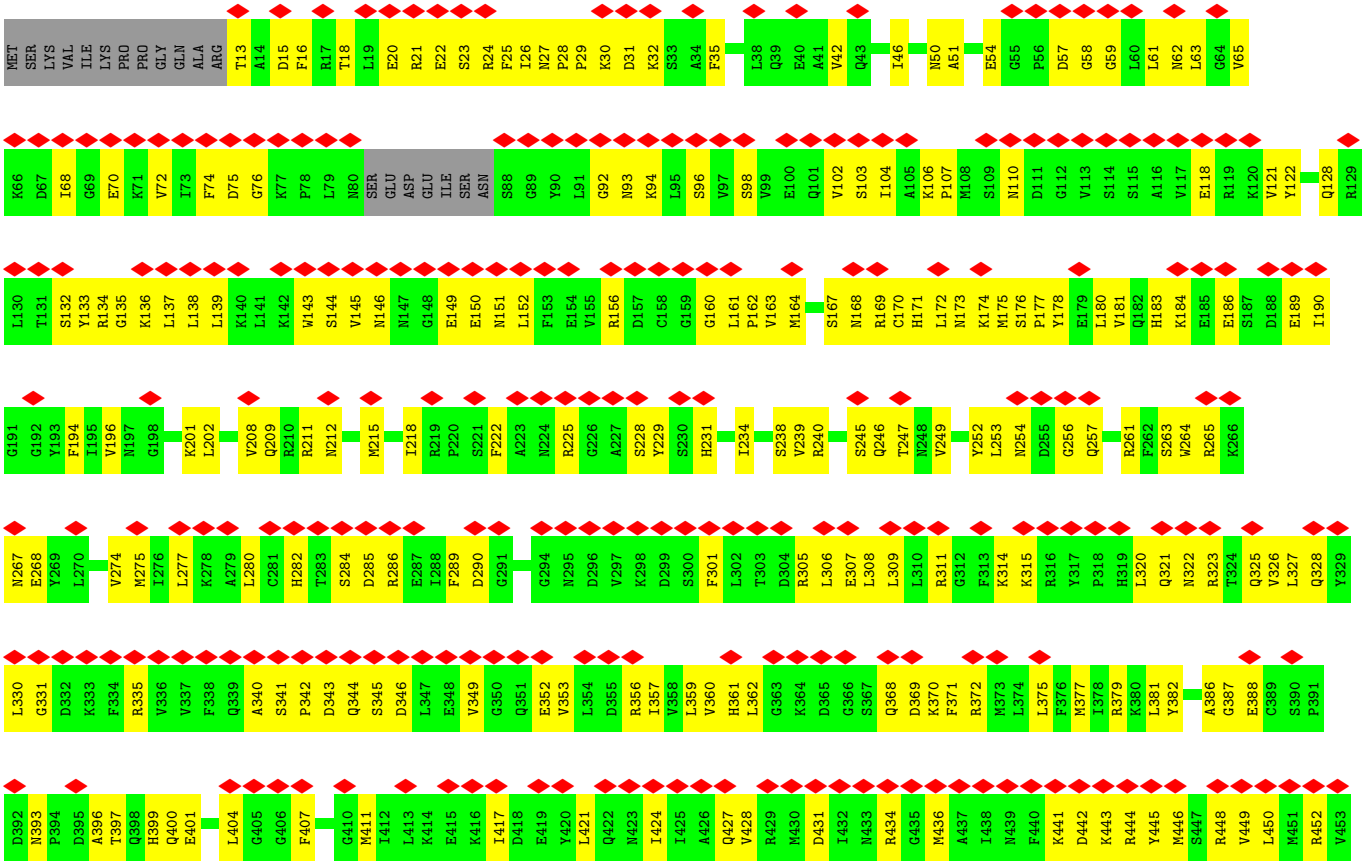
R606 V607 N610 E611 K612 T613 L614 R615 L616 H617 Y618 A619 N620 T621 G622 A623 Y624 N625 A626 D627 F628 D629 G630 D631 E632 M633 N634 M635 H636 N640 E641 N642 A643 R644 A645 E646 A647 L648 N649 L650 A651 N652 T653 D654 S655 Q656 Y657 L658 T659 G663 S664 P665 V666 R667 G668 L669 I670
Q671 D672 S675 A676 T681 S682 K683 D684 S685 R689 E690 Q691 Y692 Q693 Q694 Y697 G698 R701 P702 E703 D704 G705 H706 T707 T708 R709 S710 K711 I712 V713 T714 P717 T718 I719 F720 K721 F722 Y723 P724 L725 W726 T727 G728 K729 Q730 I731 I732 T733 T734 V735 L736 L737 N738 V739
T740 P741 P742 D743 M744 P745 G746 I747 N748 L749 I750 S751 K752 N753 K756 N757 E758 Y759 K762 L765 E766 N767 E768 V769 L770 F771 K772 D773 G774 A775 L776 L777 L781 D782 K783 Y786 G787 A788 S789 K790 Y791 G792 I793 L797 V800 P803 E804 V805 A806 A807 K808 V809
L810 S811 V812 R815 T824 A825 F826 T827 C828 G829 M830 D831 D832 L833 R834 L835 T836 A837 E838 G839 N840 K841 W842 R843 T844 D845 I846 L847 K848 T849 S850 V851 D852 T853 G854 R855 E856 A857 A858 A859 E860 V861 T862 N863 L864 D865 K866 D867 T868 P869 A870 D871 D872 P873 E874 L875 L876 K877
R878 L879 Q880 E881 I882 L883 R884 D885 N886 N887 K888 S889 G890 I891 A894 K899 A902 I903 T904 S905 Q906 V907 V908 S909 K910 P913 D914 G915 T916 M917 K918 K919 F920 P921 S924 L930 S936 N937 V938 S941 Q942 I943 M944 C945 L946 Q949 Q950 E953 G954 R955
R956 M960 V961 S962 G963 K964 T965 L966 P967 S968 F969 Y972 E973 T974 D975 A976 M977 A978 G979 G980 Y981 V982 K983 G984 R985 F986 Y987 S988 E994 Y995 Y996 M1000 G1005 L1006 I1007 D1008 T1009 A1010 VAL LYS THR SER ARG SER G1017 Y1018 L1019 Q1020 R1021 C1022 L1023 T1024 K1025 E1028
G1029 V1030 H1031 Y1034 D1035 N1036 R1039 D1040 A1041 D1042 G1043 T1044 L1045 V1046 Q1047 F1048 M1049 Y1050 G1051 G1052 D1053 A1054 I1055 D1056 I1057 T1058 K1059 E1060 S1061 H1062 M1063 T1064 Q1065 F1066 E1067 L1070 Y1074 K1078 K1079 Y1080 N1081 P1082 S1083 A1084 L1085 I1086 E1087 H1088 L1089 D1090 V1091 E1092 S1093 A1094 L1095
K1096 Y1097 S1098 K1099 K1100 T1101 L1102 K1103 Y1104 R1105 K1106 K1107 H1108 S1109 K1110 E1111 P1112 H1113 Y1114 K1115 Q1116 S1117 V1118 K1119 Y1120 D1121 L1124 A1125 K1126 Y1127 N1128 P1129 A1130 K1131 Y1132 L1133 G1134 S1135 V1136 S1137 E1138 N1139 F1140 Q1141 D1142 S1146 F1147 L1148 D1149 K1150 N1151 S1152 K1153 L1154 F1155 K1156 S1157 S1158
D1159 G1160 V1161 N1162 E1163 K1164 K1165 F1166 R1167 L1172 K1173 Y1174 M1175 R1176 E1183 A1184 V1185 G1186 I1187 I1188 A1189 S1190 Q1191 S1192 V1193 G1194 E1195 P1196 S1197 T1198 Q1199 M1200 T1201 L1202 N1203 T1204 F1205 HIS PHE ALA GLY HIS GLY ALA A1213 N1214 V1215 T1216 L1217 R1221 L1222 R1223 E1224 I1225 V1226 M1227 T1228
A1229 S1230 A1231 A1232 I1233 K1234 T1235 P1236 Q1237 M1238 T1239 L1240 P1241 I1242 W1243 N1244 D1245 V1246 S1247 D1248 E1249 Q1250 A1251 D1252 T1253 F1254 C1255 K1256 S1257 I1258 S1259 K1260 V1261 L1262 L1263 S1264 E1265 V1266 I1267 D1268 K1269 V1270 I1271 V1272 T1273 E1274 T1275 T1276 GLY THR SER ASN THR ALA GLY GLY ASN A1286 A1287 R1288
S1289 Y1290 V1291 I1292 H1293 M1294 R1295 F1296 F1297 D1298 N1299 N1300 E1301 Y1302 S1303 E1304 E1305 Y1306 D1307 V1308 S1309 K1310 E1311 E1312 L1313 Q1314 N1315 V1316 I1317 S1318 N1319 Q1320 F1321 I1322 H1323 L1324 L1325 E1326 A1327 A1328 I1329 V1330 K1331 E1332 I1333 K1334 K1335 Q1336 K1337 ARG THR THR GLY PRO ASP ILE GLY VAL ALA VAL
PRO ARG LEU GLN THR ASP VAL ALA ASN SER SER SER ASN SER LYS ARG LEU GLU GLU ASP ASN ASP GLU GLU GLN SER HIS LYS LYS THR LYS GLN ALA VAL SER TYR ASP GLU PRO ASP GLU GLU ASP GLU ILE GLU THR MET ARG GLU ALA GLU LYS SER SER ASP GLU GLU GLY ILE ASP



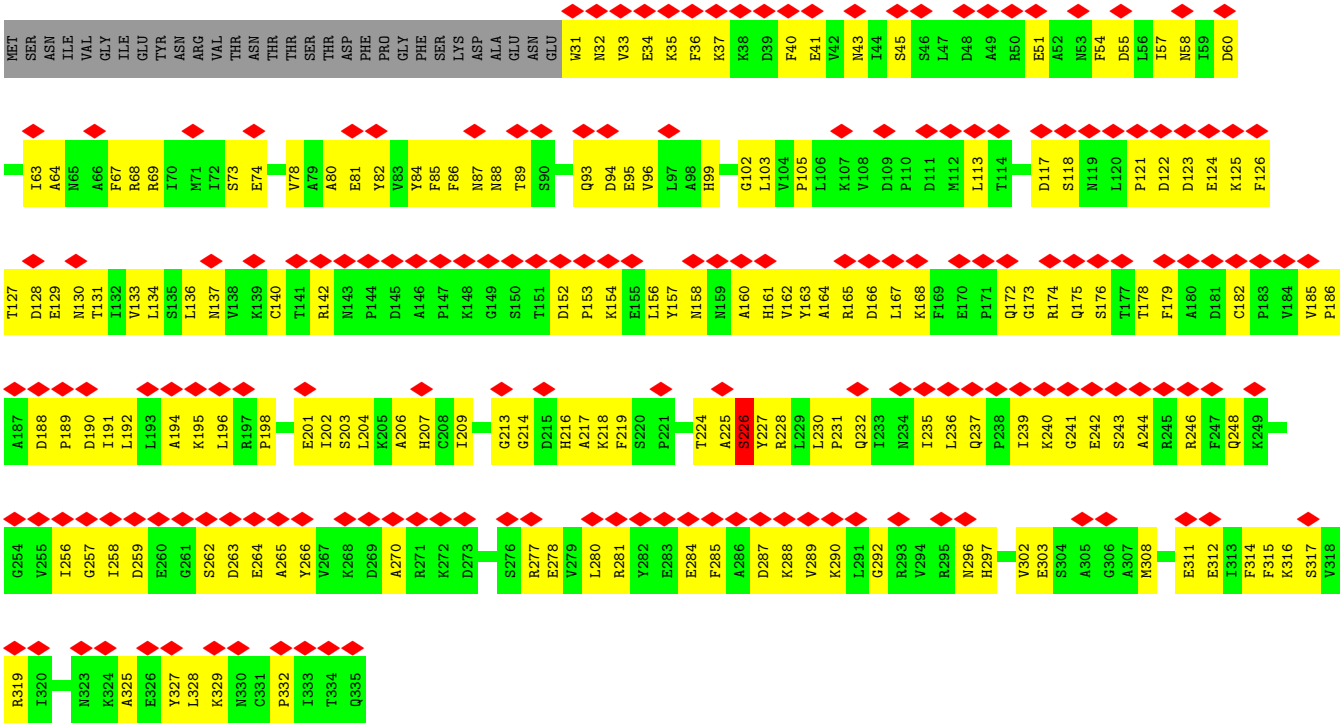
• Molecule 2: DNA-directed RNA polymerase I subunit RPA135

Chain B:



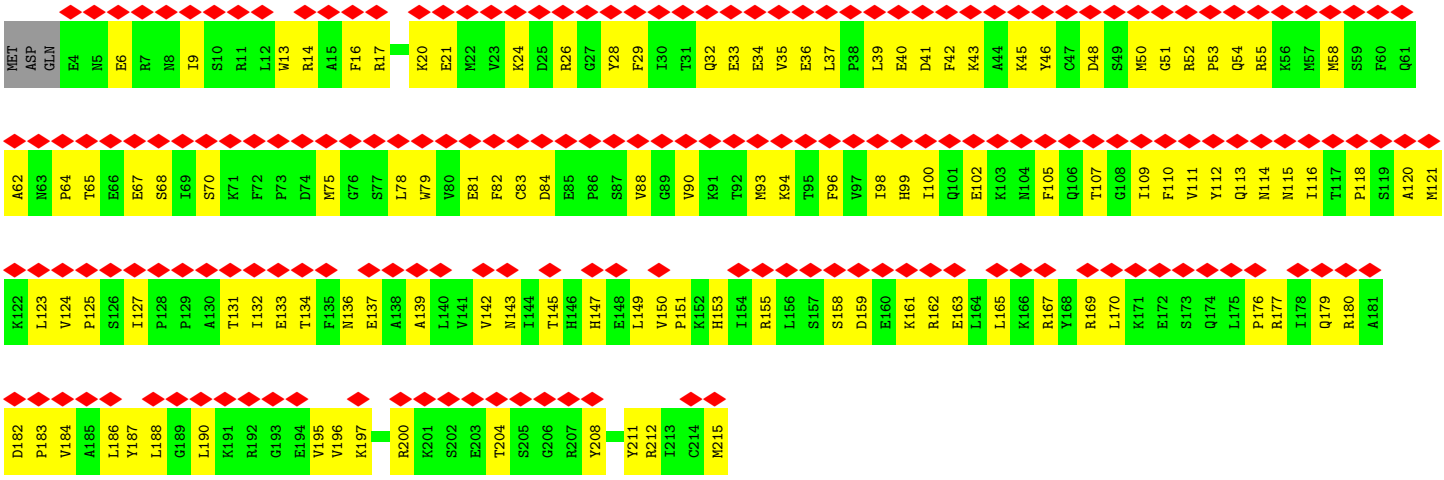
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



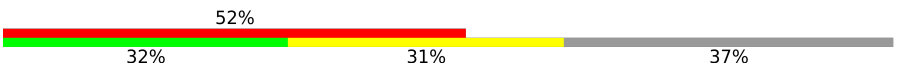
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

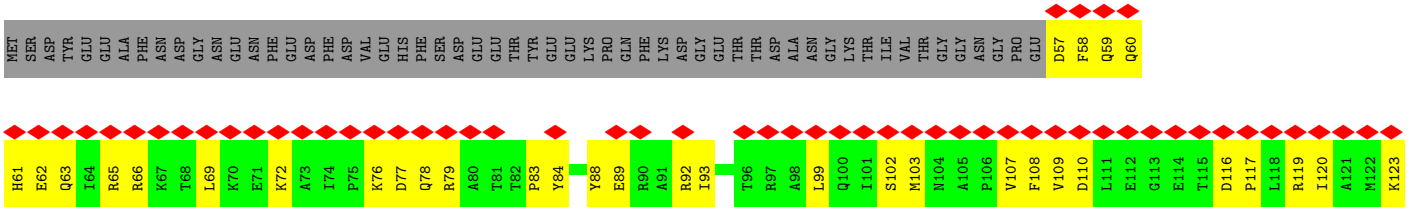
Chain E:

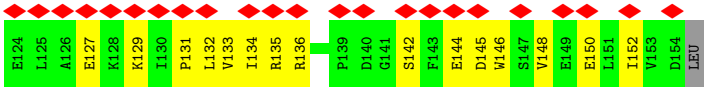


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:

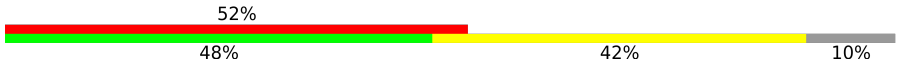


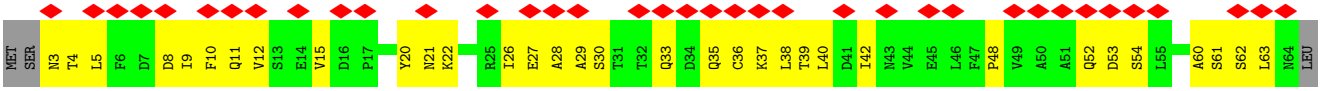


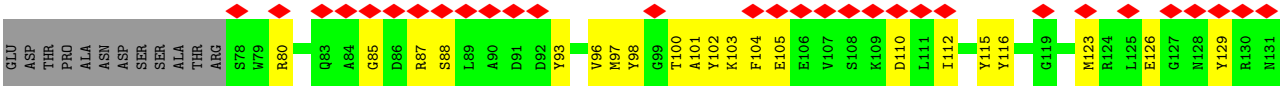


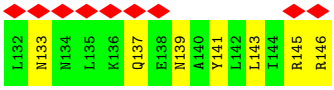
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



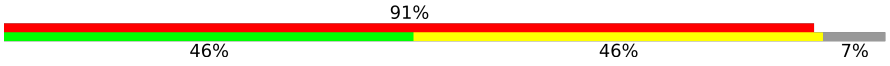


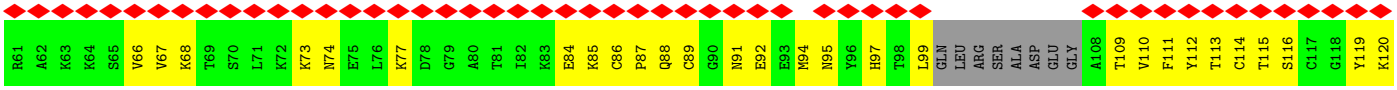


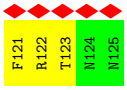


• Molecule 7: DNA-directed RNA polymerase I subunit RPA12

Chain I:

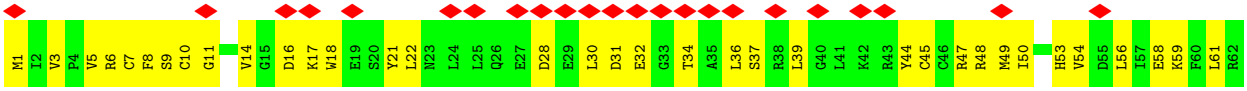


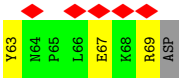




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

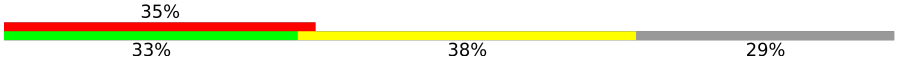
Chain J:

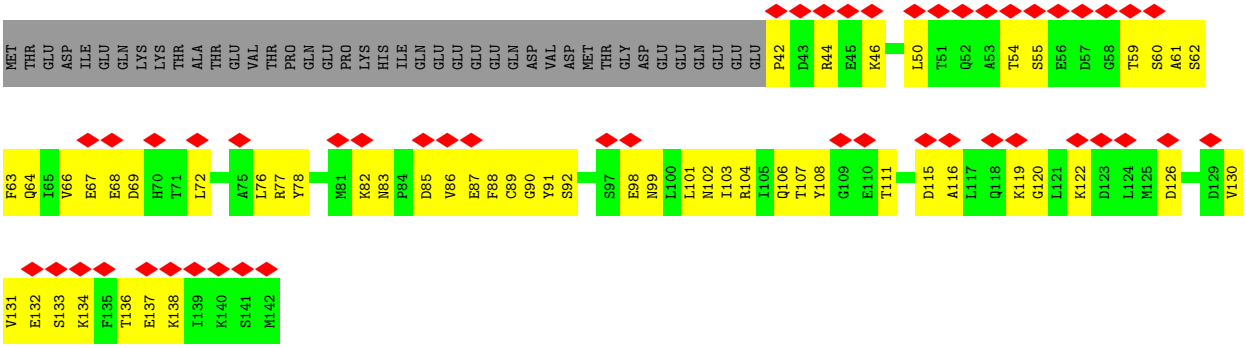




• Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC2

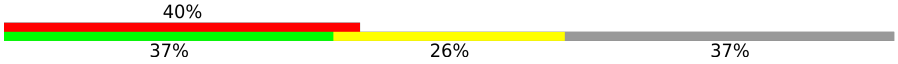
Chain K:

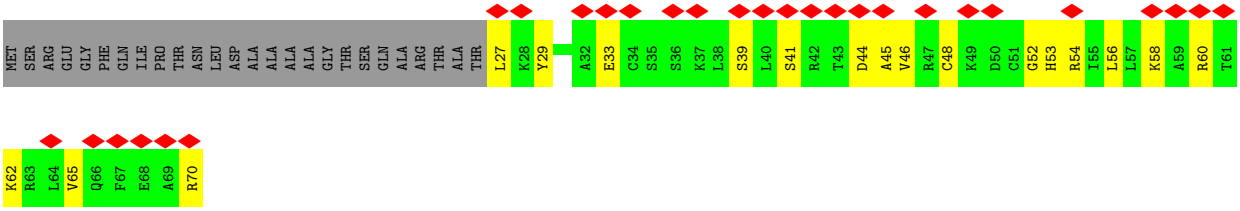




• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

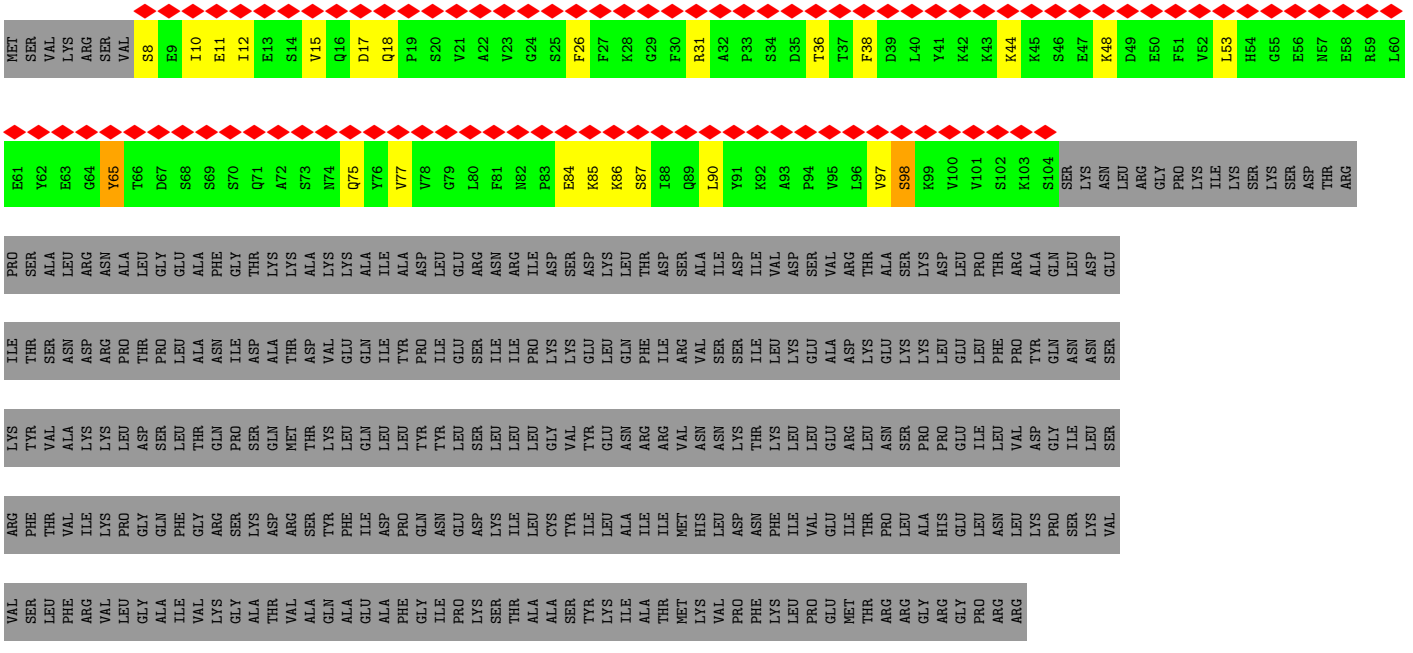
Chain L:





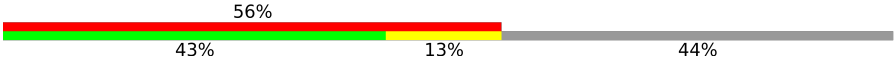
• Molecule 11: DNA-directed RNA polymerase I subunit RPA49

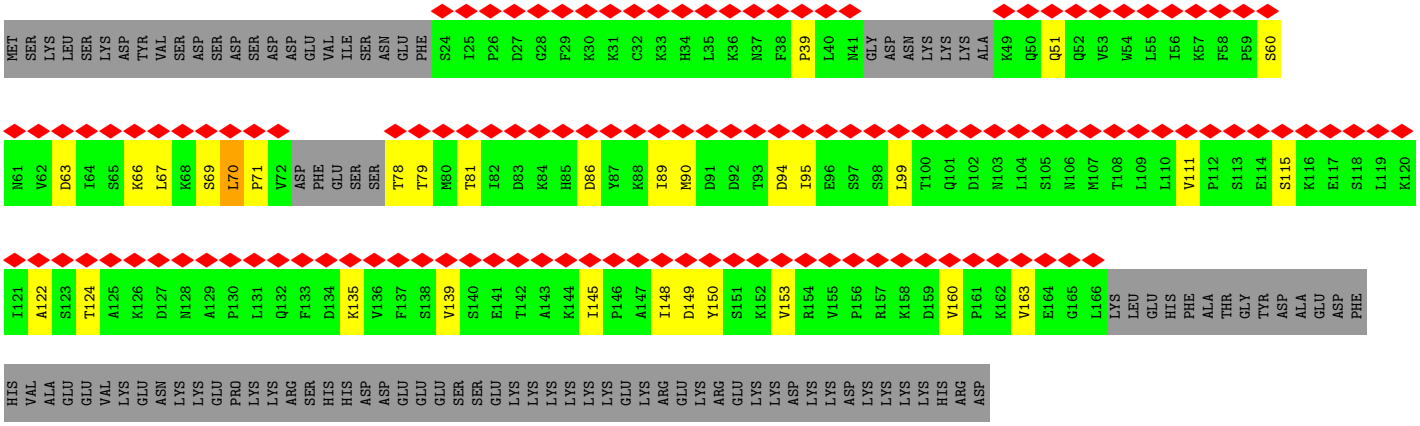
Chain M:



• Molecule 12: DNA-directed RNA polymerase I subunit RPA34

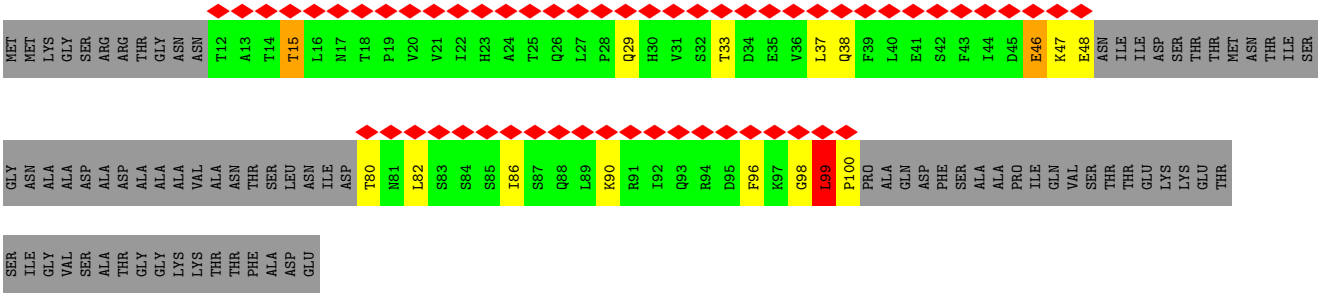
Chain N:





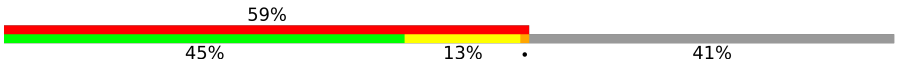
• Molecule 13: DNA-directed RNA polymerase I subunit RPA14

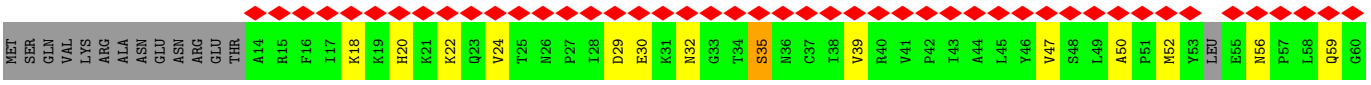
Chain D:

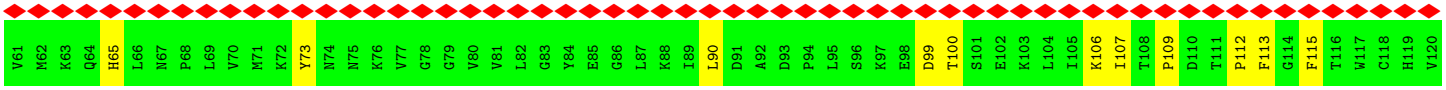


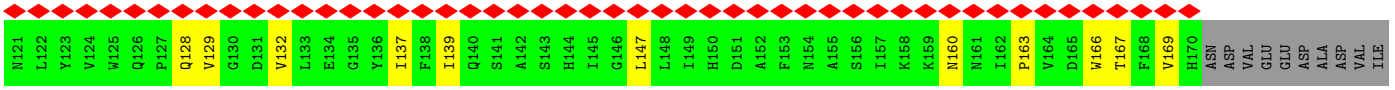
• Molecule 14: DNA-directed RNA polymerase I subunit RPA43

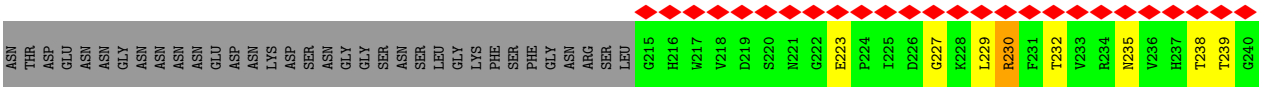
Chain G:

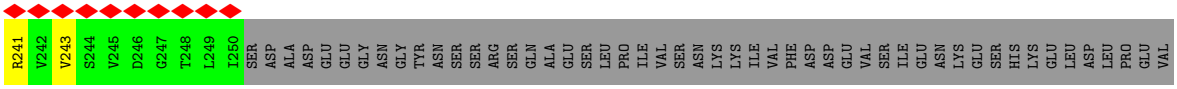












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94000	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 ($e^-/Å^2$)	56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.152	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	241.49998, 241.49998, 241.49998	wwPDB
Map dimensions	230, 230, 230	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/11770	0.51	0/15895
2	B	0.45	0/9471	0.53	0/12805
3	C	0.45	0/2475	0.51	0/3354
4	E	0.40	0/1771	0.50	0/2383
5	F	0.37	0/821	0.48	0/1106
6	H	0.46	0/1070	0.54	0/1449
7	I	0.38	0/895	0.49	0/1205
8	J	0.50	0/578	0.53	0/775
9	K	0.45	0/804	0.55	0/1083
10	L	0.40	0/354	0.53	0/468
11	M	0.40	0/786	0.55	0/1057
12	N	0.39	0/1052	0.55	0/1418
13	D	0.40	0/465	0.58	0/630
14	G	0.37	0/1555	0.66	3/2113 (0.1%)
All	All	0.42	0/33867	0.53	3/45741 (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
1	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	241	ARG	NE-CZ-NH1	11.80	126.20	120.30
14	G	241	ARG	NE-CZ-NH2	-11.62	114.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	G	241	ARG	CD-NE-CZ	6.08	132.12	123.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1649	VAL	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	A	11558	0	11642	651	0
2	B	9266	0	9151	558	0
3	C	2423	0	2412	156	0
4	E	1735	0	1764	98	0
5	F	807	0	827	45	0
6	H	1052	0	1021	47	0
7	I	883	0	879	60	0
8	J	569	0	585	36	0
9	K	793	0	790	56	0
10	L	352	0	374	20	0
11	M	771	0	755	11	0
12	N	1035	0	1069	29	0
13	D	459	0	462	8	0
14	G	1518	0	1528	31	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
16	B	5	0	0	8	0
All	All	33233	0	33259	1613	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 24.

The worst 5 of 1613 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:B:656:LEU:O	12:N:153:VAL:HG11	1.62	0.97
3:C:225:ALA:O	3:C:226:SER:HB2	1.63	0.95
1:A:1501:ILE:HG22	1:A:1502:PRO:HD2	1.49	0.94
2:B:894:LYS:HG2	10:L:54:ARG:HH21	1.33	0.94
5:F:66:ARG:HA	5:F:69:LEU:HD12	1.50	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1448/1664 (87%)	1364 (94%)	75 (5%)	9 (1%)	25 63
2	B	1158/1203 (96%)	1110 (96%)	41 (4%)	7 (1%)	25 63
3	C	303/335 (90%)	283 (93%)	19 (6%)	1 (0%)	41 75
4	E	210/215 (98%)	202 (96%)	8 (4%)	0	100 100
5	F	96/155 (62%)	94 (98%)	2 (2%)	0	100 100
6	H	127/146 (87%)	124 (98%)	3 (2%)	0	100 100
7	I	112/125 (90%)	108 (96%)	4 (4%)	0	100 100
8	J	67/70 (96%)	61 (91%)	6 (9%)	0	100 100
9	K	99/142 (70%)	95 (96%)	4 (4%)	0	100 100
10	L	42/70 (60%)	38 (90%)	4 (10%)	0	100 100
11	M	95/415 (23%)	86 (90%)	7 (7%)	2 (2%)	7 39
12	N	125/233 (54%)	108 (86%)	13 (10%)	4 (3%)	4 31
13	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	3 28
14	G	186/326 (57%)	171 (92%)	13 (7%)	2 (1%)	14 51
All	All	4122/5236 (79%)	3894 (94%)	201 (5%)	27 (1%)	26 61

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	946	LEU
2	B	657	PRO
2	B	658	LEU
2	B	659	ASP
3	C	226	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	A	1292/1465 (88%)	1288 (100%)	4 (0%)	92 95
2	B	1022/1053 (97%)	1020 (100%)	2 (0%)	93 96
3	C	269/296 (91%)	268 (100%)	1 (0%)	91 94
4	E	194/197 (98%)	194 (100%)	0	100 100
5	F	88/137 (64%)	88 (100%)	0	100 100
6	H	115/128 (90%)	115 (100%)	0	100 100
7	I	103/110 (94%)	103 (100%)	0	100 100
8	J	64/65 (98%)	64 (100%)	0	100 100
9	K	91/130 (70%)	91 (100%)	0	100 100
10	L	39/57 (68%)	39 (100%)	0	100 100
11	M	88/371 (24%)	79 (90%)	9 (10%)	7 28
12	N	124/220 (56%)	120 (97%)	4 (3%)	39 62
13	D	55/116 (47%)	49 (89%)	6 (11%)	6 26
14	G	170/291 (58%)	158 (93%)	12 (7%)	14 42
All	All	3714/4636 (80%)	3676 (99%)	38 (1%)	77 86

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	G	35	SER
14	G	230	ARG

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Mol	Chain	Res	Type
14	G	39	VAL
14	G	167	THR
14	G	243	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	587	GLN
3	C	58	ASN
9	K	99	ASN
2	B	686	HIS
2	B	1008	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
16	SO4	B	1301	-	4,4,4	0.20	0	6,6,6	0.35	0

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.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1301	SO4	8	0

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.

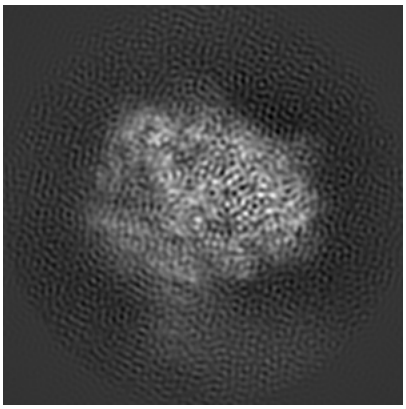
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4148. These allow visual inspection of the internal detail of the map and identification of artifacts.

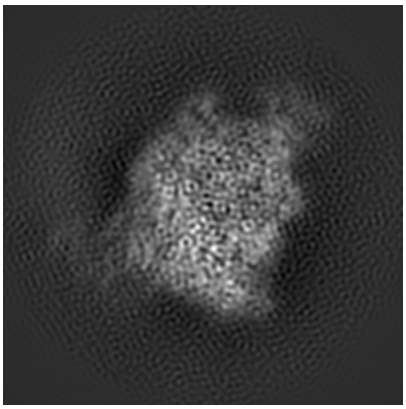
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

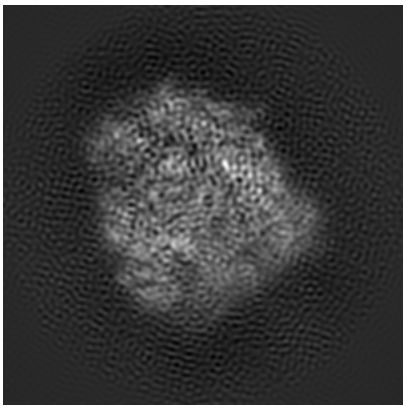
6.1.1 Primary map



X

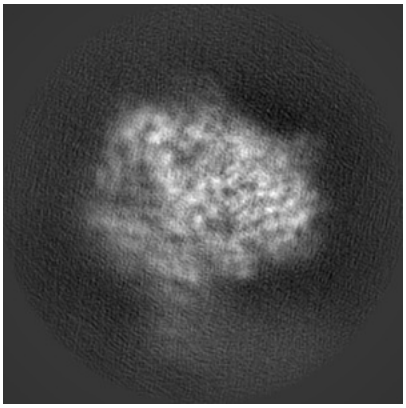


Y

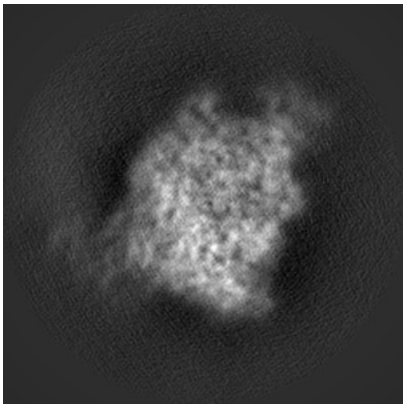


Z

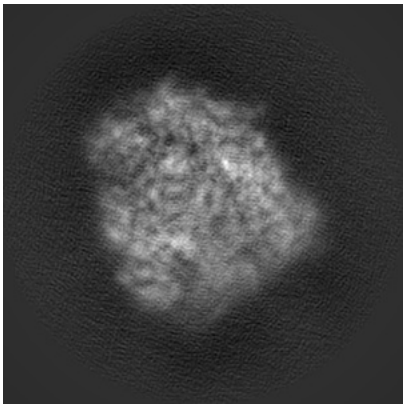
6.1.2 Raw map



X



Y

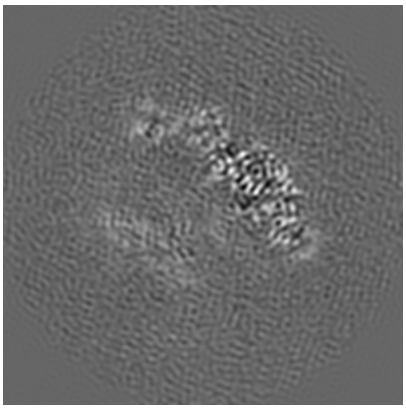


Z

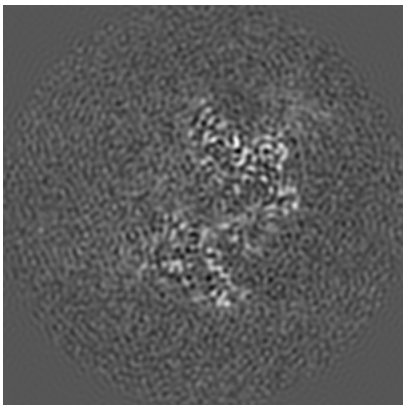
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

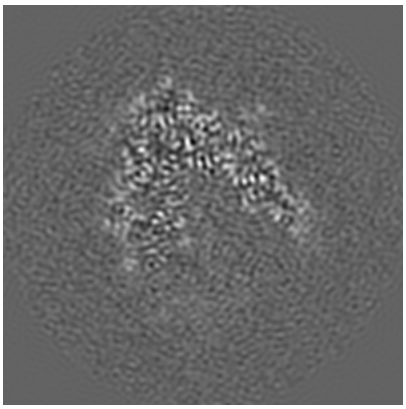
6.2.1 Primary map



X Index: 115

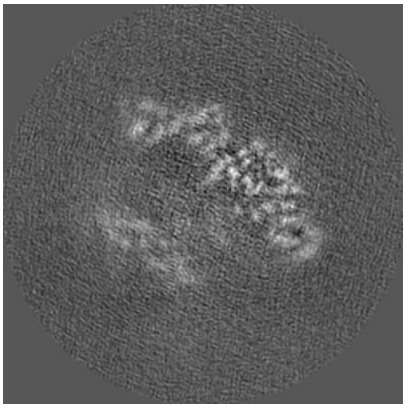


Y Index: 115

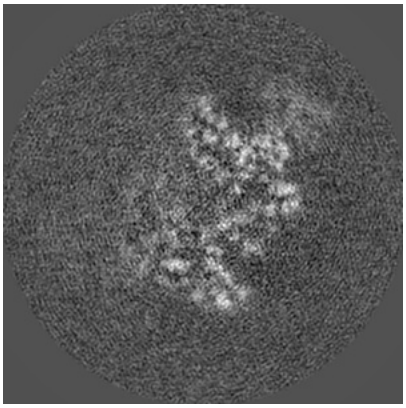


Z Index: 115

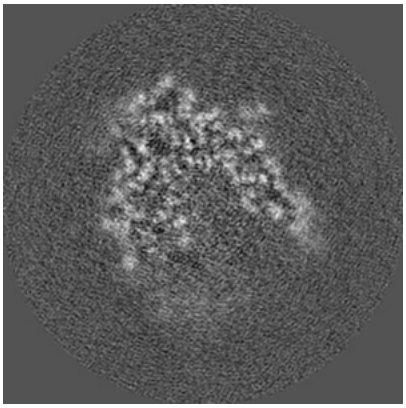
6.2.2 Raw map



X Index: 115



Y Index: 115

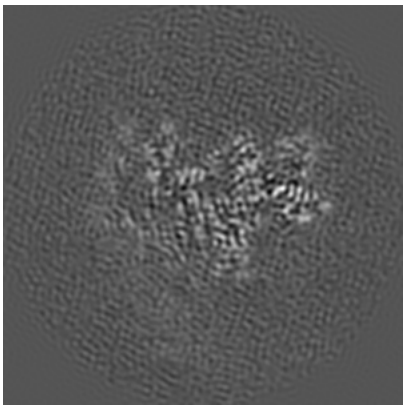


Z Index: 115

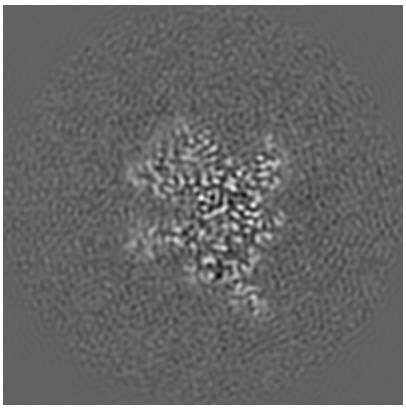
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

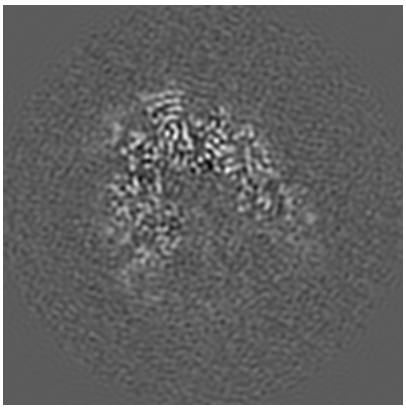
6.3.1 Primary map



X Index: 95

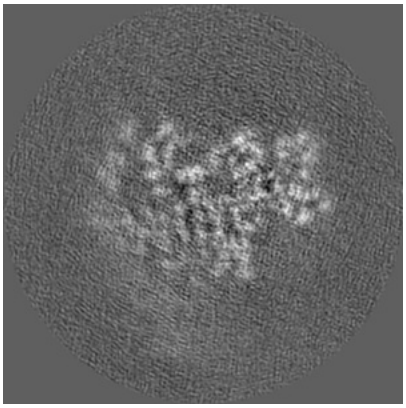


Y Index: 137

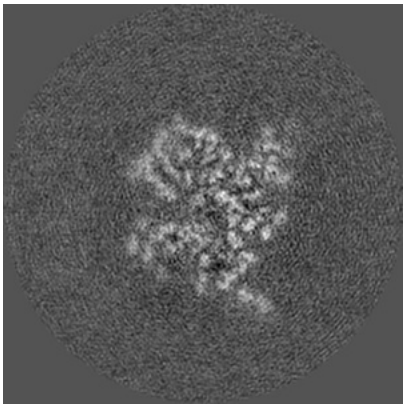


Z Index: 120

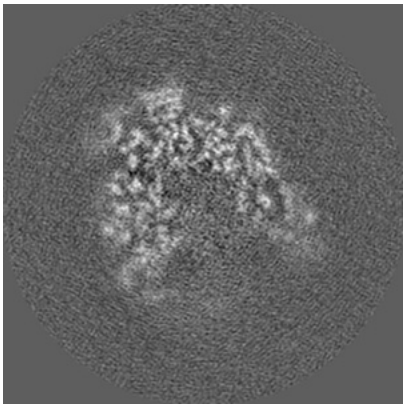
6.3.2 Raw map



X Index: 96



Y Index: 134

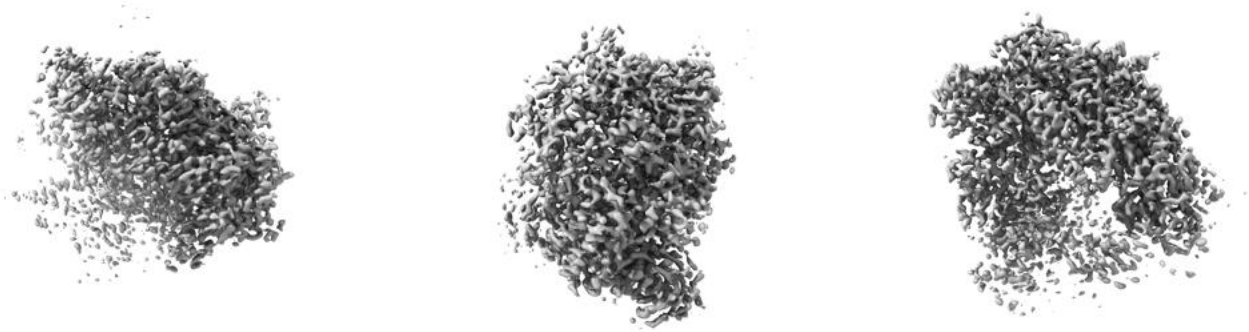


Z Index: 120

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

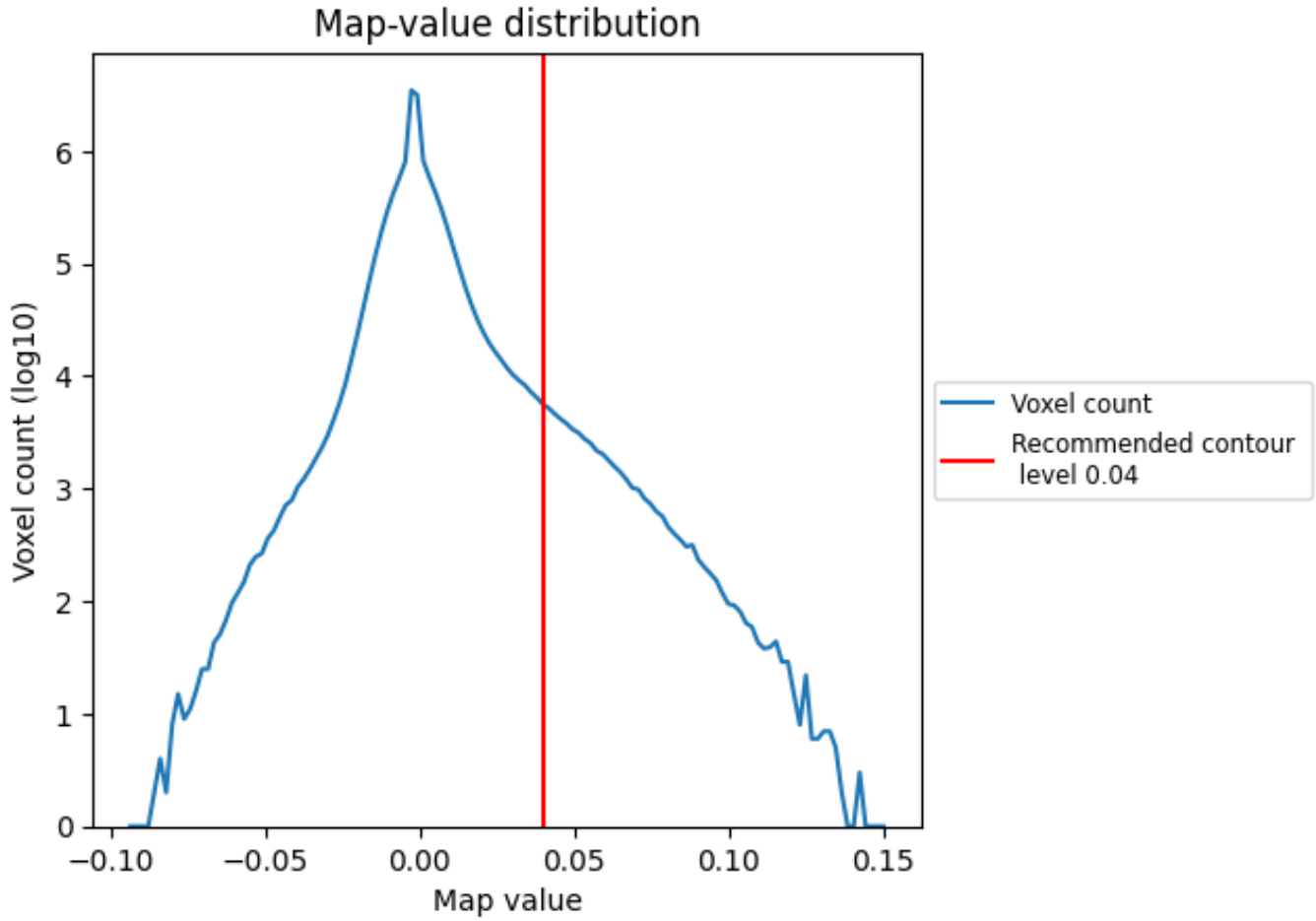
6.5 Mask visualisation (i)

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

7 Map analysis

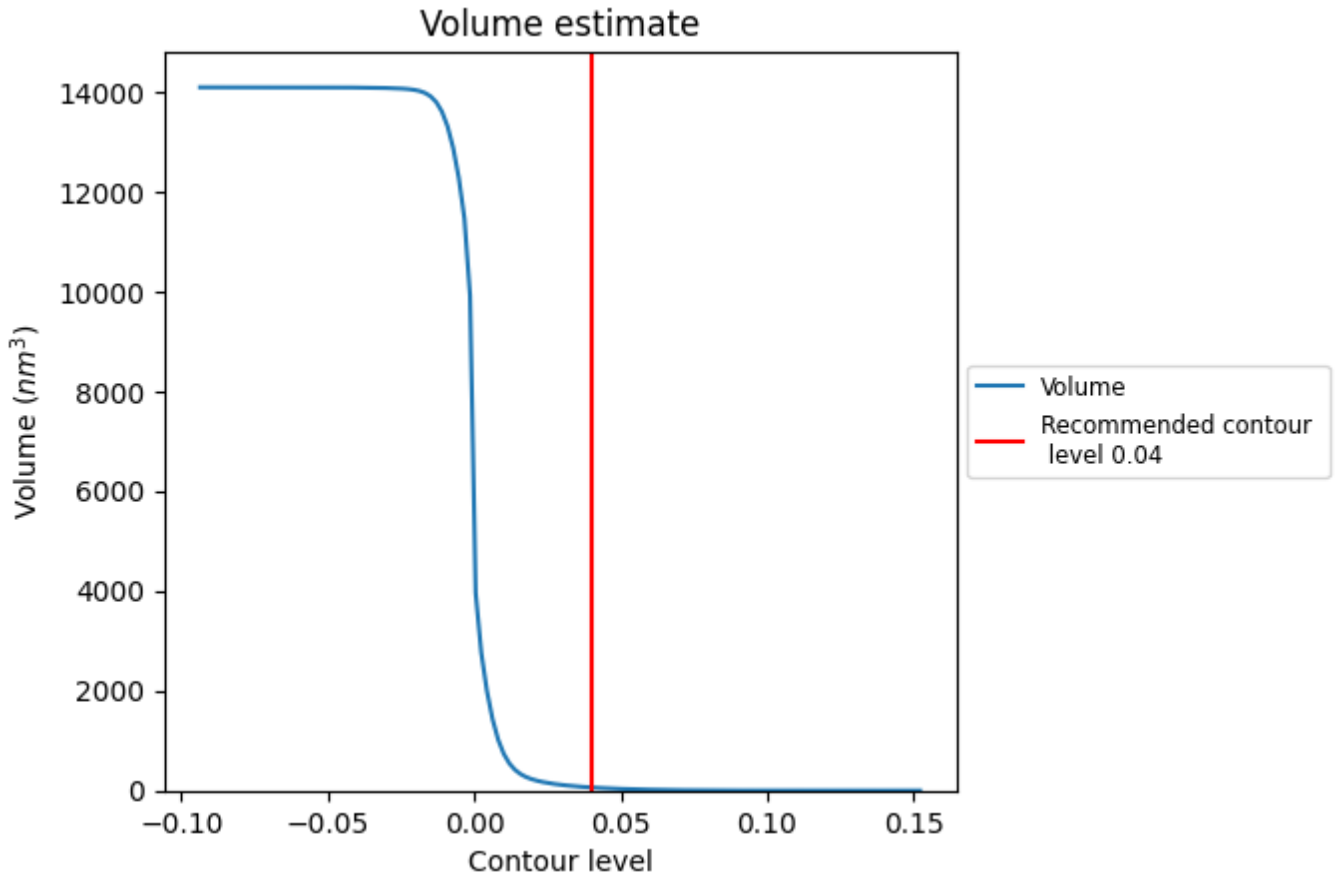
This section contains the results of statistical analysis of the map.

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.

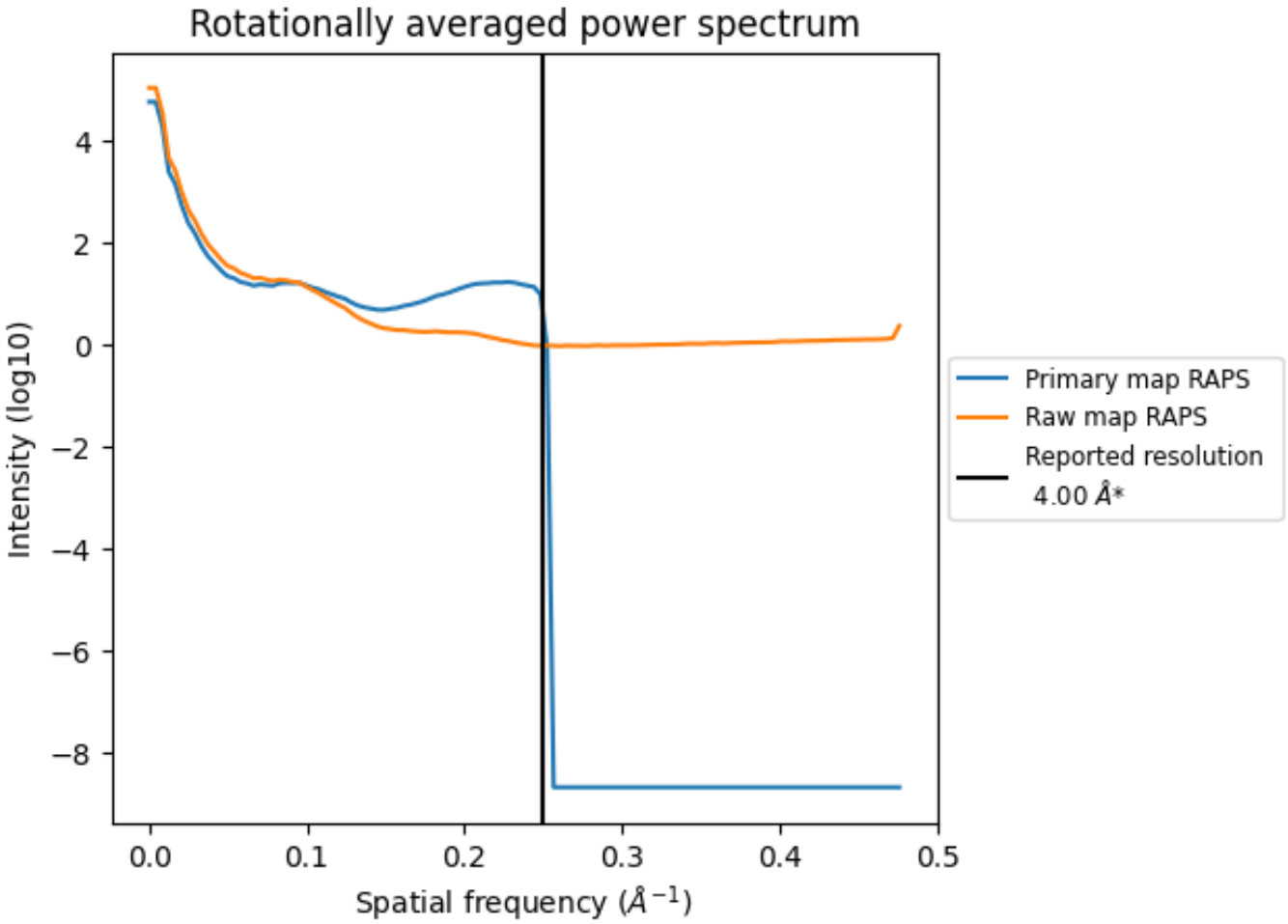
7.2 Volume estimate (i)



The volume at the recommended contour level is 62 nm^3; this corresponds to an approximate mass of 56 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)

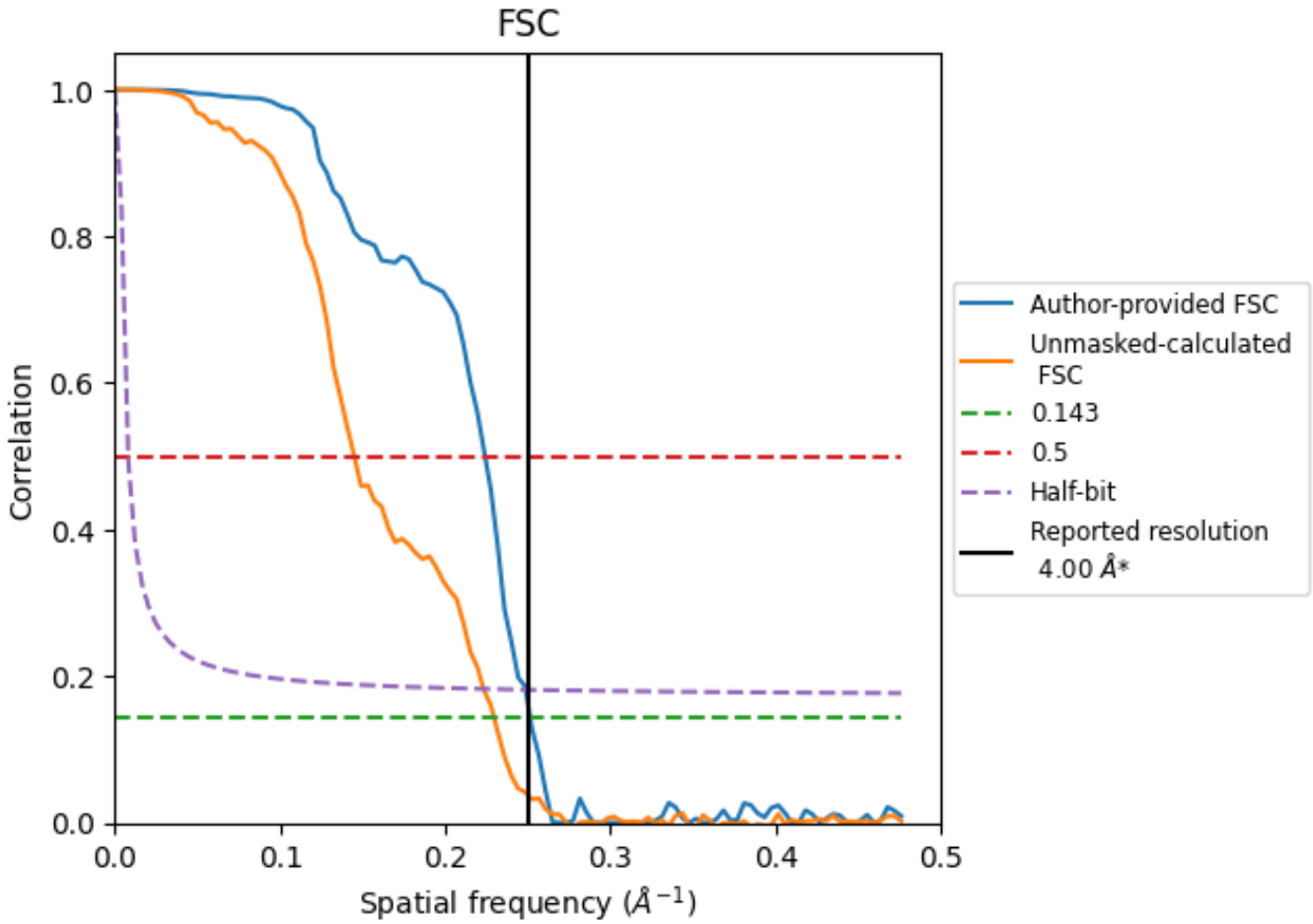


*Reported resolution corresponds to spatial frequency of 0.250 Å^{-1}

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 0.250 $Å^{-1}$

8.2 Resolution estimates (i)

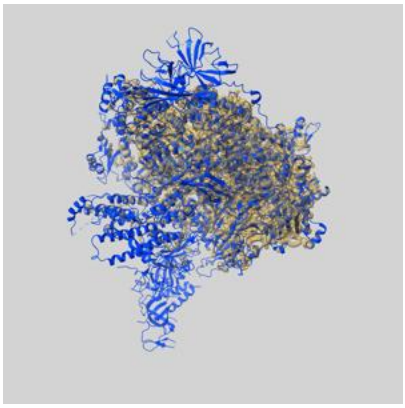
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.98	4.46	4.02
Unmasked-calculated*	4.35	6.89	4.48

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

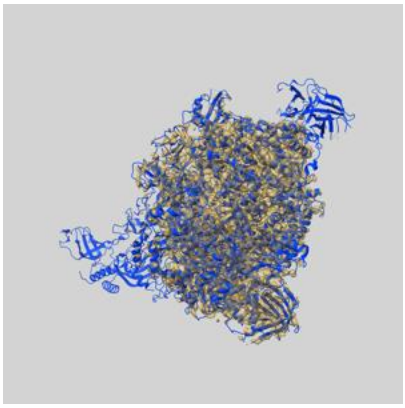
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4148 and PDB model 5M3M. Per-residue inclusion information can be found in section 3 on page 7.

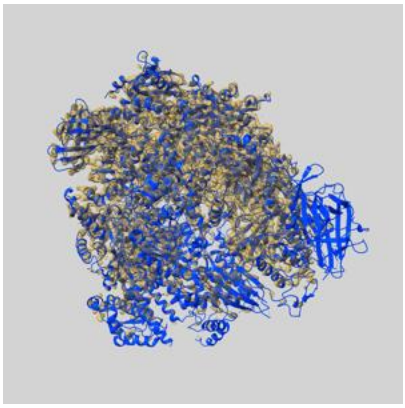
9.1 Map-model overlay



X



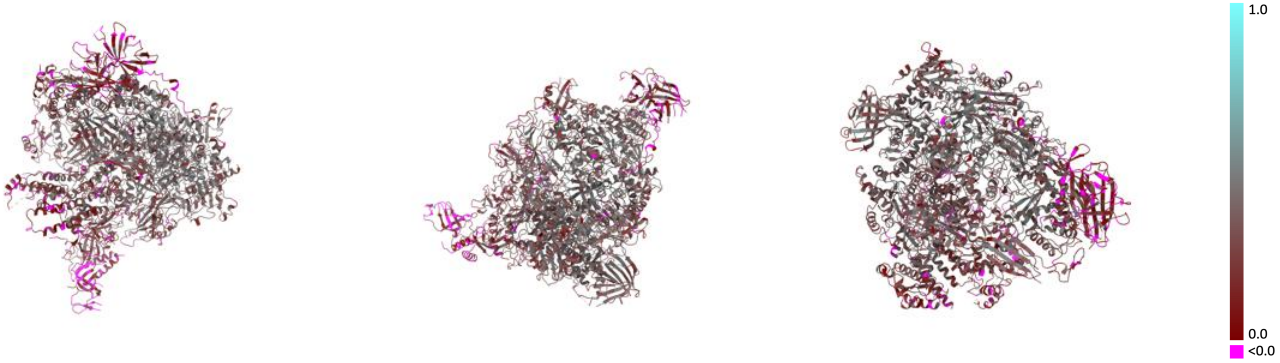
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

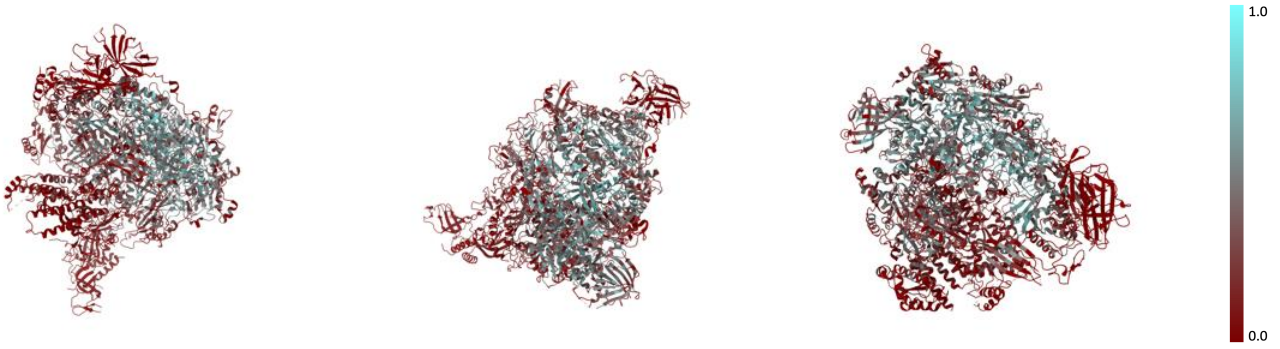
9.2 Q-score mapped to coordinate model



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.

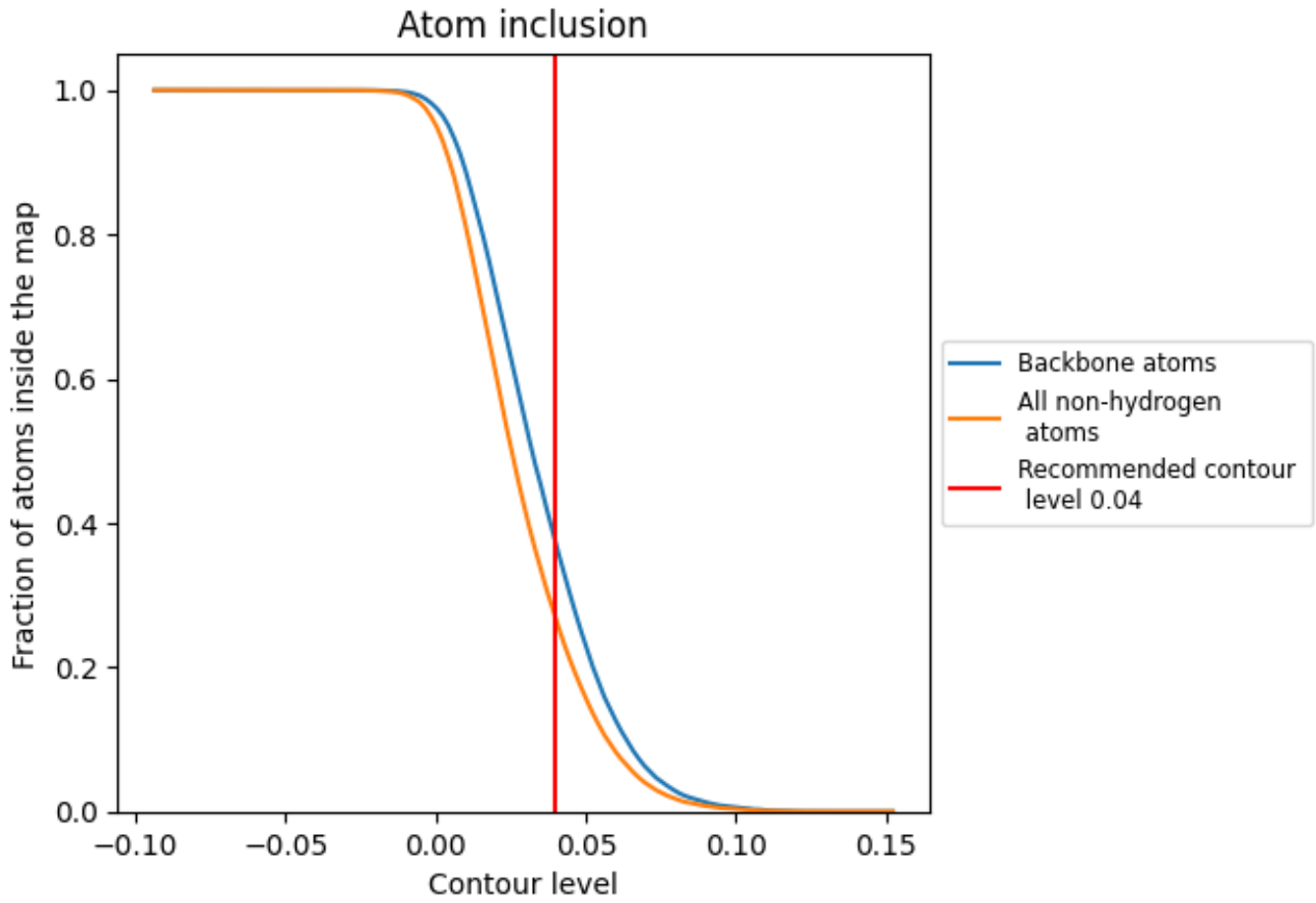
9.3 Atom inclusion mapped to coordinate model



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 (0.04).

9.4 Atom inclusion (i)



At the recommended contour level, 37% of all backbone atoms, 27% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2669	0.3090
A	0.2526	0.3180
B	0.3859	0.3650
C	0.3501	0.3600
D	0.0044	0.0810
E	0.1454	0.2700
F	0.1924	0.2950
G	0.0080	0.1250
H	0.3411	0.3680
I	0.0627	0.2470
J	0.4728	0.3920
K	0.3929	0.3660
L	0.3353	0.3610
M	0.0026	0.1250
N	0.0000	0.0710