



## wwPDB EM Validation Summary Report ⓘ

May 6, 2024 – 06:29 AM JST

PDB ID : 8K5P  
EMDB ID : EMD-36908  
Title : Cryo-EM structure of yeast Rat1-bound Pol II pre-termination transcription complex 2 (Pol II Rat1-PTTC2)  
Authors : Zeng, Y.; Zhang, Y.  
Deposited on : 2023-07-23  
Resolution : 2.80 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.dev92  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

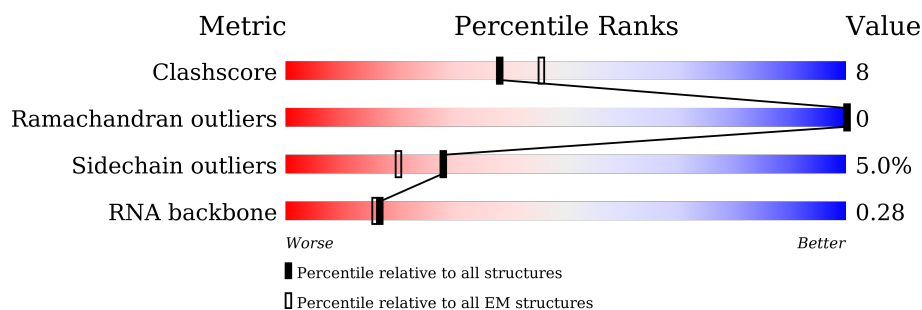
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 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.







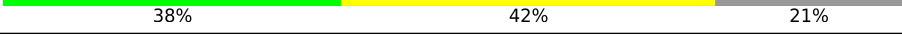
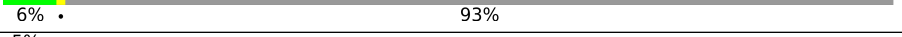
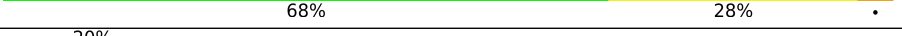


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	1733	
2	B	1259	
3	C	318	
4	E	215	
5	F	155	
6	H	146	
7	I	122	

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Mol	Chain	Length	Quality of chain
8	J	70	
9	K	120	
10	L	70	
11	N	48	
12	P	20	
13	T	48	
14	W	1070	
15	D	221	
16	G	171	
17	M	1019	
18	O	387	

## 2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 42713 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1408	Total	C	N	O	S	0	0
			11046	6963	1934	2092	57		

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1157	Total	C	N	O	S	0	0
			9187	5816	1601	1714	56		

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1225	GLU	-	expression tag	UNP P08518
B	1226	ASN	-	expression tag	UNP P08518
B	1227	LEU	-	expression tag	UNP P08518
B	1228	TYR	-	expression tag	UNP P08518
B	1229	PHE	-	expression tag	UNP P08518
B	1230	GLN	-	expression tag	UNP P08518
B	1231	GLY	-	expression tag	UNP P08518
B	1232	HIS	-	expression tag	UNP P08518
B	1233	HIS	-	expression tag	UNP P08518
B	1234	HIS	-	expression tag	UNP P08518
B	1235	HIS	-	expression tag	UNP P08518
B	1236	HIS	-	expression tag	UNP P08518
B	1237	HIS	-	expression tag	UNP P08518
B	1238	ASP	-	expression tag	UNP P08518
B	1239	TYR	-	expression tag	UNP P08518
B	1240	LYS	-	expression tag	UNP P08518
B	1241	ASP	-	expression tag	UNP P08518
B	1242	HIS	-	expression tag	UNP P08518
B	1243	ASP	-	expression tag	UNP P08518
B	1244	GLY	-	expression tag	UNP P08518
B	1245	ASP	-	expression tag	UNP P08518

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1246	TYR	-	expression tag	UNP P08518
B	1247	LYS	-	expression tag	UNP P08518
B	1248	ASP	-	expression tag	UNP P08518
B	1249	HIS	-	expression tag	UNP P08518
B	1250	ASP	-	expression tag	UNP P08518
B	1251	ILE	-	expression tag	UNP P08518
B	1252	ASP	-	expression tag	UNP P08518
B	1253	TYR	-	expression tag	UNP P08518
B	1254	LYS	-	expression tag	UNP P08518
B	1255	ASP	-	expression tag	UNP P08518
B	1256	ASP	-	expression tag	UNP P08518
B	1257	ASP	-	expression tag	UNP P08518
B	1258	ASP	-	expression tag	UNP P08518
B	1259	LYS	-	expression tag	UNP P08518

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	270	Total	C	N	O	S	0	0
			2125	1336	353	422	14		

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	215	Total	C	N	O	S	0	0
			1704	1080	305	310	9		

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	428	113	126	3		

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	144	Total	C	N	O	S	0	0
			1104	695	184	221	4		

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	115	Total	C	N	O	S	0	0
			871	542	147	171	11		

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	66	Total	C	N	O	S	0	0
			540	345	94	95	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	111	Total	C	N	O	S	0	0
			895	575	152	166	2		

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	46	Total	C	N	O	S	0	0
			364	224	72	64	4		

- Molecule 11 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	38	Total	C	N	O	P	0	0
			788	374	148	228	38		

- Molecule 12 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	P	20	Total	C	N	O	P	0	0
			430	192	80	138	20		

- Molecule 13 is a DNA chain called DNA (38-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	38	Total	C	N	O	P	0	0
			770	368	136	228	38		

- Molecule 14 is a protein called Transcription elongation factor SPT5.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	W	71	Total	C	N	O	0	0
			565	349	111	105		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-6	MET	-	initiating methionine	UNP P27692
W	-5	HIS	-	expression tag	UNP P27692
W	-4	HIS	-	expression tag	UNP P27692
W	-3	HIS	-	expression tag	UNP P27692
W	-2	HIS	-	expression tag	UNP P27692
W	-1	HIS	-	expression tag	UNP P27692
W	0	HIS	-	expression tag	UNP P27692

- Molecule 15 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	180	Total	C	N	O	S	0	0
			1455	899	262	292	2		

- Molecule 16 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	G	171	Total	C	N	O	S	0	0
			1340	861	222	249	8		

- Molecule 17 is a protein called 5'-3' exoribonuclease 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	744	Total	C	N	O	S	0	0
			6006	3860	1021	1100	25		

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-12	MET	-	initiating methionine	UNP Q02792
M	-11	GLY	-	expression tag	UNP Q02792
M	-10	SER	-	expression tag	UNP Q02792
M	-9	SER	-	expression tag	UNP Q02792
M	-8	HIS	-	expression tag	UNP Q02792
M	-7	HIS	-	expression tag	UNP Q02792
M	-6	HIS	-	expression tag	UNP Q02792

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-5	HIS	-	expression tag	UNP Q02792
M	-4	HIS	-	expression tag	UNP Q02792
M	-3	HIS	-	expression tag	UNP Q02792
M	-2	SER	-	expression tag	UNP Q02792
M	-1	GLN	-	expression tag	UNP Q02792
M	0	ASP	-	expression tag	UNP Q02792

- Molecule 18 is a protein called Decapping nuclease RAI1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	346	Total	C	N	O	S	0	0
			2842	1817	478	539	8		

- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	
19	C	1	Total	Zn	0
			1	1	
19	I	2	Total	Zn	0
			2	2	
19	J	1	Total	Zn	0
			1	1	
19	L	1	Total	Zn	0
			1	1	

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

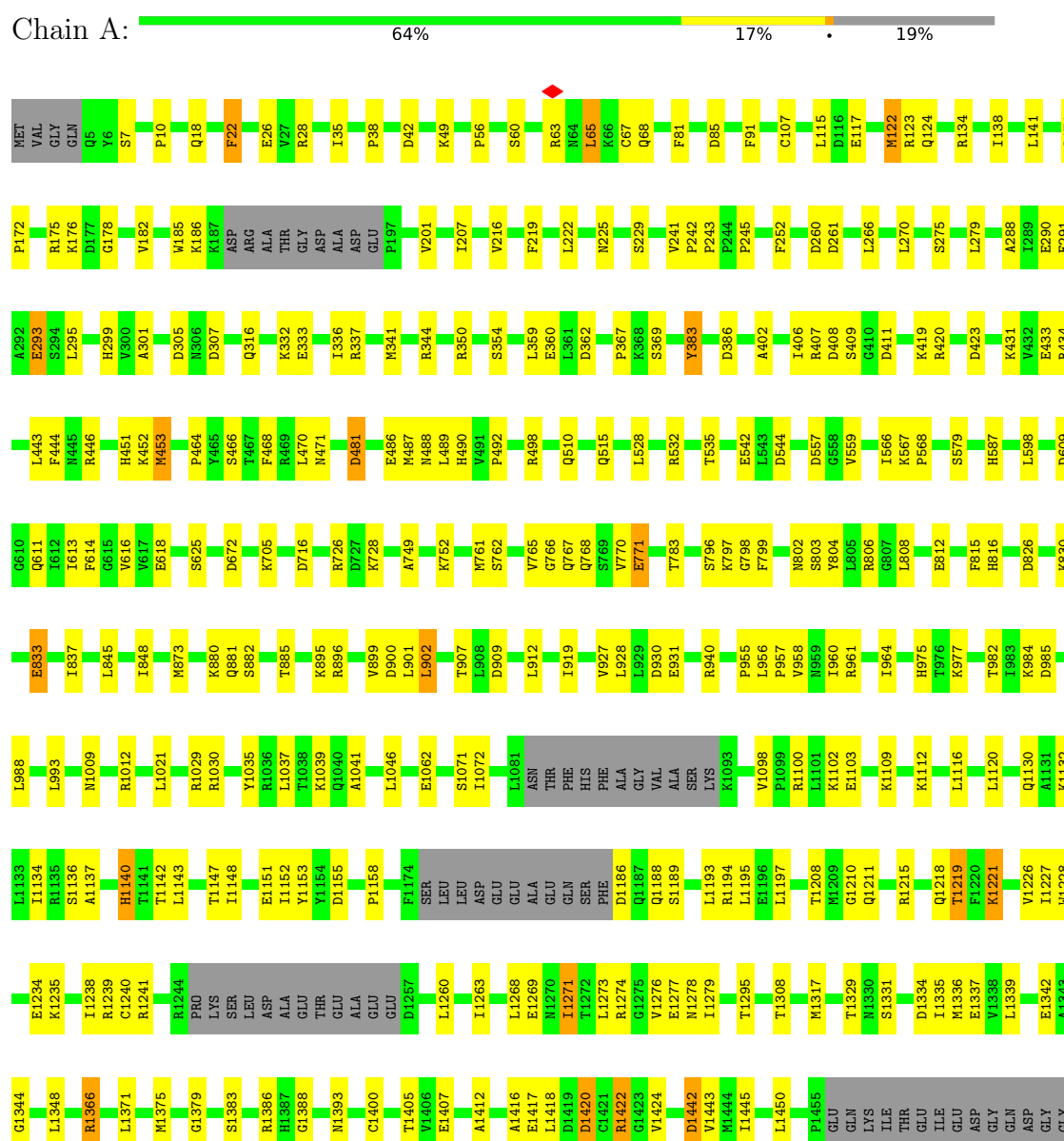
Mol	Chain	Residues	Atoms		AltConf
20	A	1	Total	Mg	0
			1	1	
20	M	1	Total	Mg	0
			1	1	
20	O	1	Total	Mg	0
			1	1	



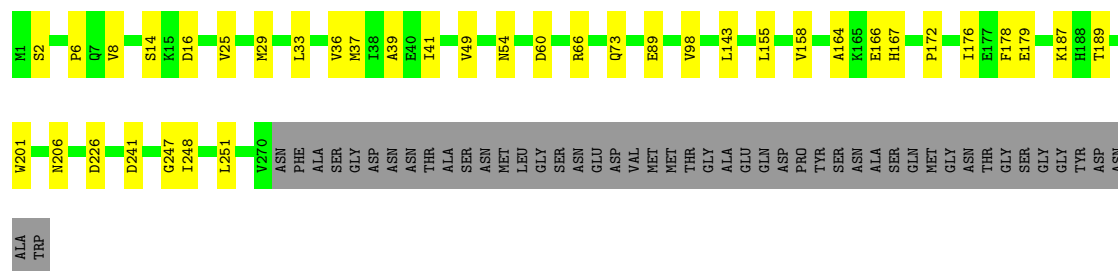
### 3 Residue-property plots

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 II subunit RPB1

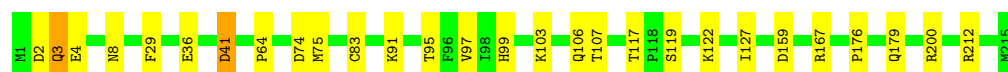






- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E: 87% 12%



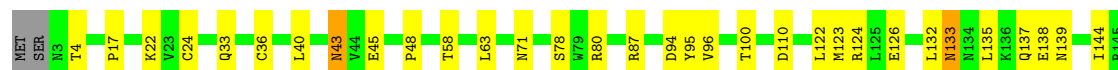
- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F: 32% 20% 46%



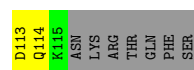
- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H: 76% 21%



- Molecule 7: DNA-directed RNA polymerase II subunit RPB9

Chain I: 62% 30% 6%



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

M1	I2	V3	Y21	E27	D28	E29	L30	D31	E32	G33	T34	L39	K42	T52	F60	L61	R62	L66	GLU	LYS	ARG	ASP
----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- |    |    |    |    |    |    |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |      |      |      |     |     |     |     |     |     |     |     |     |
|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| M1 | N2 | A3 | P4 | D5 | R6 | L12 | S17 | K18 | N44 | L45 | I46 | R47 | A48 | E49 | L50 | L51 | R54 | K55 | V56 | L57 | F58 | Q76 | T77 | T78 | E79 | I94 | L101 | K102 | T103 | N104 | F105 | L131 | GLN | THR | LEU | ALA | ALA | ASP | ASP | ALA | PRO |
|----|----|----|----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | SER | ARG | GLY | PHE | GLN | ILE | PRO | THR | ASN | LEU | ASP | ALA | ALA | ALA | GLY | THR | SER | GLN | ALA | ALA | ARG | THR | A25 | L40 | R47 | C48 | K49 | V65 | Q66 | F67 | E68 | A69 | R70 |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- |    |      |
|----|------|
| DG | C-16 |
| DC | A-13 |
| DG | G-12 |
| DT | G-11 |
| DG | A-10 |
| DT | T-9  |
| DC | C-8  |
| DT | G-7  |
| DA | G-2  |
| DG | T-1  |
|    | T5   |
|    | G6   |
|    | T11  |
|    | C12  |
|    | G13  |
|    | G14  |
|    | T15  |
|    | A16  |
|    | G17  |
|    | A18  |
|    | G21  |

- |      |      |      |      |      |      |      |      |      |      |      |     |     |     |
|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|
| A-20 | C-19 | A-18 | G-17 | A-16 | U-15 | G-14 | U-13 | C-12 | C-11 | U-10 | C-9 | G-8 | A-1 |
|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|

- |      |      |      |      |     |     |     |     |     |     |     |    |    |    |    |    |    |    |    |    |     |     |     |     |     |    |    |    |    |    |    |    |    |    |    |
|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|----|----|----|----|----|----|----|----|----|----|
| C-21 | G-12 | A-11 | T-10 | A-9 | A-8 | G-7 | C-6 | A-5 | G-4 | T-1 | T0 | A1 | C2 | C3 | T4 | C5 | T6 | C7 | G8 | C12 | T13 | G14 | T15 | G16 | DC | DT | DA | DG | DA | DC | DA | DC | DG | DC |
|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|----|----|----|----|----|----|----|----|----|-----|-----|-----|-----|-----|----|----|----|----|----|----|----|----|----|----|

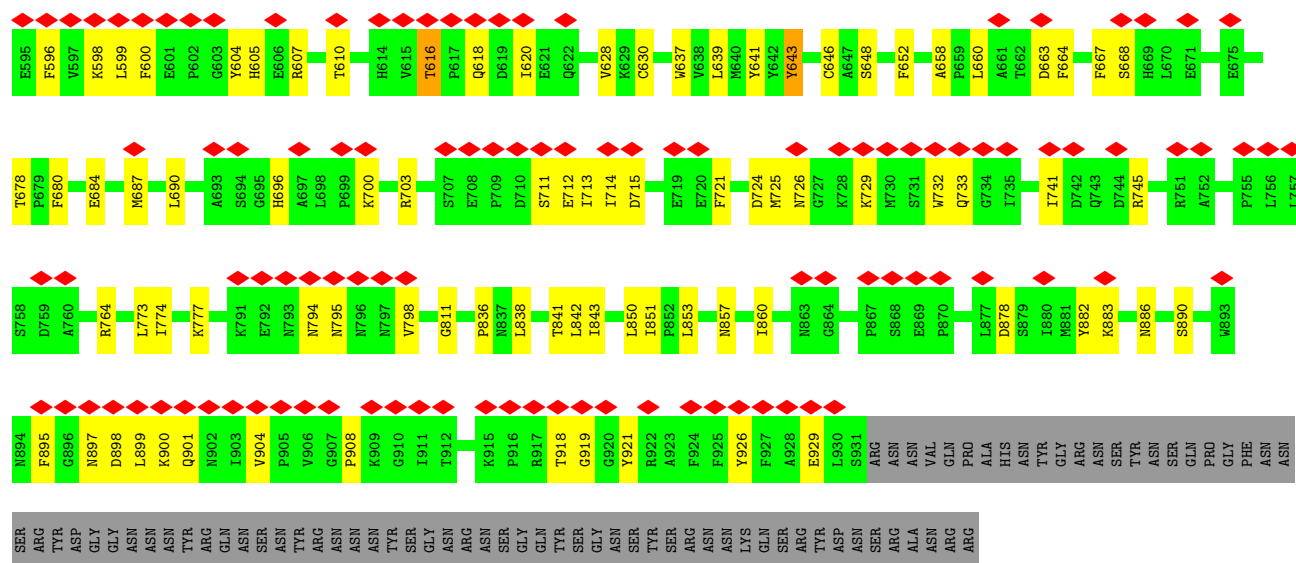
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | HIS | HIS | HIS | HIS | HIS | HIS | HIS | MET | SER | ASP | ASN | SER | ASP | THR | ASN | VAL | GLN | GLN | GLN | PHE | ALA | ASP | PRO | VAL | VAL | VAL | VAL | PRO | GLN | SER | SER | THR | ASP | THR | ASP | LYS | ASP | GLU | THR | ASN | SER | ASP | LYS | VAL | THR | ASN | THR | THR | THR | GLU | SER | SER | THR | THR | THR |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

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

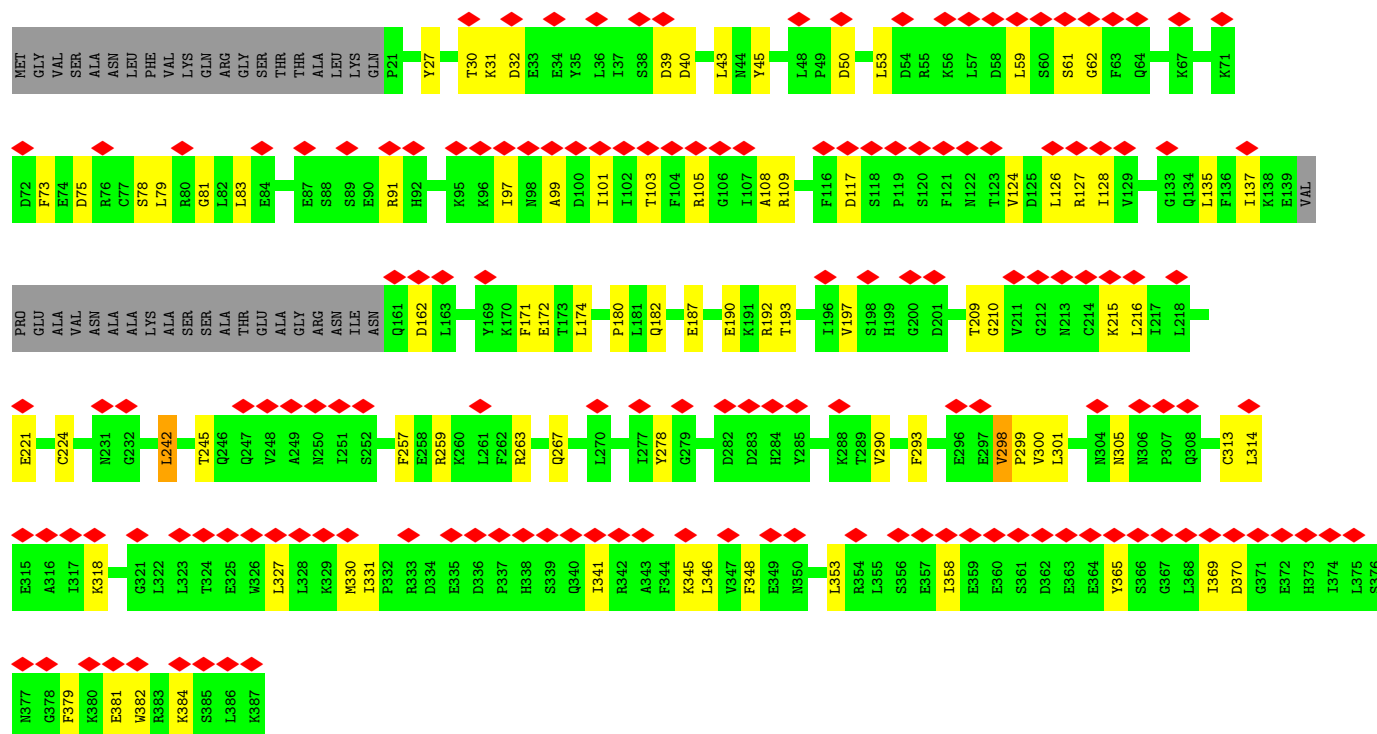
- Molecule 15: DNA-directed RNA polymerase II subunit RPB4

[illegible]





• Molecule 18: Decapping nuclease RAI1



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	265756	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.367	Depositor
Minimum map value	-0.945	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.047	Depositor
Recommended contour level	0.15	Depositor
Map size ( $\text{\AA}$ )	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.25	0/11244	0.48	0/15213
2	B	0.25	0/9370	0.50	0/12640
3	C	0.25	0/2163	0.45	0/2930
4	E	0.25	0/1739	0.49	0/2347
5	F	0.37	0/682	0.64	0/922
6	H	0.29	0/1123	0.53	0/1529
7	I	0.32	0/889	0.60	0/1207
8	J	0.27	0/549	0.55	0/738
9	K	0.26	0/913	0.49	0/1232
10	L	0.28	0/366	0.69	0/485
11	N	0.48	0/885	0.88	0/1366
12	P	0.17	0/481	0.73	0/748
13	T	0.51	0/861	0.90	0/1324
14	W	0.22	0/571	0.51	0/762
15	D	0.25	0/1466	0.57	0/1963
16	G	0.29	0/1368	0.56	0/1844
17	M	0.24	0/6166	0.47	0/8372
18	O	0.24	0/2902	0.45	0/3910
All	All	0.27	0/43738	0.53	0/59532

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 [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	11046	0	11086	171	0
2	B	9187	0	9171	133	0
3	C	2125	0	2090	28	0
4	E	1704	0	1687	17	0
5	F	670	0	688	27	0
6	H	1104	0	1047	20	0
7	I	871	0	777	32	0
8	J	540	0	553	9	0
9	K	895	0	903	18	0
10	L	364	0	386	6	0
11	N	788	0	429	14	0
12	P	430	0	217	4	0
13	T	770	0	429	16	0
14	W	565	0	580	6	0
15	D	1455	0	1477	50	0
16	G	1340	0	1357	35	0
17	M	6006	0	5878	104	0
18	O	2842	0	2802	40	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	C	1	0	0	0	0
19	I	2	0	0	0	0
19	J	1	0	0	0	0
19	L	1	0	0	0	0
20	A	1	0	0	0	0
20	M	1	0	0	0	0
20	O	1	0	0	0	0
All	All	42713	0	41557	672	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 8.

The worst 5 of 672 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)
10:L:49:LYS:HE3	10:L:49:LYS:HA	1.63	0.78
7:I:55:THR:OG1	7:I:56:ALA:N	2.20	0.75
6:H:137:GLN:HG2	6:H:138:GLU:HG3	1.69	0.74
1:A:1142:THR:HG22	1:A:1273:LEU:HG	1.71	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:216:ARG:O	18:O:182:GLN:NE2	2.22	0.72

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	1398/1733 (81%)	1343 (96%)	55 (4%)	0	100	100
2	B	1147/1259 (91%)	1107 (96%)	40 (4%)	0	100	100
3	C	268/318 (84%)	263 (98%)	5 (2%)	0	100	100
4	E	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
5	F	81/155 (52%)	77 (95%)	4 (5%)	0	100	100
6	H	142/146 (97%)	130 (92%)	12 (8%)	0	100	100
7	I	113/122 (93%)	101 (89%)	12 (11%)	0	100	100
8	J	64/70 (91%)	61 (95%)	3 (5%)	0	100	100
9	K	109/120 (91%)	107 (98%)	2 (2%)	0	100	100
10	L	44/70 (63%)	43 (98%)	1 (2%)	0	100	100
14	W	69/1070 (6%)	64 (93%)	5 (7%)	0	100	100
15	D	176/221 (80%)	165 (94%)	11 (6%)	0	100	100
16	G	169/171 (99%)	153 (90%)	16 (10%)	0	100	100
17	M	740/1019 (73%)	702 (95%)	38 (5%)	0	100	100
18	O	342/387 (88%)	325 (95%)	17 (5%)	0	100	100
All	All	5075/7076 (72%)	4846 (96%)	229 (4%)	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	1222/1520 (80%)	1160 (95%)	62 (5%)	24	55
2	B	997/1094 (91%)	957 (96%)	40 (4%)	31	65
3	C	238/274 (87%)	235 (99%)	3 (1%)	69	91
4	E	181/197 (92%)	174 (96%)	7 (4%)	32	66
5	F	73/137 (53%)	68 (93%)	5 (7%)	16	42
6	H	116/128 (91%)	110 (95%)	6 (5%)	23	55
7	I	95/116 (82%)	85 (90%)	10 (10%)	7	20
8	J	61/65 (94%)	58 (95%)	3 (5%)	25	57
9	K	96/102 (94%)	93 (97%)	3 (3%)	40	74
10	L	40/57 (70%)	37 (92%)	3 (8%)	13	37
14	W	59/883 (7%)	58 (98%)	1 (2%)	60	87
15	D	162/200 (81%)	154 (95%)	8 (5%)	25	57
16	G	152/152 (100%)	137 (90%)	15 (10%)	8	23
17	M	651/909 (72%)	612 (94%)	39 (6%)	19	48
18	O	315/346 (91%)	296 (94%)	19 (6%)	19	48
All	All	4458/6180 (72%)	4234 (95%)	224 (5%)	28	56

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	118	LEU
18	O	358	ILE
15	D	12	ARG
18	O	300	VAL
17	M	899	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
6	H	52	GLN
17	M	743	GLN
9	K	92	ASN
17	M	650	ASN
18	O	179	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	P	19/20 (95%)	9 (47%)	0

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	P	-18	A
12	P	-17	G
12	P	-16	A
12	P	-13	U
12	P	-12	C

There are no RNA pucker outliers to report.

## 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 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

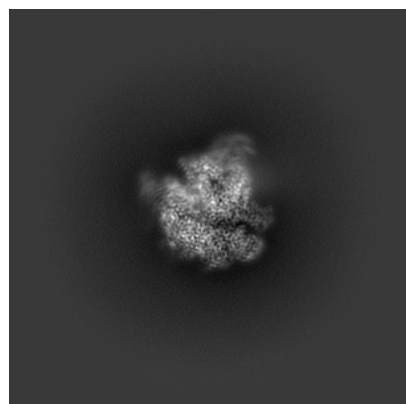
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36908. These allow visual inspection of the internal detail of the map and identification of artifacts.

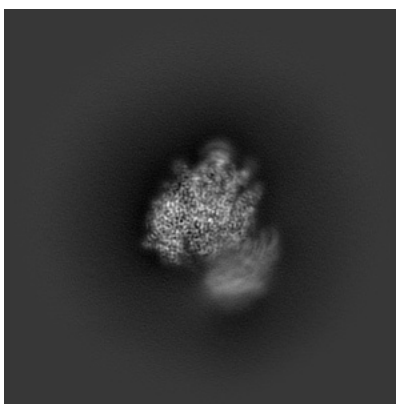
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

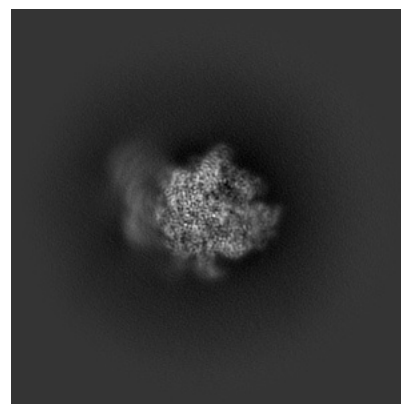
#### 6.1.1 Primary map



X

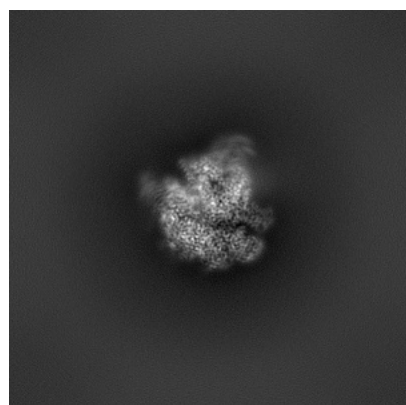


Y

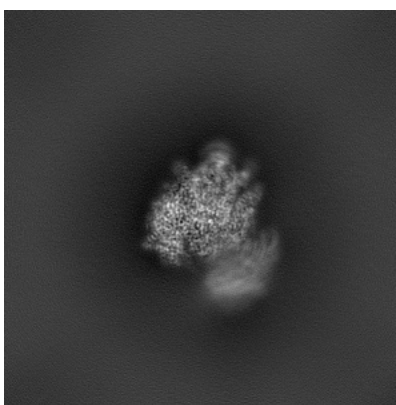


Z

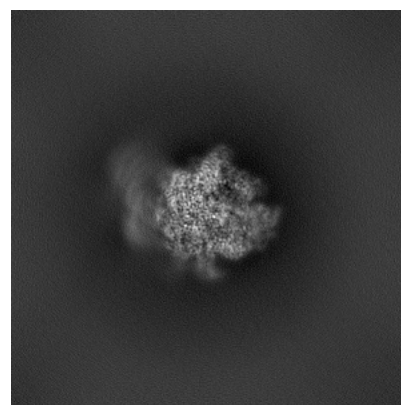
#### 6.1.2 Raw map



X



Y

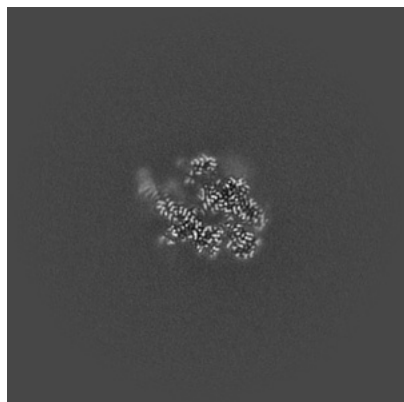


Z

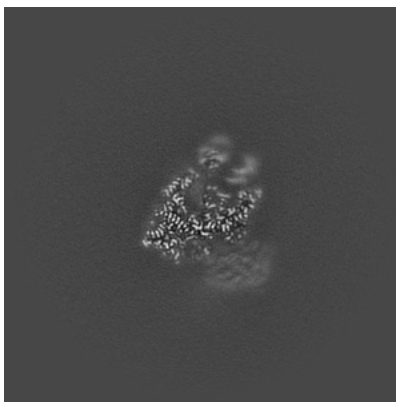
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

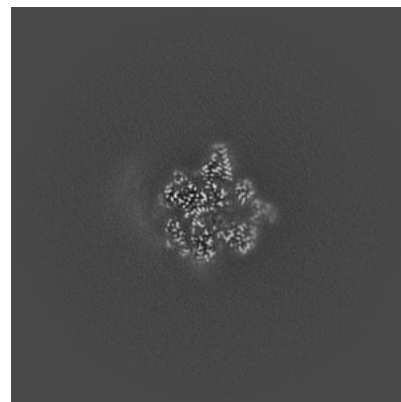
### 6.2.1 Primary map



X Index: 200

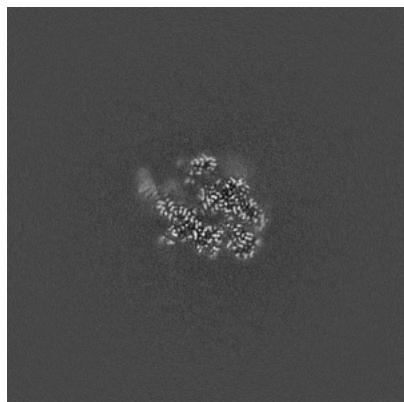


Y Index: 200

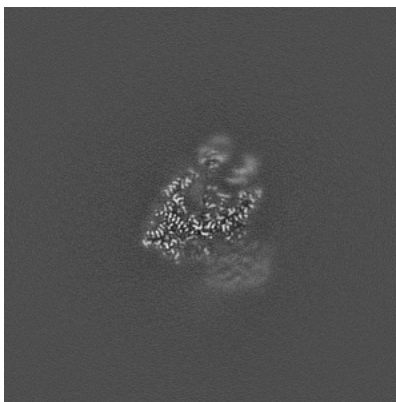


Z Index: 200

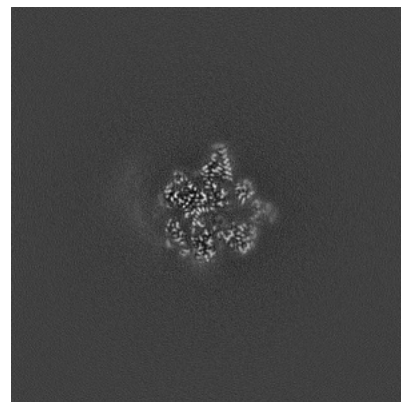
### 6.2.2 Raw map



X Index: 200



Y Index: 200



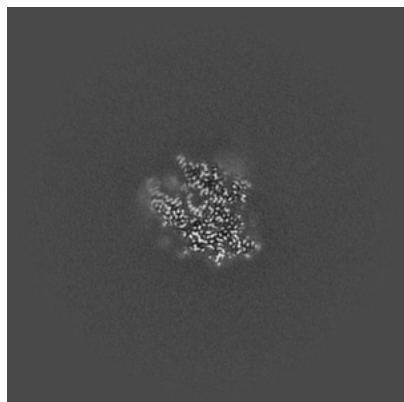
Z Index: 200

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

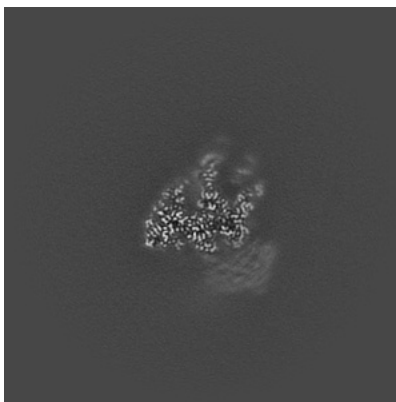


## 6.3 Largest variance slices [i](#)

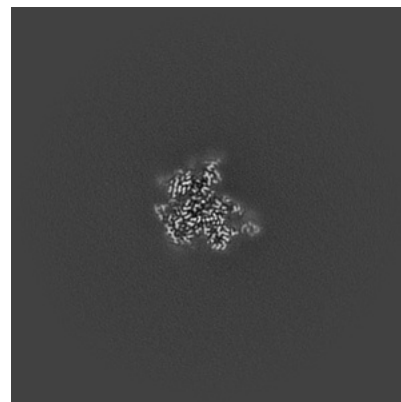
### 6.3.1 Primary map



X Index: 188

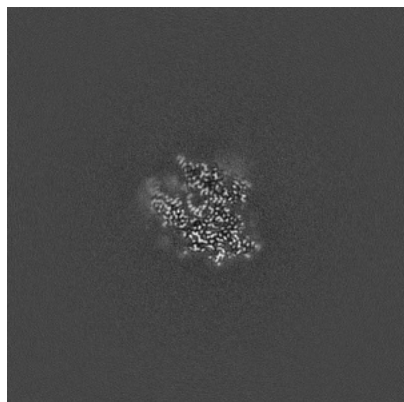


Y Index: 205

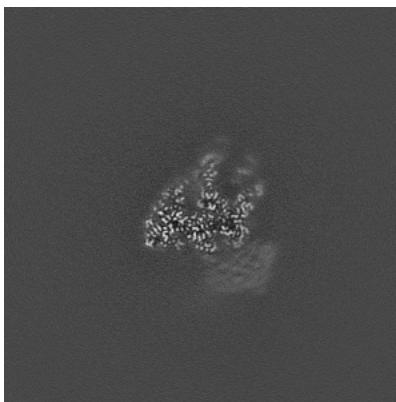


Z Index: 173

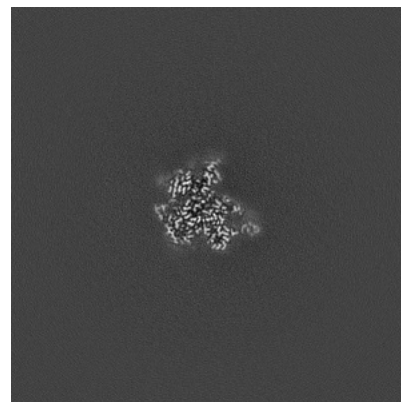
### 6.3.2 Raw map



X Index: 188



Y Index: 205

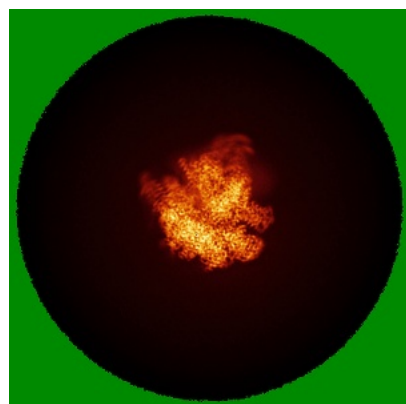


Z Index: 173

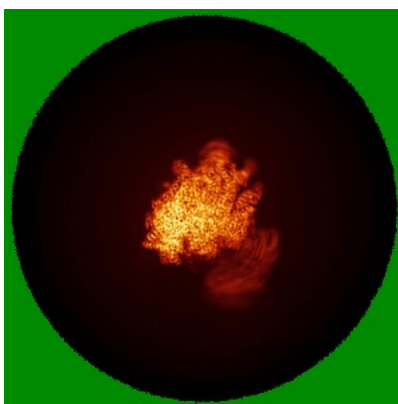
The images above show the largest variance slices of the map in three orthogonal directions.

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

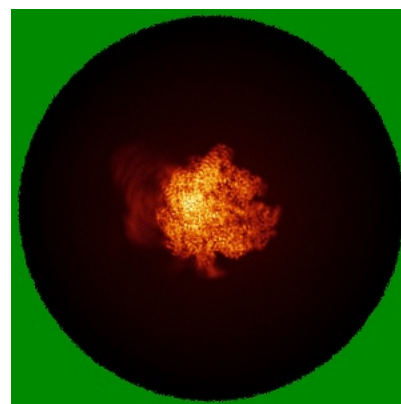
### 6.4.1 Primary map



X

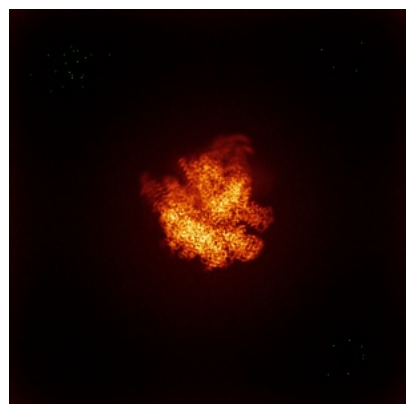


Y

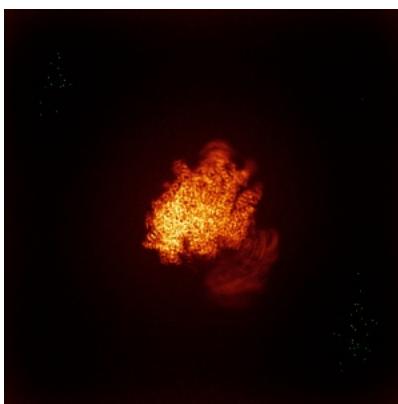


Z

### 6.4.2 Raw map



X



Y

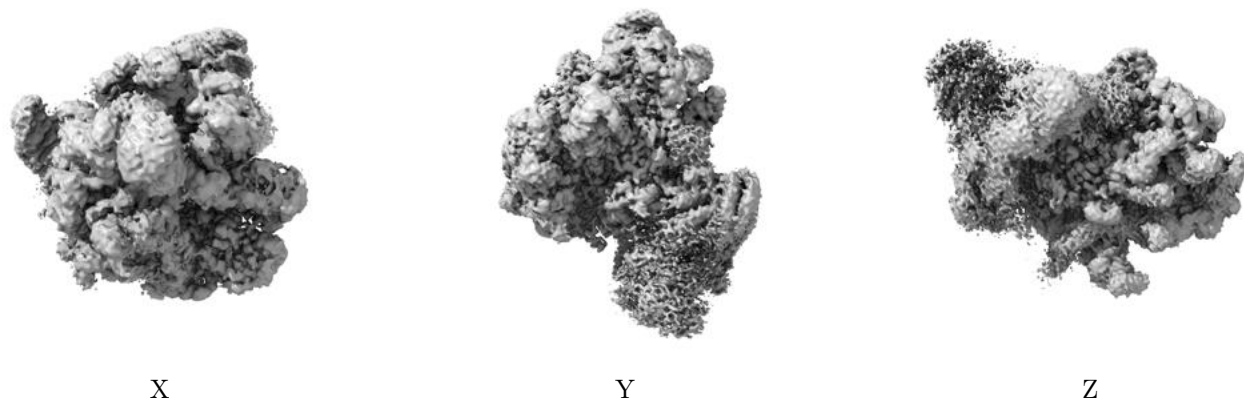


Z

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.

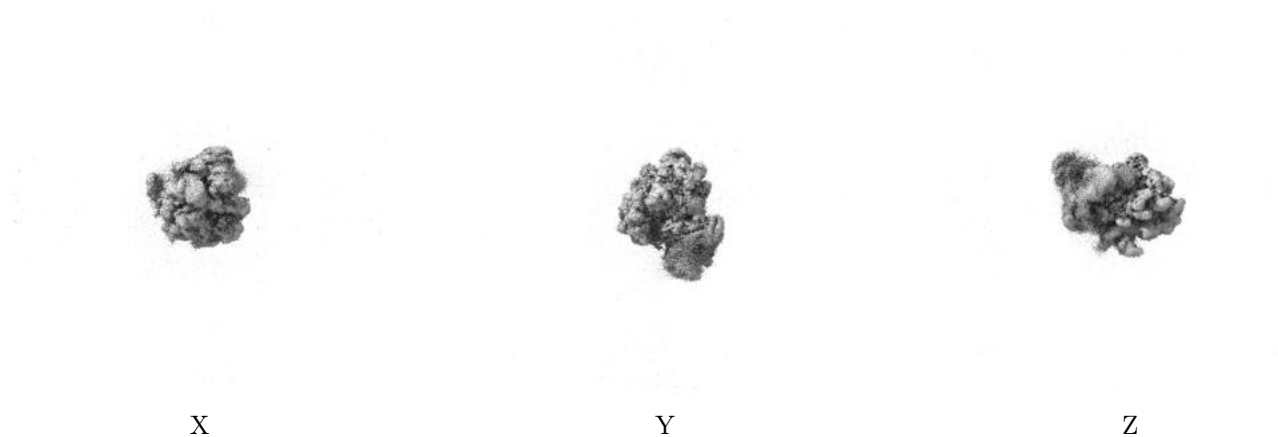
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

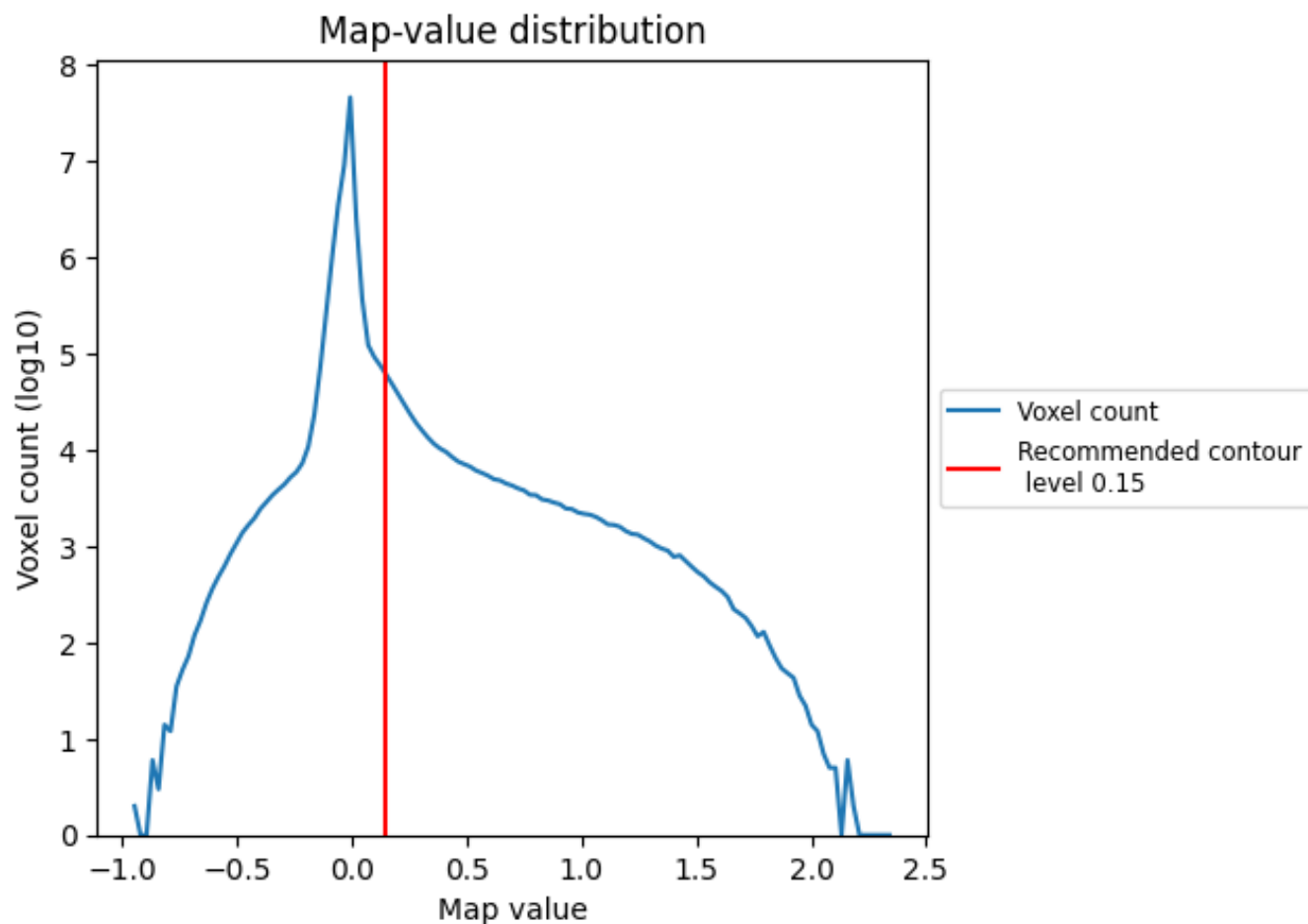
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

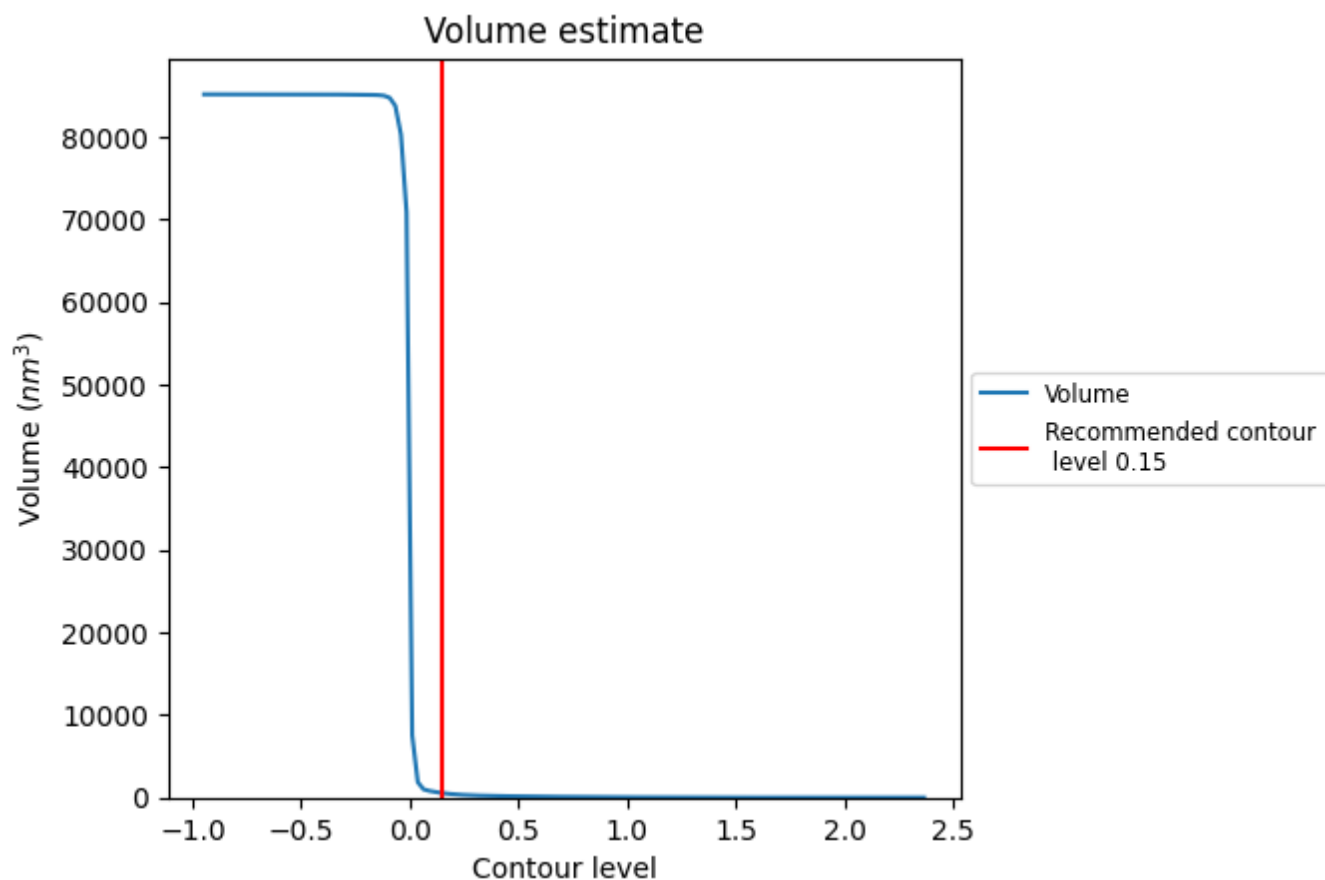
This section contains the results of statistical analysis of the map.

### 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.

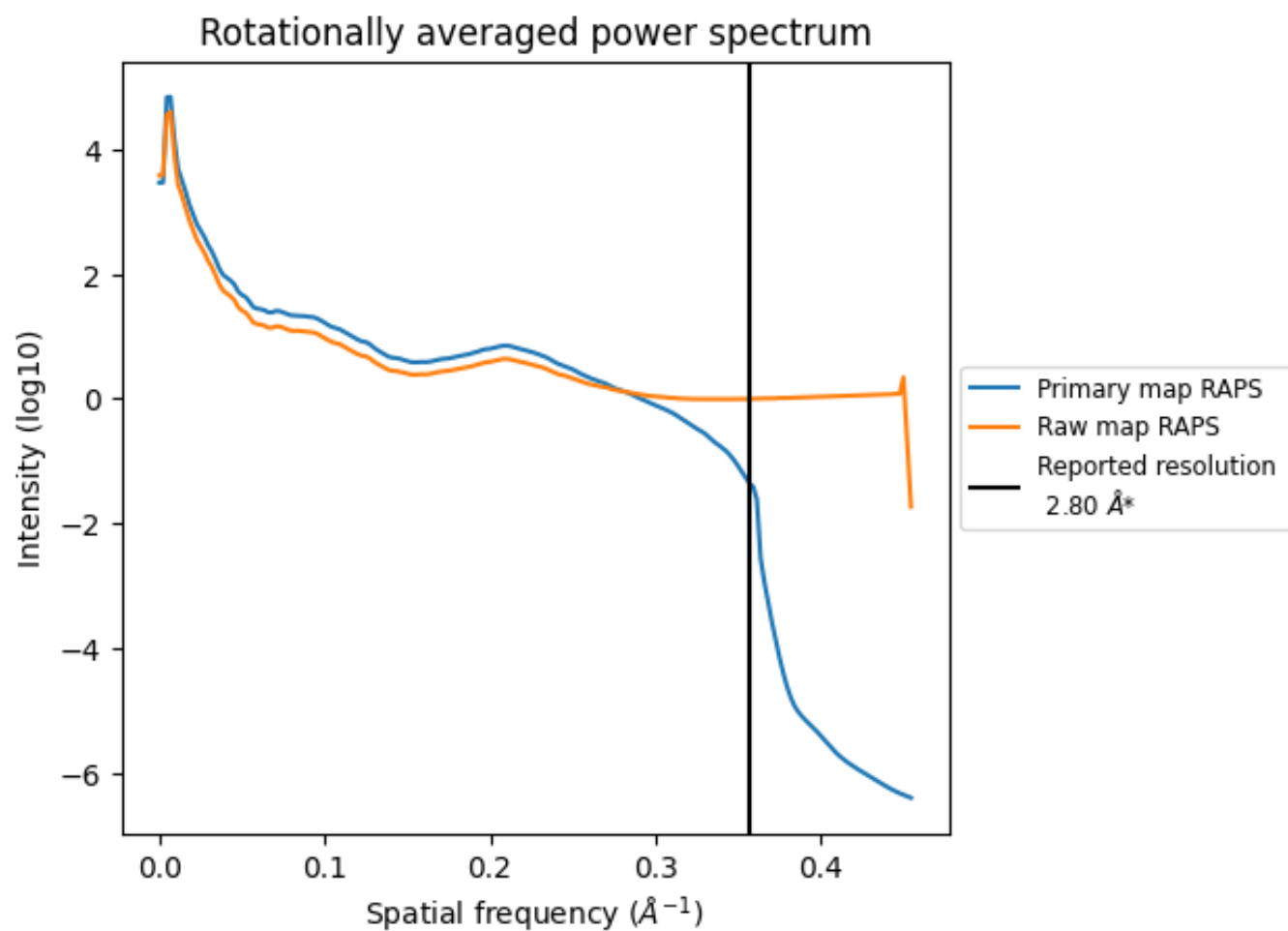
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 546 nm<sup>3</sup>; this corresponds to an approximate mass of 494 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 ⓘ

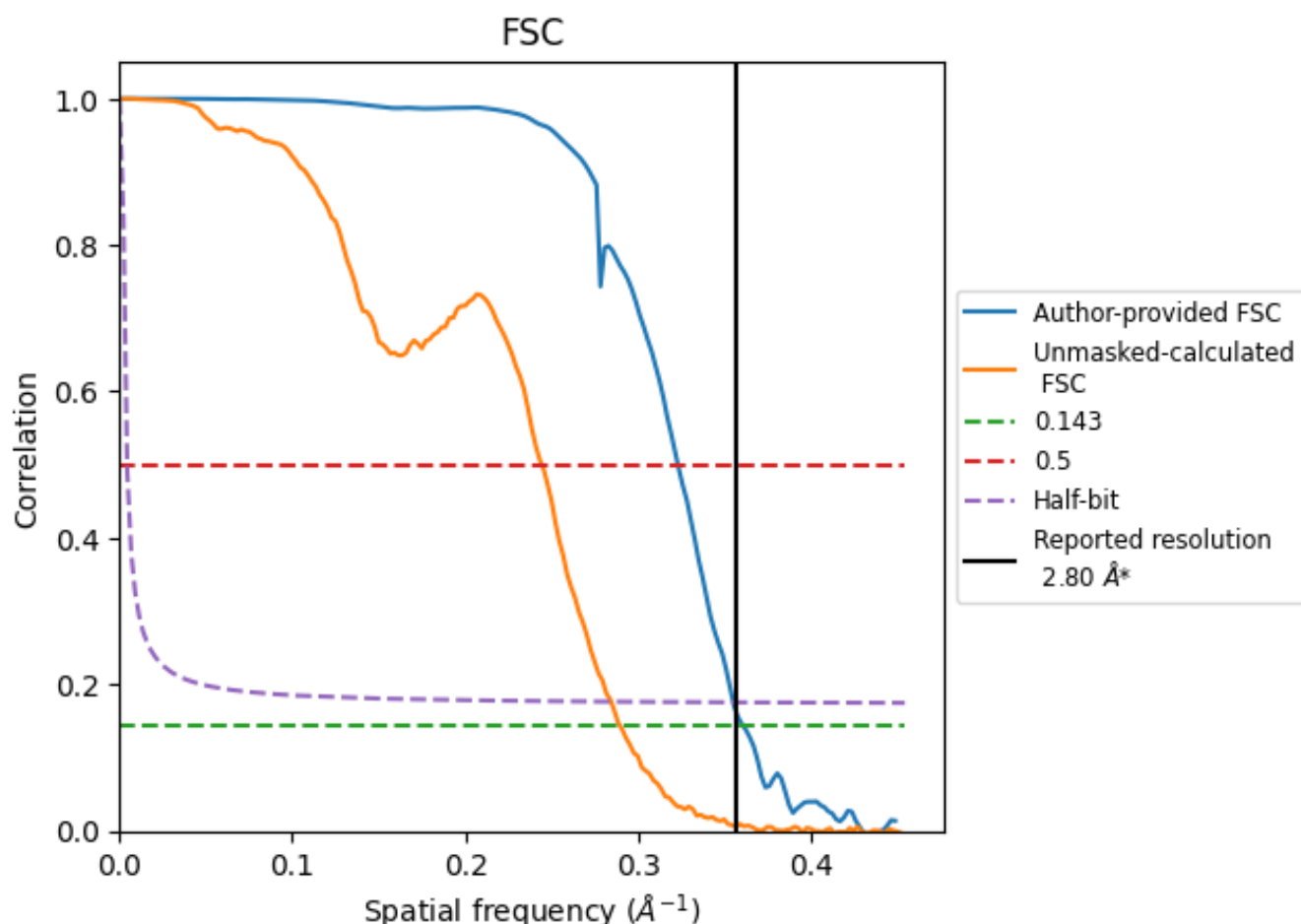


\*Reported resolution corresponds to spatial frequency of 0.357  $\text{\AA}^{-1}$

## 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 0.357  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.77	3.10	2.82
Unmasked-calculated*	3.45	4.09	3.51

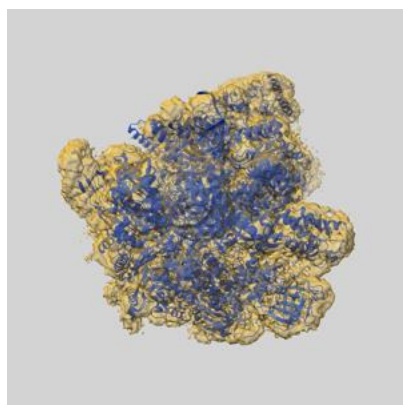
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.45 differs from the reported value 2.8 by more than 10 %



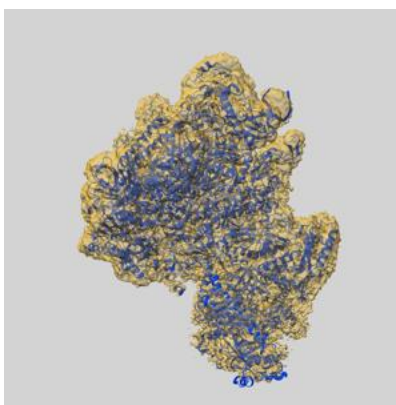
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36908 and PDB model 8K5P. Per-residue inclusion information can be found in section [3](#) on page [9](#).

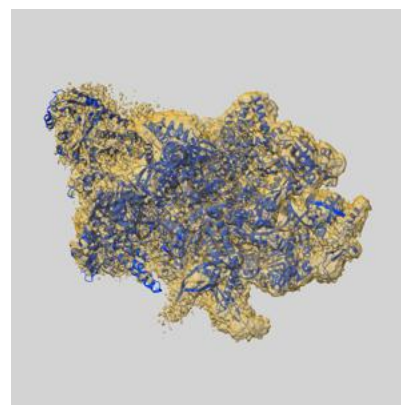
### 9.1 Map-model overlay [i](#)



X



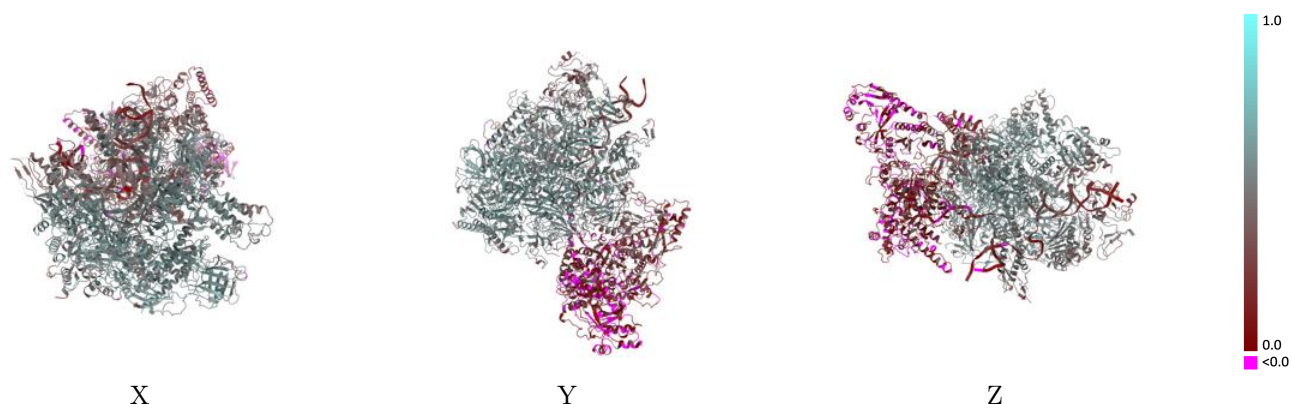
Y



Z

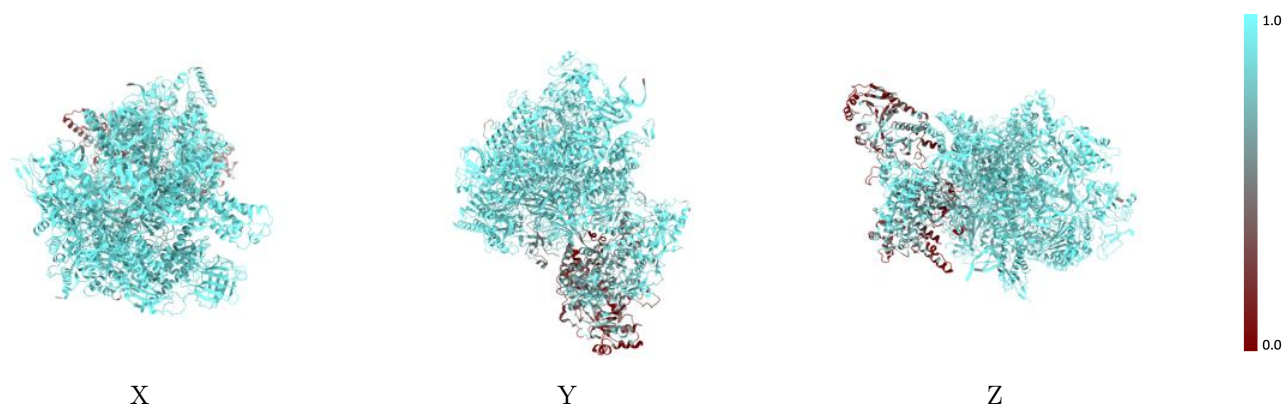
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



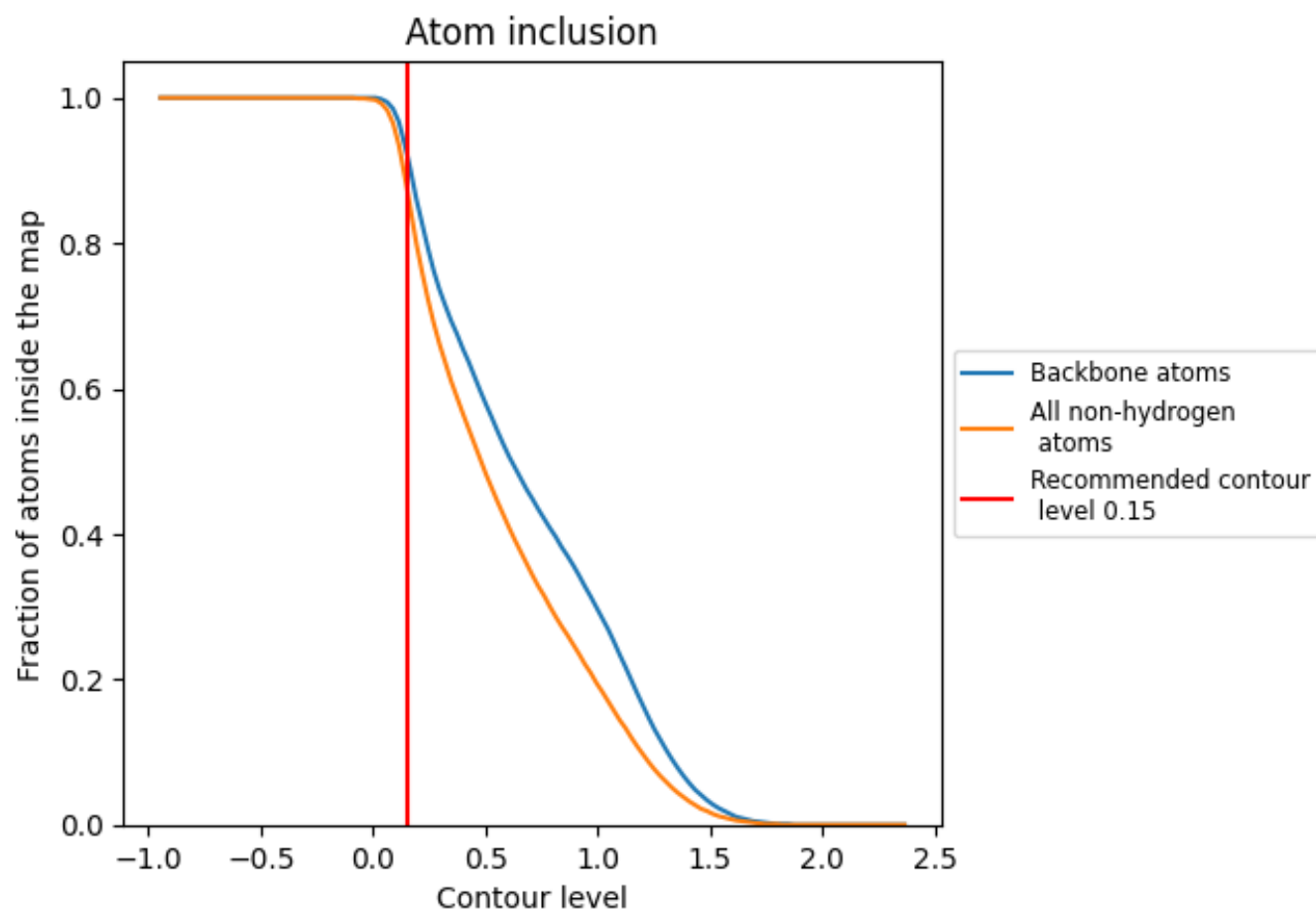
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8780	 0.4120
A	 0.9730	 0.5140
B	 0.9680	 0.5250
C	 0.9840	 0.5550
D	 0.8600	 0.2370
E	 0.9860	 0.5140
F	 0.9690	 0.5490
G	 0.9070	 0.3550
H	 0.9870	 0.5220
I	 0.9740	 0.4460
J	 0.9890	 0.5610
K	 0.9750	 0.5550
L	 0.9690	 0.5180
M	 0.6300	 0.1500
N	 0.8920	 0.1930
O	 0.4720	 0.0750
P	 0.8140	 0.2570
T	 0.9300	 0.3160
W	 0.6180	 0.4680

