



# wwPDB EM Validation Summary Report ⓘ

Jul 3, 2023 – 12:29 PM JST

PDB ID : 8IUE  
EMDB ID : EMD-35719  
Title : RNA polymerase III pre-initiation complex melting complex 1  
Authors : Hou, H.; Jin, Q.; Ren, Y.; Wang, Q.; Xu, Y.  
Deposited on : 2023-03-24  
Resolution : 4.10 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](mailto: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>.

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

EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

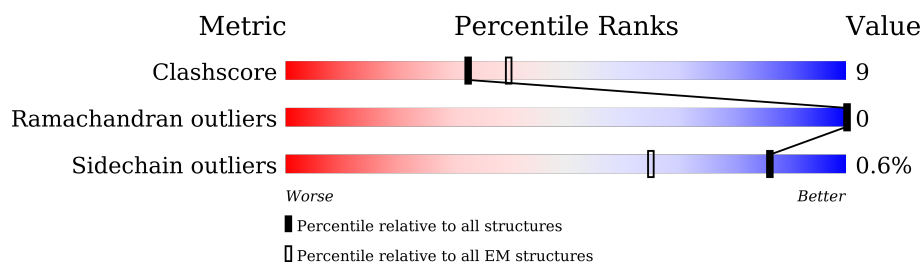
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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  $\geq 3$ , 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  $\leq 5\%$ . 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	1390	 78% 21% .
2	B	1133	 74% 23% .
3	C	346	 79% 20% .
4	D	148	 14% 57% 26% 18%
5	E	210	 6% 78% 21%
6	F	127	 55% 5% 40%
7	G	204	 5% 57% 25% 19%
8	H	150	 8% 83% 15% .

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Mol	Chain	Length	Quality of chain
9	I	108	
10	J	67	
11	K	133	
12	L	58	
13	M	708	
14	N	317	
15	O	534	
16	P	316	
17	Q	223	
18	X	464	
19	Y	464	
20	1	368	
21	3	411	
22	4	1469	
23	U	339	
24	V	419	
25	W	2624	

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 57927 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
1	A	1378	Total	C	N	O	S	0	0
			10814	6850	1886	2005	73		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1105	Total	C	N	O	S	0	0
			8741	5538	1529	1605	69		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	107	Total	C	N	O	S	0	0
			848	525	157	153	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	24	ALA	SER	variant	UNP Q9Y2Y1

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

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

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

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

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

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

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

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

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

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

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	THR	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	GLN	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	HIS	deletion	UNP P05423
N	?	-	SER	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	PHE	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASN	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	TRP	deletion	UNP P05423
N	?	-	LEU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	GLY	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	ILE	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	VAL	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423
N	?	-	ASP	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	GLU	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	MET	deletion	UNP P05423

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	PRO	deletion	UNP P05423
N	?	-	LYS	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ALA	deletion	UNP P05423
N	?	-	ARG	deletion	UNP P05423

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

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

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

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

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

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

- Molecule 18 is a DNA chain called Human gene for U 6 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	74	Total	C	N	O	P	0	0
			1517	727	263	453	74		

- Molecule 19 is a DNA chain called DNA (74-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	70	Total	C	N	O	P	0	0
			1437	686	271	410	70		

- Molecule 20 is a protein called snRNA-activating protein complex subunit 1.



Mol	Chain	Residues	Atoms					AltConf	Trace
20	1	146	Total	C	N	O	S	0	0
			1233	804	212	209	8		

- Molecule 21 is a protein called snRNA-activating protein complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	3	374	Total	C	N	O	S	0	0
			3037	1925	521	570	21		

- Molecule 22 is a protein called snRNA-activating protein complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4	365	Total	C	N	O	S	0	0
			3058	1921	573	555	9		

- Molecule 23 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	176	Total	C	N	O	S	1	0
			1396	907	244	238	7		

- Molecule 24 is a protein called Transcription factor IIIB 50 kDa subunit.

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

- Molecule 25 is a protein called Transcription factor TFIIB component B'' homolog.

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

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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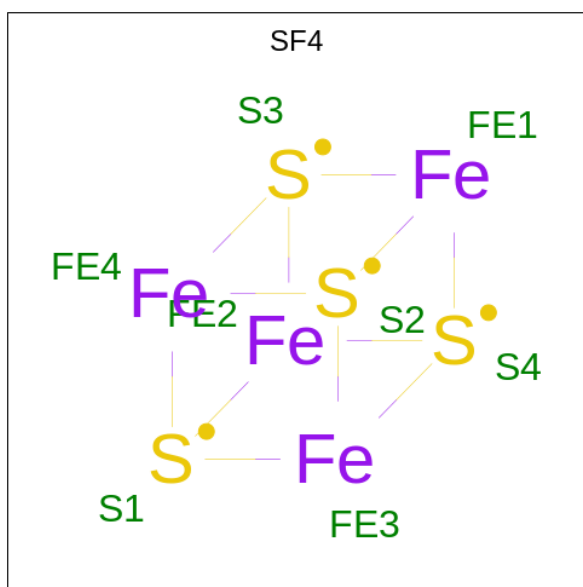
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Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	V	1	Total	Zn	0
			1	1	

- Molecule 27 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



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

### 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.

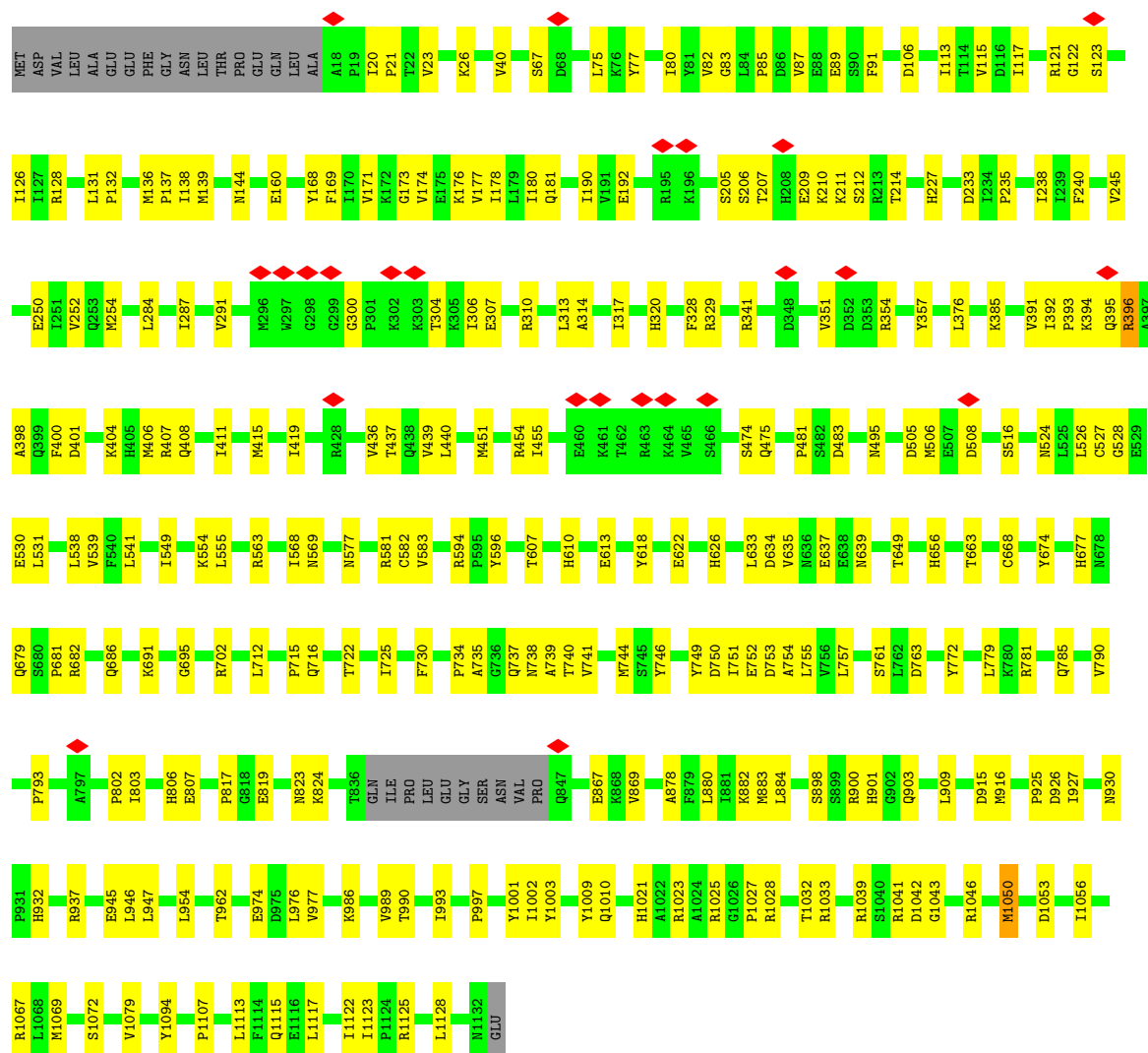
- Molecule 1: DNA-directed RNA polymerase III subunit RPC1





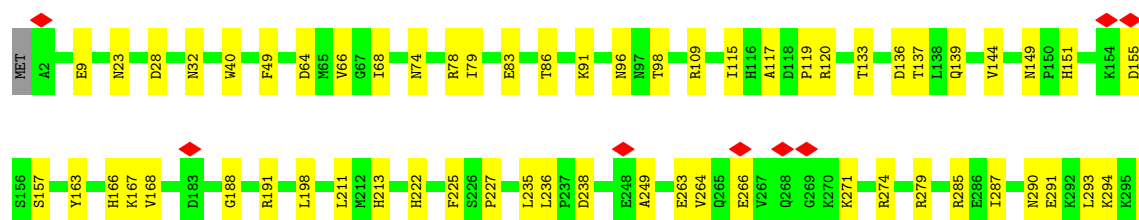
• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

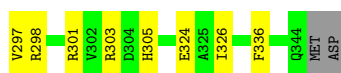
Chain B: 74% 23%



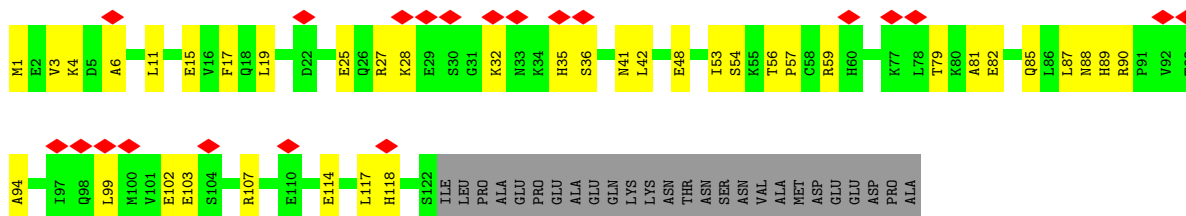
• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 79% 20%

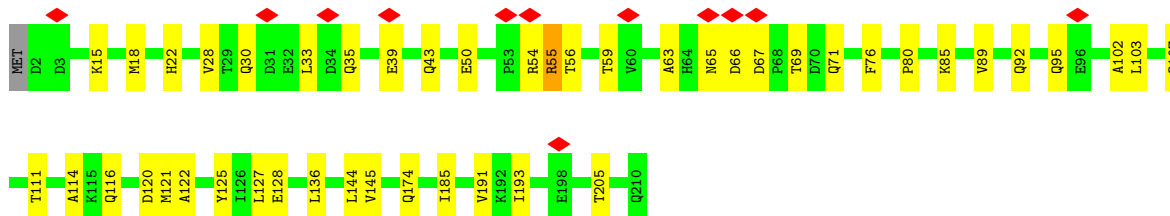
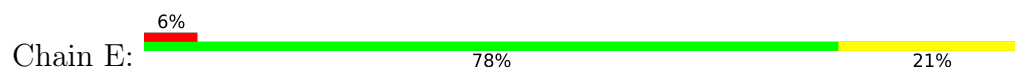




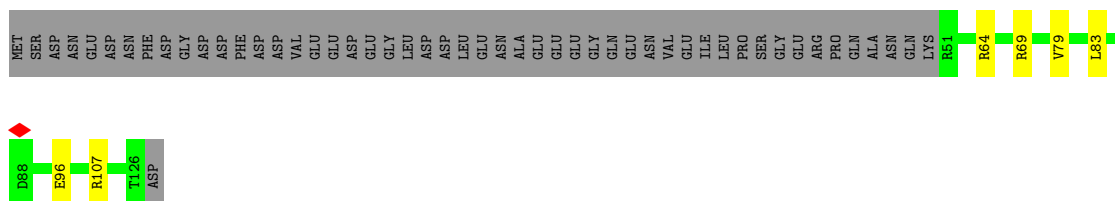
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



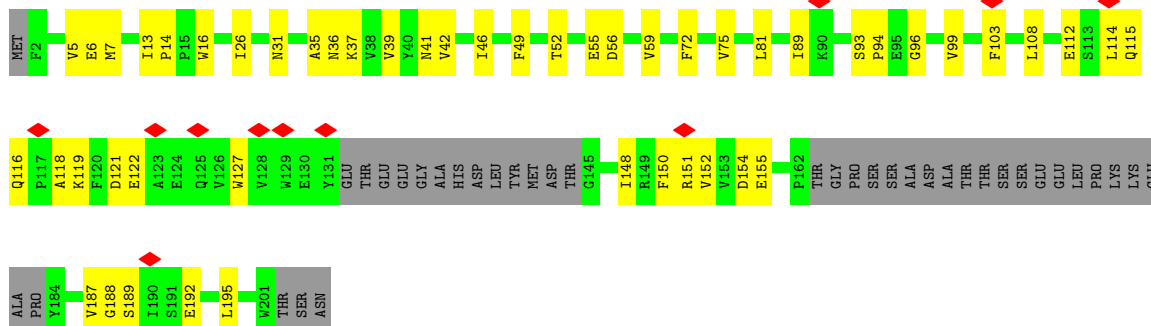
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



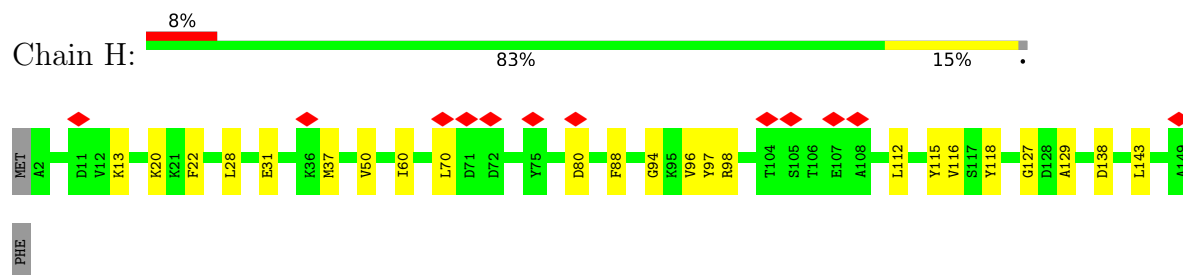
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



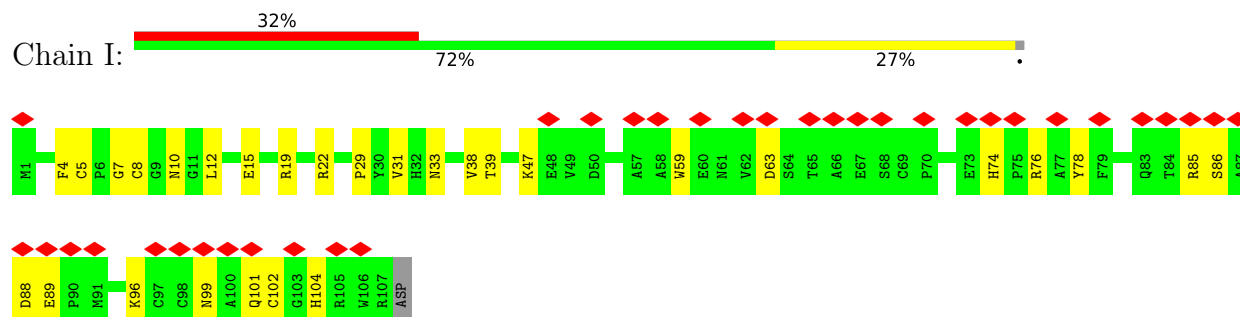
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8



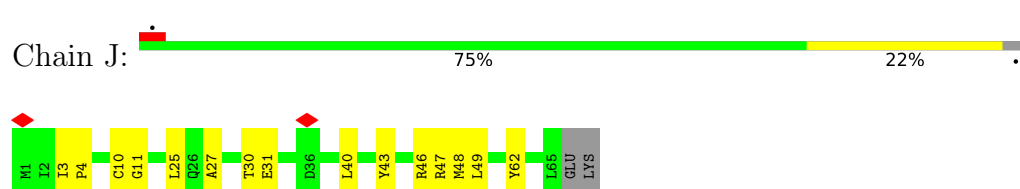
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



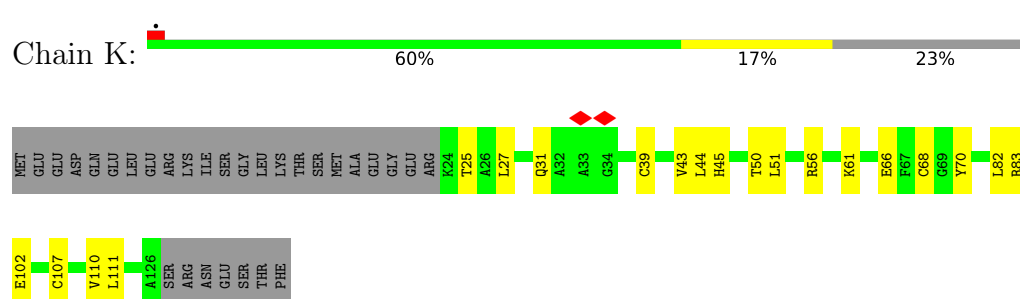
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



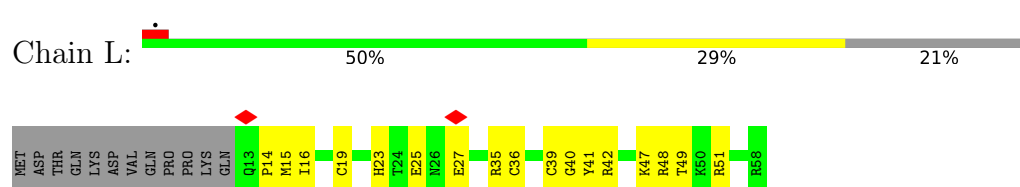
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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



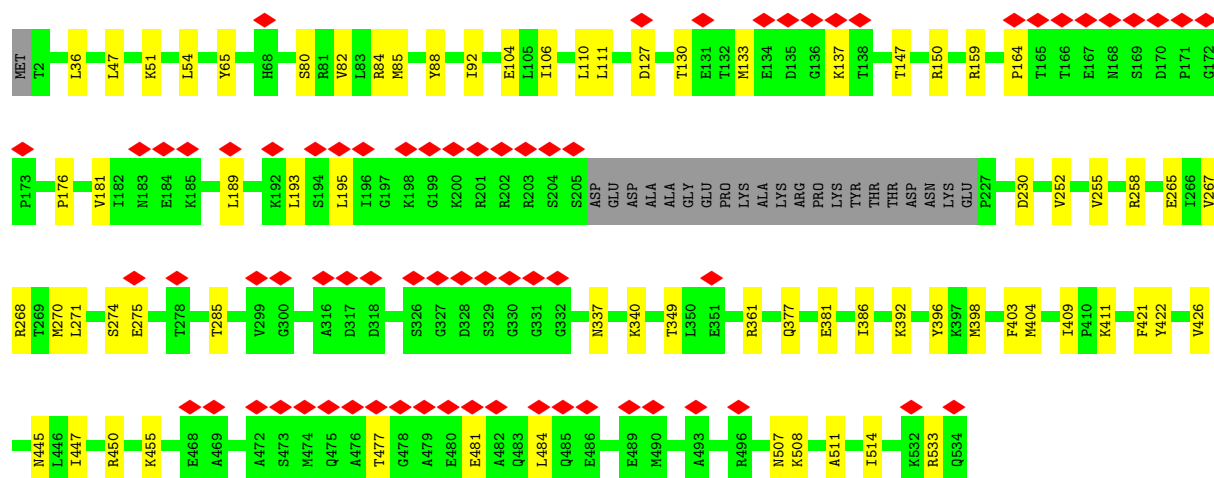
- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



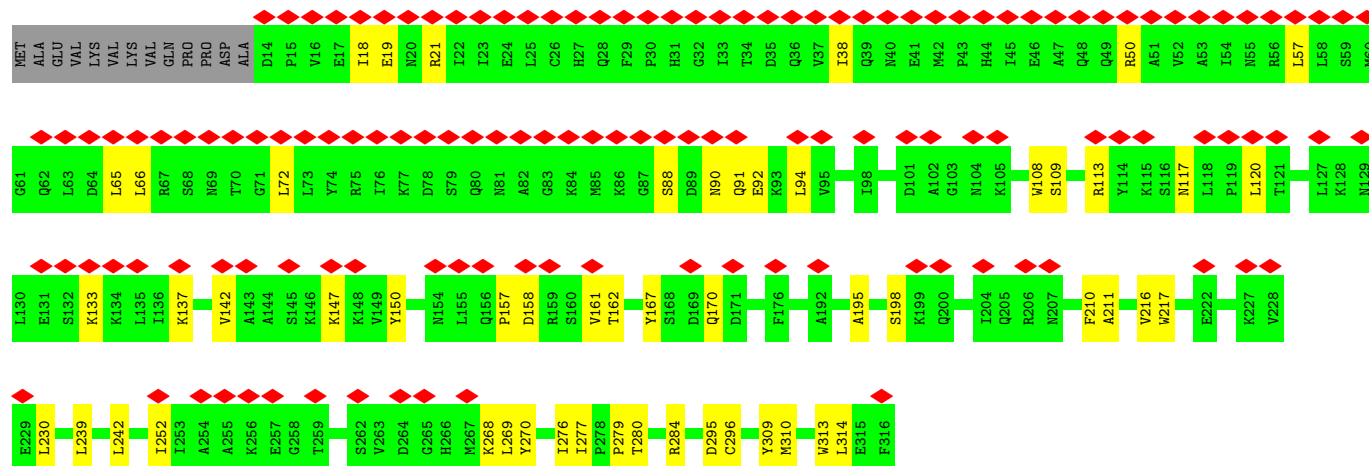
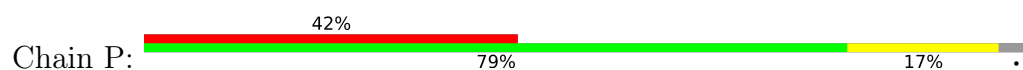
- Molecule 13: DNA-directed RNA polymerase III subunit RPC5



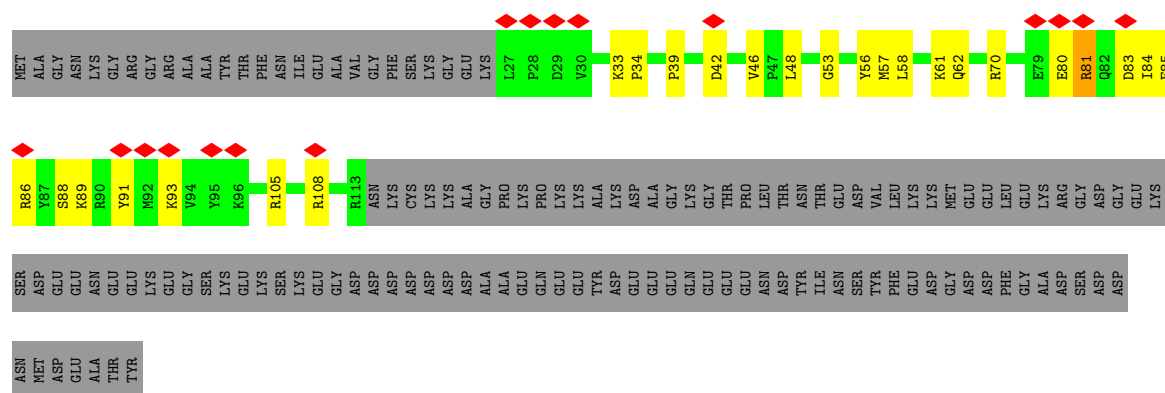




- Molecule 16: DNA-directed RNA polymerase III subunit RPC6



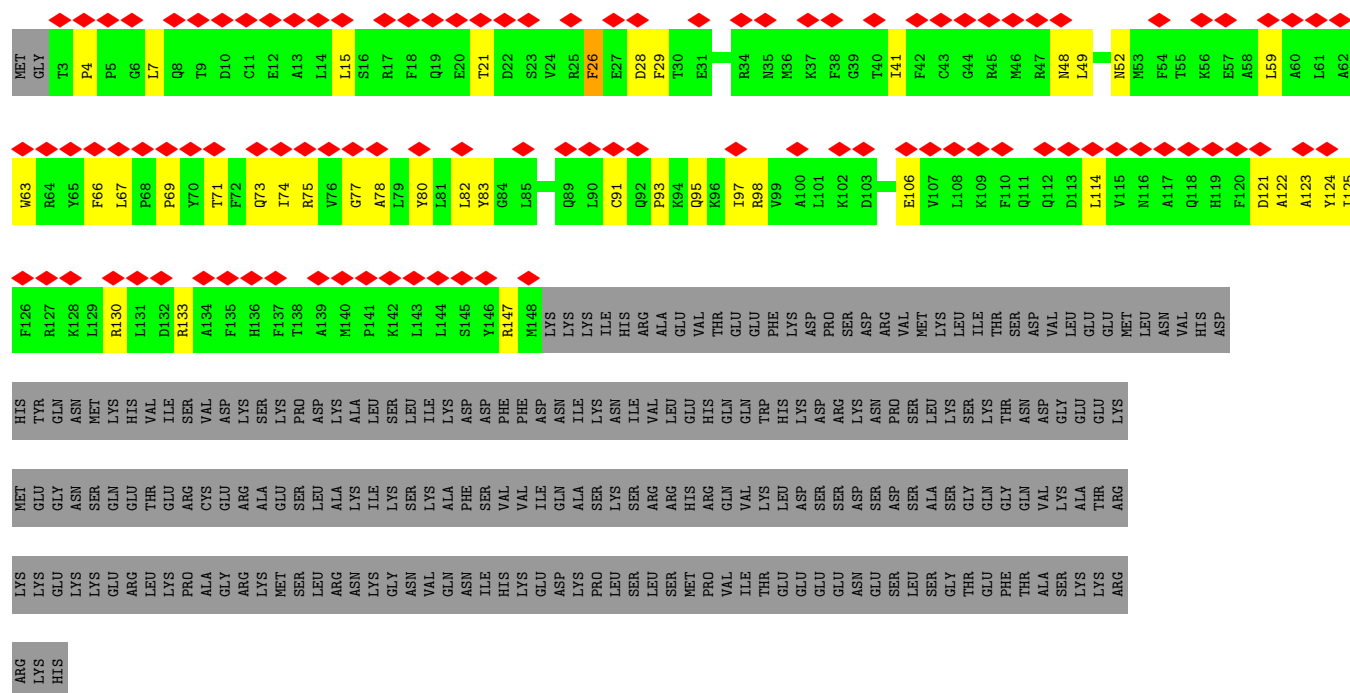
- Molecule 17: DNA-directed RNA polymerase III subunit RPC7



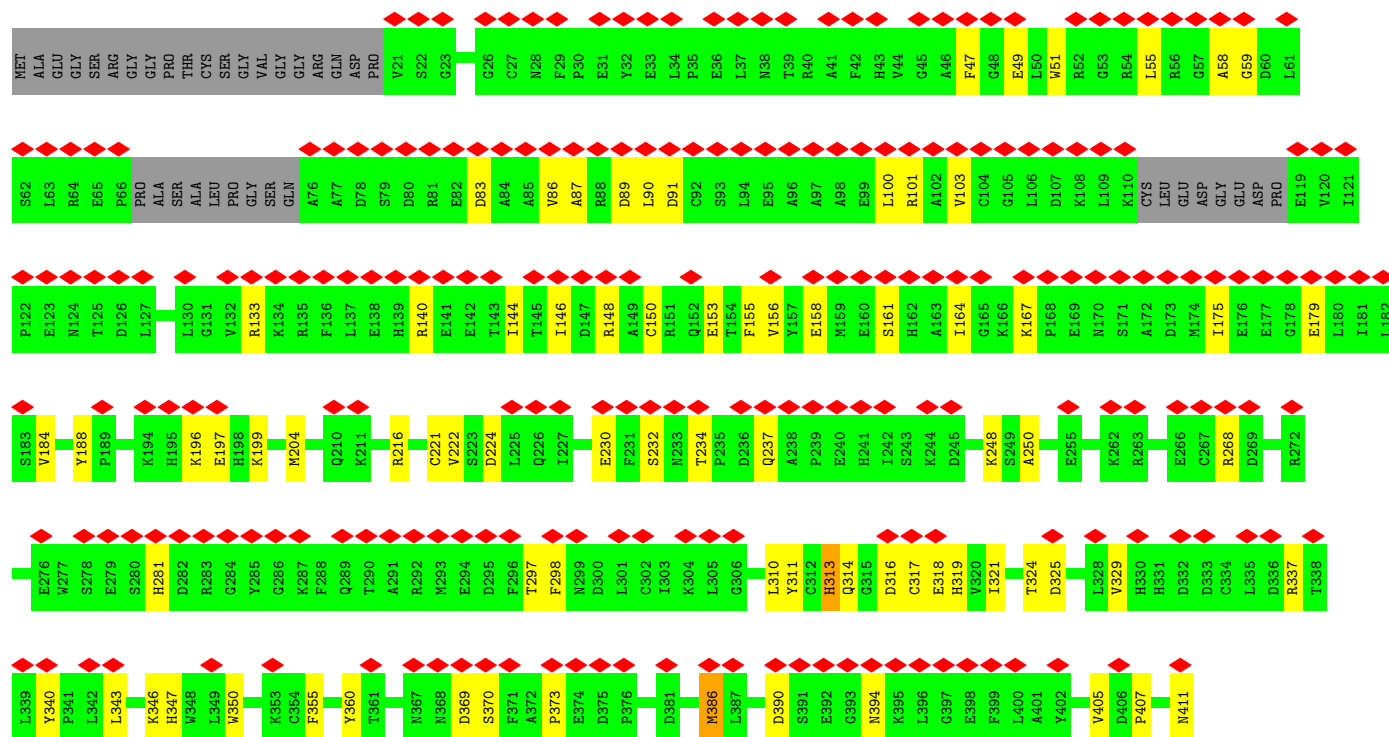
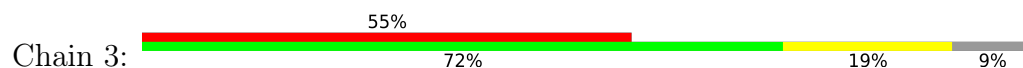
- Molecule 18: Human gene for U 6 RNA







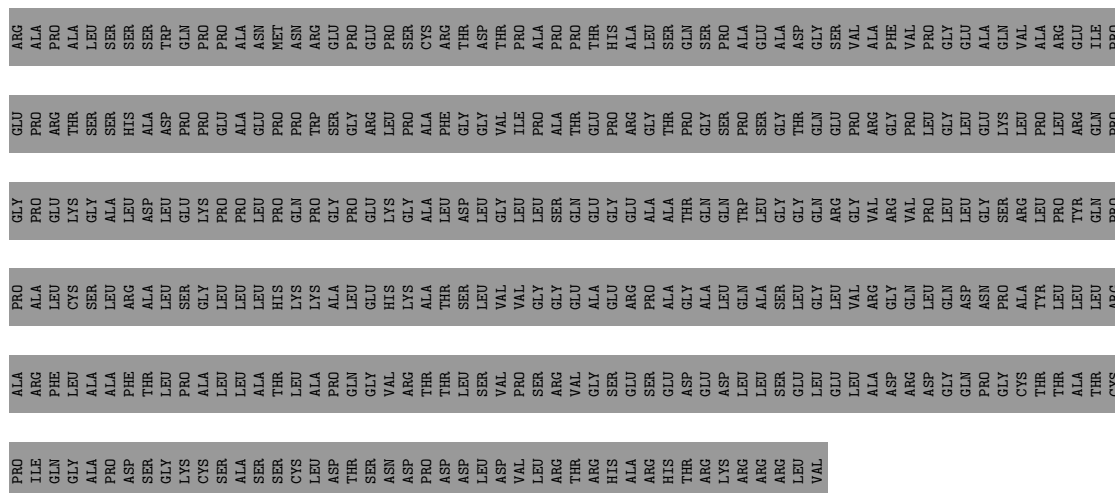
- Molecule 21: snRNA-activating protein complex subunit 3



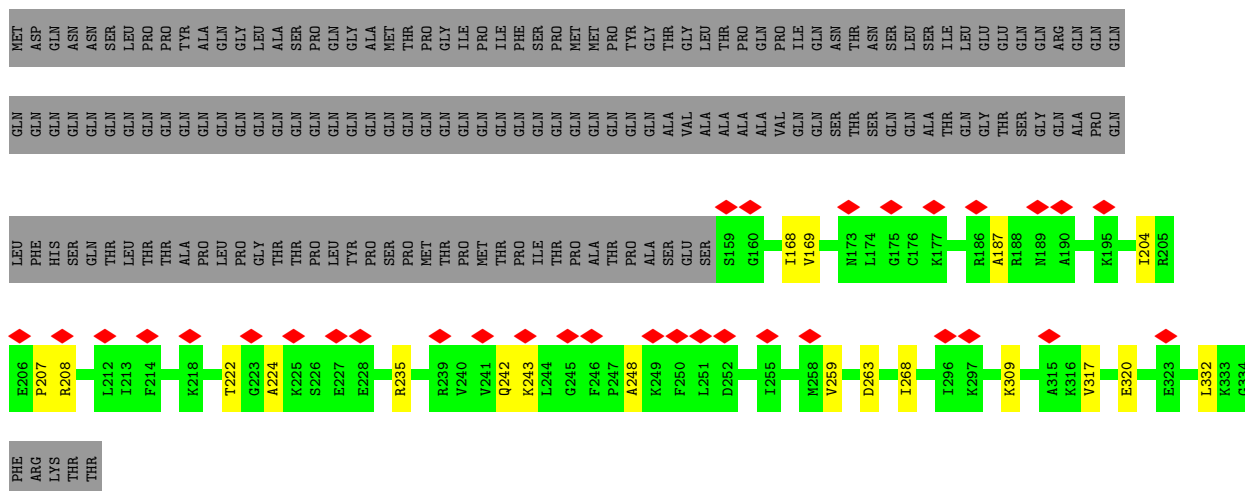
- Molecule 22: snRNA-activating protein complex subunit 4



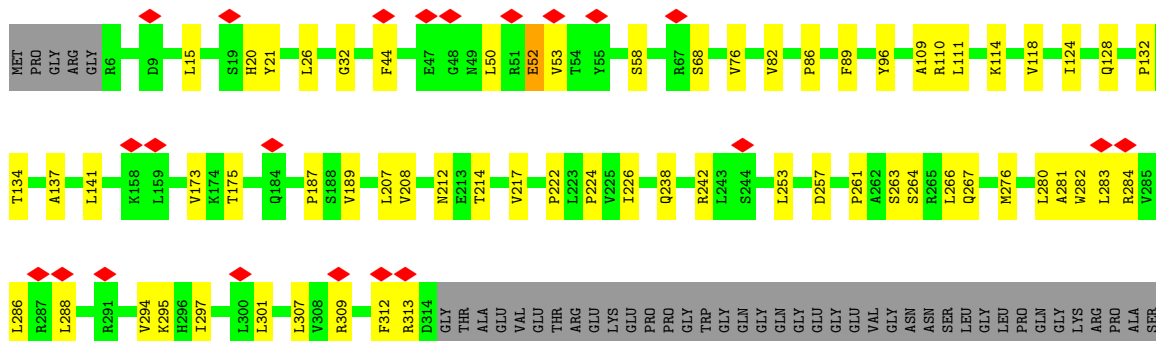


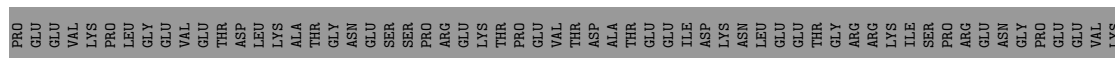


- Molecule 23: TATA-box-binding protein



- Molecule 24: Transcription factor IIIB 50 kDa subunit







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

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37656	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.184	Depositor
Minimum map value	-0.056	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	426.88, 426.88, 426.88	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	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: SF4, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.24	0/11008	0.40	0/14842
2	B	0.24	0/8910	0.40	0/12018
3	C	0.24	0/2790	0.40	0/3782
4	D	0.23	0/997	0.39	0/1343
5	E	0.23	0/1745	0.40	0/2358
6	F	0.23	0/620	0.39	0/839
7	G	0.24	0/1374	0.42	0/1868
8	H	0.24	0/1207	0.43	0/1628
9	I	0.24	0/869	0.44	0/1174
10	J	0.23	0/521	0.37	0/703
11	K	0.23	0/837	0.41	0/1129
12	L	0.23	0/394	0.41	0/524
13	M	0.23	0/3455	0.38	0/4673
14	N	0.23	0/1137	0.44	0/1530
15	O	0.23	0/4141	0.39	0/5592
16	P	0.23	0/2446	0.37	0/3301
17	Q	0.24	0/777	0.39	0/1050
18	X	1.10	1/1697 (0.1%)	1.00	3/2616 (0.1%)
19	Y	0.47	0/1614	0.86	0/2485
20	1	0.24	0/1266	0.38	0/1708
21	3	0.24	0/3112	0.41	0/4206
22	4	0.23	0/3121	0.39	0/4181
23	U	0.24	0/1424	0.43	0/1918
24	V	0.23	0/2904	0.39	0/3941
25	W	0.24	0/967	0.38	0/1293
All	All	0.30	1/59333 (0.0%)	0.45	3/80702 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	-21	DC	O3'-P	-39.90	1.13	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	-21	DC	O3'-P-O5'	-8.67	87.53	104.00
18	X	-21	DC	P-O3'-C3'	-7.90	110.22	119.70
18	X	-19	DT	C1'-O4'-C4'	-5.64	104.46	110.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10814	0	11057	221	0
2	B	8741	0	8867	214	0
3	C	2736	0	2712	54	0
4	D	985	0	1006	33	0
5	E	1715	0	1733	38	0
6	F	610	0	642	6	0
7	G	1337	0	1306	46	0
8	H	1186	0	1147	16	0
9	I	848	0	811	47	0
10	J	512	0	525	13	0
11	K	822	0	810	18	0
12	L	388	0	395	19	0
13	M	3382	0	3376	56	0
14	N	1128	0	1181	33	0
15	O	4075	0	4149	49	0
16	P	2403	0	2409	46	0
17	Q	754	0	759	23	0
18	X	1517	0	844	61	0
19	Y	1437	0	789	32	0
20	1	1233	0	1231	35	0
21	3	3037	0	2911	80	0
22	4	3058	0	3064	68	0
23	U	1396	0	1490	14	0
24	V	2853	0	2892	53	0
25	W	943	0	924	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	2	0	0	0	0
26	B	1	0	0	0	0
26	I	2	0	0	0	0
26	J	1	0	0	0	0
26	L	1	0	0	0	0
26	V	1	0	0	0	0
27	A	1	0	0	0	0
28	P	8	0	0	1	0
All	All	57927	0	57030	1067	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 9.

The worst 5 of 1067 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)
9:I:76:ARG:CD	9:I:99:ASN:HB2	1.23	1.60
2:B:741:VAL:CG2	2:B:1009:TYR:CE2	1.87	1.55
18:X:-21:DC:O3'	18:X:-20:DT:P	1.13	1.52
2:B:741:VAL:HG21	2:B:1009:TYR:CZ	1.36	1.52
9:I:76:ARG:CD	9:I:99:ASN:CB	1.99	1.38

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	1376/1390 (99%)	1342 (98%)	34 (2%)	0	100	100
2	B	1101/1133 (97%)	1072 (97%)	29 (3%)	0	100	100
3	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	120/148 (81%)	115 (96%)	5 (4%)	0	100	100
5	E	207/210 (99%)	205 (99%)	2 (1%)	0	100	100
6	F	74/127 (58%)	73 (99%)	1 (1%)	0	100	100
7	G	160/204 (78%)	151 (94%)	9 (6%)	0	100	100
8	H	146/150 (97%)	146 (100%)	0	0	100	100
9	I	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
10	J	63/67 (94%)	61 (97%)	2 (3%)	0	100	100
11	K	101/133 (76%)	100 (99%)	1 (1%)	0	100	100
12	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
13	M	418/708 (59%)	403 (96%)	15 (4%)	0	100	100
14	N	140/317 (44%)	140 (100%)	0	0	100	100
15	O	508/534 (95%)	497 (98%)	11 (2%)	0	100	100
16	P	301/316 (95%)	295 (98%)	6 (2%)	0	100	100
17	Q	85/223 (38%)	82 (96%)	3 (4%)	0	100	100
20	1	144/368 (39%)	142 (99%)	2 (1%)	0	100	100
21	3	368/411 (90%)	356 (97%)	12 (3%)	0	100	100
22	4	363/1469 (25%)	350 (96%)	13 (4%)	0	100	100
23	U	175/339 (52%)	173 (99%)	2 (1%)	0	100	100
24	V	358/419 (85%)	349 (98%)	9 (2%)	0	100	100
25	W	109/2624 (4%)	105 (96%)	4 (4%)	0	100	100
All	All	6807/11802 (58%)	6636 (98%)	171 (2%)	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	A	1200/1212 (99%)	1195 (100%)	5 (0%)	91	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	964/988 (98%)	961 (100%)	3 (0%)	92	95
3	C	299/302 (99%)	298 (100%)	1 (0%)	92	95
4	D	114/136 (84%)	114 (100%)	0	100	100
5	E	191/192 (100%)	189 (99%)	2 (1%)	76	85
6	F	66/111 (60%)	66 (100%)	0	100	100
7	G	149/181 (82%)	149 (100%)	0	100	100
8	H	129/131 (98%)	129 (100%)	0	100	100
9	I	92/93 (99%)	92 (100%)	0	100	100
10	J	53/56 (95%)	53 (100%)	0	100	100
11	K	92/119 (77%)	92 (100%)	0	100	100
12	L	43/55 (78%)	42 (98%)	1 (2%)	50	70
13	M	377/622 (61%)	376 (100%)	1 (0%)	92	95
14	N	131/276 (48%)	130 (99%)	1 (1%)	81	88
15	O	458/476 (96%)	455 (99%)	3 (1%)	84	90
16	P	269/280 (96%)	269 (100%)	0	100	100
17	Q	84/195 (43%)	82 (98%)	2 (2%)	49	69
20	1	130/334 (39%)	129 (99%)	1 (1%)	81	88
21	3	330/356 (93%)	320 (97%)	10 (3%)	41	64
22	4	321/1213 (26%)	318 (99%)	3 (1%)	78	87
23	U	152/293 (52%)	152 (100%)	0	100	100
24	V	325/365 (89%)	323 (99%)	2 (1%)	86	92
25	W	102/2381 (4%)	101 (99%)	1 (1%)	76	85
All	All	6071/10367 (59%)	6035 (99%)	36 (1%)	86	92

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	3	355	PHE
25	W	309	ASP
21	3	386	MET
22	4	461	GLU
13	M	319	MET

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

Mol	Chain	Res	Type
13	M	315	GLN
24	V	206	GLN
16	P	117	ASN
24	V	129	HIS
22	4	438	GLN

### 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 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
28	SF4	P	401	-	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
28	SF4	P	401	-	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	P	401	SF4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	-21:DC	O3'	-20:DT	P	1.13

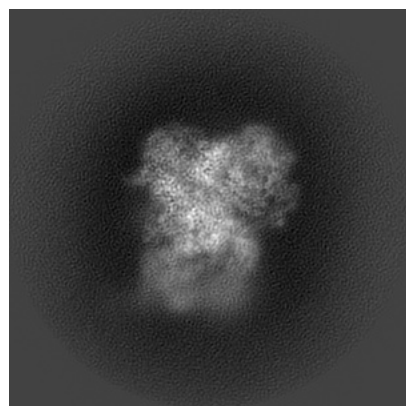
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35719. These allow visual inspection of the internal detail of the map and identification of artifacts.

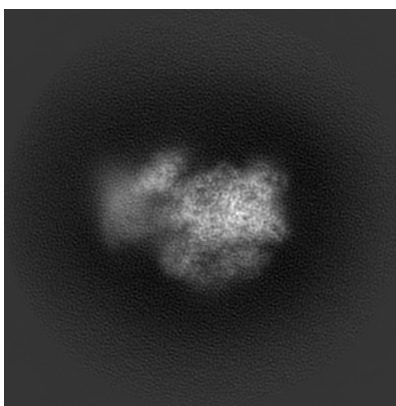
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

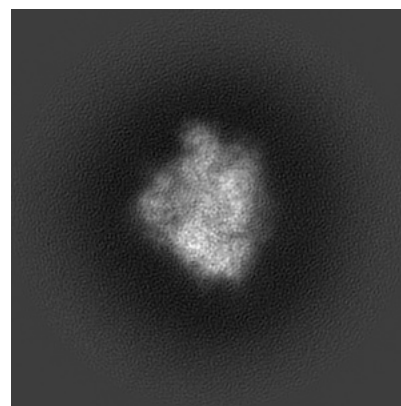
#### 6.1.1 Primary map



X

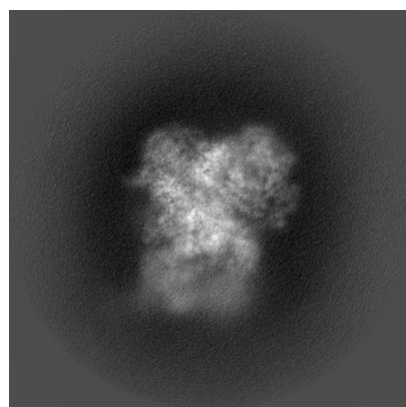


Y

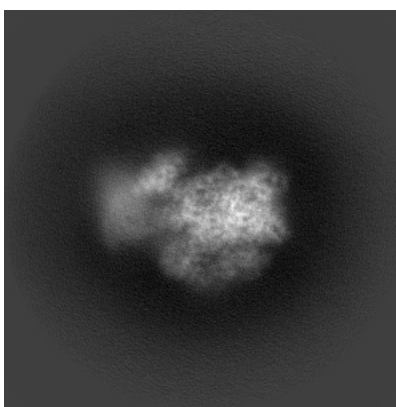


Z

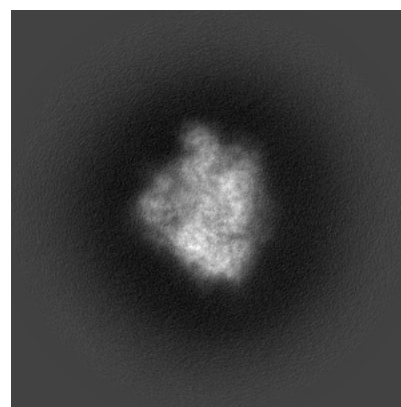
#### 6.1.2 Raw map



X



Y



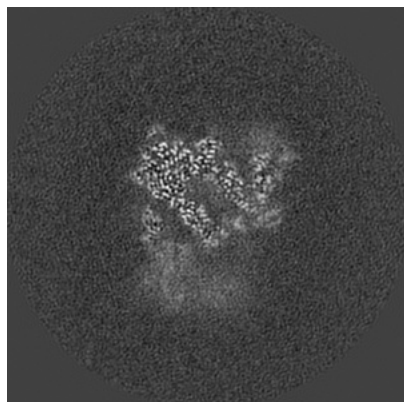
Z

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

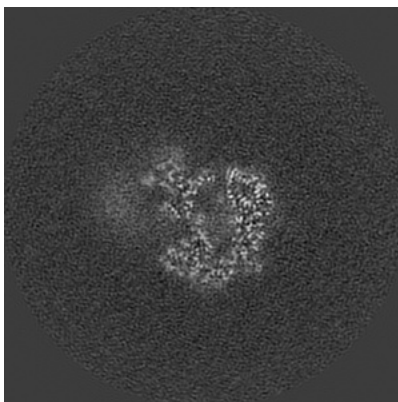


## 6.2 Central slices [i](#)

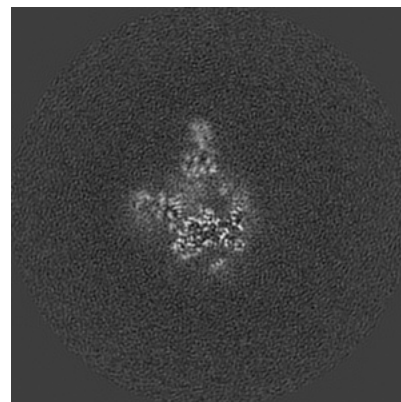
### 6.2.1 Primary map



X Index: 160

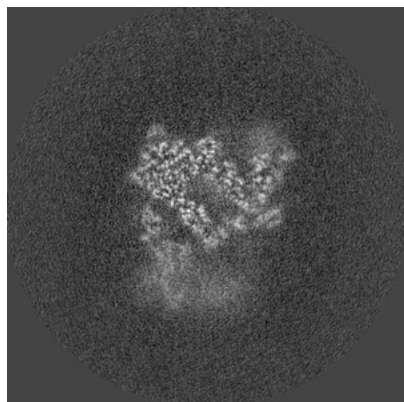


Y Index: 160

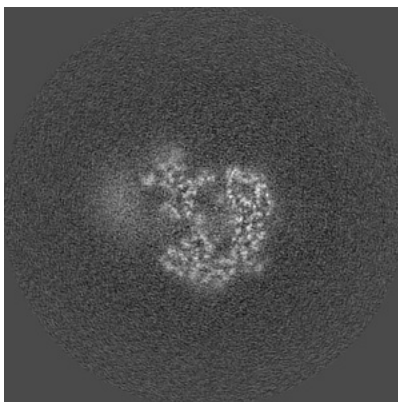


Z Index: 160

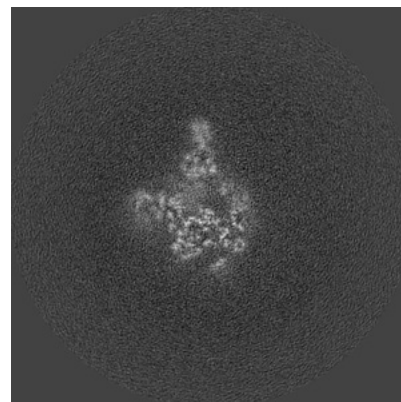
### 6.2.2 Raw map



X Index: 160



Y Index: 160

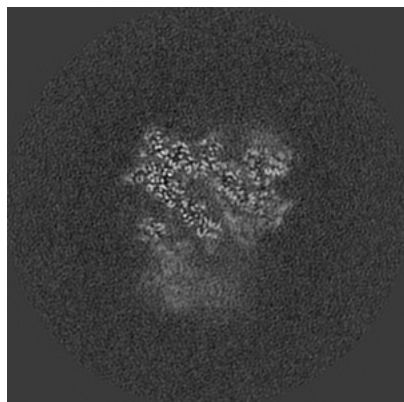


Z Index: 160

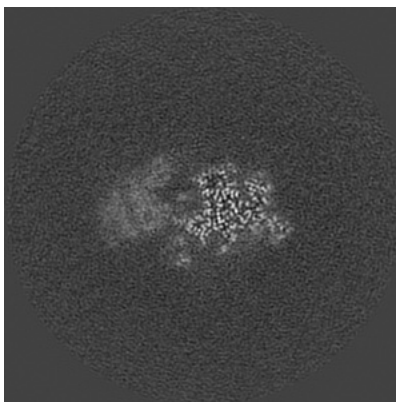
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

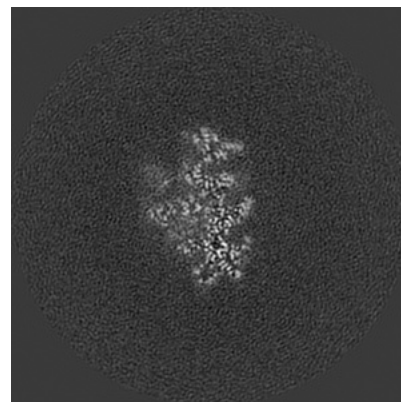
### 6.3.1 Primary map



X Index: 156

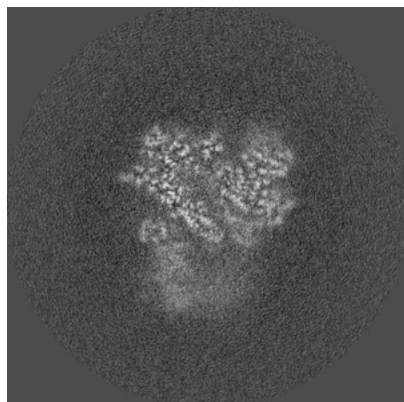


Y Index: 130

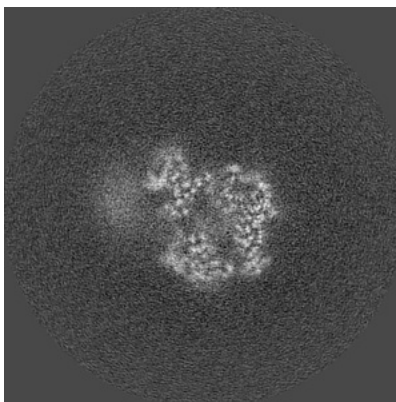


Z Index: 186

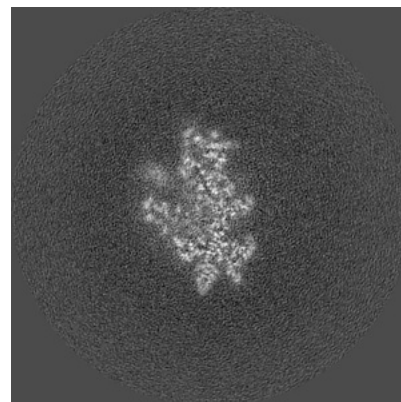
### 6.3.2 Raw map



X Index: 154



Y Index: 164

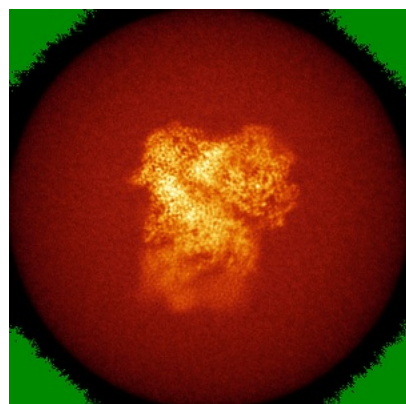


Z Index: 182

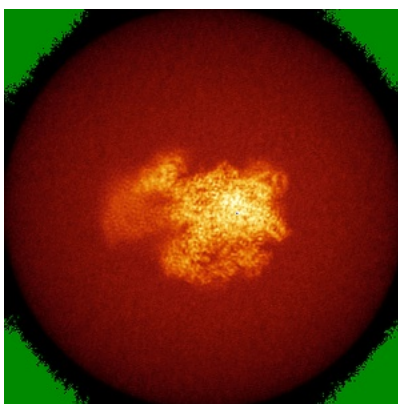
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

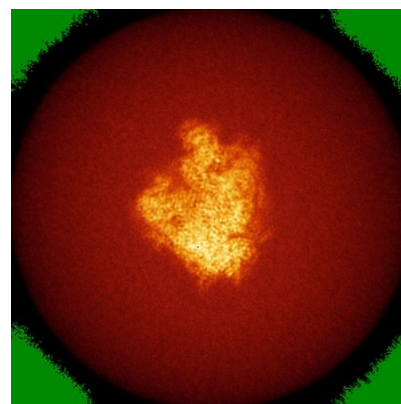
### 6.4.1 Primary map



X

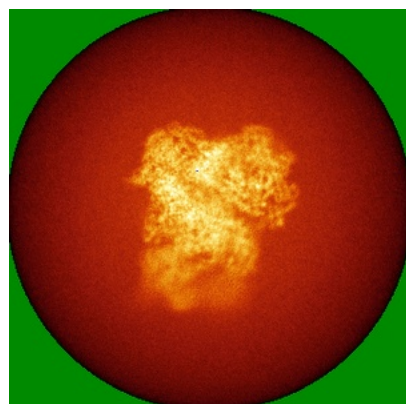


Y

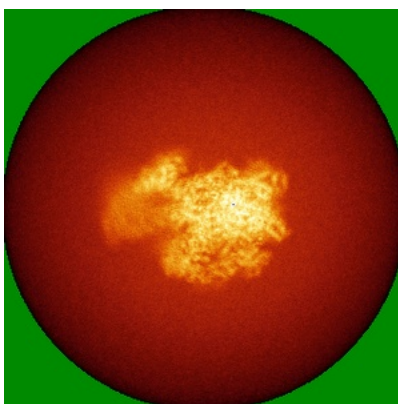


Z

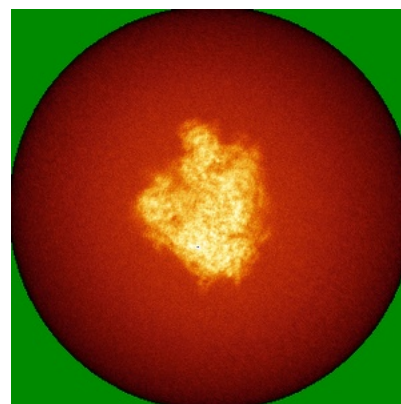
### 6.4.2 Raw map



X



Y



Z

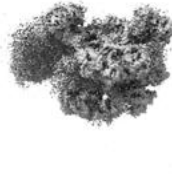
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 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 0.024. 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.

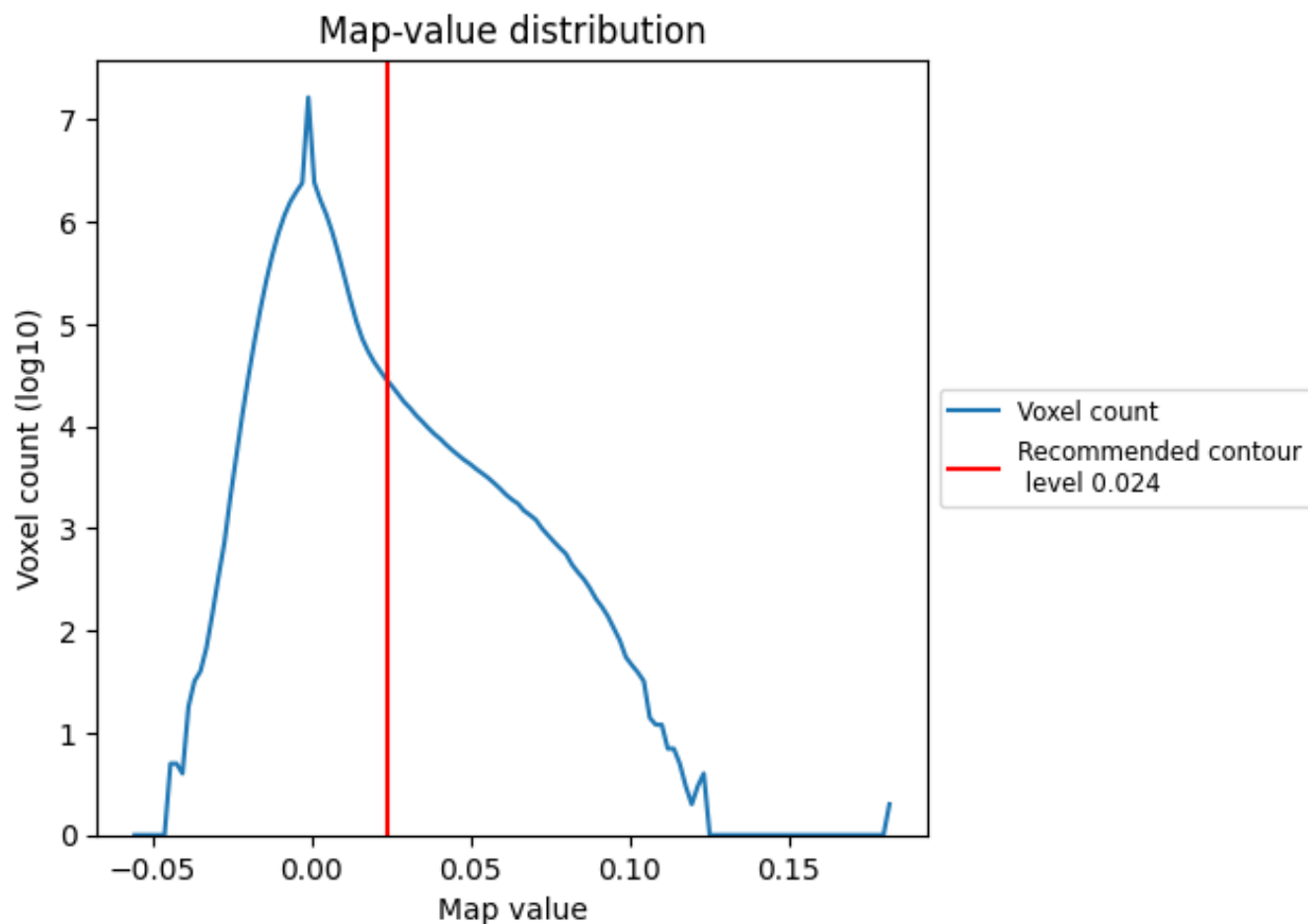
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

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

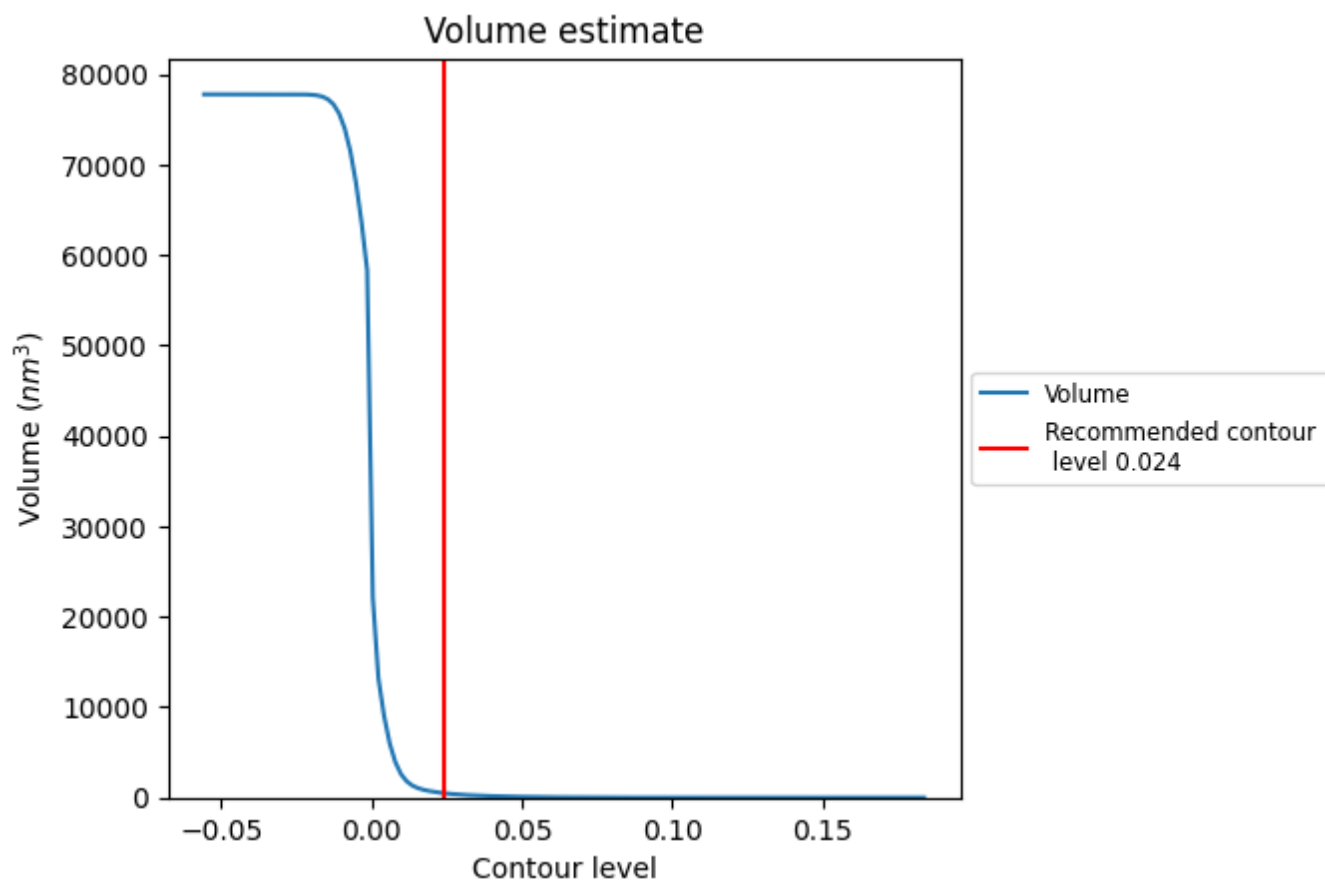
### 7.1 Map-value distribution [i](#)



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.



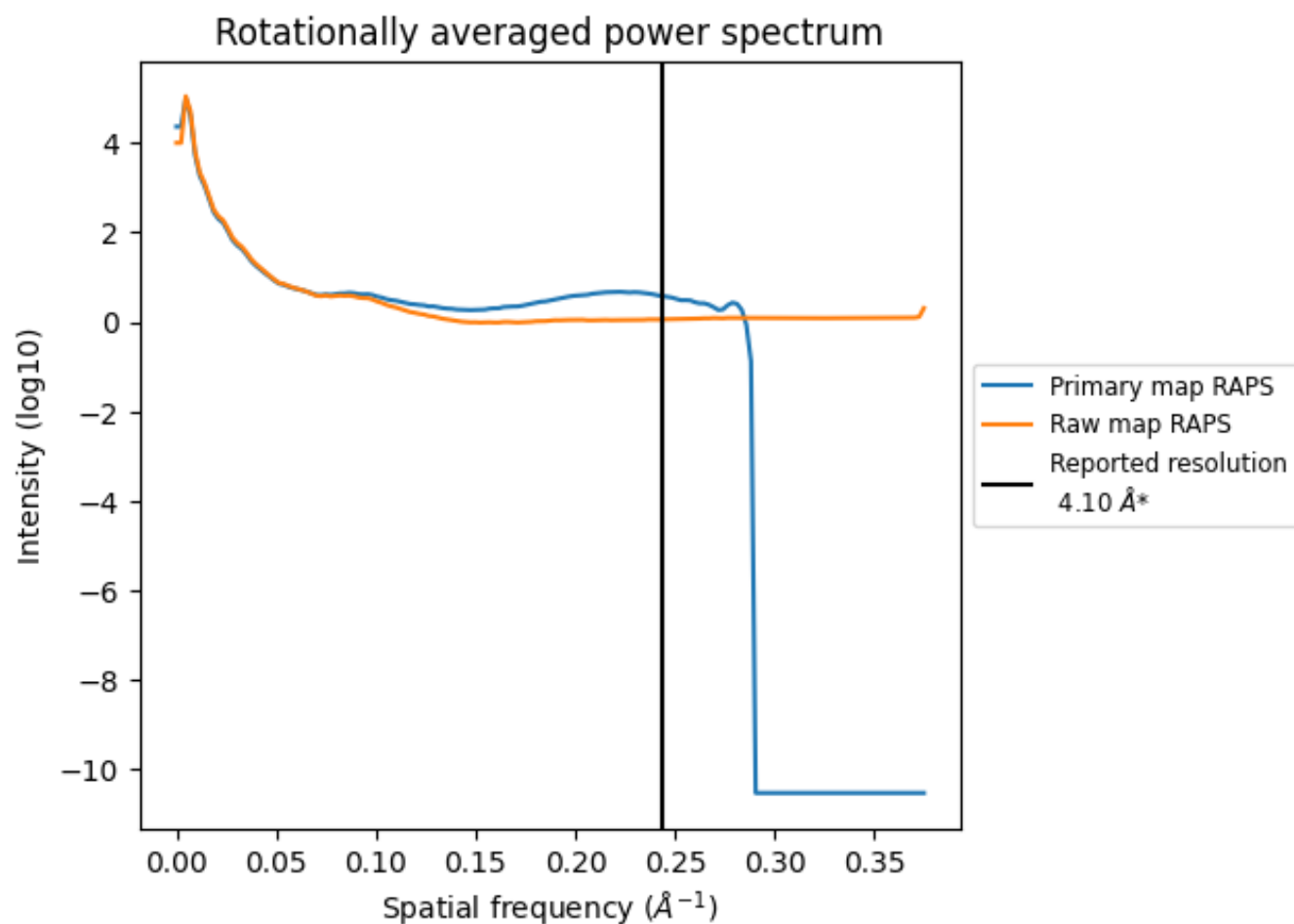
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 491 nm<sup>3</sup>; this corresponds to an approximate mass of 443 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 ⓘ

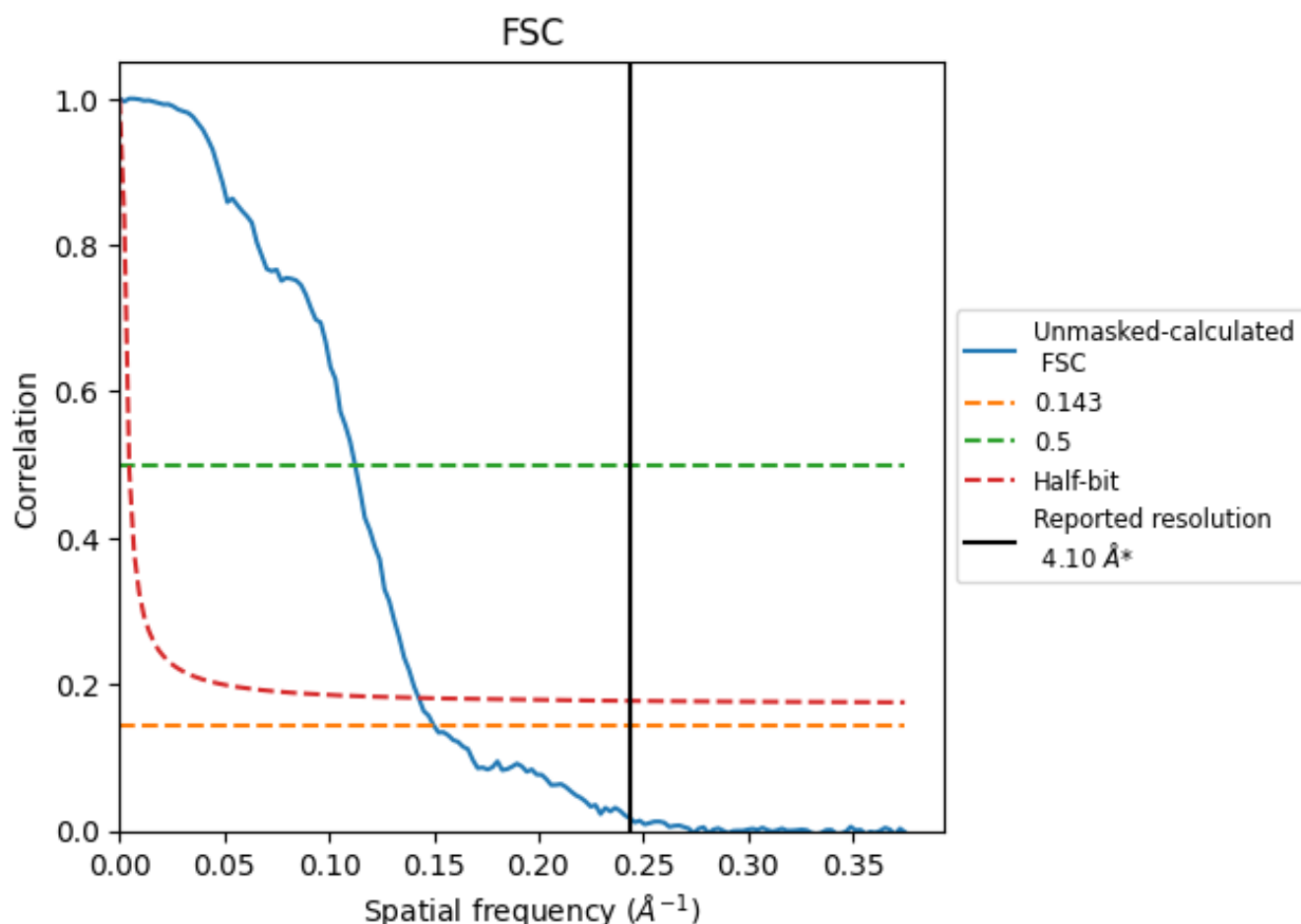


\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.244 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

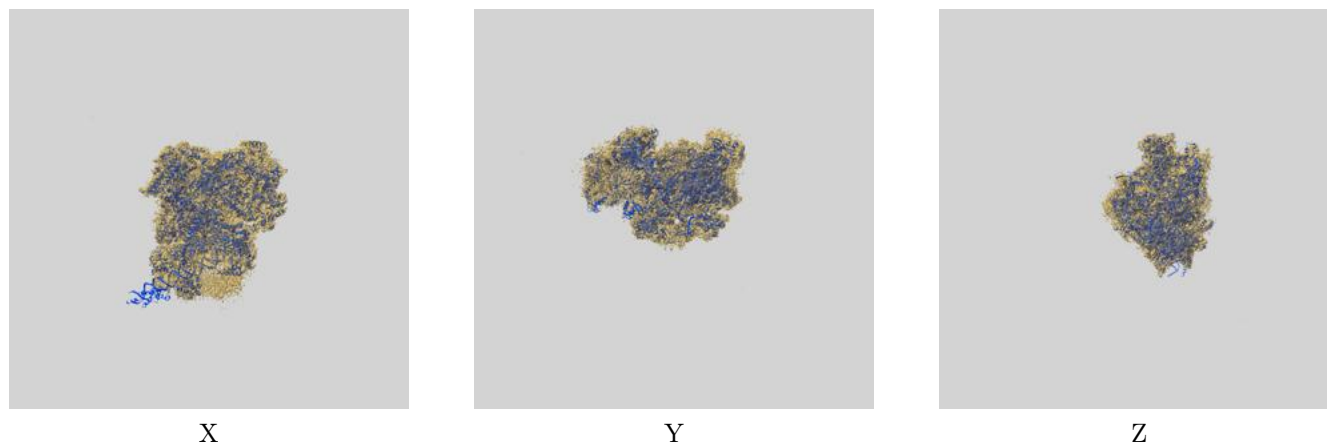
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.66	8.89	7.00

\*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 6.66 differs from the reported value 4.1 by more than 10 %

## 9 Map-model fit [i](#)

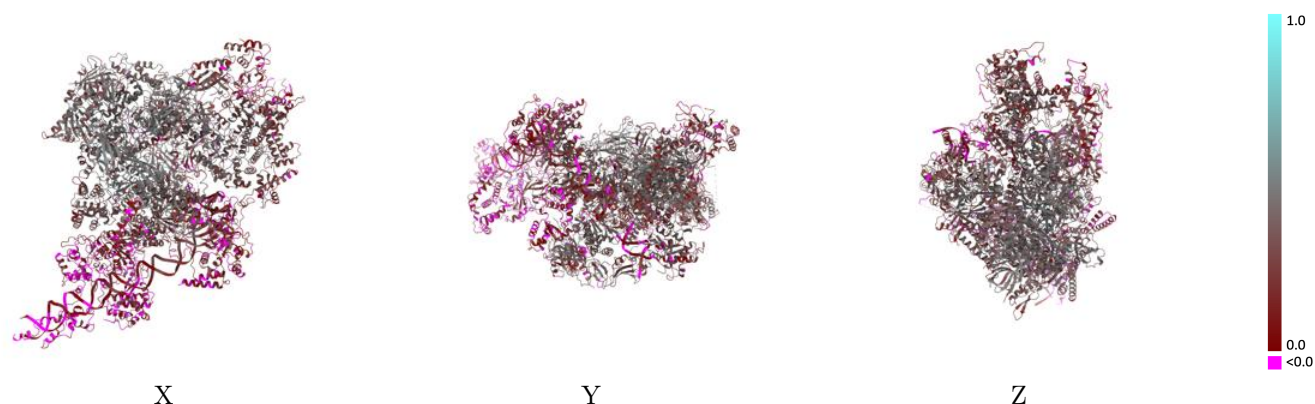
This section contains information regarding the fit between EMDB map EMD-35719 and PDB model 8IUE. Per-residue inclusion information can be found in section [3](#) on page [11](#).

### 9.1 Map-model overlay [i](#)



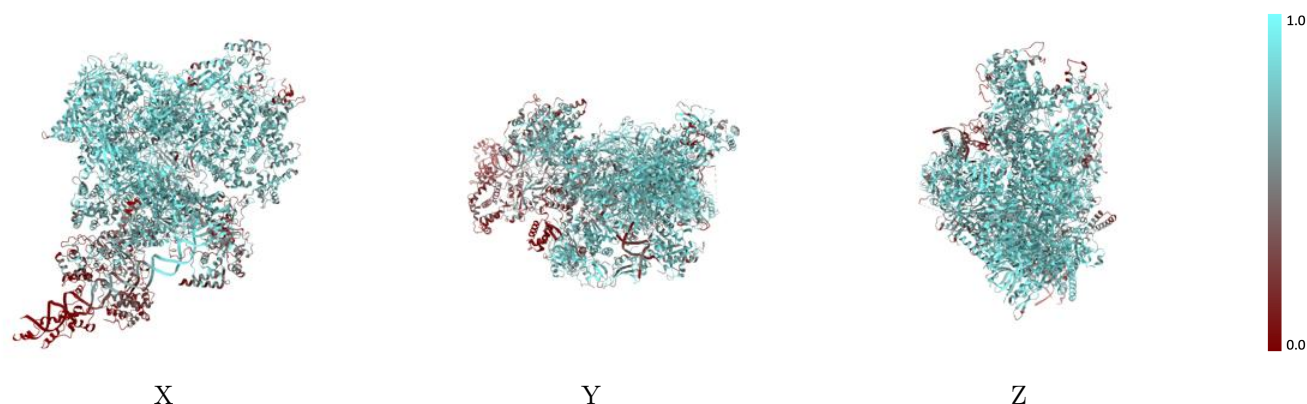
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



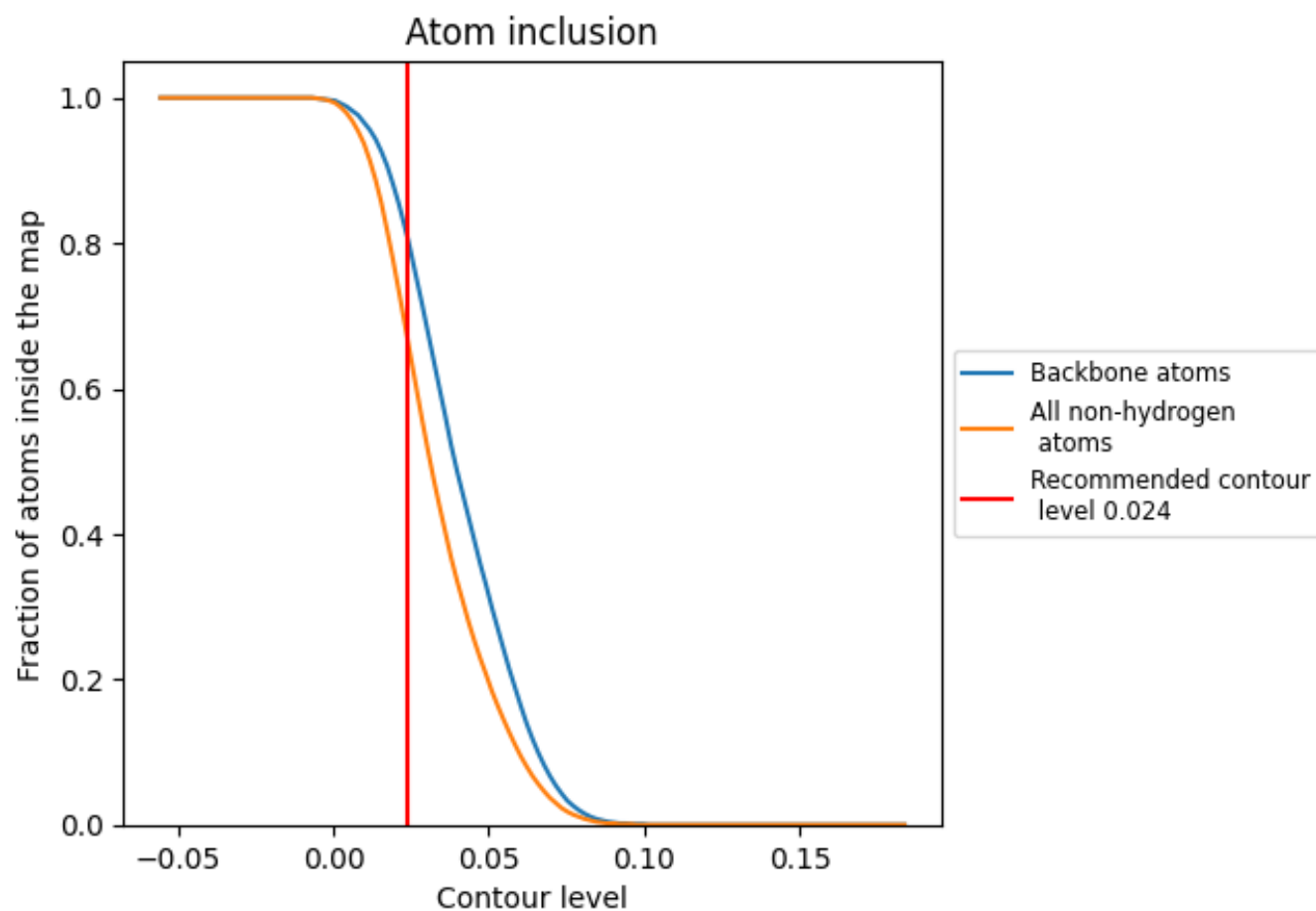
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.024).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 66% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6640	 0.2910
1	 0.2820	 0.0650
3	 0.3490	 0.0760
4	 0.2470	 0.0710
A	 0.8020	 0.3840
B	 0.8210	 0.4140
C	 0.8060	 0.4180
D	 0.6290	 0.2170
E	 0.7260	 0.3030
F	 0.8490	 0.4310
G	 0.7610	 0.2970
H	 0.7430	 0.3900
I	 0.5820	 0.2510
J	 0.8360	 0.4250
K	 0.8050	 0.4080
L	 0.8120	 0.3960
M	 0.6600	 0.2980
N	 0.6300	 0.2830
O	 0.6900	 0.3000
P	 0.4530	 0.1740
Q	 0.6580	 0.2710
U	 0.6290	 0.2020
V	 0.6670	 0.2600
W	 0.5160	 0.1200
X	 0.4920	 0.1070
Y	 0.5000	 0.1160

