



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:00 AM UTC

PDB ID : 8IUH / pdb_00008iuh
EMDB ID : EMD-35722
Title : RNA polymerase III pre-initiation complex open complex 1
Authors : Hou, H.; Jin, Q.; Ren, Y.; Wang, Q.; Xu, Y.
Deposited on : 2023-03-24
Resolution : 3.40 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:

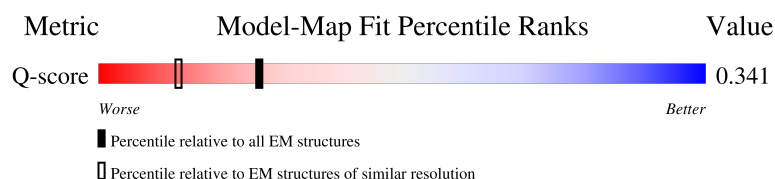
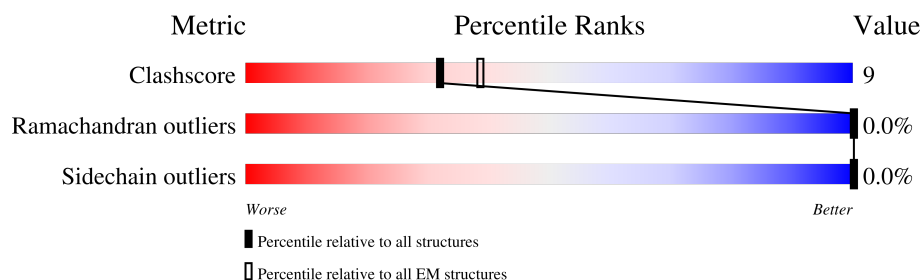
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.40 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.



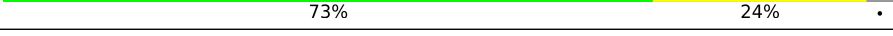
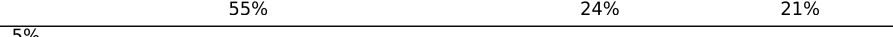
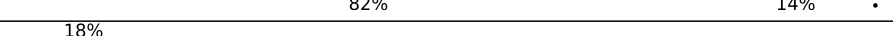
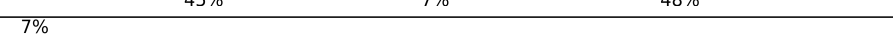
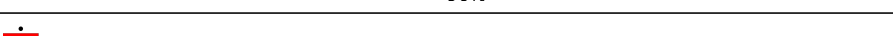
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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 $\leq 5\%$. 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	1	368	
2	3	411	
3	4	1469	
4	A	1390	

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Mol	Chain	Length	Quality of chain
5	B	1133	
6	C	346	
7	D	148	
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	317	
18	O	534	
19	P	316	
20	Q	223	
21	U	339	
22	V	419	
23	W	2624	
24	X	464	
25	Y	464	

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 58239 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
1	1	146	Total	C	N	O	S	0	0
			1233	804	212	209	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	374	Total	C	N	O	S	0	0
			3037	1925	521	570	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	365	Total	C	N	O	S	0	0
			3058	1921	573	555	9		

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

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

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

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

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

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

- 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	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 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		

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 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	176	Total	C	N	O	S	1	0
			1396	907	244	238	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 (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	81	Total	C	N	O	P	0	0
			1661	795	288	497	81		

- Molecule 25 is a DNA chain called DNA (81-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	81	Total	C	N	O	P	0	0
			1666	793	317	475	81		

- Molecule 26 is ZINC ION (CCD ID: 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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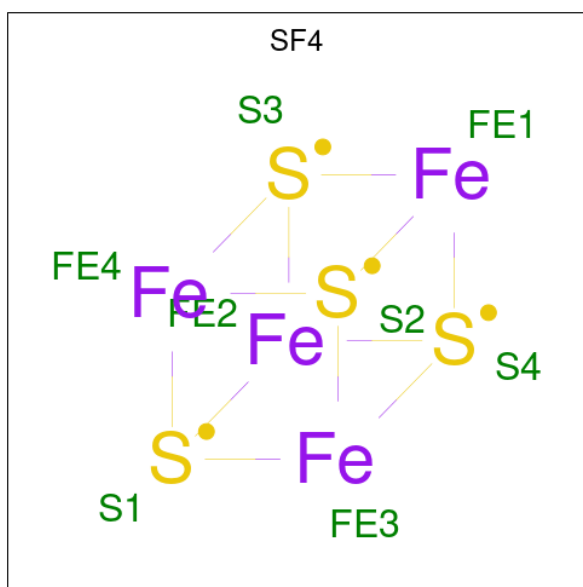
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Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	V	1	Total	Zn	0
			1	1	

- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 28 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

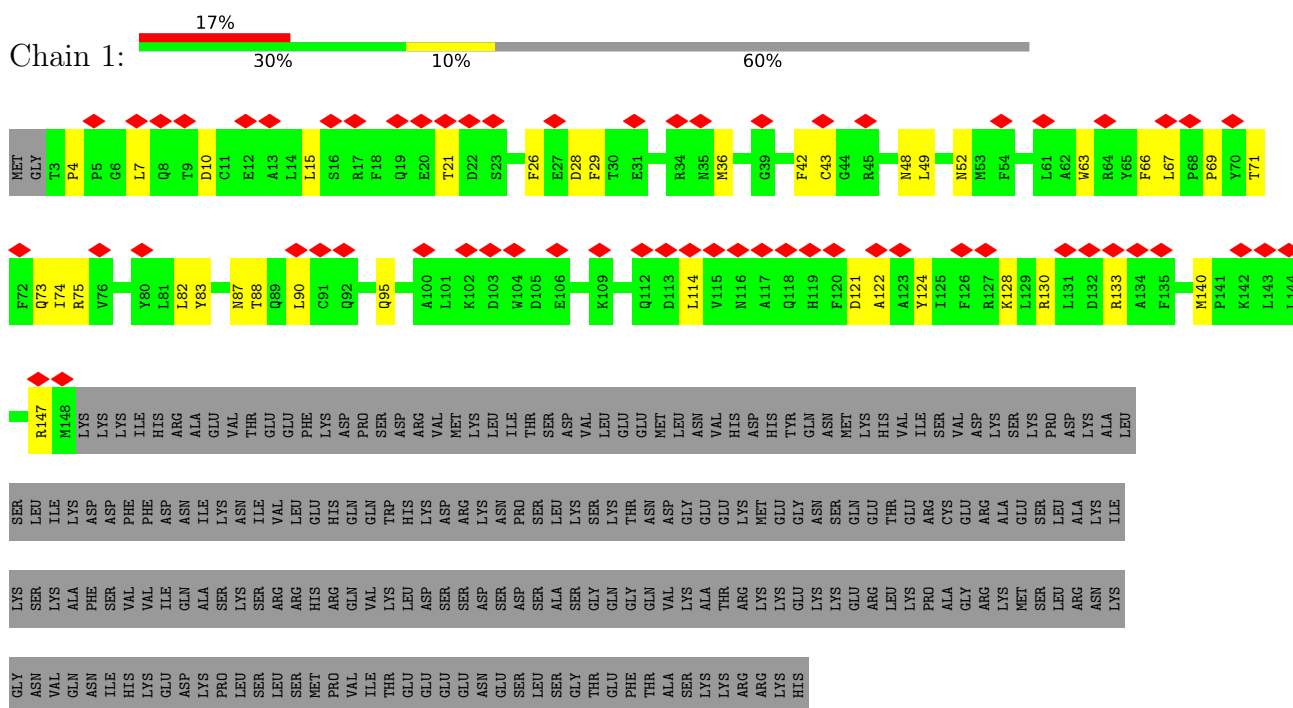


Mol	Chain	Residues	Atoms			AltConf
28	P	1	Total	Fe	S	0
			8	4	4	

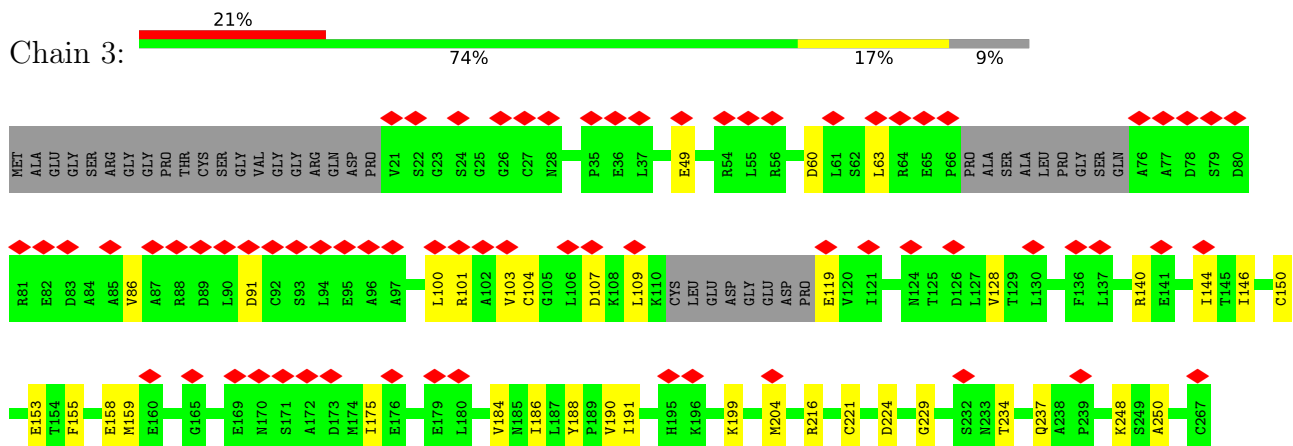
3 Residue-property plots

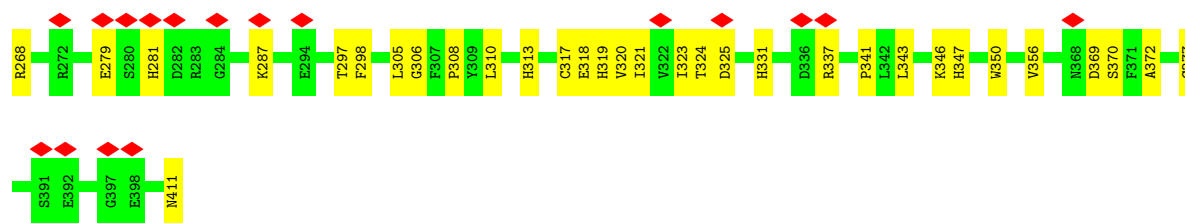
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

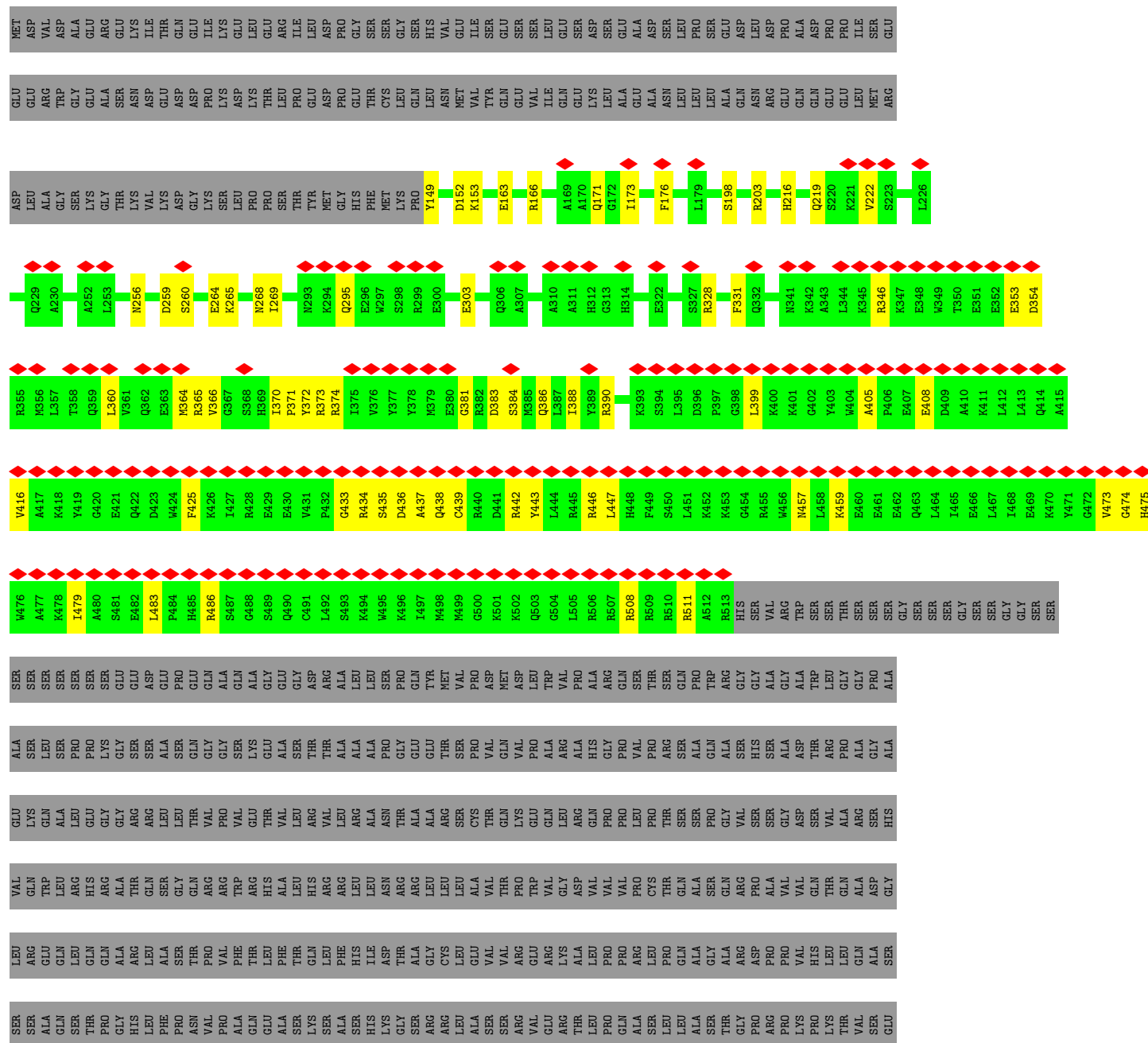


• Molecule 2: snRNA-activating protein complex subunit 3



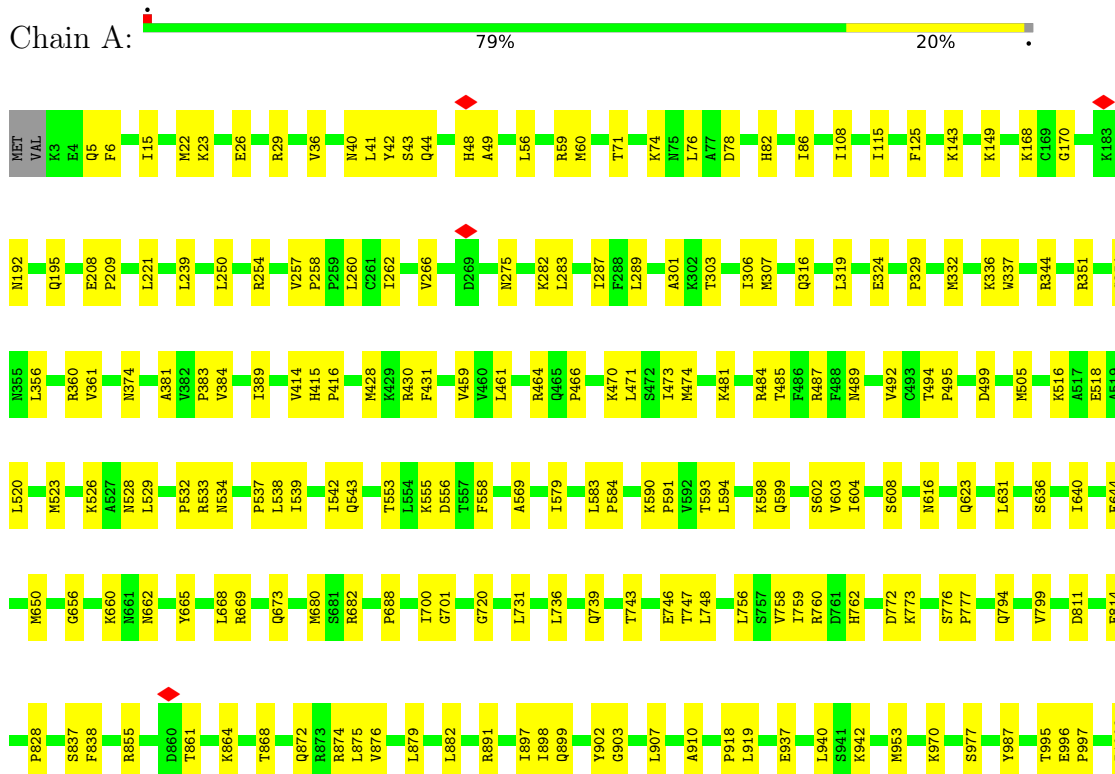


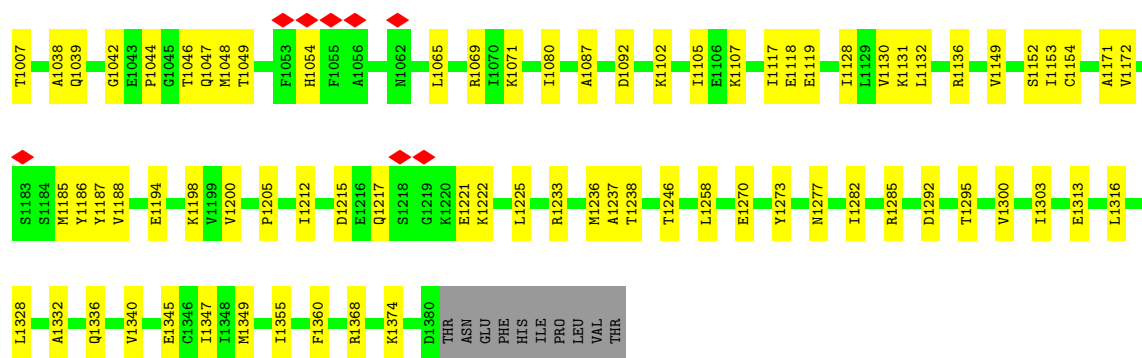
• Molecule 3: snRNA-activating protein complex subunit 4



[illegible]

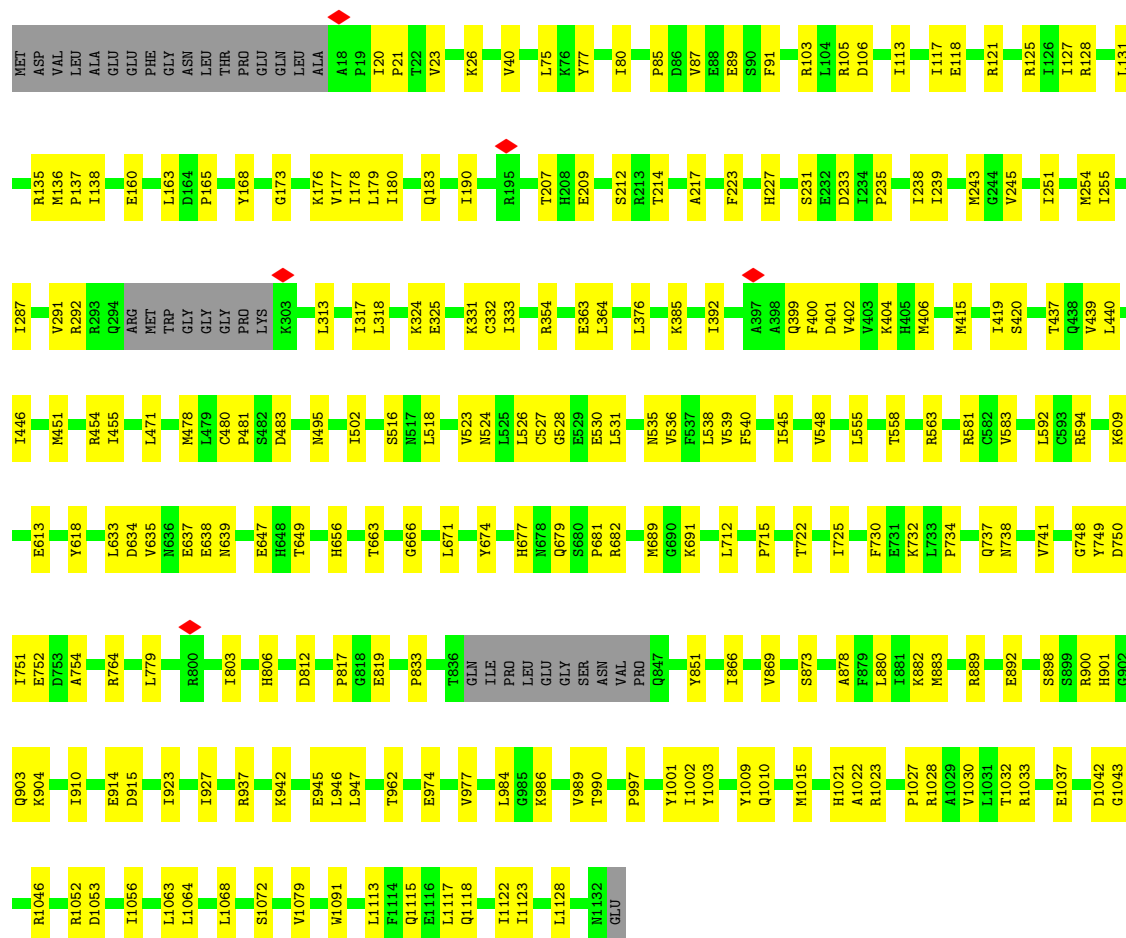
- Molecule 4: DNA-directed RNA polymerase III subunit RPC1





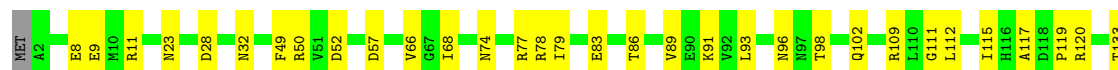
• Molecule 5: DNA-directed RNA polymerase III subunit RPC2

Chain B: 76% 20%



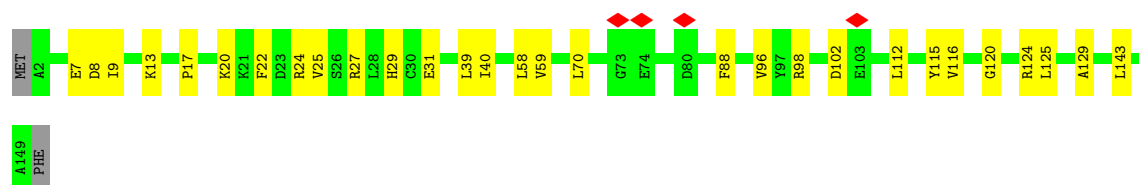
• Molecule 6: DNA-directed RNA polymerases I and III subunit RPAC1

Chain C: 77% 22%



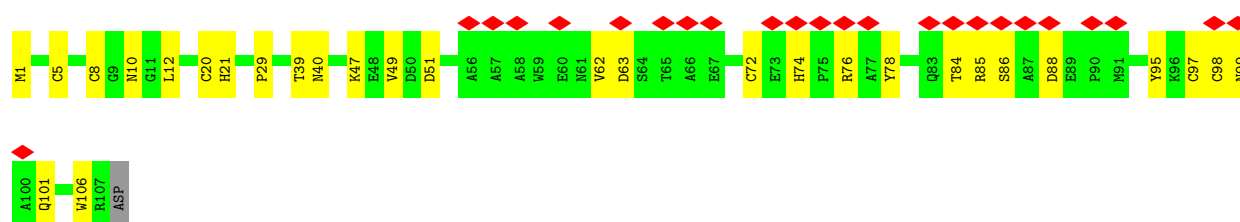
- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 



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

Chain I: 



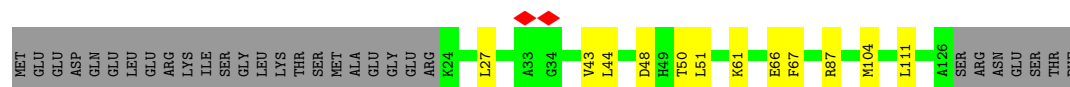
- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J: 



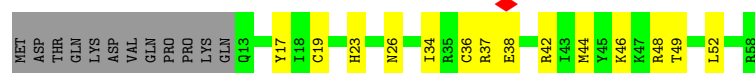
- Molecule 14: DNA-directed RNA polymerases I and III subunit RPAC2

Chain K: 



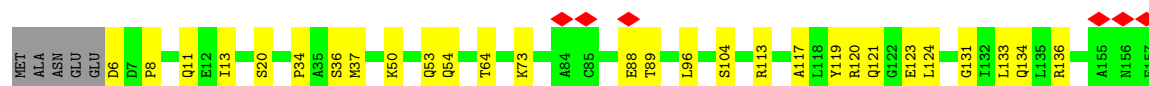
- Molecule 15: DNA-directed RNA polymerases I, II, and III subunit RPABC4

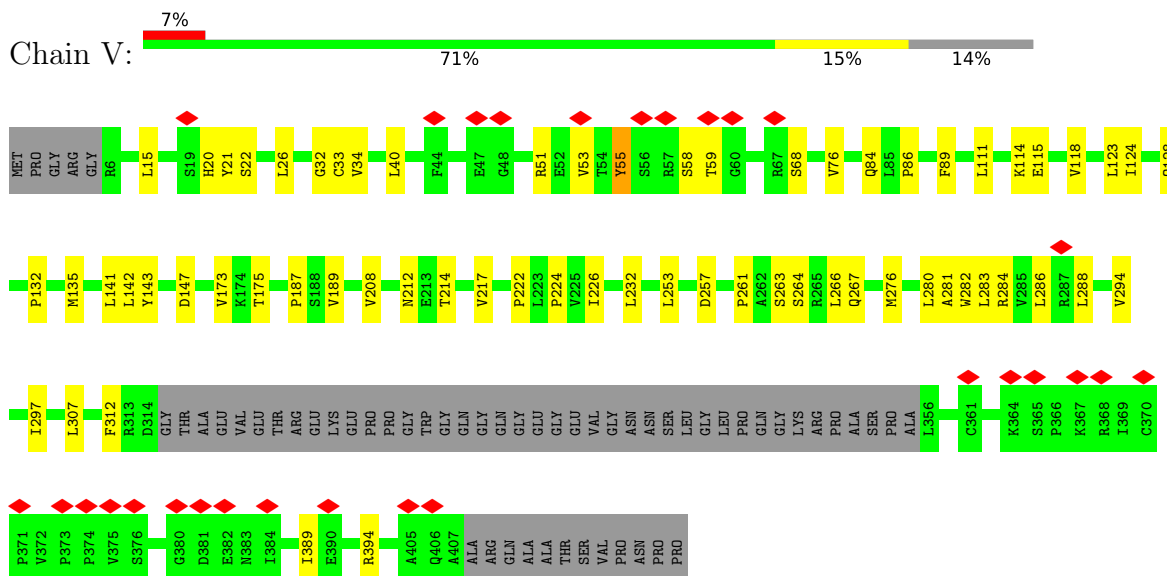
Chain L: 



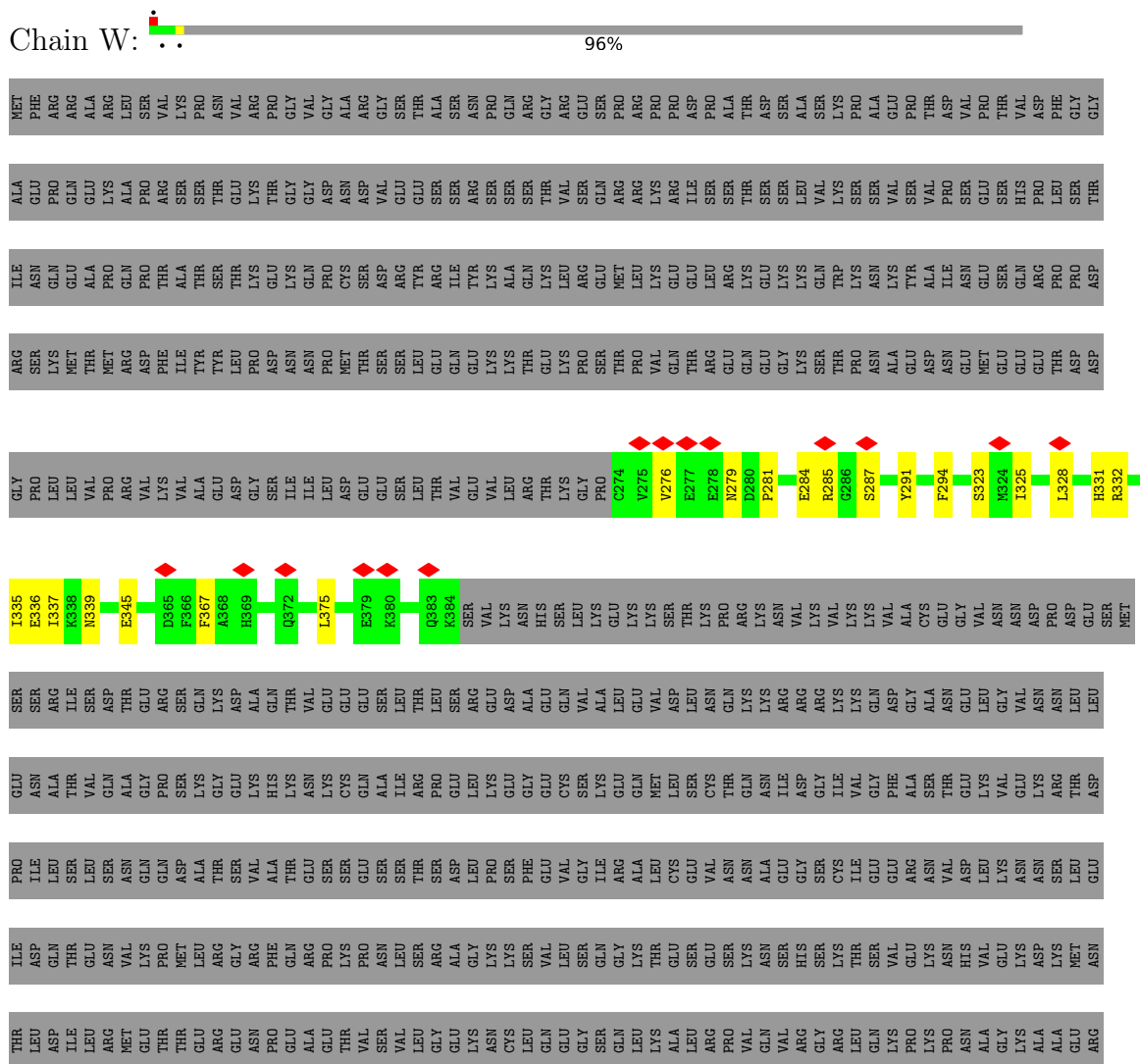
- Molecule 16: DNA-directed RNA polymerase III subunit RPC5

Chain M: 





- Molecule 23: Transcription factor TFIIB component B'' homolog





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

- Molecule 24: DNA (81-MER)

[illegible]

DC DA DT DG DG DG DA DA DA DT DA DG DG DC DC DC DT DC DT DT DC DC DT DG DC DC DC DG DA DC DC DT DT

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	107630	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	0.271	Depositor
Minimum map value	-0.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	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, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.13	0/1266	0.28	0/1708
2	3	0.12	0/3112	0.33	0/4206
3	4	0.11	0/3121	0.31	0/4181
4	A	0.10	0/11008	0.28	0/14842
5	B	0.09	0/8845	0.27	0/11930
6	C	0.10	0/2790	0.29	0/3782
7	D	0.10	0/997	0.31	0/1343
8	E	0.09	0/1745	0.26	0/2358
9	F	0.10	0/620	0.29	0/839
10	G	0.11	0/1374	0.30	0/1868
11	H	0.09	0/1207	0.28	0/1628
12	I	0.12	0/869	0.31	0/1174
13	J	0.09	0/521	0.27	0/703
14	K	0.11	0/837	0.32	0/1129
15	L	0.11	0/394	0.35	0/524
16	M	0.09	0/3455	0.27	0/4673
17	N	0.09	0/1137	0.26	0/1530
18	O	0.09	0/4141	0.27	0/5592
19	P	0.09	0/2446	0.26	0/3301
20	Q	0.10	0/777	0.28	0/1050
21	U	0.11	0/1424	0.29	0/1918
22	V	0.11	0/2904	0.31	0/3941
23	W	0.09	0/967	0.30	0/1293
24	X	0.17	0/1858	0.38	0/2865
25	Y	0.14	0/1872	0.31	0/2884
All	All	0.10	0/59687	0.29	0/81262

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1233	0	1231	47	0
2	3	3037	0	2911	78	0
3	4	3058	0	3064	55	0
4	A	10814	0	11057	227	0
5	B	8680	0	8805	185	0
6	C	2736	0	2712	56	0
7	D	985	0	1006	26	0
8	E	1715	0	1733	21	0
9	F	610	0	642	5	0
10	G	1337	0	1306	34	0
11	H	1186	0	1147	18	0
12	I	848	0	809	21	0
13	J	512	0	525	16	0
14	K	822	0	810	11	0
15	L	388	0	394	10	0
16	M	3382	0	3376	53	0
17	N	1128	0	1181	27	0
18	O	4075	0	4149	48	0
19	P	2403	0	2409	46	0
20	Q	754	0	759	14	0
21	U	1396	0	1490	19	0
22	V	2853	0	2892	76	0
23	W	943	0	924	16	0
24	X	1661	0	922	62	0
25	Y	1666	0	911	32	0
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	0	0
All	All	58239	0	57165	988	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 988 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)
2:3:191:ILE:HB	3:4:176:PHE:CZ	1.59	1.36
22:V:111:LEU:HD13	24:X:-17:DT:OP2	1.24	1.30
1:1:63:TRP:HE3	1:1:82:LEU:CD1	1.51	1.24
5:B:113:ILE:HD11	5:B:136:MET:CB	1.73	1.17
2:3:101:ARG:HA	2:3:104:CYS:SG	1.83	1.16

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%)	142 (99%)	2 (1%)	0	100	100
2	3	368/411 (90%)	352 (96%)	15 (4%)	1 (0%)	36	65
3	4	363/1469 (25%)	353 (97%)	10 (3%)	0	100	100
4	A	1376/1390 (99%)	1350 (98%)	26 (2%)	0	100	100
5	B	1091/1133 (96%)	1062 (97%)	29 (3%)	0	100	100
6	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
7	D	120/148 (81%)	115 (96%)	5 (4%)	0	100	100
8	E	207/210 (99%)	203 (98%)	4 (2%)	0	100	100
9	F	74/127 (58%)	72 (97%)	2 (3%)	0	100	100
10	G	160/204 (78%)	144 (90%)	16 (10%)	0	100	100
11	H	146/150 (97%)	145 (99%)	1 (1%)	0	100	100
12	I	105/108 (97%)	98 (93%)	7 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	J	63/67 (94%)	62 (98%)	1 (2%)	0	100	100
14	K	101/133 (76%)	97 (96%)	4 (4%)	0	100	100
15	L	44/58 (76%)	42 (96%)	2 (4%)	0	100	100
16	M	418/708 (59%)	405 (97%)	13 (3%)	0	100	100
17	N	140/317 (44%)	139 (99%)	1 (1%)	0	100	100
18	O	508/534 (95%)	497 (98%)	11 (2%)	0	100	100
19	P	301/316 (95%)	296 (98%)	5 (2%)	0	100	100
20	Q	85/223 (38%)	84 (99%)	1 (1%)	0	100	100
21	U	175/339 (52%)	171 (98%)	4 (2%)	0	100	100
22	V	358/419 (85%)	352 (98%)	6 (2%)	0	100	100
23	W	109/2624 (4%)	105 (96%)	4 (4%)	0	100	100
All	All	6797/11802 (58%)	6622 (97%)	174 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	3	341	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	130/334 (39%)	130 (100%)	0	100	100
2	3	330/356 (93%)	330 (100%)	0	100	100
3	4	321/1213 (26%)	321 (100%)	0	100	100
4	A	1200/1212 (99%)	1200 (100%)	0	100	100
5	B	959/988 (97%)	959 (100%)	0	100	100
6	C	299/302 (99%)	299 (100%)	0	100	100
7	D	114/136 (84%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	149 (100%)	0	100	100
11	H	129/131 (98%)	129 (100%)	0	100	100
12	I	92/93 (99%)	92 (100%)	0	100	100
13	J	53/56 (95%)	53 (100%)	0	100	100
14	K	92/119 (77%)	92 (100%)	0	100	100
15	L	43/55 (78%)	43 (100%)	0	100	100
16	M	377/622 (61%)	377 (100%)	0	100	100
17	N	131/276 (48%)	131 (100%)	0	100	100
18	O	458/476 (96%)	458 (100%)	0	100	100
19	P	269/280 (96%)	269 (100%)	0	100	100
20	Q	84/195 (43%)	84 (100%)	0	100	100
21	U	152/293 (52%)	152 (100%)	0	100	100
22	V	325/365 (89%)	324 (100%)	1 (0%)	86	84
23	W	102/2381 (4%)	102 (100%)	0	100	100
All	All	6066/10367 (58%)	6065 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
22	V	55	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
12	I	61	ASN
18	O	377	GLN
12	I	99	ASN
16	M	322	GLN
18	O	497	GLN

5.3.3 RNA ⓘ

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 oligosaccharides 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

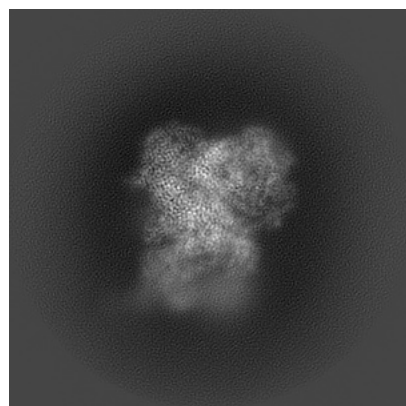
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35722. These allow visual inspection of the internal detail of the map and identification of artifacts.

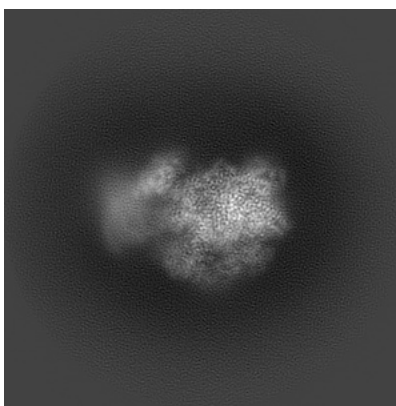
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

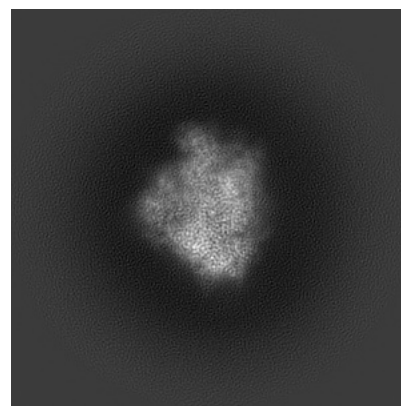
6.1.1 Primary map



X

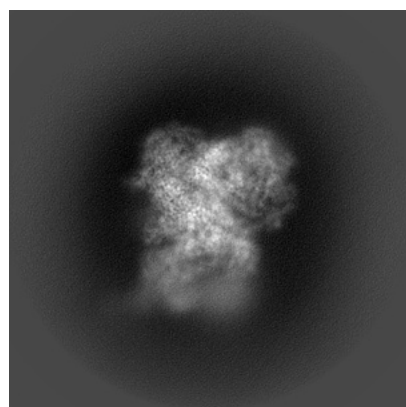


Y

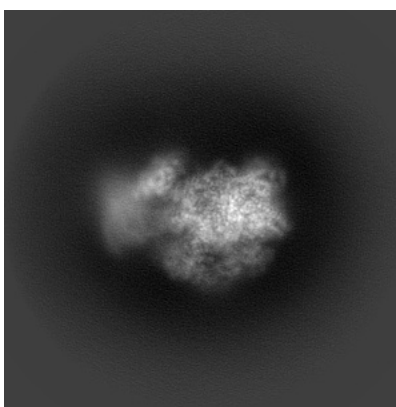


Z

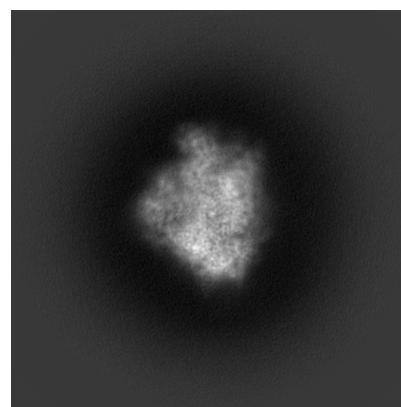
6.1.2 Raw map



X



Y

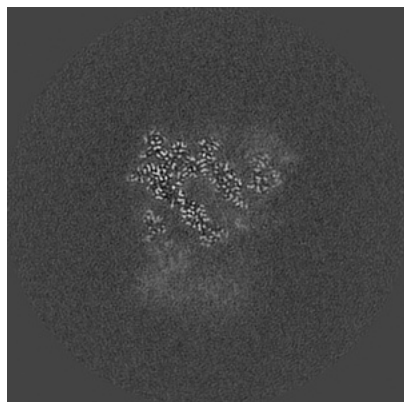


Z

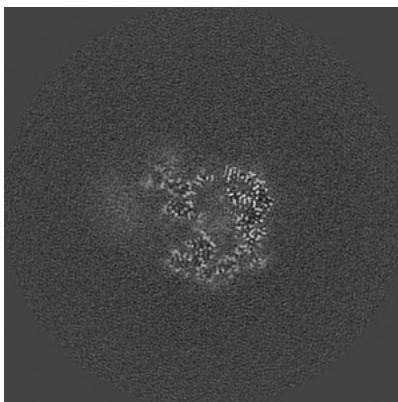
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

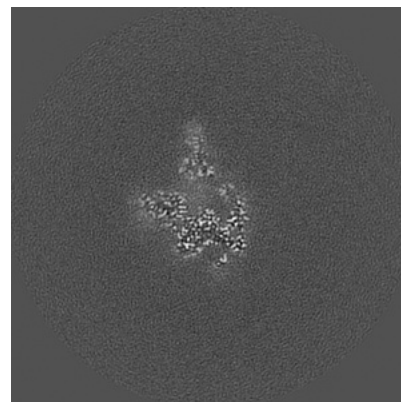
6.2.1 Primary map



X Index: 160

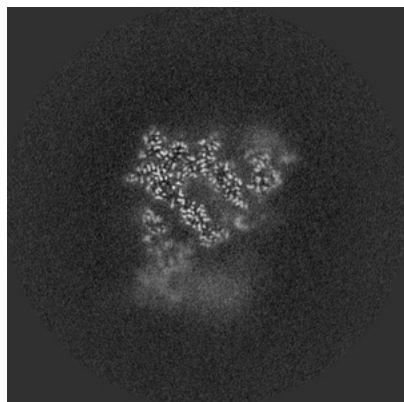


Y Index: 160

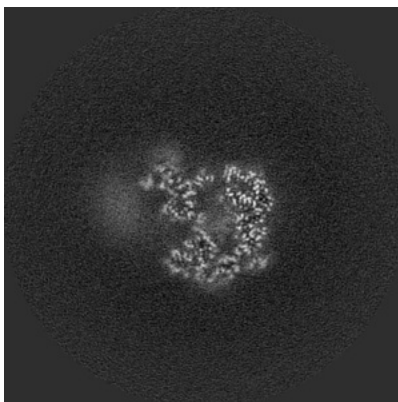


Z Index: 160

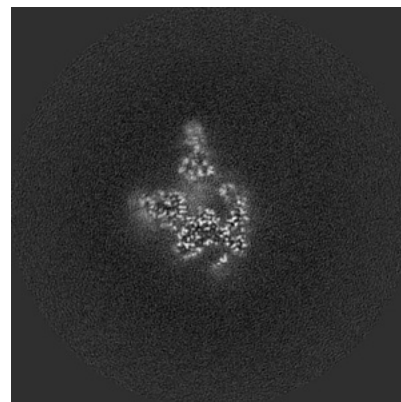
6.2.2 Raw map



X Index: 160



Y Index: 160

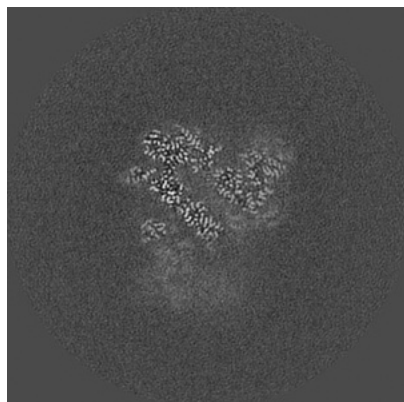


Z Index: 160

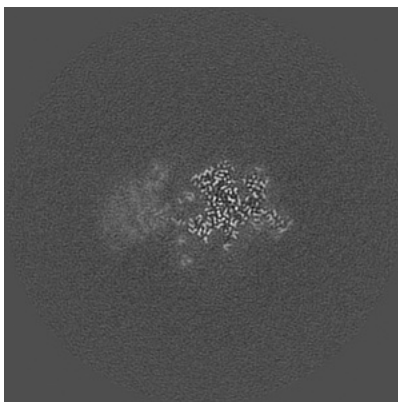
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

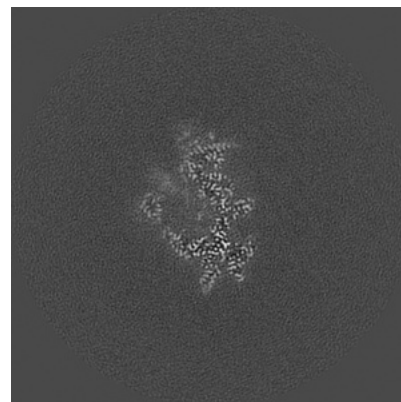
6.3.1 Primary map



X Index: 155

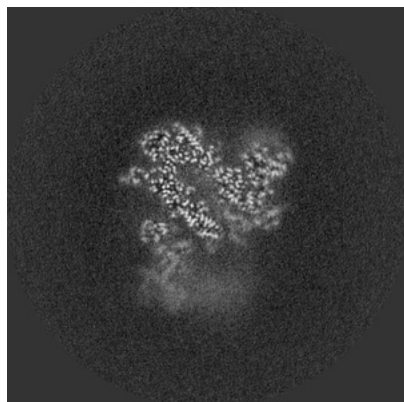


Y Index: 129

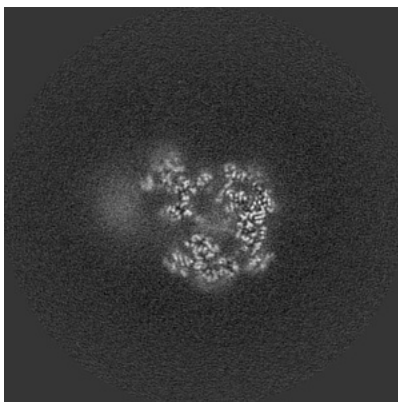


Z Index: 181

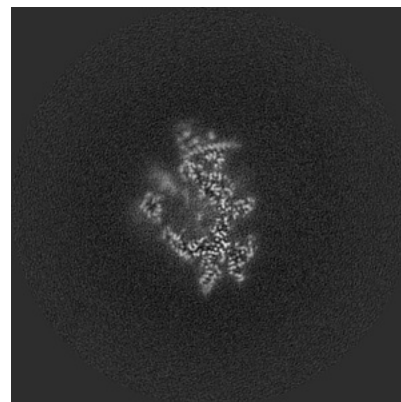
6.3.2 Raw map



X Index: 154



Y Index: 162

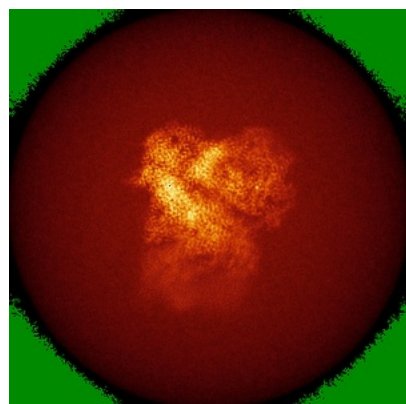


Z Index: 181

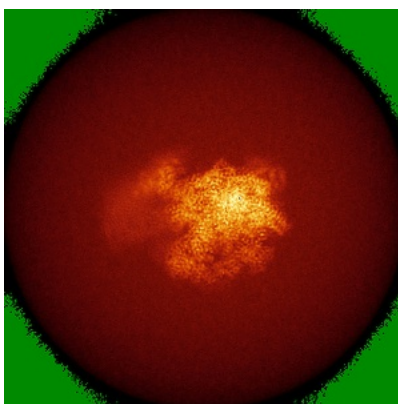
The images above show the largest variance slices of the map in three orthogonal directions.

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

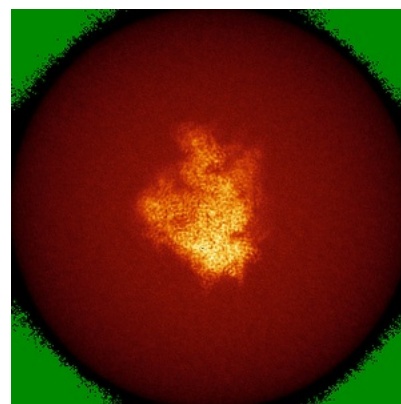
6.4.1 Primary map



X

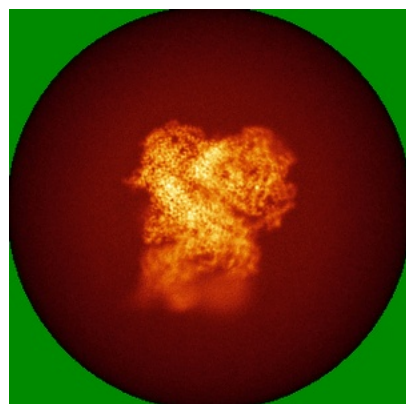


Y

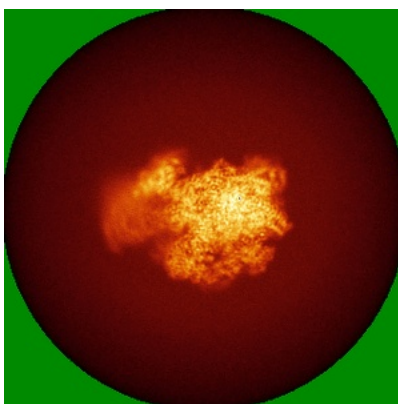


Z

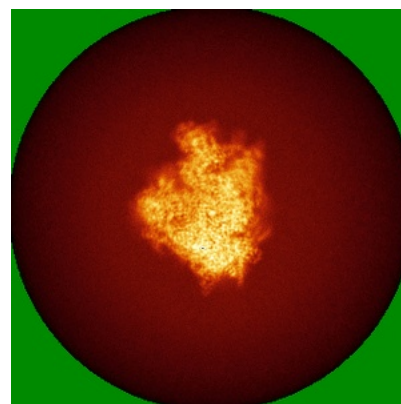
6.4.2 Raw map



X



Y

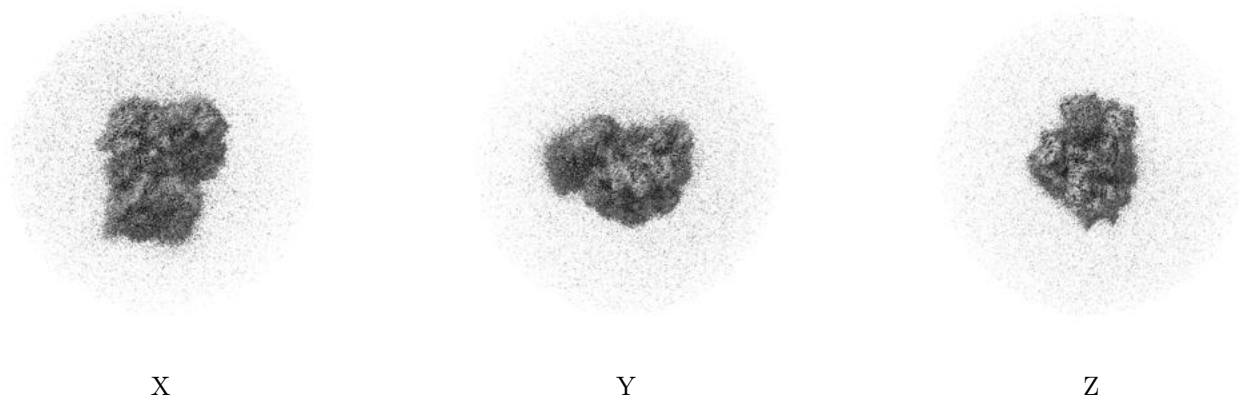


Z

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.

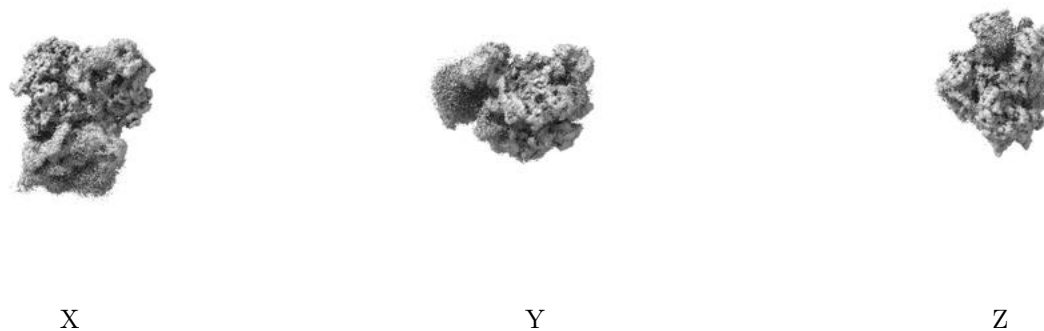
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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



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.

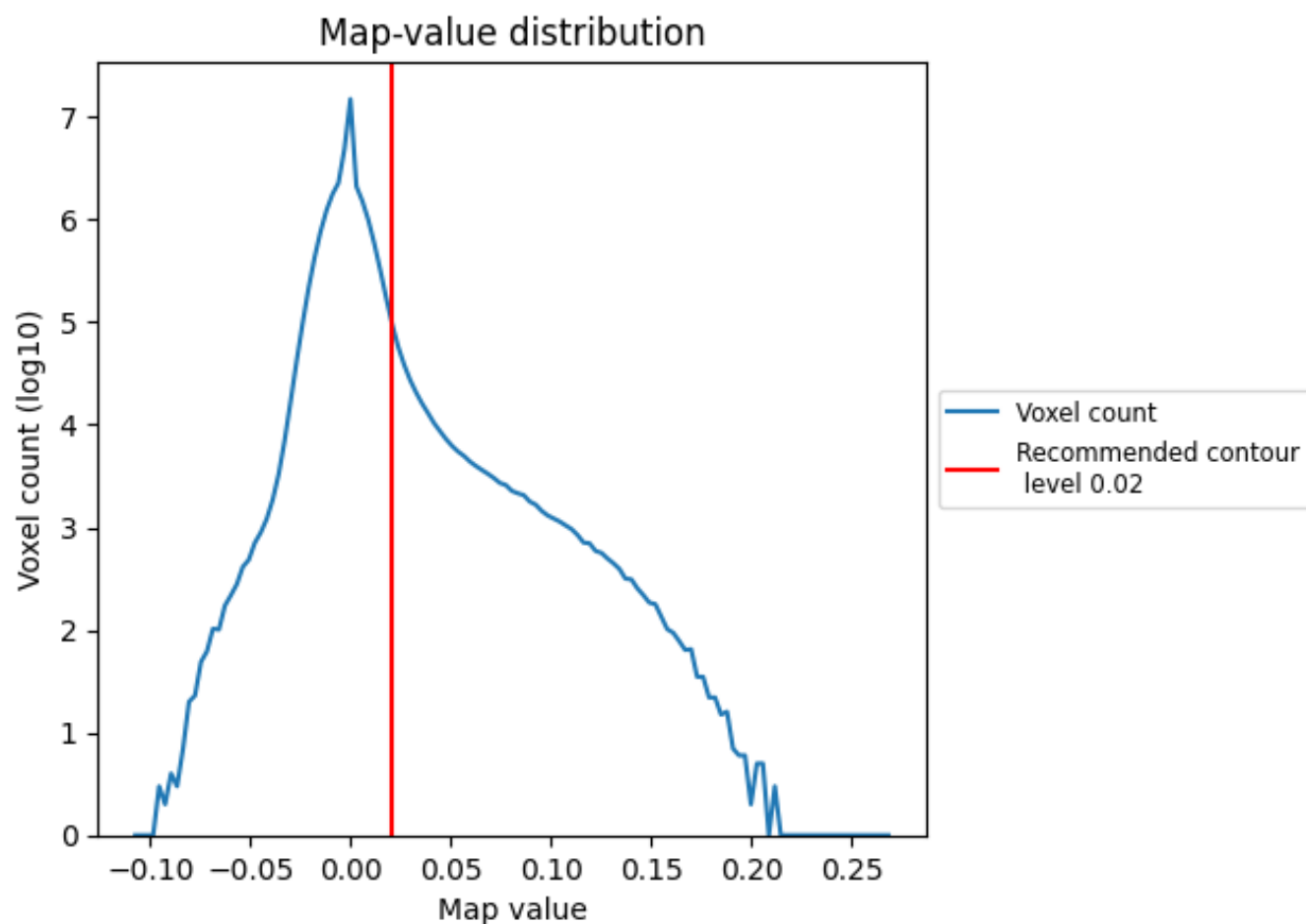
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

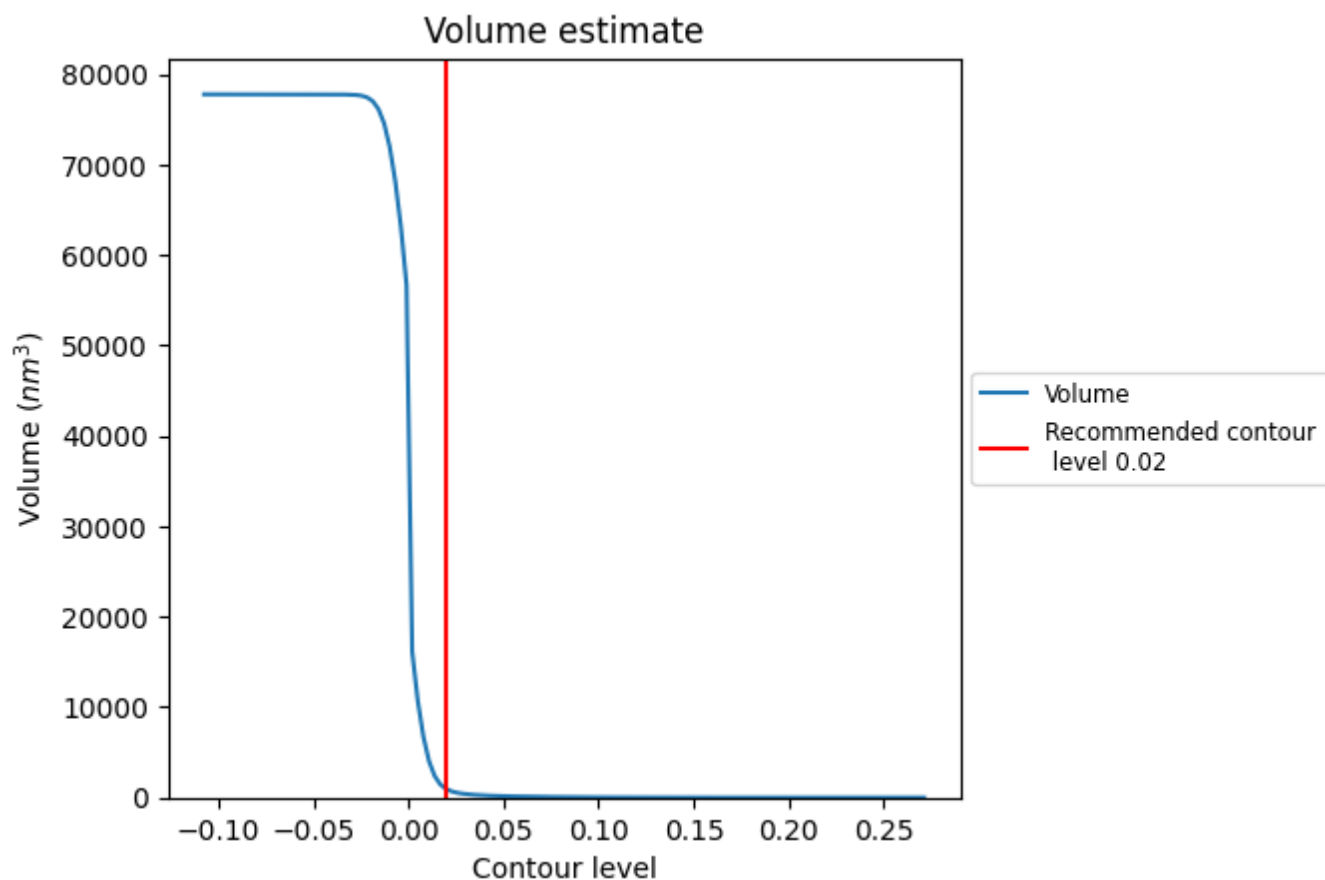
This section contains the results of statistical analysis of the map.

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.

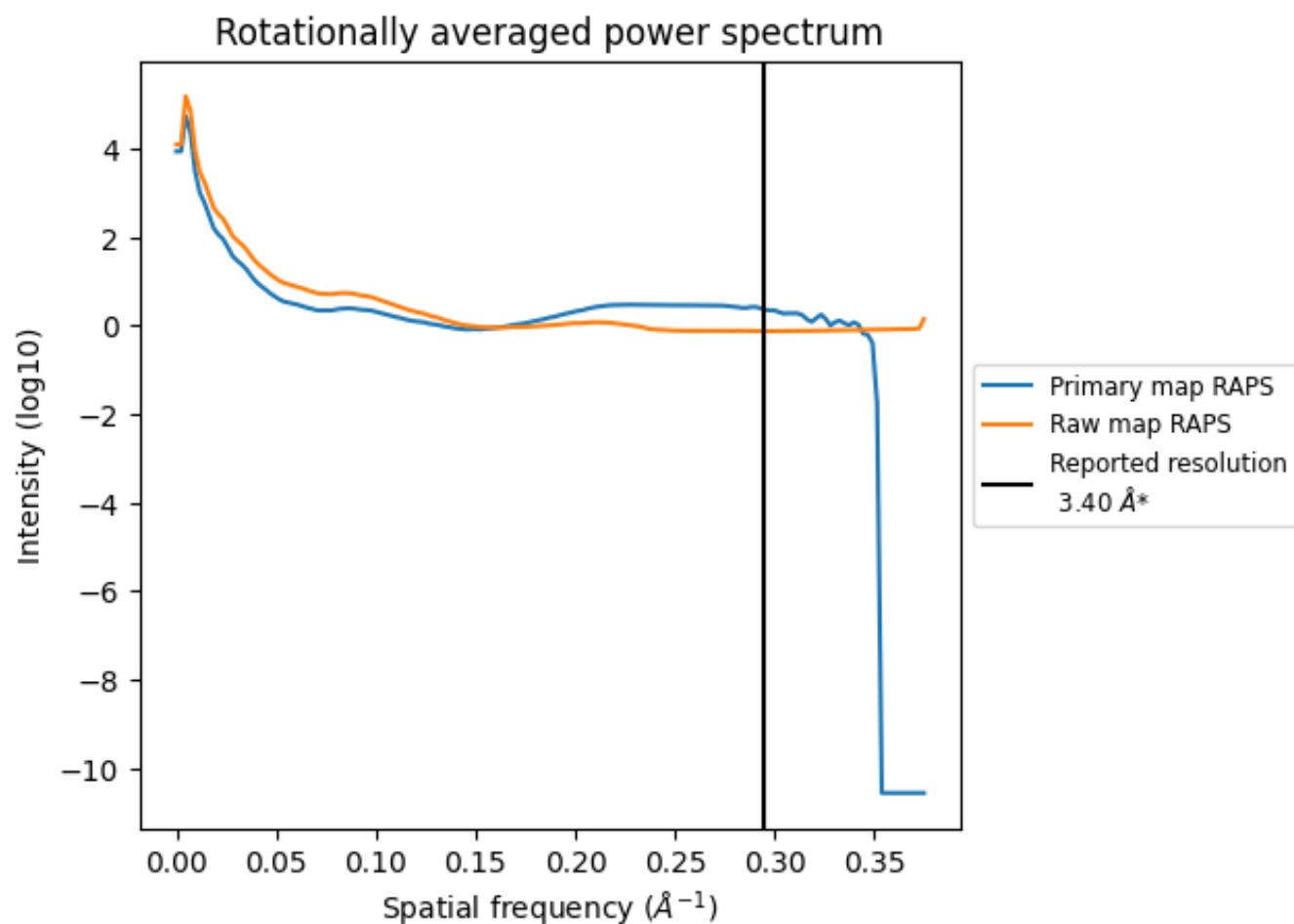
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 931 nm^3 ; this corresponds to an approximate mass of 841 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 ⓘ

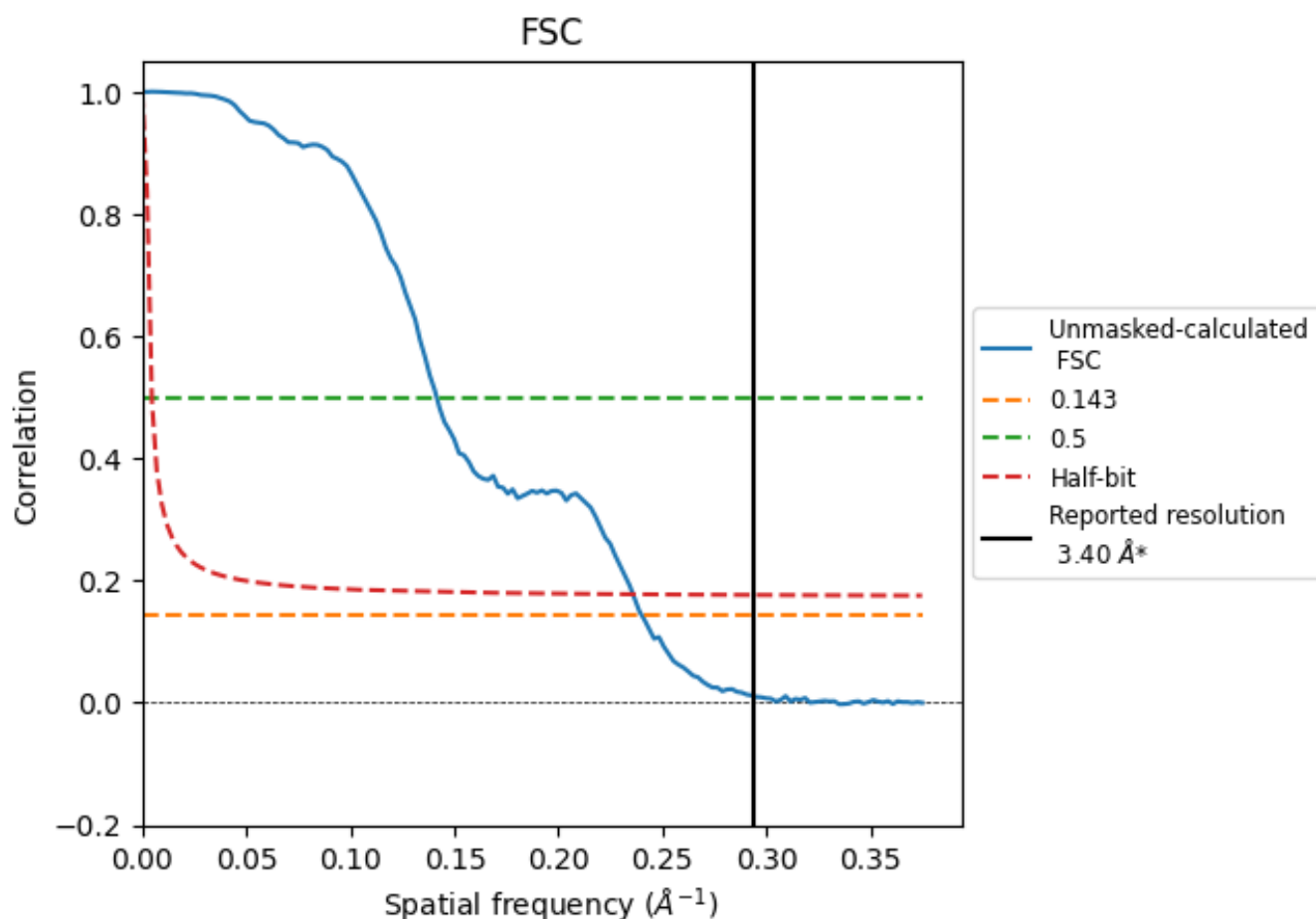


*Reported resolution corresponds to spatial frequency of 0.294 $\text{\AA}^{-1}$

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

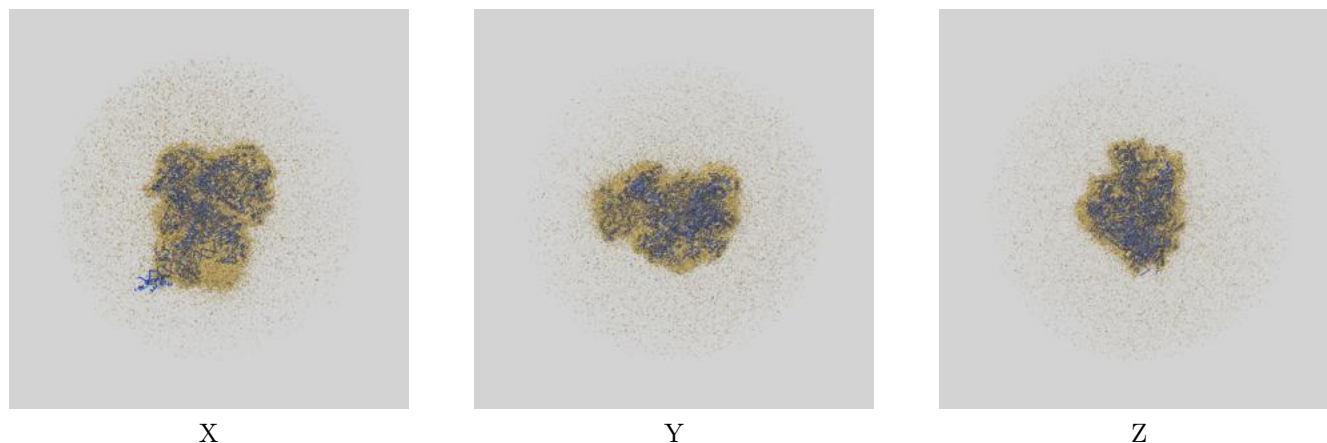
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.16	7.07	4.24

*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 4.16 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

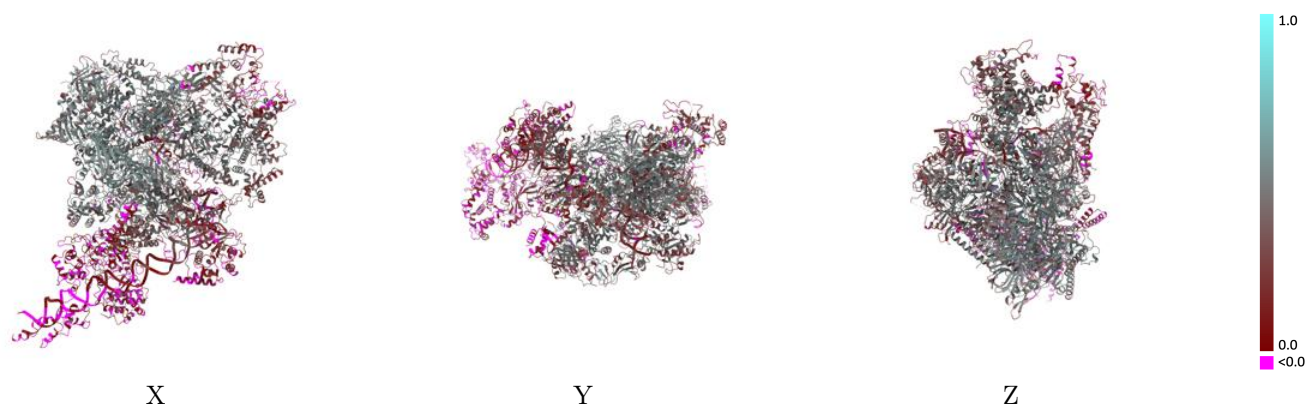
This section contains information regarding the fit between EMDB map EMD-35722 and PDB model 8IUH. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



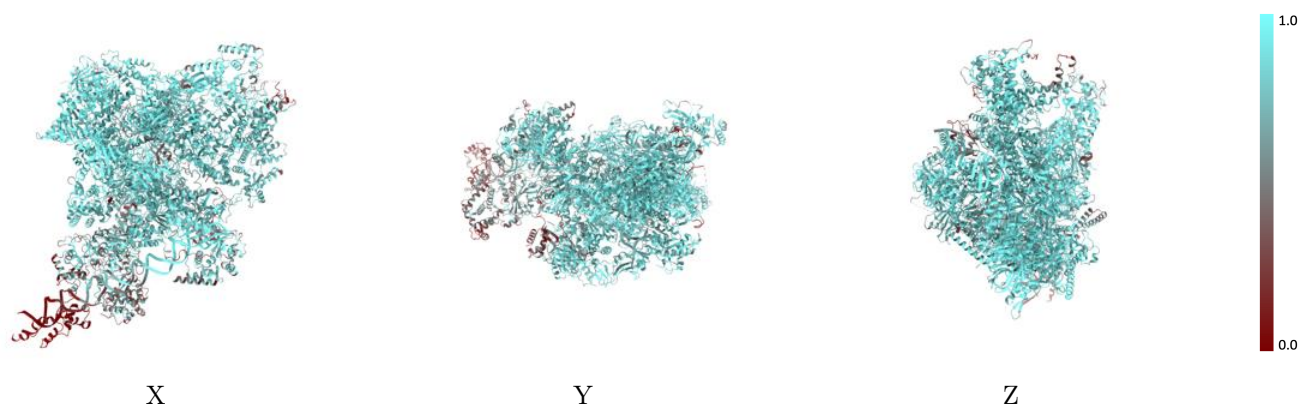
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



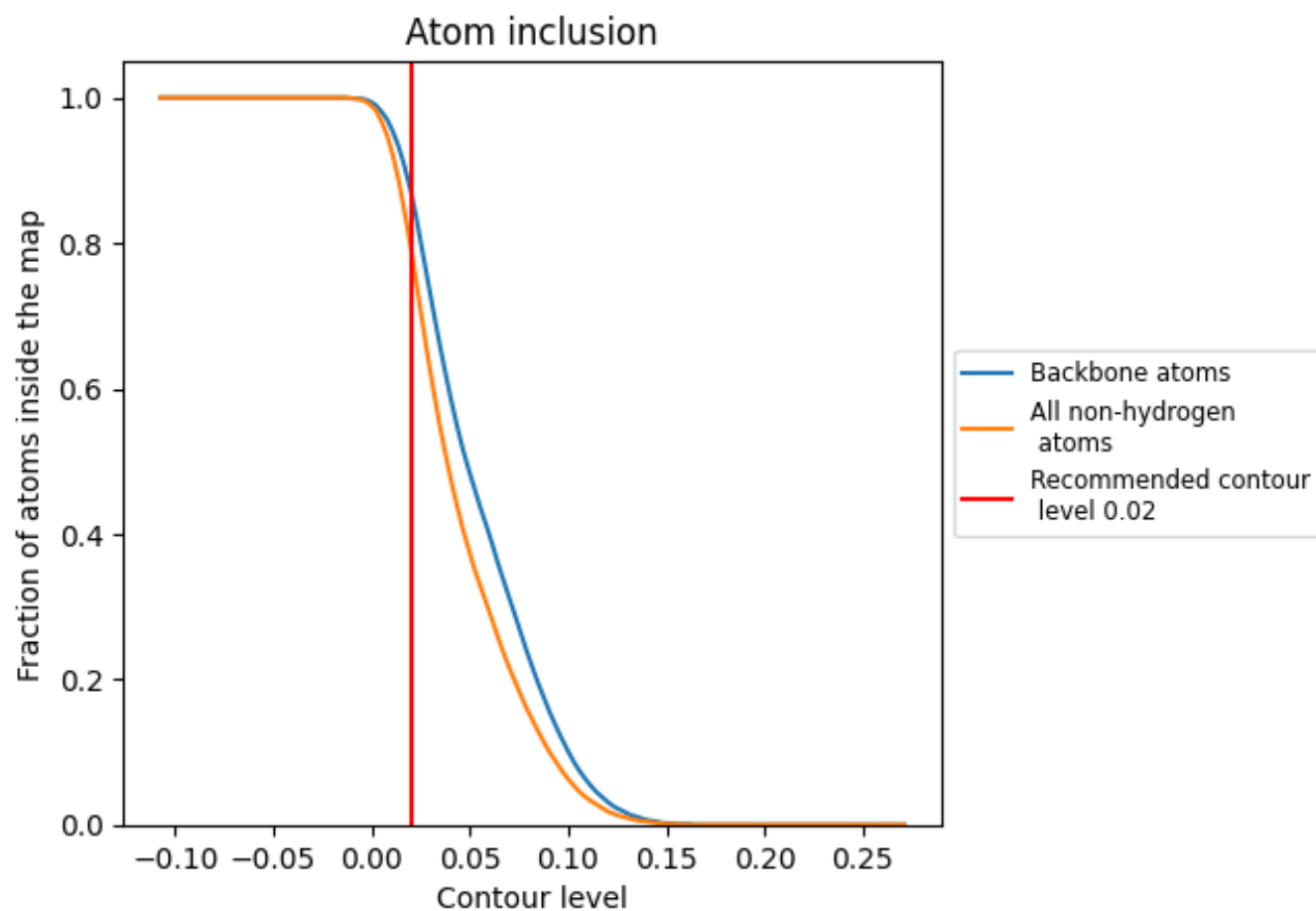
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 79% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7920	 0.3410
1	 0.4990	 0.0360
3	 0.5890	 0.1040
4	 0.4030	 0.0500
A	 0.8950	 0.4600
B	 0.9140	 0.4830
C	 0.9040	 0.4850
D	 0.7710	 0.2470
E	 0.8480	 0.3780
F	 0.9270	 0.4910
G	 0.8450	 0.3380
H	 0.8590	 0.4510
I	 0.6760	 0.2470
J	 0.9340	 0.5060
K	 0.8920	 0.4660
L	 0.8840	 0.4070
M	 0.8080	 0.3730
N	 0.7700	 0.3590
O	 0.8160	 0.3640
P	 0.6880	 0.2380
Q	 0.7570	 0.2920
U	 0.8210	 0.2440
V	 0.7790	 0.2980
W	 0.6760	 0.1300
X	 0.6490	 0.1050
Y	 0.6490	 0.1450

