



## wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 07:08 am BST

PDB ID : 6HQA  
EMDB ID : EMD-0251  
Title : Molecular structure of promoter-bound yeast TFIID  
Authors : Kolesnikova, O.; Ben-Shem, A.; Luo, J.; Ranish, J.; Schultz, P.; Papai, G.  
Deposited on : 2018-09-24  
Resolution : 7.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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>.

---

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

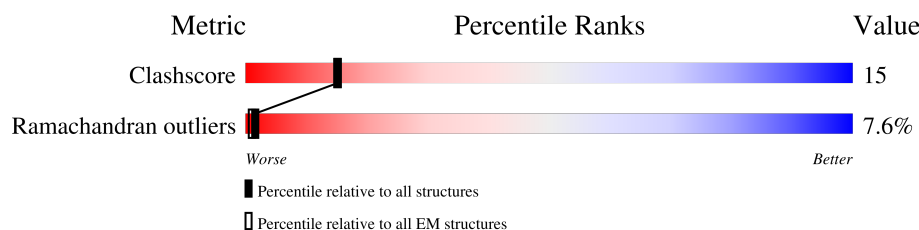
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 7.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835

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	1756	
2	B	722	
2	C	722	
3	D	485	
3	E	485	
4	F	153	
5	G	75	
6	I	64	
7	H	68	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	K	609	<div><div><div>6%</div><div>10%</div></div><div><div></div><div></div></div><div>88%</div></div>
9	J	553	<div><div><div>5%</div><div>8%</div></div><div><div></div><div></div></div><div>91%</div></div>

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12700 atoms, of which 63 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 Taf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	887	Total	C	N	O	0	0
			4396	2622	887	887		

- Molecule 2 is a protein called Subunit (90 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	522	Total	C	N	O	0	0
			2578	1534	522	522		
2	C	136	Total	C	N	O	0	0
			672	400	136	136		

- Molecule 3 is a protein called Subunit (60 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	254	Total	C	N	O	0	0
			1257	749	254	254		
3	E	320	Total	C	N	O	0	0
			1585	945	320	320		

- Molecule 4 is a protein called Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	F	103	Total	C	N	O	0	0
			511	305	103	103		

- Molecule 5 is a protein called Taf8.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	G	75	Total	C	N	O	0	0
			375	225	75	75		

- Molecule 6 is a protein called Histone-fold.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	64	Total	C	H	N	O	0	0
			383	192	63	64	64		

- Molecule 7 is a protein called Histone-fold.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	H	68	Total	C	N	O	0	0
			340	204	68	68		

- Molecule 8 is a protein called Subunit (61/68 kDa) of TFIID and SAGA complexes.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	K	71	Total	C	N	O	0	0
			351	209	71	71		

- Molecule 9 is a protein called TFIID subunit (48 kDa).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	J	51	Total	C	N	O	0	0
			252	150	51	51		

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-141	MET	-	initiating methionine	UNP C4R420
J	-140	SER	-	expression tag	UNP C4R420
J	-139	ARG	-	expression tag	UNP C4R420
J	-138	LYS	-	expression tag	UNP C4R420
J	-137	PRO	-	expression tag	UNP C4R420
J	-136	GLU	-	expression tag	UNP C4R420
J	-135	ARG	-	expression tag	UNP C4R420
J	-134	ARG	-	expression tag	UNP C4R420
J	-133	ARG	-	expression tag	UNP C4R420
J	-132	GLN	-	expression tag	UNP C4R420
J	-131	PRO	-	expression tag	UNP C4R420
J	-130	ARG	-	expression tag	UNP C4R420
J	-129	LEU	-	expression tag	UNP C4R420
J	-128	PHE	-	expression tag	UNP C4R420
J	-127	SER	-	expression tag	UNP C4R420
J	-126	ASN	-	expression tag	UNP C4R420
J	-125	ASP	-	expression tag	UNP C4R420
J	-124	MET	-	expression tag	UNP C4R420
J	-123	ARG	-	expression tag	UNP C4R420

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
J	-122	THR	-	expression tag	UNP C4R420
J	-121	LEU	-	expression tag	UNP C4R420
J	-120	LEU	-	expression tag	UNP C4R420
J	-119	PHE	-	expression tag	UNP C4R420
J	-118	ALA	-	expression tag	UNP C4R420
J	-117	TYR	-	expression tag	UNP C4R420
J	-116	GLY	-	expression tag	UNP C4R420
J	-115	ASP	-	expression tag	UNP C4R420
J	-114	VAL	-	expression tag	UNP C4R420
J	-113	GLN	-	expression tag	UNP C4R420
J	-112	GLN	-	expression tag	UNP C4R420
J	-111	PRO	-	expression tag	UNP C4R420
J	-110	GLN	-	expression tag	UNP C4R420
J	-109	LEU	-	expression tag	UNP C4R420
J	-108	GLU	-	expression tag	UNP C4R420
J	-107	THR	-	expression tag	UNP C4R420
J	-106	ILE	-	expression tag	UNP C4R420
J	-105	GLN	-	expression tag	UNP C4R420
J	-104	ALA	-	expression tag	UNP C4R420
J	-103	LEU	-	expression tag	UNP C4R420
J	-102	GLU	-	expression tag	UNP C4R420
J	-101	ASP	-	expression tag	UNP C4R420
J	-100	VAL	-	expression tag	UNP C4R420
J	-99	MET	-	expression tag	UNP C4R420
J	-98	ILE	-	expression tag	UNP C4R420
J	-97	VAL	-	expression tag	UNP C4R420
J	-96	PHE	-	expression tag	UNP C4R420
J	-95	MET	-	expression tag	UNP C4R420
J	-94	THR	-	expression tag	UNP C4R420
J	-93	ASP	-	expression tag	UNP C4R420
J	-92	LEU	-	expression tag	UNP C4R420
J	-91	CYS	-	expression tag	UNP C4R420
J	-90	HIS	-	expression tag	UNP C4R420
J	-89	GLU	-	expression tag	UNP C4R420
J	-88	ALA	-	expression tag	UNP C4R420
J	-87	MET	-	expression tag	UNP C4R420
J	-86	THR	-	expression tag	UNP C4R420
J	-85	TYR	-	expression tag	UNP C4R420
J	-84	ALA	-	expression tag	UNP C4R420
J	-83	THR	-	expression tag	UNP C4R420
J	-82	TYR	-	expression tag	UNP C4R420
J	-81	GLN	-	expression tag	UNP C4R420

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
J	-80	GLY	-	expression tag	UNP C4R420
J	-79	ARG	-	expression tag	UNP C4R420
J	-78	LYS	-	expression tag	UNP C4R420
J	-77	HIS	-	expression tag	UNP C4R420
J	-76	LYS	-	expression tag	UNP C4R420
J	-75	LEU	-	expression tag	UNP C4R420
J	-74	LYS	-	expression tag	UNP C4R420
J	-73	MET	-	expression tag	UNP C4R420
J	-72	GLU	-	expression tag	UNP C4R420
J	-71	ASP	-	expression tag	UNP C4R420
J	-70	PHE	-	expression tag	UNP C4R420
J	-69	LYS	-	expression tag	UNP C4R420
J	-68	PHE	-	expression tag	UNP C4R420
J	-67	ALA	-	expression tag	UNP C4R420
J	-66	LEU	-	expression tag	UNP C4R420
J	-65	ARG	-	expression tag	UNP C4R420
J	-64	LYS	-	expression tag	UNP C4R420
J	-63	ASP	-	expression tag	UNP C4R420
J	-62	ARG	-	expression tag	UNP C4R420
J	-61	LEU	-	expression tag	UNP C4R420
J	-60	LYS	-	expression tag	UNP C4R420
J	-59	LEU	-	expression tag	UNP C4R420
J	-58	GLY	-	expression tag	UNP C4R420
J	-57	ARG	-	expression tag	UNP C4R420
J	-56	VAL	-	expression tag	UNP C4R420
J	-55	GLU	-	expression tag	UNP C4R420
J	-54	GLU	-	expression tag	UNP C4R420
J	-53	LEU	-	expression tag	UNP C4R420
J	-52	MET	-	expression tag	UNP C4R420
J	-51	ASN	-	expression tag	UNP C4R420
J	-50	LYS	-	expression tag	UNP C4R420
J	-49	GLN	-	expression tag	UNP C4R420
J	-48	LYS	-	expression tag	UNP C4R420
J	-47	GLU	-	expression tag	UNP C4R420
J	-46	ILE	-	expression tag	UNP C4R420
J	-45	GLN	-	expression tag	UNP C4R420
J	-44	GLU	-	expression tag	UNP C4R420
J	-43	ALA	-	expression tag	UNP C4R420
J	-42	ARG	-	expression tag	UNP C4R420
J	-41	LYS	-	expression tag	UNP C4R420
J	-40	LEU	-	expression tag	UNP C4R420
J	-39	PHE	-	expression tag	UNP C4R420

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
J	-38	ASP	-	expression tag	UNP C4R420
J	-37	SER	-	expression tag	UNP C4R420
J	-36	ASN	-	expression tag	UNP C4R420
J	-35	GLU	-	expression tag	UNP C4R420
J	-34	LYS	-	expression tag	UNP C4R420
J	-33	GLU	-	expression tag	UNP C4R420
J	-32	THR	-	expression tag	UNP C4R420
J	-31	LYS	-	expression tag	UNP C4R420
J	-30	ASP	-	expression tag	UNP C4R420
J	-29	ASP	-	expression tag	UNP C4R420
J	-28	ASP	-	expression tag	UNP C4R420
J	-27	ILE	-	expression tag	UNP C4R420
J	-26	GLU	-	expression tag	UNP C4R420
J	-25	LYS	-	expression tag	UNP C4R420
J	-24	LYS	-	expression tag	UNP C4R420
J	-23	ARG	-	expression tag	UNP C4R420
J	-22	ARG	-	expression tag	UNP C4R420
J	-21	LYS	-	expression tag	UNP C4R420
J	-20	GLU	-	expression tag	UNP C4R420
J	-19	ALA	-	expression tag	UNP C4R420
J	-18	LYS	-	expression tag	UNP C4R420
J	-17	ARG	-	expression tag	UNP C4R420
J	-16	ALA	-	expression tag	UNP C4R420
J	-15	ILE	-	expression tag	UNP C4R420
J	-14	LYS	-	expression tag	UNP C4R420
J	-13	GLU	-	expression tag	UNP C4R420
J	-12	ALA	-	expression tag	UNP C4R420
J	-11	LYS	-	expression tag	UNP C4R420
J	-10	LYS	-	expression tag	UNP C4R420
J	-9	LEU	-	expression tag	UNP C4R420
J	-8	LYS	-	expression tag	UNP C4R420
J	-7	LEU	-	expression tag	UNP C4R420
J	-6	SER	-	expression tag	UNP C4R420
J	-5	LYS	-	expression tag	UNP C4R420
J	-4	GLY	-	expression tag	UNP C4R420
J	-3	ASP	-	expression tag	UNP C4R420
J	-2	THR	-	expression tag	UNP C4R420
J	-1	ALA	-	expression tag	UNP C4R420
J	0	PHE	-	expression tag	UNP C4R420

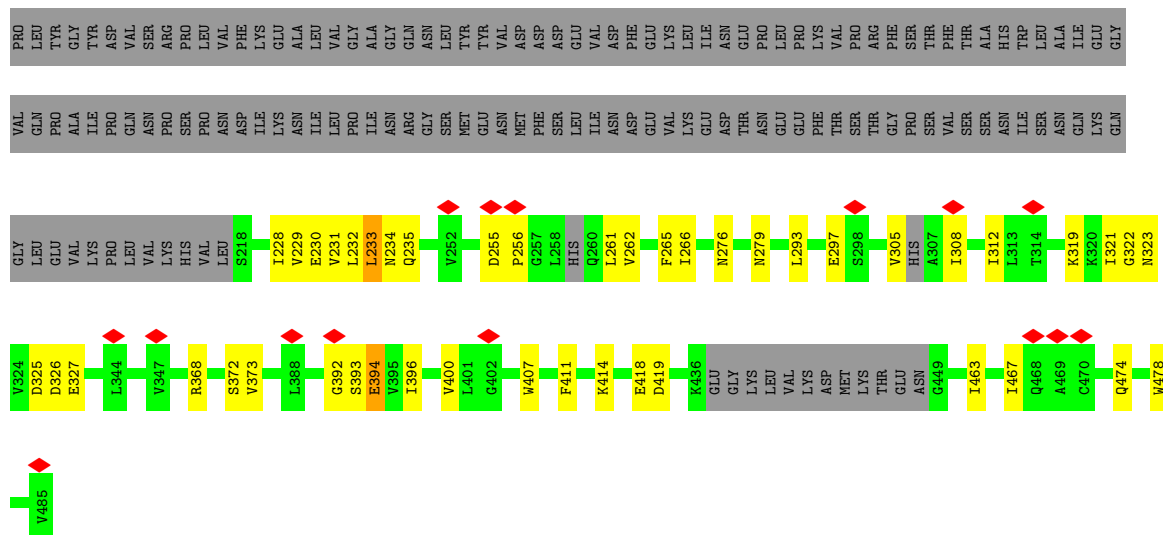




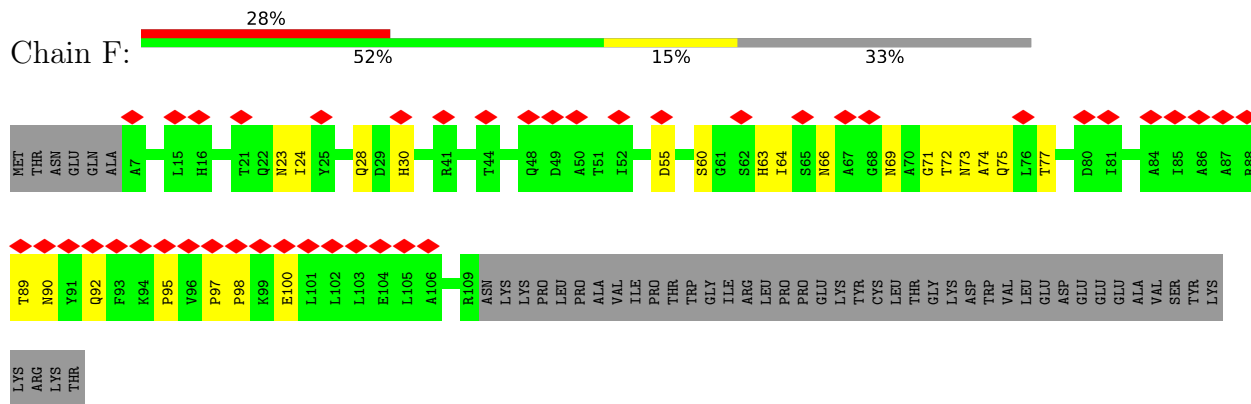




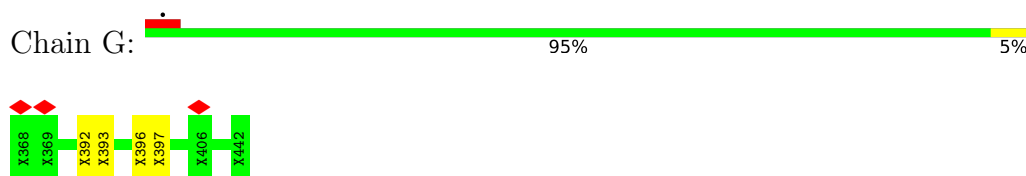




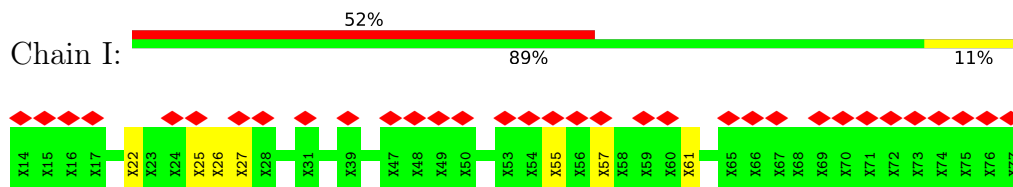
- Molecule 4: Subunit (17 kDa) of TFIID and SAGA complexes, involved in RNA polymerase II transcription initiation



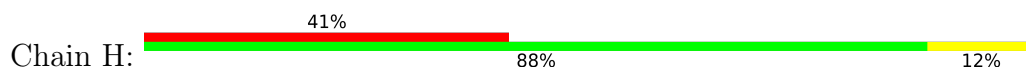
- Molecule 5: Taf8

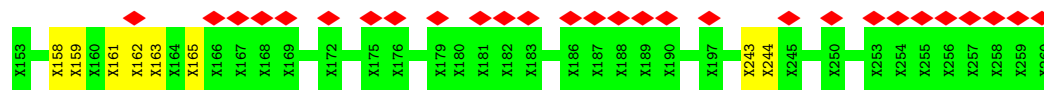


- Molecule 6: Histone-fold

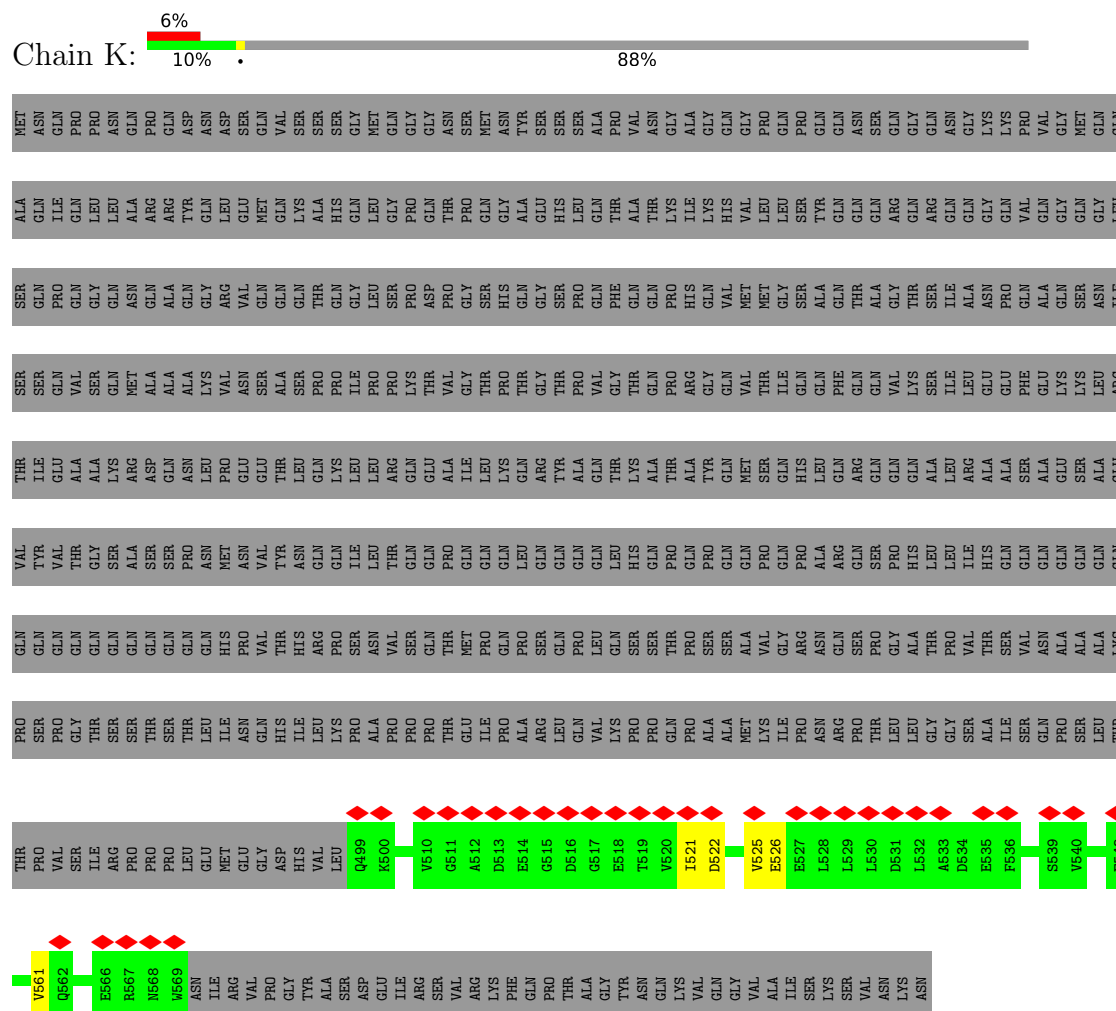


- Molecule 7: Histone-fold

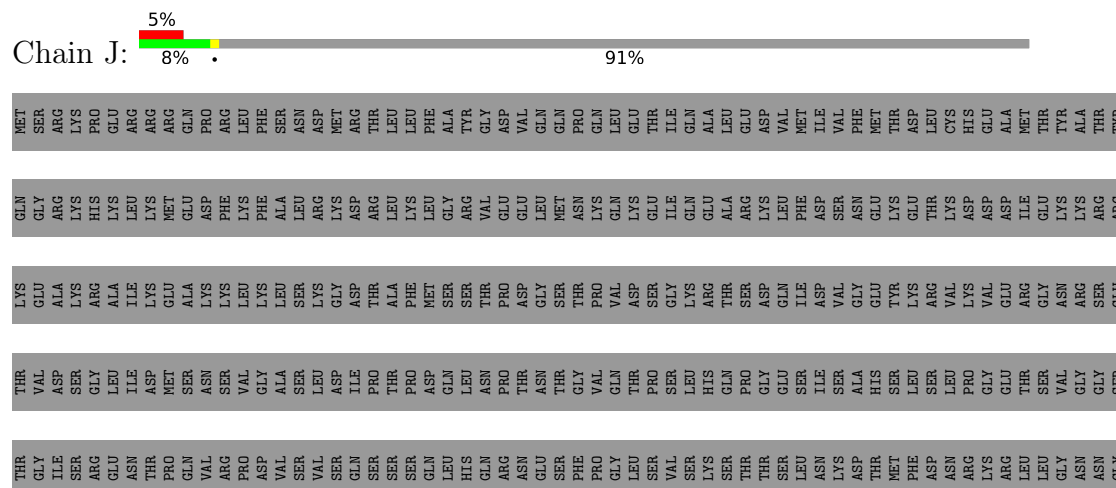


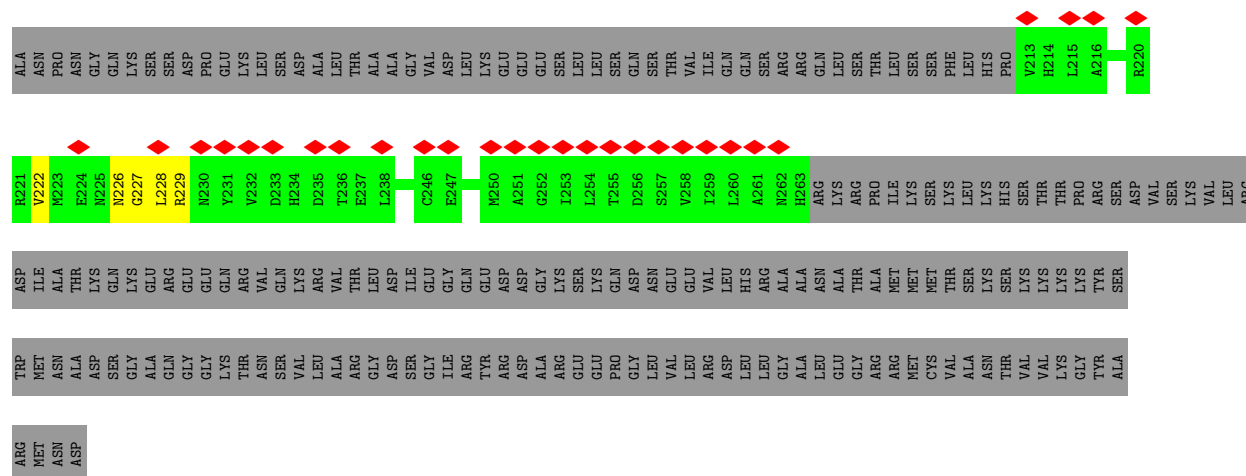


• Molecule 8: Subunit (61/68 kDa) of TFIID and SAGA complexes



• Molecule 9: TFIID subunit (48 kDa)





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	180823	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 ( $e^-/\text{\AA}^2$ )	52.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	4900	Depositor
Magnification	45454	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.022	Depositor
Minimum map value	-0.014	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.004	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	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	0.23	0/4156	0.41	0/5771
2	B	0.23	0/2572	0.40	0/3572
2	C	0.23	0/671	0.40	0/933
3	D	0.23	0/1254	0.37	0/1743
3	E	0.22	0/1582	0.37	0/2201
4	F	0.23	0/510	0.40	0/710
8	K	0.23	0/349	0.37	0/483
9	J	0.23	0/251	0.35	0/348
All	All	0.23	0/11345	0.39	0/15761

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	4396	0	1883	79	0
2	B	2578	0	1144	102	0
2	C	672	0	290	4	0
3	D	1257	0	548	29	0
3	E	1585	0	703	29	0
4	F	511	0	246	9	0
5	G	375	0	84	2	0
6	I	320	63	67	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	340	0	72	4	0
8	K	351	0	156	3	0
9	J	252	0	116	2	0
All	All	12637	63	5309	263	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 15.

The worst 5 of 263 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)
1:A:67:SER:HA	1:A:167:LEU:O	1.27	1.30
1:A:45:ASP:CA	1:A:50:THR:O	1.85	1.24
2:B:592:ARG:HA	2:B:608:ILE:O	1.32	1.23
2:B:550:THR:HA	2:B:566:ILE:O	1.29	1.23
2:B:466:ARG:HA	2:B:482:LEU:O	1.40	1.18

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	813/1756 (46%)	623 (77%)	131 (16%)	59 (7%)	1	10
2	B	511/722 (71%)	352 (69%)	99 (19%)	60 (12%)	0	4
2	C	134/722 (19%)	109 (81%)	14 (10%)	11 (8%)	1	9
3	D	248/485 (51%)	201 (81%)	32 (13%)	15 (6%)	1	13
3	E	314/485 (65%)	268 (85%)	35 (11%)	11 (4%)	3	20
4	F	101/153 (66%)	71 (70%)	20 (20%)	10 (10%)	0	7
8	K	67/609 (11%)	59 (88%)	6 (9%)	2 (3%)	3	23

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	J	49/553 (9%)	43 (88%)	5 (10%)	1 (2%)	6	32
All	All	2237/5485 (41%)	1726 (77%)	342 (15%)	169 (8%)	1	10

5 of 169 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	PRO
1	A	81	VAL
1	A	168	PRO
1	A	184	PRO
1	A	333	PRO

### 5.3.2 Protein sidechains [i](#)

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

### 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6
2	B	4
3	D	1
5	G	1
8	K	1

The worst 5 of 13 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	357:ASN	C	358:ASP	N	14.12
1	B	372:SER	C	373:ALA	N	6.29
1	D	394:GLU	C	395:VAL	N	5.84
1	A	930:PHE	C	931:GLN	N	5.73
1	A	802:ASP	C	803:ALA	N	5.20

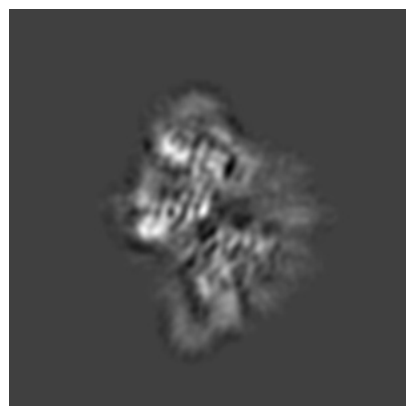
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0251. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

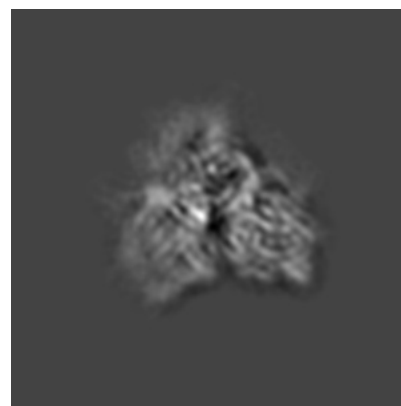
#### 6.1.1 Primary map



X

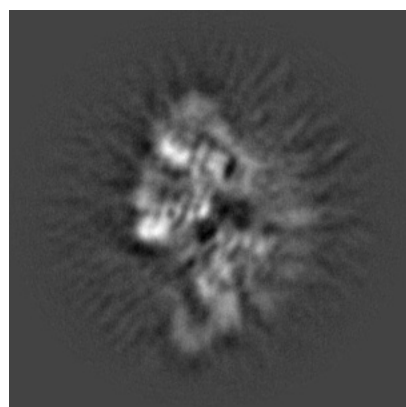


Y

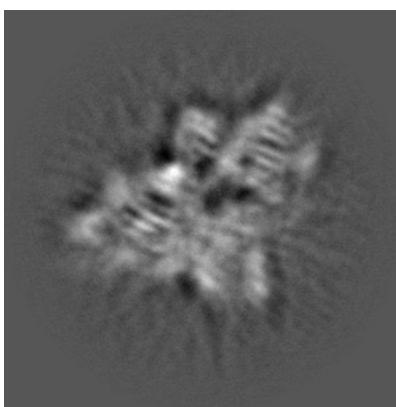


Z

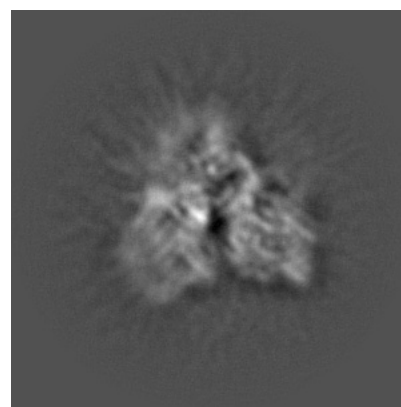
#### 6.1.2 Raw map



X



Y



Z

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

## 6.2 Central slices [i](#)

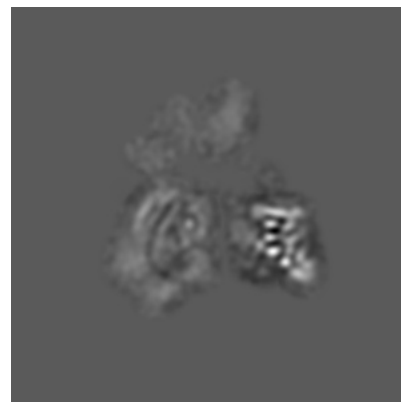
### 6.2.1 Primary map



X Index: 160

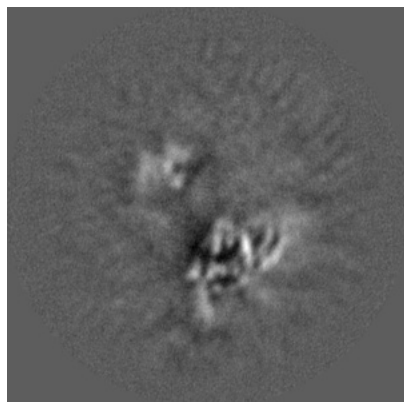


Y Index: 160

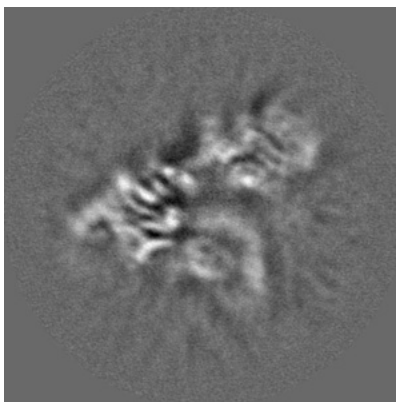


Z Index: 160

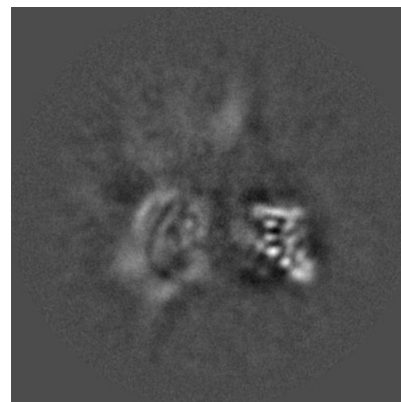
### 6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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

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

### 6.3.1 Primary map



X Index: 183

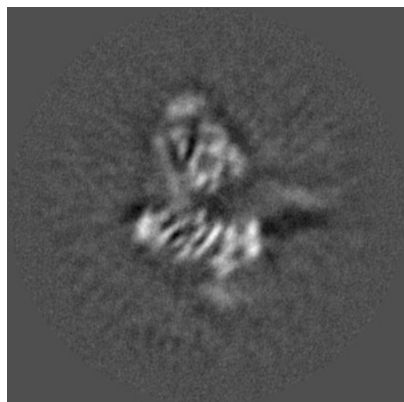


Y Index: 156

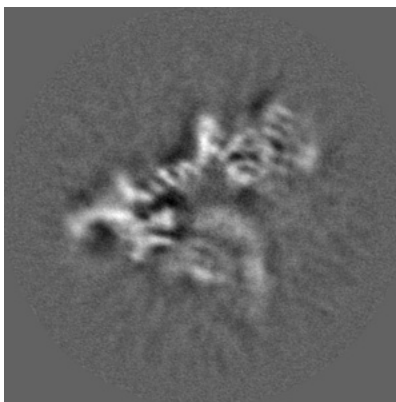


Z Index: 137

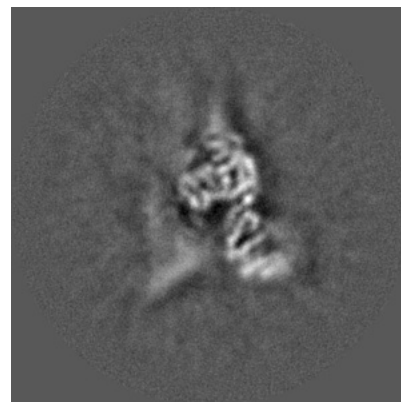
### 6.3.2 Raw map



X Index: 188



Y Index: 156

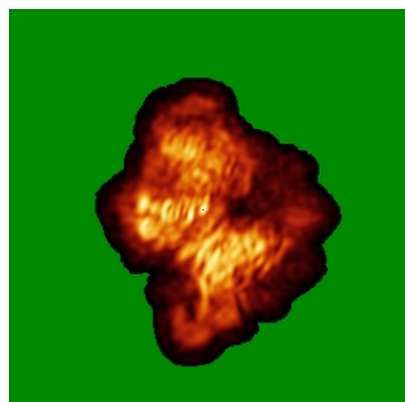


Z Index: 138

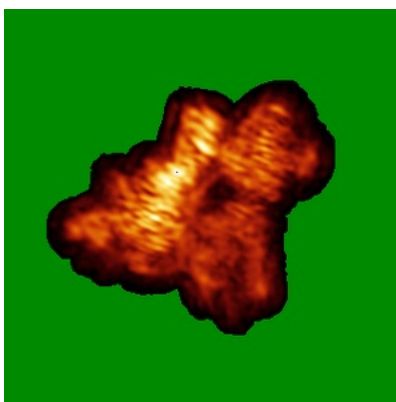
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



X

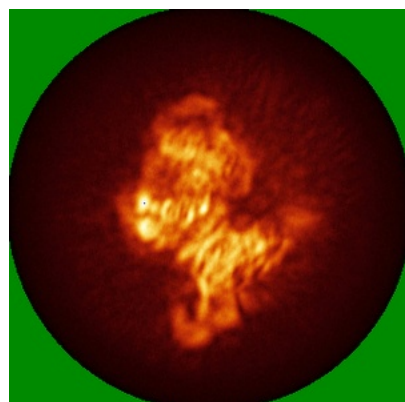


Y

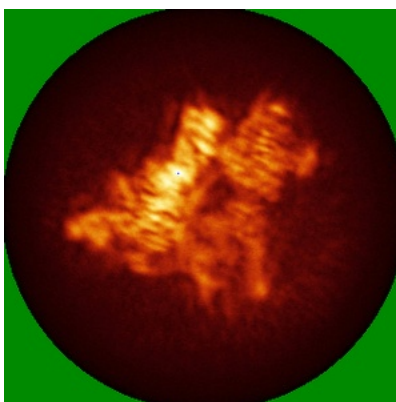


Z

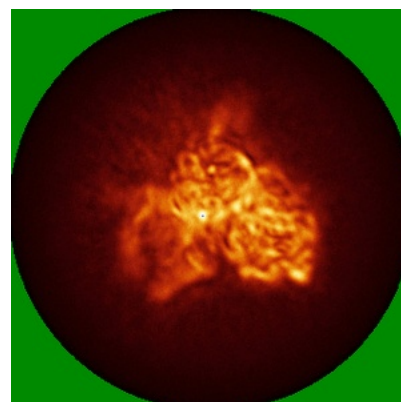
### 6.4.2 Raw map



X



Y



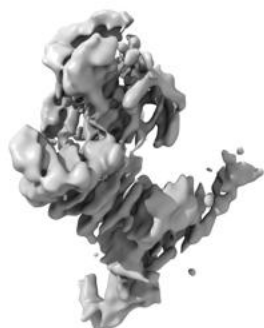
Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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

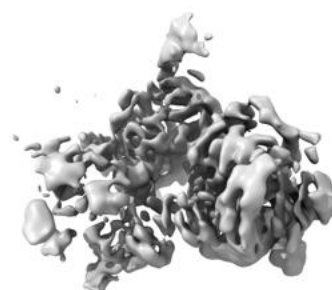
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.004. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

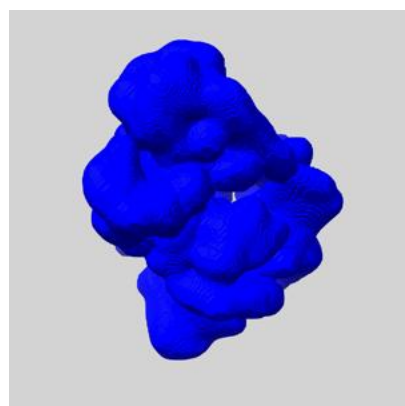
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

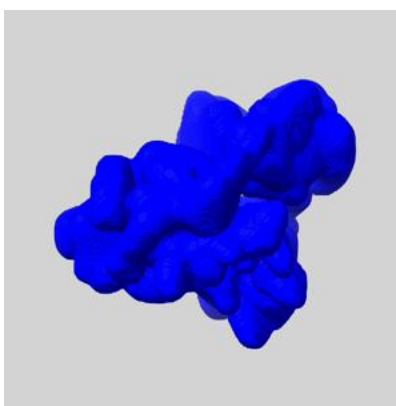
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

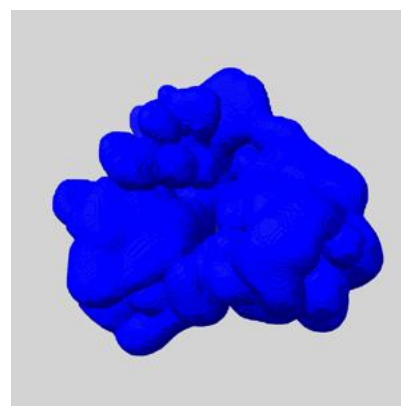
### 6.6.1 emd\_0251\_msk\_1.map [i](#)



X



Y

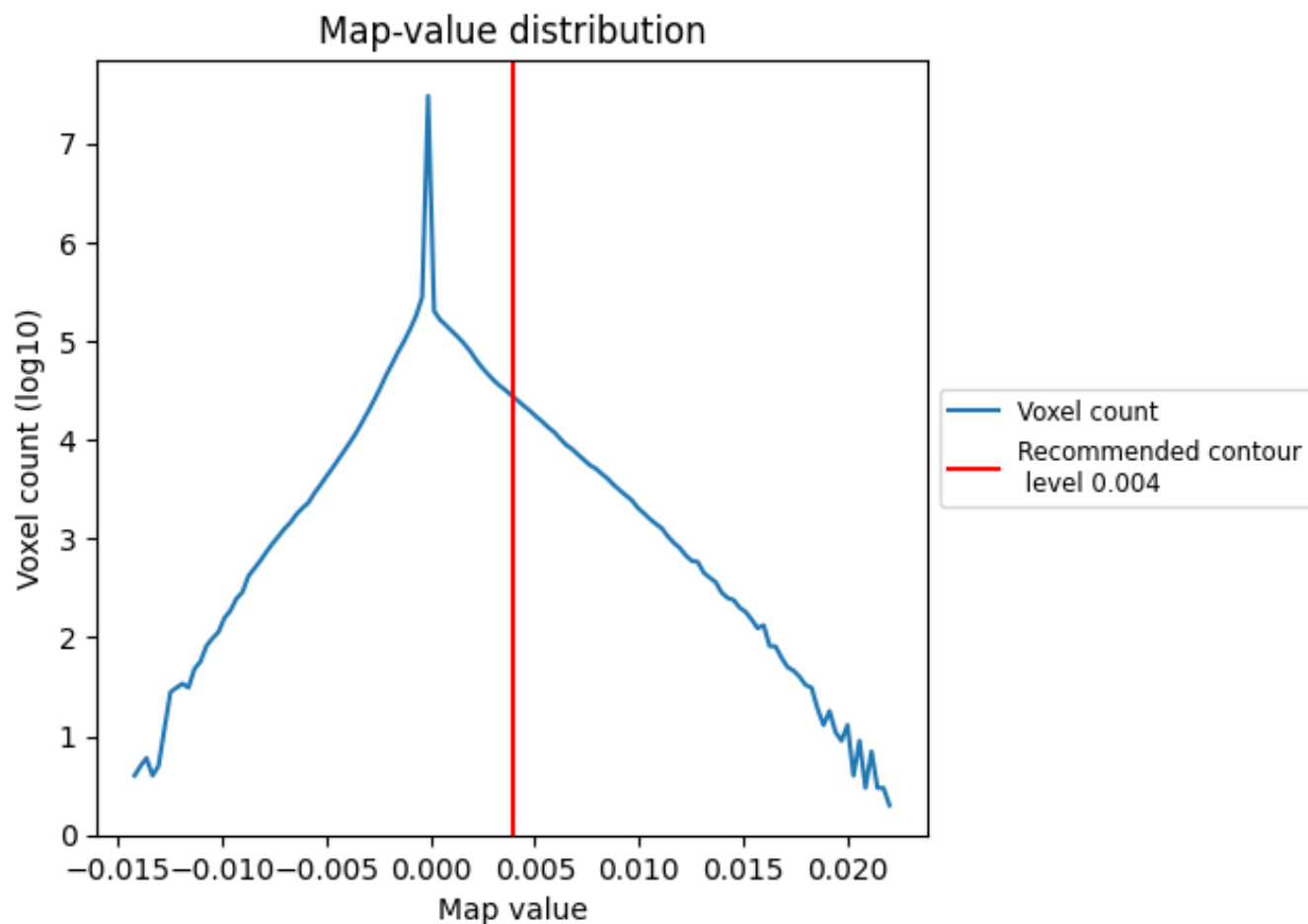


Z

## 7 Map analysis [i](#)

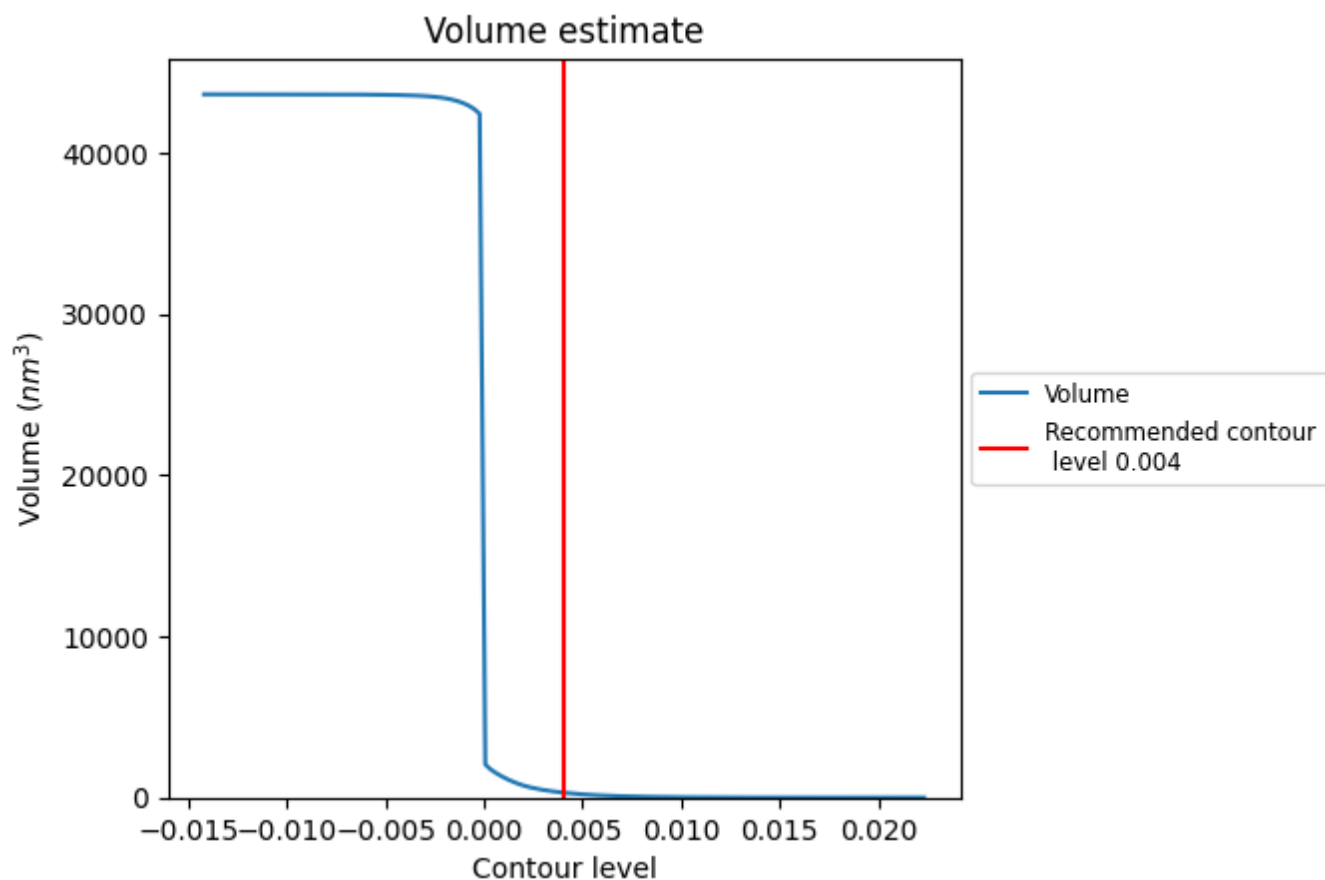
This section contains the results of statistical analysis of the map.

### 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.

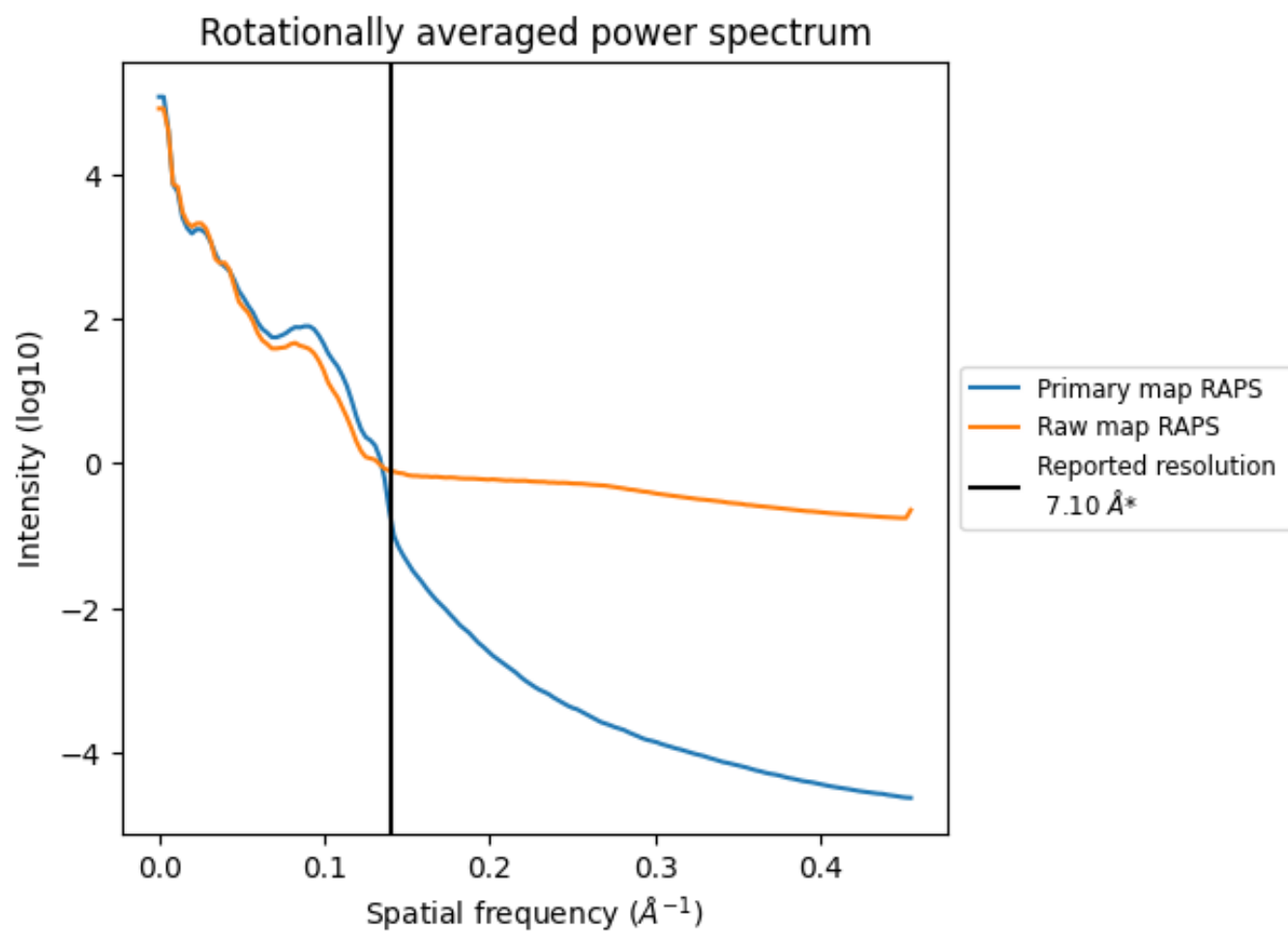
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 308 nm<sup>3</sup>; this corresponds to an approximate mass of 278 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 ⓘ

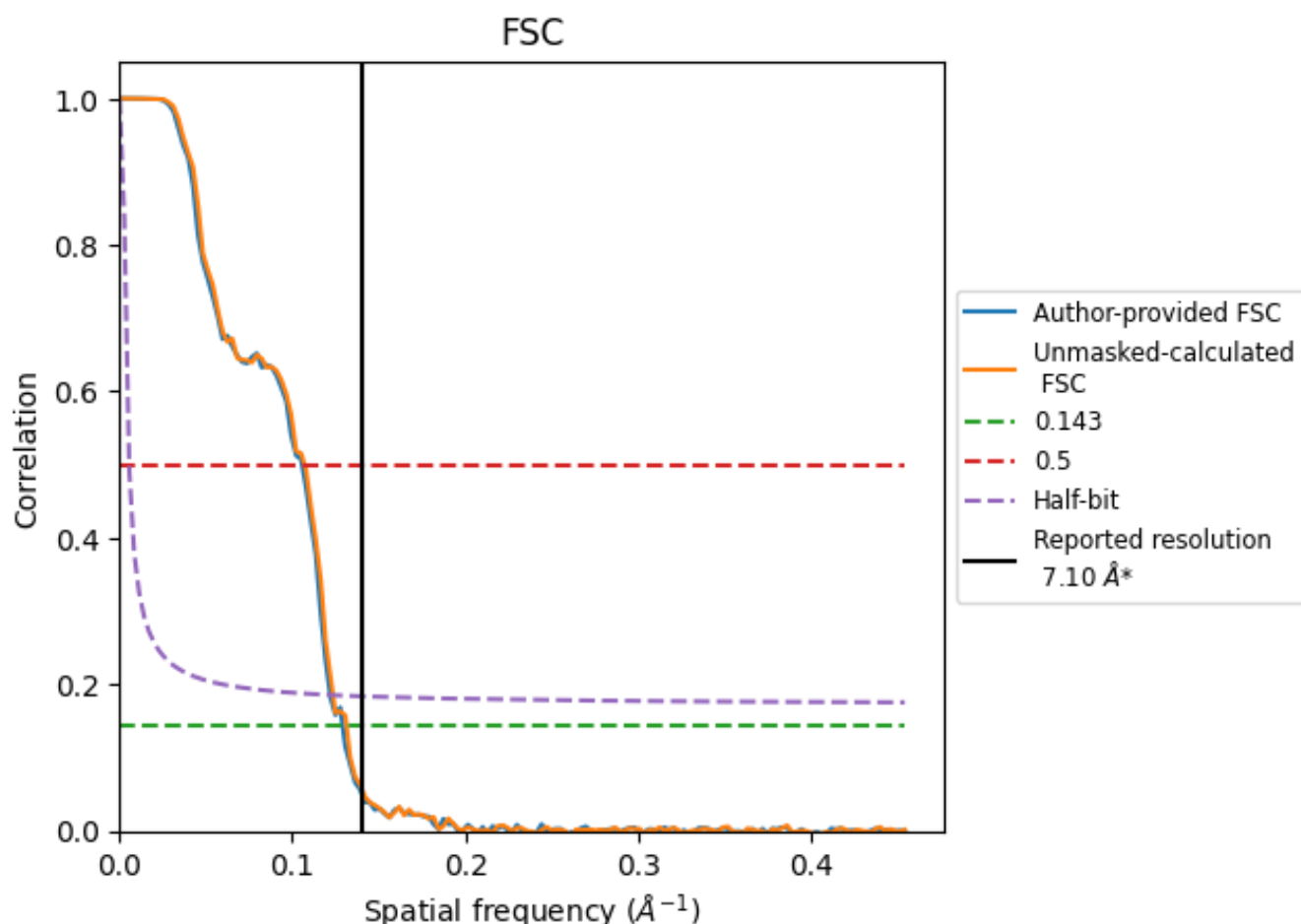


\*Reported resolution corresponds to spatial frequency of 0.141  $\text{\AA}^{-1}$

## 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 0.141 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

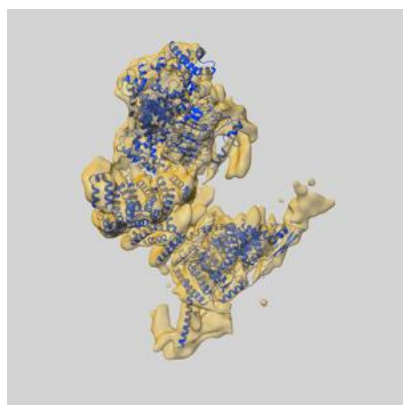
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.10	-	-
Author-provided FSC curve	7.74	9.46	8.20
Unmasked-calculated*	7.61	9.35	8.09

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

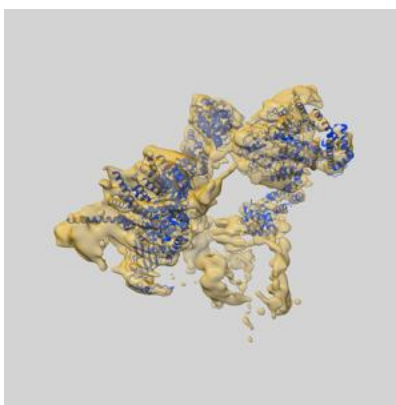
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0251 and PDB model 6HQA. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

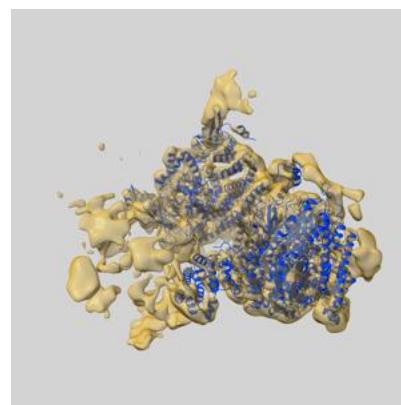
### 9.1 Map-model overlay [i](#)



X



Y

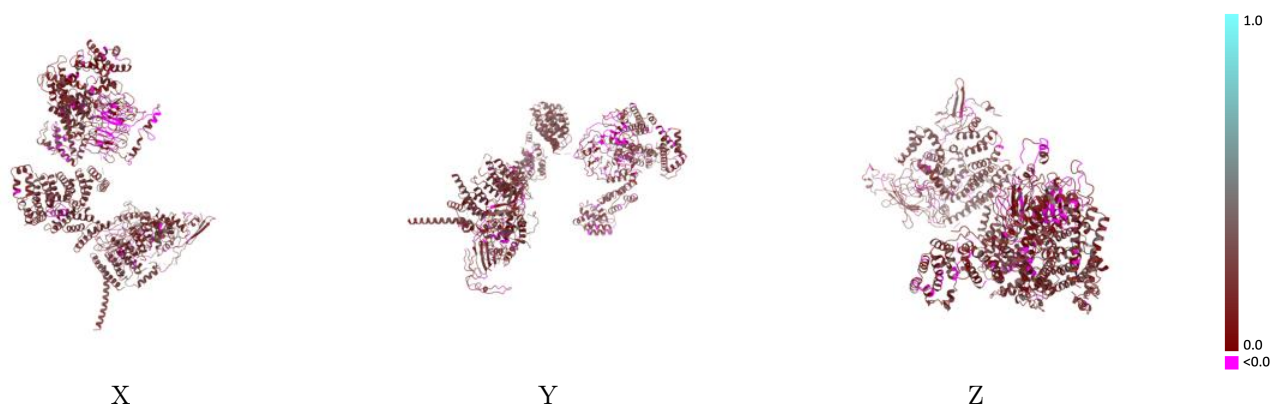


Z

The images above show the 3D surface view of the map at the recommended contour level 0.004 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.

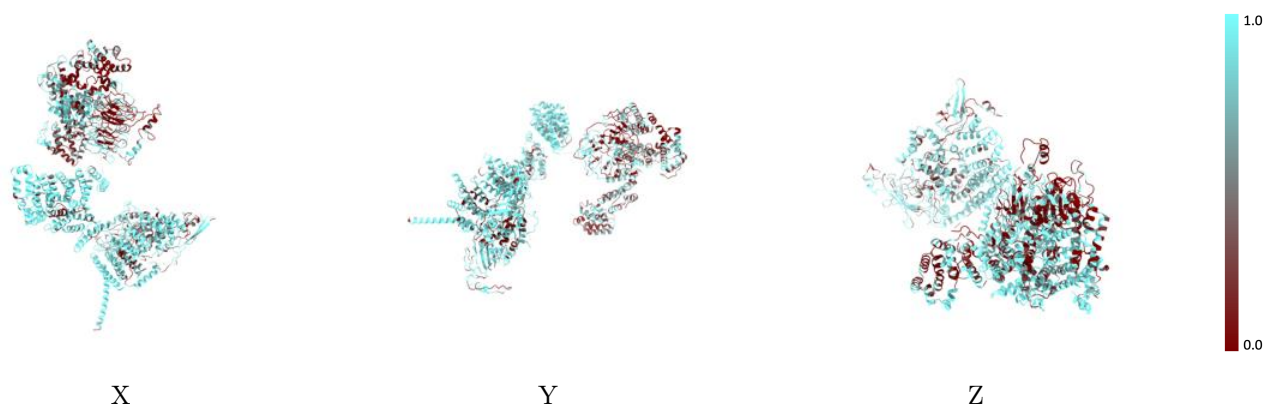


## 9.2 Q-score mapped to coordinate model [i](#)



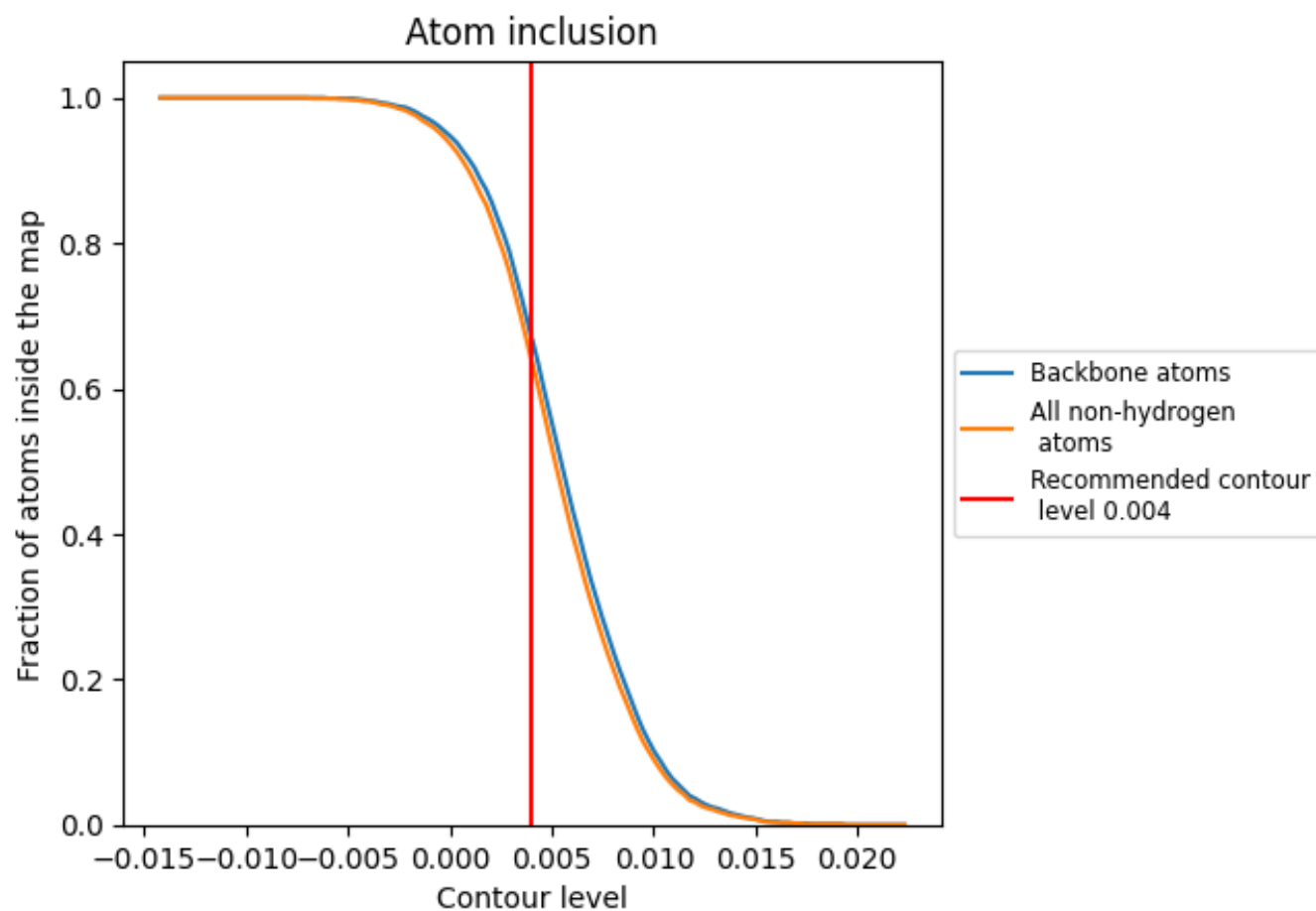
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.004).

























## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 64% 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 (0.004) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6390	 0.1780
A	 0.7010	 0.1920
B	 0.4280	 0.0980
C	 0.4720	 0.1600
D	 0.8090	 0.2040
E	 0.8290	 0.2250
F	 0.5460	 0.2020
G	 0.9520	 0.2540
H	 0.5530	 0.2110
I	 0.4870	 0.2040
J	 0.4440	 0.1520
K	 0.4160	 0.1590

