



## wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 04:06 AM JST

PDB ID : 7EGH  
EMDB ID : EMD-31117  
Title : TFIID lobe C subcomplex  
Authors : Chen, X.; Wu, Z.; Li, J.; Zhao, D.; Xu, Y.  
Deposited on : 2021-03-24  
Resolution : 3.04 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

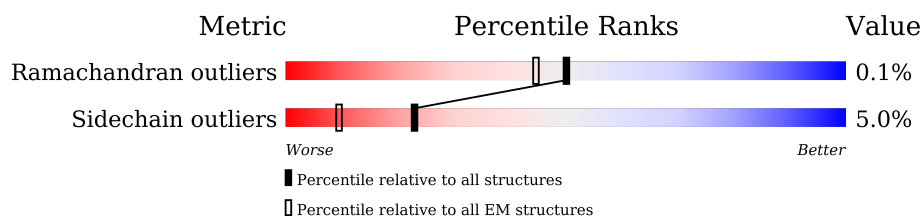
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.04 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	1872	
2	B	1199	
3	F	677	
3	f	677	
4	G	349	
5	H	310	
6	X	72	
7	Y	94	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20543 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 Transcription initiation factor TFIID subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	630	Total	C	N	O	S	0	0
			5199	3303	923	944	29		

- Molecule 2 is a protein called Transcription initiation factor TFIID subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	963	Total	C	N	O	S	0	0
			7796	5011	1315	1412	58		

- Molecule 3 is a protein called Transcription initiation factor TFIID subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	267	Total	C	N	O	S	0	0
			2006	1265	362	368	11		
3	f	260	Total	C	N	O	S	0	0
			1946	1227	348	360	11		

- Molecule 4 is a protein called Transcription initiation factor TFIID subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	144	Total	C	N	O	S	0	0
			1171	742	215	210	4		

- Molecule 5 is a protein called Transcription initiation factor TFIID subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	72	Total	C	N	O	S	0	0
			580	370	100	109	1		

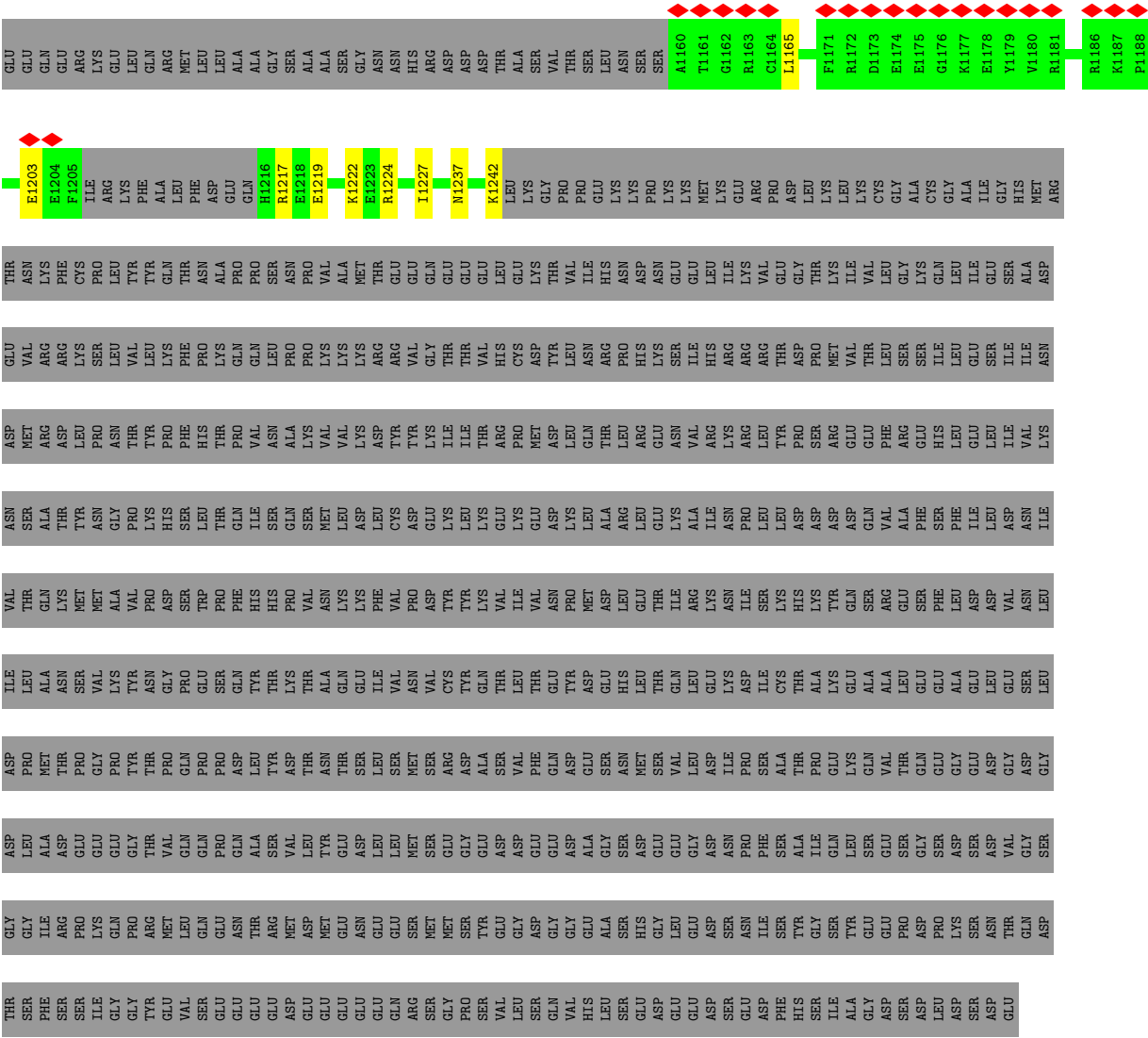
- Molecule 6 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	X	45	Total	C	N	O	P	0	0
			918	434	172	267	45		

- Molecule 7 is a DNA chain called DNA (45-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	45	Total	C	N	O	P	0	0
			927	438	171	273	45		



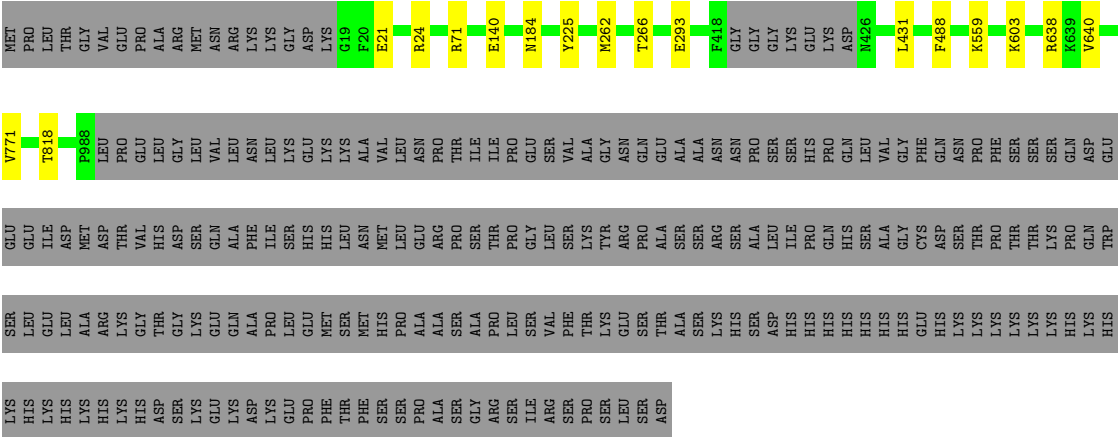


● Molecule 2: Transcription initiation factor TFIID subunit 2

Chain B: 

79%

20%







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	121285	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.396	Depositor
Minimum map value	-3.106	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.222	Depositor
Map size (Å)	540.16, 540.16, 540.16	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.055, 1.055, 1.055	Depositor

## 5 Model quality [i](#)

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

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	0.50	0/5320	0.66	0/7165
2	B	0.46	0/7993	0.60	0/10836
3	F	0.53	0/2040	0.75	0/2775
3	f	0.45	0/1979	0.67	0/2694
4	G	0.50	0/1190	0.62	0/1601
5	H	0.32	0/592	0.55	0/803
6	X	0.73	0/1029	0.91	0/1584
7	Y	0.68	0/1039	0.92	0/1603
All	All	0.50	0/21182	0.68	0/29061

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 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	610/1872 (33%)	583 (96%)	25 (4%)	2 (0%)	37	68
2	B	959/1199 (80%)	911 (95%)	48 (5%)	0	100	100
3	F	265/677 (39%)	251 (95%)	13 (5%)	1 (0%)	30	62
3	f	258/677 (38%)	252 (98%)	6 (2%)	0	100	100
4	G	138/349 (40%)	135 (98%)	3 (2%)	0	100	100
5	H	70/310 (23%)	67 (96%)	3 (4%)	0	100	100
All	All	2300/5084 (45%)	2199 (96%)	98 (4%)	3 (0%)	50	79

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	502	LEU
3	F	411	VAL
1	A	998	LEU

### 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	564/1665 (34%)	510 (90%)	54 (10%)	7	25
2	B	876/1083 (81%)	859 (98%)	17 (2%)	52	76
3	F	202/574 (35%)	187 (93%)	15 (7%)	11	36
3	f	195/574 (34%)	187 (96%)	8 (4%)	26	57
4	G	132/322 (41%)	124 (94%)	8 (6%)	15	43
5	H	64/270 (24%)	64 (100%)	0	100	100
All	All	2033/4488 (45%)	1931 (95%)	102 (5%)	23	50

5 of 102 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	140	GLU
3	F	219	GLU

*Continued on next page...*

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Mol	Chain	Res	Type
3	f	326	HIS
2	B	225	TYR
2	B	559	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	439	HIS
3	F	273	GLN
2	B	521	GLN
4	G	48	HIS
2	B	916	ASN

### 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](#)

There are no ligands in this entry.

## 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.

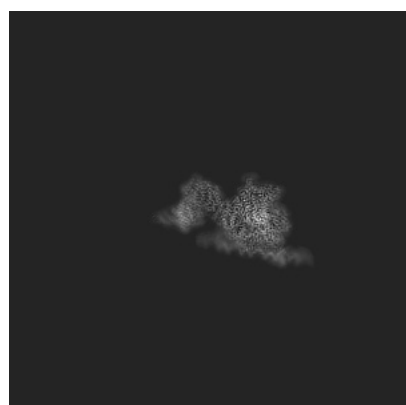
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31117. These allow visual inspection of the internal detail of the map and identification of artifacts.

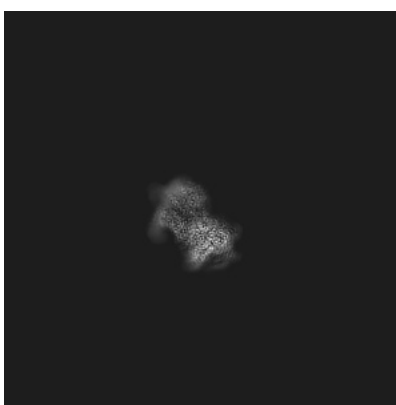
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

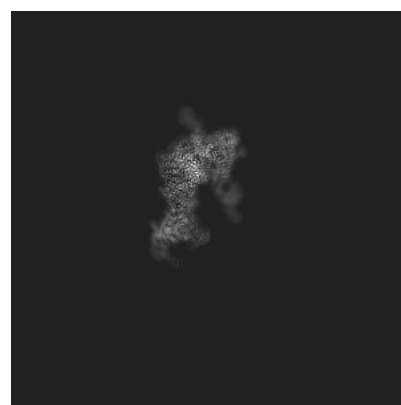
#### 6.1.1 Primary map



X



Y

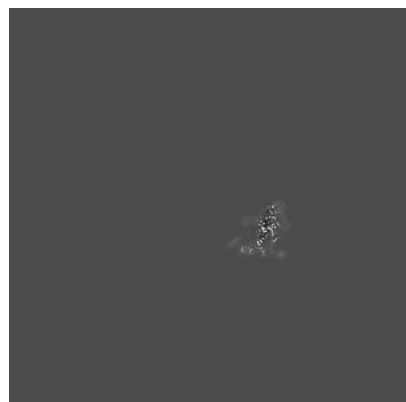


Z

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

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

#### 6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

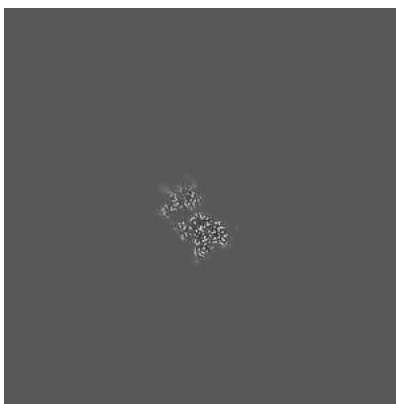
The images above show central slices of the map in three orthogonal directions.

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

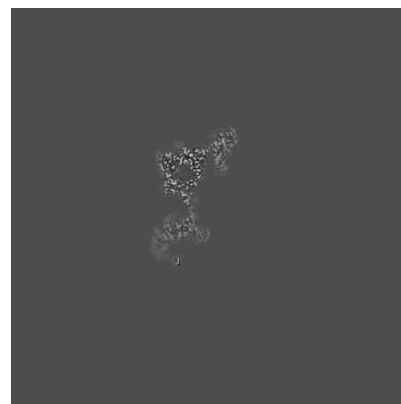
### 6.3.1 Primary map



X Index: 231



Y Index: 321

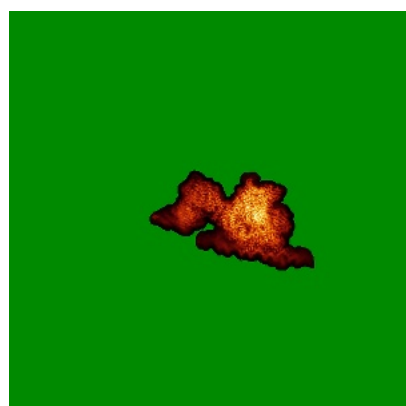


Z Index: 248

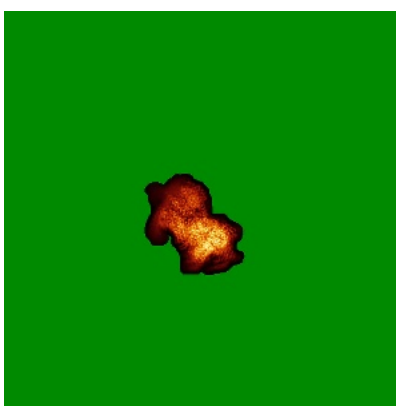
The images above show the largest variance slices of the map in three orthogonal directions.

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

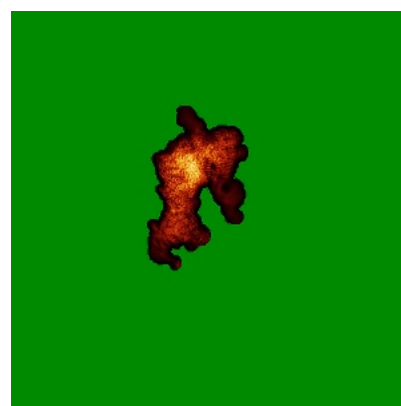
### 6.4.1 Primary map



X



Y

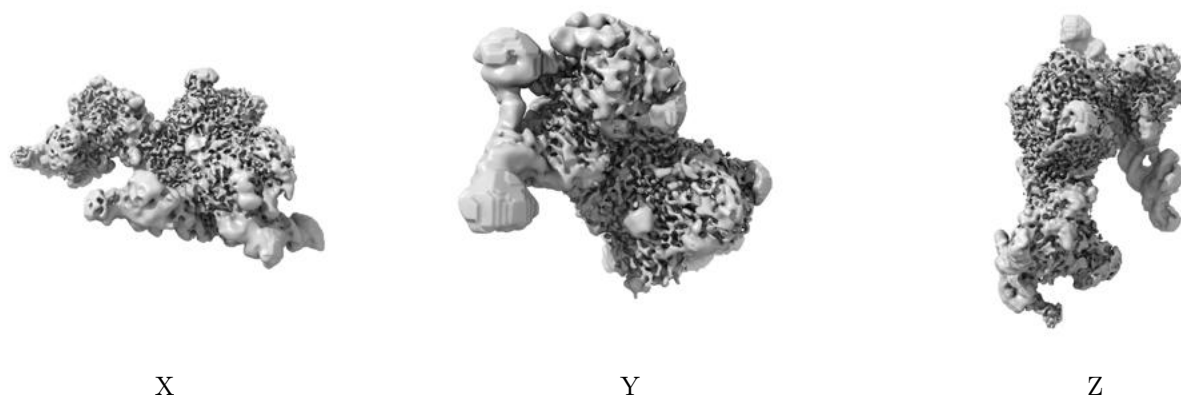


Z

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

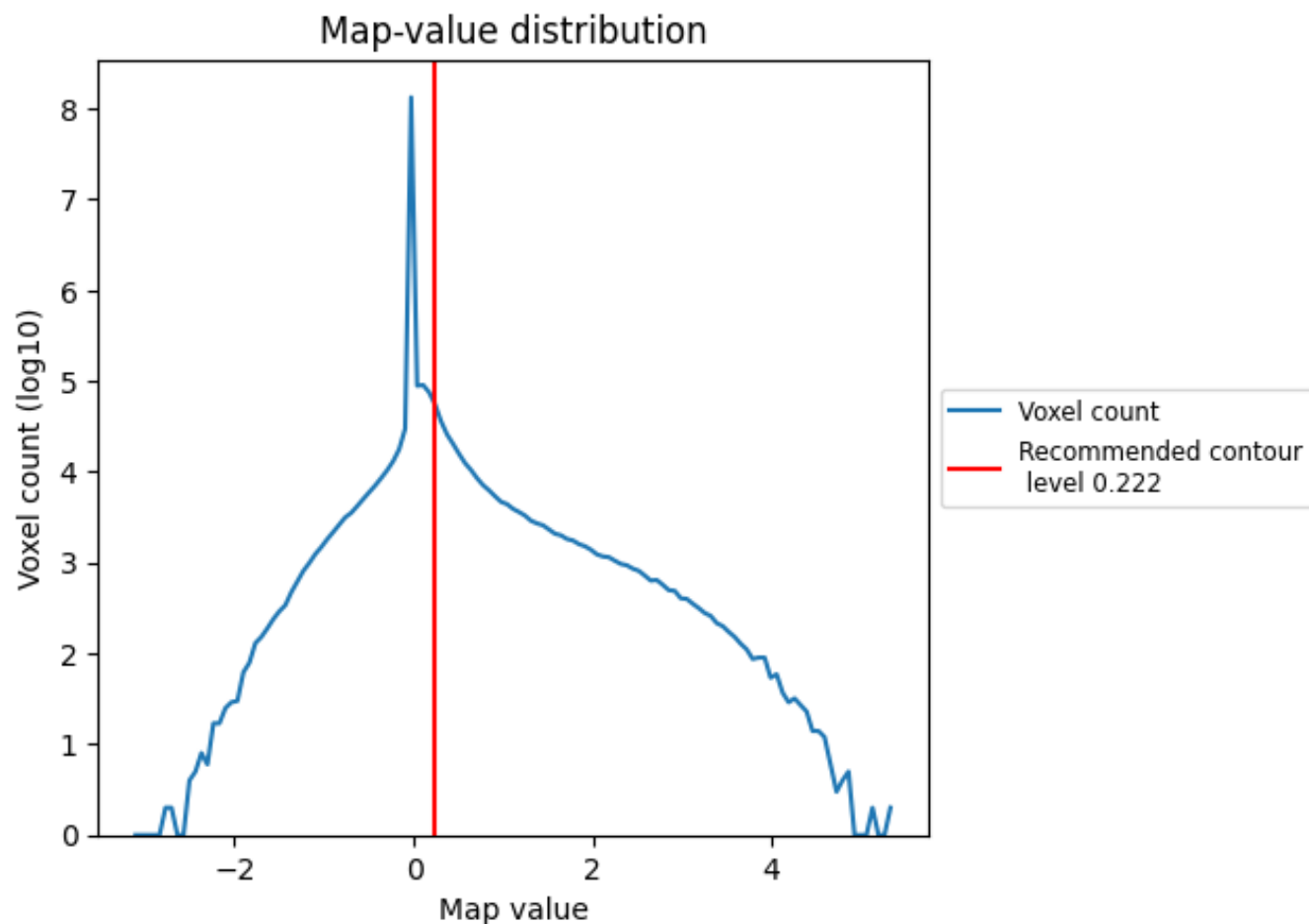
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

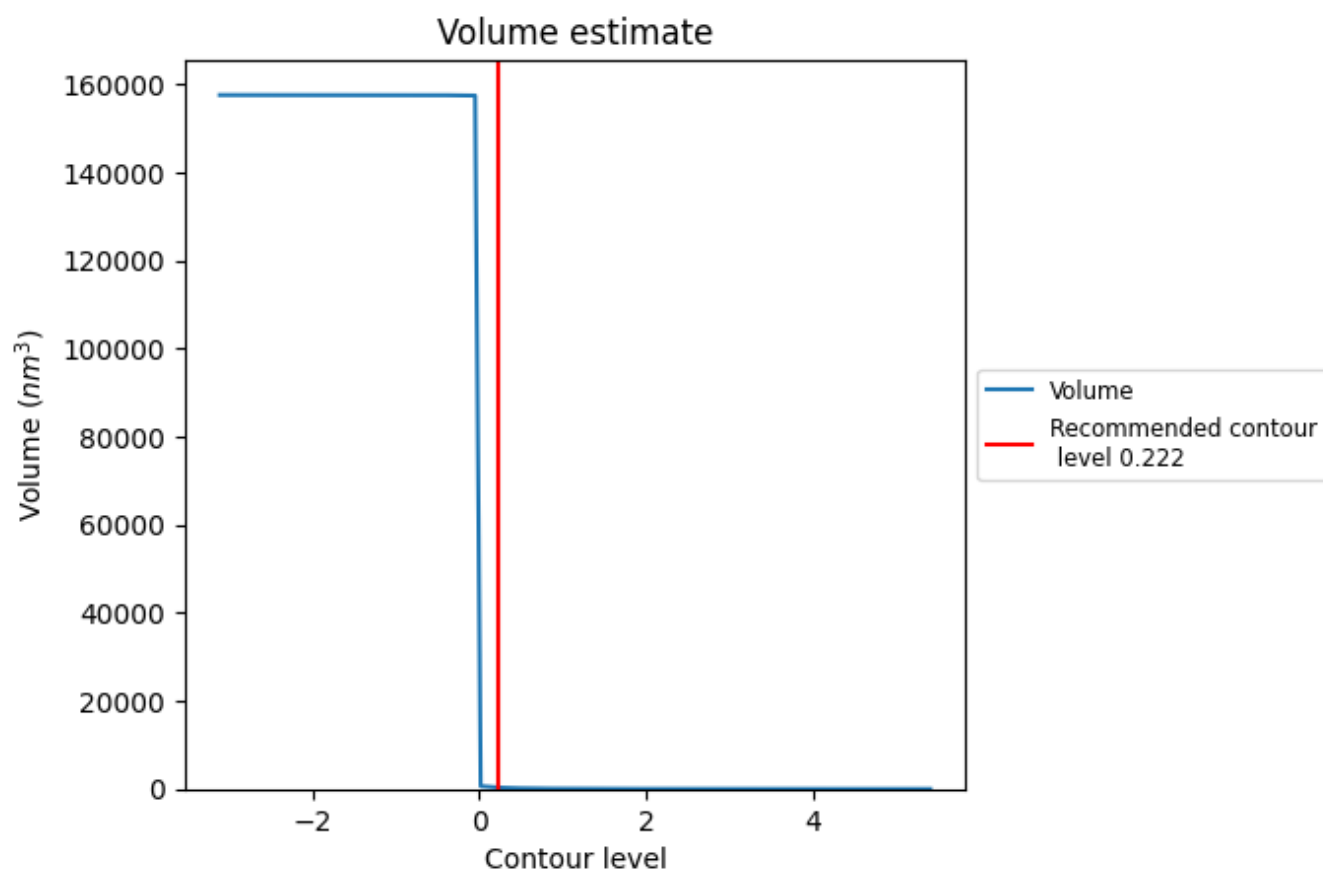
This section contains the results of statistical analysis of the map.

### 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.

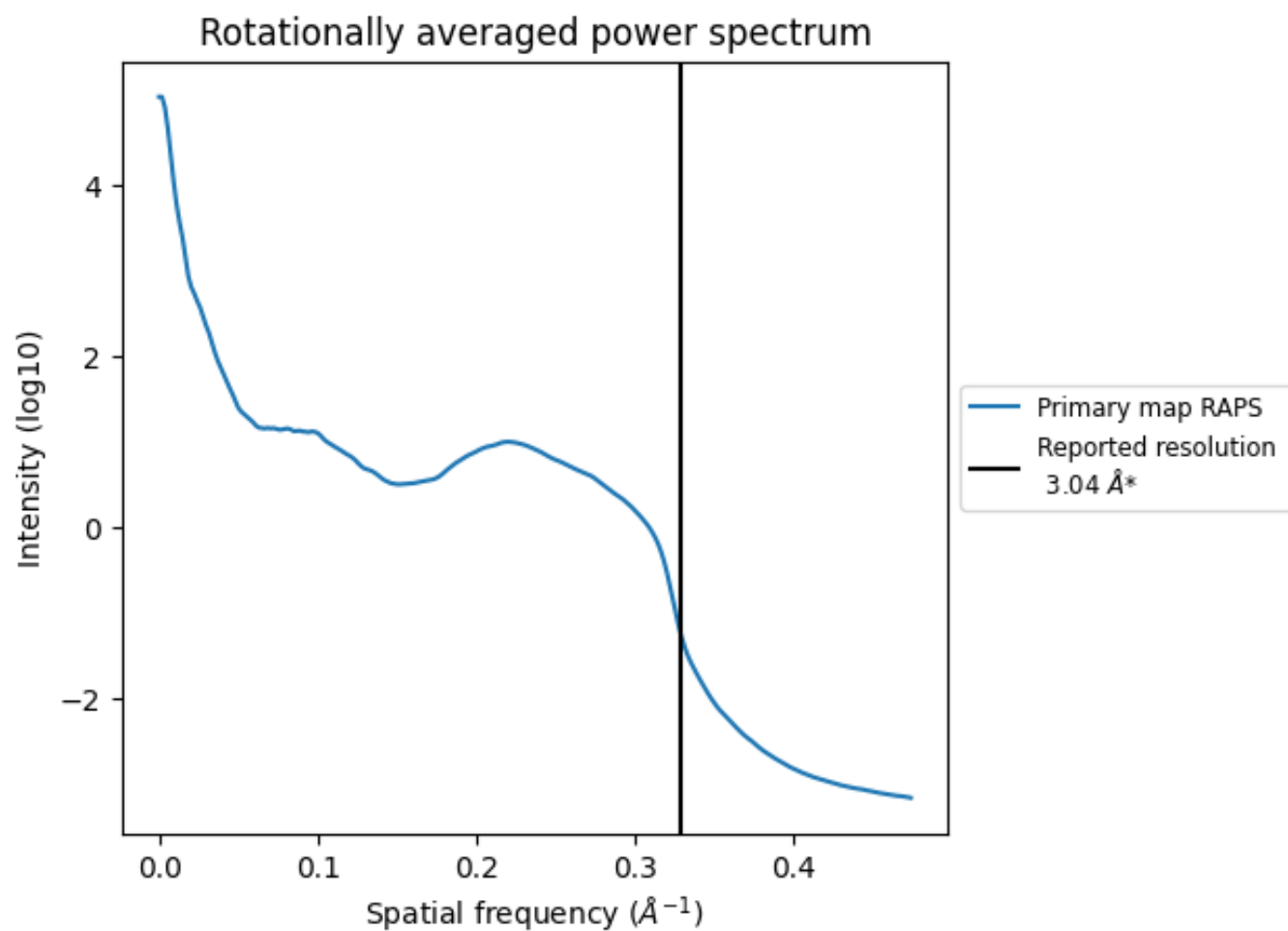
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331  $\text{nm}^3$ ; this corresponds to an approximate mass of 299 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 0.329 Å<sup>-1</sup>

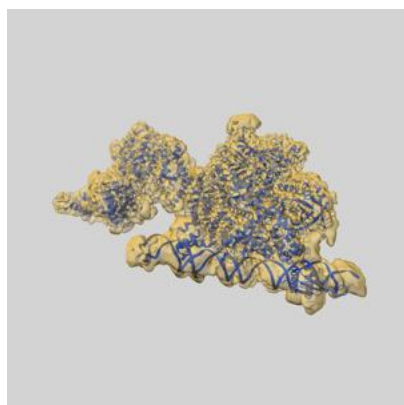
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

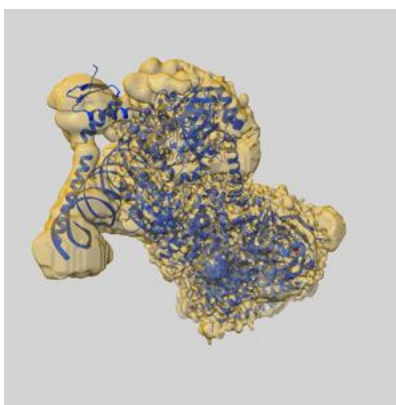
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31117 and PDB model 7EGH. Per-residue inclusion information can be found in section [3](#) on page [5](#).

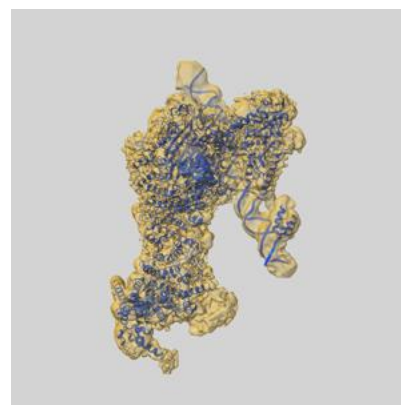
### 9.1 Map-model overlay [i](#)



X



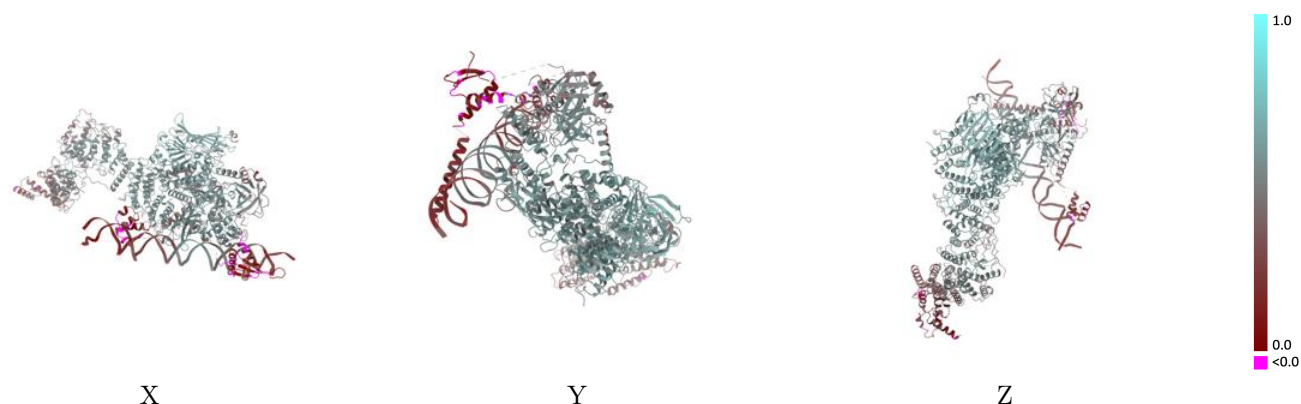
Y



Z

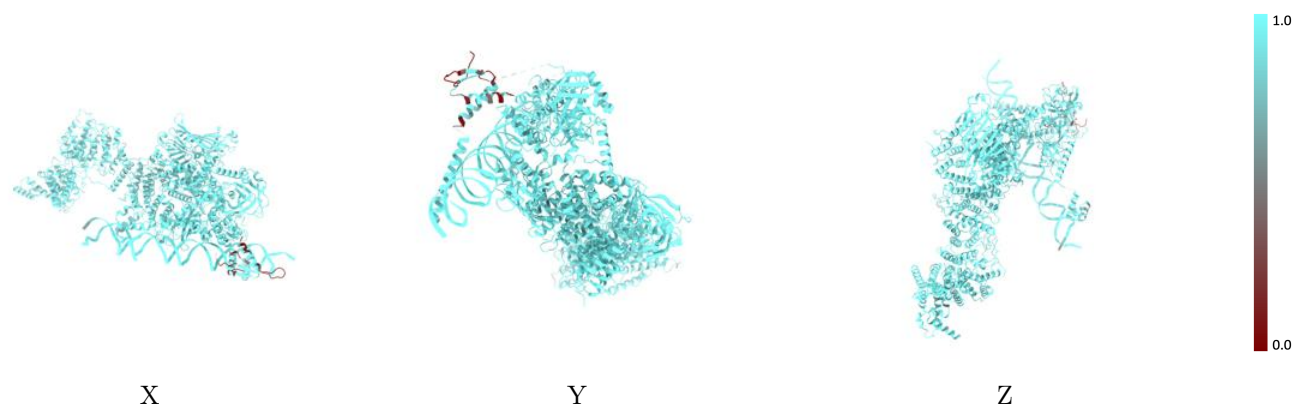
The images above show the 3D surface view of the map at the recommended contour level 0.222 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



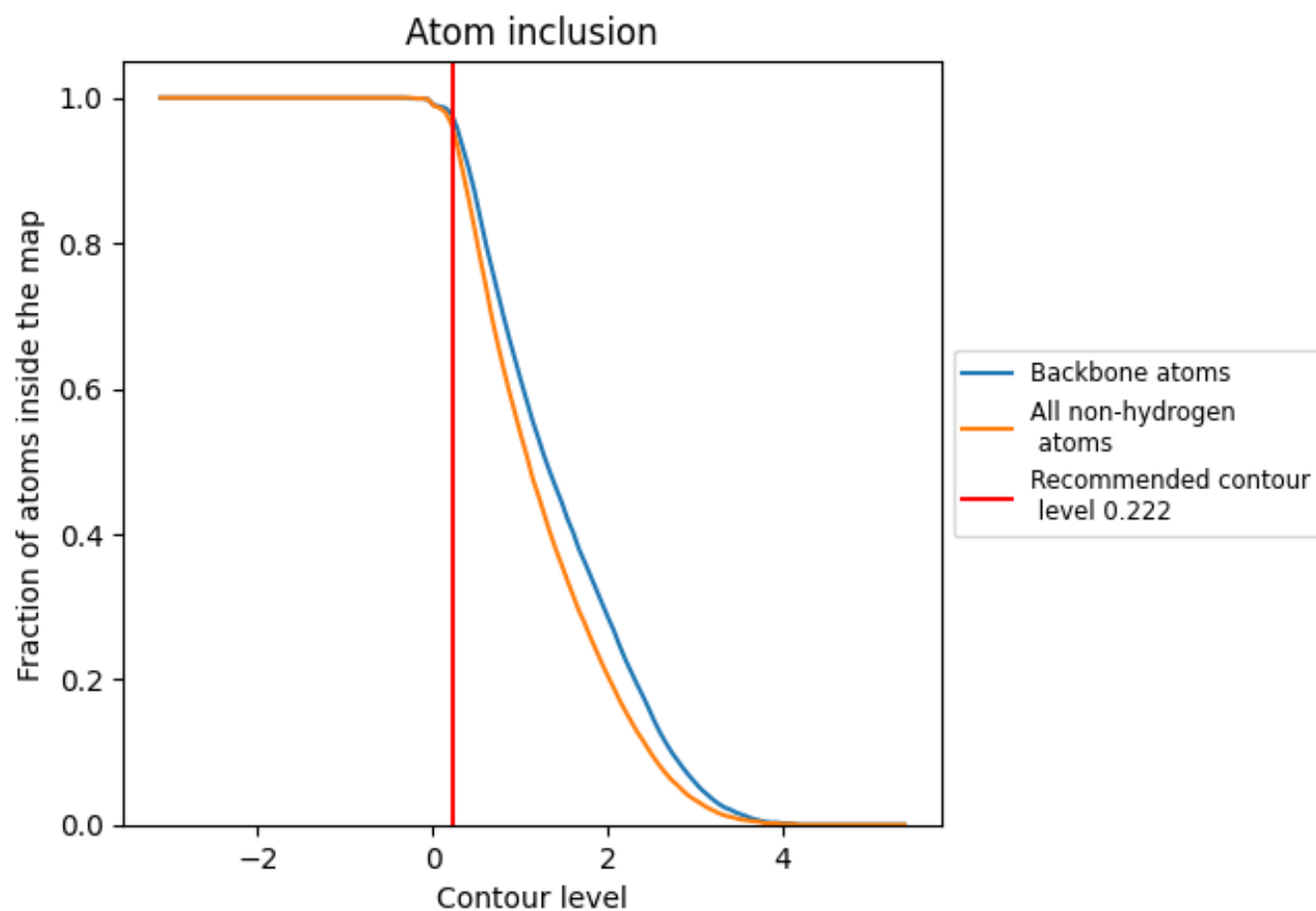
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.222).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.222) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9630</div>	<div><div></div>0.4810</div>
A	<div><div></div>0.9340</div>	<div><div></div>0.4360</div>
B	<div><div></div>0.9850</div>	<div><div></div>0.5790</div>
F	<div><div></div>0.9530</div>	<div><div></div>0.3690</div>
G	<div><div></div>0.8900</div>	<div><div></div>0.4040</div>
H	<div><div></div>0.9770</div>	<div><div></div>0.5400</div>
X	<div><div></div>0.9890</div>	<div><div></div>0.3420</div>
Y	<div><div></div>0.9800</div>	<div><div></div>0.3520</div>
f	<div><div></div>0.9790</div>	<div><div></div>0.4790</div>

1.0

0.0

<0.0