wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 06:50 pm GMT

PDB ID	:	7AST
EMDB ID	:	EMD-11904
Title	:	Apo Human RNA Polymerase III
Authors	:	Ramsay, E.P.; Abascal-Palacios, G.; Daiss, J.L.; King, H.; Gouge, J.; Pilsl, M.; Beuron, F.; Morris, E.; Gunkel, P.; Engel, C.; Vannini, A.
Deposited on	:	2020-10-28
Resolution	:	4.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

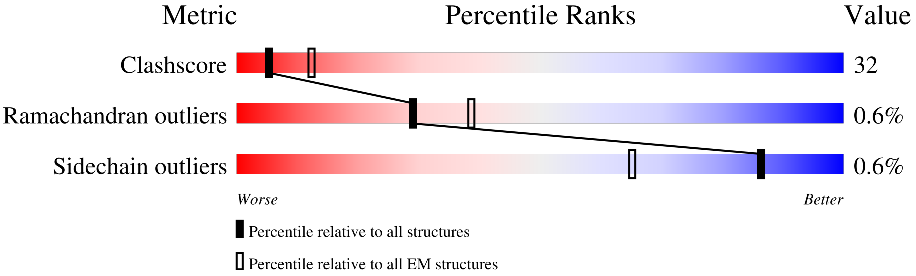
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

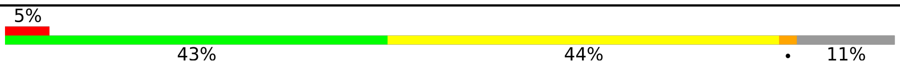
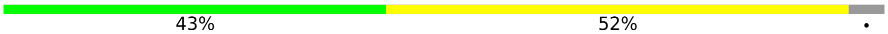
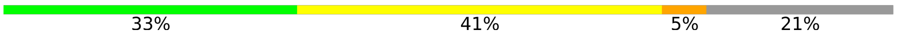
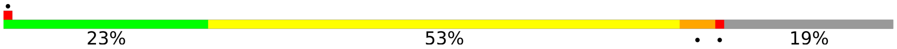
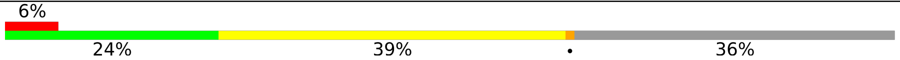
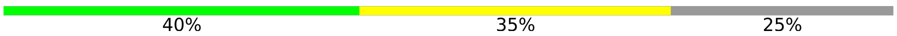
The reported resolution of this entry is 4.00 Å.

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	N	1390	
2	A	108	
3	B	67	
4	C	58	
5	D	150	
6	E	127	
7	F	210	
8	G	133	

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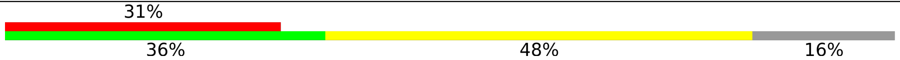
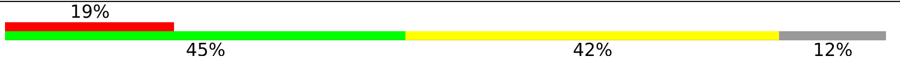
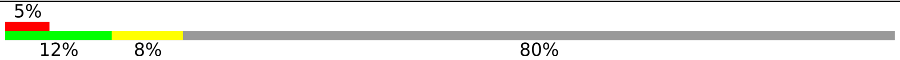
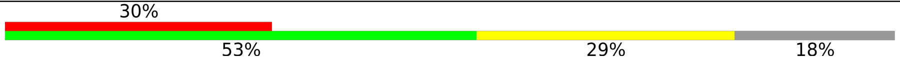
Mol	Chain	Length	Quality of chain
9	H	346	 38% 55% 5%
10	I	148	 31% 36% 48% 16%
11	J	204	 19% 45% 42% 12%
12	K	708	 8% 10% 81%
13	L	398	 7% 13% 79%
14	M	1133	 43% 53%
15	Z	316	 5% 12% 8% 80%
16	X	534	 30% 53% 29% 18%
17	Y	36	 47% 72% 28%

2 Entry composition ⓘ

There are 17 unique types of molecules in this entry. The entry contains 34518 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 III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	N	1238	9385	5928	1643	1746	68	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	37	288	179	55	49	5	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	64	507	328	86	87	6	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	C	46	388	241	75	66	6	0	0

- Molecule 5 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		
5	D	121	972	627	160	179	6	0	0

- Molecule 6 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		
6	E	81	649	414	111	119	5	0	0

- Molecule 7 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		
7	F	209	1715	1083	300	324	8	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	100	794	493	142	152	7	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	329	2635	1663	472	489	11	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	125	1008	631	175	199	3	0	0

- Molecule 11 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	179	1442	938	226	271	7	0	0

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	137	1119	718	192	204	5	0	0

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	L	82	620	397	104	115	4	0	0

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	M	1114	8811	5581	1540	1621	69	0	0

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	Z	63	518	337	78	99	4	0	0

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	X	440	3487	2193	607	665	22	0	0

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC7-beta.

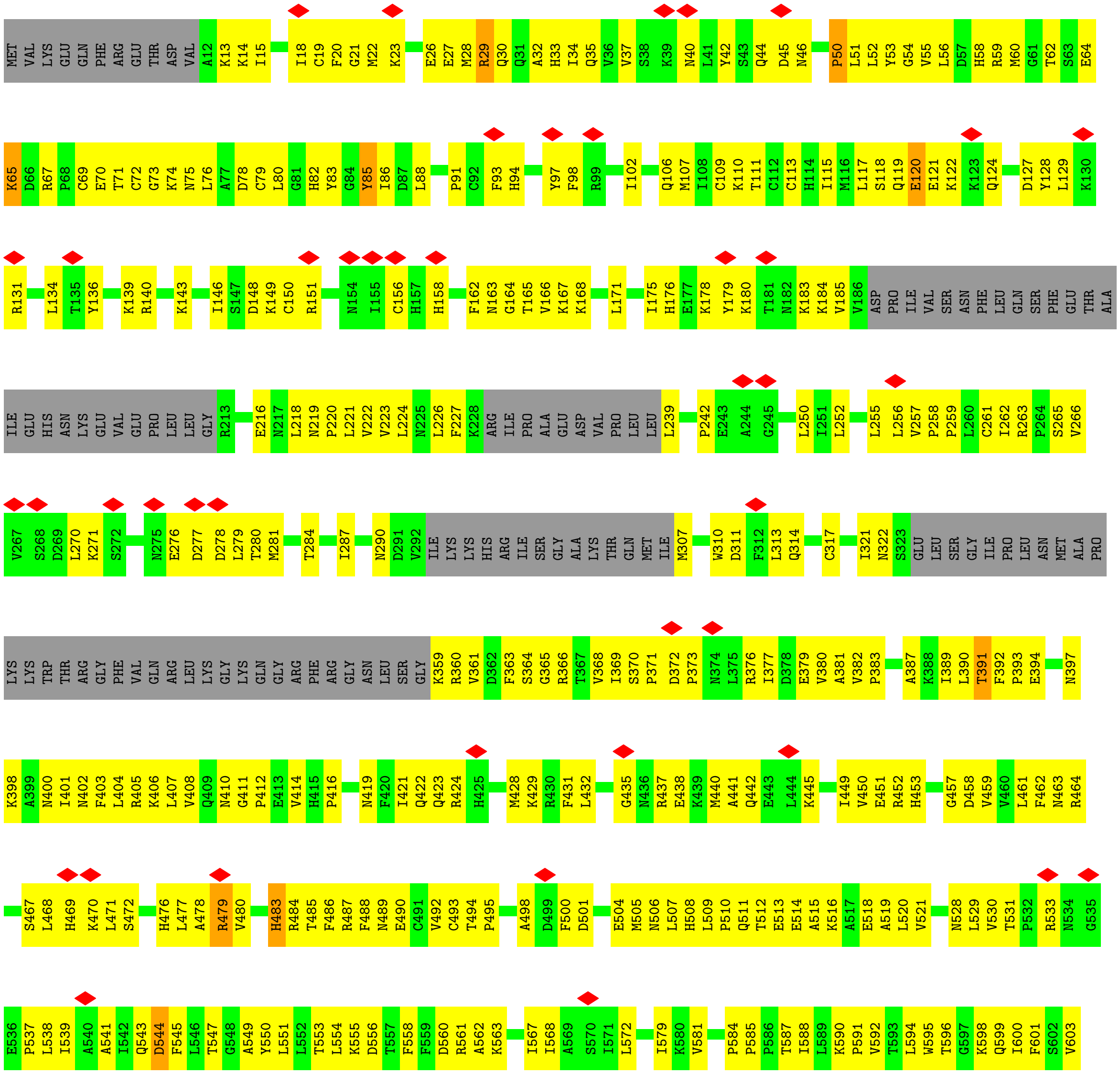
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
17	Y	36	180	108	36	36	0	0

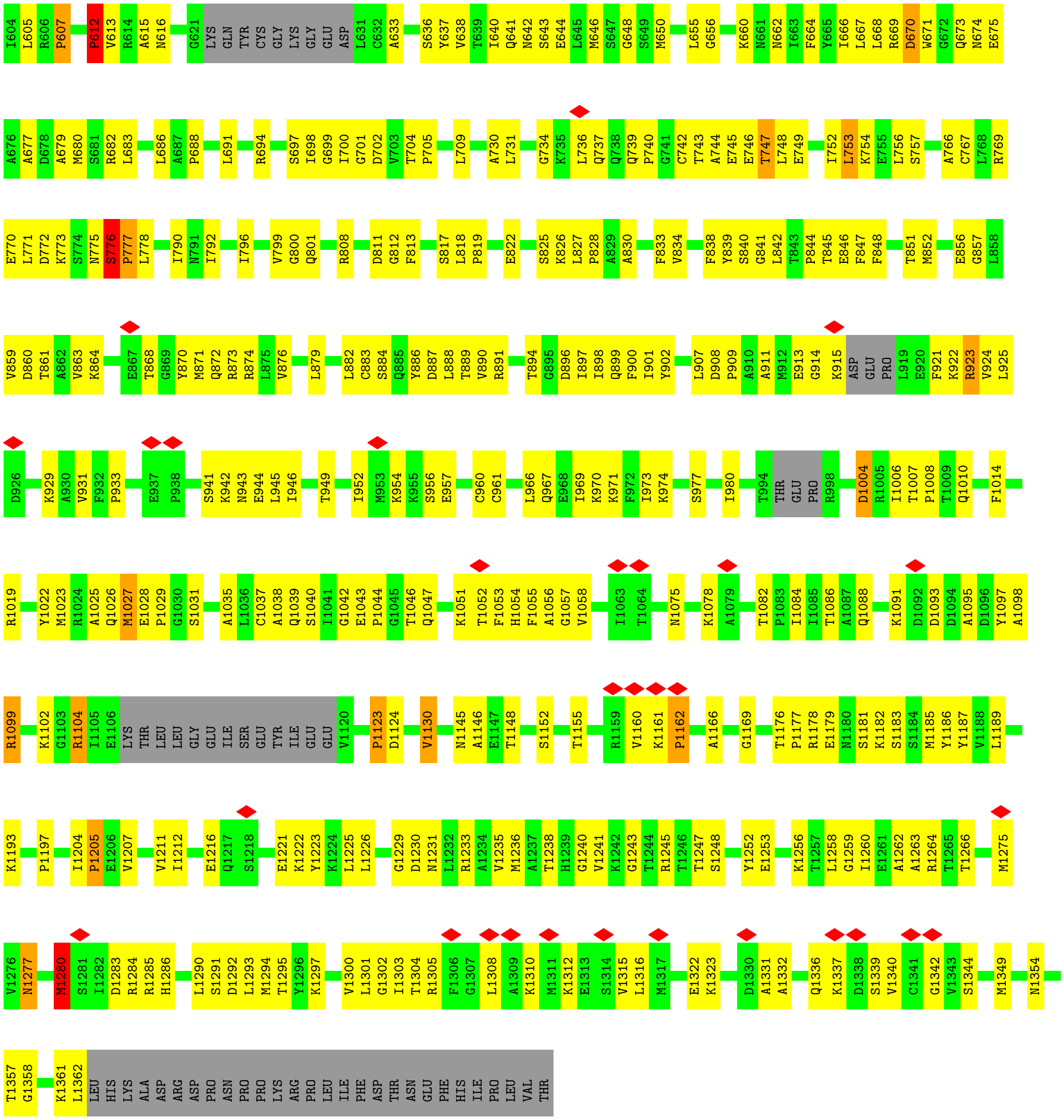
3 Residue-property plots ⓘ

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

- Molecule 1: DNA-directed RNA polymerase III subunit RPC1

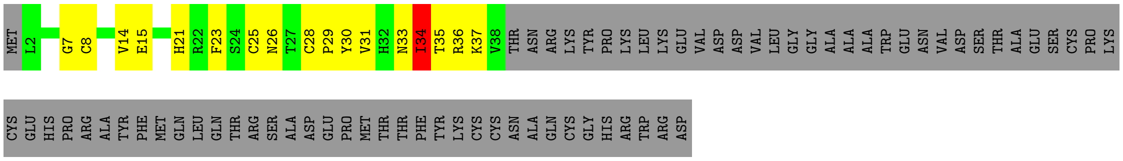
Chain N:





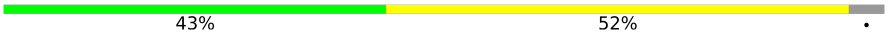
- Molecule 2: DNA-directed RNA polymerase III subunit RPC10

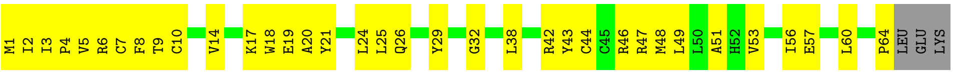
Chain A:



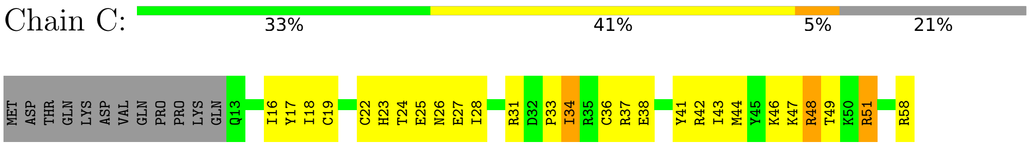
- Molecule 3: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain B:

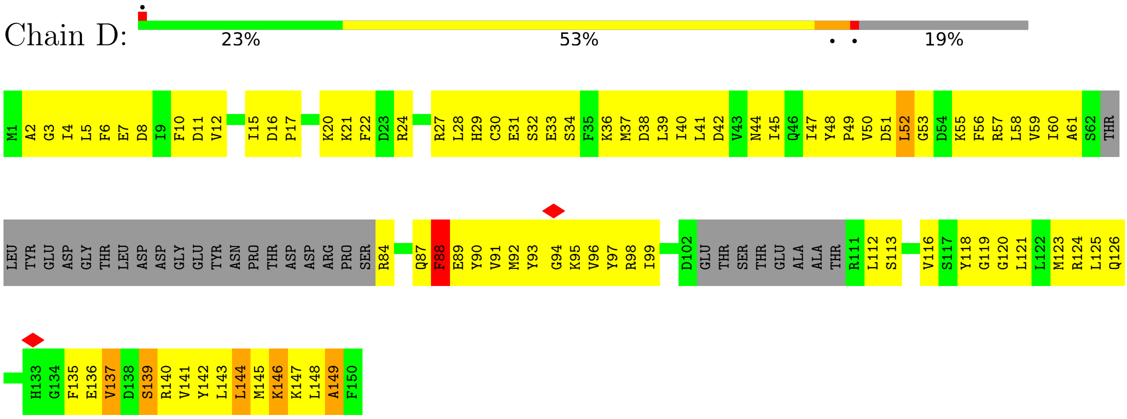




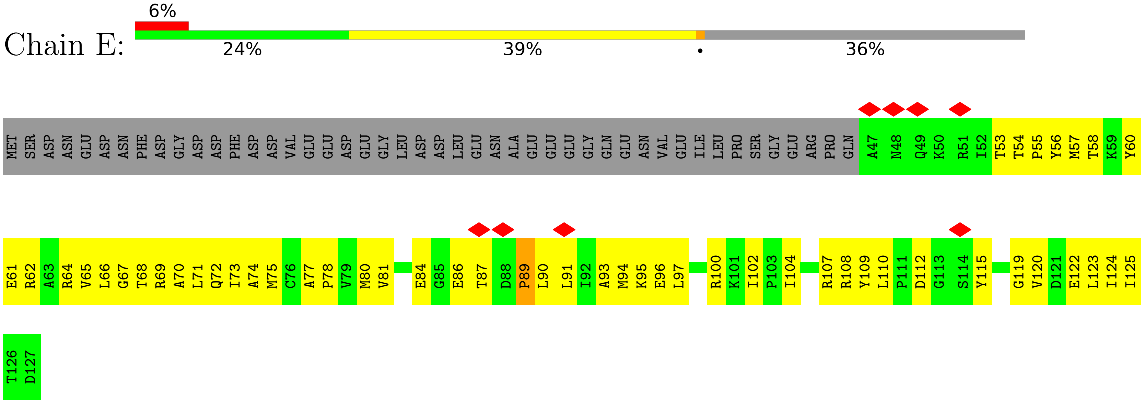
- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC4



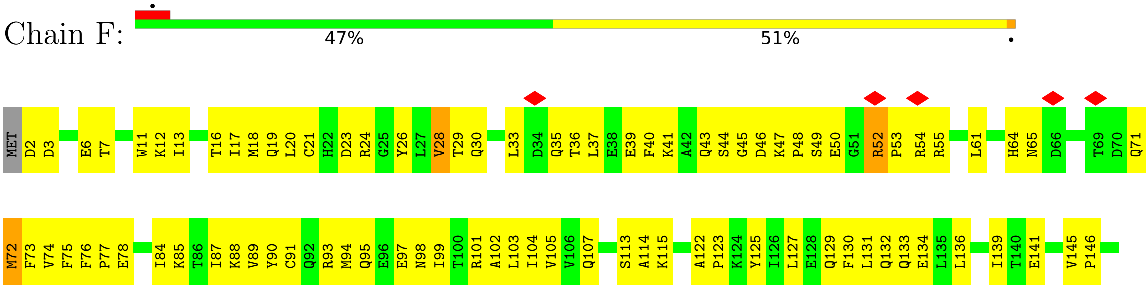
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC3

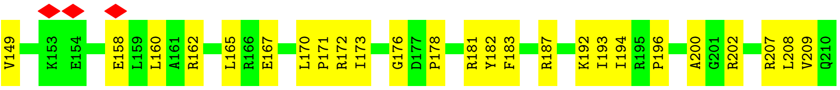


- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



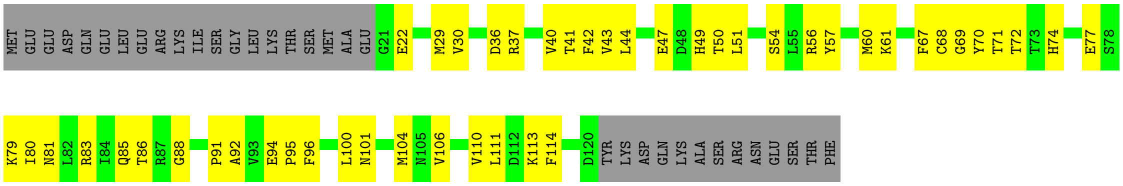
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1





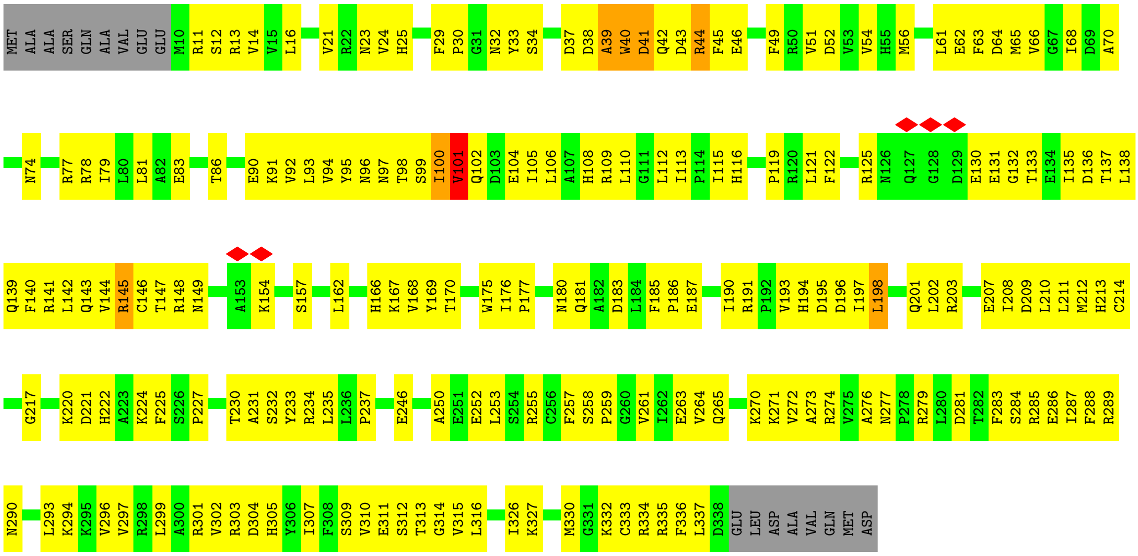
- Molecule 8: DNA-directed RNA polymerases I and III subunit RPAC2

Chain G:



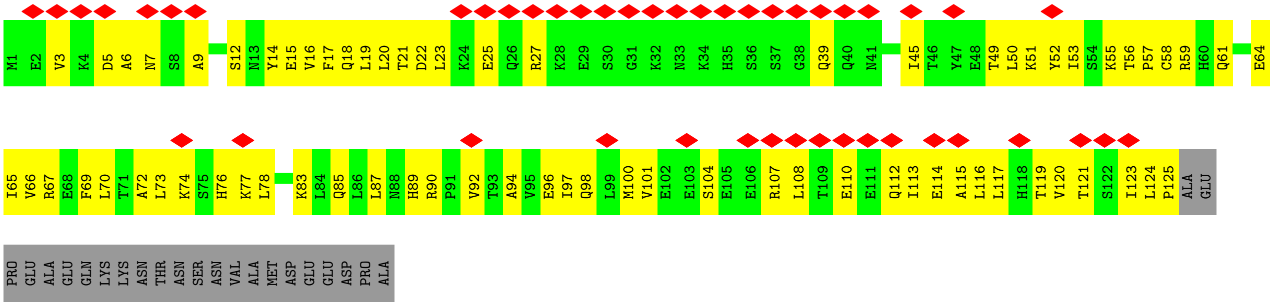
- Molecule 9: DNA-directed RNA polymerases I and III subunit RPAC1

Chain H:

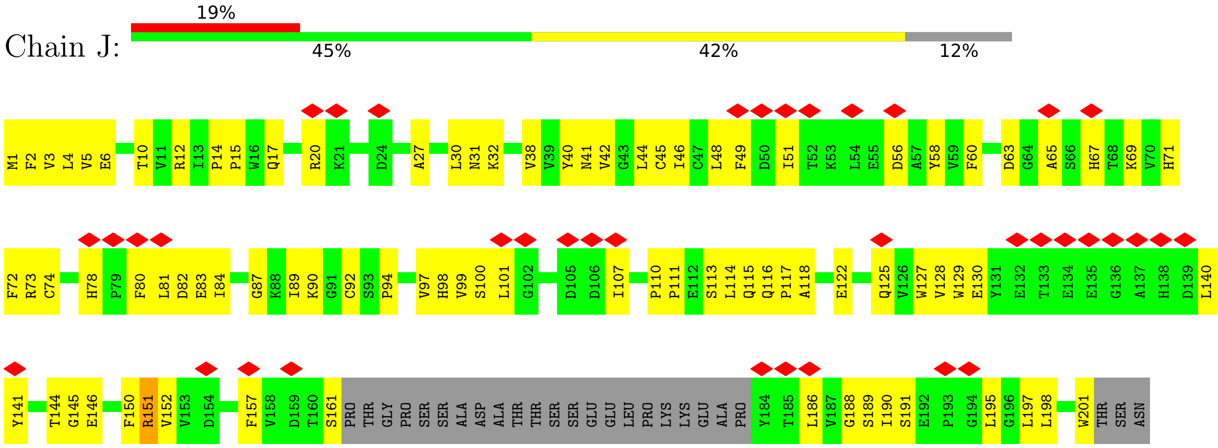


- Molecule 10: DNA-directed RNA polymerase III subunit RPC9

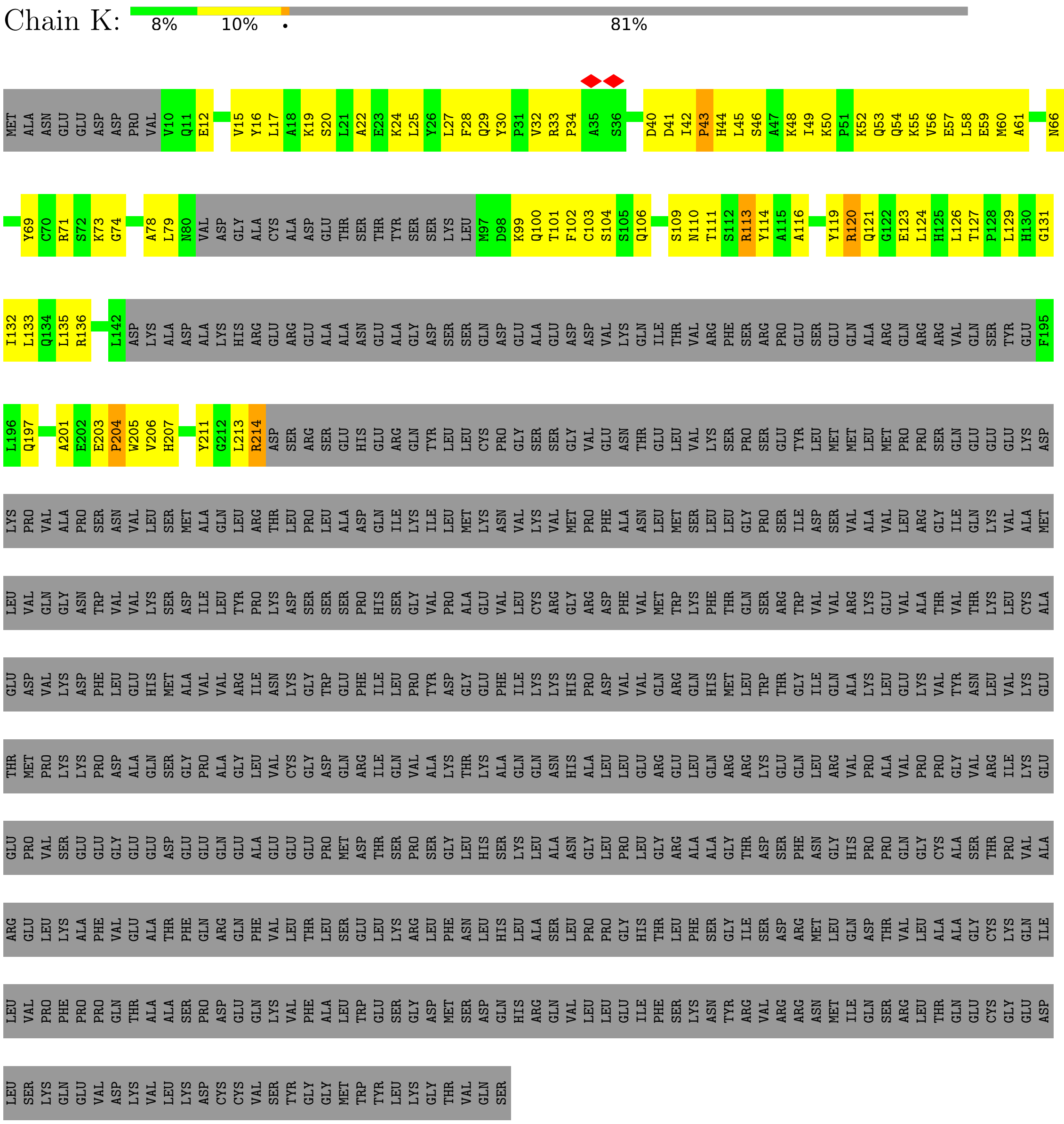
Chain I:



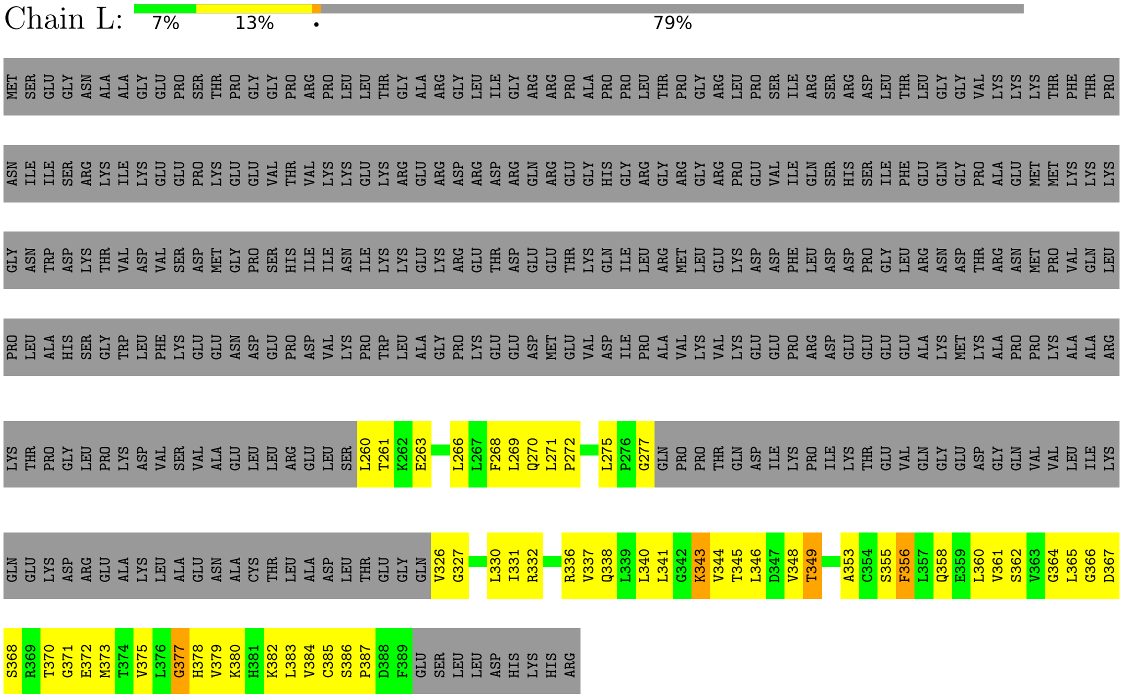
- Molecule 11: DNA-directed RNA polymerase III subunit RPC8



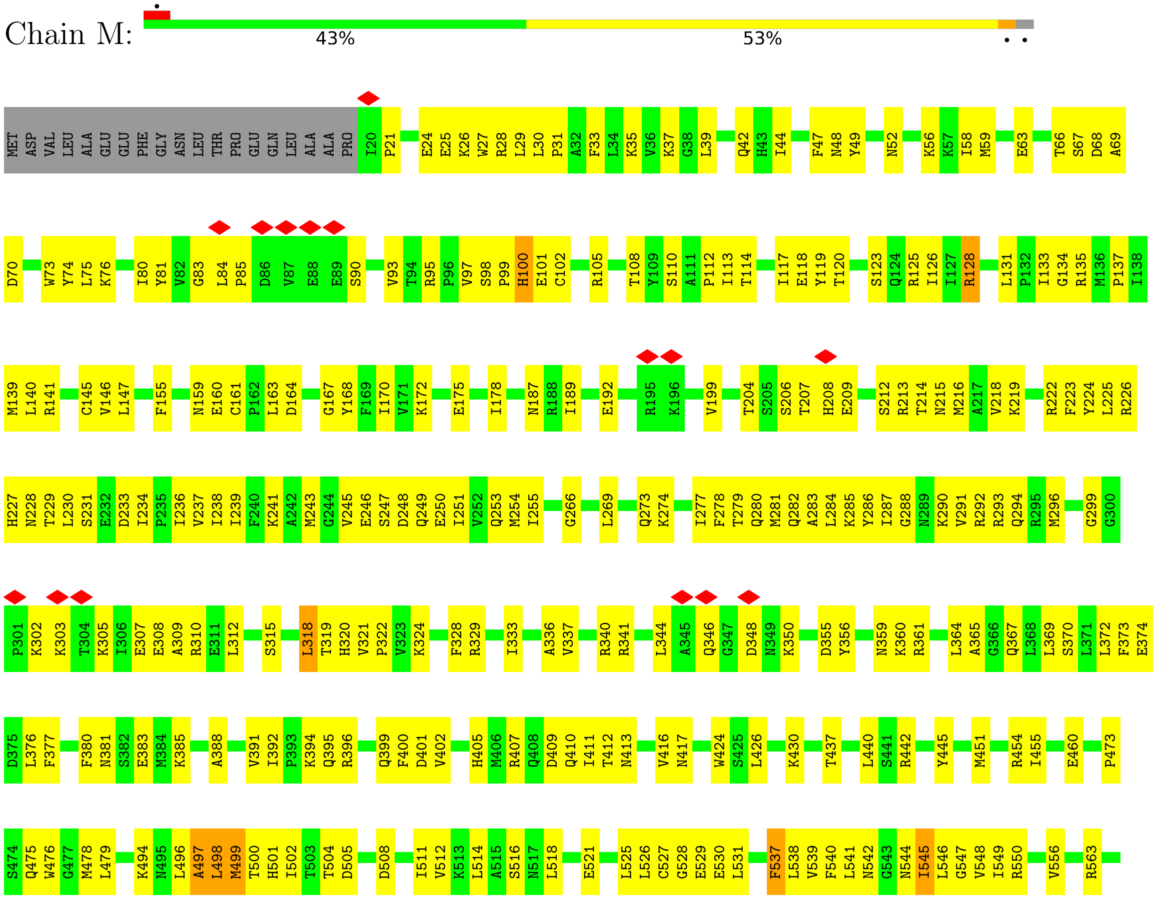
- Molecule 12: DNA-directed RNA polymerase III subunit RPC5

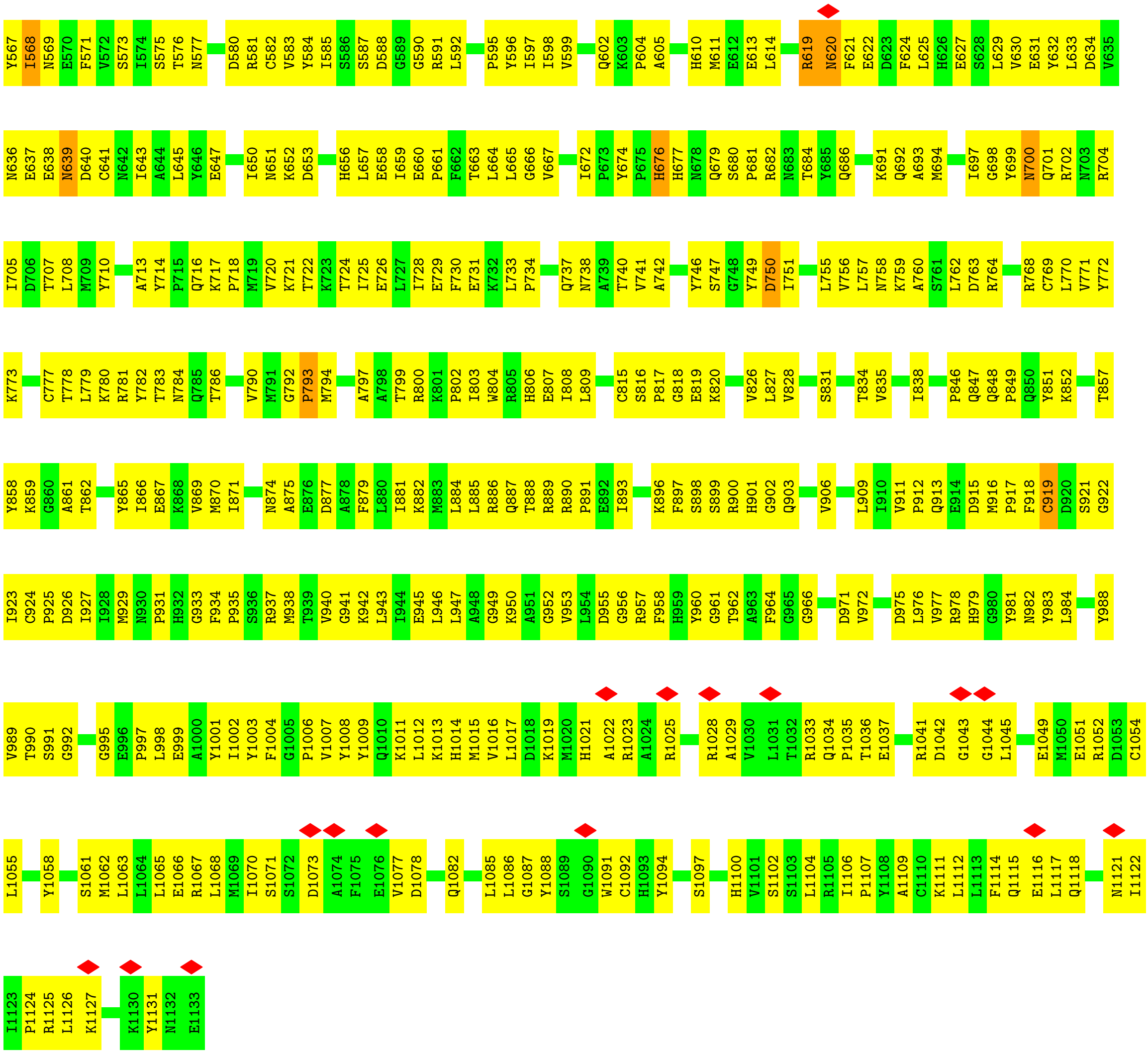


- Molecule 13: DNA-directed RNA polymerase III subunit RPC4

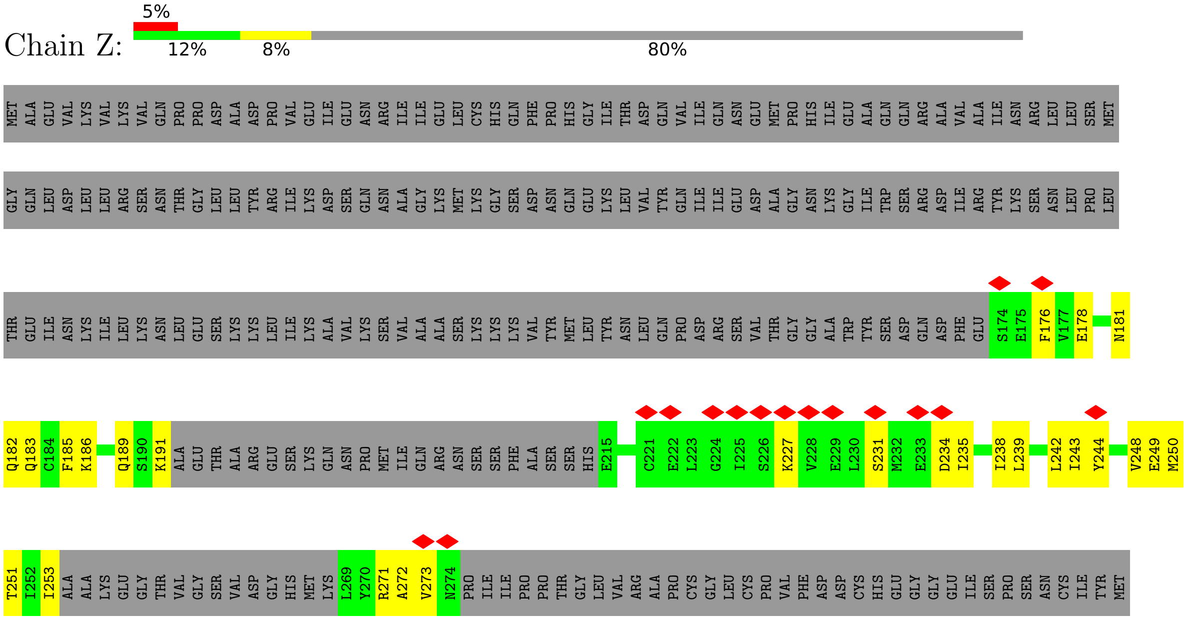


- Molecule 14: DNA-directed RNA polymerase III subunit RPC2



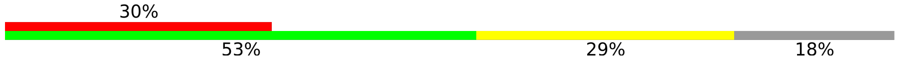


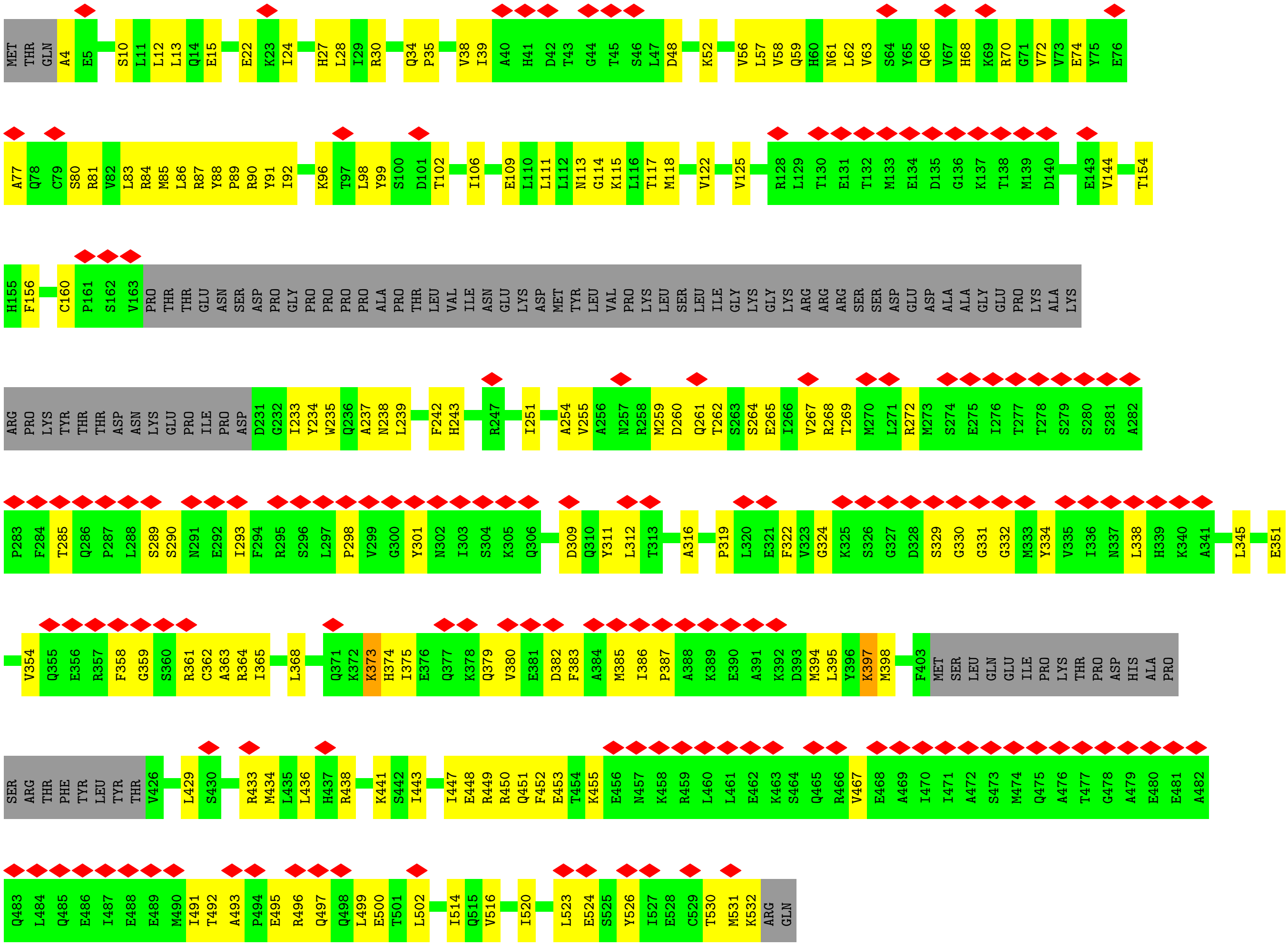
- Molecule 15: DNA-directed RNA polymerase III subunit RPC6



- Molecule 16: DNA-directed RNA polymerase III subunit RPC3

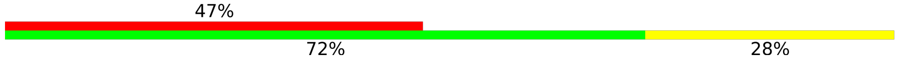
Chain X:

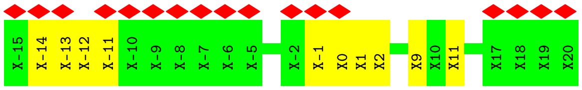




- Molecule 17: DNA-directed RNA polymerase III subunit RPC7-beta

Chain Y:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	40.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	75000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.365	Depositor
Minimum map value	-0.253	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	383.40002, 383.40002, 383.40002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	N	1.06	8/9535 (0.1%)	0.63	11/12862 (0.1%)
2	A	0.33	0/294	0.71	0/396
3	B	0.45	0/516	0.67	0/696
4	C	0.31	0/394	0.69	0/524
5	D	2.96	7/988 (0.7%)	0.89	5/1323 (0.4%)
6	E	0.31	0/659	0.62	0/891
7	F	0.27	0/1745	0.55	2/2358 (0.1%)
8	G	0.39	0/808	0.54	0/1090
9	H	0.35	0/2689	0.62	1/3644 (0.0%)
10	I	0.24	0/1021	0.51	0/1377
11	J	0.28	0/1481	0.54	0/2013
12	K	0.27	0/1146	0.55	0/1549
13	L	0.26	0/626	0.62	0/842
14	M	0.36	0/8982	0.63	1/12118 (0.0%)
15	Z	0.25	0/523	0.53	0/701
16	X	0.24	0/3534	0.46	0/4766
All	All	0.79	15/34941 (0.0%)	0.61	20/47150 (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	N	0	16
2	A	0	1
3	B	0	1
4	C	0	1
5	D	0	5
6	E	0	1
7	F	0	2
9	H	0	7
12	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	L	0	4
14	M	0	16
16	X	0	1
All	All	0	58

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	29	ARG	CB-CG	64.17	3.25	1.52
5	D	146	LYS	CD-CE	63.43	3.09	1.51
1	N	85	TYR	CD2-CE2	39.90	1.99	1.39
1	N	85	TYR	CD1-CE1	38.31	1.96	1.39
5	D	88	PHE	CE1-CZ	30.63	1.95	1.37

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	146	LYS	CG-CD-CE	9.84	141.41	111.90
1	N	29	ARG	CA-CB-CG	9.73	134.80	113.40
1	N	391	THR	C-N-CA	9.00	144.21	121.70
1	N	29	ARG	CB-CG-CD	8.77	134.41	111.60
5	D	146	LYS	CD-CE-NZ	8.33	130.87	111.70

There are no chirality outliers.

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	120	GLU	Peptide
1	N	480	VAL	Peptide
1	N	483	HIS	Peptide
1	N	563	LYS	Peptide
1	N	572	LEU	Peptide

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	N	9385	0	9273	666	0
2	A	288	0	279	24	0
3	B	507	0	525	52	0
4	C	388	0	395	34	0
5	D	972	0	959	154	0
6	E	649	0	678	59	0
7	F	1715	0	1733	98	0
8	G	794	0	780	49	0
9	H	2635	0	2620	201	0
10	I	1008	0	1035	72	0
11	J	1442	0	1396	77	0
12	K	1119	0	1109	83	0
13	L	620	0	660	62	0
14	M	8811	0	8937	653	0
15	Z	518	0	525	25	0
16	X	3487	0	3523	134	0
17	Y	180	0	41	5	0
All	All	34518	0	34468	2177	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 32.

The worst 5 of 2177 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)
1:N:85:TYR:CZ	1:N:85:TYR:CE2	1.75	1.70
1:N:85:TYR:CZ	1:N:85:TYR:CE1	1.75	1.60
5:D:88:PHE:CE1	5:D:88:PHE:CZ	1.95	1.54
1:N:85:TYR:CE1	1:N:85:TYR:CD1	1.96	1.53
5:D:88:PHE:CZ	5:D:88:PHE:CE2	1.95	1.53

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	1220/1390 (88%)	948 (78%)	258 (21%)	14 (1%)	14	51
2	A	35/108 (32%)	23 (66%)	11 (31%)	1 (3%)	4	32
3	B	62/67 (92%)	54 (87%)	8 (13%)	0	100	100
4	C	44/58 (76%)	32 (73%)	11 (25%)	1 (2%)	6	37
5	D	115/150 (77%)	77 (67%)	38 (33%)	0	100	100
6	E	79/127 (62%)	56 (71%)	22 (28%)	1 (1%)	12	48
7	F	207/210 (99%)	182 (88%)	24 (12%)	1 (0%)	29	67
8	G	98/133 (74%)	71 (72%)	27 (28%)	0	100	100
9	H	327/346 (94%)	246 (75%)	80 (24%)	1 (0%)	41	75
10	I	123/148 (83%)	113 (92%)	10 (8%)	0	100	100
11	J	175/204 (86%)	138 (79%)	37 (21%)	0	100	100
12	K	131/708 (18%)	92 (70%)	38 (29%)	1 (1%)	19	58
13	L	78/398 (20%)	60 (77%)	17 (22%)	1 (1%)	12	48
14	M	1112/1133 (98%)	831 (75%)	276 (25%)	5 (0%)	34	71
15	Z	57/316 (18%)	50 (88%)	7 (12%)	0	100	100
16	X	434/534 (81%)	405 (93%)	29 (7%)	0	100	100
All	All	4297/6030 (71%)	3378 (79%)	893 (21%)	26 (1%)	29	63

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	607	PRO
1	N	612	PRO
1	N	777	PRO
1	N	1162	PRO
1	N	1205	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	983/1212 (81%)	976 (99%)	7 (1%)	84	90
2	A	33/94 (35%)	33 (100%)	0	100	100
3	B	53/56 (95%)	53 (100%)	0	100	100
4	C	43/55 (78%)	41 (95%)	2 (5%)	26	53
5	D	103/131 (79%)	102 (99%)	1 (1%)	76	86
6	E	70/111 (63%)	70 (100%)	0	100	100
7	F	191/192 (100%)	191 (100%)	0	100	100
8	G	89/119 (75%)	89 (100%)	0	100	100
9	H	289/302 (96%)	285 (99%)	4 (1%)	67	81
10	I	117/136 (86%)	117 (100%)	0	100	100
11	J	160/181 (88%)	158 (99%)	2 (1%)	69	82
12	K	122/622 (20%)	120 (98%)	2 (2%)	62	79
13	L	72/347 (21%)	72 (100%)	0	100	100
14	M	973/988 (98%)	971 (100%)	2 (0%)	93	96
15	Z	60/280 (21%)	60 (100%)	0	100	100
16	X	386/476 (81%)	383 (99%)	3 (1%)	81	89
All	All	3744/5302 (71%)	3721 (99%)	23 (1%)	86	92

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	71	HIS
12	K	214	ARG
12	K	120	ARG
14	M	128	ARG
1	N	1284	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	1034	GLN
14	M	1115	GLN
16	X	497	GLN
9	H	180	ASN
9	H	32	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

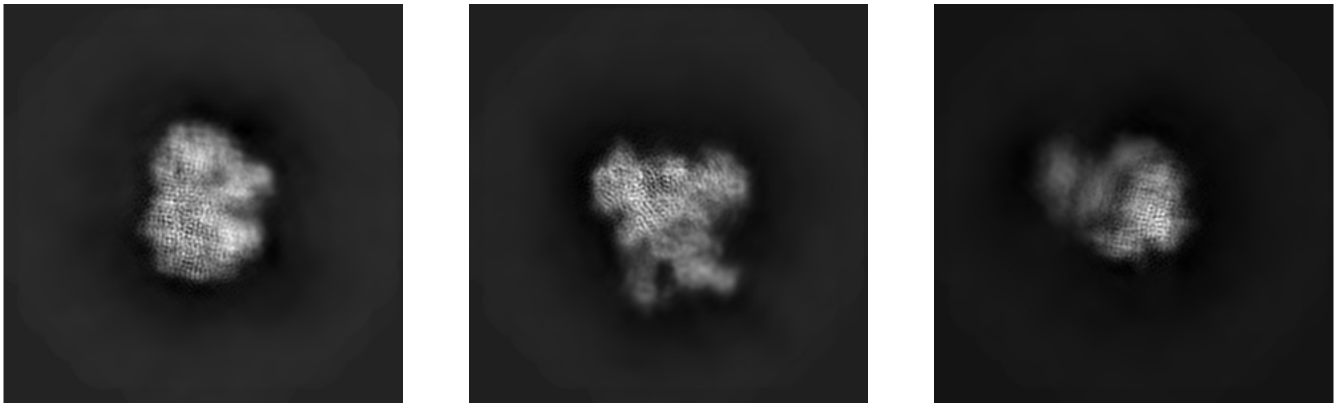
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11904. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map

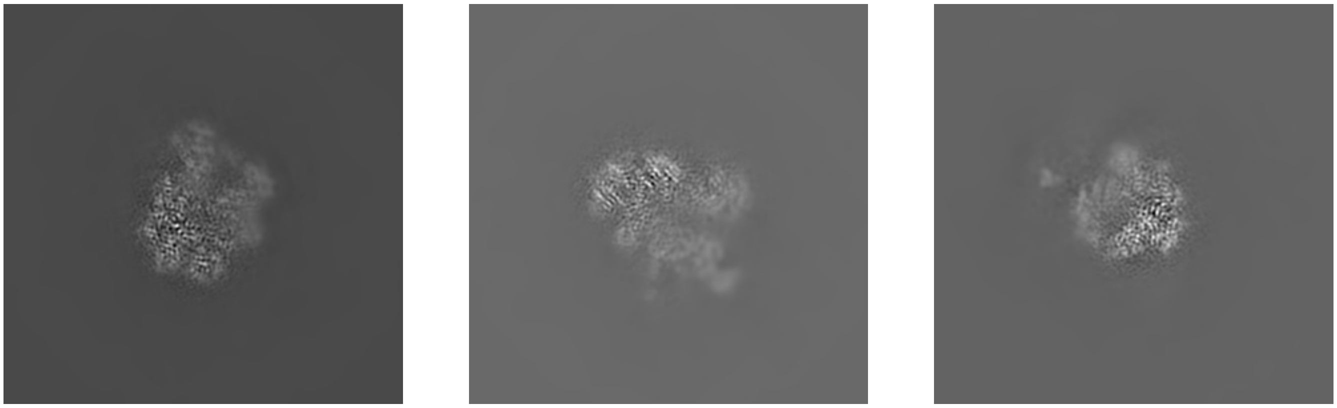


X Y Z

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

6.2 Central slices

6.2.1 Primary map

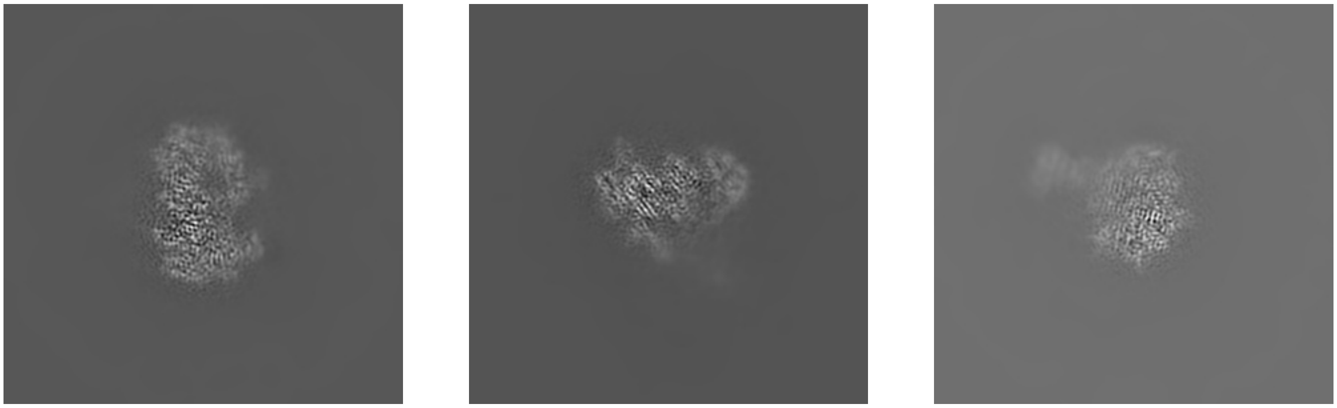


X Index: 180 Y Index: 180 Z Index: 180

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

6.3 Largest variance slices ⓘ

6.3.1 Primary map

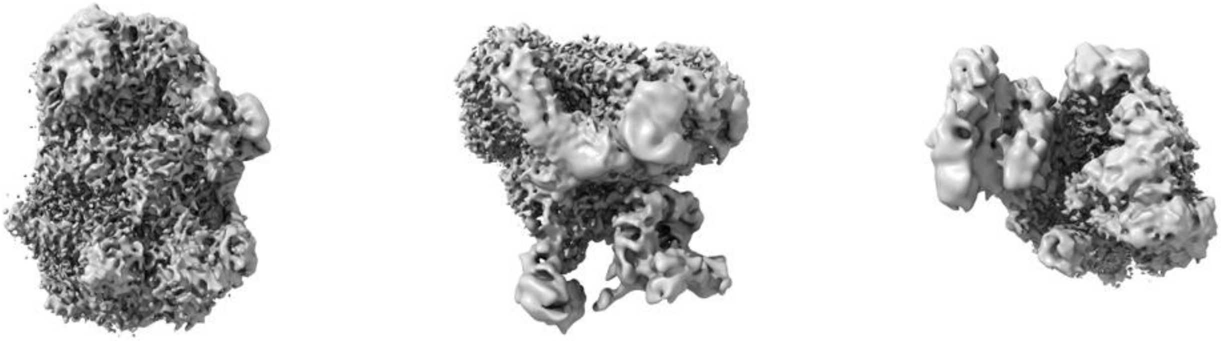


X Index: 202 Y Index: 157 Z Index: 150

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

6.4 Orthogonal surface views ⓘ

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.027. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

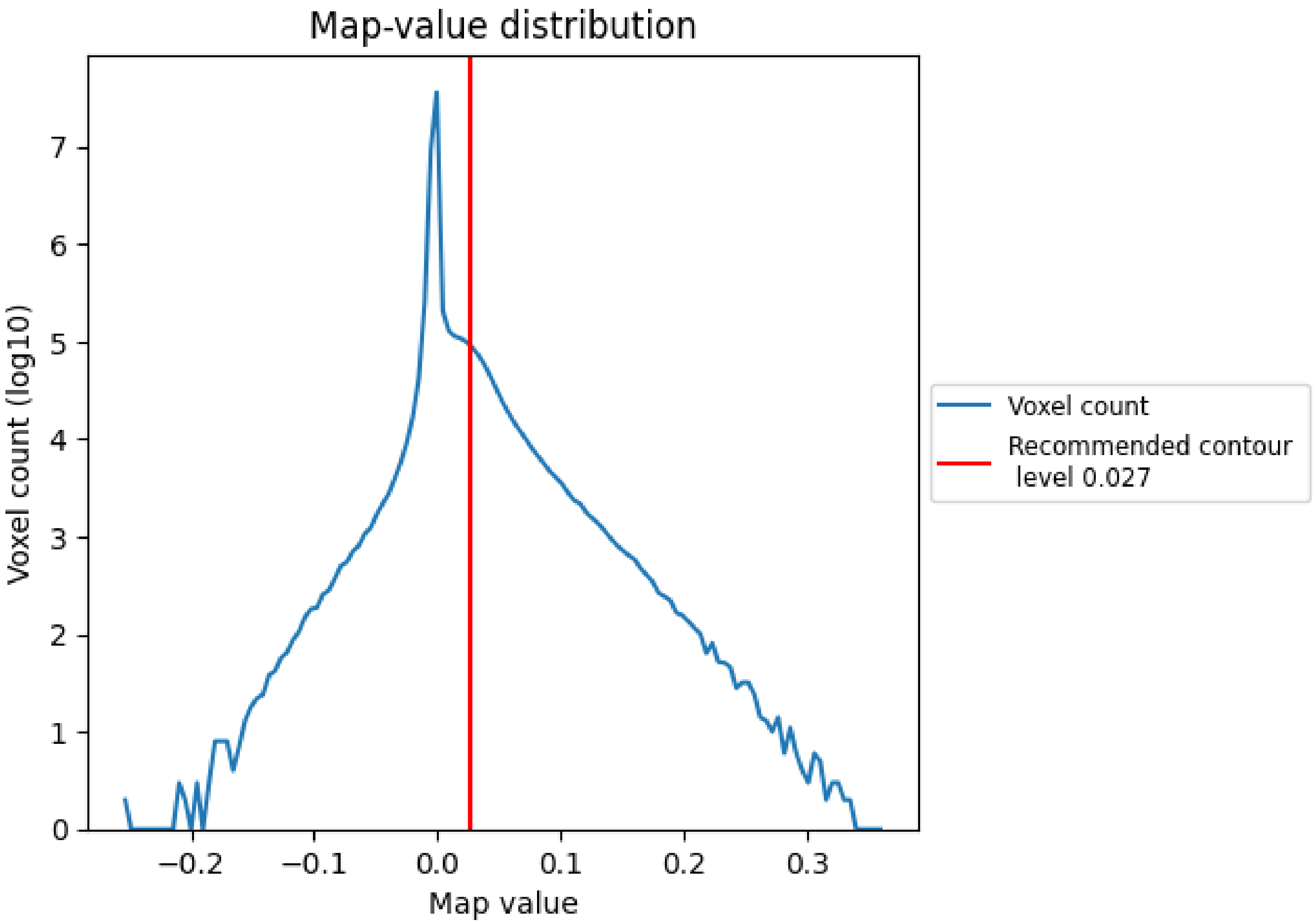
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

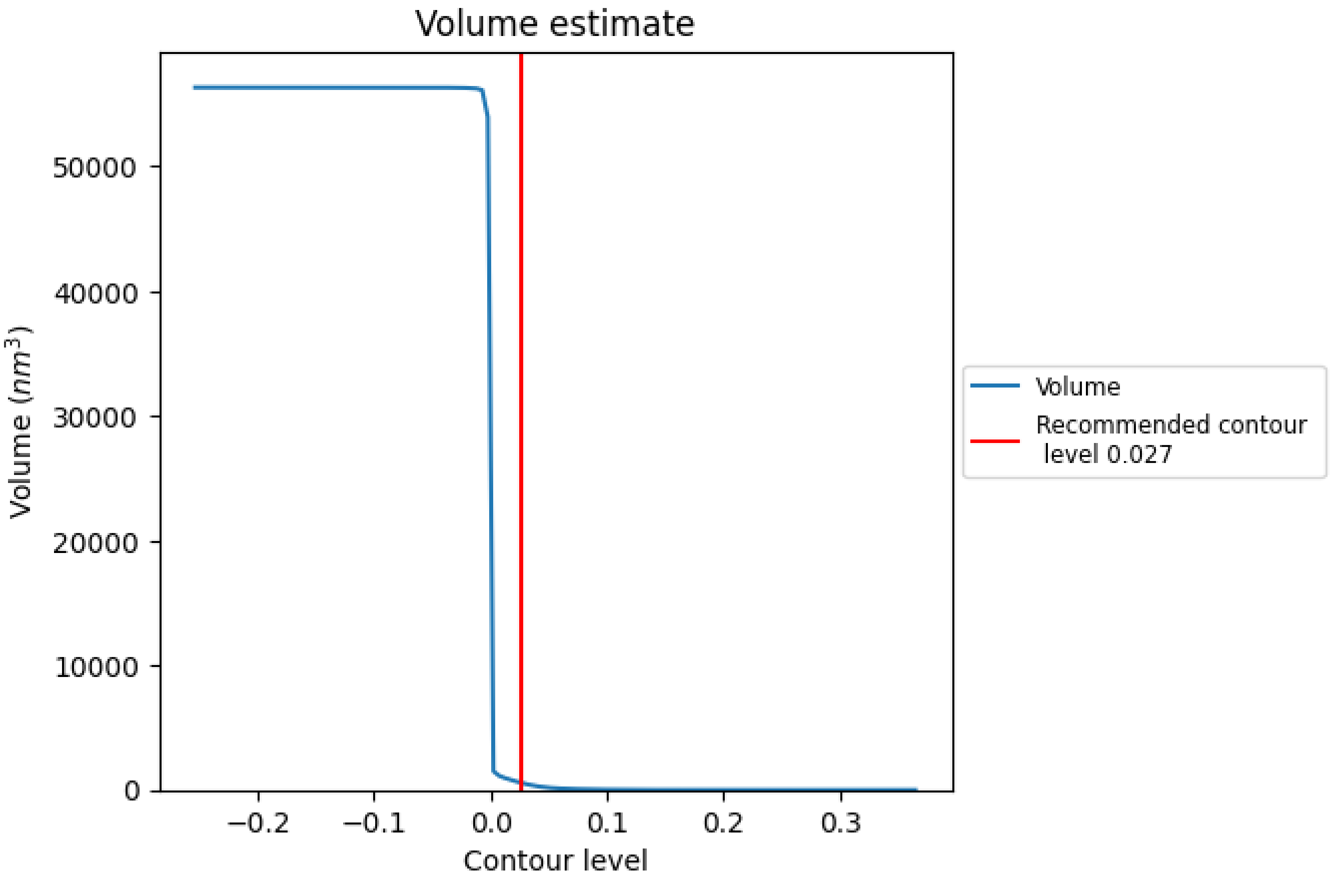
This section contains the results of statistical analysis of the map.

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.

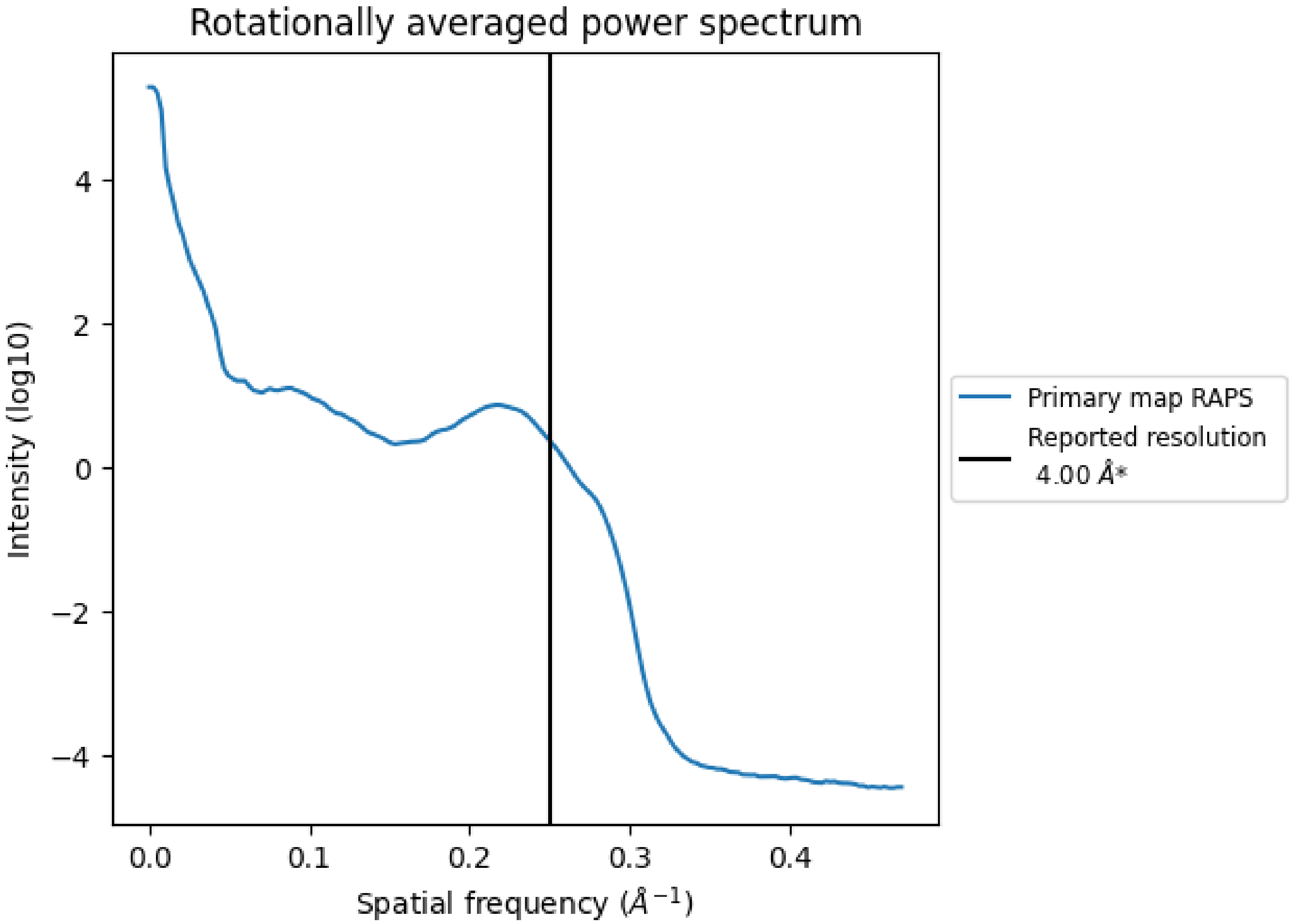
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 555 nm^3; this corresponds to an approximate mass of 501 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

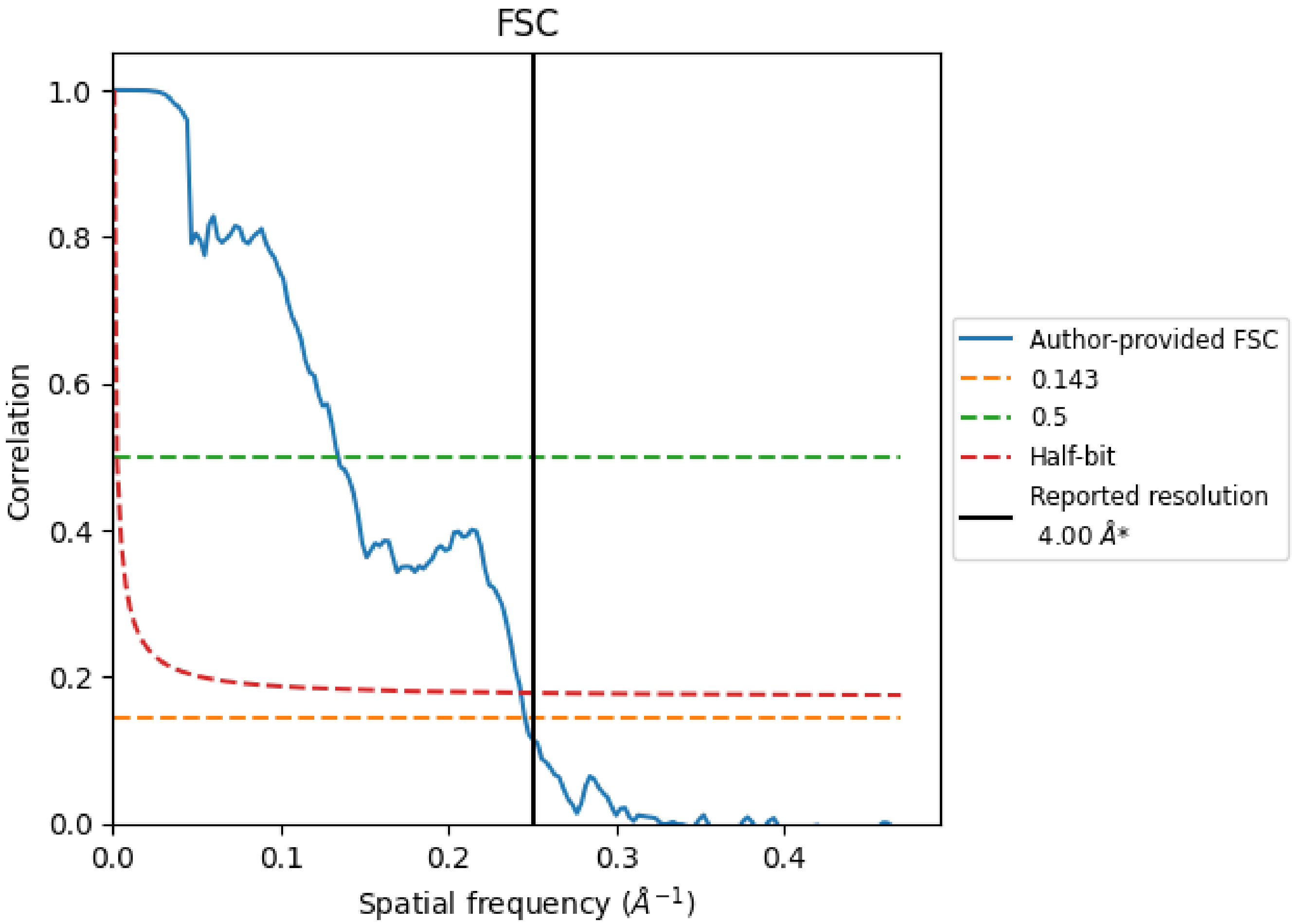


*Reported resolution corresponds to spatial frequency of 0.250 $\AA^{-1}$

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 $\AA^{-1}$

8.2 Resolution estimates ⓘ

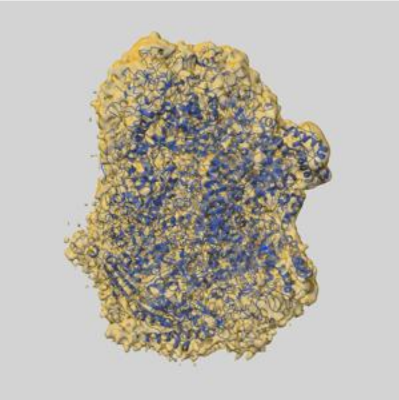
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.07	7.45	4.11
Unmasked-calculated*	-	-	-

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

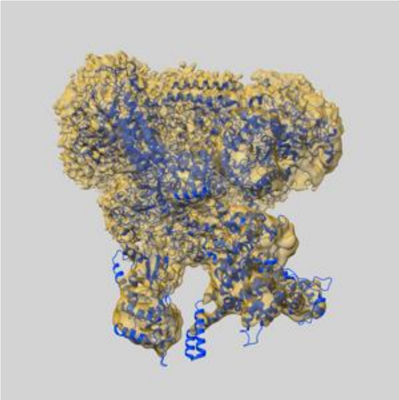
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-11904 and PDB model 7AST. Per-residue inclusion information can be found in section 3 on page 7.

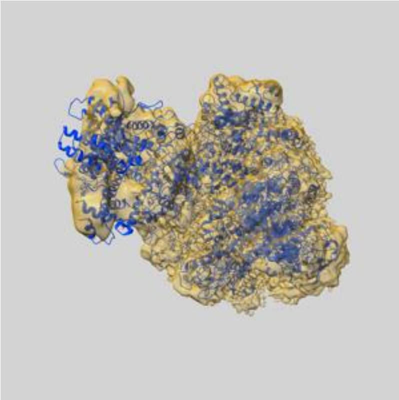
9.1 Map-model overlay ⓘ



X



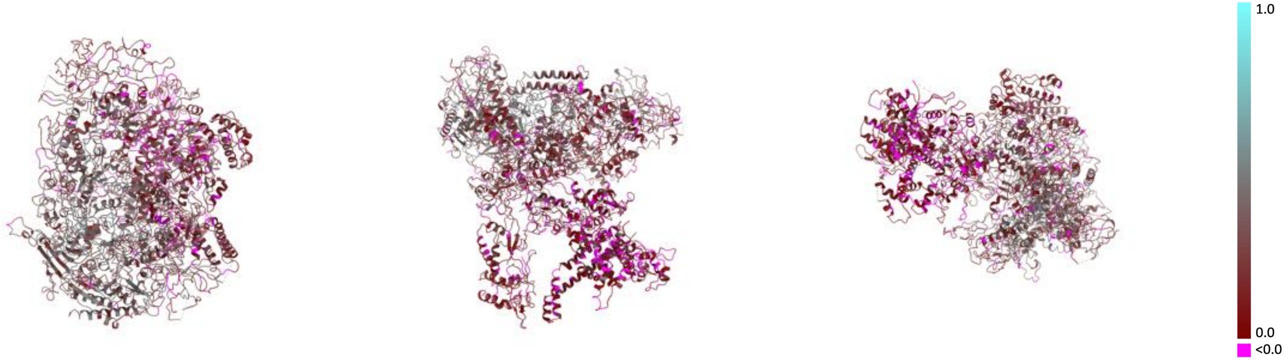
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.027 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.

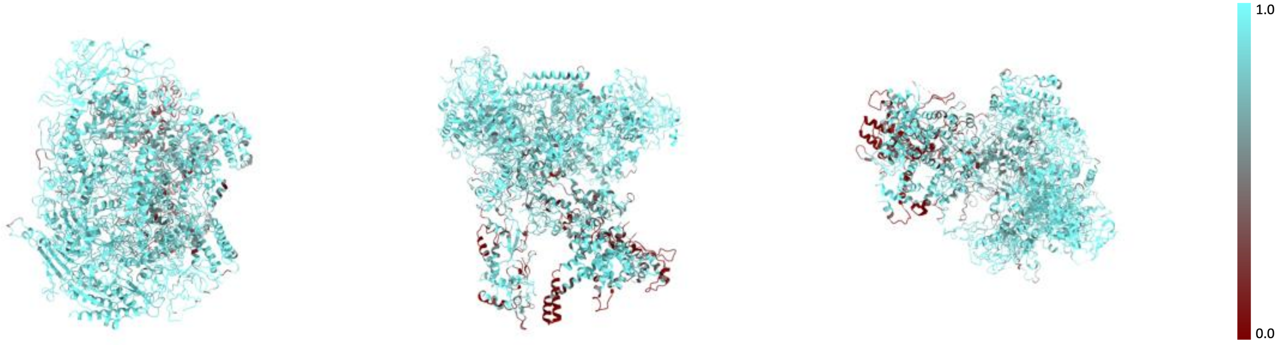
9.2 Q-score mapped to coordinate model ⓘ



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.

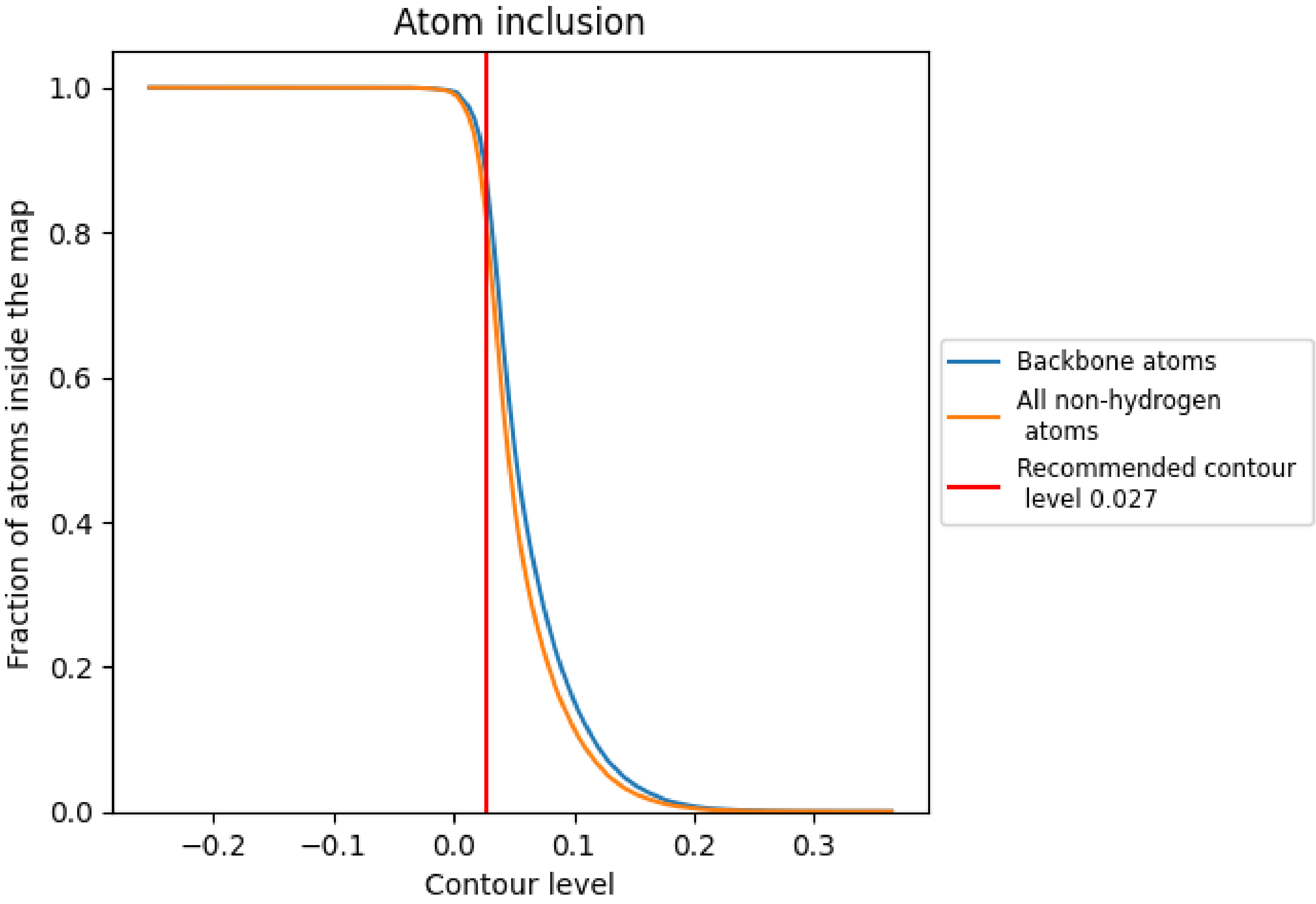
9.3 Atom inclusion mapped to coordinate model ⓘ



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 (0.027).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	■ 0.8201	■ 0.2400
A	■ 0.9964	■ 0.2280
B	■ 0.9190	■ 0.3890
C	■ 0.9272	■ 0.2890
D	■ 0.8980	■ 0.2860
E	■ 0.8175	■ 0.2110
F	■ 0.8751	■ 0.1970
G	■ 0.9244	■ 0.3620
H	■ 0.9175	■ 0.3520
I	■ 0.5668	■ 0.1330
J	■ 0.6800	■ 0.1370
K	■ 0.9380	■ 0.2130
L	■ 0.9479	■ 0.2860
M	■ 0.8717	■ 0.3090
N	■ 0.8272	■ 0.2280
X	■ 0.5860	■ 0.0820
Y	■ 0.5278	■ 0.0640
Z	■ 0.7227	■ 0.0750