



## wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 11:00 PM EDT

PDB ID : 7K61  
EMDB ID : EMD-22686  
Title : Cryo-EM structure of 197bp nucleosome aided by scFv  
Authors : Zhou, B.-R.; Bai, Y.  
Deposited on : 2020-09-17  
Resolution : 2.85 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

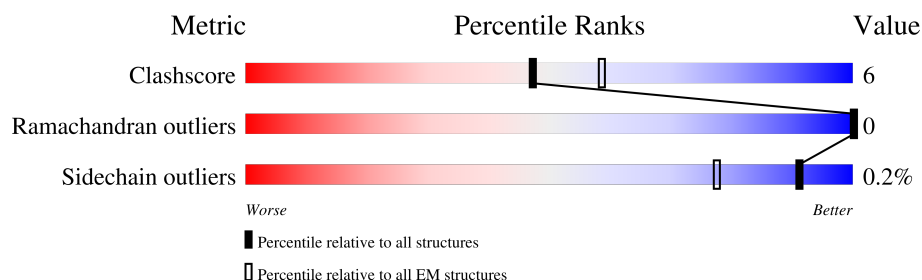
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.85 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

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	136	
1	E	136	
2	B	103	
2	F	103	
3	C	130	
3	G	130	
4	D	126	
4	H	126	

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Mol	Chain	Length	Quality of chain
5	I	197	
6	J	197	
7	M	270	
7	N	270	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 17723 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 Histone H3.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	97	Total	C	N	O	S	0	0
			799	505	153	137	4		
1	E	97	Total	C	N	O	S	0	0
			799	505	153	137	4		

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	83	Total	C	N	O	S	0	0
			662	418	129	114	1		
2	F	83	Total	C	N	O	S	0	0
			662	418	129	114	1		

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	109	Total	C	N	O	0	0
			840	529	166	145		
3	G	109	Total	C	N	O	0	0
			840	529	166	145		

- Molecule 4 is a protein called Histone H2B type 1-J.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	95	Total	C	N	O	S	0	0
			745	468	136	139	2		
4	H	95	Total	C	N	O	S	0	0
			745	468	136	139	2		

- Molecule 5 is a DNA chain called DNA (197-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	197	Total	C	N	O	P	0	0
			4015	1904	733	1181	197		

- Molecule 6 is a DNA chain called DNA (197-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	197	Total	C	N	O	P	0	0
			4062	1920	762	1183	197		

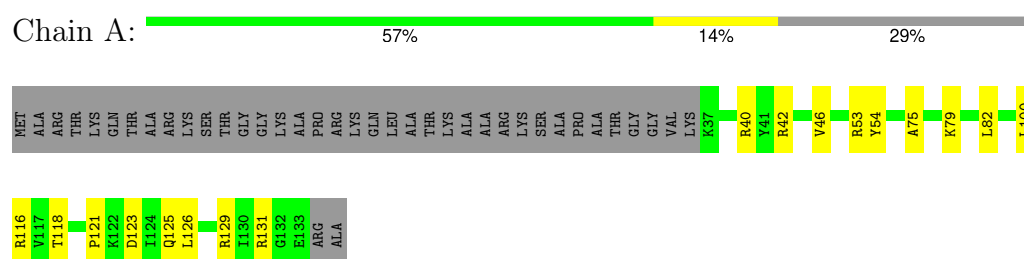
- Molecule 7 is a protein called scFv20.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	227	Total	C	N	O	S	0	0
			1777	1120	290	358	9		
7	N	227	Total	C	N	O	S	0	0
			1777	1120	290	358	9		

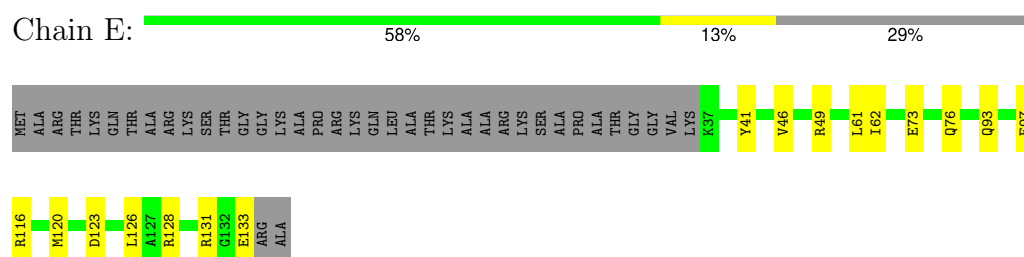
### 3 Residue-property plots [i](#)

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.

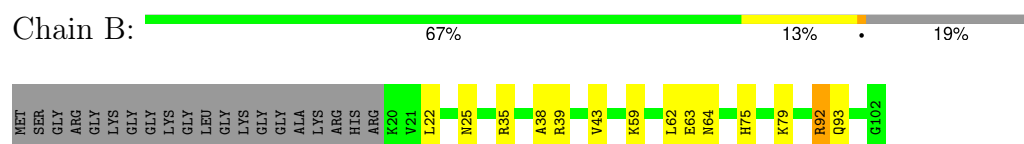
#### • Molecule 1: Histone H3.1



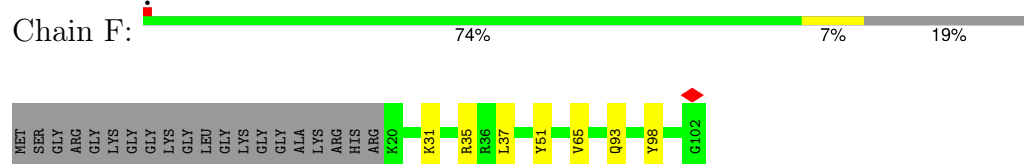
#### • Molecule 1: Histone H3.1



#### • Molecule 2: Histone H4



#### • Molecule 2: Histone H4



#### • Molecule 3: Histone H2A type 1-B/E

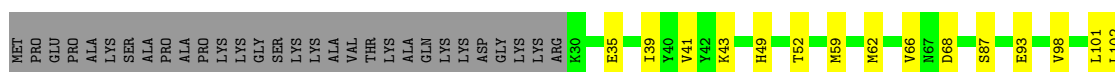




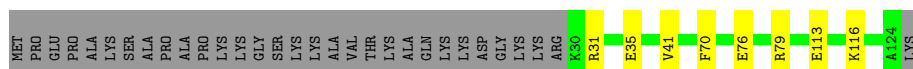
- Molecule 3: Histone H2A type 1-B/E



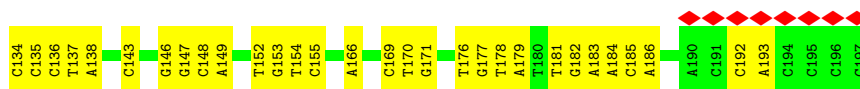
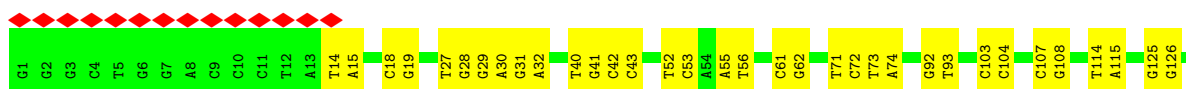
- Molecule 4: Histone H2B type 1-J



- Molecule 4: Histone H2B type 1-J



- Molecule 5: DNA (197-MER)



- Molecule 6: DNA (197-MER)



Q154	Q155	Q156	Q157	Q158	Q159	Q160	Q161	Q162	Q163	Q164	Q165	Q166	Q167	Q168	Q169	Q170	Q171	Q172	Q173	Q174	Q175	Q176	Q177	Q178	Q179	Q180	Q181	Q182	Q183	Q184	Q185	Q186	Q187	Q188	Q189	Q190	Q191	Q192	Q193	Q194	Q195	Q196	Q197	Q198	Q199	Q200	Q201	Q202	Q203	Q204	Q205	Q206	Q207	Q208	Q209	Q210	Q211	Q212	Q213	Q214	Q215	Q216	Q217	Q218	Q219	Q220	Q221	Q222	Q223	Q224	Q225	Q226	Q227	Q228	Q229	Q230	Q231	Q232	Q233	Q234	Q235	Q236	Q237	Q238	Q239	Q240	Q241	Q242	Q243	Q244	Q245	Q246	Q247	Q248	Q249	Q250	Q251	Q252	Q253	Q254	Q255	Q256	Q257	Q258	Q259	Q260	Q261	Q262	Q263	Q264	Q265	Q266	Q267	Q268	Q269	Q270	Q271	Q272	Q273	Q274	Q275	Q276	Q277	Q278	Q279	Q280	Q281	Q282	Q283	Q284	Q285	Q286	Q287	Q288	Q289	Q290	Q291	Q292	Q293	Q294	Q295	Q296	Q297	Q298	Q299	Q300	Q301	Q302	Q303	Q304	Q305	Q306	Q307	Q308	Q309	Q310	Q311	Q312	Q313	Q314	Q315	Q316	Q317	Q318	Q319	Q320	Q321	Q322	Q323	Q324	Q325	Q326	Q327	Q328	Q329	Q330	Q331	Q332	Q333	Q334	Q335	Q336	Q337	Q338	Q339	Q340	Q341	Q342	Q343	Q344	Q345	Q346	Q347	Q348	Q349	Q350	Q351	Q352	Q353	Q354	Q355	Q356	Q357	Q358	Q359	Q360	Q361	Q362	Q363	Q364	Q365	Q366	Q367	Q368	Q369	Q370	Q371	Q372	Q373	Q374	Q375	Q376	Q377	Q378	Q379	Q380	Q381	Q382	Q383	Q384	Q385	Q386	Q387	Q388	Q389	Q390	Q391	Q392	Q393	Q394	Q395	Q396	Q397	Q398	Q399	Q400	Q401	Q402	Q403	Q404	Q405	Q406	Q407	Q408	Q409	Q410	Q411	Q412	Q413	Q414	Q415	Q416	Q417	Q418	Q419	Q420	Q421	Q422	Q423	Q424	Q425	Q426	Q427	Q428	Q429	Q430	Q431	Q432	Q433	Q434	Q435	Q436	Q437	Q438	Q439	Q440	Q441	Q442	Q443	Q444	Q445	Q446	Q447	Q448	Q449	Q450	Q451	Q452	Q453	Q454	Q455	Q456	Q457	Q458	Q459	Q460	Q461	Q462	Q463	Q464	Q465	Q466	Q467	Q468	Q469	Q470	Q471	Q472	Q473	Q474	Q475	Q476	Q477	Q478	Q479	Q480	Q481	Q482	Q483	Q484	Q485	Q486	Q487	Q488	Q489	Q490	Q491	Q492	Q493	Q494	Q495	Q496	Q497	Q498	Q499	Q500	Q501	Q502	Q503	Q504	Q505	Q506	Q507	Q508	Q509	Q510	Q511	Q512	Q513	Q514	Q515	Q516	Q517	Q518	Q519	Q520	Q521	Q522	Q523	Q524	Q525	Q526	Q527	Q528	Q529	Q530	Q531	Q532	Q533	Q534	Q535	Q536	Q537	Q538	Q539	Q540	Q541	Q542	Q543	Q544	Q545	Q546	Q547	Q548	Q549	Q550	Q551	Q552	Q553	Q554	Q555	Q556	Q557	Q558	Q559	Q560	Q561	Q562	Q563	Q564	Q565	Q566	Q567	Q568	Q569	Q570	Q571	Q572	Q573	Q574	Q575	Q576	Q577	Q578	Q579	Q580	Q581	Q582	Q583	Q584	Q585	Q586	Q587	Q588	Q589	Q590	Q591	Q592	Q593	Q594	Q595	Q596	Q597	Q598	Q599	Q600	Q601	Q602	Q603	Q604	Q605	Q606	Q607	Q608
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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	194456	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 ( $e^-/\text{\AA}^2$ )	40	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	44.818	Depositor
Minimum map value	-17.282	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.8	Depositor
Map size ( $\text{\AA}$ )	340.352, 340.352, 340.352	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0636, 1.0636, 1.0636	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	0.43	0/811	0.48	0/1088
1	E	0.43	0/811	0.47	0/1088
2	B	0.42	0/669	0.49	0/894
2	F	0.43	0/669	0.50	0/894
3	C	0.38	0/850	0.46	0/1146
3	G	0.39	0/850	0.46	0/1146
4	D	0.42	0/756	0.49	0/1015
4	H	0.41	0/756	0.47	0/1015
5	I	0.76	0/4499	0.92	0/6935
6	J	0.76	0/4561	0.91	0/7044
7	M	0.41	0/1819	0.49	0/2464
7	N	0.41	0/1819	0.49	0/2464
All	All	0.61	0/18870	0.74	0/27193

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	799	0	838	14	0
1	E	799	0	838	14	0
2	B	662	0	709	10	0
2	F	662	0	709	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	840	0	902	11	0
3	G	840	0	902	9	0
4	D	745	0	771	19	0
4	H	745	0	771	7	0
5	I	4015	0	2208	40	0
6	J	4062	0	2209	40	0
7	M	1777	0	1717	26	0
7	N	1777	0	1717	21	0
All	All	17723	0	14291	186	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 6.

The worst 5 of 186 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)
7:N:197:ILE:HG21	7:N:230:MET:HE3	1.61	0.80
7:M:197:ILE:HG21	7:M:230:MET:HE3	1.68	0.74
4:H:31:ARG:NH1	6:J:150:DG:OP1	2.21	0.73
1:A:121:PRO:O	1:A:125:GLN:HG3	1.89	0.73
2:B:59:LYS:O	2:B:63:GLU:HG3	1.91	0.70

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	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
1	E	95/136 (70%)	94 (99%)	1 (1%)	0	100	100
2	B	81/103 (79%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	81/103 (79%)	79 (98%)	2 (2%)	0	100	100
3	C	107/130 (82%)	106 (99%)	1 (1%)	0	100	100
3	G	107/130 (82%)	107 (100%)	0	0	100	100
4	D	93/126 (74%)	93 (100%)	0	0	100	100
4	H	93/126 (74%)	93 (100%)	0	0	100	100
7	M	223/270 (83%)	216 (97%)	7 (3%)	0	100	100
7	N	223/270 (83%)	218 (98%)	5 (2%)	0	100	100
All	All	1198/1530 (78%)	1180 (98%)	18 (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	85/111 (77%)	84 (99%)	1 (1%)	67	84
1	E	85/111 (77%)	85 (100%)	0	100	100
2	B	68/79 (86%)	67 (98%)	1 (2%)	60	81
2	F	68/79 (86%)	68 (100%)	0	100	100
3	C	85/100 (85%)	85 (100%)	0	100	100
3	G	85/100 (85%)	85 (100%)	0	100	100
4	D	81/105 (77%)	81 (100%)	0	100	100
4	H	81/105 (77%)	81 (100%)	0	100	100
7	M	200/225 (89%)	200 (100%)	0	100	100
7	N	200/225 (89%)	200 (100%)	0	100	100
All	All	1038/1240 (84%)	1036 (100%)	2 (0%)	91	97

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ARG
2	B	92	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	93	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.

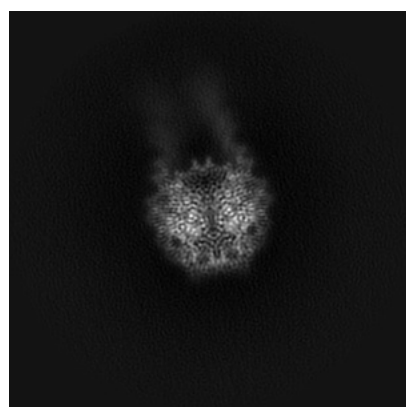
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22686. These allow visual inspection of the internal detail of the map and identification of artifacts.

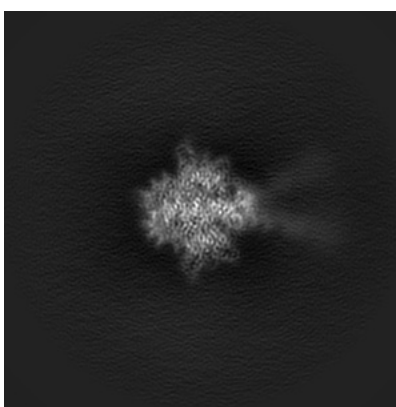
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

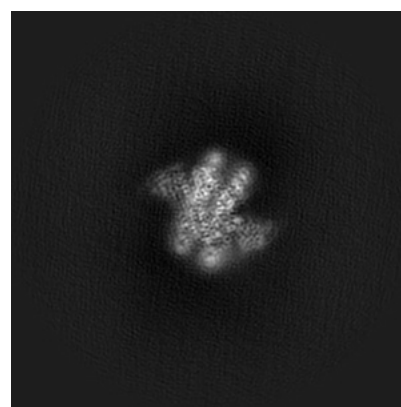
#### 6.1.1 Primary map



X



Y

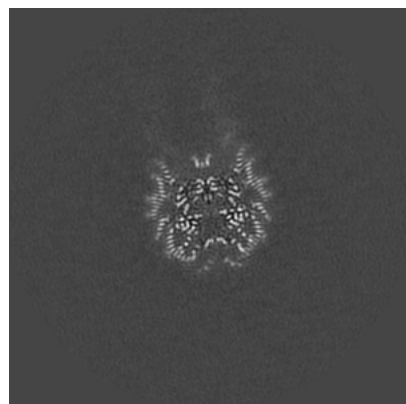


Z

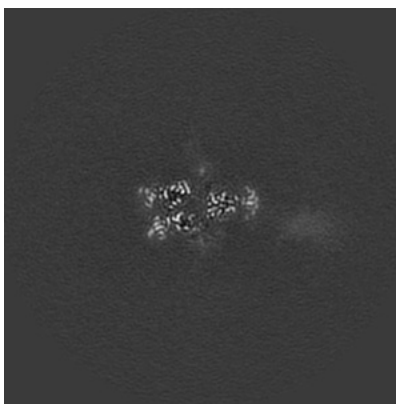
The images above show the map projected in three orthogonal directions.

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

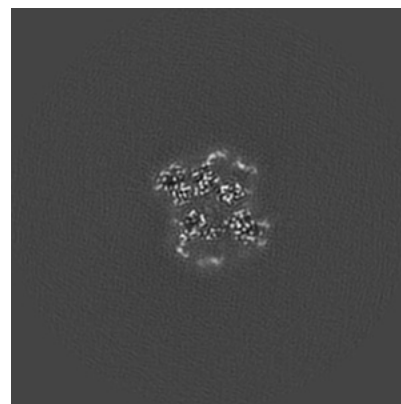
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

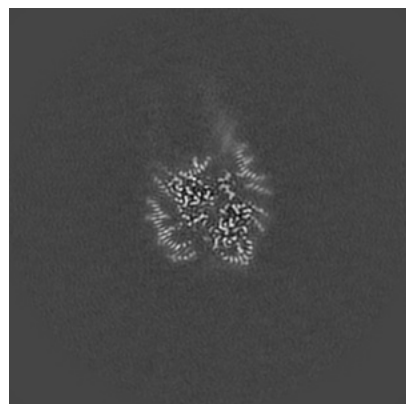


Z Index: 160

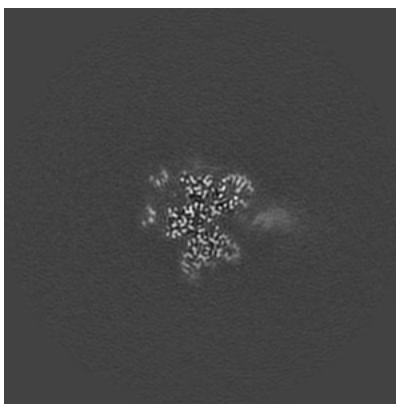
The images above show central slices of the map in three orthogonal directions.

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

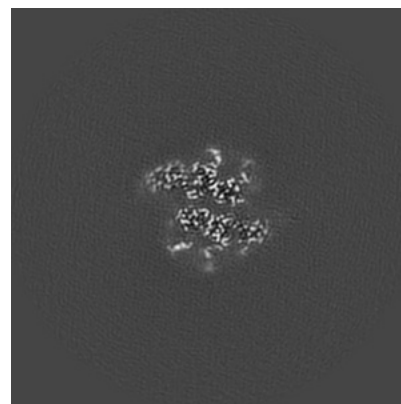
### 6.3.1 Primary map



X Index: 156



Y Index: 177

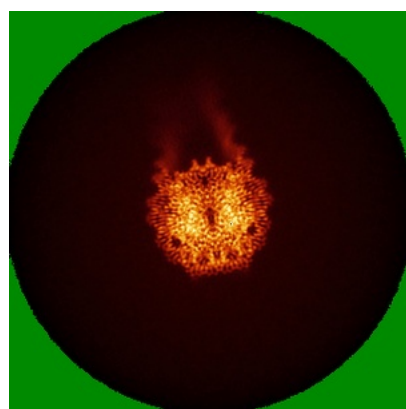


Z Index: 153

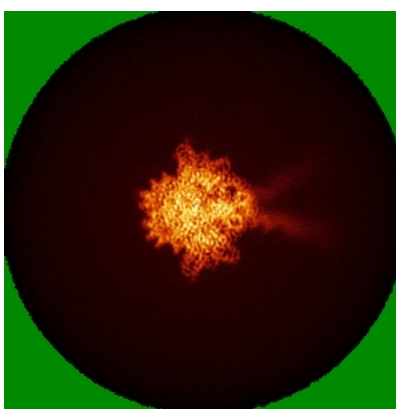
The images above show the largest variance slices of the map in three orthogonal directions.

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

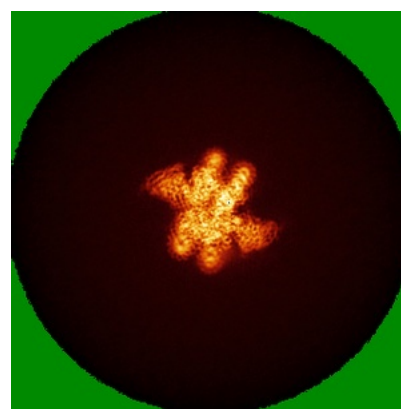
### 6.4.1 Primary map



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



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.8. 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](#)

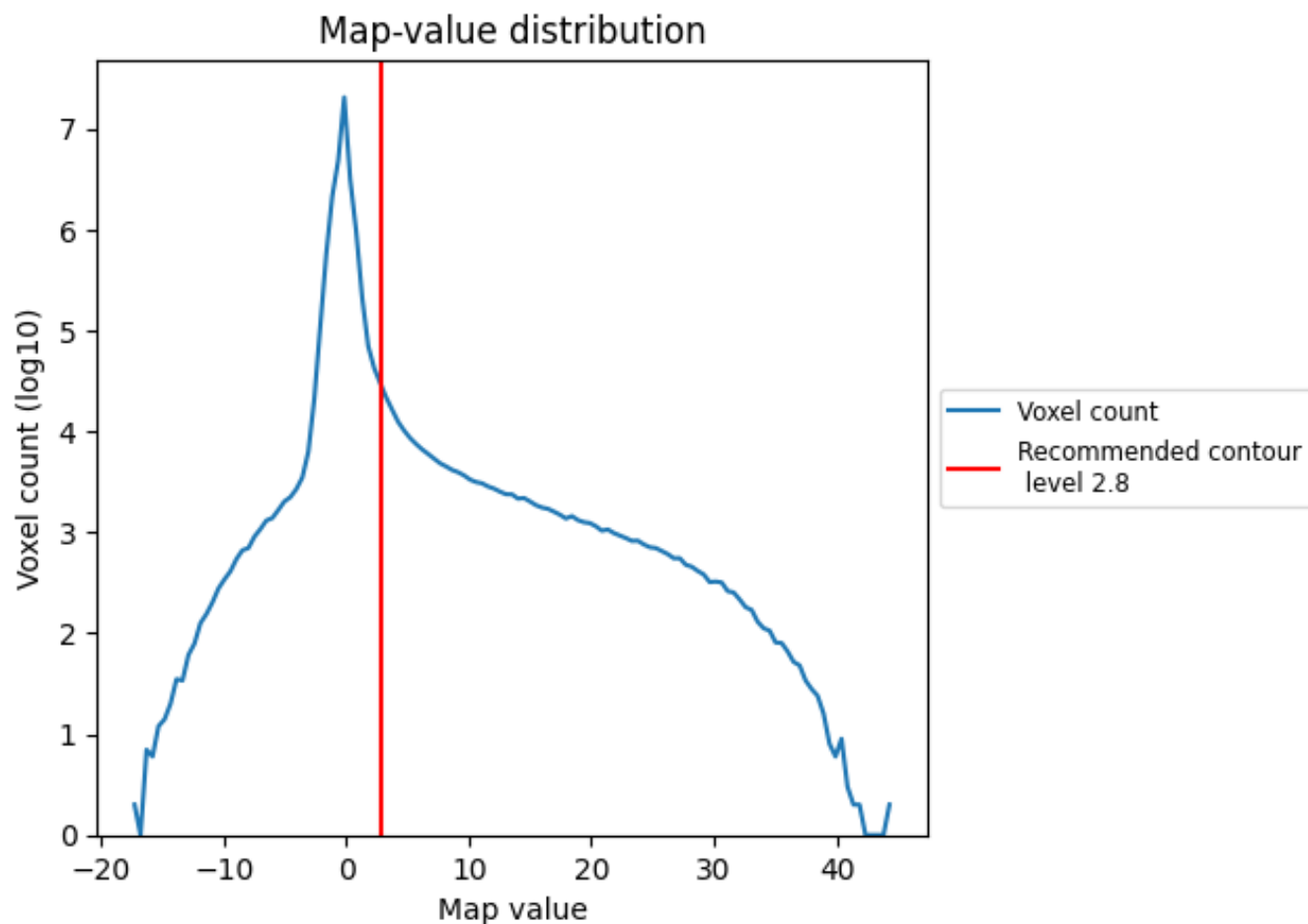
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

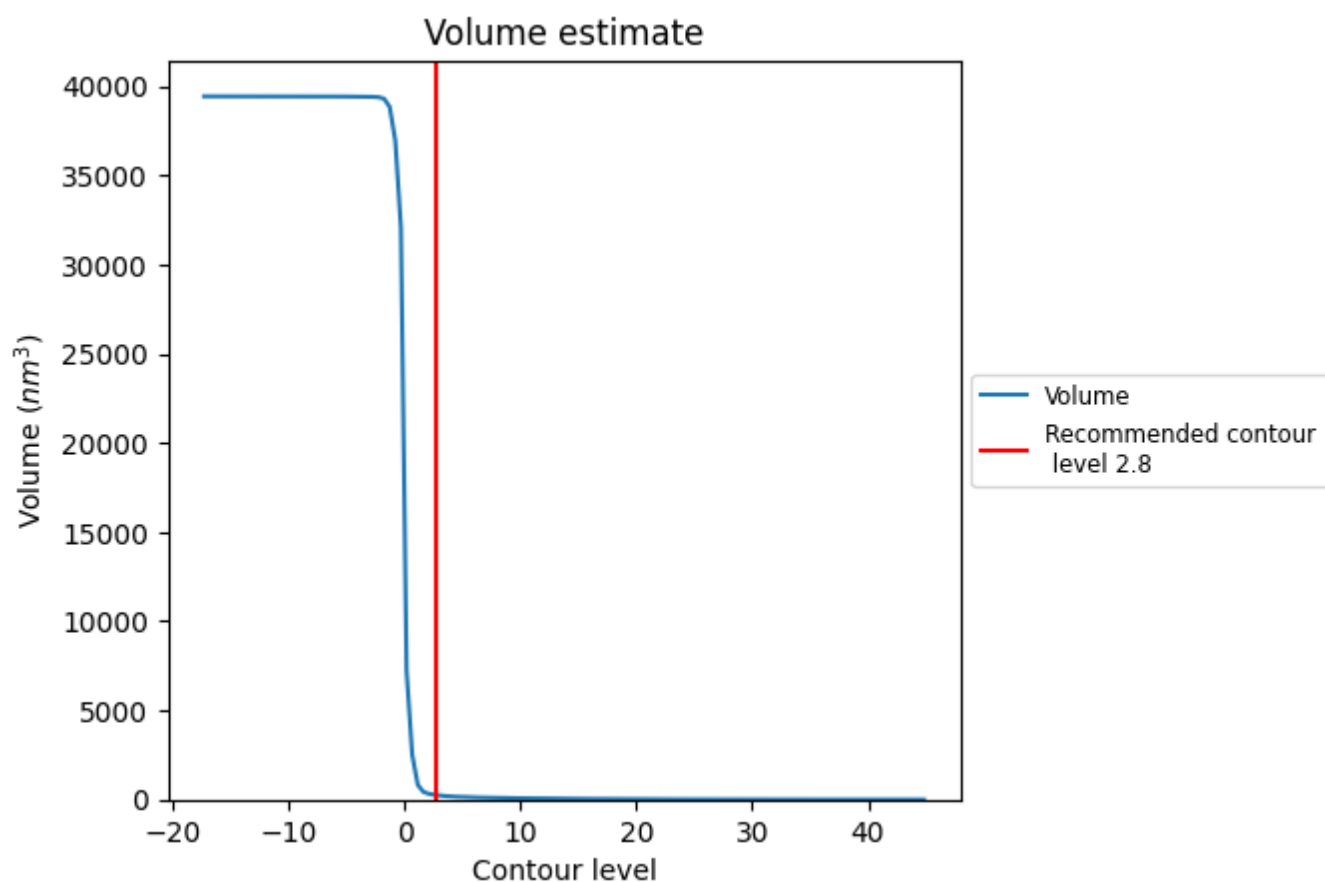
This section contains the results of statistical analysis of the map.

### 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.

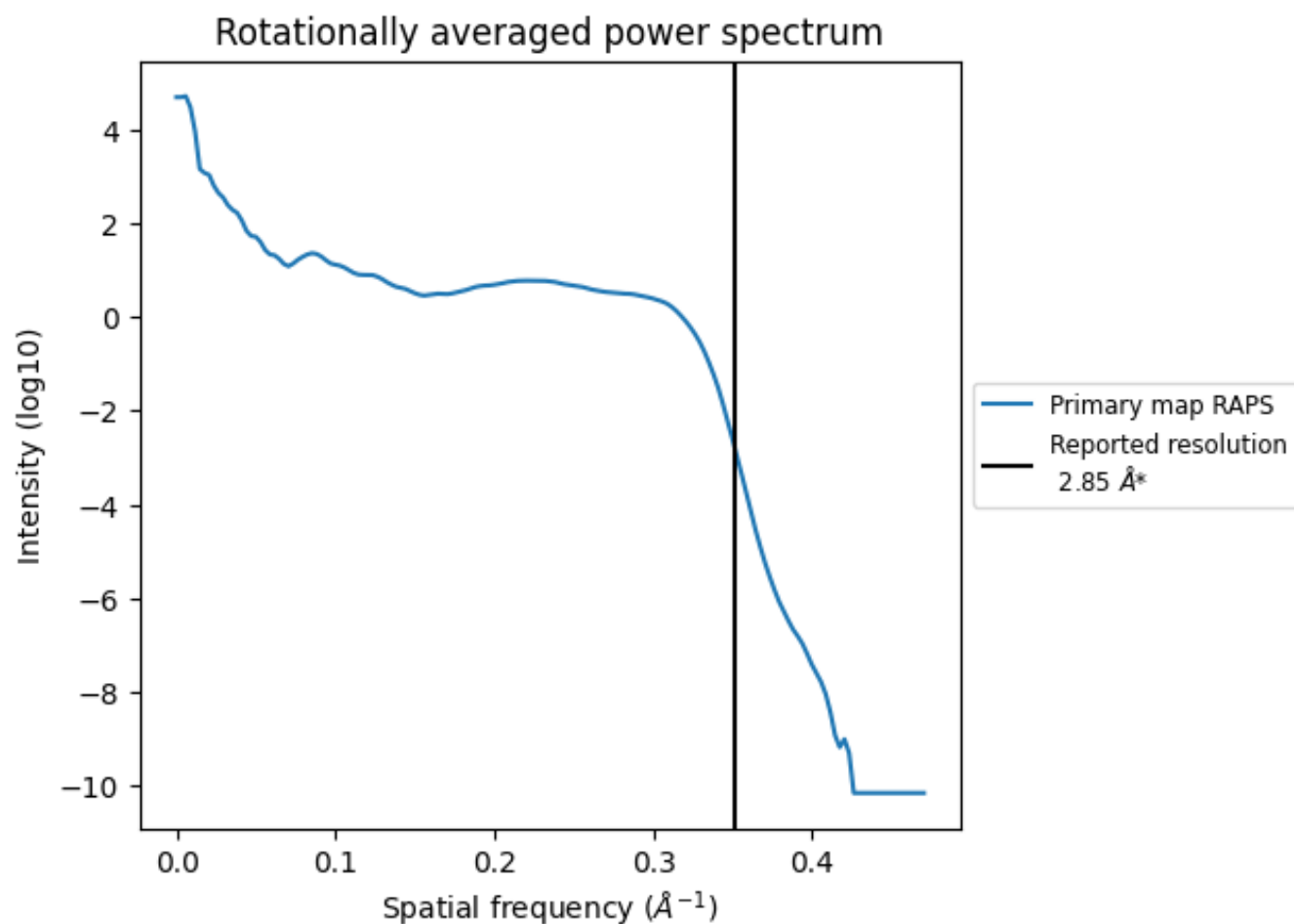
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247  $\text{nm}^3$ ; this corresponds to an approximate mass of 223 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 ⓘ

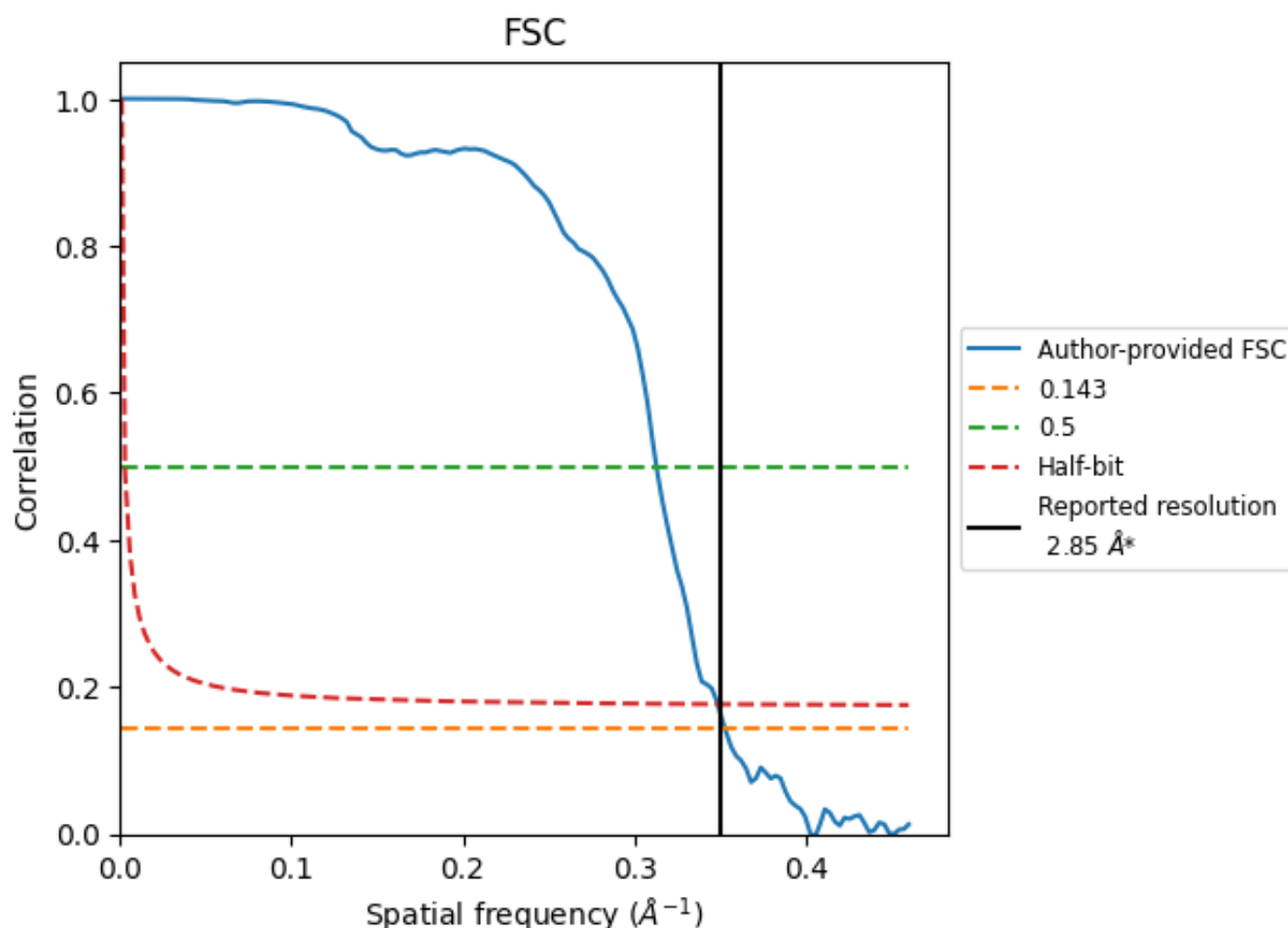


\*Reported resolution corresponds to spatial frequency of 0.351 Å<sup>-1</sup>

## 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 0.351 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

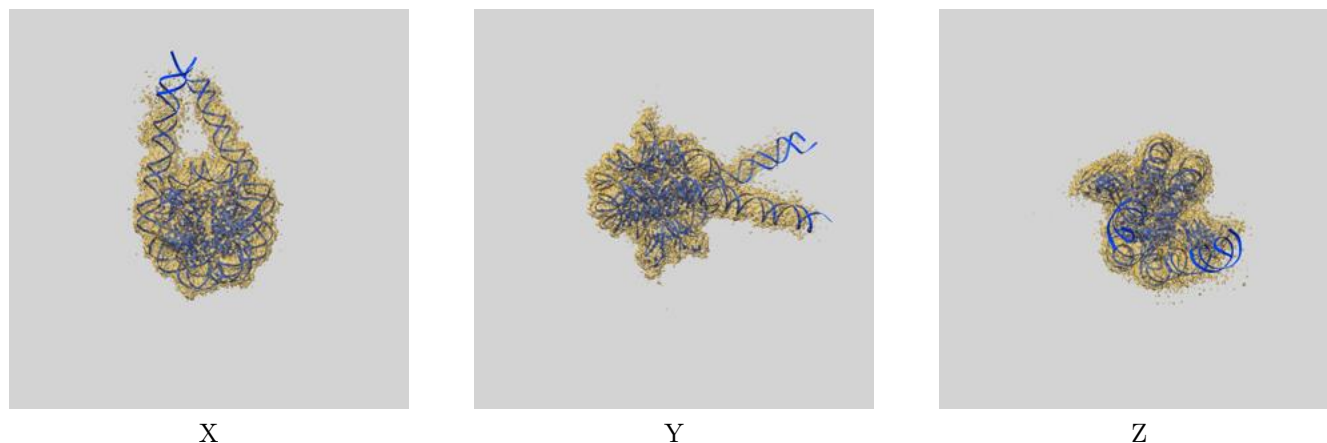
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.85	-	-
Author-provided FSC curve	2.83	3.19	2.87
Unmasked-calculated*	-	-	-

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

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

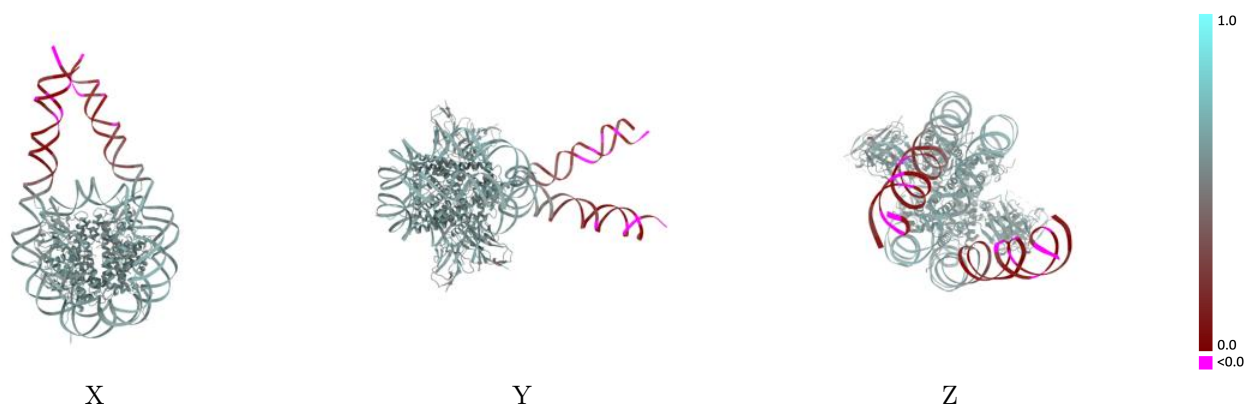
This section contains information regarding the fit between EMDB map EMD-22686 and PDB model 7K61. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

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



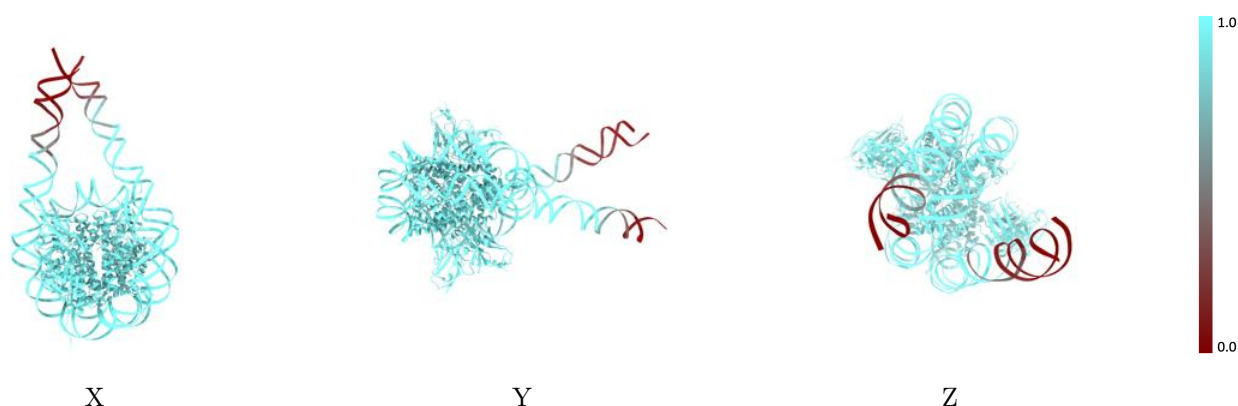
The images above show the 3D surface view of the map at the recommended contour level 2.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



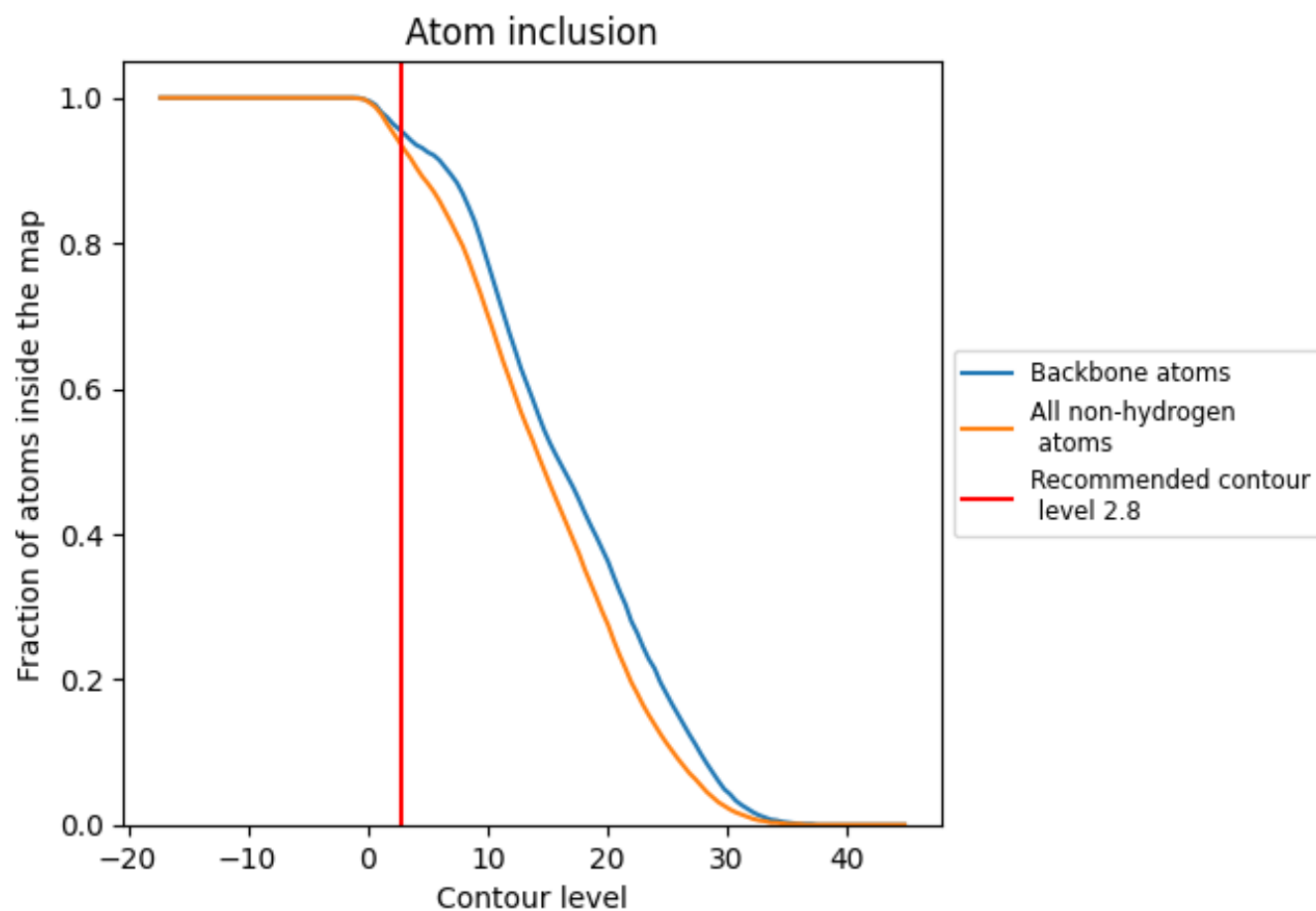
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.8).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (2.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9350</div>	<div><div></div>0.5290</div>
A	<div><div></div>0.9860</div>	<div><div></div>0.5880</div>
B	<div><div></div>0.9940</div>	<div><div></div>0.5900</div>
C	<div><div></div>0.9930</div>	<div><div></div>0.5940</div>
D	<div><div></div>0.9860</div>	<div><div></div>0.5760</div>
E	<div><div></div>0.9870</div>	<div><div></div>0.5870</div>
F	<div><div></div>0.9840</div>	<div><div></div>0.5900</div>
G	<div><div></div>0.9950</div>	<div><div></div>0.5920</div>
H	<div><div></div>0.9900</div>	<div><div></div>0.5790</div>
I	<div><div></div>0.8750</div>	<div><div></div>0.4700</div>
J	<div><div></div>0.8690</div>	<div><div></div>0.4720</div>
M	<div><div></div>0.9890</div>	<div><div></div>0.5610</div>
N	<div><div></div>0.9880</div>	<div><div></div>0.5620</div>

1.0

0.0

<0.0