wwPDB EM Validation Summary Report

Mar 29, 2023 – 04:42 pm BST

PDB ID	:	7Z31
EMDB ID	:	EMD-14470
Title	:	Structure of yeast RNA Polymerase III-Ty1 integrase complex at 2.7 A (focus subunit C11, no C11 C-terminal Zn-ribbon in the funnel pore).
Authors	:	Nguyen, P.Q.; Huecas, S.; Plaza-Pegueroles, A.; Fernandez-Tornero, C.
Deposited on	:	2022-03-01
Resolution	:	2.76 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:

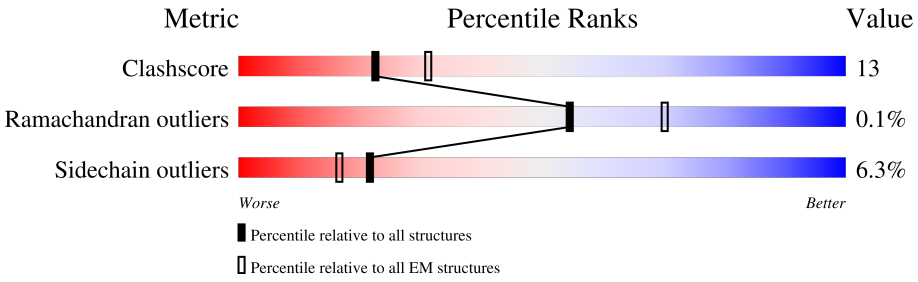
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.76 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	1460	29% 67% 28%
2	B	1149	13% 67% 28%
3	C	335	5% 77% 21%
4	D	161	85% 52% 33% 5% 10%
5	E	215	42% 73% 26%
6	F	155	42% 12% 46%
7	G	212	60% 52% 35% 10%
8	H	146	8% 66% 27% 5%

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Mol	Chain	Length	Quality of chain
9	I	110	25% 25% 18% 57%
10	J	70	79% 17%
11	K	142	54% 15% 29%
12	L	70	20% 46% 24% 29%
13	M	282	45% 42% 21% 35%
14	N	422	25% 22% 13% 64%
15	O	654	86% 46% 36% 5% 13%
16	P	317	43% 28% 13% 57%
17	Q	268	39% 29% 10% 61%
18	W	635	97%
19	X	13	77% 77% 23%

2 Entry composition (i)

There are 22 unique types of molecules in this entry. The entry contains 40156 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	A	1419	11123	7013	1962	2089	59	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1102	8701	5507	1499	1635	60	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	335	2655	1681	454	511	9	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	145	1140	723	191	220	6	0	0

- Molecule 5 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		
5	E	215	1759	1116	310	321	12	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	F	83	671	429	114	125	3	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	191	Total	C	N	O	S	0	0
			1544	1007	250	281	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	138	Total	C	N	O	S	0	0
			1103	694	186	218	5		

- Molecule 9 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	47	Total	C	N	O	S	0	0
			365	233	57	69	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			549	350	95	98	6		

- Molecule 11 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			792	496	130	161	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	50	Total	C	N	O	S	0	0
			381	235	76	66	4		

- Molecule 13 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	183	Total	C	N	O	S	0	0
			1492	953	250	288	1		

- Molecule 14 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	151	Total	C	N	O	S	0	0
			1169	738	215	213	3		

- Molecule 15 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	568	Total	C	N	O	S	0	0
			4558	2897	784	858	19		

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	136	Total	C	N	O	S	0	0
			1126	736	175	211	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0
			829	535	137	154	3		

- Molecule 18 is a protein called Integrase.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	W	17	Total	C	N	O	S	0	0
			141	86	27	27	1		

- Molecule 19 is a protein called Unknown RNA polymerase III chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	10	Total	C	N	O	0	0
			50	30	10	10		

- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms	AltConf
20	J	1	Total Zn 1 1	0
20	L	1	Total Zn 1 1	0

- Molecule 21 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 22 is water.

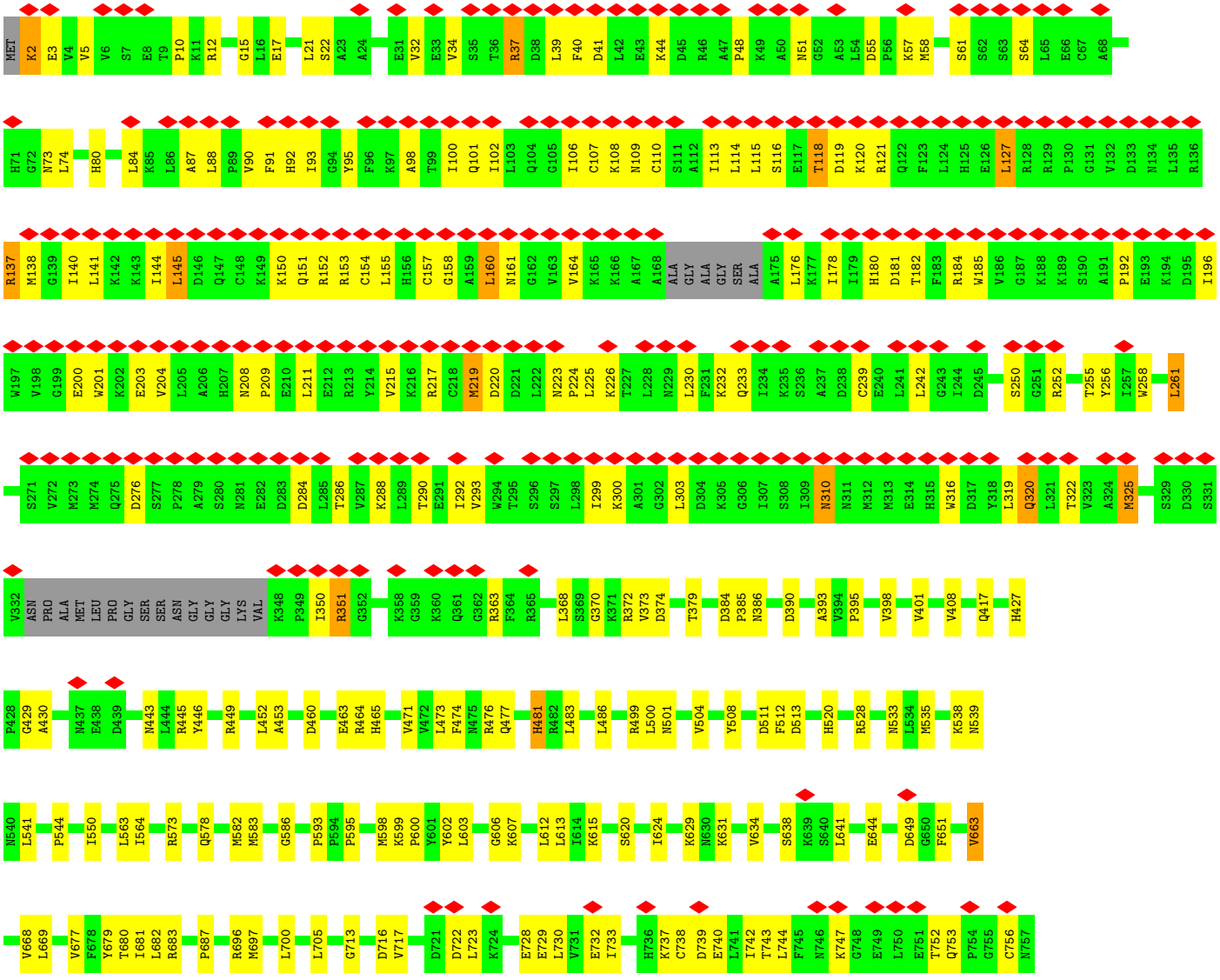
Mol	Chain	Residues	Atoms	AltConf
22	A	1	Total O 1 1	0

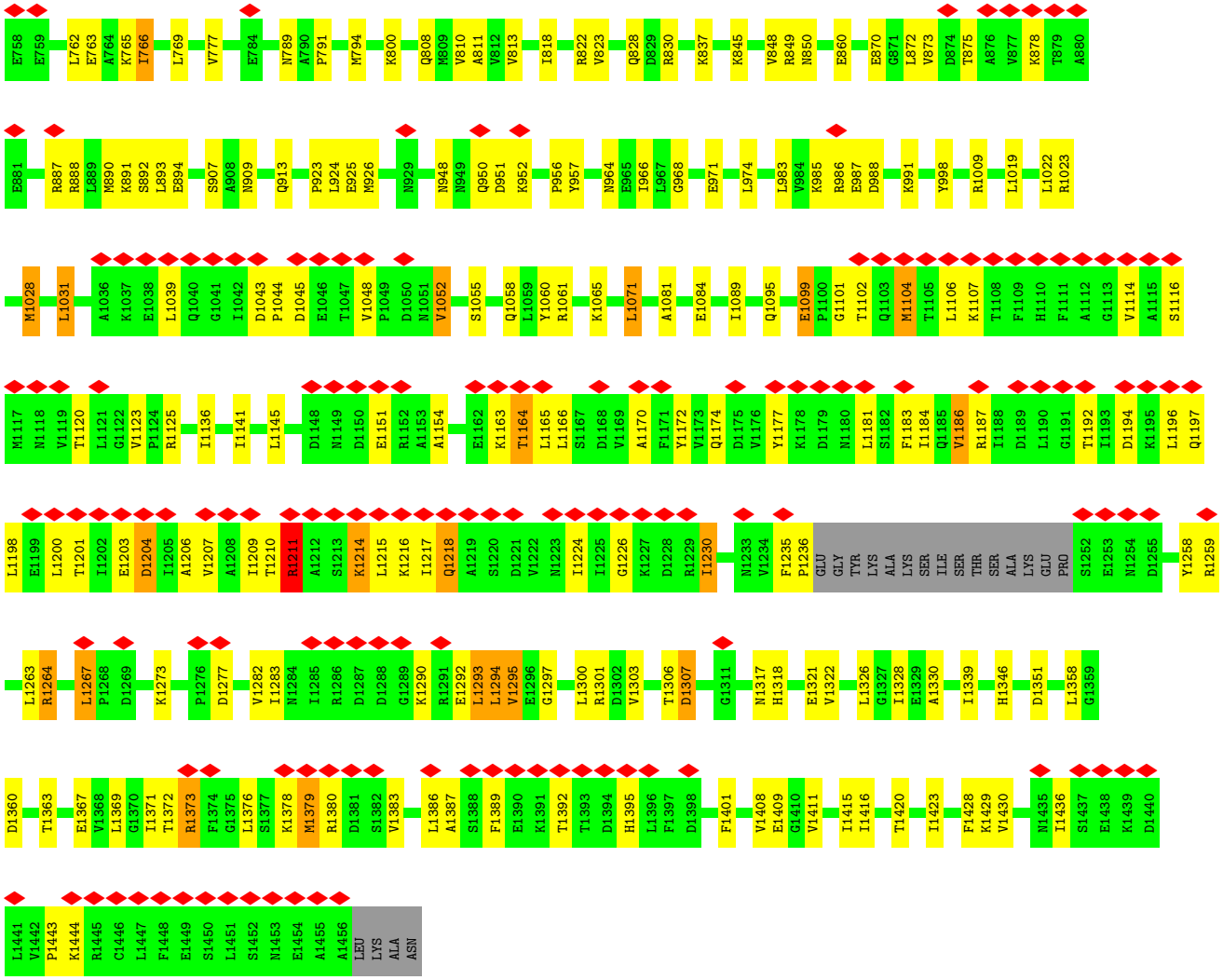
3 Residue-property plots (i)

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 III subunit RPC1

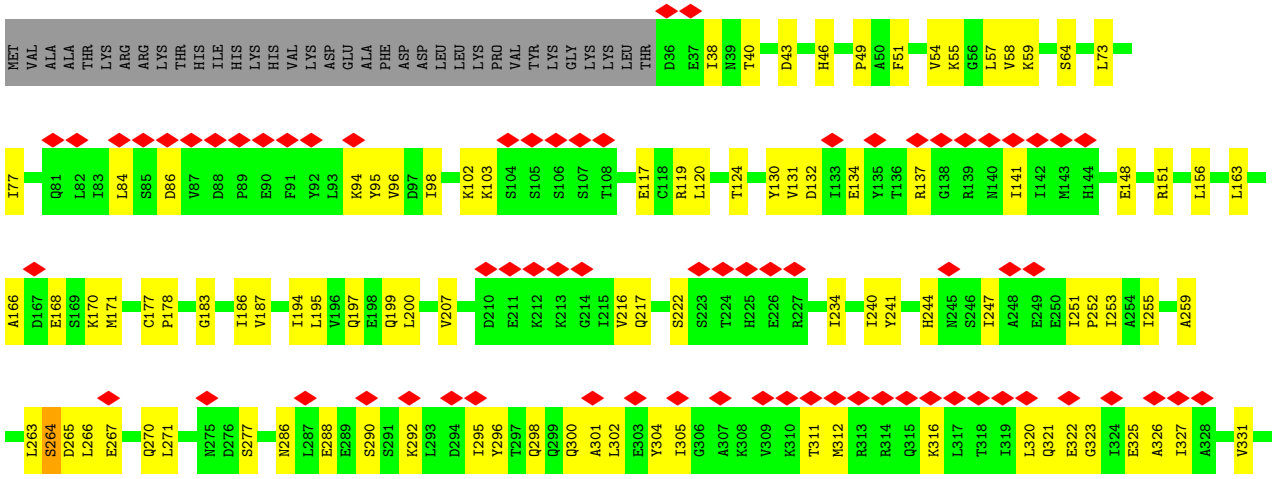
Chain A:

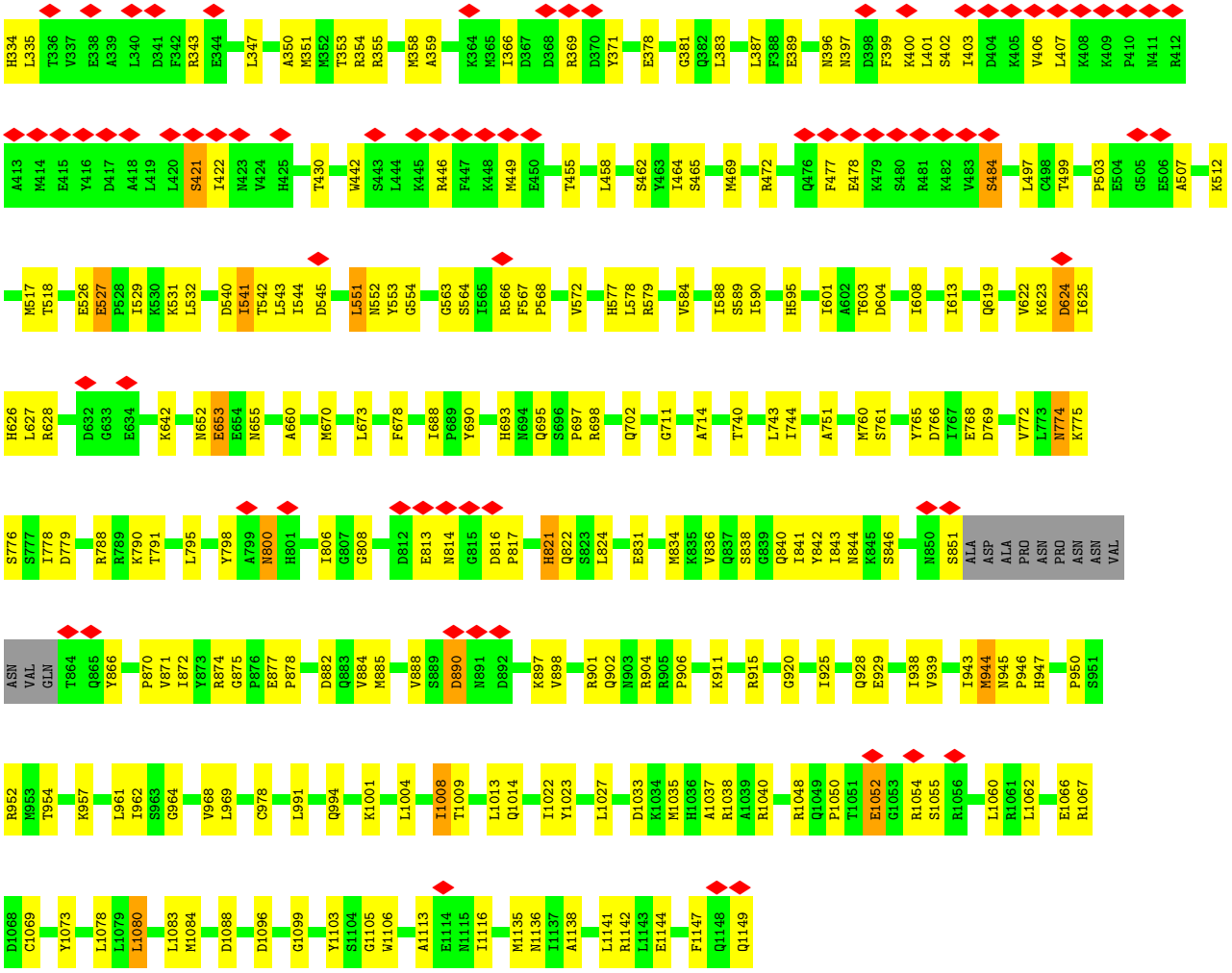




• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

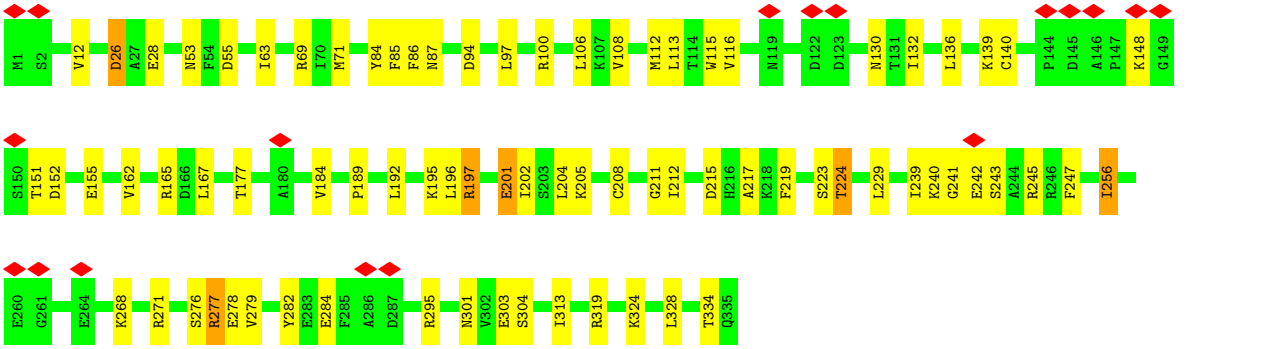
Chain B:





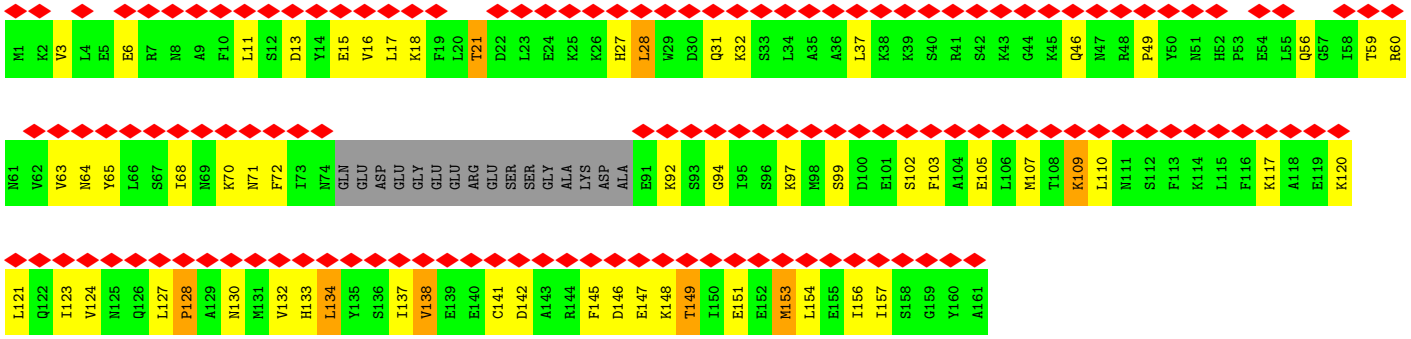
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



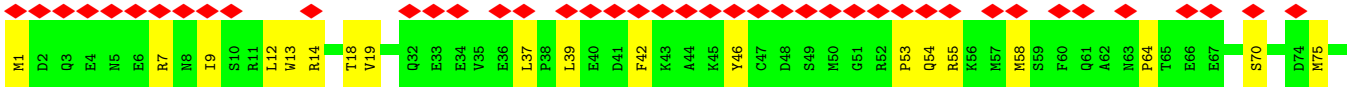
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9

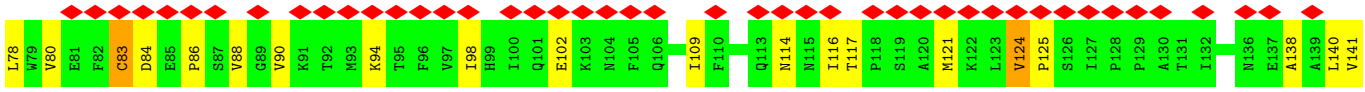
Chain D:

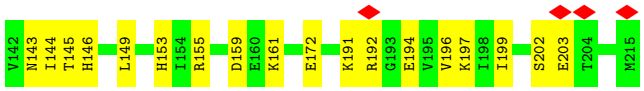


• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:

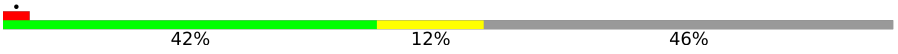






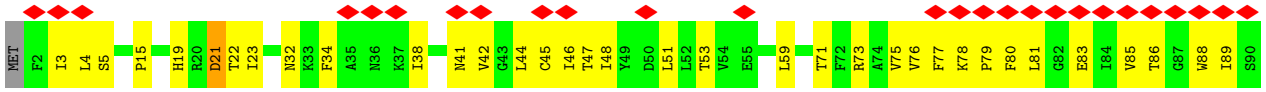
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

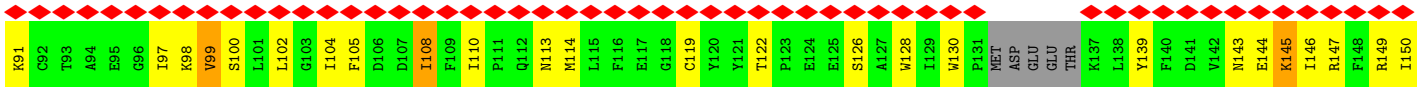
Chain F:

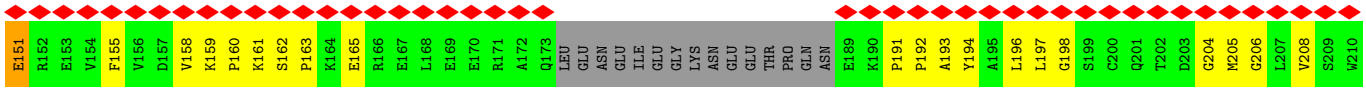


• Molecule 7: DNA-directed RNA polymerase III subunit RPC8

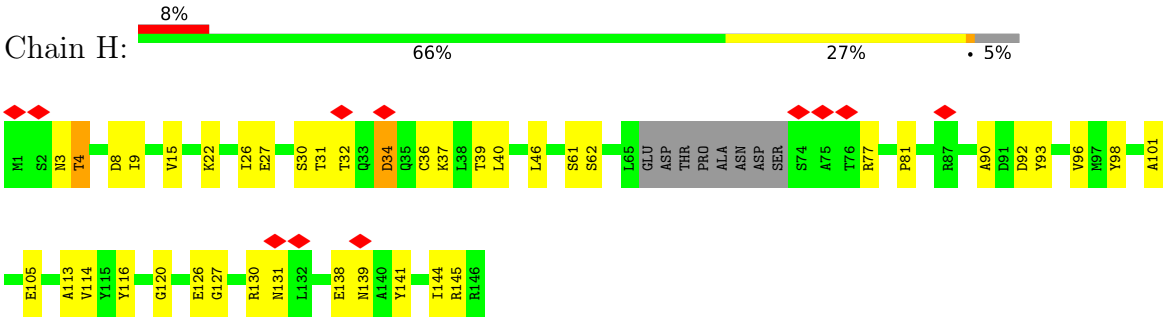
Chain G:



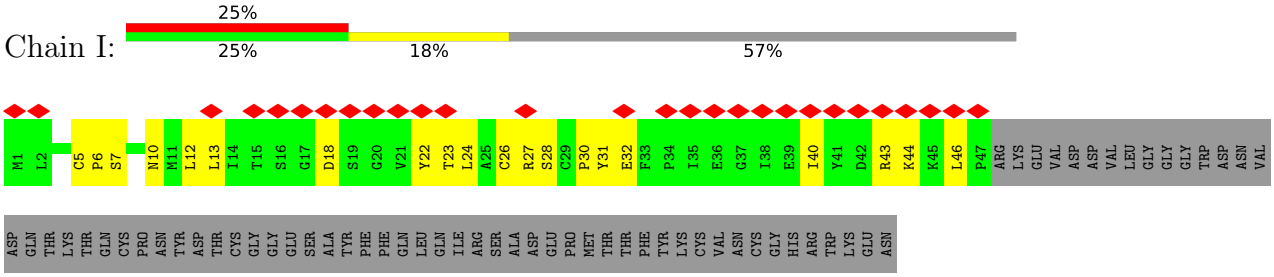




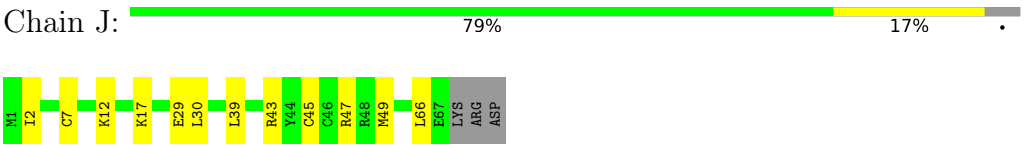
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



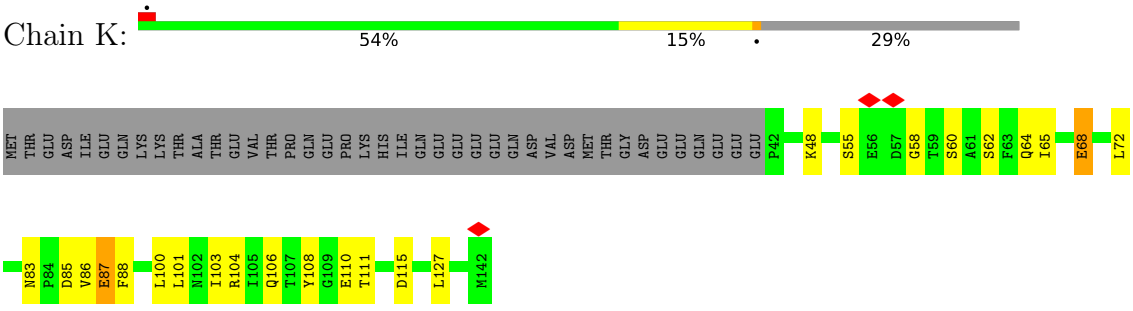
• Molecule 9: DNA-directed RNA polymerase III subunit RPC10



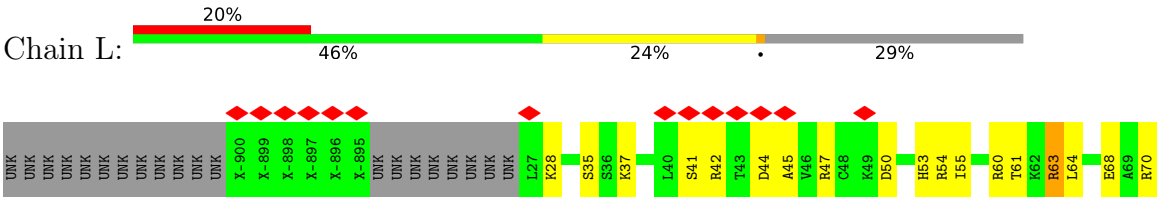
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



• Molecule 11: DNA-directed RNA polymerases I and III subunit RPAC2

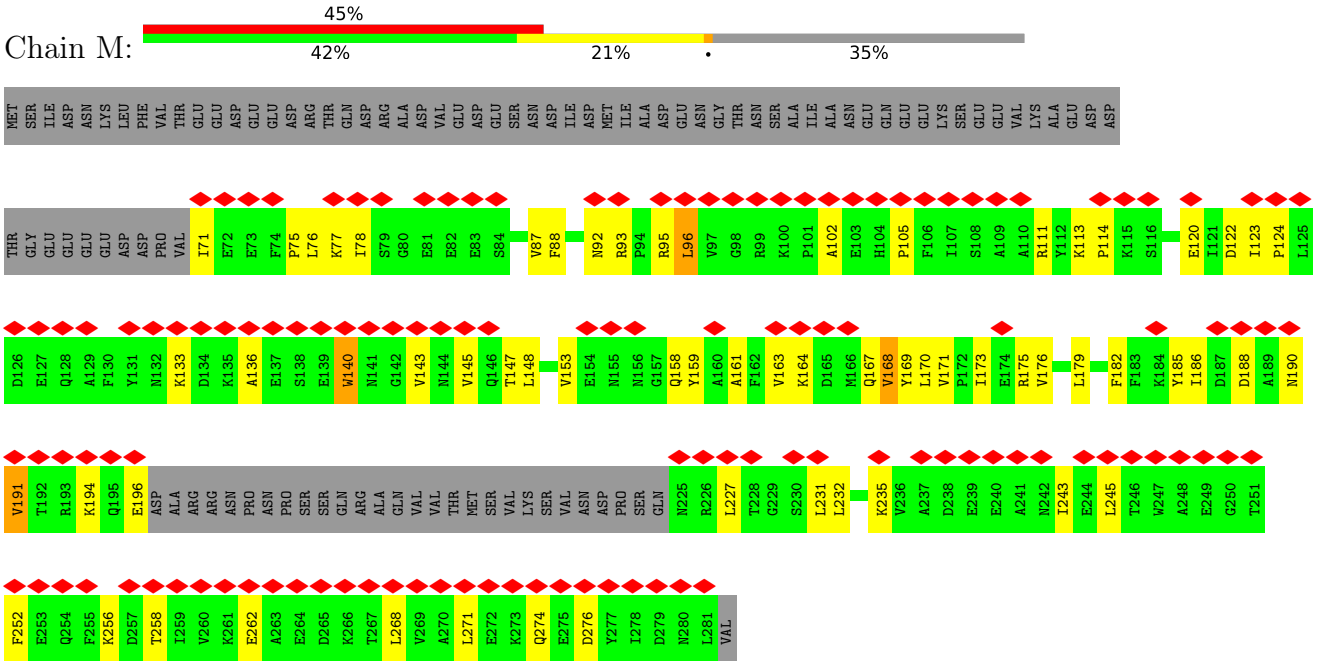


• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



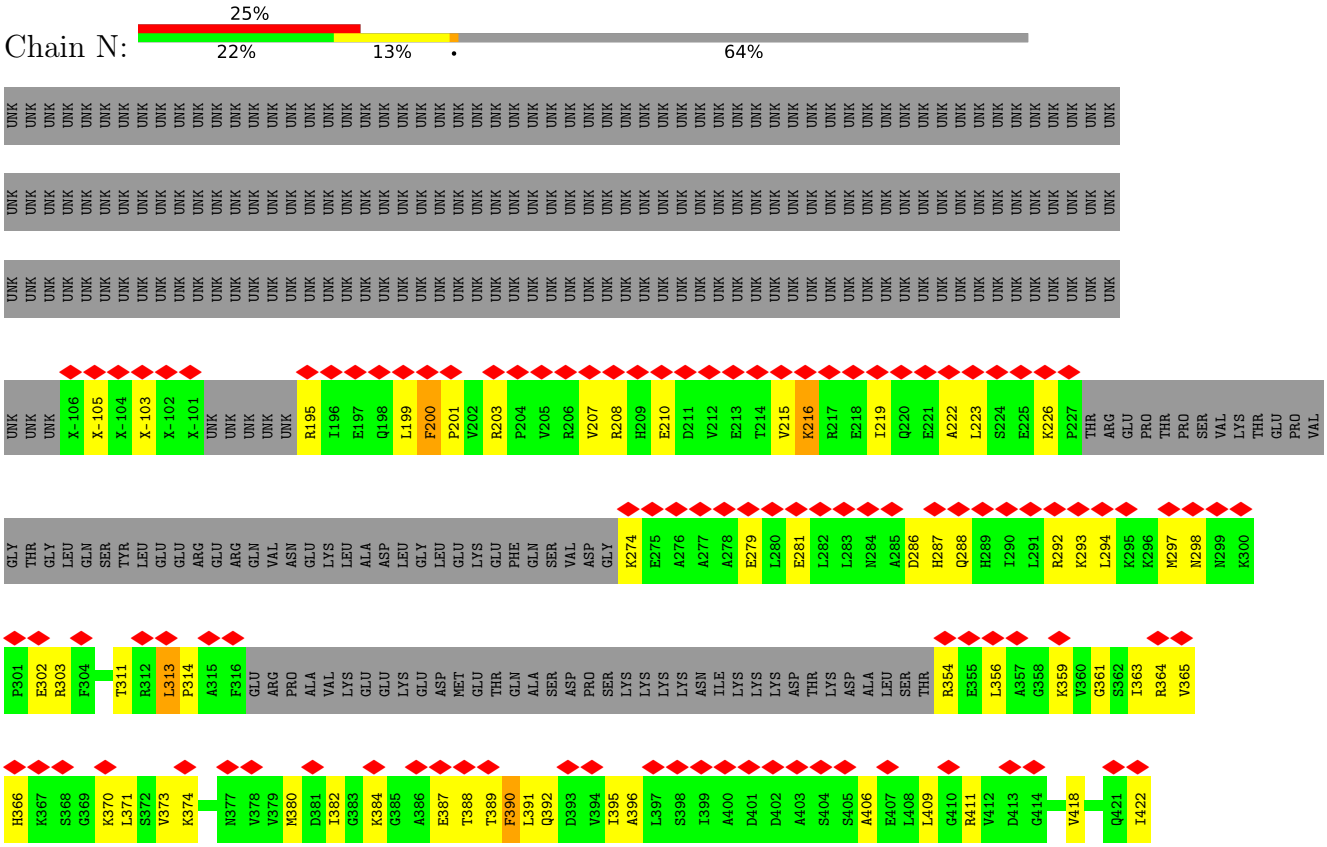
• Molecule 13: DNA-directed RNA polymerase III subunit RPC5

Chain M:



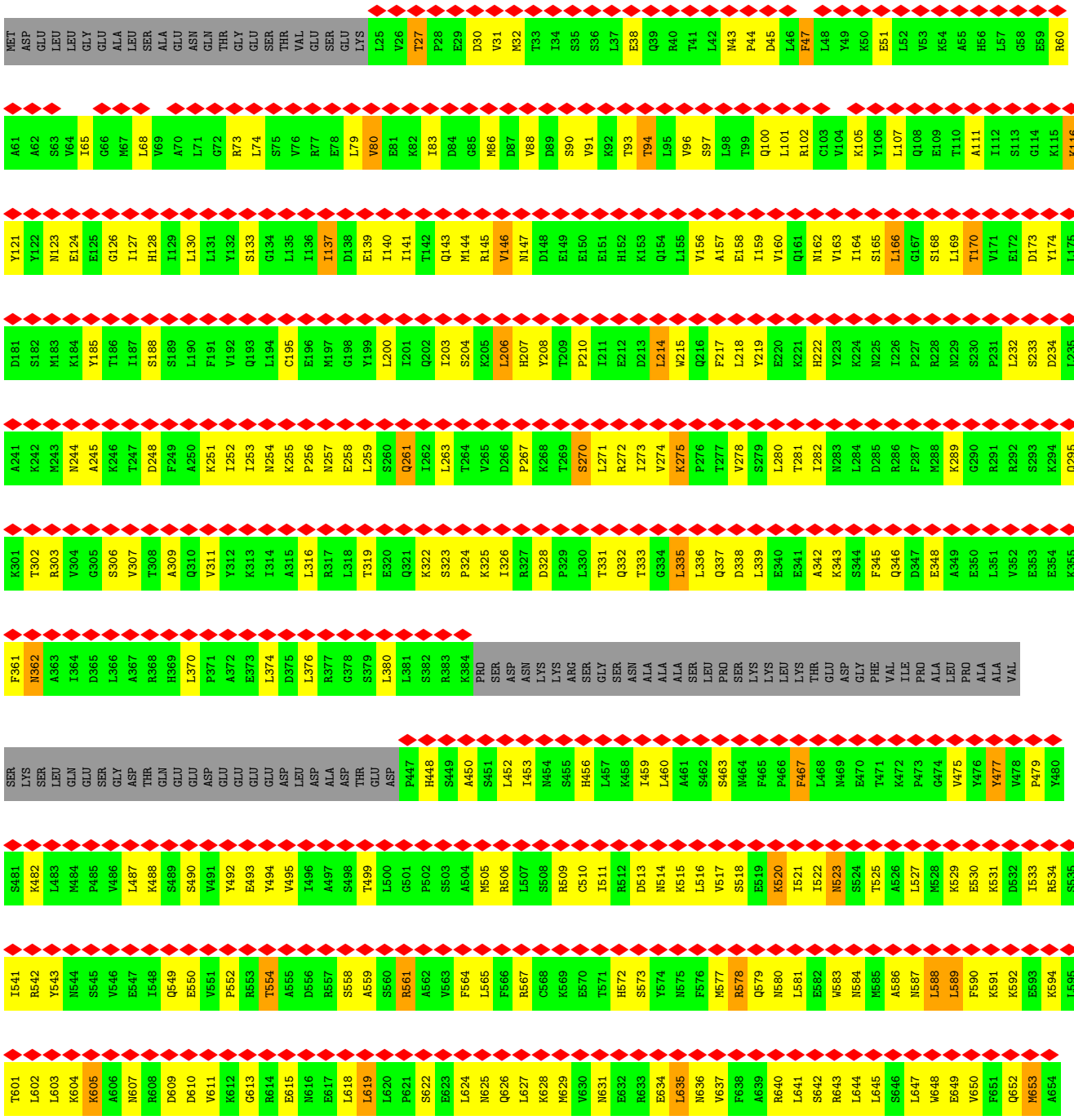
• Molecule 14: DNA-directed RNA polymerase III subunit RPC4

Chain N:

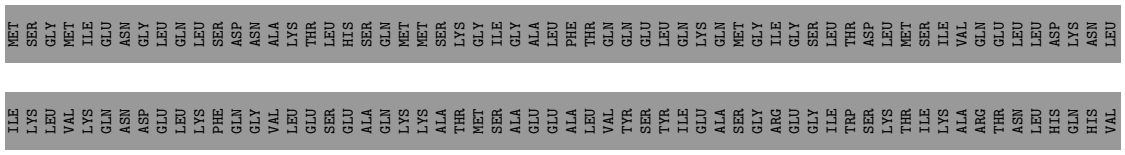


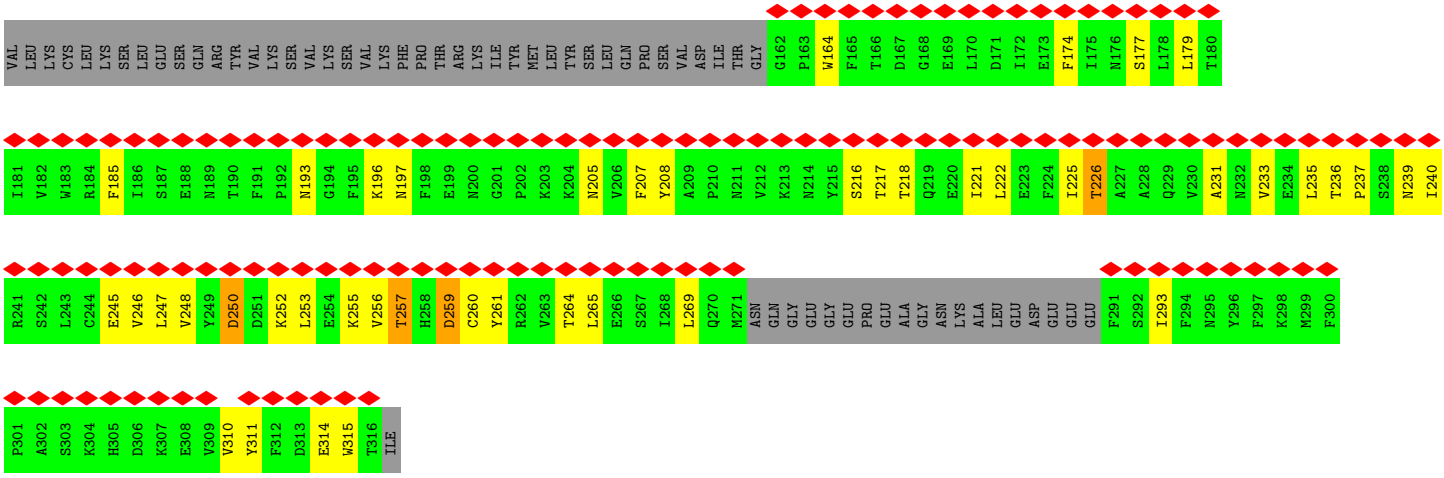
• Molecule 15: DNA-directed RNA polymerase III subunit RPC3

Chain O:



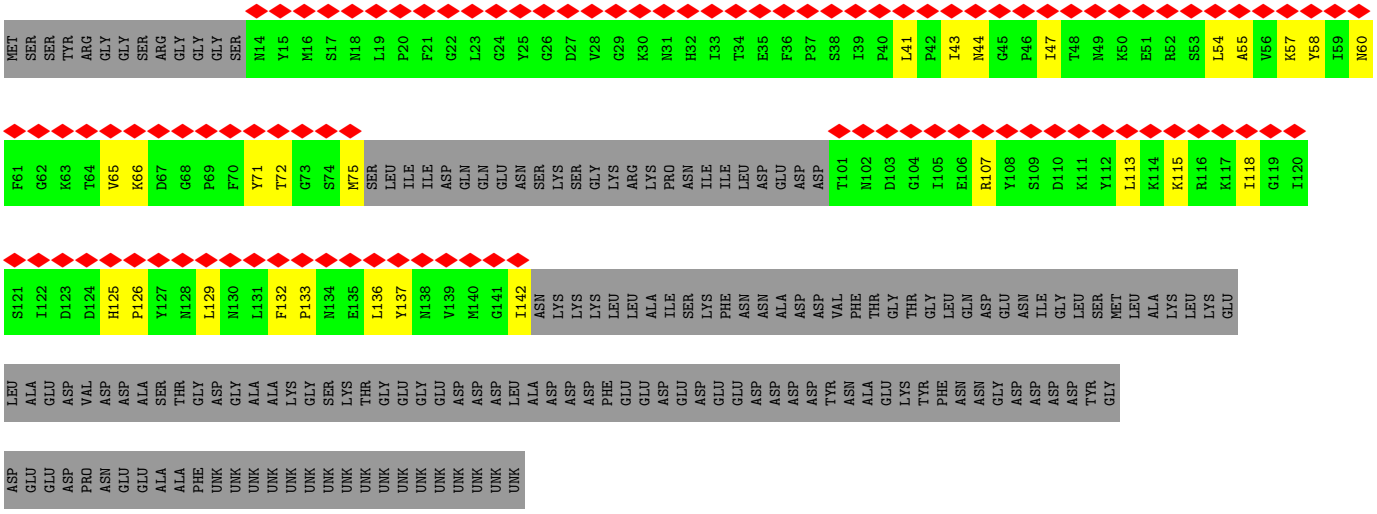
• Molecule 16: DNA-directed RNA polymerase III subunit RPC6





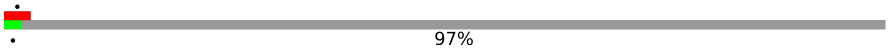
• Molecule 17: DNA-directed RNA polymerase III subunit RPC7

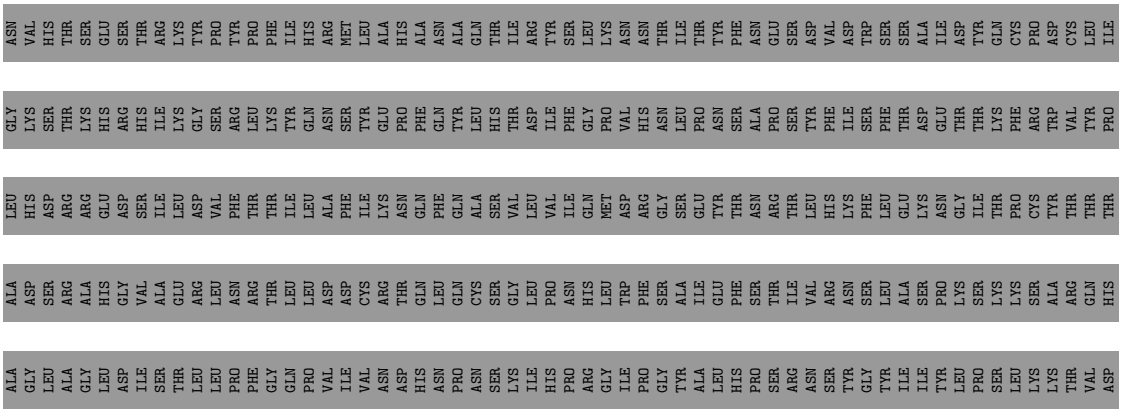
Chain Q:

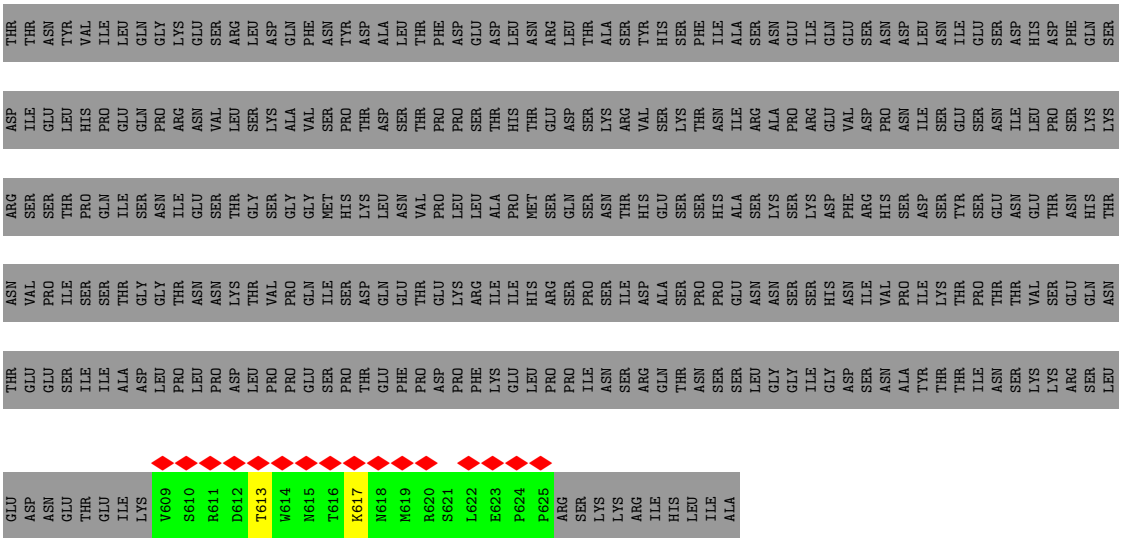


• Molecule 18: Integrase

Chain W:

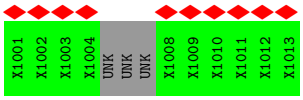






• Molecule 19: Unknown RNA polymerase III chain

Chain X:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	273119	Depositor
Resolution determination method	FSC 0.5 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42.45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.162	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0255	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.34	0/11322	0.53	0/15295
2	B	0.37	0/8853	0.53	0/11940
3	C	0.39	0/2711	0.53	0/3676
4	D	0.27	0/1158	0.48	0/1550
5	E	0.31	0/1795	0.53	0/2416
6	F	0.37	0/683	0.52	0/923
7	G	0.29	0/1583	0.51	0/2146
8	H	0.41	0/1121	0.59	0/1517
9	I	0.30	0/373	0.53	0/504
10	J	0.39	0/558	0.56	0/750
11	K	0.43	0/803	0.54	0/1083
12	L	0.33	0/353	0.60	0/468
13	M	0.29	0/1524	0.49	0/2061
14	N	0.29	0/1152	0.57	0/1546
15	O	0.27	0/4627	0.52	0/6243
16	P	0.26	0/1157	0.46	0/1571
17	Q	0.28	0/850	0.46	0/1148
18	W	0.23	0/144	0.54	0/195
All	All	0.34	0/40767	0.53	0/55032

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1211	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11123	0	11245	298	0
2	B	8701	0	8822	240	0
3	C	2655	0	2628	55	0
4	D	1140	0	1112	42	0
5	E	1759	0	1788	28	0
6	F	671	0	692	12	0
7	G	1544	0	1540	64	0
8	H	1103	0	1079	31	0
9	I	365	0	360	16	0
10	J	549	0	559	10	0
11	K	792	0	790	18	0
12	L	381	0	383	15	0
13	M	1492	0	1456	43	0
14	N	1169	0	1208	41	0
15	O	4558	0	4735	195	0
16	P	1126	0	1079	34	0
17	Q	829	0	819	22	0
18	W	141	0	137	0	0
19	X	50	0	16	0	0
20	A	2	0	0	0	0
20	B	1	0	0	0	0
20	I	1	0	0	0	0
20	J	1	0	0	0	0
20	L	1	0	0	0	0
21	A	1	0	0	0	0
22	A	1	0	0	0	0
All	All	40156	0	40448	1017	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 13.

The worst 5 of 1017 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)
15:O:203:ILE:HD11	15:O:208:TYR:CE2	1.97	0.99
1:A:890:MET:O	1:A:894:GLU:HB2	1.70	0.90
15:O:203:ILE:HD11	15:O:208:TYR:HE2	1.33	0.88
1:A:1214:LYS:HA	1:A:1218:GLN:HA	1.53	0.88
2:B:1105:GLY:HA2	2:B:1116:ILE:HG21	1.57	0.85

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	1411/1460 (97%)	1316 (93%)	95 (7%)	0	100	100
2	B	1098/1149 (96%)	1030 (94%)	68 (6%)	0	100	100
3	C	333/335 (99%)	314 (94%)	19 (6%)	0	100	100
4	D	141/161 (88%)	122 (86%)	16 (11%)	3 (2%)	7	12
5	E	213/215 (99%)	203 (95%)	10 (5%)	0	100	100
6	F	81/155 (52%)	78 (96%)	3 (4%)	0	100	100
7	G	185/212 (87%)	160 (86%)	25 (14%)	0	100	100
8	H	134/146 (92%)	118 (88%)	16 (12%)	0	100	100
9	I	45/110 (41%)	41 (91%)	4 (9%)	0	100	100
10	J	65/70 (93%)	62 (95%)	3 (5%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	42/70 (60%)	37 (88%)	5 (12%)	0	100	100
13	M	179/282 (64%)	165 (92%)	14 (8%)	0	100	100
14	N	139/422 (33%)	130 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	O	564/654 (86%)	531 (94%)	33 (6%)	0	100	100
16	P	132/317 (42%)	122 (92%)	10 (8%)	0	100	100
17	Q	100/268 (37%)	87 (87%)	13 (13%)	0	100	100
18	W	15/635 (2%)	14 (93%)	1 (7%)	0	100	100
All	All	4976/6803 (73%)	4622 (93%)	351 (7%)	3 (0%)	54	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	37	LEU
4	D	46	GLN
4	D	49	PRO

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	1230/1257 (98%)	1147 (93%)	83 (7%)	16	28
2	B	965/1006 (96%)	925 (96%)	40 (4%)	30	50
3	C	296/296 (100%)	280 (95%)	16 (5%)	22	38
4	D	123/145 (85%)	108 (88%)	15 (12%)	5	7
5	E	197/197 (100%)	184 (93%)	13 (7%)	16	29
6	F	73/137 (53%)	72 (99%)	1 (1%)	67	79
7	G	170/190 (90%)	157 (92%)	13 (8%)	13	23
8	H	121/128 (94%)	118 (98%)	3 (2%)	47	67
9	I	43/98 (44%)	40 (93%)	3 (7%)	15	26
10	J	62/65 (95%)	61 (98%)	1 (2%)	62	77
11	K	91/130 (70%)	86 (94%)	5 (6%)	21	37
12	L	39/39 (100%)	36 (92%)	3 (8%)	13	22
13	M	159/249 (64%)	150 (94%)	9 (6%)	20	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	N	125/200 (62%)	110 (88%)	15 (12%)	5 8
15	O	521/593 (88%)	474 (91%)	47 (9%)	9 16
16	P	126/285 (44%)	120 (95%)	6 (5%)	25 44
17	Q	92/212 (43%)	88 (96%)	4 (4%)	29 48
18	W	17/586 (3%)	15 (88%)	2 (12%)	5 8
All	All	4450/5813 (77%)	4171 (94%)	279 (6%)	21 31

5 of 279 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	O	166	LEU
15	O	237	LYS
15	O	589	LEU
2	B	464	ILE
2	B	421	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	64	ASN
15	O	161	GLN
10	J	53	HIS
13	M	234	HIS
15	O	599	ASN

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 7 ligands modelled in this entry, 7 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.

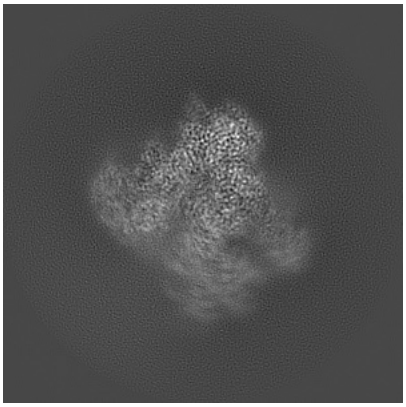
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14470. These allow visual inspection of the internal detail of the map and identification of artifacts.

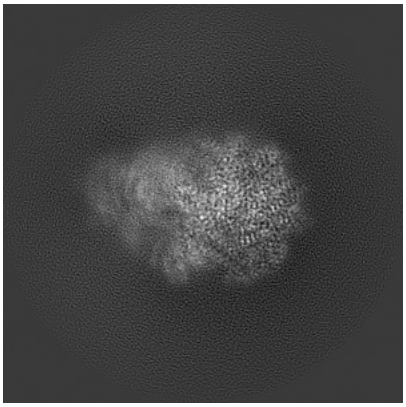
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

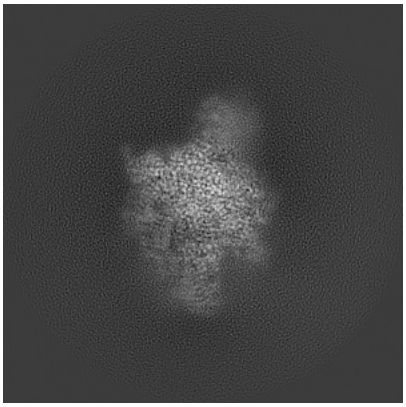
6.1.1 Primary map



X



Y

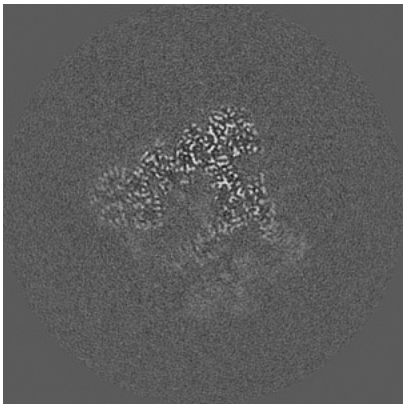


Z

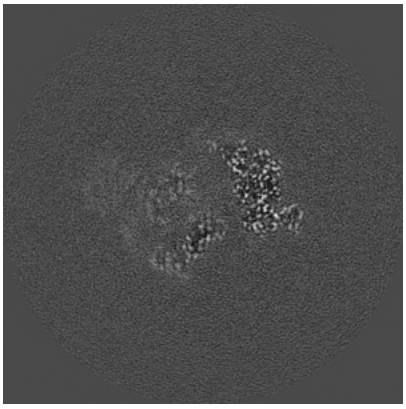
The images above show the map projected in three orthogonal directions.

6.2 Central slices

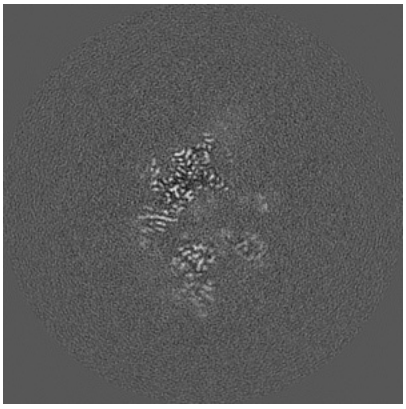
6.2.1 Primary map



X Index: 150



Y Index: 150

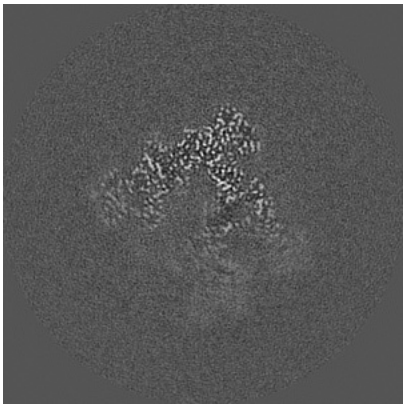


Z Index: 150

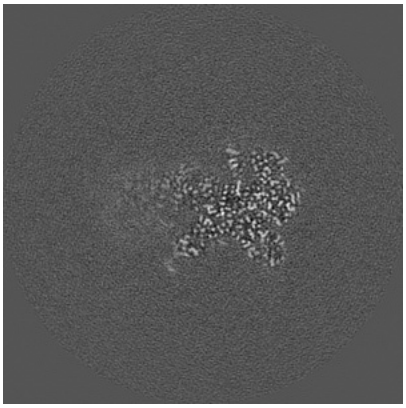
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

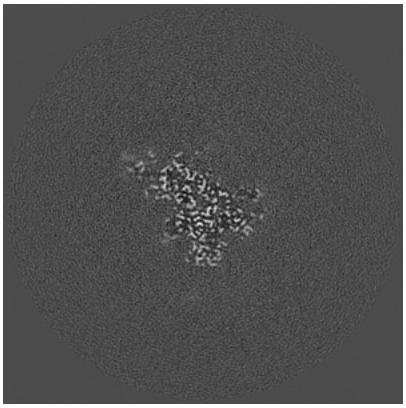
6.3.1 Primary map



X Index: 154



Y Index: 163

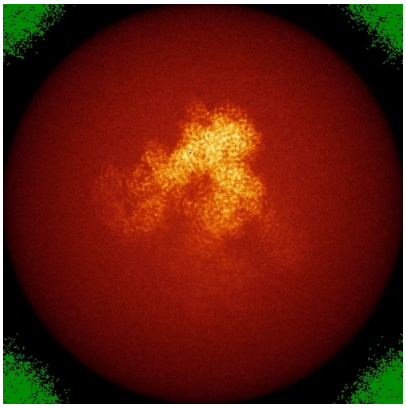


Z Index: 184

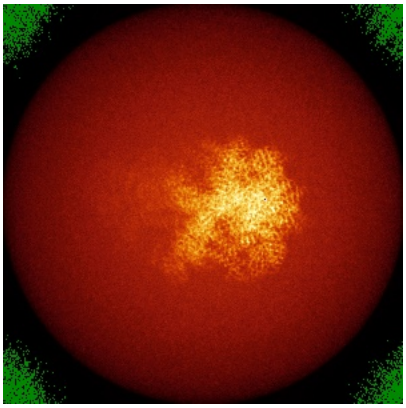
The images above show the largest variance slices of the map in three orthogonal directions.

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

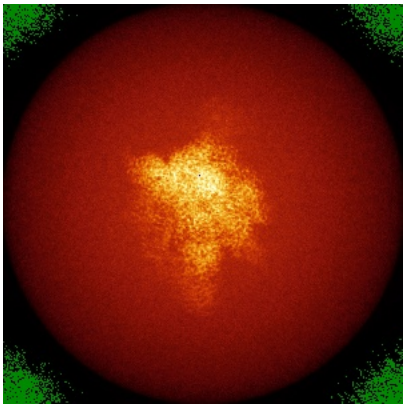
6.4.1 Primary map



X



Y

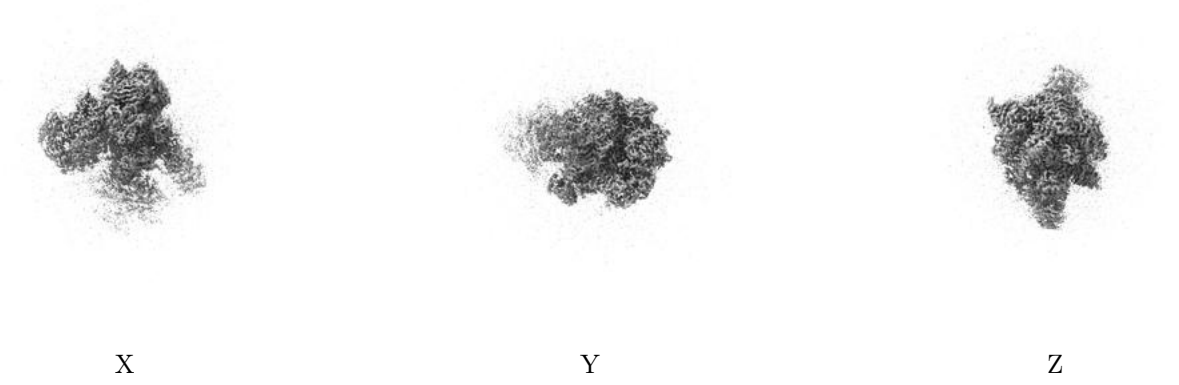


Z

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 0.0255. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

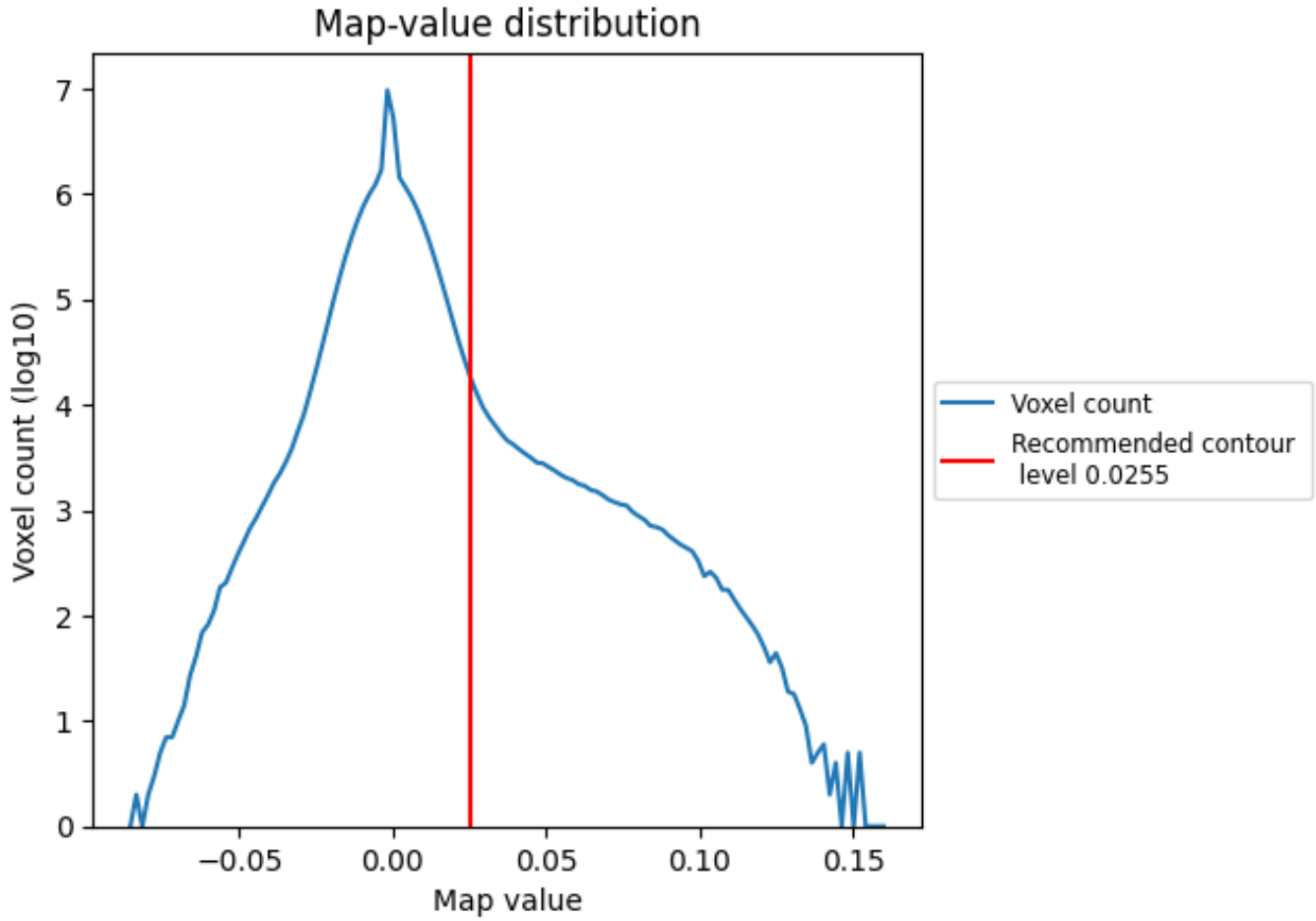
6.6 Mask visualisation (i)

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

7 Map analysis

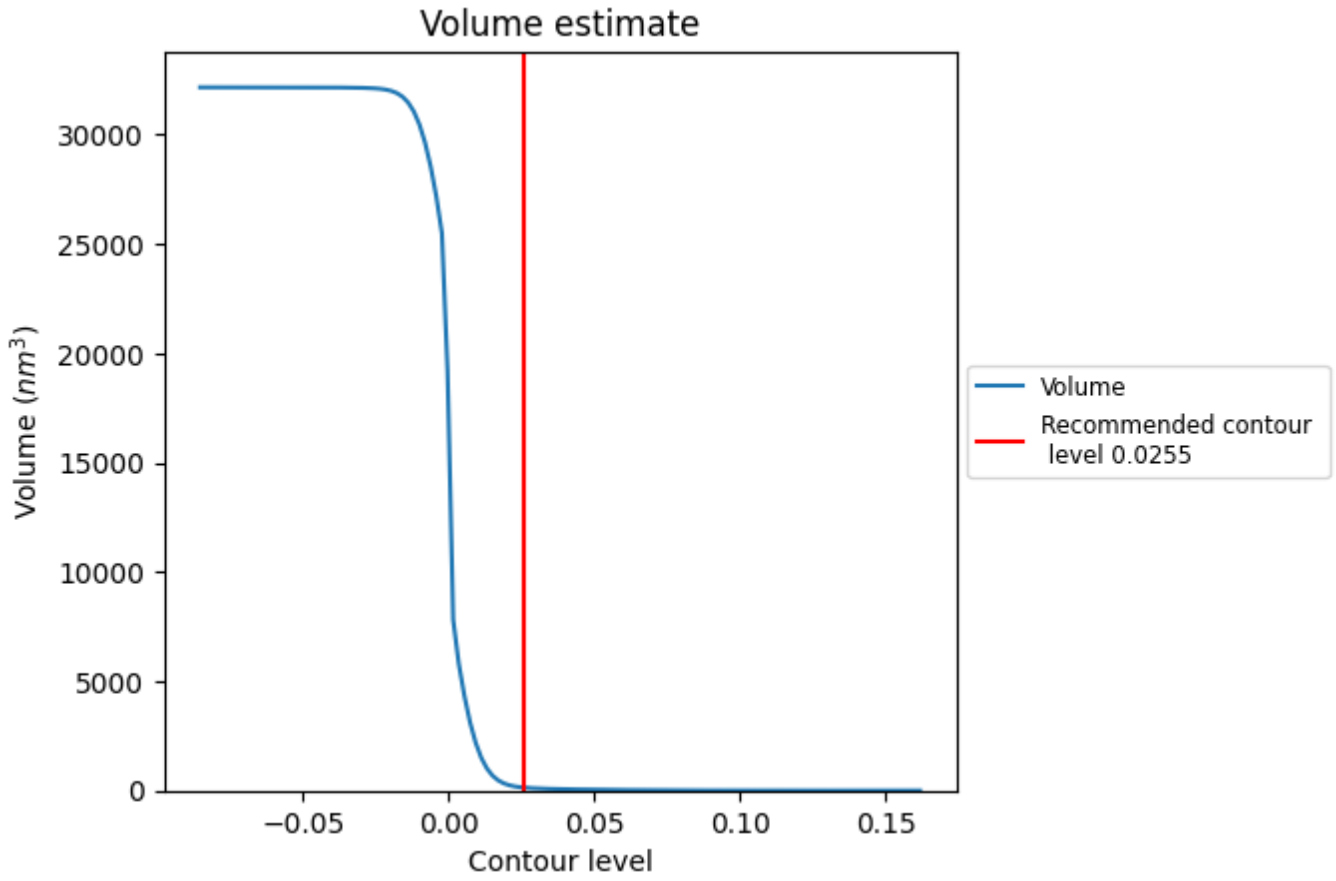
This section contains the results of statistical analysis of the map.

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.

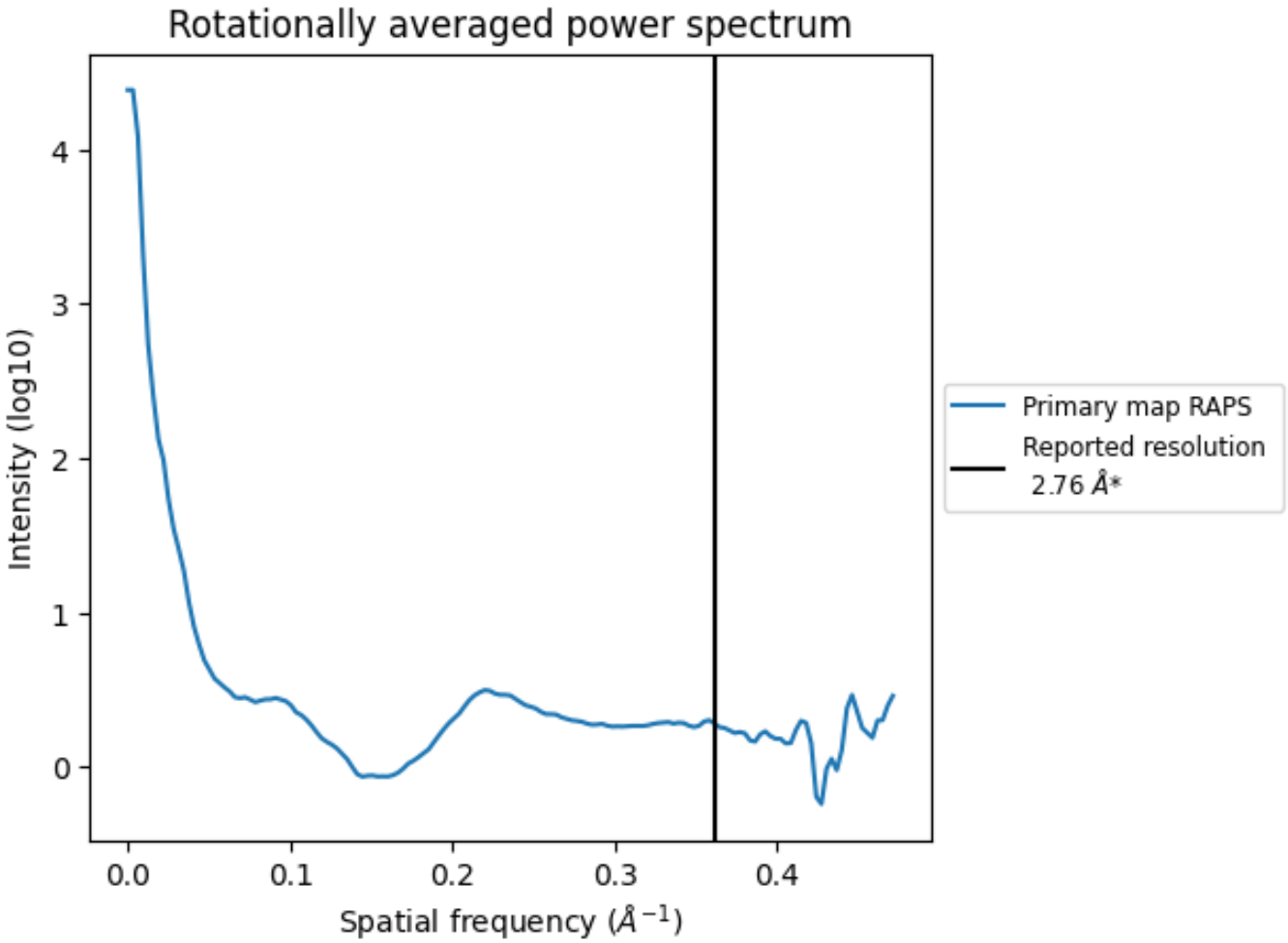
7.2 Volume estimate (i)



The volume at the recommended contour level is 141 nm^3; this corresponds to an approximate mass of 127 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)

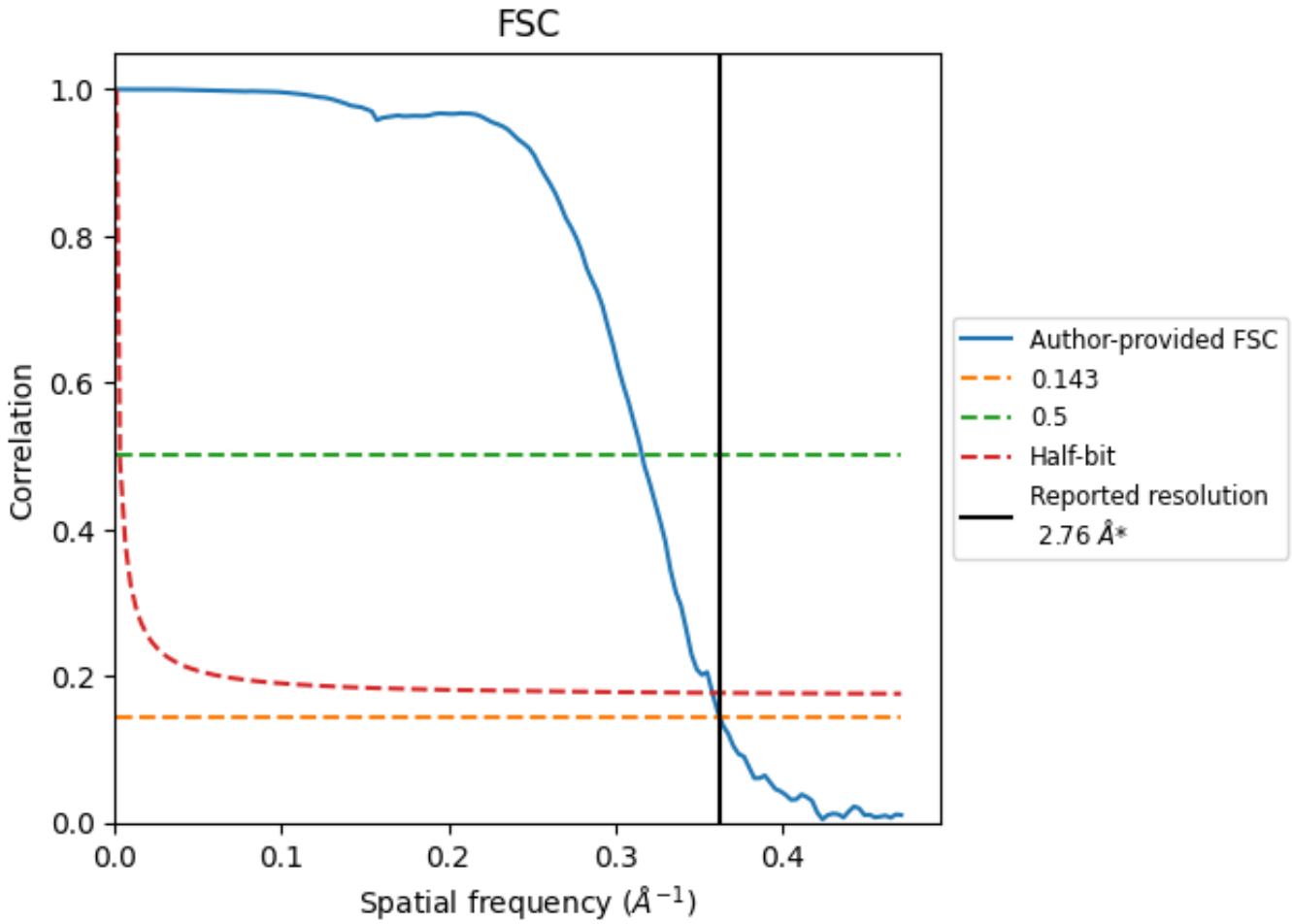


*Reported resolution corresponds to spatial frequency of 0.362 Å^{-1}

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 0.362 Å^{-1}

8.2 Resolution estimates (i)

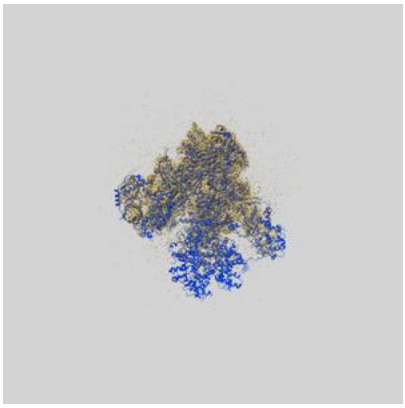
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	2.76	-
Author-provided FSC curve	2.75	3.16	2.79
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.5 CUT-OFF 3.16 differs from the reported value 2.76 by more than 10 %

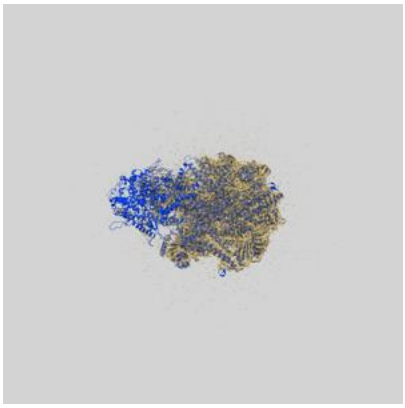
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14470 and PDB model 7Z31. Per-residue inclusion information can be found in section 3 on page 8.

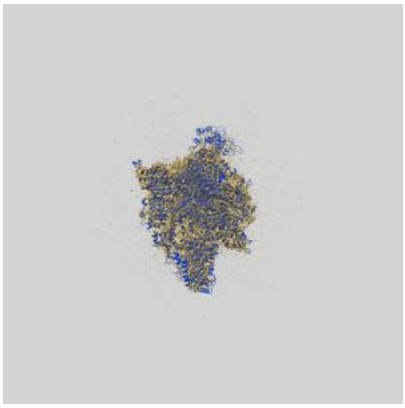
9.1 Map-model overlay



X



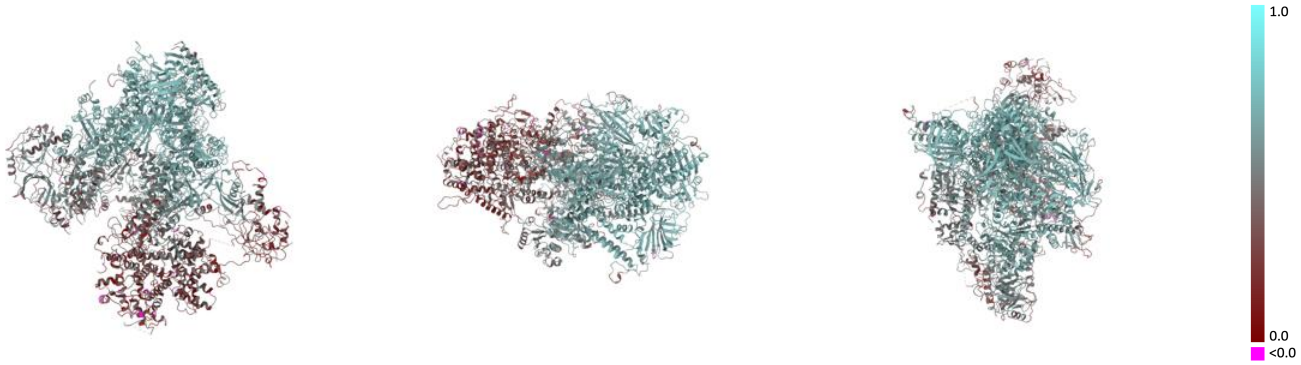
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0255 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.

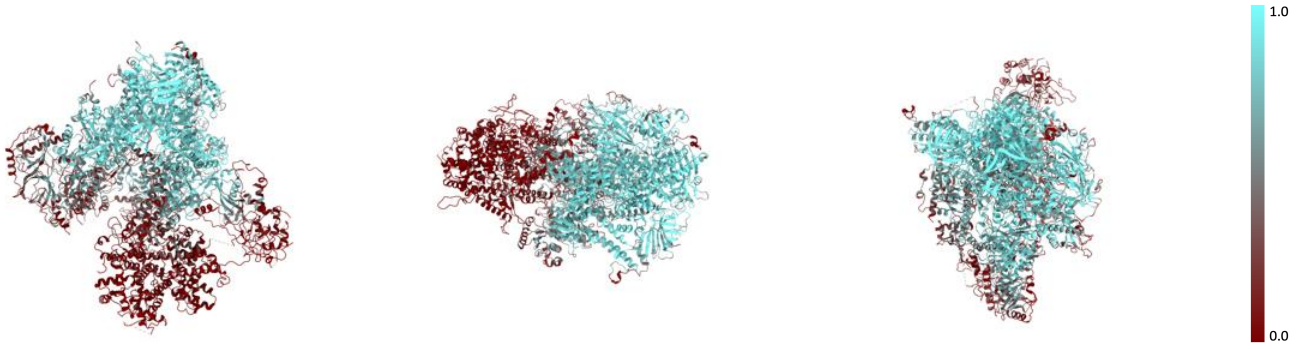
9.2 Q-score mapped to coordinate model (i)



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.

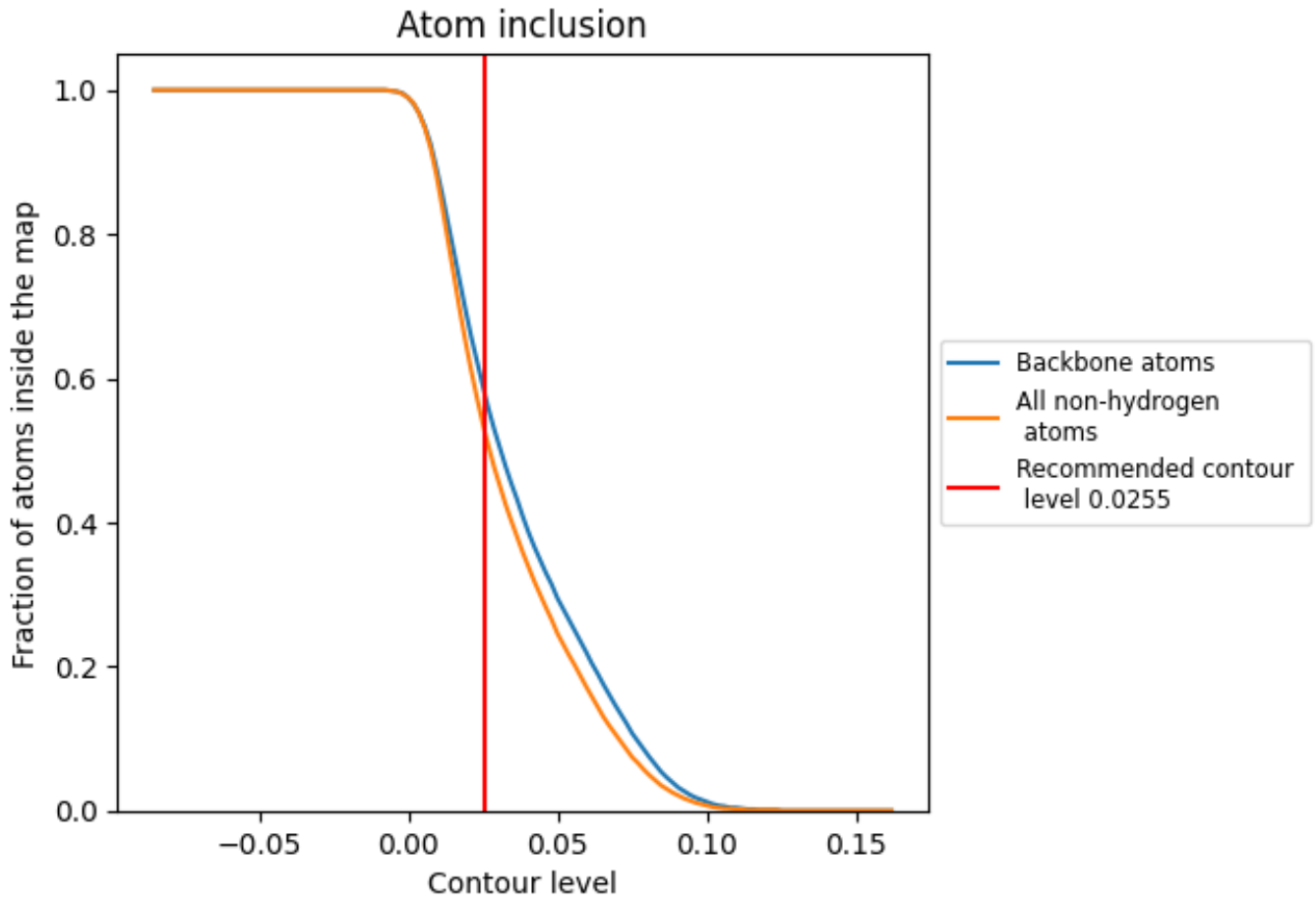
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0255).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 52% 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 (0.0255) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5250	0.5190
A	0.6220	0.5570
B	0.7490	0.6080
C	0.8440	0.6420
D	0.0950	0.3100
E	0.5030	0.5200
F	0.8450	0.6480
G	0.2910	0.4220
H	0.7980	0.6130
I	0.3870	0.4920
J	0.9040	0.6660
K	0.8580	0.6460
L	0.6450	0.5820
M	0.2970	0.4650
N	0.2530	0.4420
O	0.0530	0.3300
P	0.0280	0.2650
Q	0.0260	0.2700
W	0.0960	0.4330
X	0.1000	0.5310