



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2024 – 05:13 PM EST

PDB ID : 9BCT  
EMDB ID : EMD-44438  
Title : Cryo-EM structure of Thermococcus kodakarensis FttA-dependent transcription pre-termination complex containing 44 nt RNA  
Authors : You, L.; Ebright, R.H.  
Deposited on : 2024-04-09  
Resolution : 2.50 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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

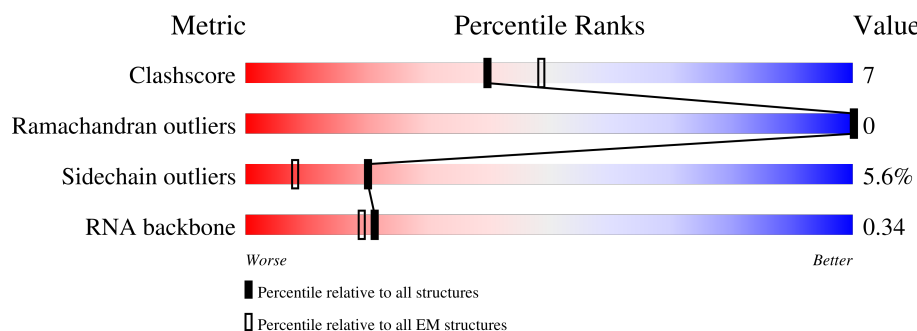
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.








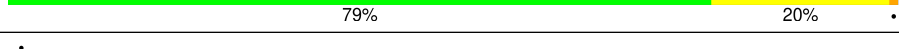
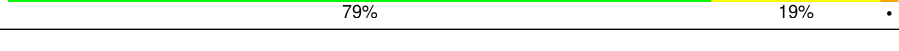
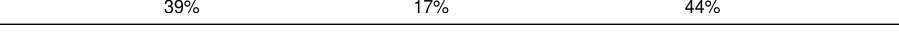
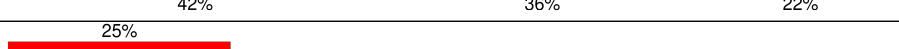
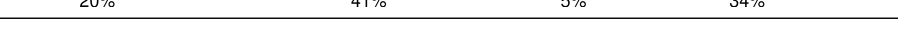
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	906	80% 19% ..
2	B	1123	76% 21% ..
3	C	391	5% 73% 22% . .
4	D	261	80% 17% ..
5	E	190	68% 26% . .
6	F	122	75% 22% ..
7	H	82	74% 18% . 6%

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Mol	Chain	Length	Quality of chain
8	K	60	
9	L	94	
10	N	65	
11	P	49	
12	G	152	
13	I	73	
14	J	648	
14	M	648	
15	5	36	
16	6	36	
17	7	44	

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 39772 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 subunit A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	900	Total	C	N	O	S	0	0
			7182	4536	1277	1330	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1103	Total	C	N	O	S	0	0
			8804	5563	1574	1631	36		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit A".

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	378	Total	C	N	O	S	0	0
			2958	1868	512	568	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	256	Total	C	N	O	S	0	0
			2053	1322	339	388	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	183	Total	C	N	O	S	0	0
			1476	946	252	269	9		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	120	Total	C	N	O	S	0	0
			1000	641	167	189	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	77	Total	C	N	O	0	0
			636	412	106	118		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	56	Total	C	N	O	S	0	0
			433	284	75	73	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	94	Total	C	N	O	S	0	0
			776	493	134	147	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	N	65	Total	C	N	O	S	0	0
			530	340	89	95	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	48	Total	C	N	O	S	0	0
			373	233	74	62	4		

- Molecule 12 is a protein called Transcription elongation factor Spt5.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	G	147	Total	C	N	O	0	0
			1142	739	190	213		

- Molecule 13 is a protein called Transcription elongation factor Spt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	65	Total	C	N	O	S	0	0
			515	321	95	95	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-5	HIS	-	expression tag	UNP Q5JIY5
I	-4	HIS	-	expression tag	UNP Q5JIY5
I	-3	HIS	-	expression tag	UNP Q5JIY5
I	-2	HIS	-	expression tag	UNP Q5JIY5
I	-1	HIS	-	expression tag	UNP Q5JIY5
I	0	HIS	-	expression tag	UNP Q5JIY5

- Molecule 14 is a protein called Transcription termination factor FttA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	645	Total	C	N	O	S	0	0
			5144	3284	903	941	16		
14	M	648	Total	C	N	O	S	0	0
			5161	3295	909	942	15		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	255	ALA	HIS	conflict	UNP Q5JH24
J	591	ALA	HIS	conflict	UNP Q5JH24
M	255	ALA	HIS	conflict	UNP Q5JH24
M	591	ALA	HIS	conflict	UNP Q5JH24

- Molecule 15 is a DNA chain called non-template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	5	20	Total	C	N	O	P	0	0
			410	196	74	120	20		

- Molecule 16 is a DNA chain called template strand DNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	6	28	Total	C	N	O	P	0	0
			575	273	102	172	28		

- Molecule 17 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	7	29	Total	C	N	O	P	0	0
			595	267	83	216	29		

- Molecule 18 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

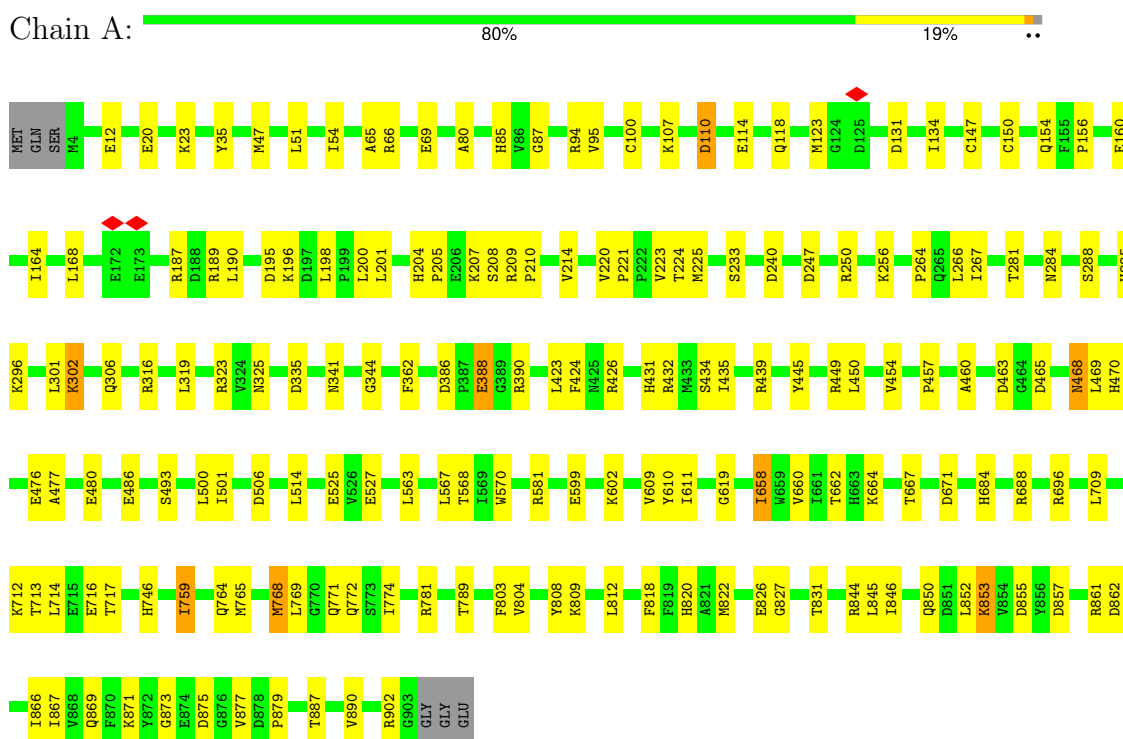
- Molecule 19 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
19	A	2	Total	Zn	0
			2	2	
19	B	1	Total	Zn	0
			1	1	
19	N	1	Total	Zn	0
			1	1	
19	P	1	Total	Zn	0
			1	1	
19	I	1	Total	Zn	0
			1	1	
19	J	1	Total	Zn	0
			1	1	
19	M	1	Total	Zn	0
			1	1	

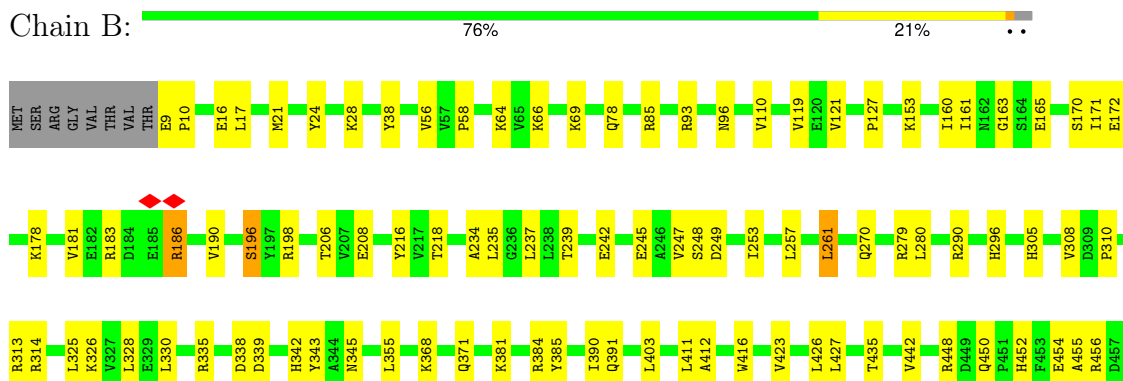
### 3 Residue-property plots

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.

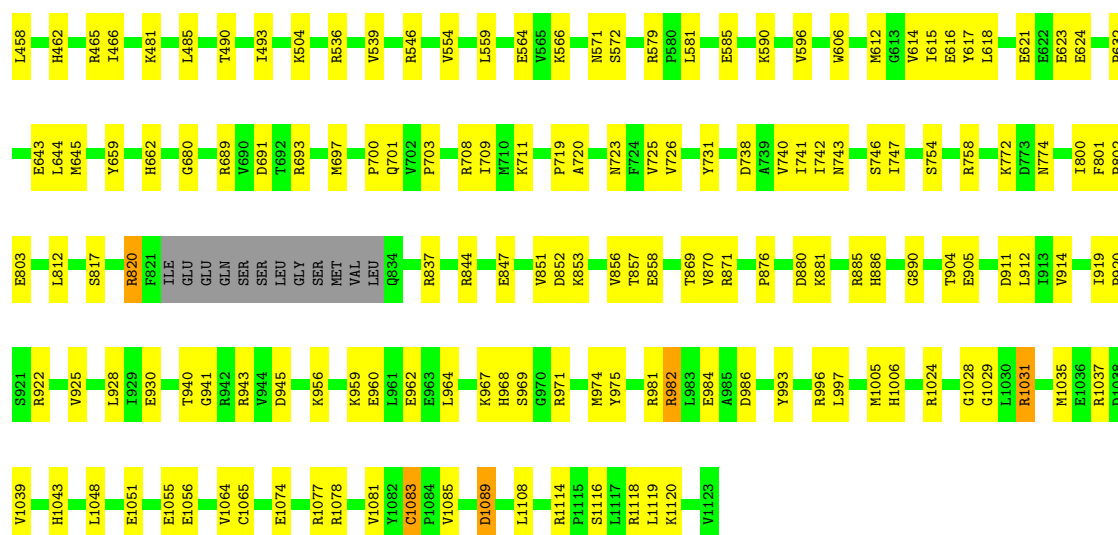
#### • Molecule 1: DNA-directed RNA polymerase subunit A'



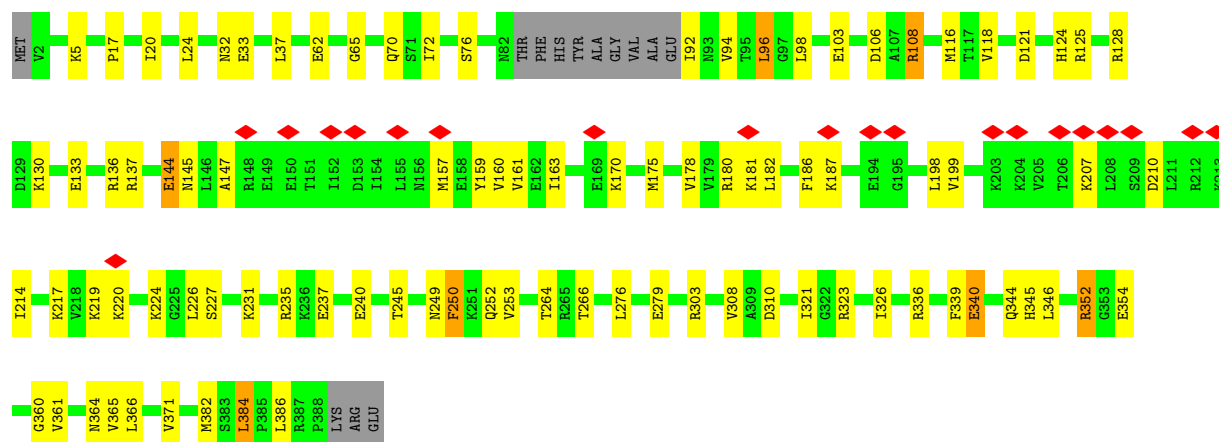
#### • Molecule 2: DNA-directed RNA polymerase subunit B



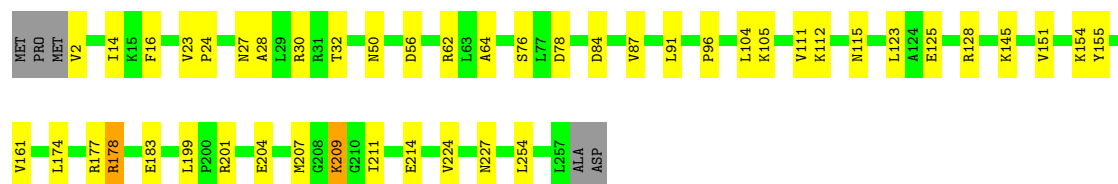
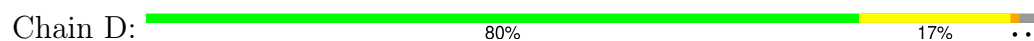




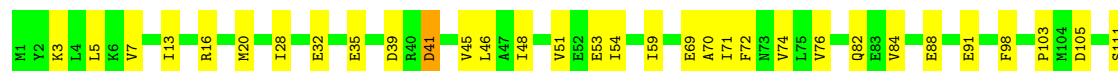
• Molecule 3: DNA-directed RNA polymerase subunit A"

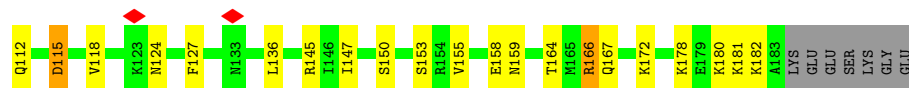


• Molecule 4: DNA-directed RNA polymerase subunit D



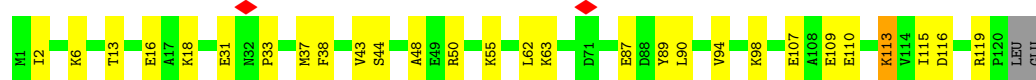
• Molecule 5: DNA-directed RNA polymerase subunit E





- Molecule 6: DNA-directed RNA polymerase subunit F

Chain F: 75% 22%



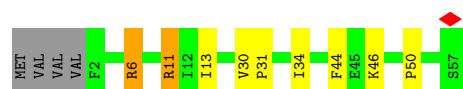
- Molecule 7: DNA-directed RNA polymerase subunit H

Chain H: 74% 18% 6%



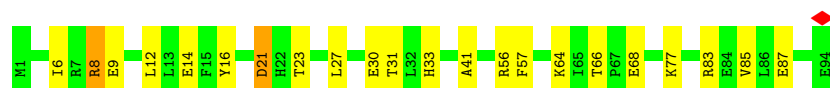
- Molecule 8: DNA-directed RNA polymerase subunit K

Chain K: 78% 12% 7%



- Molecule 9: DNA-directed RNA polymerase subunit L

Chain L: 77% 21%



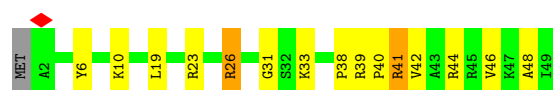
- Molecule 10: DNA-directed RNA polymerase subunit N

Chain N: 78% 20%




- Molecule 11: DNA-directed RNA polymerase subunit P

Chain P: 67% 27%



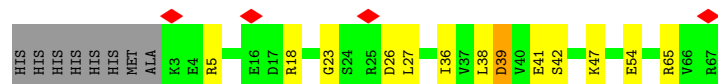
- Molecule 12: Transcription elongation factor Spt5

Chain G: 




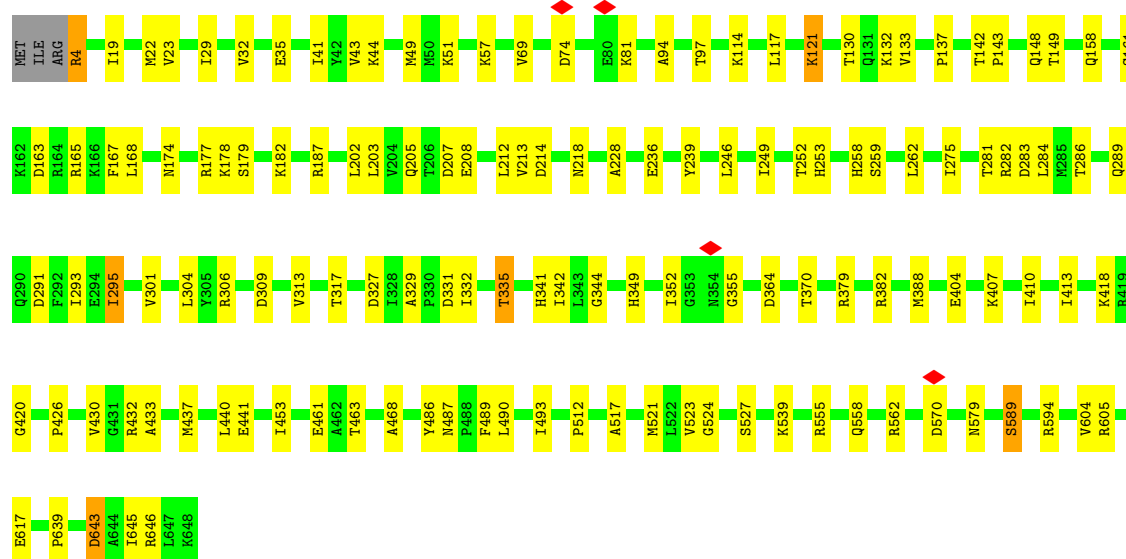
- Molecule 13: Transcription elongation factor Spt4

Chain I: 




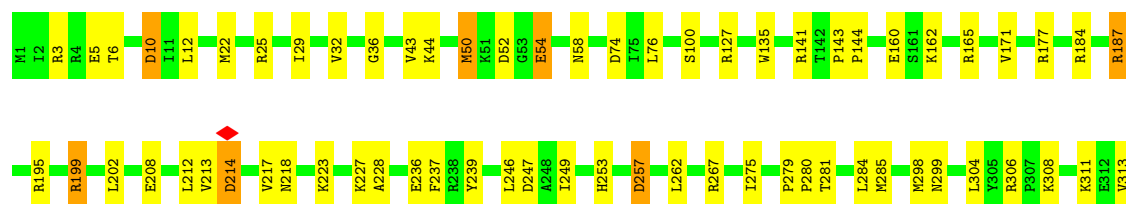
- Molecule 14: Transcription termination factor FttA

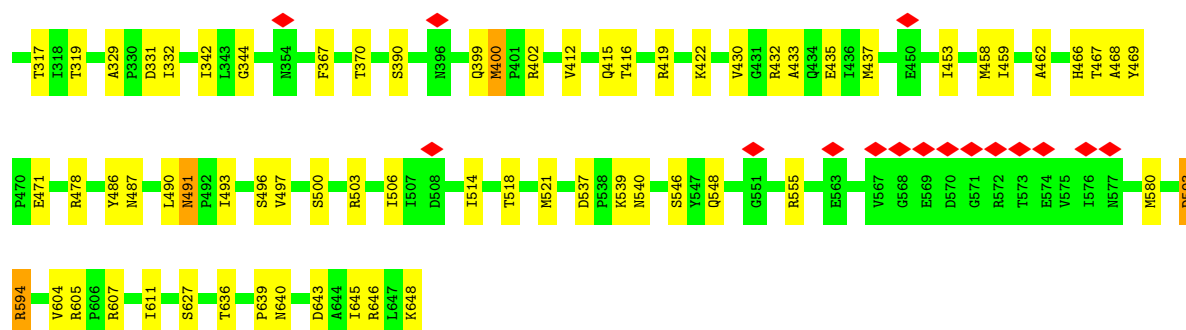
Chain J: 



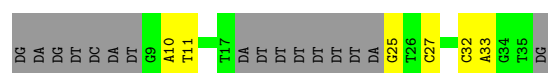
- Molecule 14: Transcription termination factor FttA

Chain M: 

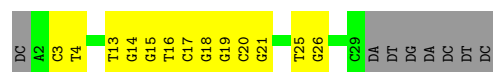




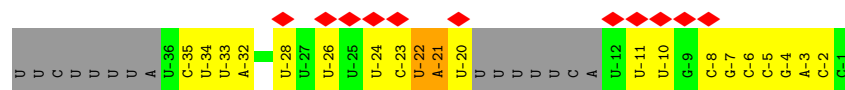
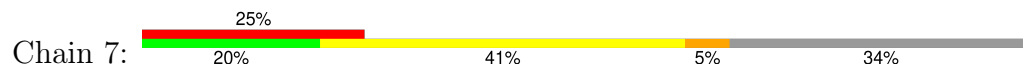
- Molecule 15: non-template strand DNA



- Molecule 16: template strand DNA



- Molecule 17: RNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171269	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	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)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.657	Depositor
Minimum map value	-0.135	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.088	Depositor
Map size ( $\text{\AA}$ )	330.0, 330.0, 330.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.825, 0.825, 0.825	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0/7325	0.50	0/9887
2	B	0.25	0/8981	0.52	0/12135
3	C	0.24	0/2994	0.50	0/4042
4	D	0.24	0/2098	0.46	0/2841
5	E	0.26	0/1502	0.53	0/2023
6	F	0.24	0/1020	0.52	0/1373
7	H	0.27	0/650	0.49	0/877
8	K	0.24	0/441	0.49	0/598
9	L	0.24	0/791	0.50	0/1066
10	N	0.26	0/539	0.48	0/723
11	P	0.27	0/378	0.63	0/507
12	G	0.25	0/1164	0.52	0/1577
13	I	0.26	0/524	0.57	0/708
14	J	0.25	0/5253	0.51	1/7115 (0.0%)
14	M	0.25	0/5270	0.52	1/7139 (0.0%)
15	5	0.47	0/458	0.91	0/702
16	6	0.47	0/643	0.90	0/991
17	7	0.14	0/657	0.74	0/1014
All	All	0.26	0/40688	0.53	2/55318 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	M	214	ASP	CB-CG-OD1	7.10	124.69	118.30
14	J	214	ASP	CB-CG-OD1	5.30	123.07	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7182	0	7247	117	0
2	B	8804	0	8858	148	0
3	C	2958	0	3077	52	0
4	D	2053	0	2063	27	0
5	E	1476	0	1512	31	0
6	F	1000	0	1000	14	0
7	H	636	0	646	11	0
8	K	433	0	466	6	0
9	L	776	0	770	14	0
10	N	530	0	540	8	0
11	P	373	0	392	11	0
12	G	1142	0	1192	20	0
13	I	515	0	506	8	0
14	J	5144	0	5246	64	0
14	M	5161	0	5264	70	0
15	5	410	0	228	4	0
16	6	575	0	317	16	0
17	7	595	0	304	13	0
18	A	1	0	0	0	0
19	A	2	0	0	0	0
19	B	1	0	0	0	0
19	I	1	0	0	0	0
19	J	1	0	0	0	0
19	M	1	0	0	0	0
19	N	1	0	0	0	0
19	P	1	0	0	0	0
All	All	39772	0	39628	543	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 7.

The worst 5 of 543 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)
5:E:112:GLN:HE22	5:E:164:THR:HA	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:SER:HG	2:B:305:HIS:HD1	1.38	0.70
14:J:329:ALA:HB3	14:J:332:ILE:HB	1.74	0.70
2:B:820:ARG:HD3	2:B:820:ARG:H	1.56	0.70
1:A:432:ARG:HA	2:B:1039:VAL:HB	1.75	0.68

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	898/906 (99%)	881 (98%)	17 (2%)	0	100	100
2	B	1099/1123 (98%)	1076 (98%)	23 (2%)	0	100	100
3	C	374/391 (96%)	363 (97%)	11 (3%)	0	100	100
4	D	254/261 (97%)	251 (99%)	3 (1%)	0	100	100
5	E	181/190 (95%)	179 (99%)	2 (1%)	0	100	100
6	F	118/122 (97%)	114 (97%)	4 (3%)	0	100	100
7	H	75/82 (92%)	75 (100%)	0	0	100	100
8	K	54/60 (90%)	50 (93%)	4 (7%)	0	100	100
9	L	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
10	N	63/65 (97%)	63 (100%)	0	0	100	100
11	P	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
12	G	145/152 (95%)	143 (99%)	2 (1%)	0	100	100
13	I	63/73 (86%)	62 (98%)	1 (2%)	0	100	100
14	J	643/648 (99%)	628 (98%)	15 (2%)	0	100	100
14	M	646/648 (100%)	625 (97%)	21 (3%)	0	100	100
All	All	4751/4864 (98%)	4644 (98%)	107 (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	774/779 (99%)	743 (96%)	31 (4%)	27	51
2	B	949/969 (98%)	908 (96%)	41 (4%)	25	48
3	C	324/334 (97%)	301 (93%)	23 (7%)	12	25
4	D	226/230 (98%)	214 (95%)	12 (5%)	19	38
5	E	160/167 (96%)	147 (92%)	13 (8%)	9	20
6	F	104/107 (97%)	97 (93%)	7 (7%)	13	28
7	H	69/72 (96%)	64 (93%)	5 (7%)	12	24
8	K	45/49 (92%)	42 (93%)	3 (7%)	13	28
9	L	81/81 (100%)	75 (93%)	6 (7%)	11	23
10	N	59/59 (100%)	54 (92%)	5 (8%)	8	18
11	P	38/40 (95%)	33 (87%)	5 (13%)	3	6
12	G	127/131 (97%)	118 (93%)	9 (7%)	12	25
13	I	56/65 (86%)	52 (93%)	4 (7%)	12	25
14	J	562/565 (100%)	530 (94%)	32 (6%)	17	35
14	M	562/565 (100%)	525 (93%)	37 (7%)	14	28
All	All	4136/4213 (98%)	3903 (94%)	233 (6%)	20	36

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	124	ASN
14	M	432	ARG
10	N	33	LYS
14	M	390	SER
14	M	50	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19

such sidechains are listed below:

Mol	Chain	Res	Type
14	J	341	HIS
14	M	399	GLN
14	M	483	HIS
14	J	579	ASN
5	E	73	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
17	7	27/44 (61%)	12 (44%)	0

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
17	7	-34	U
17	7	-33	U
17	7	-32	A
17	7	-28	U
17	7	-26	U

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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

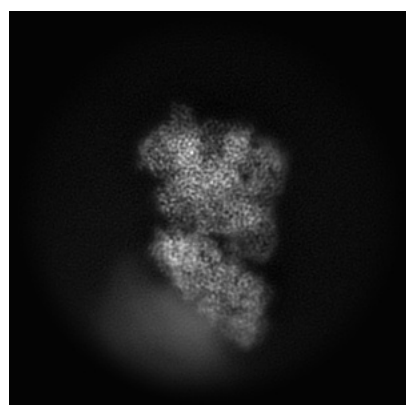
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44438. These allow visual inspection of the internal detail of the map and identification of artifacts.

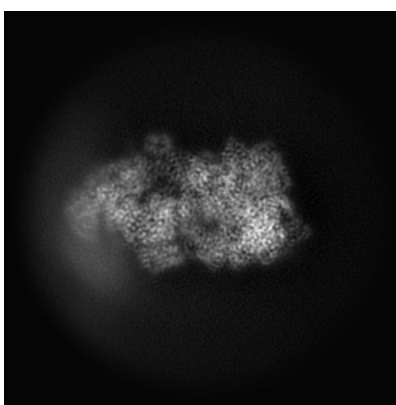
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

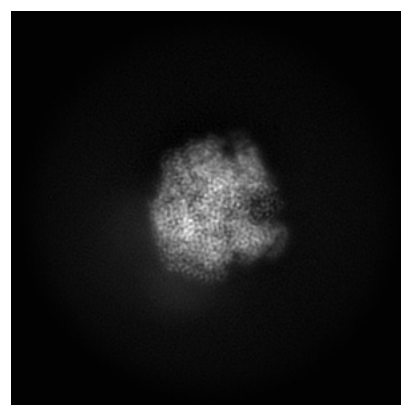
#### 6.1.1 Primary map



X



Y

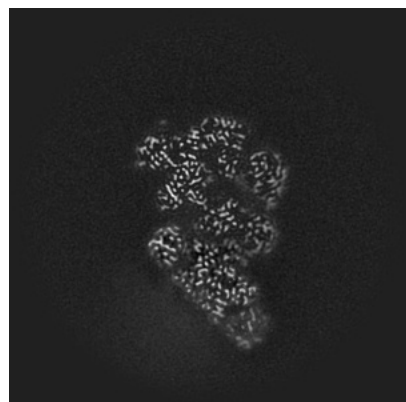


Z

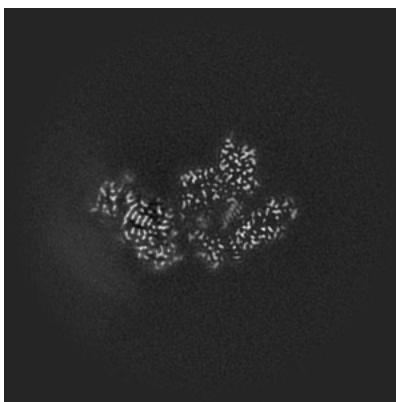
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

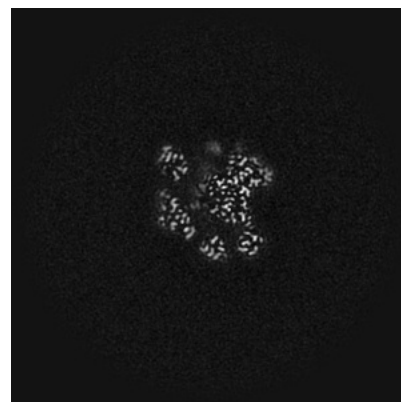
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

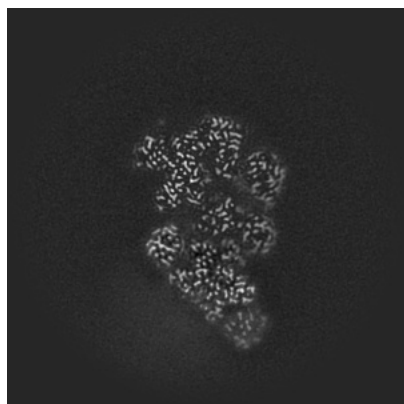


Z Index: 200

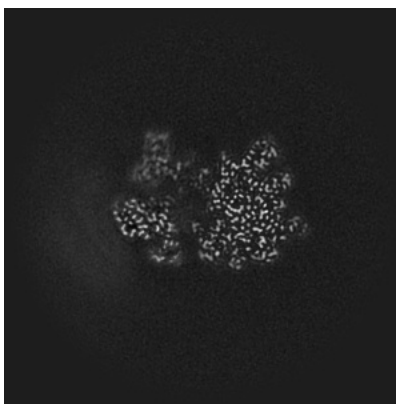
The images above show central slices of the map in three orthogonal directions.

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

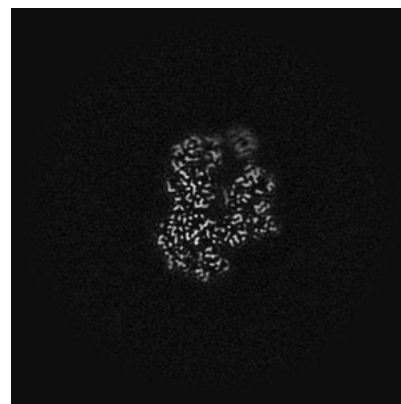
### 6.3.1 Primary map



X Index: 199



Y Index: 183

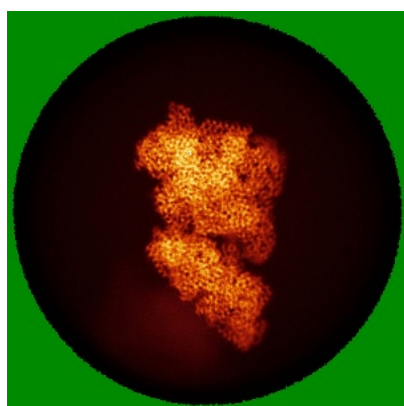


Z Index: 249

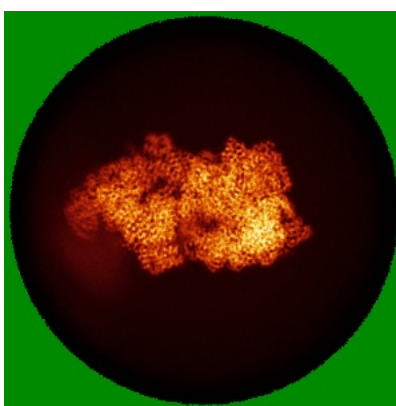
The images above show the largest variance slices of the map in three orthogonal directions.

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

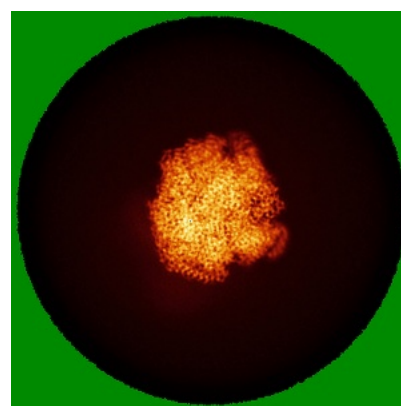
### 6.4.1 Primary map



X



Y

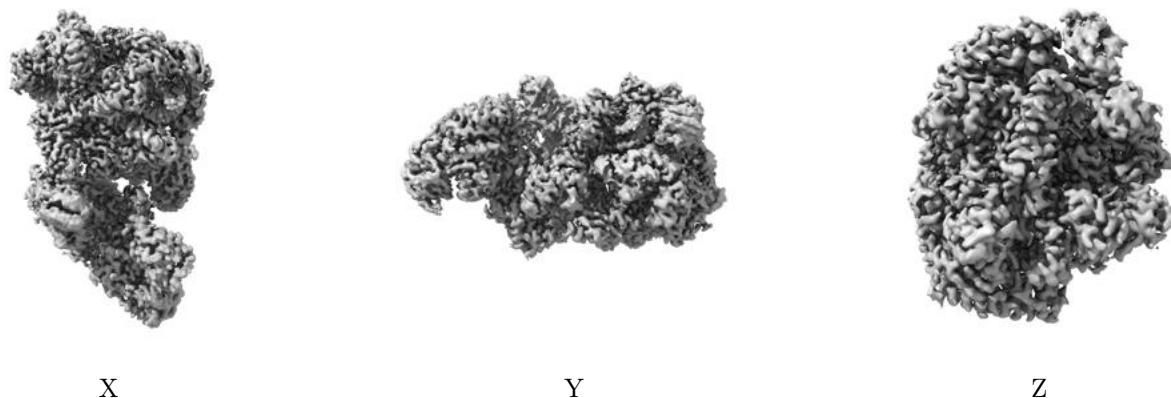


Z

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 0.088. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

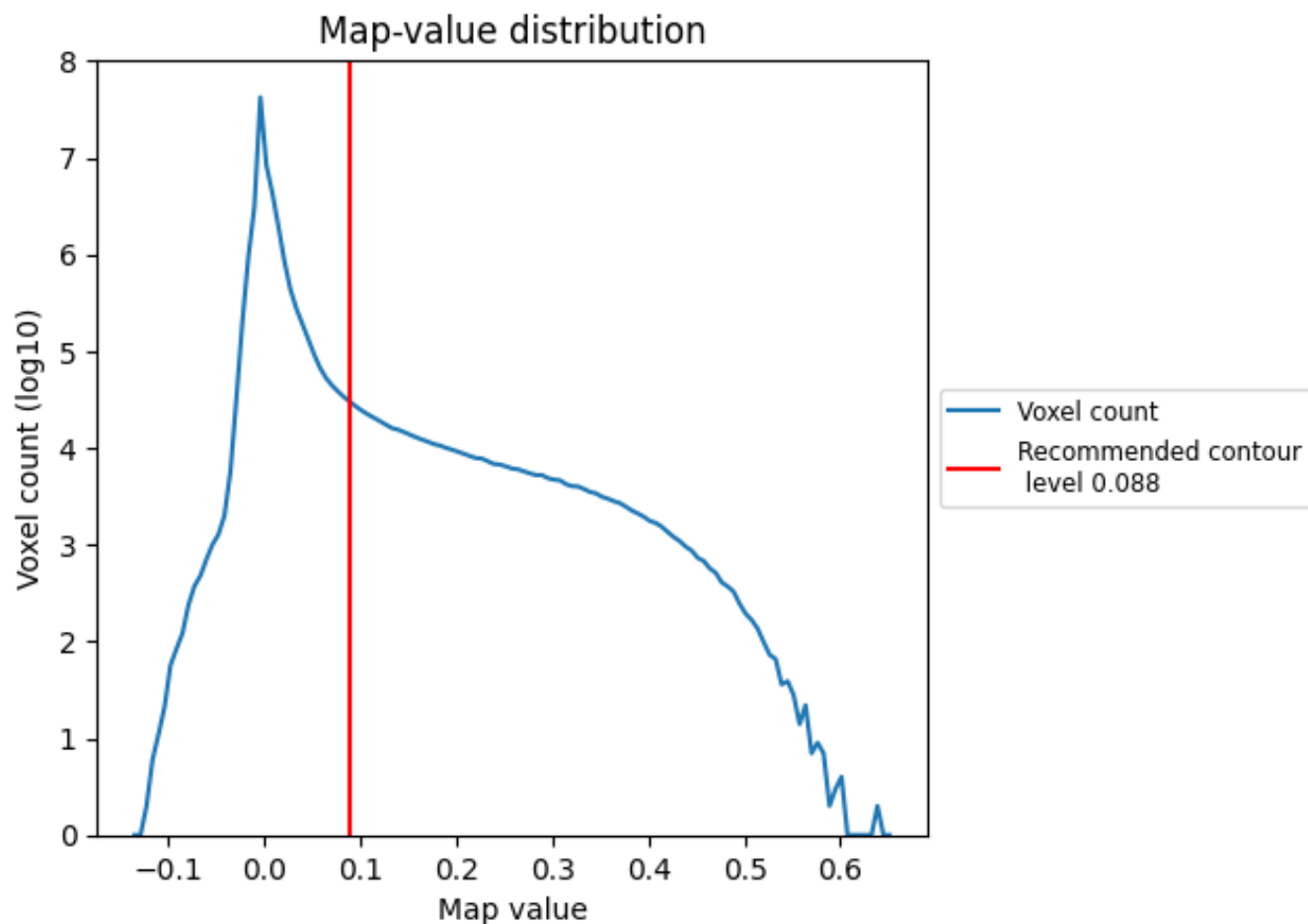
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

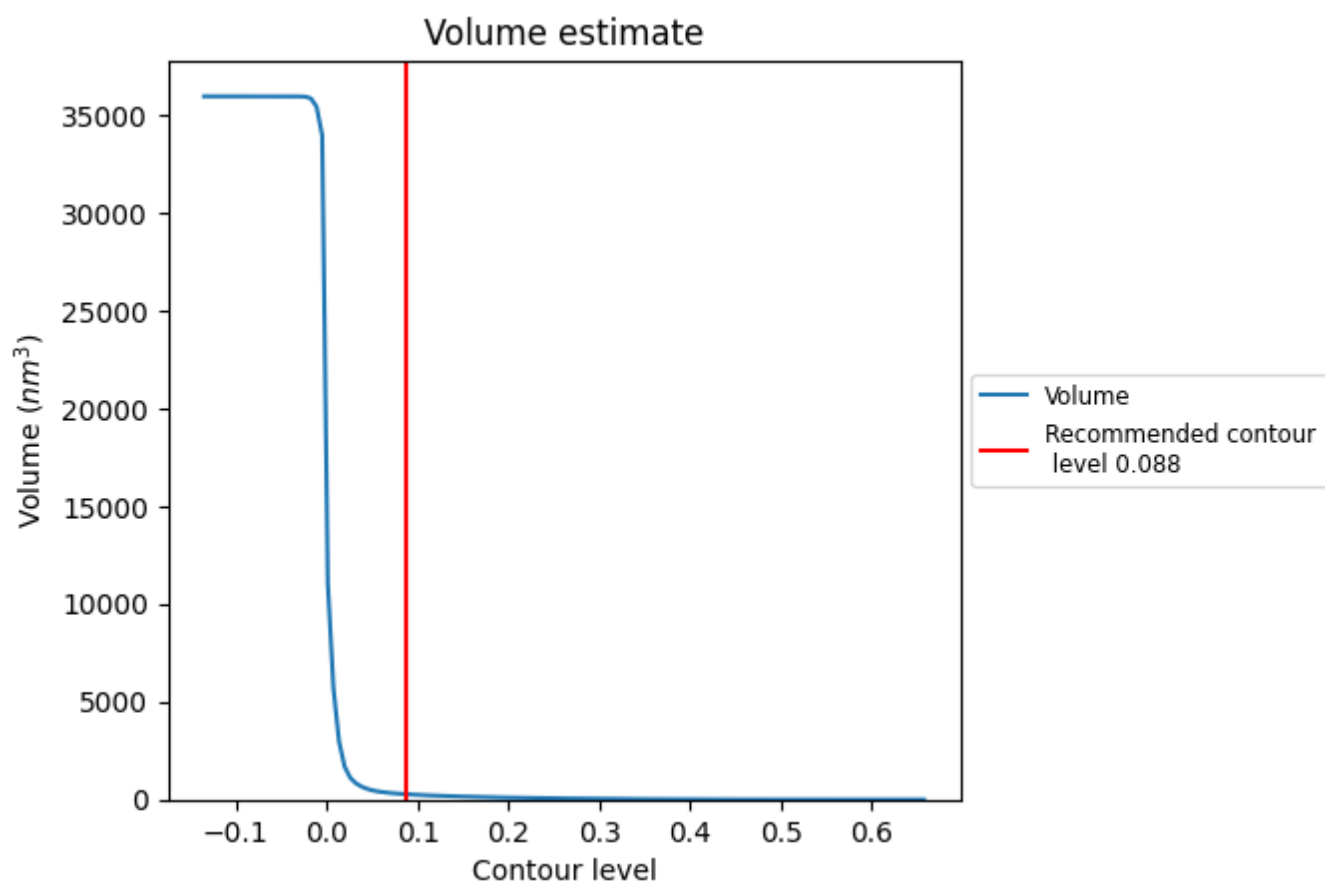
This section contains the results of statistical analysis of the map.

### 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](#)

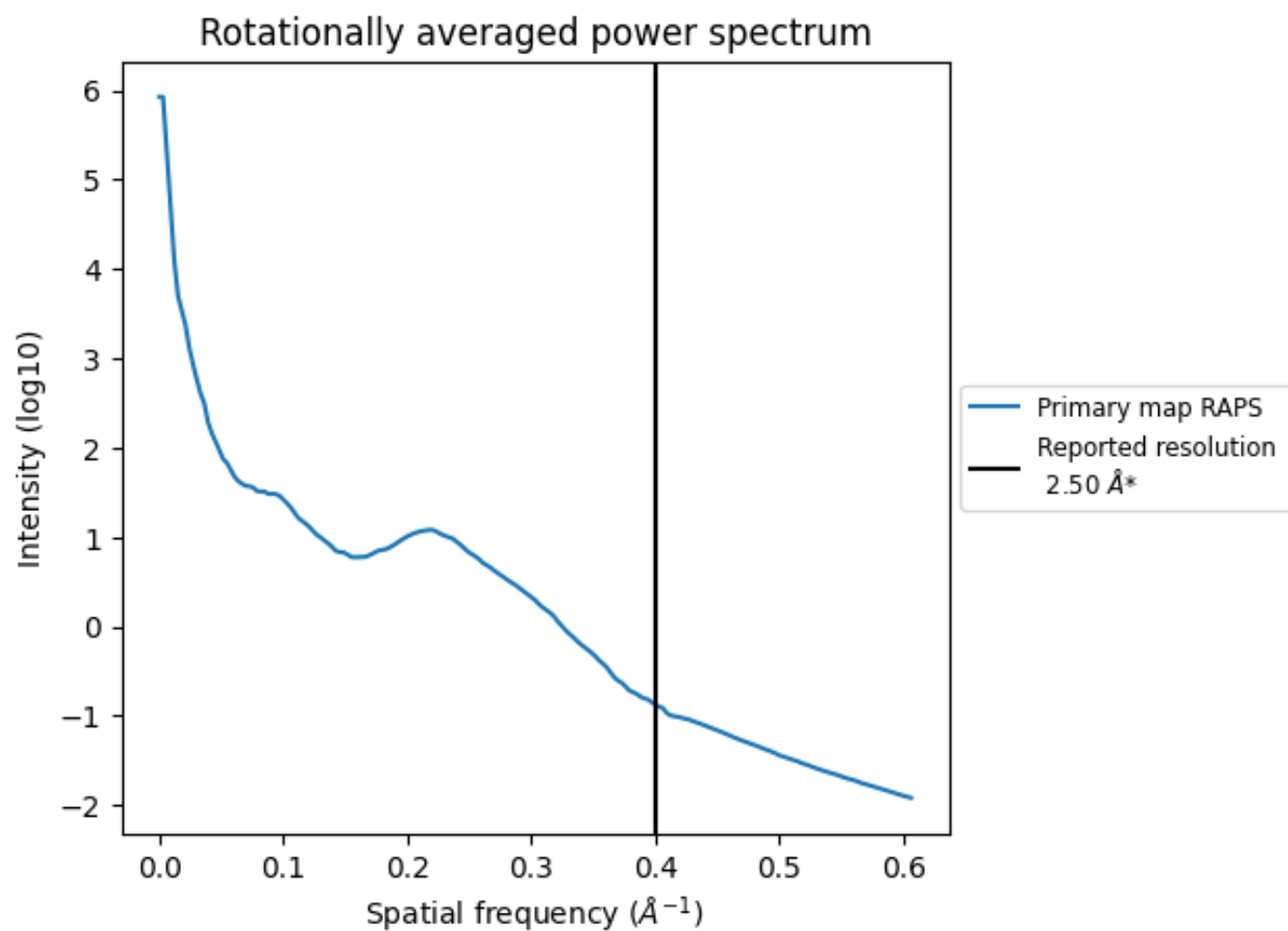


The volume at the recommended contour level is 270 nm<sup>3</sup>; this corresponds to an approximate mass of 244 kDa.

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 ⓘ

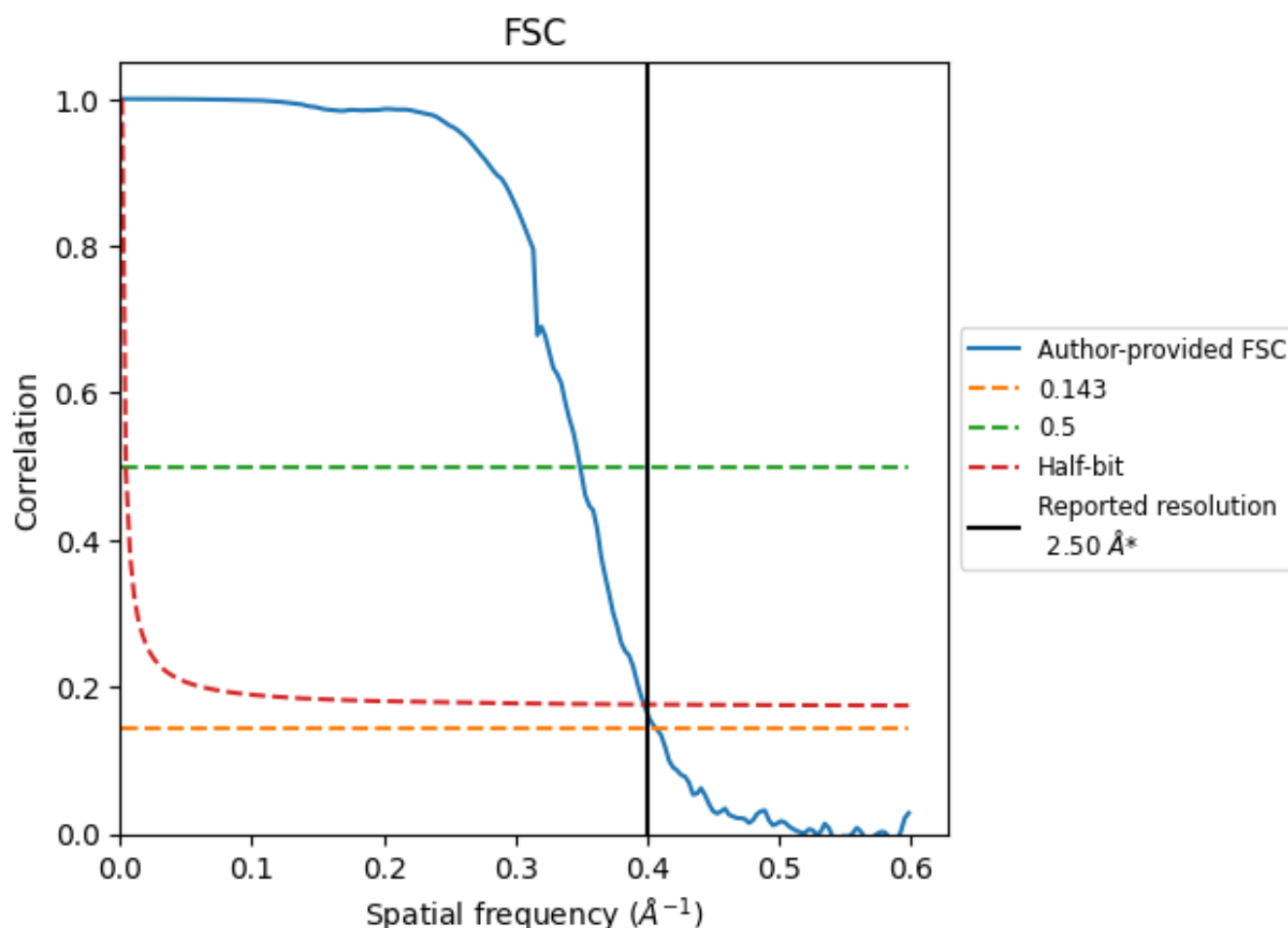


\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

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

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

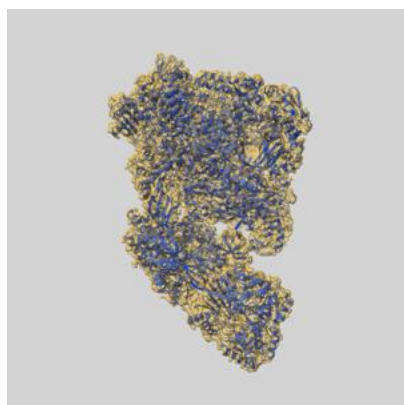
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.46	2.87	2.51
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

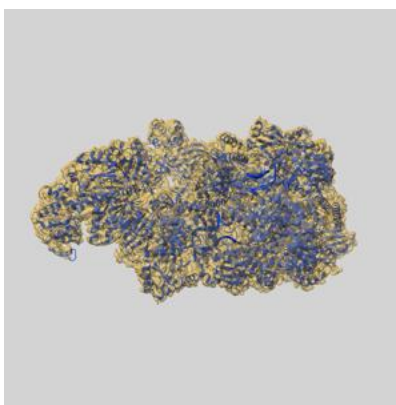
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44438 and PDB model 9BCT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

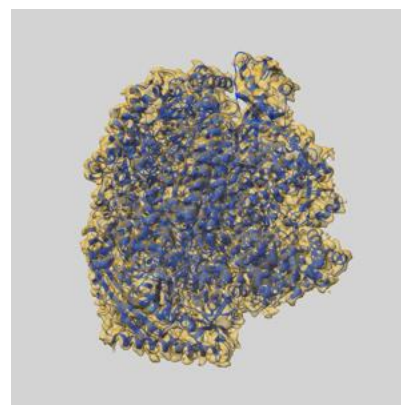
### 9.1 Map-model overlay [i](#)



X



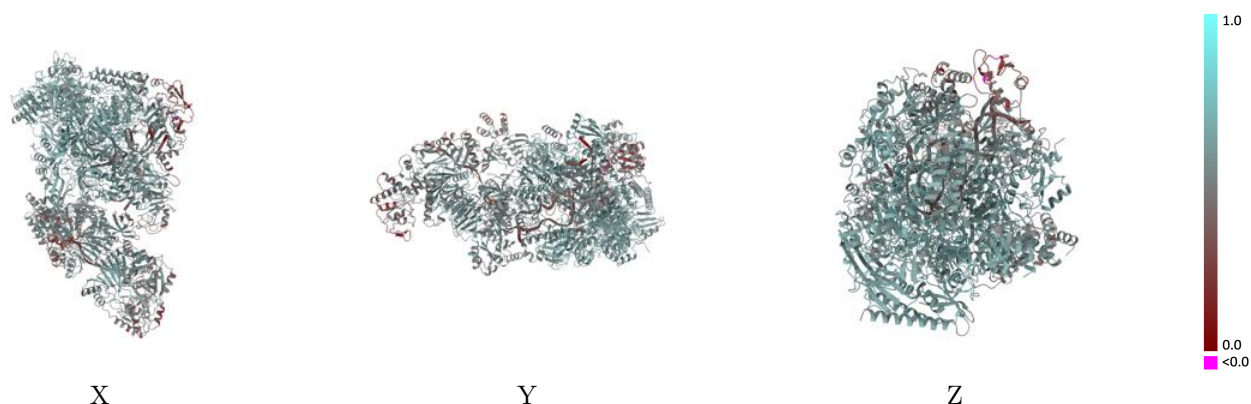
Y



Z

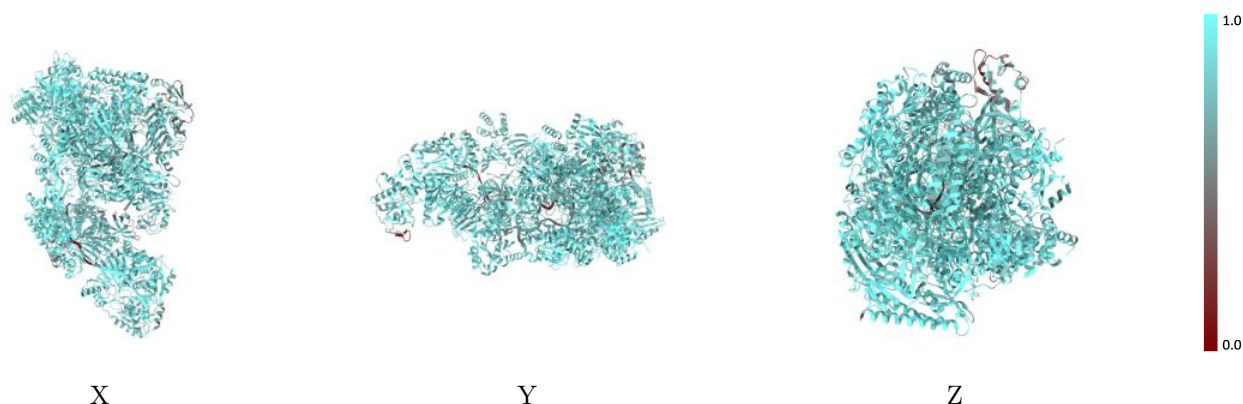
The images above show the 3D surface view of the map at the recommended contour level 0.088 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



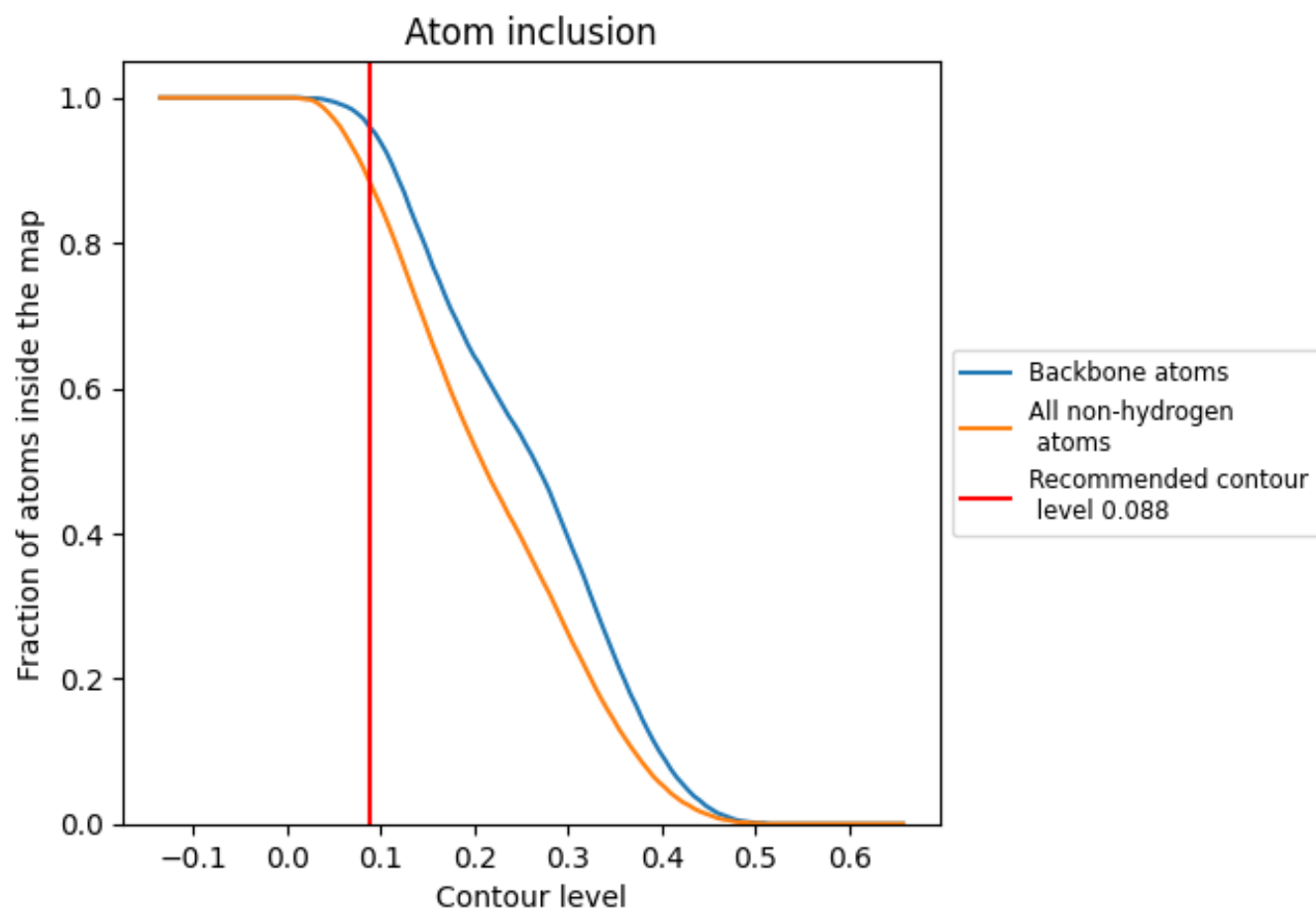
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.088).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8850	 0.5540
5	 0.7540	 0.3700
6	 0.7860	 0.3940
7	 0.5630	 0.4440
A	 0.9210	 0.5990
B	 0.9150	 0.5920
C	 0.8340	 0.5180
D	 0.9310	 0.6070
E	 0.8580	 0.5120
F	 0.8220	 0.4320
G	 0.7920	 0.5200
H	 0.9260	 0.5960
I	 0.7500	 0.4140
J	 0.9110	 0.5610
K	 0.9360	 0.5970
L	 0.9270	 0.6020
M	 0.8590	 0.5020
N	 0.9280	 0.6110
P	 0.9220	 0.5660

