wwPDB EM Validation Summary Report

May 6, 2024 – 06:30 AM JST

PDB ID	:	8JCH
EMDB ID	:	EMD-36162
Title	:	Cryo-EM structure of yeast Rat1-bound Pol II pre-termination transcription complex 1 (Pol II Rat1-PTTC1)
Authors	:	Zeng, Y.; Zhang, Y.
Deposited on	:	2023-05-11
Resolution	:	2.70 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:

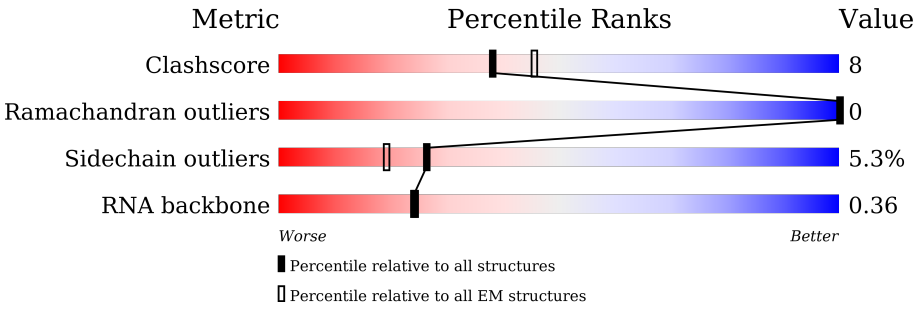
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1733	65% 16% • 18%
2	B	1259	76% 15% • 8%
3	C	318	73% 12% 15%
4	D	221	5% 53% 24% • 19%
5	E	215	81% 18% •
6	F	155	43% 10% 46%
7	G	171	• 64% 33% •

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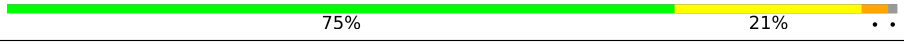
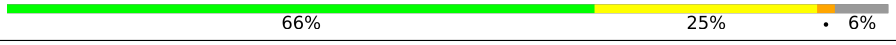
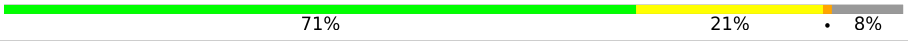
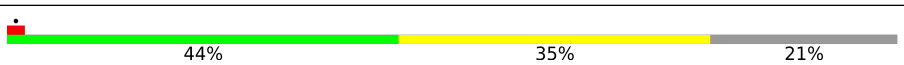
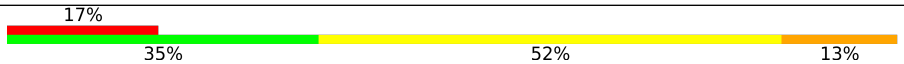
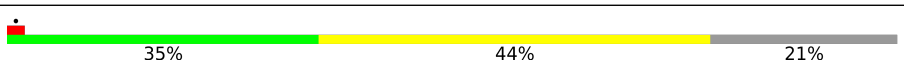
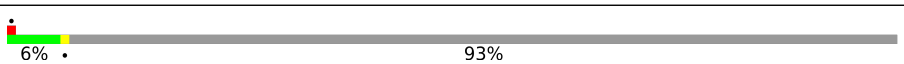
Mol	Chain	Length	Quality of chain
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	M	1019	
14	N	48	
15	O	387	
16	P	23	
17	T	48	
18	W	1063	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 42732 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 RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1419	11132	7019	1949	2106	58	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1157	9193	5819	1604	1714	56	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	GLU	-	expression tag	UNP P08518
B	1226	ASN	-	expression tag	UNP P08518
B	1227	LEU	-	expression tag	UNP P08518
B	1228	TYR	-	expression tag	UNP P08518
B	1229	PHE	-	expression tag	UNP P08518
B	1230	GLN	-	expression tag	UNP P08518
B	1231	GLY	-	expression tag	UNP P08518
B	1232	HIS	-	expression tag	UNP P08518
B	1233	HIS	-	expression tag	UNP P08518
B	1234	HIS	-	expression tag	UNP P08518
B	1235	HIS	-	expression tag	UNP P08518
B	1236	HIS	-	expression tag	UNP P08518
B	1237	HIS	-	expression tag	UNP P08518
B	1238	ASP	-	expression tag	UNP P08518
B	1239	TYR	-	expression tag	UNP P08518
B	1240	LYS	-	expression tag	UNP P08518
B	1241	ASP	-	expression tag	UNP P08518
B	1242	HIS	-	expression tag	UNP P08518
B	1243	ASP	-	expression tag	UNP P08518
B	1244	GLY	-	expression tag	UNP P08518
B	1245	ASP	-	expression tag	UNP P08518

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1246	TYR	-	expression tag	UNP P08518
B	1247	LYS	-	expression tag	UNP P08518
B	1248	ASP	-	expression tag	UNP P08518
B	1249	HIS	-	expression tag	UNP P08518
B	1250	ASP	-	expression tag	UNP P08518
B	1251	ILE	-	expression tag	UNP P08518
B	1252	ASP	-	expression tag	UNP P08518
B	1253	TYR	-	expression tag	UNP P08518
B	1254	LYS	-	expression tag	UNP P08518
B	1255	ASP	-	expression tag	UNP P08518
B	1256	ASP	-	expression tag	UNP P08518
B	1257	ASP	-	expression tag	UNP P08518
B	1258	ASP	-	expression tag	UNP P08518
B	1259	LYS	-	expression tag	UNP P08518

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2125	1336	353	422	14		

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	180	Total	C	N	O	S	0	0
			1455	899	262	292	2		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	215	Total	C	N	O	S	0	0
			1704	1080	305	310	9		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	83	Total	C	N	O	S	0	0
			670	428	113	126	3		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	144	Total	C	N	O	S	0	0
			1104	695	184	221	4		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	115	Total	C	N	O	S	0	0
			871	542	147	171	11		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	111	Total	C	N	O	S	0	0
			895	575	152	166	2		

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 13 is a protein called 5'-3' exoribonuclease 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	721	Total	C	N	O	S	0	0
			5834	3756	994	1059	25		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	MET	-	initiating methionine	UNP Q02792
M	-11	GLY	-	expression tag	UNP Q02792
M	-10	SER	-	expression tag	UNP Q02792
M	-9	SER	-	expression tag	UNP Q02792
M	-8	HIS	-	expression tag	UNP Q02792
M	-7	HIS	-	expression tag	UNP Q02792
M	-6	HIS	-	expression tag	UNP Q02792
M	-5	HIS	-	expression tag	UNP Q02792
M	-4	HIS	-	expression tag	UNP Q02792
M	-3	HIS	-	expression tag	UNP Q02792
M	-2	SER	-	expression tag	UNP Q02792
M	-1	GLN	-	expression tag	UNP Q02792
M	0	ASP	-	expression tag	UNP Q02792

- Molecule 14 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	38	Total	C	N	O	P	0	0
			787	375	141	233	38		

- Molecule 15 is a protein called Decapping nuclease RAI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	350	Total	C	N	O	S	0	0
			2880	1841	487	544	8		

- Molecule 16 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	23	Total	C	N	O	P	0	0
			493	220	90	160	23		

- Molecule 17 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	38	Total	C	N	O	P	0	0
			769	367	137	227	38		

- Molecule 18 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	W	71	Total	C	N	O	0	0
			565	349	111	105		

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

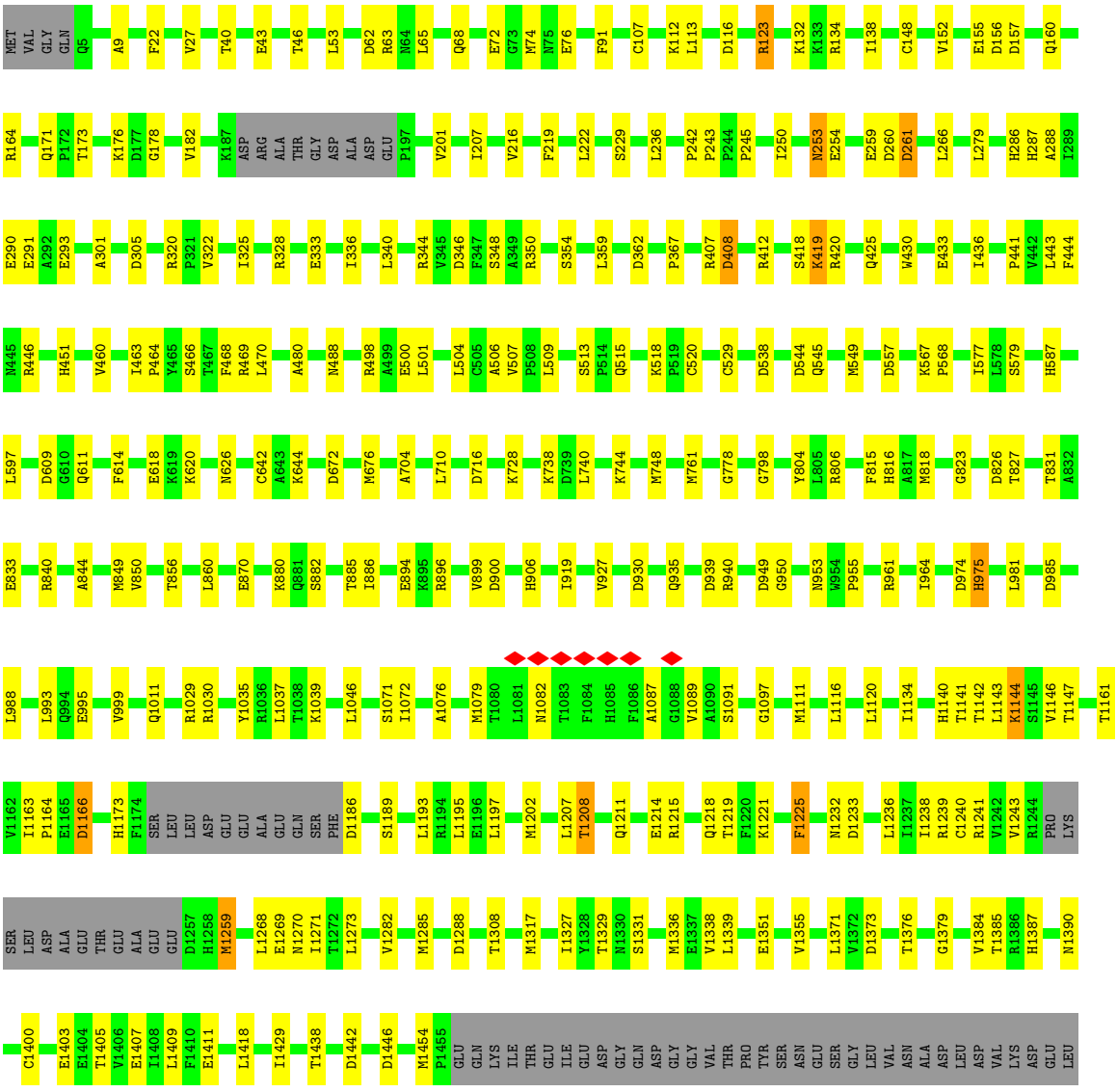
Mol	Chain	Residues	Atoms	AltConf
20	A	1	Total Mg 1 1	0
20	M	1	Total Mg 1 1	0
20	O	1	Total Mg 1 1	0

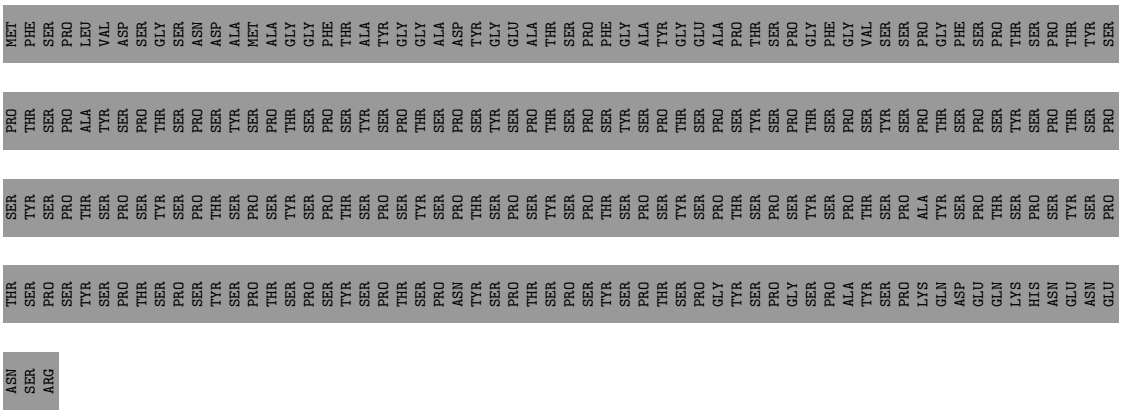
3 Residue-property plots (i)

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 RPB1

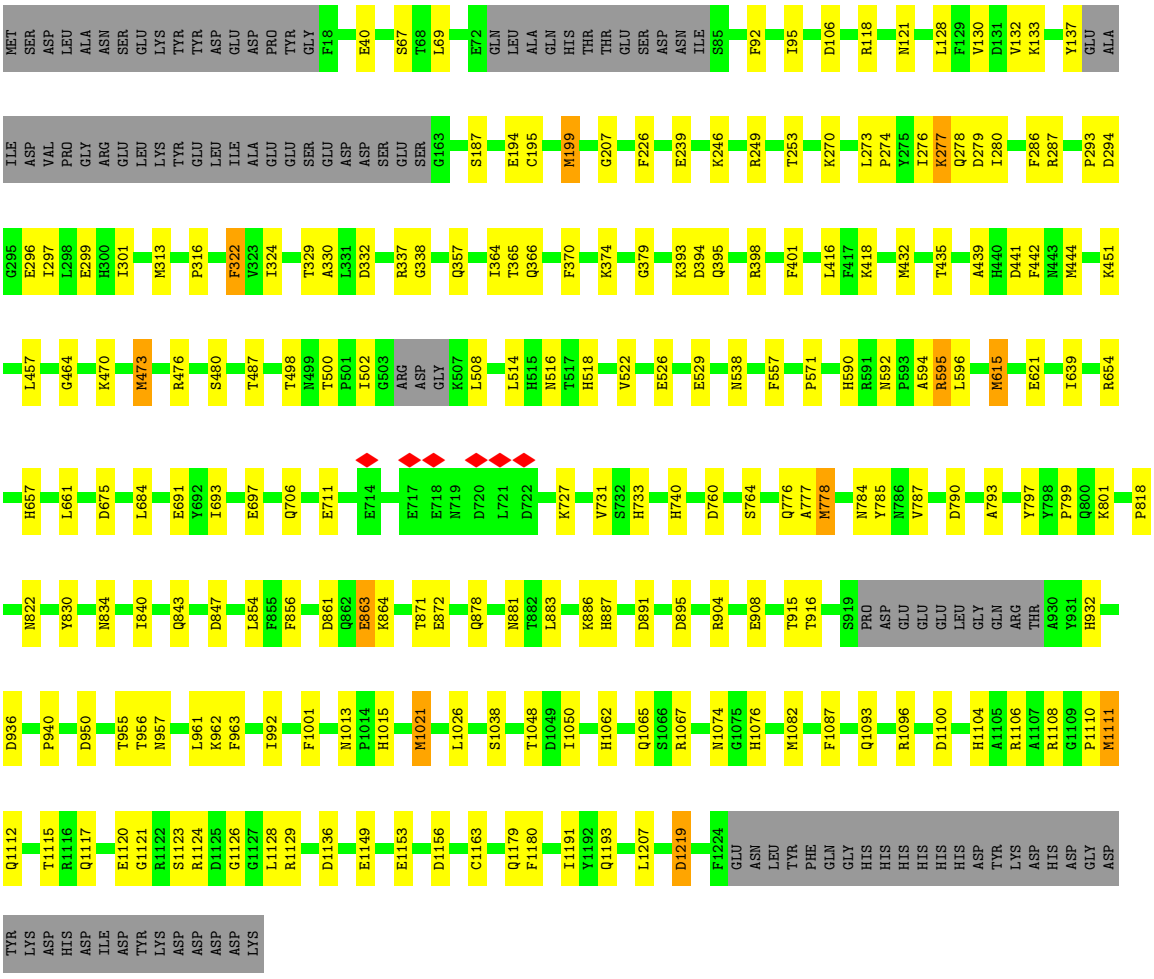
Chain A:





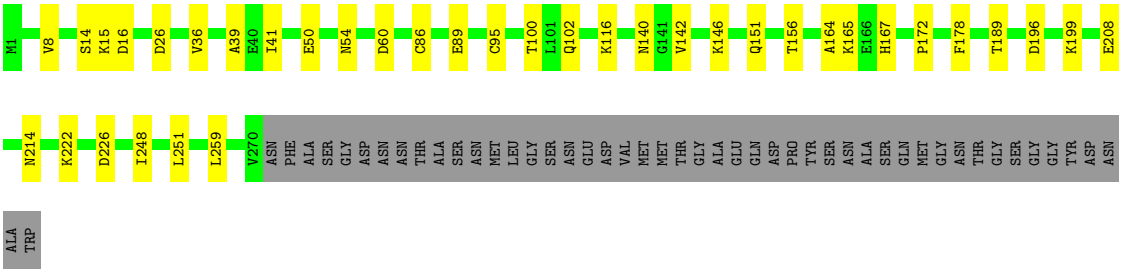
• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

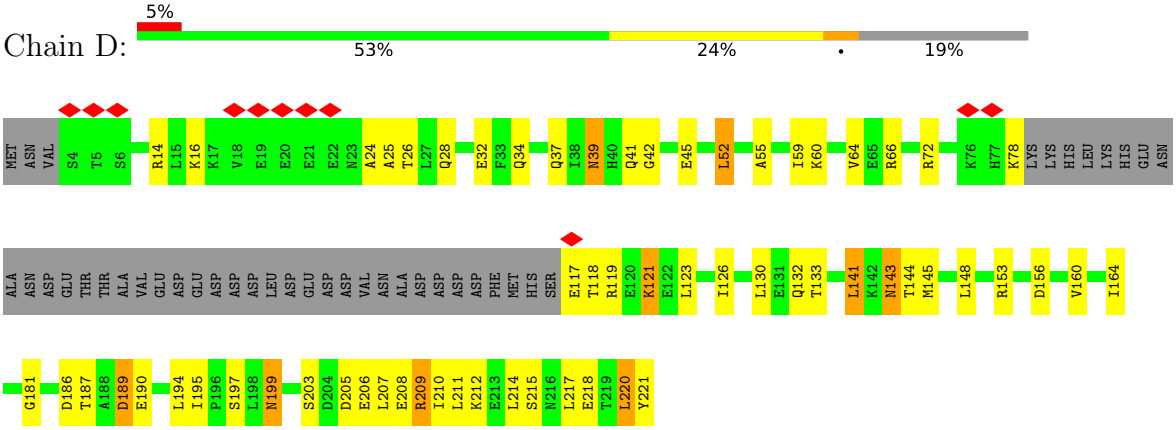


• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

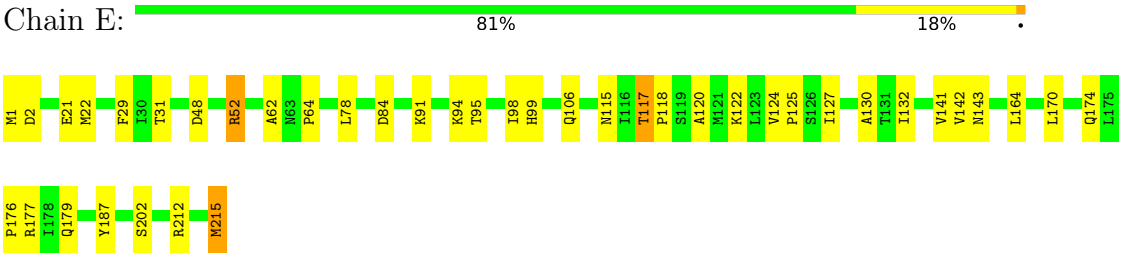
Chain C:



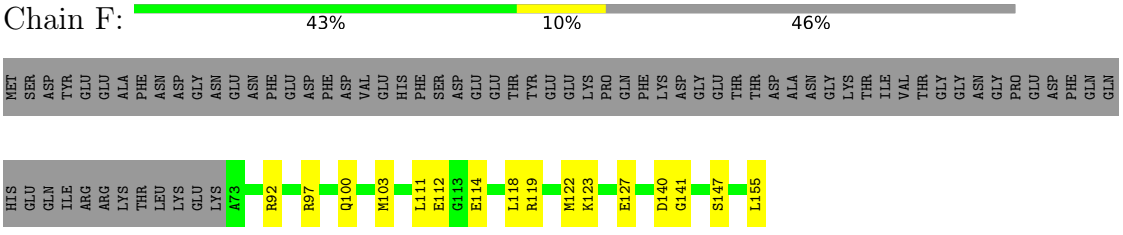
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



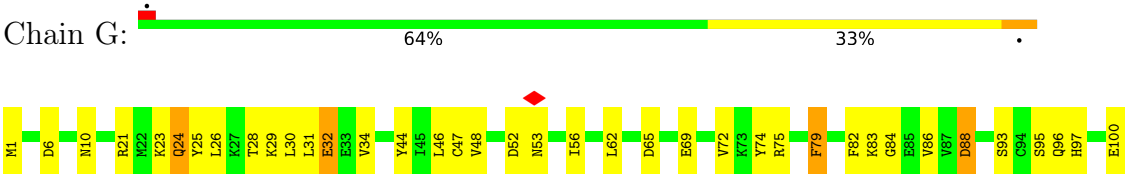
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

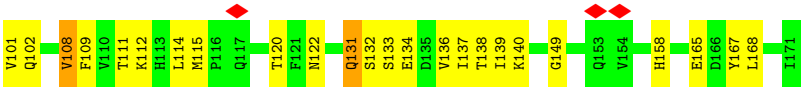


• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



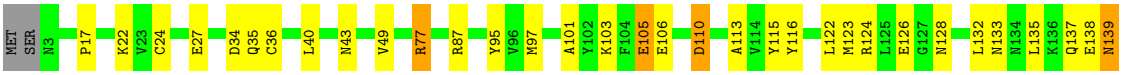
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7





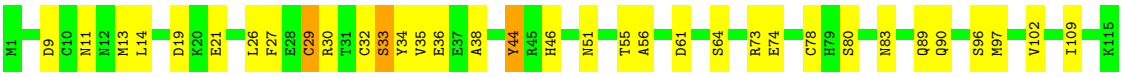
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



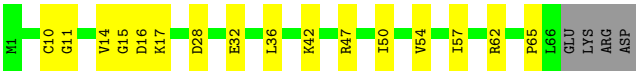
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



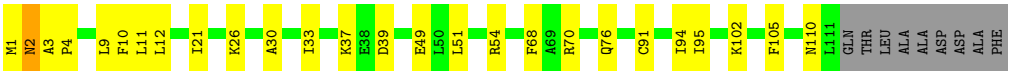
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



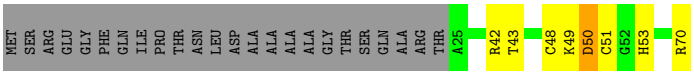
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



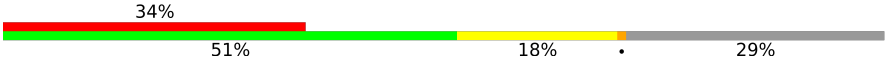
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

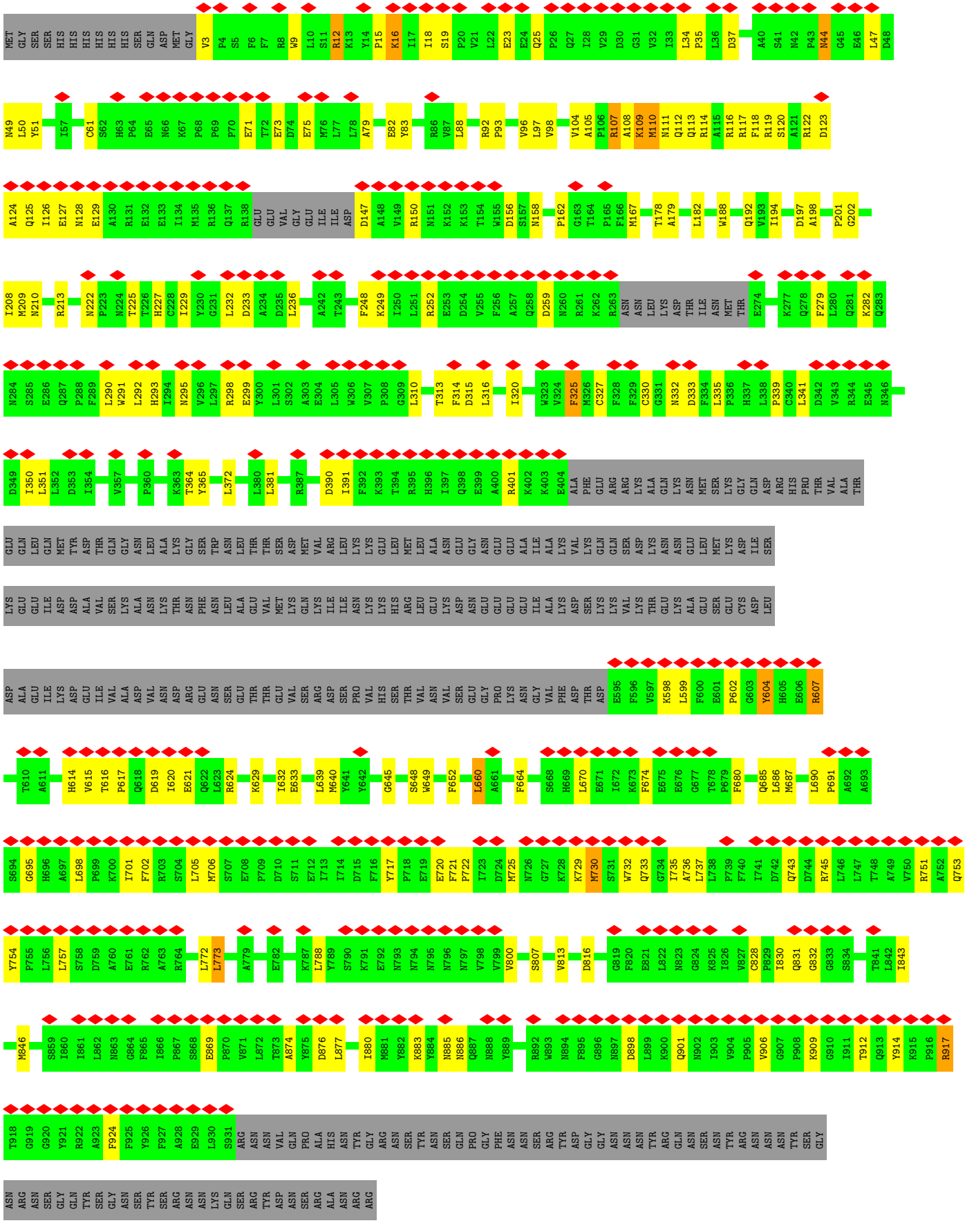
Chain L:



• Molecule 13: 5'-3' exoribonuclease 2

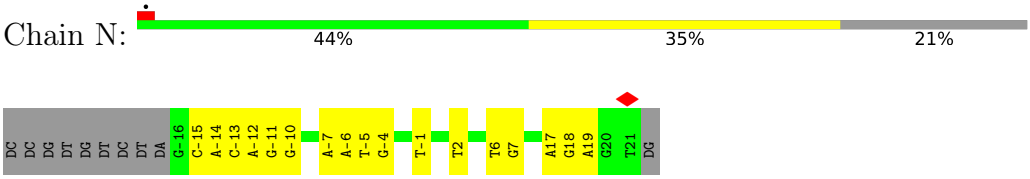
Chain M:




MET GLY SER SER HIS HIS HIS HIS HIS HIS SER GLN ASP MET GLY V3 P4 S5 F6 F7 R8 W9 L10 S11 R12 K13 Y14 P15 K16 I17 I18 S19 P20 V21 L22 E23 E24 Q25 P26 Q27 I28 V29 D30 G31 V32 I33 L34 P35 L36 D37 A40 S41 N42 P43 N44 G45 E46 L47 D48
N49 L50 Y51 T57 C61 S62 H63 P64 E65 N66 K67 P68 P69 P70 E71 T72 E73 D74 E75 W76 L77 L78 A79 E82 Y83 R86 V87 L88 R92 P93 V96 L97 V98 V104 A105 P106 R107 A108 K109 M110 N111 Q112 Q113 R114 A115 R116 R117 F118 R119 S120 A121 R122 D123
A124 Q125 I126 E127 N128 E129 A130 R131 E132 E133 I134 M135 R136 Q137 R138 GLU GLU VAL GLY GLU ILE ILE ASP D147 A148 V149 R150 N151 K152 K153 T154 W155 D156 S157 N158 P162 G163 T164 P165 F166 M167 T178 A179 L182 W188 Q192 V193 I194 D197 A198 P201 G202
I208 M209 N210 R213 N222 P223 N224 T225 T226 H227 C228 I229 Y230 G231 L232 D233 A234 D235 L236 A242 T243 F248 K249 I250 L251 R252 E253 D254 V255 F256 A257 Q258 D259 N260 R261 K262 R263 ASN ASN LEU LYS ASP THR ILE ASN MET THR E274 K277 Q278 F279 L280 Q281 K282 Q283
N284 S285 E286 Q287 P288 F289 L290 W291 L292 H293 I294 N295 V296 L297 R298 E299 Y300 L301 S302 A303 E304 L305 W306 V307 P308 G309 L310 T313 F314 D315 L316 I320 W323 V324 F325 M326 C327 F328 F329 C330 G331 N332 D333 F334 L335 P336 H337 L338 P339 C340 L341 D342 V343 R344 E345 N346
D349 I350 L351 L352 D353 I354 V357 P360 K363 T364 Y365 L372 L380 L381 R387 D390 I391 F392 K393 T394 R395 H396 I397 Q398 E399 A400 R401 K402 K403 E404 ALA PHE GLU ARG ARG LYS ALA GLN LYS ASN MET SER LYS GLY GLN ASP ARG HIS PRO THR VAL ALA THR
GLU GLN LEU GLN MET TYR ASP THR GLN GLY ASN LEU ALA LYS GLY SER TRP ASN LEU THR THR SER ASP MET VAL ARG LEU LYS LYS GLU LEU MET LEU ALA ASN GLU GLY ASN GLU GLU ALA ILE ALA LYS VAL LYS GLN GLN SER ASP LYS ASN ASN GLU LEU MET LYS ASP ILE SER
LYS GLU GLU ILE ASP ASP ALA VAL SER LYS ALA ASN LYS THR ASN PHE ASN LEU ALA GLU VAL MET LYS GLN LYS ILE ILE ASN LYS LYS HIS ARG LEU GLU LYS ASP ASN GLU GLU GLU GLU ILE ALA LYS ASP SER LYS LYS VAL LYS THR GLU LYS ALA GLU SER GLU CYS ASP LEU
ASP ALA GLU ILE LYS ASP GLU ILE VAL ALA ASP VAL ASN ASP ARG GLU ASN SER GLU THR THR GLU VAL SER ARG ASP SER PRO VAL HIS SER THR VAL ASN VAL SER GLU GLY PRO LYS ASN GLY VAL PHE ASP THR ASP E595 F596 V597 K598 L599 F600 E601 P602 G603 Y604 H605 E606 R607
T610 A611 H614 V615 T616 P617 Q618 D619 I620 E621 Q622 L623 R624 K629 I632 E633 L639 M640 Y641 Y642 G645 S648 W649 F652 L660 A661 F664 S668 H669 L670 E671 I672 K673 F674 E675 E676 G677 T678 P679 F680 Q685 L686 M687 L690 P691 A692 A693
S694 G695 H696 A697 L698 P699 K700 I701 F702 R703 S704 L705 M706 S707 E708 P709 D710 S711 E712 I713 I714 D715 F716 Y717 P718 E719 E720 F721 P722 I723 D724 M725 N726 G727 K728 H729 M730 S731 W732 Q733 G734 I735 A736 L737 L738 P739 F740 I741 D742 Q743 D744 R745 L746 L747 T748 A749 V750 R751 A752 Q753
Y754 P755 L756 L757 S758 D759 A760 E761 R762 A763 R764 L772 L773 A779 E782 K787 L788 Y789 S790 K791 E792 N793 N794 N795 N796 N797 V798 V799 V800 S807 V813 D816 G819 F820 E821 L822 N823 G824 K825 I826 V827 C828 P829 I830 Q831 G832 G833 S834 T841 L842 I843
M846 S859 I860 I861 L862 N863 G864 F865 I866 P867 S868 E869 P870 V871 L872 T873 A874 Y875 D876 L877 I880 M881 Y882 K883 Y884 N885 N886 Q887 N888 Y889 R892 W893 N894 P895 G896 N897 D898 L899 K900 Q901 N902 I903 V904 P905 V906 G907 P908 K909 G910 I911 T912 Q913 Y914 K915 P916 R917
T918 G919 G920 Y921 R922 A923 F924 F925 Y926 F927 A928 E929 L930 S931 ARG ASN ASN VAL GLN PRO ALA HIS ASN TYR GLY ARG ASN SER TYR ASN SER GLN PRO GLY PHE ASN ASN SER ARG TYR ASP GLY GLY ASN ASN ASN TYR ARG GLN ASN SER ASN TYR ARG ASN ASN ASN TYR SER GLY
ASN ARG ASN SER GLY GLN TYR SER GLY ASN SER TYR SER ARG ASN LYS GLN SER ARG TYR ASP ASN SER ARG ALA ASN ARG ARG

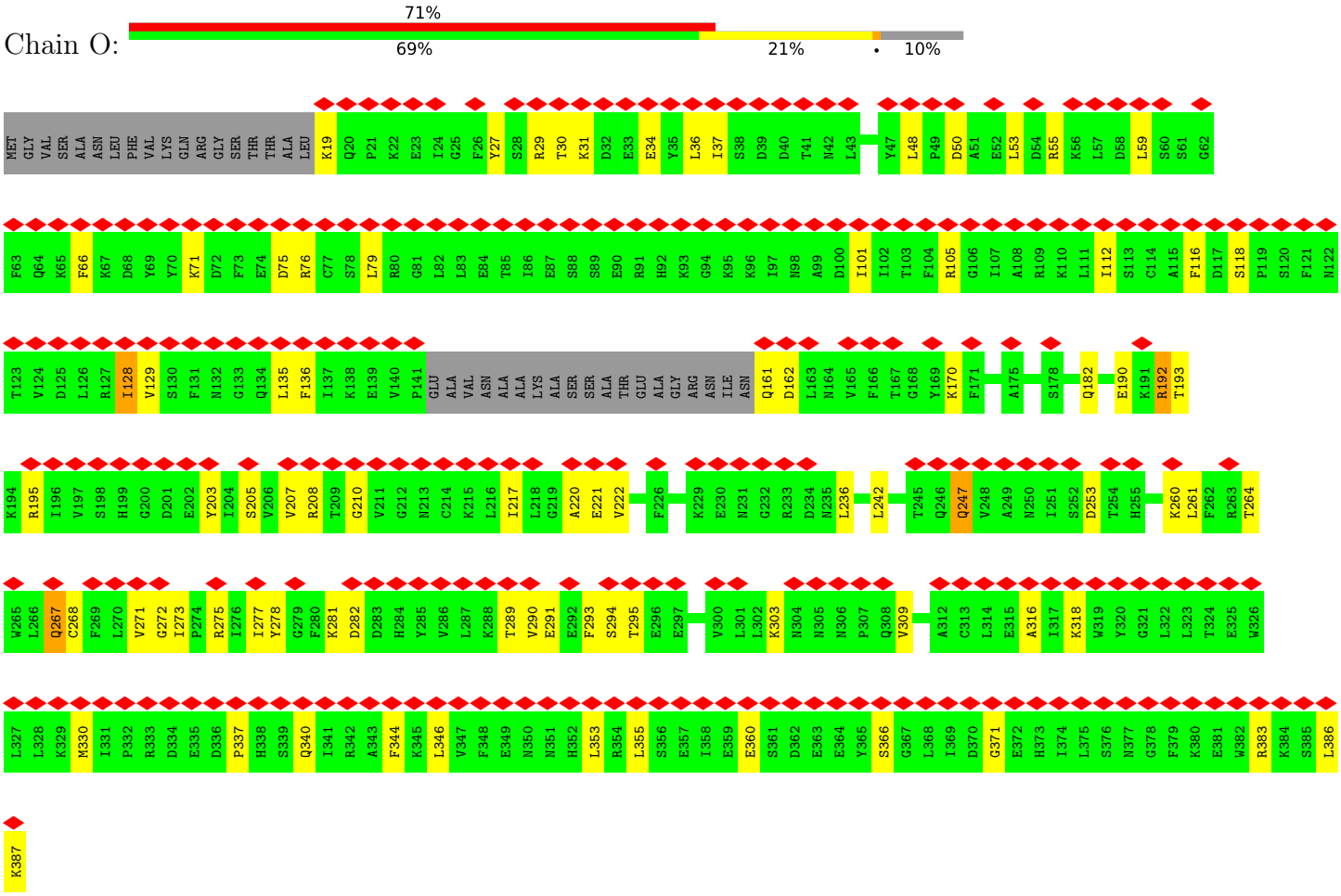
• Molecule 14: DNA (38-MER)

Chain N:



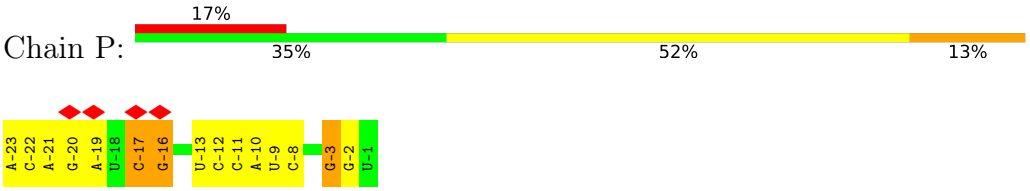
• Molecule 15: Decapping nuclease RAI1

Chain O:



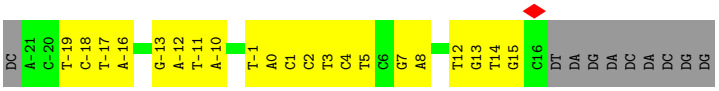
• Molecule 16: RNA

Chain P:



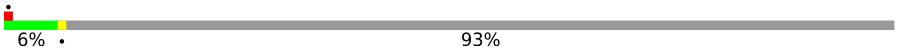
• Molecule 17: DNA (38-MER)

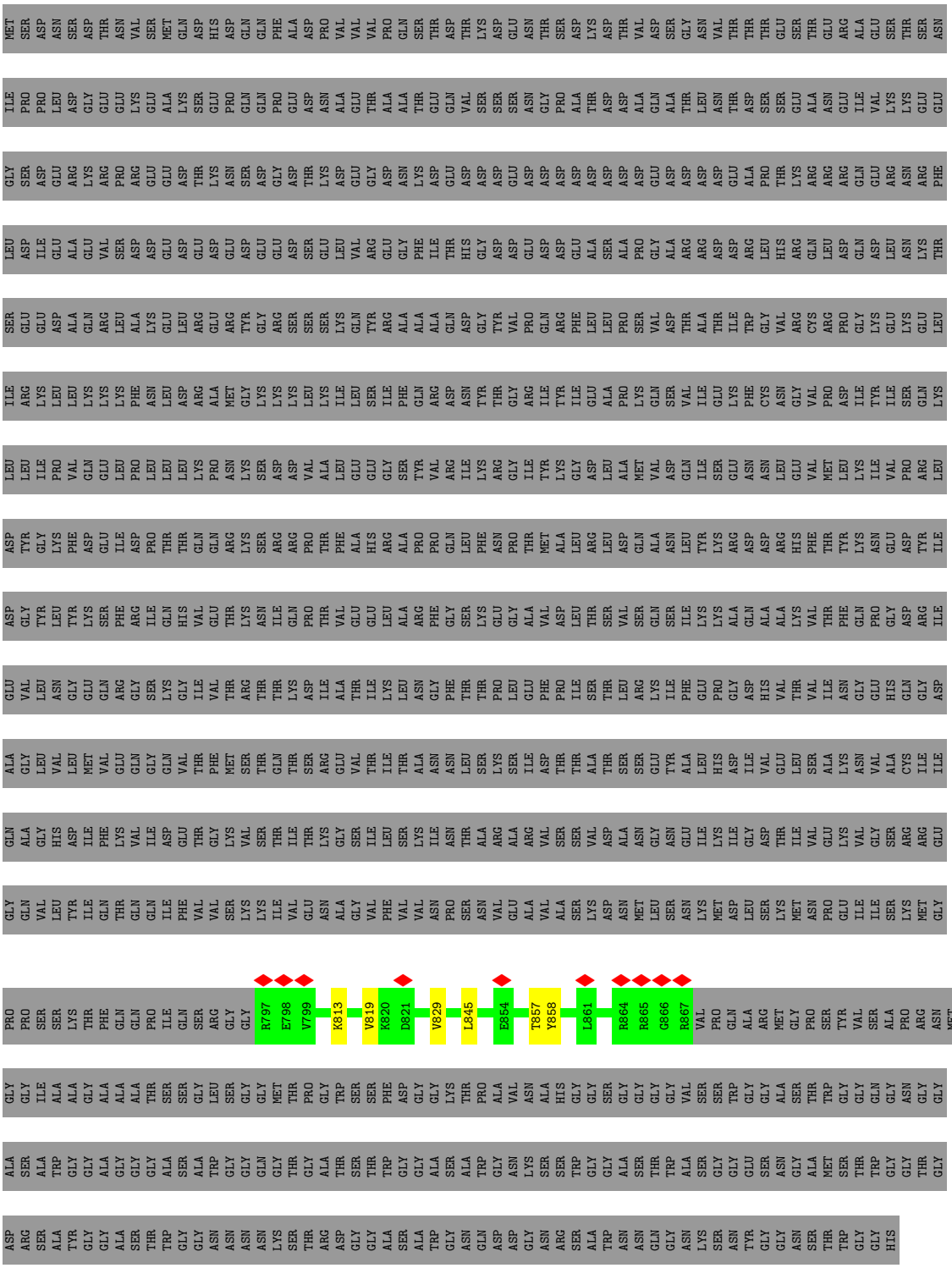
Chain T:



• Molecule 18: Transcription elongation factor SPT5

Chain W:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	416223	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.352	Depositor
Minimum map value	-0.895	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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, 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	A	0.25	0/11334	0.48	0/15335
2	B	0.25	0/9376	0.50	0/12647
3	C	0.24	0/2163	0.44	0/2930
4	D	0.24	0/1466	0.53	0/1963
5	E	0.25	0/1739	0.51	0/2347
6	F	0.24	0/682	0.54	0/922
7	G	0.27	0/1368	0.54	0/1844
8	H	0.26	0/1123	0.54	0/1529
9	I	0.26	0/889	0.53	0/1207
10	J	0.27	0/549	0.57	0/738
11	K	0.25	0/913	0.44	0/1232
12	L	0.27	0/366	0.64	0/485
13	M	0.27	0/5991	0.49	0/8129
14	N	0.50	0/882	0.92	0/1362
15	O	0.24	0/2941	0.47	0/3963
16	P	0.29	0/551	0.93	0/857
17	T	0.54	0/860	0.90	0/1322
18	W	0.22	0/571	0.52	0/762
All	All	0.27	0/43764	0.53	0/59574

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11132	0	11172	181	0
2	B	9193	0	9182	117	0
3	C	2125	0	2090	25	0
4	D	1455	0	1477	41	0
5	E	1704	0	1687	20	0
6	F	670	0	688	10	0
7	G	1340	0	1357	32	0
8	H	1104	0	1047	19	0
9	I	871	0	777	18	0
10	J	540	0	553	11	0
11	K	895	0	903	18	0
12	L	364	0	386	5	0
13	M	5834	0	5727	135	0
14	N	787	0	432	15	0
15	O	2880	0	2849	47	0
16	P	493	0	248	16	0
17	T	769	0	428	18	0
18	W	565	0	580	3	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
20	A	1	0	0	0	0
20	M	1	0	0	0	0
20	O	1	0	0	0	0
All	All	42732	0	41583	678	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 8.

The worst 5 of 678 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)
13:M:107:ARG:HG2	13:M:652:PHE:HB3	1.58	0.86
13:M:110:MET:HE2	13:M:685:GLN:HG3	1.63	0.81
13:M:615:VAL:HG23	13:M:620:ILE:HG22	1.66	0.77
8:H:35:GLN:N	8:H:35:GLN:OE1	2.20	0.75

Continued on next page...

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:113:GLN:HG3	13:M:116:ARG:HH22	1.53	0.73

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	1411/1733 (81%)	1356 (96%)	55 (4%)	0	100	100
2	B	1147/1259 (91%)	1106 (96%)	41 (4%)	0	100	100
3	C	268/318 (84%)	261 (97%)	7 (3%)	0	100	100
4	D	176/221 (80%)	168 (96%)	8 (4%)	0	100	100
5	E	213/215 (99%)	206 (97%)	7 (3%)	0	100	100
6	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
7	G	169/171 (99%)	154 (91%)	15 (9%)	0	100	100
8	H	142/146 (97%)	132 (93%)	10 (7%)	0	100	100
9	I	113/122 (93%)	103 (91%)	10 (9%)	0	100	100
10	J	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
11	K	109/120 (91%)	108 (99%)	1 (1%)	0	100	100
12	L	44/70 (63%)	41 (93%)	3 (7%)	0	100	100
13	M	713/1019 (70%)	677 (95%)	36 (5%)	0	100	100
15	O	346/387 (89%)	333 (96%)	13 (4%)	0	100	100
18	W	69/1063 (6%)	64 (93%)	5 (7%)	0	100	100
All	All	5065/7069 (72%)	4847 (96%)	218 (4%)	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	A	1231/1520 (81%)	1185 (96%)	46 (4%)	34 63
2	B	998/1094 (91%)	945 (95%)	53 (5%)	22 48
3	C	238/274 (87%)	233 (98%)	5 (2%)	53 80
4	D	162/200 (81%)	146 (90%)	16 (10%)	8 18
5	E	181/197 (92%)	170 (94%)	11 (6%)	18 41
6	F	73/137 (53%)	69 (94%)	4 (6%)	21 46
7	G	152/152 (100%)	131 (86%)	21 (14%)	3 8
8	H	116/128 (91%)	105 (90%)	11 (10%)	8 20
9	I	95/116 (82%)	87 (92%)	8 (8%)	11 25
10	J	61/65 (94%)	59 (97%)	2 (3%)	38 67
11	K	96/102 (94%)	92 (96%)	4 (4%)	30 58
12	L	40/57 (70%)	37 (92%)	3 (8%)	13 31
13	M	632/909 (70%)	600 (95%)	32 (5%)	24 50
15	O	320/346 (92%)	302 (94%)	18 (6%)	21 45
18	W	59/876 (7%)	58 (98%)	1 (2%)	60 84
All	All	4454/6173 (72%)	4219 (95%)	235 (5%)	26 48

5 of 235 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	197	SER
15	O	79	LEU
7	G	79	PHE
15	O	71	LYS
13	M	325	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	137	ASN
15	O	267	GLN
9	I	87	GLN
15	O	42	ASN
13	M	685	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
16	P	22/23 (95%)	7 (31%)	0

5 of 7 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
16	P	-19	A
16	P	-17	C
16	P	-16	G
16	P	-13	U
16	P	-12	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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)

There are no chain breaks in this entry.

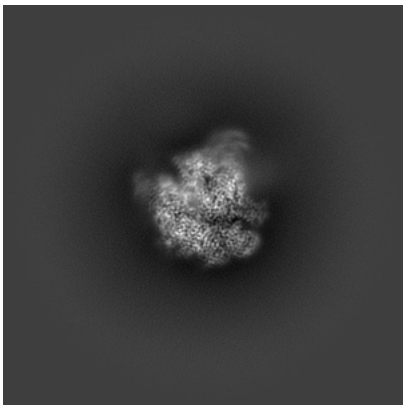
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36162. These allow visual inspection of the internal detail of the map and identification of artifacts.

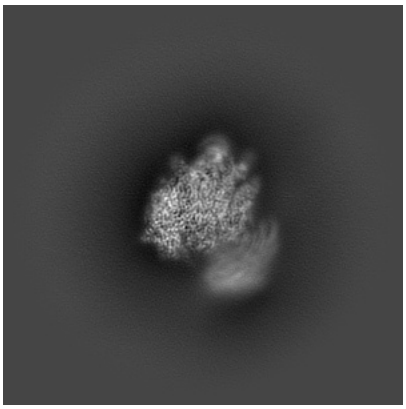
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

6.1.1 Primary map



X



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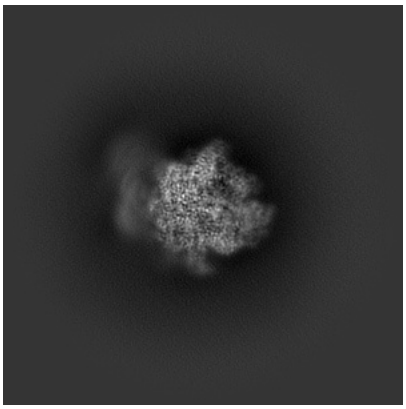
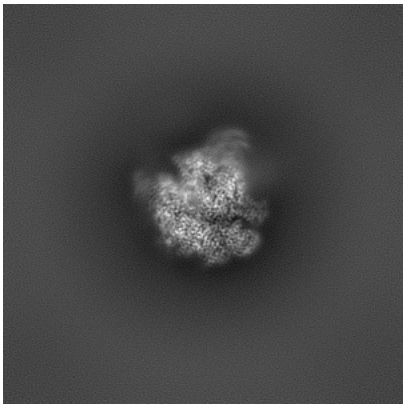


Z

6.1.2 Raw map



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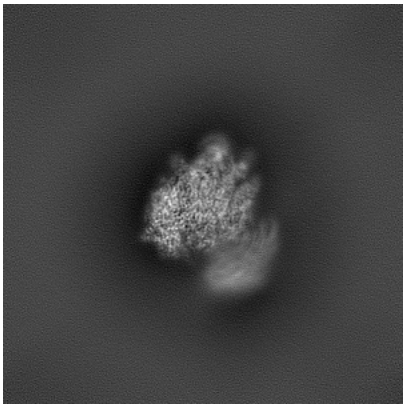
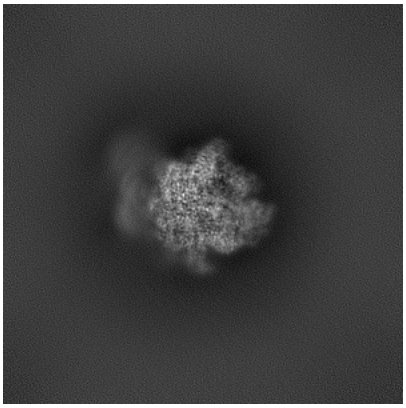


Y

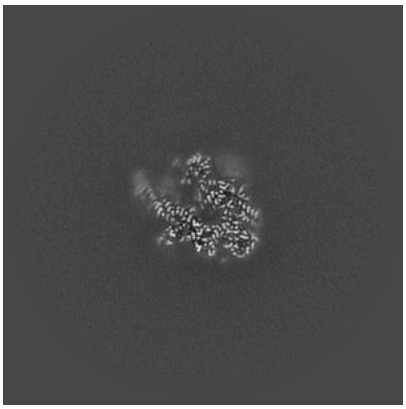


Z

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

6.2 Central slices (i)

6.2.1 Primary map



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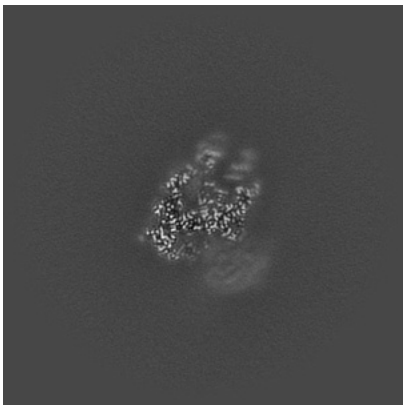
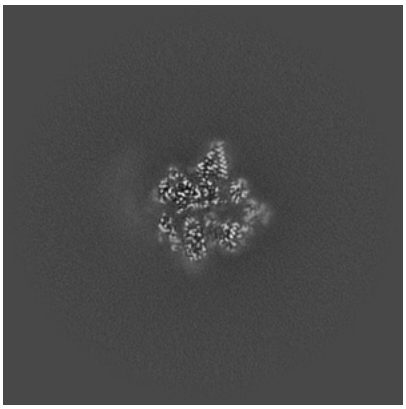
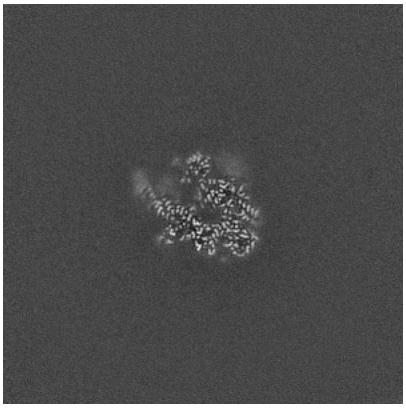


Y Index: 200

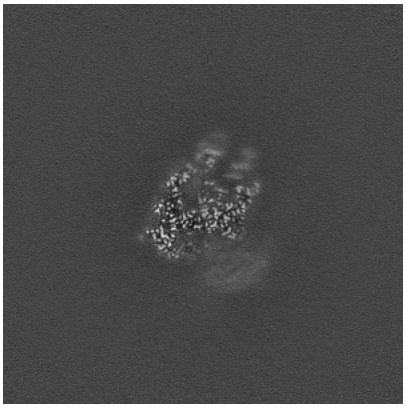


Z Index: 200

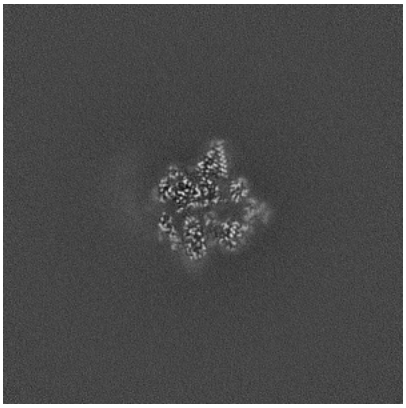
6.2.2 Raw map



X Index: 200



Y Index: 200

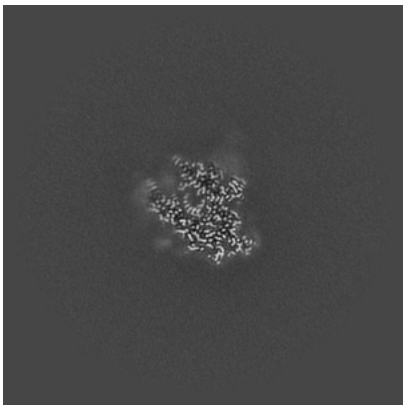


Z Index: 200

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

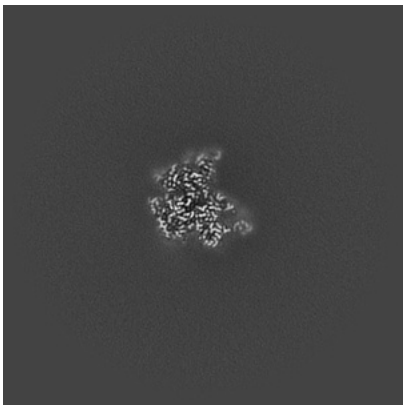
6.3 Largest variance slices (i)

6.3.1 Primary map



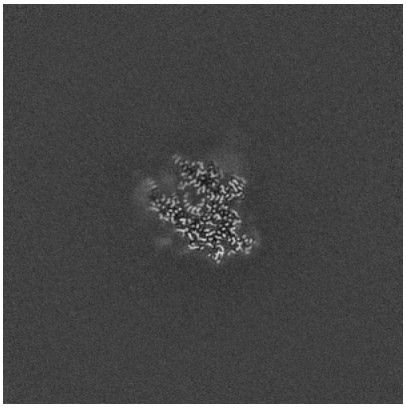
X Index: 190

Y Index: 195



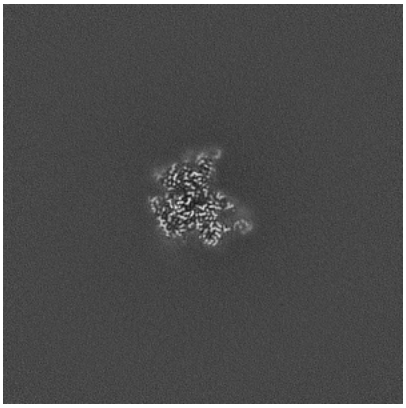
Z Index: 171

6.3.2 Raw map



X Index: 190

Y Index: 195

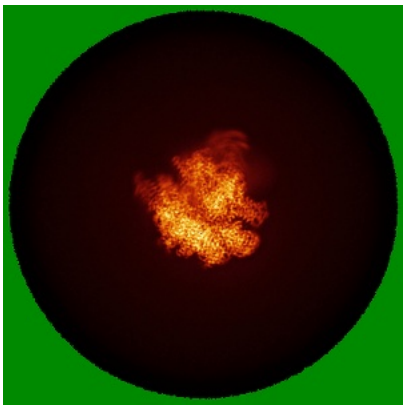


Z Index: 171

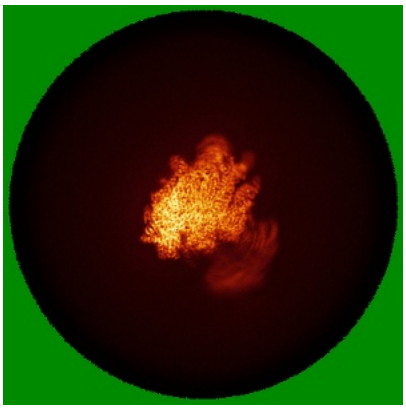
The images above show the largest variance slices of the map in three orthogonal directions.

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

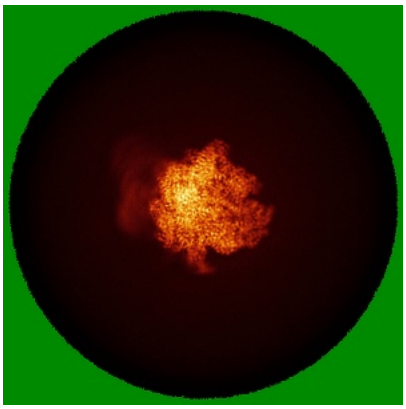
6.4.1 Primary map



X

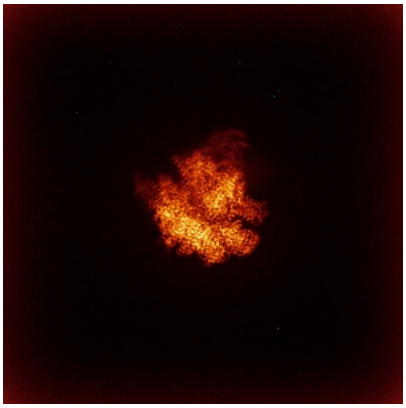


Y

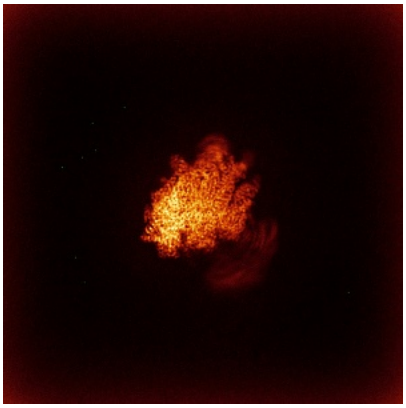


Z

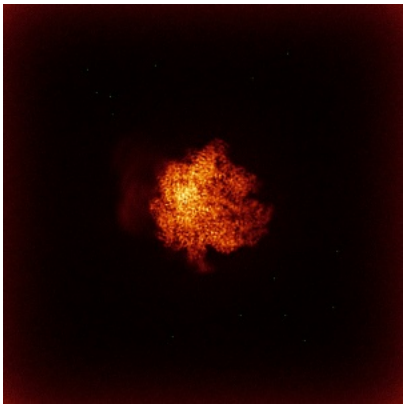
6.4.2 Raw map



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 0.15. 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.

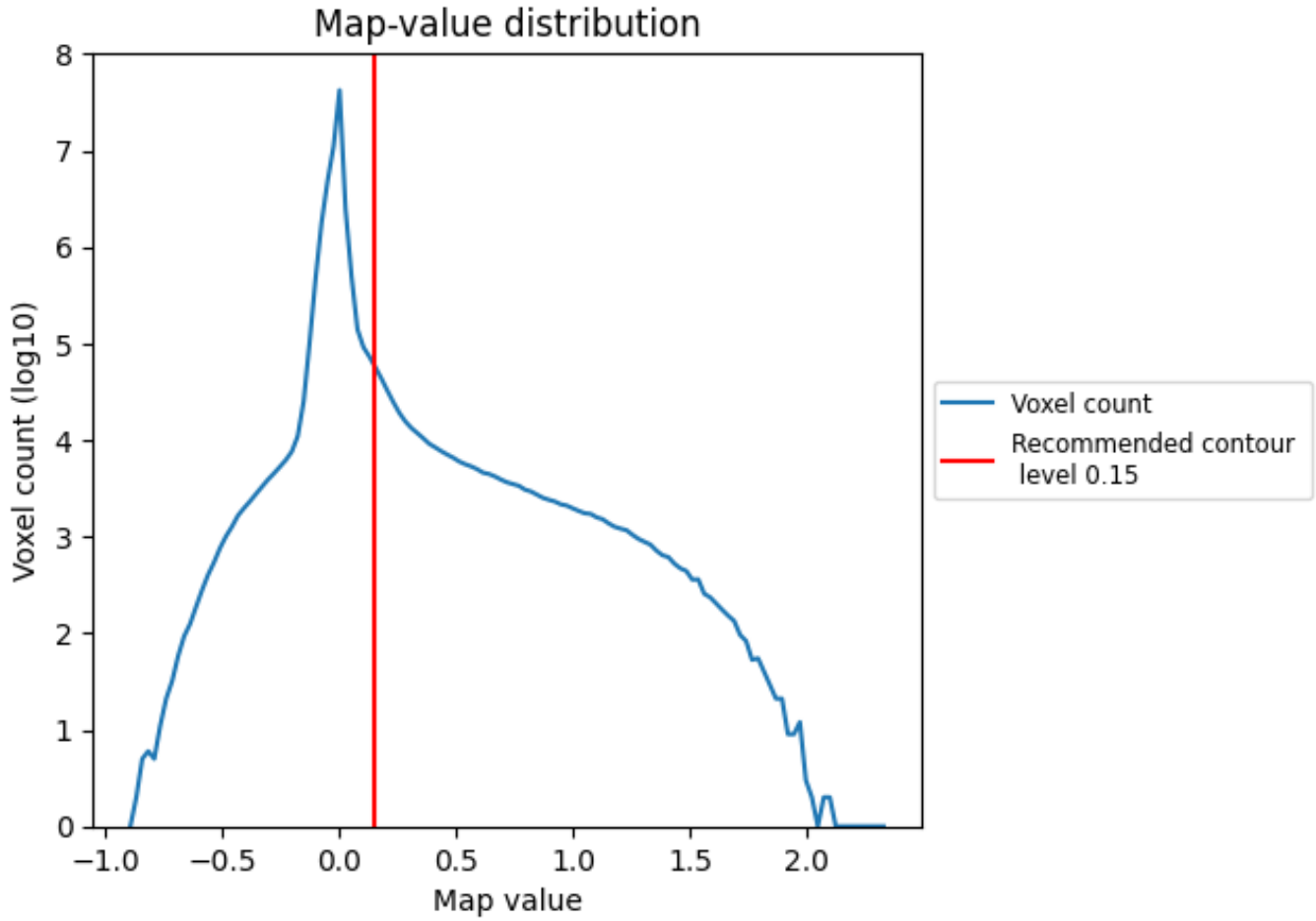
6.6 Mask visualisation (i)

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

7 Map analysis

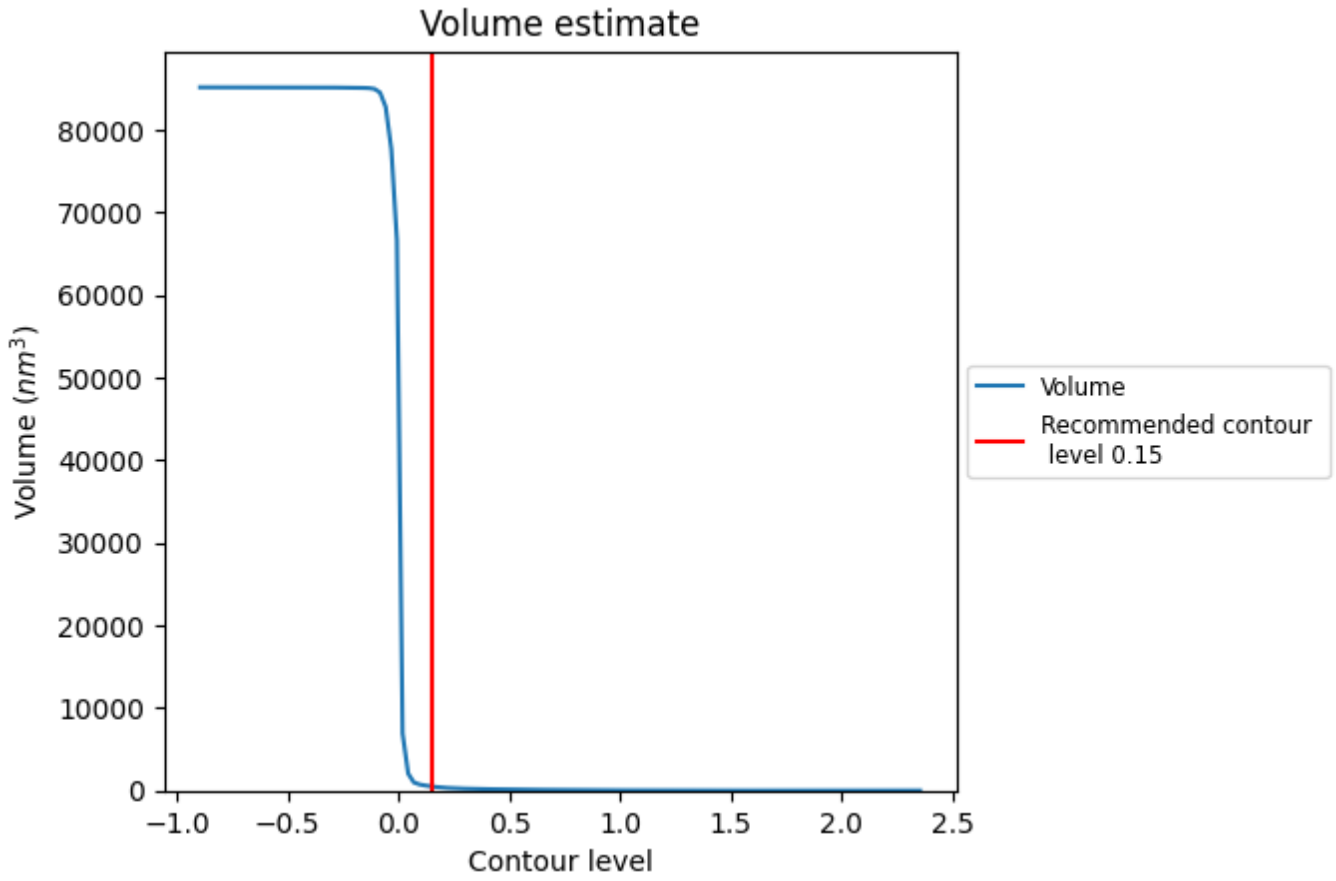
This section contains the results of statistical analysis of the map.

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.

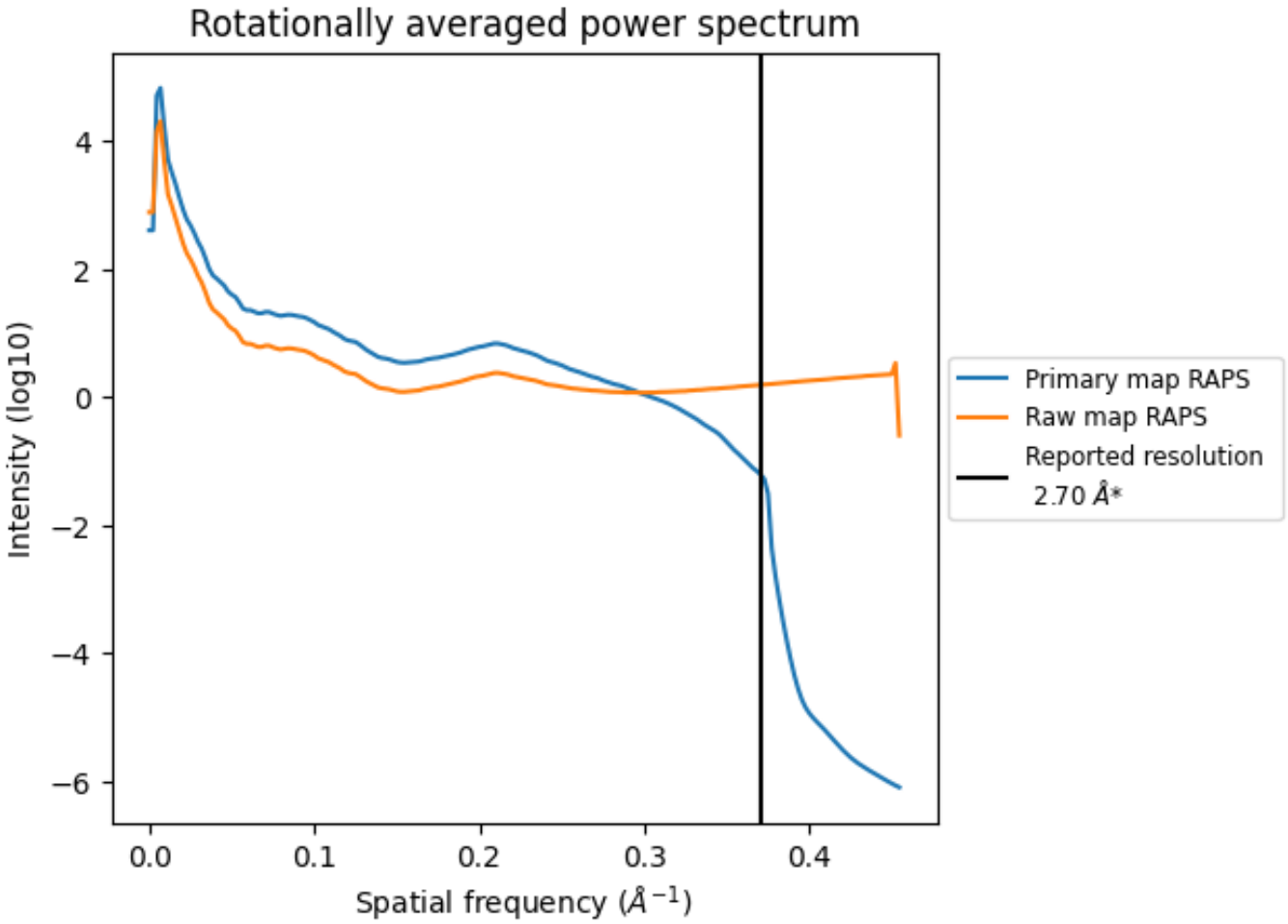
7.2 Volume estimate (i)



The volume at the recommended contour level is 493 nm^3; this corresponds to an approximate mass of 445 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)

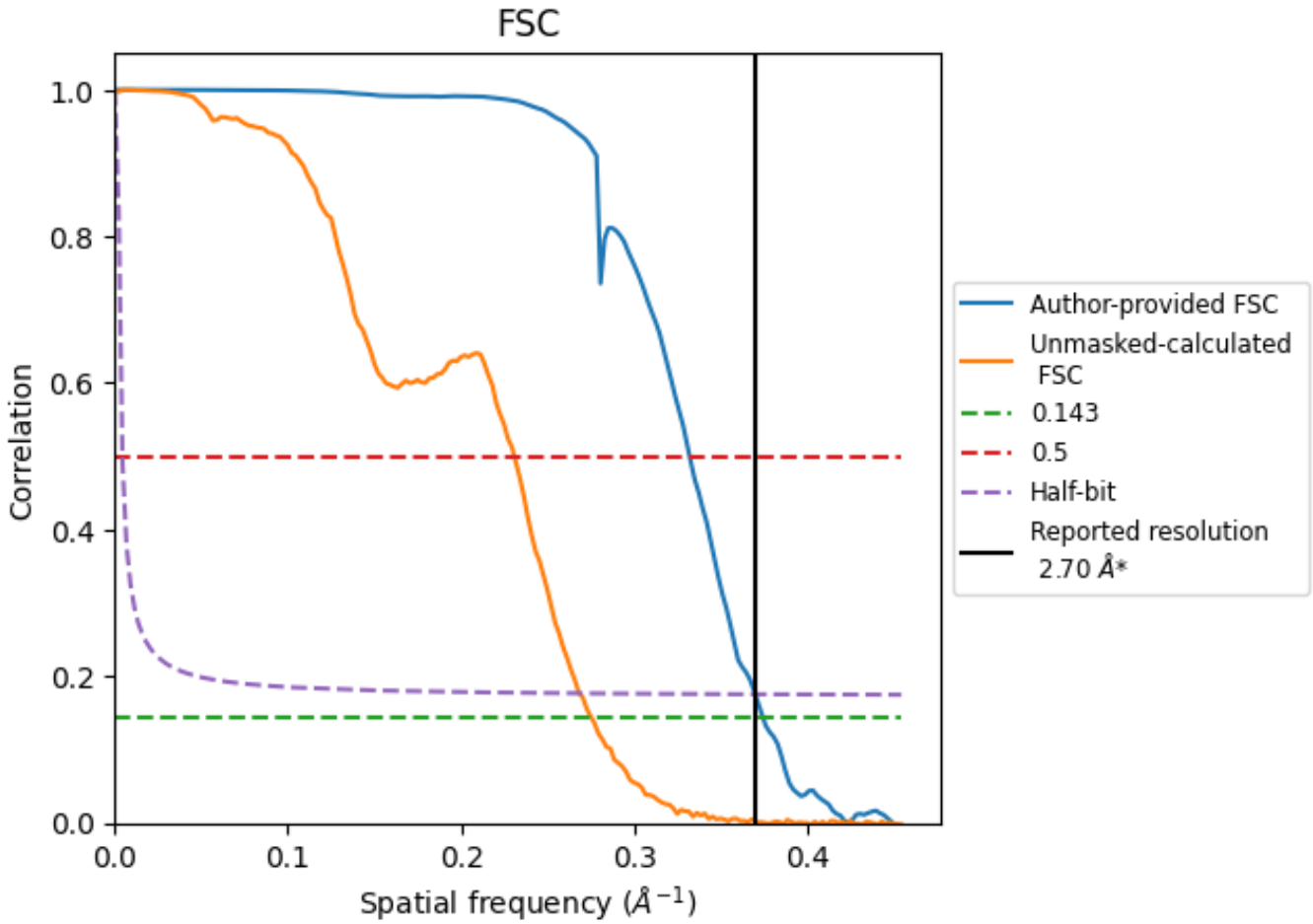


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

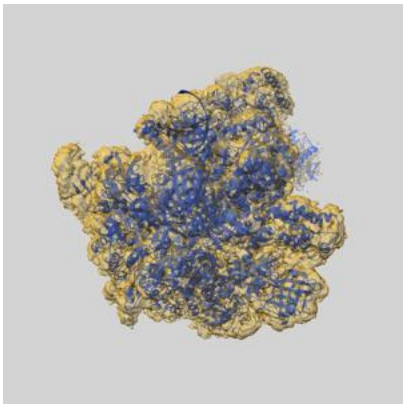
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.67	3.01	2.70
Unmasked-calculated*	3.63	4.33	3.73

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.63 differs from the reported value 2.7 by more than 10 %

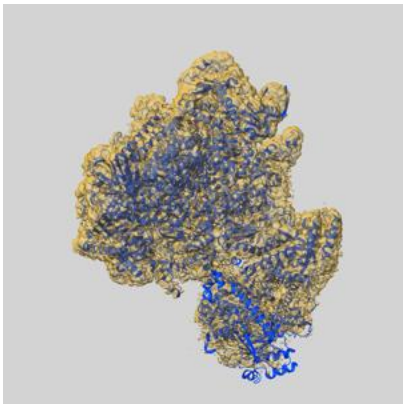
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36162 and PDB model 8JCH. Per-residue inclusion information can be found in section 3 on page 9.

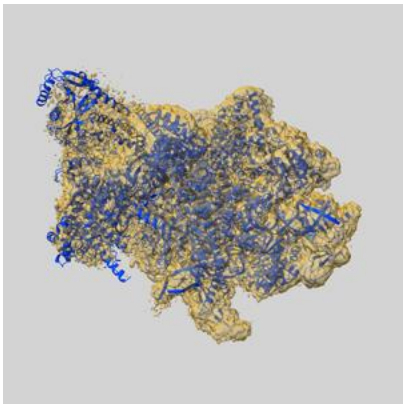
9.1 Map-model overlay



X



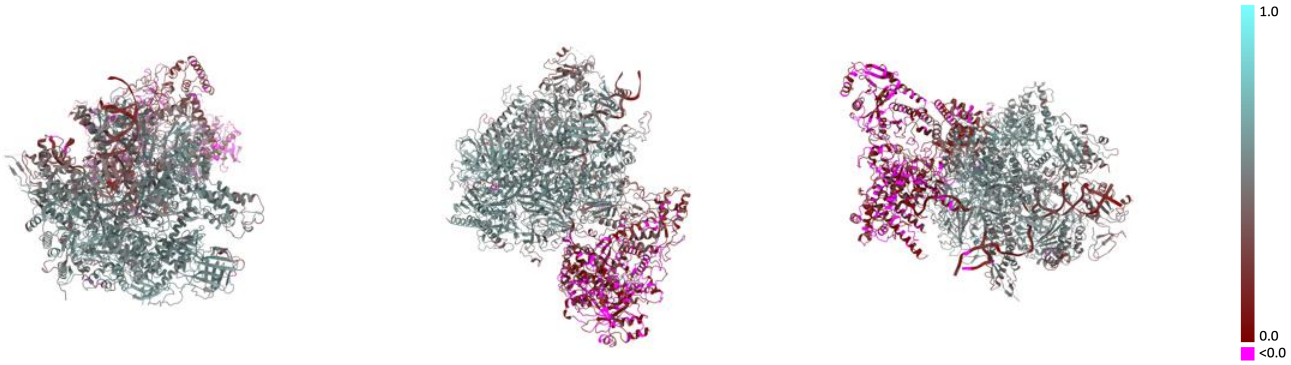
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

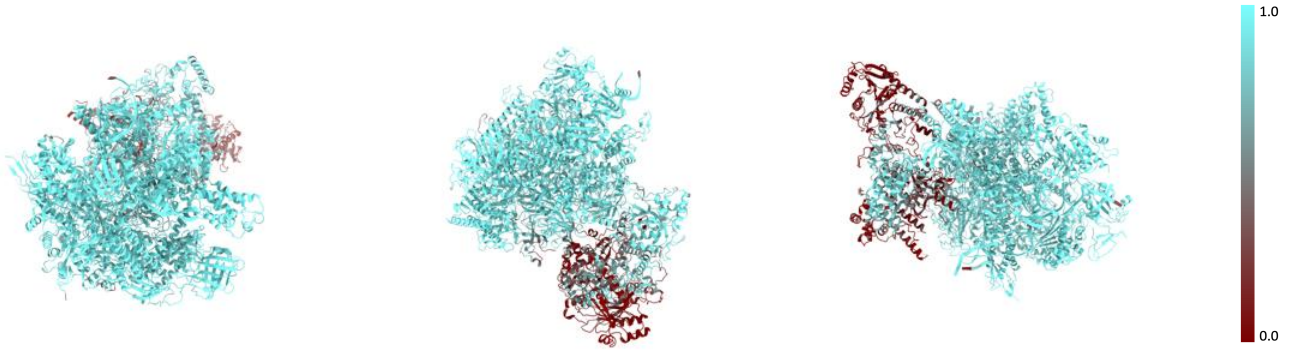
9.2 Q-score mapped to coordinate model (i)



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.

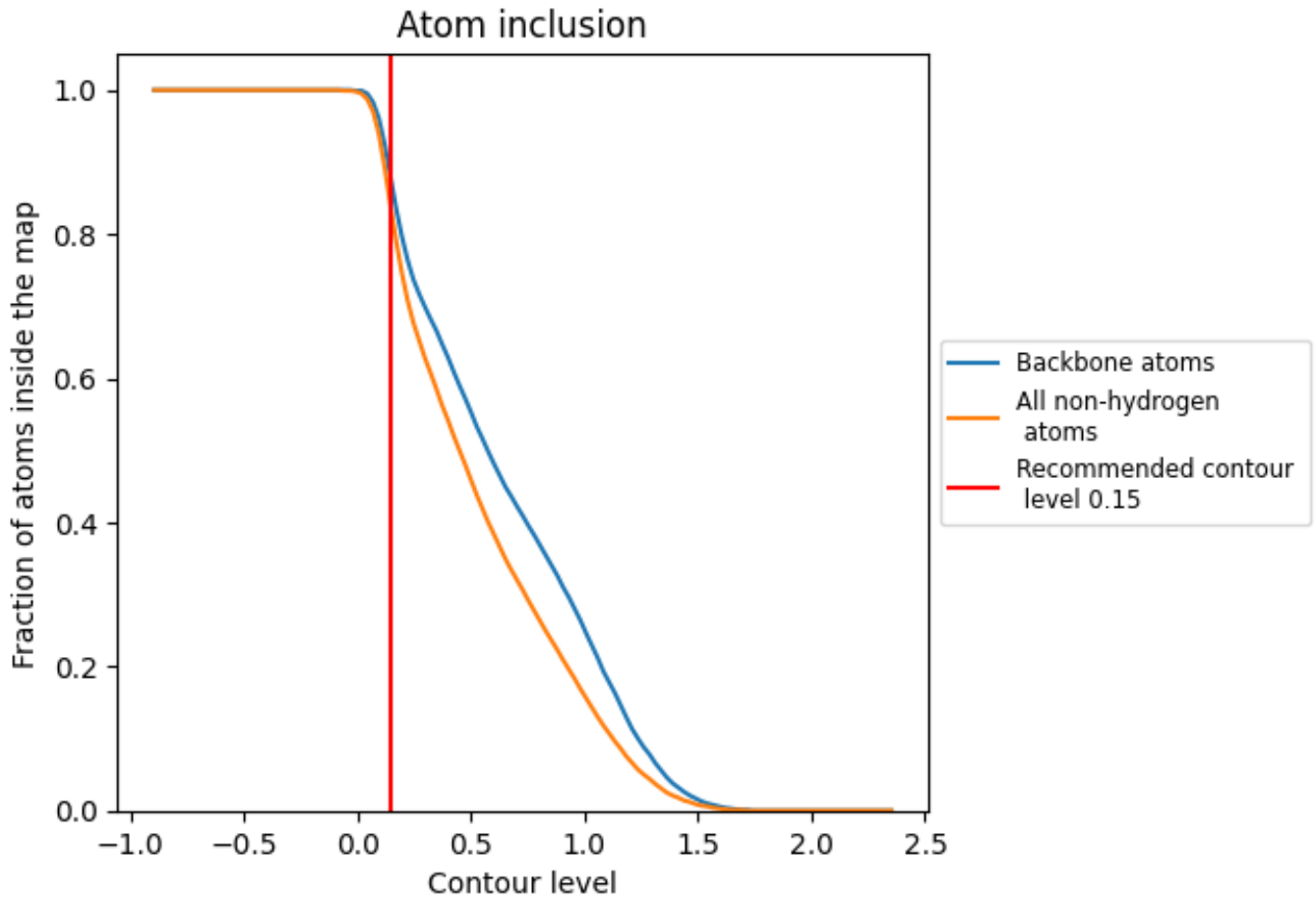
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 83% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8300	0.4030
A	0.9650	0.5180
B	0.9660	0.5310
C	0.9860	0.5660
D	0.7970	0.2000
E	0.9870	0.5190
F	0.9760	0.5550
G	0.8830	0.2850
H	0.9830	0.5160
I	0.9780	0.4450
J	0.9910	0.5730
K	0.9750	0.5730
L	0.9460	0.5030
M	0.4500	0.0850
N	0.9080	0.2150
O	0.2250	0.0740
P	0.6770	0.2550
T	0.8970	0.3010
W	0.6400	0.4680