wwPDB EM Validation Summary Report

Apr 10, 2025 – 01:40 PM JST

PDB ID	:	9K3U / pdb_00009k3u
EMDB ID	:	EMD-62029
Title	:	Human RNA Polymerase III de novo transcribing complex 5 (TC5)
Authors	:	Wang, Q.; Ren, Y.; Jin, Q.; Chen, X.; Xu, Y.
Deposited on	:	2024-10-20
Resolution	:	3.00 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

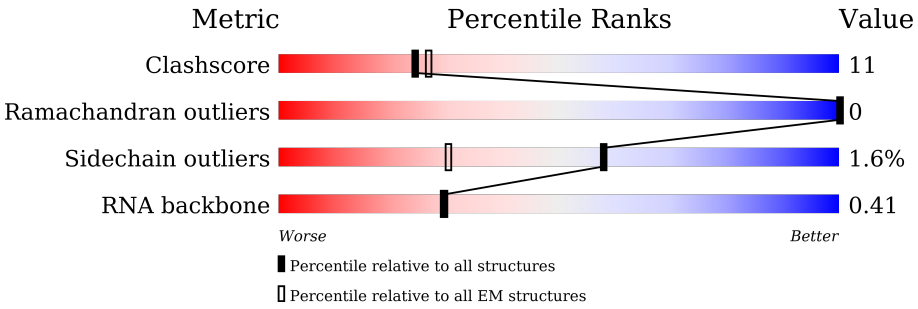
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1	368	37% 28% 11% · 60%
2	3	411	78% 75% 14% · 9%
3	4	1469	10% 14% · 83%
4	A	1390	84% 15% ·
5	B	1133	82% 14% ·
6	C	346	82% 17% ·
7	D	148	67% 16% 18%

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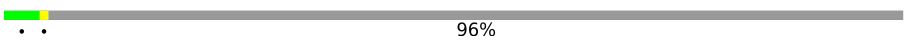
Mol	Chain	Length	Quality of chain
8	E	210	
9	F	127	
10	G	204	
11	H	150	
12	I	108	
13	J	67	
14	K	133	
15	L	58	
16	M	708	
17	N	398	
18	O	534	
19	P	316	
20	Q	223	
21	U	339	
22	V	419	
23	W	2624	
24	X	97	
25	Y	97	
26	Z	4	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	SF4	P	401	-	-	X	-
30	GTP	Z	101	-	-	X	-

2 Entry composition (i)

There are 30 unique types of molecules in this entry. The entry contains 56785 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 snRNA-activating protein complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	146	1233	804	212	209	8	0	0

- Molecule 2 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3	374	3038	1925	521	571	21	0	0

- Molecule 3 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	247	2066	1295	378	388	5	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase III subunit RPC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	1378	10814	6850	1886	2005	73	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase III subunit RPC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	B	1097	8680	5499	1516	1597	68	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I and III subunit RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	C	343	2736	1723	488	514	11	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase III subunit RPC9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	122	Total	C	N	O	S	0	0
			985	614	172	196	3		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	209	Total	C	N	O	S	0	0
			1715	1083	300	324	8		

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	76	Total	C	N	O	S	0	0
			610	392	103	110	5		

- Molecule 10 is a protein called DNA-directed RNA polymerase III subunit RPC8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	166	Total	C	N	O	S	0	0
			1337	876	211	245	5		

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	148	Total	C	N	O	S	0	0
			1186	750	194	237	5		

- Molecule 12 is a protein called DNA-directed RNA polymerase III subunit RPC10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	54	Total	C	N	O	S	0	0
			426	267	79	74	6		

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	65	Total	C	N	O	S	0	0
			512	331	87	88	6		

- Molecule 14 is a protein called DNA-directed RNA polymerases I and III subunit RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	103	Total	C	N	O	S	0	0
			822	513	145	157	7		

- Molecule 15 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

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

- Molecule 16 is a protein called DNA-directed RNA polymerase III subunit RPC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	422	Total	C	N	O	S	0	0
			3382	2138	588	636	20		

- Molecule 17 is a protein called DNA-directed RNA polymerase III subunit RPC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	146	Total	C	N	O	S	0	0
			1128	710	191	221	6		

- Molecule 18 is a protein called DNA-directed RNA polymerase III subunit RPC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	512	Total	C	N	O	S	0	0
			4075	2565	712	774	24		

- Molecule 19 is a protein called DNA-directed RNA polymerase III subunit RPC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	303	Total	C	N	O	S	0	0
			2403	1516	411	460	16		

- Molecule 20 is a protein called DNA-directed RNA polymerase III subunit RPC7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Q	87	Total	C	N	O	S	0	0
			754	488	126	134	6		

- Molecule 21 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	178	Total	C	N	O	S	1	0
			1411	915	246	243	7		

- Molecule 22 is a protein called Transcription factor IIIB 50 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	361	Total	C	N	O	S	1	0
			2853	1792	507	531	23		

- Molecule 23 is a protein called Transcription factor TFIIIB component B" homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			943	606	163	170	4		

- Molecule 24 is a DNA chain called DNA (97-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	77	Total	C	N	O	P	0	0
			1577	757	275	468	77		

- Molecule 25 is a DNA chain called DNA (97-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	77	Total	C	N	O	P	0	0
			1580	756	291	456	77		

- Molecule 26 is a RNA chain called RNA (5'-R(P*UP*GP*CP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	4	Total	C	N	O	P	0	0
			83	37	12	30	4		

- Molecule 27 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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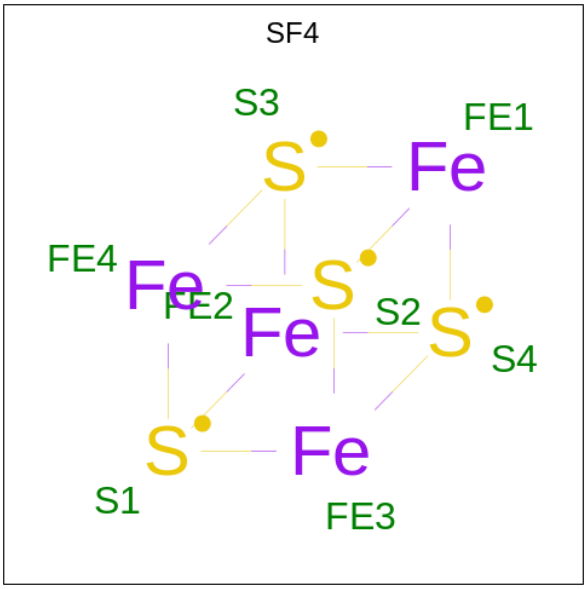
Mol	Chain	Residues	Atoms	AltConf
27	J	1	Total Zn 1 1	0
27	L	1	Total Zn 1 1	0
27	V	1	Total Zn 1 1	0

- Molecule 28 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

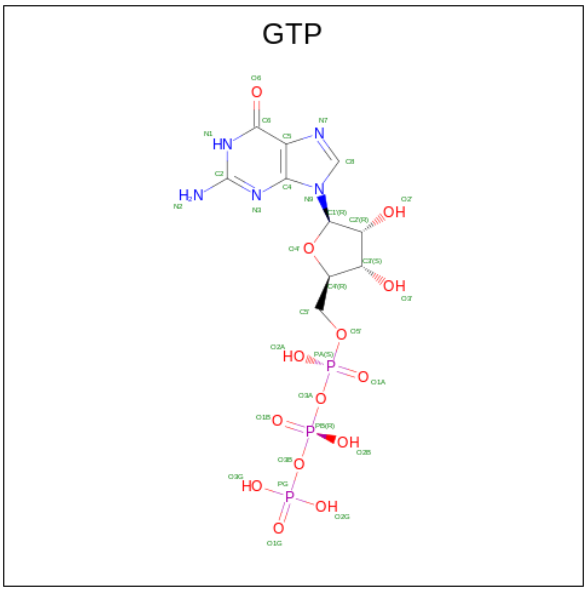
Mol	Chain	Residues	Atoms	AltConf
28	A	1	Total Mg 1 1	0

- Molecule 29 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
29	P	1	Total Fe S 8 4 4	0

- Molecule 30 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



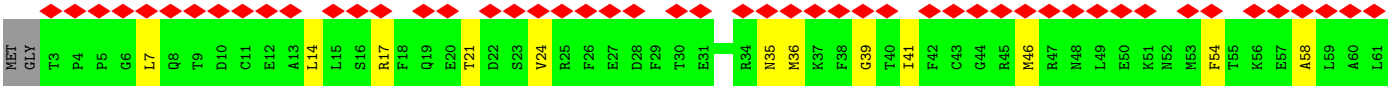
Mol	Chain	Residues	Atoms					AltConf
30	Z	1	Total	C	N	O	P	0
			32	10	5	14	3	

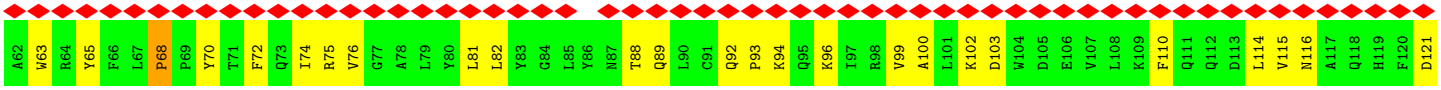
3 Residue-property plots (i)

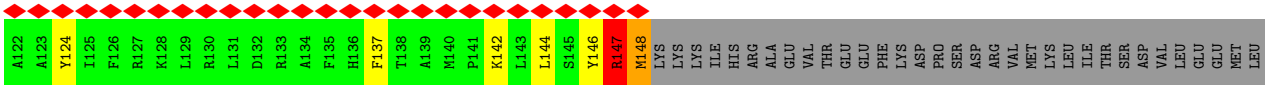
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: snRNA-activating protein complex subunit 1

Chain 1:

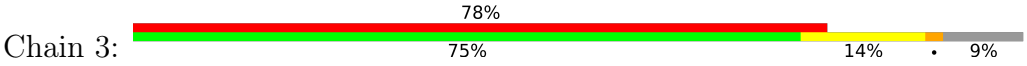


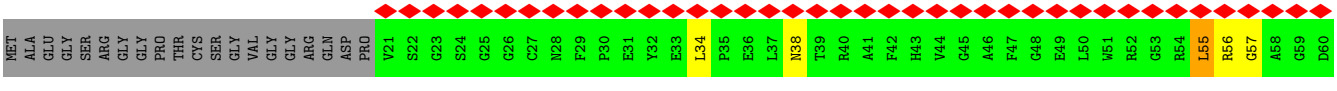


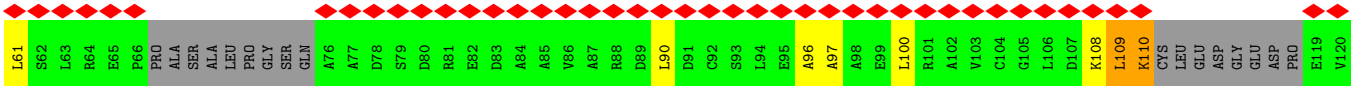


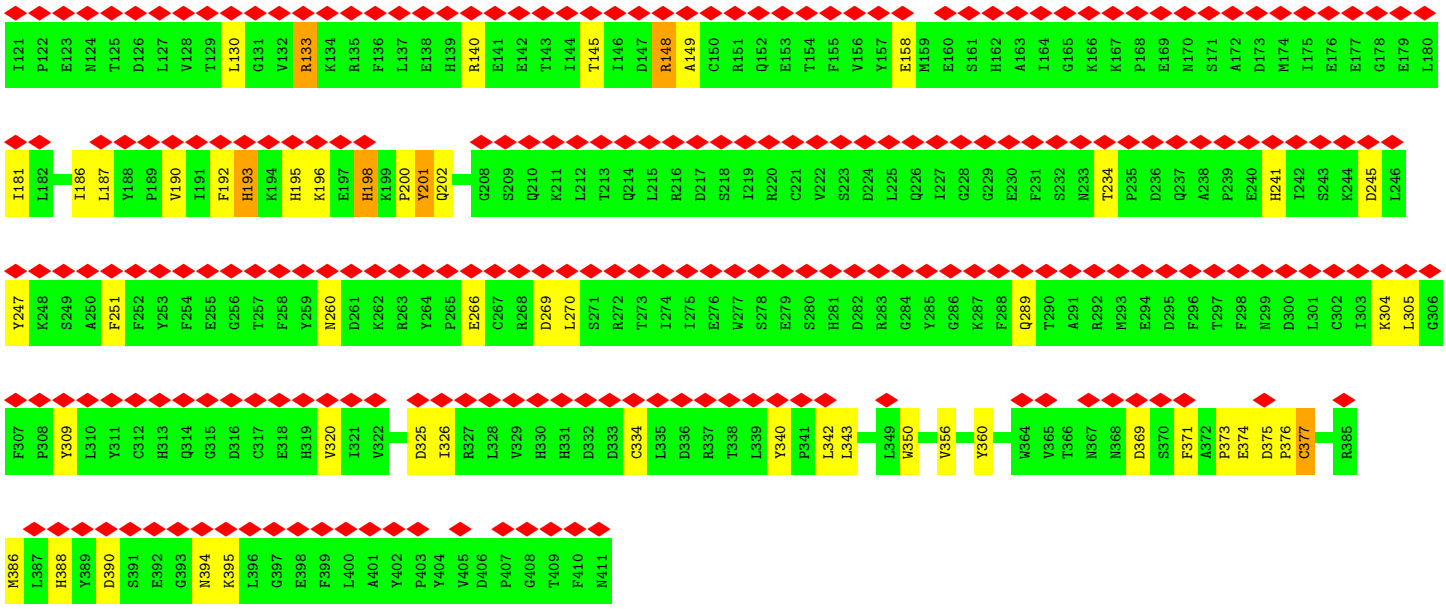
• Molecule 2: snRNA-activating protein complex subunit 3

Chain 3:



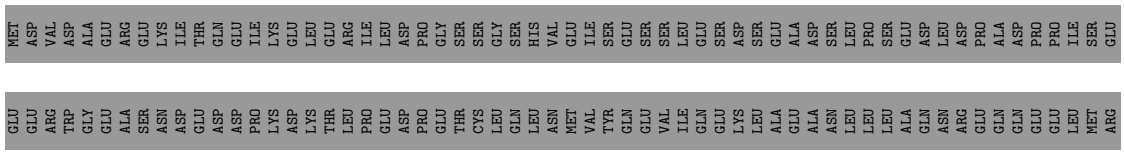


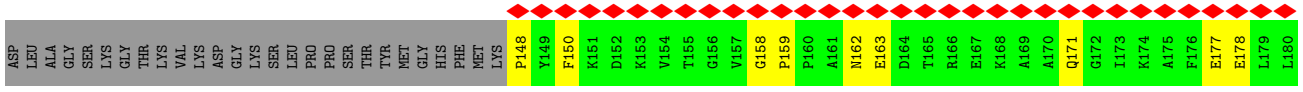


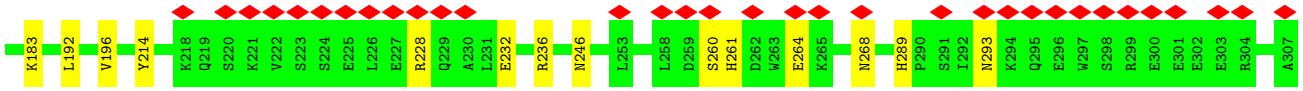


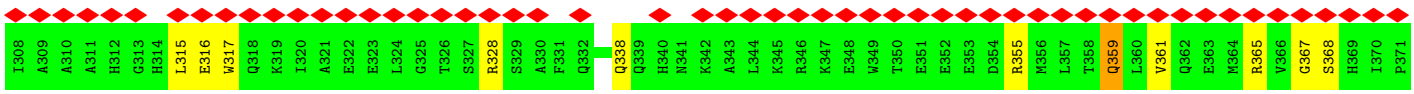
• Molecule 3: snRNA-activating protein complex subunit 4

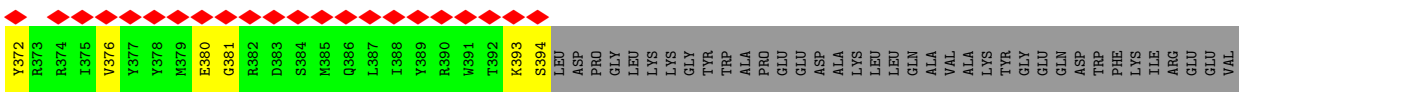
Chain 4:

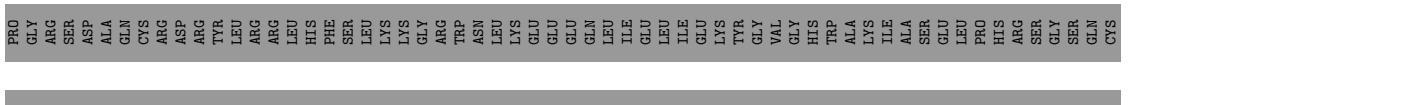


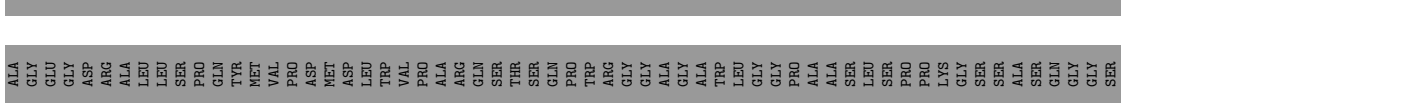


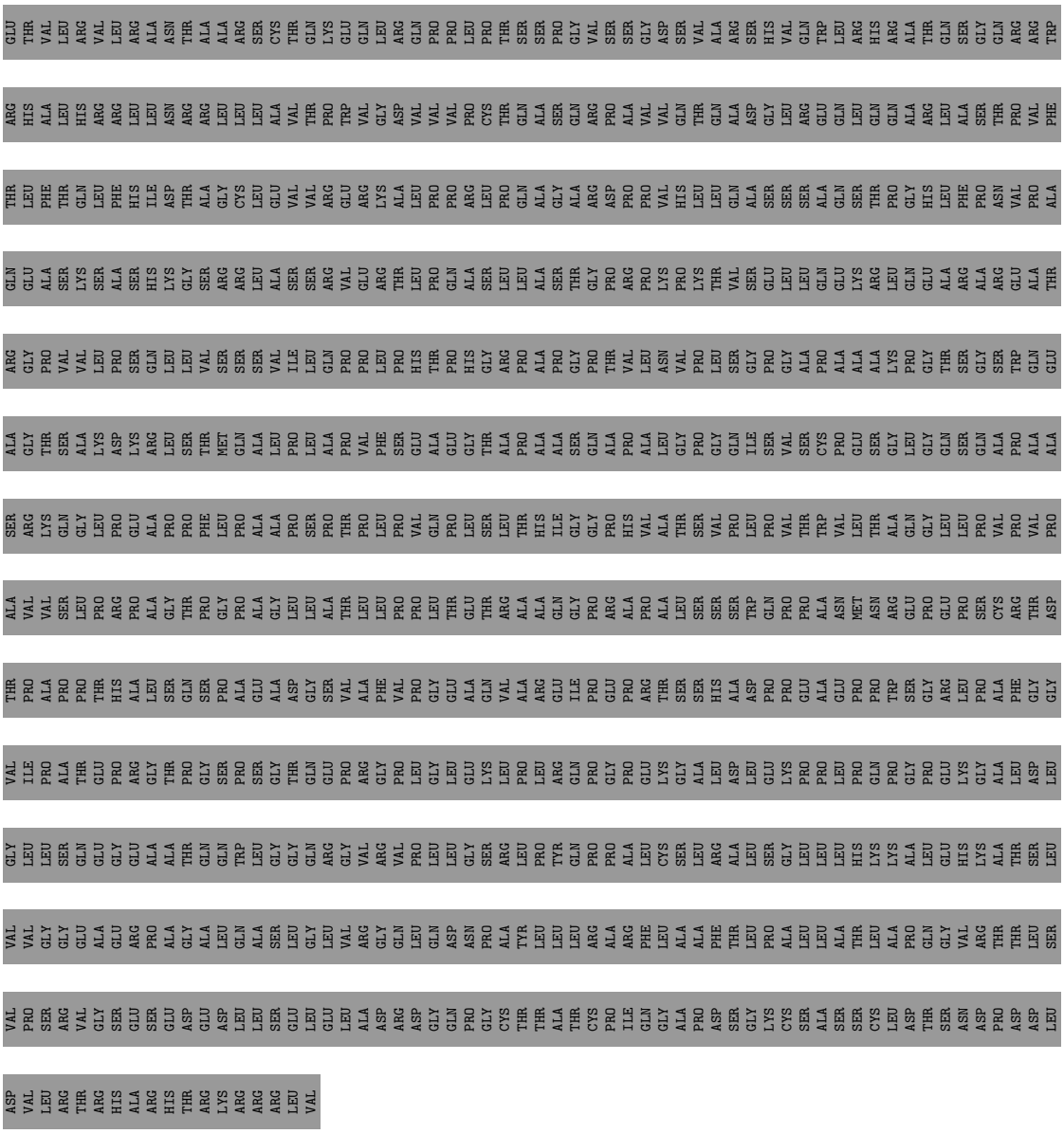






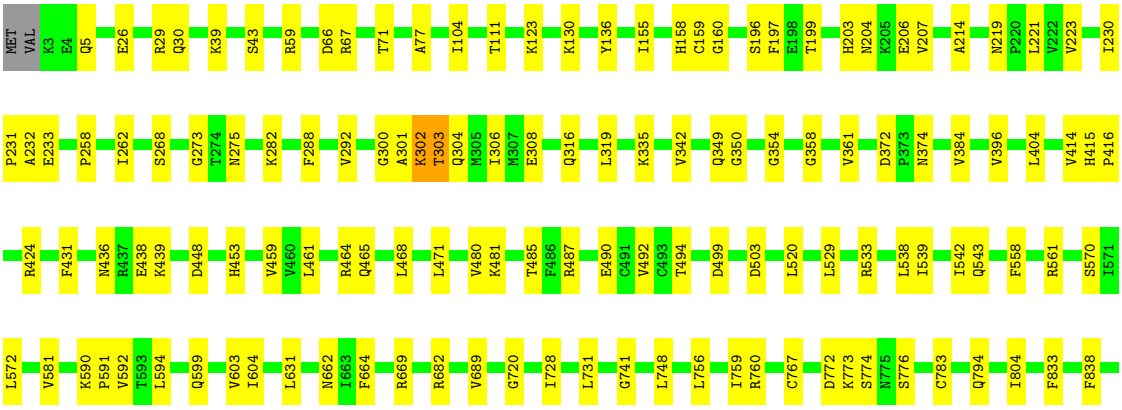


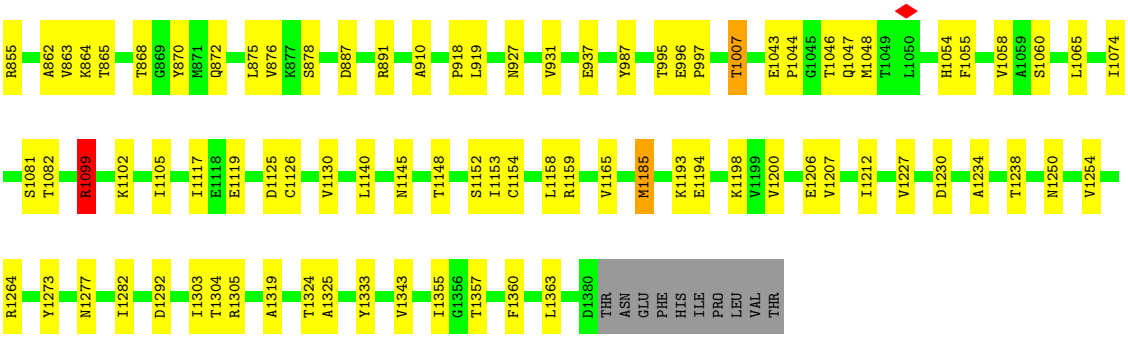




• Molecule 4: DNA-directed RNA polymerase III subunit RPC1

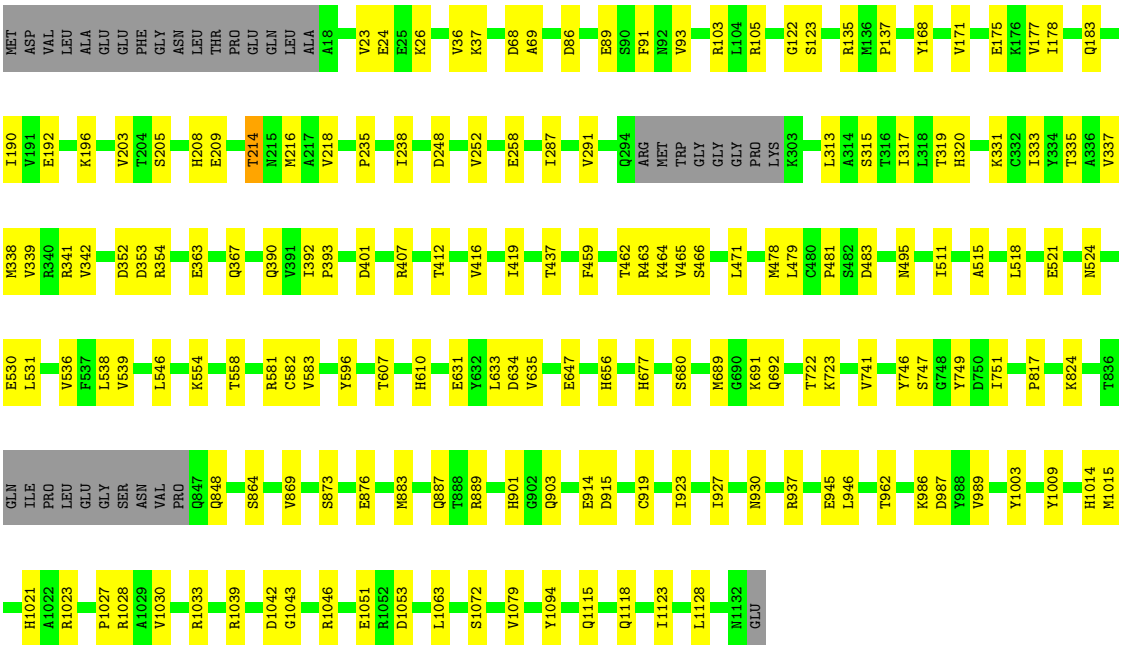
Chain A:





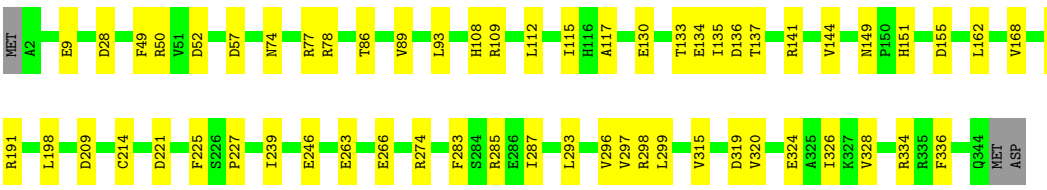
• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

Chain B:



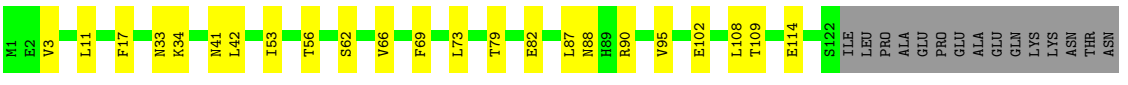
• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C:



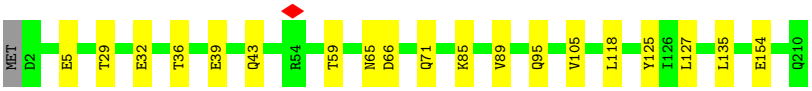
• Molecule 7: DNA-directed RNA polymerase III subunit RPC9

Chain D:



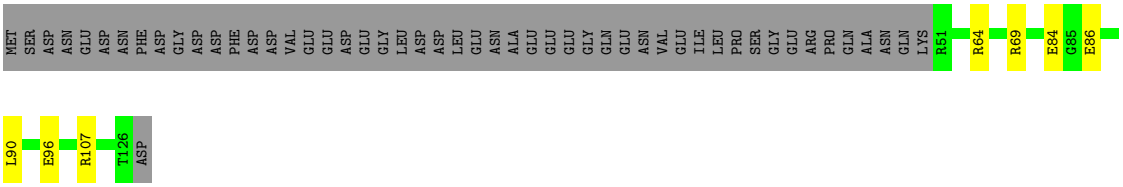
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



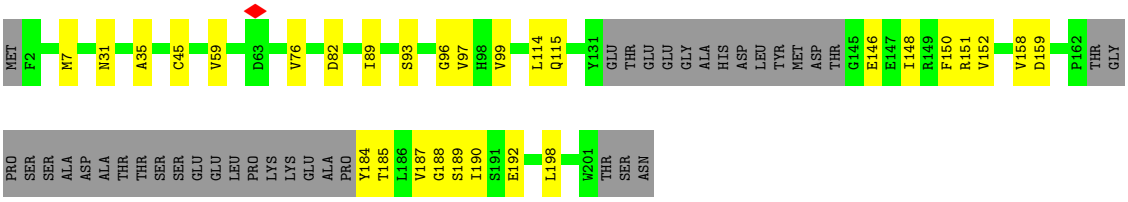
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



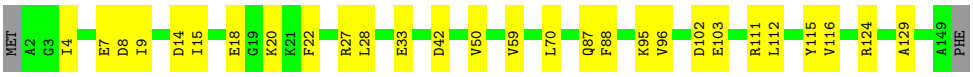
• Molecule 10: DNA-directed RNA polymerase III subunit RPC8

Chain G:



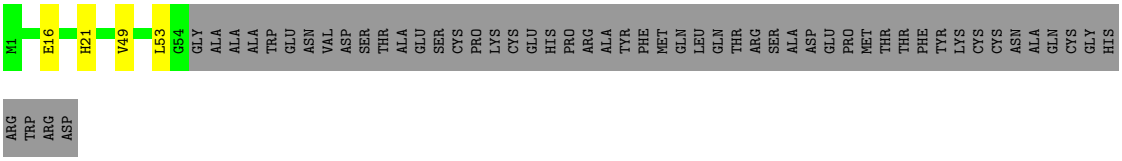
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



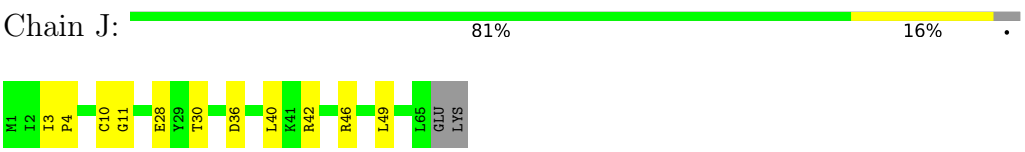
• Molecule 12: DNA-directed RNA polymerase III subunit RPC10

Chain I:



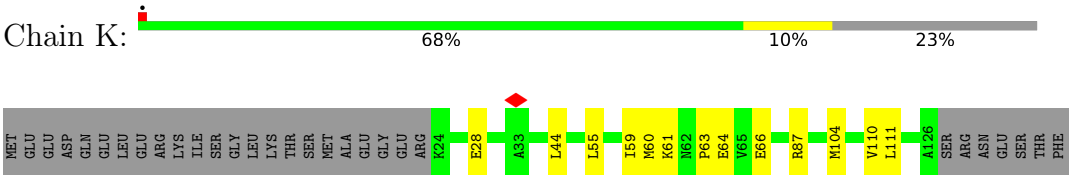
• Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



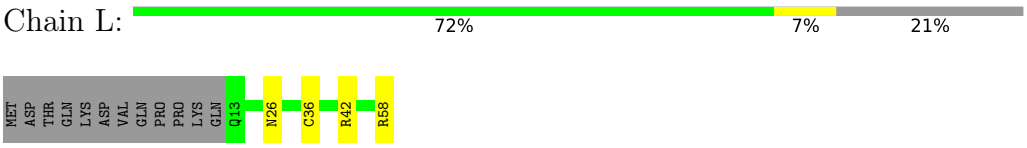
• Molecule 14: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K:



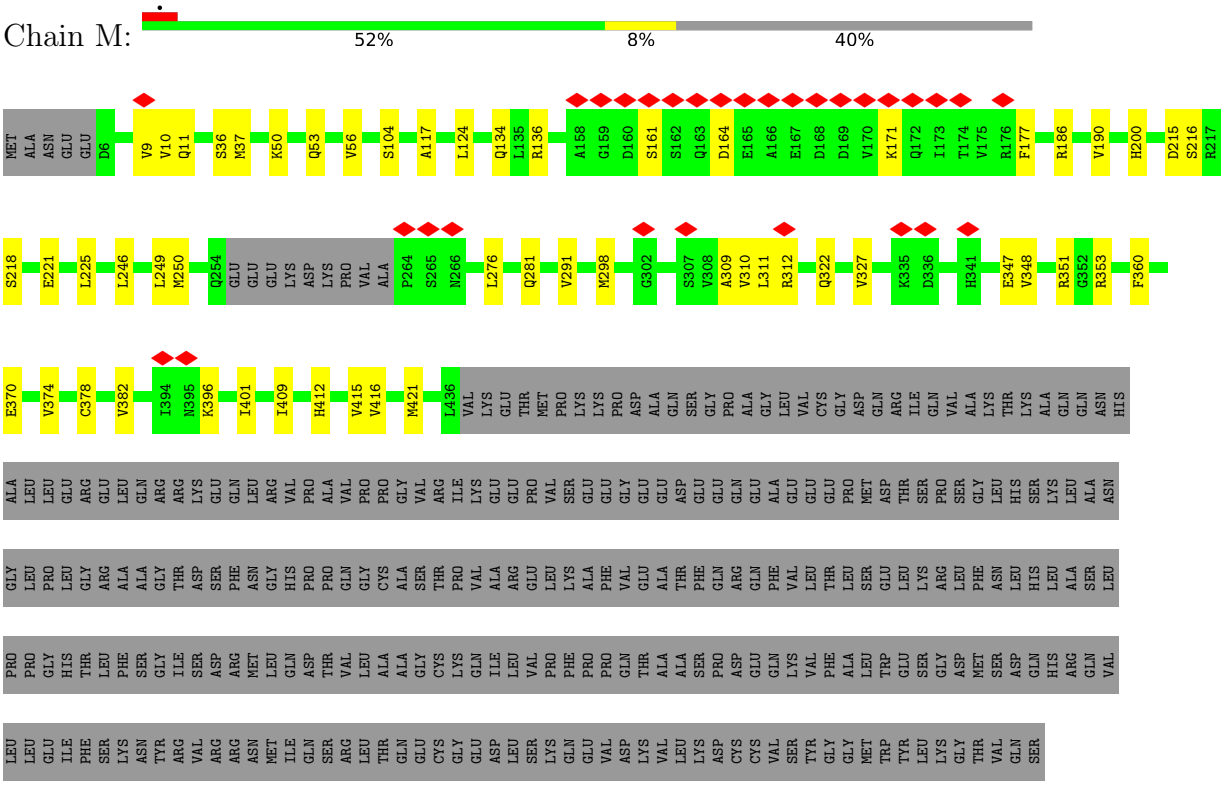
• Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:



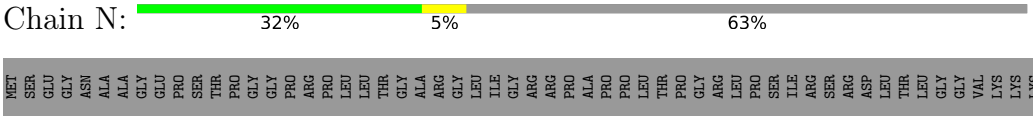
• Molecule 16: DNA-directed RNA polymerase III subunit RPC5

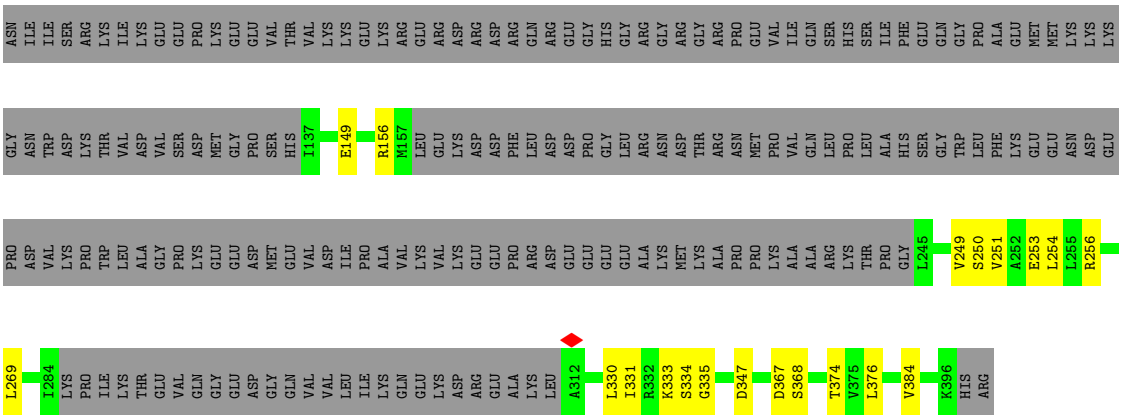
Chain M:



• Molecule 17: DNA-directed RNA polymerase III subunit RPC4

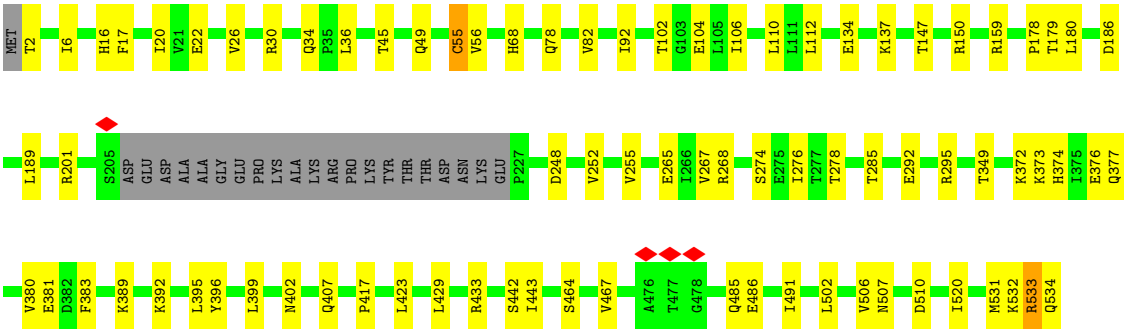
Chain N:





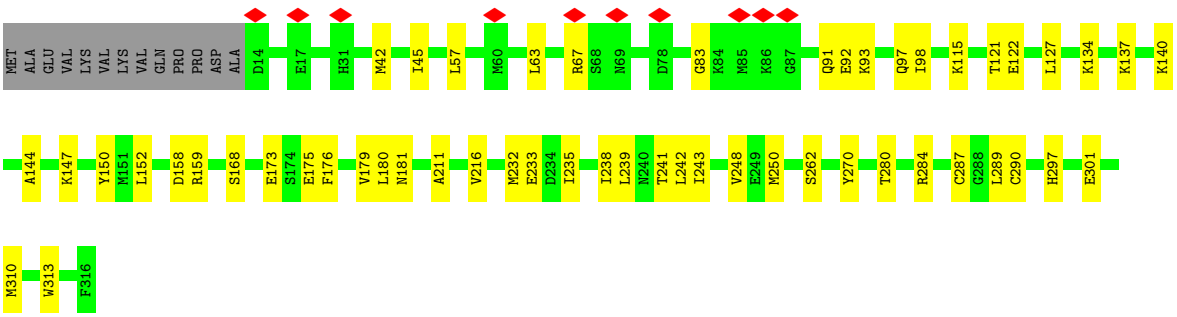
• Molecule 18: DNA-directed RNA polymerase III subunit RPC3

Chain O:



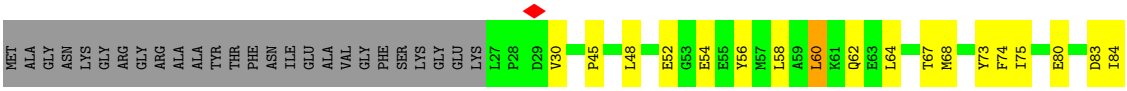
• Molecule 19: DNA-directed RNA polymerase III subunit RPC6

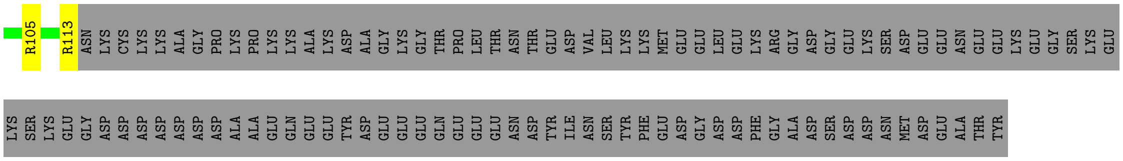
Chain P:



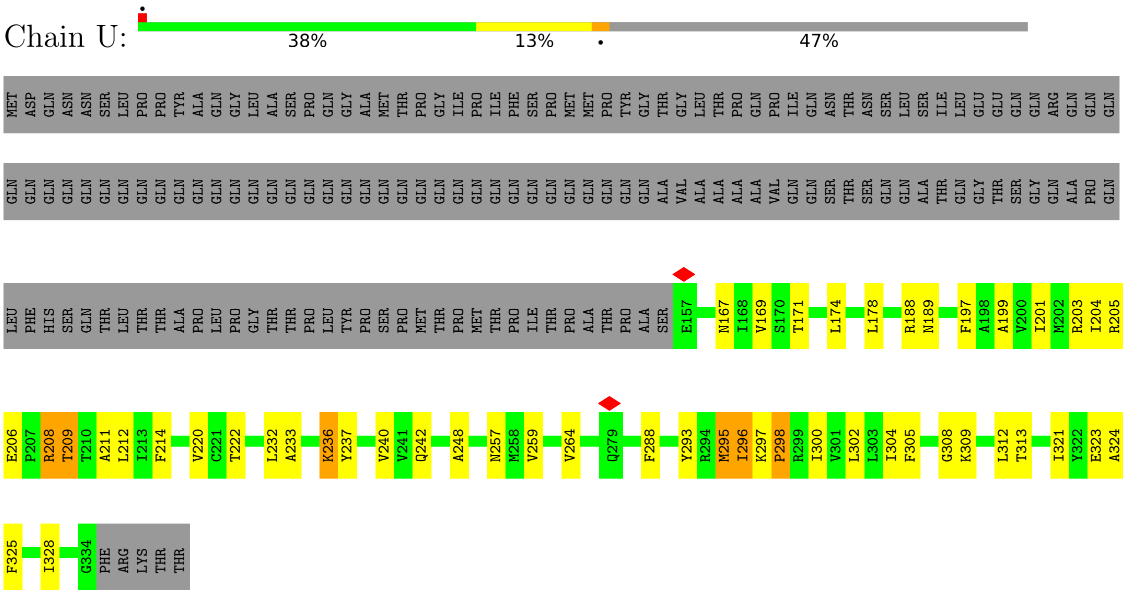
• Molecule 20: DNA-directed RNA polymerase III subunit RPC7

Chain Q:

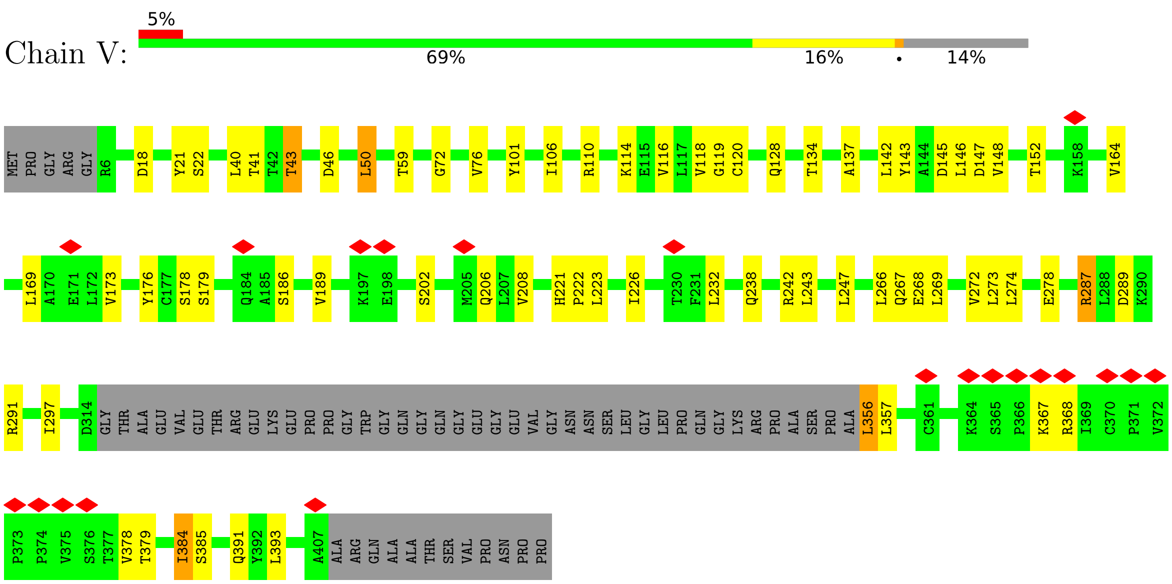




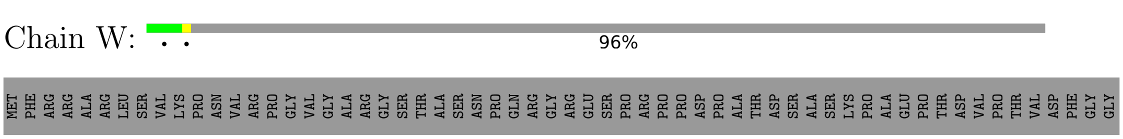
- Molecule 21: TATA-box-binding protein

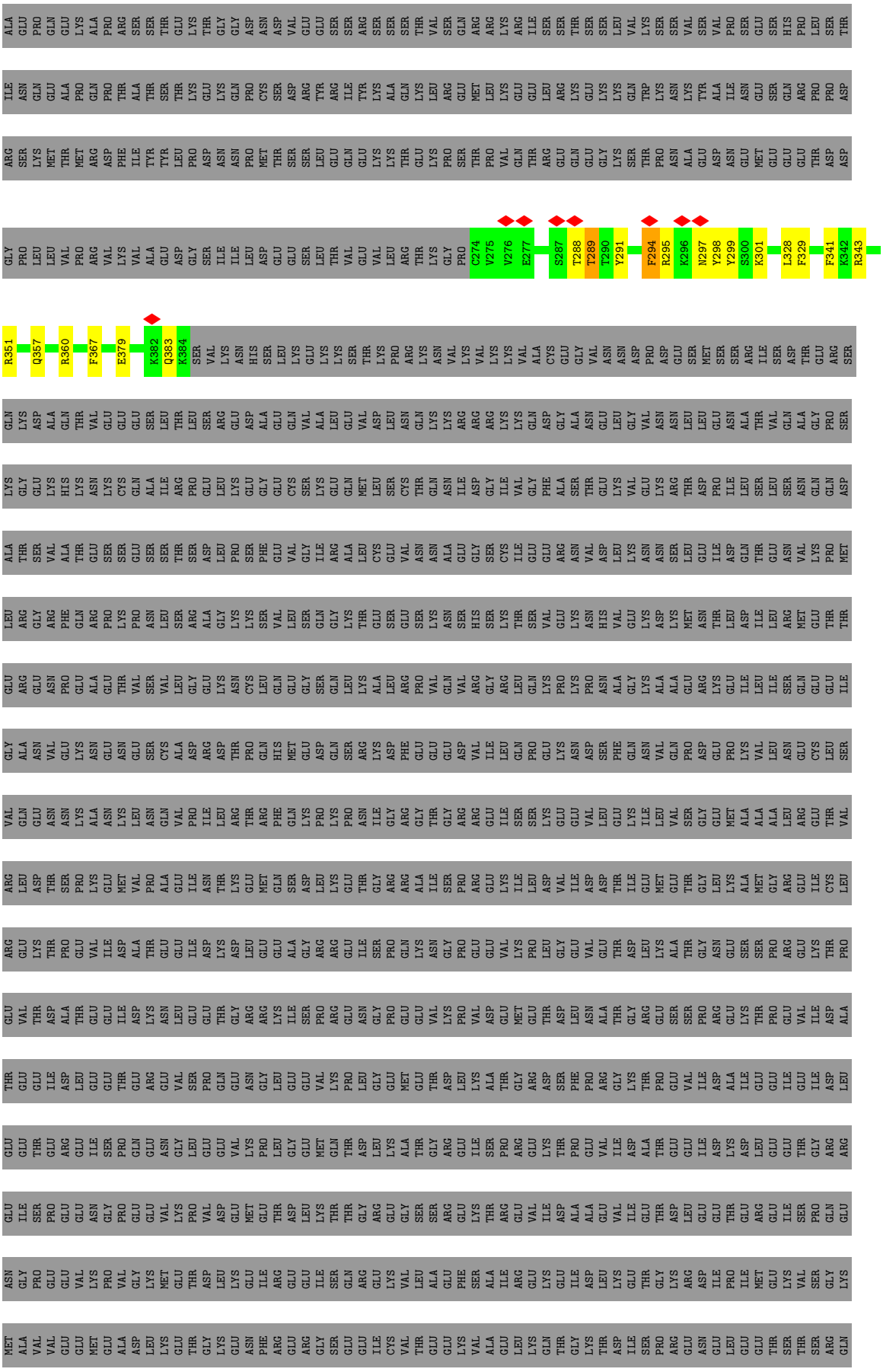


- Molecule 22: Transcription factor IIIB 50 kDa subunit



- Molecule 23: Transcription factor TFIIIB component B” homolog




C274
V275
V276
E277
S287
T288
T289
T290
Y291
F294
R295
K296
N297
Y298
Y299
S300
K301
L328
F329
F341
K342
R343
R351
Q357
R360
F367
E379
K382
Q383
K384

THR ASP THR HIS LEU MET GLN SER GLY SER ASN ASP PHE SER ALA VAL PRO SER LEU ASP ILE GLN ASN ILE SER SER GLU VAL LEU SER MET MET HIS THR PRO VAL GLU GLU LYS ARG ASN SER GLU LYS GLU VAL SER SER HIS PHE SER HIS PHE LYS ILE SER SER GLN THR HIS

GLU SER ASP LYS THR GLU VAL GLN GLY ILE GLN SER PRO ASP VAL PRO GLU GLN PHE SER ASP ILE ASN LEU SER LYS SER LEU PRO GLN GLU GLN LYS PRO LEU GLU ILE LYS PRO ALA PRO PHE VAL ARG SER ARG PHE LYS ARG PRO LYS PRO ASN LEU ALA ARG ALA ALA LEU LYS

ARG GLU THR THR GLU SER GLU LYS TYR ILE TYR GLU LYS LYS SER GLU THR LYS LYS MET GLU THR ILE VAL MET GLN GLU ASN ASN GLU GLN THR ASP THR LEU PRO SER GLN HIS ASP GLU ALA SER LEU MET ILE SER ARG GLU LYS ASP THR LEU GLY HIS ARG ASN GLU GLU ALA

VAL ILE LEU PRO CYS THR GLN THR GLU ARG ASN LEU SER PRO SER ASN SER CYS GLU PRO LYS GLU GLU SER GLN SER ALA PRO VAL GLN LYS ASN ASP SER VAL VAL SER VAL GLY THR ASN ASN VAL ASN THR PHE GLN GLN GLU MET LYS GLU SER VAL ILE GLN THR ALA ARG GLN

VAL ARG GLY ARG LEU GLN ARG PRO ARG PRO ASN ILE ARG LYS THR GLY GLN ARG GLN ILE VAL ASP LYS GLY GLU ALA LYS GLY ILE ILE LYS GLU GLY ARG THR ILE LEU PRO LYS ASP GLU THR GLU LYS LYS VAL LEU THR VAL SER ASN SER GLN ILE GLU THR GLU ILE GLU VAL

PRO SER SER ALA VAL PRO GLU HIS ARG MET TYR GLU ASN GLN SER GLN VAL VAL LEU VAL GLU ASN LEU HIS VAL ASN LYS THR ASN GLU THR ILE ARG HIS GLU ASN LYS PRO TYR VAL PRO SER SER ALA GLN MET THR ARG ARG LYS PHE GLN LYS ALA LYS PRO ASN LEU GLY ARG

ALA HIS SER LYS LYS GLU GLU PRO VAL LEU GLU LYS VAL THR THR ASP GLN SER LYS GLU GLY LYS PRO GLU ASP HIS LEU LEU GLN LYS GLY ALA SER ASN THR GLN LEU LEU LEU LYS GLU LYS ALA GLU LEU LEU THR SER LEU GLU VAL SER ALA ARG LYS ASP CYS VAL GLY SER

LYS GLU SER ALA LEU ALA LYS ILE ASP ALA GLU LEU GLU GLU VAL GLY PRO SER ARG ARG VAL GLY GLU THR VAL GLY ASP ASN SER PRO SER SER VAL VAL GLU GLU GLN TYR LEU ASN LYS LEU THR SER CYS PRO GLN PRO LEU ASN GLU THR SER TYR SER LYS ILE ALA LEU

ASP GLY LYS THR THR ILE SER SER THR SER GLU TYR GLU ARG ASN ARG GLY GLU ARG ARG SER HIS LYS LYS PHE LYS PRO ASN VAL THR ARG GLY ARG GLY SER LYS ARG VAL ARG GLY LYS THR SER LYS LYS GLU PRO ARG ALA SER LYS ALA MET LEU VAL THR LEU ARG ALA SER

GLN GLU GLU ASP ASP ALA ASP ASP PHE GLU SER ASP TYR GLU GLU GLU SER TYR HIS LEU ALA PRO GLU GLU VAL ASN LYS ALA PRO VAL PHE VAL PRO VAL GLY LEU ARG SER PRO GLU PRO VAL SER ALA GLN ILE GLU GLU THR MET GLU GLU LEU GLU ILE THR VAL ASN VAL

PRO ASP VAL GLY CYS ILE ALA VAL VAL GLU HIS GLU LEU PRO ASN THR ASP VAL THR THR GLU GLU MET LYS GLN GLU GLU ASN LEU SER VAL PRO PHE GLU MET THR THR SER GLU HIS ILE GLN ASP GLU PRO GLY THR ASN ASP GLY SER THR GLU ALA ALA ILE THR LEU LEU THR

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ALA SER PHE GLU GLU ASN LYS ILE VAL LEU GLU GLU GLN SER SER ARG GLU GLU ILE SER LEU MET GLU LYS VAL LYS GLU ASN ALA THR PRO THR ARG ASN THR ILE SER LYS VAL THR SER ASN LEU ARG ILE ARG SER ARG LEU ALA LYS PRO LYS PRO ASN LEU GLU LYS THR LEU

GLY THR ASN ARG LEU ASP ASP TYR GLN GLU VAL SER SER LEU CYS VAL THR LYS GLY ALA GLU MET GLU THR GLN ARG GLU THR GLU LYS ASN ALA SER LYS ALA THR GLU LEU GLU ASN LYS ASN LEU GLY PRO VAL THR THR ALA GLU ASN LYS ASP GLN SER LYS LEU ALA CYS VAL

HIS GLY ILE LYS GLY THR SER ILE SER SER GLU VAL ASN LEU THR GLU ARG ASN GLU ASN GLN GLU GLU SER SER GLN GLU VAL HIS MET LEU SER VAL ALA PRO VAL ALA SER SER GLU THR GLY PRO CYS THR LEU GLY LEU ASP ARG GLY LEU GLY GLU ASN SER VAL GLU GLU PRO

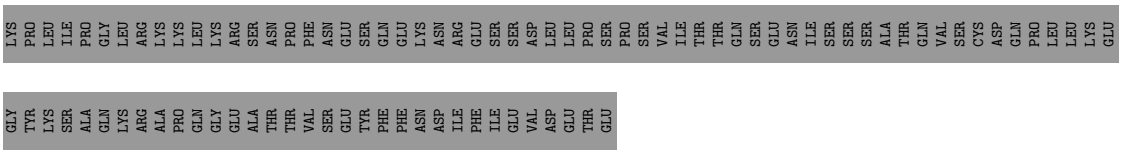
GLN ILE LYS ASP SER LYS GLY ASP SER VAL LEU THR LEU PRO VAL PRO GLU TYR THR PRO THR SER ILE PRO GLU VAL GLN GLN GLU ASN ILE ILE ASN PRO GLN ASP LEU THR VAL ASN LEU VAL ALA ASN VAL PRO GLN ASP GLY GLU ASP GLU GLN ALA PHE ILE LEU THR LEU VAL

GLU ILE PRO ALA ASN ALA VAL GLU GLU PHE THR ASP ALA THR ALA GLN PHE MET PRO ASN PRO LEU LEU PRO ALA PRO ILE LEU VAL LYS SER VAL ASN THR GLU GLU ARG GLY ASP MET SER ILE CYS LEU PRO ALA THR SER VAL GLY GLN ASP ALA MET GLY LEU SER ILE SER GLY

ARG ASP ASN SER LYS LYS PRO PRO ASP ASN LEU ASP LEU VAL SER ARG LYS ARG PHE GLN CYS ARG LEU ASP LYS ASN ASP HIS ILE PRO PRO ALA LYS LYS ARG SER LEU THR LEU ARG ASP ASP CYS GLN GLU TYR THR THR GLU VAL HIS SER LYS GLU LEU THR ASN VAL PHE GLU

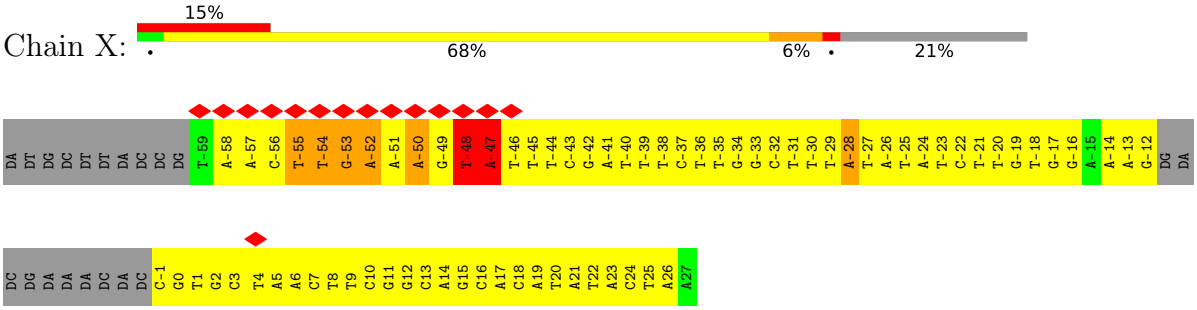
GLU THR GLY GLU SER HIS LYS GLY GLN ASP ILE PHE LEU THR SER GLY SER THR LEU THR THR PRO GLU PRO GLN ARG GLN GLN VAL GLU ALA ALA PHE GLN SER ARG GLY SER ARG SER PRO ASP ALA CYS MET ASP LYS ASN VAL PRO GLN LEU PRO GLN ASP GLU MET ILE VAL SER

ASP LYS GLU GLU ARG THR ASP ALA ALA PRO LYS SER GLN GLN MET ASP SER ARG THR SER SER SER LYS ALA SER LEU SER ARG PRO GLY ARG ARG PRO LEU GLY PHE LEU SER LEU ILE CYS SER LYS ASN SER LEU GLU SER ASP GLU PRO MET GLN VAL HIS SER LYS ARG LEU



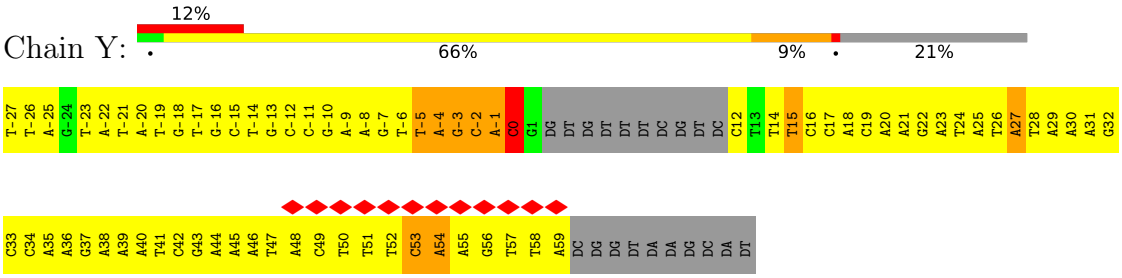
• Molecule 24: DNA (97-MER)

Chain X:



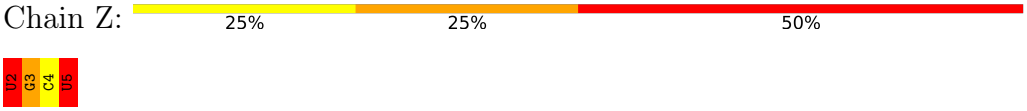
• Molecule 25: DNA (97-MER)

Chain Y:



• Molecule 26: RNA (5'-R(P*UP*GP*CP*U)-3')

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	397000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	10.367	Depositor
Minimum map value	-5.842	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.139	Depositor
Recommended contour level	0.172	Depositor
Map size (Å)	429.07724, 429.07724, 429.07724	wwPDB
Map dimensions	322, 322, 322	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.332538, 1.332538, 1.332538	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SF4, GTP, 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	1	0.27	0/1266	0.45	1/1708 (0.1%)
2	3	0.28	0/3113	0.50	1/4206 (0.0%)
3	4	0.23	0/2107	0.38	0/2828
4	A	0.24	0/11008	0.40	0/14842
5	B	0.24	0/8845	0.40	0/11930
6	C	0.24	0/2790	0.40	0/3782
7	D	0.24	0/997	0.38	0/1343
8	E	0.24	0/1745	0.40	0/2358
9	F	0.24	0/620	0.39	0/839
10	G	0.25	0/1374	0.41	0/1868
11	H	0.24	0/1207	0.42	0/1628
12	I	0.25	0/434	0.42	0/584
13	J	0.25	0/521	0.38	0/703
14	K	0.24	0/837	0.40	0/1129
15	L	0.25	0/394	0.42	0/524
16	M	0.23	0/3455	0.38	0/4673
17	N	0.24	0/1137	0.43	0/1530
18	O	0.24	0/4141	0.39	0/5592
19	P	0.24	0/2446	0.37	0/3301
20	Q	0.25	0/777	0.38	0/1050
21	U	0.28	0/1439	0.51	0/1938
22	V	0.32	0/2904	0.44	1/3941 (0.0%)
23	W	0.26	0/967	0.38	0/1293
24	X	0.74	6/1765 (0.3%)	1.23	21/2720 (0.8%)
25	Y	0.92	10/1773 (0.6%)	1.13	16/2731 (0.6%)
26	Z	2.12	3/91 (3.3%)	2.51	6/139 (4.3%)
All	All	0.33	19/58153 (0.0%)	0.51	46/79180 (0.1%)

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	1	0	1
4	A	0	1
24	X	0	2
25	Y	0	1
All	All	0	5

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	15	DT	C4'-O4'	16.19	1.61	1.45
24	X	-56	DC	O3'-P	-11.80	1.47	1.61
25	Y	0	DC	O3'-P	-11.66	1.47	1.61
26	Z	5	U	C3'-O3'	10.86	1.57	1.42
24	X	-53	DG	O3'-P	9.52	1.72	1.61

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	-52	DA	P-O3'-C3'	16.47	139.47	119.70
25	Y	54	DA	O3'-P-O5'	-13.89	77.62	104.00
24	X	-47	DA	C5'-C4'-O4'	12.73	133.49	109.30
26	Z	3	G	O5'-P-OP1	-12.12	94.79	105.70
24	X	-54	DT	OP2-P-O3'	12.02	131.65	105.20

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	147	ARG	Sidechain
4	A	1099	ARG	Sidechain
24	X	-47	DA	Sidechain
24	X	-48	DT	Sidechain
25	Y	0	DC	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	1	1233	0	1231	42	0
2	3	3038	0	2911	91	0
3	4	2066	0	2049	31	0
4	A	10814	0	11059	216	0
5	B	8680	0	8805	119	0
6	C	2736	0	2712	43	0
7	D	985	0	1006	16	0
8	E	1715	0	1733	11	0
9	F	610	0	642	7	0
10	G	1337	0	1306	22	0
11	H	1186	0	1147	22	0
12	I	426	0	429	4	0
13	J	512	0	525	7	0
14	K	822	0	810	11	0
15	L	388	0	393	3	0
16	M	3382	0	3376	72	0
17	N	1128	0	1181	17	0
18	O	4075	0	4149	115	0
19	P	2403	0	2408	70	0
20	Q	754	0	759	31	0
21	U	1411	0	1501	55	0
22	V	2853	0	2890	50	0
23	W	943	0	924	19	0
24	X	1577	0	877	212	0
25	Y	1580	0	871	196	0
26	Z	83	0	42	29	0
27	A	2	0	0	0	0
27	B	1	0	0	0	0
27	I	1	0	0	0	0
27	J	1	0	0	0	0
27	L	1	0	0	0	0
27	V	1	0	0	0	0
28	A	1	0	0	0	0
29	P	8	0	0	2	0
30	Z	32	0	11	20	0
All	All	56785	0	55747	1182	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 11.

The worst 5 of 1182 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)
24:X:-55:DT:C6	24:X:-54:DT:H71	1.52	1.42
24:X:-49:DG:H22	25:Y:49:DC:N4	1.15	1.42
24:X:-49:DG:N2	25:Y:49:DC:H42	1.09	1.40
26:Z:2:U:OP1	30:Z:101:GTP:C3'	1.82	1.28
26:Z:2:U:P	30:Z:101:GTP:O3'	2.00	1.20

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	1	144/368 (39%)	131 (91%)	13 (9%)	0	100	100
2	3	368/411 (90%)	350 (95%)	18 (5%)	0	100	100
3	4	245/1469 (17%)	234 (96%)	11 (4%)	0	100	100
4	A	1376/1390 (99%)	1348 (98%)	28 (2%)	0	100	100
5	B	1091/1133 (96%)	1058 (97%)	33 (3%)	0	100	100
6	C	341/346 (99%)	335 (98%)	6 (2%)	0	100	100
7	D	120/148 (81%)	117 (98%)	3 (2%)	0	100	100
8	E	207/210 (99%)	204 (99%)	3 (1%)	0	100	100
9	F	74/127 (58%)	70 (95%)	4 (5%)	0	100	100
10	G	160/204 (78%)	150 (94%)	10 (6%)	0	100	100
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	52/108 (48%)	51 (98%)	1 (2%)	0	100	100
13	J	63/67 (94%)	60 (95%)	3 (5%)	0	100	100
14	K	101/133 (76%)	98 (97%)	3 (3%)	0	100	100
15	L	44/58 (76%)	41 (93%)	3 (7%)	0	100	100
16	M	418/708 (59%)	404 (97%)	14 (3%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	N	140/398 (35%)	140 (100%)	0	0	100	100
18	O	508/534 (95%)	495 (97%)	13 (3%)	0	100	100
19	P	301/316 (95%)	294 (98%)	7 (2%)	0	100	100
20	Q	85/223 (38%)	83 (98%)	2 (2%)	0	100	100
21	U	177/339 (52%)	174 (98%)	3 (2%)	0	100	100
22	V	358/419 (85%)	347 (97%)	11 (3%)	0	100	100
23	W	109/2624 (4%)	101 (93%)	8 (7%)	0	100	100
All	All	6628/11883 (56%)	6430 (97%)	198 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	1	130/334 (39%)	121 (93%)	9 (7%)	13	42
2	3	330/356 (93%)	312 (94%)	18 (6%)	18	50
3	4	221/1213 (18%)	213 (96%)	8 (4%)	30	64
4	A	1200/1212 (99%)	1187 (99%)	13 (1%)	70	87
5	B	959/988 (97%)	955 (100%)	4 (0%)	89	95
6	C	299/302 (99%)	298 (100%)	1 (0%)	91	96
7	D	114/136 (84%)	114 (100%)	0	100	100
8	E	191/192 (100%)	191 (100%)	0	100	100
9	F	66/111 (60%)	66 (100%)	0	100	100
10	G	149/181 (82%)	148 (99%)	1 (1%)	81	91
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	48/93 (52%)	48 (100%)	0	100	100
13	J	53/56 (95%)	52 (98%)	1 (2%)	52	79
14	K	92/119 (77%)	91 (99%)	1 (1%)	70	87

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
15	L	43/55 (78%)	43 (100%)	0	100 100
16	M	377/622 (61%)	377 (100%)	0	100 100
17	N	131/347 (38%)	130 (99%)	1 (1%)	79 90
18	O	458/476 (96%)	456 (100%)	2 (0%)	89 95
19	P	269/280 (96%)	267 (99%)	2 (1%)	81 91
20	Q	84/195 (43%)	82 (98%)	2 (2%)	44 74
21	U	154/293 (53%)	145 (94%)	9 (6%)	17 48
22	V	325/365 (89%)	313 (96%)	12 (4%)	29 63
23	W	102/2381 (4%)	94 (92%)	8 (8%)	10 36
All	All	5924/10438 (57%)	5832 (98%)	92 (2%)	58 82

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	O	55	CYS
21	U	323	GLU
19	P	93	LYS
21	U	208	ARG
22	V	128	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
18	O	534	GLN
19	P	182	GLN
22	V	112	GLN
4	A	17	HIS
3	4	369	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	Z	4/4 (100%)	1 (25%)	1 (25%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
26	Z	5	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	Z	2	U

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
30	GTP	Z	101	-	26,34,34	1.64	4 (15%)	32,54,54	3.64	16 (50%)
29	SF4	P	401	19	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	GTP	Z	101	-	-	4/18/38/38	0/3/3/3
29	SF4	P	401	19	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Z	101	GTP	C6-N1	-5.48	1.29	1.37
30	Z	101	GTP	C5-C6	-3.22	1.40	1.47
30	Z	101	GTP	C2-N1	-2.63	1.31	1.37
30	Z	101	GTP	C3'-C4'	-2.32	1.47	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	Z	101	GTP	C3'-C2'-C1'	9.36	115.08	100.98
30	Z	101	GTP	O4'-C1'-C2'	-8.59	94.38	106.93
30	Z	101	GTP	PB-O3B-PG	-7.19	108.17	132.83
30	Z	101	GTP	PA-O3A-PB	-7.08	108.54	132.83
30	Z	101	GTP	O6-C6-C5	-4.95	114.70	124.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	Z	101	GTP	C5'-O5'-PA-O3A
30	Z	101	GTP	O4'-C4'-C5'-O5'
30	Z	101	GTP	C3'-C4'-C5'-O5'
30	Z	101	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

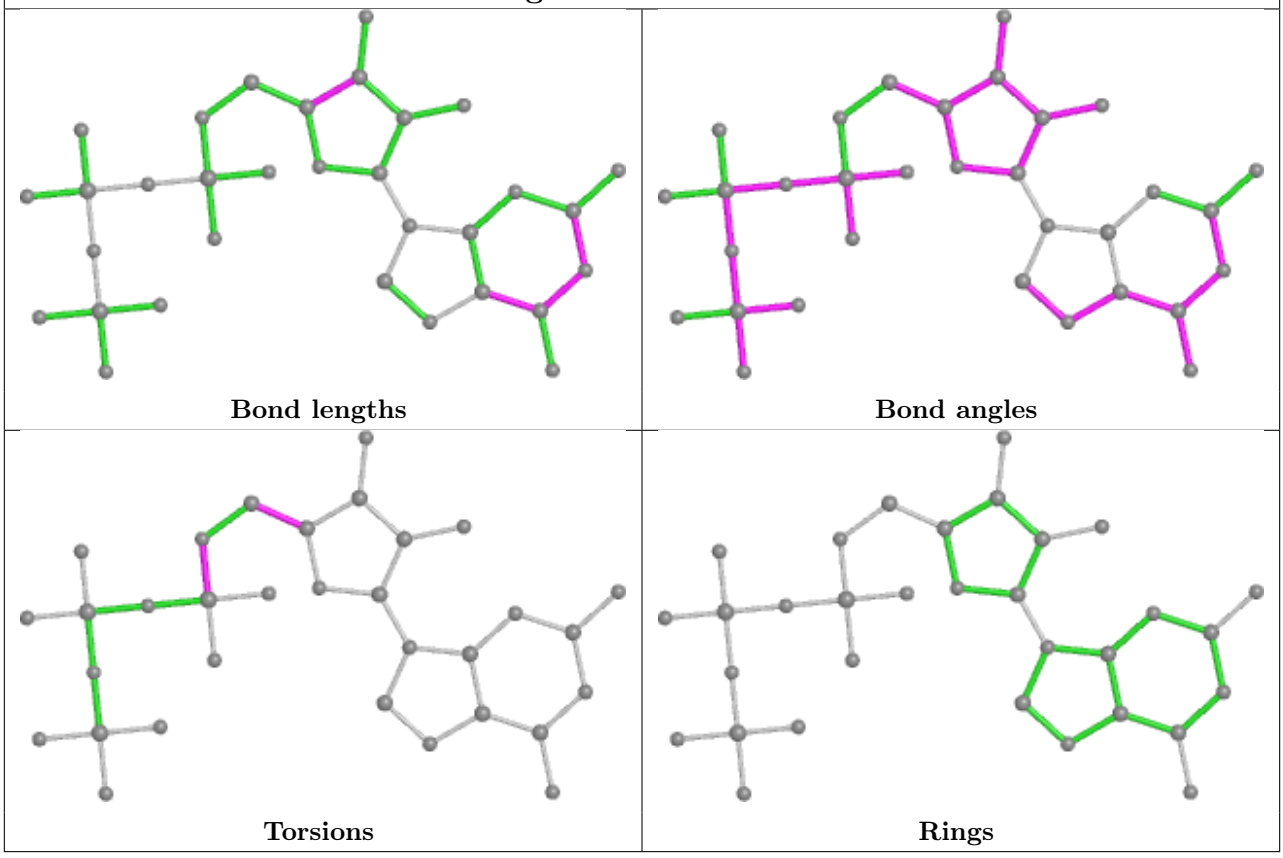
2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	Z	101	GTP	20	0
29	P	401	SF4	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand GTP Z 101



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.

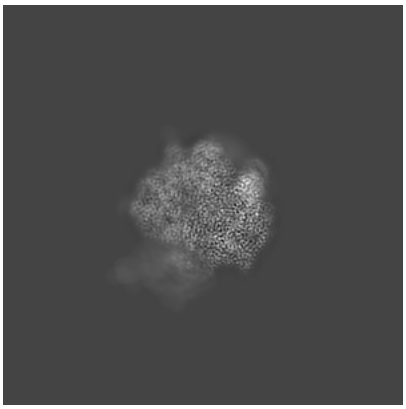
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-62029. These allow visual inspection of the internal detail of the map and identification of artifacts.

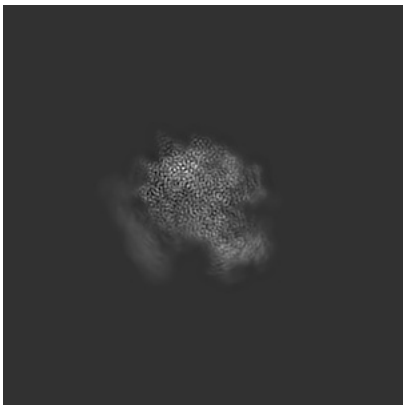
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

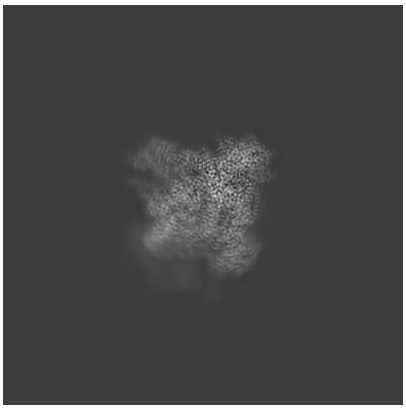
6.1.1 Primary map



X

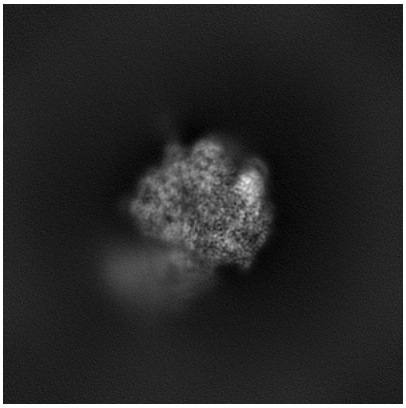


Y

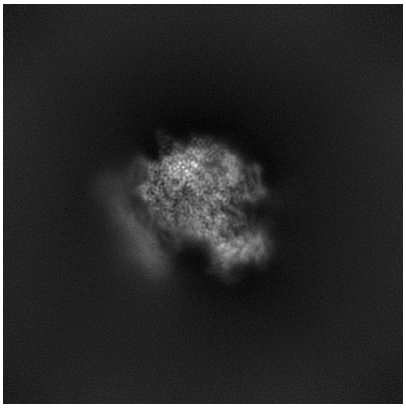


Z

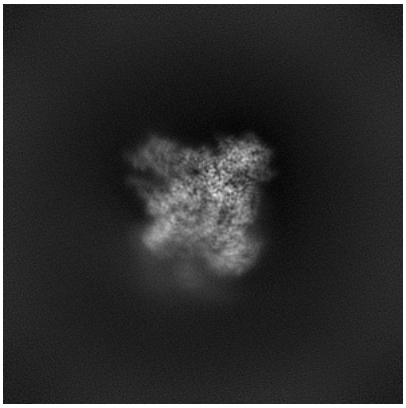
6.1.2 Raw map



X



Y



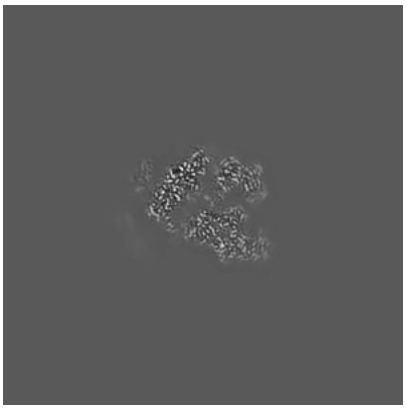
Z

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

6.2 Central slices (i)

6.2.1 Primary map

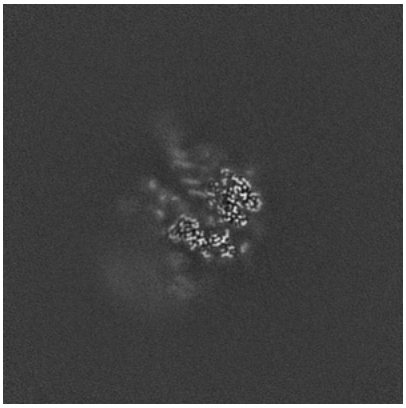
X Index: 161



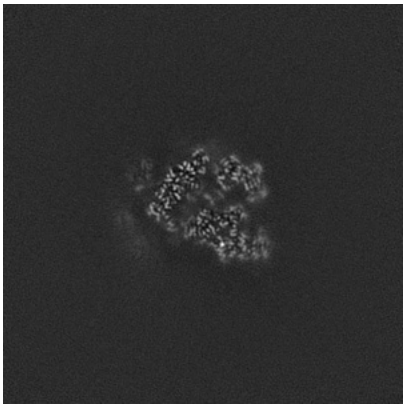
Y Index: 161

Z Index: 161

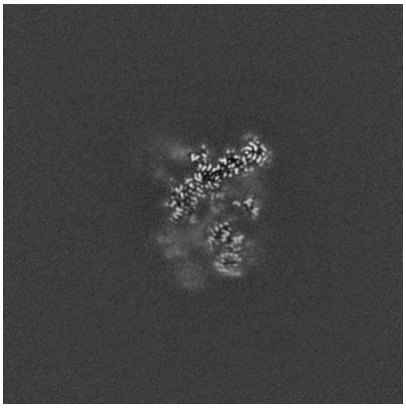
6.2.2 Raw map



X Index: 161



Y Index: 161

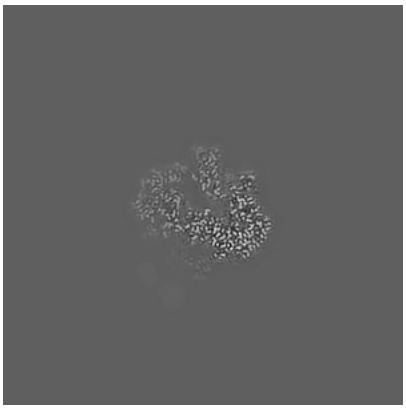


Z Index: 161

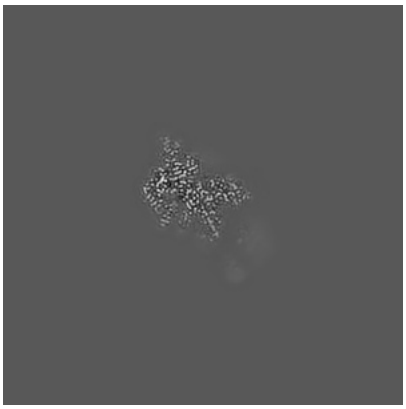
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

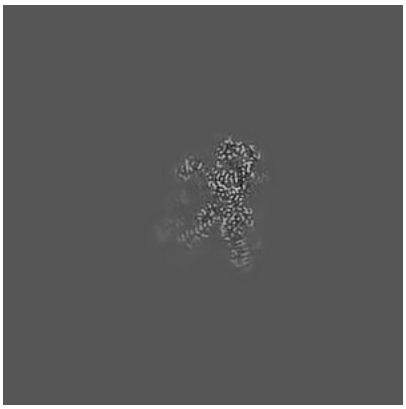
6.3.1 Primary map



X Index: 182

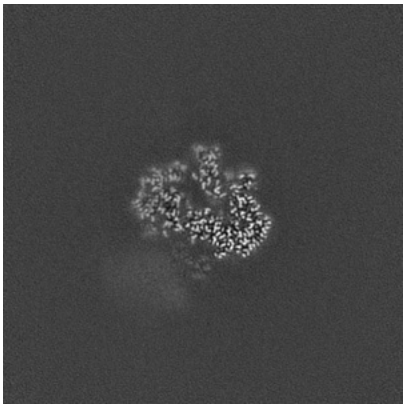


Y Index: 181

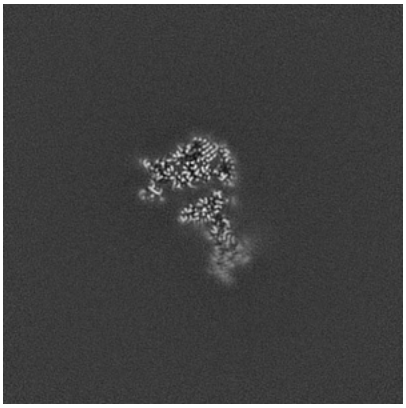


Z Index: 142

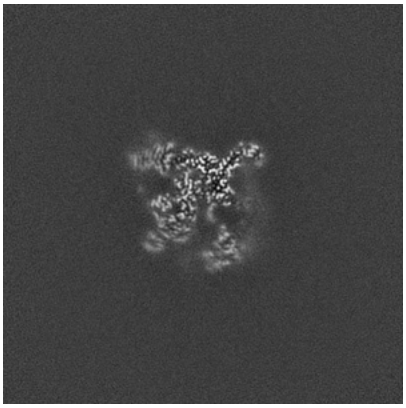
6.3.2 Raw map



X Index: 182



Y Index: 198

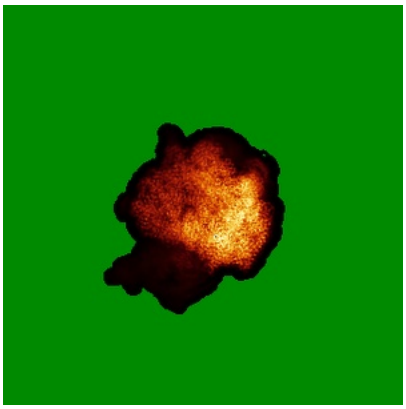


Z Index: 174

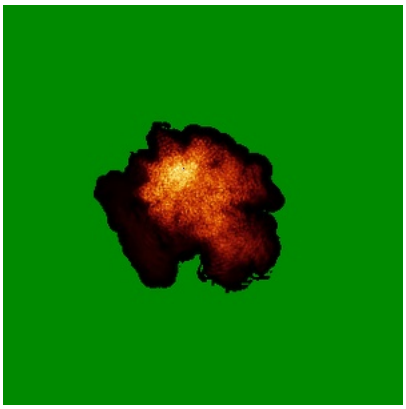
The images above show the largest variance slices of the map in three orthogonal directions.

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

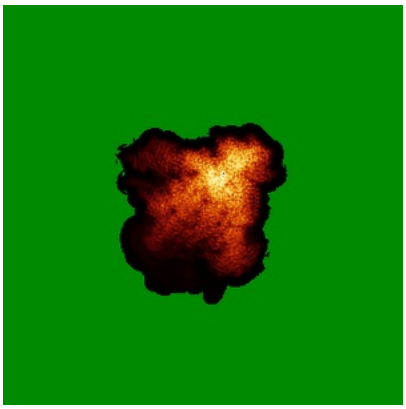
6.4.1 Primary map



X

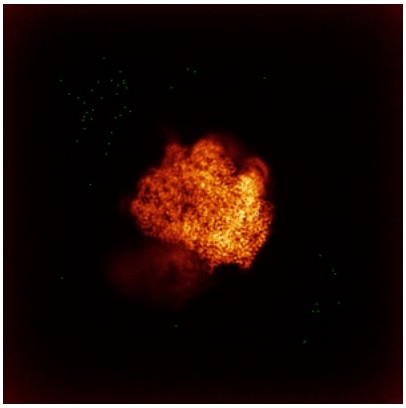


Y

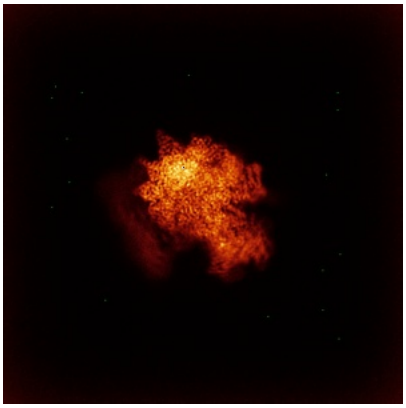


Z

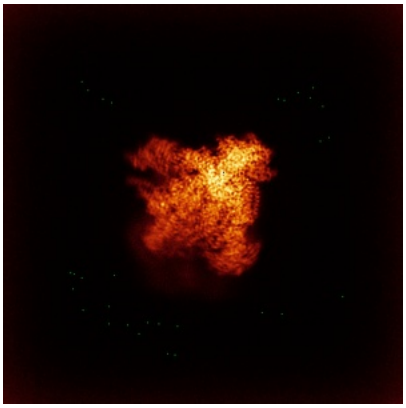
6.4.2 Raw map



X



Y

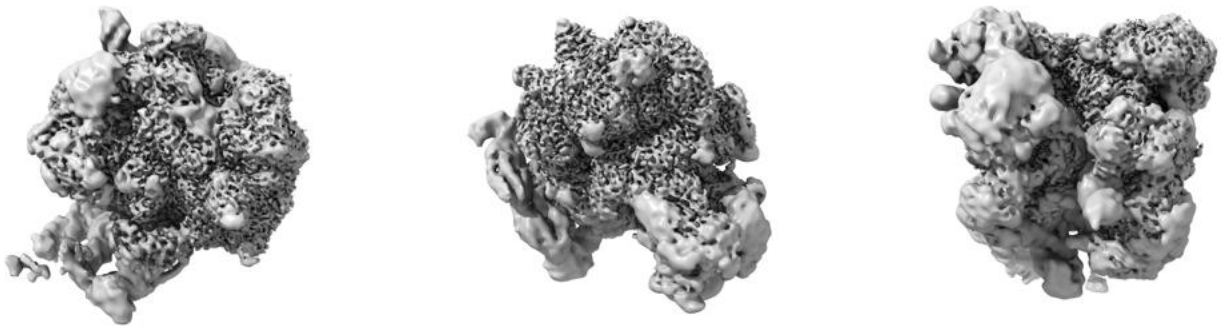


Z

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)

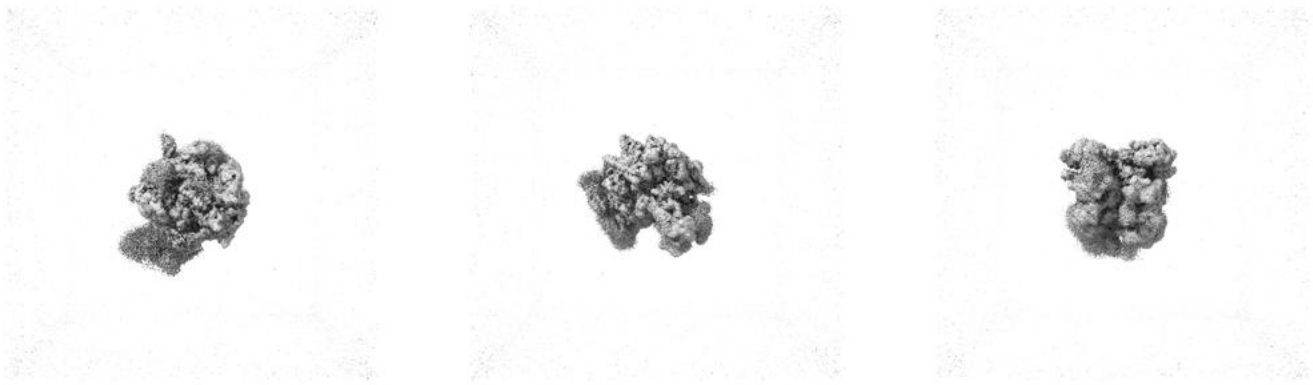
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.172. 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.

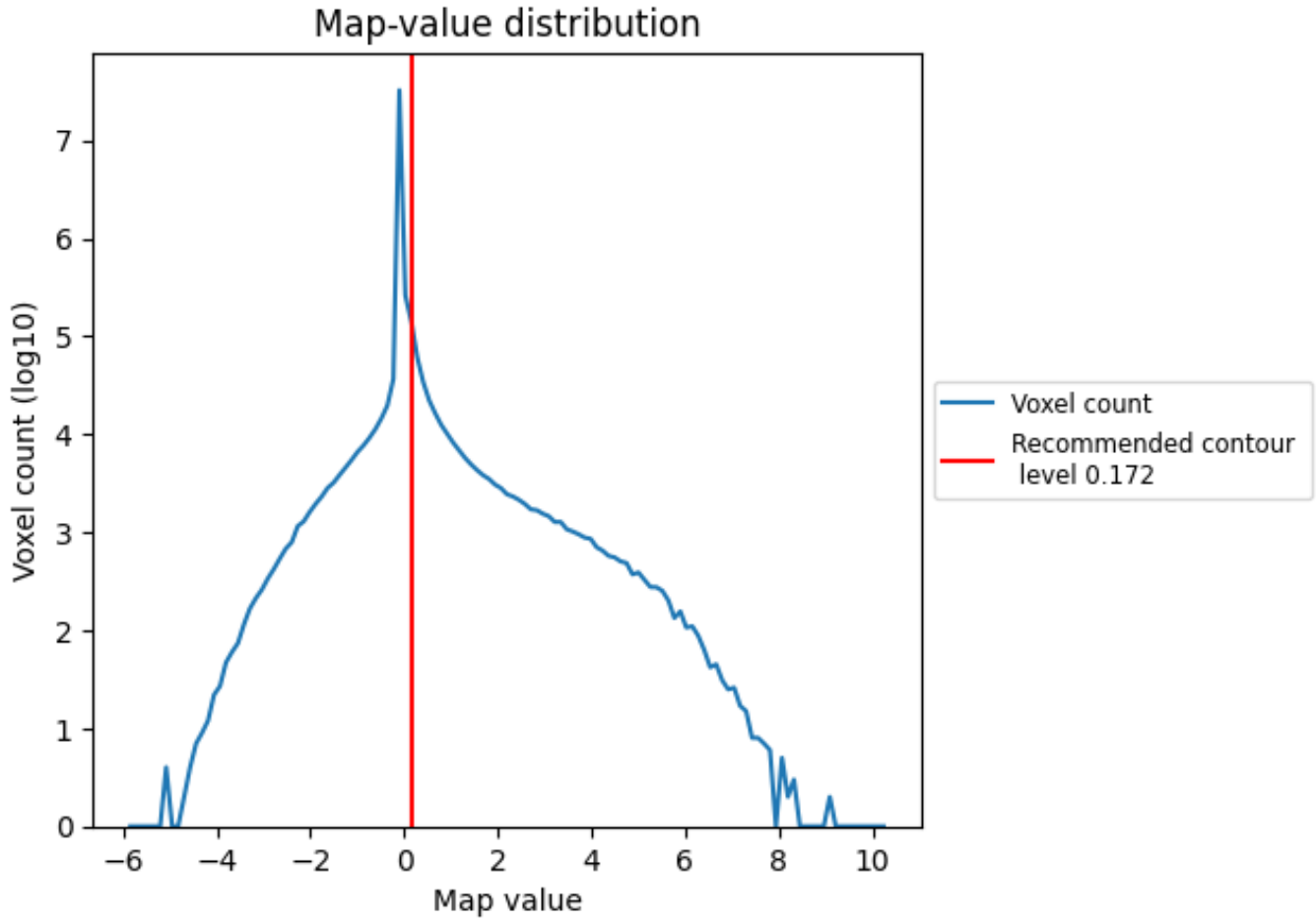
6.6 Mask visualisation (i)

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

7 Map analysis

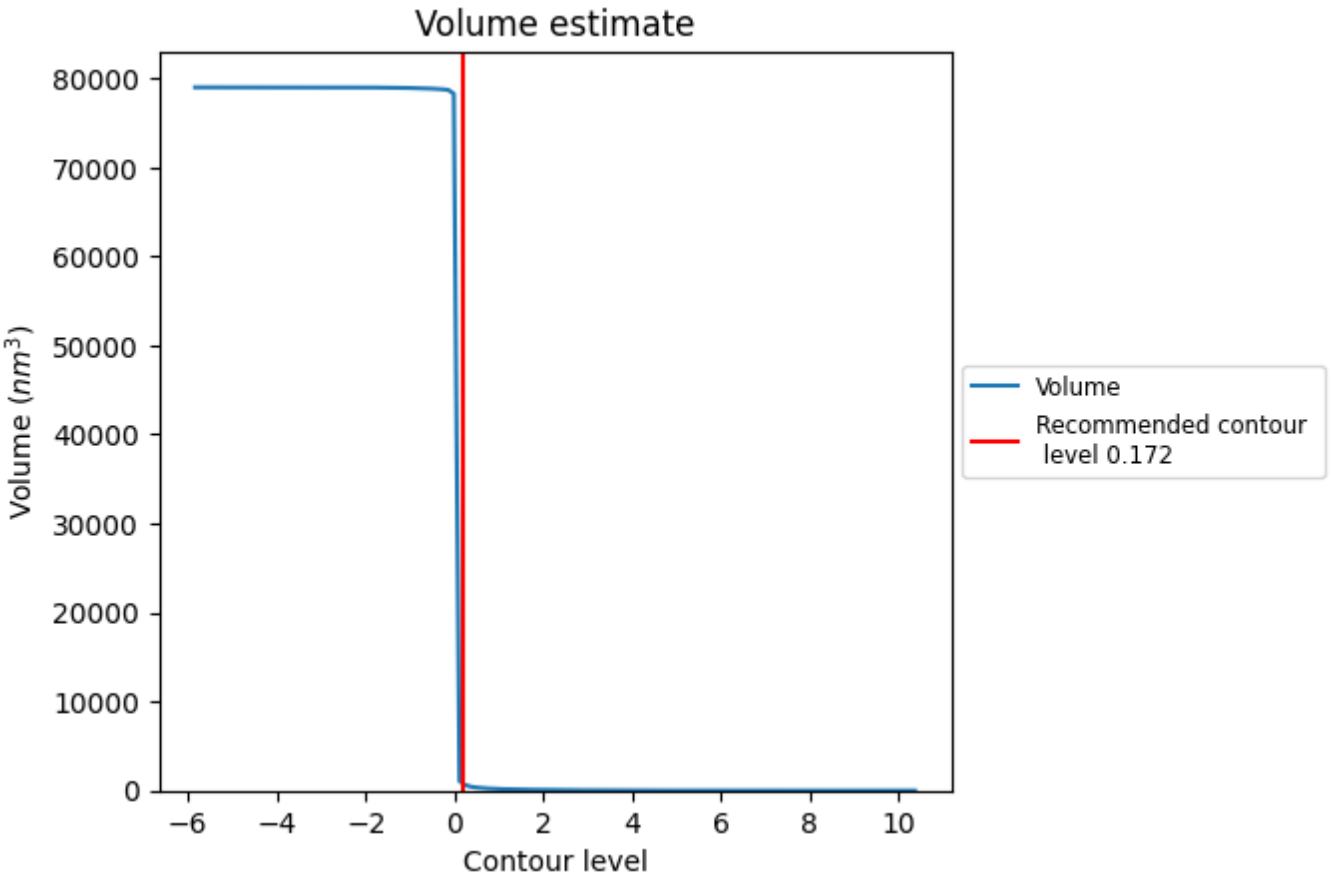
This section contains the results of statistical analysis of the map.

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.

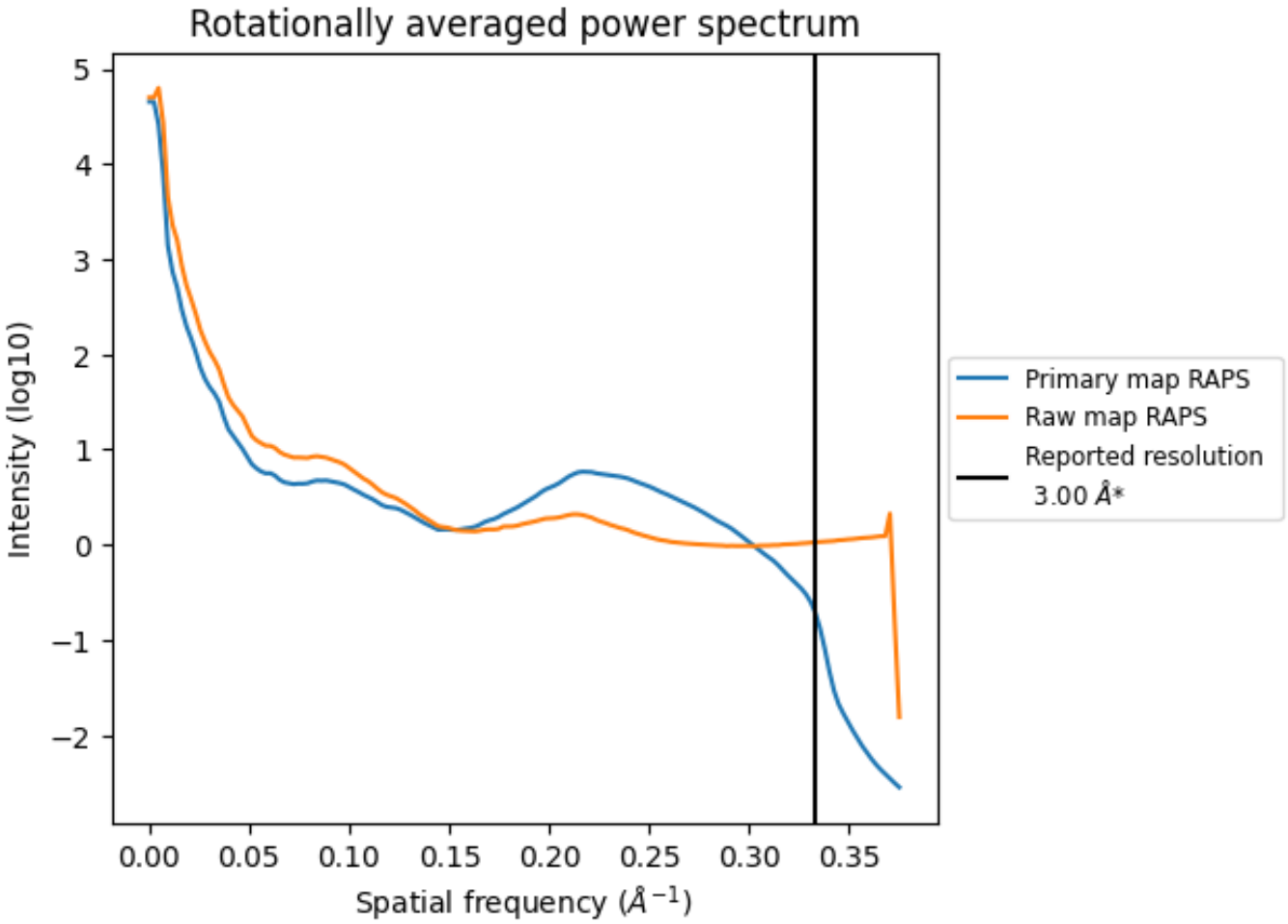
7.2 Volume estimate (i)



The volume at the recommended contour level is 857 nm^3; this corresponds to an approximate mass of 774 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)

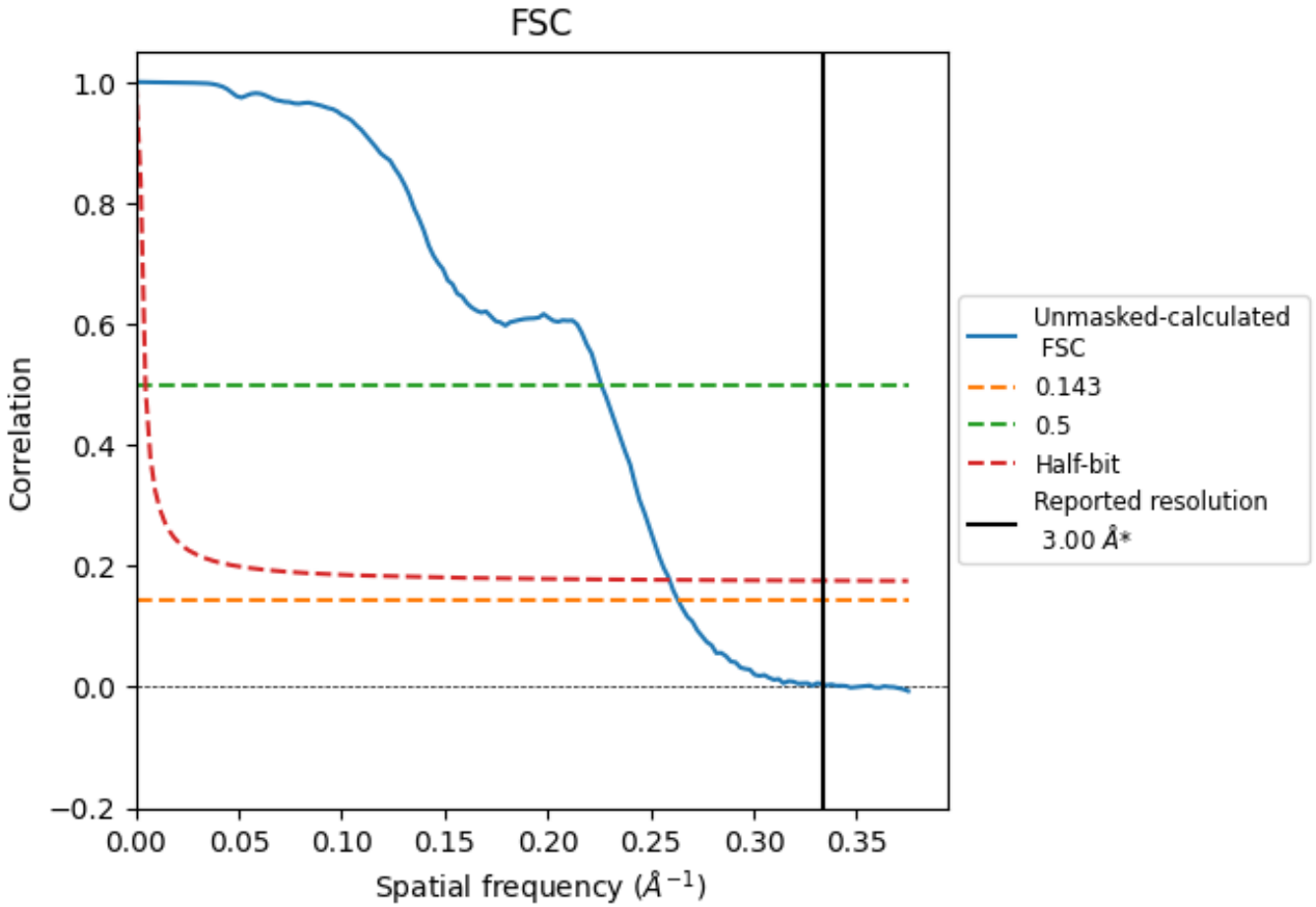


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

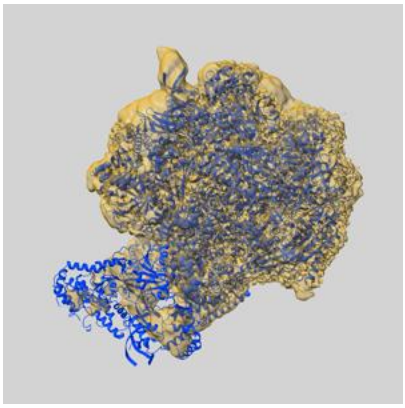
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.80	4.42	3.86

*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 3.80 differs from the reported value 3.0 by more than 10 %

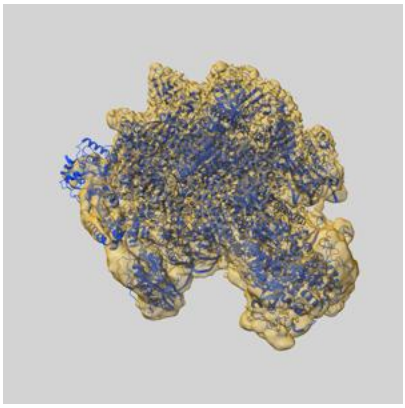
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-62029 and PDB model 9K3U. Per-residue inclusion information can be found in section 3 on page 10.

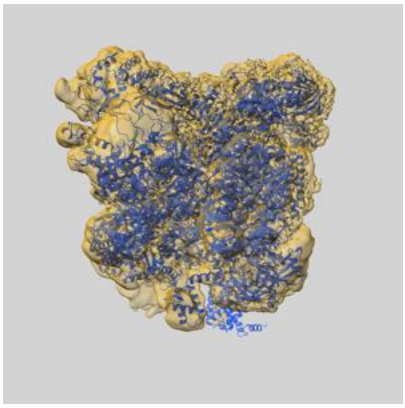
9.1 Map-model overlay



X



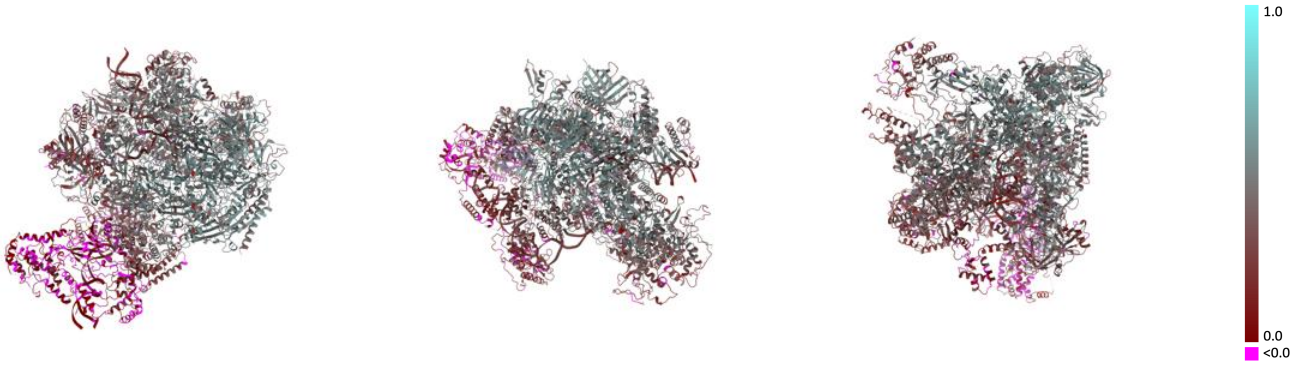
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.172 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.

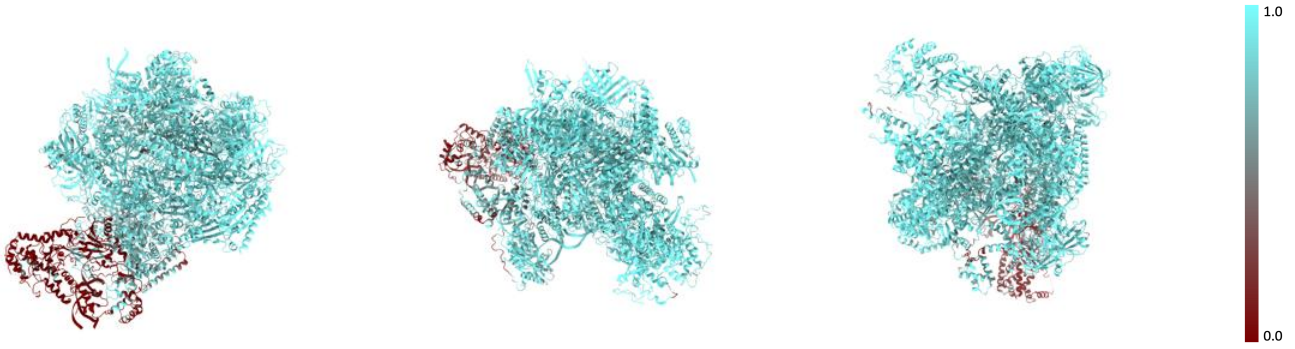
9.2 Q-score mapped to coordinate model (i)



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.

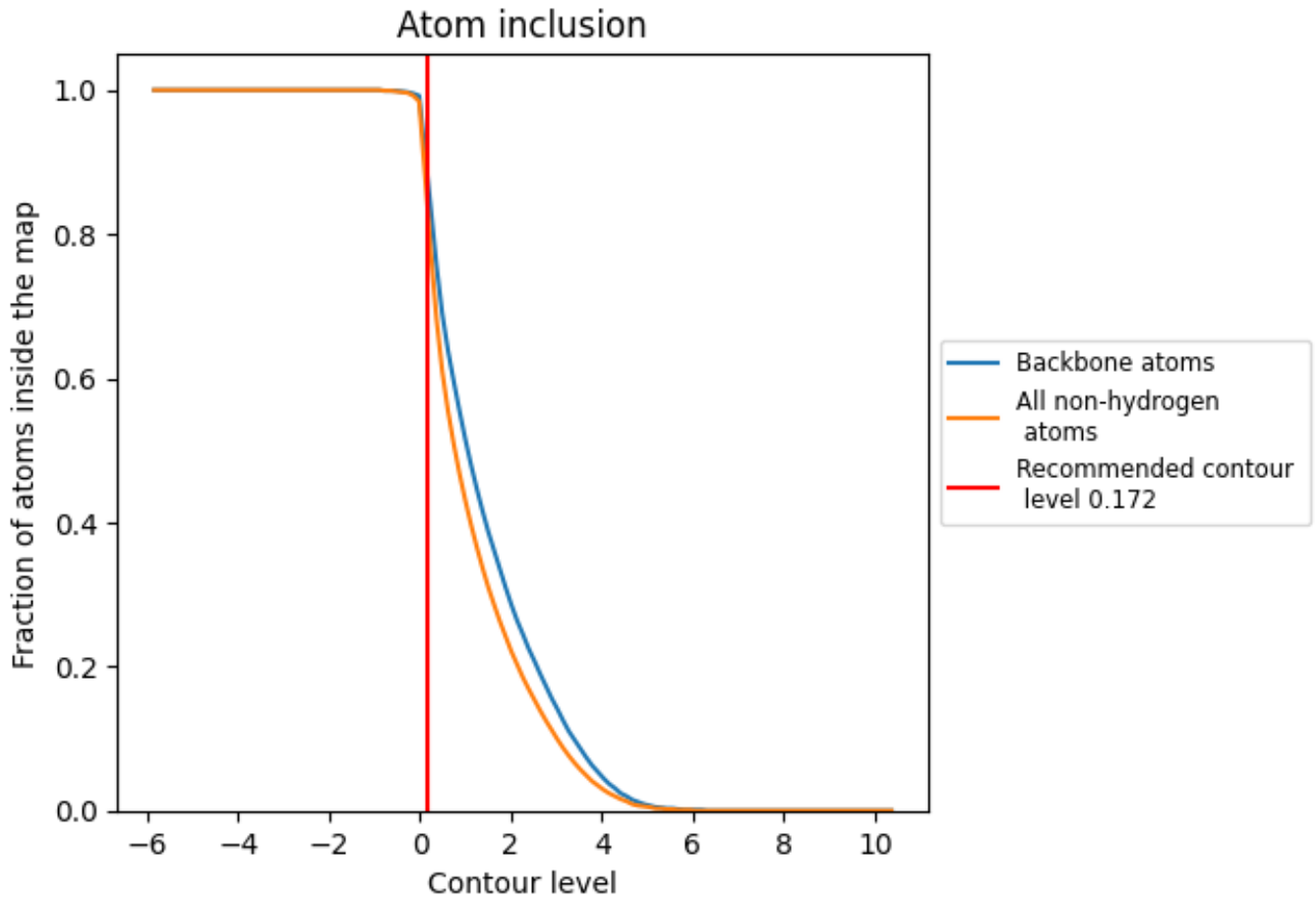
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.172).

9.4 Atom inclusion (i)



At the recommended contour level, 88% 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 (0.172) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8330	0.3510
1	0.0730	0.0290
3	0.1280	0.0030
4	0.3660	0.0610
A	0.9390	0.4700
B	0.9450	0.4830
C	0.9540	0.4980
D	0.9560	0.2740
E	0.9370	0.4000
F	0.9510	0.4930
G	0.9480	0.3600
H	0.9530	0.4770
I	0.9620	0.4360
J	0.9480	0.4840
K	0.9380	0.4720
L	0.9460	0.4070
M	0.8180	0.3470
N	0.9220	0.3070
O	0.9490	0.3940
P	0.9090	0.2670
Q	0.9400	0.3450
U	0.9030	0.1670
V	0.8360	0.2700
W	0.8280	0.1260
X	0.7550	0.1720
Y	0.7830	0.2070
Z	0.9220	0.5250