



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:20 AM UTC

PDB ID : 8IUE / pdb_00008iue
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

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:

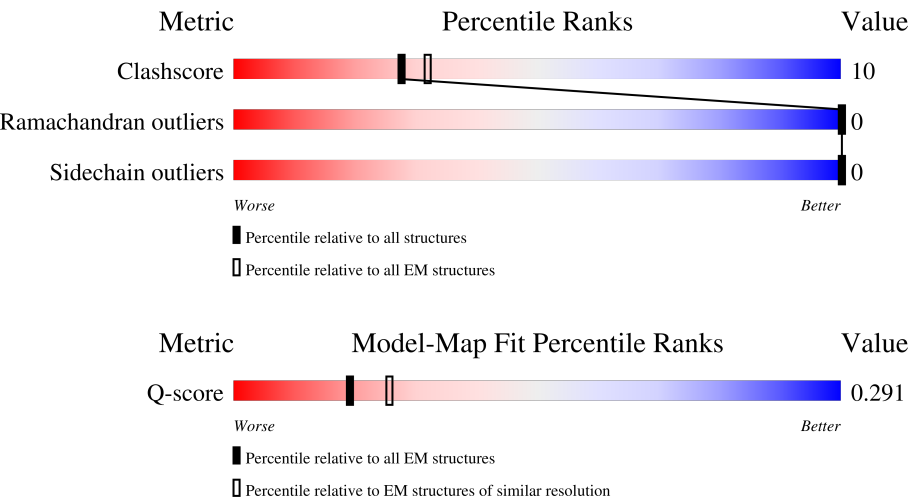
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	A	1390	77% 23%
2	B	1133	74% 23%
3	C	346	80% 19%
4	D	148	14% 56% 26% 18%

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Mol	Chain	Length	Quality of chain
5	E	210	
6	F	127	
7	G	204	
8	H	150	
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 (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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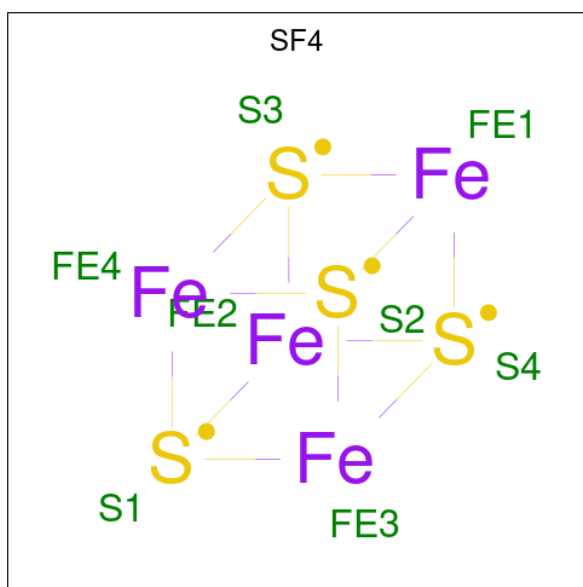
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Mol	Chain	Residues	Atoms		AltConf
26	J	1	Total	Zn	0
			1	1	
26	L	1	Total	Zn	0
			1	1	
26	V	1	Total	Zn	0
			1	1	

- 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).

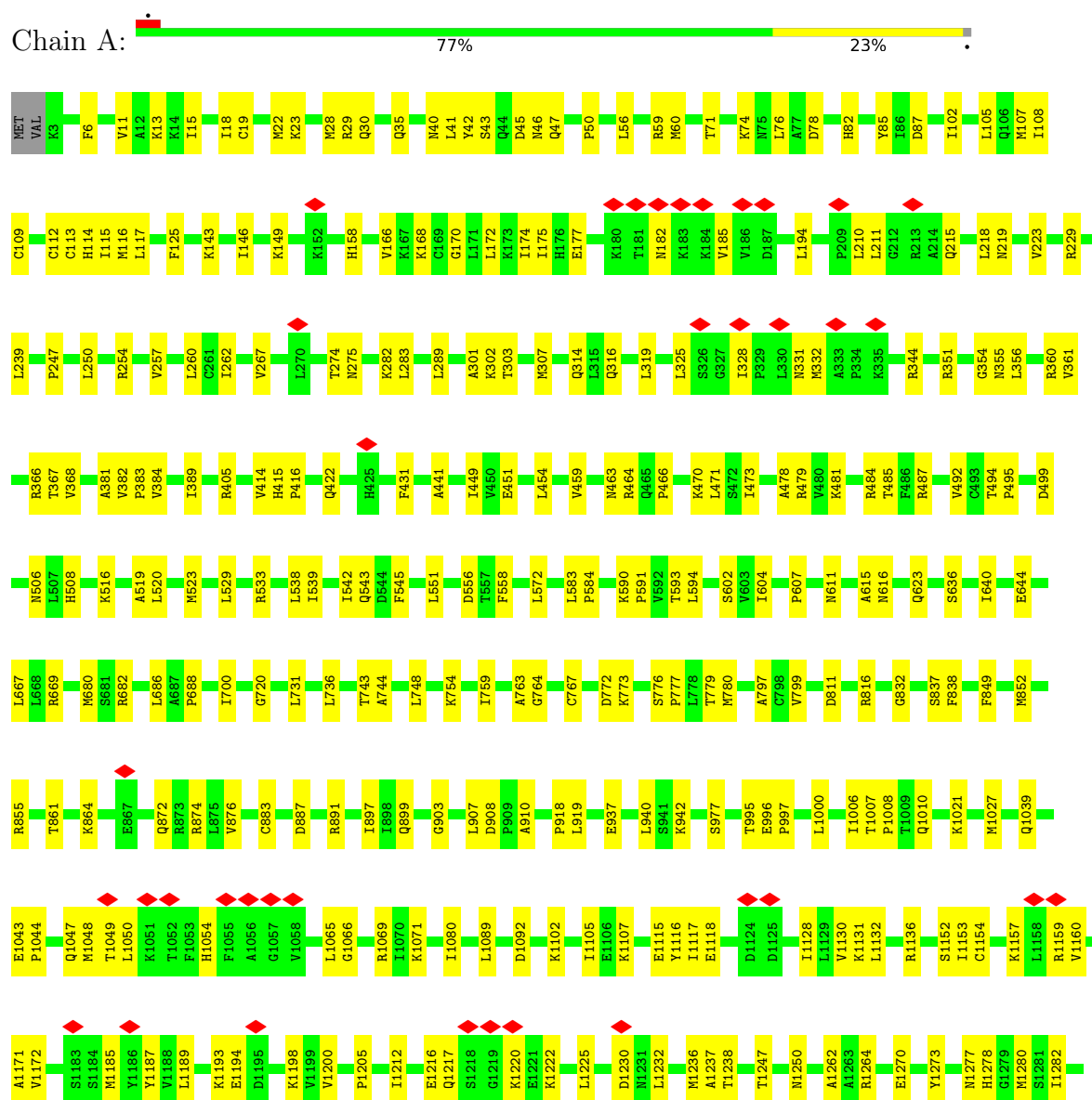


Mol	Chain	Residues	Atoms			AltConf
28	P	1	Total	Fe	S	0
			8	4	4	

3 Residue-property plots

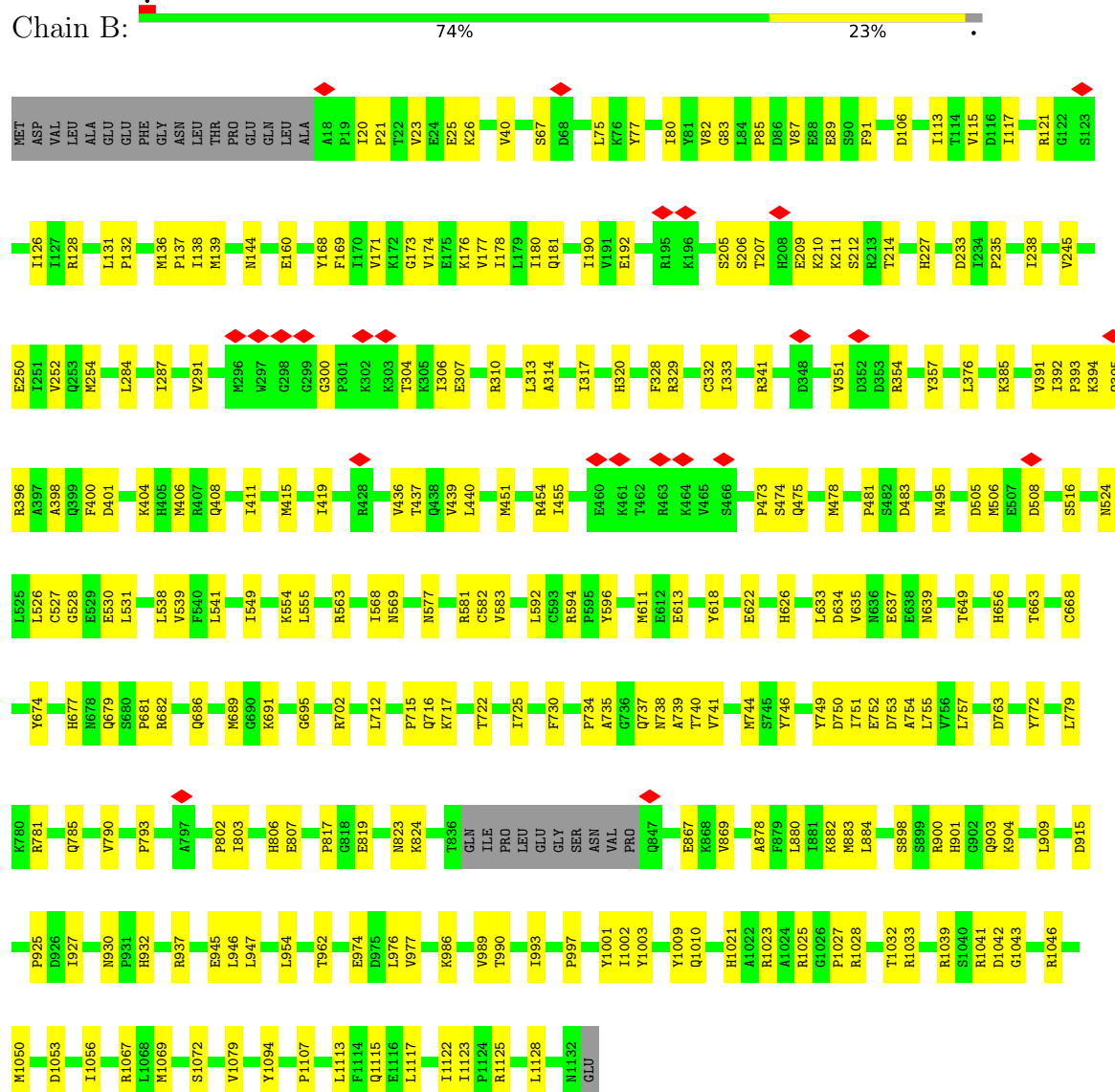
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: DNA-directed RNA polymerase III subunit RPC1

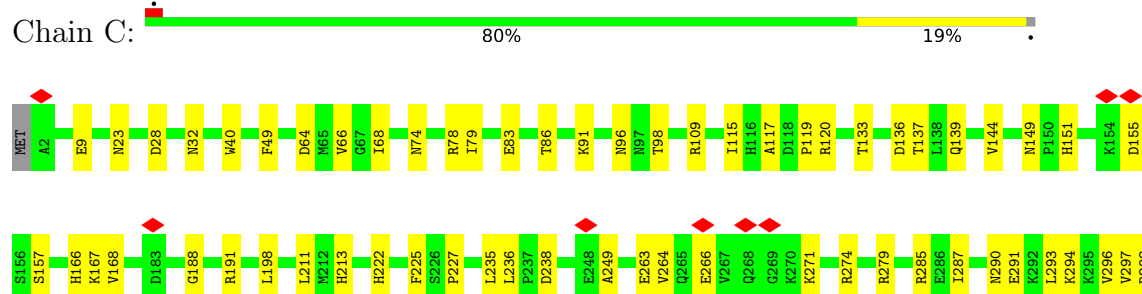


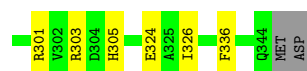


• Molecule 2: DNA-directed RNA polymerase III subunit RPC2

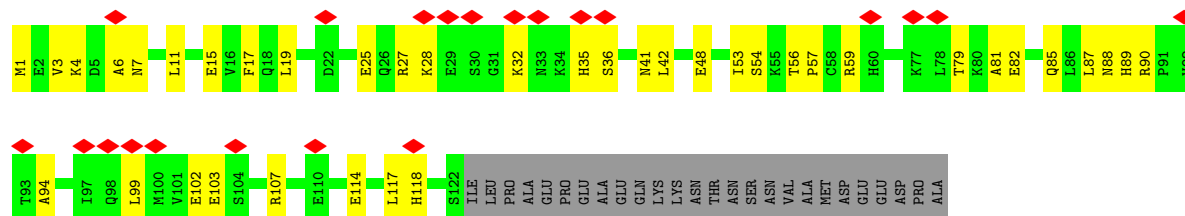


• Molecule 3: DNA-directed RNA polymerases I and III subunit RPAC1

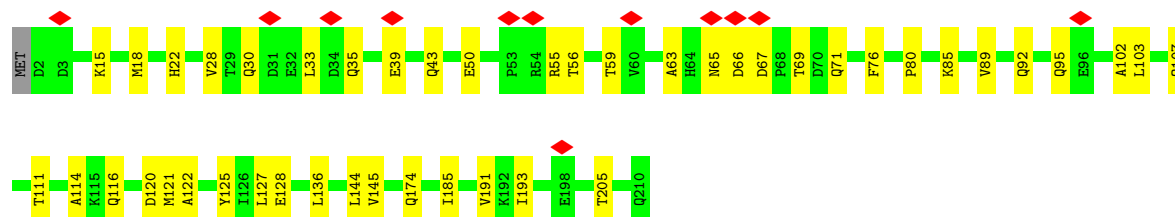
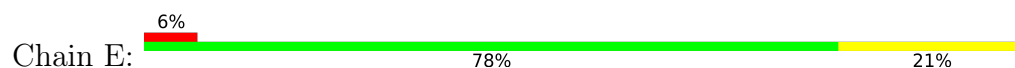




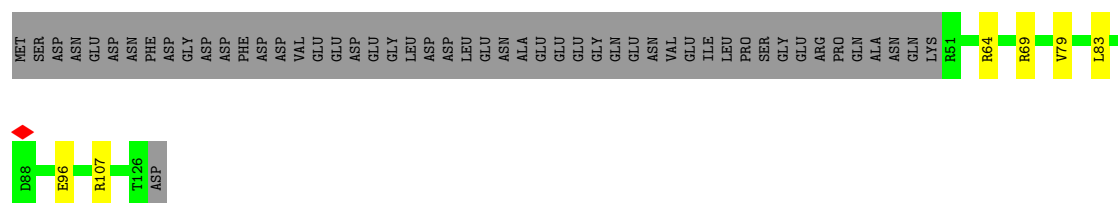
• Molecule 4: DNA-directed RNA polymerase III subunit RPC9



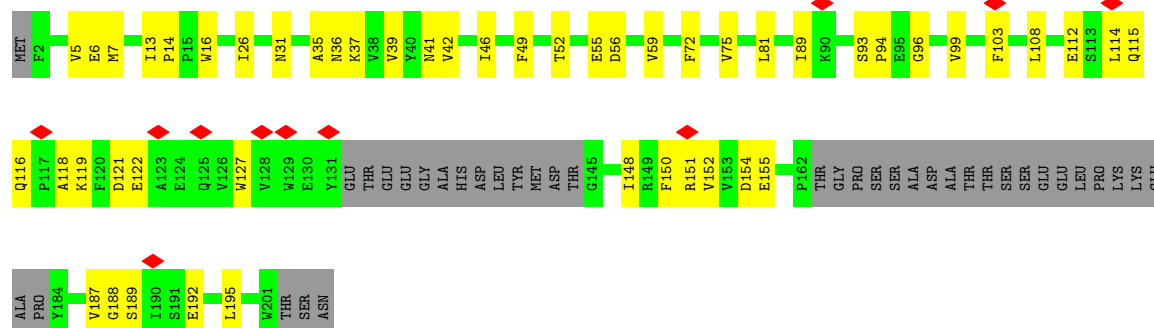
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



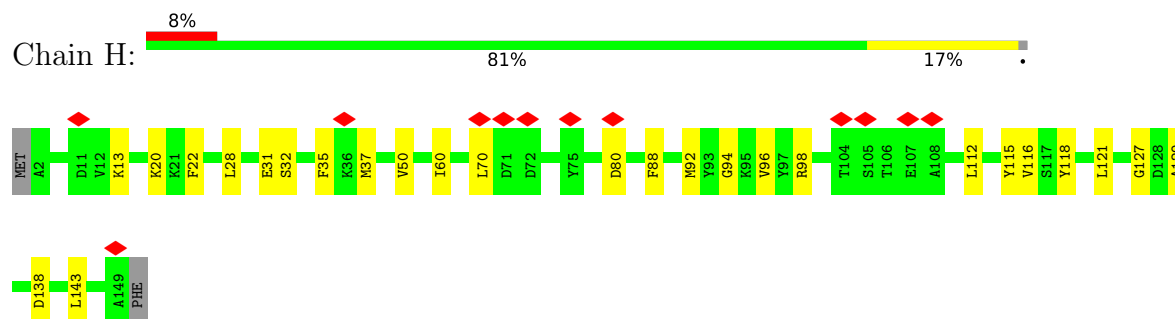
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



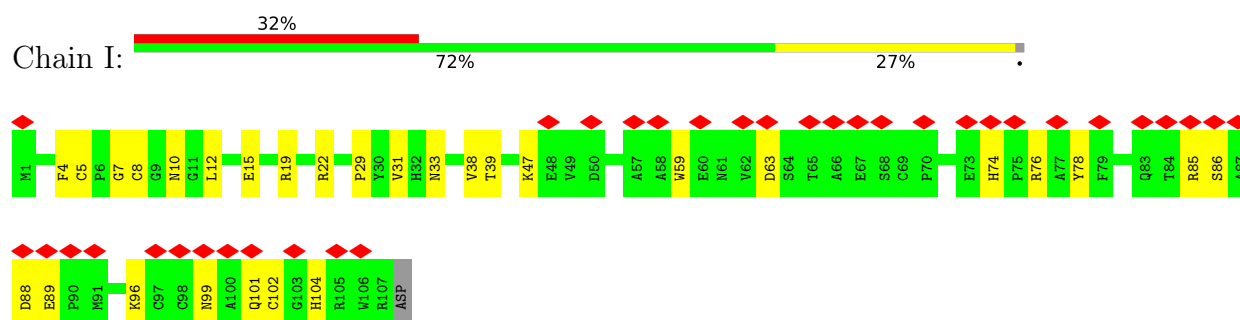
• Molecule 7: DNA-directed RNA polymerase III subunit RPC8



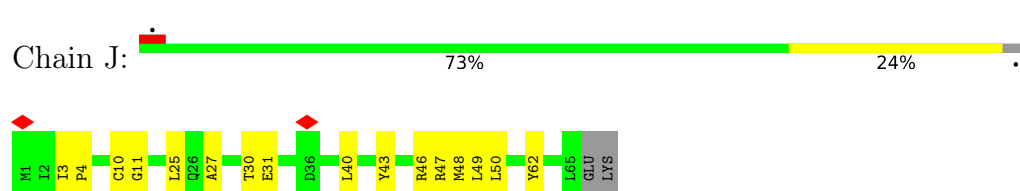
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



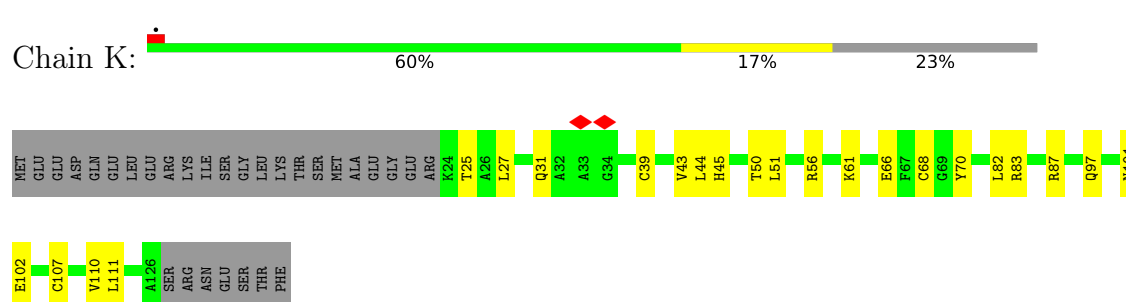
- Molecule 9: DNA-directed RNA polymerase III subunit RPC10



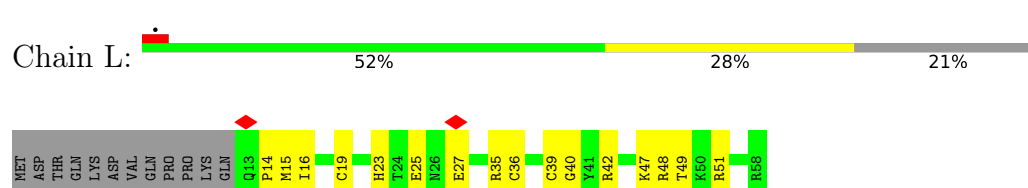
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5



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

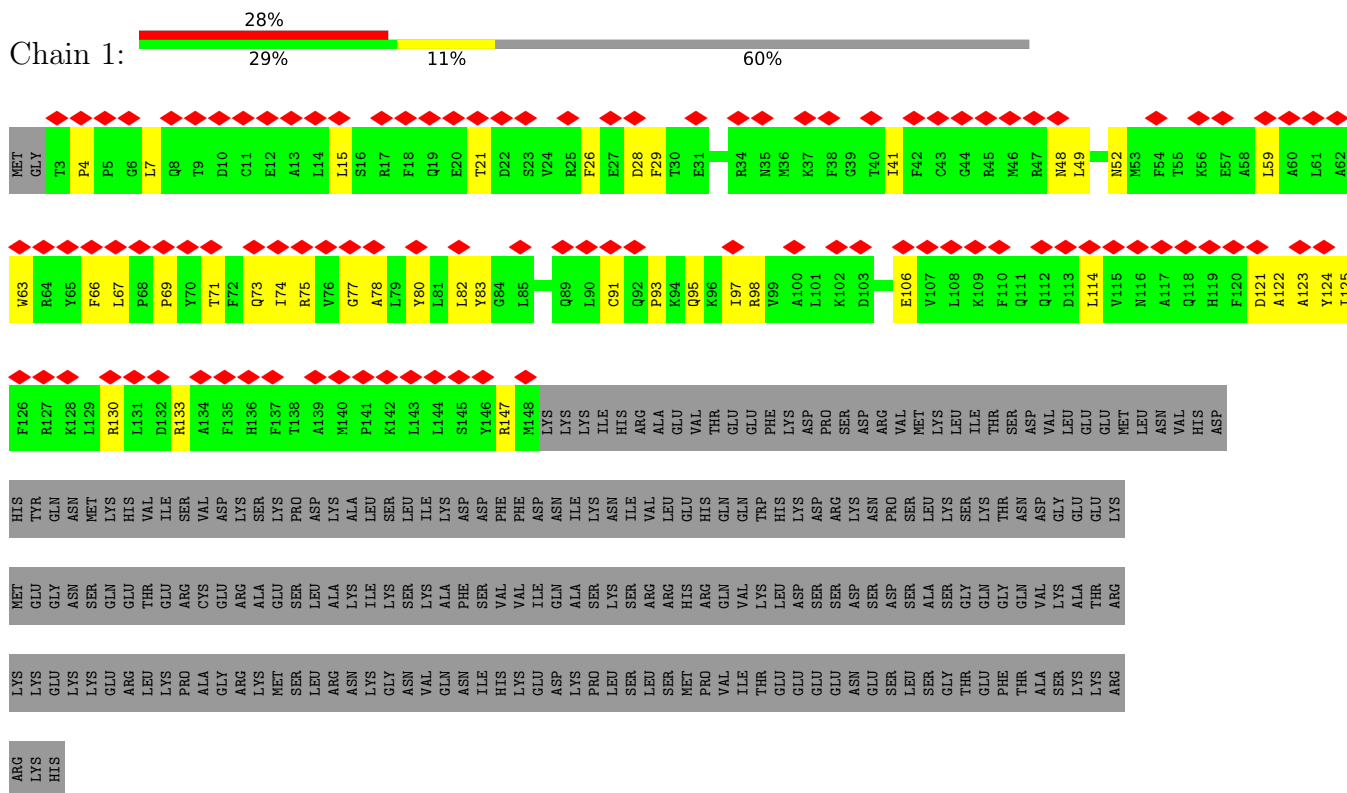


- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

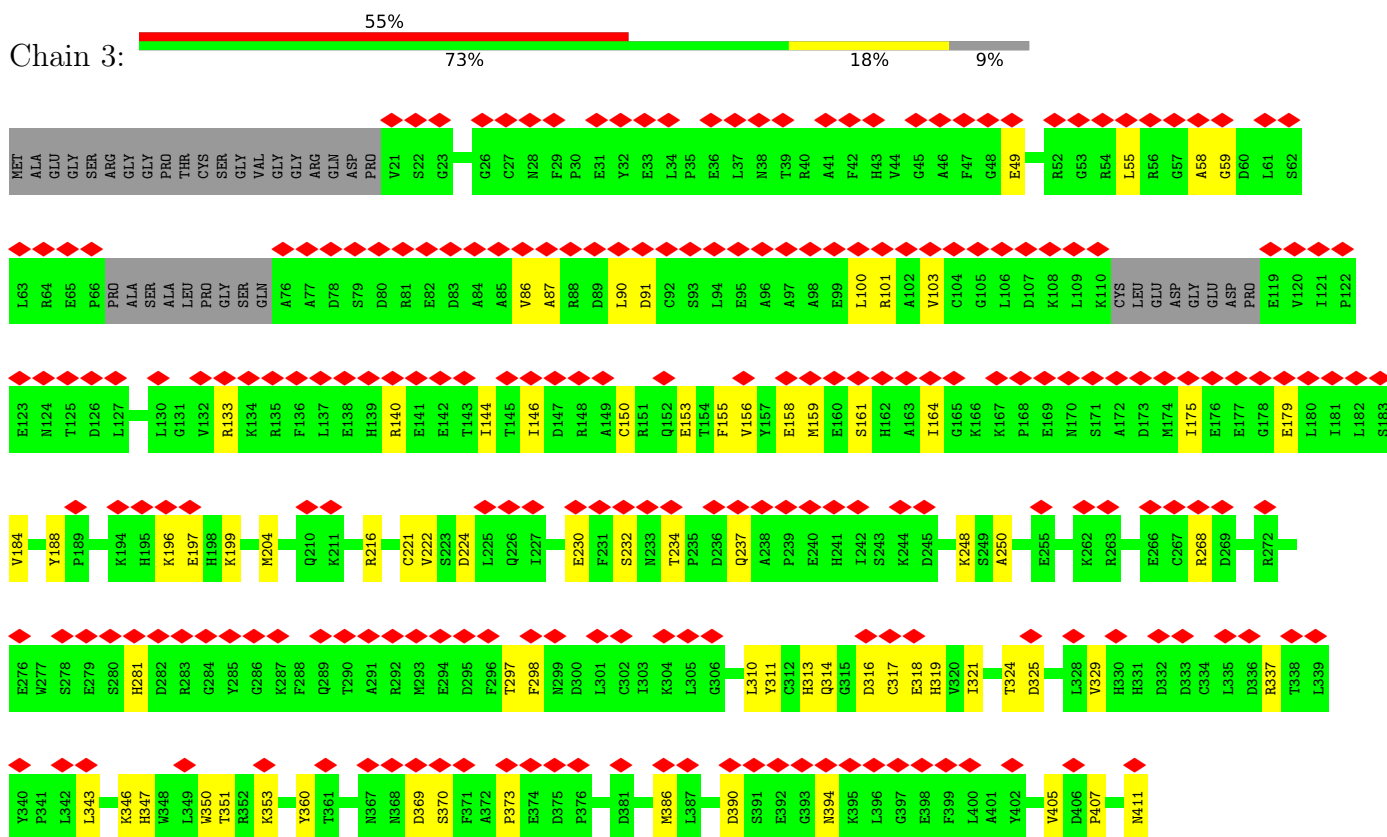


- Molecule 13: DNA-directed RNA polymerase III subunit RPC5





- Molecule 21: snRNA-activating protein complex subunit 3



- Molecule 22: snRNA-activating protein complex subunit 4



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

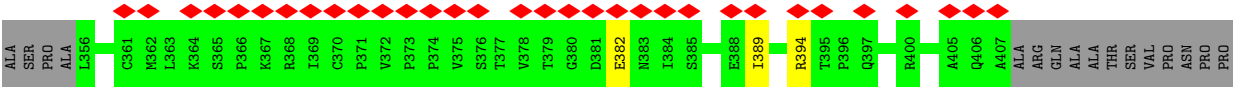
- Molecule 23: TATA-box-binding protein

[illegible]

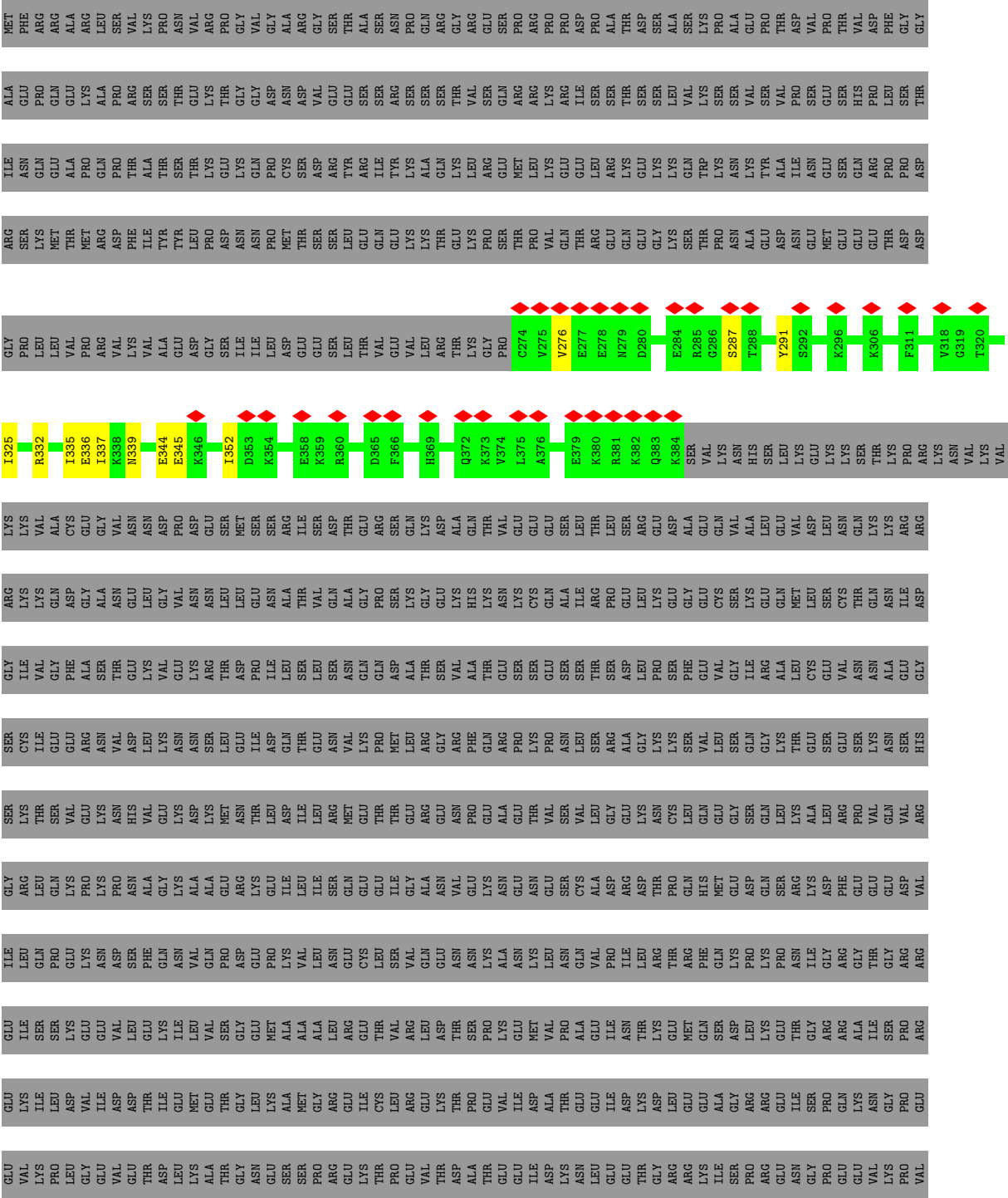
- Molecule 24: Transcription factor IIIB 50 kDa subunit



R284	R285	L286	R287	L288	R291	V294	R295	R296	L297	L300	L301	L307	V308	R309	F312	R313	D314	THR	GLY	ALA	GLU	VAL	THR	THR	ARG	GLU	GLU	LYS	GLY	PRO	PRO	GLY	TRP	GLY	GLN	GLN	GLY	GLY	GLY	VAL	GLY	ASN	ASN	SER	GLY	LEU	PRO	GLN	LYS	ARG	PRO
L133	T134	M135	G136	A137	L141	K158	L159	V173	K174	T175	Q184	P187	S188	V189	L207	V208	N212	E213	T214	V217	P222	L223	P224	V225	I226	Q238	R242	L243	S244	L253	D257	P261	A262	S263	S264	V265	L266	Q267	N276	L280	A281	W282	L283								
Met	Pro	Gly	Arg	Gly	R6	D9	L15	S19	H20	Y21	L26	G32	F44	E47	G48	N49	L50	R51	E52	V53	T54	Y55	S58	R67	S68	V76	V82	P86	F89	Y96	A109	R110	L111	K114	V118	L123	I124	Q128	T130												



• Molecule 25: Transcription factor TFIIB component B' homolog





[illegible]

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: MG, SF4, 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	0.10	0/11008	0.29	0/14842
2	B	0.10	0/8910	0.30	0/12018
3	C	0.10	0/2790	0.30	0/3782
4	D	0.10	0/997	0.29	0/1343
5	E	0.10	0/1745	0.30	0/2358
6	F	0.11	0/620	0.27	0/839
7	G	0.12	0/1374	0.33	0/1868
8	H	0.11	0/1207	0.31	0/1628
9	I	0.14	0/869	0.34	0/1174
10	J	0.10	0/521	0.28	0/703
11	K	0.10	0/837	0.31	0/1129
12	L	0.12	0/394	0.34	0/524
13	M	0.10	0/3455	0.28	0/4673
14	N	0.10	0/1137	0.29	0/1530
15	O	0.10	0/4141	0.28	0/5592
16	P	0.10	0/2446	0.30	0/3301
17	Q	0.11	0/777	0.31	0/1050
18	X	0.80	1/1697 (0.1%)	0.52	4/2616 (0.2%)
19	Y	0.14	0/1614	0.30	0/2485
20	1	0.13	0/1266	0.28	0/1708
21	3	0.12	0/3112	0.33	0/4206
22	4	0.11	0/3121	0.31	0/4181
23	U	0.11	0/1424	0.29	0/1918
24	V	0.11	0/2904	0.31	0/3941
25	W	0.10	0/967	0.29	0/1293
All	All	0.17	1/59333 (0.0%)	0.31	4/80702 (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	-31.92	1.13	1.61

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	X	-21	DC	O3'-P-O5'	-10.98	87.53	104.00
18	X	-18	DG	C4'-C3'-O3'	7.94	121.91	110.00
18	X	-21	DC	P-O3'-C3'	-6.65	110.22	120.20
18	X	-19	DT	C2'-C3'-O3'	-5.90	102.65	111.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10814	0	11057	234	0
2	B	8741	0	8867	217	0
3	C	2736	0	2712	54	0
4	D	985	0	1006	34	0
5	E	1715	0	1733	38	0
6	F	610	0	642	6	0
7	G	1337	0	1306	45	0
8	H	1186	0	1147	17	0
9	I	848	0	811	47	0
10	J	512	0	525	14	0
11	K	822	0	810	18	0
12	L	388	0	395	19	0
13	M	3382	0	3376	60	0
14	N	1128	0	1181	35	0
15	O	4075	0	4149	54	0
16	P	2403	0	2409	48	0
17	Q	754	0	759	25	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	84	0
22	4	3058	0	3064	70	0
23	U	1396	0	1490	15	0
24	V	2853	0	2892	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	W	943	0	924	8	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	1	0
All	All	57927	0	57030	1104	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 10.

The worst 5 of 1104 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	341/346 (99%)	336 (98%)	5 (2%)	0	100	100
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%)	1200 (100%)	0	100	100
2	B	964/988 (98%)	964 (100%)	0	100	100
3	C	299/302 (99%)	299 (100%)	0	100	100
4	D	114/136 (84%)	114 (100%)	0	100	100
5	E	191/192 (100%)	191 (100%)	0	100	100
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%)	43 (100%)	0	100	100
13	M	377/622 (61%)	377 (100%)	0	100	100
14	N	131/276 (48%)	131 (100%)	0	100	100
15	O	458/476 (96%)	458 (100%)	0	100	100
16	P	269/280 (96%)	269 (100%)	0	100	100
17	Q	84/195 (43%)	84 (100%)	0	100	100
20	1	130/334 (39%)	130 (100%)	0	100	100
21	3	330/356 (93%)	330 (100%)	0	100	100
22	4	321/1213 (26%)	321 (100%)	0	100	100
23	U	152/293 (52%)	152 (100%)	0	100	100
24	V	325/365 (89%)	325 (100%)	0	100	100
25	W	102/2381 (4%)	102 (100%)	0	100	100
All	All	6071/10367 (59%)	6071 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	395	HIS
20	1	95	GLN
15	O	60	HIS
15	O	498	GLN
21	3	314	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 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.

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

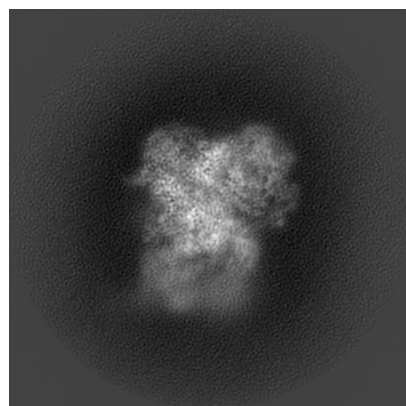
6 Map visualisation [i](#)

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.

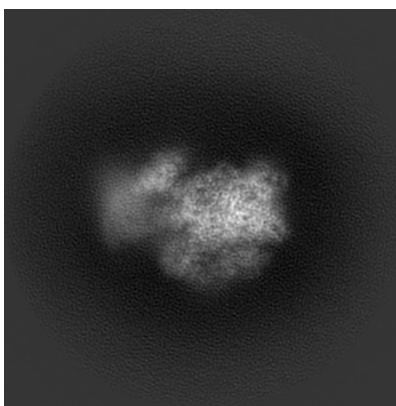
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

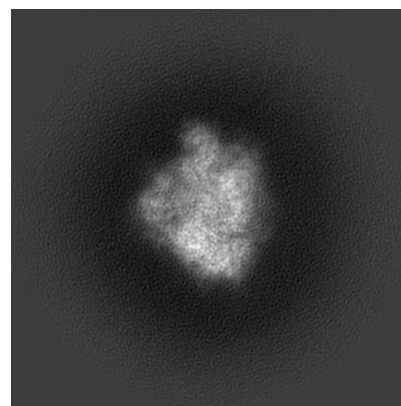
6.1.1 Primary map



X

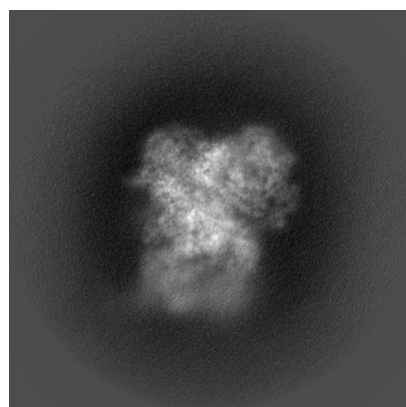


Y

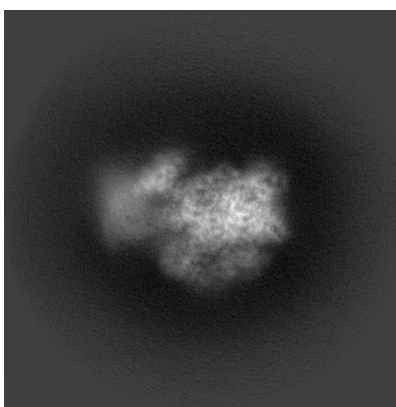


Z

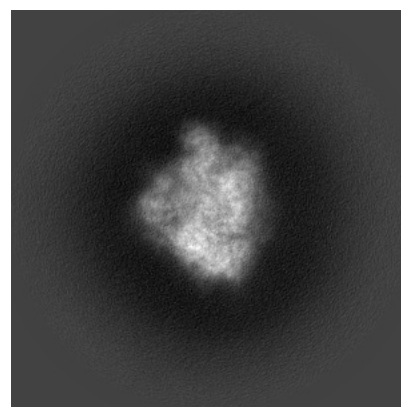
6.1.2 Raw map



X



Y

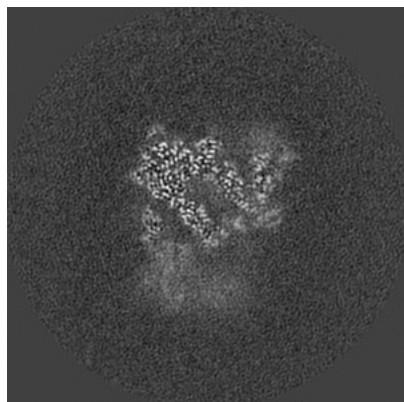


Z

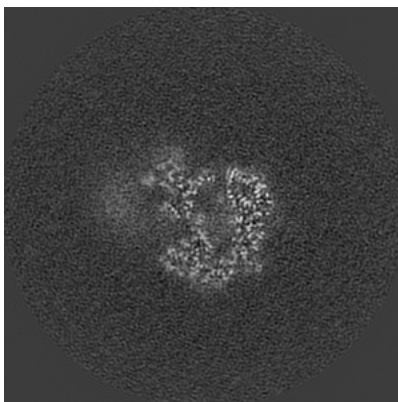
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

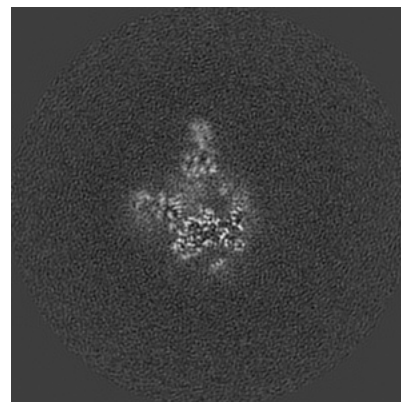
6.2.1 Primary map



X Index: 160

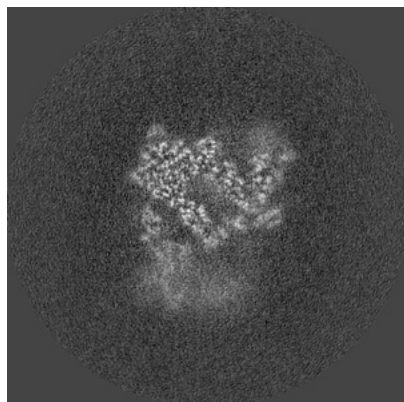


Y Index: 160

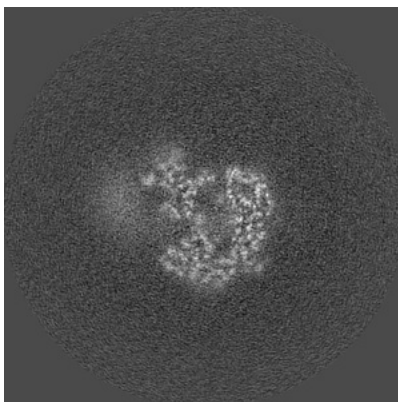


Z Index: 160

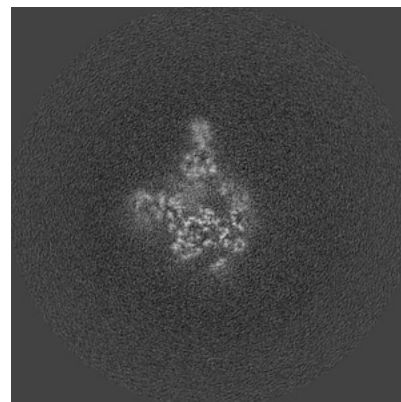
6.2.2 Raw map



X Index: 160



Y Index: 160

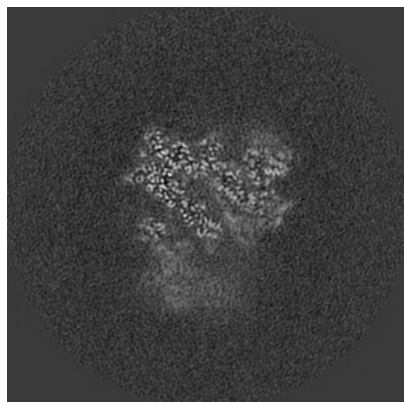


Z Index: 160

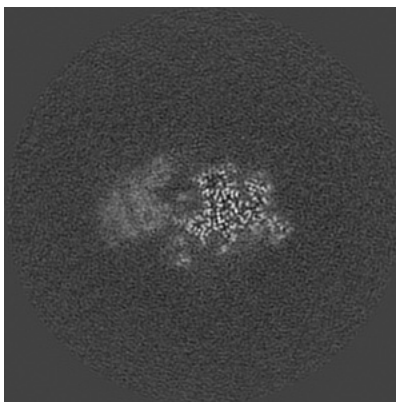
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

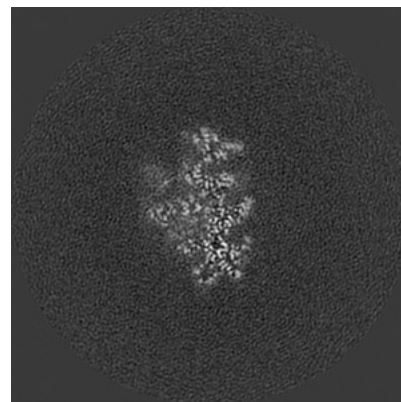
6.3.1 Primary map



X Index: 156

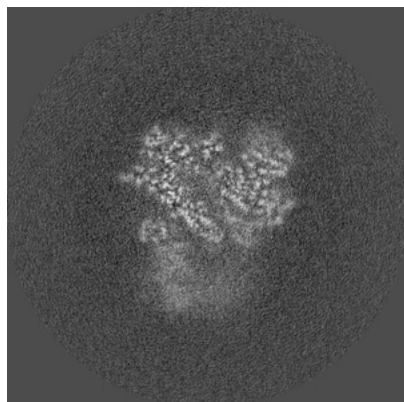


Y Index: 130

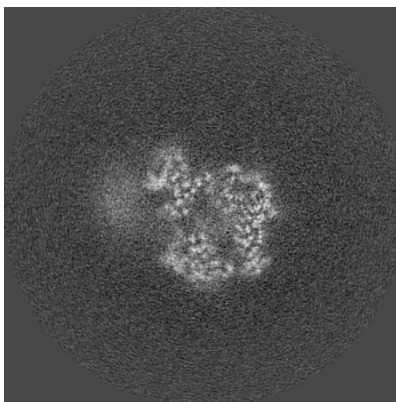


Z Index: 186

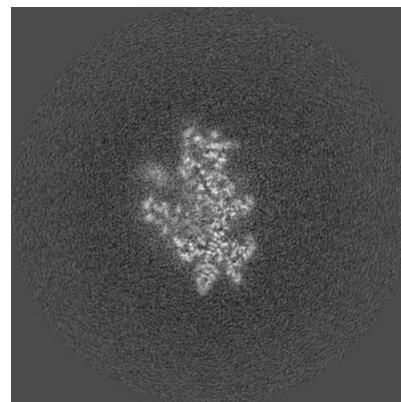
6.3.2 Raw map



X Index: 154



Y Index: 164

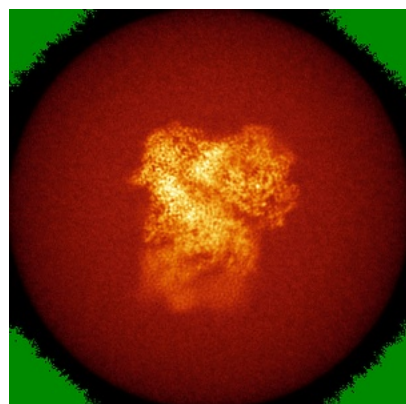


Z Index: 182

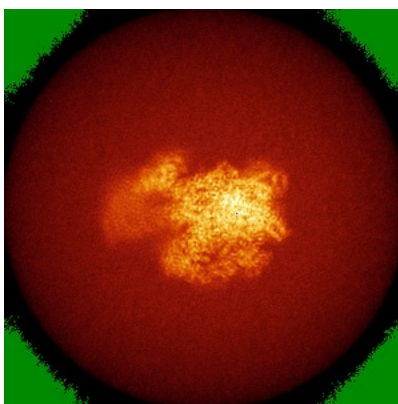
The images above show the largest variance slices of the map in three orthogonal directions.

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

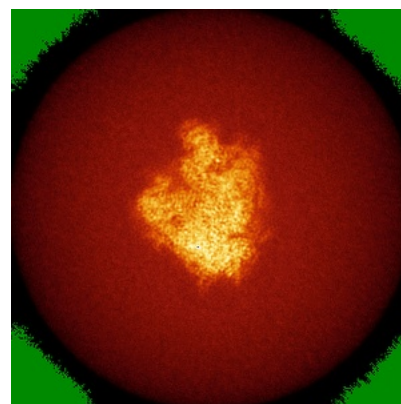
6.4.1 Primary map



X

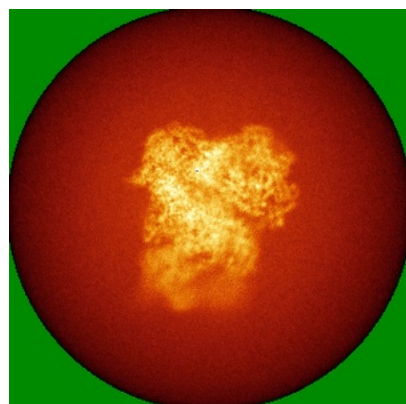


Y

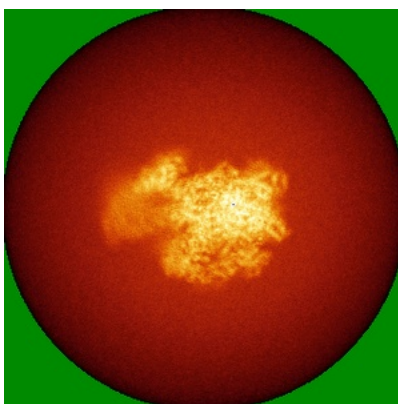


Z

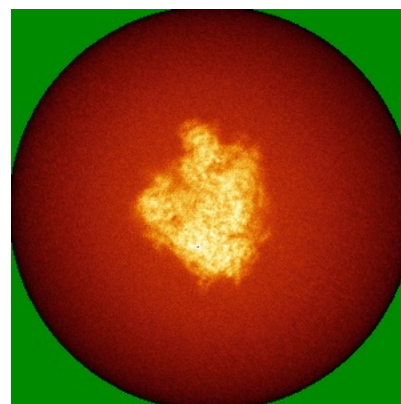
6.4.2 Raw map



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.

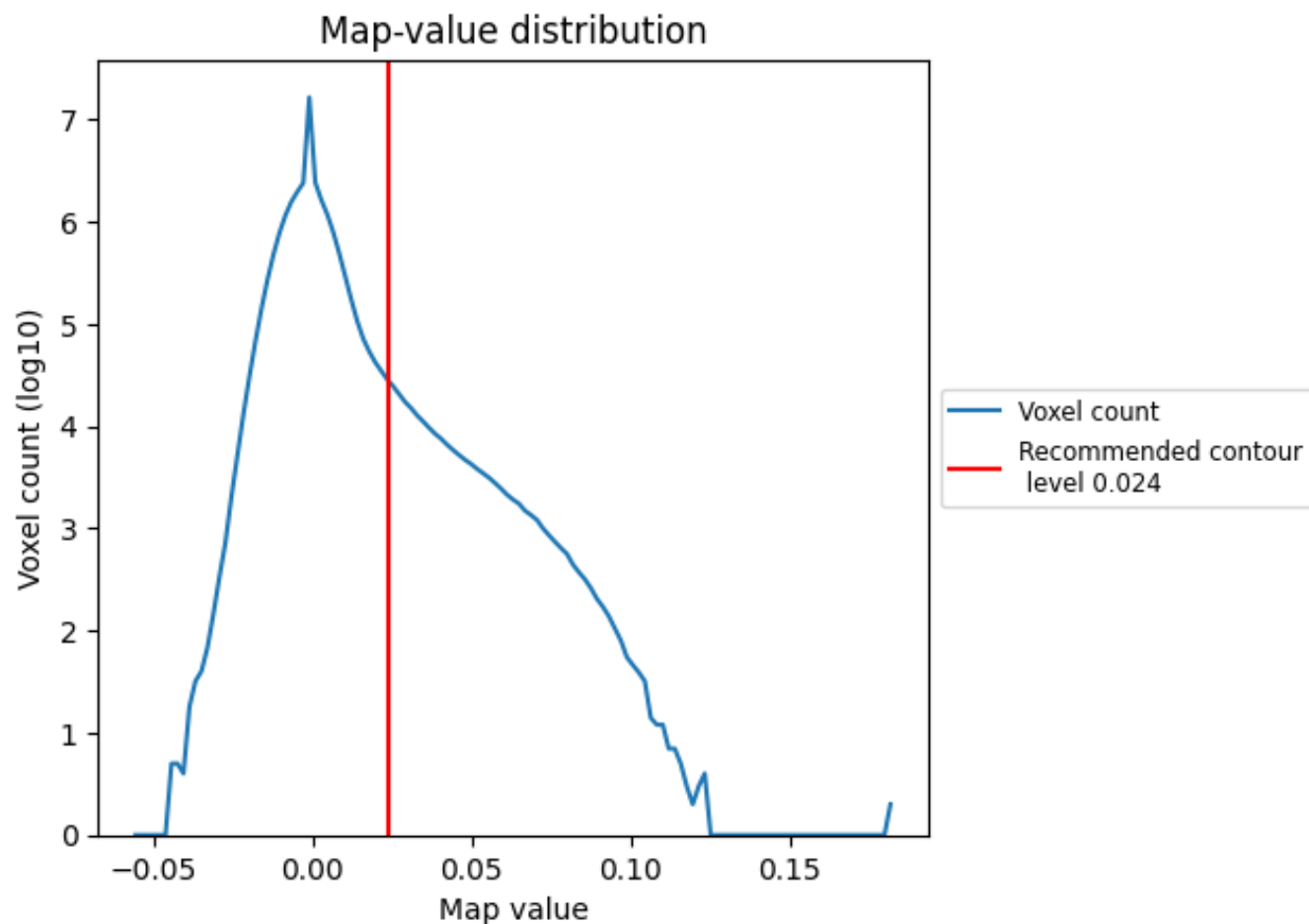
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

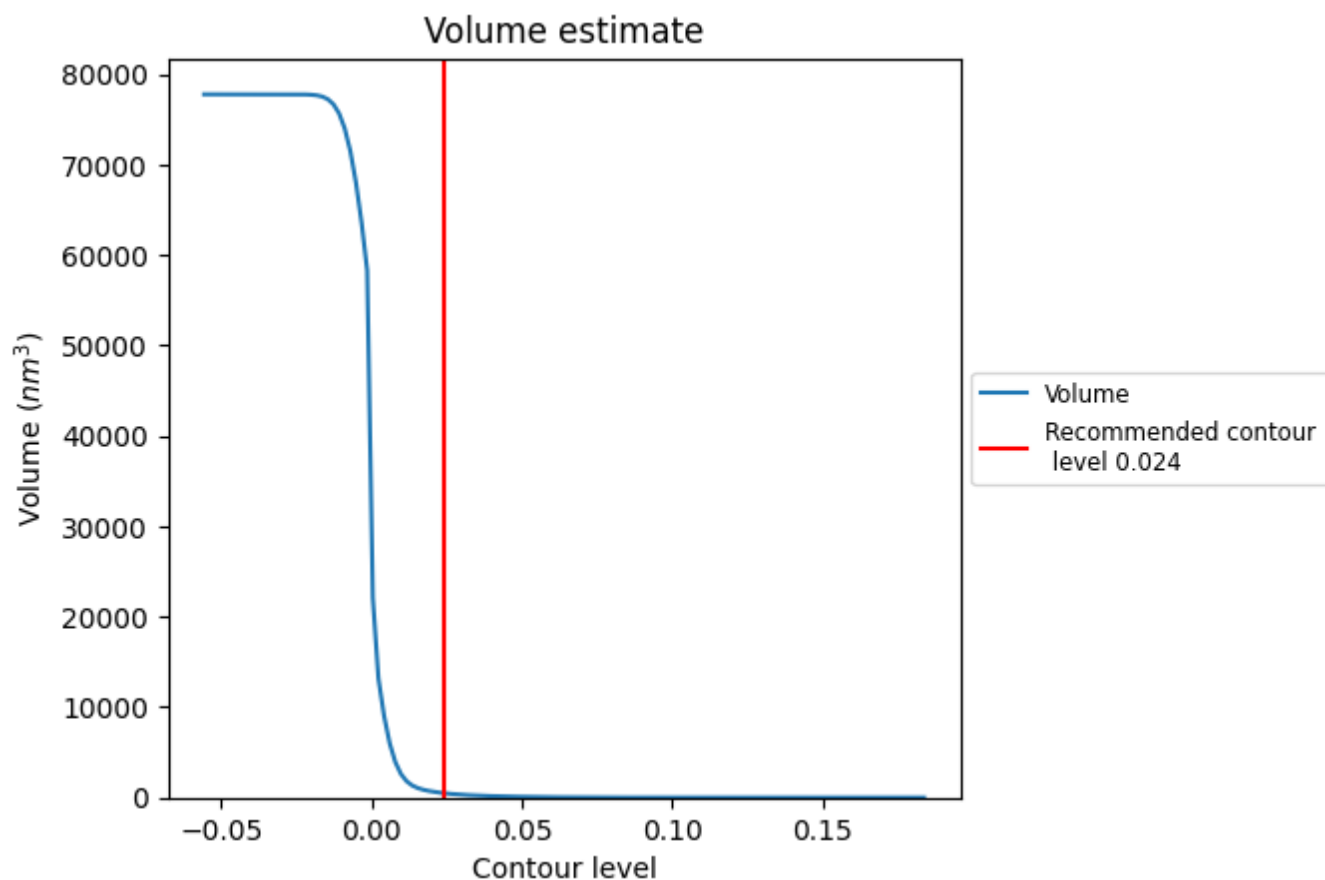
This section contains the results of statistical analysis of the map.

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.

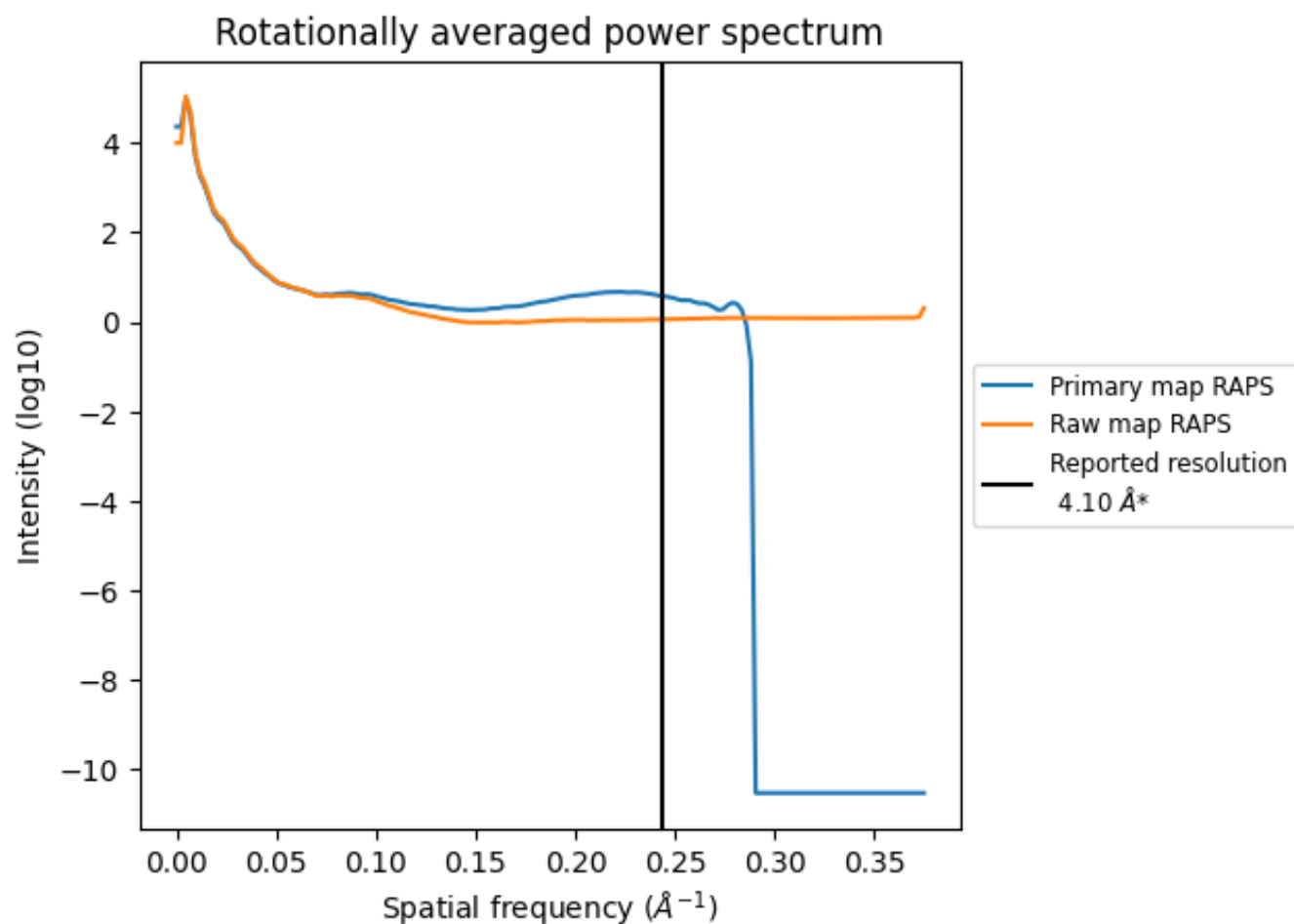
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 491 nm³; 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 ⓘ

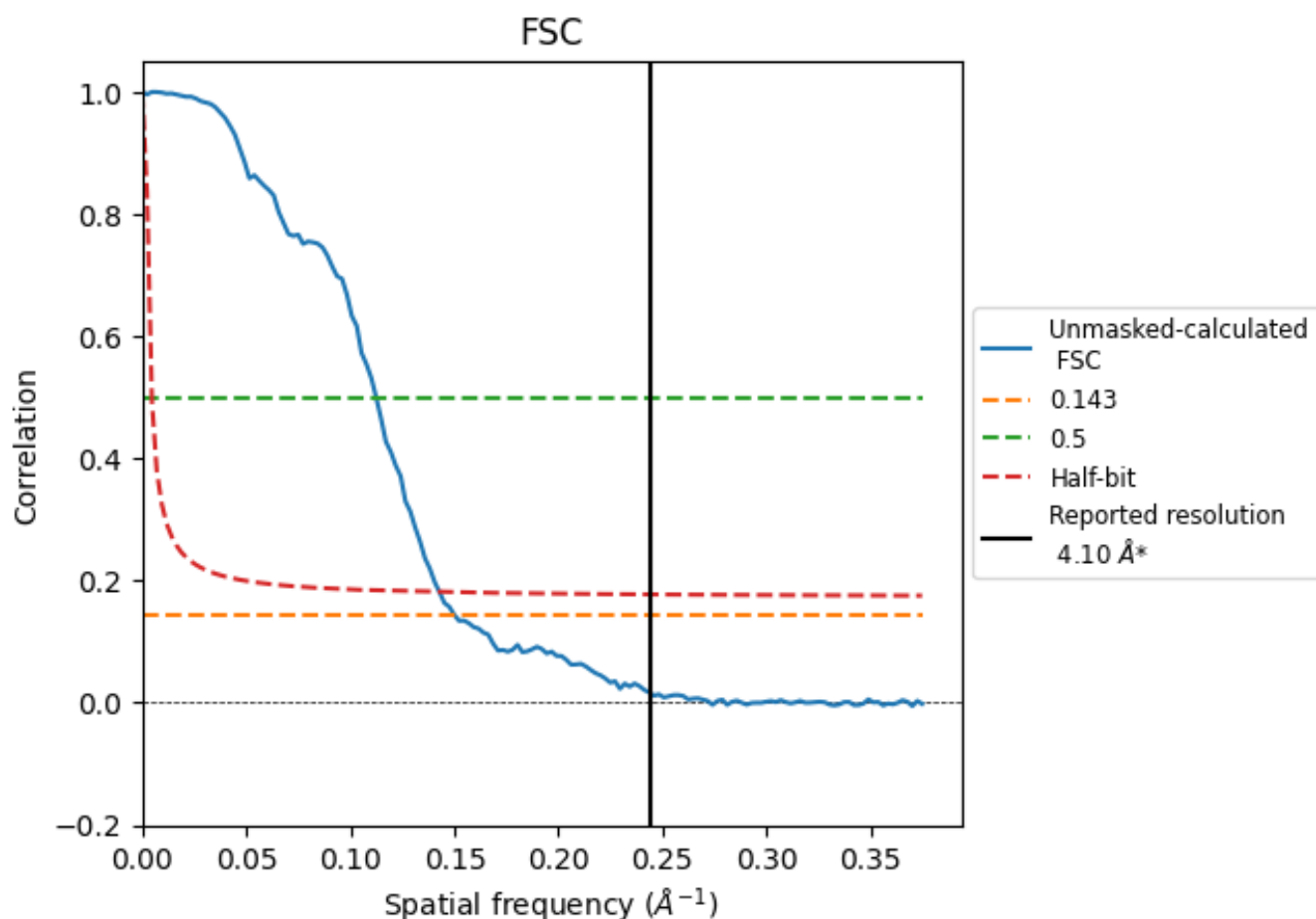


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

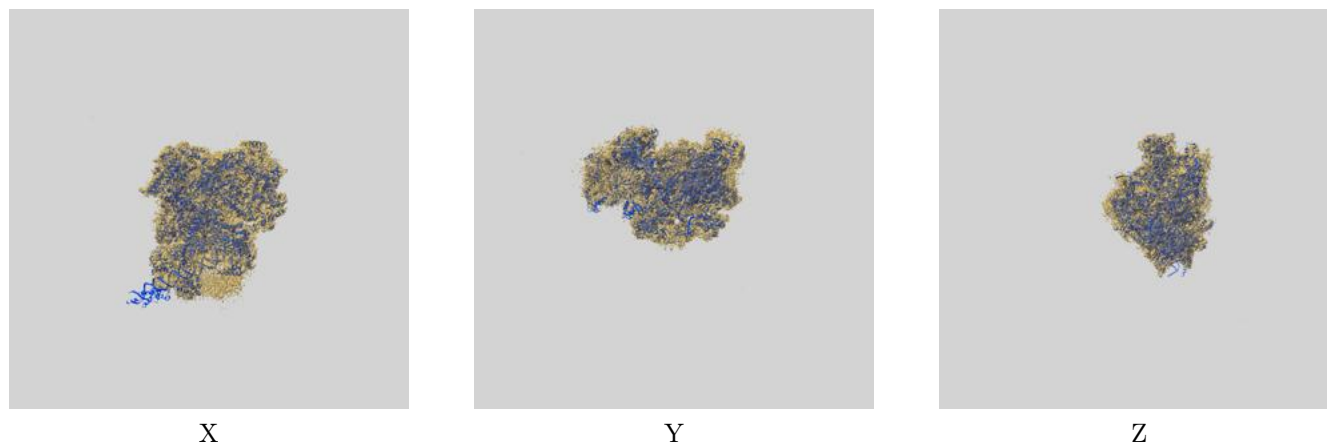
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.66	8.89	7.00

*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](#)

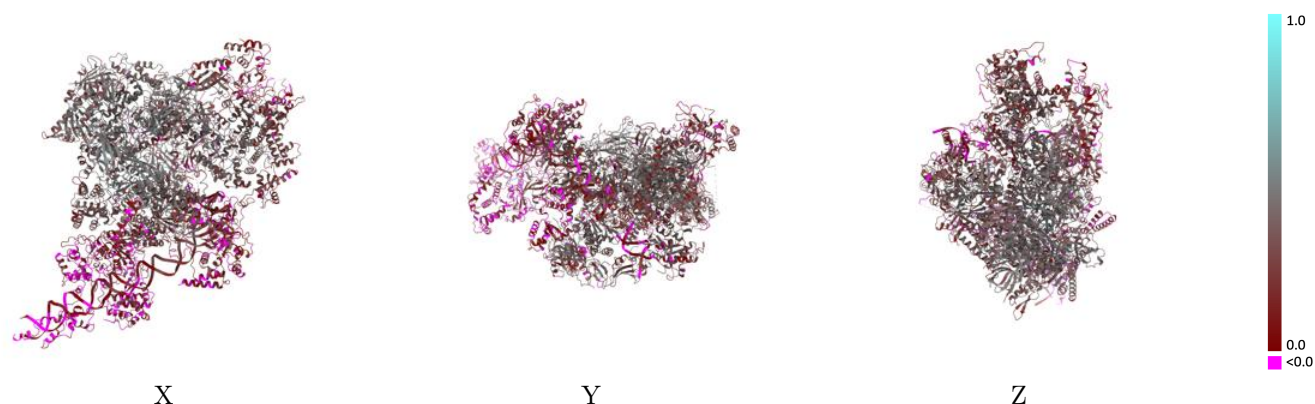
This section contains information regarding the fit between EMDB map EMD-35719 and PDB model 8IUE. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



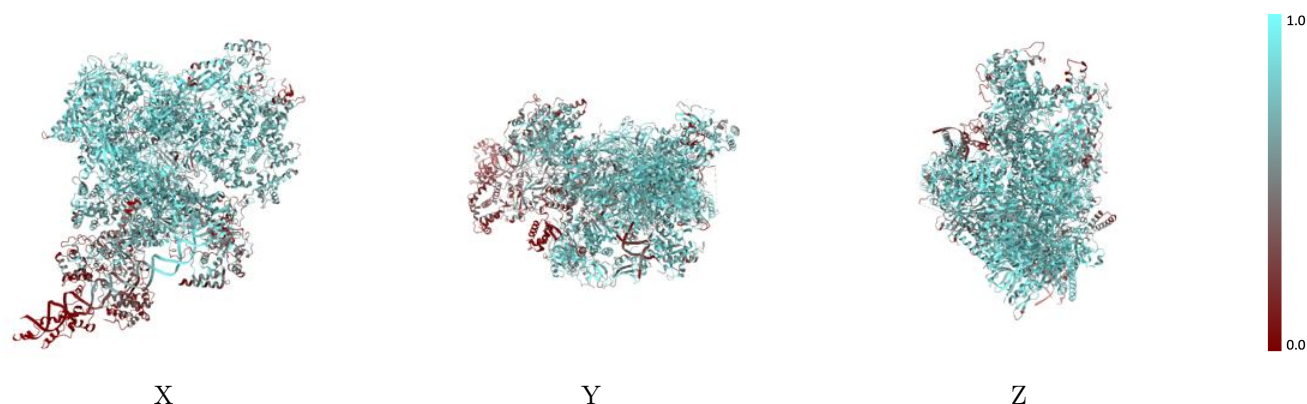
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



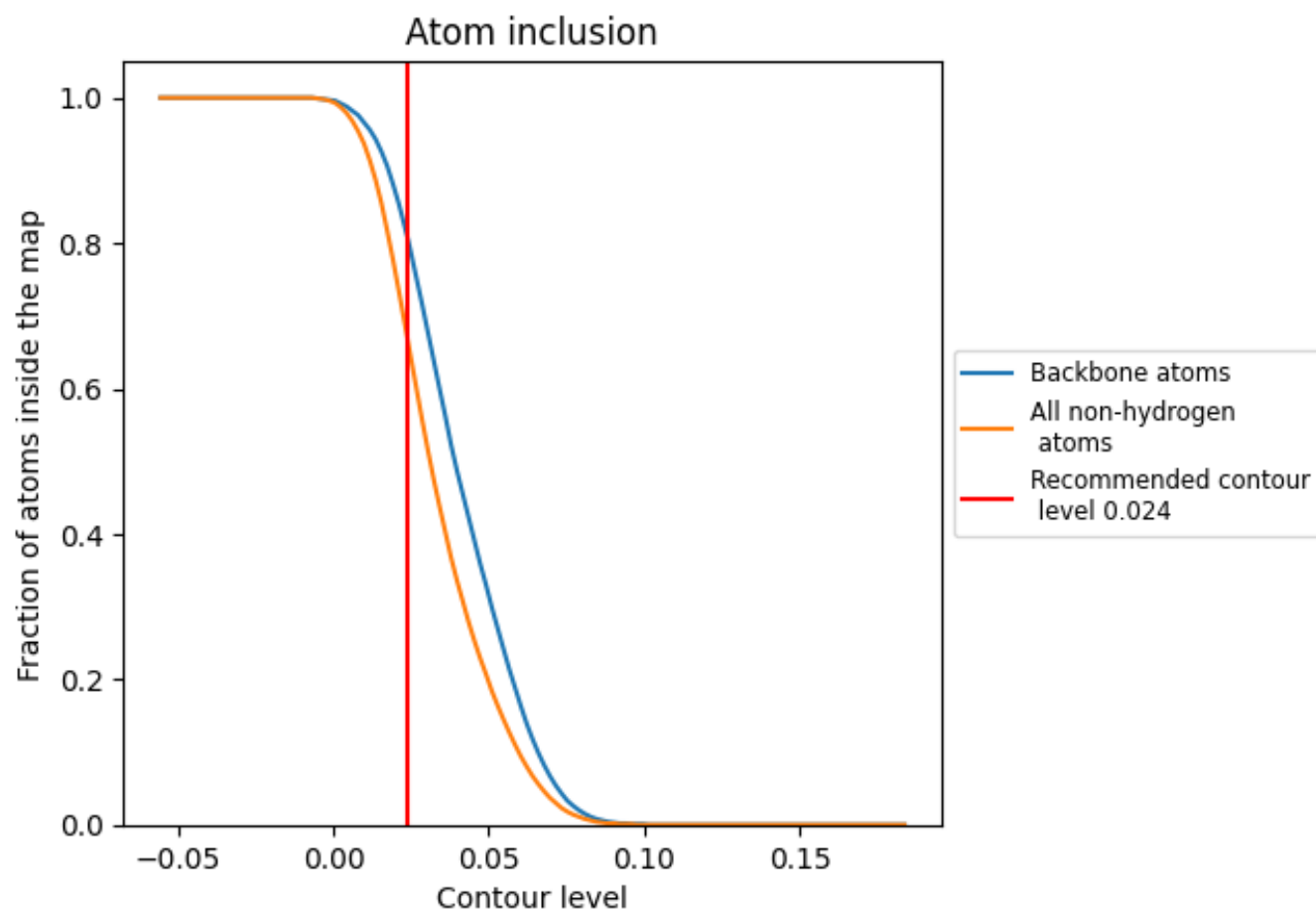
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.4300
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

